



wwPDB EM Validation Summary Report ⓘ

Sep 16, 2026 – 12:36 PM JST

PDB ID : 7DR2 / pdb_00007dr2
EMDB ID : EMD-30823
Title : Structure of GraFix PSI tetramer from *Cyanophora paradoxa*
Authors : Kato, K.; Nagao, R.; Akita, F.; Miyazaki, N.; Shen, J.R.
Deposited on : 2020-12-25
Resolution : 3.80 Å(reported)

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:

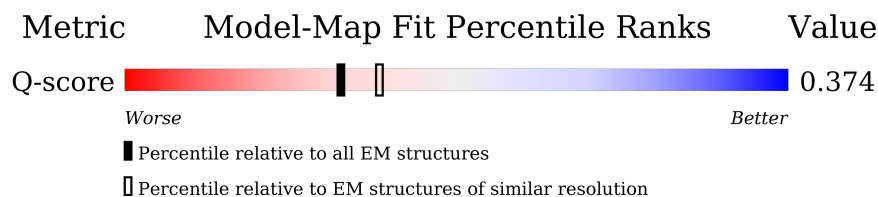
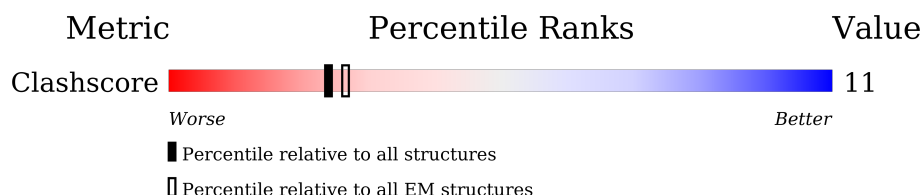
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using 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

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

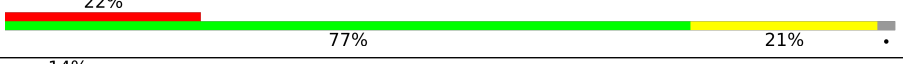
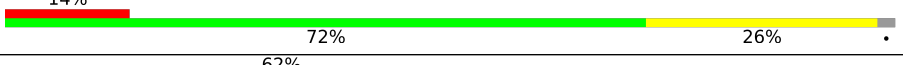
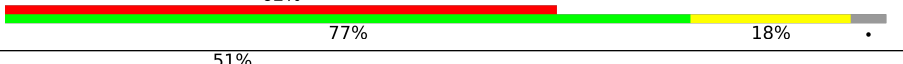
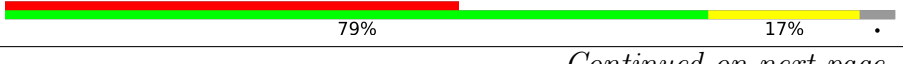
The reported resolution of this entry is 3.80 Å.

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	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	752	
1	bA	752	
1	cA	752	
1	dA	752	
2	aB	737	
2	bB	737	

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Mol	Chain	Length	Quality of chain
2	cB	737	
2	dB	737	
3	aC	81	
3	bC	81	
3	cC	81	
3	dC	81	
4	aD	220	
4	bD	220	
4	cD	220	
4	dD	220	
5	aE	70	
5	bE	70	
5	cE	70	
5	dE	70	
6	aF	186	
6	bF	186	
6	cF	186	
6	dF	186	
7	aI	35	
7	bI	35	
7	cI	35	
7	dI	35	
8	aJ	40	
8	bJ	40	
8	cJ	40	

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Mol	Chain	Length	Quality of chain
8	dJ	40	 88% 75% 18% 8%
9	aK	157	 6% 34% 10% 56%
9	cK	157	 6% 35% 9% 56%
10	aL	146	 32% 66% 21% 12%
10	bL	146	 19% 69% 21% 10%
10	cL	146	 34% 68% 19% 12%
10	dL	146	 23% 70% 20% 10%
11	aM	31	 74% 68% 26% 6%
11	bM	31	 71% 77% 16% 6%
11	cM	31	 77% 65% 29% 6%
11	dM	31	 74% 77% 16% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
17	SF4	aB	802	-	-	X	-
17	SF4	aC	102	-	-	X	-
17	SF4	cB	802	-	-	X	-
17	SF4	cC	102	-	-	X	-

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 89952 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	aA	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		
1	bA	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		
1	cA	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		
1	dA	739	Total	C	N	O	S	0	0
			5803	3794	987	999	23		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	706	Total	C	N	O	S	0	0
			5622	3688	950	972	12		
2	bB	706	Total	C	N	O	S	0	0
			5622	3688	950	972	12		
2	cB	706	Total	C	N	O	S	0	0
			5622	3688	950	972	12		
2	dB	706	Total	C	N	O	S	0	0
			5622	3688	950	972	12		

- 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
			601	367	106	117	11		
3	bC	80	Total	C	N	O	S	0	0
			601	367	106	117	11		
3	cC	80	Total	C	N	O	S	0	0
			601	367	106	117	11		
3	dC	80	Total	C	N	O	S	0	0
			601	367	106	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	139	Total	C	N	O	S	0	0
			1082	691	190	199	2		
4	bD	139	Total	C	N	O	S	0	0
			1082	691	190	199	2		
4	cD	139	Total	C	N	O	S	0	0
			1082	691	190	199	2		
4	dD	139	Total	C	N	O	S	0	0
			1082	691	190	199	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	62	Total	C	N	O	S	0	0
			508	322	87	98	1		
5	bE	62	Total	C	N	O	S	0	0
			508	322	87	98	1		
5	cE	62	Total	C	N	O	S	0	0
			508	322	87	98	1		
5	dE	62	Total	C	N	O	S	0	0
			508	322	87	98	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	161	Total	C	N	O	S	0	0
			1255	795	220	238	2		
6	bF	161	Total	C	N	O	S	0	0
			1255	795	220	238	2		
6	cF	161	Total	C	N	O	S	0	0
			1255	795	220	238	2		
6	dF	161	Total	C	N	O	S	0	0
			1255	795	220	238	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	30	Total	C	N	O	S	0	0
			228	155	31	40	2		
7	bI	30	Total	C	N	O	S	0	0
			228	155	31	40	2		
7	cI	30	Total	C	N	O	S	0	0
			228	155	31	40	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	dI	30	Total	C	N	O	S	0	0
			228	155	31	40	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	37	Total	C	N	O		0	0
			292	199	43	50			
8	bJ	37	Total	C	N	O		0	0
			292	199	43	50			
8	cJ	37	Total	C	N	O		0	0
			292	199	43	50			
8	dJ	37	Total	C	N	O		0	0
			292	199	43	50			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	69	Total	C	N	O	S	0	0
			490	322	79	87	2		
9	cK	69	Total	C	N	O	S	0	0
			490	322	79	87	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	128	Total	C	N	O	S	0	0
			943	612	155	174	2		
10	bL	131	Total	C	N	O	S	0	0
			965	626	160	177	2		
10	cL	128	Total	C	N	O	S	0	0
			943	612	155	174	2		
10	dL	131	Total	C	N	O	S	0	0
			965	626	160	177	2		

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

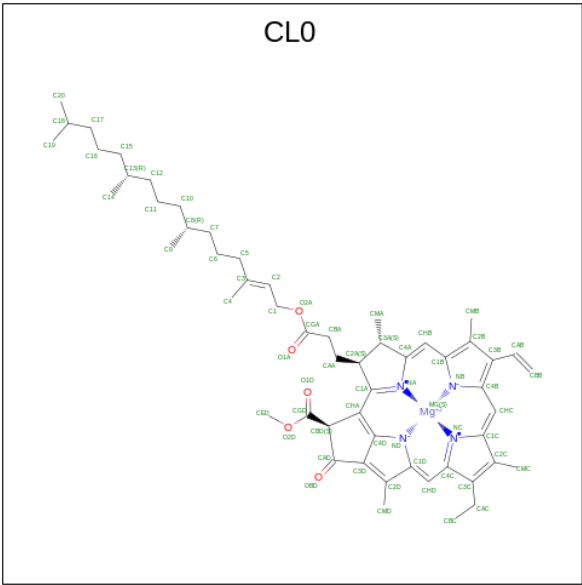
Mol	Chain	Residues	Atoms				AltConf	Trace
11	aM	29	Total	C	N	O	0	0
			215	145	34	36		
11	bM	29	Total	C	N	O	0	0
			215	145	34	36		

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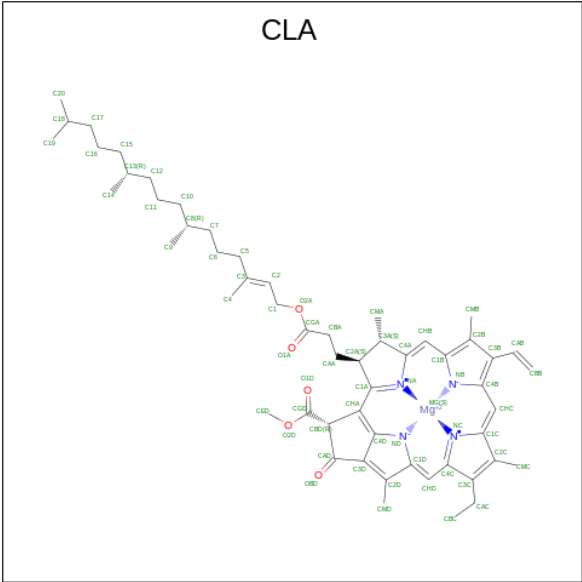
Mol	Chain	Residues	Atoms				AltConf	Trace
11	cM	29	Total	C	N	O	0	0
			215	145	34	36		
11	dM	29	Total	C	N	O	0	0
			215	145	34	36		

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

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



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

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

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Mol	Chain	Residues	Atoms					AltConf
13	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	aA	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aA	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aB	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	aB	1	Total 59	C 49	Mg 1	N 4	O 5	0
13	aB	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	aB	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aB	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aF	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	aF	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	aJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aK	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	aK	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	aK	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	aL	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	aL	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	bA	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	bA	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bA	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 56	C 46	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bB	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	bB	1	Total 59	C 49	Mg 1	N 4	O 5	0
13	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	bB	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bB	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bF	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	bF	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	bL	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	cA	1	Total 61	C 51	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	cA	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	cA	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cA	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cB	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	cB	1	Total 59	C 49	Mg 1	N 4	O 5	0
13	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	cB	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cB	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cF	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	cF	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cK	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	cK	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	cK	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	cL	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	cL	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	dA	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	dA	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	dA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	dA	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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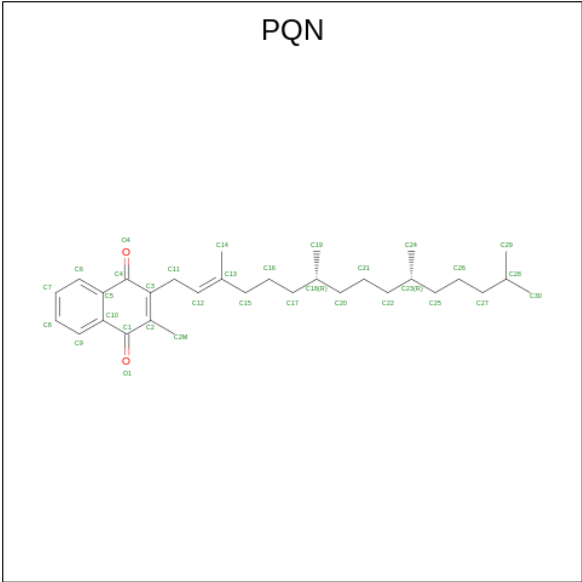
Mol	Chain	Residues	Atoms					AltConf
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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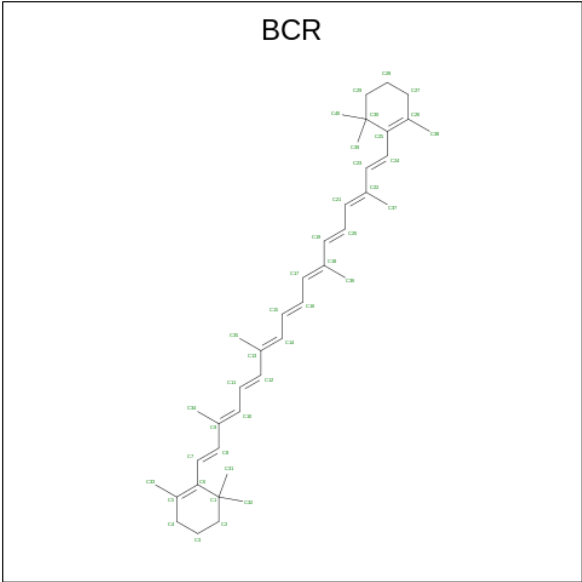
Mol	Chain	Residues	Atoms					AltConf
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dF	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	dF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	dL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	dL	1	Total	C	Mg	N	O	0
			52	42	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
15	aA	1	Total	C	0
			40	40	
15	aA	1	Total	C	0
			40	40	
15	aA	1	Total	C	0
			40	40	
15	aA	1	Total	C	0
			40	40	
15	aA	1	Total	C	0
			40	40	
15	aB	1	Total	C	0
			40	40	
15	aB	1	Total	C	0
			40	40	
15	aB	1	Total	C	0
			40	40	
15	aF	1	Total	C	0
			40	40	
15	aF	1	Total	C	0
			40	40	
15	aI	1	Total	C	0
			40	40	
15	aJ	1	Total	C	0
			40	40	
15	aJ	1	Total	C	0
			40	40	
15	aJ	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
15	aK	1	Total C 40 40	0
15	aK	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aL	1	Total C 40 40	0
15	aM	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bA	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bB	1	Total C 40 40	0
15	bF	1	Total C 40 40	0
15	bF	1	Total C 40 40	0
15	bI	1	Total C 40 40	0
15	bI	1	Total C 40 40	0
15	bJ	1	Total C 40 40	0
15	bJ	1	Total C 40 40	0

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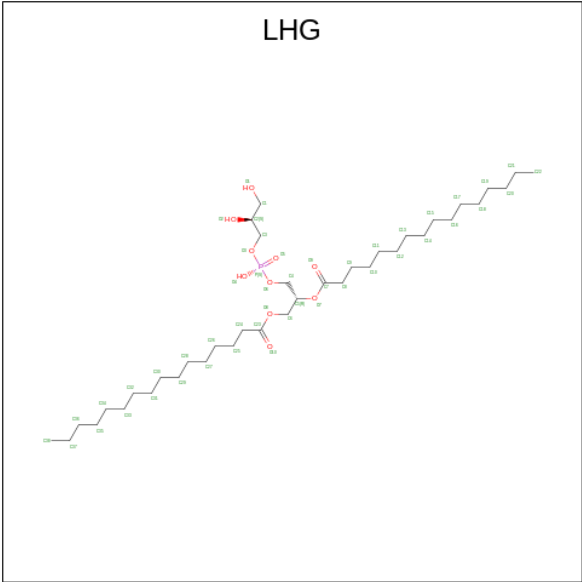
Mol	Chain	Residues	Atoms	AltConf
15	bJ	1	Total C 40 40	0
15	bL	1	Total C 40 40	0
15	bM	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cA	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cB	1	Total C 40 40	0
15	cF	1	Total C 40 40	0
15	cF	1	Total C 40 40	0
15	cI	1	Total C 40 40	0
15	cJ	1	Total C 40 40	0
15	cJ	1	Total C 40 40	0
15	cJ	1	Total C 40 40	0
15	cK	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0
15	cL	1	Total C 40 40	0

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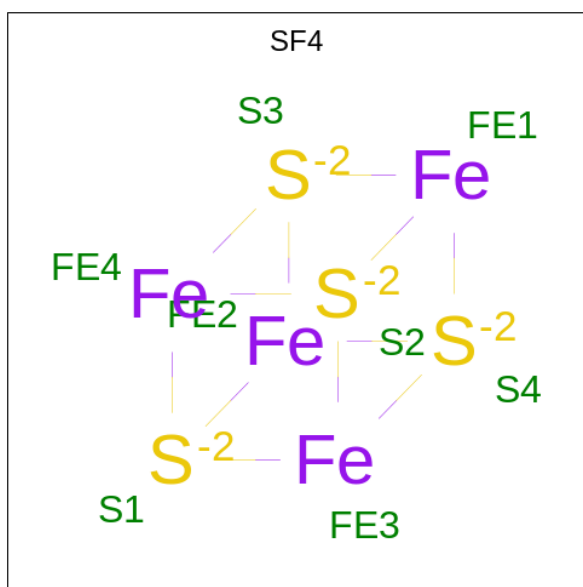
Mol	Chain	Residues	Atoms	AltConf
15	cM	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dA	1	Total C 40 40	0
15	dB	1	Total C 40 40	0
15	dB	1	Total C 40 40	0
15	dB	1	Total C 40 40	0
15	dF	1	Total C 40 40	0
15	dF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

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



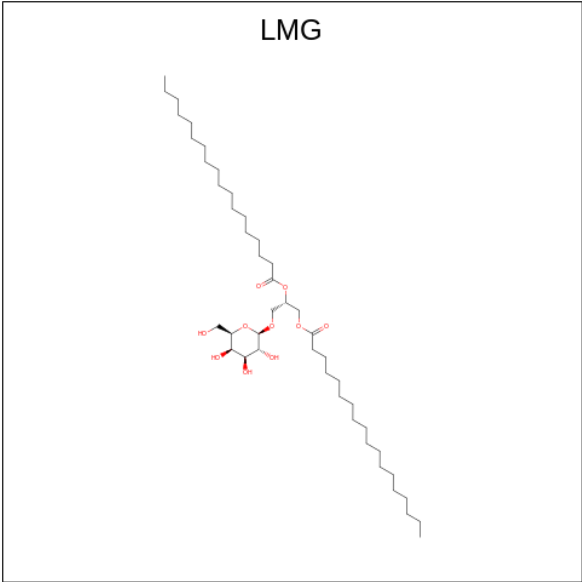
Mol	Chain	Residues	Atoms				AltConf
16	aA	1	Total	C	O	P	0
			49	38	10	1	
16	aA	1	Total	C	O	P	0
			27	16	10	1	
16	bA	1	Total	C	O	P	0
			49	38	10	1	
16	bA	1	Total	C	O	P	0
			27	16	10	1	
16	cA	1	Total	C	O	P	0
			49	38	10	1	
16	cA	1	Total	C	O	P	0
			27	16	10	1	
16	dA	1	Total	C	O	P	0
			49	38	10	1	
16	dA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

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
17	aB	1	Total	Fe	S	0
			8	4	4	
17	aC	1	Total	Fe	S	0
			8	4	4	
17	aC	1	Total	Fe	S	0
			8	4	4	
17	bB	1	Total	Fe	S	0
			8	4	4	
17	bC	1	Total	Fe	S	0
			8	4	4	
17	bC	1	Total	Fe	S	0
			8	4	4	
17	cB	1	Total	Fe	S	0
			8	4	4	
17	cC	1	Total	Fe	S	0
			8	4	4	
17	cC	1	Total	Fe	S	0
			8	4	4	
17	dB	1	Total	Fe	S	0
			8	4	4	
17	dC	1	Total	Fe	S	0
			8	4	4	
17	dC	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).

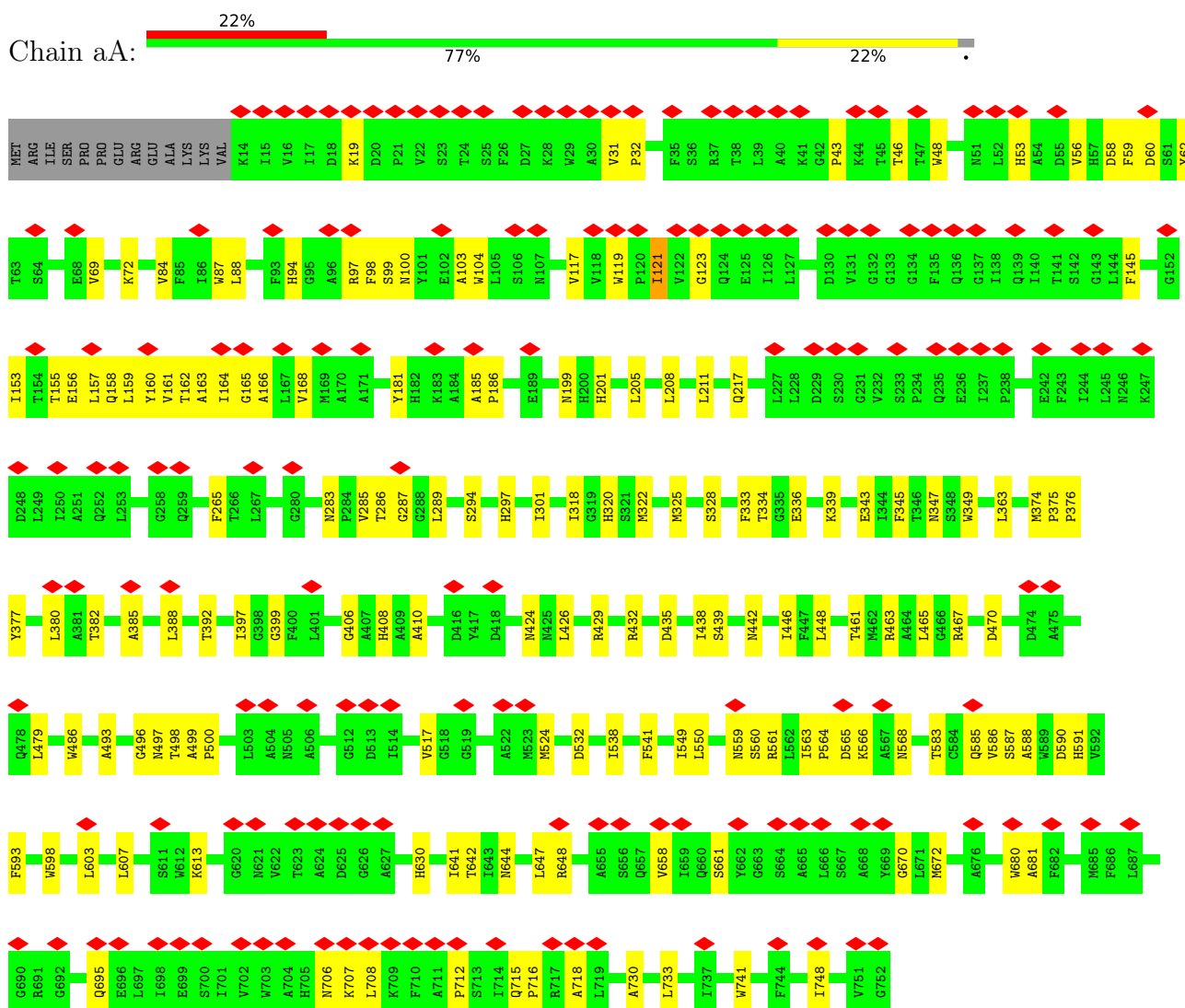


Mol	Chain	Residues	Atoms			AltConf
18	aB	1	Total	C	O	0
			55	45	10	
18	bB	1	Total	C	O	0
			55	45	10	
18	cB	1	Total	C	O	0
			55	45	10	
18	dB	1	Total	C	O	0
			55	45	10	

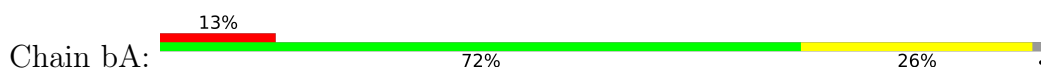
3 Residue-property plots

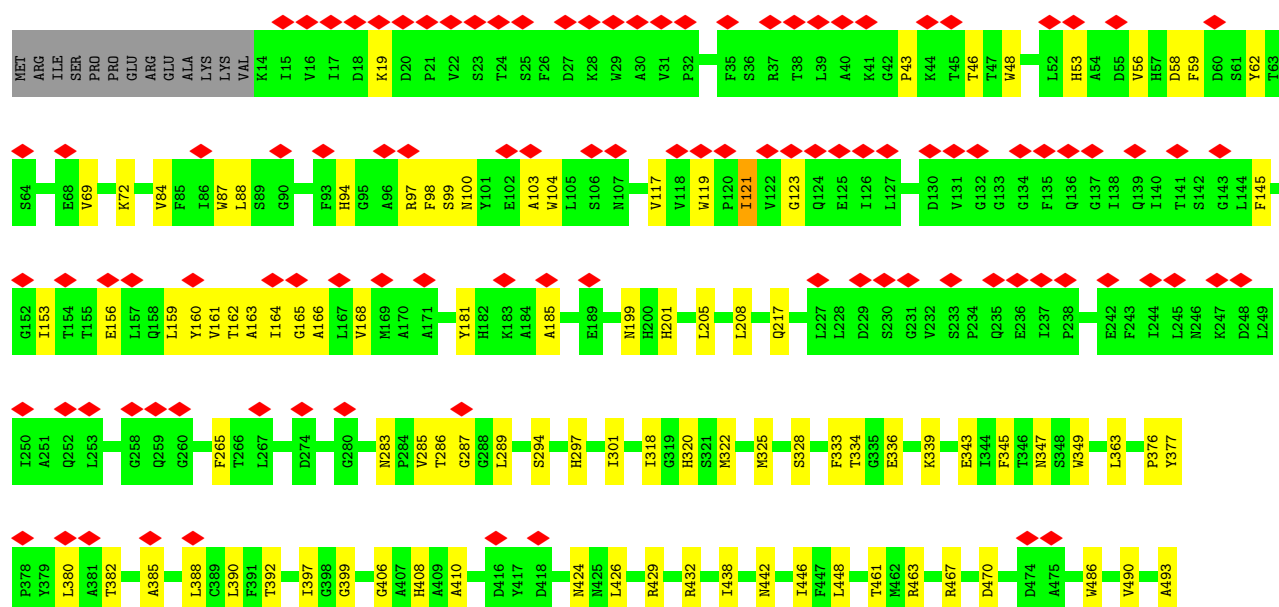
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

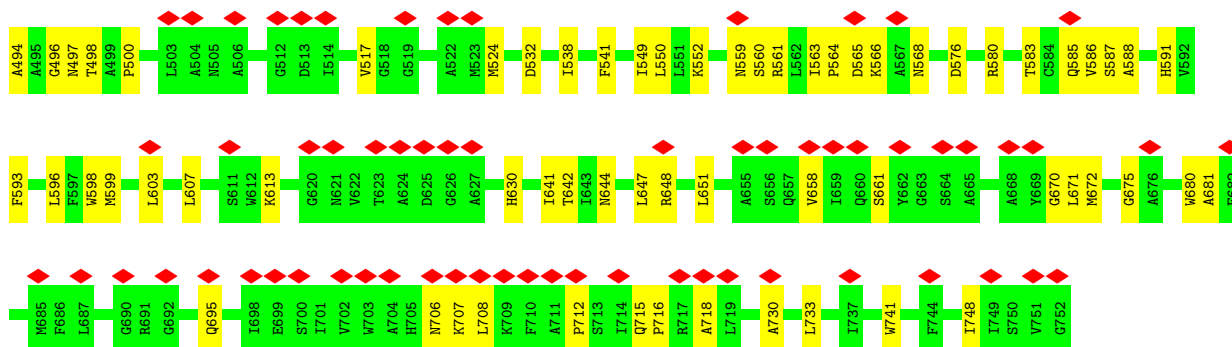
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



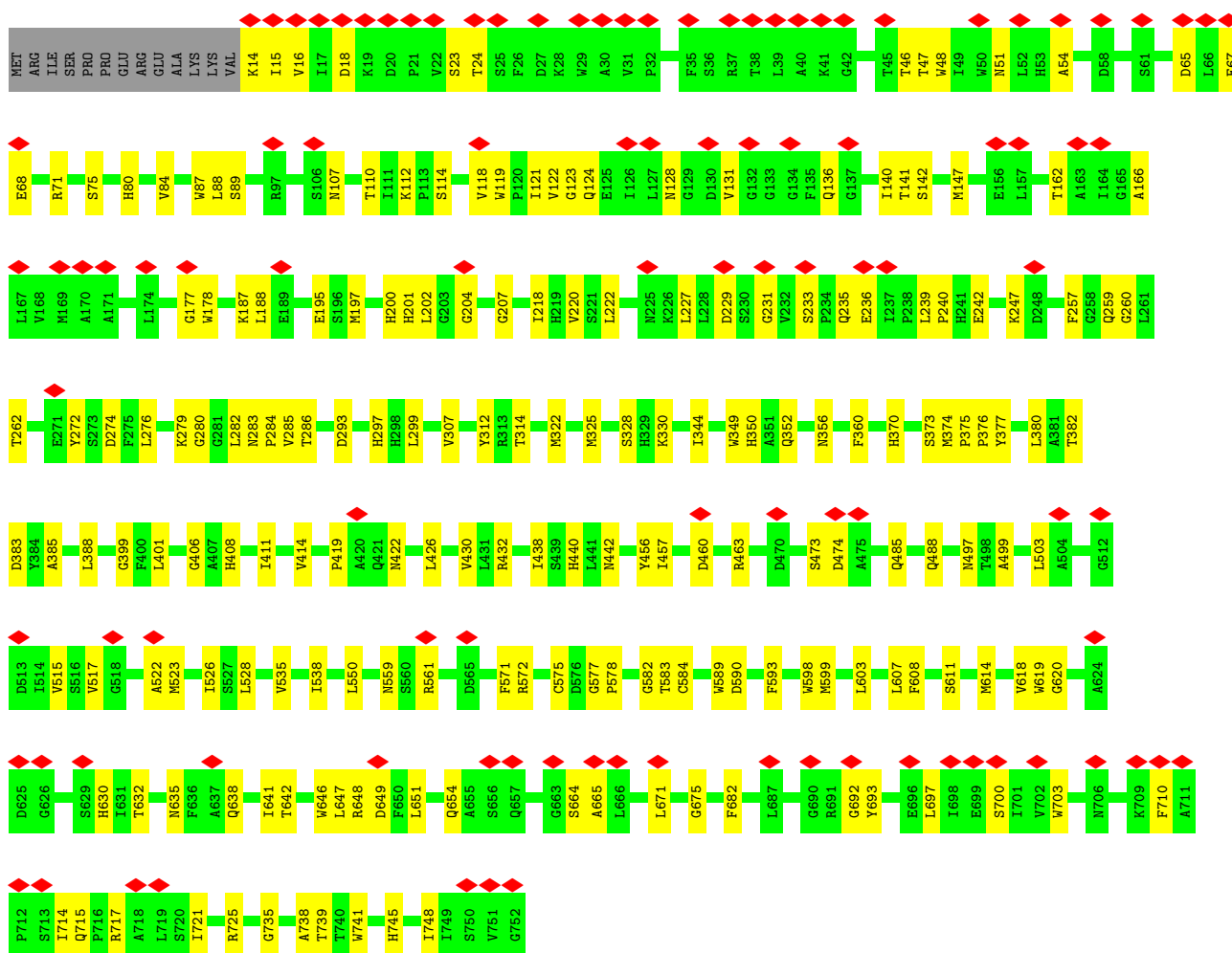
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



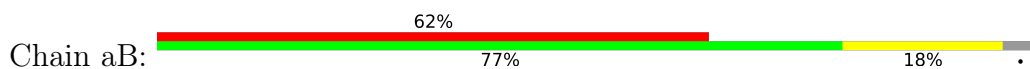


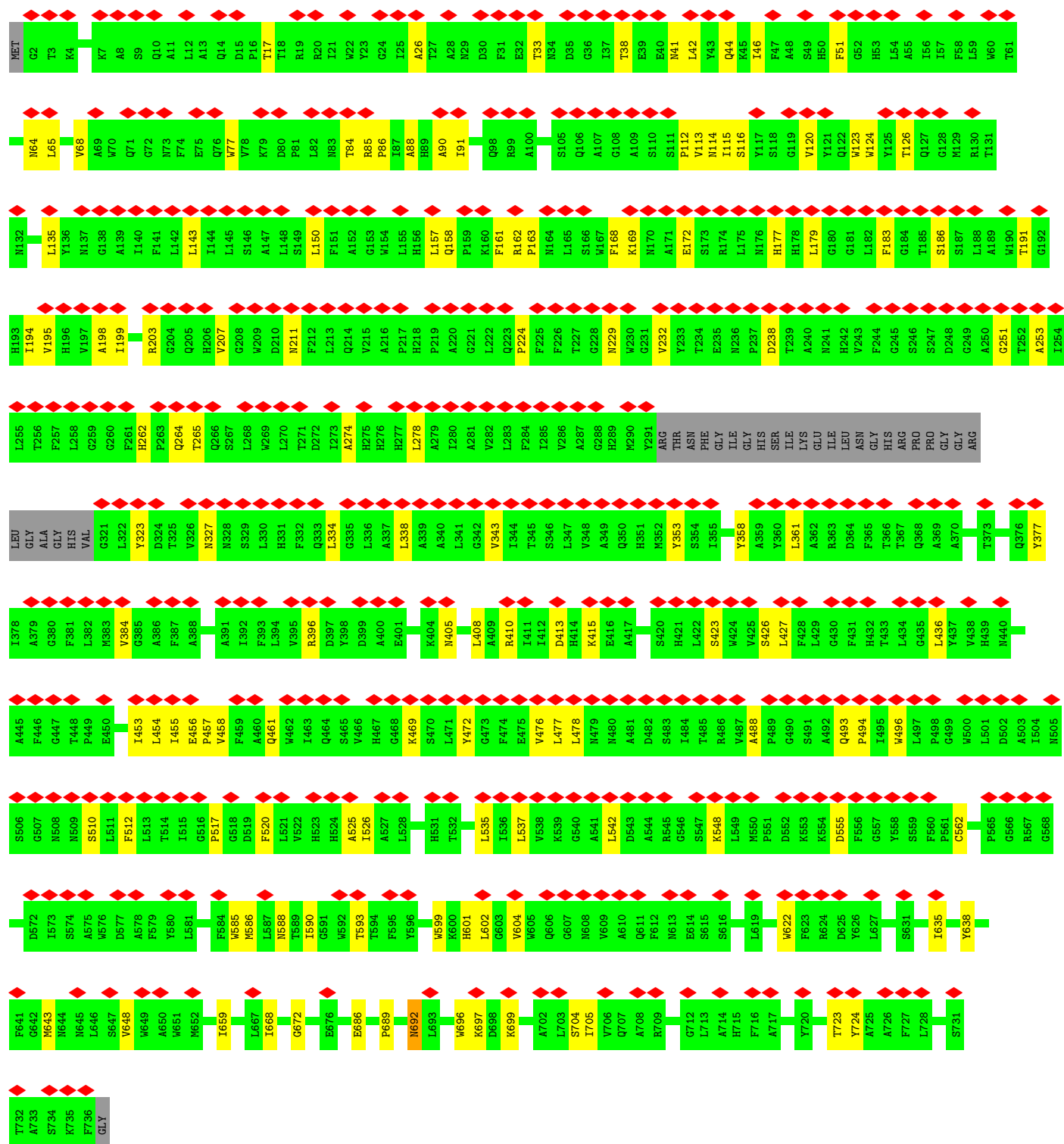


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

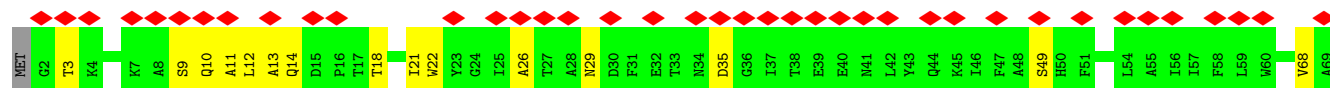
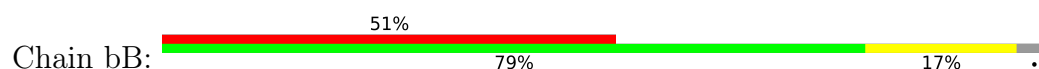


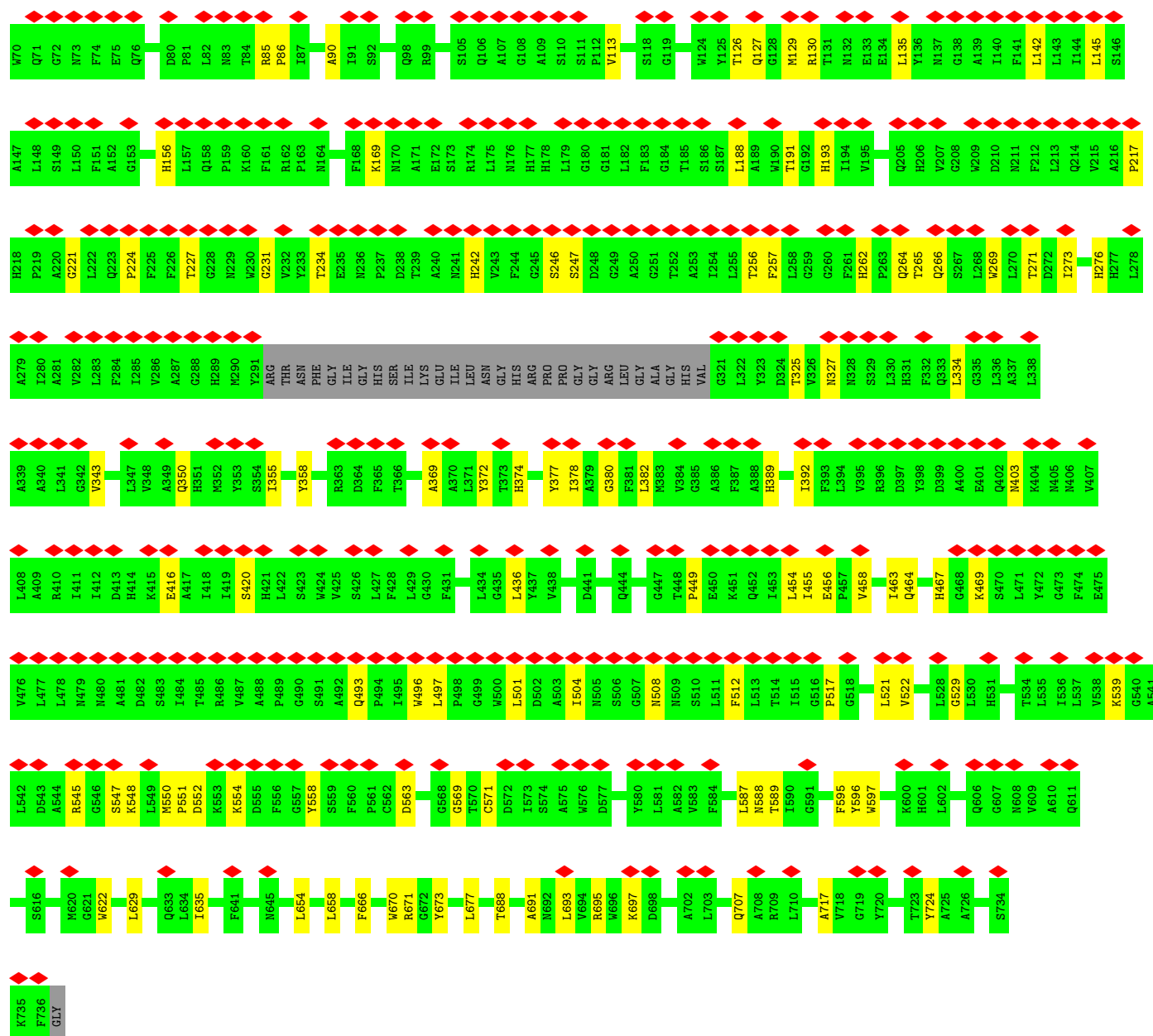
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



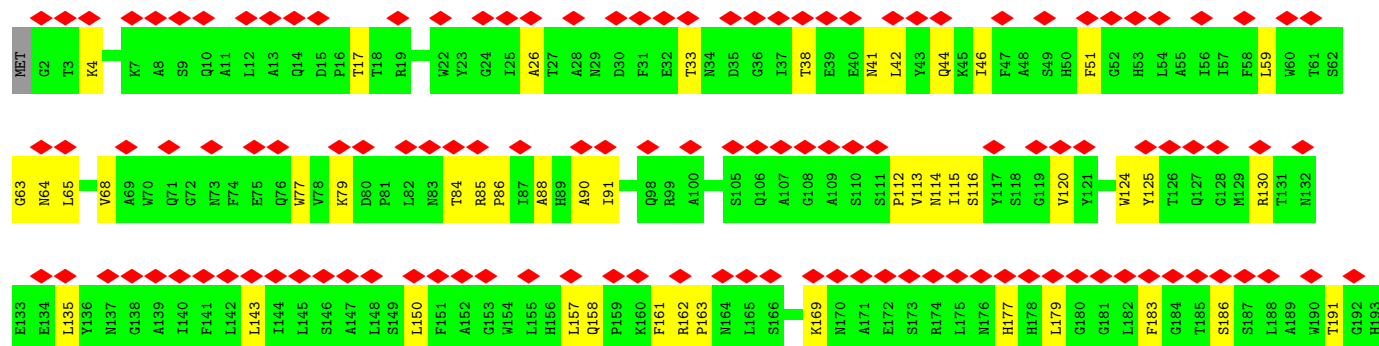
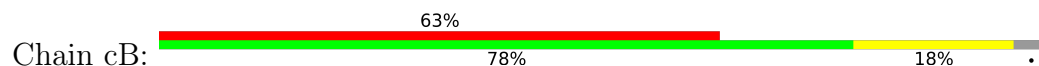


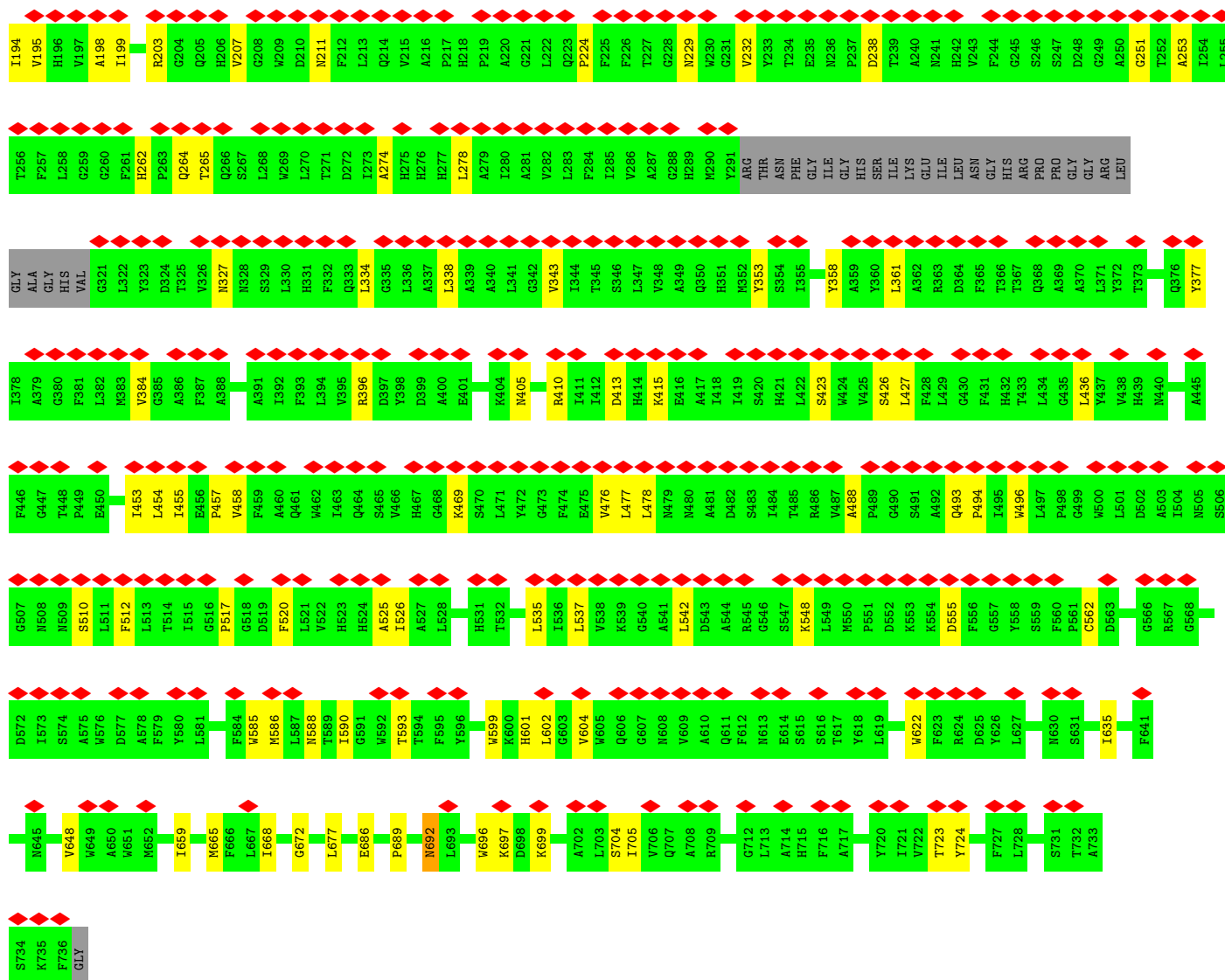
● Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



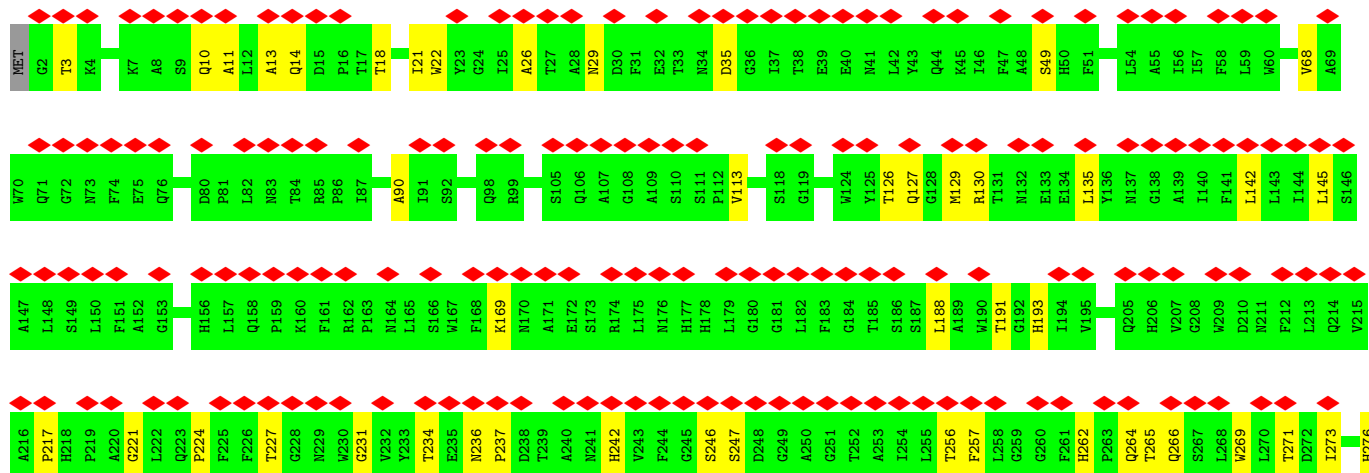
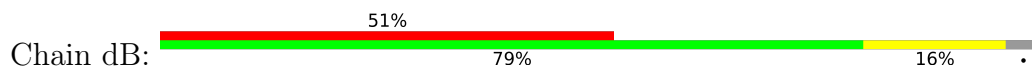


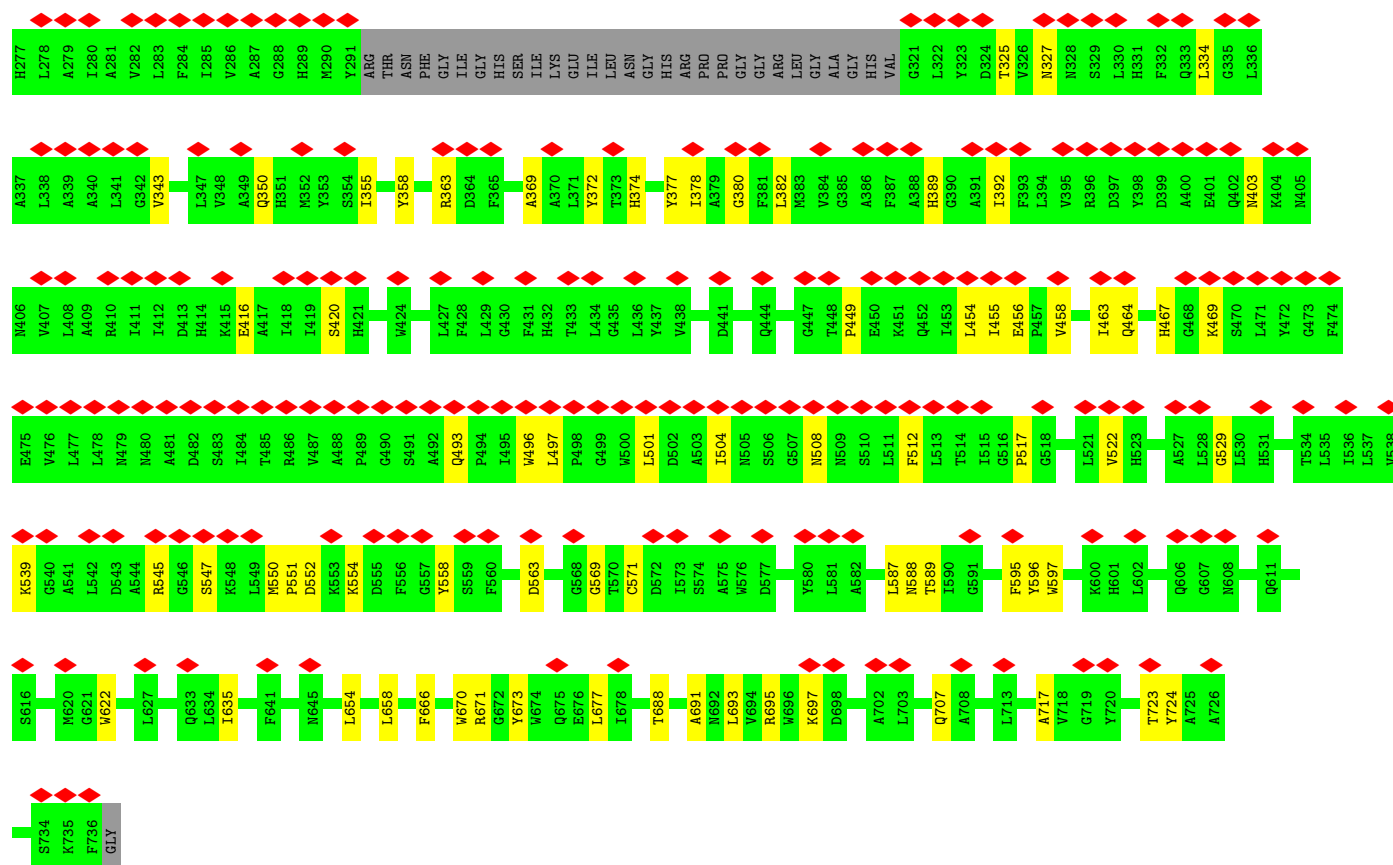
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



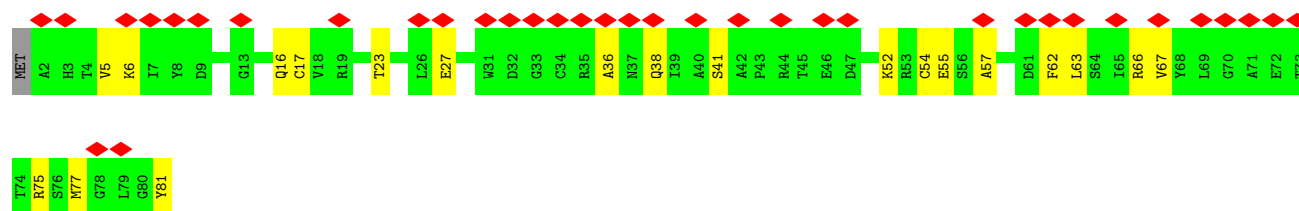
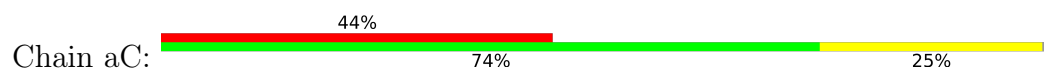


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

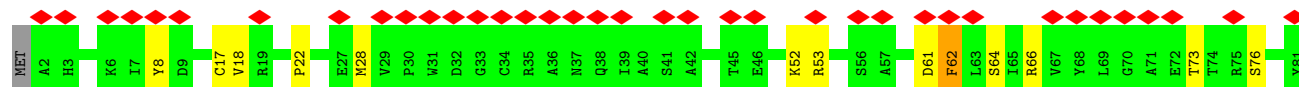
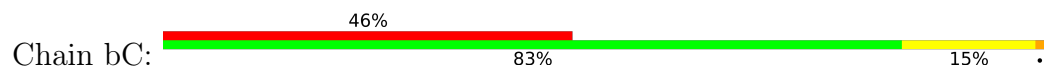




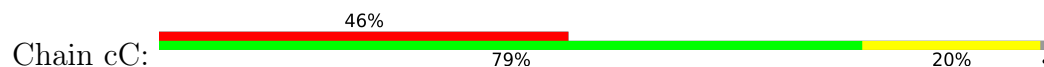
• Molecule 3: Photosystem I iron-sulfur center



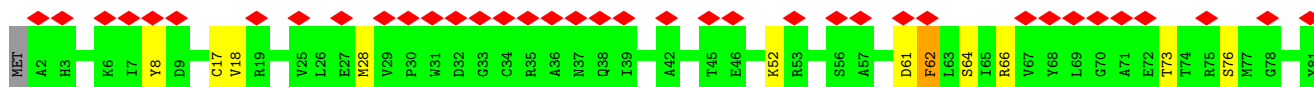
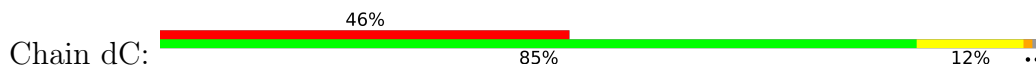
• Molecule 3: Photosystem I iron-sulfur center



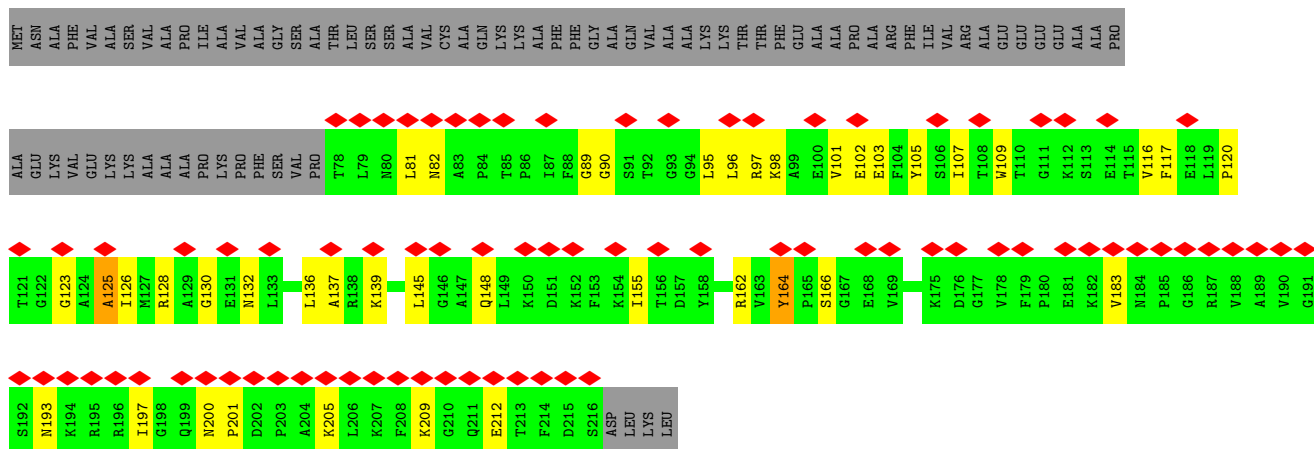
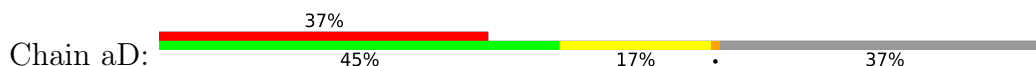
• Molecule 3: Photosystem I iron-sulfur center



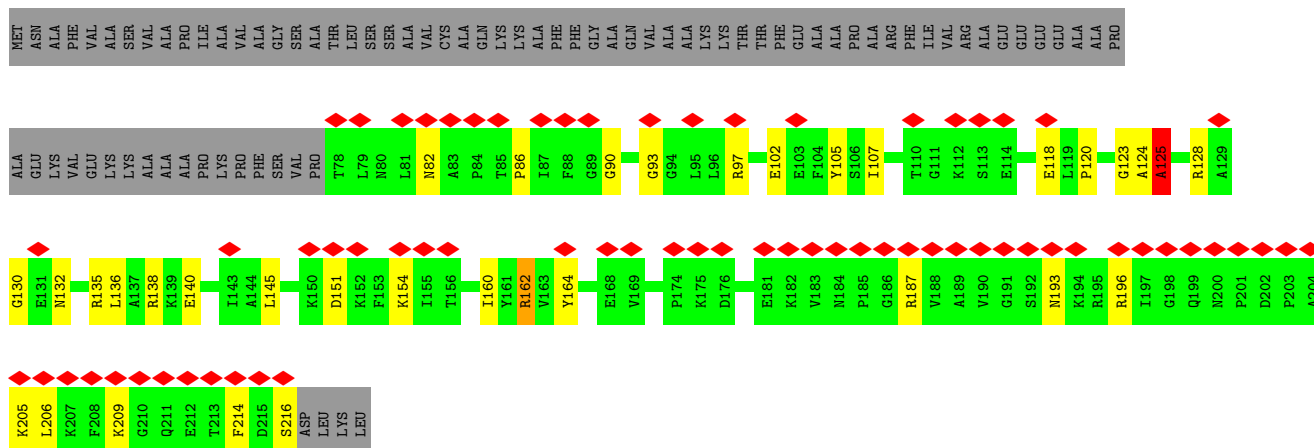
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II, cyanelle



- Molecule 4: Photosystem I reaction center subunit II, cyanelle

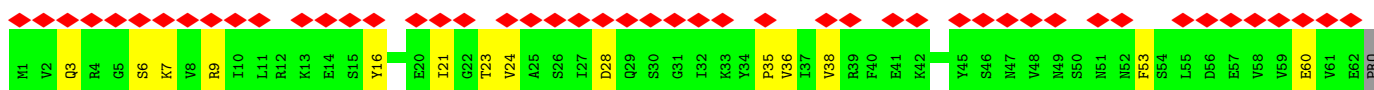


- Molecule 4: Photosystem I reaction center subunit II, cyanobacteria

PRO
SER
LYS
LYS
LYS
ALA

• Molecule 5: Photosystem I reaction center subunit IV

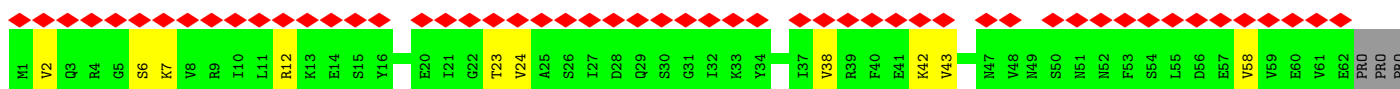
Chain cE: 



PRO
PRO
SER
LYS
LYS
LYS
ALA

• Molecule 5: Photosystem I reaction center subunit IV

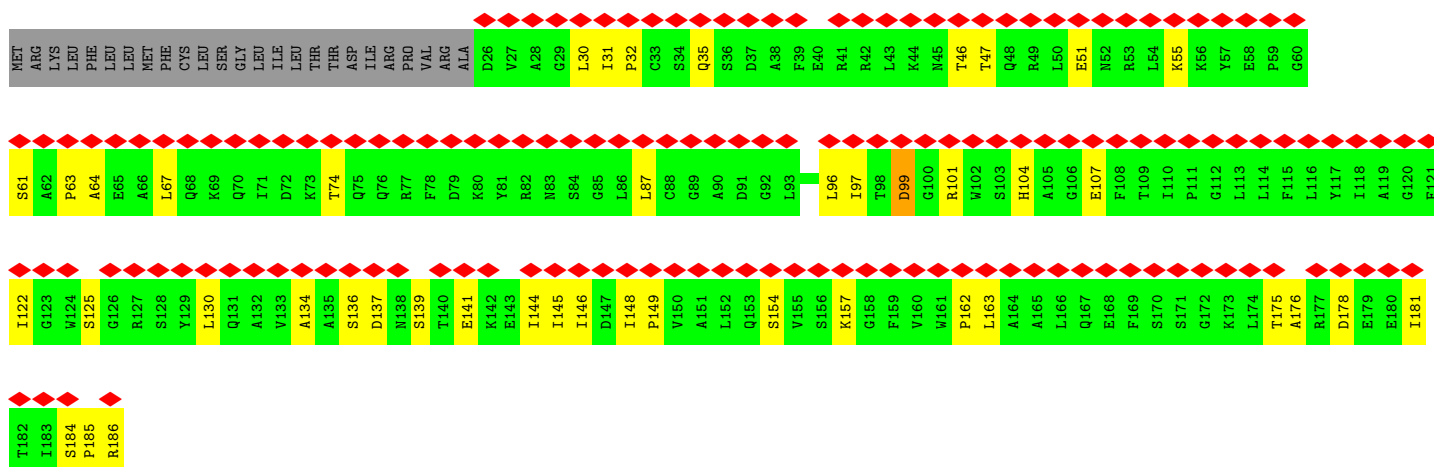
Chain dE: 



SER
LYS
LYS
LYS
ALA

• Molecule 6: Photosystem I reaction center subunit III

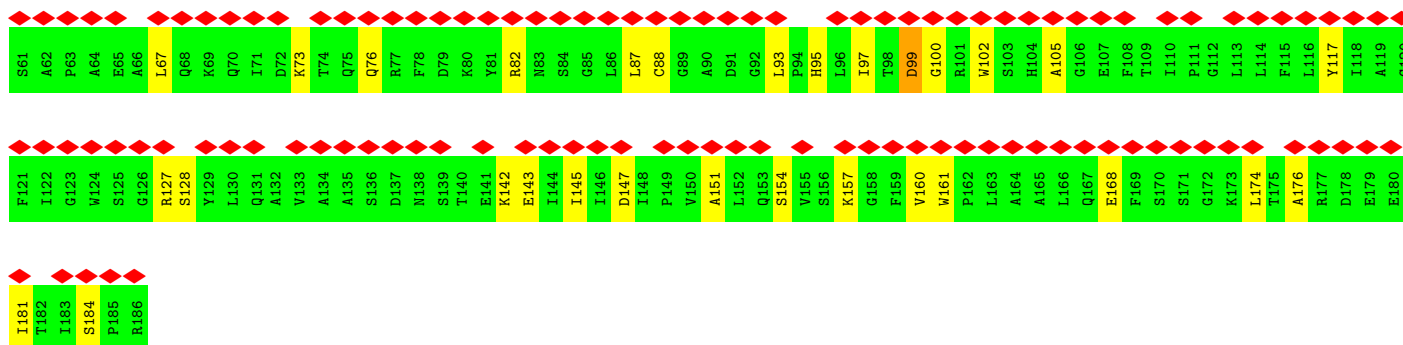
Chain aF: 



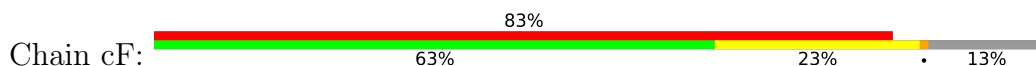
• Molecule 6: Photosystem I reaction center subunit III

Chain bF: 

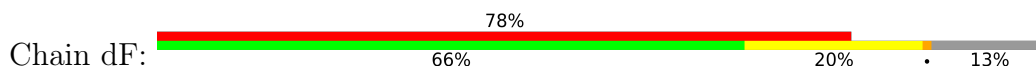




• Molecule 6: Photosystem I reaction center subunit III

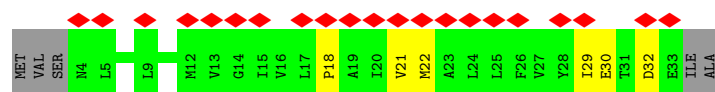


• Molecule 6: Photosystem I reaction center subunit III

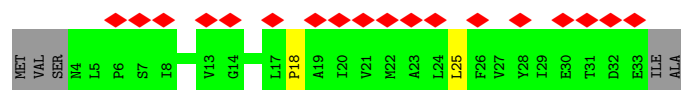
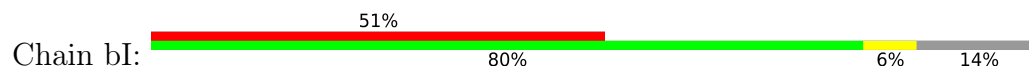


• Molecule 7: Photosystem I reaction center subunit VIII

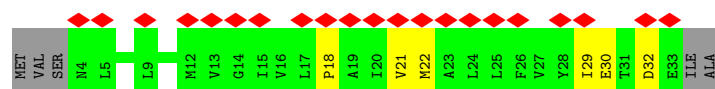




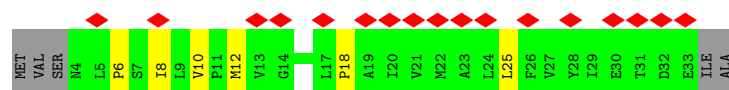
- Molecule 7: Photosystem I reaction center subunit VIII



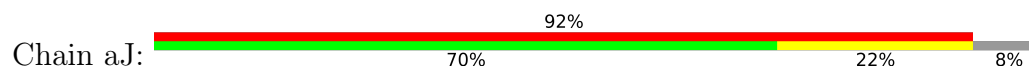
- Molecule 7: Photosystem I reaction center subunit VIII



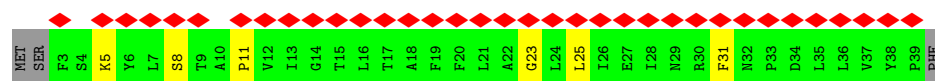
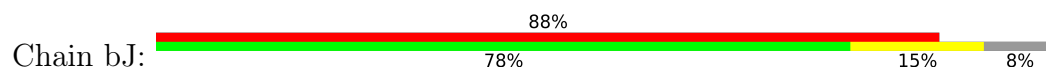
- Molecule 7: Photosystem I reaction center subunit VIII



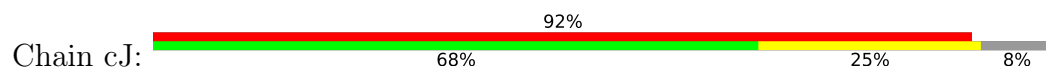
- Molecule 8: Photosystem I reaction center subunit IX



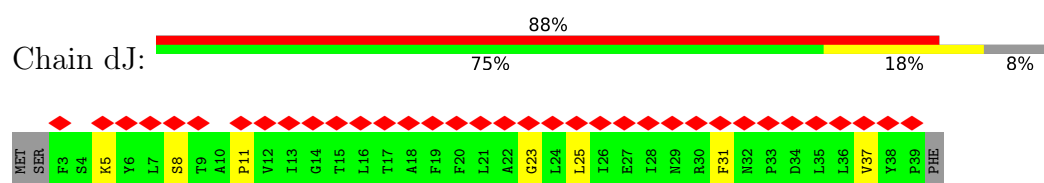
- Molecule 8: Photosystem I reaction center subunit IX



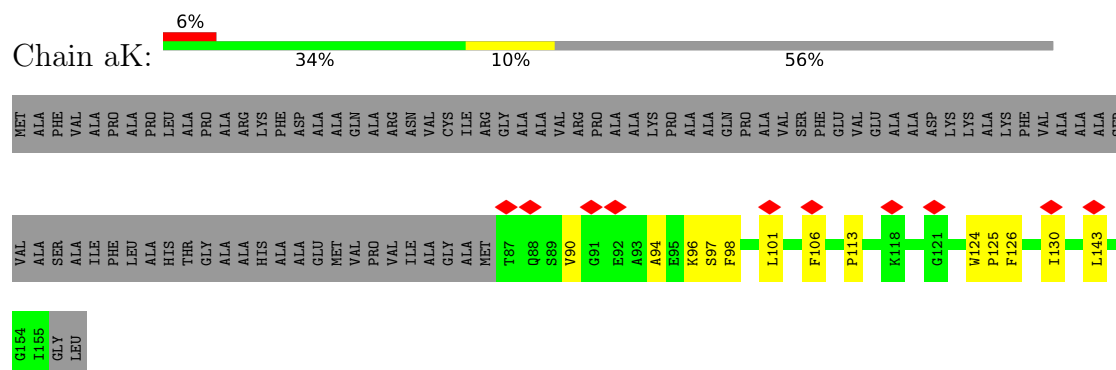
- Molecule 8: Photosystem I reaction center subunit IX



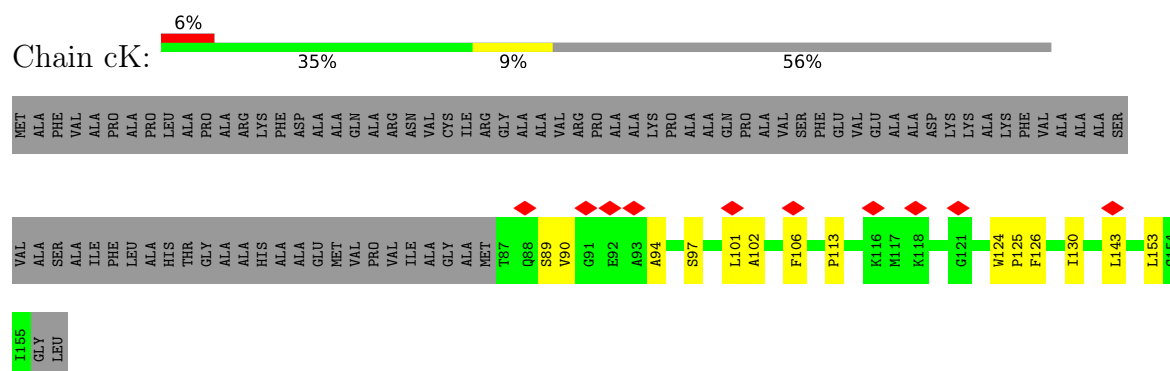
- Molecule 8: Photosystem I reaction center subunit IX



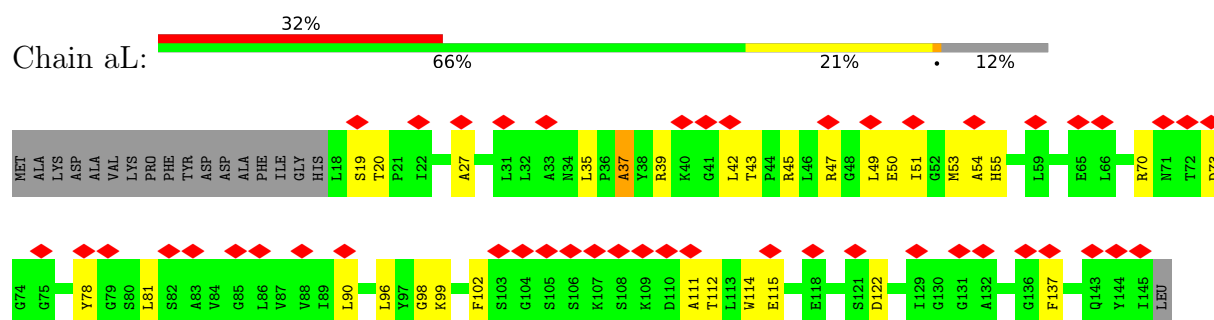
- Molecule 9: Photosystem I reaction center subunit PsaK 1



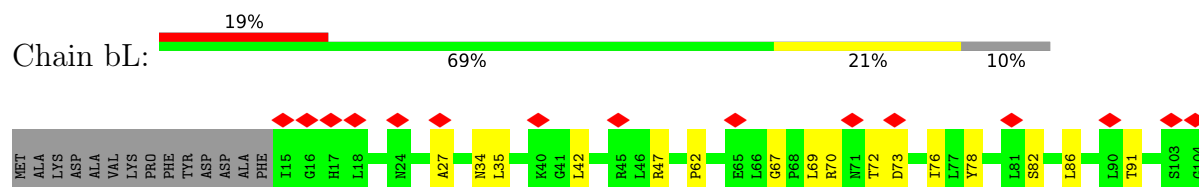
- Molecule 9: Photosystem I reaction center subunit PsaK 1

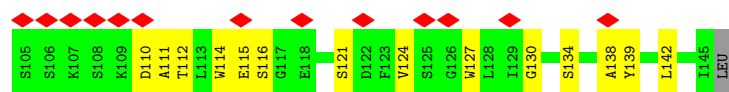


- Molecule 10: Photosystem I reaction center subunit XI

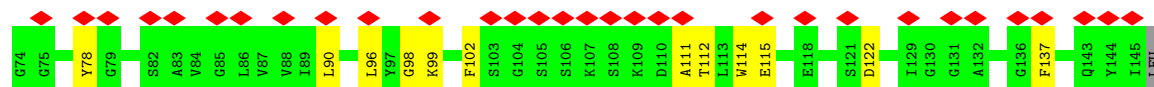


- Molecule 10: Photosystem I reaction center subunit XI

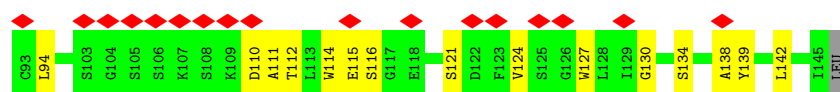
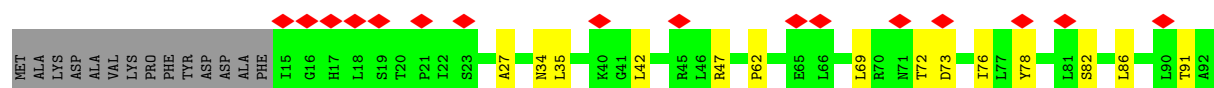
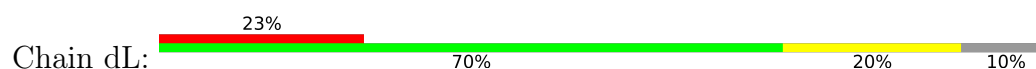




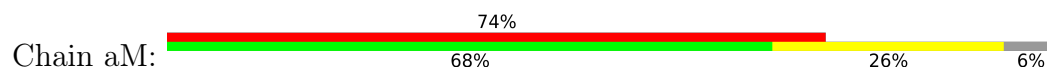
- Molecule 10: Photosystem I reaction center subunit XI



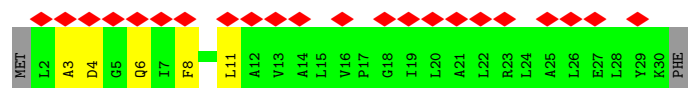
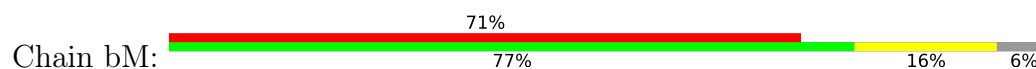
- Molecule 10: Photosystem I reaction center subunit XI



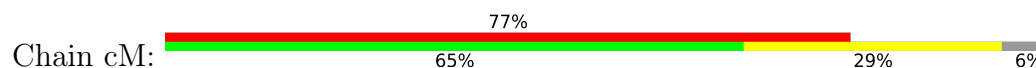
- Molecule 11: Photosystem I reaction center subunit XII



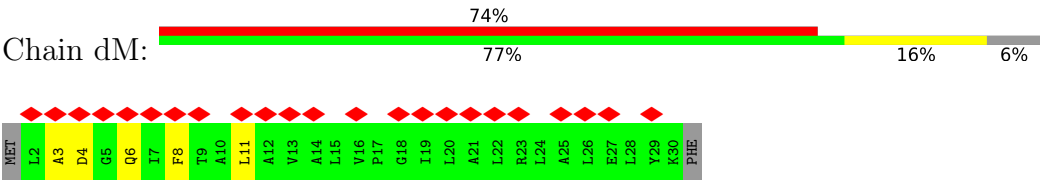
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40679	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.220	Depositor
Minimum map value	-0.104	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	450.316, 450.316, 450.316	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.093, 1.093, 1.093	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	aA	0.33	0/6000	0.58	2/8177 (0.0%)
1	bA	0.42	0/6000	0.57	0/8177
1	cA	0.33	0/6000	0.58	2/8177 (0.0%)
1	dA	0.42	0/6000	0.57	0/8177
2	aB	0.34	0/5820	0.92	5/7955 (0.1%)
2	bB	0.37	0/5820	0.83	3/7955 (0.0%)
2	cB	0.34	0/5820	0.92	5/7955 (0.1%)
2	dB	0.37	0/5820	0.83	3/7955 (0.0%)
3	aC	0.37	0/611	1.07	2/828 (0.2%)
3	bC	0.39	0/611	0.96	4/828 (0.5%)
3	cC	0.37	0/611	1.07	2/828 (0.2%)
3	dC	0.39	0/611	0.96	4/828 (0.5%)
4	aD	0.31	0/1105	0.91	7/1489 (0.5%)
4	bD	0.32	0/1105	0.86	4/1489 (0.3%)
4	cD	0.31	0/1105	0.90	7/1489 (0.5%)
4	dD	0.32	0/1105	0.86	4/1489 (0.3%)
5	aE	0.24	0/516	0.60	0/696
5	bE	0.27	0/516	0.57	0/696
5	cE	0.24	0/516	0.60	0/696
5	dE	0.27	0/516	0.57	0/696
6	aF	0.25	0/1281	0.63	0/1733
6	bF	0.26	0/1281	0.61	1/1733 (0.1%)
6	cF	0.25	0/1281	0.63	0/1733
6	dF	0.26	0/1281	0.61	1/1733 (0.1%)
7	aI	0.31	0/232	0.83	0/319
7	bI	0.53	0/232	0.80	0/319
7	cI	0.31	0/232	0.83	0/319
7	dI	0.54	0/232	0.83	0/319
8	aJ	0.23	0/300	0.54	0/410
8	bJ	0.28	0/300	0.62	0/410
8	cJ	0.23	0/300	0.54	0/410
8	dJ	0.28	0/300	0.62	0/410

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	aK	0.38	0/502	0.63	0/682
9	cK	0.38	0/502	0.64	0/682
10	aL	0.26	0/965	0.75	5/1311 (0.4%)
10	bL	0.38	0/988	0.73	2/1342 (0.1%)
10	cL	0.26	0/965	0.75	5/1311 (0.4%)
10	dL	0.41	0/988	0.74	2/1342 (0.1%)
11	aM	0.21	0/217	0.61	0/295
11	bM	0.29	0/217	0.61	0/295
11	cM	0.21	0/217	0.61	0/295
11	dM	0.29	0/217	0.61	0/295
All	All	0.35	0/69238	0.74	70/94278 (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	2
1	cA	0	2
2	aB	0	2
2	bB	0	1
2	cB	0	2
2	dB	0	1
4	aD	0	3
4	bD	0	6
4	cD	0	3
4	dD	0	6
6	aF	0	1
6	bF	0	1
6	cF	0	1
6	dF	0	1
10	aL	0	1
10	cL	0	1
All	All	0	34

There are no bond length outliers.

The worst 5 of 70 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	aD	130	GLY	CA-C-N	7.55	135.29	121.70
4	aD	130	GLY	C-N-CA	7.55	135.29	121.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	cD	130	GLY	CA-C-N	7.55	135.28	121.70
4	cD	130	GLY	C-N-CA	7.55	135.28	121.70
3	aC	62	PHE	CA-C-N	7.00	134.92	121.54

There are no chirality outliers.

5 of 34 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	aA	121	ILE	Peptide
1	aA	328	SER	Peptide
2	aB	478	LEU	Peptide
2	aB	493	GLN	Peptide
4	aD	123	GLY	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	5803	0	5621	137	0
1	bA	5803	0	5621	147	0
1	cA	5803	0	5621	143	0
1	dA	5803	0	5621	150	0
2	aB	5622	0	5406	96	0
2	bB	5622	0	5406	92	0
2	cB	5622	0	5406	95	0
2	dB	5622	0	5406	89	0
3	aC	601	0	576	17	0
3	bC	601	0	576	9	0
3	cC	601	0	576	14	0
3	dC	601	0	576	8	0
4	aD	1082	0	1099	27	0
4	bD	1082	0	1099	22	0
4	cD	1082	0	1099	27	0
4	dD	1082	0	1099	24	0
5	aE	508	0	507	8	0
5	bE	508	0	507	10	0
5	cE	508	0	507	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	dE	508	0	507	8	0
6	aF	1255	0	1249	32	0
6	bF	1255	0	1249	23	0
6	cF	1255	0	1249	32	0
6	dF	1255	0	1249	25	0
7	aI	228	0	247	5	0
7	bI	228	0	247	3	0
7	cI	228	0	247	6	0
7	dI	228	0	247	5	0
8	aJ	292	0	302	10	0
8	bJ	292	0	302	5	0
8	cJ	292	0	302	11	0
8	dJ	292	0	302	6	0
9	aK	490	0	502	41	0
9	cK	490	0	502	36	0
10	aL	943	0	949	26	0
10	bL	965	0	970	26	0
10	cL	943	0	949	24	0
10	dL	965	0	970	24	0
11	aM	215	0	239	6	0
11	bM	215	0	239	5	0
11	cM	215	0	239	7	0
11	dM	215	0	239	5	0
12	aA	65	0	72	4	0
12	bA	65	0	72	2	0
12	cA	65	0	72	4	0
12	dA	65	0	72	2	0
13	aA	2390	0	2321	115	0
13	aB	1945	0	1960	93	0
13	aF	96	0	74	6	0
13	aJ	45	0	33	2	0
13	aK	132	0	93	18	0
13	aL	152	0	134	6	0
13	bA	2421	0	2320	115	0
13	bB	1835	0	1855	84	0
13	bF	96	0	74	1	0
13	bJ	45	0	33	2	0
13	bL	117	0	115	14	0
13	cA	2390	0	2321	102	0
13	cB	1945	0	1960	95	0
13	cF	96	0	74	6	0
13	cJ	45	0	33	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	cK	132	0	93	16	0
13	cL	152	0	134	5	0
13	dA	2421	0	2320	106	0
13	dB	1835	0	1855	84	0
13	dF	96	0	74	1	0
13	dJ	45	0	33	2	0
13	dL	117	0	115	9	0
14	aA	33	0	46	5	0
14	aB	33	0	46	9	0
14	bA	33	0	46	2	0
14	bB	33	0	46	4	0
14	cA	33	0	46	5	0
14	cB	33	0	46	7	0
14	dA	33	0	46	2	0
14	dB	33	0	46	4	0
15	aA	200	0	280	11	0
15	aB	120	0	168	8	0
15	aF	80	0	112	12	0
15	aI	40	0	56	5	0
15	aJ	120	0	168	9	0
15	aK	80	0	112	6	0
15	aL	120	0	168	14	0
15	aM	40	0	56	2	0
15	bA	240	0	336	15	0
15	bB	120	0	168	5	0
15	bF	80	0	112	6	0
15	bI	80	0	112	5	0
15	bJ	120	0	168	11	0
15	bL	40	0	56	3	0
15	bM	40	0	56	8	0
15	cA	200	0	280	14	0
15	cB	120	0	168	8	0
15	cF	80	0	112	11	0
15	cI	40	0	56	5	0
15	cJ	120	0	168	10	0
15	cK	40	0	56	1	0
15	cL	120	0	168	12	0
15	cM	40	0	56	3	0
15	dA	240	0	336	19	0
15	dB	120	0	168	6	0
15	dF	80	0	112	8	0
15	dI	80	0	112	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	dJ	120	0	168	10	0
15	dL	80	0	112	6	0
15	dM	40	0	56	8	0
16	aA	76	0	98	4	0
16	bA	76	0	98	1	0
16	cA	76	0	98	5	0
16	dA	76	0	98	1	0
17	aB	8	0	0	2	0
17	aC	16	0	0	2	0
17	bB	8	0	0	1	0
17	bC	16	0	0	0	0
17	cB	8	0	0	2	0
17	cC	16	0	0	2	0
17	dB	8	0	0	1	0
17	dC	16	0	0	0	0
18	aB	55	0	86	6	0
18	bB	55	0	86	2	0
18	cB	55	0	86	6	0
18	dB	55	0	86	2	0
All	All	89952	0	89498	1940	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 11.

The worst 5 of 1940 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)
1:cA:153:ILE:CG2	1:cA:159:LEU:HD21	1.28	1.59
1:cA:153:ILE:HG21	1:cA:159:LEU:CD2	1.30	1.56
13:aK:204:CLA:C2D	9:cK:126:PHE:CE2	2.06	1.35
9:aK:113:PRO:HB3	10:bL:27:ALA:CB	1.54	1.35
1:cA:153:ILE:CG2	1:cA:159:LEU:CD2	1.94	1.32

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

438 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	CLA	cA	805	1	49,53,73	2.38	18 (36%)	59,89,113	3.35	26 (44%)
13	CLA	aA	819	1	58,62,73	2.17	18 (31%)	69,99,113	3.04	31 (44%)
13	CLA	aA	818	1	69,73,73	1.92	18 (26%)	83,113,113	2.94	30 (36%)
13	CLA	cB	823	2	69,73,73	2.01	19 (27%)	83,113,113	2.81	27 (32%)
13	CLA	cB	828	2	49,53,73	2.43	21 (42%)	59,89,113	3.17	27 (45%)
13	CLA	cB	817	2	59,63,73	2.25	21 (35%)	71,101,113	3.14	30 (42%)
13	CLA	aA	816	1	49,53,73	2.40	17 (34%)	59,89,113	3.27	27 (45%)
13	CLA	bB	818	2	64,68,73	2.11	19 (29%)	77,107,113	2.96	32 (41%)
13	CLA	cA	839	1	60,64,73	2.10	18 (30%)	72,102,113	2.99	28 (38%)
16	LHG	aA	851	13	26,26,48	0.91	0	29,32,54	1.35	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	bB	832	2	69,73,73	2.01	20 (28%)	83,113,113	2.83	31 (37%)
13	CLA	bA	833	1	69,73,73	2.01	18 (26%)	83,113,113	2.87	30 (36%)
13	CLA	aA	838	1	55,59,73	2.21	20 (36%)	66,96,113	3.14	30 (45%)
15	BCR	aM	101	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	dB	817	2	63,67,73	2.12	20 (31%)	75,105,113	3.10	26 (34%)
13	CLA	dA	835	1	69,73,73	1.95	18 (26%)	83,113,113	2.92	32 (38%)
13	CLA	bA	803	-	49,53,73	2.36	19 (38%)	59,89,113	3.13	28 (47%)
13	CLA	dA	821	1	65,69,73	2.04	19 (29%)	78,108,113	2.94	31 (39%)
15	BCR	dI	102	-	41,41,41	1.22	2 (4%)	56,56,56	1.39	8 (14%)
13	CLA	bA	832	1	54,58,73	2.22	19 (35%)	65,95,113	3.11	34 (52%)
13	CLA	aA	841	1	69,73,73	2.05	21 (30%)	83,113,113	2.84	30 (36%)
13	CLA	aB	815	2	60,64,73	2.22	20 (33%)	72,102,113	2.99	28 (38%)
13	CLA	aA	802	-	69,73,73	1.97	20 (28%)	83,113,113	2.93	34 (40%)
13	CLA	aL	202	10	50,54,73	2.36	20 (40%)	60,90,113	3.30	26 (43%)
13	CLA	dA	813	1	58,62,73	2.15	19 (32%)	69,99,113	2.94	29 (42%)
14	PQN	cA	844	-	34,34,34	1.51	2 (5%)	42,45,45	1.12	4 (9%)
15	BCR	cM	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	cA	812	1	69,73,73	2.02	21 (30%)	83,113,113	2.93	29 (34%)
13	CLA	aB	804	-	69,73,73	1.92	19 (27%)	83,113,113	2.84	32 (38%)
13	CLA	aA	824	1	55,59,73	2.17	18 (32%)	66,96,113	3.21	30 (45%)
13	CLA	bA	841	1	69,73,73	2.03	18 (26%)	83,113,113	2.84	28 (33%)
13	CLA	dF	204	6	49,53,73	2.42	20 (40%)	59,89,113	3.35	27 (45%)
15	BCR	aK	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
13	CLA	dA	830	1	69,73,73	1.99	19 (27%)	83,113,113	2.77	30 (36%)
13	CLA	dB	802	2	69,73,73	1.97	18 (26%)	83,113,113	2.86	34 (40%)
13	CLA	dB	829	2	69,73,73	2.01	20 (28%)	83,113,113	2.86	33 (39%)
15	BCR	aB	838	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	cA	825	1	51,55,73	2.29	18 (35%)	61,91,113	3.32	29 (47%)
13	CLA	bB	820	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	30 (36%)
13	CLA	aA	811	1	49,53,73	2.34	19 (38%)	59,89,113	3.37	29 (49%)
13	CLA	aA	813	1	58,62,73	2.17	19 (32%)	69,99,113	2.98	28 (40%)
13	CLA	bB	811	2	69,73,73	1.97	20 (28%)	83,113,113	2.80	38 (45%)
13	CLA	dA	837	1	49,53,73	2.35	19 (38%)	59,89,113	3.41	30 (50%)
17	SF4	dC	102	3	0,12,12	-	-	-	-	-
13	CLA	bA	838	1	55,59,73	2.23	18 (32%)	66,96,113	3.17	30 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	dA	807	1	69,73,73	1.99	18 (26%)	83,113,113	2.88	31 (37%)
15	BCR	dF	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	8 (14%)
13	CLA	cA	804	1	49,53,73	2.43	19 (38%)	59,89,113	3.28	30 (50%)
13	CLA	dB	831	-	69,73,73	1.96	19 (27%)	83,113,113	2.87	32 (38%)
13	CLA	dB	824	2	53,57,73	2.35	19 (35%)	62,93,113	3.32	29 (46%)
13	CLA	dB	810	2	69,73,73	1.96	18 (26%)	83,113,113	2.80	32 (38%)
14	PQN	bA	845	-	34,34,34	1.57	2 (5%)	42,45,45	1.04	3 (7%)
13	CLA	dA	823	1	50,54,73	2.29	18 (36%)	60,90,113	3.28	26 (43%)
13	CLA	cB	820	-	50,54,73	2.44	22 (44%)	60,90,113	3.50	32 (53%)
13	CLA	dB	820	2	69,73,73	2.05	20 (28%)	83,113,113	2.79	30 (36%)
13	CLA	aA	807	1	69,73,73	1.97	19 (27%)	83,113,113	2.90	31 (37%)
14	PQN	aB	835	-	34,34,34	1.51	3 (8%)	42,45,45	1.31	3 (7%)
15	BCR	aA	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.49	11 (19%)
13	CLA	aB	826	2	69,73,73	2.04	21 (30%)	83,113,113	2.89	31 (37%)
13	CLA	aB	829	-	49,53,73	2.48	20 (40%)	59,89,113	3.22	28 (47%)
13	CLA	bB	807	2	69,73,73	2.01	22 (31%)	83,113,113	2.93	33 (39%)
13	CLA	bA	818	1	69,73,73	1.94	18 (26%)	83,113,113	2.93	29 (34%)
13	CLA	cB	827	2	62,66,73	2.14	18 (29%)	74,104,113	3.16	30 (40%)
13	CLA	dA	834	1	69,73,73	1.98	19 (27%)	83,113,113	2.81	34 (40%)
13	CLA	cA	829	1	69,73,73	1.95	18 (26%)	83,113,113	2.92	31 (37%)
13	CLA	aA	825	1	51,55,73	2.29	18 (35%)	61,91,113	3.31	29 (47%)
15	BCR	bF	202	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	8 (14%)
13	CLA	cA	821	1	65,69,73	2.00	18 (27%)	78,108,113	2.89	28 (35%)
13	CLA	dB	827	2	49,53,73	2.44	20 (40%)	59,89,113	3.37	29 (49%)
13	CLA	cB	809	2	69,73,73	2.00	20 (28%)	83,113,113	2.78	29 (34%)
13	CLA	aB	833	-	69,73,73	2.02	20 (28%)	83,113,113	2.89	29 (34%)
17	SF4	dC	101	3	0,12,12	-	-	-	-	-
13	CLA	bB	802	2	69,73,73	1.97	18 (26%)	83,113,113	2.85	34 (40%)
13	CLA	bB	823	2	69,73,73	1.98	18 (26%)	83,113,113	2.72	27 (32%)
13	CLA	aB	805	-	69,73,73	1.92	20 (28%)	83,113,113	2.74	29 (34%)
13	CLA	cA	832	1	54,58,73	2.23	18 (33%)	65,95,113	3.14	33 (50%)
15	BCR	aA	845	-	41,41,41	1.15	3 (7%)	56,56,56	1.31	10 (17%)
13	CLA	cA	841	1	69,73,73	2.05	21 (30%)	83,113,113	2.84	30 (36%)
13	CLA	bA	812	1	69,73,73	2.01	21 (30%)	83,113,113	2.87	32 (38%)
13	CLA	aA	810	1	49,53,73	2.40	22 (44%)	59,89,113	3.19	25 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	bB	813	2	69,73,73	2.01	20 (28%)	83,113,113	2.84	27 (32%)
13	CLA	bB	831	-	69,73,73	1.96	20 (28%)	83,113,113	2.86	32 (38%)
13	CLA	aA	840	1	69,73,73	1.95	19 (27%)	83,113,113	2.84	31 (37%)
13	CLA	aB	801	-	69,73,73	1.96	18 (26%)	83,113,113	2.73	32 (38%)
13	CLA	cB	832	2	51,55,73	2.34	20 (39%)	61,91,113	3.34	29 (47%)
13	CLA	aA	823	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	28 (33%)
13	CLA	aA	828	1	69,73,73	1.98	18 (26%)	83,113,113	2.85	31 (37%)
13	CLA	aB	834	2	69,73,73	2.02	19 (27%)	83,113,113	2.80	30 (36%)
13	CLA	dA	814	1	49,53,73	2.32	18 (36%)	59,89,113	3.25	27 (45%)
13	CLA	bB	828	2	50,54,73	2.33	21 (42%)	60,90,113	3.32	30 (50%)
13	CLA	dA	841	1	69,73,73	2.03	18 (26%)	83,113,113	2.84	28 (33%)
13	CLA	bA	808	1	55,59,73	2.24	20 (36%)	66,96,113	3.22	32 (48%)
13	CLA	aA	836	1	58,62,73	2.15	19 (32%)	69,99,113	3.01	29 (42%)
15	BCR	dA	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.47	9 (16%)
13	CLA	cB	803	2	69,73,73	1.99	21 (30%)	83,113,113	2.95	33 (39%)
15	BCR	aB	837	-	41,41,41	1.07	2 (4%)	56,56,56	1.37	8 (14%)
15	BCR	bA	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.47	9 (16%)
13	CLA	aA	821	1	65,69,73	2.00	18 (27%)	78,108,113	2.89	28 (35%)
13	CLA	dA	805	1	49,53,73	2.37	18 (36%)	59,89,113	3.45	29 (49%)
13	CLA	bB	821	2	69,73,73	1.95	20 (28%)	83,113,113	2.98	31 (37%)
13	CLA	bA	827	-	59,63,73	2.10	18 (30%)	71,101,113	3.14	35 (49%)
13	CLA	aB	816	2	49,53,73	2.45	21 (42%)	59,89,113	3.19	27 (45%)
13	CLA	bA	837	1	49,53,73	2.35	19 (38%)	59,89,113	3.41	30 (50%)
13	CLA	cA	827	-	59,63,73	2.14	18 (30%)	71,101,113	3.12	32 (45%)
15	BCR	dA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.48	10 (17%)
13	CLA	bA	820	1	69,73,73	2.00	19 (27%)	83,113,113	2.71	31 (37%)
13	CLA	bB	803	-	69,73,73	1.92	19 (27%)	83,113,113	2.92	35 (42%)
13	CLA	aB	824	2	69,73,73	2.04	20 (28%)	83,113,113	2.86	31 (37%)
16	LHG	dA	853	13	26,26,48	0.90	1 (3%)	29,32,54	1.38	4 (13%)
13	CLA	aF	201	-	55,59,73	2.32	21 (38%)	66,96,113	3.12	28 (42%)
13	CLA	aA	803	-	49,53,73	2.37	19 (38%)	59,89,113	3.15	28 (47%)
15	BCR	bL	201	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	6 (10%)
13	CLA	cA	840	1	69,73,73	1.95	19 (27%)	83,113,113	2.84	31 (37%)
13	CLA	cA	802	-	69,73,73	1.97	20 (28%)	83,113,113	2.93	34 (40%)
13	CLA	bA	825	1	51,55,73	2.24	18 (35%)	61,91,113	3.36	31 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	aB	827	2	62,66,73	2.14	18 (29%)	74,104,113	3.16	30 (40%)
13	CLA	cA	815	1	49,53,73	2.43	18 (36%)	59,89,113	3.34	29 (49%)
12	CL0	bA	801	1	69,73,73	2.00	18 (26%)	83,113,113	3.01	36 (43%)
13	CLA	dB	822	2	69,73,73	2.01	19 (27%)	83,113,113	2.77	31 (37%)
13	CLA	bA	834	1	69,73,73	1.98	19 (27%)	83,113,113	2.81	34 (40%)
13	CLA	cA	810	1	49,53,73	2.41	22 (44%)	59,89,113	3.20	25 (42%)
15	BCR	bI	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.16	5 (8%)
15	BCR	cA	848	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	7 (12%)
13	CLA	bB	816	2	59,63,73	2.22	21 (35%)	71,101,113	3.13	29 (40%)
13	CLA	dA	819	1	58,62,73	2.15	19 (32%)	69,99,113	2.82	29 (42%)
13	CLA	bB	825	2	69,73,73	2.03	20 (28%)	83,113,113	3.05	31 (37%)
15	BCR	cJ	104	-	41,41,41	1.09	2 (4%)	56,56,56	1.33	8 (14%)
13	CLA	dA	816	1	49,53,73	2.35	20 (40%)	59,89,113	3.30	27 (45%)
15	BCR	aF	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.31	7 (12%)
15	BCR	dB	835	-	41,41,41	1.08	3 (7%)	56,56,56	1.34	7 (12%)
13	CLA	dA	828	1	69,73,73	1.92	19 (27%)	83,113,113	2.90	31 (37%)
13	CLA	dA	817	-	53,57,73	2.30	19 (35%)	62,93,113	3.18	28 (45%)
13	CLA	cA	826	-	69,73,73	1.92	18 (26%)	83,113,113	2.74	29 (34%)
13	CLA	aA	842	1	69,73,73	2.01	20 (28%)	83,113,113	2.79	28 (33%)
13	CLA	dA	818	1	69,73,73	1.95	18 (26%)	83,113,113	2.94	29 (34%)
13	CLA	aK	203	-	49,53,73	2.37	20 (40%)	59,89,113	3.35	29 (49%)
13	CLA	dA	820	1	69,73,73	2.00	19 (27%)	83,113,113	2.71	31 (37%)
13	CLA	dA	844	16	56,60,73	2.14	16 (28%)	67,97,113	3.32	35 (52%)
15	BCR	cJ	103	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
13	CLA	dB	815	2	49,53,73	2.37	21 (42%)	59,89,113	3.31	28 (47%)
17	SF4	bC	101	3	0,12,12	-	-	-	-	-
15	BCR	cF	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.31	7 (12%)
15	BCR	dI	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.16	5 (8%)
13	CLA	cB	807	2	69,73,73	2.05	20 (28%)	83,113,113	2.84	32 (38%)
13	CLA	bB	819	-	50,54,73	2.39	20 (40%)	60,90,113	3.37	31 (51%)
15	BCR	bB	836	-	41,41,41	1.23	2 (4%)	56,56,56	1.15	3 (5%)
13	CLA	dA	839	1	60,64,73	2.10	18 (30%)	72,102,113	2.91	28 (38%)
13	CLA	bA	815	1	49,53,73	2.34	20 (40%)	59,89,113	3.22	28 (47%)
13	CLA	cA	824	1	55,59,73	2.17	18 (32%)	66,96,113	3.21	30 (45%)
13	CLA	bA	822	-	69,73,73	1.92	18 (26%)	83,113,113	2.70	28 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	cA	837	1	49,53,73	2.37	20 (40%)	59,89,113	3.40	27 (45%)
13	CLA	dA	829	1	69,73,73	1.97	19 (27%)	83,113,113	2.80	33 (39%)
15	BCR	bA	849	-	41,41,41	1.16	2 (4%)	56,56,56	1.48	10 (17%)
13	CLA	cA	820	1	69,73,73	2.04	19 (27%)	83,113,113	2.75	31 (37%)
13	CLA	dA	831	1	69,73,73	1.94	19 (27%)	83,113,113	2.84	32 (38%)
13	CLA	bB	806	2	69,73,73	2.02	20 (28%)	83,113,113	2.93	31 (37%)
16	LHG	cA	851	13	26,26,48	0.91	0	29,32,54	1.35	3 (10%)
13	CLA	cA	813	1	58,62,73	2.17	19 (32%)	69,99,113	2.98	28 (40%)
14	PQN	bB	833	-	34,34,34	1.56	2 (5%)	42,45,45	1.25	4 (9%)
15	BCR	cL	201	-	41,41,41	1.21	2 (4%)	56,56,56	1.26	4 (7%)
15	BCR	dJ	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.42	9 (16%)
13	CLA	cB	831	2	69,73,73	2.02	19 (27%)	83,113,113	2.77	30 (36%)
13	CLA	dA	843	-	69,73,73	1.92	18 (26%)	83,113,113	2.76	30 (36%)
13	CLA	bL	203	-	56,60,73	2.20	18 (32%)	67,97,113	3.36	34 (50%)
13	CLA	bA	807	1	69,73,73	1.99	18 (26%)	83,113,113	2.88	31 (37%)
13	CLA	dA	824	1	55,59,73	2.16	19 (34%)	66,96,113	3.17	29 (43%)
13	CLA	dB	814	2	60,64,73	2.17	20 (33%)	72,102,113	3.01	28 (38%)
13	CLA	aB	828	2	49,53,73	2.42	20 (40%)	59,89,113	3.17	27 (45%)
13	CLA	aB	817	2	59,63,73	2.25	20 (33%)	71,101,113	3.14	30 (42%)
13	CLA	cB	830	2	50,54,73	2.35	20 (40%)	60,90,113	3.27	30 (50%)
13	CLA	dA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.20	29 (49%)
13	CLA	aB	808	2	69,73,73	2.00	21 (30%)	83,113,113	2.92	33 (39%)
13	CLA	dB	808	2	69,73,73	1.97	19 (27%)	83,113,113	2.77	32 (38%)
13	CLA	dA	826	-	69,73,73	1.91	20 (28%)	83,113,113	2.75	31 (37%)
13	CLA	aA	831	1	69,73,73	1.95	18 (26%)	83,113,113	2.81	30 (36%)
13	CLA	dB	830	2	51,55,73	2.31	22 (43%)	61,91,113	3.20	27 (44%)
13	CLA	cF	204	6	49,53,73	2.47	21 (42%)	59,89,113	3.33	30 (50%)
15	BCR	aL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.33	8 (14%)
15	BCR	cA	845	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	10 (17%)
15	BCR	cF	203	-	41,41,41	1.03	2 (4%)	56,56,56	1.33	12 (21%)
13	CLA	bA	844	16	56,60,73	2.14	16 (28%)	67,97,113	3.32	35 (52%)
13	CLA	cB	826	2	69,73,73	2.05	20 (28%)	83,113,113	2.90	31 (37%)
13	CLA	bA	823	1	50,54,73	2.30	18 (36%)	60,90,113	3.28	26 (43%)
13	CLA	aL	203	10	69,73,73	1.98	19 (27%)	83,113,113	2.85	30 (36%)
12	CL0	cA	801	1	69,73,73	2.01	19 (27%)	83,113,113	2.80	36 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	cA	828	1	69,73,73	1.97	18 (26%)	83,113,113	2.85	31 (37%)
14	PQN	cB	835	-	34,34,34	1.51	3 (8%)	42,45,45	1.31	3 (7%)
13	CLA	dA	827	-	59,63,73	2.09	18 (30%)	71,101,113	3.14	35 (49%)
13	CLA	bB	826	2	62,66,73	2.09	19 (30%)	74,104,113	3.15	33 (44%)
15	BCR	dA	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	7 (12%)
15	BCR	dJ	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	8 (14%)
15	BCR	bM	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	dJ	104	-	41,41,41	1.10	2 (4%)	56,56,56	1.36	7 (12%)
13	CLA	cB	834	2	69,73,73	2.02	19 (27%)	83,113,113	2.80	30 (36%)
13	CLA	dA	811	1	49,53,73	2.35	18 (36%)	59,89,113	3.40	29 (49%)
15	BCR	cB	836	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	4 (7%)
13	CLA	bA	804	1	49,53,73	2.39	19 (38%)	59,89,113	3.39	29 (49%)
15	BCR	cJ	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	9 (16%)
13	CLA	aB	832	2	51,55,73	2.34	20 (39%)	61,91,113	3.35	29 (47%)
17	SF4	cC	102	3	0,12,12	-	-	-	-	-
15	BCR	dA	851	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	7 (12%)
13	CLA	aA	827	-	59,63,73	2.14	18 (30%)	71,101,113	3.13	32 (45%)
13	CLA	bA	843	-	69,73,73	1.92	18 (26%)	83,113,113	2.77	30 (36%)
13	CLA	aB	810	2	69,73,73	2.03	20 (28%)	83,113,113	2.85	32 (38%)
13	CLA	aA	837	1	49,53,73	2.37	19 (38%)	59,89,113	3.40	27 (45%)
15	BCR	bA	846	-	41,41,41	1.19	3 (7%)	56,56,56	1.41	13 (23%)
13	CLA	dB	819	-	50,54,73	2.39	20 (40%)	60,90,113	3.37	31 (51%)
13	CLA	aB	806	2	58,62,73	2.21	20 (34%)	69,99,113	3.12	32 (46%)
13	CLA	aA	835	1	69,73,73	2.02	19 (27%)	83,113,113	2.91	28 (33%)
13	CLA	bA	817	-	53,57,73	2.30	19 (35%)	62,93,113	3.18	28 (45%)
15	BCR	dB	834	-	41,41,41	1.12	3 (7%)	56,56,56	1.30	5 (8%)
13	CLA	aA	826	-	69,73,73	1.92	18 (26%)	83,113,113	2.75	29 (34%)
15	BCR	dL	201	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	6 (10%)
13	CLA	bA	840	1	54,58,73	2.18	18 (33%)	65,95,113	3.26	34 (52%)
16	LHG	aA	850	-	48,48,48	0.63	0	51,54,54	1.29	6 (11%)
13	CLA	aA	809	1	69,73,73	2.00	21 (30%)	83,113,113	2.84	31 (37%)
13	CLA	aB	821	2	69,73,73	2.05	19 (27%)	83,113,113	2.94	30 (36%)
13	CLA	cA	822	-	69,73,73	1.99	19 (27%)	83,113,113	2.73	26 (31%)
13	CLA	dA	840	1	54,58,73	2.18	18 (33%)	65,95,113	3.26	34 (52%)
15	BCR	bA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.42	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CL0	dA	801	1	69,73,73	2.00	18 (26%)	83,113,113	3.02	36 (43%)
13	CLA	bA	813	1	58,62,73	2.14	19 (32%)	69,99,113	2.94	29 (42%)
13	CLA	bA	835	1	69,73,73	1.95	18 (26%)	83,113,113	2.92	32 (38%)
13	CLA	dB	804	-	69,73,73	1.90	18 (26%)	83,113,113	2.65	27 (32%)
15	BCR	dB	836	-	41,41,41	1.23	2 (4%)	56,56,56	1.15	3 (5%)
13	CLA	bA	814	1	49,53,73	2.31	18 (36%)	59,89,113	3.25	27 (45%)
13	CLA	aB	803	2	69,73,73	1.99	21 (30%)	83,113,113	2.95	33 (39%)
13	CLA	aA	817	-	53,57,73	2.35	19 (35%)	62,93,113	3.24	27 (43%)
15	BCR	aA	849	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	11 (19%)
14	PQN	dA	845	-	34,34,34	1.56	2 (5%)	42,45,45	1.04	3 (7%)
13	CLA	bB	817	2	63,67,73	2.12	20 (31%)	75,105,113	3.11	27 (36%)
15	BCR	cK	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
13	CLA	cA	806	1	69,73,73	1.95	19 (27%)	83,113,113	2.83	30 (36%)
13	CLA	cB	825	2	53,57,73	2.31	19 (35%)	62,93,113	3.31	27 (43%)
13	CLA	aA	834	1	69,73,73	1.98	19 (27%)	83,113,113	2.84	32 (38%)
13	CLA	bA	805	1	49,53,73	2.37	18 (36%)	59,89,113	3.44	29 (49%)
15	BCR	aA	848	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	7 (12%)
13	CLA	bA	826	-	69,73,73	1.92	20 (28%)	83,113,113	2.76	31 (37%)
13	CLA	dB	825	2	69,73,73	2.03	21 (30%)	83,113,113	3.05	31 (37%)
13	CLA	aA	832	1	54,58,73	2.23	18 (33%)	65,95,113	3.14	33 (50%)
13	CLA	dA	803	-	49,53,73	2.36	19 (38%)	59,89,113	3.12	28 (47%)
15	BCR	aJ	104	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	8 (14%)
13	CLA	cB	806	2	58,62,73	2.22	20 (34%)	69,99,113	3.12	32 (46%)
15	BCR	cB	838	-	41,41,41	1.21	3 (7%)	56,56,56	1.26	8 (14%)
15	BCR	cA	849	-	41,41,41	1.03	1 (2%)	56,56,56	1.47	11 (19%)
13	CLA	dB	806	2	69,73,73	2.02	20 (28%)	83,113,113	2.93	31 (37%)
13	CLA	dB	805	2	58,62,73	2.15	19 (32%)	69,99,113	3.07	31 (44%)
17	SF4	aC	102	3	0,12,12	-	-	-	-	-
13	CLA	aB	819	2	64,68,73	2.13	20 (31%)	77,107,113	2.91	34 (44%)
13	CLA	cB	822	2	69,73,73	2.04	21 (30%)	83,113,113	2.82	30 (36%)
13	CLA	dB	826	2	62,66,73	2.09	20 (32%)	74,104,113	3.15	33 (44%)
13	CLA	bB	827	2	49,53,73	2.44	20 (40%)	59,89,113	3.36	29 (49%)
15	BCR	bB	834	-	41,41,41	1.12	2 (4%)	56,56,56	1.30	5 (8%)
12	CL0	aA	801	1	69,73,73	2.01	19 (27%)	83,113,113	2.81	36 (43%)
13	CLA	aJ	101	8	49,53,73	2.45	20 (40%)	59,89,113	3.26	27 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	bA	819	1	58,62,73	2.15	19 (32%)	69,99,113	2.82	29 (42%)
13	CLA	bA	809	1	69,73,73	1.96	19 (27%)	83,113,113	2.84	31 (37%)
13	CLA	cA	843	16	56,60,73	2.24	19 (33%)	67,97,113	3.16	32 (47%)
13	CLA	dA	802	-	69,73,73	1.96	18 (26%)	83,113,113	2.96	33 (39%)
13	CLA	aB	818	2	63,67,73	2.17	20 (31%)	75,105,113	3.00	30 (40%)
13	CLA	dB	818	2	64,68,73	2.11	19 (29%)	77,107,113	2.96	31 (40%)
13	CLA	bA	831	1	69,73,73	1.94	19 (27%)	83,113,113	2.84	32 (38%)
13	CLA	cA	842	1	69,73,73	2.00	20 (28%)	83,113,113	2.79	28 (33%)
13	CLA	cB	815	2	60,64,73	2.22	20 (33%)	72,102,113	2.99	28 (38%)
13	CLA	dA	815	1	49,53,73	2.34	20 (40%)	59,89,113	3.22	30 (50%)
13	CLA	dA	842	1	69,73,73	1.99	21 (30%)	83,113,113	2.89	30 (36%)
16	LHG	bA	852	-	48,48,48	0.69	2 (4%)	51,54,54	1.27	6 (11%)
13	CLA	cA	831	1	69,73,73	1.95	18 (26%)	83,113,113	2.80	30 (36%)
15	BCR	cL	206	-	41,41,41	1.01	2 (4%)	56,56,56	1.33	8 (14%)
13	CLA	cA	835	1	69,73,73	2.02	19 (27%)	83,113,113	2.92	28 (33%)
13	CLA	cB	804	-	69,73,73	1.92	20 (28%)	83,113,113	2.83	31 (37%)
13	CLA	bB	809	2	69,73,73	1.99	20 (28%)	83,113,113	2.90	32 (38%)
15	BCR	dA	848	-	41,41,41	1.10	2 (4%)	56,56,56	1.43	10 (17%)
13	CLA	cB	816	2	49,53,73	2.45	20 (40%)	59,89,113	3.19	27 (45%)
15	BCR	bI	102	-	41,41,41	1.22	2 (4%)	56,56,56	1.39	8 (14%)
15	BCR	aJ	103	-	41,41,41	1.03	2 (4%)	56,56,56	1.37	8 (14%)
13	CLA	cA	817	-	53,57,73	2.35	19 (35%)	62,93,113	3.25	27 (43%)
17	SF4	aC	101	3	0,12,12	-	-	-	-	-
13	CLA	cL	202	10	50,54,73	2.36	20 (40%)	60,90,113	3.30	26 (43%)
15	BCR	dF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	7 (12%)
13	CLA	cB	824	2	69,73,73	2.05	20 (28%)	83,113,113	2.87	31 (37%)
13	CLA	cA	814	1	49,53,73	2.33	19 (38%)	59,89,113	3.36	27 (45%)
13	CLA	cK	201	9	46,49,73	2.31	19 (41%)	55,83,113	3.42	27 (49%)
15	BCR	bJ	104	-	41,41,41	1.10	2 (4%)	56,56,56	1.37	7 (12%)
15	BCR	dM	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.20	5 (8%)
13	CLA	cL	204	-	45,49,73	2.43	18 (40%)	54,84,113	3.48	27 (50%)
13	CLA	cB	818	2	63,67,73	2.17	20 (31%)	75,105,113	3.01	30 (40%)
13	CLA	dB	816	2	59,63,73	2.22	21 (35%)	71,101,113	3.13	29 (40%)
13	CLA	cB	810	2	69,73,73	2.03	20 (28%)	83,113,113	2.84	32 (38%)
13	CLA	aB	830	2	50,54,73	2.35	20 (40%)	60,90,113	3.27	30 (50%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	dL	203	-	56,60,73	2.21	18 (32%)	67,97,113	3.37	33 (49%)
13	CLA	bA	829	1	69,73,73	1.98	19 (27%)	83,113,113	2.81	33 (39%)
13	CLA	cA	809	1	69,73,73	1.99	20 (28%)	83,113,113	2.85	31 (37%)
13	CLA	aB	813	2	49,53,73	2.47	21 (42%)	59,89,113	3.26	27 (45%)
13	CLA	dF	201	-	55,59,73	2.25	21 (38%)	66,96,113	3.26	32 (48%)
13	CLA	aB	812	2	69,73,73	2.00	18 (26%)	83,113,113	2.86	35 (42%)
15	BCR	aI	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.35	9 (16%)
13	CLA	cA	830	1	69,73,73	1.96	19 (27%)	83,113,113	2.72	31 (37%)
13	CLA	dA	808	1	55,59,73	2.24	20 (36%)	66,96,113	3.22	32 (48%)
13	CLA	cK	203	-	49,53,73	2.37	20 (40%)	59,89,113	3.35	29 (49%)
17	SF4	bC	102	3	0,12,12	-	-	-	-	-
15	BCR	cA	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.47	11 (19%)
13	CLA	aB	820	-	50,54,73	2.44	22 (44%)	60,90,113	3.50	32 (53%)
13	CLA	cB	814	2	69,73,73	2.02	20 (28%)	83,113,113	2.93	30 (36%)
13	CLA	aB	811	2	69,73,73	1.99	18 (26%)	83,113,113	2.76	33 (39%)
16	LHG	dA	852	-	48,48,48	0.69	2 (4%)	51,54,54	1.27	6 (11%)
13	CLA	dB	823	2	69,73,73	1.97	18 (26%)	83,113,113	2.72	27 (32%)
13	CLA	dB	828	2	50,54,73	2.33	21 (42%)	60,90,113	3.32	30 (50%)
15	BCR	bB	835	-	41,41,41	1.07	3 (7%)	56,56,56	1.35	7 (12%)
13	CLA	cB	808	2	69,73,73	2.00	21 (30%)	83,113,113	2.92	33 (39%)
13	CLA	aA	829	1	69,73,73	1.95	18 (26%)	83,113,113	2.93	31 (37%)
15	BCR	aF	203	-	41,41,41	1.03	2 (4%)	56,56,56	1.34	12 (21%)
15	BCR	cL	205	-	41,41,41	1.15	2 (4%)	56,56,56	1.36	9 (16%)
13	CLA	bJ	101	8	49,53,73	2.43	19 (38%)	59,89,113	3.35	28 (47%)
18	LMG	cB	839	-	55,55,55	0.75	1 (1%)	63,63,63	1.38	8 (12%)
17	SF4	aB	802	2,1	0,12,12	-	-	-	-	-
13	CLA	cB	813	2	49,53,73	2.47	21 (42%)	59,89,113	3.26	27 (45%)
13	CLA	aB	809	2	69,73,73	2.00	20 (28%)	83,113,113	2.79	29 (34%)
13	CLA	cB	812	2	69,73,73	2.00	19 (27%)	83,113,113	2.86	35 (42%)
13	CLA	dB	821	2	69,73,73	1.95	19 (27%)	83,113,113	2.98	31 (37%)
15	BCR	aK	205	-	41,41,41	1.10	2 (4%)	56,56,56	1.35	5 (8%)
13	CLA	bB	808	2	69,73,73	1.97	19 (27%)	83,113,113	2.76	31 (37%)
13	CLA	dB	813	2	69,73,73	2.00	20 (28%)	83,113,113	2.84	27 (32%)
13	CLA	bA	816	1	49,53,73	2.36	20 (40%)	59,89,113	3.30	27 (45%)
13	CLA	aA	812	1	69,73,73	2.02	21 (30%)	83,113,113	2.93	29 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	bB	812	2	49,53,73	2.45	21 (42%)	59,89,113	3.32	27 (45%)
15	BCR	cB	837	-	41,41,41	1.07	2 (4%)	56,56,56	1.37	8 (14%)
13	CLA	cA	834	1	69,73,73	1.98	19 (27%)	83,113,113	2.84	32 (38%)
13	CLA	dA	833	1	69,73,73	2.01	18 (26%)	83,113,113	2.87	29 (34%)
13	CLA	cB	833	-	69,73,73	2.02	20 (28%)	83,113,113	2.89	29 (34%)
13	CLA	aA	830	1	69,73,73	1.96	19 (27%)	83,113,113	2.73	32 (38%)
13	CLA	dB	812	2	49,53,73	2.44	21 (42%)	59,89,113	3.32	26 (44%)
13	CLA	cB	821	2	69,73,73	2.05	19 (27%)	83,113,113	2.94	30 (36%)
13	CLA	cF	201	-	55,59,73	2.32	21 (38%)	66,96,113	3.12	28 (42%)
13	CLA	cA	819	1	58,62,73	2.17	18 (31%)	69,99,113	3.04	31 (44%)
13	CLA	aA	839	1	60,64,73	2.10	18 (30%)	72,102,113	3.00	28 (38%)
13	CLA	bA	842	1	69,73,73	1.99	21 (30%)	83,113,113	2.88	30 (36%)
13	CLA	aA	806	1	69,73,73	1.95	19 (27%)	83,113,113	2.83	30 (36%)
13	CLA	aA	808	1	55,59,73	2.27	20 (36%)	66,96,113	3.26	30 (45%)
17	SF4	dB	801	2,1	0,12,12	-	-	-	-	-
13	CLA	bA	811	1	49,53,73	2.35	18 (36%)	59,89,113	3.40	29 (49%)
13	CLA	dB	807	2	69,73,73	2.01	22 (31%)	83,113,113	2.93	34 (40%)
15	BCR	bA	851	-	41,41,41	1.11	3 (7%)	56,56,56	1.30	7 (12%)
13	CLA	bA	802	-	69,73,73	1.95	18 (26%)	83,113,113	2.96	33 (39%)
13	CLA	cA	833	1	69,73,73	2.03	18 (26%)	83,113,113	2.82	30 (36%)
13	CLA	aK	201	9	46,49,73	2.31	19 (41%)	55,83,113	3.42	26 (47%)
13	CLA	bB	815	2	49,53,73	2.38	21 (42%)	59,89,113	3.31	28 (47%)
13	CLA	cB	819	2	64,68,73	2.13	20 (31%)	77,107,113	2.91	34 (44%)
13	CLA	bF	204	6	49,53,73	2.42	20 (40%)	59,89,113	3.34	27 (45%)
18	LMG	dB	837	-	55,55,55	0.84	3 (5%)	63,63,63	1.46	7 (11%)
18	LMG	aB	839	-	55,55,55	0.75	1 (1%)	63,63,63	1.38	8 (12%)
13	CLA	aA	822	-	69,73,73	1.99	19 (27%)	83,113,113	2.72	26 (31%)
16	LHG	cA	850	-	48,48,48	0.63	0	51,54,54	1.29	6 (11%)
15	BCR	aB	836	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	bA	824	1	55,59,73	2.16	19 (34%)	66,96,113	3.17	29 (43%)
13	CLA	aA	820	1	69,73,73	2.04	18 (26%)	83,113,113	2.75	32 (38%)
13	CLA	cB	801	-	69,73,73	1.96	18 (26%)	83,113,113	2.73	32 (38%)
13	CLA	dA	809	1	69,73,73	1.95	21 (30%)	83,113,113	2.83	31 (37%)
13	CLA	bA	810	1	49,53,73	2.38	21 (42%)	59,89,113	3.19	30 (50%)
13	CLA	aB	831	2	69,73,73	2.03	19 (27%)	83,113,113	2.77	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	dA	804	1	49,53,73	2.38	19 (38%)	59,89,113	3.39	29 (49%)
13	CLA	cA	803	-	49,53,73	2.38	18 (36%)	59,89,113	3.16	28 (47%)
13	CLA	dB	811	2	69,73,73	1.98	20 (28%)	83,113,113	2.80	38 (45%)
14	PQN	aA	844	-	34,34,34	1.51	2 (5%)	42,45,45	1.12	4 (9%)
13	CLA	bB	805	2	58,62,73	2.15	19 (32%)	69,99,113	3.07	31 (44%)
15	BCR	cI	101	-	41,41,41	1.07	3 (7%)	56,56,56	1.35	9 (16%)
16	LHG	bA	853	13	26,26,48	0.90	1 (3%)	29,32,54	1.37	4 (13%)
13	CLA	aB	807	2	69,73,73	2.05	20 (28%)	83,113,113	2.84	32 (38%)
13	CLA	cA	836	1	58,62,73	2.15	19 (32%)	69,99,113	3.01	29 (42%)
13	CLA	bA	821	1	65,69,73	2.04	19 (29%)	78,108,113	2.94	31 (39%)
13	CLA	dB	809	2	69,73,73	1.99	20 (28%)	83,113,113	2.90	32 (38%)
13	CLA	cB	829	-	49,53,73	2.48	20 (40%)	59,89,113	3.22	28 (47%)
13	CLA	aK	204	10	50,54,73	2.36	21 (42%)	60,90,113	3.32	28 (46%)
13	CLA	bB	814	2	60,64,73	2.17	20 (33%)	72,102,113	3.01	28 (38%)
13	CLA	dA	825	1	51,55,73	2.24	18 (35%)	61,91,113	3.36	31 (50%)
13	CLA	bB	824	2	53,57,73	2.34	19 (35%)	62,93,113	3.32	29 (46%)
15	BCR	aJ	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	9 (16%)
13	CLA	dJ	101	8	49,53,73	2.43	19 (38%)	59,89,113	3.35	28 (47%)
13	CLA	aA	804	1	49,53,73	2.43	19 (38%)	59,89,113	3.28	29 (49%)
13	CLA	bB	804	-	69,73,73	1.90	18 (26%)	83,113,113	2.65	27 (32%)
13	CLA	bB	810	2	69,73,73	1.96	18 (26%)	83,113,113	2.80	32 (38%)
13	CLA	bA	839	1	60,64,73	2.11	18 (30%)	72,102,113	2.92	28 (38%)
13	CLA	aA	843	16	56,60,73	2.23	18 (32%)	67,97,113	3.15	32 (47%)
13	CLA	aB	822	2	69,73,73	2.04	21 (30%)	83,113,113	2.81	30 (36%)
13	CLA	dA	832	1	54,58,73	2.22	18 (33%)	65,95,113	3.12	33 (50%)
13	CLA	cK	204	10	50,54,73	2.36	21 (42%)	60,90,113	3.33	28 (46%)
13	CLA	dB	803	-	69,73,73	1.92	19 (27%)	83,113,113	2.92	35 (42%)
13	CLA	cJ	101	8	49,53,73	2.45	20 (40%)	59,89,113	3.25	27 (45%)
13	CLA	cA	838	1	55,59,73	2.22	20 (36%)	66,96,113	3.14	30 (45%)
13	CLA	dA	836	1	58,62,73	2.17	18 (31%)	69,99,113	3.06	32 (46%)
13	CLA	cA	807	1	69,73,73	1.96	19 (27%)	83,113,113	2.89	31 (37%)
13	CLA	cA	816	1	49,53,73	2.40	19 (38%)	59,89,113	3.27	26 (44%)
17	SF4	bB	801	2,1	0,12,12	-	-	-	-	-
13	CLA	dA	806	1	69,73,73	1.95	18 (26%)	83,113,113	2.85	30 (36%)
15	BCR	cA	846	-	41,41,41	1.11	2 (4%)	56,56,56	1.49	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	cB	805	-	69,73,73	1.92	21 (30%)	83,113,113	2.75	29 (34%)
15	BCR	aL	205	-	41,41,41	1.15	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	aL	204	-	45,49,73	2.42	18 (40%)	54,84,113	3.47	27 (50%)
15	BCR	bA	847	-	41,41,41	1.15	3 (7%)	56,56,56	1.24	7 (12%)
18	LMG	bB	837	-	55,55,55	0.84	3 (5%)	63,63,63	1.47	7 (11%)
13	CLA	aA	814	1	49,53,73	2.33	19 (38%)	59,89,113	3.36	27 (45%)
13	CLA	dB	832	2	69,73,73	2.00	20 (28%)	83,113,113	2.83	31 (37%)
15	BCR	aL	201	-	41,41,41	1.21	2 (4%)	56,56,56	1.26	4 (7%)
13	CLA	cA	811	1	49,53,73	2.34	19 (38%)	59,89,113	3.37	29 (49%)
13	CLA	bA	830	1	69,73,73	1.99	19 (27%)	83,113,113	2.76	30 (36%)
13	CLA	dA	822	-	69,73,73	1.92	18 (26%)	83,113,113	2.70	28 (33%)
15	BCR	bF	203	-	41,41,41	1.08	2 (4%)	56,56,56	1.36	8 (14%)
13	CLA	cA	823	1	69,73,73	1.98	20 (28%)	83,113,113	2.74	28 (33%)
13	CLA	cA	818	1	69,73,73	1.92	18 (26%)	83,113,113	2.93	30 (36%)
13	CLA	aF	204	6	49,53,73	2.46	21 (42%)	59,89,113	3.33	30 (50%)
13	CLA	bB	829	2	69,73,73	2.01	20 (28%)	83,113,113	2.86	34 (40%)
13	CLA	dA	812	1	69,73,73	2.01	21 (30%)	83,113,113	2.87	32 (38%)
13	CLA	bA	806	1	69,73,73	1.95	18 (26%)	83,113,113	2.85	30 (36%)
14	PQN	dB	833	-	34,34,34	1.56	2 (5%)	42,45,45	1.25	4 (9%)
13	CLA	aA	805	1	49,53,73	2.39	18 (36%)	59,89,113	3.35	26 (44%)
13	CLA	cL	203	10	69,73,73	1.97	19 (27%)	83,113,113	2.85	30 (36%)
15	BCR	aA	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.46	11 (19%)
13	CLA	aB	823	2	69,73,73	2.02	19 (27%)	83,113,113	2.81	27 (32%)
13	CLA	aB	825	2	53,57,73	2.31	19 (35%)	62,93,113	3.30	27 (43%)
13	CLA	bF	201	-	55,59,73	2.25	21 (38%)	66,96,113	3.26	32 (48%)
17	SF4	cC	101	3	0,12,12	-	-	-	-	-
13	CLA	dL	202	10	69,73,73	1.90	19 (27%)	83,113,113	2.89	29 (34%)
15	BCR	dL	204	-	41,41,41	1.10	3 (7%)	56,56,56	1.35	6 (10%)
13	CLA	bA	828	1	69,73,73	1.92	19 (27%)	83,113,113	2.90	31 (37%)
13	CLA	cA	808	1	55,59,73	2.27	20 (36%)	66,96,113	3.26	31 (46%)
13	CLA	cB	811	2	69,73,73	1.99	18 (26%)	83,113,113	2.76	33 (39%)
13	CLA	bB	830	2	51,55,73	2.31	22 (43%)	61,91,113	3.20	27 (44%)
13	CLA	aA	833	1	69,73,73	2.03	18 (26%)	83,113,113	2.82	30 (36%)
15	BCR	dA	846	-	41,41,41	1.19	3 (7%)	56,56,56	1.41	13 (23%)
13	CLA	aB	814	2	69,73,73	2.02	20 (28%)	83,113,113	2.93	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	bA	836	1	58,62,73	2.17	18 (31%)	69,99,113	3.06	32 (46%)
15	BCR	bJ	102	-	41,41,41	1.04	2 (4%)	56,56,56	1.30	8 (14%)
17	SF4	cB	802	2,1	0,12,12	-	-	-	-	-
13	CLA	dA	838	1	55,59,73	2.23	18 (32%)	66,96,113	3.17	30 (45%)
15	BCR	bJ	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.42	9 (16%)
13	CLA	aA	815	1	49,53,73	2.43	18 (36%)	59,89,113	3.34	29 (49%)
13	CLA	bB	822	2	69,73,73	2.01	19 (27%)	83,113,113	2.77	31 (37%)
13	CLA	bL	202	10	69,73,73	1.90	19 (27%)	83,113,113	2.89	29 (34%)

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
13	CLA	cA	805	1	-	2/15/91/115	-
13	CLA	aA	819	1	-	12/26/102/115	-
13	CLA	aA	818	1	-	12/39/115/115	-
13	CLA	cB	823	2	-	15/39/115/115	-
13	CLA	cB	828	2	-	3/15/91/115	-
13	CLA	cB	817	2	-	14/27/103/115	-
13	CLA	aA	816	1	-	8/15/91/115	-
13	CLA	bB	818	2	-	9/33/109/115	-
13	CLA	cA	839	1	-	9/29/105/115	-
16	LHG	aA	851	13	-	8/31/31/53	-
13	CLA	bB	832	2	-	18/39/115/115	-
13	CLA	bA	833	1	-	14/39/115/115	-
13	CLA	aA	838	1	-	11/23/99/115	-
15	BCR	aM	101	-	-	19/29/63/63	0/2/2/2
13	CLA	dB	817	2	-	15/32/108/115	-
13	CLA	dA	835	1	-	17/39/115/115	-
13	CLA	bA	803	-	-	8/15/91/115	-
13	CLA	dA	821	1	-	11/35/111/115	-
15	BCR	dI	102	-	-	16/29/63/63	0/2/2/2
13	CLA	bA	832	1	-	4/21/97/115	-
13	CLA	aA	841	1	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	aB	815	2	-	9/29/105/115	-
13	CLA	aA	802	-	-	9/39/115/115	-
13	CLA	aL	202	10	-	6/17/93/115	-
13	CLA	dA	813	1	-	11/26/102/115	-
14	PQN	cA	844	-	-	6/23/43/43	0/2/2/2
15	BCR	cM	101	-	-	19/29/63/63	0/2/2/2
13	CLA	cA	812	1	-	12/39/115/115	-
13	CLA	aB	804	-	-	8/39/115/115	-
13	CLA	aA	824	1	-	9/23/99/115	-
13	CLA	bA	841	1	-	19/39/115/115	-
13	CLA	dF	204	6	-	4/15/91/115	-
15	BCR	aK	202	-	-	13/29/63/63	0/2/2/2
13	CLA	dA	830	1	-	14/39/115/115	-
13	CLA	dB	802	2	-	16/39/115/115	-
13	CLA	dB	829	2	-	18/39/115/115	-
15	BCR	aB	838	-	-	15/29/63/63	0/2/2/2
13	CLA	cA	825	1	-	8/18/94/115	-
13	CLA	bB	820	2	-	12/39/115/115	-
13	CLA	aA	811	1	-	5/15/91/115	-
13	CLA	aA	813	1	-	11/26/102/115	-
13	CLA	bB	811	2	-	11/39/115/115	-
13	CLA	dA	837	1	-	8/15/91/115	-
17	SF4	dC	102	3	-	-	0/6/5/5
13	CLA	bA	838	1	-	13/23/99/115	-
13	CLA	dA	807	1	-	18/39/115/115	-
15	BCR	dF	202	-	-	20/29/63/63	0/2/2/2
13	CLA	cA	804	1	-	7/15/91/115	-
13	CLA	dB	831	-	-	11/39/115/115	-
13	CLA	dB	824	2	-	12/20/96/115	-
13	CLA	dB	810	2	-	10/39/115/115	-
14	PQN	bA	845	-	-	10/23/43/43	0/2/2/2
13	CLA	dA	823	1	-	9/17/93/115	-
13	CLA	cB	820	-	-	8/17/93/115	-
13	CLA	dB	820	2	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	aA	807	1	-	18/39/115/115	-
14	PQN	aB	835	-	-	8/23/43/43	0/2/2/2
15	BCR	aA	846	-	-	20/29/63/63	0/2/2/2
13	CLA	aB	826	2	-	10/39/115/115	-
13	CLA	aB	829	-	-	5/15/91/115	-
13	CLA	bB	807	2	-	17/39/115/115	-
13	CLA	bA	818	1	-	15/39/115/115	-
13	CLA	cB	827	2	-	13/31/107/115	-
13	CLA	dA	834	1	-	16/39/115/115	-
13	CLA	cA	829	1	-	18/39/115/115	-
13	CLA	aA	825	1	-	8/18/94/115	-
15	BCR	bF	202	-	-	20/29/63/63	0/2/2/2
13	CLA	cA	821	1	-	13/35/111/115	-
13	CLA	dB	827	2	-	9/15/91/115	-
13	CLA	cB	809	2	-	5/39/115/115	-
13	CLA	aB	833	-	-	15/39/115/115	-
17	SF4	dC	101	3	-	-	0/6/5/5
13	CLA	bB	802	2	-	16/39/115/115	-
13	CLA	bB	823	2	-	20/39/115/115	-
13	CLA	aB	805	-	-	7/39/115/115	-
13	CLA	cA	832	1	-	7/21/97/115	-
15	BCR	aA	845	-	-	18/29/63/63	0/2/2/2
13	CLA	cA	841	1	-	12/39/115/115	-
13	CLA	bA	812	1	-	16/39/115/115	-
13	CLA	aA	810	1	-	7/15/91/115	-
13	CLA	bB	813	2	-	16/39/115/115	-
13	CLA	bB	831	-	-	11/39/115/115	-
13	CLA	aA	840	1	-	16/39/115/115	-
13	CLA	aB	801	-	-	13/39/115/115	-
13	CLA	cB	832	2	-	5/18/94/115	-
13	CLA	aA	823	1	-	17/39/115/115	-
13	CLA	aA	828	1	-	15/39/115/115	-
13	CLA	aB	834	2	-	24/39/115/115	-
13	CLA	dA	814	1	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	bB	828	2	-	6/17/93/115	-
13	CLA	dA	841	1	-	19/39/115/115	-
13	CLA	bA	808	1	-	6/23/99/115	-
13	CLA	aA	836	1	-	13/26/102/115	-
15	BCR	dA	850	-	-	18/29/63/63	0/2/2/2
13	CLA	cB	803	2	-	18/39/115/115	-
15	BCR	aB	837	-	-	18/29/63/63	0/2/2/2
15	BCR	bA	850	-	-	18/29/63/63	0/2/2/2
13	CLA	aA	821	1	-	13/35/111/115	-
13	CLA	dA	805	1	-	8/15/91/115	-
13	CLA	bB	821	2	-	18/39/115/115	-
13	CLA	bA	827	-	-	10/27/103/115	-
13	CLA	aB	816	2	-	7/15/91/115	-
13	CLA	bA	837	1	-	8/15/91/115	-
13	CLA	cA	827	-	-	9/27/103/115	-
15	BCR	dA	849	-	-	13/29/63/63	0/2/2/2
13	CLA	bA	820	1	-	14/39/115/115	-
13	CLA	bB	803	-	-	8/39/115/115	-
13	CLA	aB	824	2	-	13/39/115/115	-
16	LHG	dA	853	13	-	11/31/31/53	-
13	CLA	aF	201	-	-	9/23/99/115	-
13	CLA	aA	803	-	-	5/15/91/115	-
15	BCR	bL	201	-	-	14/29/63/63	0/2/2/2
13	CLA	cA	840	1	-	16/39/115/115	-
13	CLA	cA	802	-	-	9/39/115/115	-
13	CLA	bA	825	1	-	6/18/94/115	-
13	CLA	aB	827	2	-	13/31/107/115	-
13	CLA	cA	815	1	-	7/15/91/115	-
12	CL0	bA	801	1	-	7/39/115/115	-
13	CLA	dB	822	2	-	13/39/115/115	-
13	CLA	bA	834	1	-	16/39/115/115	-
13	CLA	cA	810	1	-	7/15/91/115	-
15	BCR	bI	101	-	-	20/29/63/63	0/2/2/2
15	BCR	cA	848	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	bB	816	2	-	10/27/103/115	-
13	CLA	dA	819	1	-	14/26/102/115	-
13	CLA	bB	825	2	-	14/39/115/115	-
15	BCR	cJ	104	-	-	15/29/63/63	0/2/2/2
13	CLA	dA	816	1	-	7/15/91/115	-
15	BCR	aF	202	-	-	18/29/63/63	0/2/2/2
15	BCR	dB	835	-	-	16/29/63/63	0/2/2/2
13	CLA	dA	828	1	-	16/39/115/115	-
13	CLA	dA	817	-	-	7/20/96/115	-
13	CLA	cA	826	-	-	19/39/115/115	-
13	CLA	aA	842	1	-	15/39/115/115	-
13	CLA	dA	818	1	-	15/39/115/115	-
13	CLA	aK	203	-	-	7/15/91/115	-
13	CLA	dA	820	1	-	14/39/115/115	-
13	CLA	dA	844	16	-	15/24/100/115	-
15	BCR	cJ	103	-	-	14/29/63/63	0/2/2/2
13	CLA	dB	815	2	-	7/15/91/115	-
17	SF4	bC	101	3	-	-	0/6/5/5
15	BCR	cF	202	-	-	18/29/63/63	0/2/2/2
15	BCR	dI	101	-	-	20/29/63/63	0/2/2/2
13	CLA	cB	807	2	-	23/39/115/115	-
13	CLA	bB	819	-	-	6/17/93/115	-
15	BCR	bB	836	-	-	15/29/63/63	0/2/2/2
13	CLA	dA	839	1	-	10/29/105/115	-
13	CLA	bA	815	1	-	6/15/91/115	-
13	CLA	cA	824	1	-	9/23/99/115	-
13	CLA	bA	822	-	-	11/39/115/115	-
13	CLA	cA	837	1	-	11/15/91/115	-
13	CLA	dA	829	1	-	18/39/115/115	-
15	BCR	bA	849	-	-	13/29/63/63	0/2/2/2
13	CLA	cA	820	1	-	16/39/115/115	-
13	CLA	dA	831	1	-	13/39/115/115	-
13	CLA	bB	806	2	-	19/39/115/115	-
16	LHG	cA	851	13	-	8/31/31/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	cA	813	1	-	11/26/102/115	-
14	PQN	bB	833	-	-	7/23/43/43	0/2/2/2
15	BCR	cL	201	-	-	9/29/63/63	0/2/2/2
15	BCR	dJ	103	-	-	17/29/63/63	0/2/2/2
13	CLA	cB	831	2	-	7/39/115/115	-
13	CLA	dA	843	-	-	19/39/115/115	-
13	CLA	bL	203	-	-	11/24/100/115	-
13	CLA	bA	807	1	-	18/39/115/115	-
13	CLA	dA	824	1	-	9/23/99/115	-
13	CLA	dB	814	2	-	12/29/105/115	-
13	CLA	aB	828	2	-	3/15/91/115	-
13	CLA	aB	817	2	-	14/27/103/115	-
13	CLA	cB	830	2	-	9/17/93/115	-
13	CLA	dA	810	1	-	8/15/91/115	-
13	CLA	aB	808	2	-	16/39/115/115	-
13	CLA	dB	808	2	-	3/39/115/115	-
13	CLA	dA	826	-	-	14/39/115/115	-
13	CLA	aA	831	1	-	16/39/115/115	-
13	CLA	dB	830	2	-	5/18/94/115	-
13	CLA	cF	204	6	-	4/15/91/115	-
15	BCR	aL	206	-	-	18/29/63/63	0/2/2/2
15	BCR	cA	845	-	-	18/29/63/63	0/2/2/2
15	BCR	cF	203	-	-	12/29/63/63	0/2/2/2
13	CLA	bA	844	16	-	15/24/100/115	-
13	CLA	cB	826	2	-	10/39/115/115	-
13	CLA	bA	823	1	-	9/17/93/115	-
13	CLA	aL	203	10	-	15/39/115/115	-
12	CL0	cA	801	1	-	4/39/115/115	-
13	CLA	cA	828	1	-	15/39/115/115	-
14	PQN	cB	835	-	-	8/23/43/43	0/2/2/2
13	CLA	dA	827	-	-	10/27/103/115	-
13	CLA	bB	826	2	-	18/31/107/115	-
15	BCR	dA	847	-	-	14/29/63/63	0/2/2/2
15	BCR	dJ	102	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	bM	101	-	-	16/29/63/63	0/2/2/2
15	BCR	dJ	104	-	-	14/29/63/63	0/2/2/2
13	CLA	cB	834	2	-	24/39/115/115	-
13	CLA	dA	811	1	-	6/15/91/115	-
15	BCR	cB	836	-	-	16/29/63/63	0/2/2/2
13	CLA	bA	804	1	-	8/15/91/115	-
15	BCR	cJ	102	-	-	20/29/63/63	0/2/2/2
13	CLA	aB	832	2	-	5/18/94/115	-
17	SF4	cC	102	3	-	-	0/6/5/5
15	BCR	dA	851	-	-	20/29/63/63	0/2/2/2
13	CLA	aA	827	-	-	9/27/103/115	-
13	CLA	bA	843	-	-	19/39/115/115	-
13	CLA	aB	810	2	-	9/39/115/115	-
13	CLA	aA	837	1	-	11/15/91/115	-
15	BCR	bA	846	-	-	14/29/63/63	0/2/2/2
13	CLA	dB	819	-	-	6/17/93/115	-
13	CLA	aB	806	2	-	7/26/102/115	-
13	CLA	aA	835	1	-	14/39/115/115	-
13	CLA	bA	817	-	-	7/20/96/115	-
15	BCR	dB	834	-	-	15/29/63/63	0/2/2/2
13	CLA	aA	826	-	-	19/39/115/115	-
15	BCR	dL	201	-	-	14/29/63/63	0/2/2/2
13	CLA	bA	840	1	-	5/21/97/115	-
16	LHG	aA	850	-	-	28/53/53/53	-
13	CLA	aA	809	1	-	19/39/115/115	-
13	CLA	aB	821	2	-	6/39/115/115	-
13	CLA	cA	822	-	-	9/39/115/115	-
13	CLA	dA	840	1	-	5/21/97/115	-
15	BCR	bA	848	-	-	9/29/63/63	0/2/2/2
12	CL0	dA	801	1	-	7/39/115/115	-
13	CLA	bA	813	1	-	11/26/102/115	-
13	CLA	bA	835	1	-	17/39/115/115	-
13	CLA	dB	804	-	-	7/39/115/115	-
15	BCR	dB	836	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	bA	814	1	-	9/15/91/115	-
13	CLA	aB	803	2	-	18/39/115/115	-
13	CLA	aA	817	-	-	4/20/96/115	-
15	BCR	aA	849	-	-	25/29/63/63	0/2/2/2
14	PQN	dA	845	-	-	10/23/43/43	0/2/2/2
13	CLA	bB	817	2	-	15/32/108/115	-
15	BCR	cK	202	-	-	13/29/63/63	0/2/2/2
13	CLA	cA	806	1	-	18/39/115/115	-
13	CLA	cB	825	2	-	13/20/96/115	-
13	CLA	aA	834	1	-	12/39/115/115	-
13	CLA	bA	805	1	-	8/15/91/115	-
15	BCR	aA	848	-	-	10/29/63/63	0/2/2/2
13	CLA	bA	826	-	-	14/39/115/115	-
13	CLA	dB	825	2	-	14/39/115/115	-
13	CLA	aA	832	1	-	7/21/97/115	-
13	CLA	dA	803	-	-	8/15/91/115	-
15	BCR	aJ	104	-	-	15/29/63/63	0/2/2/2
13	CLA	cB	806	2	-	7/26/102/115	-
15	BCR	cB	838	-	-	15/29/63/63	0/2/2/2
15	BCR	cA	849	-	-	25/29/63/63	0/2/2/2
13	CLA	dB	806	2	-	19/39/115/115	-
13	CLA	dB	805	2	-	6/26/102/115	-
17	SF4	aC	102	3	-	-	0/6/5/5
13	CLA	aB	819	2	-	10/33/109/115	-
13	CLA	cB	822	2	-	14/39/115/115	-
13	CLA	dB	826	2	-	18/31/107/115	-
13	CLA	bB	827	2	-	9/15/91/115	-
15	BCR	bB	834	-	-	15/29/63/63	0/2/2/2
12	CL0	aA	801	1	-	4/39/115/115	-
13	CLA	aJ	101	8	-	6/15/91/115	-
13	CLA	bA	819	1	-	14/26/102/115	-
13	CLA	bA	809	1	-	16/39/115/115	-
13	CLA	cA	843	16	-	12/24/100/115	-
13	CLA	dA	802	-	-	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	aB	818	2	-	15/32/108/115	-
13	CLA	dB	818	2	-	9/33/109/115	-
13	CLA	bA	831	1	-	13/39/115/115	-
13	CLA	cA	842	1	-	15/39/115/115	-
13	CLA	cB	815	2	-	9/29/105/115	-
13	CLA	dA	815	1	-	6/15/91/115	-
13	CLA	dA	842	1	-	18/39/115/115	-
16	LHG	bA	852	-	-	30/53/53/53	-
13	CLA	cA	831	1	-	16/39/115/115	-
15	BCR	cL	206	-	-	18/29/63/63	0/2/2/2
13	CLA	cA	835	1	-	14/39/115/115	-
13	CLA	cB	804	-	-	8/39/115/115	-
13	CLA	bB	809	2	-	9/39/115/115	-
15	BCR	dA	848	-	-	9/29/63/63	0/2/2/2
13	CLA	cB	816	2	-	7/15/91/115	-
15	BCR	bI	102	-	-	16/29/63/63	0/2/2/2
15	BCR	aJ	103	-	-	14/29/63/63	0/2/2/2
13	CLA	cA	817	-	-	4/20/96/115	-
17	SF4	aC	101	3	-	-	0/6/5/5
13	CLA	cL	202	10	-	6/17/93/115	-
15	BCR	dF	203	-	-	15/29/63/63	0/2/2/2
13	CLA	cB	824	2	-	13/39/115/115	-
13	CLA	cA	814	1	-	7/15/91/115	-
13	CLA	cK	201	9	-	5/9/81/115	-
15	BCR	bJ	104	-	-	14/29/63/63	0/2/2/2
15	BCR	dM	101	-	-	16/29/63/63	0/2/2/2
13	CLA	cL	204	-	-	5/10/86/115	-
13	CLA	cB	818	2	-	15/32/108/115	-
13	CLA	dB	816	2	-	10/27/103/115	-
13	CLA	cB	810	2	-	9/39/115/115	-
13	CLA	aB	830	2	-	9/17/93/115	-
13	CLA	dL	203	-	-	11/24/100/115	-
13	CLA	bA	829	1	-	18/39/115/115	-
13	CLA	cA	809	1	-	19/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	aB	813	2	-	3/15/91/115	-
13	CLA	dF	201	-	-	6/23/99/115	-
13	CLA	aB	812	2	-	4/39/115/115	-
15	BCR	aI	101	-	-	9/29/63/63	0/2/2/2
13	CLA	cA	830	1	-	15/39/115/115	-
13	CLA	dA	808	1	-	6/23/99/115	-
13	CLA	cK	203	-	-	7/15/91/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
15	BCR	cA	847	-	-	12/29/63/63	0/2/2/2
13	CLA	aB	820	-	-	8/17/93/115	-
13	CLA	cB	814	2	-	15/39/115/115	-
13	CLA	aB	811	2	-	11/39/115/115	-
16	LHG	dA	852	-	-	30/53/53/53	-
13	CLA	dB	823	2	-	20/39/115/115	-
13	CLA	dB	828	2	-	6/17/93/115	-
15	BCR	bB	835	-	-	16/29/63/63	0/2/2/2
13	CLA	cB	808	2	-	16/39/115/115	-
13	CLA	aA	829	1	-	18/39/115/115	-
15	BCR	aF	203	-	-	12/29/63/63	0/2/2/2
15	BCR	cL	205	-	-	16/29/63/63	0/2/2/2
13	CLA	bJ	101	8	-	8/15/91/115	-
18	LMG	cB	839	-	-	25/50/70/70	0/1/1/1
17	SF4	aB	802	2,1	-	-	0/6/5/5
13	CLA	cB	813	2	-	3/15/91/115	-
13	CLA	aB	809	2	-	5/39/115/115	-
13	CLA	cB	812	2	-	4/39/115/115	-
13	CLA	dB	821	2	-	18/39/115/115	-
15	BCR	aK	205	-	-	20/29/63/63	0/2/2/2
13	CLA	bB	808	2	-	3/39/115/115	-
13	CLA	dB	813	2	-	16/39/115/115	-
13	CLA	bA	816	1	-	7/15/91/115	-
13	CLA	aA	812	1	-	12/39/115/115	-
13	CLA	bB	812	2	-	3/15/91/115	-
15	BCR	cB	837	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	cA	834	1	-	12/39/115/115	-
13	CLA	dA	833	1	-	14/39/115/115	-
13	CLA	cB	833	-	-	15/39/115/115	-
13	CLA	aA	830	1	-	15/39/115/115	-
13	CLA	dB	812	2	-	3/15/91/115	-
13	CLA	cB	821	2	-	6/39/115/115	-
13	CLA	cF	201	-	-	9/23/99/115	-
13	CLA	cA	819	1	-	12/26/102/115	-
13	CLA	aA	839	1	-	9/29/105/115	-
13	CLA	bA	842	1	-	18/39/115/115	-
13	CLA	aA	806	1	-	18/39/115/115	-
13	CLA	aA	808	1	-	3/23/99/115	-
17	SF4	dB	801	2,1	-	-	0/6/5/5
13	CLA	bA	811	1	-	6/15/91/115	-
13	CLA	dB	807	2	-	17/39/115/115	-
15	BCR	bA	851	-	-	20/29/63/63	0/2/2/2
13	CLA	bA	802	-	-	10/39/115/115	-
13	CLA	cA	833	1	-	10/39/115/115	-
13	CLA	aK	201	9	-	5/9/81/115	-
13	CLA	bB	815	2	-	7/15/91/115	-
13	CLA	cB	819	2	-	10/33/109/115	-
13	CLA	bF	204	6	-	4/15/91/115	-
18	LMG	dB	837	-	-	25/50/70/70	0/1/1/1
18	LMG	aB	839	-	-	25/50/70/70	0/1/1/1
13	CLA	aA	822	-	-	9/39/115/115	-
16	LHG	cA	850	-	-	28/53/53/53	-
15	BCR	aB	836	-	-	16/29/63/63	0/2/2/2
13	CLA	bA	824	1	-	9/23/99/115	-
13	CLA	aA	820	1	-	16/39/115/115	-
13	CLA	cB	801	-	-	13/39/115/115	-
13	CLA	dA	809	1	-	16/39/115/115	-
13	CLA	bA	810	1	-	8/15/91/115	-
13	CLA	aB	831	2	-	7/39/115/115	-
13	CLA	dA	804	1	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	cA	803	-	-	5/15/91/115	-
13	CLA	dB	811	2	-	11/39/115/115	-
14	PQN	aA	844	-	-	6/23/43/43	0/2/2/2
13	CLA	bB	805	2	-	6/26/102/115	-
15	BCR	cI	101	-	-	9/29/63/63	0/2/2/2
16	LHG	bA	853	13	-	11/31/31/53	-
13	CLA	aB	807	2	-	23/39/115/115	-
13	CLA	cA	836	1	-	13/26/102/115	-
13	CLA	bA	821	1	-	11/35/111/115	-
13	CLA	dB	809	2	-	9/39/115/115	-
13	CLA	cB	829	-	-	5/15/91/115	-
13	CLA	aK	204	10	-	9/17/93/115	-
13	CLA	bB	814	2	-	12/29/105/115	-
13	CLA	dA	825	1	-	6/18/94/115	-
13	CLA	bB	824	2	-	12/20/96/115	-
15	BCR	aJ	102	-	-	20/29/63/63	0/2/2/2
13	CLA	dJ	101	8	-	8/15/91/115	-
13	CLA	aA	804	1	-	7/15/91/115	-
13	CLA	bB	804	-	-	7/39/115/115	-
13	CLA	bB	810	2	-	10/39/115/115	-
13	CLA	bA	839	1	-	10/29/105/115	-
13	CLA	aA	843	16	-	12/24/100/115	-
13	CLA	aB	822	2	-	15/39/115/115	-
13	CLA	dA	832	1	-	4/21/97/115	-
13	CLA	cK	204	10	-	9/17/93/115	-
13	CLA	dB	803	-	-	8/39/115/115	-
13	CLA	cJ	101	8	-	6/15/91/115	-
13	CLA	cA	838	1	-	11/23/99/115	-
13	CLA	dA	836	1	-	3/26/102/115	-
13	CLA	cA	807	1	-	18/39/115/115	-
13	CLA	cA	816	1	-	8/15/91/115	-
17	SF4	bB	801	2,1	-	-	0/6/5/5
13	CLA	dA	806	1	-	15/39/115/115	-
15	BCR	cA	846	-	-	20/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	cB	805	-	-	7/39/115/115	-
15	BCR	aL	205	-	-	16/29/63/63	0/2/2/2
13	CLA	aL	204	-	-	4/10/86/115	-
15	BCR	bA	847	-	-	14/29/63/63	0/2/2/2
18	LMG	bB	837	-	-	25/50/70/70	0/1/1/1
13	CLA	aA	814	1	-	7/15/91/115	-
13	CLA	dB	832	2	-	18/39/115/115	-
15	BCR	aL	201	-	-	9/29/63/63	0/2/2/2
13	CLA	cA	811	1	-	5/15/91/115	-
13	CLA	bA	830	1	-	14/39/115/115	-
13	CLA	dA	822	-	-	11/39/115/115	-
15	BCR	bF	203	-	-	15/29/63/63	0/2/2/2
13	CLA	cA	823	1	-	17/39/115/115	-
13	CLA	cA	818	1	-	12/39/115/115	-
13	CLA	aF	204	6	-	4/15/91/115	-
13	CLA	bB	829	2	-	18/39/115/115	-
13	CLA	dA	812	1	-	16/39/115/115	-
13	CLA	bA	806	1	-	15/39/115/115	-
14	PQN	dB	833	-	-	7/23/43/43	0/2/2/2
13	CLA	aA	805	1	-	2/15/91/115	-
13	CLA	cL	203	10	-	15/39/115/115	-
15	BCR	aA	847	-	-	12/29/63/63	0/2/2/2
13	CLA	aB	823	2	-	15/39/115/115	-
13	CLA	aB	825	2	-	12/20/96/115	-
13	CLA	bF	201	-	-	6/23/99/115	-
17	SF4	cC	101	3	-	-	0/6/5/5
13	CLA	dL	202	10	-	22/39/115/115	-
15	BCR	dL	204	-	-	20/29/63/63	0/2/2/2
13	CLA	bA	828	1	-	16/39/115/115	-
13	CLA	cA	808	1	-	3/23/99/115	-
13	CLA	cB	811	2	-	11/39/115/115	-
13	CLA	bB	830	2	-	5/18/94/115	-
13	CLA	aA	833	1	-	10/39/115/115	-
15	BCR	dA	846	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	aB	814	2	-	15/39/115/115	-
13	CLA	bA	836	1	-	3/26/102/115	-
15	BCR	bJ	102	-	-	14/29/63/63	0/2/2/2
17	SF4	cB	802	2,1	-	-	0/6/5/5
13	CLA	dA	838	1	-	13/23/99/115	-
15	BCR	bJ	103	-	-	17/29/63/63	0/2/2/2
13	CLA	aA	815	1	-	7/15/91/115	-
13	CLA	bB	822	2	-	13/39/115/115	-
13	CLA	bL	202	10	-	23/39/115/115	-

The worst 5 of 6573 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	bA	845	PQN	C3-C2	7.57	1.49	1.35
14	dA	845	PQN	C3-C2	7.55	1.49	1.35
14	bB	833	PQN	C3-C2	7.39	1.48	1.35
14	dB	833	PQN	C3-C2	7.37	1.48	1.35
14	aA	844	PQN	C3-C2	7.25	1.48	1.35

The worst 5 of 10620 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	aA	818	CLA	C1D-ND-C4D	-10.51	98.87	106.33
13	cA	818	CLA	C1D-ND-C4D	-10.47	98.90	106.33
13	dA	823	CLA	C1D-ND-C4D	-10.16	99.12	106.33
13	bA	823	CLA	C1D-ND-C4D	-10.16	99.12	106.33
13	aB	820	CLA	C1D-ND-C4D	-10.15	99.13	106.33

There are no chirality outliers.

5 of 5122 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	aA	802	CLA	CHA-CBD-CGD-O1D
13	aA	802	CLA	CHA-CBD-CGD-O2D
13	aA	805	CLA	C4B-C3B-CAB-CBB
13	aA	806	CLA	C1A-C2A-CAA-CBA
13	aA	806	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

375 monomers are involved in 960 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	aA	819	CLA	2	0
13	aA	818	CLA	2	0
13	cB	823	CLA	3	0
13	cB	817	CLA	1	0
13	bB	818	CLA	4	0
13	cA	839	CLA	2	0
13	bB	832	CLA	9	0
13	bA	833	CLA	3	0
15	aM	101	BCR	2	0
13	dB	817	CLA	2	0
13	dA	835	CLA	3	0
13	dA	821	CLA	2	0
15	dI	102	BCR	4	0
13	bA	832	CLA	2	0
13	aA	841	CLA	4	0
13	aB	815	CLA	2	0
13	aA	802	CLA	5	0
13	dA	813	CLA	1	0
14	cA	844	PQN	5	0
15	cM	101	BCR	3	0
13	cA	812	CLA	1	0
13	aB	804	CLA	4	0
13	bA	841	CLA	4	0
15	aK	202	BCR	3	0
13	dA	830	CLA	1	0
13	dB	802	CLA	5	0
13	dB	829	CLA	4	0
15	aB	838	BCR	4	0
13	bB	820	CLA	3	0
13	aA	813	CLA	1	0
13	bB	811	CLA	1	0
13	dA	837	CLA	5	0
13	dA	807	CLA	6	0
15	dF	202	BCR	6	0
13	cA	804	CLA	1	0
13	dB	831	CLA	2	0
13	dB	824	CLA	2	0
13	dB	810	CLA	4	0
14	bA	845	PQN	2	0
13	dA	823	CLA	1	0
13	cB	820	CLA	1	0
13	dB	820	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	aA	807	CLA	2	0
14	aB	835	PQN	9	0
15	aA	846	BCR	2	0
13	aB	826	CLA	6	0
13	bB	807	CLA	7	0
13	bA	818	CLA	2	0
13	cB	827	CLA	3	0
13	dA	834	CLA	5	0
13	cA	829	CLA	8	0
15	bF	202	BCR	5	0
13	cA	821	CLA	2	0
13	dB	827	CLA	4	0
13	cB	809	CLA	4	0
13	aB	833	CLA	10	0
13	bB	802	CLA	4	0
13	bB	823	CLA	4	0
13	aB	805	CLA	8	0
13	cA	832	CLA	1	0
15	aA	845	BCR	2	0
13	cA	841	CLA	4	0
13	bA	812	CLA	3	0
13	aA	810	CLA	1	0
13	bB	813	CLA	2	0
13	bB	831	CLA	3	0
13	aA	840	CLA	4	0
13	aB	801	CLA	6	0
13	cB	832	CLA	1	0
13	aA	823	CLA	2	0
13	aA	828	CLA	4	0
13	aB	834	CLA	10	0
13	dA	814	CLA	2	0
13	dA	841	CLA	4	0
13	bA	808	CLA	2	0
13	aA	836	CLA	5	0
15	dA	850	BCR	3	0
13	cB	803	CLA	4	0
15	aB	837	BCR	1	0
15	bA	850	BCR	3	0
13	aA	821	CLA	4	0
13	dA	805	CLA	1	0
13	bB	821	CLA	3	0
13	bA	827	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	bA	837	CLA	8	0
13	cA	827	CLA	5	0
15	dA	849	BCR	2	0
13	bA	820	CLA	2	0
13	bB	803	CLA	2	0
13	aB	824	CLA	6	0
13	aF	201	CLA	5	0
13	aA	803	CLA	3	0
15	bL	201	BCR	3	0
13	cA	840	CLA	4	0
13	cA	802	CLA	5	0
13	aB	827	CLA	3	0
13	cA	815	CLA	4	0
12	bA	801	CL0	2	0
13	dB	822	CLA	4	0
13	bA	834	CLA	5	0
13	cA	810	CLA	1	0
15	bI	101	BCR	1	0
15	cA	848	BCR	4	0
13	bB	816	CLA	1	0
13	dA	819	CLA	5	0
13	bB	825	CLA	5	0
15	cJ	104	BCR	4	0
13	dA	816	CLA	1	0
15	aF	202	BCR	8	0
15	dB	835	BCR	1	0
13	dA	828	CLA	4	0
13	cA	826	CLA	3	0
13	aA	842	CLA	5	0
13	dA	818	CLA	2	0
13	aK	203	CLA	1	0
13	dA	820	CLA	3	0
13	dA	844	CLA	2	0
15	cJ	103	BCR	2	0
13	dB	815	CLA	2	0
15	cF	202	BCR	8	0
15	dI	101	BCR	1	0
13	cB	807	CLA	5	0
13	bB	819	CLA	4	0
15	bB	836	BCR	4	0
13	bA	815	CLA	1	0
13	bA	822	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	cA	837	CLA	1	0
13	dA	829	CLA	7	0
15	bA	849	BCR	1	0
13	cA	820	CLA	6	0
13	dA	831	CLA	3	0
13	bB	806	CLA	1	0
14	bB	833	PQN	4	0
15	cL	201	BCR	3	0
15	dJ	103	BCR	5	0
13	cB	831	CLA	2	0
13	dA	843	CLA	6	0
13	bL	203	CLA	6	0
13	bA	807	CLA	5	0
13	dA	824	CLA	11	0
13	dA	810	CLA	1	0
13	aB	808	CLA	5	0
13	dB	808	CLA	6	0
13	dA	826	CLA	2	0
13	aA	831	CLA	1	0
13	cF	204	CLA	1	0
15	aL	206	BCR	5	0
15	cA	845	BCR	3	0
15	cF	203	BCR	3	0
13	bA	844	CLA	1	0
13	cB	826	CLA	5	0
13	bA	823	CLA	1	0
13	aL	203	CLA	6	0
12	cA	801	CL0	4	0
13	cA	828	CLA	4	0
14	cB	835	PQN	7	0
13	dA	827	CLA	1	0
13	bB	826	CLA	2	0
15	dA	847	BCR	5	0
15	dJ	102	BCR	3	0
15	bM	101	BCR	8	0
15	dJ	104	BCR	2	0
13	cB	834	CLA	11	0
13	dA	811	CLA	1	0
15	cB	836	BCR	3	0
13	bA	804	CLA	2	0
15	cJ	102	BCR	4	0
13	aB	832	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	cC	102	SF4	2	0
15	dA	851	BCR	3	0
13	aA	827	CLA	5	0
13	bA	843	CLA	7	0
13	aB	810	CLA	3	0
13	aA	837	CLA	2	0
15	bA	846	BCR	2	0
13	dB	819	CLA	4	0
13	aB	806	CLA	1	0
13	aA	835	CLA	4	0
15	dB	834	BCR	1	0
13	aA	826	CLA	4	0
15	dL	201	BCR	4	0
13	bA	840	CLA	1	0
16	aA	850	LHG	4	0
13	aA	809	CLA	4	0
13	cA	822	CLA	2	0
13	dA	840	CLA	1	0
15	bA	848	BCR	3	0
12	dA	801	CL0	2	0
13	bA	813	CLA	2	0
13	bA	835	CLA	3	0
13	dB	804	CLA	6	0
15	dB	836	BCR	4	0
13	bA	814	CLA	2	0
13	aB	803	CLA	5	0
15	aA	849	BCR	3	0
14	dA	845	PQN	2	0
13	bB	817	CLA	2	0
15	cK	202	BCR	1	0
13	cA	806	CLA	4	0
13	cB	825	CLA	3	0
13	aA	834	CLA	6	0
13	bA	805	CLA	1	0
15	aA	848	BCR	3	0
13	bA	826	CLA	1	0
13	dB	825	CLA	4	0
13	aA	832	CLA	1	0
15	aJ	104	BCR	5	0
13	cB	806	CLA	1	0
15	cB	838	BCR	4	0
15	cA	849	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	dB	806	CLA	1	0
13	dB	805	CLA	2	0
17	aC	102	SF4	2	0
13	cB	822	CLA	3	0
13	dB	826	CLA	2	0
13	bB	827	CLA	4	0
12	aA	801	CL0	4	0
13	aJ	101	CLA	2	0
13	bA	819	CLA	4	0
13	bA	809	CLA	5	0
13	cA	843	CLA	13	0
13	dA	802	CLA	5	0
13	dB	818	CLA	3	0
13	bA	831	CLA	2	0
13	cA	842	CLA	5	0
13	cB	815	CLA	2	0
13	dA	815	CLA	1	0
13	dA	842	CLA	3	0
16	bA	852	LHG	1	0
13	cA	831	CLA	1	0
15	cL	206	BCR	4	0
13	cA	835	CLA	5	0
13	cB	804	CLA	4	0
13	bB	809	CLA	5	0
15	dA	848	BCR	5	0
15	bI	102	BCR	4	0
13	cL	202	CLA	1	0
15	dF	203	BCR	2	0
13	cB	824	CLA	6	0
13	cA	814	CLA	1	0
13	cK	201	CLA	2	0
15	bJ	104	BCR	2	0
15	dM	101	BCR	8	0
13	dB	816	CLA	2	0
13	cB	810	CLA	3	0
13	dL	203	CLA	2	0
13	bA	829	CLA	7	0
13	cA	809	CLA	3	0
13	aB	813	CLA	2	0
13	dF	201	CLA	1	0
13	aB	812	CLA	3	0
15	aI	101	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	cA	830	CLA	7	0
13	dA	808	CLA	2	0
15	cA	847	BCR	2	0
13	aB	820	CLA	1	0
13	cB	814	CLA	2	0
13	aB	811	CLA	4	0
16	dA	852	LHG	1	0
13	dB	823	CLA	4	0
15	bB	835	BCR	1	0
13	cB	808	CLA	4	0
13	aA	829	CLA	8	0
15	aF	203	BCR	4	0
15	cL	205	BCR	5	0
13	bJ	101	CLA	2	0
18	cB	839	LMG	6	0
17	aB	802	SF4	2	0
13	cB	813	CLA	2	0
13	aB	809	CLA	5	0
13	cB	812	CLA	3	0
13	dB	821	CLA	3	0
15	aK	205	BCR	3	0
13	bB	808	CLA	6	0
13	dB	813	CLA	2	0
13	bA	816	CLA	1	0
13	aA	812	CLA	1	0
13	bB	812	CLA	1	0
15	cB	837	BCR	1	0
13	cA	834	CLA	5	0
13	dA	833	CLA	4	0
13	cB	833	CLA	10	0
13	aA	830	CLA	7	0
13	cF	201	CLA	5	0
13	cA	819	CLA	2	0
13	aA	839	CLA	1	0
13	bA	842	CLA	3	0
13	aA	806	CLA	4	0
13	aA	808	CLA	2	0
17	dB	801	SF4	1	0
13	bA	811	CLA	1	0
13	dB	807	CLA	7	0
15	bA	851	BCR	3	0
13	bA	802	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	cA	833	CLA	2	0
13	aK	201	CLA	2	0
13	bB	815	CLA	2	0
13	cB	819	CLA	1	0
18	dB	837	LMG	2	0
18	aB	839	LMG	6	0
13	aA	822	CLA	3	0
16	cA	850	LHG	5	0
15	aB	836	BCR	3	0
13	bA	824	CLA	19	0
13	aA	820	CLA	6	0
13	cB	801	CLA	7	0
13	dA	809	CLA	3	0
13	bA	810	CLA	2	0
13	aB	831	CLA	2	0
13	dA	804	CLA	2	0
13	cA	803	CLA	3	0
13	dB	811	CLA	5	0
14	aA	844	PQN	5	0
13	bB	805	CLA	2	0
15	cI	101	BCR	5	0
13	aB	807	CLA	6	0
13	cA	836	CLA	3	0
13	bA	821	CLA	1	0
13	dB	809	CLA	5	0
13	aK	204	CLA	15	0
13	bB	824	CLA	3	0
15	aJ	102	BCR	4	0
13	dJ	101	CLA	2	0
13	aA	804	CLA	1	0
13	bB	804	CLA	6	0
13	bB	810	CLA	4	0
13	bA	839	CLA	1	0
13	aA	843	CLA	20	0
13	aB	822	CLA	4	0
13	dA	832	CLA	2	0
13	cK	204	CLA	14	0
13	dB	803	CLA	1	0
13	cJ	101	CLA	2	0
13	dA	836	CLA	1	0
13	cA	807	CLA	2	0
17	bB	801	SF4	1	0

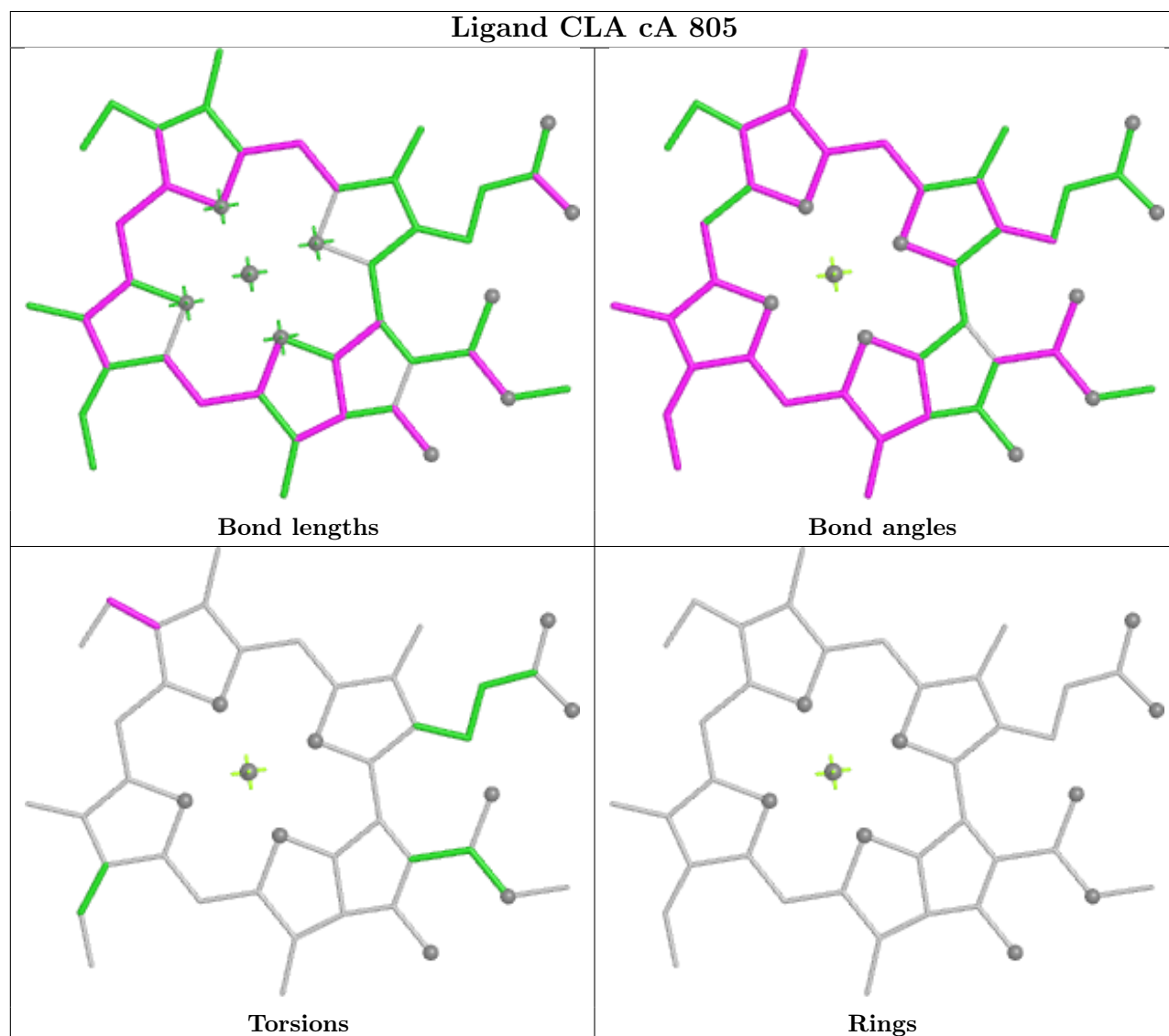
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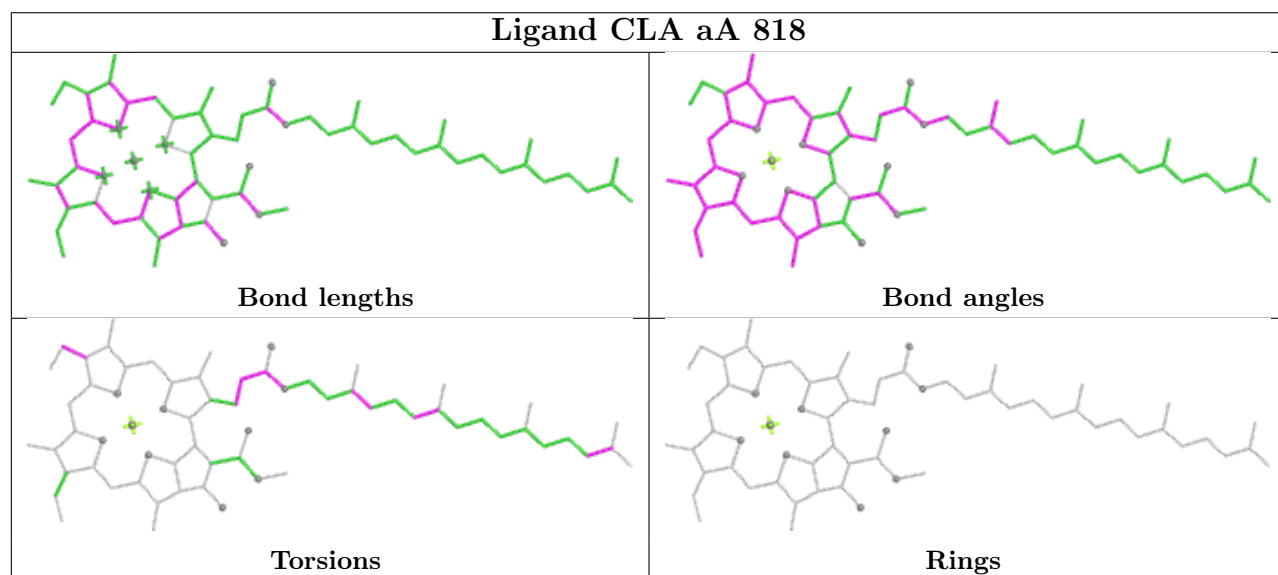
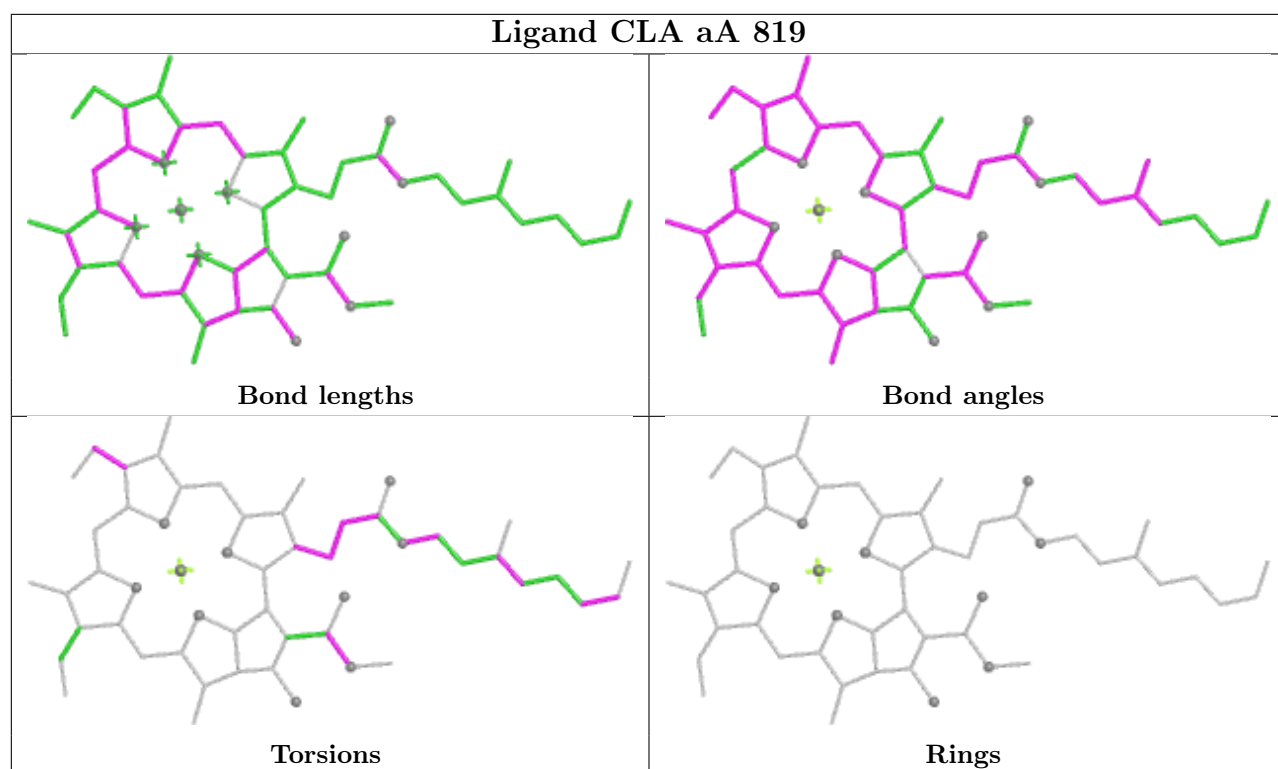
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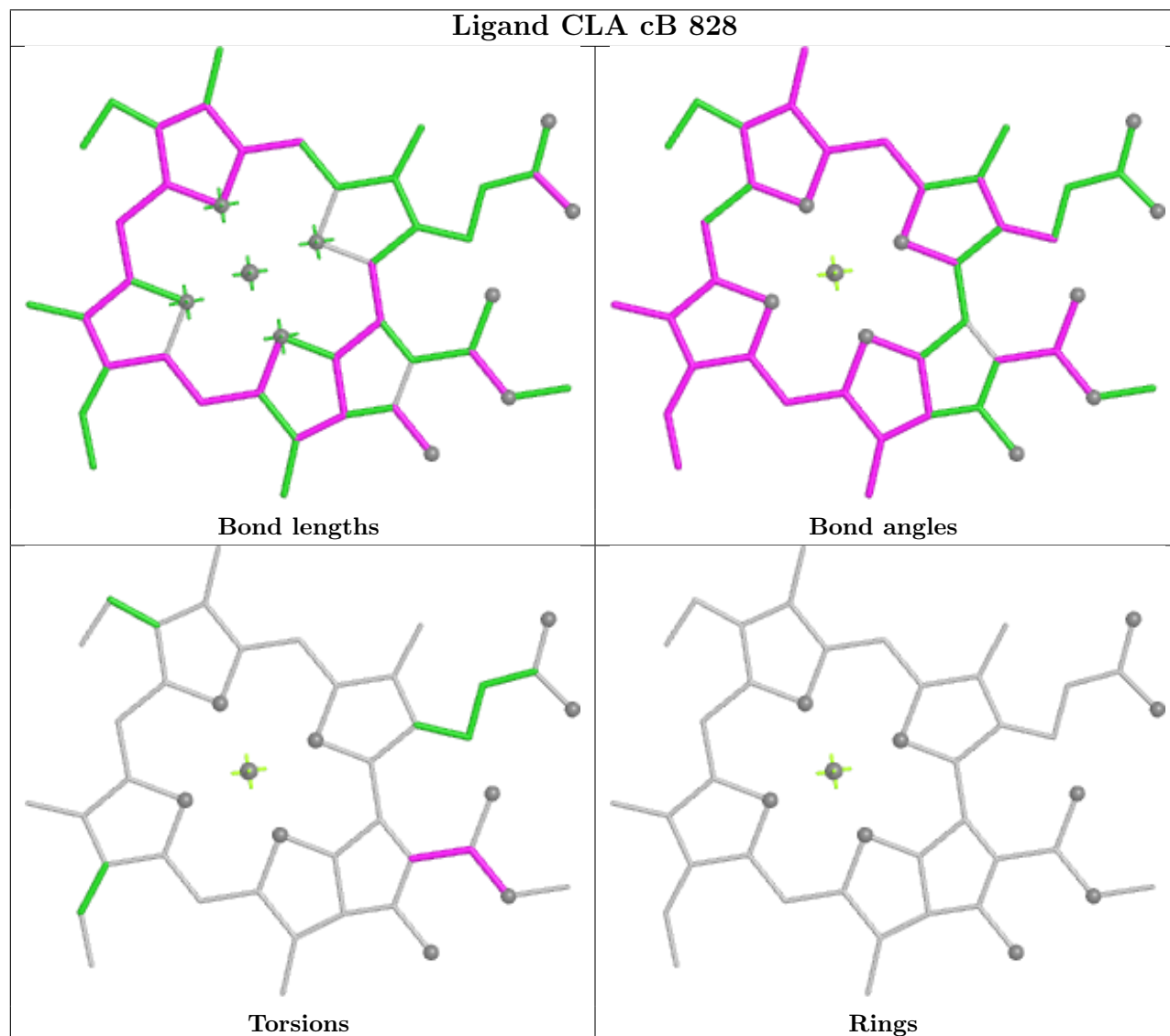
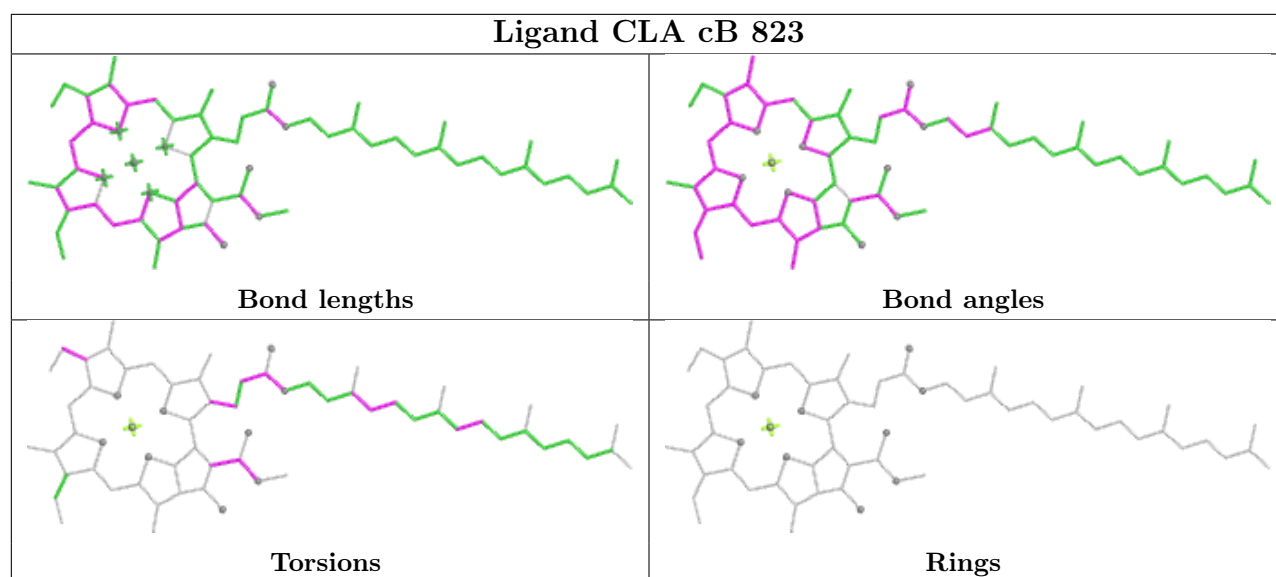
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	dA	806	CLA	6	0
15	cA	846	BCR	2	0
13	cB	805	CLA	10	0
15	aL	205	BCR	5	0
15	bA	847	BCR	3	0
18	bB	837	LMG	2	0
13	aA	814	CLA	1	0
13	dB	832	CLA	9	0
15	aL	201	BCR	4	0
13	bA	830	CLA	1	0
13	dA	822	CLA	6	0
15	bF	203	BCR	1	0
13	cA	823	CLA	1	0
13	cA	818	CLA	2	0
13	aF	204	CLA	1	0
13	bB	829	CLA	2	0
13	dA	812	CLA	2	0
13	bA	806	CLA	6	0
14	dB	833	PQN	4	0
13	cL	203	CLA	4	0
15	aA	847	BCR	1	0
13	aB	823	CLA	4	0
13	aB	825	CLA	3	0
13	bF	201	CLA	1	0
13	dL	202	CLA	7	0
15	dL	204	BCR	2	0
13	bA	828	CLA	4	0
13	cA	808	CLA	2	0
13	cB	811	CLA	5	0
13	aA	833	CLA	3	0
15	dA	846	BCR	2	0
13	aB	814	CLA	2	0
13	bA	836	CLA	1	0
15	bJ	102	BCR	4	0
17	cB	802	SF4	2	0
15	bJ	103	BCR	5	0
13	aA	815	CLA	1	0
13	bB	822	CLA	6	0
13	bL	202	CLA	8	0

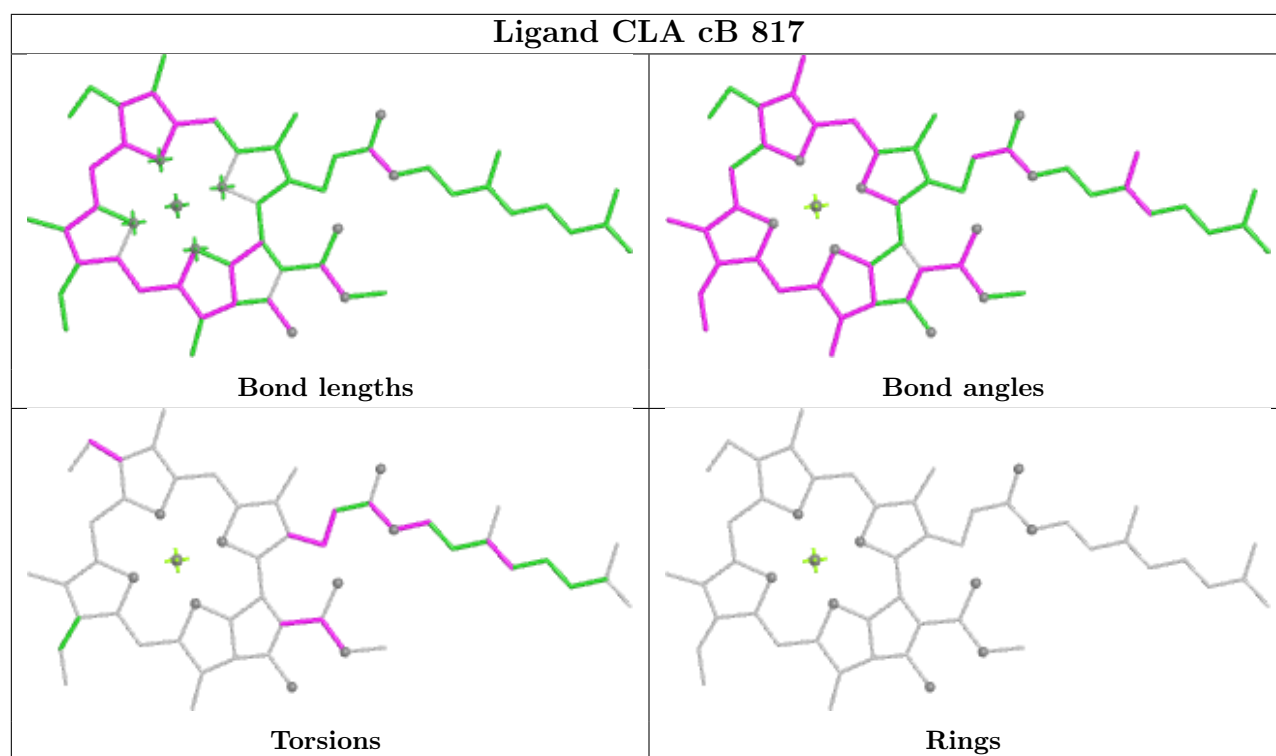
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.

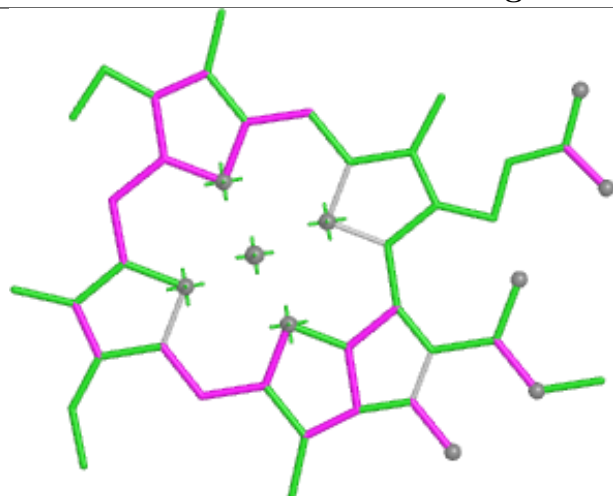




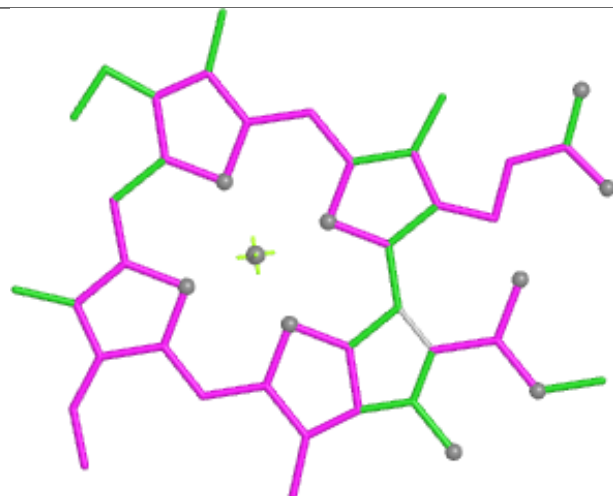




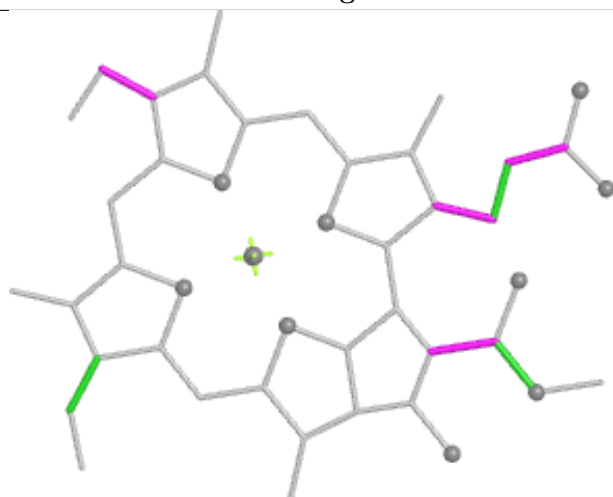
Ligand CLA aA 816



Bond lengths



Bond angles

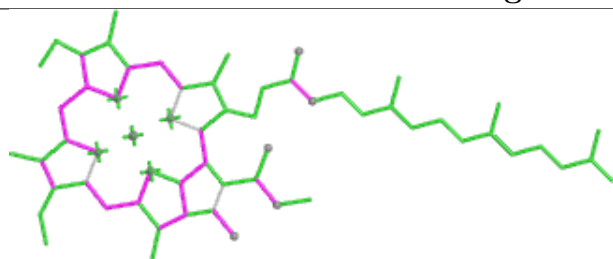


Torsions

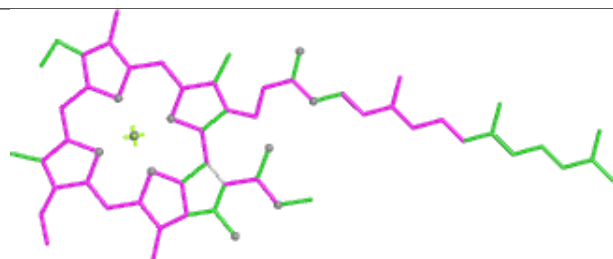


Rings

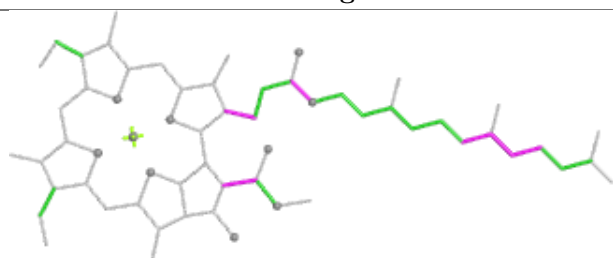
Ligand CLA bB 818



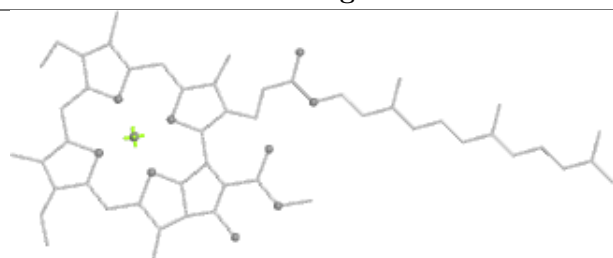
Bond lengths



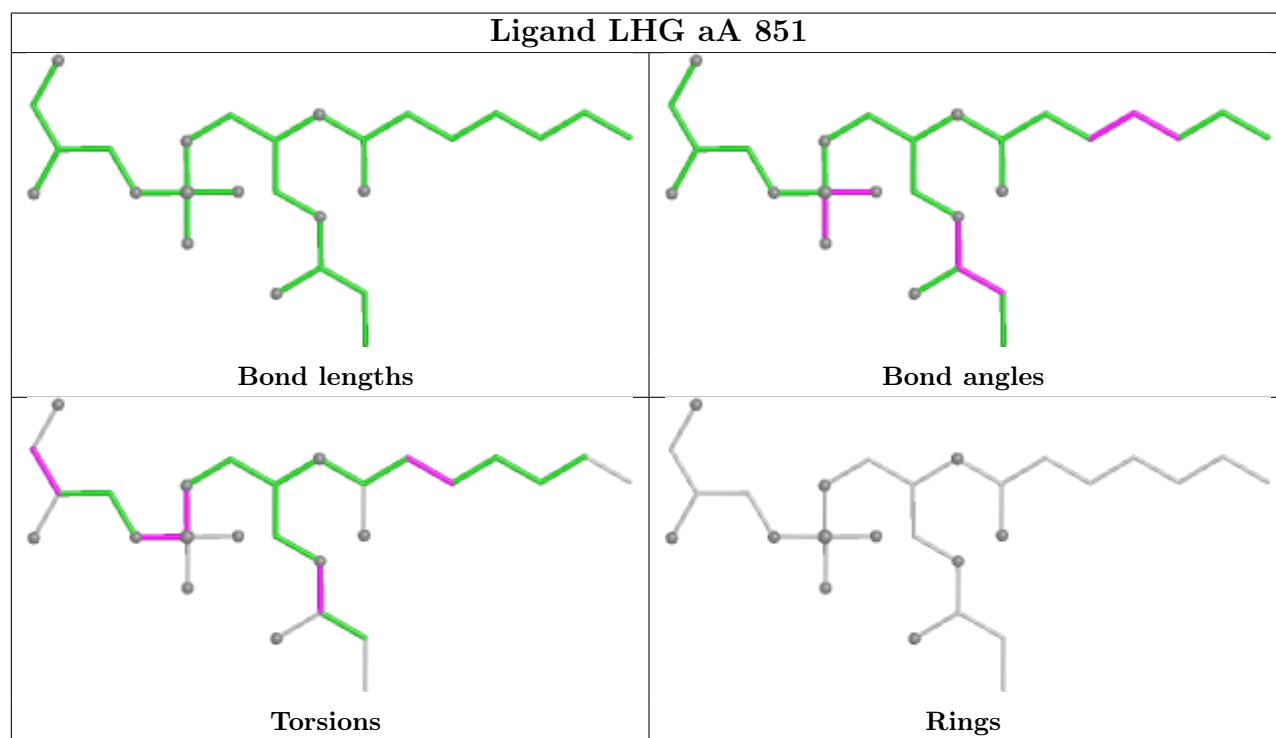
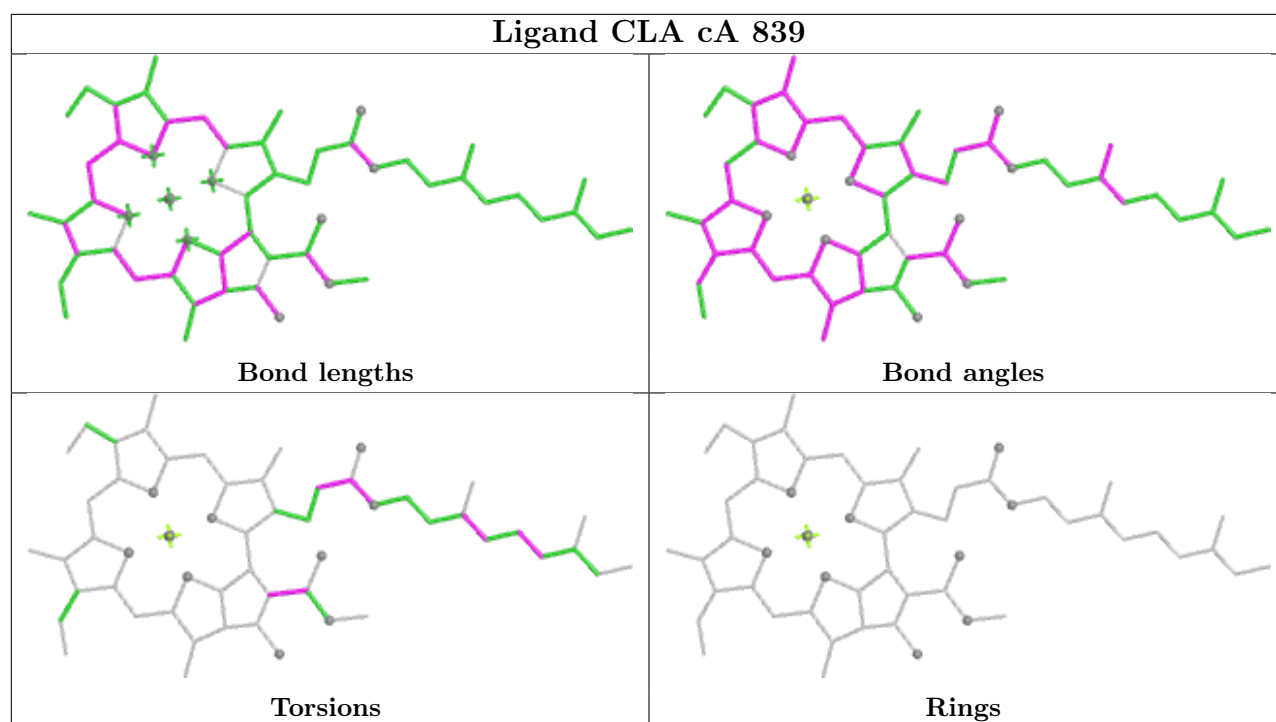
Bond angles

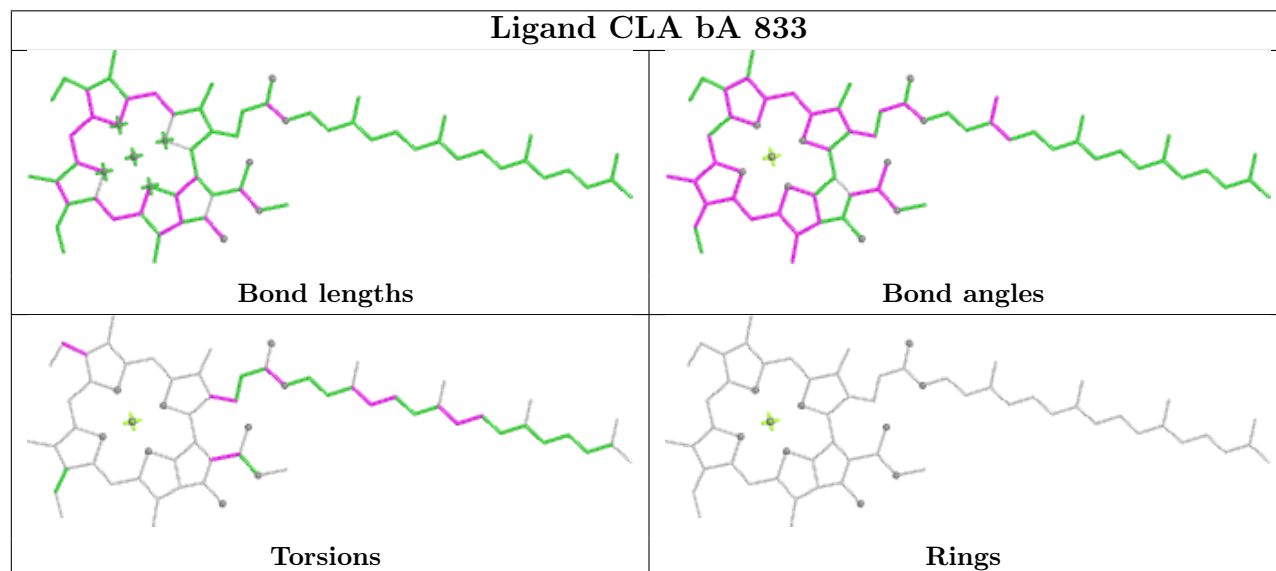
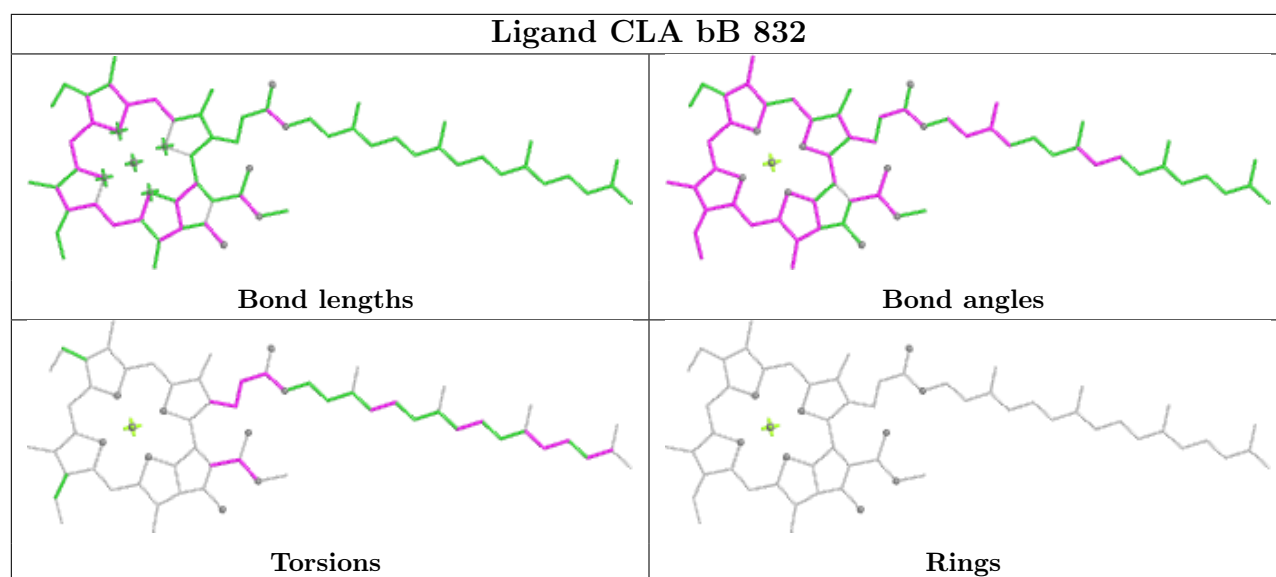


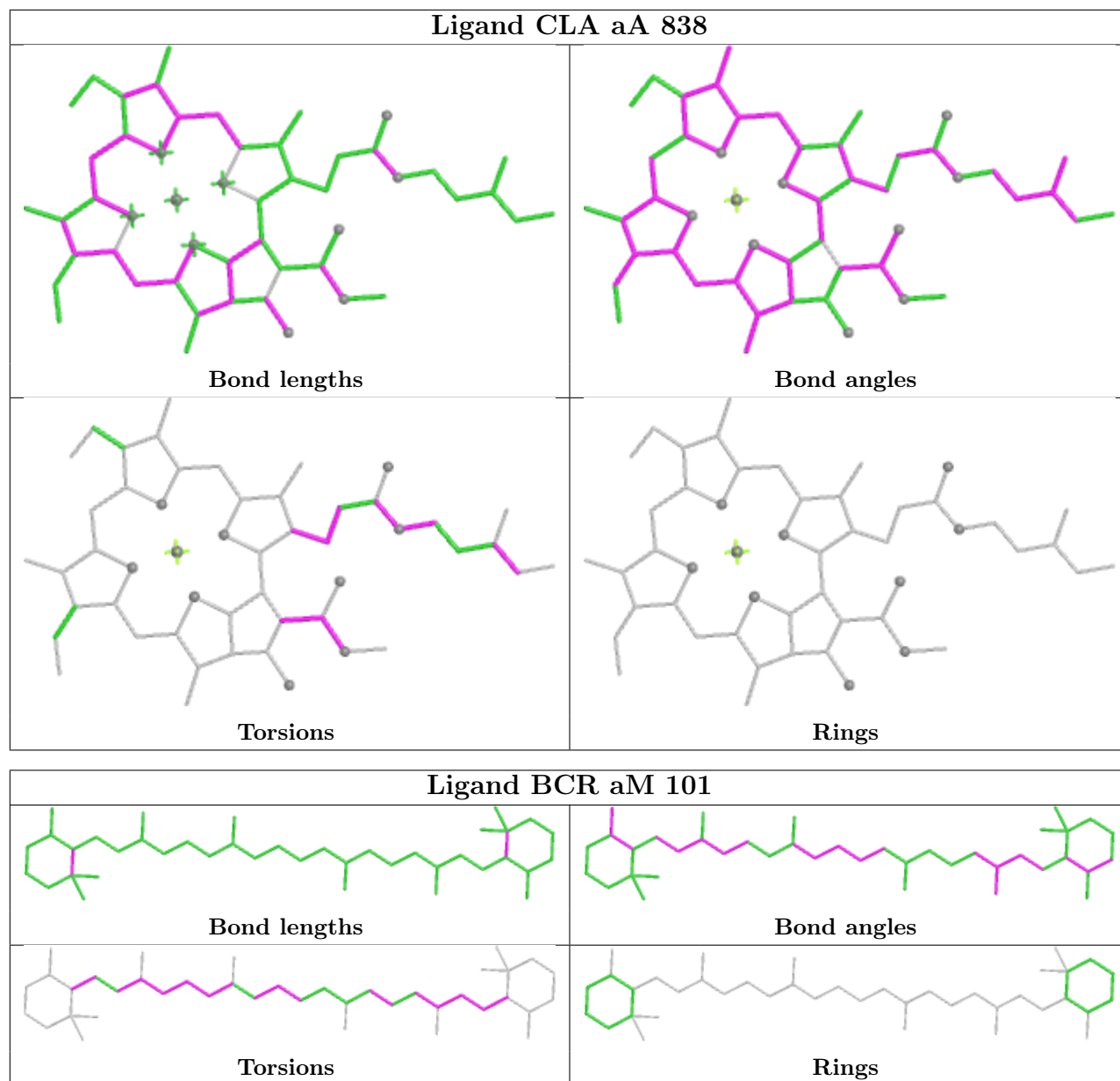
Torsions



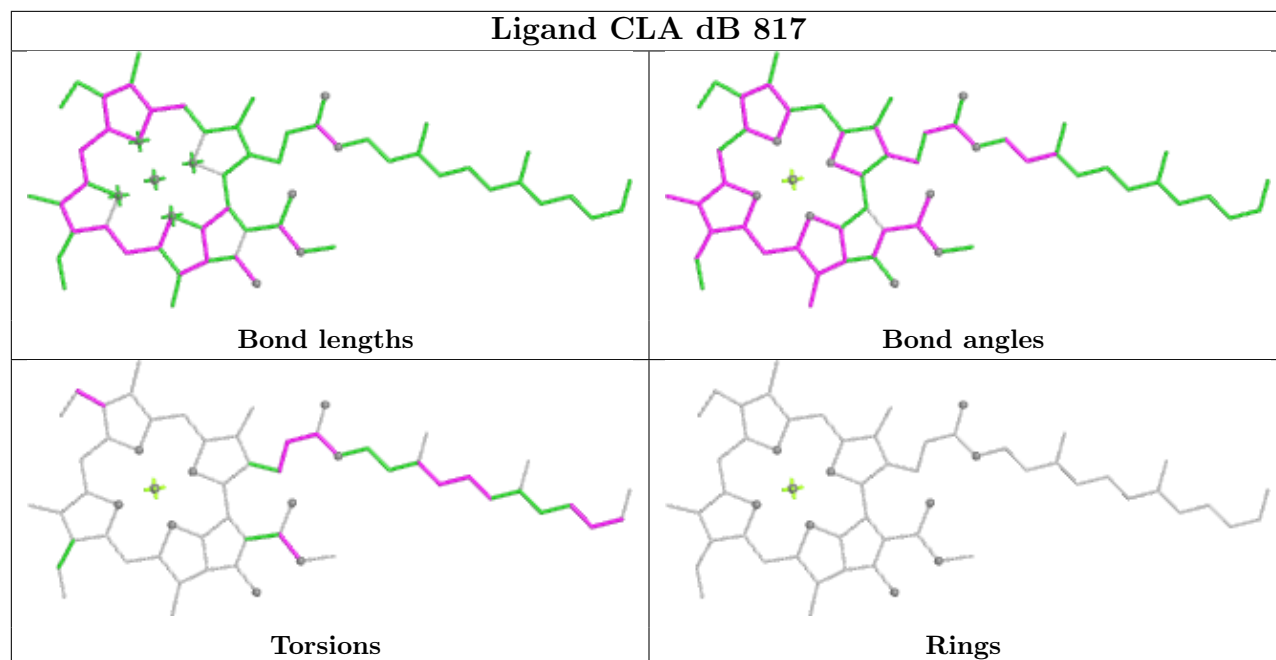
Rings



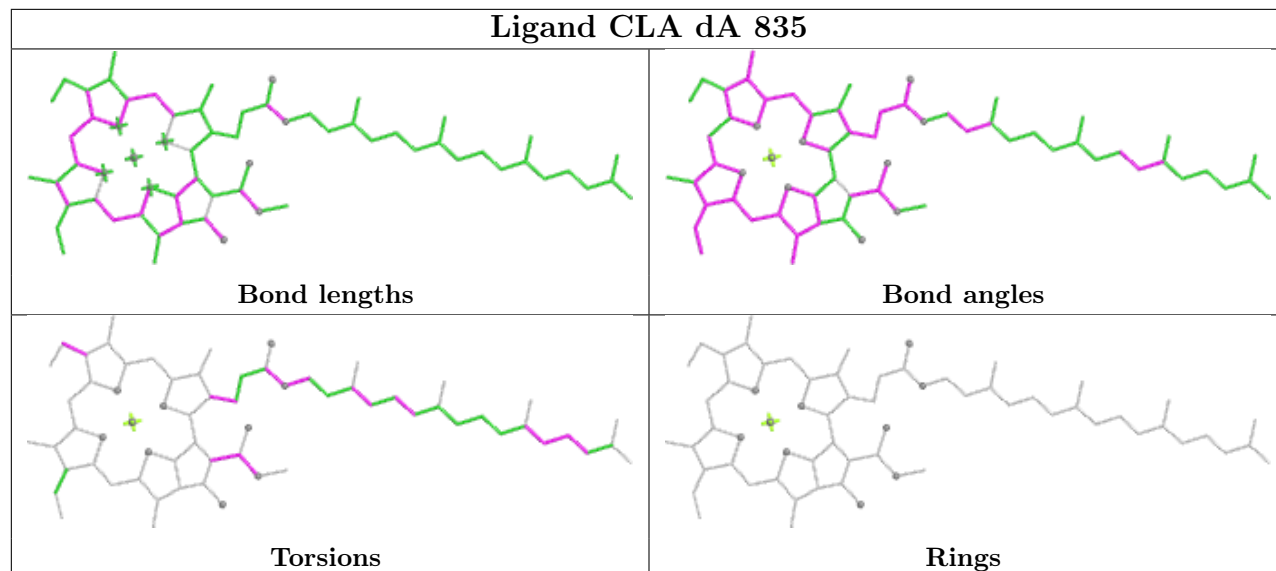




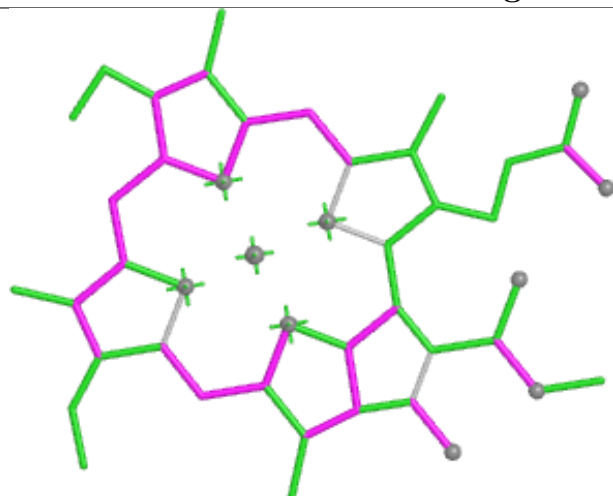
Ligand CLA dB 817



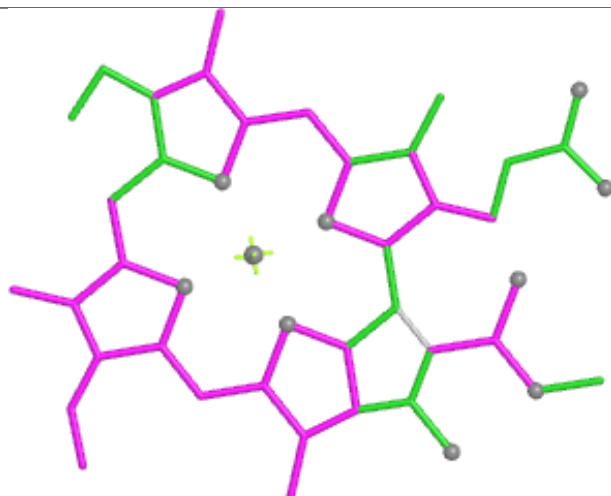
Ligand CLA dA 835



Ligand CLA bA 803



Bond lengths



Bond angles

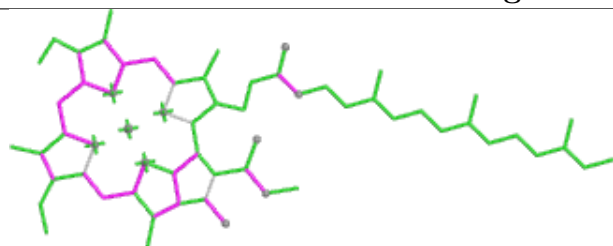


Torsions

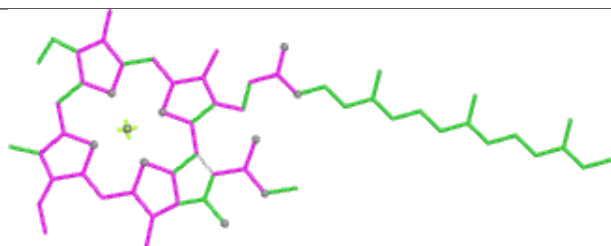


Rings

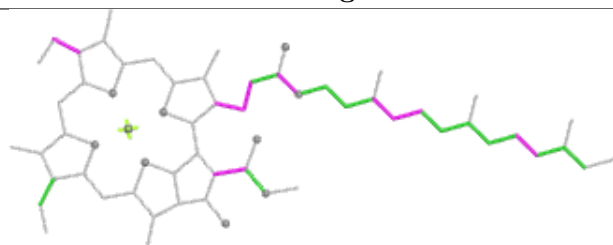
Ligand CLA dA 821



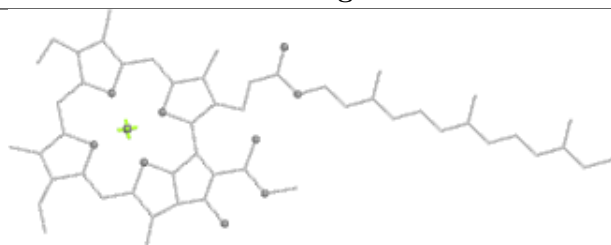
Bond lengths



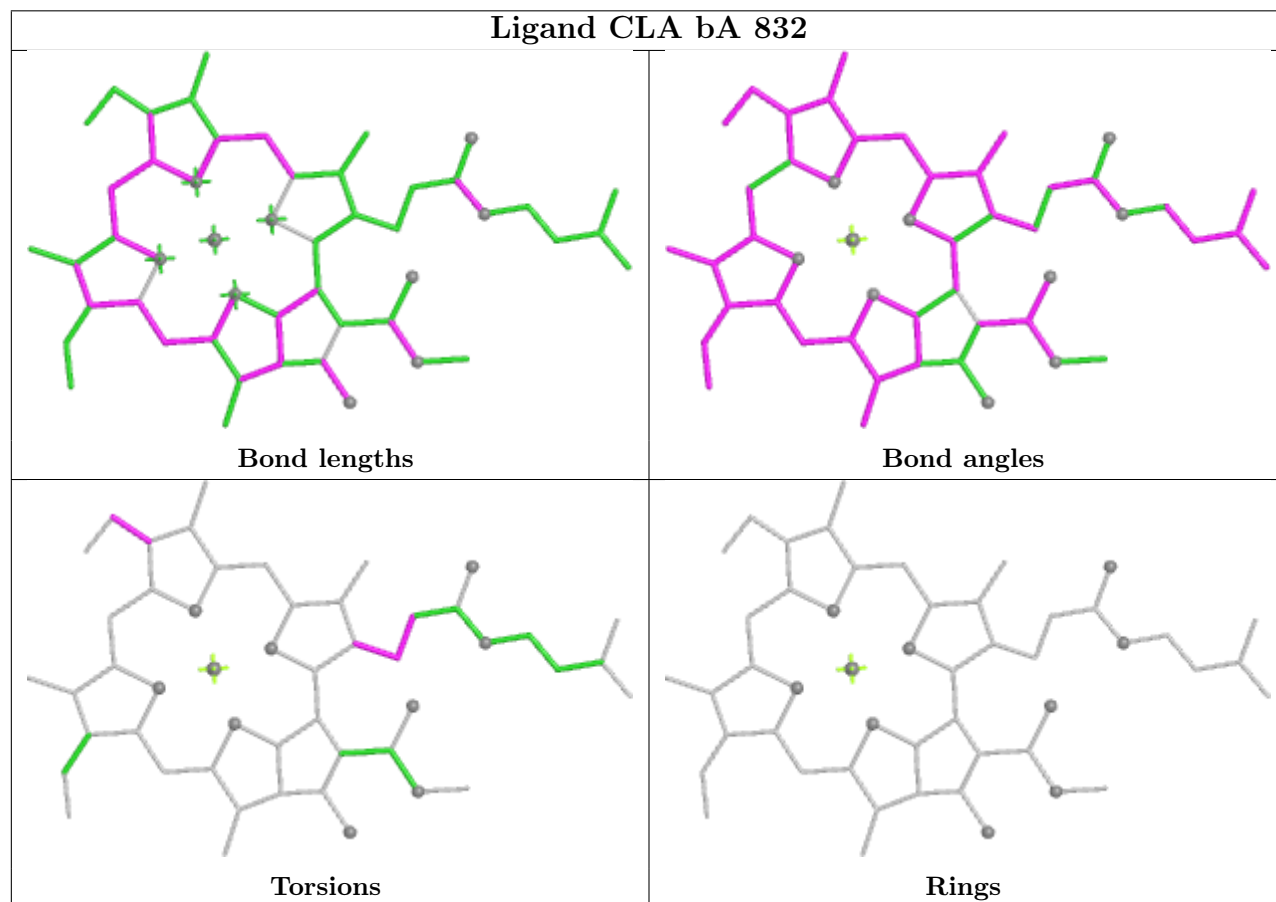
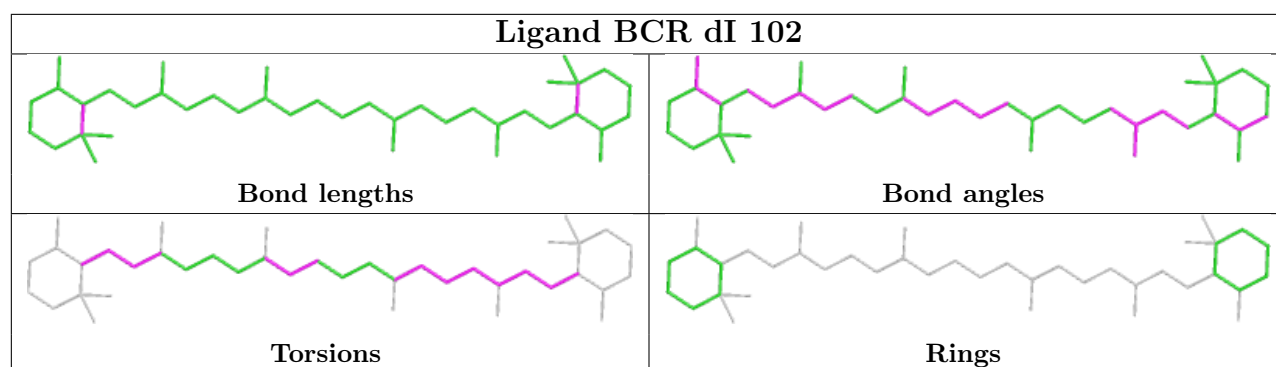
Bond angles

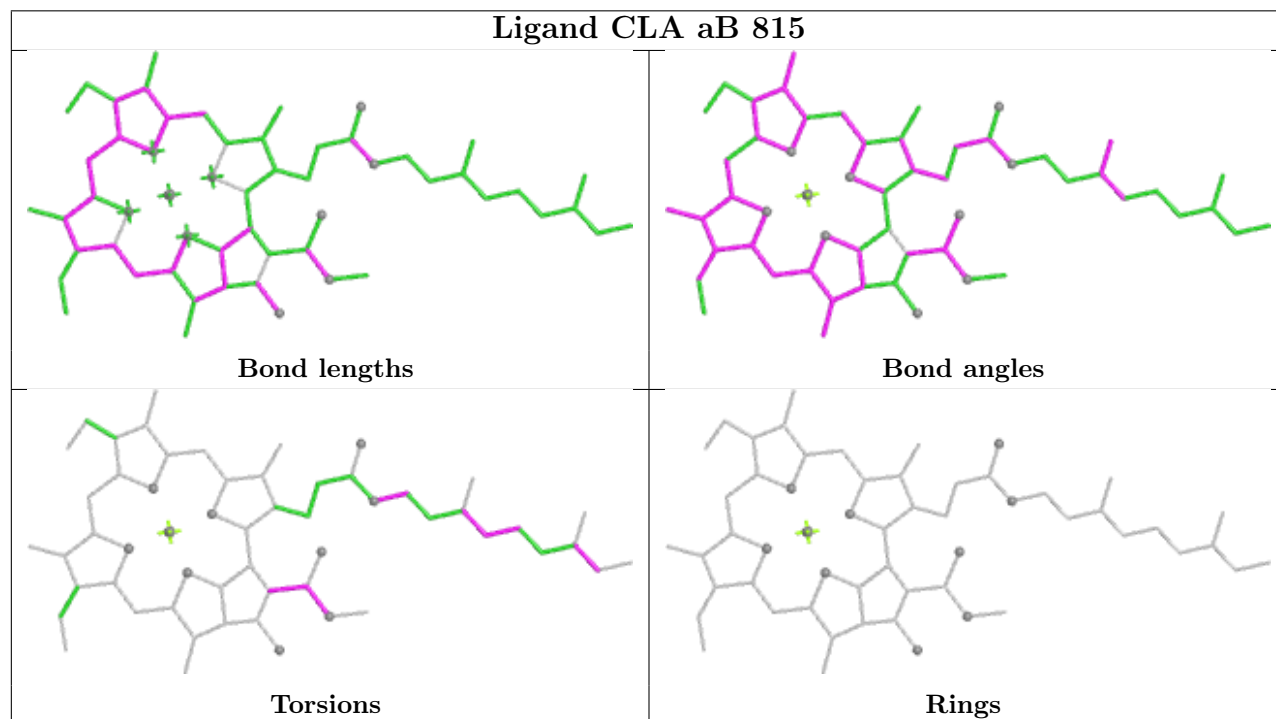
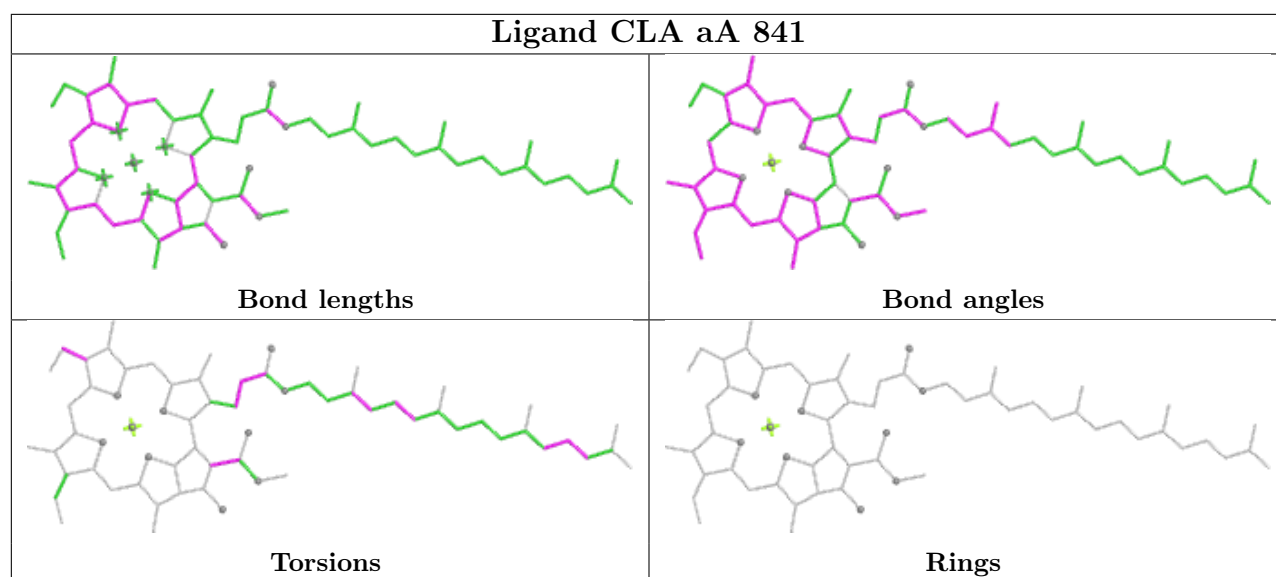


Torsions

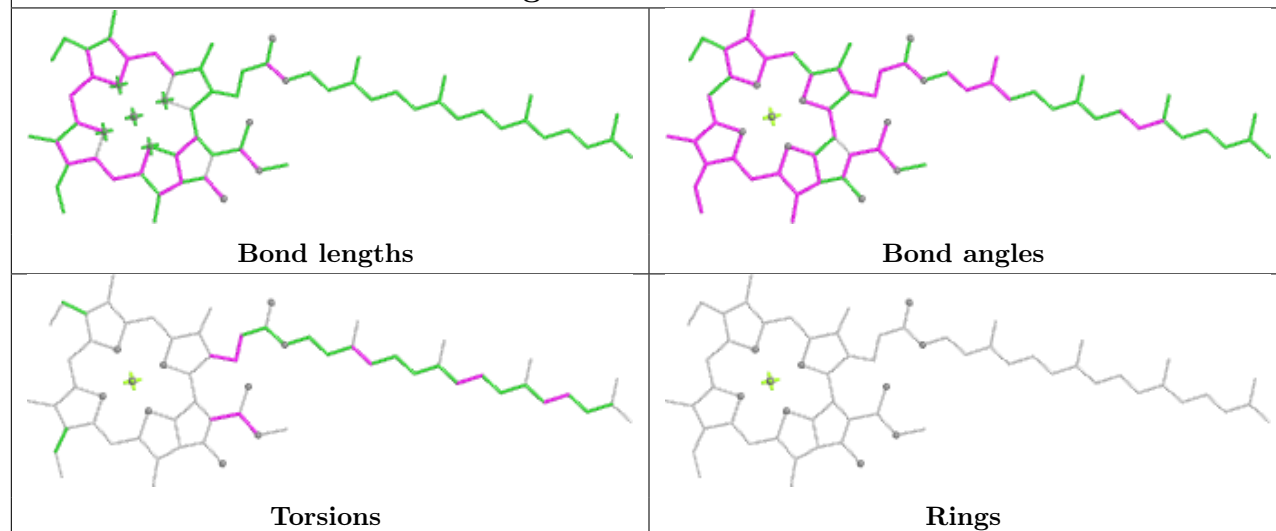


Rings

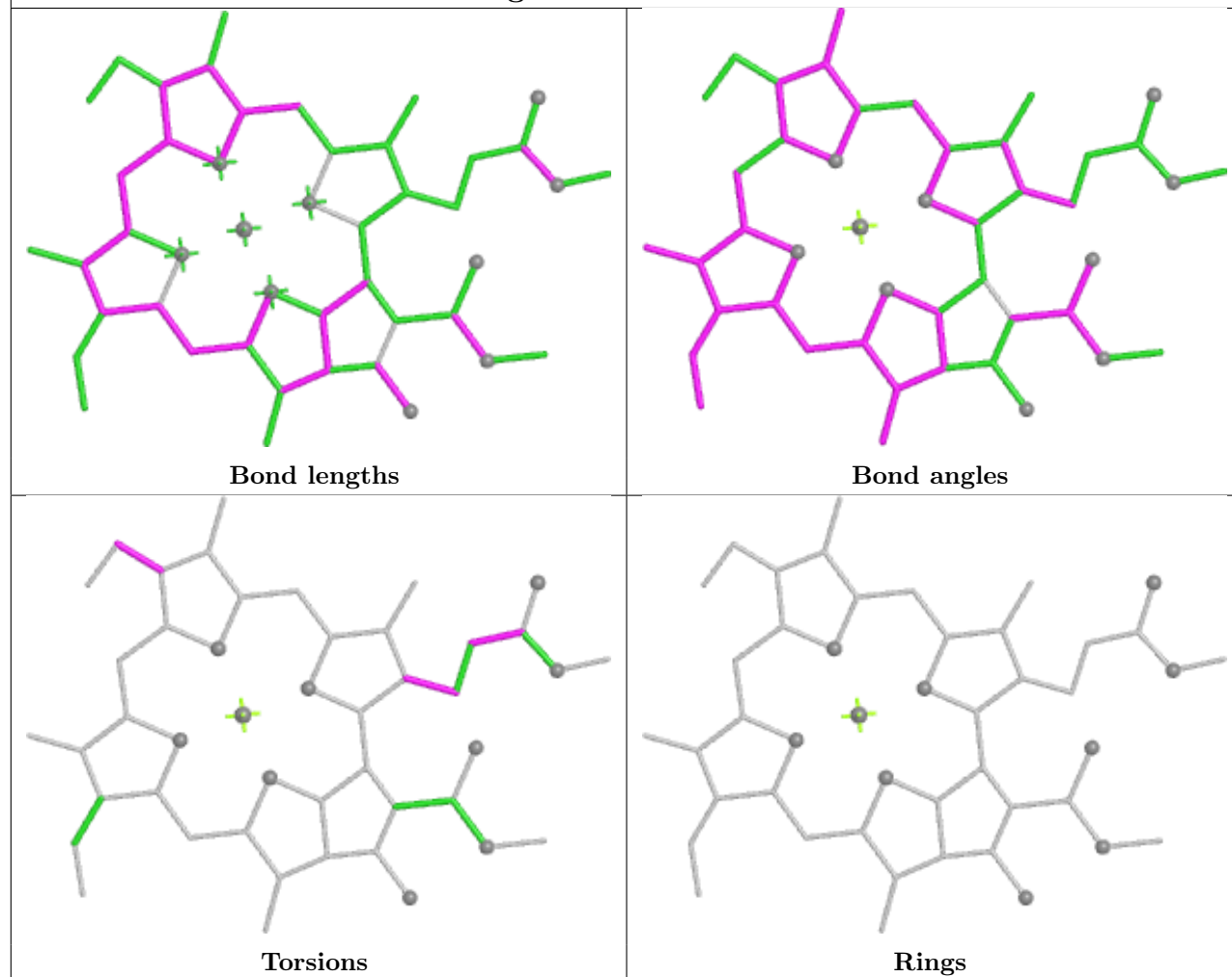


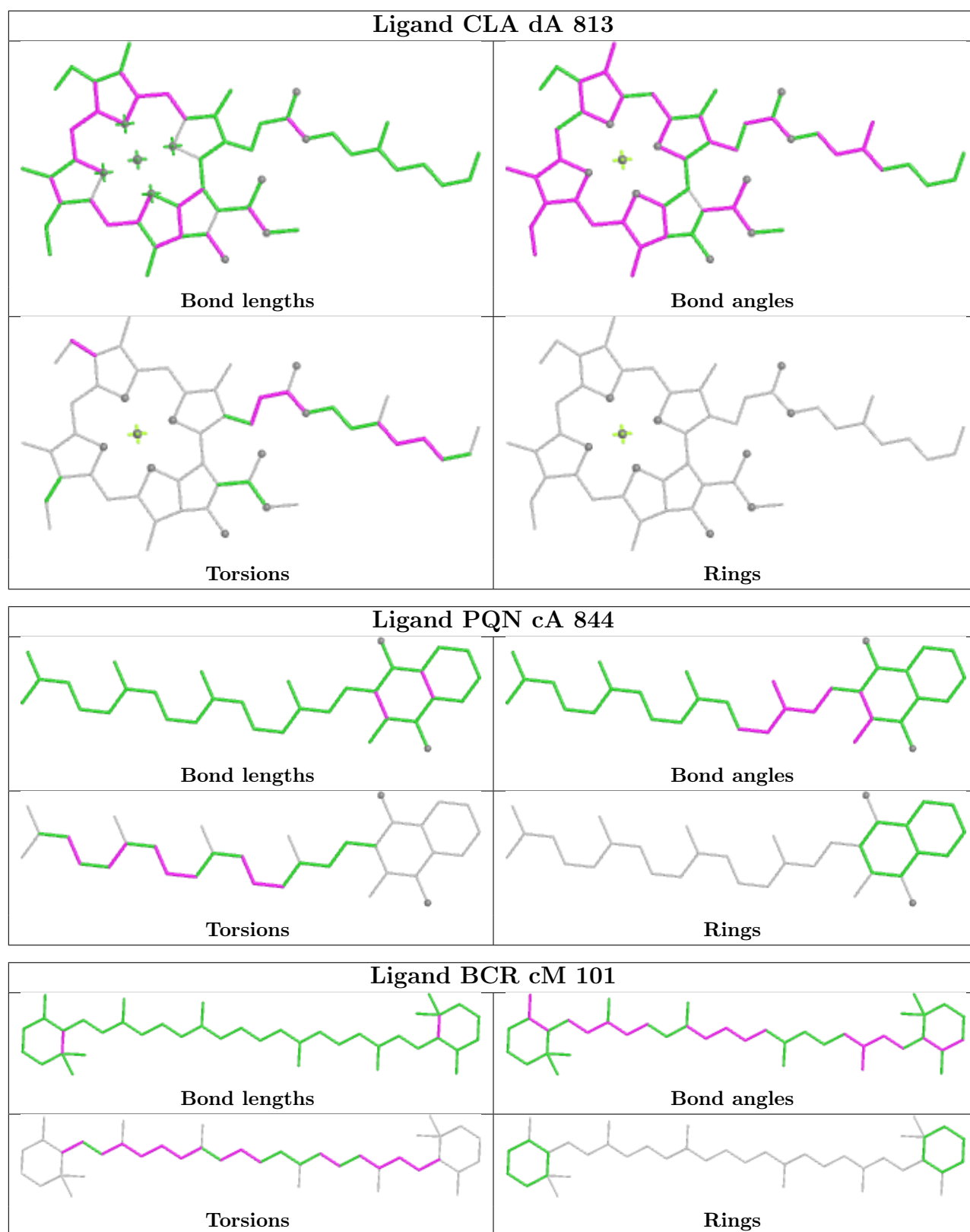


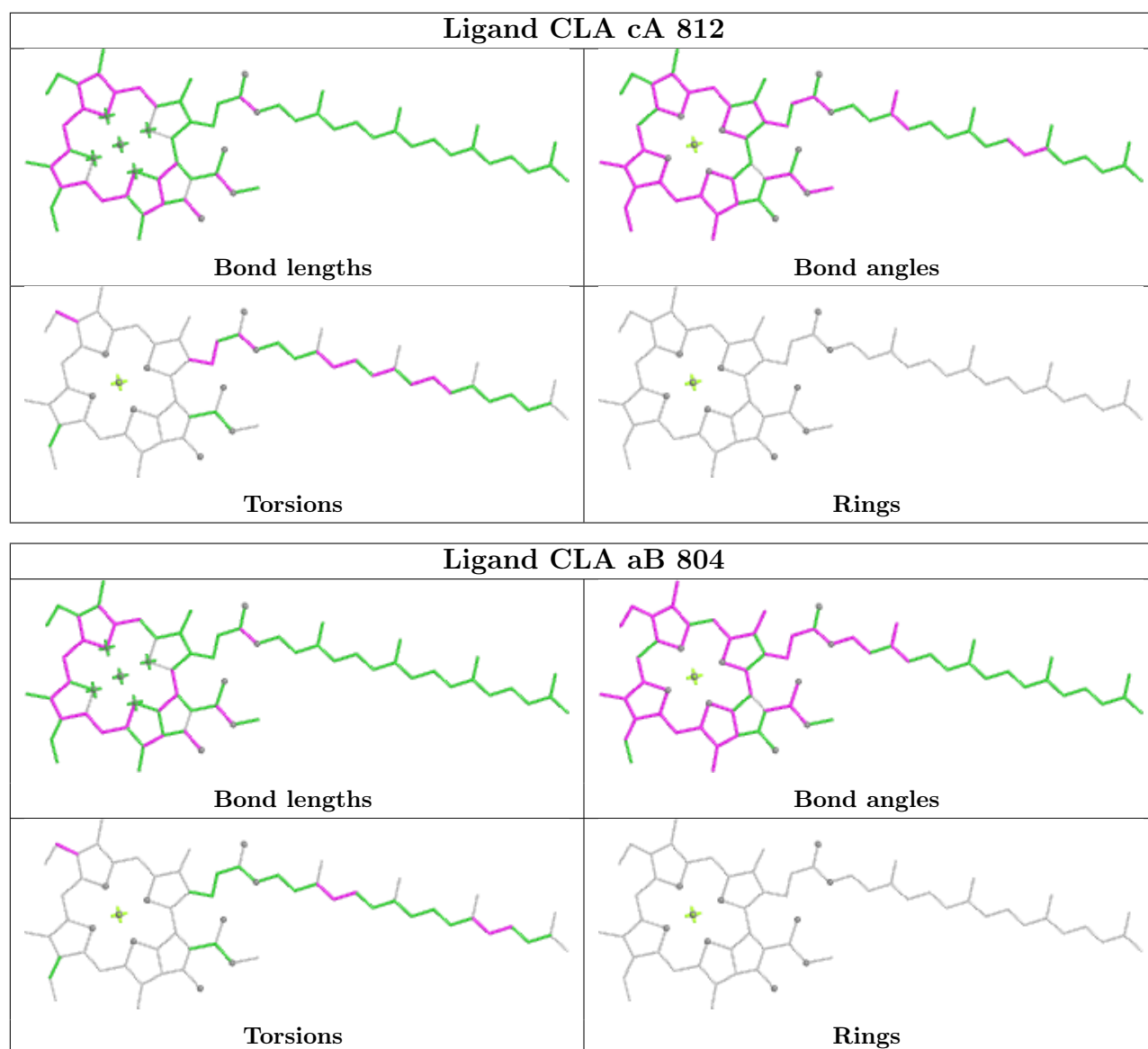
Ligand CLA aA 802

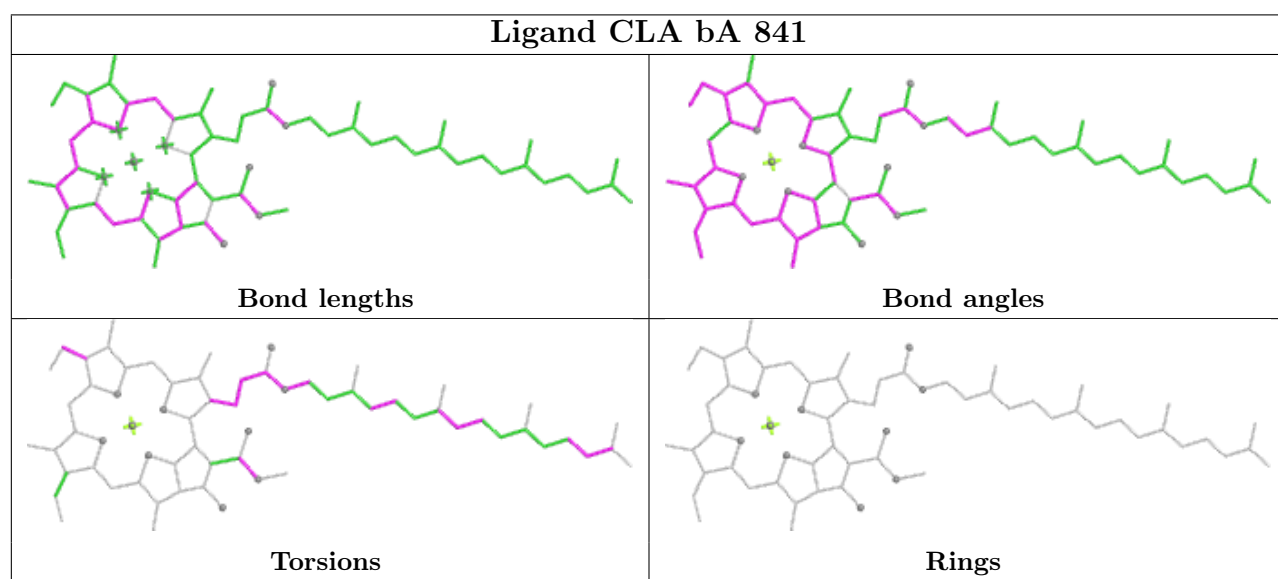
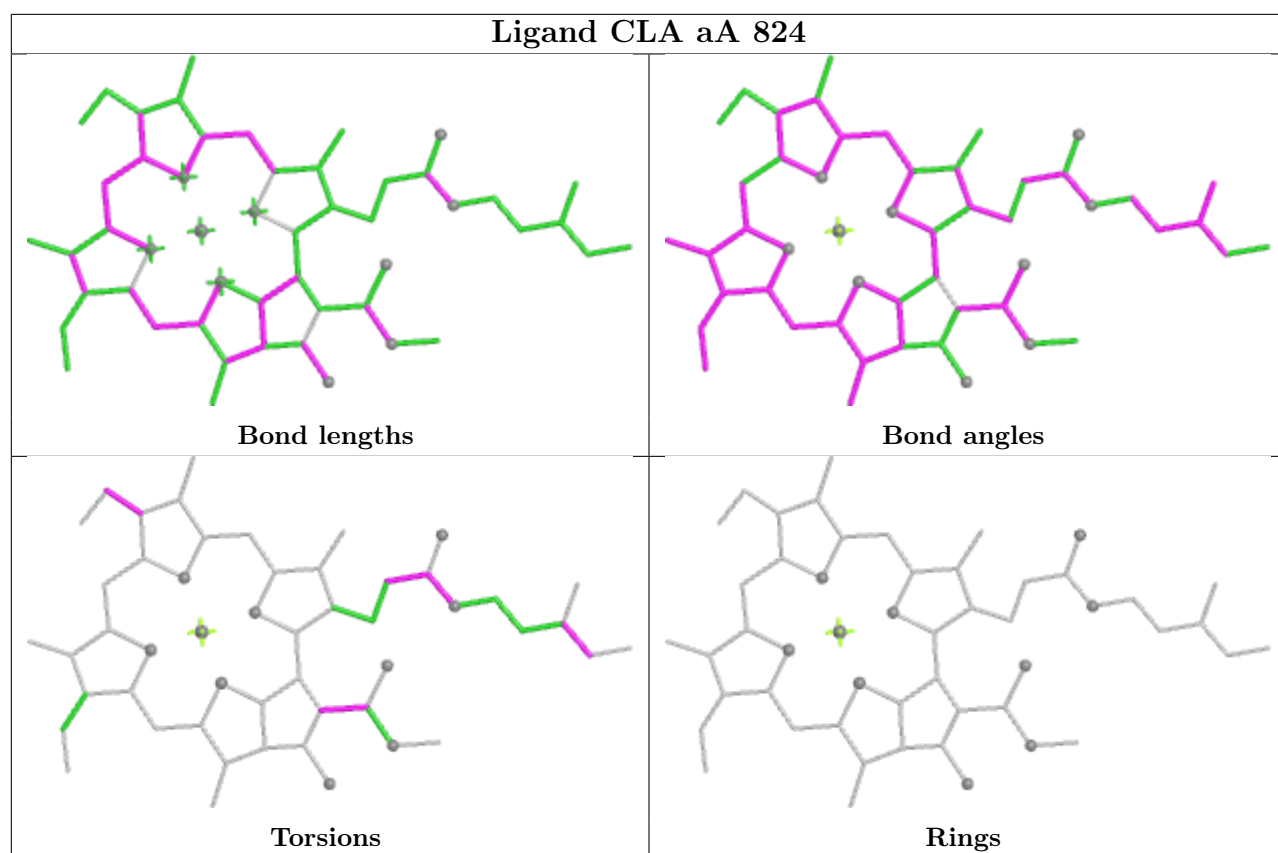


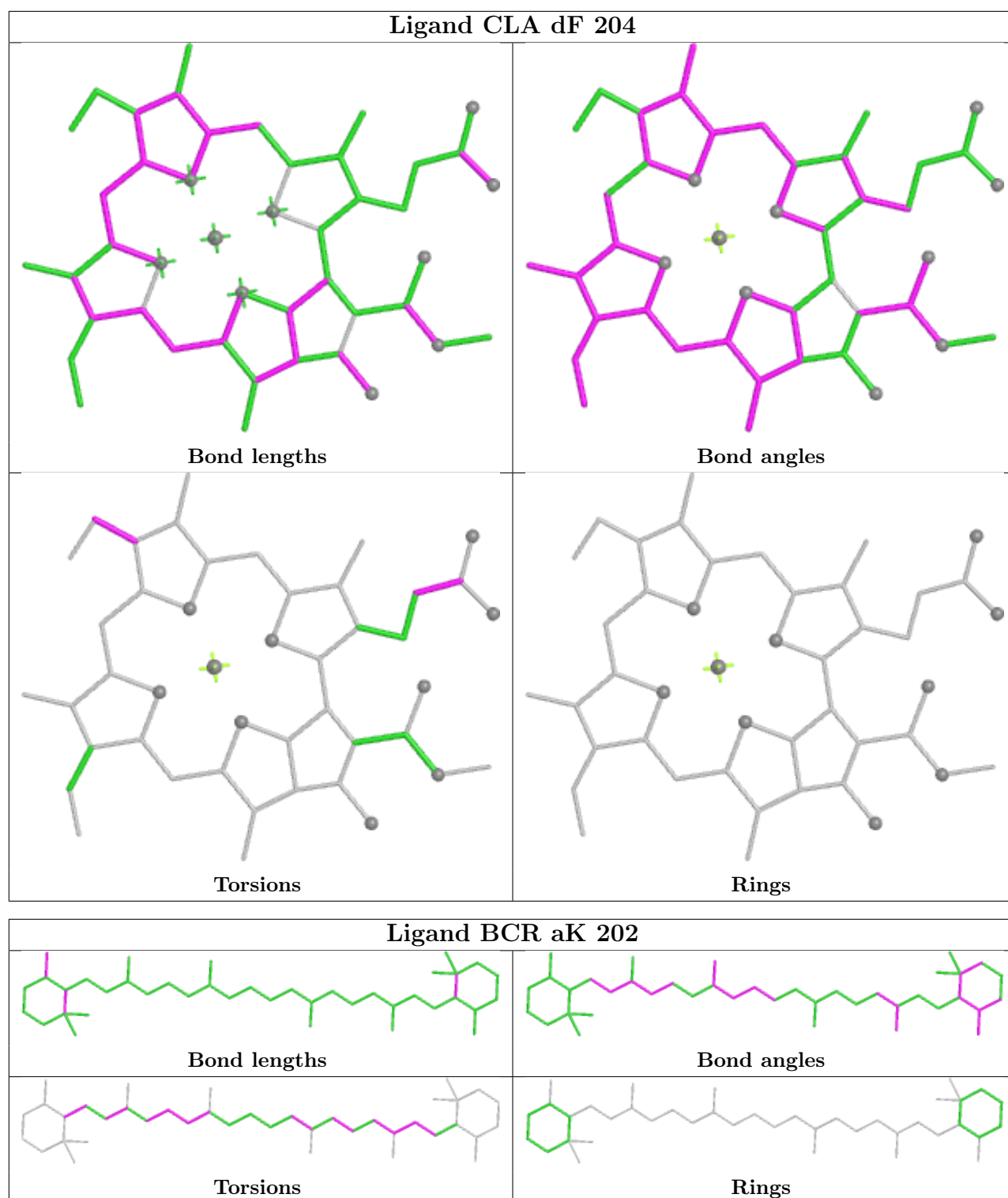
Ligand CLA aL 202

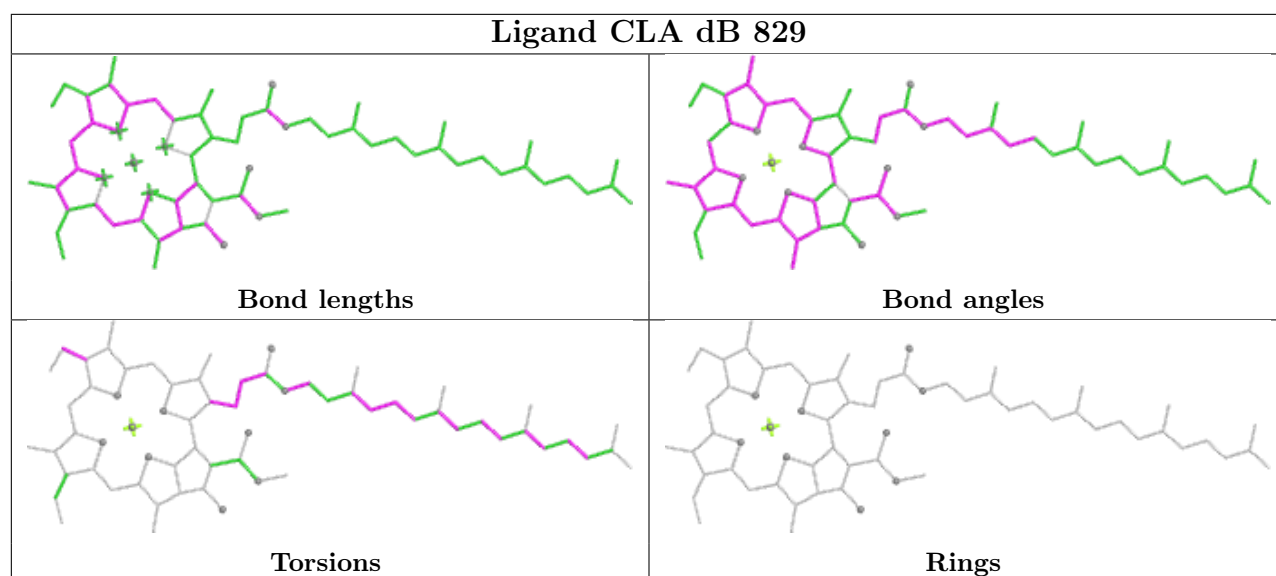
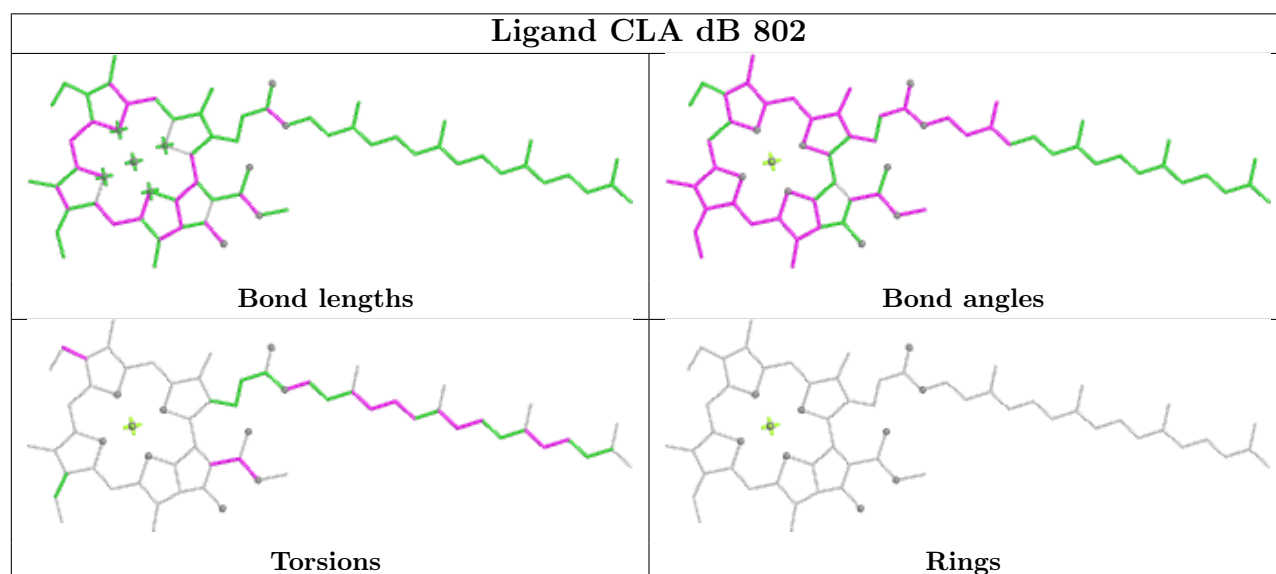
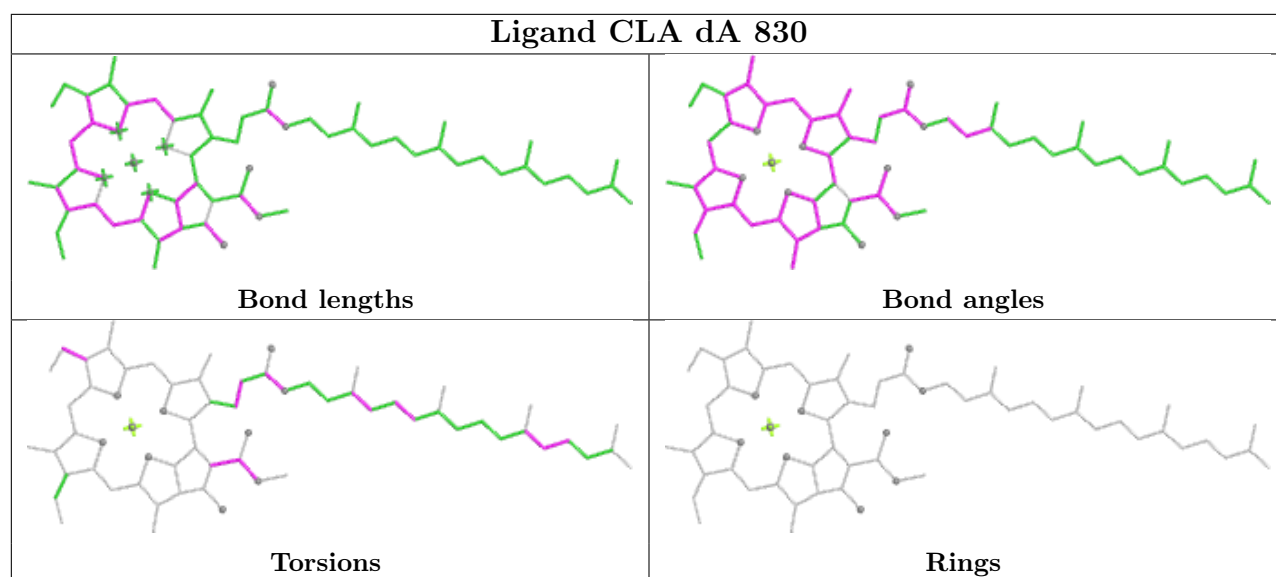


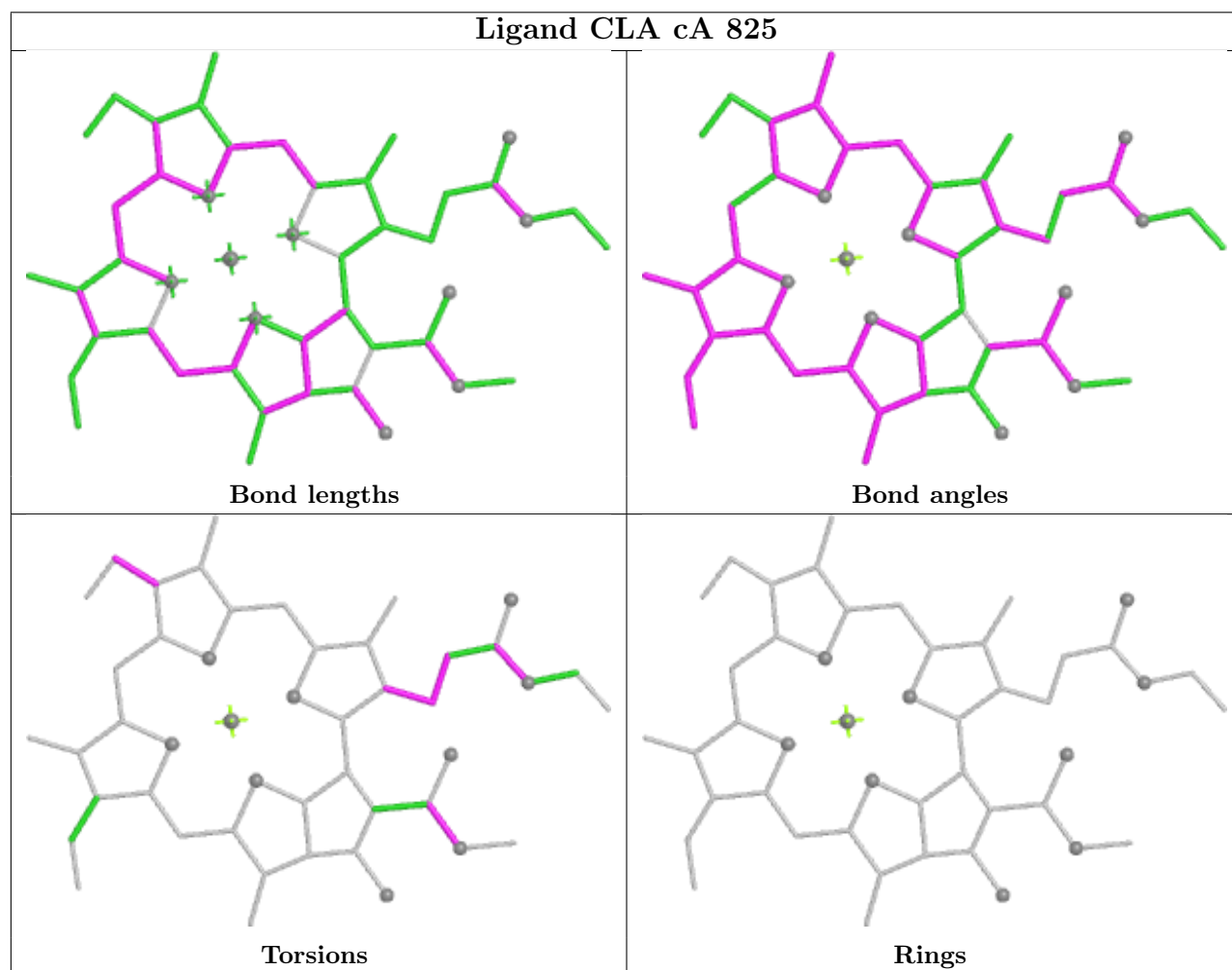
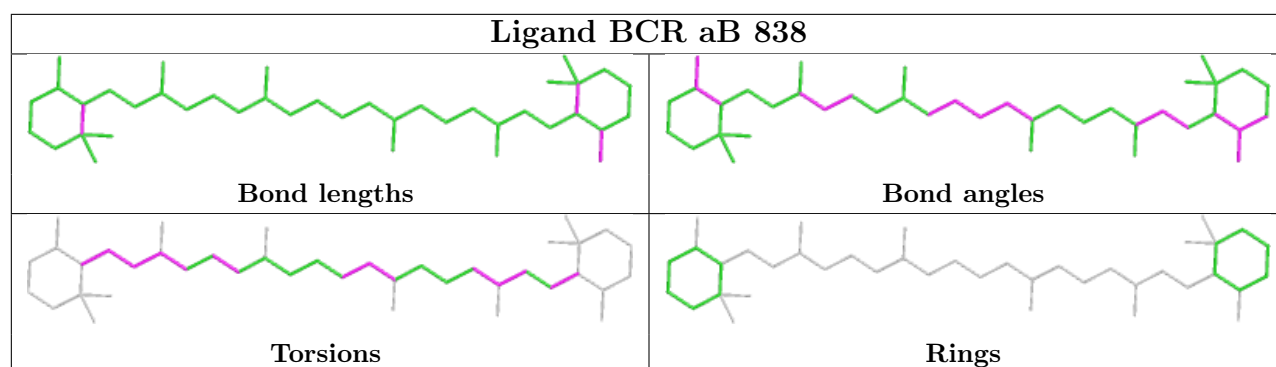




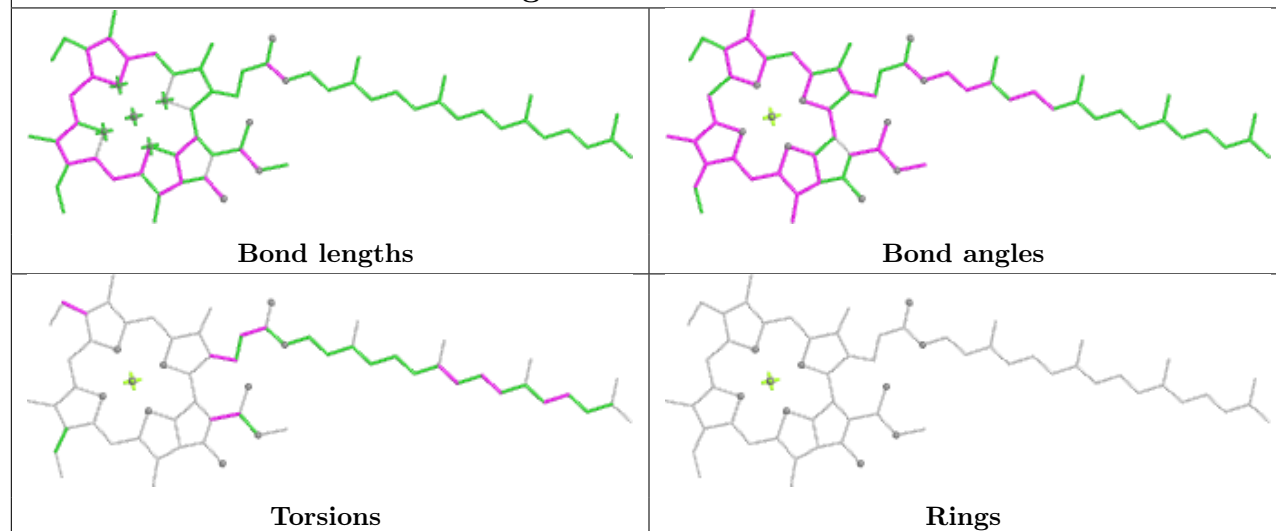




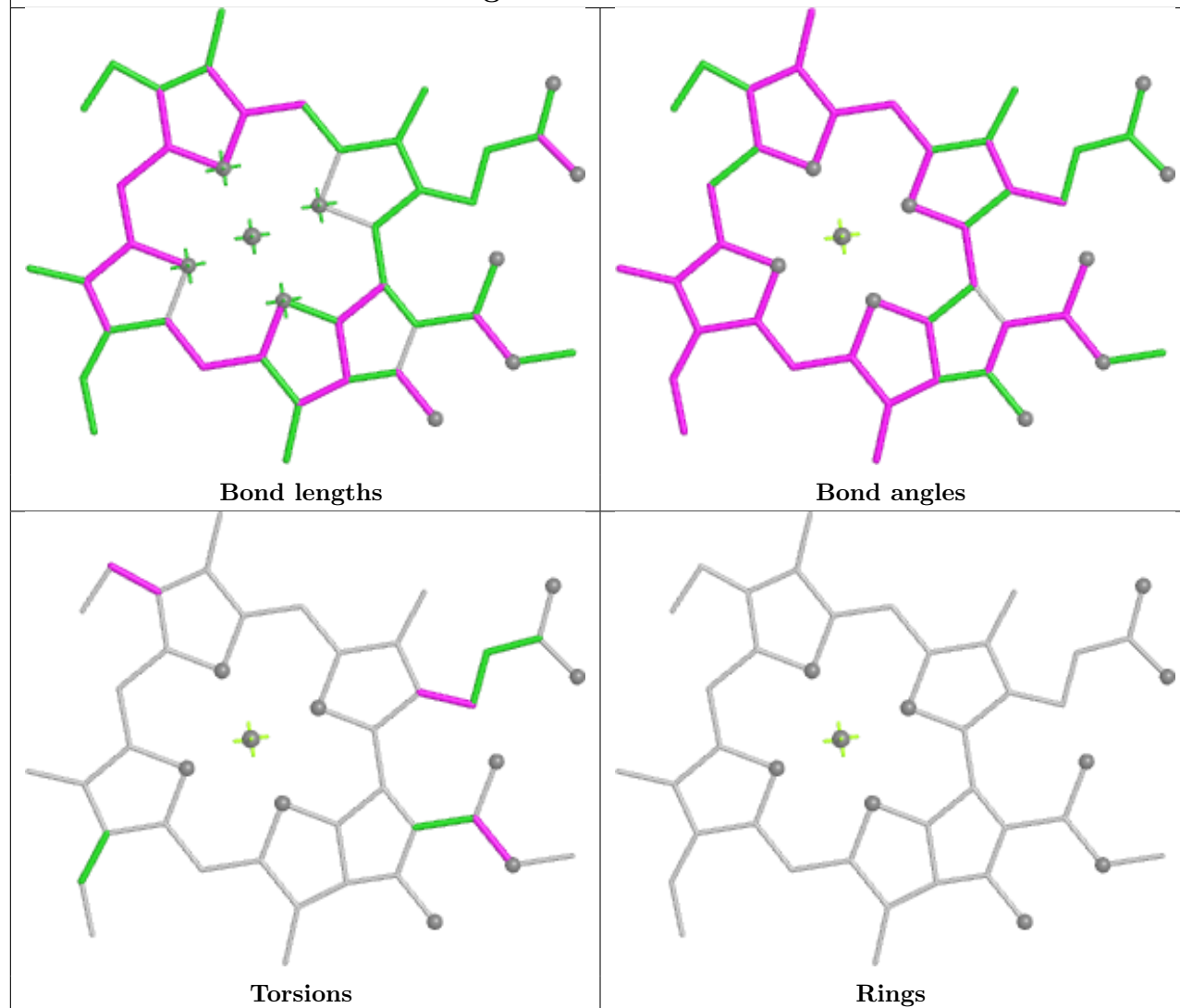


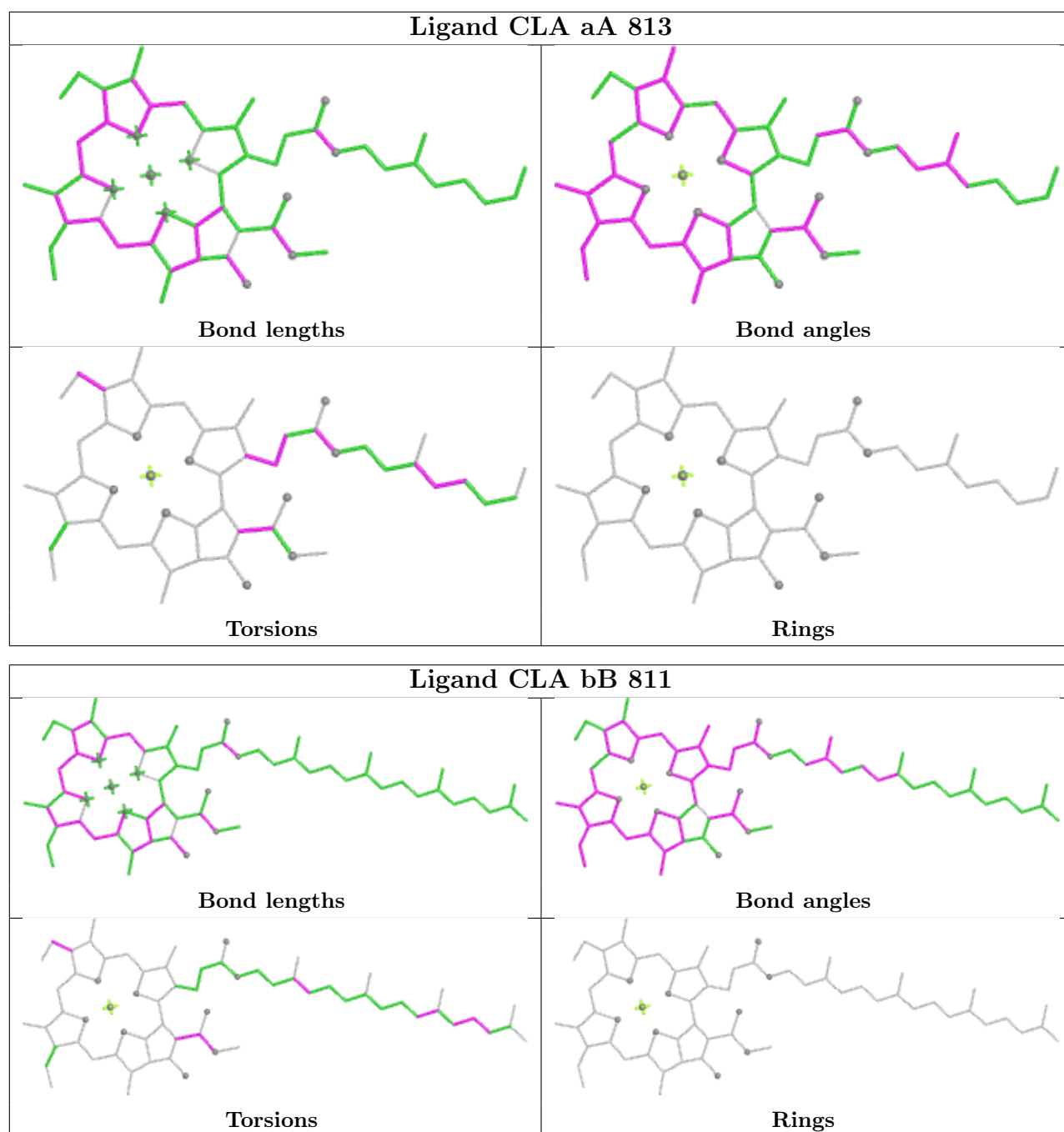


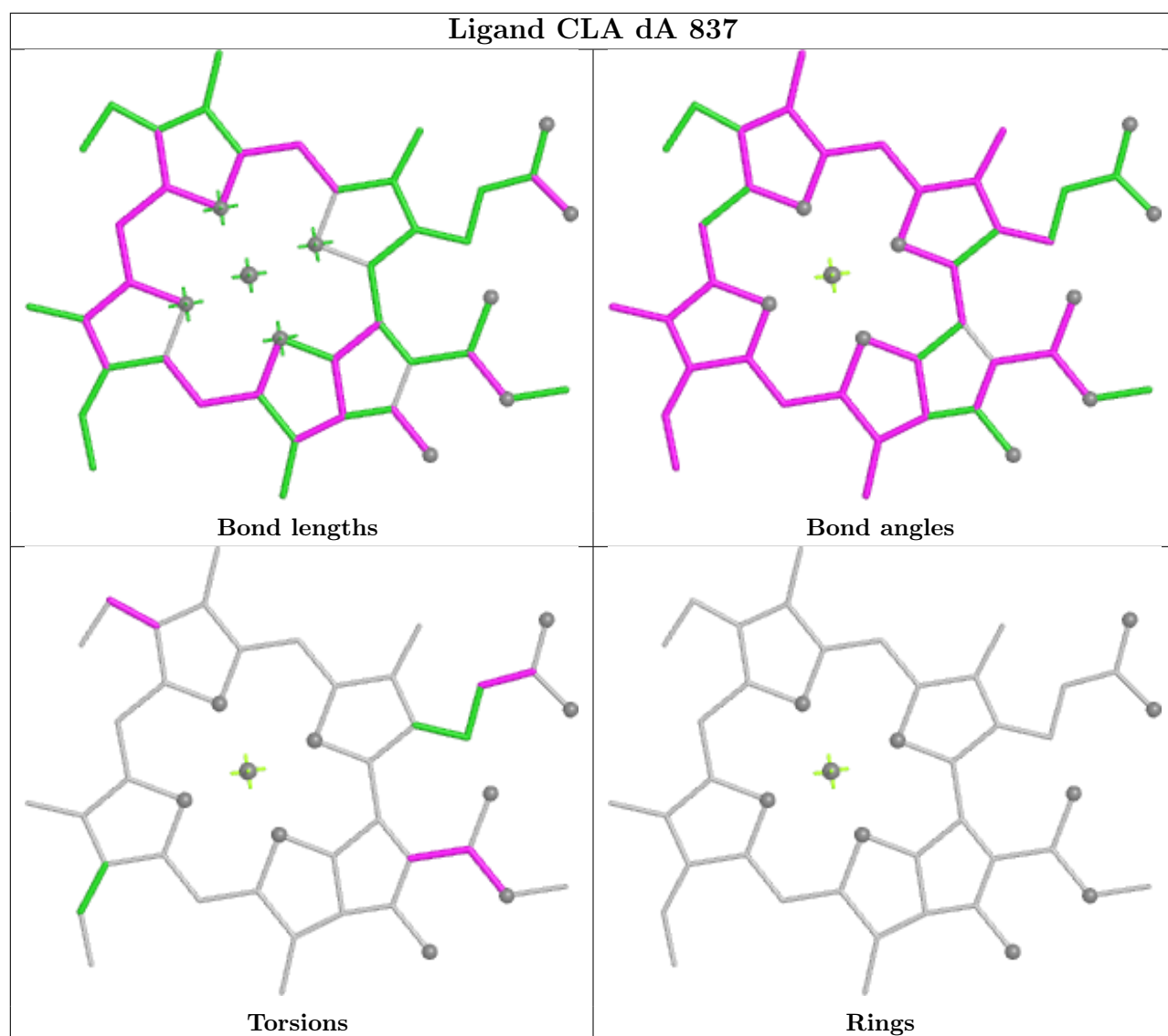
Ligand CLA bB 820

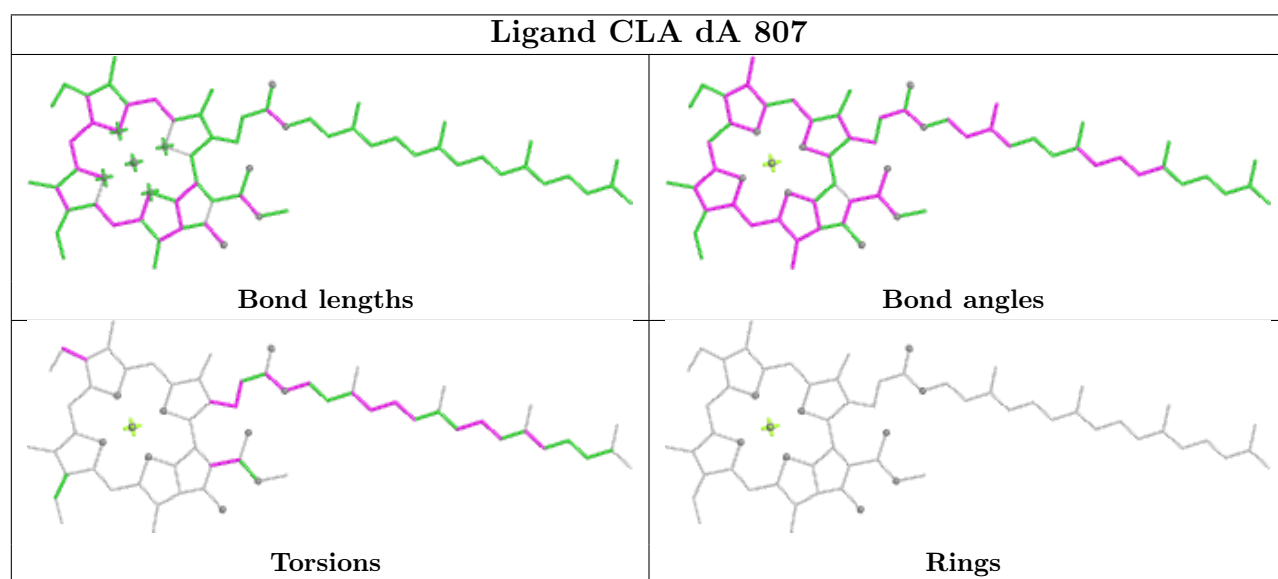
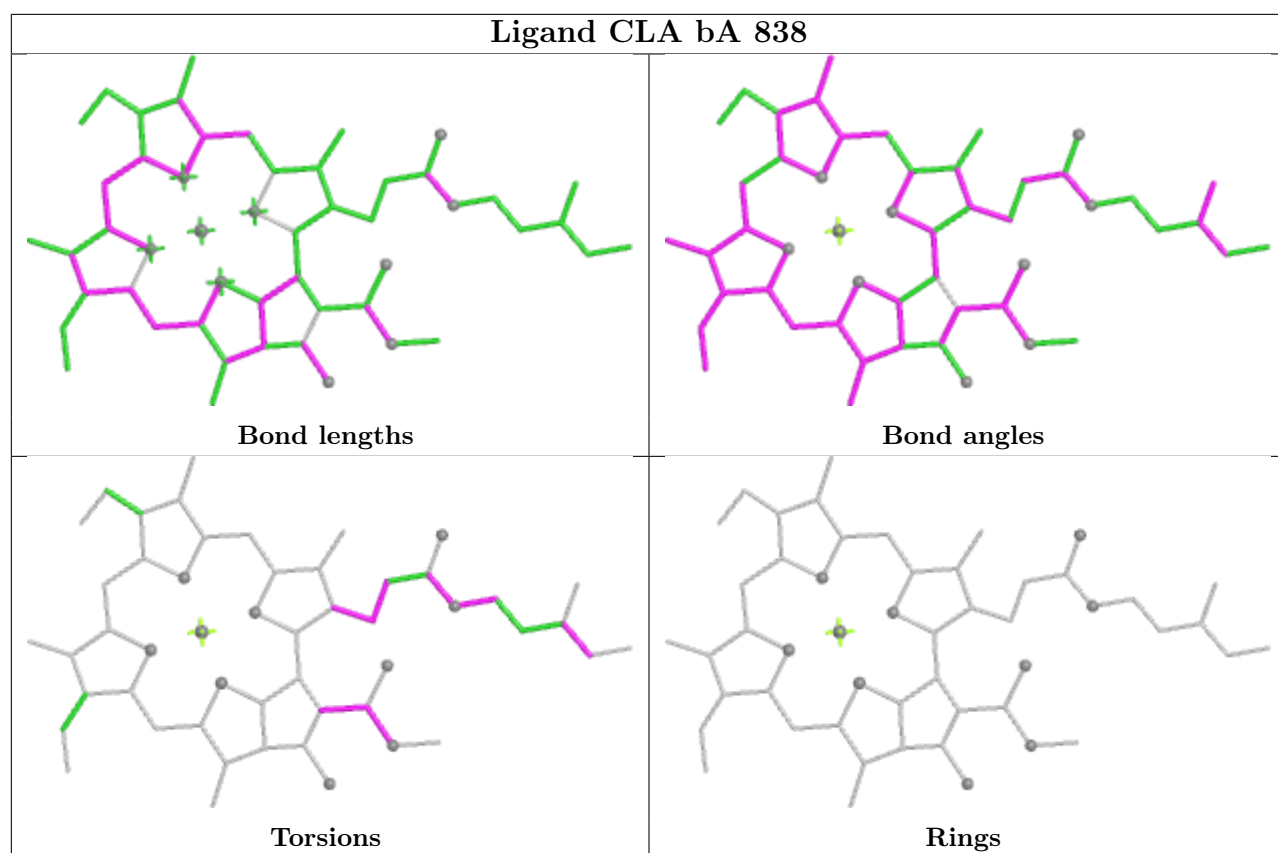


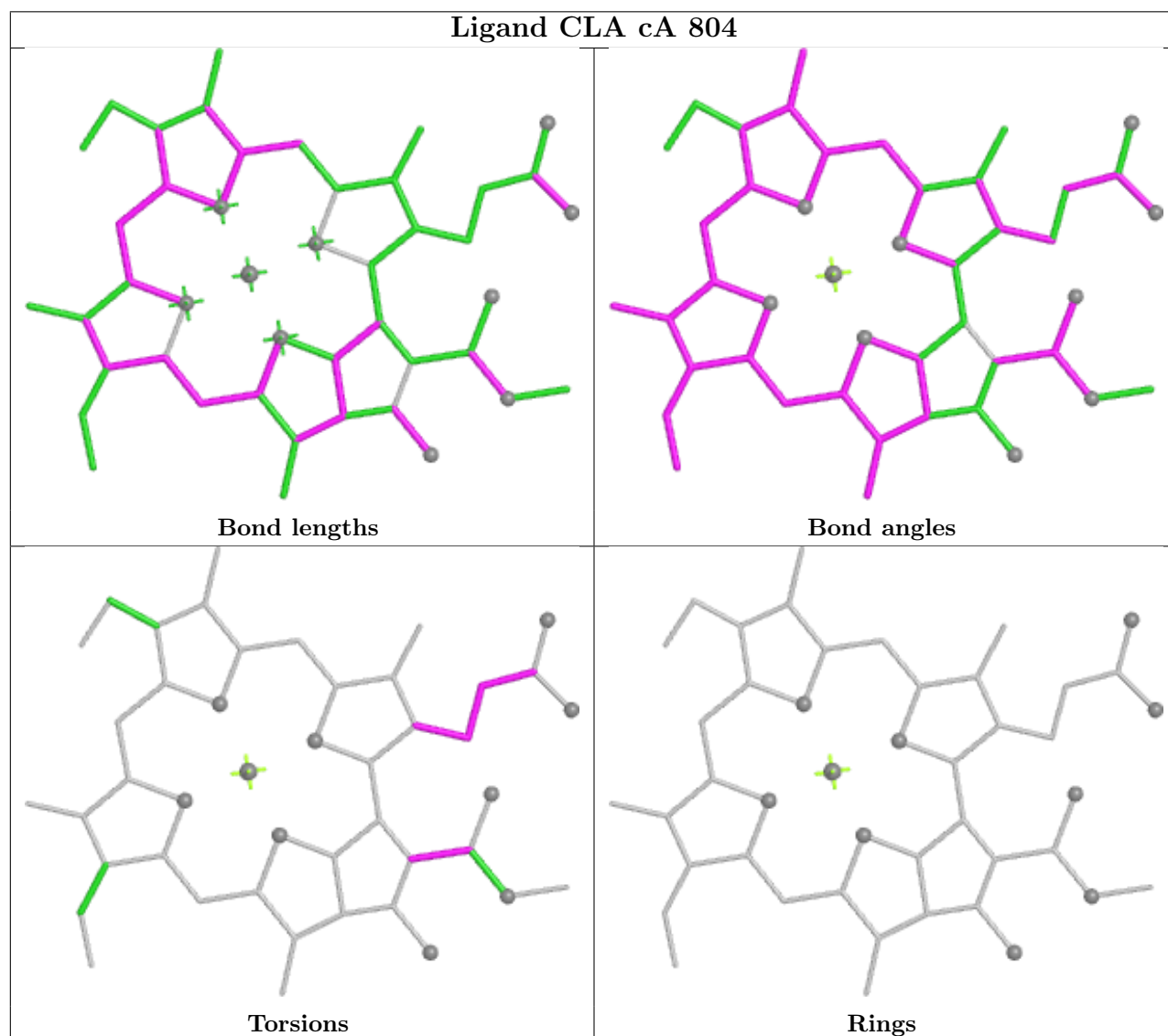
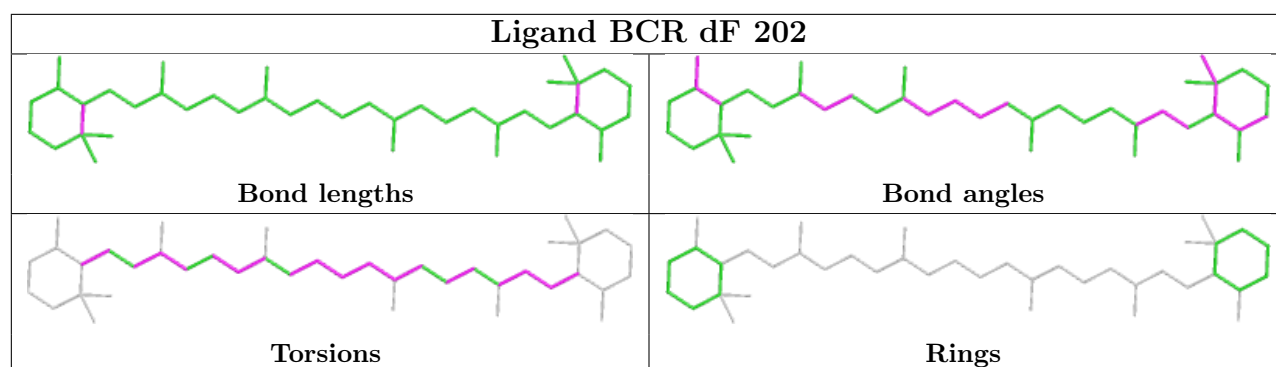
Ligand CLA aA 811

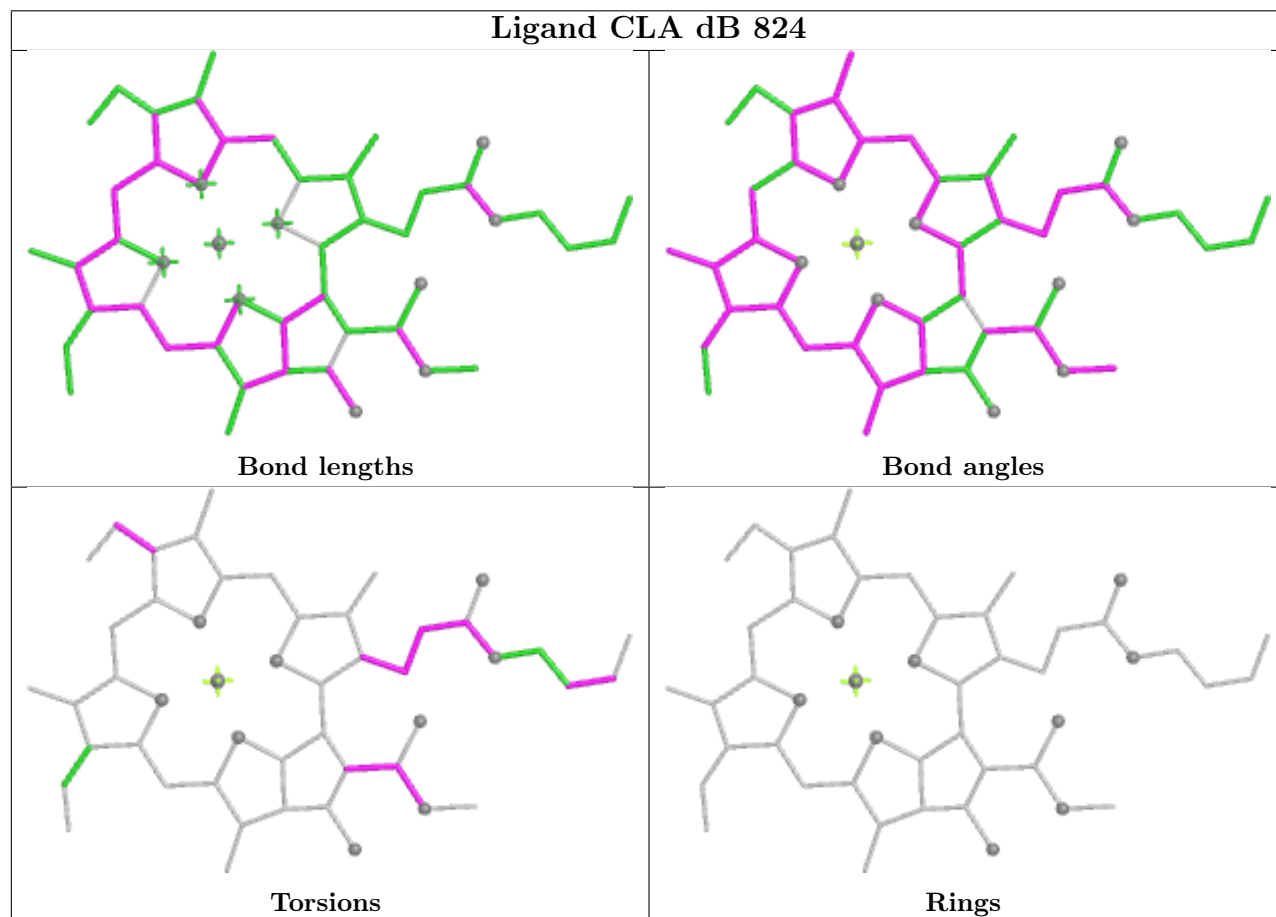
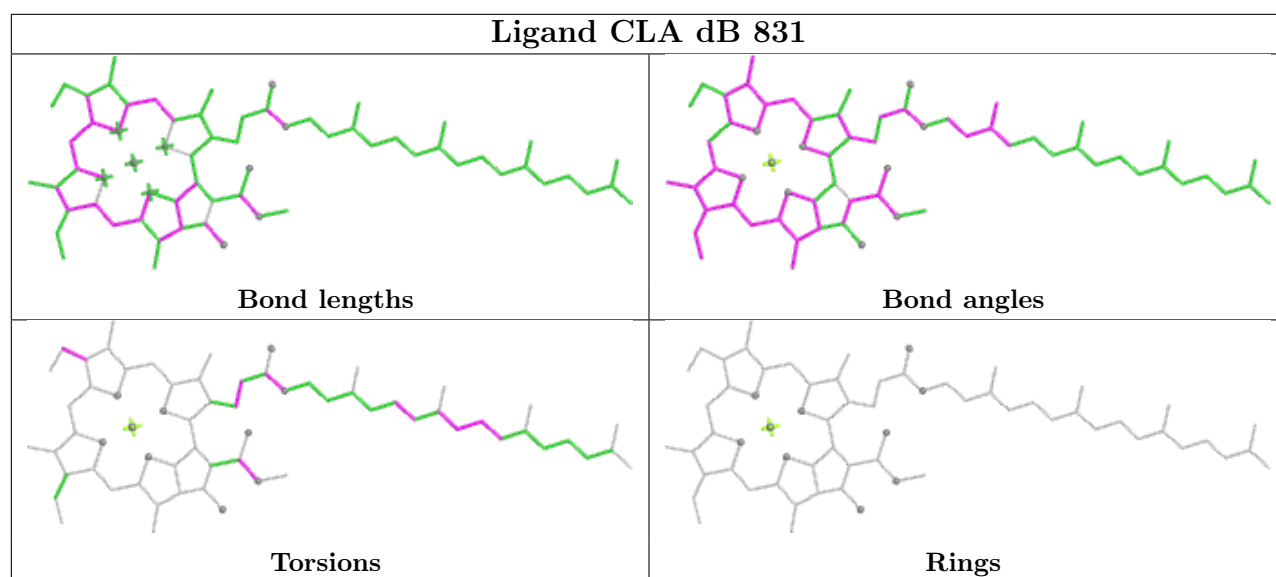


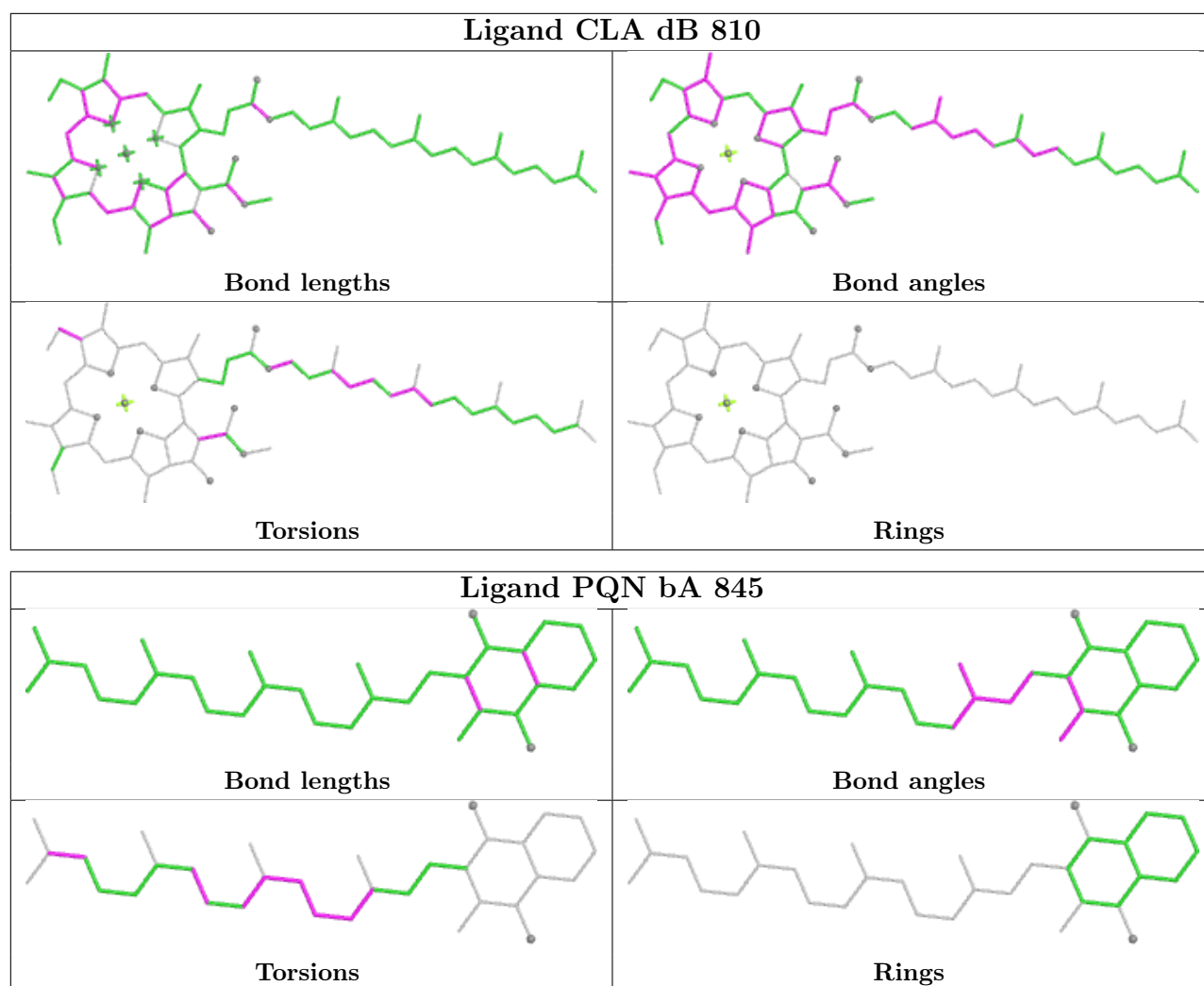


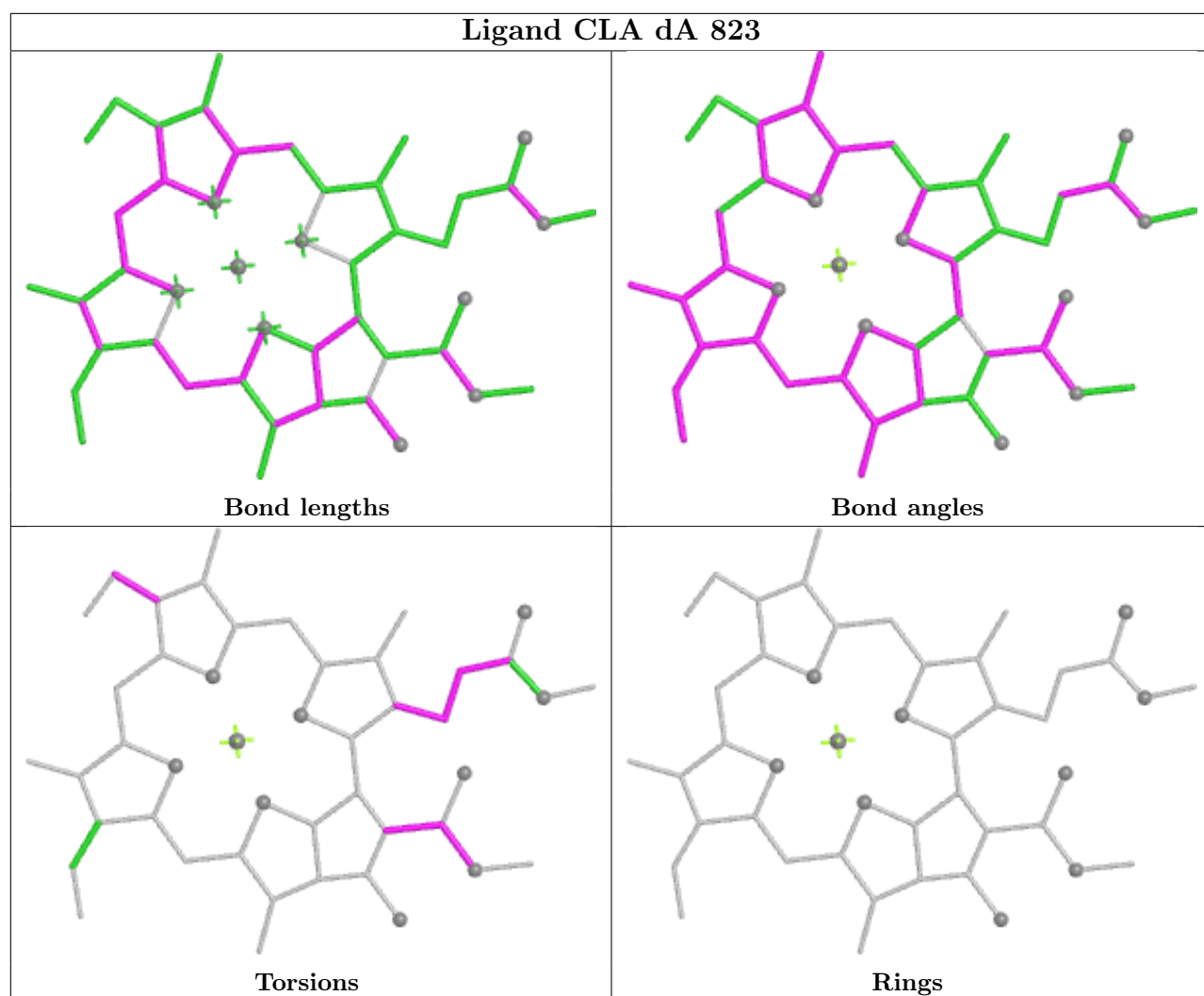


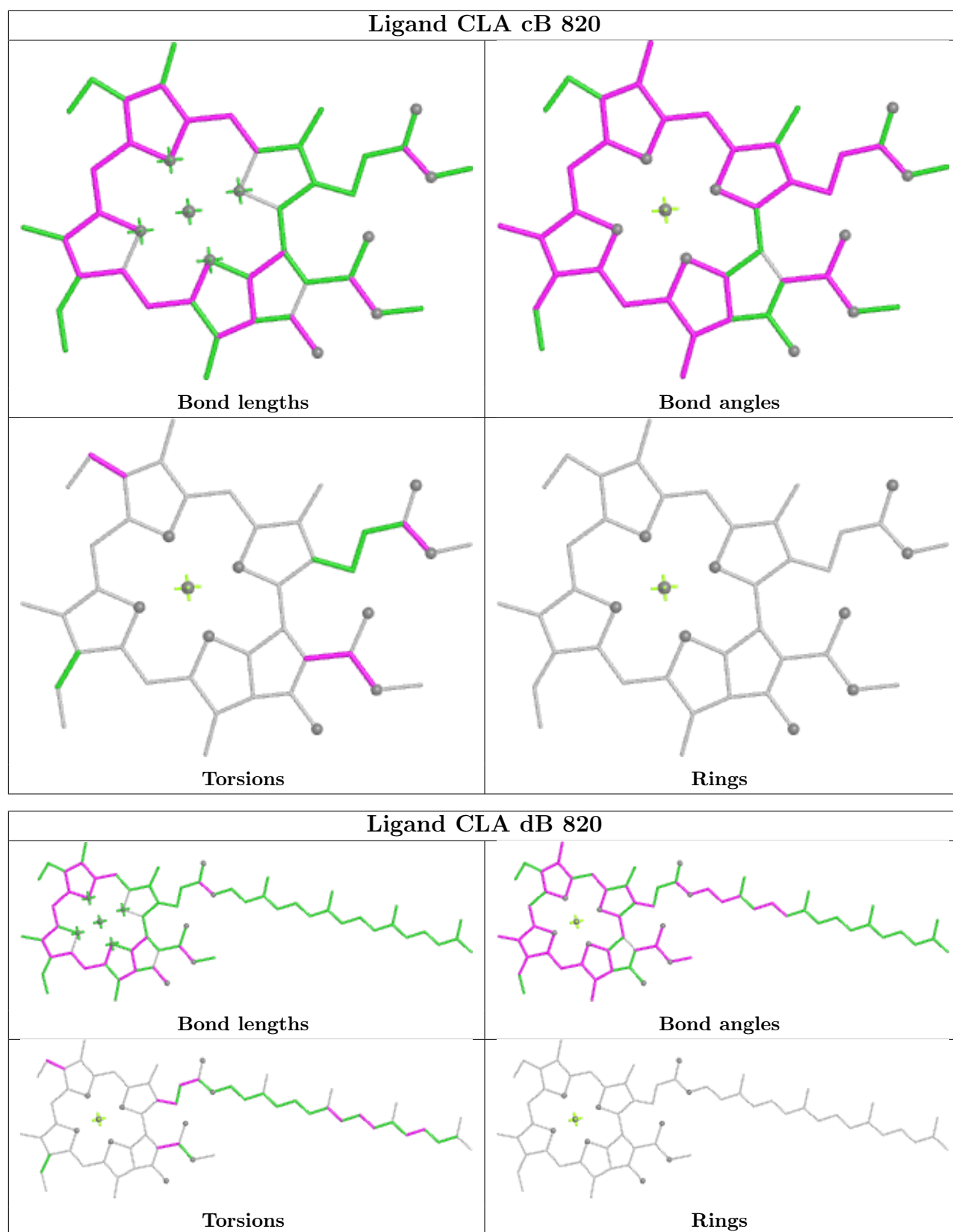


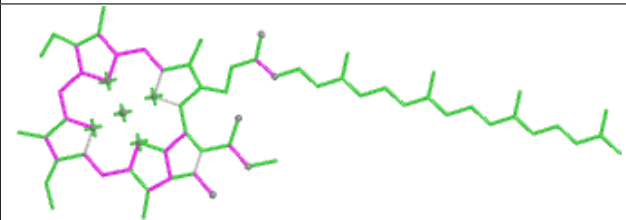
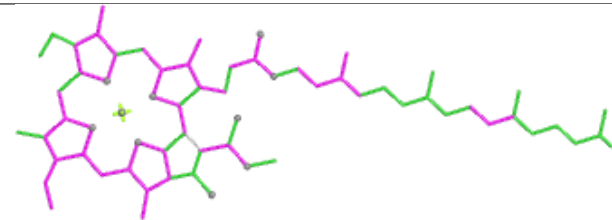
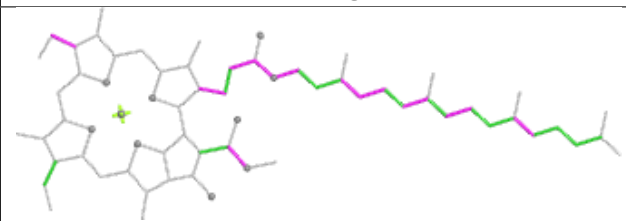
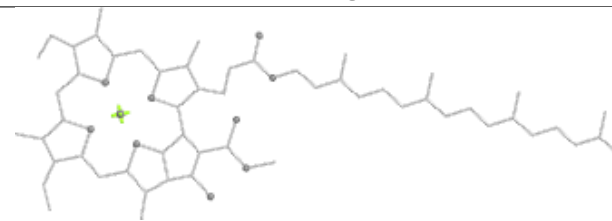


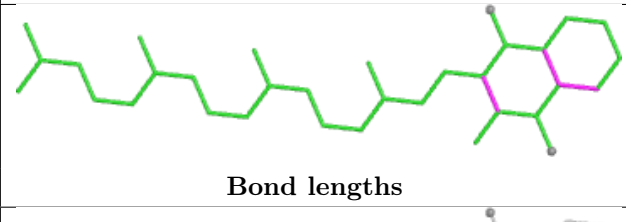
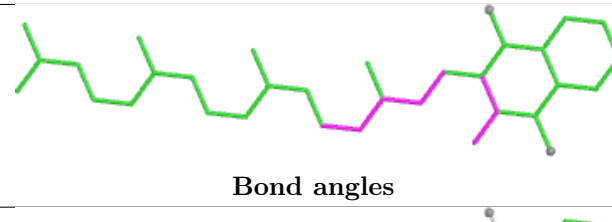
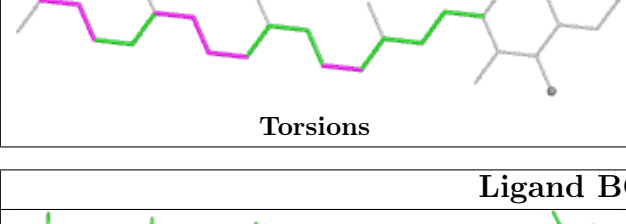


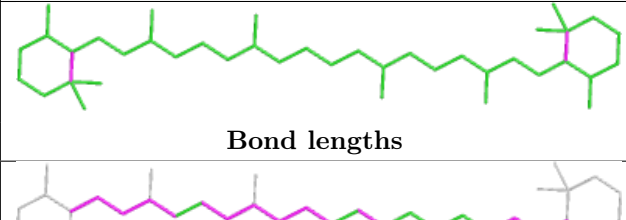
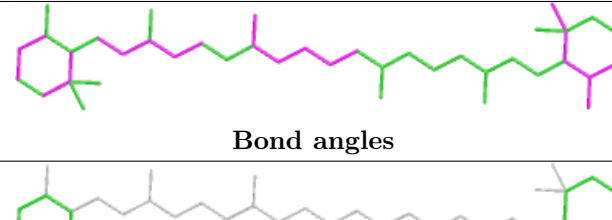


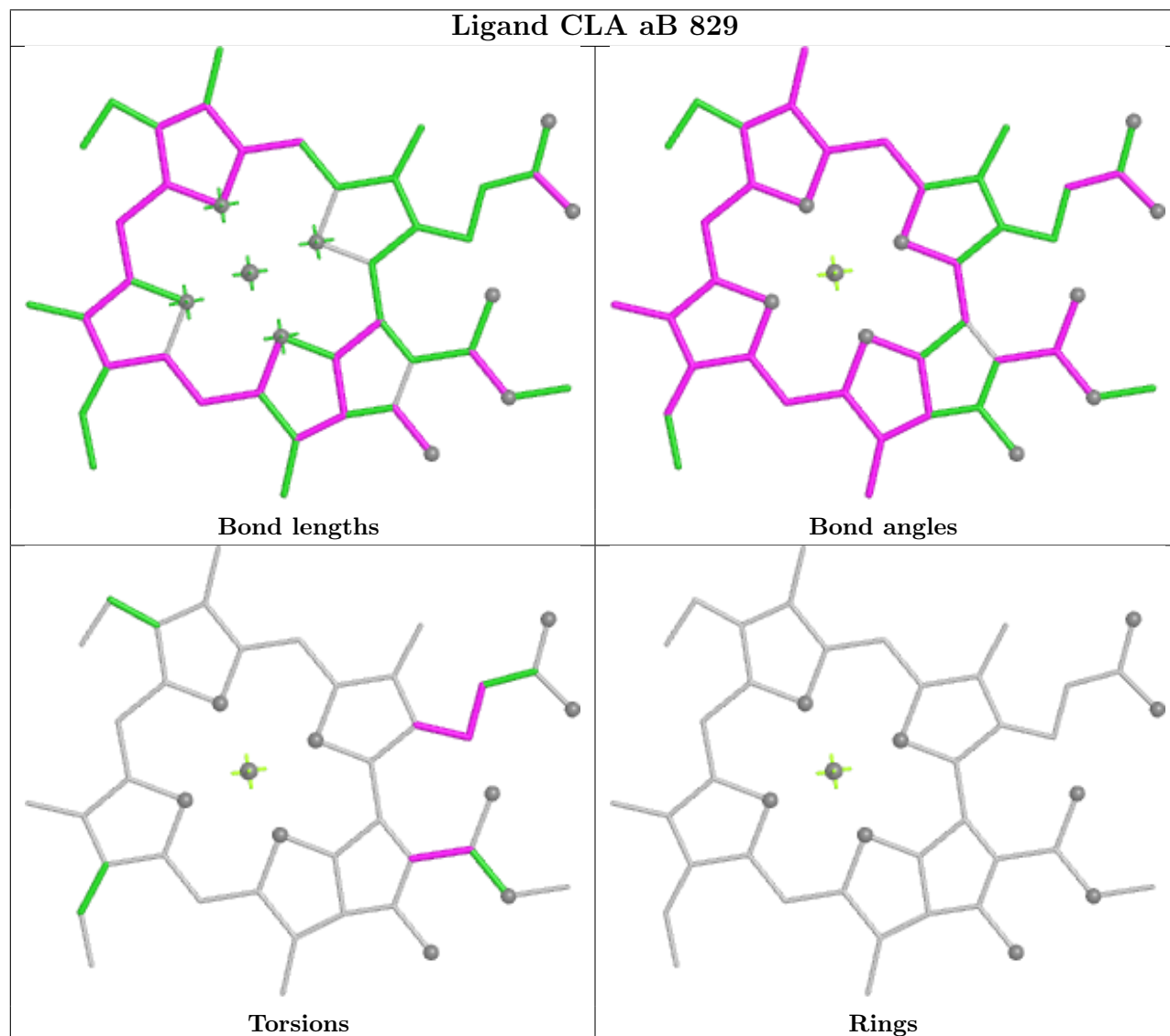
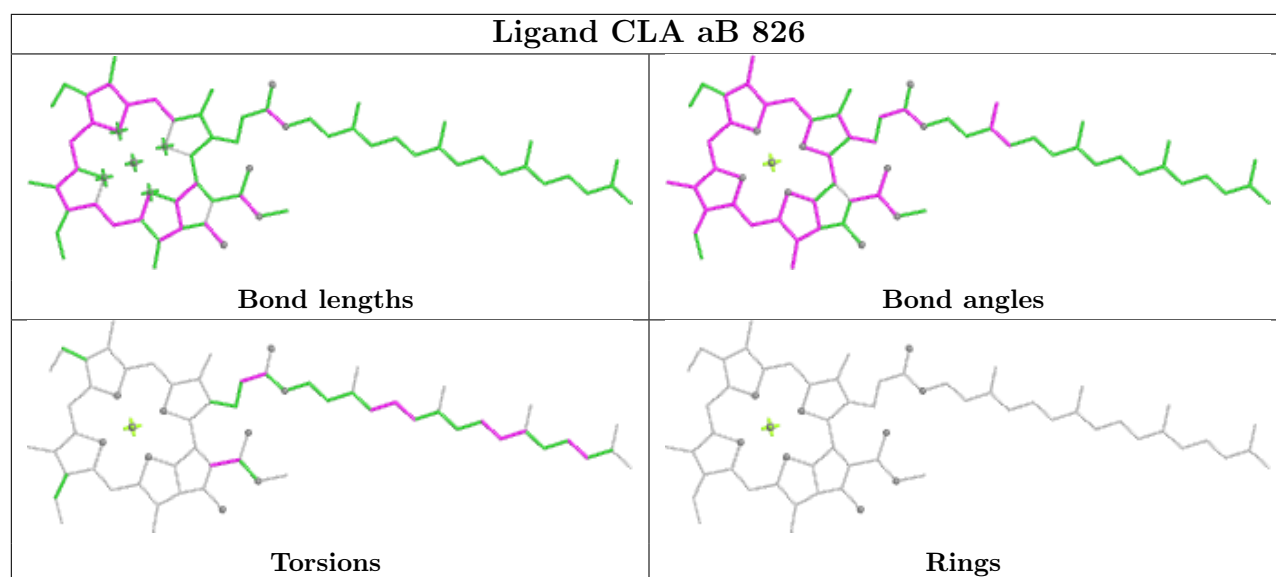


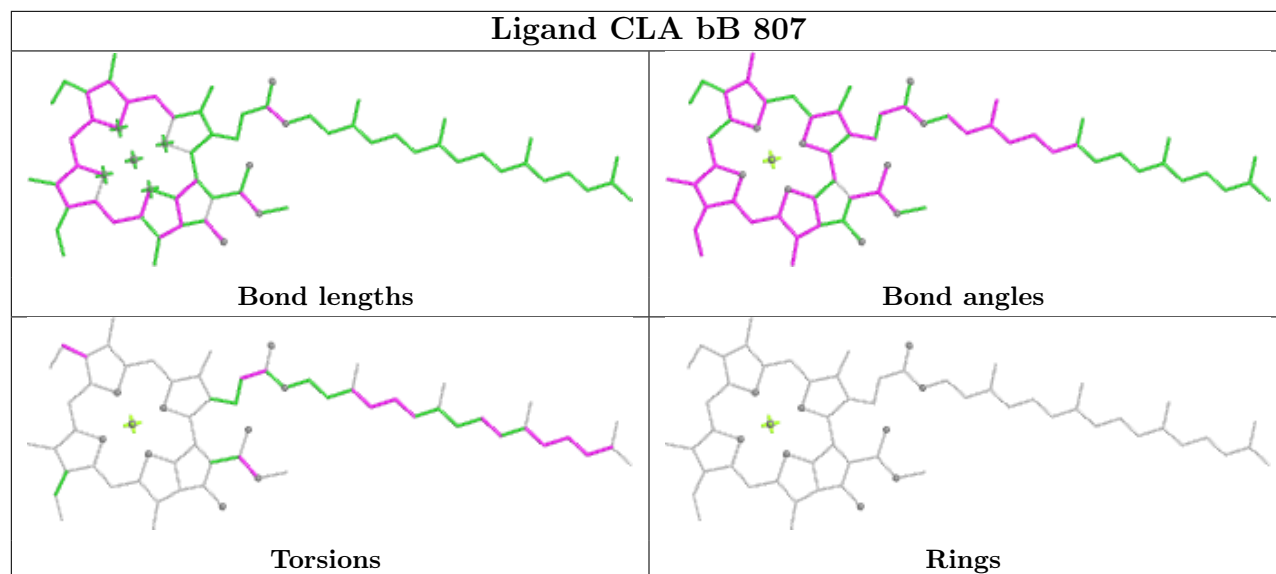
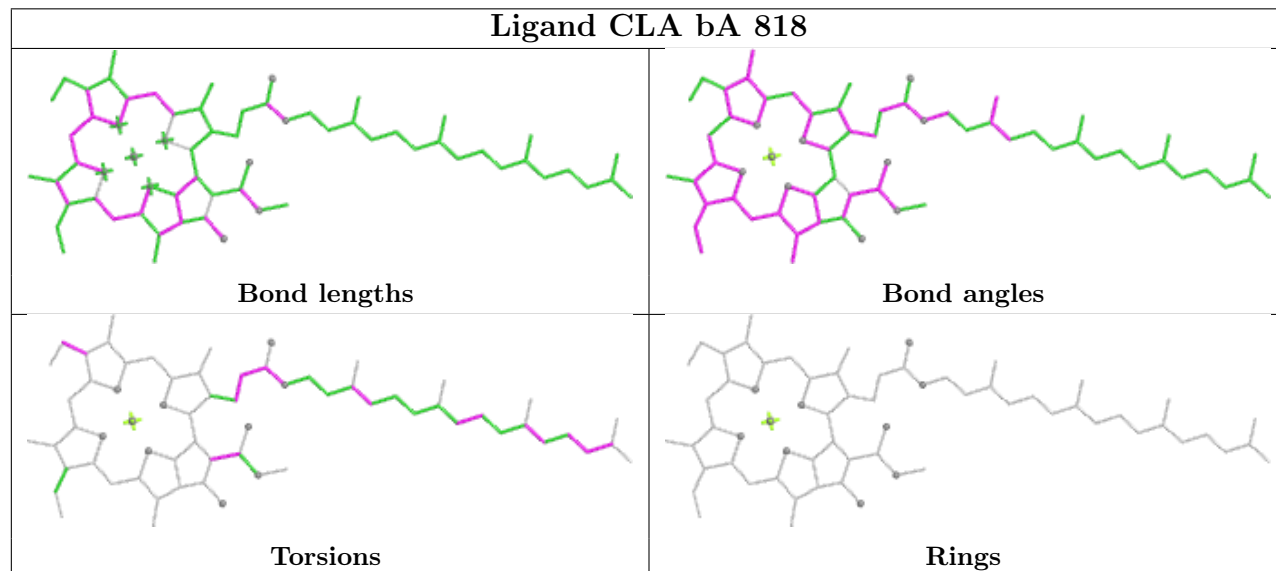


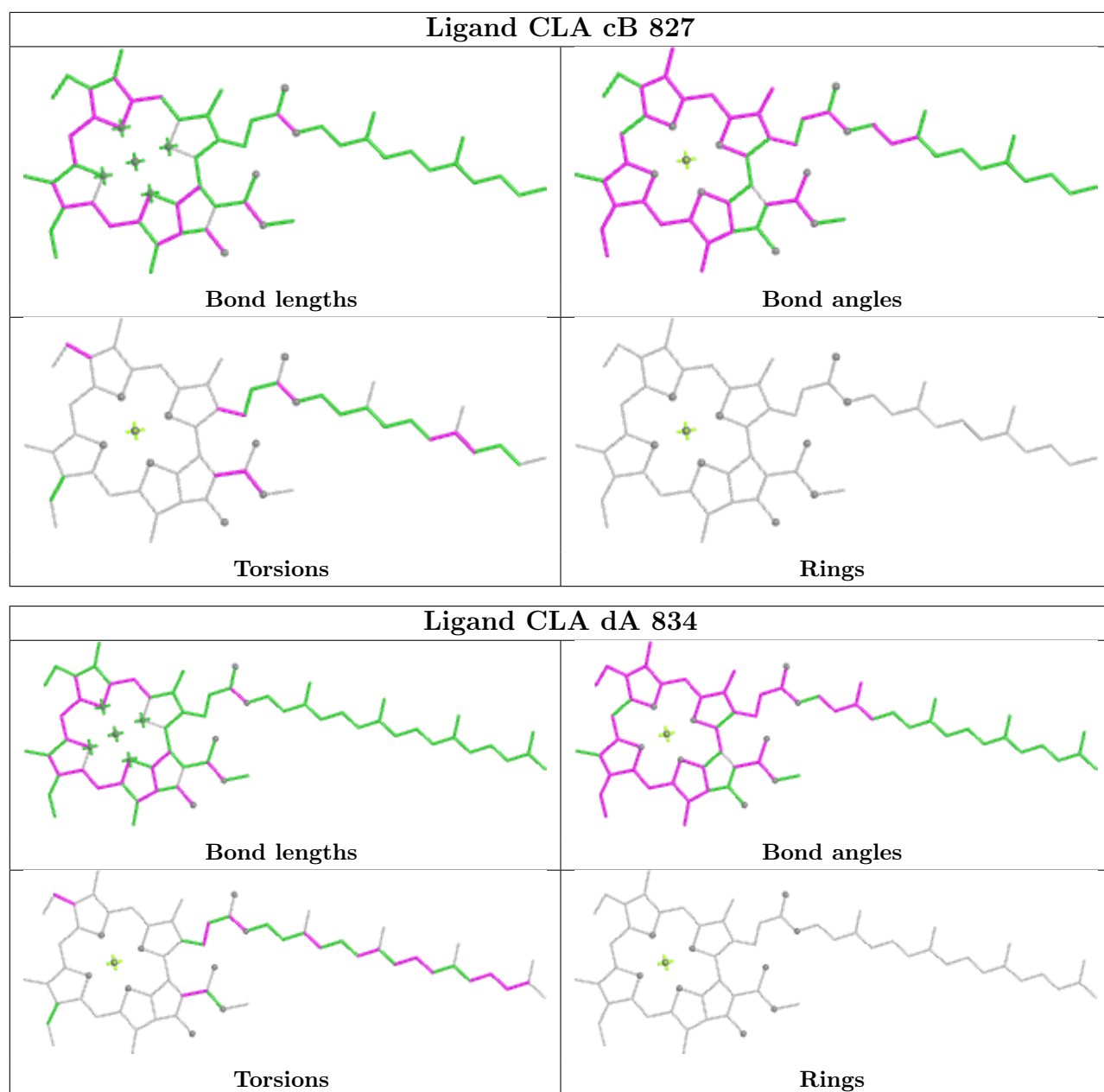
Ligand CLA aA 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

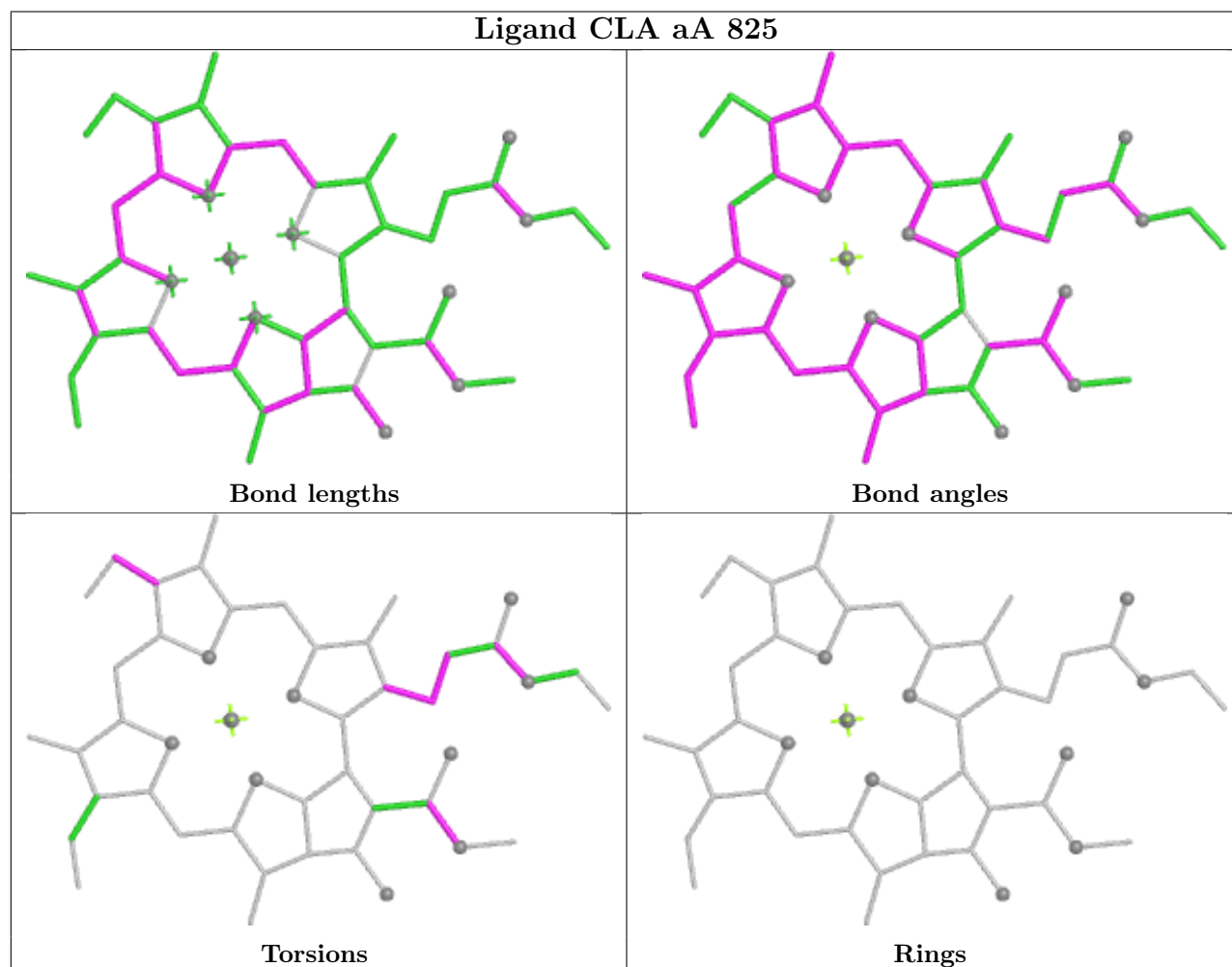
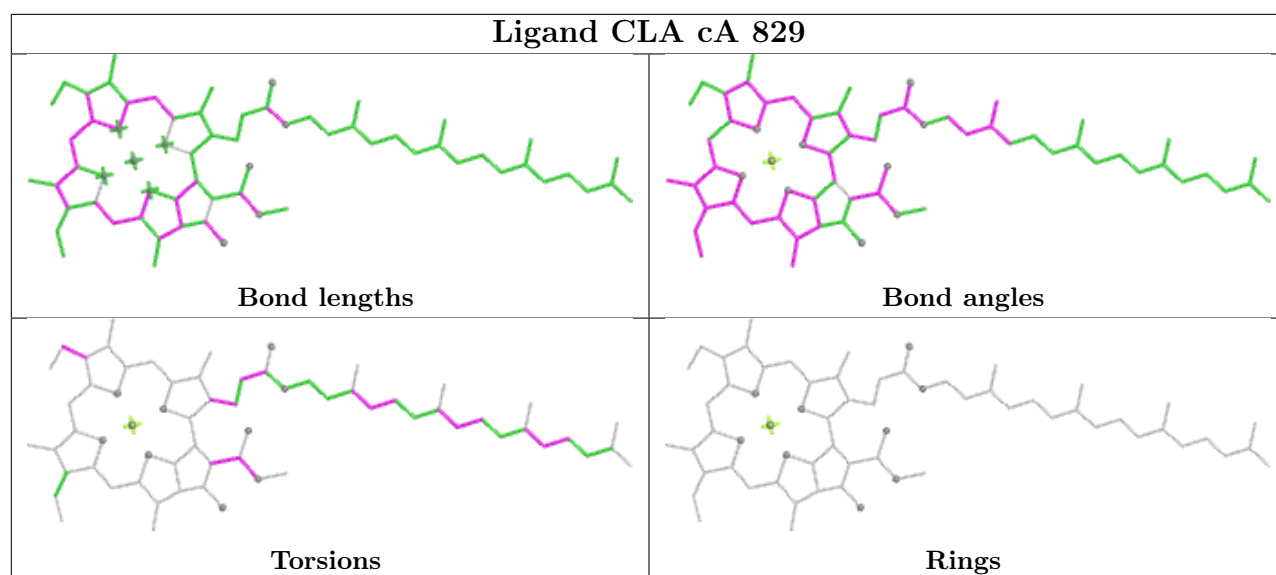
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Bond lengths	Bond angles
	
Torsions	Rings

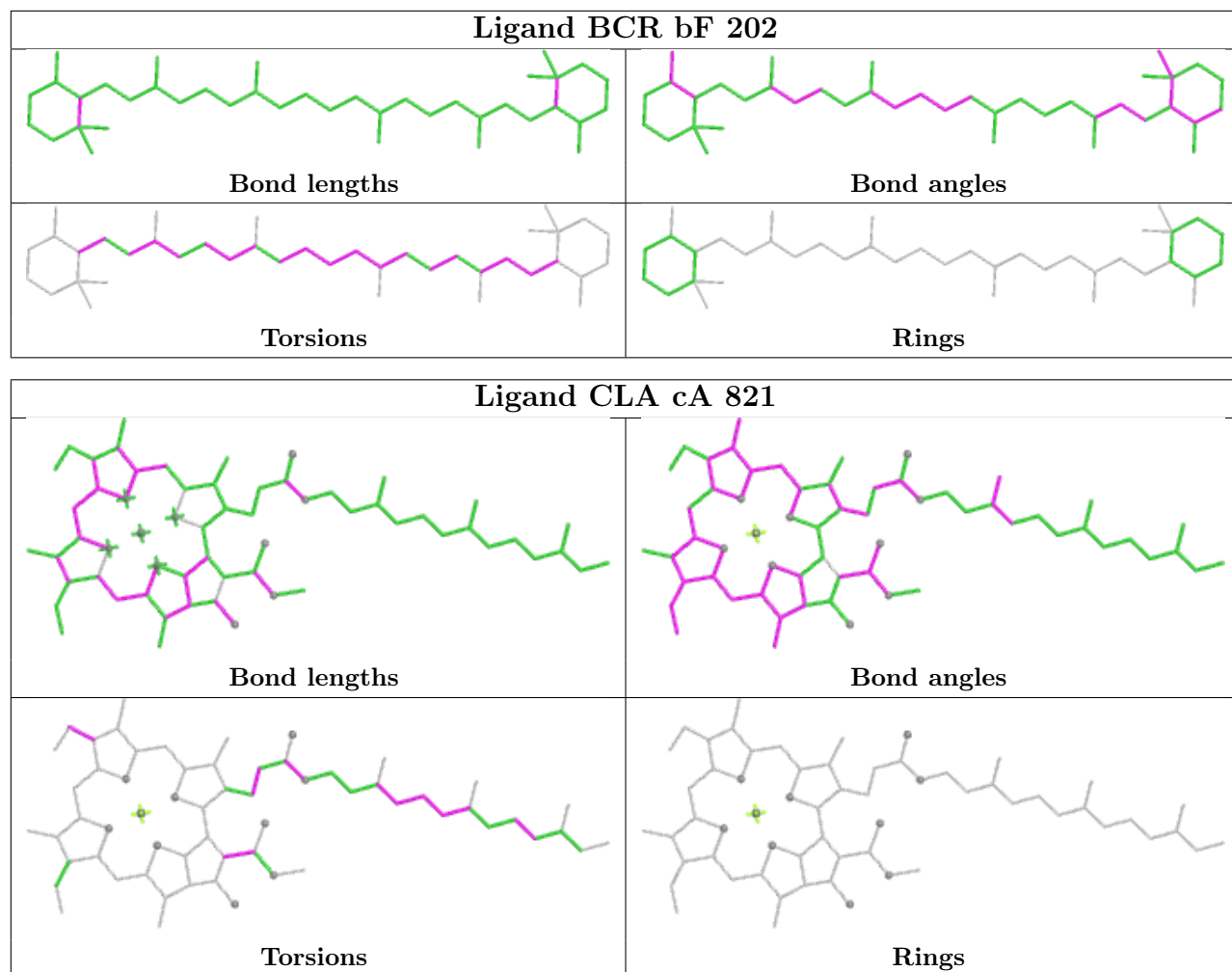
Ligand BCR aA 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

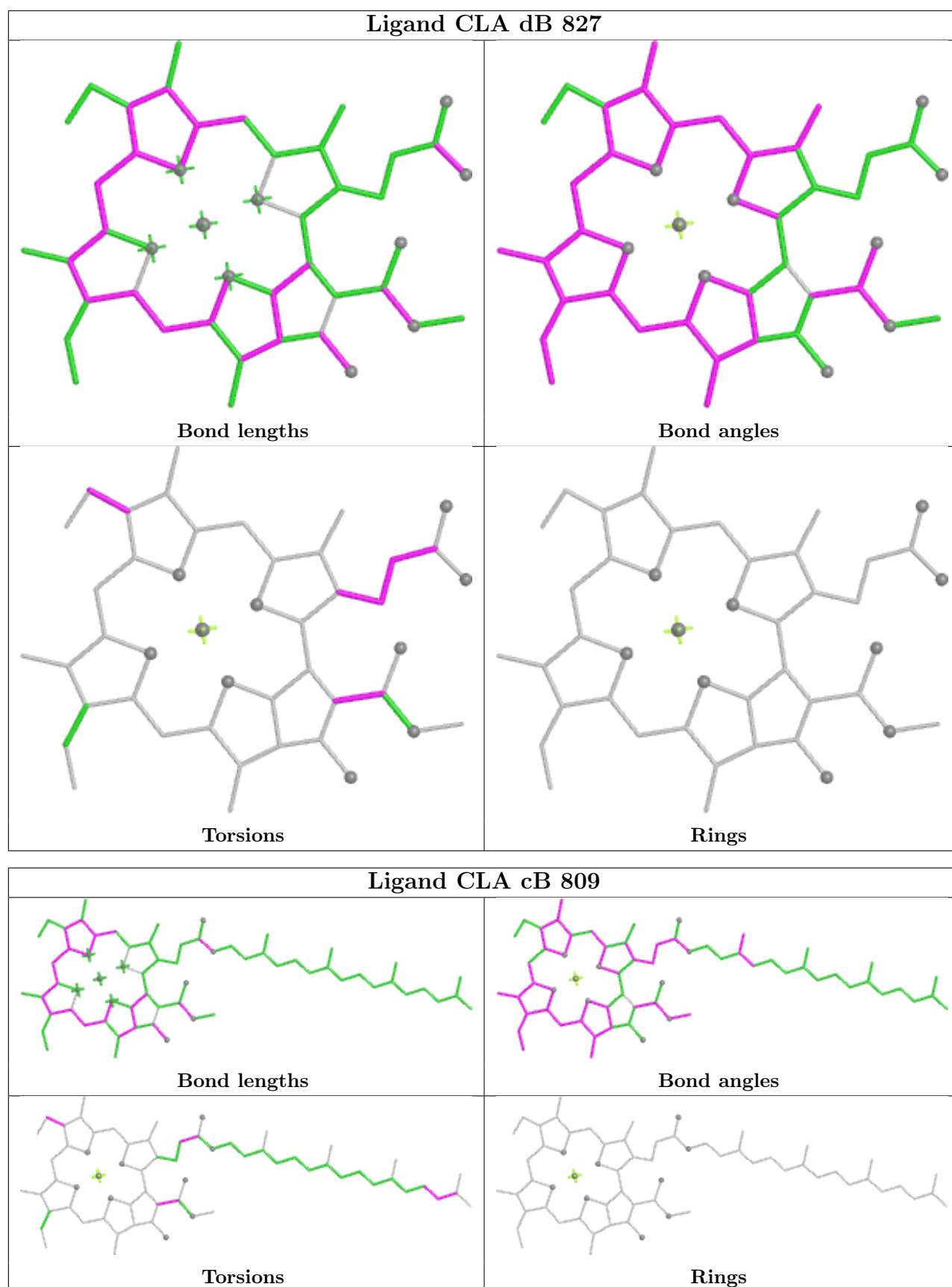


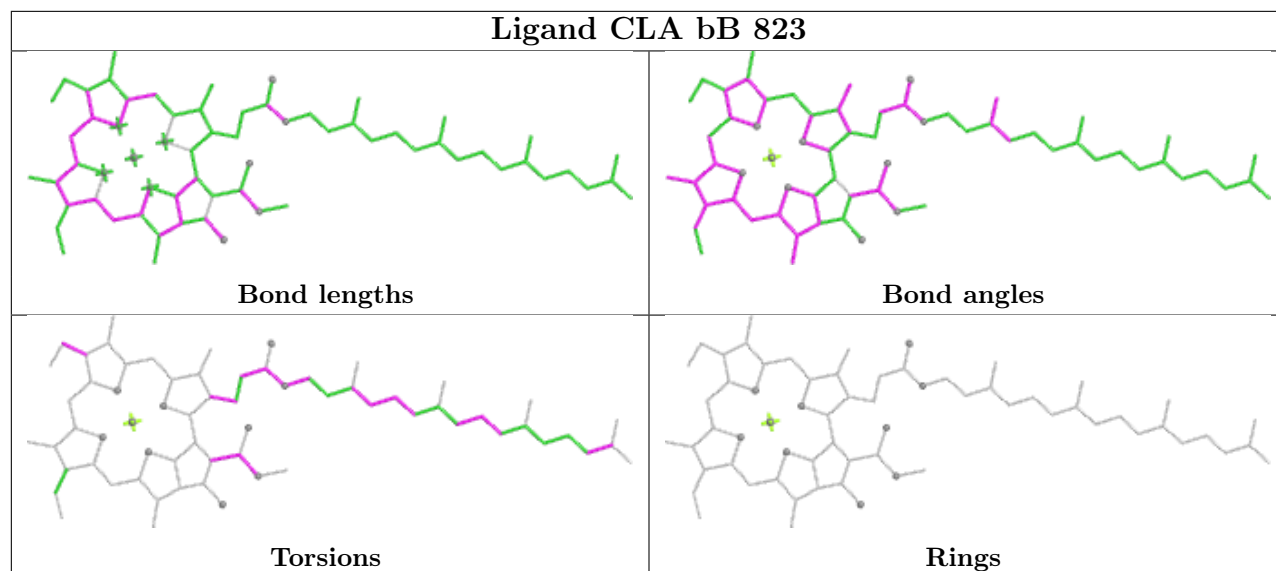
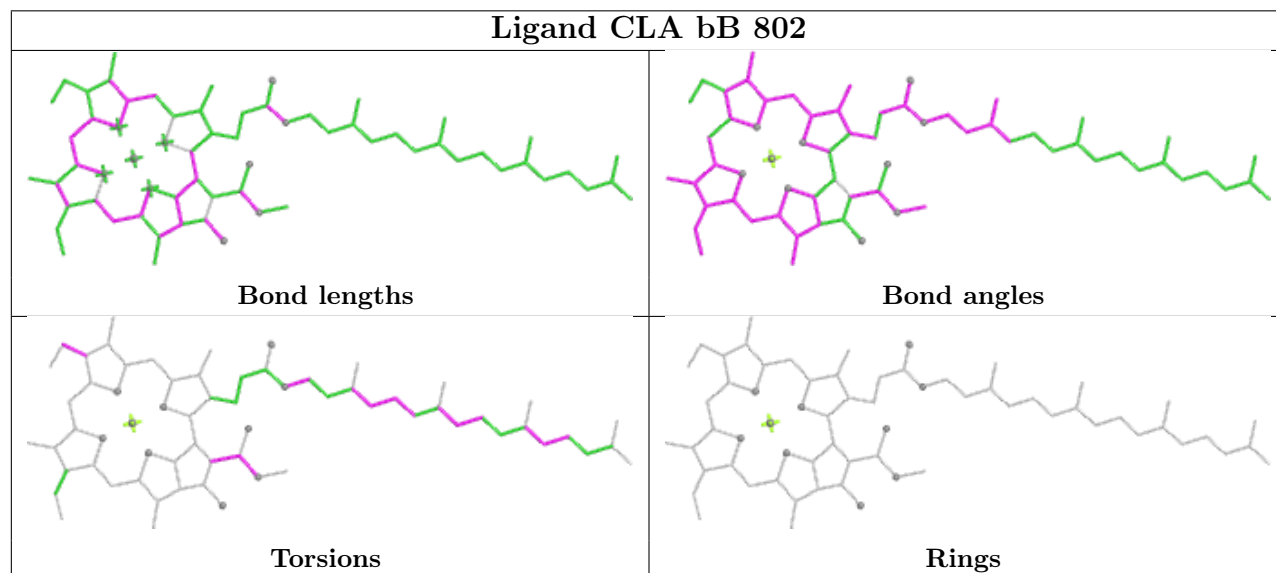
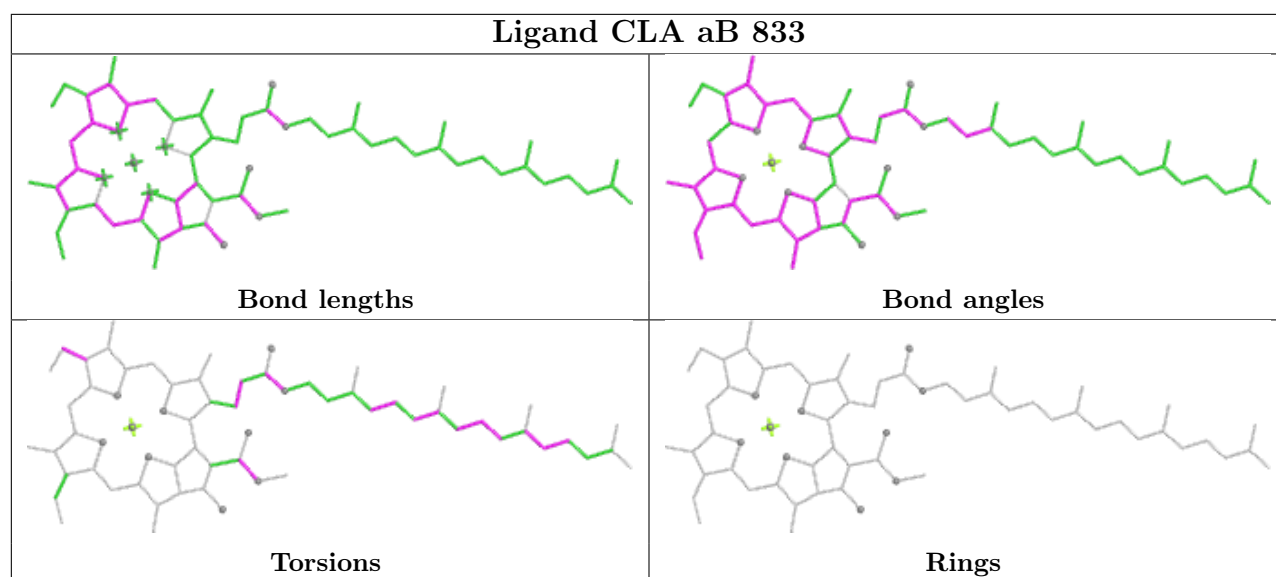
Ligand CLA bB 807**Ligand CLA bA 818**

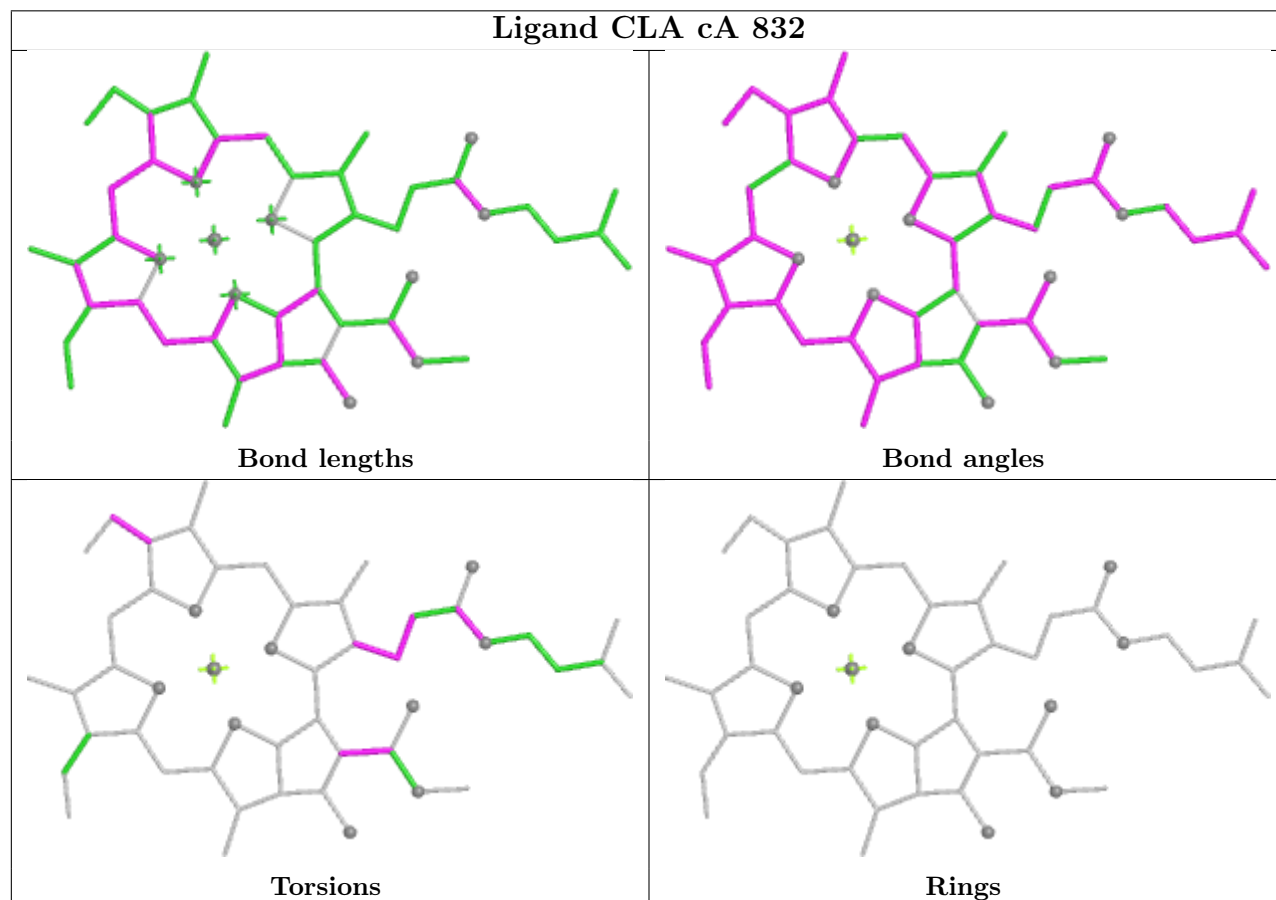
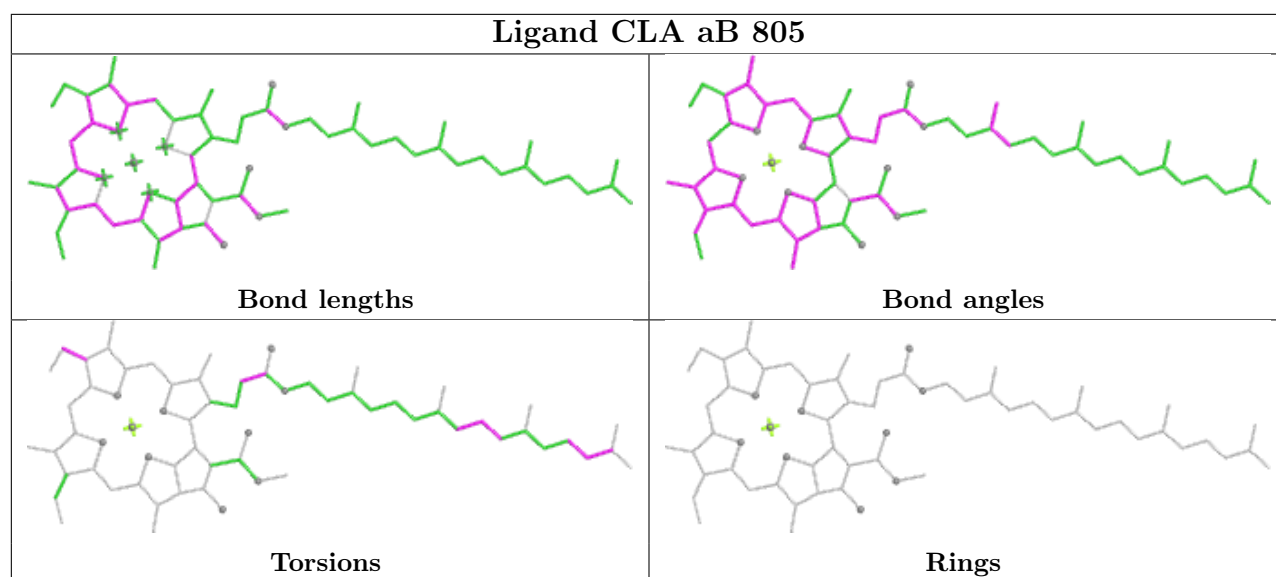


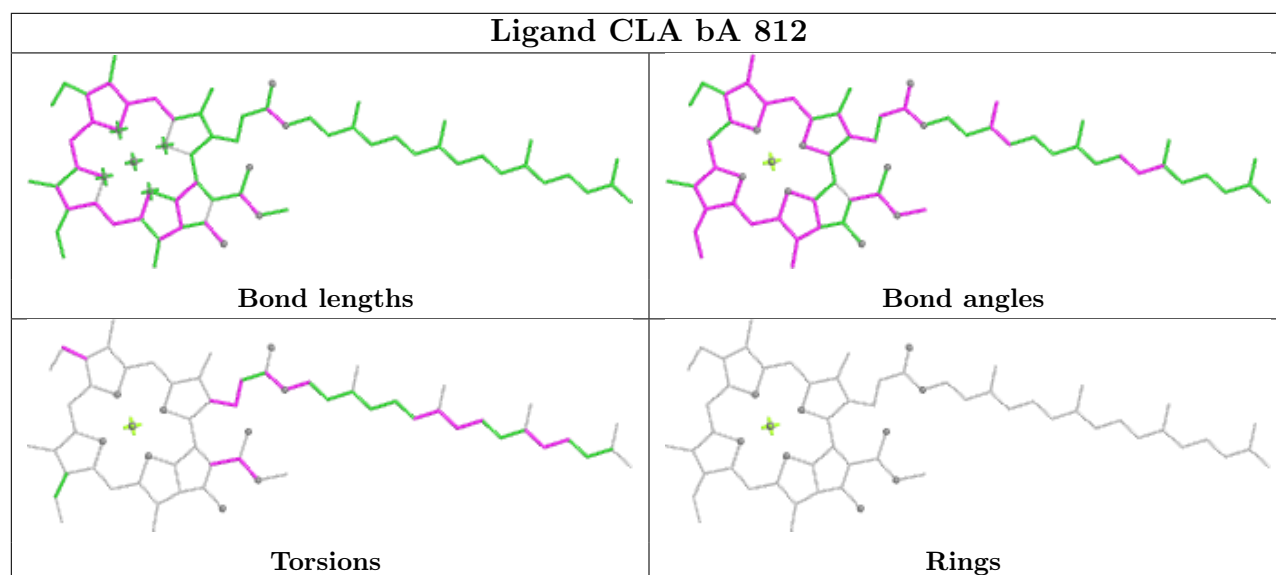
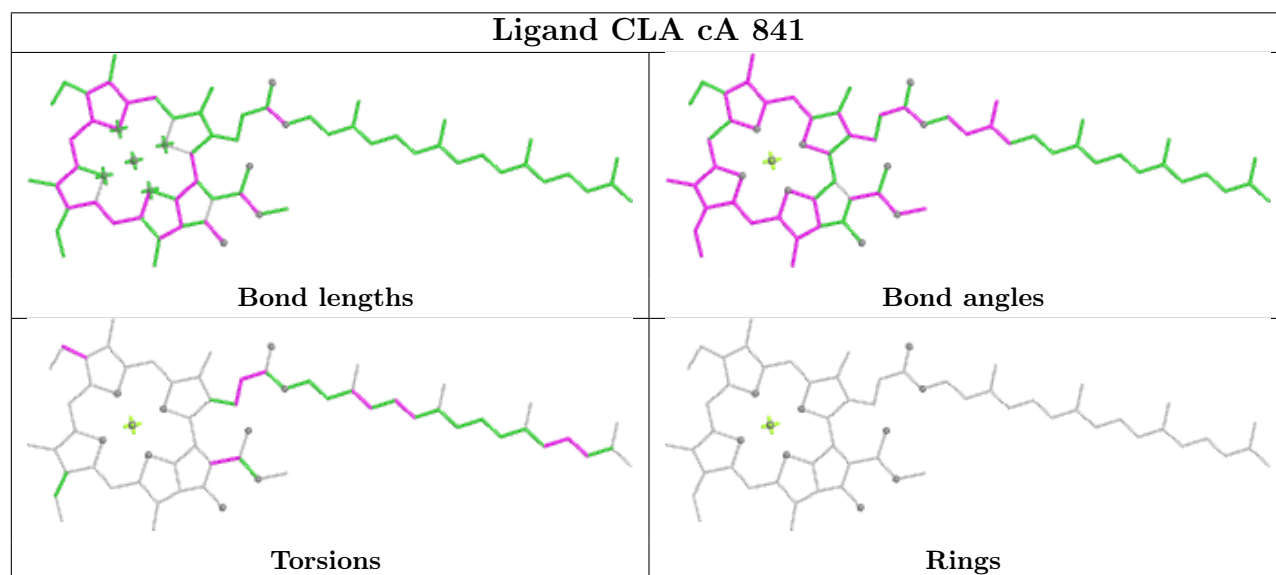
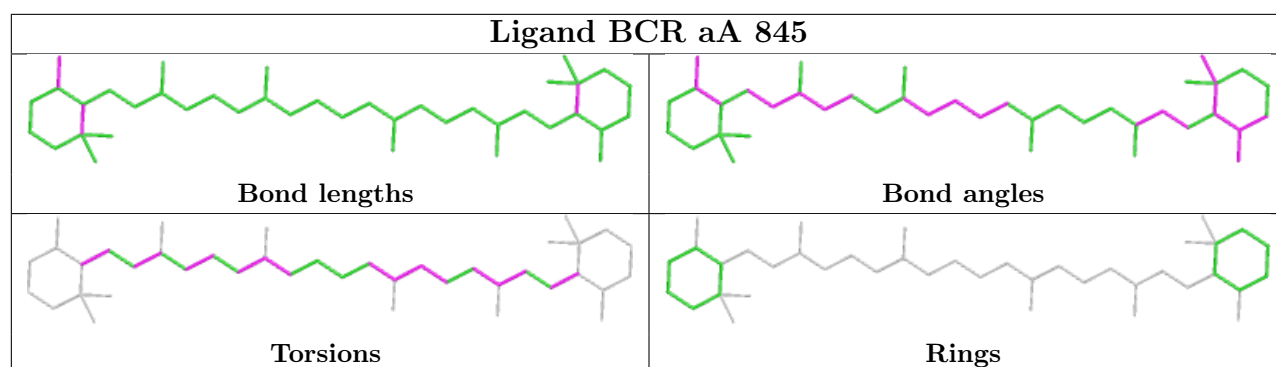


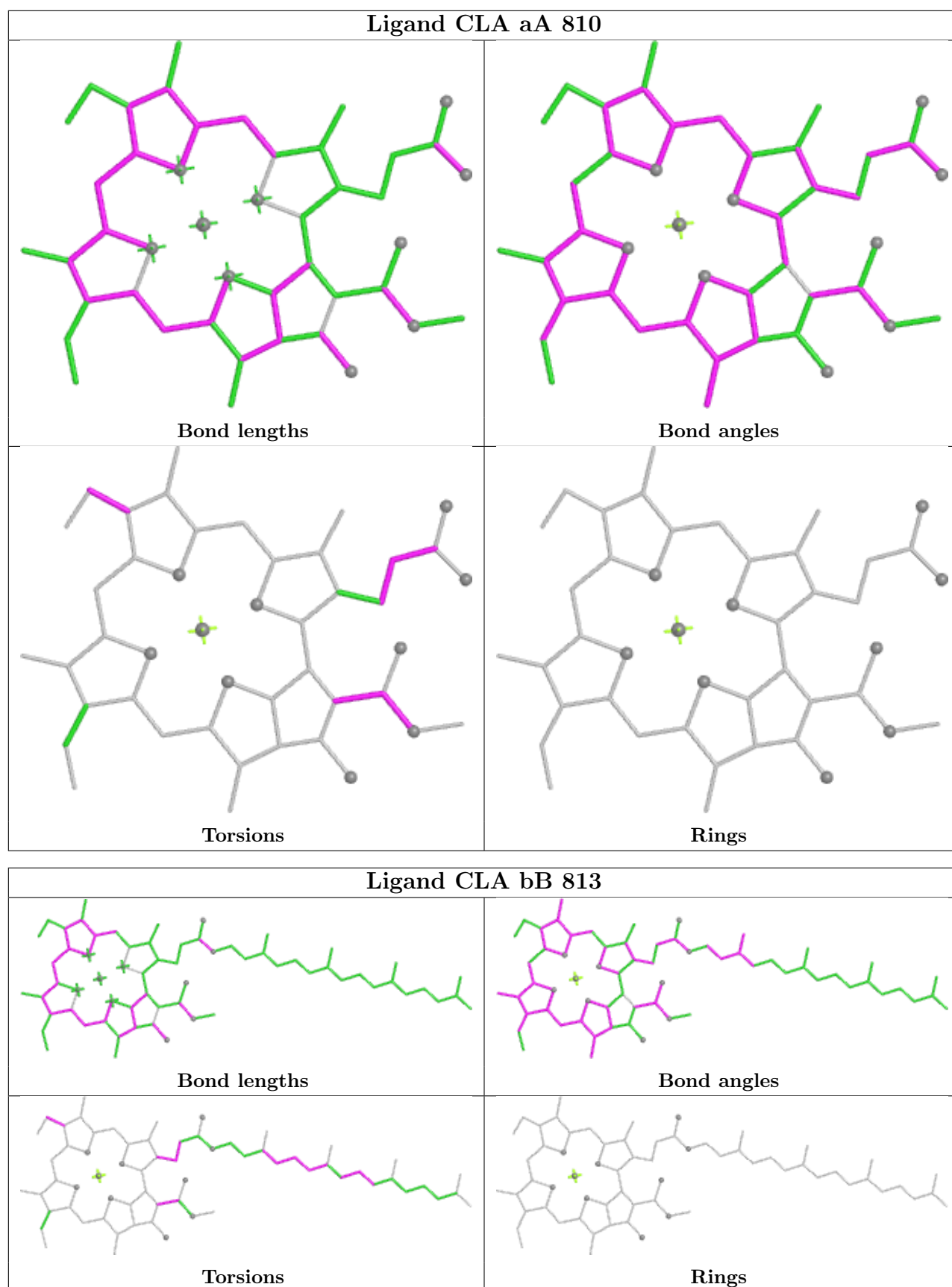


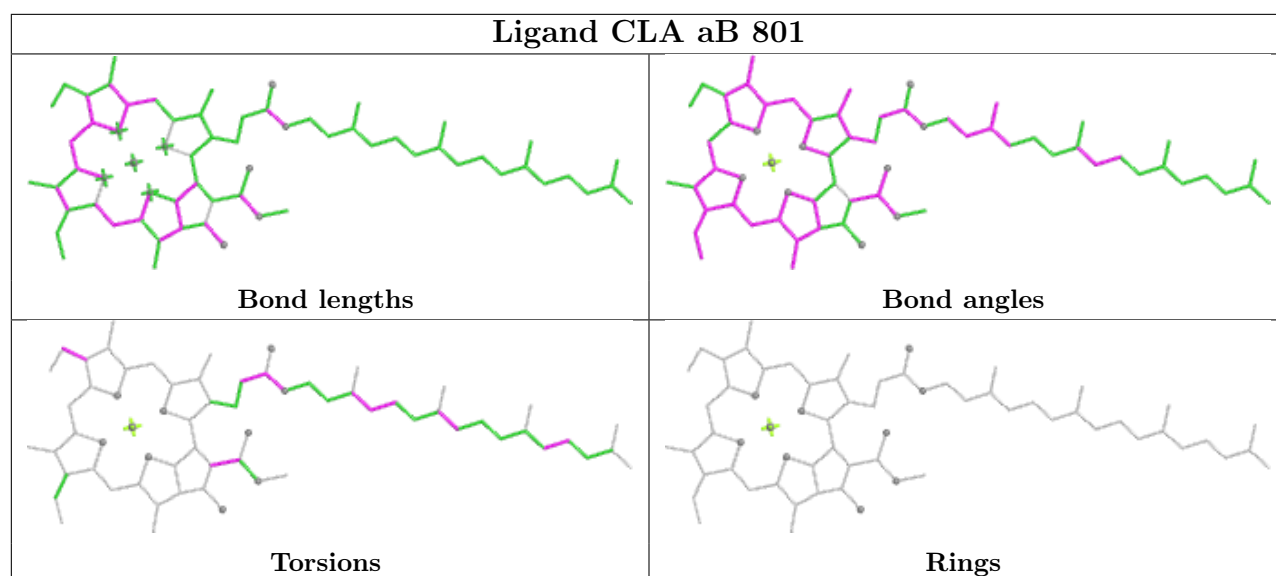
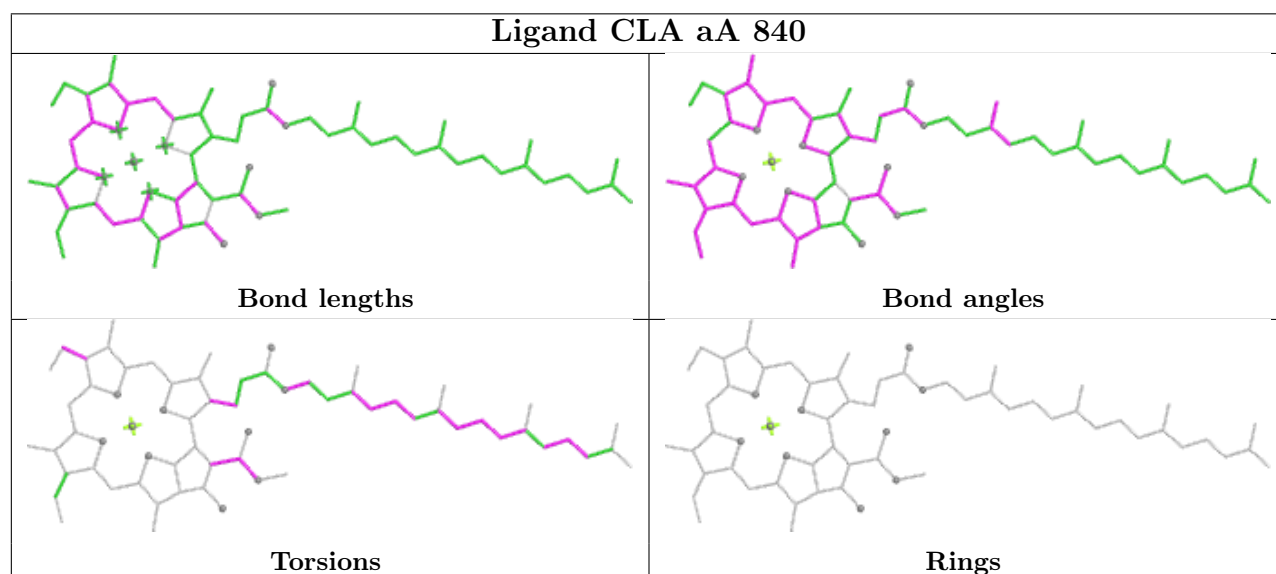
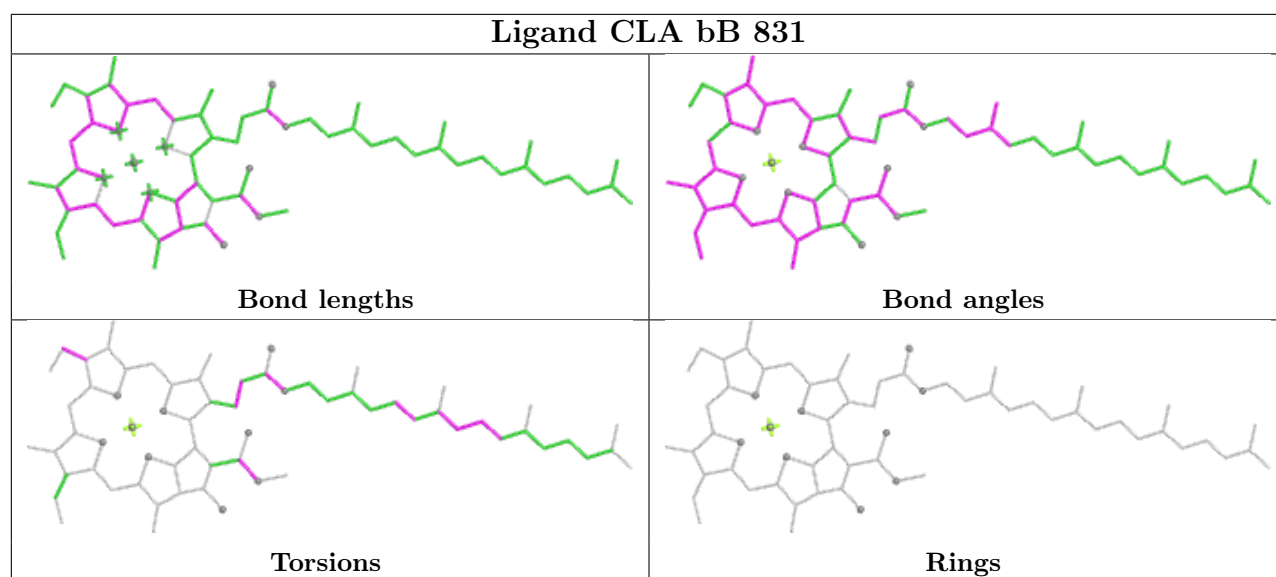


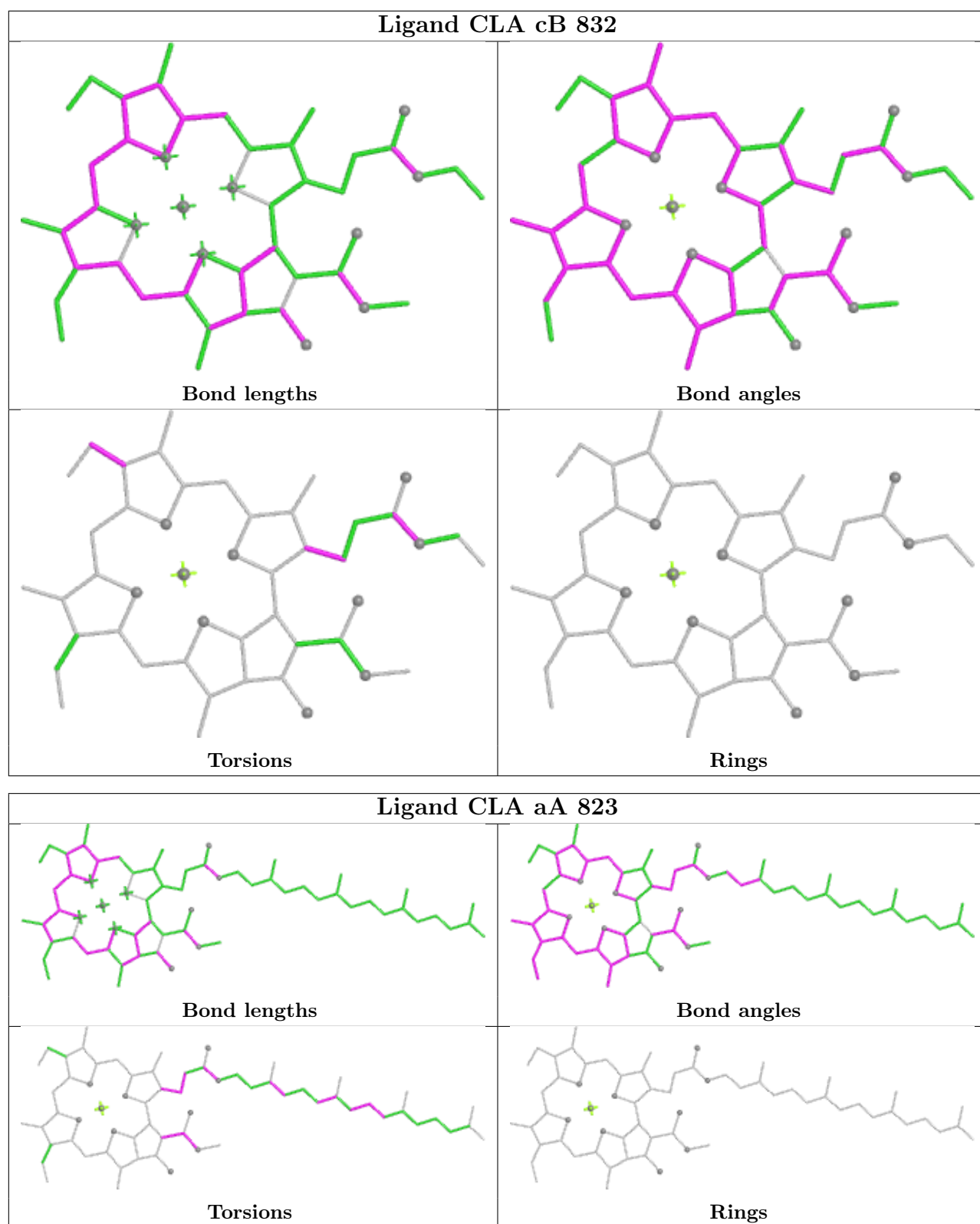


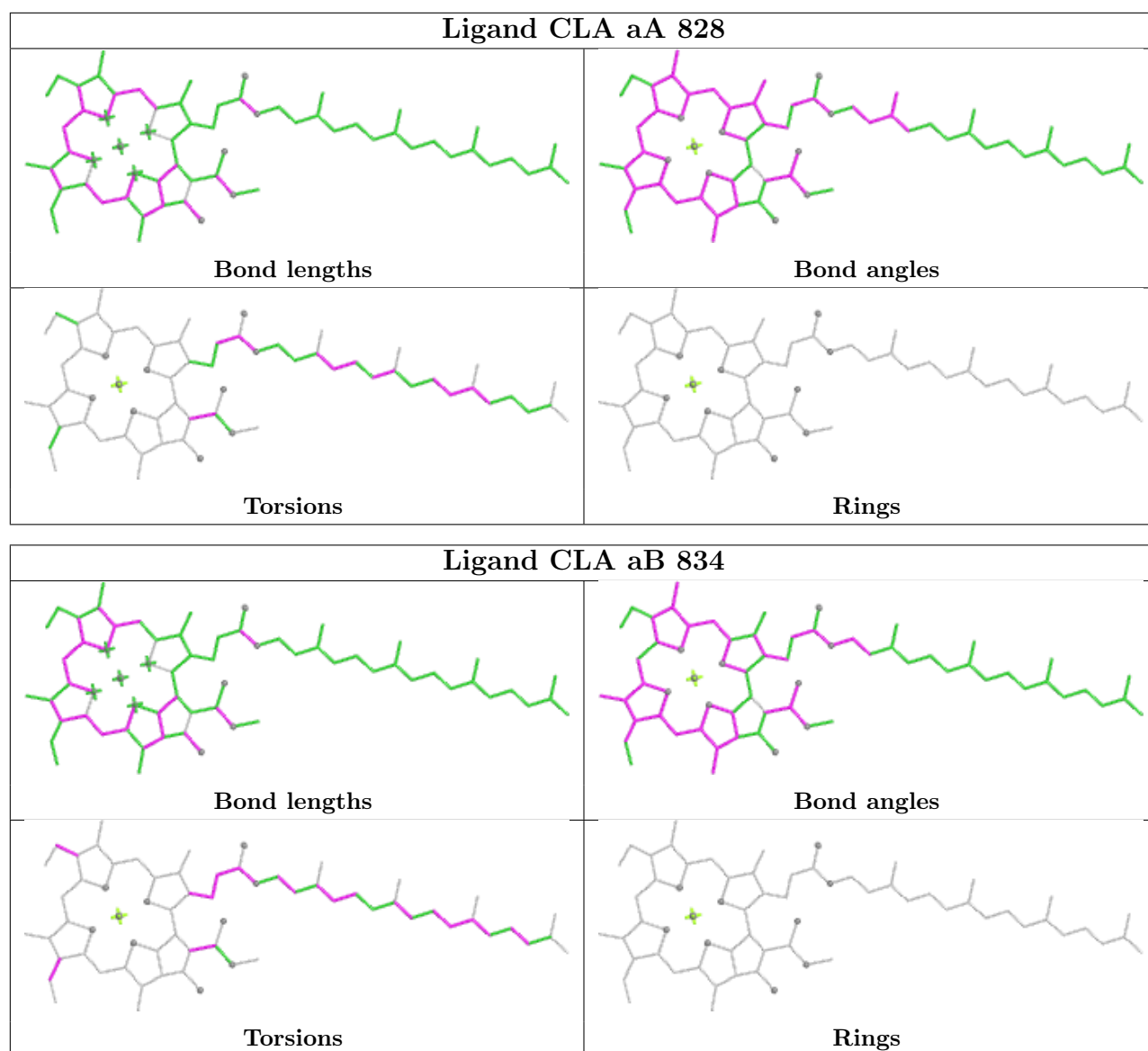


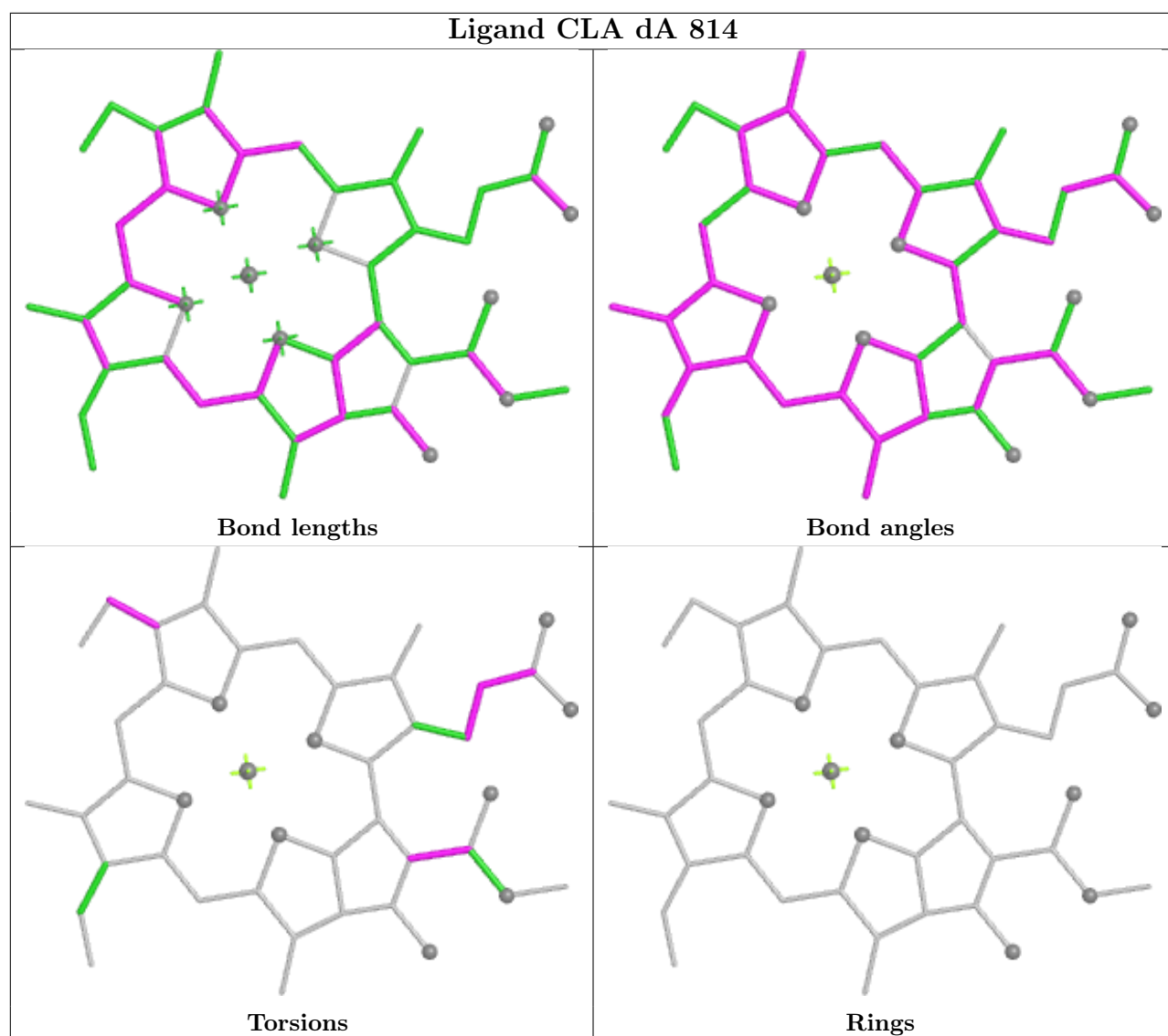




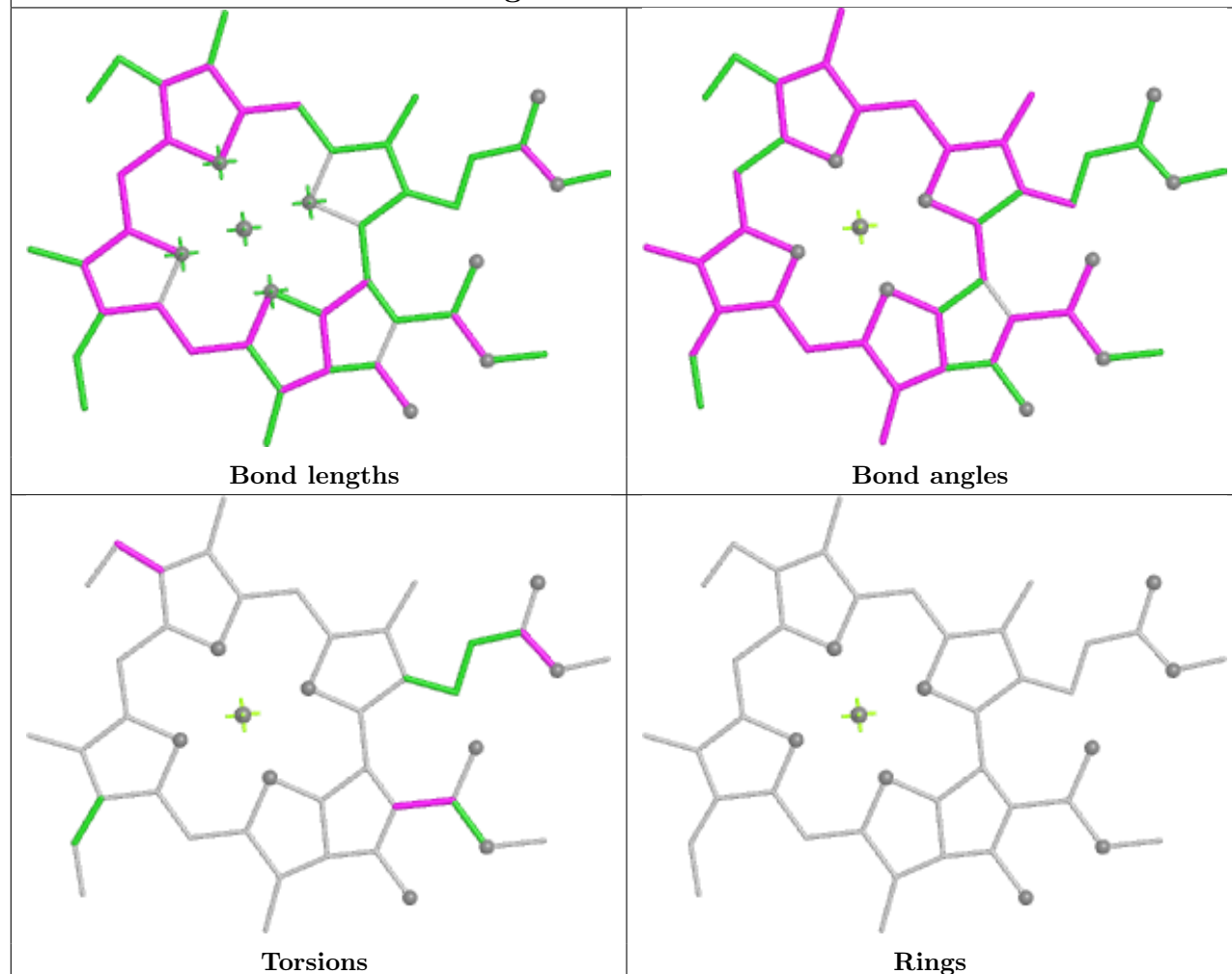




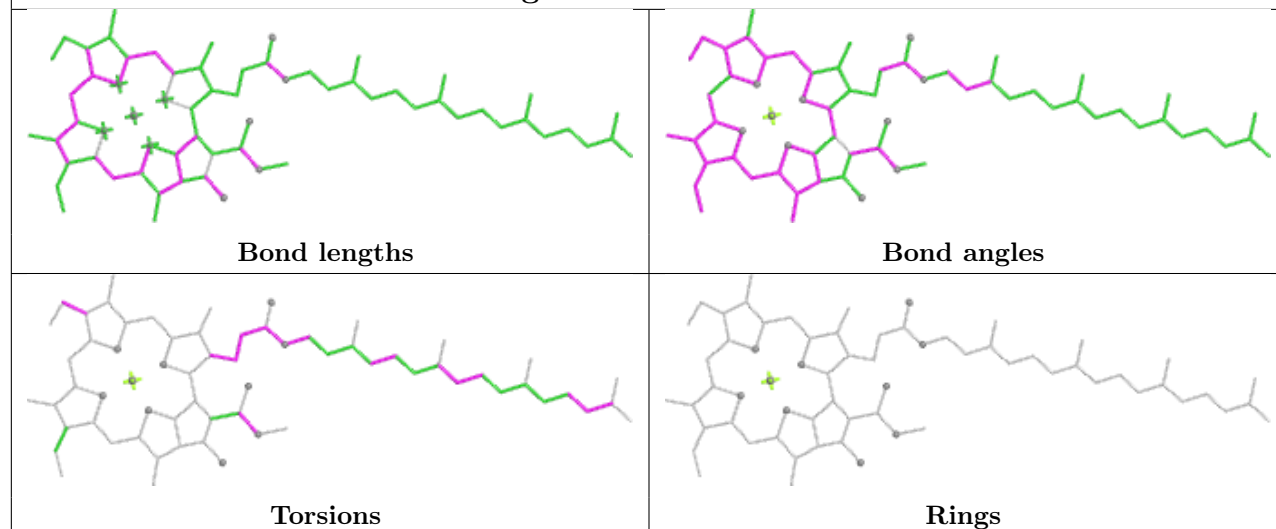




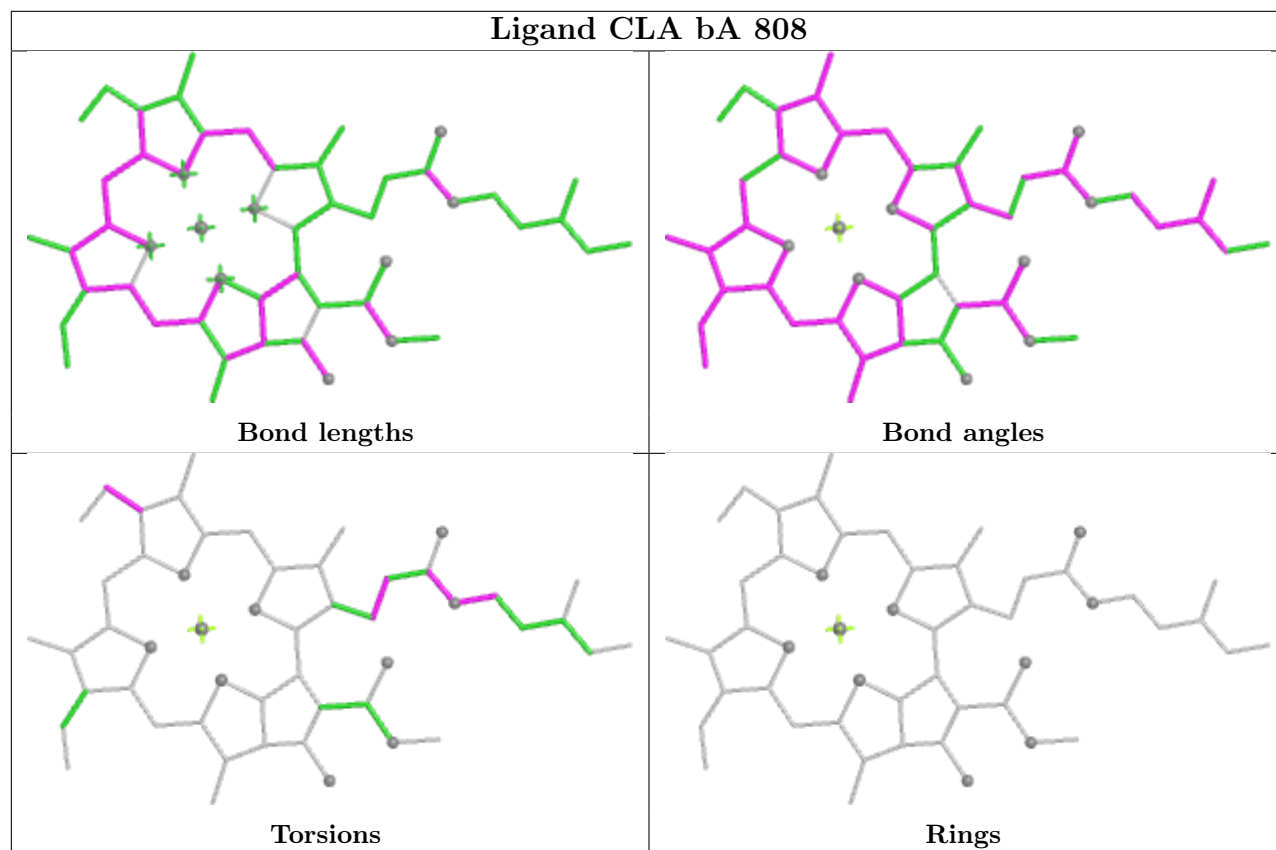
Ligand CLA bB 828



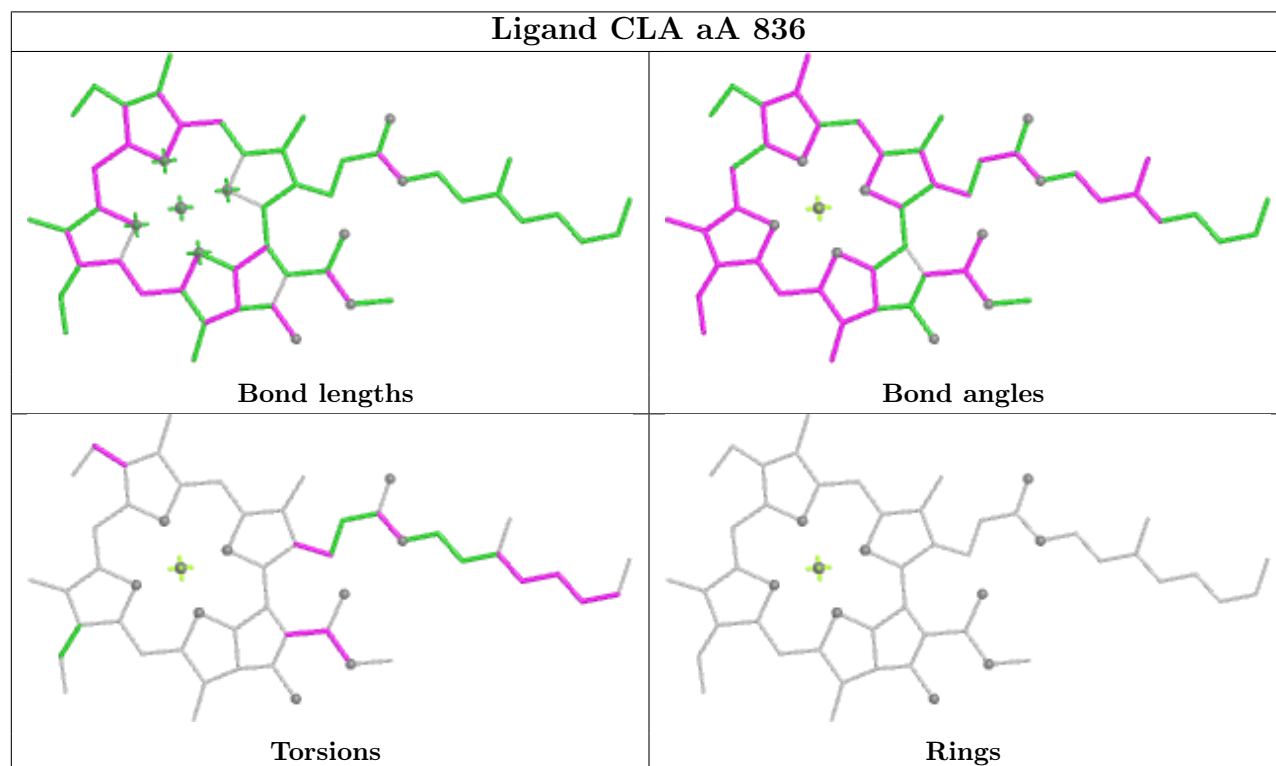
Ligand CLA dA 841

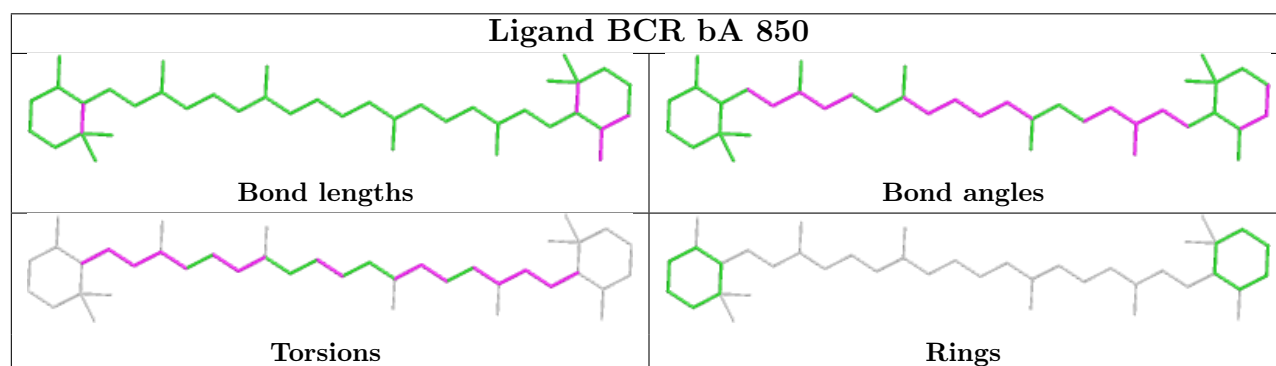
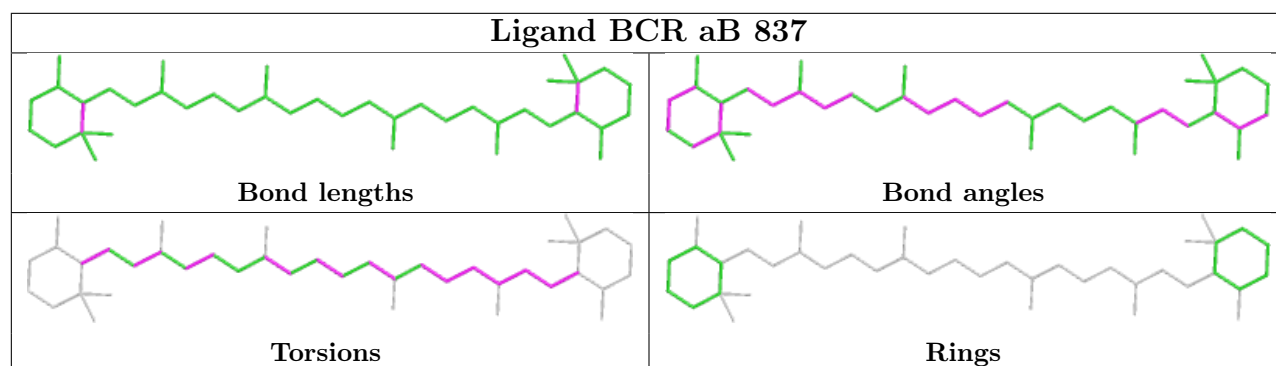
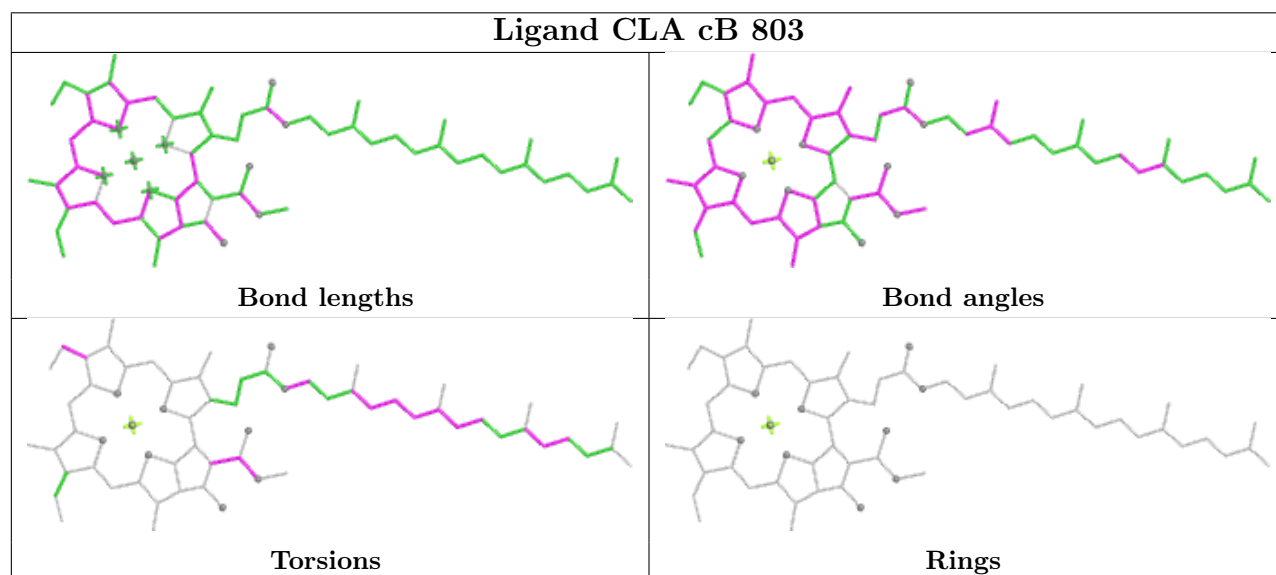
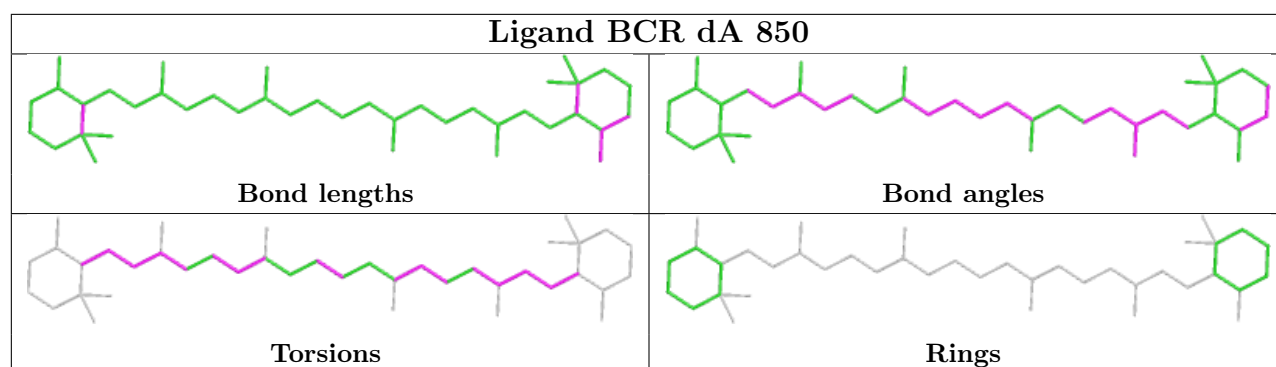


Ligand CLA bA 808

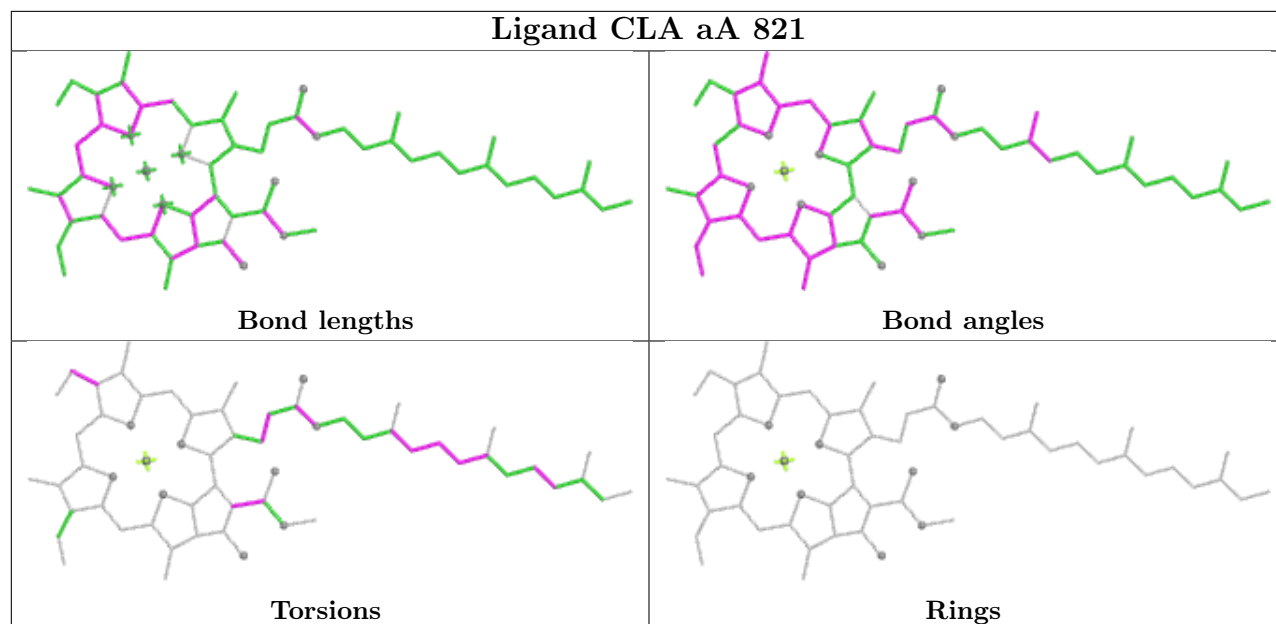


Ligand CLA aA 836

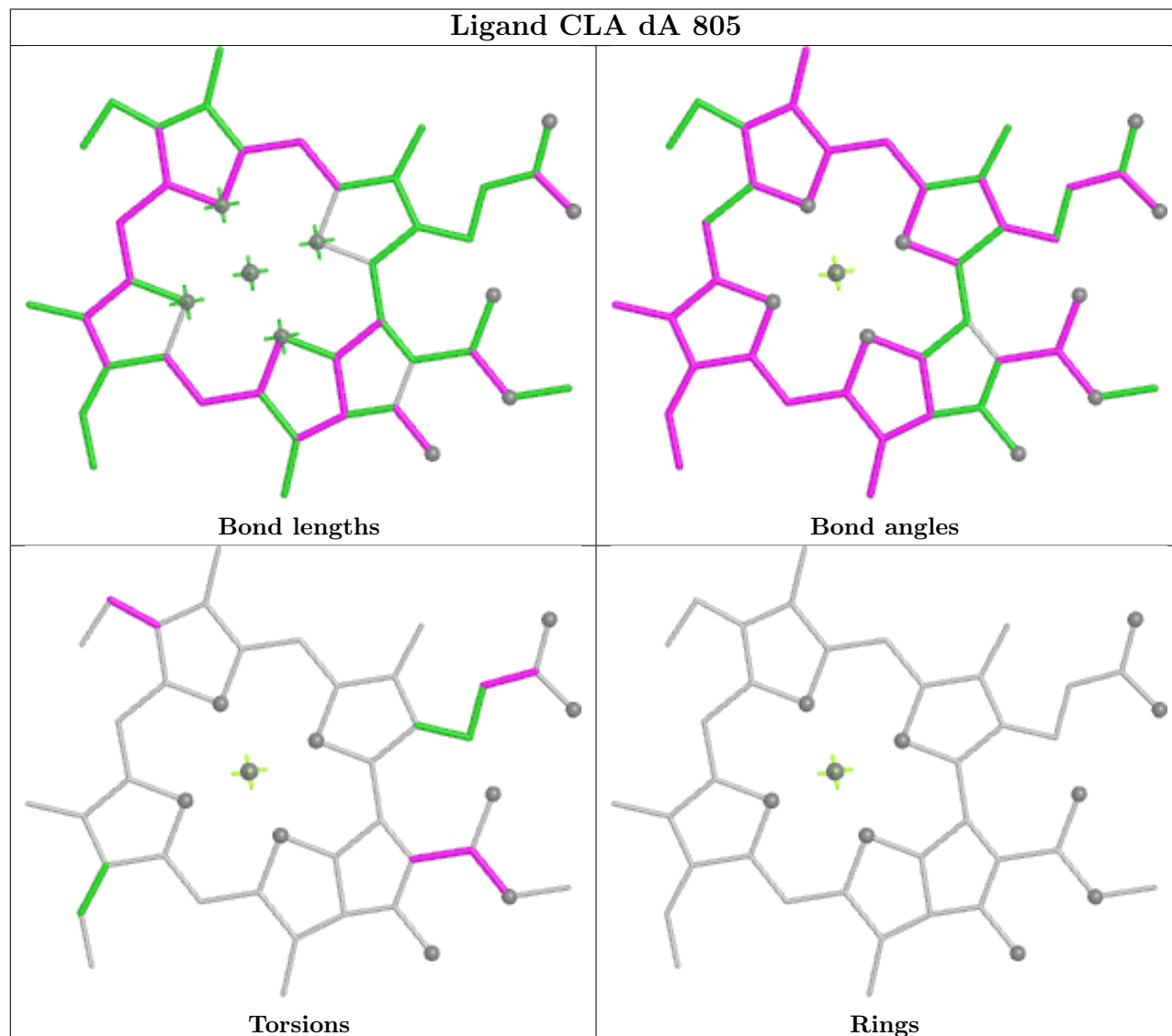


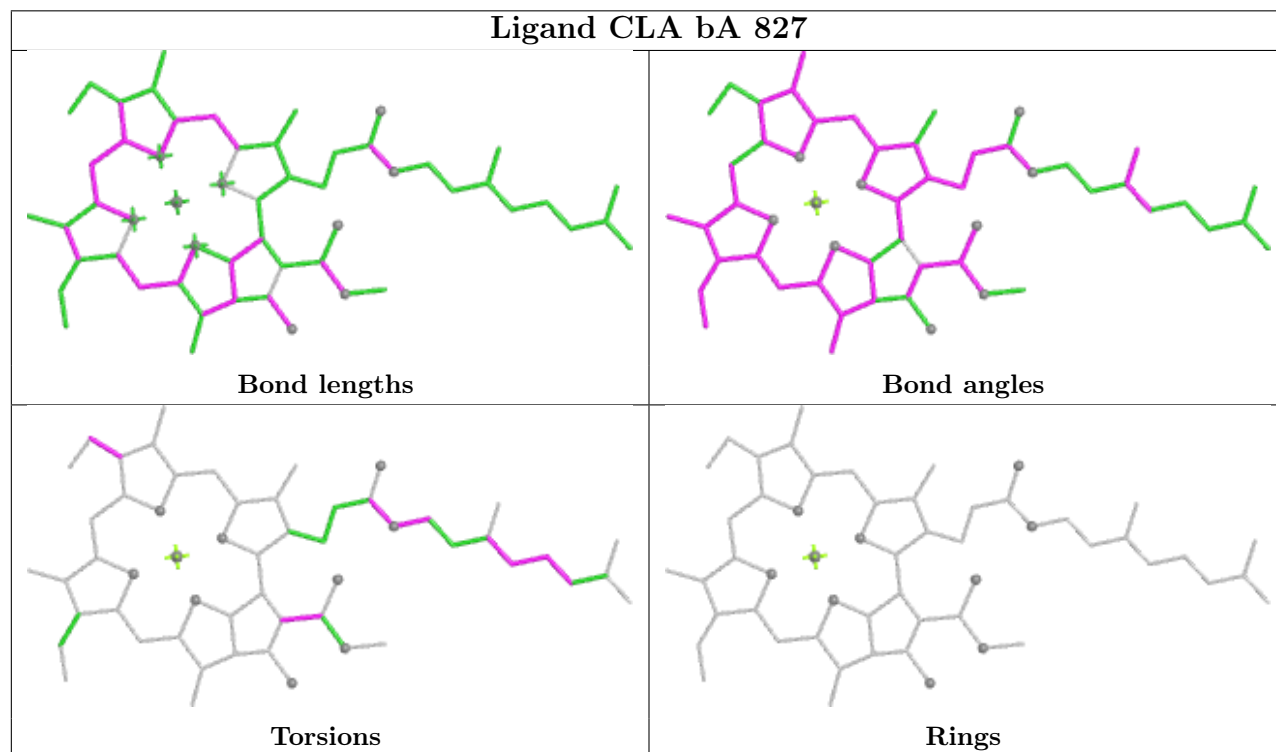
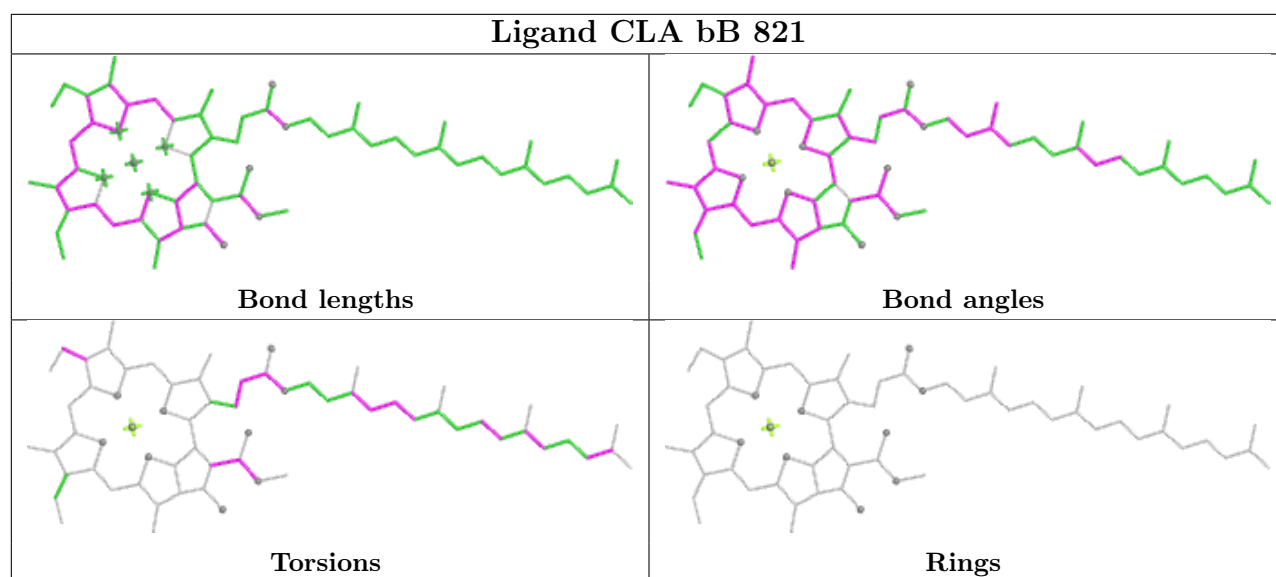


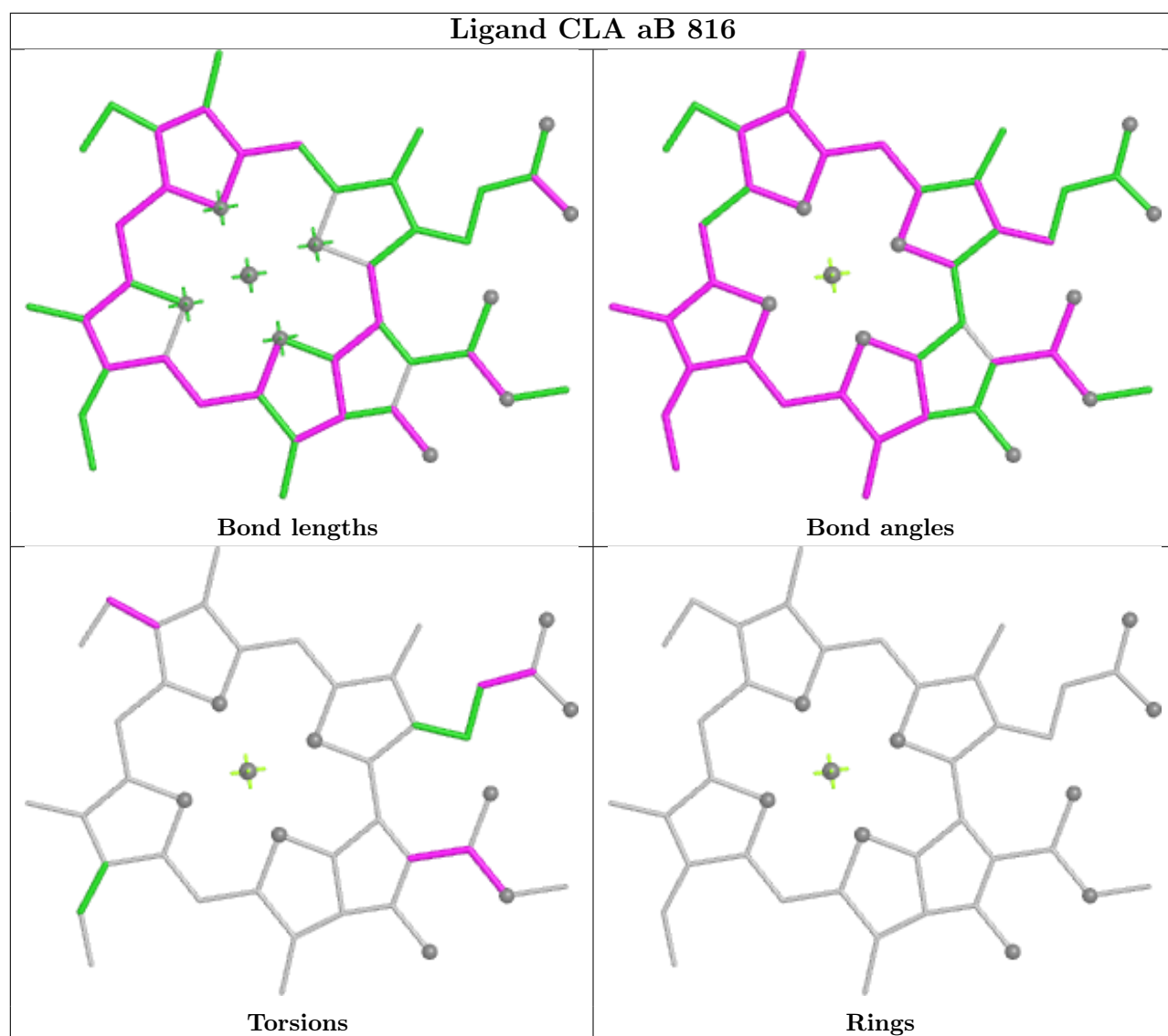
Ligand CLA aA 821



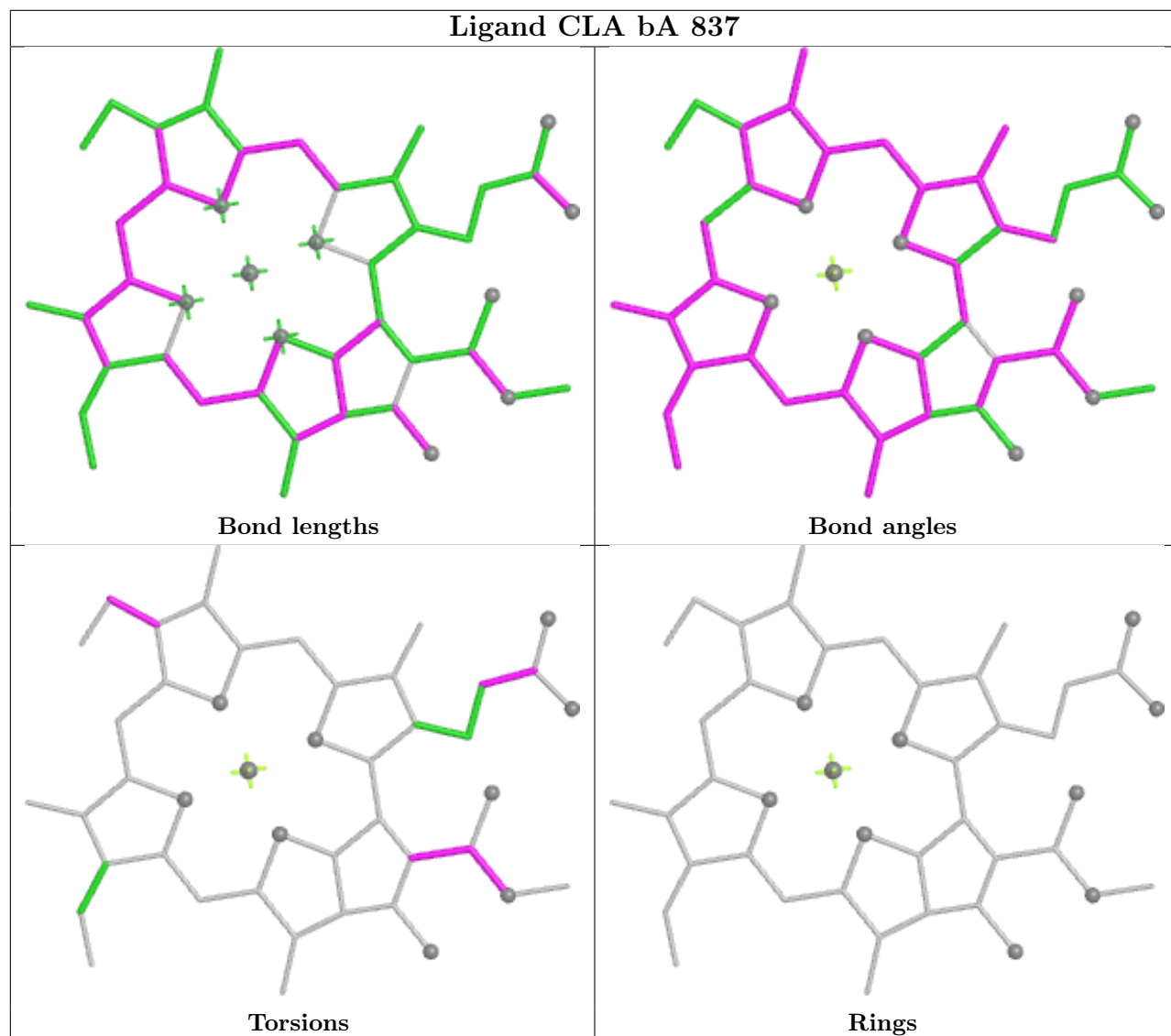
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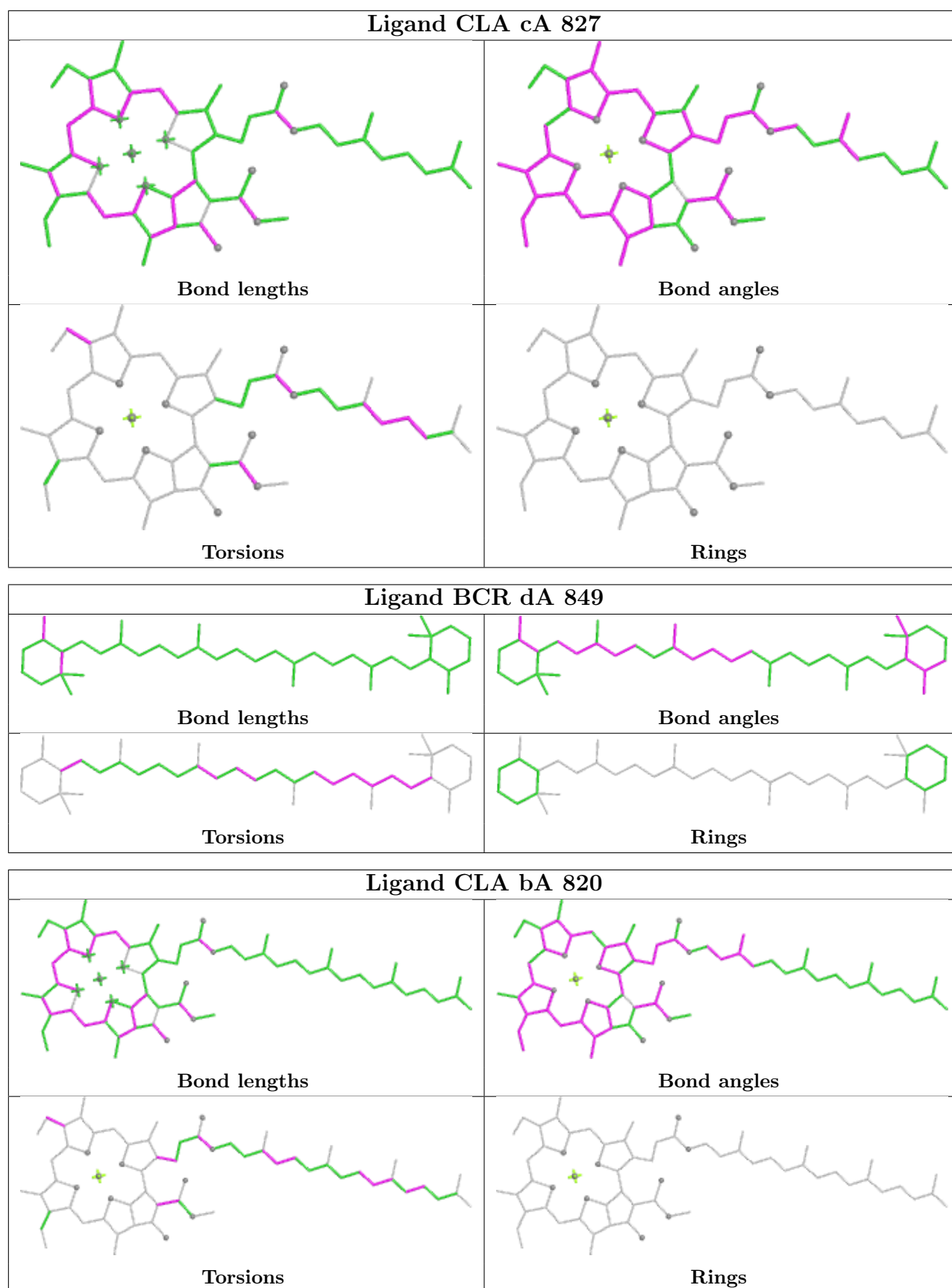


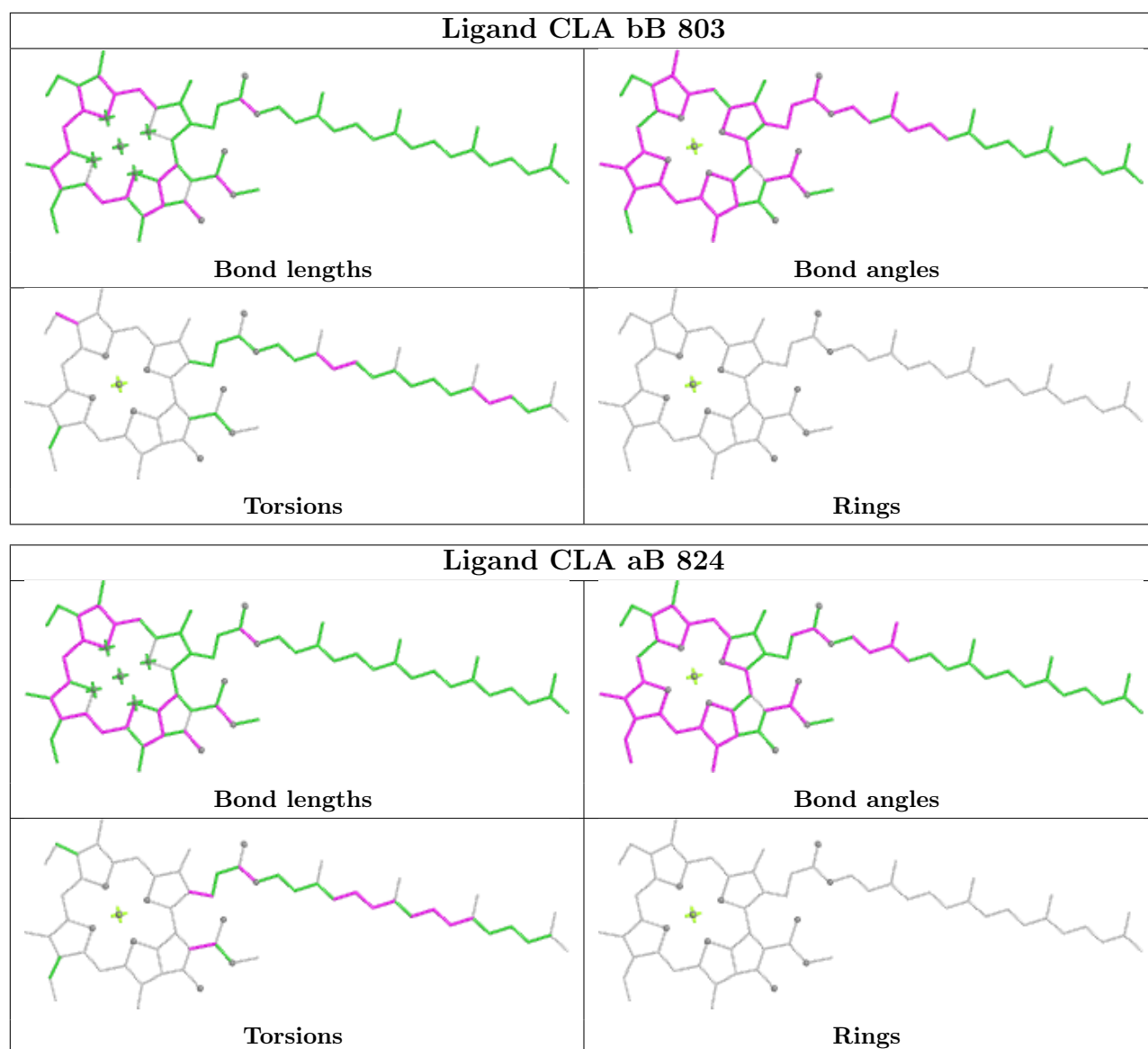


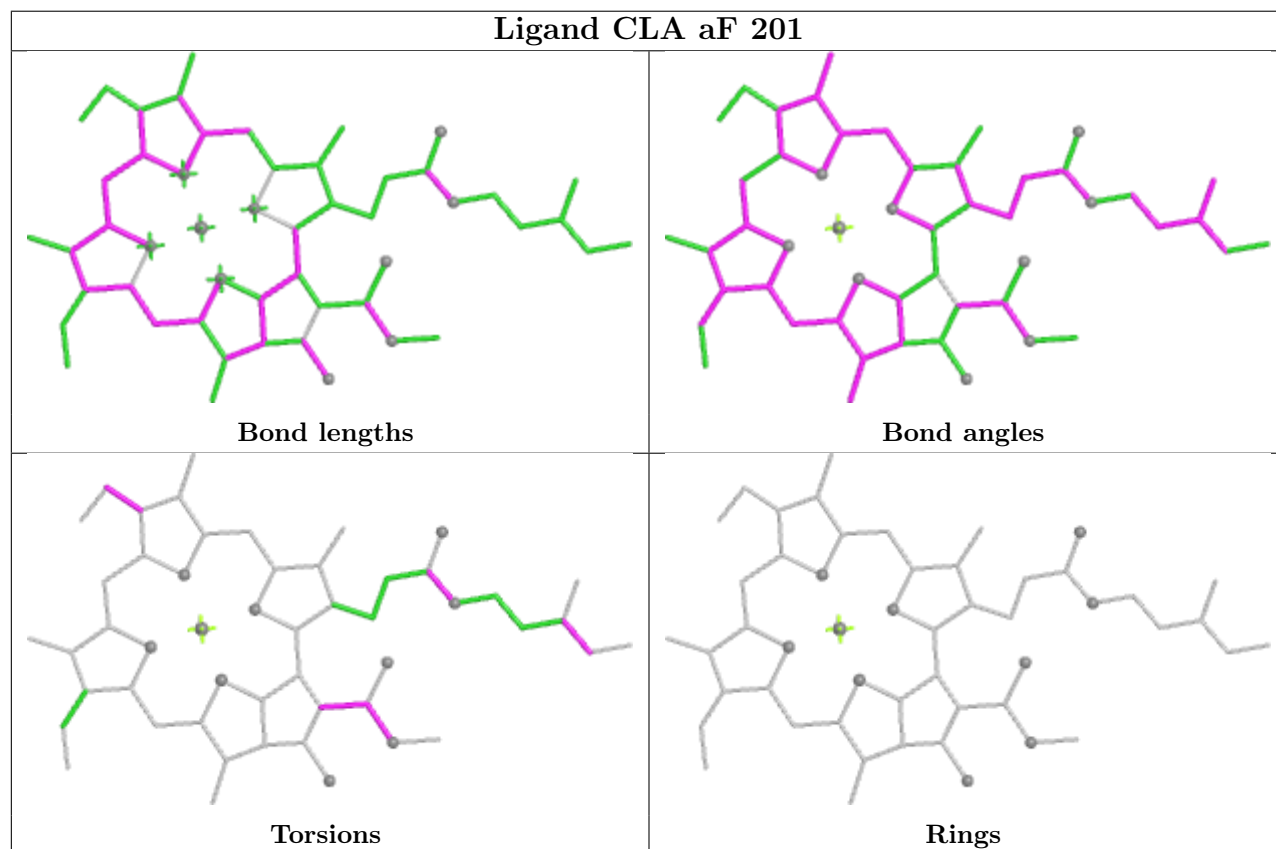
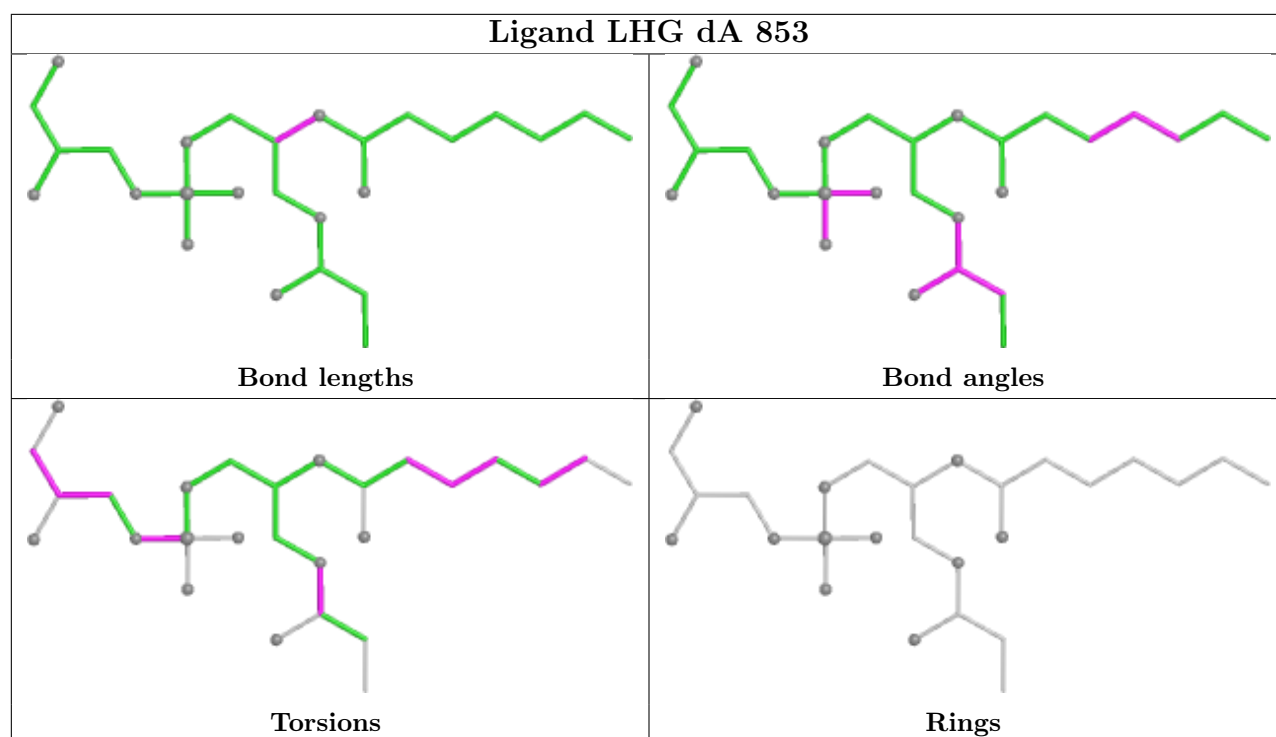


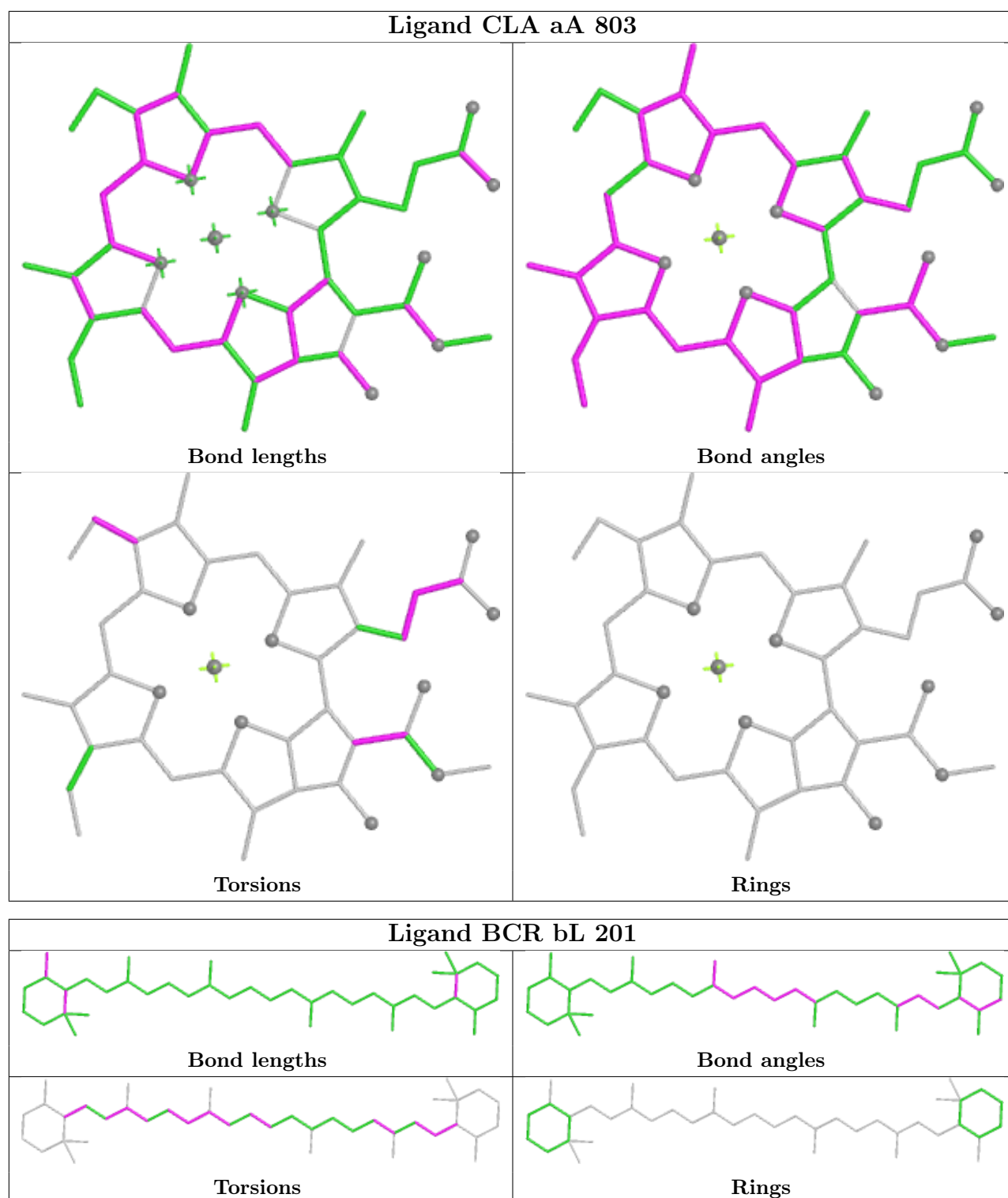
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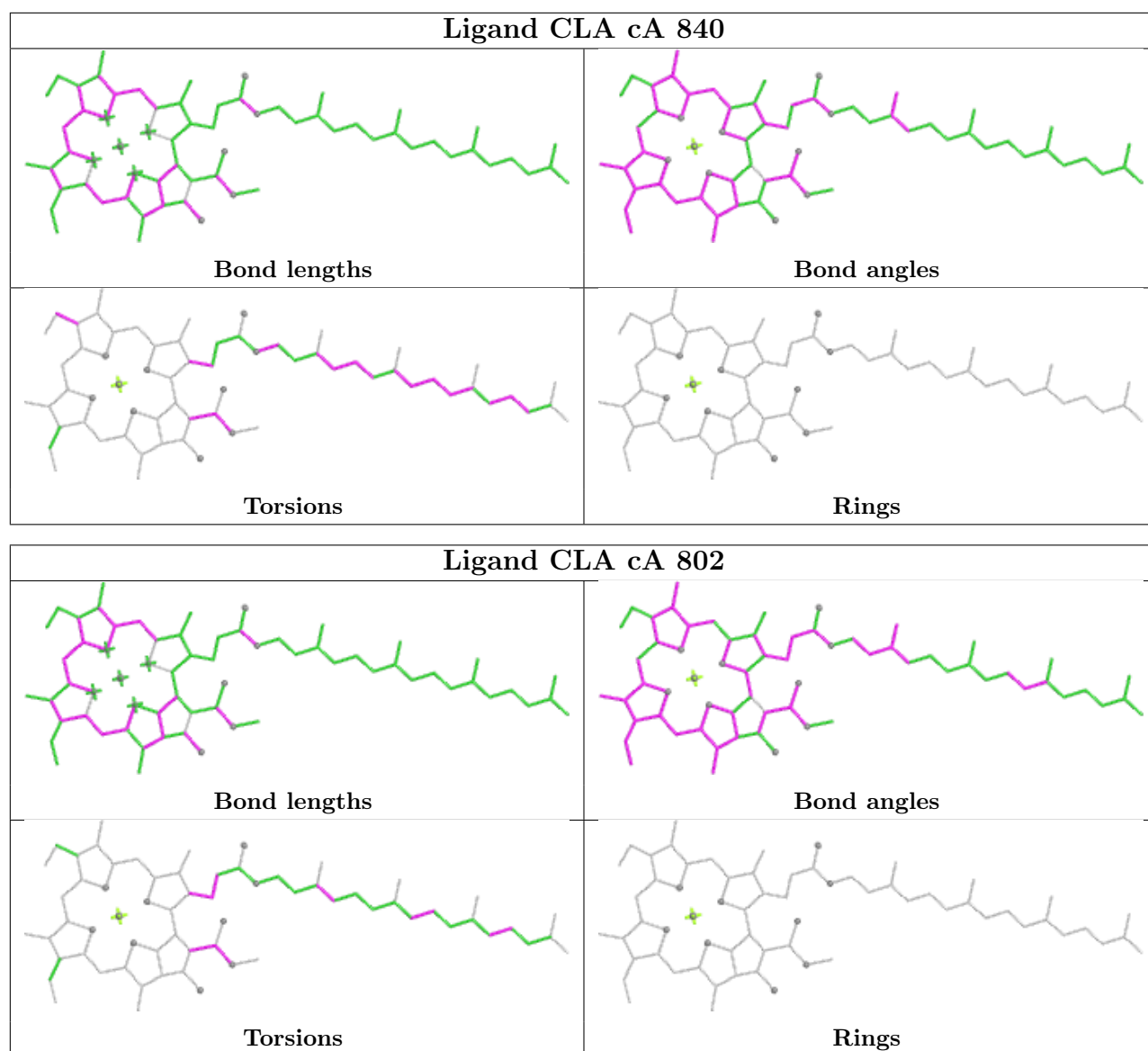




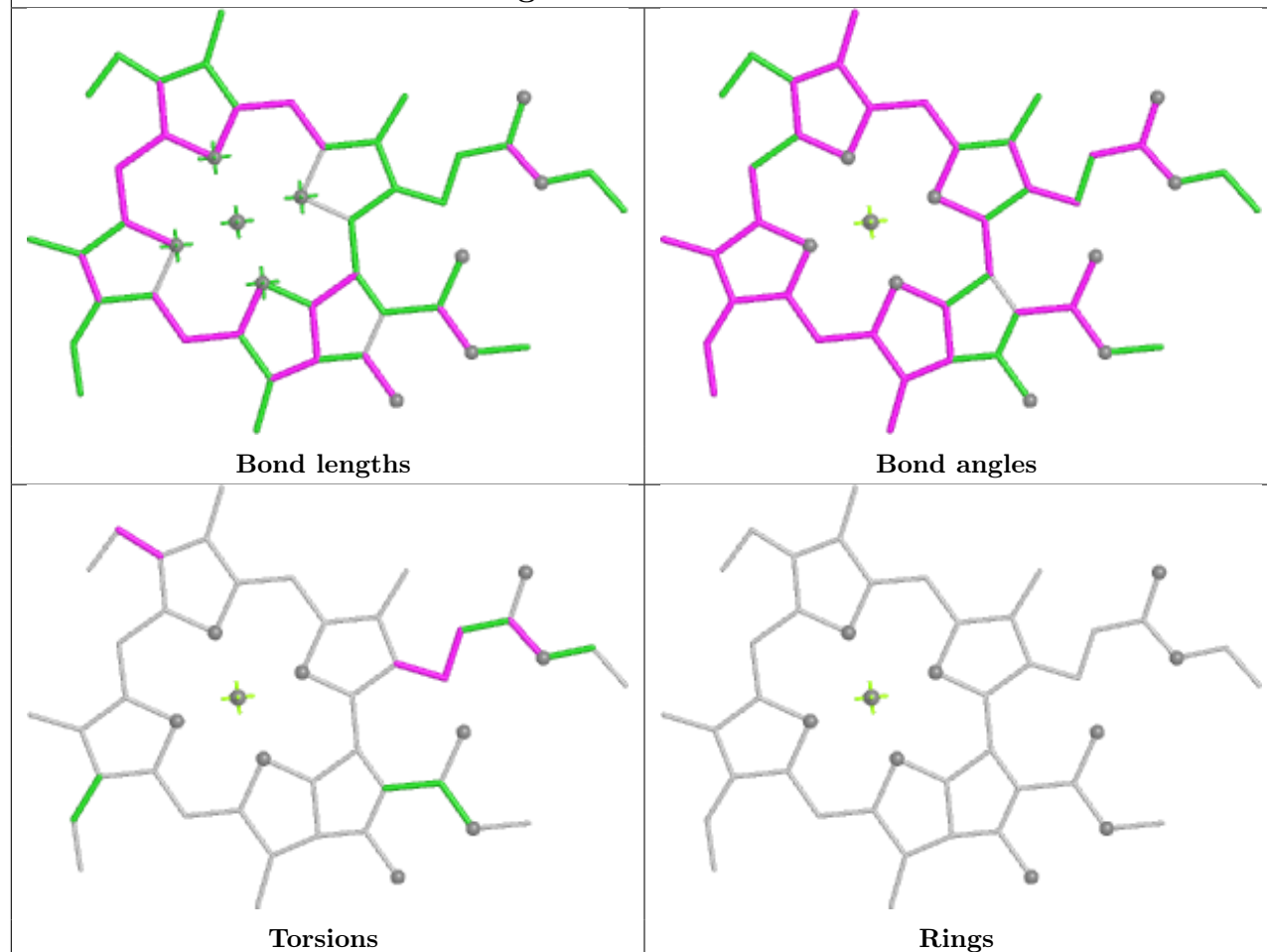




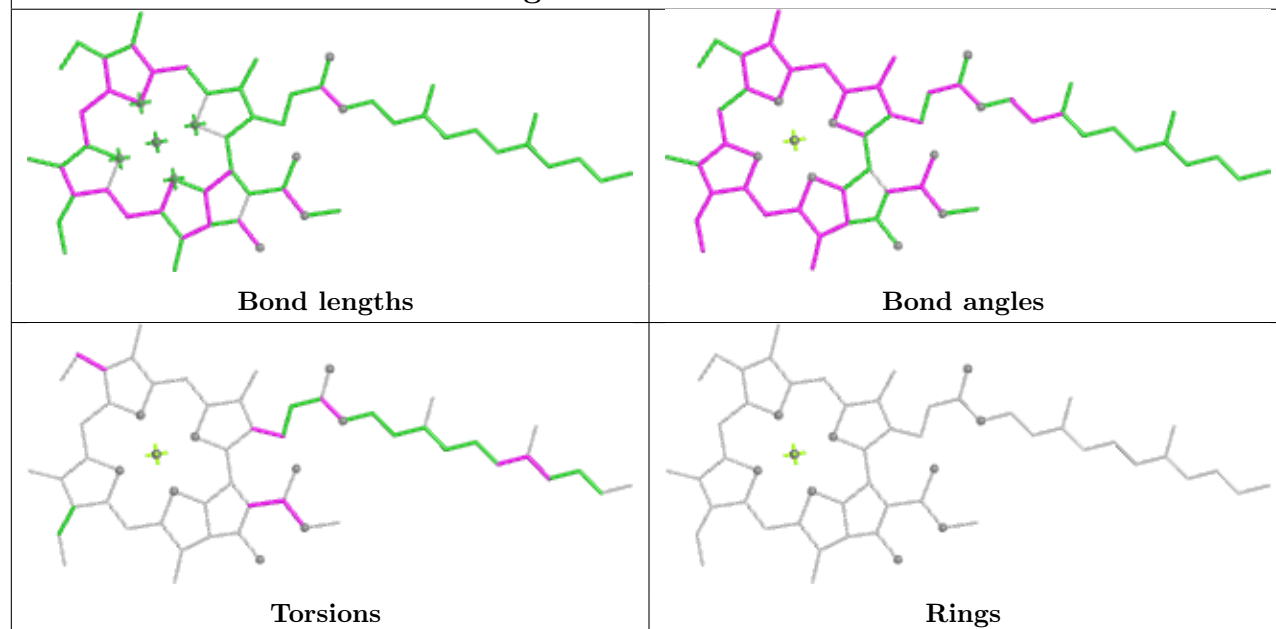


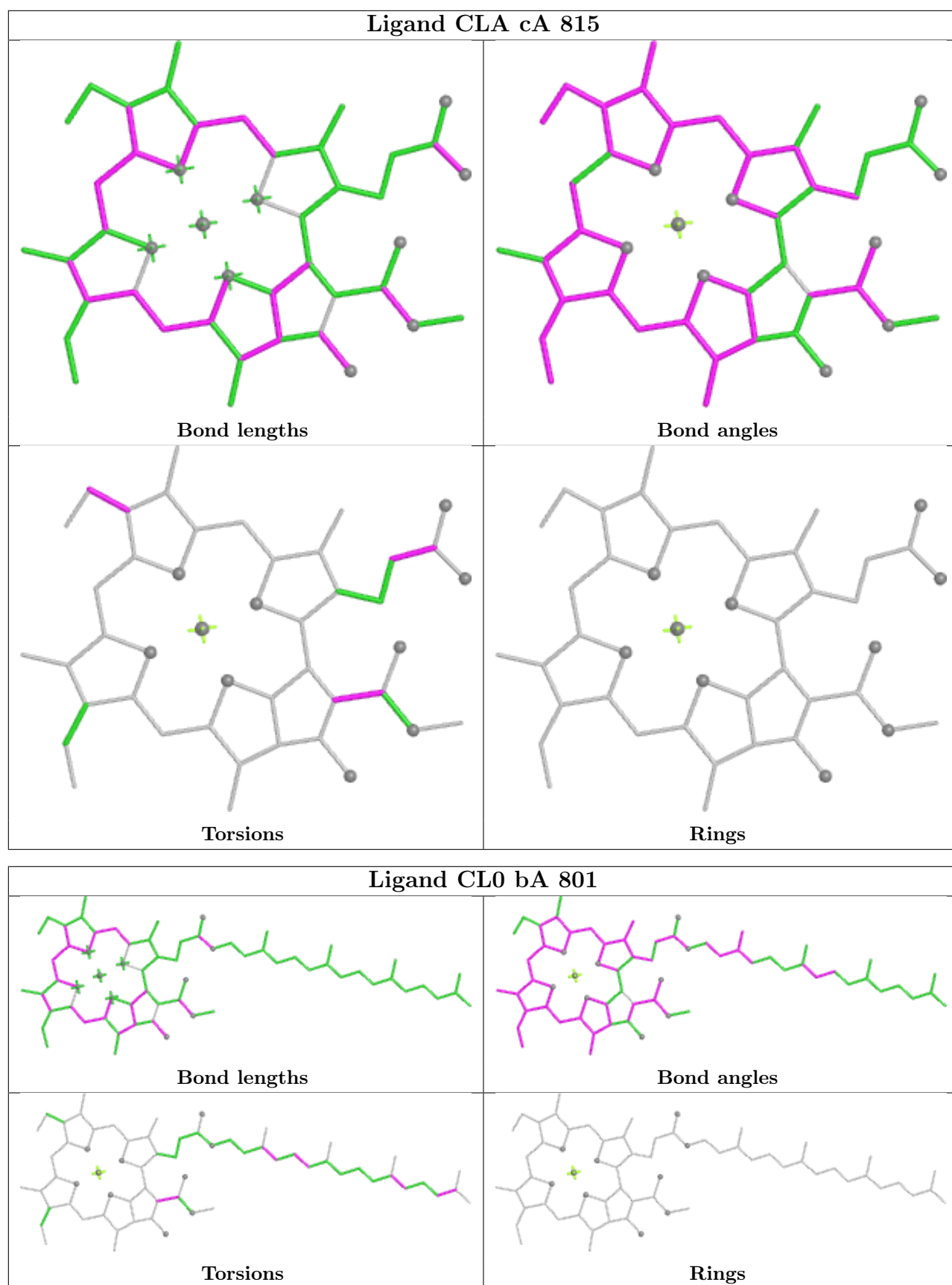


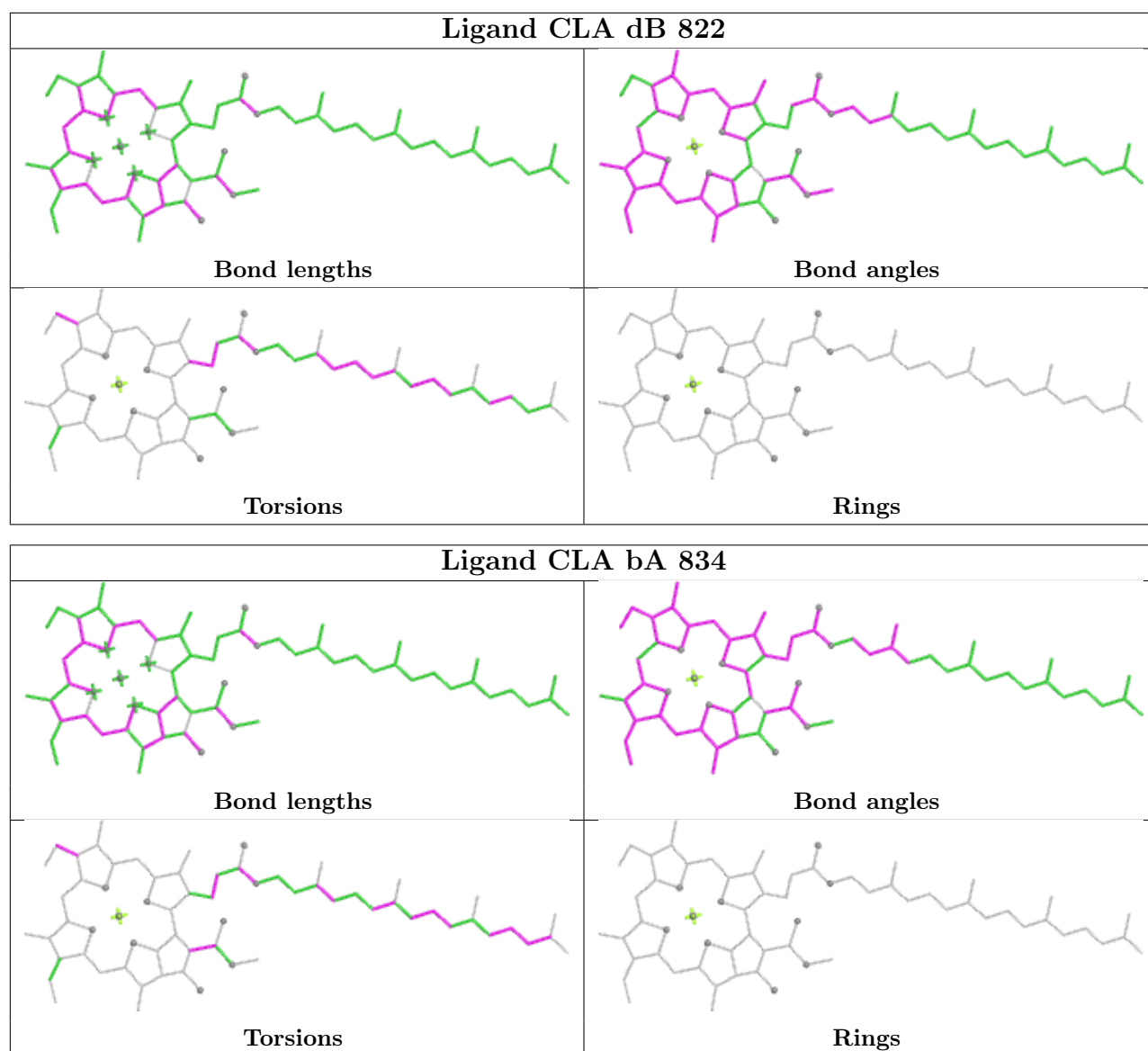
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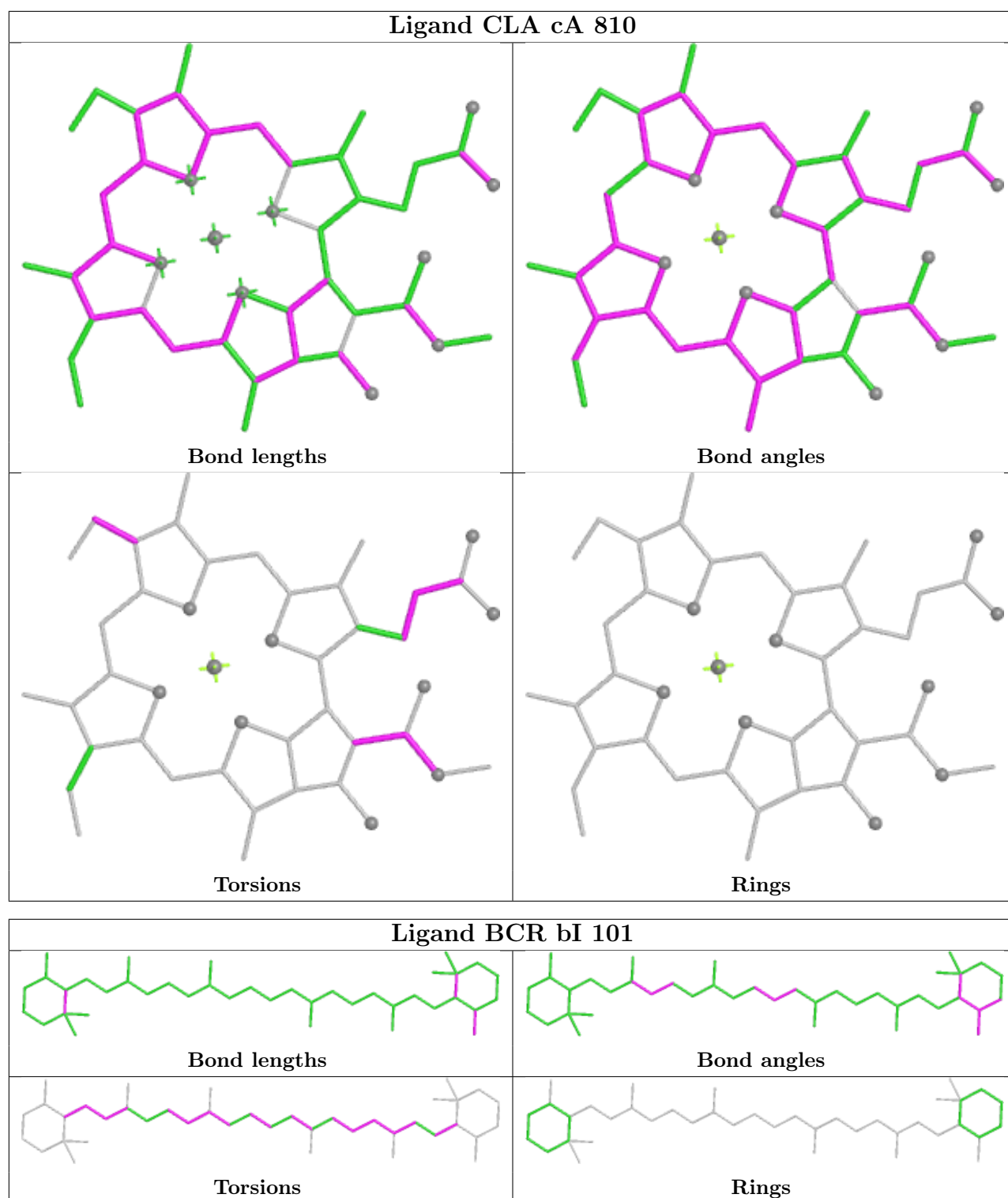


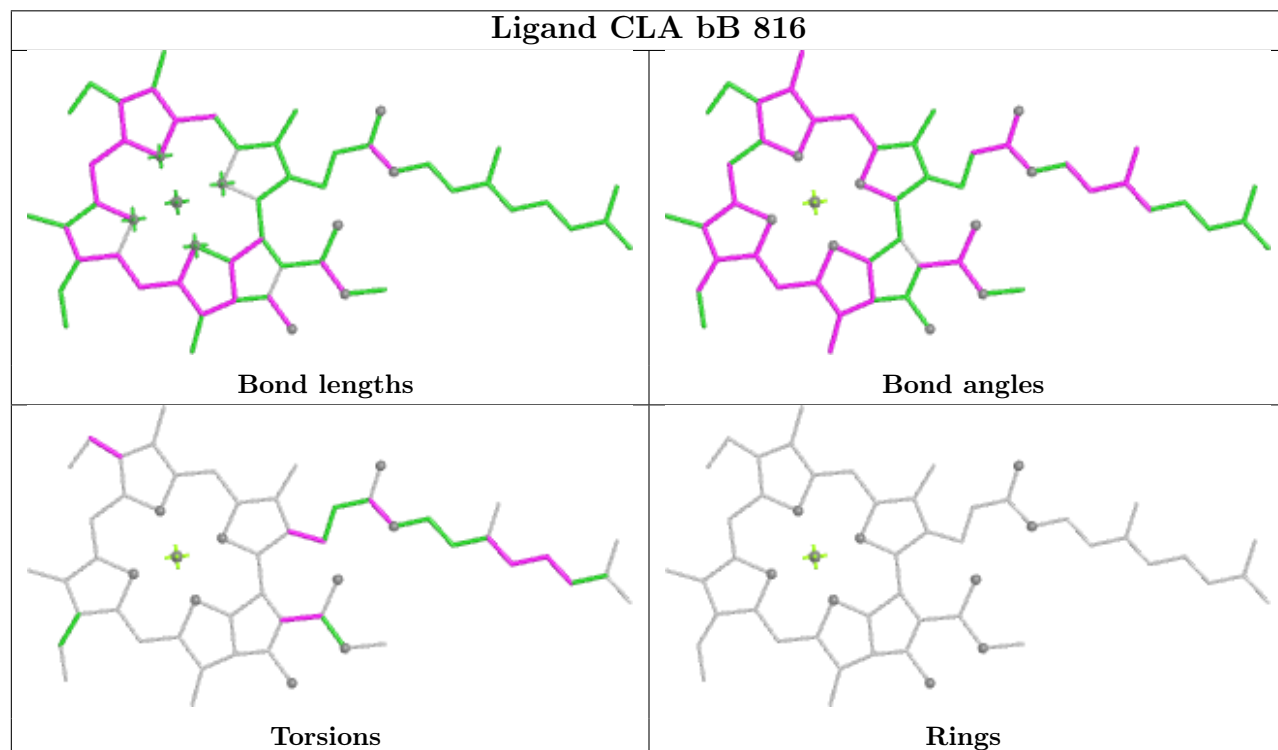
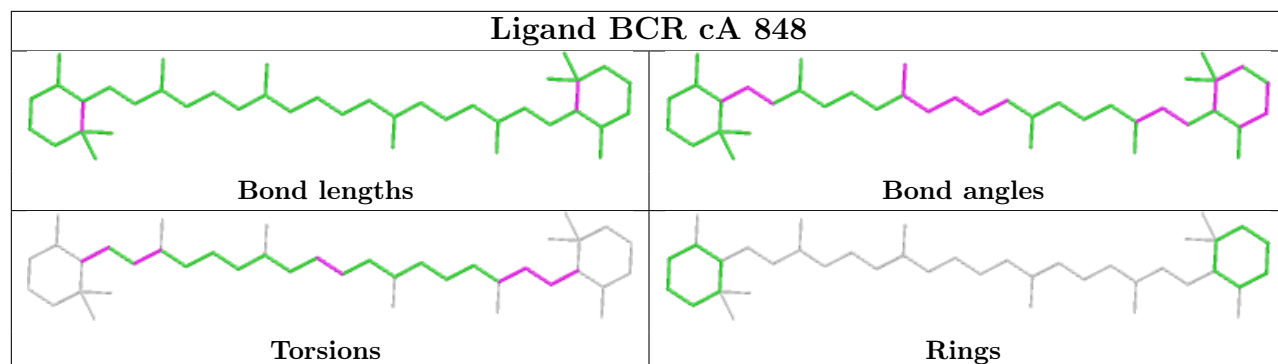
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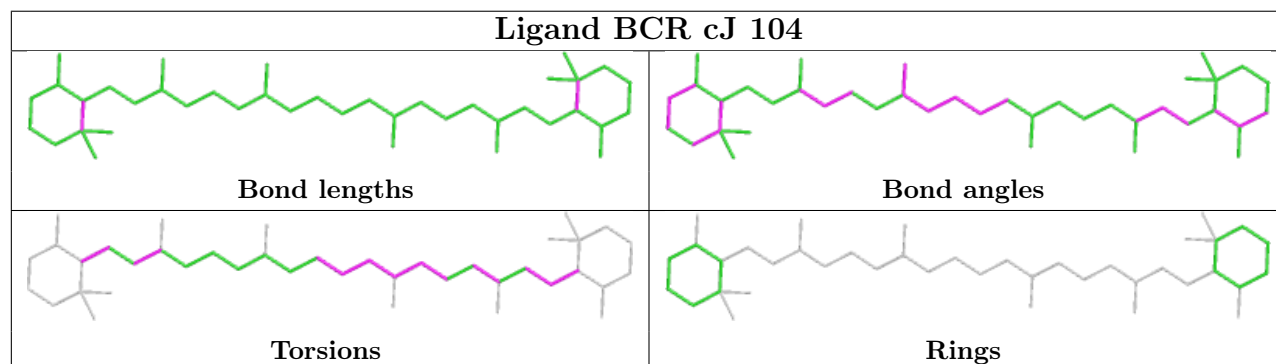
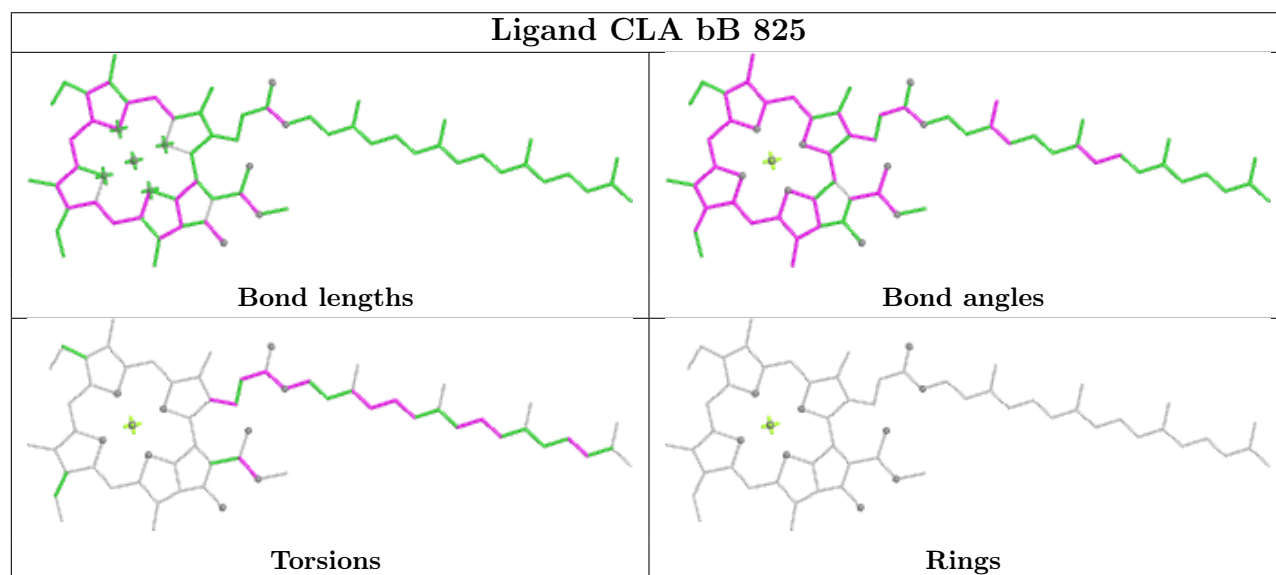
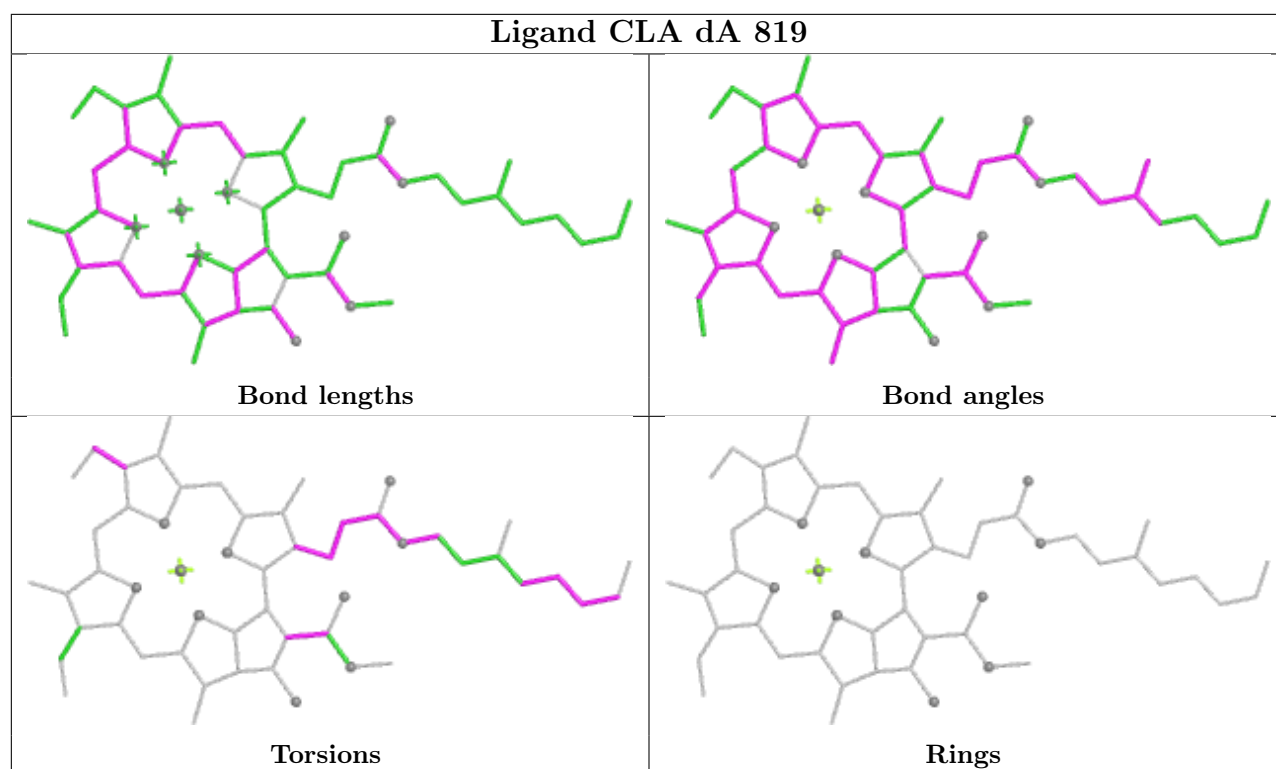


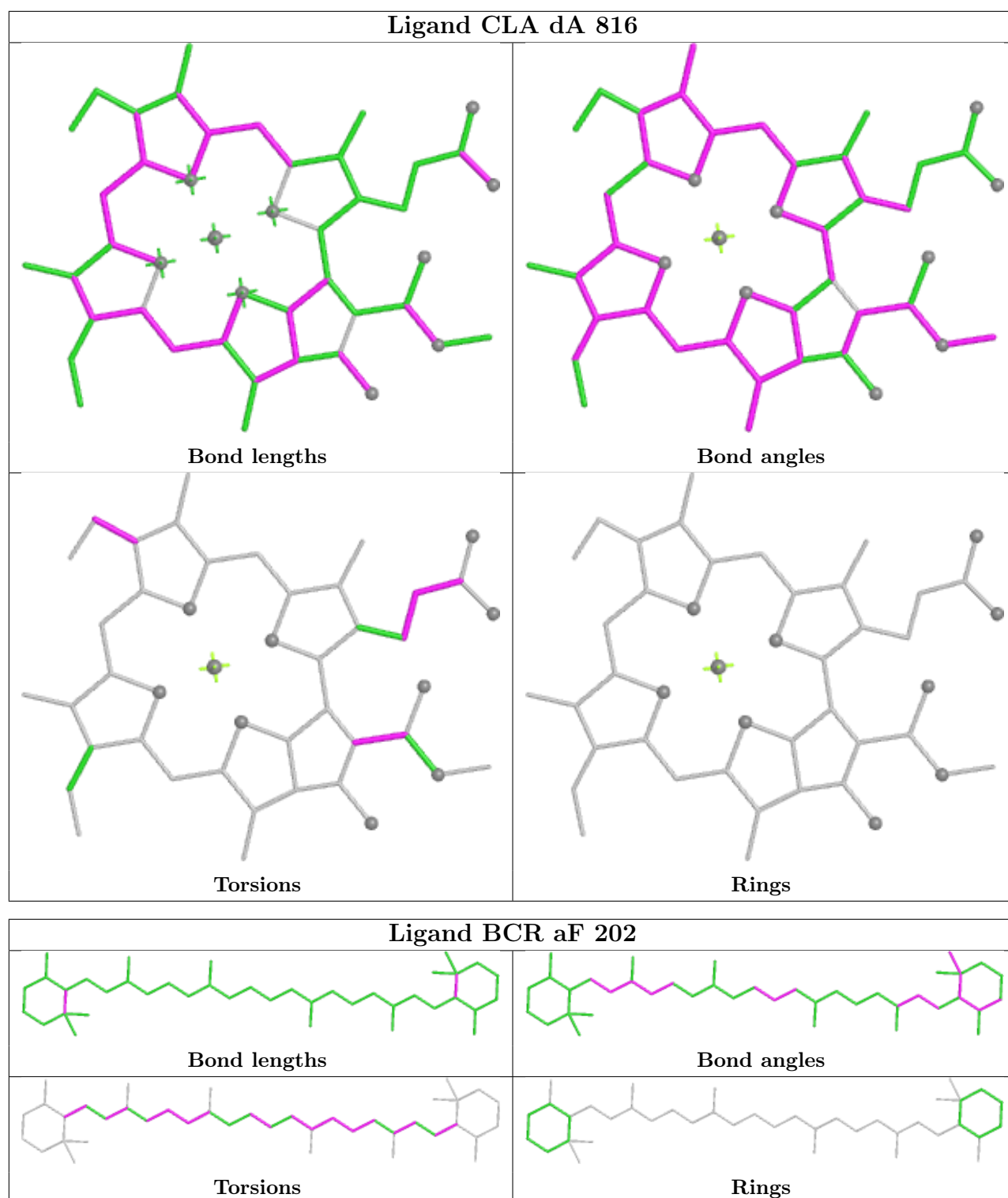


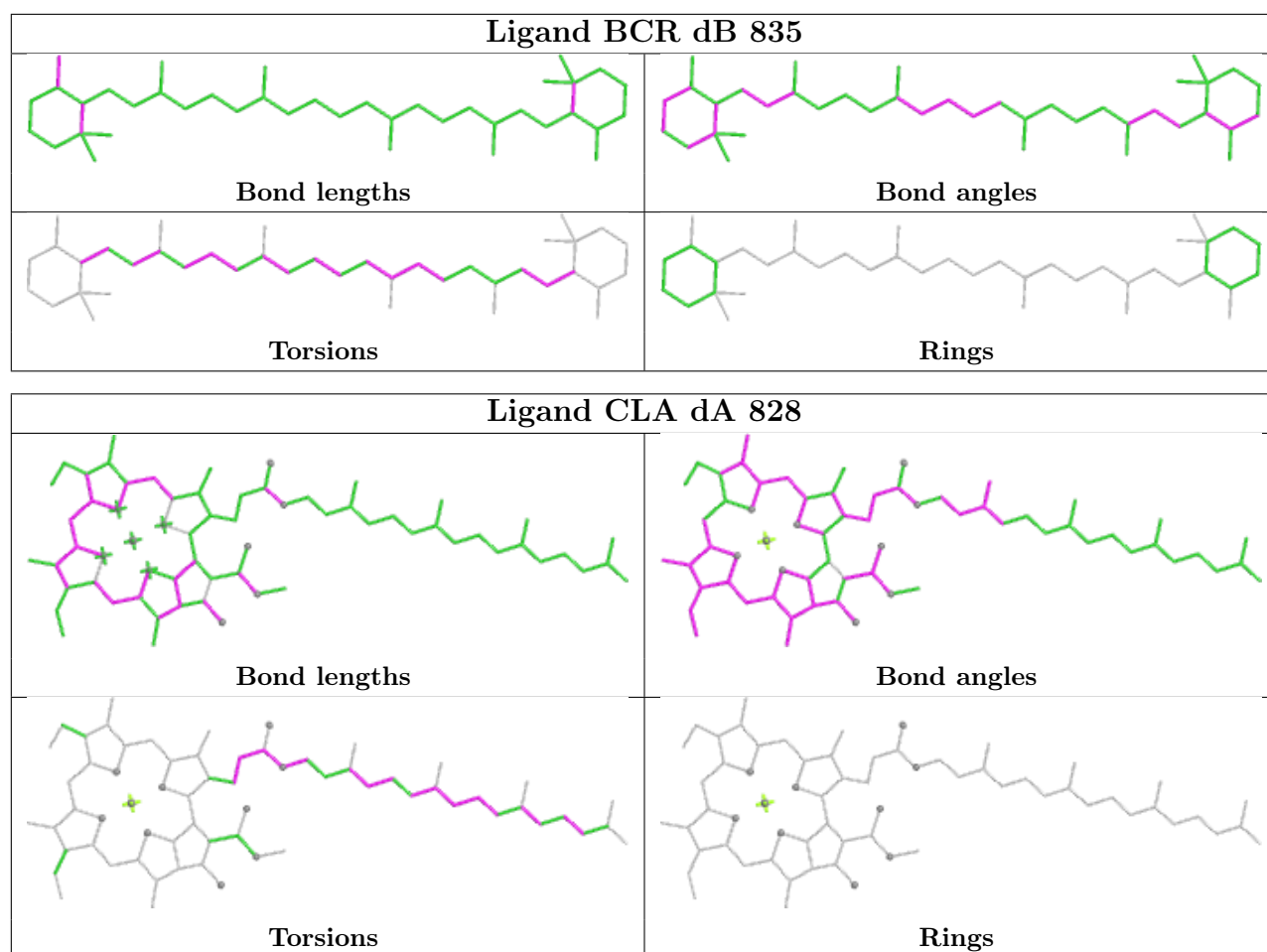




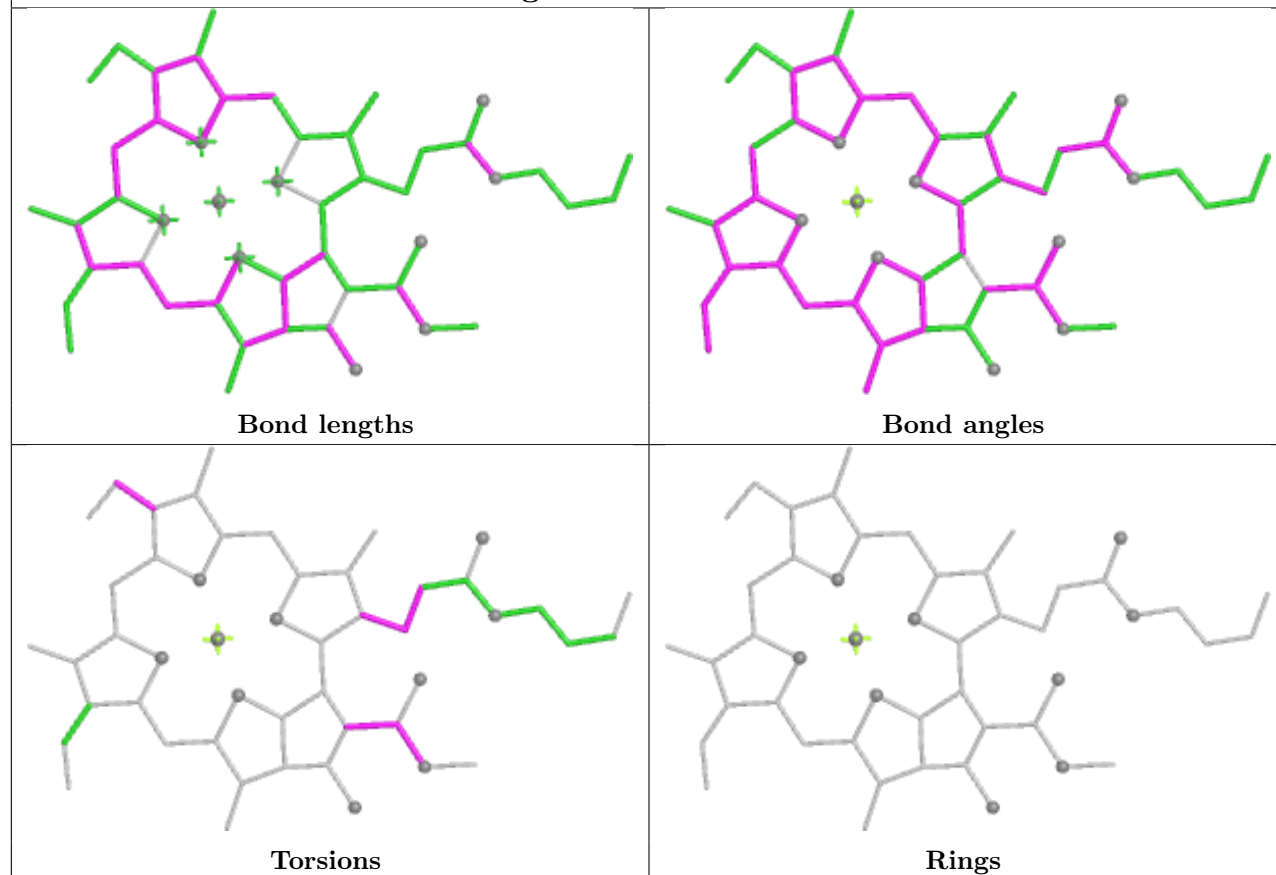




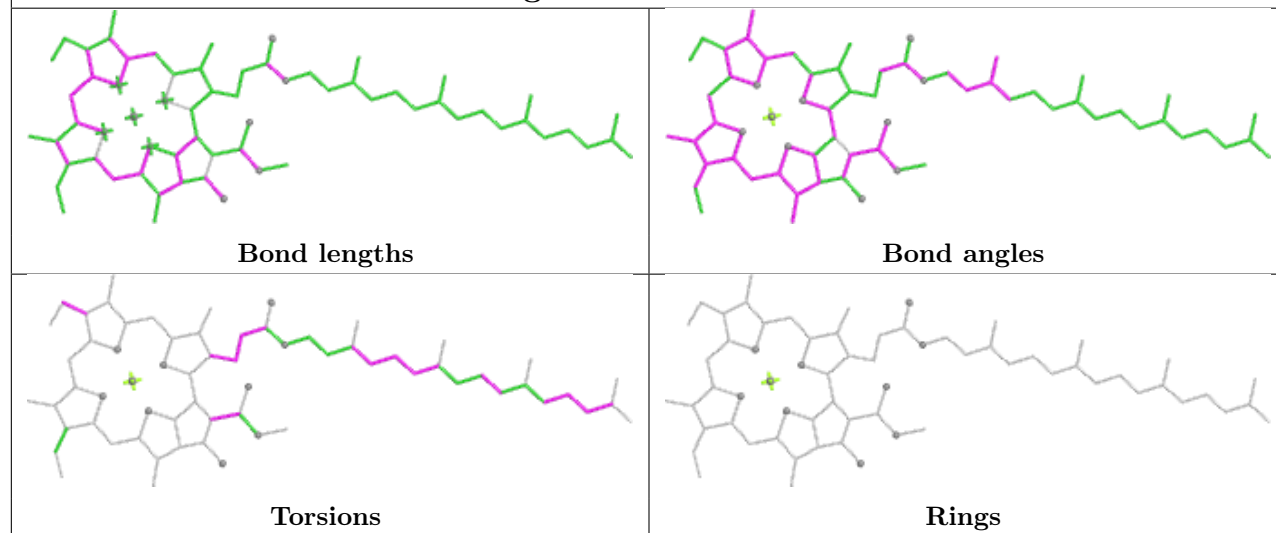


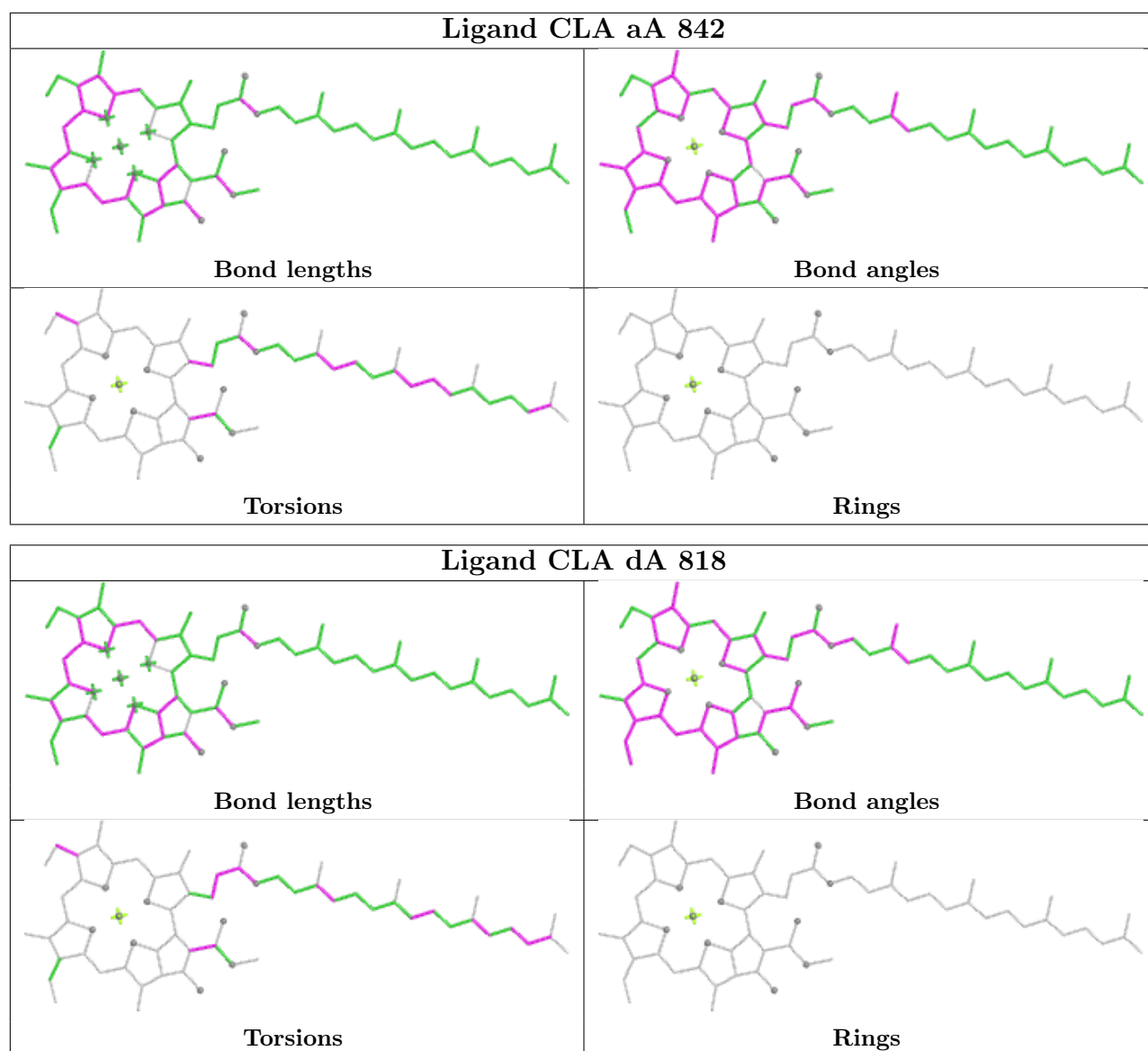


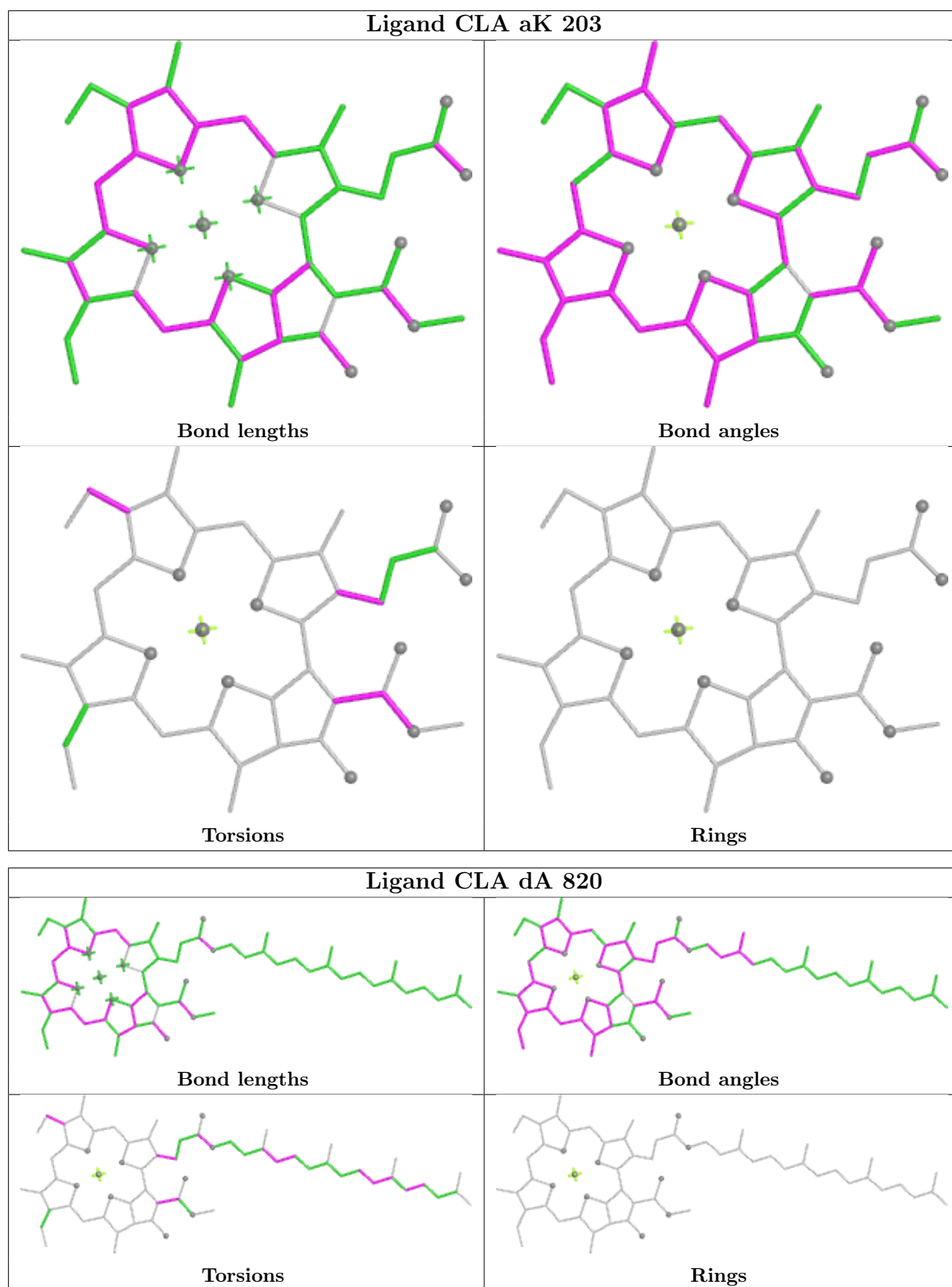
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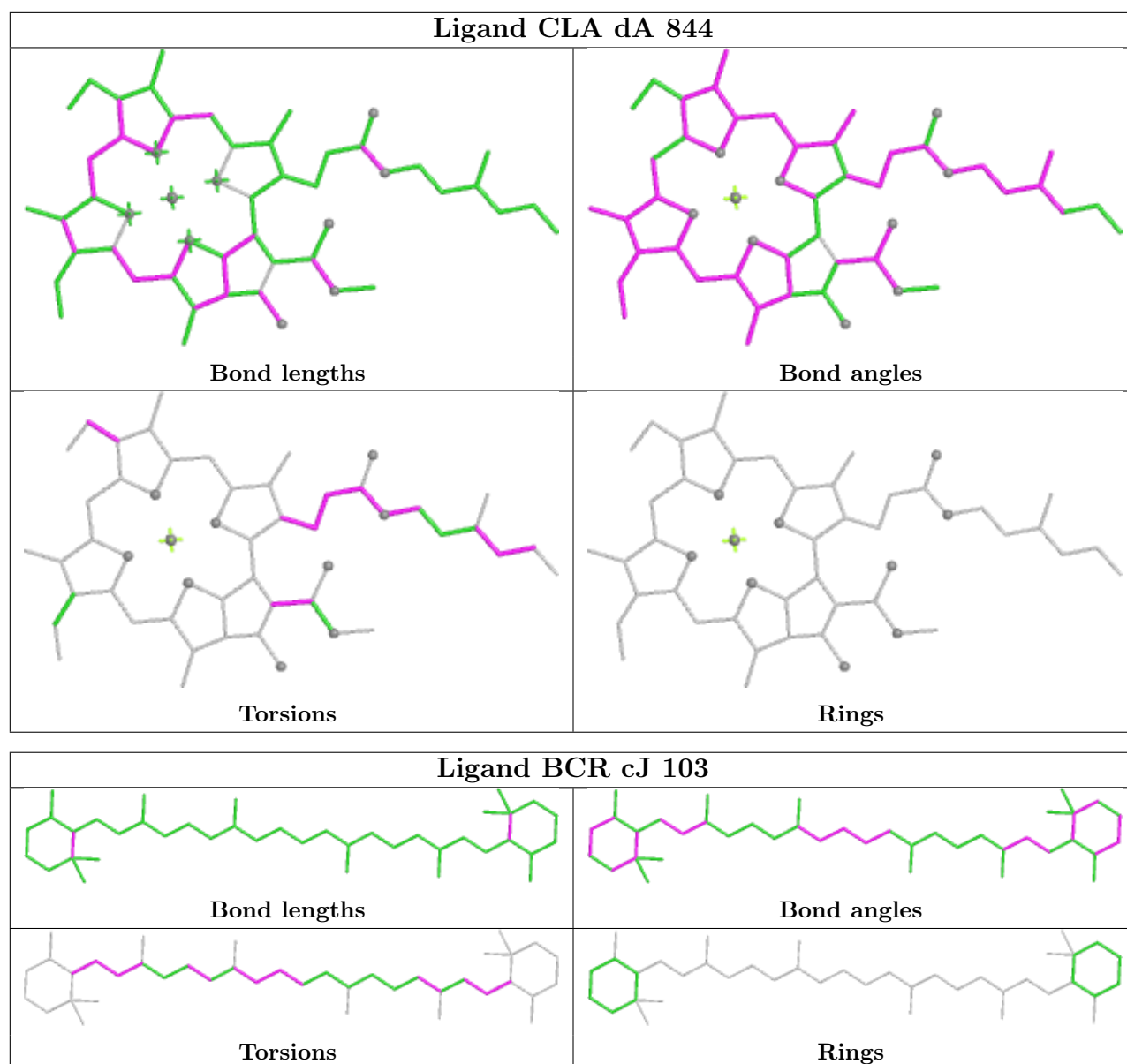


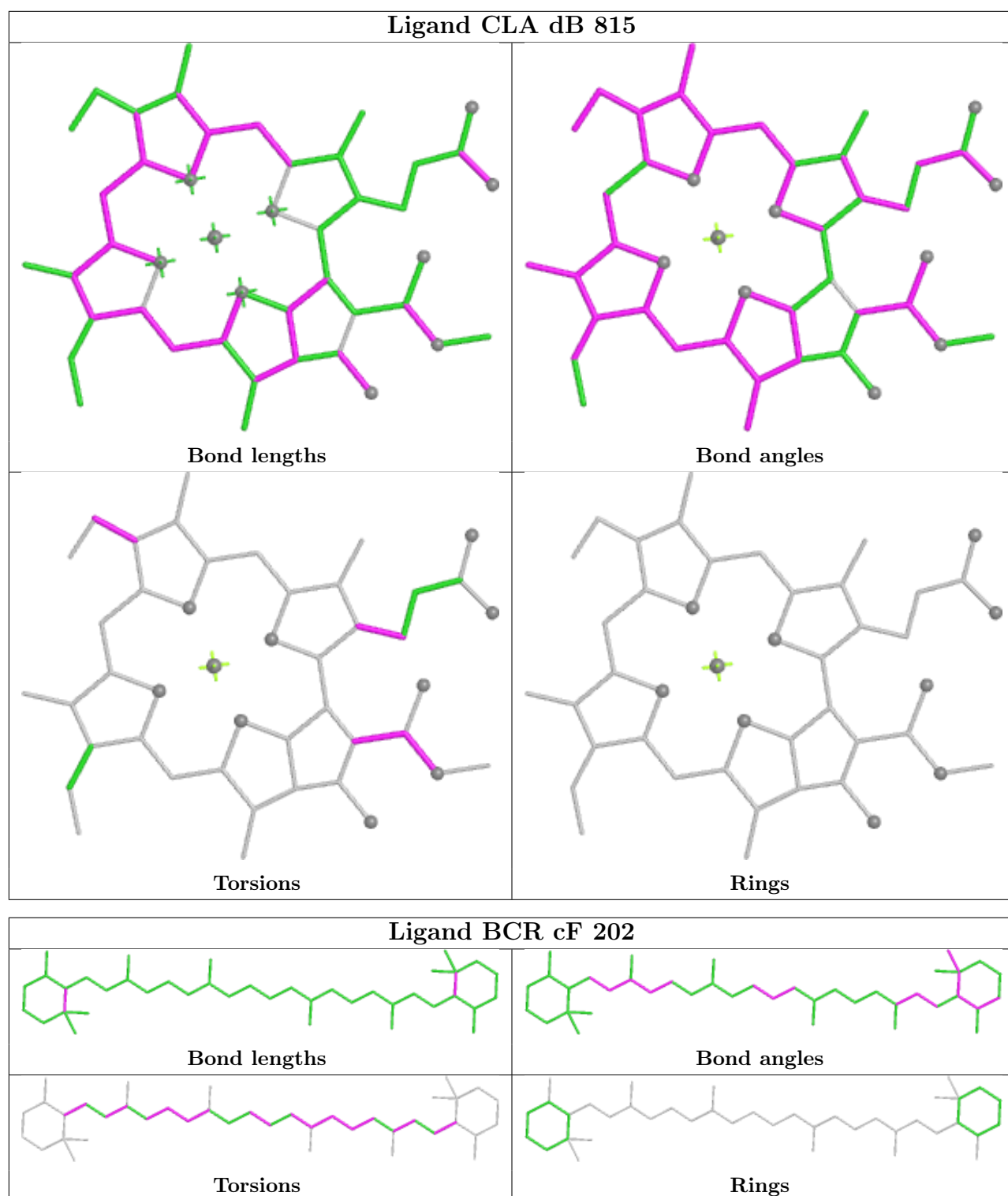
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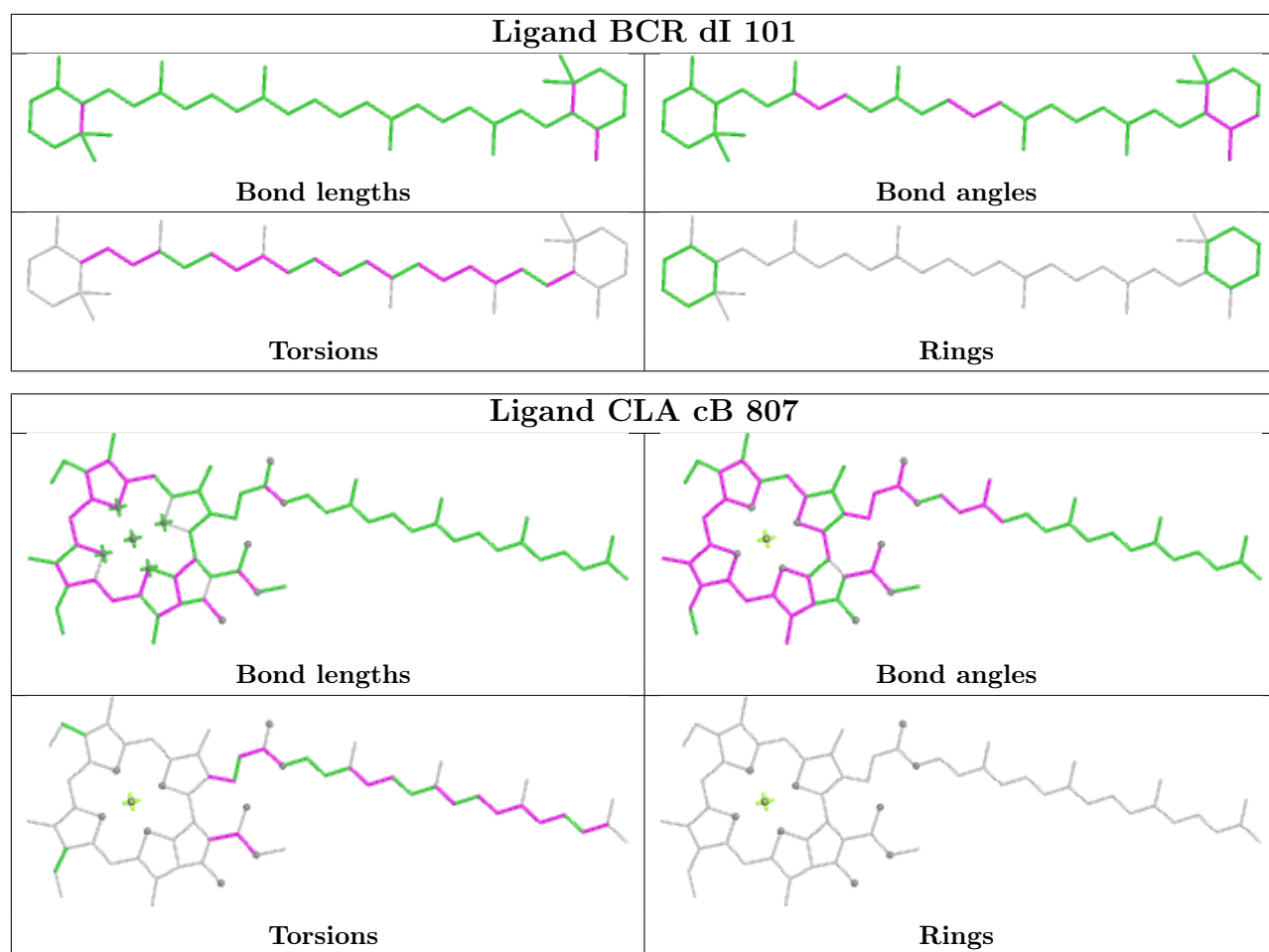


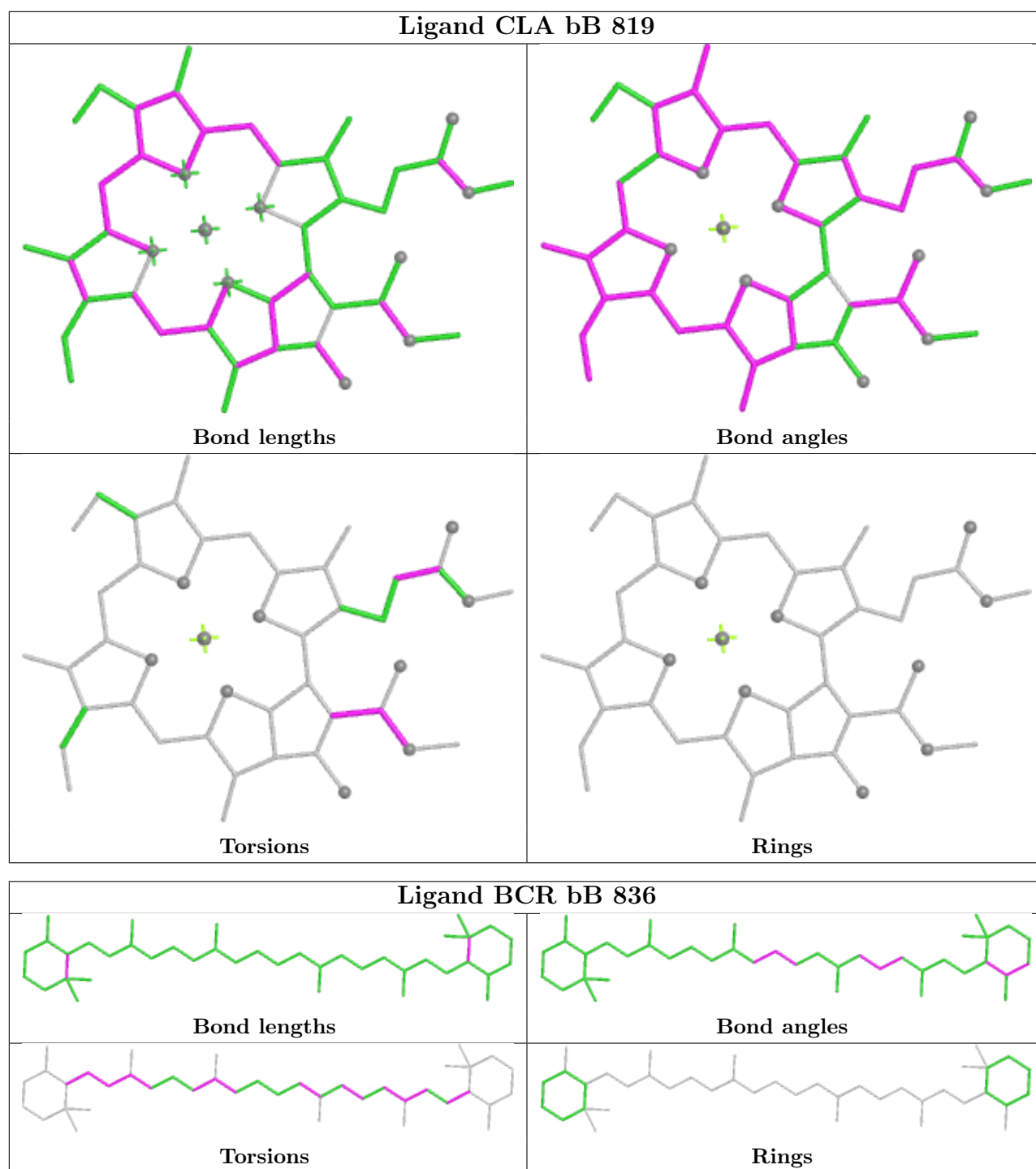


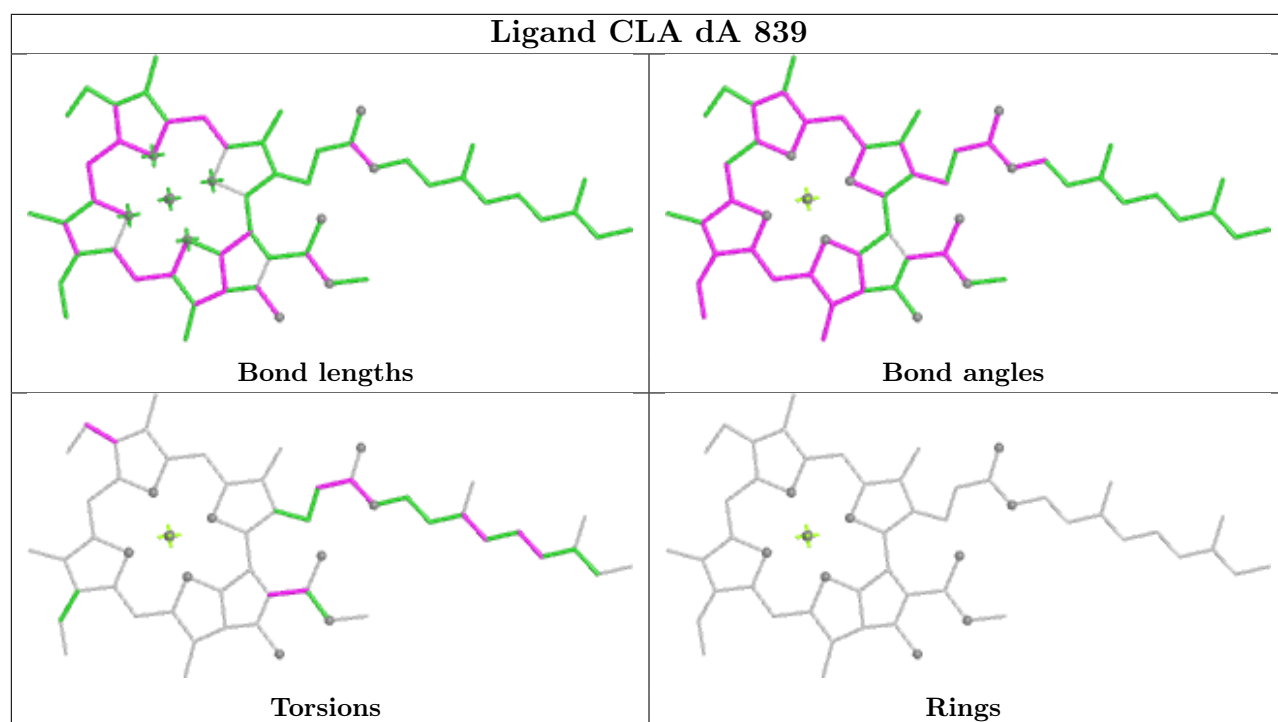


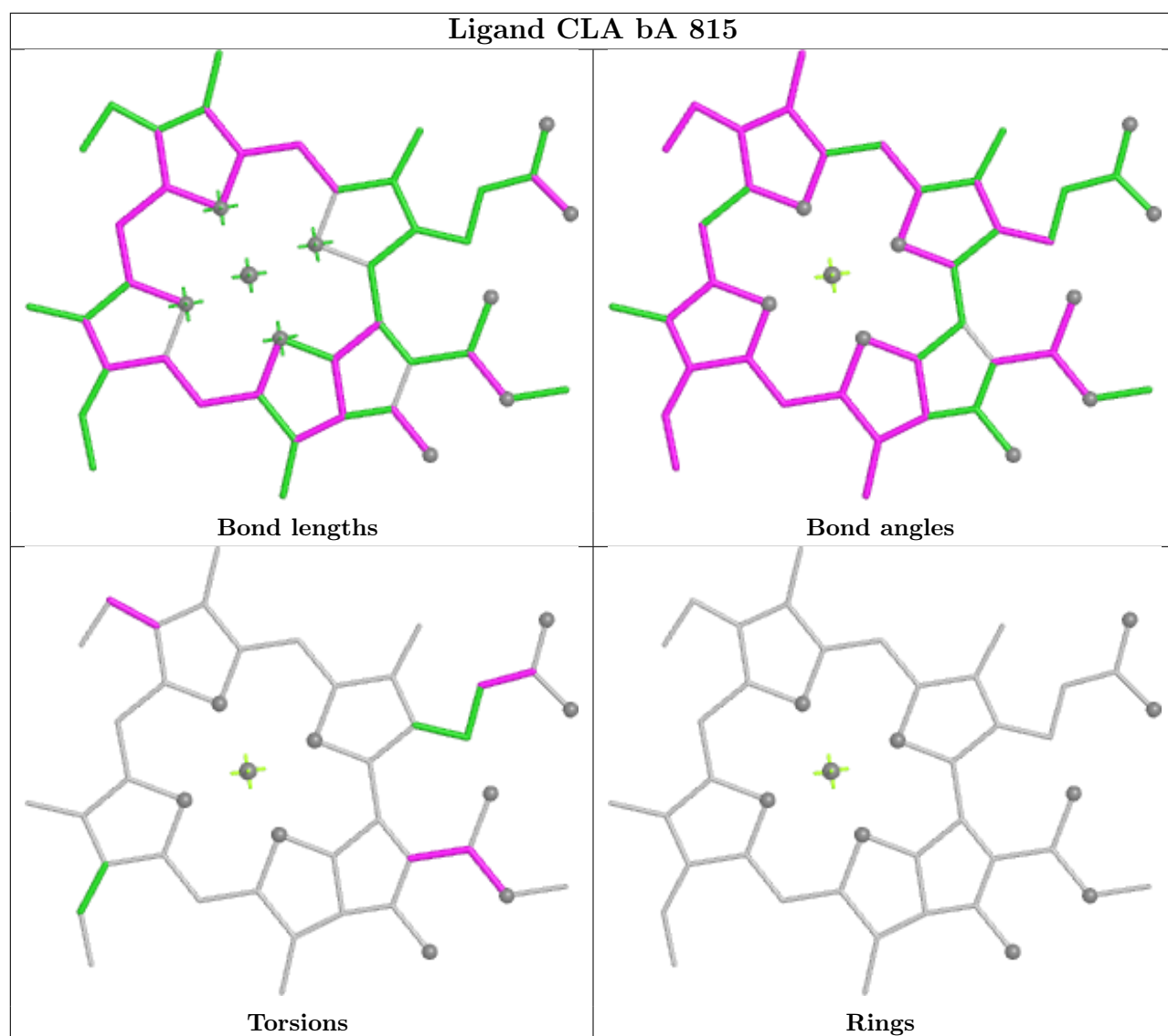


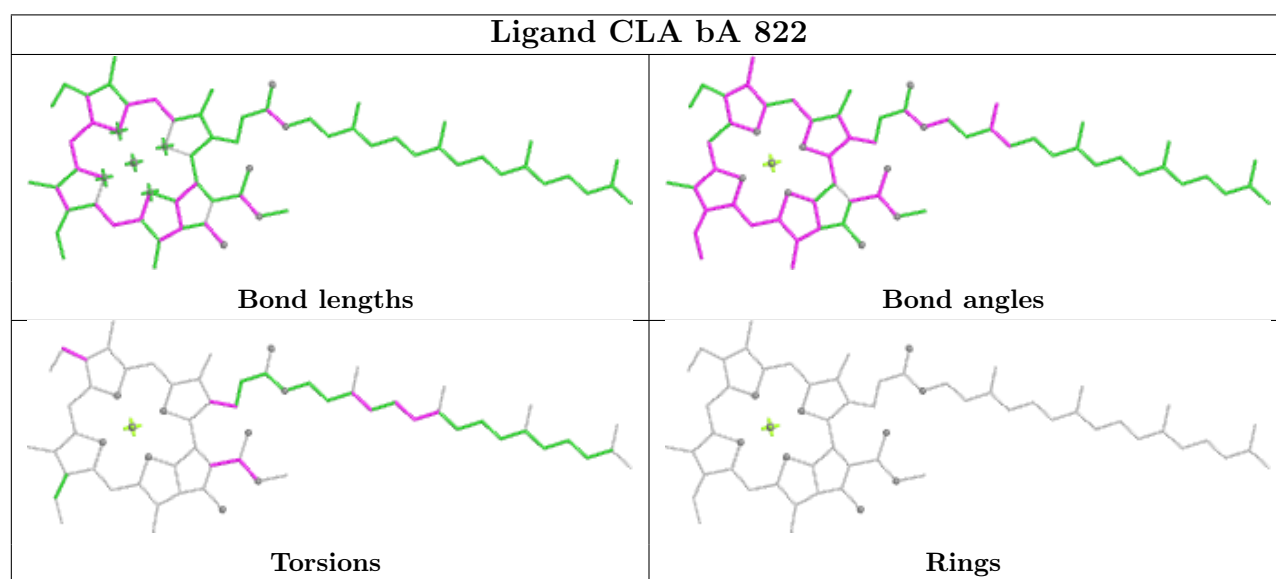
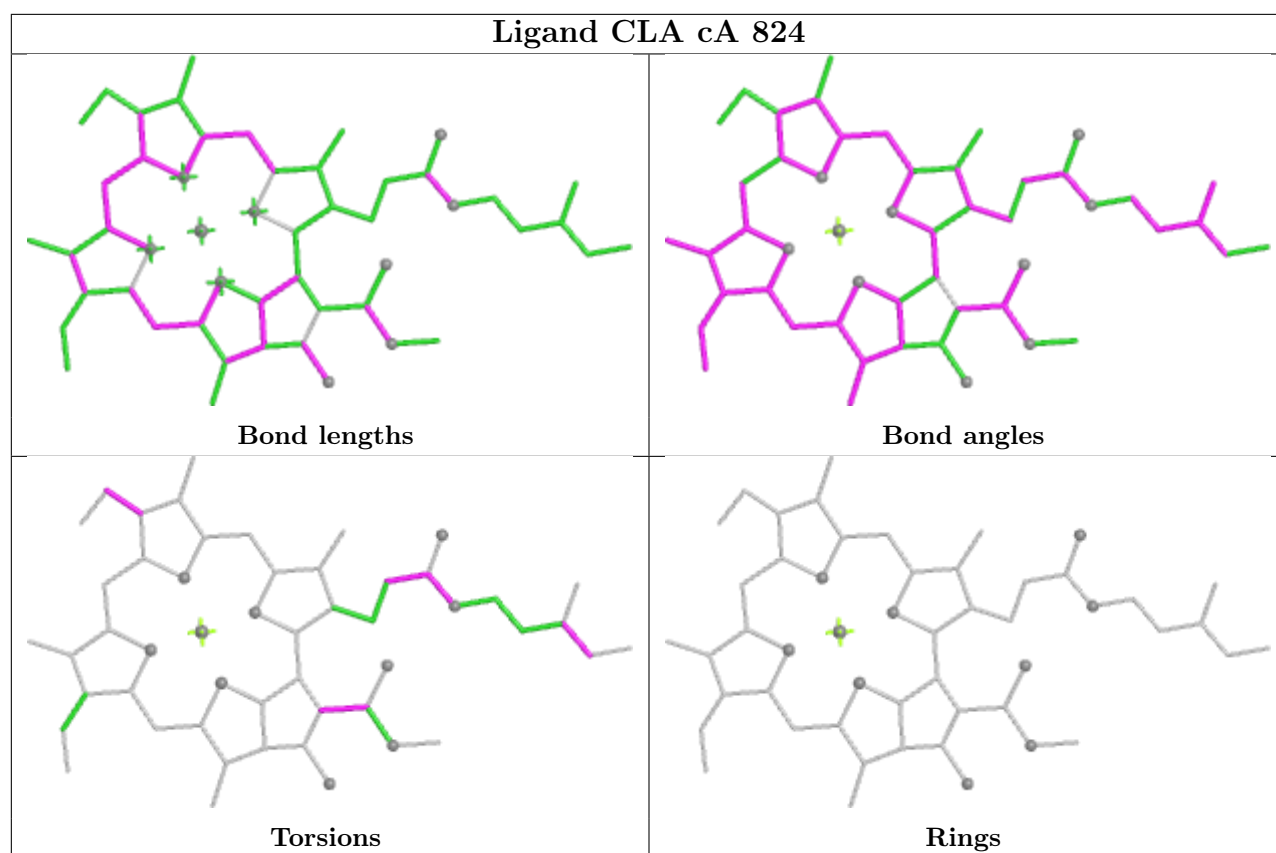


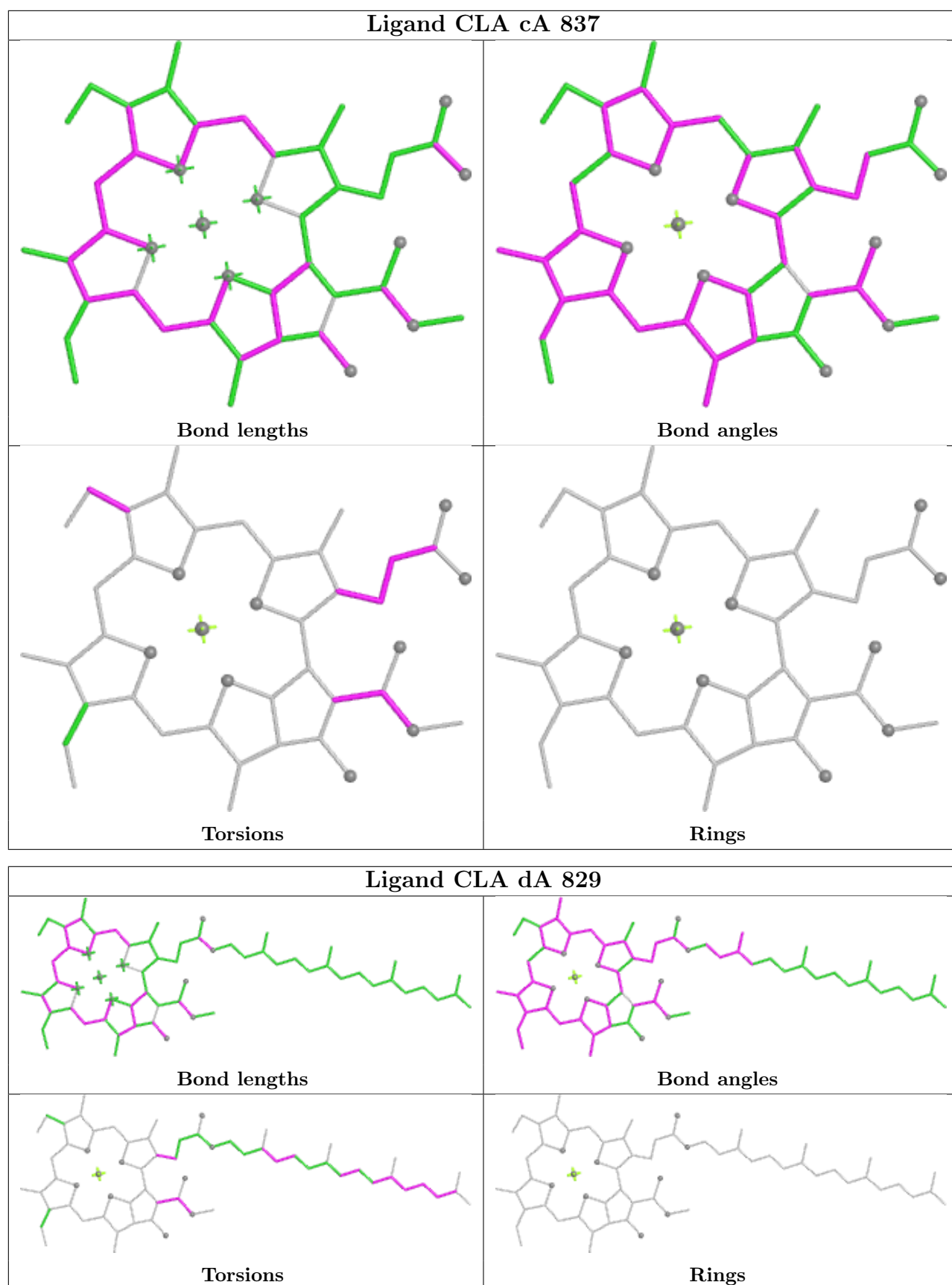


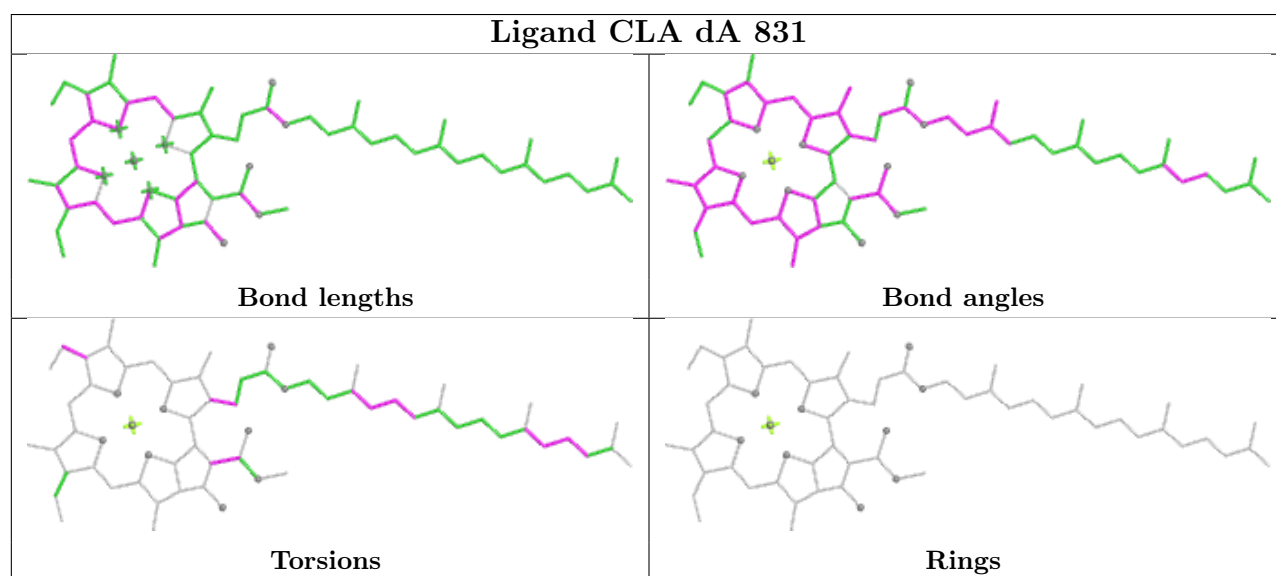
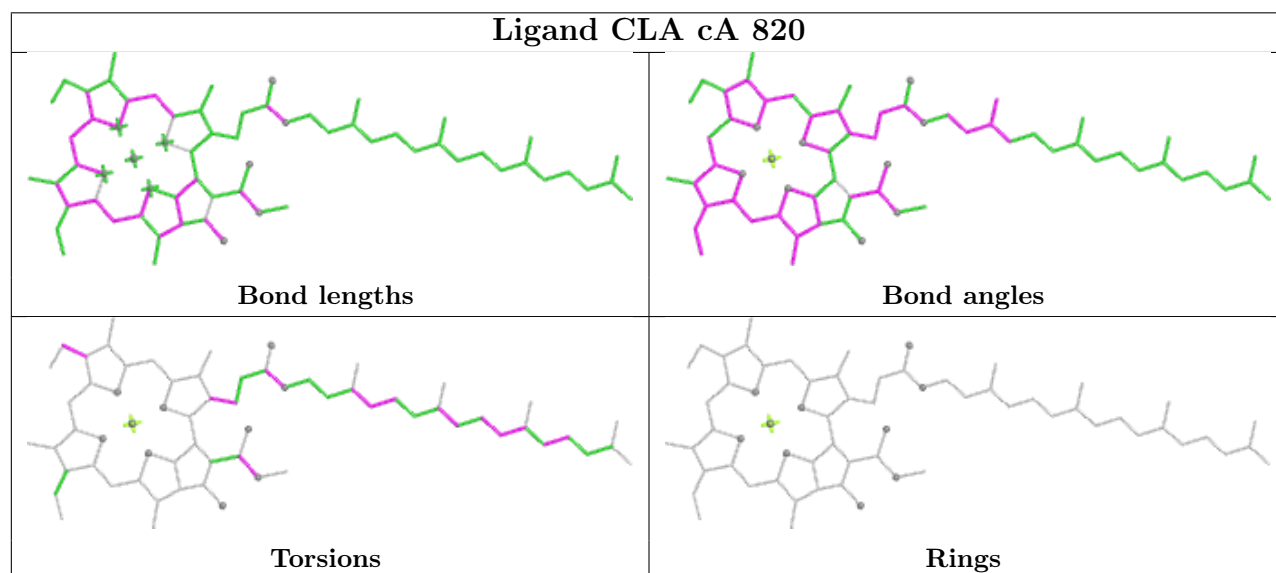
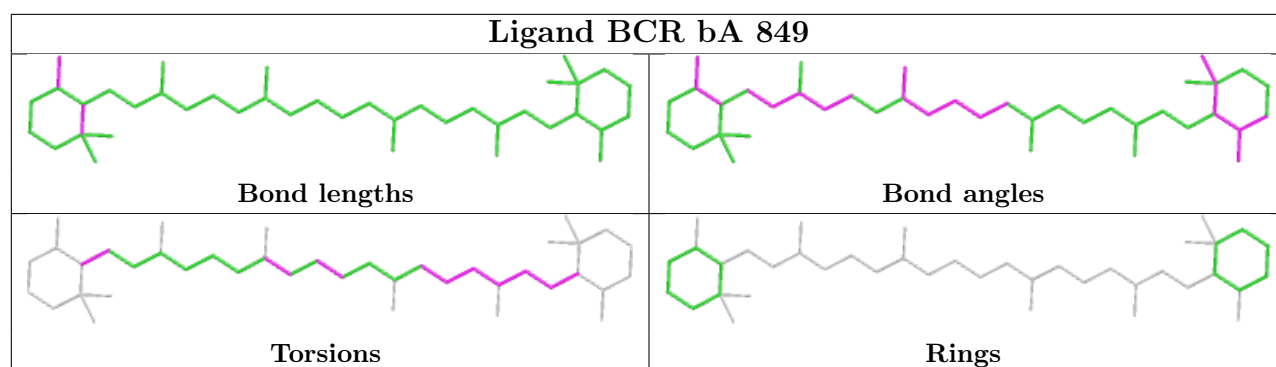


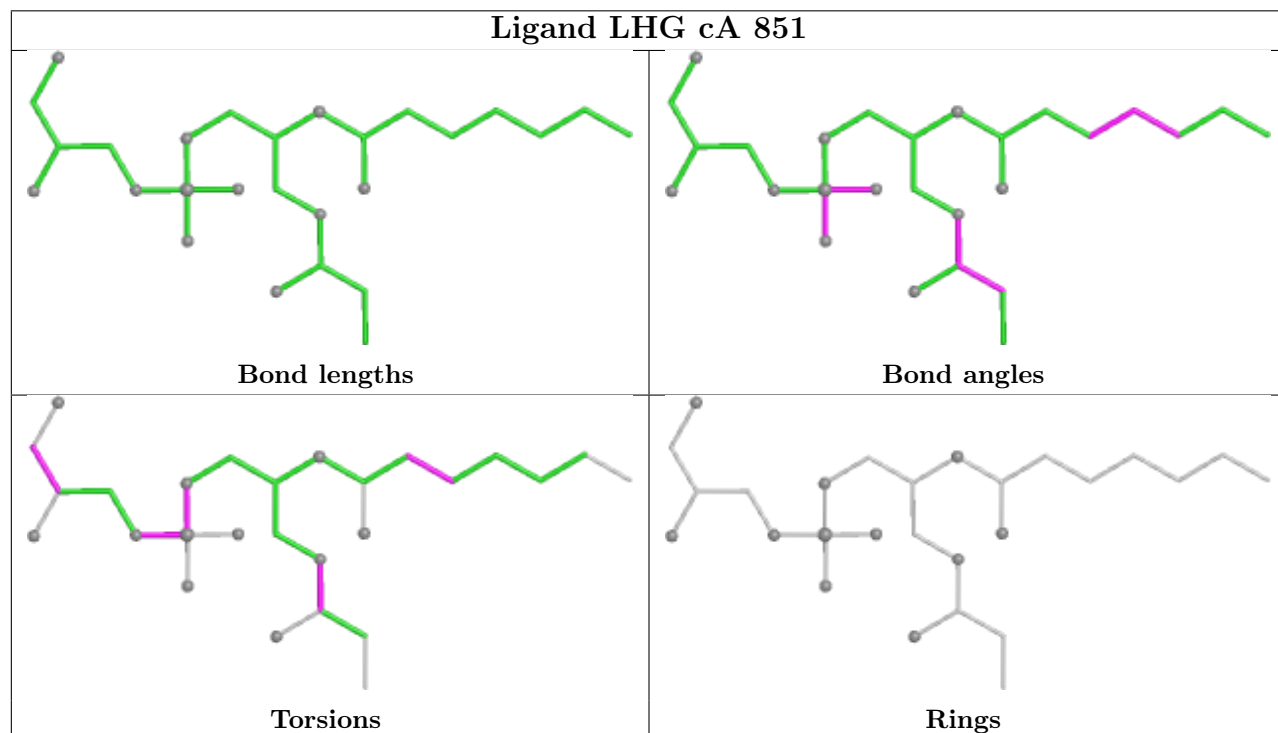
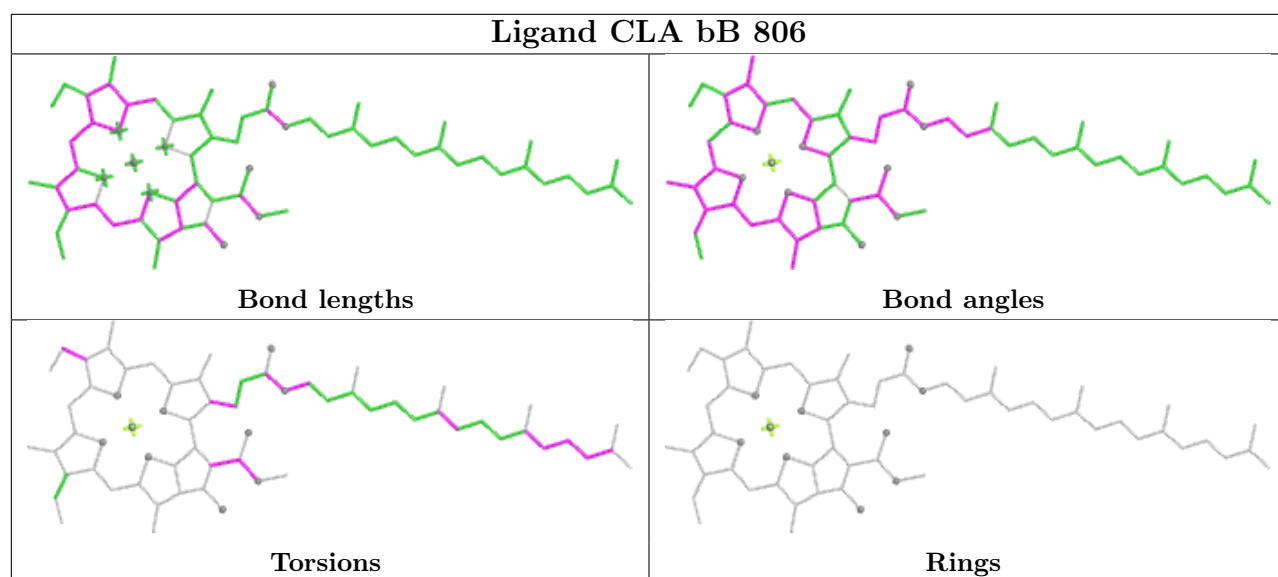


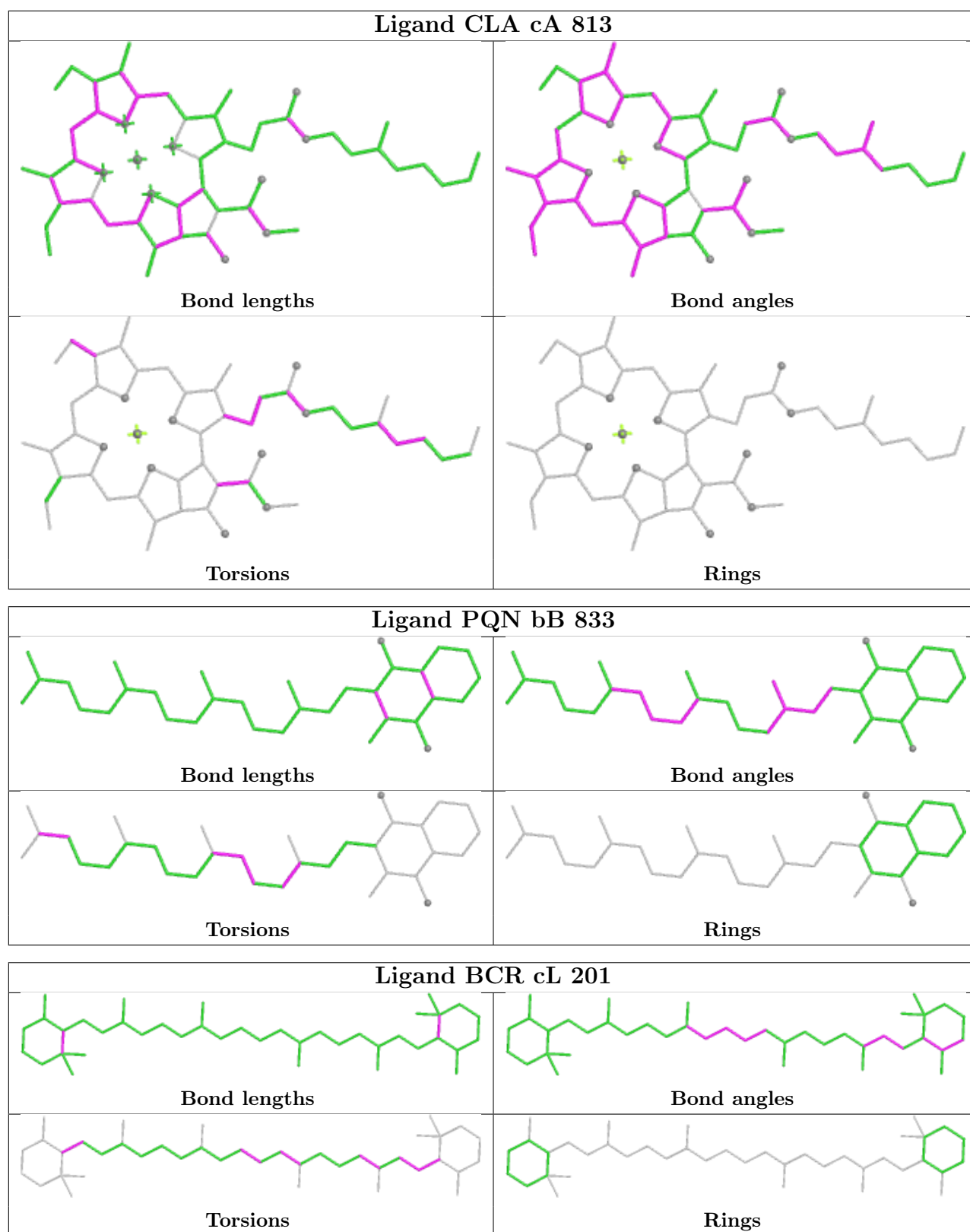


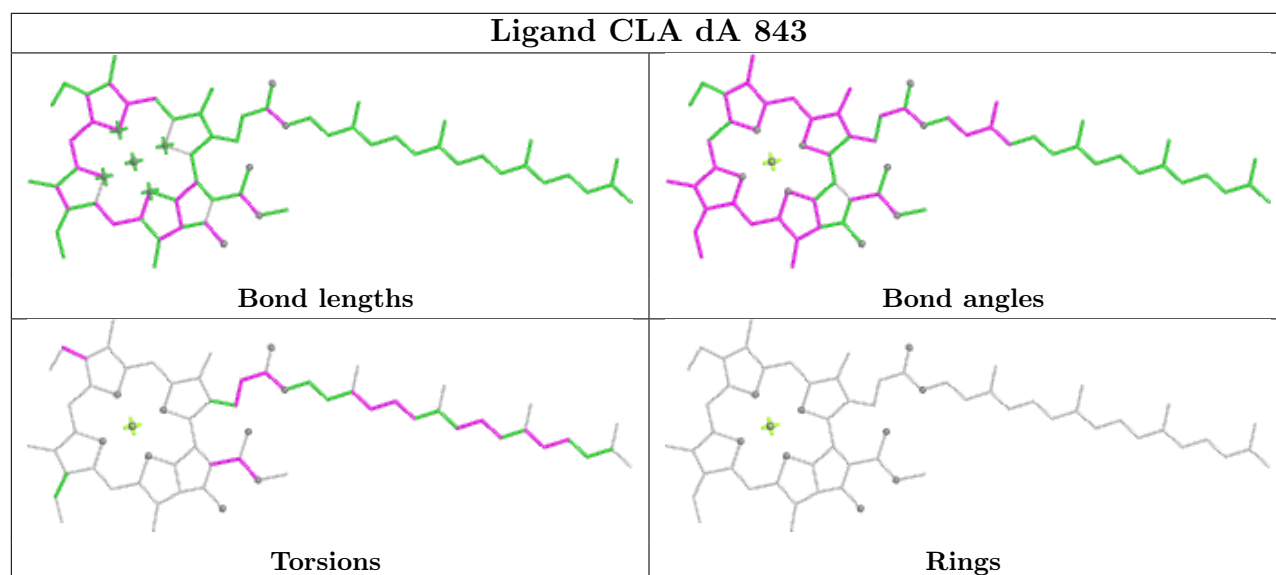
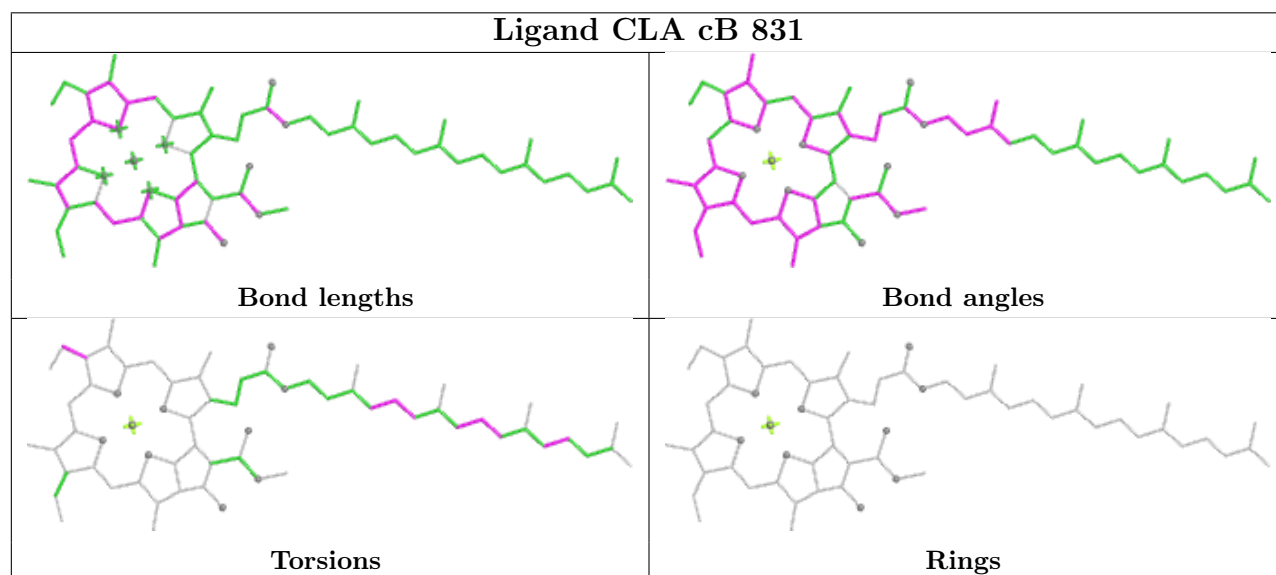
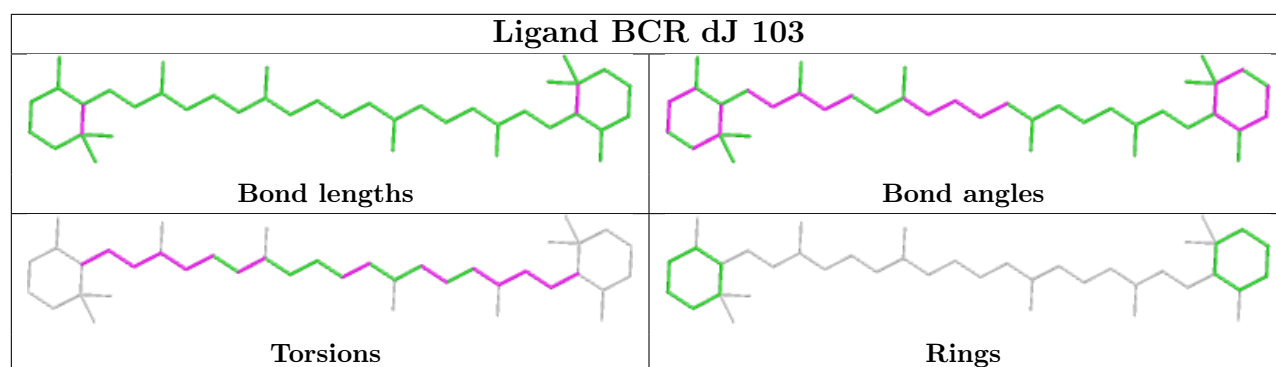


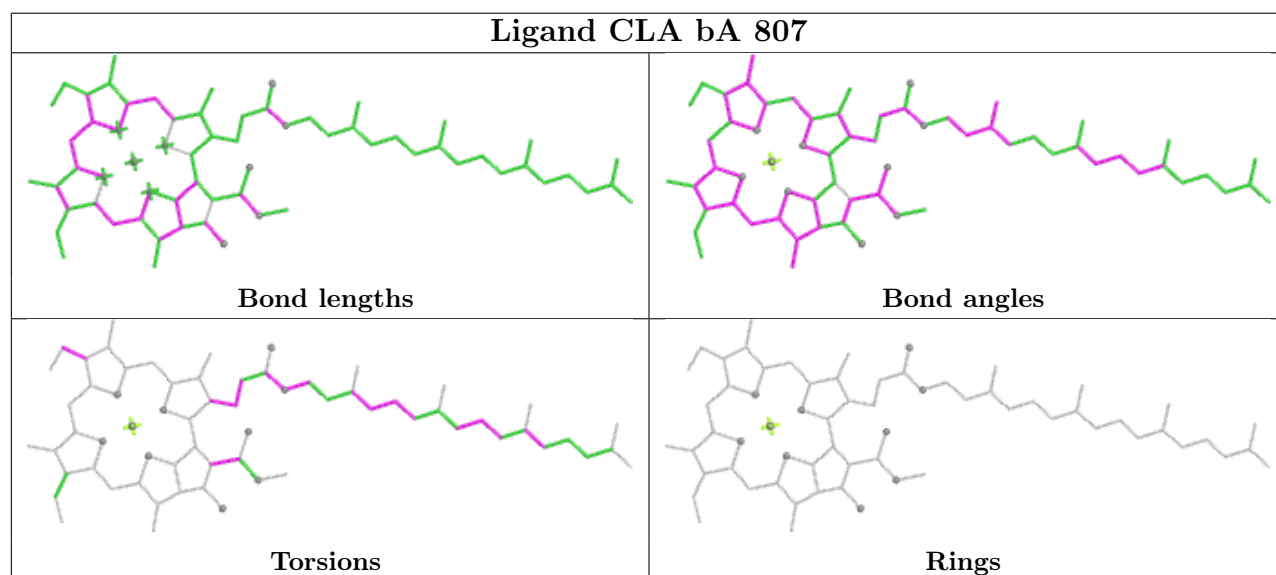
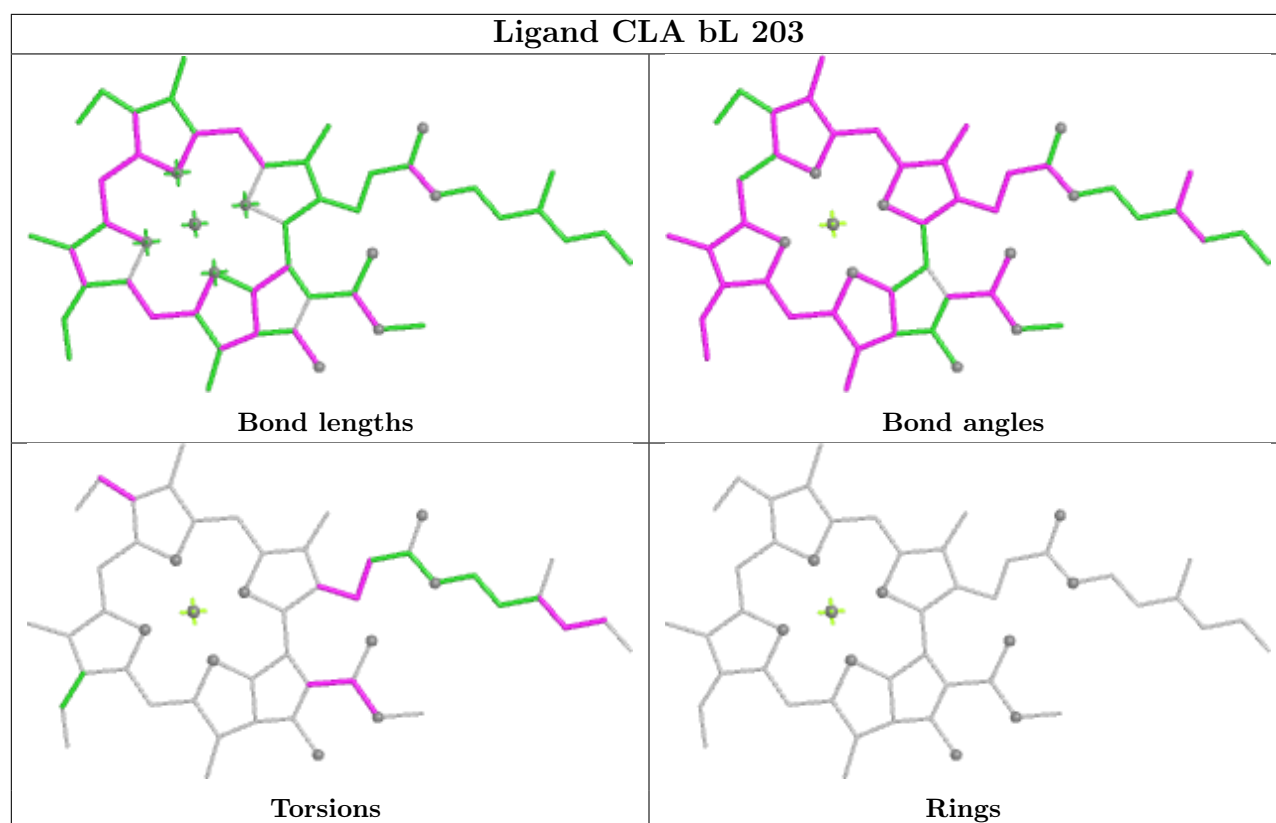




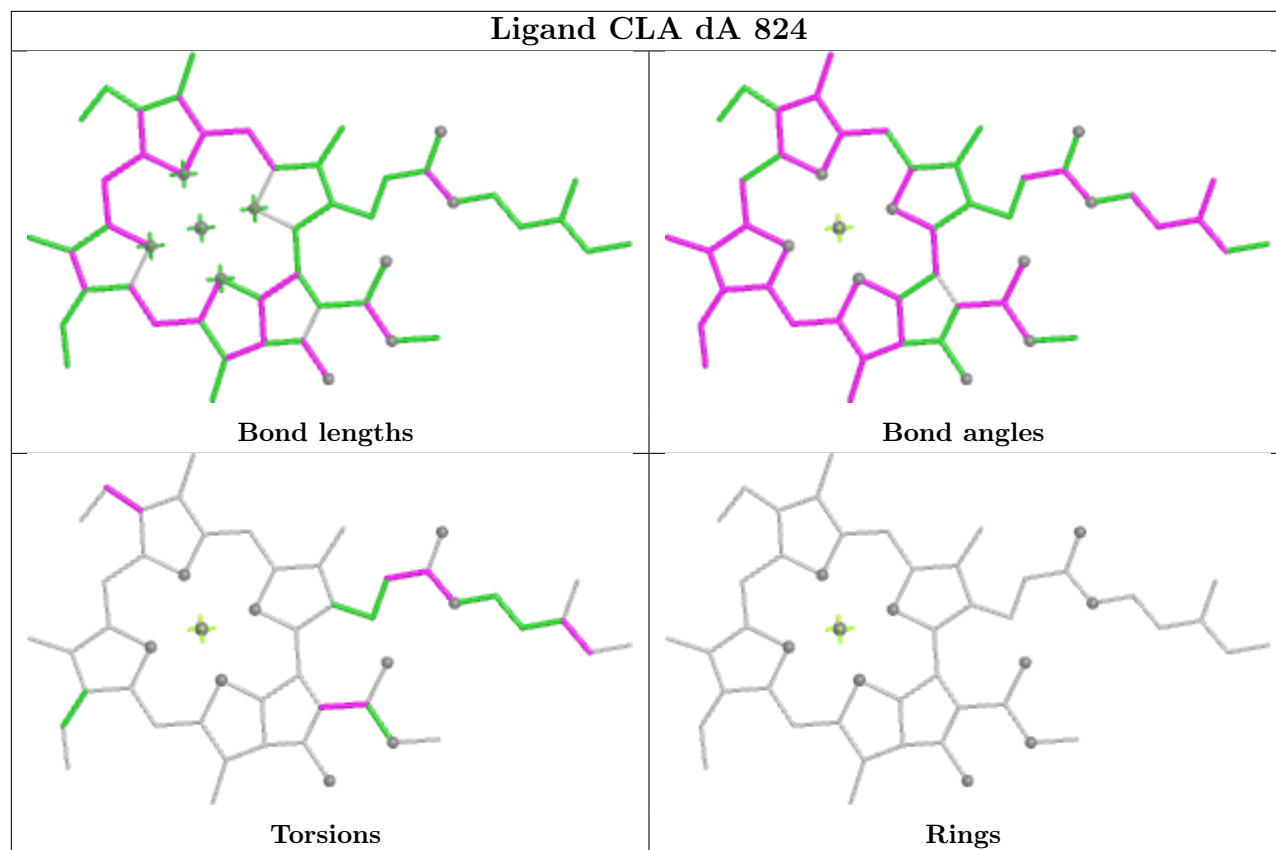




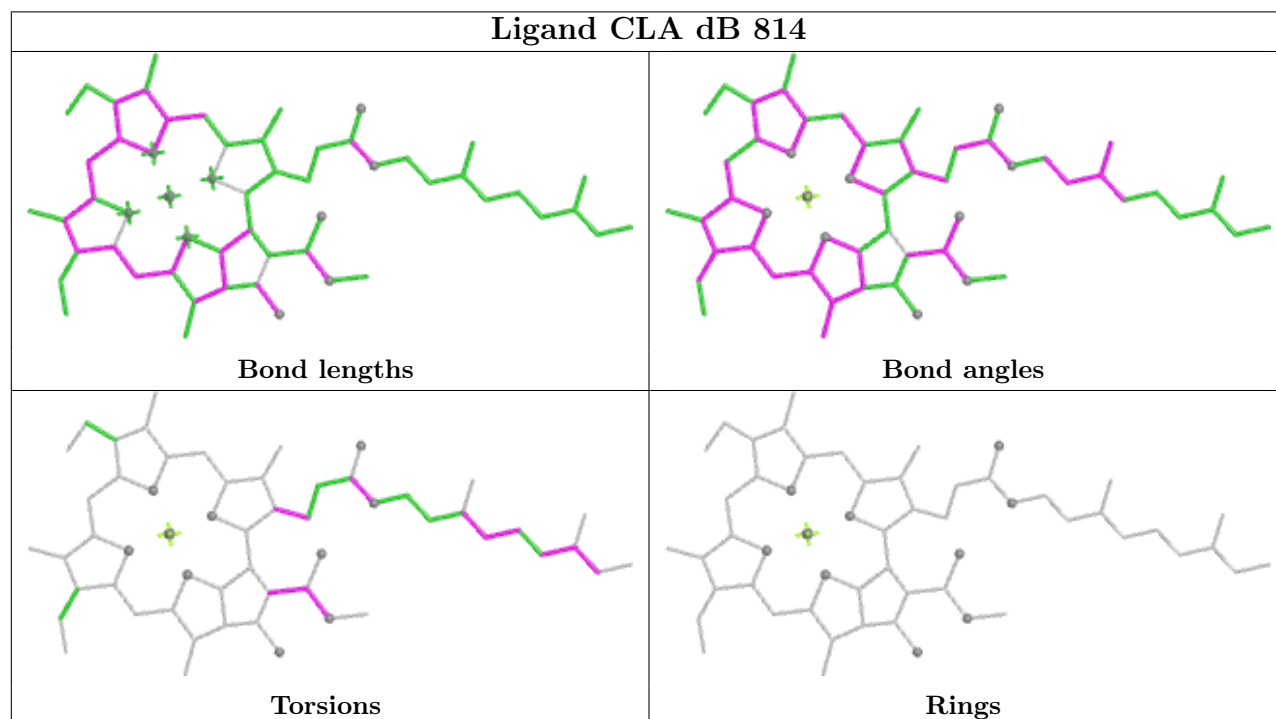


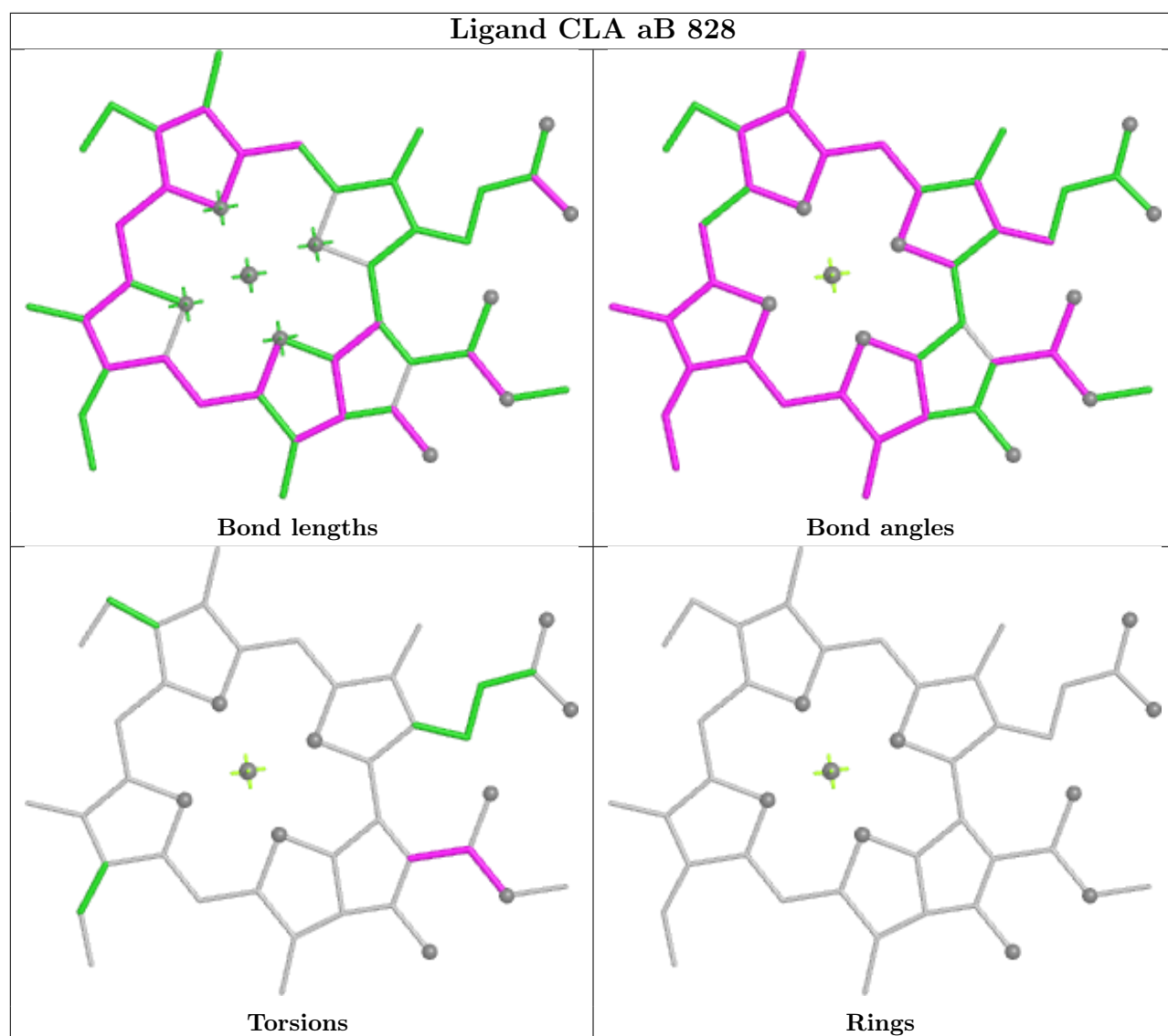


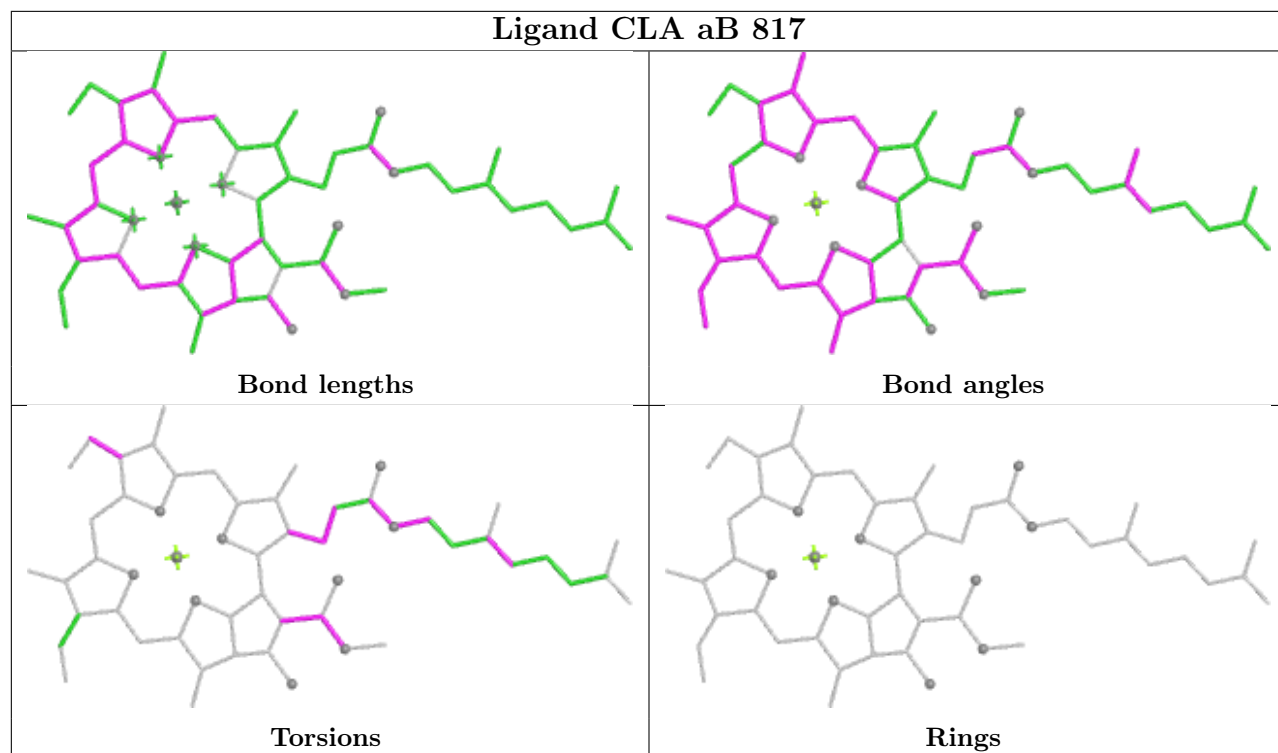
Ligand CLA dA 824

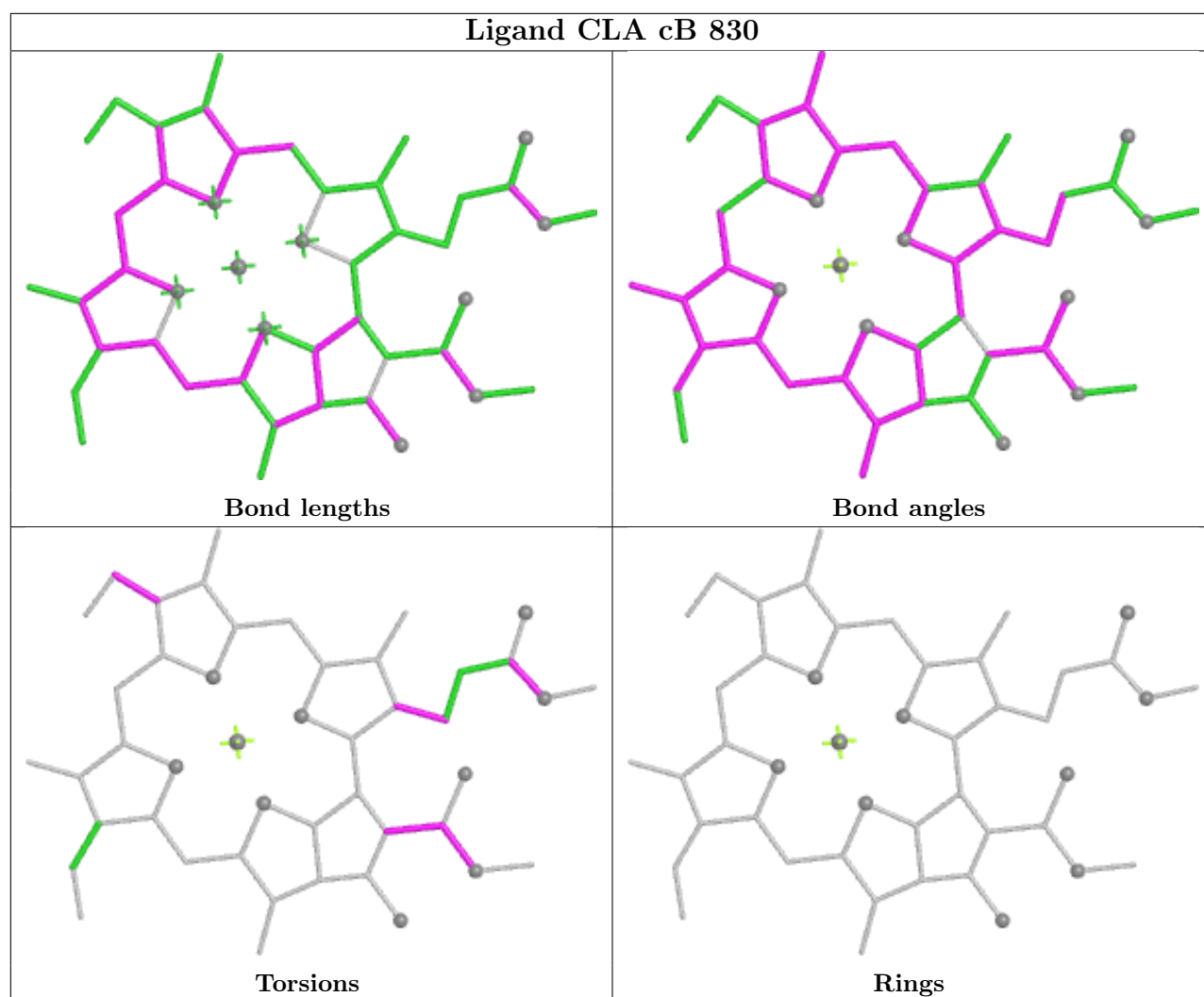


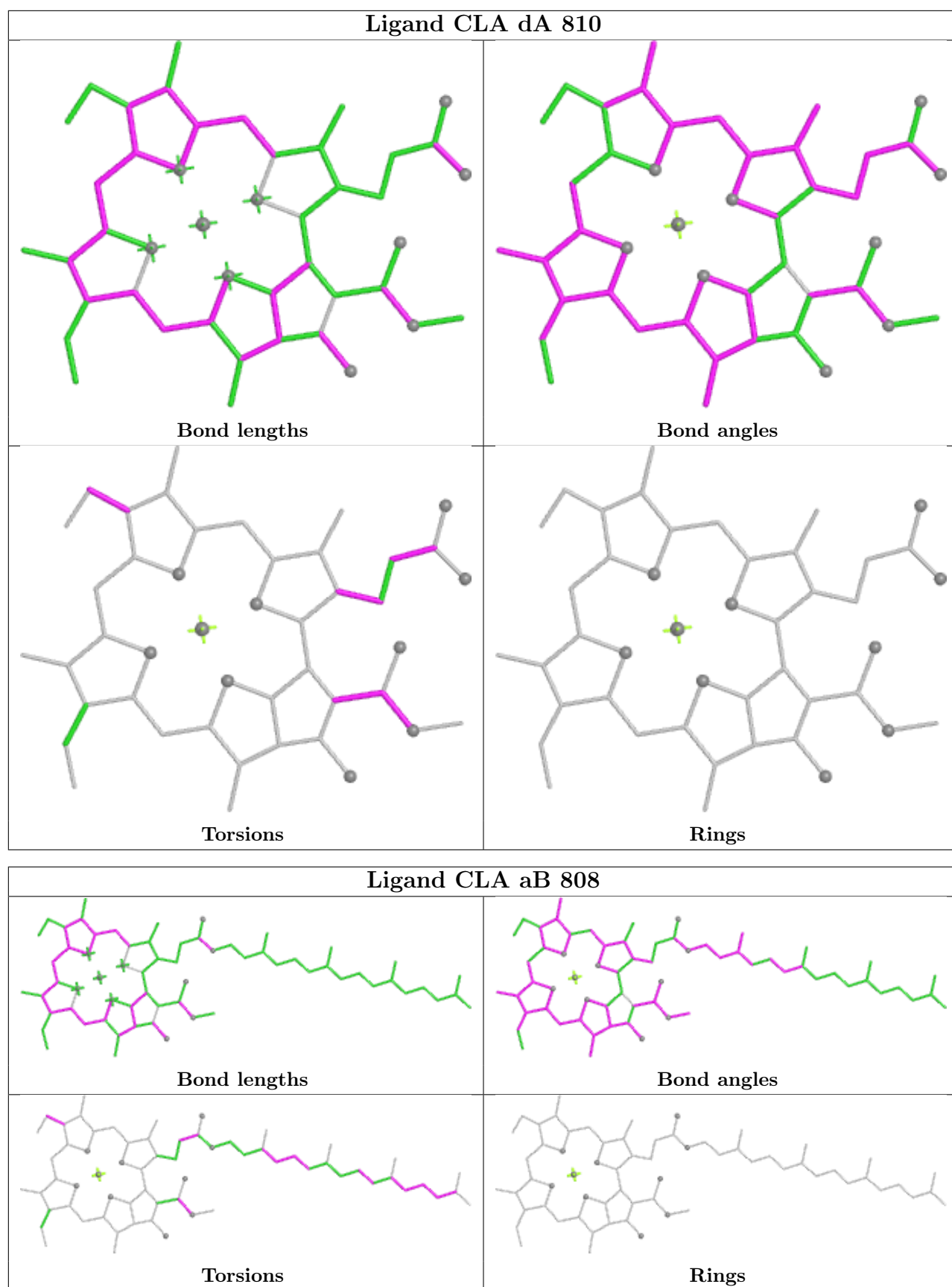
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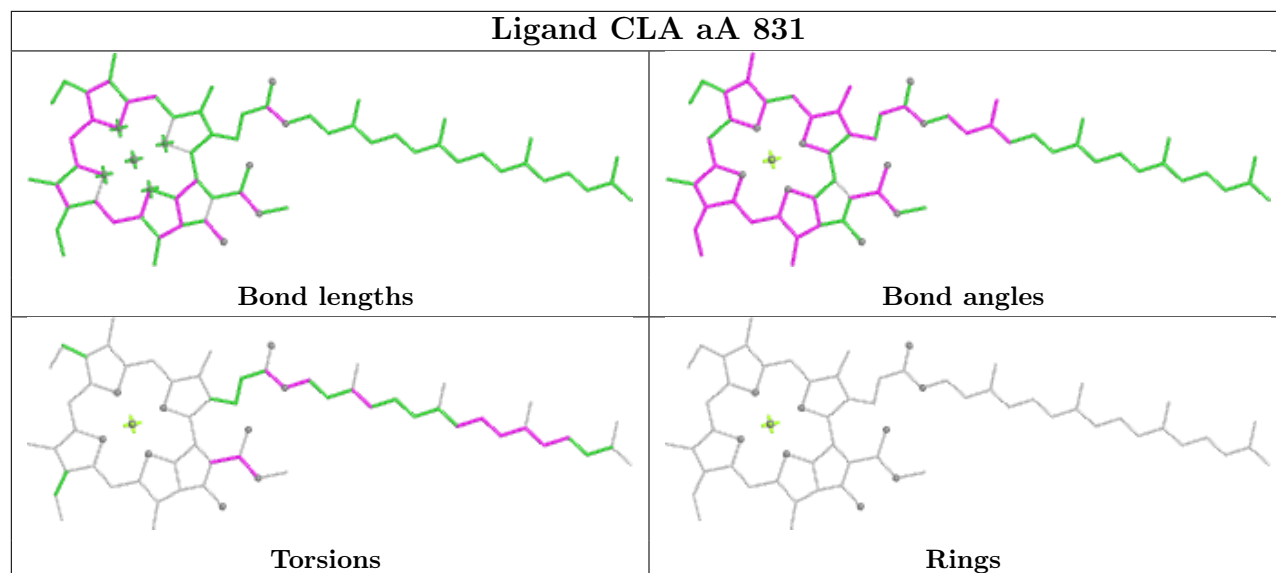
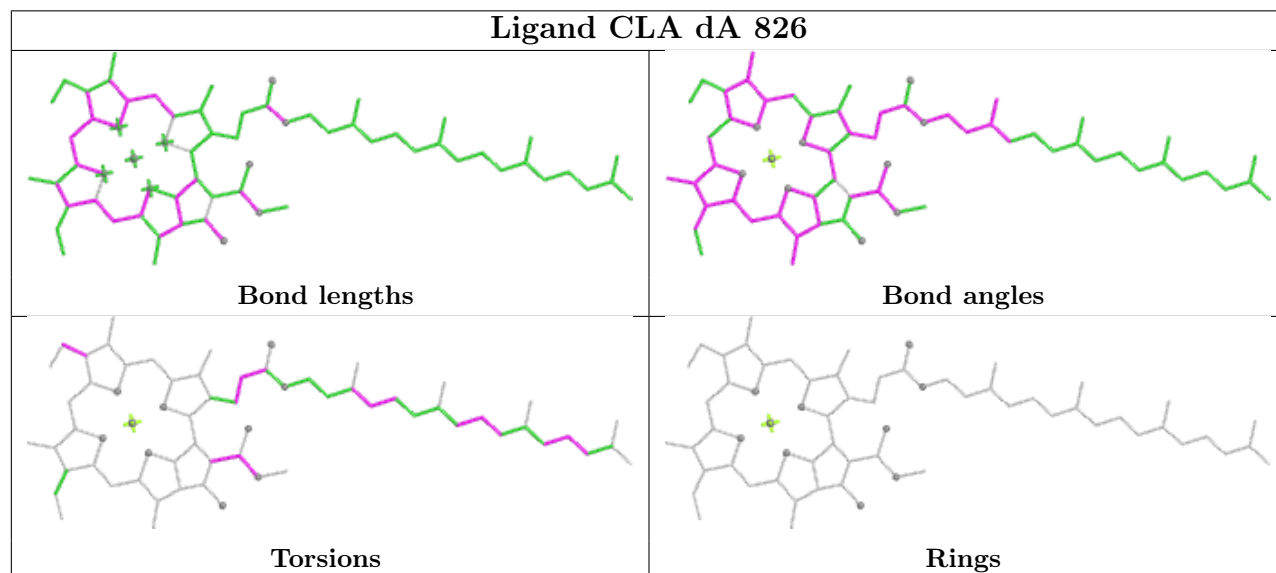
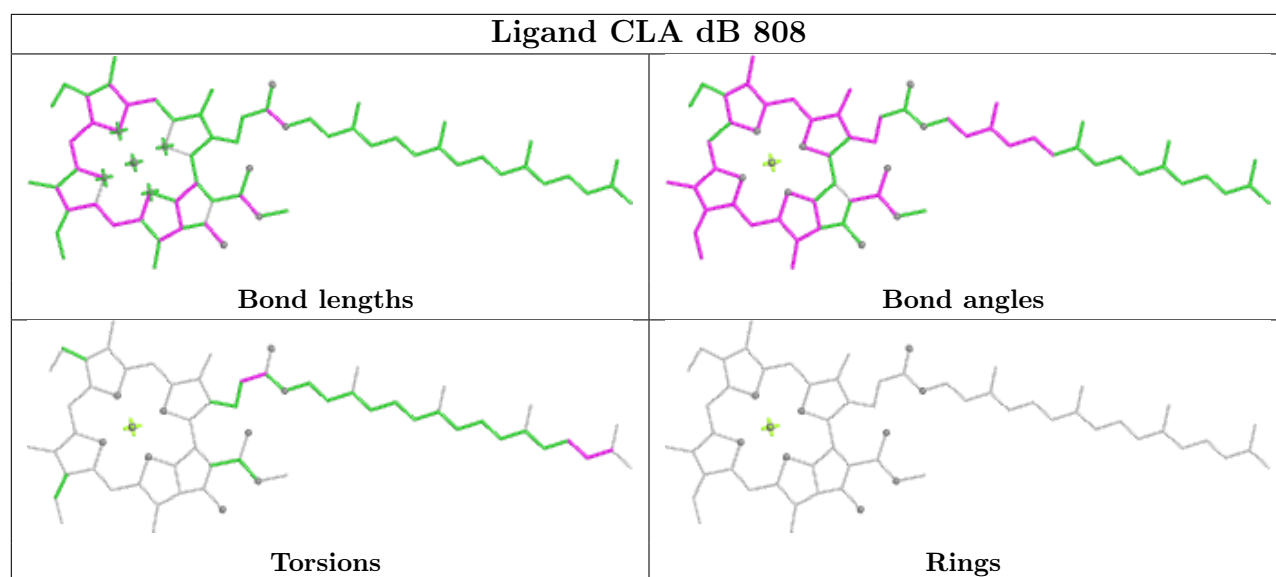


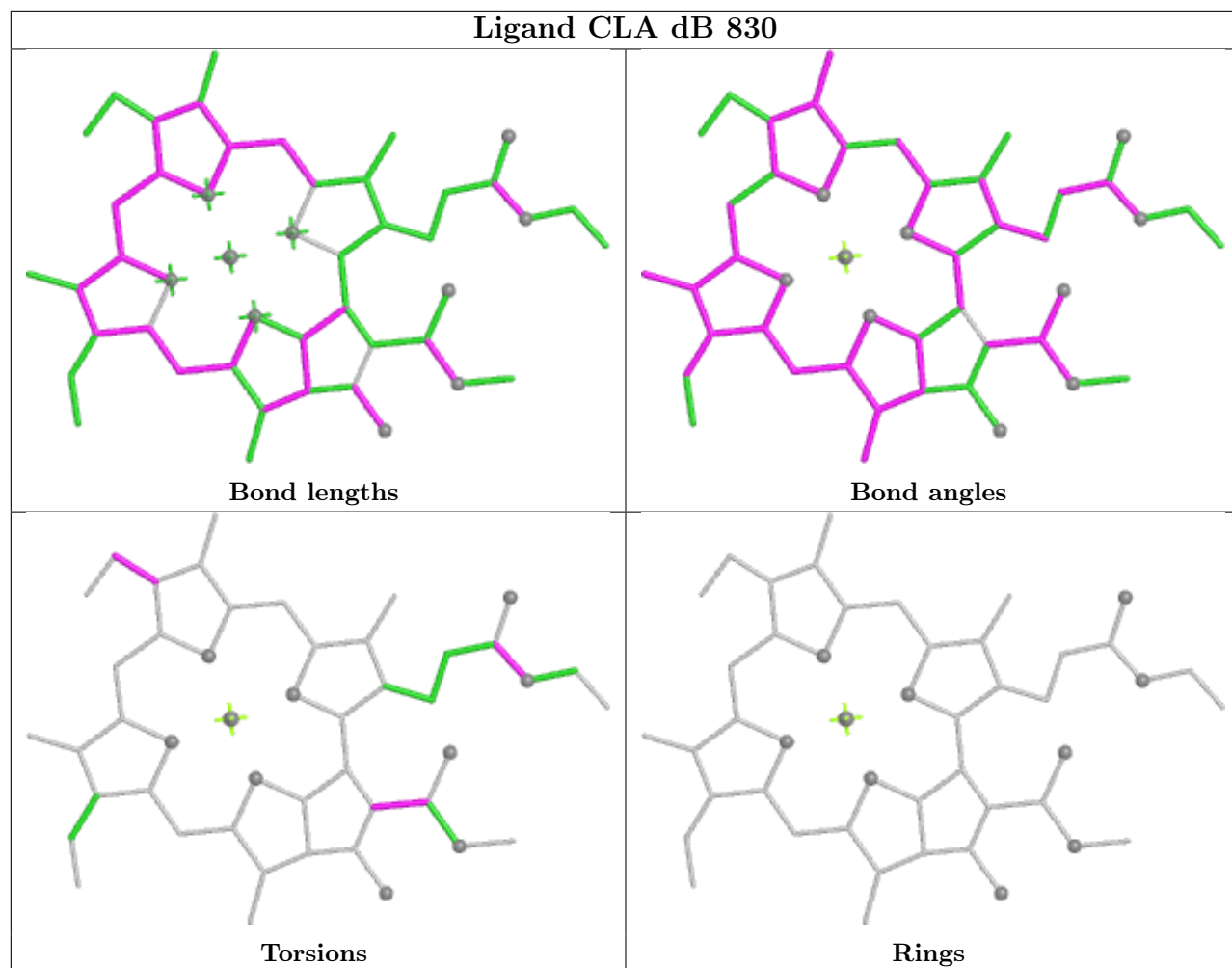


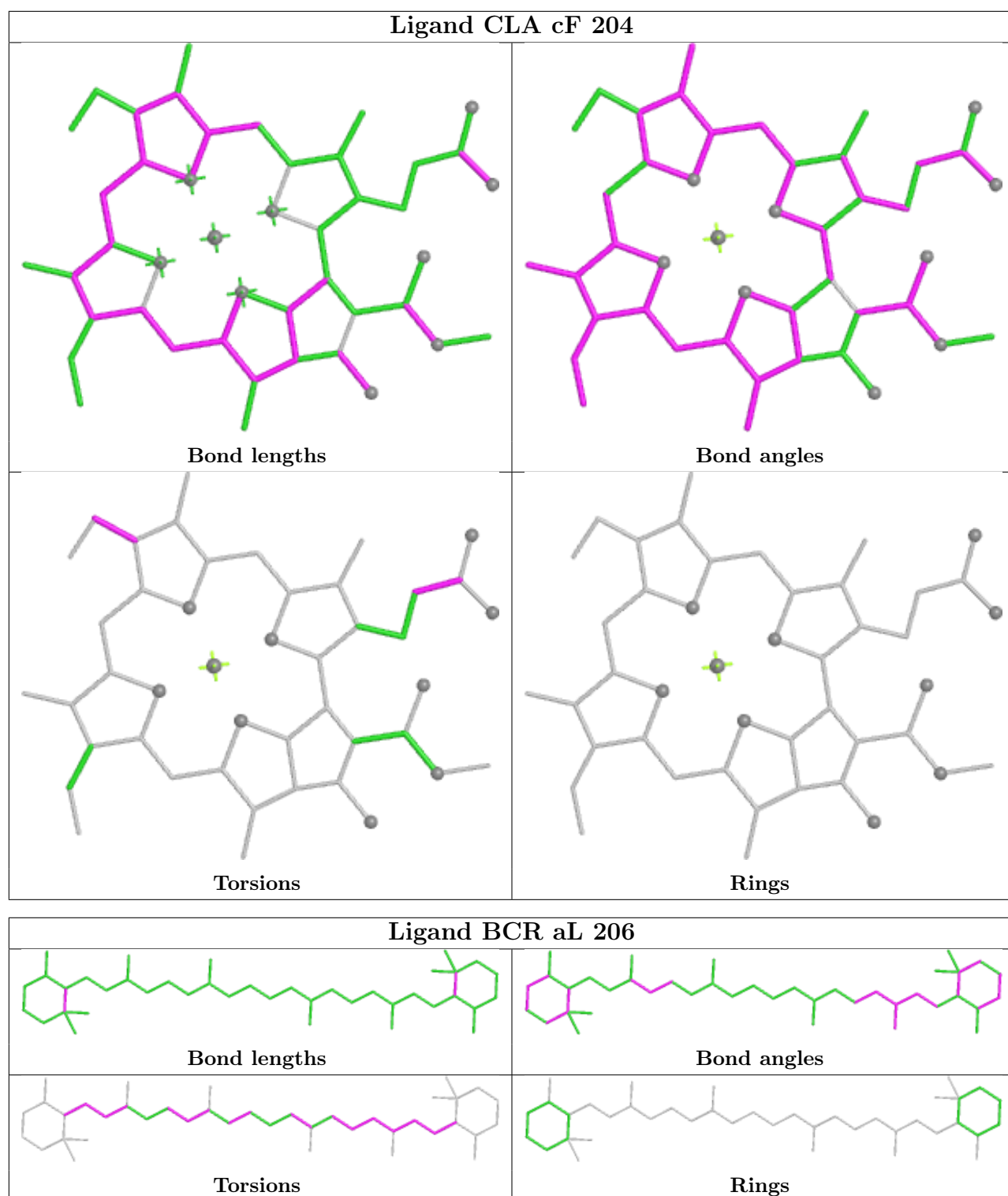


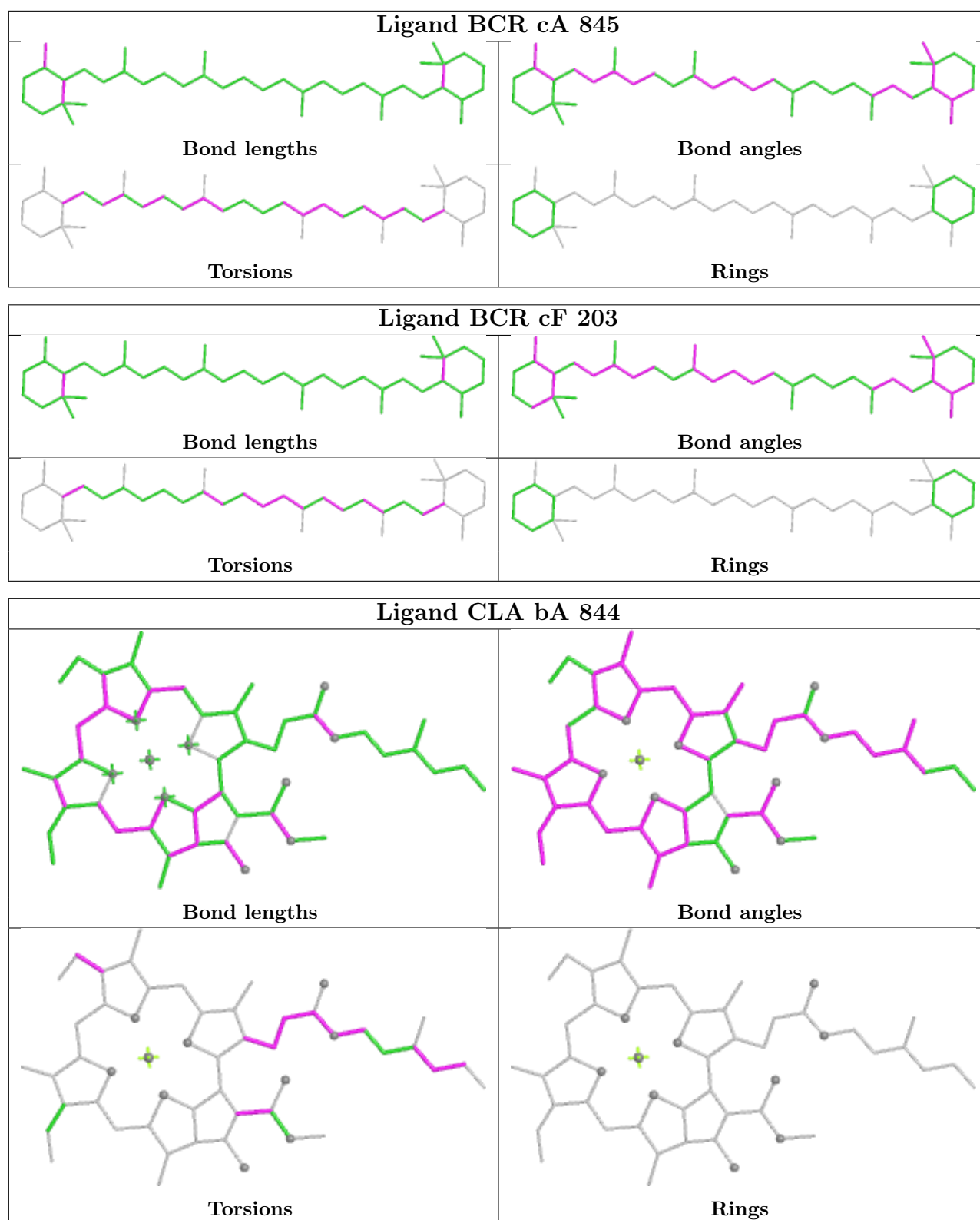


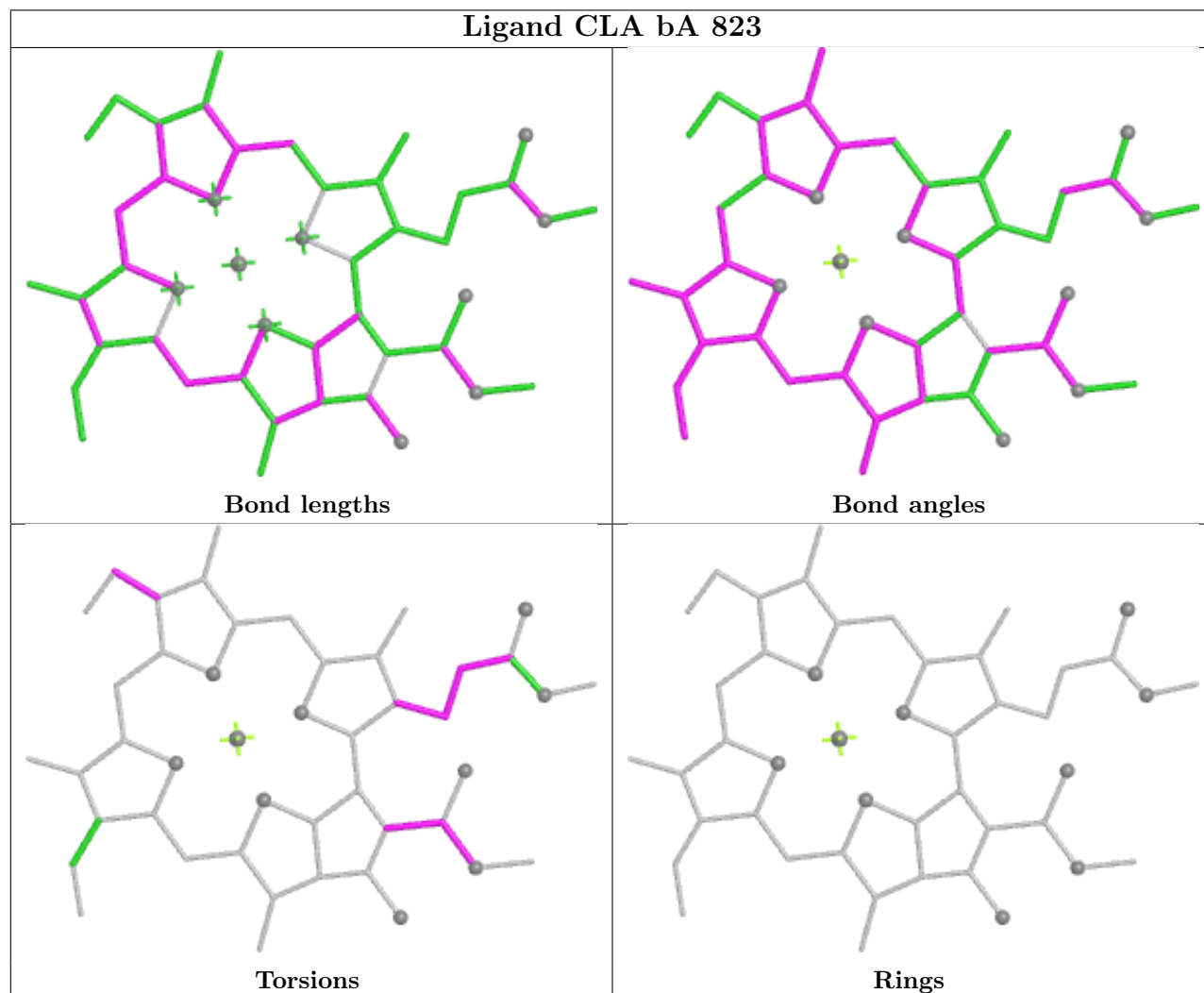
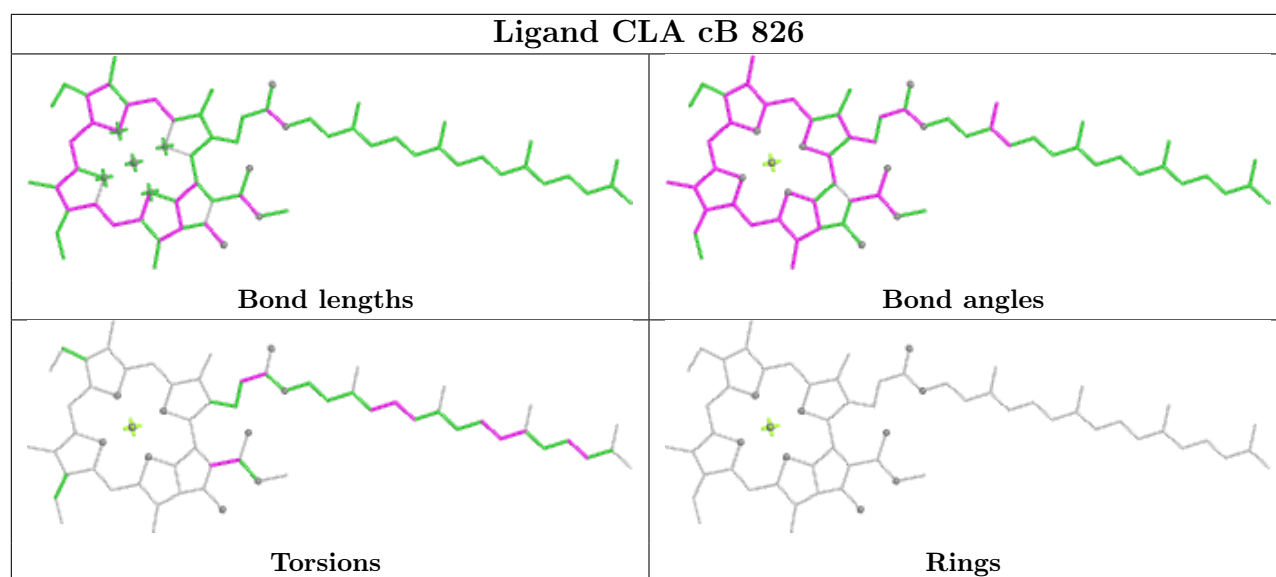


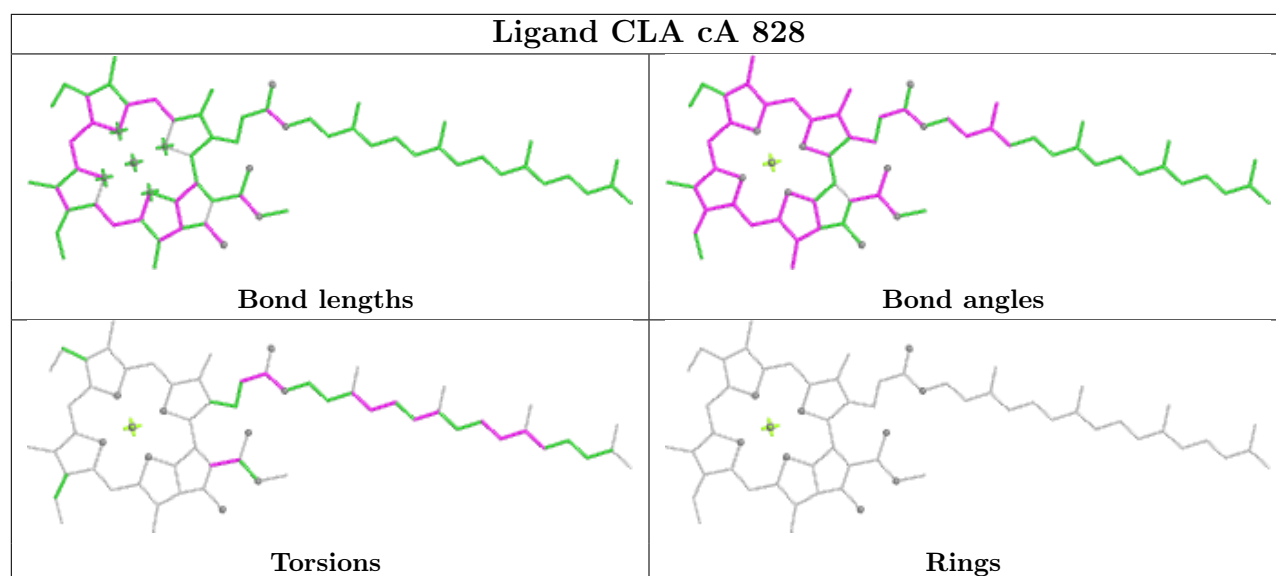
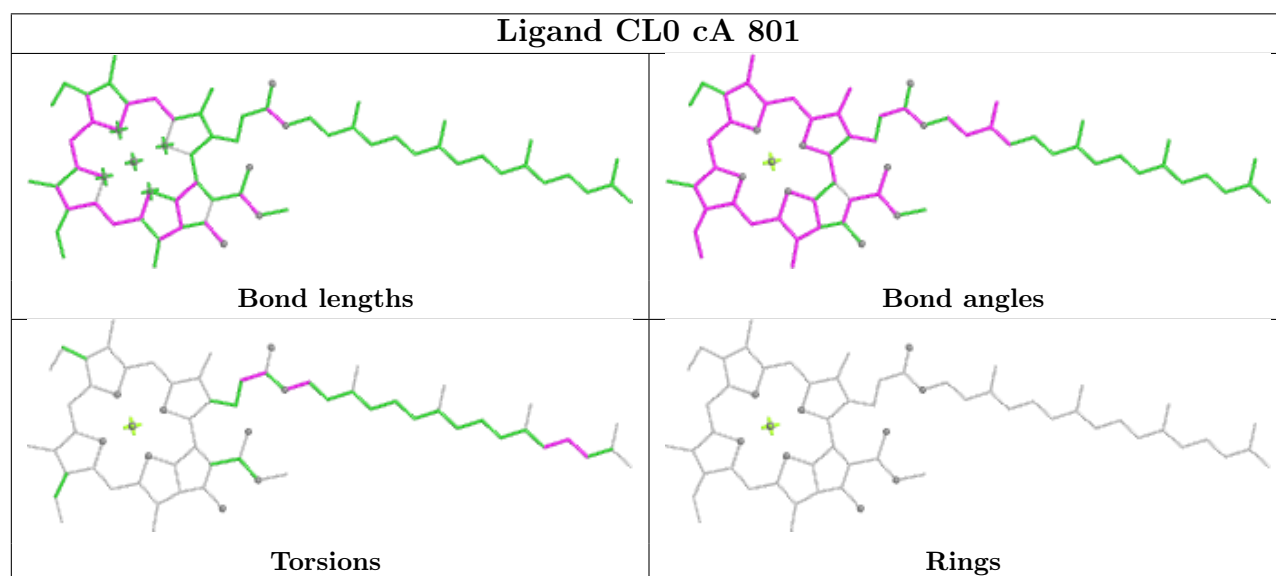
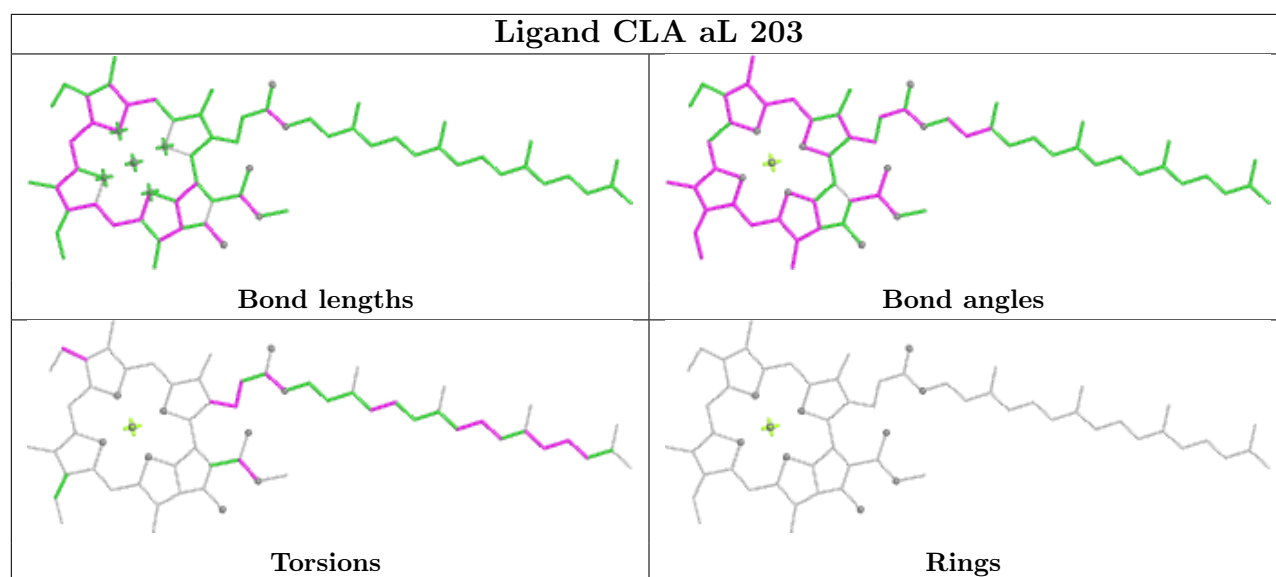


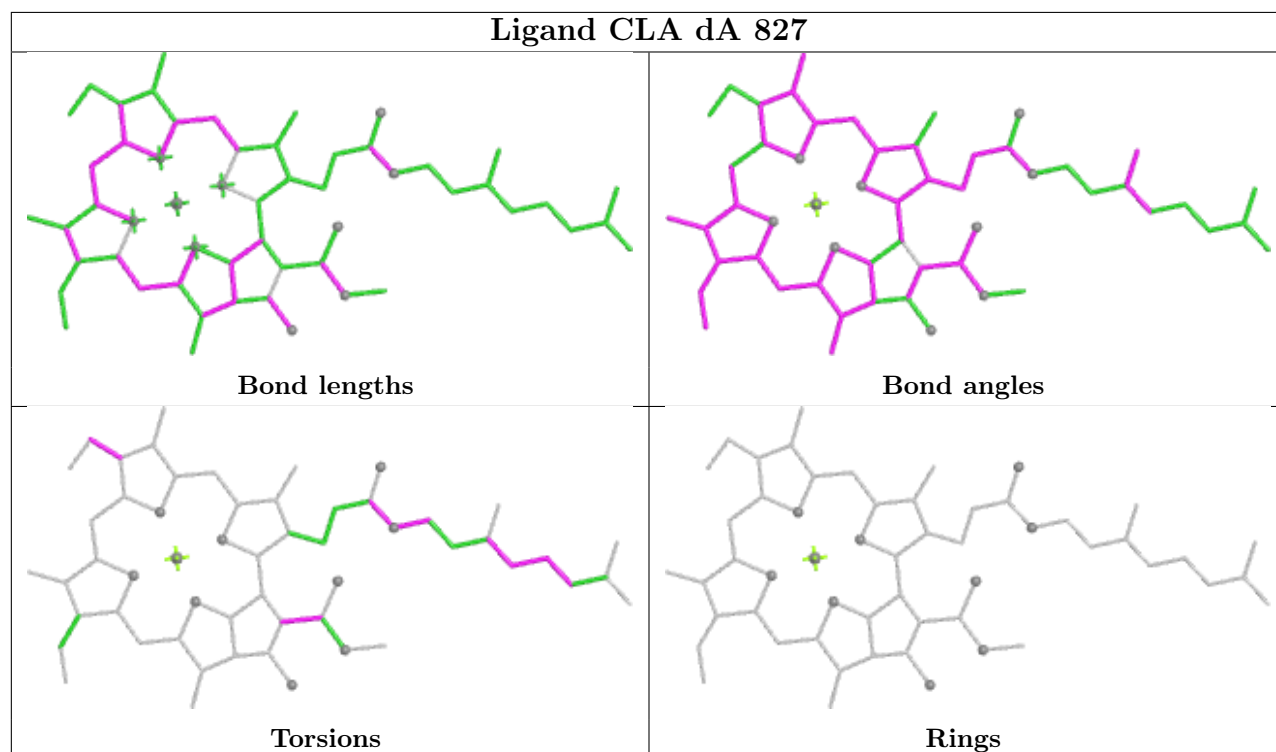
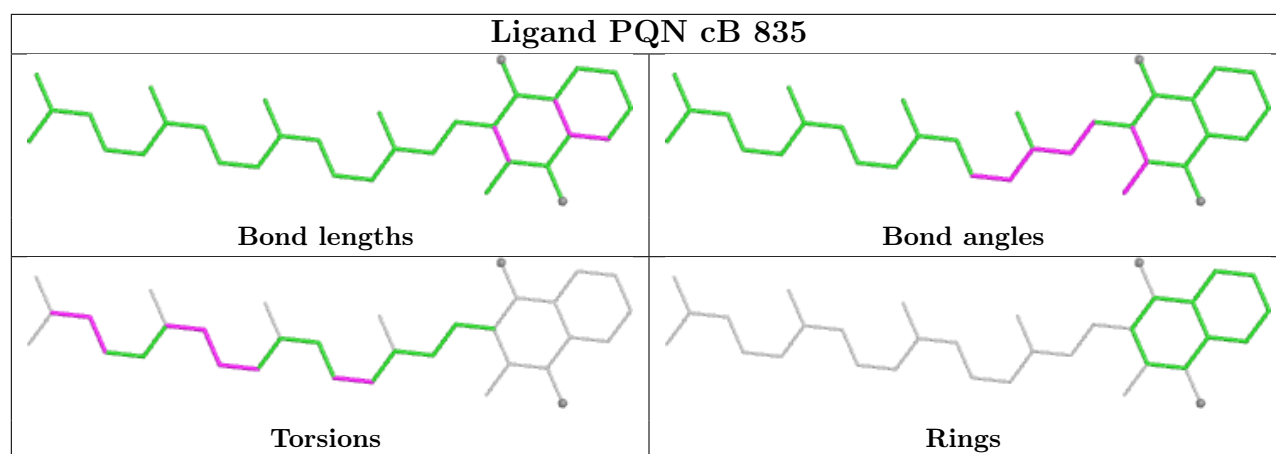


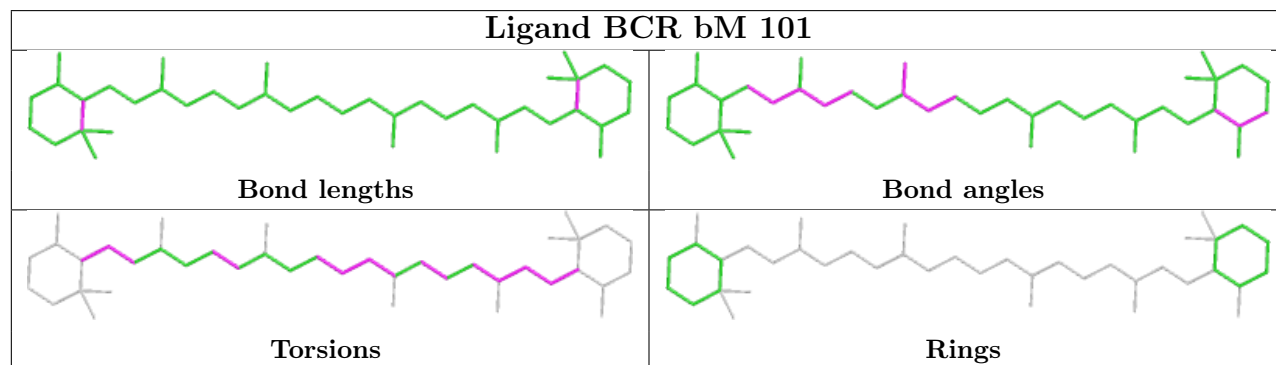
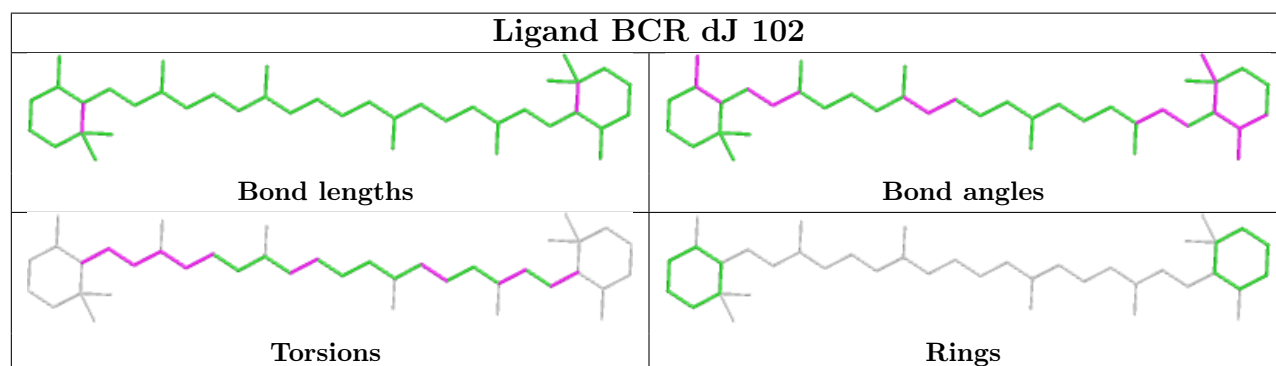
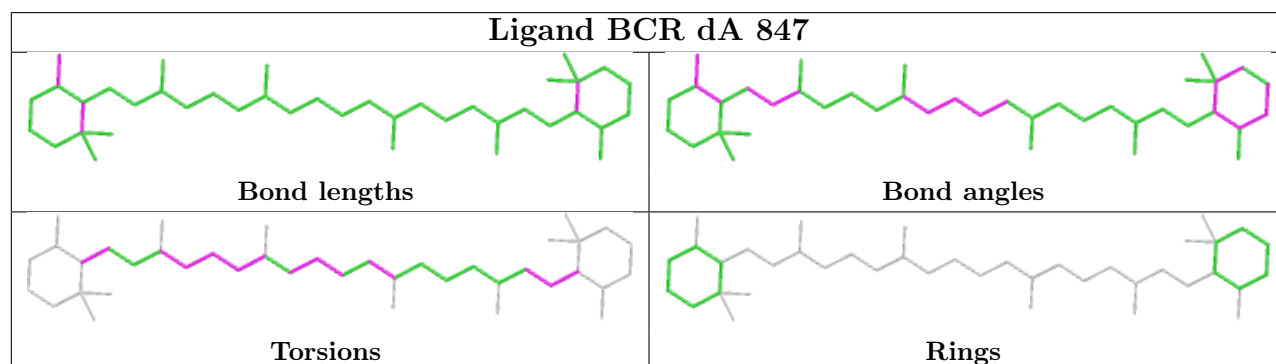
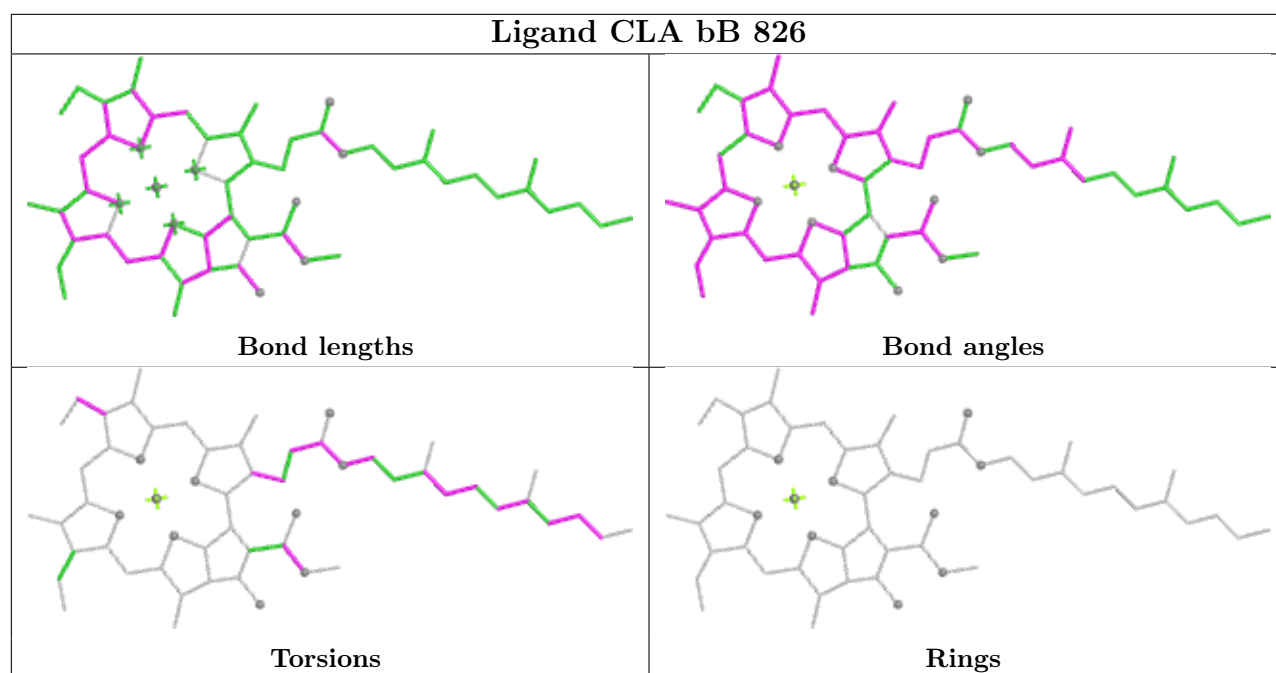


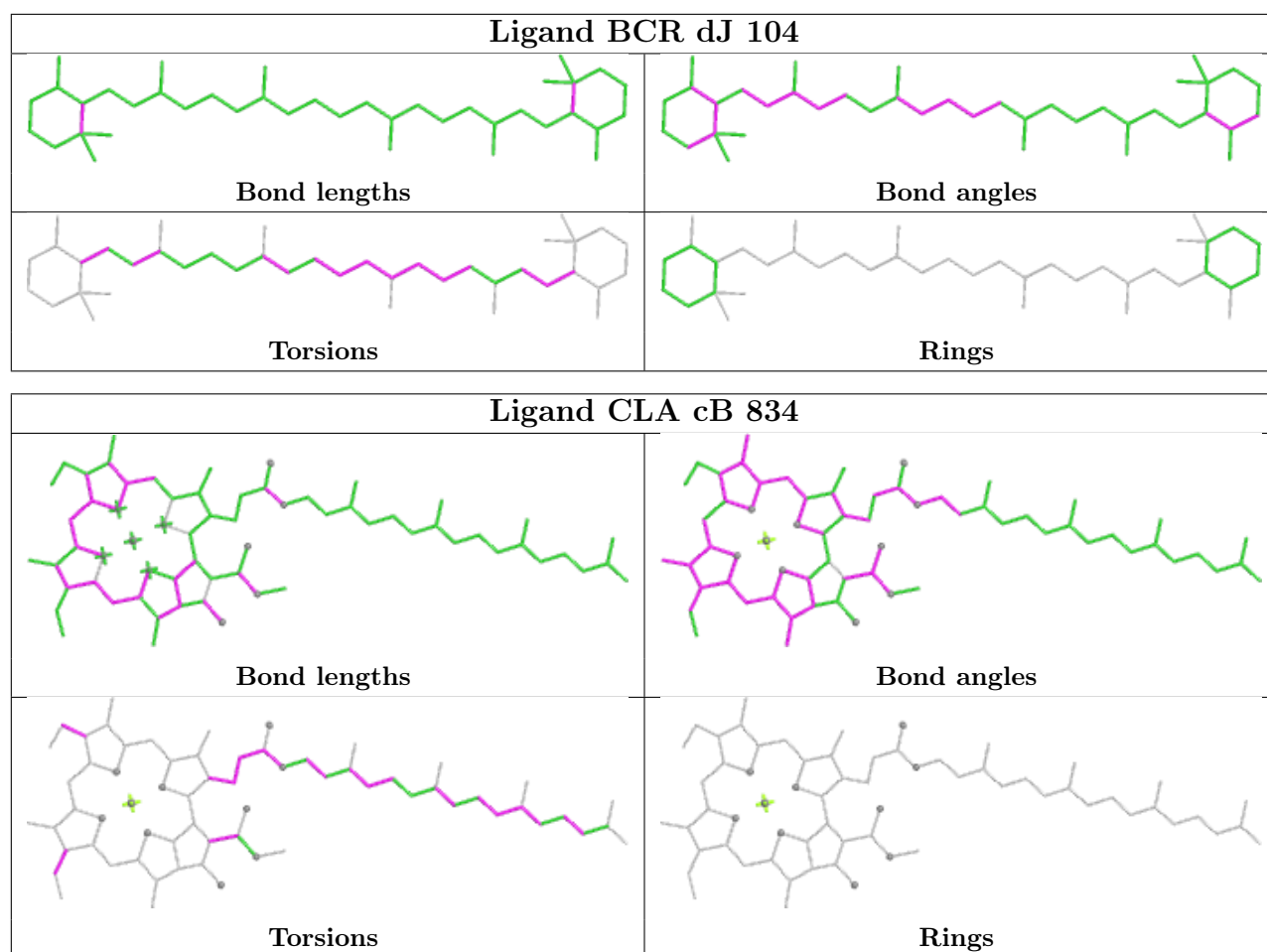


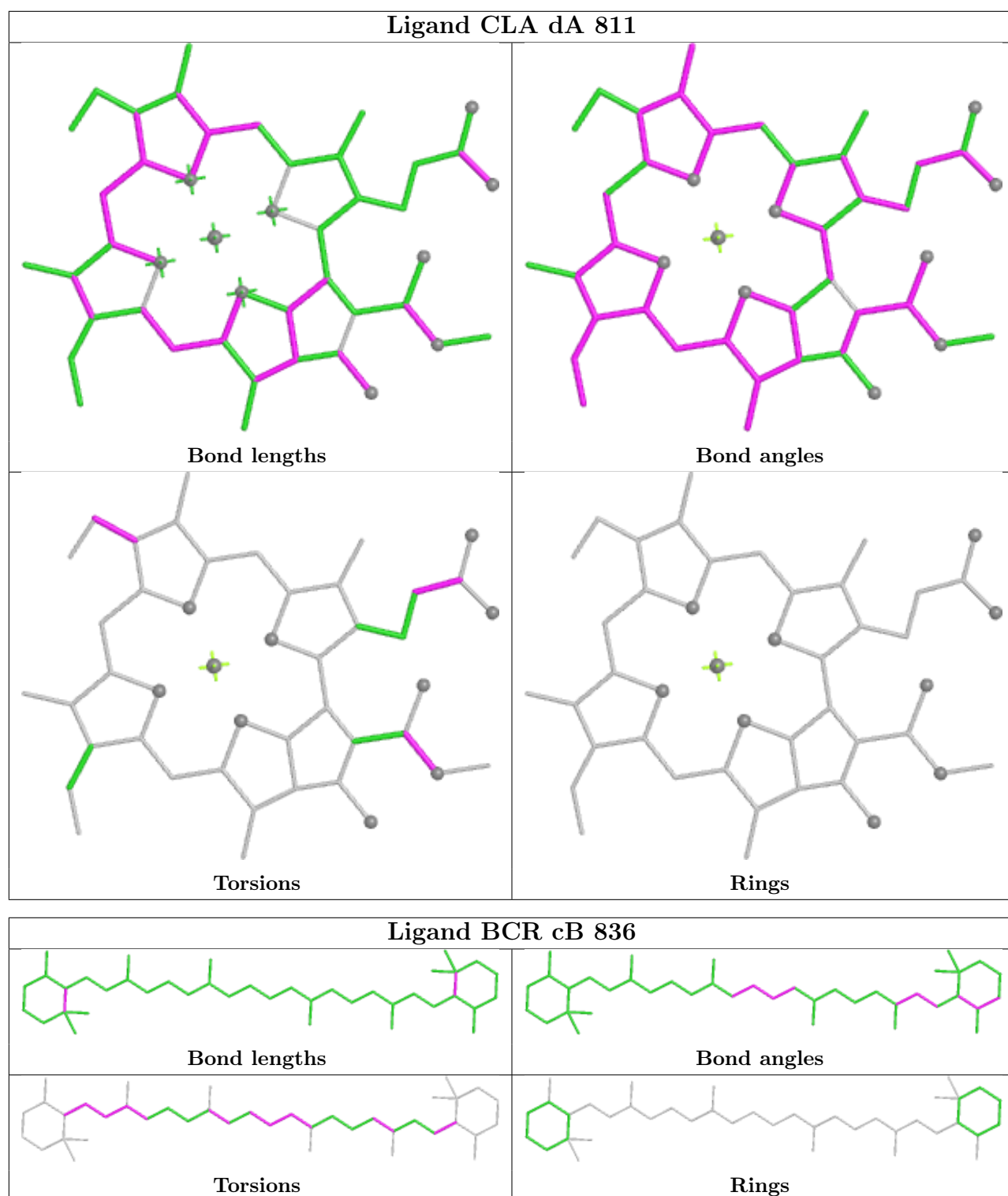


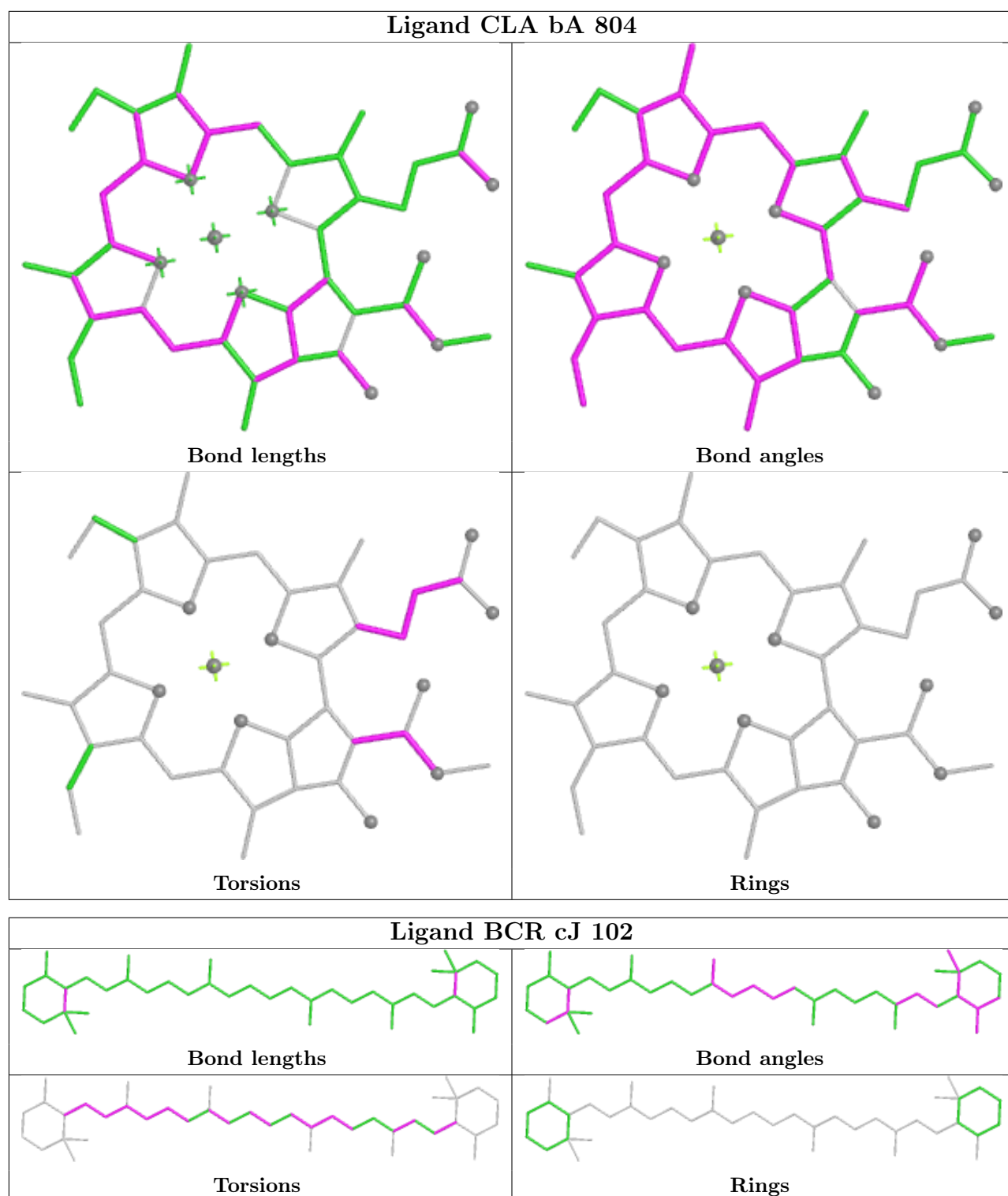


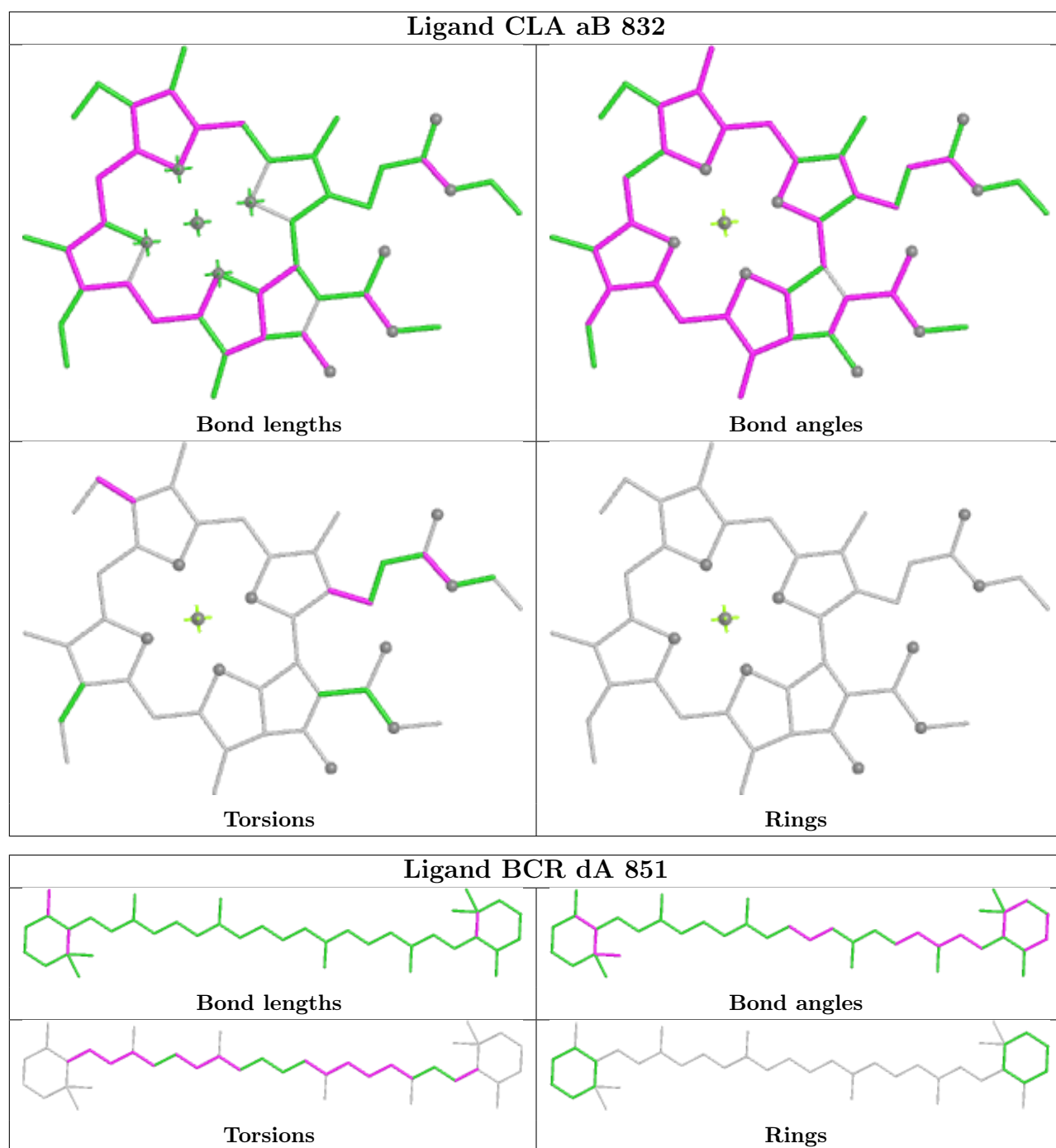




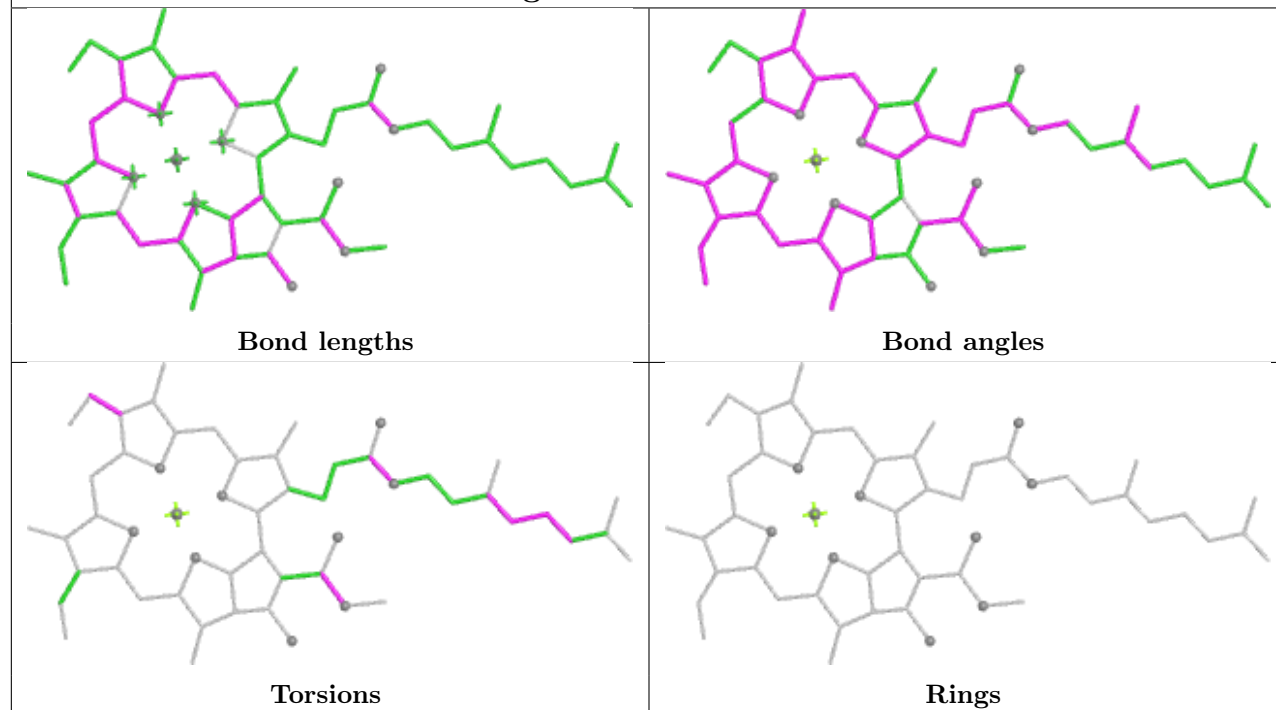




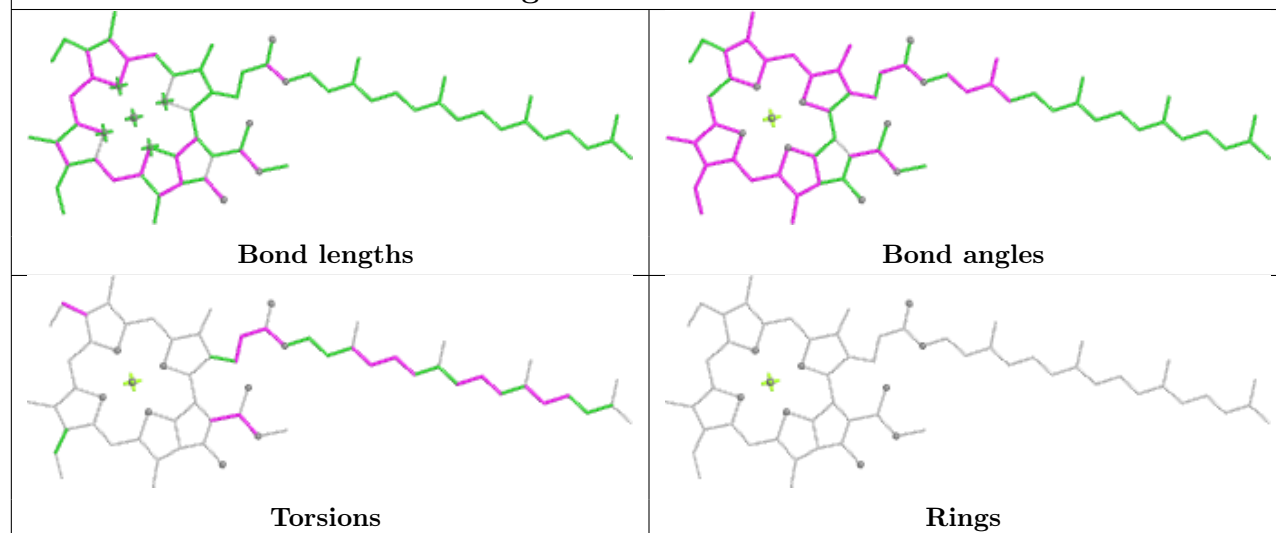


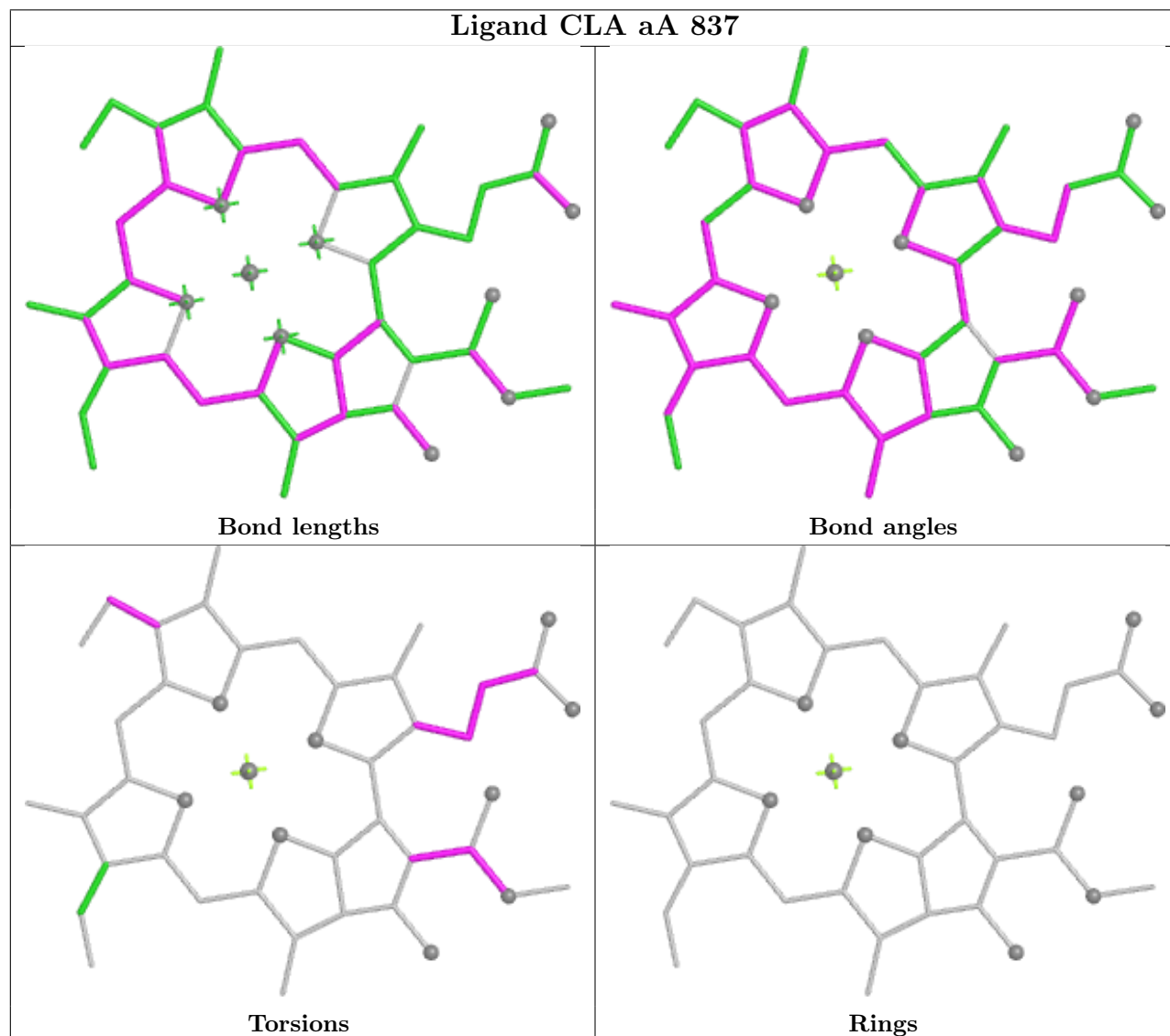
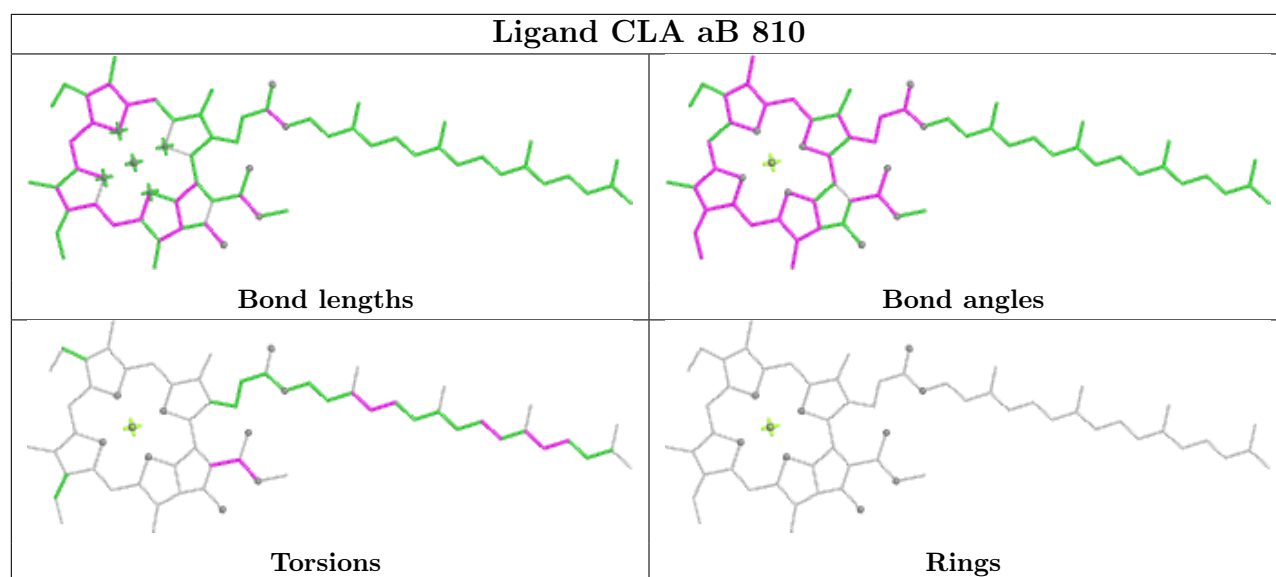


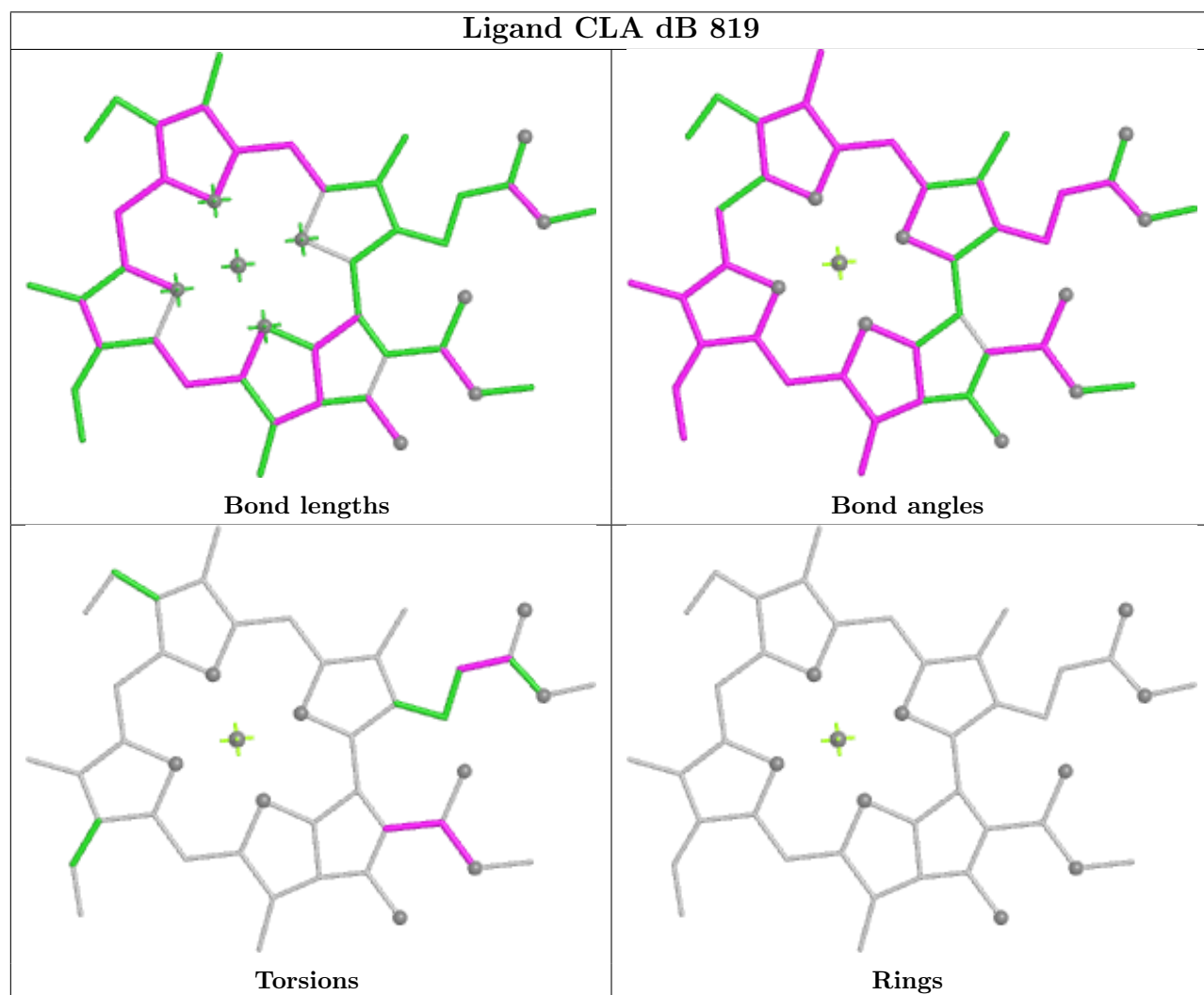
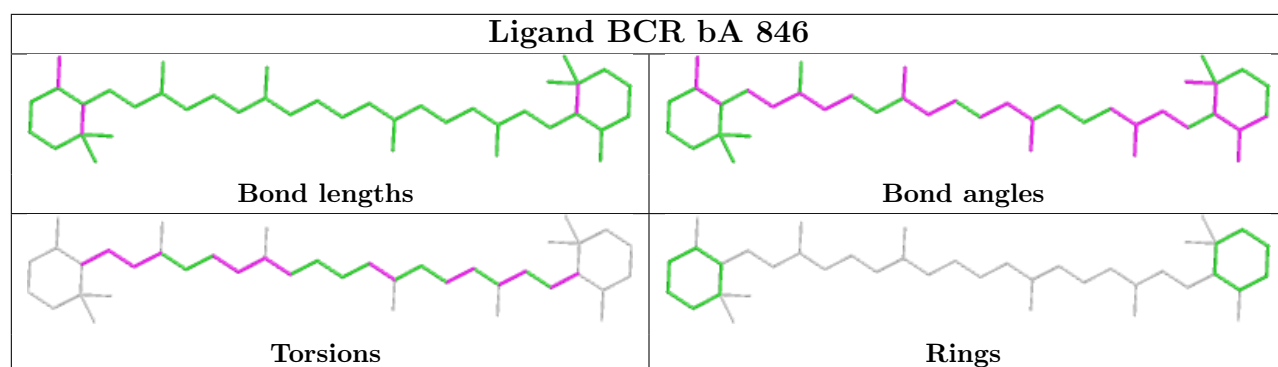
Ligand CLA aA 827

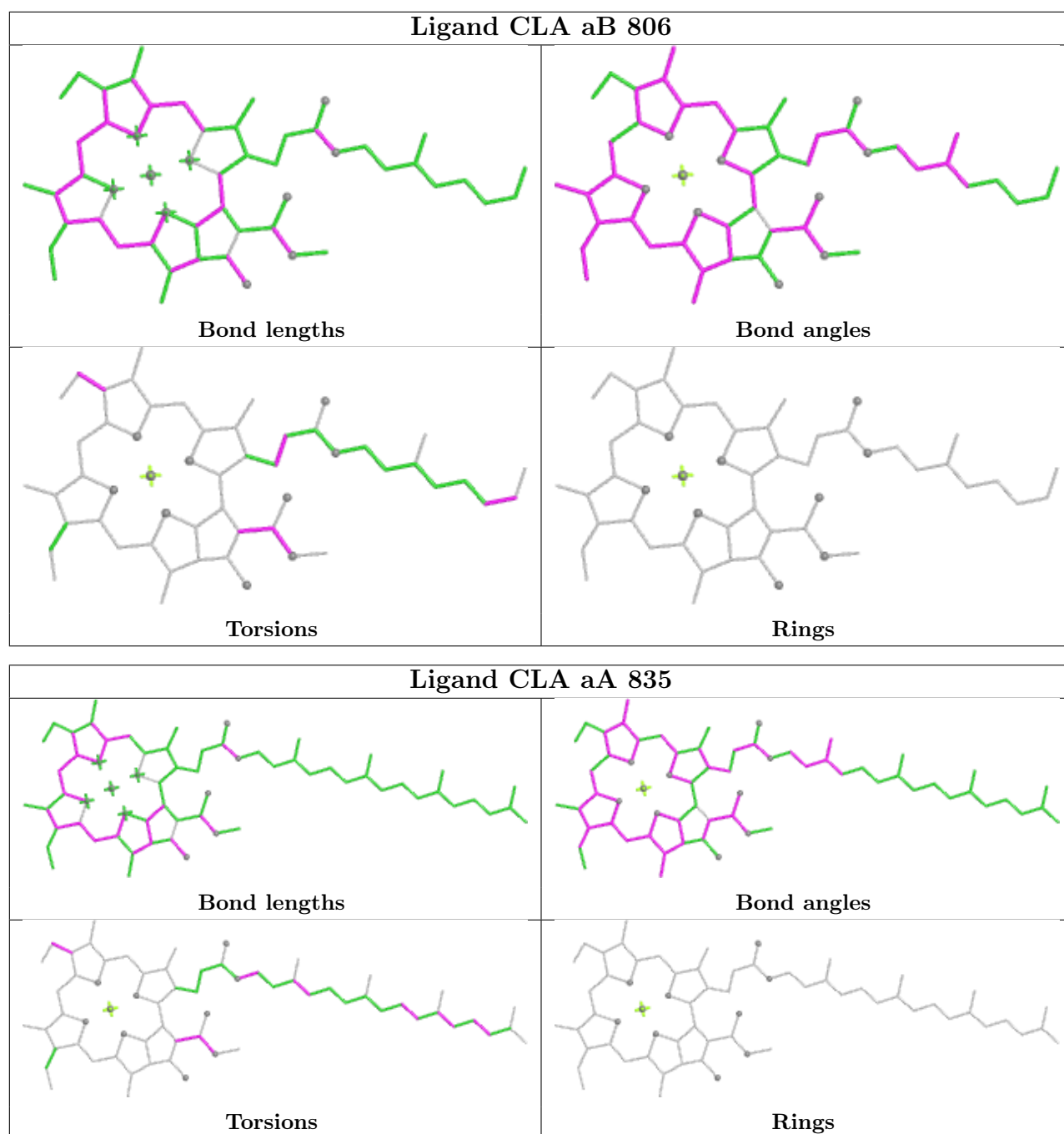


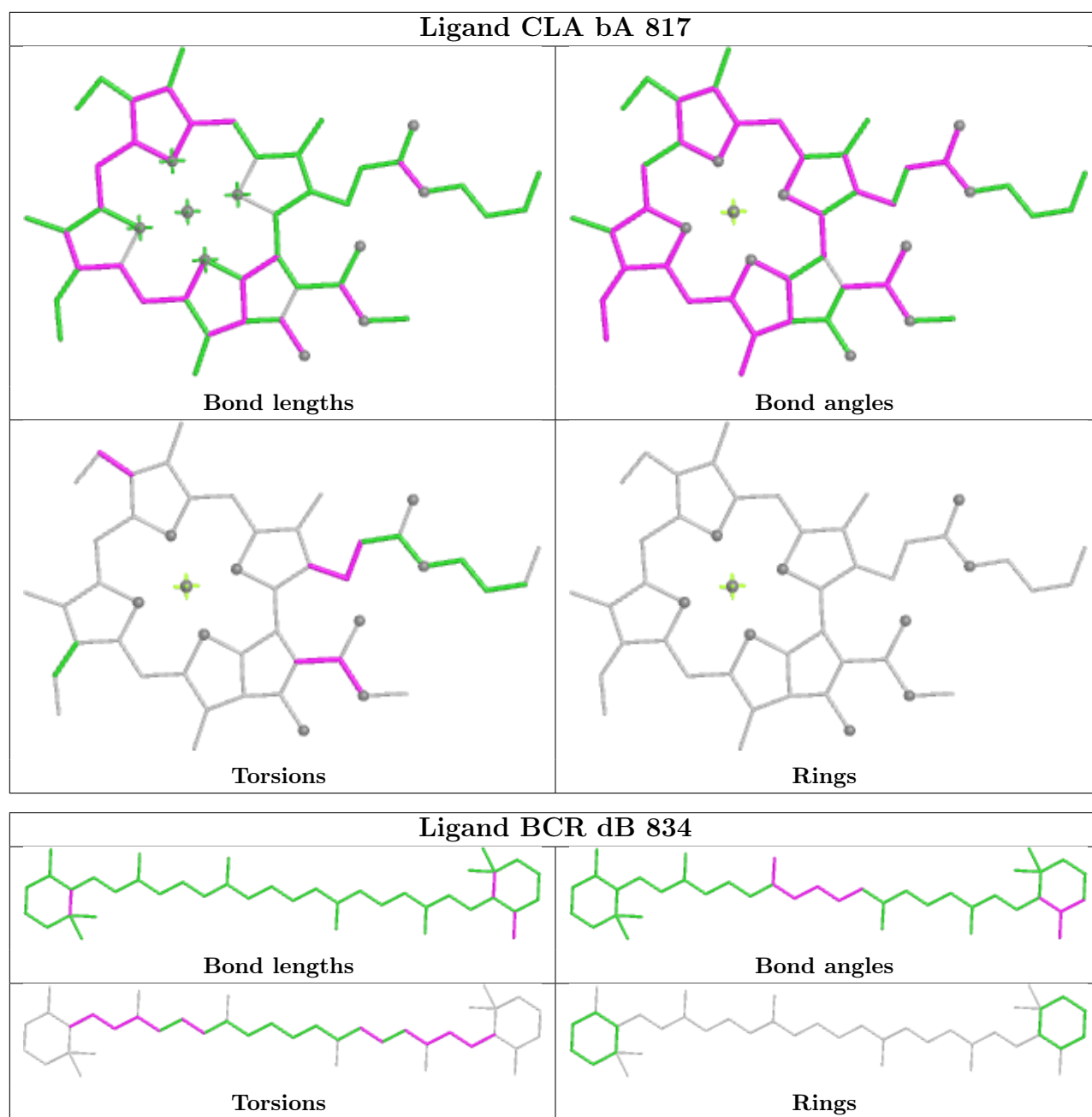
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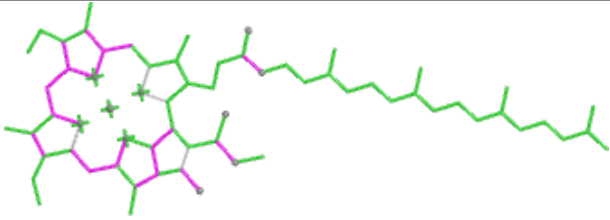
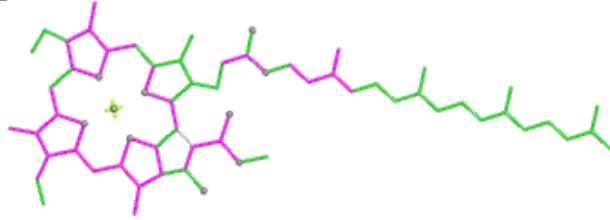
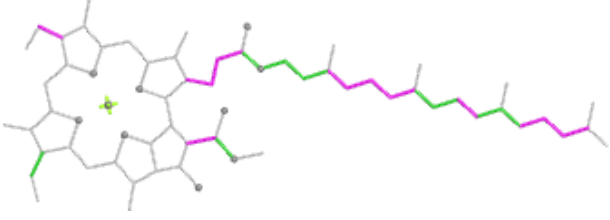
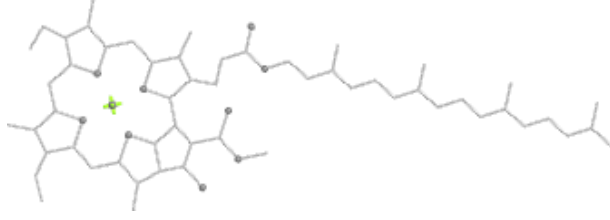


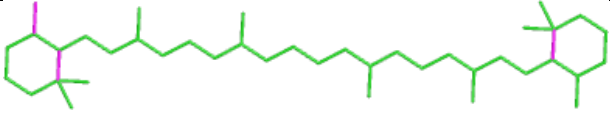
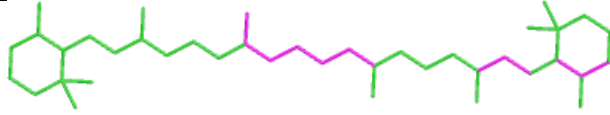
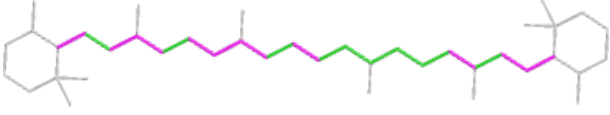
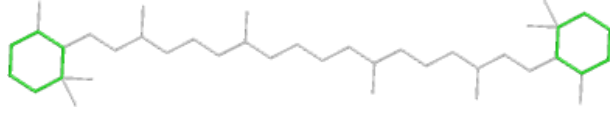


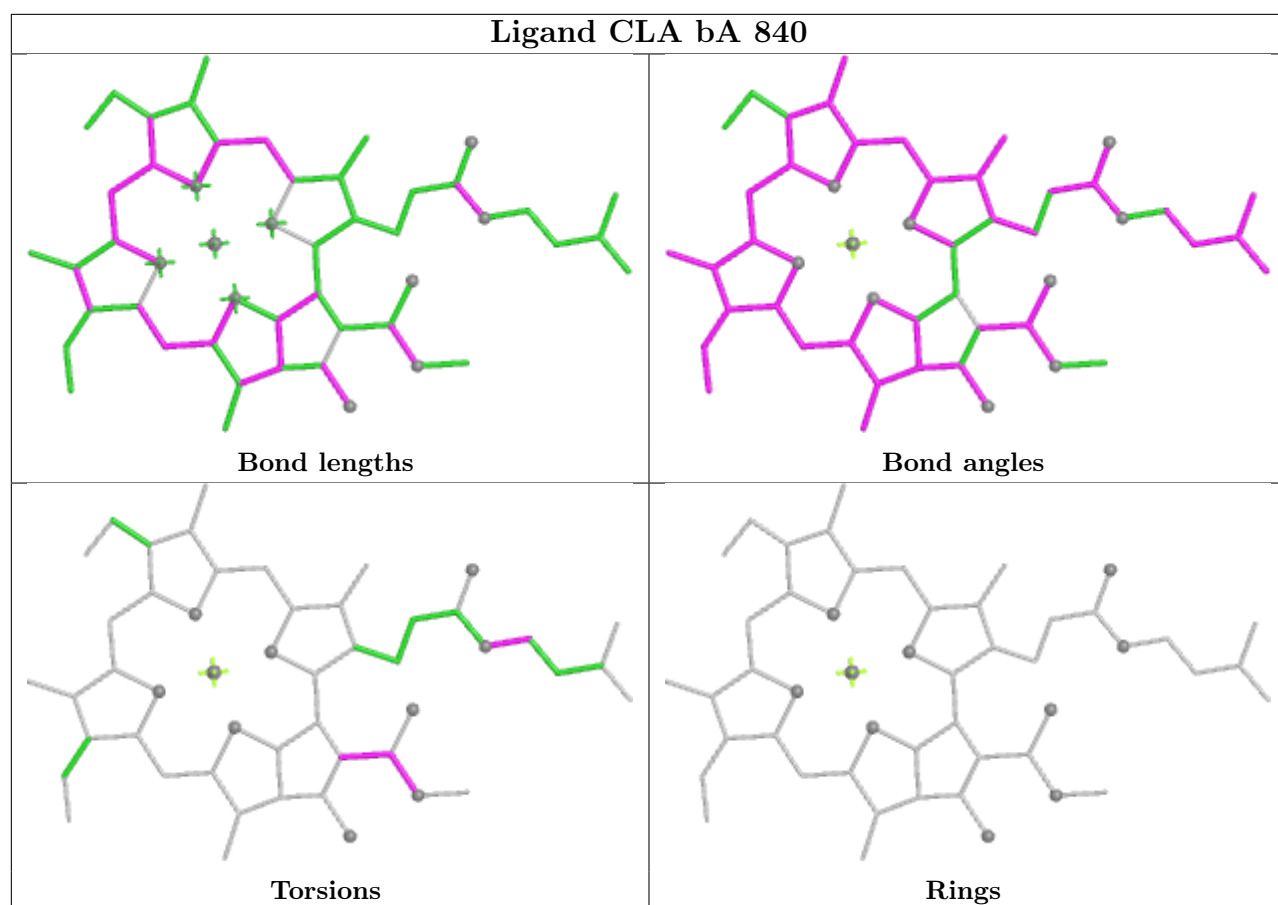


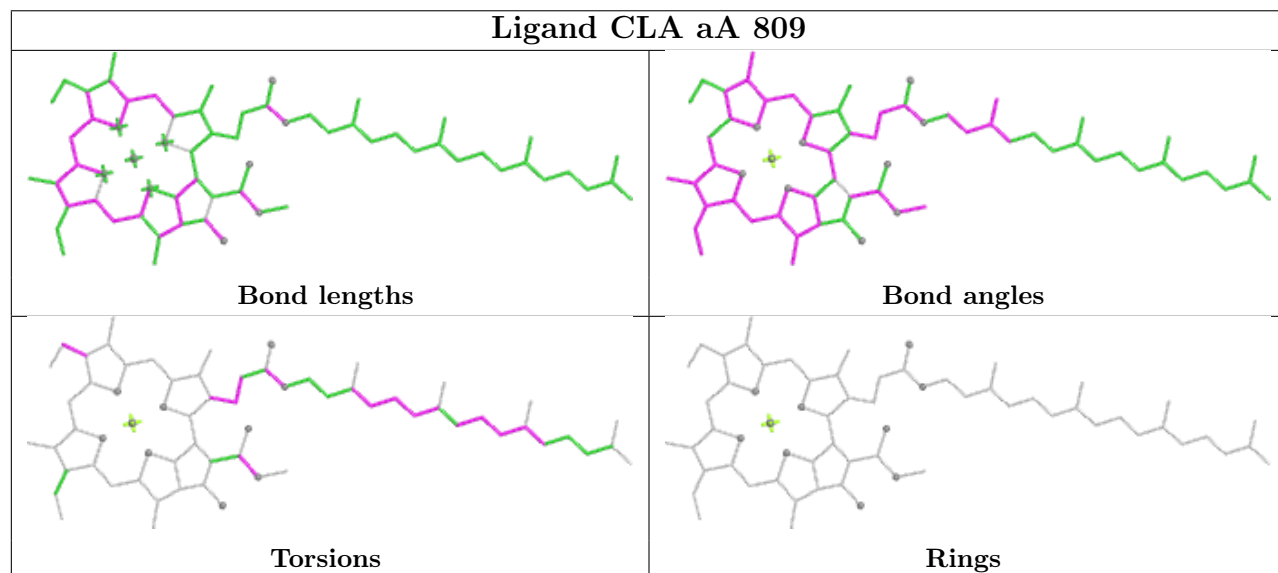
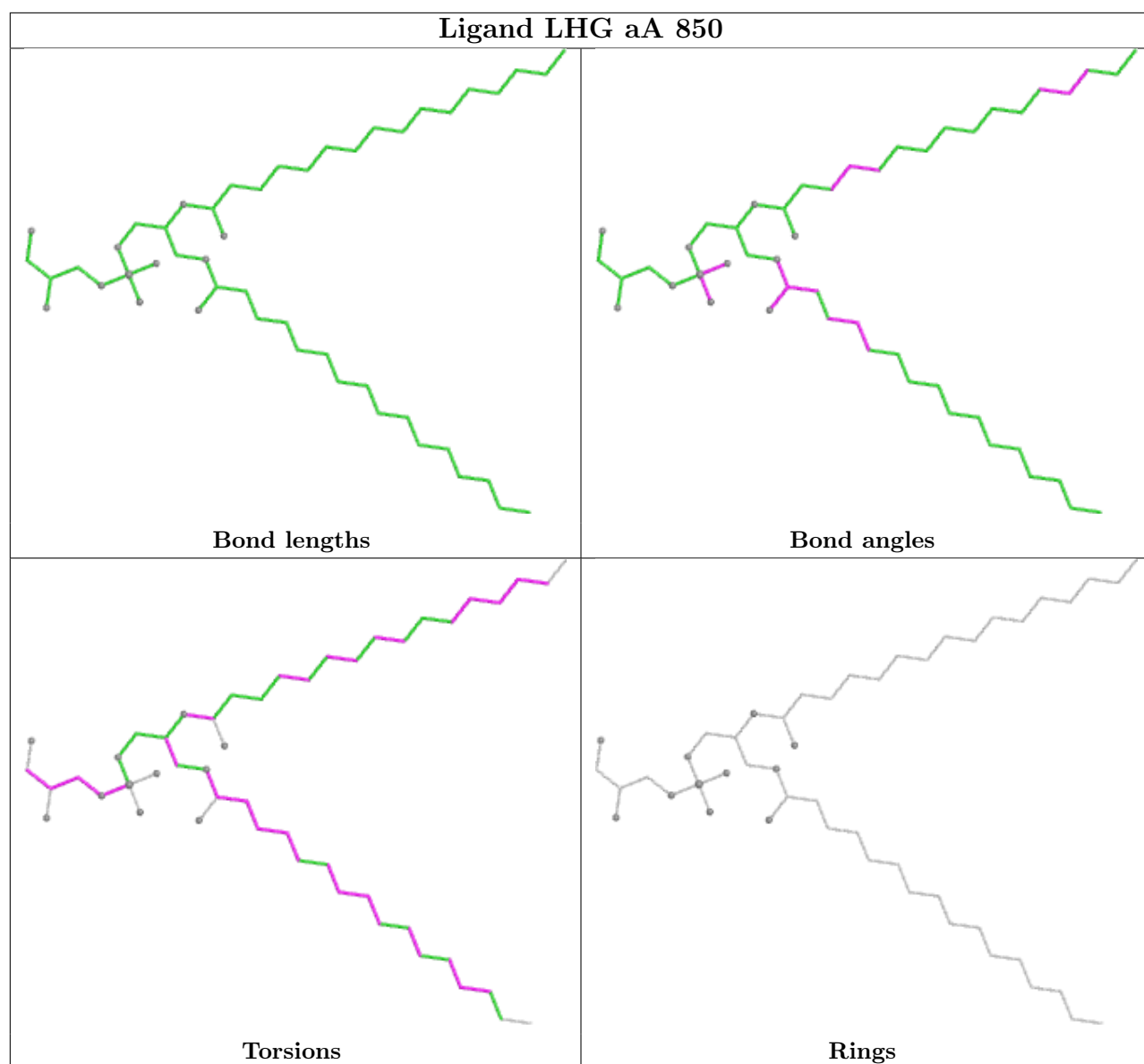


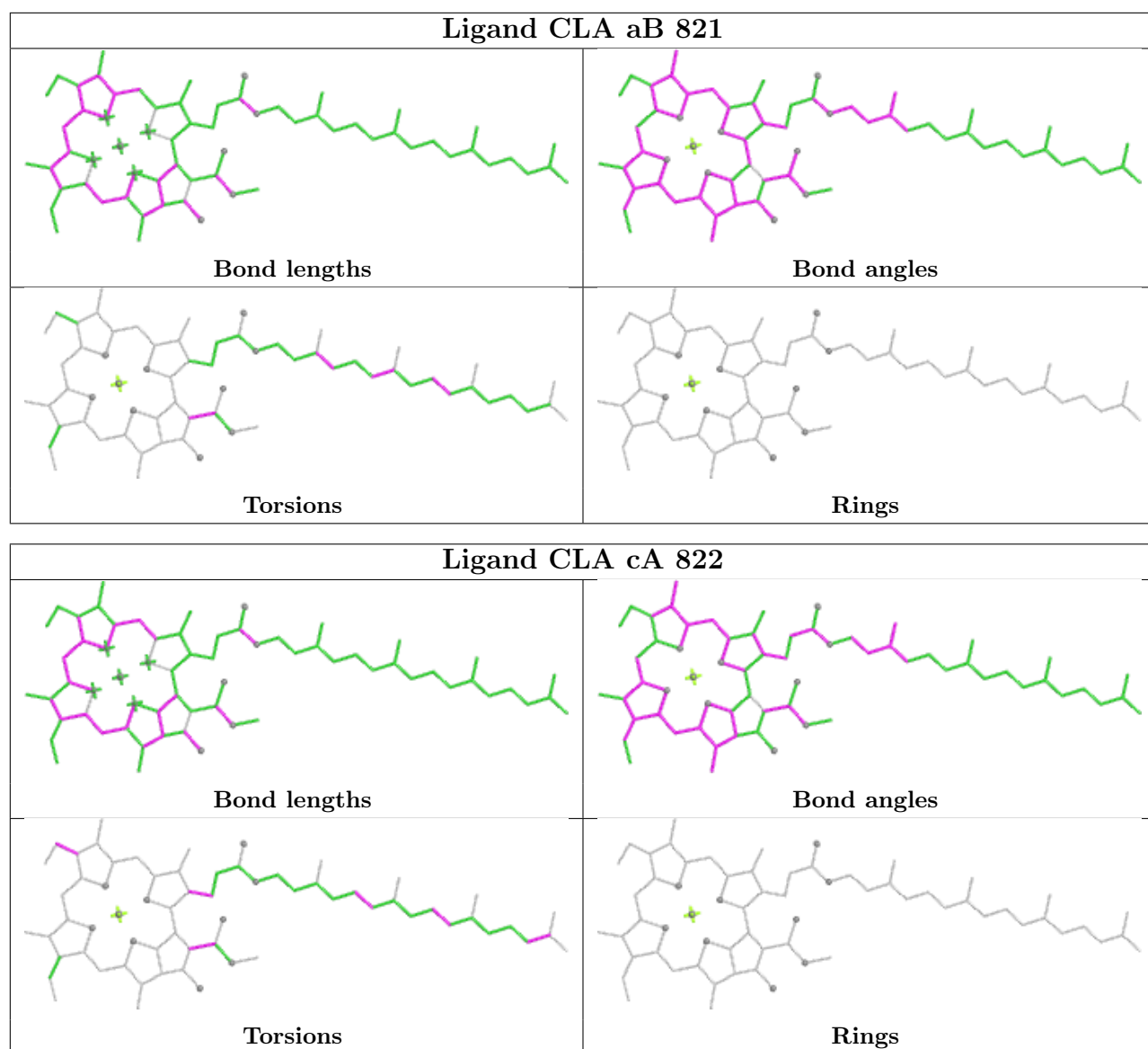


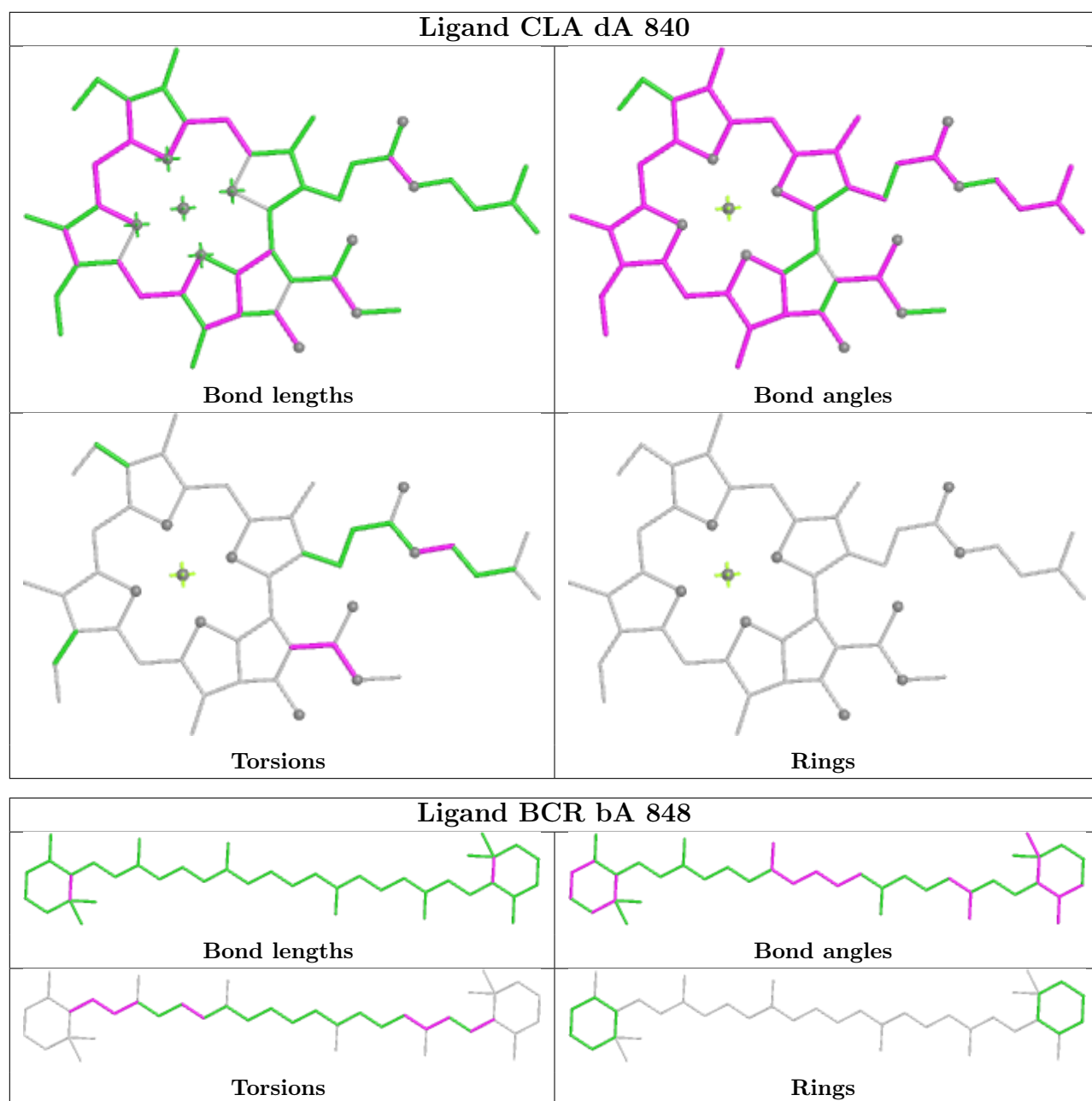
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Bond lengths	Bond angles		
			
Torsions	Rings		

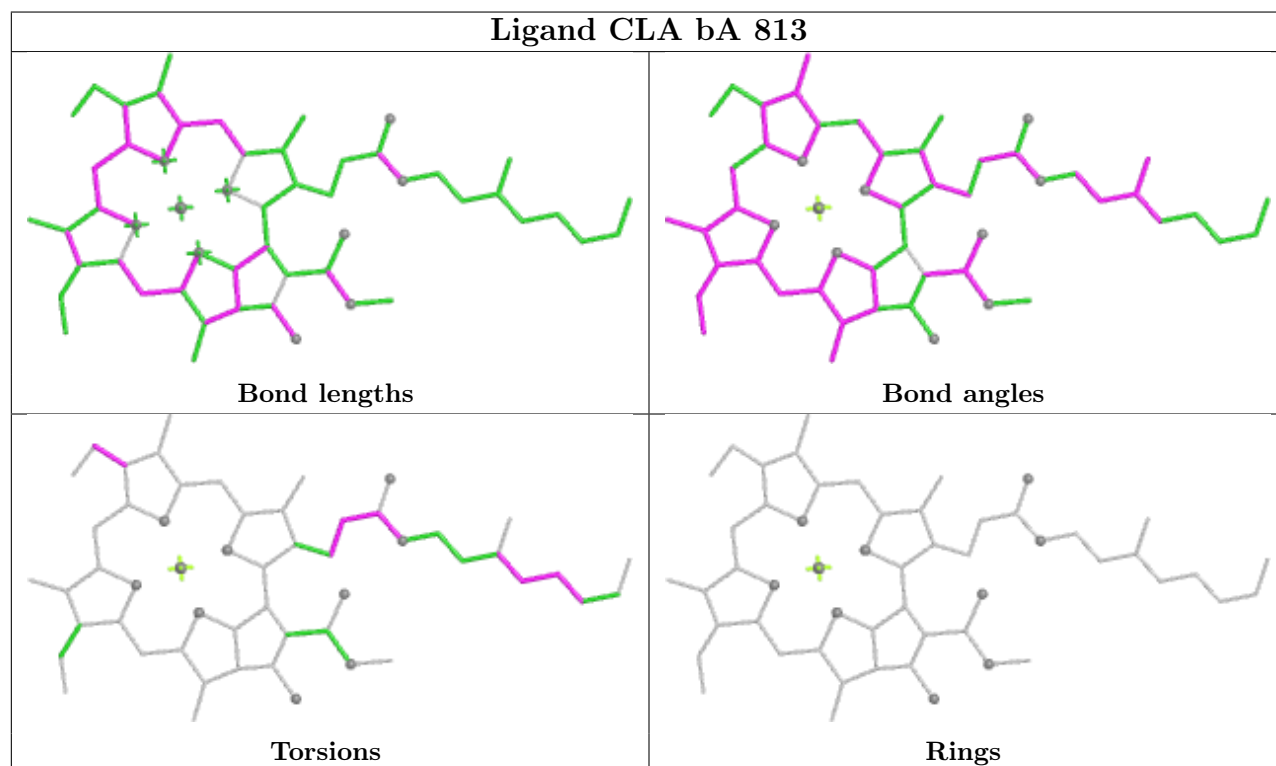
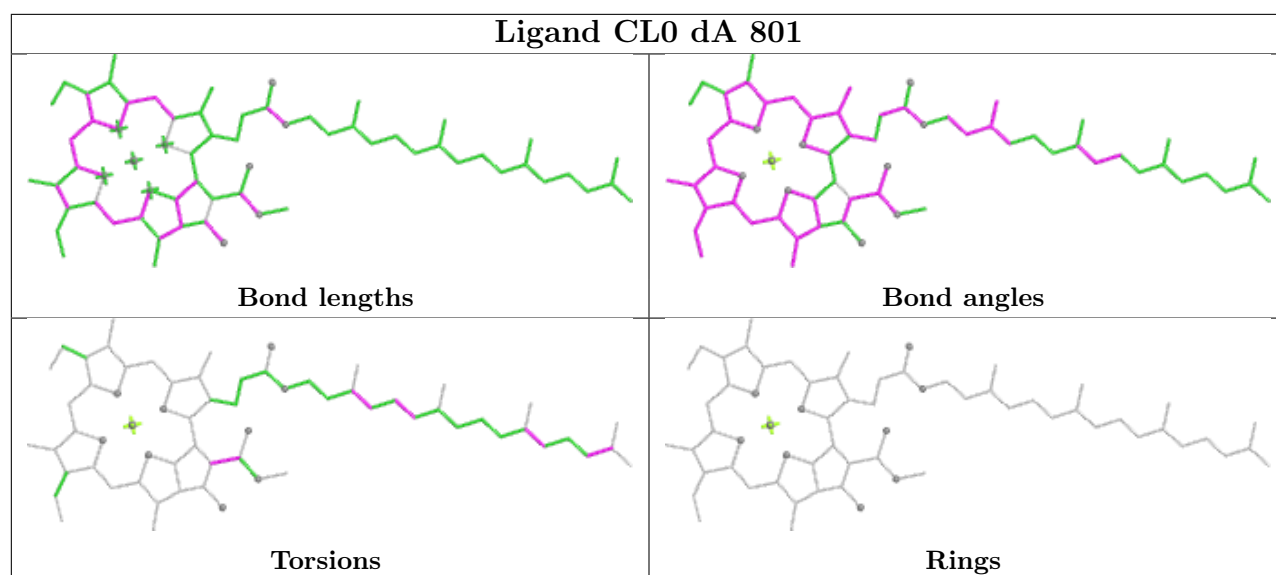
Ligand BCR dL 201			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

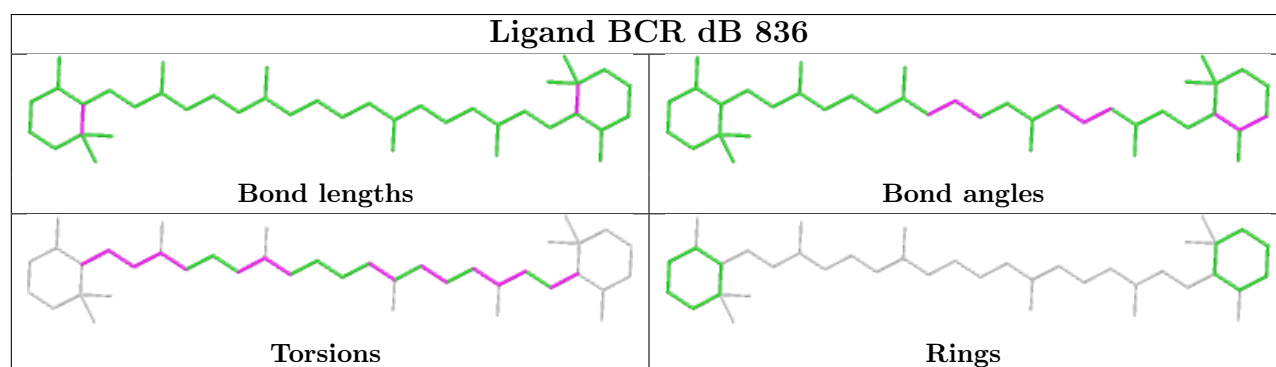
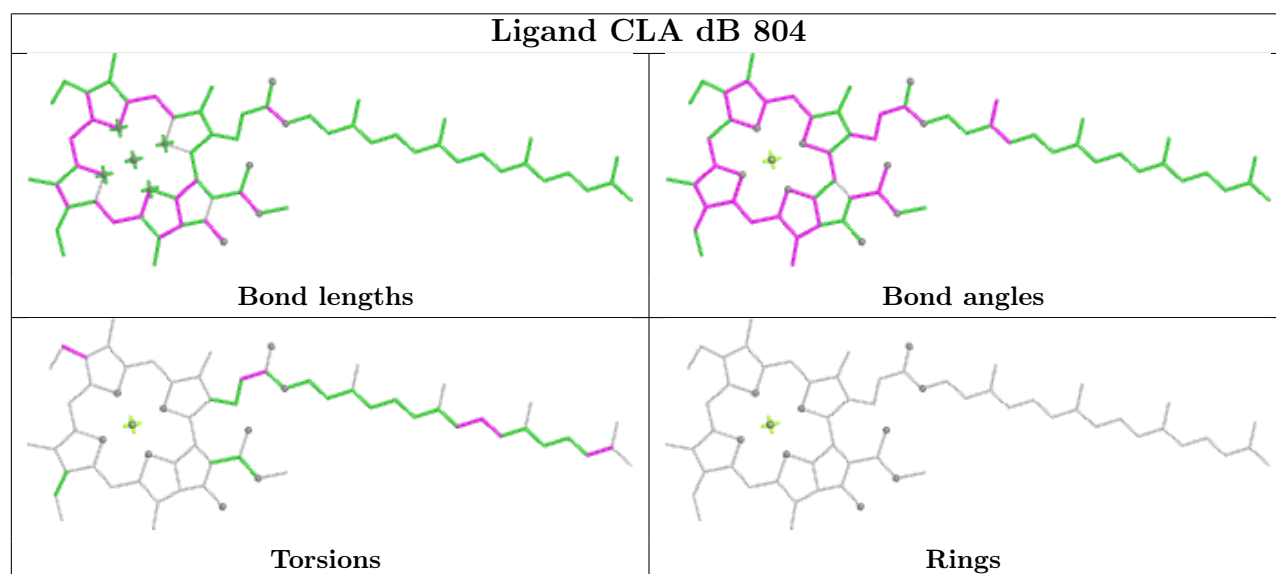
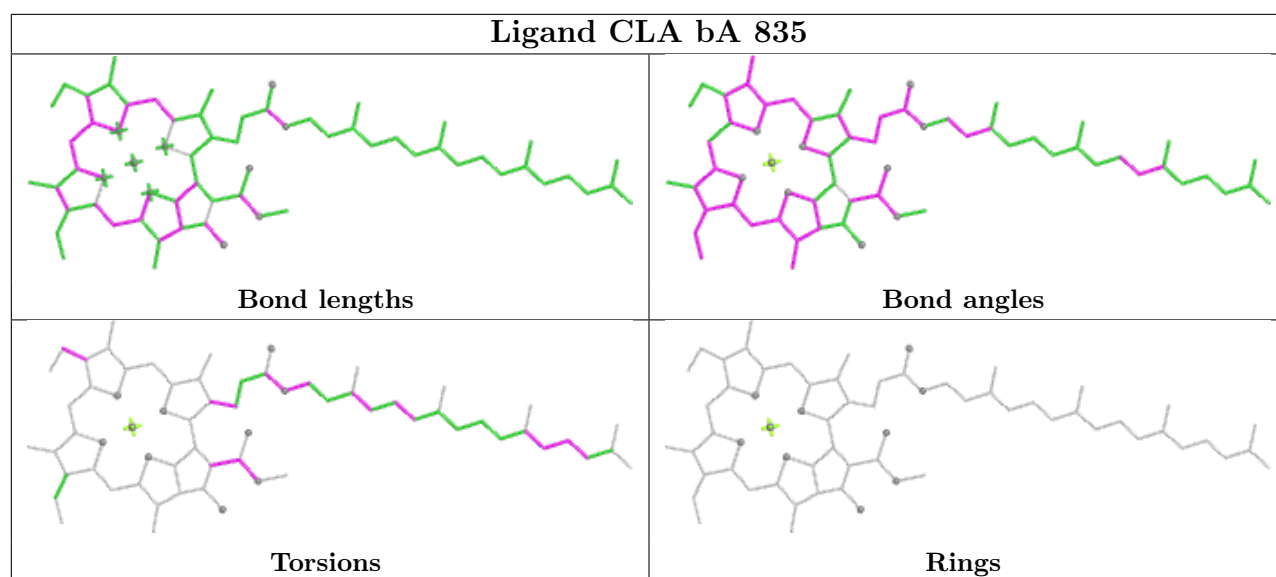


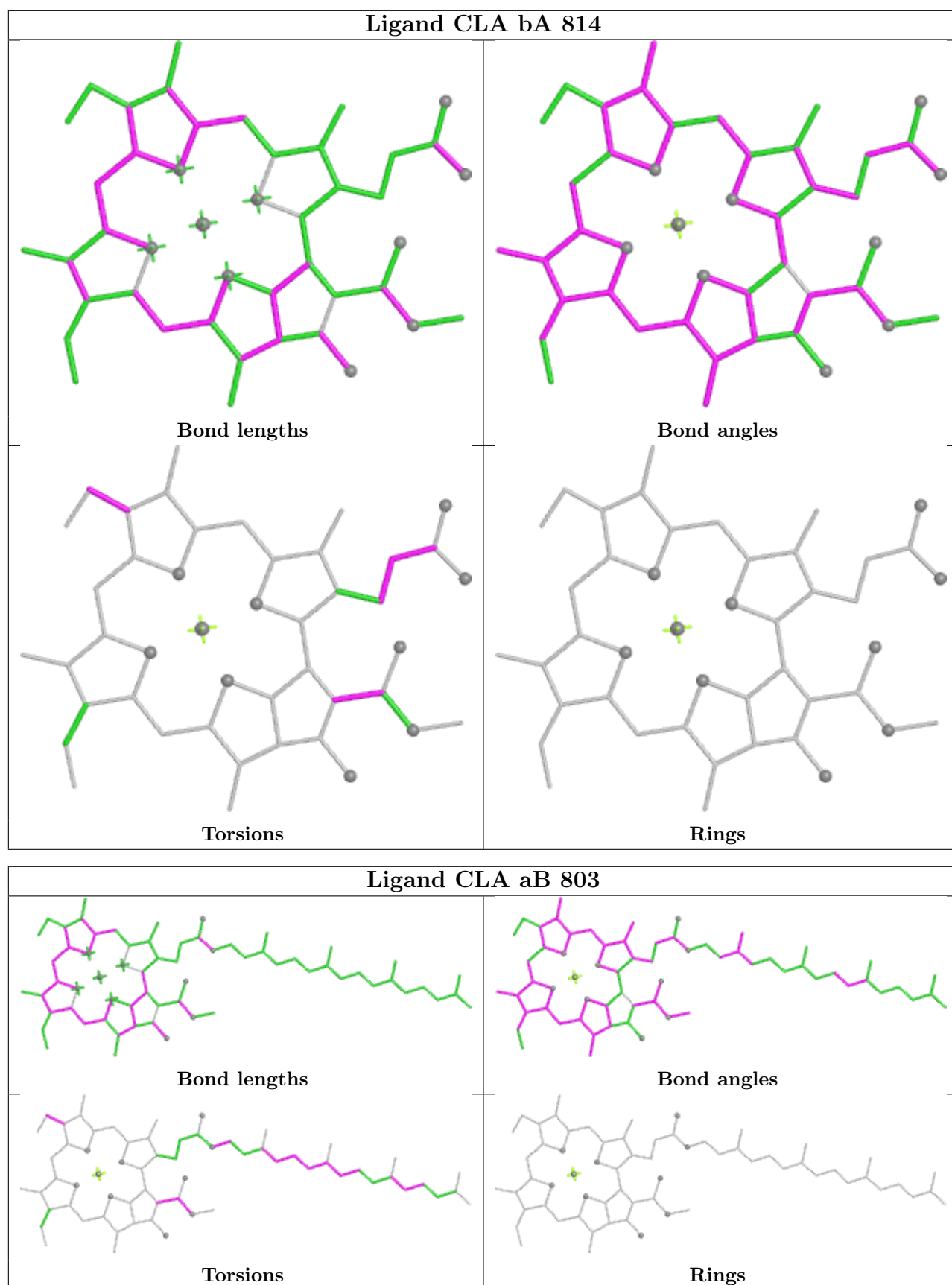


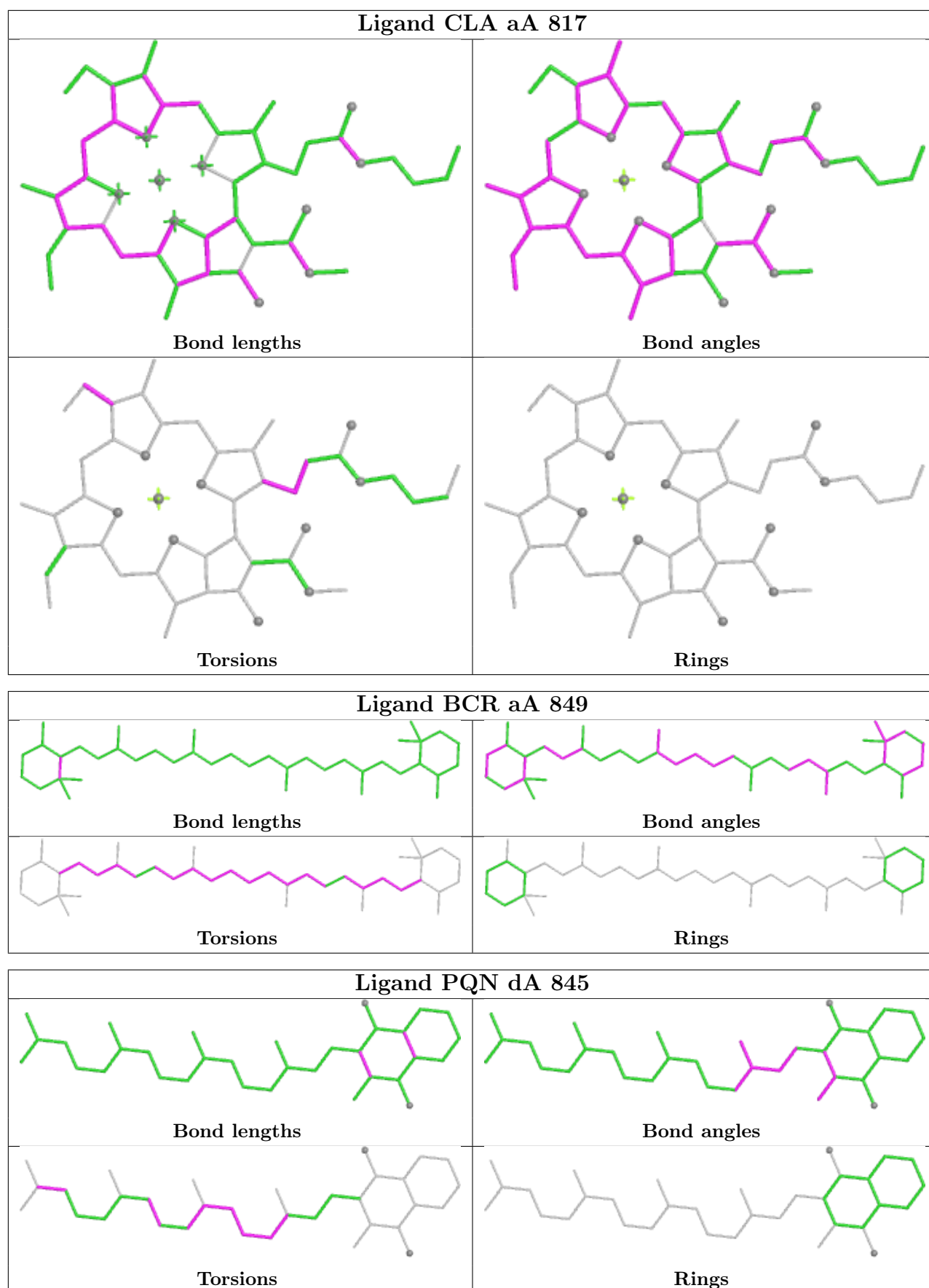


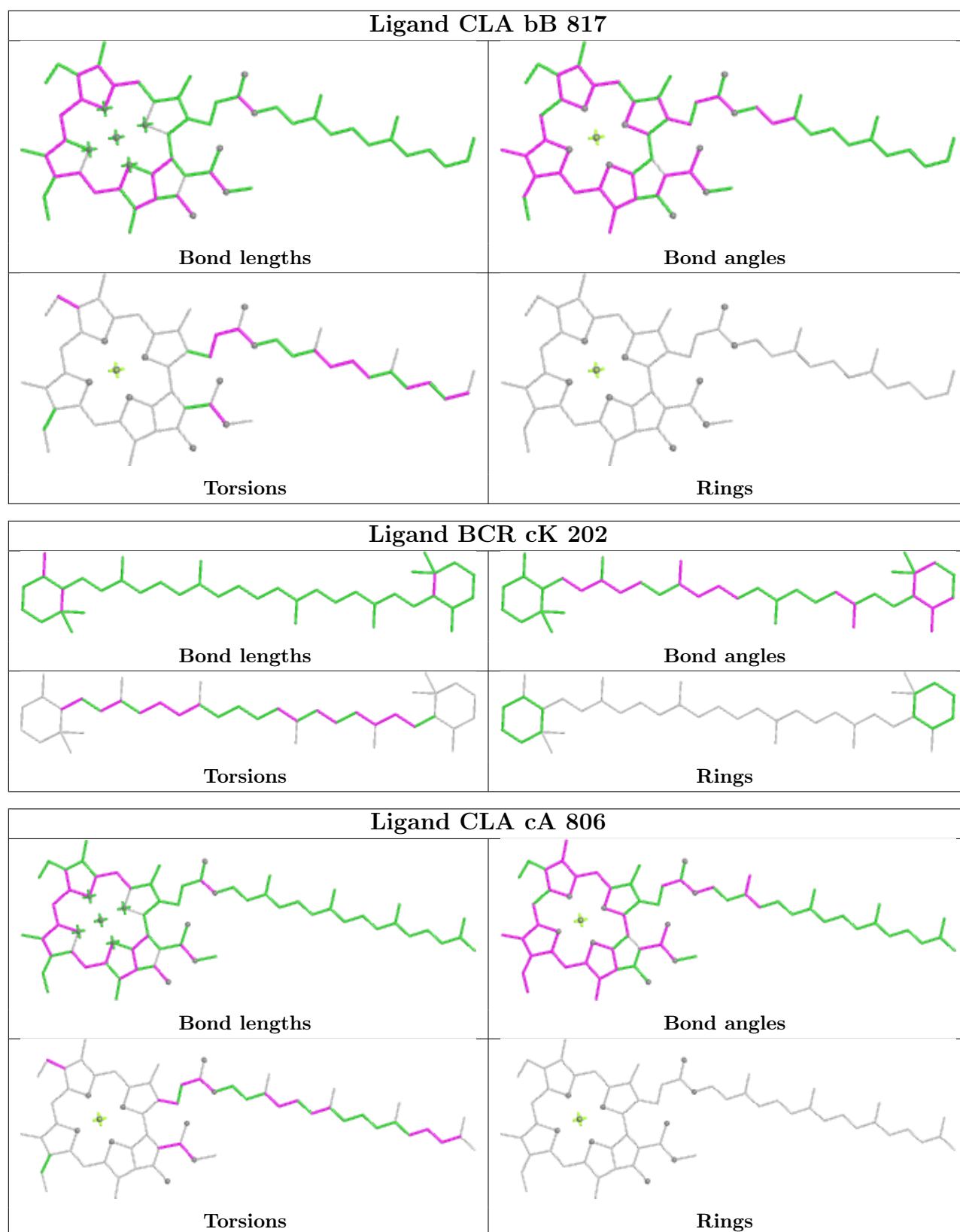




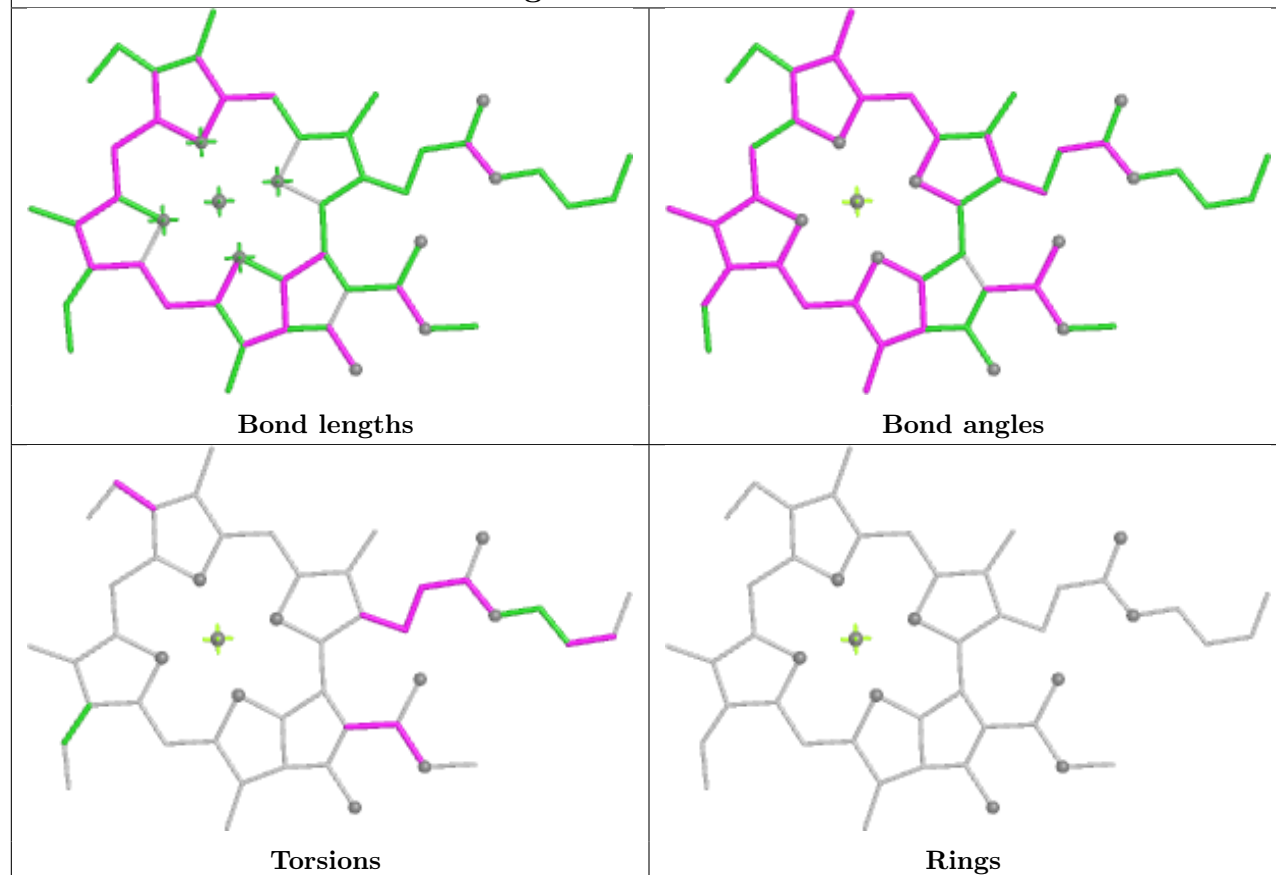




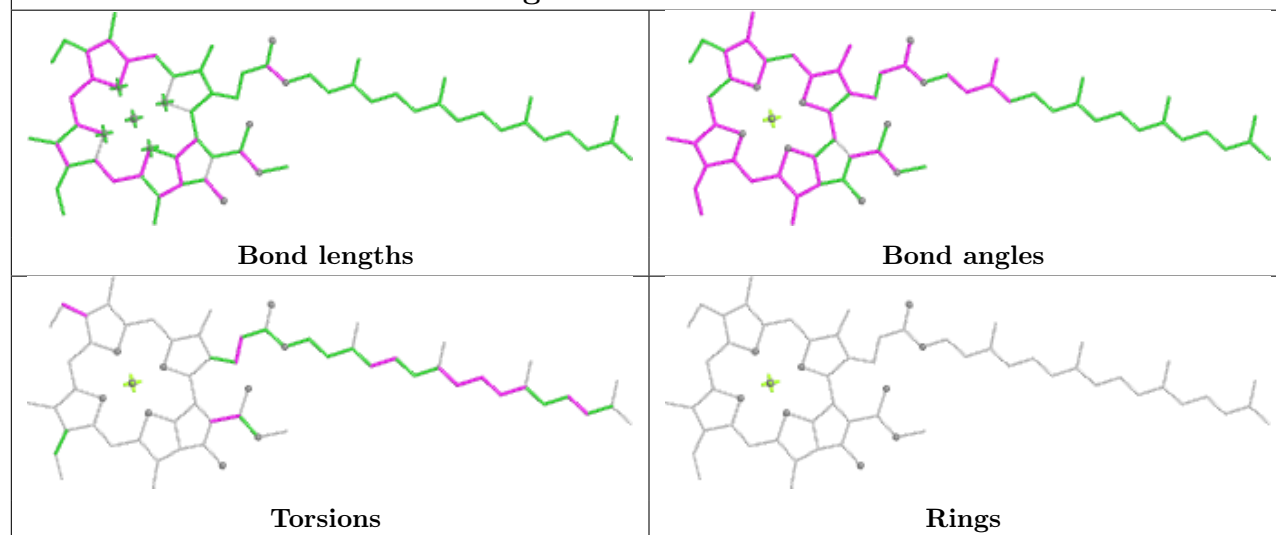


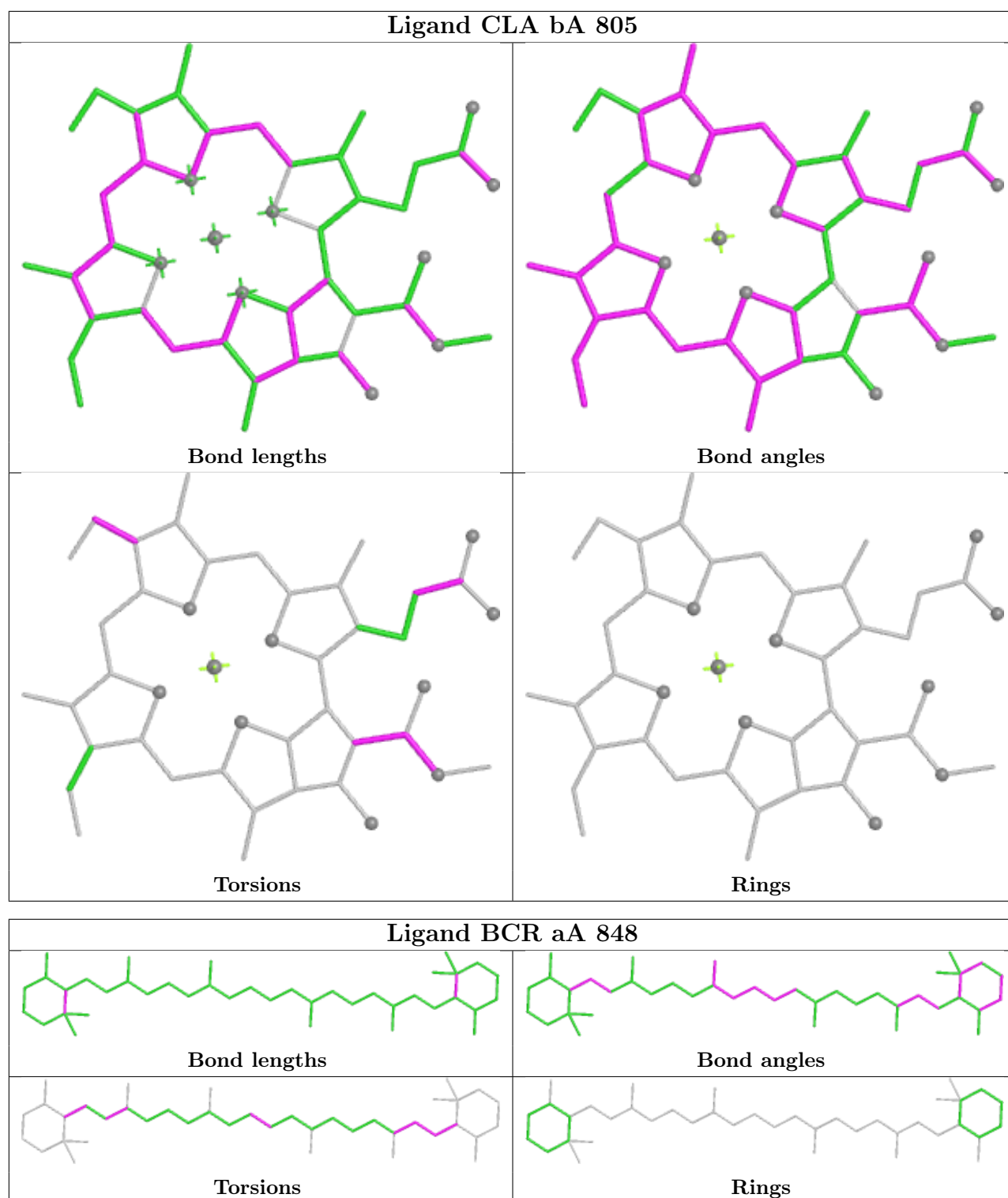


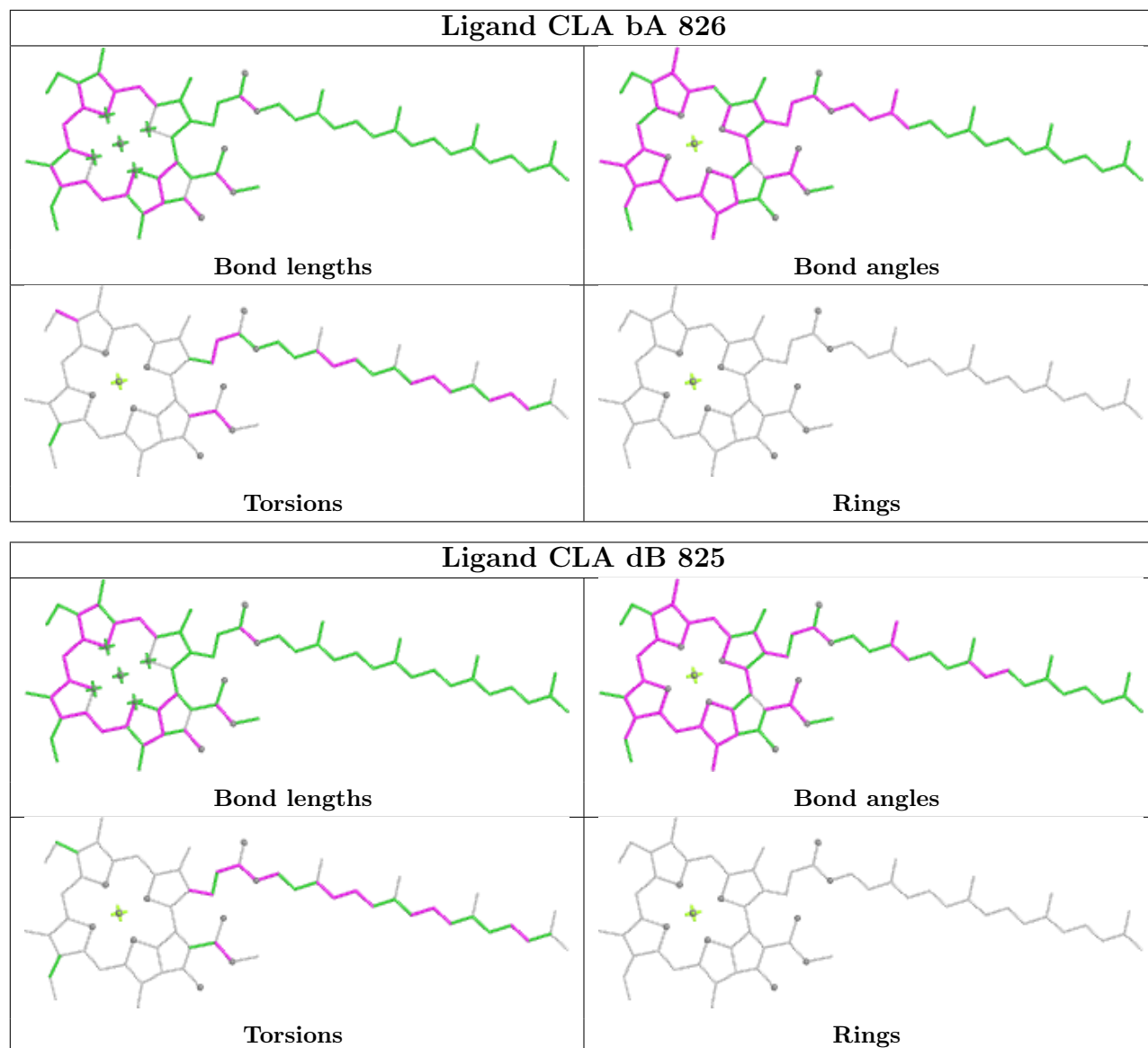
Ligand CLA cB 825

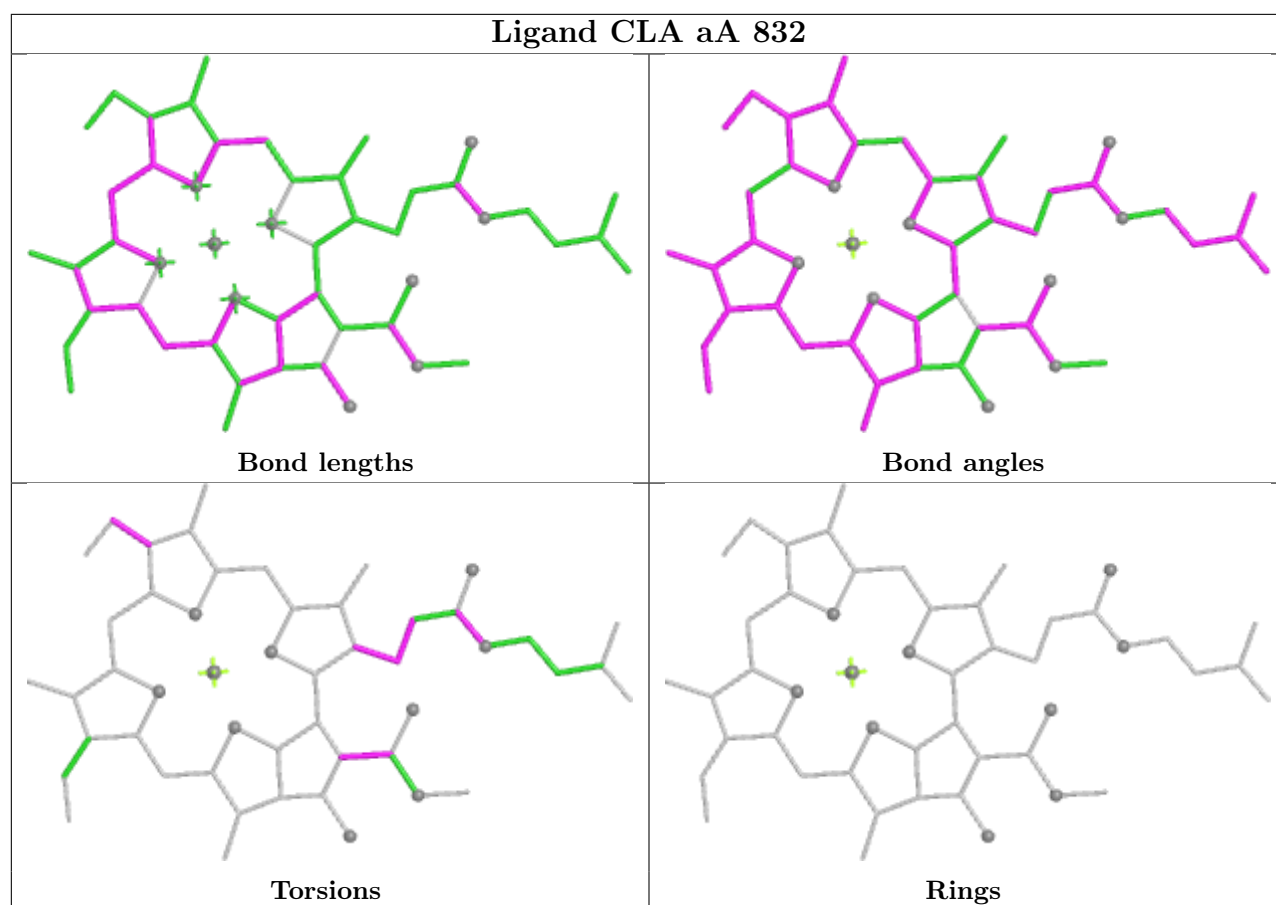


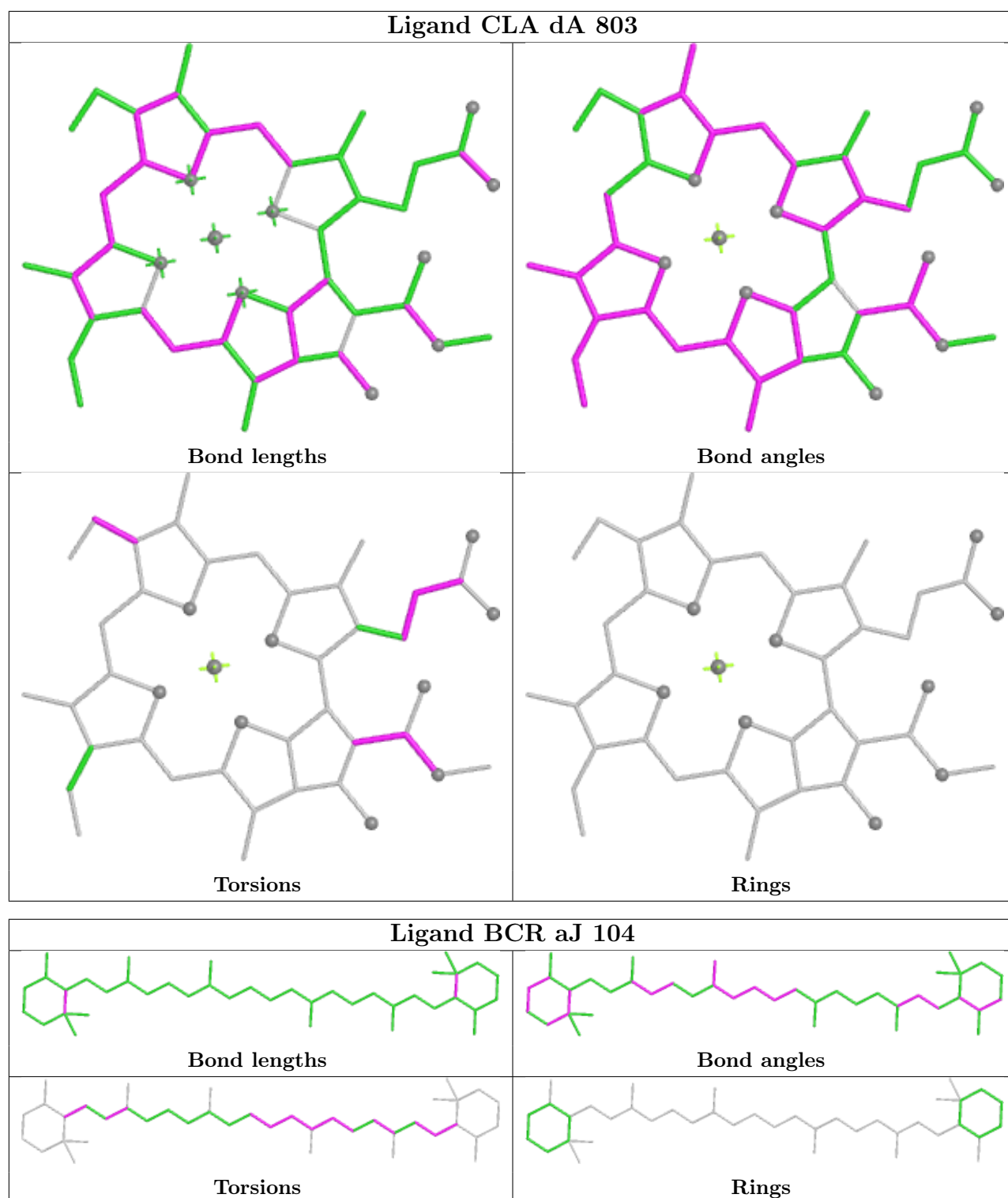
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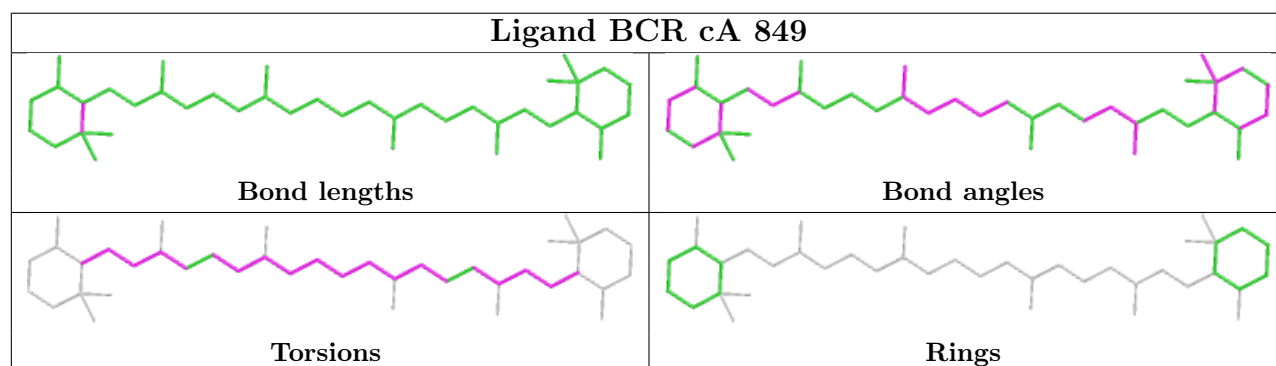
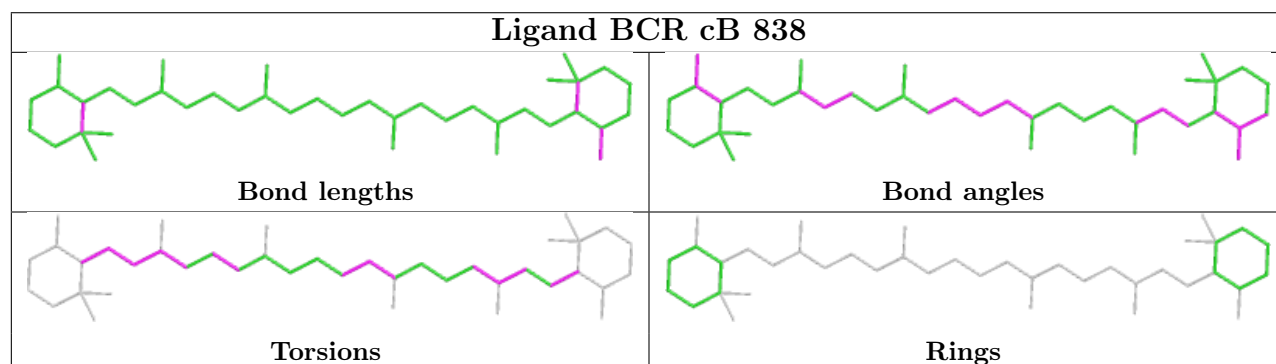
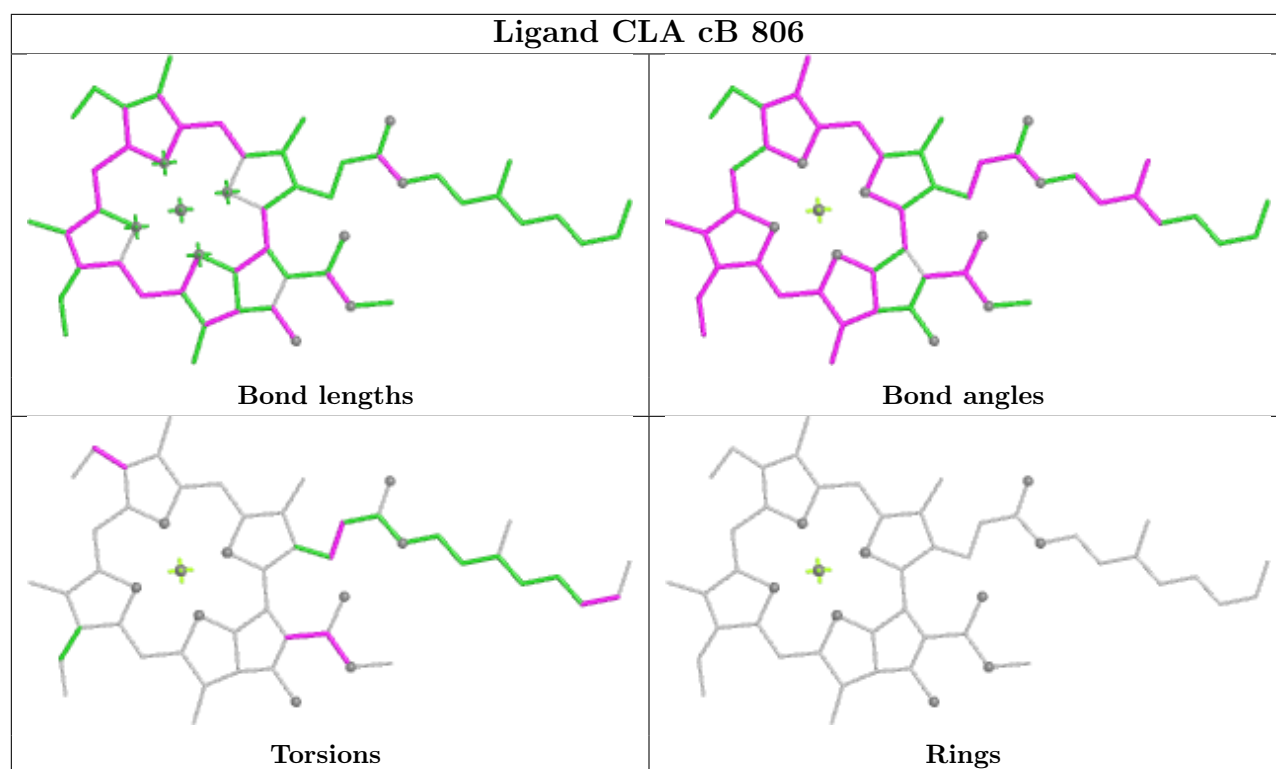


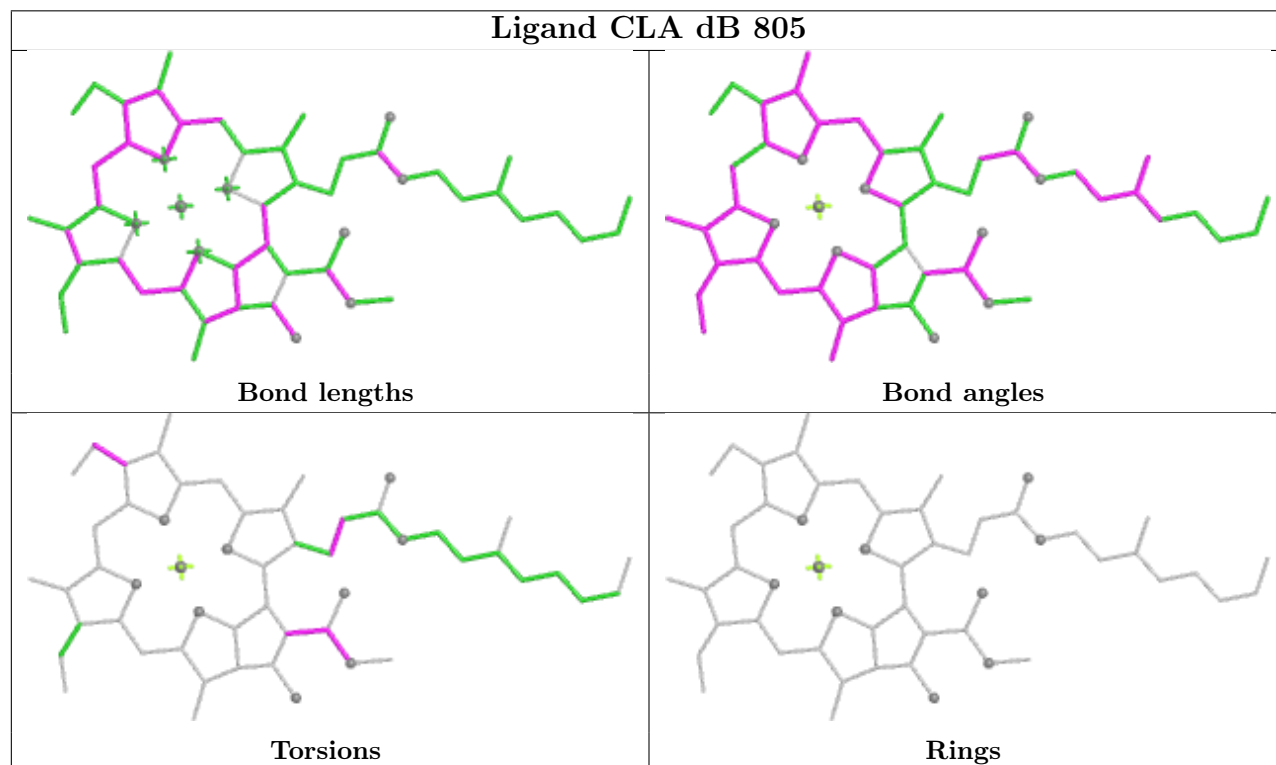
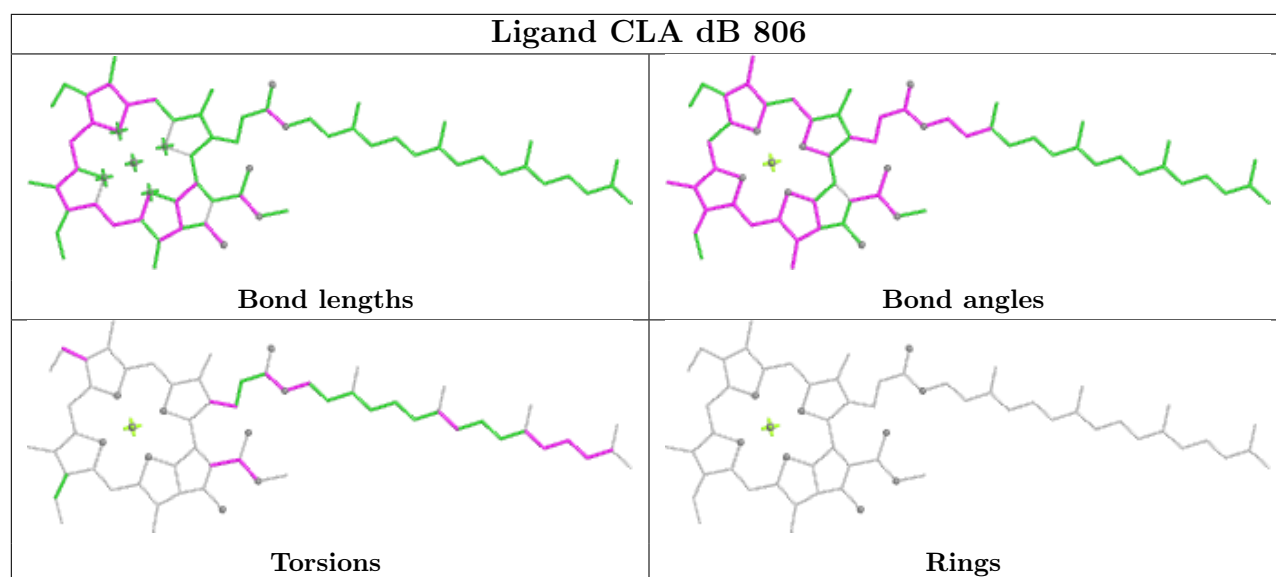


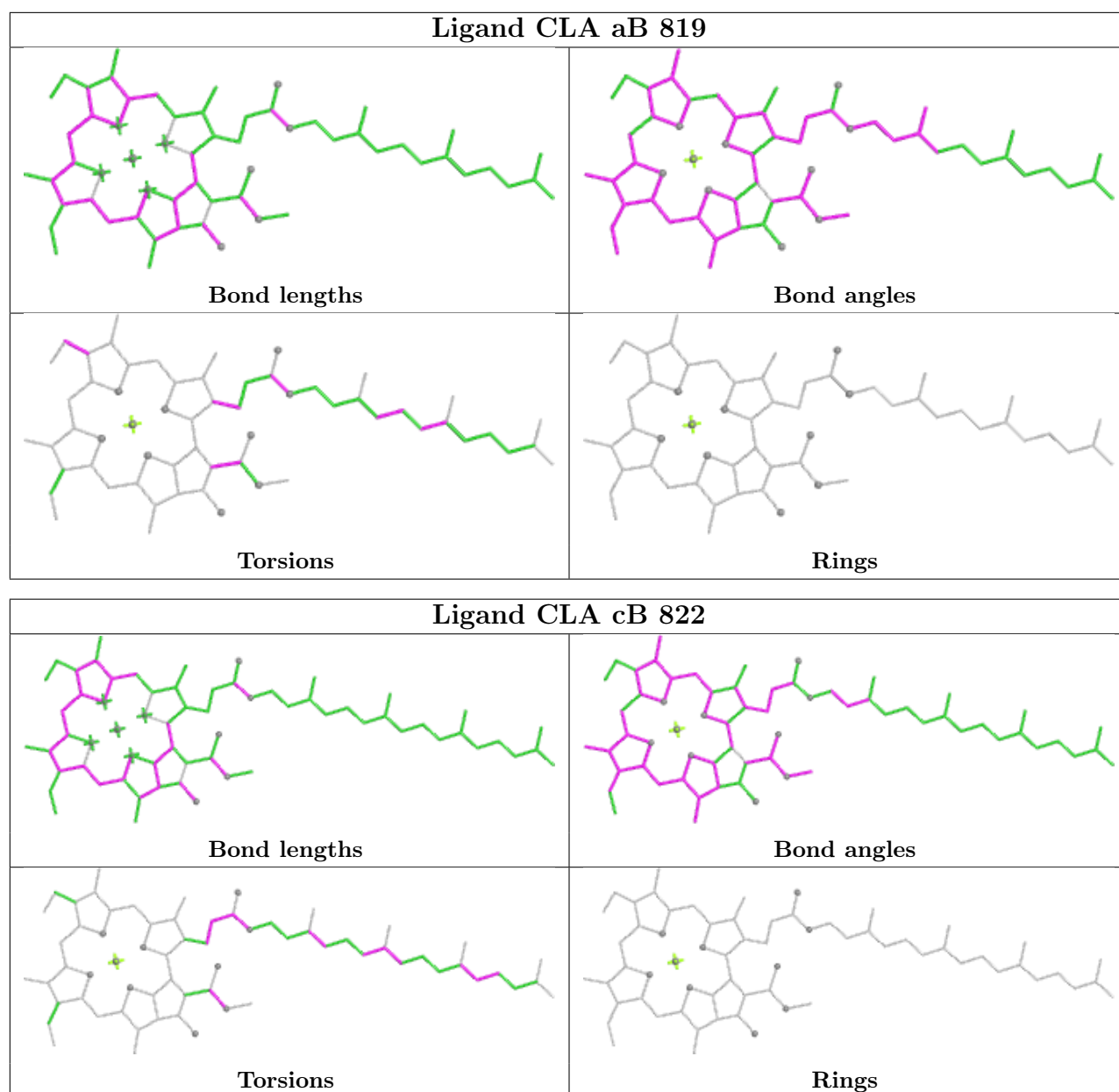




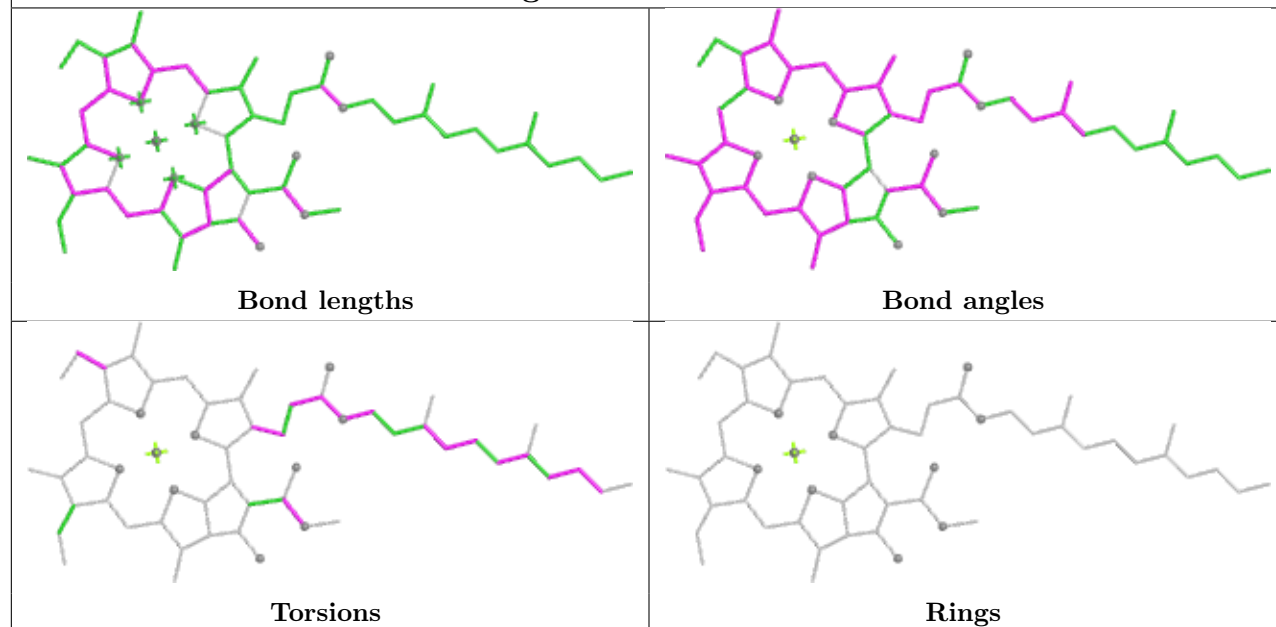




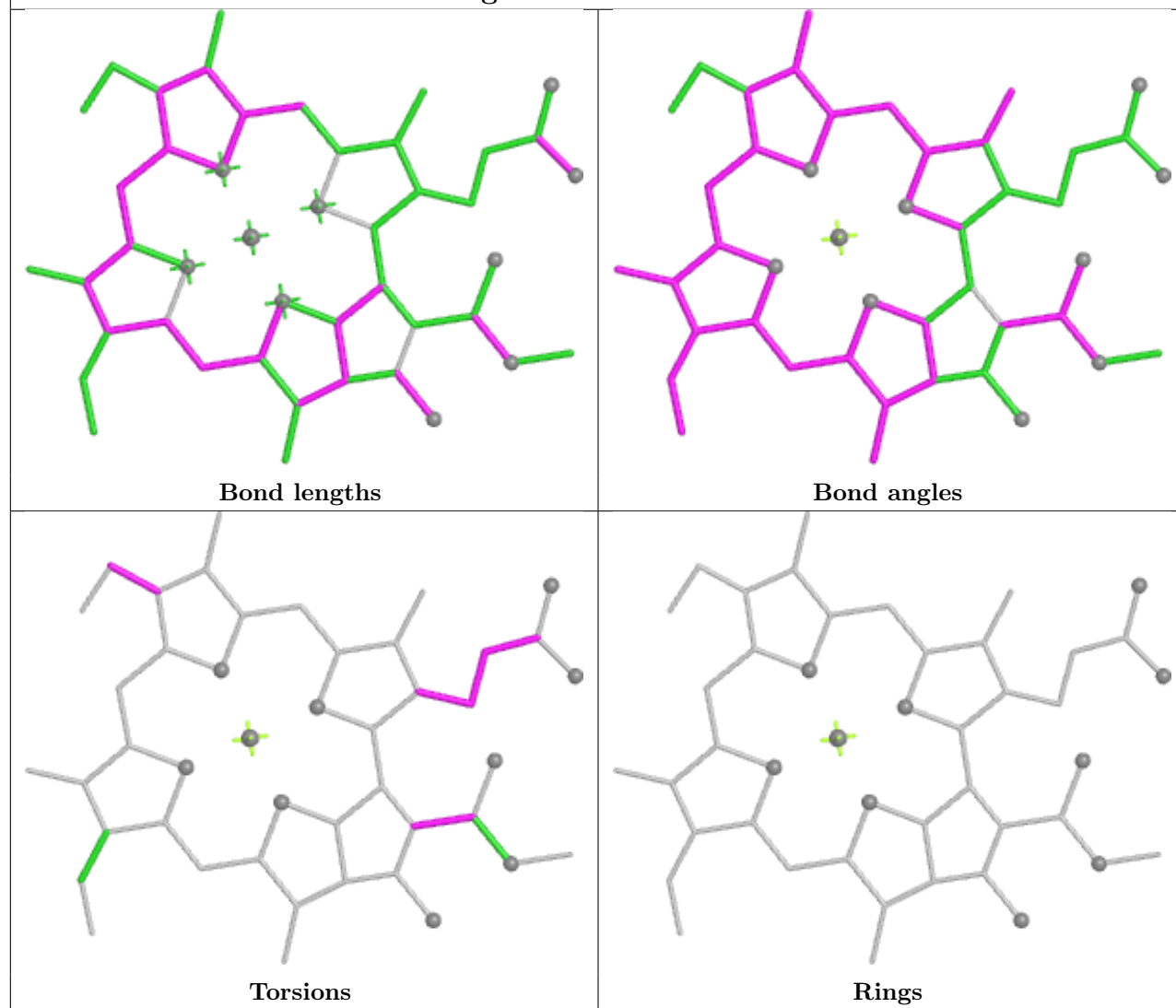


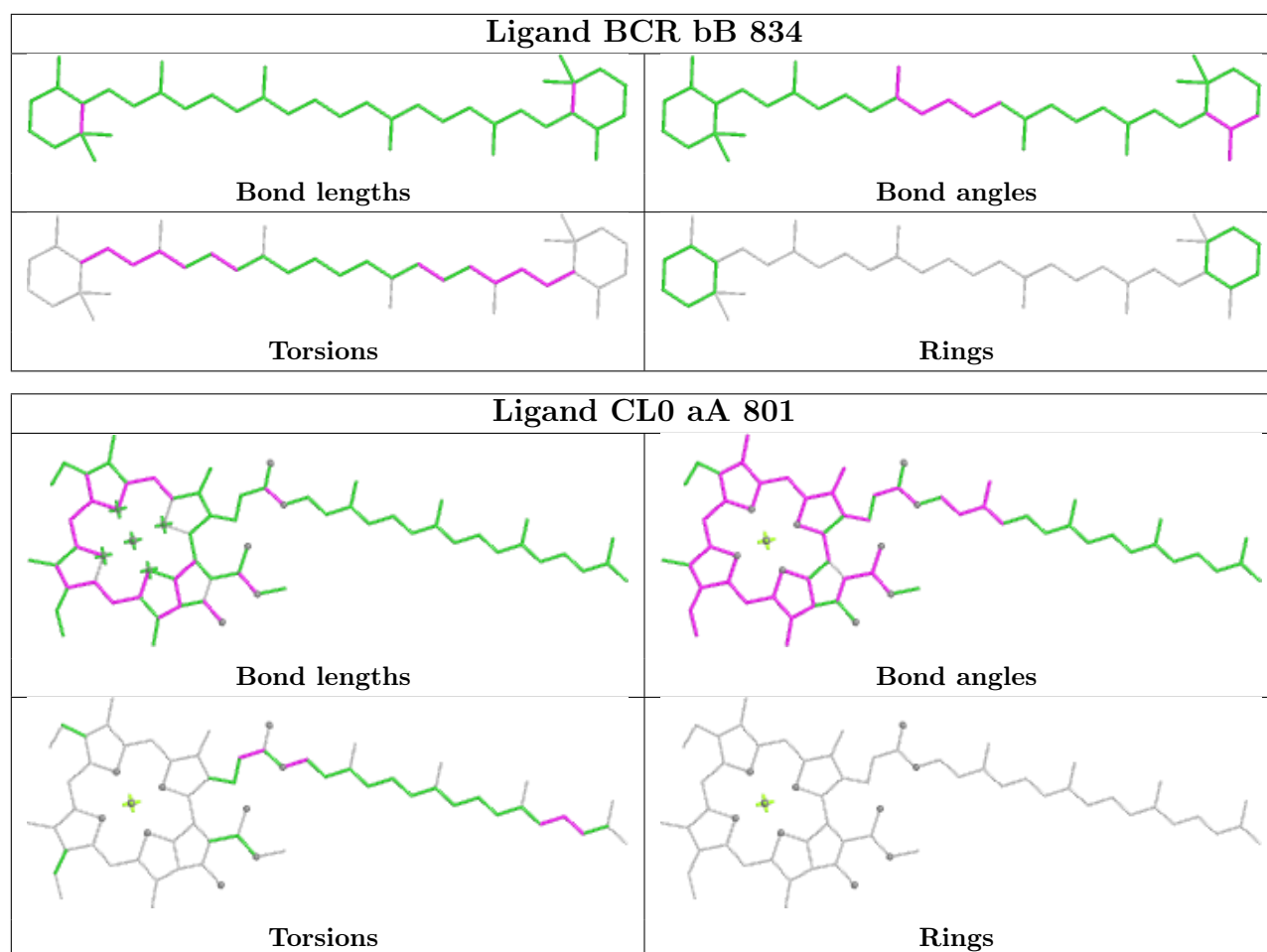


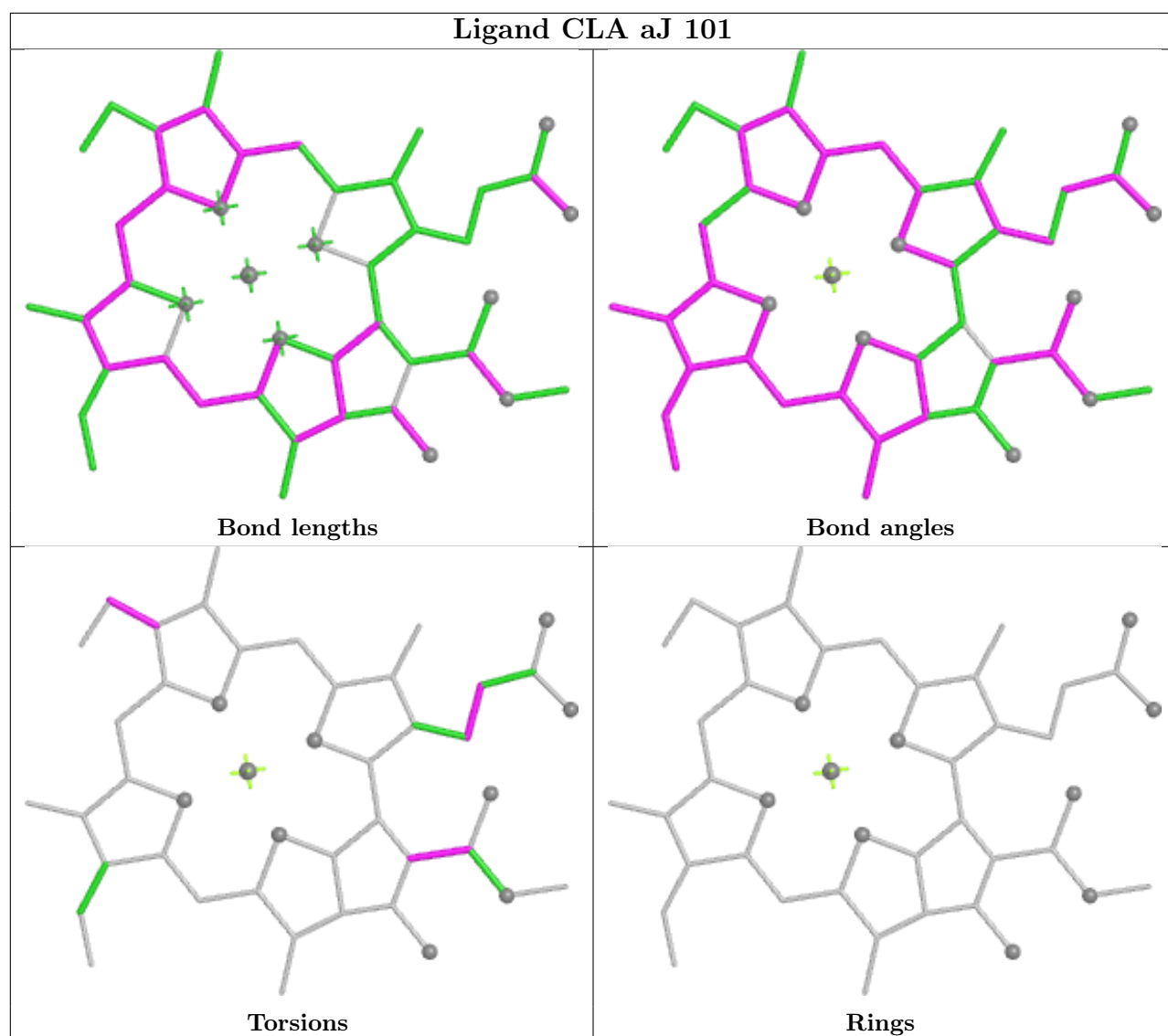
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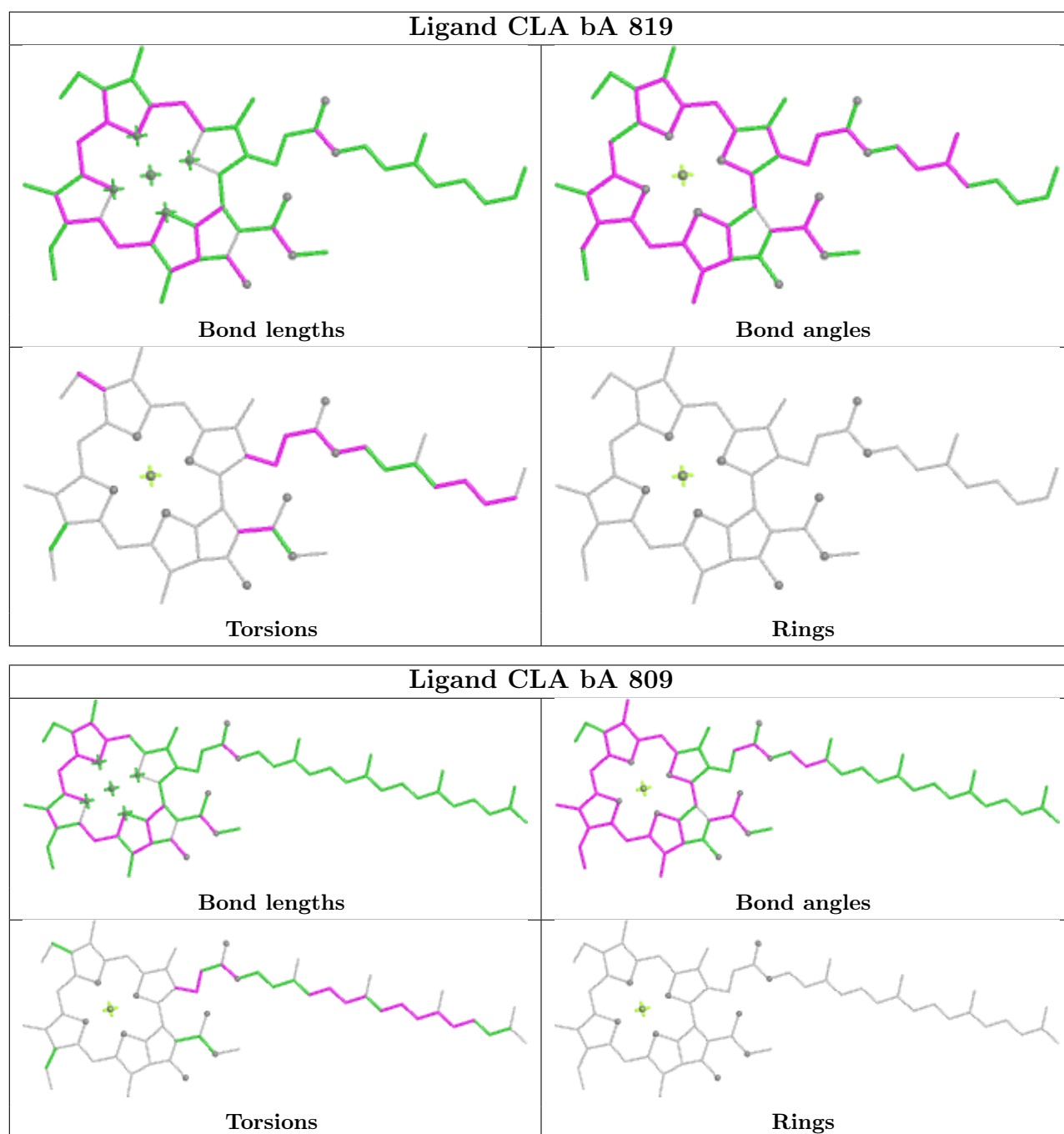


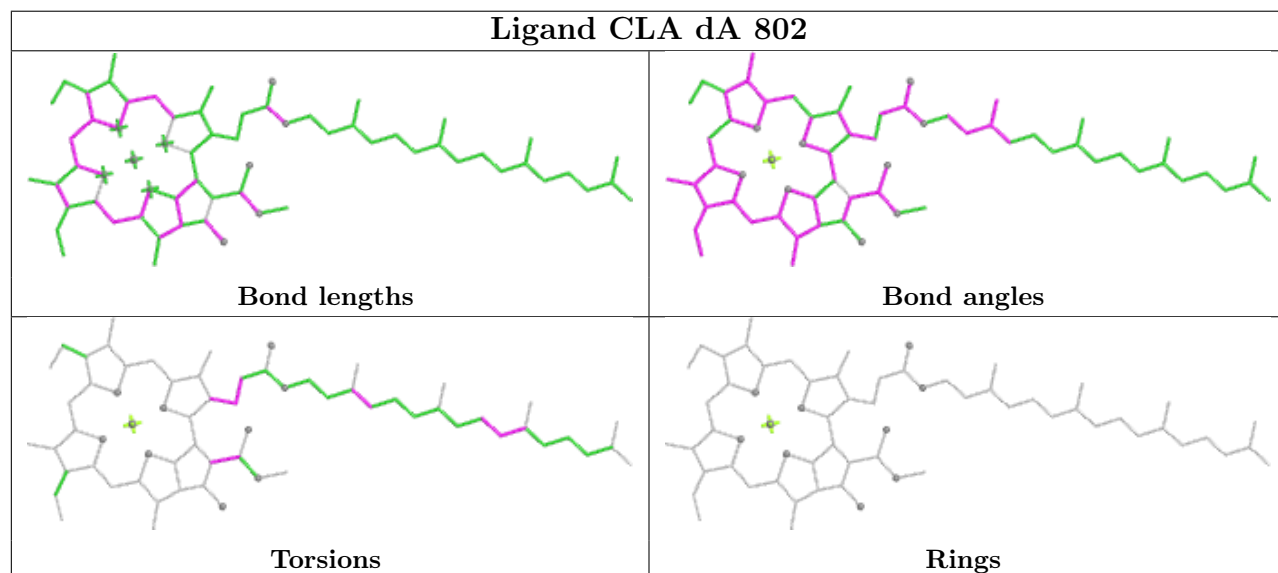
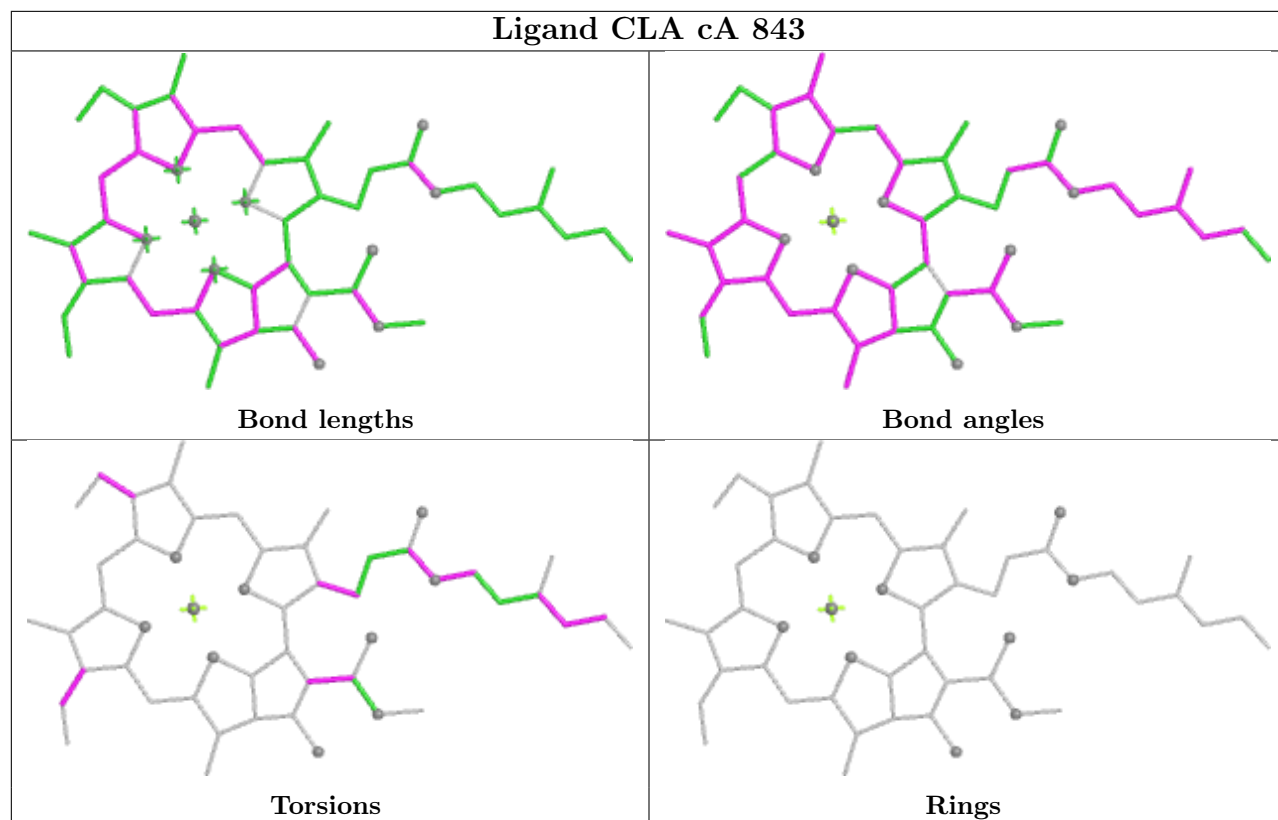
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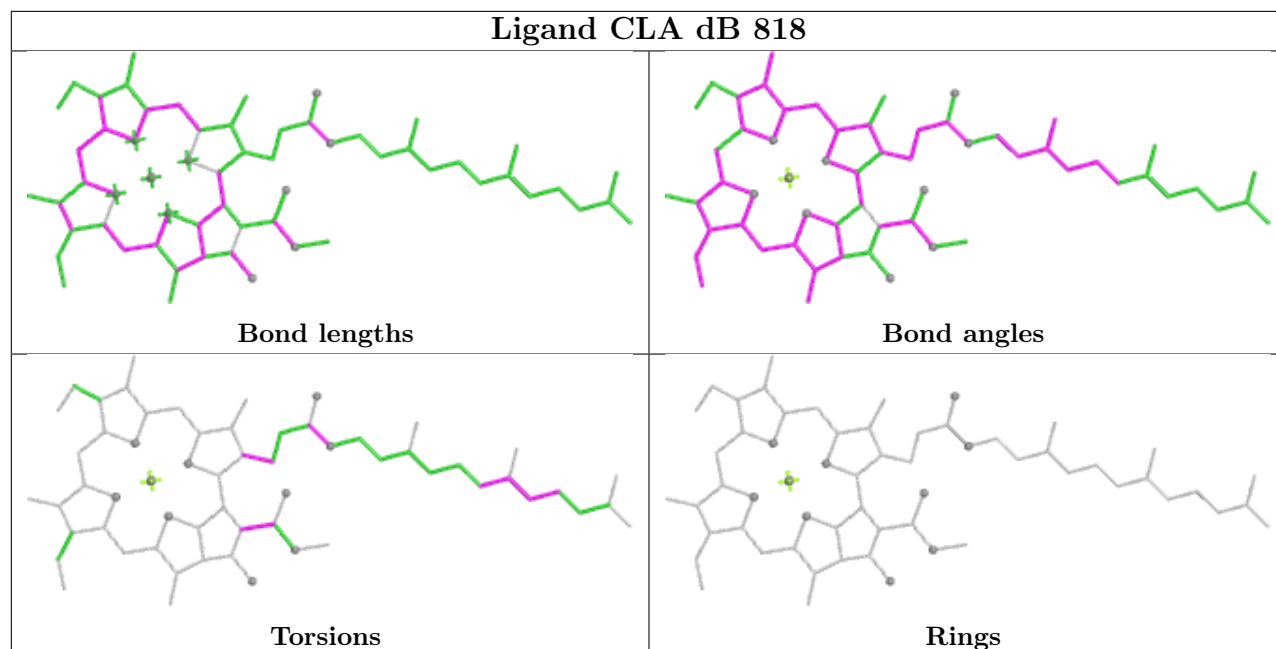
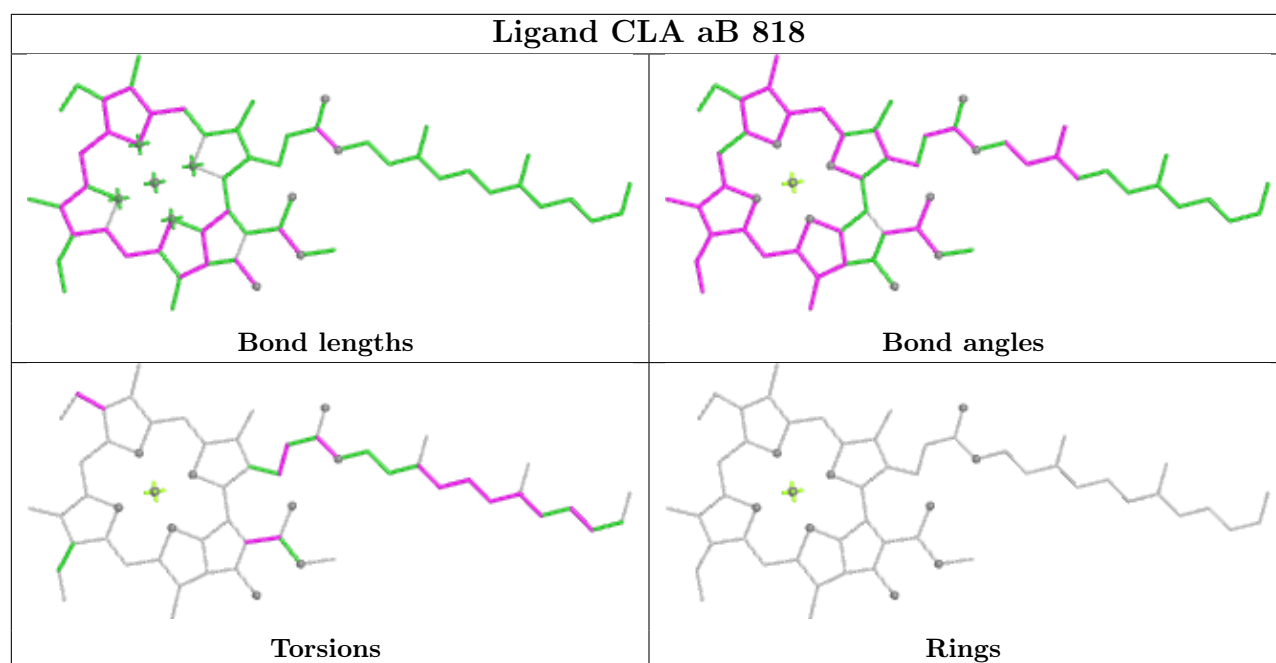


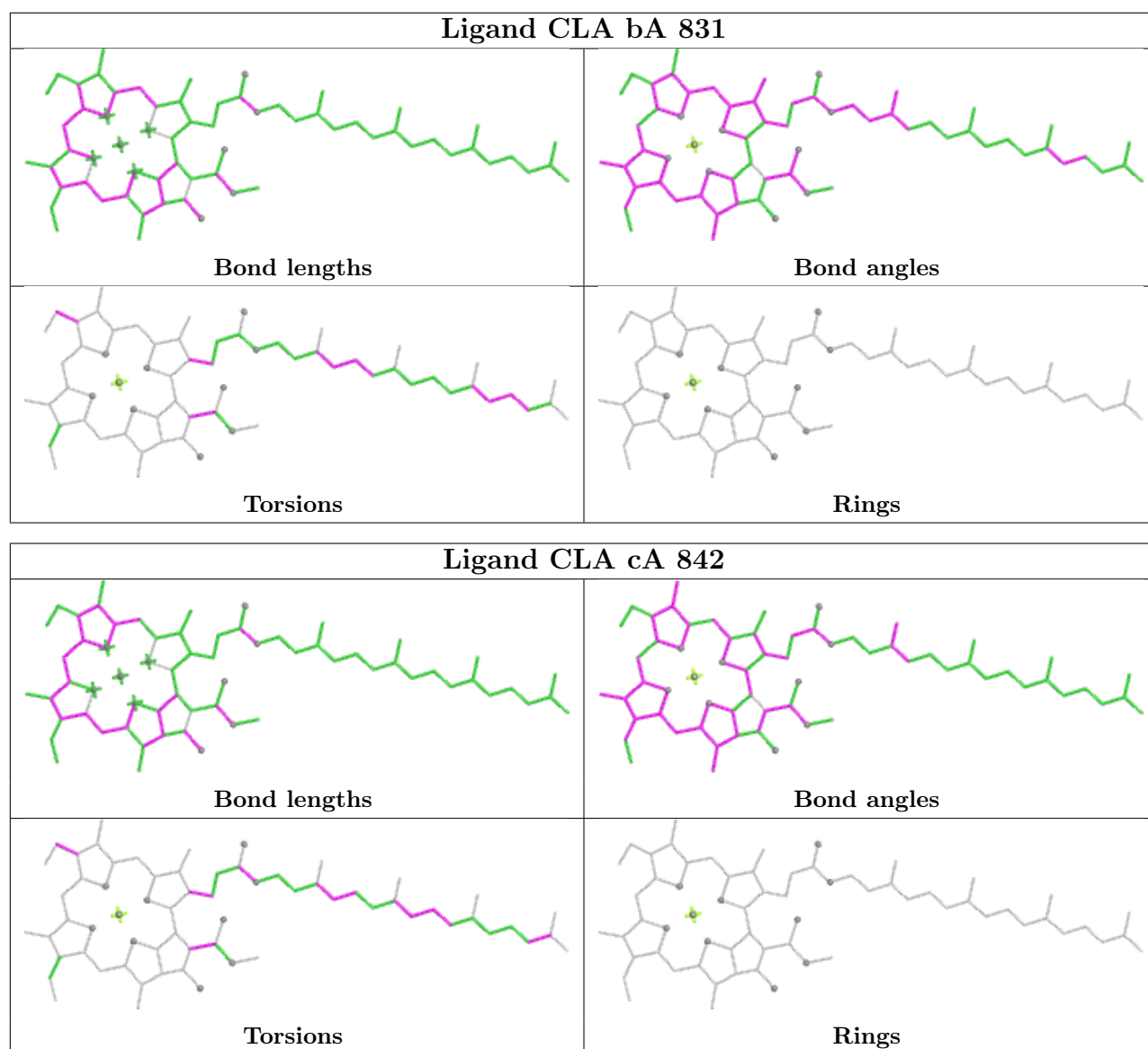


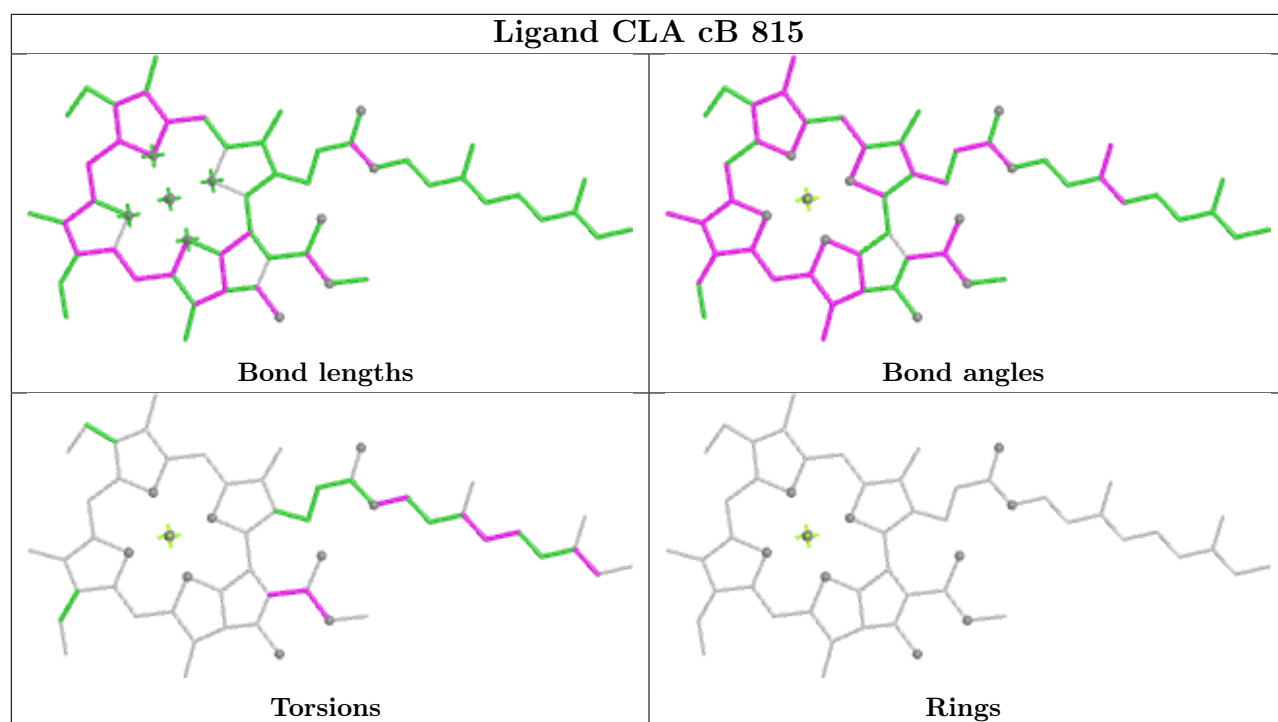


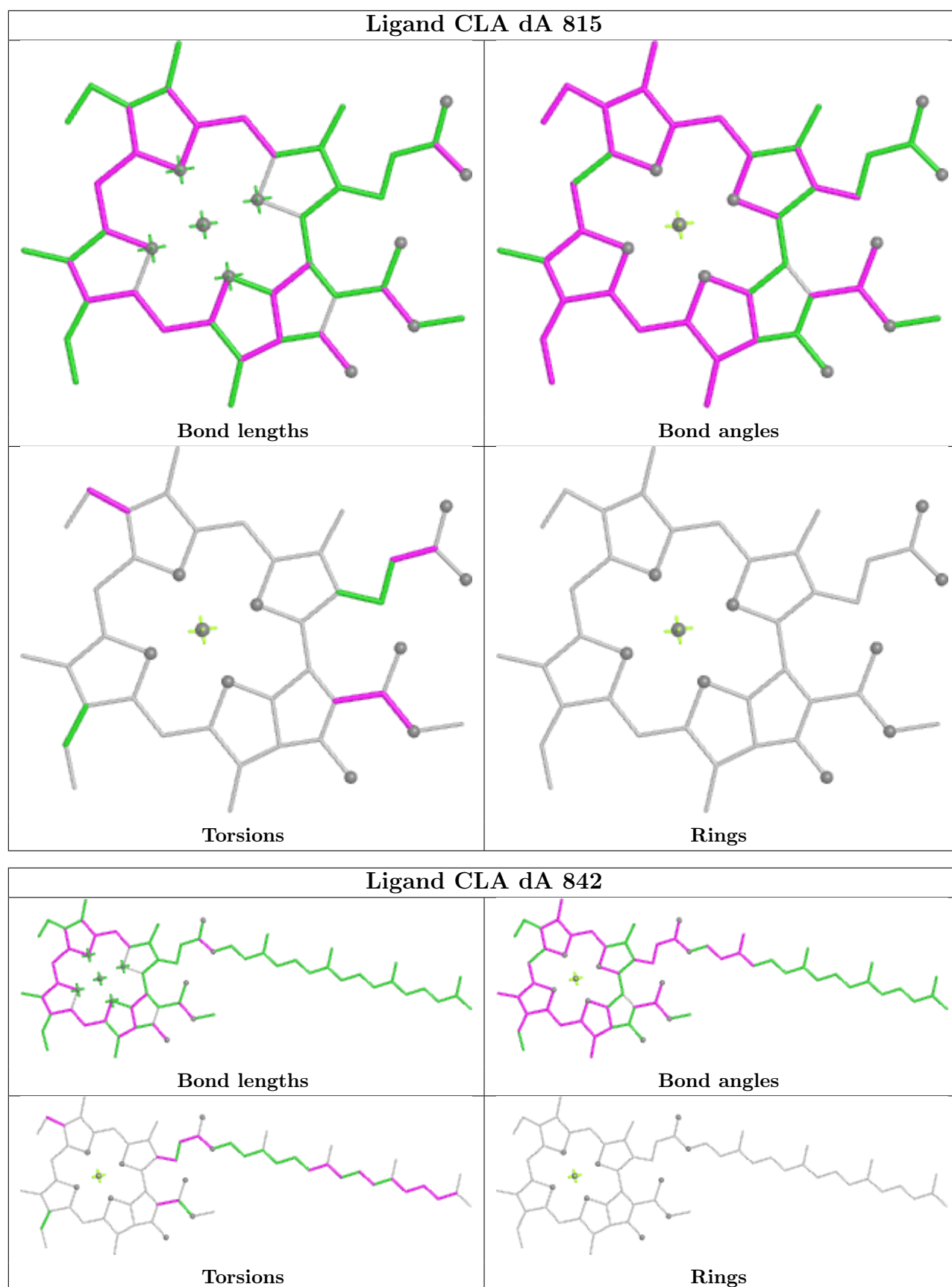


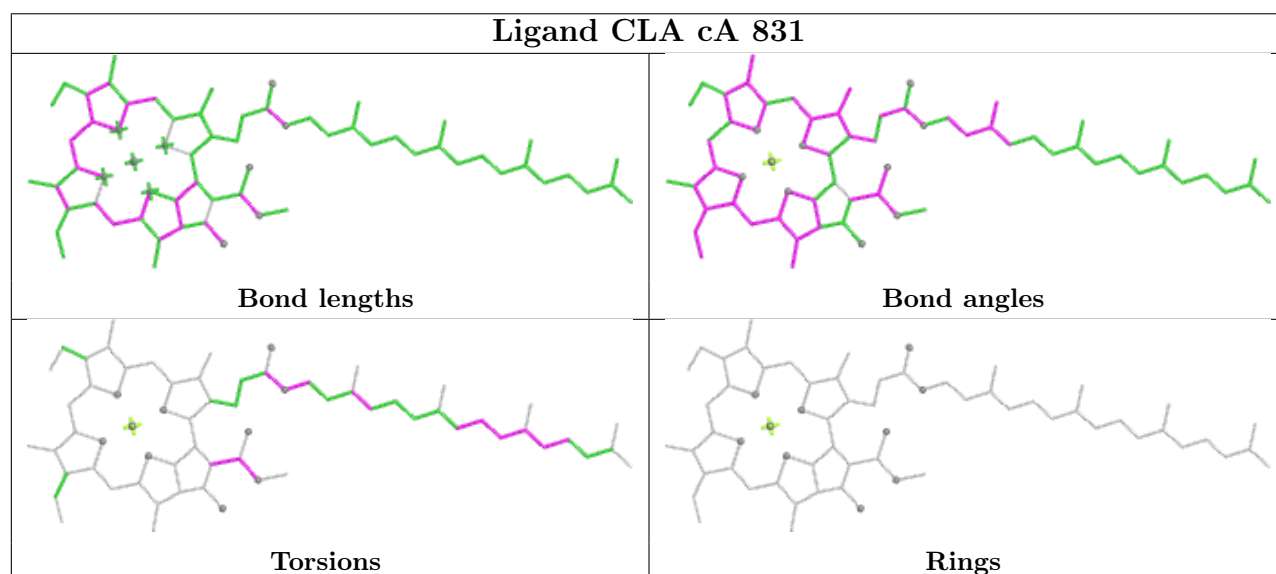
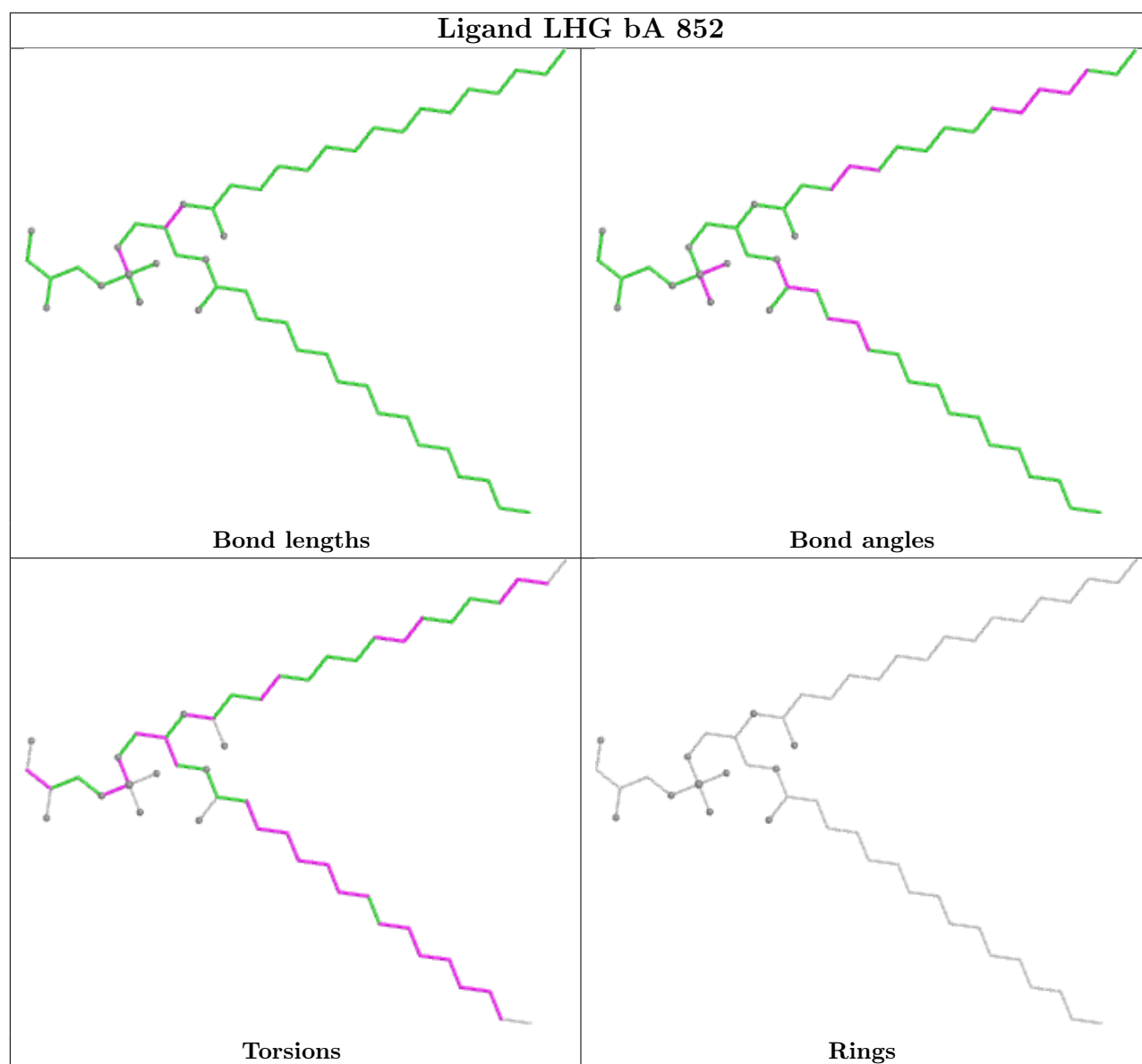


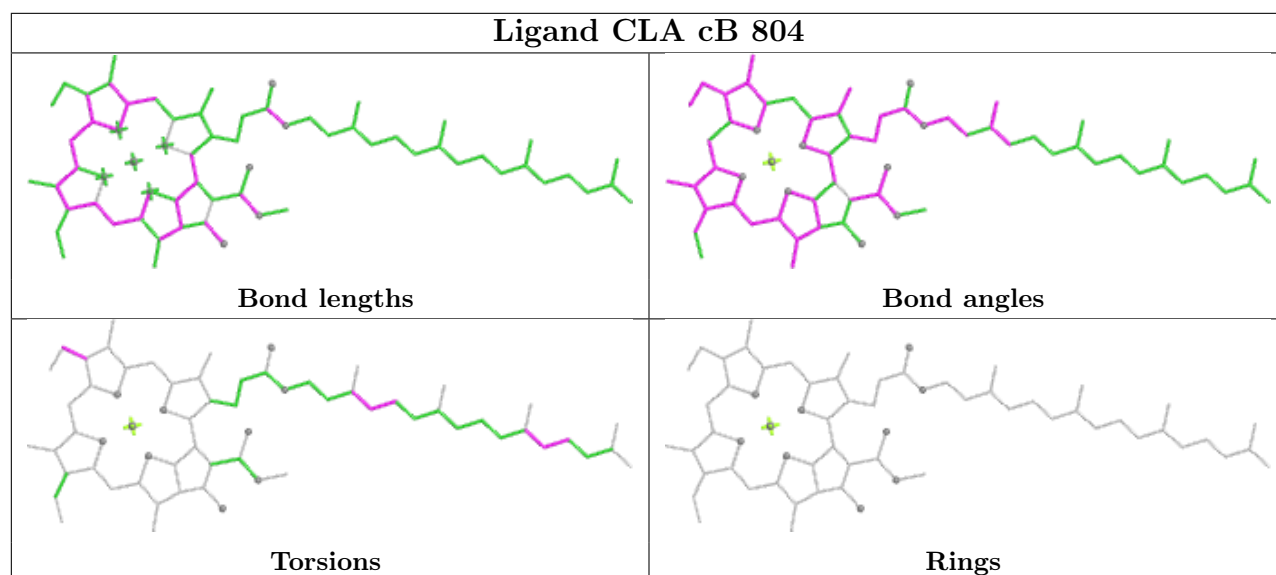
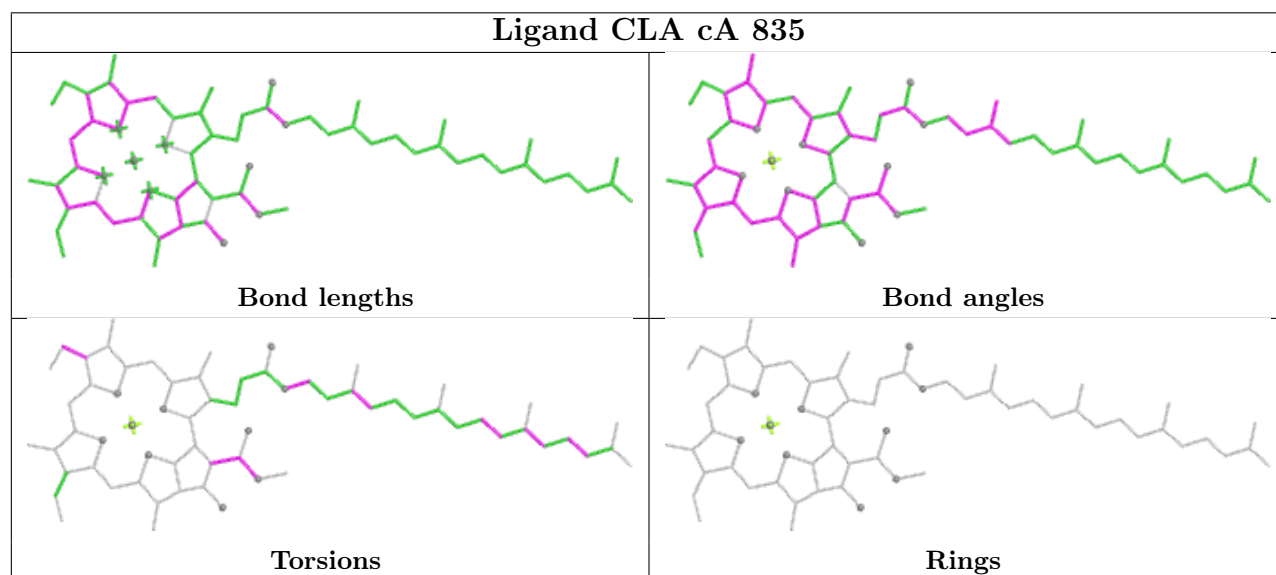
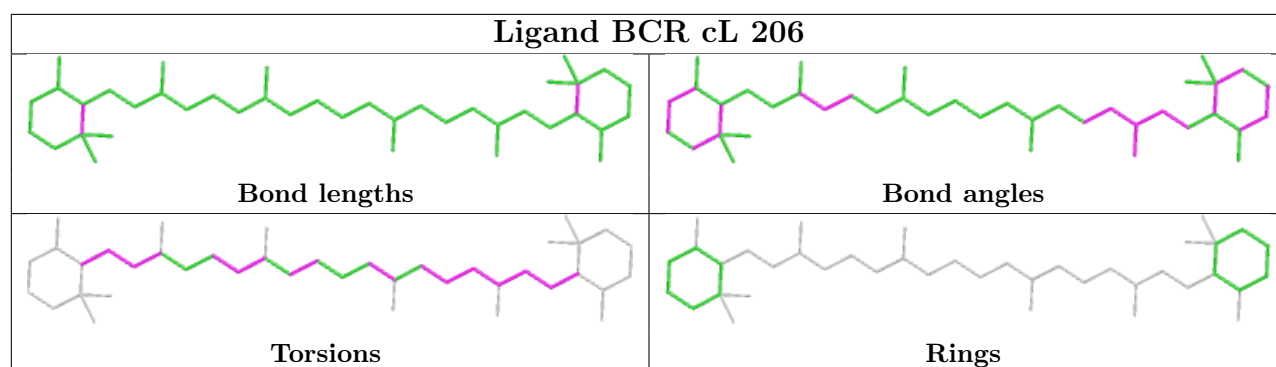


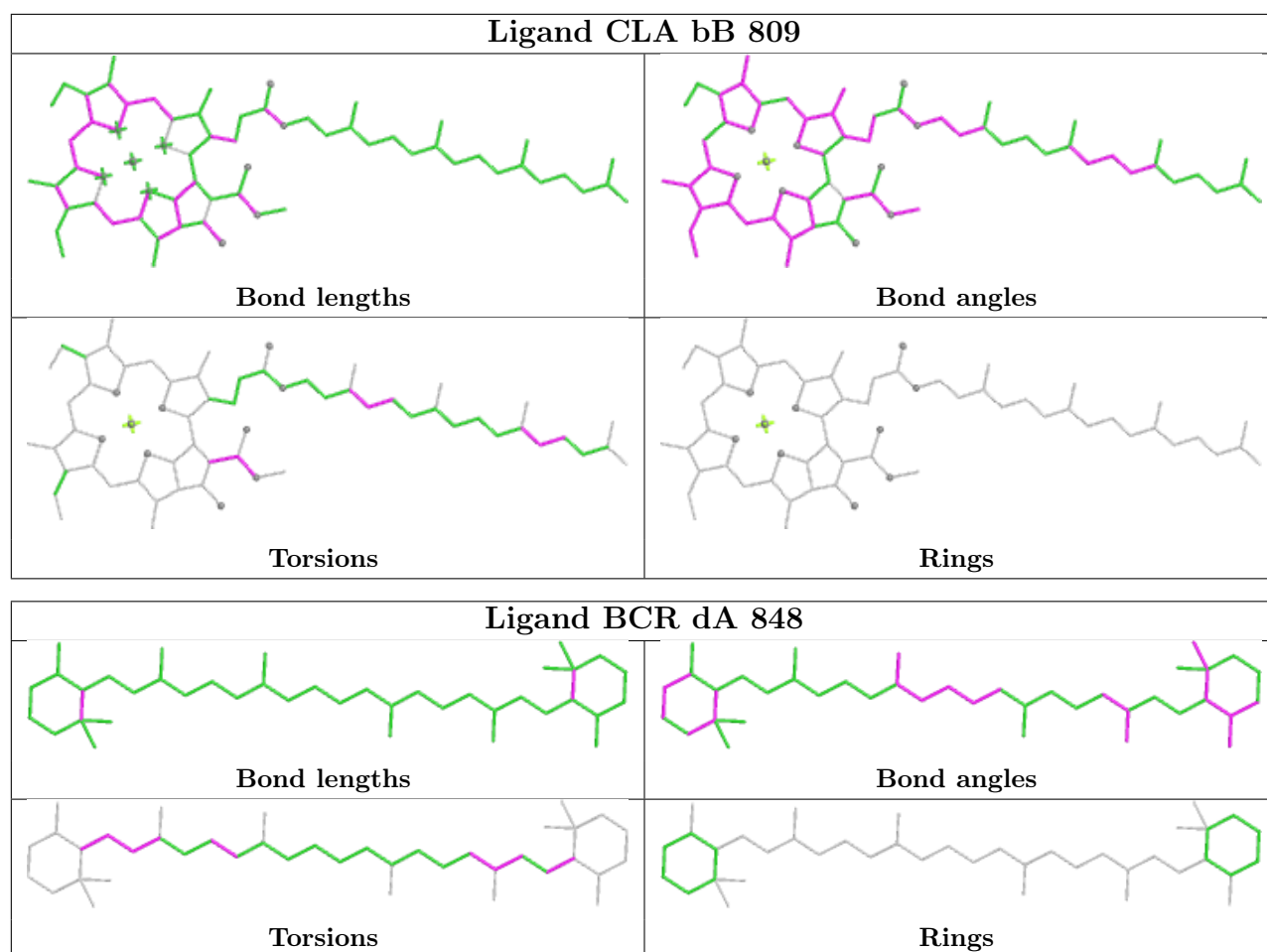


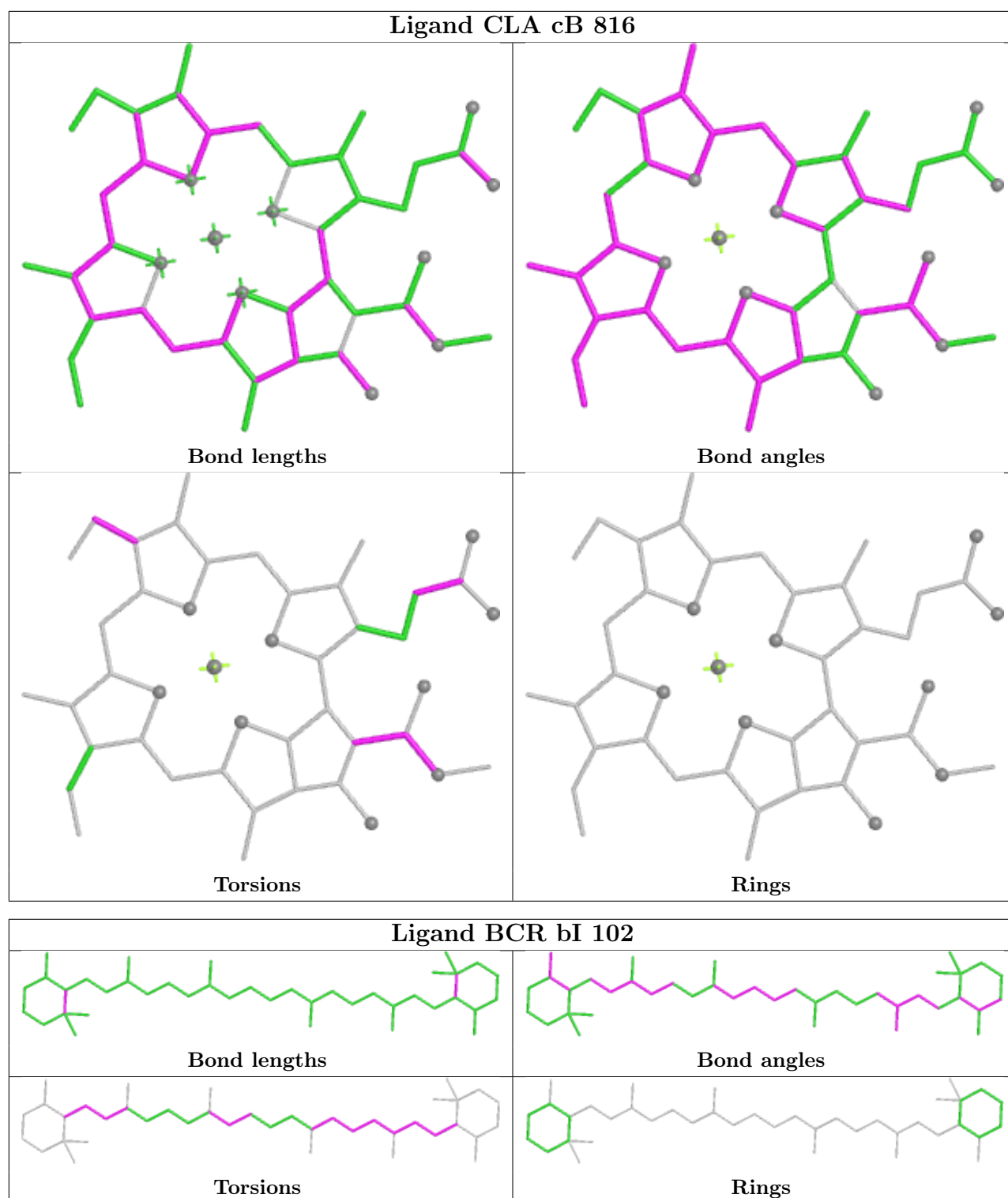


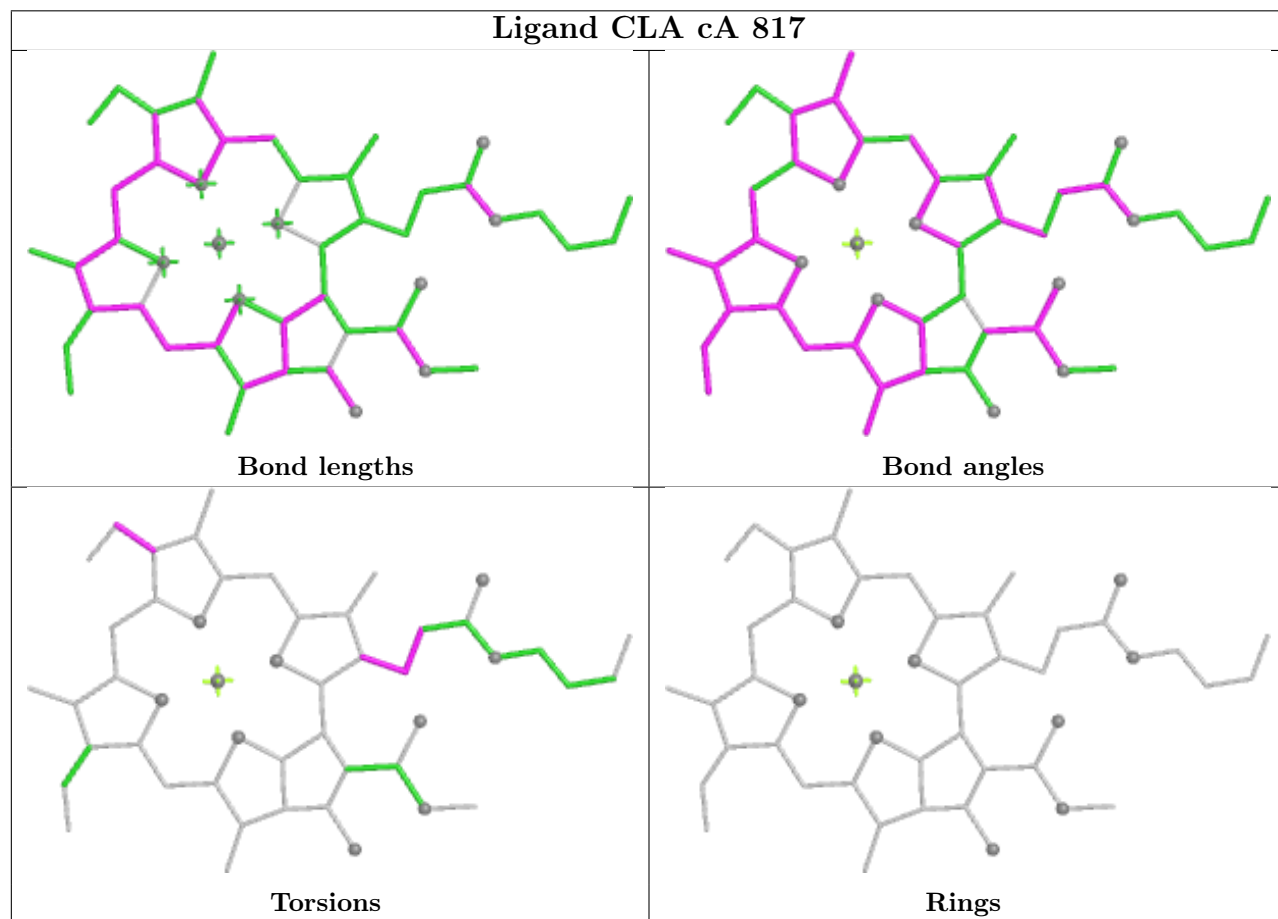
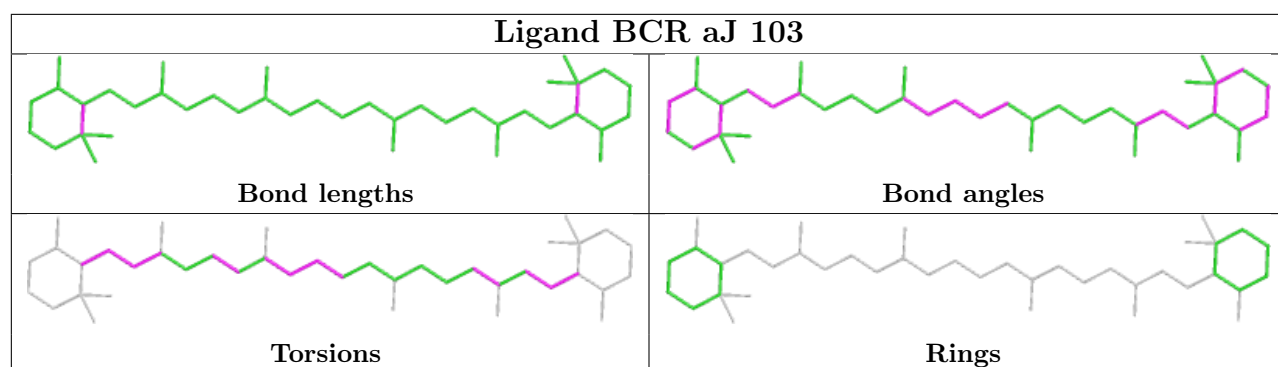


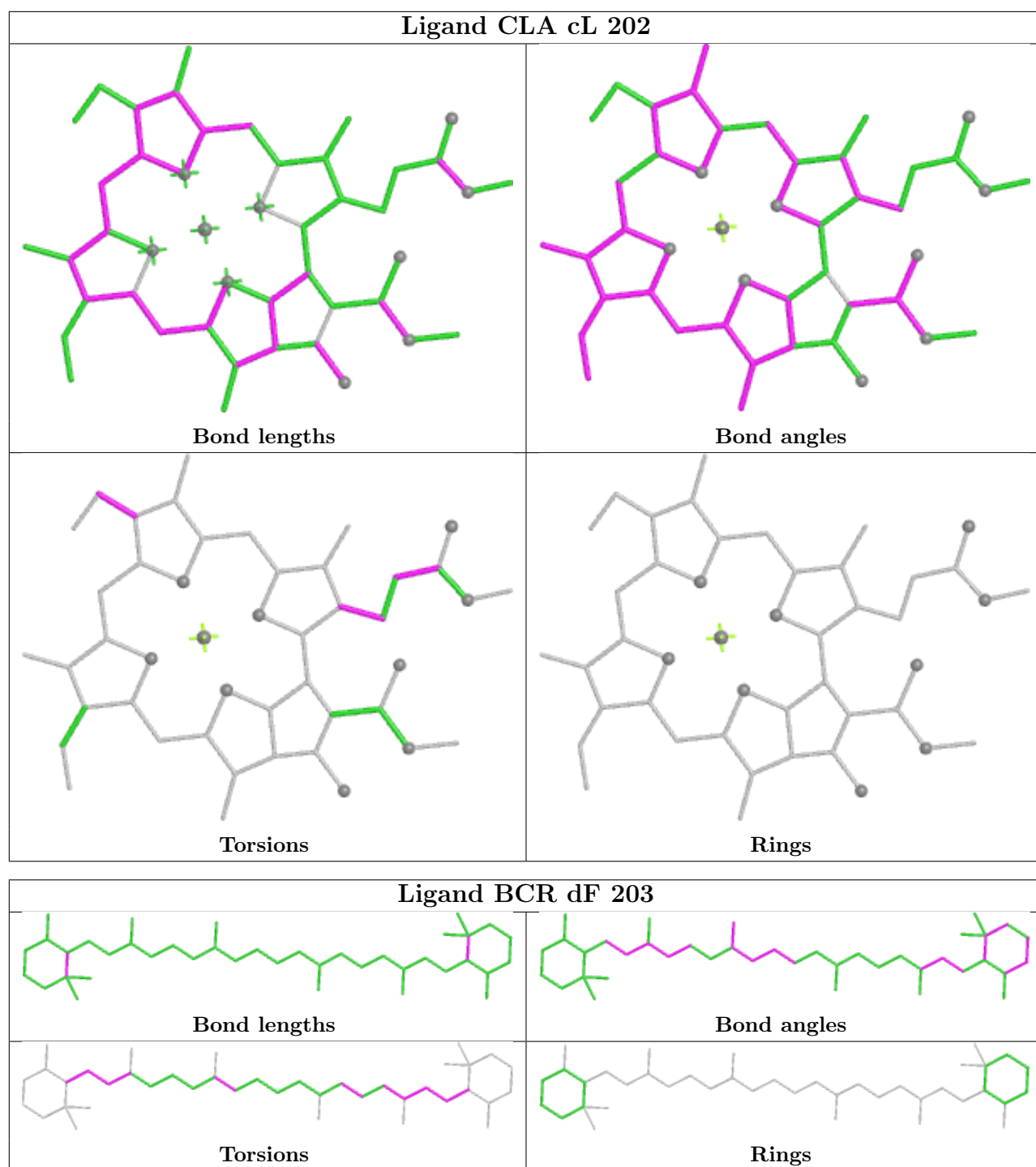


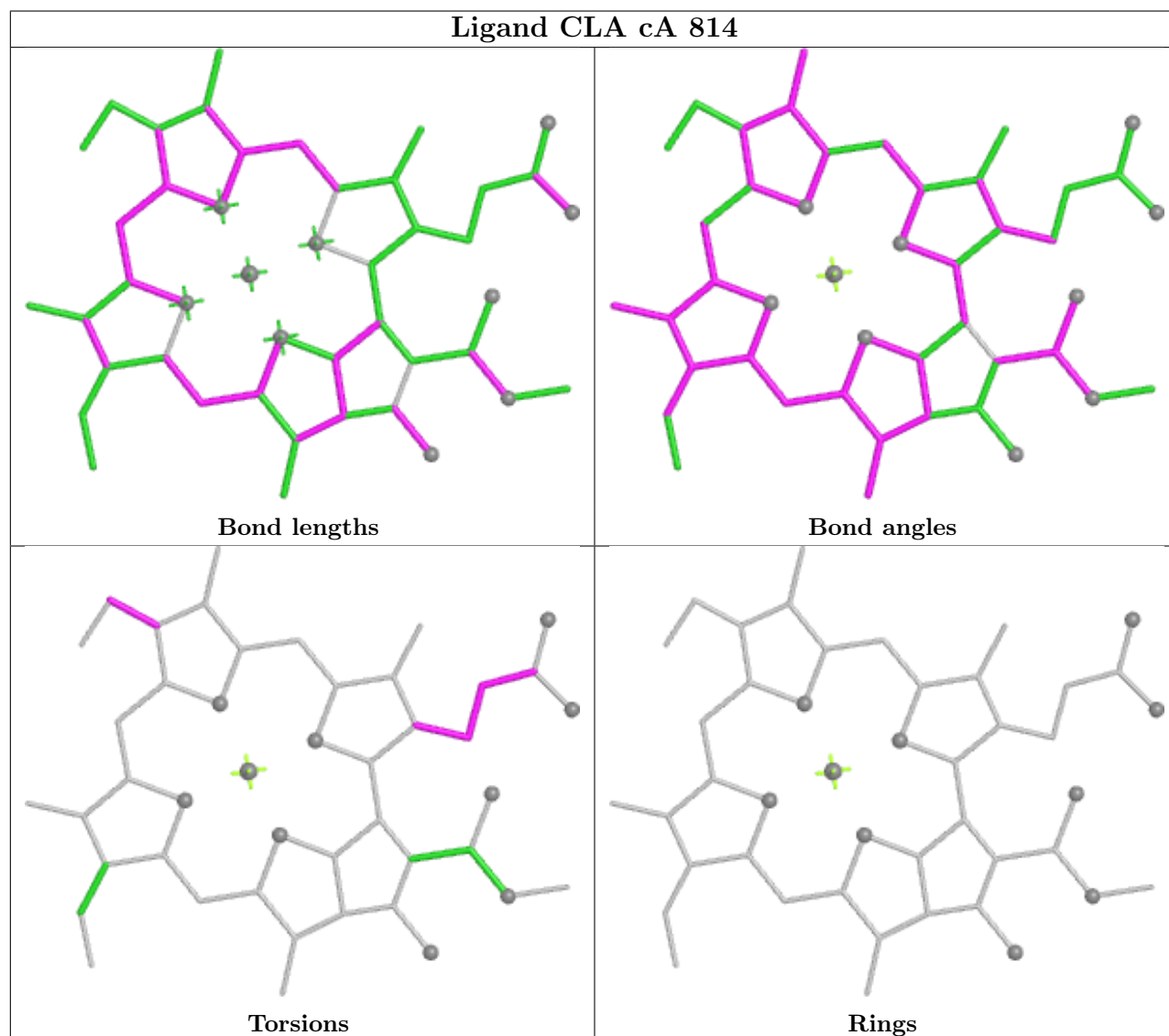
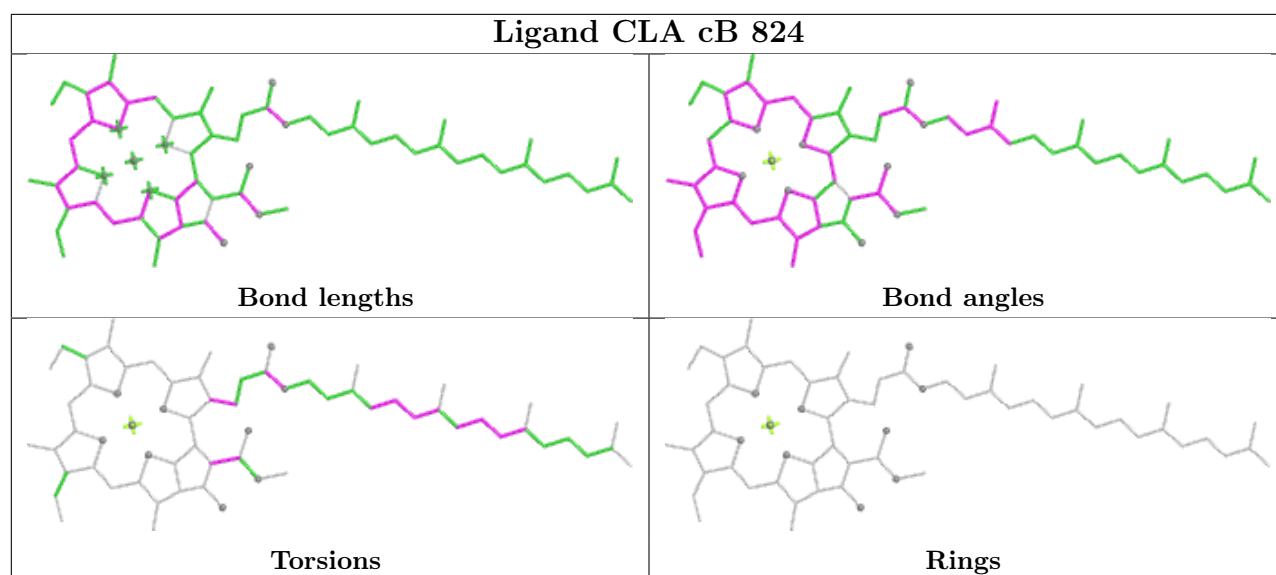


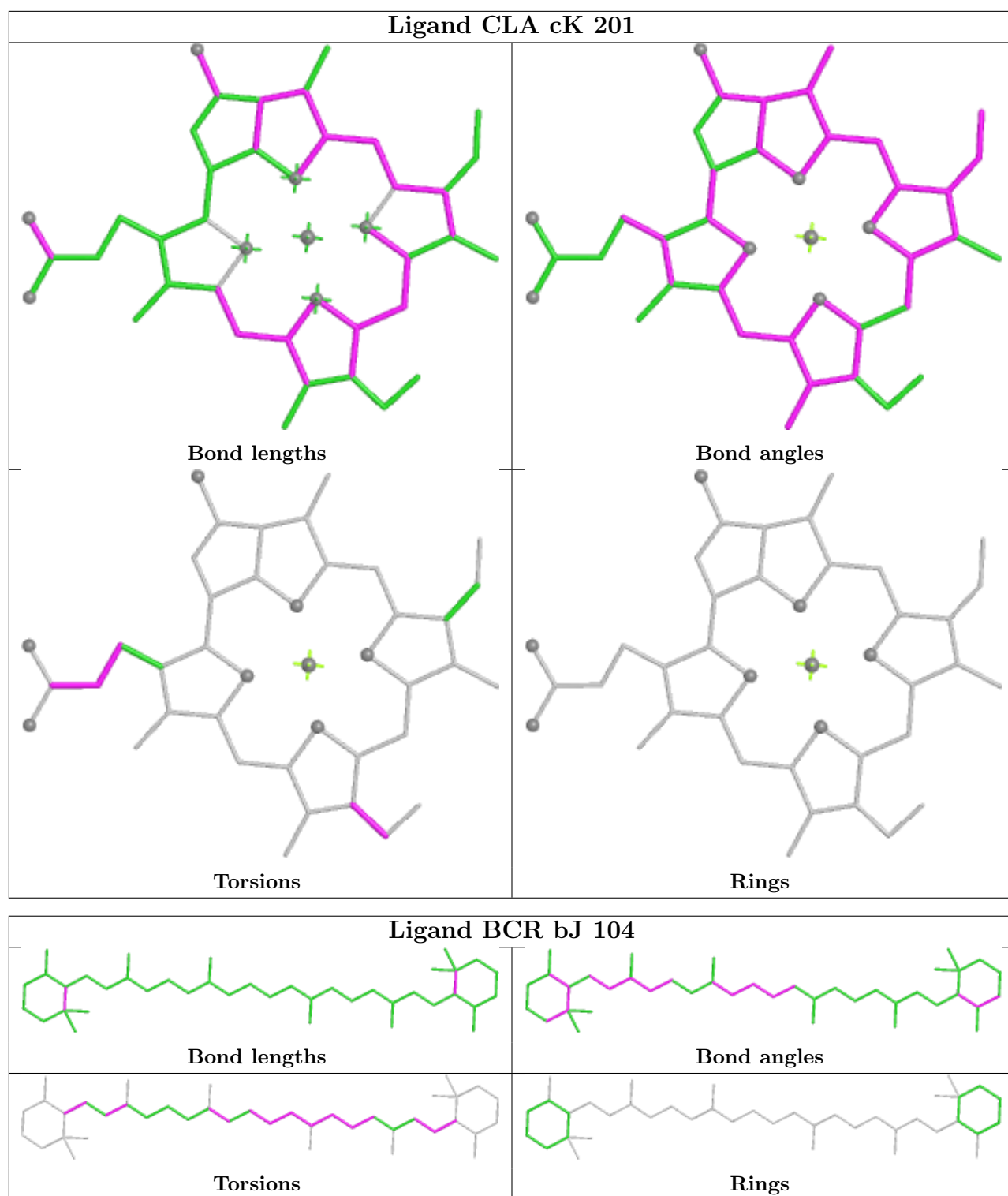


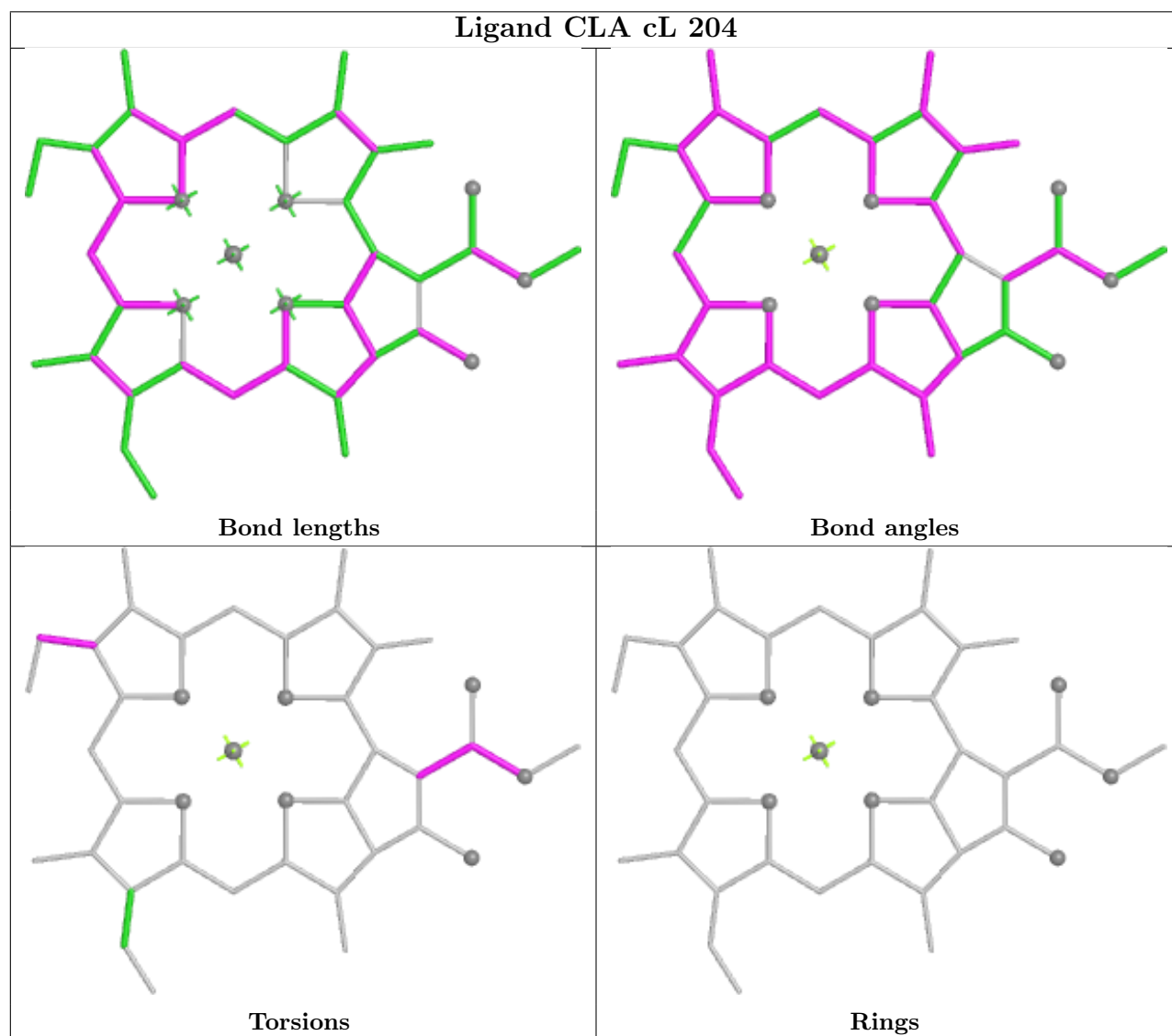
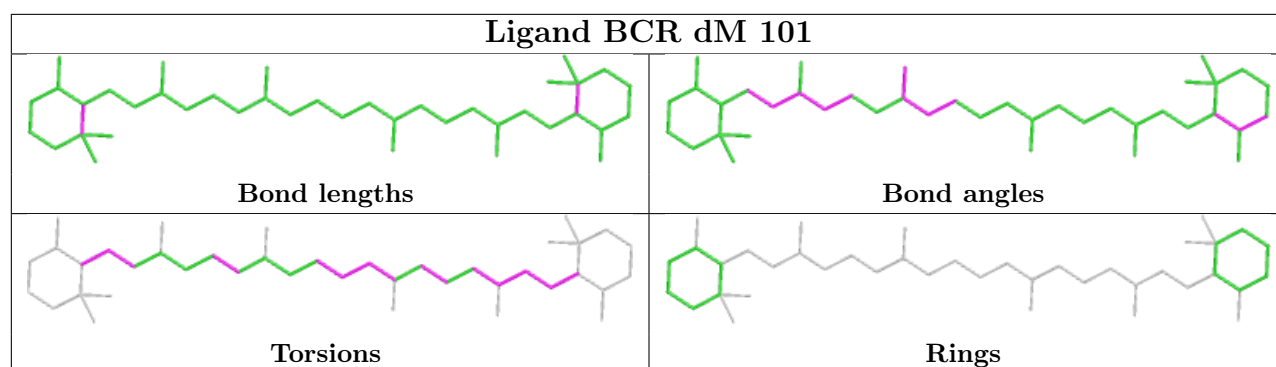


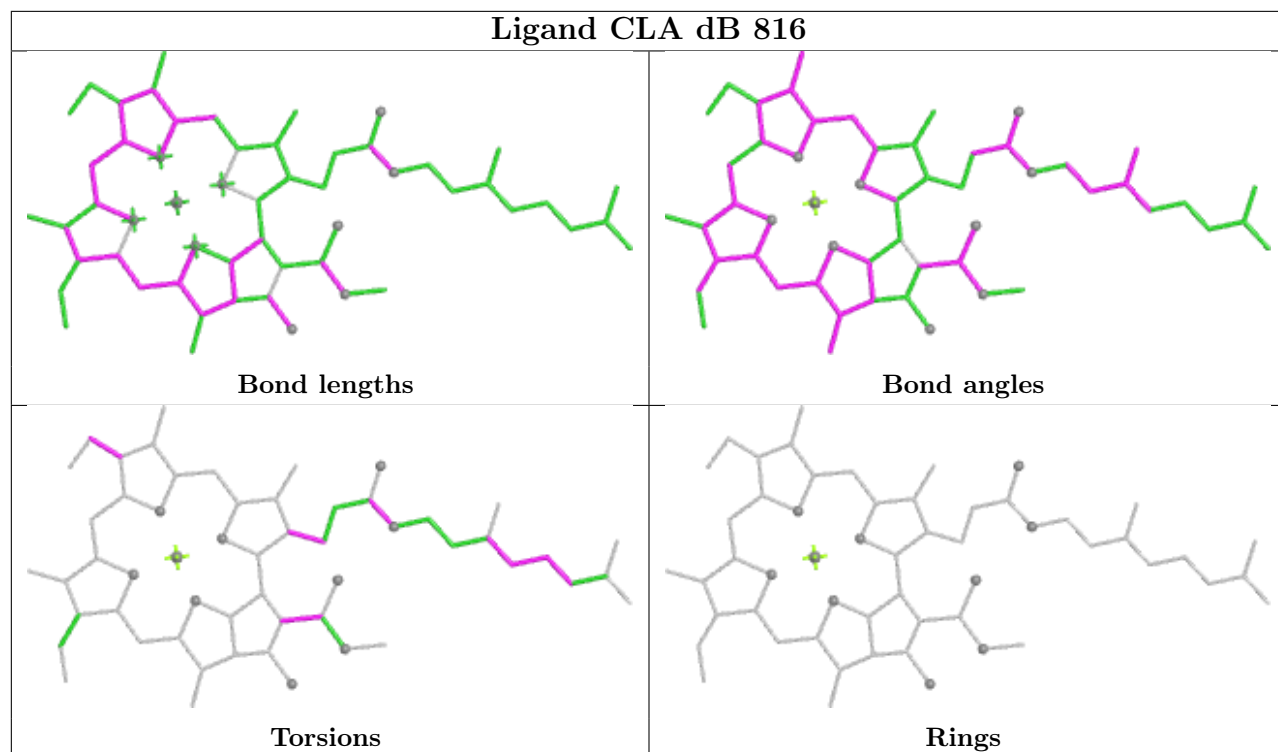
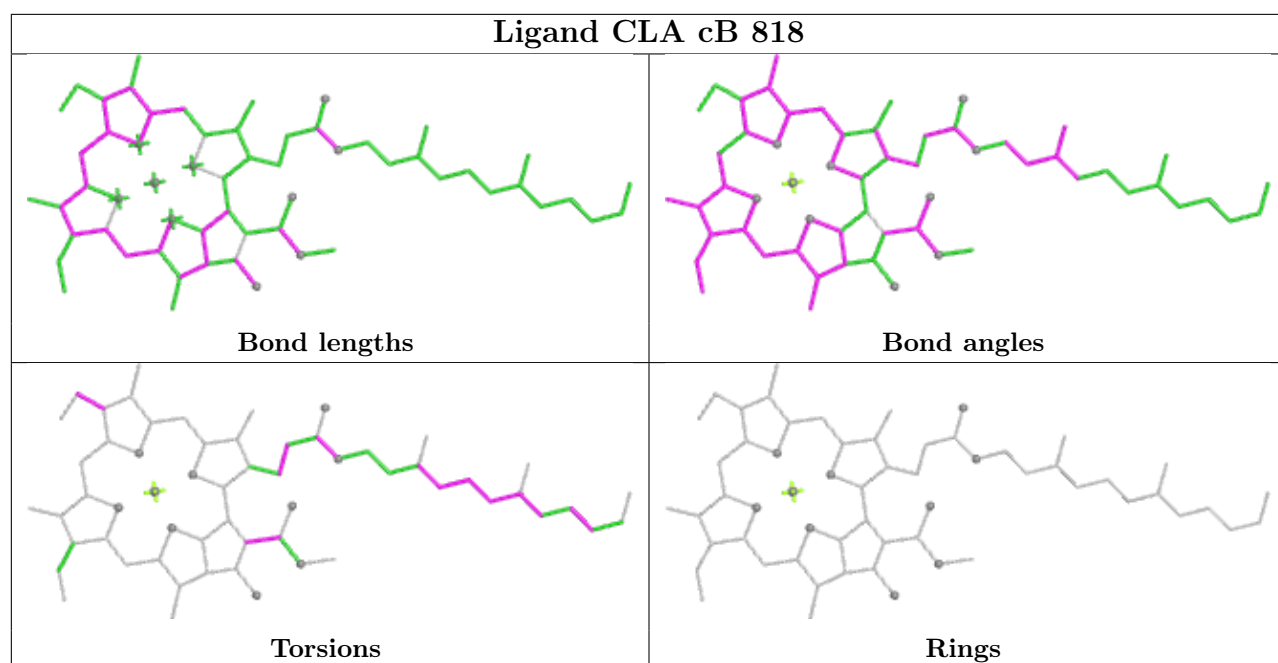


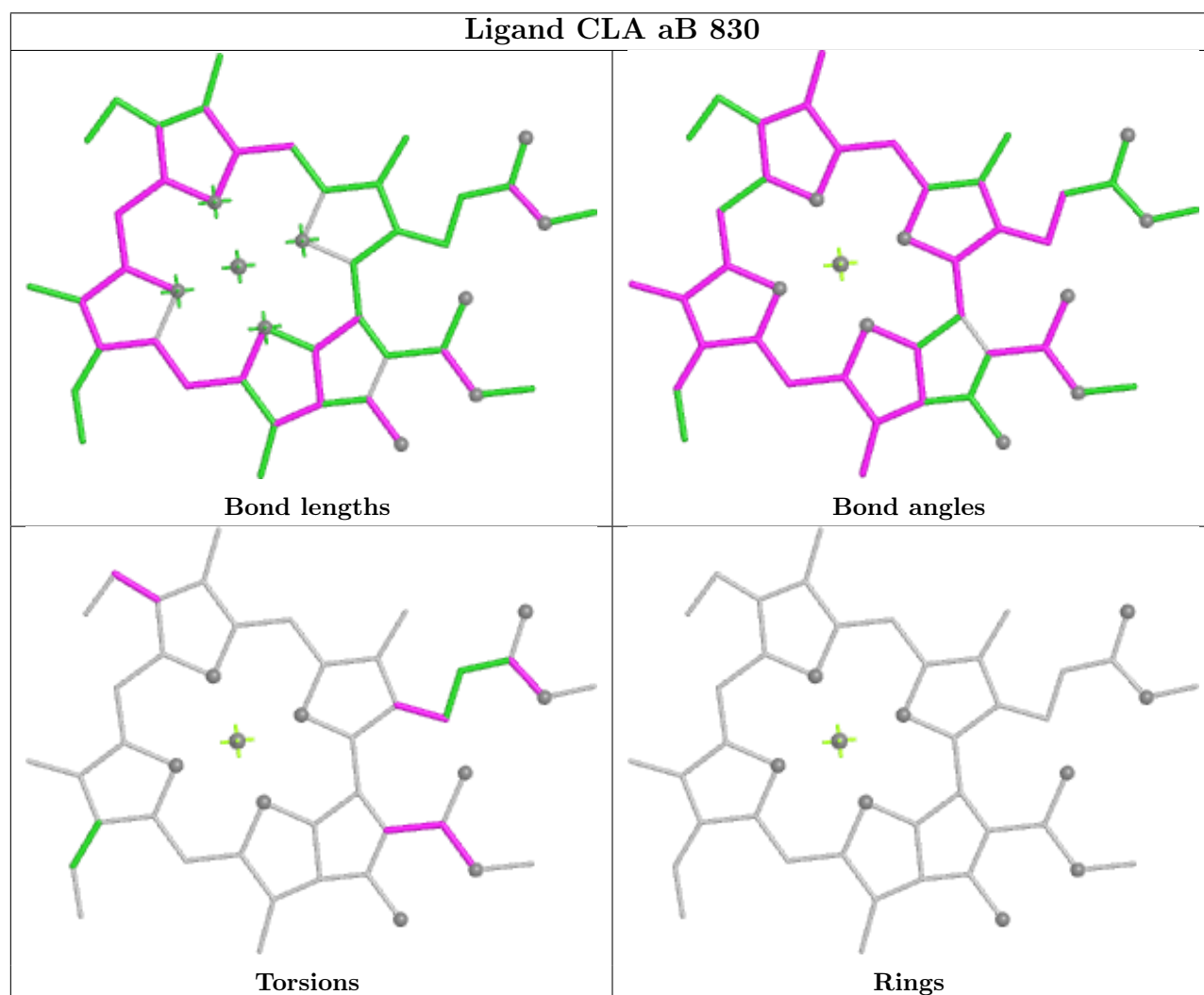
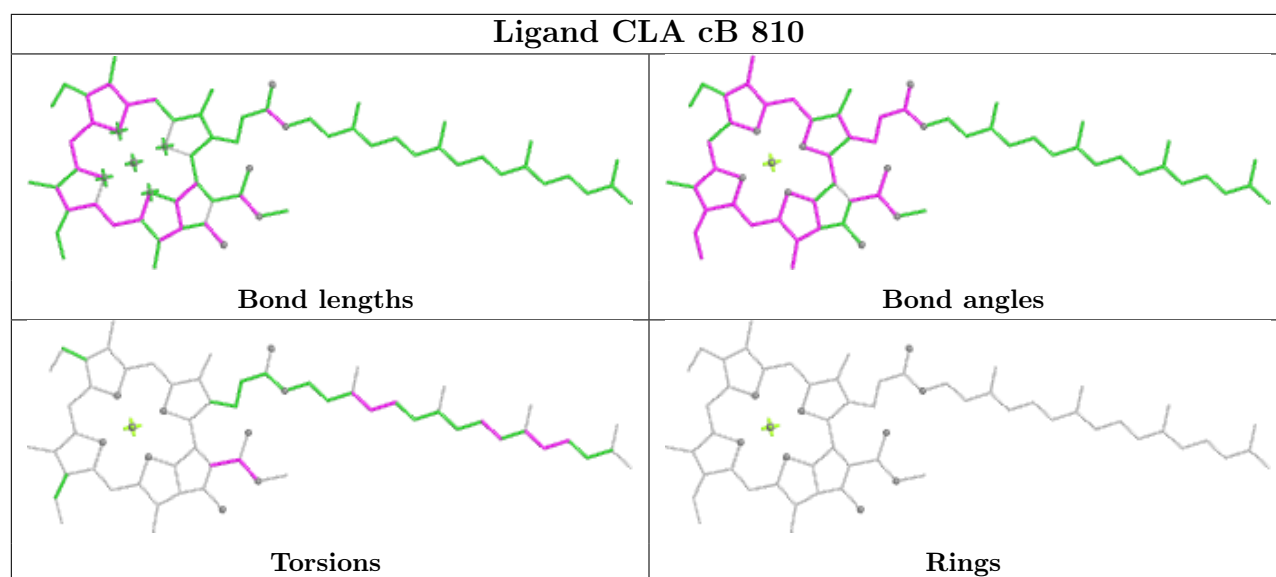


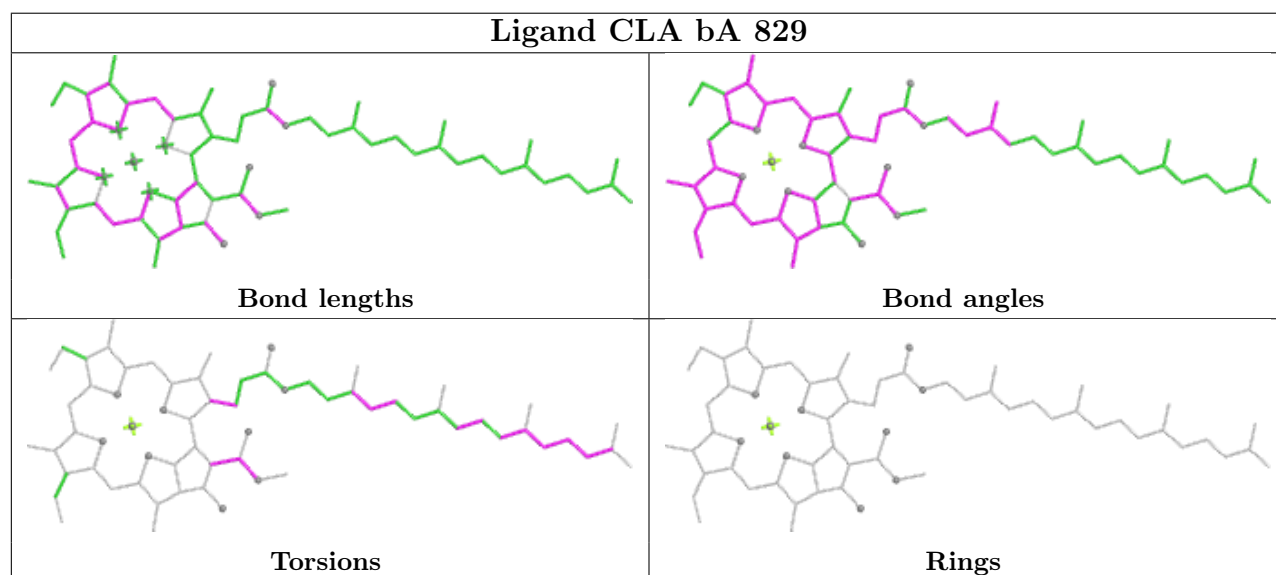
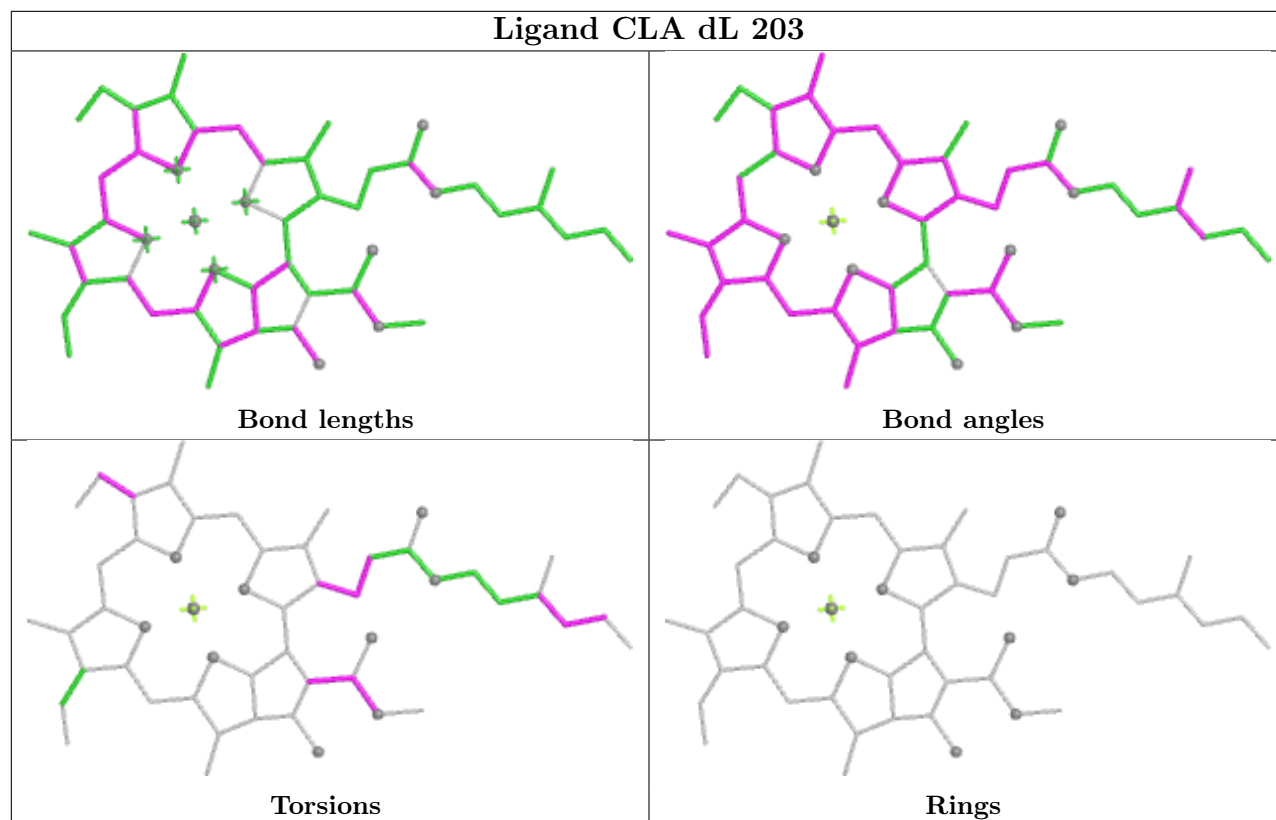


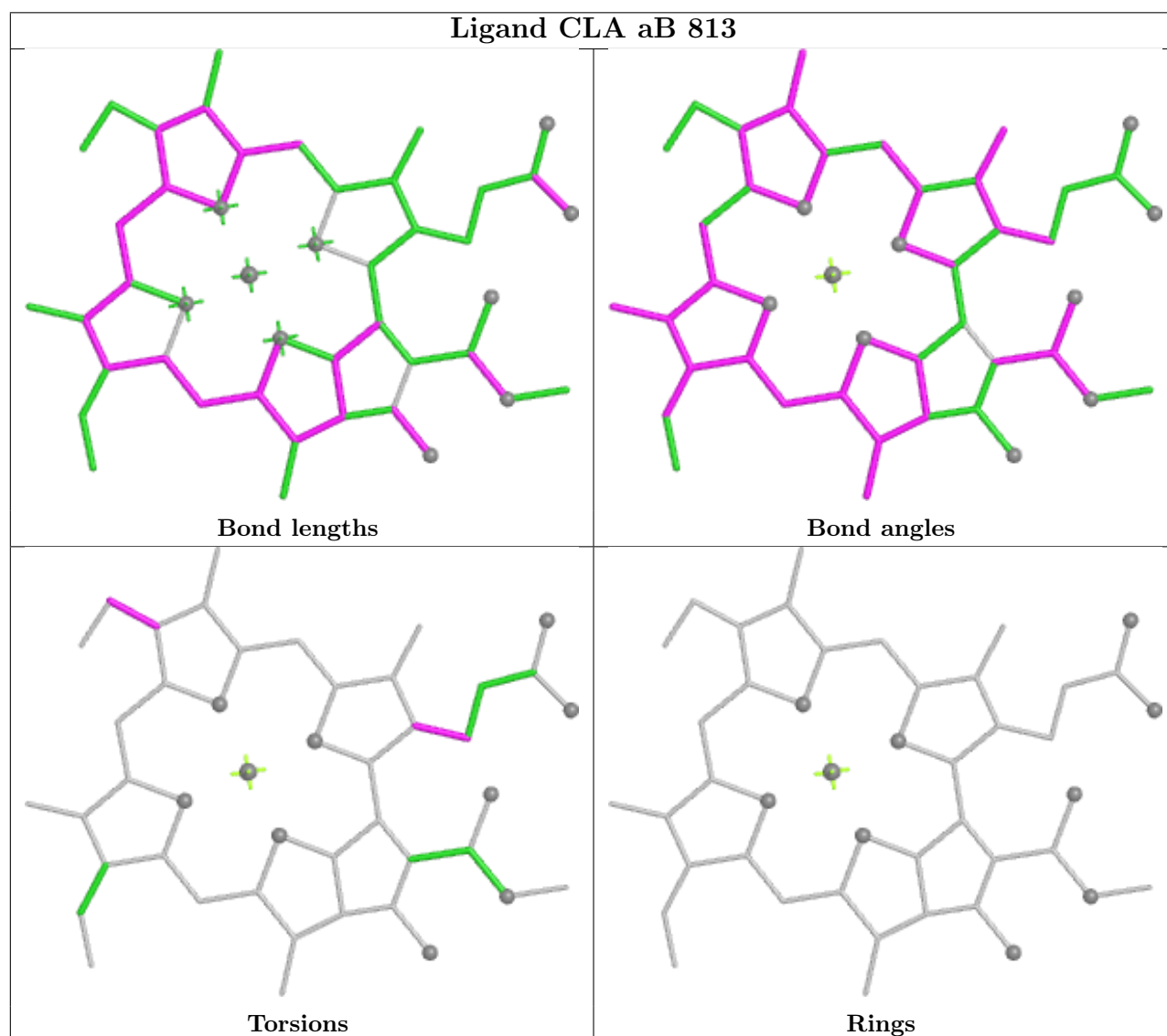
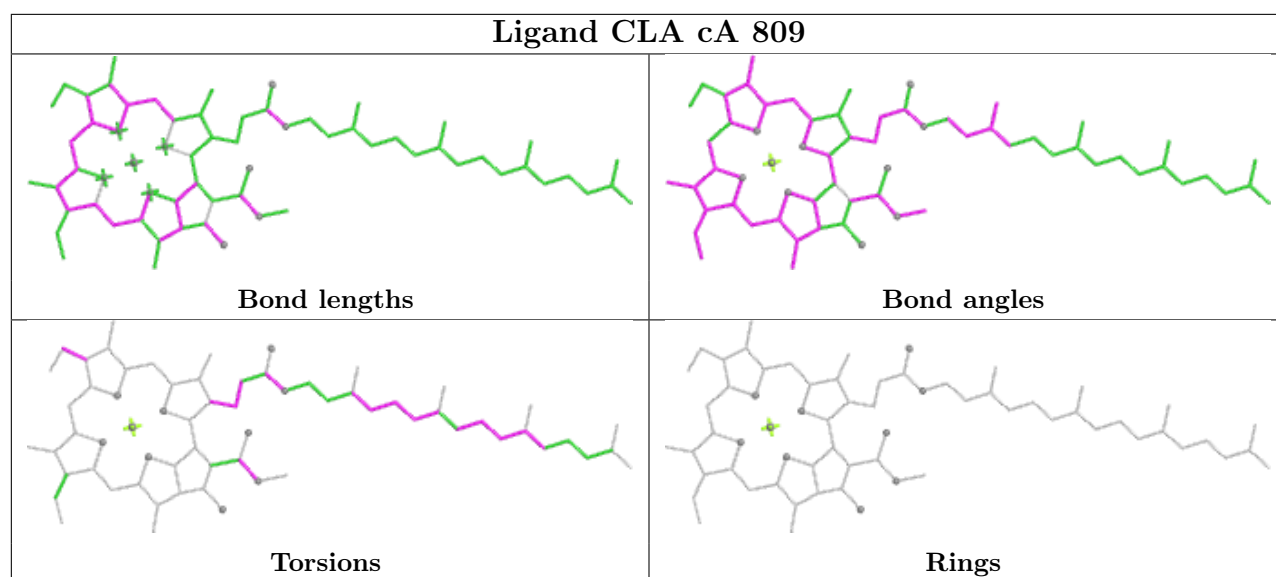


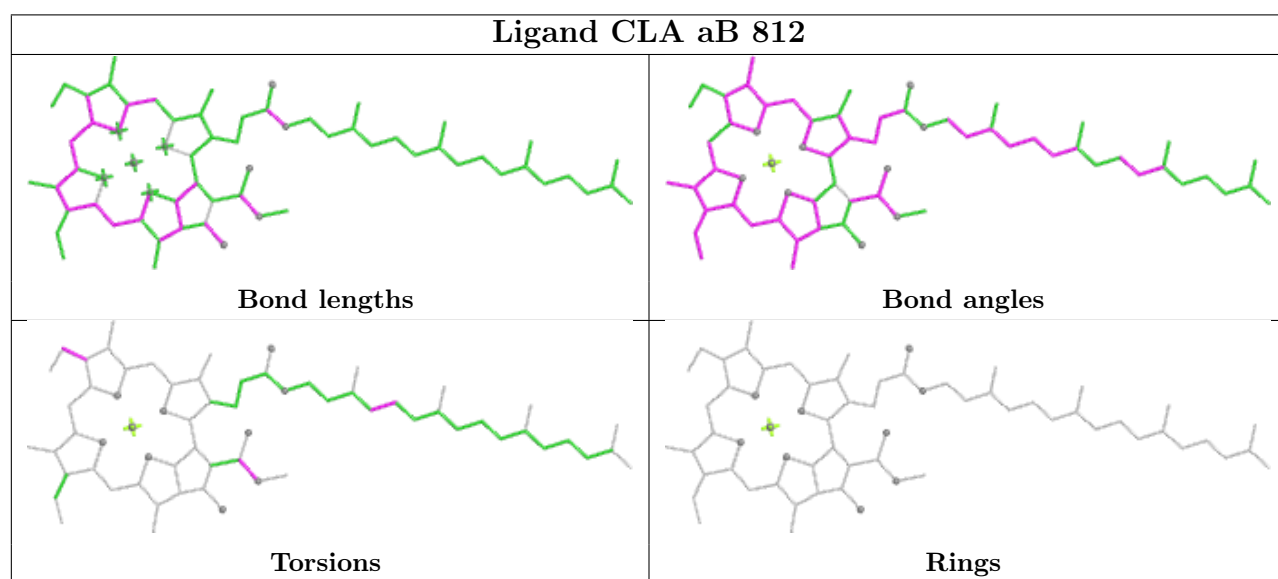
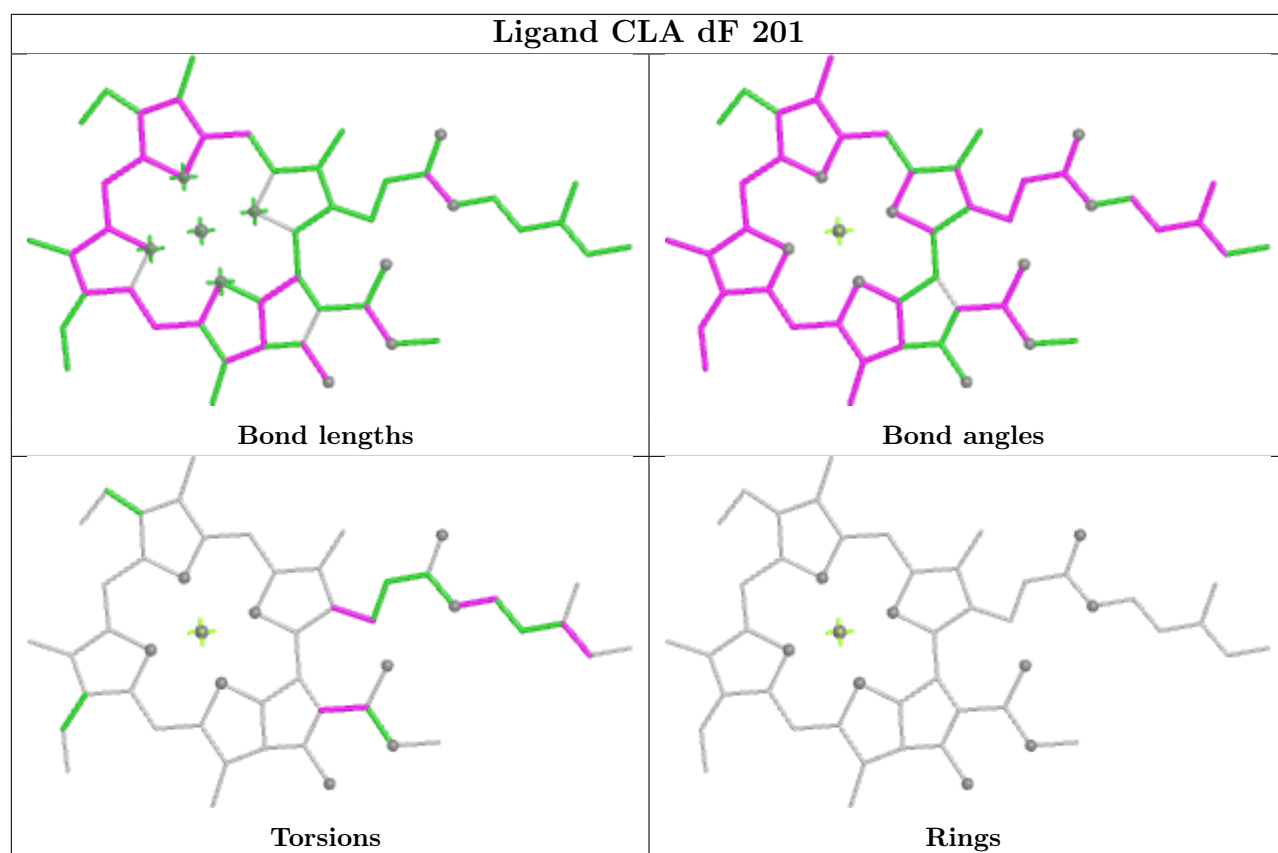


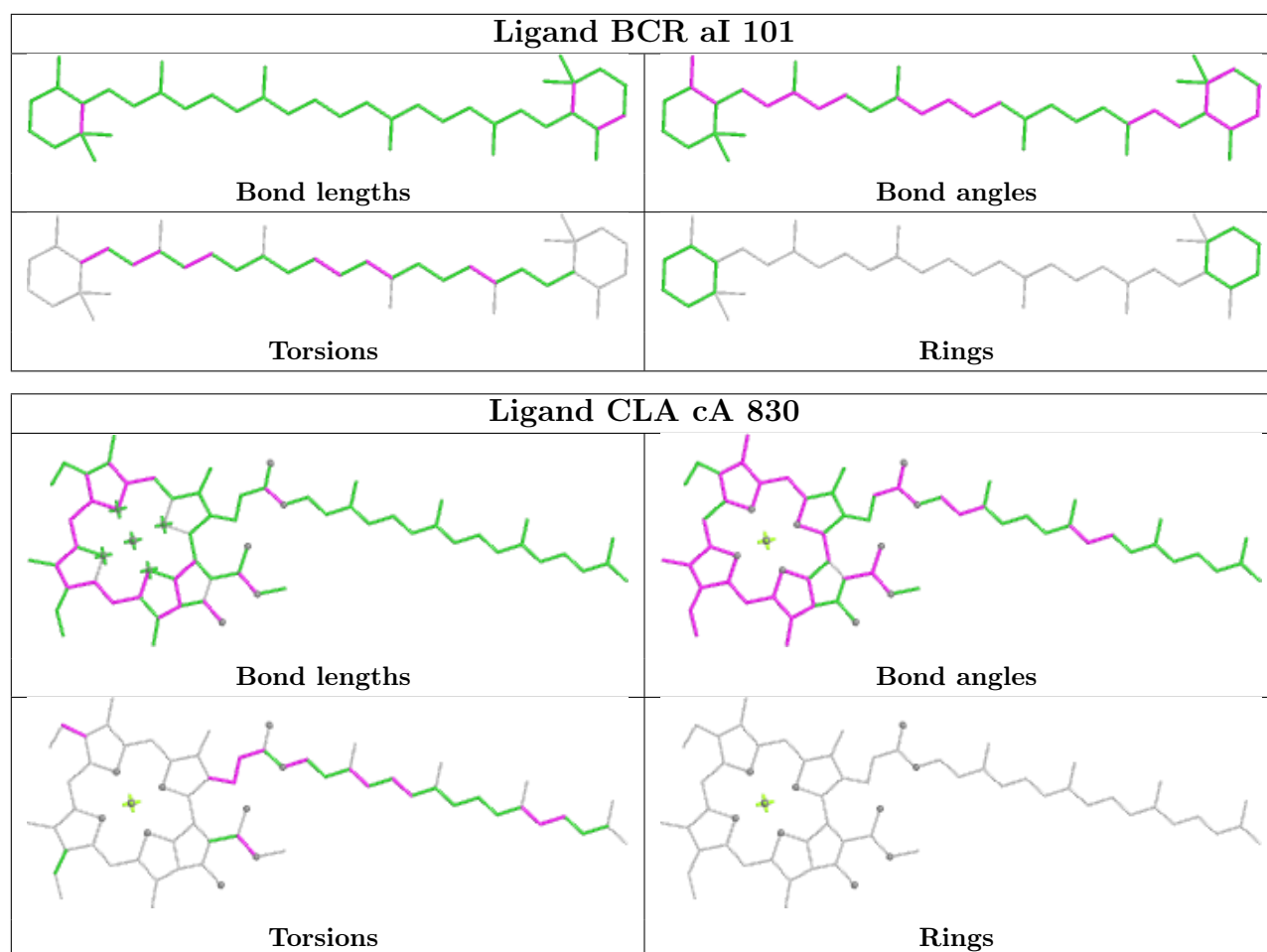


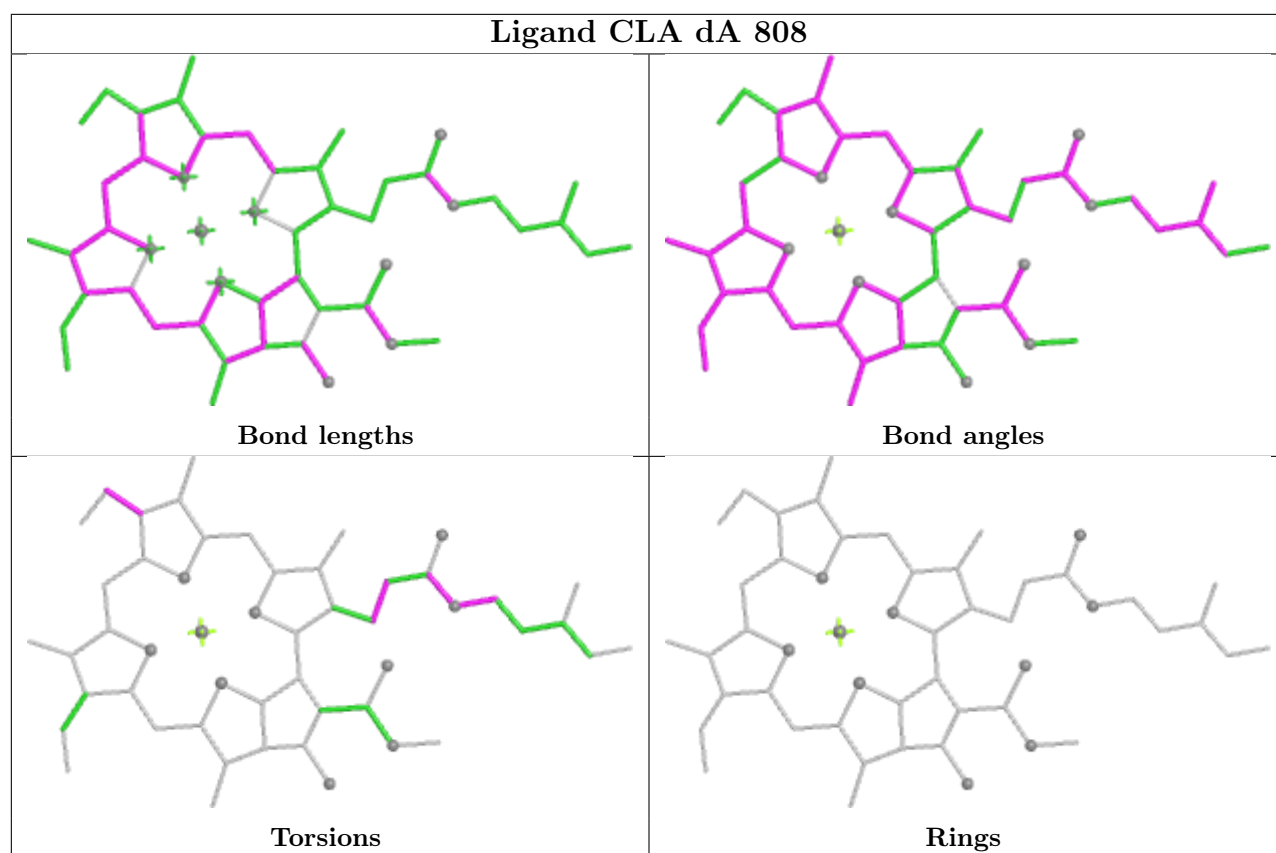


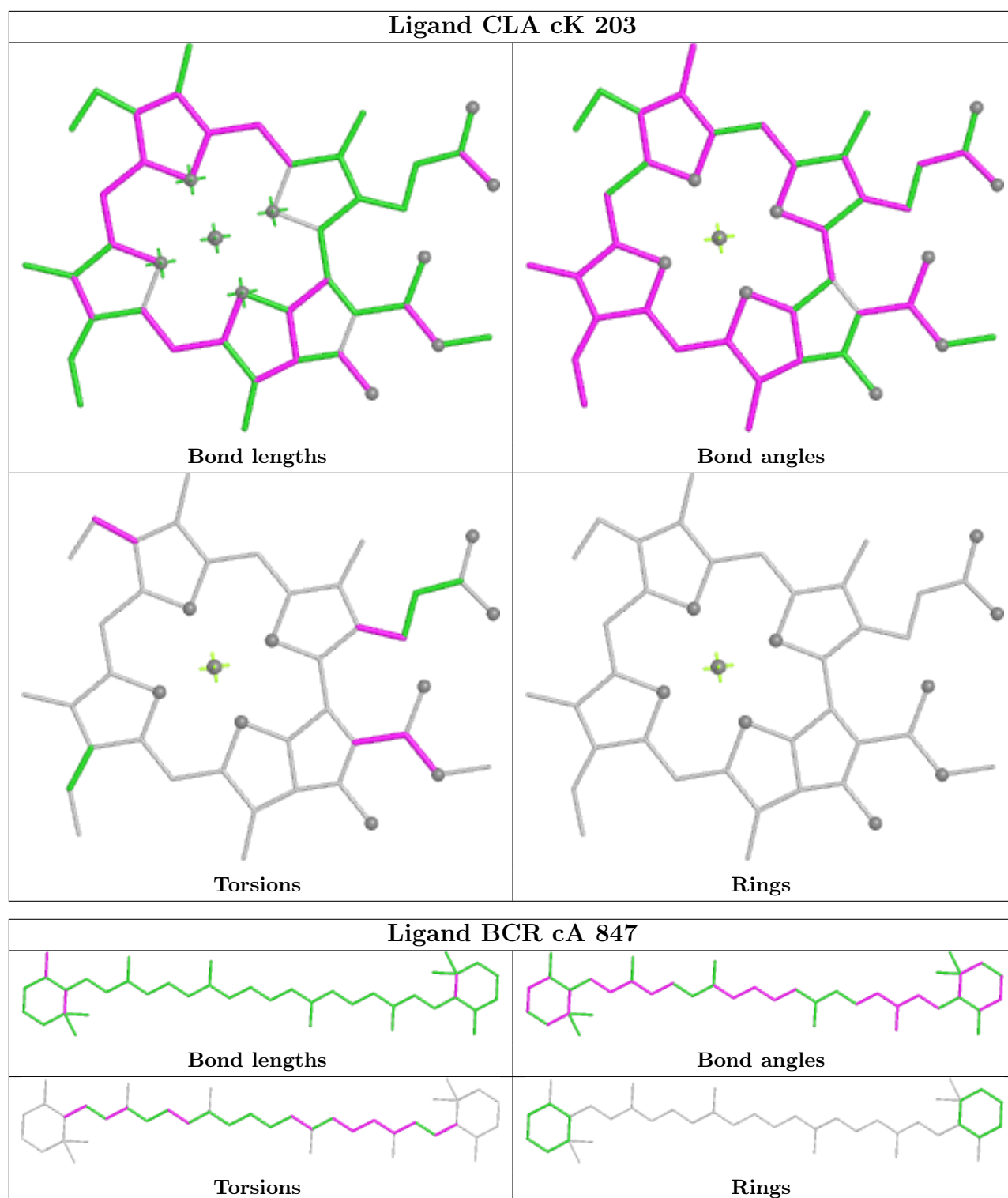




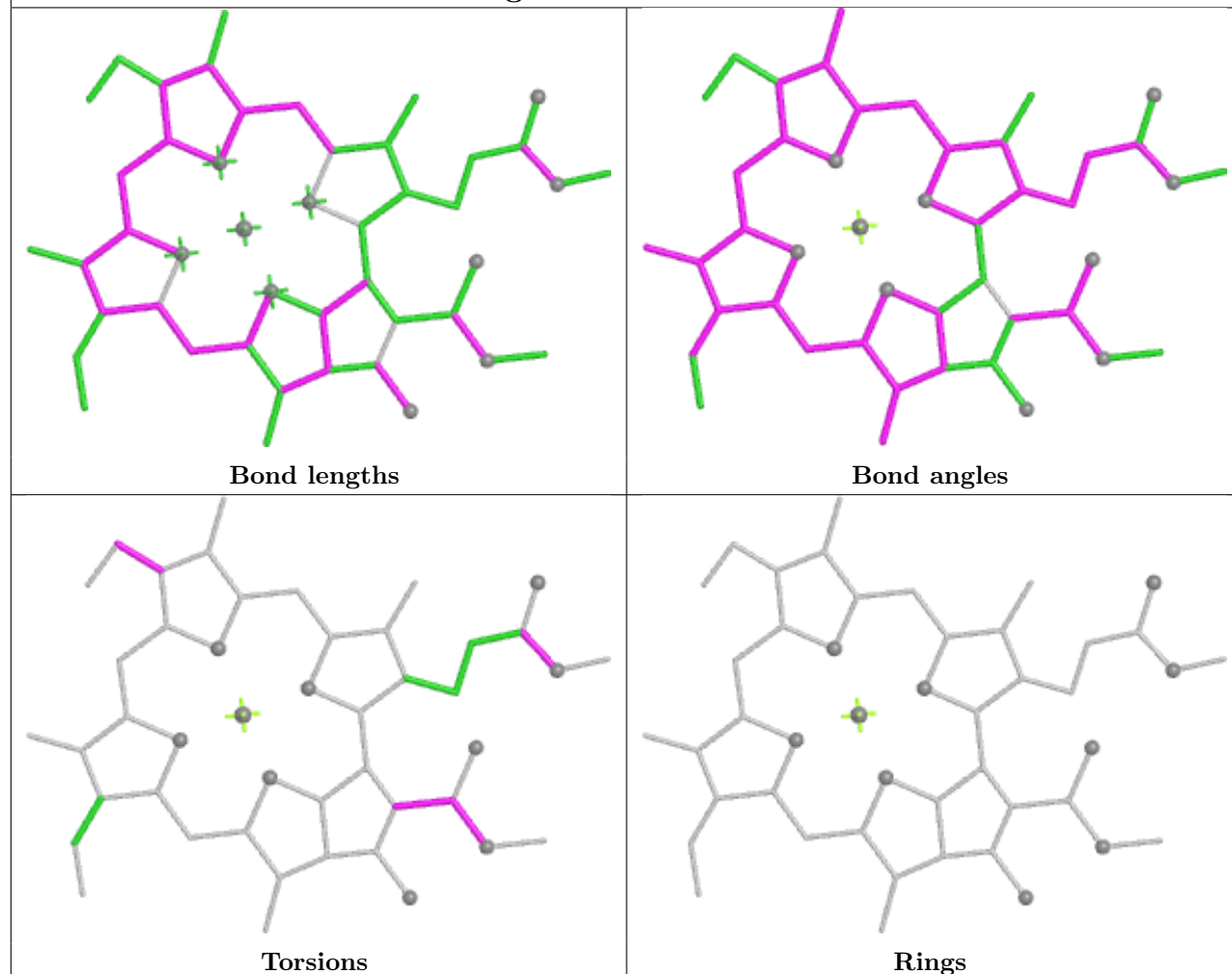




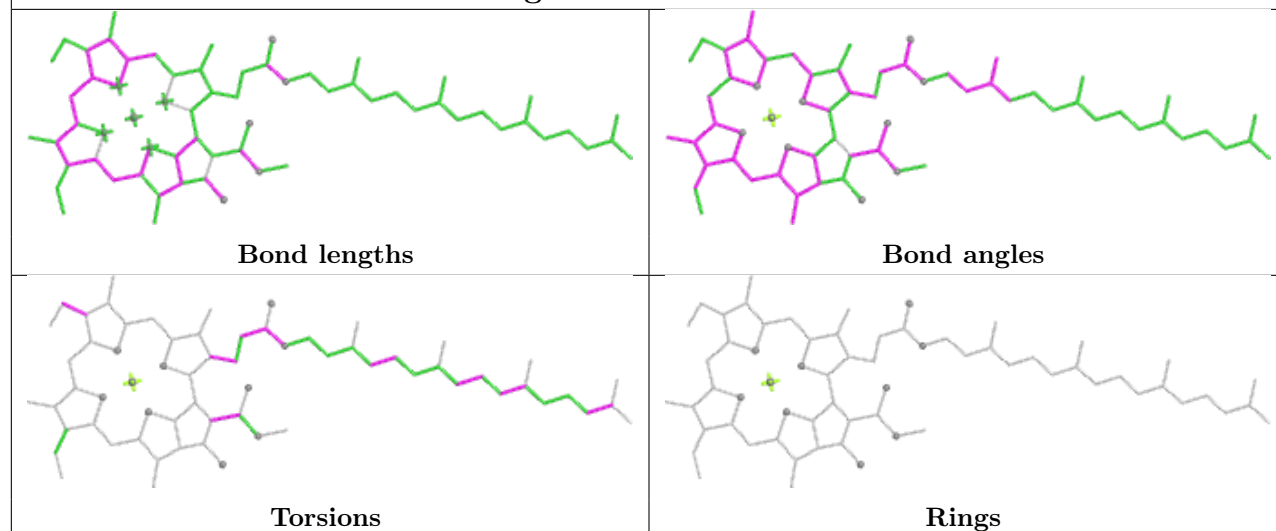


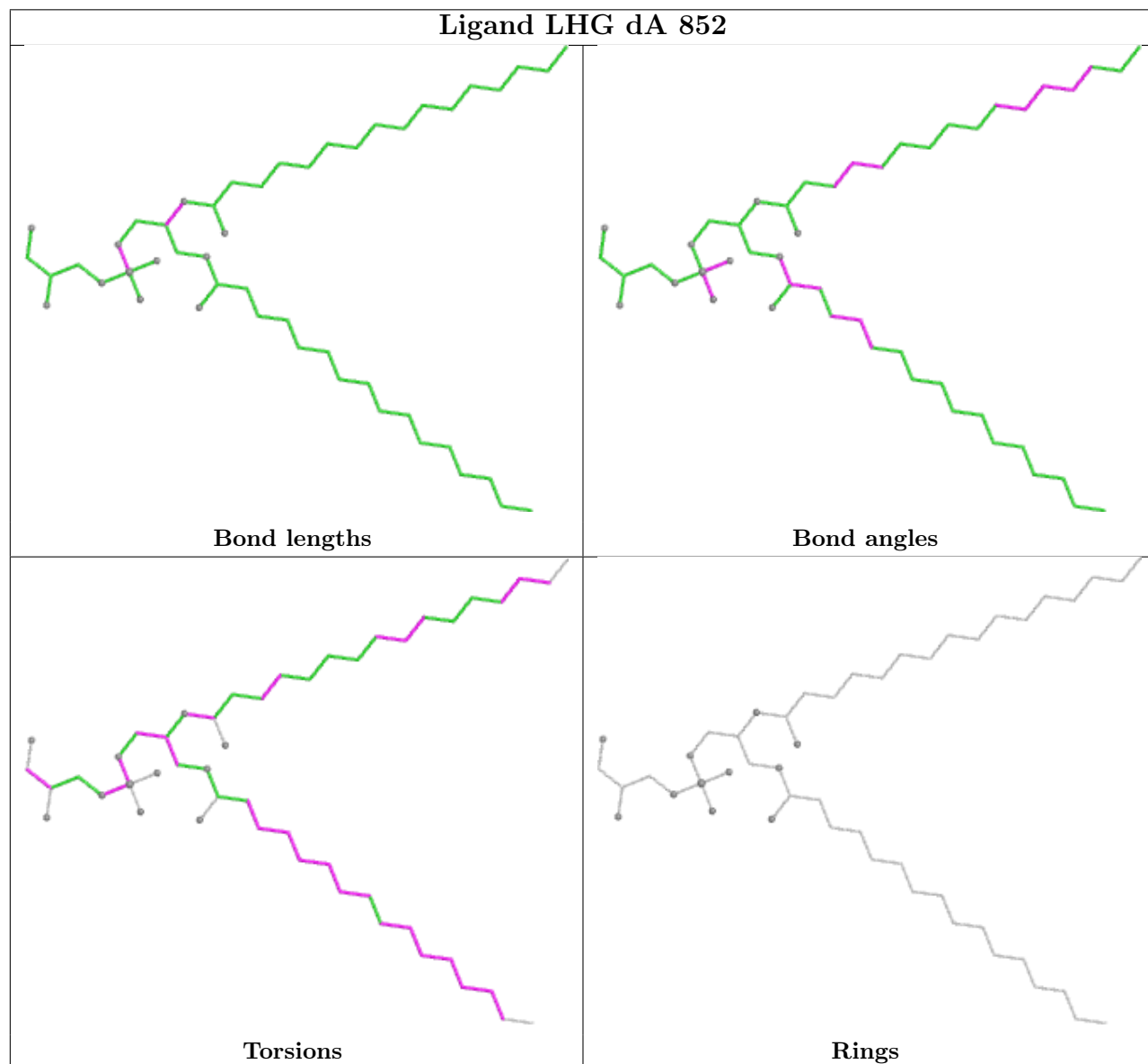
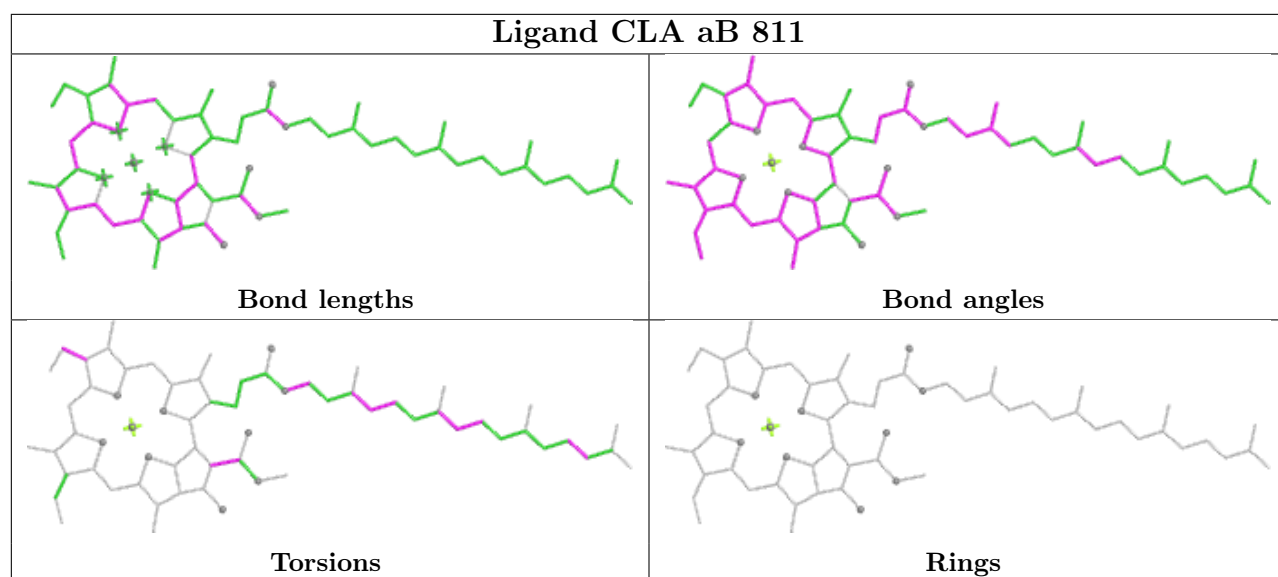


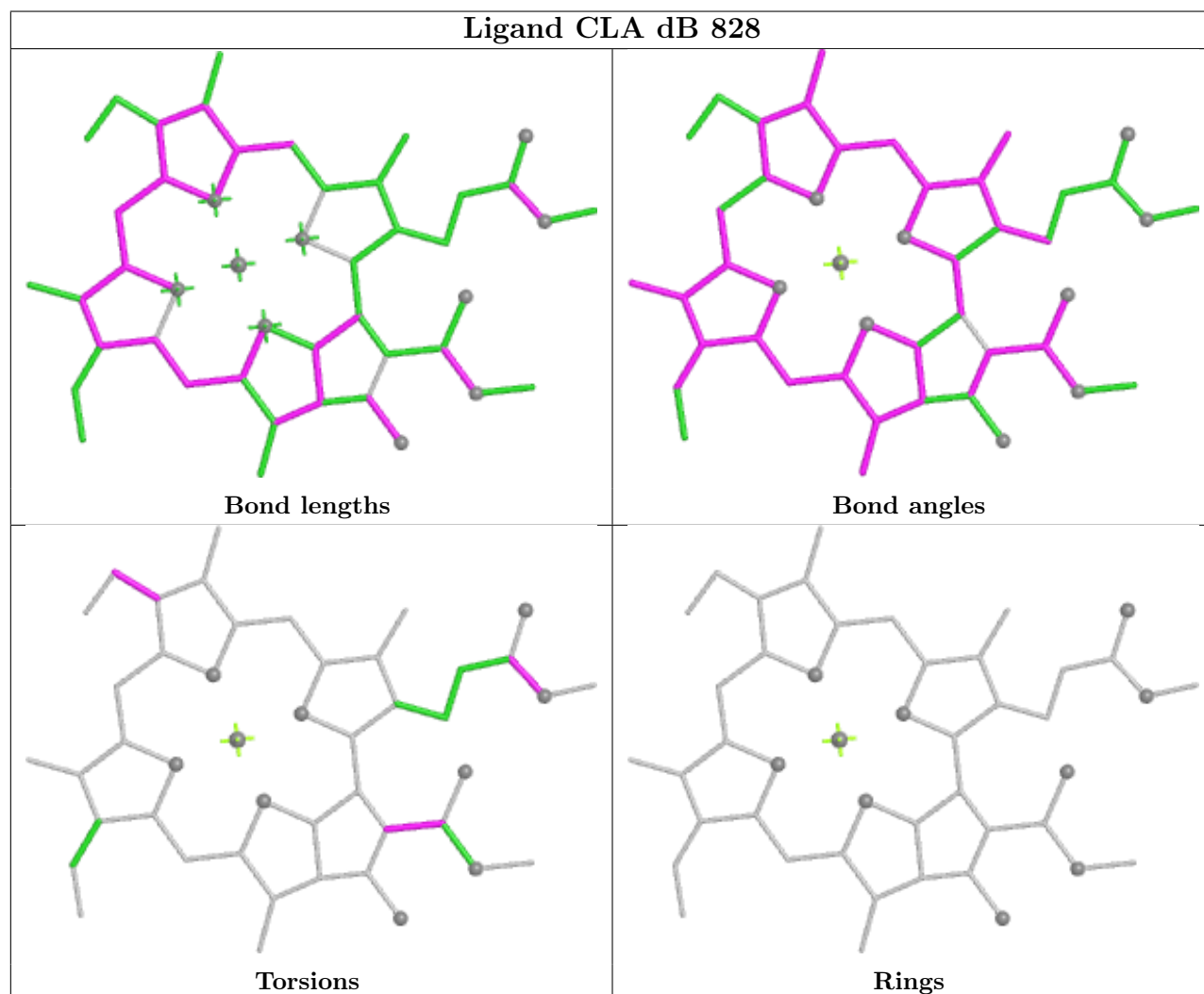
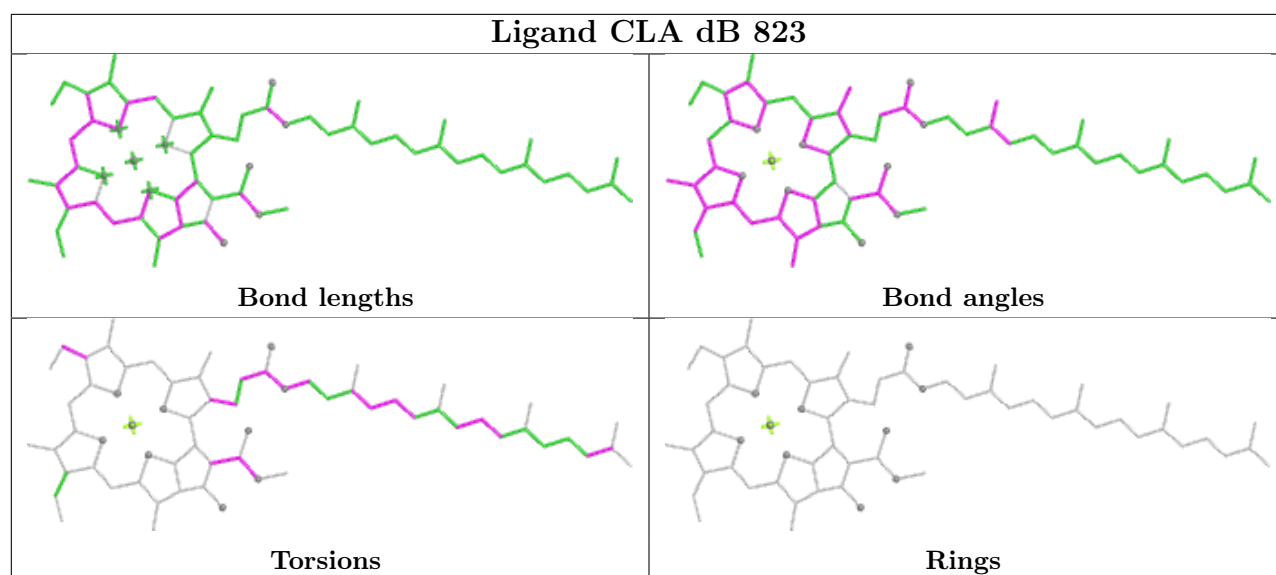
Ligand CLA aB 820

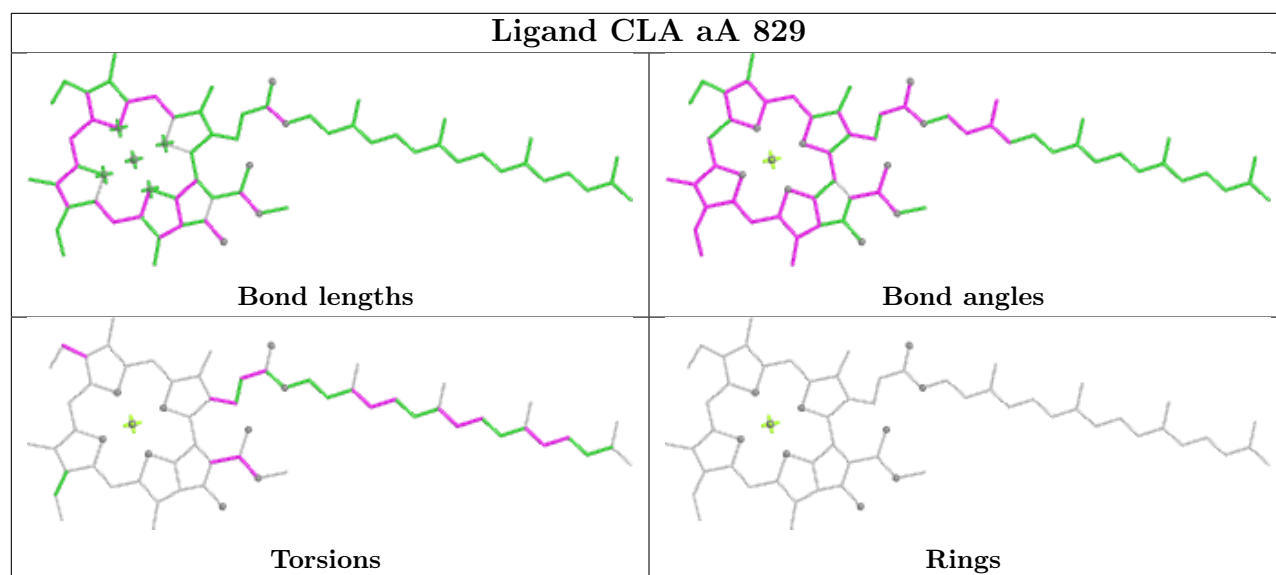
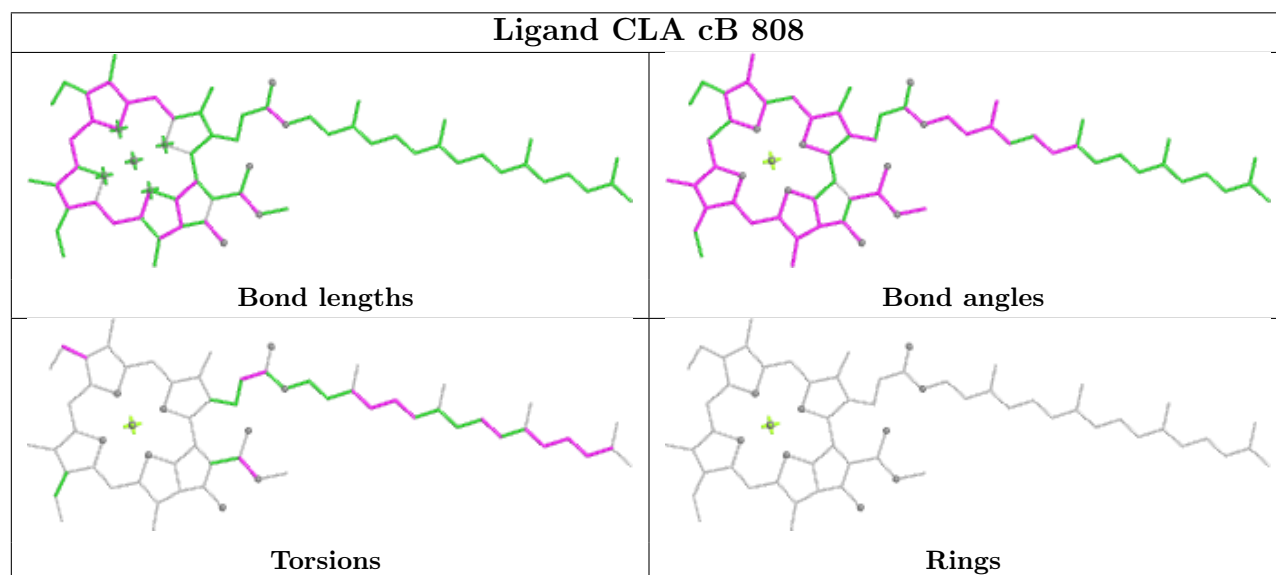
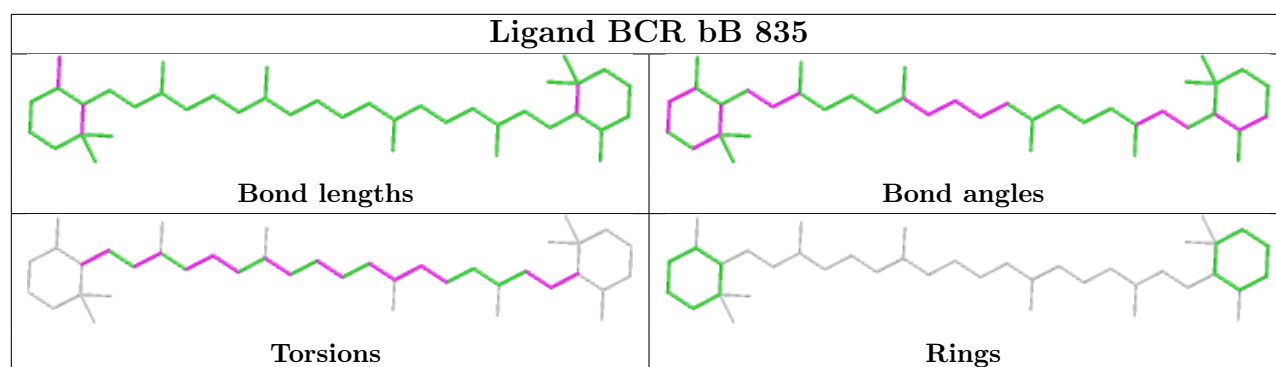


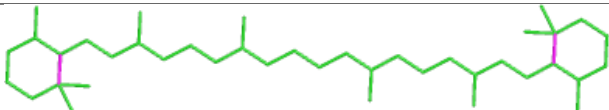
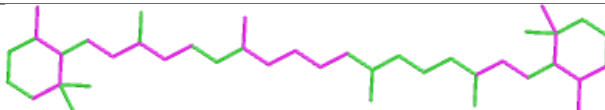
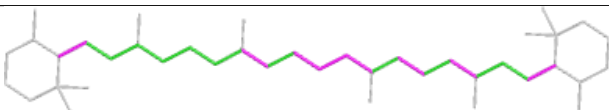
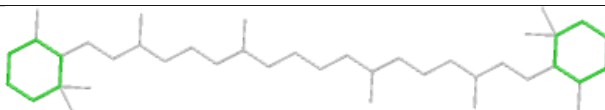
Ligand CLA cB 814

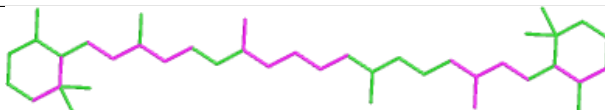
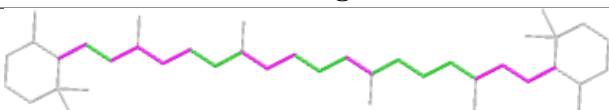
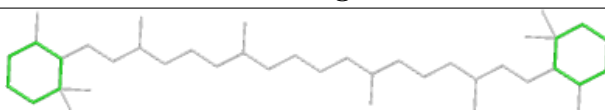


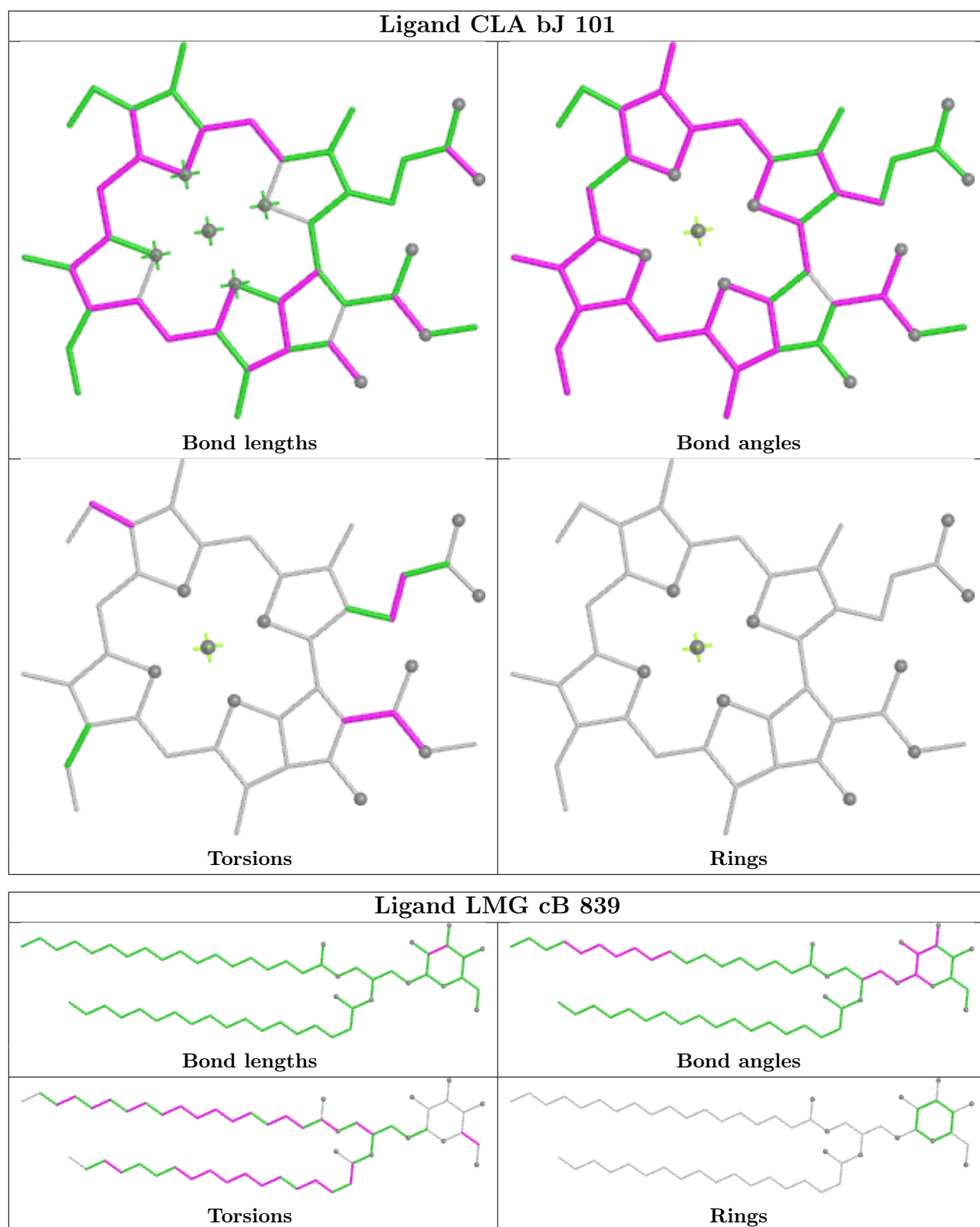


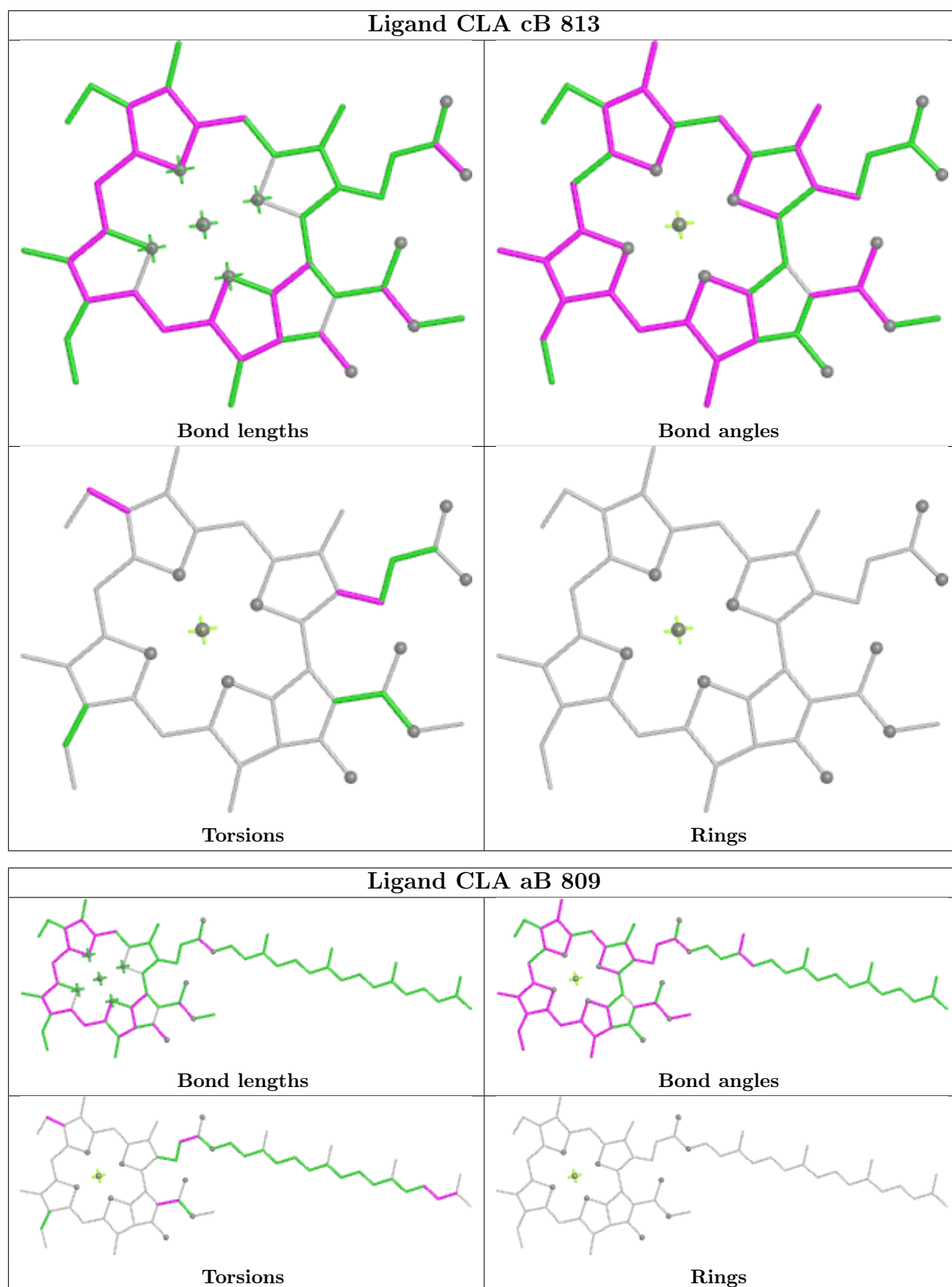


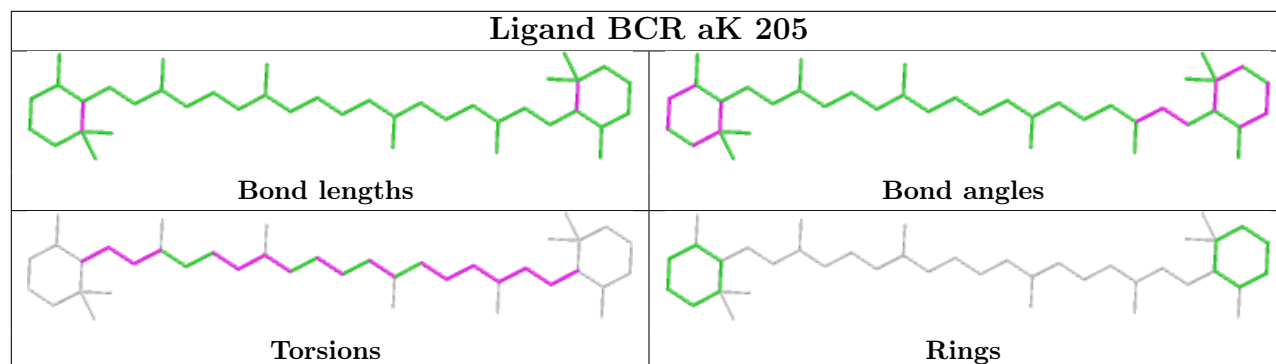
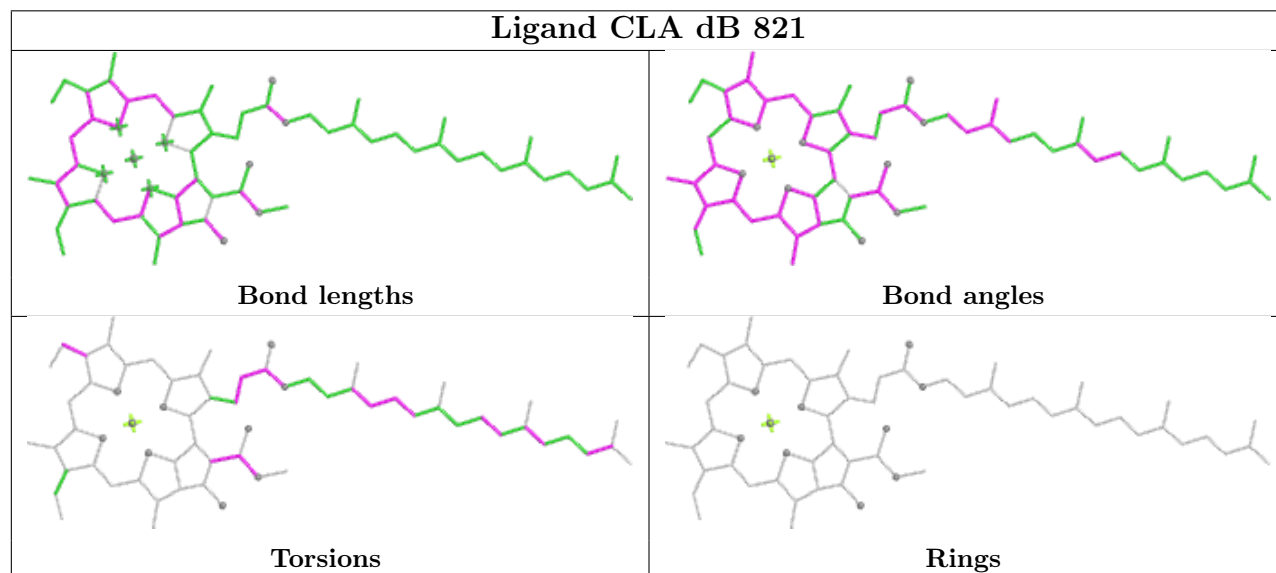
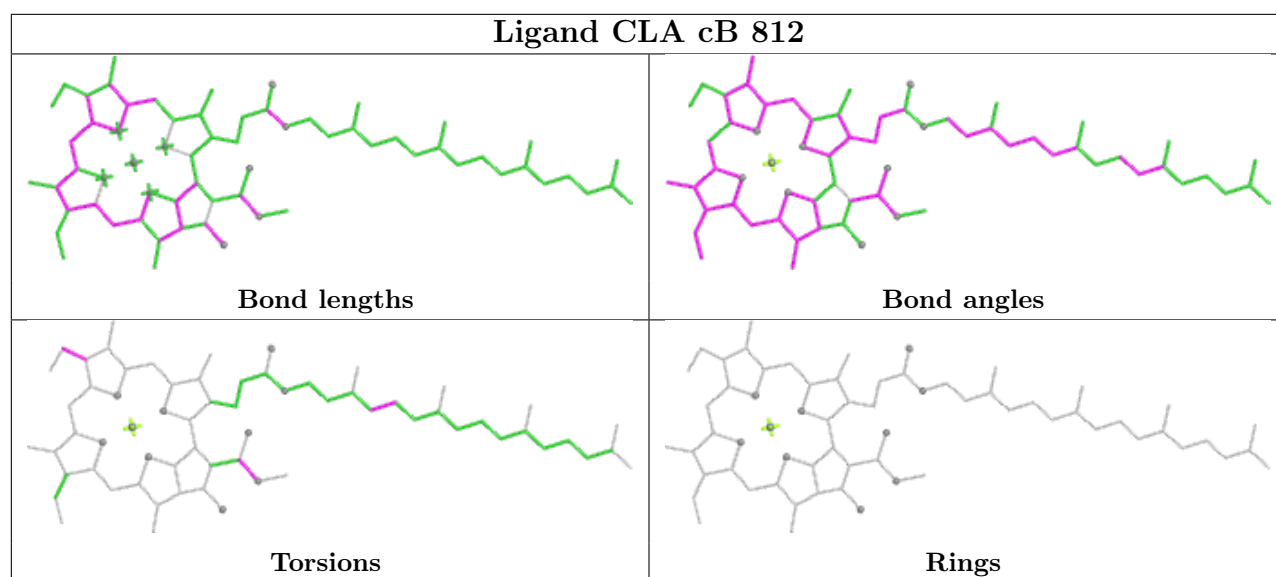


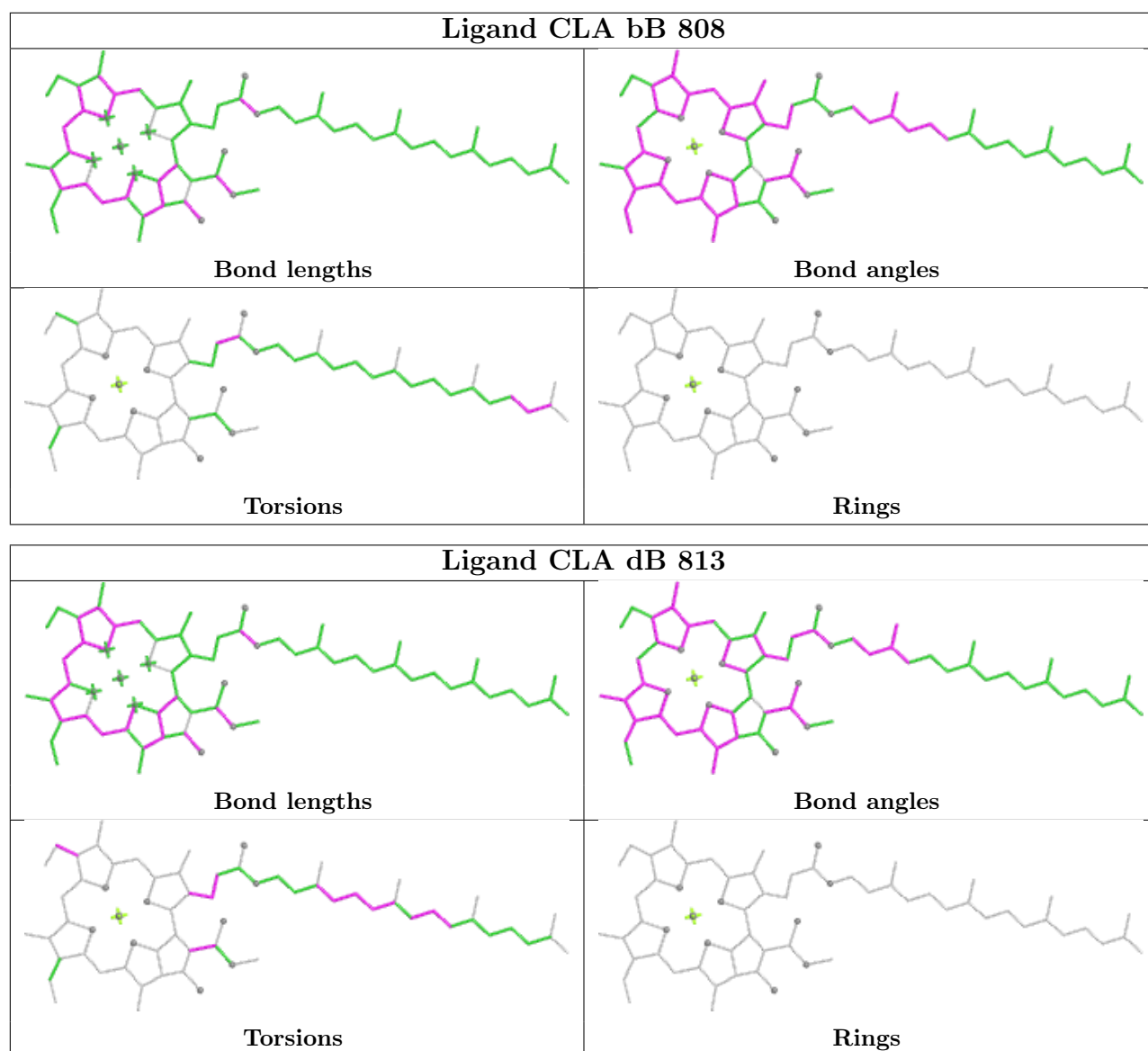
Ligand BCR aF 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR cL 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

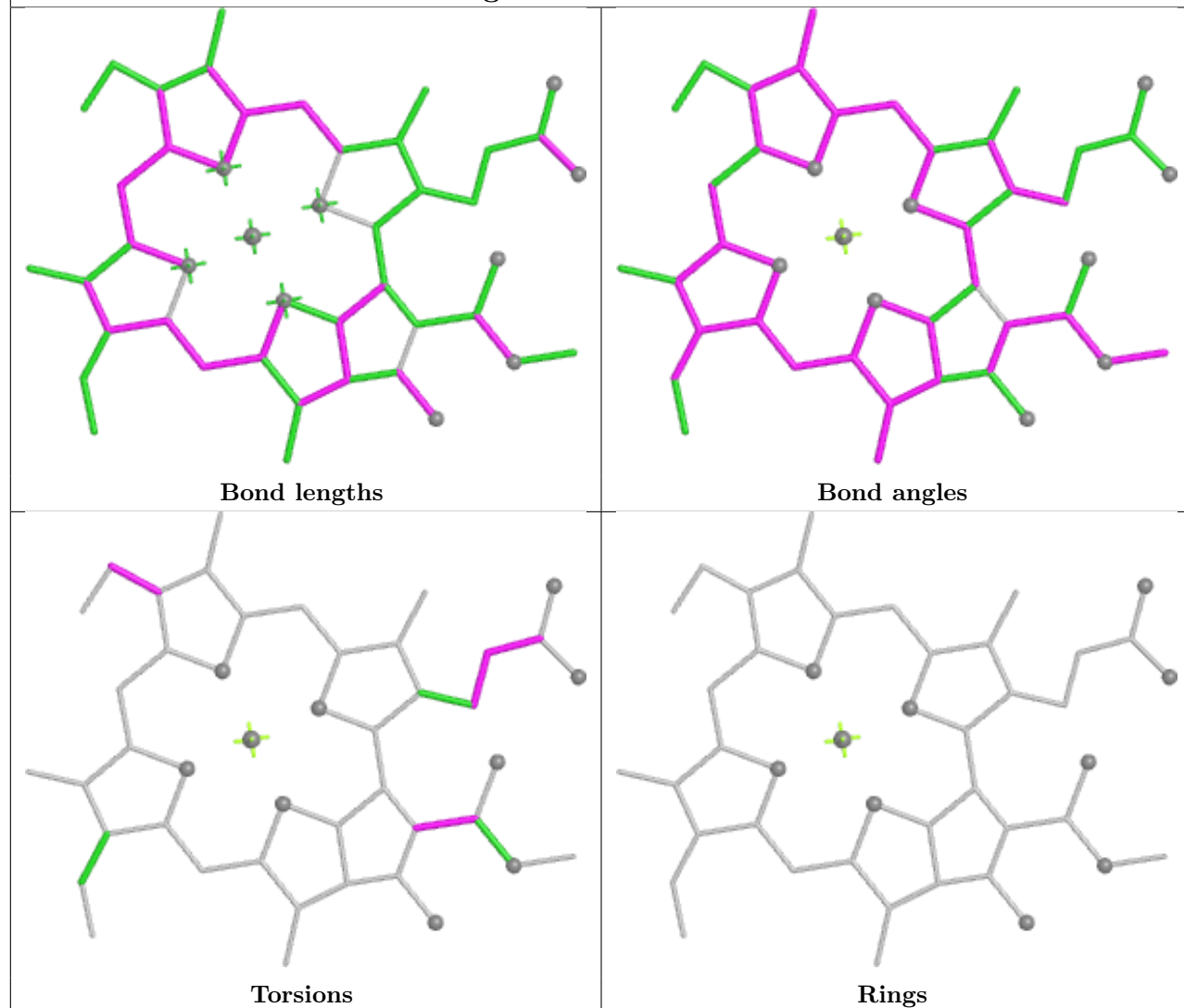




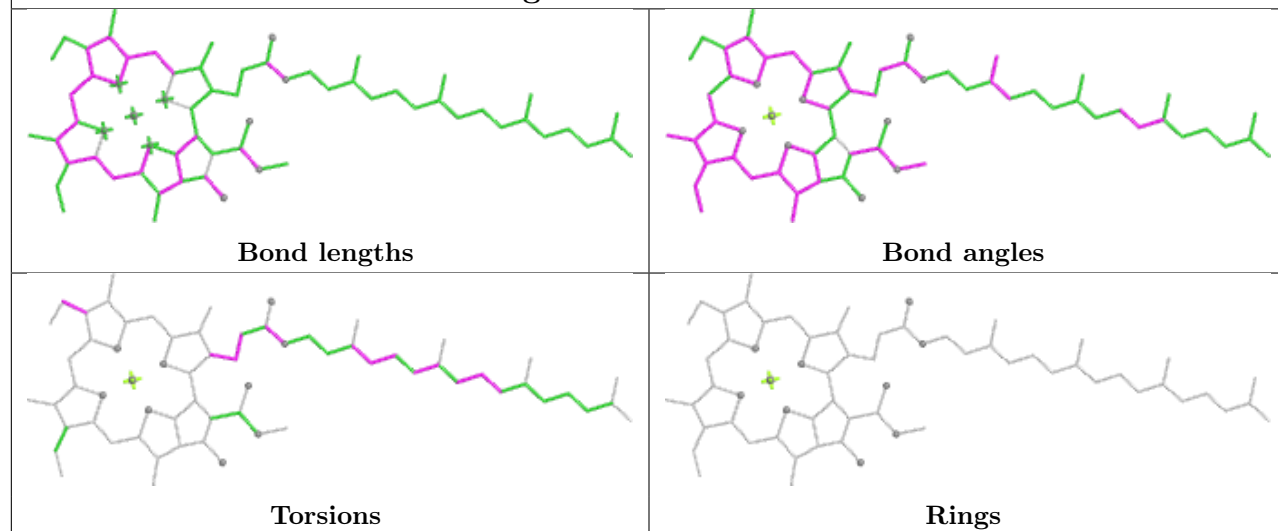


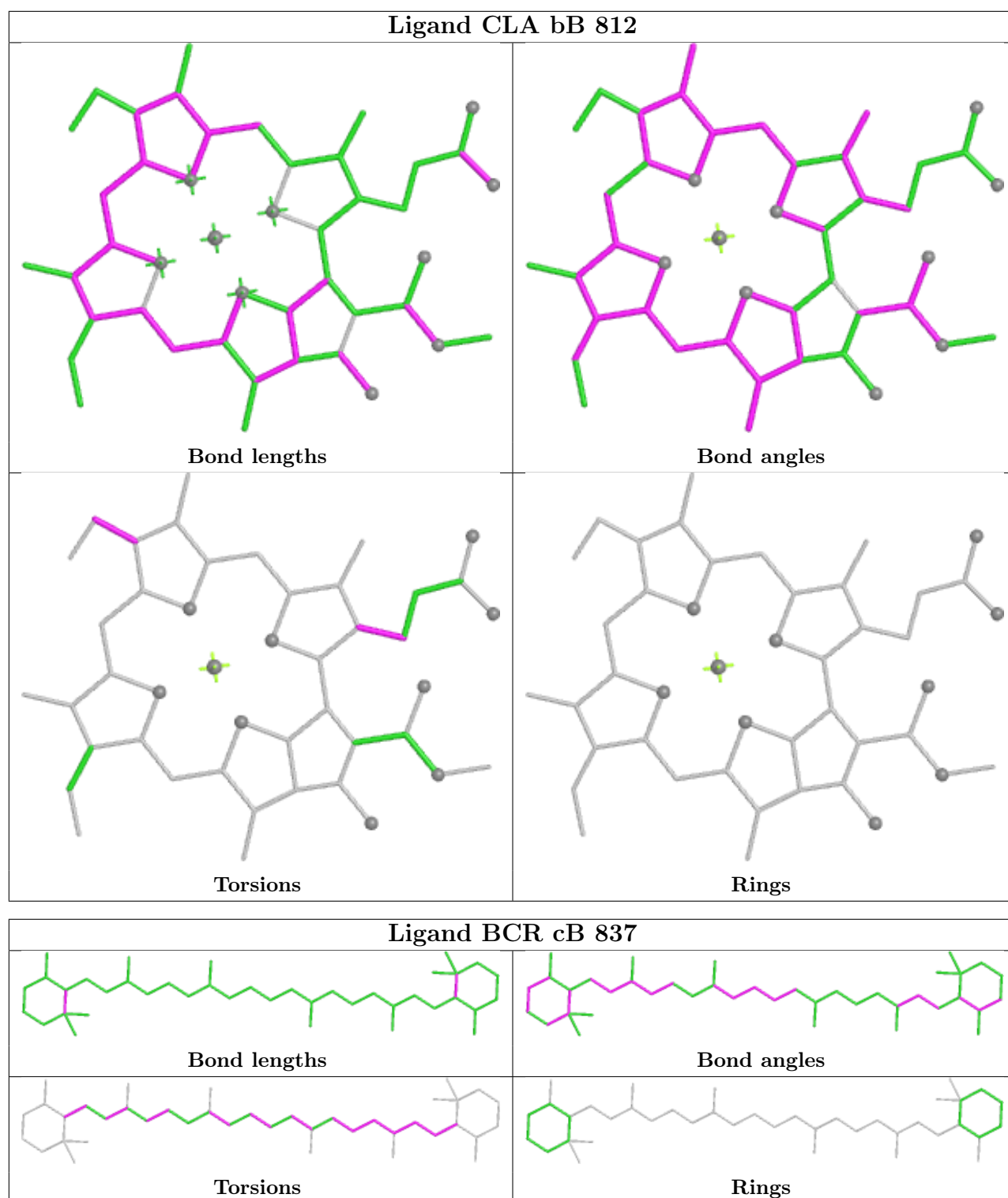


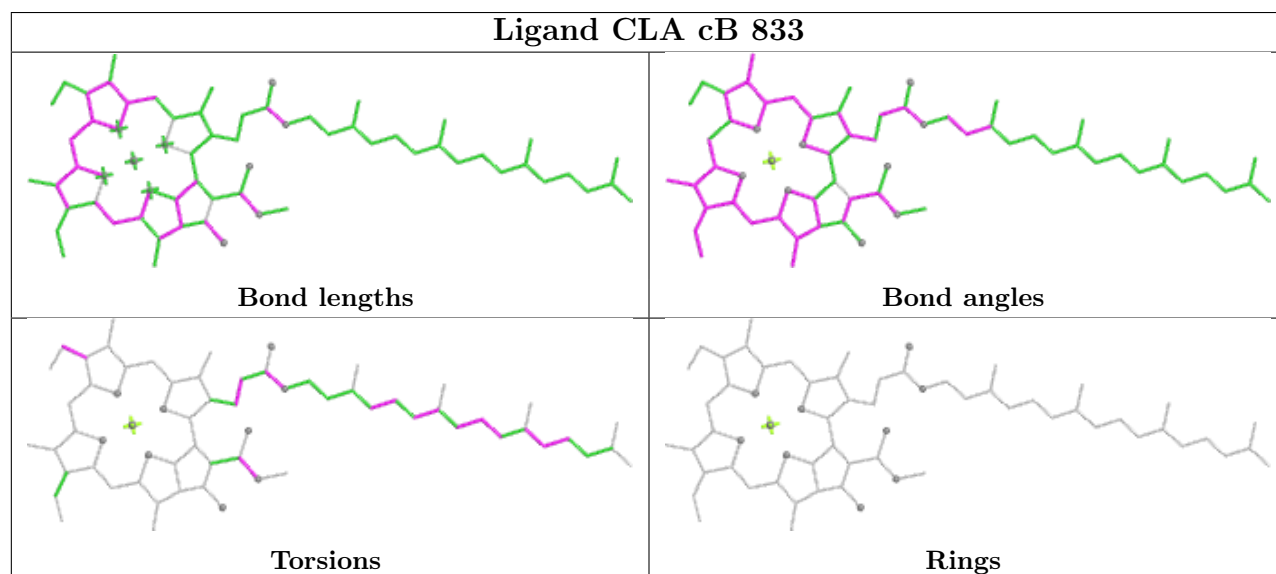
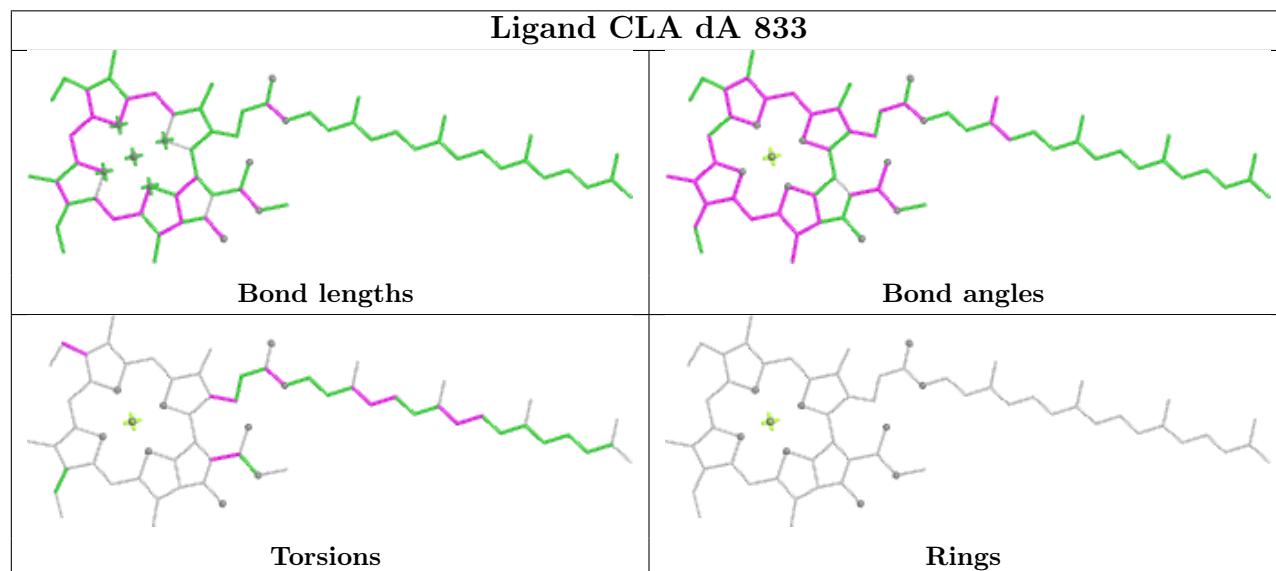
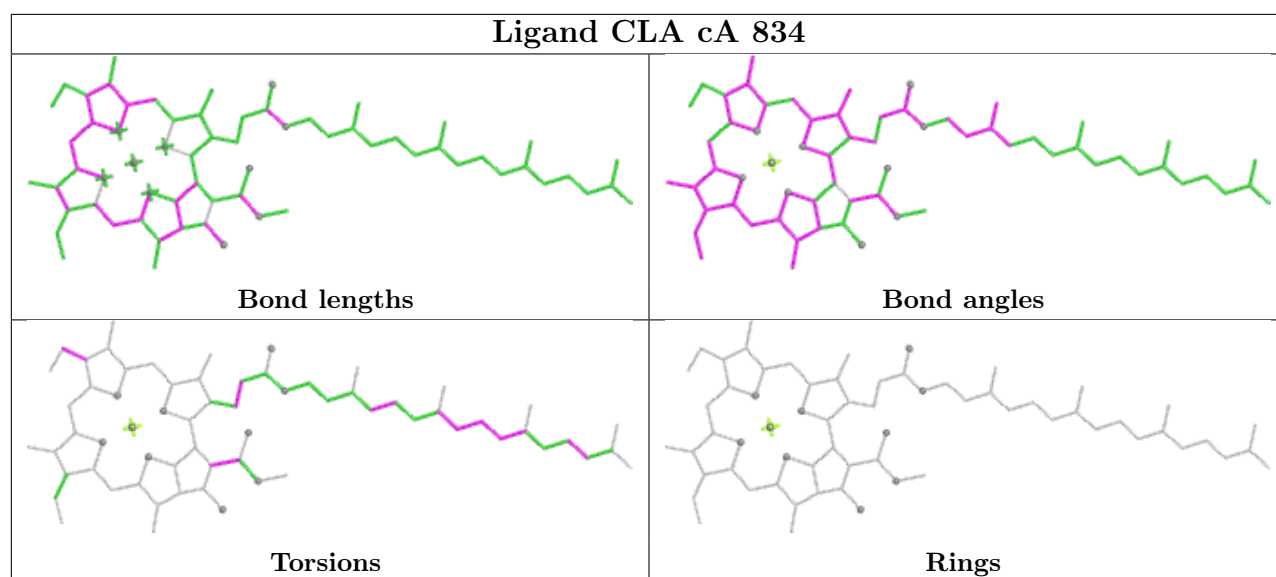
Ligand CLA bA 816

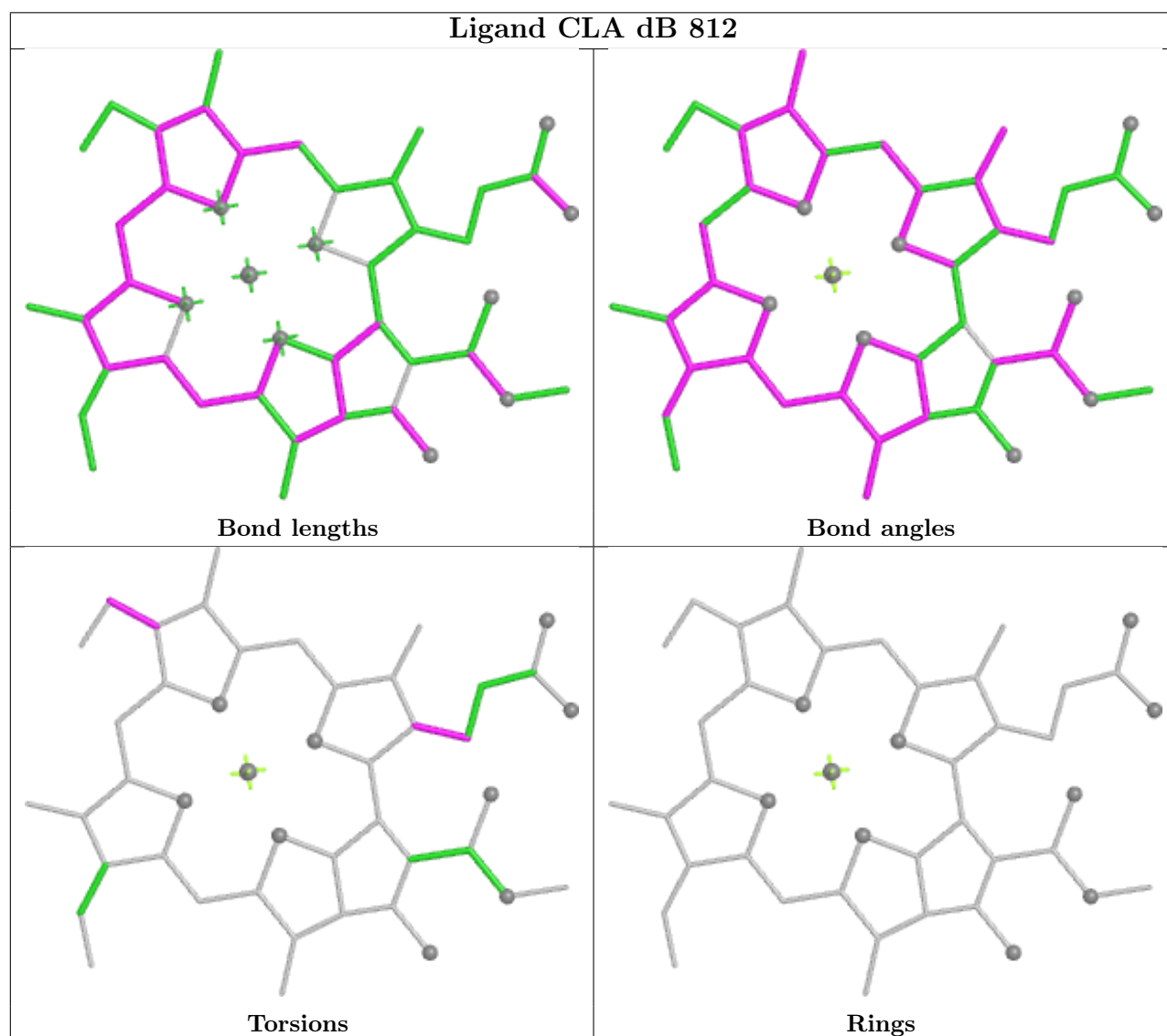
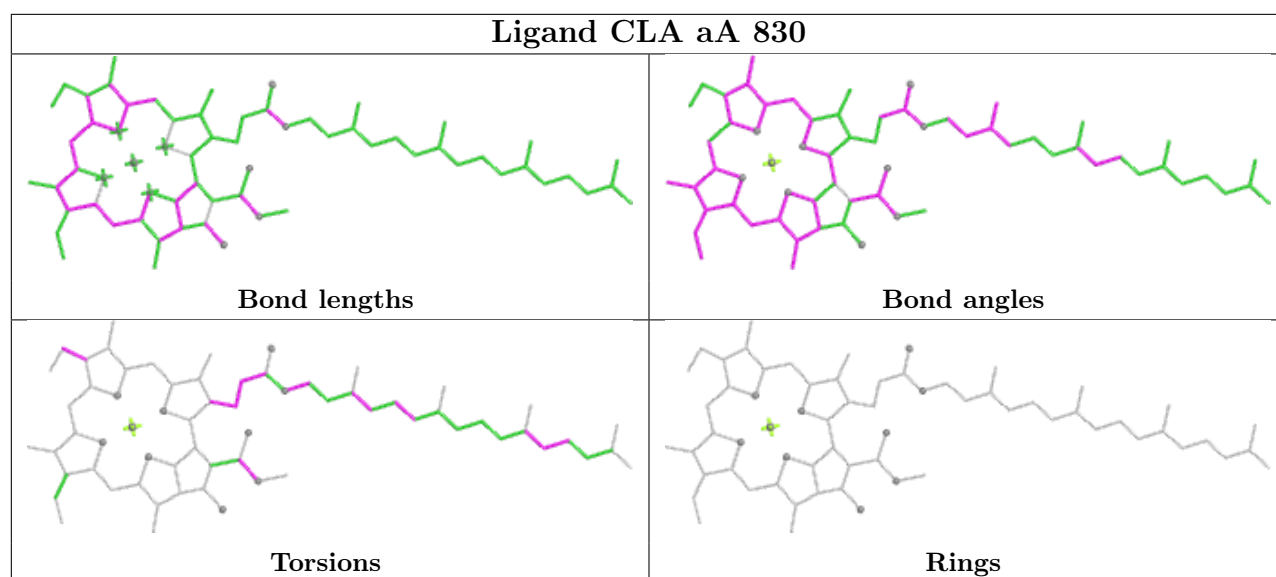


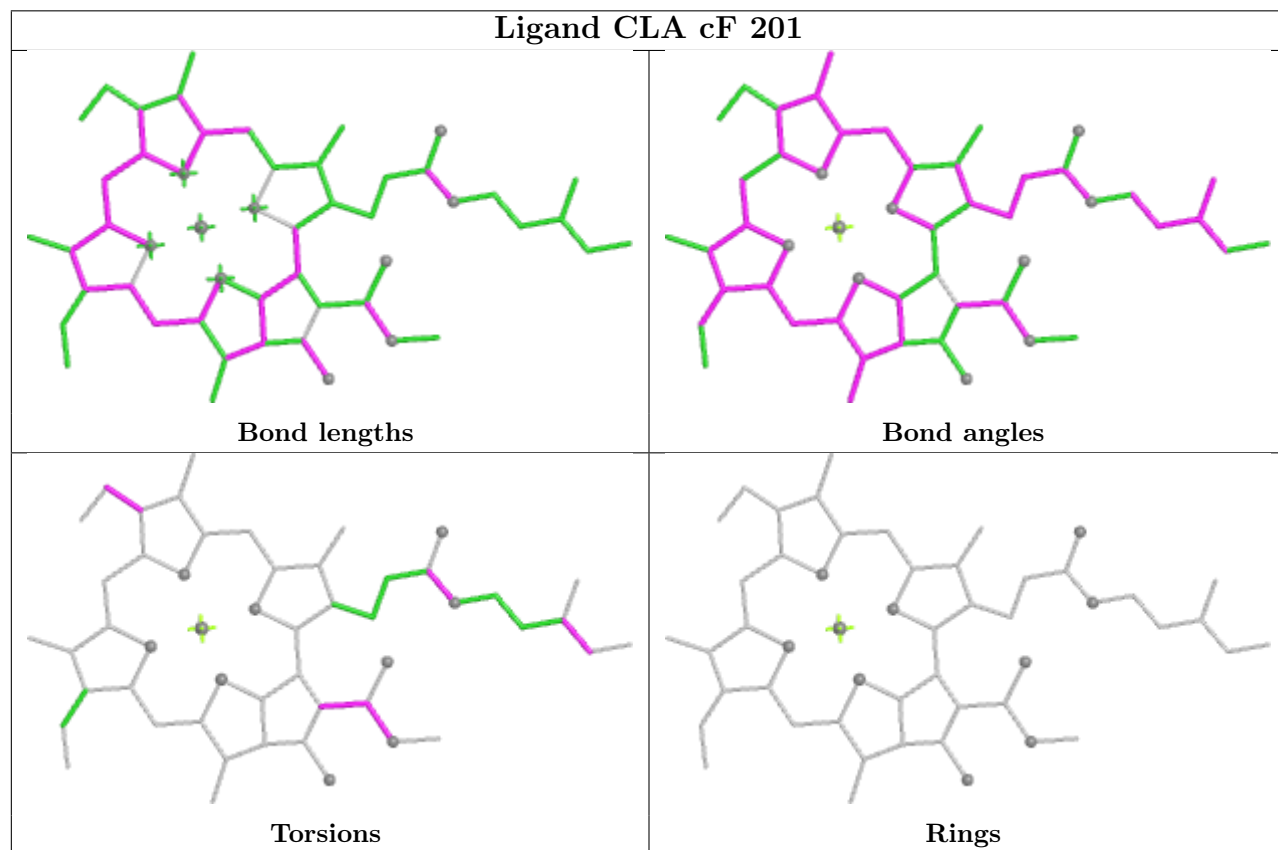
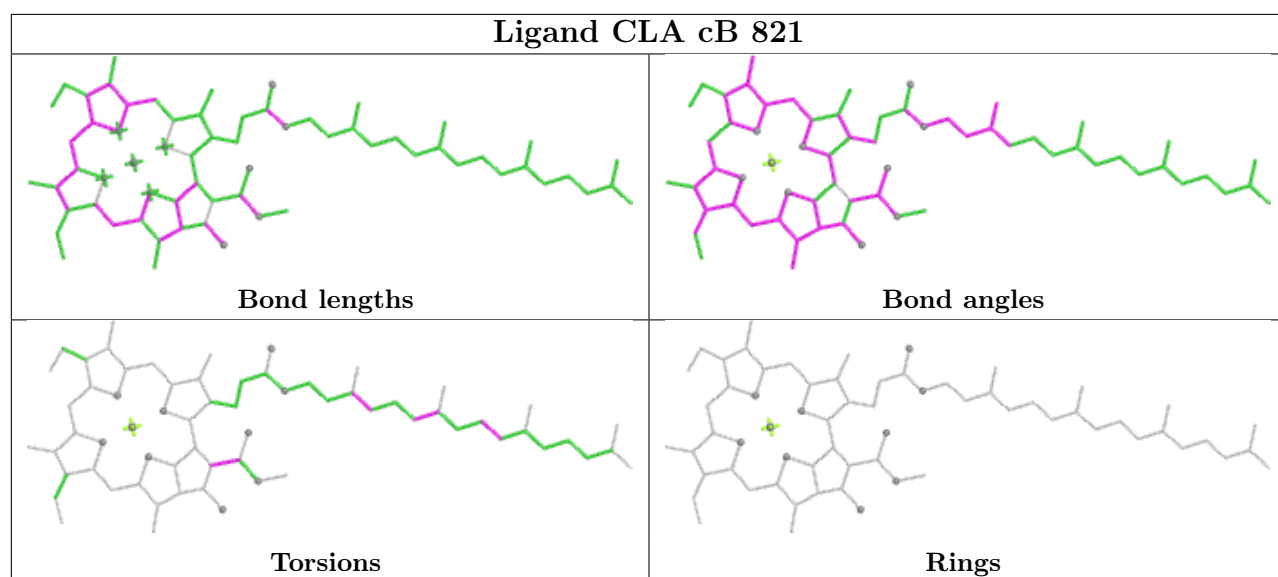
Ligand CLA aA 812

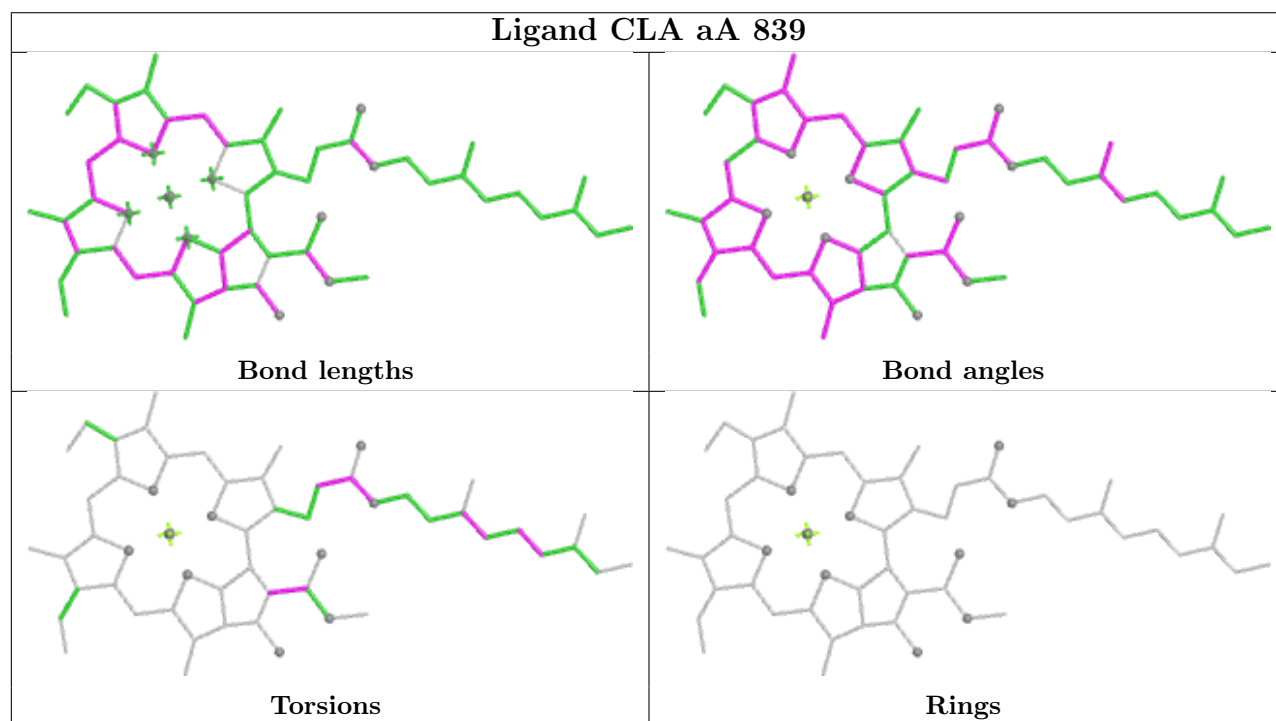
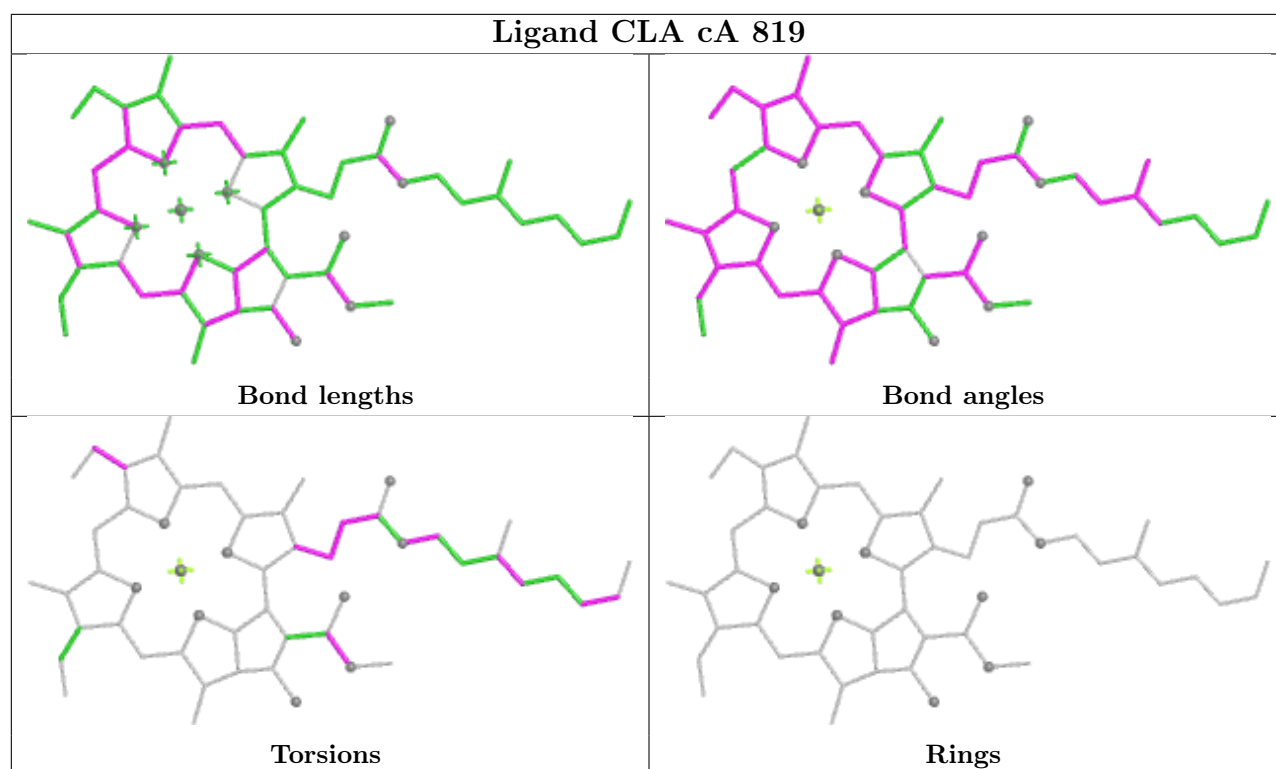


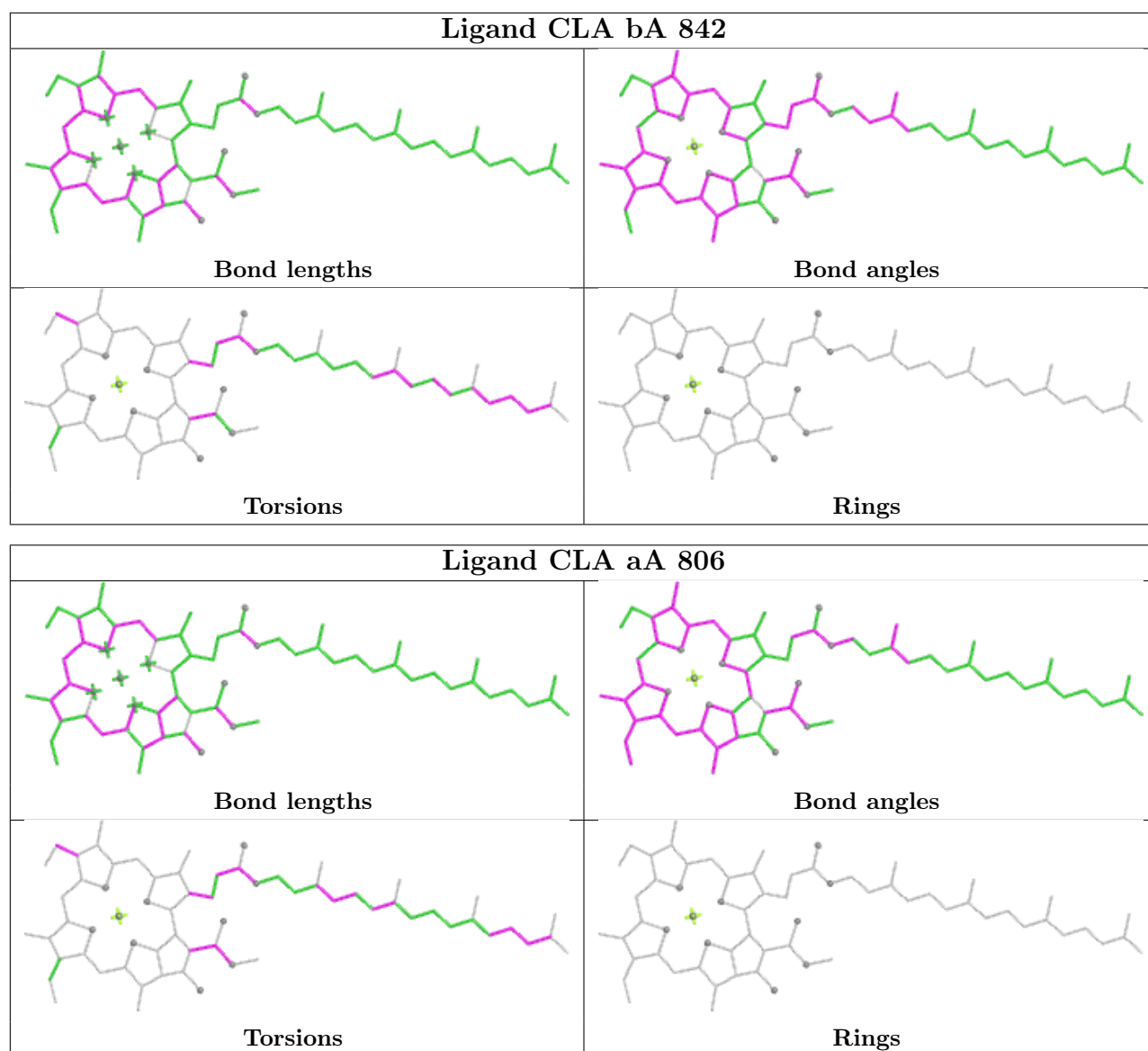


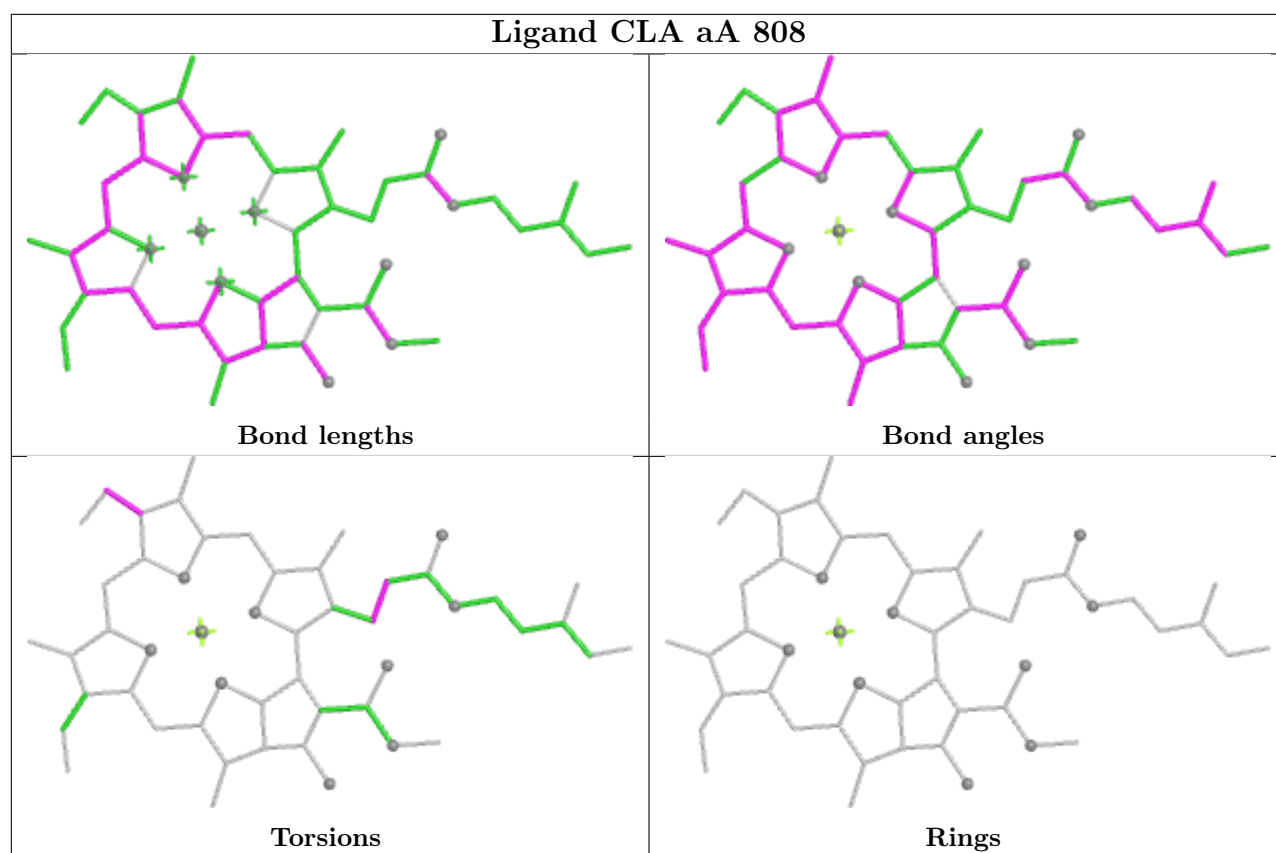




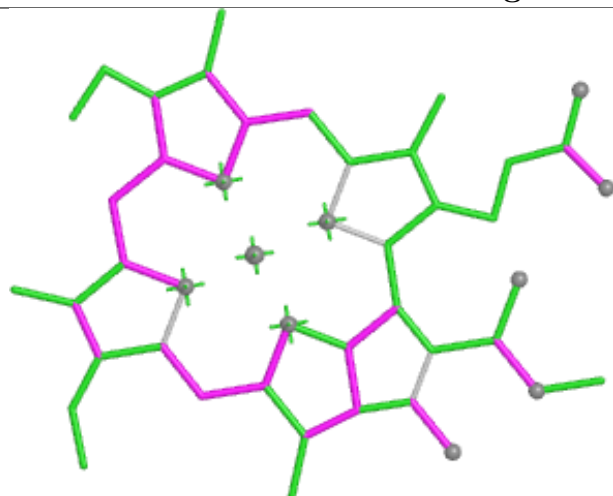




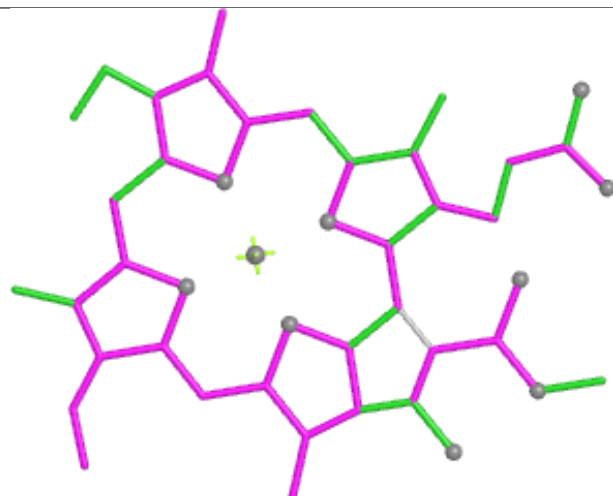




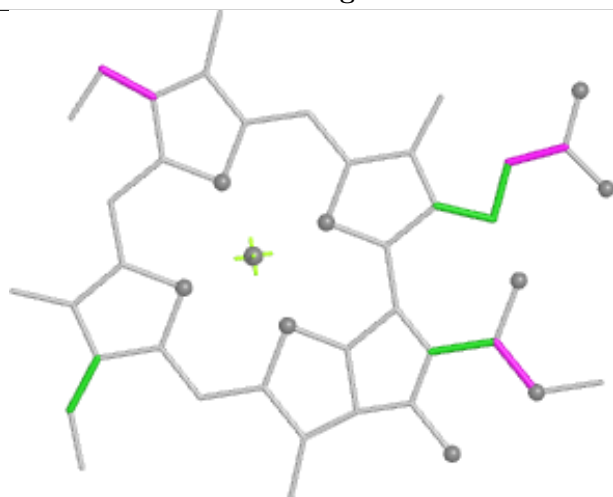
Ligand CLA bA 811



Bond lengths



Bond angles

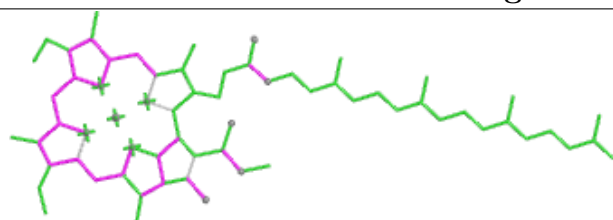


Torsions

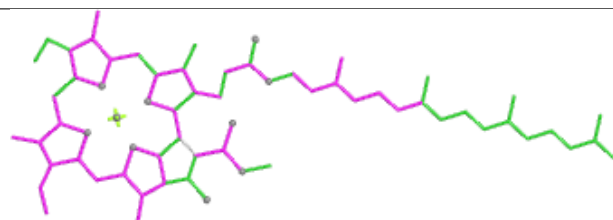


Rings

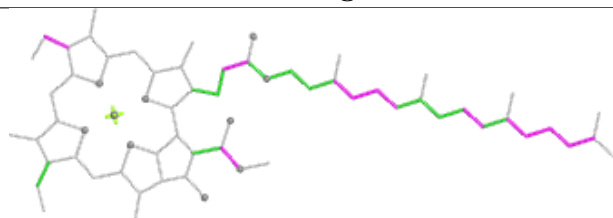
Ligand CLA dB 807



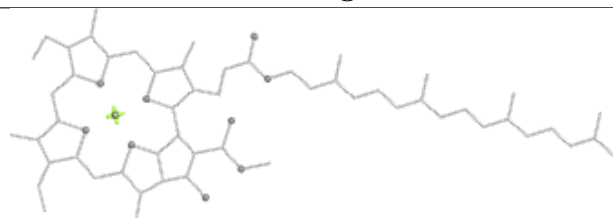
Bond lengths



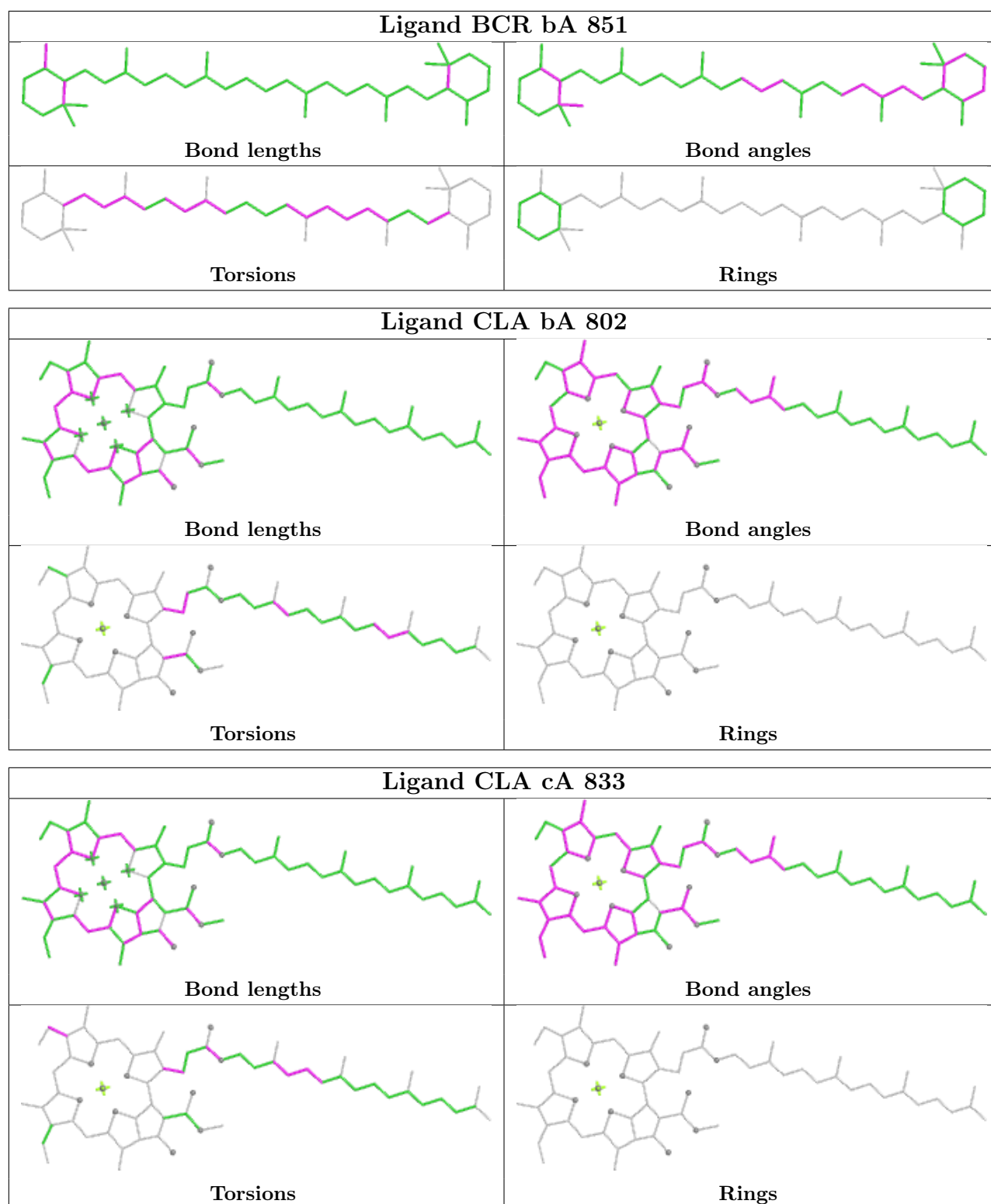
Bond angles

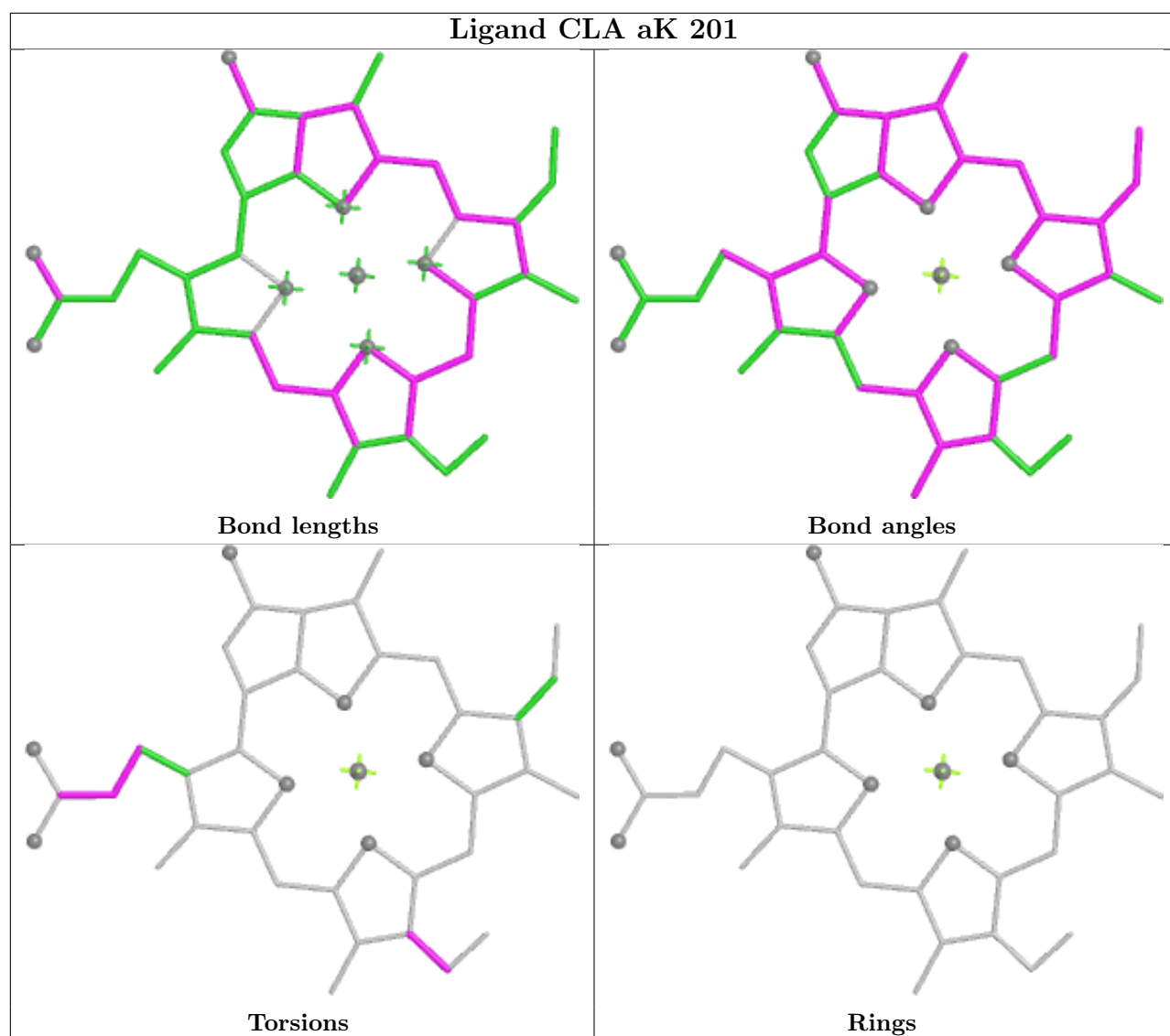


Torsions

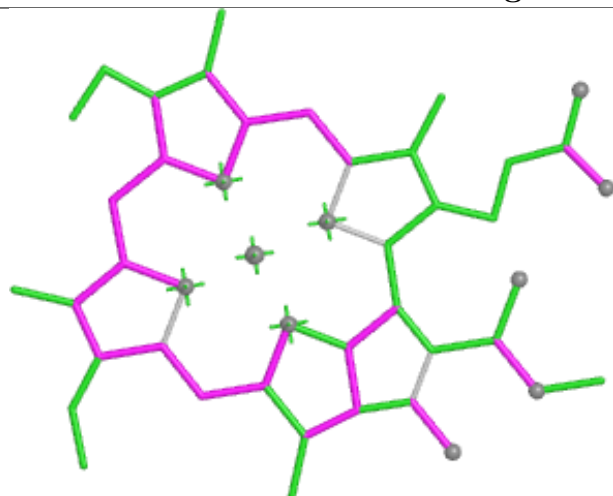


Rings

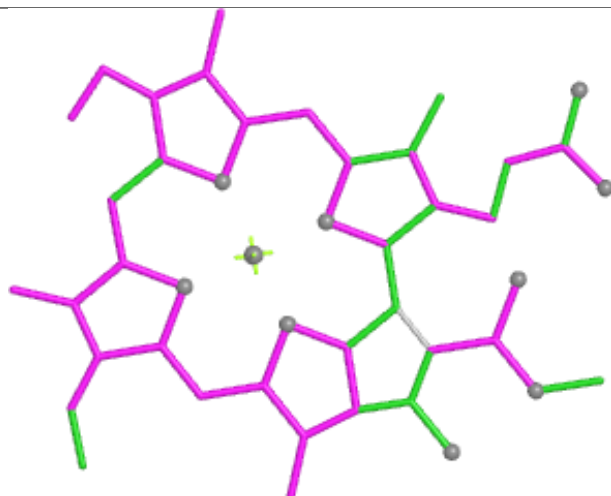




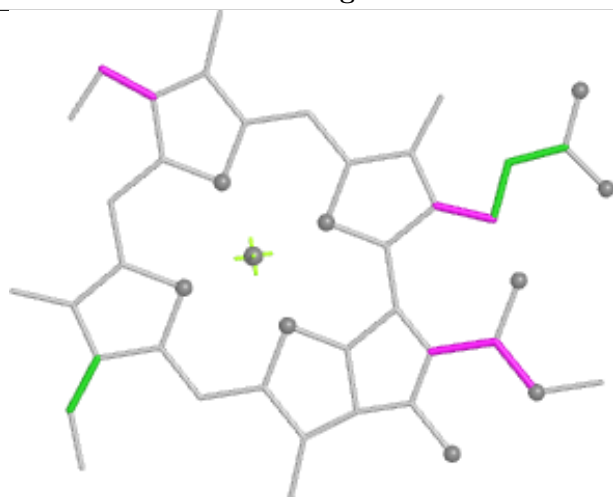
Ligand CLA bB 815



Bond lengths



Bond angles

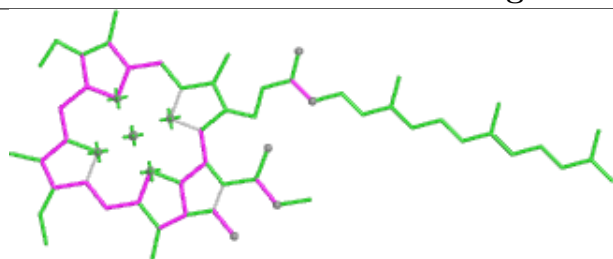


Torsions

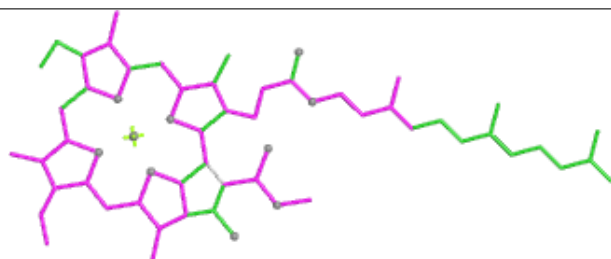


Rings

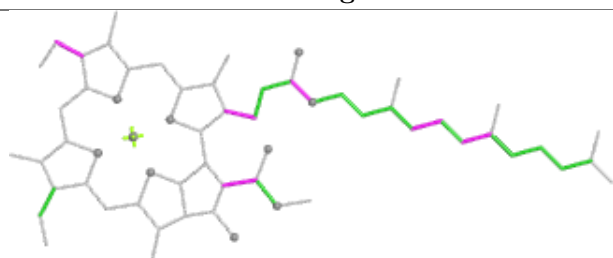
Ligand CLA cB 819



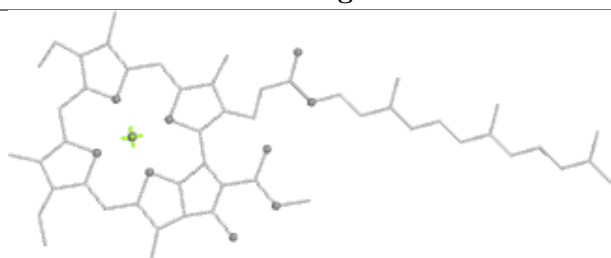
Bond lengths



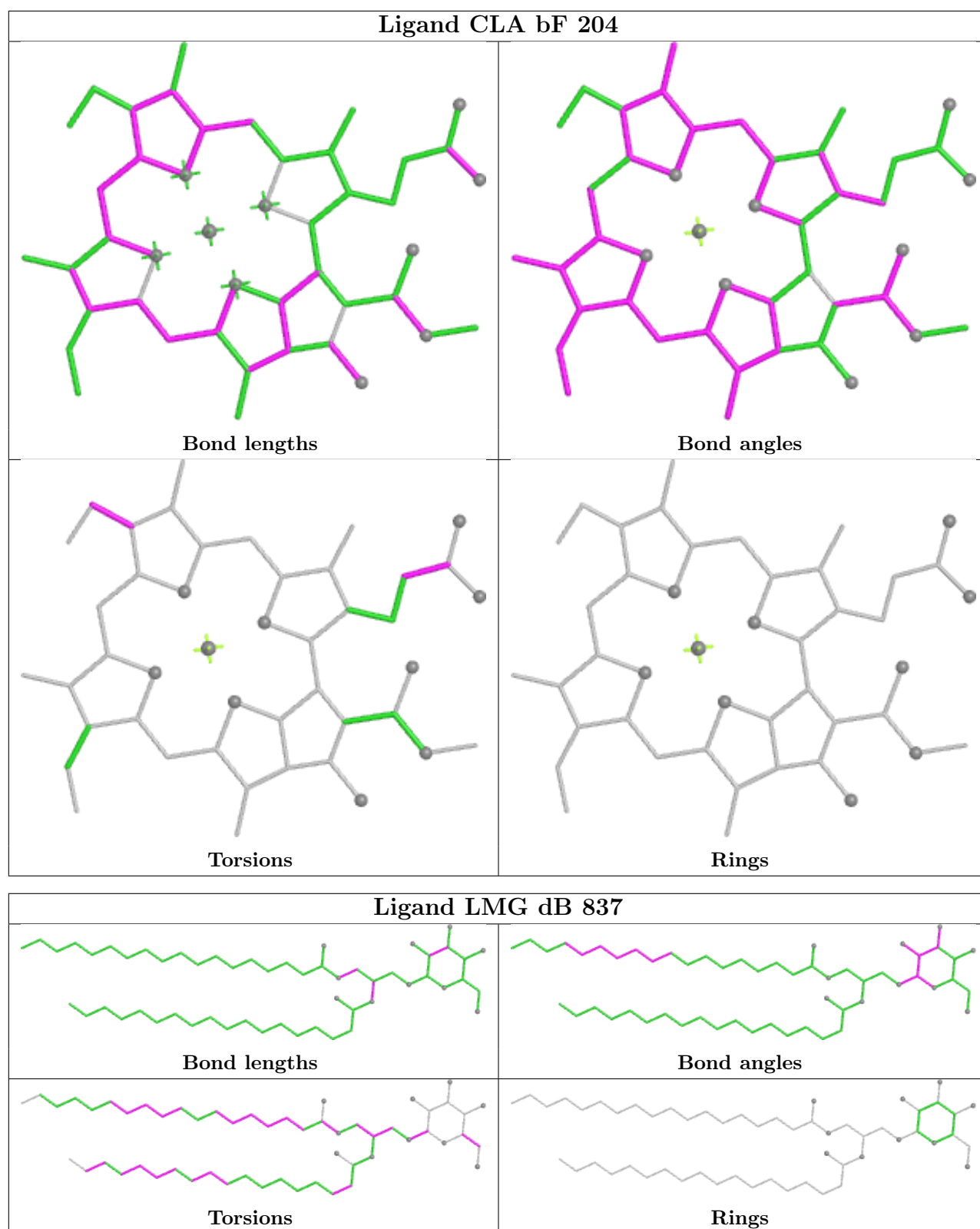
Bond angles

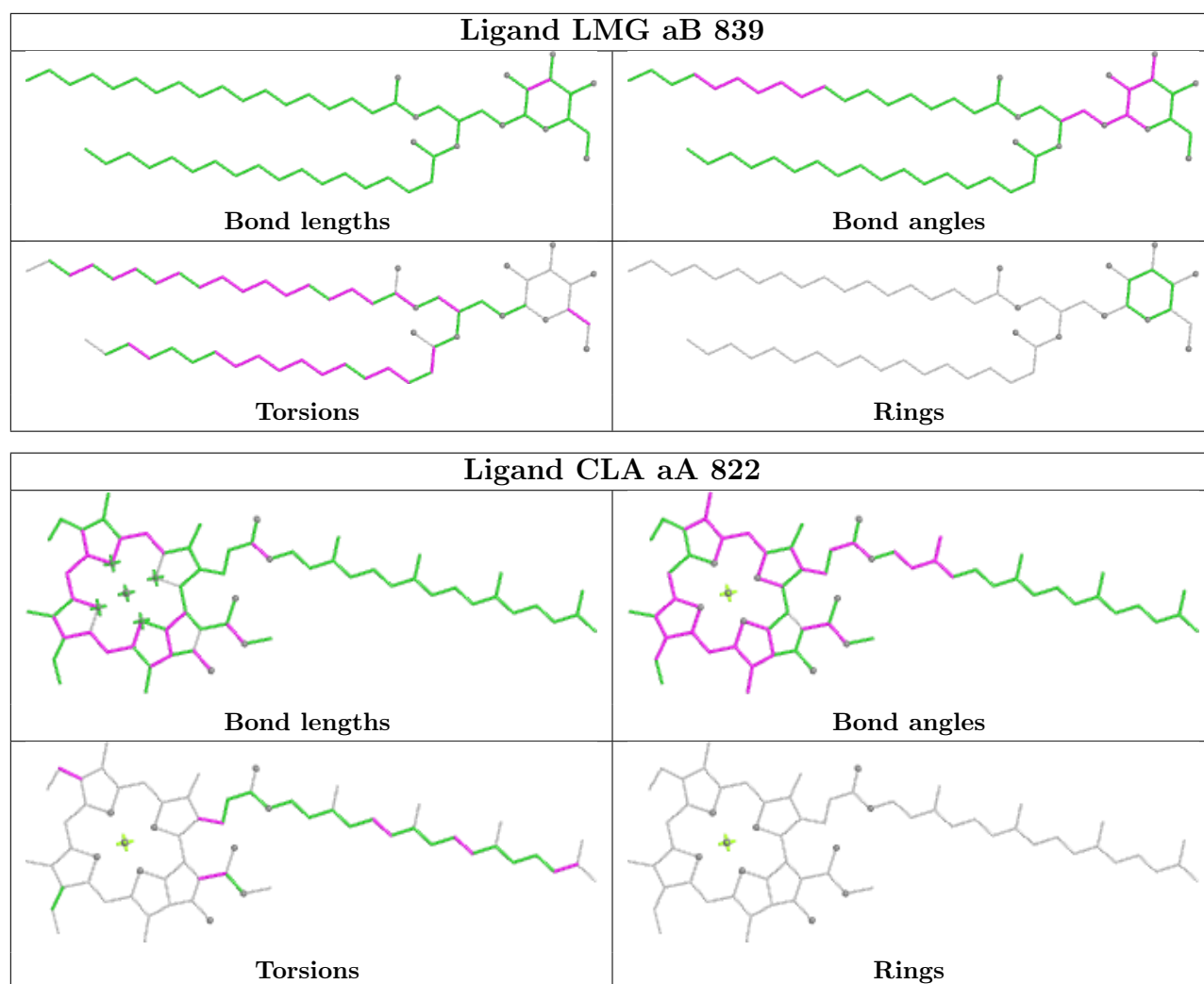


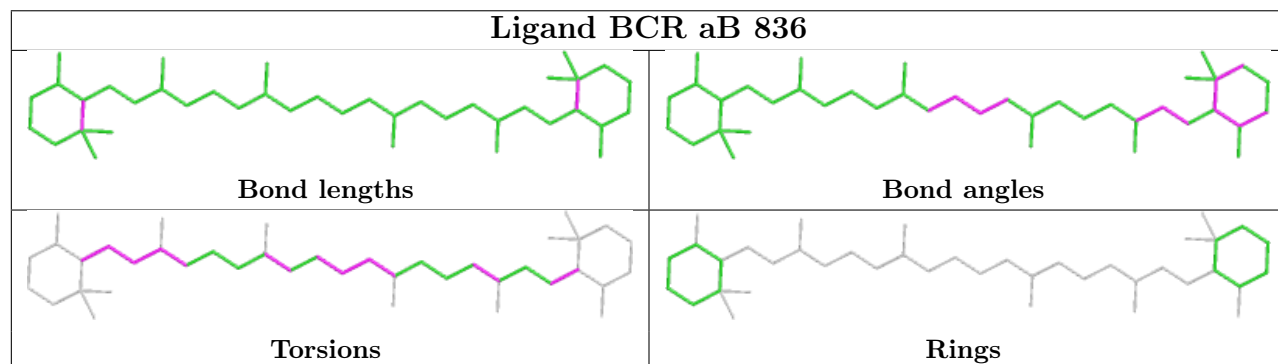
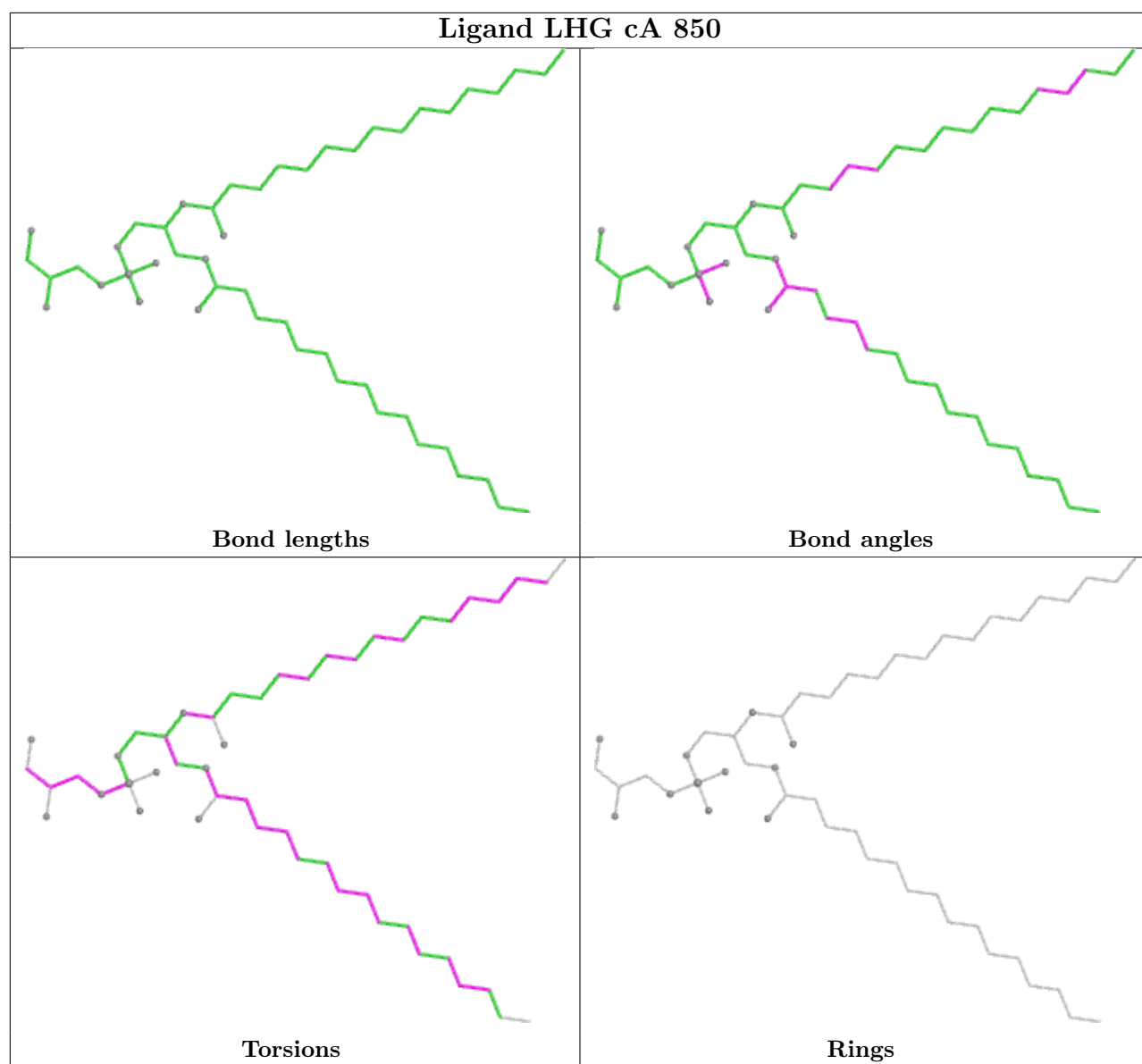
Torsions

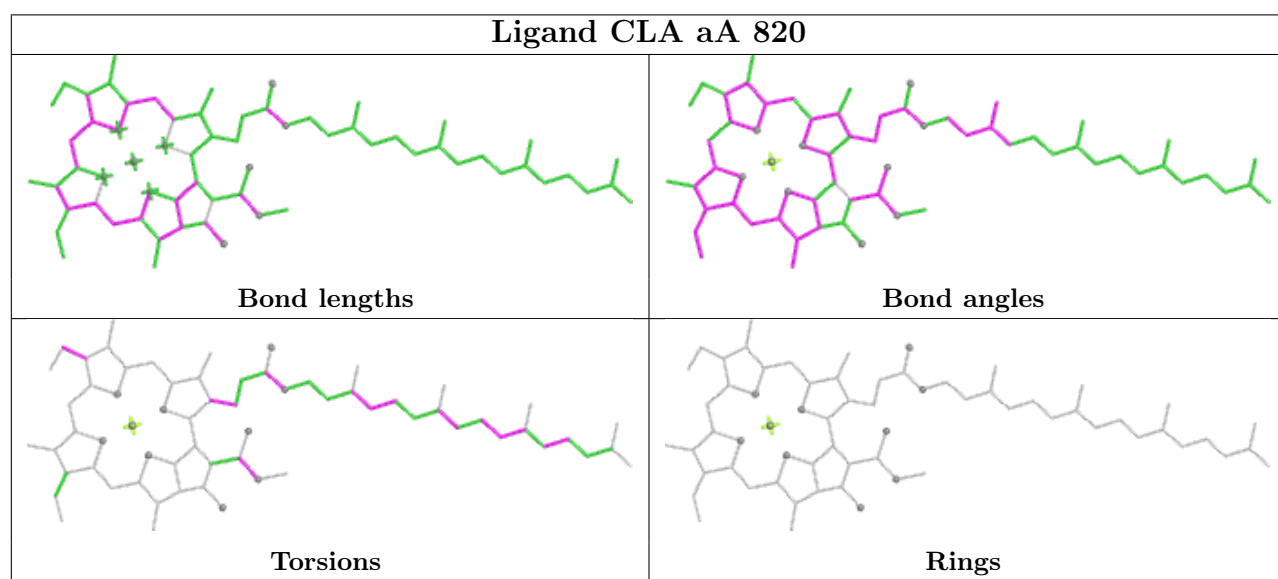
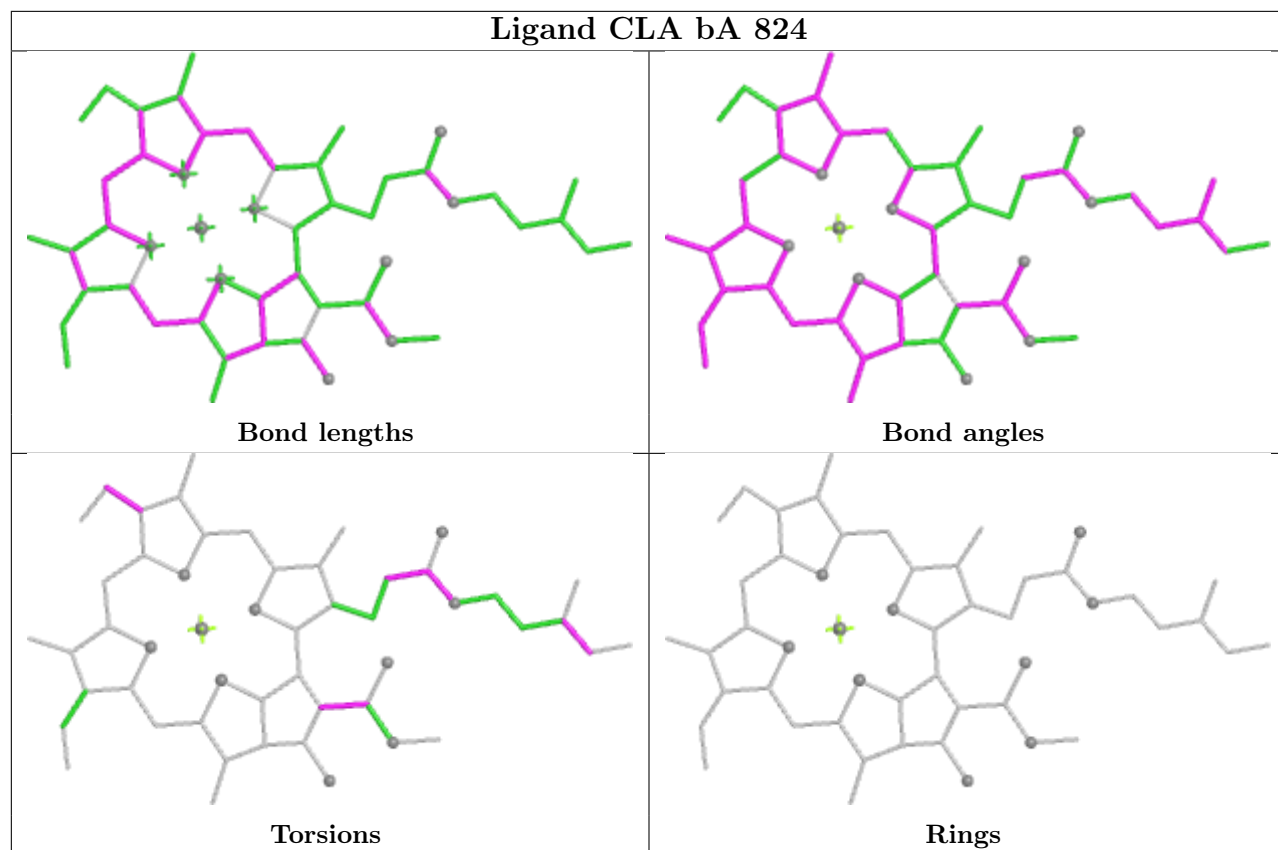


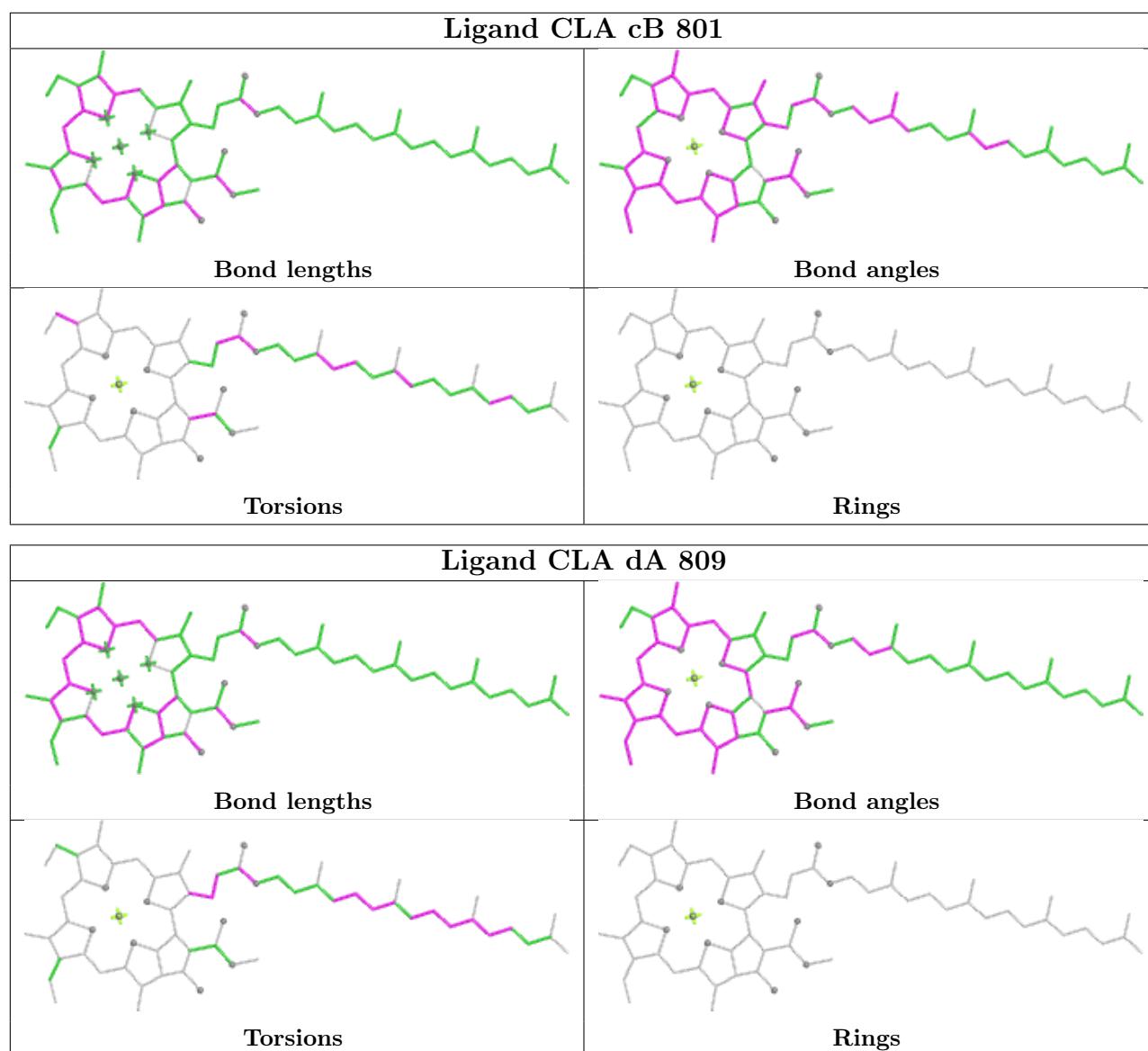
Rings

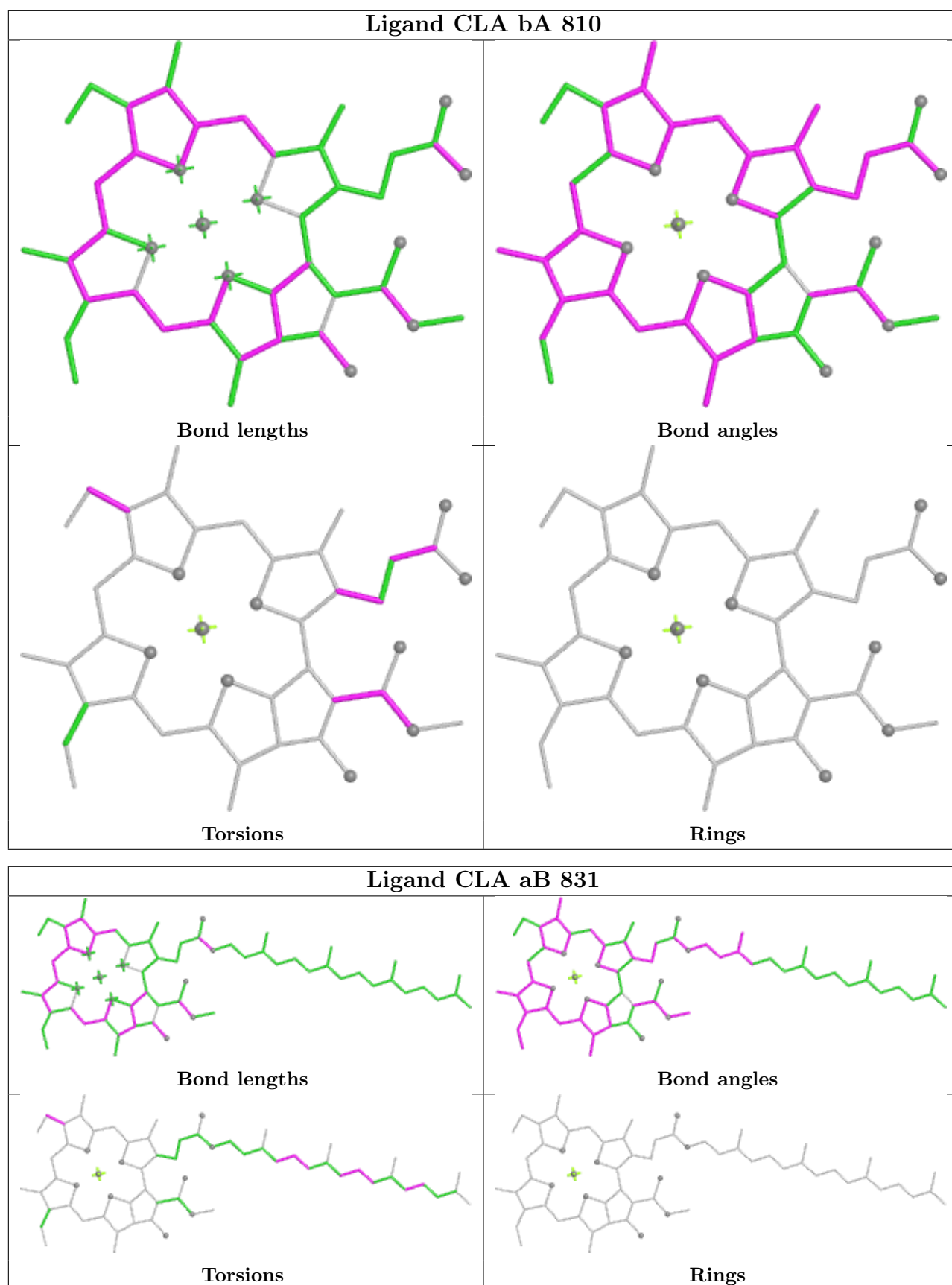


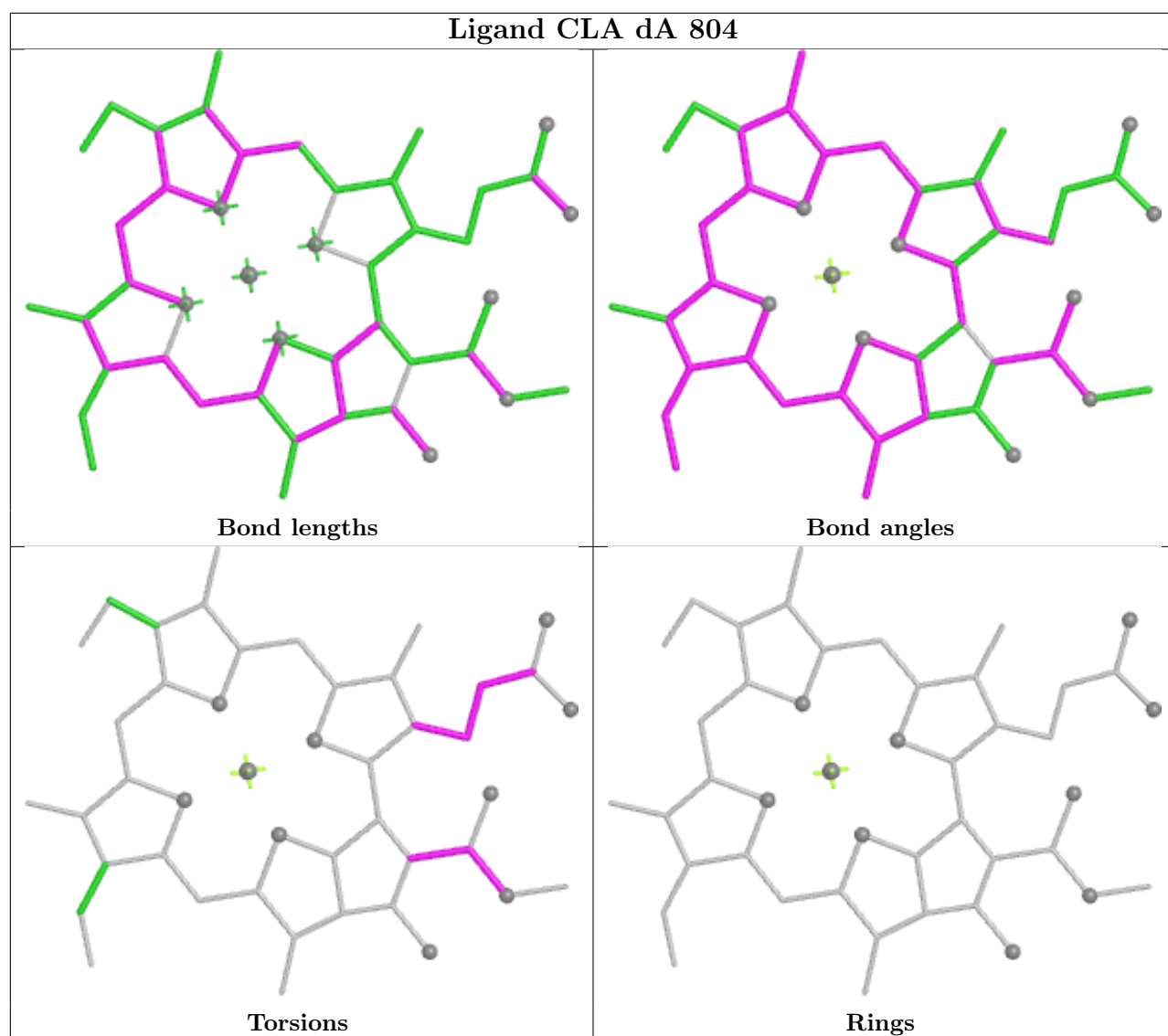


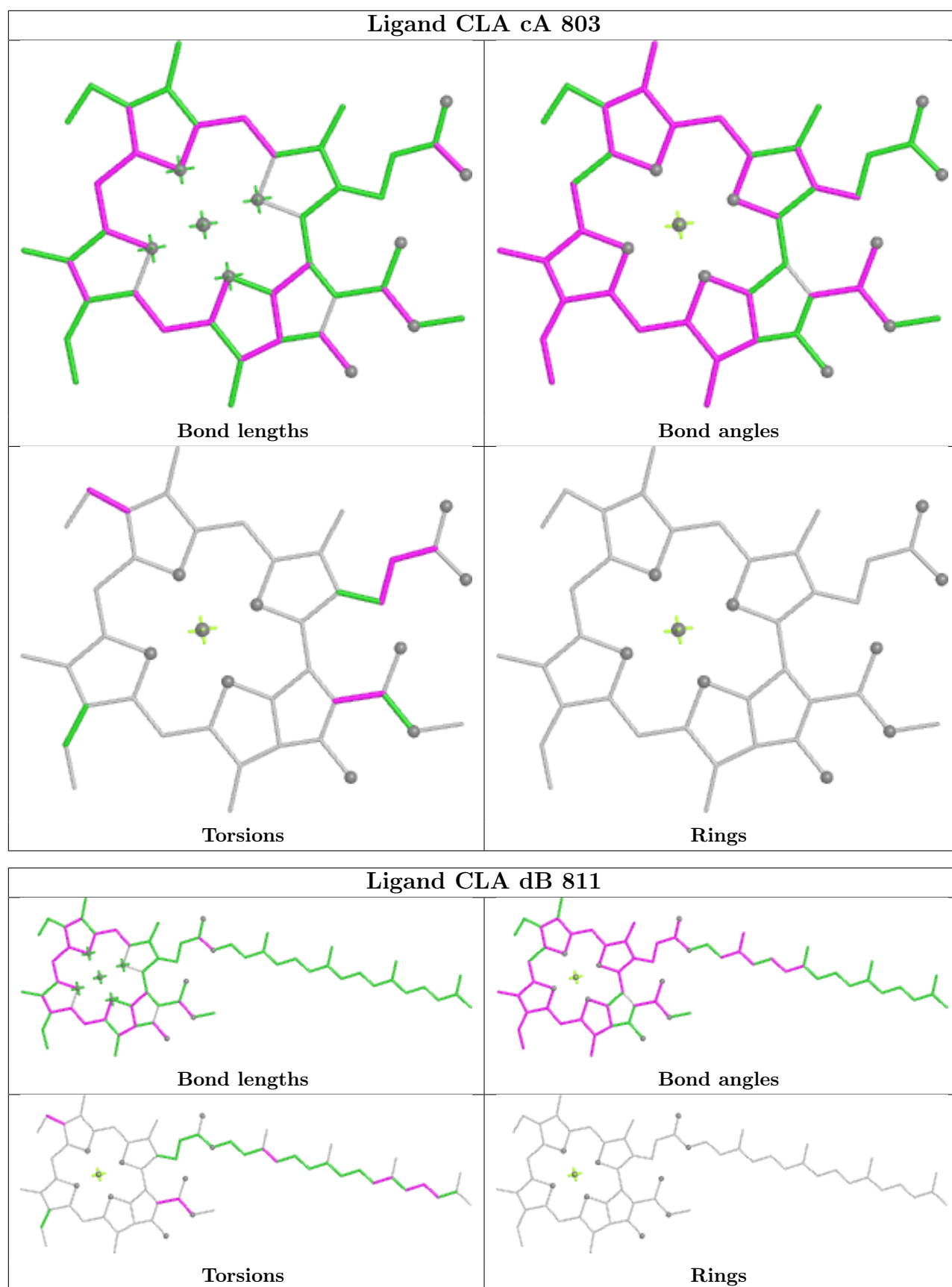


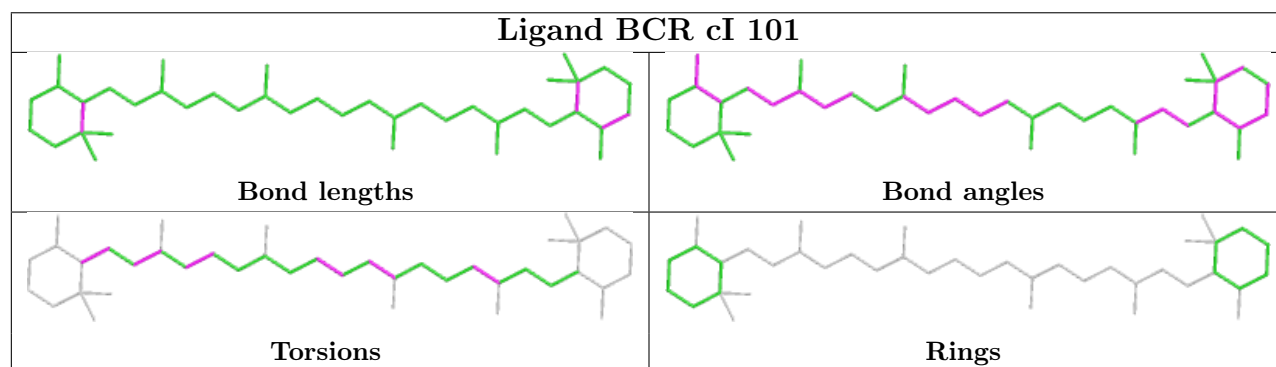
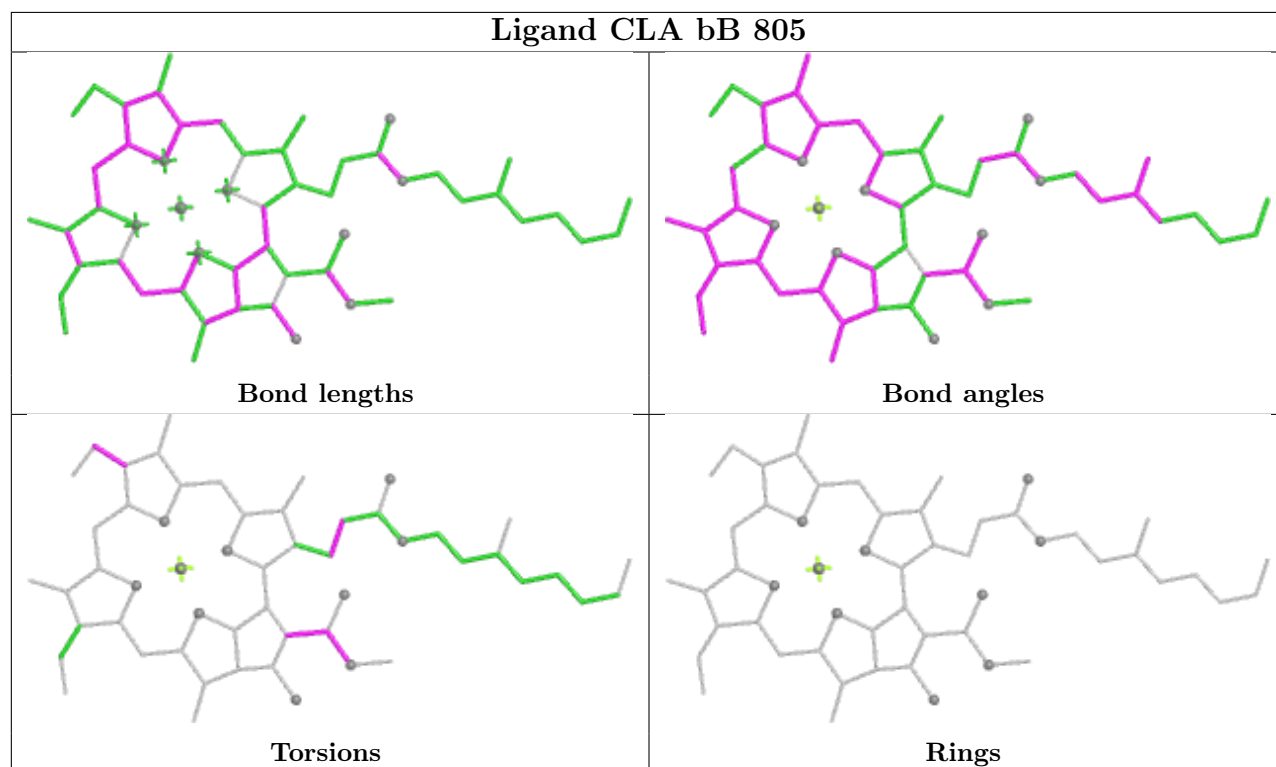
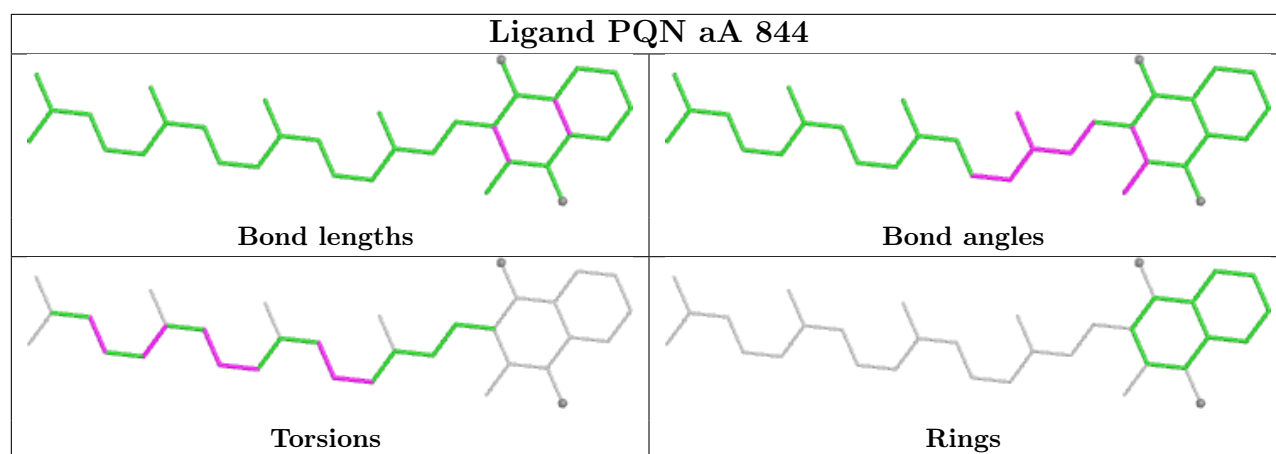


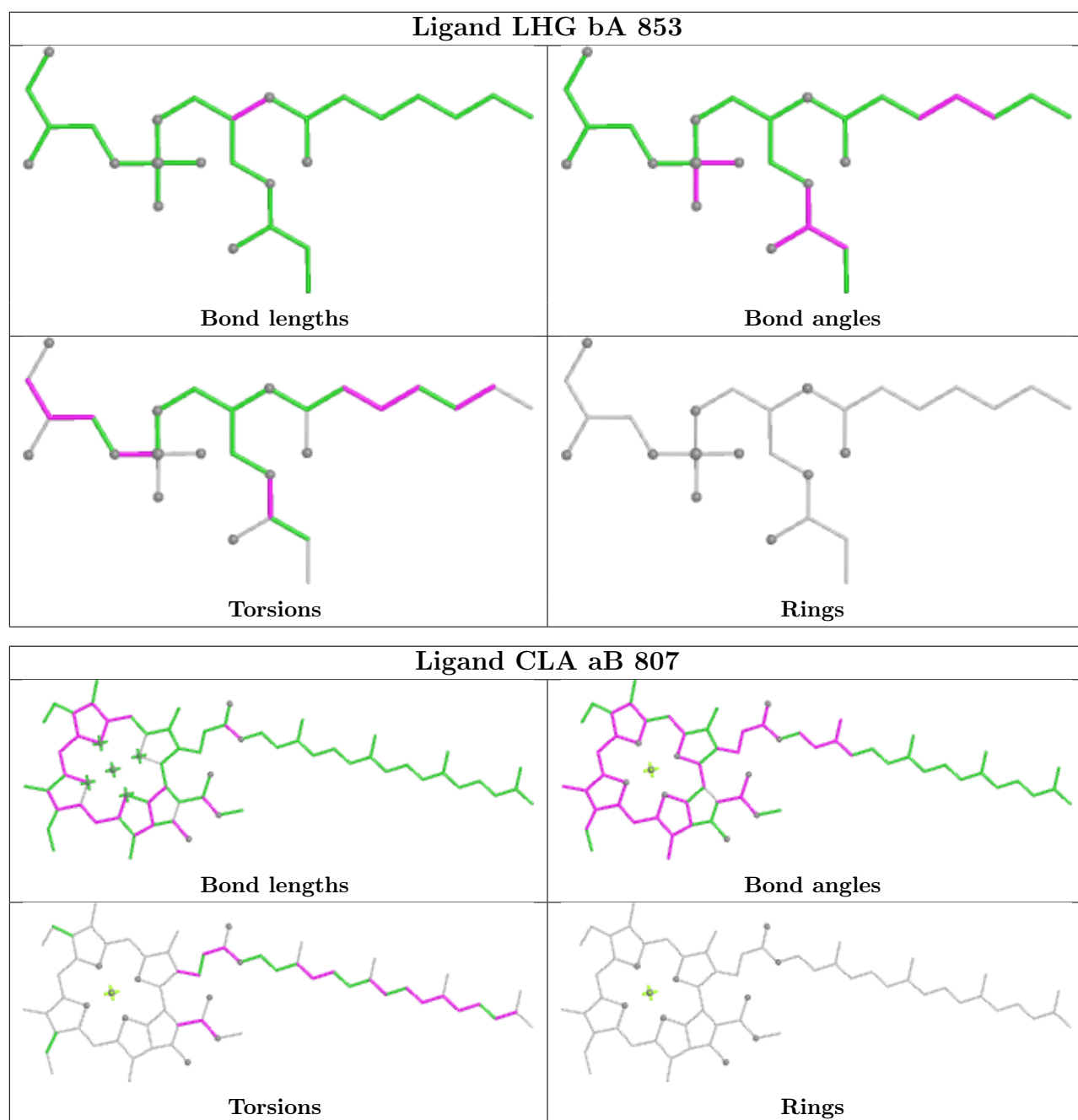


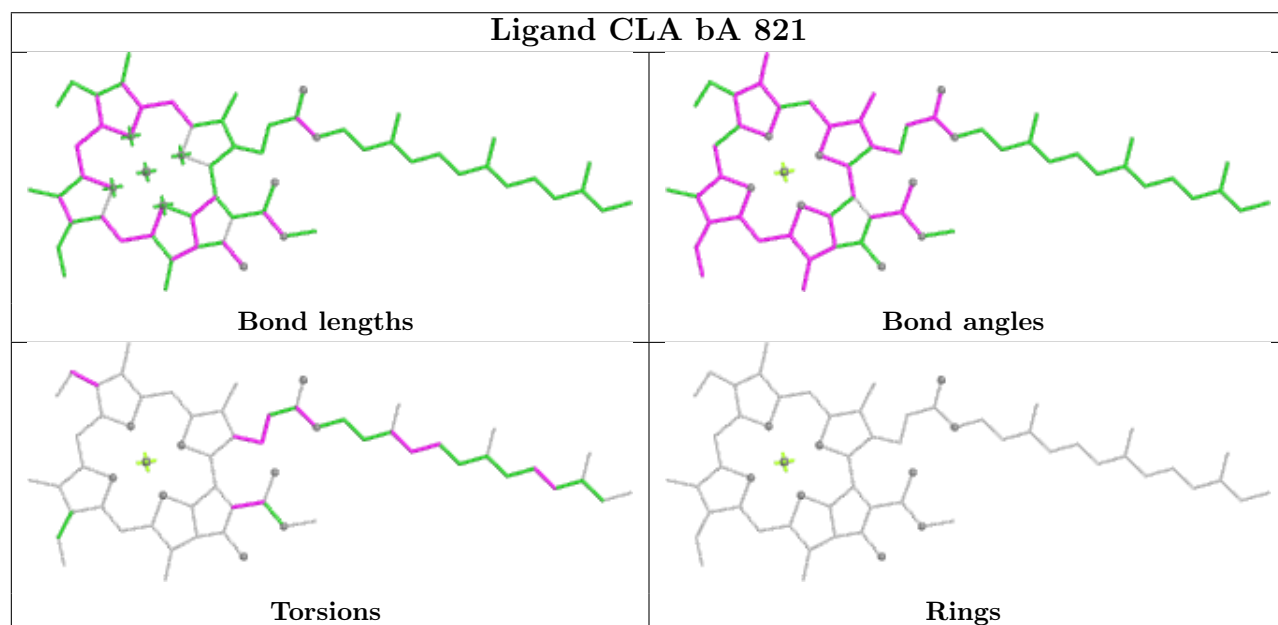
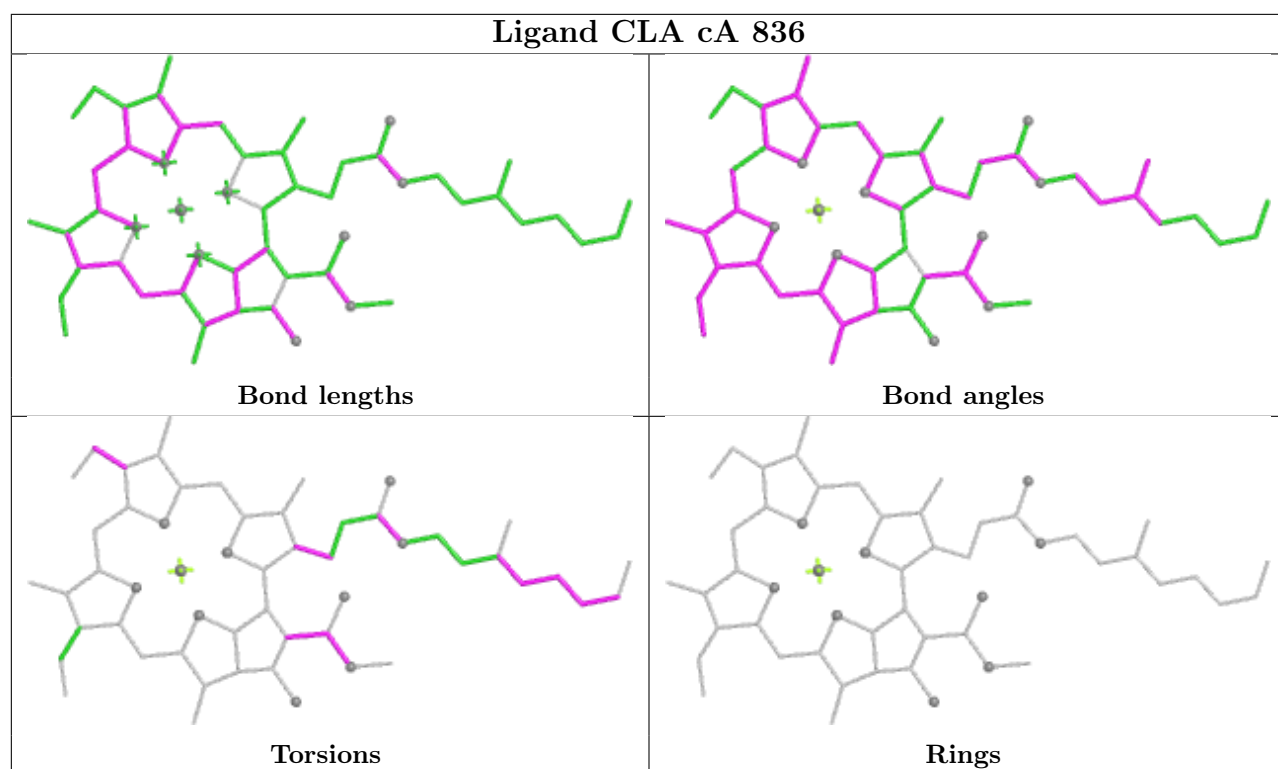


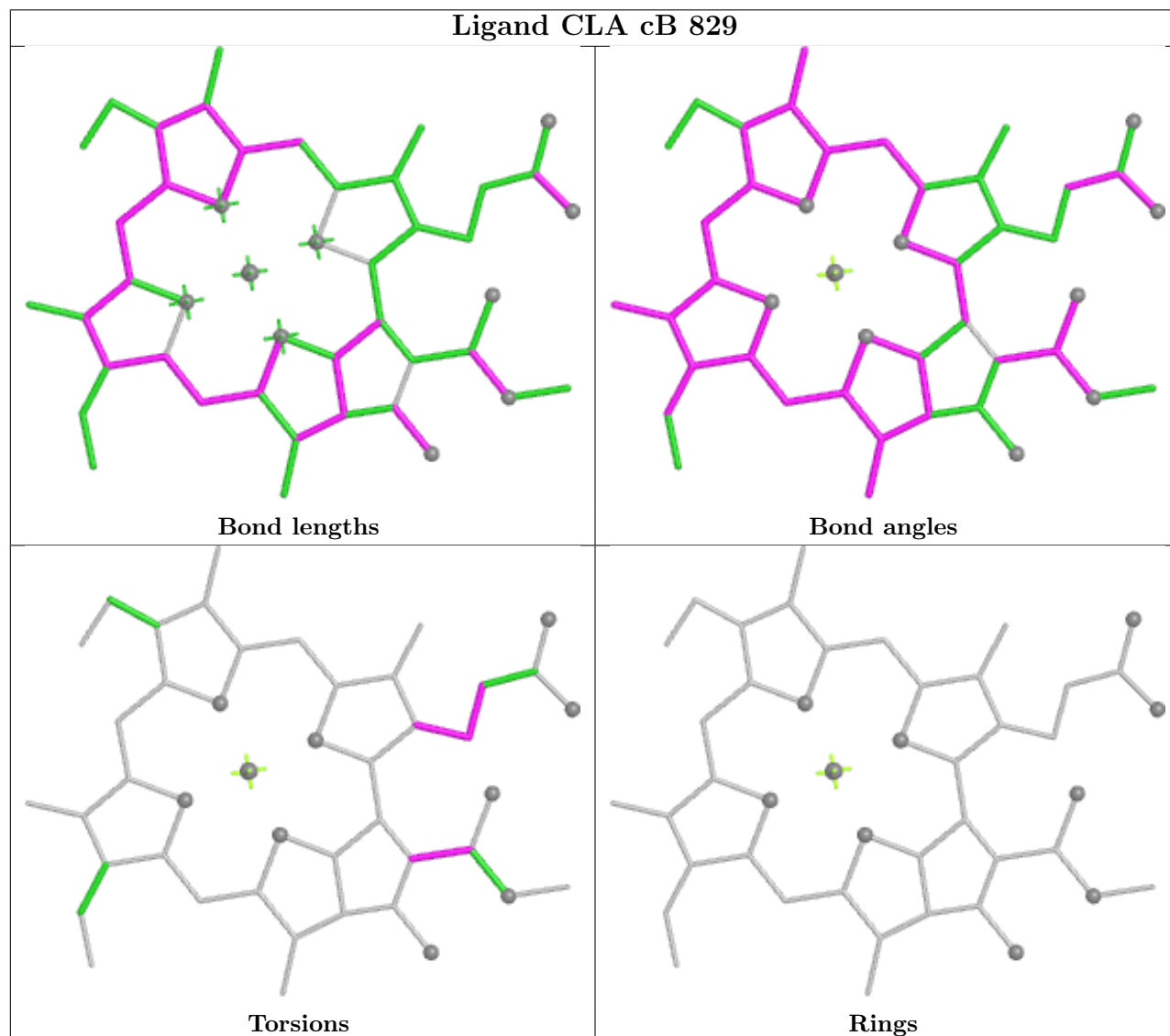
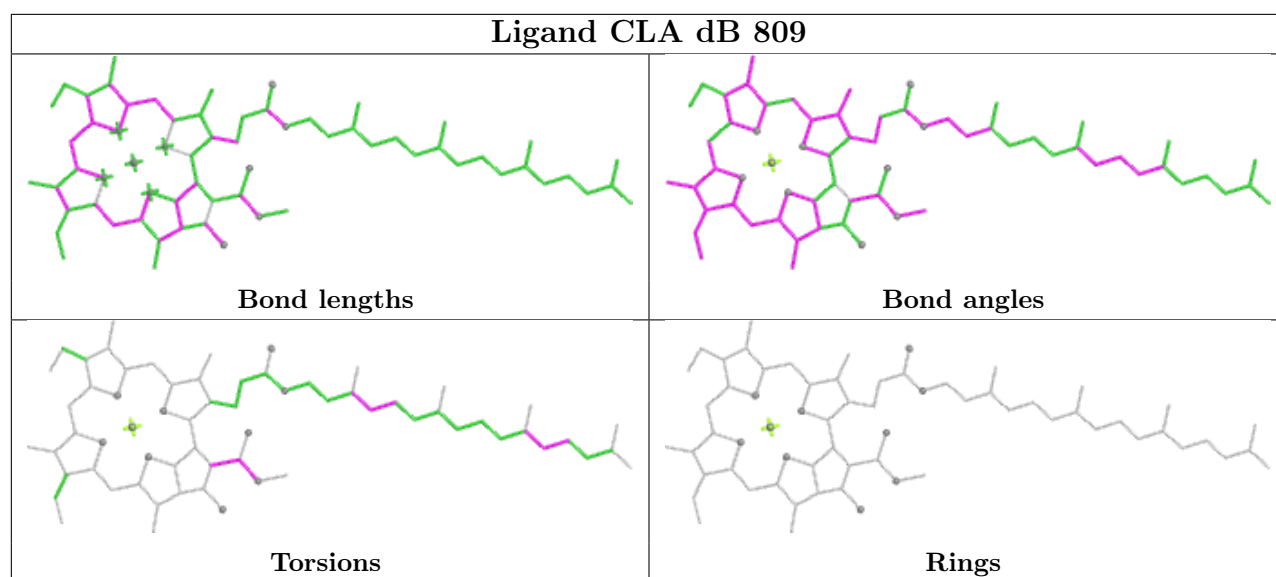




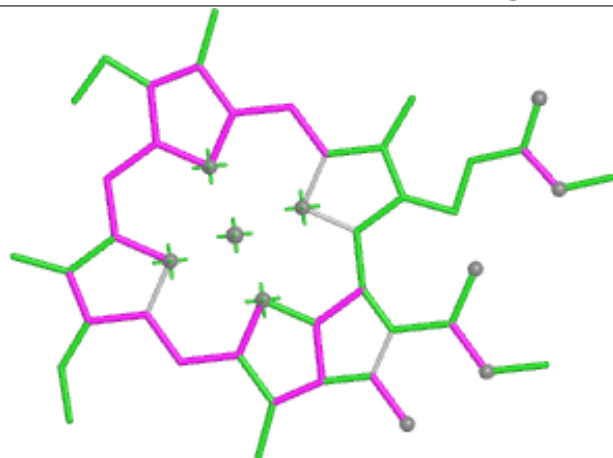




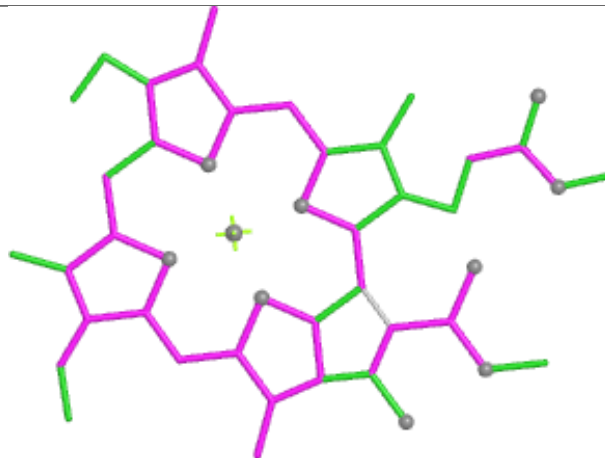




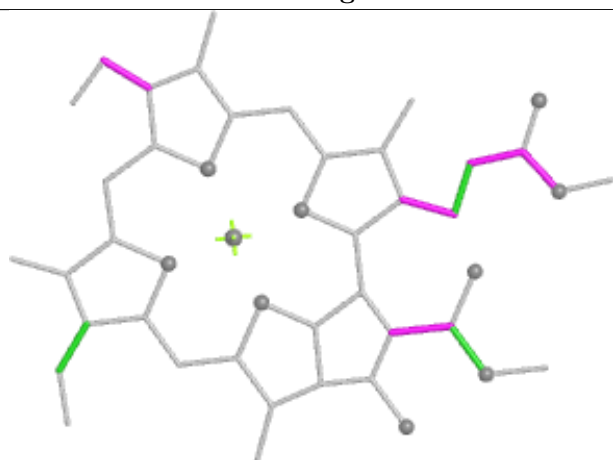
Ligand CLA aK 204



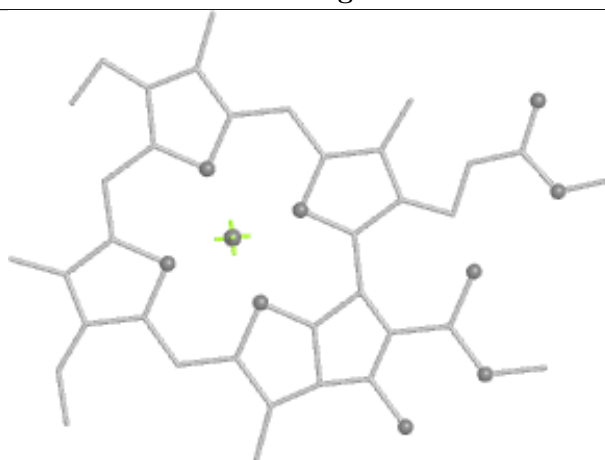
Bond lengths



Bond angles

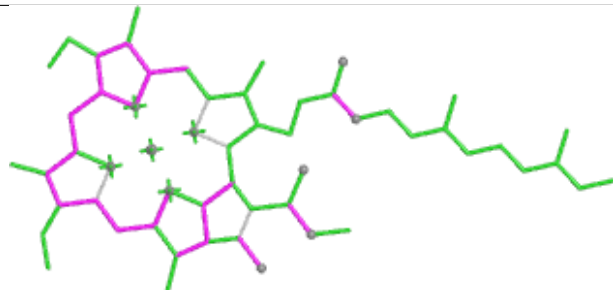


Torsions

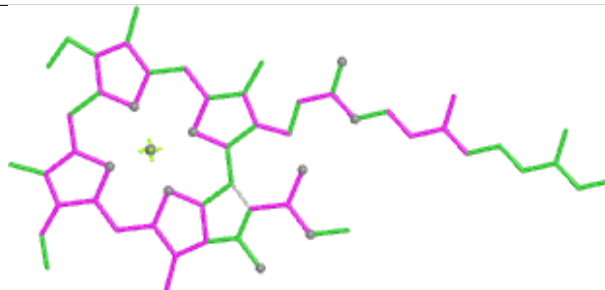


Rings

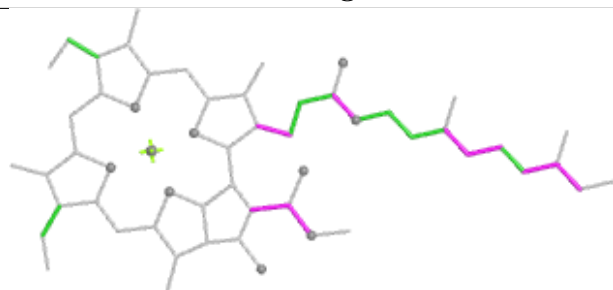
Ligand CLA bB 814



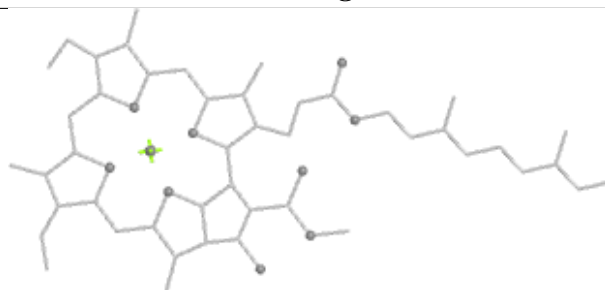
Bond lengths



Bond angles

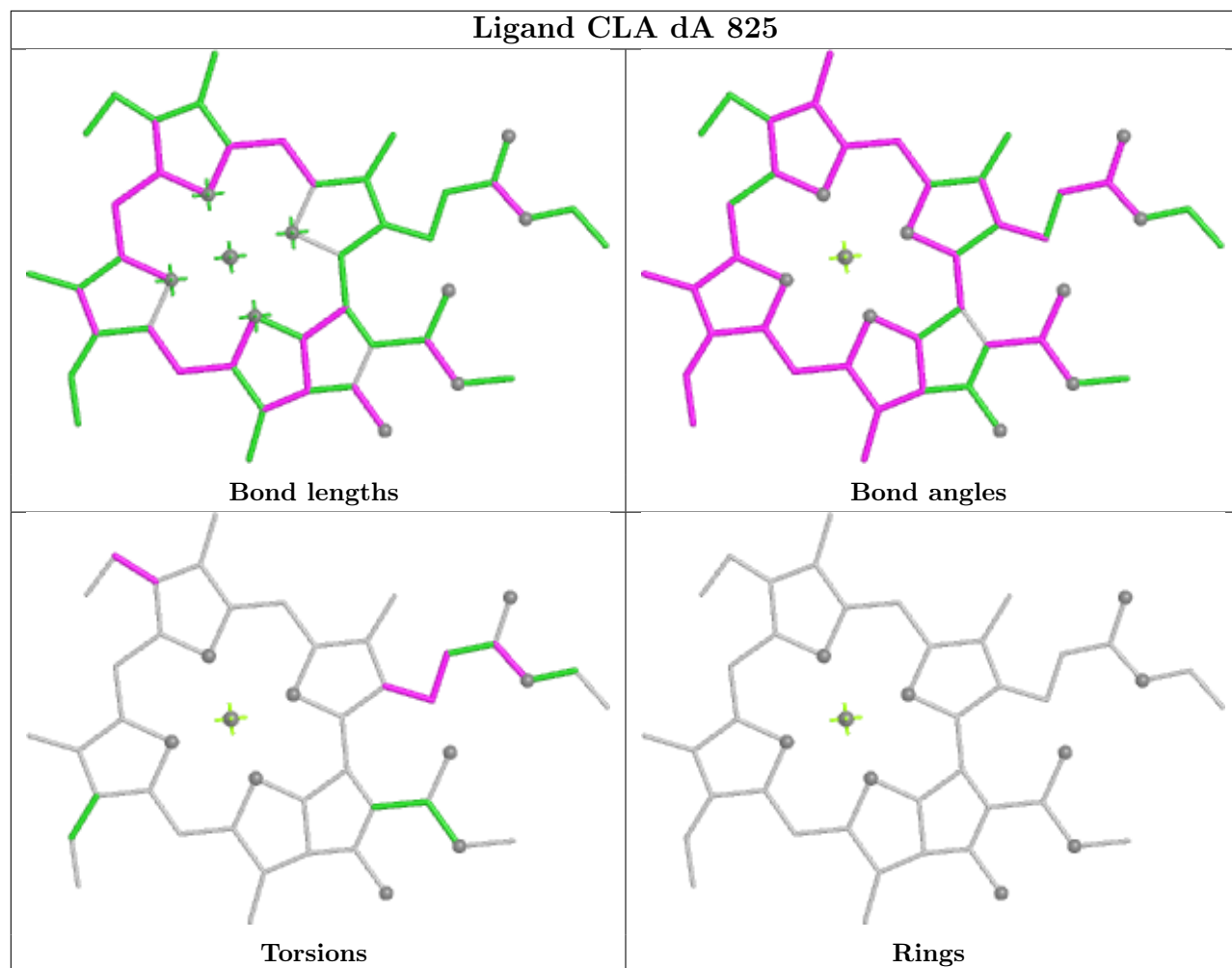


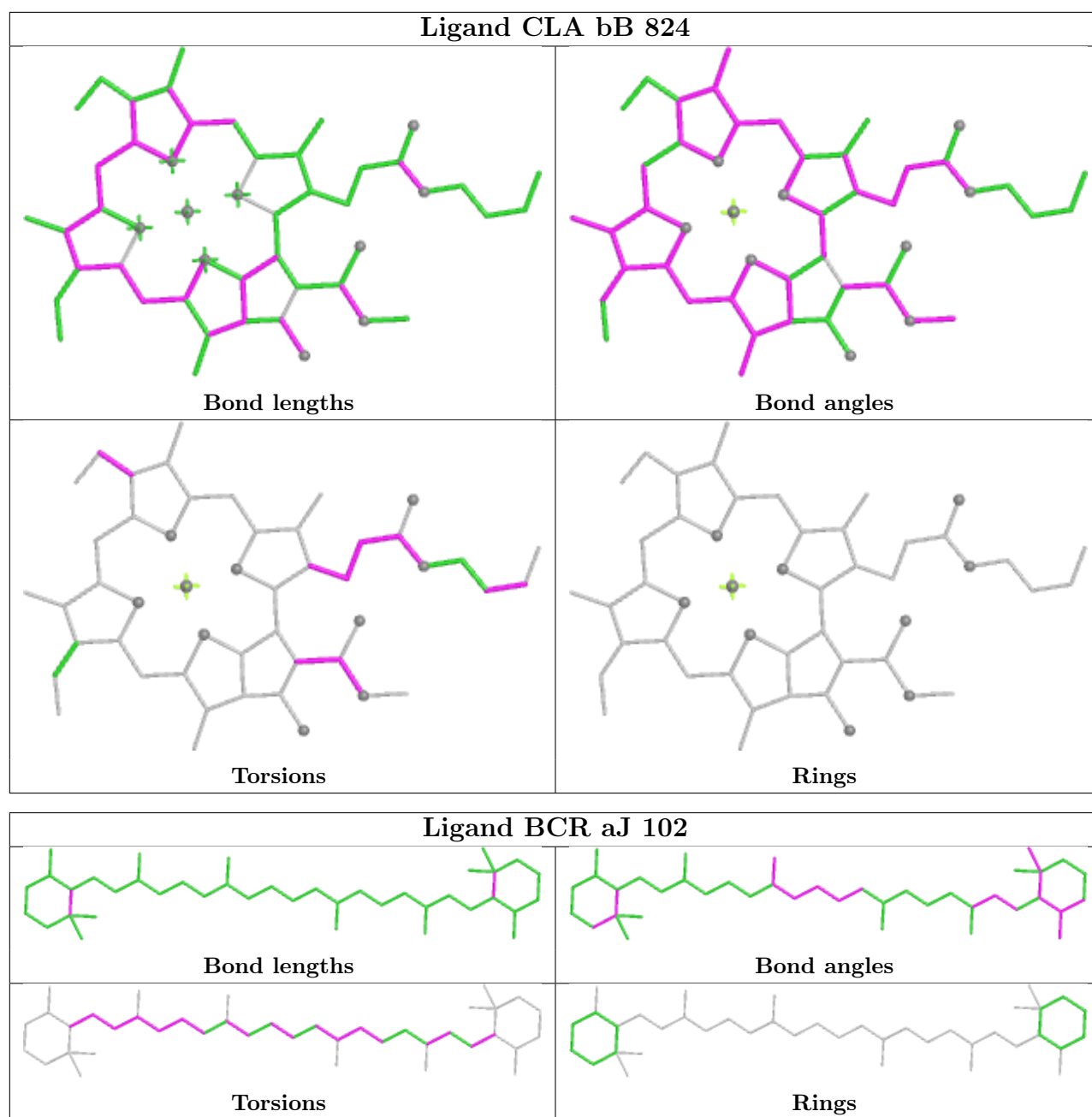
Torsions

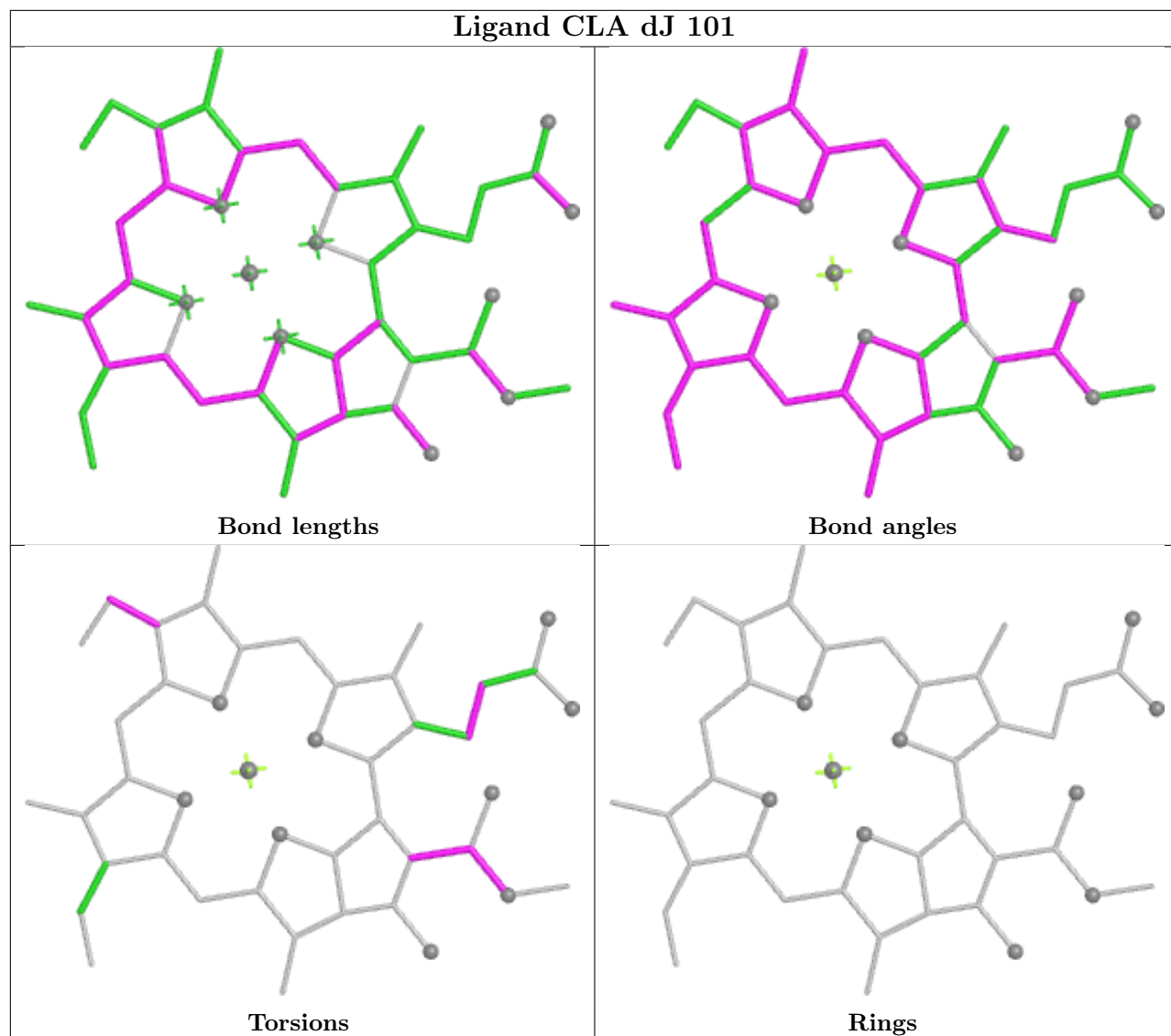


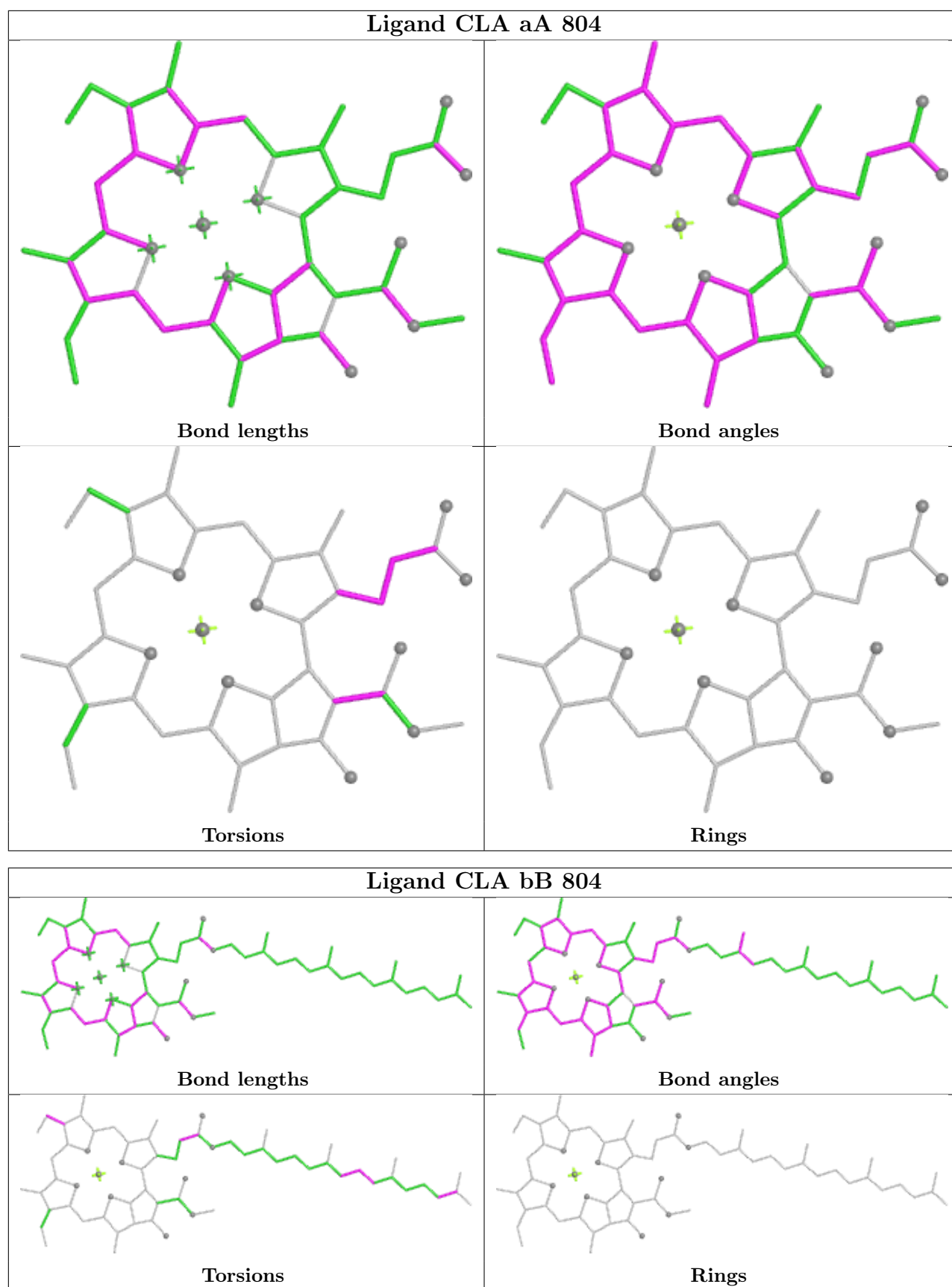
Rings

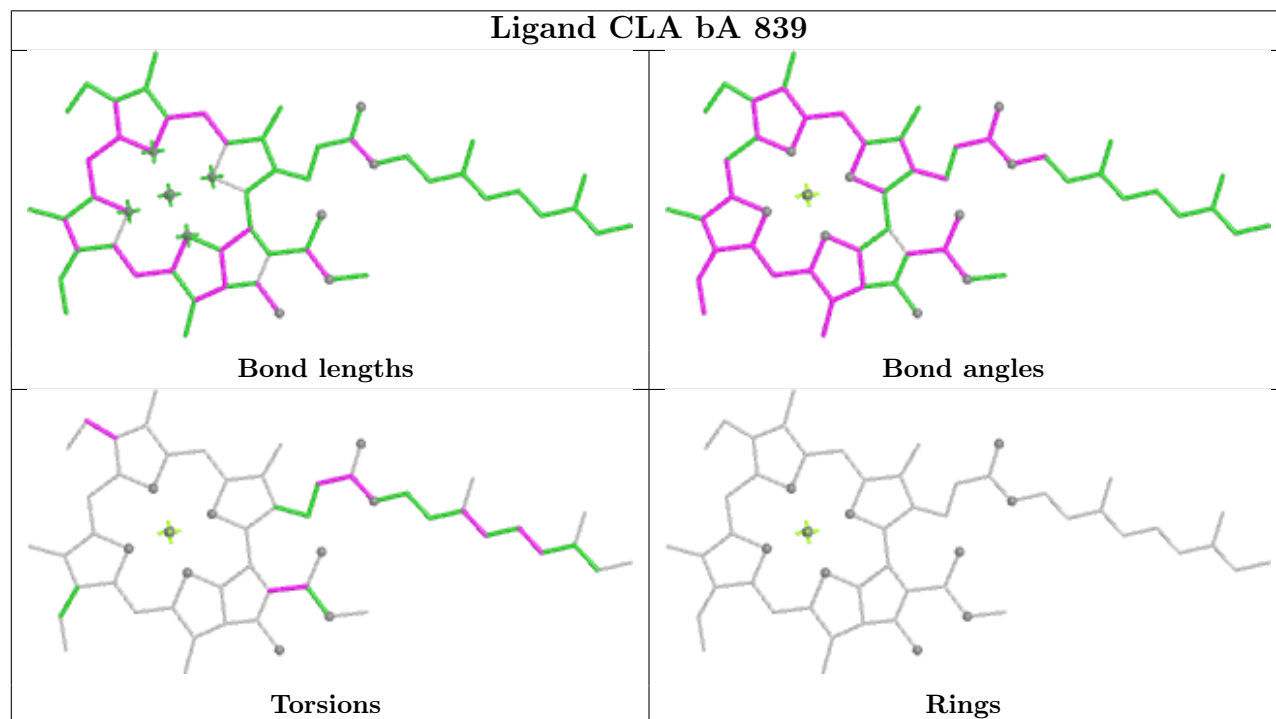
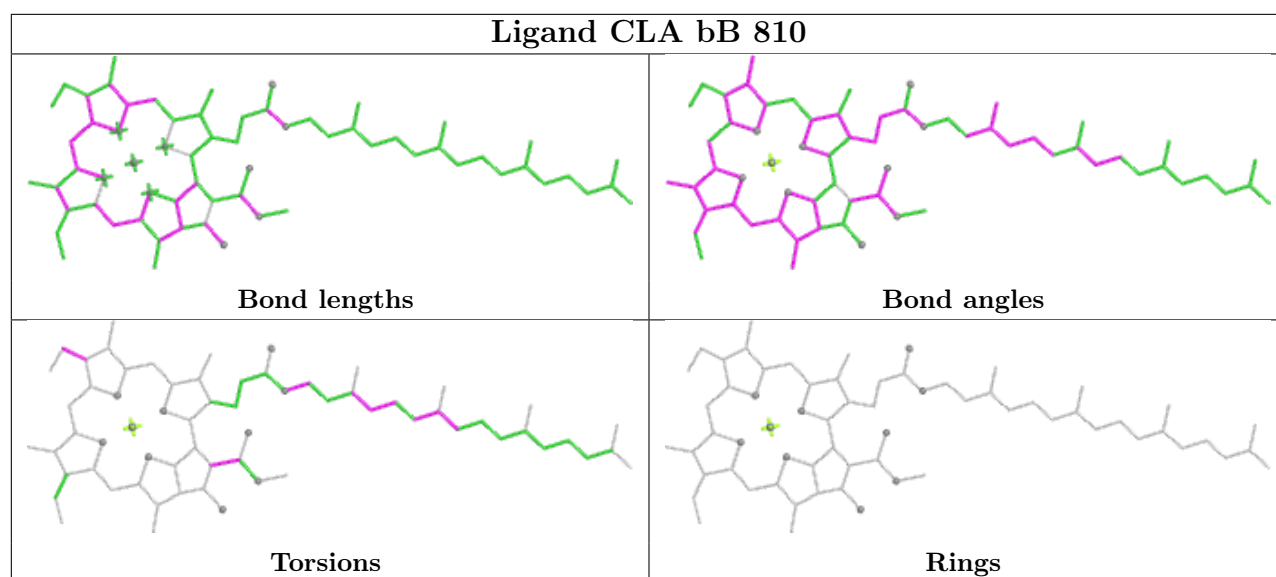
Ligand CLA dA 825

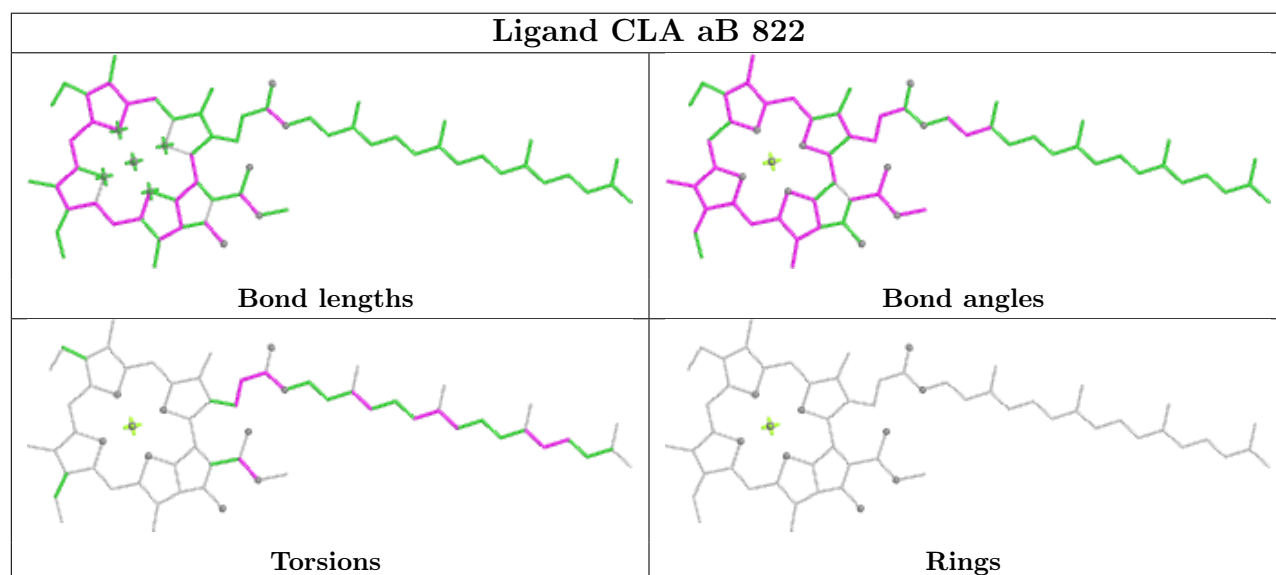
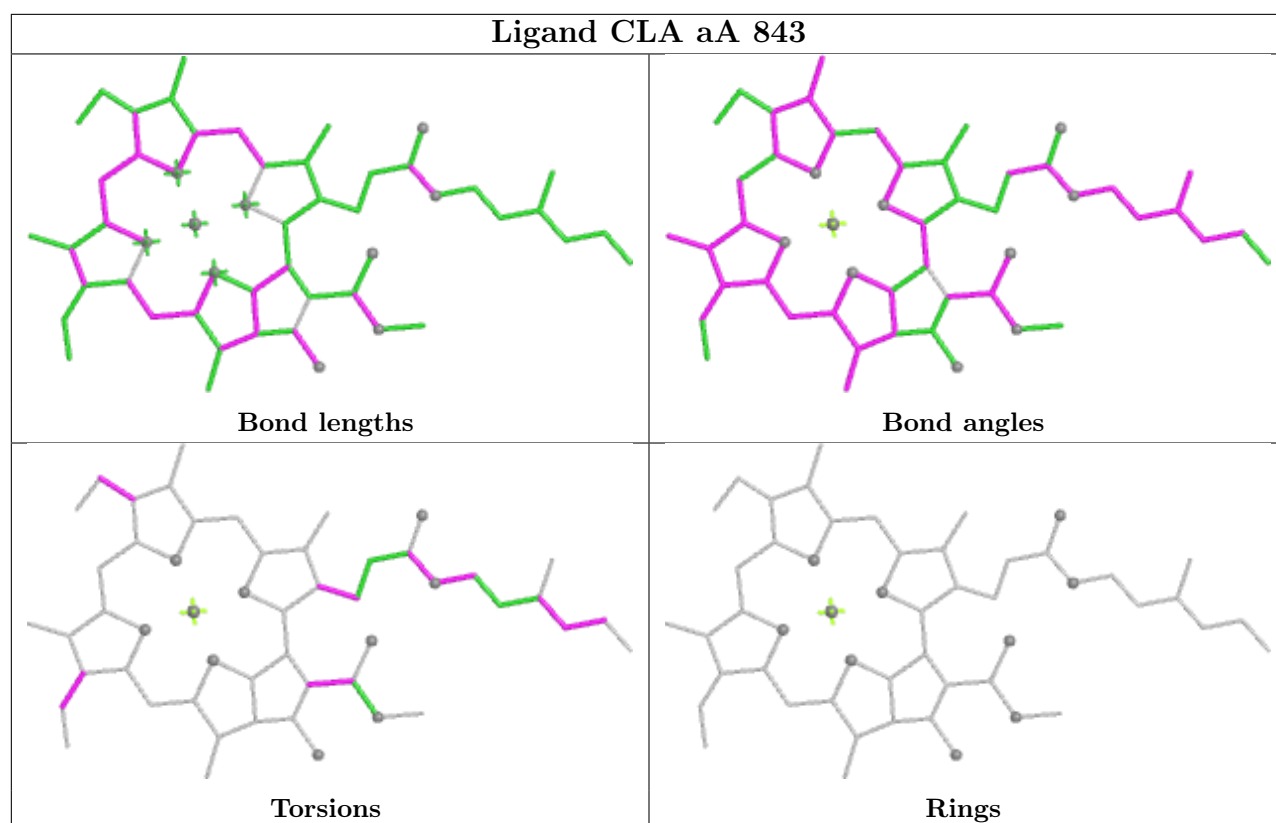


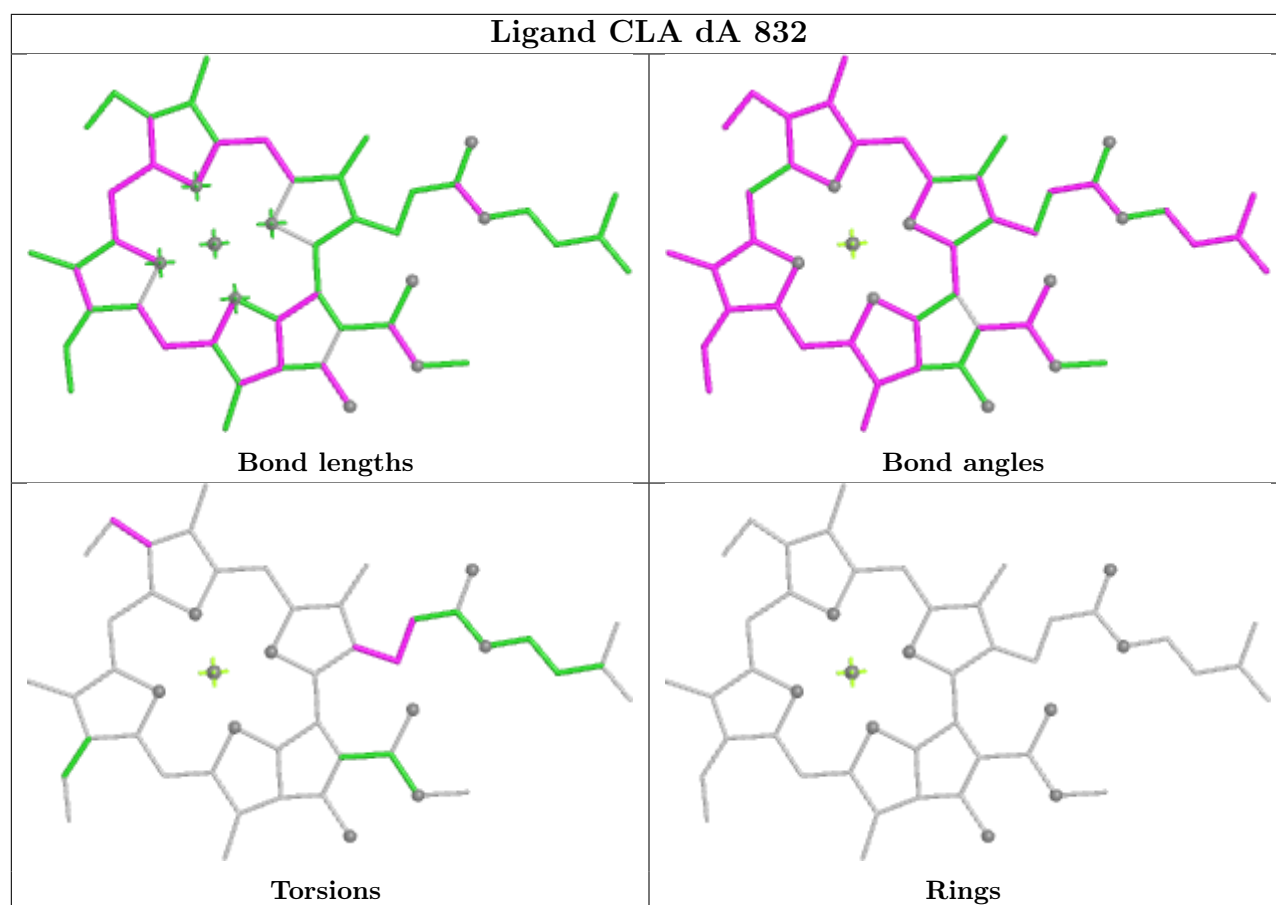




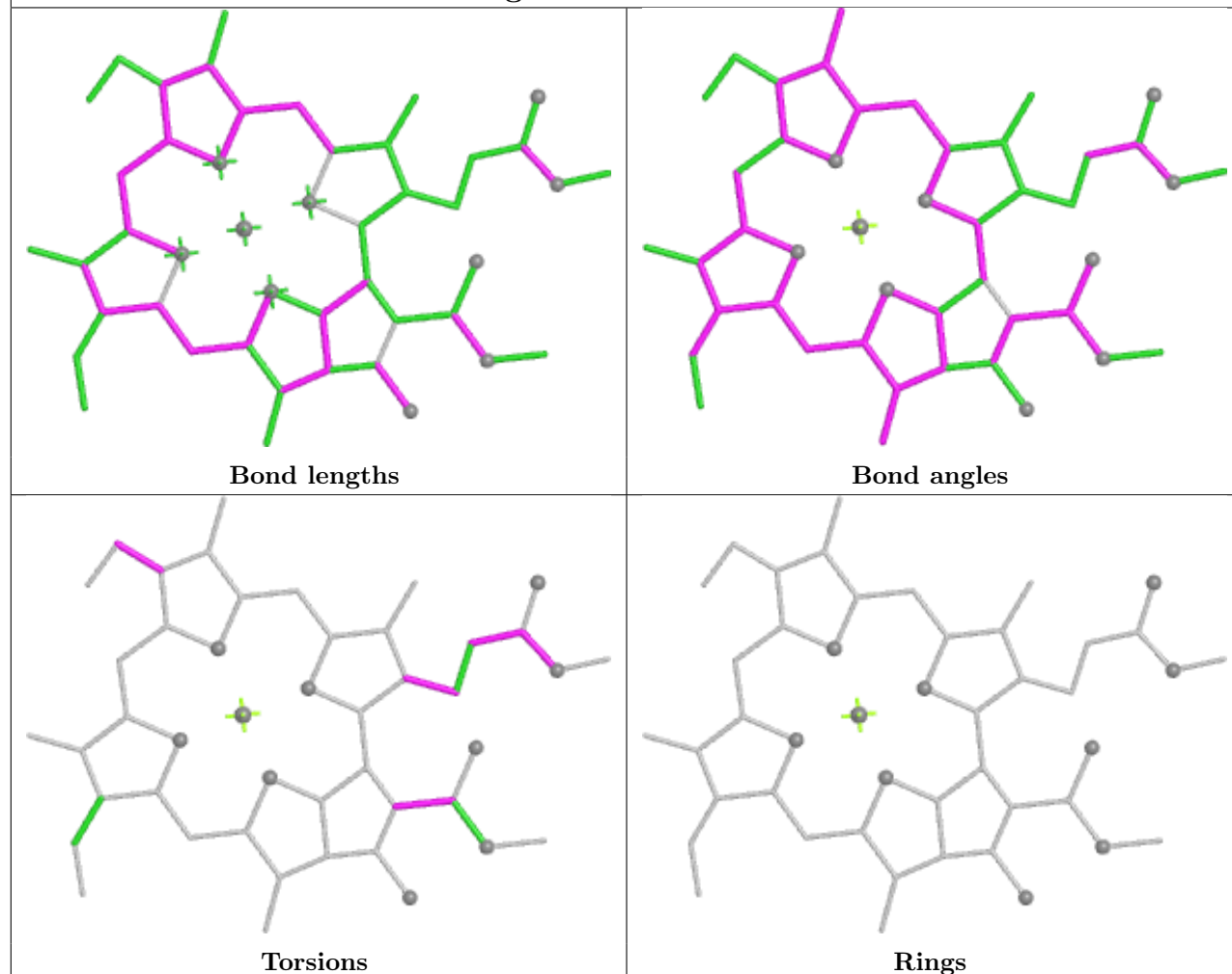




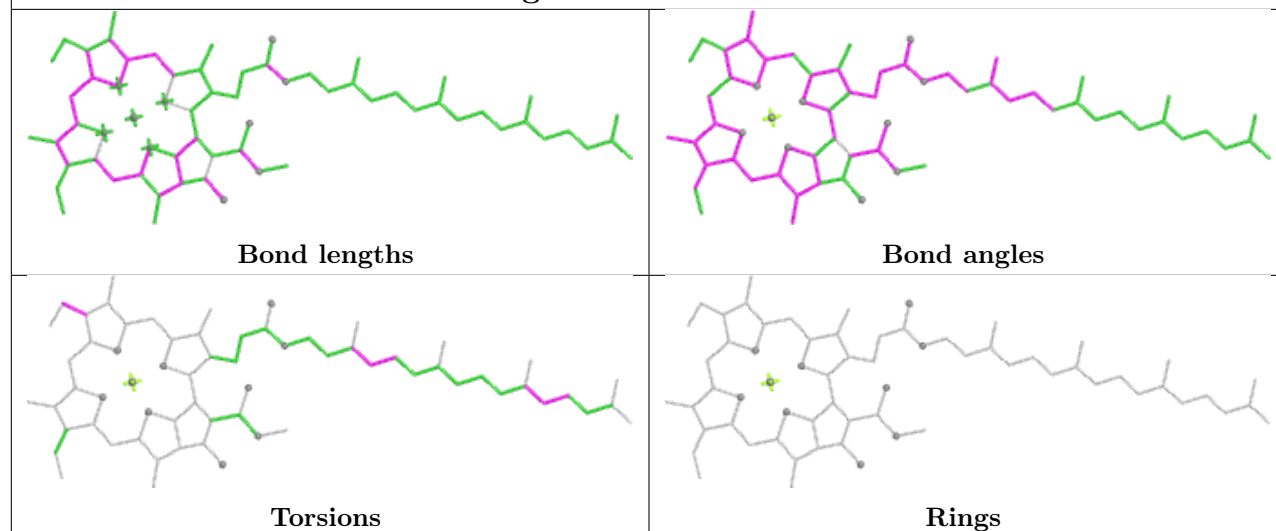


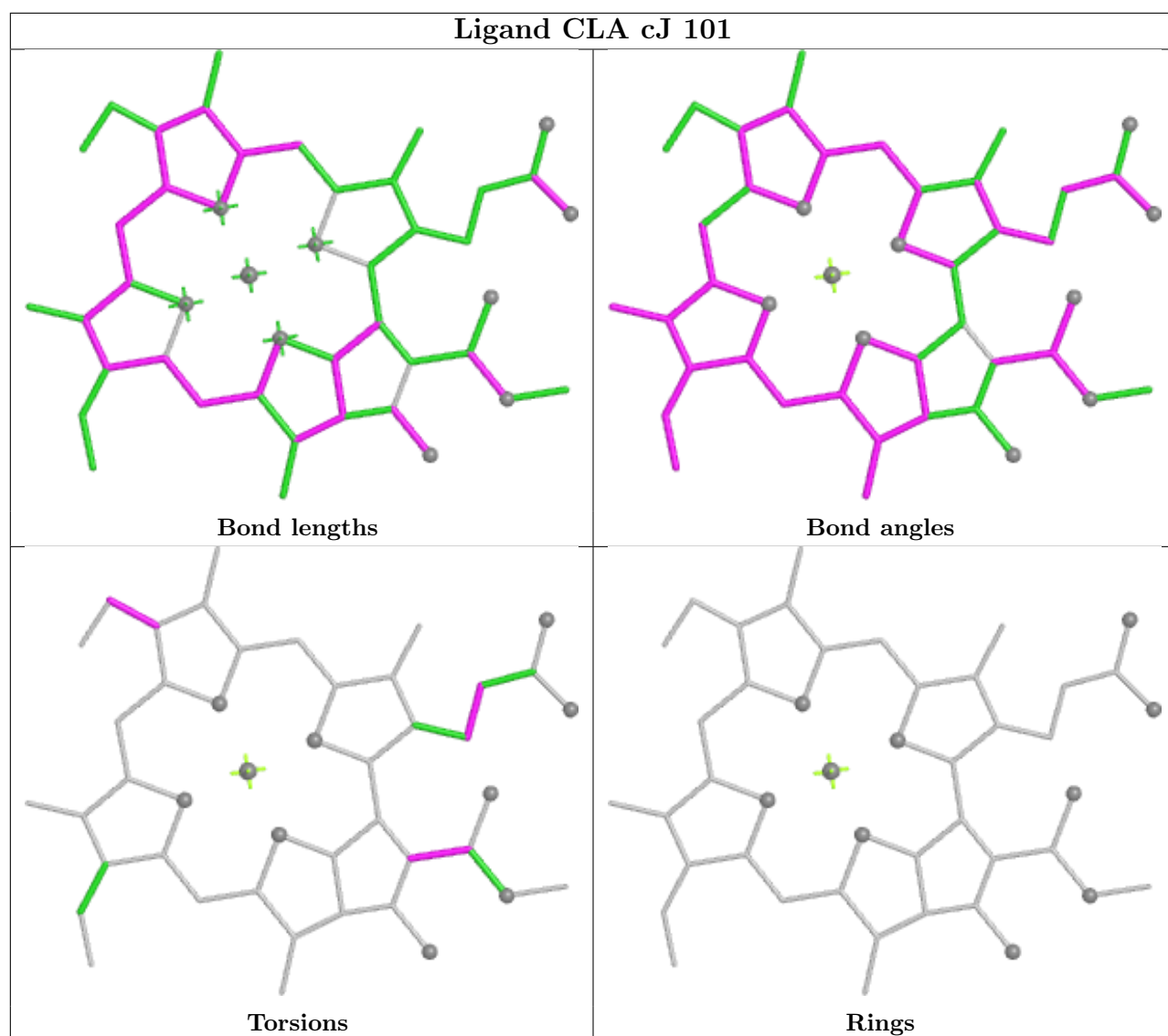


Ligand CLA cK 204

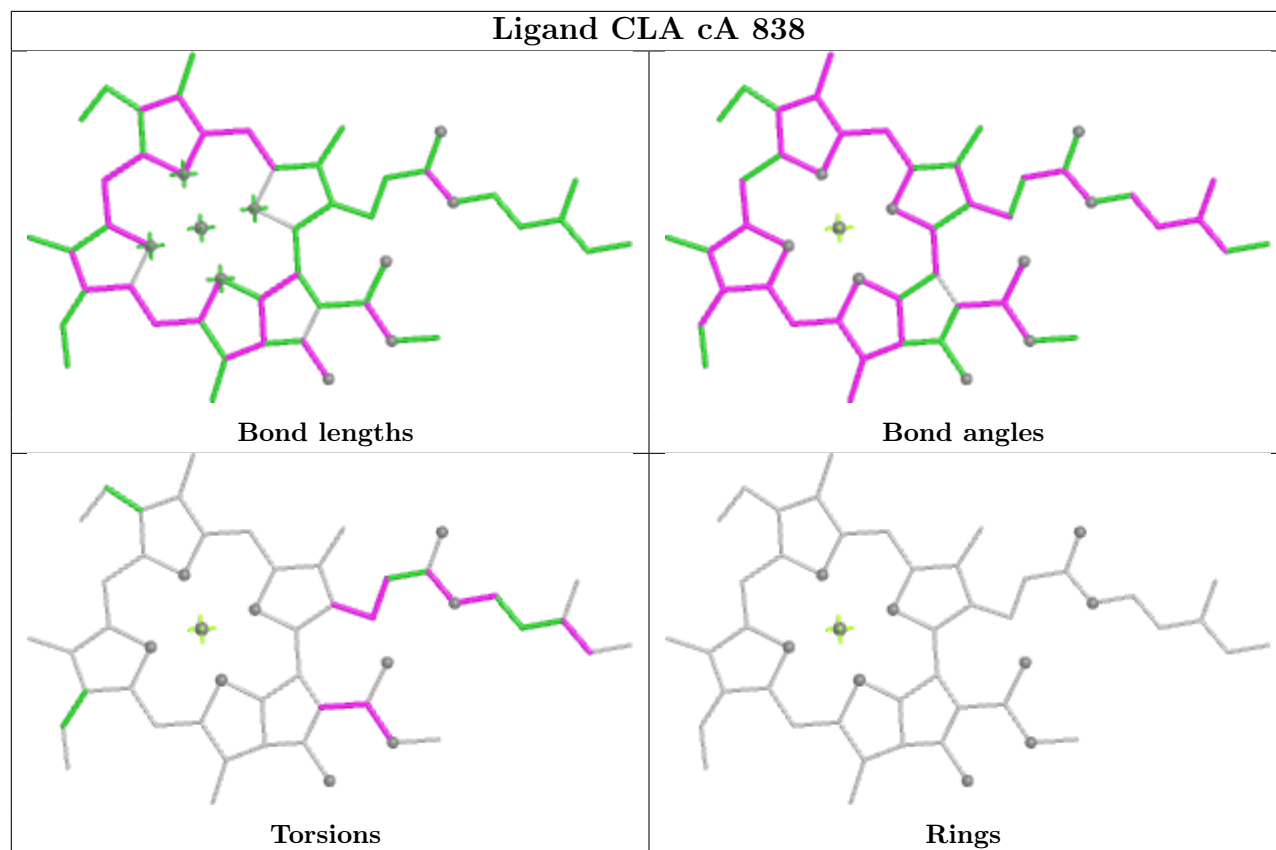


Ligand CLA dB 803

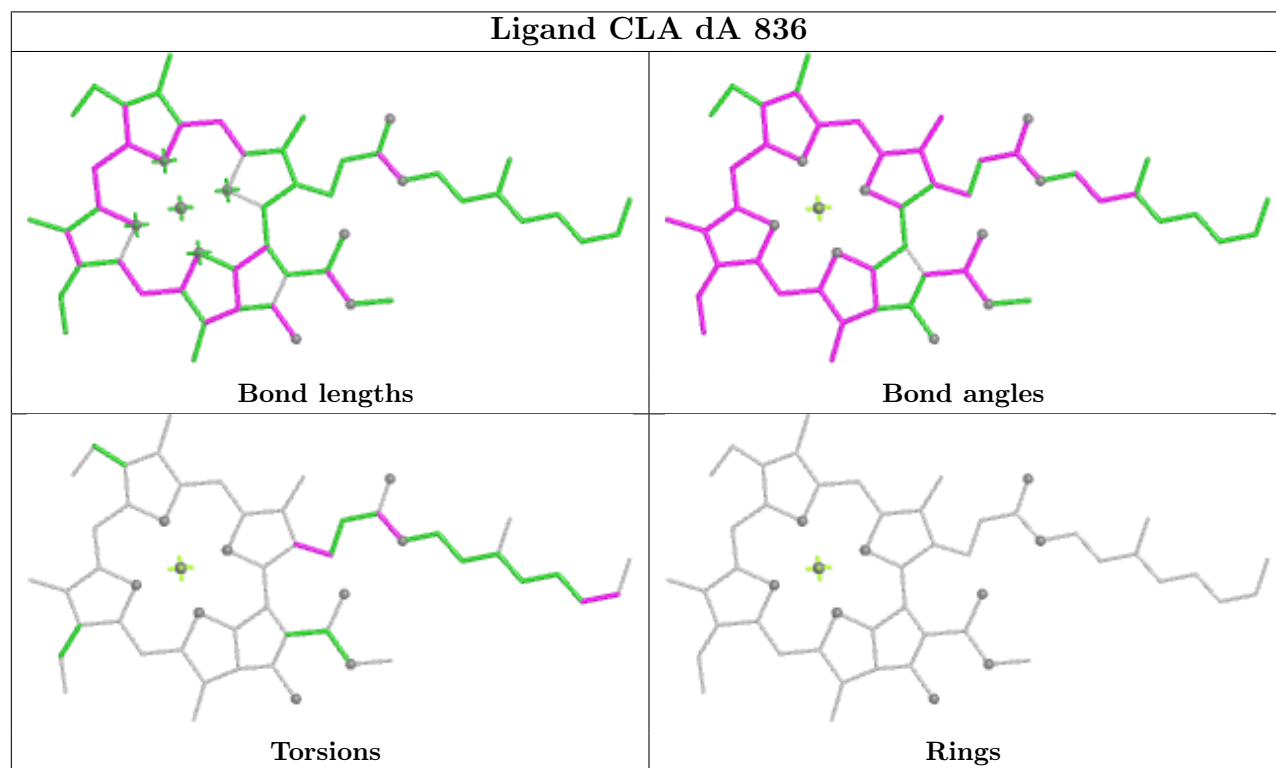


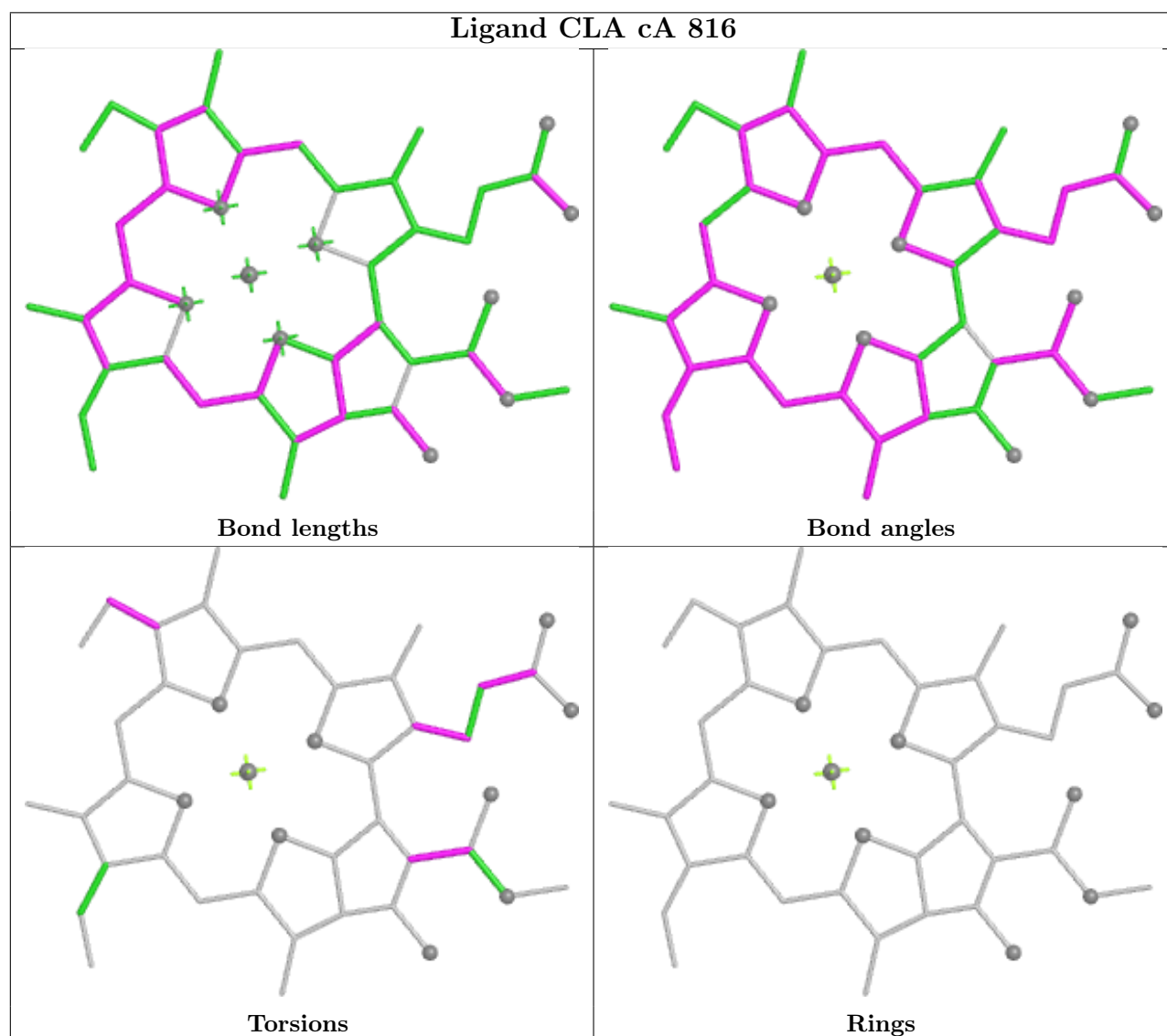
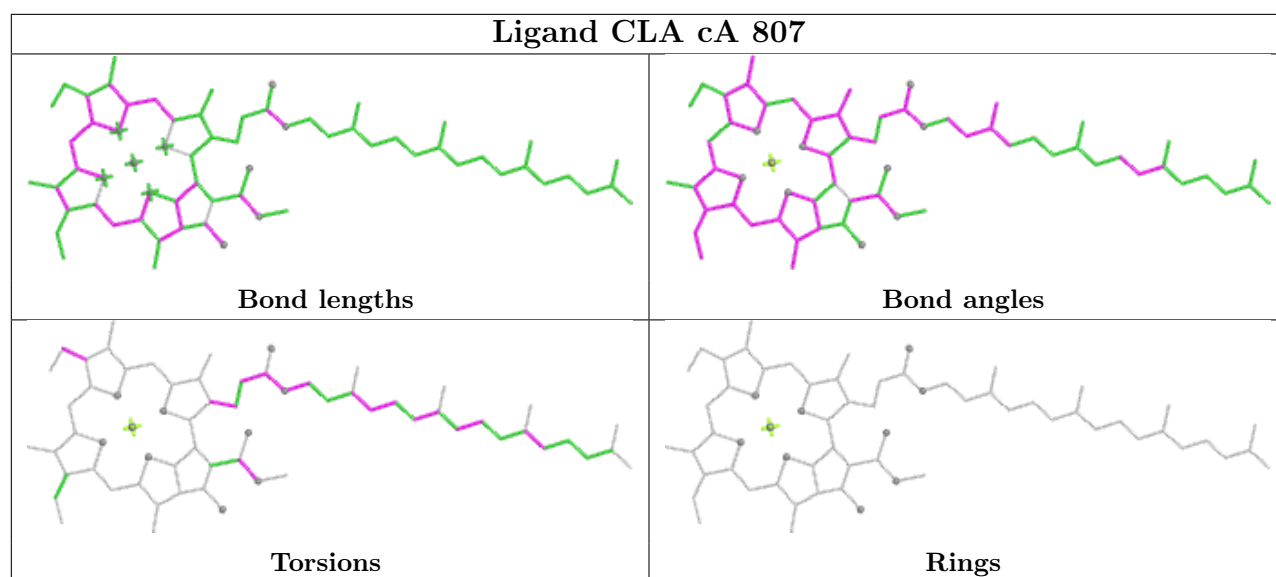


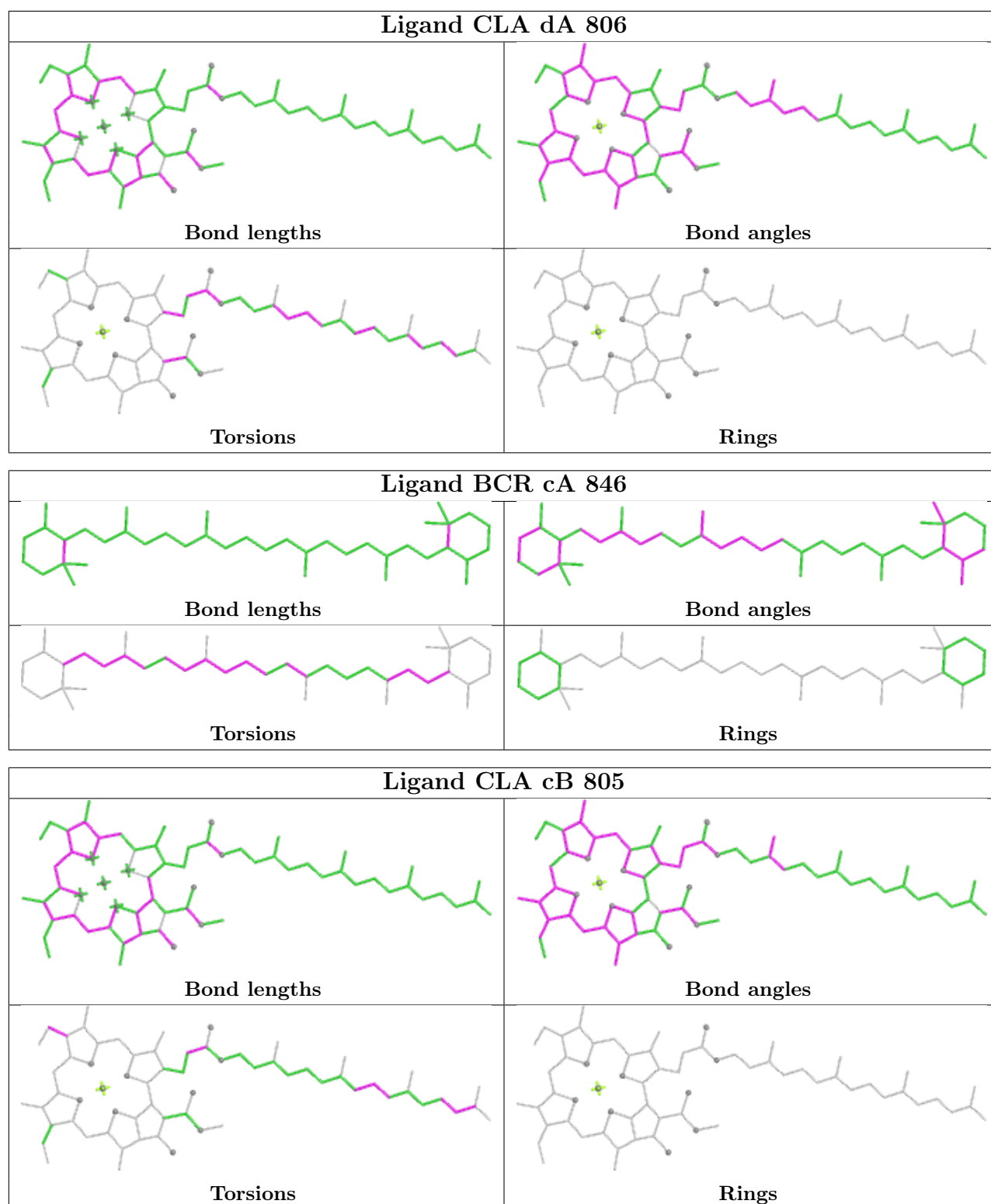
Ligand CLA cA 838

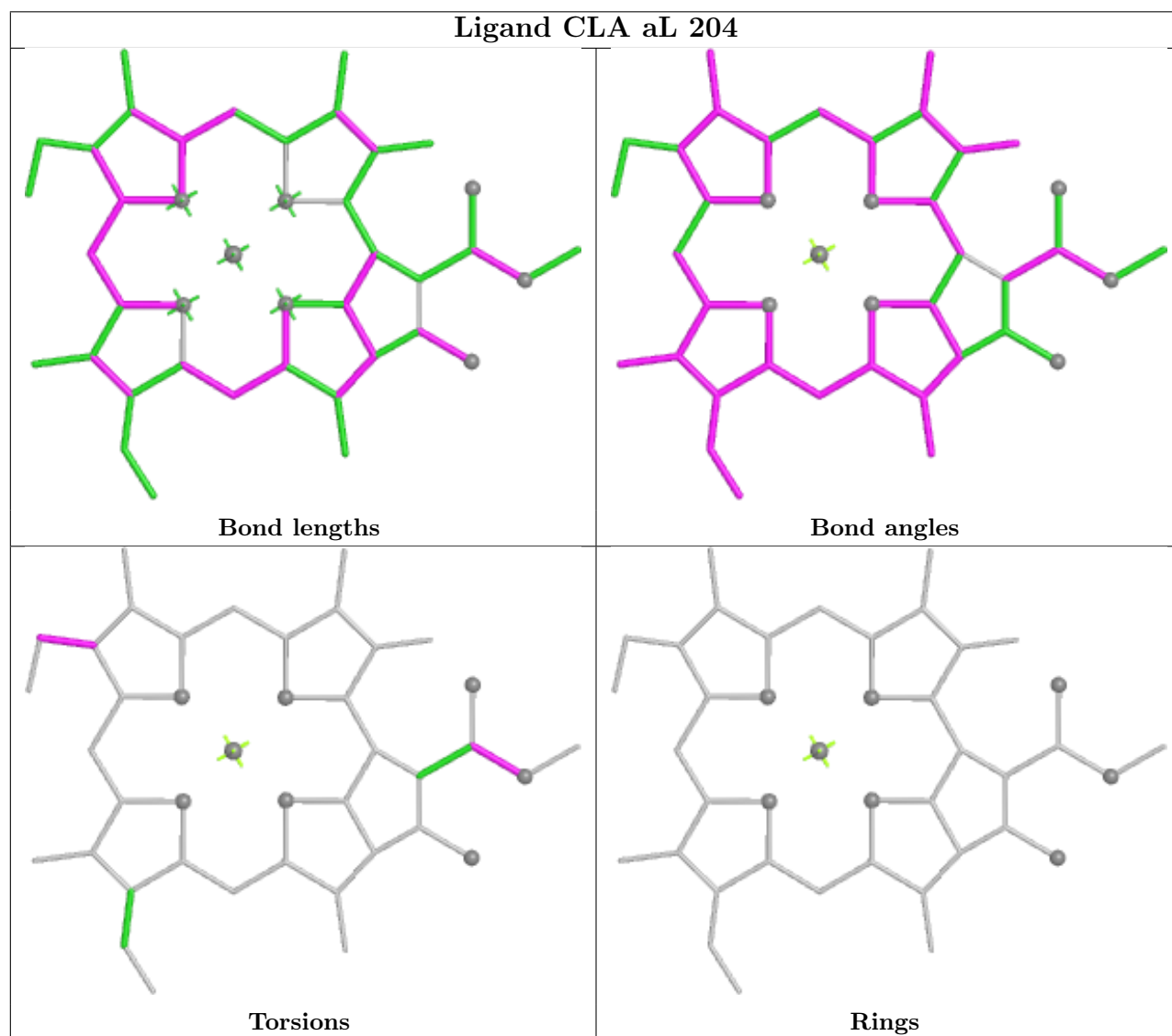
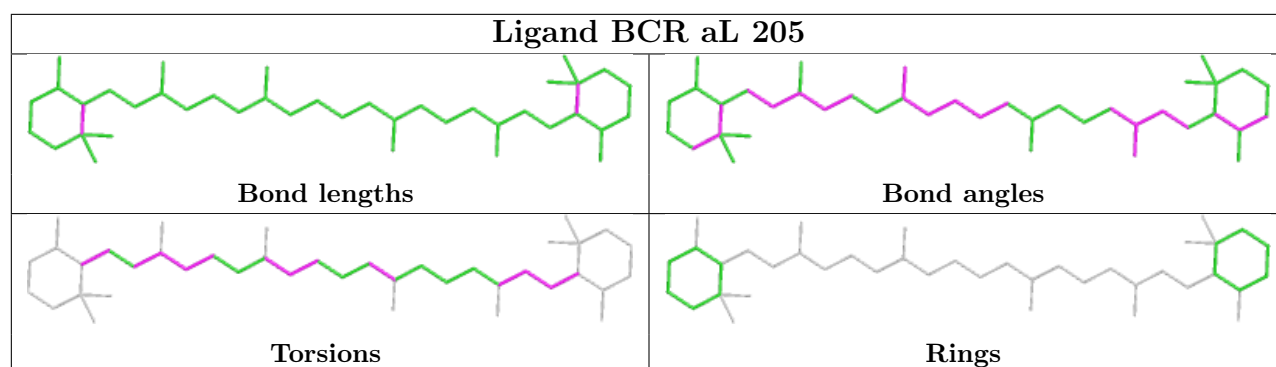


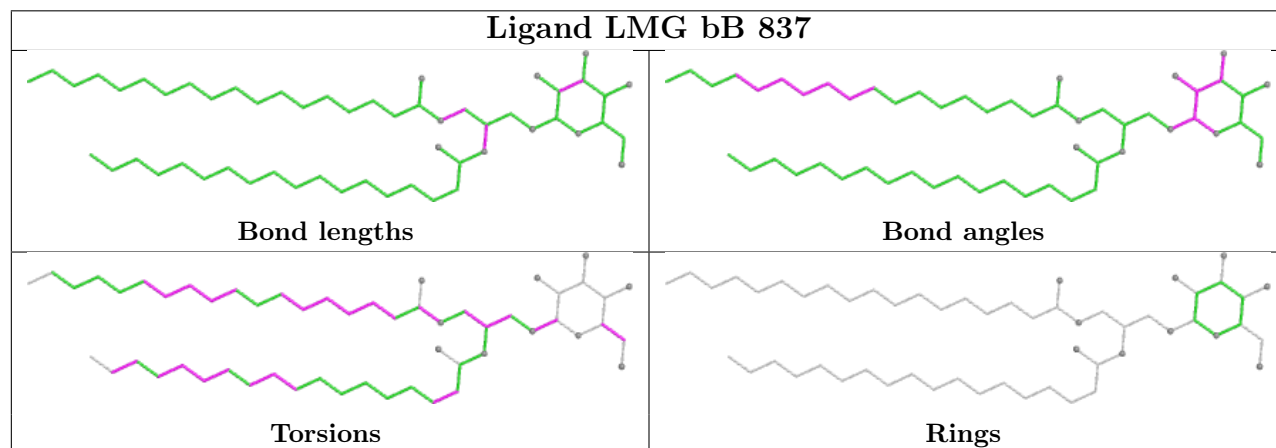
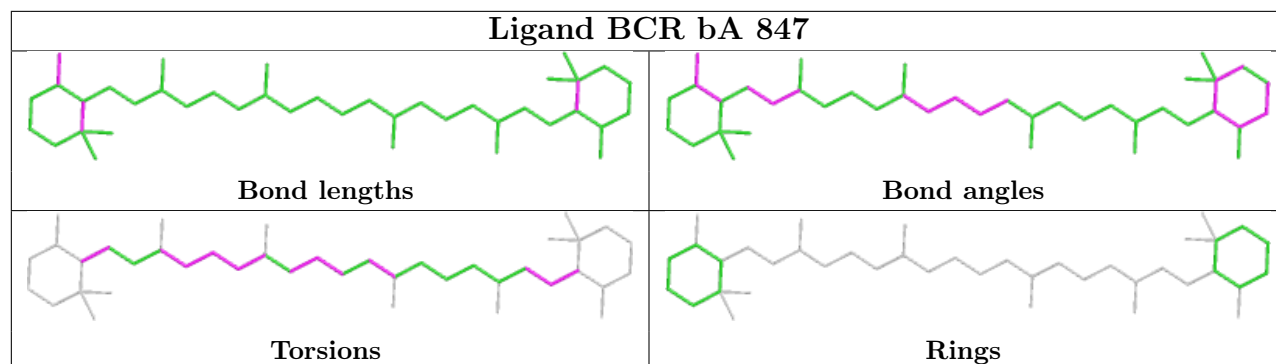
Ligand CLA dA 836

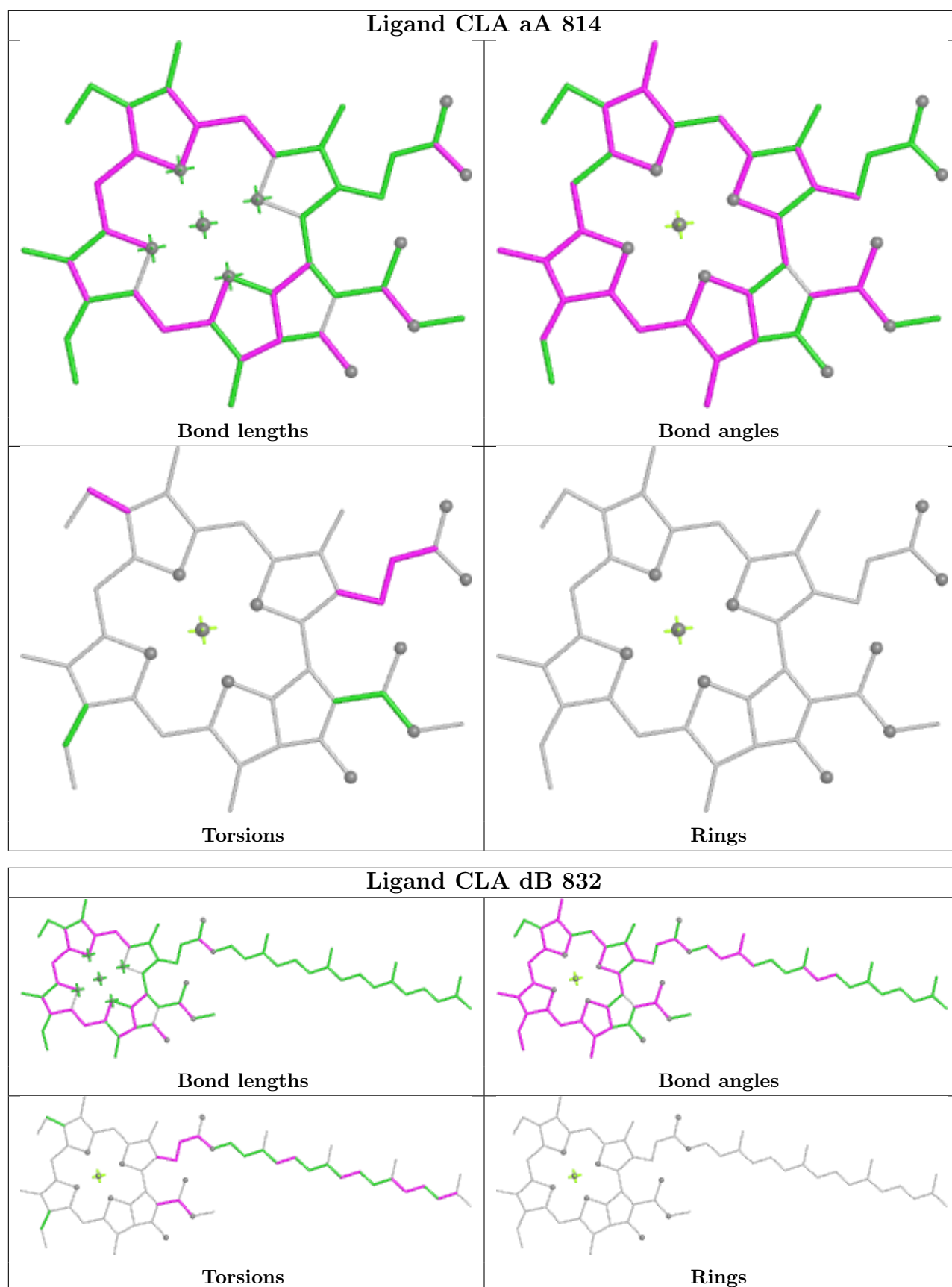


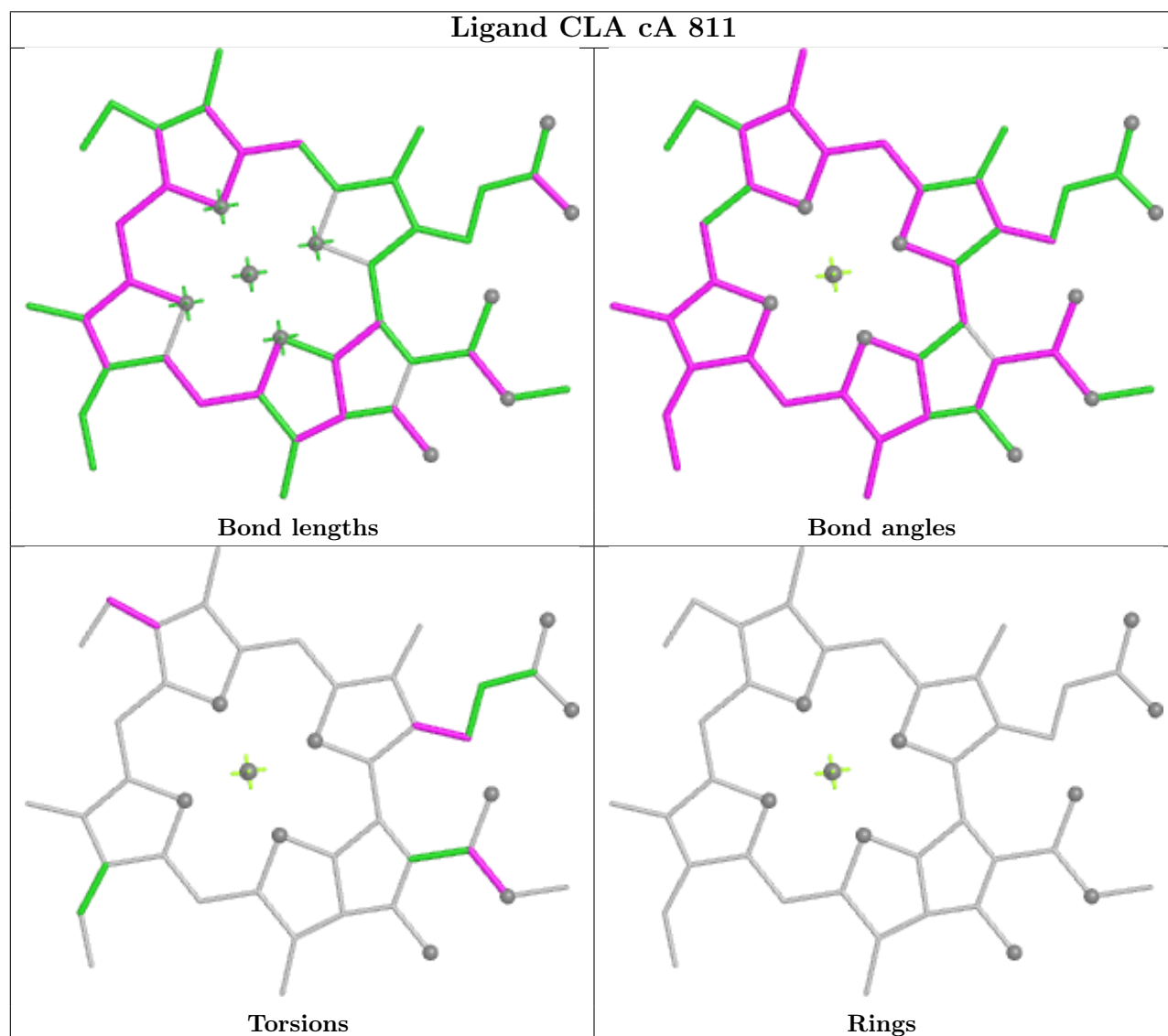
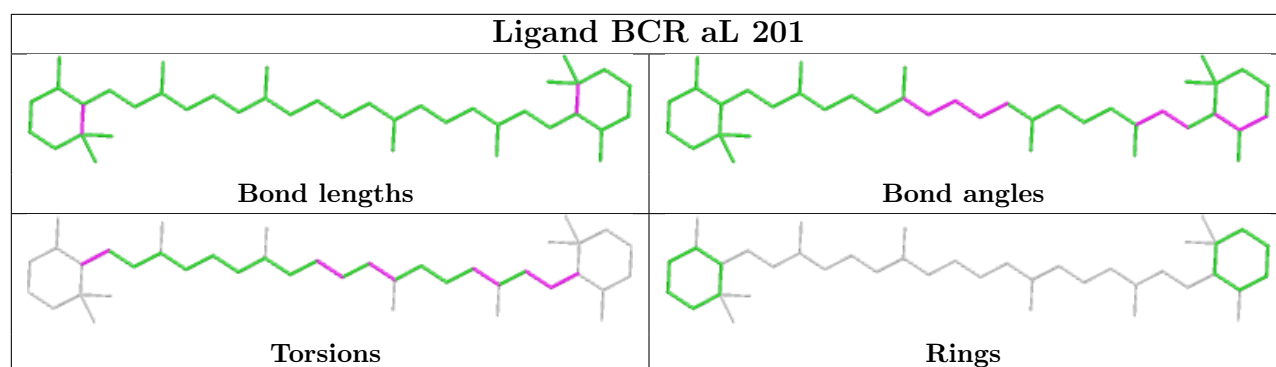


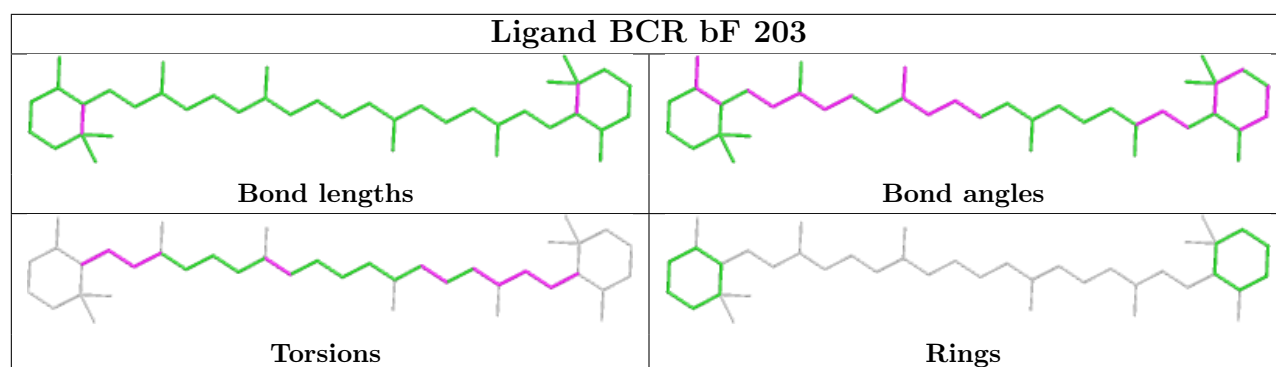
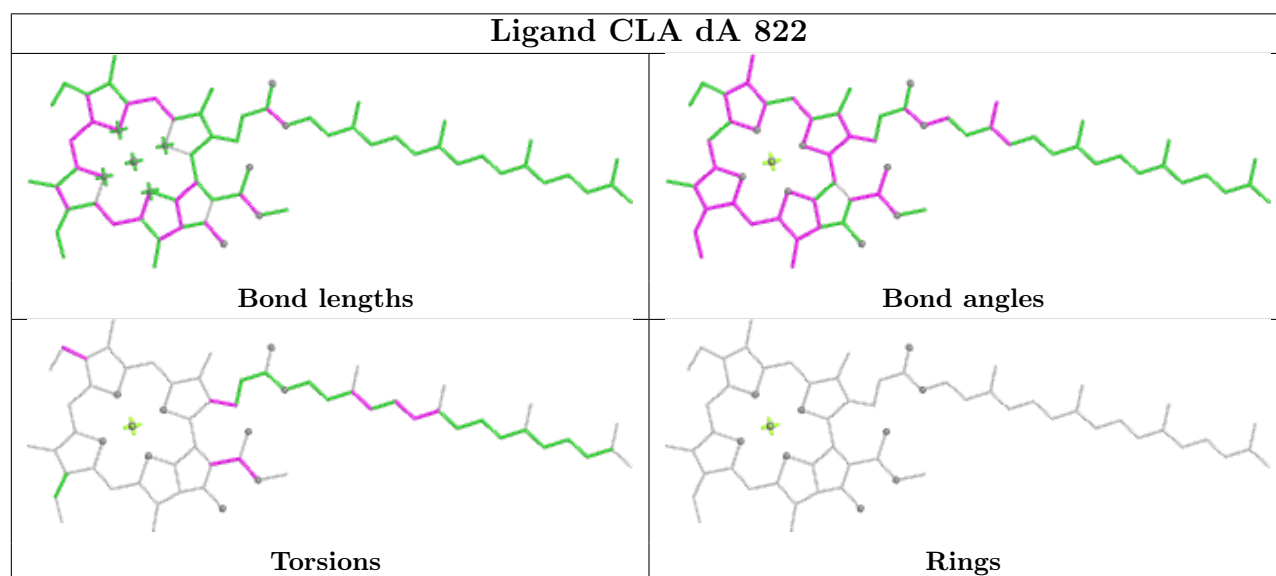
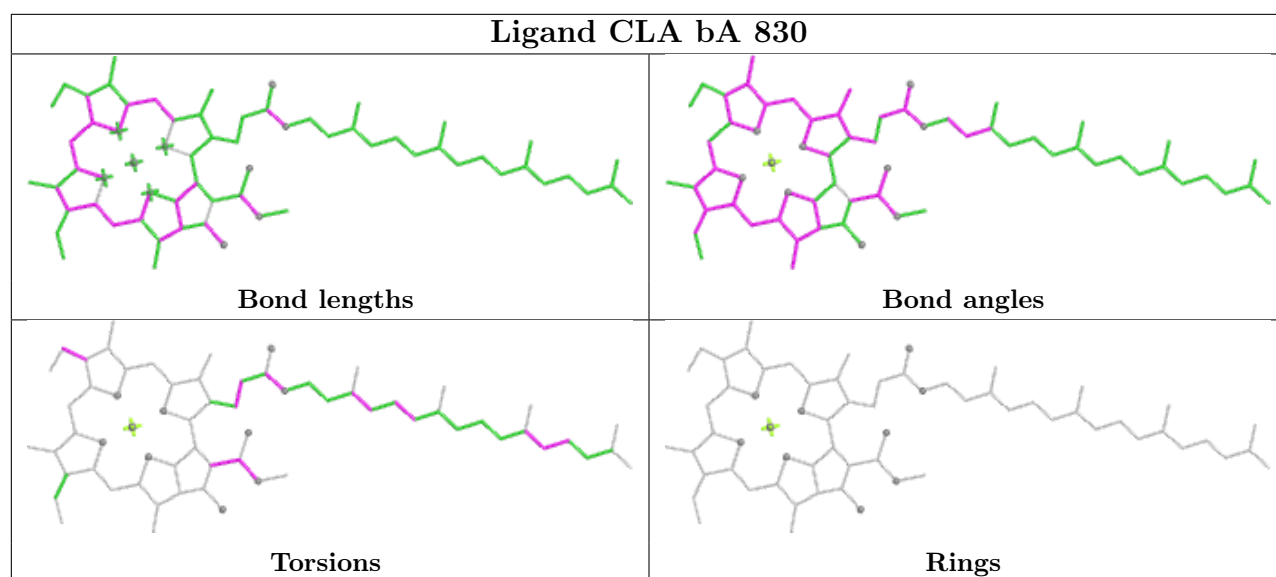


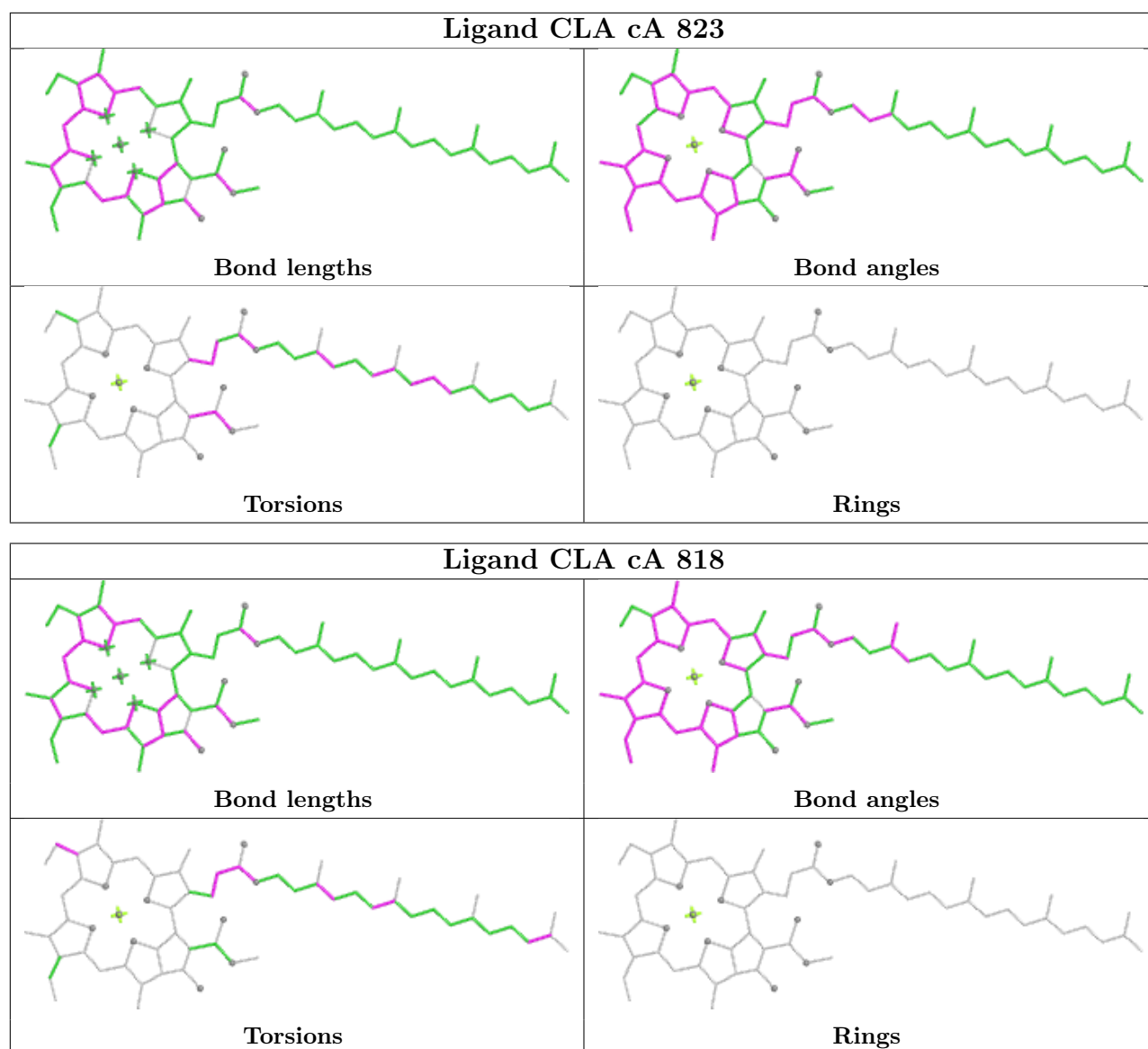


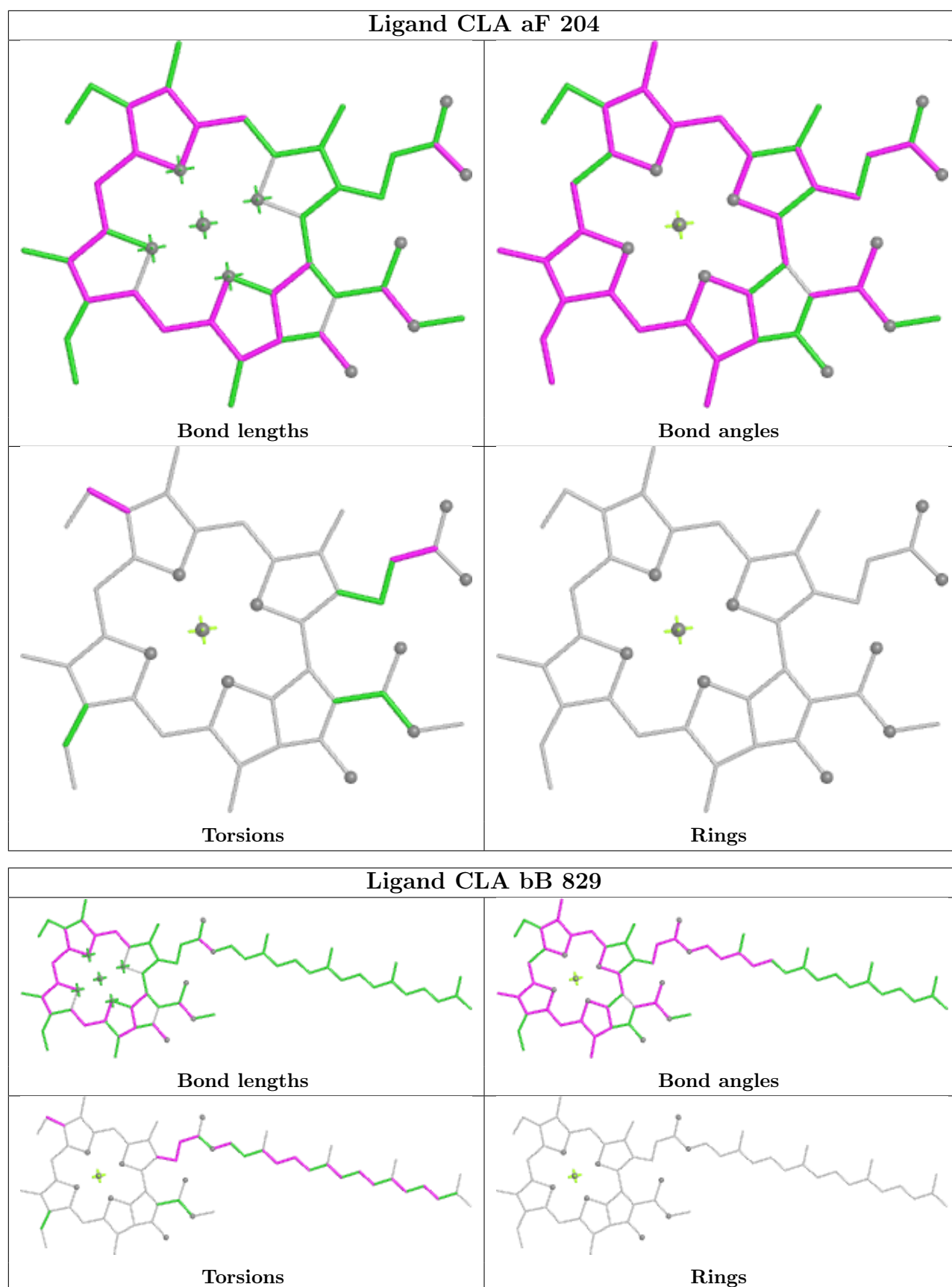


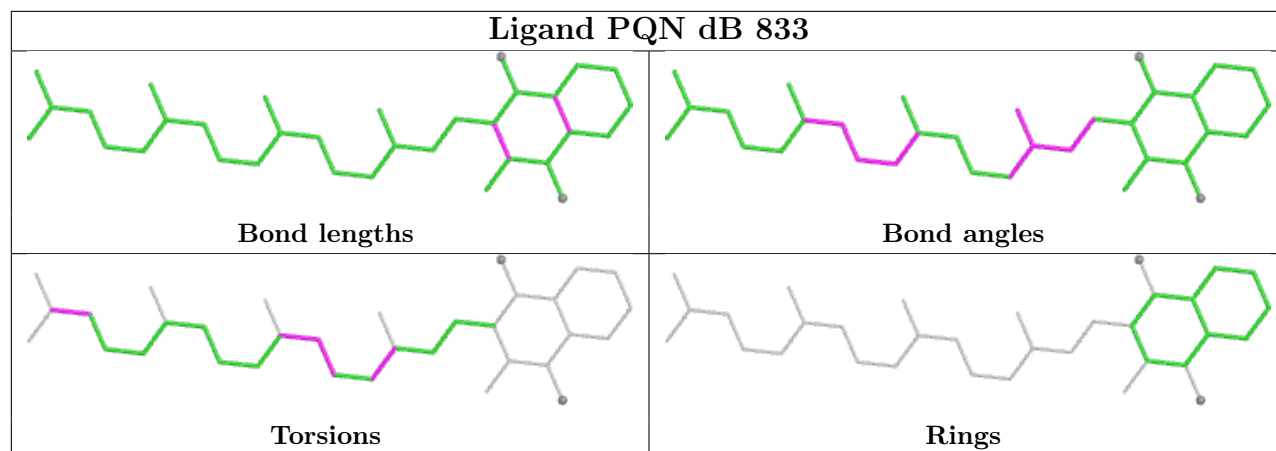
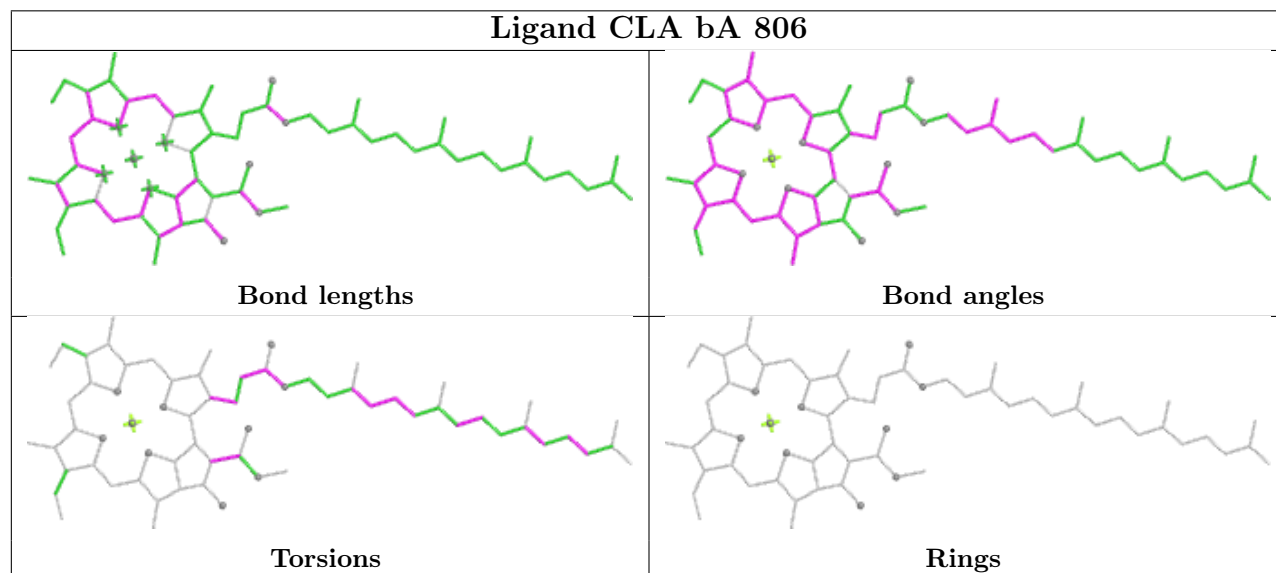
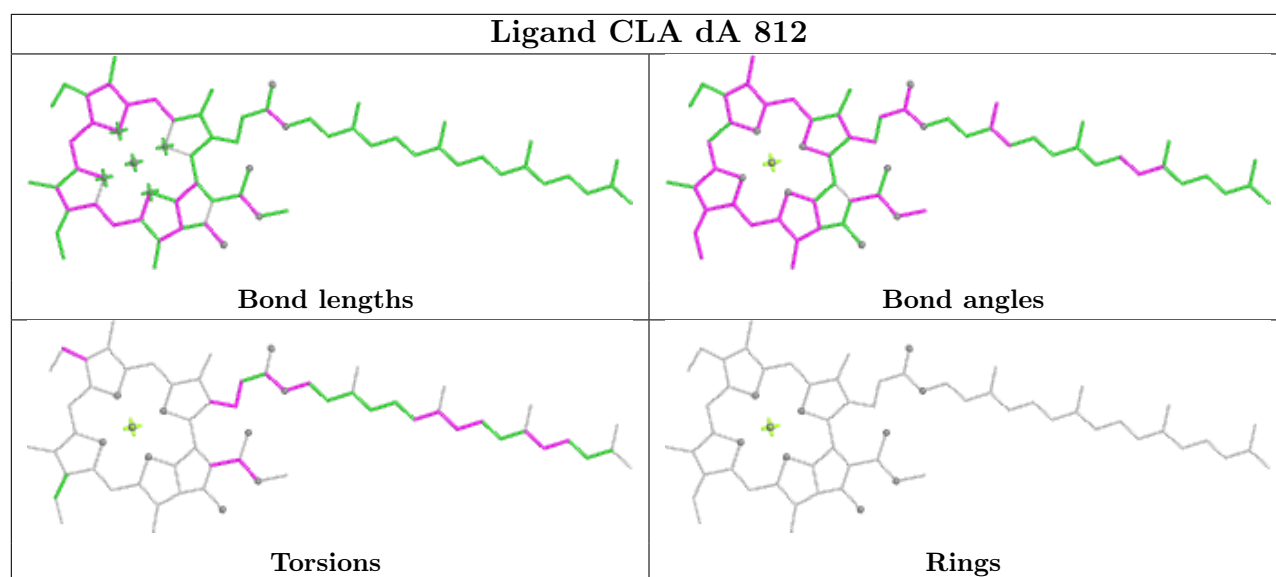




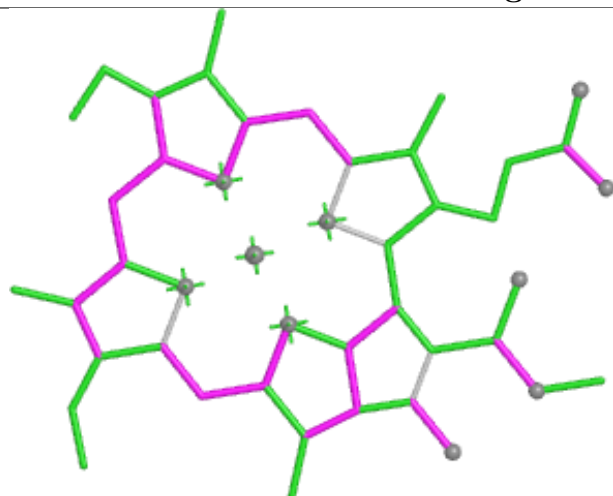




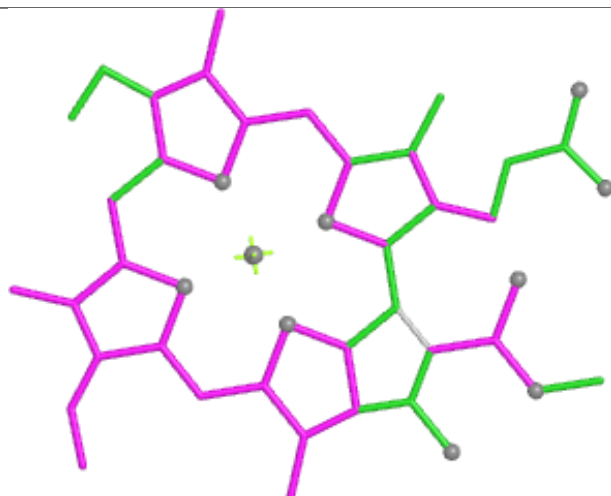




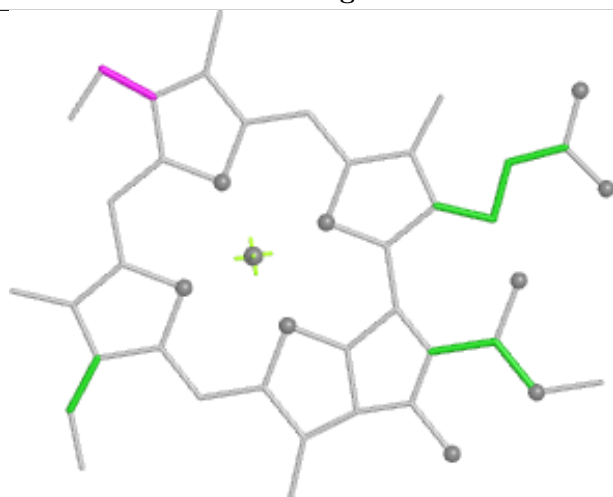
Ligand CLA aA 805



Bond lengths



Bond angles

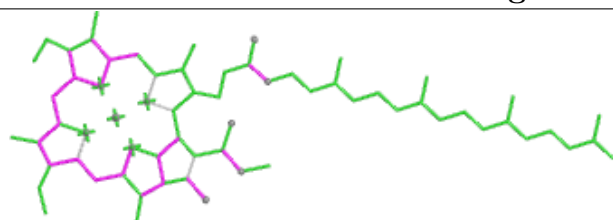


Torsions

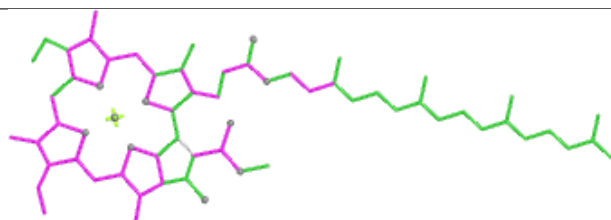


Rings

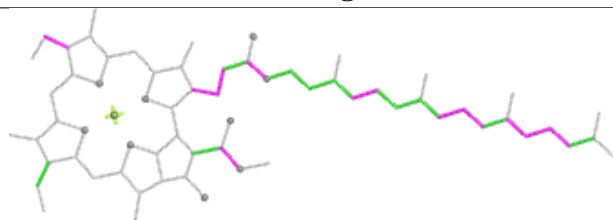
Ligand CLA cL 203



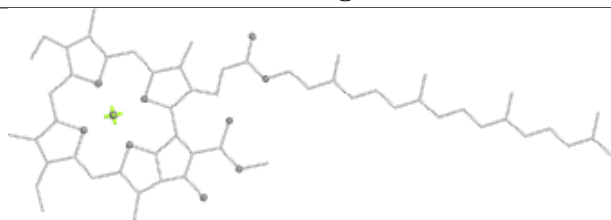
Bond lengths



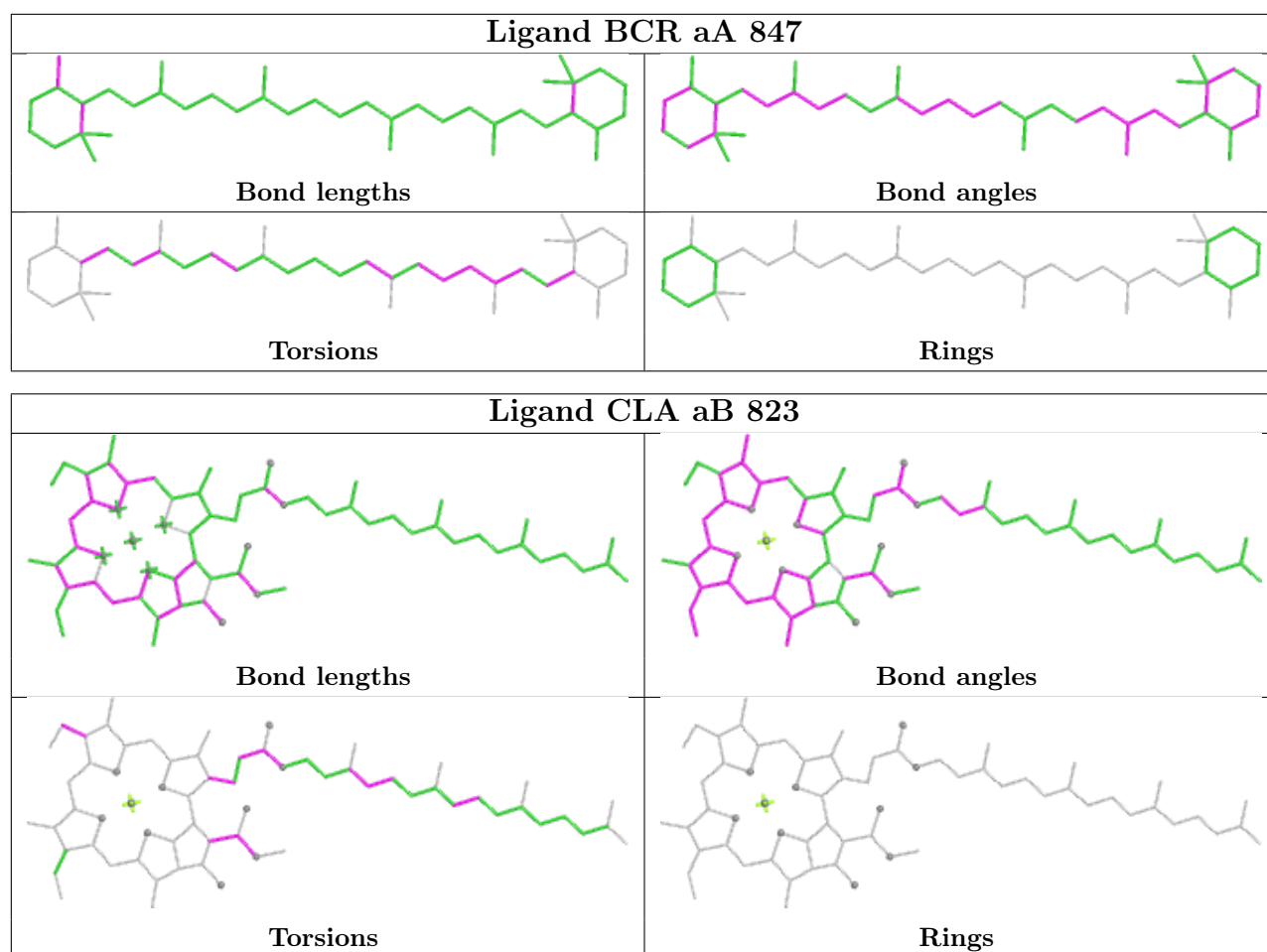
Bond angles



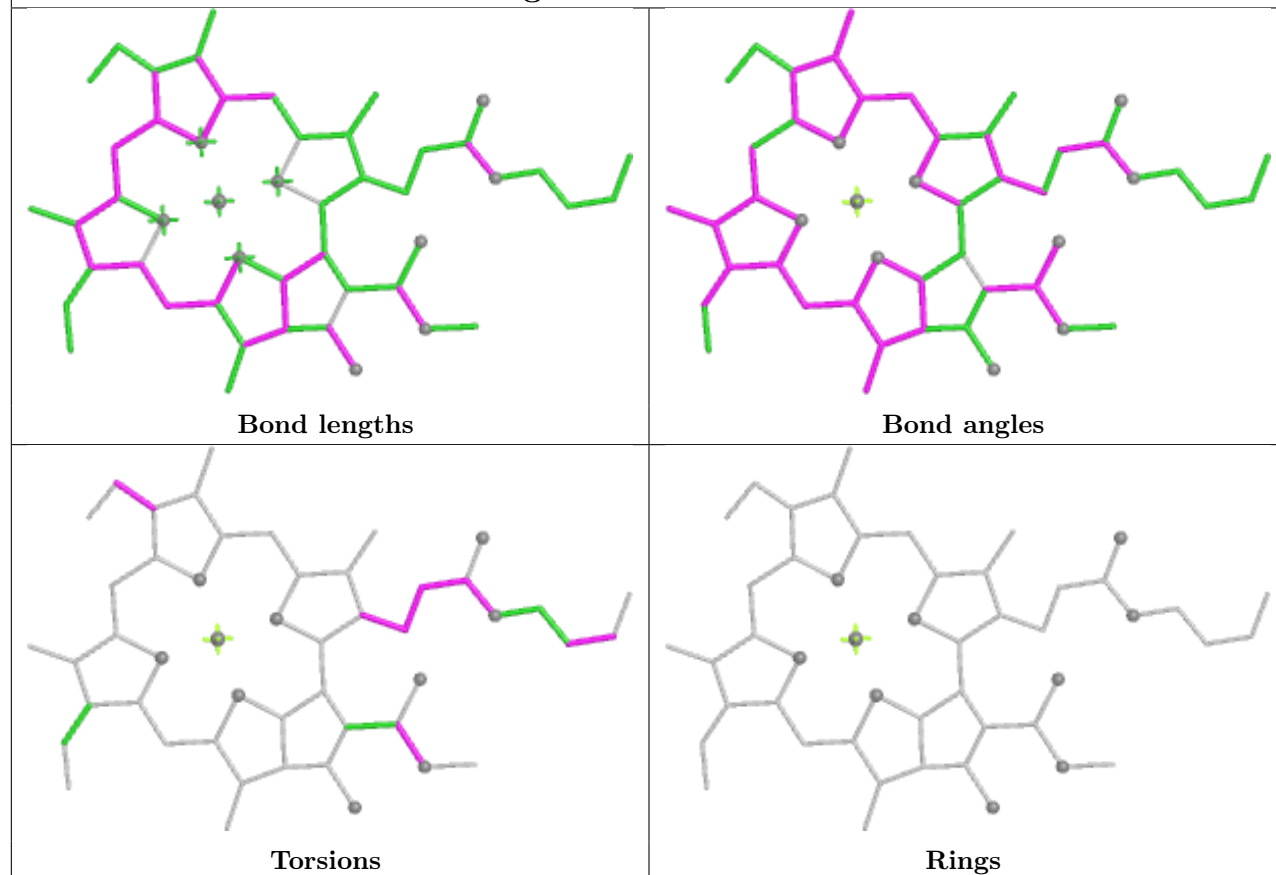
Torsions



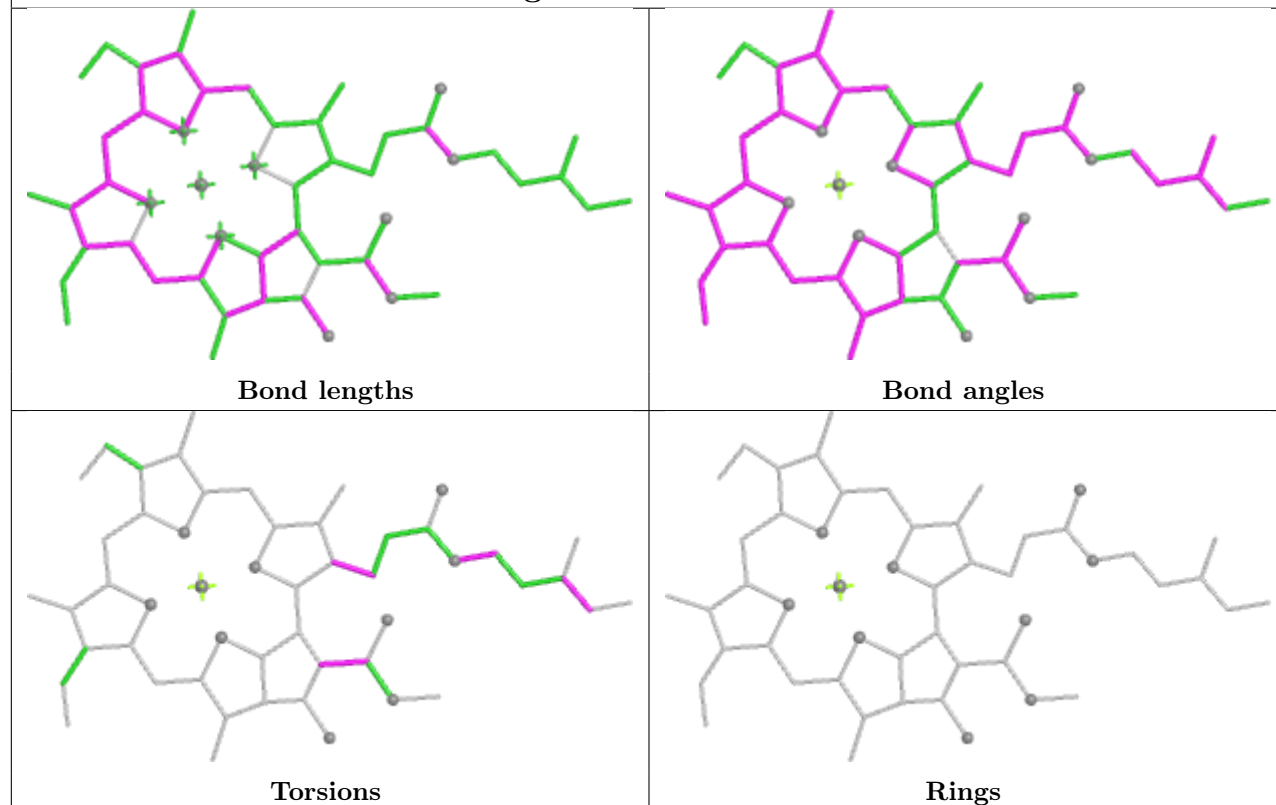
Rings

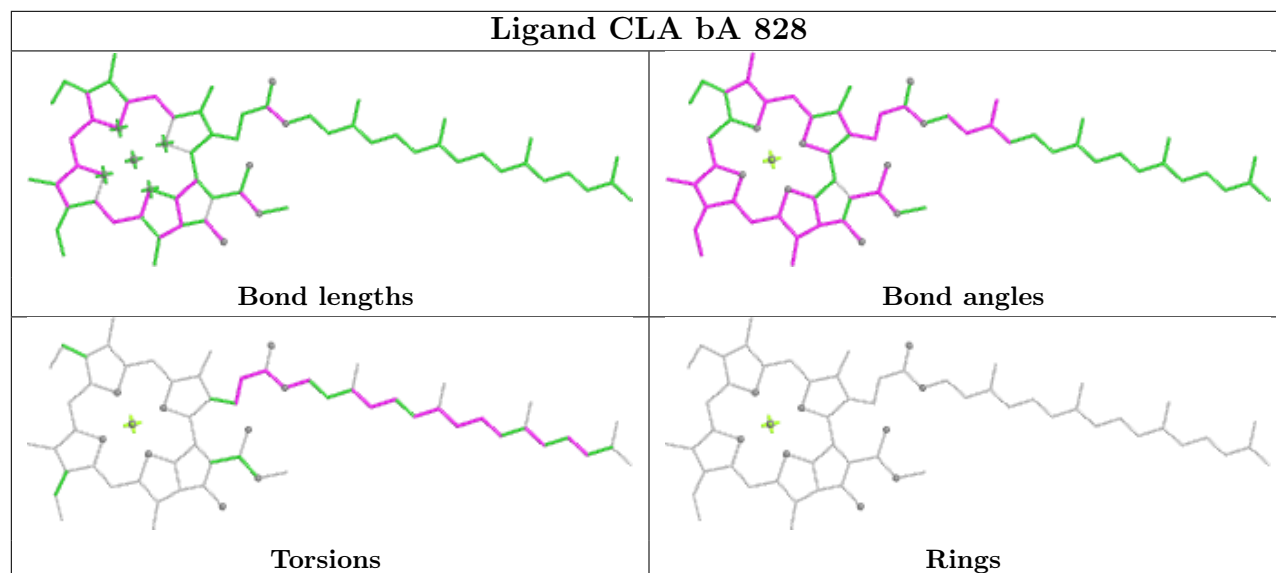
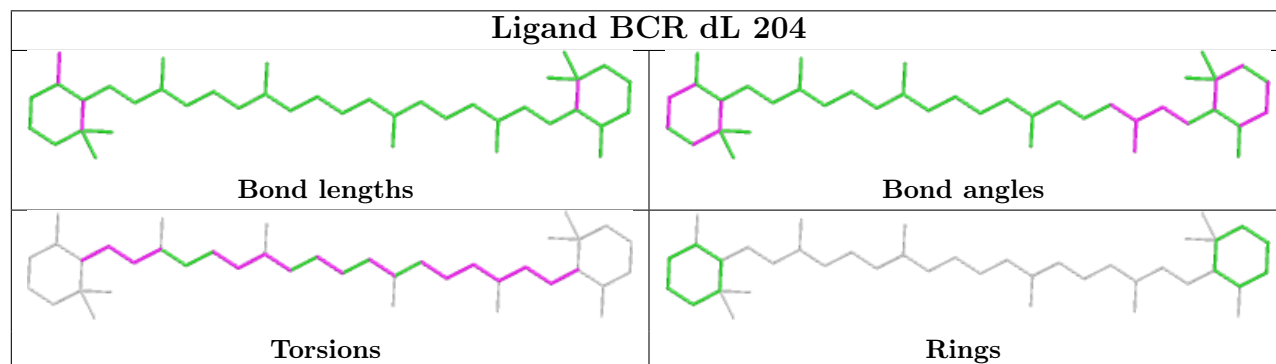
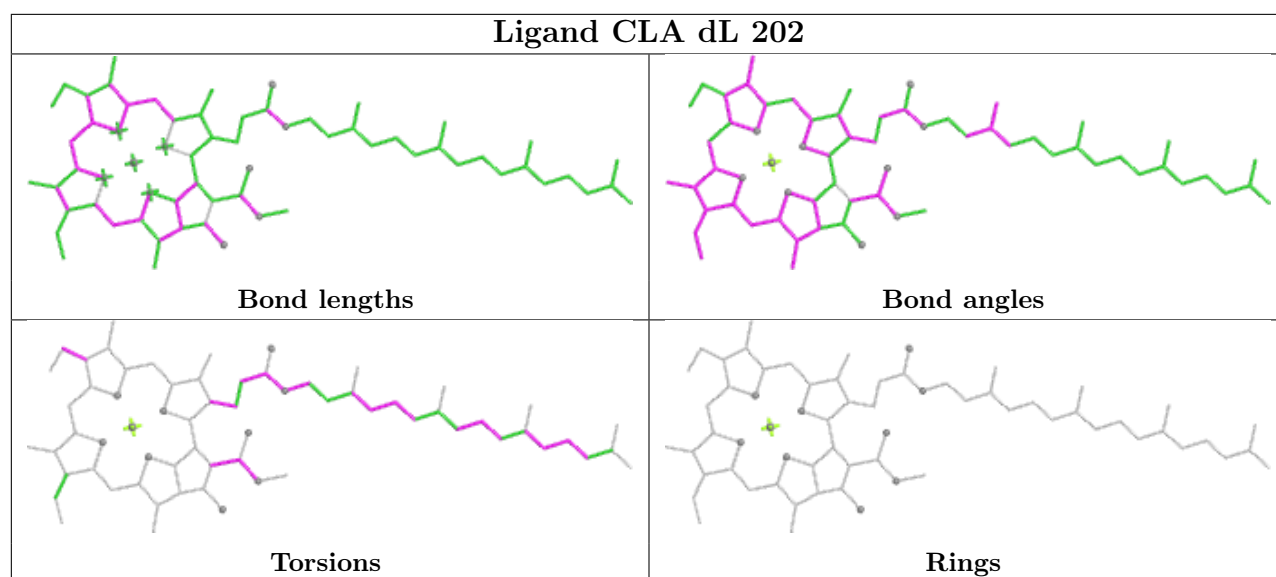


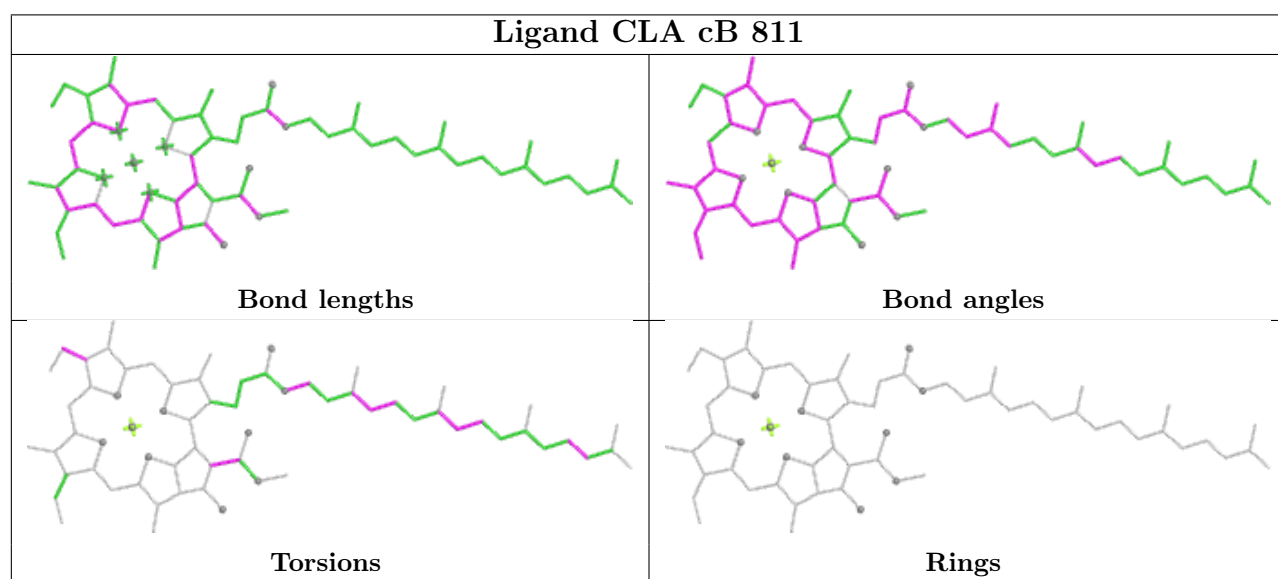
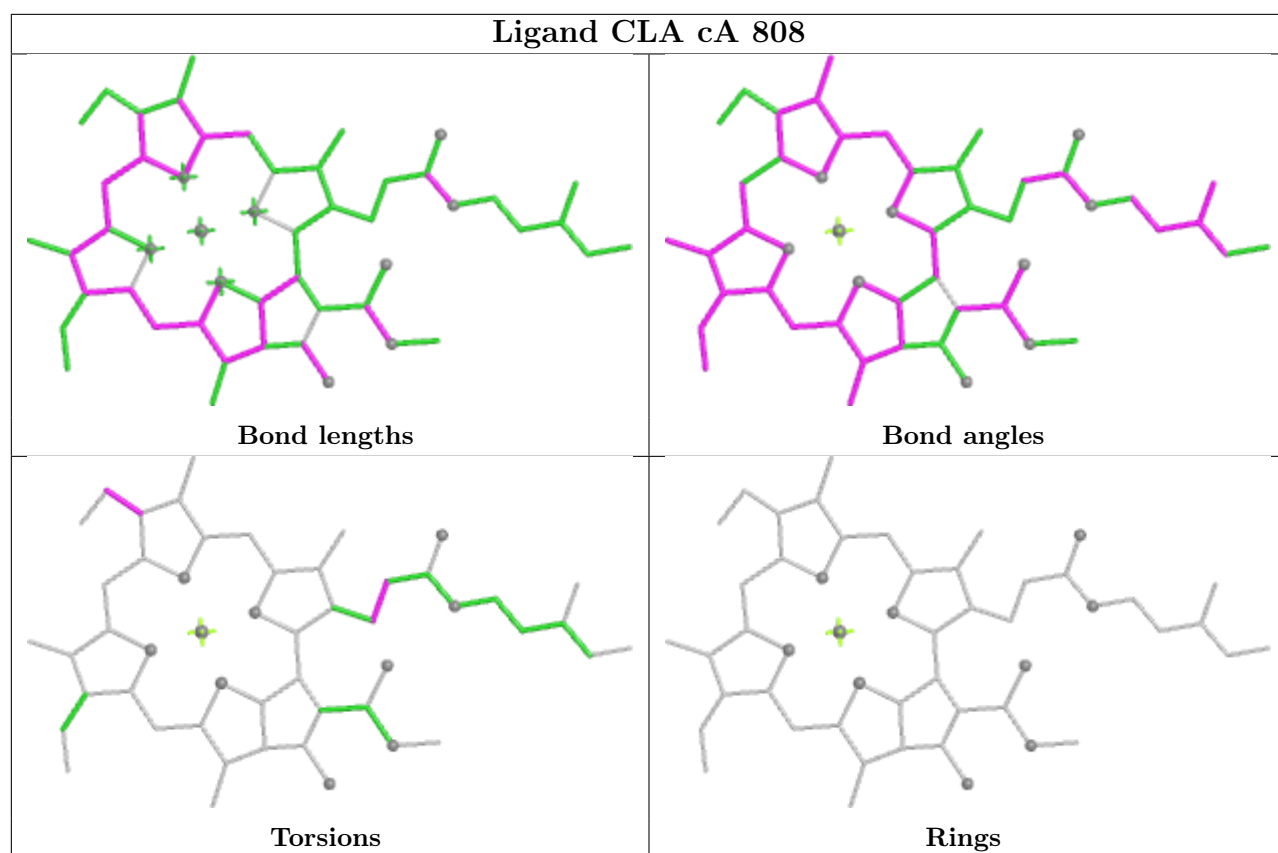
Ligand CLA aB 825



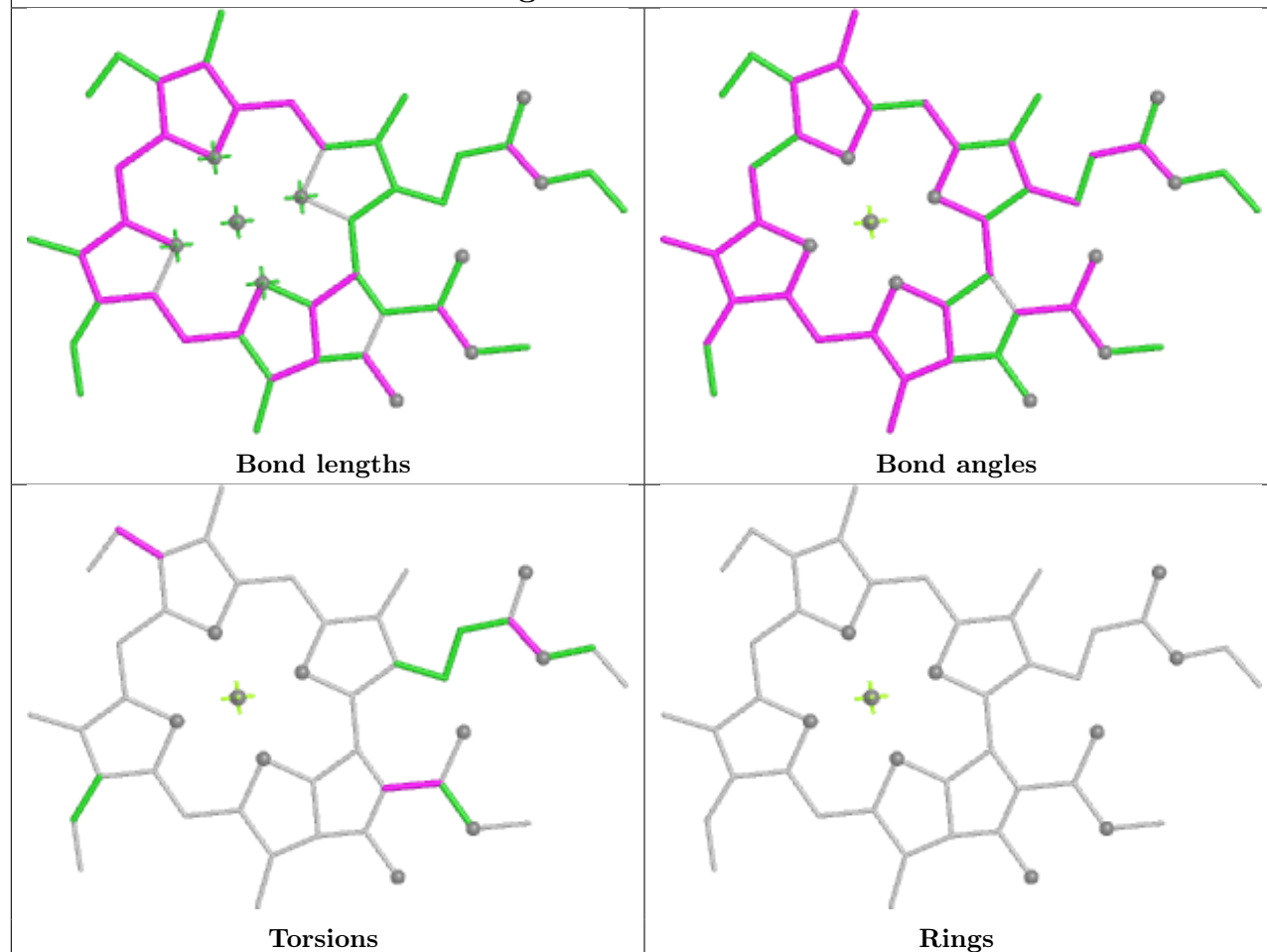
Ligand CLA bF 201



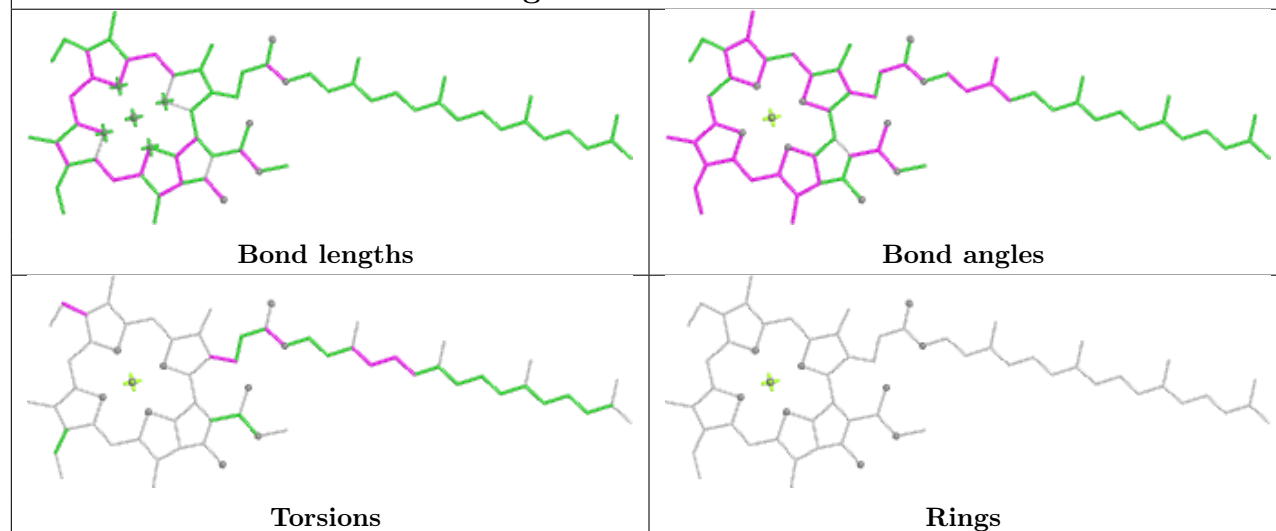


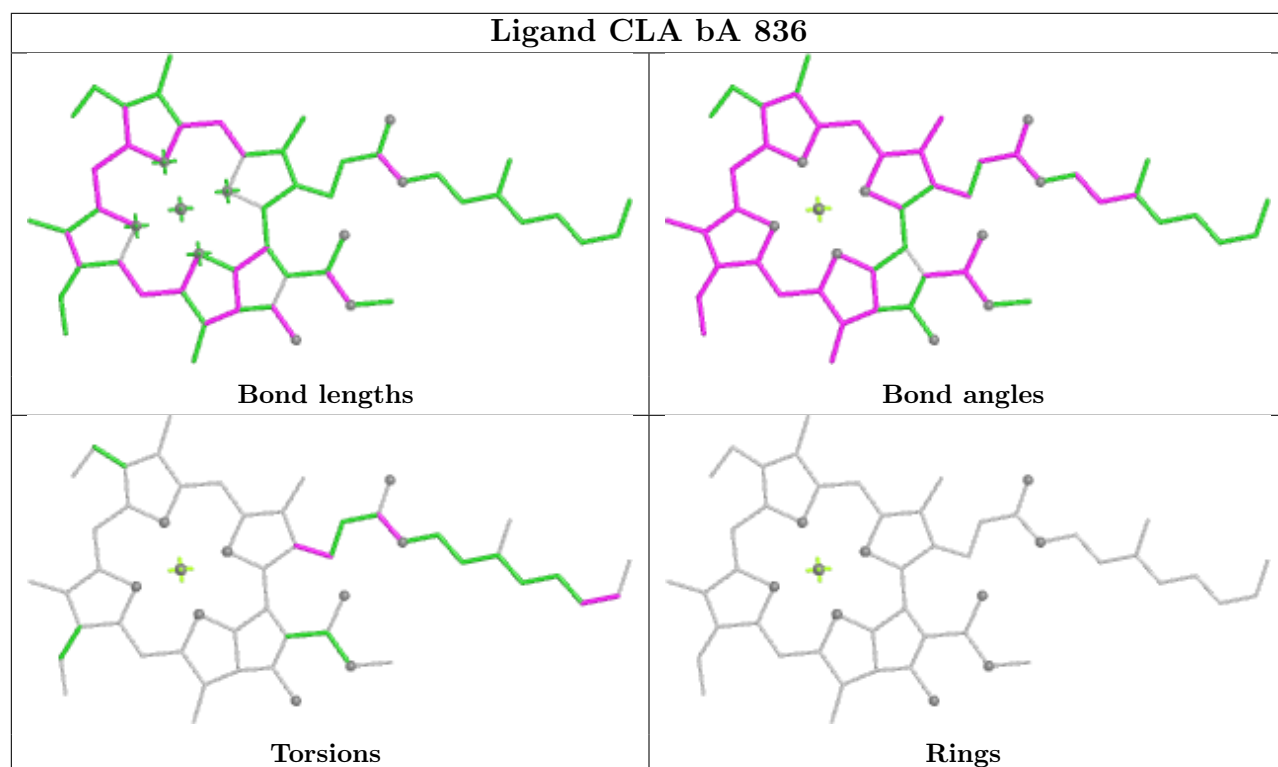
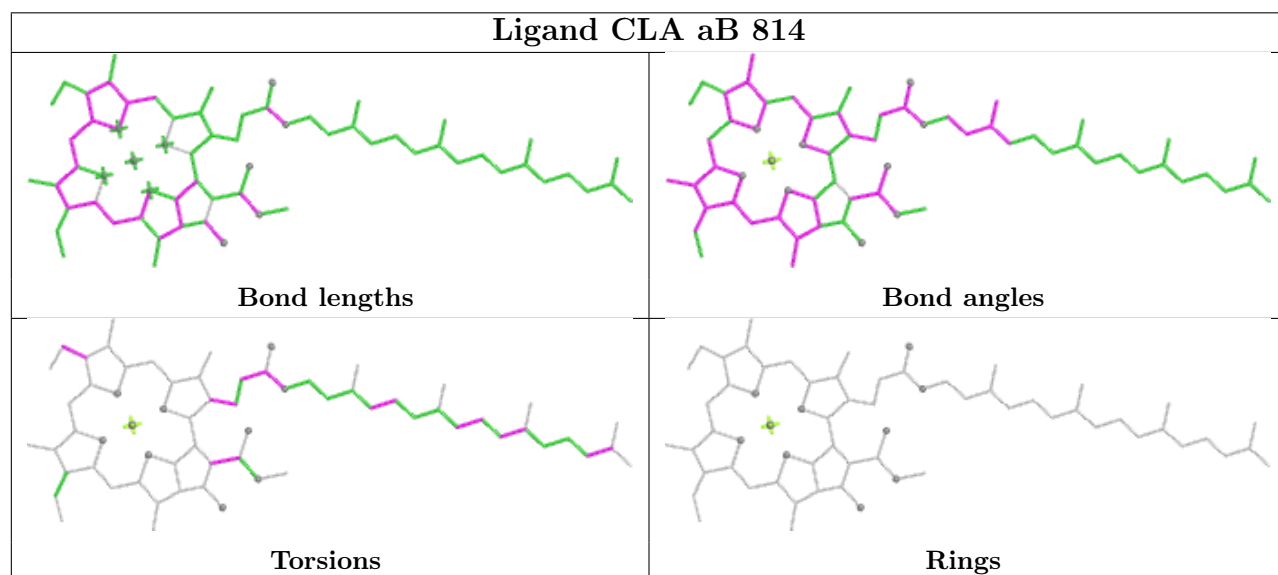
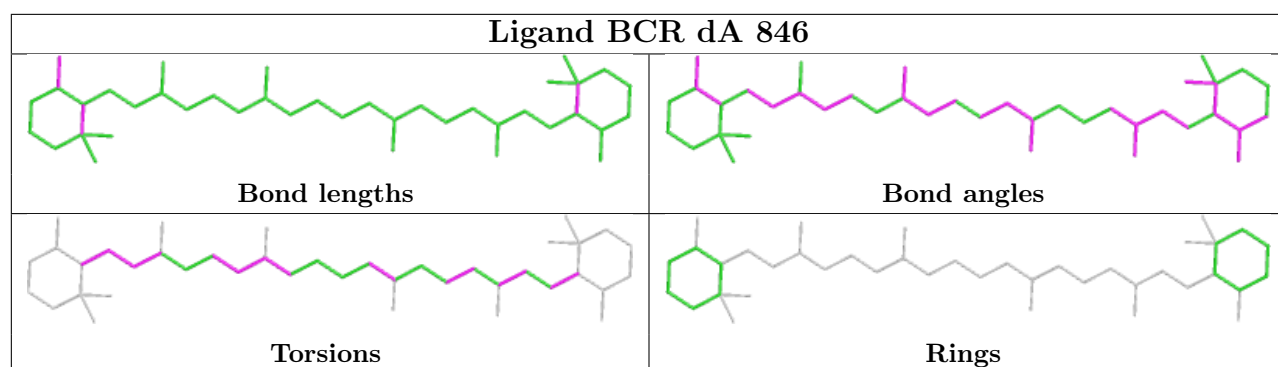


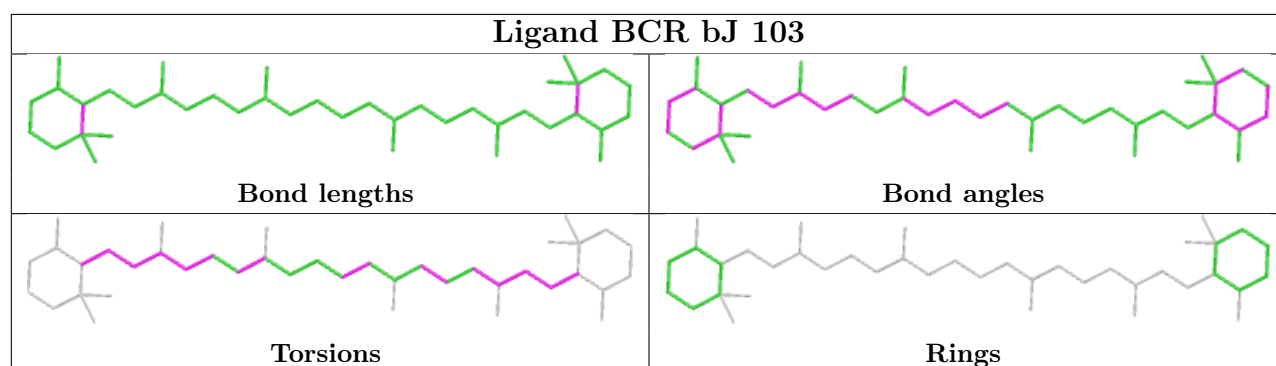
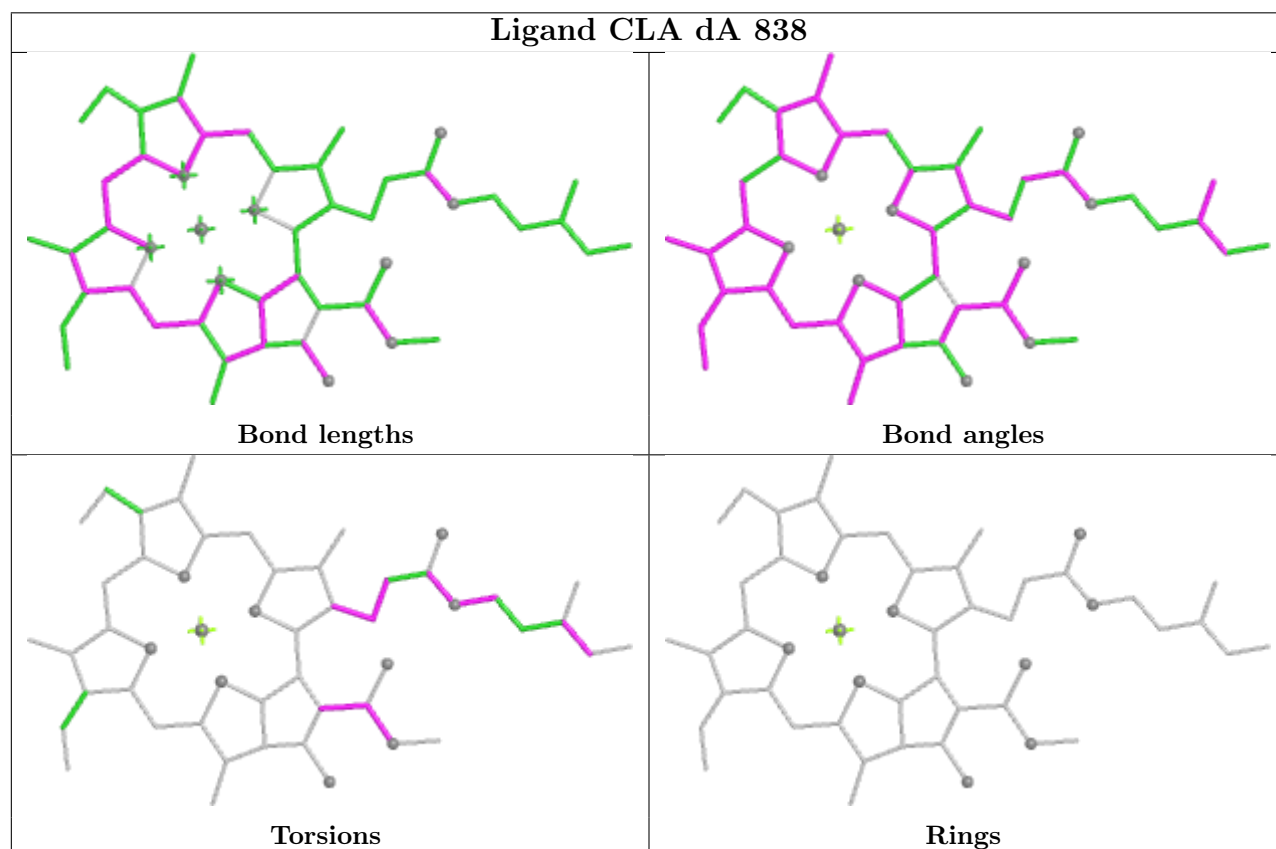
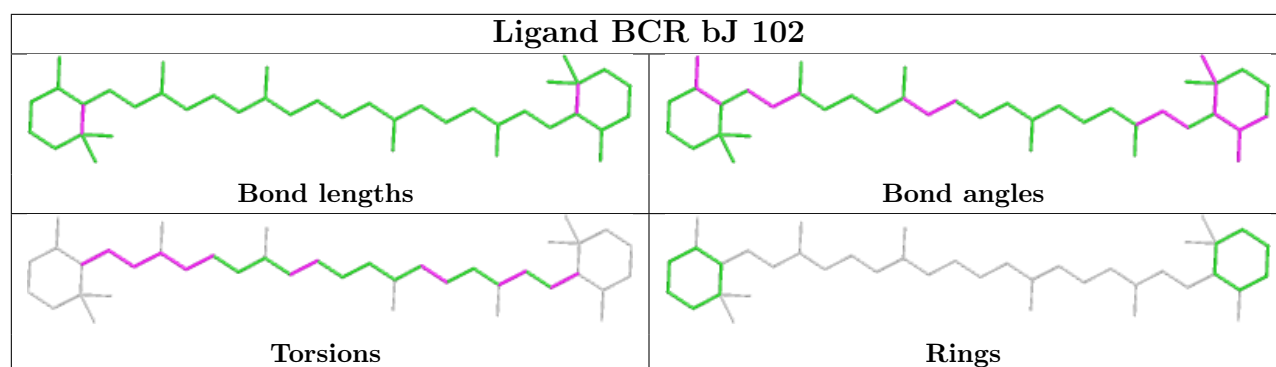
Ligand CLA bB 830



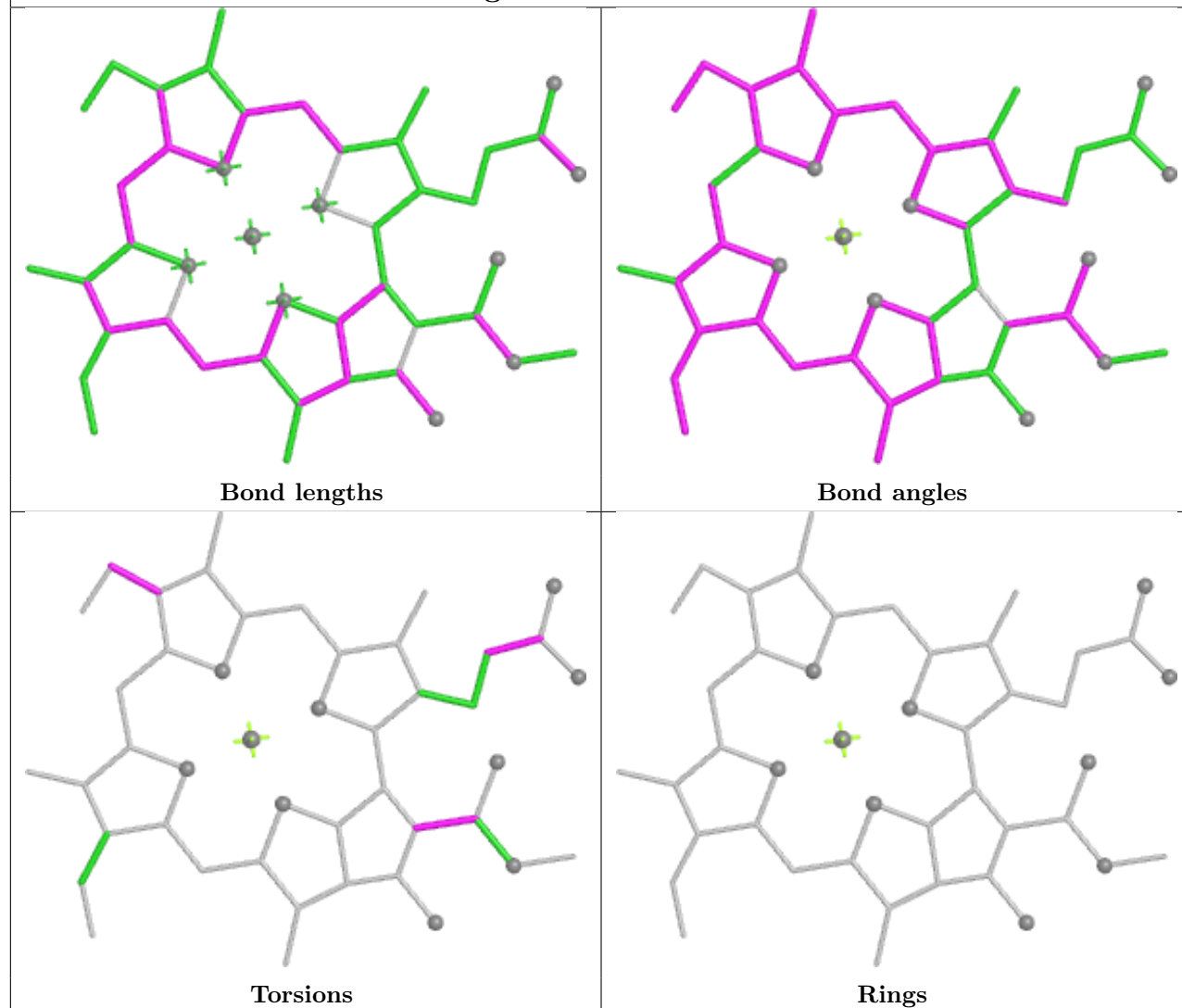
Ligand CLA aA 833



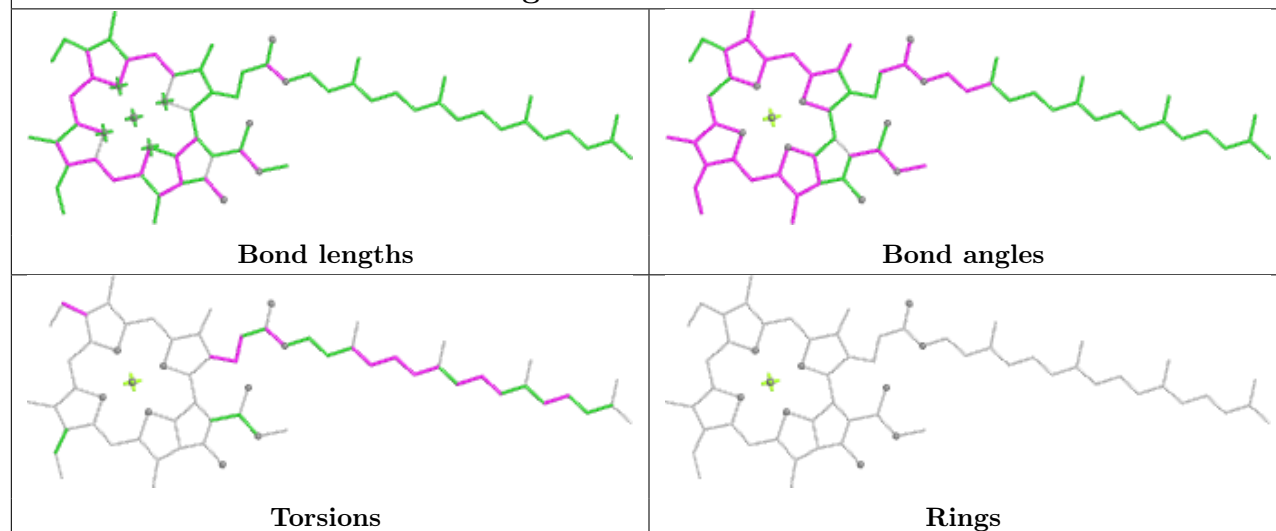


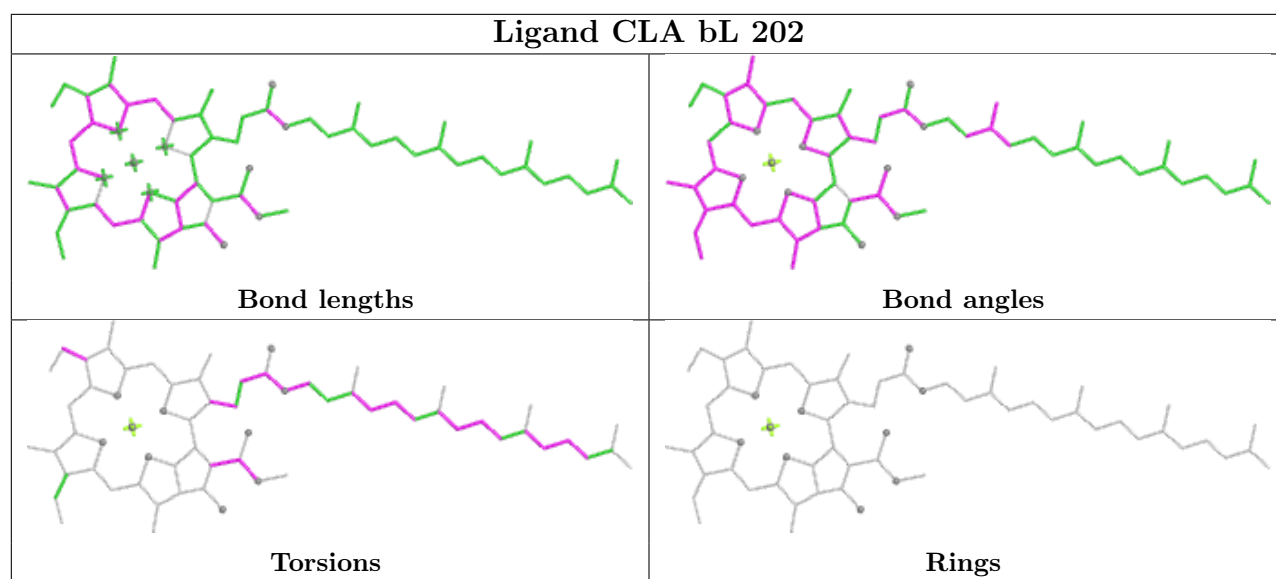


Ligand CLA aA 815



Ligand CLA bB 822





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

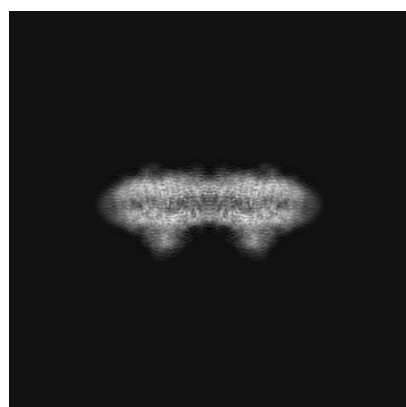
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-30823. These allow visual inspection of the internal detail of the map and identification of artifacts.

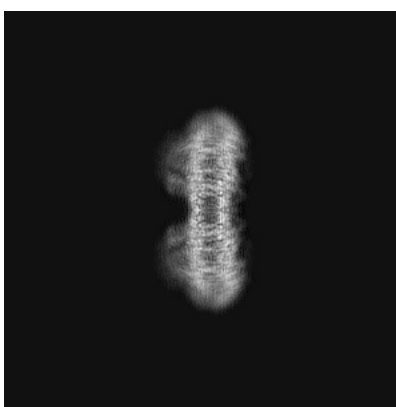
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

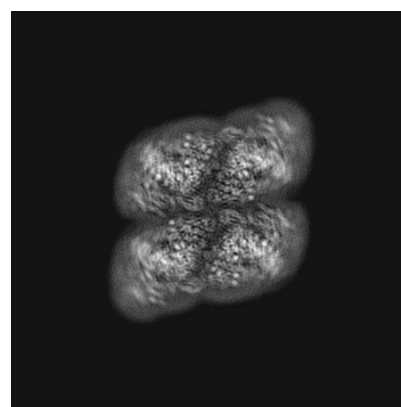
6.1.1 Primary map



X



Y

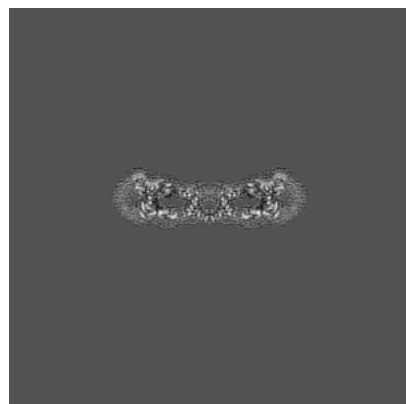


Z

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

6.2 Central slices [i](#)

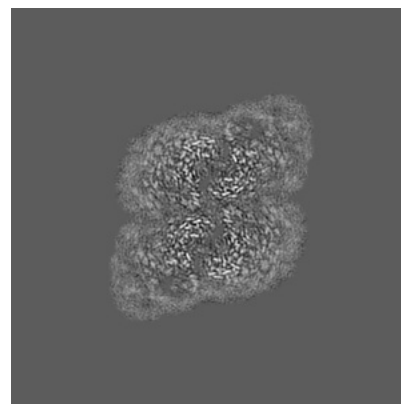
6.2.1 Primary map



X Index: 206



Y Index: 206



Z Index: 206

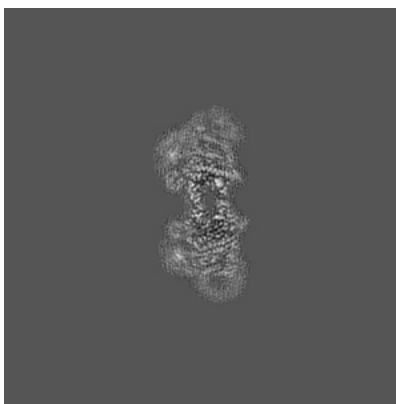
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

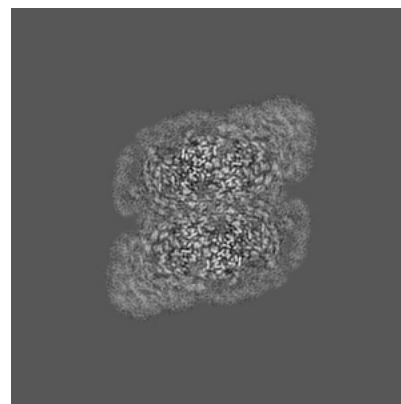
6.3.1 Primary map



X Index: 229



Y Index: 252

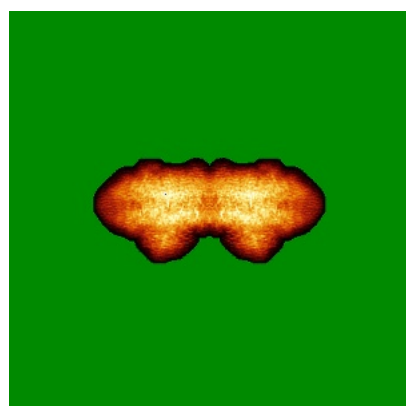


Z Index: 223

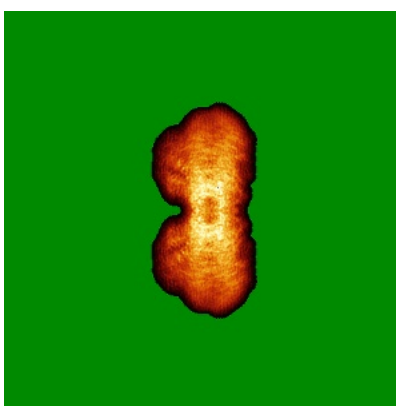
The images above show the largest variance slices of the map in three orthogonal directions.

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

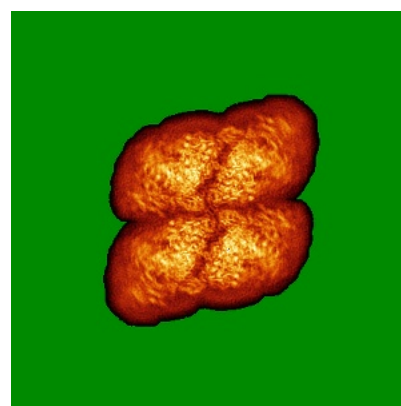
6.4.1 Primary map



X



Y

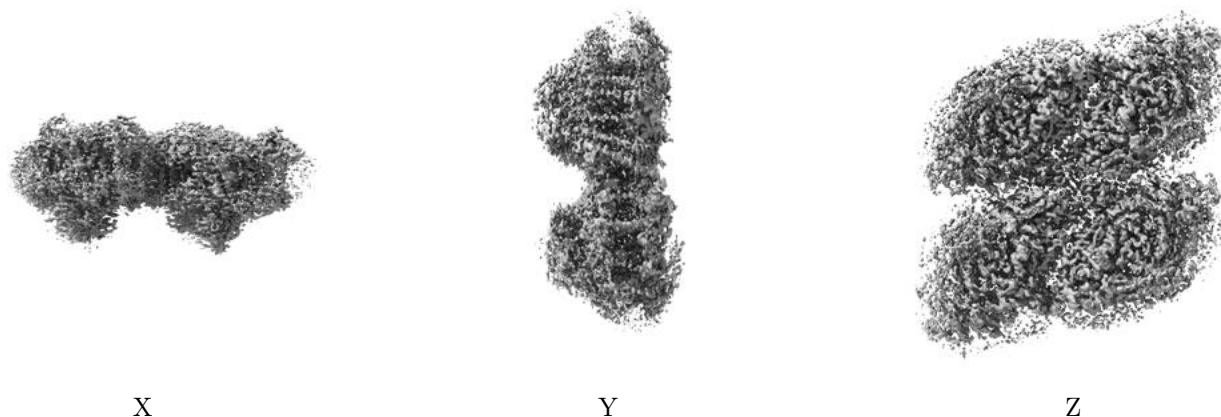


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

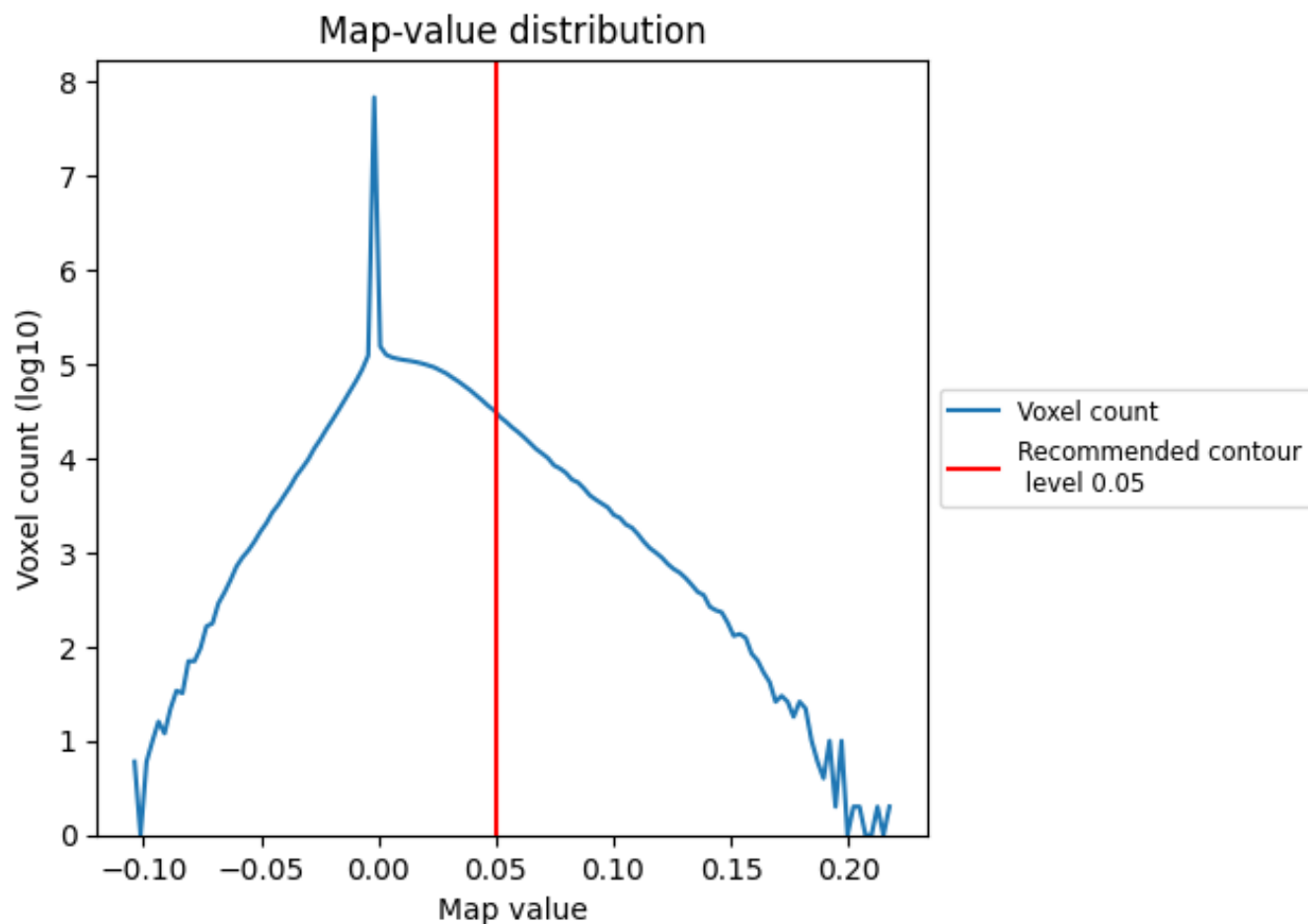
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

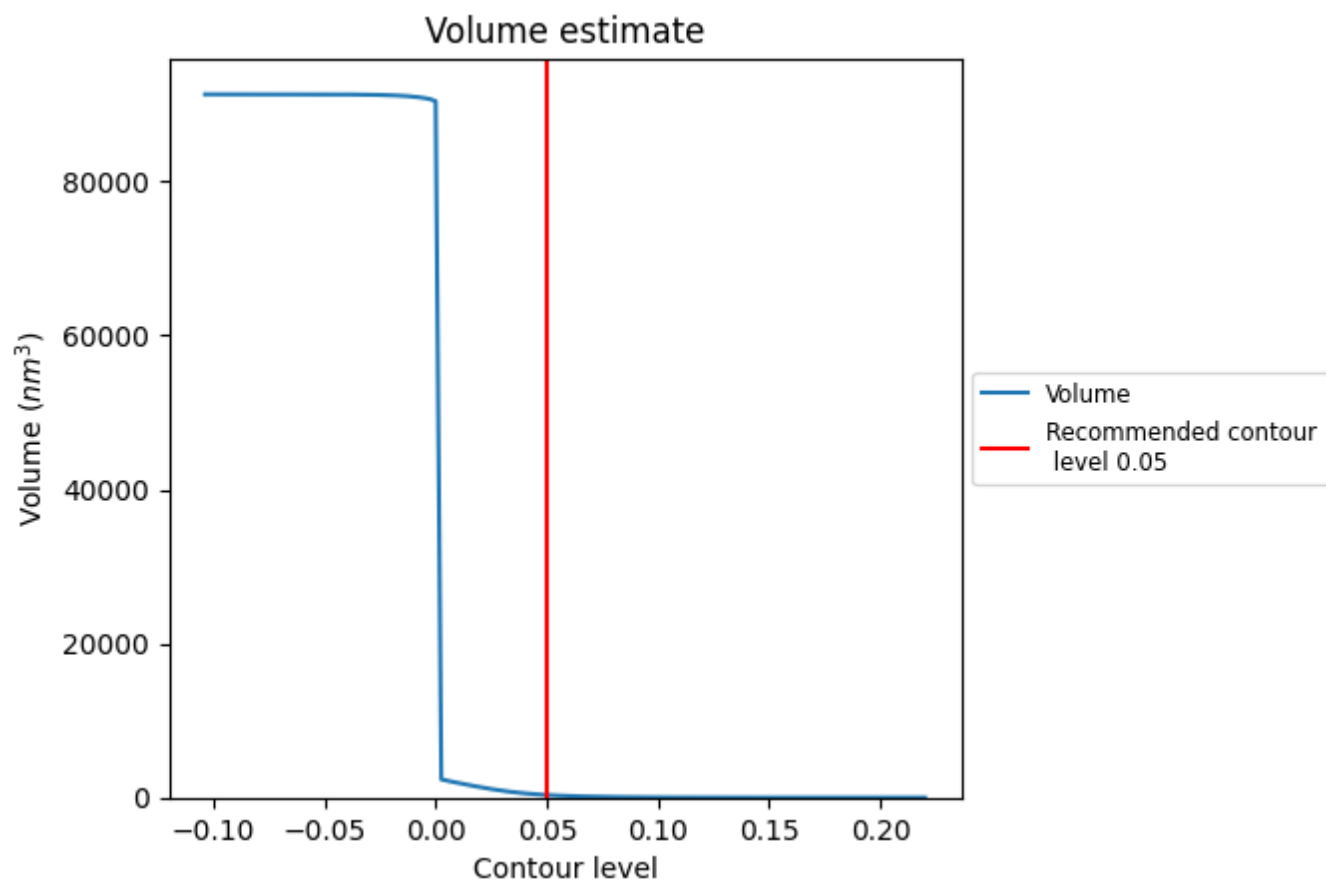
This section contains the results of statistical analysis of the map.

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.

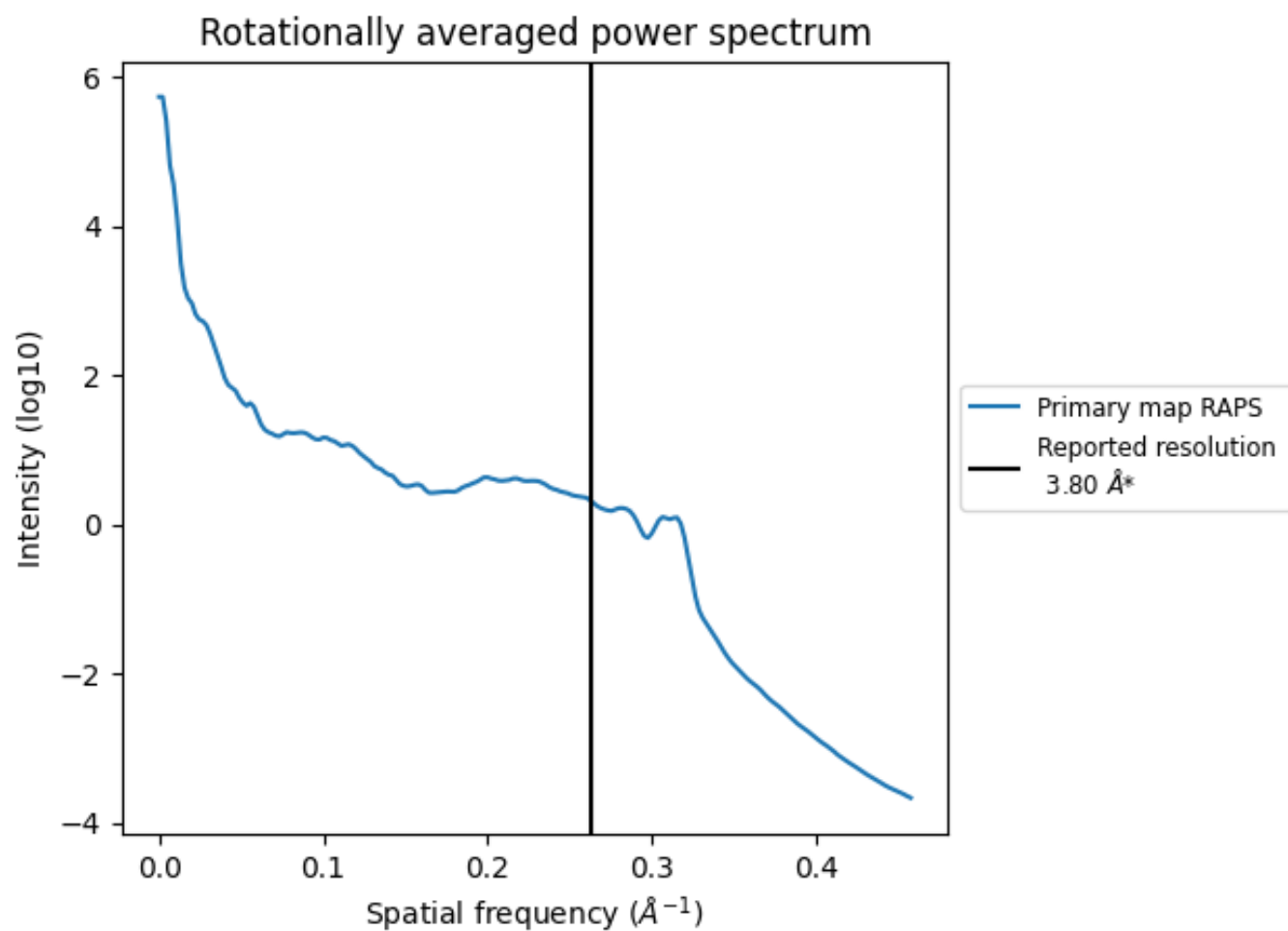
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 330 nm^3 ; this corresponds to an approximate mass of 298 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 ⓘ

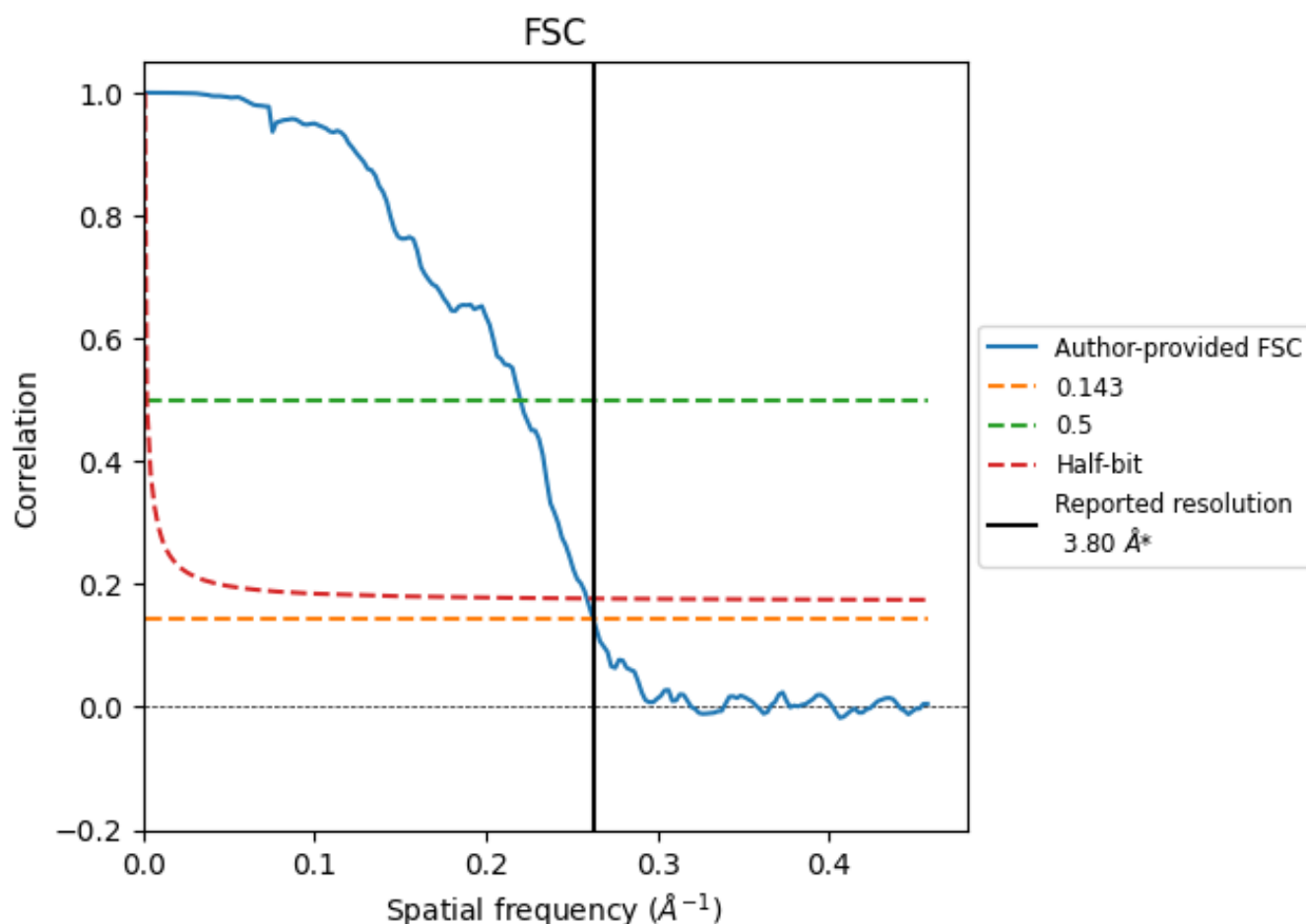


*Reported resolution corresponds to spatial frequency of 0.263 Å⁻¹

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

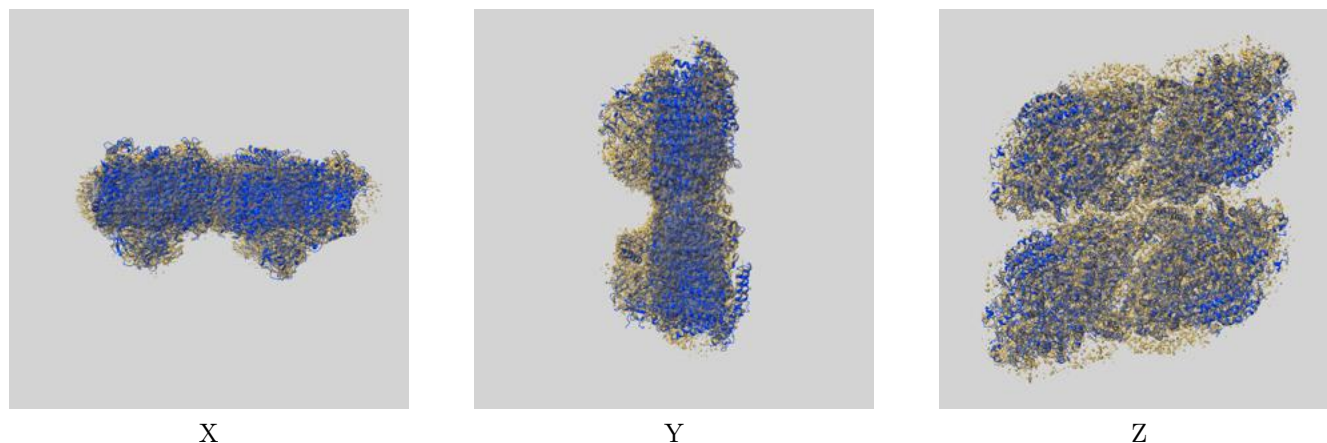
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.81	4.54	3.86
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

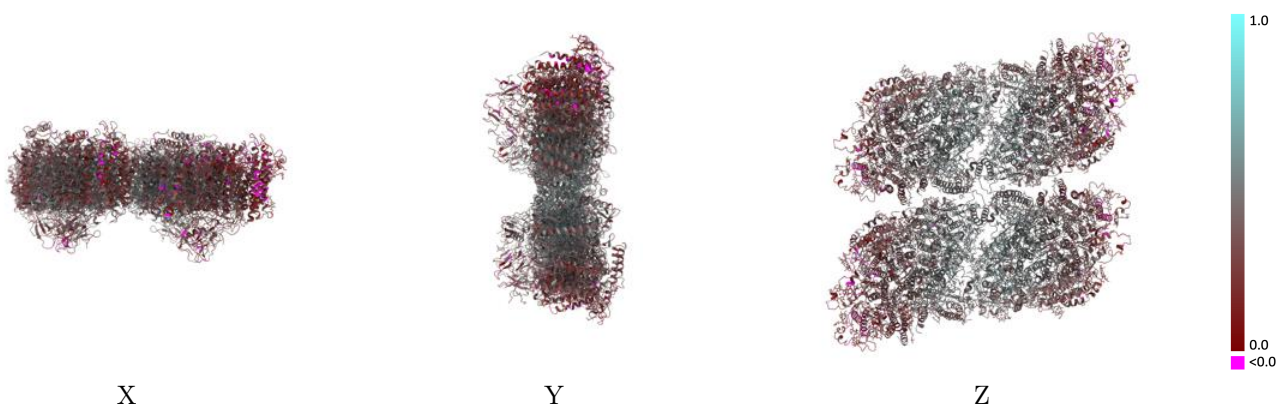
This section contains information regarding the fit between EMDB map EMD-30823 and PDB model 7DR2. Per-residue inclusion information can be found in section [3](#) on page [33](#).

9.1 Map-model overlay [i](#)



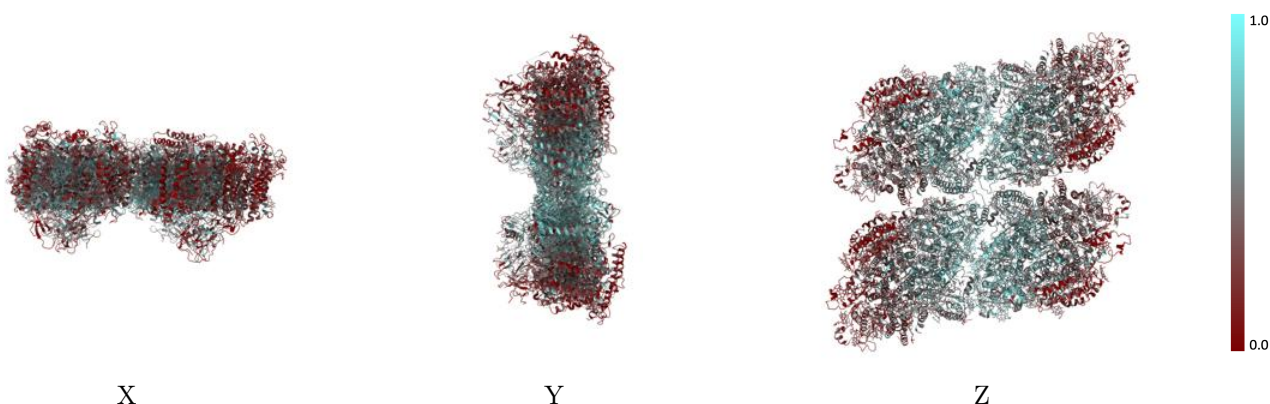
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



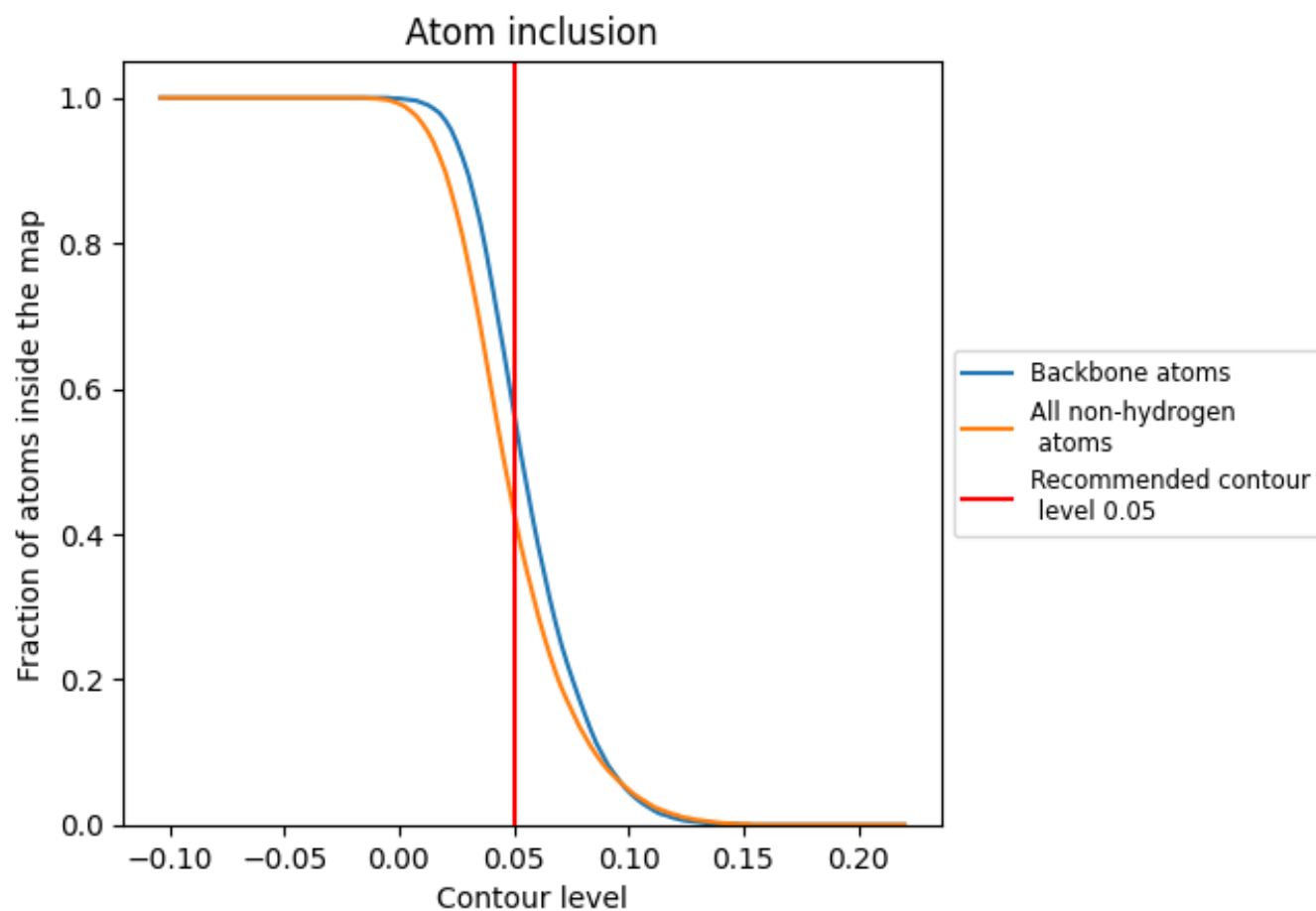
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 57% of all backbone atoms, 43% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4310	 0.3740
aA	 0.5590	 0.4470
aB	 0.3080	 0.2770
aC	 0.4630	 0.2700
aD	 0.3620	 0.3420
aE	 0.2340	 0.2770
aF	 0.1300	 0.2700
aI	 0.2660	 0.3170
aJ	 0.0690	 0.2940
aK	 0.5690	 0.4570
aL	 0.4630	 0.3930
aM	 0.2060	 0.3030
bA	 0.6170	 0.4730
bB	 0.3830	 0.3390
bC	 0.4460	 0.3080
bD	 0.3930	 0.3690
bE	 0.2040	 0.3430
bF	 0.1760	 0.3210
bI	 0.3320	 0.3840
bJ	 0.1510	 0.3320
bL	 0.5780	 0.4420
bM	 0.2620	 0.3160
cA	 0.5580	 0.4430
cB	 0.3050	 0.2740
cC	 0.4530	 0.2730
cD	 0.3660	 0.3380
cE	 0.2420	 0.2770
cF	 0.1260	 0.2650
cI	 0.2730	 0.3140
cJ	 0.0760	 0.2890
cK	 0.5840	 0.4560
cL	 0.4560	 0.3910
cM	 0.2020	 0.2940
dA	 0.6090	 0.4670
dB	 0.3790	 0.3360



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Chain	Atom inclusion	Q-score
dC	 0.4440	 0.2990
dD	 0.3950	 0.3650
dE	 0.1900	 0.3340
dF	 0.1660	 0.3110
dI	 0.3450	 0.3900
dJ	 0.1290	 0.3240
dL	 0.5540	 0.4390
dM	 0.2340	 0.3150