



wwPDB EM Validation Summary Report ⓘ

Aug 6, 2026 – 04:00 AM JST

PDB ID : 6K33 / pdb_00006k33
EMDB ID : EMD-9908
Title : Structure of PSI-isiA supercomplex from *Thermosynechococcus vulcanus*
Authors : Akita, F.; Nagao, R.; Kato, K.; Shen, J.R.; Miyazaki, N.
Deposited on : 2019-05-16
Resolution : 2.74 Å (reported)
Based on initial model : 1JB0

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

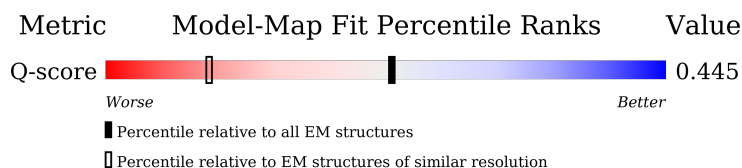
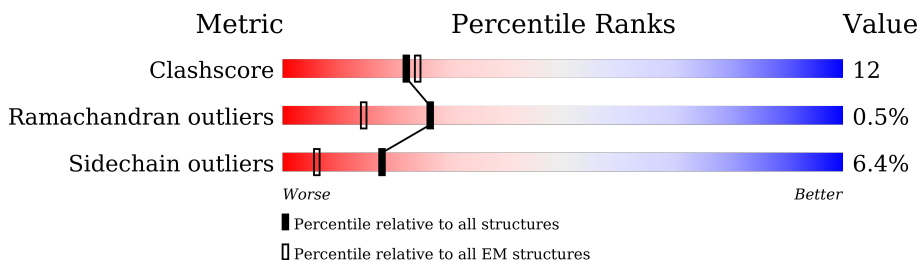
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 Å.

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



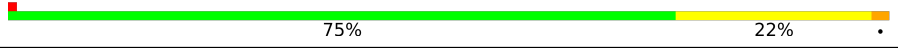
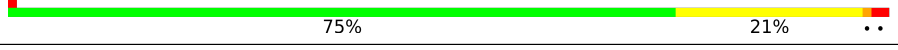
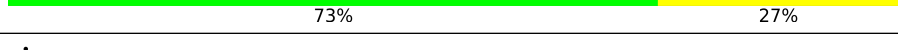
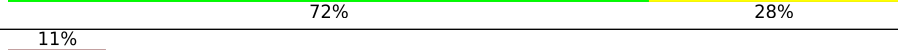
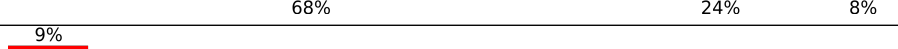
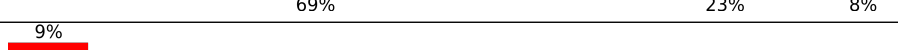
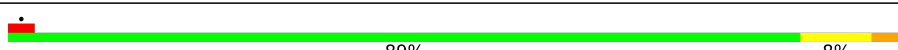
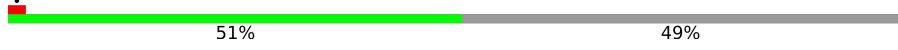
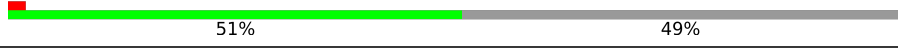
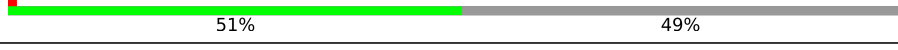
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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	755	
1	bA	755	
1	cA	755	
2	aB	740	

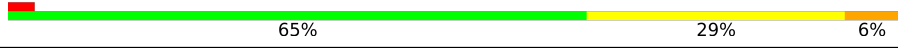
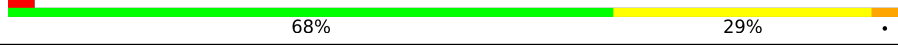
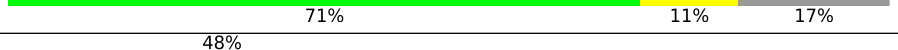
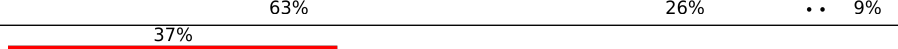
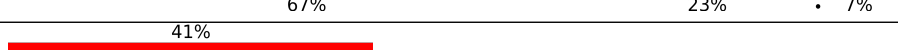
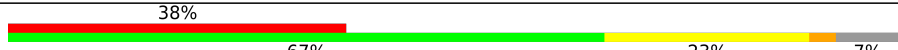
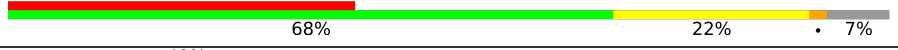
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Mol	Chain	Length	Quality of chain
2	bB	740	
2	cB	740	
3	aC	80	
3	bC	80	
3	cC	80	
4	aD	138	
4	bD	138	
4	cD	138	
5	aE	75	
5	bE	75	
5	cE	75	
6	aF	164	
6	bF	164	
6	cF	164	
7	aI	38	
7	bI	38	
7	cI	38	
8	aJ	41	
8	bJ	41	
8	cJ	41	
9	aK	85	
9	bK	85	
9	cK	85	
10	aL	154	
10	bL	154	

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Mol	Chain	Length	Quality of chain
10	cL	154	
11	aM	31	
11	bM	31	
11	cM	31	
12	aX	35	
12	bX	35	
12	cX	35	
13	a1	358	
13	a2	358	
13	a3	358	
13	a4	358	
13	a5	358	
13	a6	358	
13	b1	358	
13	b2	358	
13	b3	358	
13	b4	358	
13	b5	358	
13	b6	358	
13	c1	358	
13	c2	358	
13	c3	358	
13	c4	358	
13	c5	358	
13	c6	358	

2 Entry composition [i](#)

There are 22 unique types of molecules in this entry. The entry contains 137634 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	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	bA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		
1	cA	742	Total	C	N	O	S	0	0
			5801	3805	991	979	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	aB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	bB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		
2	cB	739	Total	C	N	O	S	0	0
			5879	3867	986	1005	21		

- 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
			598	367	103	117	11		
3	bC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	cC	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	aD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	bD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	cD	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	aE	69	Total	C	N	O		0	0
			539	342	93	104			
5	bE	69	Total	C	N	O		0	0
			539	342	93	104			
5	cE	69	Total	C	N	O		0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	aF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	bF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	cF	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	aI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	bI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		
7	cI	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	aJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		
8	bJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	cJ	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	aK	43	Total	C	N	O		0	0
			208	122	43	43			
9	bK	43	Total	C	N	O		0	0
			208	122	43	43			
9	cK	43	Total	C	N	O		0	0
			208	122	43	43			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	aL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	bL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		
10	cL	151	Total	C	N	O	S	0	0
			1119	735	179	201	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	aM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	bM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	cM	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

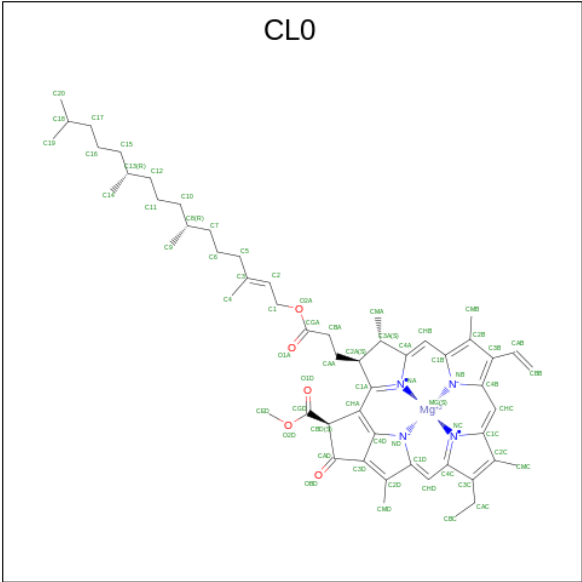
- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	aX	29	Total	C	N	O		0	0
			233	164	34	35			
12	bX	29	Total	C	N	O		0	0
			233	164	34	35			
12	cX	29	Total	C	N	O		0	0
			233	164	34	35			

- Molecule 13 is a protein called Iron stress in-duced protein A.

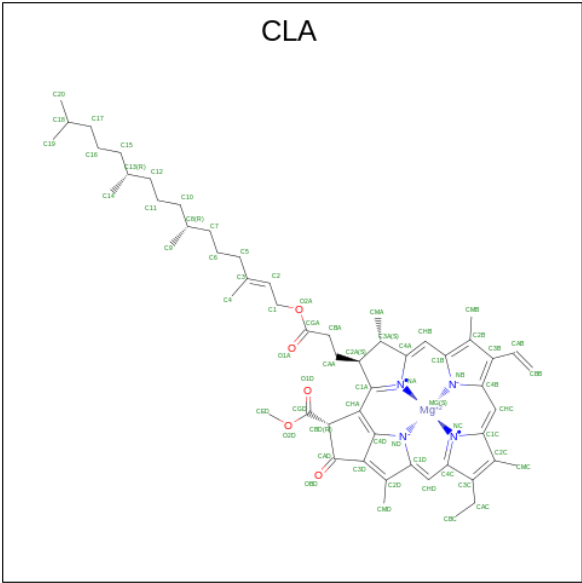
Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	a2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	a3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	a5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	b2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	b3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	b5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	b6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	c2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	c3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	c5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	c6	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		

- Molecule 14 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	aA	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aA	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	aA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	aA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	aA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aA	1	Total 49	C 39	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
15	aA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	aB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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Mol	Chain	Residues	Atoms					AltConf
15	aB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
15	aK	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	aX	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a1	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a1	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a1	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a2	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a2	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a2	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a3	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a3	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a3	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a4	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a4	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a4	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a5	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a5	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a5	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a6	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	a6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a6	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a6	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	bA	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	bA	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	bA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 47	C 37	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	bA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bA	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	bA	1	Total 52	C 42	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
15	bB	1	Total 58	C 48	Mg 1	N 4	O 5	0
15	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bB	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 47	C 37	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bF	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
15	bK	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	bX	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b1	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	b1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b1	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	b1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
15	b2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
15	b2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
15	b3	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	b3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b3	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	b3	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b4	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	b4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	b4	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b5	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	b5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b5	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	b5	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b6	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b6	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	b6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b6	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	b6	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	cA	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 61	C 51	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	cA	1	Total 59	C 49	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	cA	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cA	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 47	C 37	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cA	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	cA	1	Total 52	C 42	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cB	1	Total 49	C 39	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 58	C 48	Mg 1	N 4	O 5	0
15	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cB	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 47	C 37	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cB	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cF	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	cF	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cJ	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cJ	1	Total 37	C 31	Mg 1	N 4	O 1	0
15	cK	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cL	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	cX	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c1	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c1	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c1	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c1	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c2	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c2	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c2	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c2	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c2	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c3	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c3	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c3	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c3	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c3	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c4	1	Total 64	C 54	Mg 1	N 4	O 5	0

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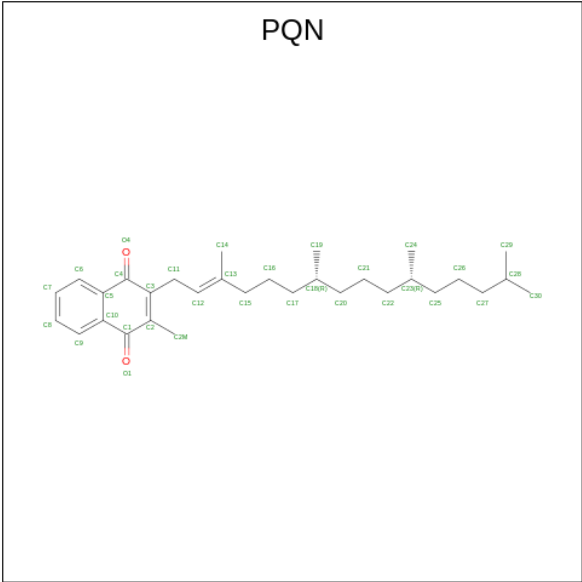
Mol	Chain	Residues	Atoms					AltConf
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c4	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c4	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c5	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 41	C 33	Mg 1	N 4	O 3	0

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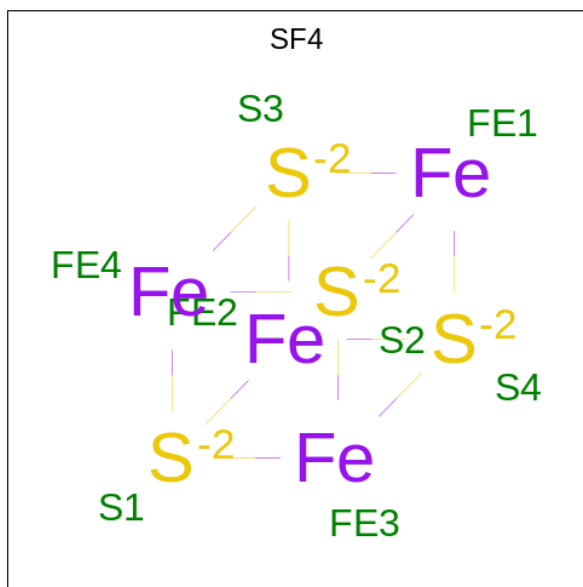
Mol	Chain	Residues	Atoms					AltConf
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c5	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 64	C 54	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c6	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c6	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c6	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



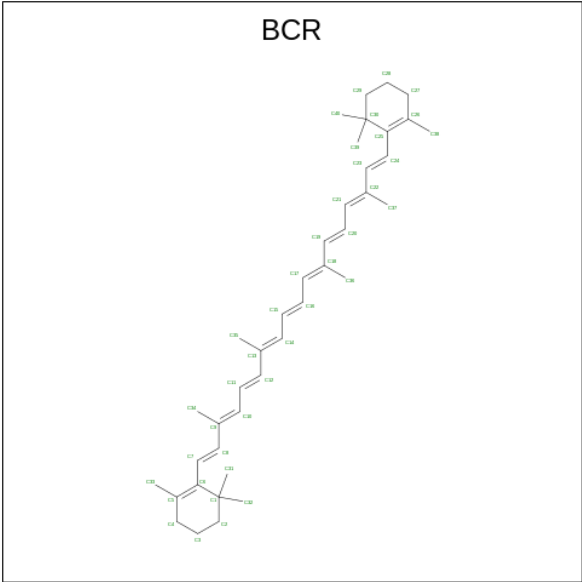
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

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



Mol	Chain	Residues	Atoms			AltConf
17	aA	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	bA	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	cA	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	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
18	aA	1	Total	C	0
			40	40	
18	aA	1	Total	C	0
			40	40	
18	aA	1	Total	C	0
			40	40	
18	aA	1	Total	C	0
			40	40	
18	aA	1	Total	C	0
			40	40	
18	aB	1	Total	C	0
			40	40	
18	aB	1	Total	C	0
			40	40	
18	aB	1	Total	C	0
			40	40	
18	aB	1	Total	C	0
			25	25	
18	aB	1	Total	C	0
			40	40	
18	aB	1	Total	C	0
			40	40	
18	aF	1	Total	C	0
			40	40	
18	aF	1	Total	C	0
			40	40	
18	aF	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aI	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aJ	1	Total C 40 40	0
18	aK	1	Total C 40 40	0
18	aL	1	Total C 40 40	0
18	aM	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a1	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a2	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0
18	a3	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a4	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a5	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	a6	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bA	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	bB	1	Total C 25 25	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bB	1	Total C 40 40	0
18	bF	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bI	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bJ	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bL	1	Total C 40 40	0
18	bM	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b1	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0
18	b2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
18	b2	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b3	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b4	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b5	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	b6	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0
18	cA	1	Total C 40 40	0

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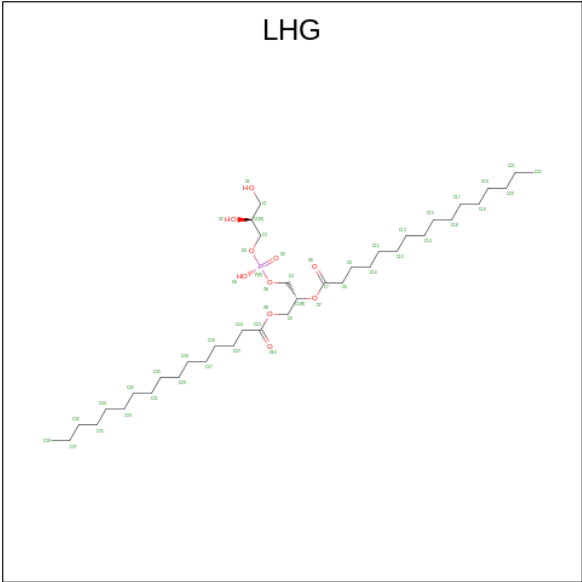
Mol	Chain	Residues	Atoms	AltConf
18	cA	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 25 25	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cJ	1	Total C 40 40	0
18	cK	1	Total C 40 40	0
18	cL	1	Total C 40 40	0
18	cM	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0
18	c1	1	Total C 40 40	0

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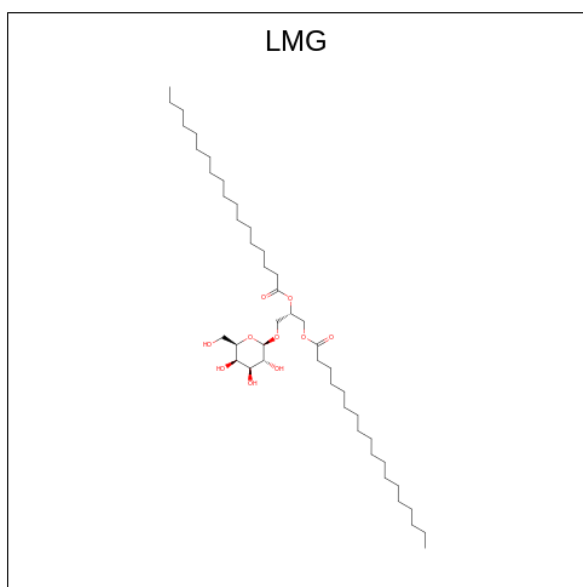
Mol	Chain	Residues	Atoms	AltConf
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c5	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0
18	c6	1	Total C 40 40	0

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
19	aA	1	Total	C	O	P	0
			49	38	10	1	
19	aA	1	Total	C	O	P	0
			27	16	10	1	
19	aX	1	Total	C	O	P	0
			23	12	10	1	
19	bA	1	Total	C	O	P	0
			49	38	10	1	
19	bA	1	Total	C	O	P	0
			27	16	10	1	
19	bX	1	Total	C	O	P	0
			23	12	10	1	
19	cA	1	Total	C	O	P	0
			49	38	10	1	
19	cA	1	Total	C	O	P	0
			27	16	10	1	
19	cX	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
21	aL	2	Total	Ca	0
			2	2	
21	bL	1	Total	Ca	0
			1	1	

- Molecule 22 is water.

Mol	Chain	Residues	Atoms		AltConf
22	aA	3	Total	O	0
			3	3	
22	aB	3	Total	O	0
			3	3	
22	aL	1	Total	O	0
			1	1	
22	bA	3	Total	O	0
			3	3	

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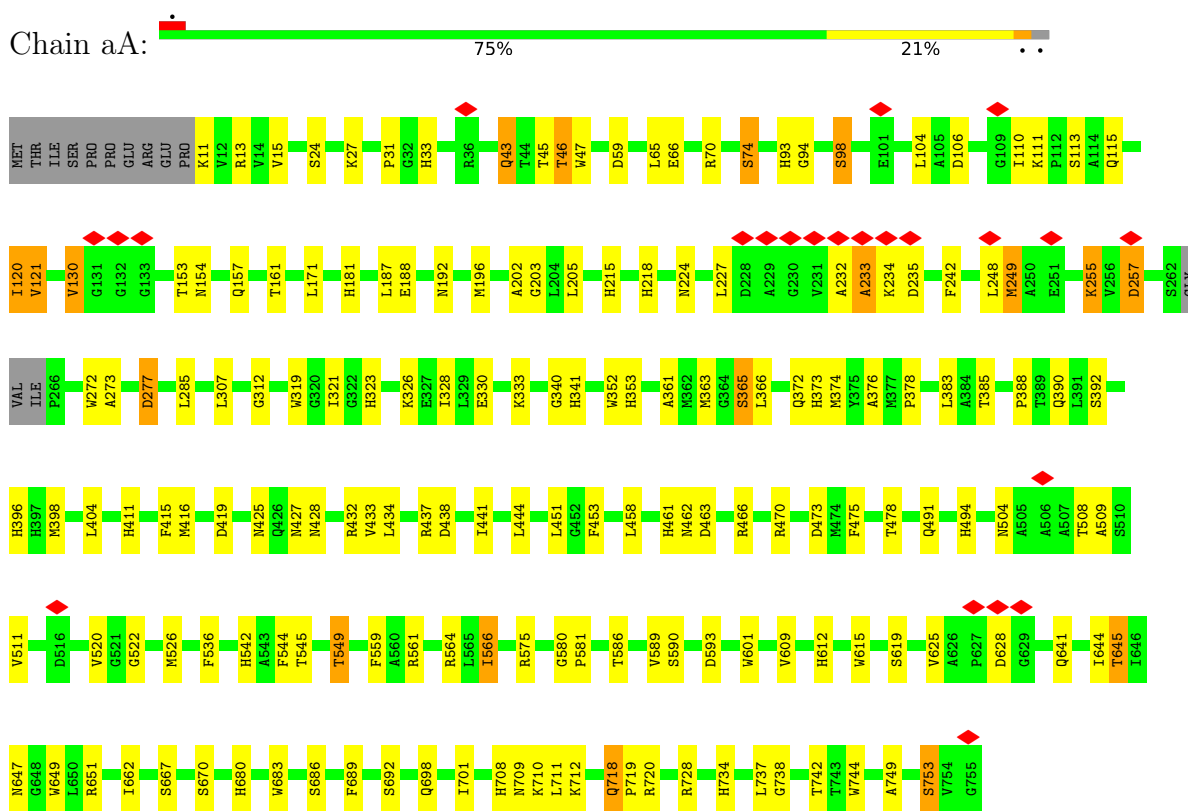
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Mol	Chain	Residues	Atoms		AltConf
22	bB	3	Total 3	O 3	0
22	bL	1	Total 1	O 1	0
22	cA	2	Total 2	O 2	0
22	cB	3	Total 3	O 3	0
22	cF	1	Total 1	O 1	0
22	cL	1	Total 1	O 1	0

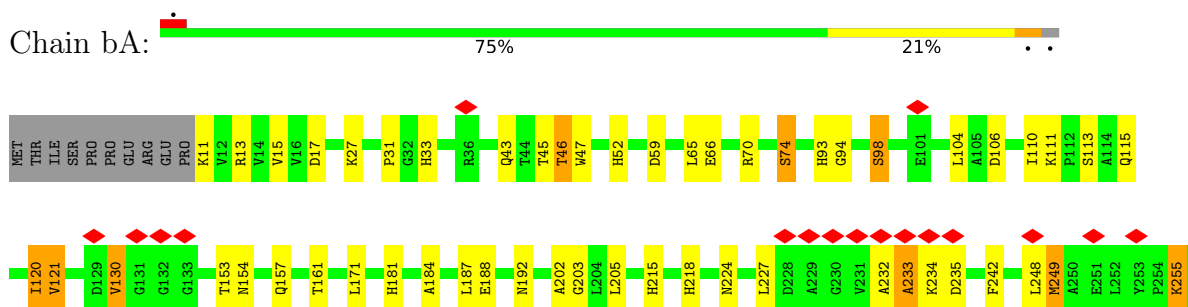
3 Residue-property plots

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

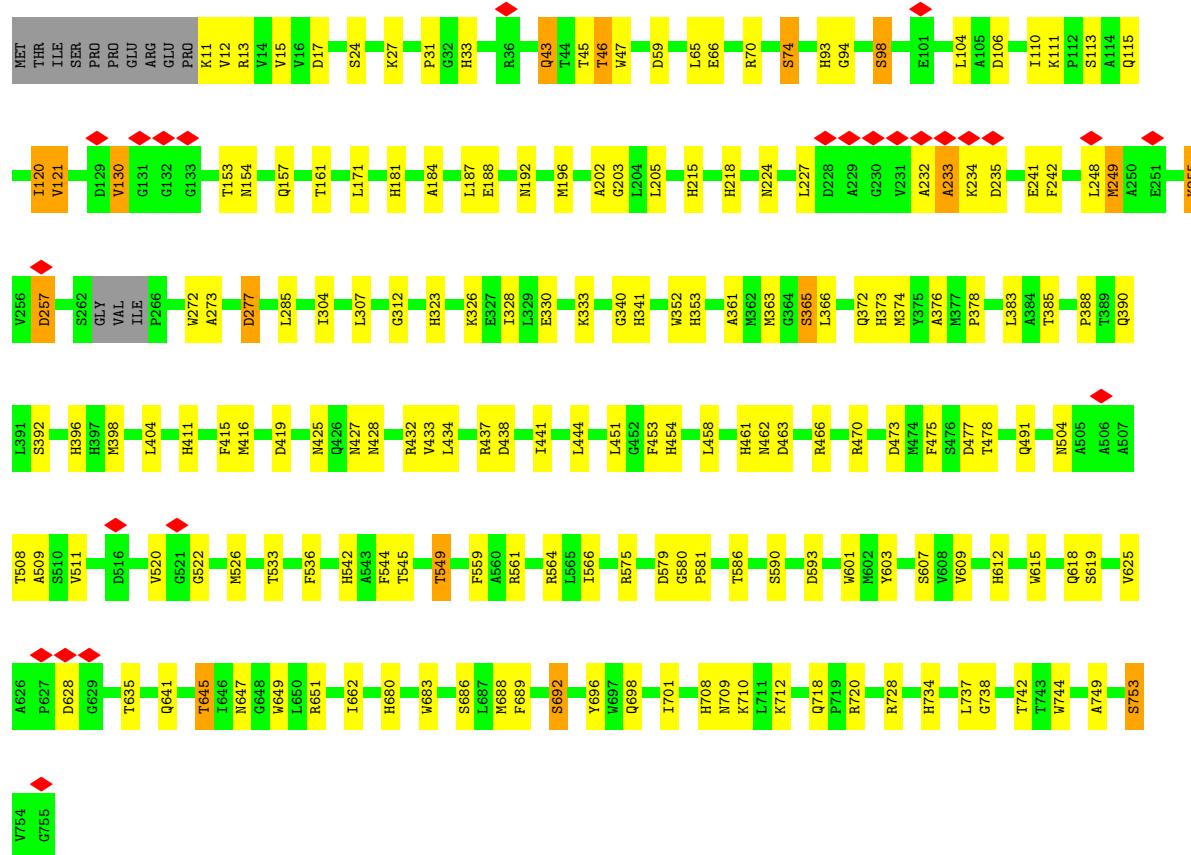
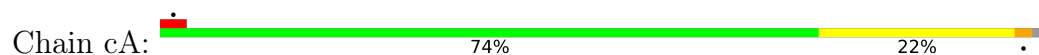
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



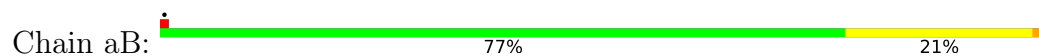
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

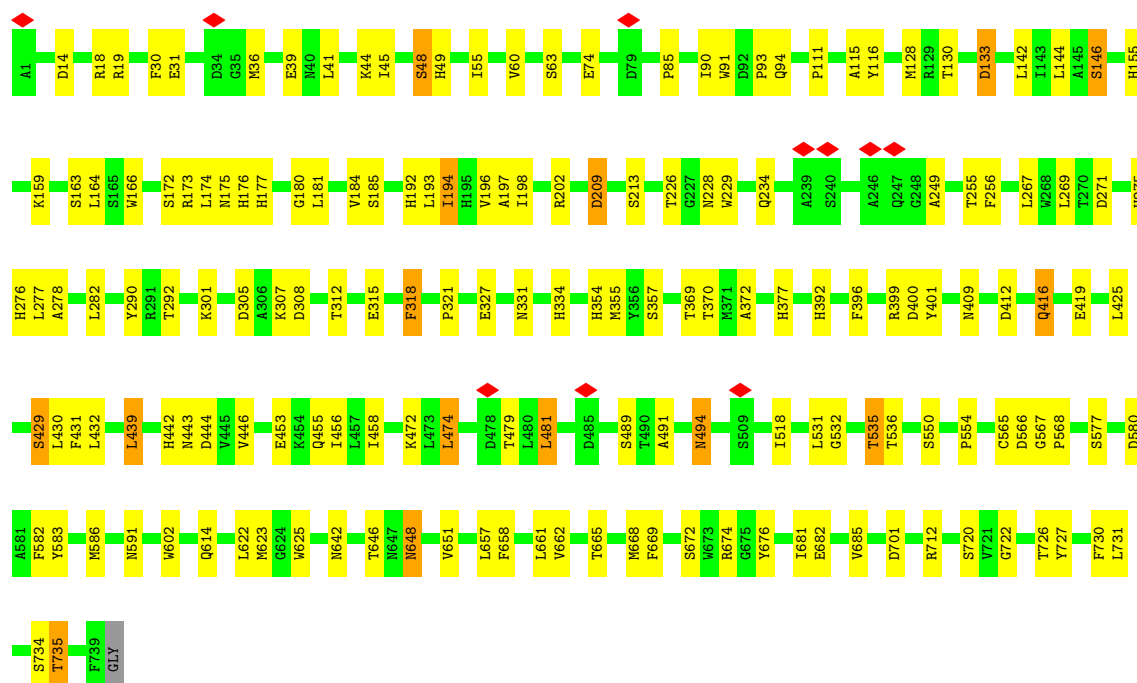


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



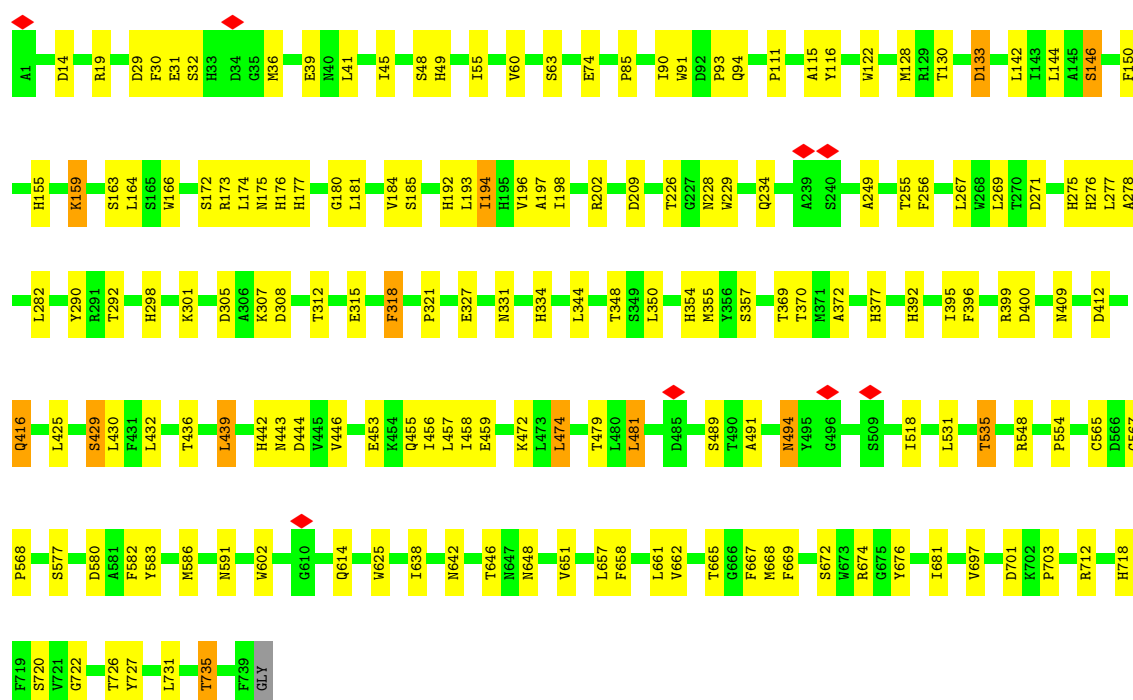
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





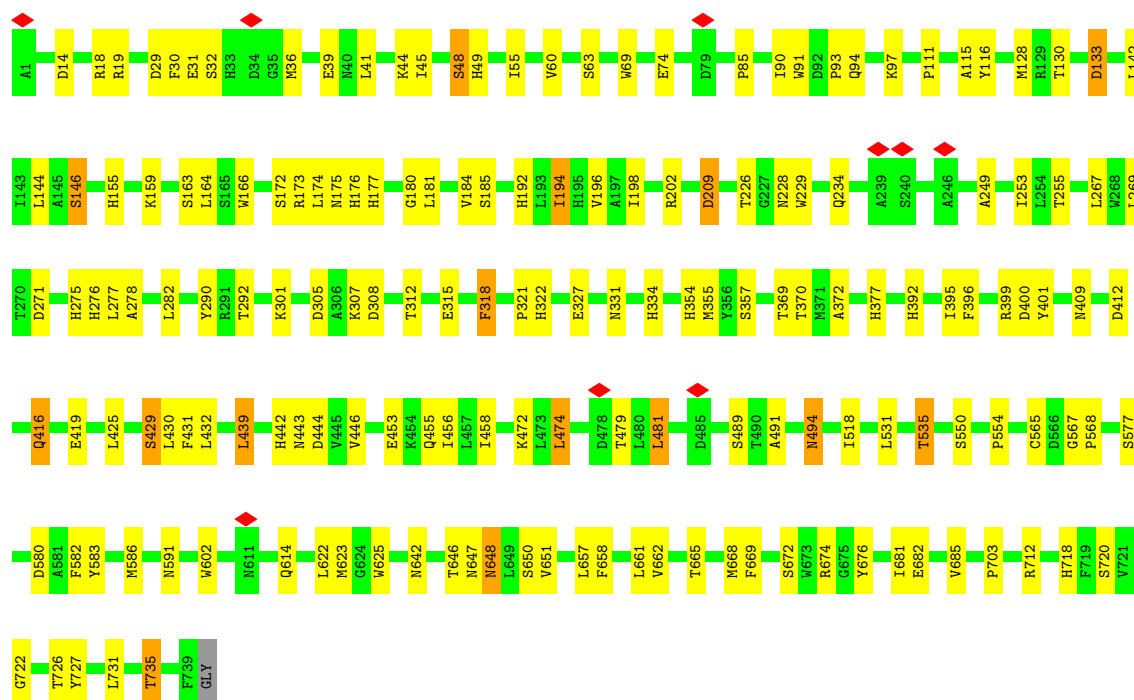
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 77% 21%

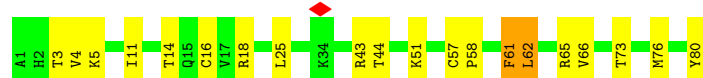
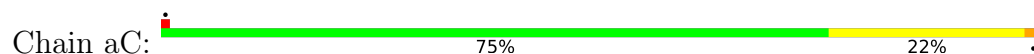


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

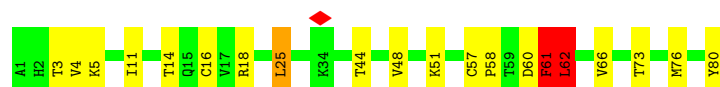
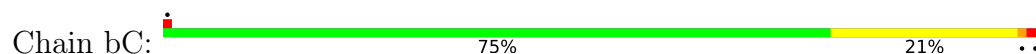
Chain cB: 77% 21%



- Molecule 3: Photosystem I iron-sulfur center



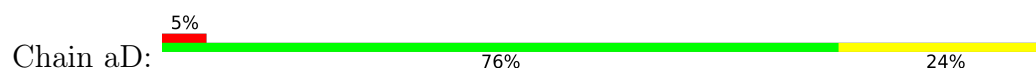
- Molecule 3: Photosystem I iron-sulfur center

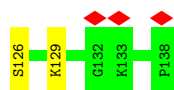


- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II





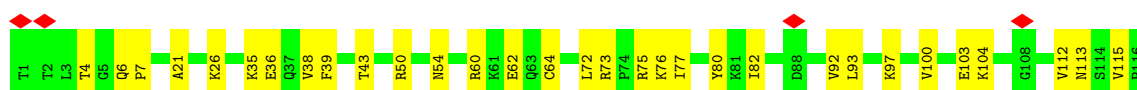
- Molecule 4: Photosystem I reaction center subunit II

Chain bD: 73% 27%



- Molecule 4: Photosystem I reaction center subunit II

Chain cD: 72% 28%



- Molecule 5: Photosystem I reaction center subunit IV

Chain aE: 11% 68% 24% 8%



- Molecule 5: Photosystem I reaction center subunit IV

Chain bE: 9% 69% 23% 8%

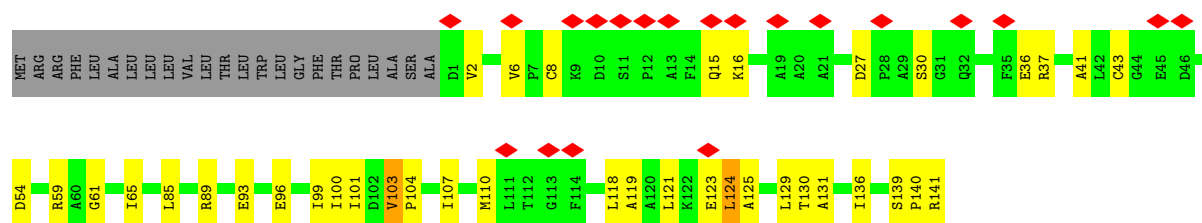


- Molecule 5: Photosystem I reaction center subunit IV

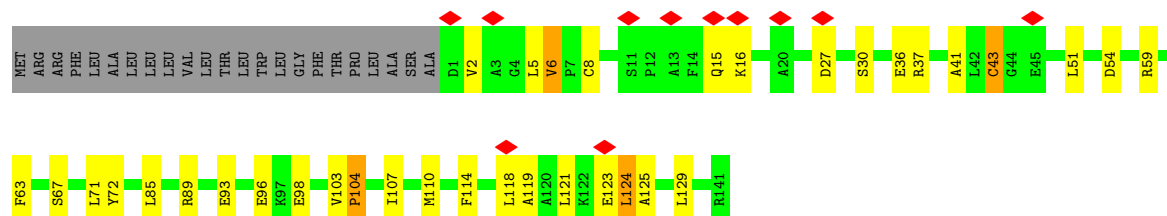
Chain cE: 9% 68% 23% 8%



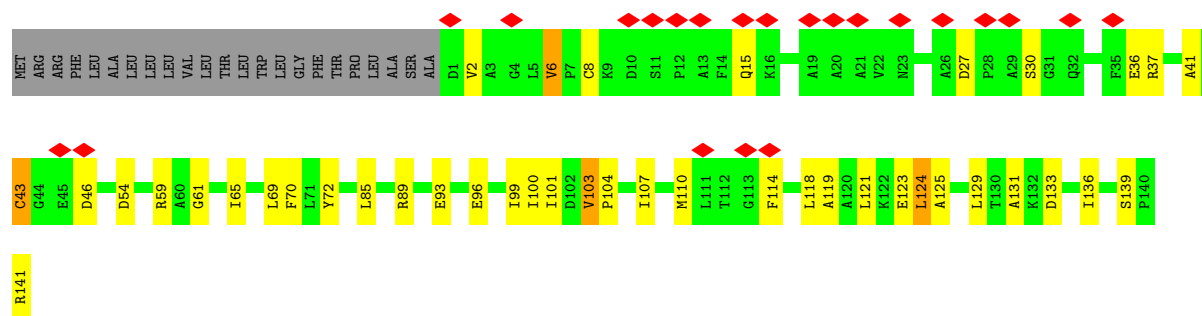
- Molecule 6: Photosystem I reaction center subunit III



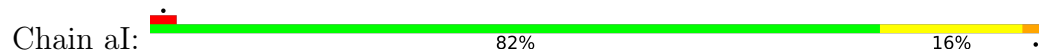
- Molecule 6: Photosystem I reaction center subunit III



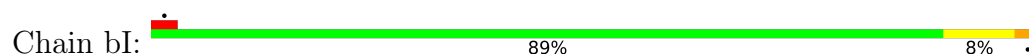
- Molecule 6: Photosystem I reaction center subunit III



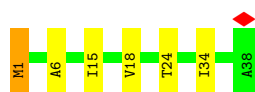
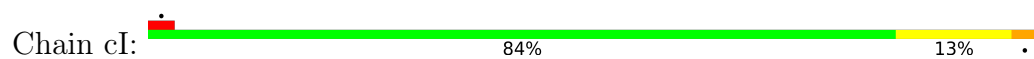
- Molecule 7: Photosystem I reaction center subunit VIII



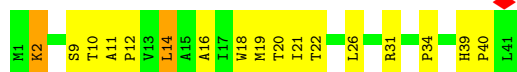
- Molecule 7: Photosystem I reaction center subunit VIII



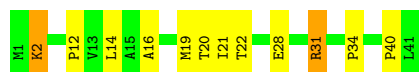
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



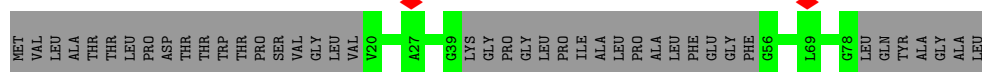
- Molecule 8: Photosystem I reaction center subunit IX



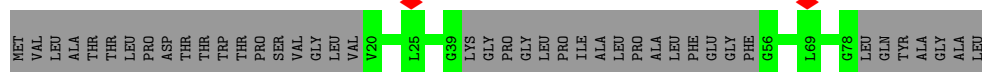
- Molecule 8: Photosystem I reaction center subunit IX



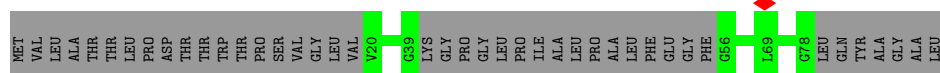
- Molecule 9: Photosystem I reaction center subunit Psak



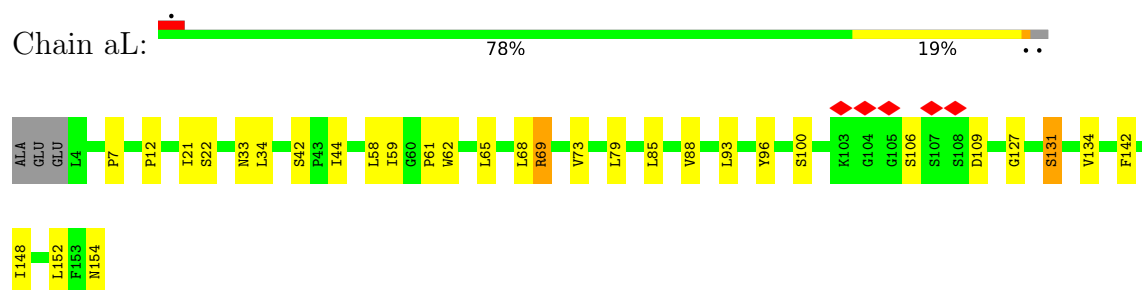
- Molecule 9: Photosystem I reaction center subunit Psak



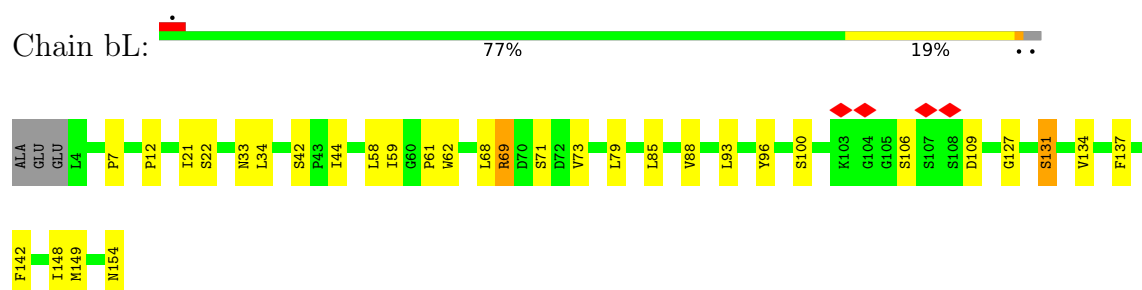
- Molecule 9: Photosystem I reaction center subunit Psak



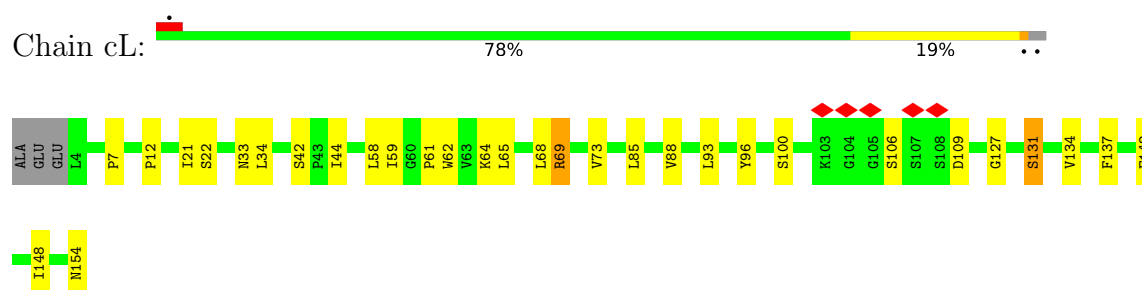
- Molecule 10: Photosystem I reaction center subunit XI



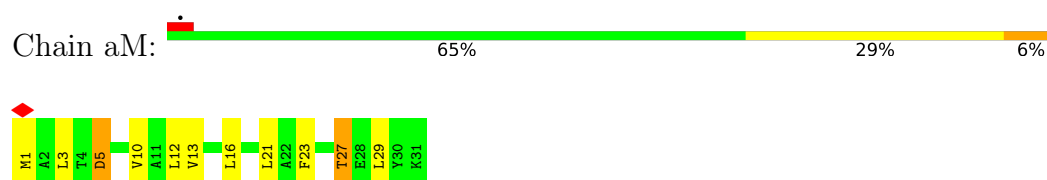
- Molecule 10: Photosystem I reaction center subunit XI



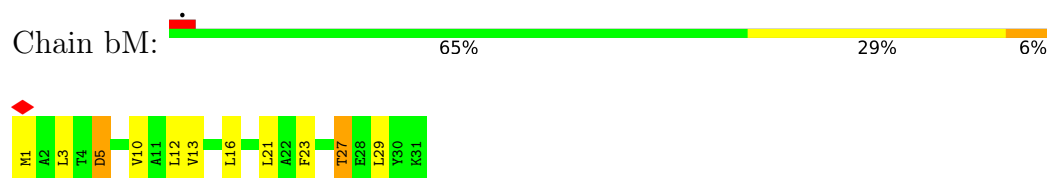
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



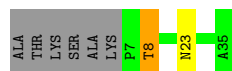
- Molecule 11: Photosystem I reaction center subunit XII





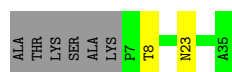
- Molecule 12: Photosystem I reaction center subunit psaX

Chain aX: 77% 17%



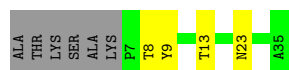
- Molecule 12: Photosystem I reaction center subunit psaX

Chain bX: 77% 6% 17%



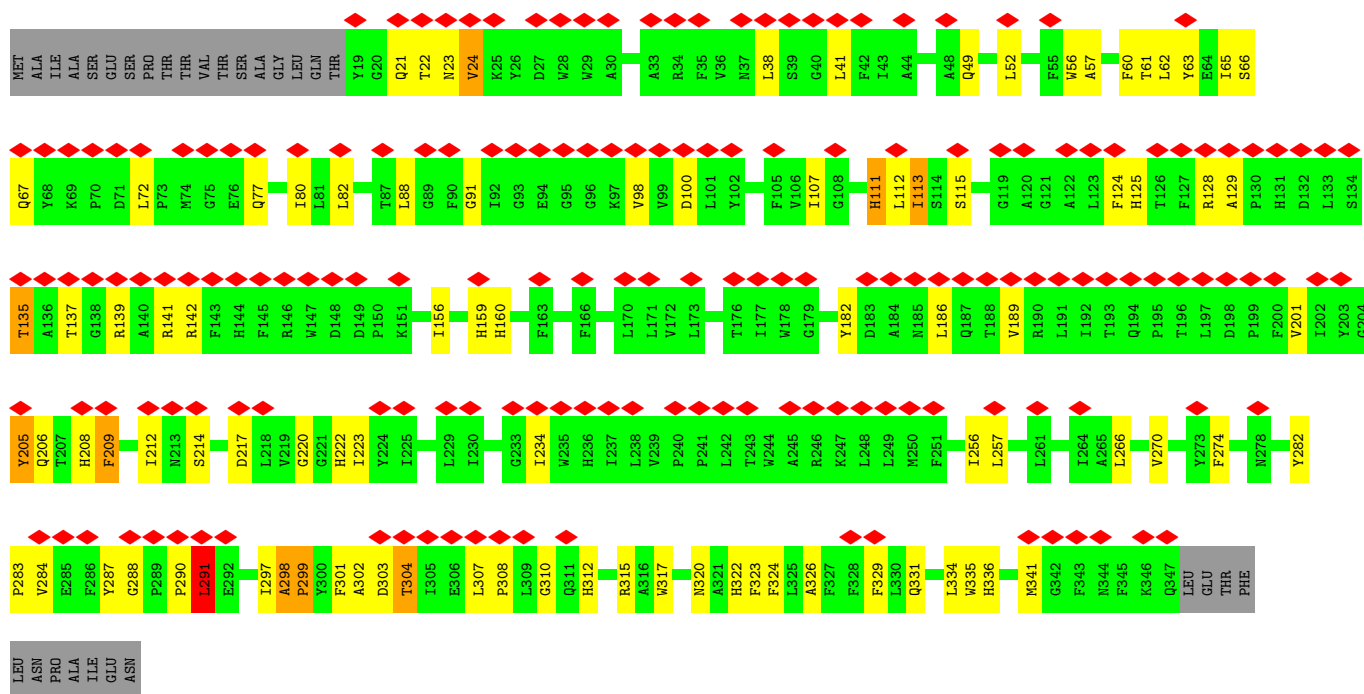
- Molecule 12: Photosystem I reaction center subunit psaX

Chain cX: 71% 11% 17%



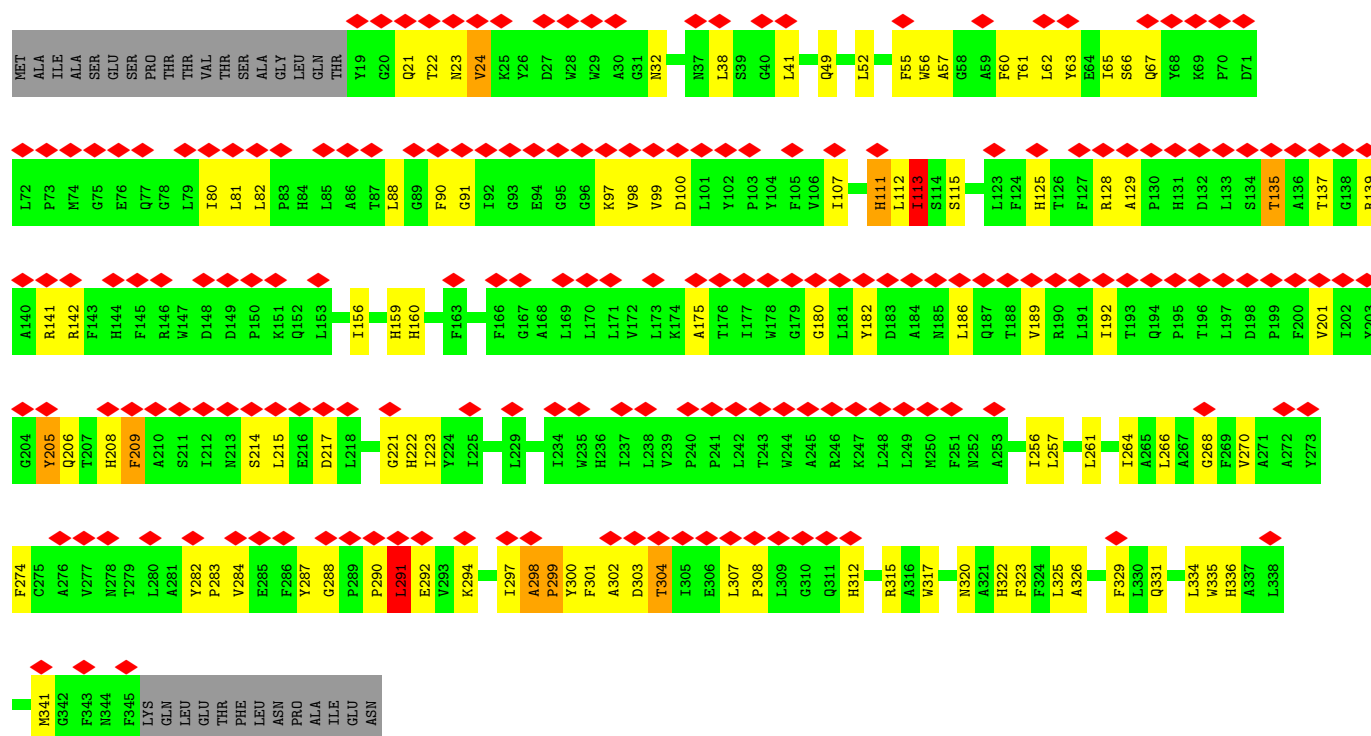
- Molecule 13: Iron stress in-duced protein A

Chain a1: 48% 66% 23% 8%



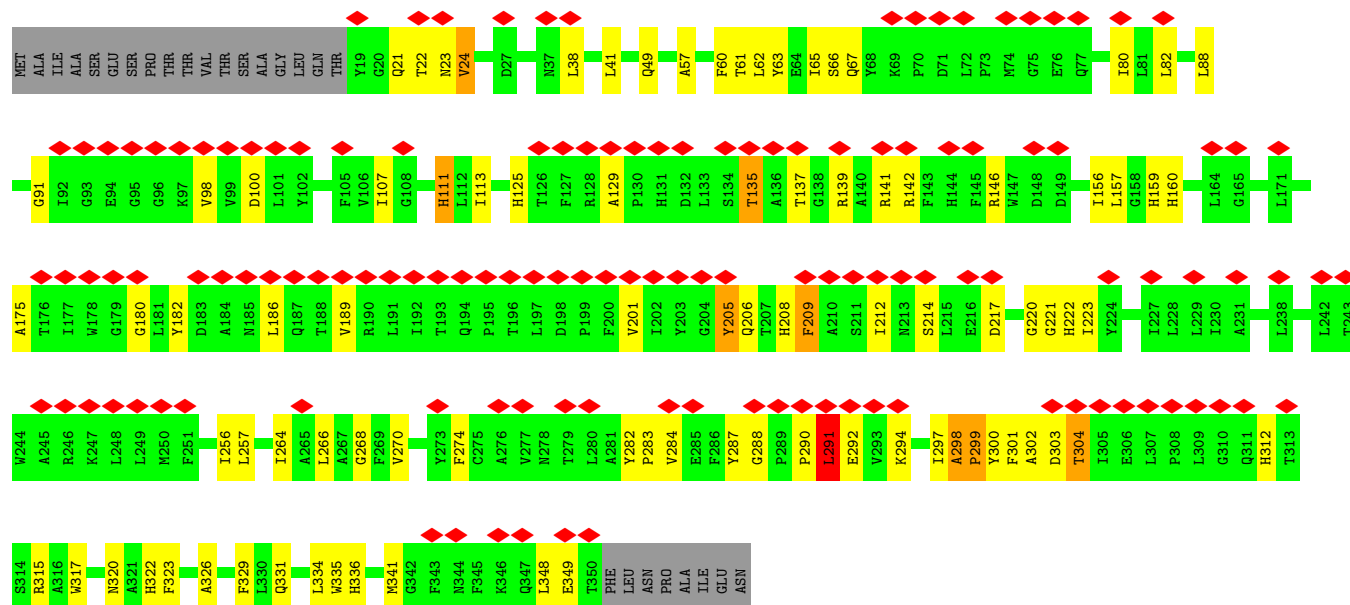
- Molecule 13: Iron stress in-duced protein A

Chain a2: 



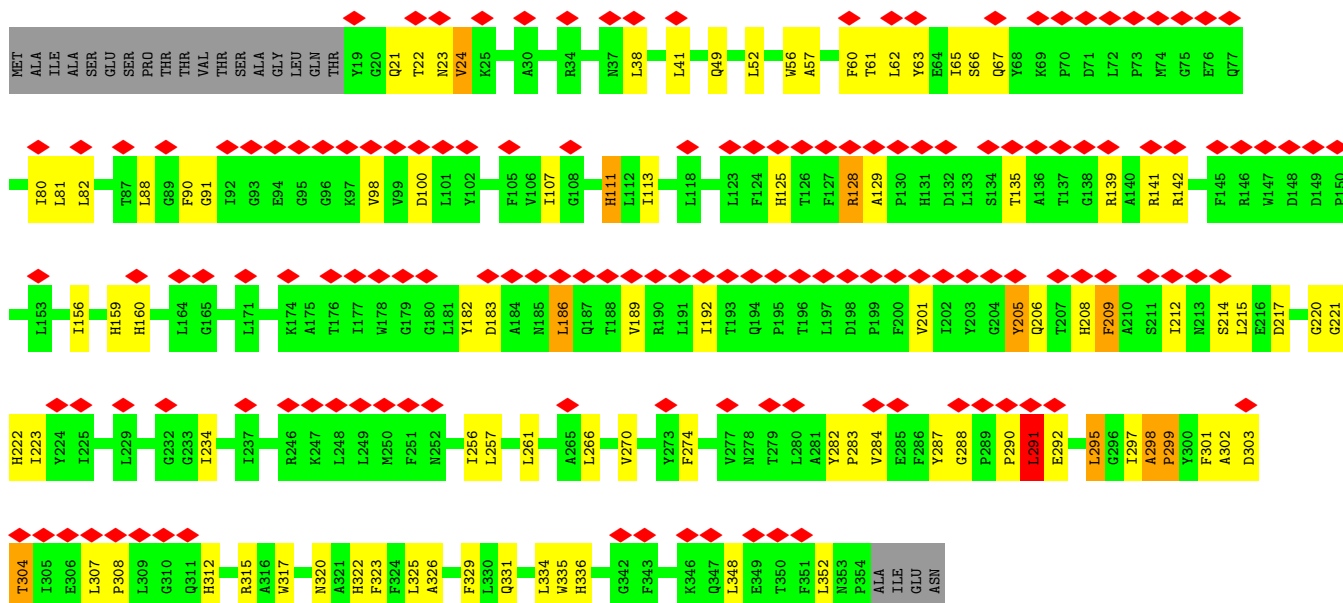
• Molecule 13: Iron stress in-duced protein A

Chain a3: 

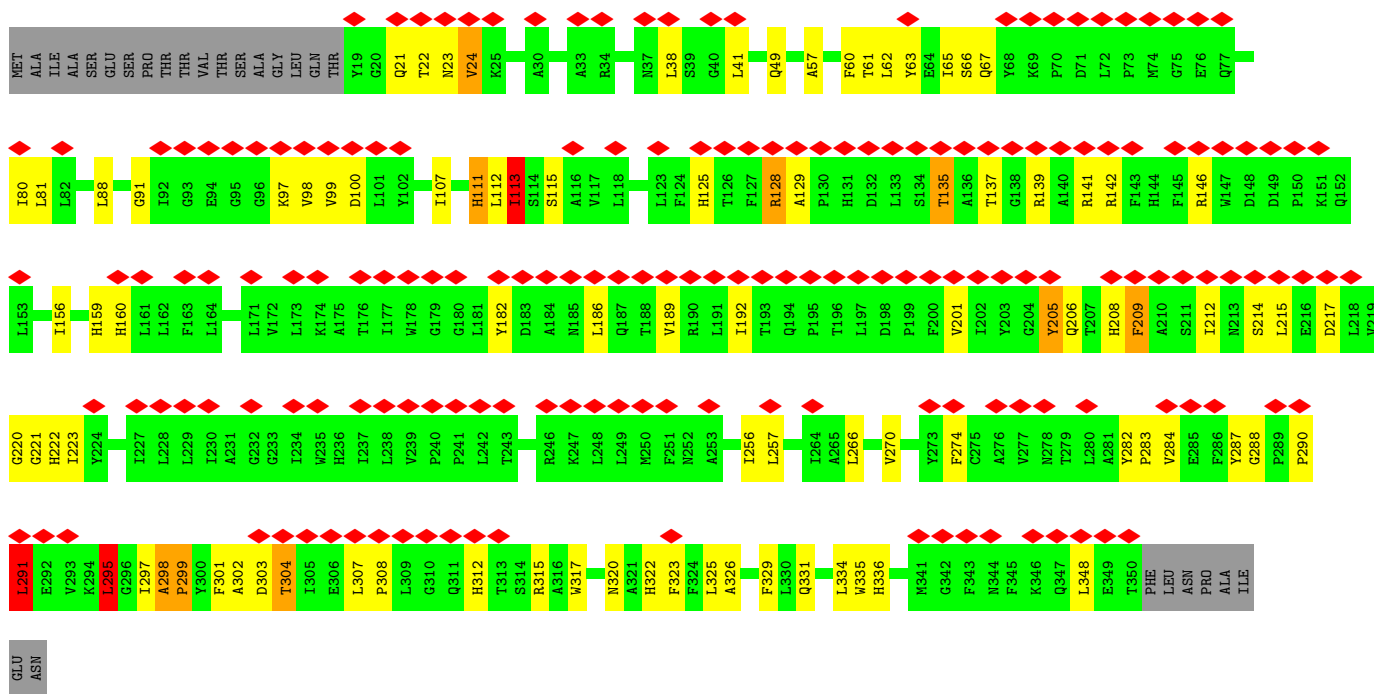


• Molecule 13: Iron stress in-duced protein A

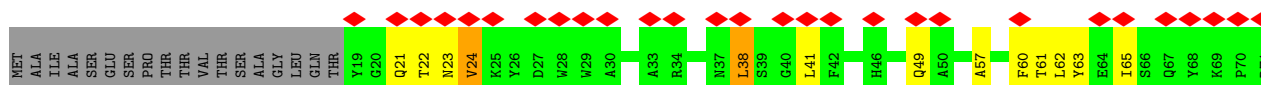
Chain a4: 

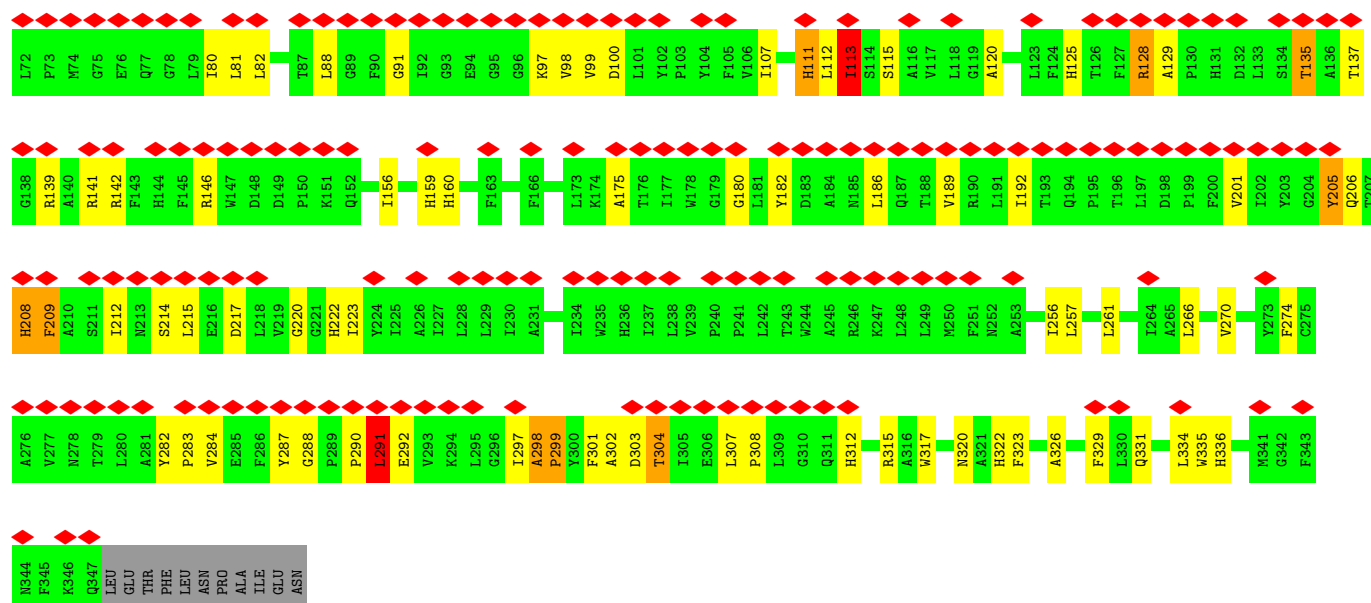


• Molecule 13: Iron stress in-duced protein A

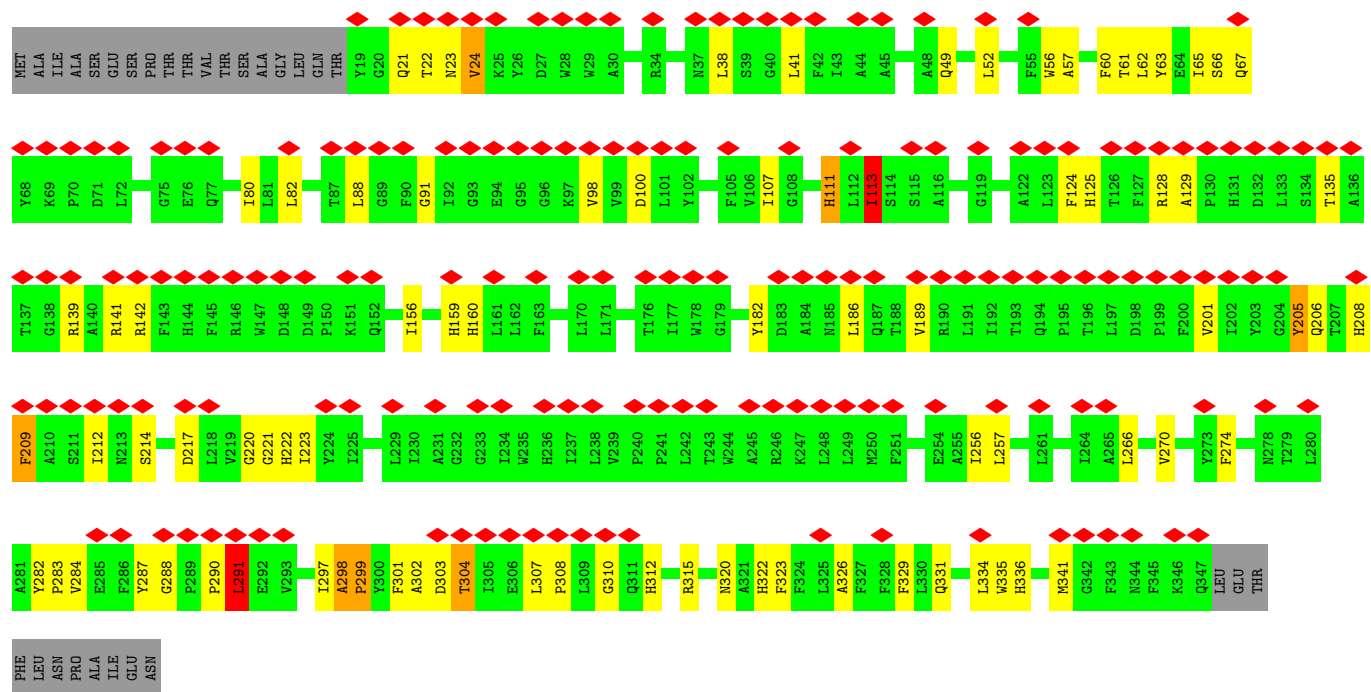


• Molecule 13: Iron stress in-duced protein A

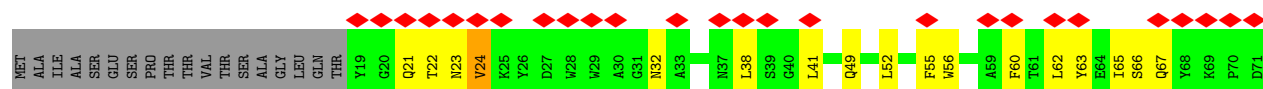


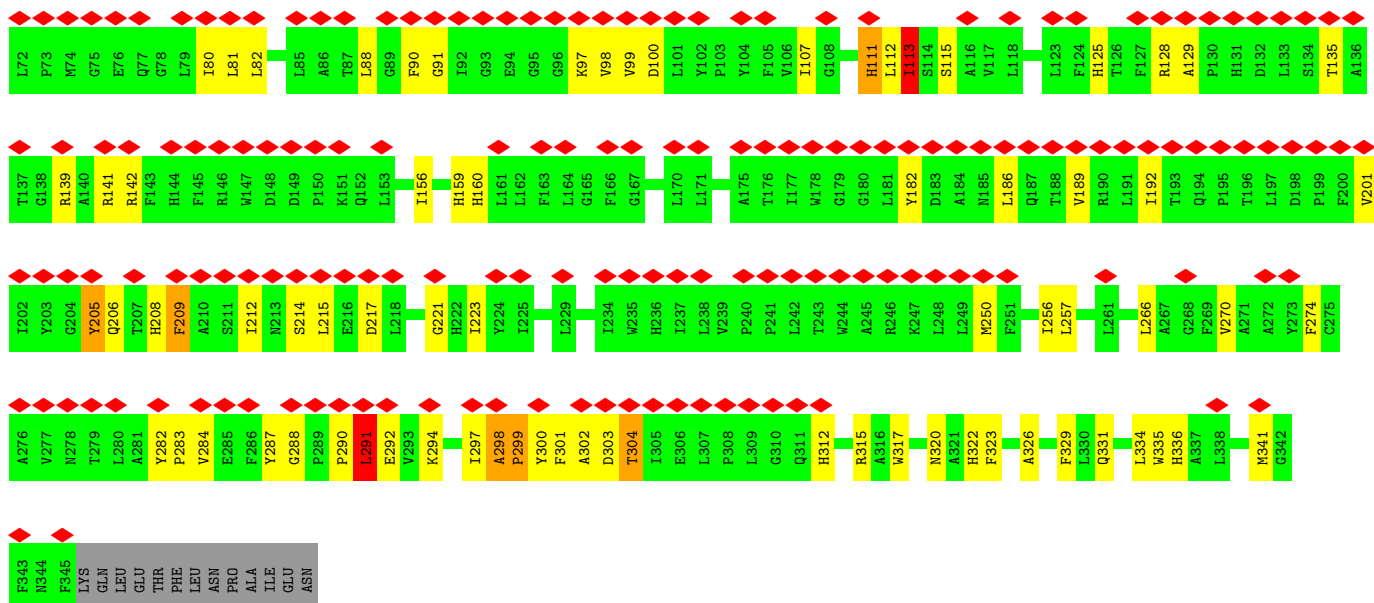


• Molecule 13: Iron stress in-duced protein A

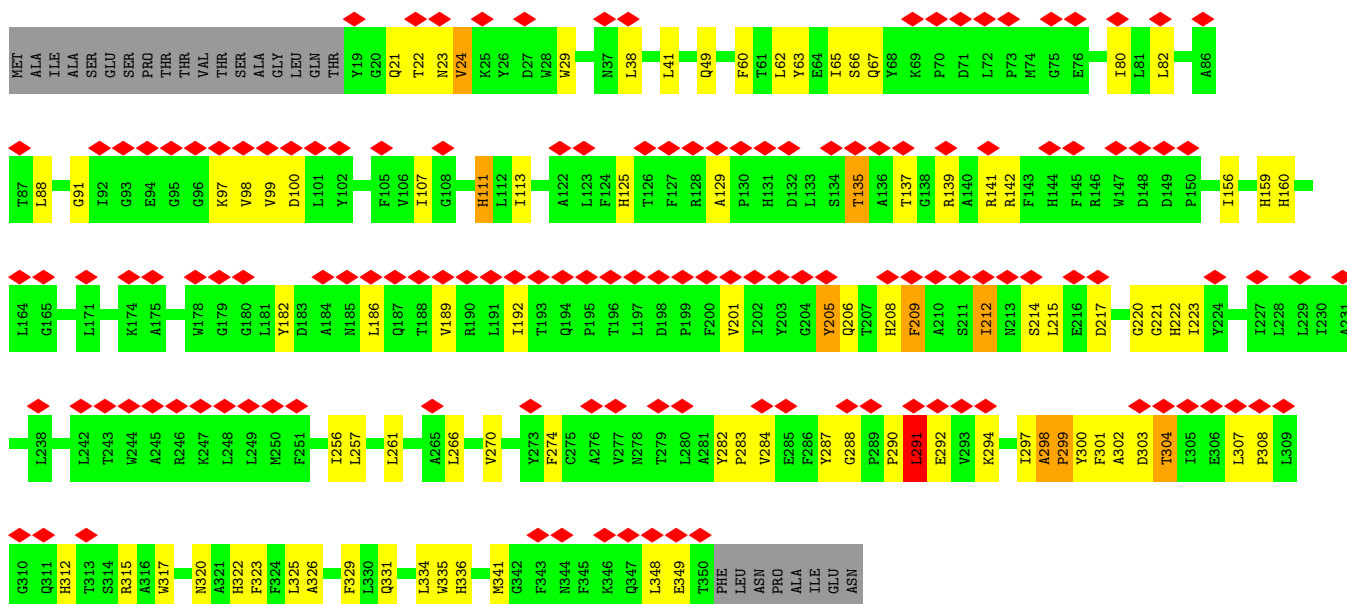


• Molecule 13: Iron stress in-duced protein A

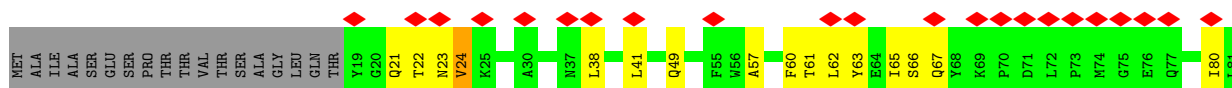
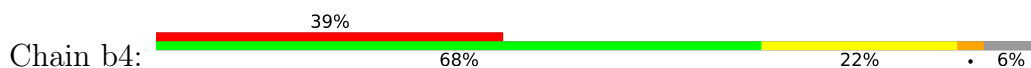


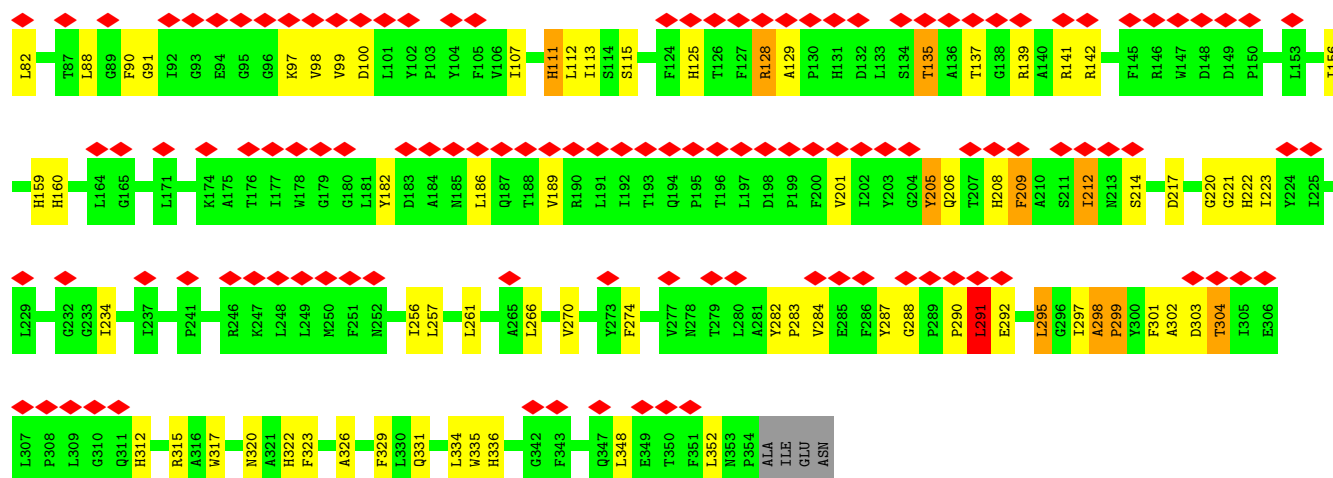


• Molecule 13: Iron stress in-duced protein A

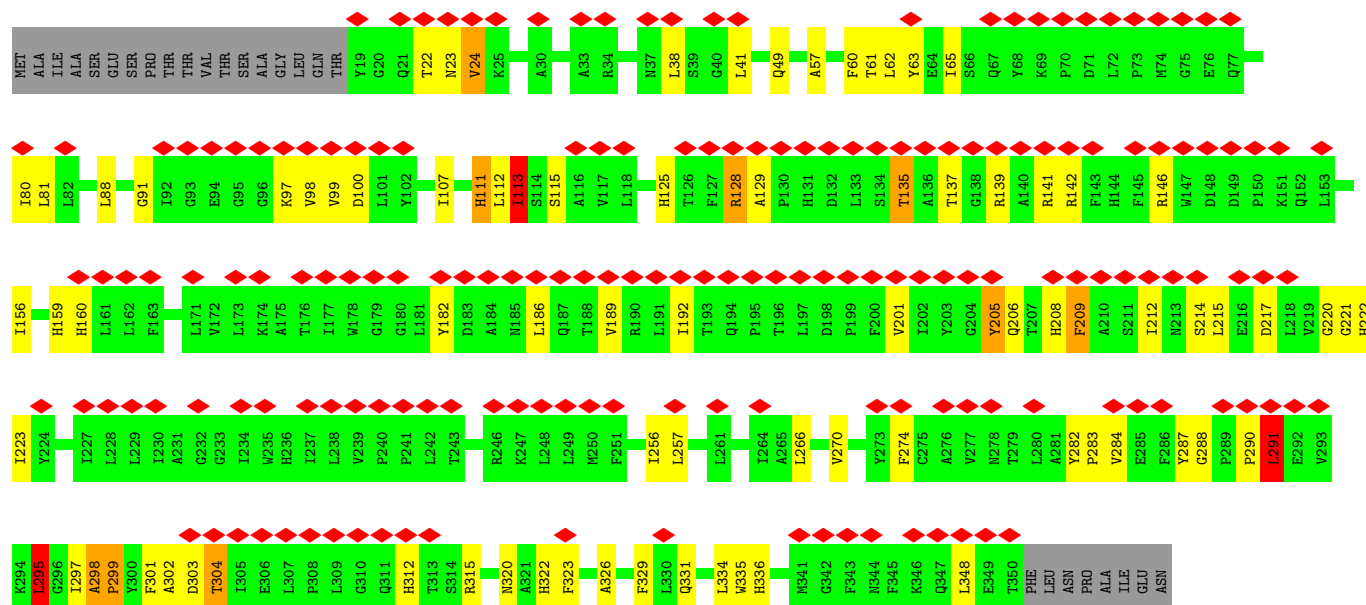


• Molecule 13: Iron stress in-duced protein A

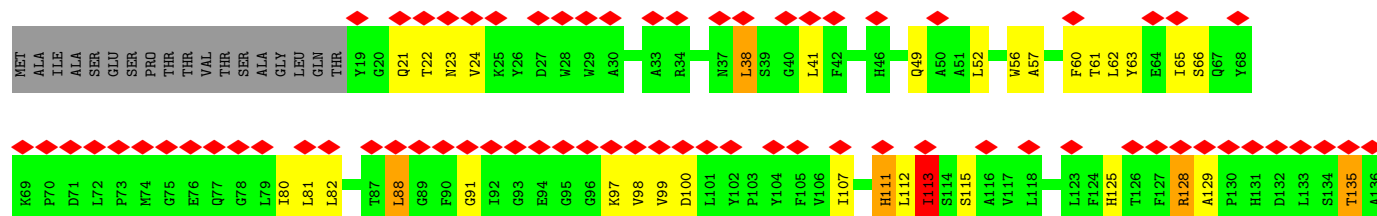


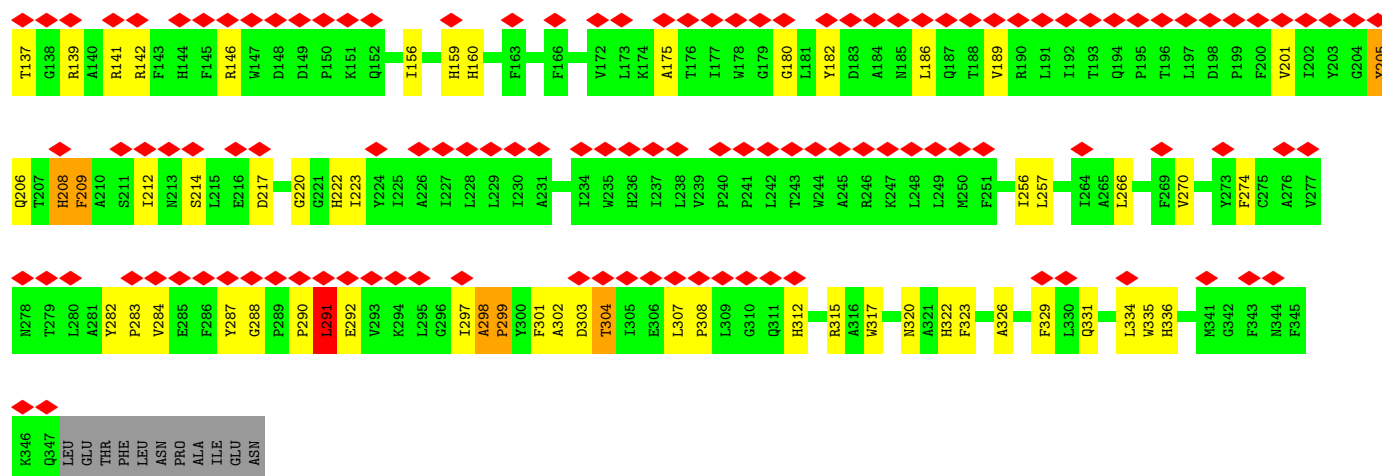


• Molecule 13: Iron stress in-duced protein A

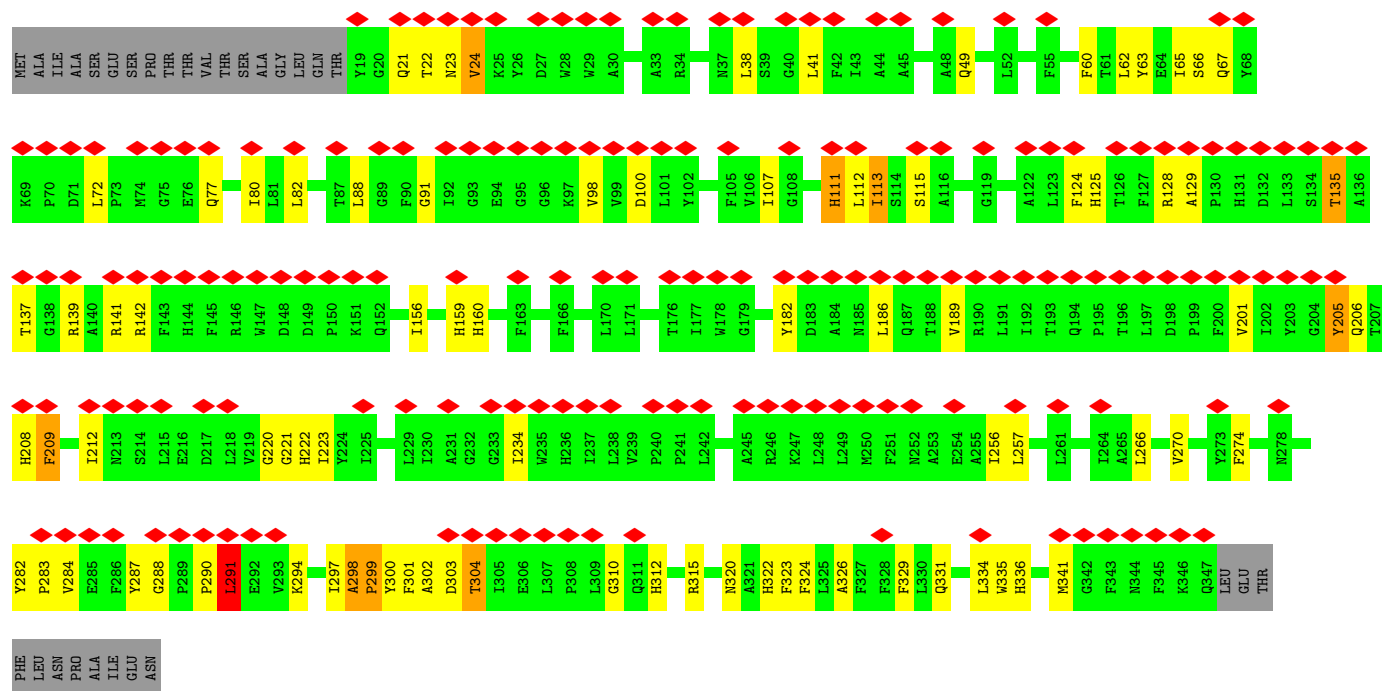


• Molecule 13: Iron stress in-duced protein A

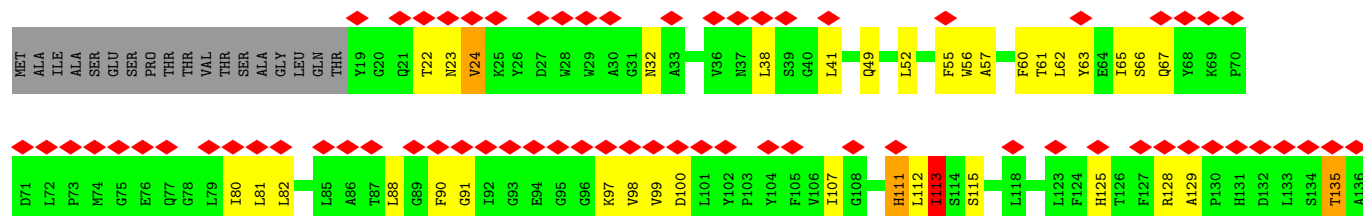


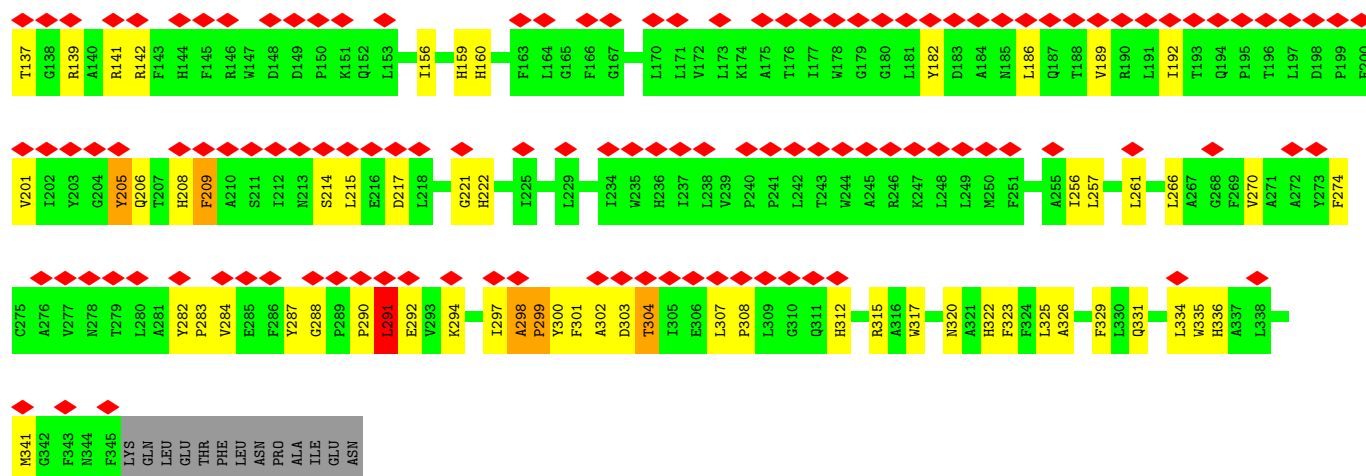


• Molecule 13: Iron stress in-duced protein A

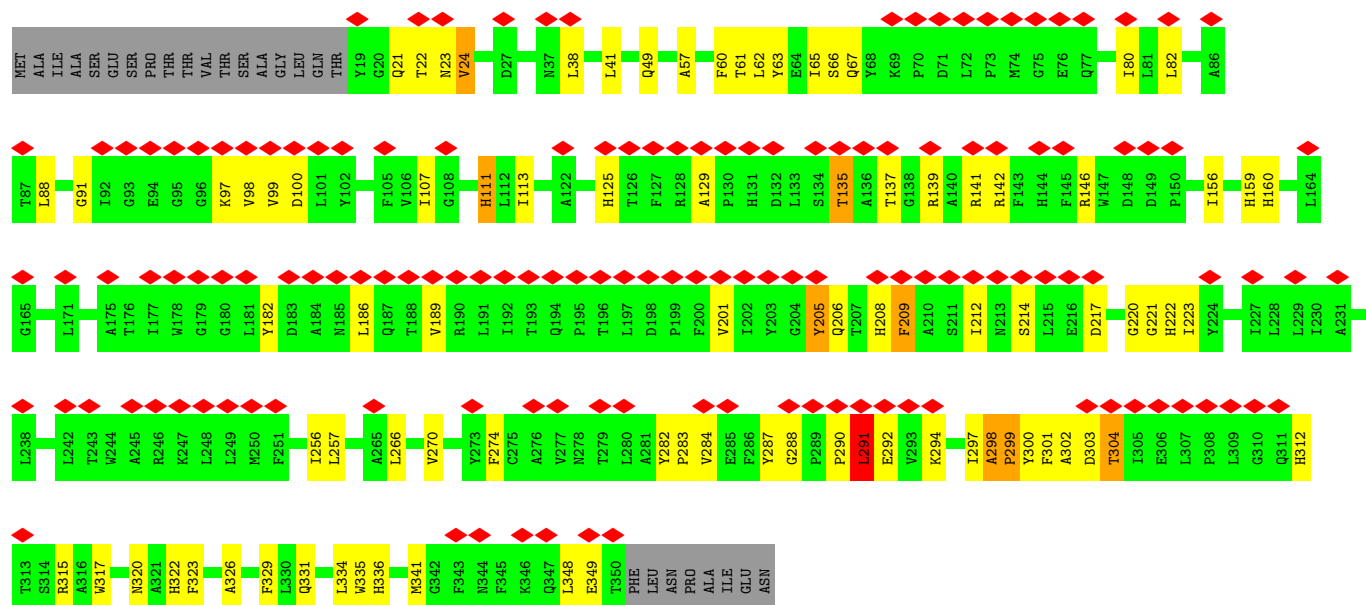
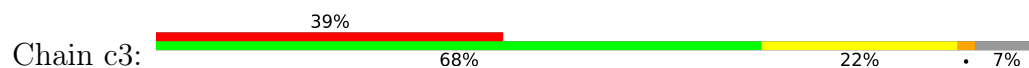


• Molecule 13: Iron stress in-duced protein A

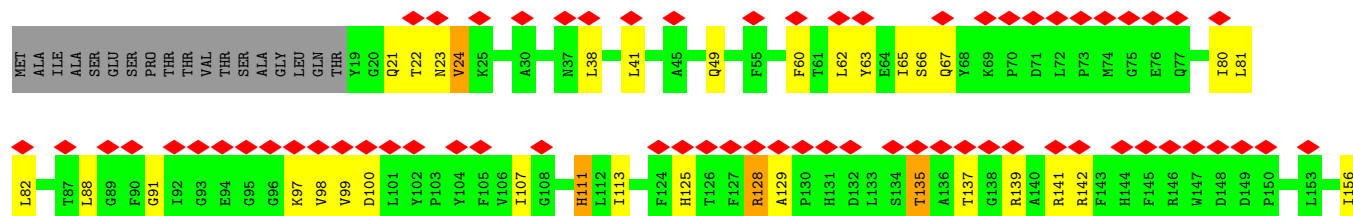
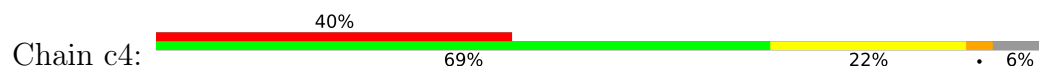


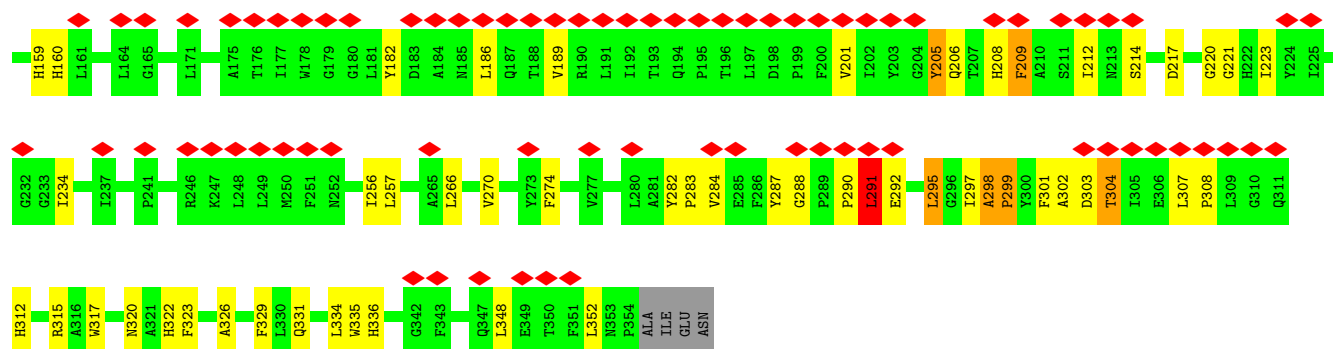


• Molecule 13: Iron stress in-duced protein A

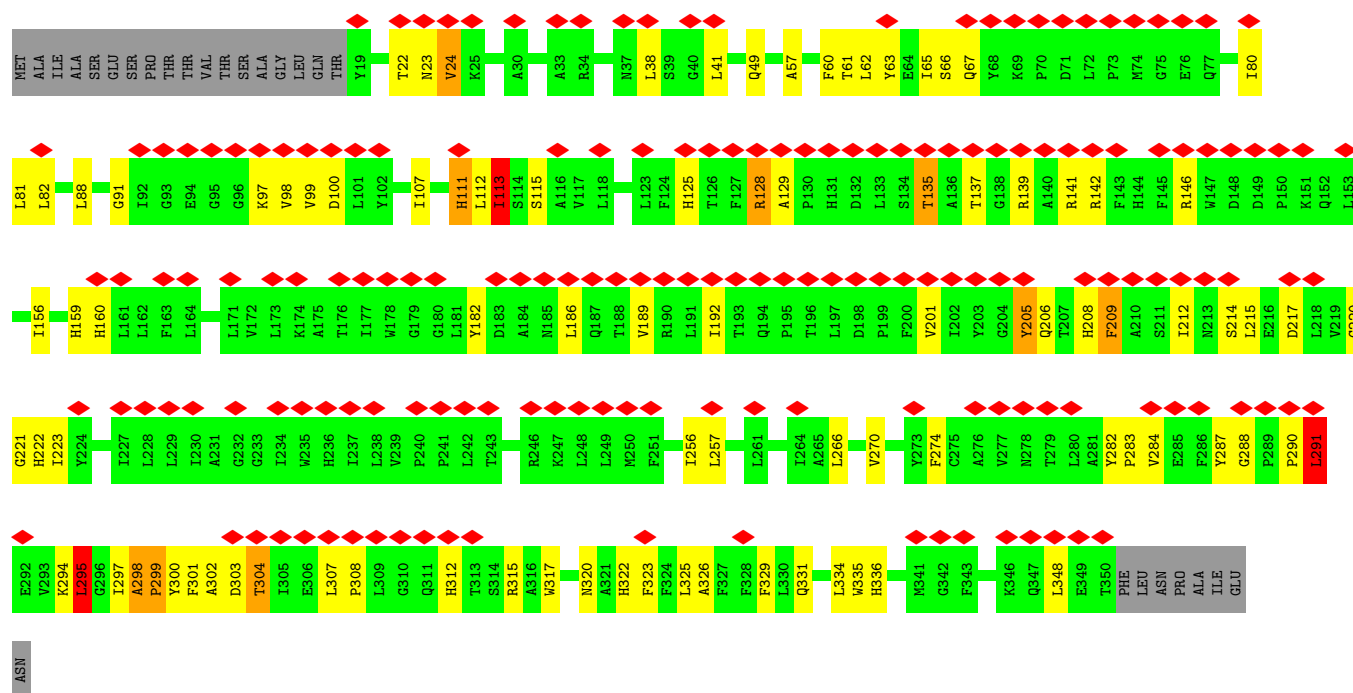


• Molecule 13: Iron stress in-duced protein A

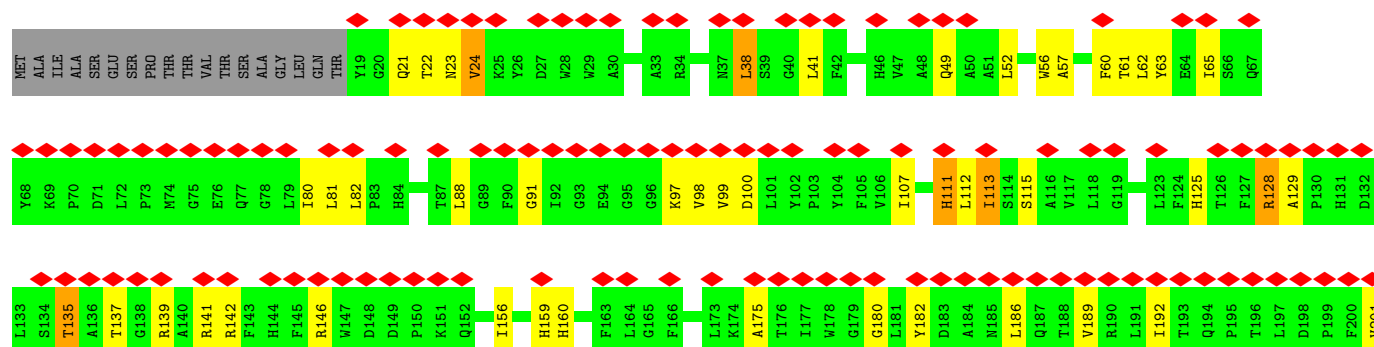


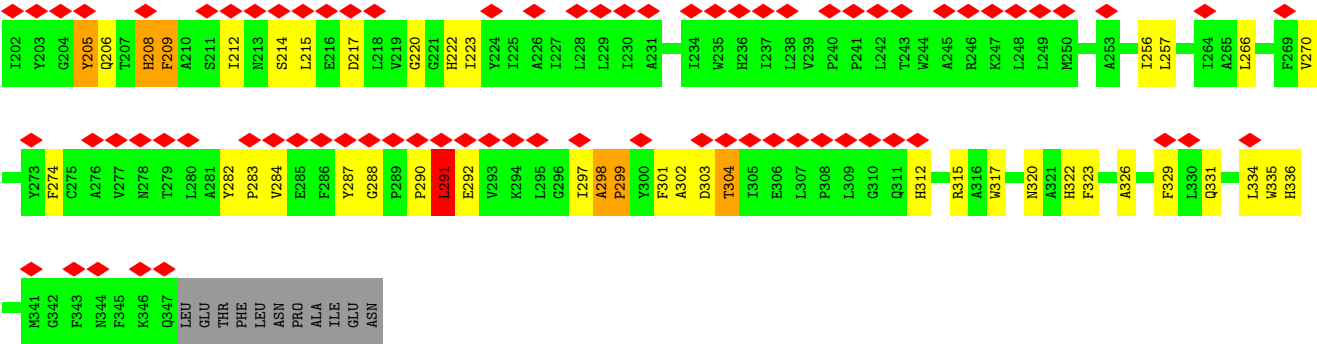


• Molecule 13: Iron stress in-duced protein A



• Molecule 13: Iron stress in-duced protein A





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	303983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.291	Depositor
Minimum map value	-0.149	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.035	Depositor
Map size (Å)	534.24, 534.24, 534.24	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.113, 1.113, 1.113	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	aA	0.53	0/6000	0.54	0/8180
1	bA	0.53	0/6000	0.54	0/8180
1	cA	0.53	0/6000	0.54	0/8180
2	aB	0.52	0/6096	0.57	0/8332
2	bB	0.52	0/6096	0.56	0/8332
2	cB	0.52	0/6096	0.57	0/8332
3	aC	0.52	0/608	0.70	2/824 (0.2%)
3	bC	0.52	0/608	0.70	2/824 (0.2%)
3	cC	0.52	0/608	0.70	2/824 (0.2%)
4	aD	0.42	0/1101	0.51	0/1492
4	bD	0.42	0/1101	0.51	0/1492
4	cD	0.42	0/1101	0.51	0/1492
5	aE	0.35	0/551	0.44	0/750
5	bE	0.35	0/551	0.44	0/750
5	cE	0.35	0/551	0.44	0/750
6	aF	0.41	0/1087	0.56	0/1476
6	bF	0.40	0/1087	0.55	0/1476
6	cF	0.41	0/1087	0.55	0/1476
7	aI	0.55	0/312	0.70	0/425
7	bI	0.55	0/312	0.70	0/425
7	cI	0.55	0/312	0.70	0/425
8	aJ	0.47	0/350	0.64	0/477
8	bJ	0.47	0/350	0.64	0/477
8	cJ	0.47	0/350	0.64	0/477
9	aK	0.23	0/206	0.34	0/281
9	bK	0.23	0/206	0.34	0/281
9	cK	0.23	0/206	0.34	0/281
10	aL	0.52	0/1148	0.54	0/1558
10	bL	0.52	0/1148	0.55	0/1558
10	cL	0.52	0/1148	0.54	0/1558
11	aM	0.44	0/244	0.60	0/332
11	bM	0.44	0/244	0.60	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	cM	0.44	0/244	0.60	0/332
12	aX	0.37	0/242	0.42	0/332
12	bX	0.37	0/242	0.42	0/332
12	cX	0.37	0/242	0.42	0/332
13	a1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	a2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	a3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	a4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	a5	0.41	1/2695 (0.0%)	0.75	15/3680 (0.4%)
13	a6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	b1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	b2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	b3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	b4	0.42	1/2731 (0.0%)	0.73	14/3730 (0.4%)
13	b5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	b6	0.40	1/2671 (0.0%)	0.74	15/3647 (0.4%)
13	c1	0.41	1/2671 (0.0%)	0.72	13/3647 (0.4%)
13	c2	0.40	1/2653 (0.0%)	0.73	14/3624 (0.4%)
13	c3	0.42	1/2695 (0.0%)	0.71	12/3680 (0.3%)
13	c4	0.42	1/2731 (0.0%)	0.72	14/3730 (0.4%)
13	c5	0.41	1/2695 (0.0%)	0.75	16/3680 (0.4%)
13	c6	0.40	1/2671 (0.0%)	0.72	14/3647 (0.4%)
All	All	0.46	18/102183 (0.0%)	0.64	256/139401 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	aB	0	1
2	bB	0	1
2	cB	0	1
6	aF	0	1
6	bF	0	1
6	cF	0	1
11	aM	0	1
11	bM	0	1
11	cM	0	1
13	a1	0	3
13	a2	0	3
13	a3	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
13	a4	0	3
13	a5	0	3
13	a6	0	3
13	b1	0	3
13	b2	0	3
13	b3	0	3
13	b4	0	3
13	b5	0	3
13	b6	0	3
13	c1	0	3
13	c2	0	3
13	c3	0	3
13	c4	0	3
13	c5	0	3
13	c6	0	3
All	All	0	63

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	b1	297	ILE	CB-CG2	-6.66	1.30	1.52
13	c4	297	ILE	CB-CG2	-6.66	1.30	1.52
13	a4	297	ILE	CB-CG2	-6.64	1.30	1.52
13	b4	297	ILE	CB-CG2	-6.64	1.30	1.52

The worst 5 of 256 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a1	113	ILE	N-CA-CB	-7.92	103.50	112.21
13	c1	113	ILE	N-CA-CB	-7.87	103.55	112.21
13	b6	113	ILE	N-CA-CB	-7.86	103.56	112.21
13	b5	113	ILE	N-CA-CB	-7.62	103.26	112.33
13	a6	113	ILE	N-CA-CB	-7.61	103.84	112.21

There are no chirality outliers.

5 of 63 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	a1	282	TYR	Peptide
13	a1	290	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	aB	234	GLN	Peptide
6	aF	125	ALA	Peptide
11	aM	29	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	aA	5801	0	5660	126	0
1	bA	5801	0	5660	126	0
1	cA	5801	0	5660	128	0
2	aB	5879	0	5627	119	0
2	bB	5879	0	5627	120	0
2	cB	5879	0	5627	121	0
3	aC	598	0	580	11	0
3	bC	598	0	580	12	0
3	cC	598	0	580	17	0
4	aD	1075	0	1077	20	0
4	bD	1075	0	1077	22	0
4	cD	1075	0	1077	24	0
5	aE	539	0	528	8	0
5	bE	539	0	528	8	0
5	cE	539	0	528	9	0
6	aF	1065	0	1077	29	0
6	bF	1065	0	1077	21	0
6	cF	1065	0	1077	30	0
7	aI	301	0	306	7	0
7	bI	301	0	306	3	0
7	cI	301	0	306	6	0
8	aJ	338	0	347	20	0
8	bJ	338	0	347	9	0
8	cJ	338	0	347	17	0
9	aK	208	0	106	0	0
9	bK	208	0	106	0	0
9	cK	208	0	106	0	0
10	aL	1119	0	1125	21	0
10	bL	1119	0	1125	23	0
10	cL	1119	0	1125	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	aM	241	0	264	6	0
11	bM	241	0	264	5	0
11	cM	241	0	264	5	0
12	aX	233	0	231	2	0
12	bX	233	0	231	2	0
12	cX	233	0	231	2	0
13	a1	2583	0	2568	69	0
13	a2	2565	0	2545	77	0
13	a3	2607	0	2590	64	0
13	a4	2641	0	2624	67	0
13	a5	2607	0	2591	67	0
13	a6	2583	0	2567	73	0
13	b1	2583	0	2568	69	0
13	b2	2565	0	2545	73	0
13	b3	2607	0	2590	65	0
13	b4	2641	0	2624	67	0
13	b5	2607	0	2591	62	0
13	b6	2583	0	2567	73	0
13	c1	2583	0	2568	69	0
13	c2	2565	0	2545	73	0
13	c3	2607	0	2590	62	0
13	c4	2641	0	2624	63	0
13	c5	2607	0	2591	68	0
13	c6	2583	0	2567	69	0
14	aA	65	0	72	4	0
14	bA	65	0	72	4	0
14	cA	65	0	72	3	0
15	a1	895	0	790	48	0
15	a2	960	0	862	64	0
15	a3	895	0	790	49	0
15	a4	895	0	792	53	0
15	a5	895	0	792	52	0
15	a6	895	0	790	53	0
15	aA	2557	0	2532	109	0
15	aB	2414	0	2369	111	0
15	aJ	127	0	91	5	0
15	aK	45	0	33	0	0
15	aL	195	0	216	11	0
15	aX	45	0	33	2	0
15	b1	830	0	720	41	0
15	b2	960	0	862	67	0
15	b3	895	0	790	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b4	895	0	792	54	0
15	b5	895	0	792	56	0
15	b6	895	0	790	53	0
15	bA	2557	0	2532	113	0
15	bB	2414	0	2369	113	0
15	bF	45	0	33	2	0
15	bJ	82	0	58	1	0
15	bK	45	0	33	0	0
15	bL	195	0	216	11	0
15	bX	45	0	33	3	0
15	c1	830	0	720	40	0
15	c2	960	0	862	65	0
15	c3	895	0	790	48	0
15	c4	895	0	792	47	0
15	c5	895	0	792	52	0
15	c6	830	0	720	43	0
15	cA	2506	0	2491	112	0
15	cB	2414	0	2369	109	0
15	cF	96	0	74	6	0
15	cJ	82	0	58	1	0
15	cK	45	0	33	0	0
15	cL	195	0	216	13	0
15	cX	45	0	33	2	0
16	aA	33	0	46	3	0
16	aB	33	0	46	3	0
16	bA	33	0	46	3	0
16	bB	33	0	46	4	0
16	cA	33	0	46	4	0
16	cB	33	0	46	3	0
17	aA	8	0	0	0	0
17	aC	16	0	0	0	0
17	bA	8	0	0	0	0
17	bC	16	0	0	0	0
17	cA	8	0	0	0	0
17	cC	16	0	0	0	0
18	a1	200	0	280	15	0
18	a2	160	0	224	14	0
18	a3	160	0	224	9	0
18	a4	160	0	224	13	0
18	a5	120	0	168	10	0
18	a6	200	0	280	14	0
18	aA	200	0	278	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	aB	225	0	313	16	0
18	aF	120	0	168	15	0
18	aI	120	0	168	10	0
18	aJ	80	0	112	8	0
18	aK	40	0	56	1	0
18	aL	40	0	56	1	0
18	aM	40	0	56	3	0
18	b1	160	0	224	13	0
18	b2	160	0	224	14	0
18	b3	160	0	224	11	0
18	b4	160	0	224	12	0
18	b5	120	0	168	9	0
18	b6	200	0	280	11	0
18	bA	240	0	334	15	0
18	bB	265	0	369	25	0
18	bF	40	0	56	5	0
18	bI	80	0	112	4	0
18	bJ	120	0	168	14	0
18	bL	120	0	168	6	0
18	bM	40	0	56	4	0
18	c1	160	0	224	12	0
18	c2	160	0	224	11	0
18	c3	160	0	224	9	0
18	c4	160	0	224	13	0
18	c5	120	0	168	9	0
18	c6	160	0	224	10	0
18	cA	200	0	278	13	0
18	cB	225	0	313	16	0
18	cF	120	0	168	17	0
18	cI	80	0	112	4	0
18	cJ	80	0	112	9	0
18	cK	40	0	56	1	0
18	cL	40	0	56	3	0
18	cM	40	0	56	4	0
19	aA	76	0	98	3	0
19	aX	23	0	16	1	0
19	bA	76	0	98	3	0
19	bX	23	0	16	0	0
19	cA	76	0	98	3	0
19	cX	23	0	16	0	0
20	aB	55	0	86	1	0
20	bB	55	0	86	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cB	55	0	86	1	0
21	aL	2	0	0	0	0
21	bL	1	0	0	0	0
22	aA	3	0	0	0	0
22	aB	3	0	0	0	0
22	aL	1	0	0	0	0
22	bA	3	0	0	0	0
22	bB	3	0	0	0	0
22	bL	1	0	0	0	0
22	cA	2	0	0	0	0
22	cB	3	0	0	0	0
22	cF	1	0	0	0	0
22	cL	1	0	0	0	0
All	All	137634	0	136044	3155	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 12.

The worst 5 of 3155 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)
13:a1:331:GLN:HE22	15:a1:414:CLA:C1B	1.70	1.04
13:c1:331:GLN:HE22	15:c1:415:CLA:C1B	1.70	1.04
13:b1:331:GLN:HE22	15:b1:415:CLA:C1B	1.71	1.03
13:b3:331:GLN:HE22	15:b3:415:CLA:C1B	1.73	1.01
13:c5:331:GLN:HE22	15:c5:415:CLA:C1B	1.74	1.00

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
1	bA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
1	cA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	69
2	aB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	bB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
2	cB	737/740 (100%)	699 (95%)	38 (5%)	0	100	100
3	aC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
3	bC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
3	cC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	6
4	aD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	bD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
4	cD	136/138 (99%)	126 (93%)	10 (7%)	0	100	100
5	aE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	bE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	cE	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
6	aF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	bF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
6	cF	139/164 (85%)	133 (96%)	6 (4%)	0	100	100
7	aI	36/38 (95%)	36 (100%)	0	0	100	100
7	bI	36/38 (95%)	36 (100%)	0	0	100	100
7	cI	36/38 (95%)	36 (100%)	0	0	100	100
8	aJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	bJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	cJ	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	aK	39/85 (46%)	39 (100%)	0	0	100	100
9	bK	39/85 (46%)	39 (100%)	0	0	100	100
9	cK	39/85 (46%)	39 (100%)	0	0	100	100
10	aL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	bL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
10	cL	149/154 (97%)	145 (97%)	4 (3%)	0	100	100
11	aM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	bM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	cM	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
12	aX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	bX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
12	cX	27/35 (77%)	26 (96%)	1 (4%)	0	100	100
13	a1	327/358 (91%)	301 (92%)	24 (7%)	2 (1%)	21	36
13	a2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	a3	330/358 (92%)	303 (92%)	24 (7%)	3 (1%)	14	26
13	a4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	a5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	a6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	b1	327/358 (91%)	299 (91%)	26 (8%)	2 (1%)	21	36
13	b2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	26
13	b3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	b4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	b5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	21	36
13	b6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	26
13	c1	327/358 (91%)	300 (92%)	25 (8%)	2 (1%)	21	36
13	c2	325/358 (91%)	298 (92%)	24 (7%)	3 (1%)	14	26
13	c3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	26
13	c4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	26
13	c5	330/358 (92%)	302 (92%)	26 (8%)	2 (1%)	21	36
13	c6	327/358 (91%)	298 (91%)	26 (8%)	3 (1%)	14	26
All	All	12561/13452 (93%)	11740 (94%)	764 (6%)	57 (0%)	26	40

5 of 57 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	aA	233	ALA
13	a1	283	PRO
13	a2	283	PRO
13	a3	283	PRO
13	a4	283	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	bA	592/604 (98%)	555 (94%)	37 (6%)	16	29
1	cA	592/604 (98%)	554 (94%)	38 (6%)	16	29
2	aB	595/597 (100%)	559 (94%)	36 (6%)	17	30
2	bB	595/597 (100%)	559 (94%)	36 (6%)	17	30
2	cB	595/597 (100%)	559 (94%)	36 (6%)	17	30
3	aC	67/67 (100%)	61 (91%)	6 (9%)	9	17
3	bC	67/67 (100%)	60 (90%)	7 (10%)	7	13
3	cC	67/67 (100%)	61 (91%)	6 (9%)	9	17
4	aD	115/115 (100%)	110 (96%)	5 (4%)	26	46
4	bD	115/115 (100%)	110 (96%)	5 (4%)	26	46
4	cD	115/115 (100%)	110 (96%)	5 (4%)	26	46
5	aE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	bE	59/64 (92%)	53 (90%)	6 (10%)	7	13
5	cE	59/64 (92%)	53 (90%)	6 (10%)	7	13
6	aF	109/128 (85%)	101 (93%)	8 (7%)	13	24
6	bF	109/128 (85%)	101 (93%)	8 (7%)	13	24
6	cF	109/128 (85%)	101 (93%)	8 (7%)	13	24
7	aI	32/32 (100%)	30 (94%)	2 (6%)	16	29
7	bI	32/32 (100%)	30 (94%)	2 (6%)	16	29
7	cI	32/32 (100%)	30 (94%)	2 (6%)	16	29
8	aJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
8	bJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
8	cJ	36/36 (100%)	32 (89%)	4 (11%)	6	11
10	aL	117/119 (98%)	110 (94%)	7 (6%)	17	31
10	bL	117/119 (98%)	110 (94%)	7 (6%)	17	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	cL	117/119 (98%)	110 (94%)	7 (6%)	17	31
11	aM	26/26 (100%)	21 (81%)	5 (19%)	1	2
11	bM	26/26 (100%)	21 (81%)	5 (19%)	1	2
11	cM	26/26 (100%)	21 (81%)	5 (19%)	1	2
12	aX	20/24 (83%)	19 (95%)	1 (5%)	22	40
12	bX	20/24 (83%)	19 (95%)	1 (5%)	22	40
12	cX	20/24 (83%)	19 (95%)	1 (5%)	22	40
13	a1	255/279 (91%)	240 (94%)	15 (6%)	18	32
13	a2	253/279 (91%)	238 (94%)	15 (6%)	18	32
13	a3	258/279 (92%)	242 (94%)	16 (6%)	16	30
13	a4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	a5	258/279 (92%)	241 (93%)	17 (7%)	15	28
13	a6	255/279 (91%)	239 (94%)	16 (6%)	16	29
13	b1	255/279 (91%)	240 (94%)	15 (6%)	18	32
13	b2	253/279 (91%)	238 (94%)	15 (6%)	18	32
13	b3	258/279 (92%)	243 (94%)	15 (6%)	18	33
13	b4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	b5	258/279 (92%)	241 (93%)	17 (7%)	15	28
13	b6	255/279 (91%)	239 (94%)	16 (6%)	16	29
13	c1	255/279 (91%)	240 (94%)	15 (6%)	18	32
13	c2	253/279 (91%)	239 (94%)	14 (6%)	19	35
13	c3	258/279 (92%)	242 (94%)	16 (6%)	16	30
13	c4	262/279 (94%)	246 (94%)	16 (6%)	17	30
13	c5	258/279 (92%)	240 (93%)	18 (7%)	14	26
13	c6	255/279 (91%)	240 (94%)	15 (6%)	18	32
All	All	9927/10458 (95%)	9291 (94%)	636 (6%)	18	29

5 of 636 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	63	SER
13	c3	88	LEU
2	cB	357	SER

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Mol	Chain	Res	Type
2	cB	48	SER
6	cF	104	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 110 such sidechains are listed below:

Mol	Chain	Res	Type
2	bB	614	GLN
13	b4	320	ASN
13	c6	320	ASN
4	cD	70	GLN
2	bB	639	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 759 ligands modelled in this entry, 3 are monoatomic - leaving 756 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	BCR	a1	417	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	aA	805	1	63,67,73	1.33	10 (15%)	75,105,113	1.54	11 (14%)
15	CLA	cA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	c5	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.65	10 (16%)
15	CLA	a4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	aX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	12 (20%)
15	CLA	cA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	bA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
18	BCR	c3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	cA	813	1	58,62,73	1.42	10 (17%)	69,99,113	1.42	10 (14%)
18	BCR	a3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.67	9 (16%)
15	CLA	c3	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.63	6 (11%)
18	BCR	bL	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	bA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	cB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
18	BCR	cB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	b3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	b5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	aB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	a3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
18	BCR	b2	401	-	41,41,41	1.24	4 (9%)	56,56,56	1.82	12 (21%)
15	CLA	bB	802	2	69,73,73	1.38	10 (14%)	83,113,113	1.50	9 (10%)
15	CLA	b3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.55	10 (16%)
15	CLA	cB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
15	CLA	aA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.58	11 (13%)
15	CLA	b3	417	13	59,63,73	1.57	8 (13%)	71,101,113	1.93	18 (25%)
15	CLA	a2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	a5	414	13	45,49,73	1.49	9 (20%)	54,84,113	1.62	7 (12%)
15	CLA	bJ	102	8	42,45,73	1.51	11 (26%)	50,78,113	1.64	5 (10%)
15	CLA	cA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	11 (14%)
15	CLA	aB	818	2	63,67,73	1.30	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	c2	408	-	49,53,73	1.48	9 (18%)	59,89,113	1.49	10 (16%)
15	CLA	b2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
18	BCR	a5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
15	CLA	aB	816	2	49,53,73	1.40	10 (20%)	59,89,113	1.73	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.60	14 (23%)
15	CLA	b6	415	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	bL	202	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
18	BCR	aL	205	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	b3	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.62	14 (23%)
15	CLA	bB	819	2	64,68,73	1.31	11 (17%)	77,107,113	1.60	10 (12%)
15	CLA	c4	405	13	49,53,73	1.55	11 (22%)	59,89,113	1.96	21 (35%)
18	BCR	bA	853	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	6 (10%)
18	BCR	b1	401	-	41,41,41	1.16	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	b3	405	13	49,53,73	1.55	11 (22%)	59,89,113	1.93	18 (30%)
15	CLA	c5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	7 (12%)
15	CLA	c1	416	13	54,58,73	1.52	11 (20%)	65,95,113	2.27	17 (26%)
15	CLA	a6	413	13	49,53,73	1.56	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	cA	827	22	69,73,73	1.31	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	a2	404	13	69,73,73	1.27	10 (14%)	83,113,113	1.40	9 (10%)
15	CLA	bA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
15	CLA	a4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
18	BCR	aB	845	-	41,41,41	1.11	3 (7%)	56,56,56	1.28	6 (10%)
15	CLA	aA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	c1	410	13,15	68,72,73	1.29	11 (16%)	81,111,113	1.60	15 (18%)
15	CLA	a2	409	13	49,53,73	1.44	9 (18%)	59,89,113	1.57	8 (13%)
15	CLA	cA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.48	10 (12%)
15	CLA	bB	811	2	69,73,73	1.29	10 (14%)	83,113,113	1.70	12 (14%)
15	CLA	aB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
15	CLA	a1	422	13	69,73,73	1.42	14 (20%)	83,113,113	1.98	20 (24%)
18	BCR	cK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
15	CLA	b1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	a1	411	13	49,53,73	1.56	11 (22%)	59,89,113	1.70	14 (23%)
15	CLA	b1	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	aB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)
15	CLA	c2	415	13	45,49,73	1.51	7 (15%)	54,84,113	1.60	5 (9%)
15	CLA	c3	402	13	69,73,73	1.24	10 (14%)	83,113,113	1.34	7 (8%)
15	CLA	aB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)
15	CLA	bB	804	-	69,73,73	1.36	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	aB	839	22	69,73,73	1.24	11 (15%)	83,113,113	1.42	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	b3	418	-	41,41,41	1.43	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	bA	842	22	55,59,73	1.41	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	b6	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	cA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
18	BCR	bB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	9 (16%)
15	CLA	c5	410	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.63	15 (18%)
15	CLA	bB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	cK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
15	CLA	b5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.37	6 (7%)
15	CLA	c3	412	13	49,53,73	1.56	10 (20%)	59,89,113	1.62	14 (23%)
18	BCR	a5	418	-	41,41,41	1.39	6 (14%)	56,56,56	1.53	10 (17%)
15	CLA	cB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	c6	414	13	49,53,73	1.52	7 (14%)	59,89,113	1.64	8 (13%)
15	CLA	b1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	c1	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	bB	827	2	69,73,73	1.29	11 (15%)	83,113,113	1.55	14 (16%)
15	CLA	b2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
15	CLA	b4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
17	SF4	bA	847	2,1	0,12,12	-	-	-	-	-
15	CLA	aA	844	-	46,49,73	1.46	8 (17%)	55,83,113	1.60	4 (7%)
15	CLA	cB	803	-	69,73,73	1.31	8 (11%)	83,113,113	1.51	14 (16%)
15	CLA	bA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	17 (25%)
15	CLA	c1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	17 (23%)
15	CLA	aA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	aB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	11 (13%)
15	CLA	a3	403	13,15	69,73,73	1.21	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	aJ	203	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
15	CLA	b4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	7 (8%)
18	BCR	cA	847	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	cJ	101	8	49,53,73	1.46	11 (22%)	59,89,113	1.64	7 (11%)
20	LMG	cB	850	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	bB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.55	9 (10%)
15	CLA	b2	402	13	69,73,73	1.25	8 (11%)	83,113,113	1.35	6 (7%)
18	BCR	aJ	205	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	aA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	10 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	12 (20%)
15	CLA	c1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
18	BCR	b4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
18	BCR	b5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.54	10 (17%)
15	CLA	c1	405	13	49,53,73	1.55	9 (18%)	59,89,113	1.91	19 (32%)
14	CL0	cA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	bA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.65	6 (10%)
15	CLA	a5	403	13,15	69,73,73	1.23	10 (14%)	83,113,113	1.42	10 (12%)
15	CLA	c6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
18	BCR	aB	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.35	9 (16%)
15	CLA	bF	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
15	CLA	a6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.62	8 (13%)
15	CLA	bA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	a3	413	13	49,53,73	1.51	11 (22%)	59,89,113	1.50	6 (10%)
15	CLA	b6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.83	11 (18%)
15	CLA	cA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)
15	CLA	cL	201	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	a2	405	13	49,53,73	1.58	8 (16%)	59,89,113	1.95	19 (32%)
15	CLA	c5	412	13	49,53,73	1.55	9 (18%)	59,89,113	1.62	14 (23%)
15	CLA	c5	405	13	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
15	CLA	aA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.48	7 (11%)
15	CLA	a3	405	13	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
18	BCR	b6	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	b2	411	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.58	15 (18%)
18	BCR	bJ	105	-	41,41,41	1.20	5 (12%)	56,56,56	1.35	9 (16%)
15	CLA	bB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.74	7 (11%)
15	CLA	a3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
18	BCR	aI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
15	CLA	cA	823	1	53,57,73	1.39	9 (16%)	62,93,113	1.47	6 (9%)
18	BCR	bJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	a1	402	13,15	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	bA	821	18,1	65,69,73	1.30	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	a6	416	13	49,53,73	1.51	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	cF	203	-	49,53,73	1.51	10 (20%)	59,89,113	1.67	11 (18%)
15	CLA	a3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	c5	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	c1	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	5 (8%)
15	CLA	a1	410	13	49,53,73	1.49	11 (22%)	59,89,113	1.65	8 (13%)
18	BCR	a1	419	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	aB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
14	CL0	bA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	a6	415	13	45,49,73	1.52	9 (20%)	54,84,113	1.59	6 (11%)
15	CLA	aA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.45	6 (9%)
15	CLA	c3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.47	7 (11%)
18	BCR	b6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
15	CLA	b6	407	13	49,53,73	1.46	9 (18%)	59,89,113	1.49	7 (11%)
18	BCR	aB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.58	8 (24%)
18	BCR	cI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.28	5 (8%)
15	CLA	a2	413	13	49,53,73	1.57	11 (22%)	59,89,113	1.65	15 (25%)
15	CLA	a5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	bB	823	-	59,63,73	1.30	10 (16%)	71,101,113	1.51	7 (9%)
17	SF4	aC	102	3	0,12,12	-	-	-	-	-
15	CLA	cA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.34	8 (9%)
15	CLA	c3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	cX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.67	11 (18%)
15	CLA	cA	803	-	69,73,73	1.28	12 (17%)	83,113,113	1.74	15 (18%)
15	CLA	bA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
15	CLA	a3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.64	10 (16%)
18	BCR	b4	420	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	aA	823	1	53,57,73	1.40	9 (16%)	62,93,113	1.46	6 (9%)
15	CLA	a3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.83	12 (20%)
15	CLA	c3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.60	10 (16%)
15	CLA	c6	407	13	49,53,73	1.45	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	c2	422	13	69,73,73	1.36	11 (15%)	83,113,113	1.80	19 (22%)
15	CLA	aA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	aA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
15	CLA	aA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	cA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.69	12 (18%)
18	BCR	aA	848	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
18	BCR	cA	849	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b3	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
18	BCR	bB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	aB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.53	8 (12%)
15	CLA	c4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	b5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.50	8 (13%)
18	BCR	c2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.52	9 (16%)
15	CLA	b1	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.92	16 (22%)
15	CLA	a5	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.62	15 (18%)
15	CLA	aA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	cA	818	1	58,62,73	1.33	10 (17%)	69,99,113	1.60	9 (13%)
18	BCR	c2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.84	11 (19%)
18	BCR	cJ	104	-	41,41,41	1.31	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	c3	416	13	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
18	BCR	bB	849	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	10 (17%)
15	CLA	c2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.58	9 (15%)
18	BCR	aA	851	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	b4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	bA	805	1	63,67,73	1.33	11 (17%)	75,105,113	1.54	11 (14%)
15	CLA	cA	816	1	49,53,73	1.47	10 (20%)	59,89,113	1.66	6 (10%)
15	CLA	c3	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.62	14 (17%)
19	LHG	bA	855	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	aB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.52	9 (10%)
15	CLA	aB	820	2,22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	a6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
15	CLA	bA	832	1	54,58,73	1.37	10 (18%)	65,95,113	1.69	8 (12%)
15	CLA	cB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.56	5 (8%)
15	CLA	aB	836	2	64,68,73	1.37	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	b1	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	8 (9%)
15	CLA	c6	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	14 (19%)
15	CLA	b2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)
15	CLA	b5	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.36	8 (9%)
18	BCR	a3	418	-	41,41,41	1.44	5 (12%)	56,56,56	1.55	10 (17%)
15	CLA	cA	807	1	69,73,73	1.36	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	a2	411	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
18	BCR	aF	201	-	41,41,41	1.31	4 (9%)	56,56,56	1.37	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	a5	405	13	49,53,73	1.55	10 (20%)	59,89,113	1.97	22 (37%)
15	CLA	a2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	cB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.43	7 (8%)
15	CLA	c3	404	13	69,73,73	1.26	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	aA	845	19	56,60,73	1.41	12 (21%)	67,97,113	2.02	18 (26%)
15	CLA	c4	403	13,15	69,73,73	1.23	8 (11%)	83,113,113	1.40	8 (9%)
15	CLA	b3	403	13,15	69,73,73	1.21	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	cA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)
15	CLA	b6	411	13,15	68,72,73	1.31	12 (17%)	81,111,113	1.57	15 (18%)
15	CLA	cA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	aA	814	1	64,68,73	1.36	11 (17%)	77,107,113	1.38	7 (9%)
15	CLA	b2	409	13	49,53,73	1.43	9 (18%)	59,89,113	1.59	10 (16%)
15	CLA	aB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	c1	415	13	49,53,73	1.47	9 (18%)	59,89,113	1.83	11 (18%)
15	CLA	aB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	a5	416	13	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
18	BCR	b1	418	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	8 (14%)
19	LHG	cX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	b1	416	13	54,58,73	1.52	9 (16%)	65,95,113	2.25	17 (26%)
15	CLA	bB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	a1	408	13	69,73,73	1.26	8 (11%)	83,113,113	1.30	9 (10%)
18	BCR	a5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	11 (19%)
18	BCR	c6	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	c2	417	13	54,58,73	1.58	11 (20%)	65,95,113	2.35	19 (29%)
15	CLA	b2	422	13	69,73,73	1.37	11 (15%)	83,113,113	1.82	19 (22%)
15	CLA	bB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.51	14 (16%)
15	CLA	aA	815	1	49,53,73	1.48	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	aA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
18	BCR	b5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.52	12 (21%)
15	CLA	c4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.59	8 (13%)
15	CLA	b1	414	13	45,49,73	1.51	9 (20%)	54,84,113	1.57	8 (14%)
15	CLA	cA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	c5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	c2	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.39	9 (10%)
15	CLA	cB	816	2	49,53,73	1.41	10 (20%)	59,89,113	1.72	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	a6	406	13	49,53,73	1.57	8 (16%)	59,89,113	1.92	19 (32%)
15	CLA	c3	403	13,15	69,73,73	1.22	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	c5	404	13	69,73,73	1.26	10 (14%)	83,113,113	1.37	9 (10%)
18	BCR	aI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	b2	405	13	49,53,73	1.59	8 (16%)	59,89,113	1.94	19 (32%)
15	CLA	b5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
18	BCR	aA	849	15	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	c4	410	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	a5	413	13	49,53,73	1.50	9 (18%)	59,89,113	1.50	5 (8%)
15	CLA	cA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.55	9 (13%)
15	CLA	a1	401	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
15	CLA	c4	402	13	69,73,73	1.22	8 (11%)	83,113,113	1.38	8 (9%)
15	CLA	cB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	a6	417	13	54,58,73	1.52	10 (18%)	65,95,113	2.28	17 (26%)
15	CLA	c3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.92	18 (25%)
15	CLA	b1	405	13	49,53,73	1.55	8 (16%)	59,89,113	1.91	20 (33%)
18	BCR	cB	848	-	41,41,41	1.33	4 (9%)	56,56,56	1.50	8 (14%)
15	CLA	aB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)
18	BCR	b3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	10 (17%)
18	BCR	b5	419	-	41,41,41	1.16	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	aA	816	1	49,53,73	1.46	11 (22%)	59,89,113	1.65	6 (10%)
15	CLA	a6	404	13,15	69,73,73	1.22	9 (13%)	83,113,113	1.42	10 (12%)
15	CLA	b3	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	cA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.36	9 (10%)
15	CLA	aB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	b1	403	13,15	69,73,73	1.24	9 (13%)	83,113,113	1.45	10 (12%)
15	CLA	bA	843	1	69,73,73	1.32	10 (14%)	83,113,113	1.50	8 (9%)
15	CLA	a3	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	18 (25%)
15	CLA	cL	202	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
15	CLA	c6	415	13	45,49,73	1.52	8 (17%)	54,84,113	1.60	6 (11%)
15	CLA	c3	405	13	49,53,73	1.56	11 (22%)	59,89,113	1.93	19 (32%)
18	BCR	b6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	b2	413	13	49,53,73	1.57	10 (20%)	59,89,113	1.66	15 (25%)
15	CLA	a5	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.55	10 (16%)
15	CLA	a5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bB	817	2	59,63,73	1.36	8 (13%)	71,101,113	1.63	14 (19%)
18	BCR	c6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.70	10 (17%)
19	LHG	aX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	bB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.53	8 (9%)
15	CLA	c4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.34	8 (9%)
18	BCR	a4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
18	BCR	cF	202	-	41,41,41	1.30	5 (12%)	56,56,56	1.37	9 (16%)
15	CLA	bA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	a3	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.60	14 (17%)
15	CLA	a4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
16	PQN	cA	845	-	34,34,34	1.40	2 (5%)	42,45,45	1.14	5 (11%)
19	LHG	aA	854	15	26,26,48	0.97	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	c3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.61	15 (18%)
15	CLA	bB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	b5	408	13	49,53,73	1.45	11 (22%)	59,89,113	1.62	9 (15%)
15	CLA	aA	803	-	69,73,73	1.27	12 (17%)	83,113,113	1.74	15 (18%)
15	CLA	a6	412	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	11 (18%)
15	CLA	b5	416	13	54,58,73	1.53	9 (16%)	65,95,113	2.27	16 (24%)
15	CLA	a4	407	-	49,53,73	1.47	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	b1	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.43	4 (6%)
15	CLA	cA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	cA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
15	CLA	b2	403	13,15	69,73,73	1.23	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	bA	811	1	49,53,73	1.45	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	b5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.93	16 (22%)
18	BCR	c6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
15	CLA	b2	406	13	69,73,73	1.41	12 (17%)	83,113,113	1.89	21 (25%)
15	CLA	cB	815	2	69,73,73	1.22	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	c3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.50	6 (10%)
15	CLA	a4	416	13	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	c1	403	13,15	69,73,73	1.24	9 (13%)	83,113,113	1.43	10 (12%)
15	CLA	cB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	a3	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.37	8 (9%)
18	BCR	a1	418	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	c1	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.56	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aJ	202	8	49,53,73	1.45	12 (24%)	59,89,113	1.65	7 (11%)
19	LHG	cA	852	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	a3	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.35	7 (8%)
15	CLA	bA	827	22	69,73,73	1.30	8 (11%)	83,113,113	1.48	13 (15%)
15	CLA	cA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.48	10 (15%)
15	CLA	aA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	7 (8%)
15	CLA	b4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)
15	CLA	a2	416	13	49,53,73	1.48	9 (18%)	59,89,113	1.81	11 (18%)
15	CLA	cA	832	1	54,58,73	1.36	10 (18%)	65,95,113	1.70	8 (12%)
15	CLA	c4	411	13	49,53,73	1.49	11 (22%)	59,89,113	1.66	9 (15%)
15	CLA	c5	406	13	49,53,73	1.45	9 (18%)	59,89,113	1.50	6 (10%)
15	CLA	c4	413	13	49,53,73	1.52	10 (20%)	59,89,113	1.49	6 (10%)
17	SF4	cA	846	2,1	0,12,12	-	-	-	-	-
15	CLA	b2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.92	15 (21%)
15	CLA	bA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	9 (13%)
15	CLA	aA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	4 (6%)
15	CLA	bA	818	1	58,62,73	1.34	11 (18%)	69,99,113	1.61	9 (13%)
15	CLA	aA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.50	12 (14%)
15	CLA	bA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	b4	410	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.60	14 (17%)
15	CLA	cA	820	1	69,73,73	1.30	10 (14%)	83,113,113	1.51	11 (13%)
15	CLA	aL	202	10	69,73,73	1.26	10 (14%)	83,113,113	1.59	11 (13%)
15	CLA	c5	407	-	49,53,73	1.46	8 (16%)	59,89,113	1.54	9 (15%)
15	CLA	bB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.64	8 (13%)
15	CLA	bB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	10 (12%)
15	CLA	bA	824	1	55,59,73	1.38	11 (20%)	66,96,113	1.46	6 (9%)
16	PQN	aB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
15	CLA	c6	411	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.57	15 (18%)
19	LHG	bX	101	-	22,22,48	0.89	1 (4%)	25,28,54	1.17	2 (8%)
15	CLA	aB	841	-	49,53,73	1.52	10 (20%)	59,89,113	1.56	9 (15%)
15	CLA	a1	403	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
18	BCR	b4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.50	9 (16%)
17	SF4	aC	101	3	0,12,12	-	-	-	-	-
15	CLA	aL	201	10	69,73,73	1.28	10 (14%)	83,113,113	1.28	8 (9%)
15	CLA	aB	827	2	69,73,73	1.28	10 (14%)	83,113,113	1.56	14 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	cB	834	2	62,66,73	1.31	11 (17%)	74,104,113	1.48	9 (12%)
15	CLA	bB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	c4	415	13	49,53,73	1.47	8 (16%)	59,89,113	1.85	12 (20%)
15	CLA	c4	416	13	54,58,73	1.54	9 (16%)	65,95,113	2.27	17 (26%)
15	CLA	b5	414	13	45,49,73	1.50	9 (20%)	54,84,113	1.64	6 (11%)
15	CLA	bA	835	1	69,73,73	1.28	10 (14%)	83,113,113	1.56	10 (12%)
15	CLA	bB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	cB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
17	SF4	bC	102	3	0,12,12	-	-	-	-	-
15	CLA	bA	825	1	63,67,73	1.31	10 (15%)	75,105,113	1.37	12 (16%)
15	CLA	b4	405	13	49,53,73	1.55	10 (20%)	59,89,113	1.97	18 (30%)
15	CLA	c1	412	13	49,53,73	1.56	11 (22%)	59,89,113	1.67	13 (22%)
15	CLA	aB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.59	7 (11%)
15	CLA	bA	817	-	53,57,73	1.40	7 (13%)	62,93,113	1.43	5 (8%)
15	CLA	aB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.62	8 (13%)
15	CLA	b6	409	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	9 (15%)
15	CLA	cA	835	1	69,73,73	1.27	9 (13%)	83,113,113	1.55	10 (12%)
15	CLA	b2	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.39	9 (10%)
15	CLA	c5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.85	17 (20%)
15	CLA	a1	412	13	49,53,73	1.51	10 (20%)	59,89,113	1.45	4 (6%)
15	CLA	bB	836	2	64,68,73	1.38	9 (14%)	77,107,113	1.49	10 (12%)
15	CLA	aB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.47	11 (13%)
15	CLA	b4	403	13,15	69,73,73	1.22	8 (11%)	83,113,113	1.40	8 (9%)
15	CLA	b5	405	13	49,53,73	1.54	10 (20%)	59,89,113	1.97	22 (37%)
18	BCR	b2	419	-	41,41,41	1.36	5 (12%)	56,56,56	1.55	9 (16%)
15	CLA	cB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.78	15 (18%)
18	BCR	b6	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.53	8 (14%)
15	CLA	bA	834	1	69,73,73	1.34	12 (17%)	83,113,113	1.56	11 (13%)
18	BCR	a6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.52	11 (19%)
15	CLA	aA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.38	7 (8%)
15	CLA	aK	102	-	49,53,73	1.47	11 (22%)	59,89,113	1.51	10 (16%)
15	CLA	a5	409	13	69,73,73	1.28	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	b4	406	13	49,53,73	1.44	9 (18%)	59,89,113	1.49	7 (11%)
15	CLA	b6	406	13	49,53,73	1.58	8 (16%)	59,89,113	1.92	19 (32%)
18	BCR	bA	851	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c4	414	13	45,49,73	1.53	9 (20%)	54,84,113	1.59	5 (9%)
15	CLA	c6	409	13	49,53,73	1.46	10 (20%)	59,89,113	1.61	9 (15%)
18	BCR	cA	851	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
18	BCR	cF	205	-	41,41,41	1.21	5 (12%)	56,56,56	1.34	8 (14%)
18	BCR	aA	852	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	6 (10%)
18	BCR	bA	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.41	9 (16%)
15	CLA	aJ	201	-	49,53,73	1.52	10 (20%)	59,89,113	1.66	11 (18%)
15	CLA	cA	821	18,1	65,69,73	1.31	12 (18%)	78,108,113	1.41	7 (8%)
19	LHG	cA	853	15	26,26,48	0.98	1 (3%)	29,32,54	1.38	3 (10%)
15	CLA	c2	414	13	49,53,73	1.52	10 (20%)	59,89,113	1.52	6 (10%)
17	SF4	bC	101	3	0,12,12	-	-	-	-	-
18	BCR	c1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.65	12 (21%)
15	CLA	cA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
15	CLA	cB	836	2	64,68,73	1.38	10 (15%)	77,107,113	1.49	10 (12%)
15	CLA	a3	416	13	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	cB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.50	10 (12%)
18	BCR	aI	103	-	41,41,41	1.31	4 (9%)	56,56,56	1.44	9 (16%)
15	CLA	a5	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.65	10 (16%)
18	BCR	bI	101	-	41,41,41	1.25	2 (4%)	56,56,56	1.29	6 (10%)
18	BCR	c2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.45	8 (14%)
18	BCR	c6	401	-	41,41,41	1.18	4 (9%)	56,56,56	1.53	11 (19%)
15	CLA	bA	823	1	53,57,73	1.41	10 (18%)	62,93,113	1.46	6 (9%)
15	CLA	c6	406	13	49,53,73	1.57	9 (18%)	59,89,113	1.93	19 (32%)
15	CLA	aA	809	1	69,73,73	1.24	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	a3	421	13	69,73,73	1.40	11 (15%)	83,113,113	1.62	15 (18%)
15	CLA	a6	414	13	49,53,73	1.50	12 (24%)	59,89,113	1.68	10 (16%)
15	CLA	cA	822	-	69,73,73	1.26	10 (14%)	83,113,113	1.43	8 (9%)
15	CLA	c2	403	13,15	69,73,73	1.23	9 (13%)	83,113,113	1.42	9 (10%)
18	BCR	c3	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.54	10 (17%)
15	CLA	bB	826	2,22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
15	CLA	a1	407	13	49,53,73	1.45	10 (20%)	59,89,113	1.59	8 (13%)
16	PQN	aA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	a5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.39	6 (7%)
15	CLA	bB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.79	15 (18%)
18	BCR	a2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.44	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	a6	402	-	41,41,41	1.24	4 (9%)	56,56,56	1.71	10 (17%)
15	CLA	a2	408	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	11 (18%)
18	BCR	aJ	204	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	b5	413	13	49,53,73	1.50	10 (20%)	59,89,113	1.49	5 (8%)
18	BCR	bB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.58	8 (24%)
15	CLA	bB	821	2	51,55,73	1.45	11 (21%)	61,91,113	1.46	4 (6%)
15	CLA	b2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.61	5 (9%)
15	CLA	a3	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	11 (18%)
18	BCR	bF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	b6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.55	9 (15%)
15	CLA	bB	806	2	69,73,73	1.26	12 (17%)	83,113,113	1.53	9 (10%)
15	CLA	cB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.68	12 (14%)
15	CLA	aB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.58	12 (14%)
15	CLA	bB	807	2	69,73,73	1.38	12 (17%)	83,113,113	1.49	9 (10%)
15	CLA	a1	405	13	49,53,73	1.46	9 (18%)	59,89,113	1.47	8 (13%)
15	CLA	cB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	a4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.68	16 (19%)
15	CLA	a4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.37	8 (9%)
15	CLA	bA	803	-	69,73,73	1.28	13 (18%)	83,113,113	1.74	15 (18%)
18	BCR	cB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
15	CLA	aA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
15	CLA	aA	807	1	69,73,73	1.35	11 (15%)	83,113,113	1.49	14 (16%)
15	CLA	bA	802	22	69,73,73	1.41	12 (17%)	83,113,113	1.44	10 (12%)
18	BCR	aF	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	10 (17%)
15	CLA	a2	415	13	45,49,73	1.51	8 (17%)	54,84,113	1.60	5 (9%)
15	CLA	cB	811	2	69,73,73	1.28	8 (11%)	83,113,113	1.70	12 (14%)
18	BCR	b3	401	-	41,41,41	1.28	4 (9%)	56,56,56	1.66	9 (16%)
15	CLA	cB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.60	7 (11%)
18	BCR	a4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)
15	CLA	aB	811	2	69,73,73	1.29	9 (13%)	83,113,113	1.69	12 (14%)
20	LMG	bB	851	-	55,55,55	1.07	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	b5	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.61	15 (18%)
15	CLA	b6	410	13	69,73,73	1.25	9 (13%)	83,113,113	1.33	9 (10%)
18	BCR	bB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
15	CLA	b3	411	13	49,53,73	1.49	10 (20%)	59,89,113	1.63	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	cB	842	-	49,53,73	1.47	8 (16%)	59,89,113	1.40	3 (5%)
18	BCR	b6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
18	BCR	bB	850	-	41,41,41	1.41	5 (12%)	56,56,56	1.30	8 (14%)
15	CLA	aB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	aA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
14	CL0	aA	801	1	69,73,73	1.92	18 (26%)	83,113,113	2.86	36 (43%)
15	CLA	a3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.62	6 (11%)
15	CLA	cA	811	1	49,53,73	1.46	11 (22%)	59,89,113	1.47	7 (11%)
15	CLA	bB	840	2	69,73,73	1.31	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	aB	803	-	69,73,73	1.32	8 (11%)	83,113,113	1.52	15 (18%)
15	CLA	bA	812	1	69,73,73	1.26	10 (14%)	83,113,113	1.35	10 (12%)
15	CLA	aA	818	1	58,62,73	1.34	10 (17%)	69,99,113	1.62	8 (11%)
15	CLA	bB	833	2	69,73,73	1.30	11 (15%)	83,113,113	1.42	12 (14%)
15	CLA	b4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	c2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
15	CLA	a6	411	13,15	68,72,73	1.32	11 (16%)	81,111,113	1.57	15 (18%)
15	CLA	bB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	b6	413	13	49,53,73	1.55	10 (20%)	59,89,113	1.59	14 (23%)
15	CLA	aB	802	2	69,73,73	1.37	10 (14%)	83,113,113	1.51	9 (10%)
15	CLA	b5	420	13	69,73,73	1.34	12 (17%)	83,113,113	1.84	17 (20%)
15	CLA	b1	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.79	11 (18%)
15	CLA	b2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.48	7 (11%)
15	CLA	cB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	bA	815	1	49,53,73	1.49	12 (24%)	59,89,113	1.53	9 (15%)
15	CLA	c5	416	13	54,58,73	1.53	9 (16%)	65,95,113	2.26	16 (24%)
18	BCR	a4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.49	11 (19%)
18	BCR	cI	102	-	41,41,41	1.37	3 (7%)	56,56,56	1.41	9 (16%)
20	LMG	aB	850	-	55,55,55	1.07	4 (7%)	63,63,63	1.62	8 (12%)
15	CLA	aA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.51	11 (13%)
15	CLA	cF	201	22	55,59,73	1.42	10 (18%)	66,96,113	1.33	8 (12%)
15	CLA	b1	407	-	49,53,73	1.46	9 (18%)	59,89,113	1.56	8 (13%)
18	BCR	cA	848	15	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
18	BCR	c1	418	-	41,41,41	1.37	5 (12%)	56,56,56	1.54	11 (19%)
18	BCR	a1	421	-	41,41,41	1.11	3 (7%)	56,56,56	1.59	9 (16%)
15	CLA	c2	416	13	49,53,73	1.49	9 (18%)	59,89,113	1.82	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bA	804	1	69,73,73	1.31	10 (14%)	83,113,113	1.51	10 (12%)
15	CLA	a6	408	-	49,53,73	1.47	9 (18%)	59,89,113	1.54	9 (15%)
15	CLA	a6	422	13	69,73,73	1.50	15 (21%)	83,113,113	2.17	21 (25%)
15	CLA	aA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	11 (13%)
18	BCR	bA	849	-	41,41,41	1.20	3 (7%)	56,56,56	1.39	6 (10%)
15	CLA	c2	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
15	CLA	aA	813	1	58,62,73	1.43	10 (17%)	69,99,113	1.42	10 (14%)
15	CLA	bA	841	1	69,73,73	1.25	10 (14%)	83,113,113	1.33	8 (9%)
15	CLA	cA	834	1	69,73,73	1.33	12 (17%)	83,113,113	1.56	11 (13%)
15	CLA	aB	840	2	69,73,73	1.30	11 (15%)	83,113,113	1.67	12 (14%)
15	CLA	aA	842	22	55,59,73	1.41	9 (16%)	66,96,113	1.33	8 (12%)
15	CLA	bK	101	-	49,53,73	1.48	11 (22%)	59,89,113	1.52	10 (16%)
18	BCR	bL	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
15	CLA	a1	416	13	59,63,73	1.54	9 (15%)	71,101,113	1.93	17 (23%)
15	CLA	cA	844	19	56,60,73	1.41	12 (21%)	67,97,113	2.01	17 (25%)
19	LHG	aA	853	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
15	CLA	b4	415	13	49,53,73	1.48	9 (18%)	59,89,113	1.86	13 (22%)
18	BCR	b1	420	-	41,41,41	1.20	4 (9%)	56,56,56	1.45	11 (19%)
15	CLA	a2	414	13	49,53,73	1.51	9 (18%)	59,89,113	1.52	5 (8%)
15	CLA	cB	802	2	69,73,73	1.38	11 (15%)	83,113,113	1.51	10 (12%)
15	CLA	bB	822	2	49,53,73	1.44	8 (16%)	59,89,113	1.62	8 (13%)
15	CLA	aB	804	-	69,73,73	1.35	10 (14%)	83,113,113	1.87	16 (19%)
15	CLA	c2	405	13	49,53,73	1.58	9 (18%)	59,89,113	1.94	19 (32%)
15	CLA	a6	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.34	9 (10%)
15	CLA	b6	417	13	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
15	CLA	cB	821	2	51,55,73	1.47	11 (21%)	61,91,113	1.46	4 (6%)
15	CLA	c1	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.45	8 (13%)
15	CLA	c4	421	13	69,73,73	1.38	14 (20%)	83,113,113	1.69	16 (19%)
15	CLA	cB	832	2	53,57,73	1.44	8 (15%)	62,93,113	1.53	8 (12%)
18	BCR	cB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
15	CLA	aA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	a1	414	13	49,53,73	1.48	9 (18%)	59,89,113	1.82	11 (18%)
15	CLA	bB	820	2,22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	bA	828	1	69,73,73	1.31	11 (15%)	83,113,113	1.37	7 (8%)
18	BCR	a2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bA	814	1	64,68,73	1.36	10 (15%)	77,107,113	1.37	7 (9%)
15	CLA	aA	833	1	69,73,73	1.29	9 (13%)	83,113,113	1.37	9 (10%)
15	CLA	c5	403	13,15	69,73,73	1.23	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	cJ	102	8	42,45,73	1.52	11 (26%)	50,78,113	1.66	5 (10%)
15	CLA	a4	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.58	8 (13%)
15	CLA	b6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.38	9 (10%)
15	CLA	aB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.48	9 (12%)
15	CLA	cB	812	2	49,53,73	1.46	9 (18%)	59,89,113	1.47	7 (11%)
15	CLA	cB	820	2,22	69,73,73	1.24	9 (13%)	83,113,113	1.37	7 (8%)
15	CLA	b5	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.66	10 (16%)
17	SF4	cC	102	3	0,12,12	-	-	-	-	-
15	CLA	a5	415	13	49,53,73	1.49	10 (20%)	59,89,113	1.85	12 (20%)
15	CLA	a5	406	13	49,53,73	1.46	9 (18%)	59,89,113	1.51	8 (13%)
15	CLA	c4	417	13	59,63,73	1.57	9 (15%)	71,101,113	1.95	16 (22%)
16	PQN	bB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
15	CLA	aB	809	2	69,73,73	1.28	11 (15%)	83,113,113	1.54	9 (10%)
15	CLA	bA	844	-	46,49,73	1.47	9 (19%)	55,83,113	1.59	5 (9%)
15	CLA	a6	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.91	14 (19%)
15	CLA	b1	411	13	49,53,73	1.49	9 (18%)	59,89,113	1.66	9 (15%)
15	CLA	cB	818	2	63,67,73	1.31	10 (15%)	75,105,113	1.48	13 (17%)
15	CLA	cB	806	2	69,73,73	1.26	11 (15%)	83,113,113	1.53	9 (10%)
17	SF4	aA	847	2,1	0,12,12	-	-	-	-	-
15	CLA	cL	203	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
15	CLA	b3	409	13	69,73,73	1.25	10 (14%)	83,113,113	1.34	10 (12%)
15	CLA	a2	417	13	54,58,73	1.57	11 (20%)	65,95,113	2.36	20 (30%)
15	CLA	a1	415	13	54,58,73	1.54	11 (20%)	65,95,113	2.28	18 (27%)
15	CLA	c2	413	13	49,53,73	1.58	10 (20%)	59,89,113	1.63	15 (25%)
15	CLA	aB	819	2	64,68,73	1.30	11 (17%)	77,107,113	1.60	10 (12%)
15	CLA	a4	404	13	69,73,73	1.27	11 (15%)	83,113,113	1.35	8 (9%)
15	CLA	a2	407	13	49,53,73	1.44	7 (14%)	59,89,113	1.47	7 (11%)
15	CLA	c6	408	-	49,53,73	1.46	9 (18%)	59,89,113	1.52	8 (13%)
18	BCR	bB	845	-	41,41,41	1.10	3 (7%)	56,56,56	1.29	6 (10%)
18	BCR	c1	420	-	41,41,41	1.19	3 (7%)	56,56,56	1.44	11 (19%)
15	CLA	c1	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.59	8 (13%)
15	CLA	c3	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.81	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	cF	204	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	a4	410	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	b3	408	13	49,53,73	1.43	10 (20%)	59,89,113	1.61	12 (20%)
15	CLA	bL	204	22	69,73,73	1.31	9 (13%)	83,113,113	1.31	9 (10%)
15	CLA	a2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	b6	404	13,15	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
18	BCR	a6	419	-	41,41,41	1.37	5 (12%)	56,56,56	1.52	10 (17%)
15	CLA	aL	203	22	69,73,73	1.31	9 (13%)	83,113,113	1.32	9 (10%)
15	CLA	bB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
18	BCR	cB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	9 (16%)
15	CLA	a4	409	13	69,73,73	1.26	8 (11%)	83,113,113	1.32	10 (12%)
15	CLA	b6	422	13	69,73,73	1.45	13 (18%)	83,113,113	2.00	20 (24%)
15	CLA	c5	408	13	49,53,73	1.45	10 (20%)	59,89,113	1.61	10 (16%)
15	CLA	b3	416	13	54,58,73	1.54	11 (20%)	65,95,113	2.24	18 (27%)
15	CLA	cB	839	22	69,73,73	1.25	11 (15%)	83,113,113	1.43	9 (10%)
15	CLA	cB	801	-	69,73,73	1.29	10 (14%)	83,113,113	1.44	10 (12%)
15	CLA	c1	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)
18	BCR	c4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aA	843	1	69,73,73	1.31	10 (14%)	83,113,113	1.52	8 (9%)
15	CLA	bA	838	1	55,59,73	1.46	10 (18%)	66,96,113	1.69	12 (18%)
15	CLA	bA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	7 (11%)
18	BCR	aF	203	-	41,41,41	1.20	4 (9%)	56,56,56	1.35	9 (16%)
15	CLA	a6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.37	8 (9%)
15	CLA	b5	415	13	49,53,73	1.49	9 (18%)	59,89,113	1.84	12 (20%)
15	CLA	c2	418	13	59,63,73	1.59	8 (13%)	71,101,113	1.93	15 (21%)
15	CLA	b2	417	13	54,58,73	1.57	11 (20%)	65,95,113	2.32	18 (27%)
15	CLA	cB	841	-	49,53,73	1.52	11 (22%)	59,89,113	1.55	9 (15%)
15	CLA	c1	409	13	69,73,73	1.25	8 (11%)	83,113,113	1.29	8 (9%)
15	CLA	b5	407	-	49,53,73	1.45	8 (16%)	59,89,113	1.55	10 (16%)
15	CLA	bB	842	-	49,53,73	1.47	7 (14%)	59,89,113	1.40	3 (5%)
18	BCR	bA	850	15	41,41,41	1.18	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	bA	808	1	55,59,73	1.39	10 (18%)	66,96,113	1.49	10 (15%)
15	CLA	aB	824	2	49,53,73	1.47	8 (16%)	59,89,113	1.49	13 (22%)
15	CLA	a1	406	-	49,53,73	1.46	9 (18%)	59,89,113	1.57	9 (15%)
15	CLA	cB	826	2,22	50,54,73	1.43	10 (20%)	60,90,113	1.75	11 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
15	CLA	cB	835	2	49,53,73	1.42	9 (18%)	59,89,113	1.72	6 (10%)
15	CLA	bA	807	1	69,73,73	1.35	12 (17%)	83,113,113	1.49	14 (16%)
15	CLA	aB	830	2	69,73,73	1.35	9 (13%)	83,113,113	1.77	15 (18%)
15	CLA	bA	820	1	69,73,73	1.29	10 (14%)	83,113,113	1.52	11 (13%)
18	BCR	aK	101	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	9 (16%)
18	BCR	c4	420	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	10 (17%)
15	CLA	b1	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.66	14 (23%)
15	CLA	b6	403	13	69,73,73	1.23	8 (11%)	83,113,113	1.34	7 (8%)
15	CLA	c5	409	13	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
15	CLA	b3	402	13	69,73,73	1.23	8 (11%)	83,113,113	1.33	7 (8%)
15	CLA	aA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	aB	815	2	69,73,73	1.23	10 (14%)	83,113,113	1.41	10 (12%)
15	CLA	bA	836	1	58,62,73	1.34	10 (17%)	69,99,113	1.40	6 (8%)
16	PQN	bA	846	-	34,34,34	1.41	2 (5%)	42,45,45	1.14	5 (11%)
15	CLA	b4	402	13	69,73,73	1.22	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	cA	842	1	69,73,73	1.32	10 (14%)	83,113,113	1.51	8 (9%)
18	BCR	a3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
15	CLA	aB	808	2	69,73,73	1.22	9 (13%)	83,113,113	1.44	7 (8%)
15	CLA	a1	409	13,15	68,72,73	1.30	11 (16%)	81,111,113	1.61	14 (17%)
15	CLA	a2	418	13	59,63,73	1.60	8 (13%)	71,101,113	1.93	15 (21%)
15	CLA	bA	826	-	69,73,73	1.25	10 (14%)	83,113,113	1.49	10 (12%)
15	CLA	c3	411	13	49,53,73	1.50	10 (20%)	59,89,113	1.63	10 (16%)
15	CLA	cA	810	1	69,73,73	1.25	11 (15%)	83,113,113	1.46	6 (7%)
18	BCR	aB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.51	8 (14%)
18	BCR	aB	849	-	41,41,41	1.40	5 (12%)	56,56,56	1.30	8 (14%)
18	BCR	a3	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.42	9 (16%)
15	CLA	bB	831	2	49,53,73	1.46	10 (20%)	59,89,113	1.55	5 (8%)
15	CLA	c6	410	13	69,73,73	1.25	8 (11%)	83,113,113	1.33	9 (10%)
15	CLA	cA	843	-	46,49,73	1.47	8 (17%)	55,83,113	1.59	5 (9%)
19	LHG	bA	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.35	7 (13%)
18	BCR	bA	852	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
15	CLA	b6	412	13	49,53,73	1.48	10 (20%)	59,89,113	1.64	11 (18%)
15	CLA	bB	835	2	49,53,73	1.42	10 (20%)	59,89,113	1.72	6 (10%)
15	CLA	bB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aA	831	1	69,73,73	1.38	10 (14%)	83,113,113	1.62	13 (15%)
15	CLA	a5	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.94	15 (21%)
18	BCR	b1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
15	CLA	c6	417	13	54,58,73	1.52	10 (18%)	65,95,113	2.28	18 (27%)
15	CLA	b3	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.52	5 (8%)
15	CLA	b4	421	13	69,73,73	1.40	15 (21%)	83,113,113	1.69	16 (19%)
15	CLA	aA	838	1	55,59,73	1.45	10 (18%)	66,96,113	1.68	12 (18%)
15	CLA	aA	837	1	49,53,73	1.46	9 (18%)	59,89,113	1.57	6 (10%)
15	CLA	cB	814	2	69,73,73	1.31	11 (15%)	83,113,113	1.60	17 (20%)
15	CLA	a4	403	13,15	69,73,73	1.23	8 (11%)	83,113,113	1.40	9 (10%)
18	BCR	b2	420	-	41,41,41	1.13	3 (7%)	56,56,56	1.45	8 (14%)
15	CLA	a5	404	13	69,73,73	1.25	9 (13%)	83,113,113	1.38	8 (9%)
15	CLA	b4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.49	5 (8%)
18	BCR	a4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	7 (12%)
18	BCR	c2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	b5	403	13,15	69,73,73	1.22	9 (13%)	83,113,113	1.42	11 (13%)
15	CLA	c6	412	13	49,53,73	1.49	10 (20%)	59,89,113	1.64	11 (18%)
15	CLA	c6	416	13	49,53,73	1.51	8 (16%)	59,89,113	1.82	11 (18%)
15	CLA	a6	407	13	49,53,73	1.45	9 (18%)	59,89,113	1.48	7 (11%)
15	CLA	cA	836	1	58,62,73	1.35	10 (17%)	69,99,113	1.41	6 (8%)
18	BCR	c3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.40	8 (14%)
18	BCR	c5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.41	11 (19%)
15	CLA	aB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	aB	807	2	69,73,73	1.39	11 (15%)	83,113,113	1.49	10 (12%)
15	CLA	cA	831	1	69,73,73	1.37	10 (14%)	83,113,113	1.63	13 (15%)
15	CLA	a4	417	13	59,63,73	1.56	9 (15%)	71,101,113	1.95	16 (22%)
15	CLA	cB	817	2	59,63,73	1.35	8 (13%)	71,101,113	1.62	13 (18%)
15	CLA	cB	829	2	69,73,73	1.26	9 (13%)	83,113,113	1.40	9 (10%)
15	CLA	c2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
18	BCR	bI	102	-	41,41,41	1.37	4 (9%)	56,56,56	1.41	9 (16%)
15	CLA	a1	404	13	49,53,73	1.54	9 (18%)	59,89,113	1.91	19 (32%)
15	CLA	cB	822	2	49,53,73	1.44	7 (14%)	59,89,113	1.63	8 (13%)
15	CLA	bA	806	1	69,73,73	1.31	9 (13%)	83,113,113	1.61	10 (12%)
15	CLA	a4	413	13	49,53,73	1.51	10 (20%)	59,89,113	1.48	5 (8%)
18	BCR	c4	418	-	41,41,41	1.42	5 (12%)	56,56,56	1.56	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	a2	419	-	41,41,41	1.38	5 (12%)	56,56,56	1.53	10 (17%)
15	CLA	cA	830	1	69,73,73	1.28	9 (13%)	83,113,113	1.50	11 (13%)
18	BCR	cL	204	-	41,41,41	1.30	4 (9%)	56,56,56	1.45	9 (16%)
15	CLA	c5	413	13	49,53,73	1.50	11 (22%)	59,89,113	1.51	5 (8%)
15	CLA	b1	408	13	49,53,73	1.44	9 (18%)	59,89,113	1.60	9 (15%)
15	CLA	a3	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	10 (16%)
15	CLA	a4	412	13	49,53,73	1.57	10 (20%)	59,89,113	1.61	14 (23%)
18	BCR	a2	401	-	41,41,41	1.26	4 (9%)	56,56,56	1.83	12 (21%)
15	CLA	bL	203	10	69,73,73	1.26	10 (14%)	83,113,113	1.60	11 (13%)
15	CLA	aB	826	2,22	50,54,73	1.43	11 (22%)	60,90,113	1.75	11 (18%)
18	BCR	cM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.34	9 (16%)
15	CLA	a5	412	13	49,53,73	1.55	10 (20%)	59,89,113	1.63	13 (22%)
15	CLA	bX	102	12	49,53,73	1.51	11 (22%)	59,89,113	1.68	11 (18%)
15	CLA	a1	413	13	45,49,73	1.49	9 (20%)	54,84,113	1.58	7 (12%)
15	CLA	a2	406	13	69,73,73	1.41	11 (15%)	83,113,113	1.89	20 (24%)
15	CLA	cA	805	1	63,67,73	1.34	11 (17%)	75,105,113	1.53	11 (14%)
18	BCR	c3	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	9 (16%)
18	BCR	cA	850	-	41,41,41	1.38	5 (12%)	56,56,56	1.34	8 (14%)
18	BCR	cB	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.36	9 (16%)
15	CLA	aB	821	2	51,55,73	1.46	11 (21%)	61,91,113	1.48	4 (6%)
15	CLA	a2	412	13	49,53,73	1.50	12 (24%)	59,89,113	1.67	10 (16%)
15	CLA	b3	421	13	69,73,73	1.39	11 (15%)	83,113,113	1.60	15 (18%)
15	CLA	b4	416	13	54,58,73	1.54	9 (16%)	65,95,113	2.26	17 (26%)
15	CLA	bB	810	2	69,73,73	1.34	10 (14%)	83,113,113	1.57	12 (14%)
15	CLA	cA	839	1	69,73,73	1.35	10 (14%)	83,113,113	1.45	7 (8%)
15	CLA	c6	404	13,15	69,73,73	1.23	8 (11%)	83,113,113	1.42	10 (12%)
15	CLA	aB	823	-	59,63,73	1.30	9 (15%)	71,101,113	1.50	7 (9%)
15	CLA	a4	415	13	49,53,73	1.48	8 (16%)	59,89,113	1.86	13 (22%)
15	CLA	bB	813	2	49,53,73	1.52	11 (22%)	59,89,113	1.61	7 (11%)
18	BCR	a6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.41	10 (17%)
18	BCR	aB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.41	6 (10%)
18	BCR	c1	401	-	41,41,41	1.16	3 (7%)	56,56,56	1.54	9 (16%)
15	CLA	c2	411	13,15	68,72,73	1.31	11 (16%)	81,111,113	1.59	15 (18%)
15	CLA	aA	810	1	69,73,73	1.24	11 (15%)	83,113,113	1.46	6 (7%)
15	CLA	b3	404	13	69,73,73	1.27	9 (13%)	83,113,113	1.38	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b4	411	13	49,53,73	1.50	11 (22%)	59,89,113	1.66	9 (15%)
15	CLA	b4	414	13	45,49,73	1.52	9 (20%)	54,84,113	1.60	6 (11%)
15	CLA	bA	840	1	51,55,73	1.52	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	cB	827	2	69,73,73	1.29	10 (14%)	83,113,113	1.55	14 (16%)
15	CLA	aB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
15	CLA	cB	828	2	69,73,73	1.31	11 (15%)	83,113,113	1.54	8 (9%)
15	CLA	c3	407	-	49,53,73	1.47	10 (20%)	59,89,113	1.54	10 (16%)
15	CLA	c4	406	13	49,53,73	1.43	9 (18%)	59,89,113	1.48	7 (11%)
18	BCR	cJ	103	-	41,41,41	1.29	3 (7%)	56,56,56	1.46	11 (19%)
18	BCR	b2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.40	9 (16%)
15	CLA	c2	402	13	69,73,73	1.24	8 (11%)	83,113,113	1.36	6 (7%)
15	CLA	c6	405	13	69,73,73	1.27	10 (14%)	83,113,113	1.39	9 (10%)
15	CLA	bB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.50	8 (11%)
15	CLA	b2	414	13	49,53,73	1.52	9 (18%)	59,89,113	1.53	6 (10%)
18	BCR	c5	401	-	41,41,41	1.21	4 (9%)	56,56,56	1.53	12 (21%)
15	CLA	cA	840	1	51,55,73	1.53	9 (17%)	61,91,113	1.83	10 (16%)
15	CLA	bB	832	2	53,57,73	1.43	8 (15%)	62,93,113	1.52	9 (14%)
15	CLA	b4	408	13	49,53,73	1.44	10 (20%)	59,89,113	1.60	8 (13%)
15	CLA	aA	819	1	58,62,73	1.39	11 (18%)	69,99,113	1.54	9 (13%)
15	CLA	b6	414	13	49,53,73	1.53	10 (20%)	59,89,113	1.69	10 (16%)
15	CLA	c5	402	13	69,73,73	1.25	9 (13%)	83,113,113	1.36	6 (7%)
15	CLA	aA	821	18,1	65,69,73	1.32	12 (18%)	78,108,113	1.41	7 (8%)
15	CLA	bB	825	2	58,62,73	1.41	10 (17%)	69,99,113	1.58	10 (14%)
15	CLA	cB	805	2	58,62,73	1.34	10 (17%)	69,99,113	1.49	8 (11%)
15	CLA	cA	814	1	64,68,73	1.35	10 (15%)	77,107,113	1.38	7 (9%)
15	CLA	b1	402	13	69,73,73	1.23	9 (13%)	83,113,113	1.36	7 (8%)
15	CLA	cB	838	2	51,55,73	1.47	10 (19%)	61,91,113	1.65	10 (16%)
15	CLA	cB	837	2	69,73,73	1.28	10 (14%)	83,113,113	1.48	9 (10%)
15	CLA	c2	412	13	49,53,73	1.51	11 (22%)	59,89,113	1.66	10 (16%)
18	BCR	bJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	c4	407	-	49,53,73	1.48	11 (22%)	59,89,113	1.55	8 (13%)
15	CLA	a4	405	13	49,53,73	1.55	10 (20%)	59,89,113	1.97	20 (33%)
18	BCR	a6	421	-	41,41,41	1.11	4 (9%)	56,56,56	1.55	9 (16%)
16	PQN	cB	843	-	34,34,34	1.43	3 (8%)	42,45,45	1.16	3 (7%)
15	CLA	cA	829	1	69,73,73	1.27	9 (13%)	83,113,113	1.49	12 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aA	812	1	69,73,73	1.26	11 (15%)	83,113,113	1.35	9 (10%)
15	CLA	a2	403	13,15	69,73,73	1.23	9 (13%)	83,113,113	1.42	8 (9%)
17	SF4	cC	101	3	0,12,12	-	-	-	-	-
15	CLA	bB	834	2	62,66,73	1.32	11 (17%)	74,104,113	1.49	9 (12%)
18	BCR	bL	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.37	10 (17%)
18	BCR	bM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
15	CLA	bB	812	2	49,53,73	1.46	10 (20%)	59,89,113	1.47	8 (13%)
18	BCR	c4	401	-	41,41,41	1.19	3 (7%)	56,56,56	1.49	10 (17%)
18	BCR	b3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.39	8 (14%)
18	BCR	aA	850	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	9 (16%)
15	CLA	b3	414	13	45,49,73	1.50	10 (22%)	54,84,113	1.63	6 (11%)
18	BCR	a1	420	-	41,41,41	1.14	3 (7%)	56,56,56	1.51	10 (17%)
15	CLA	bA	809	1	69,73,73	1.25	11 (15%)	83,113,113	1.44	9 (10%)
15	CLA	aA	802	22	69,73,73	1.41	11 (15%)	83,113,113	1.44	11 (13%)
15	CLA	bJ	101	8	49,53,73	1.46	12 (24%)	59,89,113	1.66	7 (11%)
15	CLA	c1	411	13	49,53,73	1.48	11 (22%)	59,89,113	1.64	9 (15%)
15	CLA	c6	413	13	49,53,73	1.56	10 (20%)	59,89,113	1.60	14 (23%)
18	BCR	aM	101	-	41,41,41	1.18	3 (7%)	56,56,56	1.33	9 (16%)
18	BCR	b4	418	-	41,41,41	1.43	6 (14%)	56,56,56	1.56	9 (16%)
15	CLA	c5	417	13	59,63,73	1.56	8 (13%)	71,101,113	1.94	15 (21%)

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
18	BCR	a1	417	-	-	9/29/63/63	0/2/2/2
15	CLA	bA	833	1	-	11/39/115/115	-
15	CLA	aA	805	1	-	11/32/108/115	-
15	CLA	cA	815	1	-	4/15/91/115	-
15	CLA	c5	411	13	-	3/15/91/115	-
15	CLA	a4	411	13	-	5/15/91/115	-
15	CLA	aX	102	12	-	8/15/91/115	-
15	CLA	cA	804	1	-	10/39/115/115	-
15	CLA	bA	829	1	-	22/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	c3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	813	1	-	8/26/102/115	-
18	BCR	a3	401	-	-	12/29/63/63	0/2/2/2
15	CLA	c3	414	13	-	4/10/86/115	-
18	BCR	bL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	bA	810	1	-	18/39/115/115	-
15	CLA	cB	825	2	-	10/26/102/115	-
18	BCR	cB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	b3	415	13	-	7/15/91/115	-
15	CLA	b5	409	13	-	6/39/115/115	-
15	CLA	aB	833	2	-	18/39/115/115	-
15	CLA	a3	412	13	-	9/15/91/115	-
18	BCR	b2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	bB	802	2	-	13/39/115/115	-
15	CLA	b3	407	-	-	7/15/91/115	-
15	CLA	cB	819	2	-	12/33/109/115	-
15	CLA	aA	834	1	-	12/39/115/115	-
15	CLA	b3	417	13	-	11/27/103/115	-
15	CLA	a2	410	13	-	6/39/115/115	-
15	CLA	a5	414	13	-	4/10/86/115	-
15	CLA	bJ	102	8	-	2/4/76/115	-
15	CLA	cA	825	1	-	17/32/108/115	-
15	CLA	aB	818	2	-	10/32/108/115	-
15	CLA	c2	408	-	-	8/15/91/115	-
15	CLA	b2	410	13	-	7/39/115/115	-
18	BCR	a5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	816	2	-	6/15/91/115	-
15	CLA	c4	412	13	-	9/15/91/115	-
15	CLA	b6	415	13	-	4/10/86/115	-
15	CLA	bL	202	10	-	15/39/115/115	-
18	BCR	aL	205	-	-	14/29/63/63	0/2/2/2
15	CLA	b3	412	13	-	9/15/91/115	-
15	CLA	bB	819	2	-	12/33/109/115	-
15	CLA	c4	405	13	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	bA	853	-	-	22/29/63/63	0/2/2/2
18	BCR	b1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	405	13	-	3/15/91/115	-
15	CLA	c5	414	13	-	4/10/86/115	-
15	CLA	c1	416	13	-	11/21/97/115	-
15	CLA	a6	413	13	-	9/15/91/115	-
15	CLA	cA	827	22	-	10/39/115/115	-
15	CLA	a2	404	13	-	12/39/115/115	-
15	CLA	bA	830	1	-	13/39/115/115	-
15	CLA	a4	414	13	-	4/10/86/115	-
18	BCR	aB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	825	1	-	17/32/108/115	-
15	CLA	c1	410	13,15	-	15/38/114/115	-
15	CLA	a2	409	13	-	5/15/91/115	-
15	CLA	cA	826	-	-	10/39/115/115	-
15	CLA	bB	811	2	-	13/39/115/115	-
15	CLA	aB	842	-	-	2/15/91/115	-
15	CLA	a1	422	13	-	16/39/115/115	-
18	BCR	cK	101	-	-	10/29/63/63	0/2/2/2
15	CLA	b1	406	13	-	4/15/91/115	-
15	CLA	a1	411	13	-	9/15/91/115	-
15	CLA	b1	410	13,15	-	14/38/114/115	-
15	CLA	aB	817	2	-	12/27/103/115	-
15	CLA	c2	415	13	-	4/10/86/115	-
15	CLA	c3	402	13	-	17/39/115/115	-
15	CLA	aB	828	2	-	21/39/115/115	-
15	CLA	bB	804	-	-	12/39/115/115	-
15	CLA	aB	839	22	-	10/39/115/115	-
18	BCR	b3	418	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	842	22	-	10/23/99/115	-
15	CLA	b6	418	13	-	11/27/103/115	-
15	CLA	cA	837	1	-	7/15/91/115	-
18	BCR	bB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	c5	410	13,15	-	13/38/114/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	841	-	-	4/15/91/115	-
15	CLA	cK	102	-	-	10/15/91/115	-
15	CLA	b5	402	13	-	17/39/115/115	-
15	CLA	c3	412	13	-	9/15/91/115	-
18	BCR	a5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	804	-	-	12/39/115/115	-
15	CLA	c6	414	13	-	4/15/91/115	-
15	CLA	b1	404	13	-	14/39/115/115	-
15	CLA	c1	414	13	-	4/10/86/115	-
15	CLA	bB	827	2	-	15/39/115/115	-
15	CLA	b2	408	-	-	7/15/91/115	-
15	CLA	b4	417	13	-	9/27/103/115	-
17	SF4	bA	847	2,1	-	-	0/6/5/5
15	CLA	aA	844	-	-	7/9/81/115	-
15	CLA	cB	803	-	-	11/39/115/115	-
15	CLA	bA	845	19	-	13/24/100/115	-
15	CLA	c1	417	13	-	9/27/103/115	-
15	CLA	aA	832	1	-	8/21/97/115	-
15	CLA	aB	801	-	-	12/39/115/115	-
15	CLA	a3	403	13,15	-	13/39/115/115	-
15	CLA	aJ	203	8	-	2/4/76/115	-
15	CLA	b4	404	13	-	12/39/115/115	-
18	BCR	cA	847	-	-	11/29/63/63	0/2/2/2
15	CLA	cJ	101	8	-	8/15/91/115	-
20	LMG	cB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	bB	809	2	-	13/39/115/115	-
15	CLA	b2	402	13	-	17/39/115/115	-
18	BCR	aJ	205	-	-	10/29/63/63	0/2/2/2
15	CLA	aA	820	1	-	18/39/115/115	-
15	CLA	bB	824	2	-	5/15/91/115	-
15	CLA	c1	402	13	-	17/39/115/115	-
18	BCR	b4	419	-	-	11/29/63/63	0/2/2/2
18	BCR	b5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c1	405	13	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CL0	cA	801	1	-	6/39/115/115	-
15	CLA	bA	816	1	-	3/15/91/115	-
15	CLA	a5	403	13,15	-	14/39/115/115	-
15	CLA	c6	403	13	-	17/39/115/115	-
18	BCR	aB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	bF	201	-	-	10/15/91/115	-
15	CLA	a6	409	13	-	5/15/91/115	-
15	CLA	bA	831	1	-	8/39/115/115	-
15	CLA	a3	413	13	-	3/15/91/115	-
15	CLA	b6	416	13	-	7/15/91/115	-
15	CLA	cA	802	22	-	16/39/115/115	-
15	CLA	cL	201	10	-	15/39/115/115	-
15	CLA	a2	405	13	-	4/15/91/115	-
15	CLA	c5	412	13	-	9/15/91/115	-
15	CLA	c5	405	13	-	4/15/91/115	-
15	CLA	aA	811	1	-	10/15/91/115	-
15	CLA	a3	405	13	-	3/15/91/115	-
18	BCR	b6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	411	13,15	-	13/38/114/115	-
18	BCR	bJ	105	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	816	2	-	6/15/91/115	-
15	CLA	a3	409	13	-	5/39/115/115	-
18	BCR	aI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	823	1	-	6/20/96/115	-
18	BCR	bJ	103	-	-	14/29/63/63	0/2/2/2
15	CLA	a1	402	13,15	-	14/39/115/115	-
15	CLA	bA	821	18,1	-	15/35/111/115	-
15	CLA	a6	416	13	-	7/15/91/115	-
15	CLA	cF	203	-	-	10/15/91/115	-
15	CLA	a3	406	13	-	4/15/91/115	-
18	BCR	c5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c1	413	13	-	4/15/91/115	-
15	CLA	a1	410	13	-	4/15/91/115	-
18	BCR	a1	419	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	835	2	-	9/15/91/115	-
14	CL0	bA	801	1	-	6/39/115/115	-
15	CLA	a6	415	13	-	4/10/86/115	-
15	CLA	aA	824	1	-	14/23/99/115	-
15	CLA	c3	406	13	-	4/15/91/115	-
18	BCR	b6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	b6	407	13	-	4/15/91/115	-
18	BCR	aB	847	-	-	9/18/35/63	0/1/1/2
18	BCR	cI	101	-	-	11/29/63/63	0/2/2/2
15	CLA	a2	413	13	-	9/15/91/115	-
15	CLA	a5	408	13	-	5/15/91/115	-
15	CLA	bB	823	-	-	5/27/103/115	-
17	SF4	aC	102	3	-	-	0/6/5/5
15	CLA	cA	841	1	-	17/39/115/115	-
15	CLA	c3	409	13	-	6/39/115/115	-
15	CLA	cX	102	12	-	8/15/91/115	-
15	CLA	cA	803	-	-	16/39/115/115	-
15	CLA	bA	819	1	-	10/26/102/115	-
15	CLA	a3	411	13	-	5/15/91/115	-
18	BCR	b4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	823	1	-	6/20/96/115	-
15	CLA	a3	415	13	-	7/15/91/115	-
15	CLA	c3	408	13	-	5/15/91/115	-
15	CLA	c6	407	13	-	4/15/91/115	-
15	CLA	c2	422	13	-	13/39/115/115	-
15	CLA	aA	804	1	-	10/39/115/115	-
15	CLA	aA	826	-	-	10/39/115/115	-
15	CLA	aA	835	1	-	14/39/115/115	-
15	CLA	cA	838	1	-	8/23/99/115	-
18	BCR	aA	848	-	-	11/29/63/63	0/2/2/2
18	BCR	cA	849	-	-	13/29/63/63	0/2/2/2
15	CLA	b3	410	13,15	-	12/38/114/115	-
18	BCR	bB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	aB	832	2	-	8/20/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c4	409	13	-	6/39/115/115	-
15	CLA	b5	406	13	-	4/15/91/115	-
18	BCR	c2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b1	417	13	-	12/27/103/115	-
15	CLA	a5	410	13,15	-	14/38/114/115	-
15	CLA	aA	827	22	-	10/39/115/115	-
15	CLA	cA	818	1	-	6/26/102/115	-
18	BCR	c2	401	-	-	12/29/63/63	0/2/2/2
18	BCR	cJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	c3	416	13	-	11/21/97/115	-
18	BCR	bB	849	-	-	14/29/63/63	0/2/2/2
15	CLA	c2	409	13	-	5/15/91/115	-
18	BCR	aA	851	-	-	8/29/63/63	0/2/2/2
15	CLA	b4	407	-	-	8/15/91/115	-
15	CLA	bA	805	1	-	11/32/108/115	-
15	CLA	cA	816	1	-	3/15/91/115	-
15	CLA	c3	410	13,15	-	12/38/114/115	-
19	LHG	bA	855	15	-	15/31/31/53	-
15	CLA	aB	806	2	-	21/39/115/115	-
15	CLA	aB	820	2,22	-	10/39/115/115	-
15	CLA	a6	403	13	-	17/39/115/115	-
15	CLA	bA	832	1	-	8/21/97/115	-
15	CLA	cB	831	2	-	8/15/91/115	-
15	CLA	aB	836	2	-	11/33/109/115	-
15	CLA	b1	409	13	-	6/39/115/115	-
15	CLA	c6	418	13	-	11/27/103/115	-
15	CLA	b2	416	13	-	7/15/91/115	-
15	CLA	b5	404	13	-	11/39/115/115	-
18	BCR	a3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	cA	807	1	-	11/39/115/115	-
15	CLA	a2	411	13,15	-	13/38/114/115	-
18	BCR	aF	201	-	-	14/29/63/63	0/2/2/2
15	CLA	a5	405	13	-	4/15/91/115	-
15	CLA	a2	422	13	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	808	2	-	14/39/115/115	-
15	CLA	c3	404	13	-	12/39/115/115	-
15	CLA	aA	845	19	-	13/24/100/115	-
15	CLA	c4	403	13,15	-	14/39/115/115	-
15	CLA	b3	403	13,15	-	13/39/115/115	-
15	CLA	cA	817	-	-	6/20/96/115	-
15	CLA	b6	411	13,15	-	14/38/114/115	-
15	CLA	cA	828	1	-	14/39/115/115	-
15	CLA	aA	814	1	-	16/33/109/115	-
15	CLA	b2	409	13	-	5/15/91/115	-
15	CLA	aB	805	2	-	5/26/102/115	-
15	CLA	c1	415	13	-	7/15/91/115	-
15	CLA	aB	838	2	-	2/18/94/115	-
15	CLA	a5	416	13	-	11/21/97/115	-
18	BCR	b1	418	-	-	9/29/63/63	0/2/2/2
19	LHG	cX	101	-	-	11/26/26/53	-
15	CLA	b1	416	13	-	11/21/97/115	-
15	CLA	bB	815	2	-	17/39/115/115	-
15	CLA	a1	408	13	-	6/39/115/115	-
18	BCR	a5	419	-	-	12/29/63/63	0/2/2/2
18	BCR	c6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c2	417	13	-	9/21/97/115	-
15	CLA	b2	422	13	-	12/39/115/115	-
15	CLA	bB	803	-	-	11/39/115/115	-
15	CLA	aA	815	1	-	4/15/91/115	-
15	CLA	aA	822	-	-	18/39/115/115	-
18	BCR	b5	401	-	-	14/29/63/63	0/2/2/2
15	CLA	c4	408	13	-	5/15/91/115	-
15	CLA	b1	414	13	-	4/10/86/115	-
15	CLA	cA	809	1	-	21/39/115/115	-
15	CLA	c5	415	13	-	7/15/91/115	-
15	CLA	c2	404	13	-	11/39/115/115	-
15	CLA	cB	816	2	-	6/15/91/115	-
15	CLA	a6	406	13	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c3	403	13,15	-	13/39/115/115	-
15	CLA	c5	404	13	-	11/39/115/115	-
18	BCR	aI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	405	13	-	4/15/91/115	-
15	CLA	b5	412	13	-	9/15/91/115	-
18	BCR	aA	849	15	-	13/29/63/63	0/2/2/2
15	CLA	c4	410	13,15	-	13/38/114/115	-
15	CLA	a5	413	13	-	3/15/91/115	-
15	CLA	cA	819	1	-	10/26/102/115	-
15	CLA	a1	401	13	-	17/39/115/115	-
15	CLA	c4	402	13	-	17/39/115/115	-
15	CLA	cB	810	2	-	16/39/115/115	-
15	CLA	a6	417	13	-	11/21/97/115	-
15	CLA	c3	417	13	-	11/27/103/115	-
15	CLA	b1	405	13	-	3/15/91/115	-
18	BCR	cB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	814	2	-	25/39/115/115	-
18	BCR	b3	420	-	-	12/29/63/63	0/2/2/2
18	BCR	b5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	816	1	-	3/15/91/115	-
15	CLA	a6	404	13,15	-	14/39/115/115	-
15	CLA	b3	406	13	-	4/15/91/115	-
15	CLA	cA	812	1	-	13/39/115/115	-
15	CLA	aB	829	2	-	16/39/115/115	-
15	CLA	b1	403	13,15	-	14/39/115/115	-
15	CLA	bA	843	1	-	14/39/115/115	-
15	CLA	a3	417	13	-	12/27/103/115	-
15	CLA	cL	202	10	-	10/39/115/115	-
15	CLA	c6	415	13	-	4/10/86/115	-
15	CLA	c3	405	13	-	3/15/91/115	-
18	BCR	b6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	413	13	-	9/15/91/115	-
15	CLA	a5	407	-	-	8/15/91/115	-
15	CLA	a5	420	13	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	817	2	-	12/27/103/115	-
18	BCR	c6	402	-	-	13/29/63/63	0/2/2/2
19	LHG	aX	101	-	-	11/26/26/53	-
15	CLA	bB	828	2	-	21/39/115/115	-
15	CLA	c4	404	13	-	11/39/115/115	-
18	BCR	a4	420	-	-	12/29/63/63	0/2/2/2
18	BCR	cF	202	-	-	14/29/63/63	0/2/2/2
15	CLA	bA	839	1	-	16/39/115/115	-
15	CLA	a3	410	13,15	-	12/38/114/115	-
15	CLA	a4	406	13	-	4/15/91/115	-
16	PQN	cA	845	-	-	5/23/43/43	0/2/2/2
19	LHG	aA	854	15	-	15/31/31/53	-
15	CLA	c3	421	13	-	12/39/115/115	-
15	CLA	bB	829	2	-	16/39/115/115	-
15	CLA	b5	408	13	-	5/15/91/115	-
15	CLA	aA	803	-	-	16/39/115/115	-
15	CLA	a6	412	13	-	4/15/91/115	-
15	CLA	b5	416	13	-	11/21/97/115	-
15	CLA	a4	407	-	-	8/15/91/115	-
15	CLA	b1	413	13	-	4/15/91/115	-
15	CLA	cA	833	1	-	11/39/115/115	-
15	CLA	cA	824	1	-	14/23/99/115	-
15	CLA	b2	403	13,15	-	14/39/115/115	-
15	CLA	bA	811	1	-	10/15/91/115	-
15	CLA	b5	417	13	-	10/27/103/115	-
18	BCR	c6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	406	13	-	10/39/115/115	-
15	CLA	cB	815	2	-	17/39/115/115	-
15	CLA	c3	413	13	-	4/15/91/115	-
15	CLA	a4	416	13	-	11/21/97/115	-
15	CLA	c1	403	13,15	-	14/39/115/115	-
15	CLA	cB	833	2	-	18/39/115/115	-
15	CLA	a3	404	13	-	12/39/115/115	-
18	BCR	a1	418	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	c1	407	-	-	8/15/91/115	-
15	CLA	aJ	202	8	-	8/15/91/115	-
19	LHG	cA	852	-	-	19/53/53/53	-
15	CLA	a3	402	13	-	17/39/115/115	-
15	CLA	bA	827	22	-	10/39/115/115	-
15	CLA	cA	808	1	-	4/23/99/115	-
15	CLA	aA	841	1	-	17/39/115/115	-
15	CLA	b4	412	13	-	9/15/91/115	-
15	CLA	a2	416	13	-	7/15/91/115	-
15	CLA	cA	832	1	-	8/21/97/115	-
15	CLA	c4	411	13	-	4/15/91/115	-
15	CLA	c5	406	13	-	4/15/91/115	-
15	CLA	c4	413	13	-	4/15/91/115	-
17	SF4	cA	846	2,1	-	-	0/6/5/5
15	CLA	b2	418	13	-	11/27/103/115	-
15	CLA	bA	813	1	-	8/26/102/115	-
15	CLA	aA	817	-	-	6/20/96/115	-
15	CLA	bA	818	1	-	6/26/102/115	-
15	CLA	aA	829	1	-	22/39/115/115	-
15	CLA	bA	822	-	-	18/39/115/115	-
15	CLA	b4	410	13,15	-	13/38/114/115	-
15	CLA	cA	820	1	-	18/39/115/115	-
15	CLA	aL	202	10	-	10/39/115/115	-
15	CLA	c5	407	-	-	8/15/91/115	-
15	CLA	bB	838	2	-	2/18/94/115	-
15	CLA	bB	837	2	-	15/39/115/115	-
15	CLA	bA	824	1	-	14/23/99/115	-
16	PQN	aB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	c6	411	13,15	-	12/38/114/115	-
19	LHG	bX	101	-	-	11/26/26/53	-
15	CLA	aB	841	-	-	4/15/91/115	-
15	CLA	a1	403	13	-	13/39/115/115	-
18	BCR	b4	401	-	-	13/29/63/63	0/2/2/2
17	SF4	aC	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aL	201	10	-	15/39/115/115	-
15	CLA	aB	827	2	-	15/39/115/115	-
15	CLA	cB	834	2	-	15/31/107/115	-
15	CLA	bB	808	2	-	14/39/115/115	-
15	CLA	c4	415	13	-	7/15/91/115	-
15	CLA	c4	416	13	-	11/21/97/115	-
15	CLA	b5	414	13	-	4/10/86/115	-
15	CLA	bA	835	1	-	14/39/115/115	-
15	CLA	bB	818	2	-	10/32/108/115	-
15	CLA	cB	809	2	-	13/39/115/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
15	CLA	bA	825	1	-	17/32/108/115	-
15	CLA	b4	405	13	-	4/15/91/115	-
15	CLA	c1	412	13	-	9/15/91/115	-
15	CLA	aB	813	2	-	4/15/91/115	-
15	CLA	bA	817	-	-	6/20/96/115	-
15	CLA	aB	822	2	-	2/15/91/115	-
15	CLA	b6	409	13	-	5/15/91/115	-
15	CLA	cA	835	1	-	14/39/115/115	-
15	CLA	b2	404	13	-	11/39/115/115	-
15	CLA	c5	420	13	-	12/39/115/115	-
15	CLA	a1	412	13	-	4/15/91/115	-
15	CLA	bB	836	2	-	11/33/109/115	-
15	CLA	aB	837	2	-	15/39/115/115	-
15	CLA	b4	403	13,15	-	14/39/115/115	-
15	CLA	b5	405	13	-	4/15/91/115	-
18	BCR	b2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	cB	830	2	-	6/39/115/115	-
18	BCR	b6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	bA	834	1	-	12/39/115/115	-
18	BCR	a6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	828	1	-	14/39/115/115	-
15	CLA	aK	102	-	-	10/15/91/115	-
15	CLA	a5	409	13	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b4	406	13	-	4/15/91/115	-
15	CLA	b6	406	13	-	3/15/91/115	-
18	BCR	bA	851	-	-	13/29/63/63	0/2/2/2
15	CLA	c4	414	13	-	4/10/86/115	-
15	CLA	c6	409	13	-	5/15/91/115	-
18	BCR	cA	851	-	-	22/29/63/63	0/2/2/2
18	BCR	cF	205	-	-	11/29/63/63	0/2/2/2
18	BCR	aA	852	-	-	22/29/63/63	0/2/2/2
18	BCR	bA	848	-	-	10/29/63/63	0/2/2/2
15	CLA	aJ	201	-	-	10/15/91/115	-
15	CLA	cA	821	18,1	-	15/35/111/115	-
19	LHG	cA	853	15	-	15/31/31/53	-
15	CLA	c2	414	13	-	4/15/91/115	-
18	BCR	c1	419	-	-	11/29/63/63	0/2/2/2
17	SF4	bC	101	3	-	-	0/6/5/5
15	CLA	cA	806	1	-	23/39/115/115	-
15	CLA	cB	836	2	-	11/33/109/115	-
15	CLA	a3	416	13	-	11/21/97/115	-
15	CLA	cB	807	2	-	15/39/115/115	-
18	BCR	aI	103	-	-	9/29/63/63	0/2/2/2
15	CLA	a5	411	13	-	3/15/91/115	-
18	BCR	bI	101	-	-	11/29/63/63	0/2/2/2
18	BCR	c2	420	-	-	11/29/63/63	0/2/2/2
18	BCR	c6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	823	1	-	6/20/96/115	-
15	CLA	c6	406	13	-	3/15/91/115	-
15	CLA	aA	809	1	-	21/39/115/115	-
15	CLA	a3	421	13	-	12/39/115/115	-
15	CLA	a6	414	13	-	4/15/91/115	-
15	CLA	cA	822	-	-	18/39/115/115	-
15	CLA	c2	403	13,15	-	14/39/115/115	-
18	BCR	c3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	826	2,22	-	8/17/93/115	-
15	CLA	a1	407	13	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	PQN	aA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	a5	402	13	-	17/39/115/115	-
15	CLA	bB	830	2	-	6/39/115/115	-
18	BCR	a2	420	-	-	11/29/63/63	0/2/2/2
18	BCR	a6	402	-	-	14/29/63/63	0/2/2/2
15	CLA	a2	408	-	-	8/15/91/115	-
18	BCR	aJ	204	-	-	14/29/63/63	0/2/2/2
15	CLA	b5	413	13	-	3/15/91/115	-
18	BCR	bB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	bB	821	2	-	13/18/94/115	-
15	CLA	b2	415	13	-	4/10/86/115	-
15	CLA	a3	408	13	-	5/15/91/115	-
18	BCR	bF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	b6	408	-	-	7/15/91/115	-
15	CLA	bB	806	2	-	21/39/115/115	-
15	CLA	cB	840	2	-	16/39/115/115	-
15	CLA	aB	810	2	-	16/39/115/115	-
15	CLA	bB	807	2	-	15/39/115/115	-
15	CLA	a1	405	13	-	4/15/91/115	-
15	CLA	cB	823	-	-	5/27/103/115	-
15	CLA	a4	421	13	-	13/39/115/115	-
15	CLA	a4	402	13	-	17/39/115/115	-
15	CLA	bA	803	-	-	16/39/115/115	-
18	BCR	cB	844	-	-	9/29/63/63	0/2/2/2
15	CLA	aA	836	1	-	8/26/102/115	-
15	CLA	aA	807	1	-	11/39/115/115	-
15	CLA	bA	802	22	-	16/39/115/115	-
18	BCR	aF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	a2	415	13	-	4/10/86/115	-
15	CLA	cB	811	2	-	13/39/115/115	-
18	BCR	b3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cB	813	2	-	4/15/91/115	-
18	BCR	a4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	aB	811	2	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	LMG	bB	851	-	-	26/50/70/70	0/1/1/1
15	CLA	b5	410	13,15	-	14/38/114/115	-
15	CLA	b6	410	13	-	6/39/115/115	-
18	BCR	bB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	b3	411	13	-	5/15/91/115	-
15	CLA	cB	842	-	-	2/15/91/115	-
18	BCR	b6	419	-	-	10/29/63/63	0/2/2/2
18	BCR	bB	850	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	831	2	-	8/15/91/115	-
15	CLA	aA	808	1	-	4/23/99/115	-
14	CL0	aA	801	1	-	6/39/115/115	-
15	CLA	a3	414	13	-	4/10/86/115	-
15	CLA	cA	811	1	-	10/15/91/115	-
15	CLA	bB	840	2	-	16/39/115/115	-
15	CLA	aB	803	-	-	11/39/115/115	-
15	CLA	bA	812	1	-	13/39/115/115	-
15	CLA	aA	818	1	-	6/26/102/115	-
15	CLA	bB	833	2	-	18/39/115/115	-
15	CLA	b4	409	13	-	6/39/115/115	-
15	CLA	c2	407	13	-	4/15/91/115	-
15	CLA	a6	411	13,15	-	13/38/114/115	-
15	CLA	bB	801	-	-	12/39/115/115	-
15	CLA	b6	413	13	-	9/15/91/115	-
15	CLA	aB	802	2	-	13/39/115/115	-
15	CLA	b5	420	13	-	12/39/115/115	-
15	CLA	b1	415	13	-	7/15/91/115	-
15	CLA	b2	407	13	-	4/15/91/115	-
15	CLA	cB	824	2	-	5/15/91/115	-
15	CLA	bA	815	1	-	4/15/91/115	-
15	CLA	c5	416	13	-	11/21/97/115	-
18	BCR	a4	401	-	-	13/29/63/63	0/2/2/2
18	BCR	cI	102	-	-	11/29/63/63	0/2/2/2
20	LMG	aB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	aA	830	1	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cF	201	22	-	10/23/99/115	-
15	CLA	b1	407	-	-	7/15/91/115	-
18	BCR	cA	848	15	-	13/29/63/63	0/2/2/2
18	BCR	c1	418	-	-	8/29/63/63	0/2/2/2
18	BCR	a1	421	-	-	14/29/63/63	0/2/2/2
15	CLA	c2	416	13	-	7/15/91/115	-
15	CLA	bA	804	1	-	10/39/115/115	-
15	CLA	a6	408	-	-	7/15/91/115	-
15	CLA	a6	422	13	-	19/39/115/115	-
15	CLA	aA	806	1	-	23/39/115/115	-
18	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	c2	410	13	-	6/39/115/115	-
15	CLA	aA	813	1	-	8/26/102/115	-
15	CLA	bA	841	1	-	17/39/115/115	-
15	CLA	cA	834	1	-	12/39/115/115	-
15	CLA	aB	840	2	-	16/39/115/115	-
15	CLA	aA	842	22	-	10/23/99/115	-
15	CLA	bK	101	-	-	10/15/91/115	-
18	BCR	bL	206	-	-	14/29/63/63	0/2/2/2
15	CLA	a1	416	13	-	10/27/103/115	-
15	CLA	cA	844	19	-	13/24/100/115	-
19	LHG	aA	853	-	-	19/53/53/53	-
15	CLA	b4	415	13	-	7/15/91/115	-
18	BCR	b1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a2	414	13	-	3/15/91/115	-
15	CLA	cB	802	2	-	13/39/115/115	-
15	CLA	bB	822	2	-	2/15/91/115	-
15	CLA	aB	804	-	-	12/39/115/115	-
15	CLA	c2	405	13	-	3/15/91/115	-
15	CLA	a6	410	13	-	6/39/115/115	-
15	CLA	b6	417	13	-	11/21/97/115	-
15	CLA	cB	821	2	-	13/18/94/115	-
15	CLA	c1	406	13	-	4/15/91/115	-
15	CLA	c4	421	13	-	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	832	2	-	8/20/96/115	-
18	BCR	cB	845	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	840	1	-	4/18/94/115	-
15	CLA	a1	414	13	-	7/15/91/115	-
15	CLA	bB	820	2,22	-	10/39/115/115	-
15	CLA	bA	828	1	-	14/39/115/115	-
18	BCR	a2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	814	1	-	16/33/109/115	-
15	CLA	aA	833	1	-	11/39/115/115	-
15	CLA	c5	403	13,15	-	14/39/115/115	-
15	CLA	cJ	102	8	-	2/4/76/115	-
15	CLA	a4	408	13	-	5/15/91/115	-
15	CLA	b6	405	13	-	11/39/115/115	-
15	CLA	aB	834	2	-	15/31/107/115	-
15	CLA	cB	812	2	-	3/15/91/115	-
15	CLA	cB	820	2,22	-	10/39/115/115	-
15	CLA	b5	411	13	-	3/15/91/115	-
17	SF4	cC	102	3	-	-	0/6/5/5
15	CLA	a5	415	13	-	7/15/91/115	-
15	CLA	a5	406	13	-	4/15/91/115	-
15	CLA	c4	417	13	-	9/27/103/115	-
16	PQN	bB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	aB	809	2	-	13/39/115/115	-
15	CLA	bA	844	-	-	7/9/81/115	-
15	CLA	a6	418	13	-	11/27/103/115	-
15	CLA	b1	411	13	-	5/15/91/115	-
15	CLA	cB	818	2	-	10/32/108/115	-
15	CLA	cB	806	2	-	21/39/115/115	-
17	SF4	aA	847	2,1	-	-	0/6/5/5
15	CLA	cL	203	22	-	15/39/115/115	-
15	CLA	b3	409	13	-	5/39/115/115	-
15	CLA	a2	417	13	-	9/21/97/115	-
15	CLA	a1	415	13	-	11/21/97/115	-
15	CLA	c2	413	13	-	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	819	2	-	12/33/109/115	-
15	CLA	a4	404	13	-	12/39/115/115	-
15	CLA	a2	407	13	-	4/15/91/115	-
15	CLA	c6	408	-	-	7/15/91/115	-
18	BCR	bB	845	-	-	12/29/63/63	0/2/2/2
18	BCR	c1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	c1	408	13	-	5/15/91/115	-
15	CLA	c3	415	13	-	7/15/91/115	-
18	BCR	cF	204	-	-	12/29/63/63	0/2/2/2
15	CLA	a4	410	13,15	-	13/38/114/115	-
15	CLA	b3	408	13	-	5/15/91/115	-
15	CLA	bL	204	22	-	15/39/115/115	-
15	CLA	a2	402	13	-	17/39/115/115	-
15	CLA	b6	404	13,15	-	14/39/115/115	-
18	BCR	a6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	aL	203	22	-	15/39/115/115	-
15	CLA	bB	839	22	-	10/39/115/115	-
18	BCR	cB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	a4	409	13	-	5/39/115/115	-
15	CLA	b6	422	13	-	17/39/115/115	-
15	CLA	c5	408	13	-	5/15/91/115	-
15	CLA	b3	416	13	-	11/21/97/115	-
15	CLA	cB	839	22	-	10/39/115/115	-
15	CLA	cB	801	-	-	12/39/115/115	-
15	CLA	c1	404	13	-	13/39/115/115	-
18	BCR	c4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	843	1	-	14/39/115/115	-
15	CLA	bA	838	1	-	8/23/99/115	-
15	CLA	bA	837	1	-	7/15/91/115	-
18	BCR	aF	203	-	-	11/29/63/63	0/2/2/2
15	CLA	a6	405	13	-	11/39/115/115	-
15	CLA	b5	415	13	-	7/15/91/115	-
15	CLA	c2	418	13	-	11/27/103/115	-
15	CLA	b2	417	13	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	841	-	-	4/15/91/115	-
15	CLA	c1	409	13	-	6/39/115/115	-
15	CLA	b5	407	-	-	8/15/91/115	-
15	CLA	bB	842	-	-	2/15/91/115	-
18	BCR	bA	850	15	-	13/29/63/63	0/2/2/2
15	CLA	bA	808	1	-	4/23/99/115	-
15	CLA	aB	824	2	-	5/15/91/115	-
15	CLA	a1	406	-	-	8/15/91/115	-
15	CLA	cB	826	2,22	-	8/17/93/115	-
15	CLA	b2	412	13	-	3/15/91/115	-
15	CLA	cB	835	2	-	9/15/91/115	-
15	CLA	bA	807	1	-	11/39/115/115	-
15	CLA	aB	830	2	-	6/39/115/115	-
15	CLA	bA	820	1	-	18/39/115/115	-
18	BCR	aK	101	-	-	10/29/63/63	0/2/2/2
18	BCR	c4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b1	412	13	-	9/15/91/115	-
15	CLA	b6	403	13	-	17/39/115/115	-
15	CLA	c5	409	13	-	6/39/115/115	-
15	CLA	b3	402	13	-	17/39/115/115	-
15	CLA	aA	839	1	-	16/39/115/115	-
15	CLA	aB	815	2	-	17/39/115/115	-
15	CLA	bA	836	1	-	8/26/102/115	-
16	PQN	bA	846	-	-	5/23/43/43	0/2/2/2
15	CLA	b4	402	13	-	17/39/115/115	-
15	CLA	cA	842	1	-	14/39/115/115	-
18	BCR	a3	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	808	2	-	14/39/115/115	-
15	CLA	a1	409	13,15	-	14/38/114/115	-
15	CLA	a2	418	13	-	11/27/103/115	-
15	CLA	bA	826	-	-	10/39/115/115	-
15	CLA	c3	411	13	-	5/15/91/115	-
15	CLA	cA	810	1	-	18/39/115/115	-
18	BCR	aB	848	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	aB	849	-	-	11/29/63/63	0/2/2/2
18	BCR	a3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bB	831	2	-	8/15/91/115	-
15	CLA	c6	410	13	-	6/39/115/115	-
15	CLA	cA	843	-	-	7/9/81/115	-
19	LHG	bA	854	-	-	19/53/53/53	-
18	BCR	bA	852	-	-	8/29/63/63	0/2/2/2
15	CLA	b6	412	13	-	4/15/91/115	-
15	CLA	bB	835	2	-	9/15/91/115	-
15	CLA	bB	814	2	-	25/39/115/115	-
15	CLA	aA	831	1	-	8/39/115/115	-
15	CLA	a5	417	13	-	9/27/103/115	-
18	BCR	b1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	c6	417	13	-	11/21/97/115	-
15	CLA	b3	413	13	-	3/15/91/115	-
15	CLA	b4	421	13	-	13/39/115/115	-
15	CLA	aA	838	1	-	8/23/99/115	-
15	CLA	aA	837	1	-	7/15/91/115	-
15	CLA	cB	814	2	-	25/39/115/115	-
15	CLA	a4	403	13,15	-	14/39/115/115	-
18	BCR	b2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	404	13	-	11/39/115/115	-
15	CLA	b4	413	13	-	4/15/91/115	-
18	BCR	a4	419	-	-	11/29/63/63	0/2/2/2
18	BCR	c2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	b5	403	13,15	-	14/39/115/115	-
15	CLA	c6	412	13	-	4/15/91/115	-
15	CLA	c6	416	13	-	7/15/91/115	-
15	CLA	a6	407	13	-	4/15/91/115	-
15	CLA	cA	836	1	-	8/26/102/115	-
18	BCR	c3	419	-	-	10/29/63/63	0/2/2/2
18	BCR	c5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	825	2	-	10/26/102/115	-
15	CLA	aB	807	2	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cA	831	1	-	8/39/115/115	-
15	CLA	a4	417	13	-	9/27/103/115	-
15	CLA	cB	817	2	-	12/27/103/115	-
15	CLA	cB	829	2	-	16/39/115/115	-
15	CLA	c2	406	13	-	11/39/115/115	-
18	BCR	bI	102	-	-	11/29/63/63	0/2/2/2
15	CLA	a1	404	13	-	3/15/91/115	-
15	CLA	cB	822	2	-	2/15/91/115	-
15	CLA	bA	806	1	-	23/39/115/115	-
15	CLA	a4	413	13	-	4/15/91/115	-
18	BCR	c4	418	-	-	9/29/63/63	0/2/2/2
18	BCR	a2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	cA	830	1	-	13/39/115/115	-
18	BCR	cL	204	-	-	9/29/63/63	0/2/2/2
15	CLA	c5	413	13	-	3/15/91/115	-
15	CLA	b1	408	13	-	5/15/91/115	-
15	CLA	a3	407	-	-	7/15/91/115	-
15	CLA	a4	412	13	-	9/15/91/115	-
18	BCR	a2	401	-	-	12/29/63/63	0/2/2/2
15	CLA	bL	203	10	-	10/39/115/115	-
15	CLA	aB	826	2,22	-	8/17/93/115	-
18	BCR	cM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	412	13	-	9/15/91/115	-
15	CLA	bX	102	12	-	8/15/91/115	-
15	CLA	a1	413	13	-	4/10/86/115	-
15	CLA	a2	406	13	-	11/39/115/115	-
15	CLA	cA	805	1	-	11/32/108/115	-
18	BCR	c3	420	-	-	12/29/63/63	0/2/2/2
18	BCR	cA	850	-	-	8/29/63/63	0/2/2/2
18	BCR	cB	846	-	-	13/29/63/63	0/2/2/2
15	CLA	aB	821	2	-	13/18/94/115	-
15	CLA	a2	412	13	-	3/15/91/115	-
15	CLA	b3	421	13	-	12/39/115/115	-
15	CLA	b4	416	13	-	11/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	810	2	-	16/39/115/115	-
15	CLA	cA	839	1	-	16/39/115/115	-
15	CLA	c6	404	13,15	-	14/39/115/115	-
15	CLA	aB	823	-	-	5/27/103/115	-
15	CLA	a4	415	13	-	7/15/91/115	-
15	CLA	bB	813	2	-	4/15/91/115	-
18	BCR	a6	420	-	-	12/29/63/63	0/2/2/2
18	BCR	aB	844	-	-	9/29/63/63	0/2/2/2
18	BCR	c1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	411	13,15	-	12/38/114/115	-
15	CLA	aA	810	1	-	18/39/115/115	-
15	CLA	b3	404	13	-	12/39/115/115	-
15	CLA	b4	411	13	-	5/15/91/115	-
15	CLA	b4	414	13	-	4/10/86/115	-
15	CLA	bA	840	1	-	5/18/94/115	-
15	CLA	cB	827	2	-	15/39/115/115	-
15	CLA	aB	812	2	-	3/15/91/115	-
15	CLA	cB	828	2	-	21/39/115/115	-
15	CLA	c3	407	-	-	7/15/91/115	-
15	CLA	c4	406	13	-	4/15/91/115	-
18	BCR	cJ	103	-	-	14/29/63/63	0/2/2/2
18	BCR	b2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	402	13	-	17/39/115/115	-
15	CLA	c6	405	13	-	11/39/115/115	-
15	CLA	bB	805	2	-	5/26/102/115	-
15	CLA	b2	414	13	-	3/15/91/115	-
18	BCR	c5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	840	1	-	5/18/94/115	-
15	CLA	bB	832	2	-	8/20/96/115	-
15	CLA	b4	408	13	-	5/15/91/115	-
15	CLA	aA	819	1	-	10/26/102/115	-
15	CLA	b6	414	13	-	4/15/91/115	-
15	CLA	c5	402	13	-	17/39/115/115	-
15	CLA	aA	821	18,1	-	15/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	825	2	-	10/26/102/115	-
15	CLA	cB	805	2	-	5/26/102/115	-
15	CLA	cA	814	1	-	16/33/109/115	-
15	CLA	b1	402	13	-	17/39/115/115	-
15	CLA	cB	838	2	-	2/18/94/115	-
15	CLA	cB	837	2	-	15/39/115/115	-
15	CLA	c2	412	13	-	3/15/91/115	-
18	BCR	bJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	c4	407	-	-	8/15/91/115	-
15	CLA	a4	405	13	-	4/15/91/115	-
18	BCR	a6	421	-	-	13/29/63/63	0/2/2/2
16	PQN	cB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	cA	829	1	-	22/39/115/115	-
15	CLA	aA	812	1	-	13/39/115/115	-
15	CLA	a2	403	13,15	-	14/39/115/115	-
17	SF4	cC	101	3	-	-	0/6/5/5
15	CLA	bB	834	2	-	15/31/107/115	-
18	BCR	bL	201	-	-	14/29/63/63	0/2/2/2
18	BCR	bM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	812	2	-	3/15/91/115	-
18	BCR	c4	401	-	-	13/29/63/63	0/2/2/2
18	BCR	b3	419	-	-	11/29/63/63	0/2/2/2
18	BCR	aA	850	-	-	13/29/63/63	0/2/2/2
15	CLA	b3	414	13	-	4/10/86/115	-
18	BCR	a1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	809	1	-	21/39/115/115	-
15	CLA	aA	802	22	-	16/39/115/115	-
15	CLA	bJ	101	8	-	8/15/91/115	-
15	CLA	c1	411	13	-	5/15/91/115	-
15	CLA	c6	413	13	-	9/15/91/115	-
18	BCR	aM	101	-	-	11/29/63/63	0/2/2/2
18	BCR	b4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	c5	417	13	-	10/27/103/115	-

The worst 5 of 6339 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	aA	846	PQN	C3-C2	6.92	1.47	1.35
16	bA	846	PQN	C3-C2	6.88	1.47	1.35
16	cA	845	PQN	C3-C2	6.86	1.47	1.35
16	cB	843	PQN	C3-C2	6.78	1.47	1.35
16	aB	843	PQN	C3-C2	6.78	1.47	1.35

The worst 5 of 7568 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	bB	804	CLA	C4A-NA-C1A	10.51	111.43	106.71
15	aB	804	CLA	C4A-NA-C1A	10.44	111.40	106.71
15	aA	803	CLA	C4A-NA-C1A	9.96	111.19	106.71
15	cA	803	CLA	C4A-NA-C1A	9.91	111.16	106.71

There are no chirality outliers.

5 of 7649 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	C1A-C2A-CAA-CBA
15	aA	804	CLA	CHA-CBD-CGD-O1D
15	aA	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

660 monomers are involved in 1881 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a1	417	BCR	4	0
15	bA	833	CLA	3	0
15	aA	805	CLA	3	0
15	cA	815	CLA	2	0
15	c5	411	CLA	1	0
15	a4	411	CLA	1	0
15	aX	102	CLA	2	0
15	cA	804	CLA	8	0
15	bA	829	CLA	6	0
18	c3	401	BCR	1	0
15	cA	813	CLA	2	0
18	a3	401	BCR	2	0
15	c3	414	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	bL	205	BCR	3	0
15	bA	810	CLA	6	0
15	cB	825	CLA	1	0
18	cB	847	BCR	2	0
15	b3	415	CLA	7	0
15	b5	409	CLA	3	0
15	aB	833	CLA	8	0
15	a3	412	CLA	2	0
18	b2	401	BCR	4	0
15	bB	802	CLA	3	0
15	cB	819	CLA	3	0
15	aA	834	CLA	5	0
15	b3	417	CLA	5	0
15	a2	410	CLA	3	0
15	a5	414	CLA	1	0
15	cA	825	CLA	5	0
15	aB	818	CLA	4	0
15	b2	410	CLA	3	0
18	a5	401	BCR	4	0
15	aB	816	CLA	1	0
15	c4	412	CLA	2	0
15	b6	415	CLA	1	0
15	bL	202	CLA	2	0
18	aL	205	BCR	1	0
15	b3	412	CLA	2	0
15	bB	819	CLA	4	0
15	c4	405	CLA	1	0
18	bA	853	BCR	4	0
18	b1	401	BCR	2	0
15	b3	405	CLA	1	0
15	c5	414	CLA	1	0
15	c1	416	CLA	4	0
15	a6	413	CLA	3	0
15	cA	827	CLA	2	0
15	a2	404	CLA	2	0
15	a4	414	CLA	1	0
18	aB	845	BCR	3	0
15	aA	825	CLA	5	0
15	c1	410	CLA	4	0
15	a2	409	CLA	1	0
15	cA	826	CLA	3	0
15	bB	811	CLA	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	aB	842	CLA	2	0
15	a1	422	CLA	8	0
18	cK	101	BCR	1	0
15	a1	411	CLA	2	0
15	b1	410	CLA	3	0
15	aB	817	CLA	4	0
15	c2	415	CLA	1	0
15	c3	402	CLA	9	0
15	aB	828	CLA	6	0
15	bB	804	CLA	4	0
15	aB	839	CLA	4	0
18	b3	418	BCR	2	0
15	bA	842	CLA	3	0
15	b6	418	CLA	5	0
15	cA	837	CLA	1	0
18	bB	846	BCR	2	0
15	c5	410	CLA	4	0
15	bB	841	CLA	1	0
15	b5	402	CLA	9	0
15	c3	412	CLA	2	0
18	a5	418	BCR	1	0
15	cB	804	CLA	4	0
15	b1	404	CLA	3	0
15	c1	414	CLA	1	0
15	bB	827	CLA	3	0
15	b4	417	CLA	5	0
15	aA	844	CLA	1	0
15	cB	803	CLA	2	0
15	bA	845	CLA	1	0
15	c1	417	CLA	2	0
15	aA	832	CLA	1	0
15	aB	801	CLA	4	0
15	a3	403	CLA	4	0
15	b4	404	CLA	3	0
18	cA	847	BCR	3	0
15	cJ	101	CLA	1	0
20	cB	850	LMG	1	0
15	bB	809	CLA	3	0
15	b2	402	CLA	8	0
18	aJ	205	BCR	3	0
15	aA	820	CLA	2	0
15	bB	824	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c1	402	CLA	9	0
18	b4	419	BCR	3	0
18	b5	418	BCR	1	0
15	c1	405	CLA	1	0
14	cA	801	CL0	3	0
15	bA	816	CLA	1	0
15	a5	403	CLA	4	0
15	c6	403	CLA	9	0
18	aB	846	BCR	1	0
15	bF	201	CLA	2	0
15	a6	409	CLA	1	0
15	bA	831	CLA	5	0
15	b6	416	CLA	8	0
15	cA	802	CLA	2	0
15	cL	201	CLA	5	0
15	a2	405	CLA	1	0
15	c5	412	CLA	3	0
15	c5	405	CLA	1	0
15	a3	405	CLA	1	0
18	b6	420	BCR	3	0
15	b2	411	CLA	3	0
18	bJ	105	BCR	4	0
15	bB	816	CLA	1	0
15	a3	409	CLA	2	0
18	bJ	103	BCR	5	0
15	a1	402	CLA	4	0
15	bA	821	CLA	3	0
15	a6	416	CLA	8	0
15	cF	203	CLA	3	0
18	c5	418	BCR	1	0
15	c1	413	CLA	1	0
15	a1	410	CLA	1	0
18	a1	419	BCR	3	0
15	aB	835	CLA	2	0
14	bA	801	CL0	4	0
15	a6	415	CLA	1	0
18	b6	402	BCR	3	0
18	aB	847	BCR	3	0
18	cI	101	BCR	1	0
15	a2	413	CLA	3	0
15	a5	408	CLA	1	0
15	cA	841	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c3	409	CLA	3	0
15	cX	102	CLA	2	0
15	cA	803	CLA	5	0
15	bA	819	CLA	1	0
15	a3	411	CLA	1	0
18	b4	420	BCR	5	0
15	a3	415	CLA	8	0
15	c3	408	CLA	1	0
15	c2	422	CLA	7	0
15	aA	804	CLA	6	0
15	aA	826	CLA	3	0
15	aA	835	CLA	5	0
15	cA	838	CLA	1	0
18	aA	848	BCR	4	0
18	cA	849	BCR	2	0
15	b3	410	CLA	4	0
18	bB	844	BCR	3	0
15	aB	832	CLA	2	0
15	c4	409	CLA	3	0
18	c2	419	BCR	1	0
15	b1	417	CLA	4	0
15	a5	410	CLA	3	0
15	aA	827	CLA	2	0
15	cA	818	CLA	2	0
18	c2	401	BCR	5	0
18	cJ	104	BCR	3	0
15	c3	416	CLA	4	0
18	bB	849	BCR	6	0
15	c2	409	CLA	1	0
18	aA	851	BCR	2	0
15	bA	805	CLA	3	0
15	cA	816	CLA	1	0
15	c3	410	CLA	3	0
15	aB	806	CLA	2	0
15	aB	820	CLA	1	0
15	a6	403	CLA	9	0
15	bA	832	CLA	1	0
15	cB	831	CLA	3	0
15	b1	409	CLA	3	0
15	c6	418	CLA	4	0
15	b2	416	CLA	8	0
15	b5	404	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	a3	418	BCR	1	0
15	cA	807	CLA	5	0
15	a2	411	CLA	3	0
18	aF	201	BCR	3	0
15	a5	405	CLA	1	0
15	a2	422	CLA	8	0
15	cB	808	CLA	5	0
15	c3	404	CLA	3	0
15	aA	845	CLA	1	0
15	c4	403	CLA	4	0
15	b3	403	CLA	4	0
15	b6	411	CLA	3	0
15	cA	828	CLA	3	0
15	aA	814	CLA	2	0
15	b2	409	CLA	1	0
15	c1	415	CLA	8	0
15	aB	838	CLA	3	0
15	a5	416	CLA	5	0
18	b1	418	BCR	3	0
15	b1	416	CLA	4	0
15	bB	815	CLA	5	0
15	a1	408	CLA	3	0
18	a5	419	BCR	5	0
18	c6	419	BCR	2	0
15	c2	417	CLA	6	0
15	b2	422	CLA	9	0
15	bB	803	CLA	4	0
15	aA	815	CLA	2	0
15	aA	822	CLA	4	0
18	b5	401	BCR	3	0
15	c4	408	CLA	1	0
15	b1	414	CLA	1	0
15	cA	809	CLA	2	0
15	c5	415	CLA	8	0
15	c2	404	CLA	3	0
15	cB	816	CLA	1	0
15	a6	406	CLA	1	0
15	c3	403	CLA	4	0
15	c5	404	CLA	3	0
18	aI	102	BCR	6	0
15	b2	405	CLA	1	0
15	b5	412	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	aA	849	BCR	2	0
15	c4	410	CLA	4	0
15	cA	819	CLA	1	0
15	a1	401	CLA	9	0
15	c4	402	CLA	8	0
15	cB	810	CLA	4	0
15	a6	417	CLA	5	0
15	c3	417	CLA	6	0
15	b1	405	CLA	1	0
18	cB	848	BCR	2	0
15	aB	814	CLA	7	0
18	b3	420	BCR	5	0
18	b5	419	BCR	5	0
15	aA	816	CLA	1	0
15	a6	404	CLA	4	0
15	cA	812	CLA	5	0
15	aB	829	CLA	5	0
15	b1	403	CLA	4	0
15	bA	843	CLA	10	0
15	a3	417	CLA	5	0
15	cL	202	CLA	3	0
15	c6	415	CLA	1	0
15	c3	405	CLA	1	0
18	b6	401	BCR	3	0
15	b2	413	CLA	2	0
15	a5	420	CLA	10	0
15	bB	817	CLA	4	0
18	c6	402	BCR	3	0
19	aX	101	LHG	1	0
15	bB	828	CLA	5	0
15	c4	404	CLA	2	0
18	a4	420	BCR	5	0
18	cF	202	BCR	5	0
15	bA	839	CLA	5	0
15	a3	410	CLA	4	0
16	cA	845	PQN	4	0
15	c3	421	CLA	6	0
15	bB	829	CLA	5	0
15	b5	408	CLA	1	0
15	aA	803	CLA	5	0
15	a6	412	CLA	1	0
15	b5	416	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cA	833	CLA	3	0
15	b2	403	CLA	5	0
15	b5	417	CLA	6	0
18	c6	420	BCR	2	0
15	b2	406	CLA	16	0
15	cB	815	CLA	5	0
15	a4	416	CLA	5	0
15	c1	403	CLA	4	0
15	cB	833	CLA	9	0
15	a3	404	CLA	3	0
18	a1	418	BCR	4	0
15	aJ	202	CLA	1	0
19	cA	852	LHG	3	0
15	a3	402	CLA	9	0
15	bA	827	CLA	4	0
15	cA	808	CLA	2	0
15	aA	841	CLA	5	0
15	b4	412	CLA	1	0
15	a2	416	CLA	8	0
15	cA	832	CLA	1	0
15	c4	411	CLA	1	0
15	b2	418	CLA	4	0
15	bA	813	CLA	2	0
15	bA	818	CLA	2	0
15	aA	829	CLA	4	0
15	bA	822	CLA	3	0
15	b4	410	CLA	4	0
15	cA	820	CLA	3	0
15	aL	202	CLA	4	0
15	bB	838	CLA	1	0
15	bB	837	CLA	7	0
16	aB	843	PQN	3	0
15	c6	411	CLA	3	0
15	aB	841	CLA	1	0
15	a1	403	CLA	2	0
18	b4	401	BCR	3	0
15	aL	201	CLA	3	0
15	aB	827	CLA	3	0
15	cB	834	CLA	1	0
15	bB	808	CLA	2	0
15	c4	415	CLA	9	0
15	c4	416	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b5	414	CLA	1	0
15	bA	835	CLA	6	0
15	bB	818	CLA	4	0
15	cB	809	CLA	3	0
15	bA	825	CLA	5	0
15	b4	405	CLA	1	0
15	c1	412	CLA	2	0
15	aB	813	CLA	3	0
15	b6	409	CLA	1	0
15	cA	835	CLA	3	0
15	b2	404	CLA	2	0
15	c5	420	CLA	8	0
15	a1	412	CLA	1	0
15	bB	836	CLA	1	0
15	aB	837	CLA	8	0
15	b4	403	CLA	5	0
15	b5	405	CLA	1	0
18	b2	419	BCR	3	0
15	cB	830	CLA	3	0
18	b6	421	BCR	1	0
15	bA	834	CLA	5	0
18	a6	401	BCR	3	0
15	aA	828	CLA	3	0
15	a5	409	CLA	3	0
15	b6	406	CLA	1	0
18	bA	851	BCR	2	0
15	c4	414	CLA	1	0
15	c6	409	CLA	1	0
18	cA	851	BCR	4	0
18	cF	205	BCR	8	0
18	aA	852	BCR	4	0
18	bA	848	BCR	2	0
15	aJ	201	CLA	4	0
15	cA	821	CLA	4	0
18	c1	419	BCR	4	0
15	cA	806	CLA	4	0
15	a3	416	CLA	4	0
15	cB	807	CLA	3	0
18	aI	103	BCR	4	0
15	a5	411	CLA	1	0
18	c2	420	BCR	2	0
18	c6	401	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c6	406	CLA	1	0
15	aA	809	CLA	2	0
15	a3	421	CLA	6	0
15	cA	822	CLA	3	0
15	c2	403	CLA	5	0
18	c3	418	BCR	1	0
15	bB	826	CLA	2	0
15	a1	407	CLA	1	0
16	aA	846	PQN	3	0
15	a5	402	CLA	9	0
15	bB	830	CLA	3	0
18	a2	420	BCR	3	0
18	a6	402	BCR	5	0
18	aJ	204	BCR	5	0
18	bB	847	BCR	4	0
15	bB	821	CLA	2	0
15	b2	415	CLA	1	0
15	a3	408	CLA	1	0
18	bF	202	BCR	5	0
15	bB	806	CLA	2	0
15	cB	840	CLA	2	0
15	aB	810	CLA	2	0
15	bB	807	CLA	4	0
15	a4	421	CLA	7	0
15	a4	402	CLA	9	0
15	bA	803	CLA	8	0
18	cB	844	BCR	2	0
15	aA	836	CLA	3	0
15	aA	807	CLA	5	0
15	bA	802	CLA	1	0
18	aF	202	BCR	7	0
15	a2	415	CLA	1	0
15	cB	811	CLA	4	0
18	b3	401	BCR	1	0
15	cB	813	CLA	3	0
18	a4	418	BCR	1	0
15	aB	811	CLA	10	0
20	bB	851	LMG	1	0
15	b5	410	CLA	4	0
15	b6	410	CLA	4	0
18	bB	848	BCR	2	0
15	b3	411	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	cB	842	CLA	2	0
18	b6	419	BCR	1	0
18	bB	850	BCR	5	0
15	aB	831	CLA	2	0
15	aA	808	CLA	2	0
14	aA	801	CL0	4	0
15	a3	414	CLA	1	0
15	bB	840	CLA	2	0
15	aB	803	CLA	1	0
15	bA	812	CLA	5	0
15	aA	818	CLA	1	0
15	bB	833	CLA	4	0
15	b4	409	CLA	3	0
15	a6	411	CLA	3	0
15	bB	801	CLA	6	0
15	b6	413	CLA	3	0
15	aB	802	CLA	2	0
15	b5	420	CLA	10	0
15	b1	415	CLA	8	0
15	cB	824	CLA	2	0
15	bA	815	CLA	1	0
15	c5	416	CLA	5	0
18	a4	401	BCR	4	0
18	cI	102	BCR	3	0
20	aB	850	LMG	1	0
15	aA	830	CLA	1	0
15	cF	201	CLA	3	0
18	cA	848	BCR	3	0
18	c1	418	BCR	2	0
18	a1	421	BCR	2	0
15	c2	416	CLA	8	0
15	bA	804	CLA	8	0
15	a6	422	CLA	11	0
15	aA	806	CLA	5	0
18	bA	849	BCR	3	0
15	c2	410	CLA	2	0
15	aA	813	CLA	2	0
15	bA	841	CLA	3	0
15	cA	834	CLA	5	0
15	aB	840	CLA	1	0
15	aA	842	CLA	3	0
18	bL	206	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a1	416	CLA	2	0
15	cA	844	CLA	3	0
19	aA	853	LHG	3	0
15	b4	415	CLA	8	0
18	b1	420	BCR	5	0
15	cB	802	CLA	3	0
15	bB	822	CLA	1	0
15	aB	804	CLA	4	0
15	c2	405	CLA	1	0
15	a6	410	CLA	3	0
15	b6	417	CLA	4	0
15	cB	821	CLA	2	0
15	c4	421	CLA	7	0
15	cB	832	CLA	2	0
18	cB	845	BCR	3	0
15	aA	840	CLA	2	0
15	a1	414	CLA	7	0
15	bB	820	CLA	1	0
15	bA	828	CLA	3	0
18	a2	421	BCR	4	0
15	bA	814	CLA	1	0
15	aA	833	CLA	2	0
15	c5	403	CLA	4	0
15	a4	408	CLA	1	0
15	b6	405	CLA	3	0
15	aB	834	CLA	1	0
15	cB	812	CLA	2	0
15	cB	820	CLA	1	0
15	b5	411	CLA	1	0
15	a5	415	CLA	8	0
15	c4	417	CLA	5	0
16	bB	843	PQN	4	0
15	aB	809	CLA	3	0
15	bA	844	CLA	1	0
15	a6	418	CLA	4	0
15	b1	411	CLA	1	0
15	cB	818	CLA	3	0
15	cB	806	CLA	2	0
15	cL	203	CLA	5	0
15	b3	409	CLA	3	0
15	a2	417	CLA	6	0
15	a1	415	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	c2	413	CLA	3	0
15	aB	819	CLA	3	0
15	a4	404	CLA	3	0
18	bB	845	BCR	3	0
18	c1	420	BCR	4	0
15	c1	408	CLA	1	0
15	c3	415	CLA	7	0
18	cF	204	BCR	5	0
15	a4	410	CLA	4	0
15	b3	408	CLA	1	0
15	bL	204	CLA	5	0
15	a2	402	CLA	9	0
15	b6	404	CLA	4	0
18	a6	419	BCR	2	0
15	aL	203	CLA	4	0
15	bB	839	CLA	4	0
18	cB	849	BCR	5	0
15	a4	409	CLA	3	0
15	b6	422	CLA	9	0
15	c5	408	CLA	1	0
15	b3	416	CLA	4	0
15	cB	839	CLA	5	0
15	cB	801	CLA	5	0
15	c1	404	CLA	2	0
18	c4	419	BCR	3	0
15	aA	843	CLA	11	0
15	bA	838	CLA	1	0
15	bA	837	CLA	1	0
18	aF	203	BCR	6	0
15	a6	405	CLA	2	0
15	b5	415	CLA	8	0
15	c2	418	CLA	4	0
15	b2	417	CLA	6	0
15	cB	841	CLA	1	0
15	c1	409	CLA	3	0
15	bB	842	CLA	2	0
18	bA	850	BCR	3	0
15	bA	808	CLA	2	0
15	aB	824	CLA	1	0
15	cB	826	CLA	3	0
15	b2	412	CLA	2	0
15	cB	835	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bA	807	CLA	5	0
15	aB	830	CLA	3	0
15	bA	820	CLA	3	0
18	aK	101	BCR	1	0
18	c4	420	BCR	5	0
15	b1	412	CLA	2	0
15	b6	403	CLA	9	0
15	c5	409	CLA	3	0
15	b3	402	CLA	9	0
15	aA	839	CLA	5	0
15	aB	815	CLA	5	0
15	bA	836	CLA	3	0
16	bA	846	PQN	3	0
15	b4	402	CLA	9	0
15	cA	842	CLA	11	0
18	a3	419	BCR	2	0
15	aB	808	CLA	5	0
15	a1	409	CLA	4	0
15	a2	418	CLA	4	0
15	bA	826	CLA	3	0
15	c3	411	CLA	1	0
15	cA	810	CLA	6	0
18	aB	848	BCR	3	0
18	aB	849	BCR	4	0
18	a3	420	BCR	4	0
15	bB	831	CLA	3	0
15	c6	410	CLA	3	0
15	cA	843	CLA	1	0
19	bA	854	LHG	3	0
18	bA	852	BCR	3	0
15	b6	412	CLA	1	0
15	bB	835	CLA	2	0
15	bB	814	CLA	8	0
15	aA	831	CLA	4	0
15	a5	417	CLA	4	0
18	b1	419	BCR	3	0
15	c6	417	CLA	5	0
15	b4	421	CLA	10	0
15	aA	838	CLA	1	0
15	aA	837	CLA	1	0
15	cB	814	CLA	7	0
15	a4	403	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	b2	420	BCR	3	0
15	a5	404	CLA	2	0
18	a4	419	BCR	3	0
18	c2	421	BCR	3	0
15	b5	403	CLA	4	0
15	c6	412	CLA	1	0
15	c6	416	CLA	8	0
15	cA	836	CLA	2	0
18	c3	419	BCR	1	0
18	c5	419	BCR	5	0
15	aB	825	CLA	1	0
15	aB	807	CLA	2	0
15	cA	831	CLA	5	0
15	a4	417	CLA	6	0
15	cB	817	CLA	4	0
15	cB	829	CLA	4	0
15	c2	406	CLA	13	0
18	bI	102	BCR	4	0
15	a1	404	CLA	1	0
15	bA	806	CLA	4	0
18	c4	418	BCR	1	0
18	a2	419	BCR	1	0
15	cA	830	CLA	1	0
18	cL	204	BCR	3	0
15	b1	408	CLA	1	0
15	a3	407	CLA	1	0
15	a4	412	CLA	2	0
18	a2	401	BCR	6	0
15	bL	203	CLA	4	0
15	aB	826	CLA	3	0
18	cM	101	BCR	4	0
15	a5	412	CLA	3	0
15	bX	102	CLA	3	0
15	a1	413	CLA	1	0
15	a2	406	CLA	11	0
15	cA	805	CLA	2	0
18	c3	420	BCR	6	0
18	cA	850	BCR	3	0
18	cB	846	BCR	2	0
15	aB	821	CLA	2	0
15	a2	412	CLA	3	0
15	b3	421	CLA	5	0

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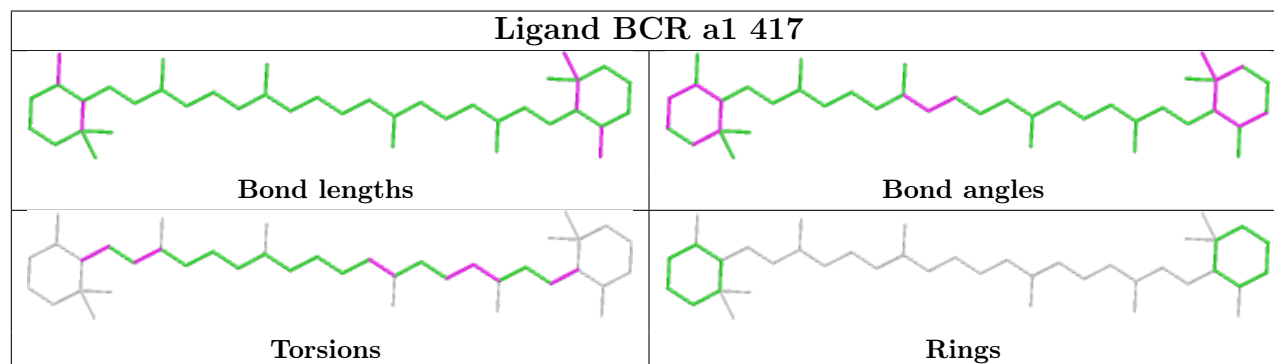
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b4	416	CLA	5	0
15	bB	810	CLA	3	0
15	cA	839	CLA	6	0
15	c6	404	CLA	4	0
15	a4	415	CLA	8	0
15	bB	813	CLA	3	0
18	a6	420	BCR	3	0
18	aB	844	BCR	2	0
18	c1	401	BCR	2	0
15	c2	411	CLA	4	0
15	aA	810	CLA	6	0
15	b3	404	CLA	3	0
15	b4	411	CLA	1	0
15	b4	414	CLA	1	0
15	bA	840	CLA	2	0
15	cB	827	CLA	3	0
15	aB	812	CLA	2	0
15	cB	828	CLA	4	0
18	cJ	103	BCR	6	0
18	b2	421	BCR	4	0
15	c2	402	CLA	9	0
15	c6	405	CLA	3	0
18	c5	401	BCR	3	0
15	cA	840	CLA	2	0
15	bB	832	CLA	4	0
15	b4	408	CLA	1	0
15	aA	819	CLA	1	0
15	c5	402	CLA	9	0
15	aA	821	CLA	4	0
15	bB	825	CLA	1	0
15	cA	814	CLA	2	0
15	b1	402	CLA	9	0
15	cB	838	CLA	3	0
15	cB	837	CLA	5	0
15	c2	412	CLA	2	0
18	bJ	104	BCR	5	0
15	a4	405	CLA	1	0
18	a6	421	BCR	1	0
16	cB	843	PQN	3	0
15	cA	829	CLA	4	0
15	aA	812	CLA	5	0
15	a2	403	CLA	5	0

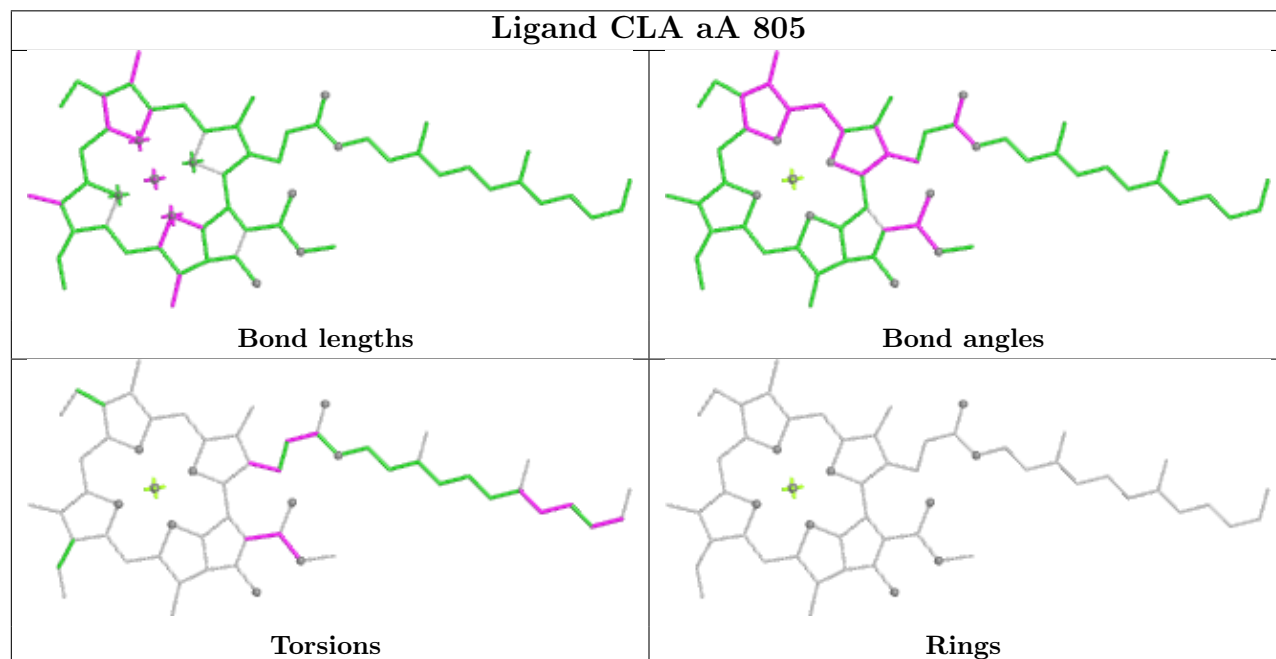
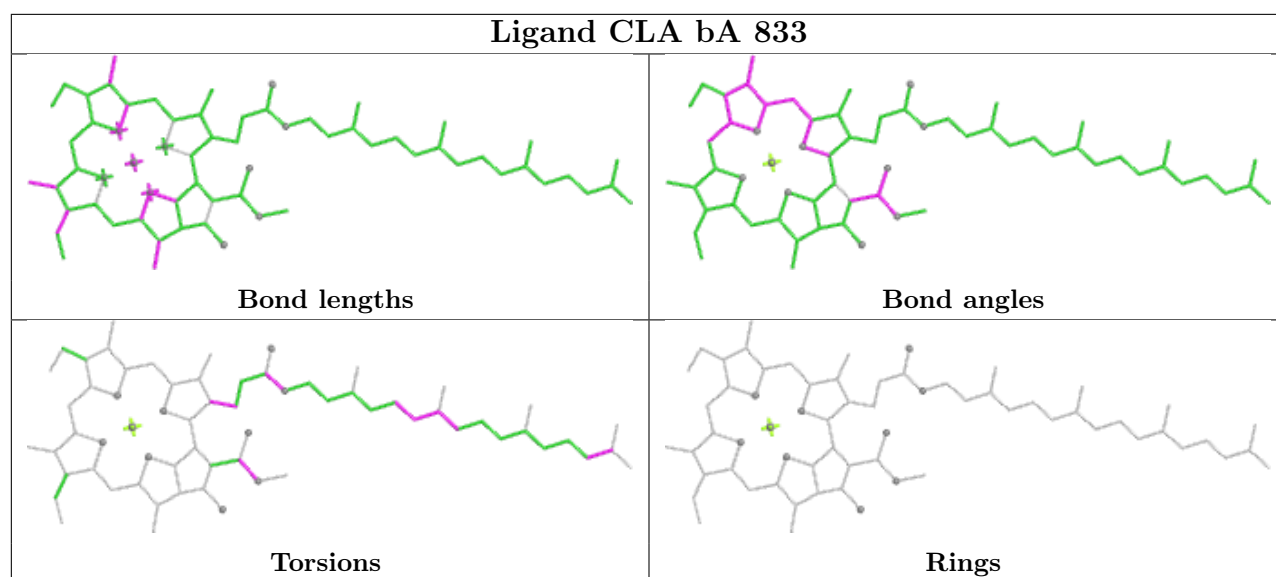
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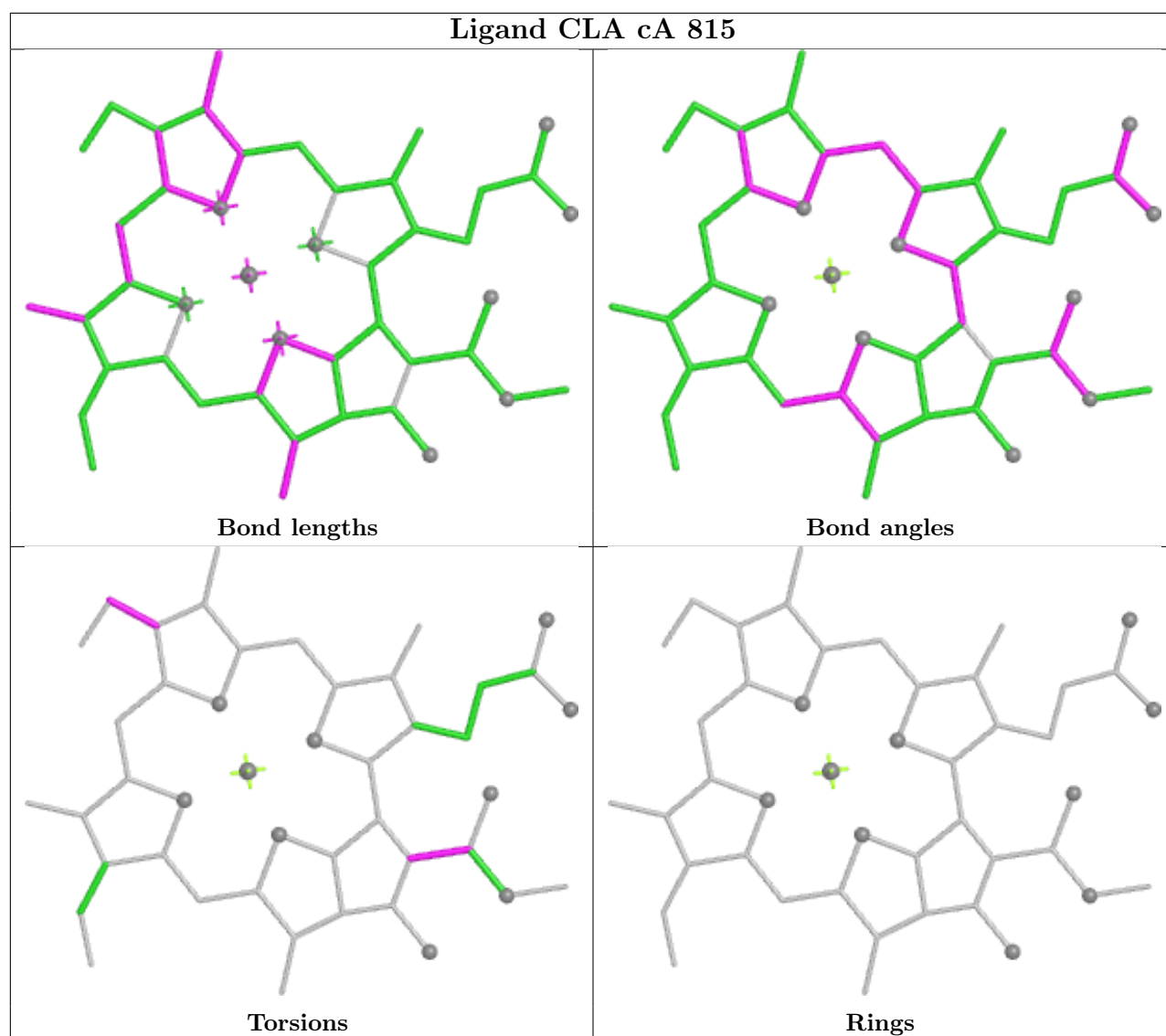
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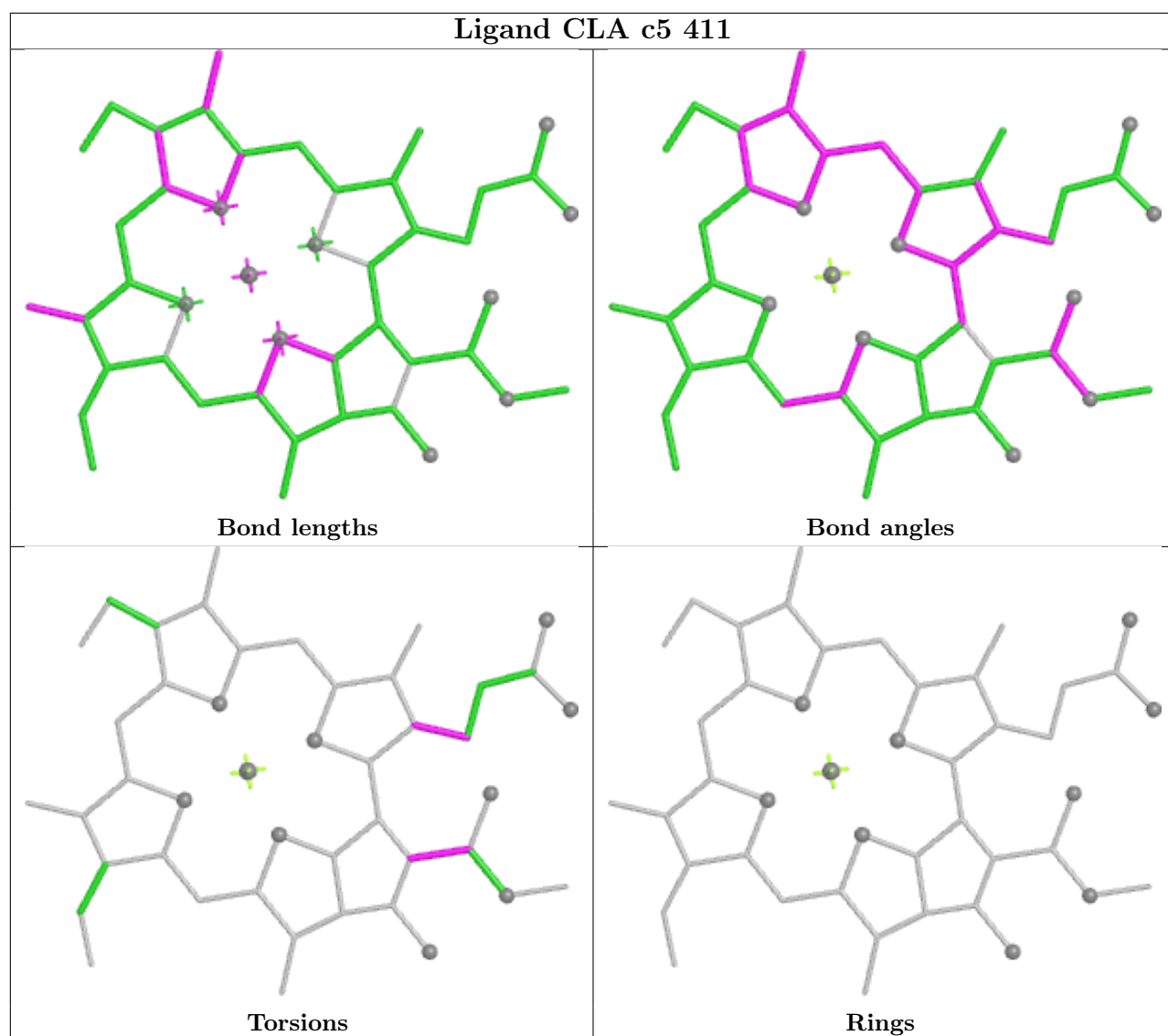
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	bB	834	CLA	1	0
18	bL	201	BCR	1	0
18	bM	101	BCR	4	0
15	bB	812	CLA	2	0
18	c4	401	BCR	4	0
18	b3	419	BCR	3	0
18	aA	850	BCR	3	0
15	b3	414	CLA	1	0
18	a1	420	BCR	2	0
15	bA	809	CLA	2	0
15	aA	802	CLA	2	0
15	bJ	101	CLA	1	0
15	c1	411	CLA	1	0
15	c6	413	CLA	3	0
18	aM	101	BCR	3	0
18	b4	418	BCR	1	0
15	c5	417	CLA	4	0

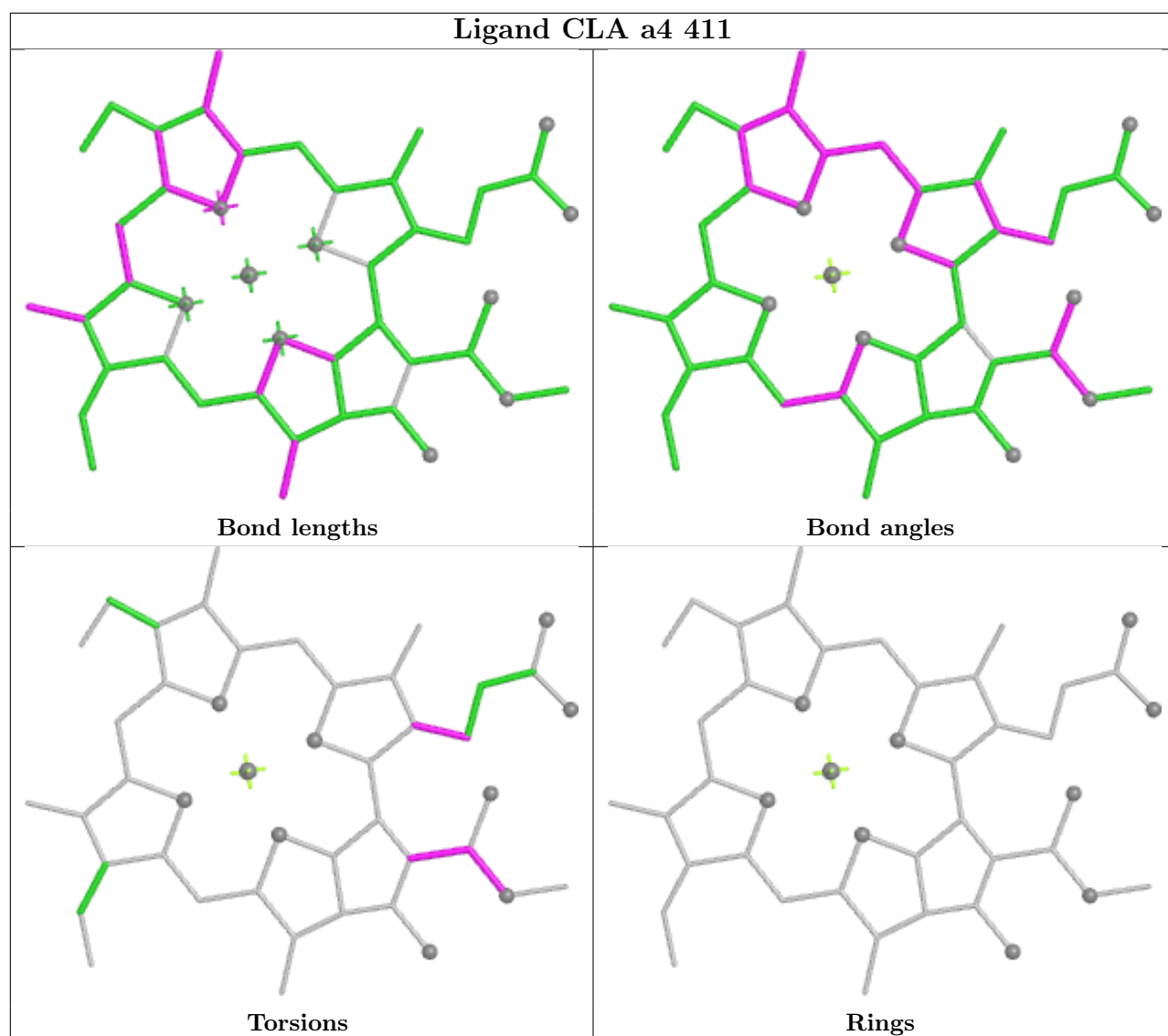
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



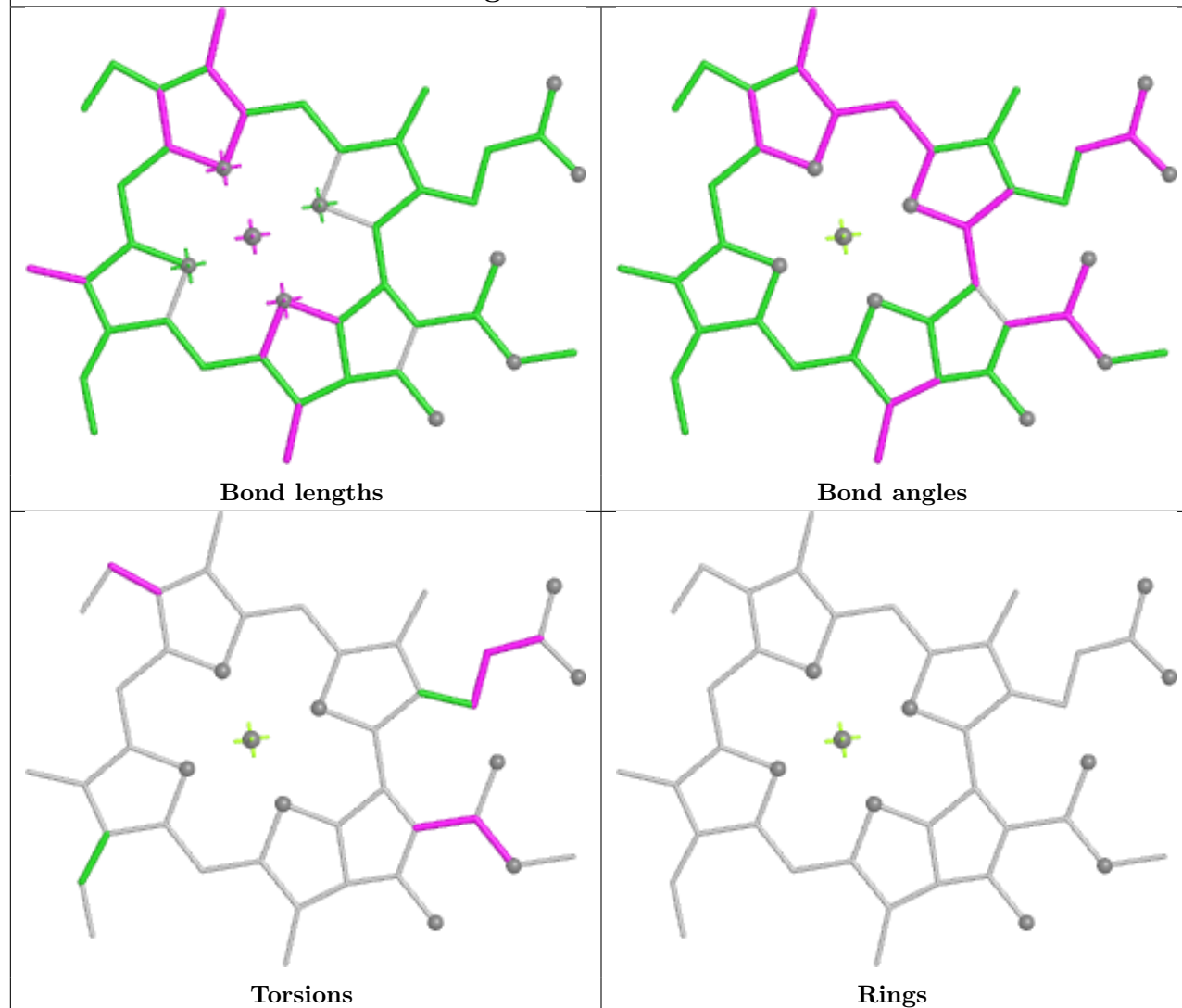




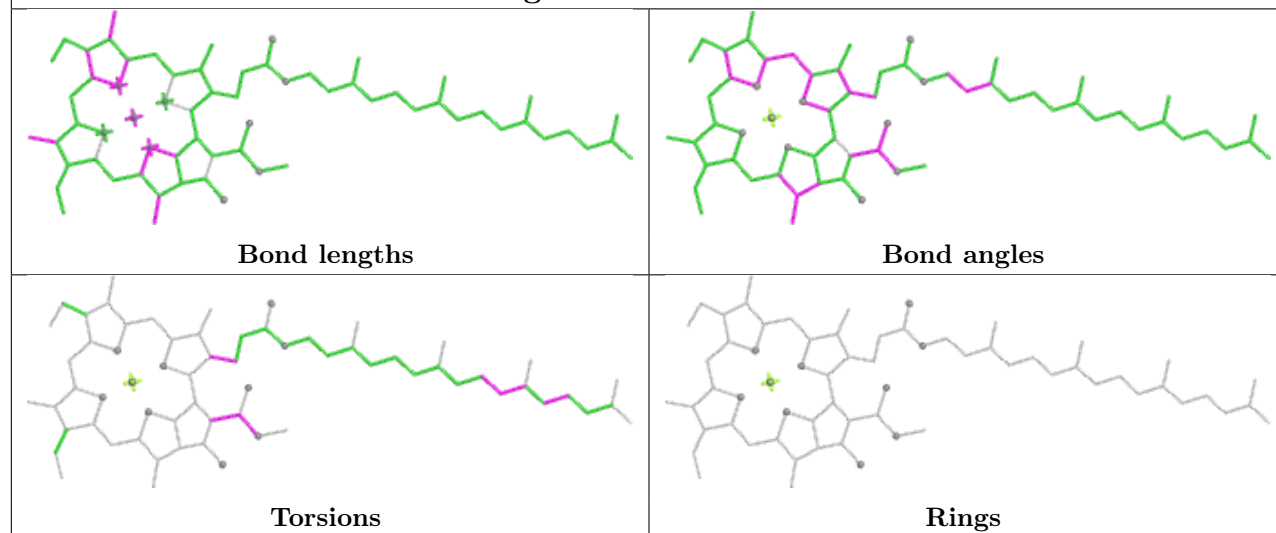


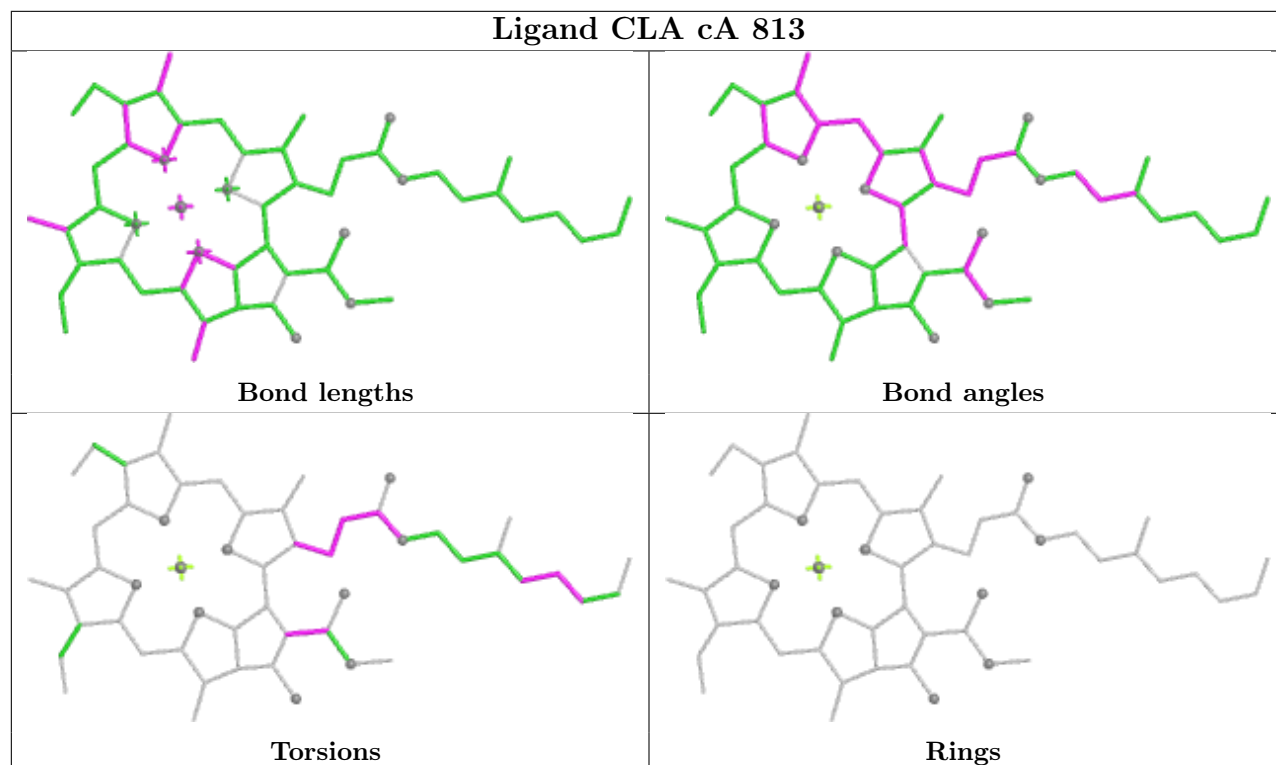
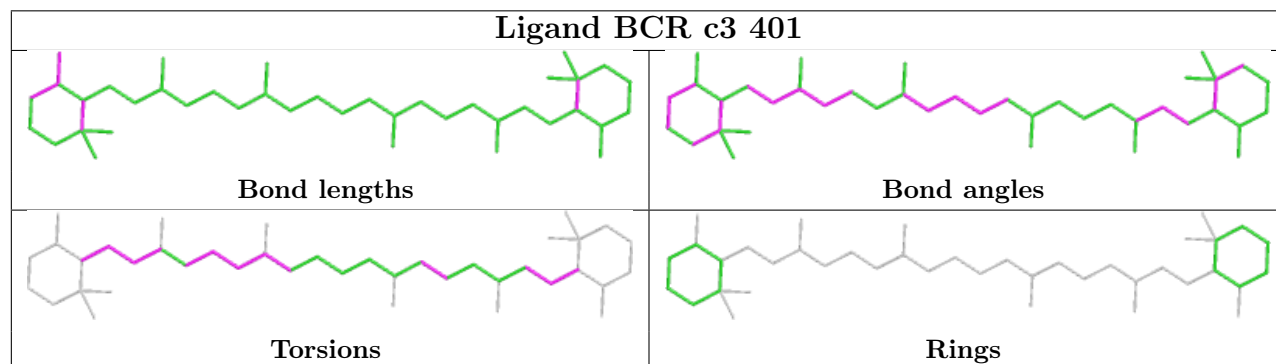
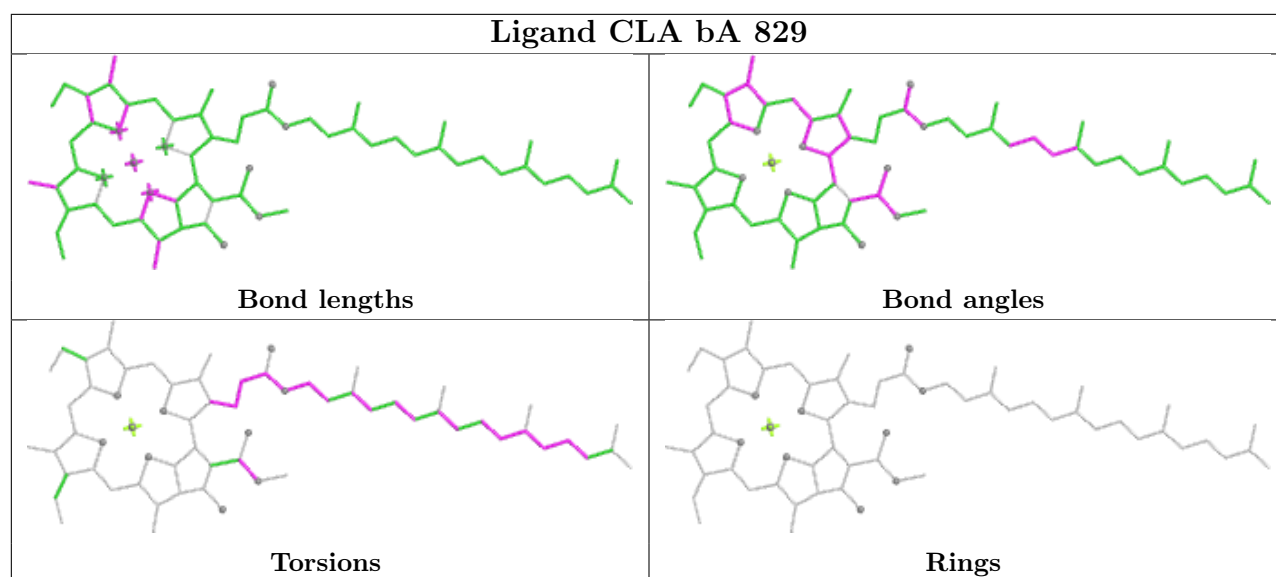


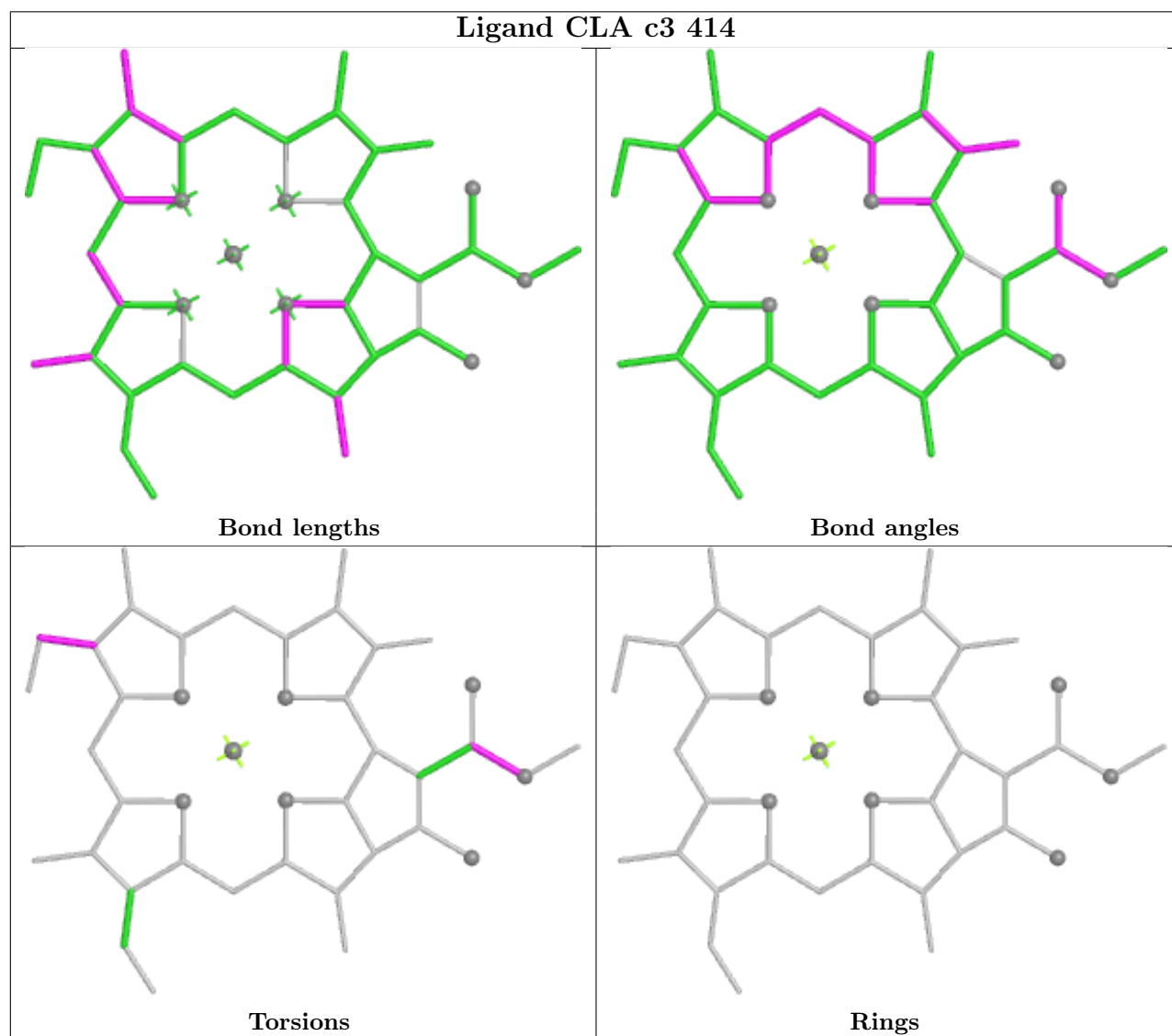
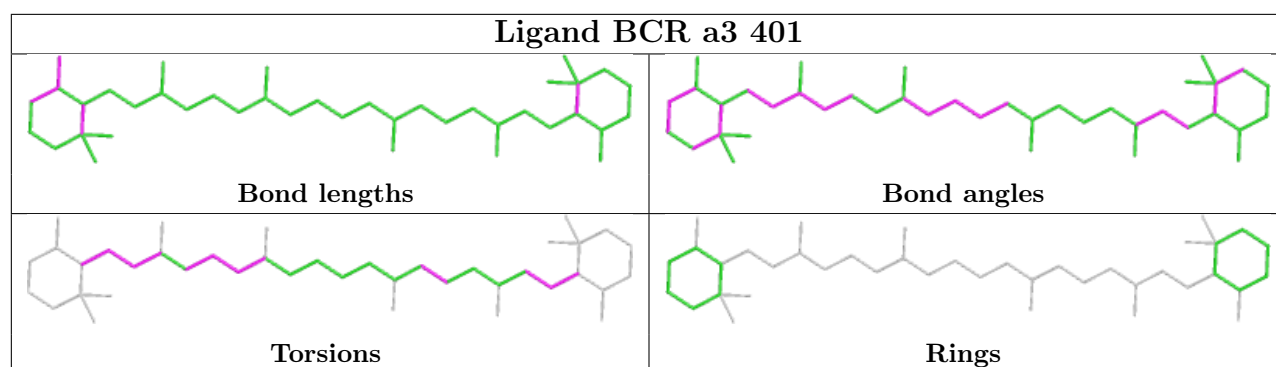
Ligand CLA aX 102

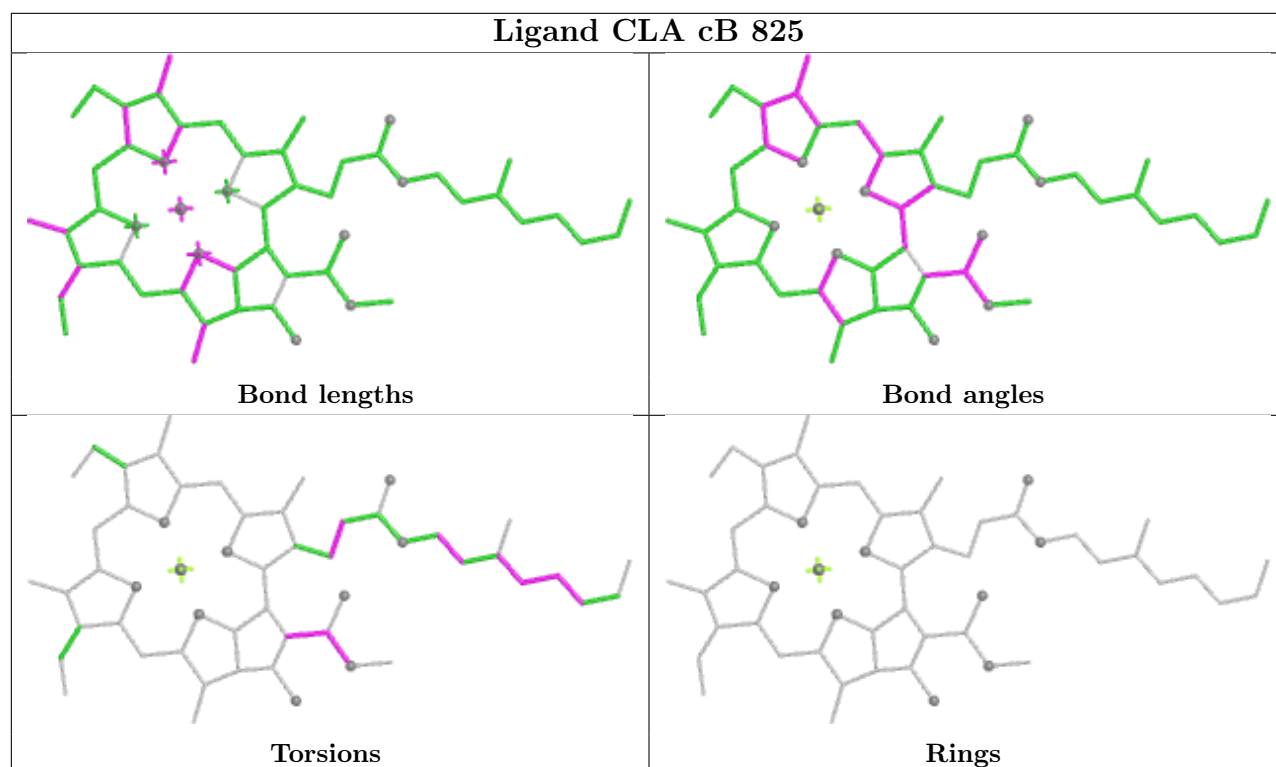
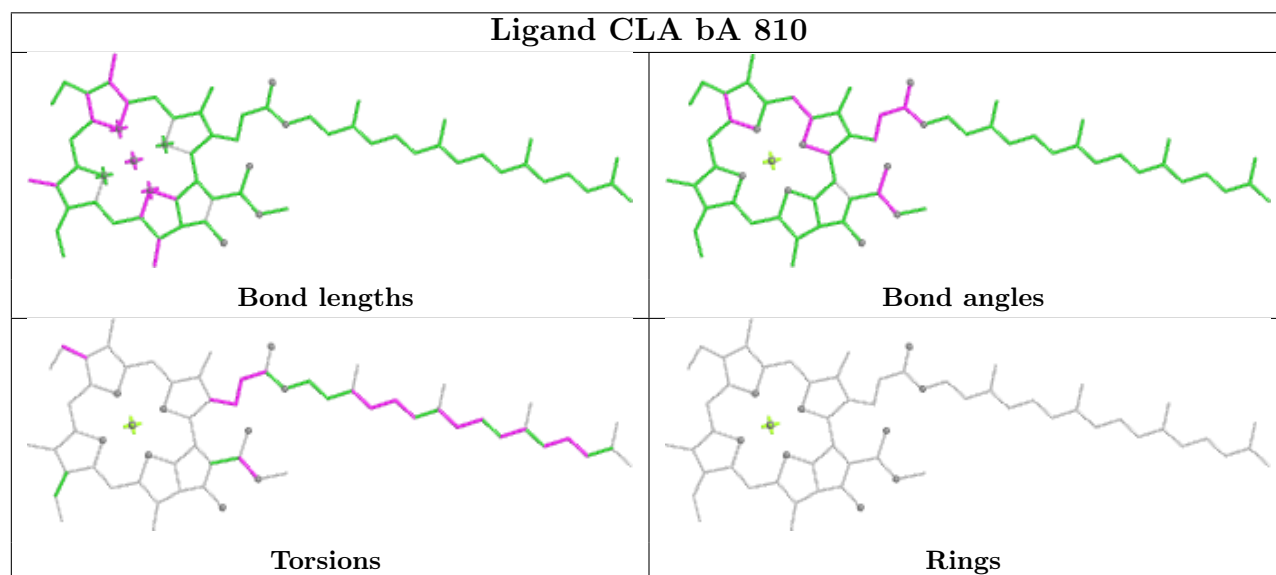
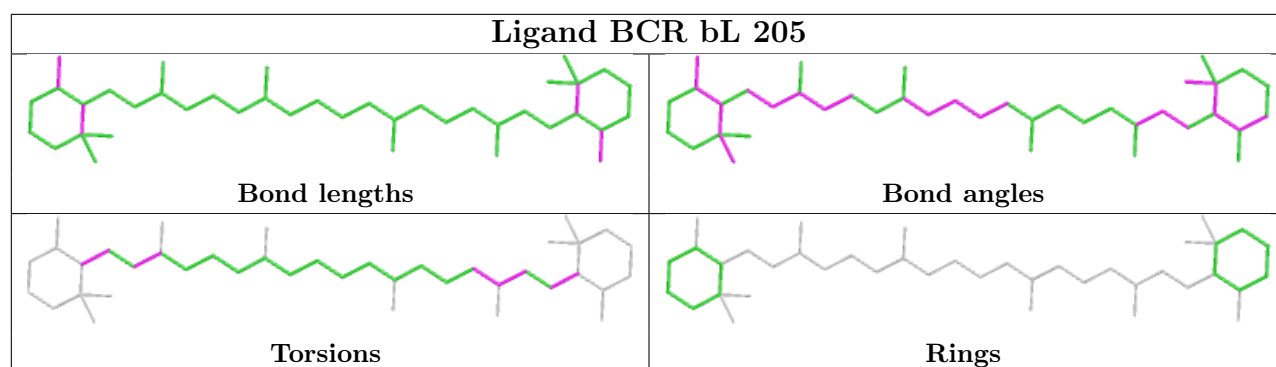


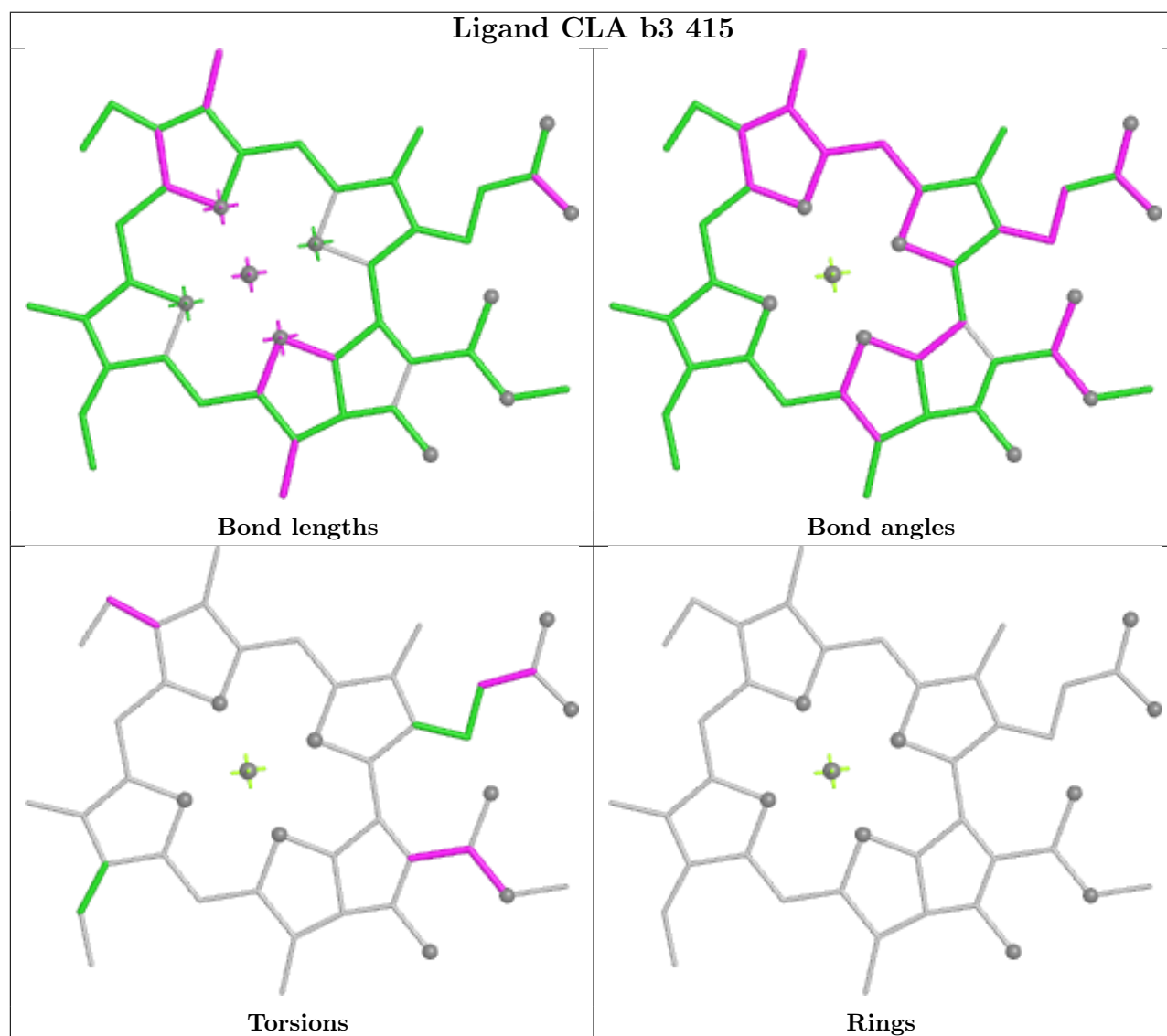
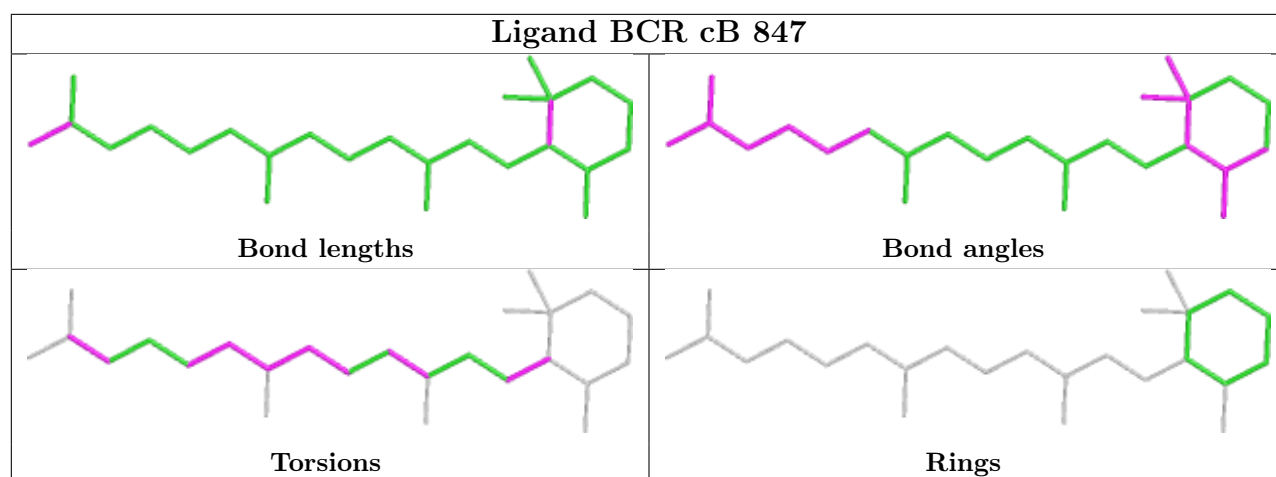
Ligand CLA cA 804

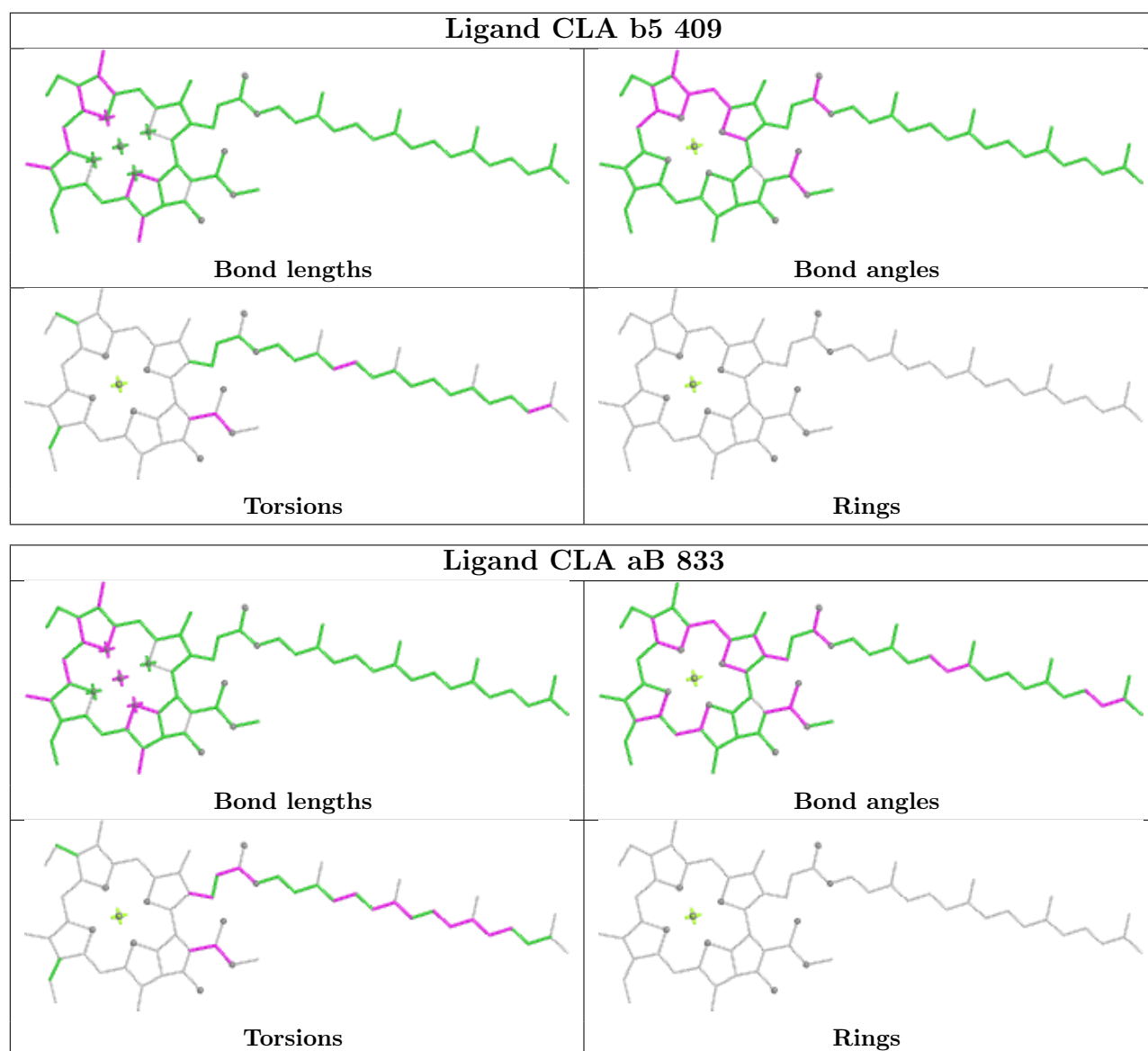


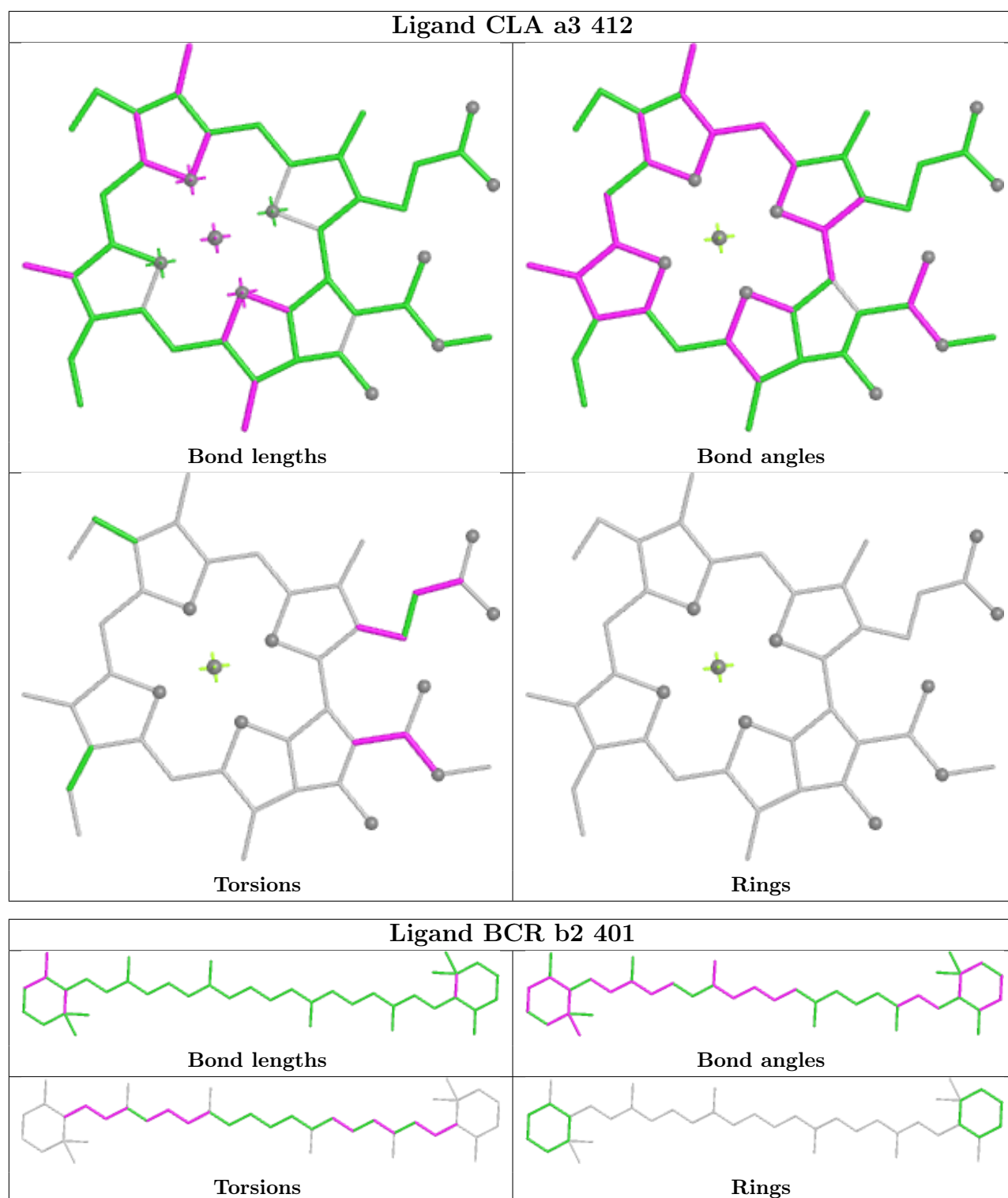


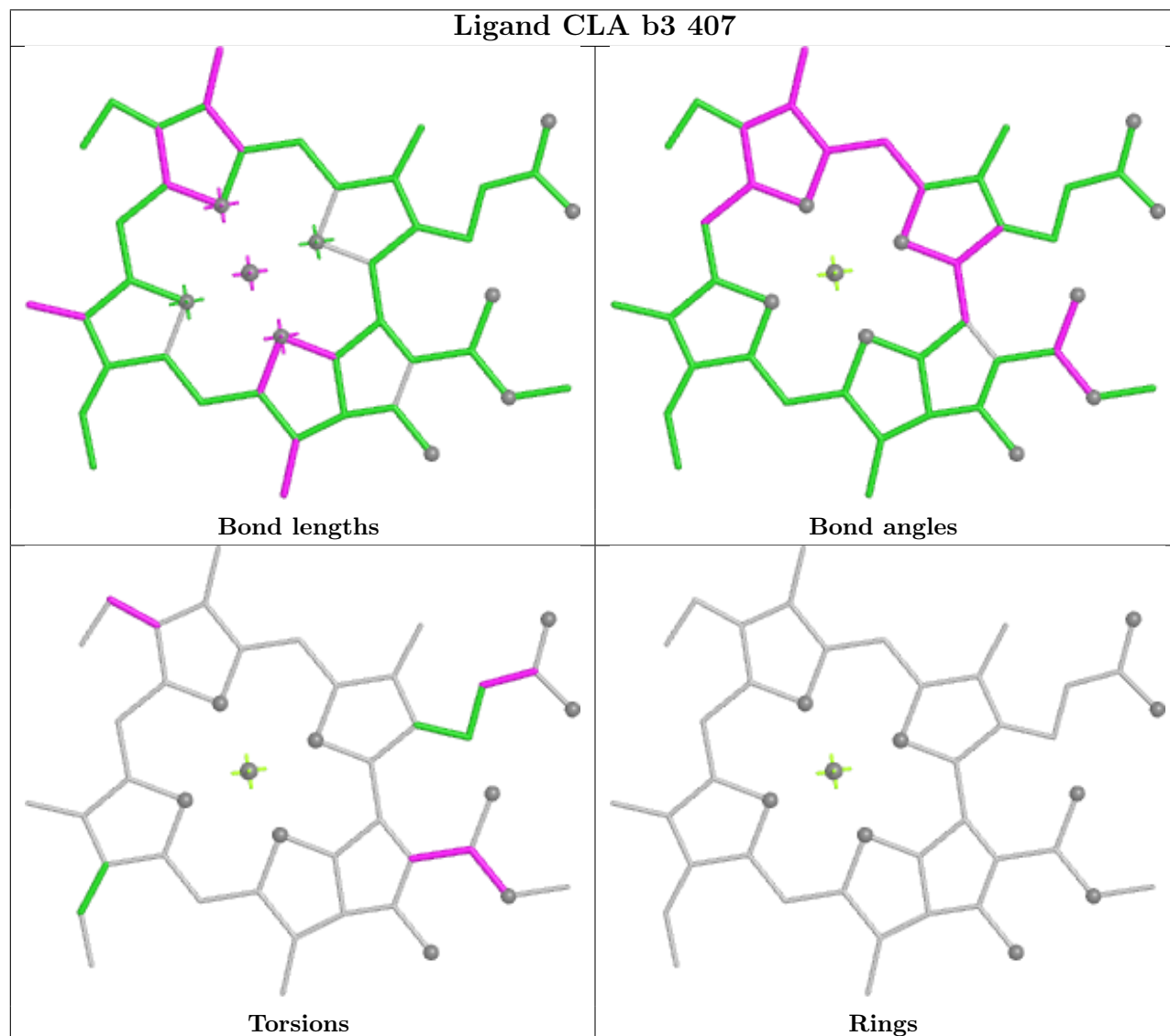
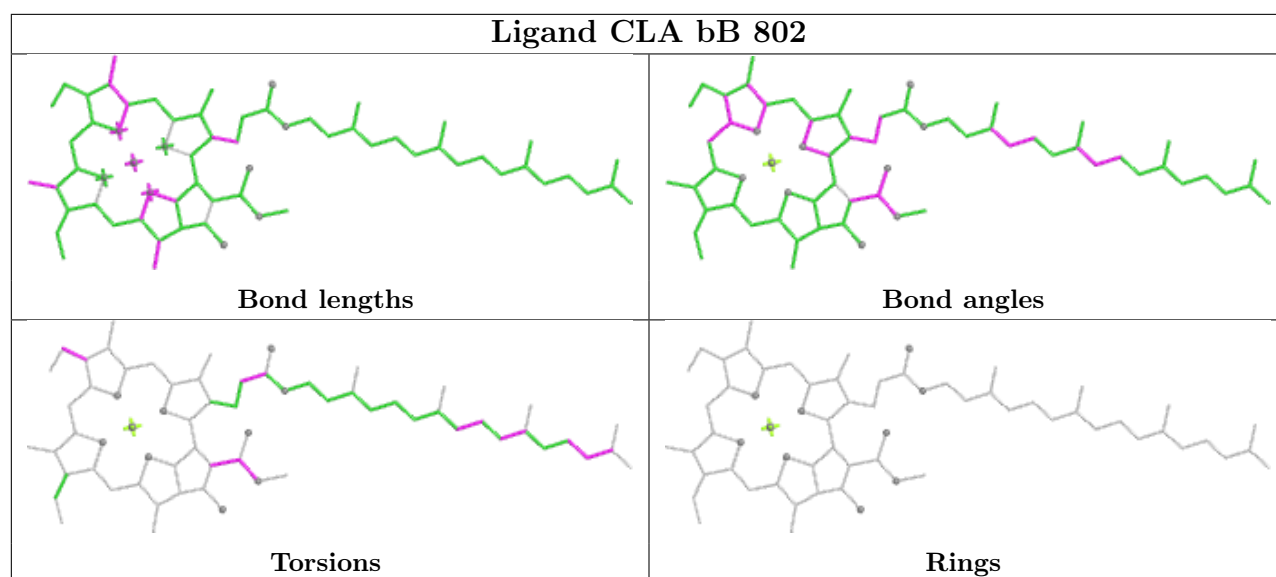


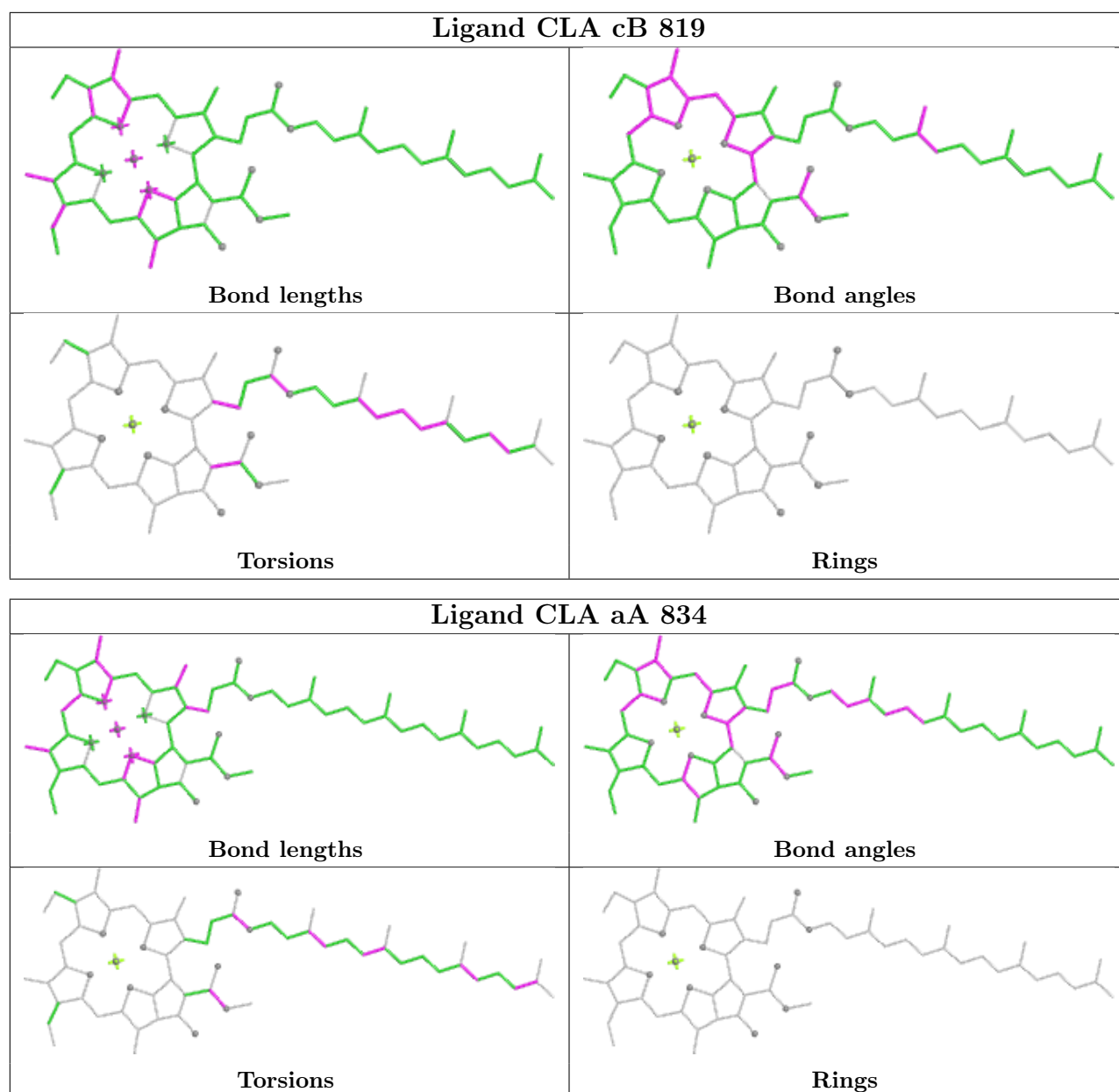


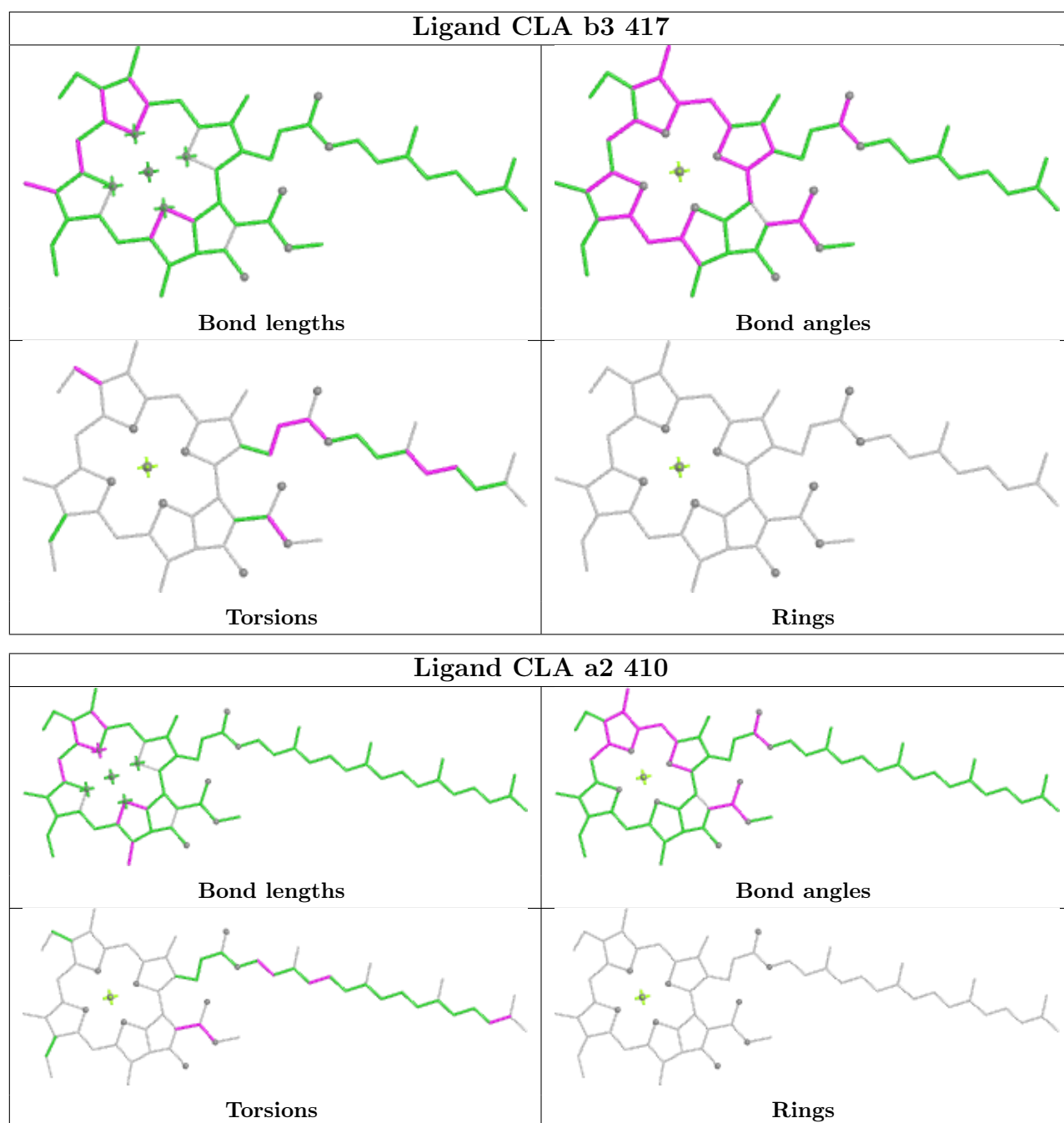


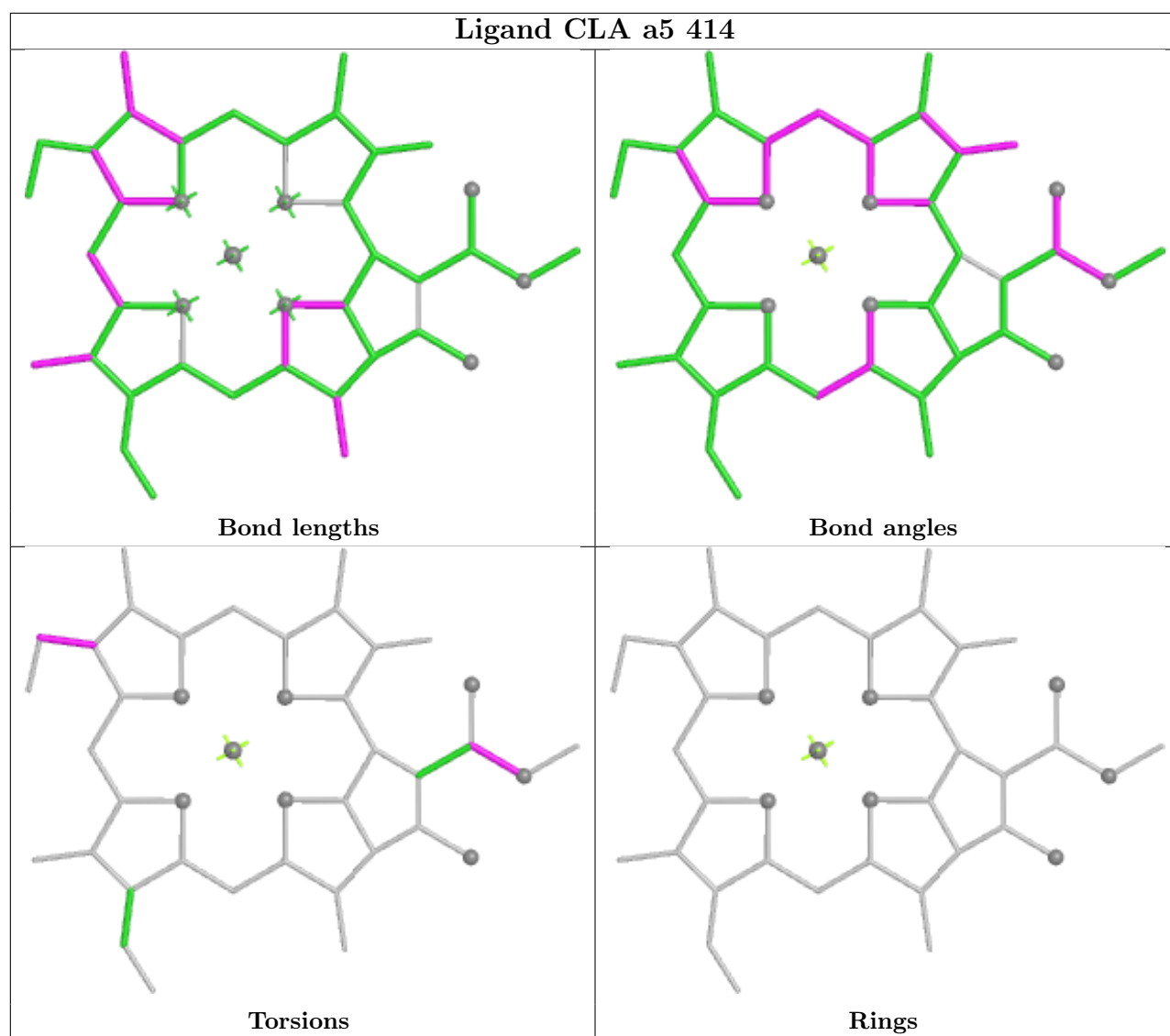


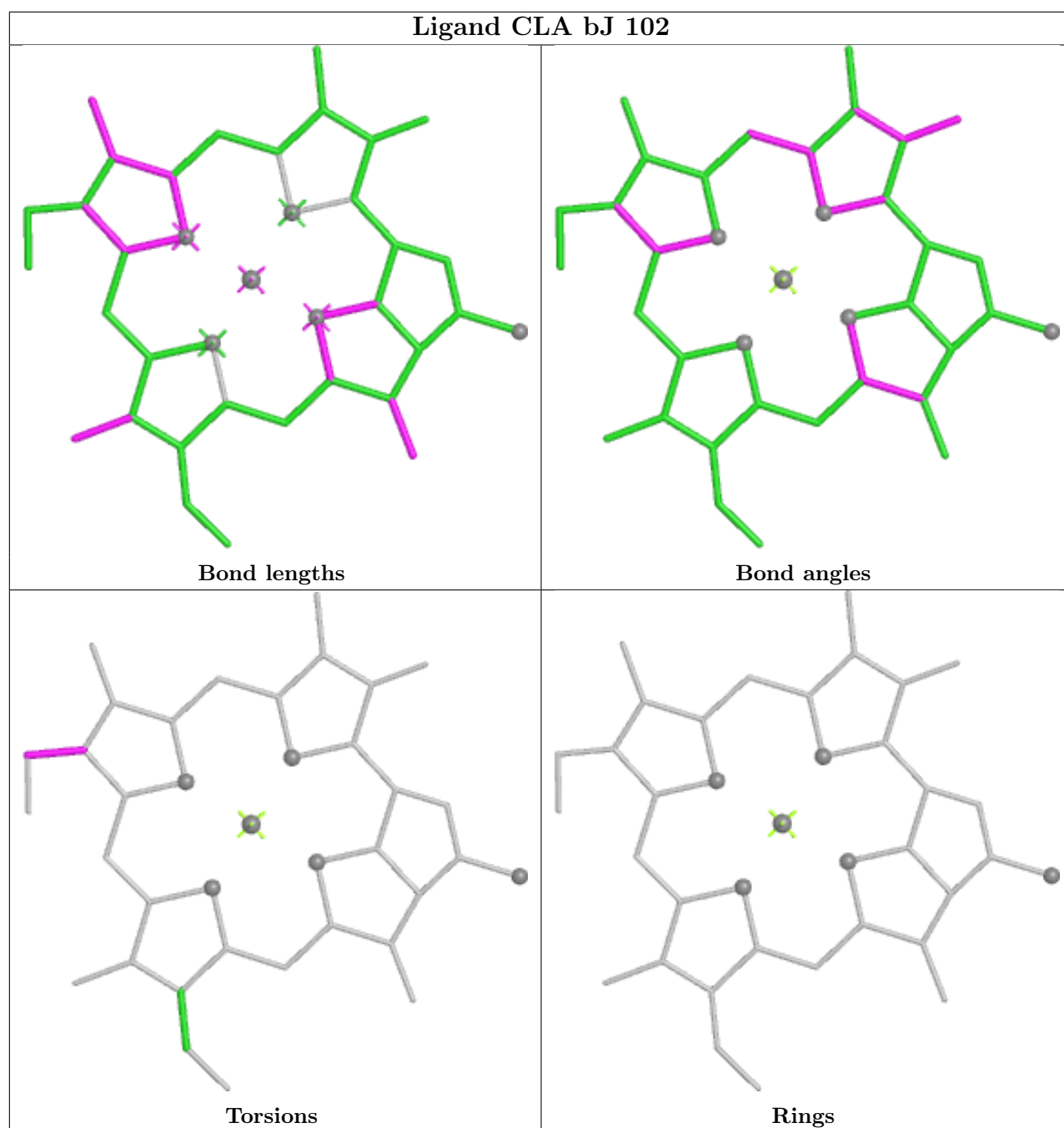


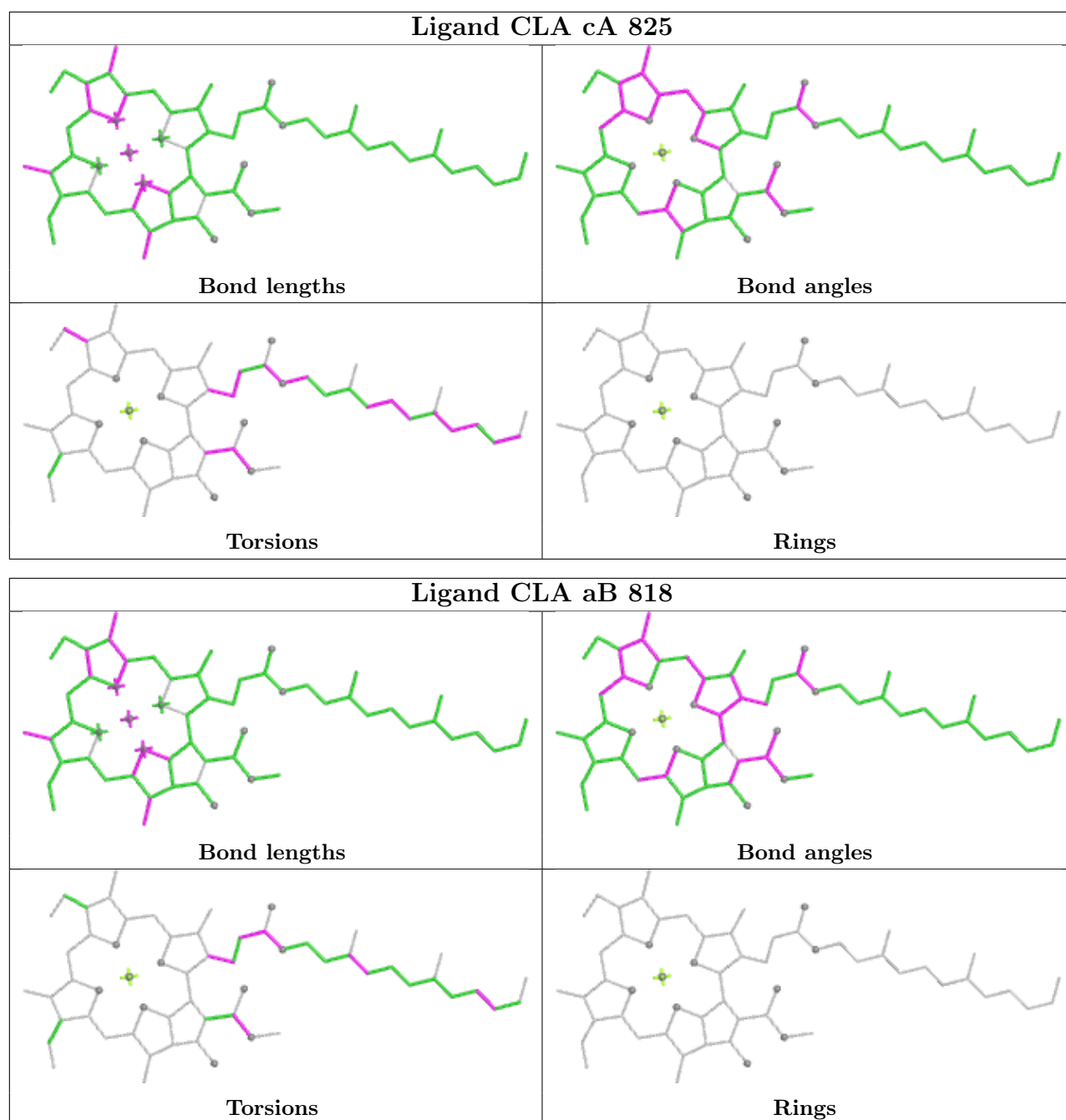


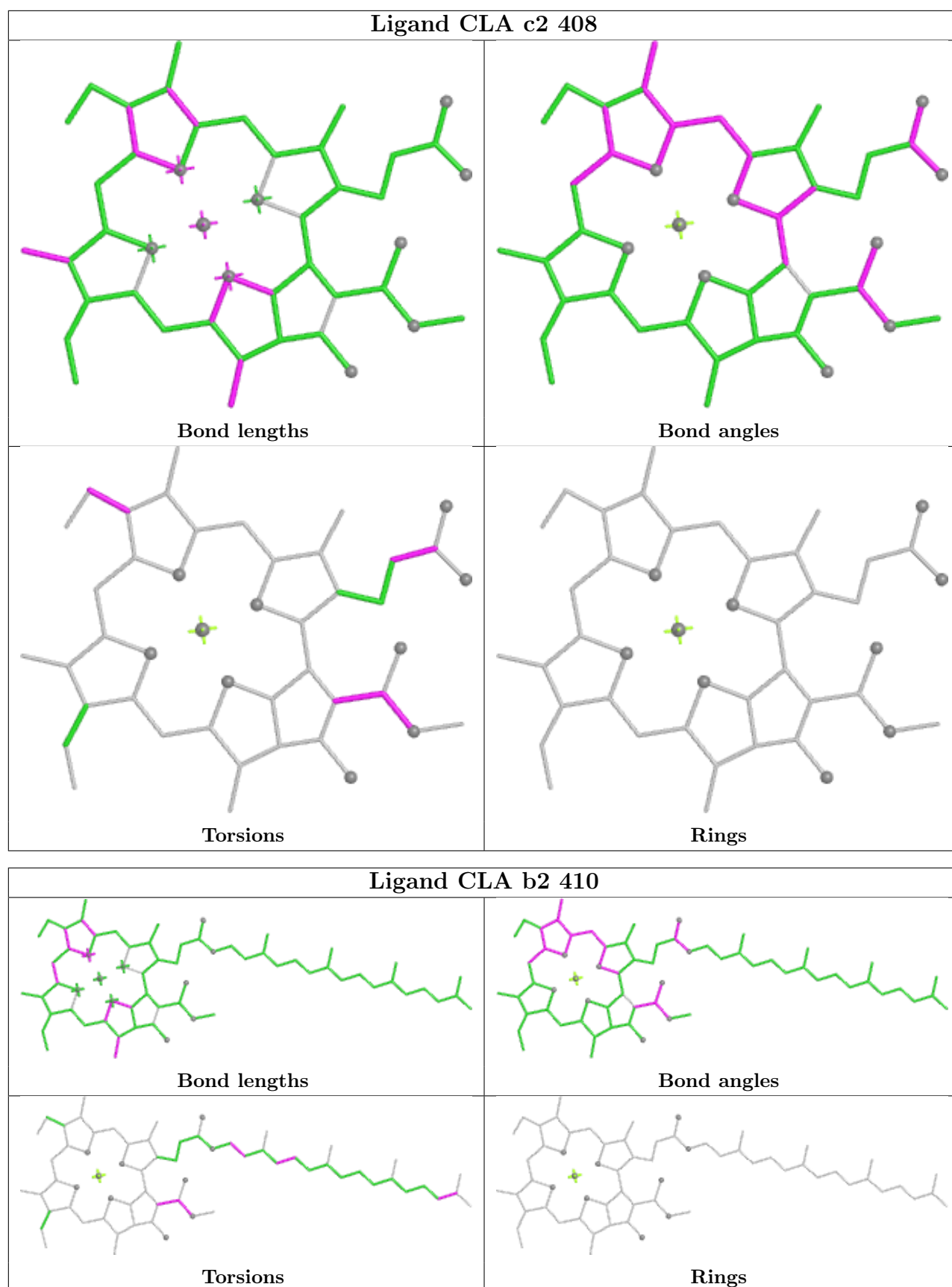


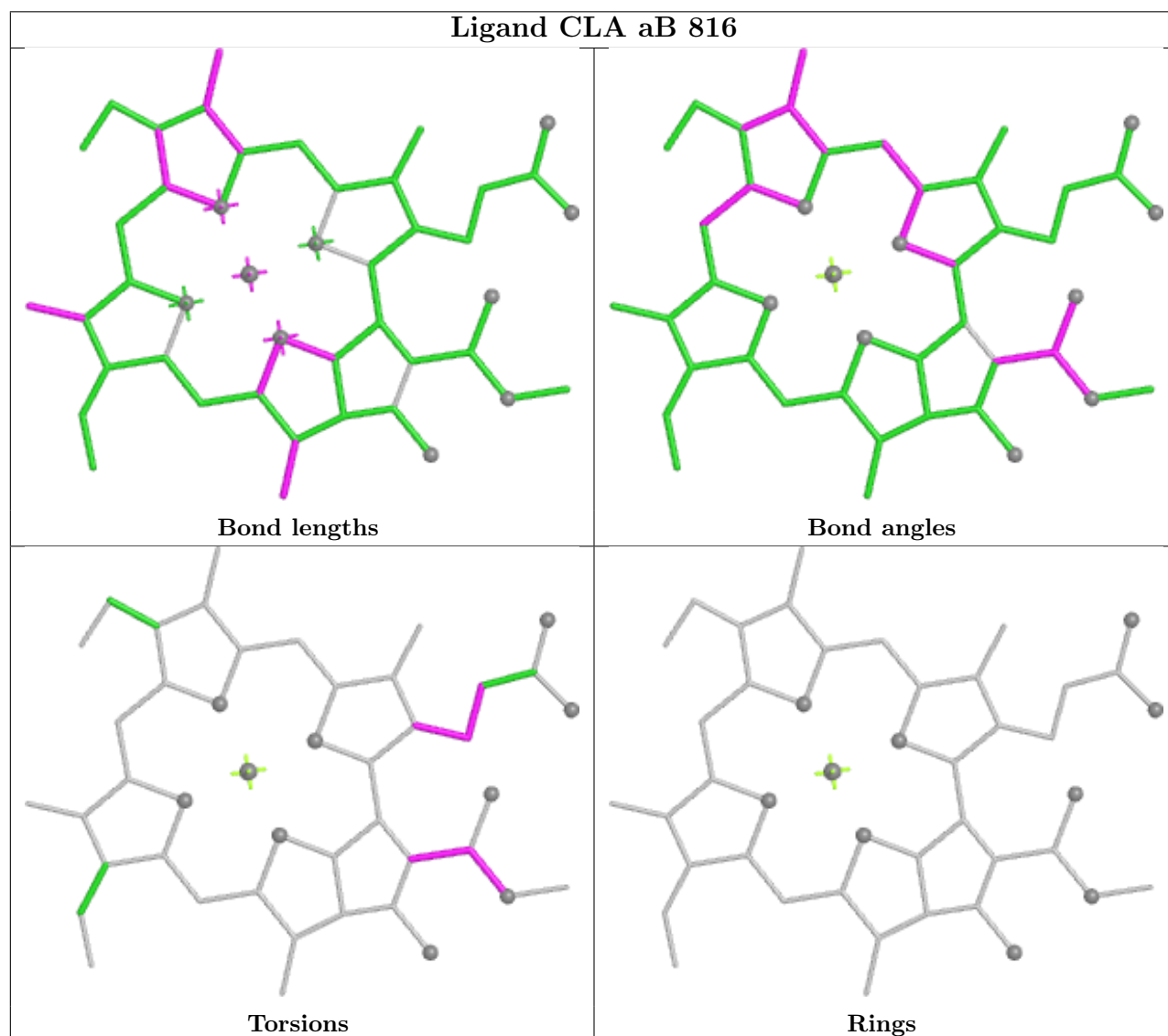
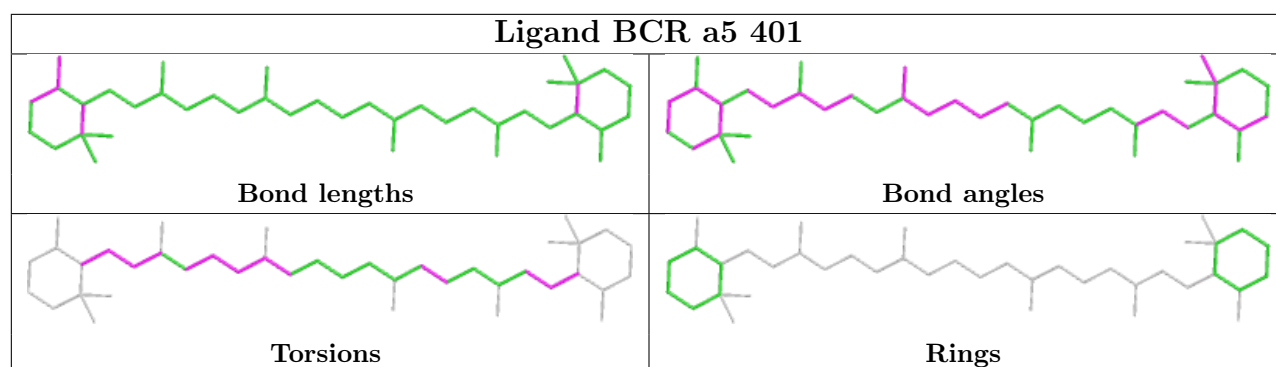


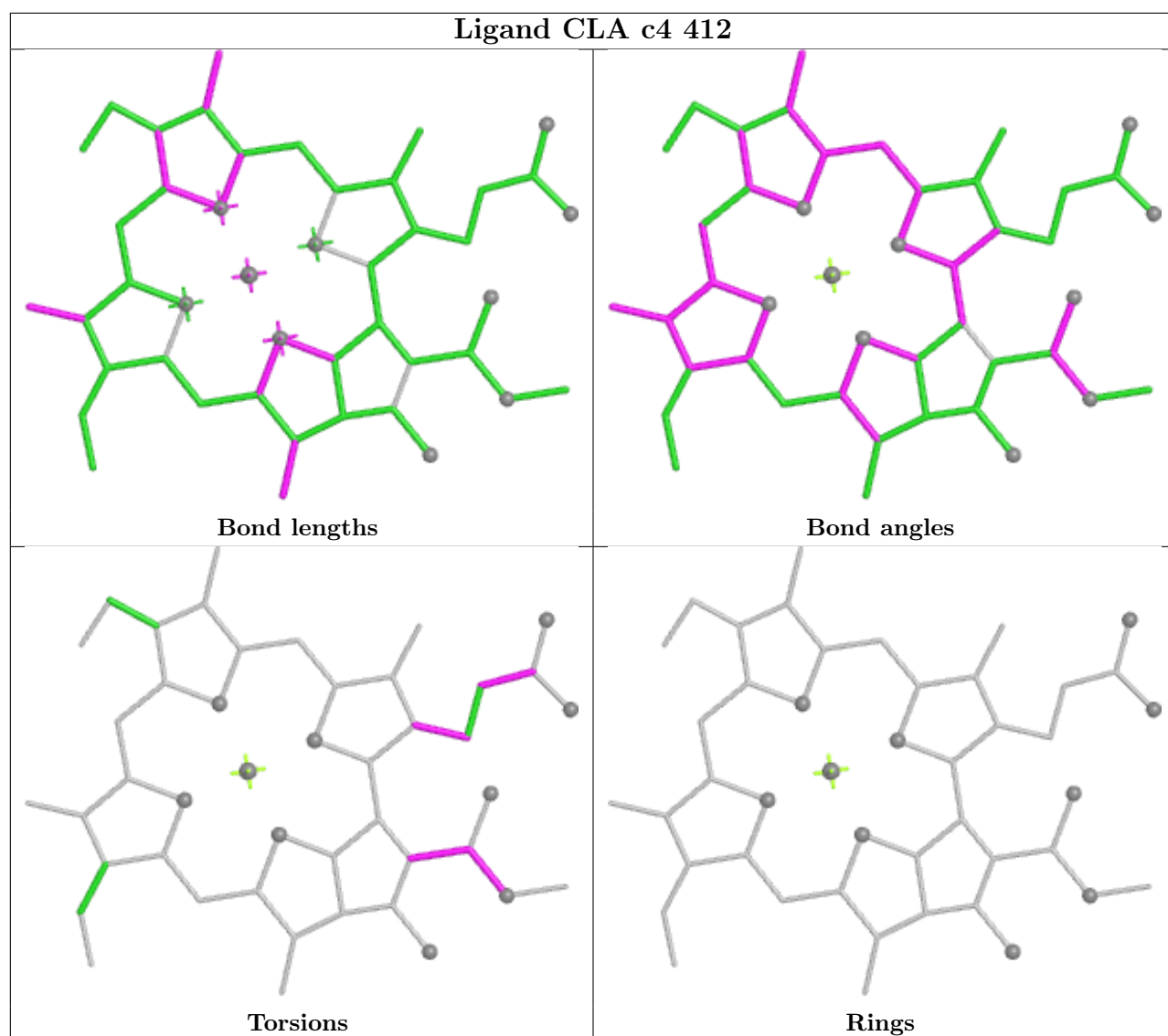


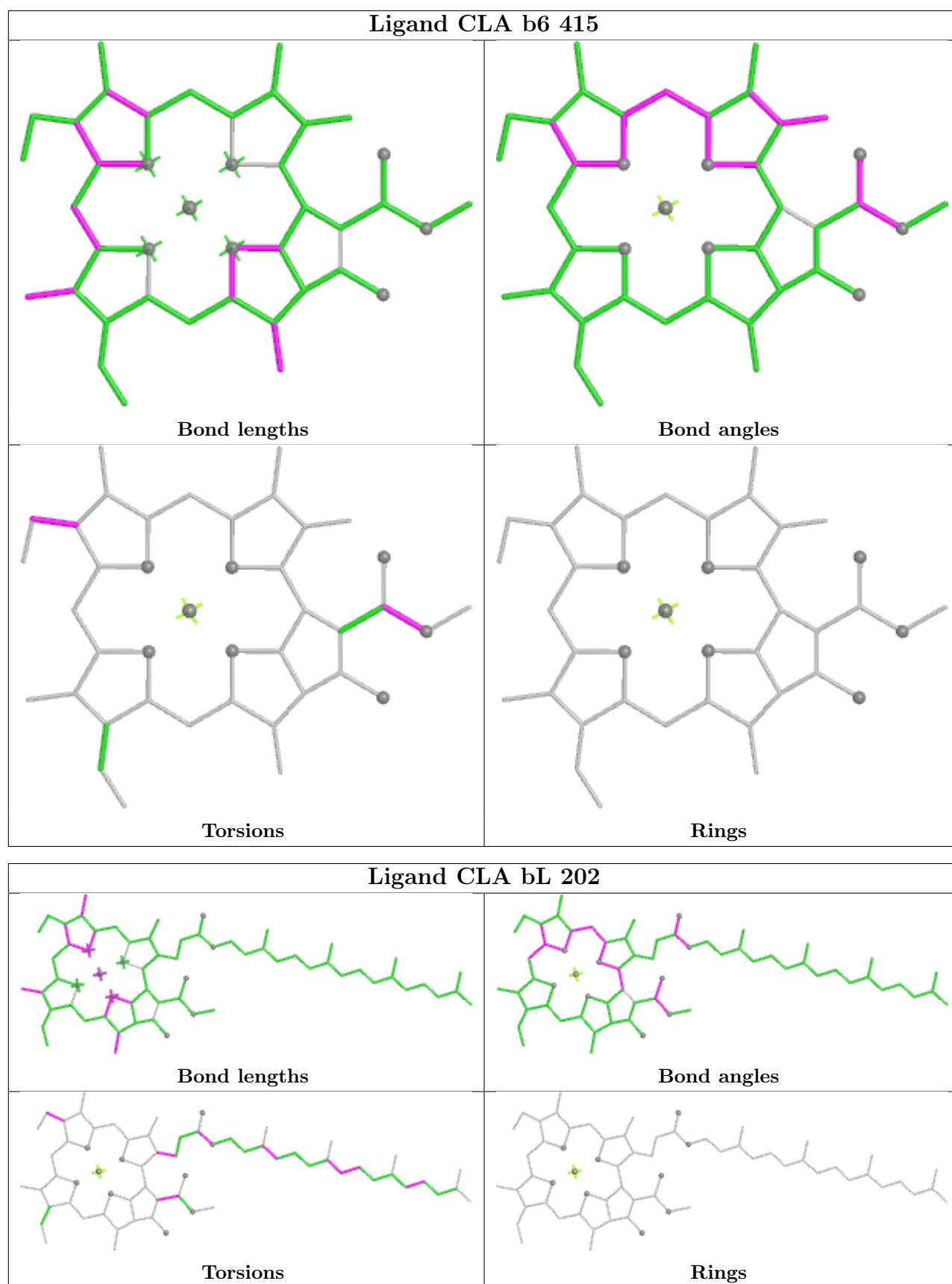


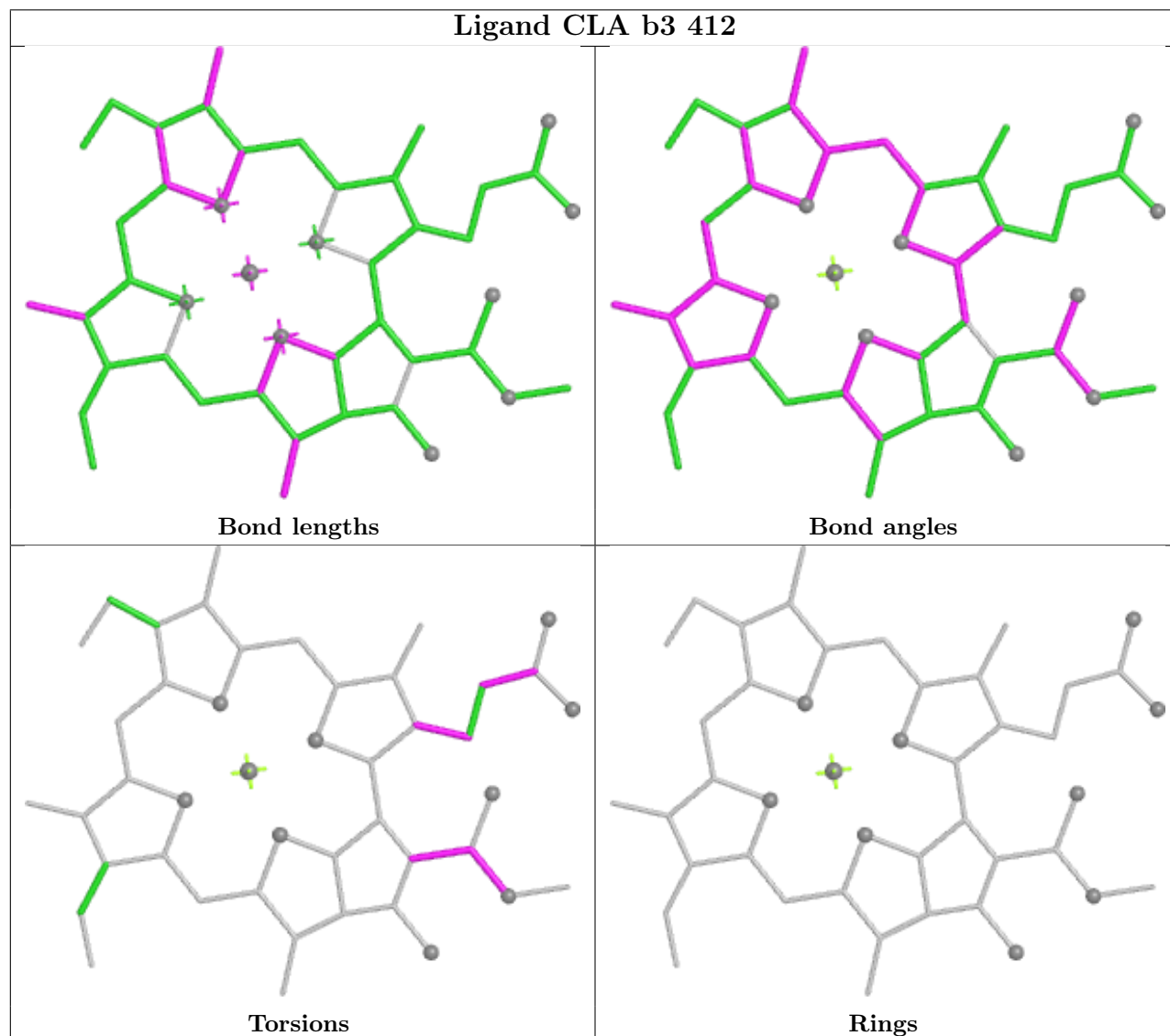
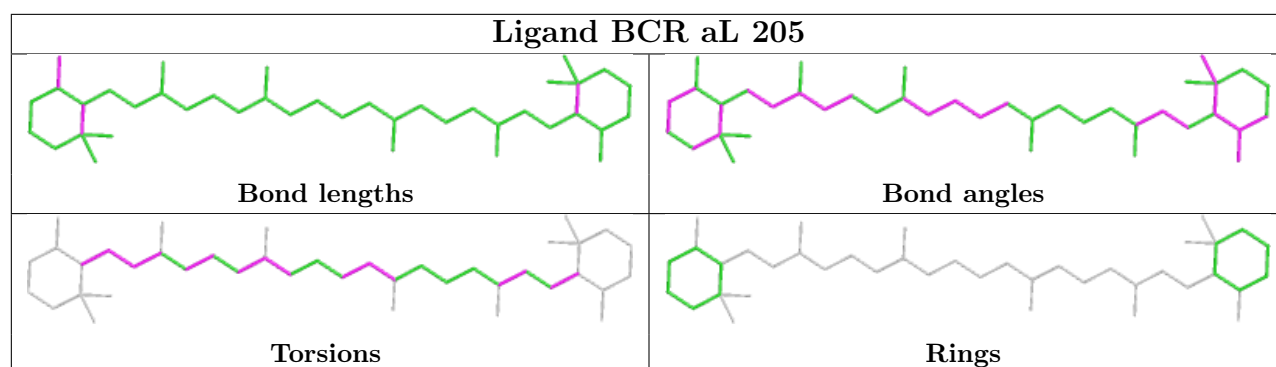




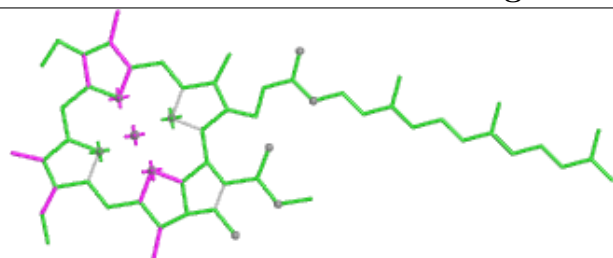




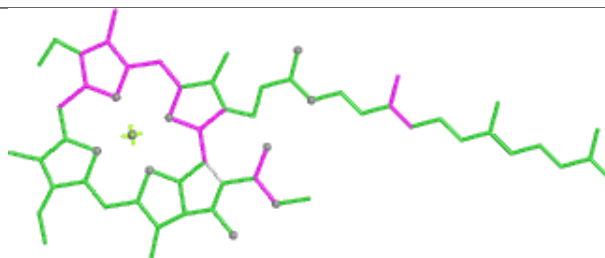




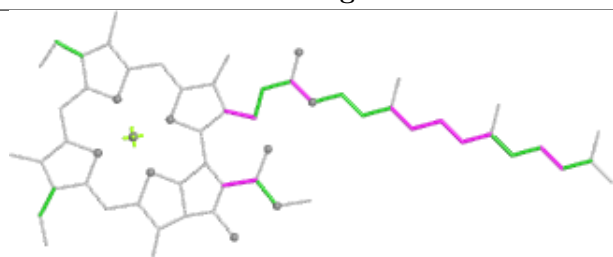
Ligand CLA bB 819



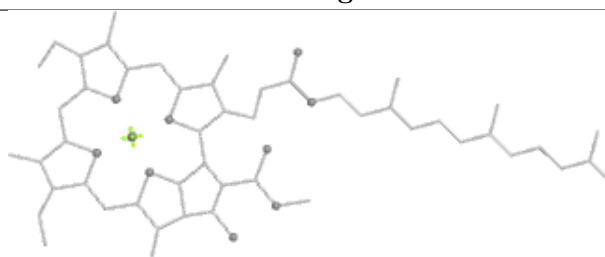
Bond lengths



Bond angles

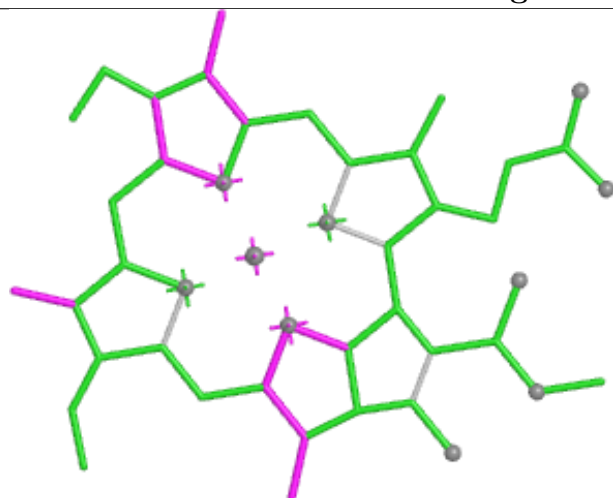


Torsions

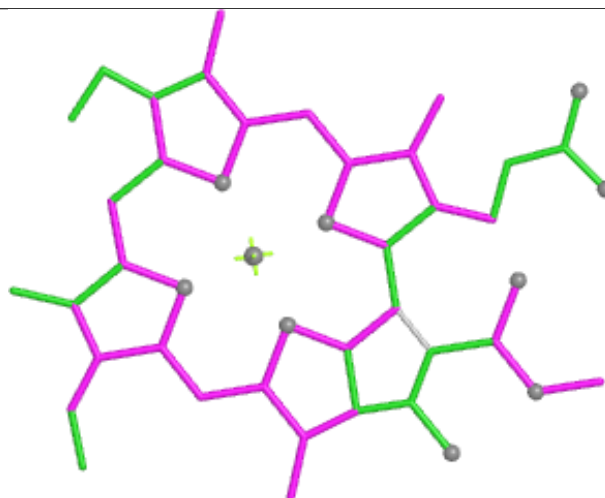


Rings

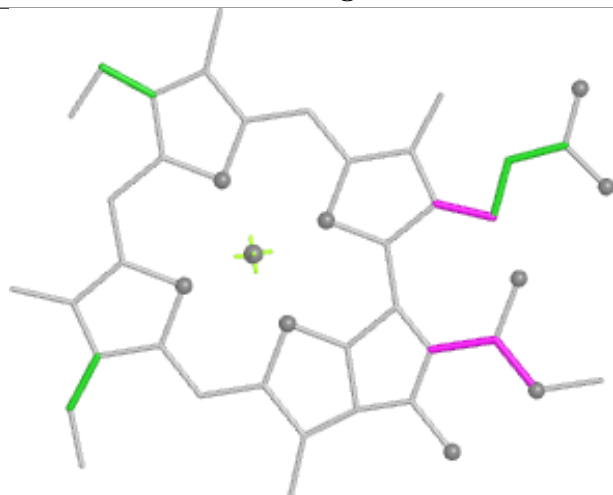
Ligand CLA c4 405



Bond lengths



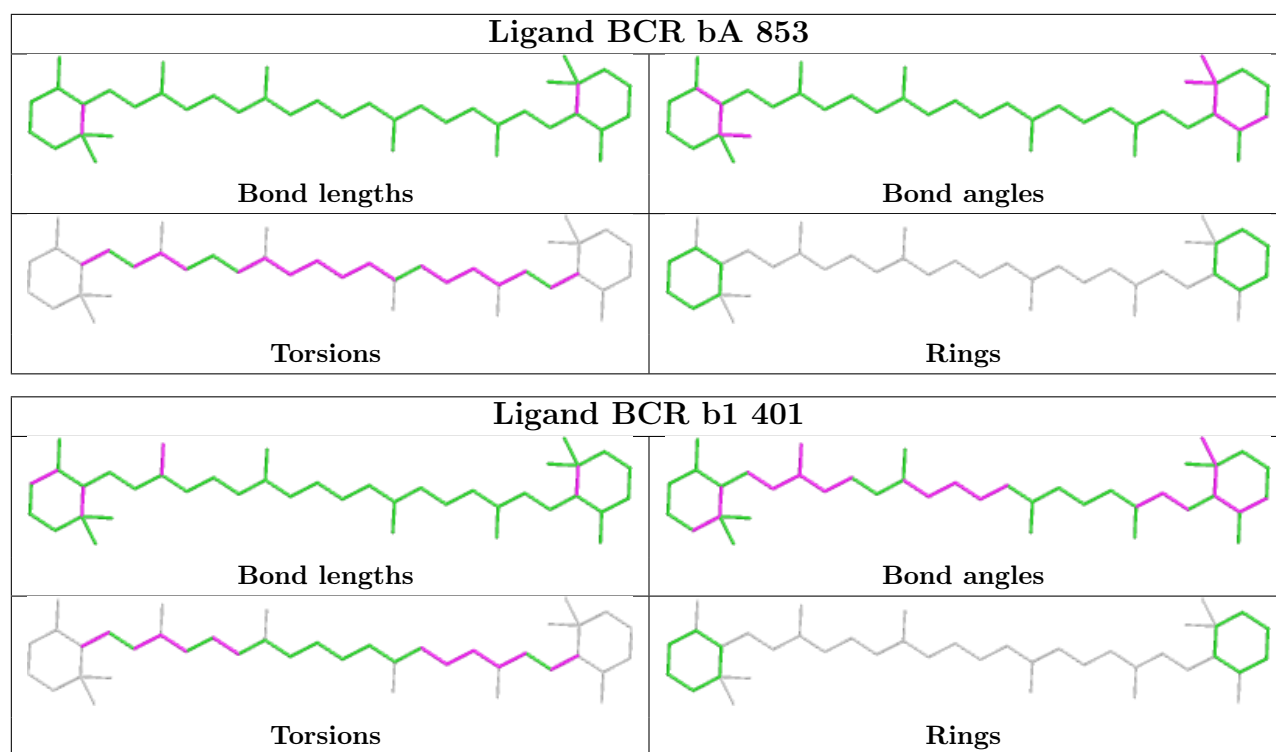
Bond angles

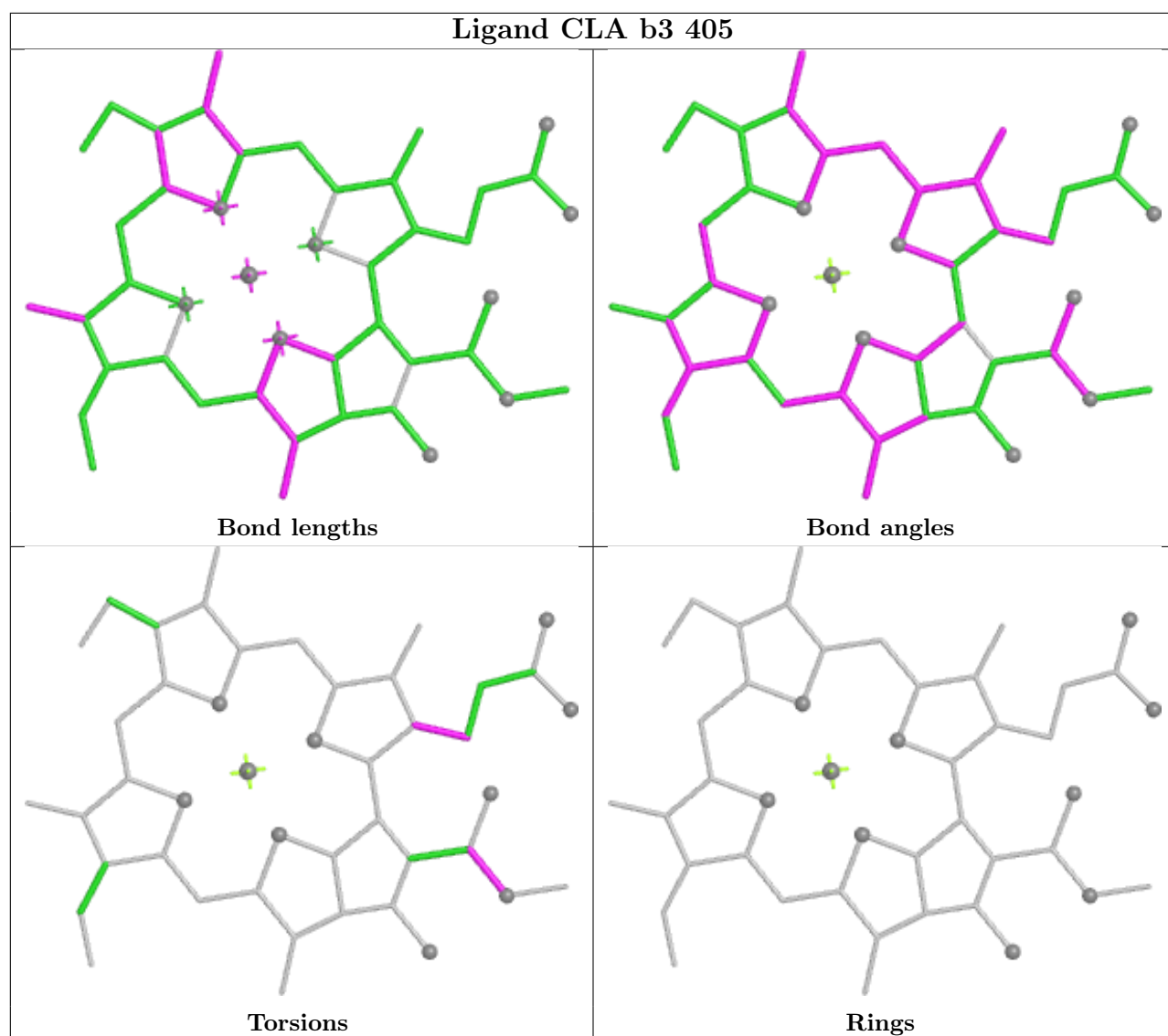


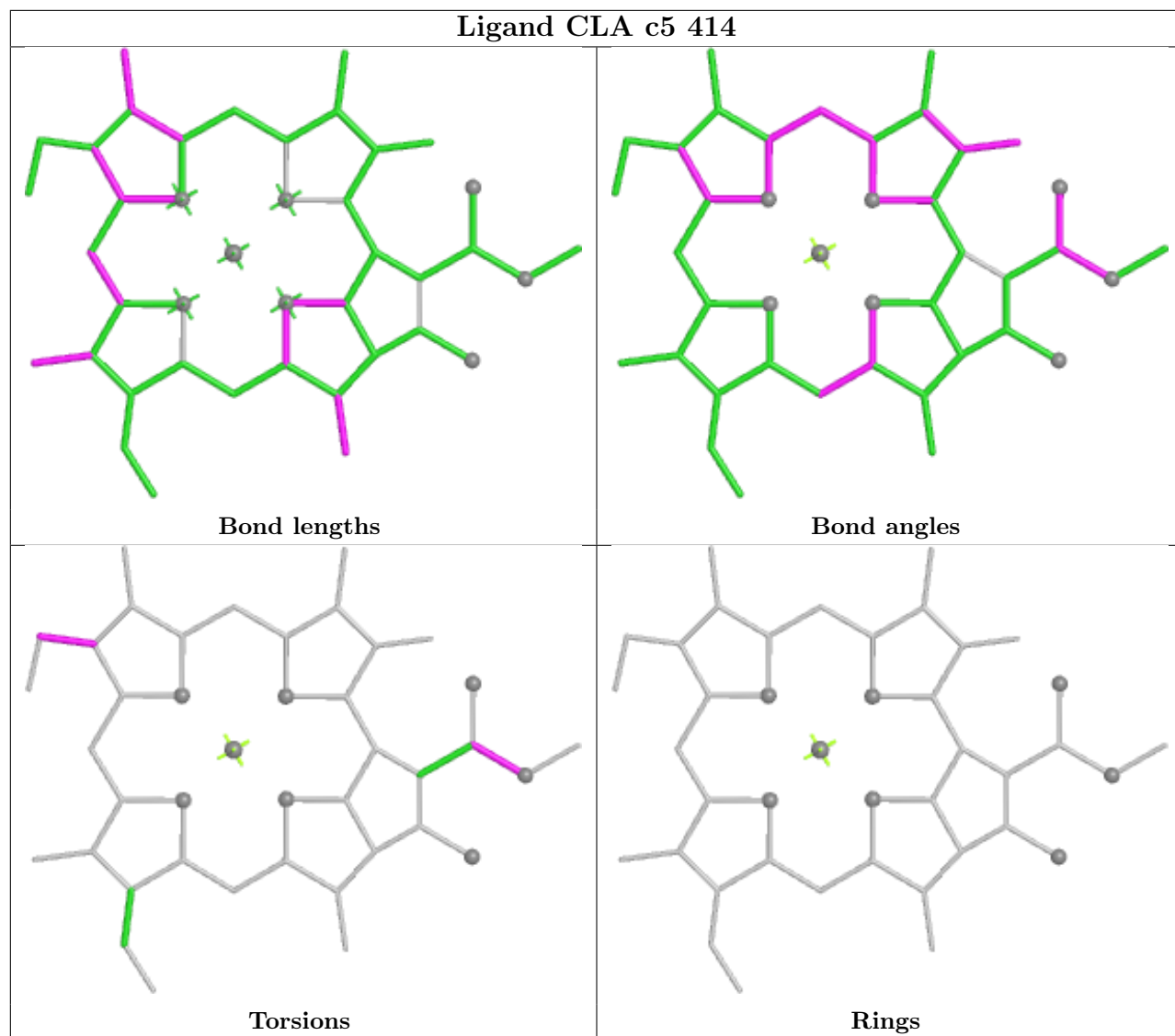
Torsions

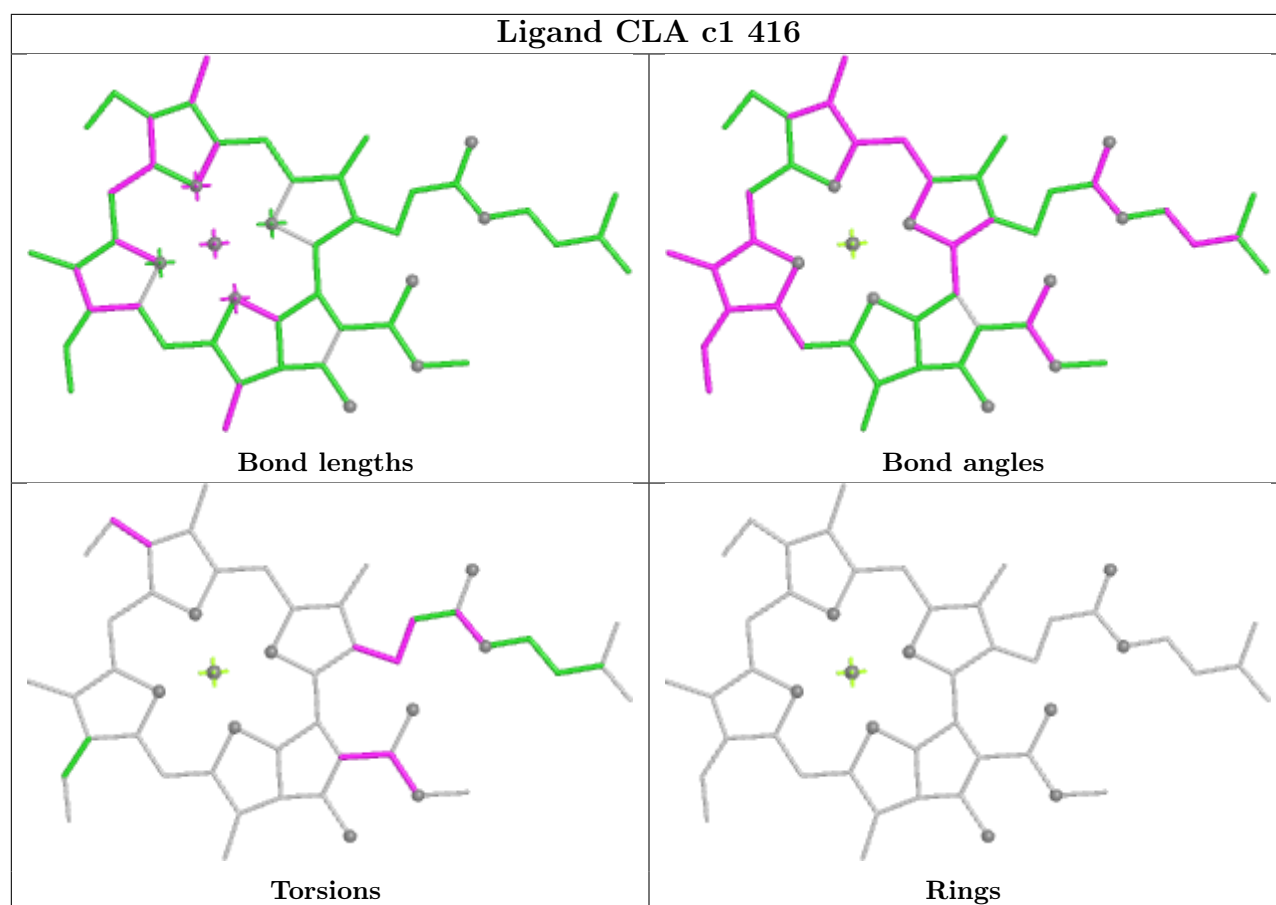


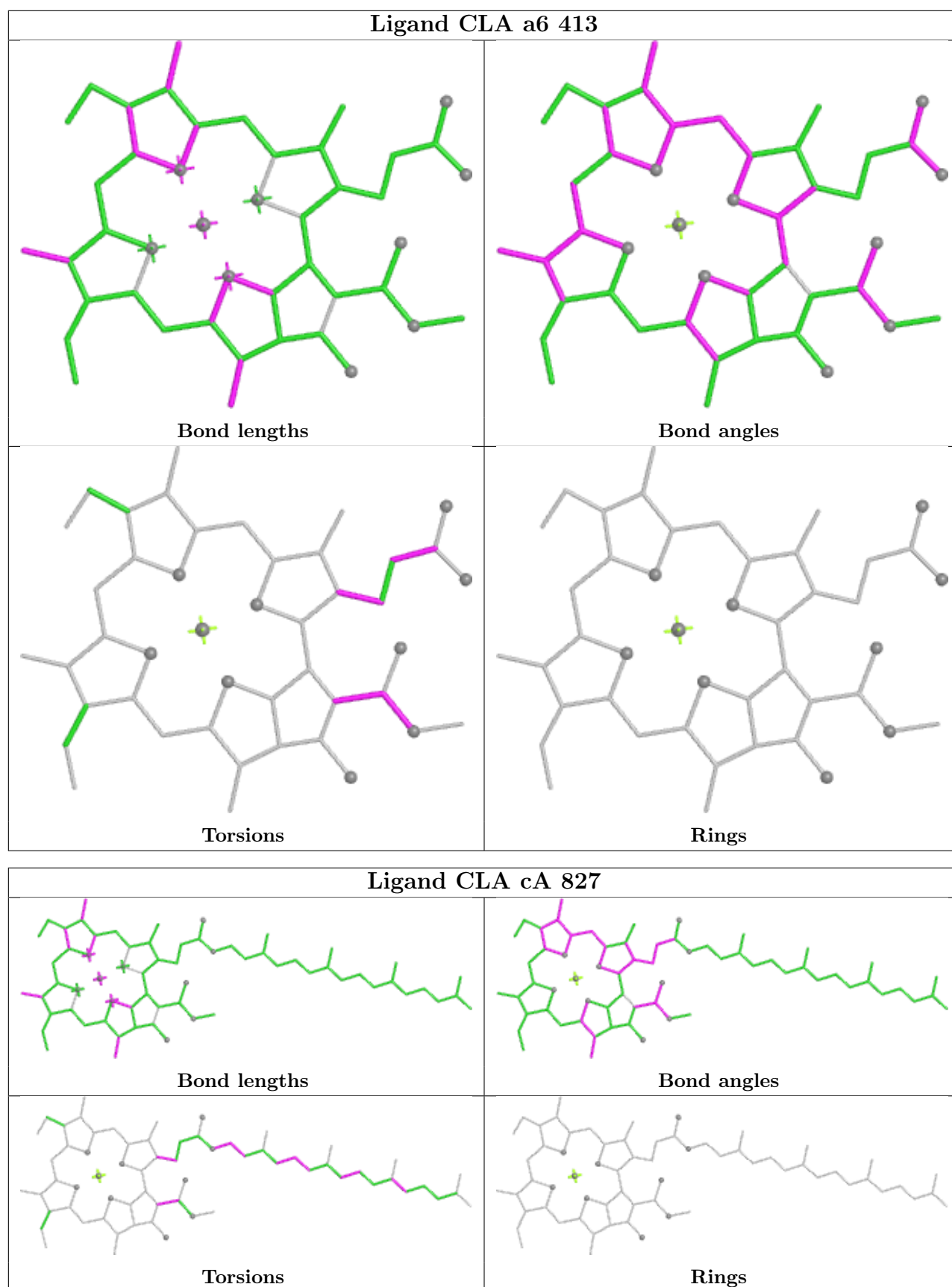
Rings

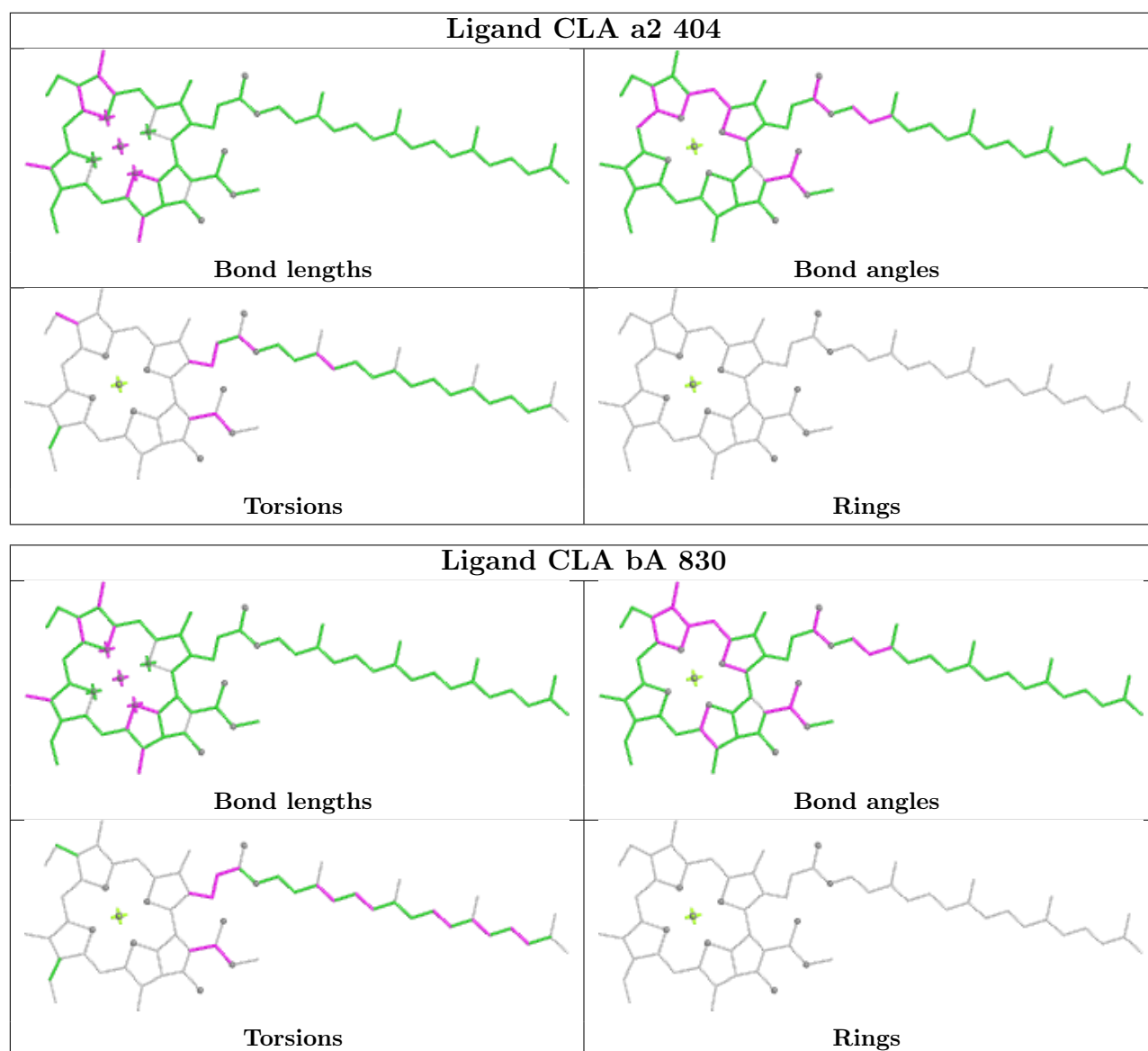


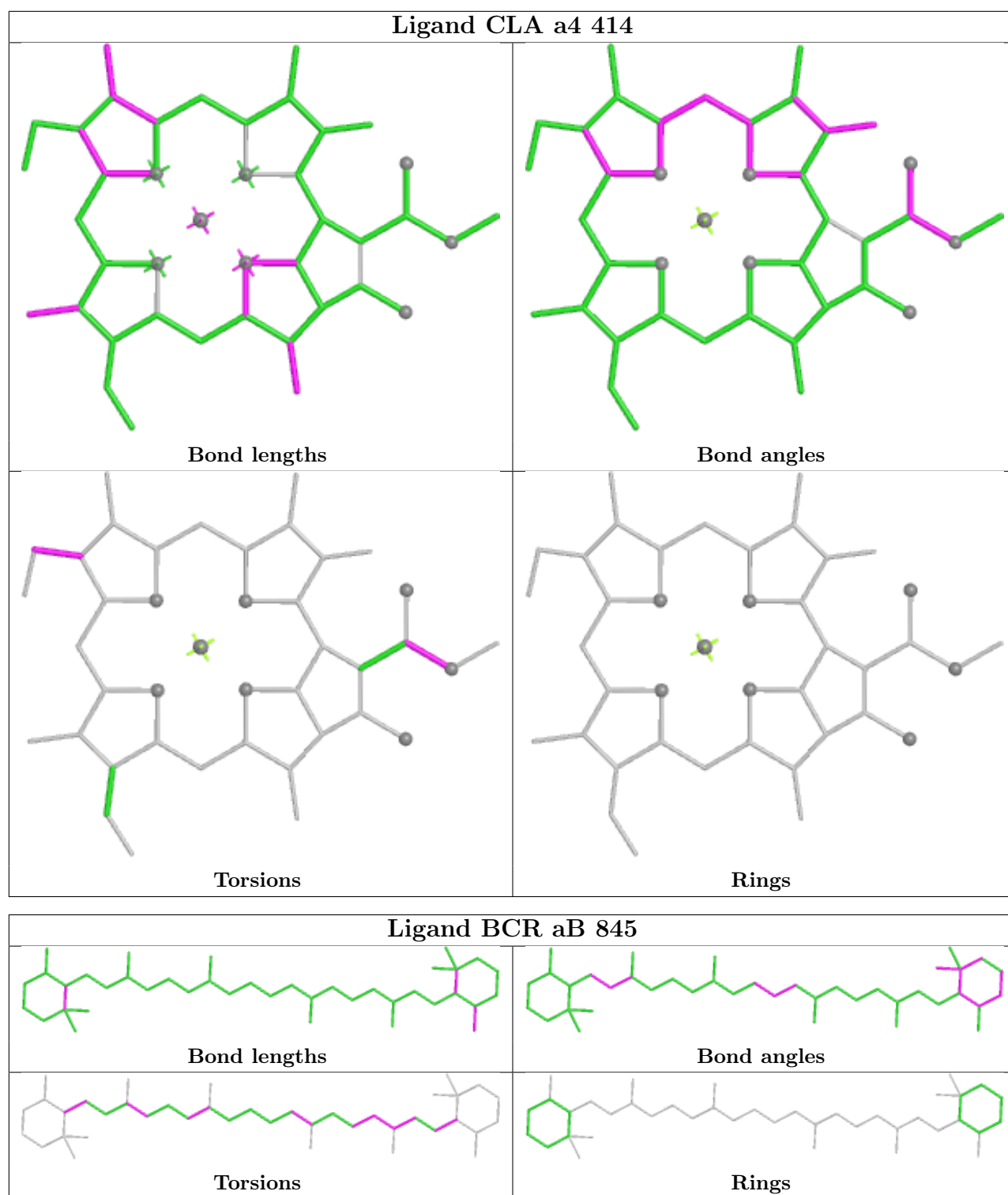


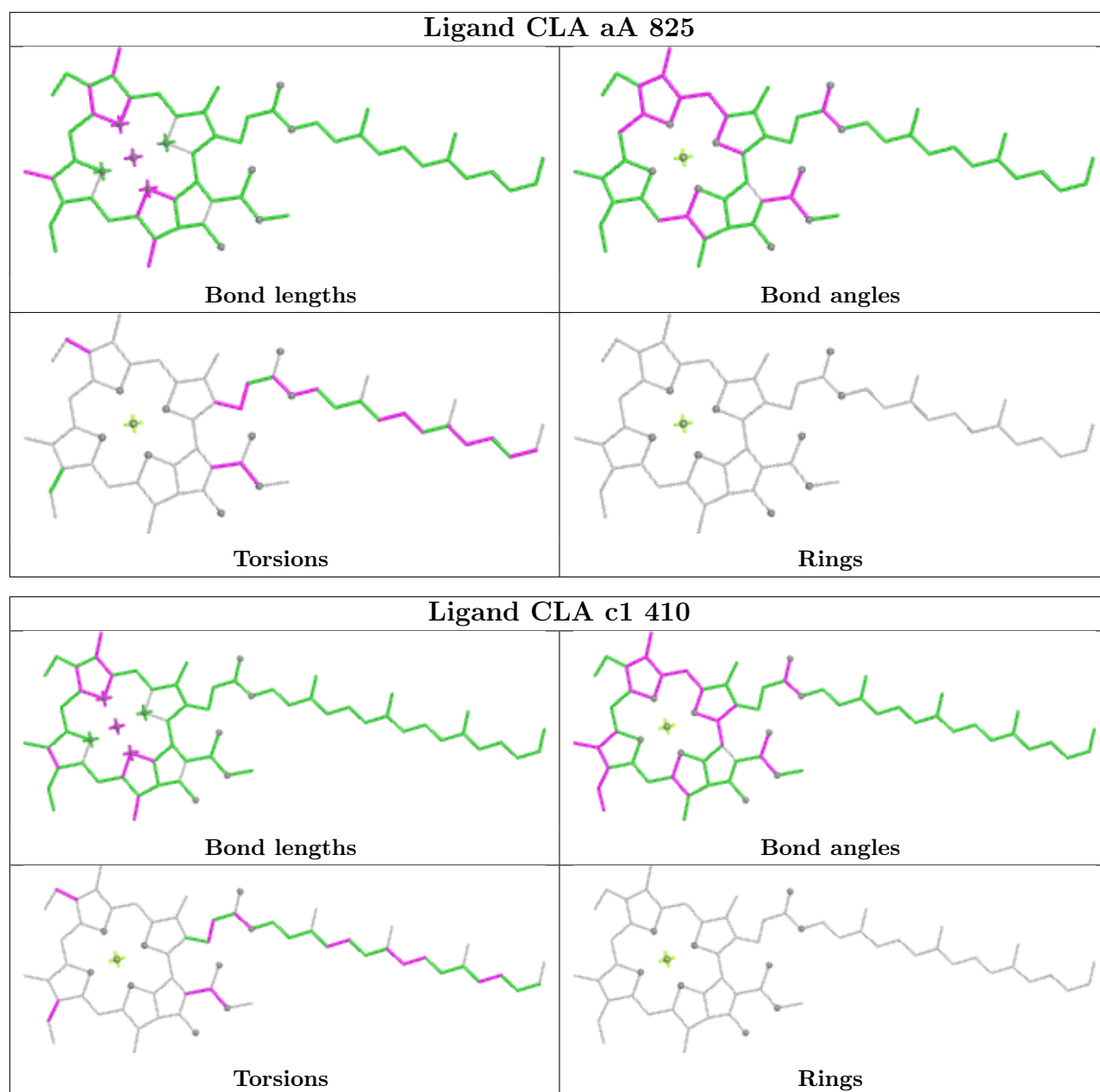


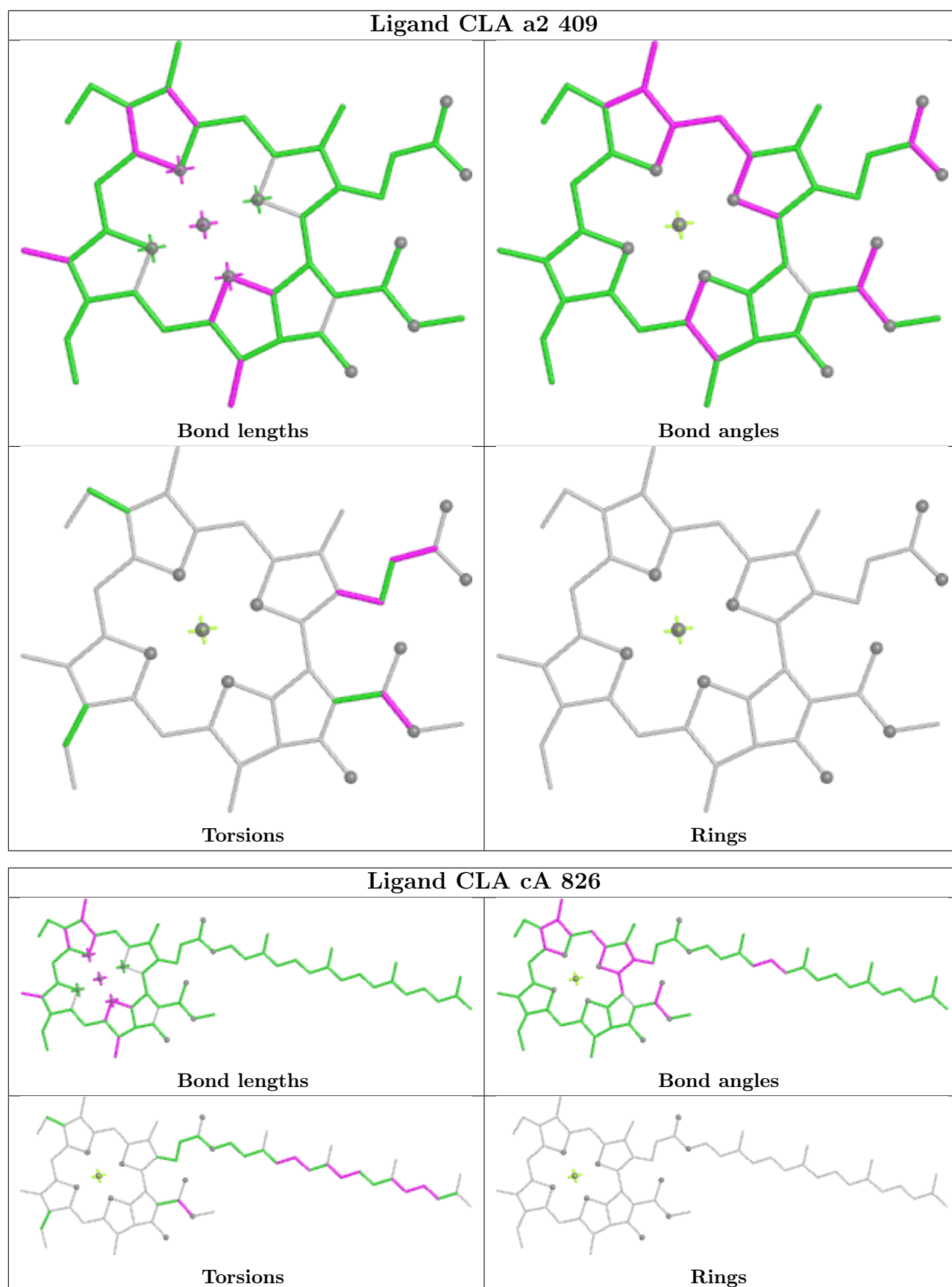


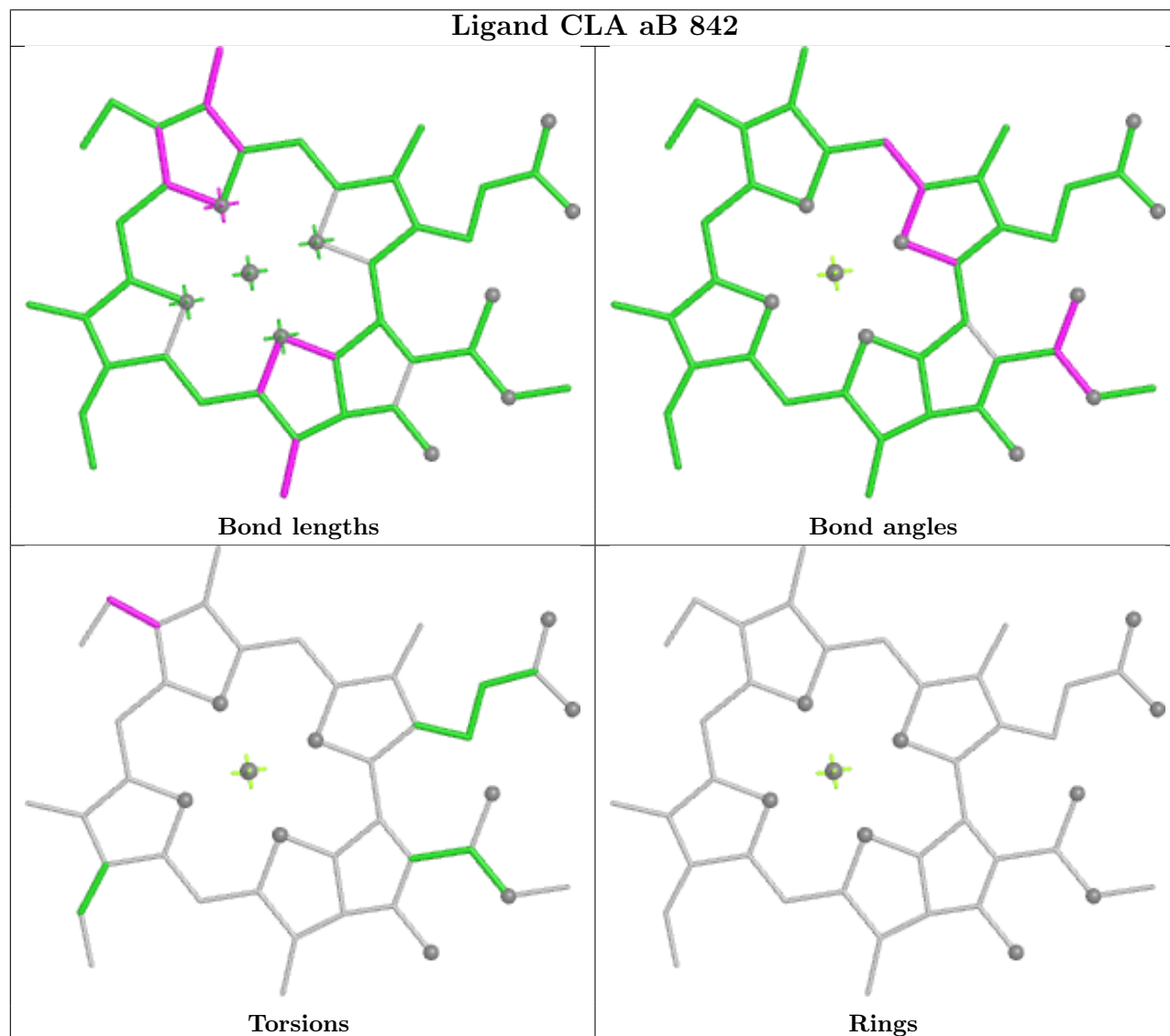
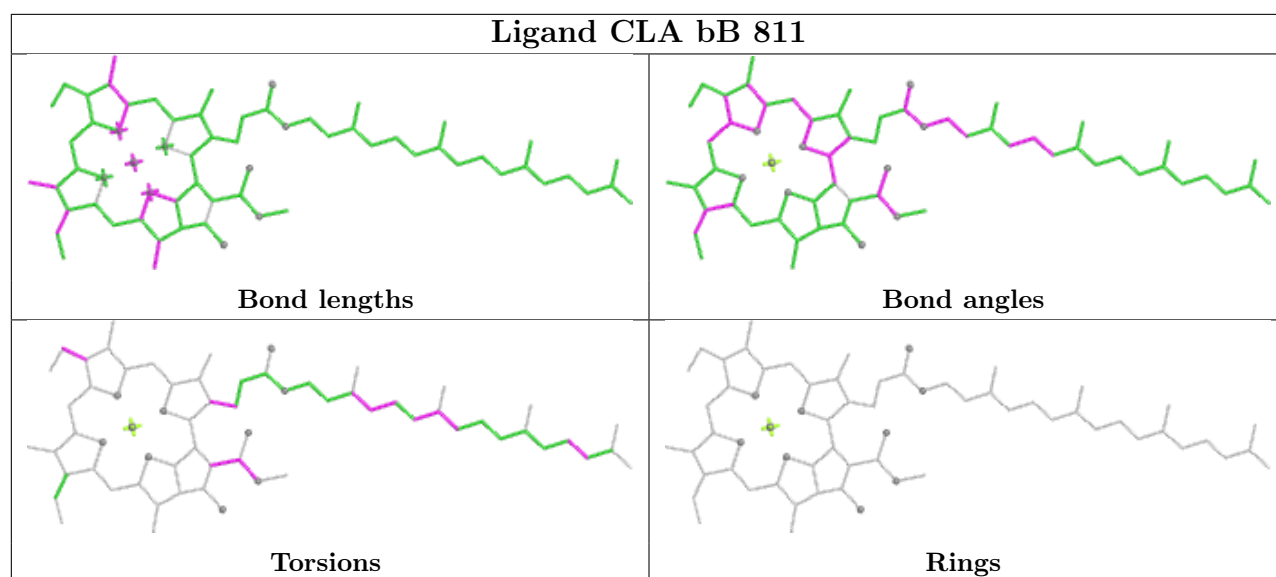


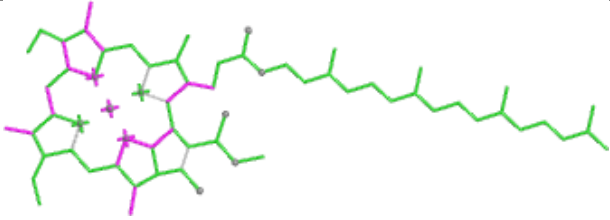
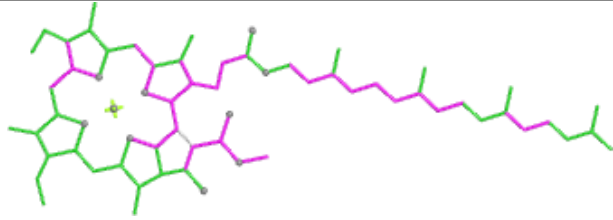
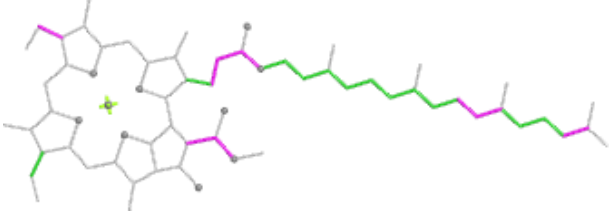
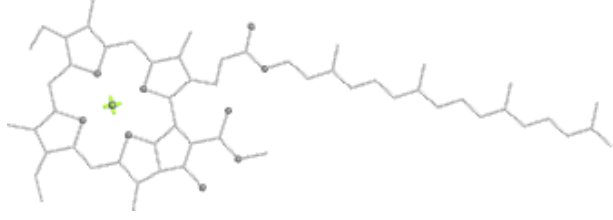


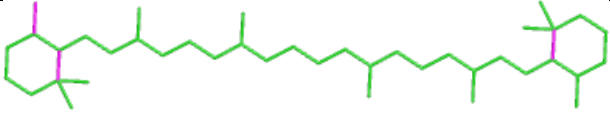
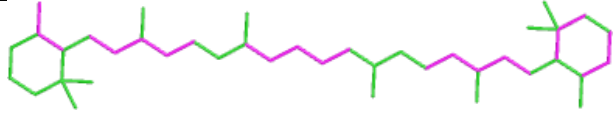
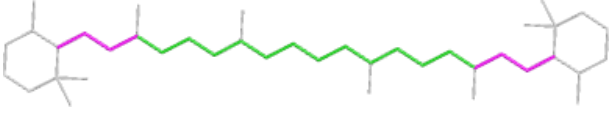
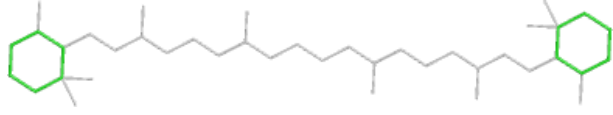


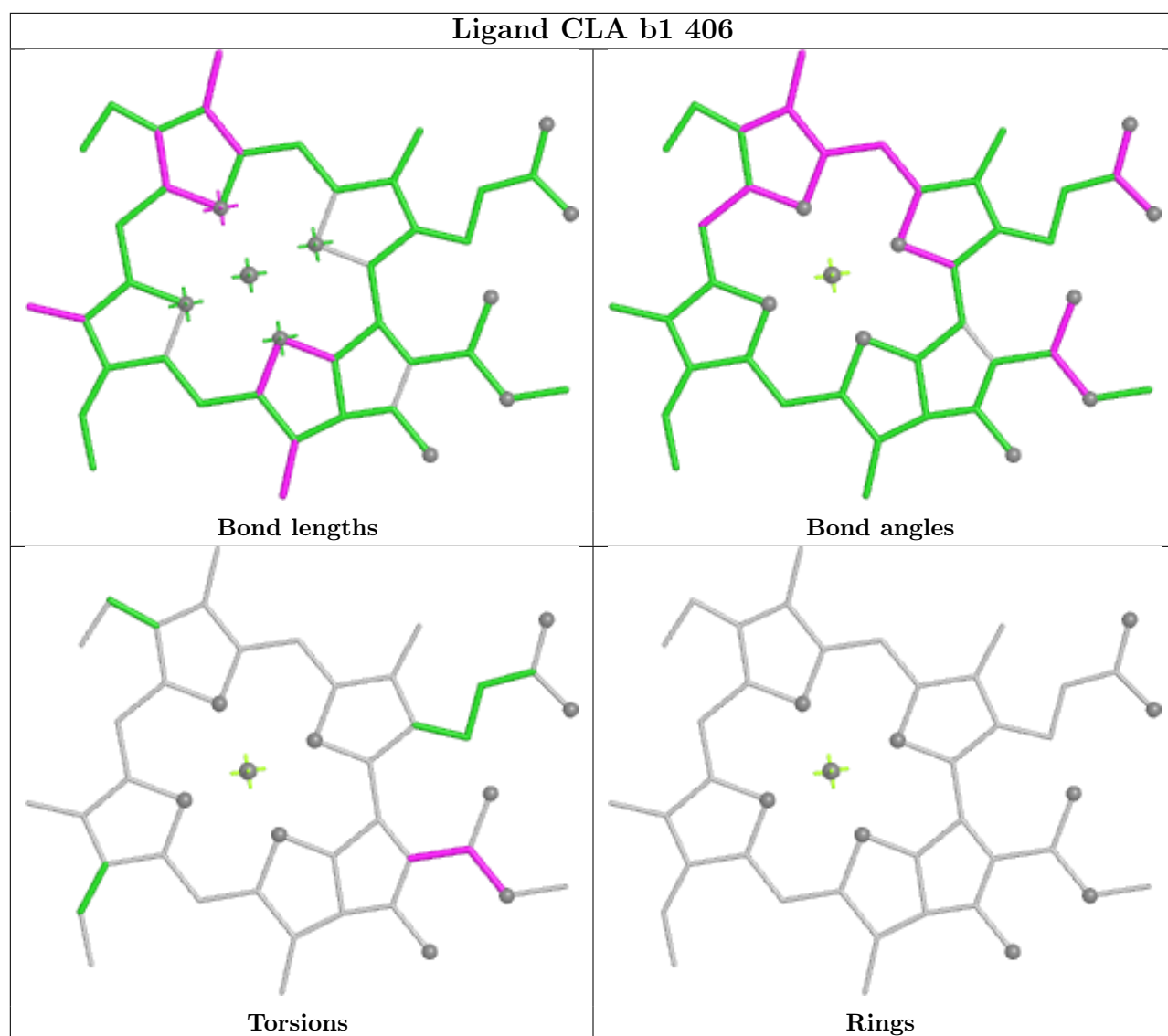


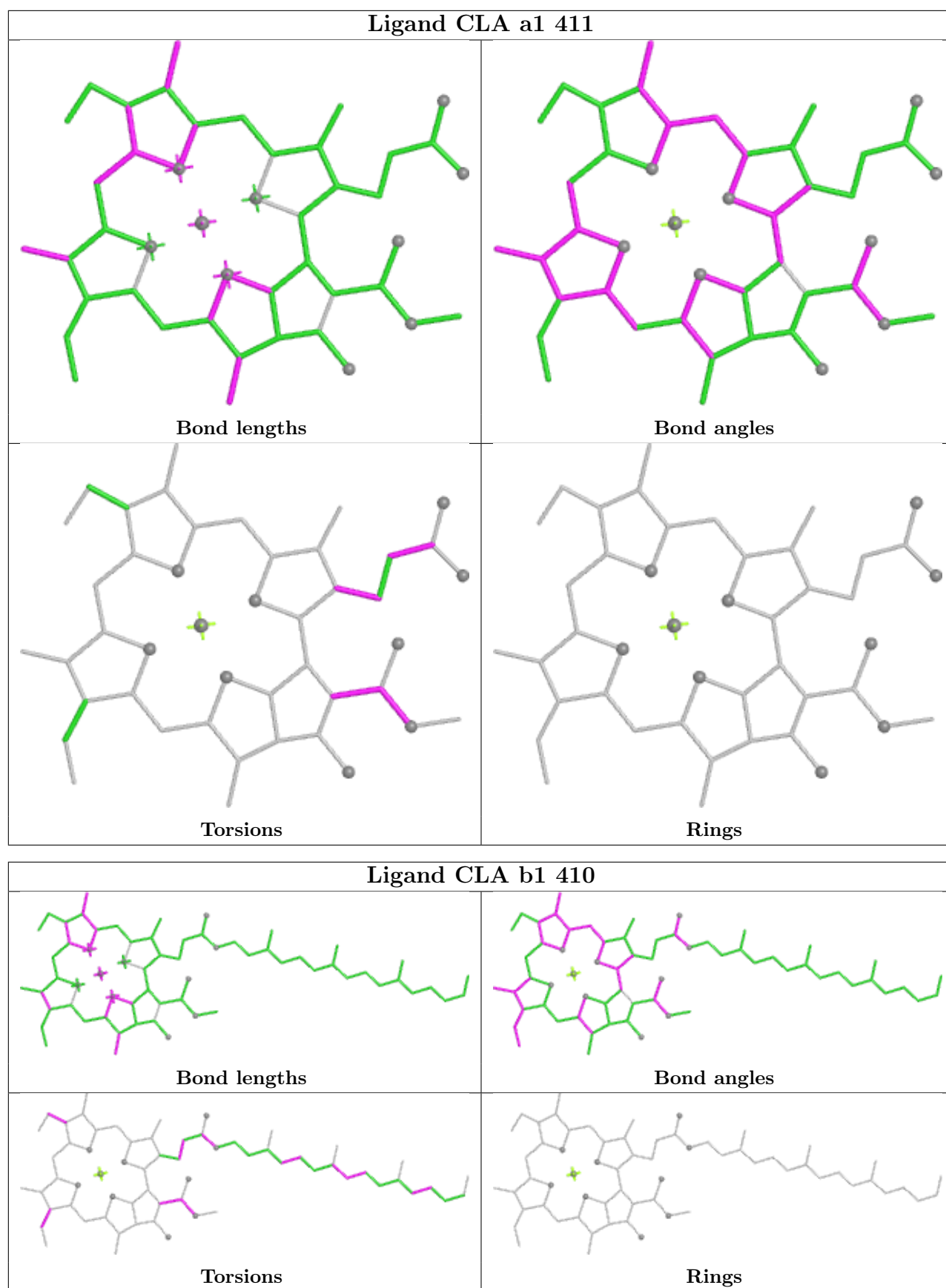


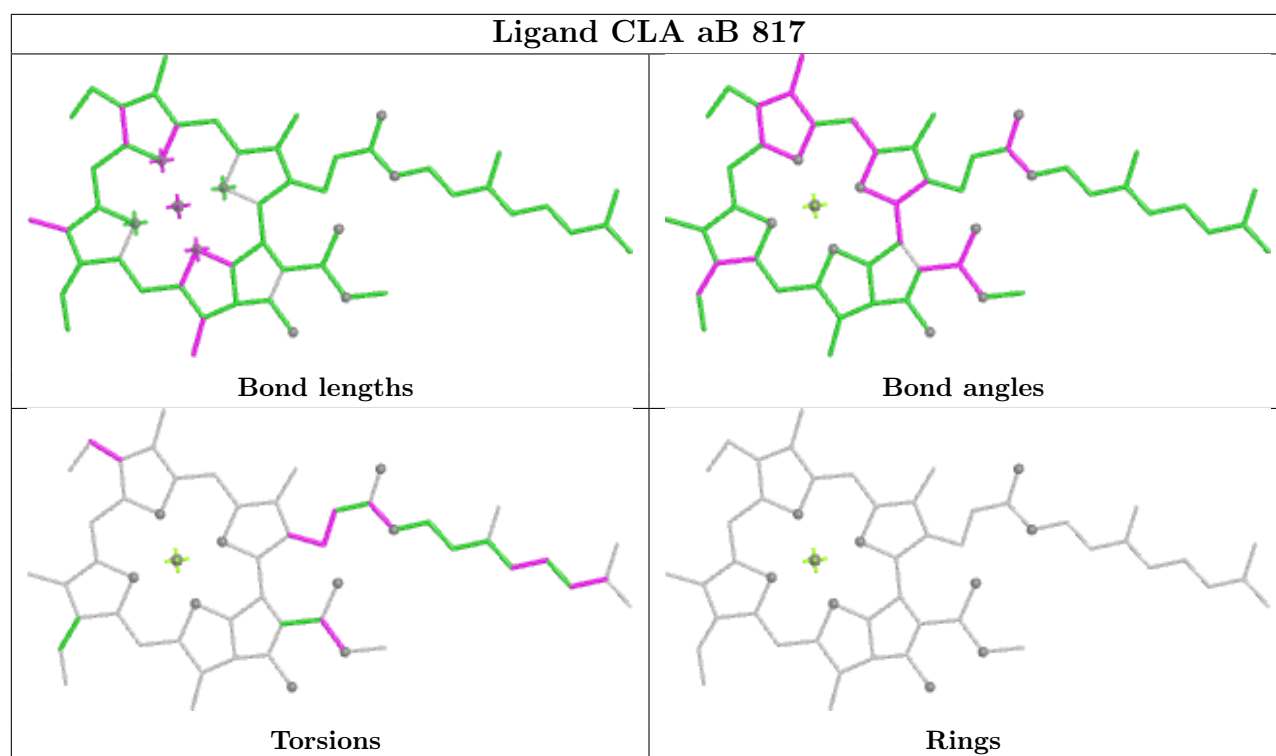


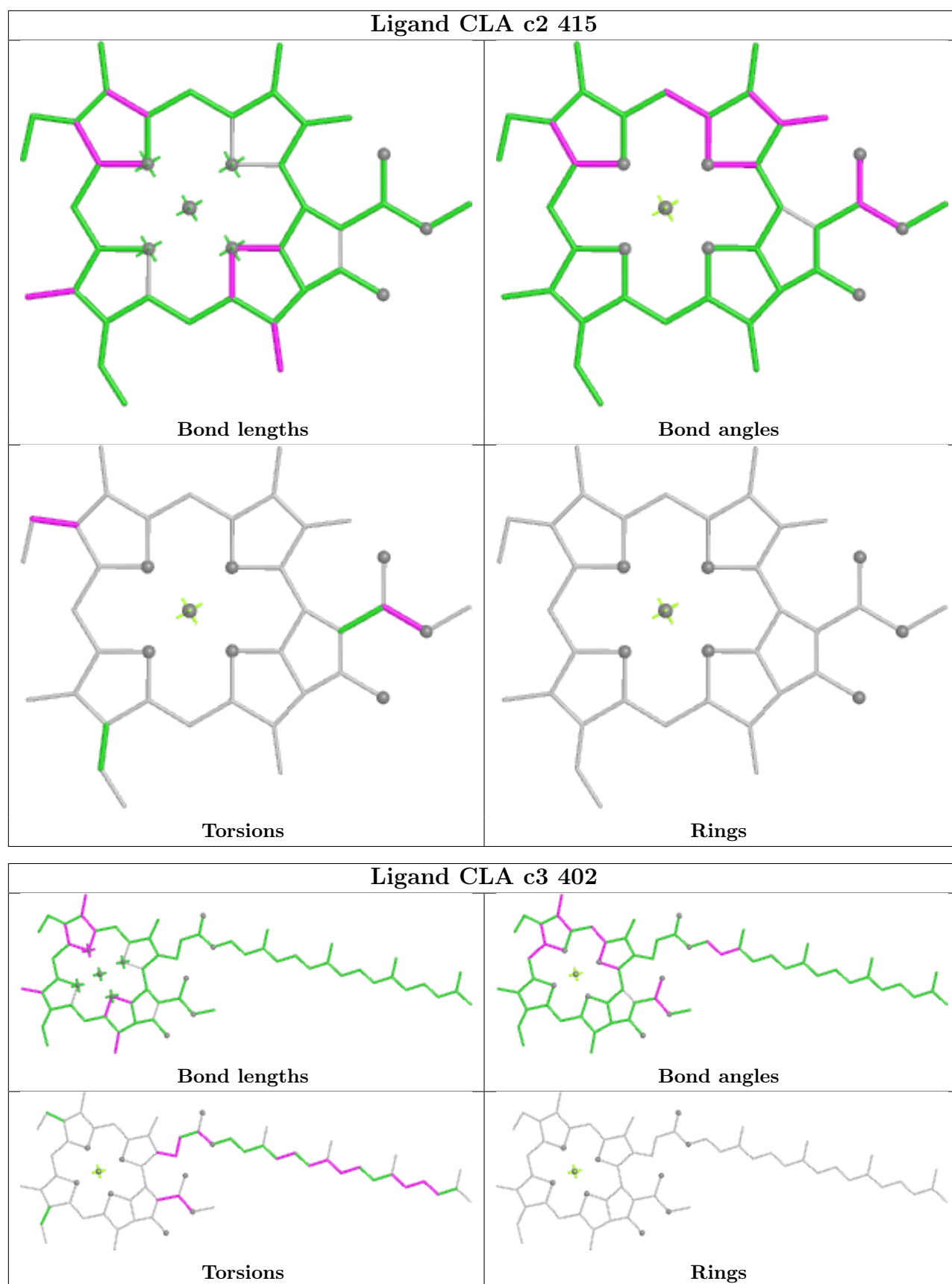
Ligand CLA a1 422			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

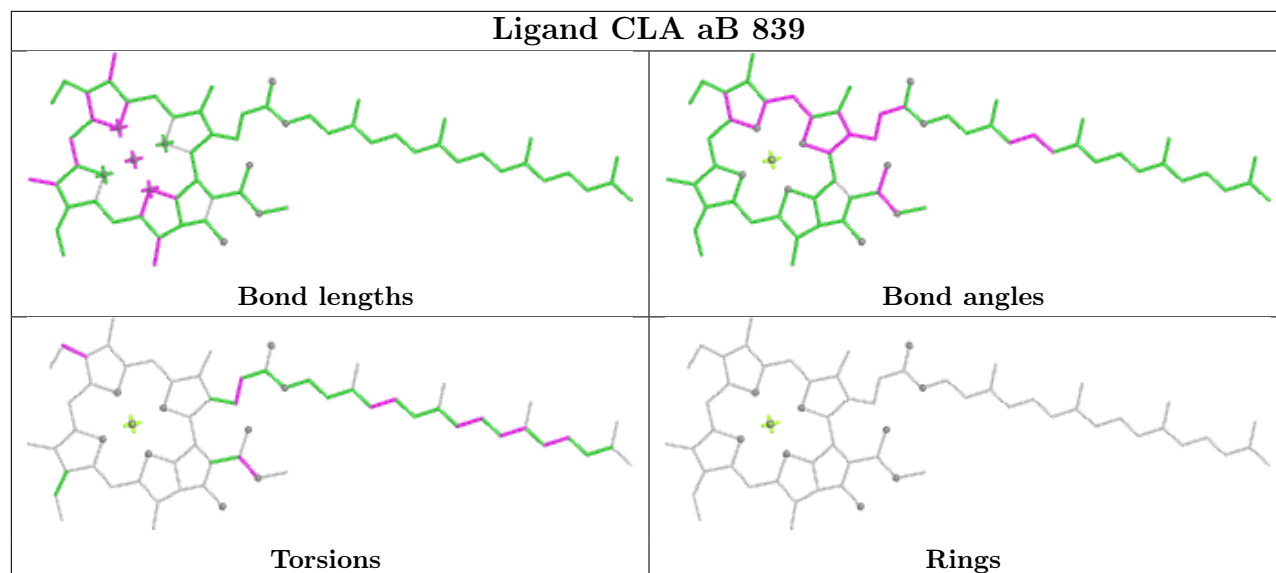
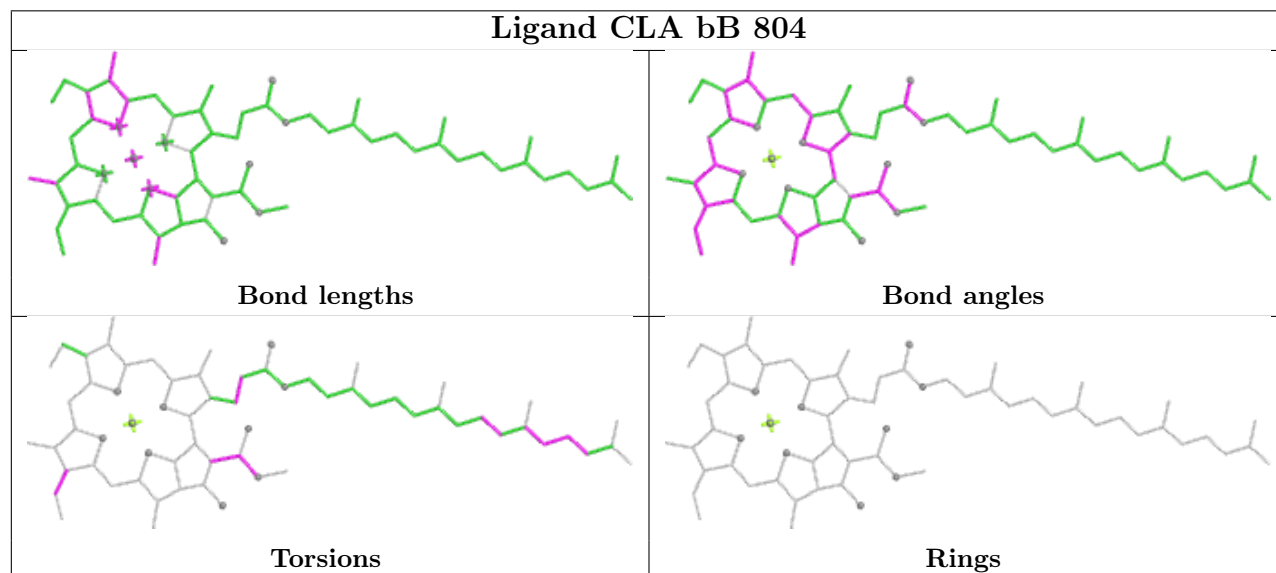
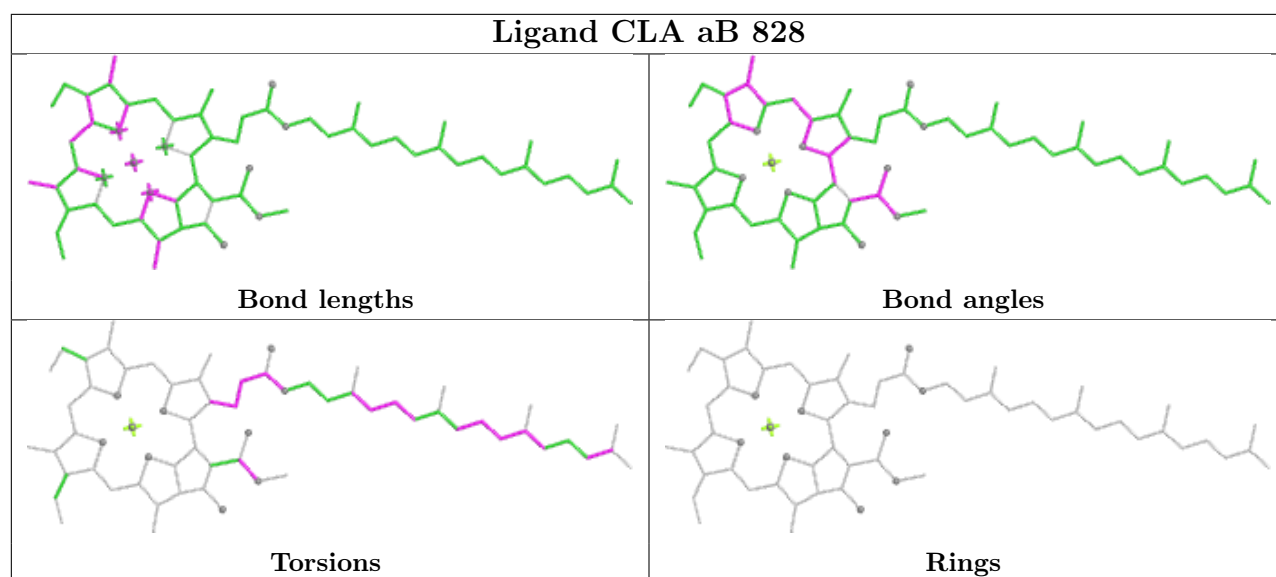
Ligand BCR cK 101			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

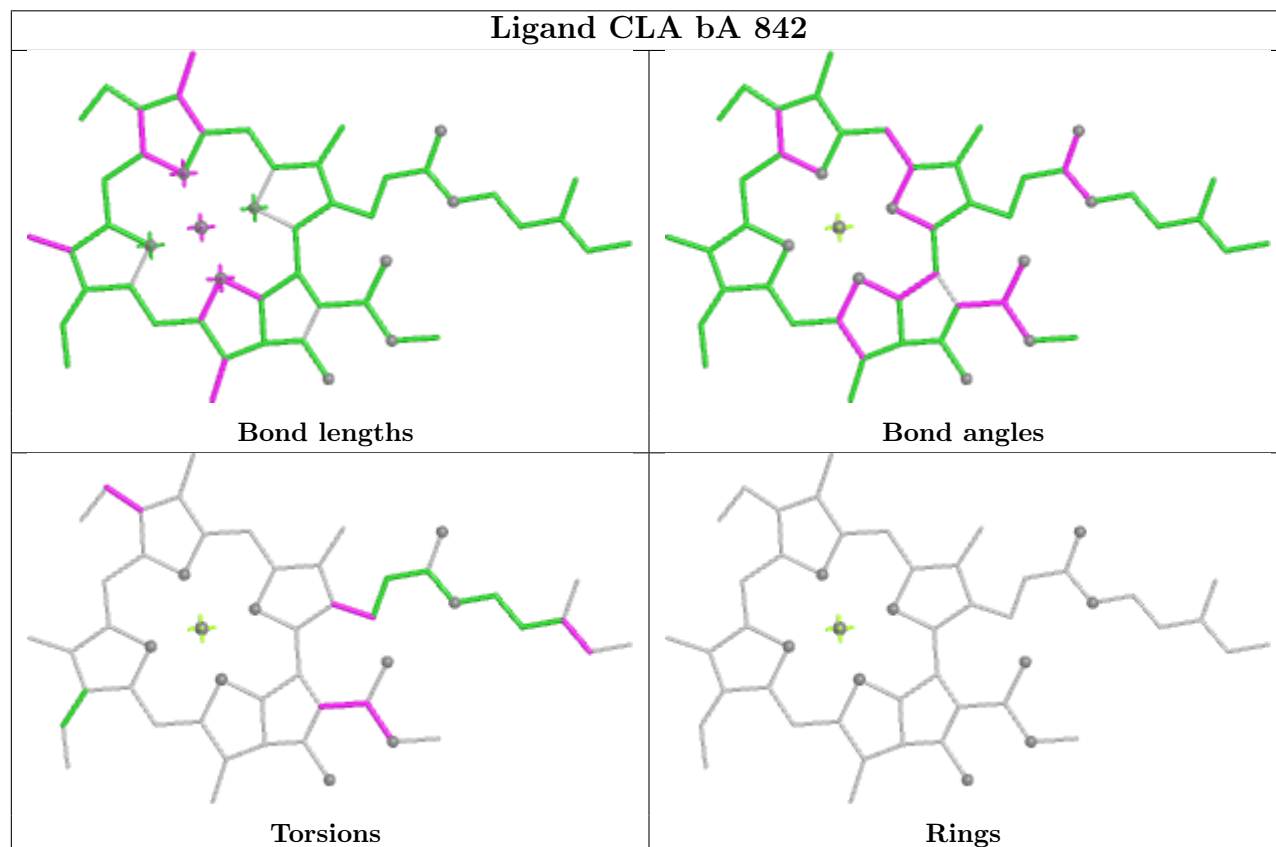
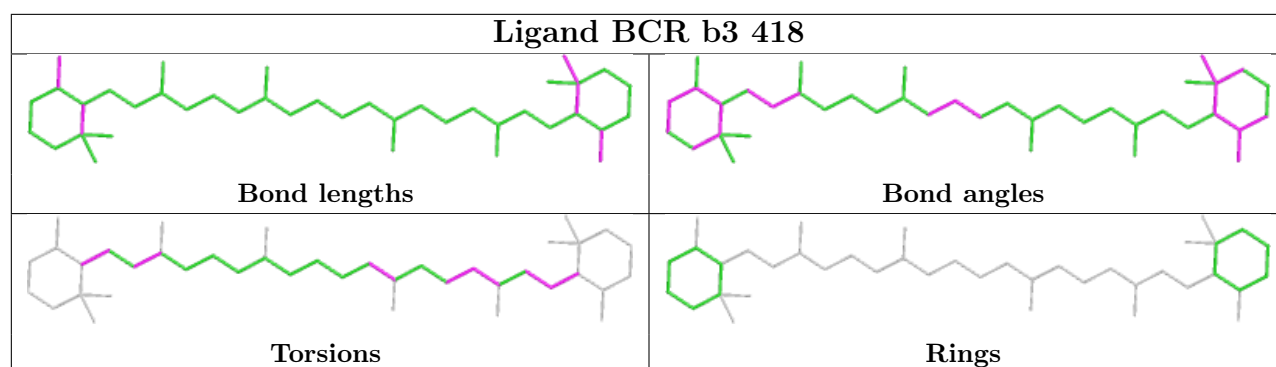


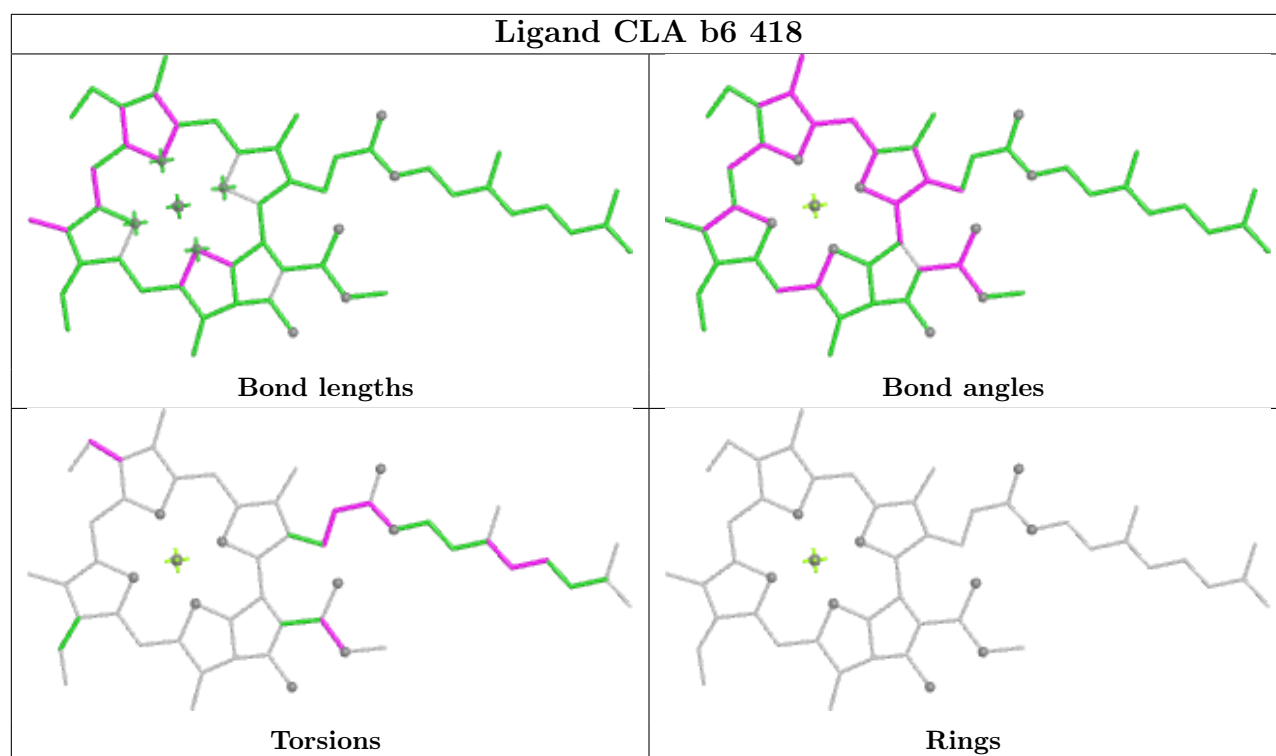


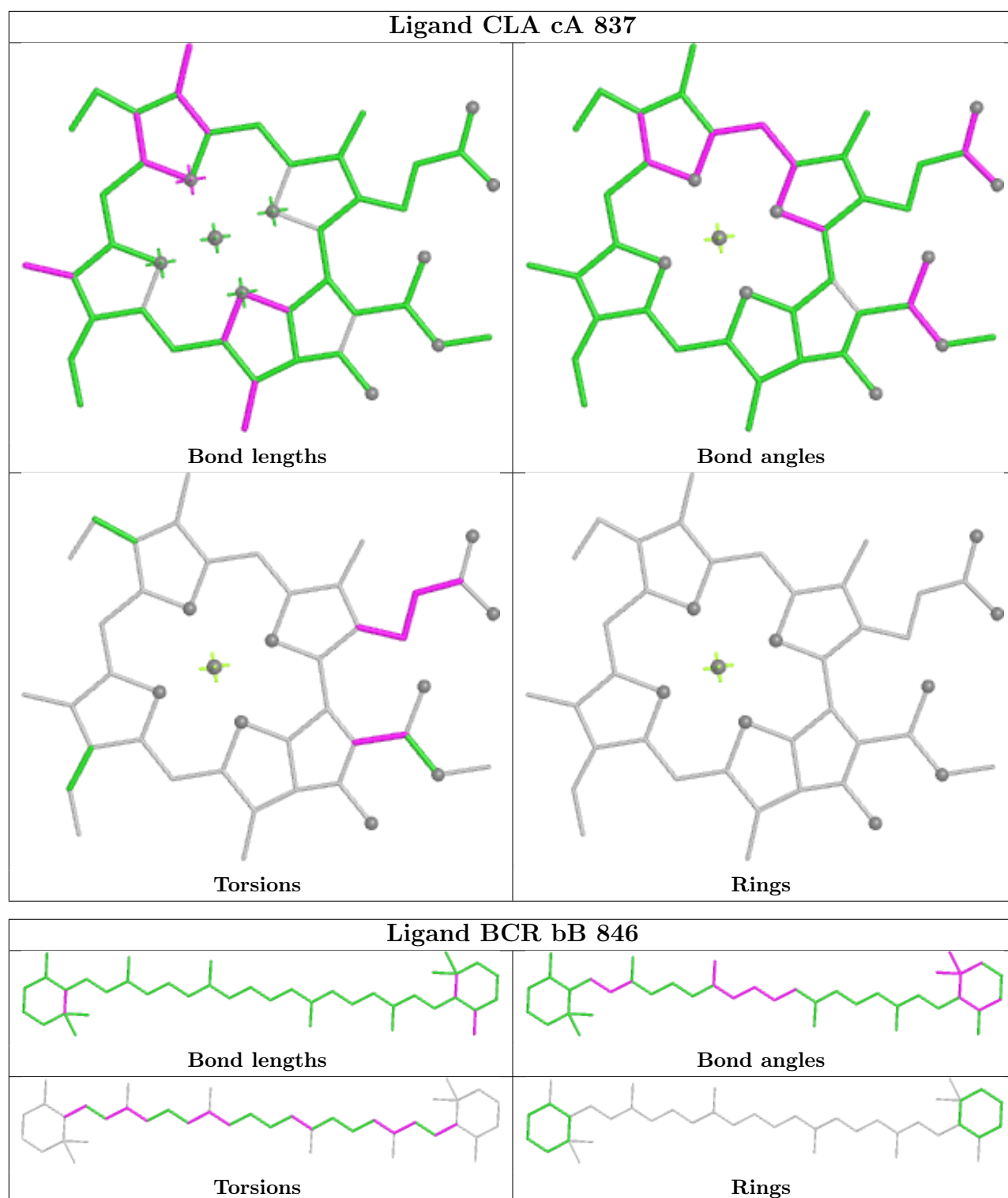


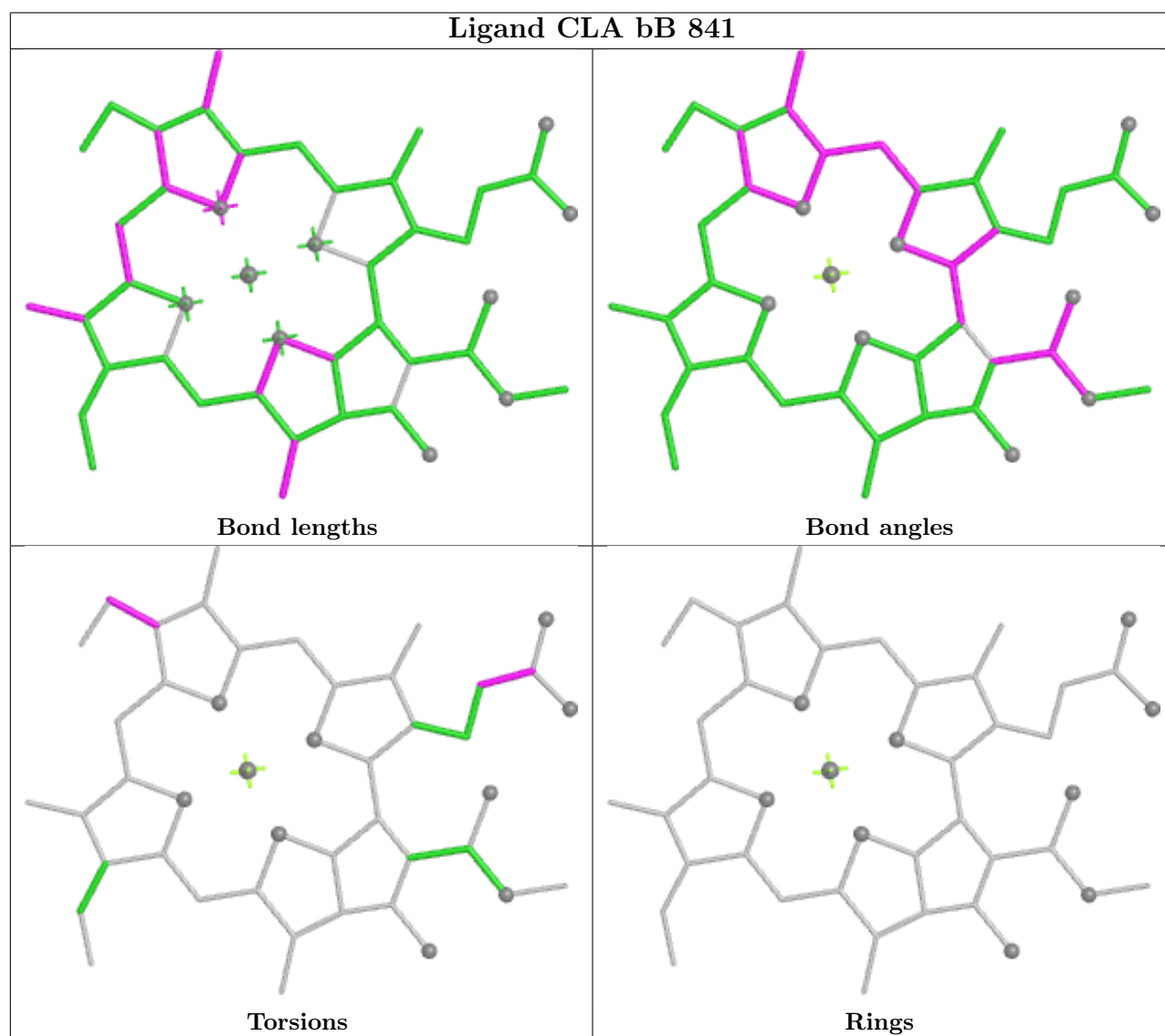
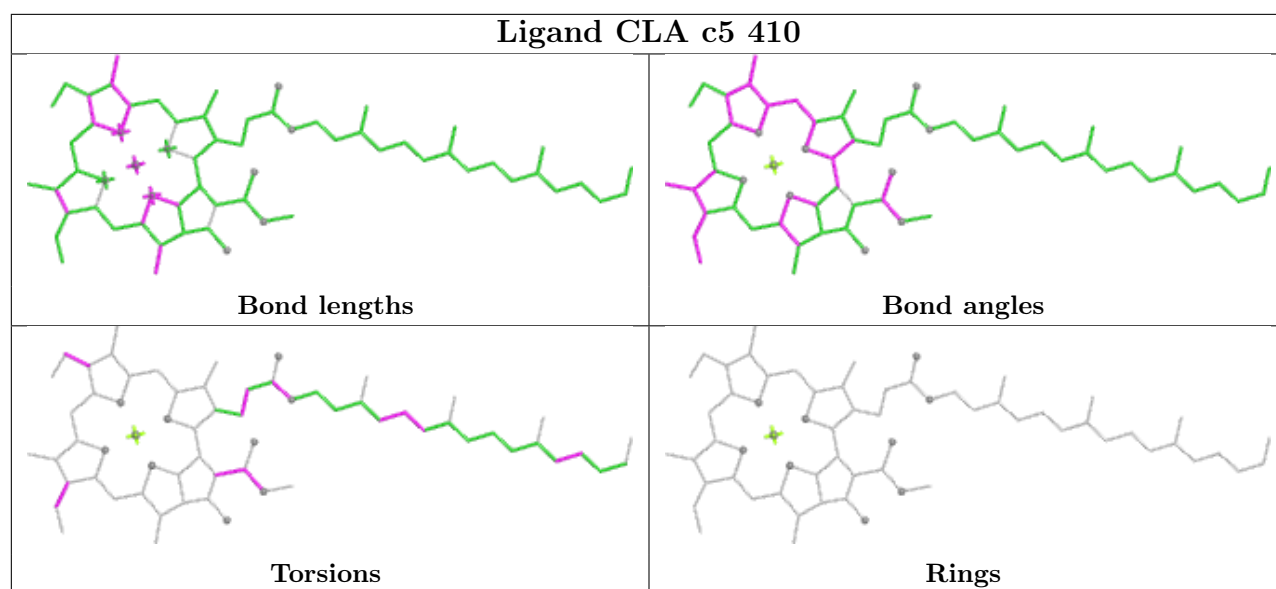


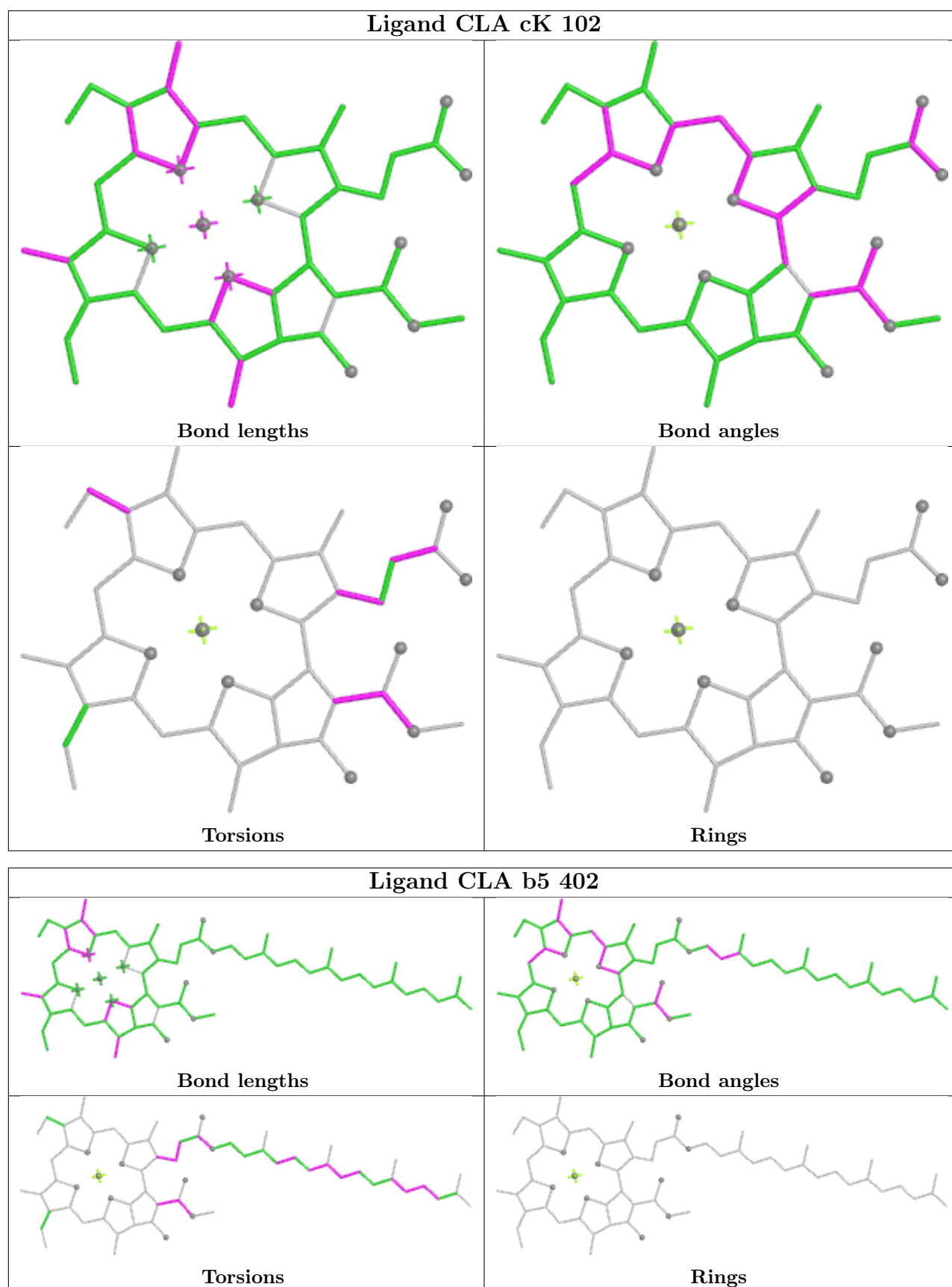


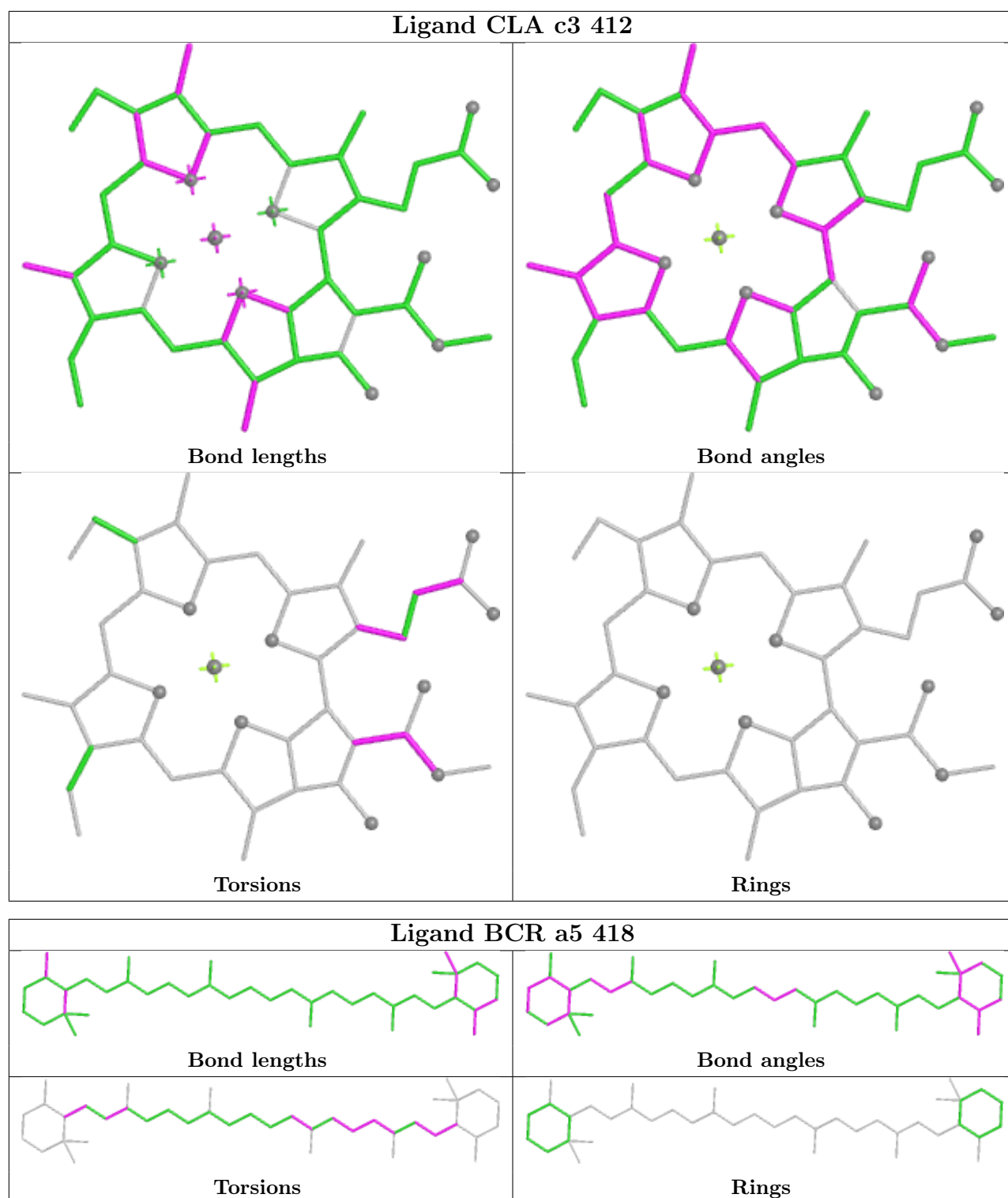


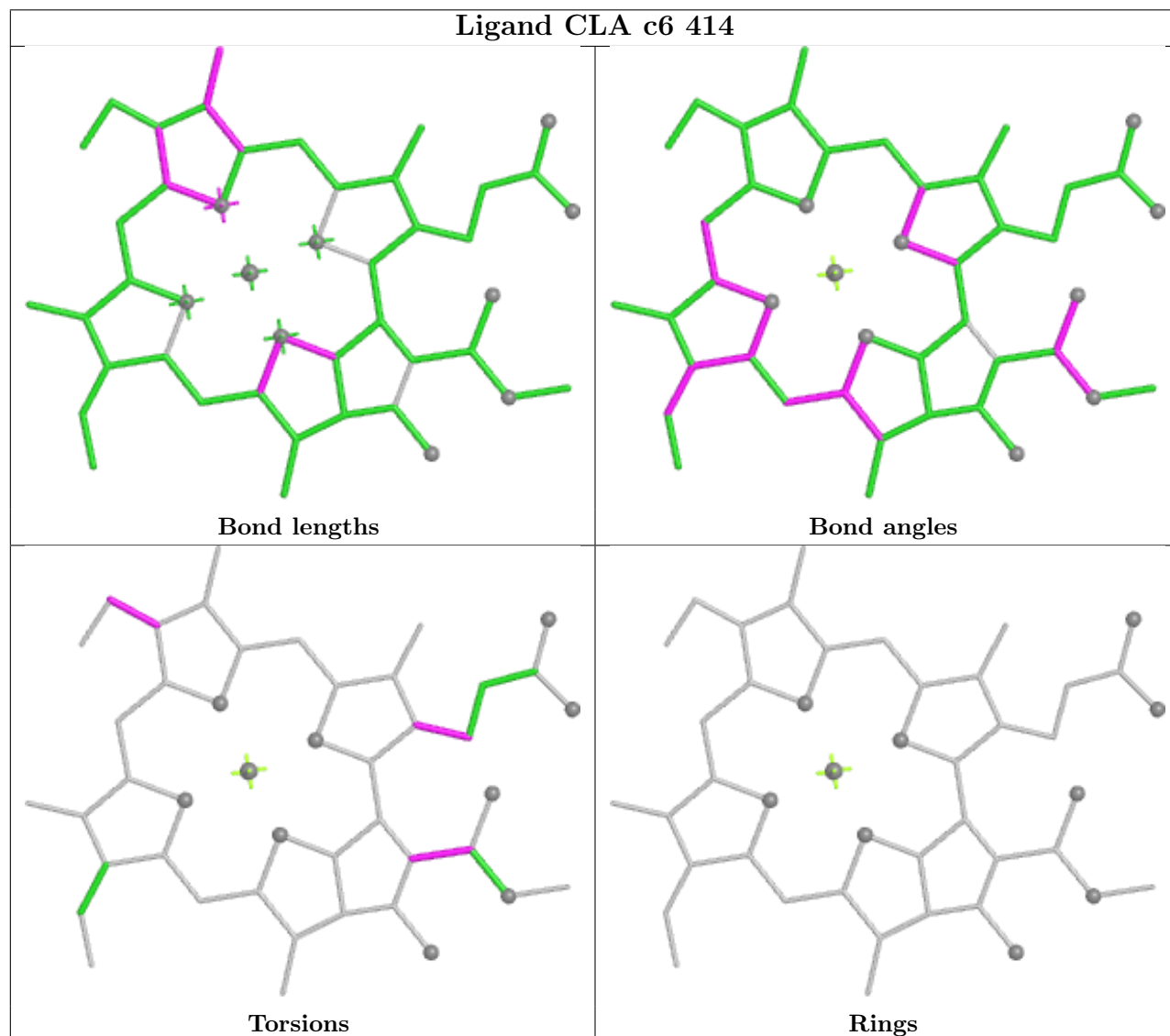
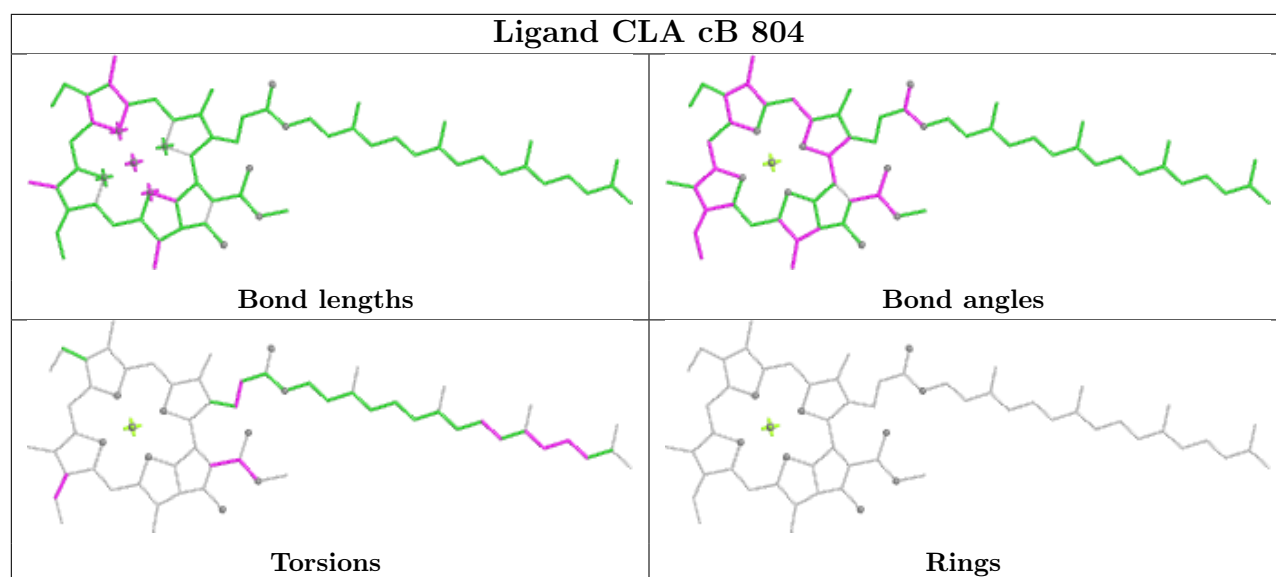


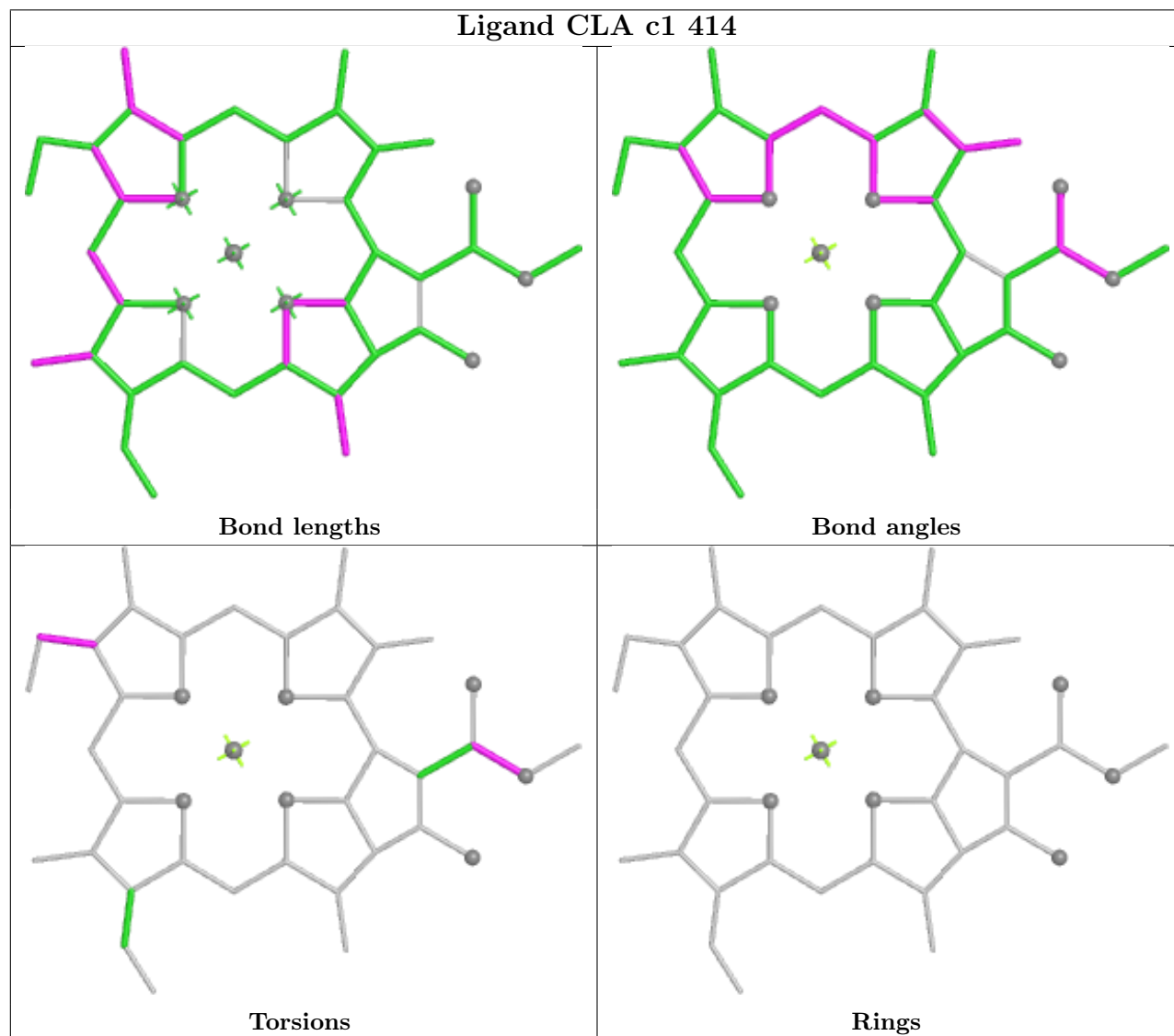
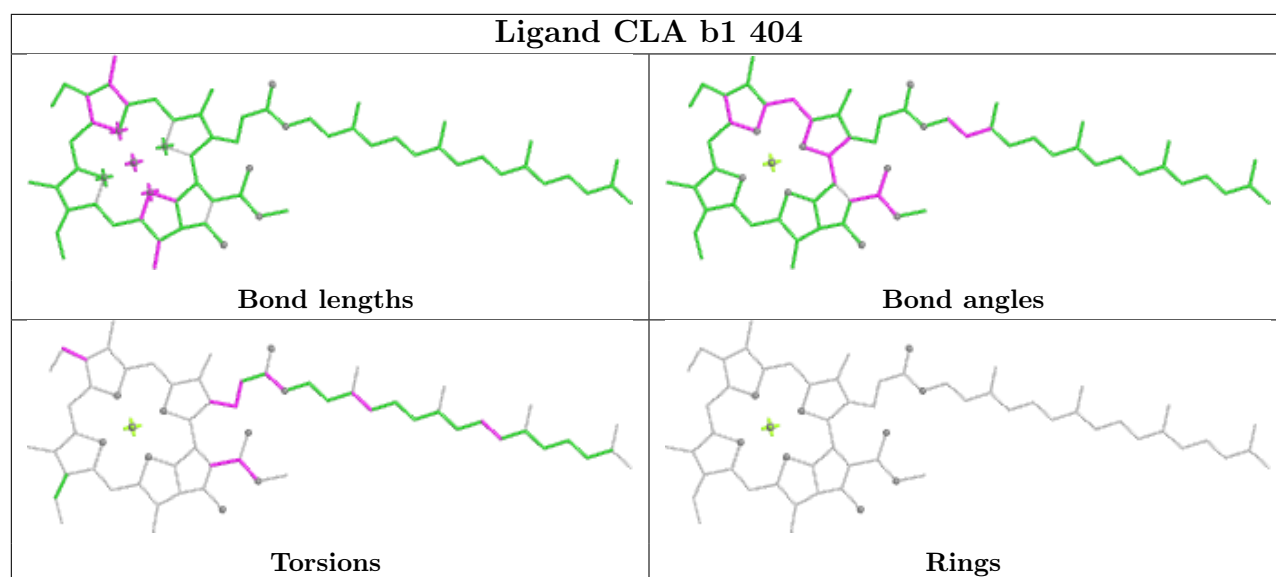




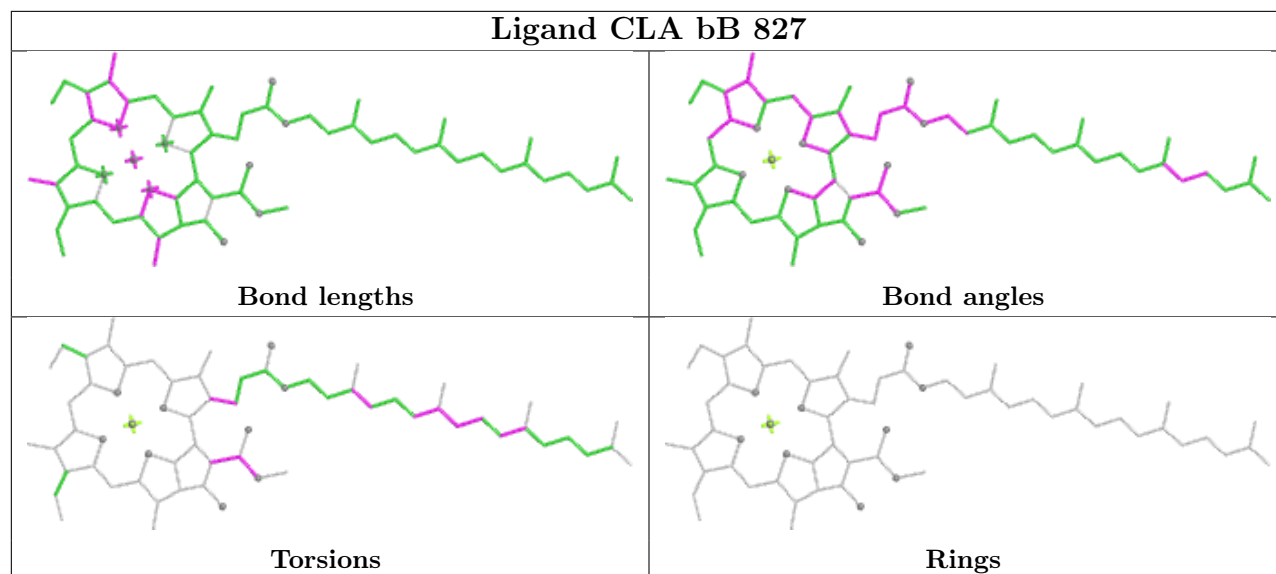




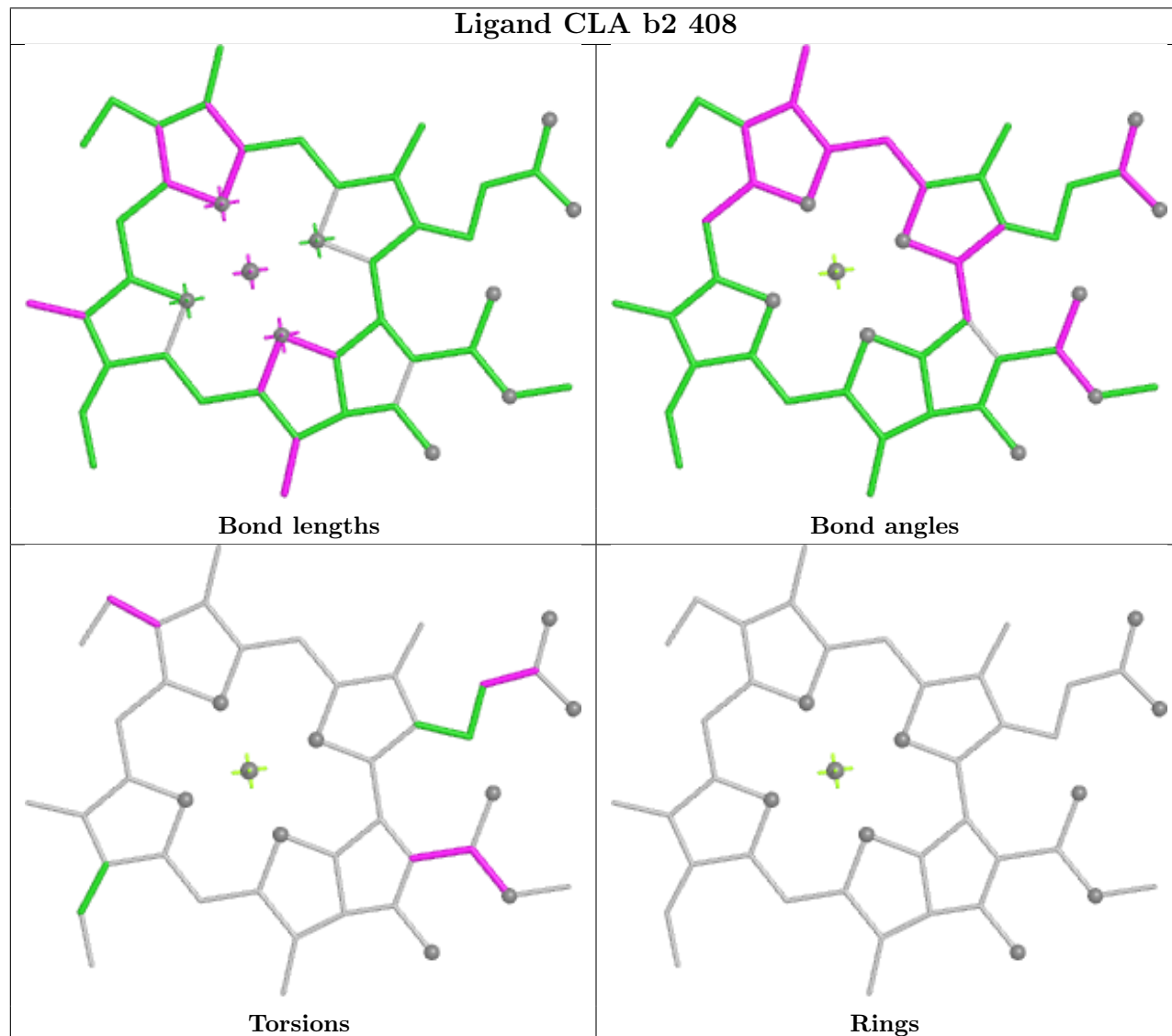


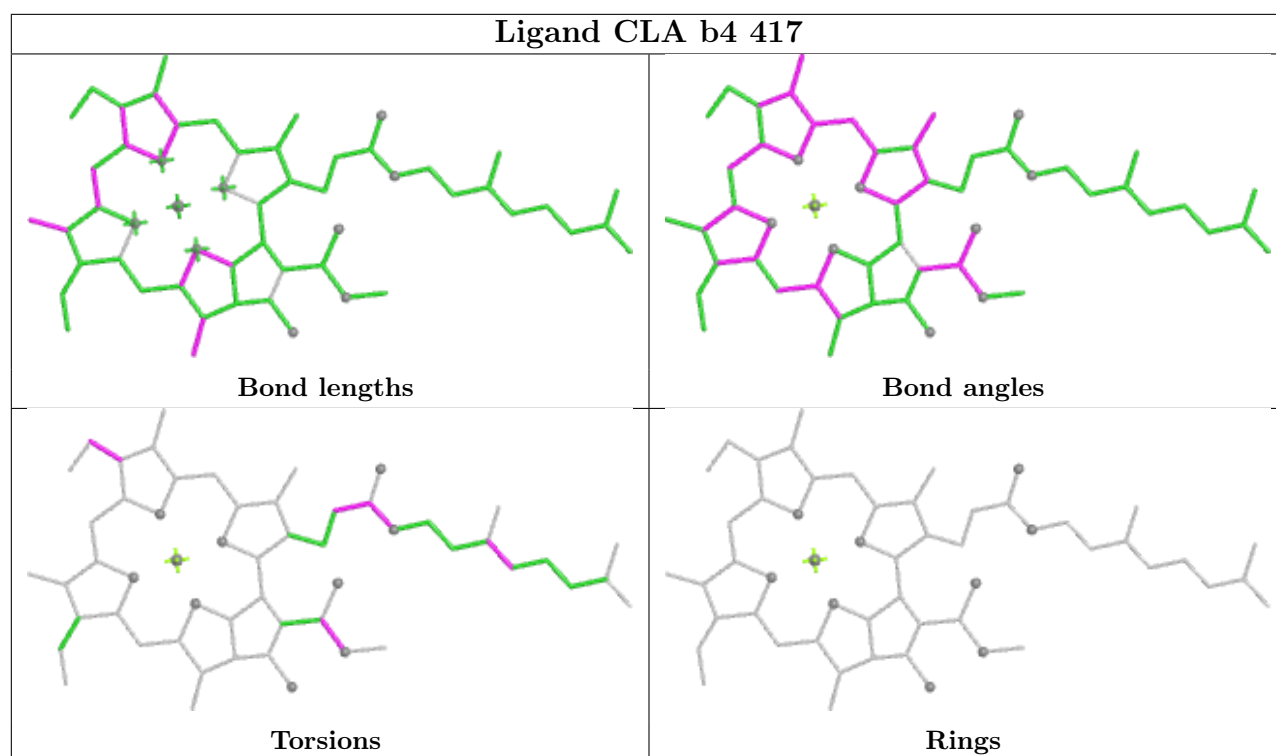


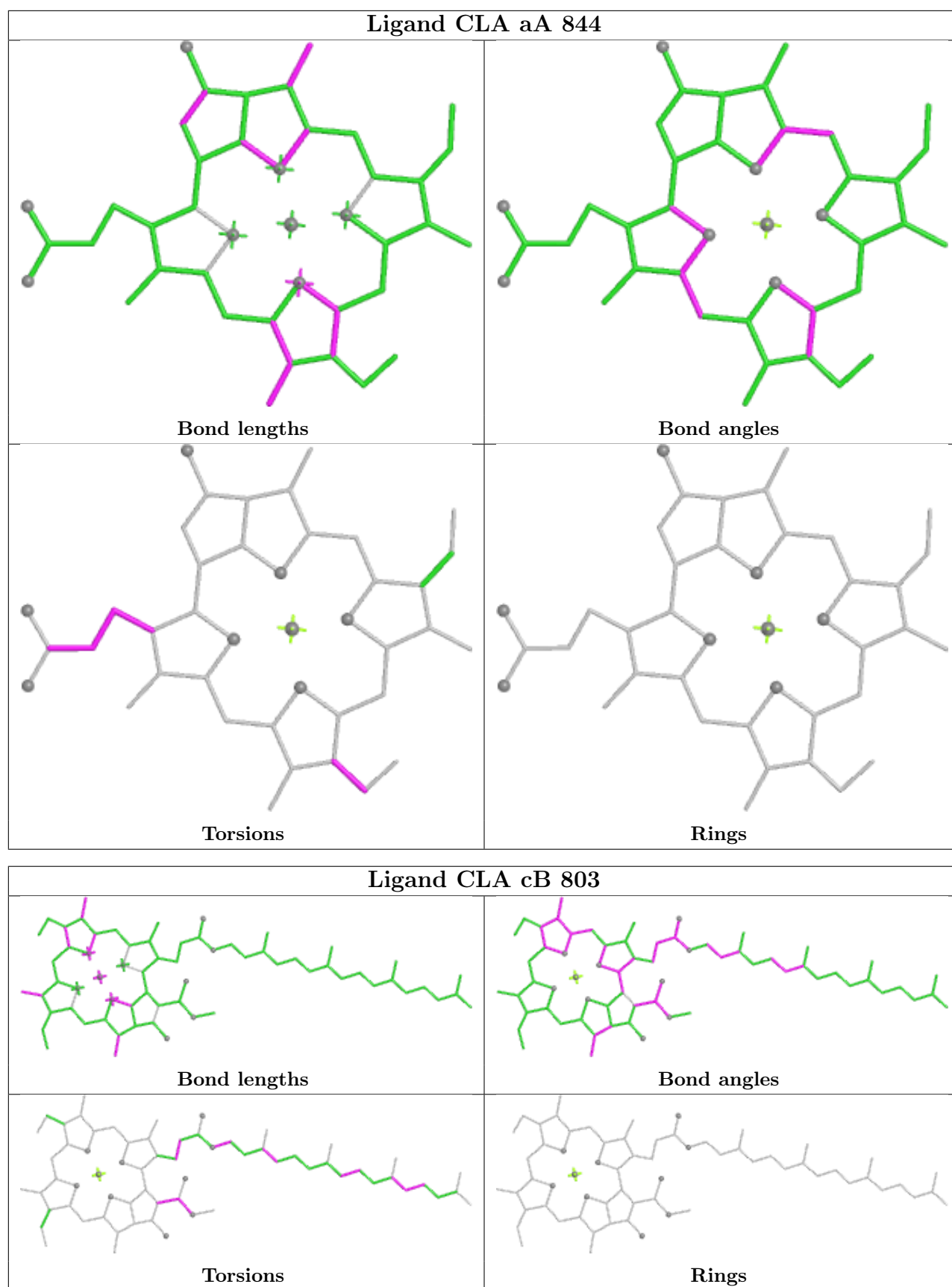
Ligand CLA bB 827



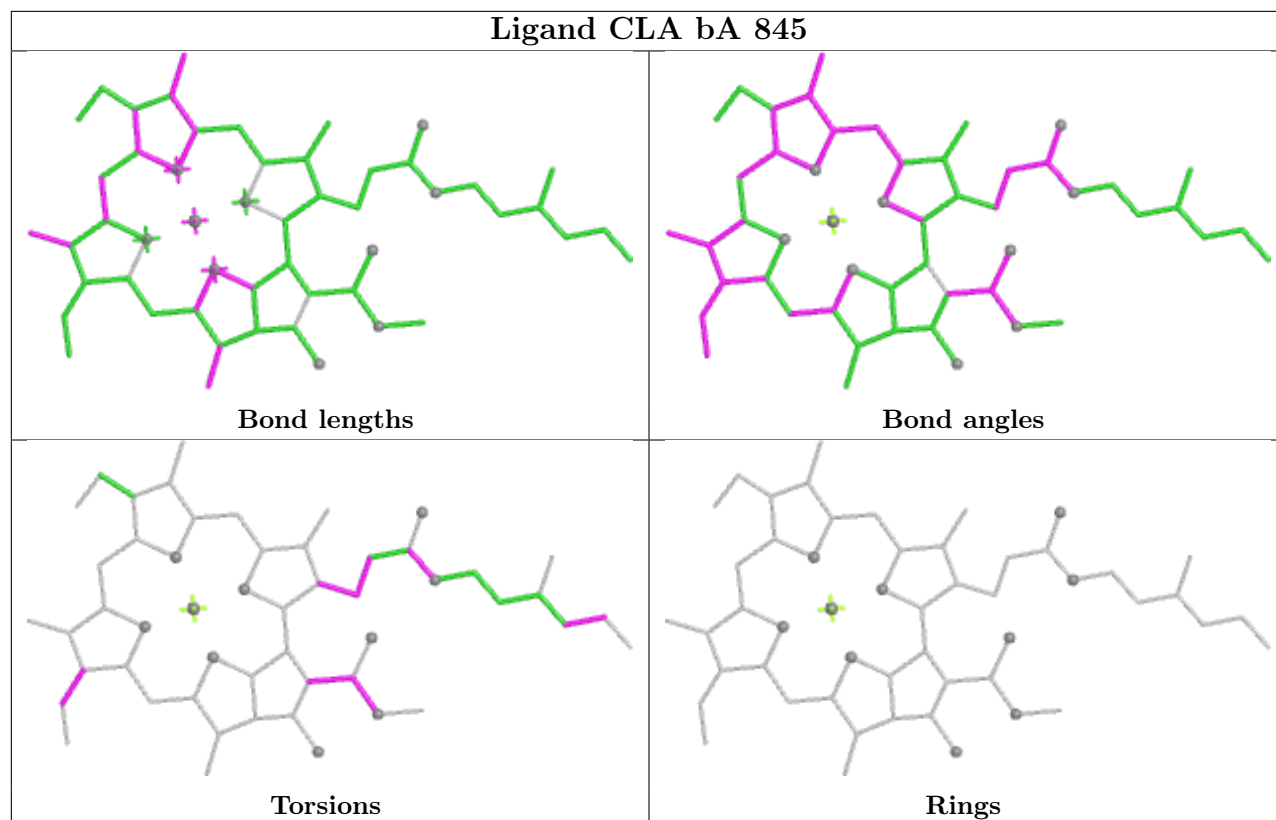
Ligand CLA b2 408



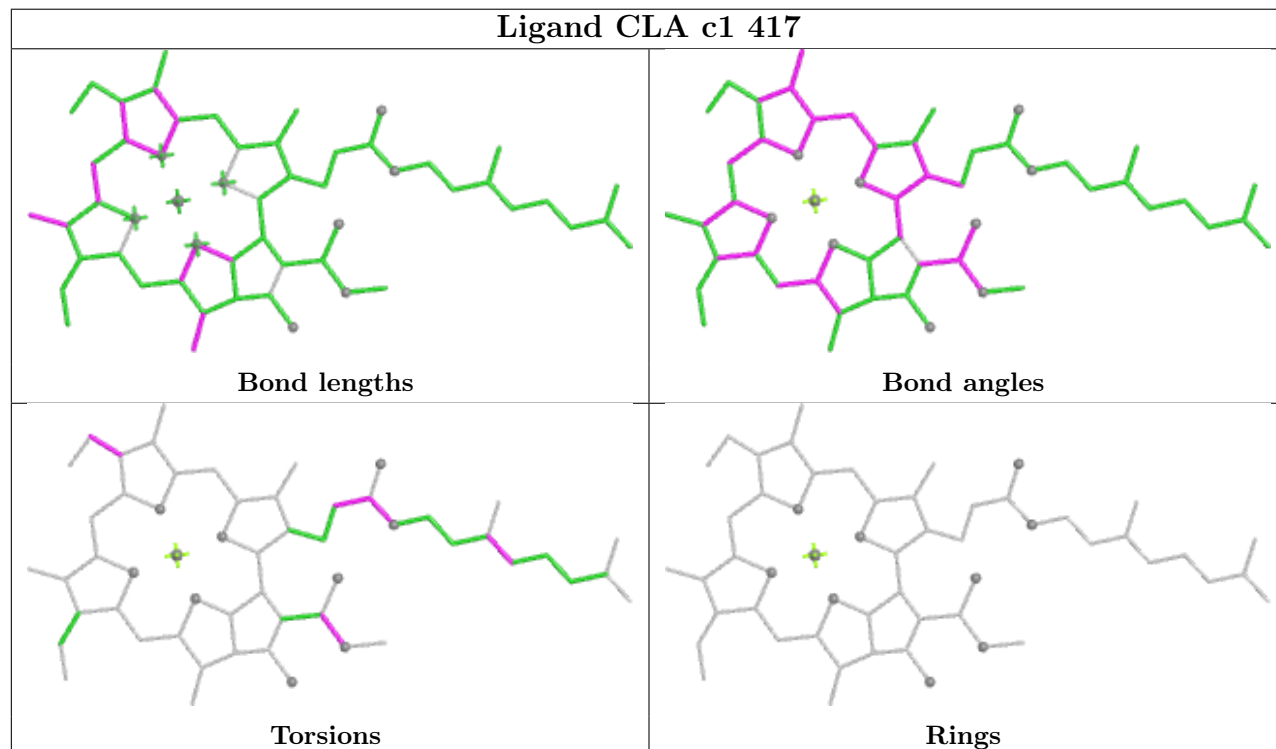


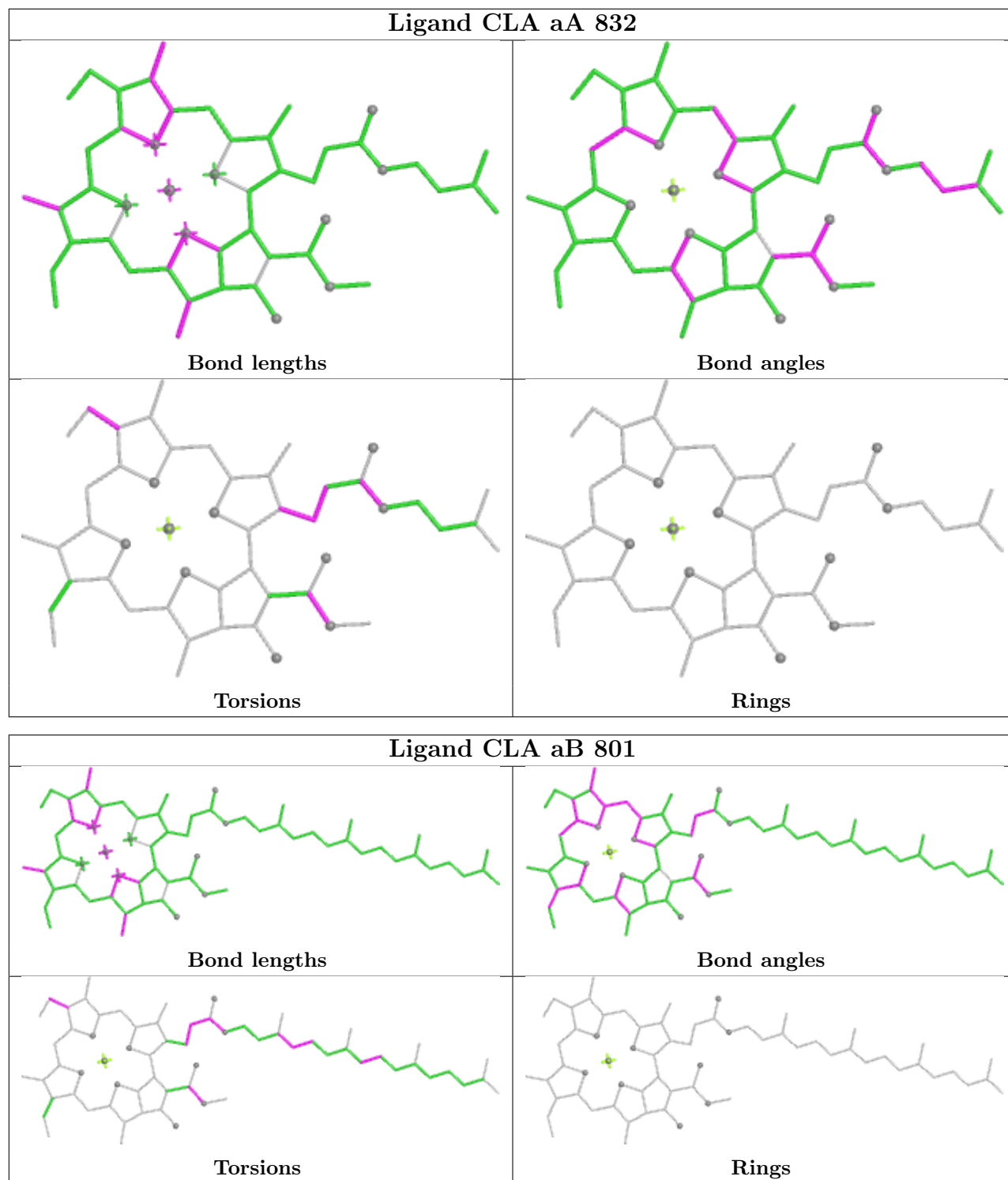


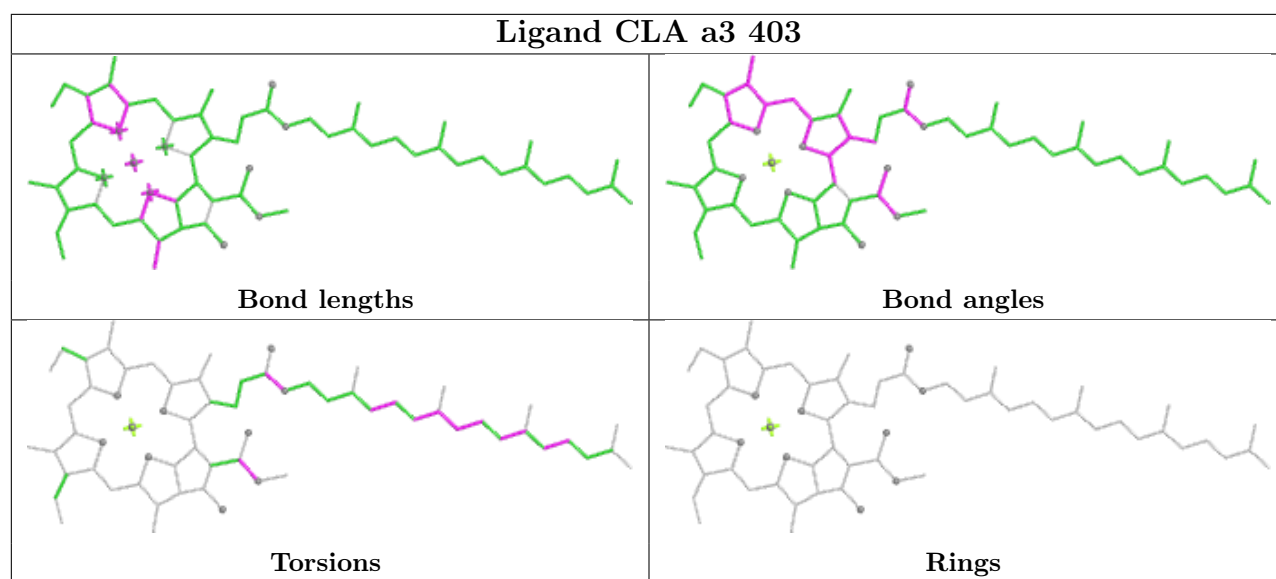
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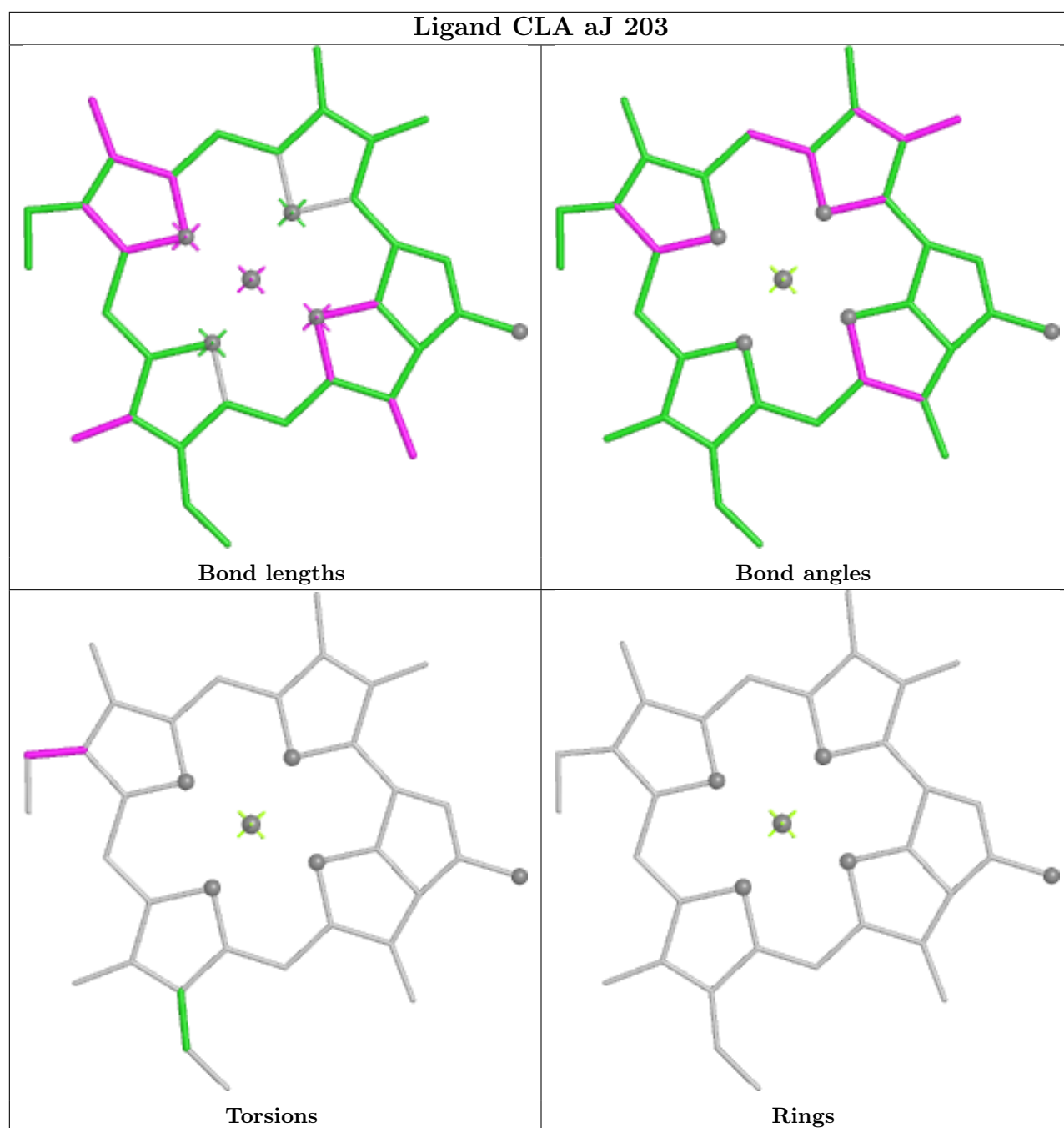


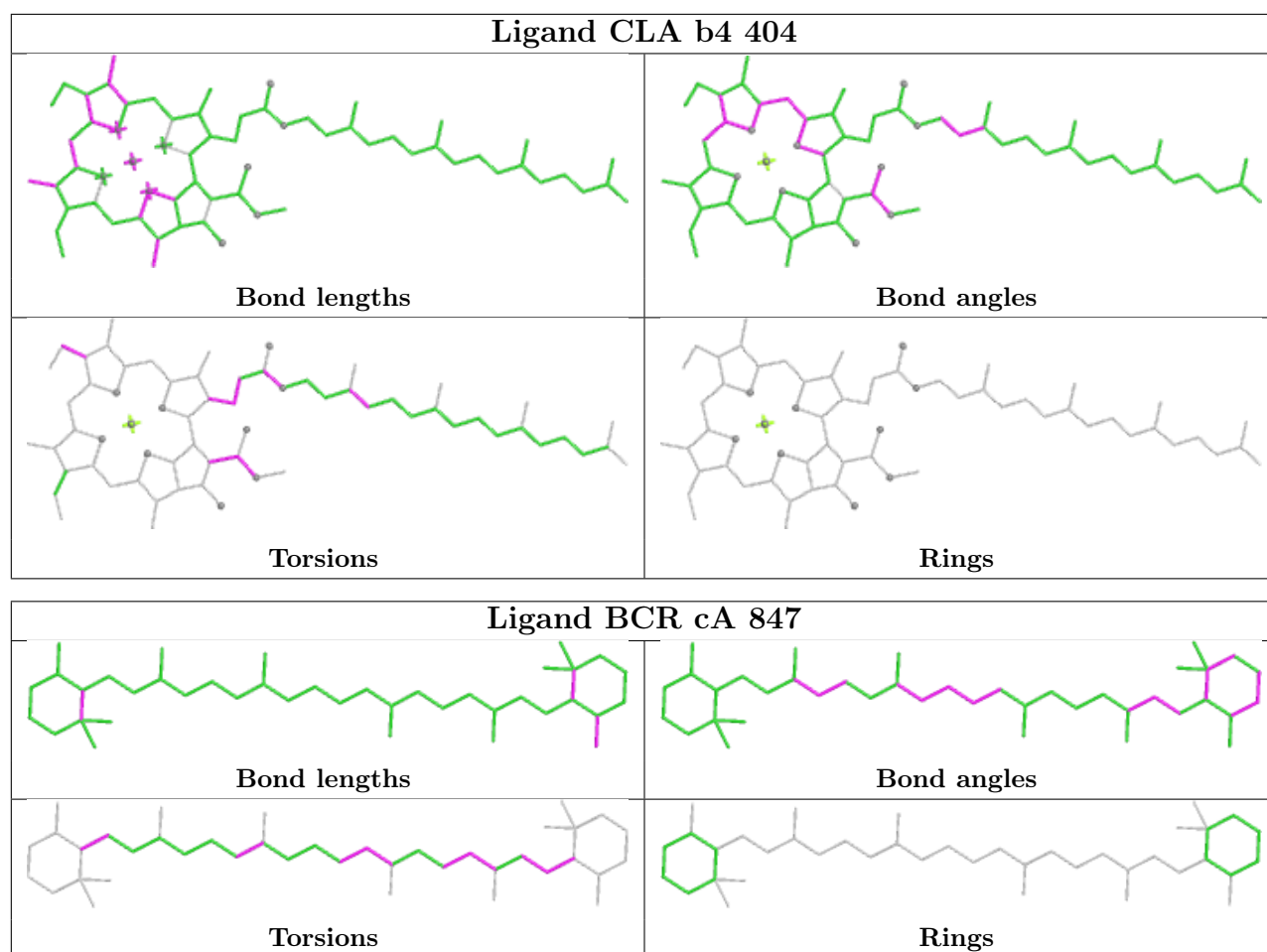
Ligand CLA c1 417

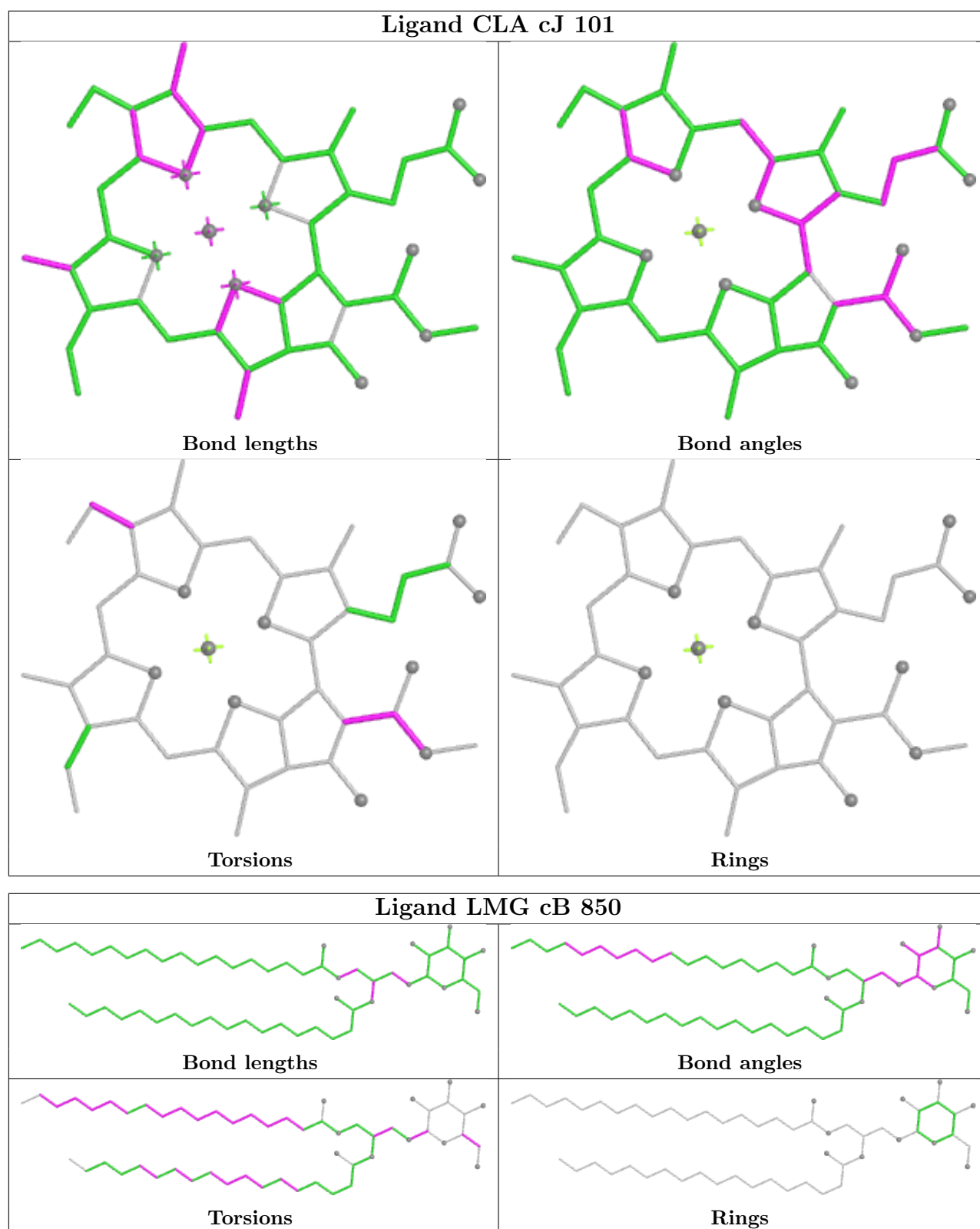


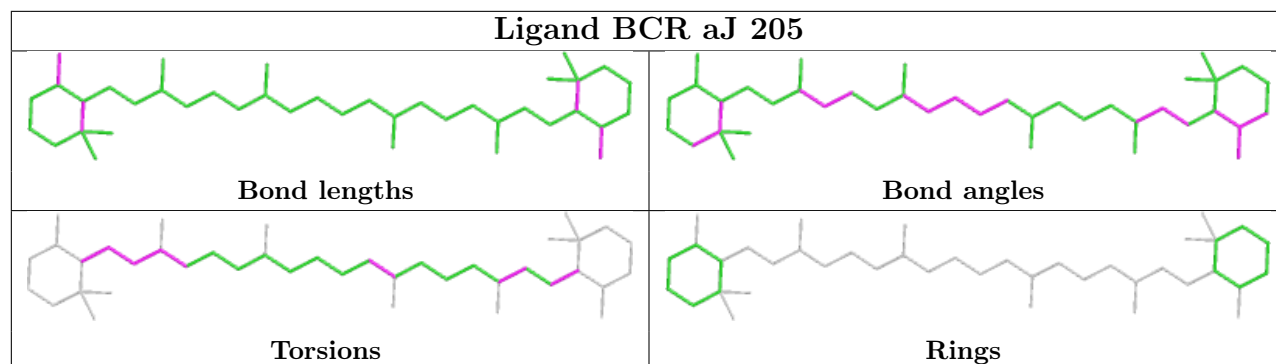
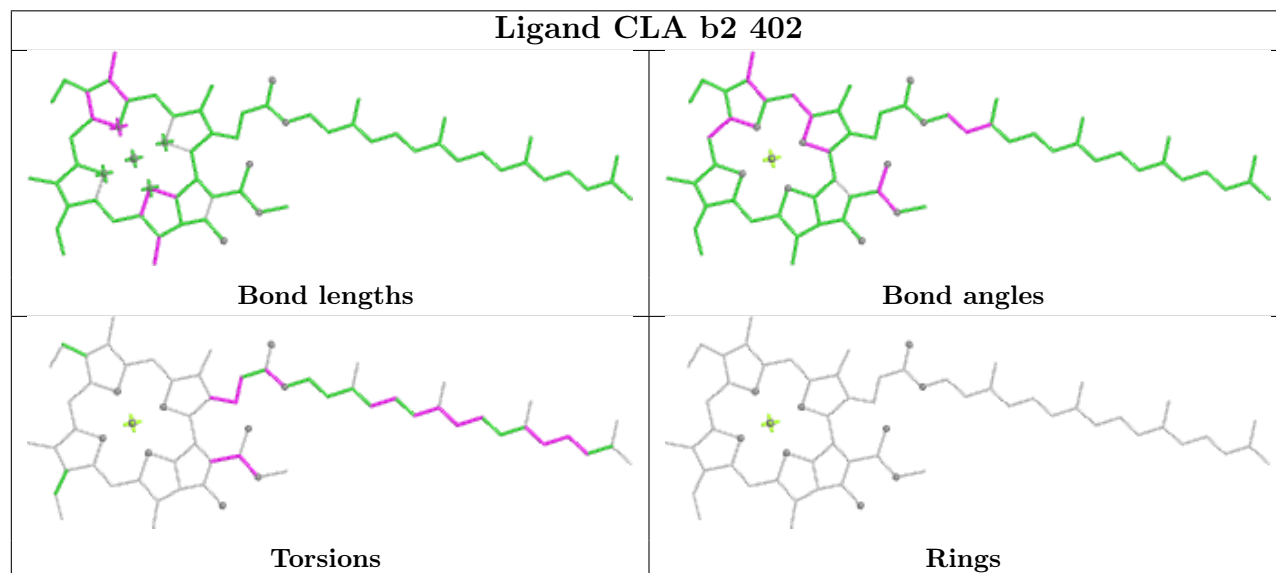
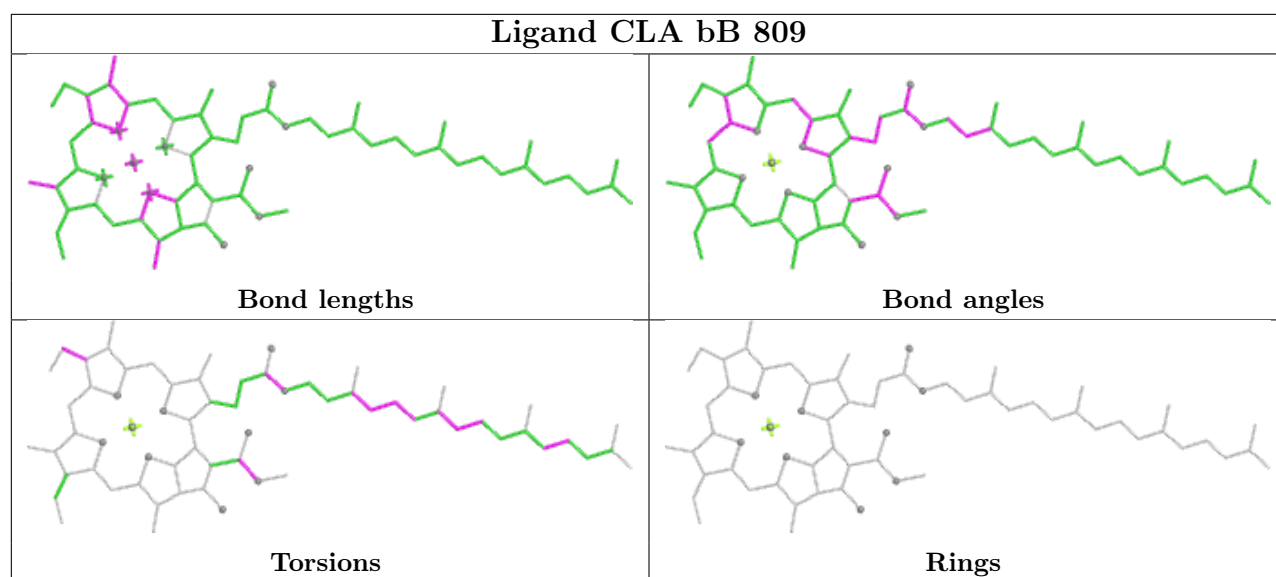


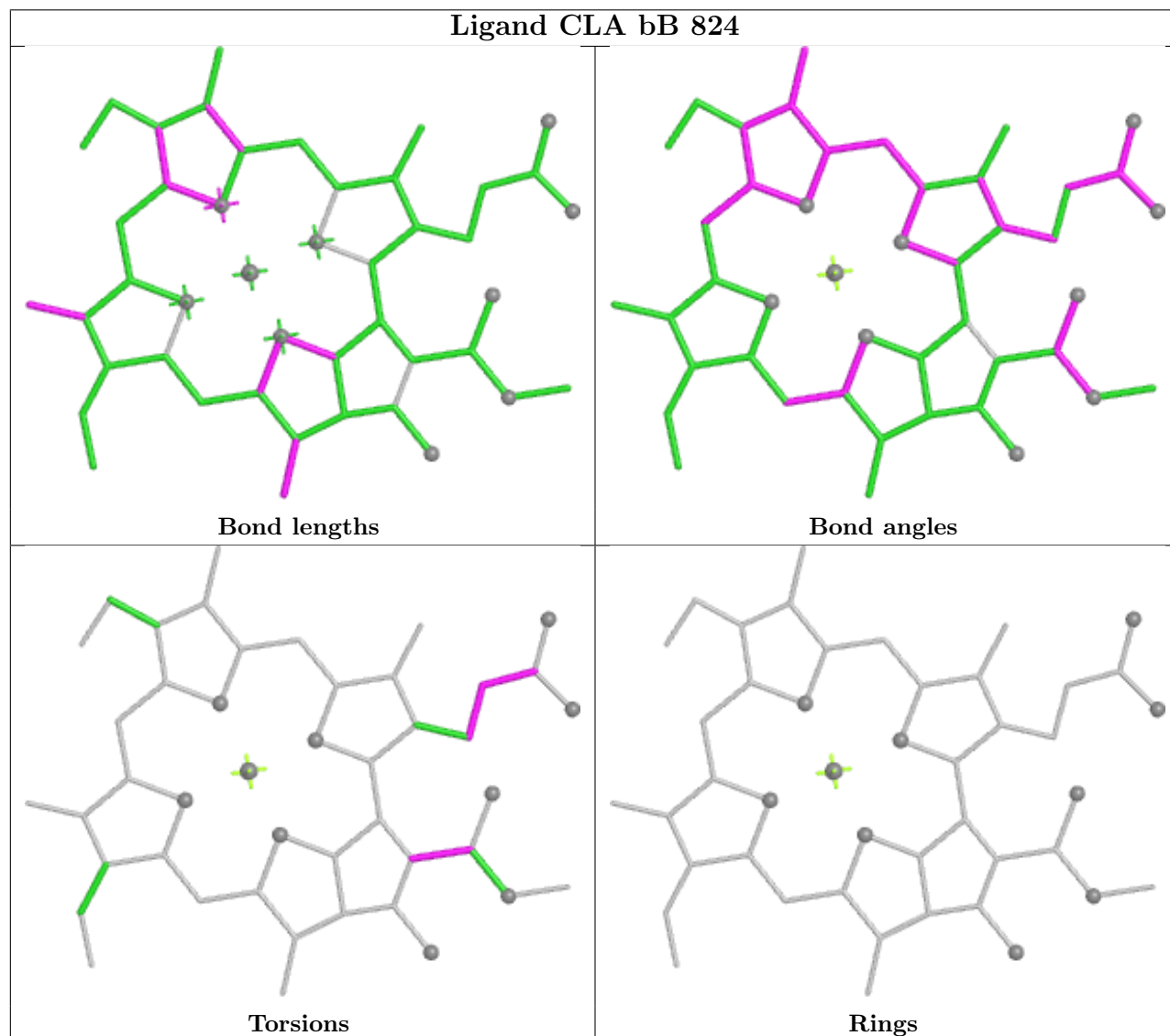
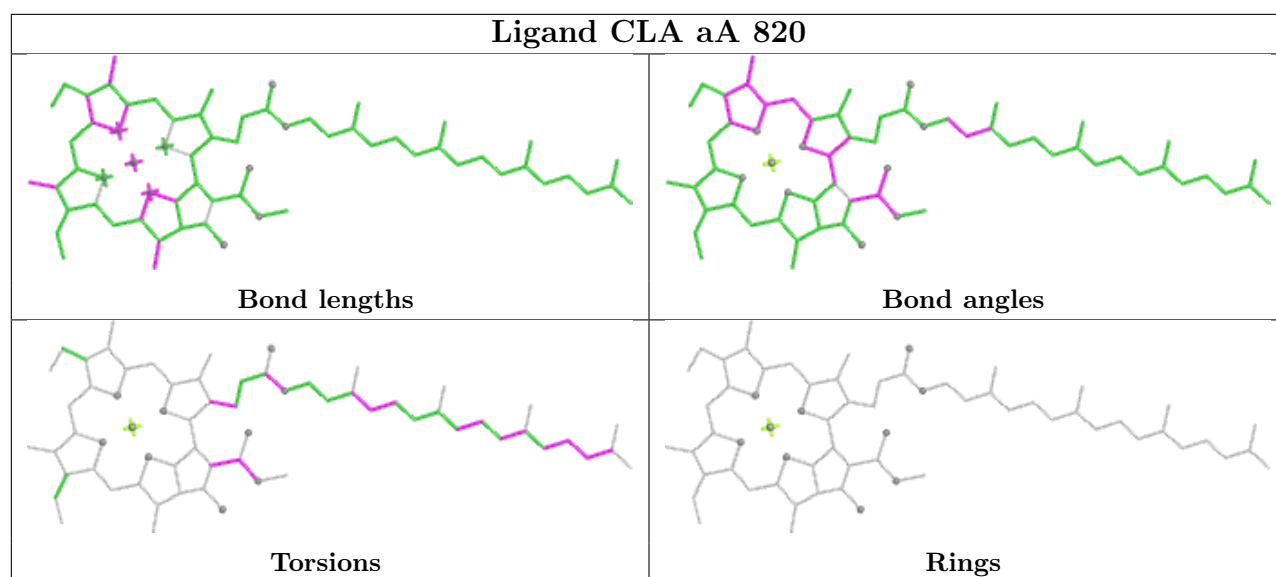


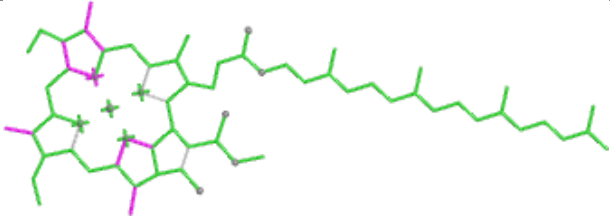
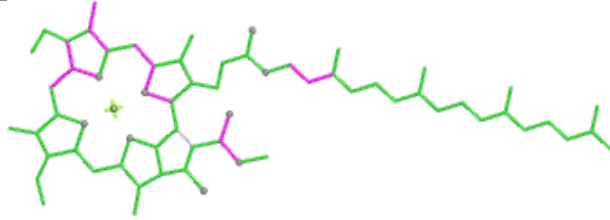
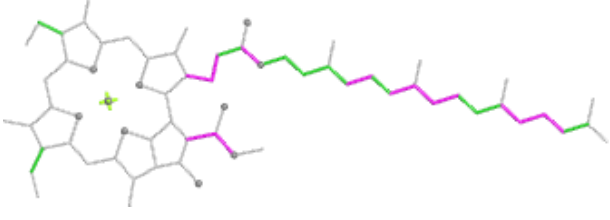
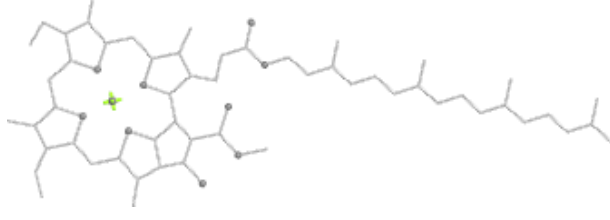
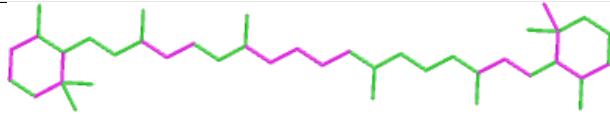
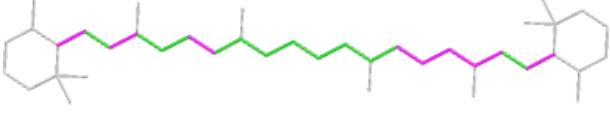
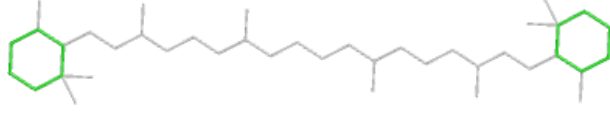
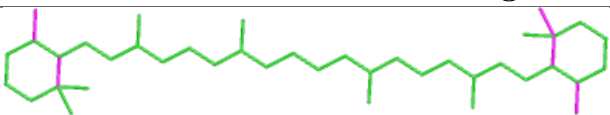
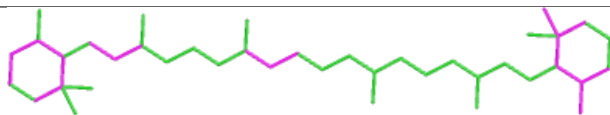
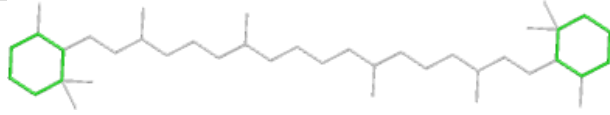


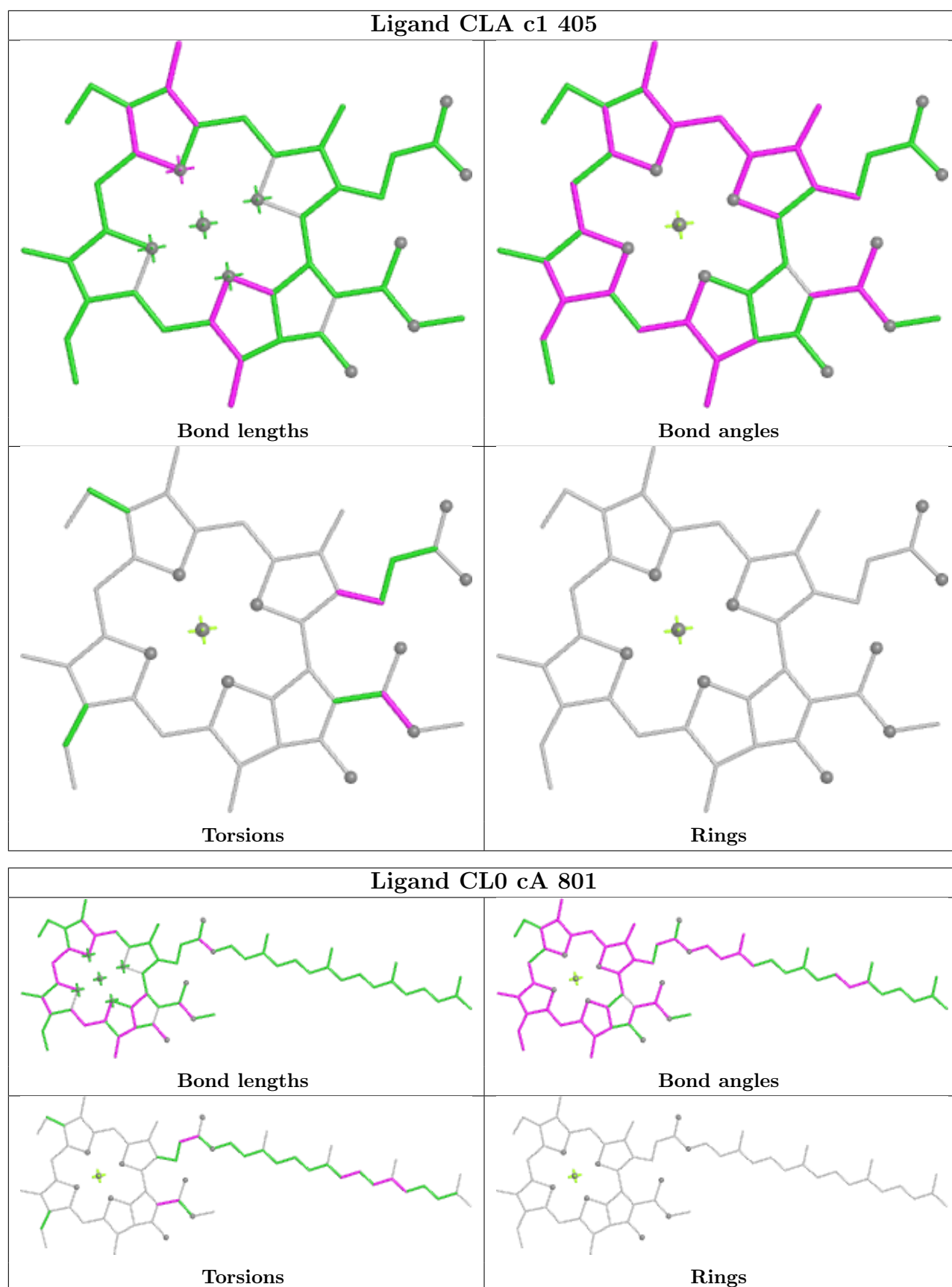




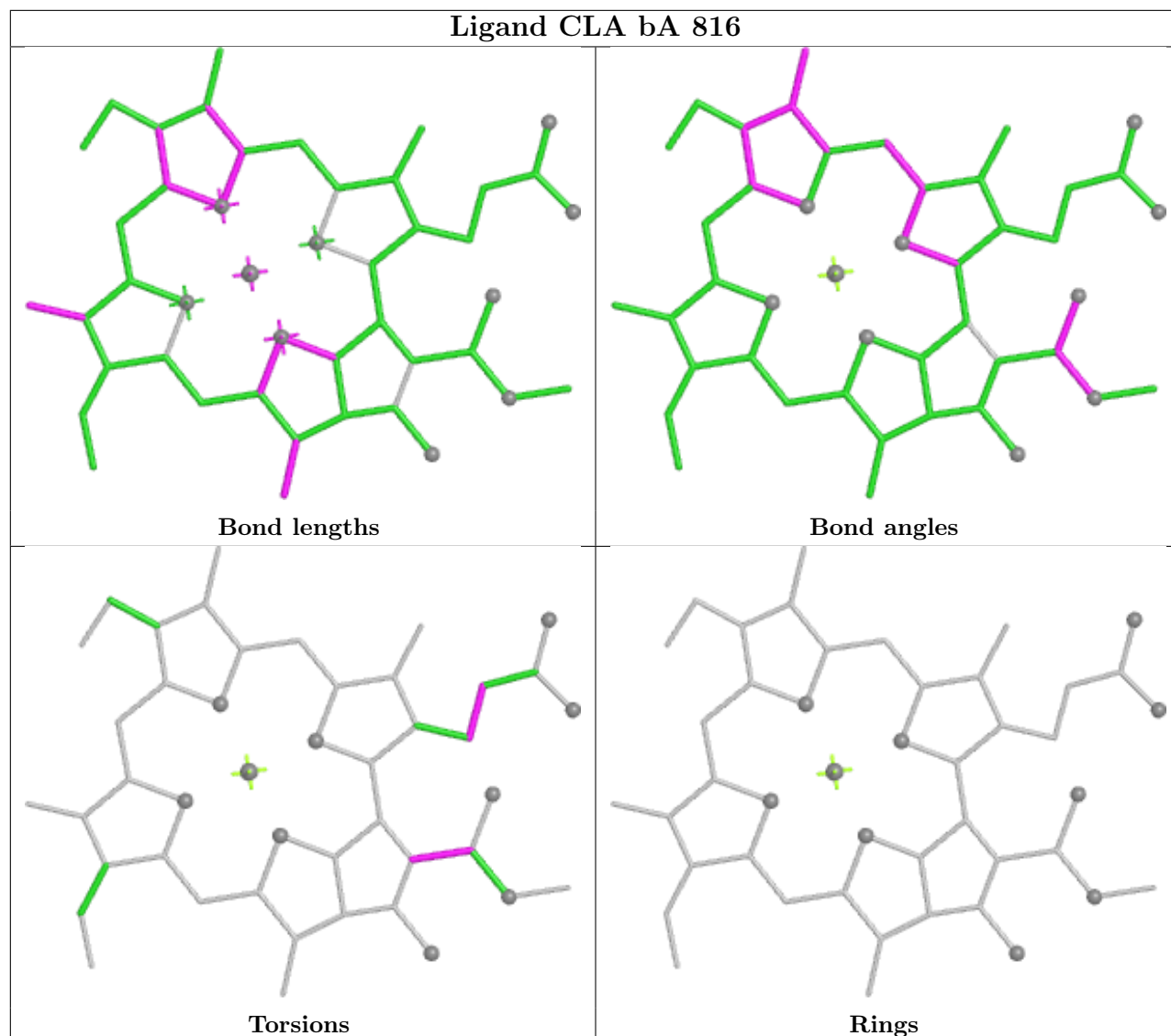




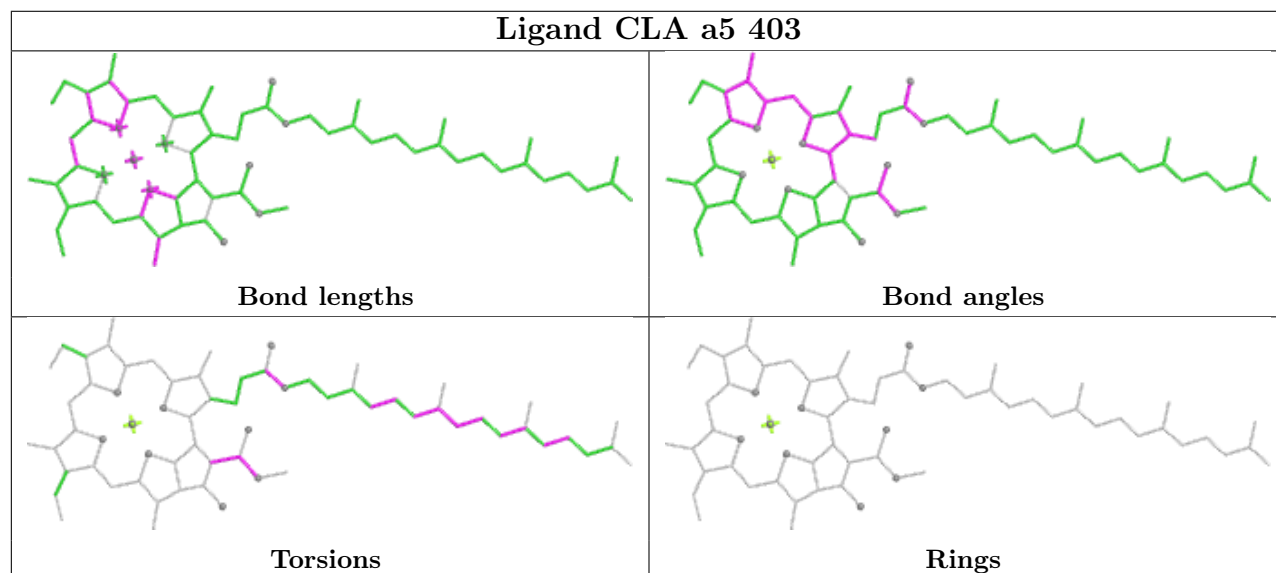
Ligand CLA c1 402	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b4 419	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b5 418	
 Bond lengths	 Bond angles
 Torsions	 Rings

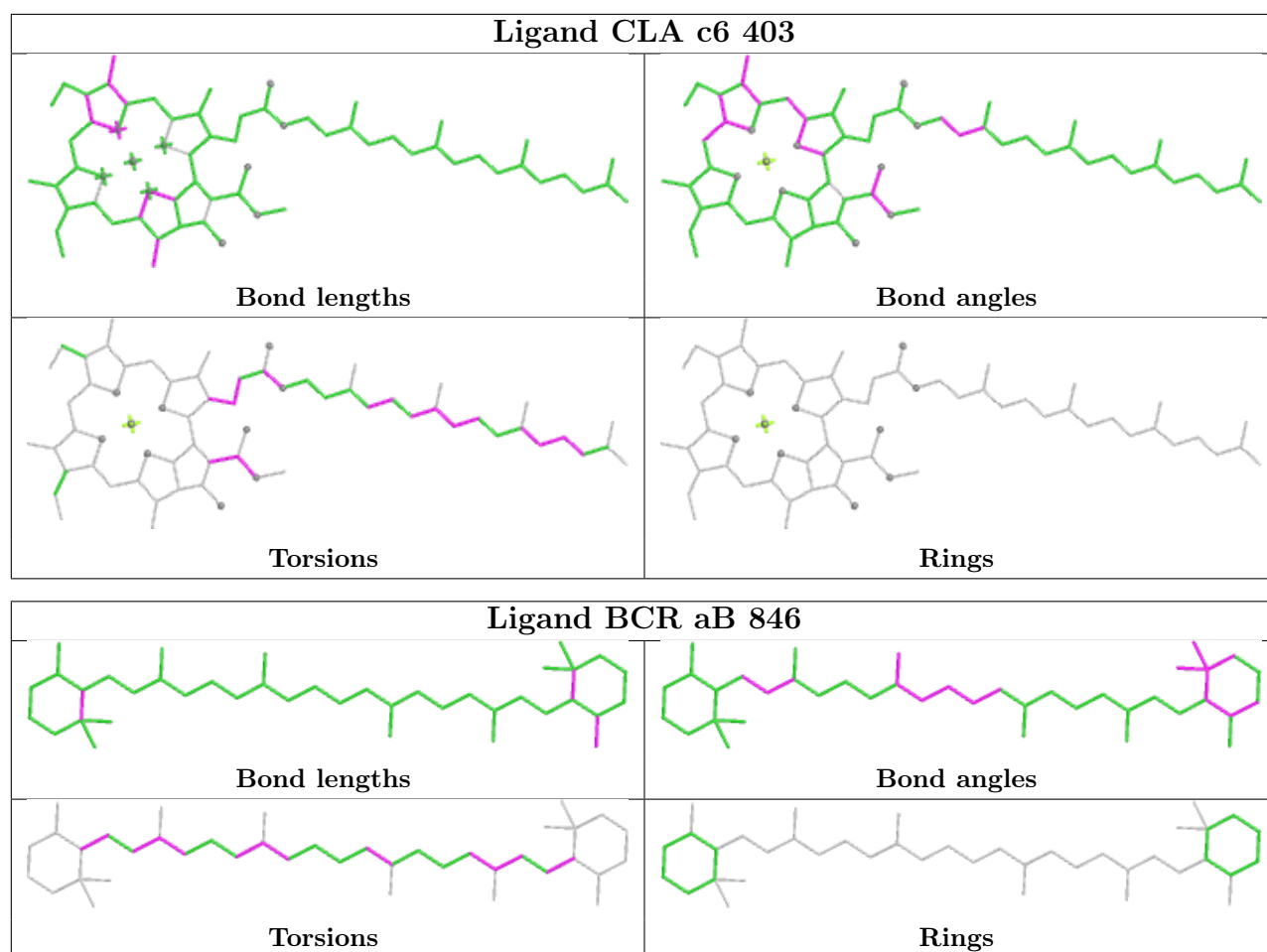


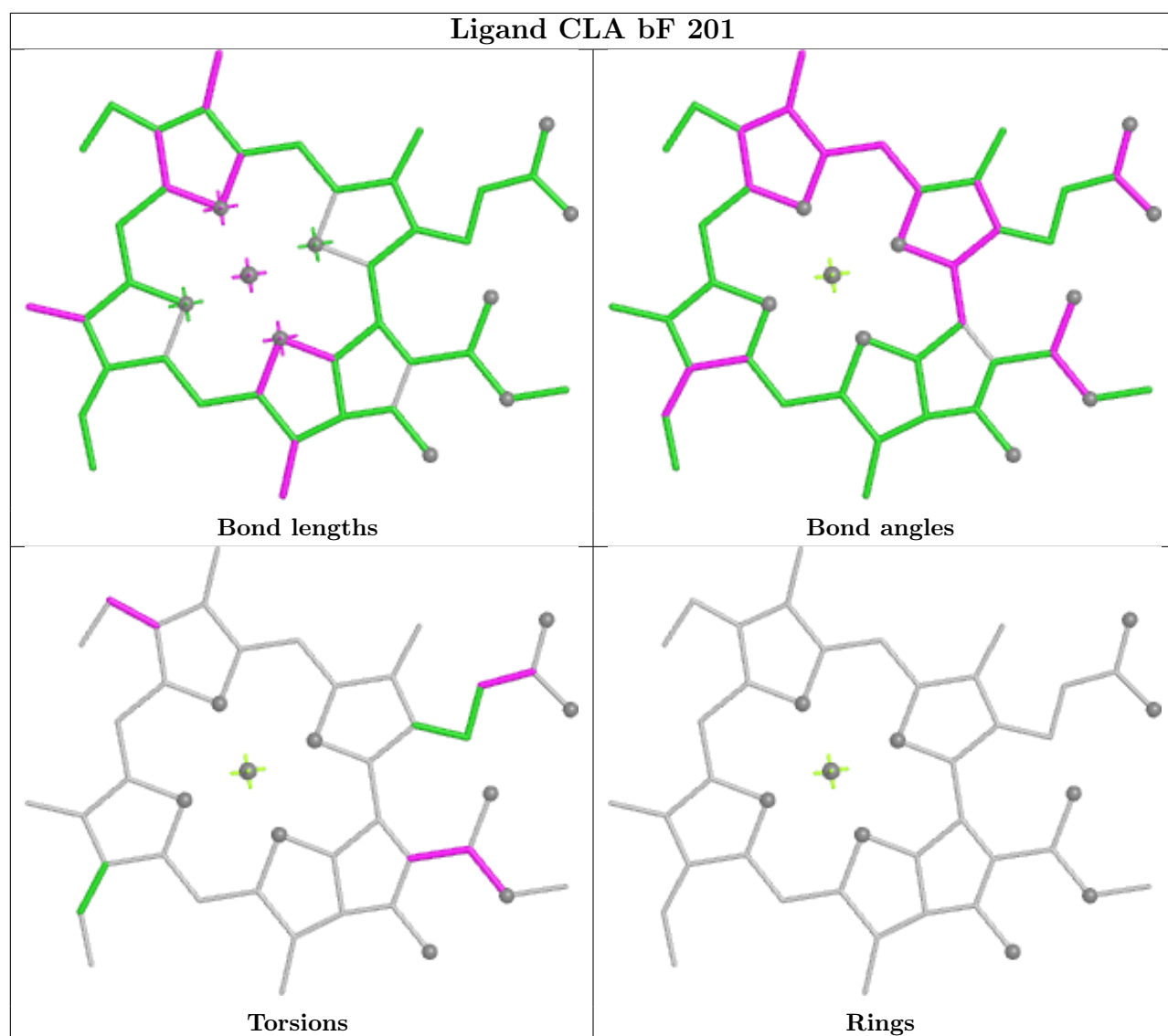
Ligand CLA bA 816

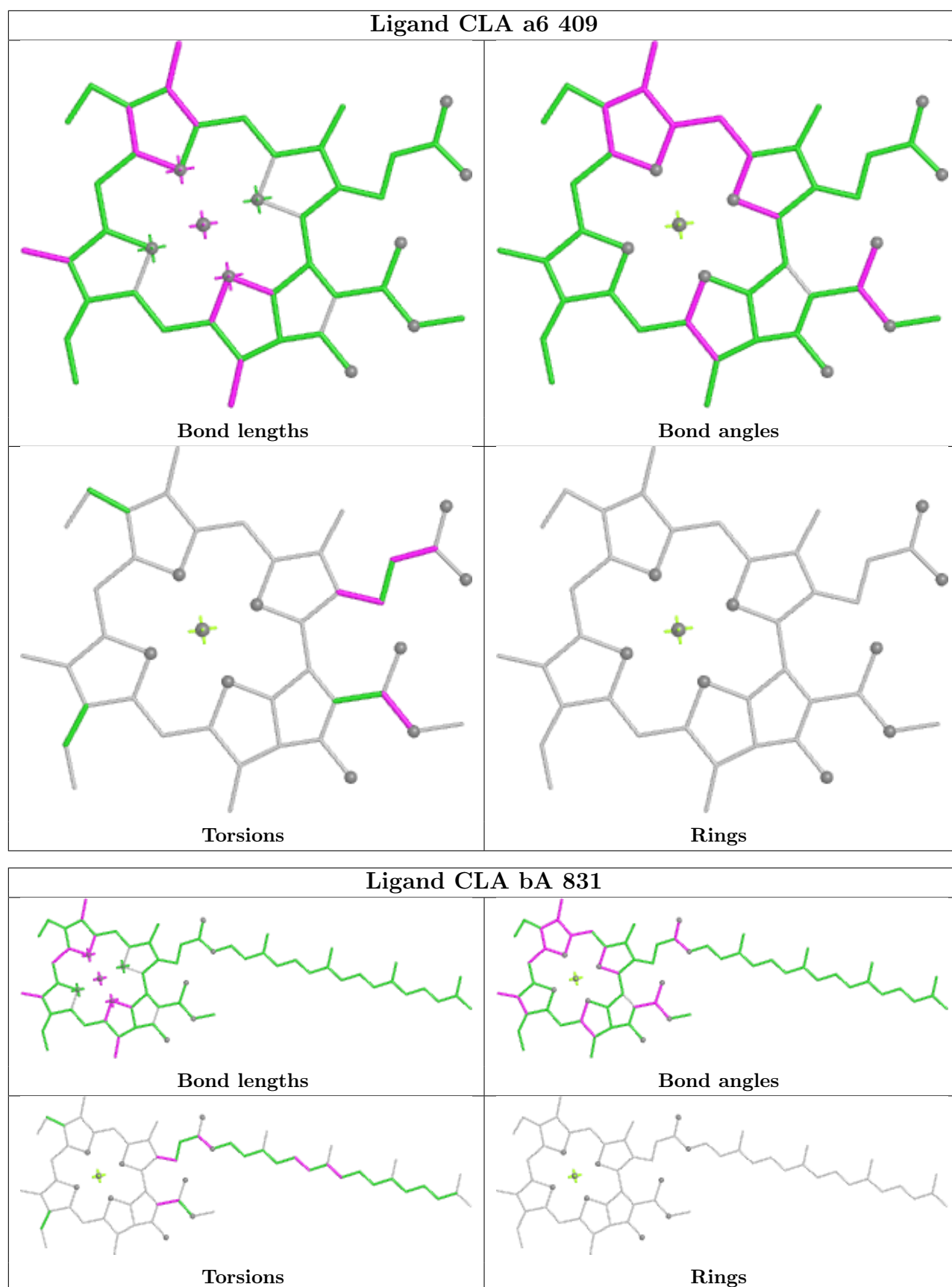


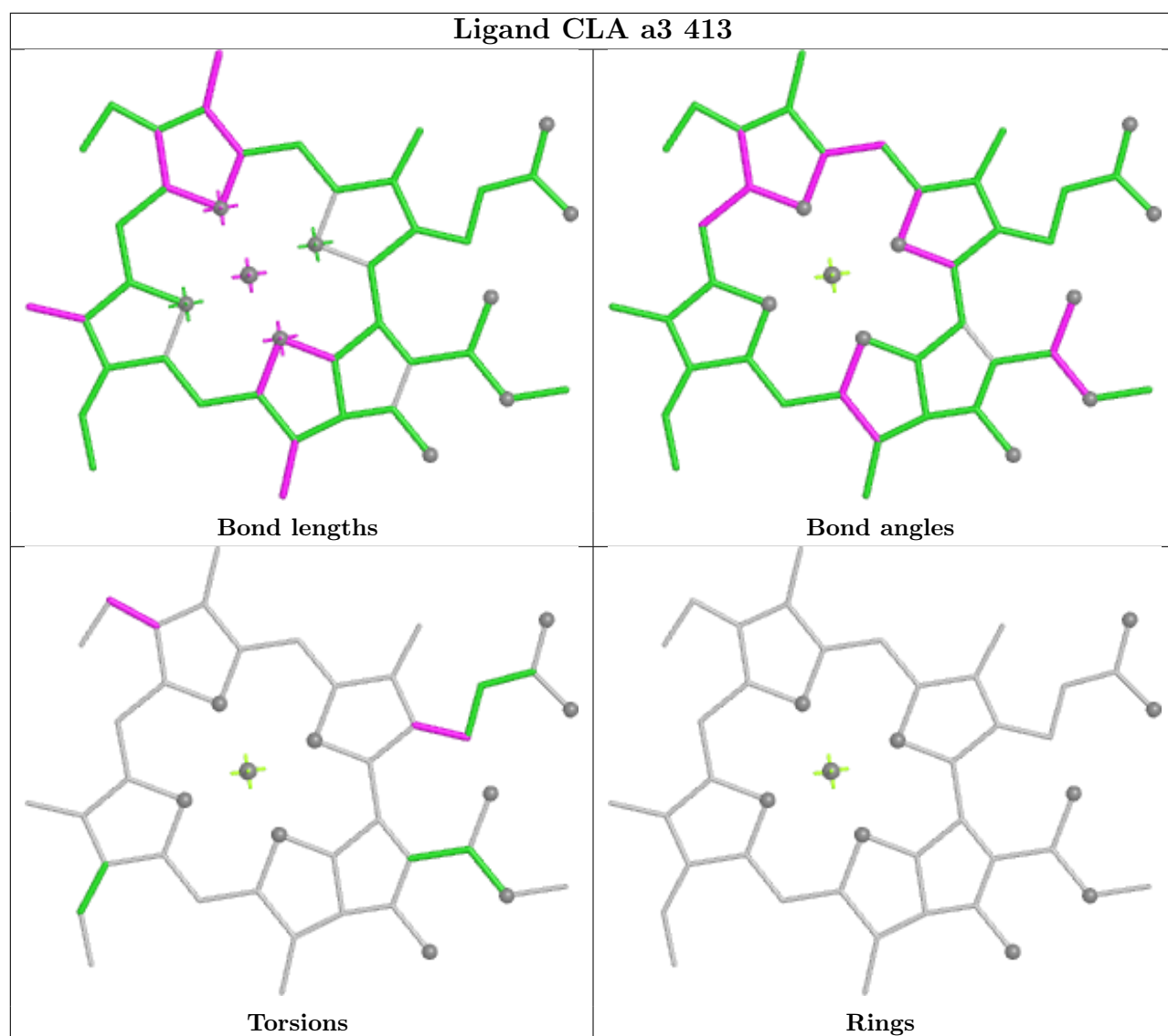
Ligand CLA a5 403

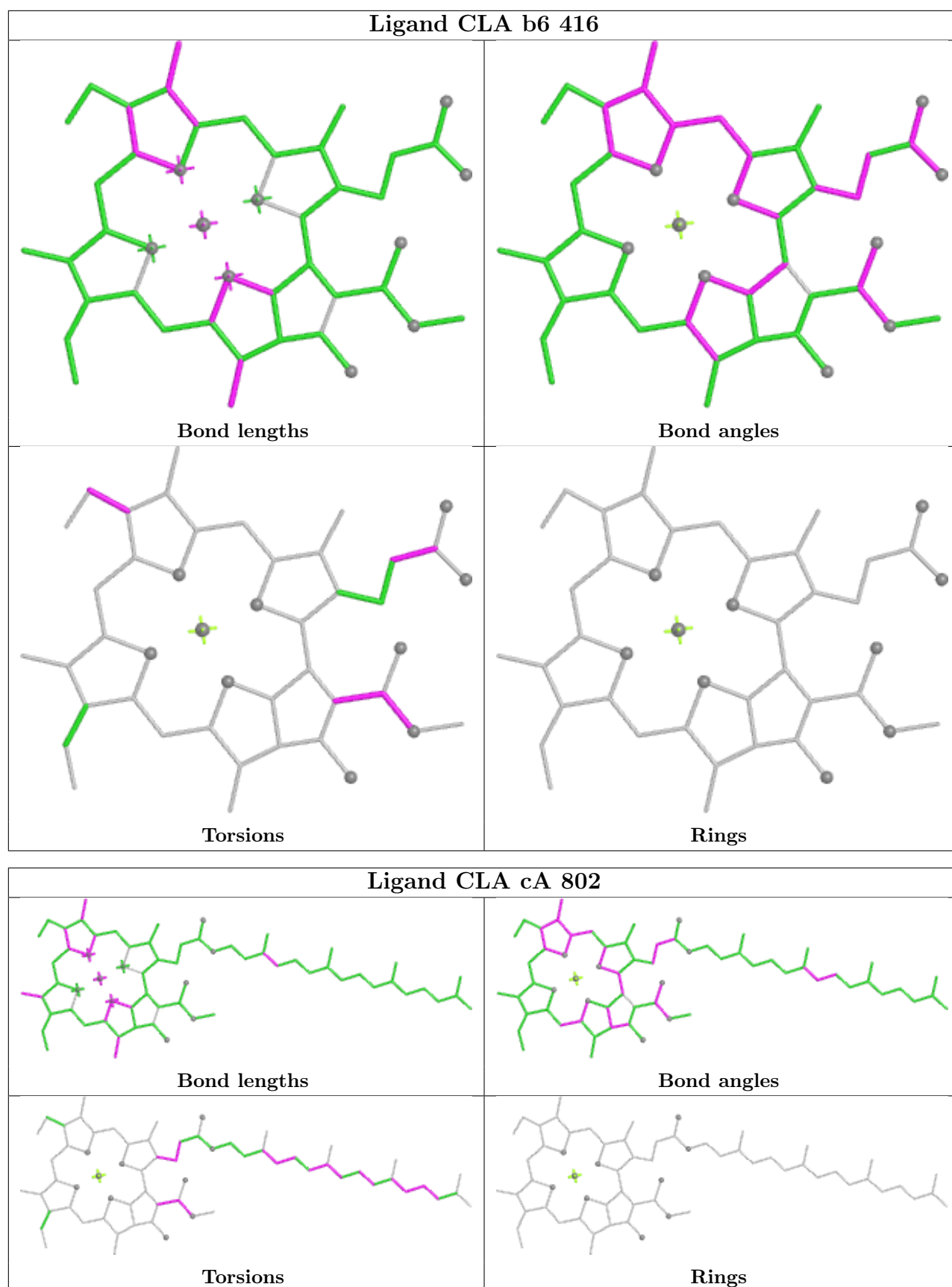


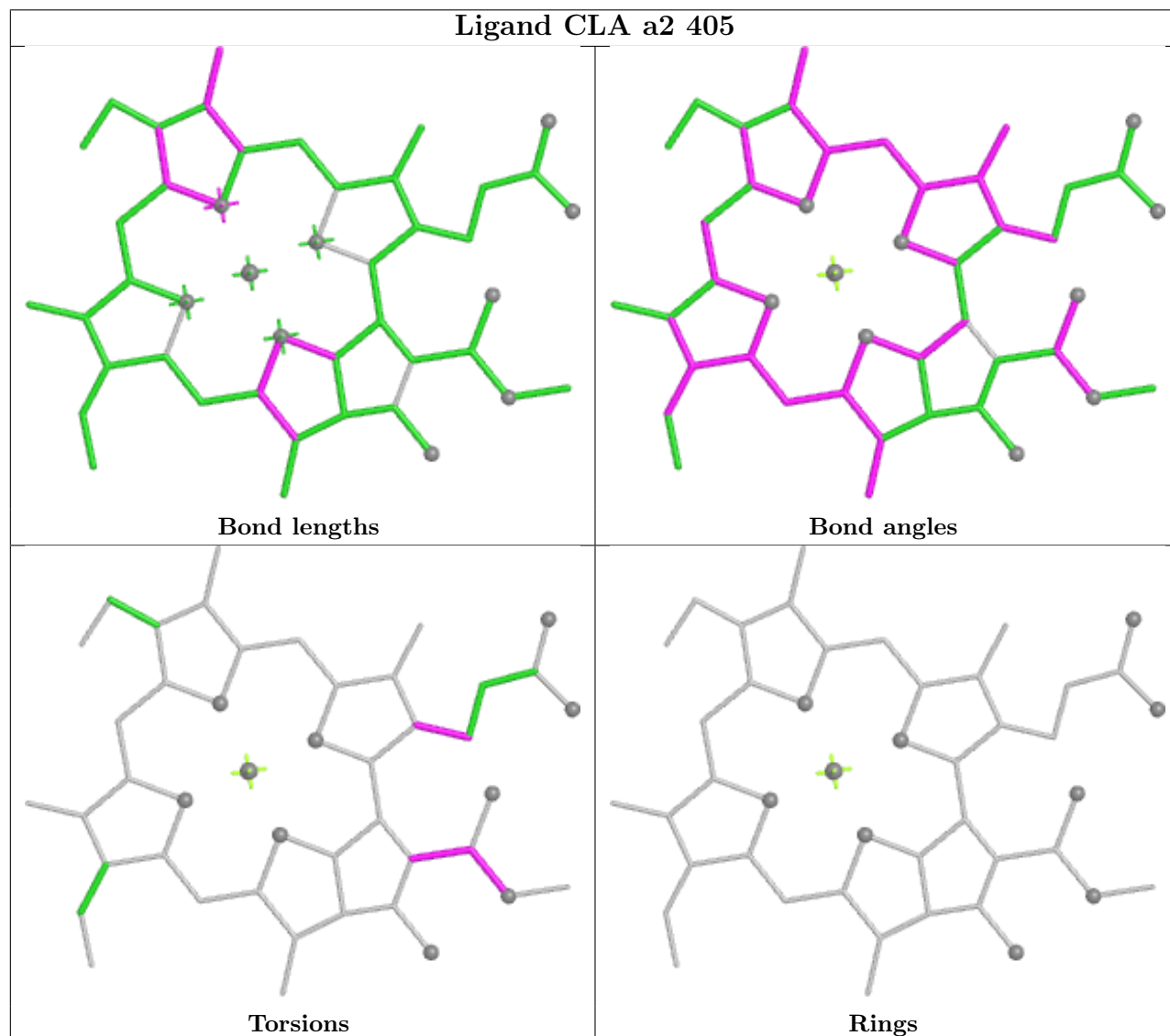
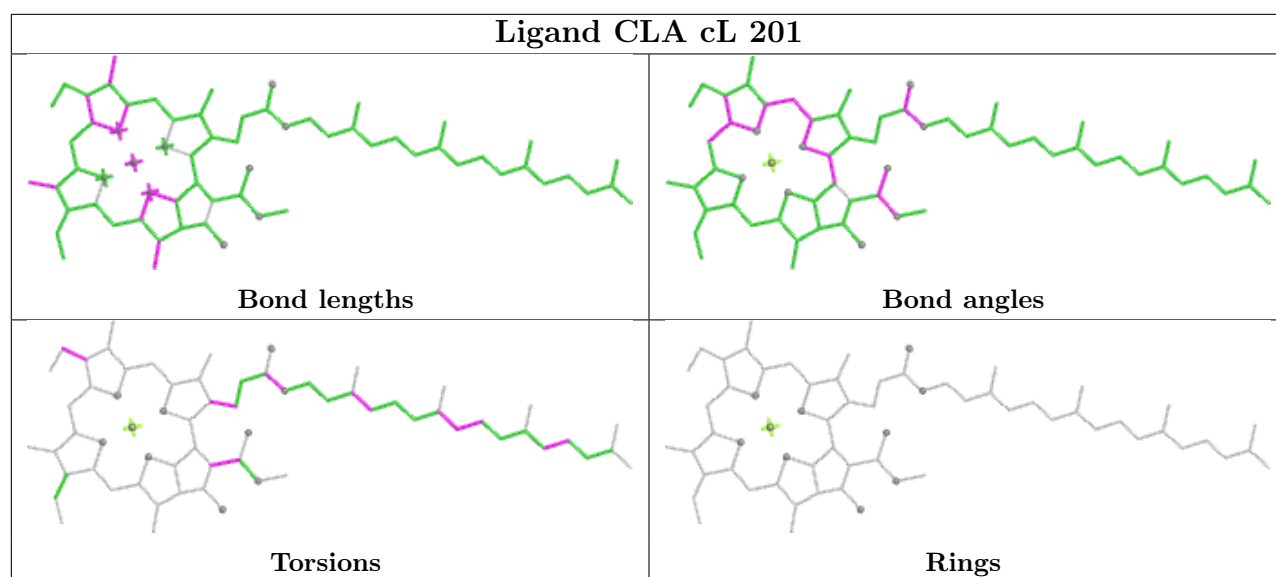


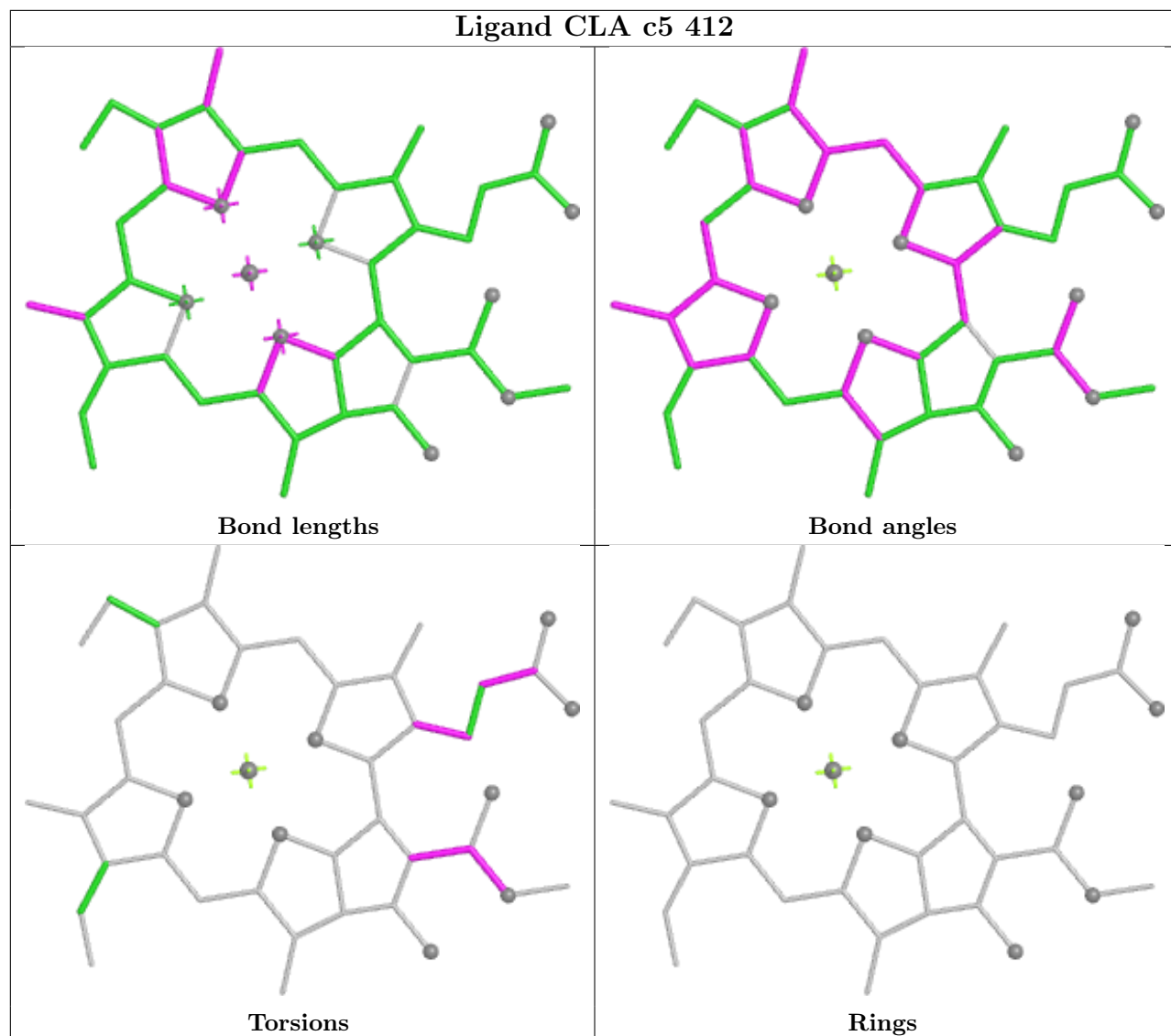


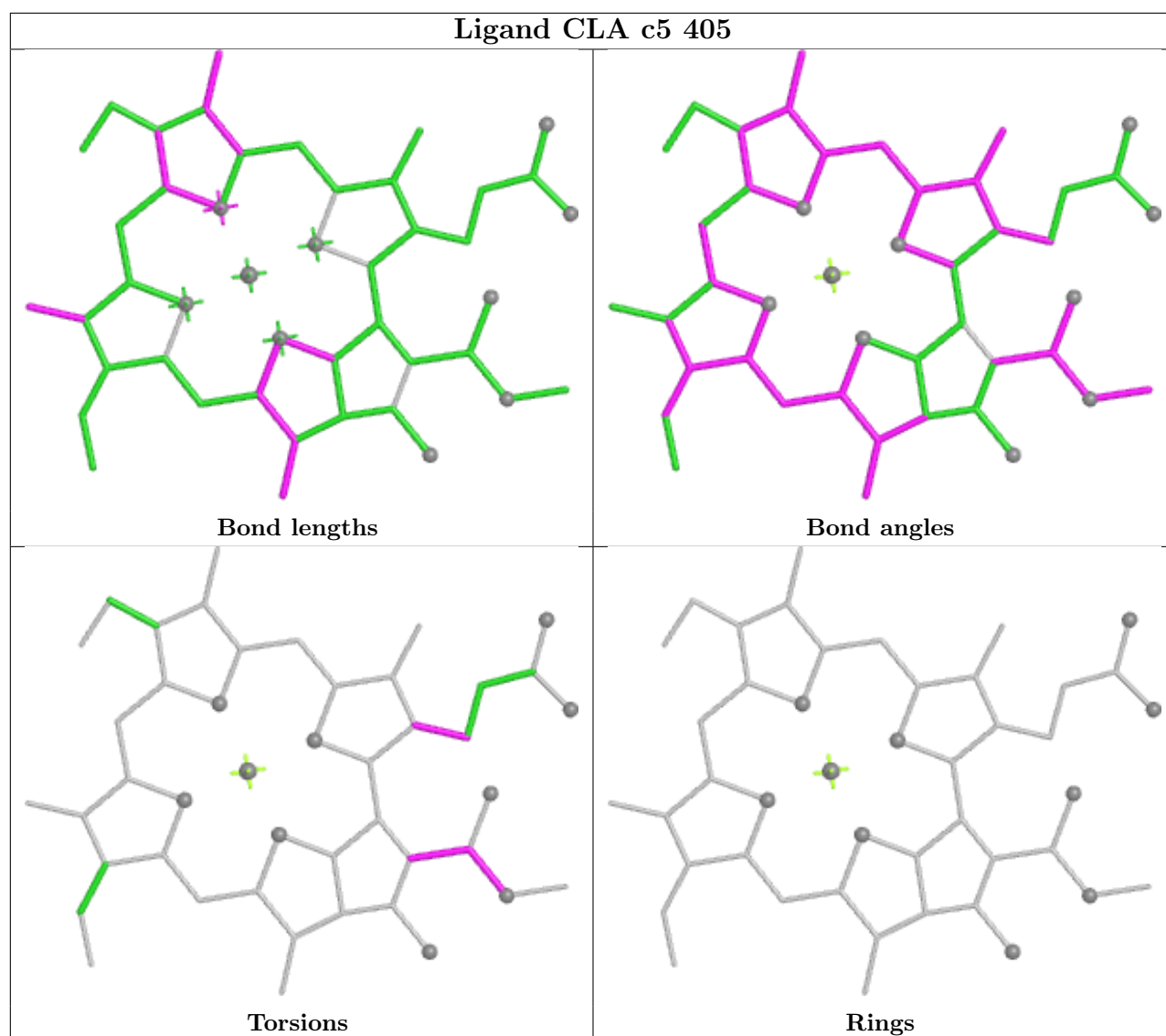


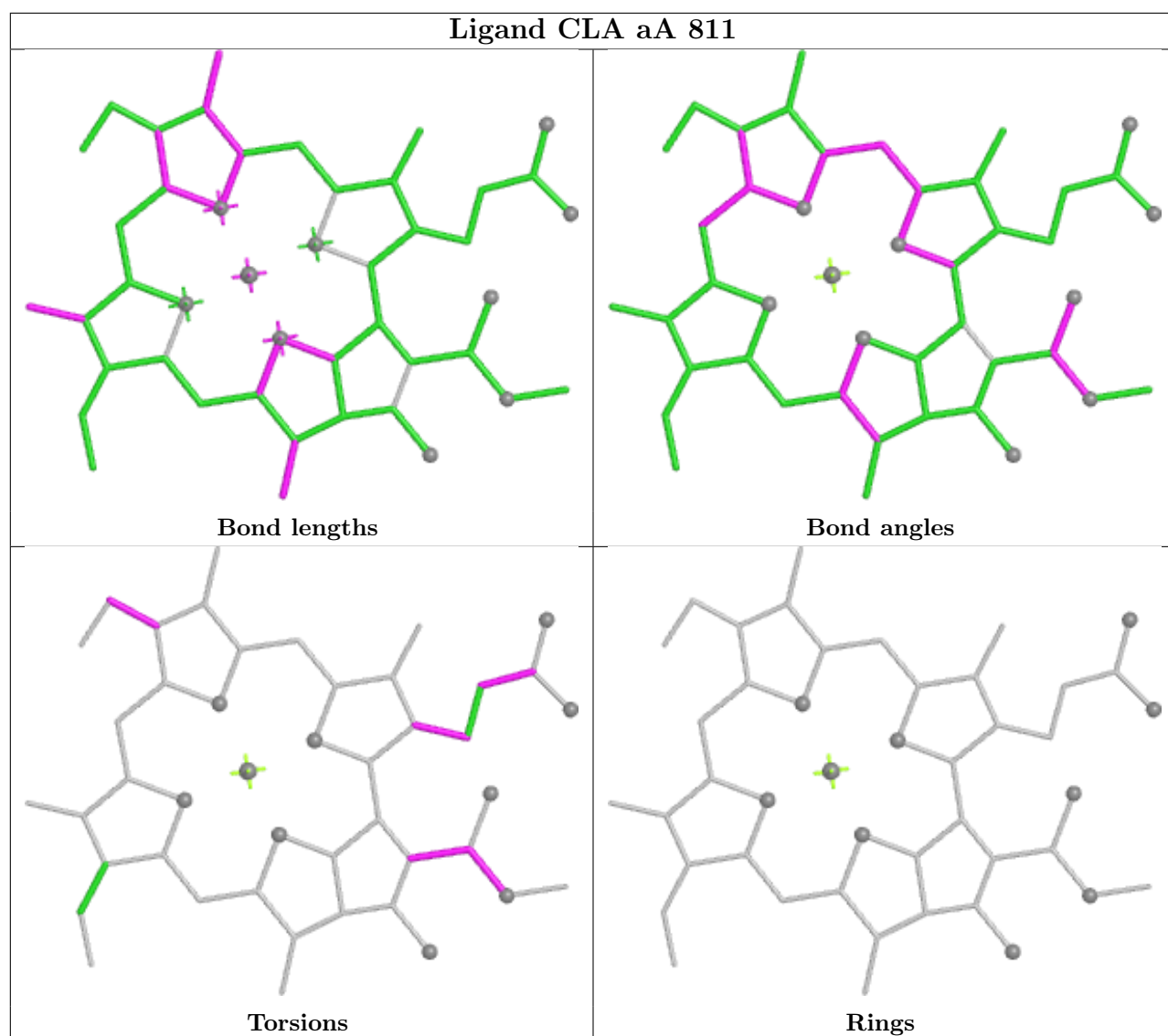


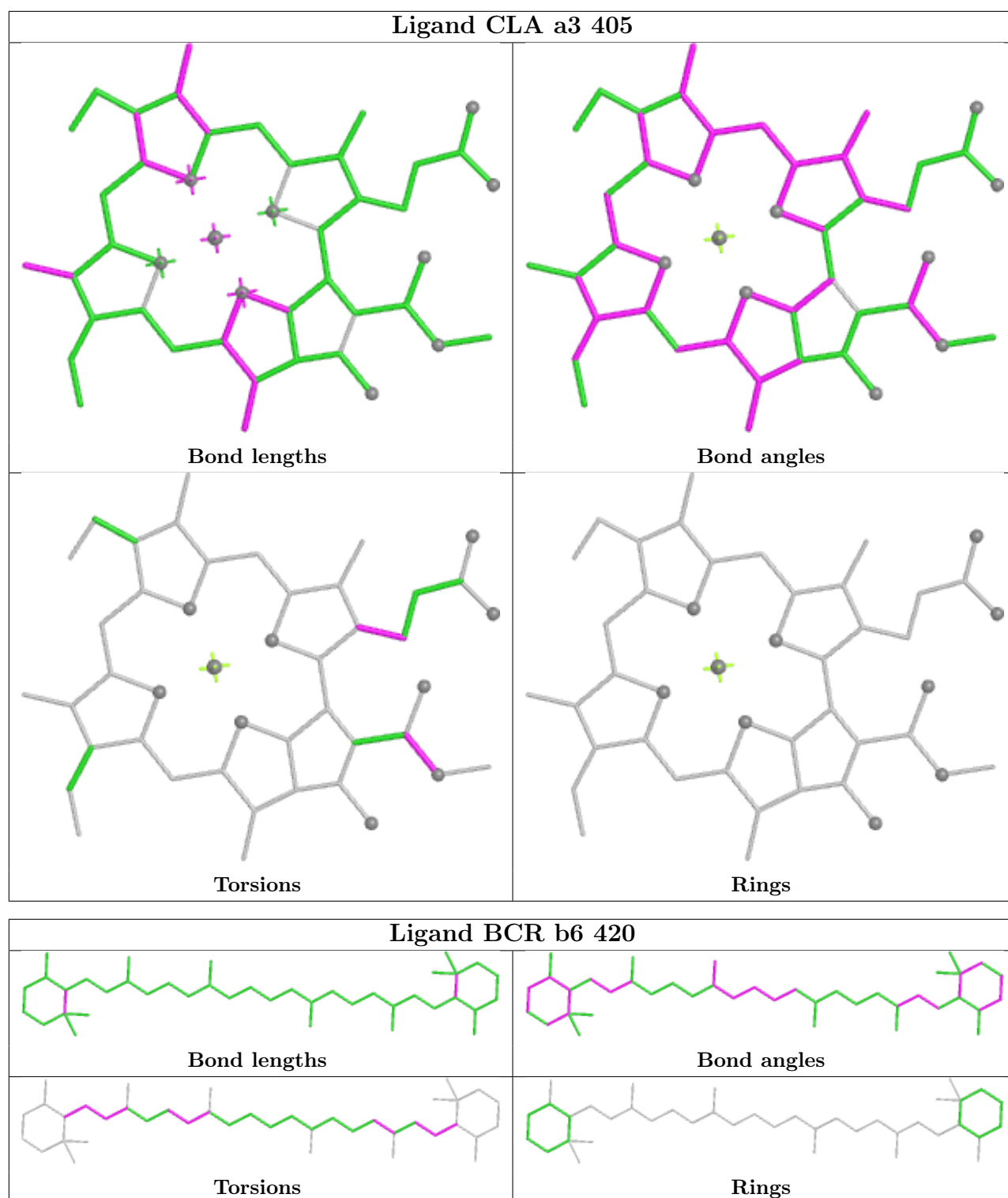


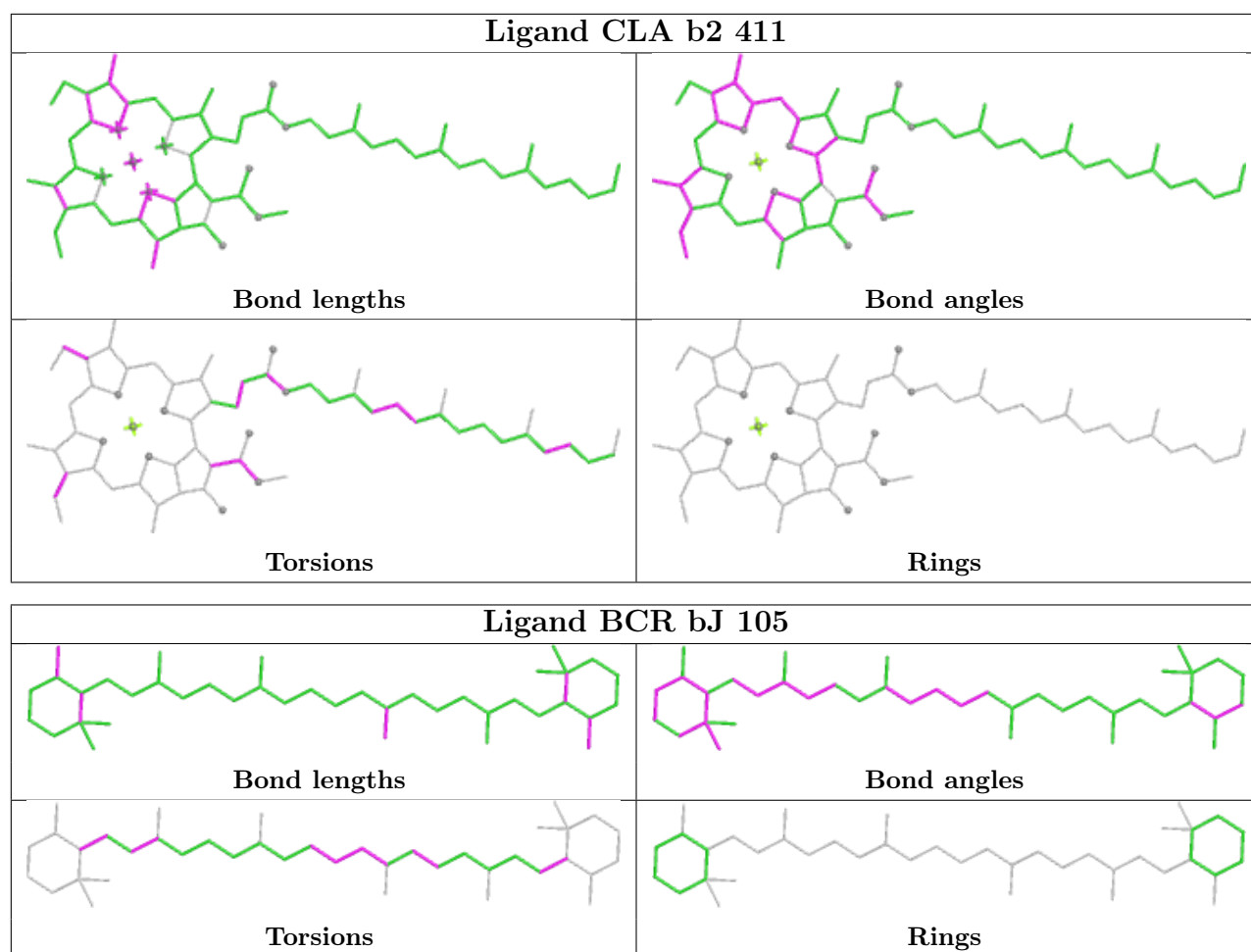




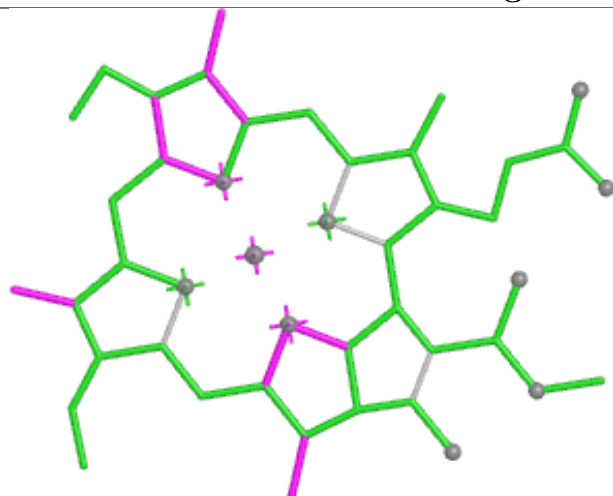




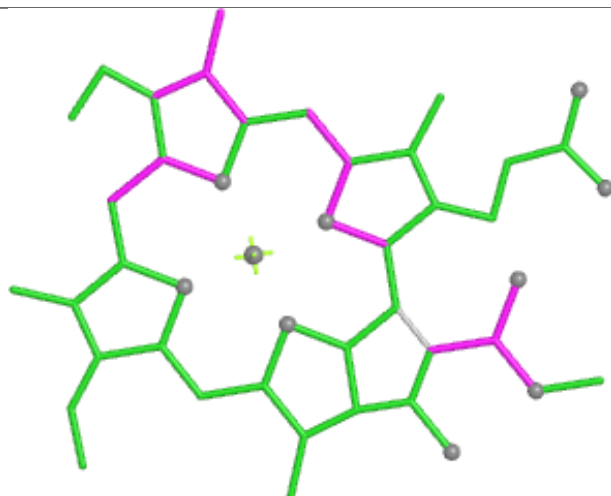




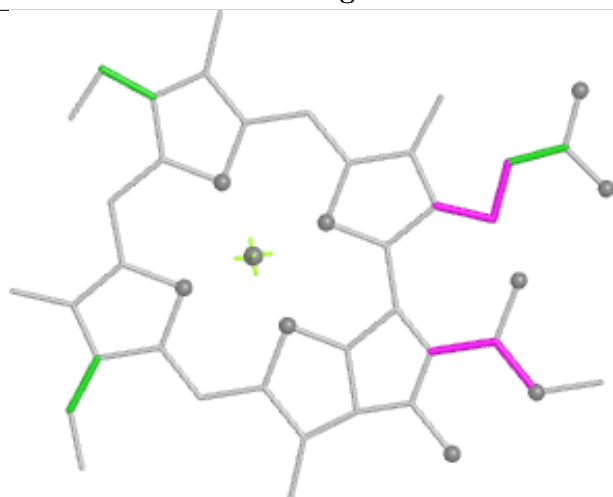
Ligand CLA bB 816



Bond lengths



Bond angles

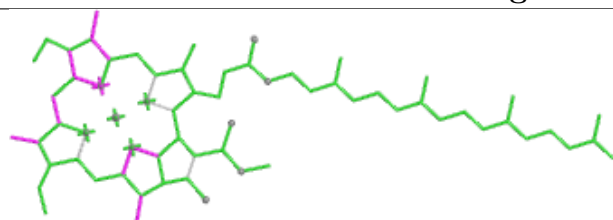


Torsions

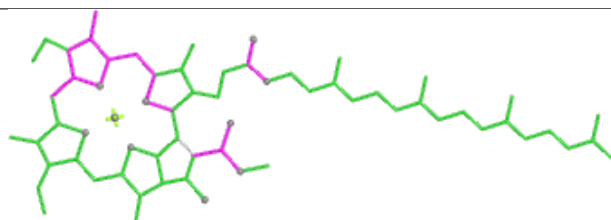


Rings

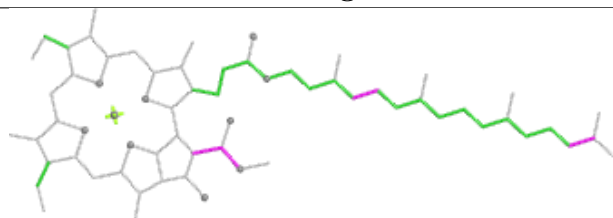
Ligand CLA a3 409



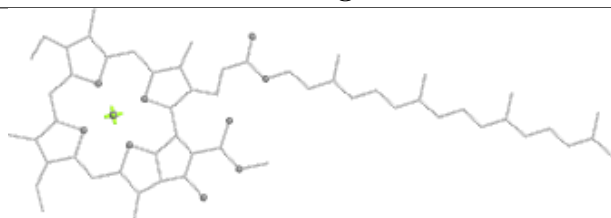
Bond lengths



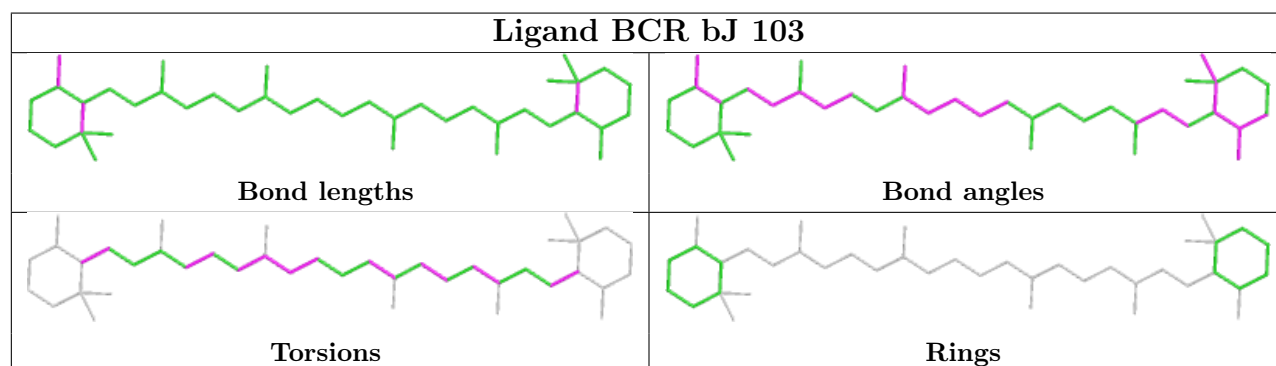
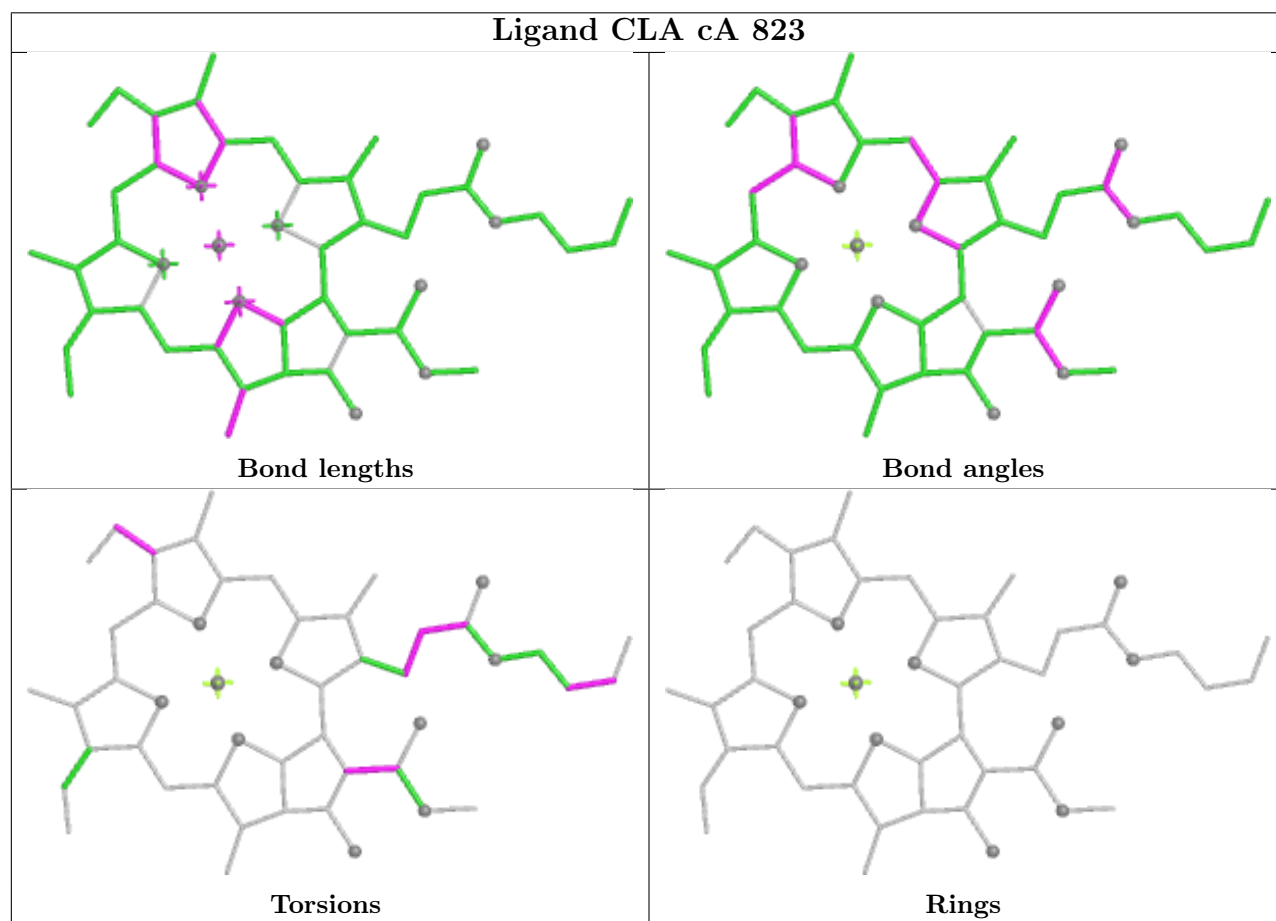
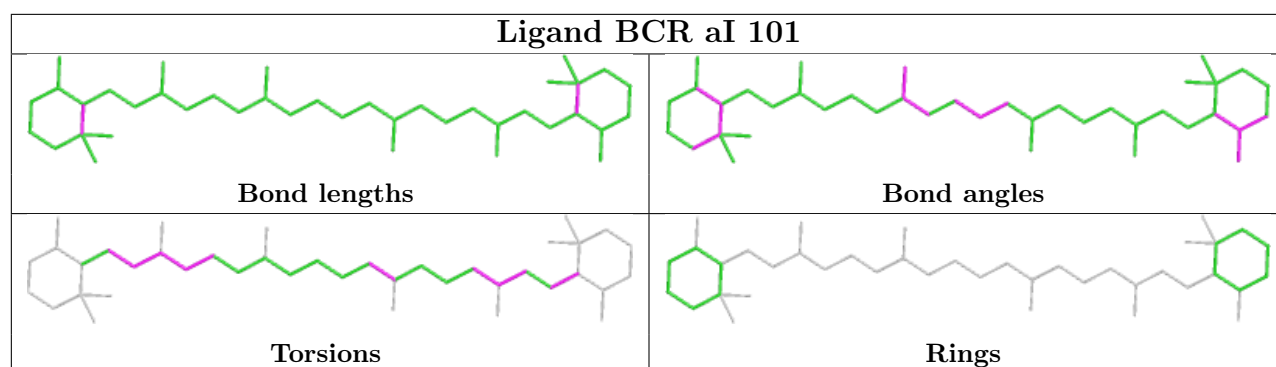
Bond angles

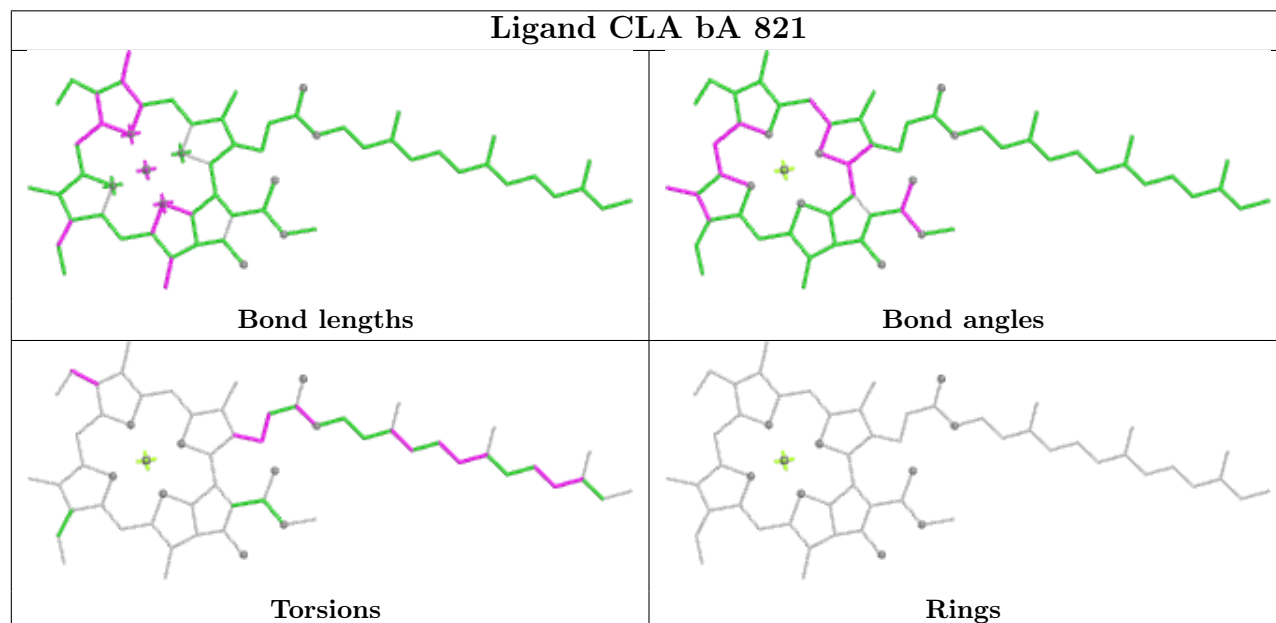
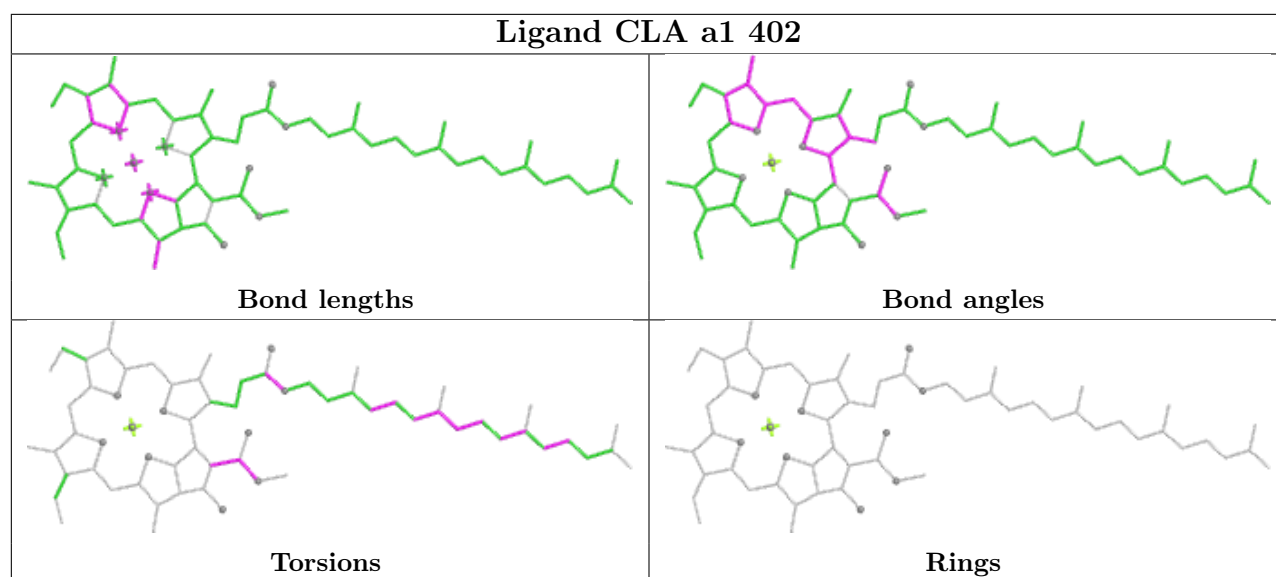


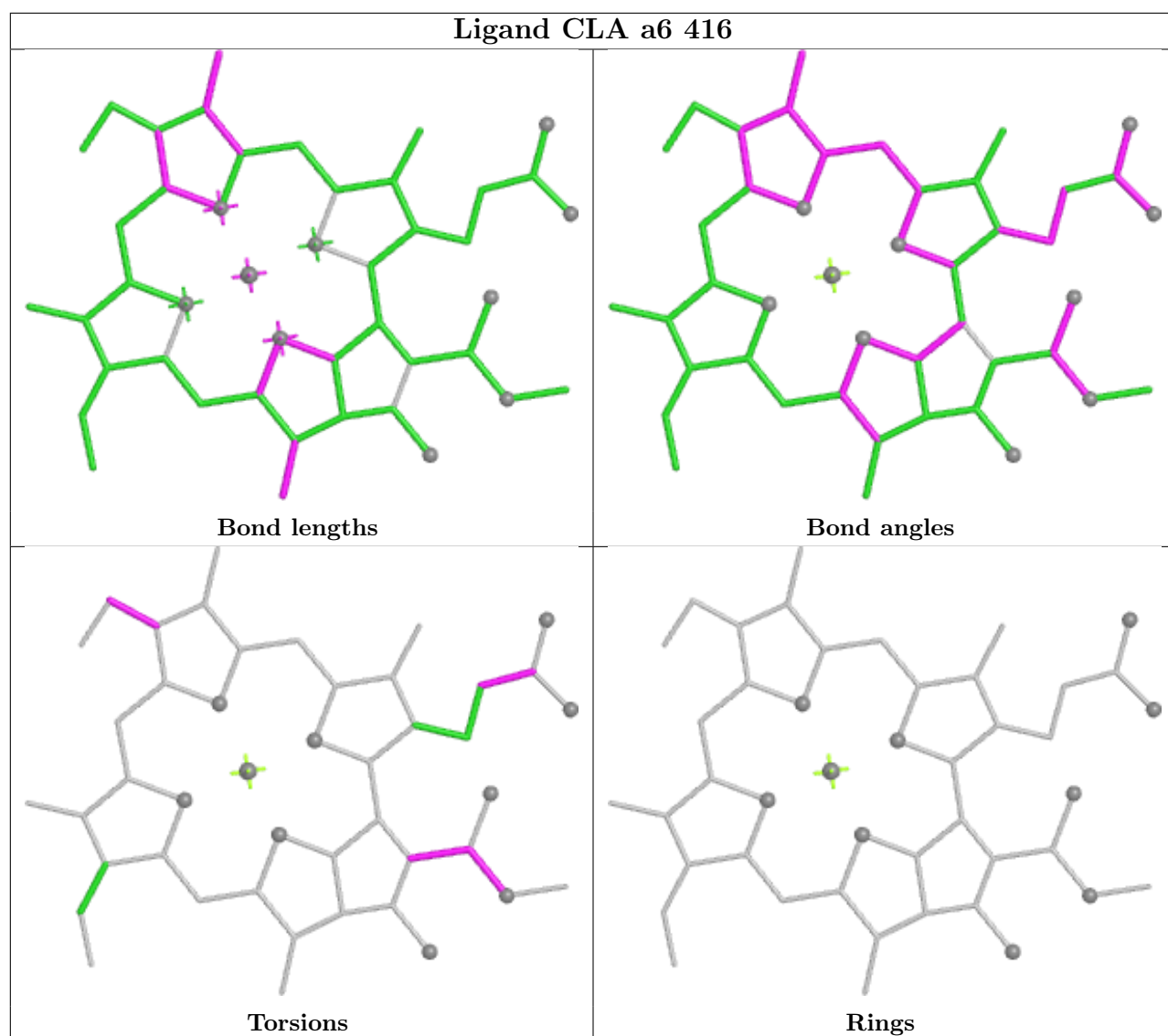
Torsions

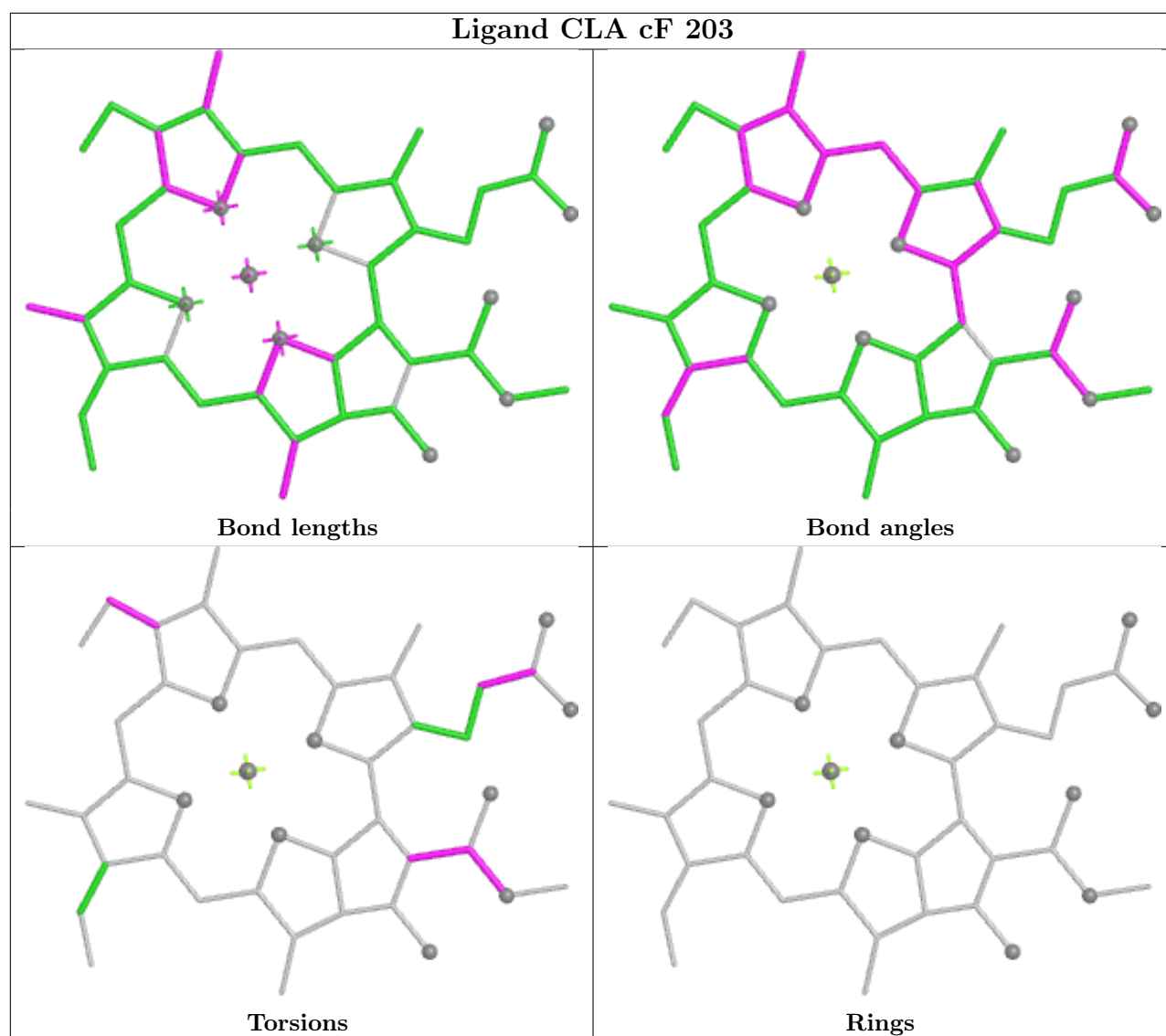


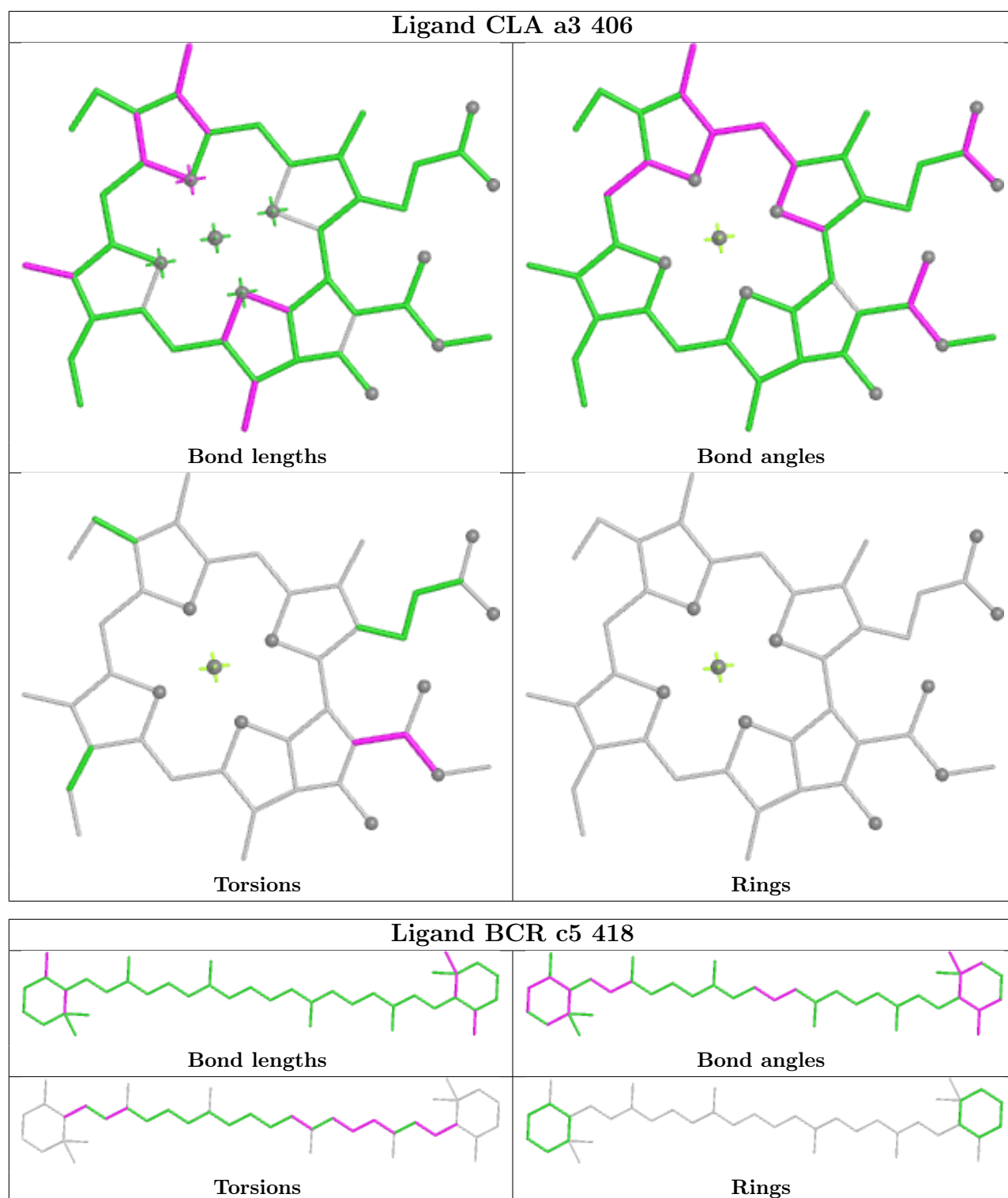
Rings

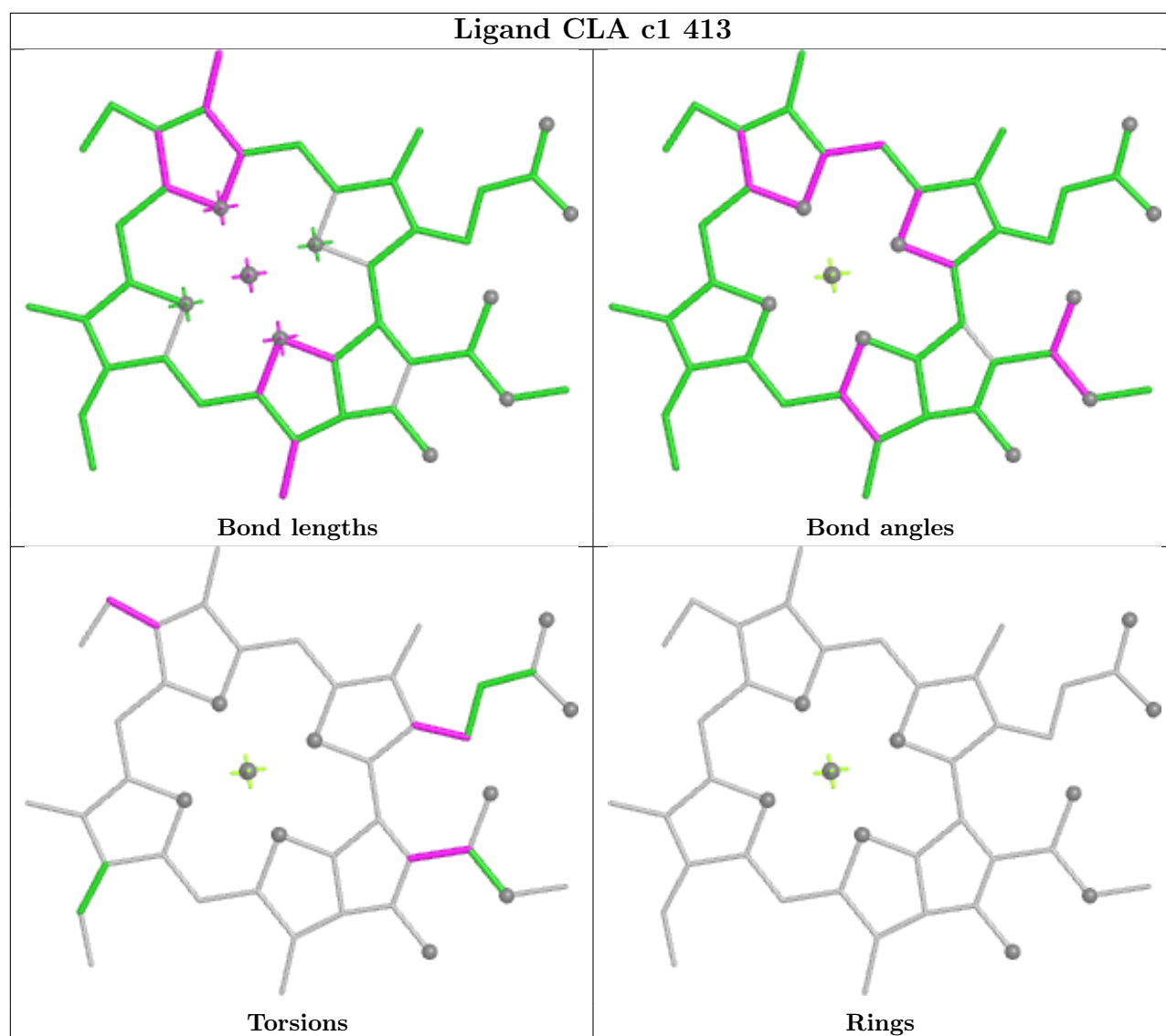


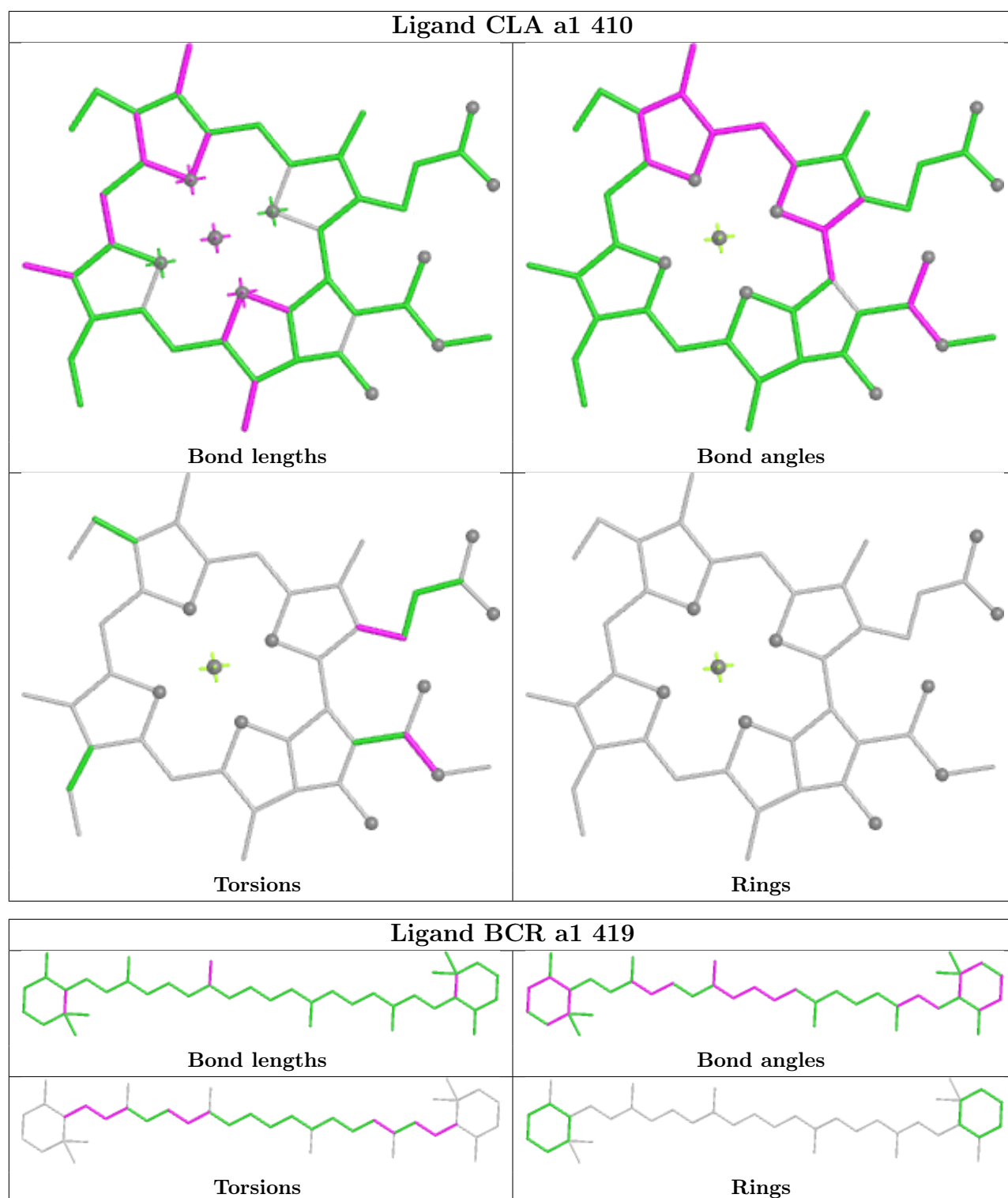


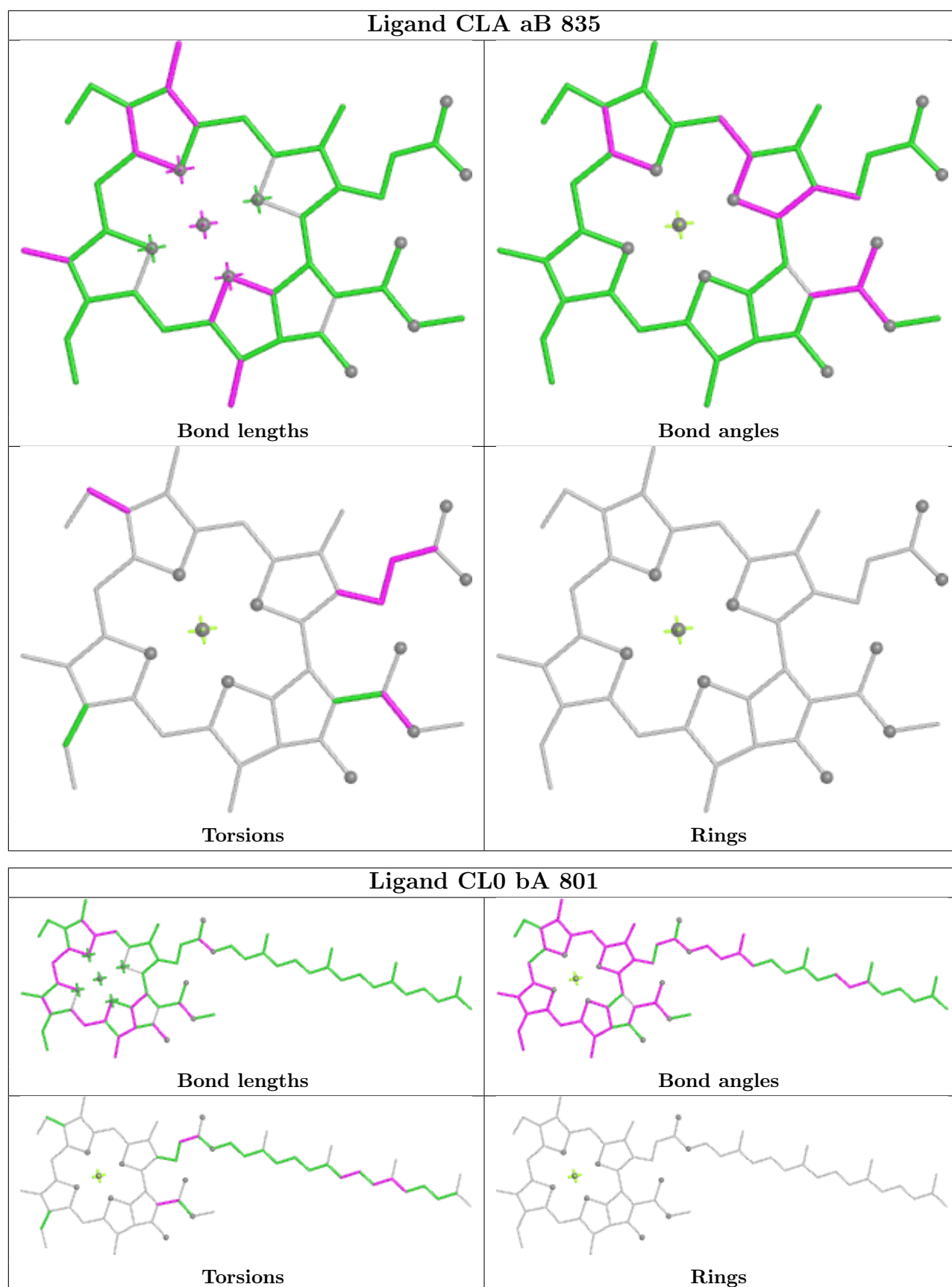


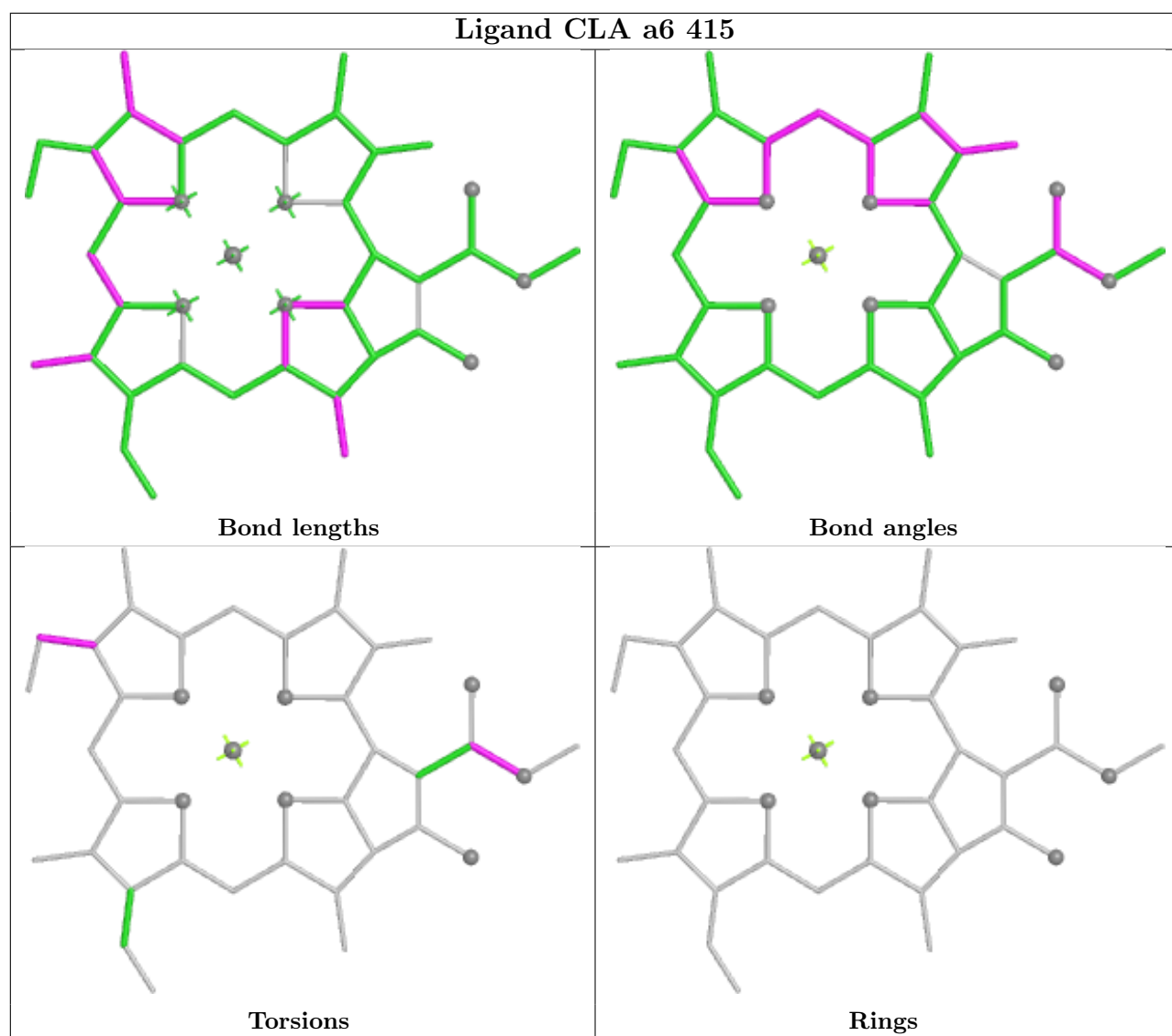


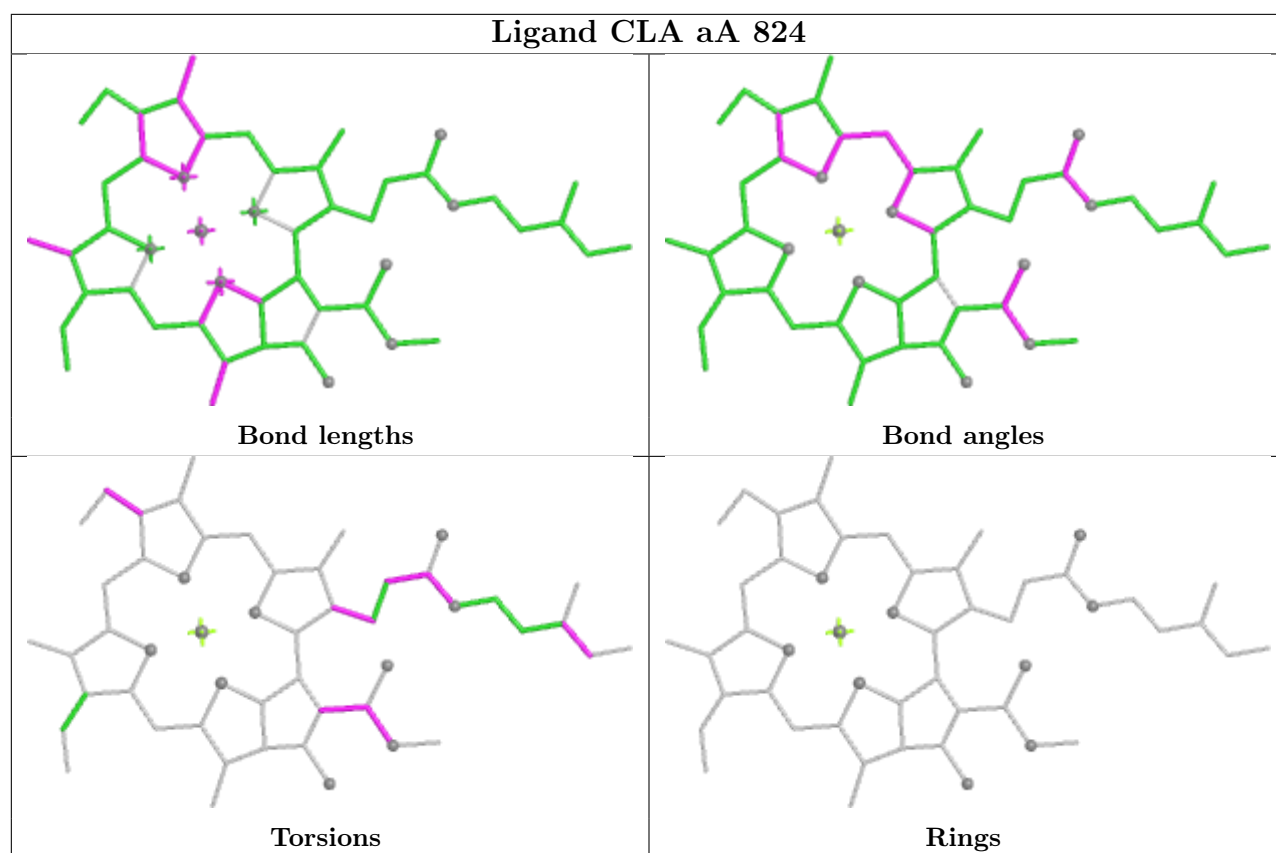


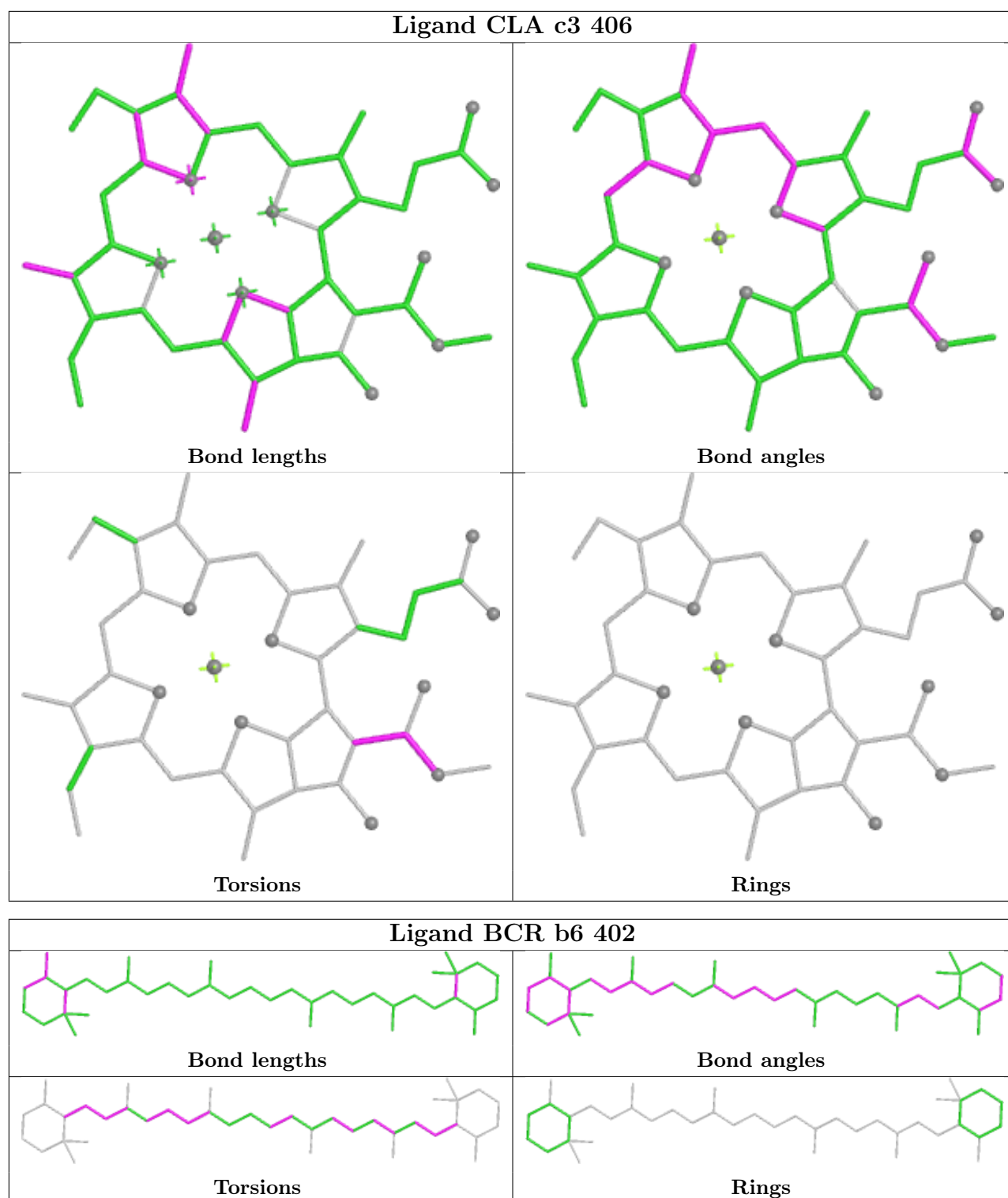


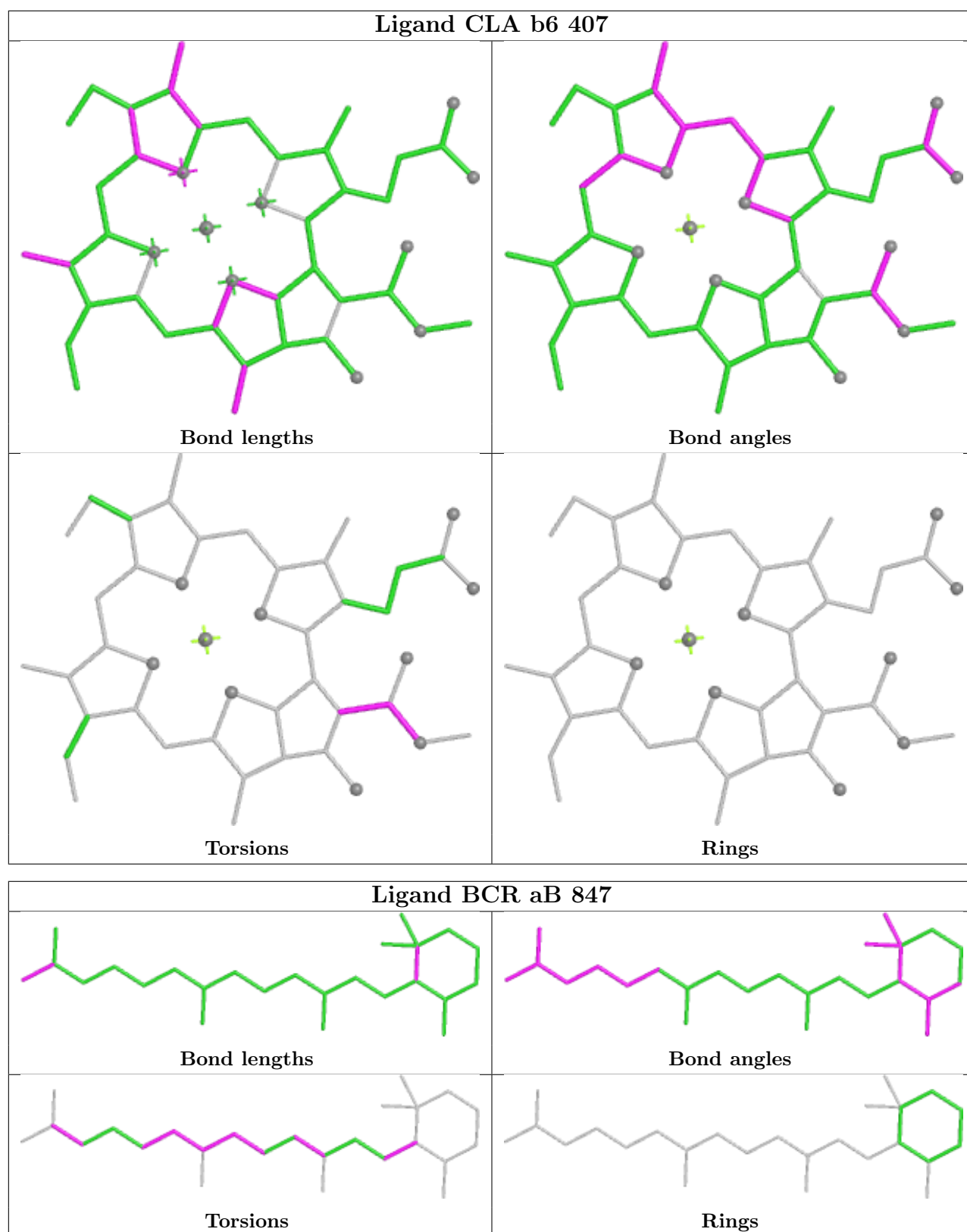


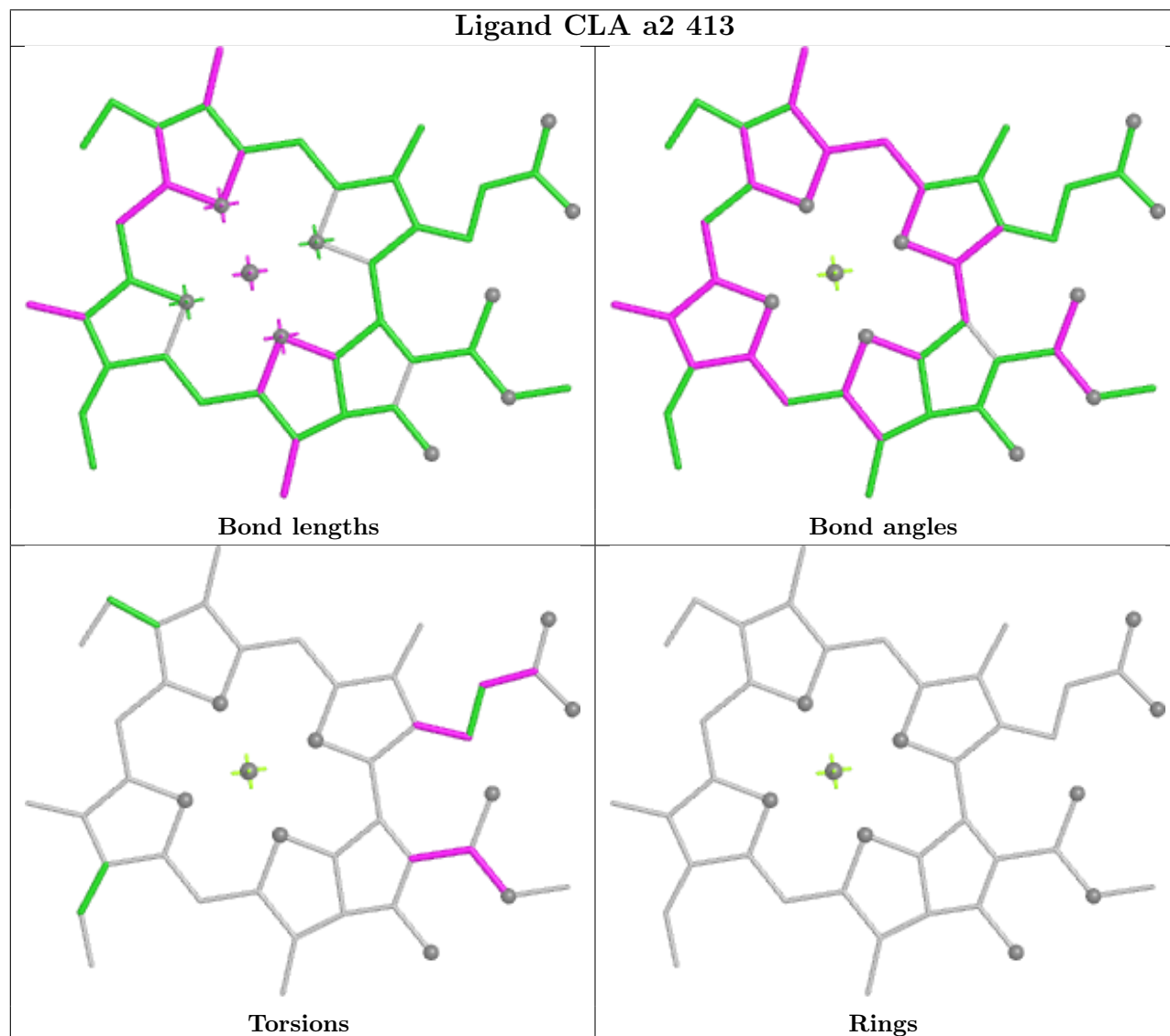
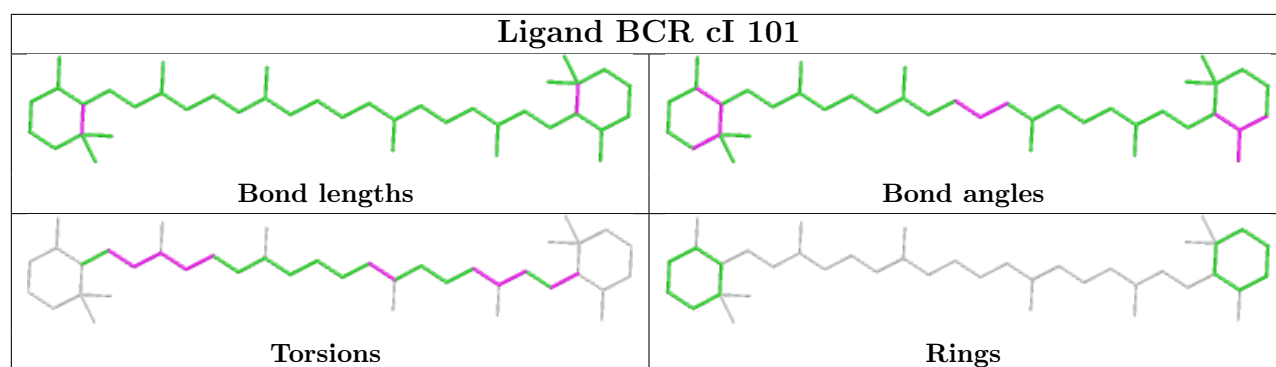


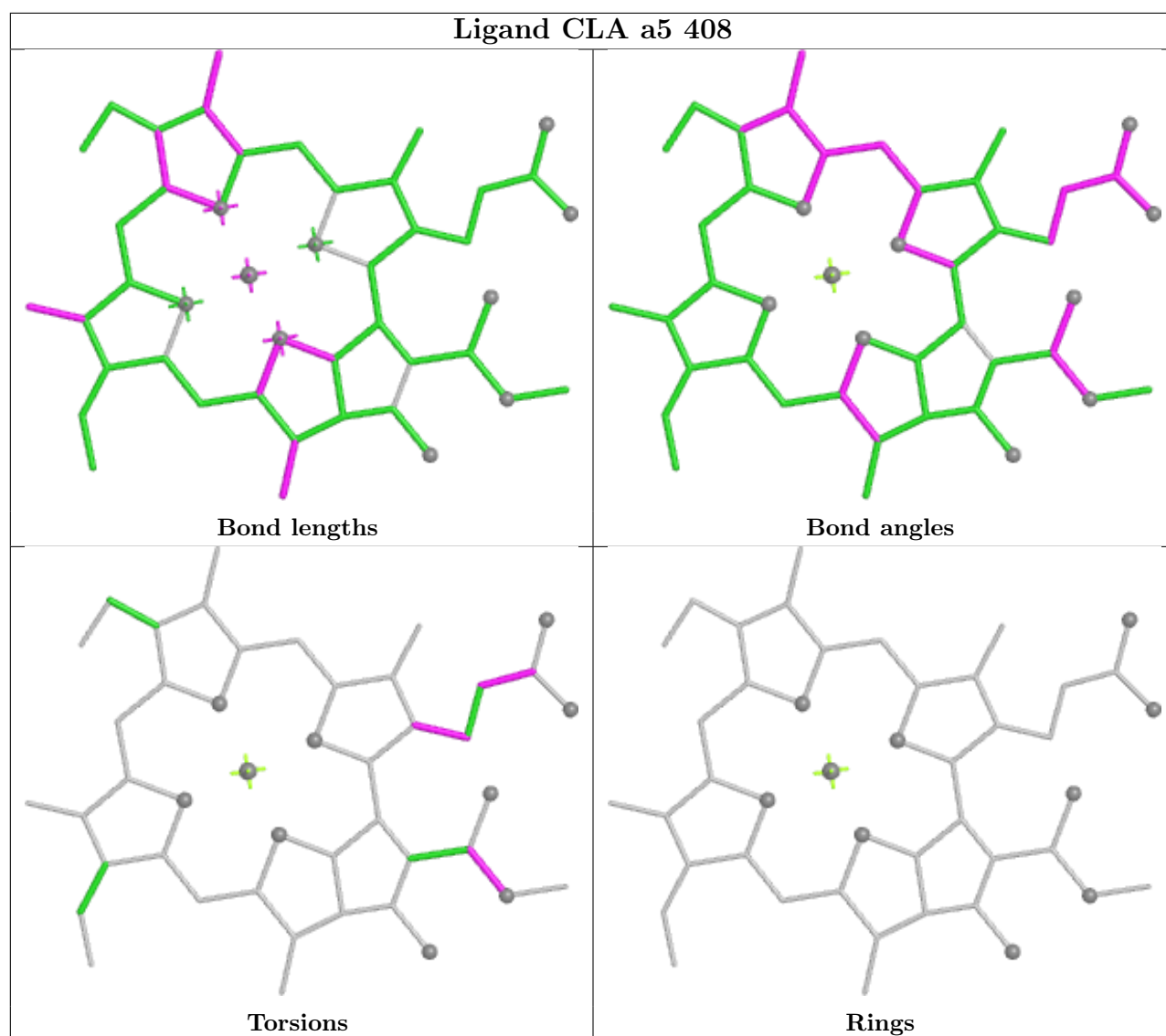


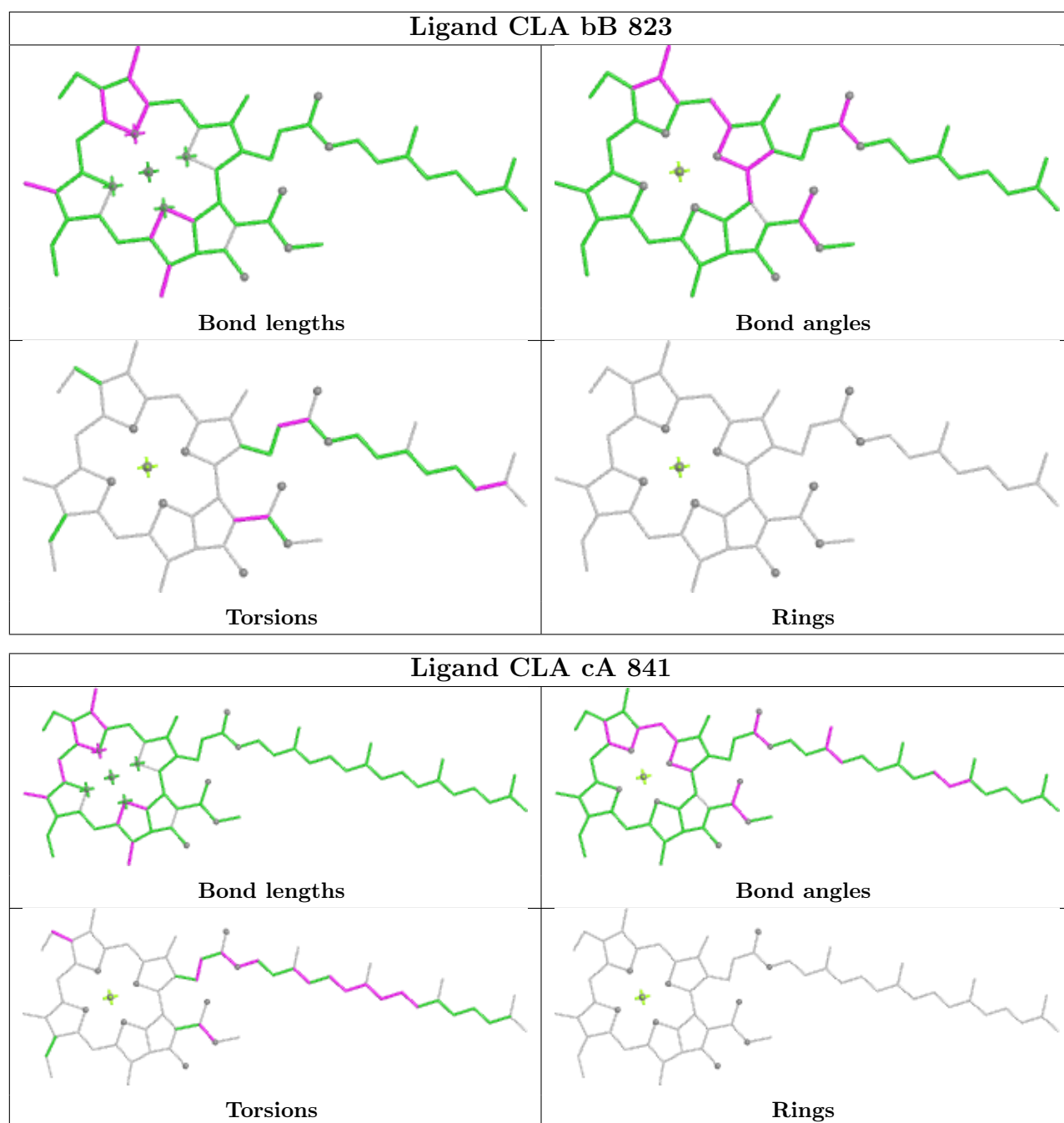


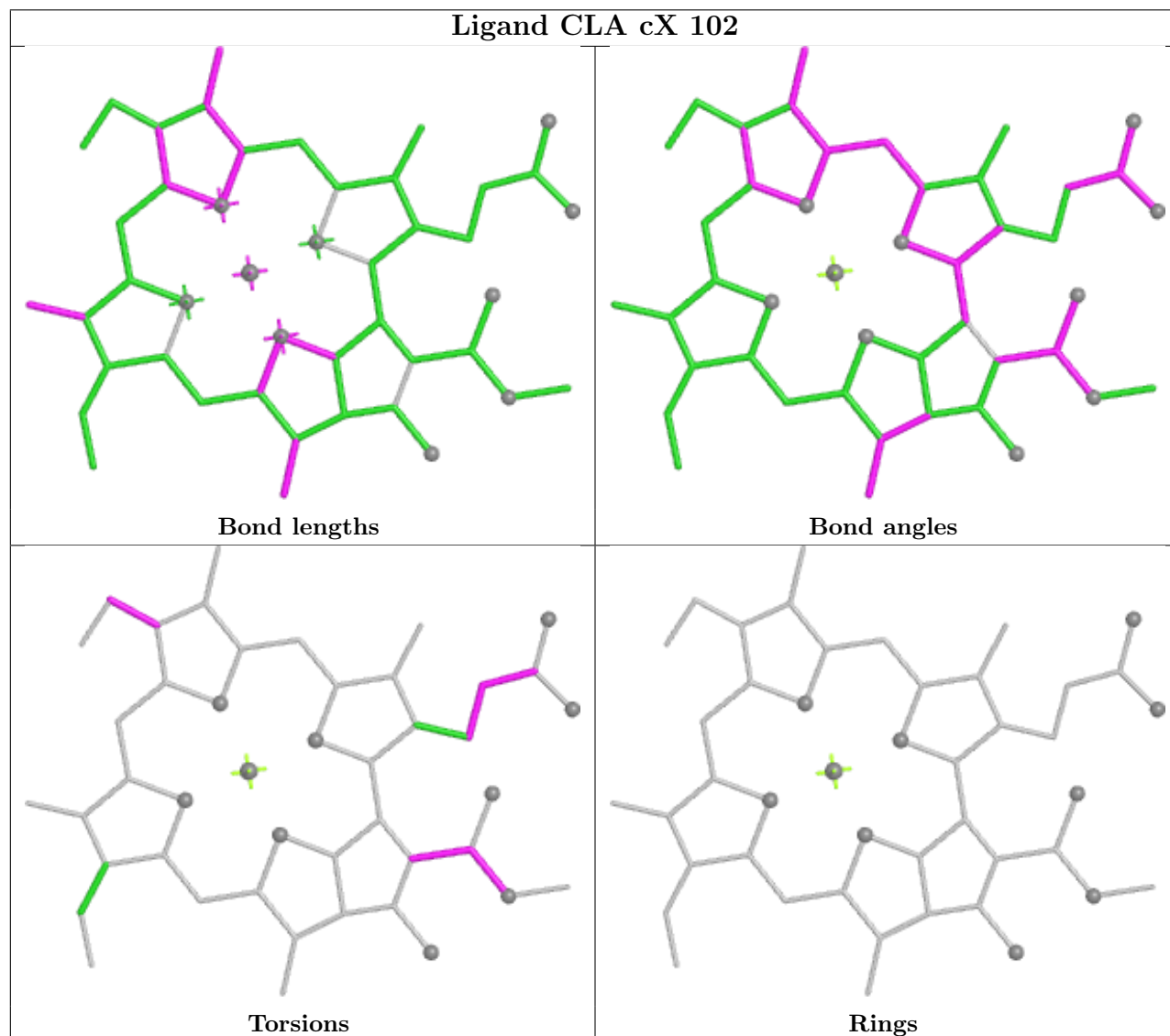
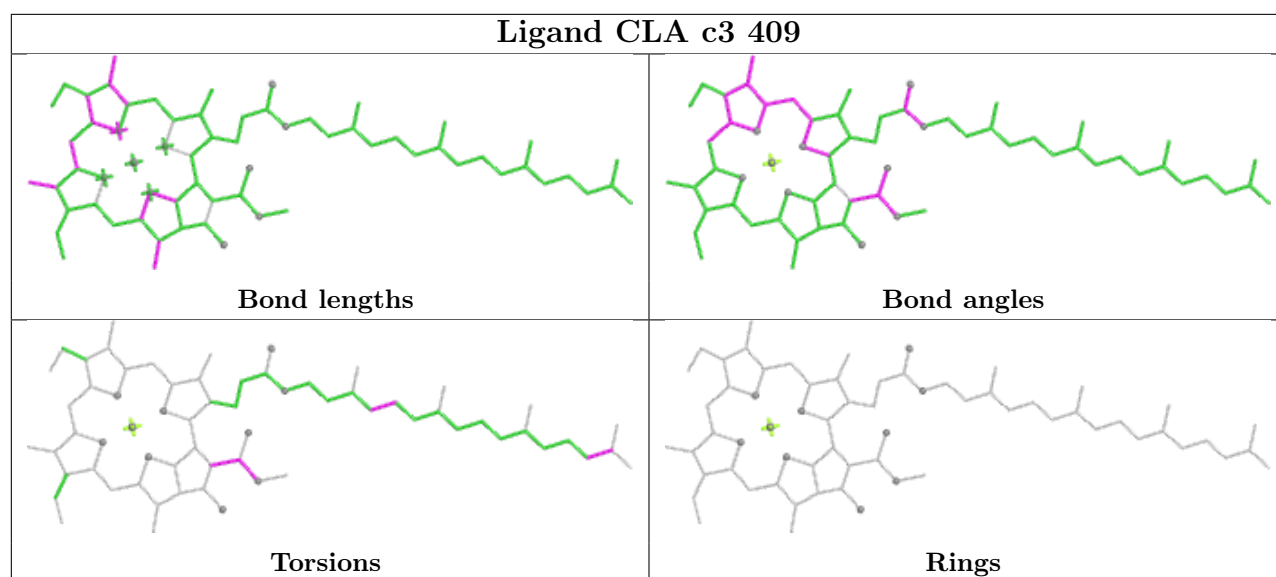


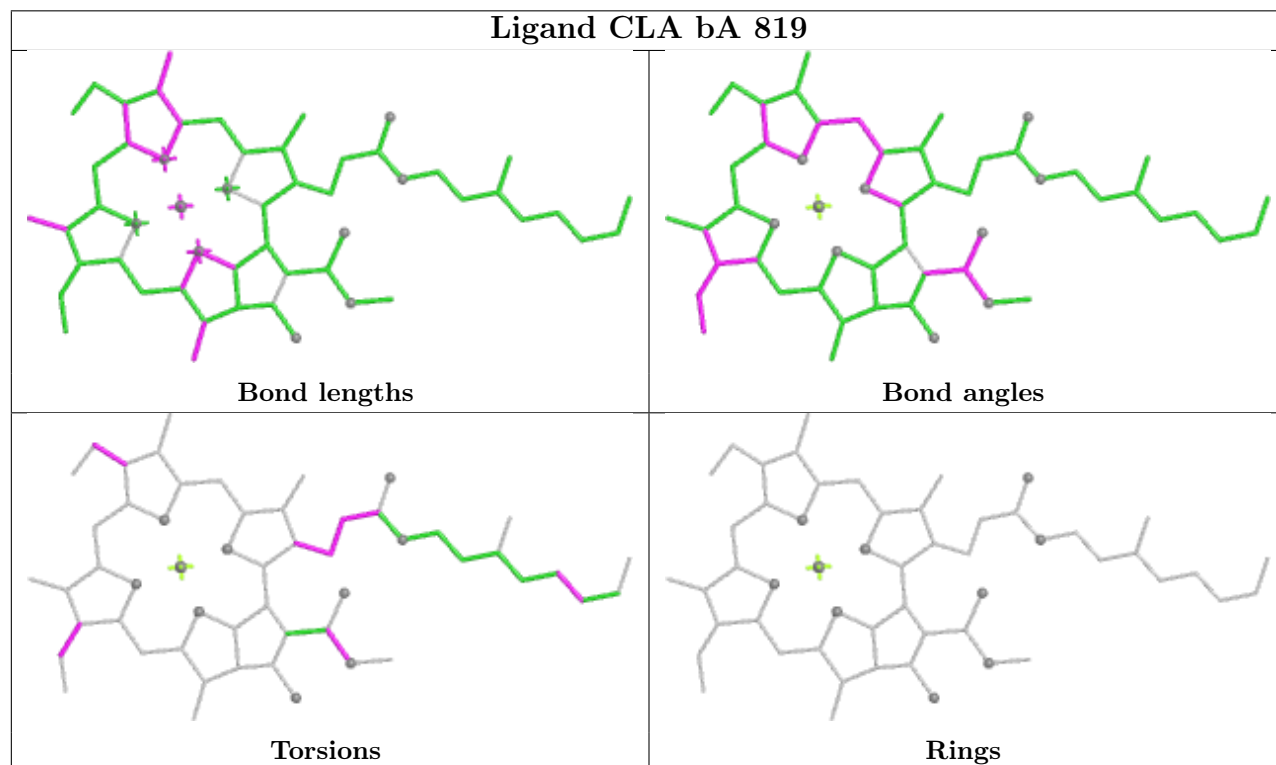
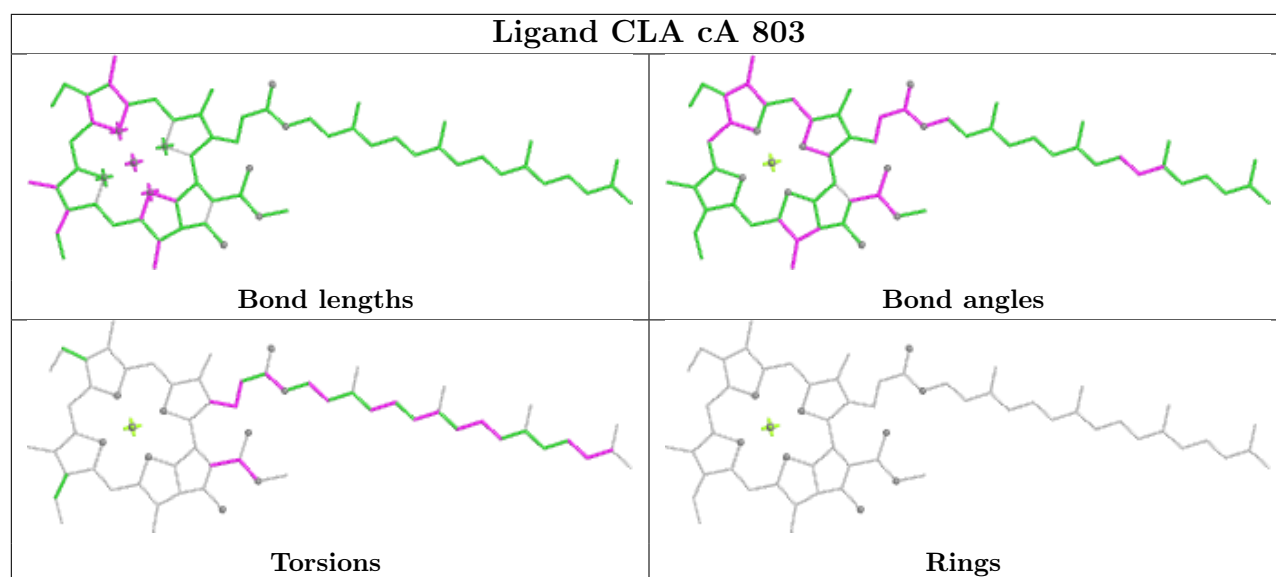


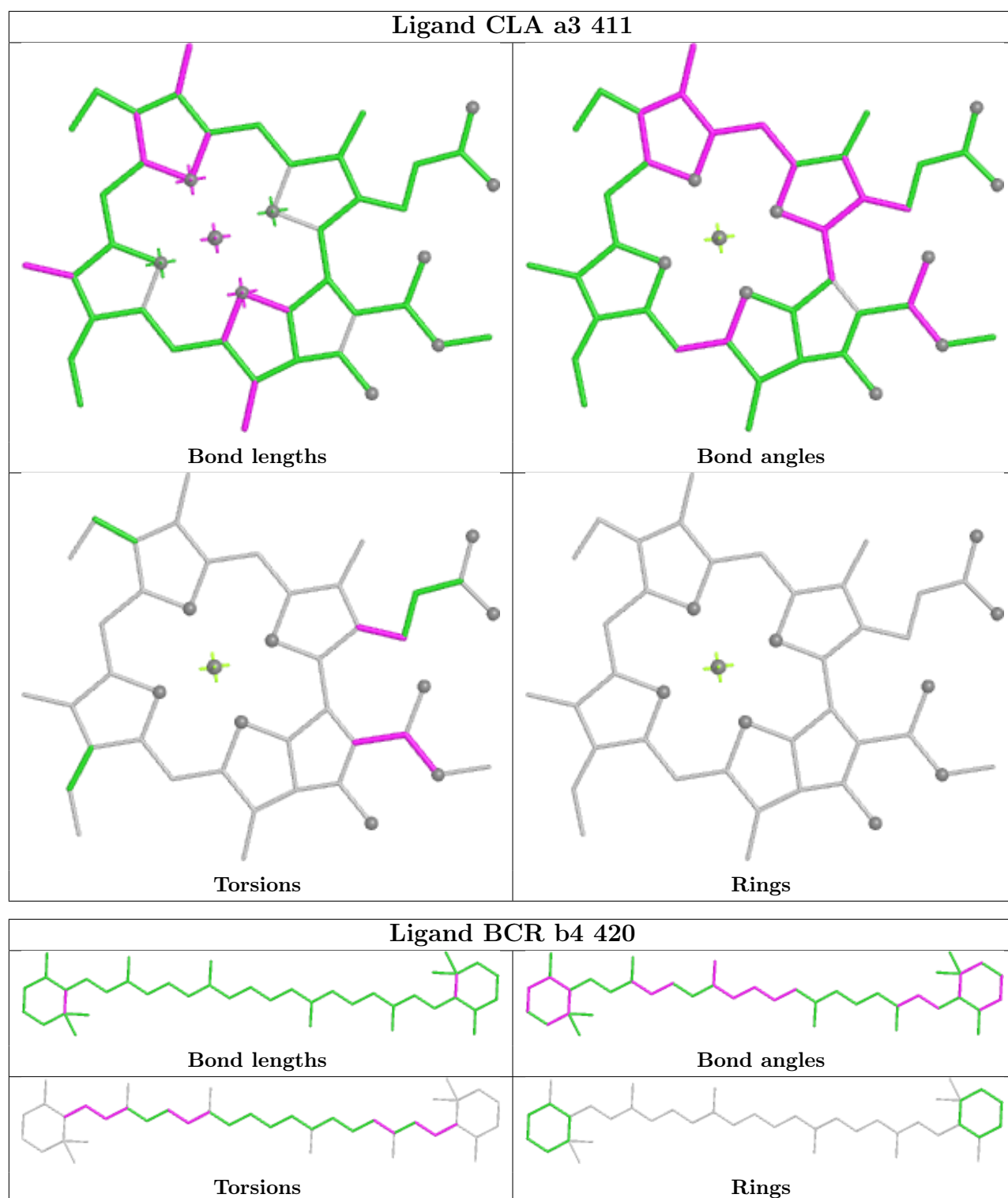


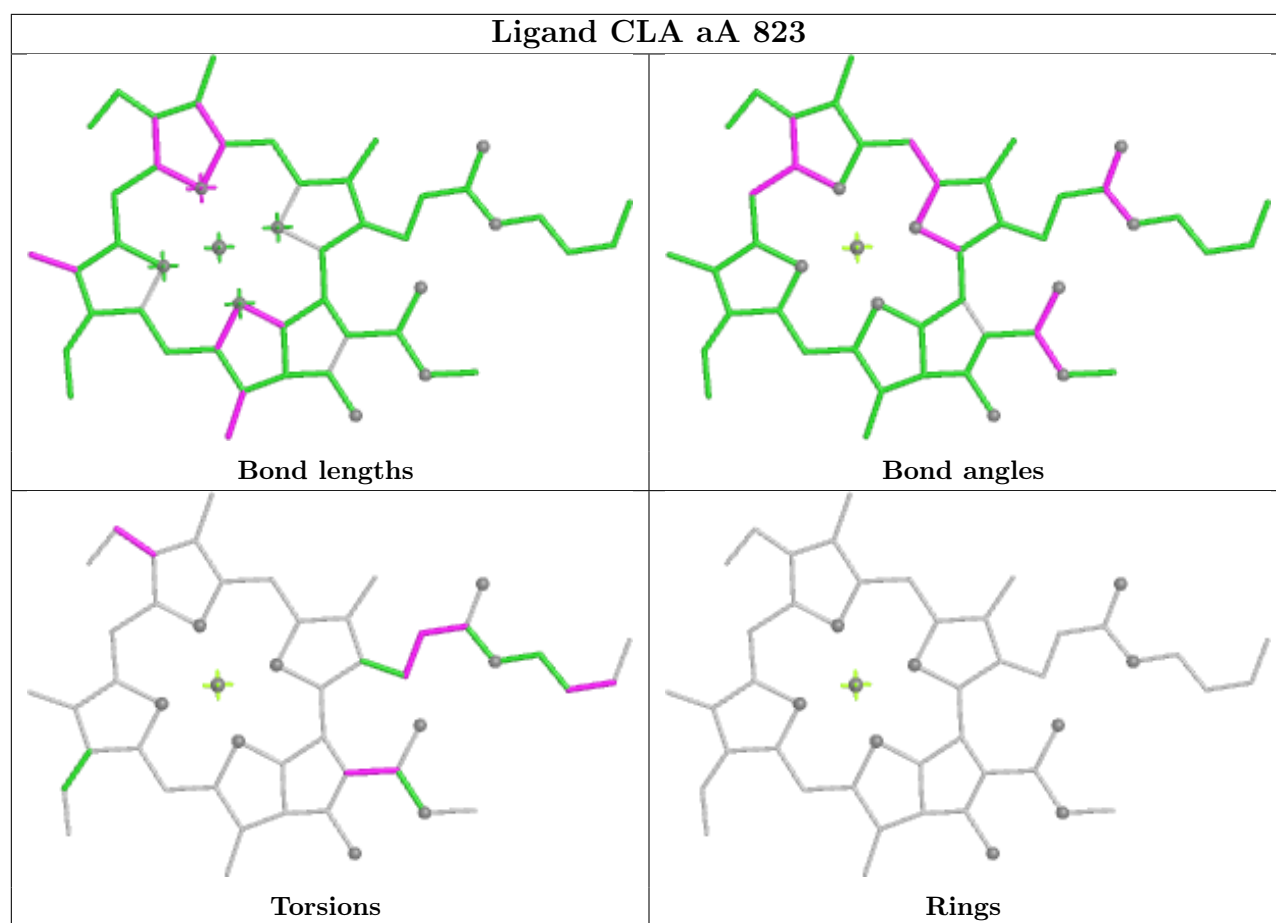


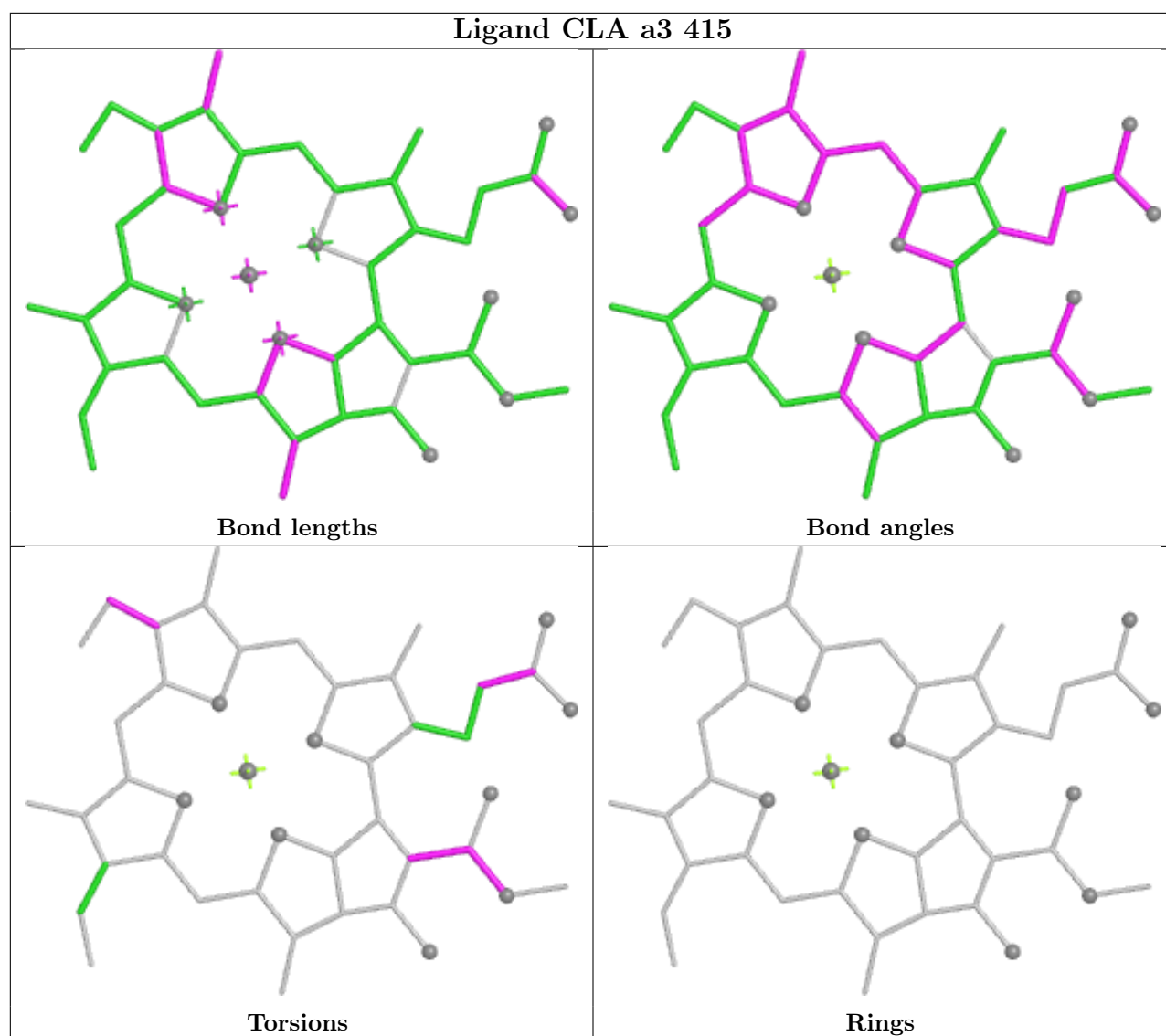


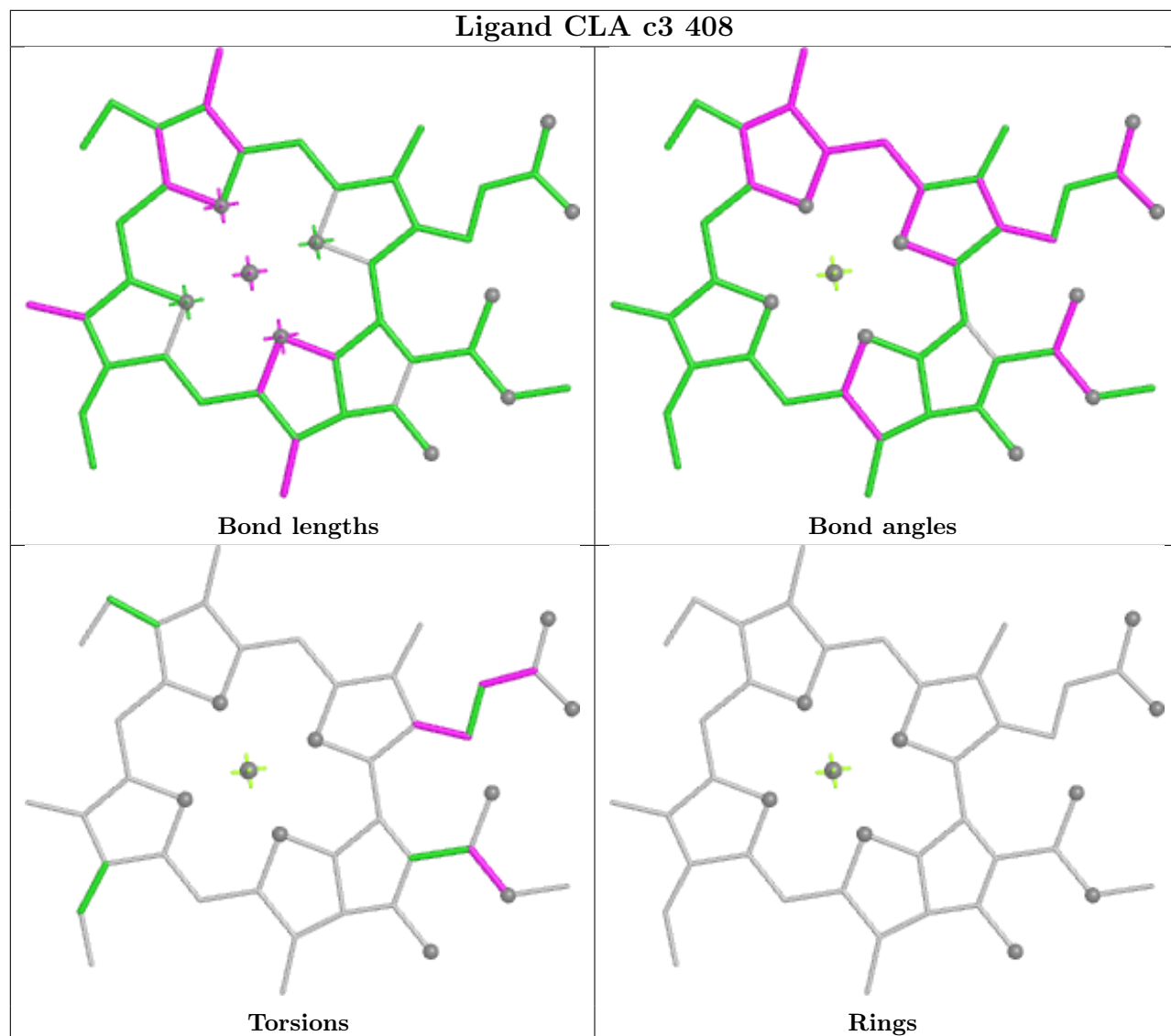


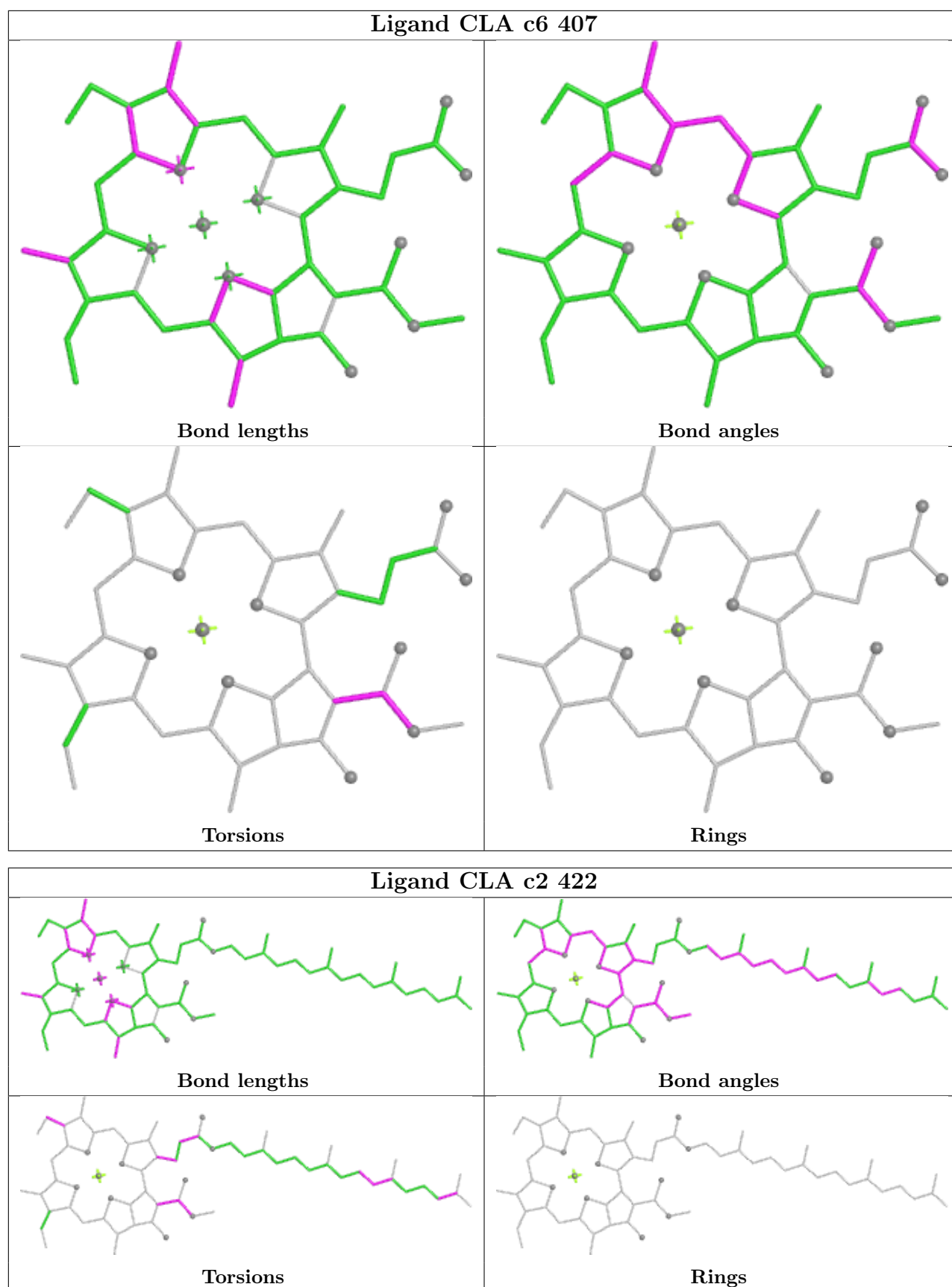


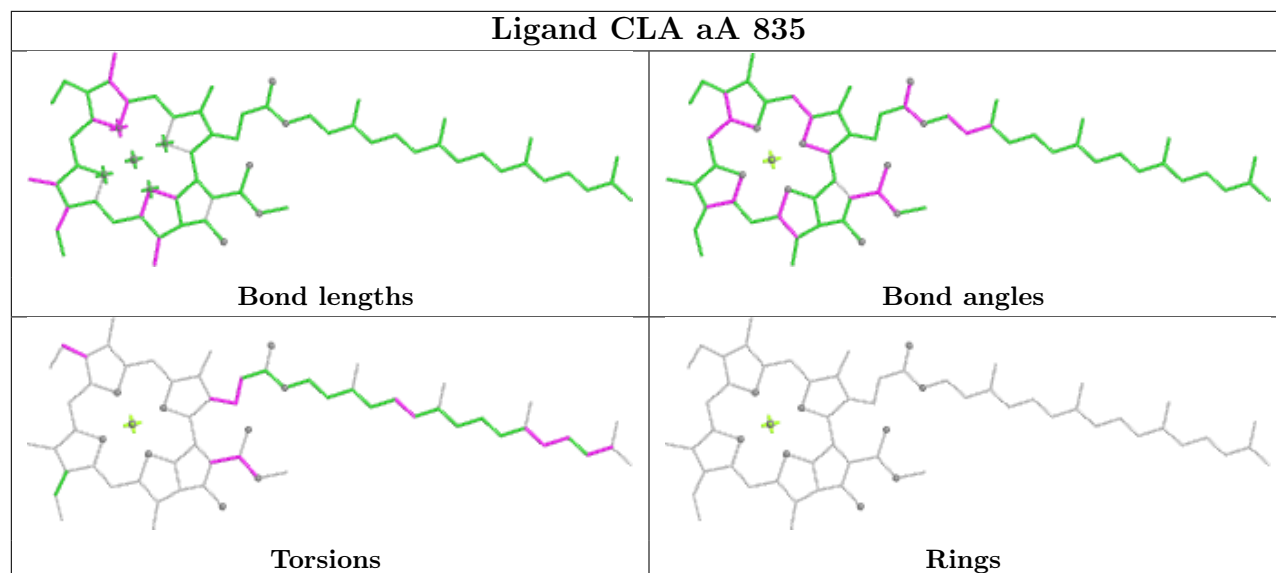
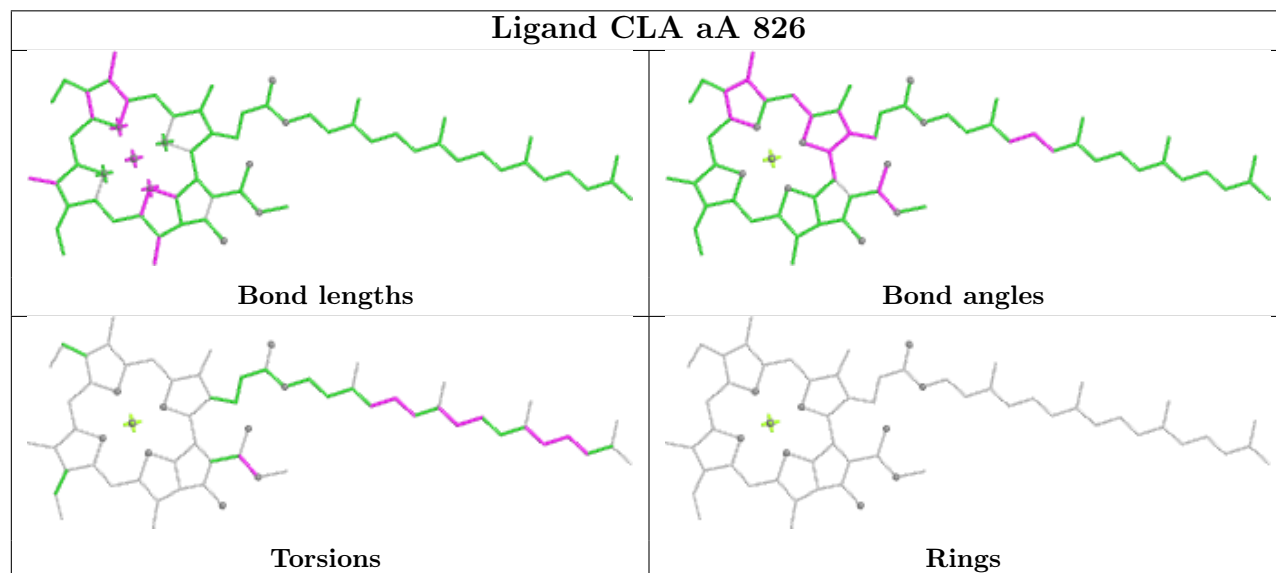
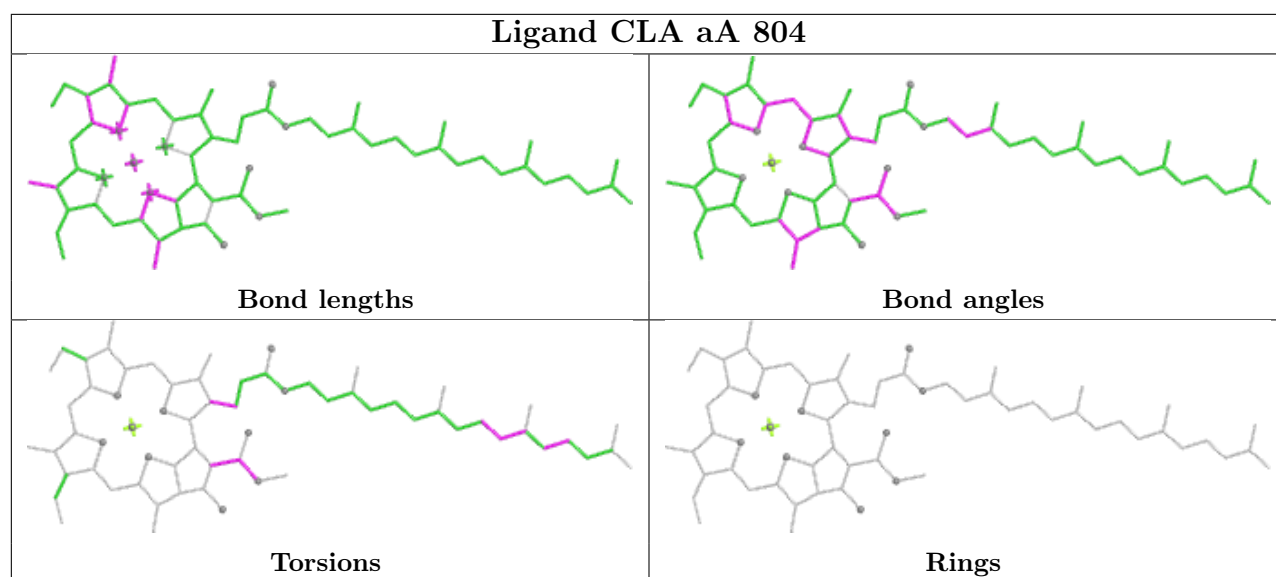


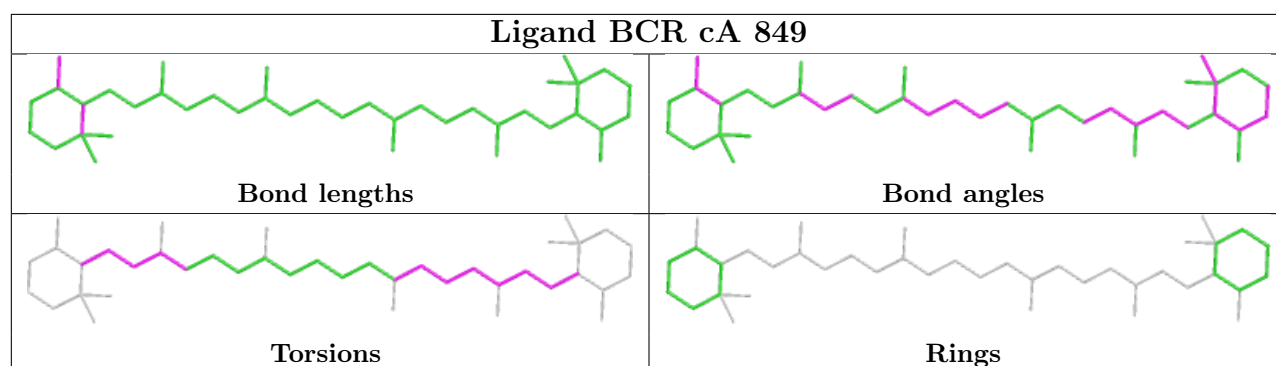
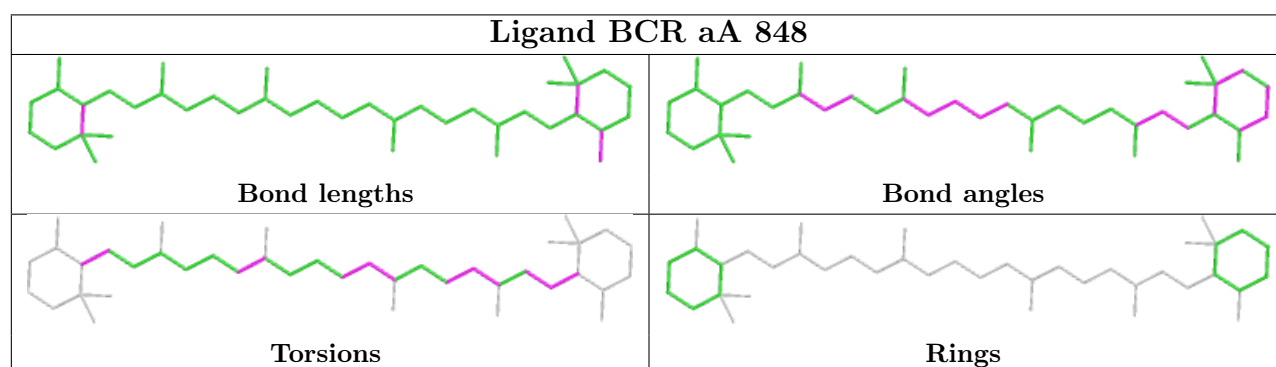
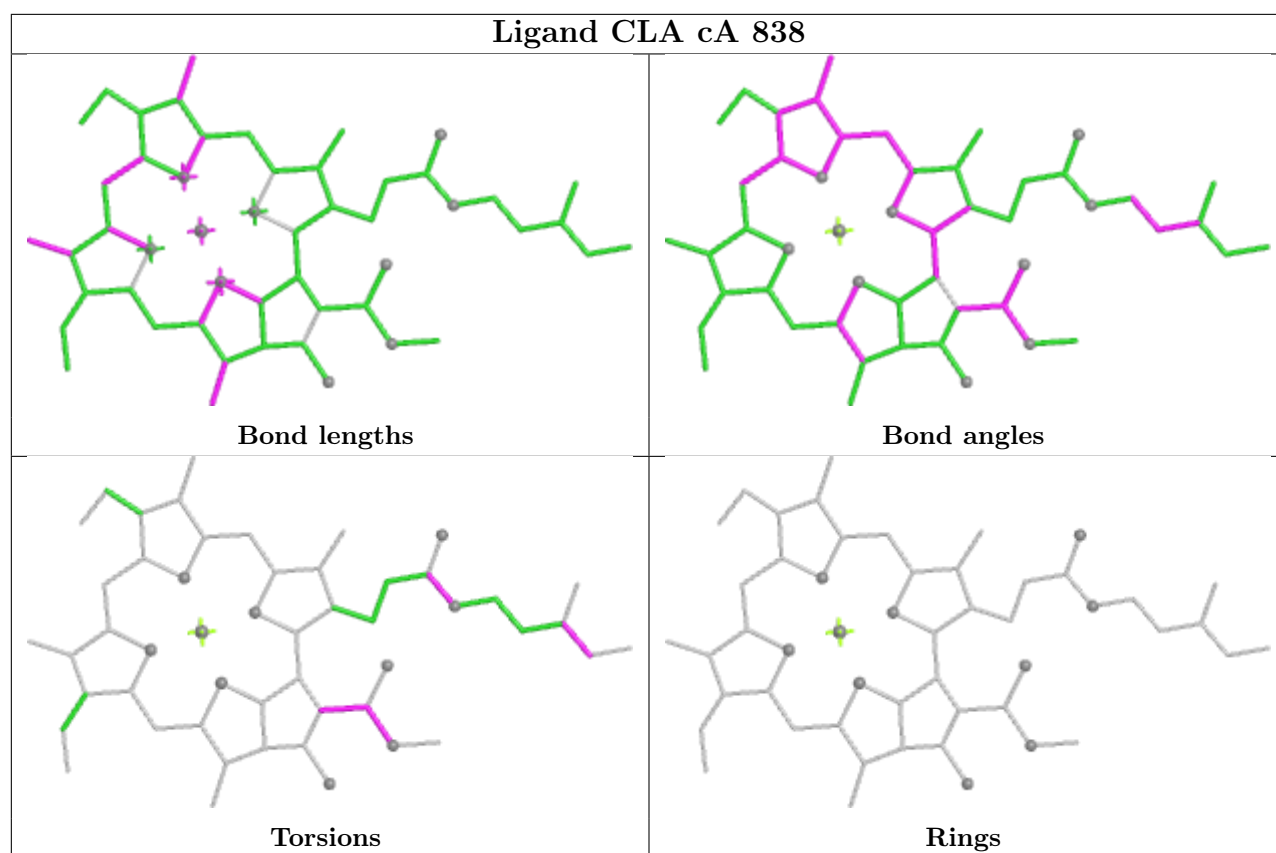


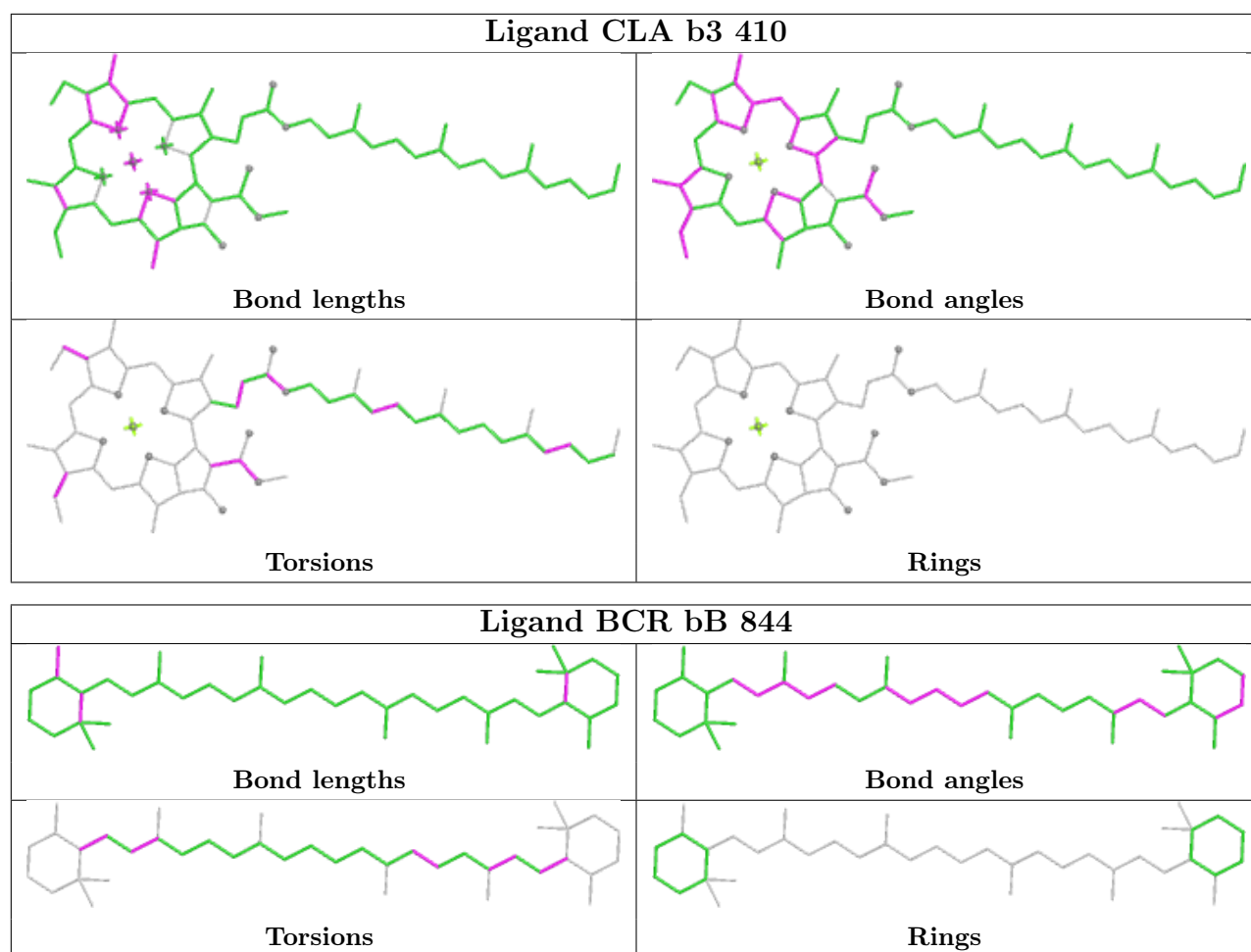




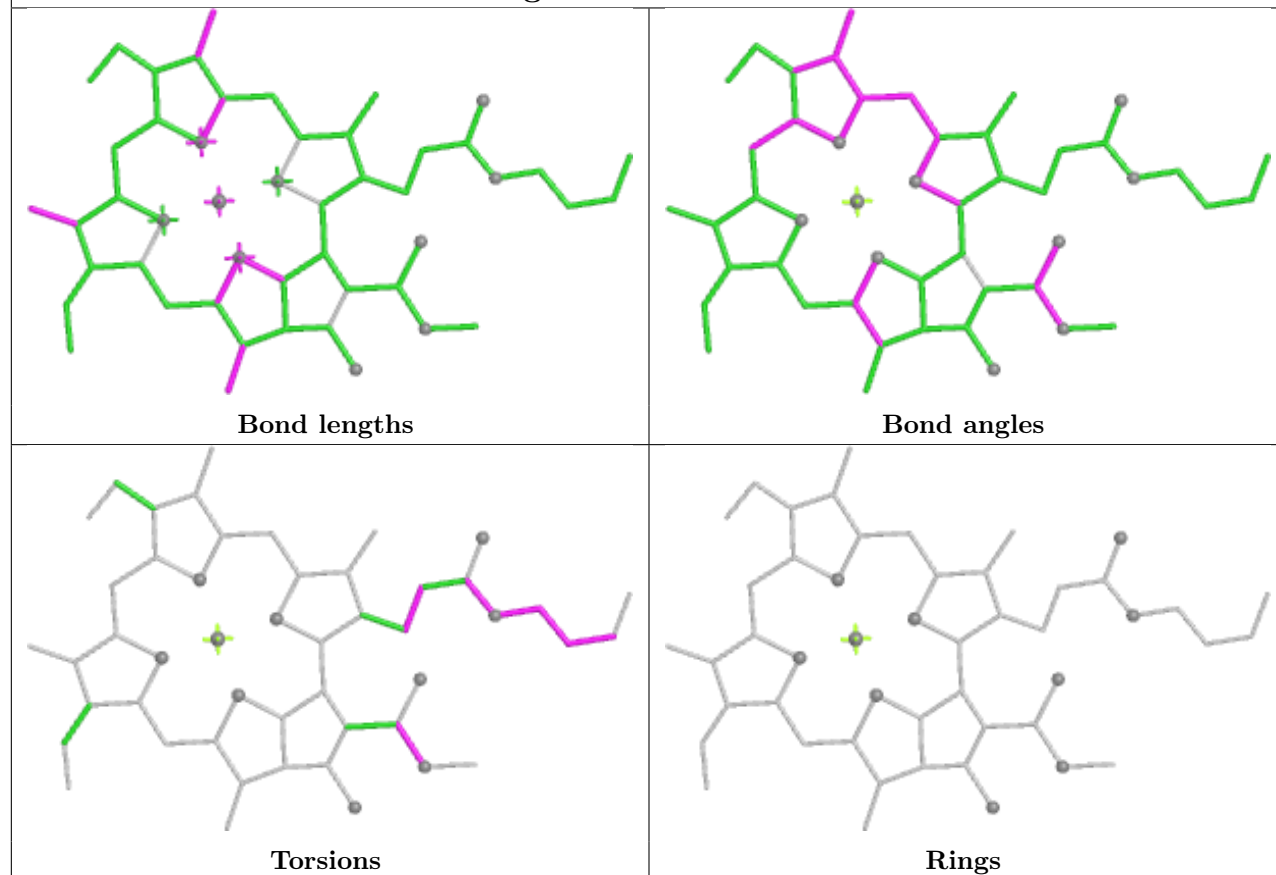




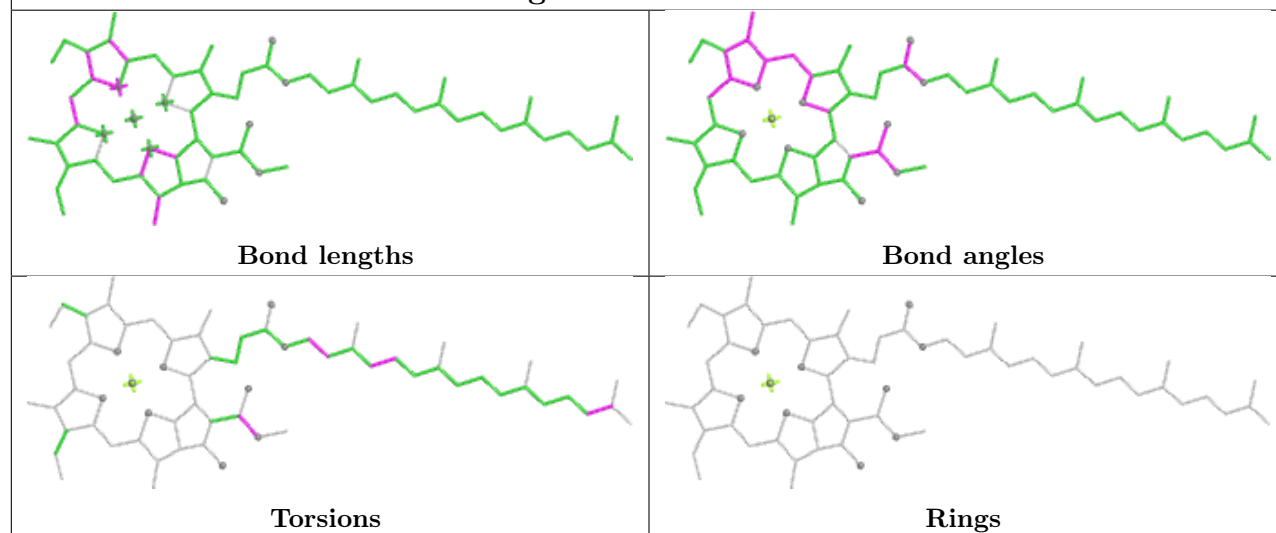


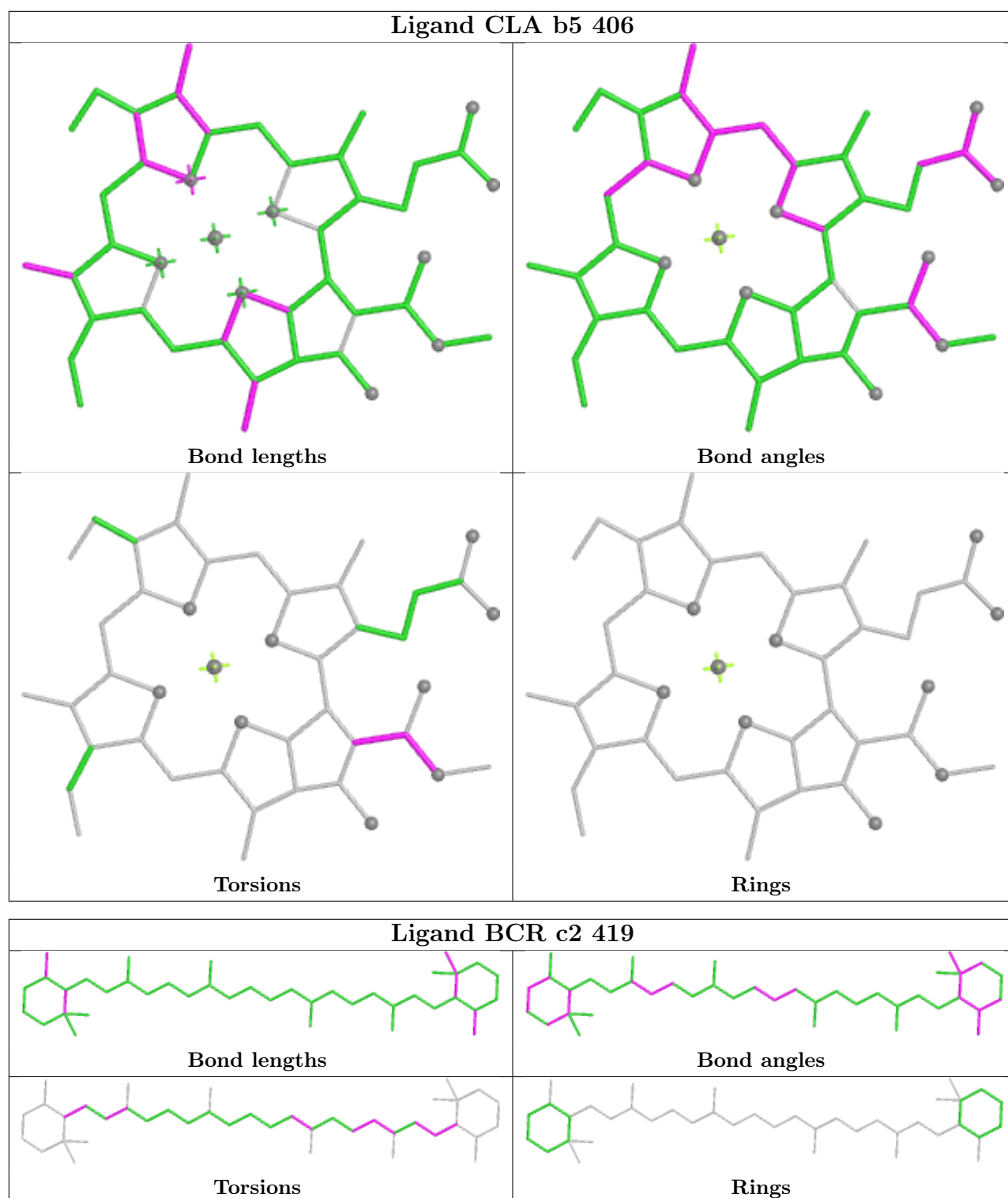


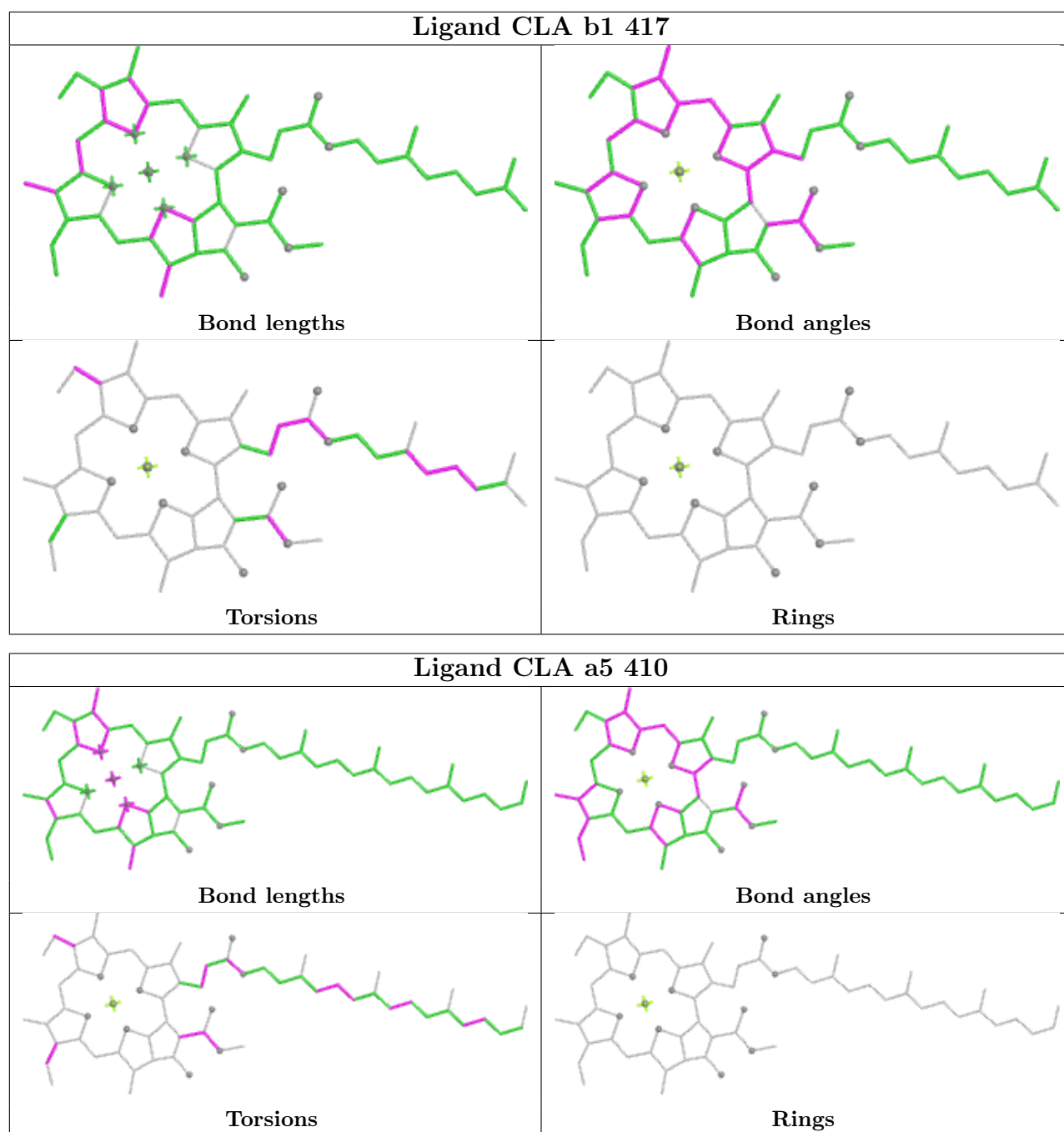
Ligand CLA aB 832

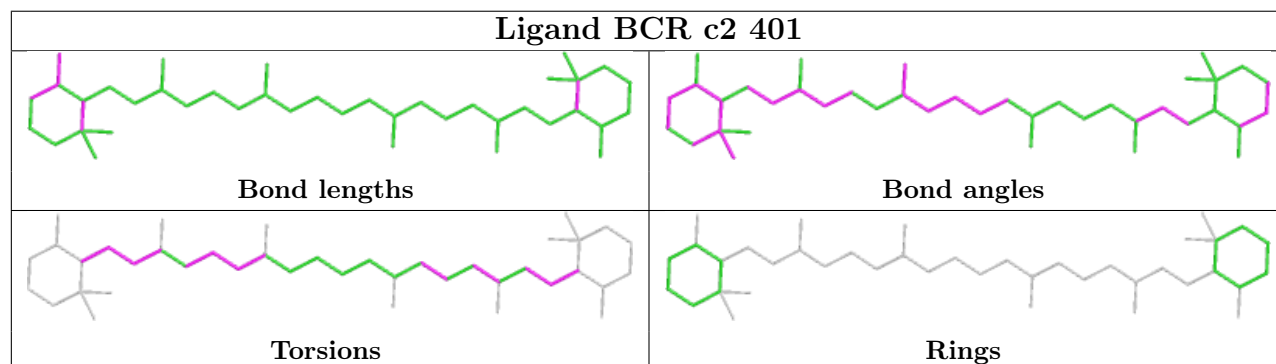
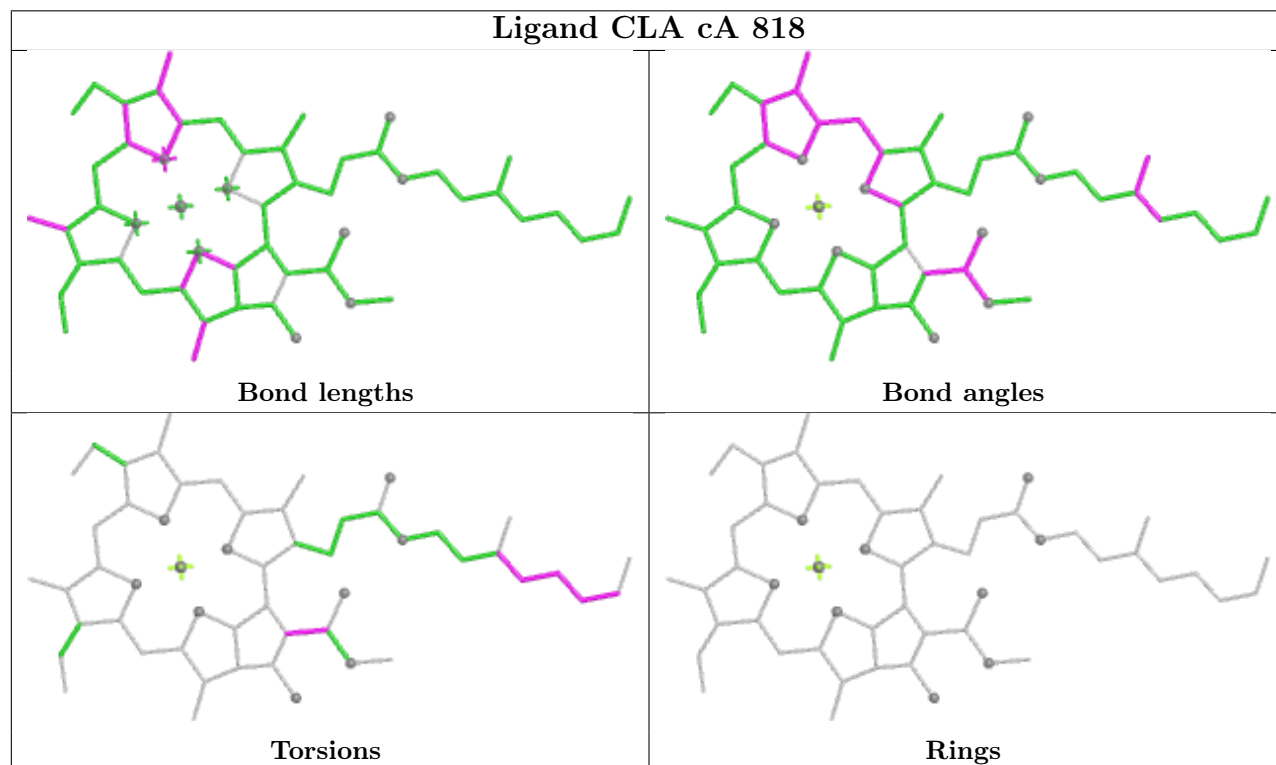
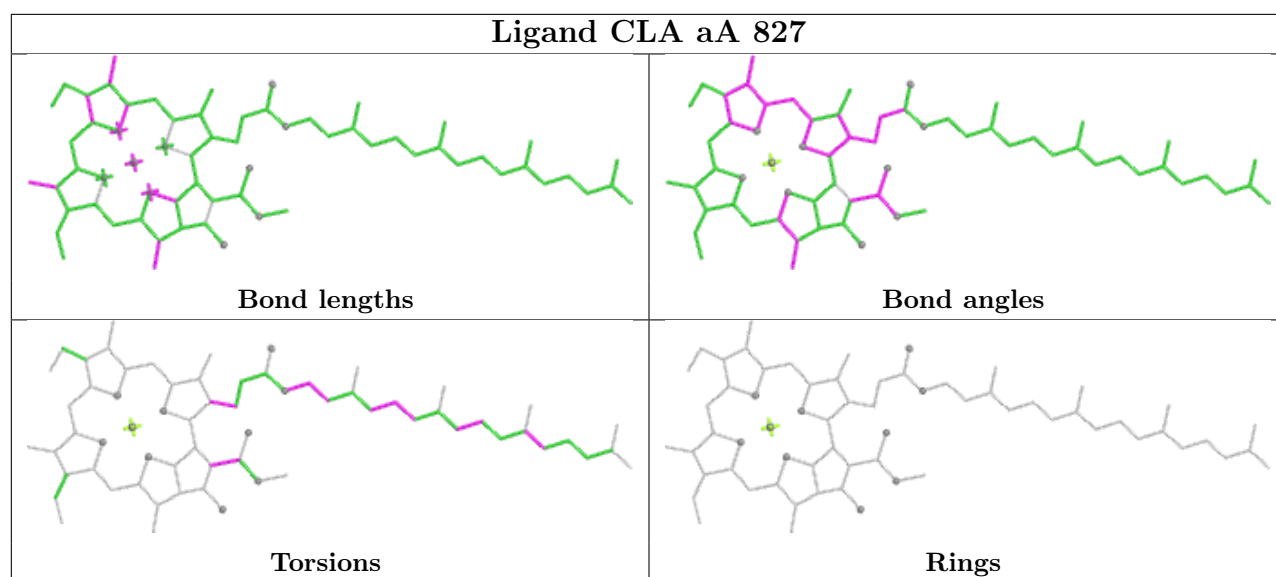


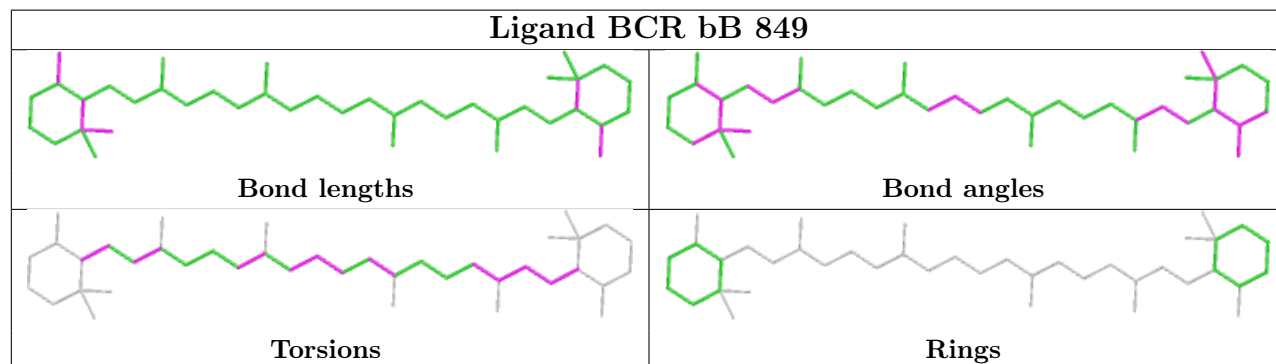
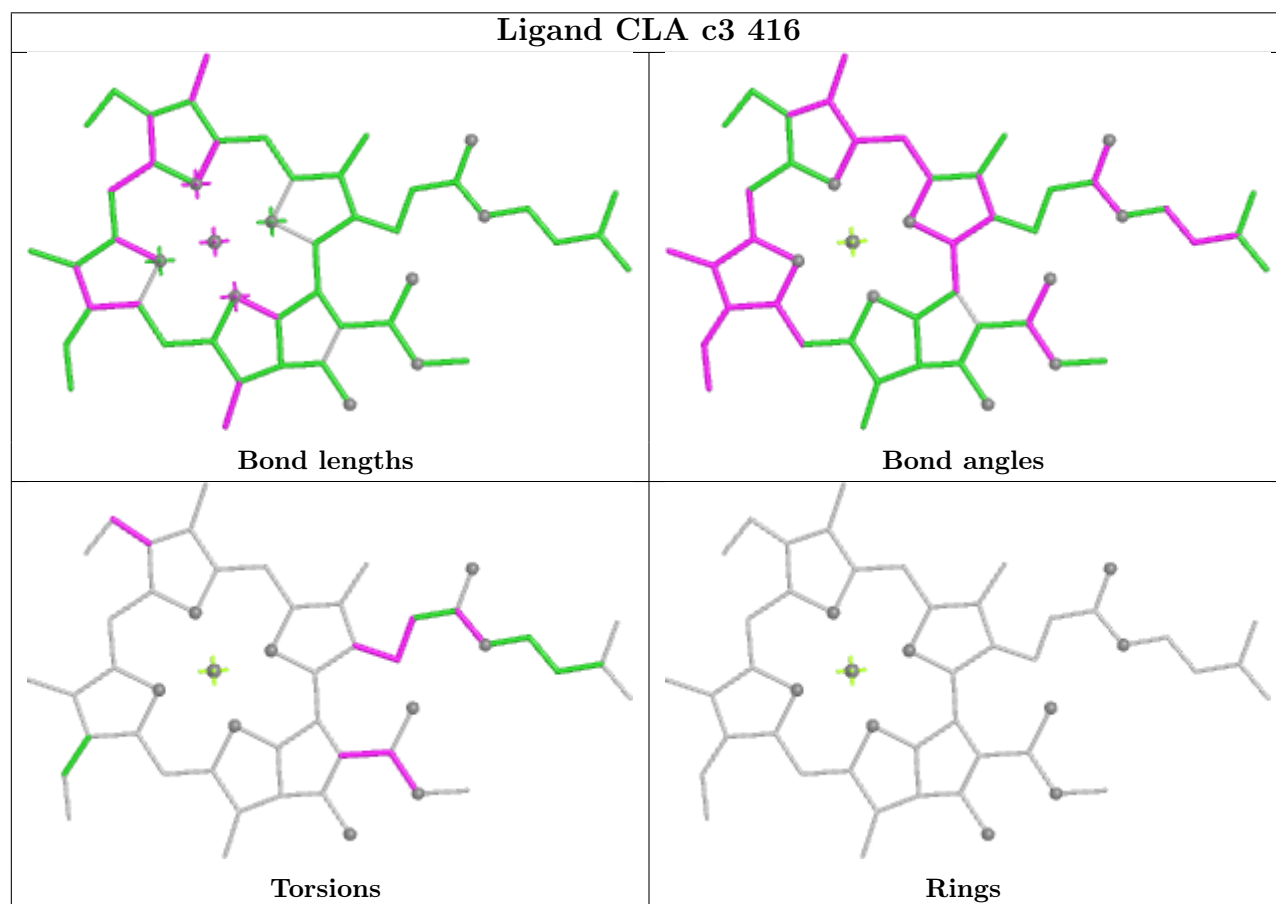
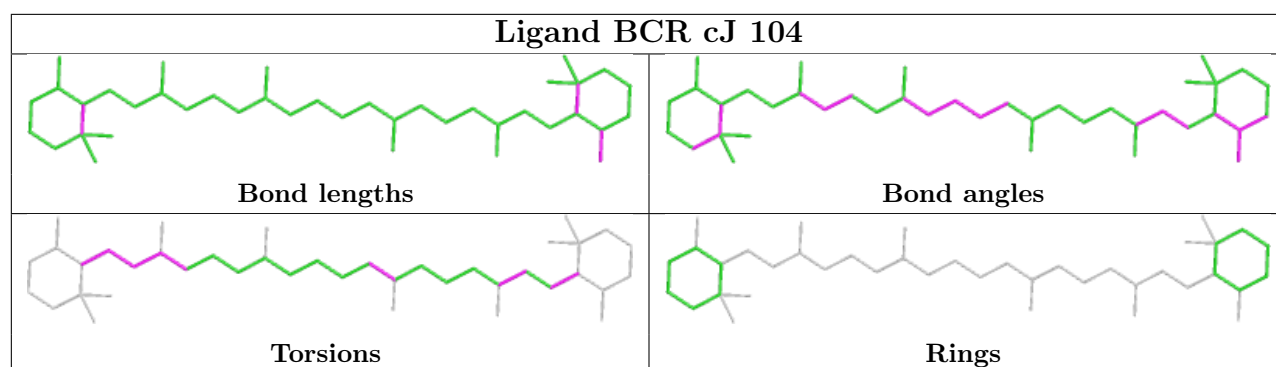
Ligand CLA c4 409

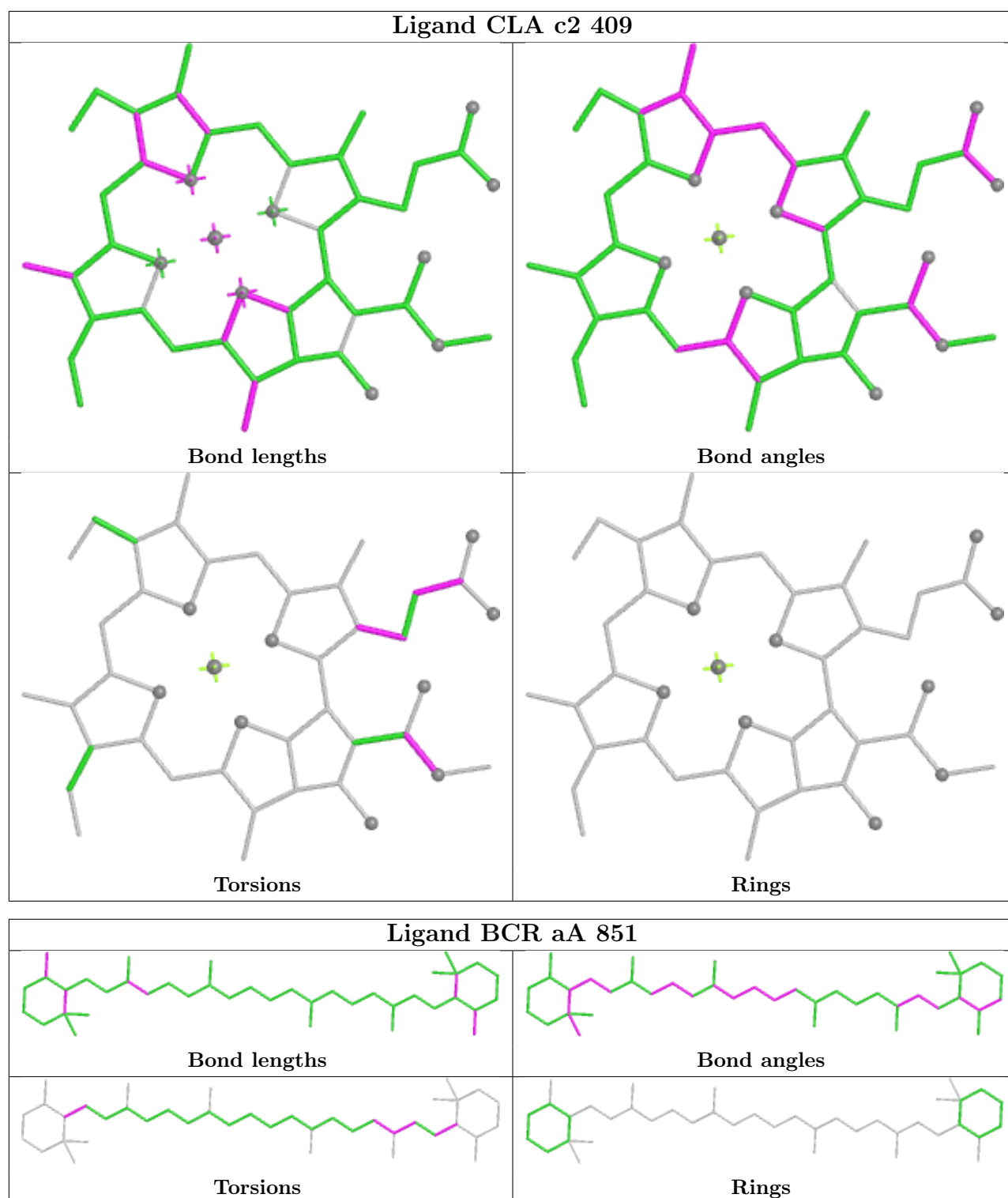


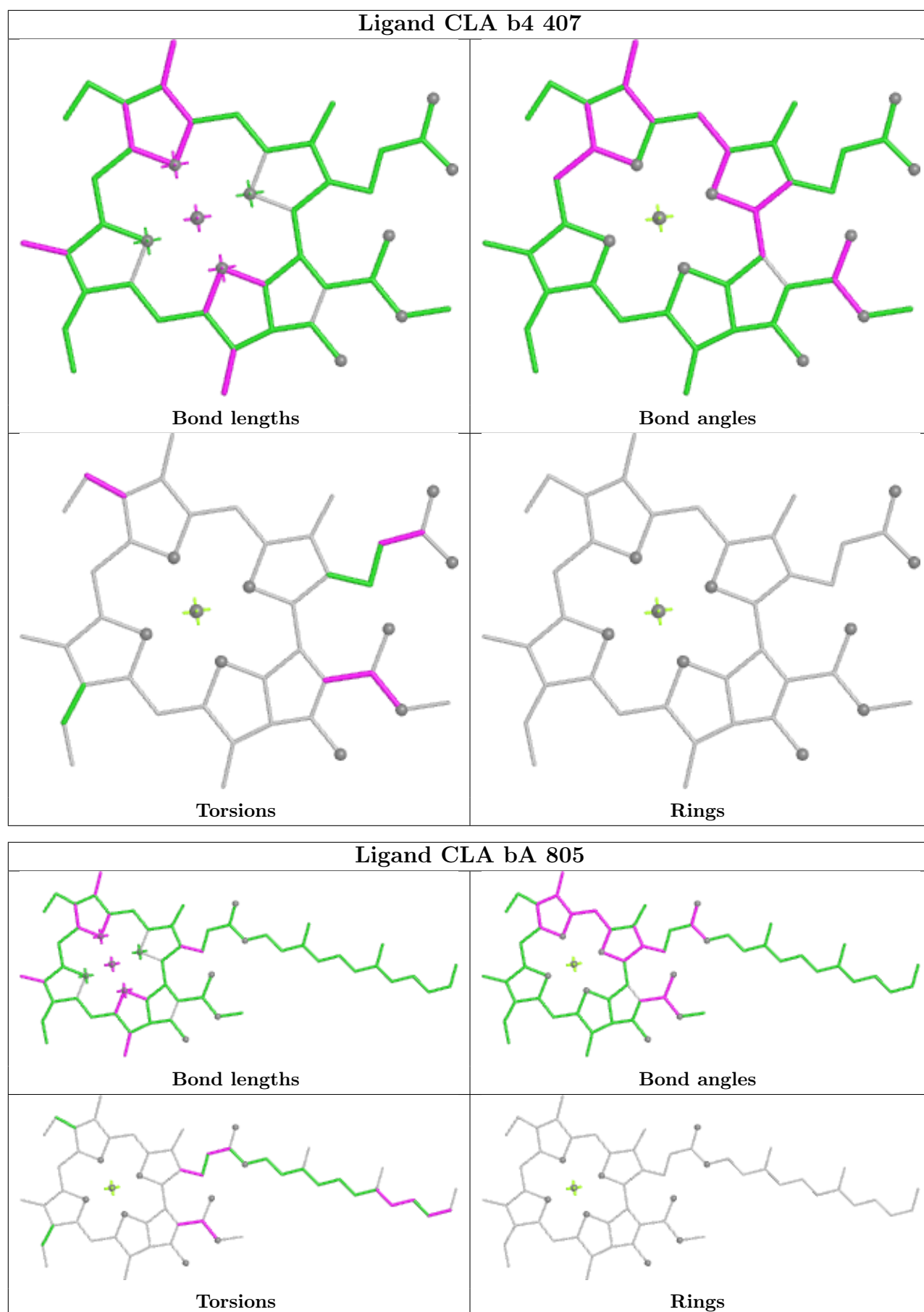


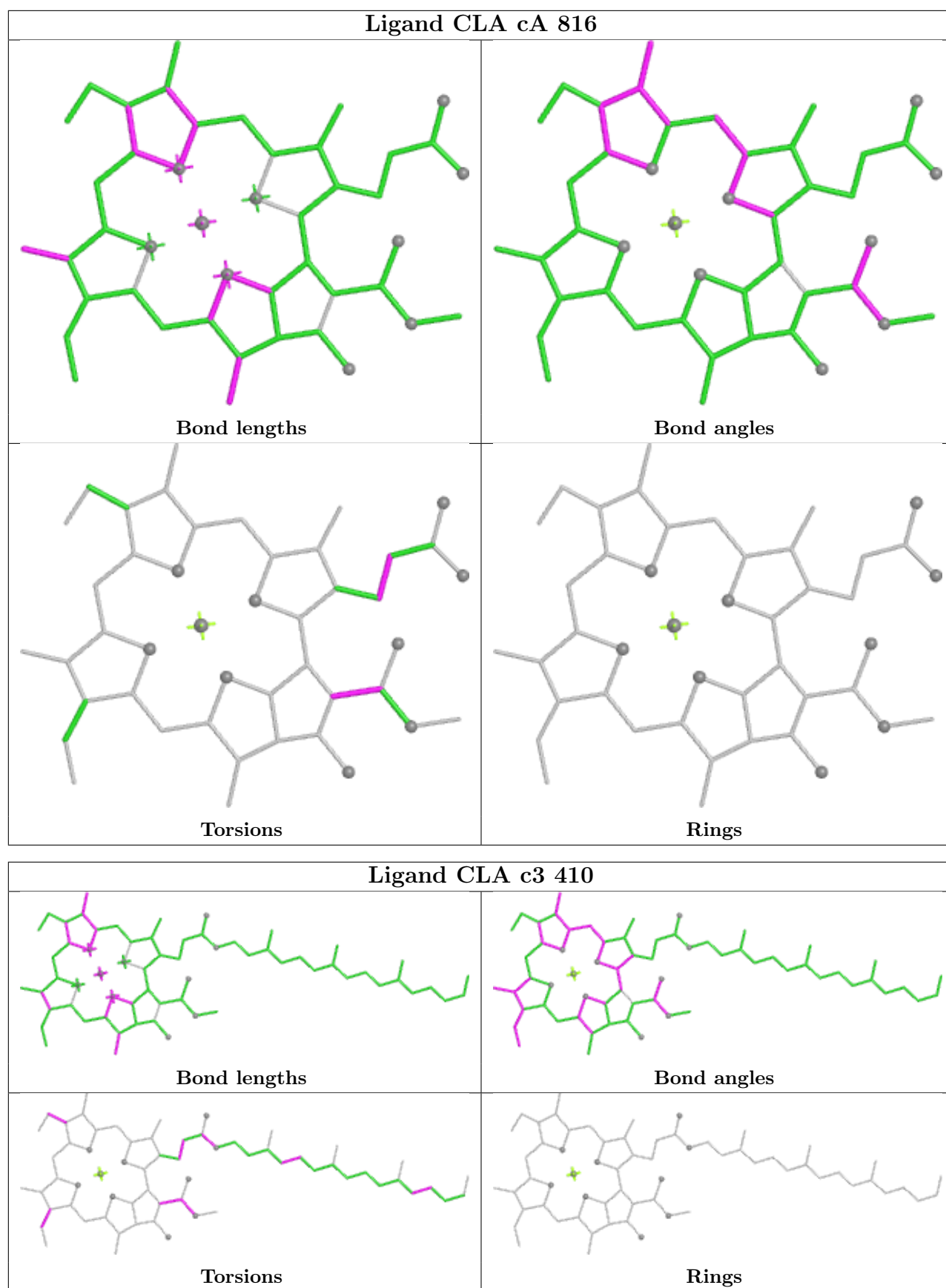


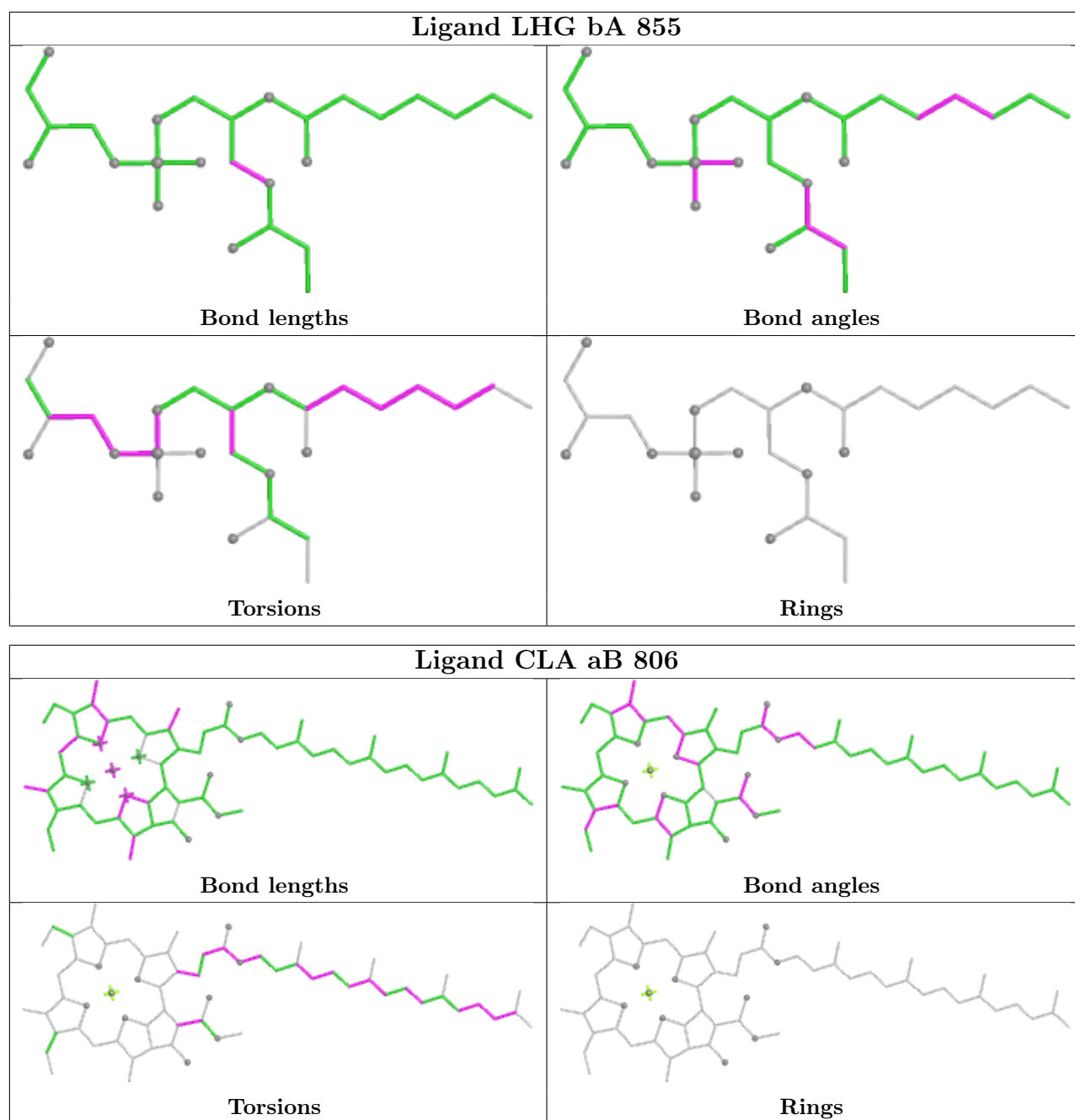


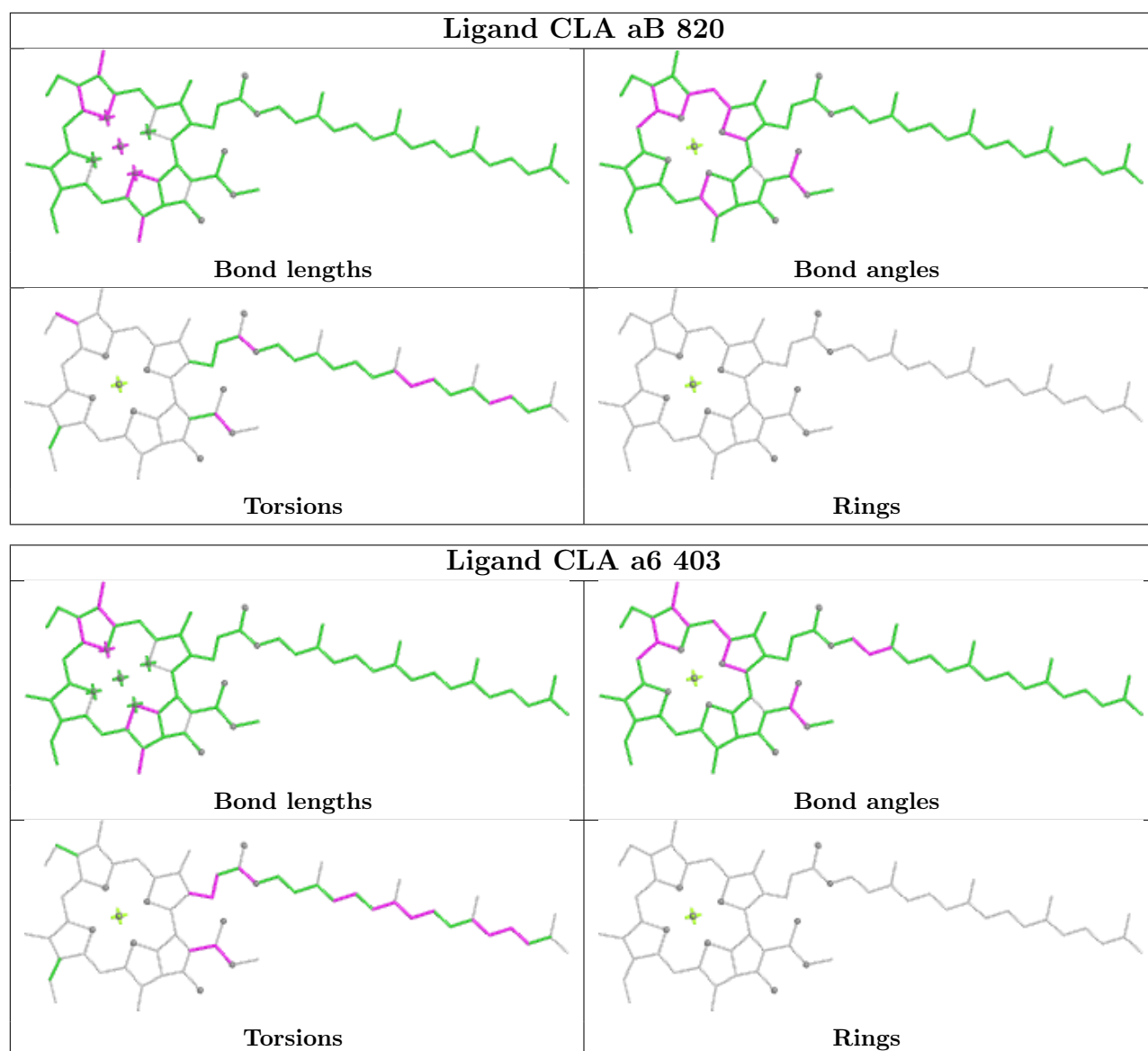


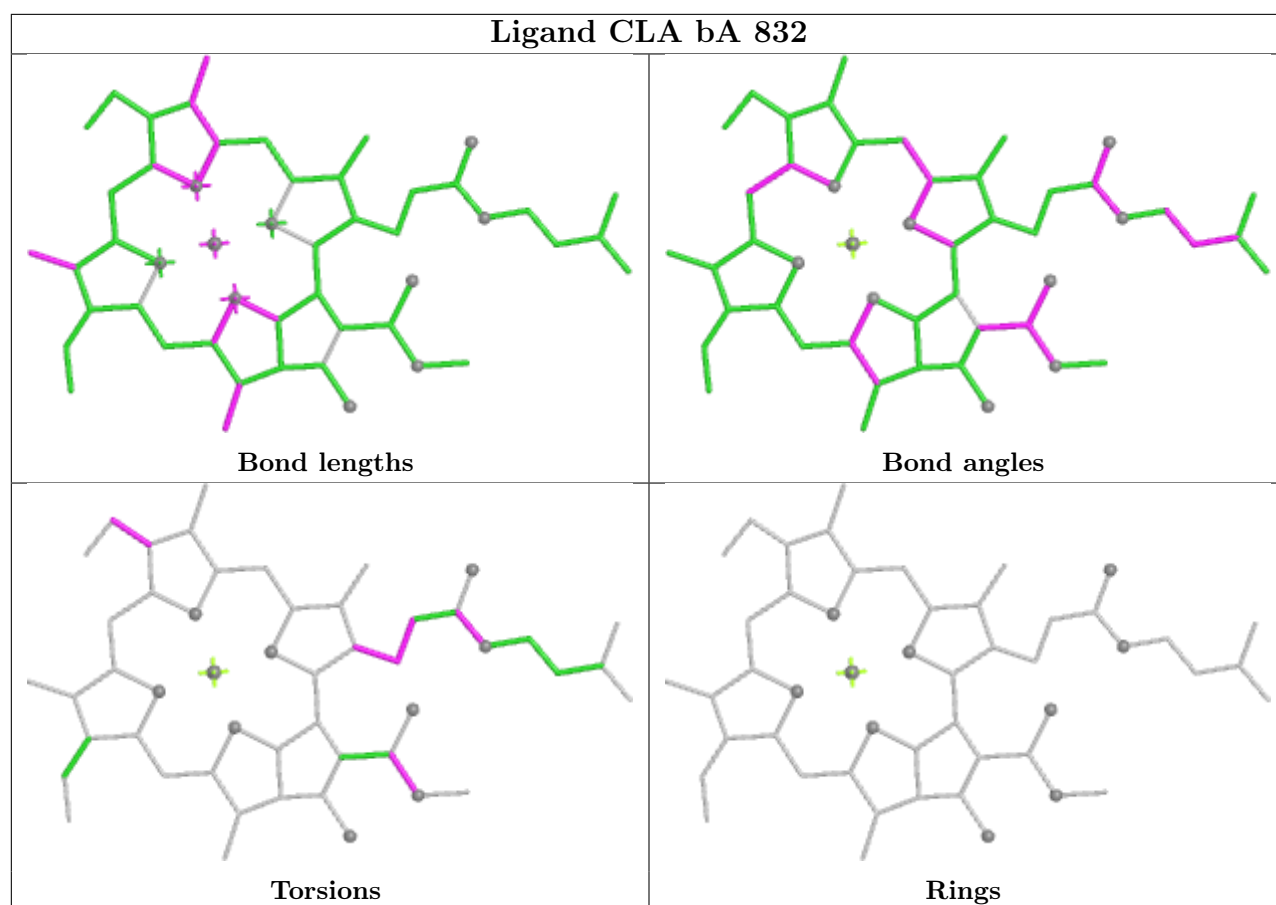




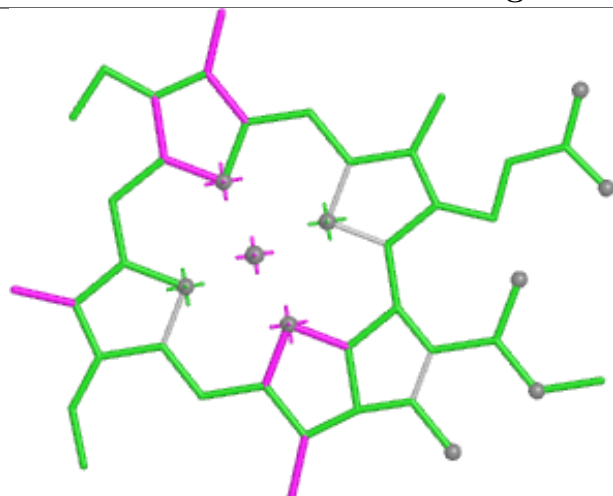




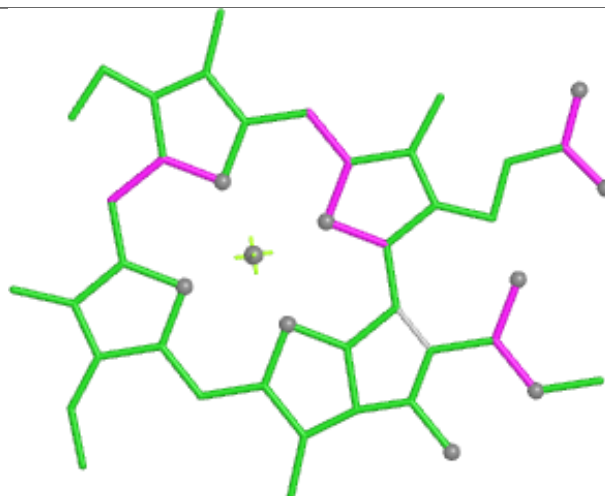




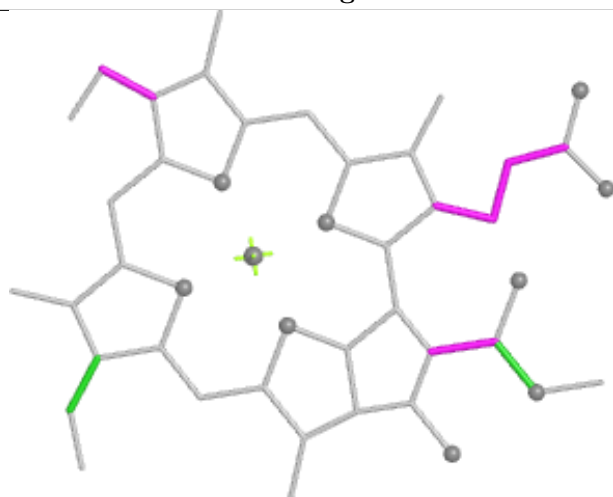
Ligand CLA cB 831



Bond lengths



Bond angles

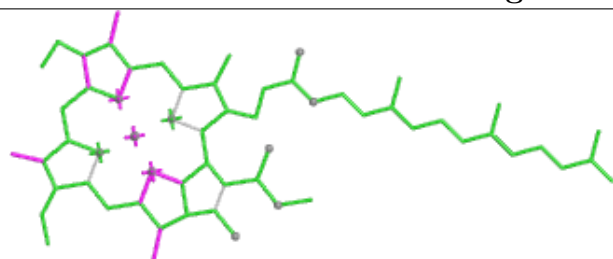


Torsions

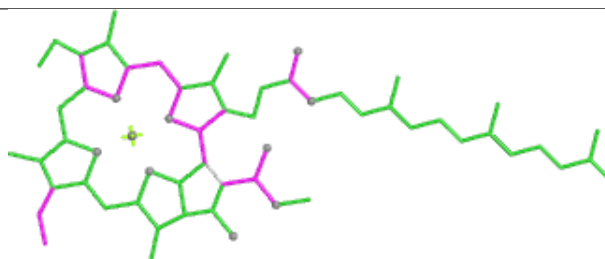


Rings

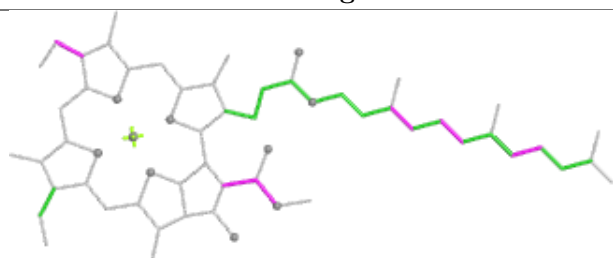
Ligand CLA aB 836



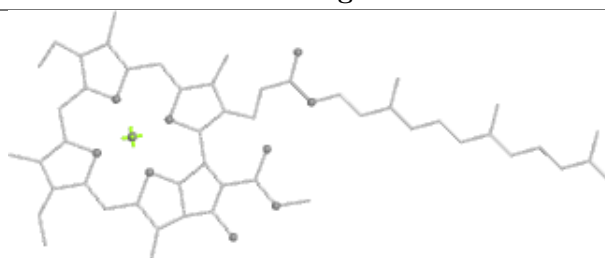
Bond lengths



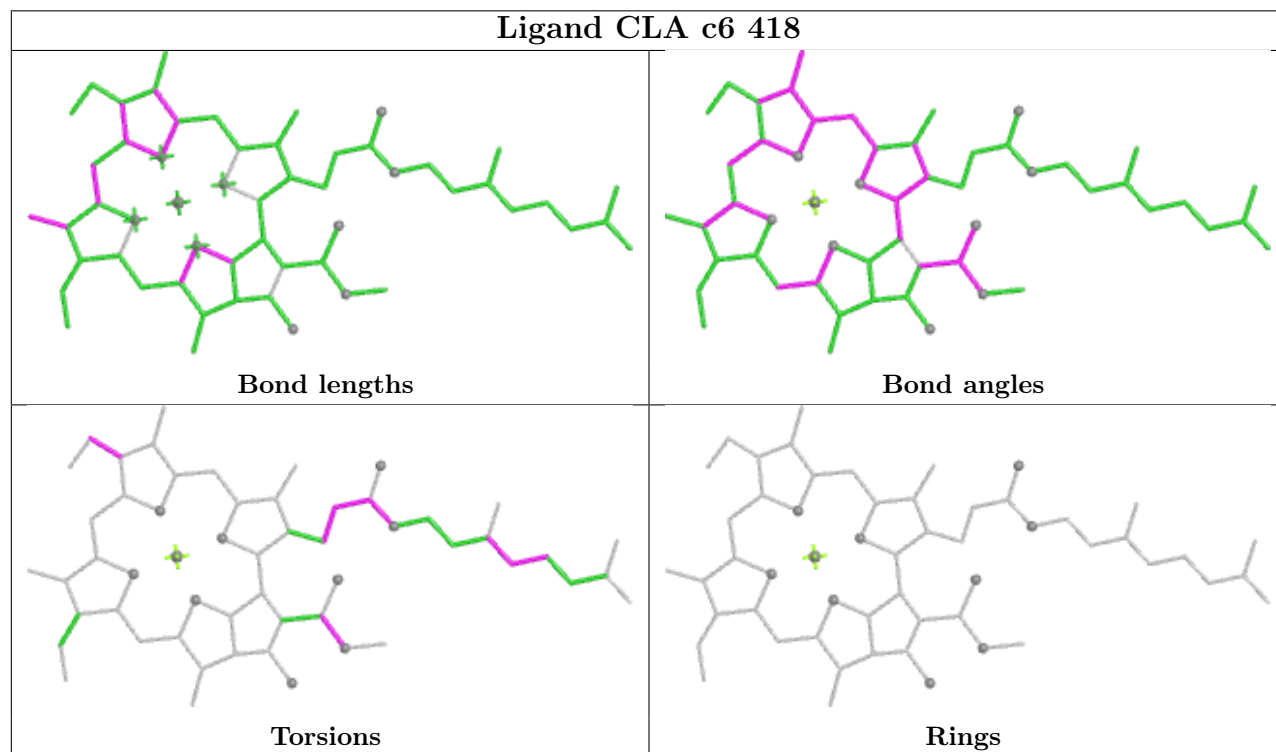
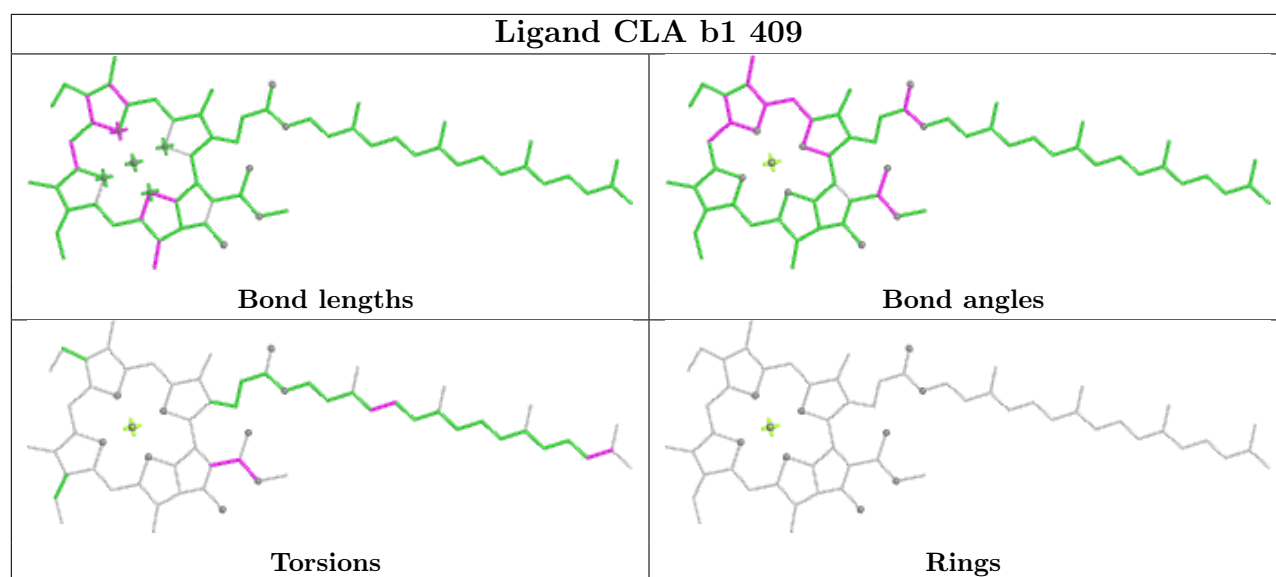
Bond angles

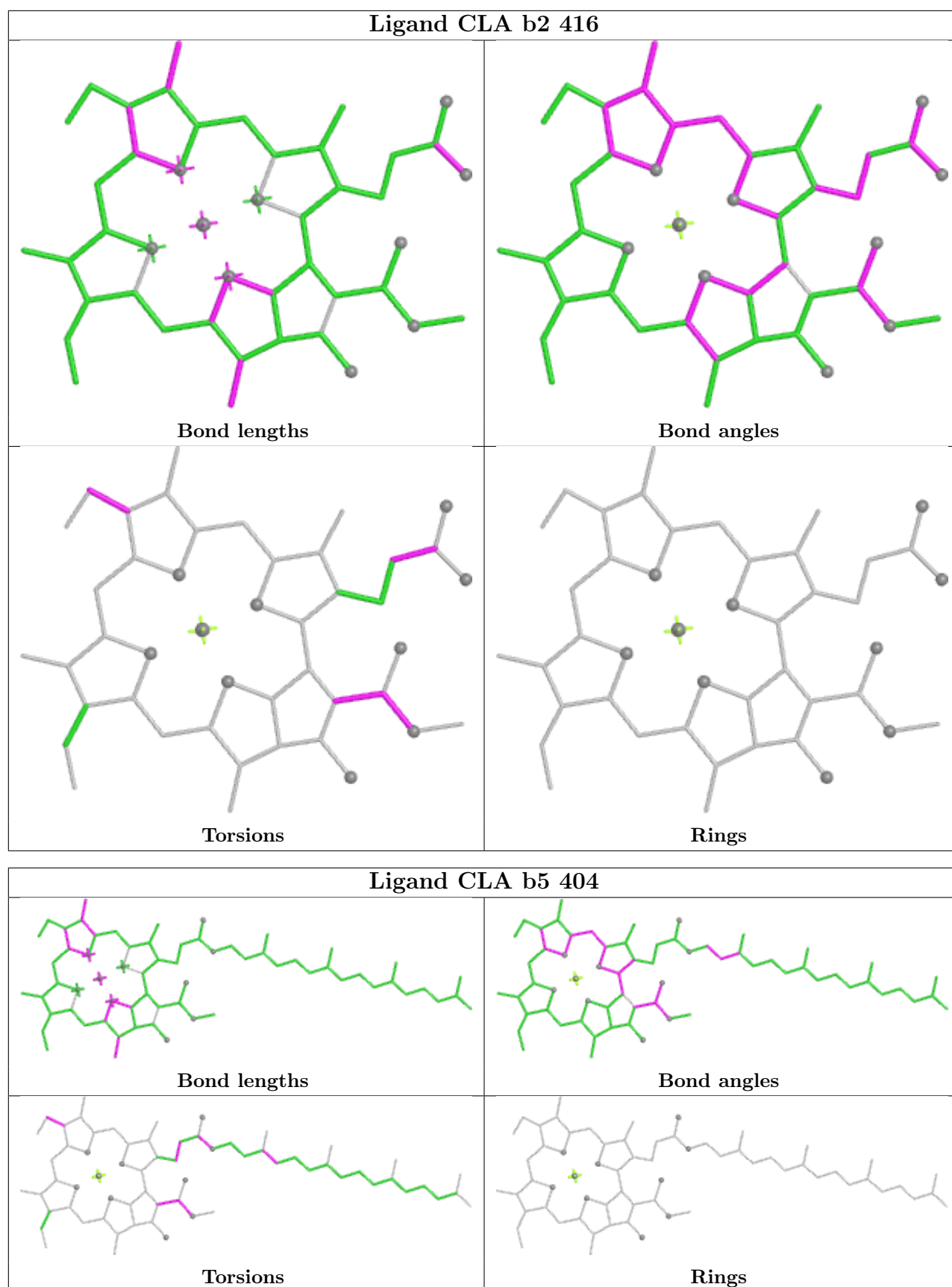


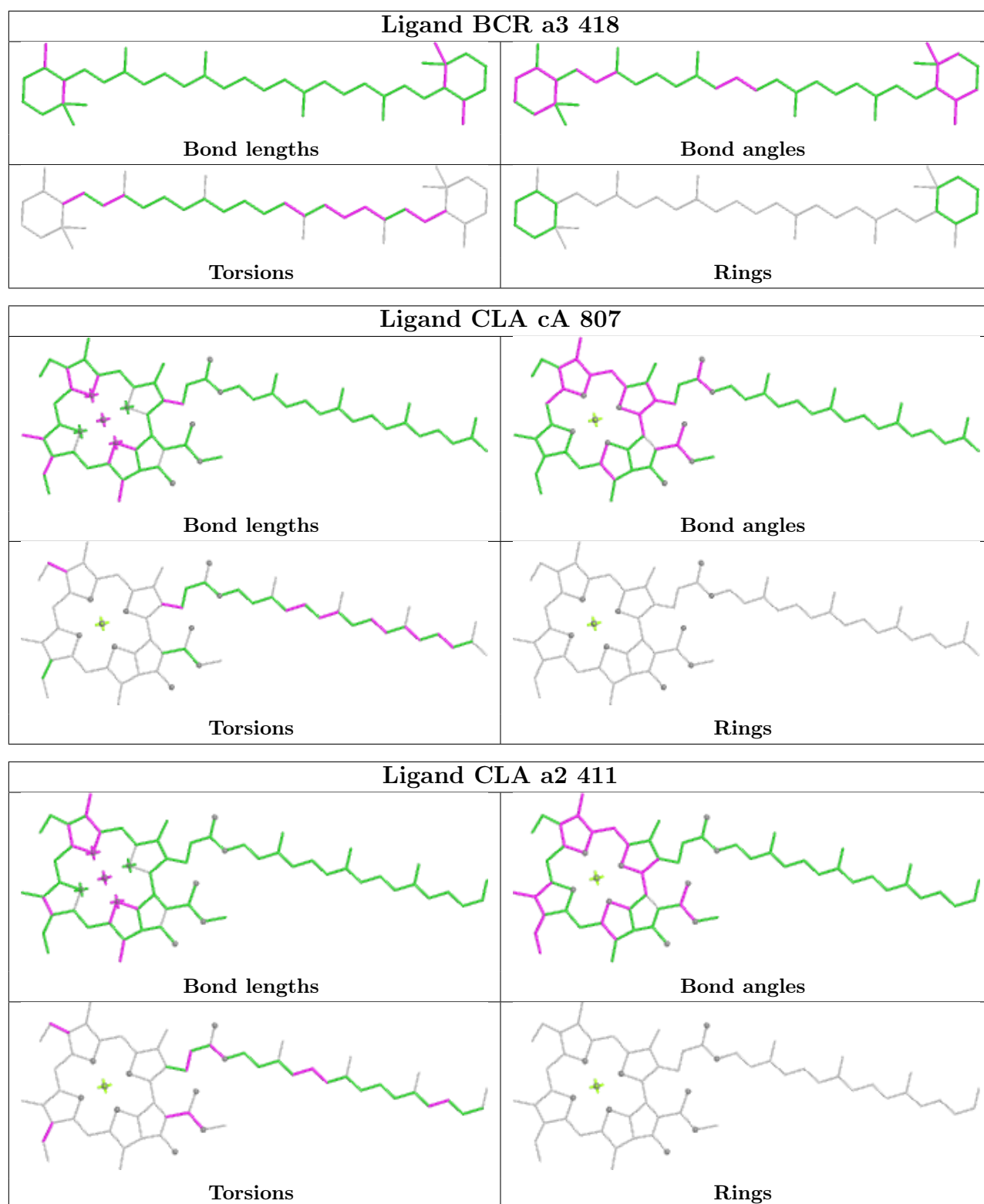
Torsions

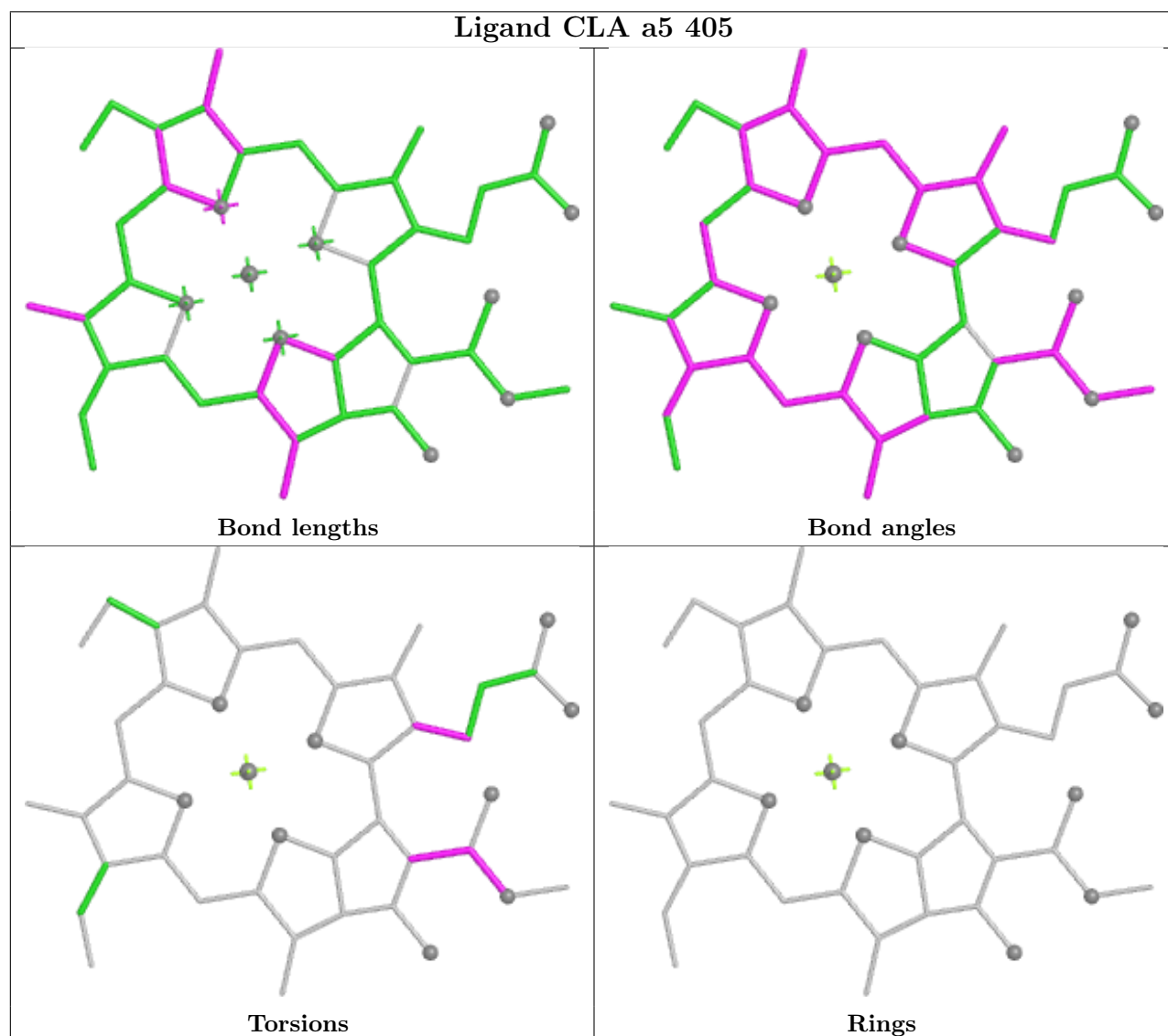
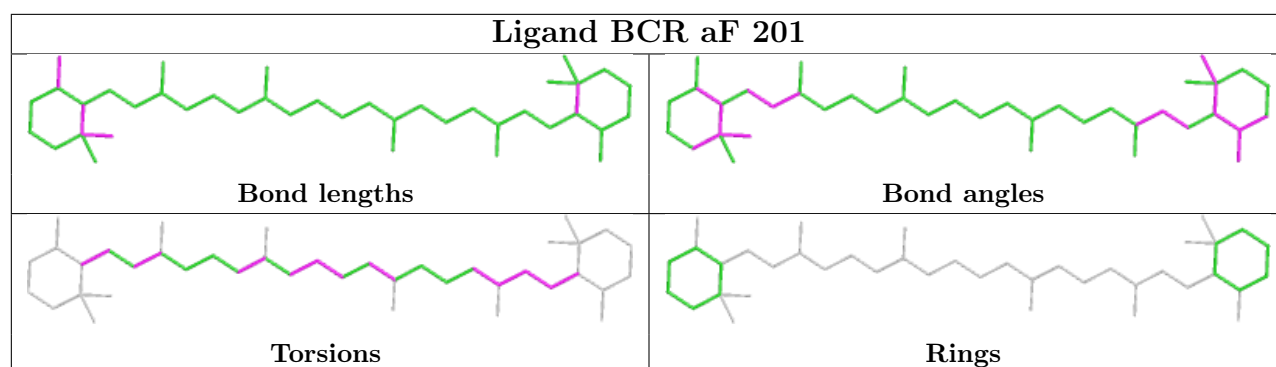


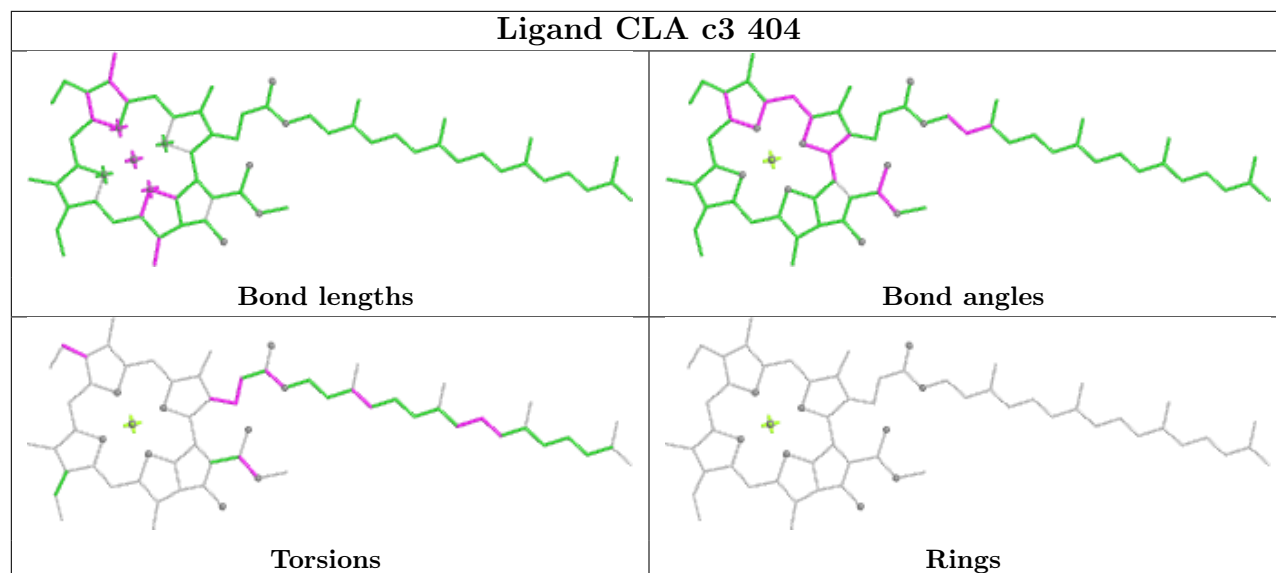
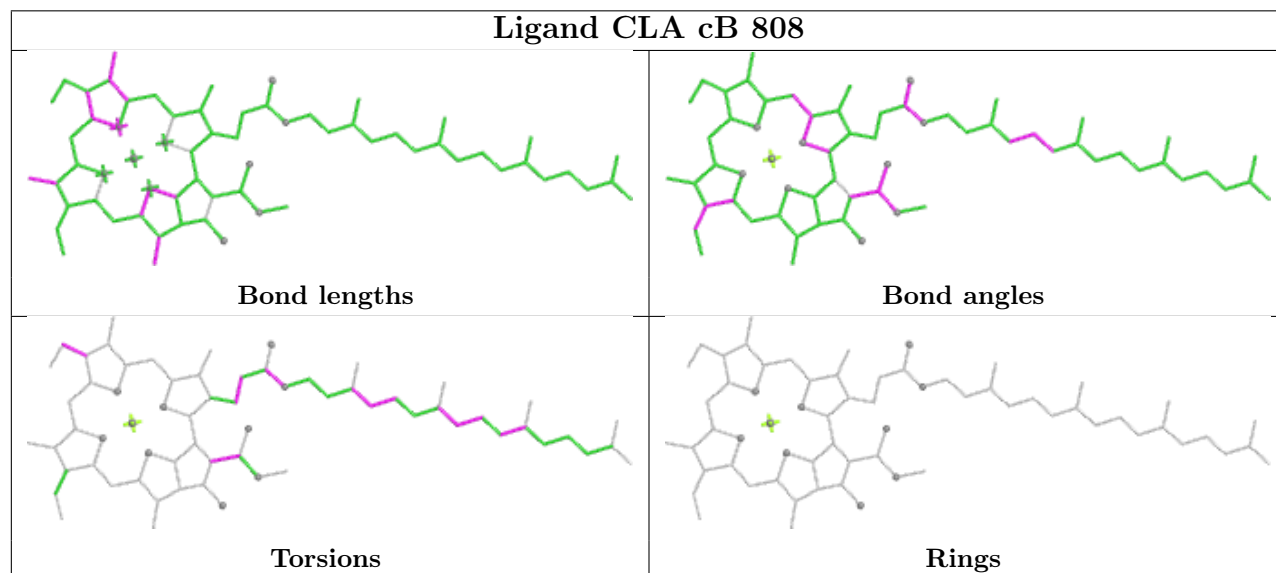
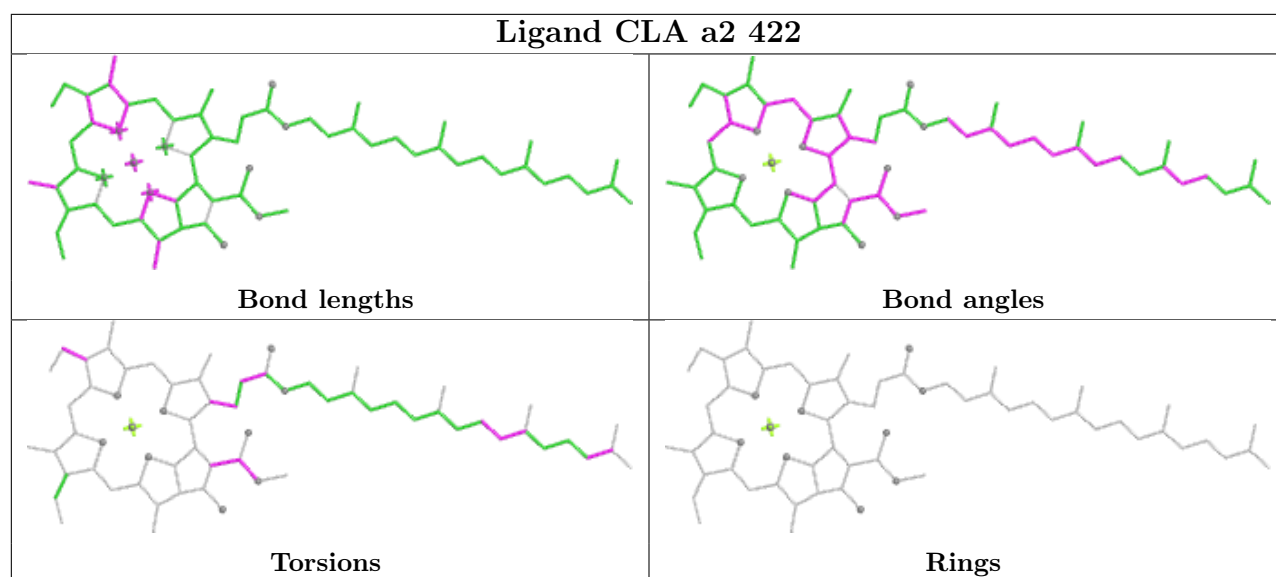
Rings

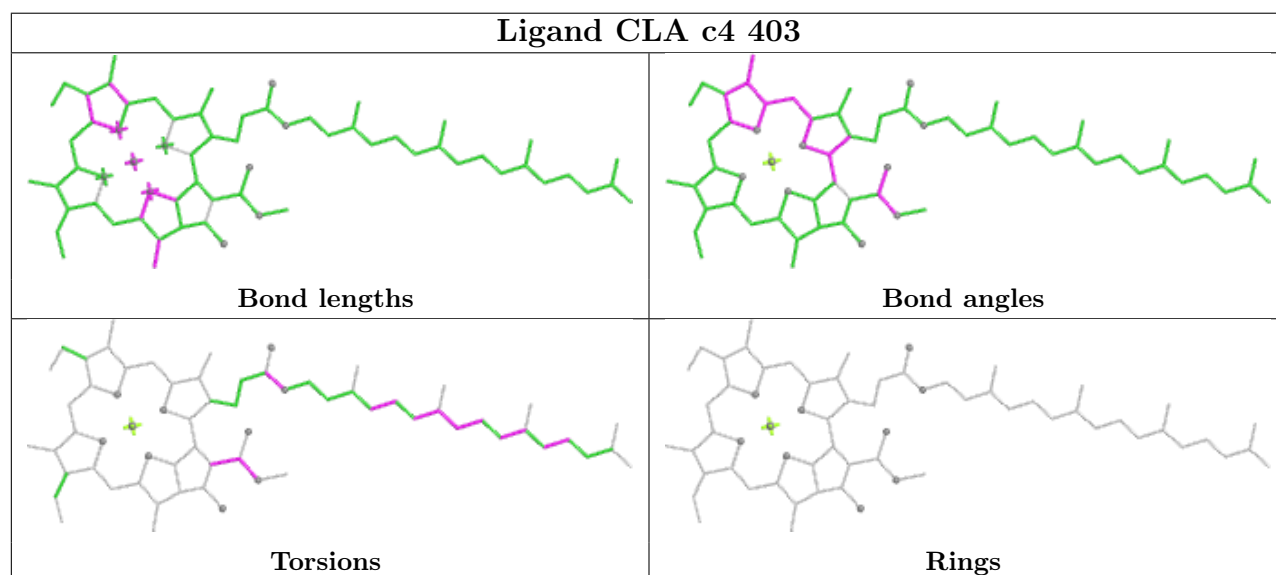
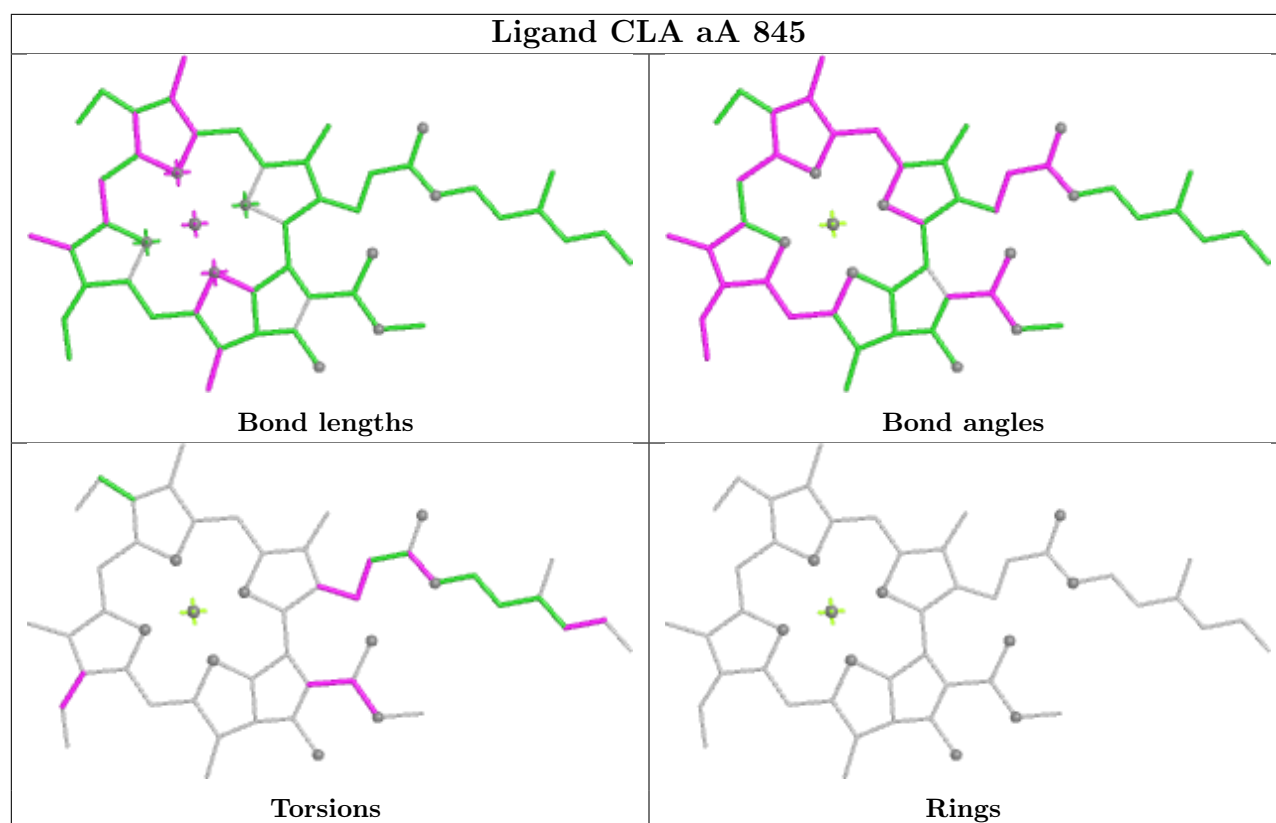


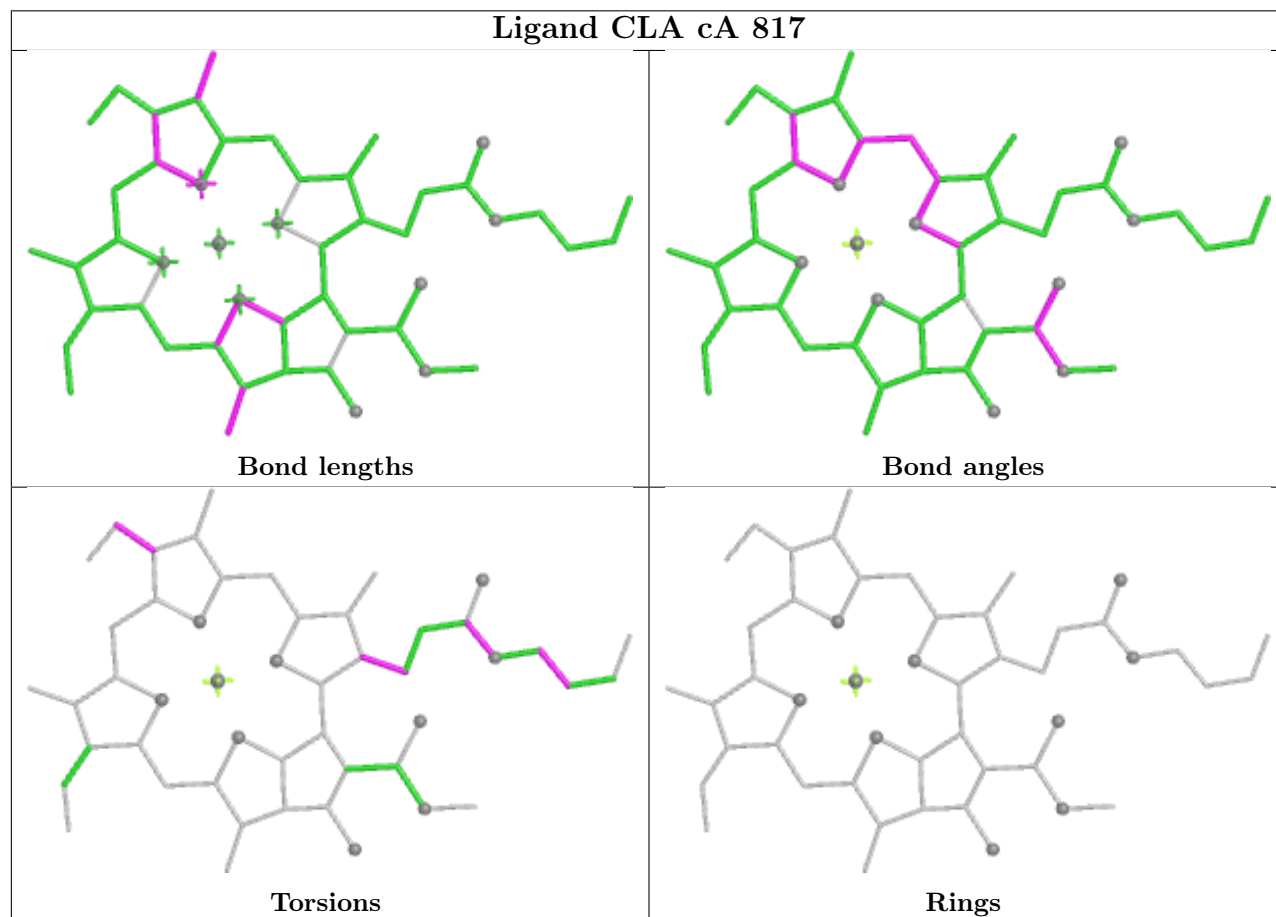
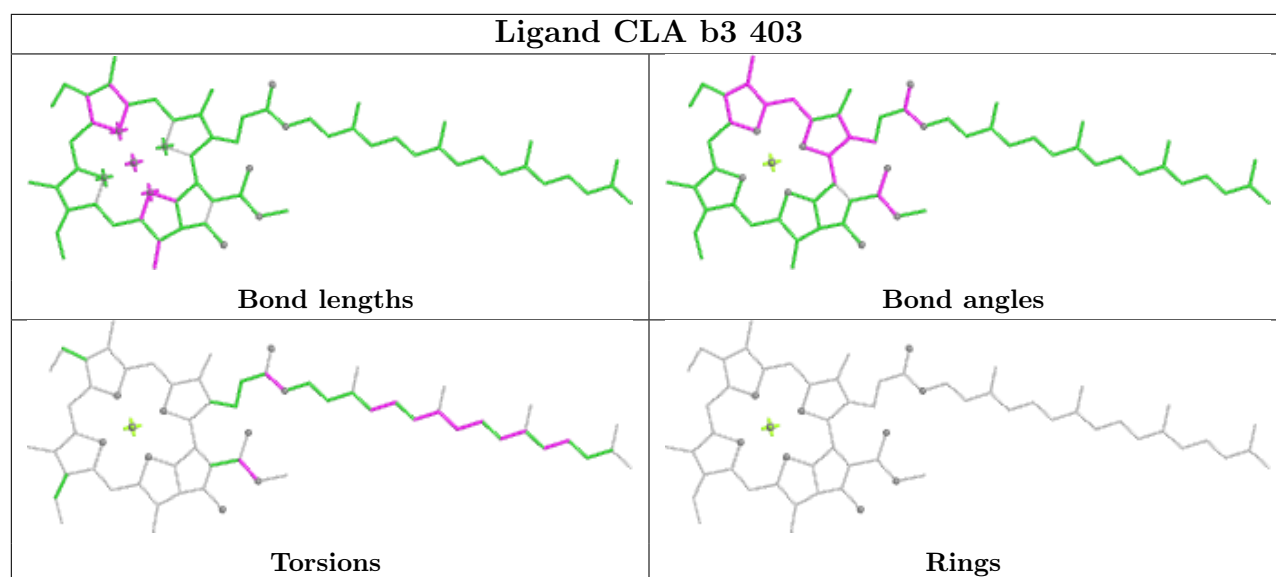


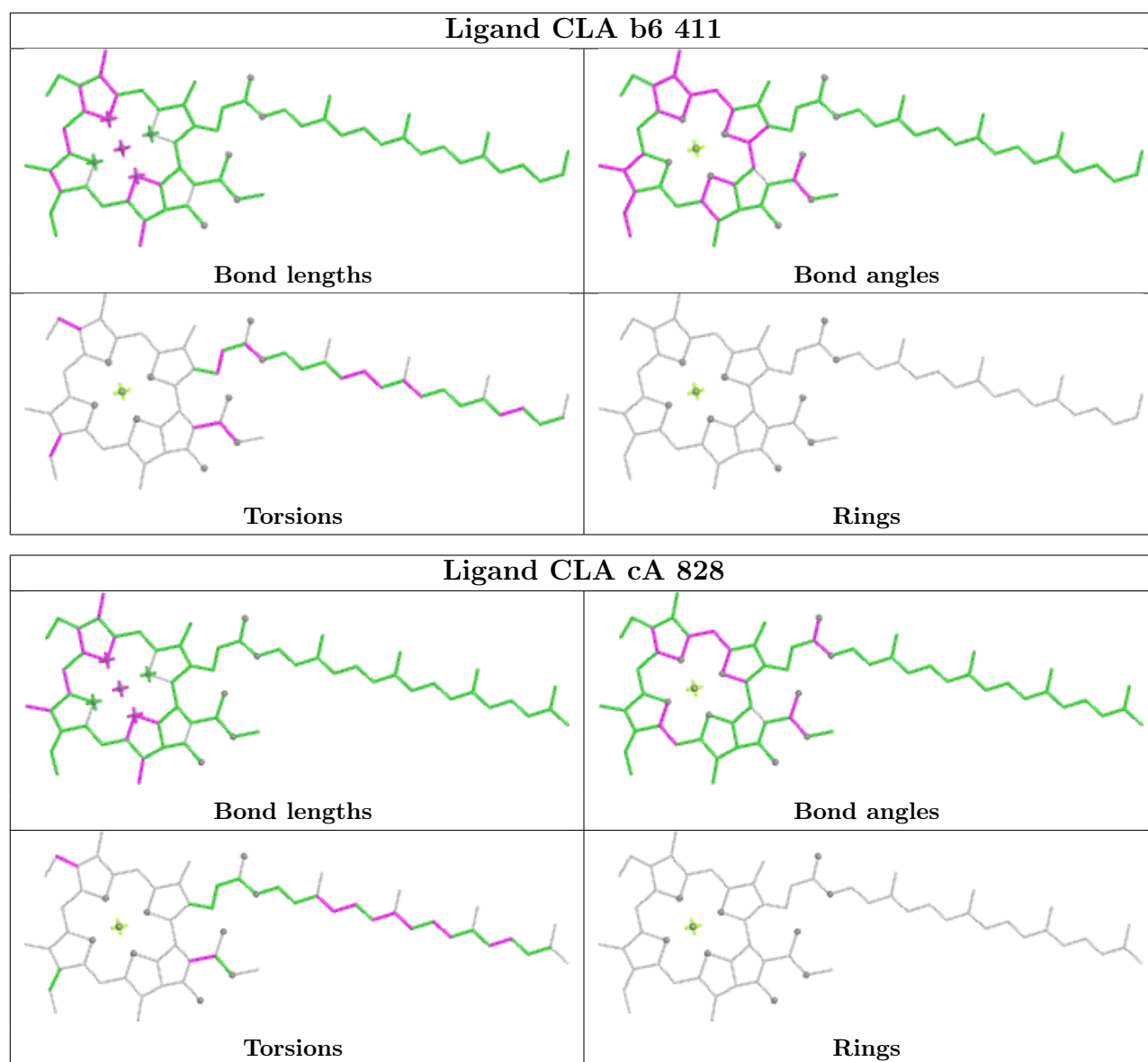


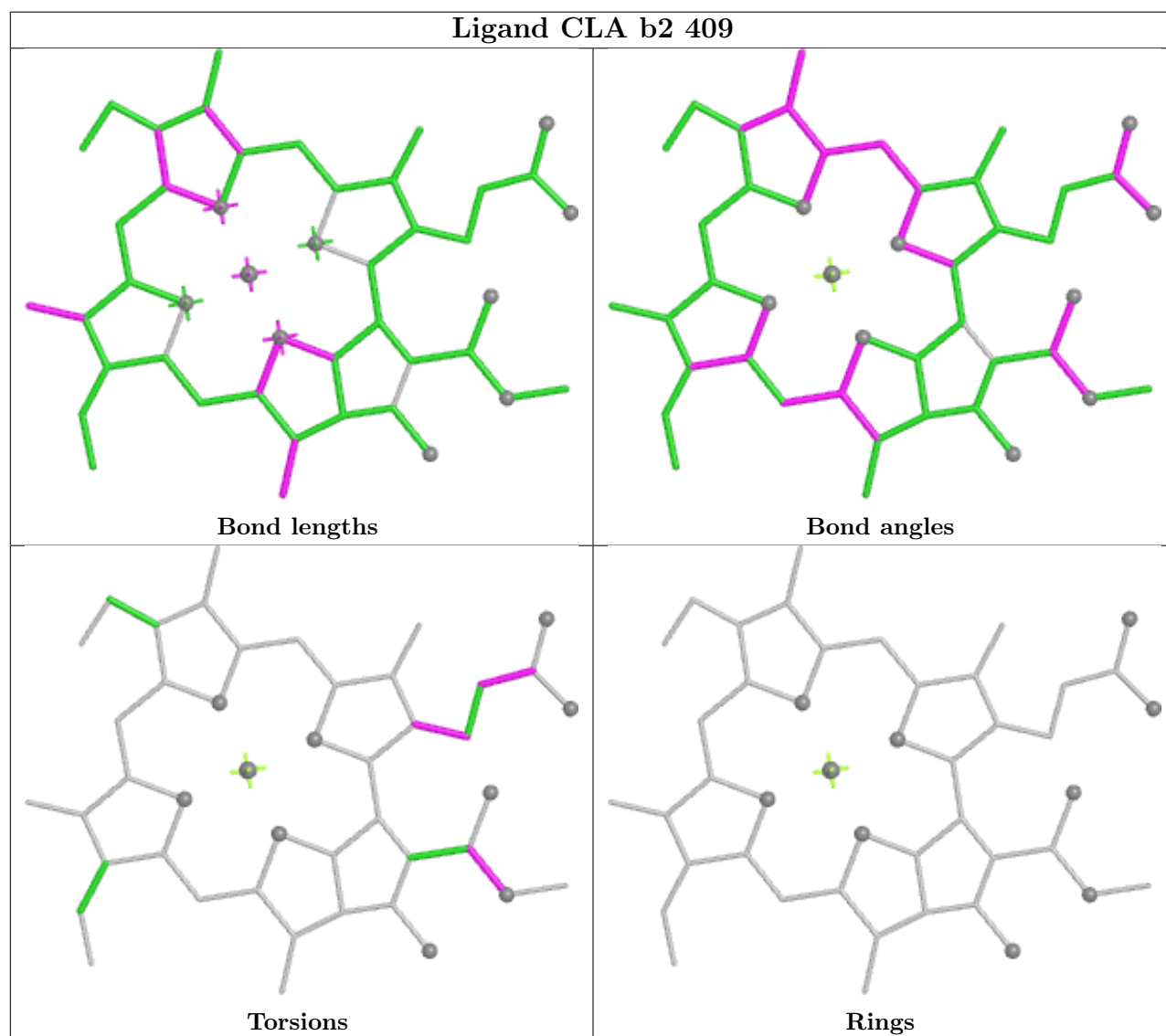
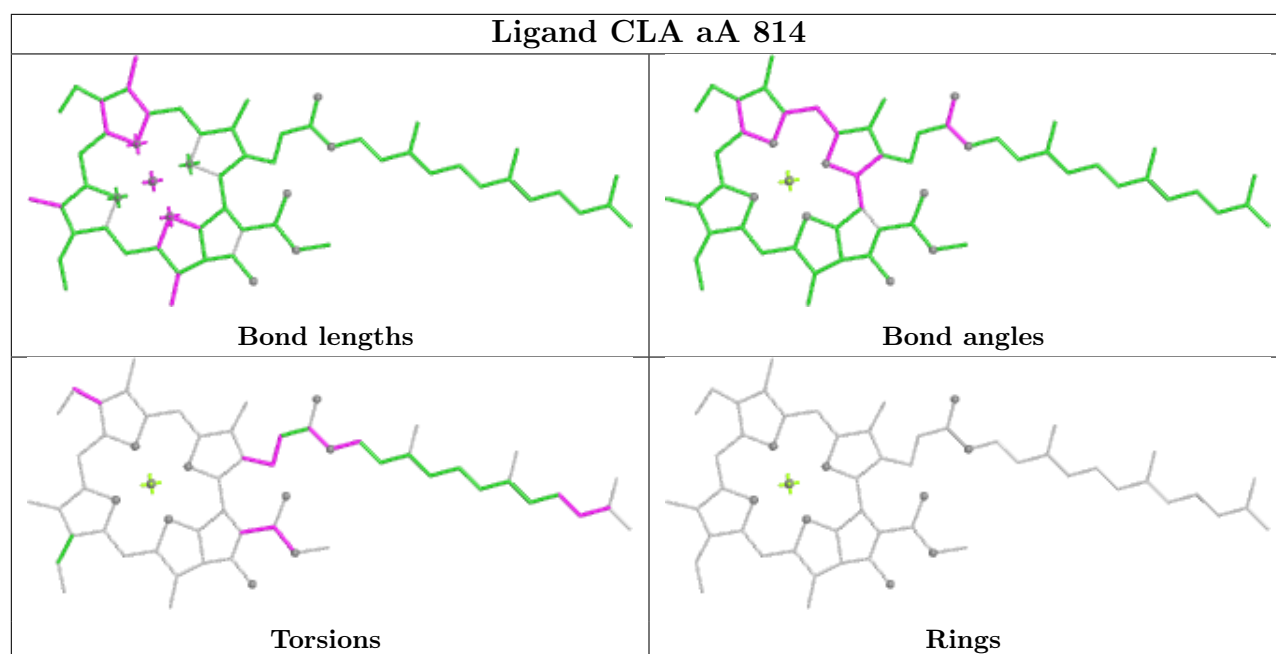


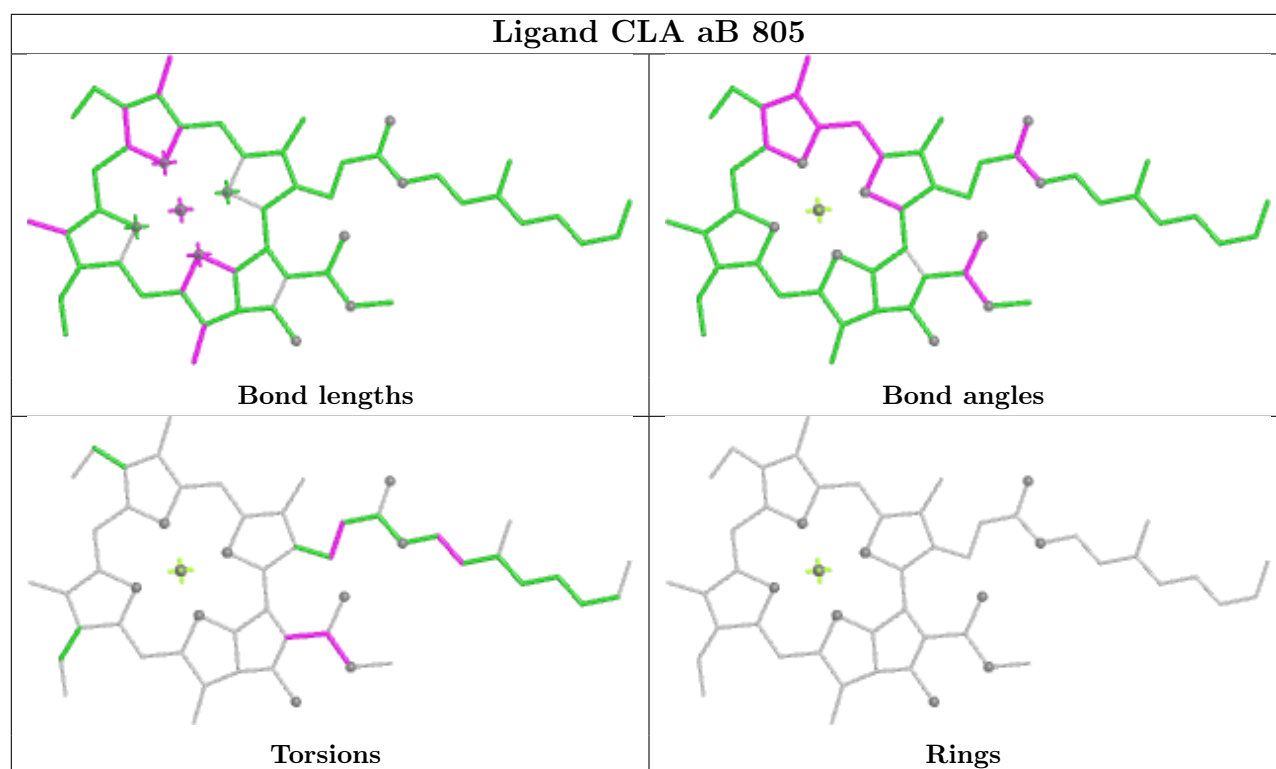


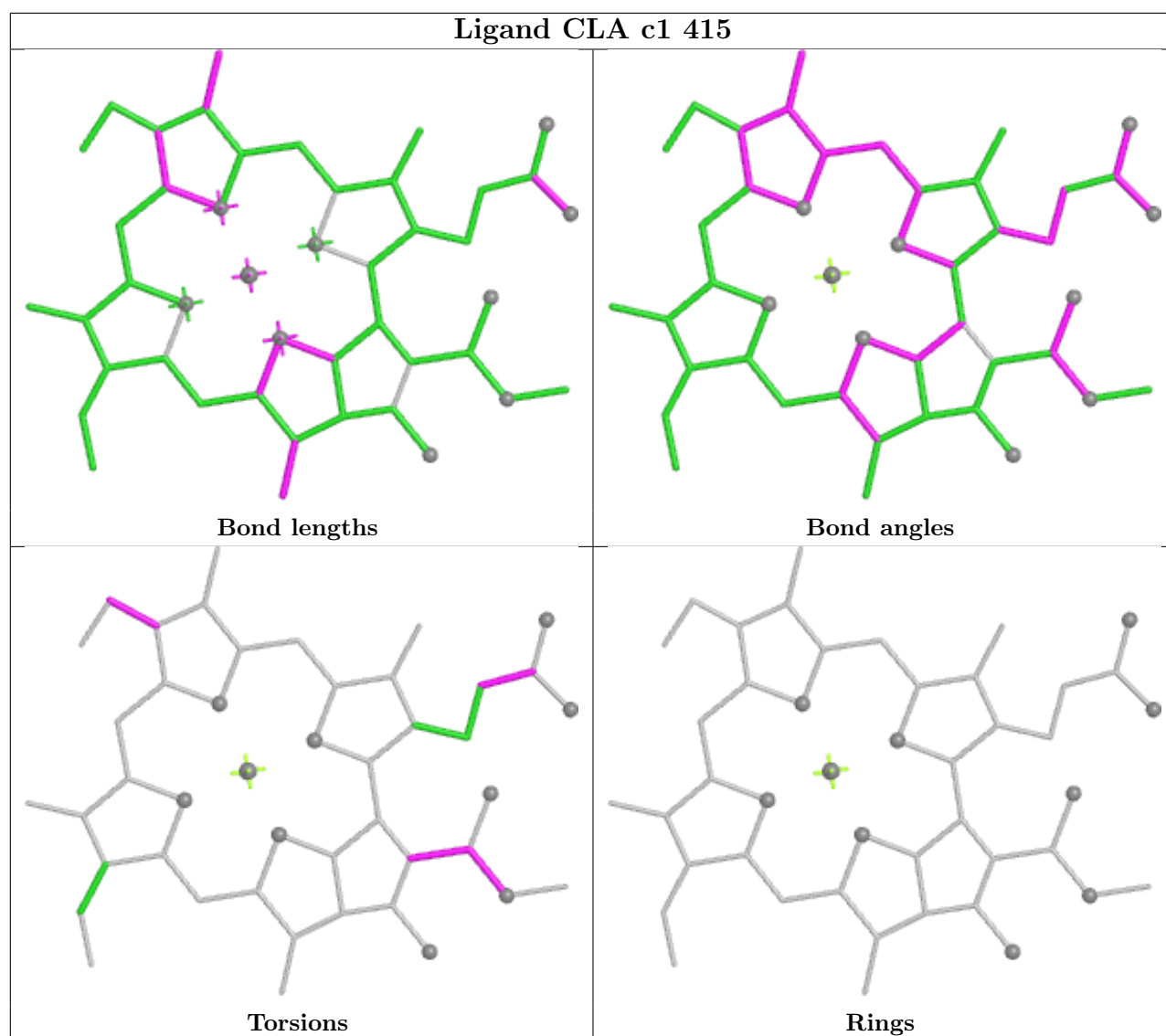


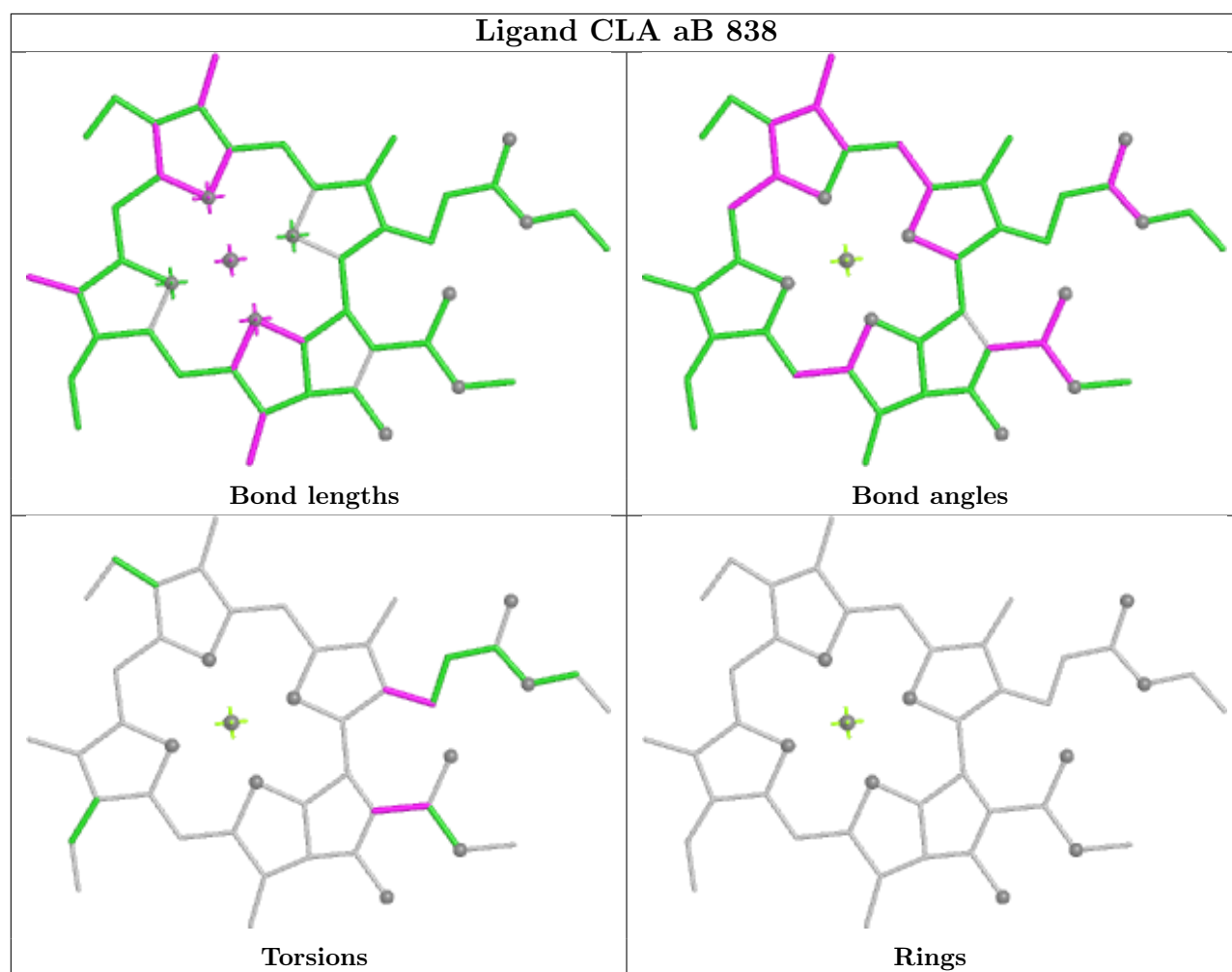


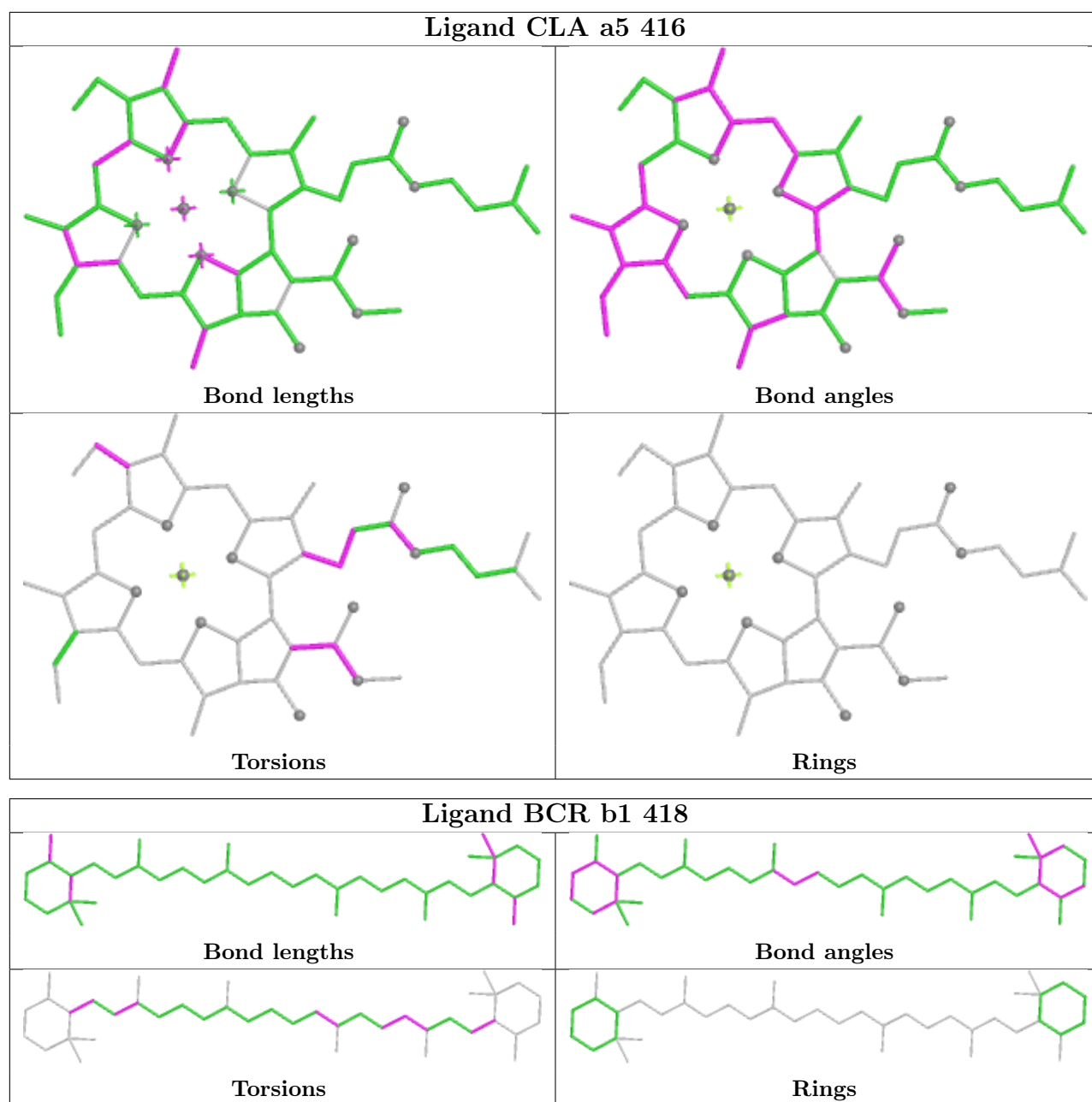


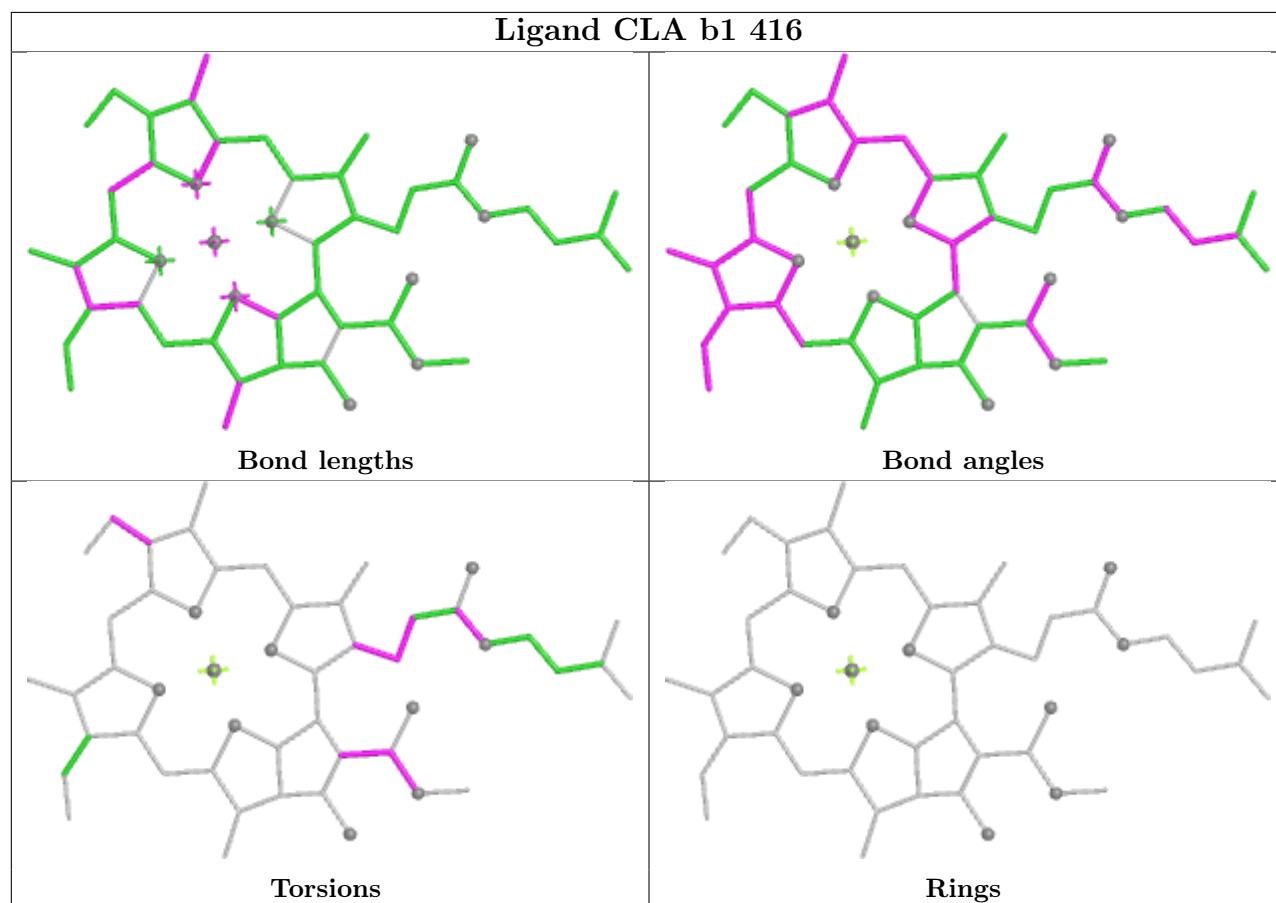
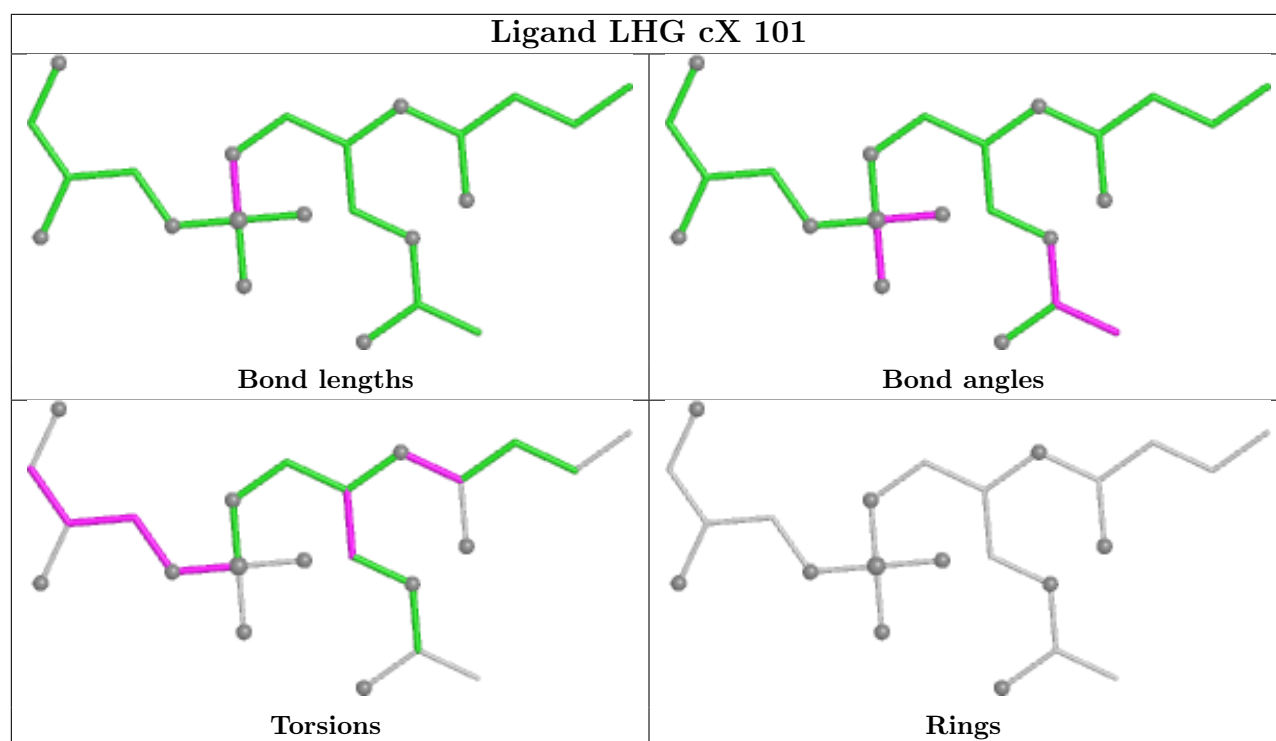


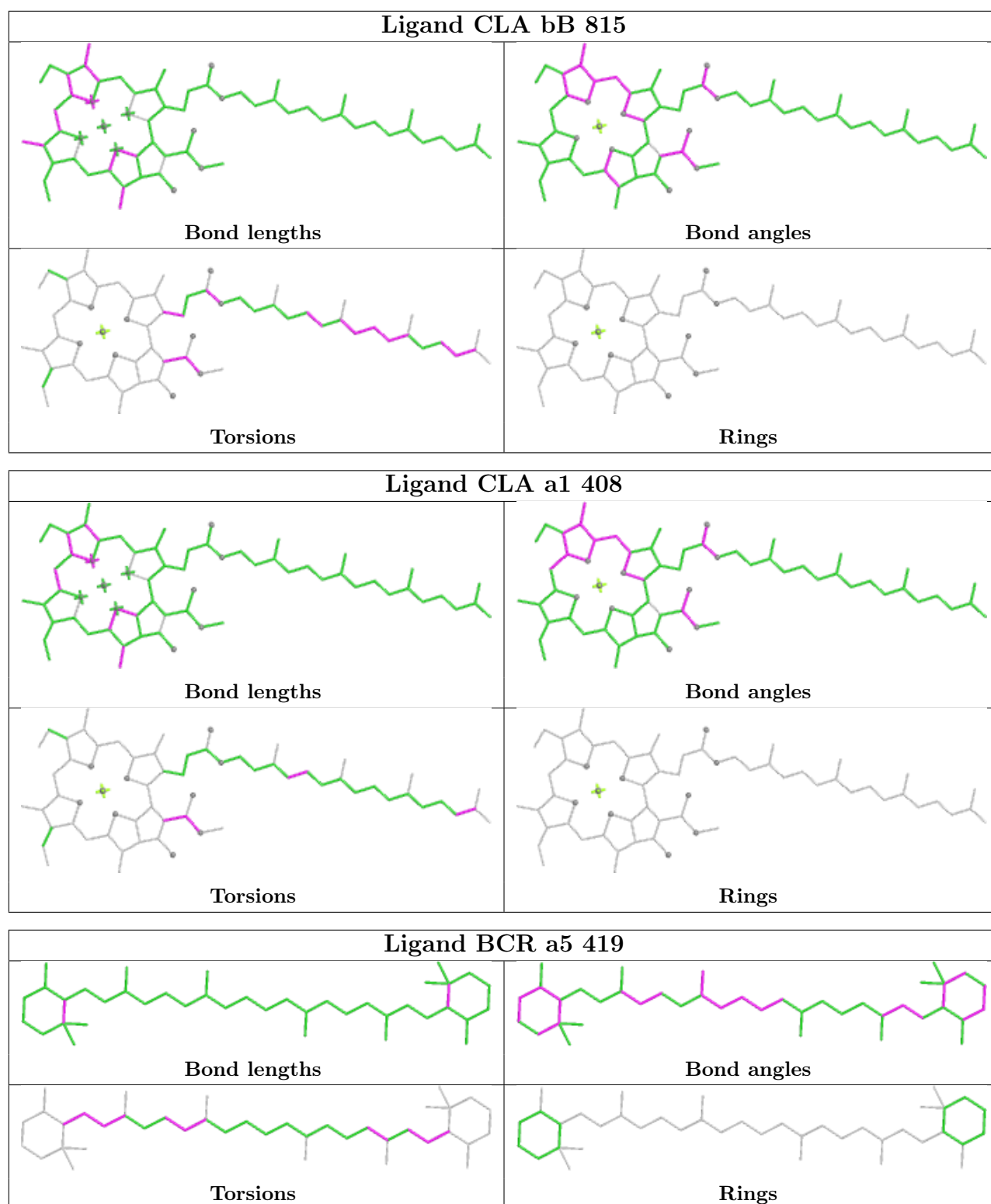


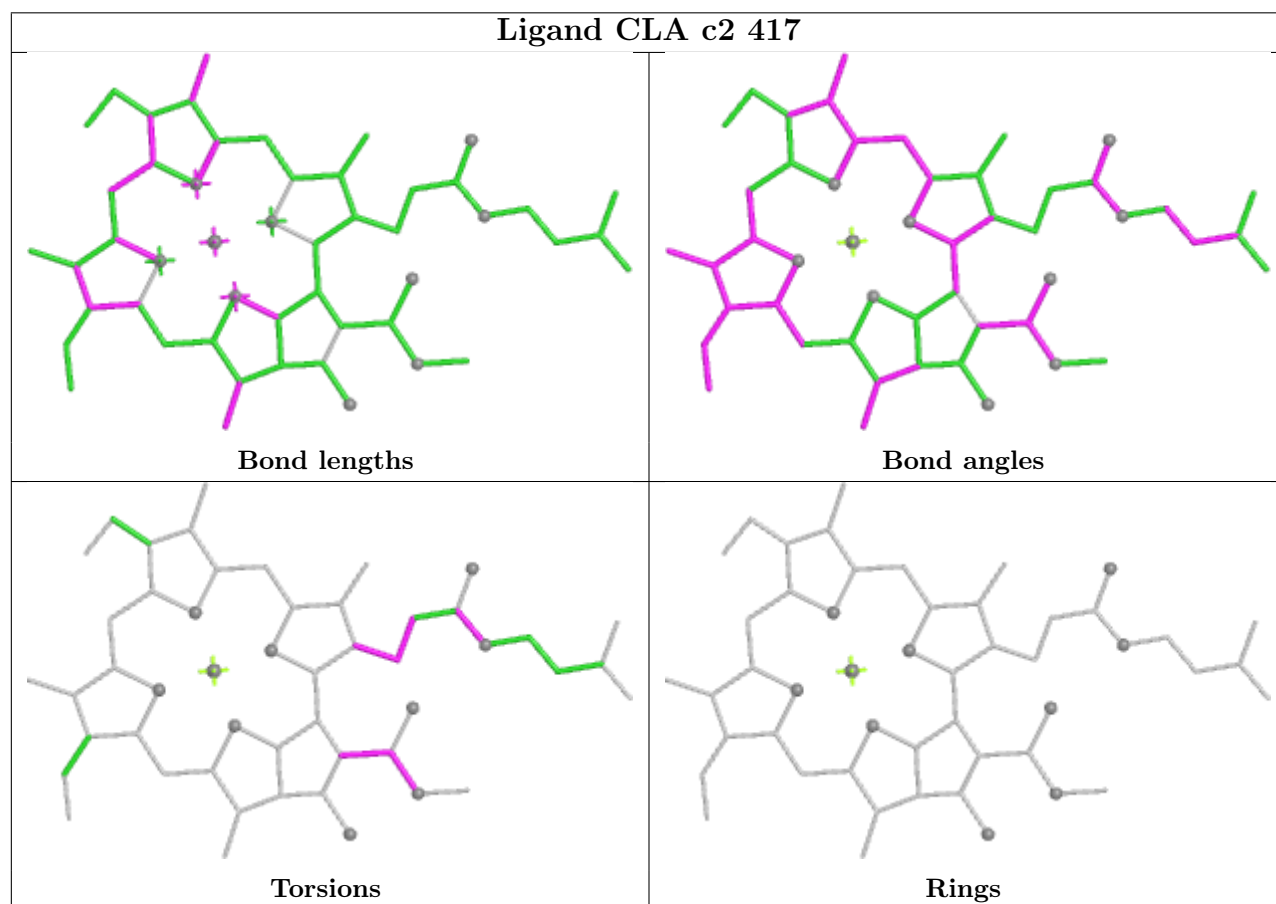
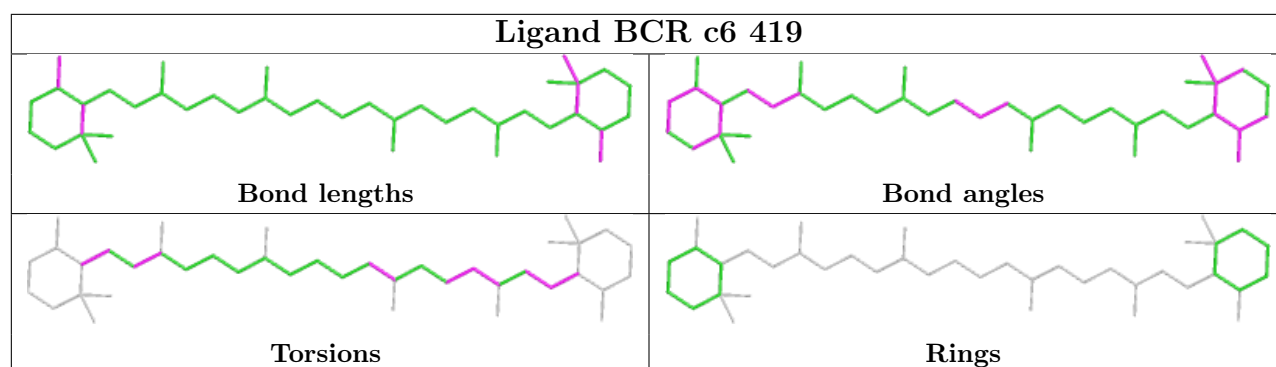


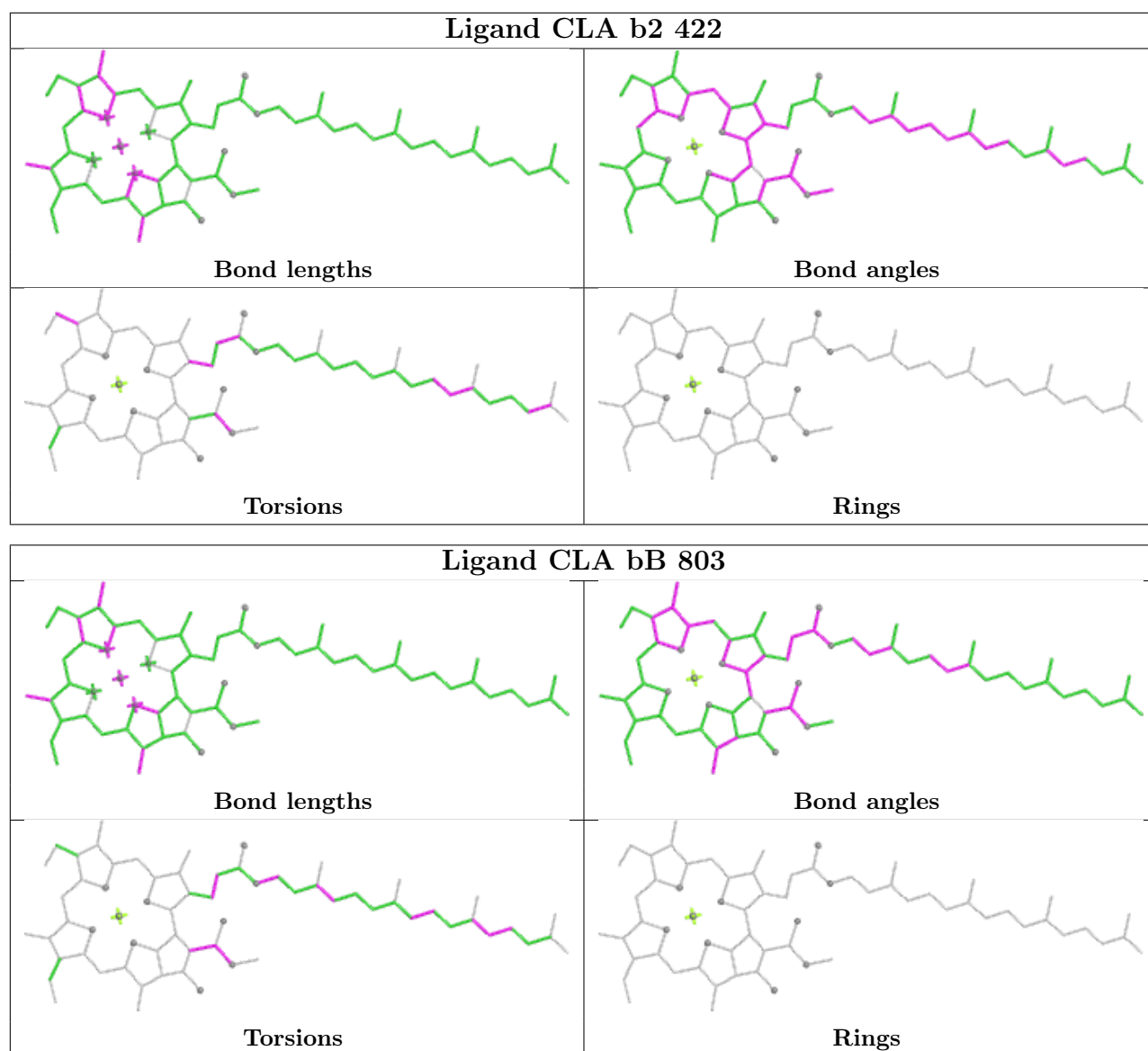




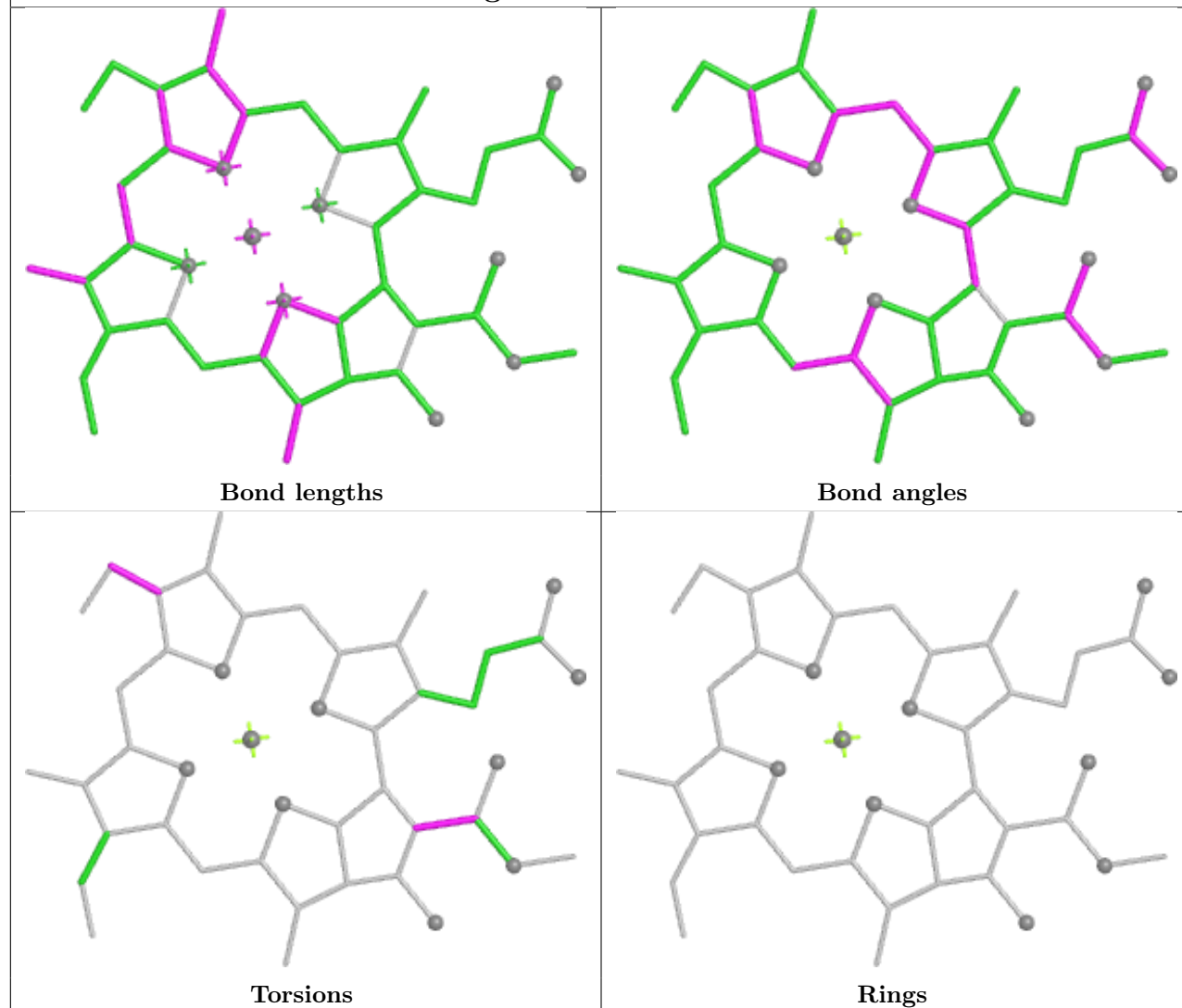




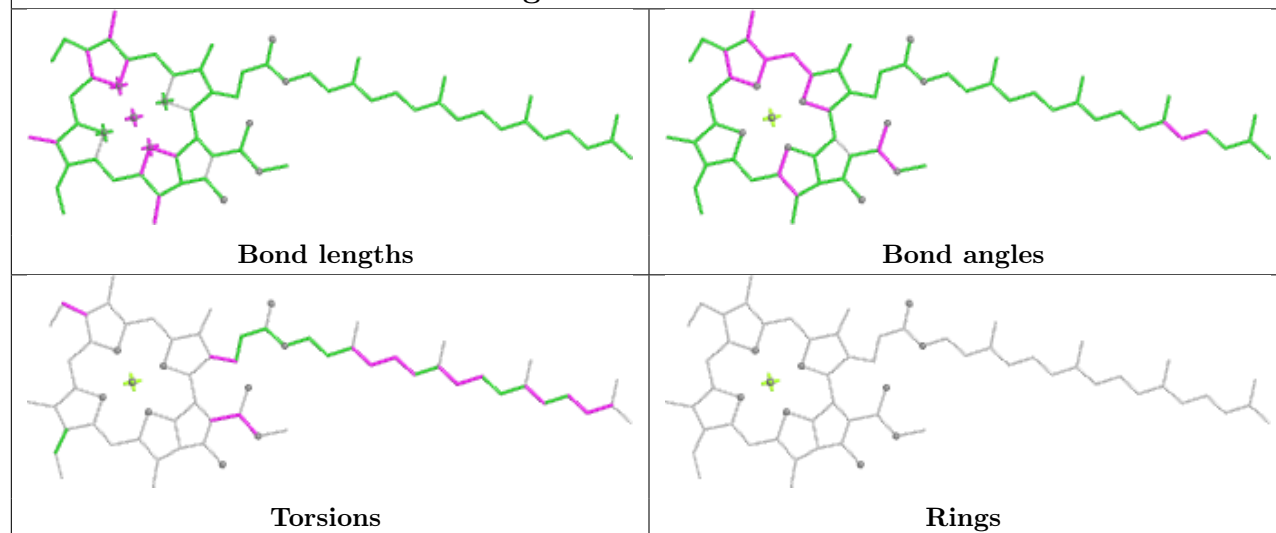


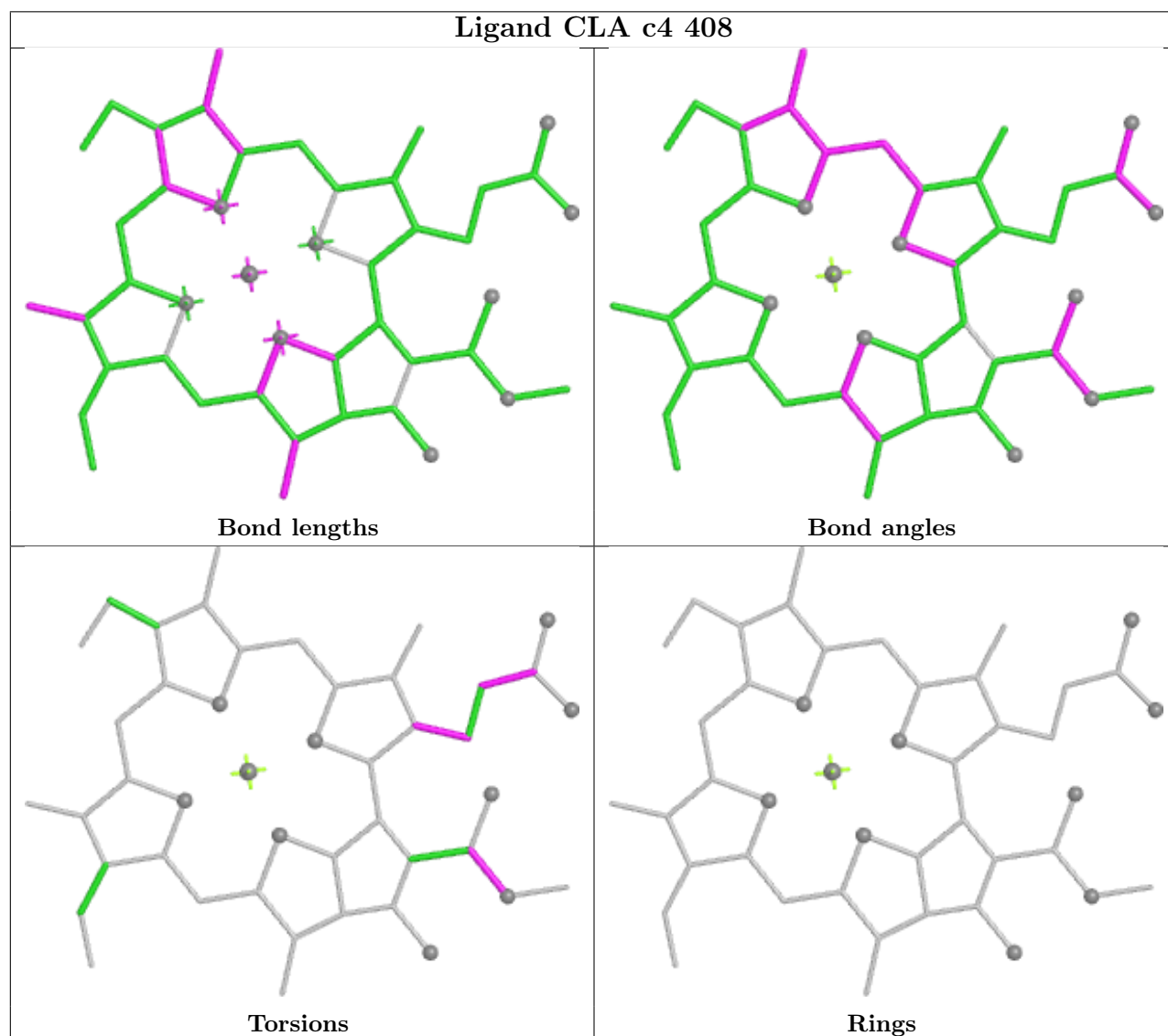
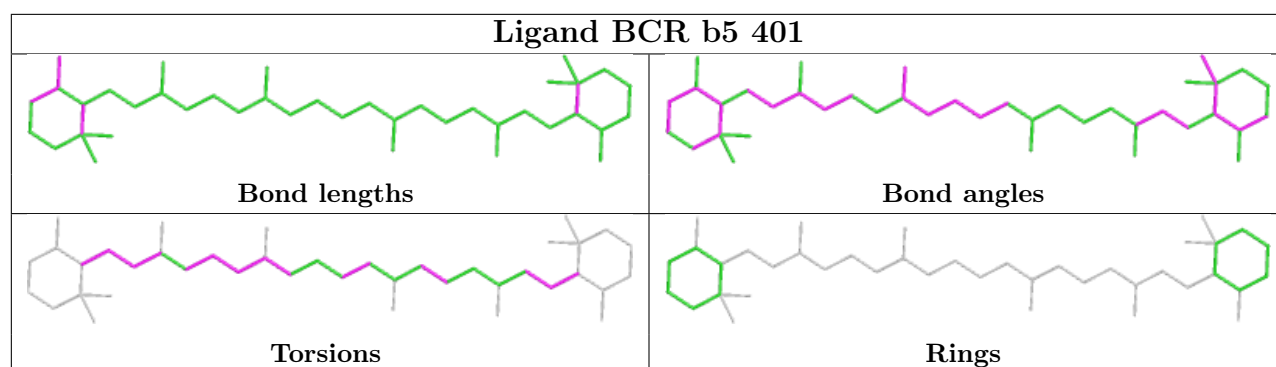


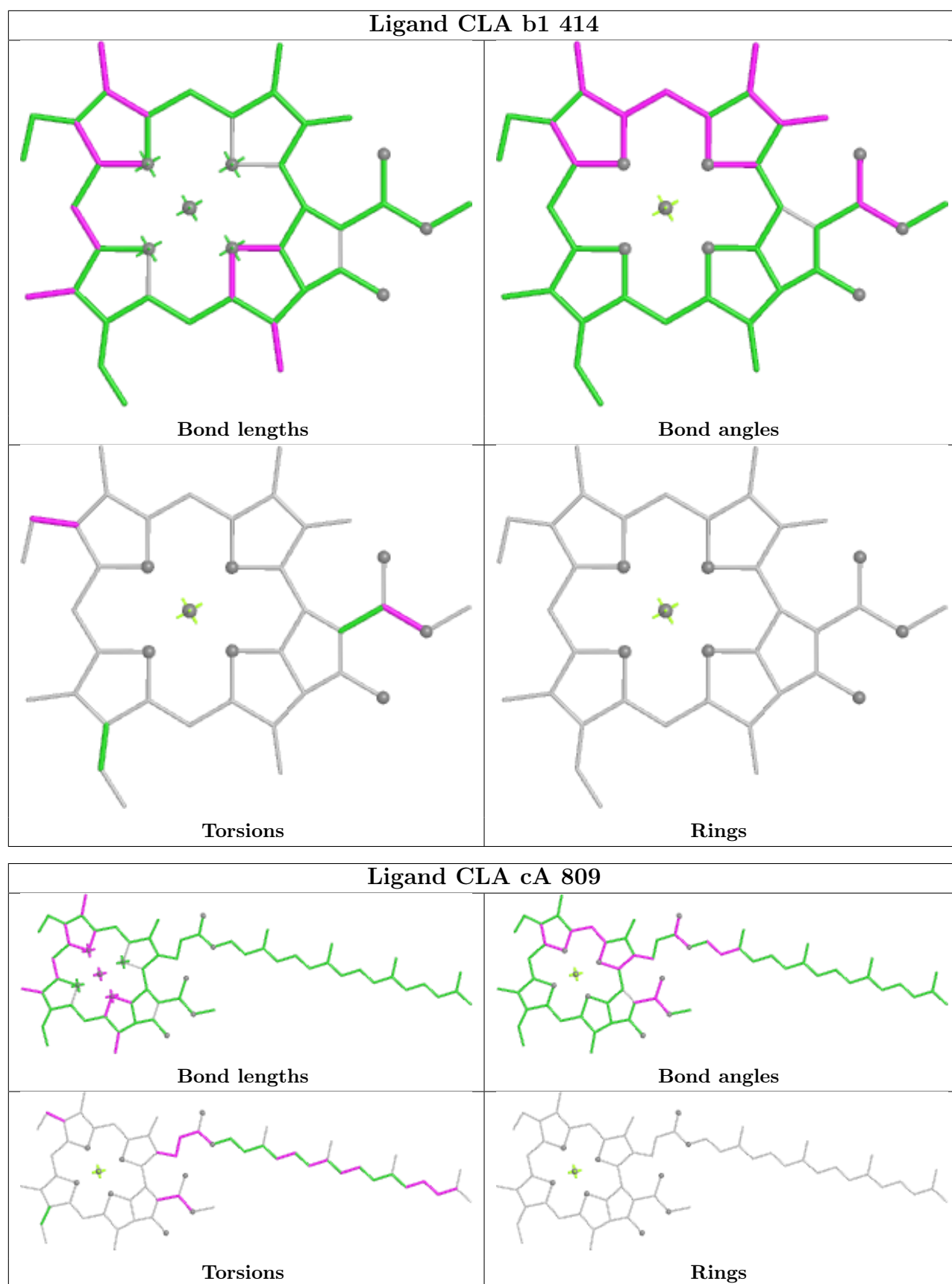
Ligand CLA aA 815

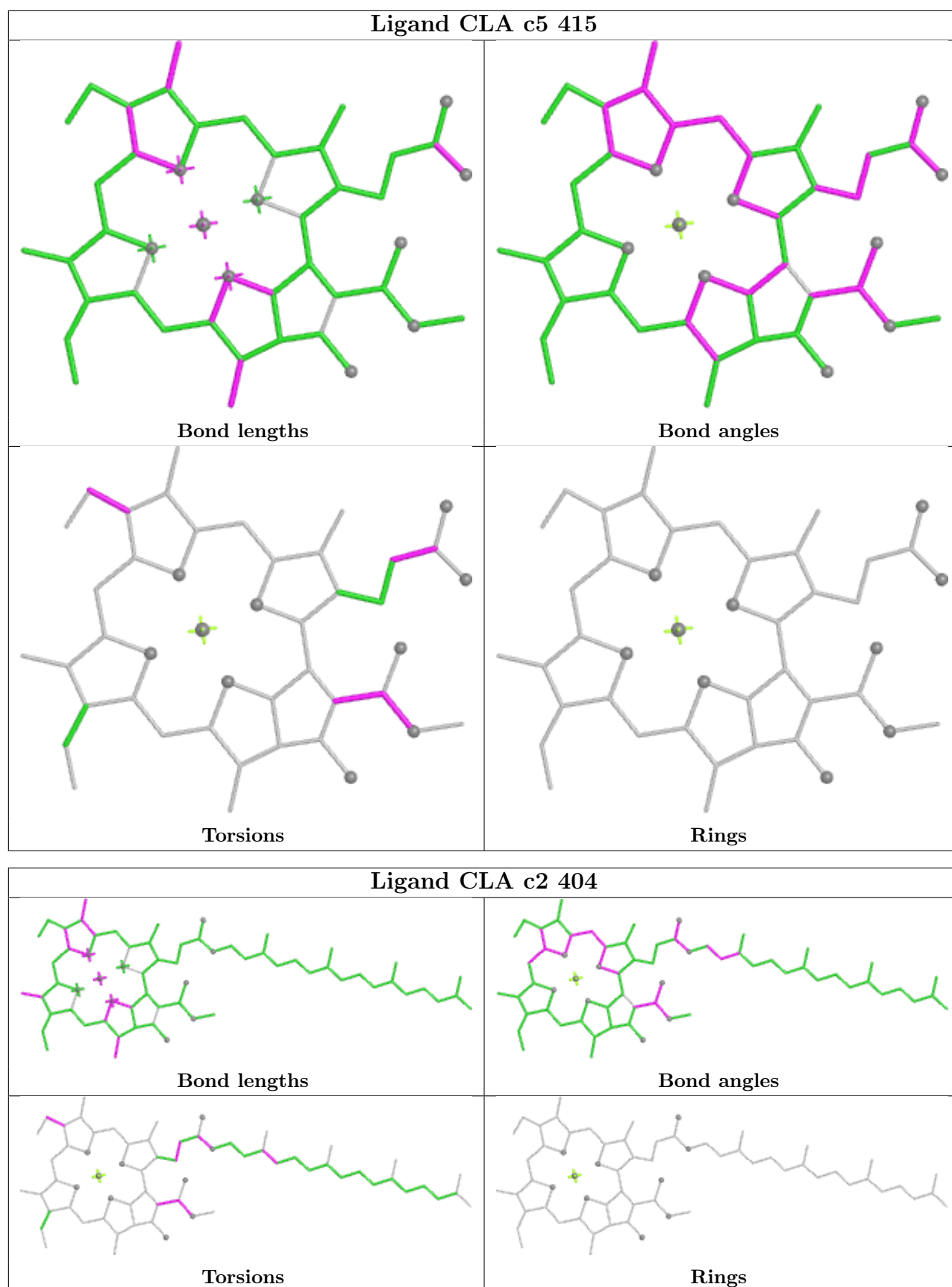


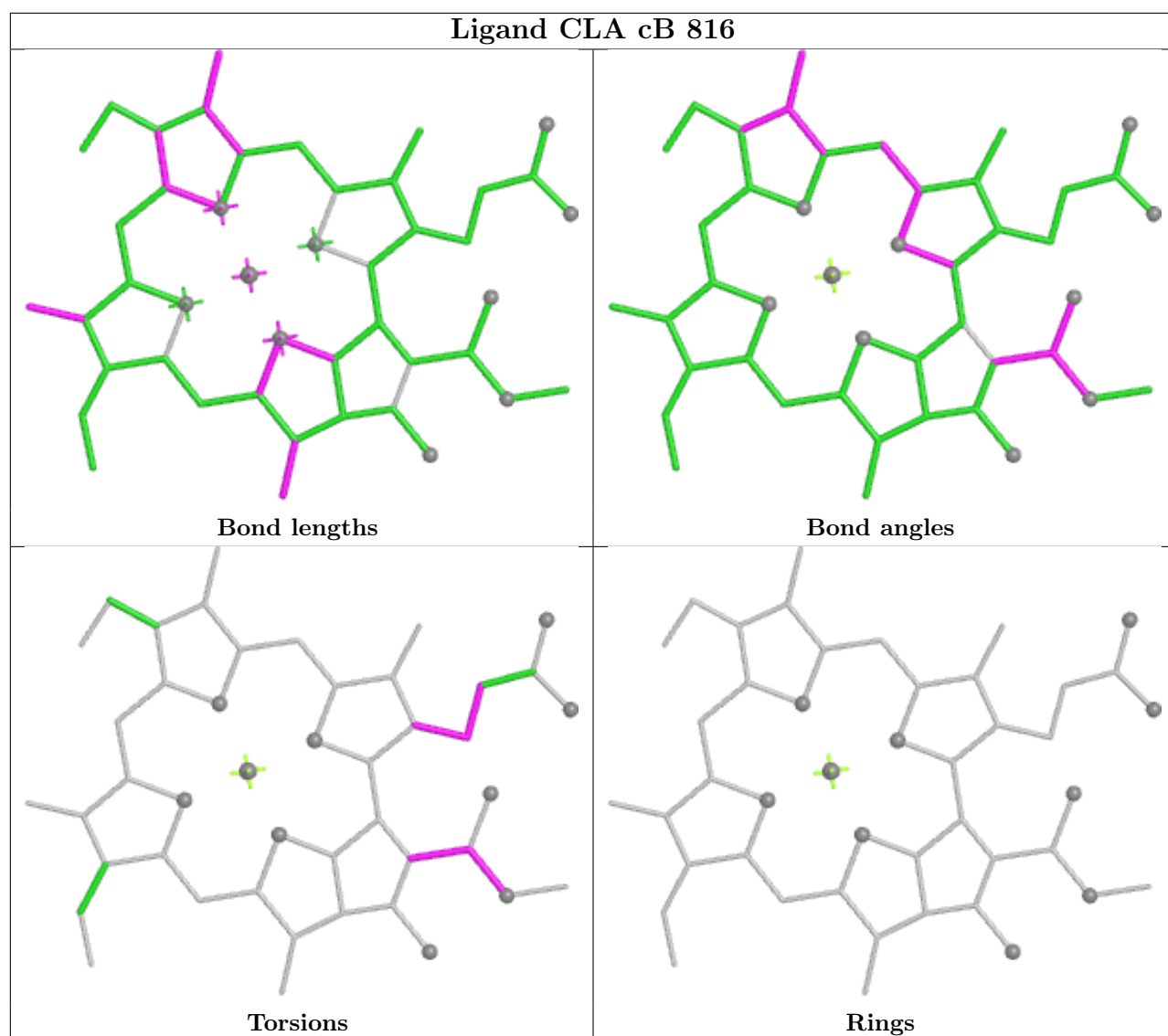
Ligand CLA aA 822

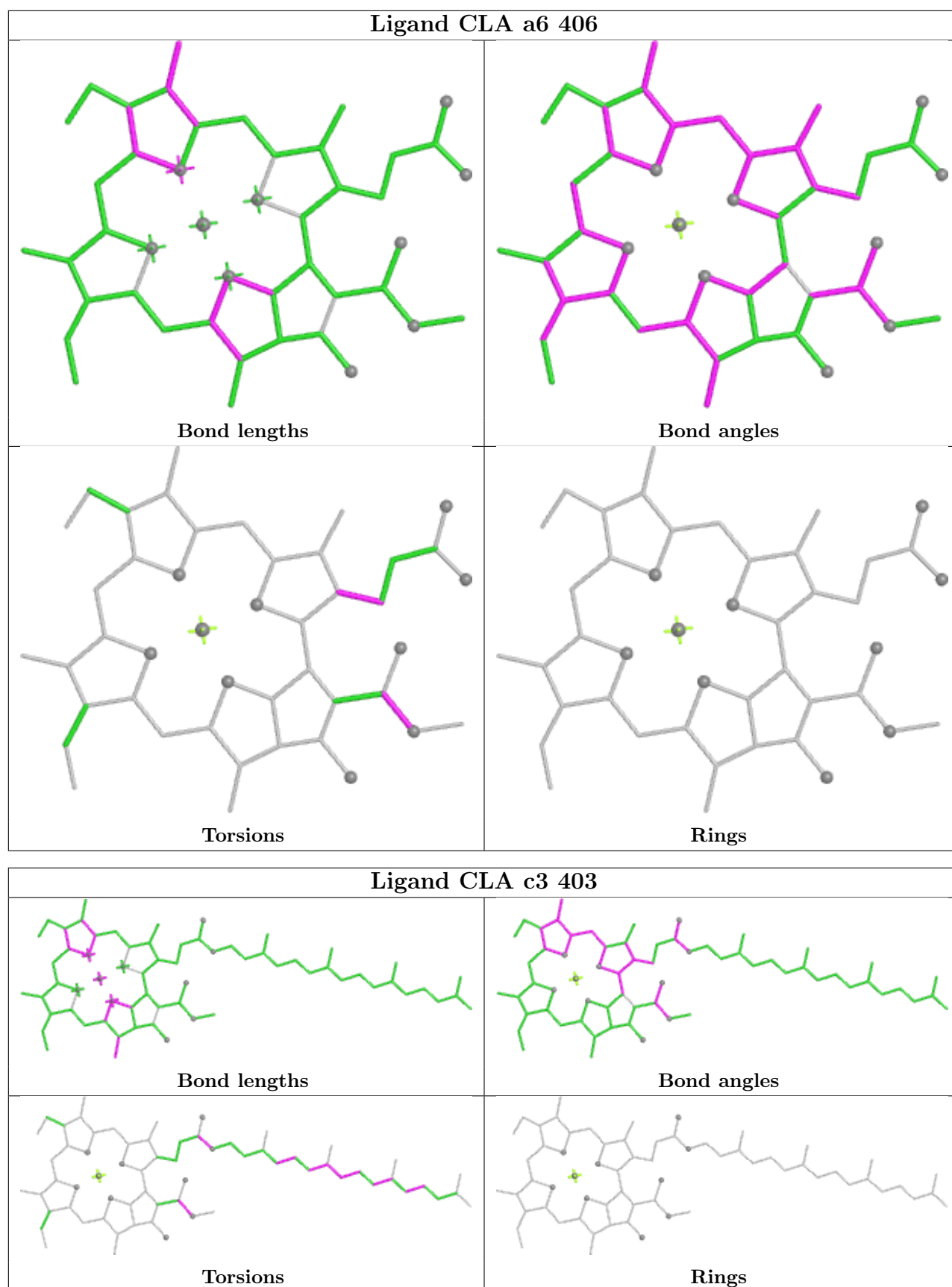


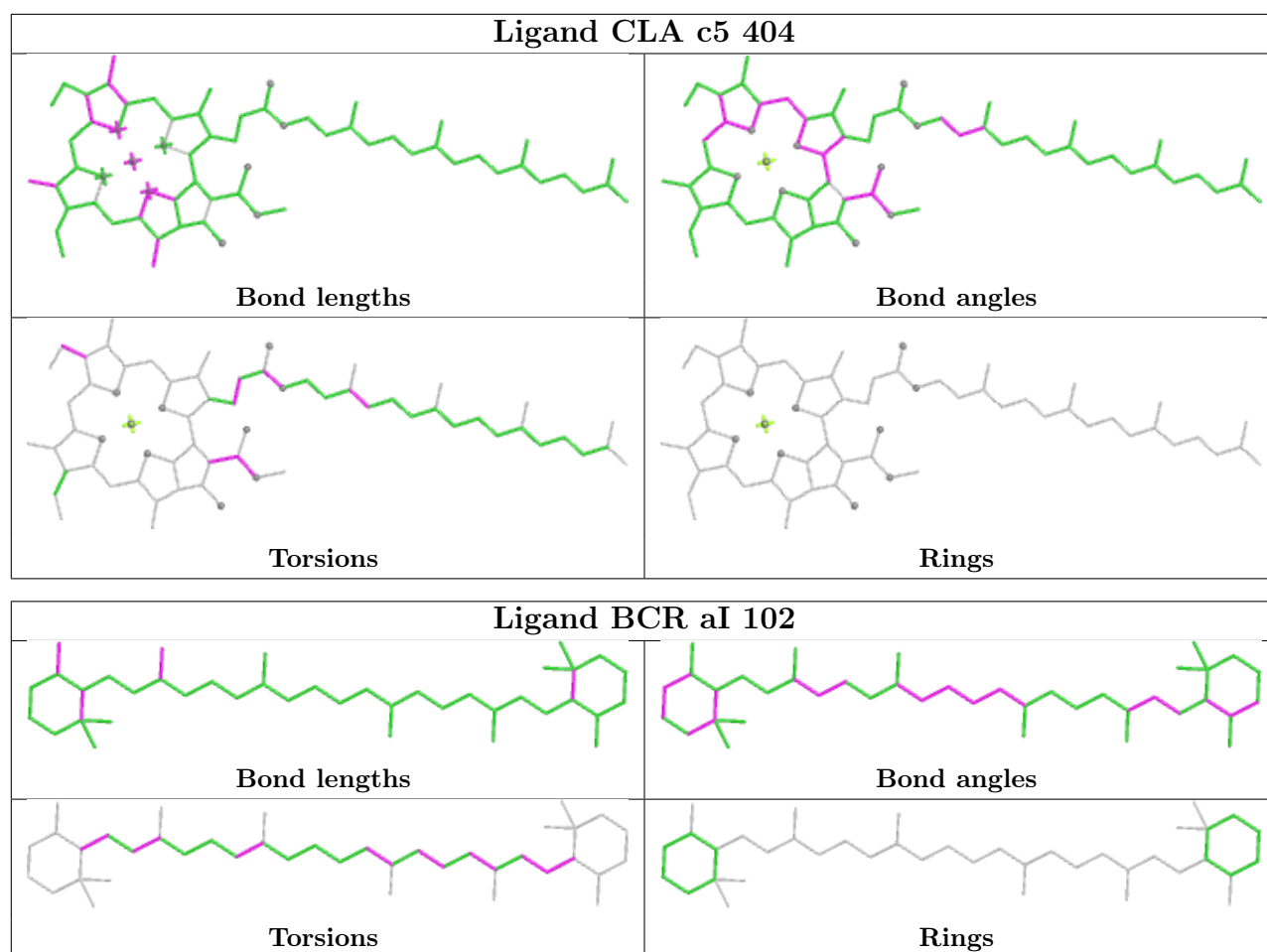


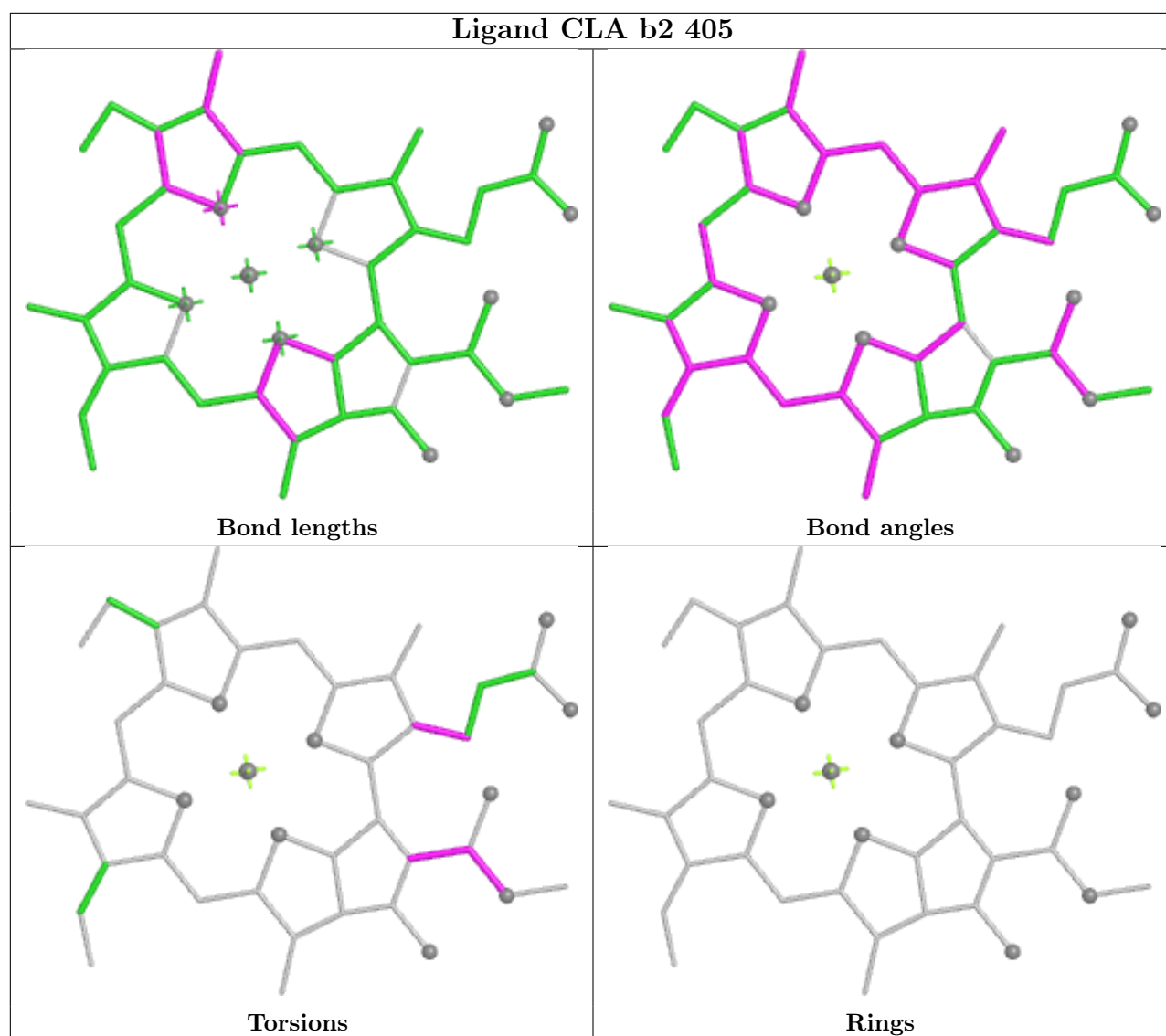


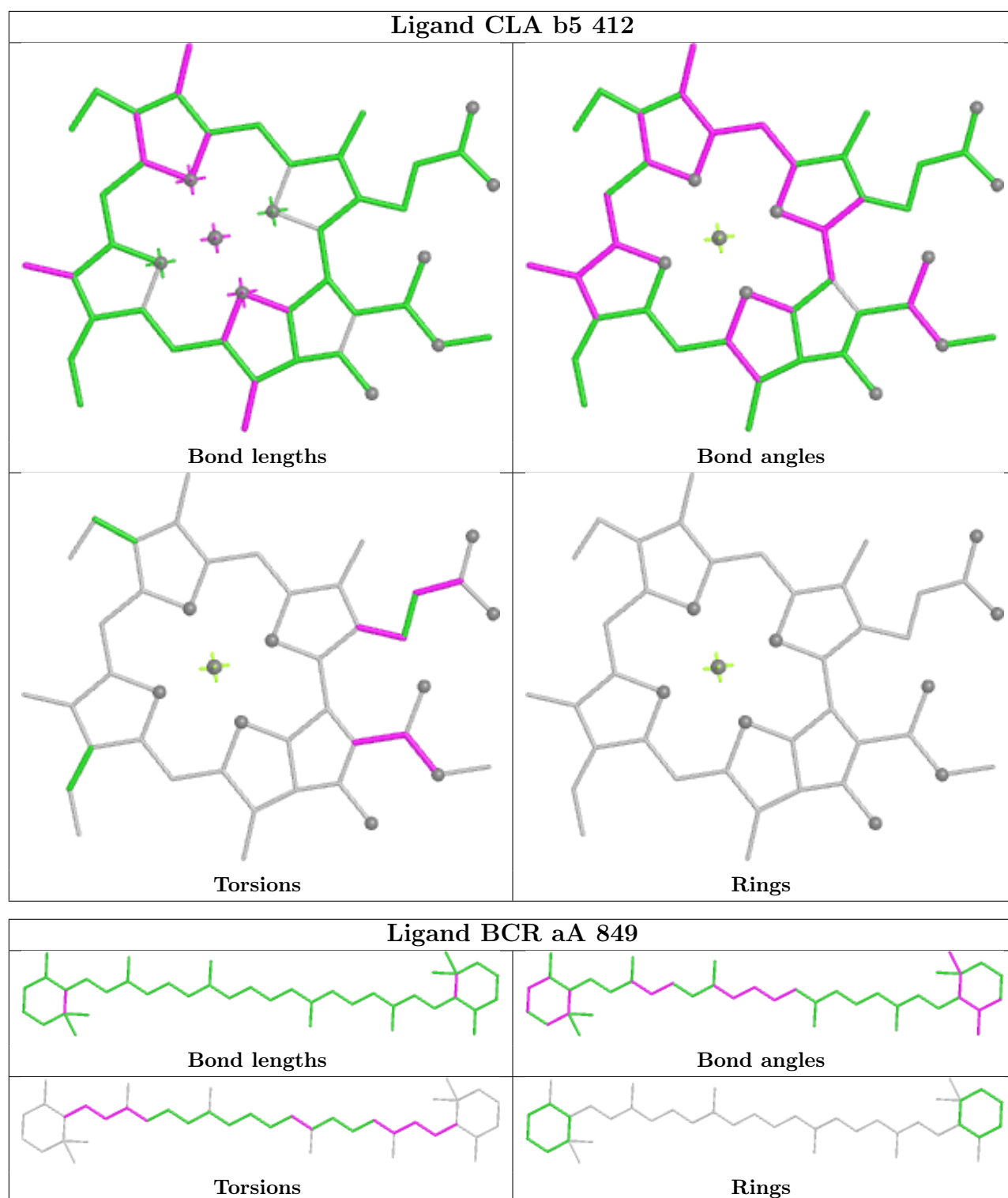


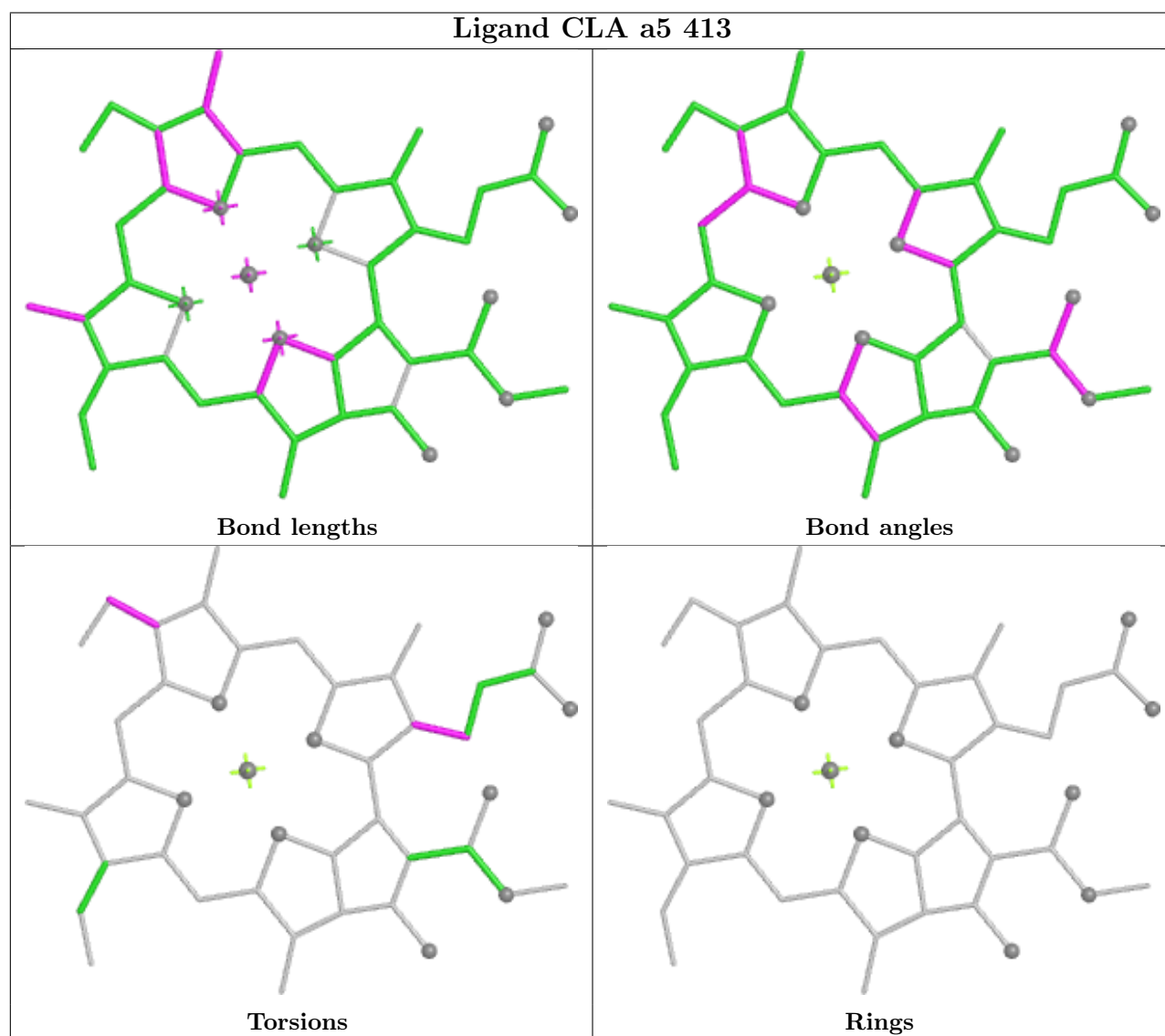
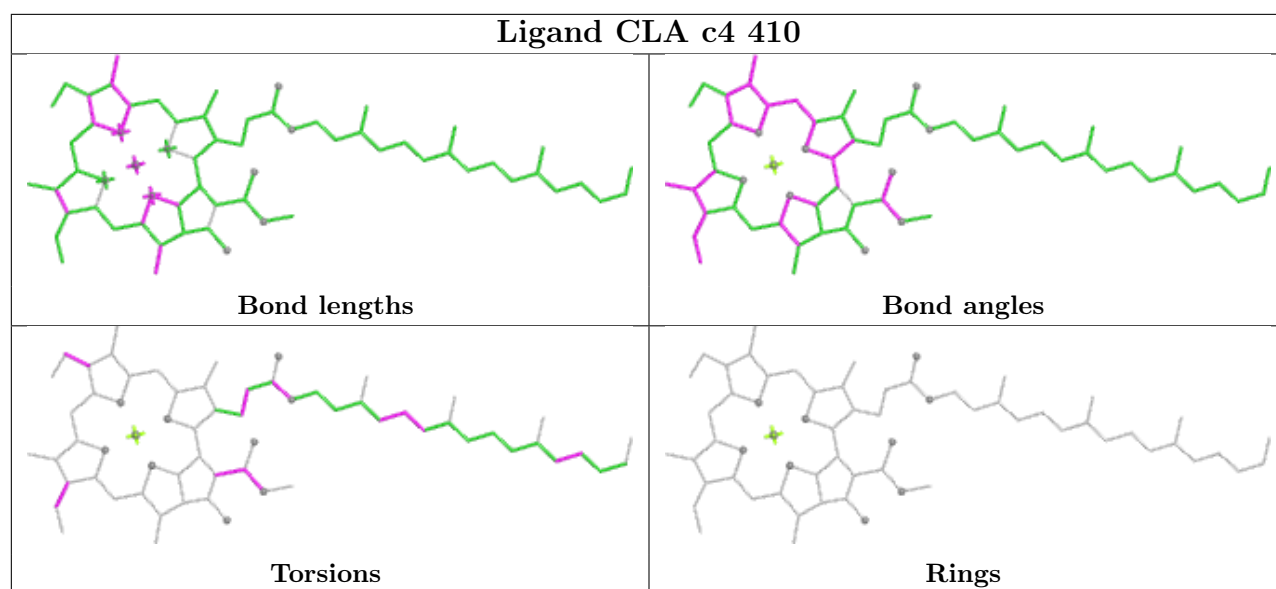


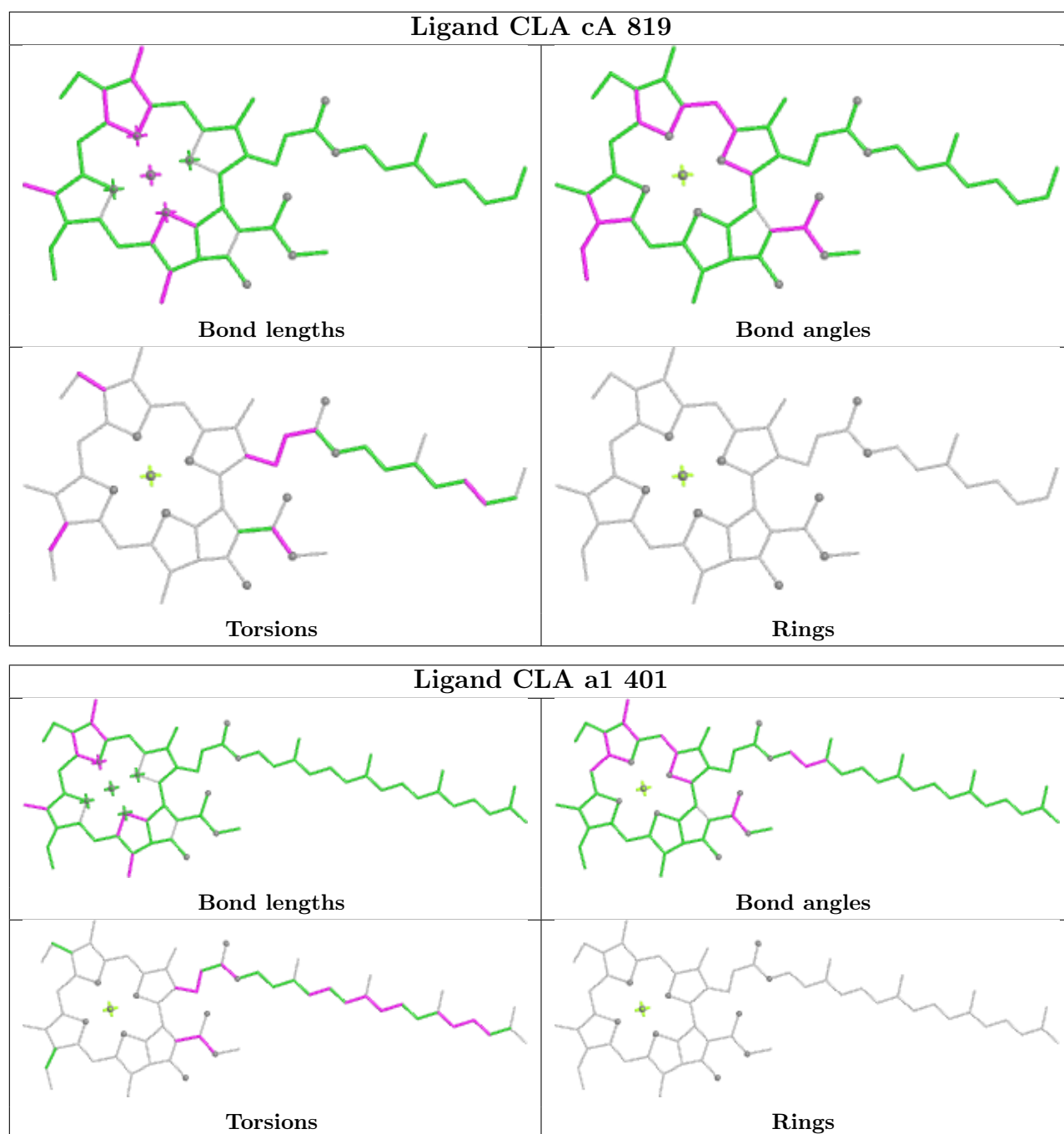


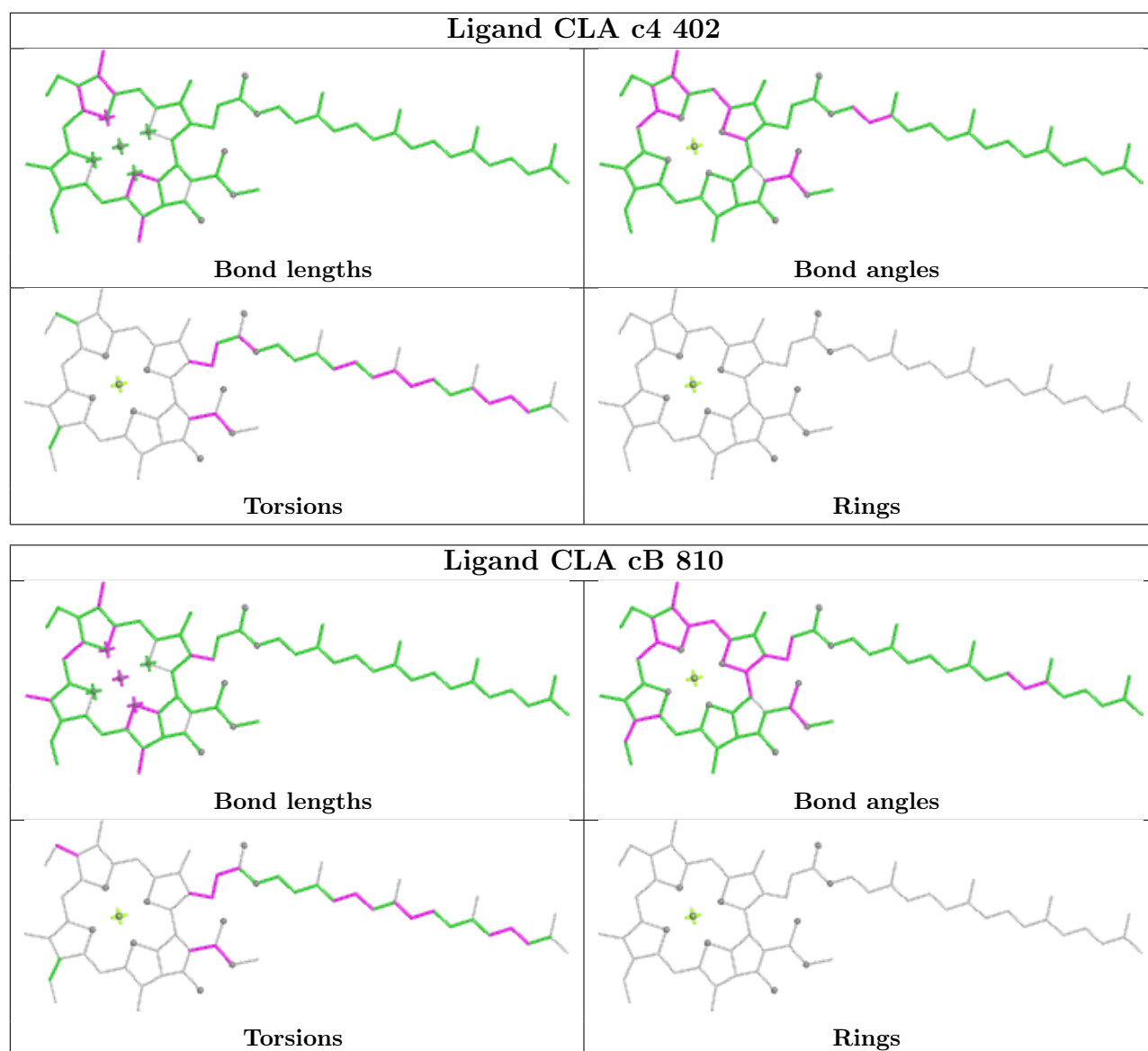


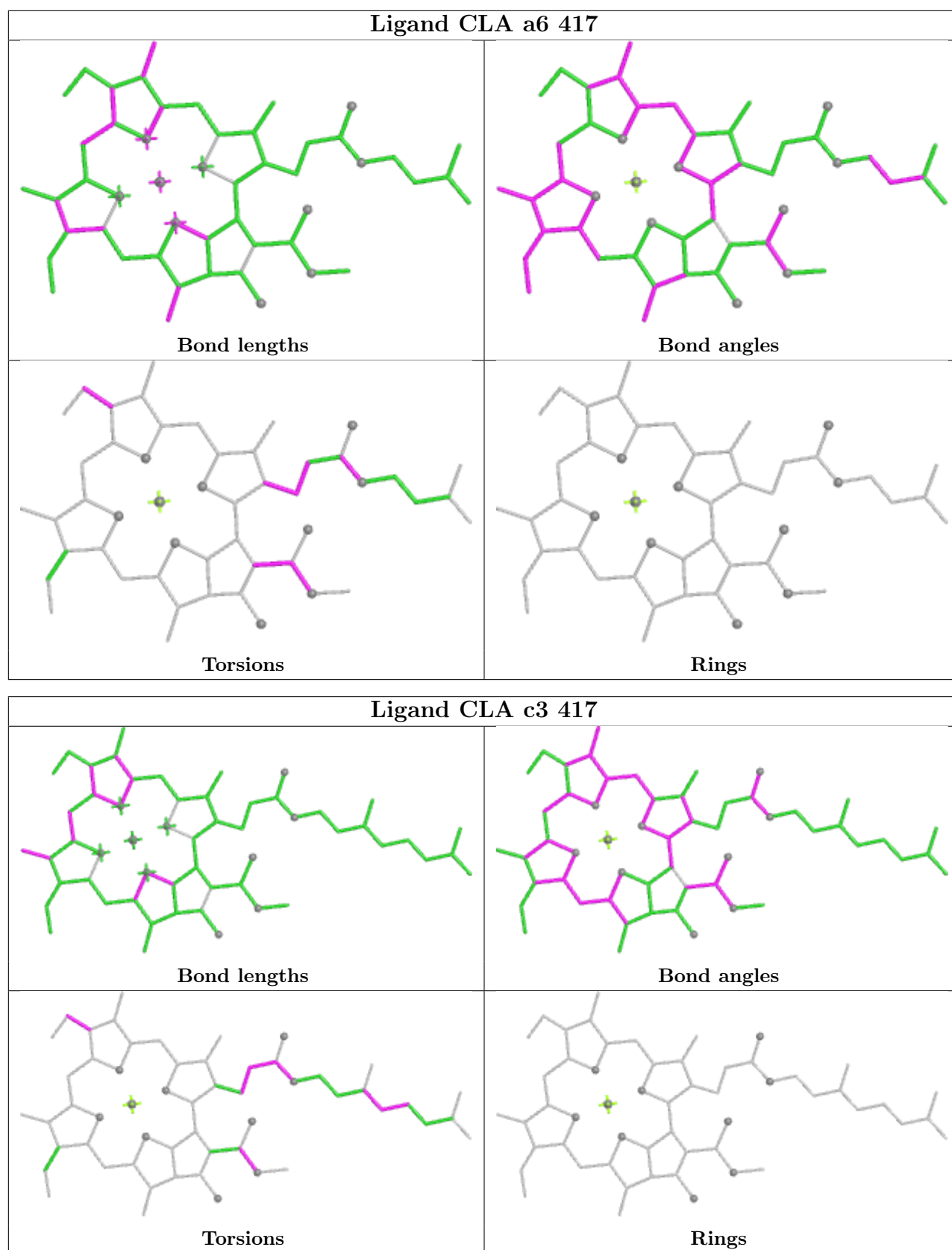


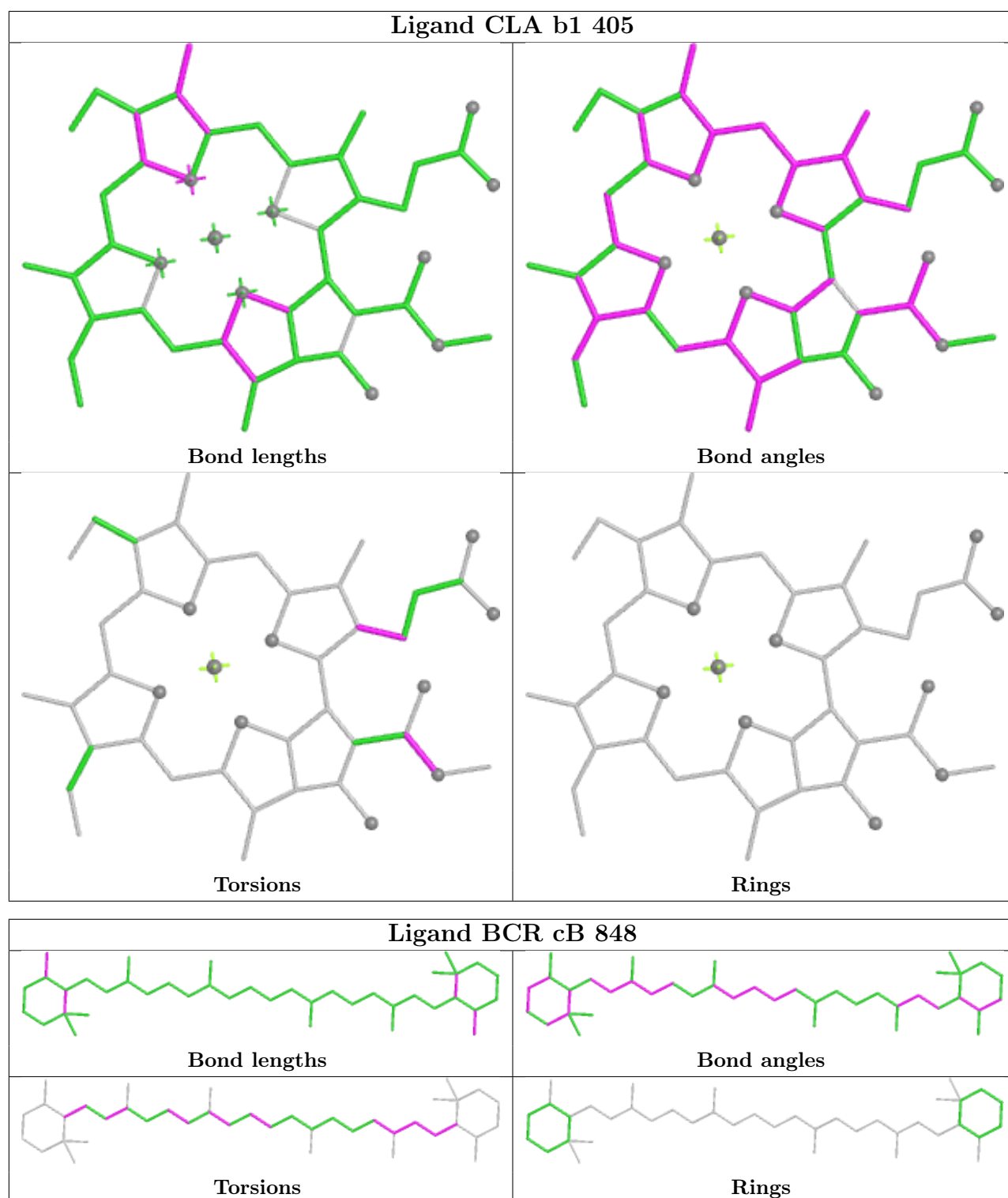


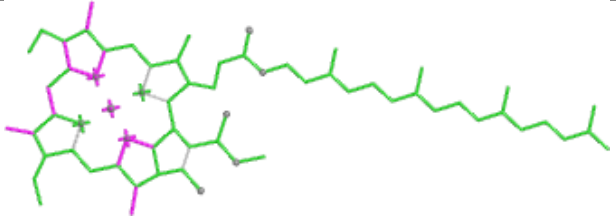
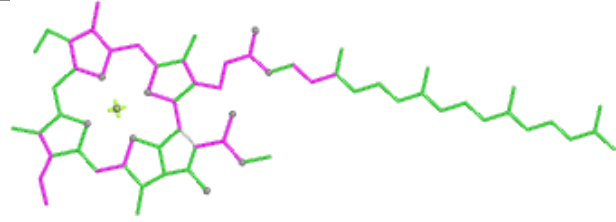
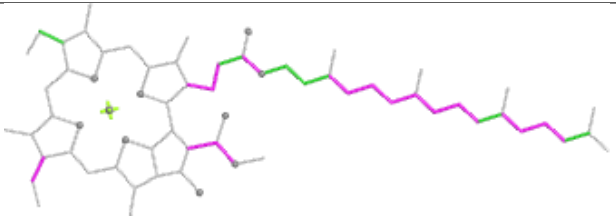
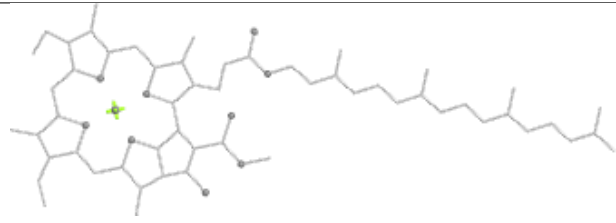
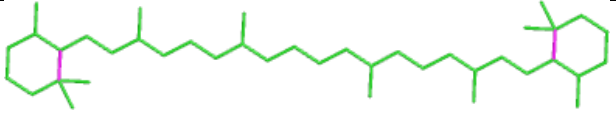
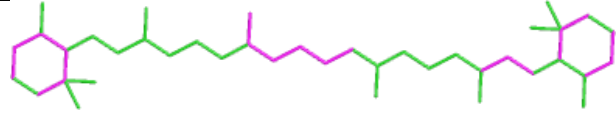
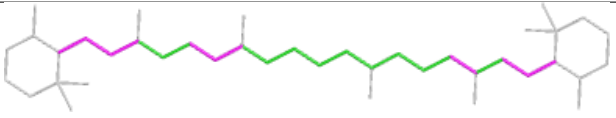
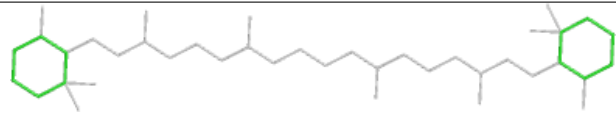
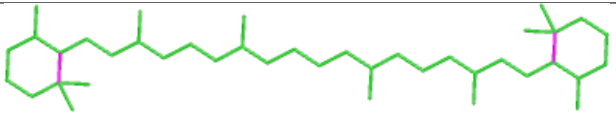
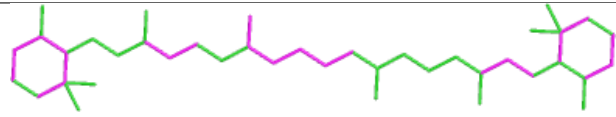
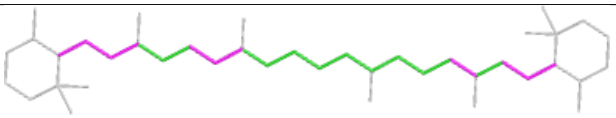
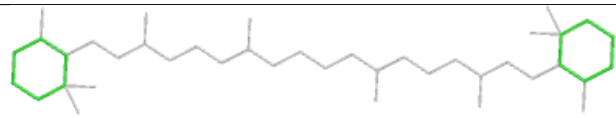




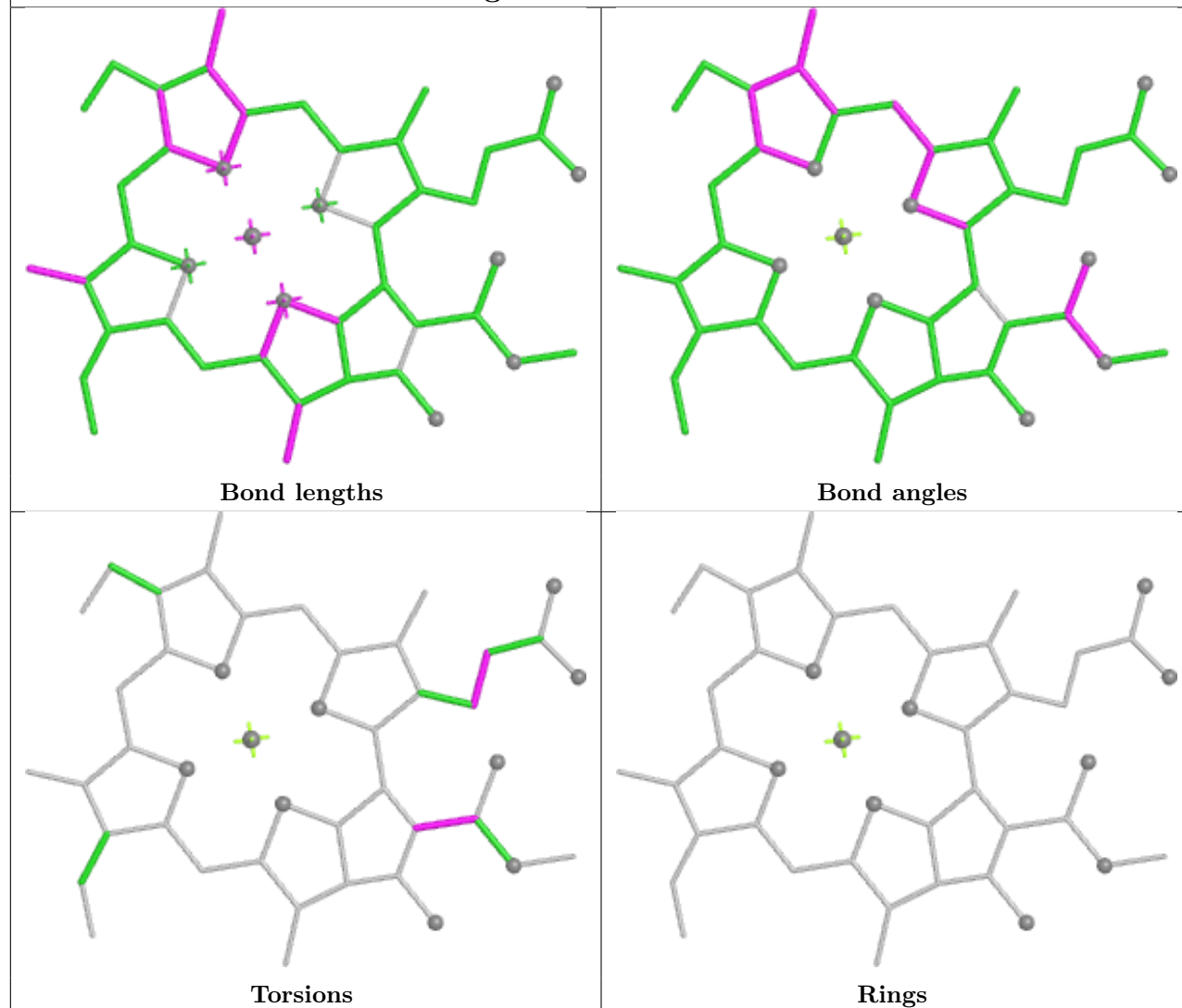




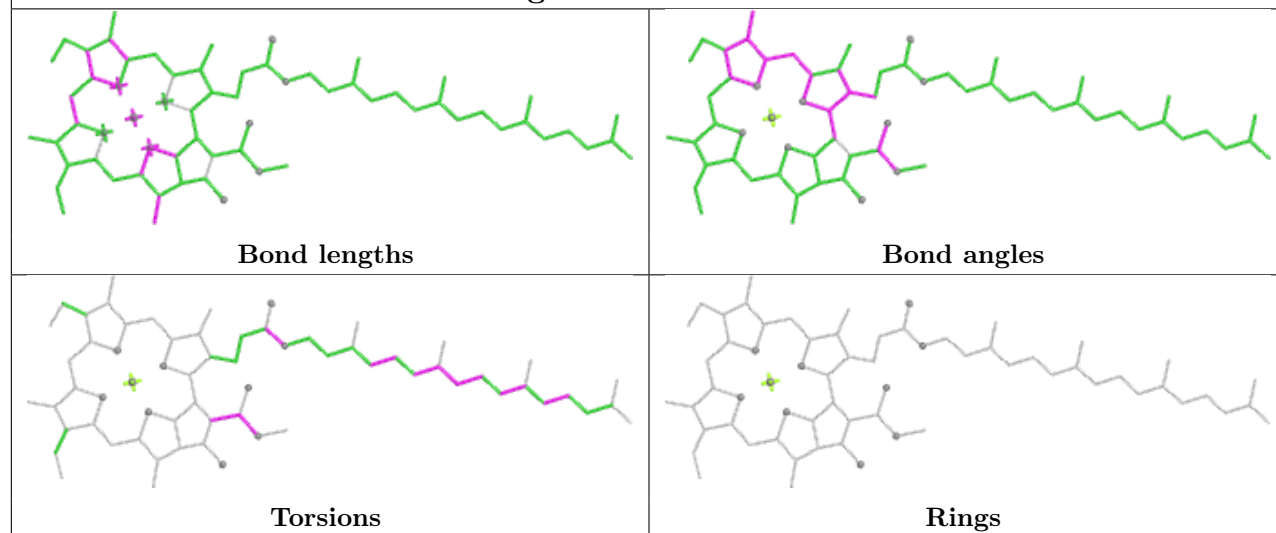


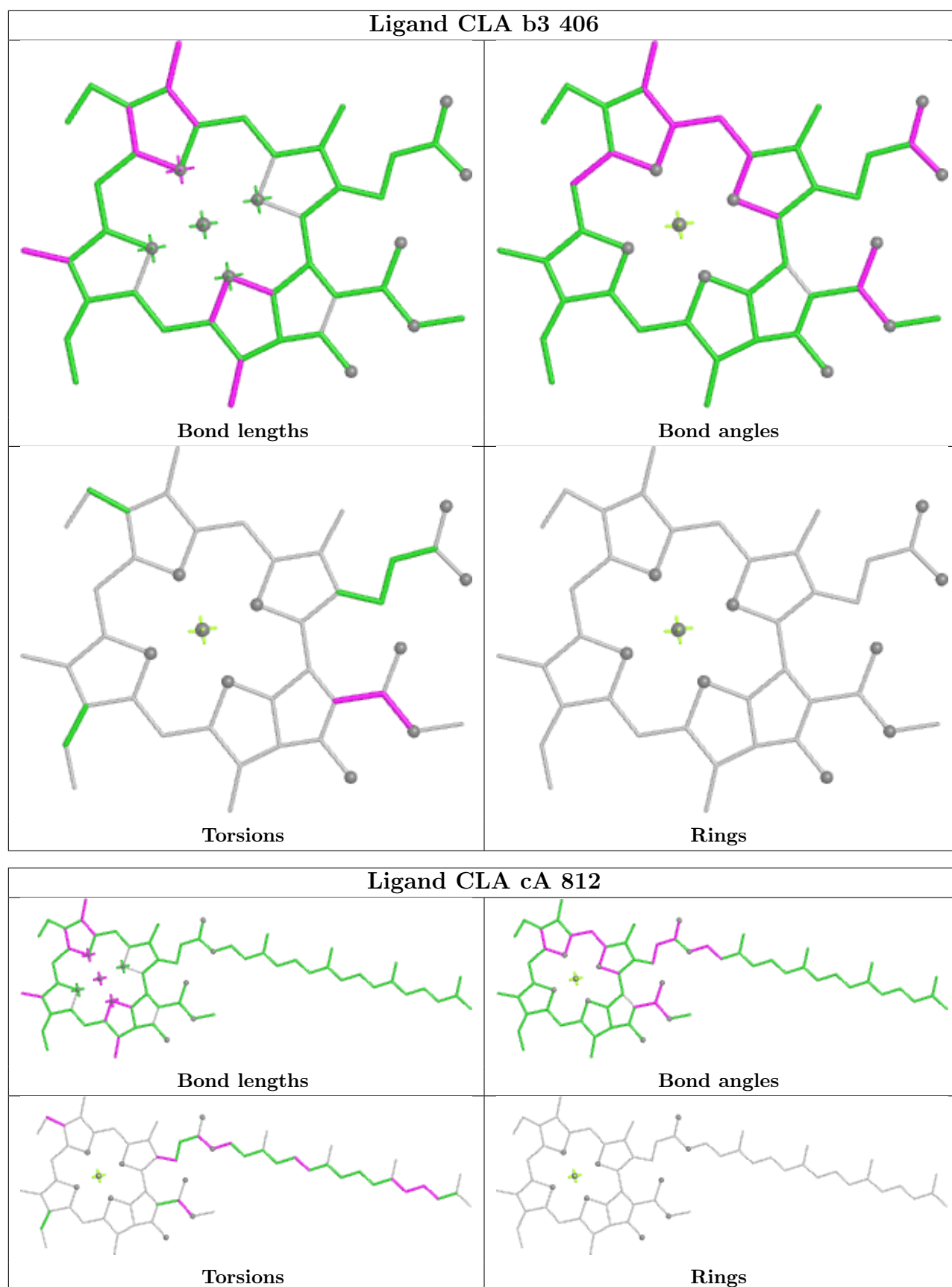
Ligand CLA aB 814	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b3 420	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b5 419	
 Bond lengths	 Bond angles
 Torsions	 Rings

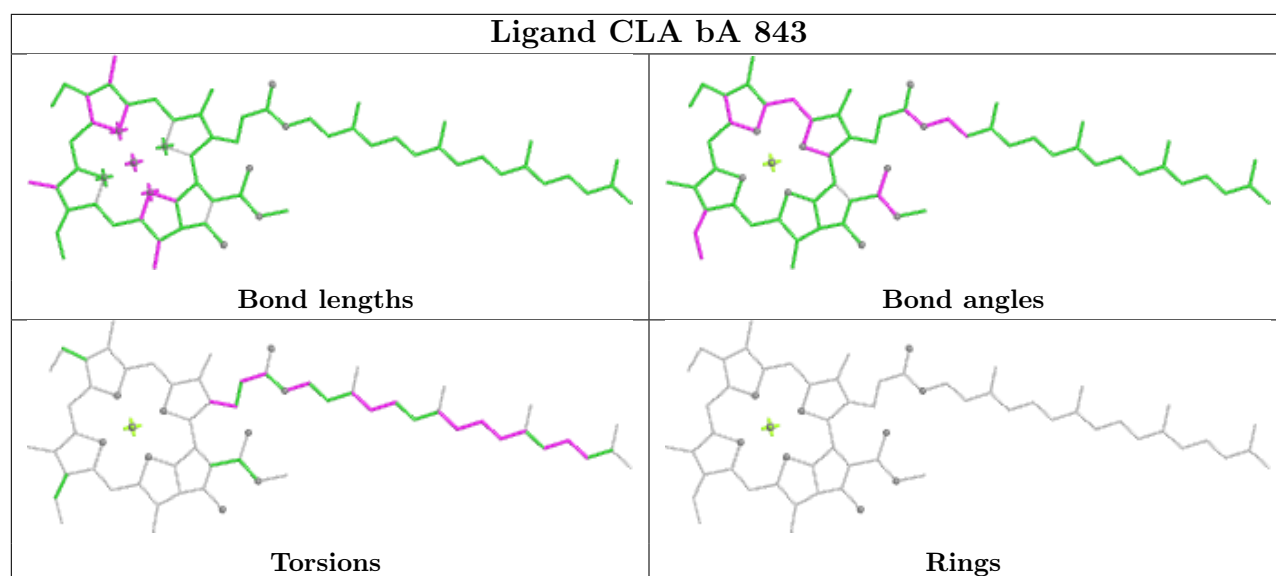
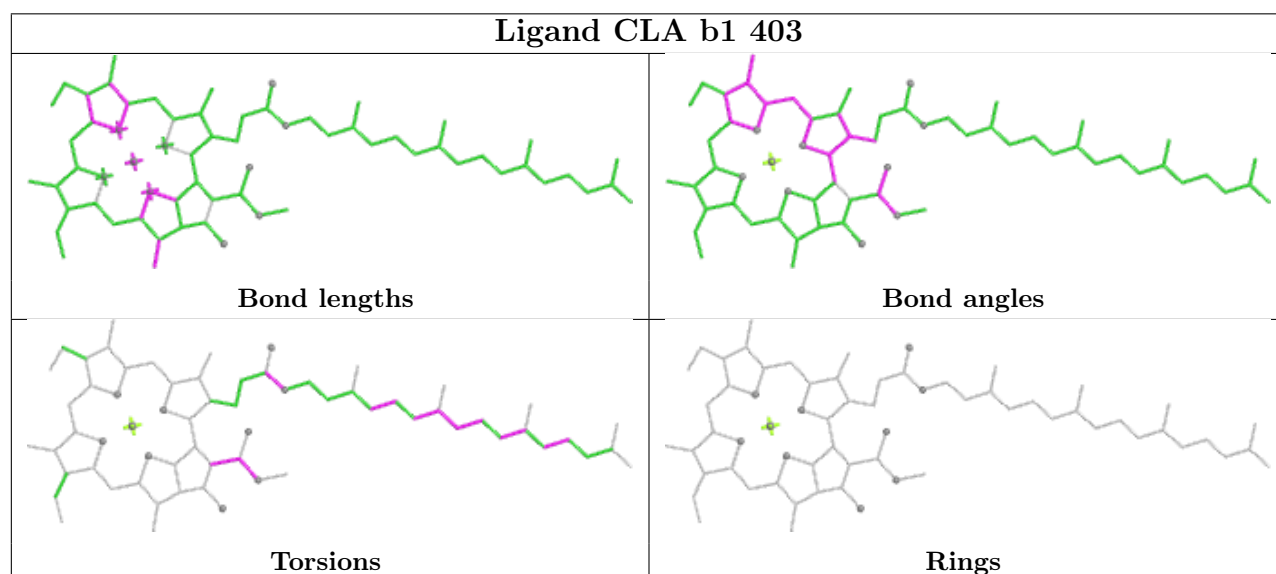
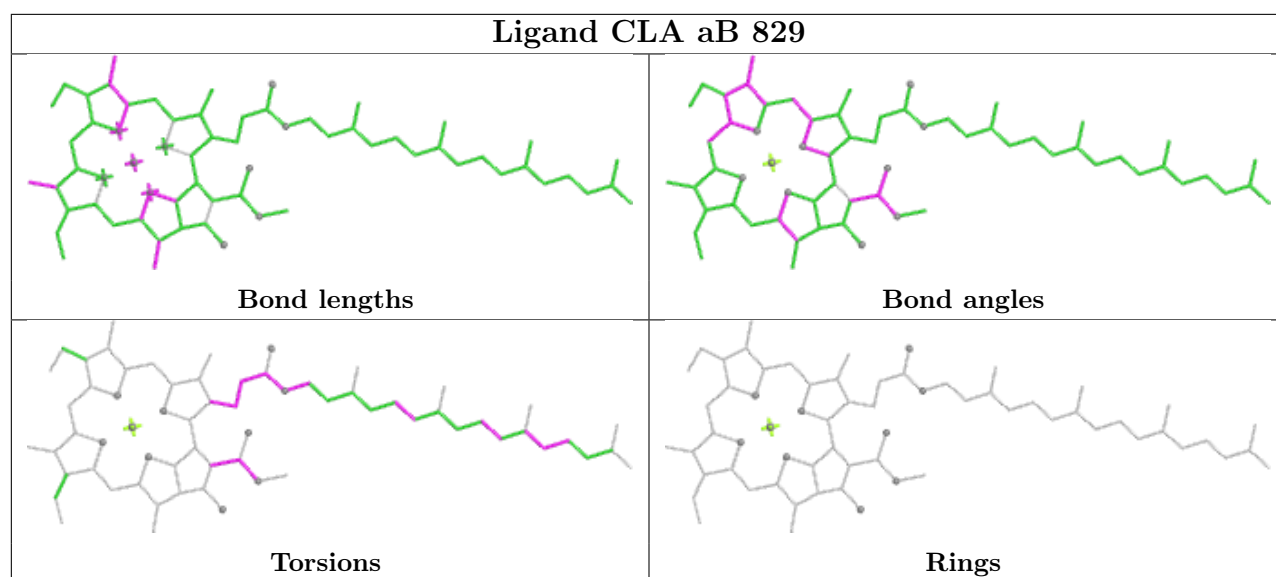
Ligand CLA aA 816

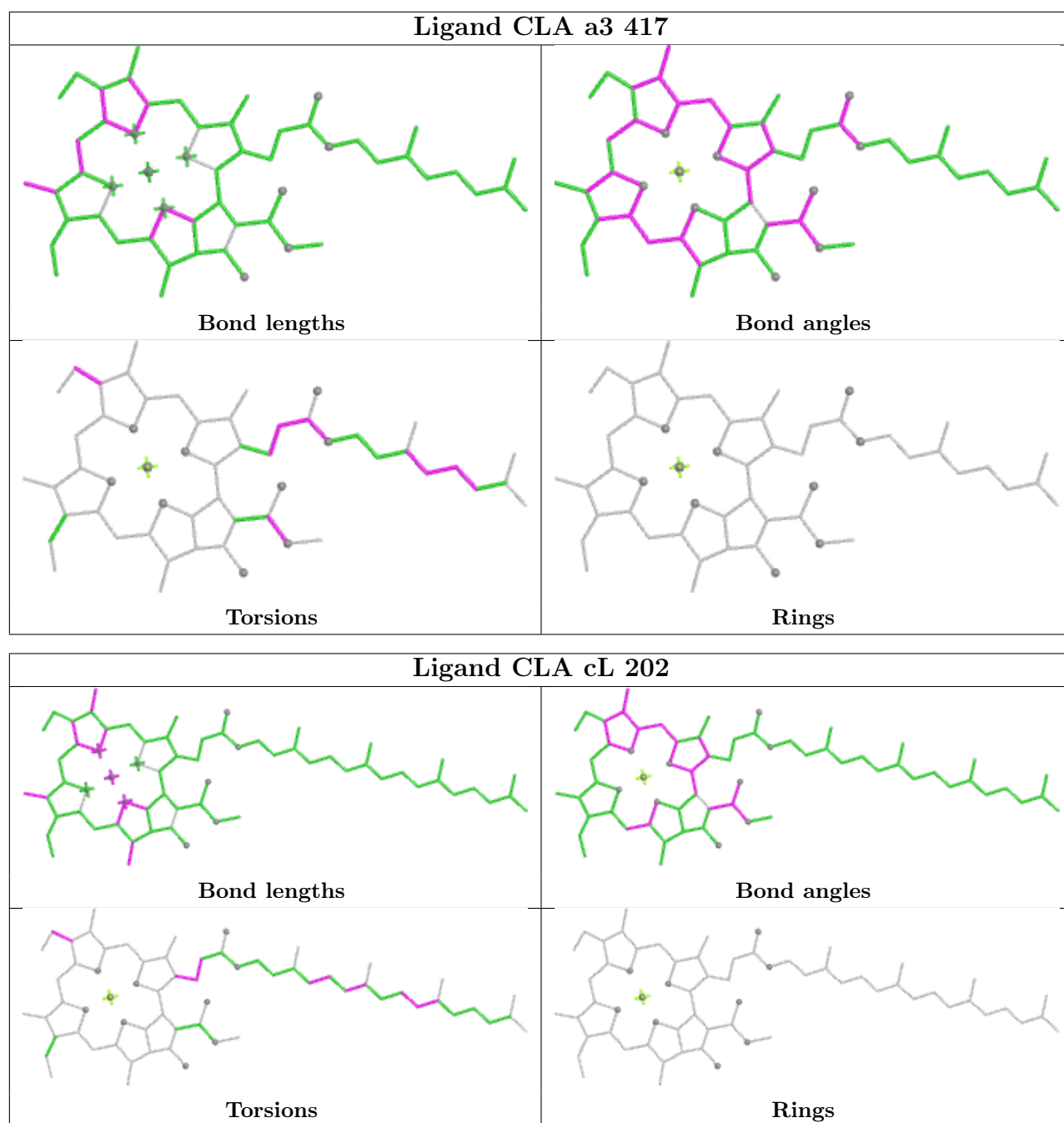


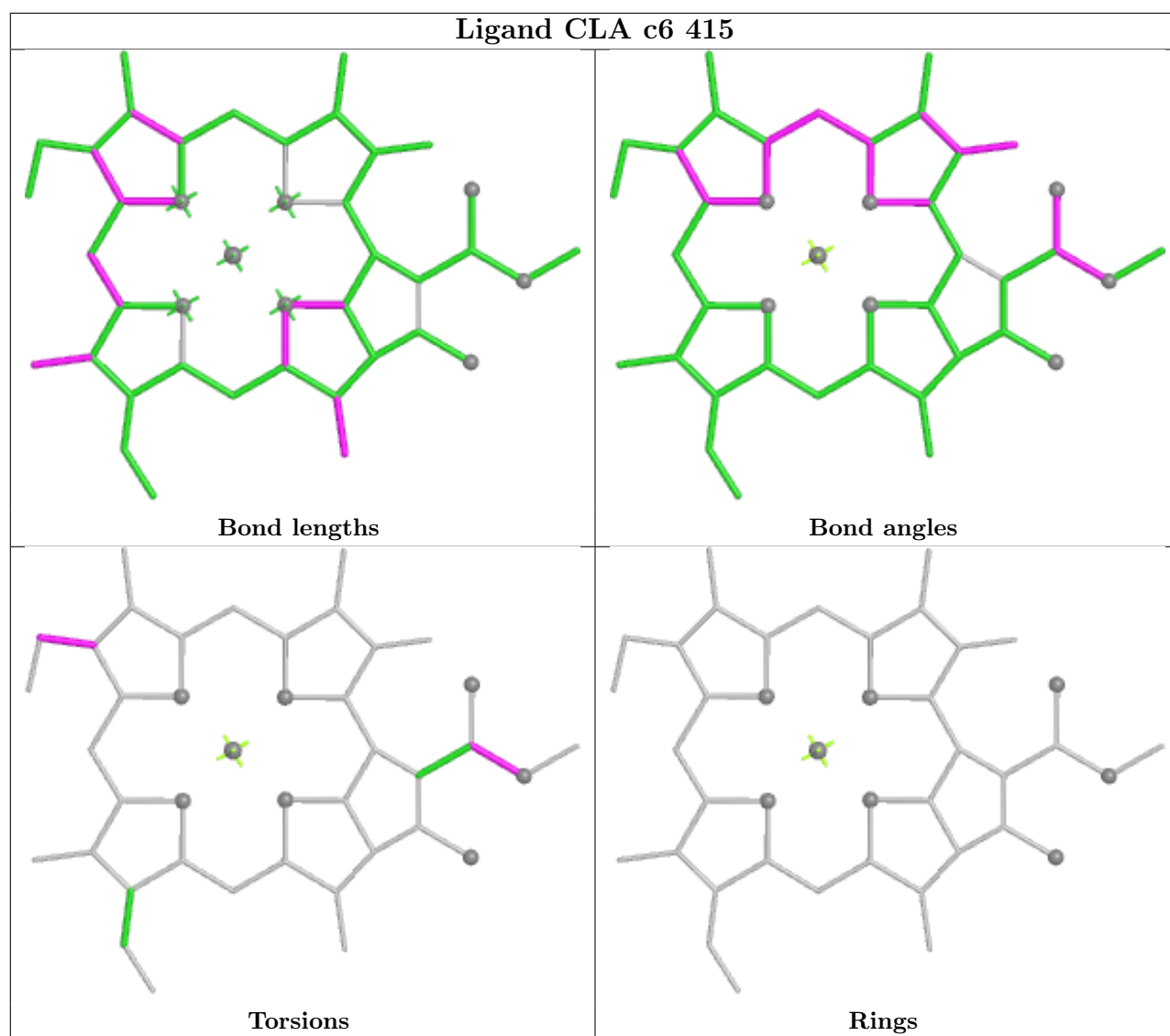
Ligand CLA a6 404

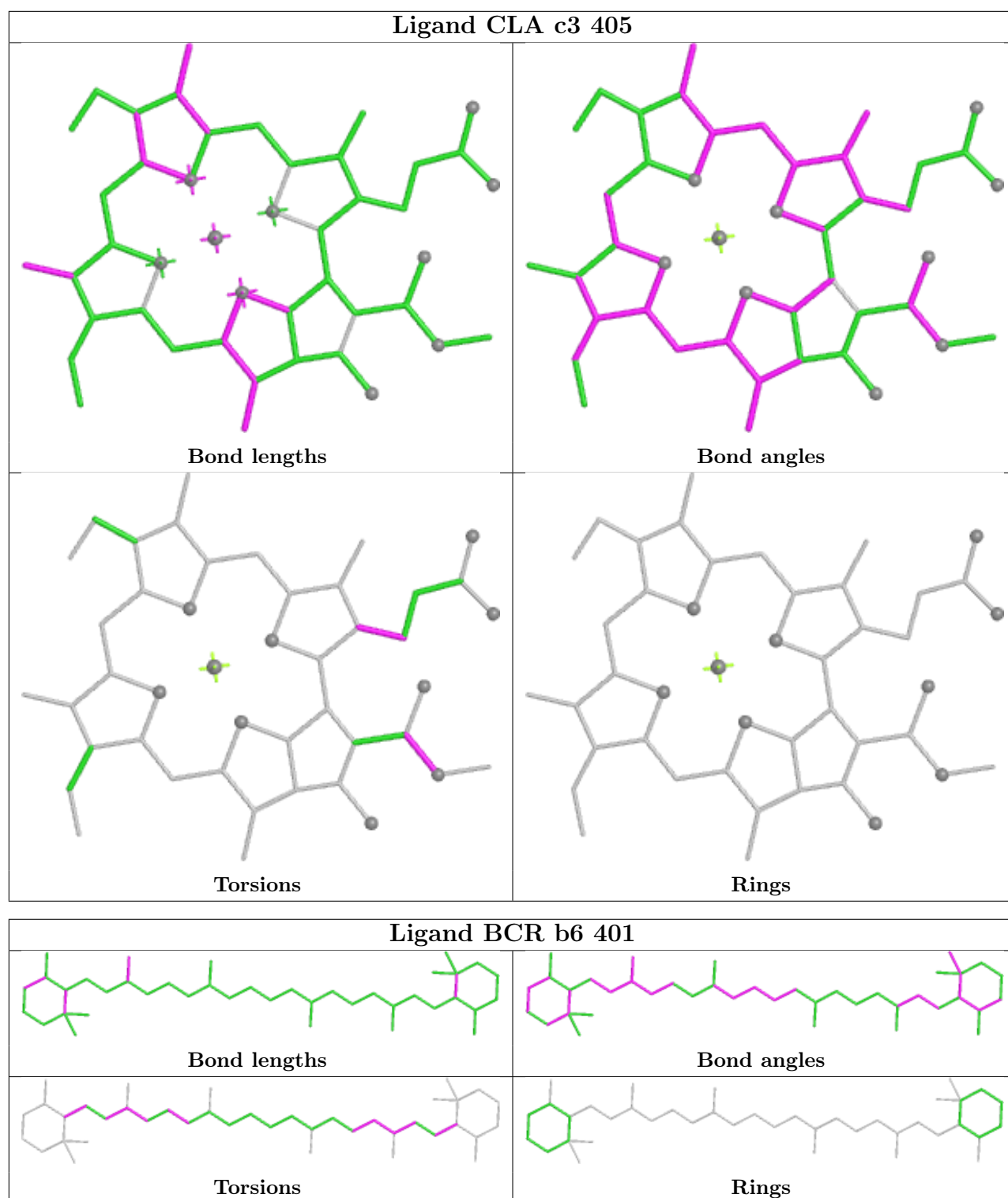


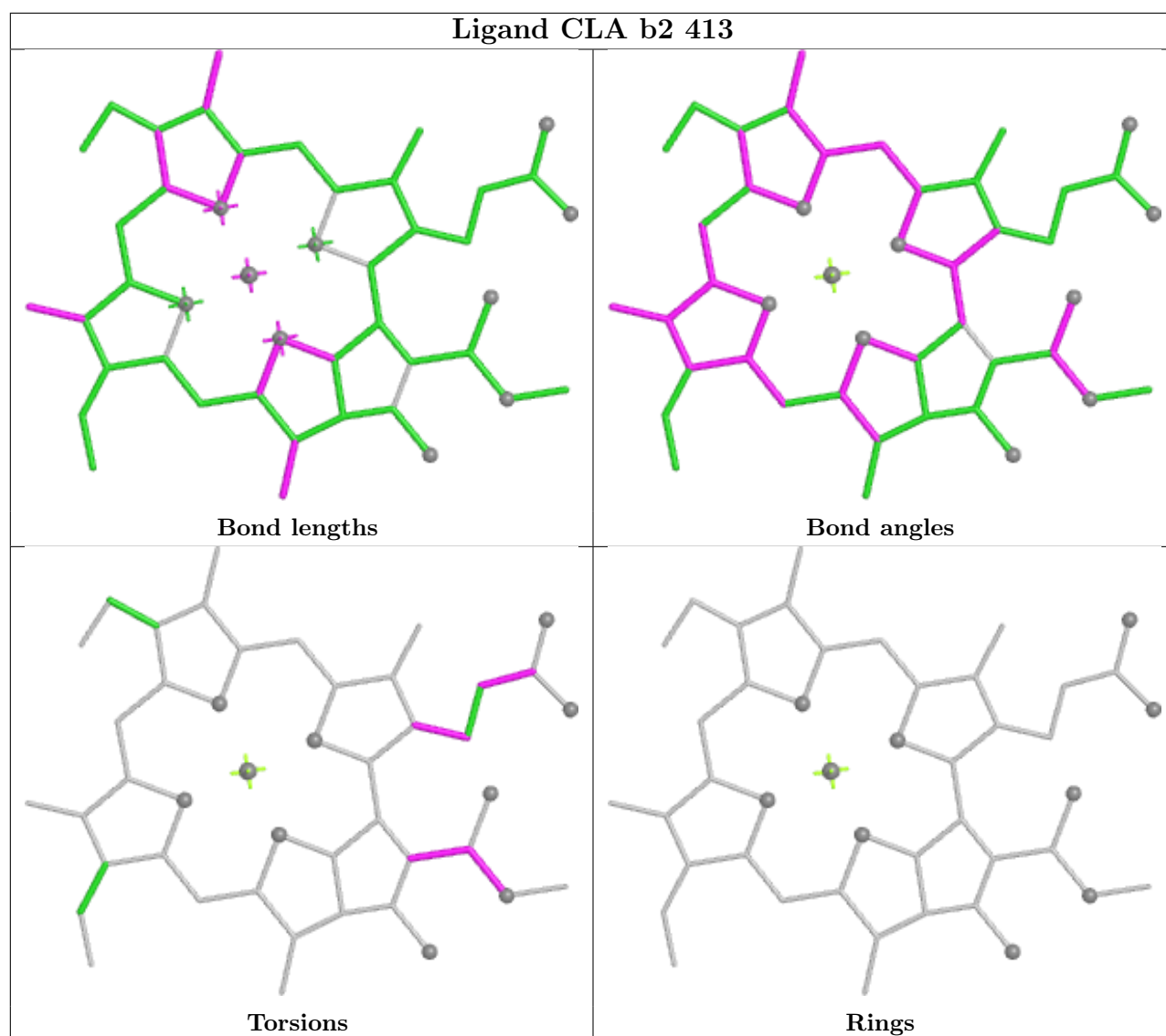


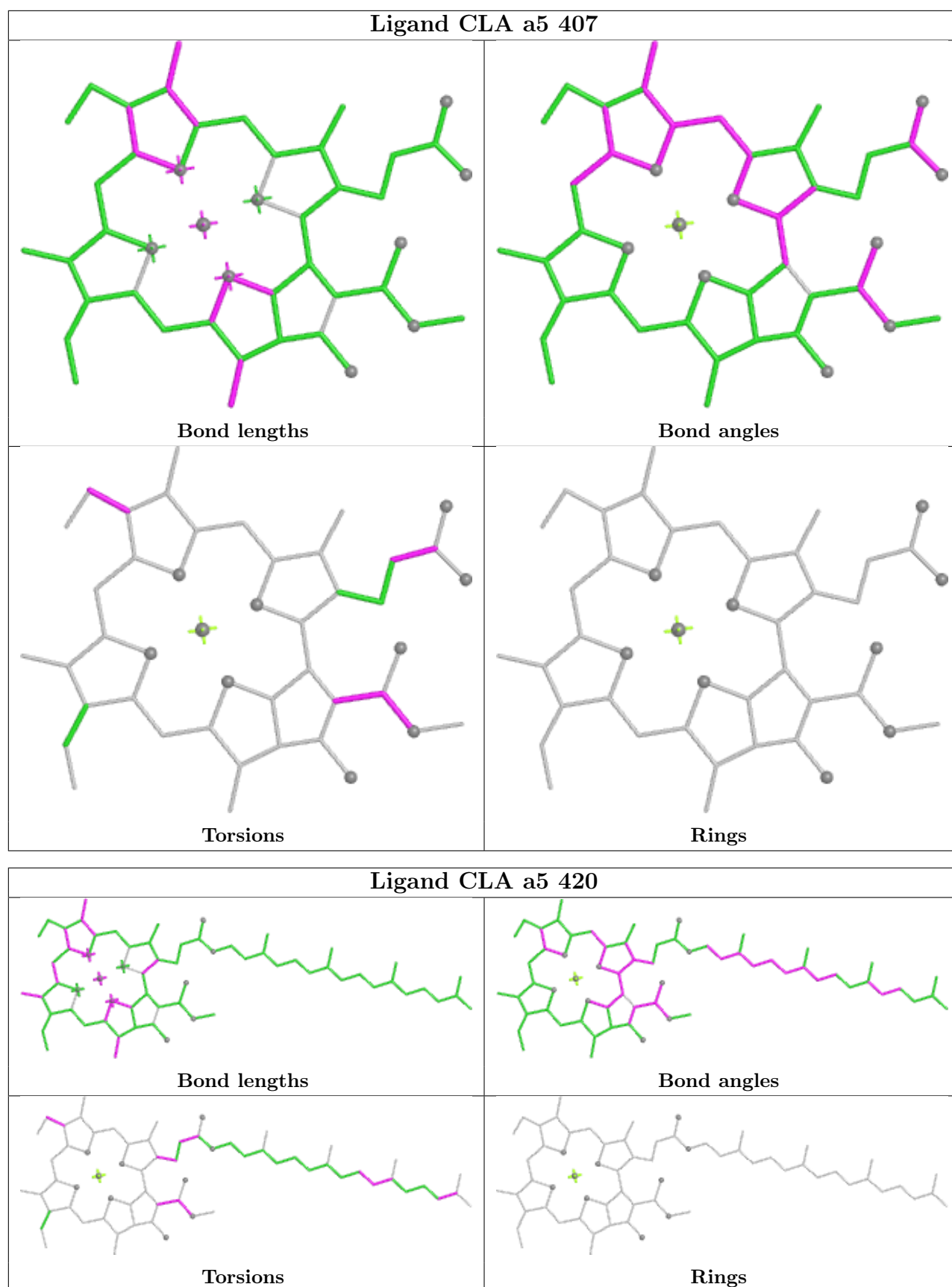


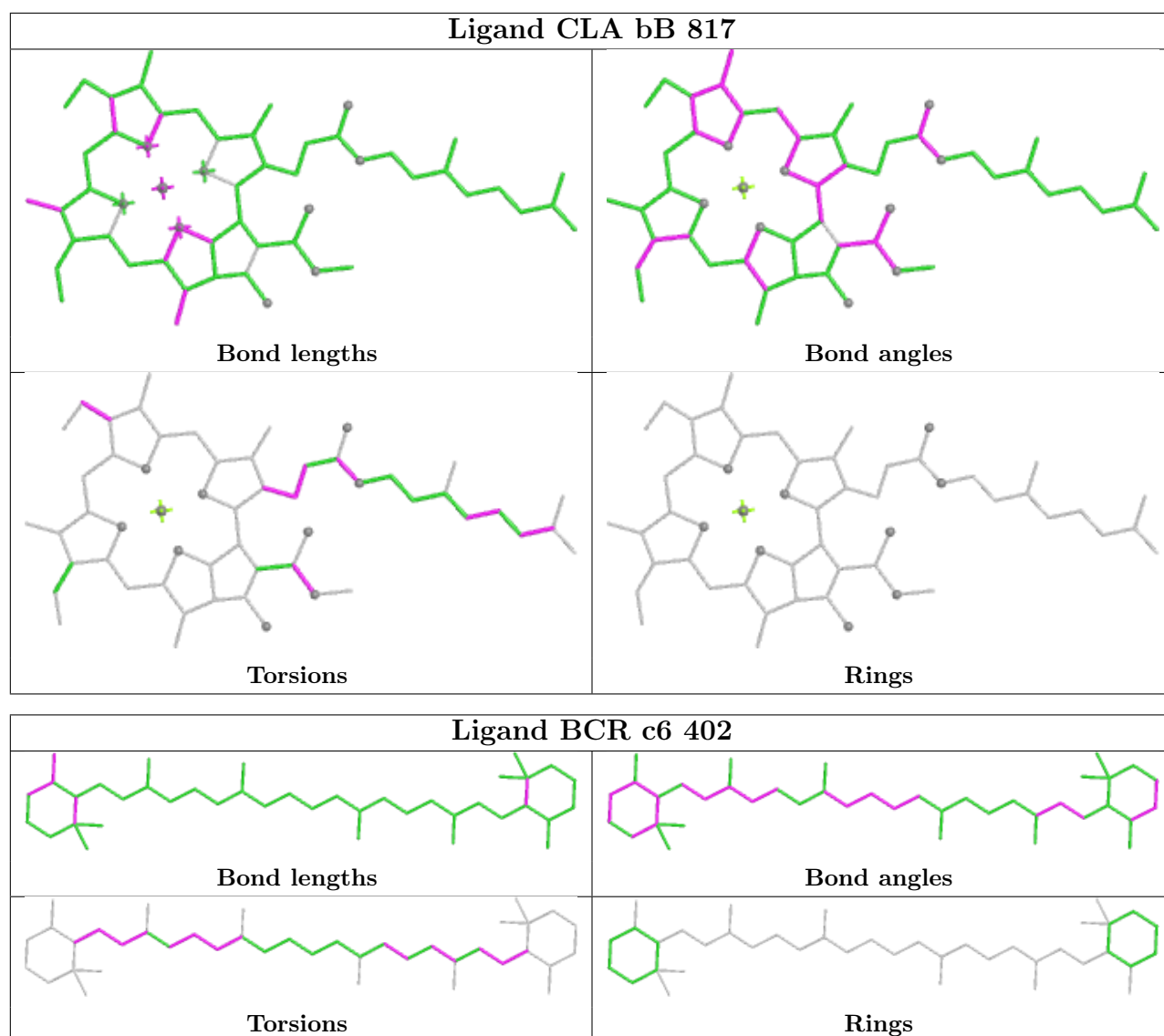


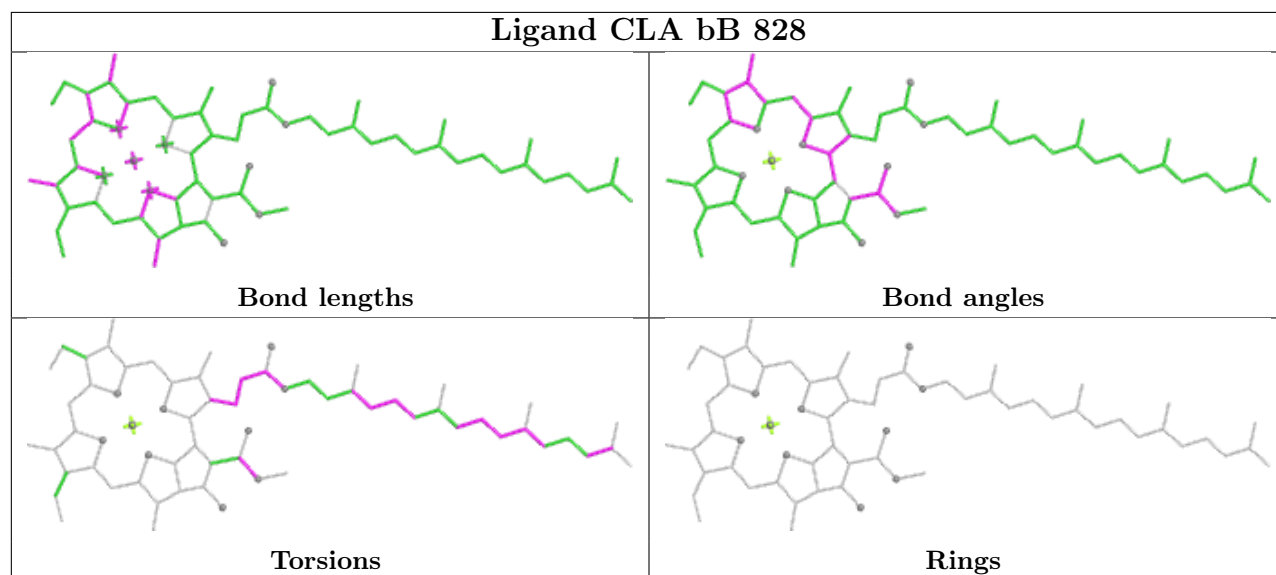
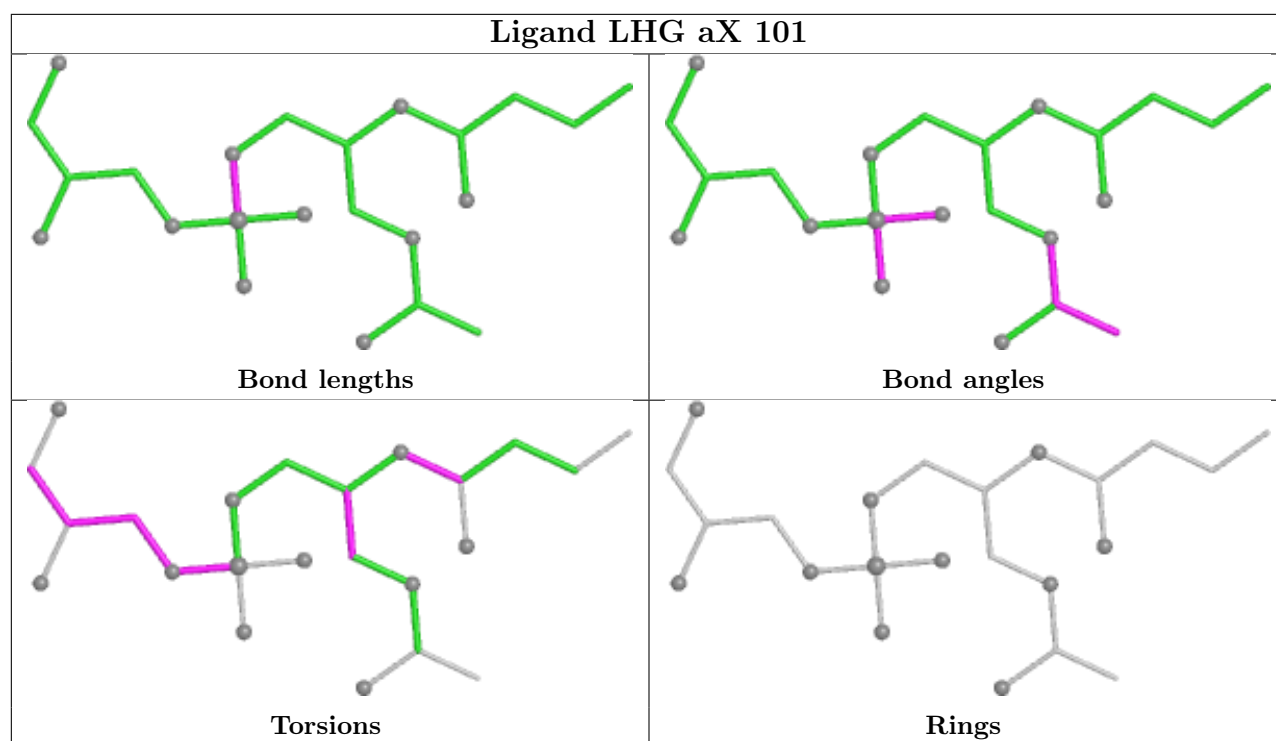


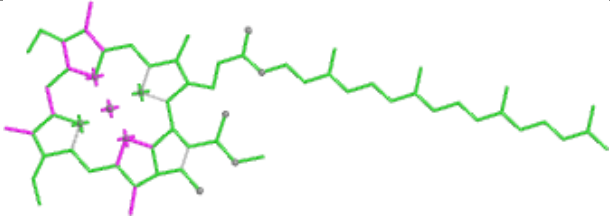
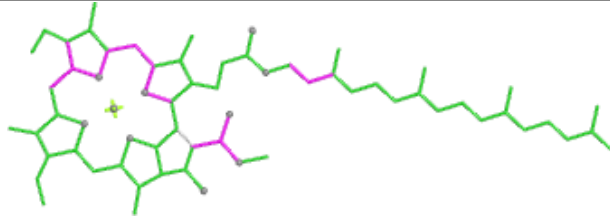
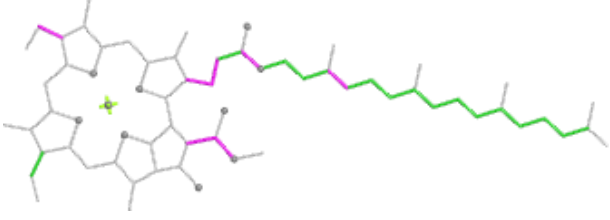
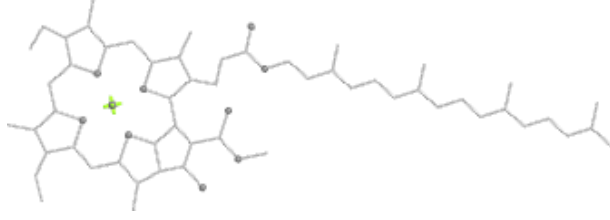
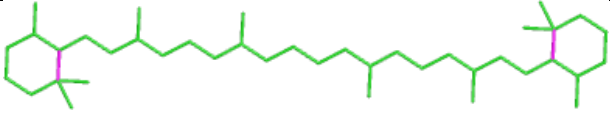
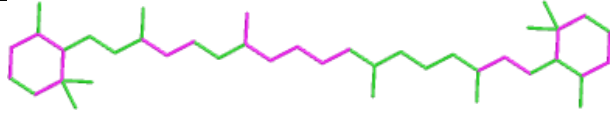
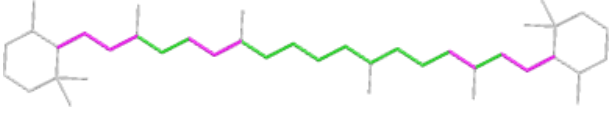
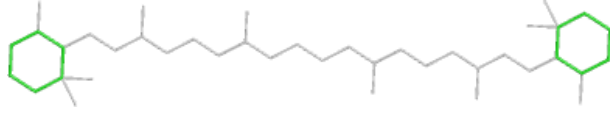
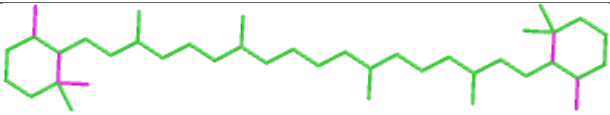
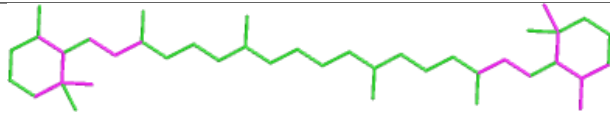
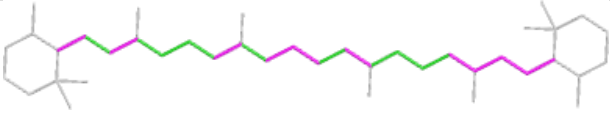
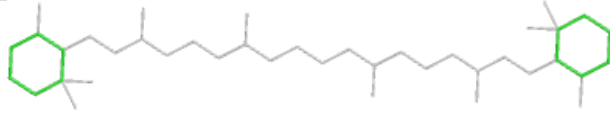


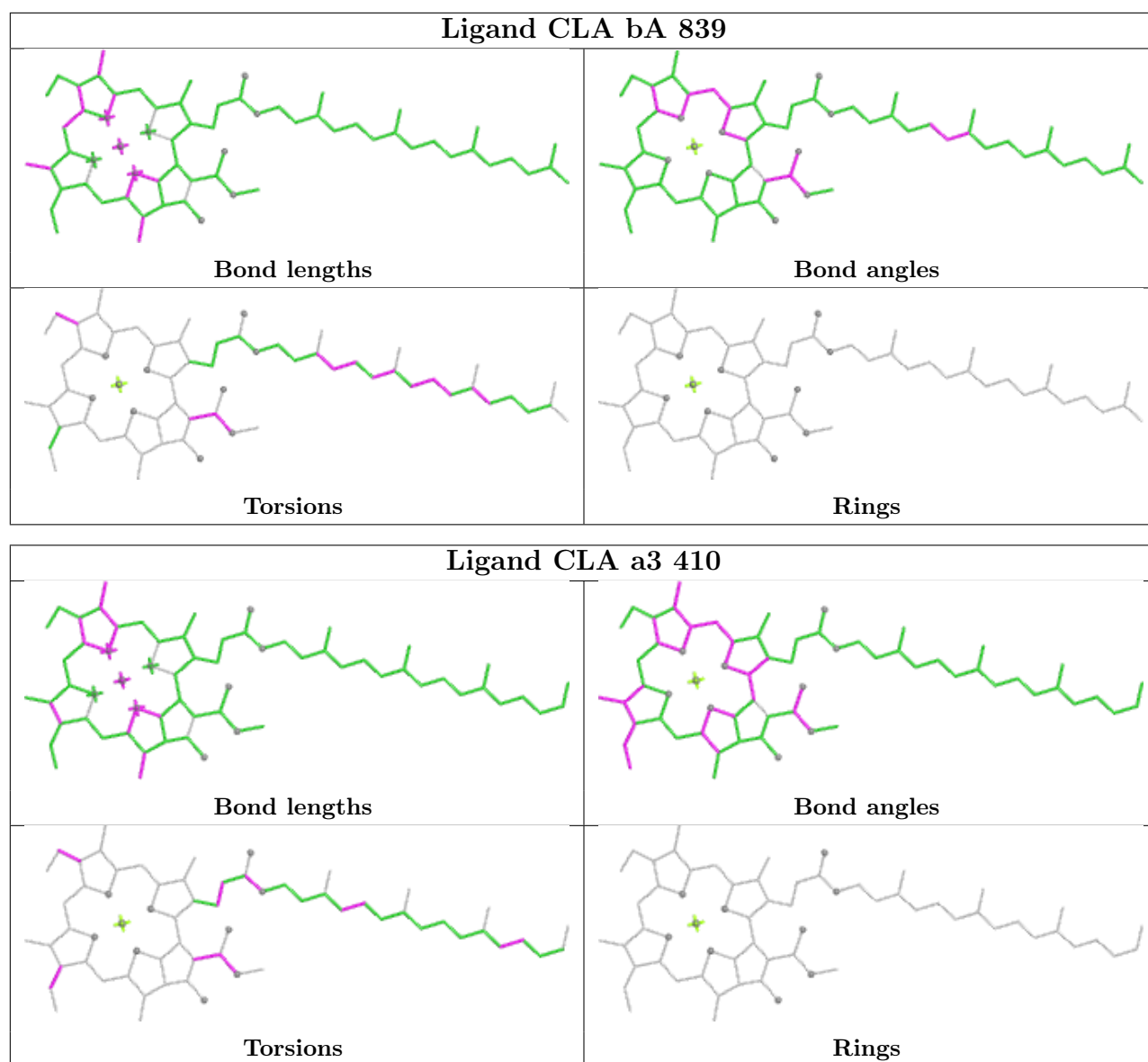


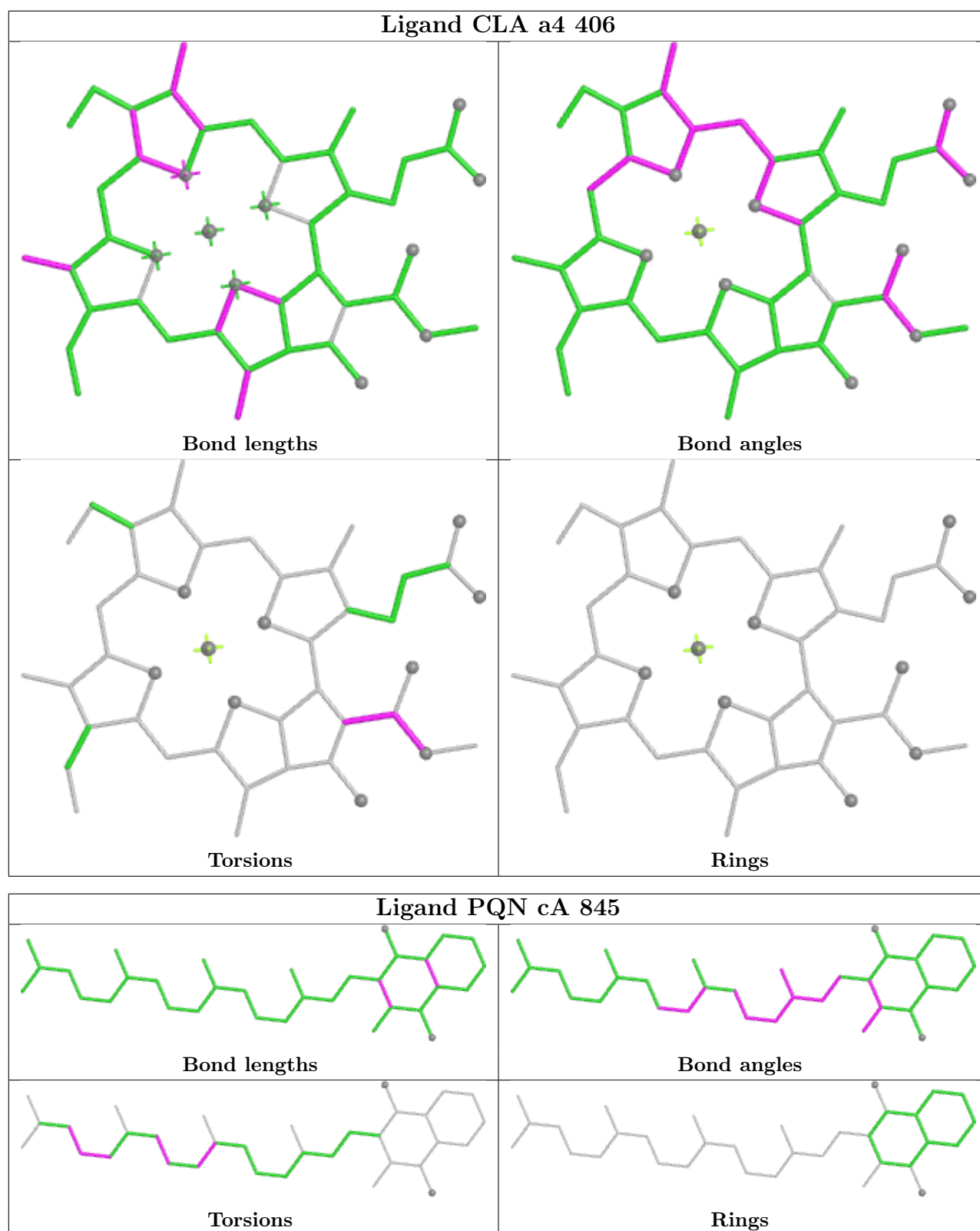


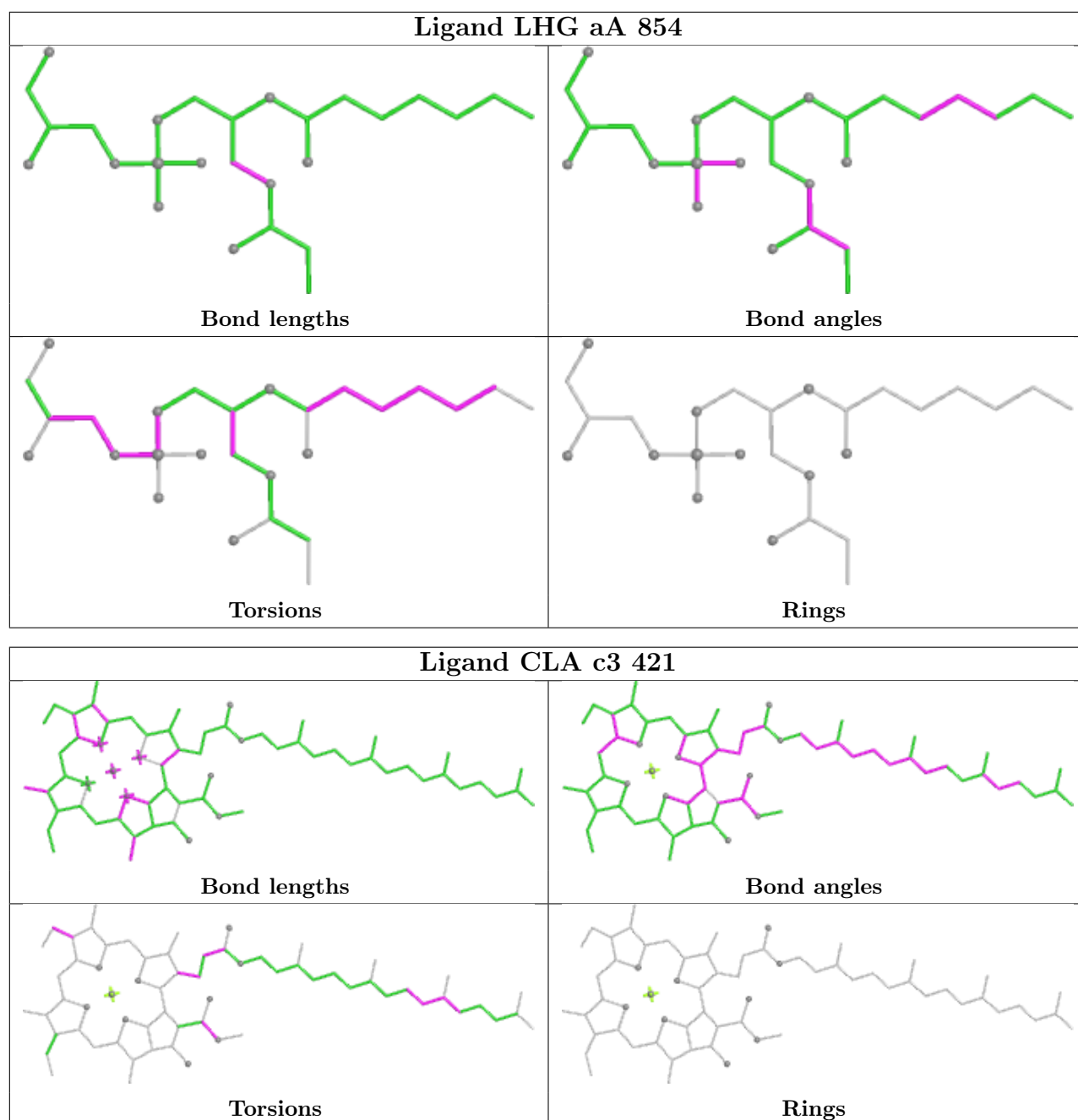




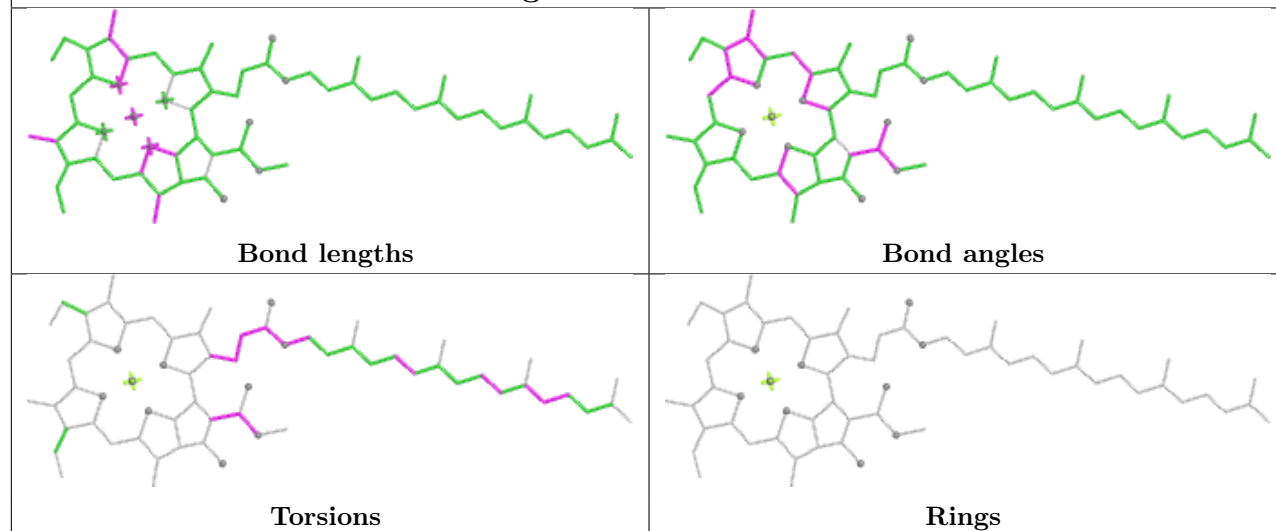
Ligand CLA c4 404	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a4 420	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR cF 202	
 Bond lengths	 Bond angles
 Torsions	 Rings



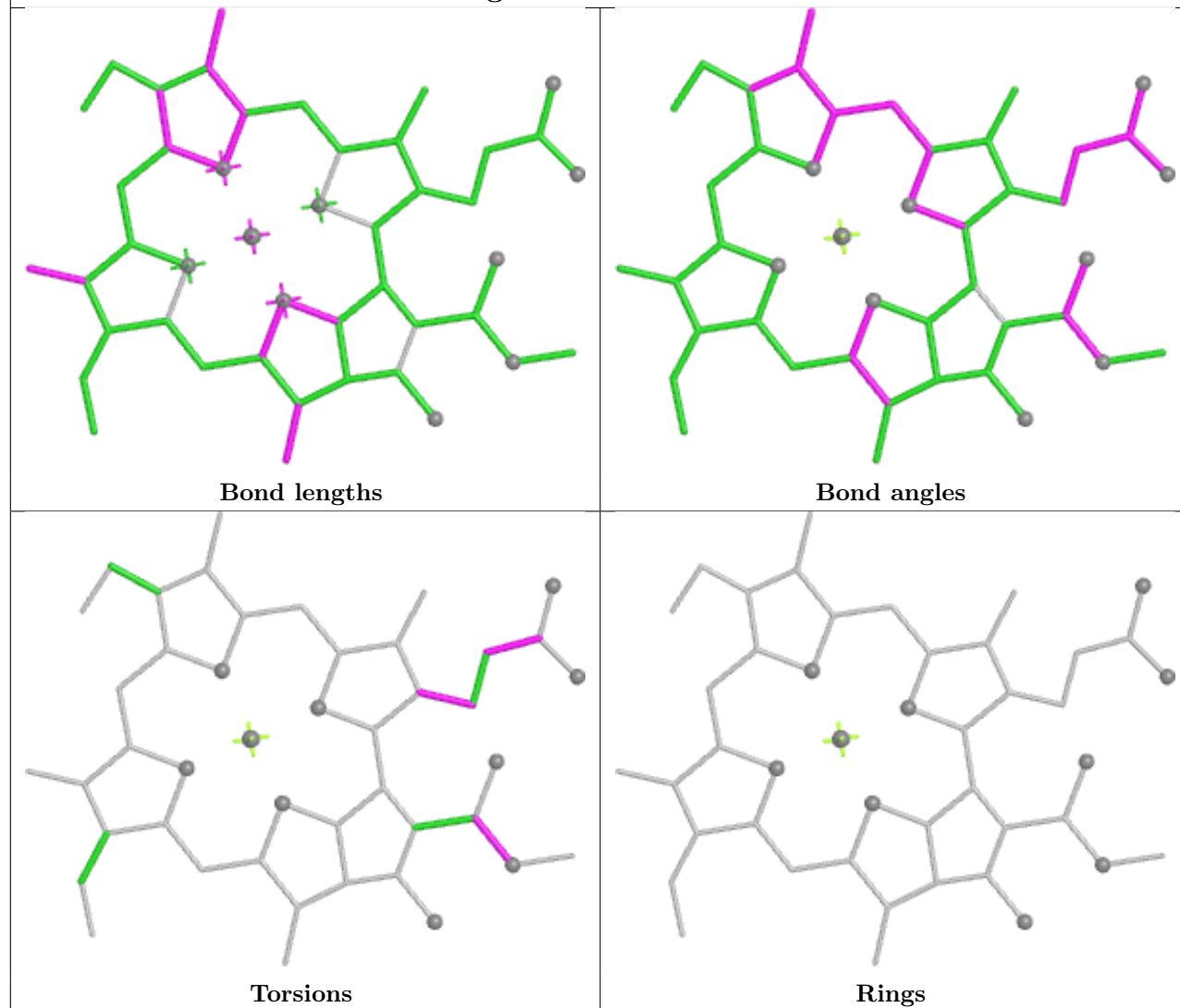


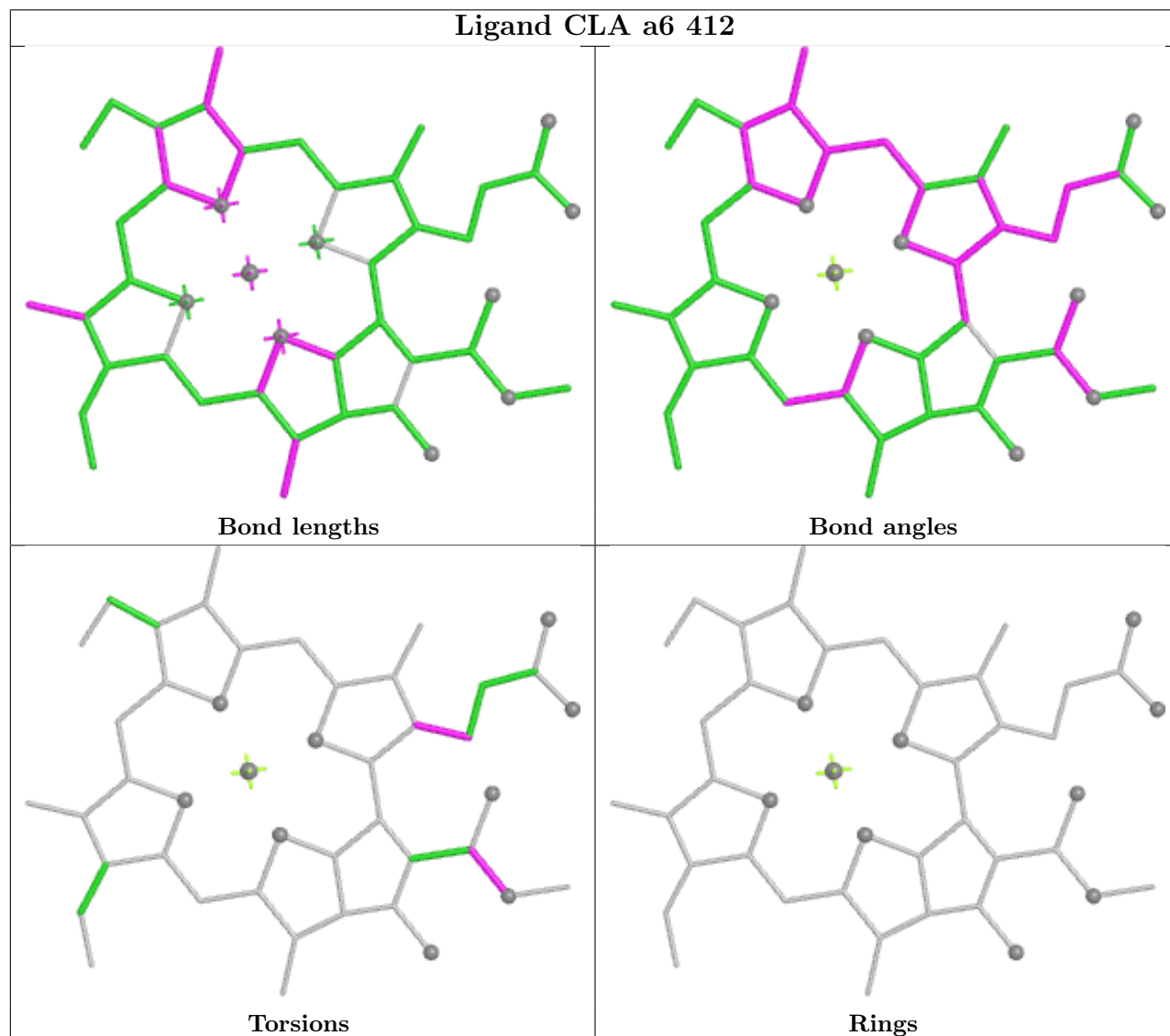
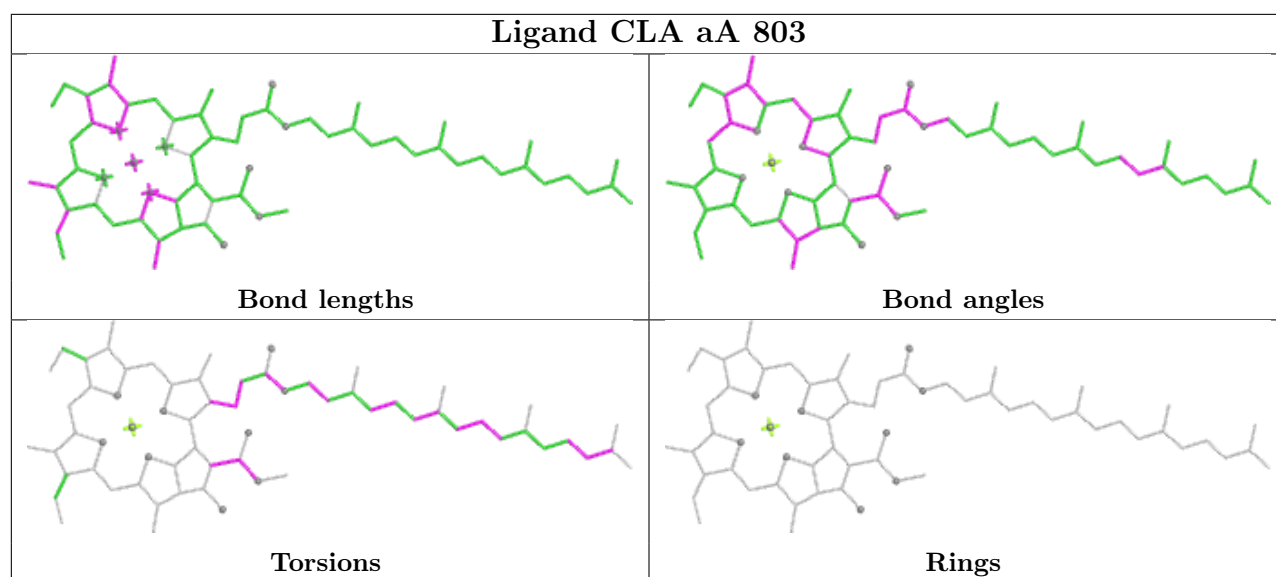


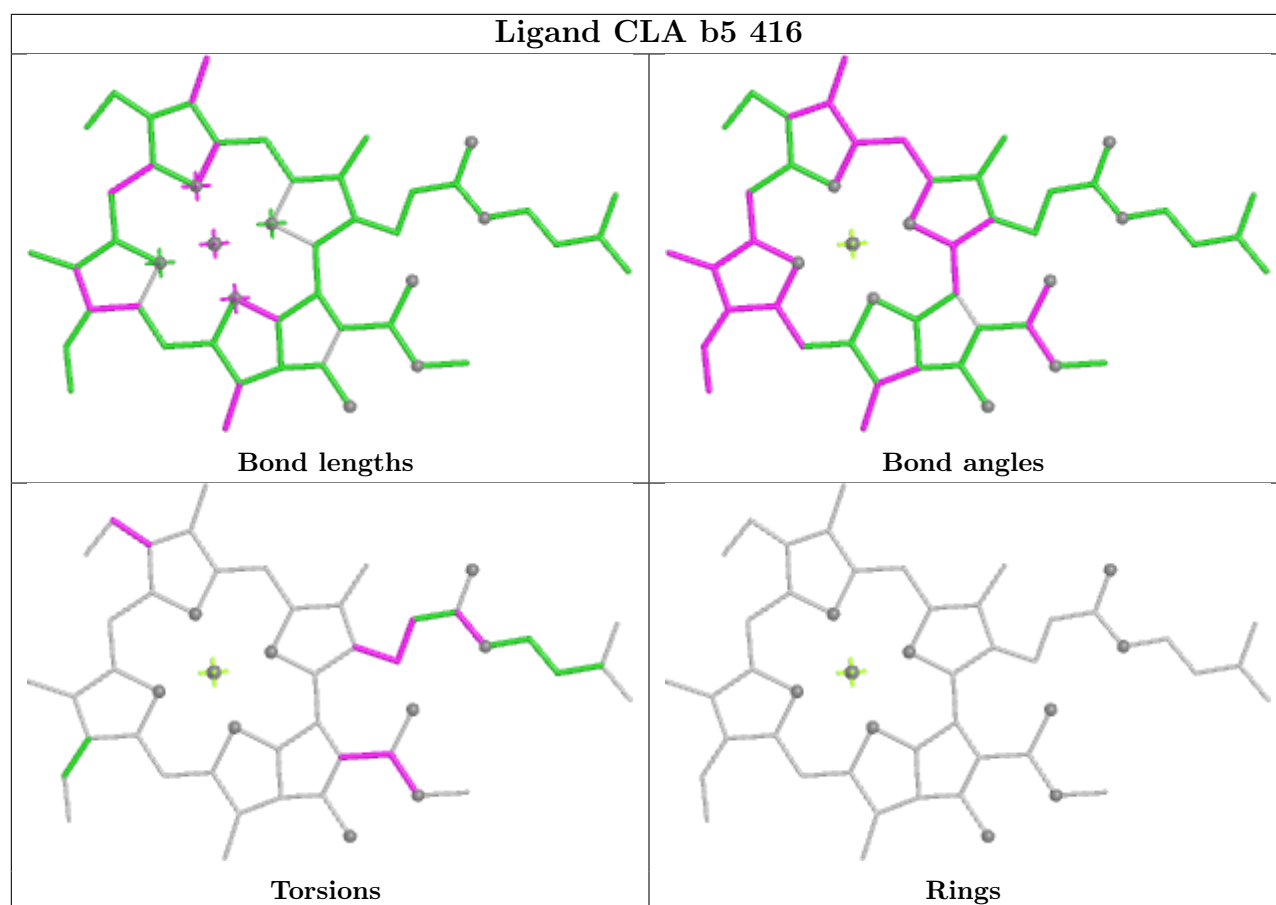
Ligand CLA bB 829

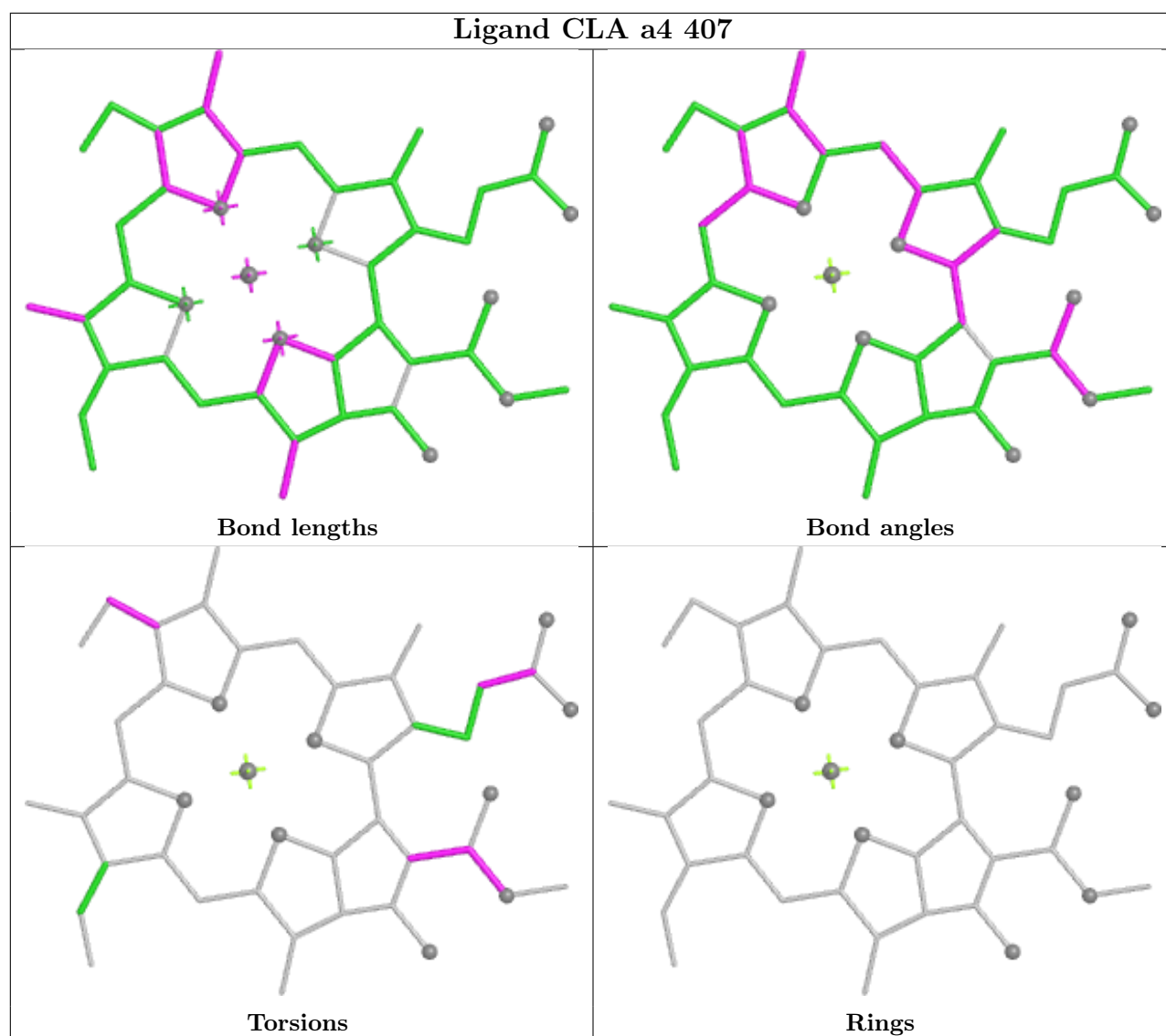


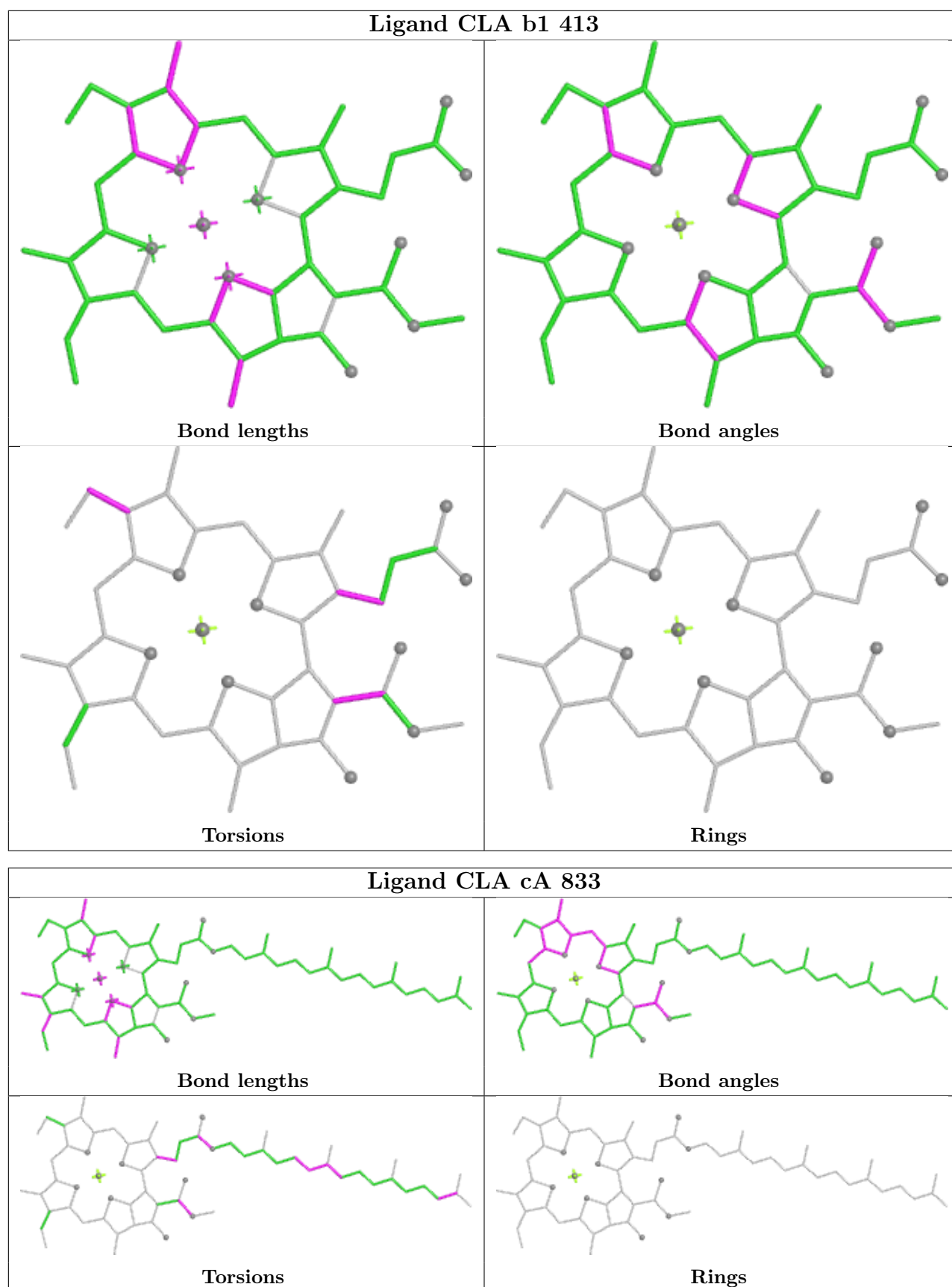
Ligand CLA b5 408

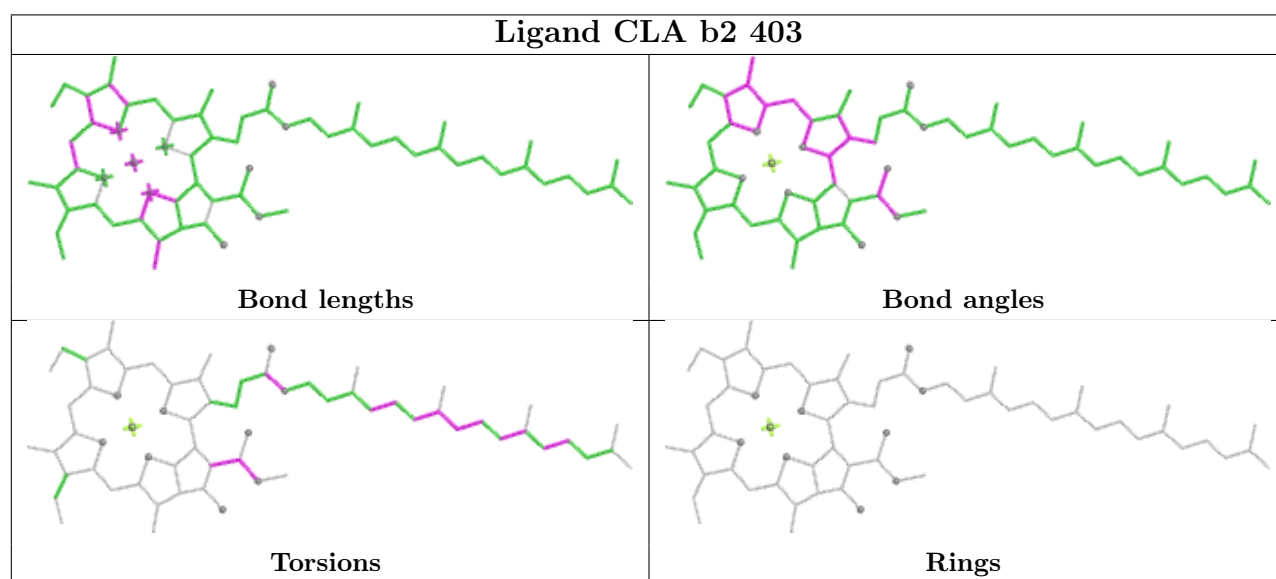
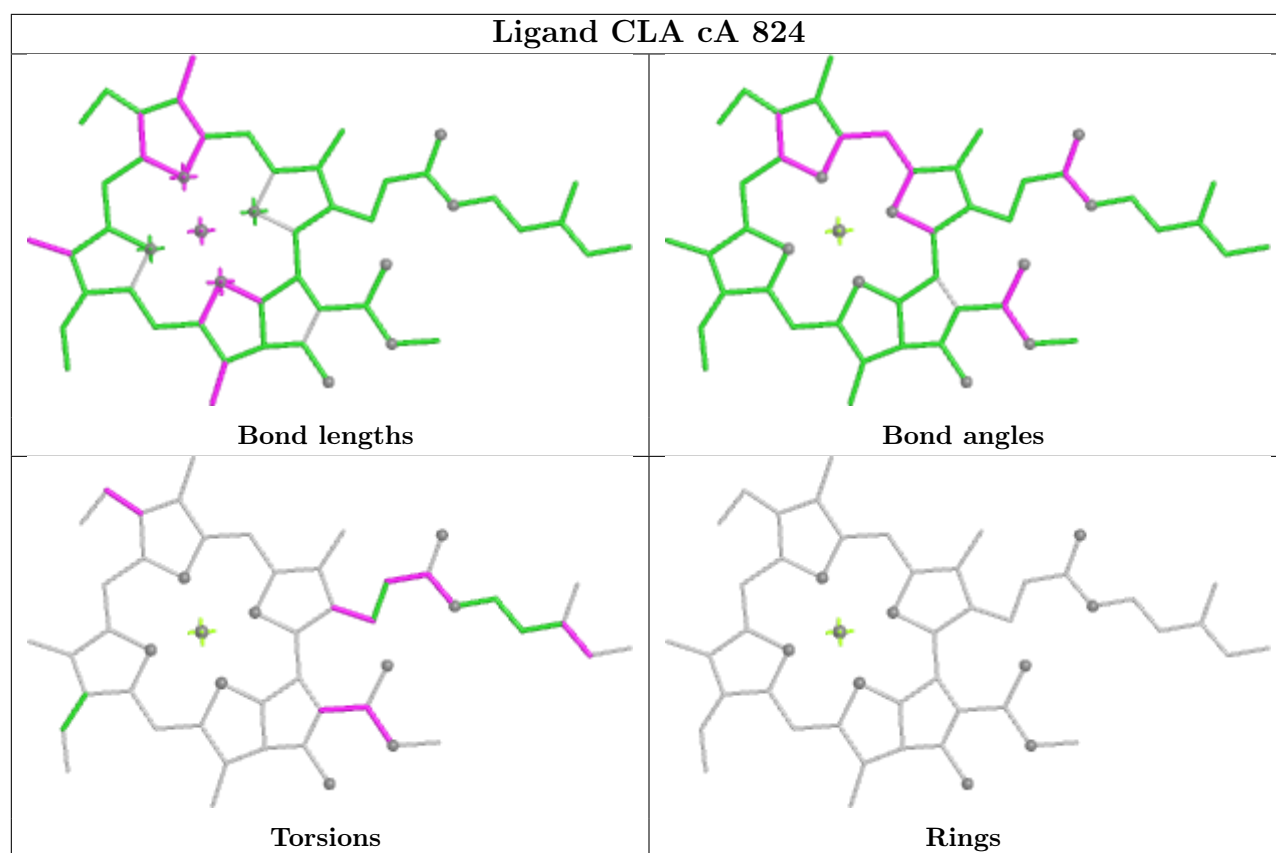




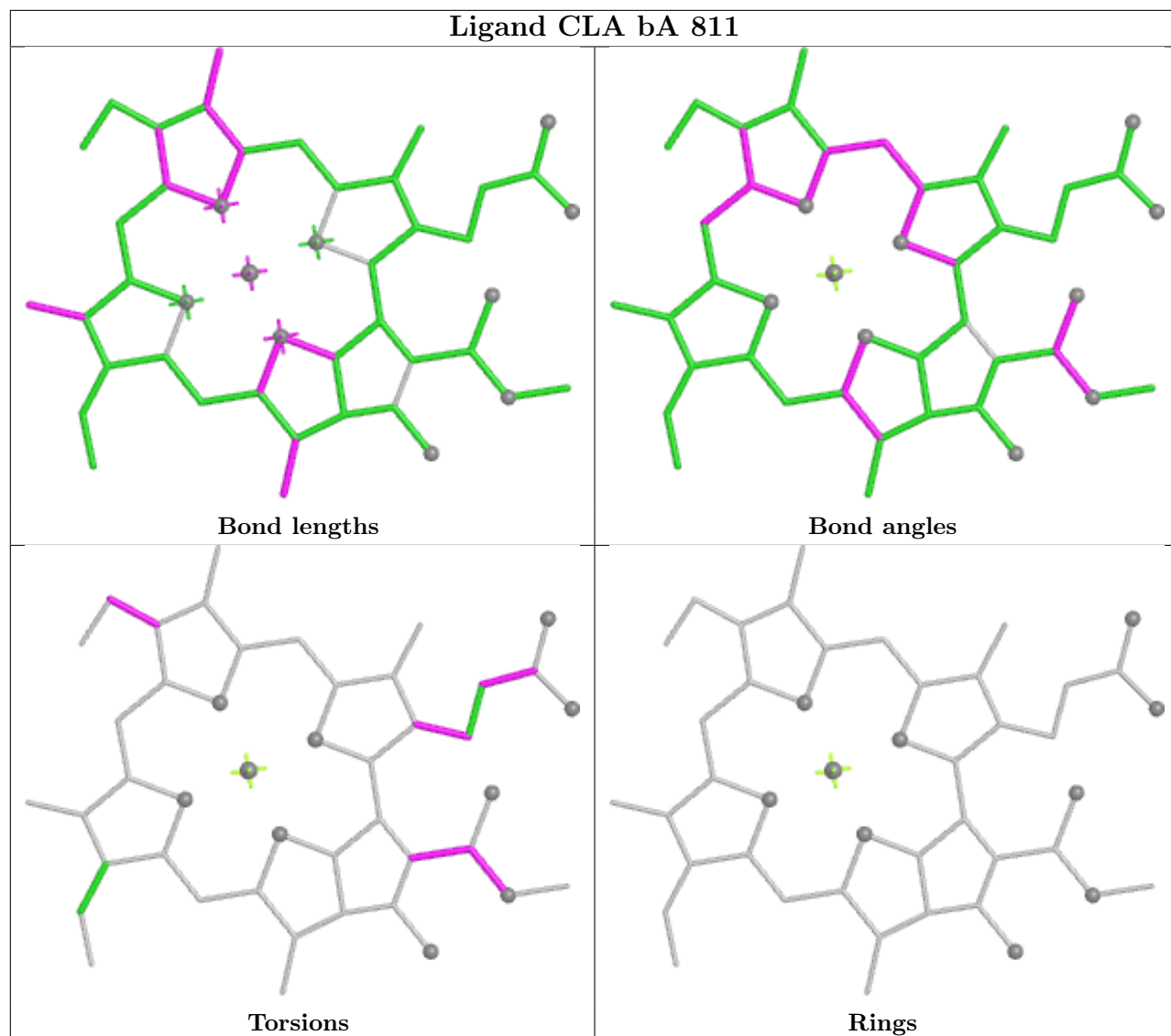


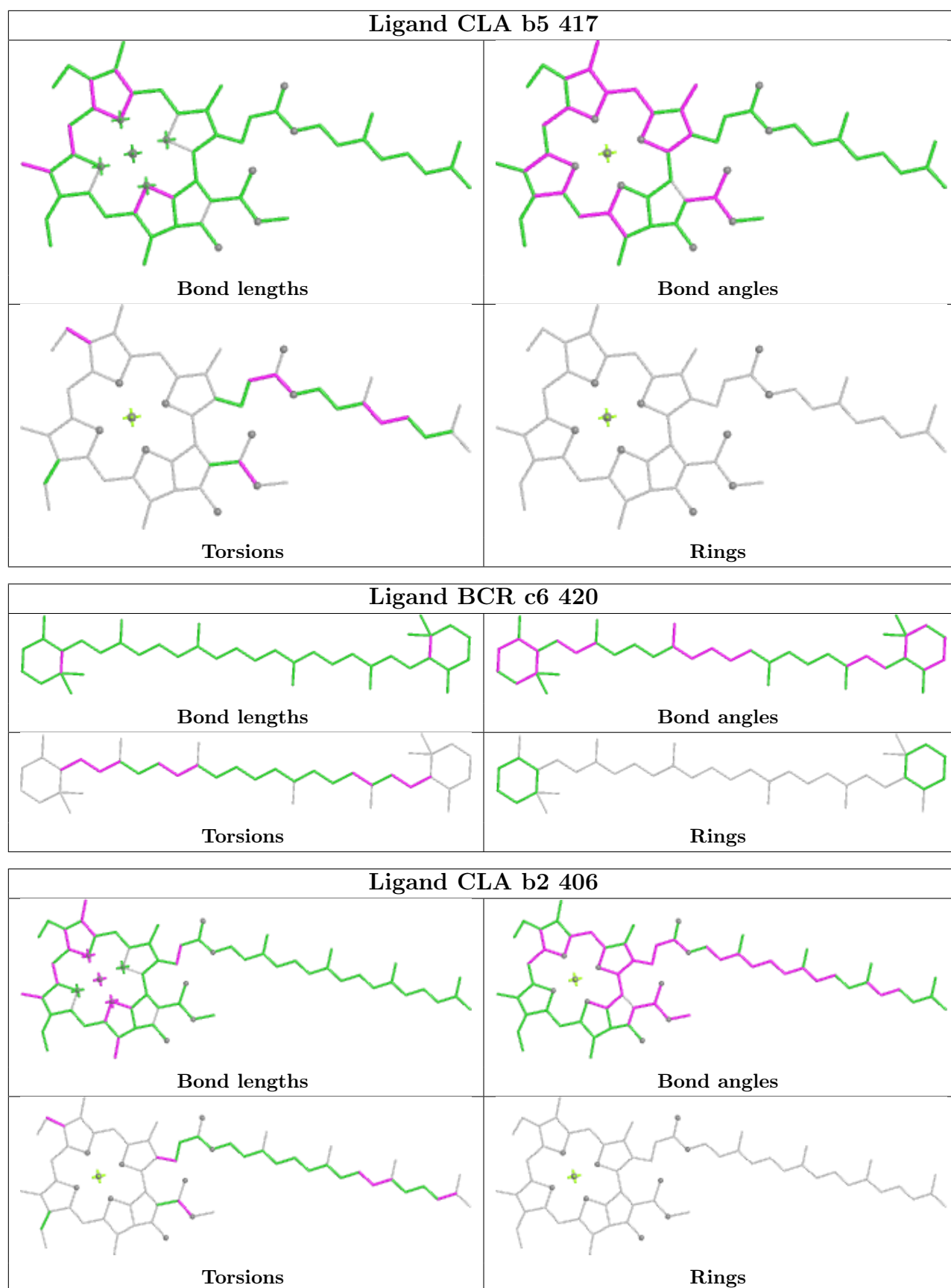


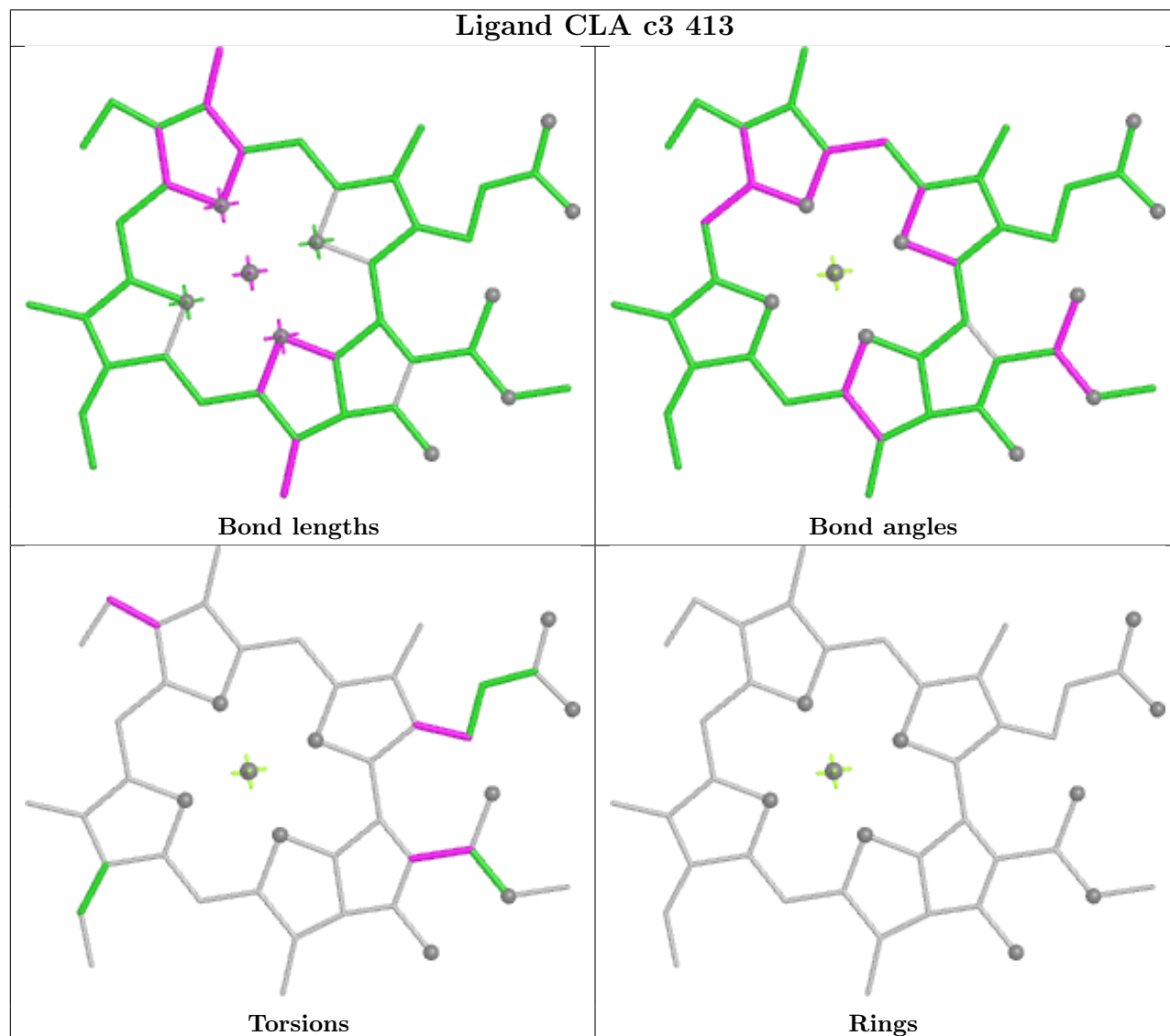
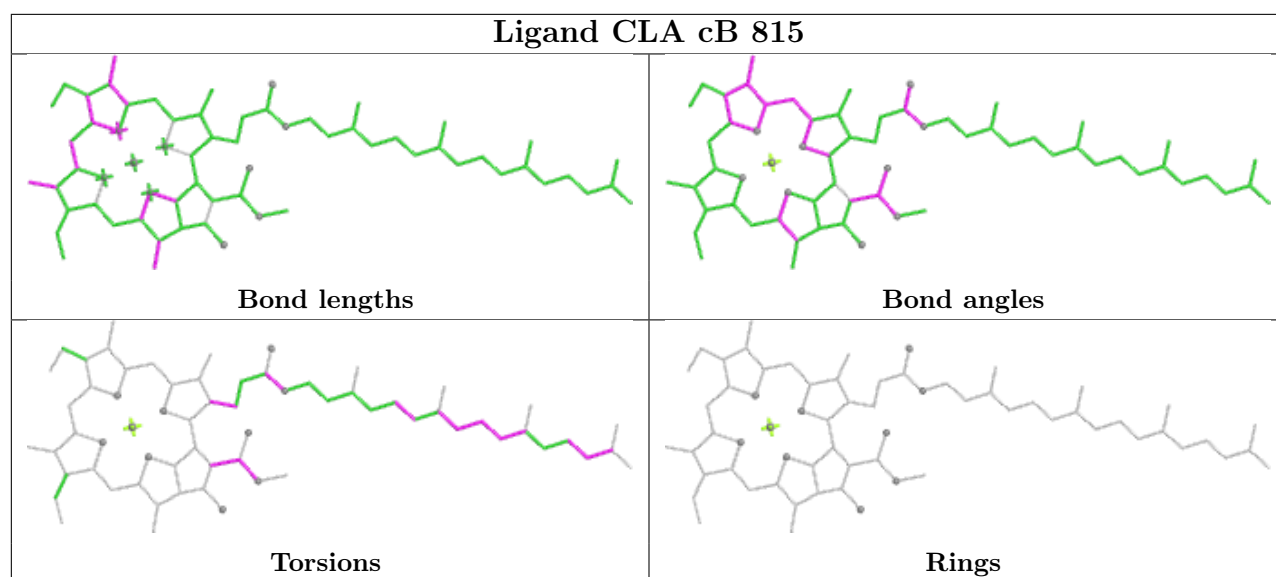


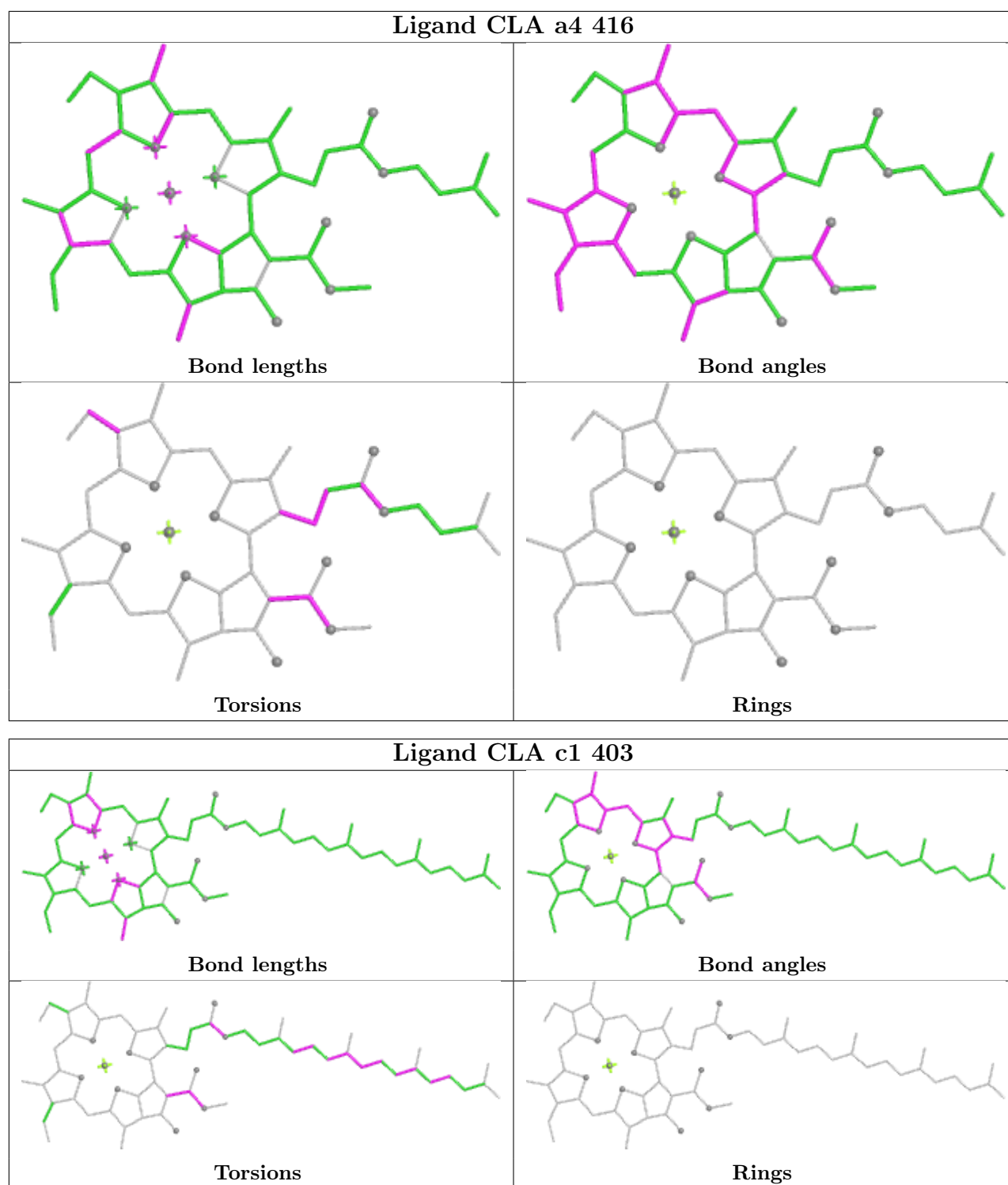


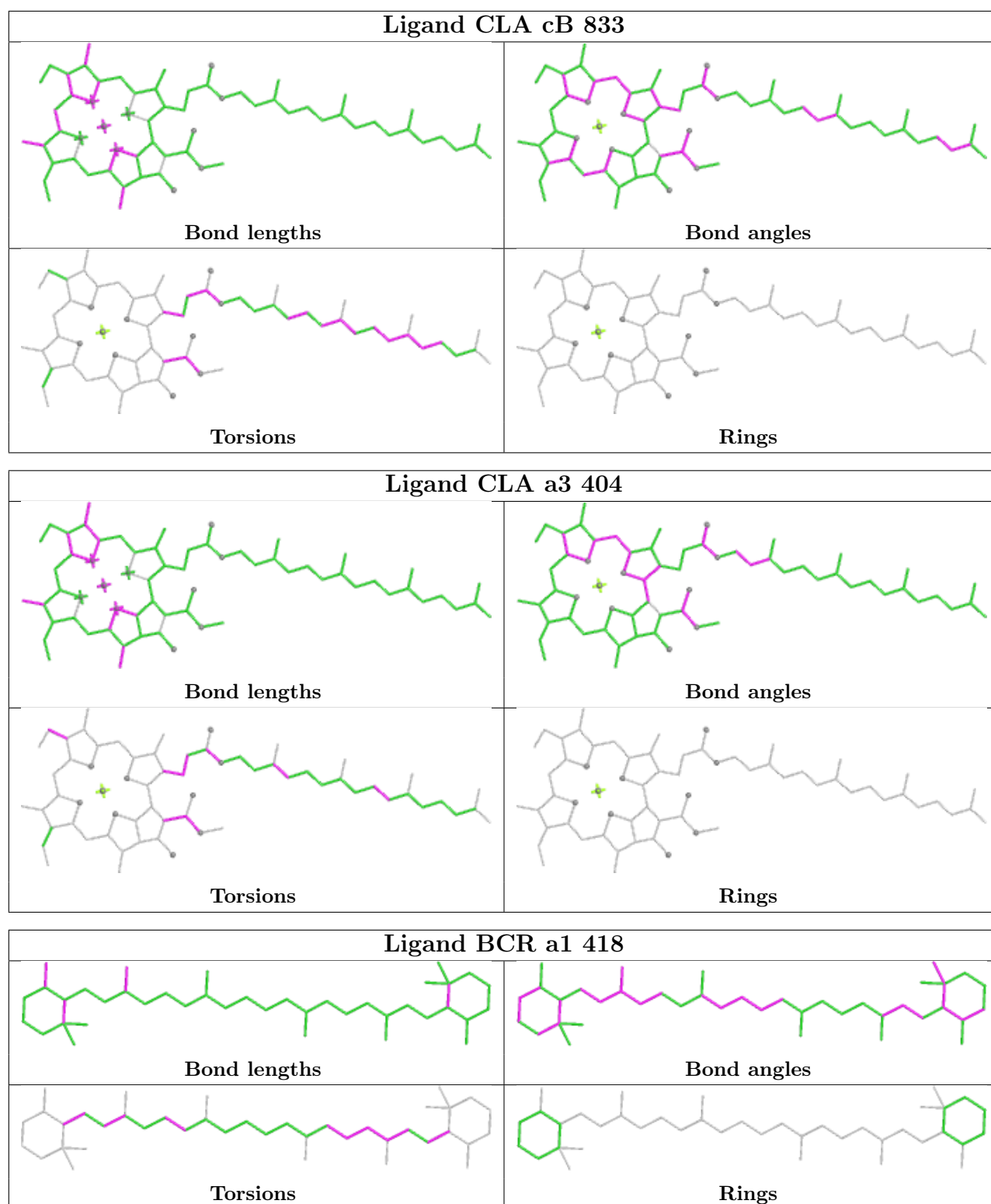
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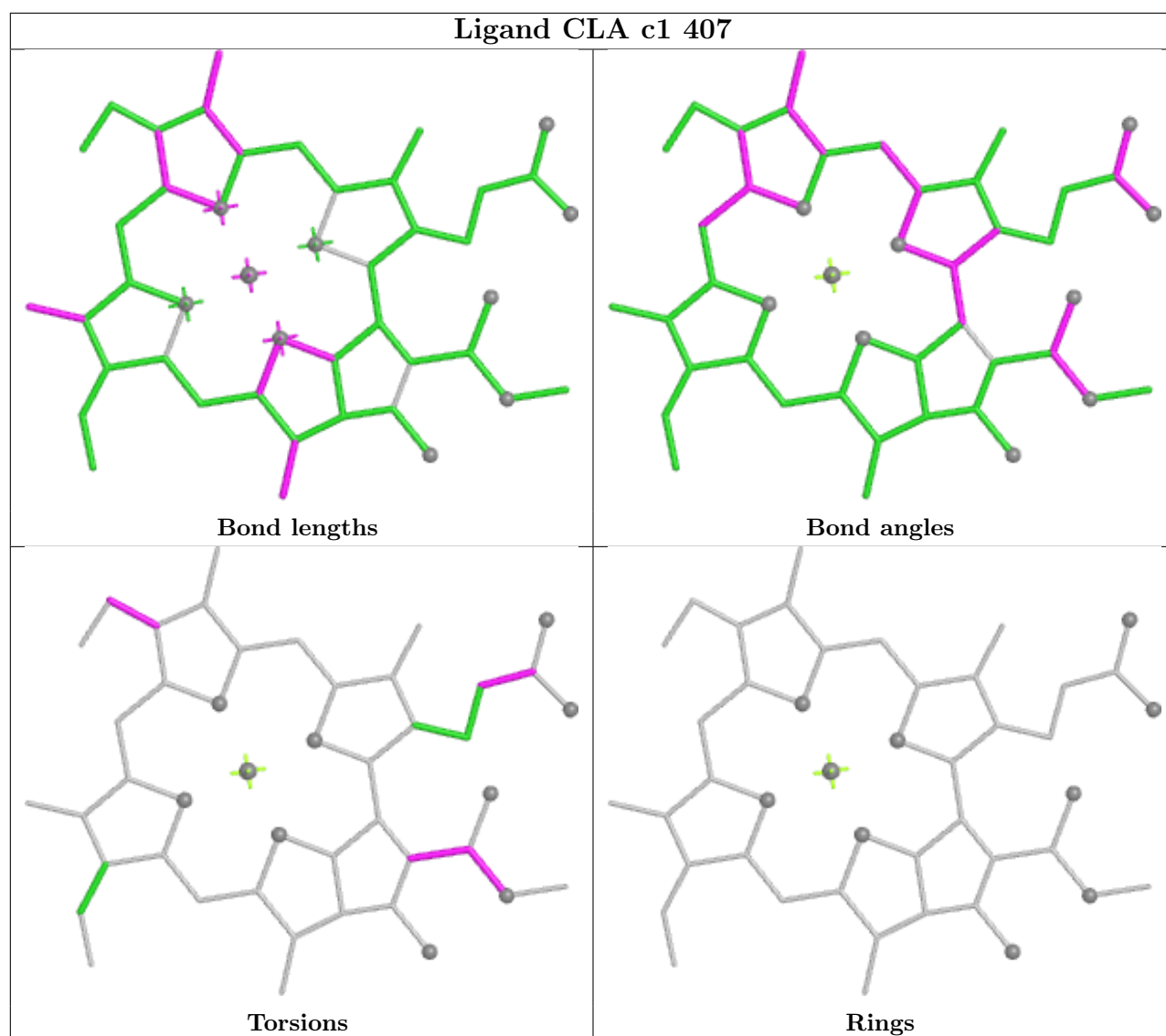


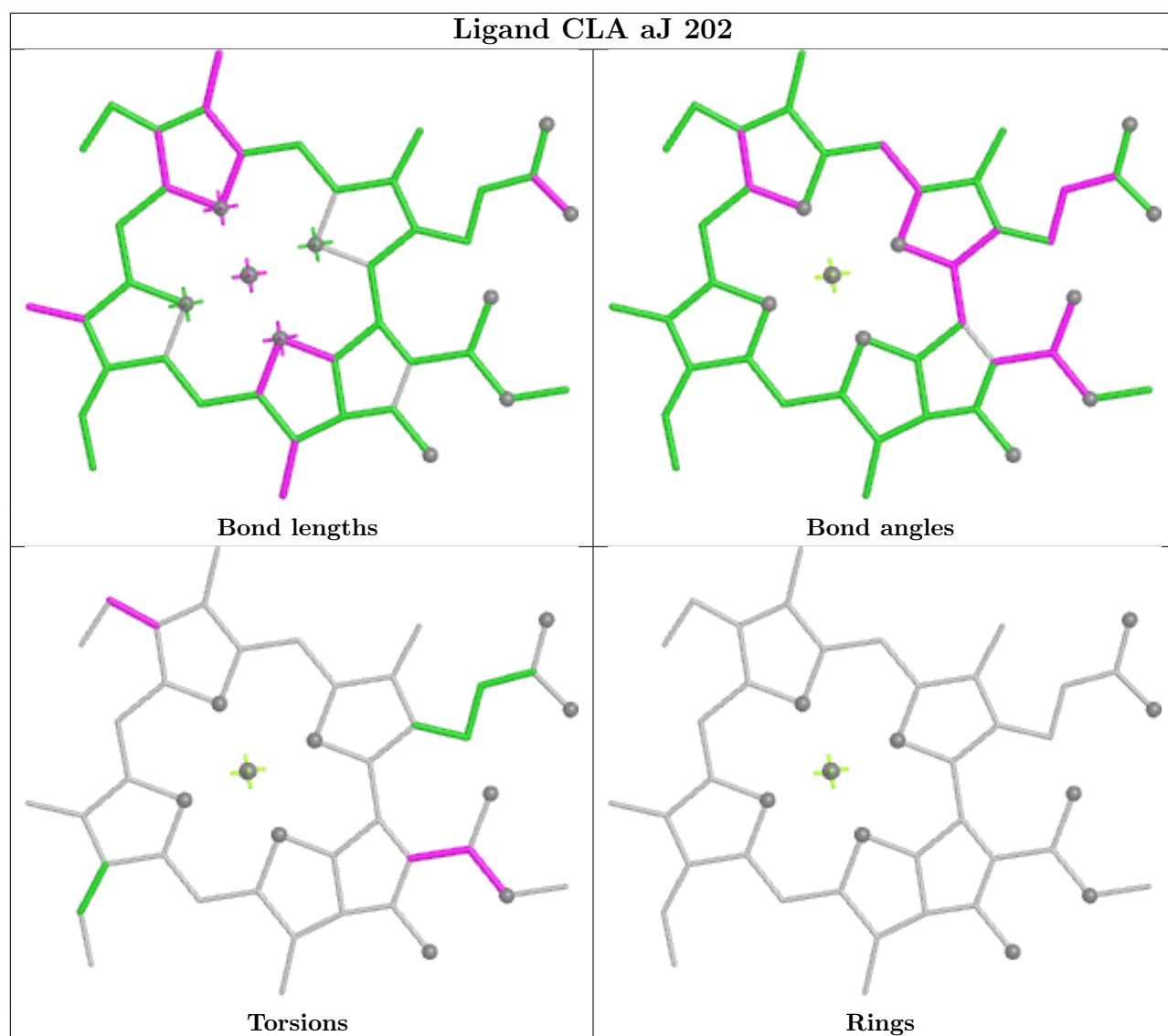


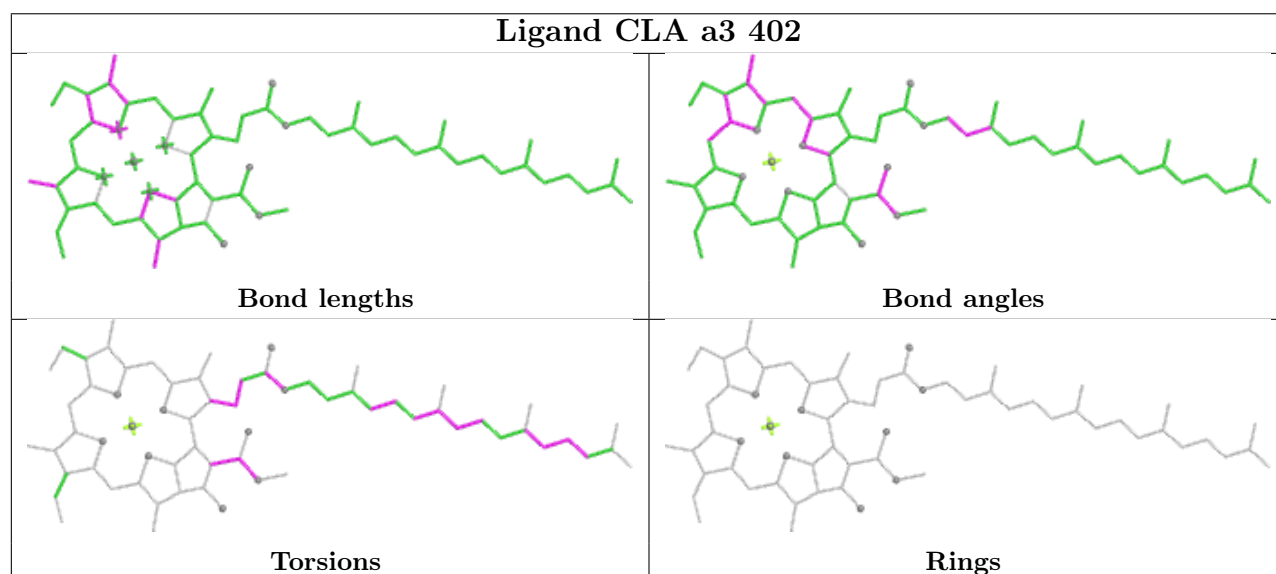
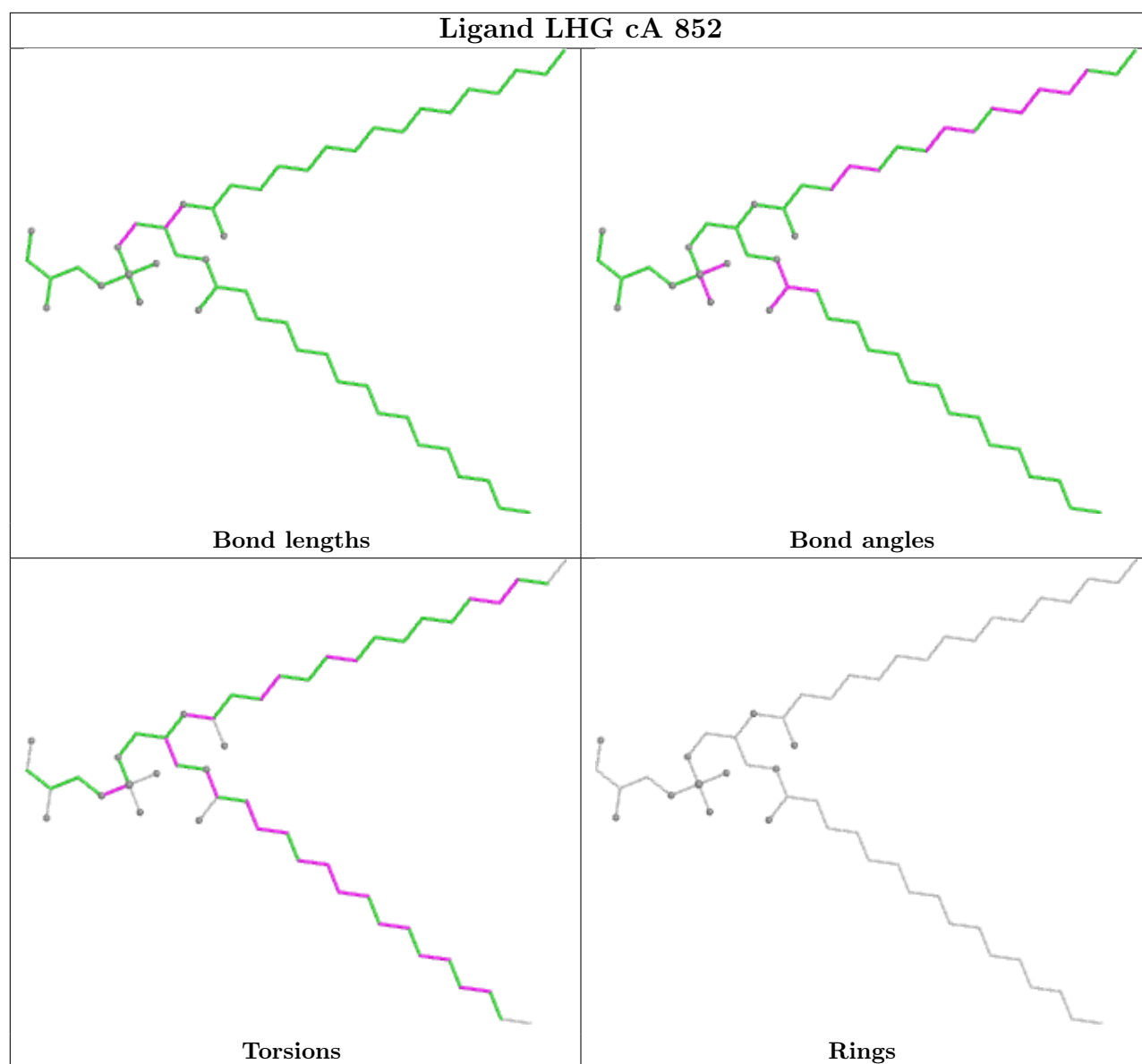


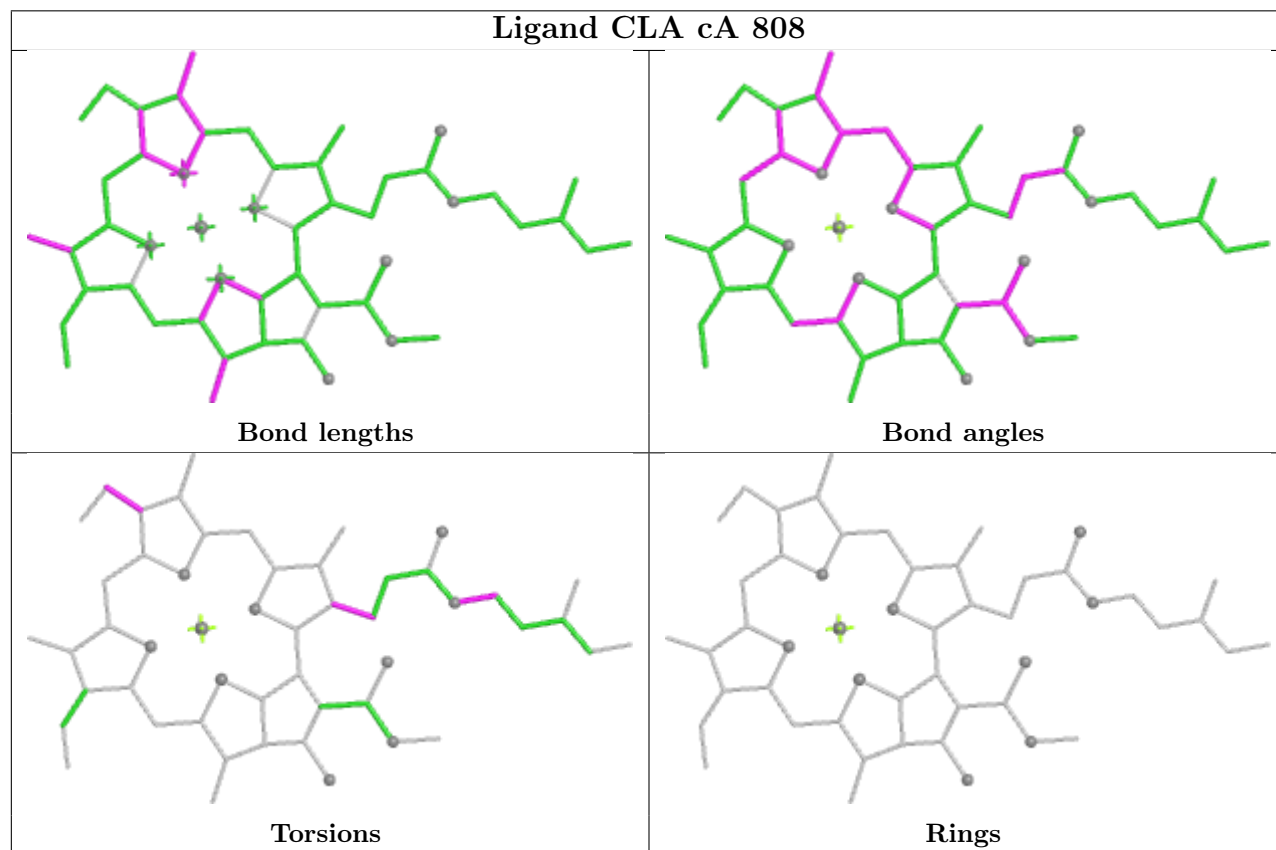
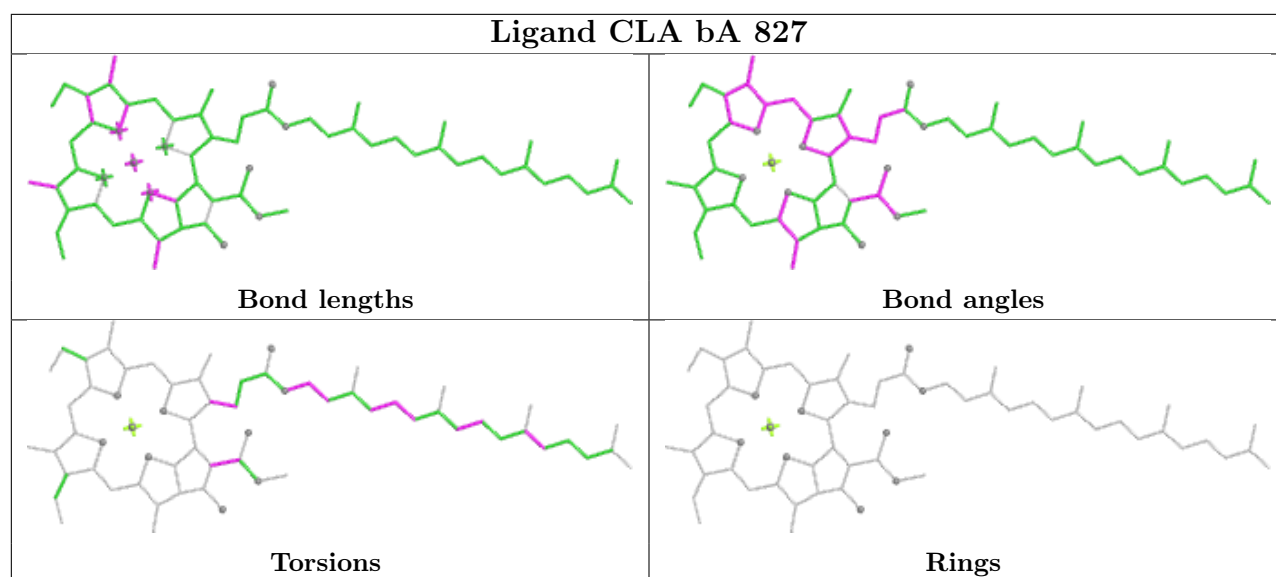


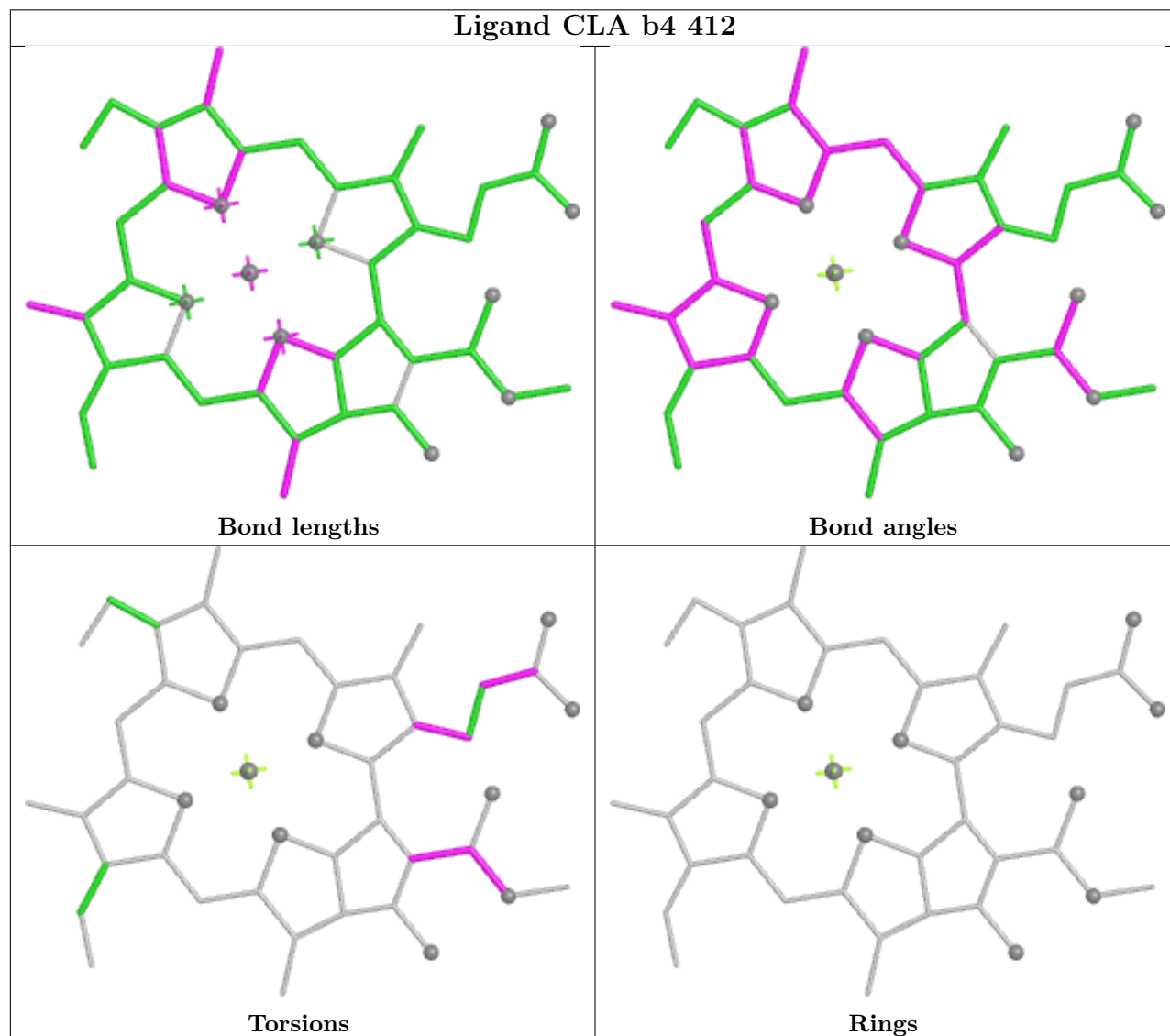
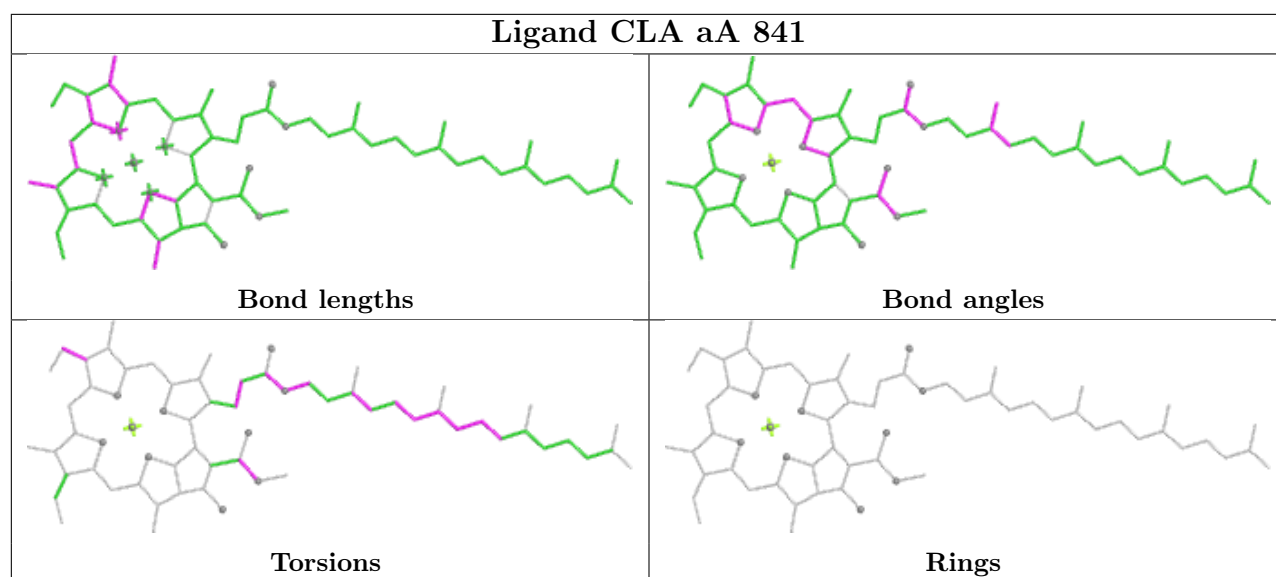


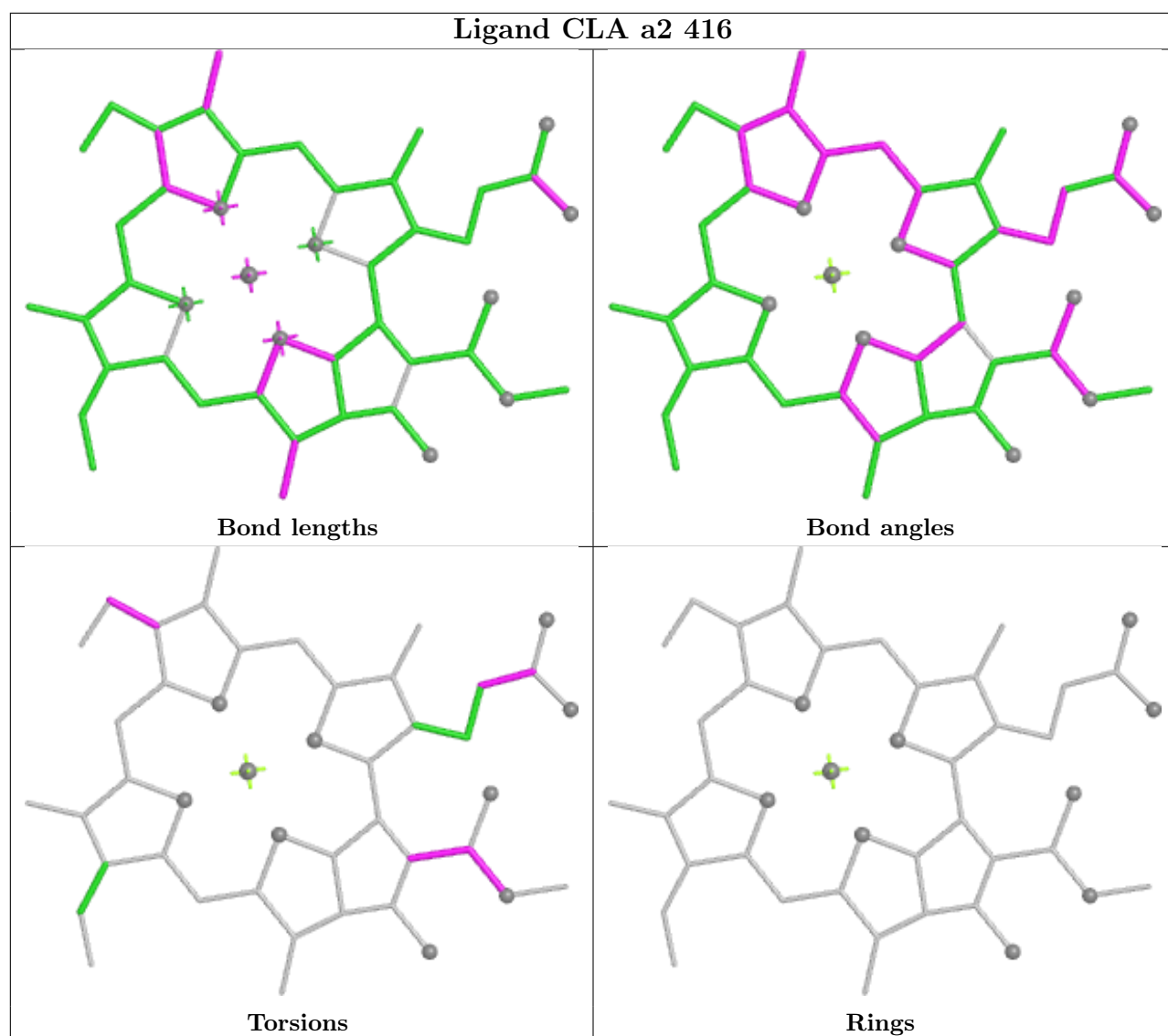


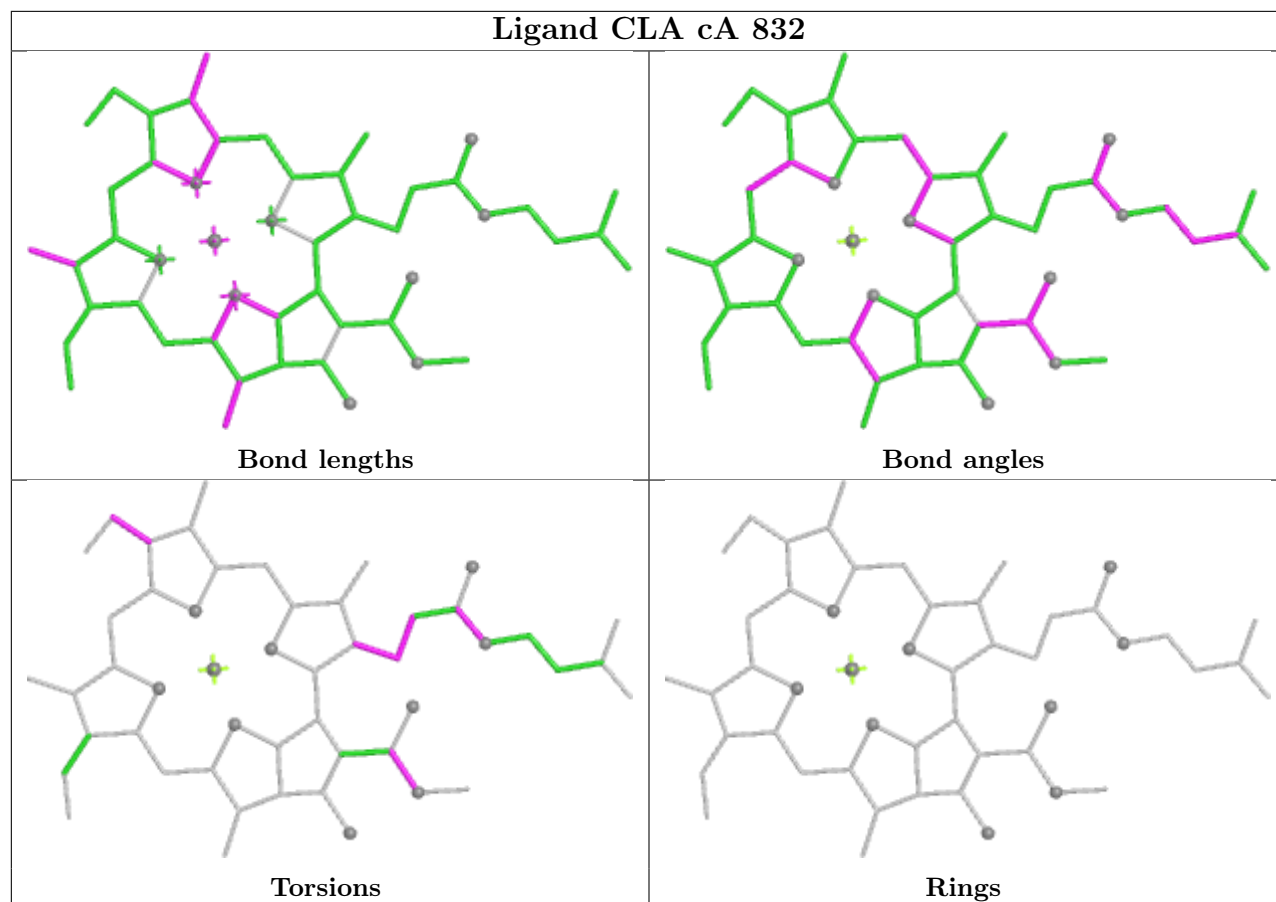


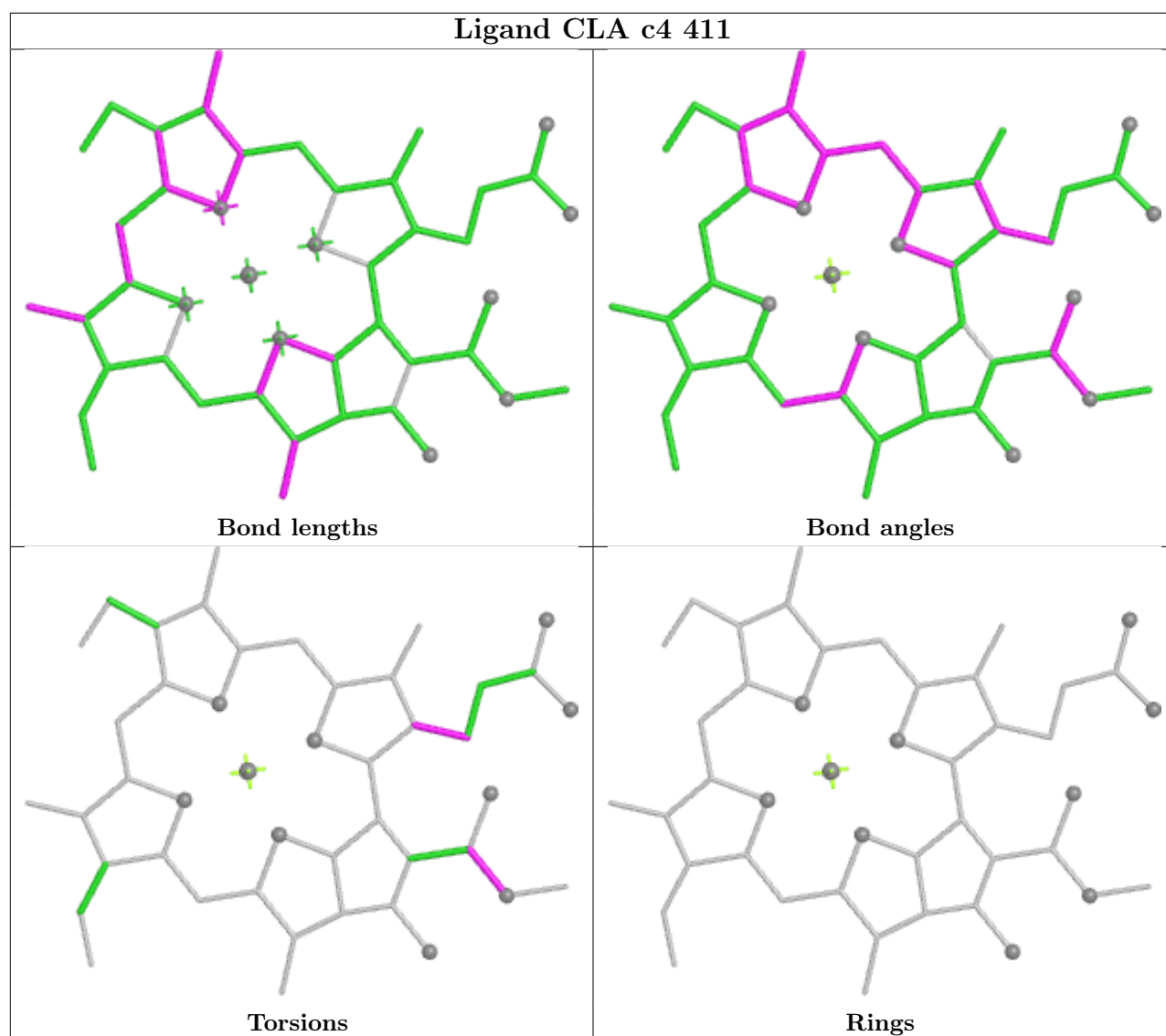


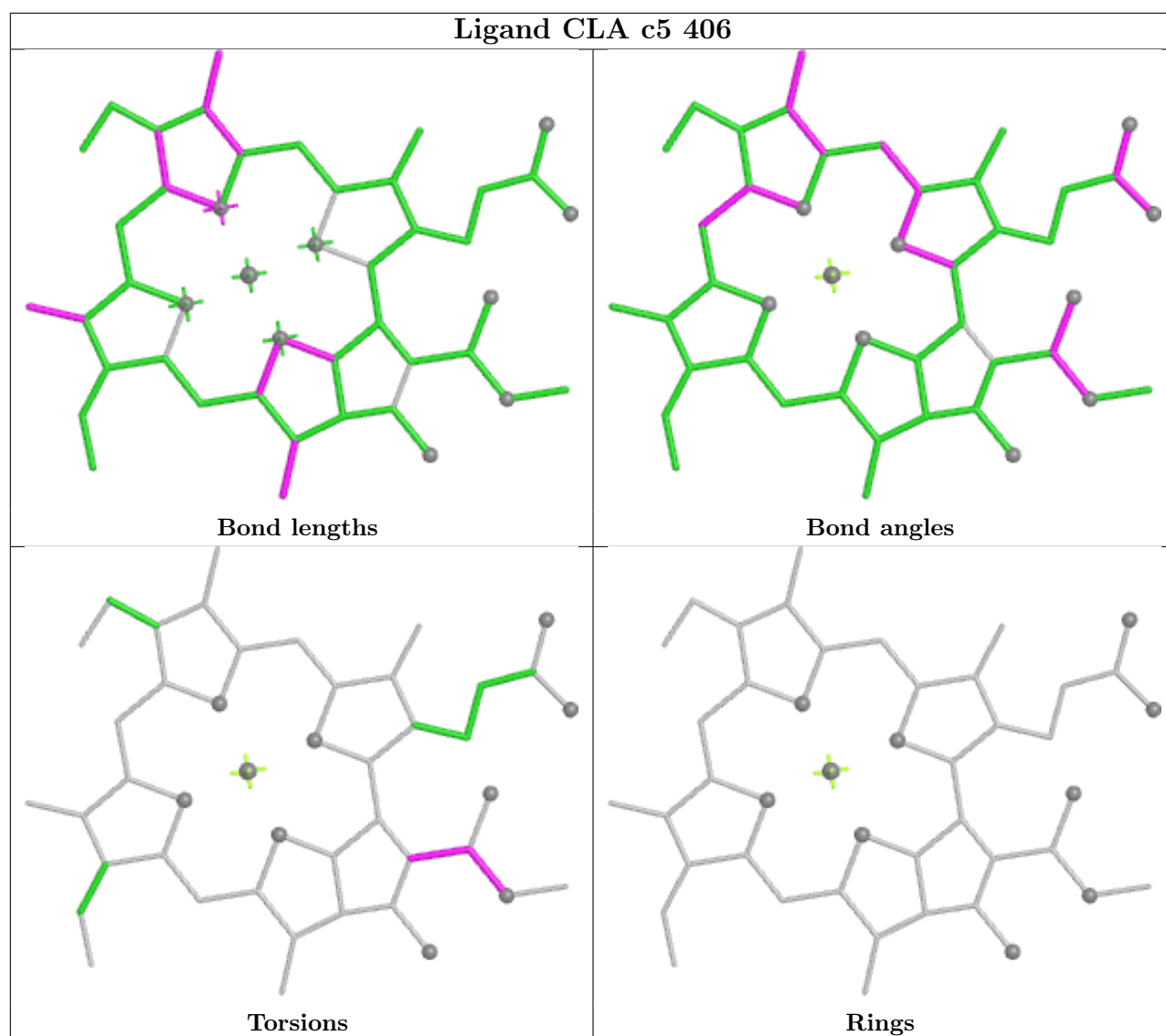


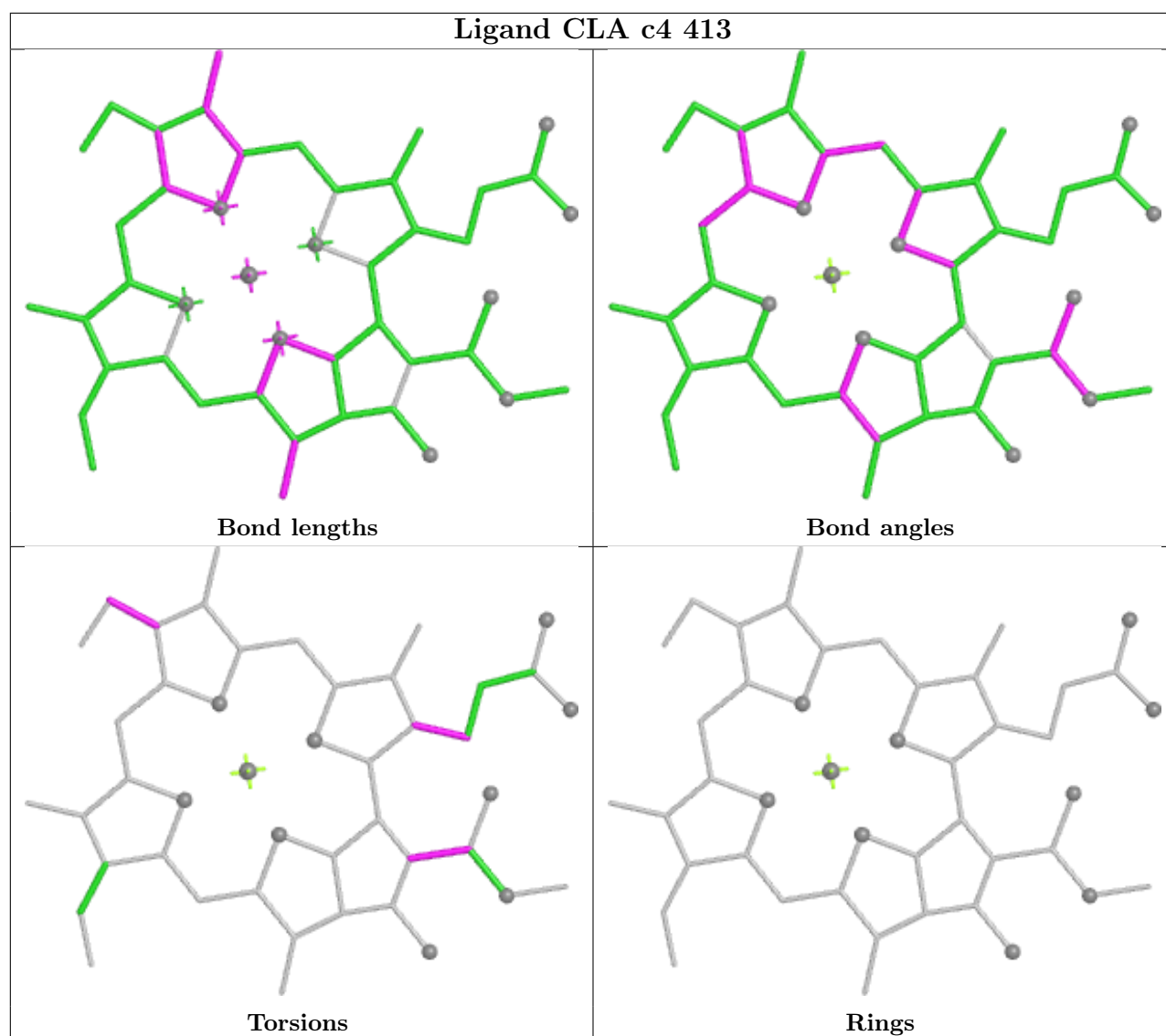


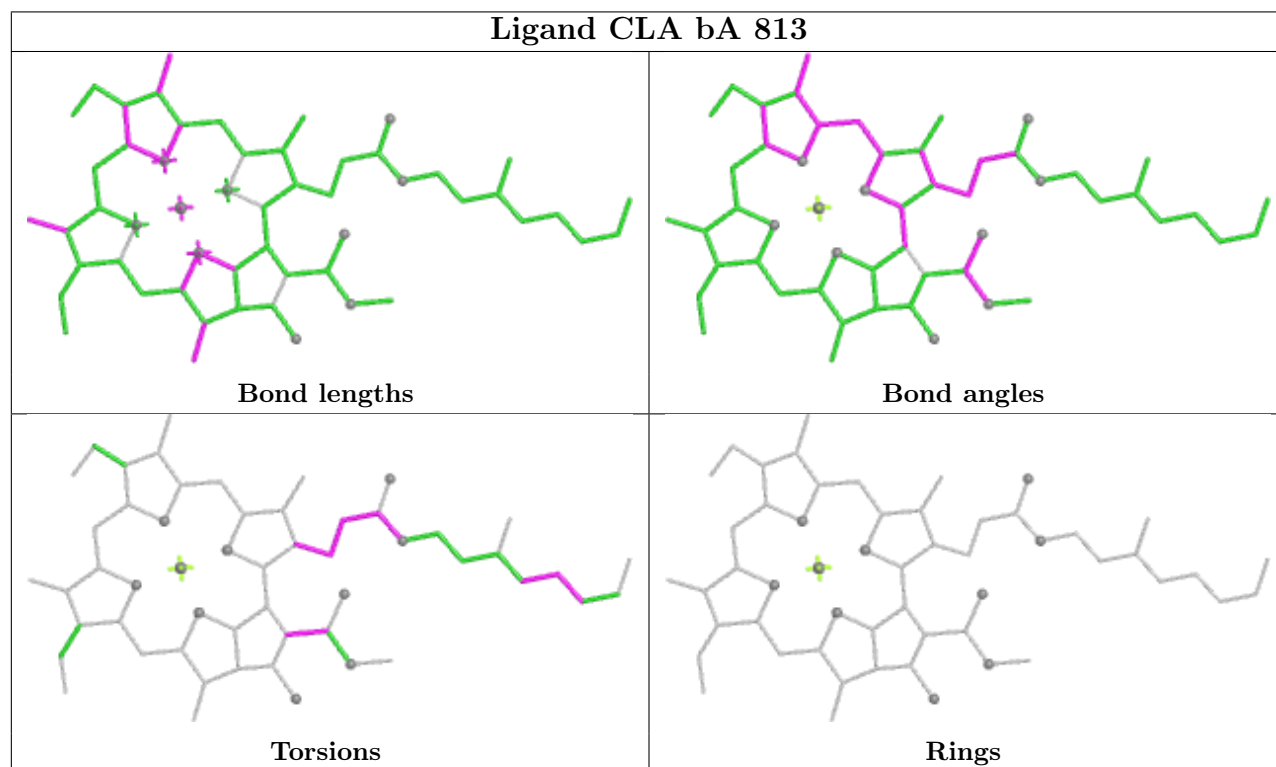
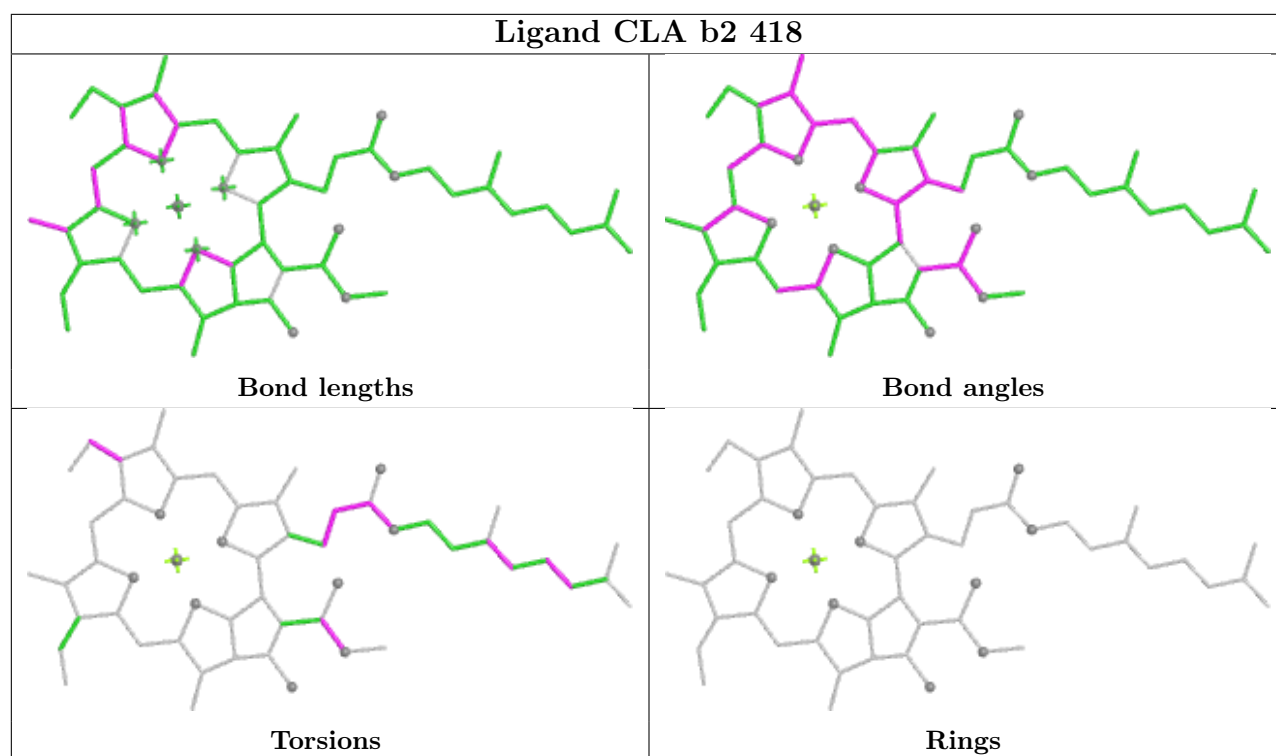




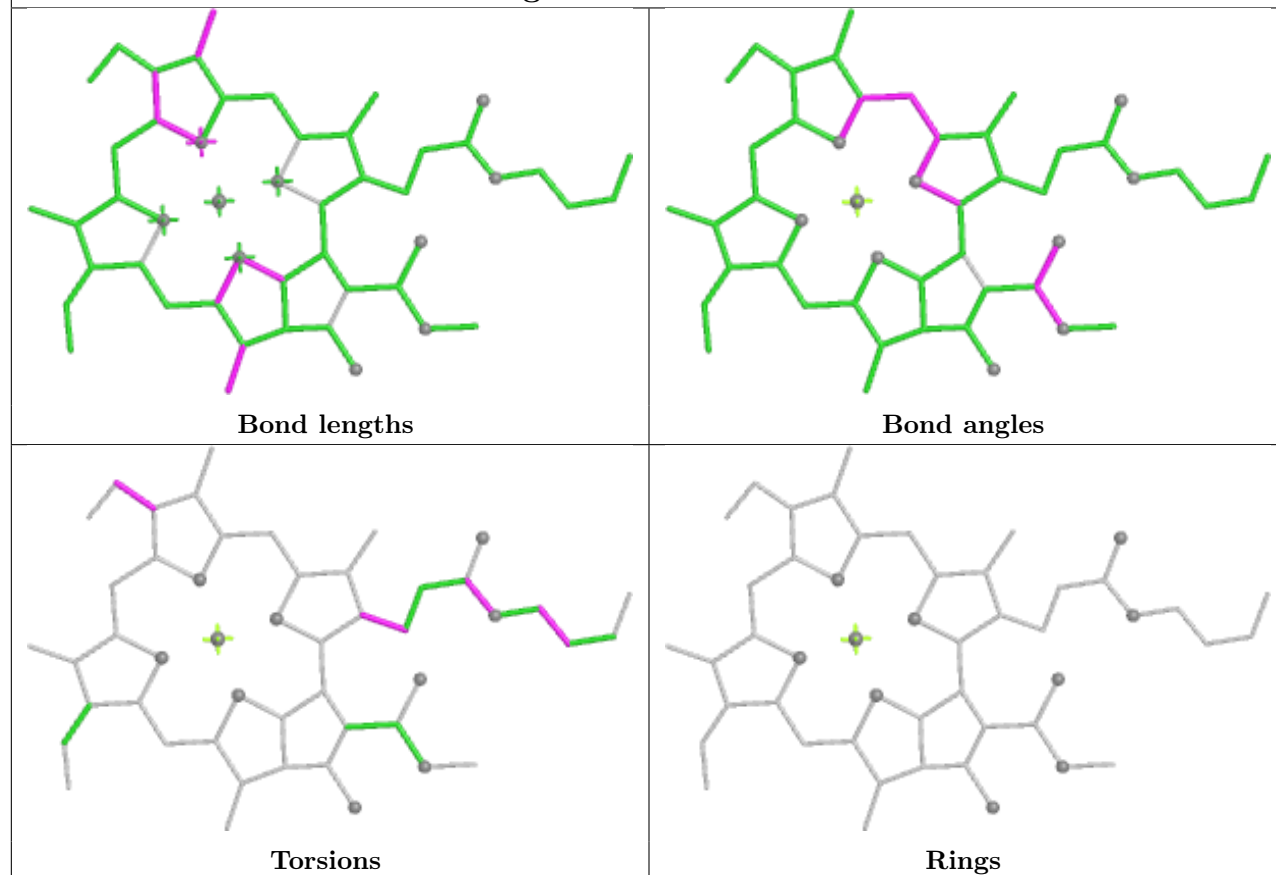




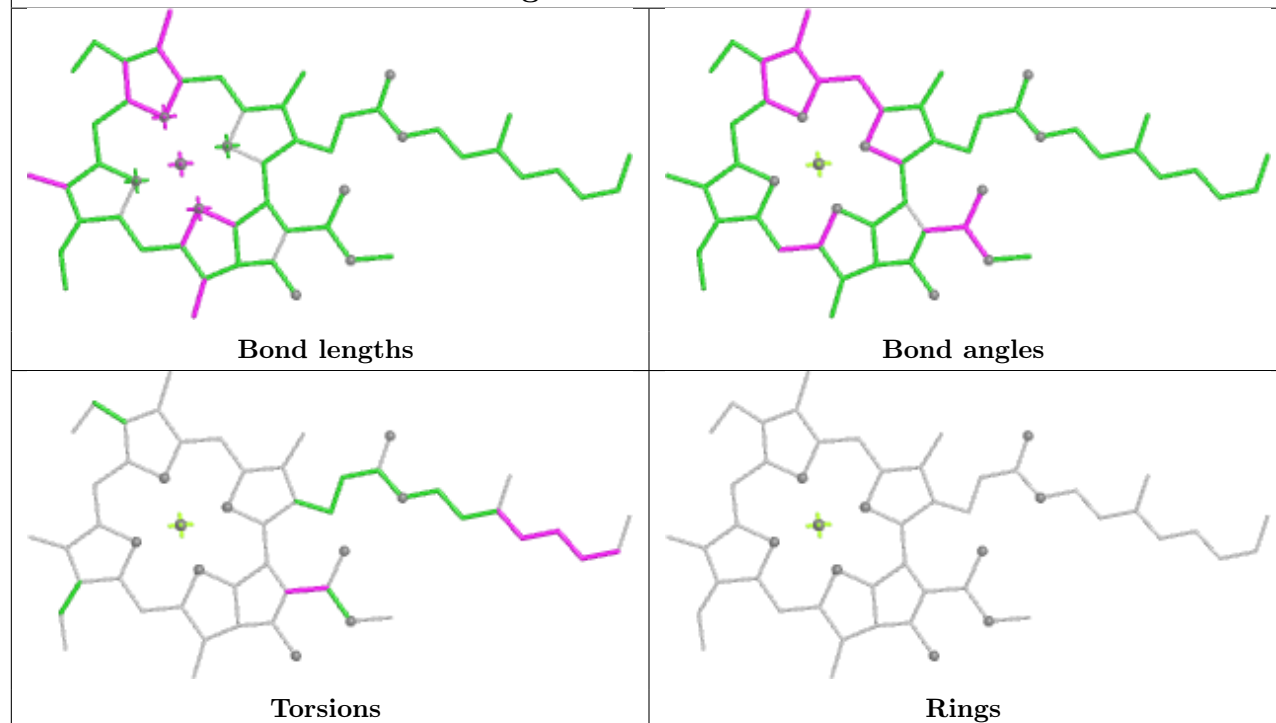


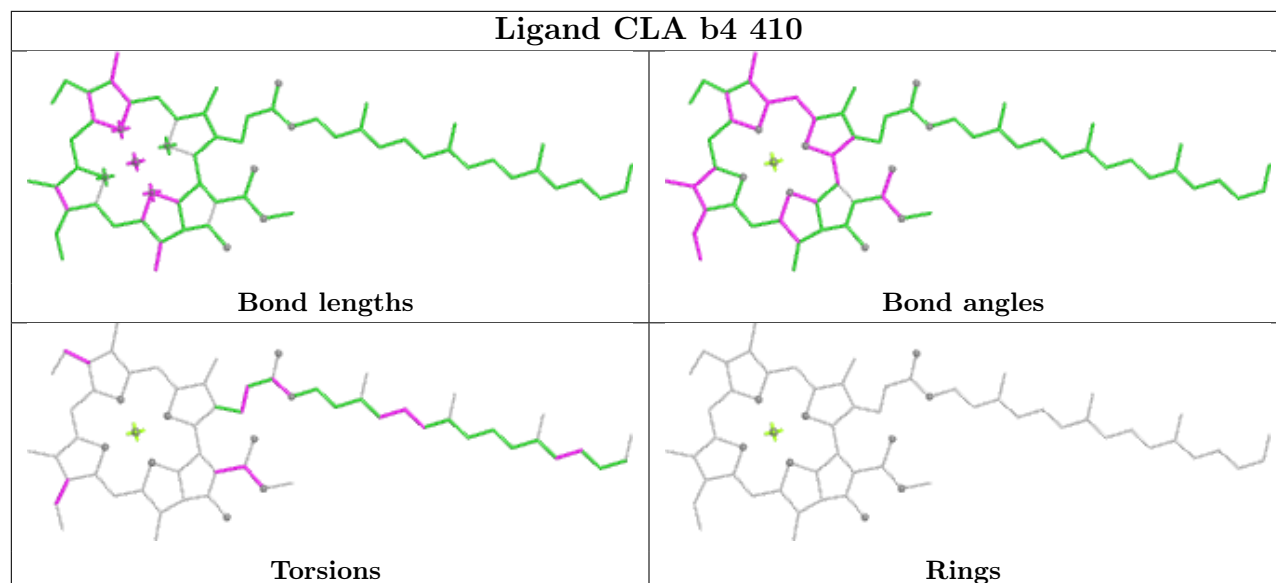
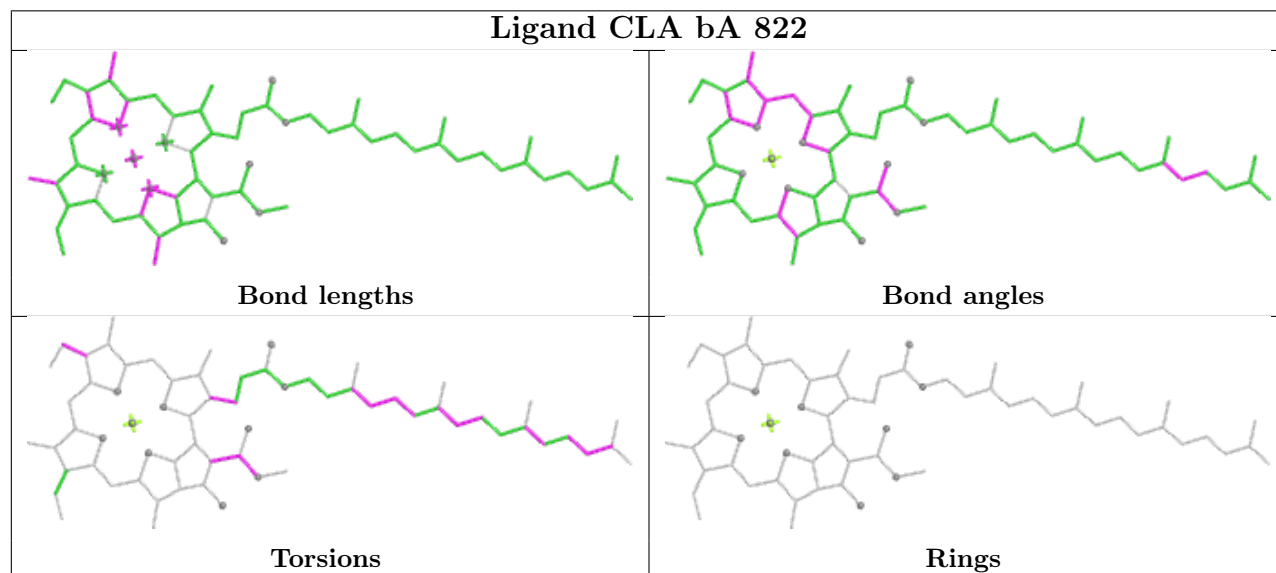
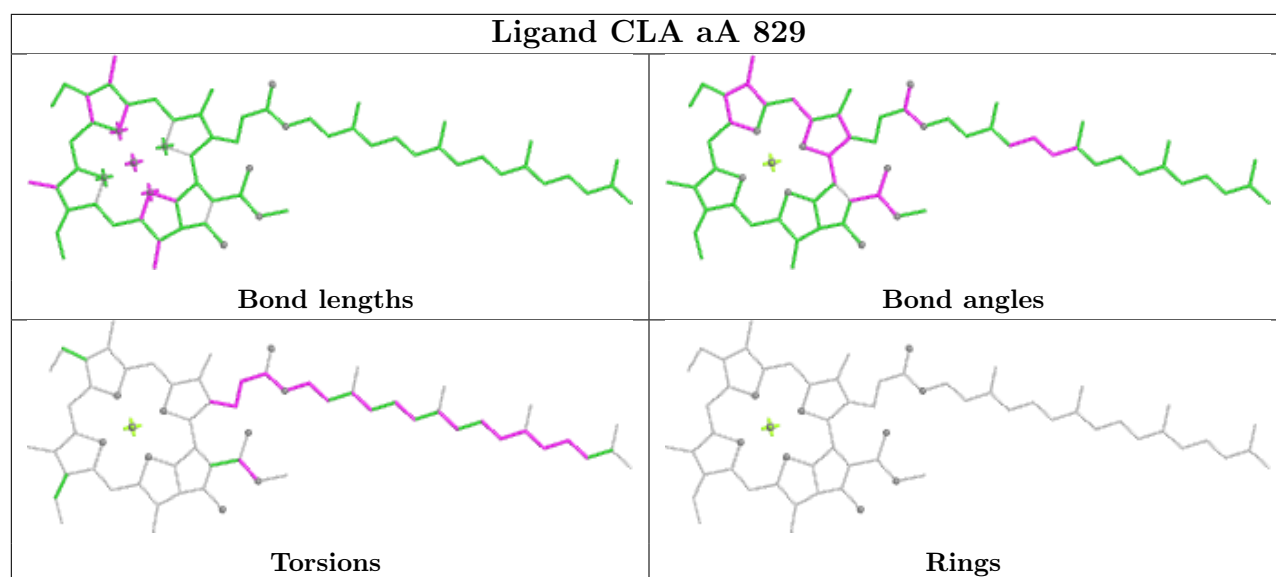


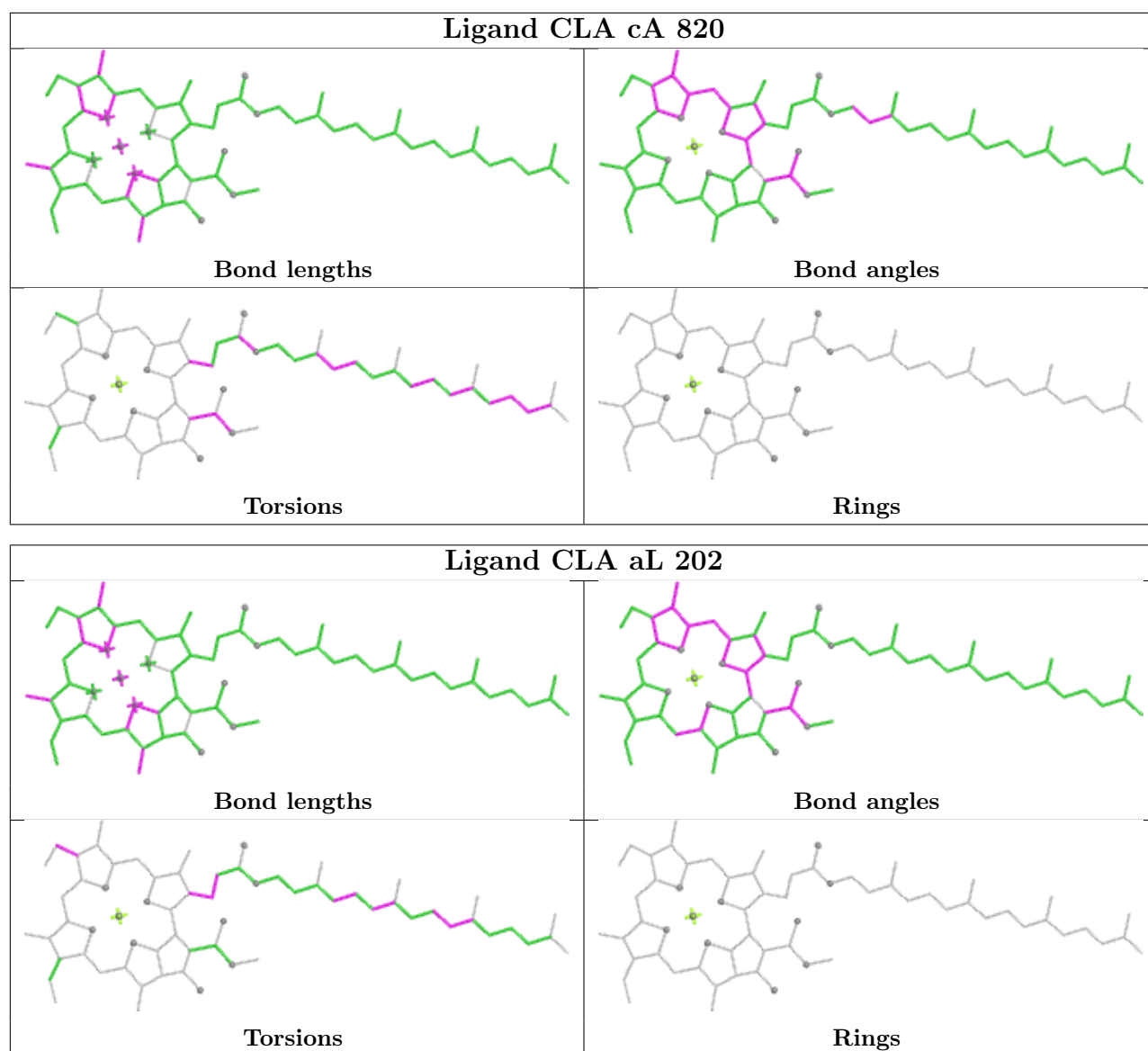
Ligand CLA aA 817

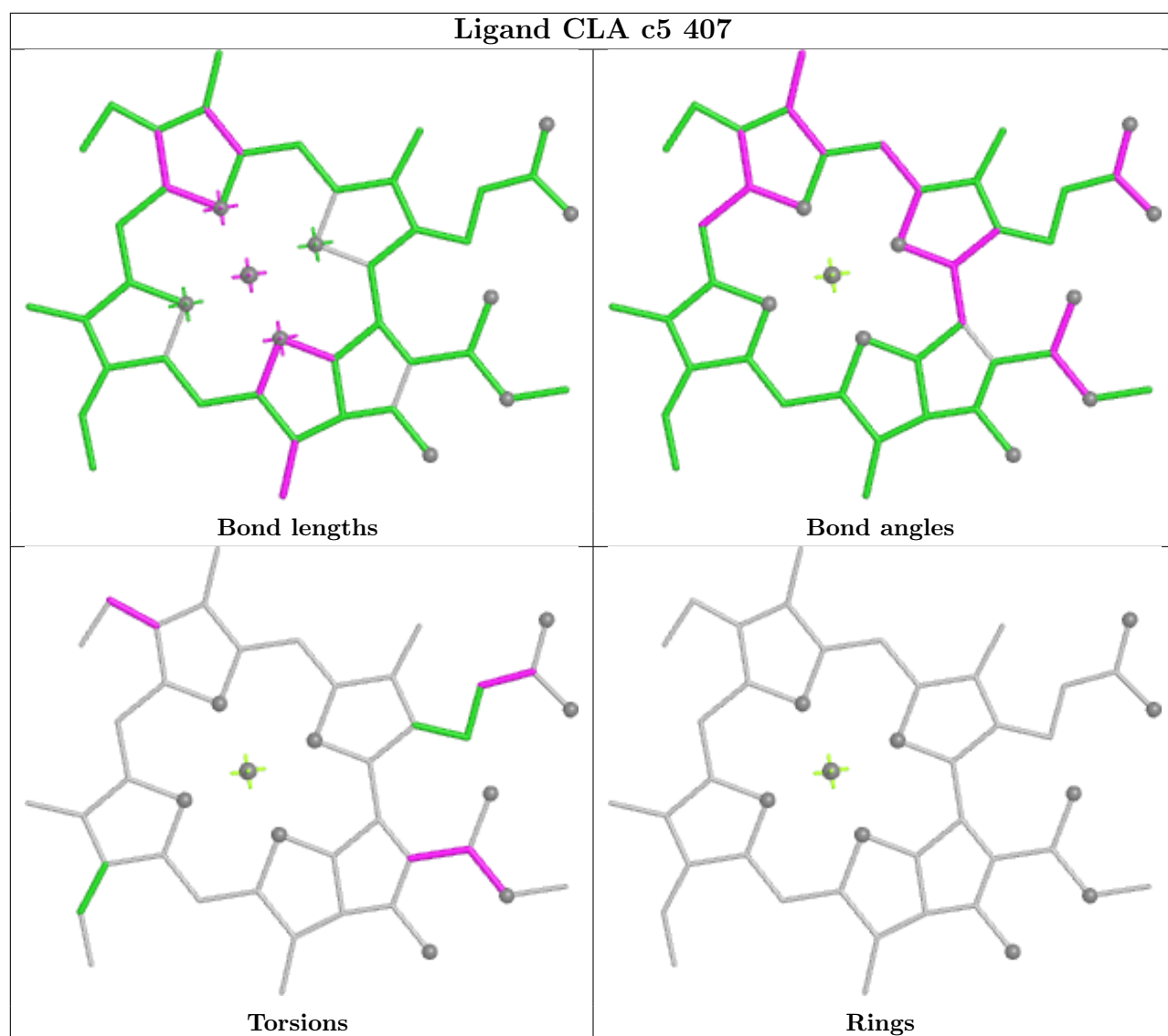


Ligand CLA bA 818

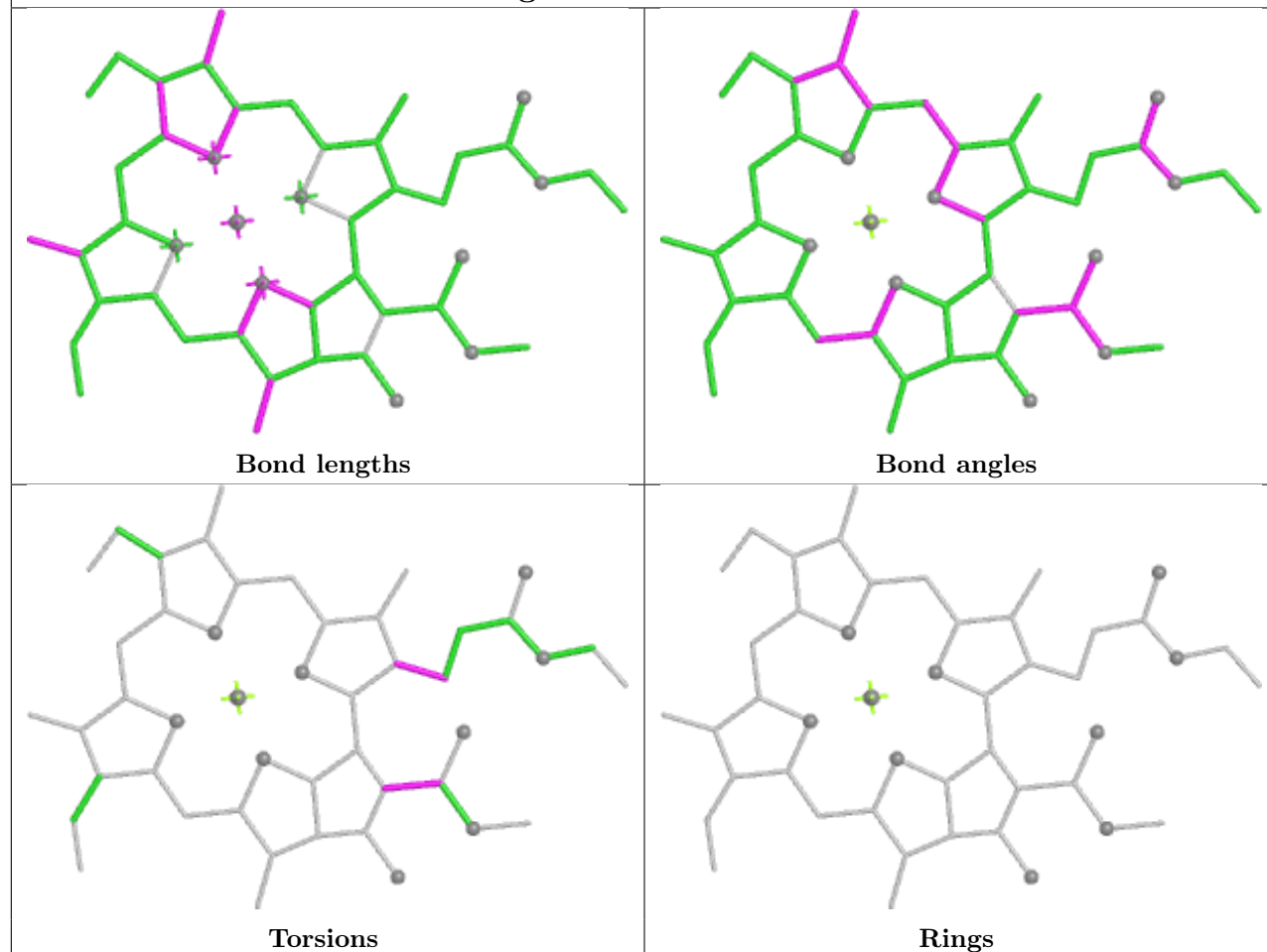




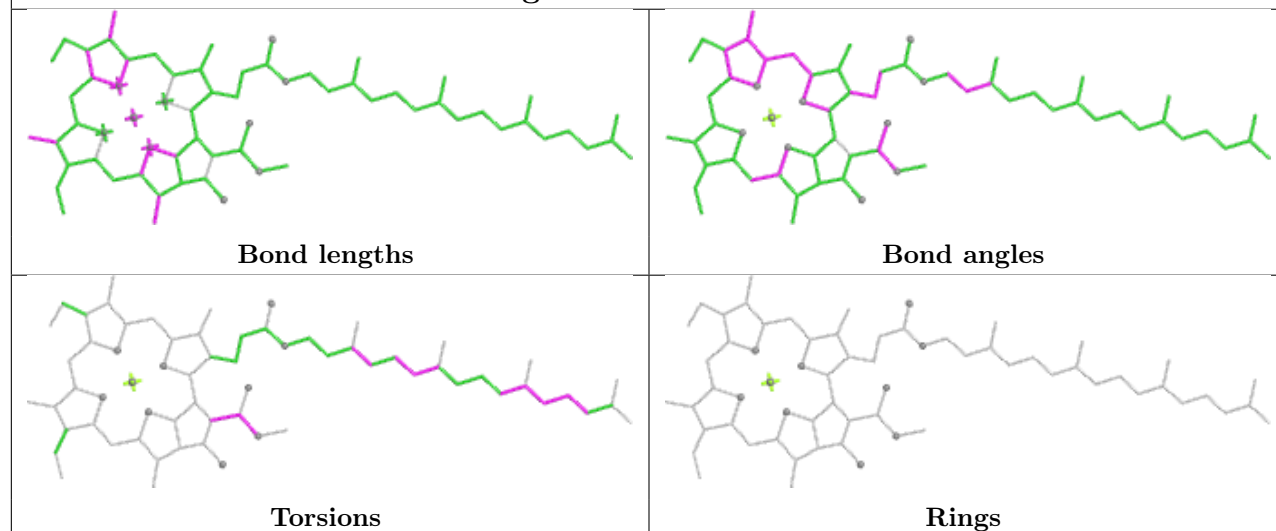


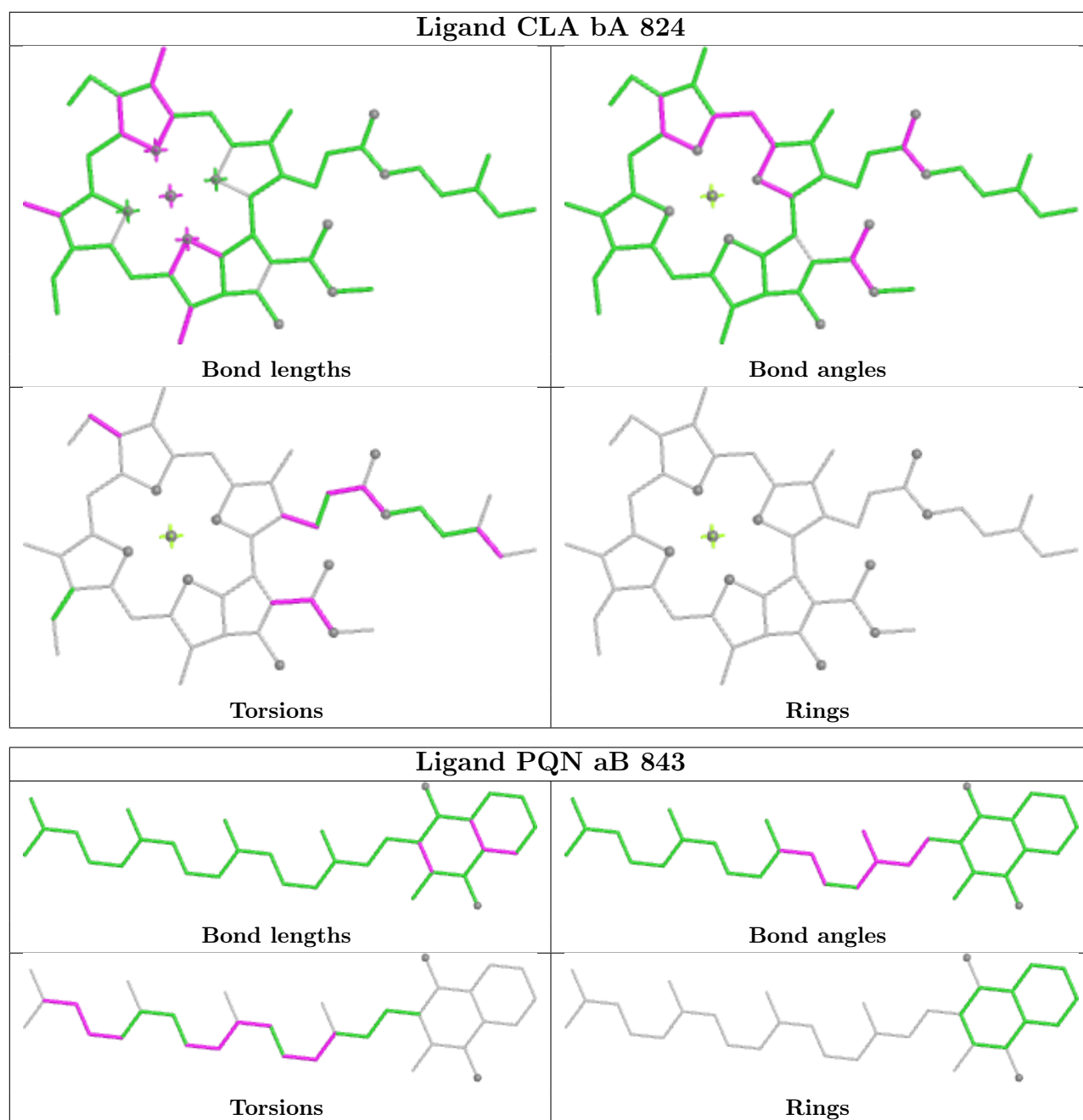


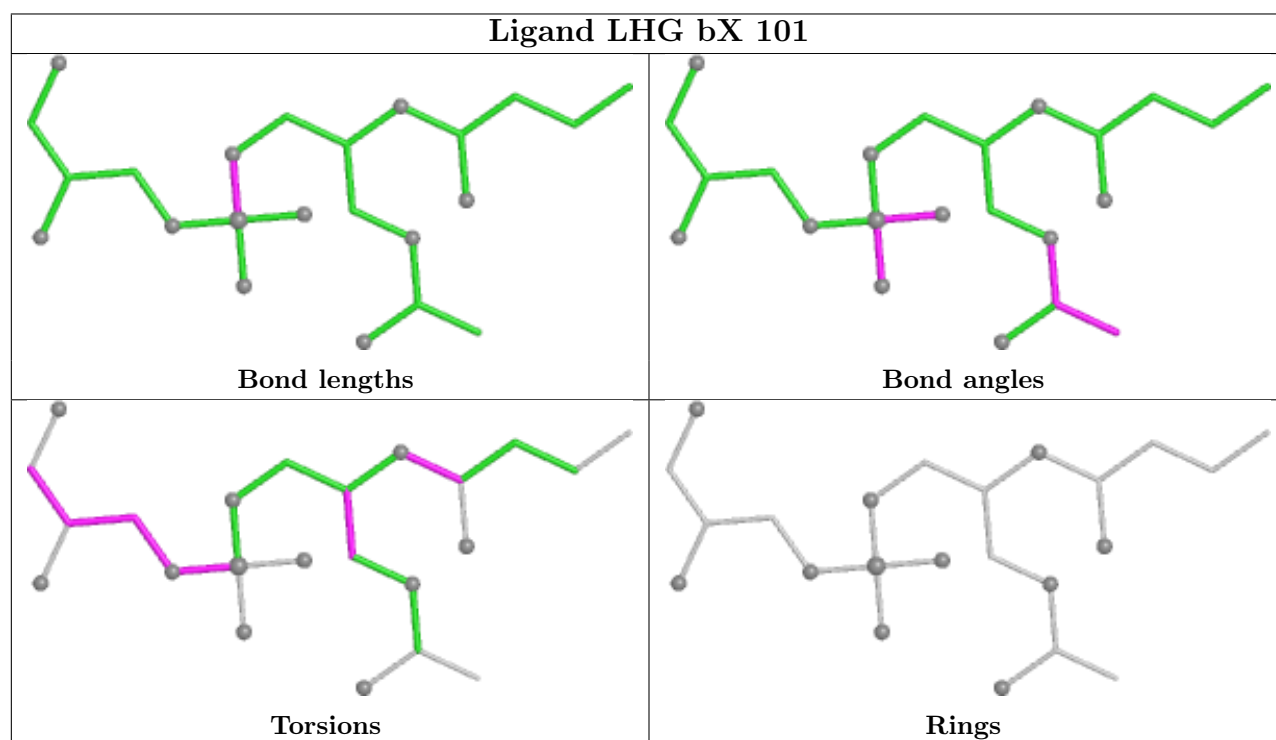
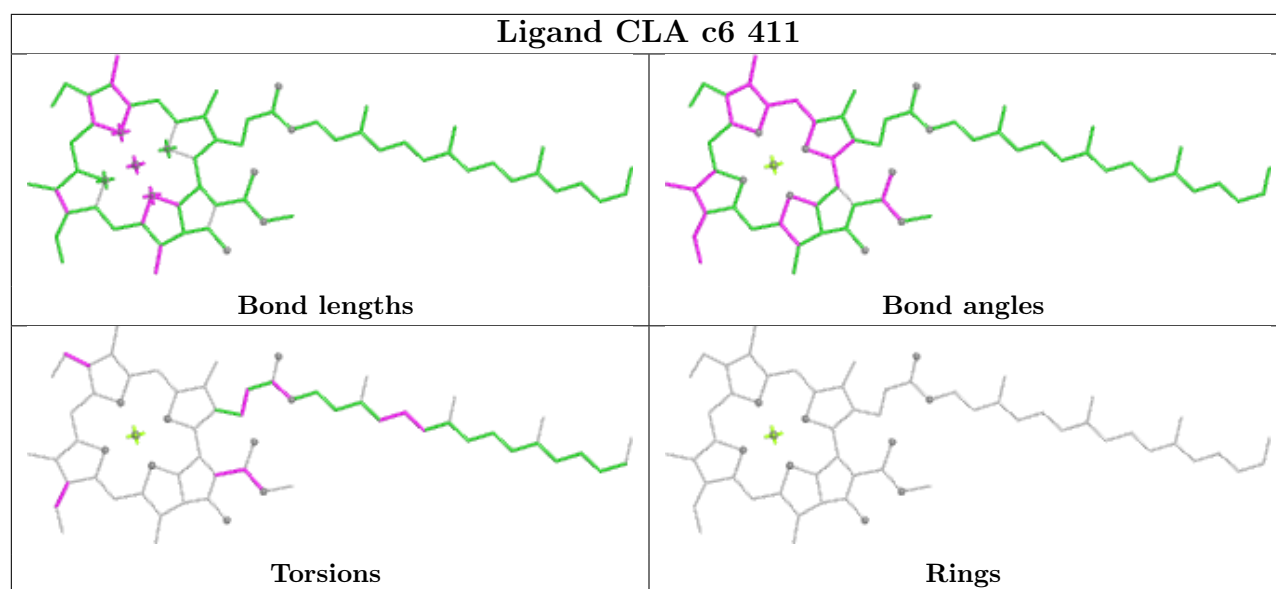
Ligand CLA bB 838

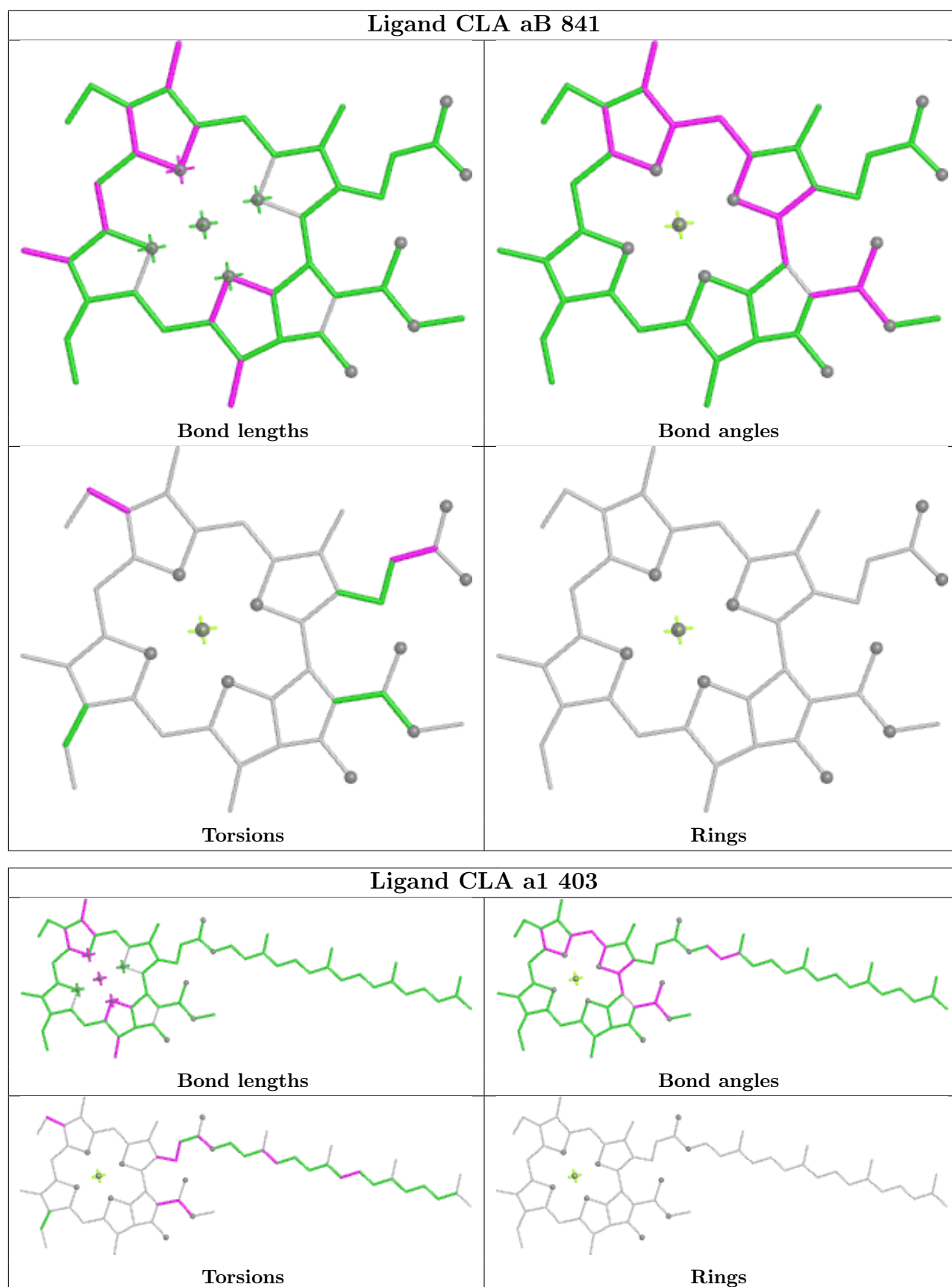


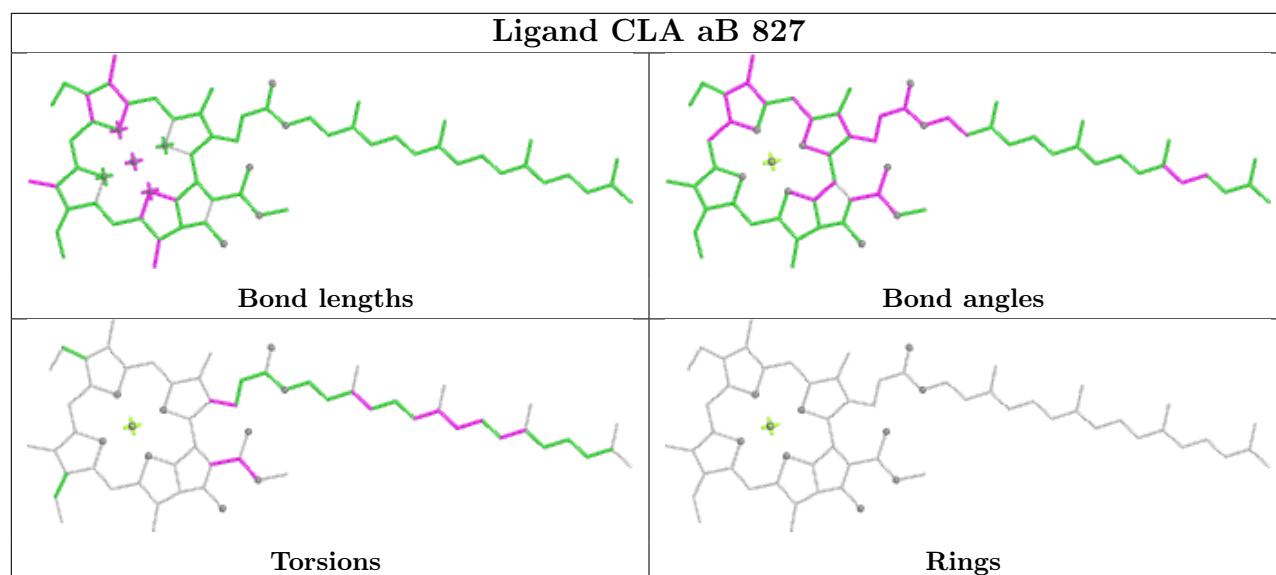
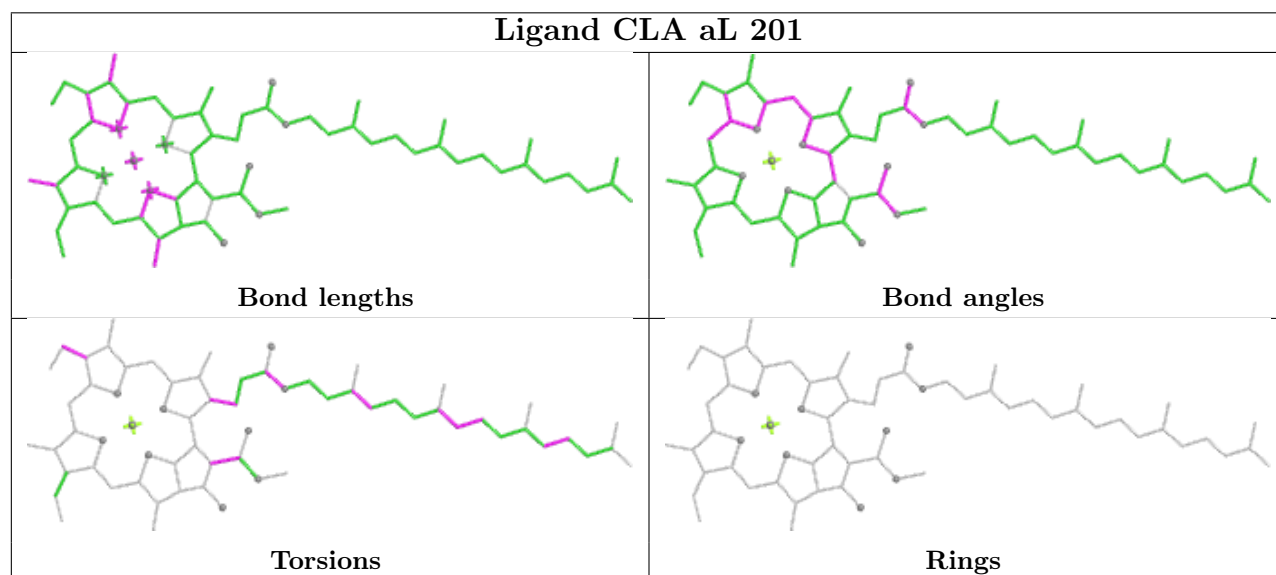
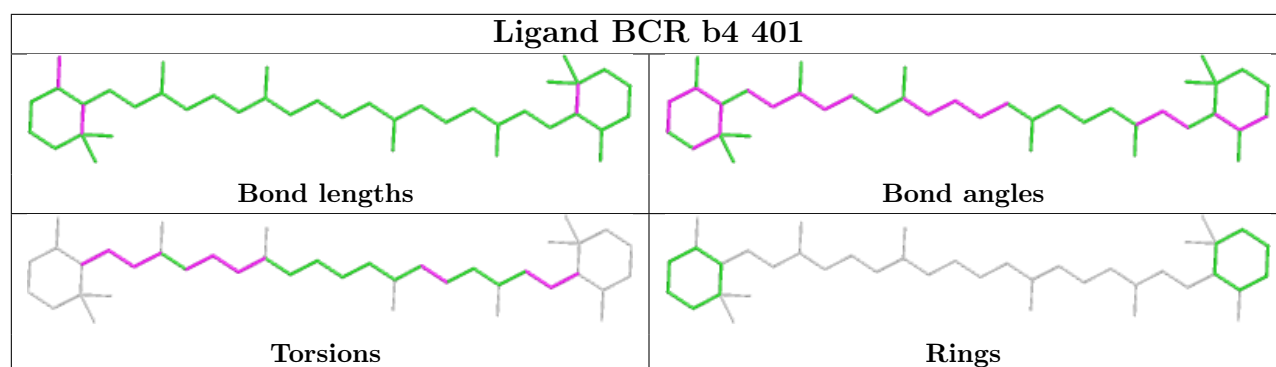
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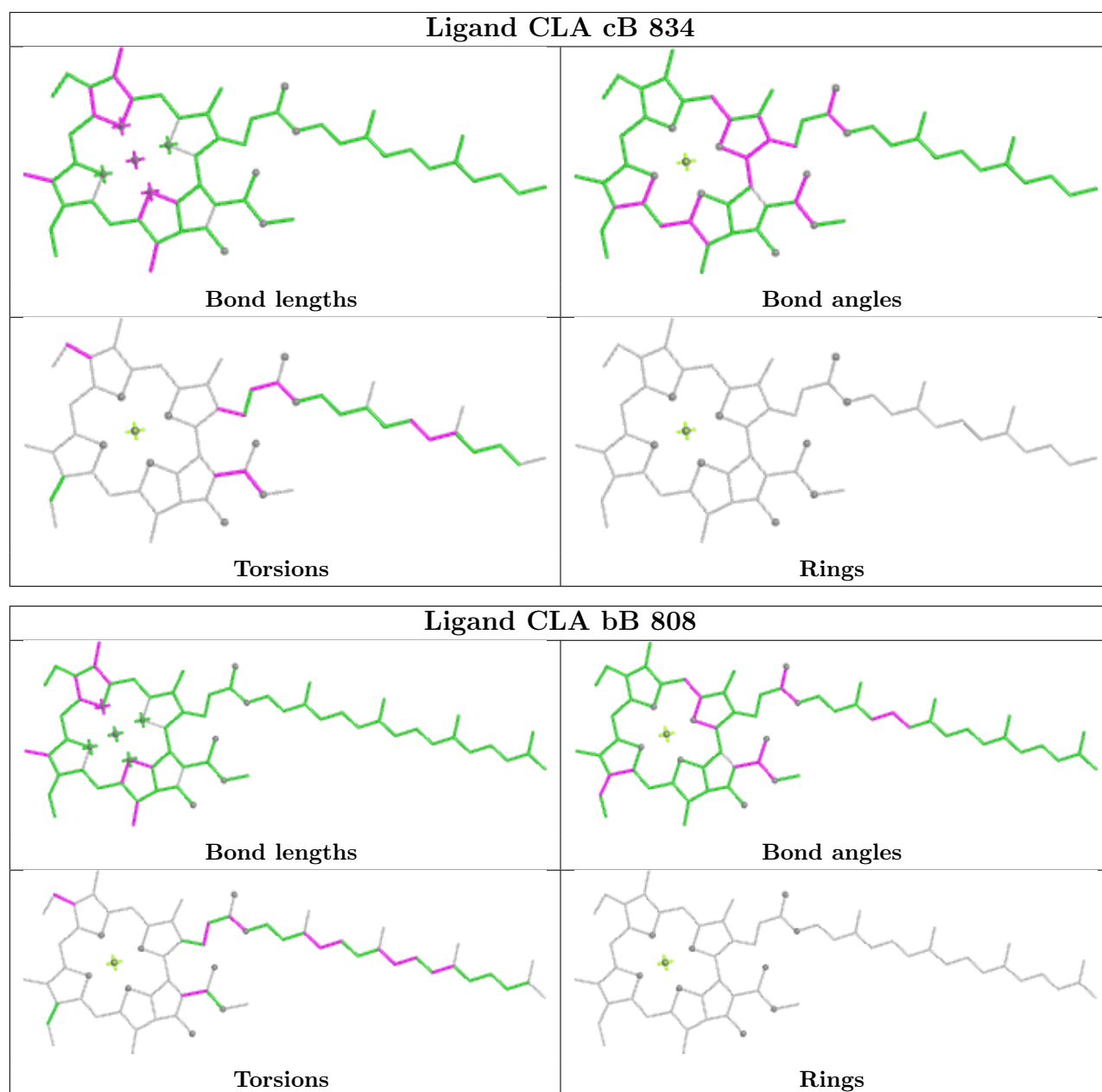


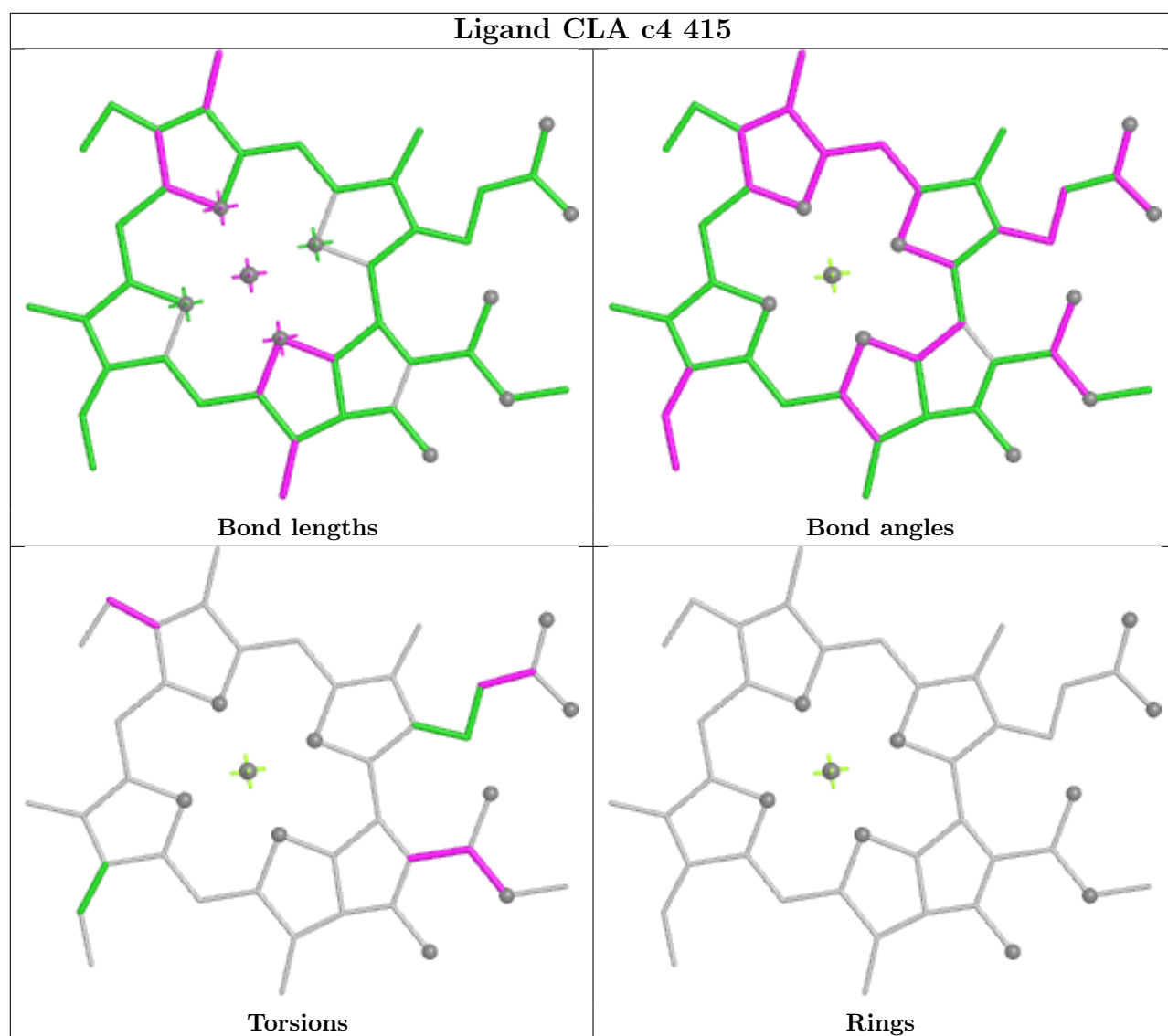


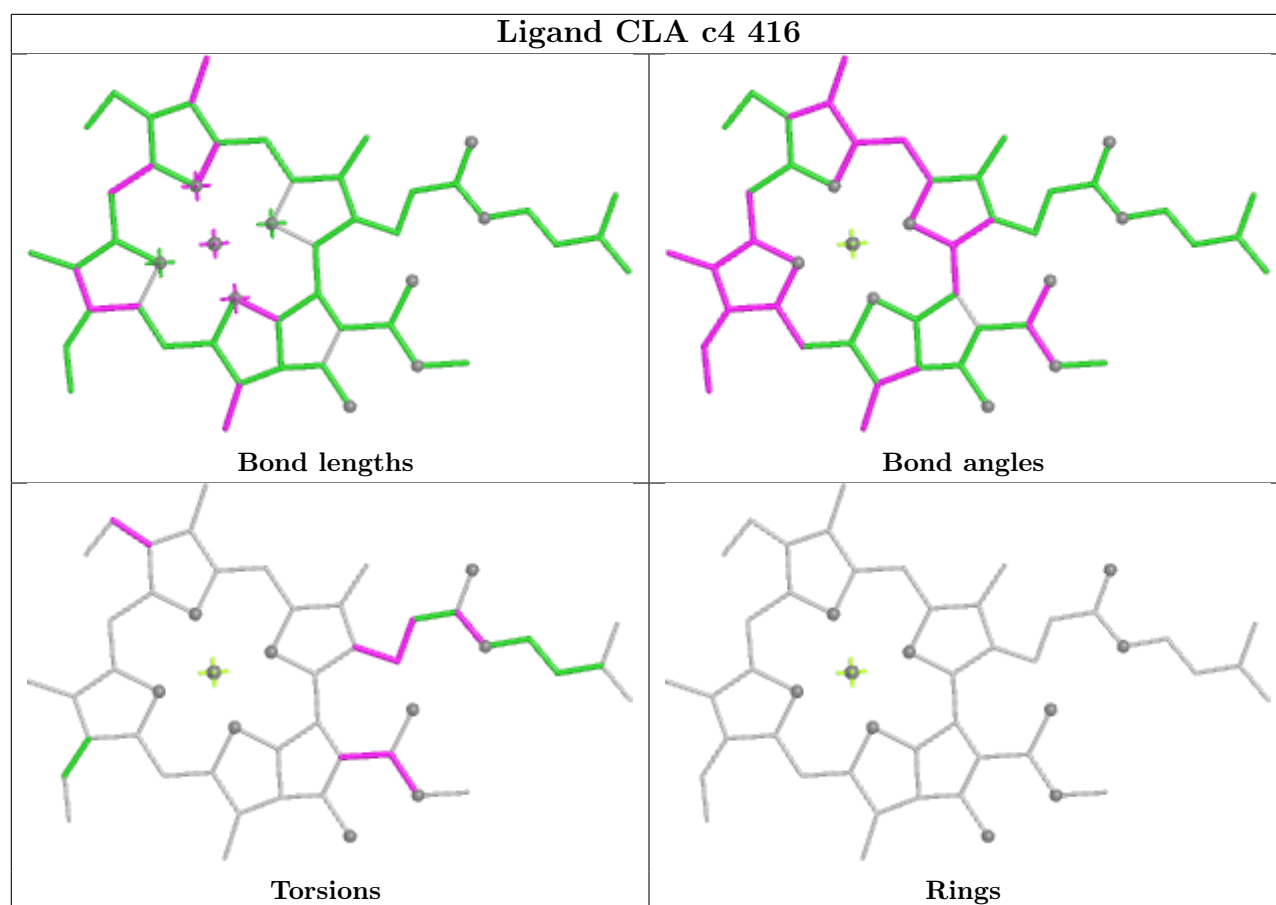


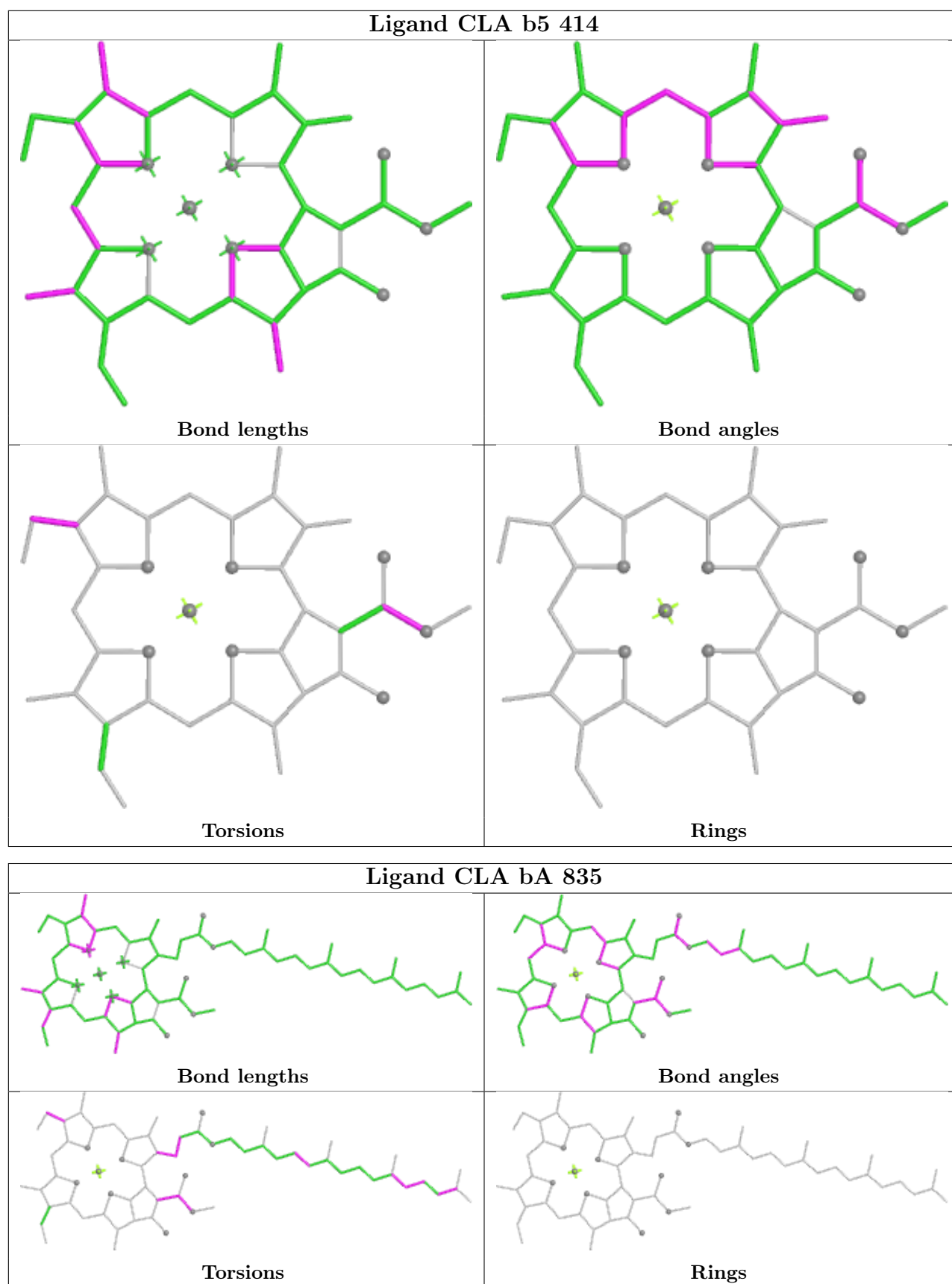


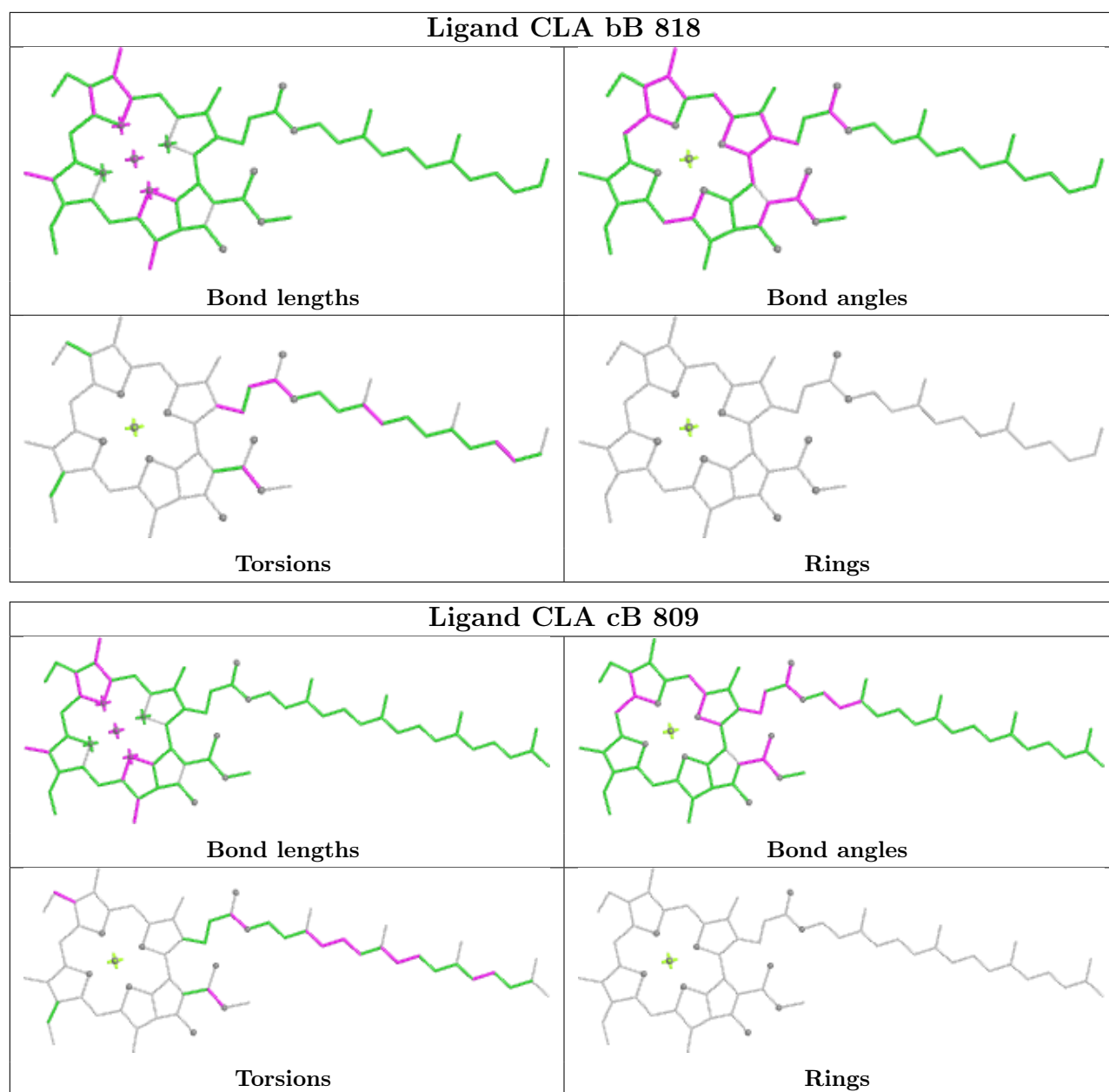




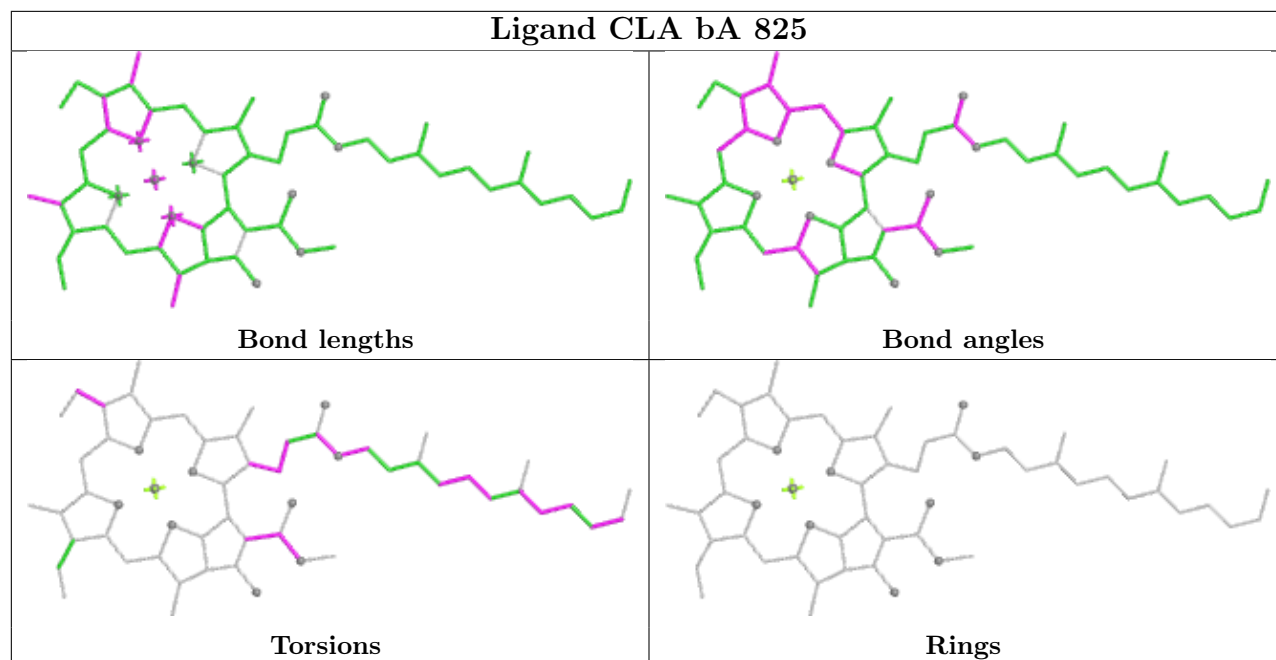




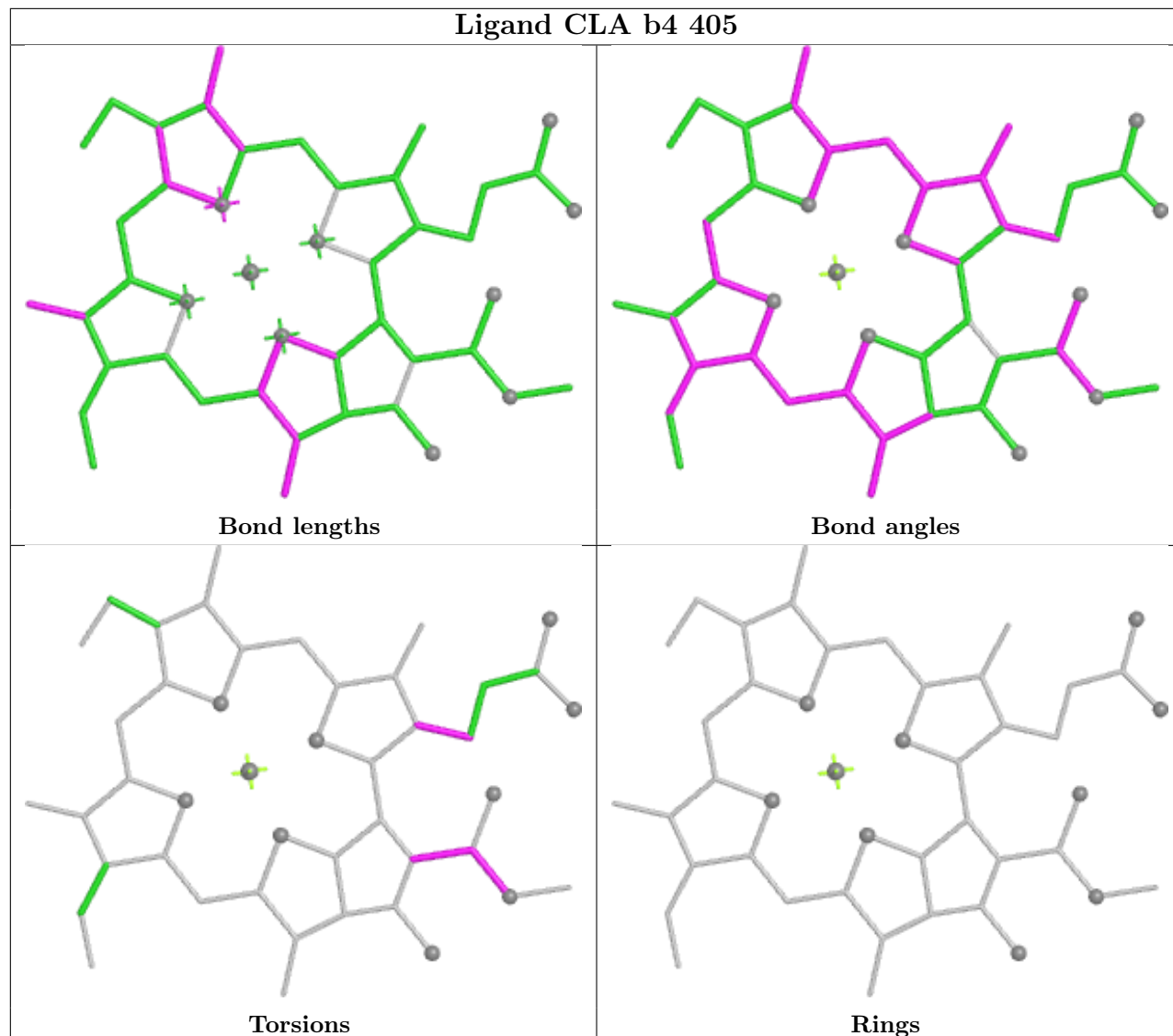


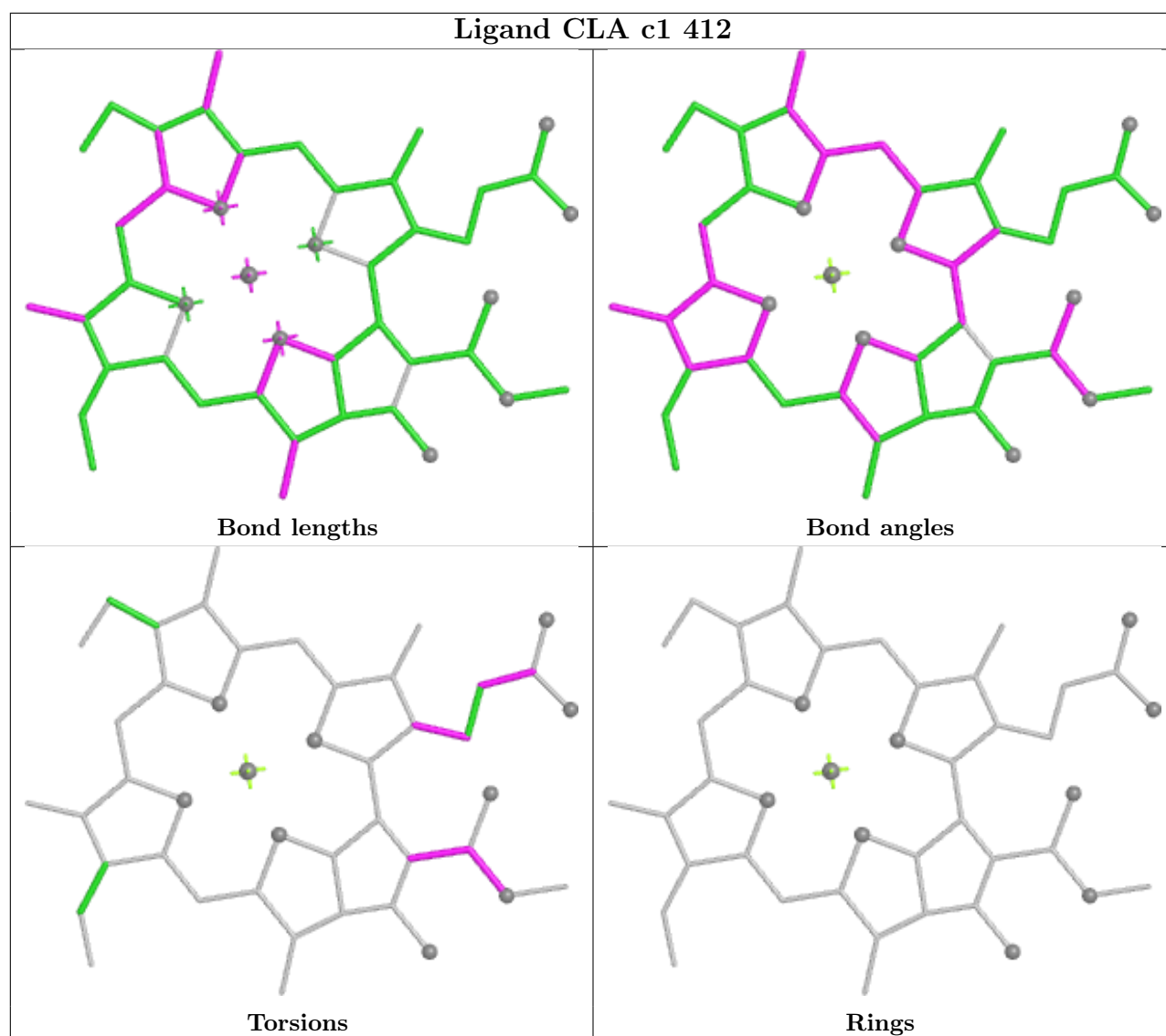


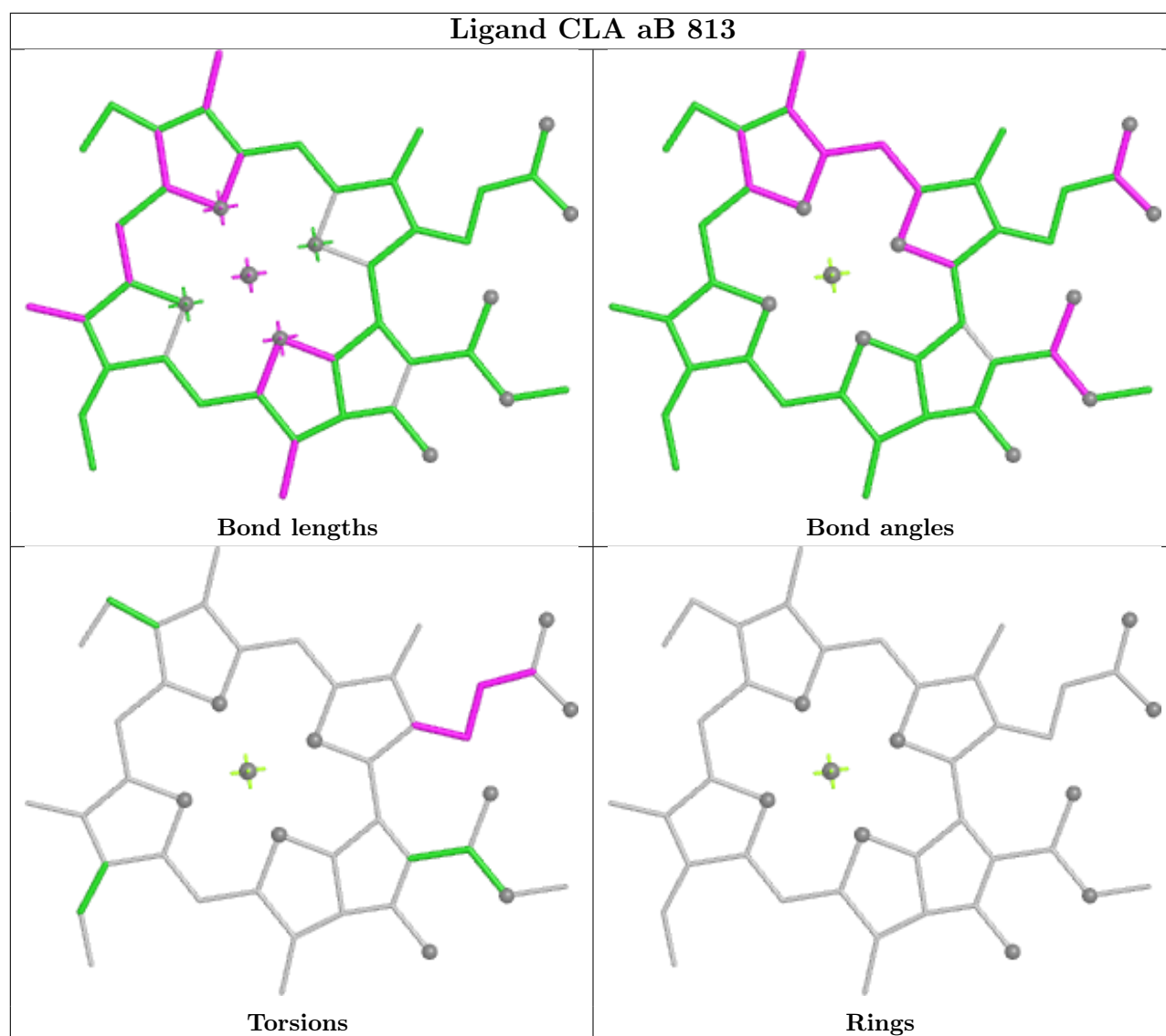
Ligand CLA bA 825

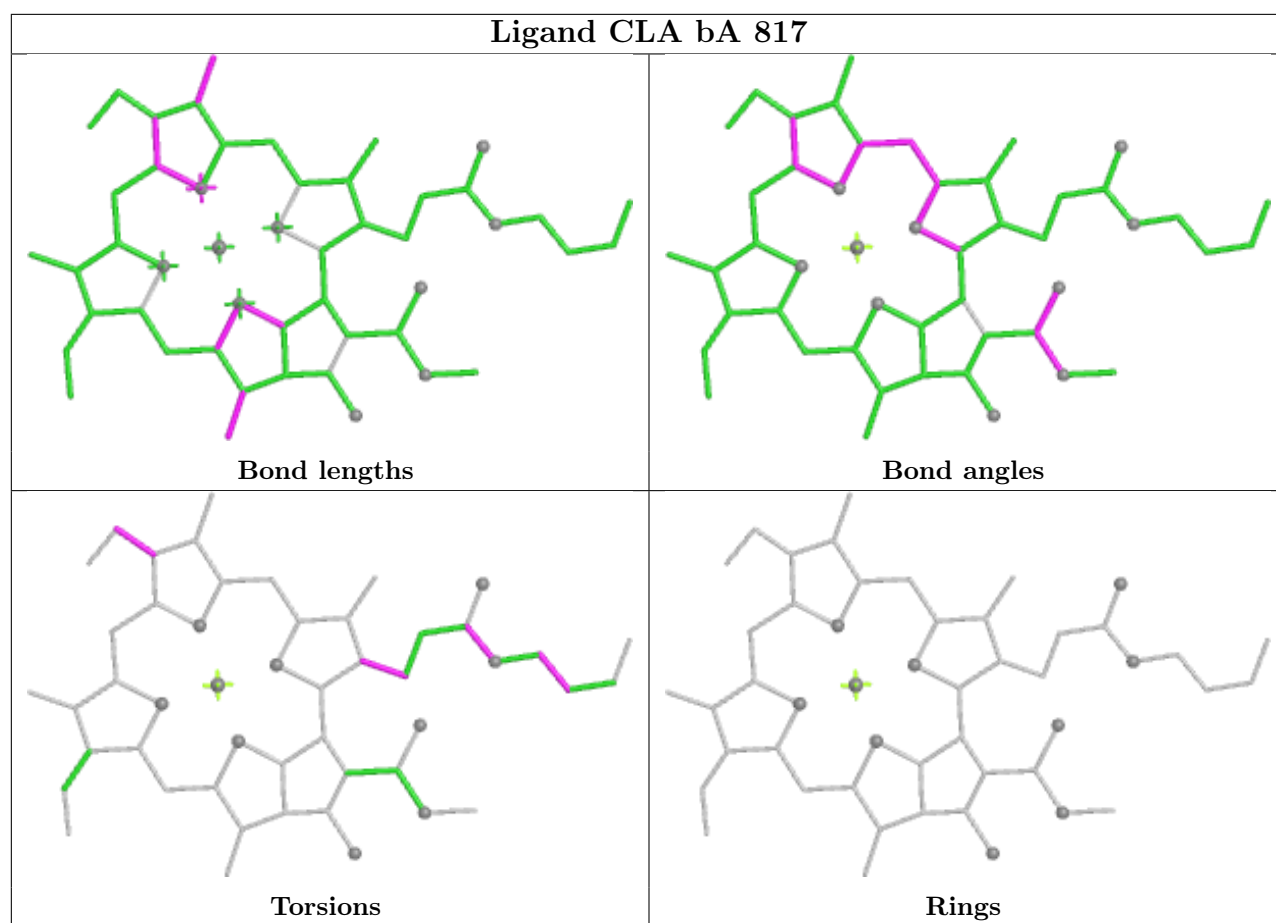


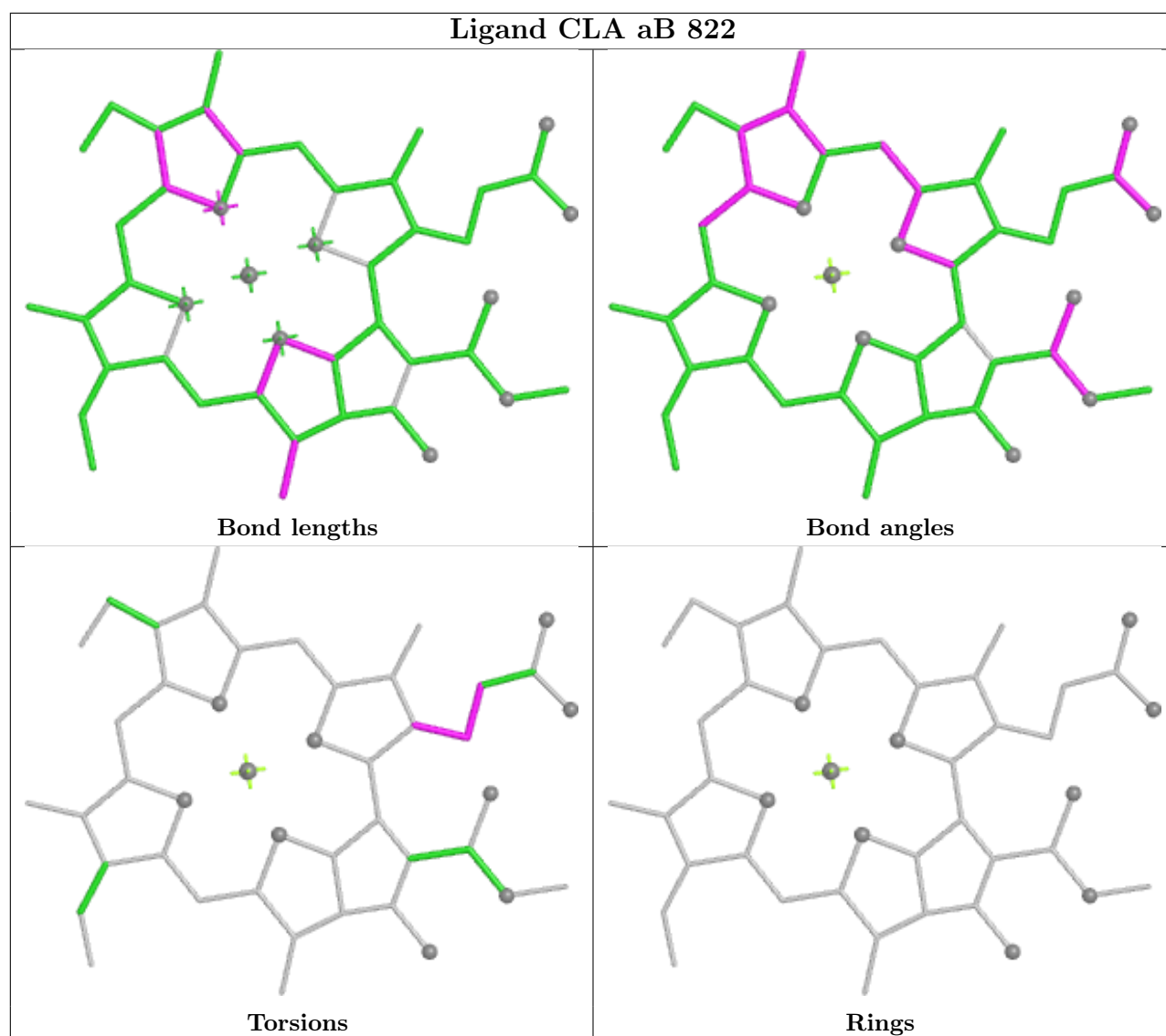
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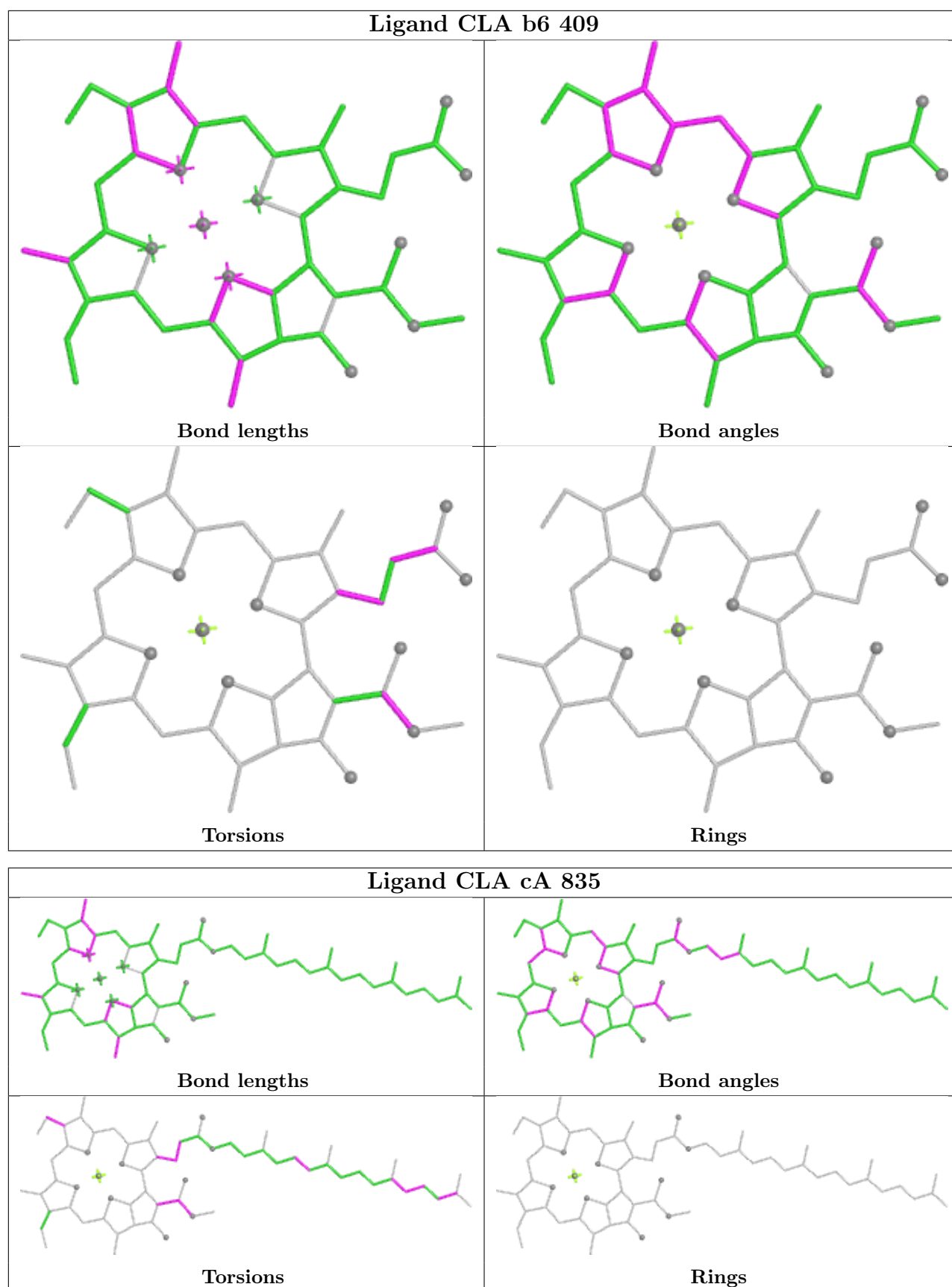


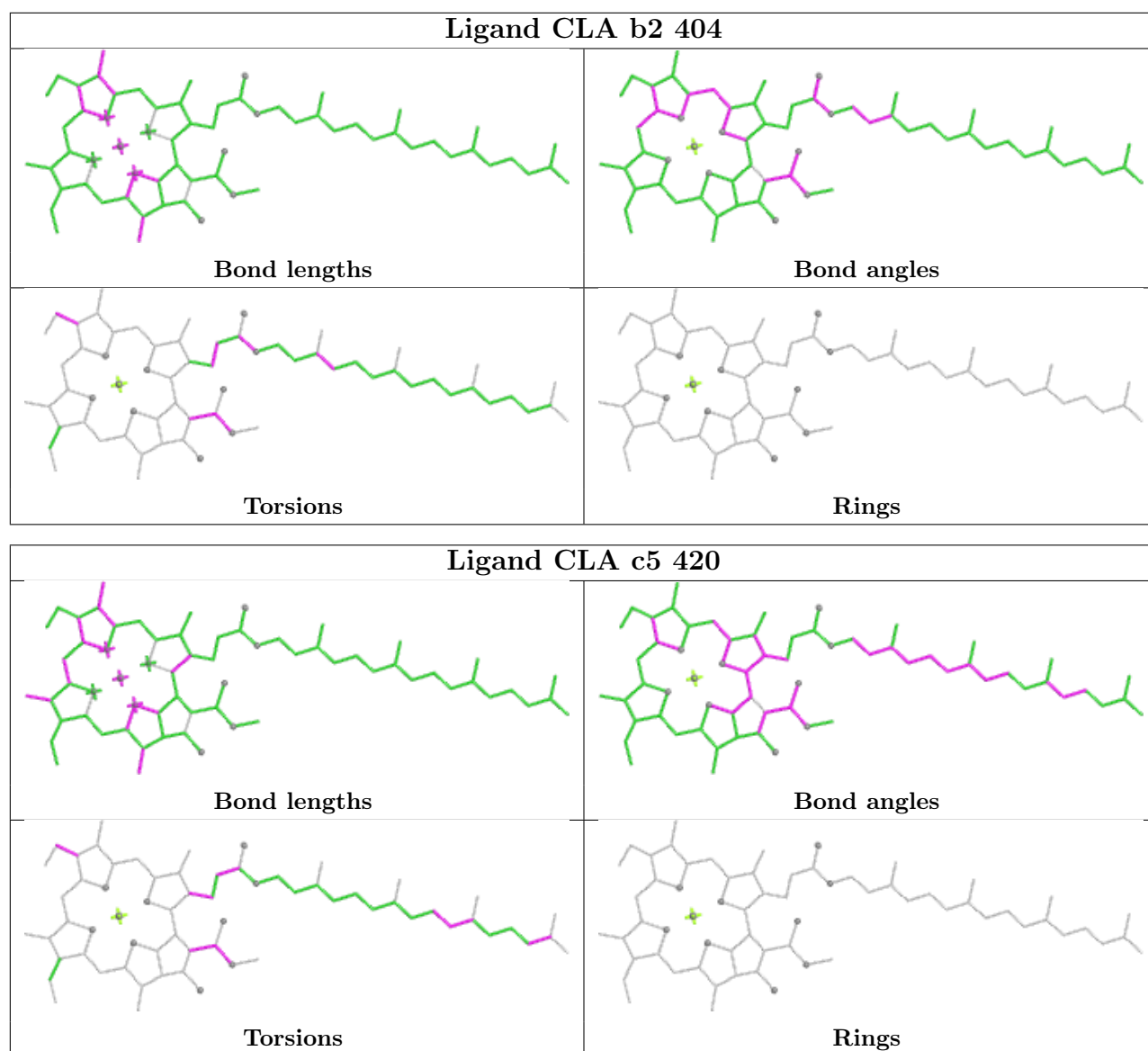


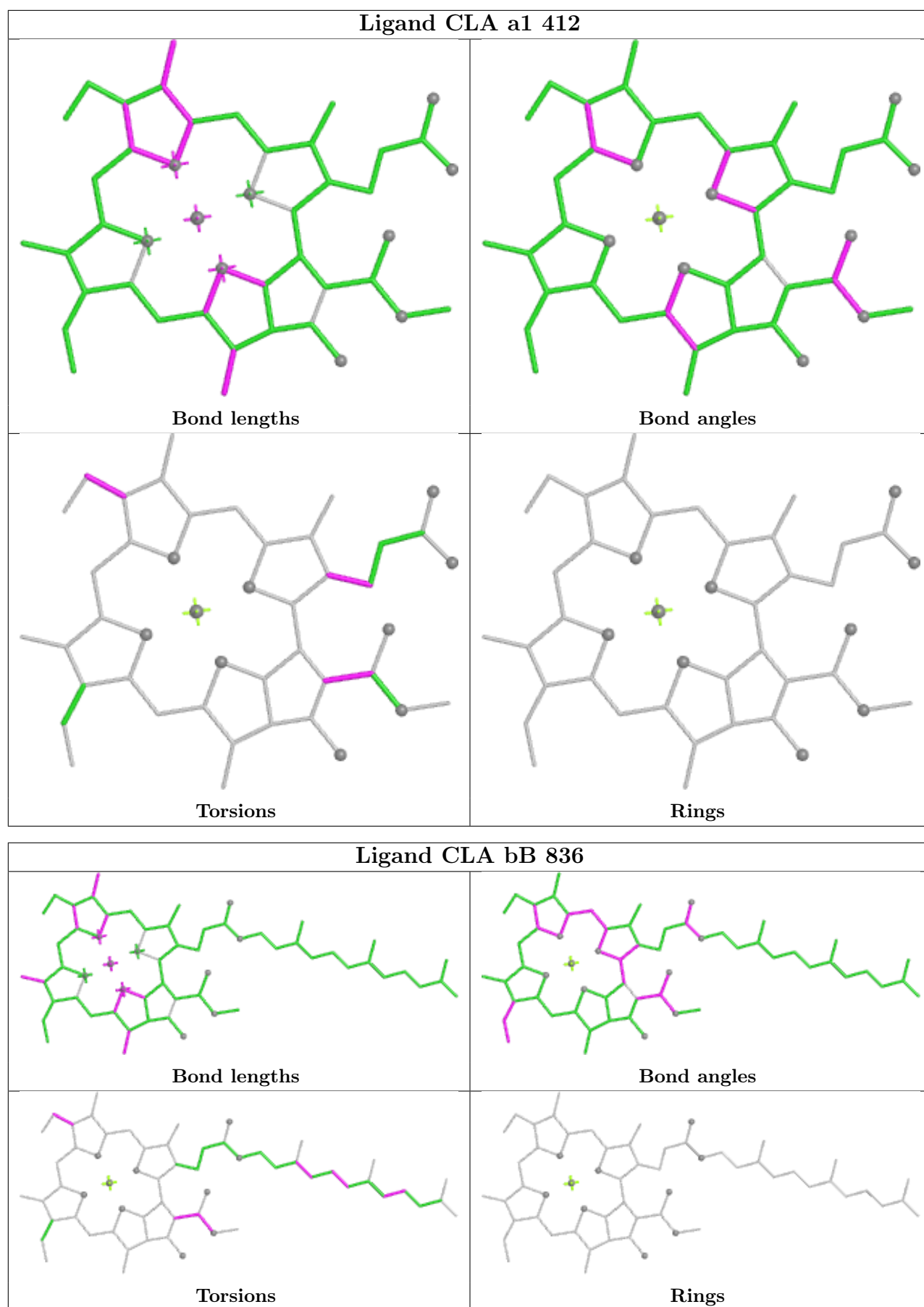


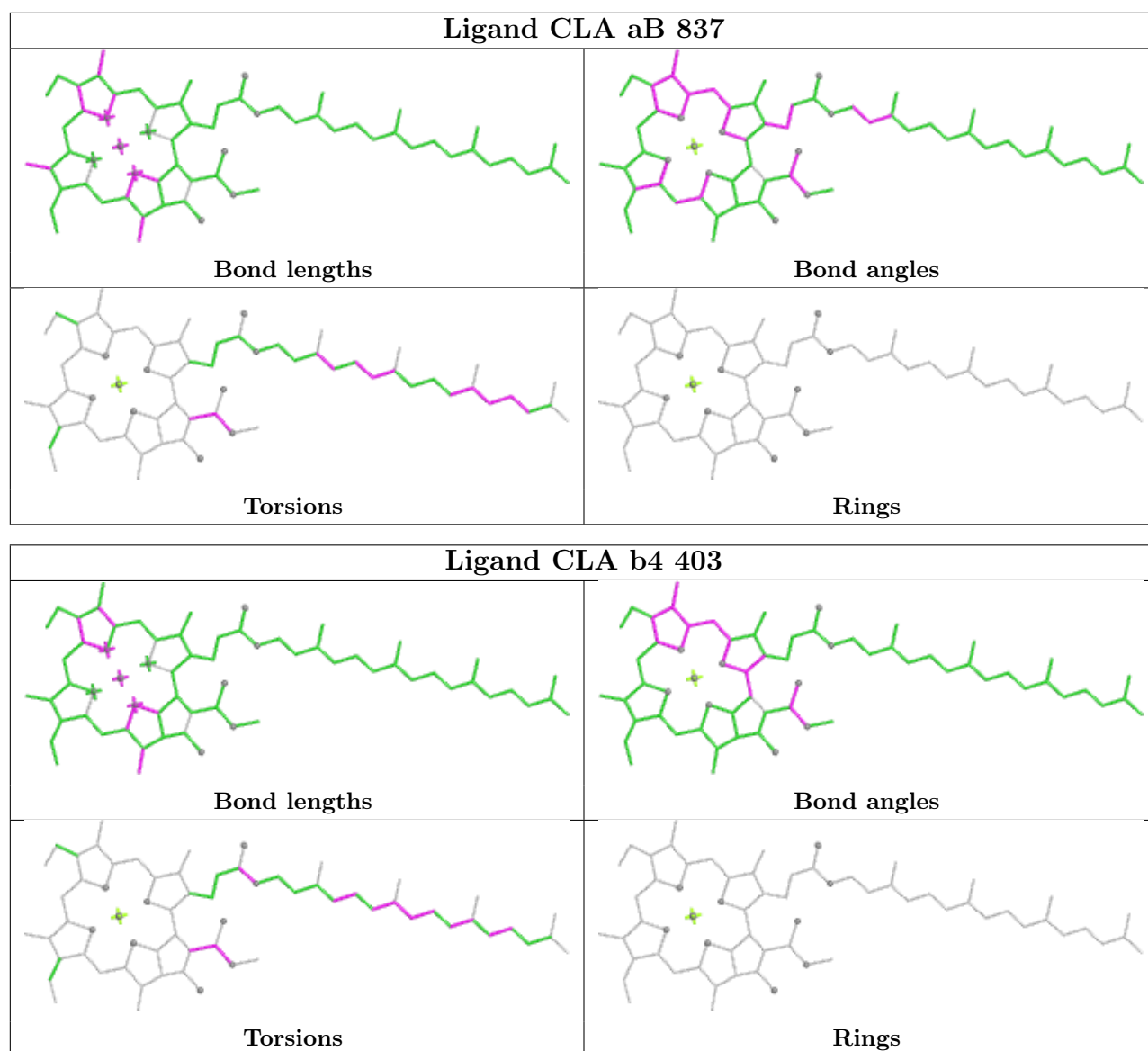


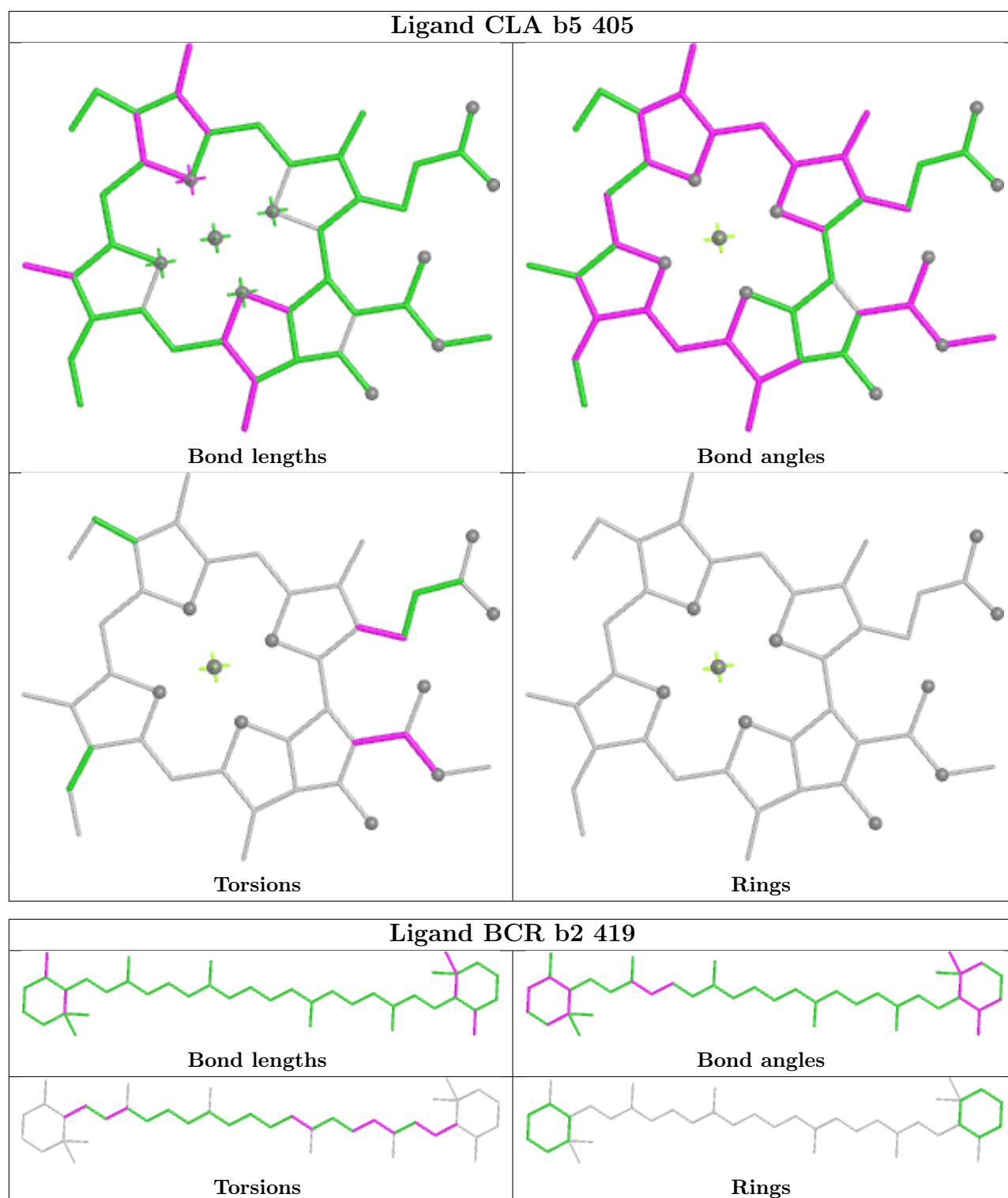


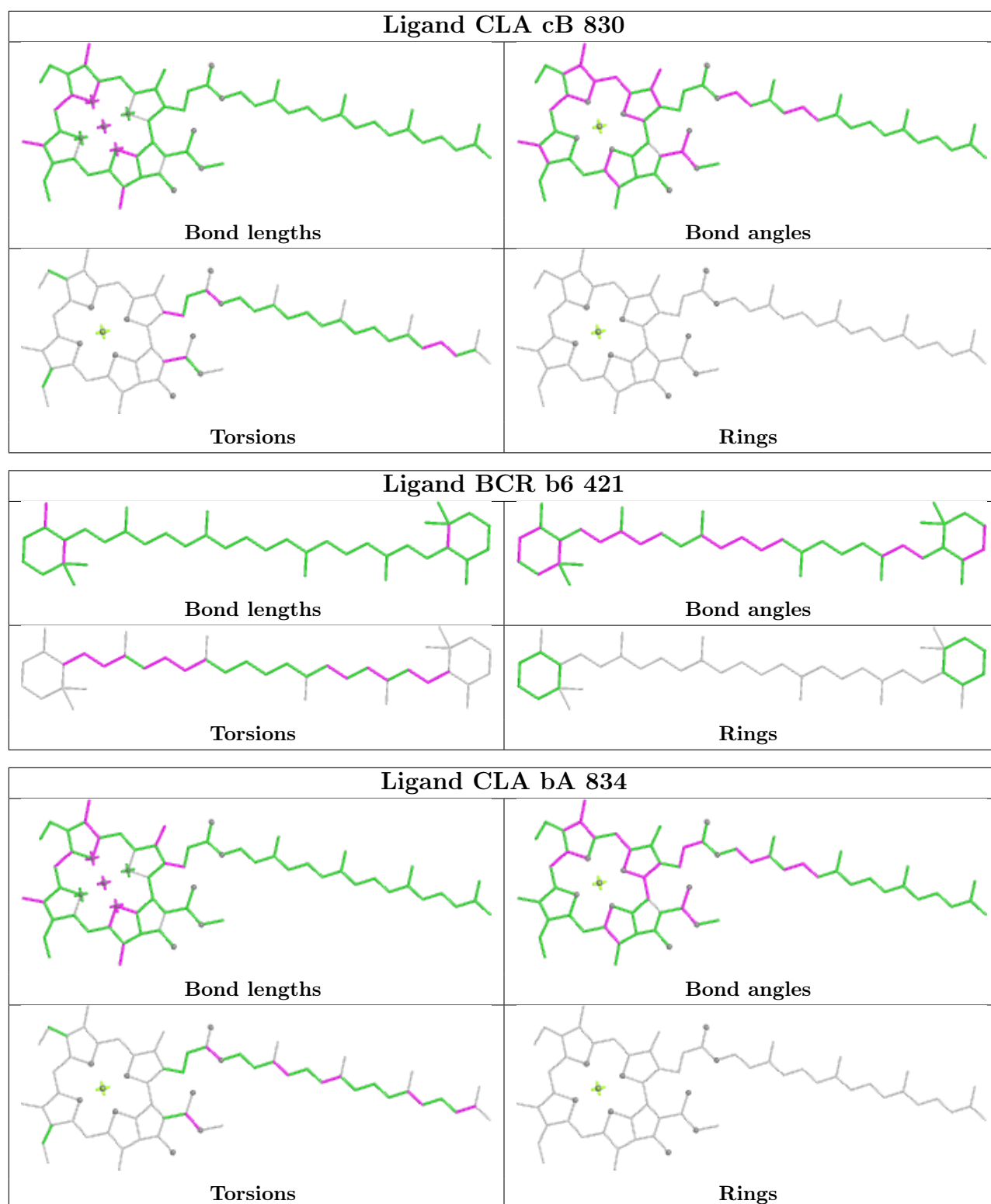


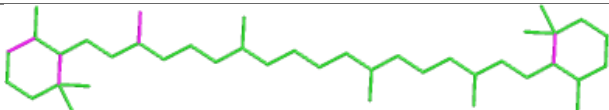
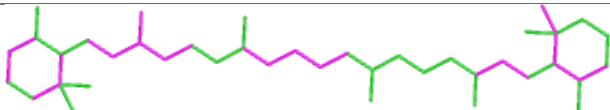
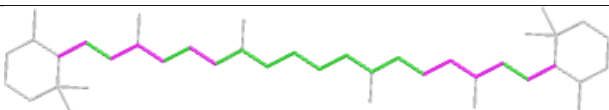
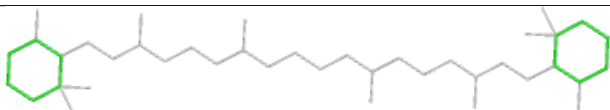


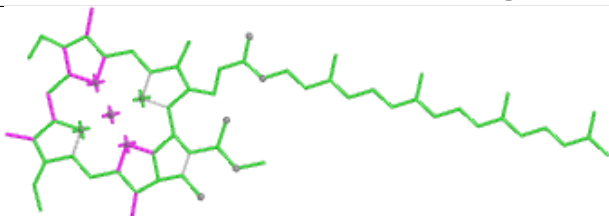
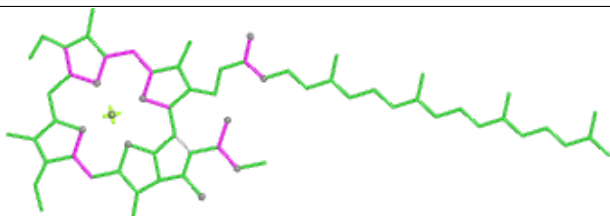
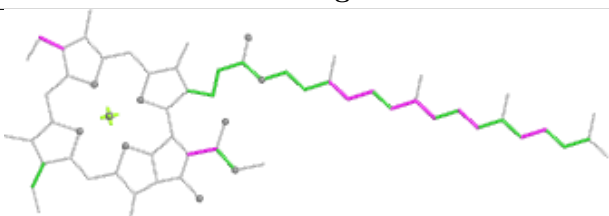
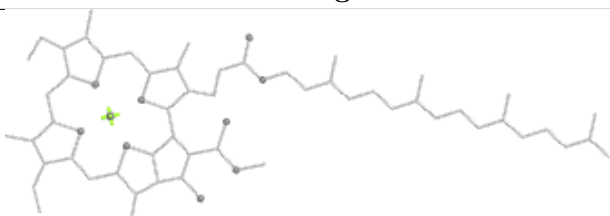




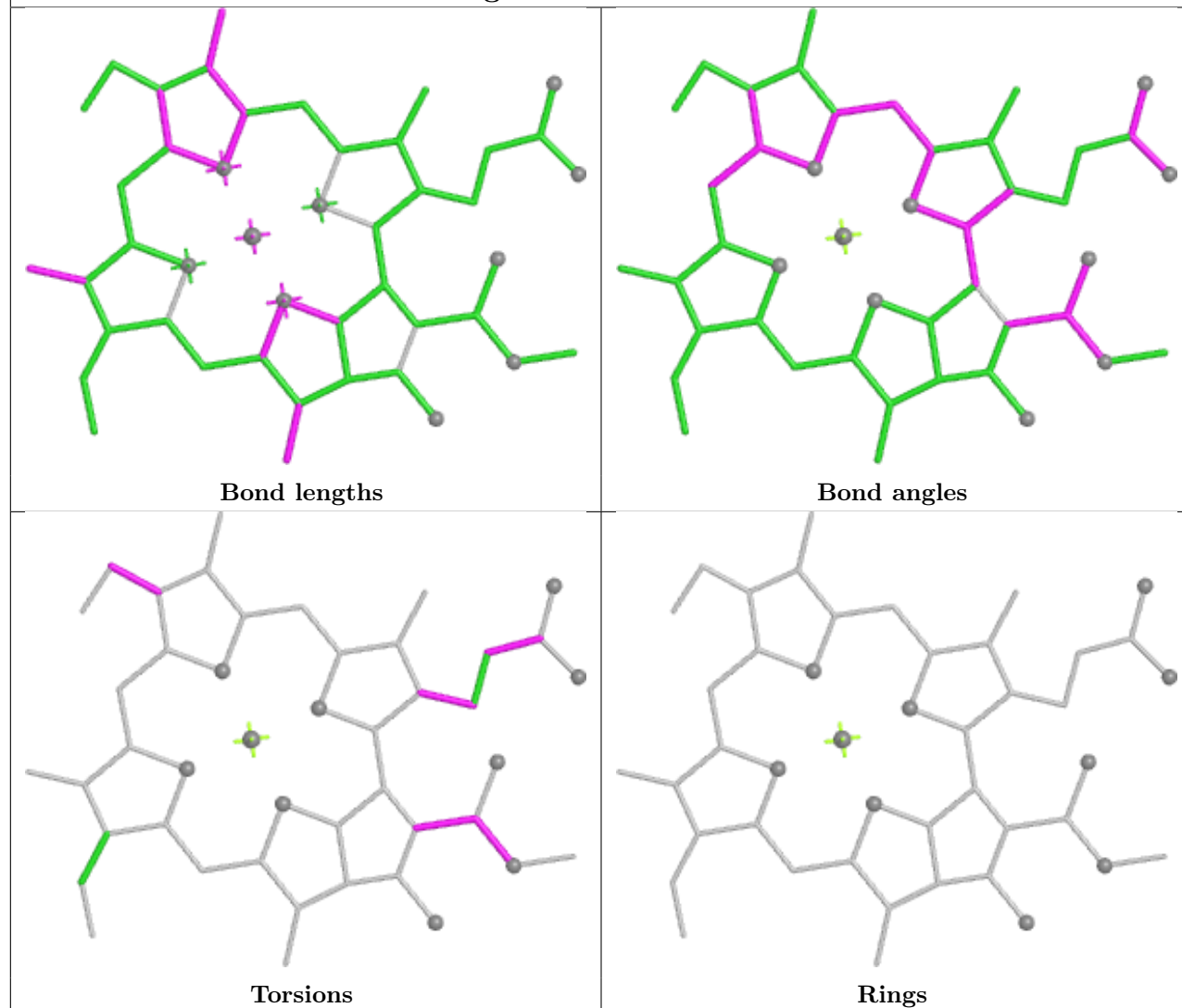




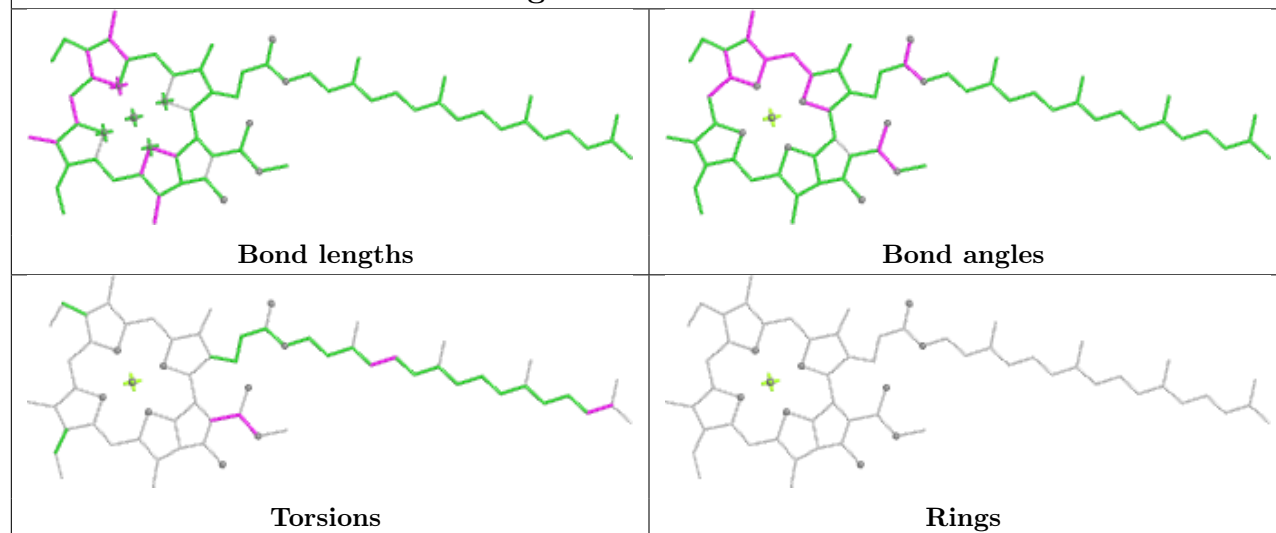
Ligand BCR a6 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

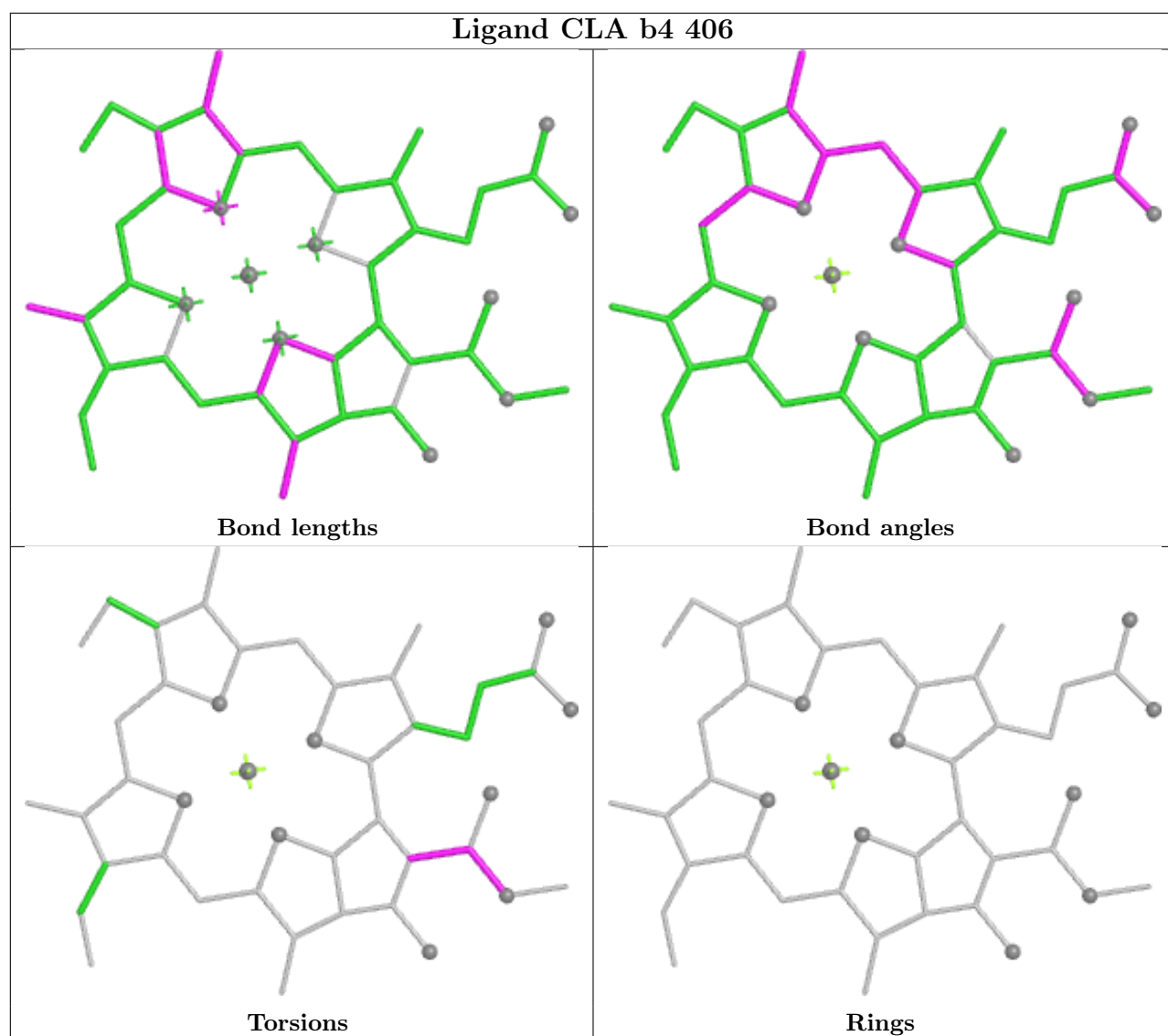
Ligand CLA aA 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

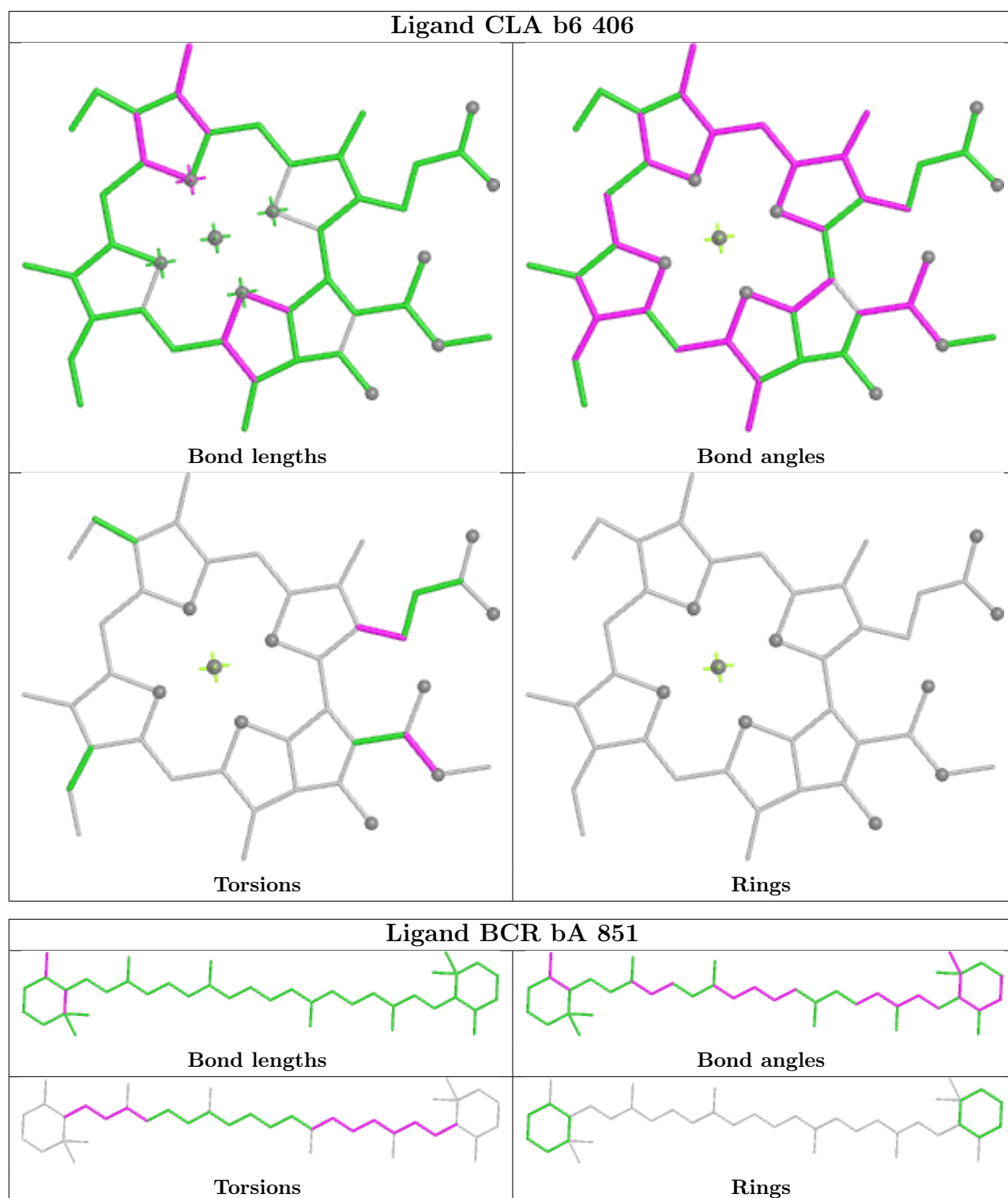
Ligand CLA aK 102

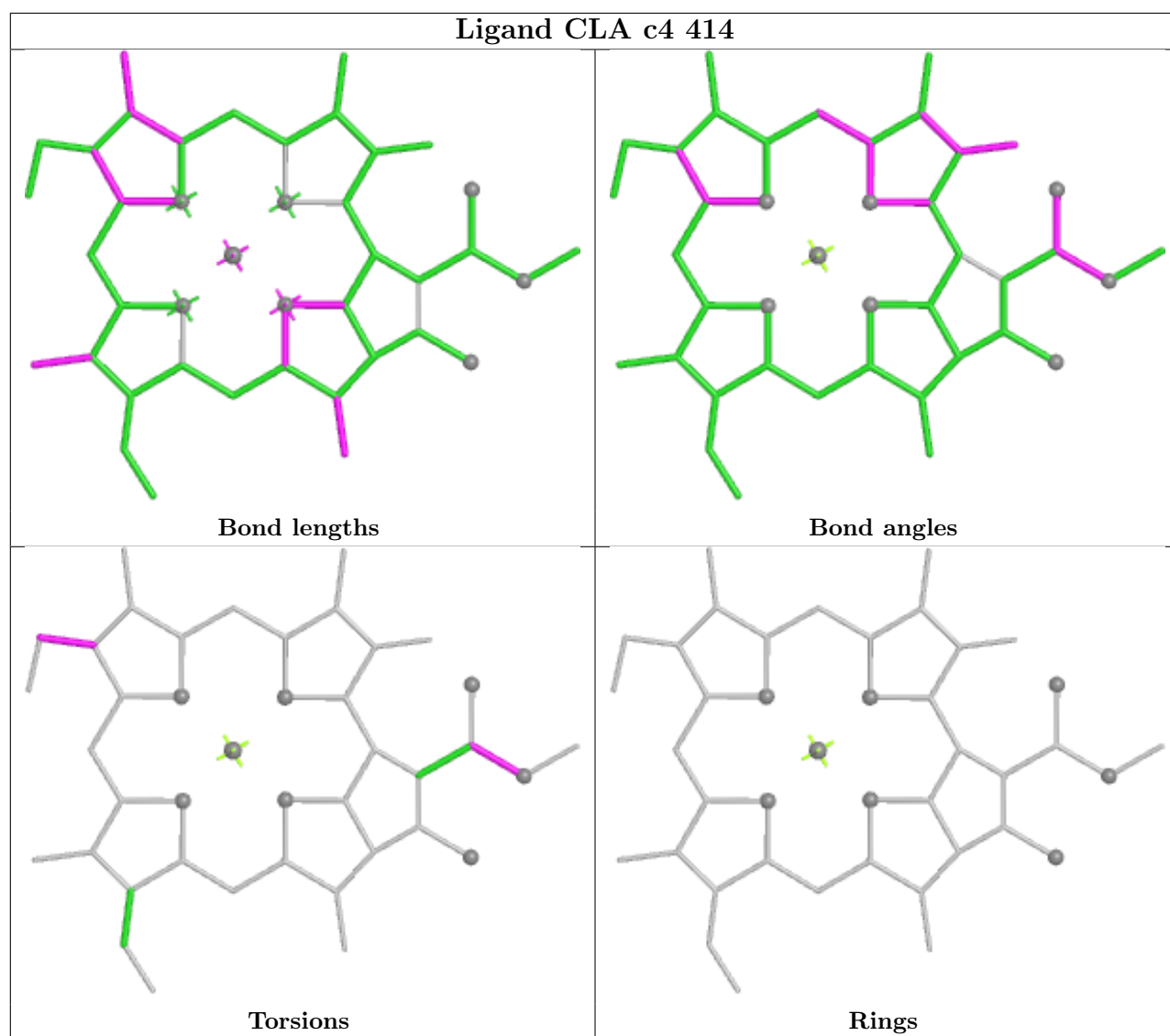


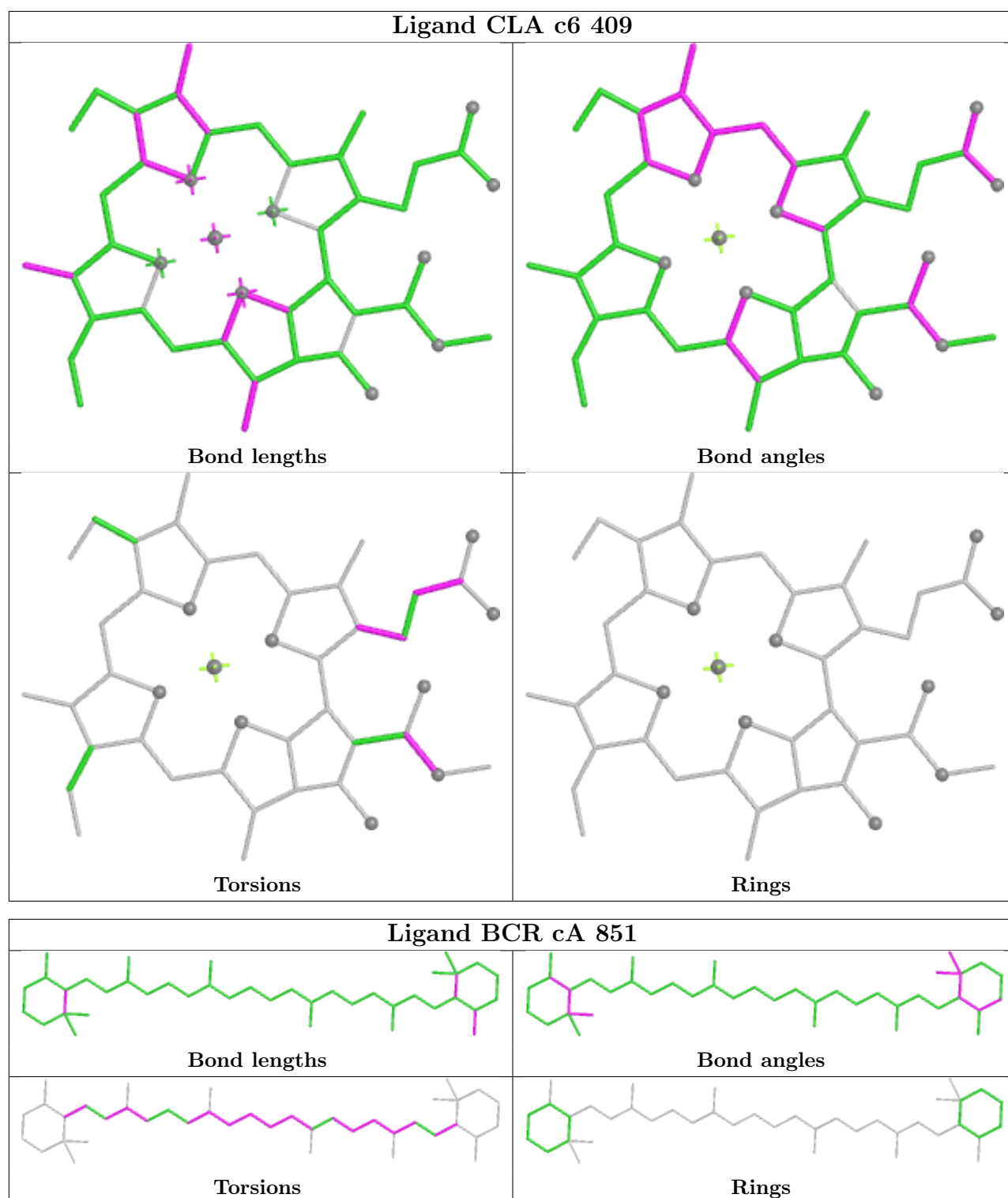
Ligand CLA a5 409

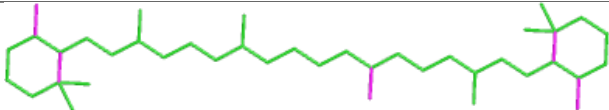
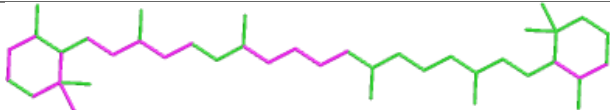
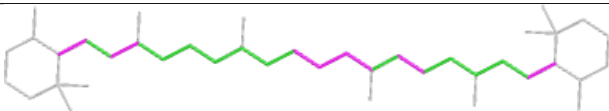
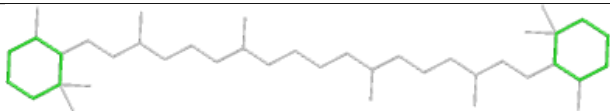


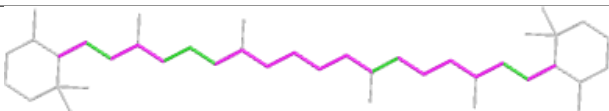
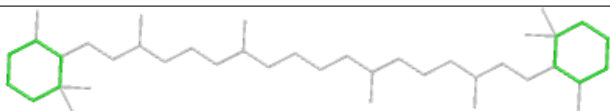


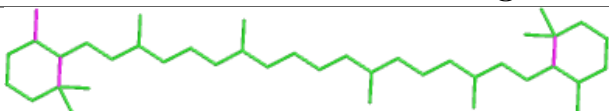
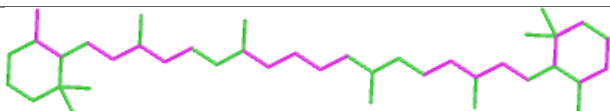
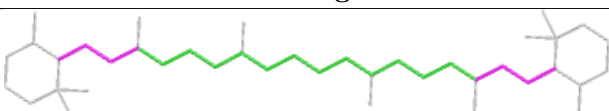
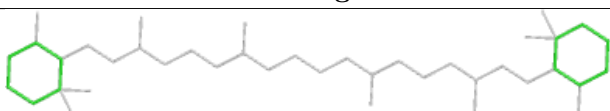


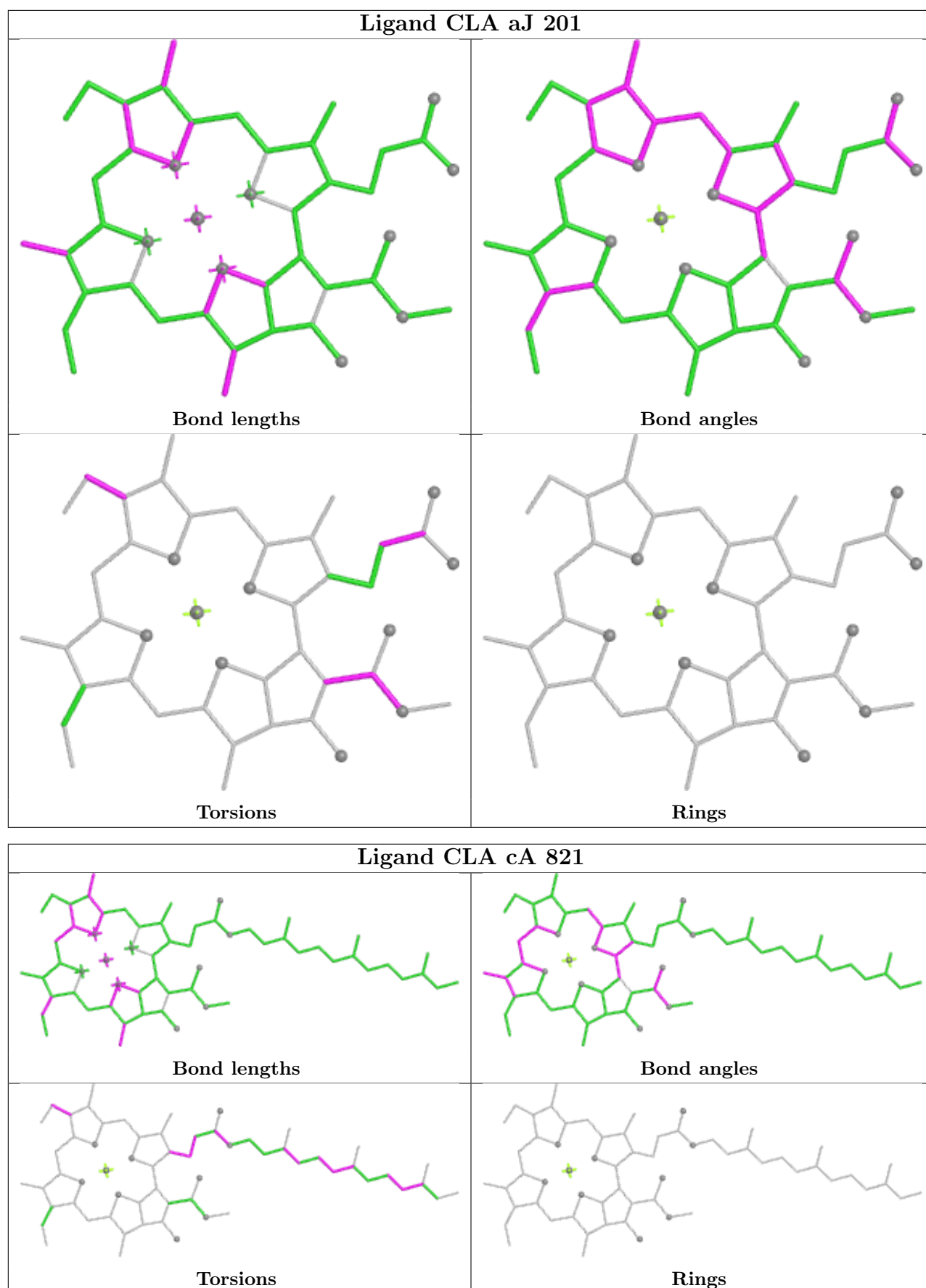


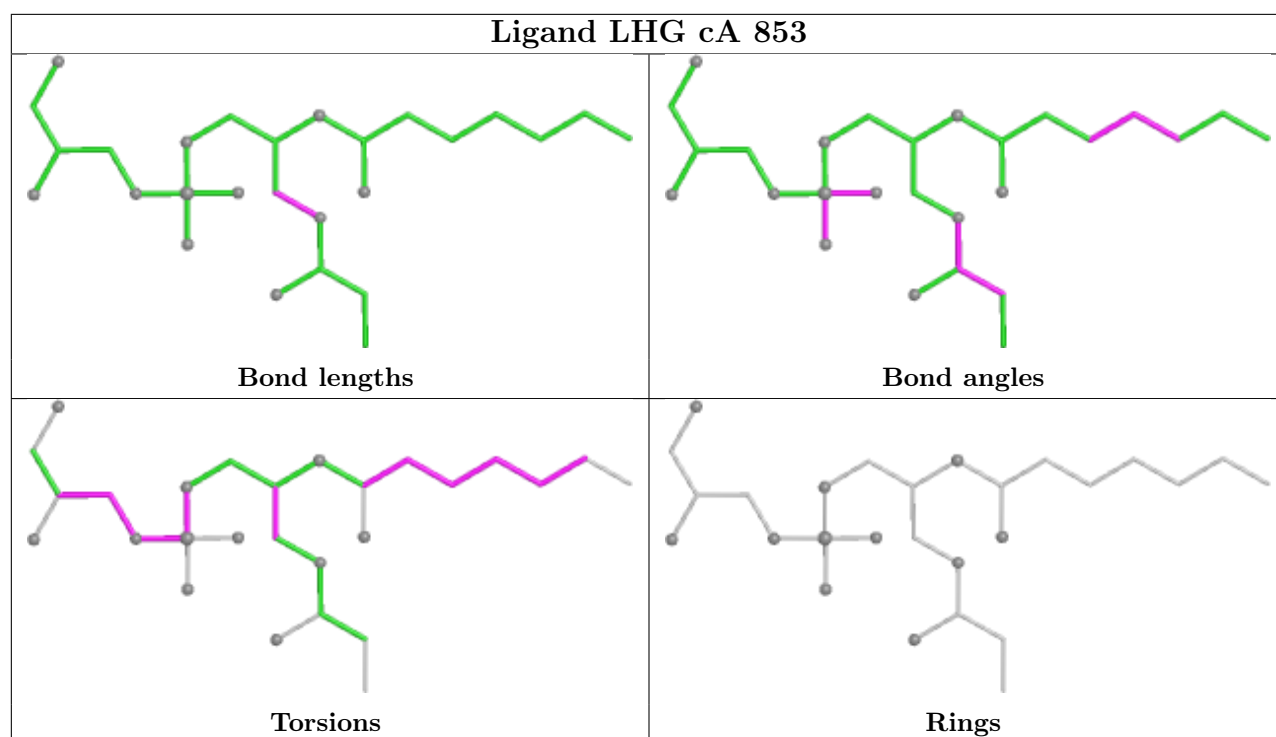


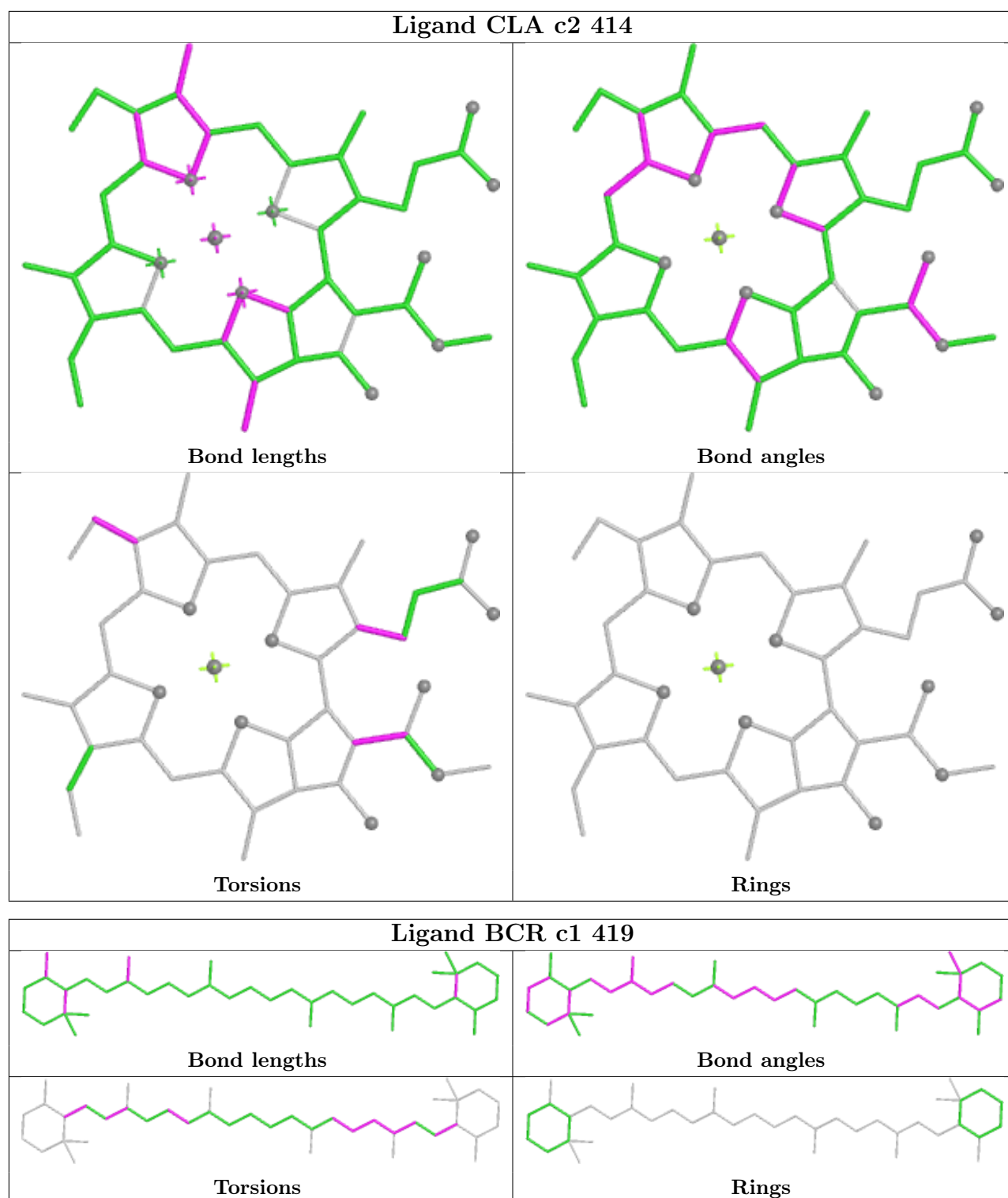
Ligand BCR cF 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

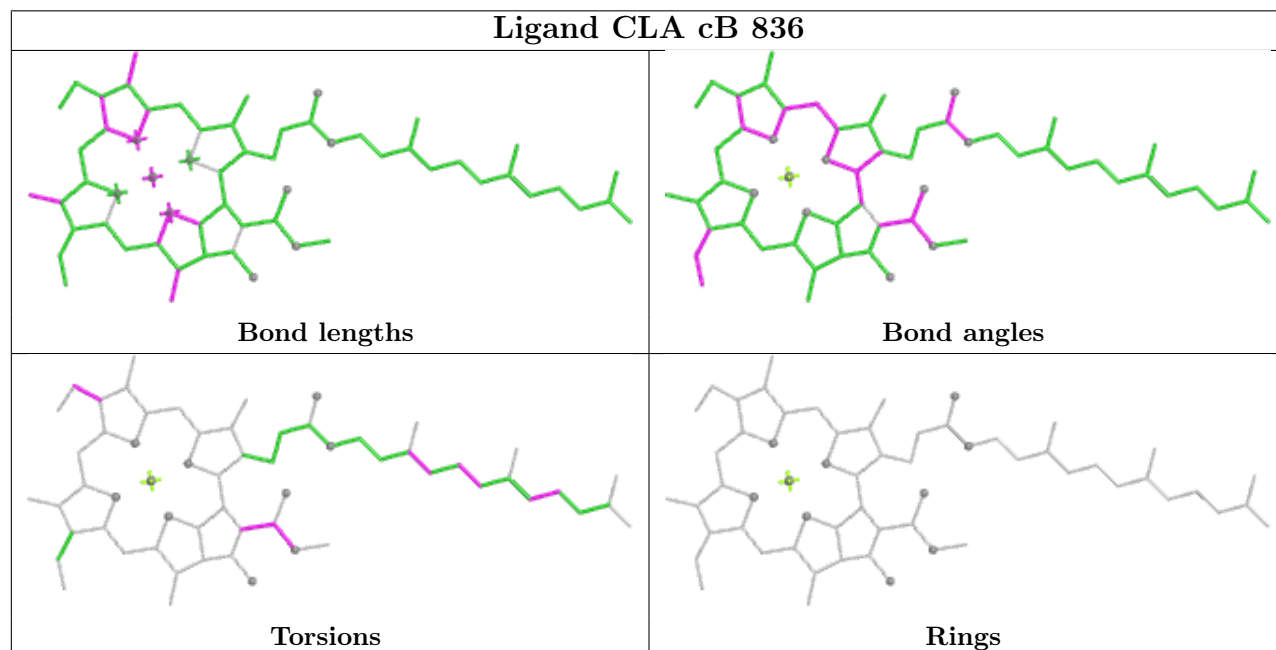
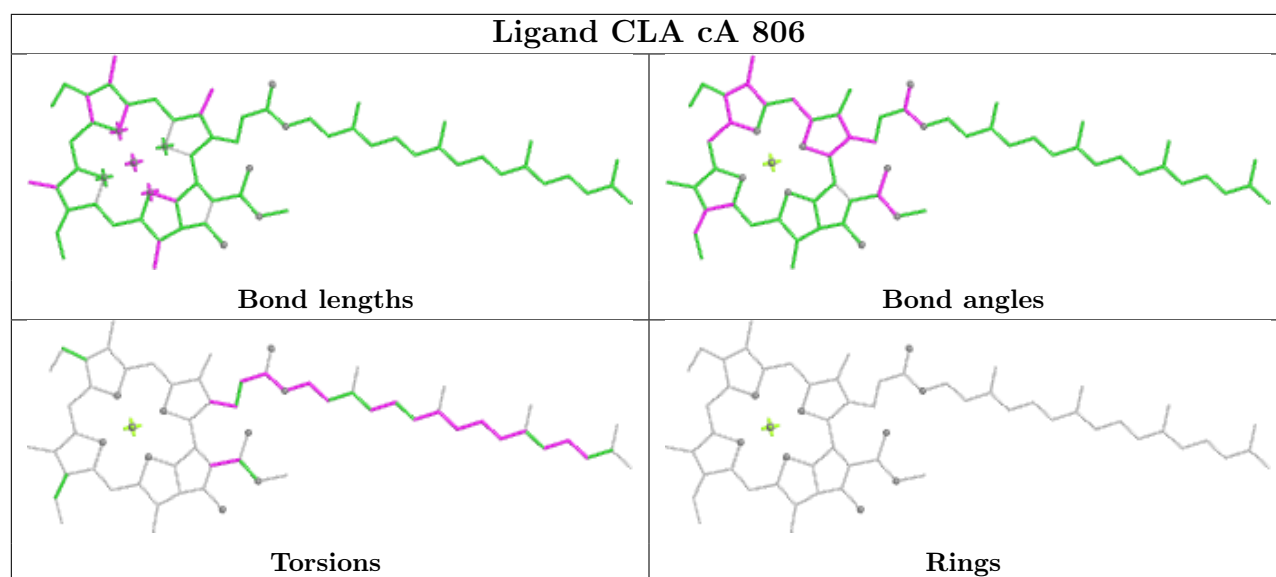
Ligand BCR aA 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

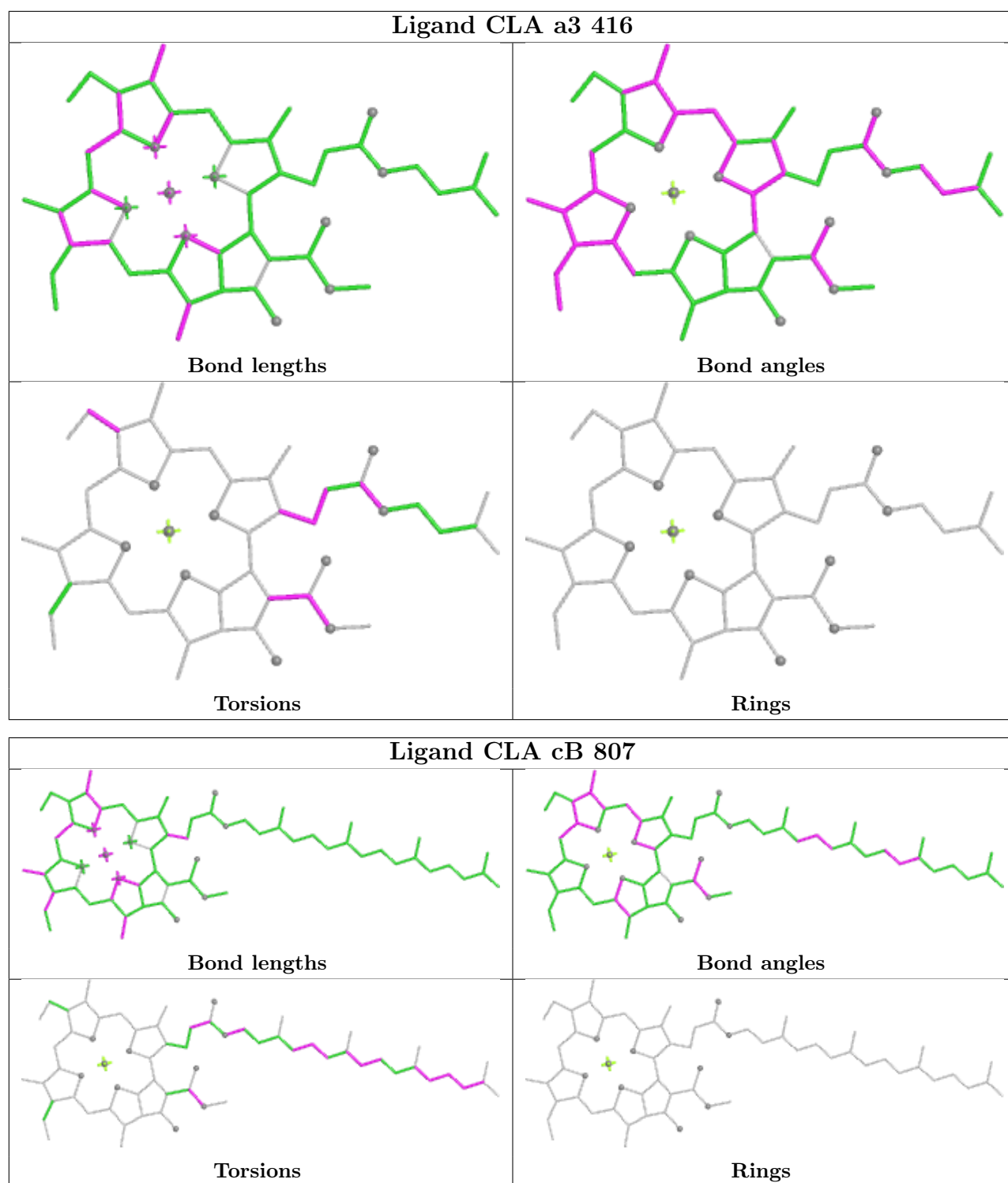
Ligand BCR bA 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

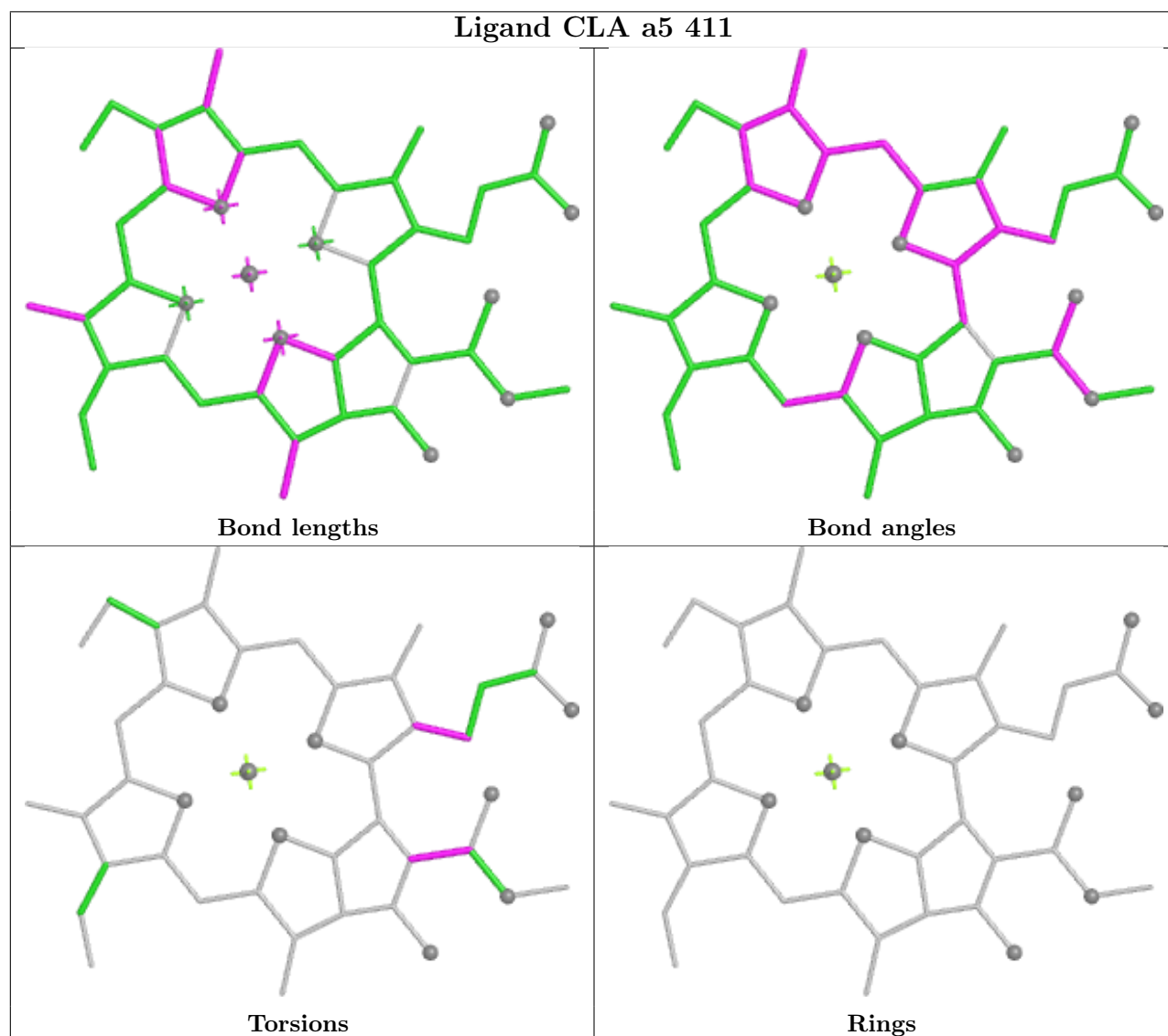
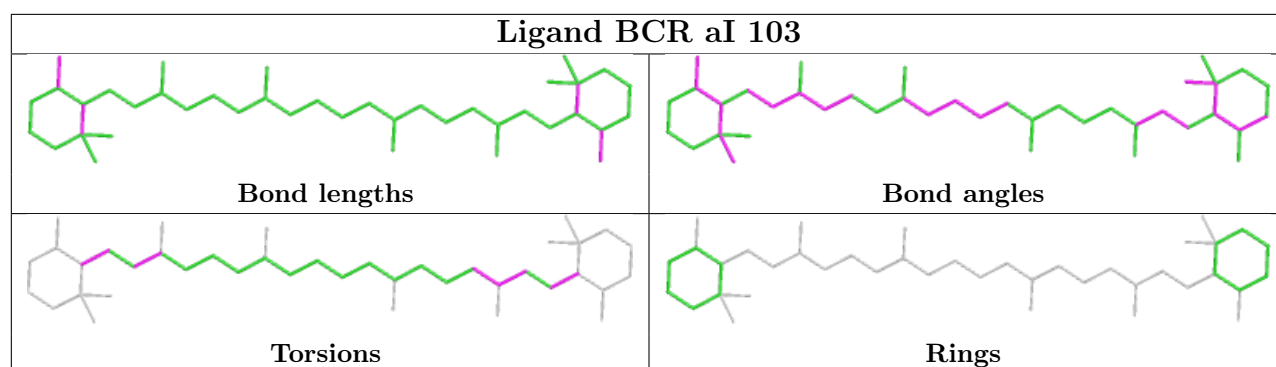


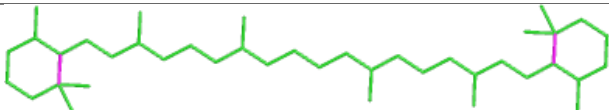
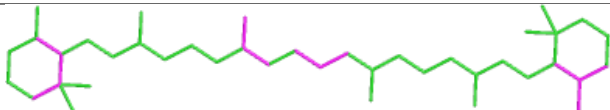
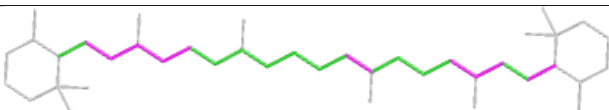
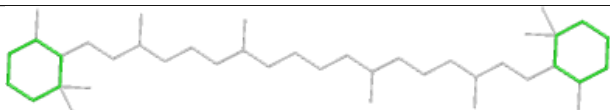


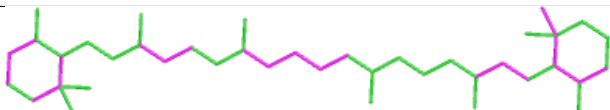
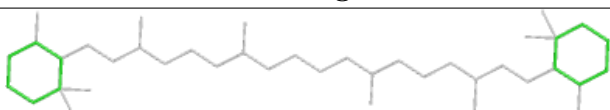


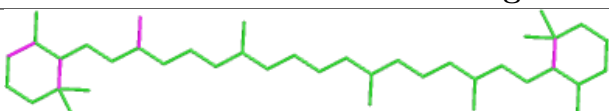
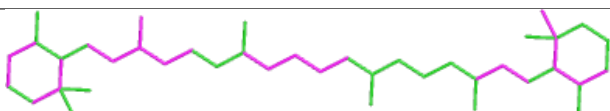
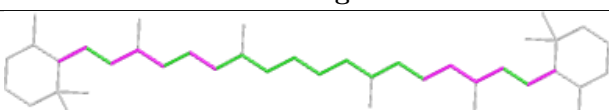
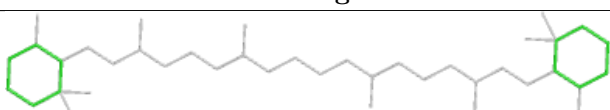


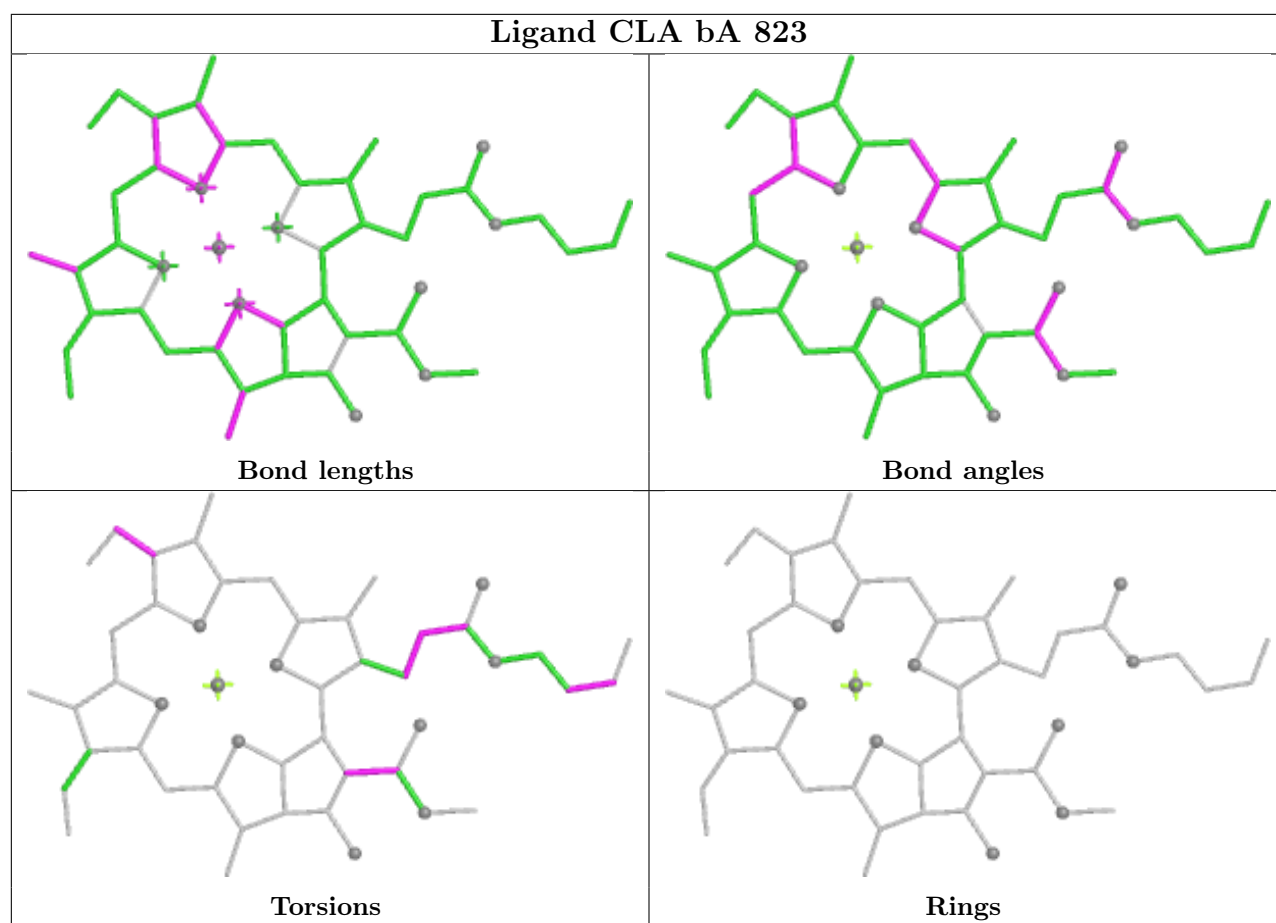


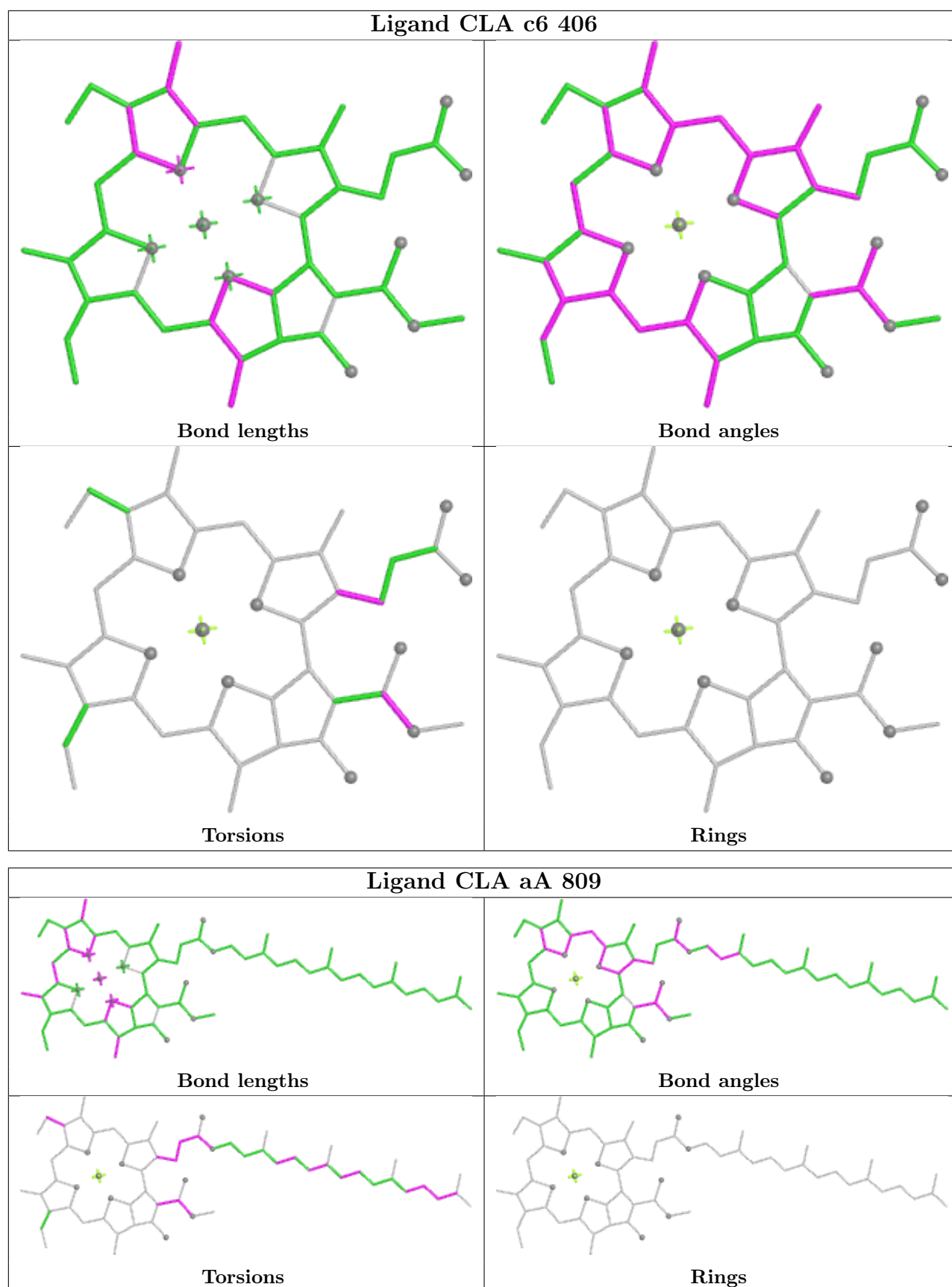


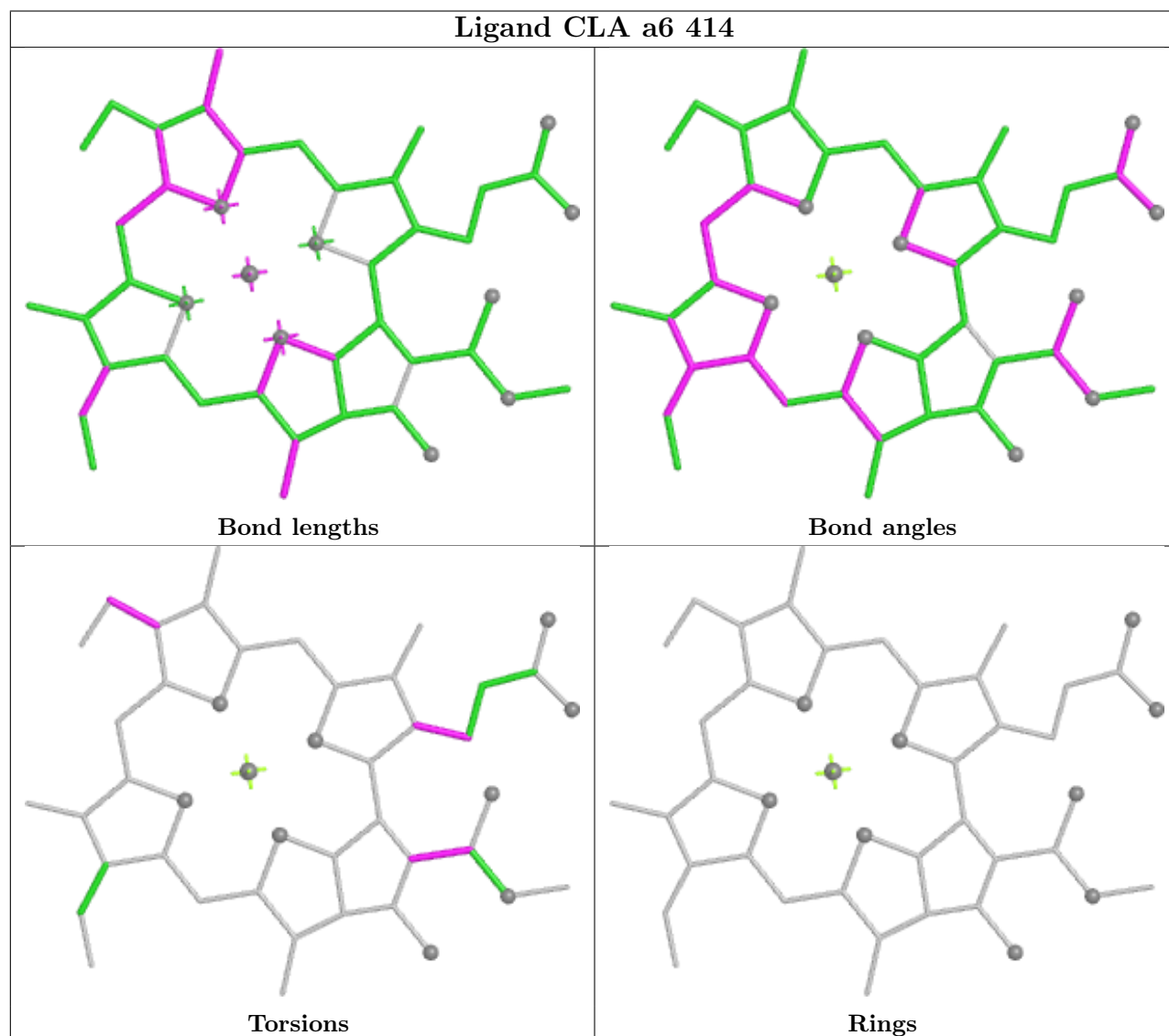
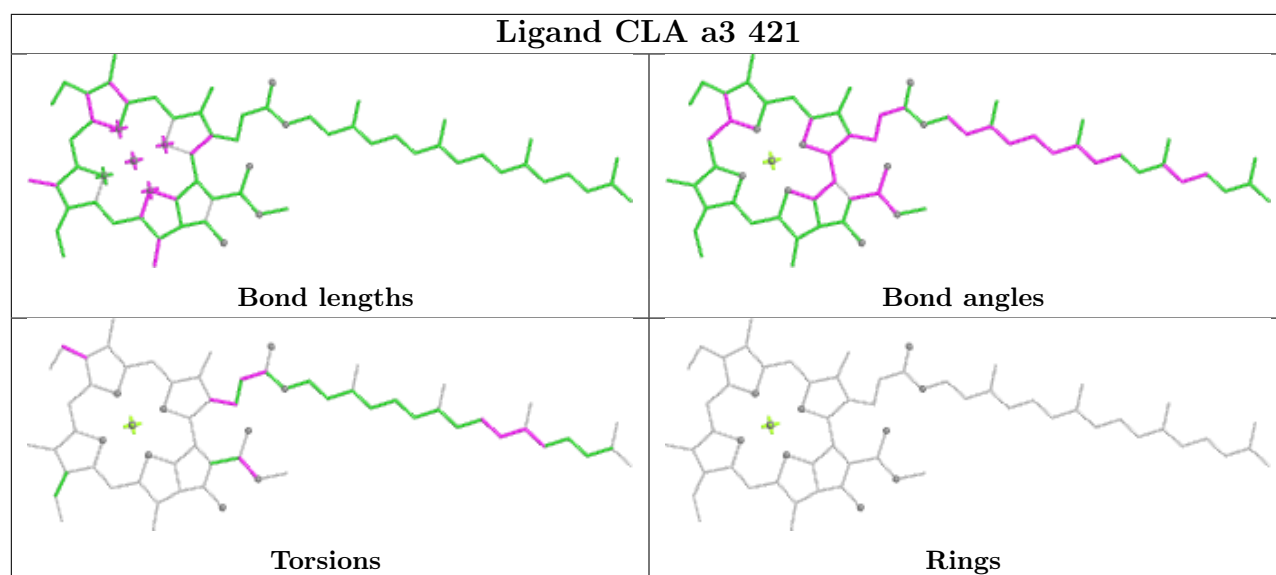
Ligand BCR bI 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

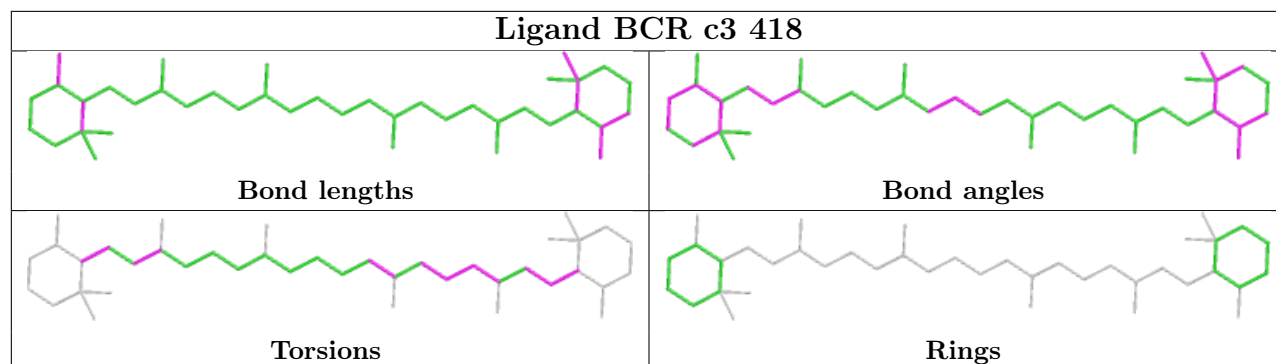
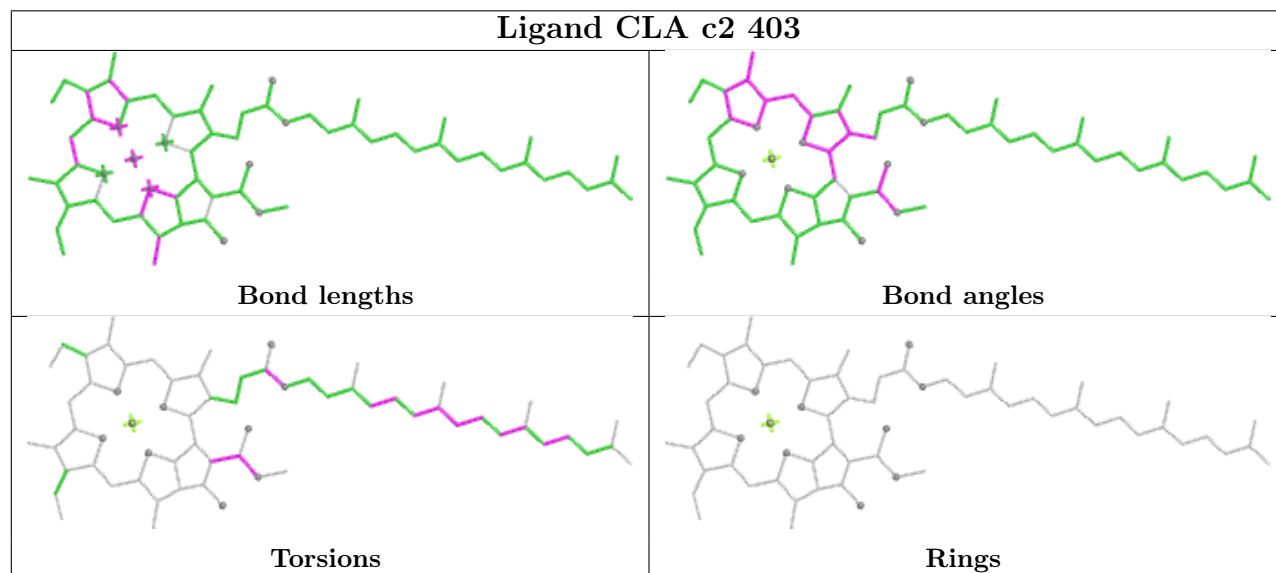
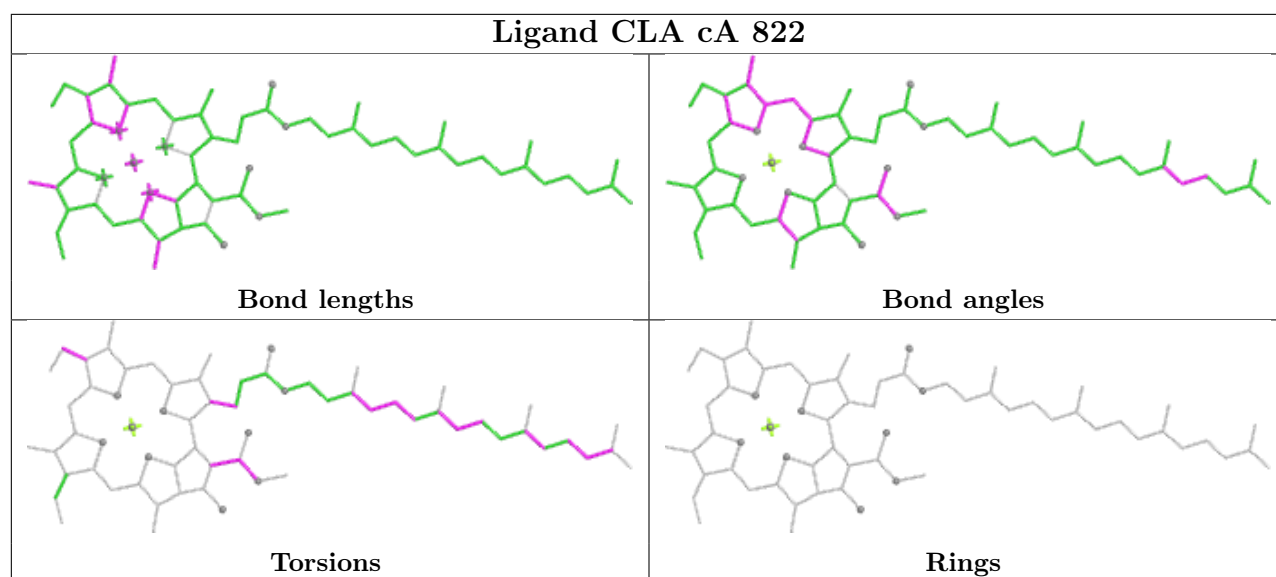
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Bond lengths	Bond angles
	
Torsions	Rings

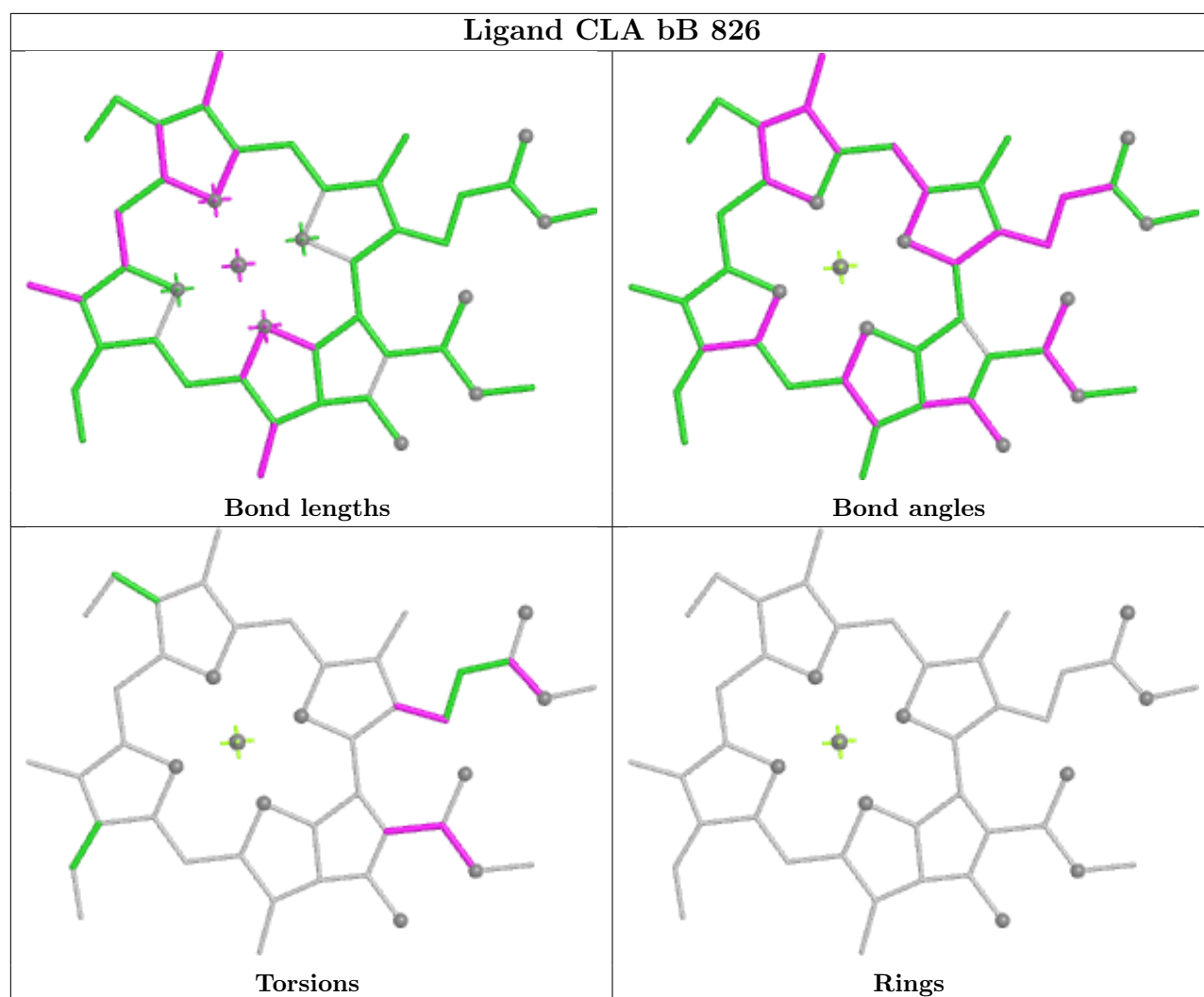
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Bond lengths	Bond angles
	
Torsions	Rings

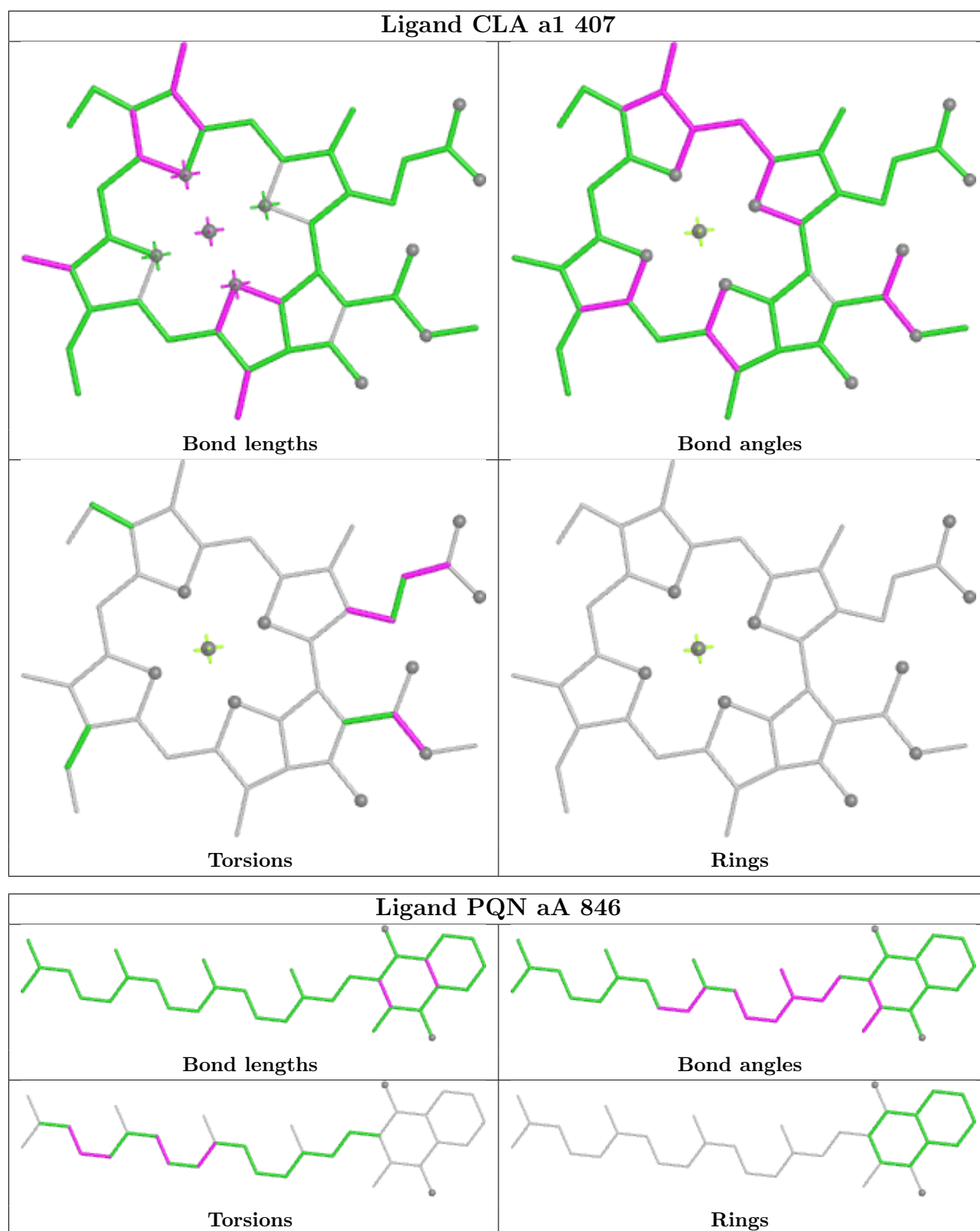


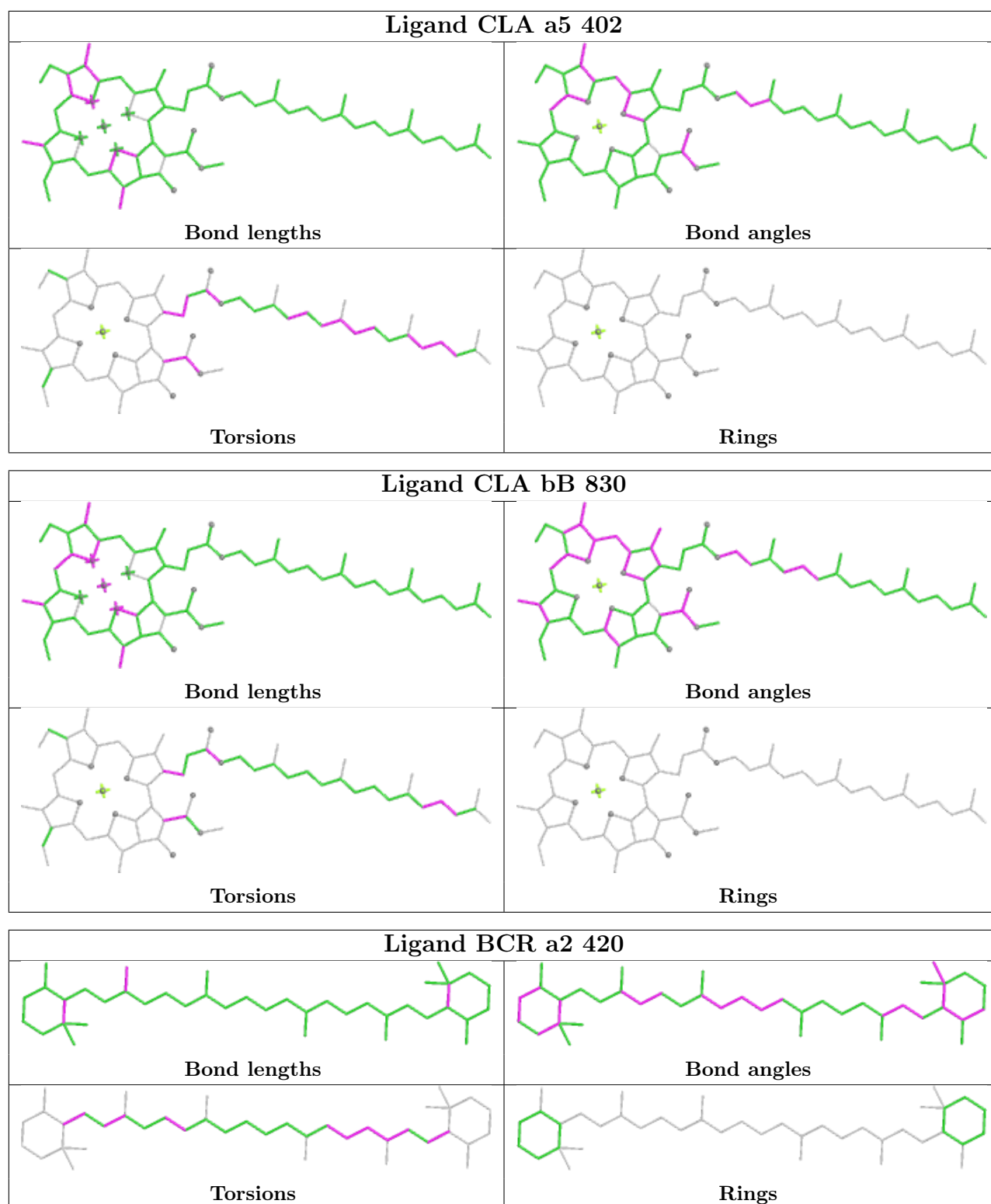


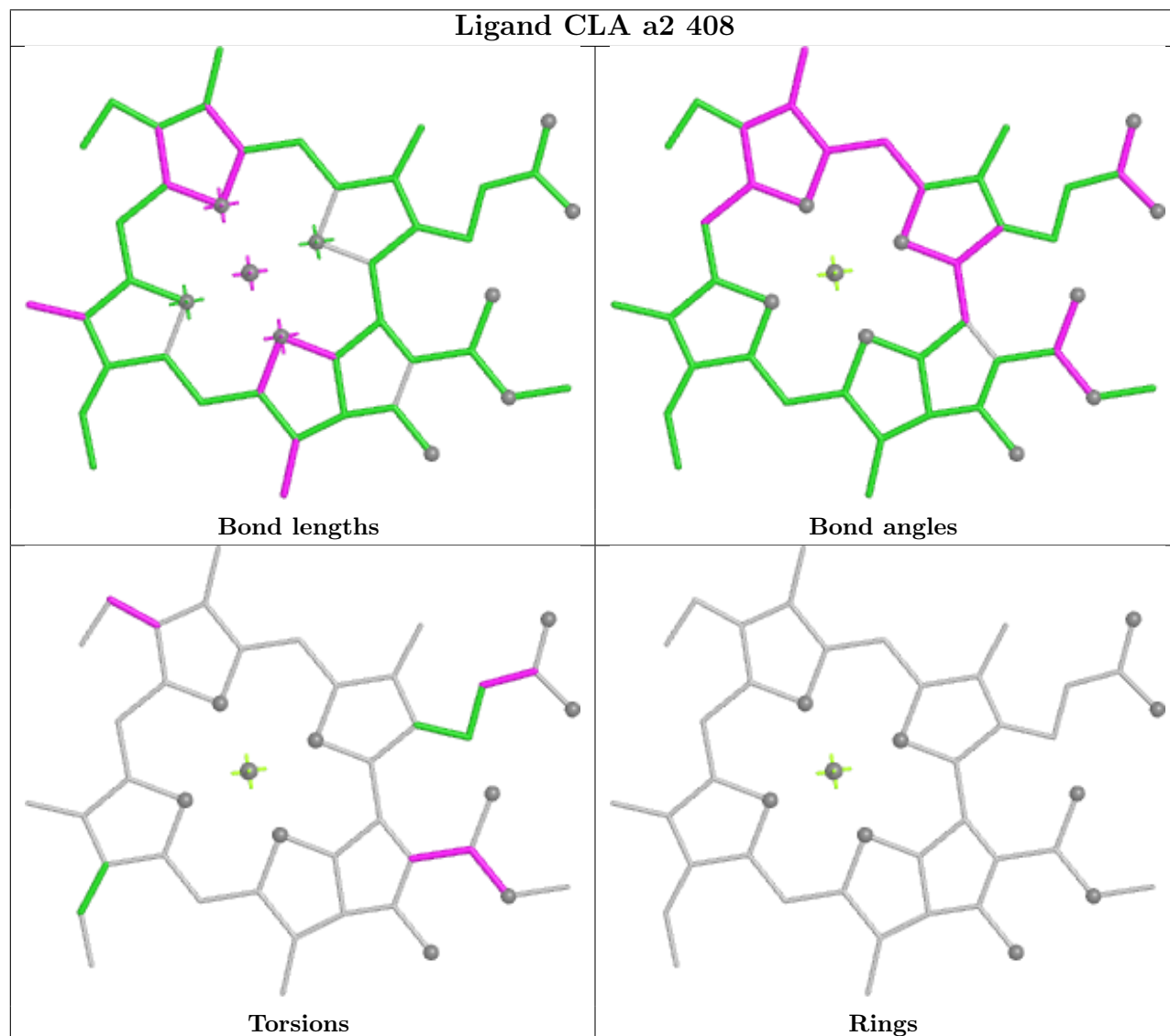
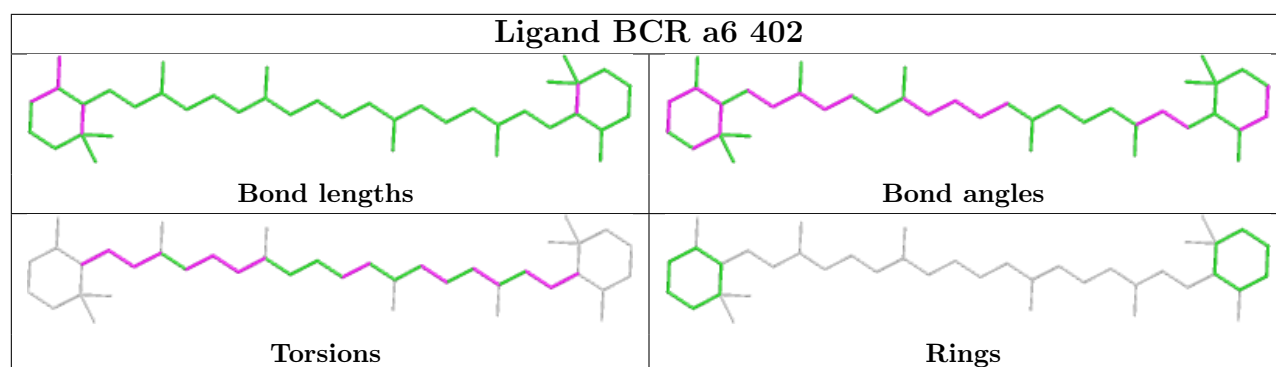


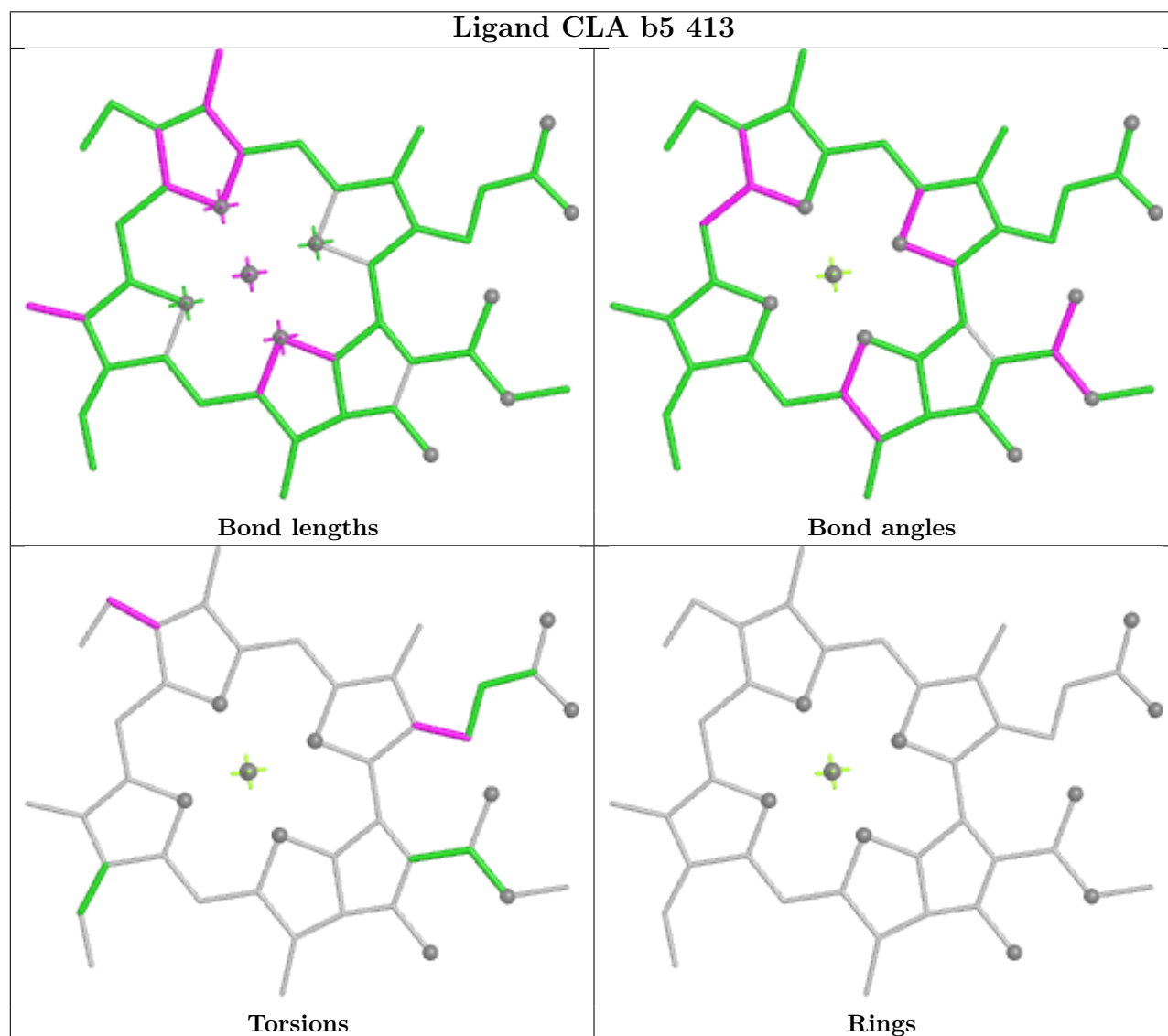
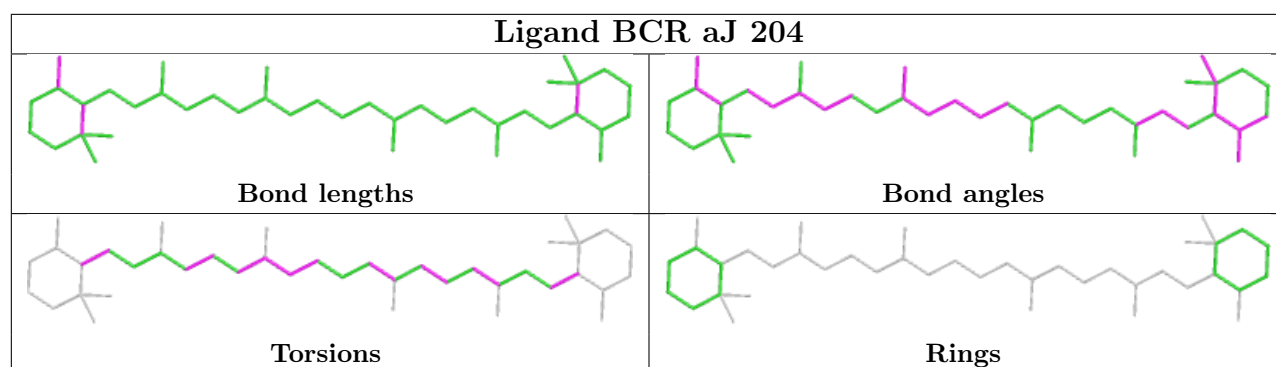


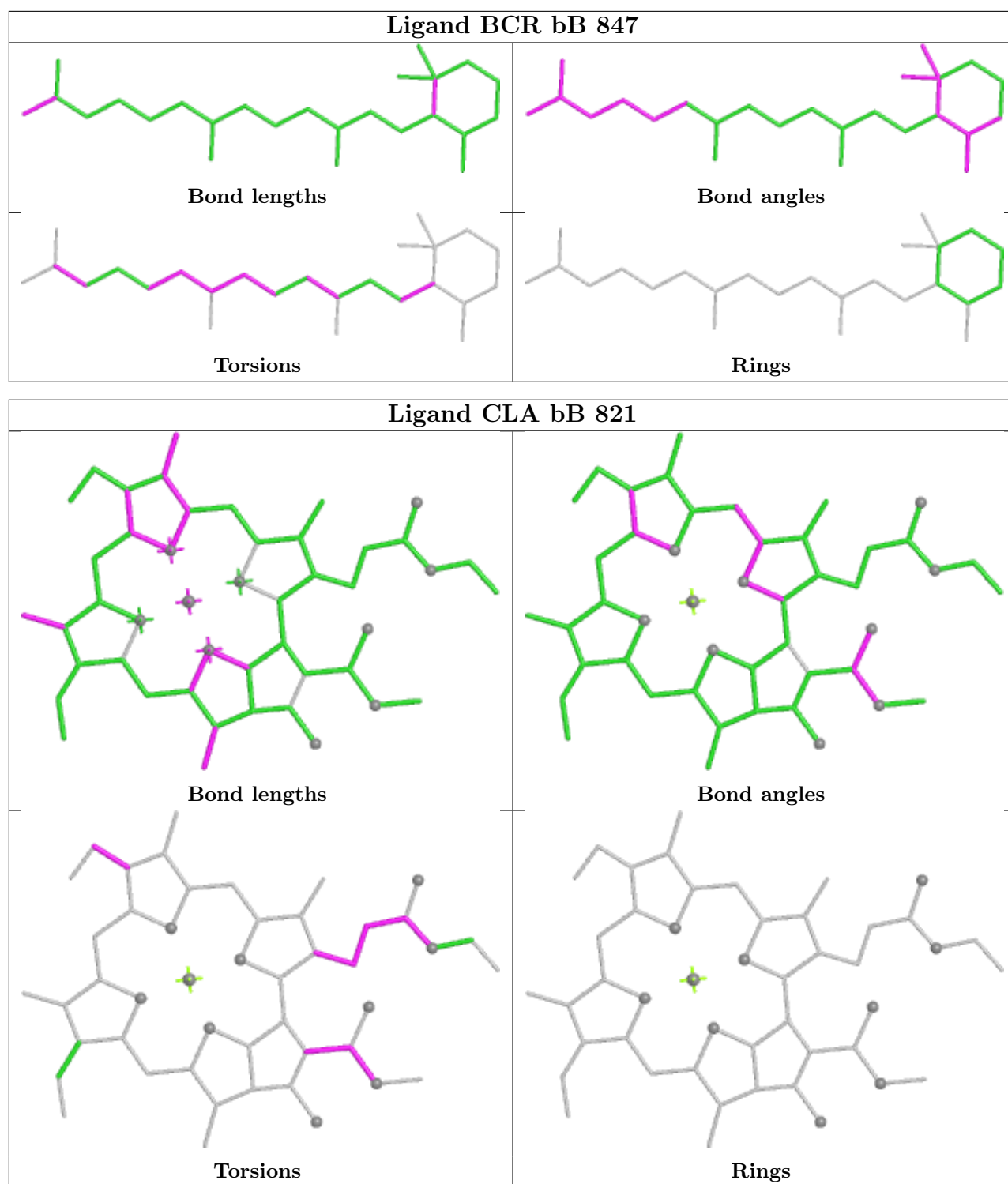


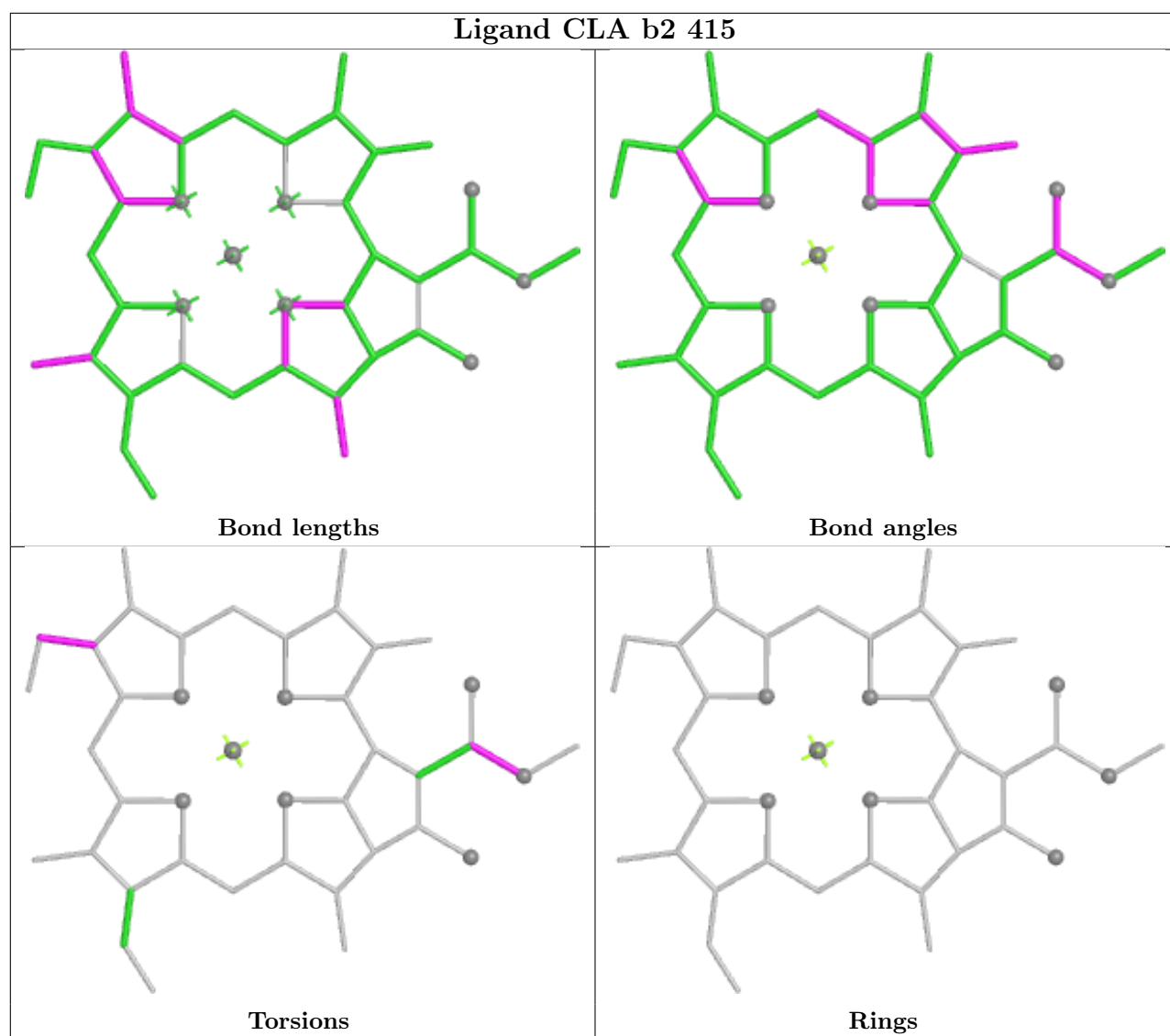


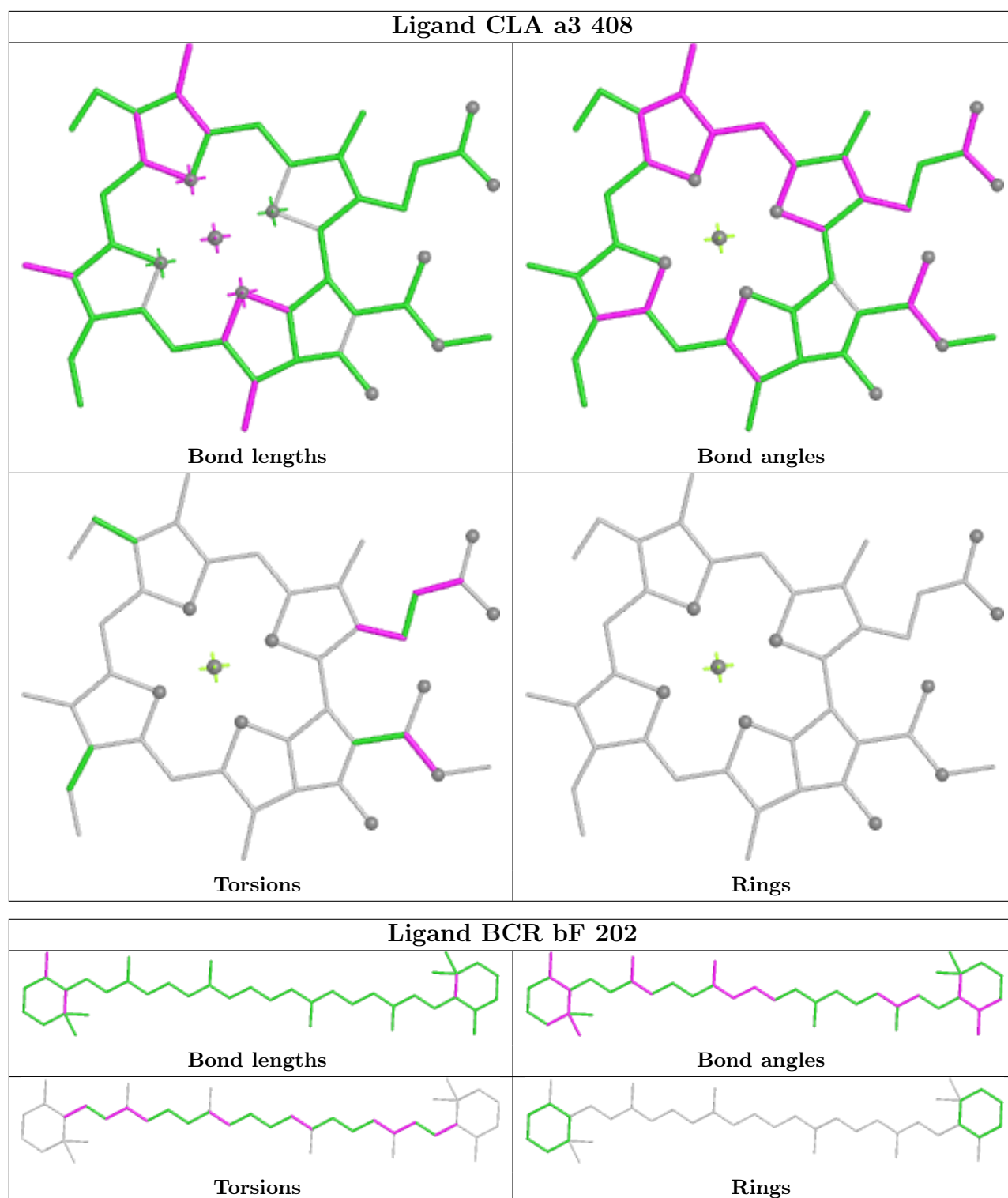


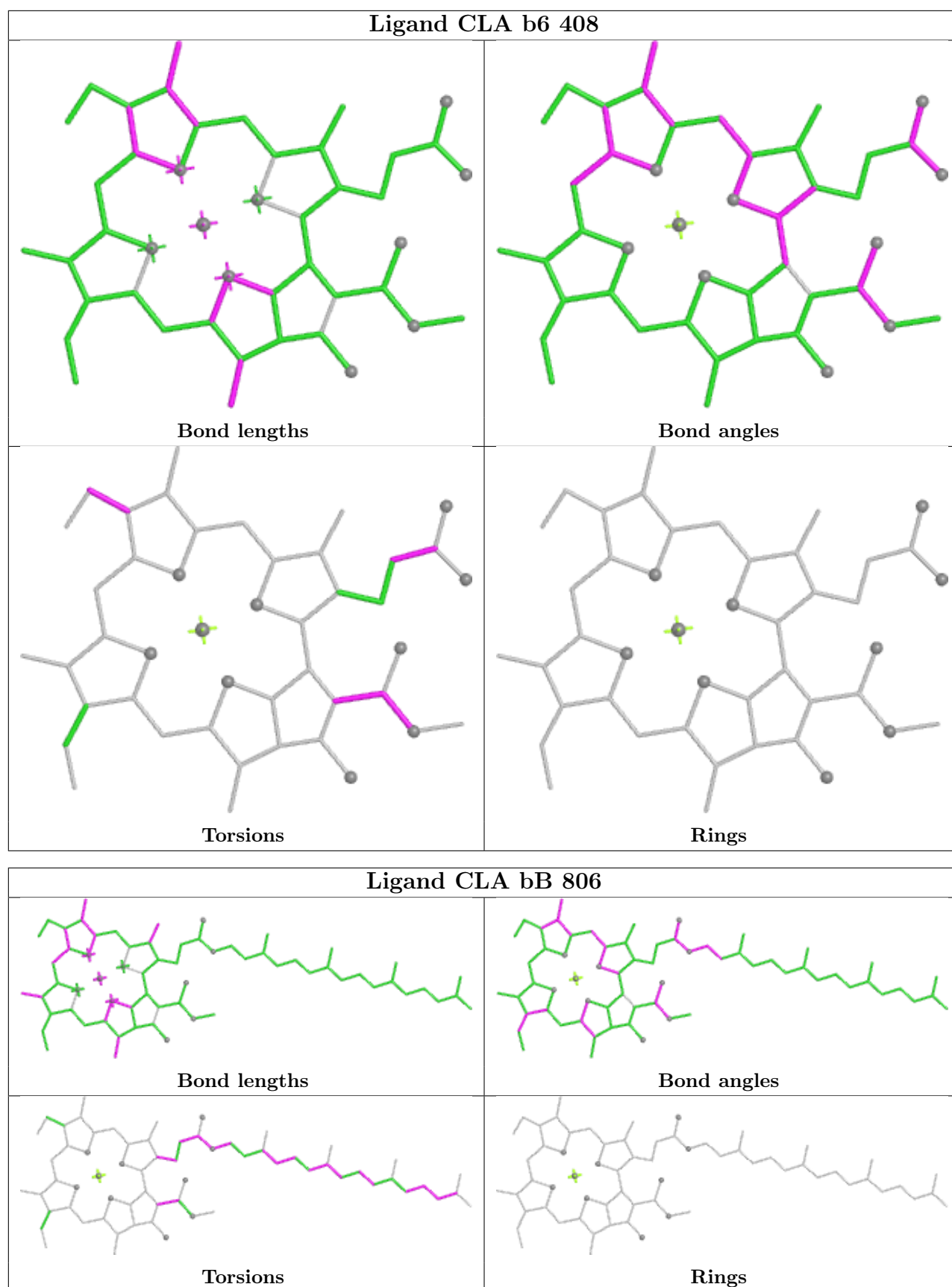


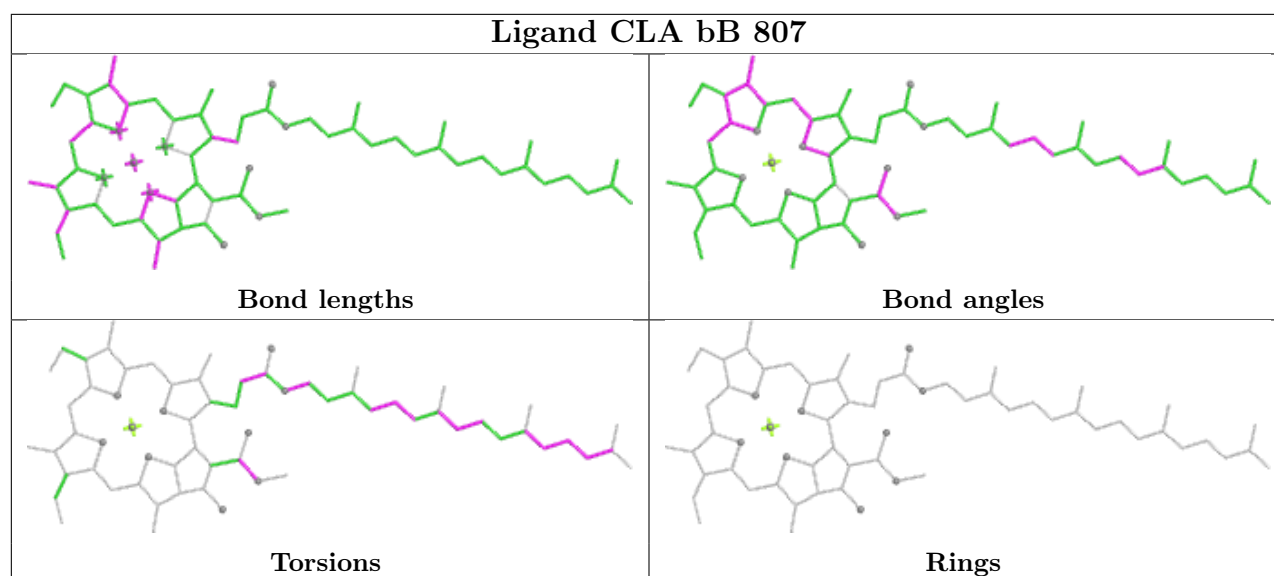
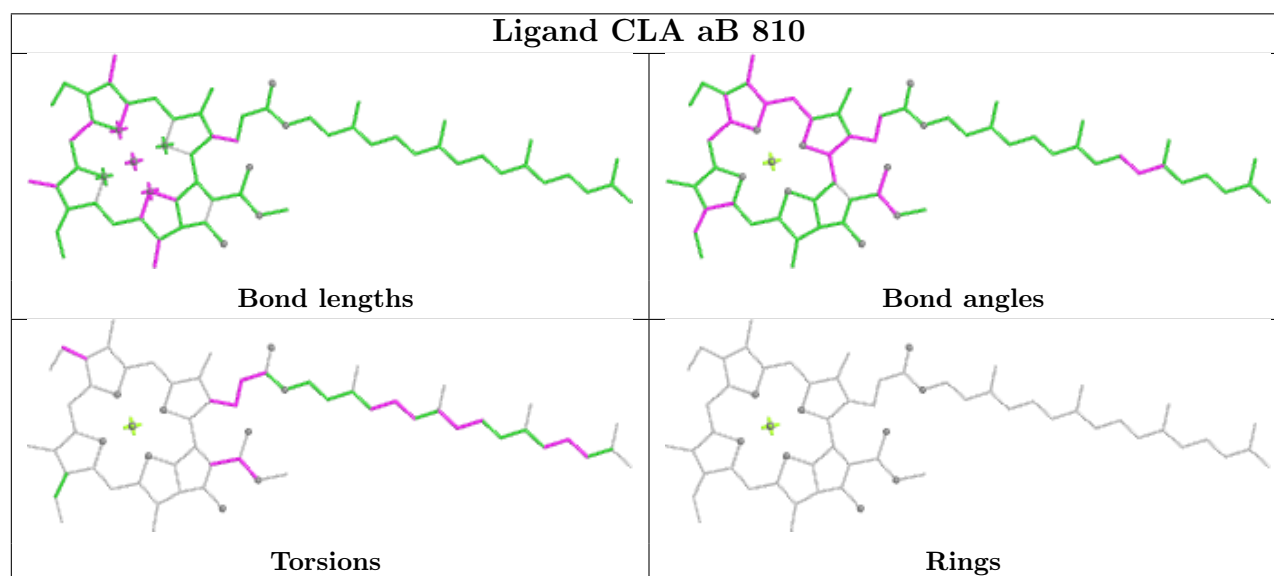
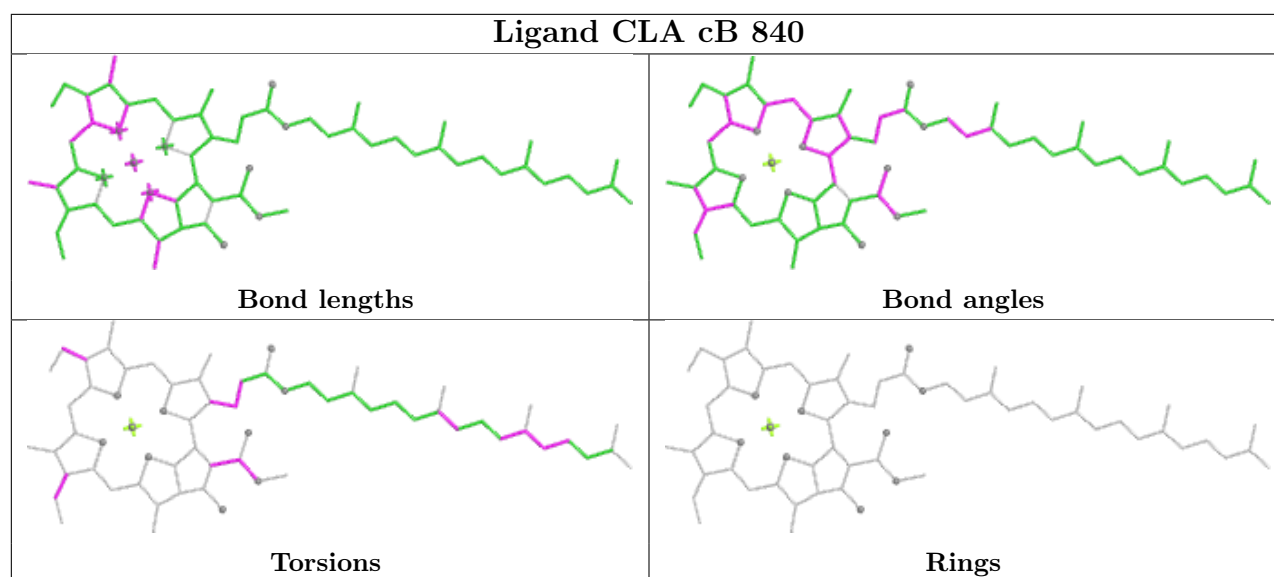


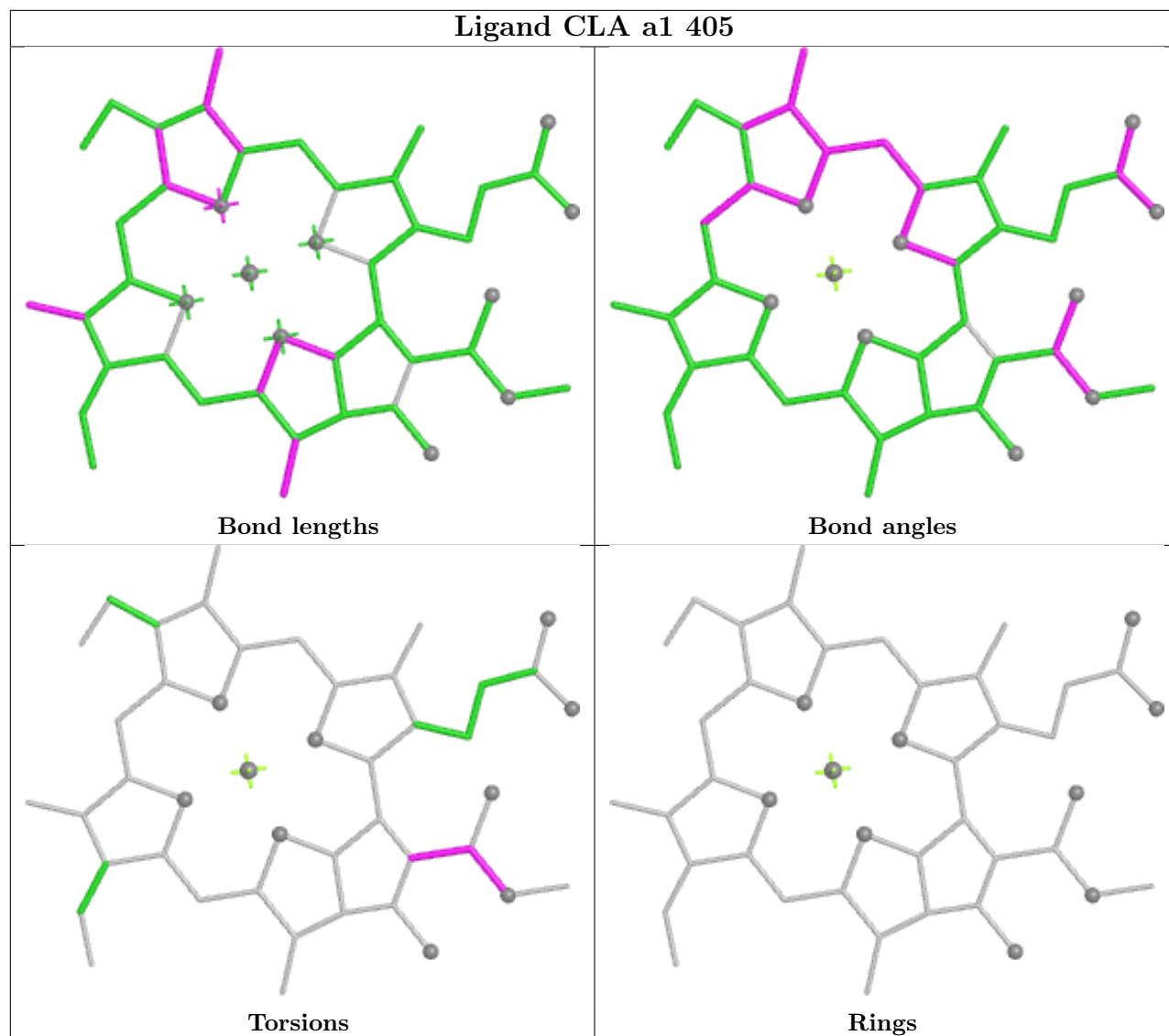


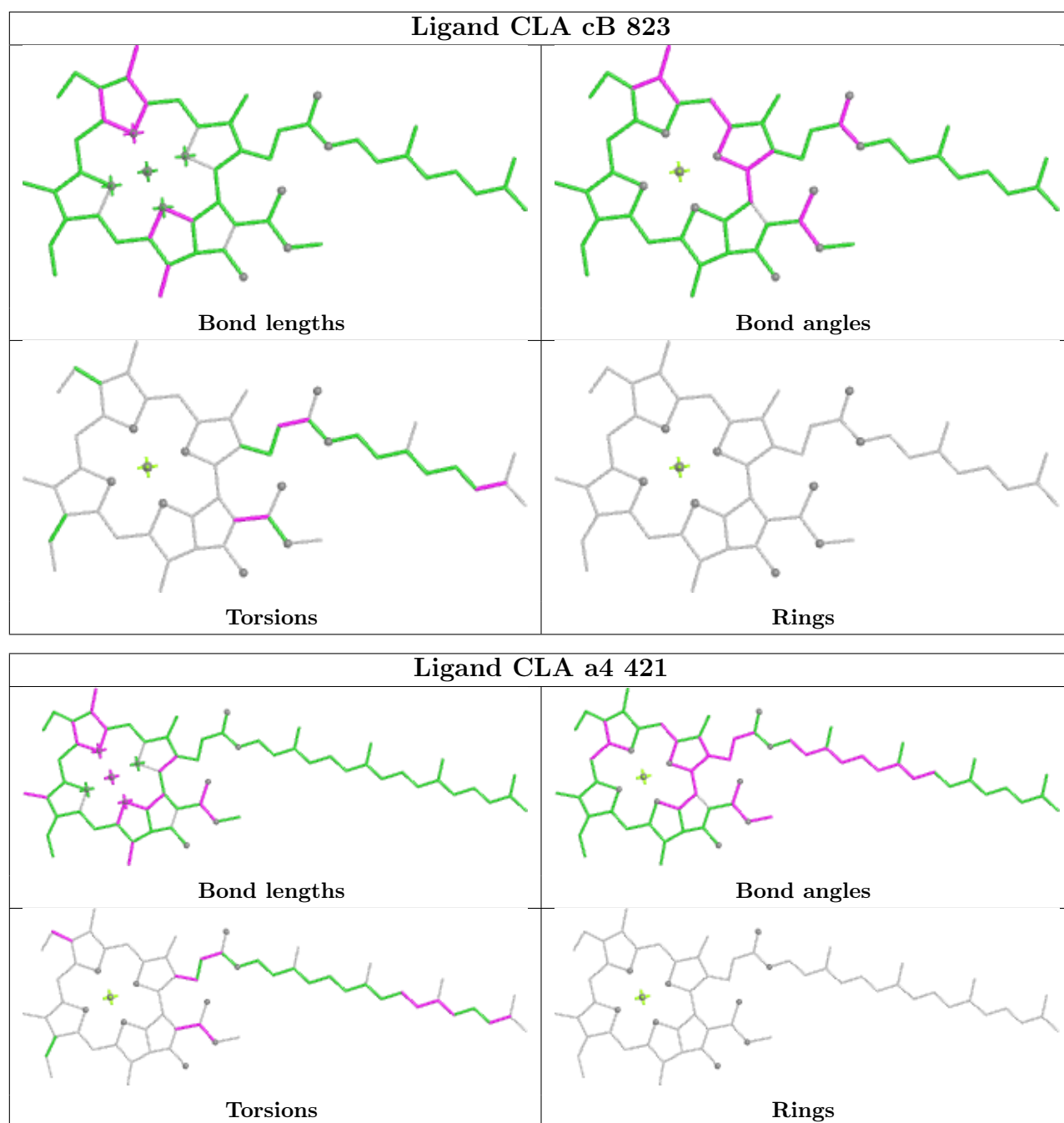


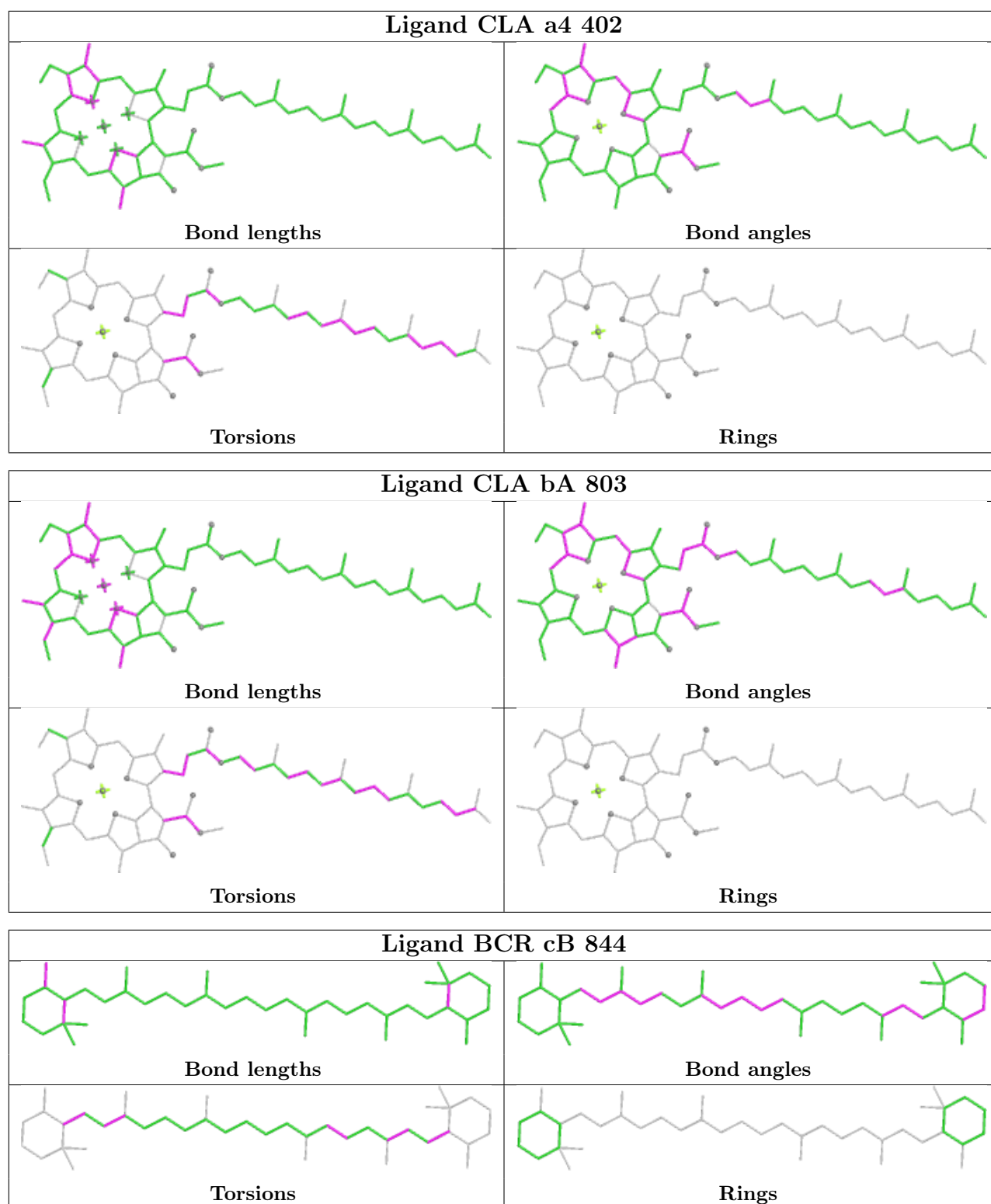


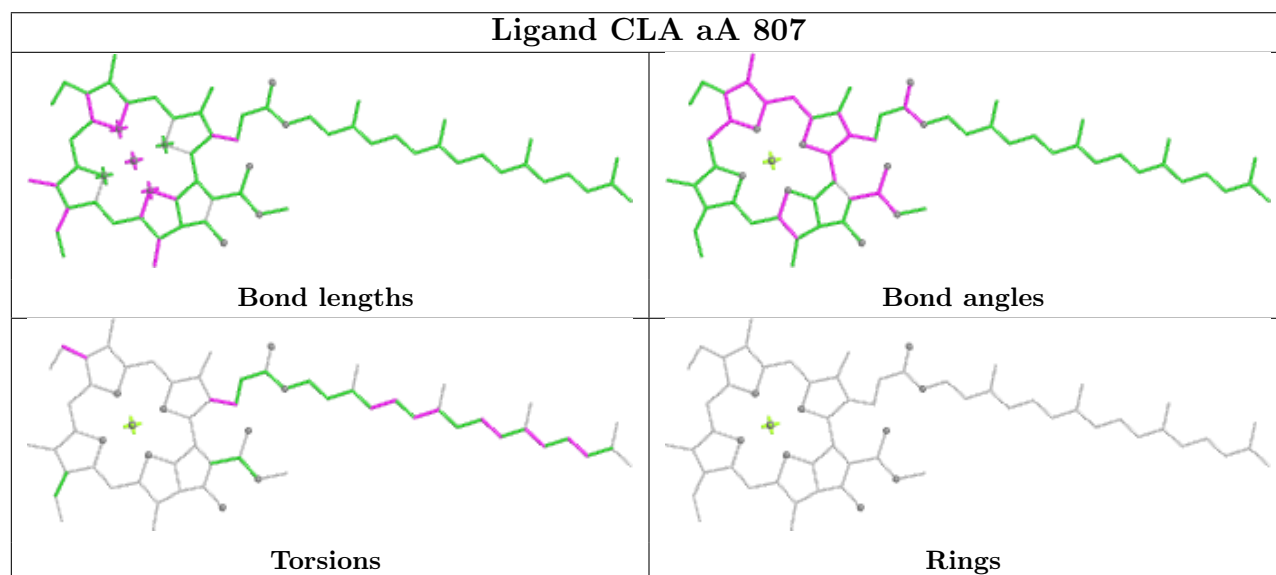
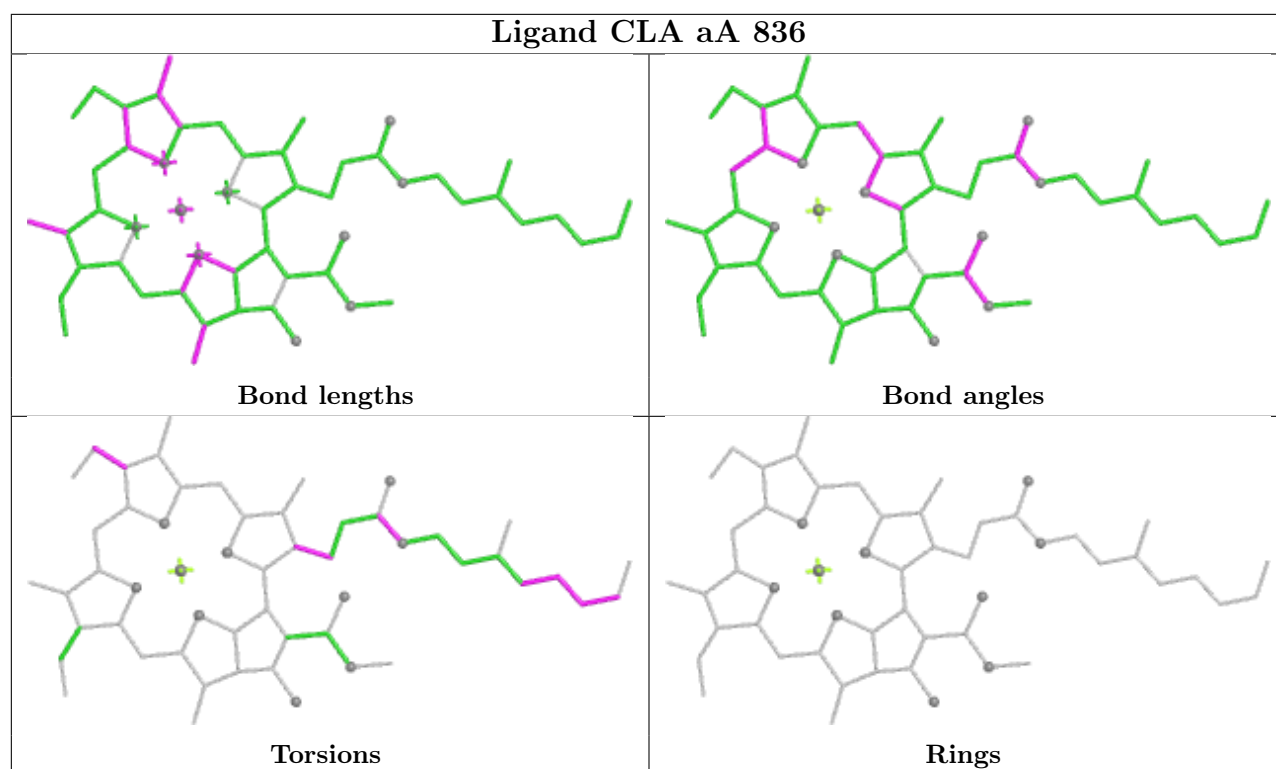


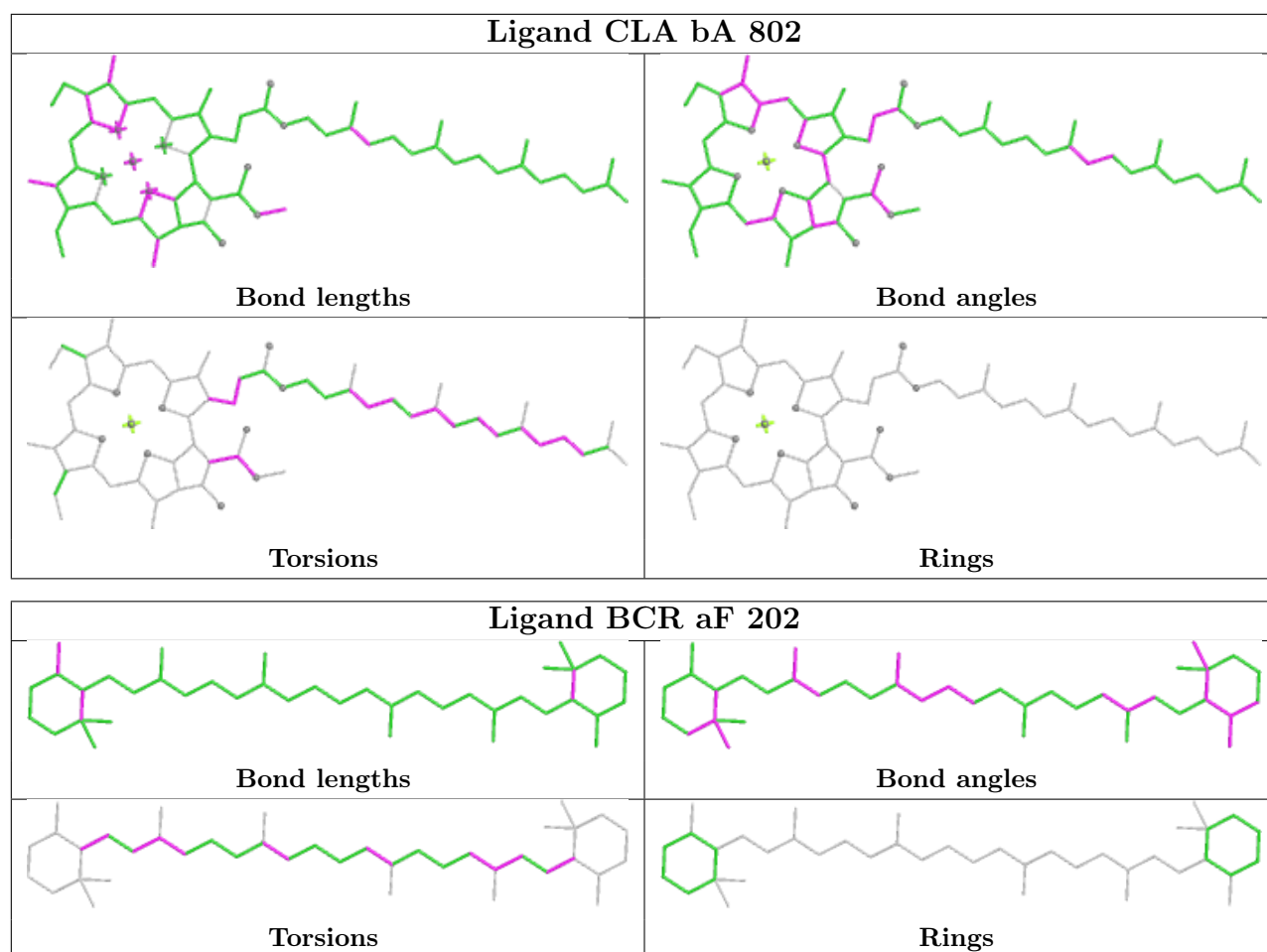


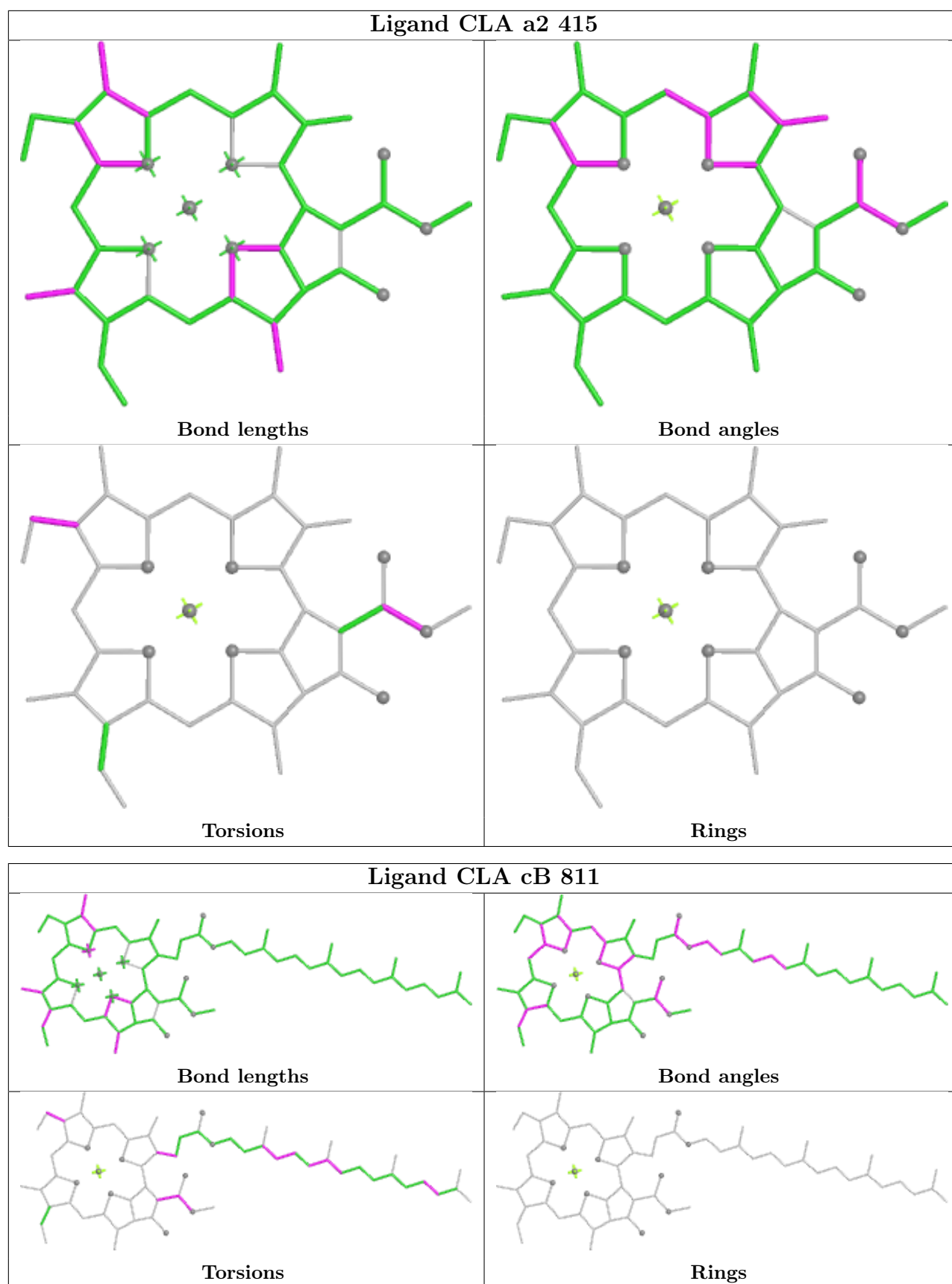


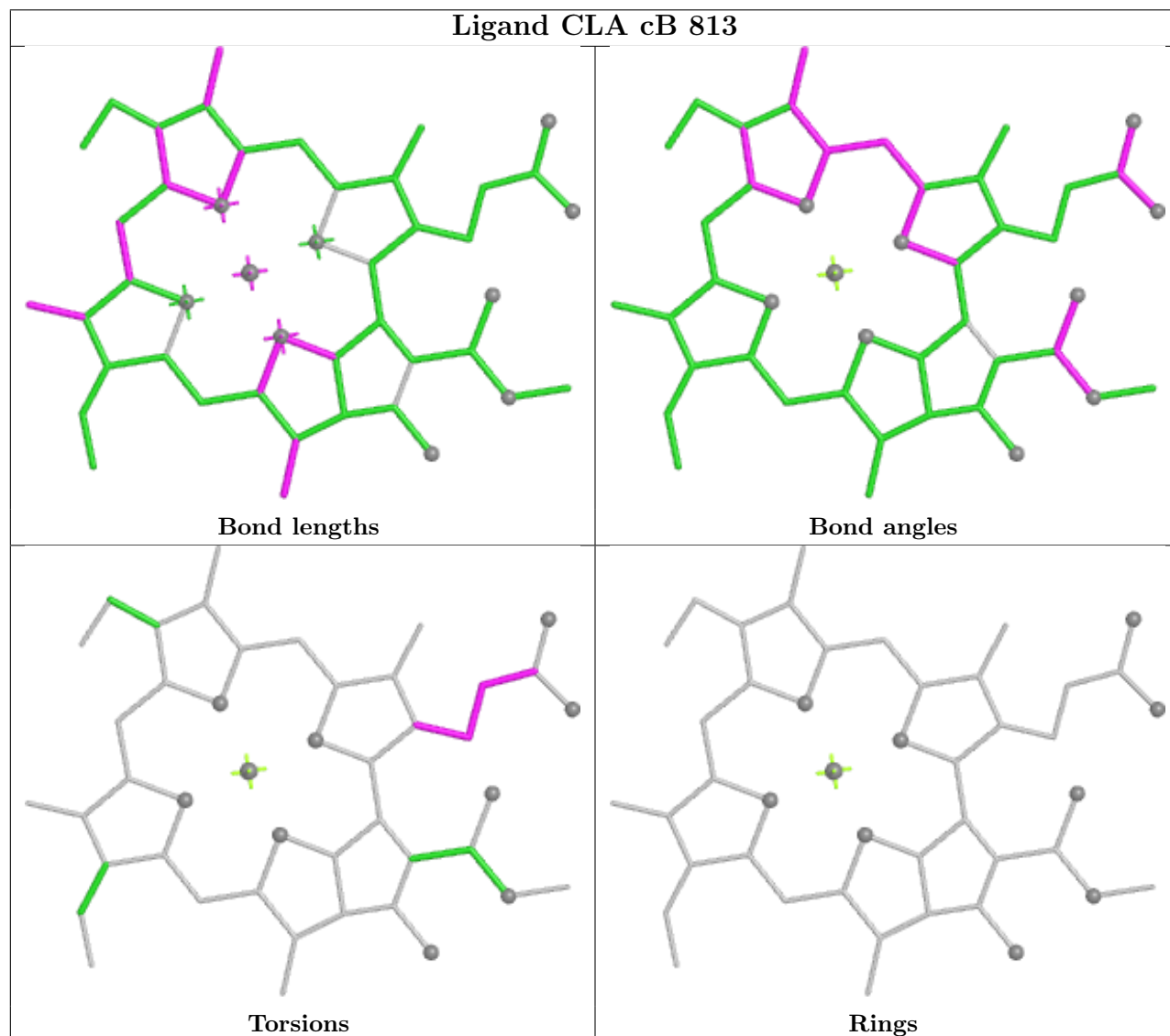
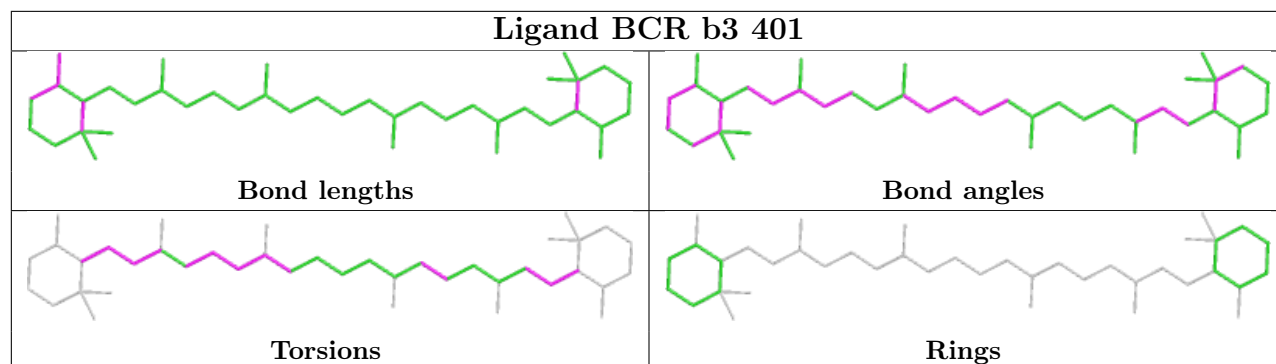


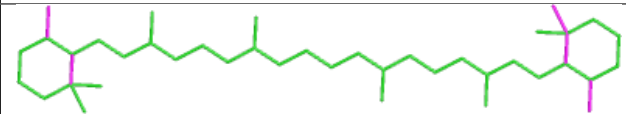
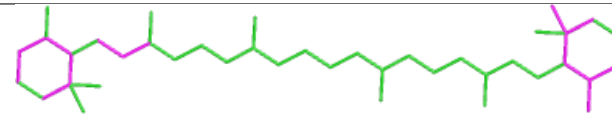
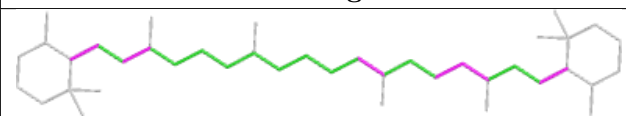
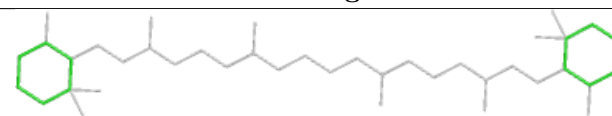


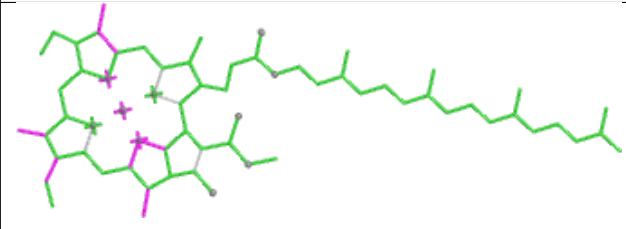
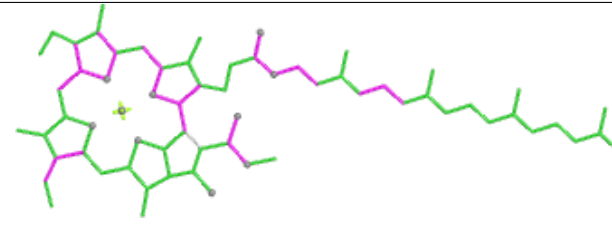
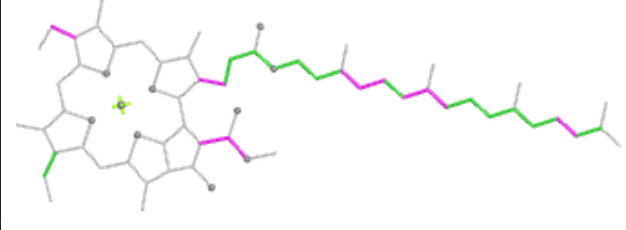
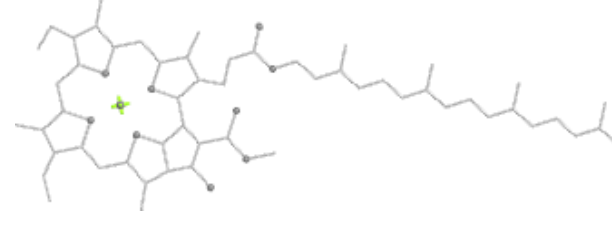


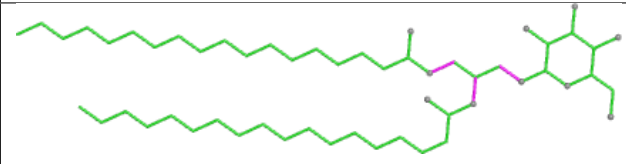
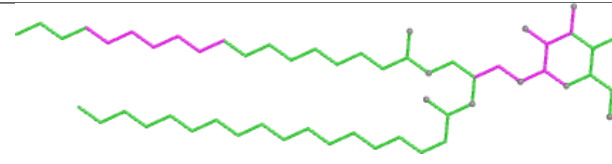
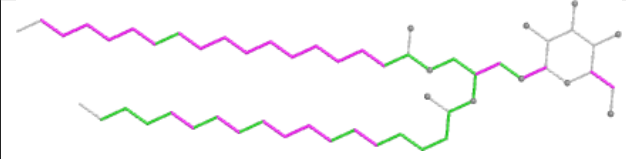
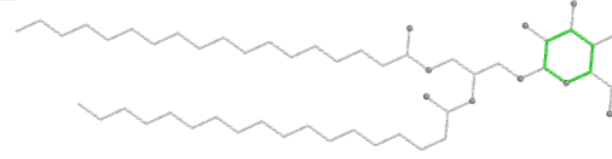


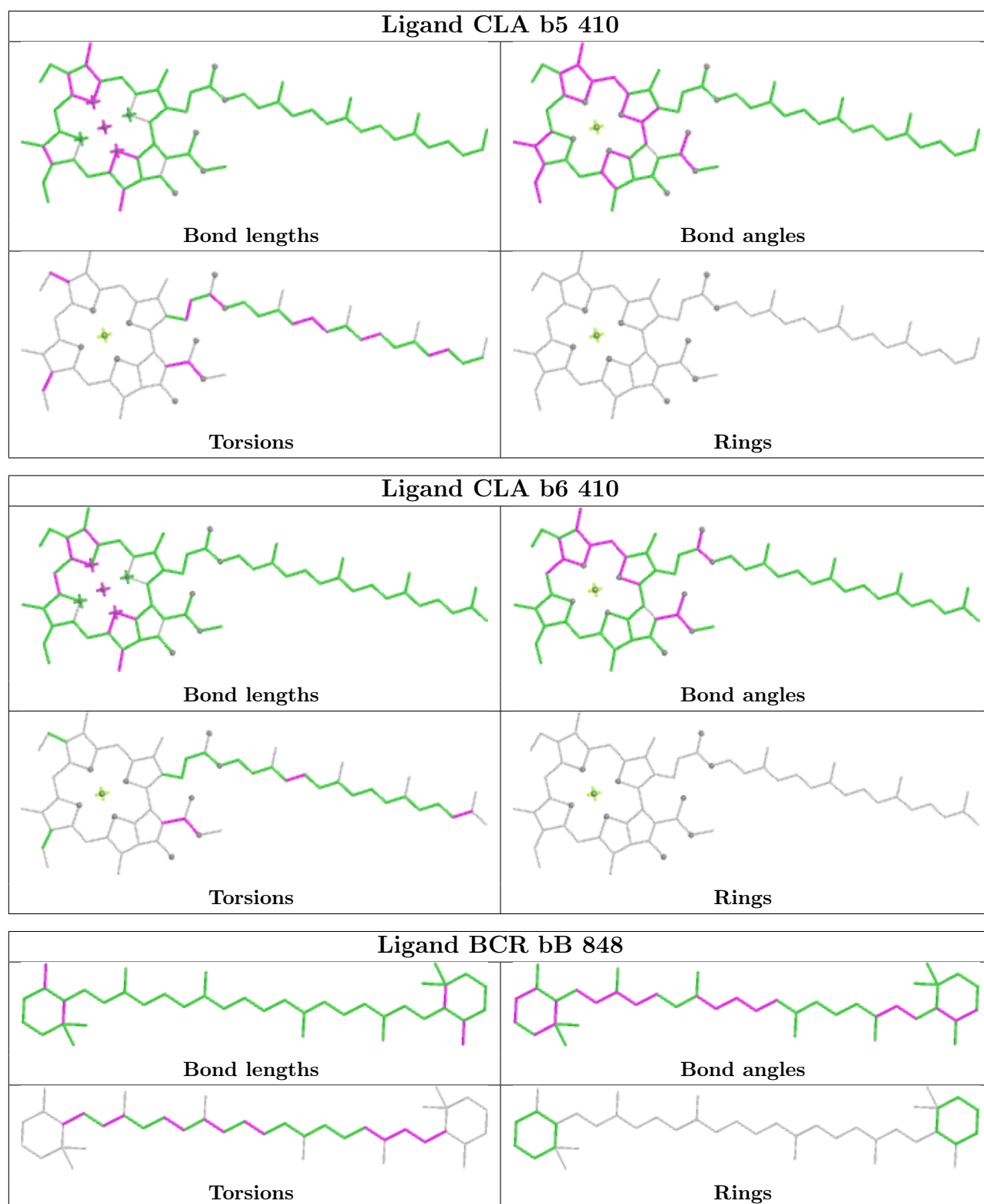


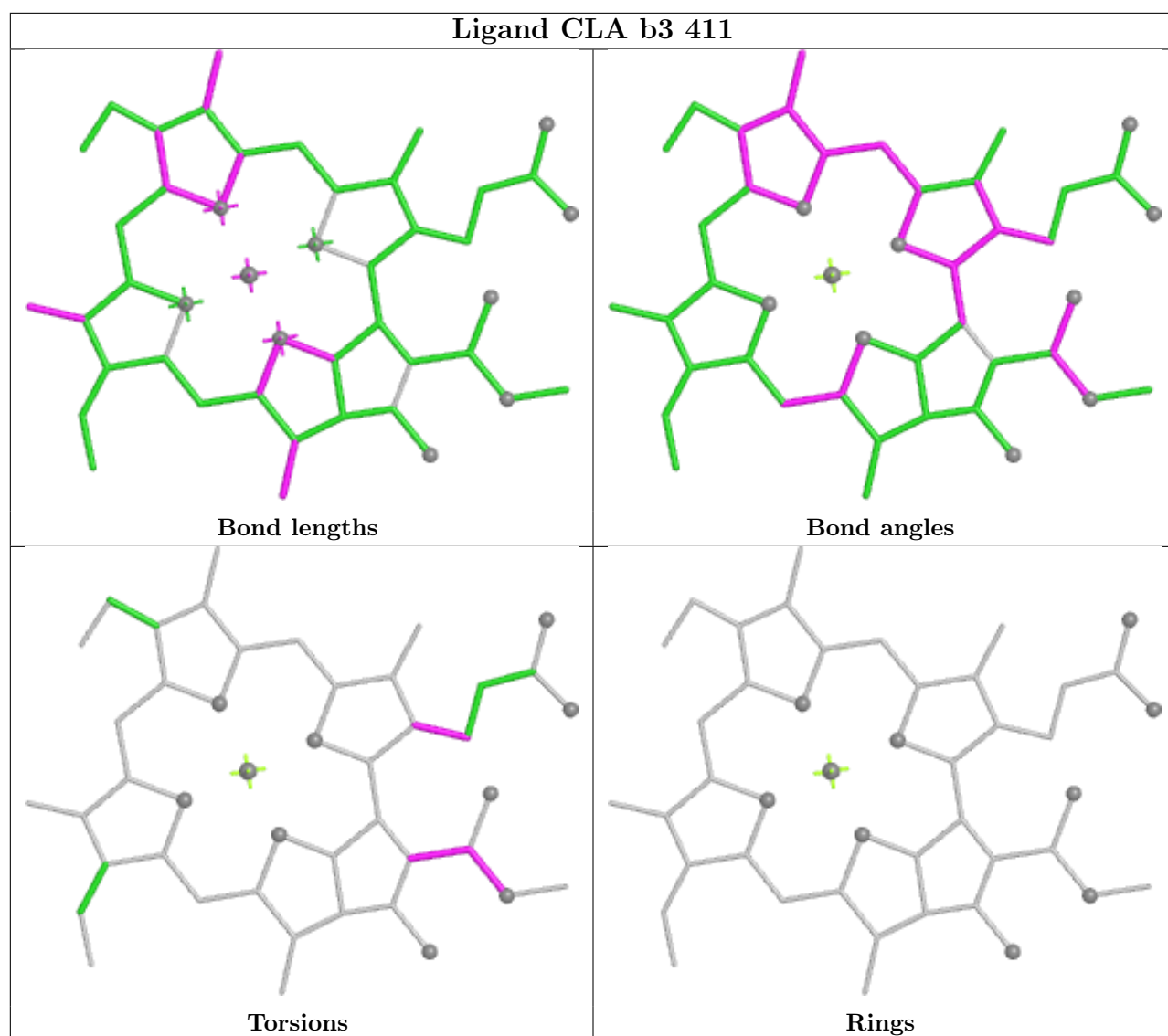


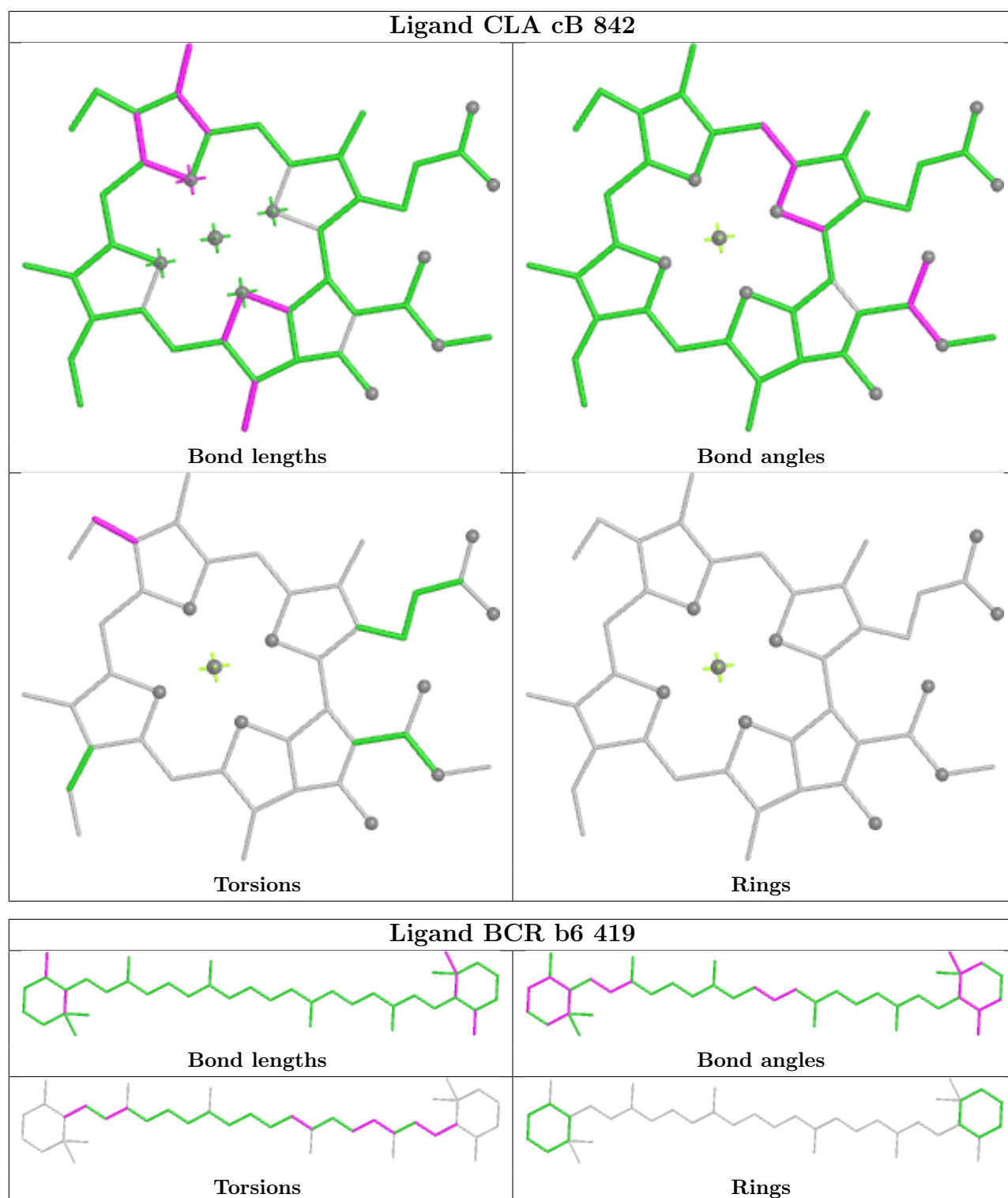
Ligand BCR a4 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

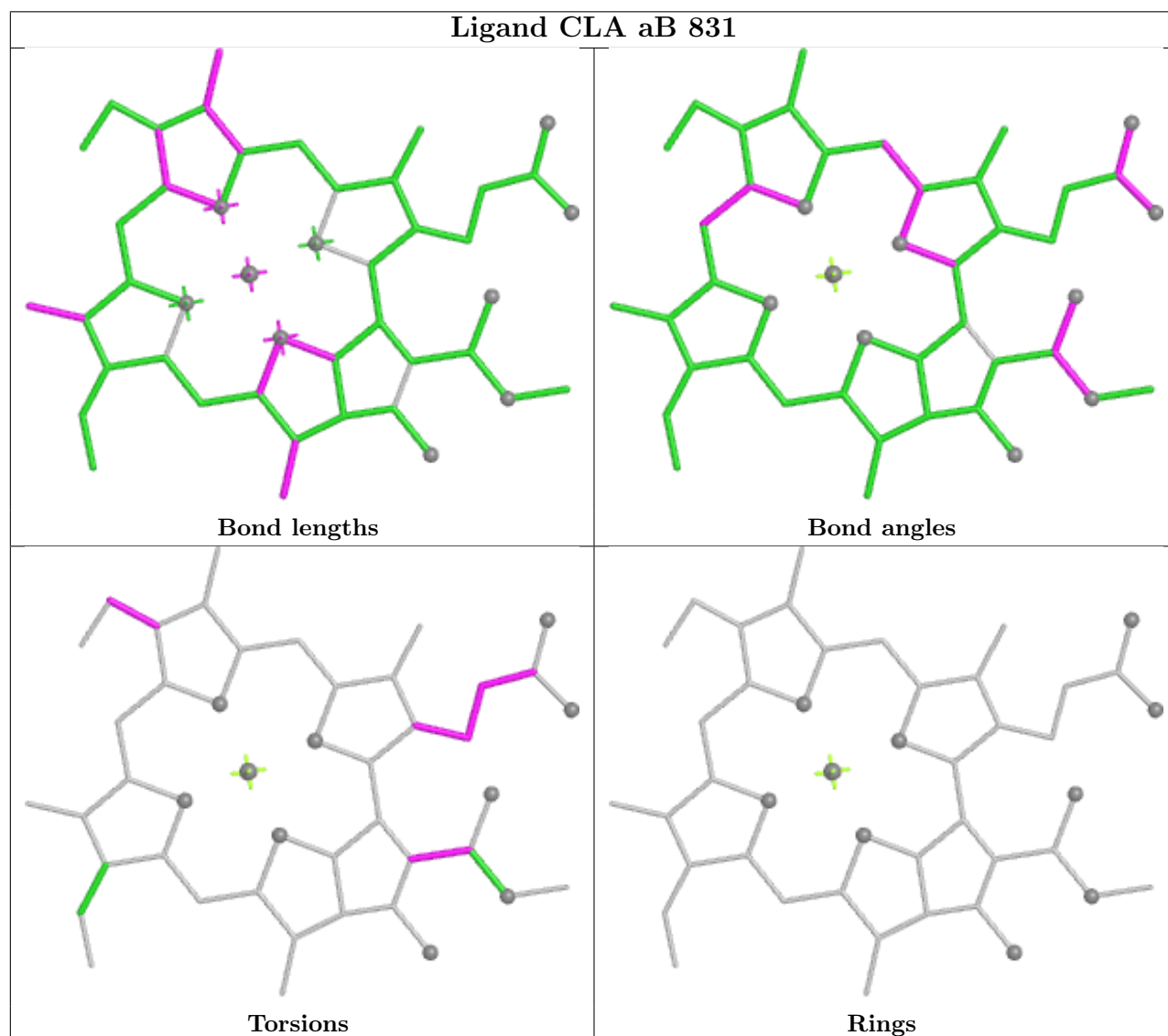
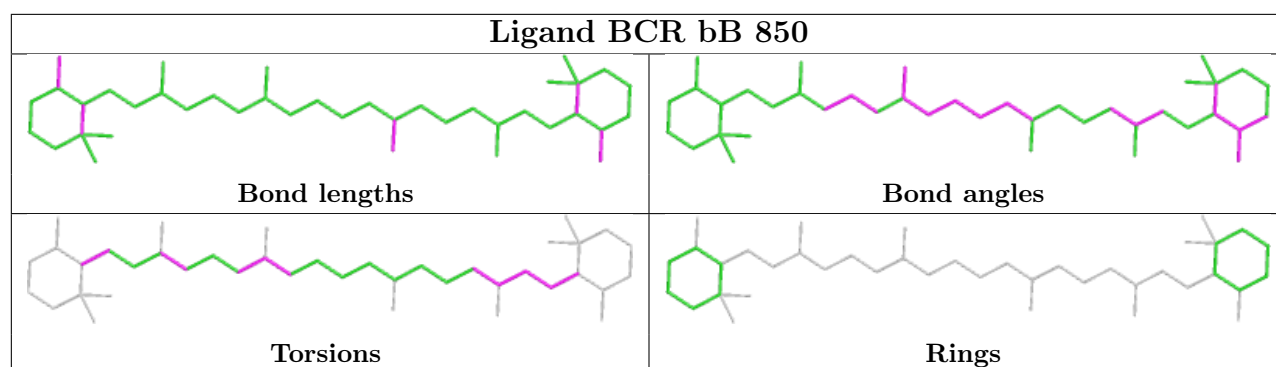
Ligand CLA aB 811	
	
Bond lengths	Bond angles
	
Torsions	Rings

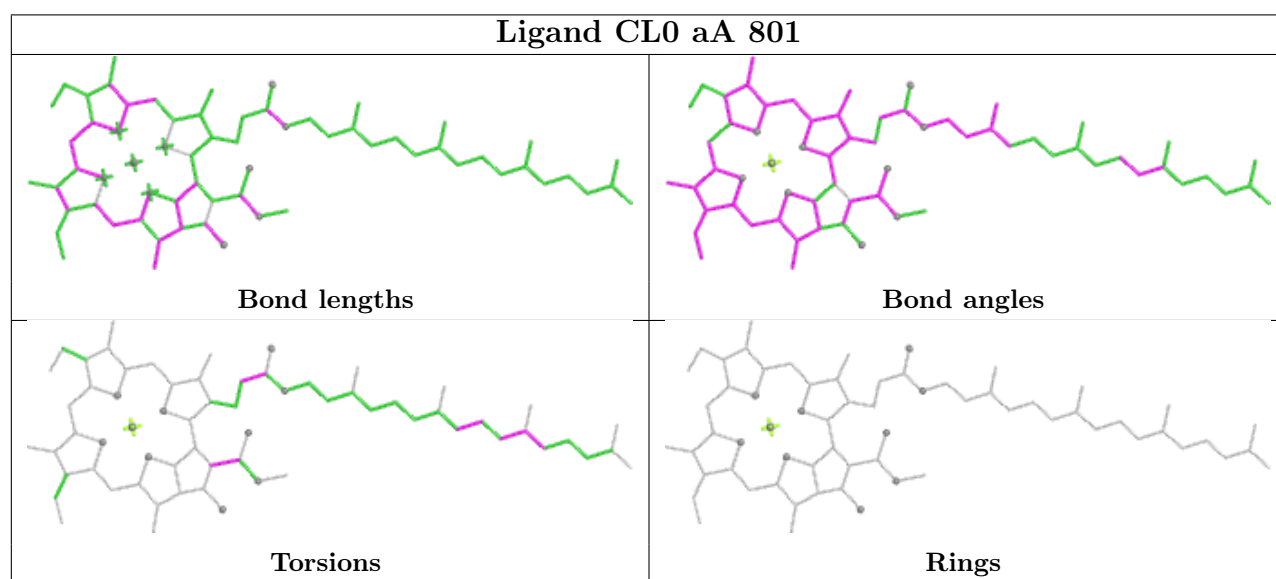
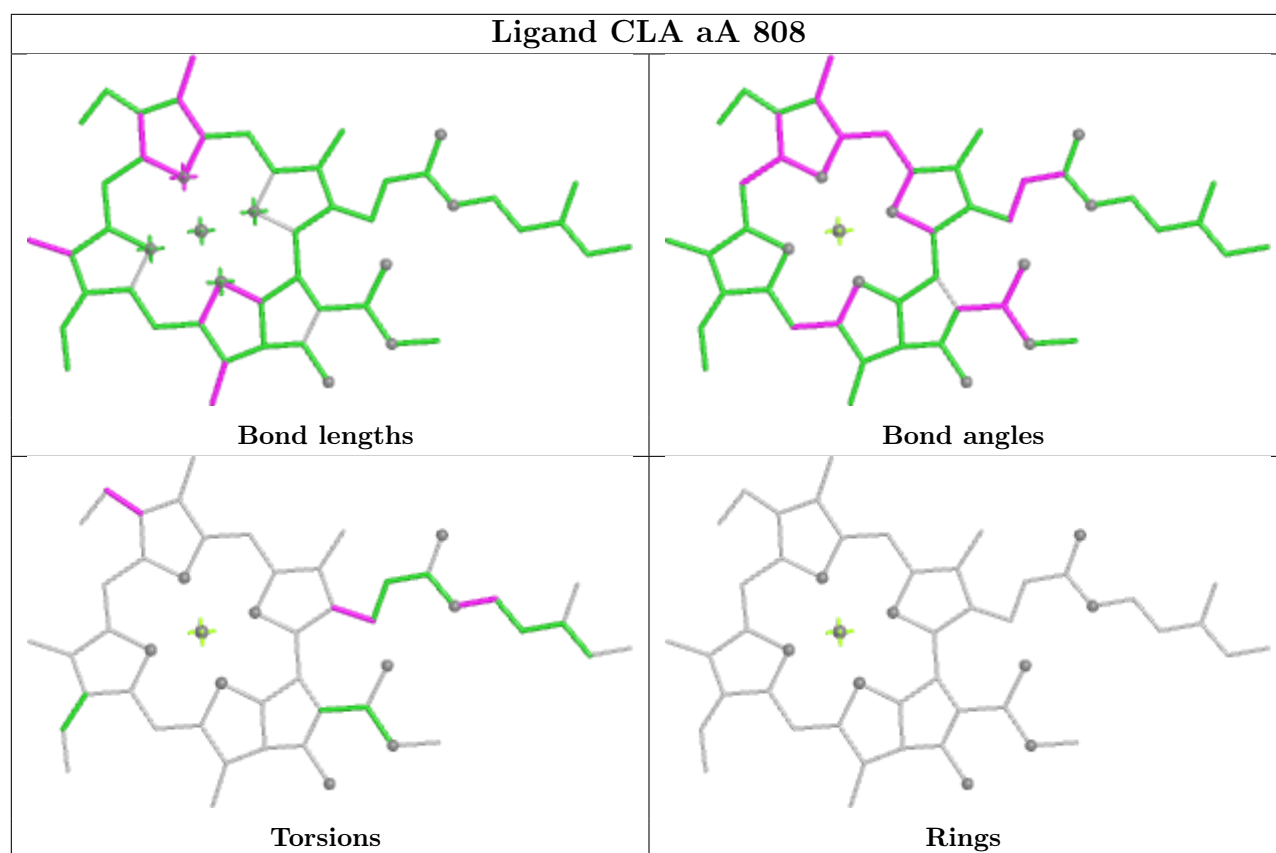
Ligand LMG bB 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

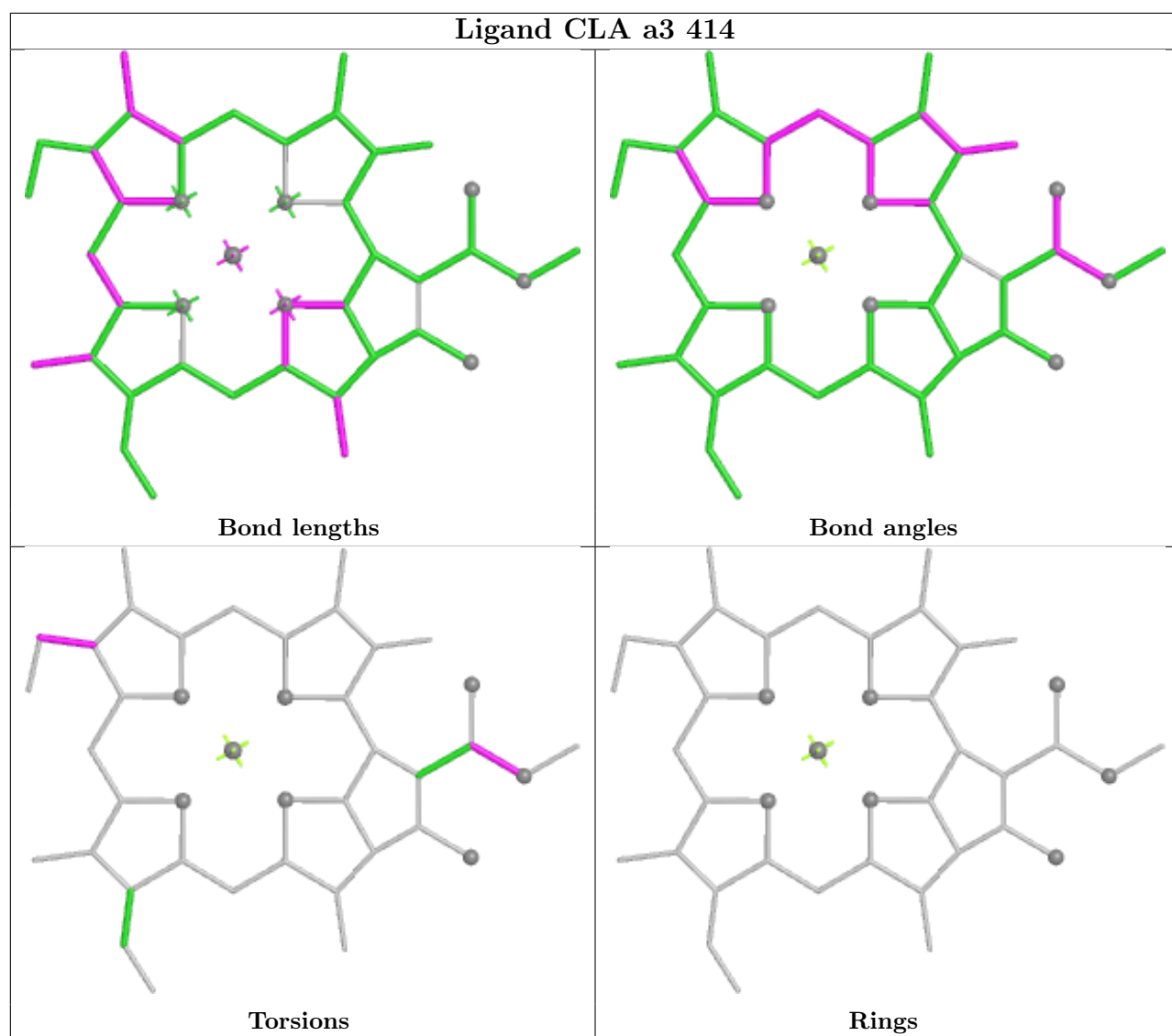


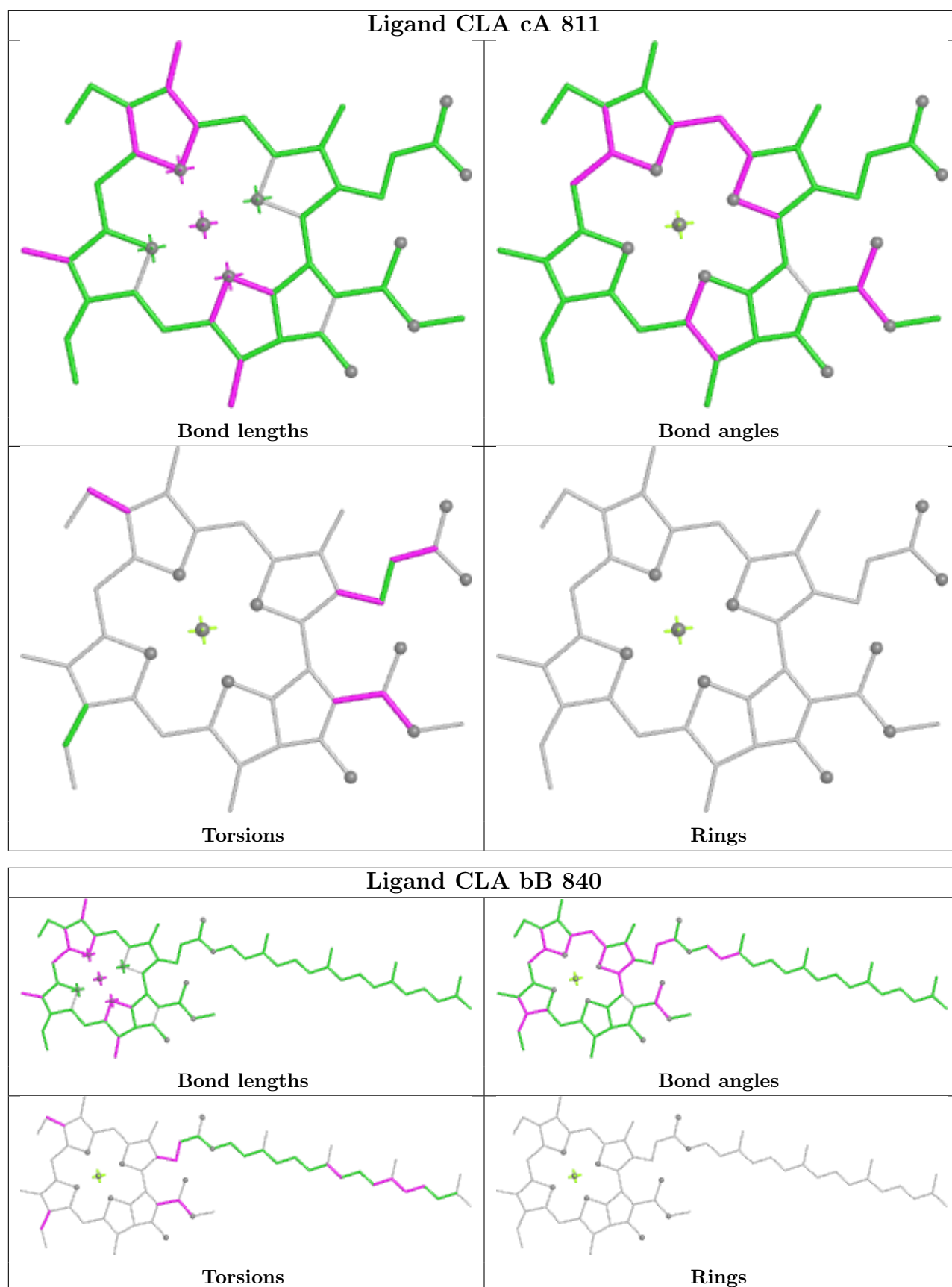


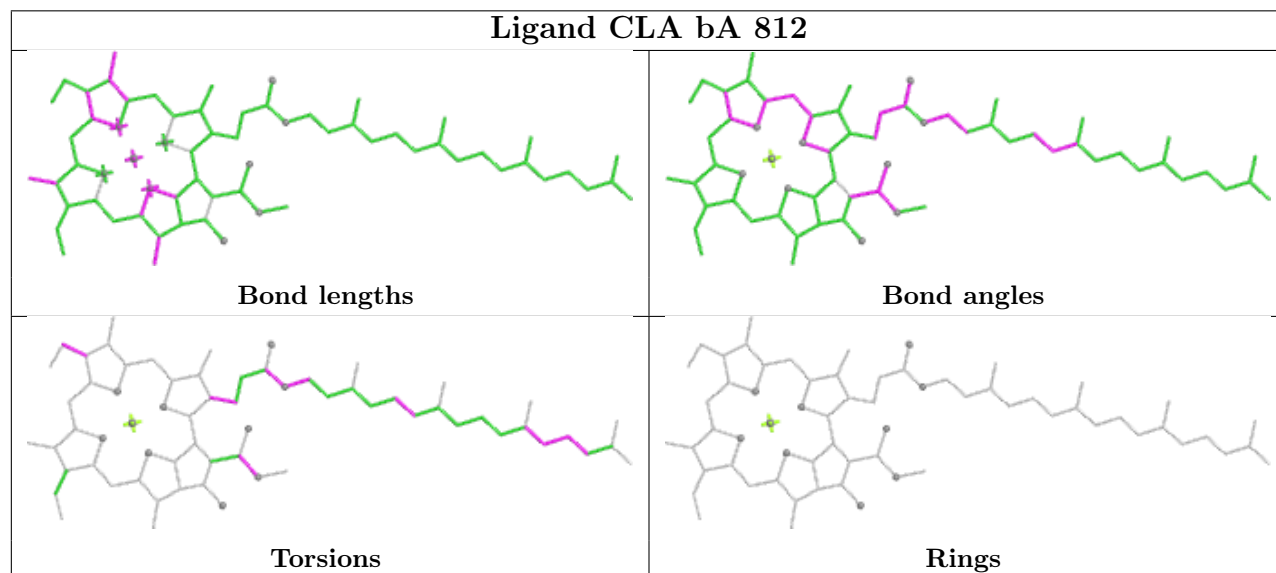
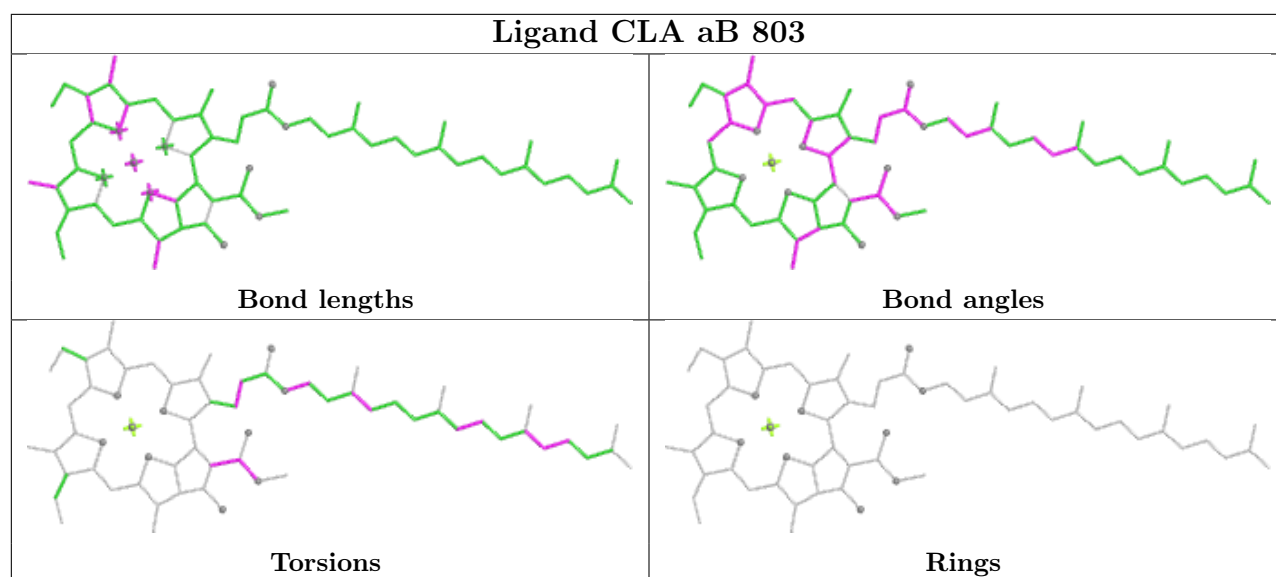


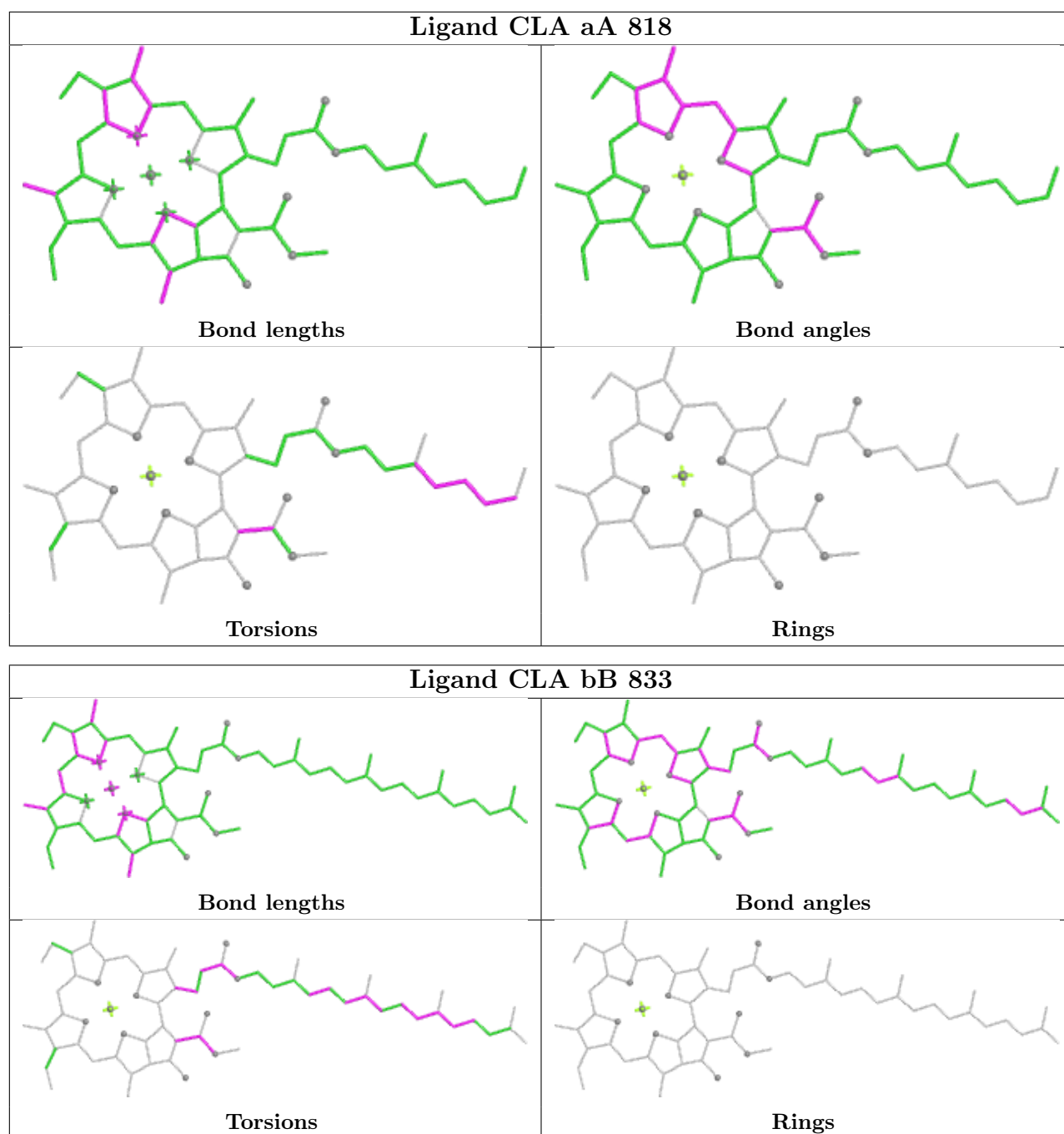


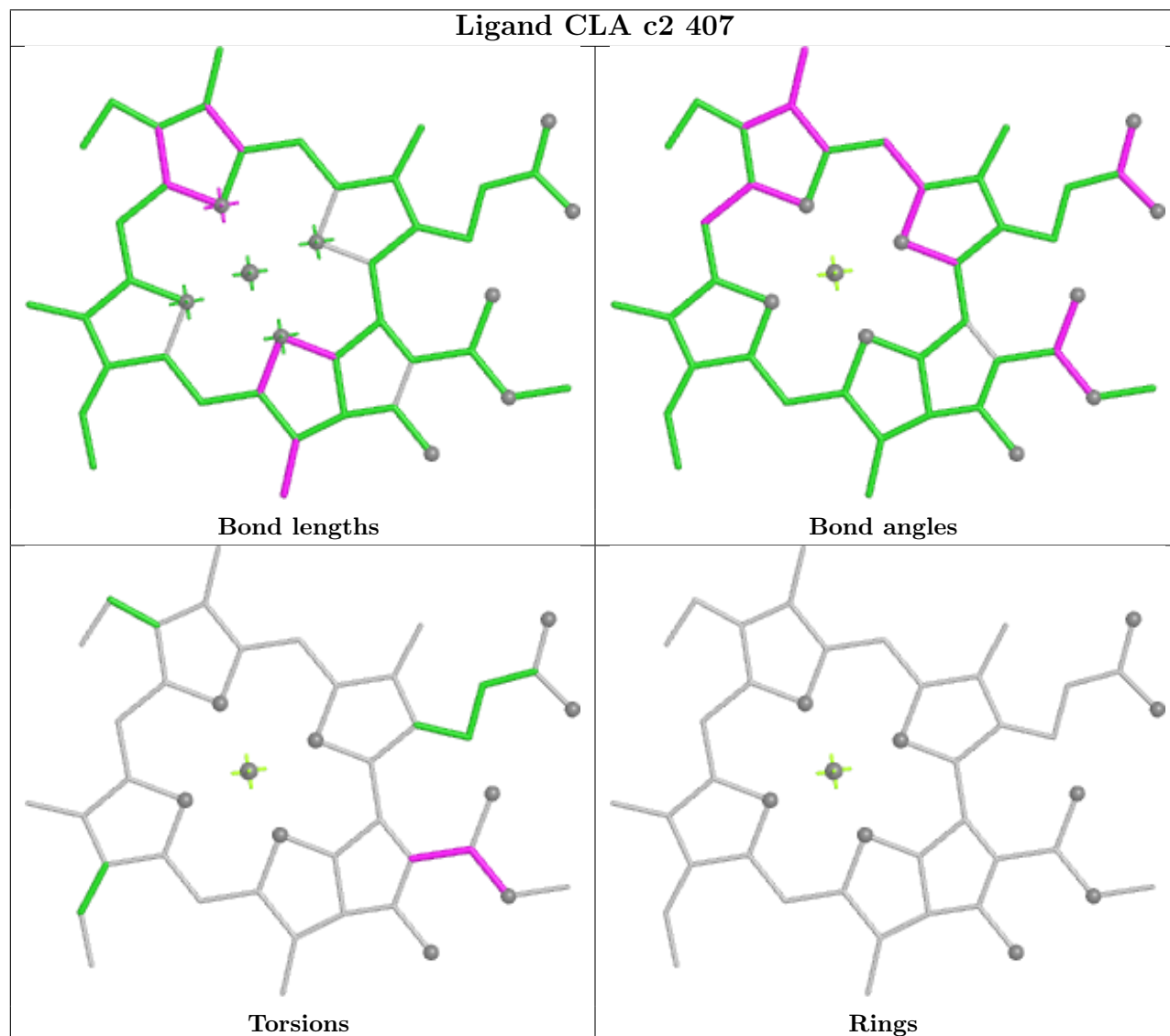
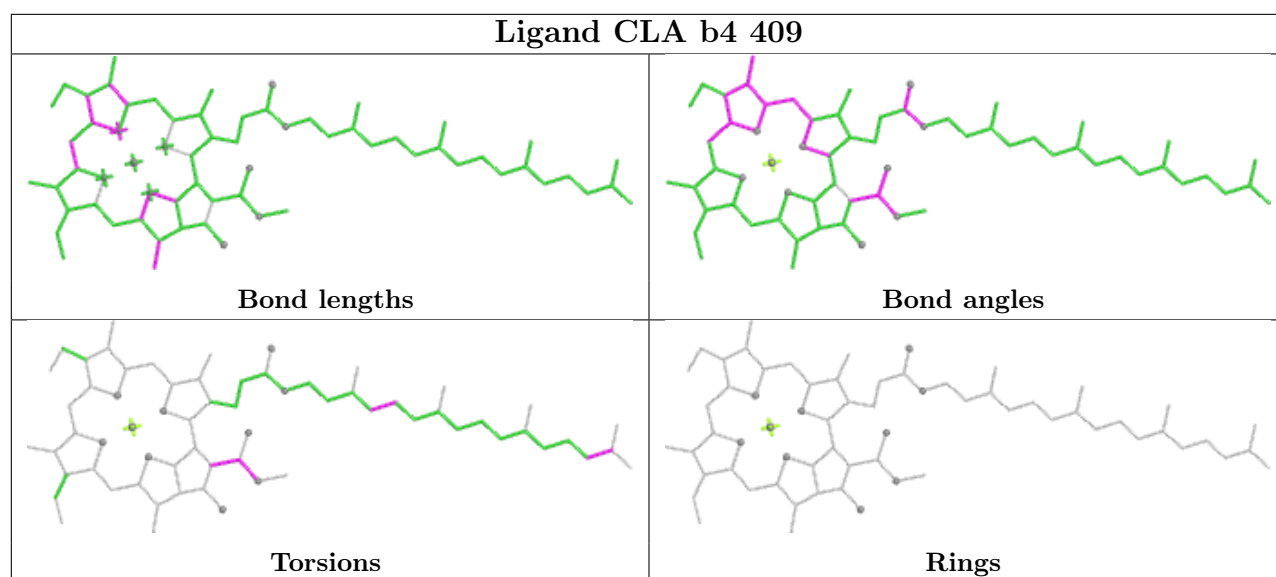


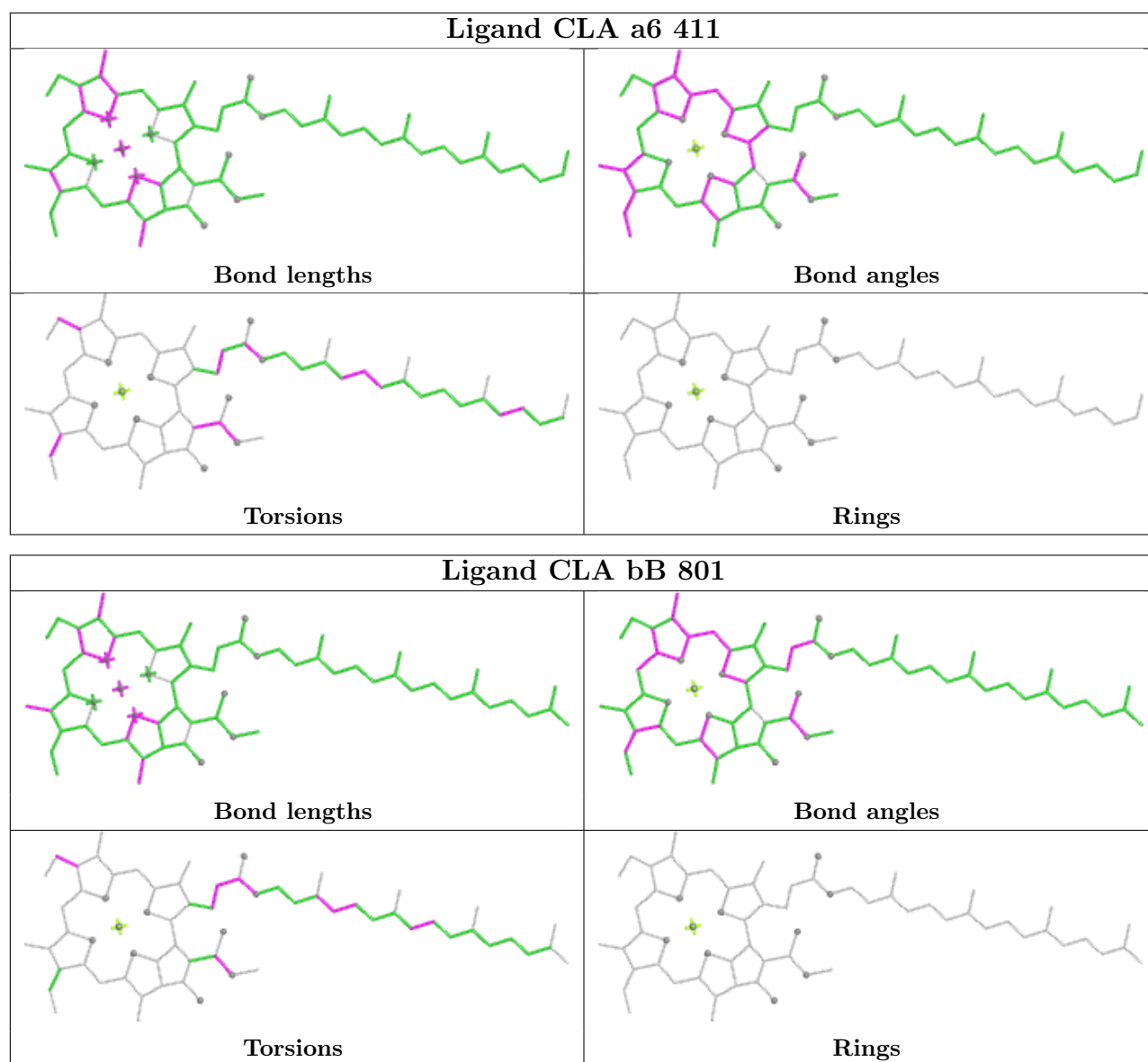


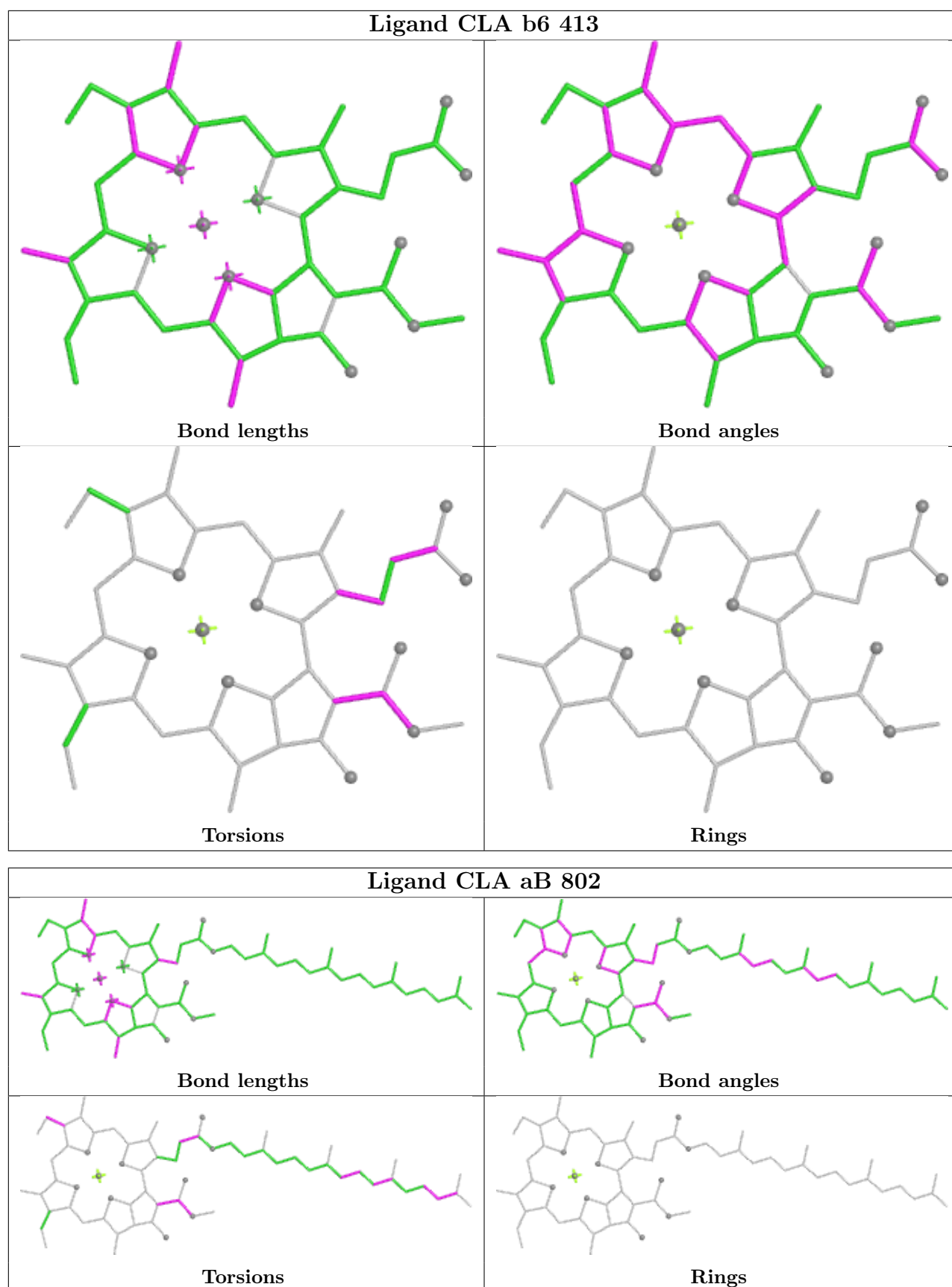


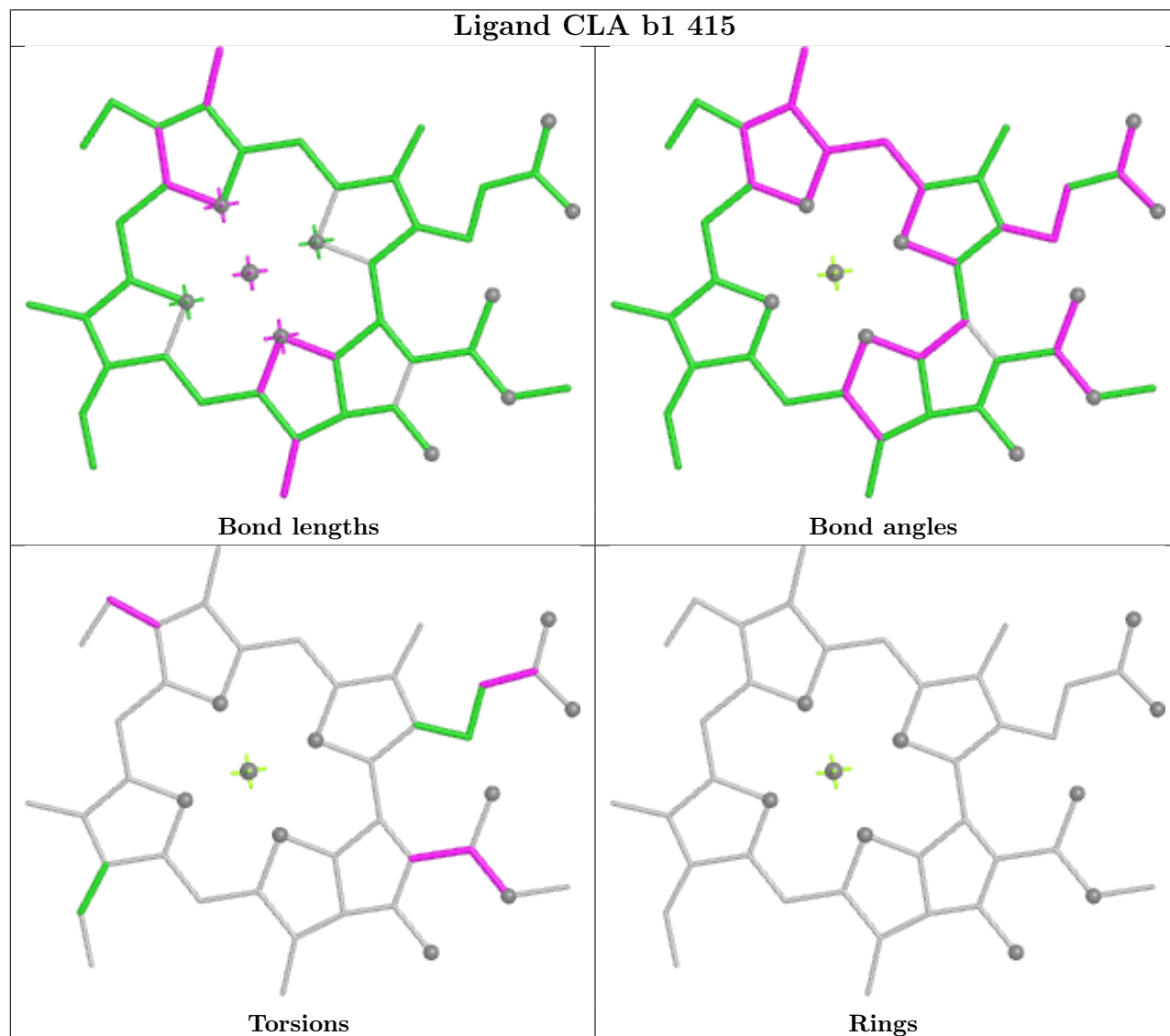
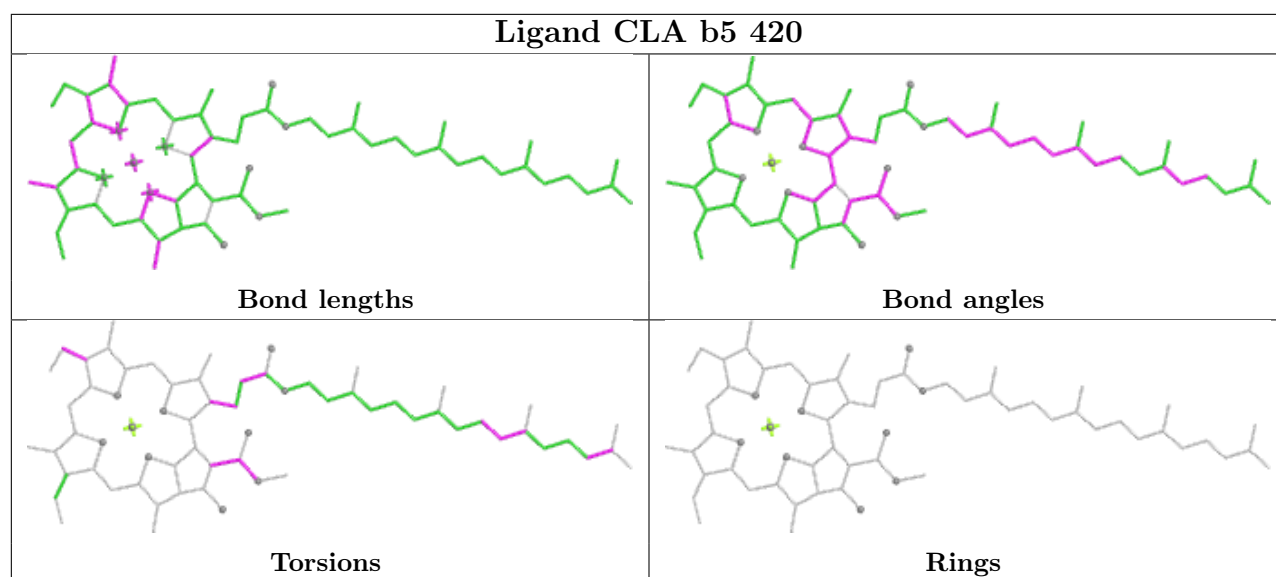


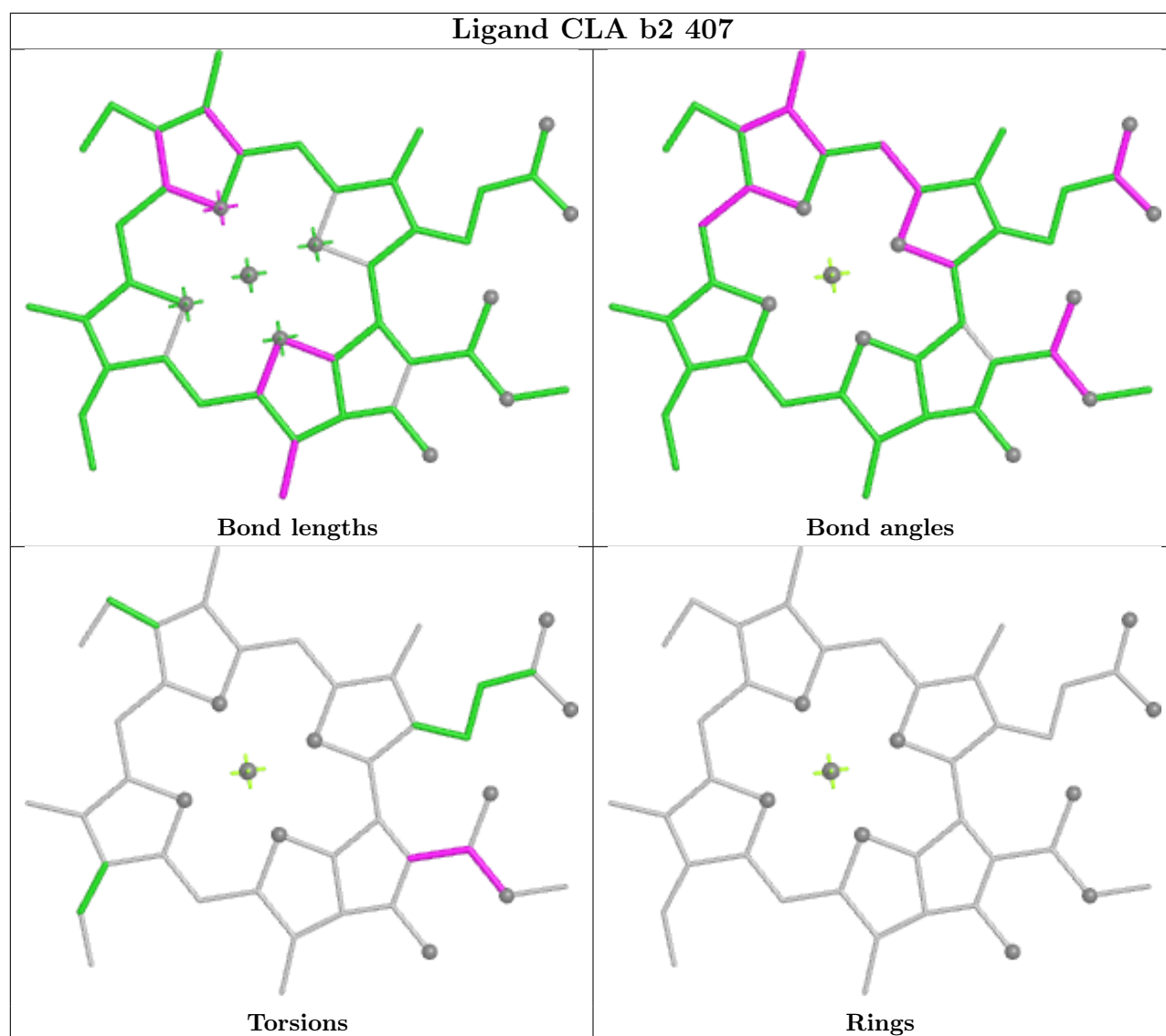


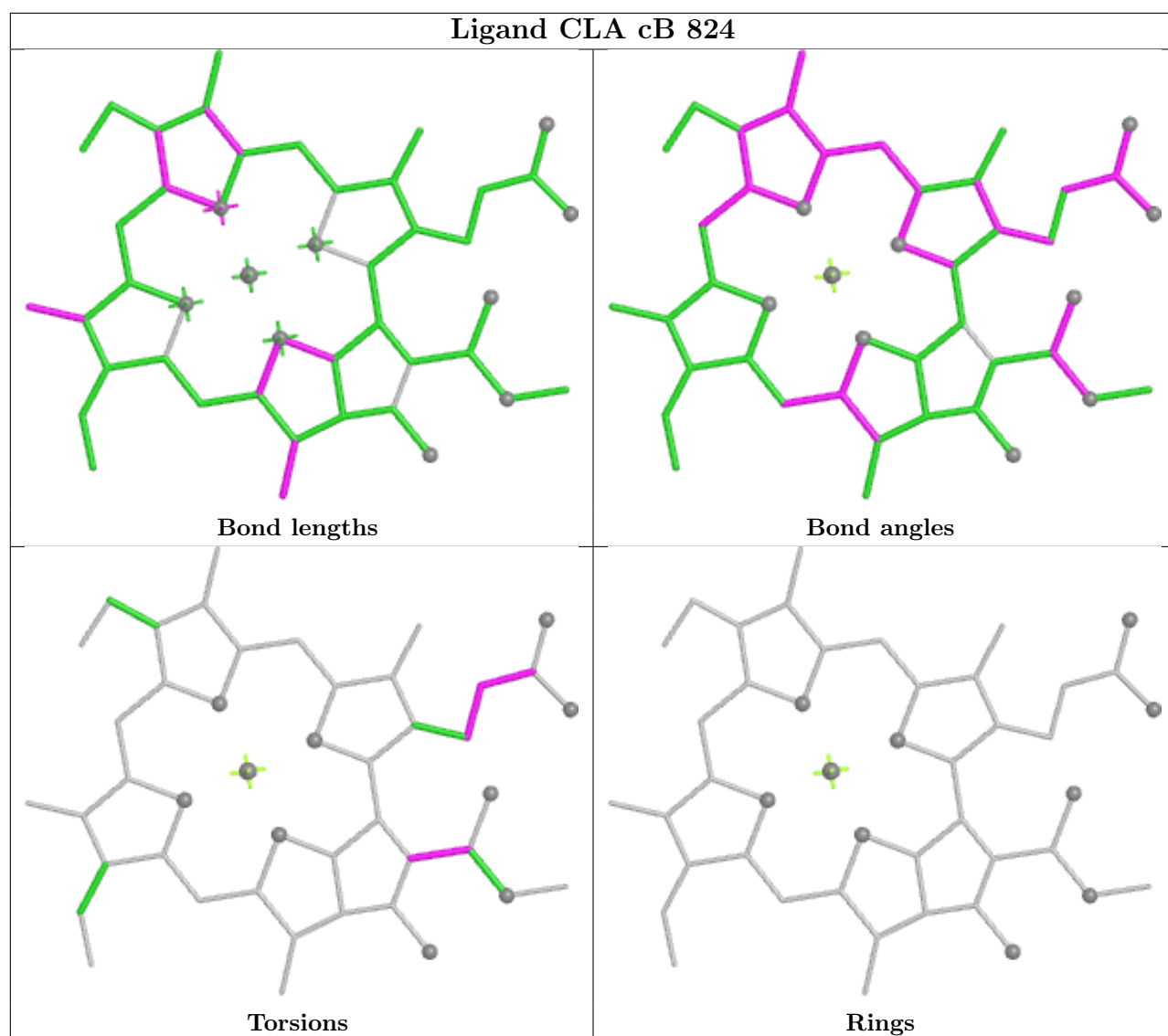




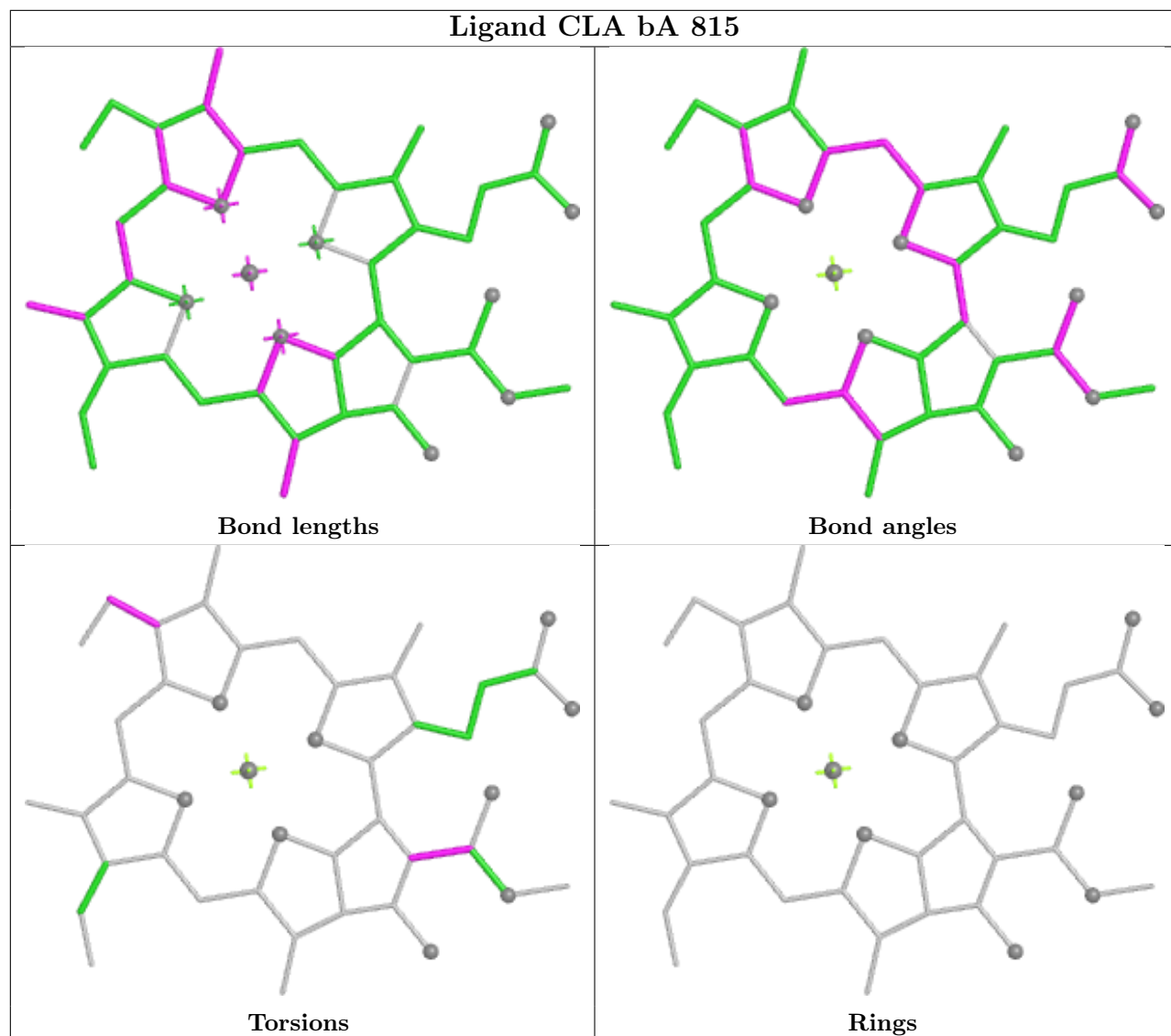


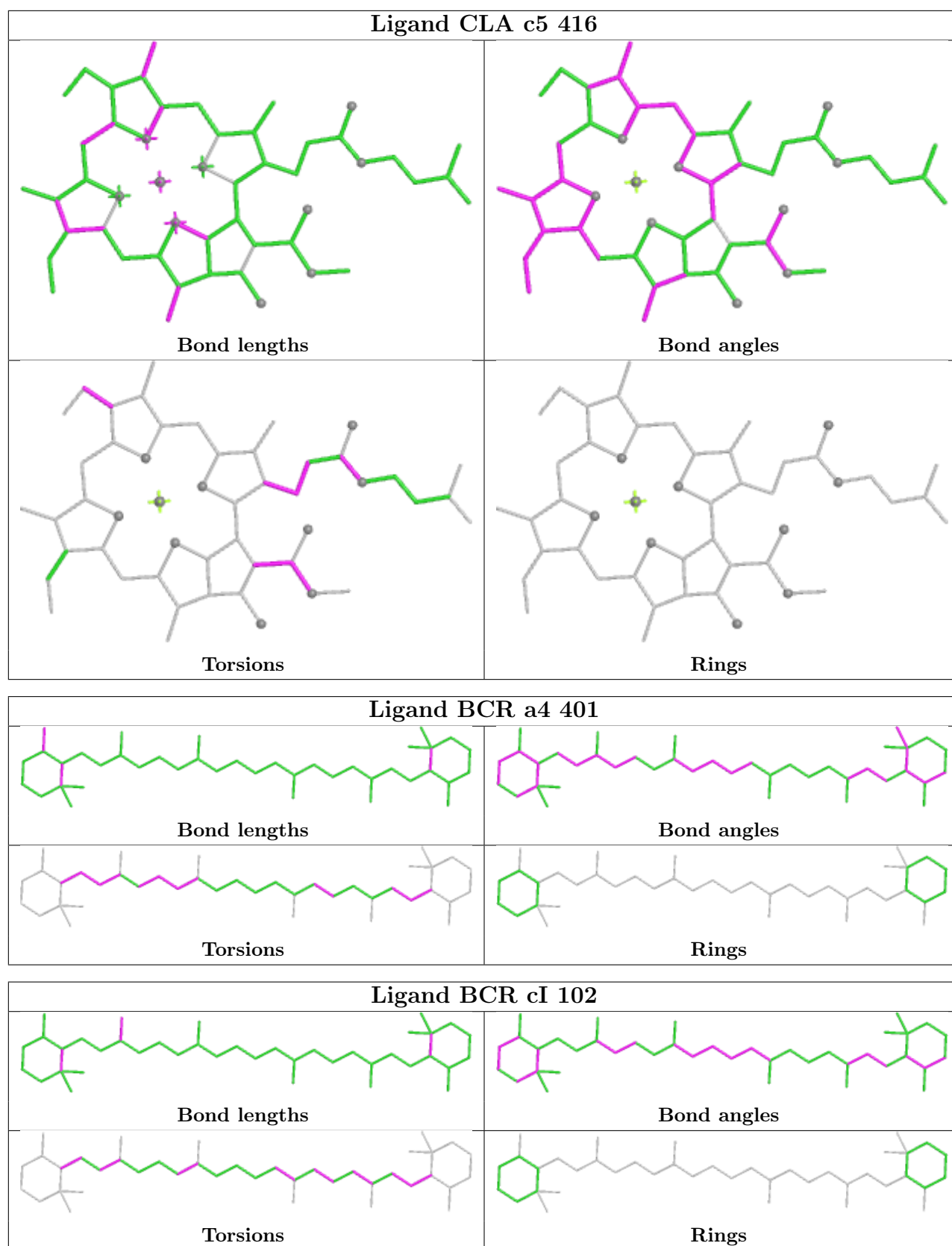


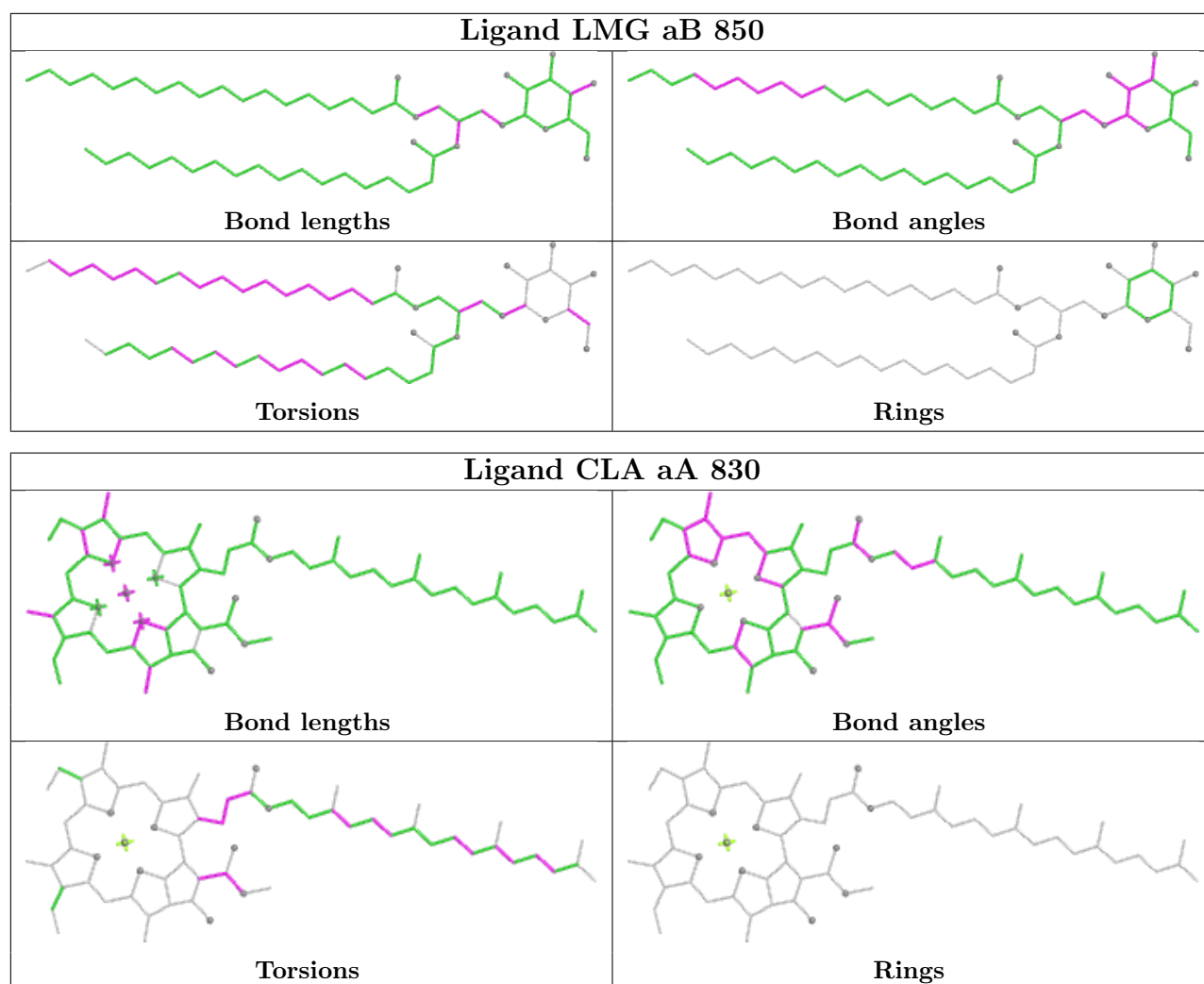


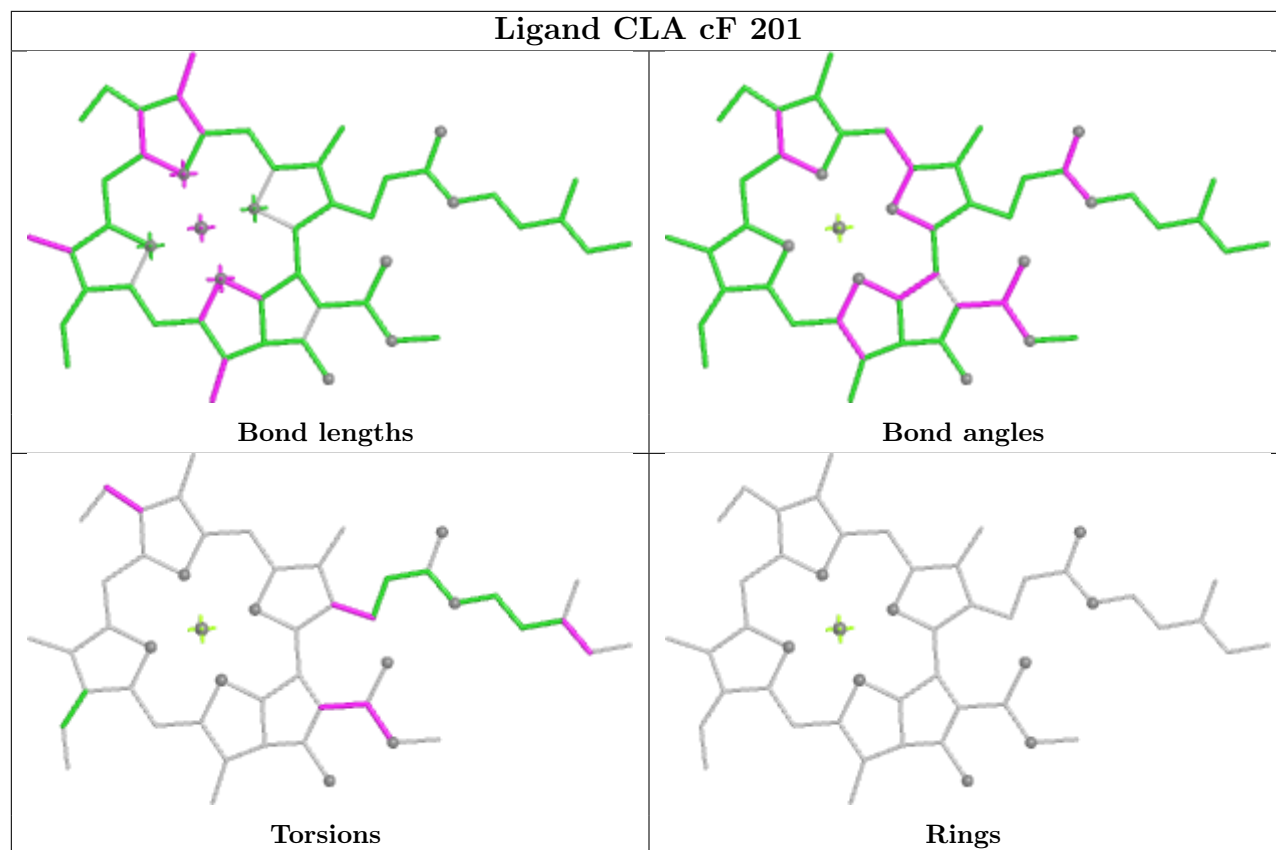


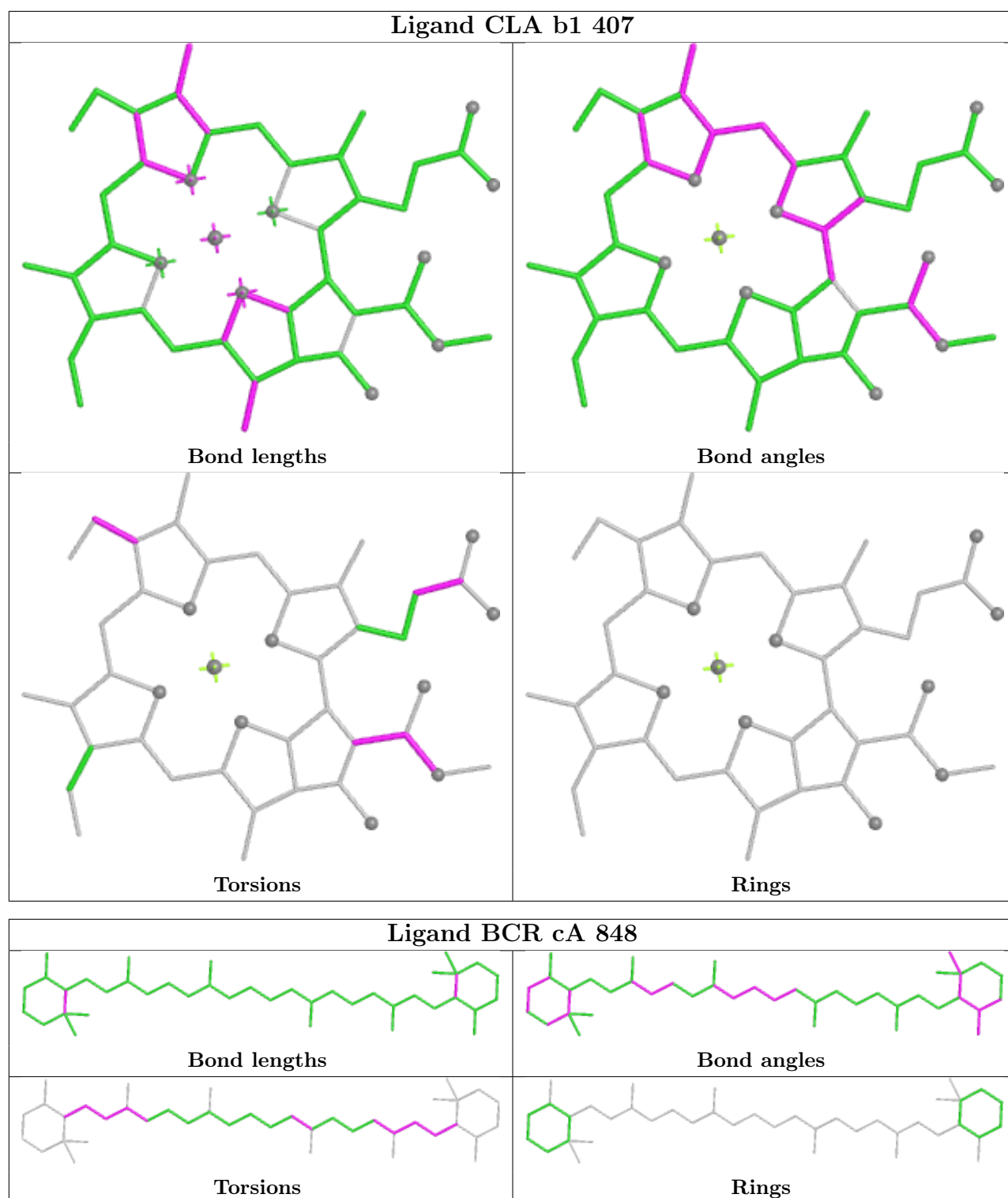
Ligand CLA bA 815

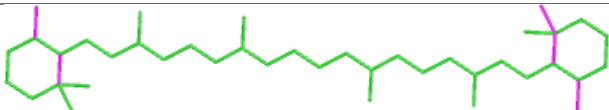
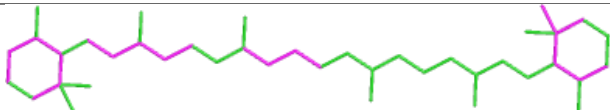
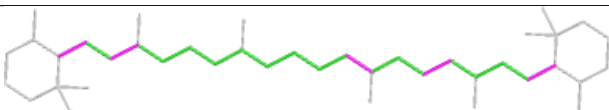
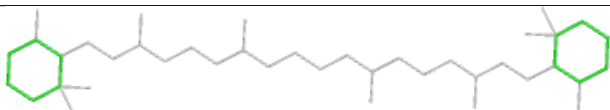


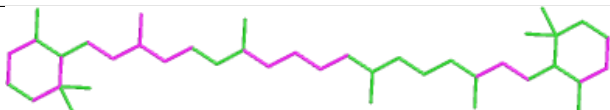
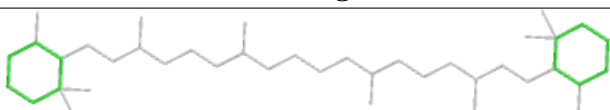


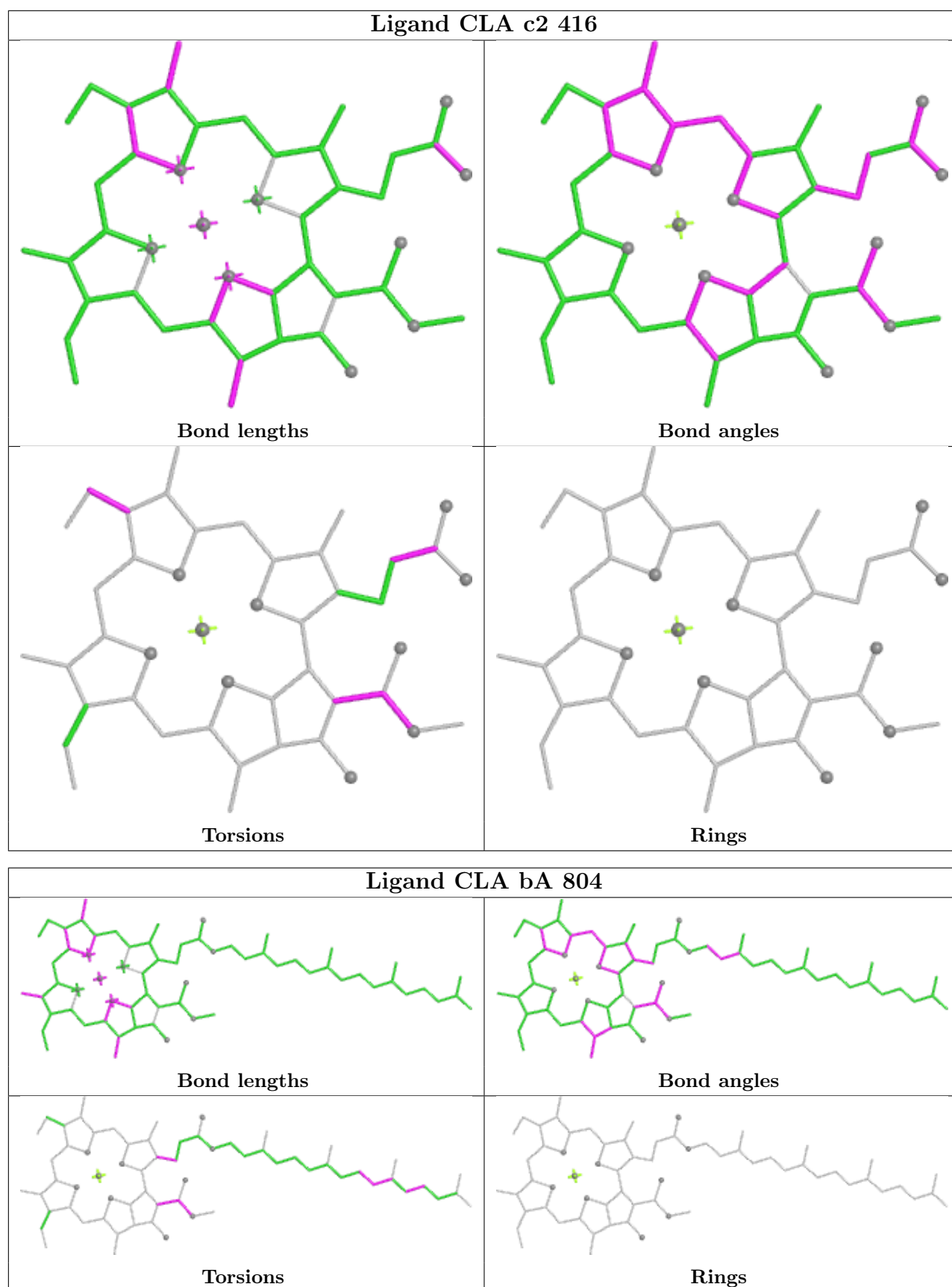


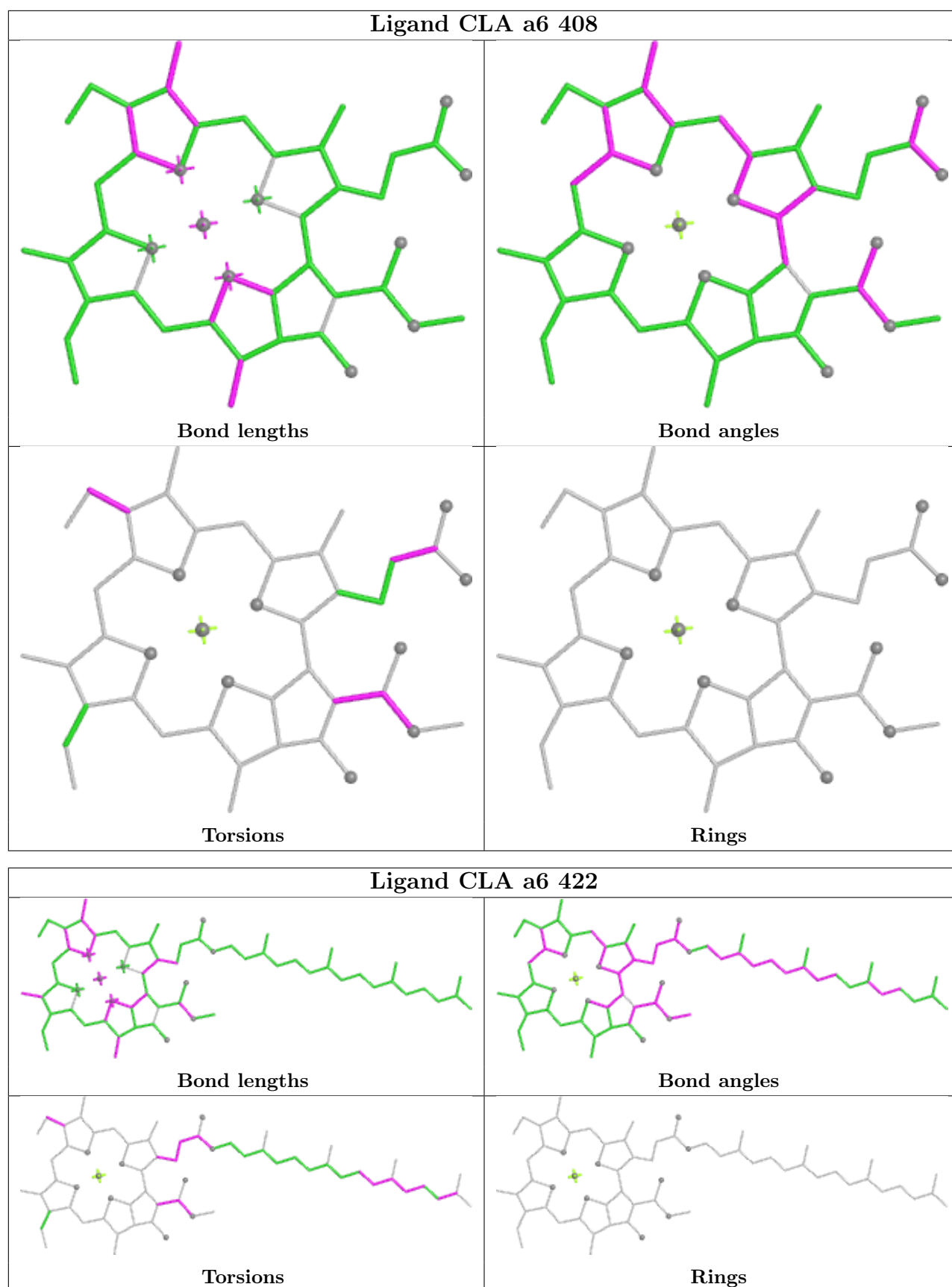


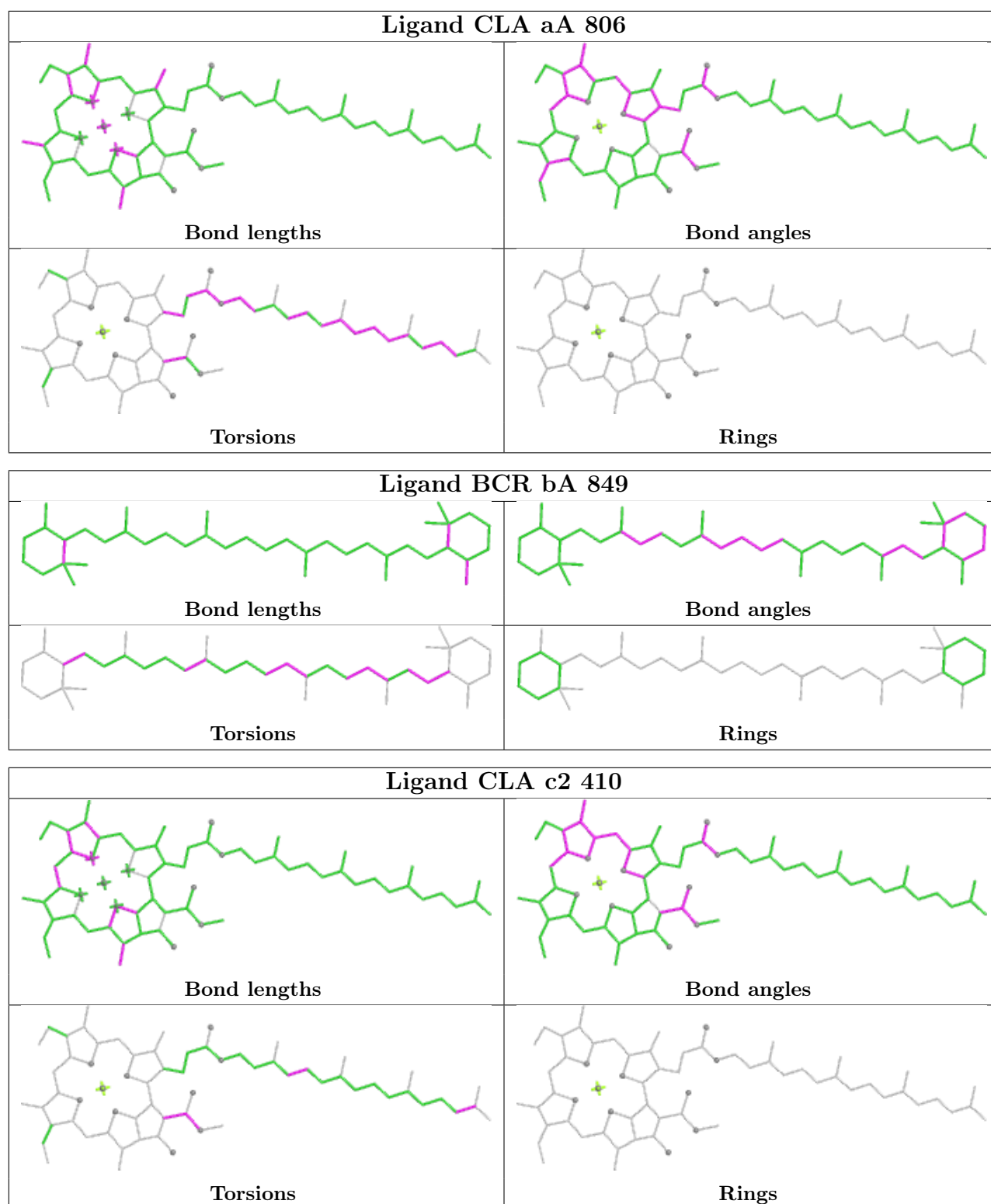


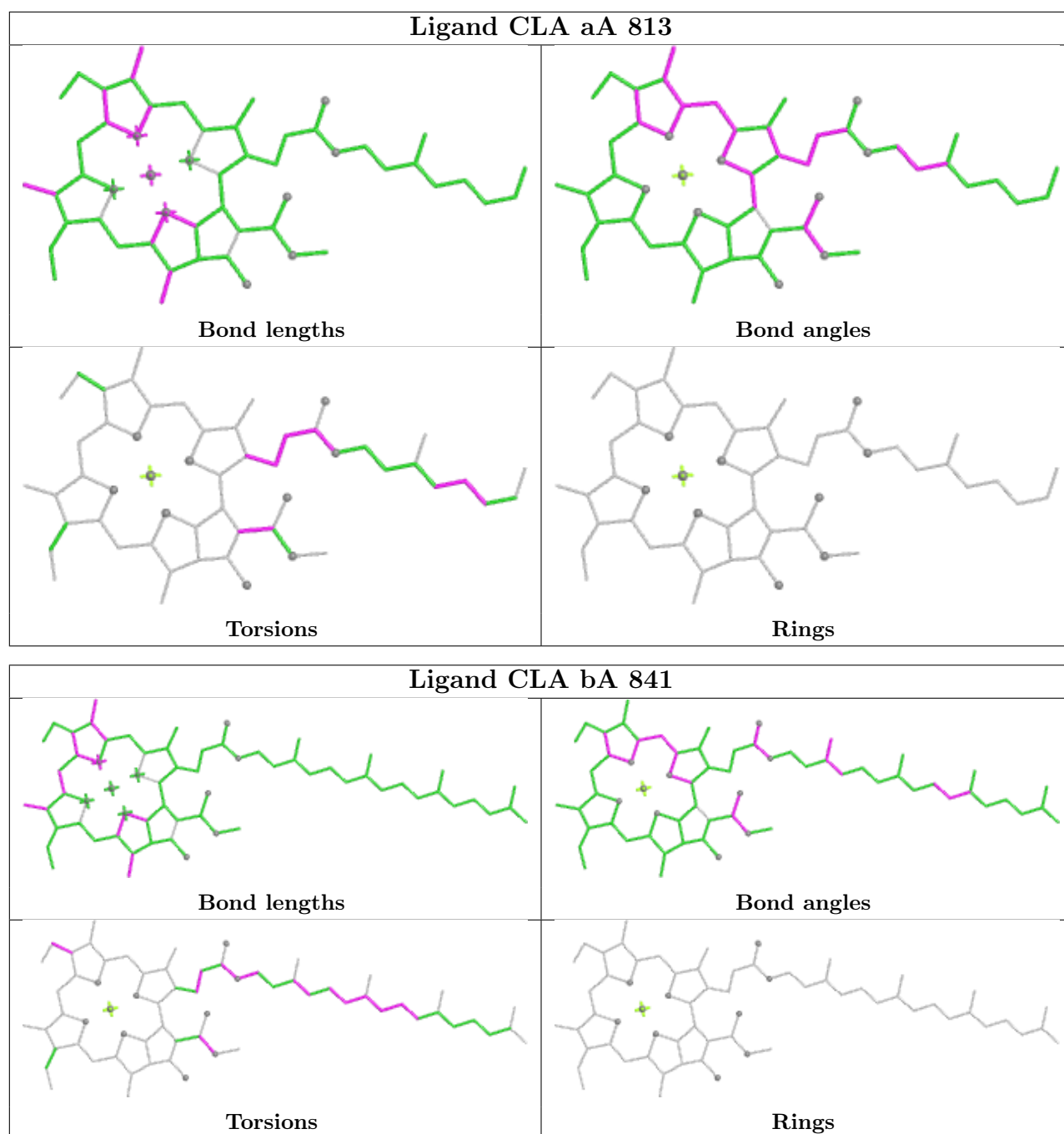
Ligand BCR c1 418			
	Bond lengths		
	Torsions		
Rings			

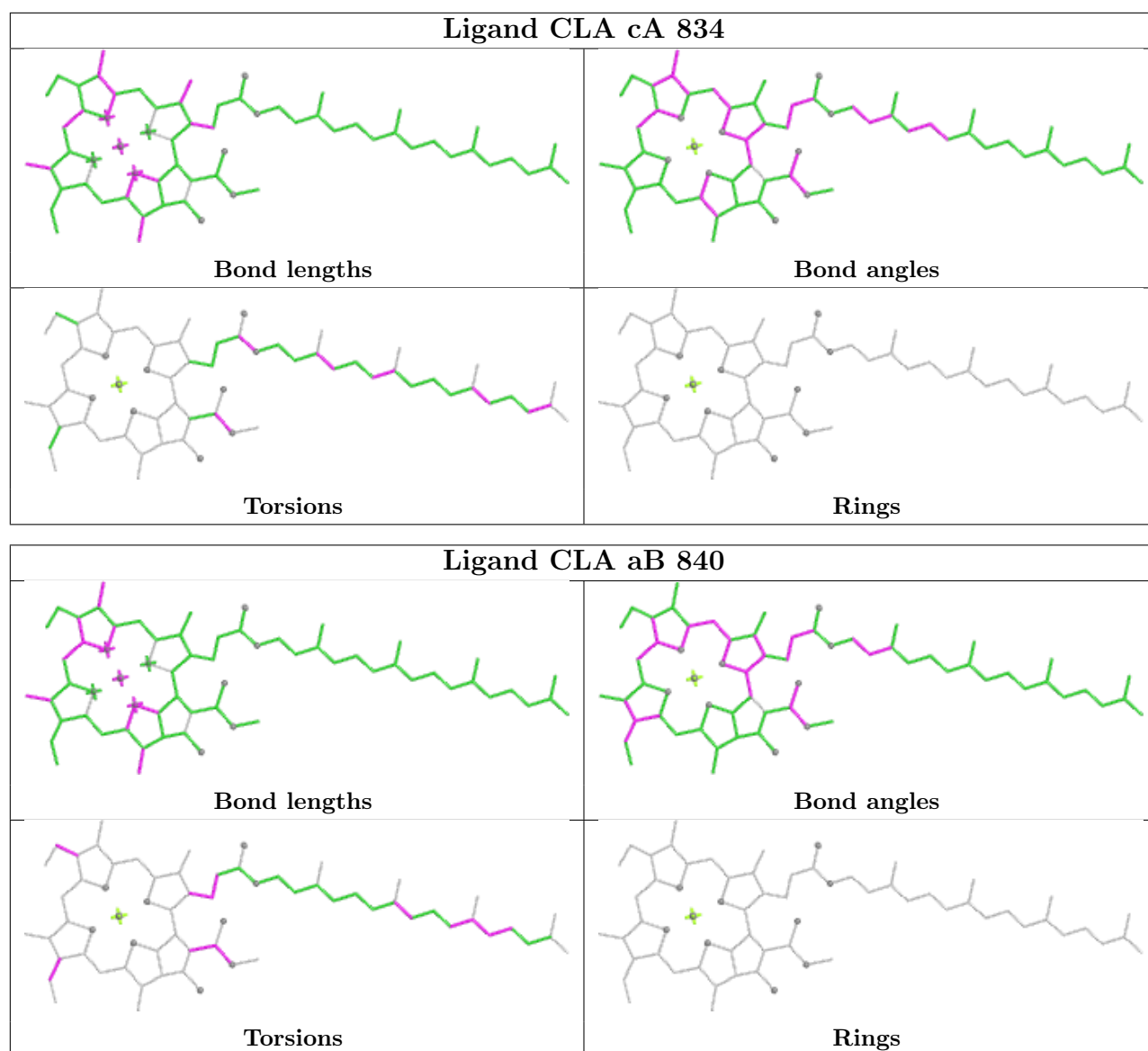
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	Torsions		
Rings			

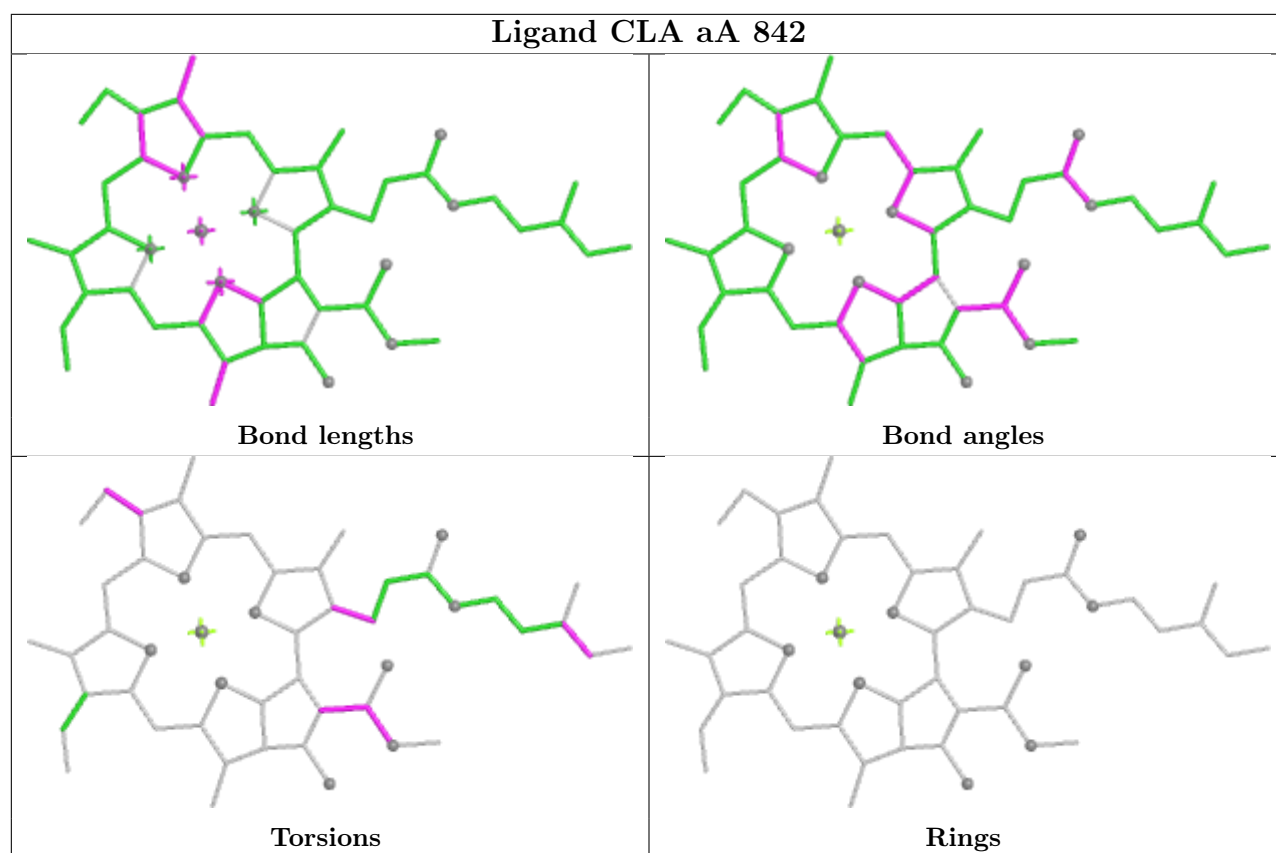


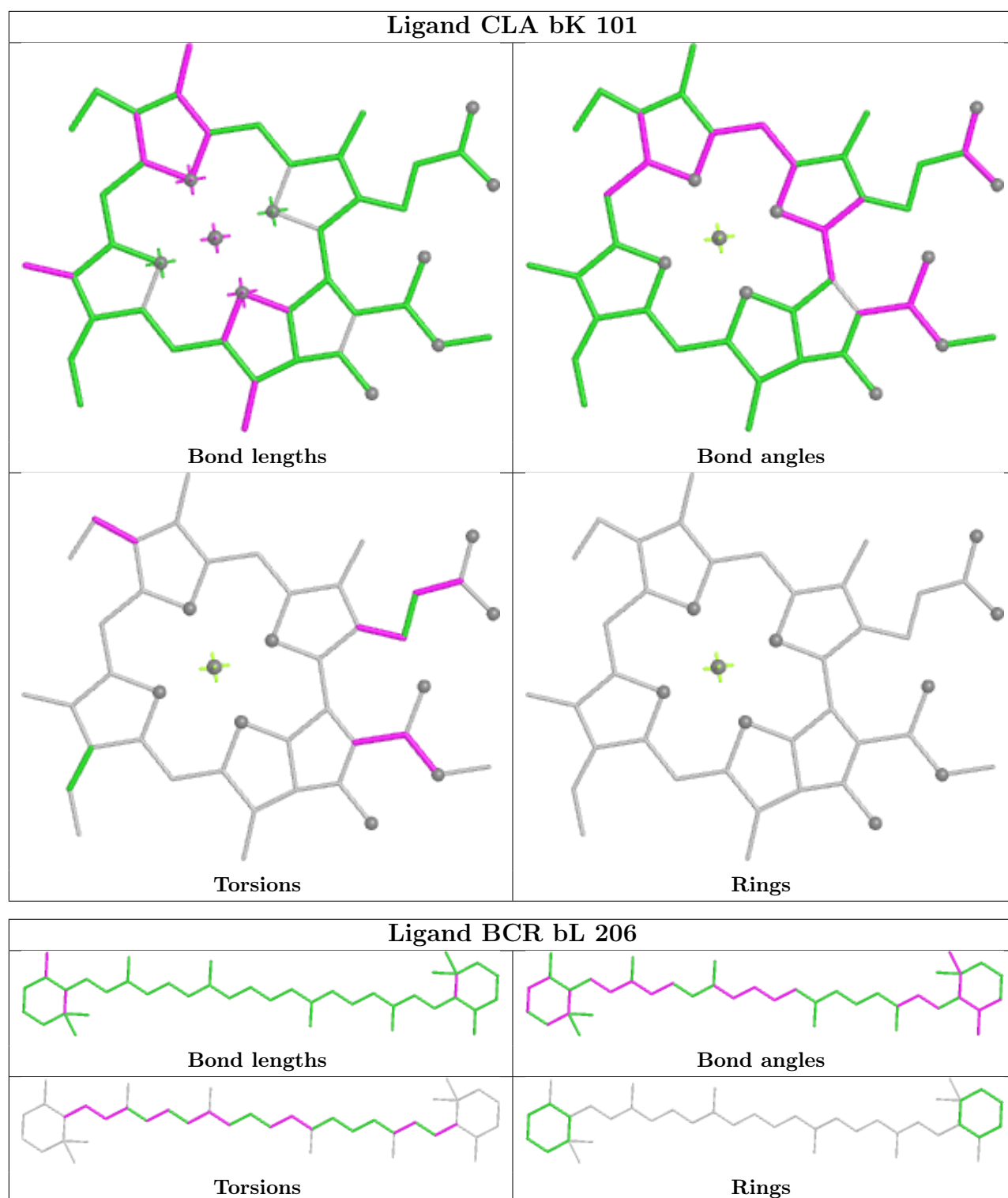


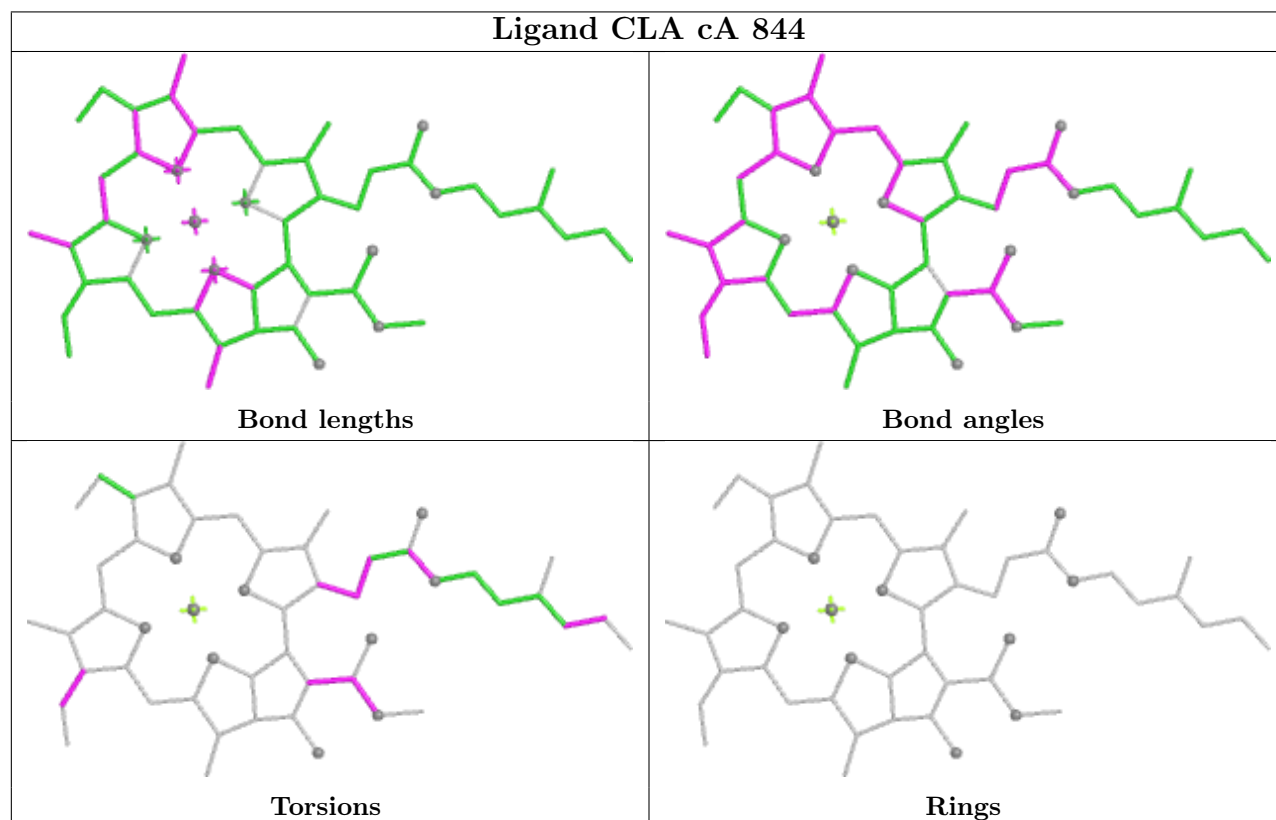
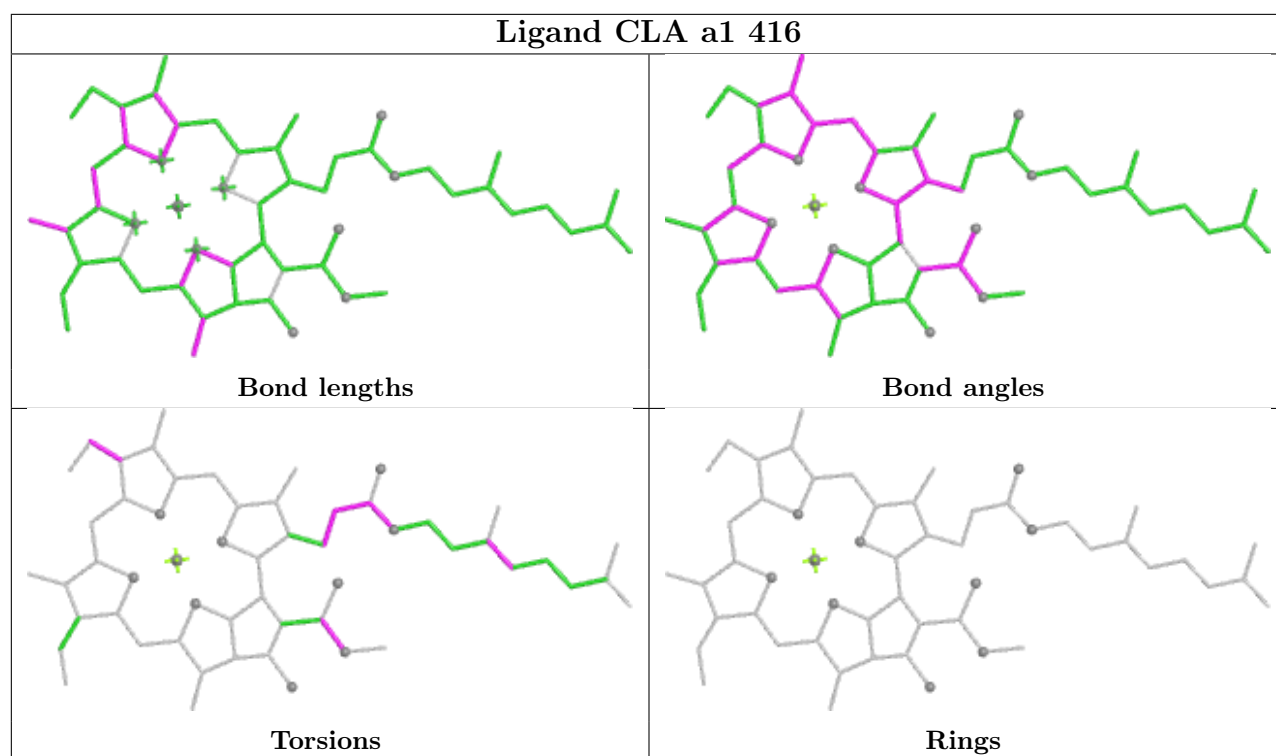


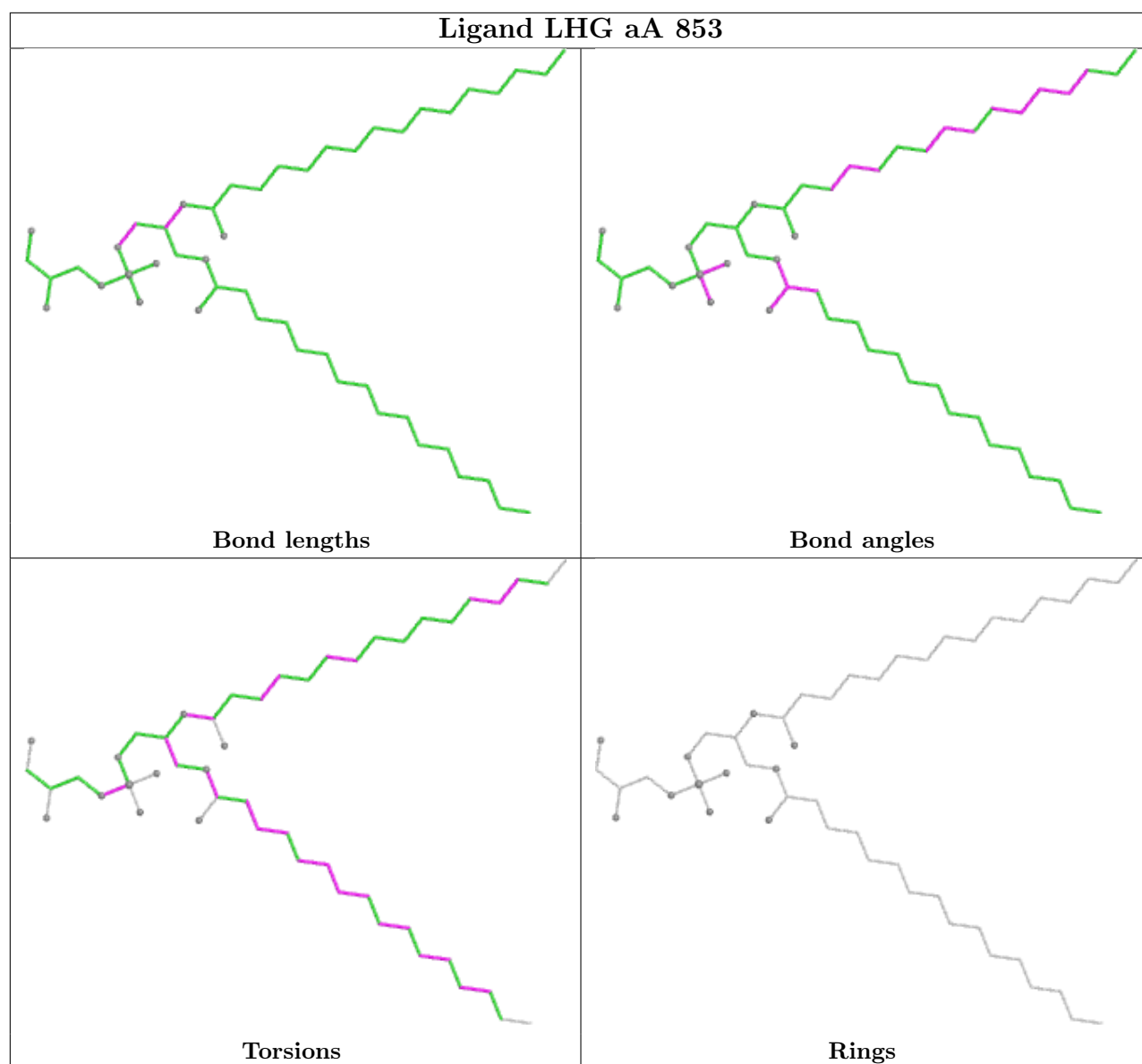


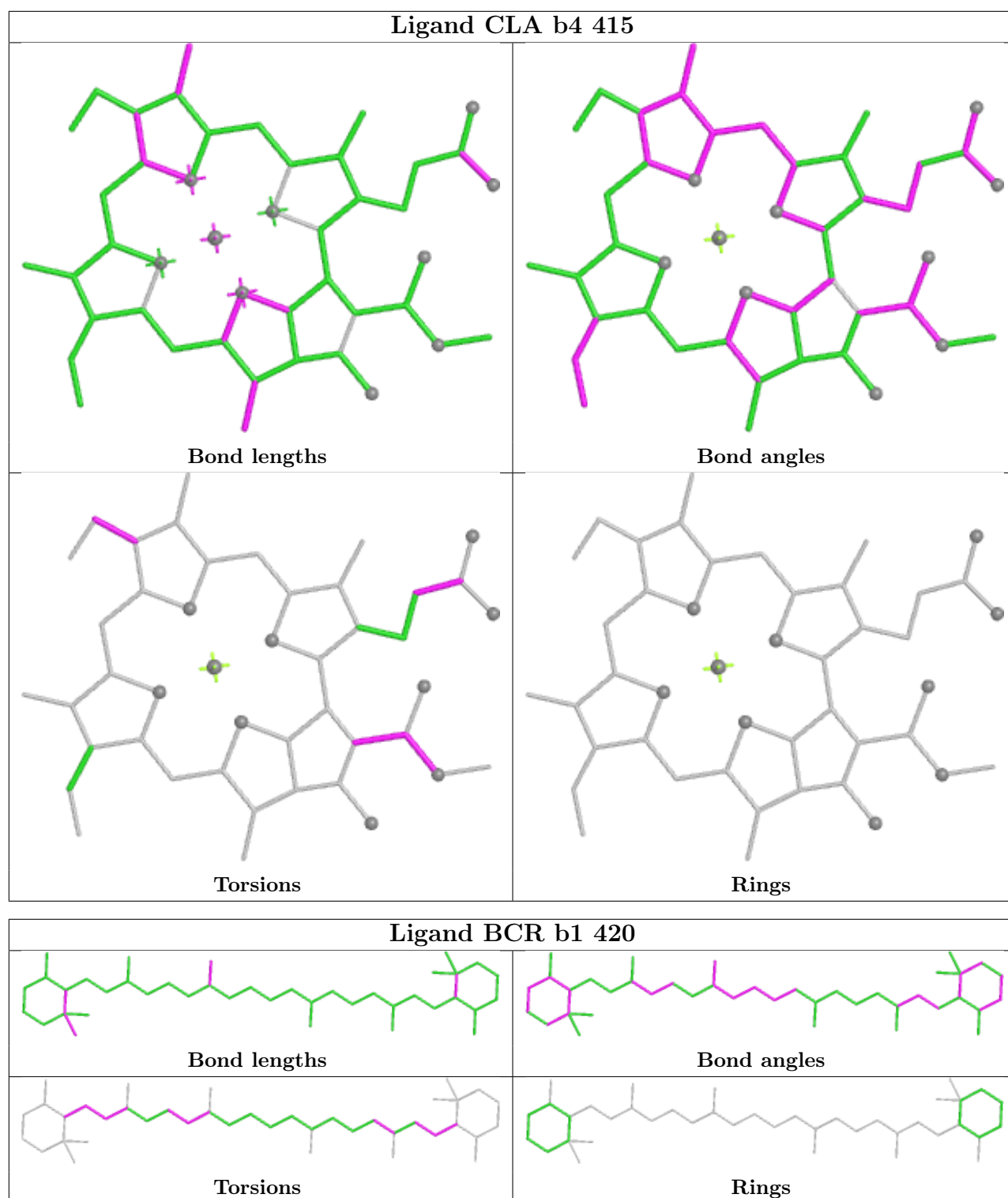


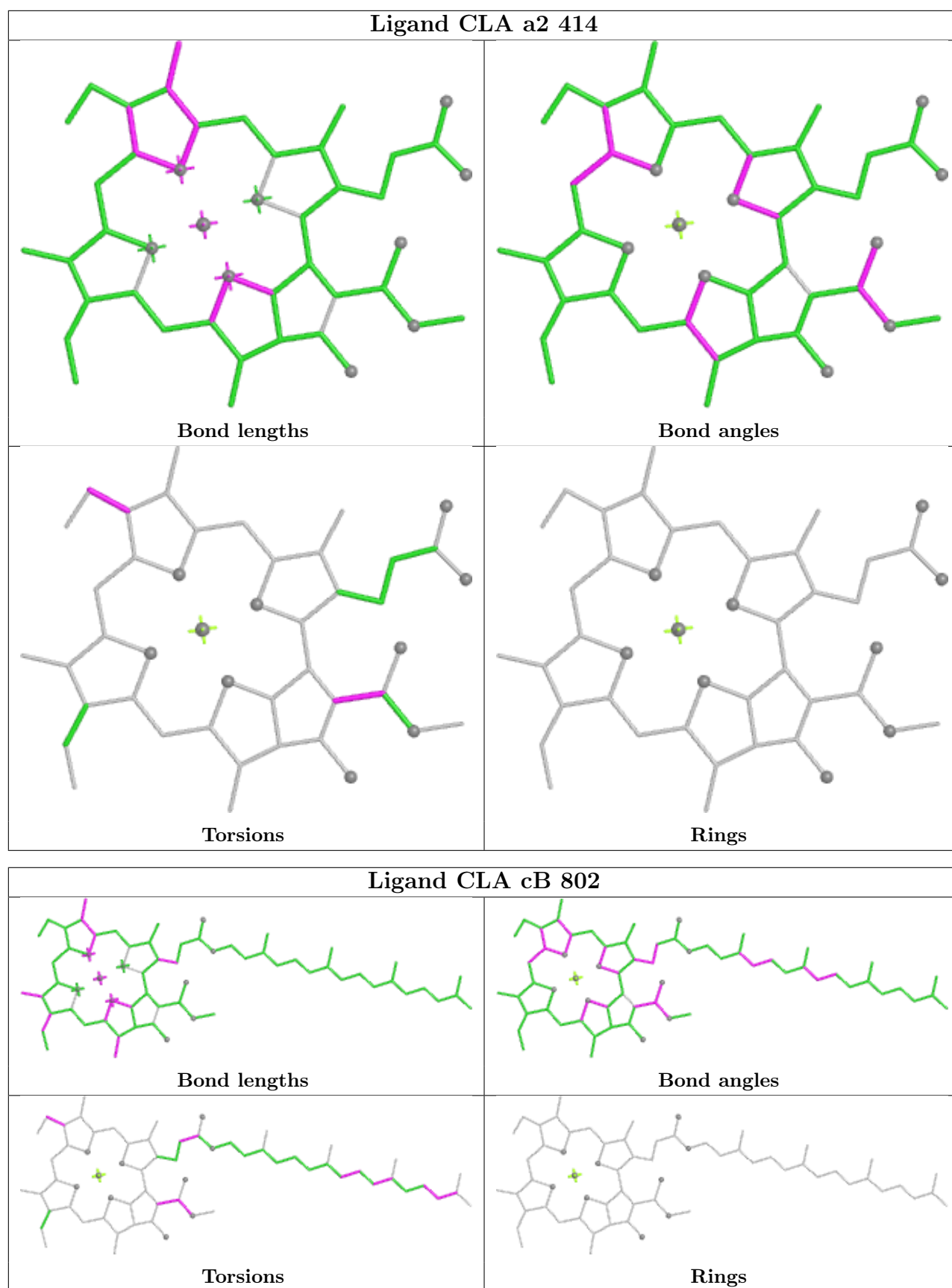


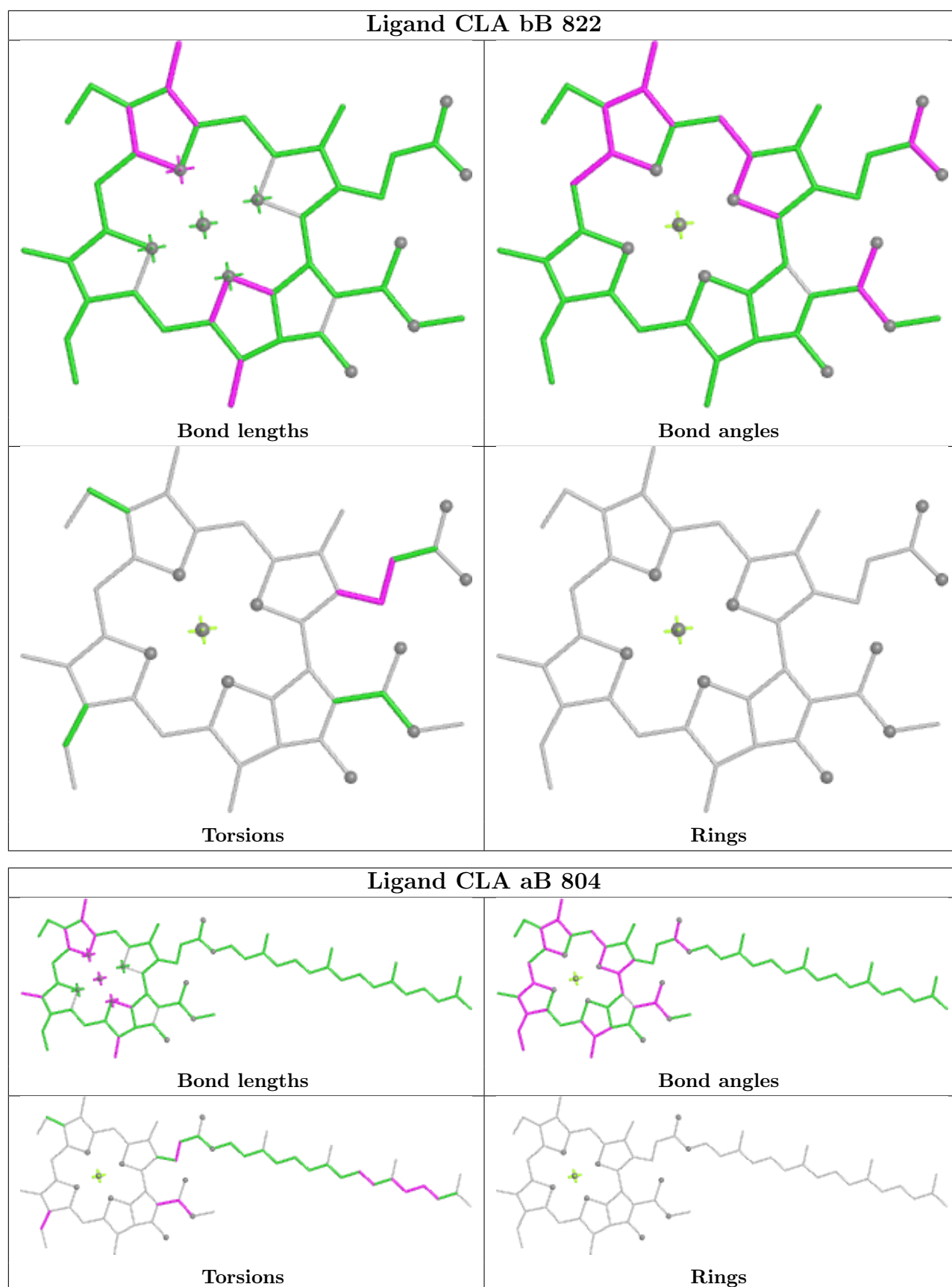


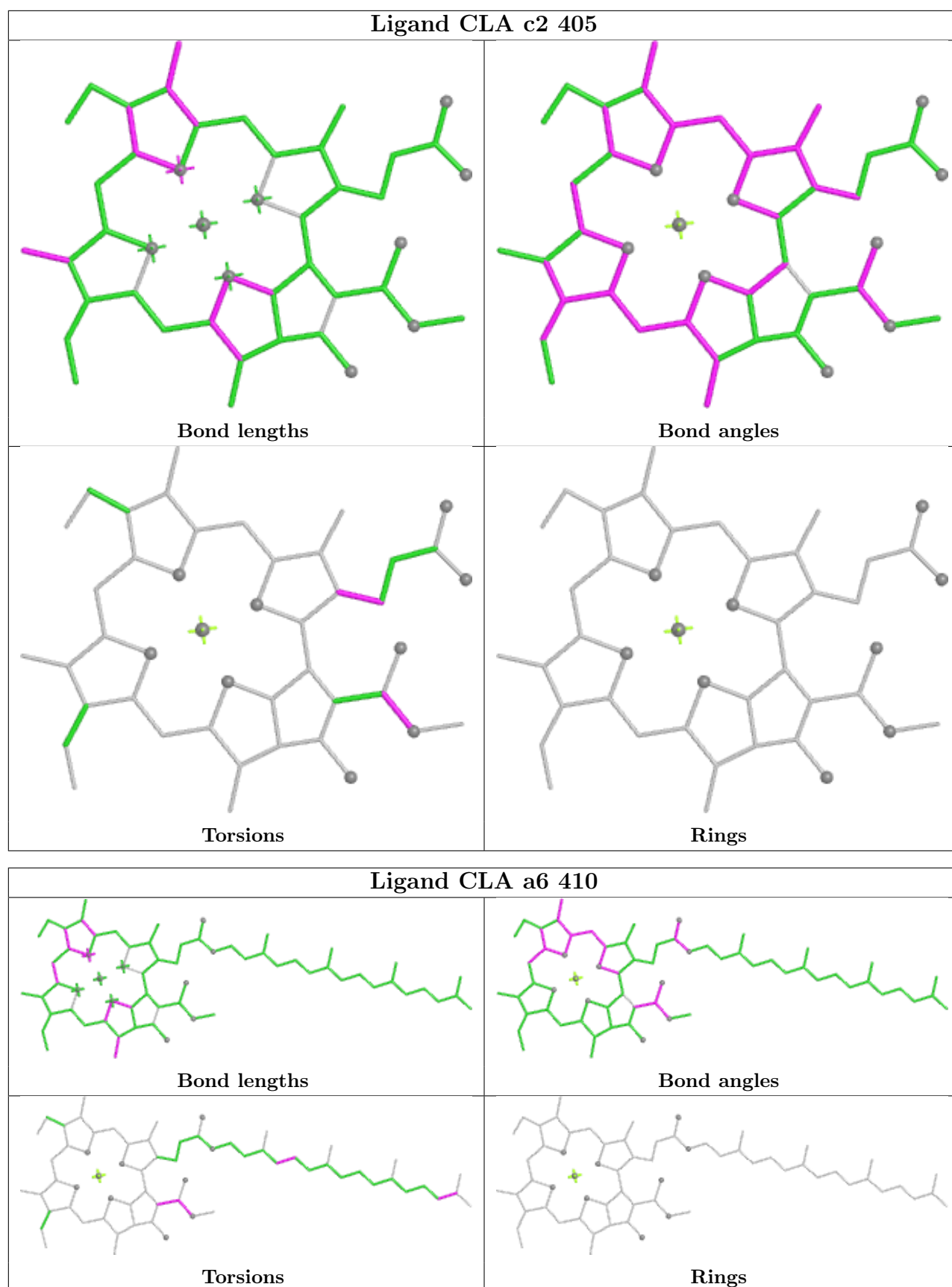


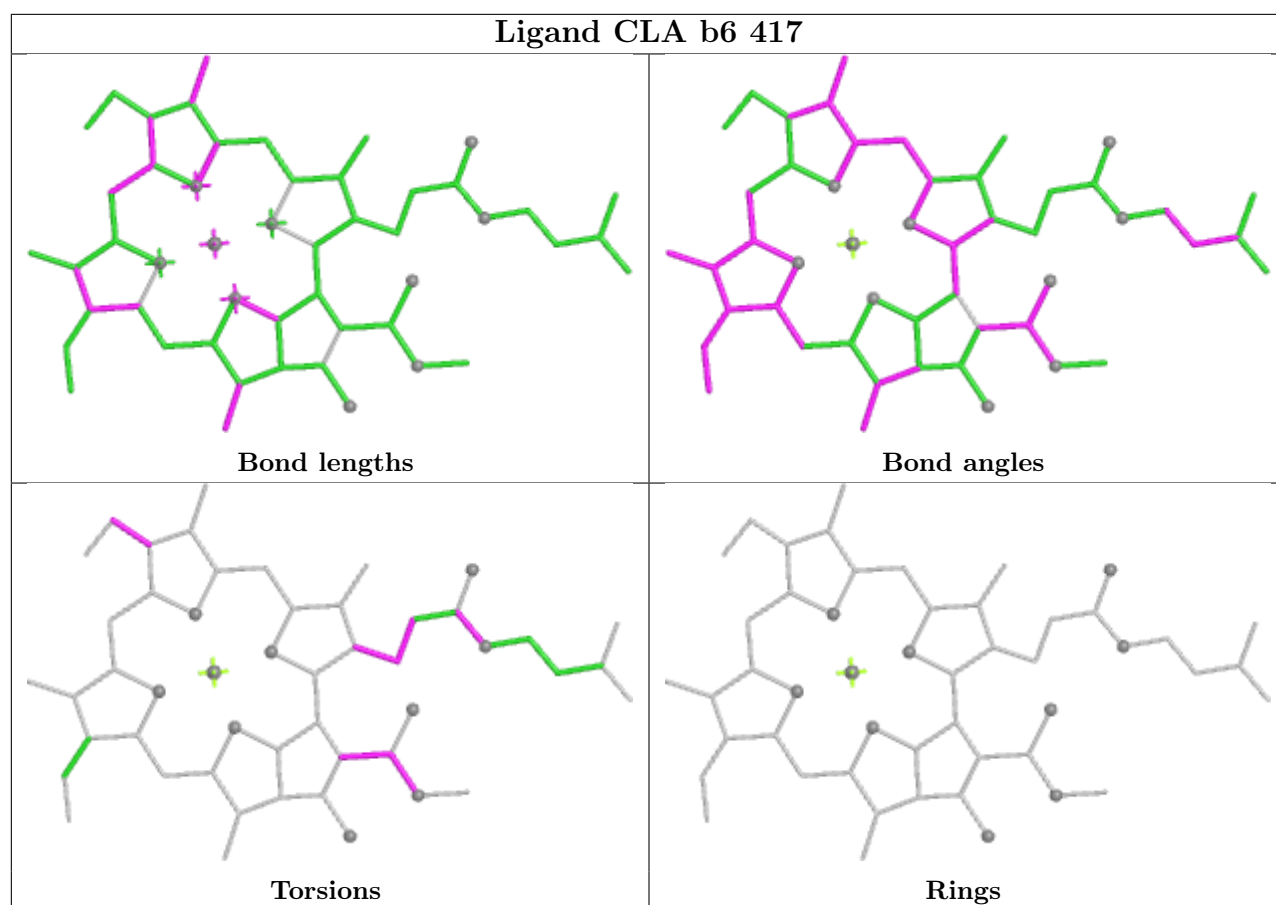


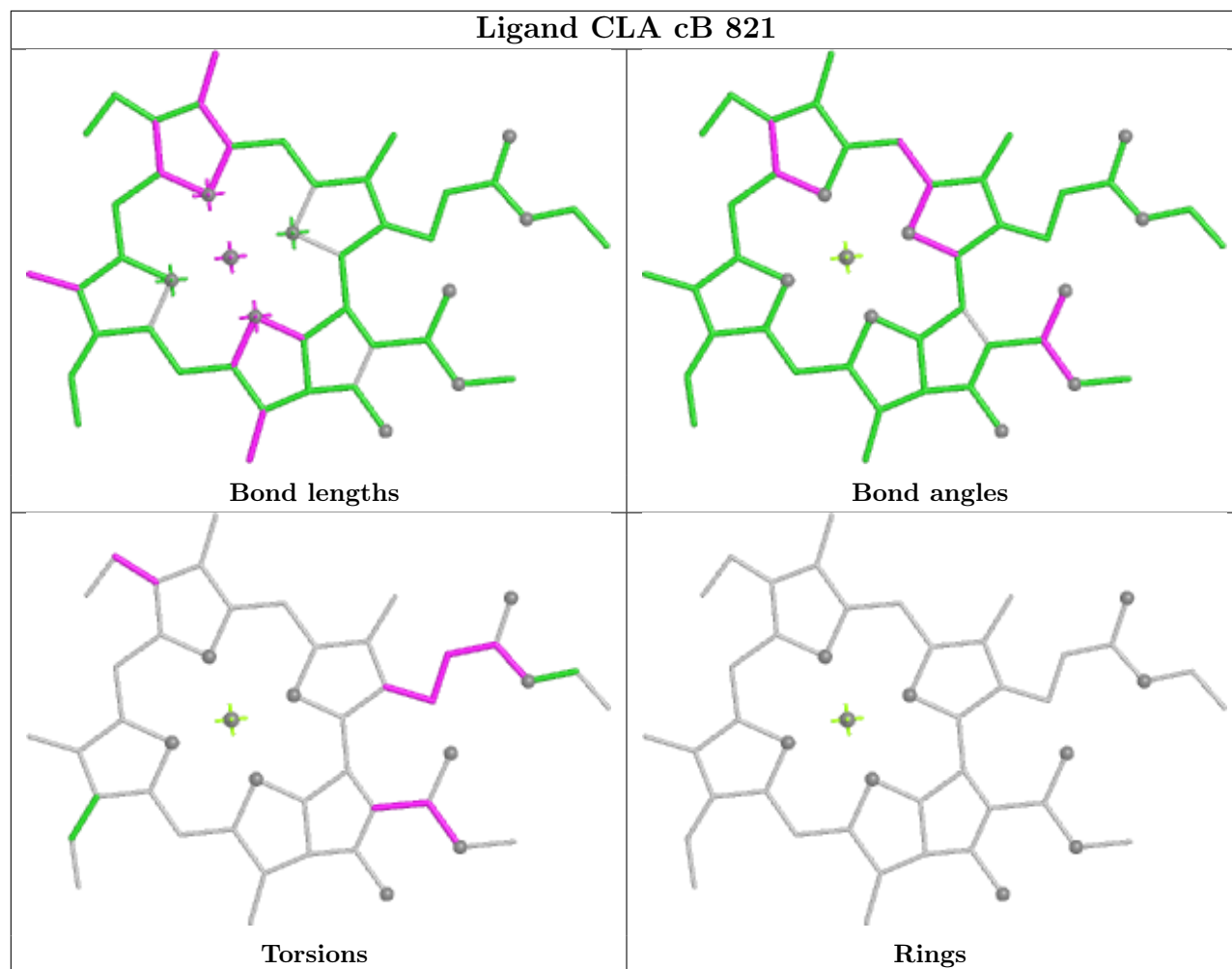


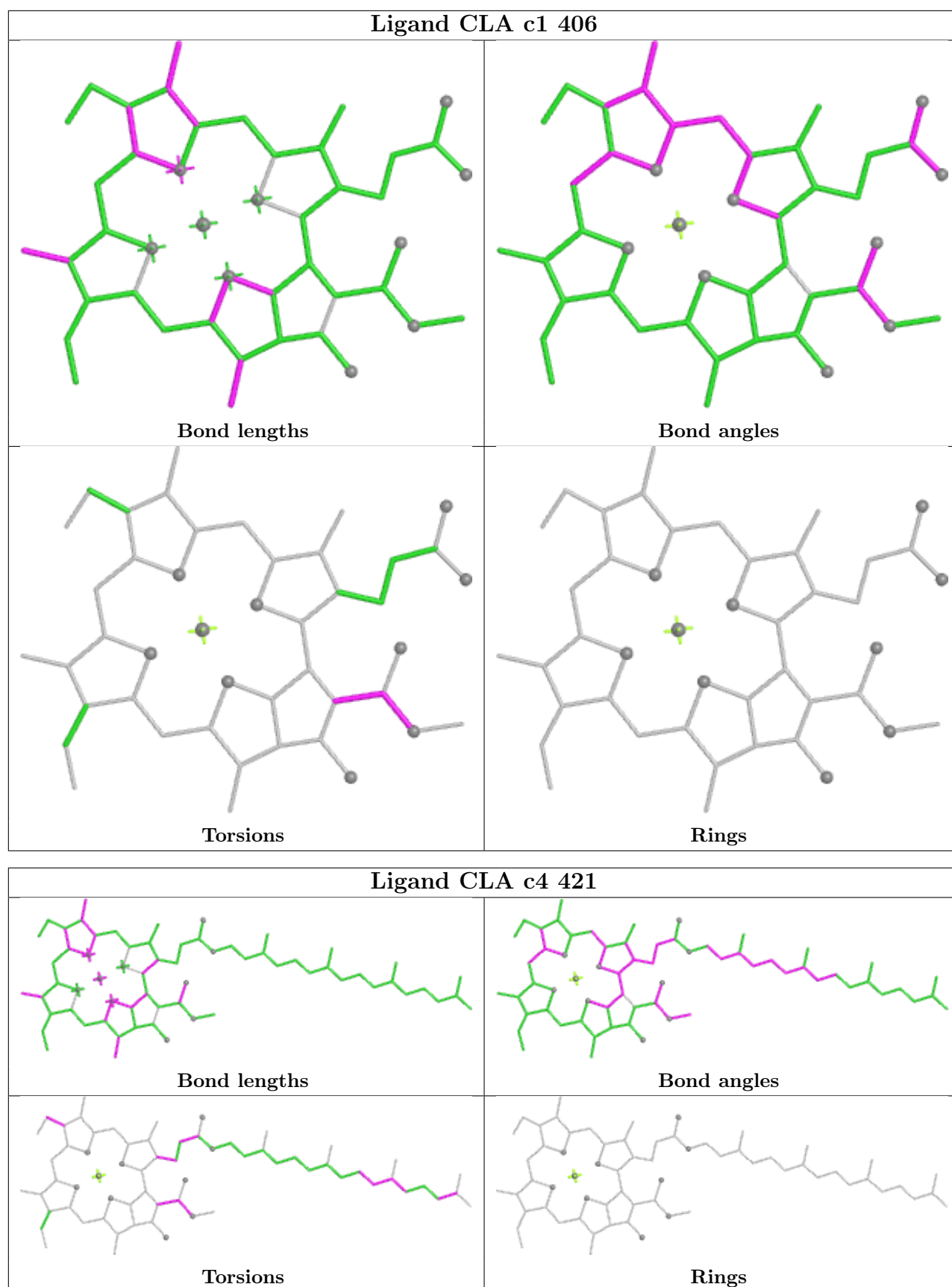


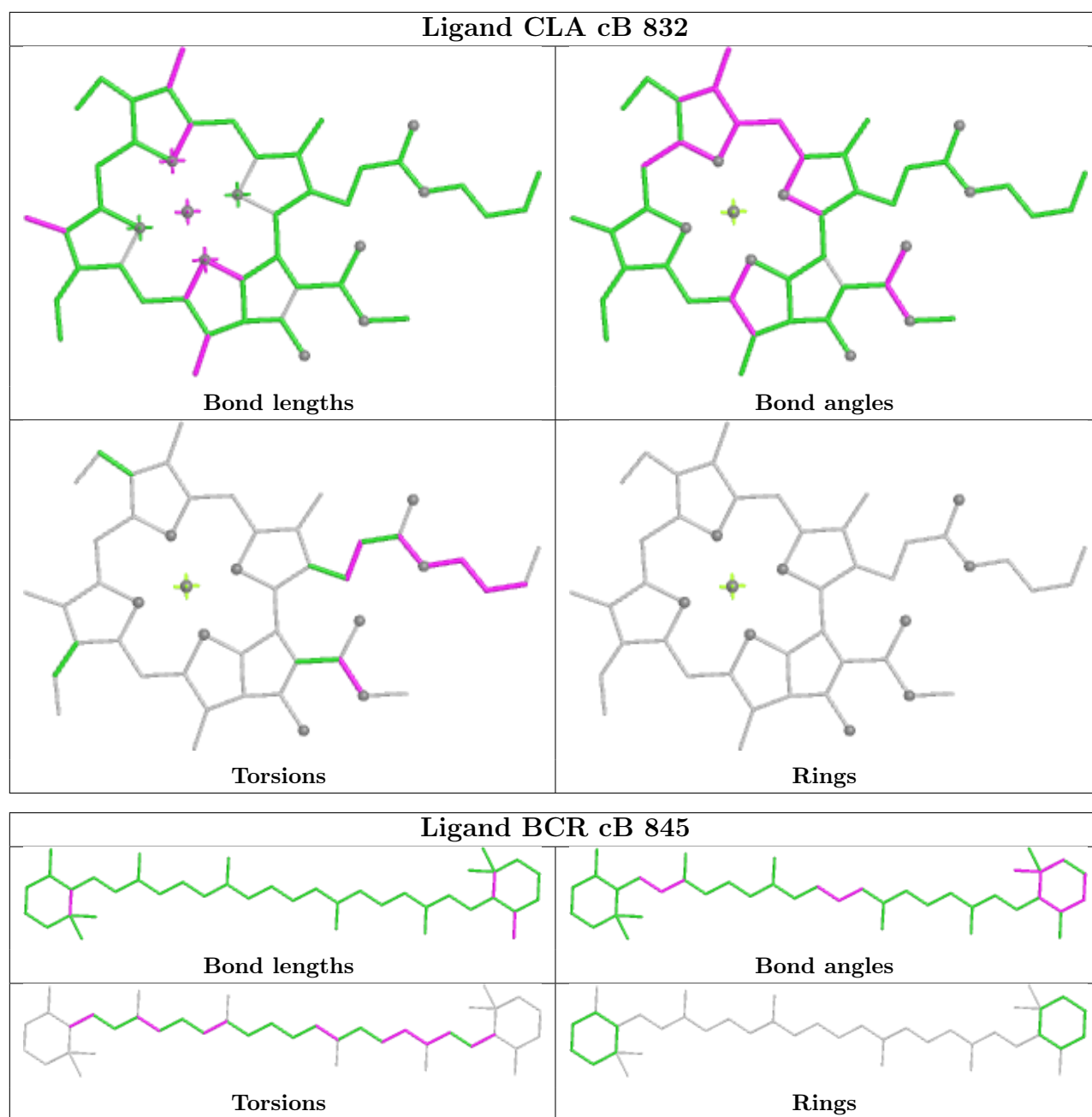


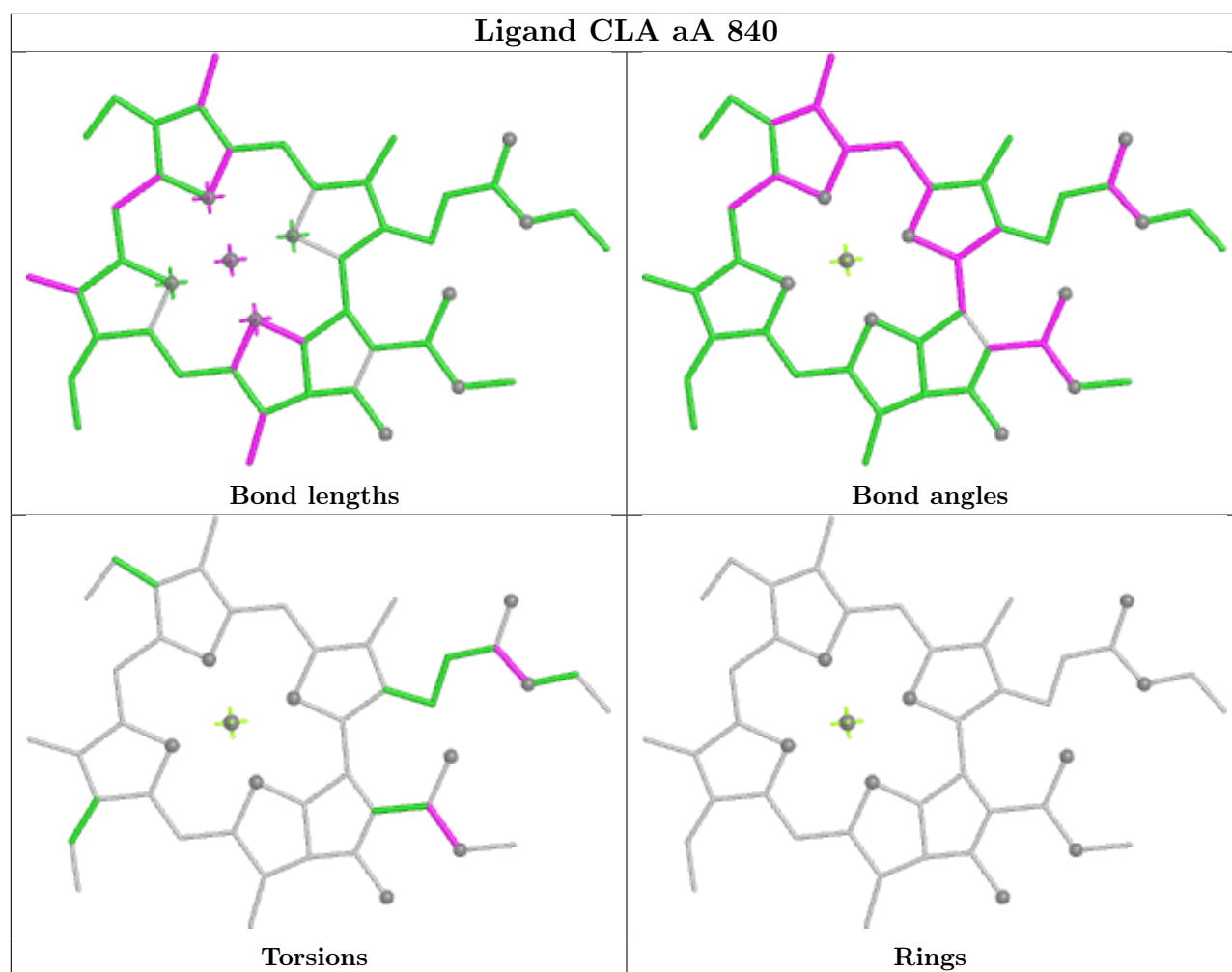


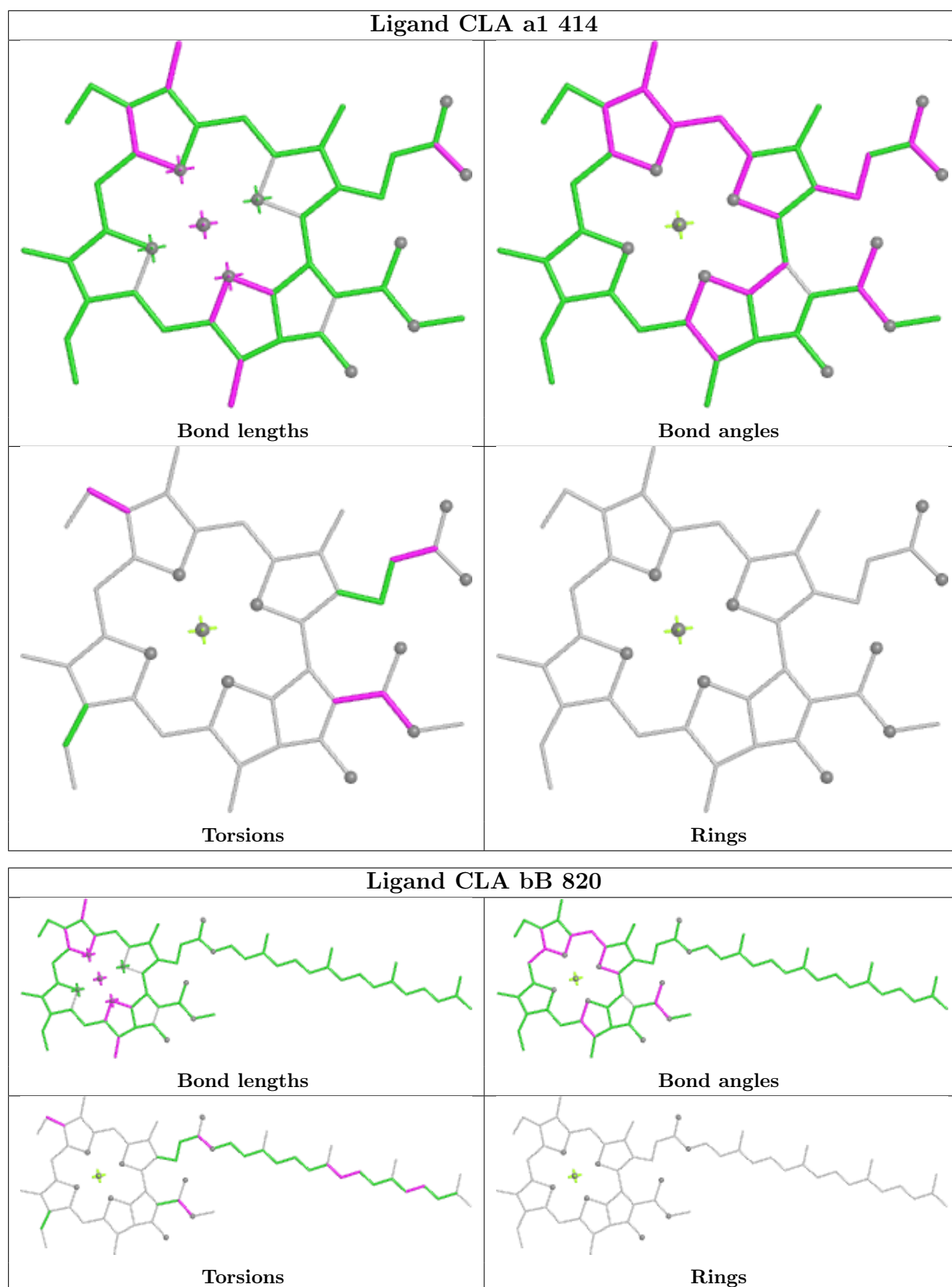


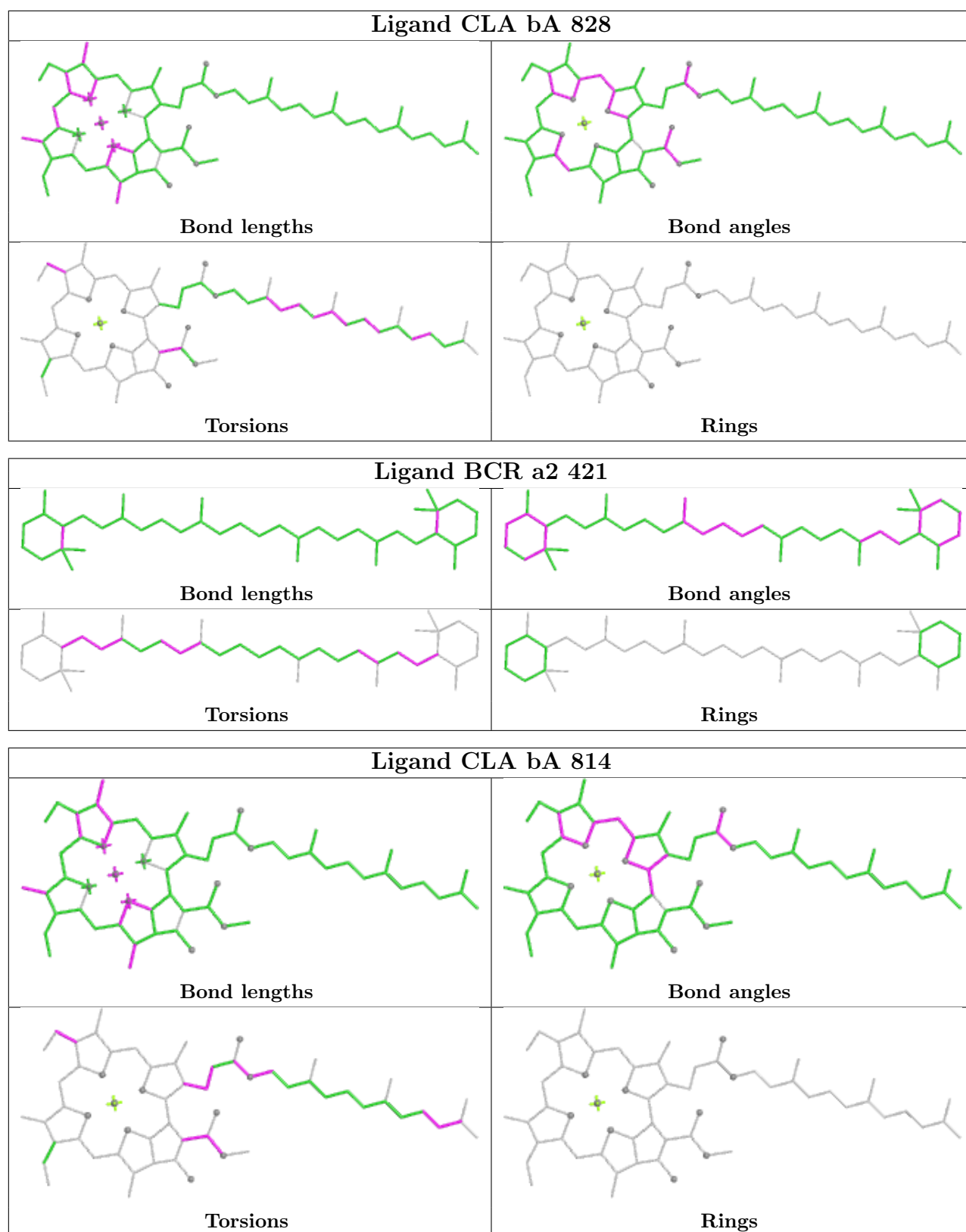


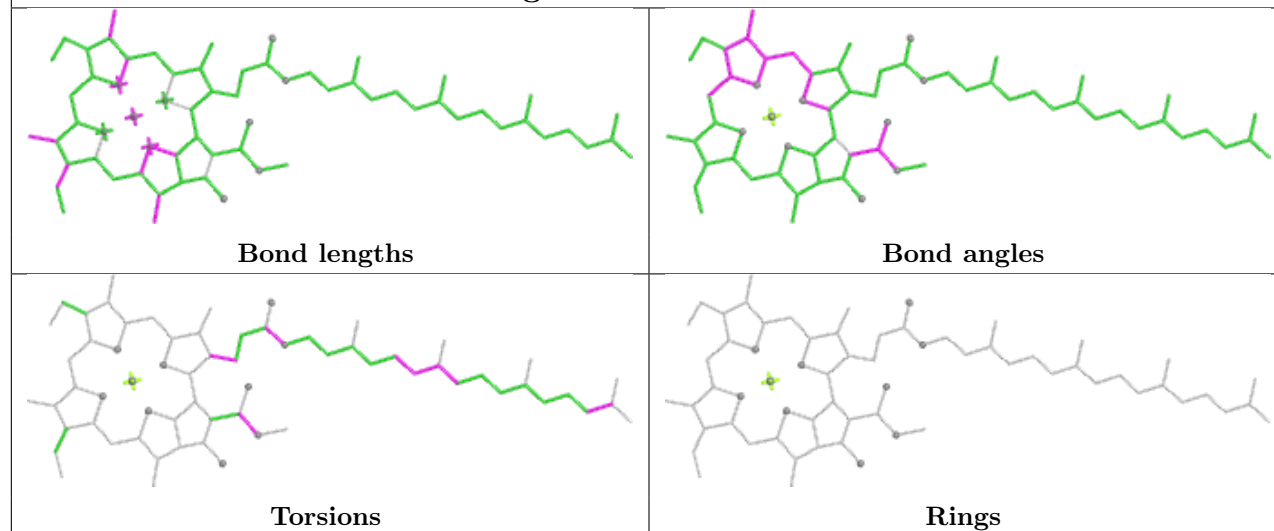
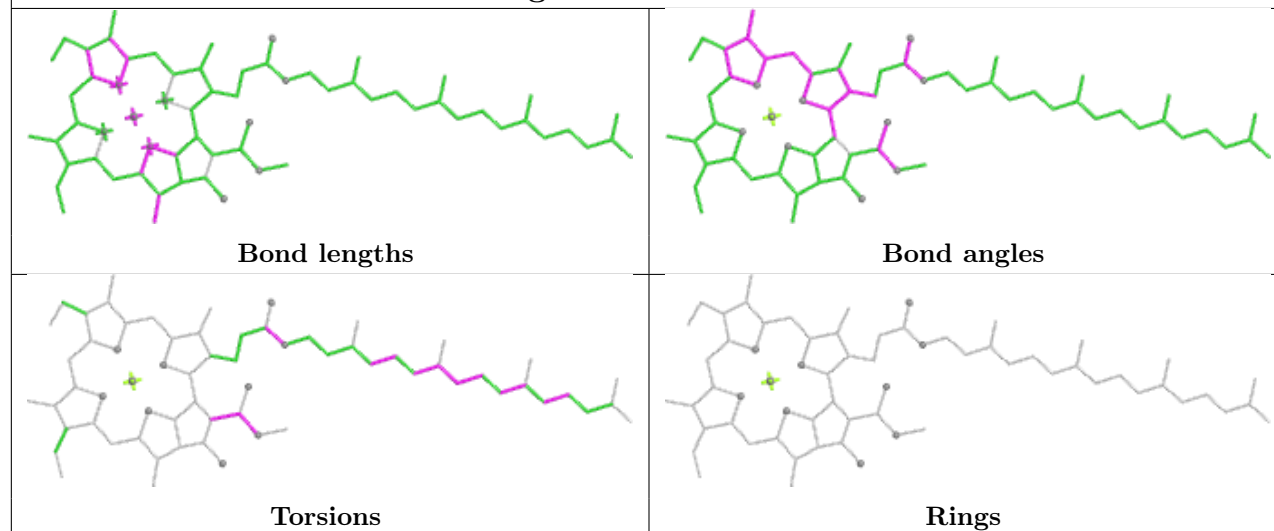


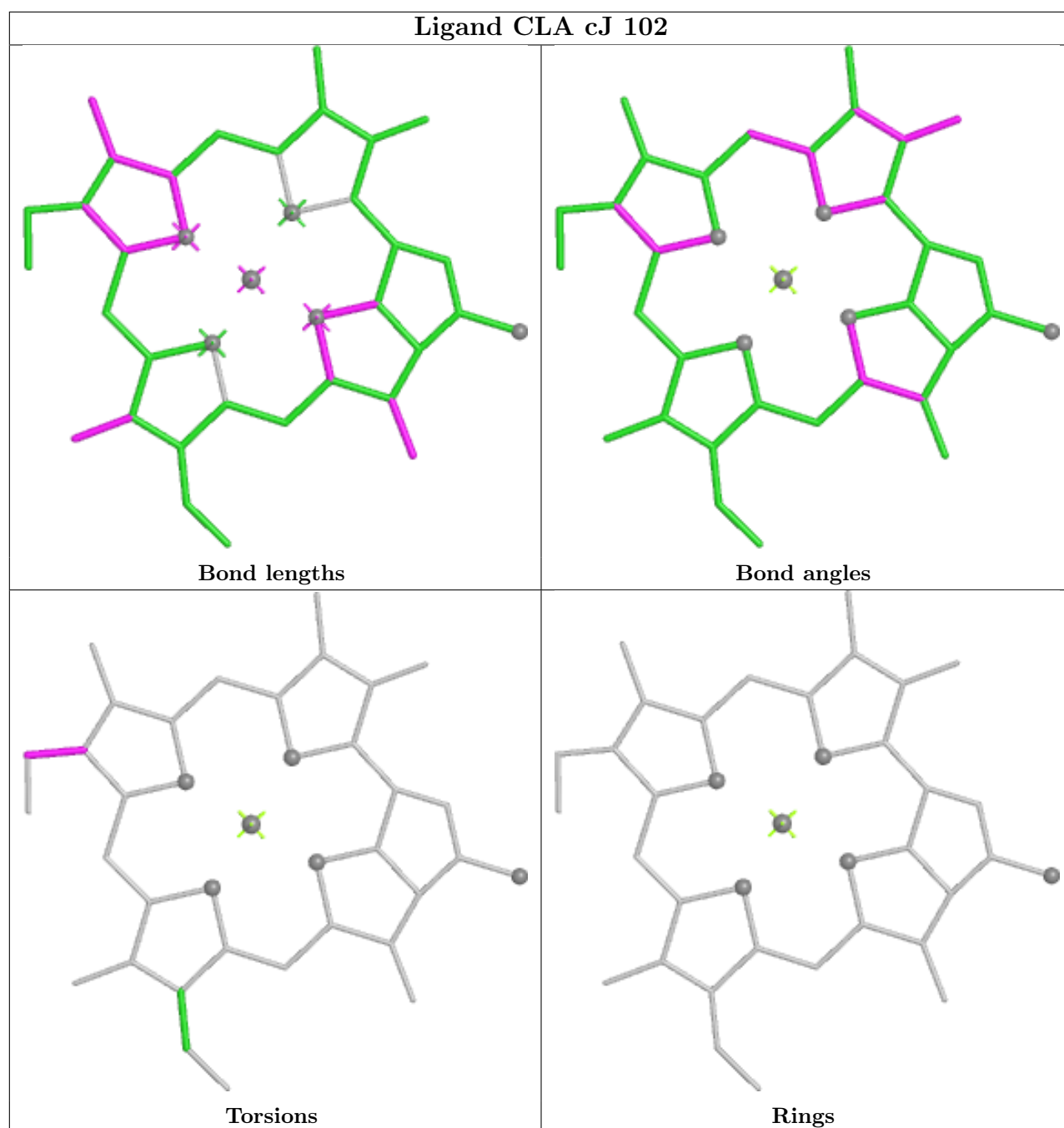


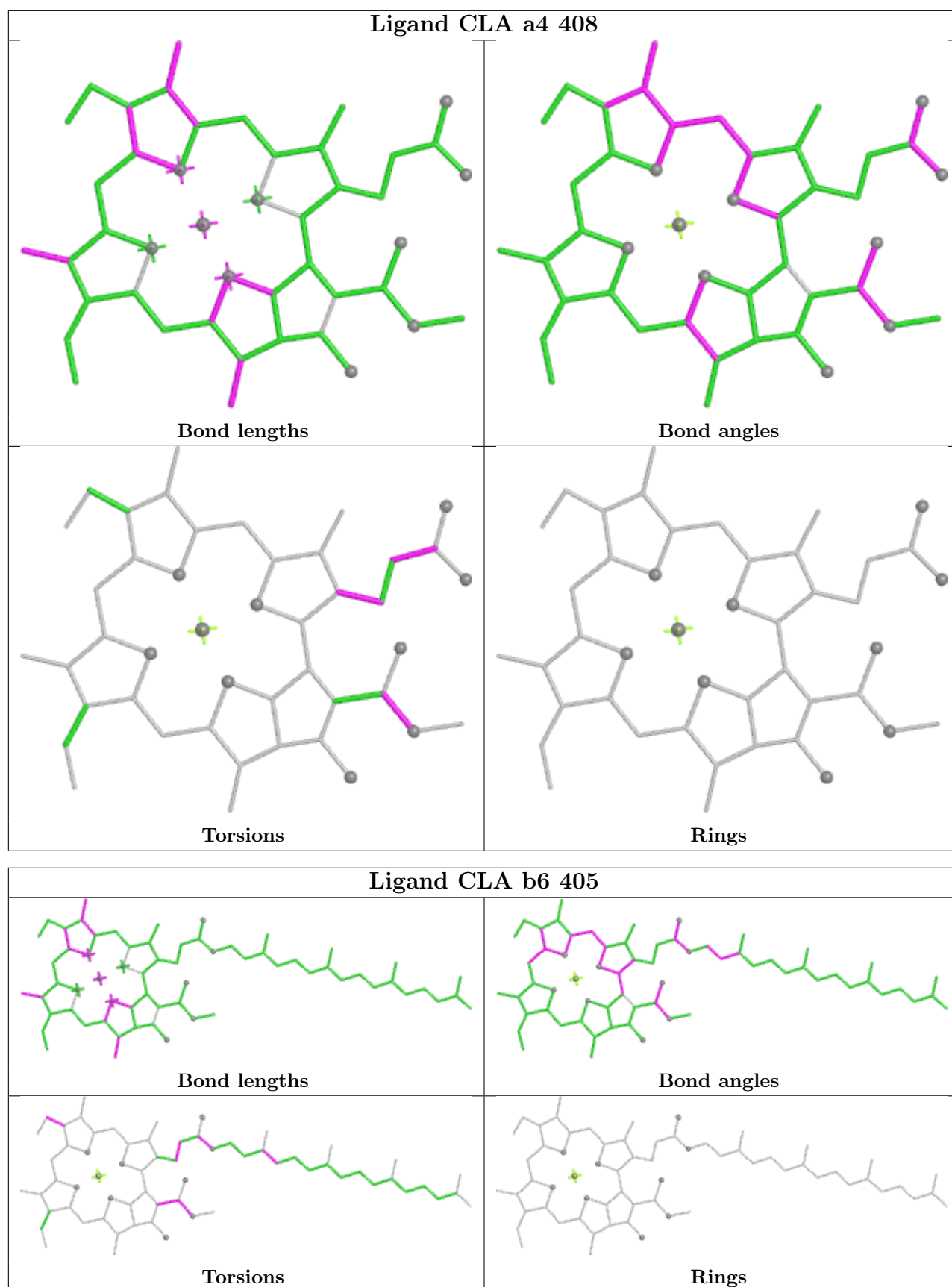




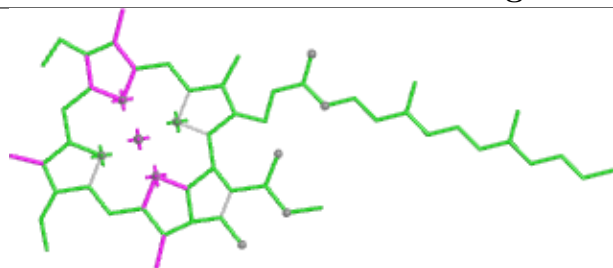


Ligand CLA aA 833**Ligand CLA c5 403**

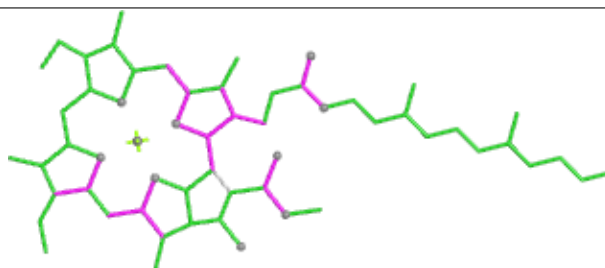




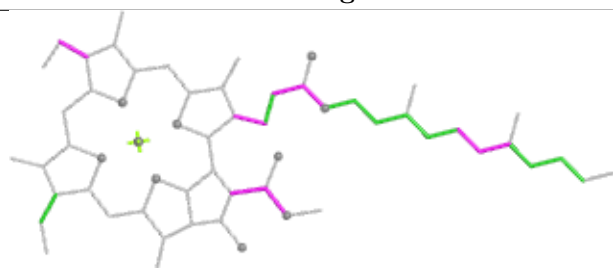
Ligand CLA aB 834



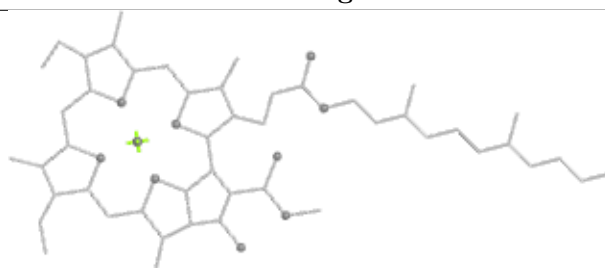
Bond lengths



Bond angles

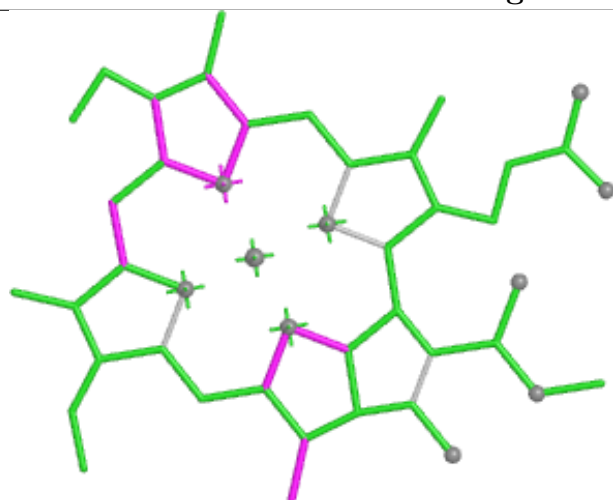


Torsions

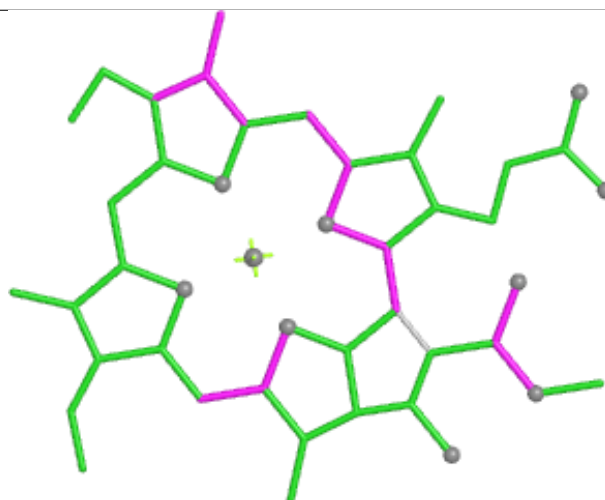


Rings

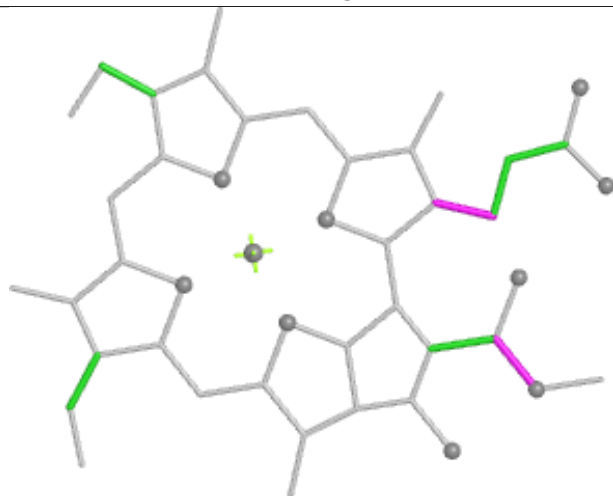
Ligand CLA cB 812



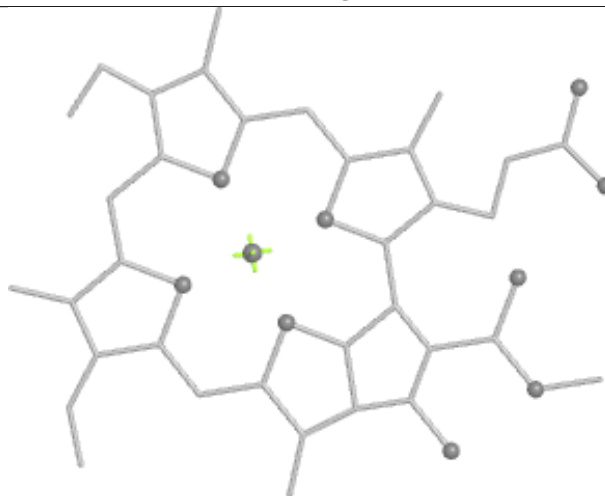
Bond lengths



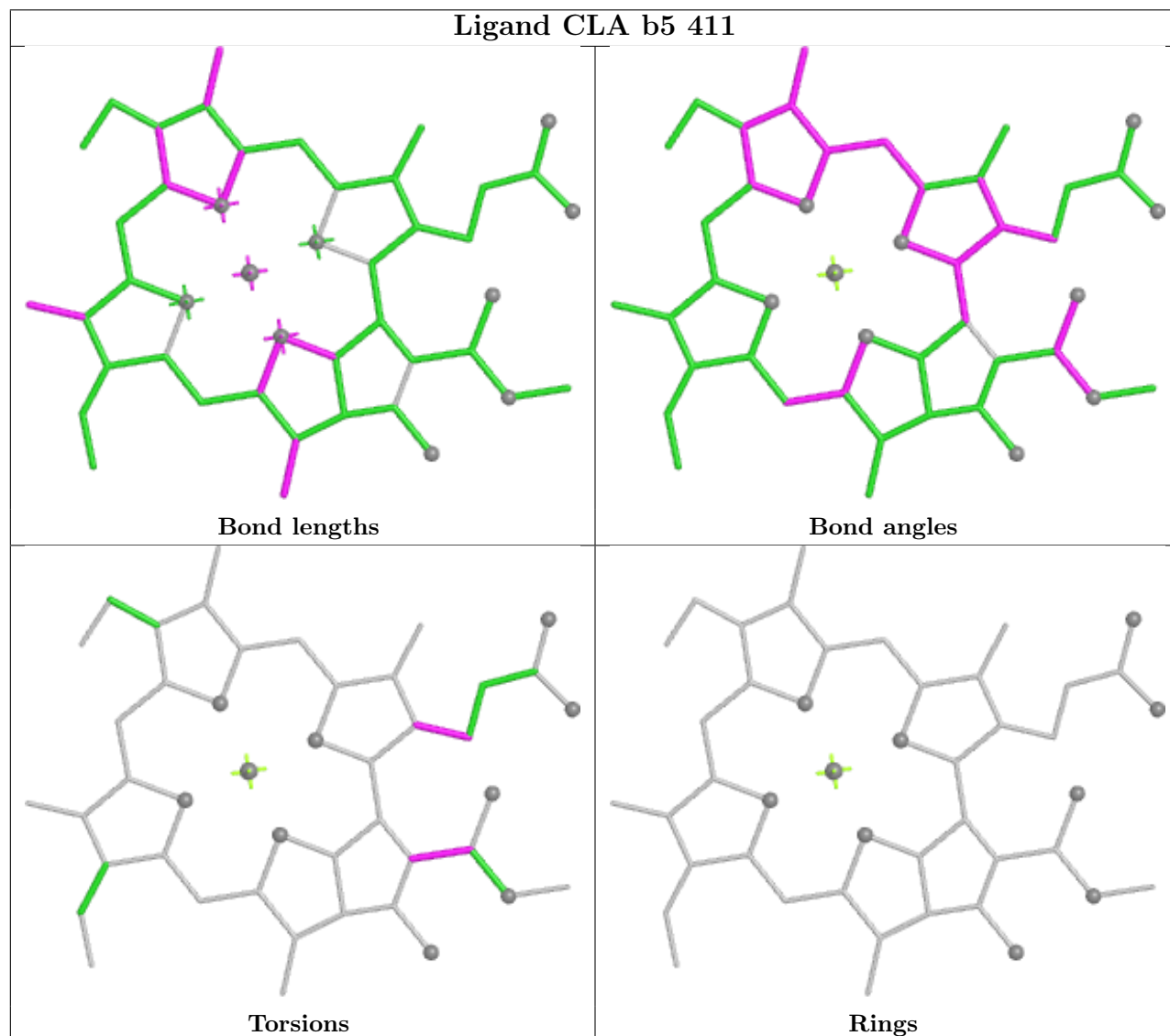
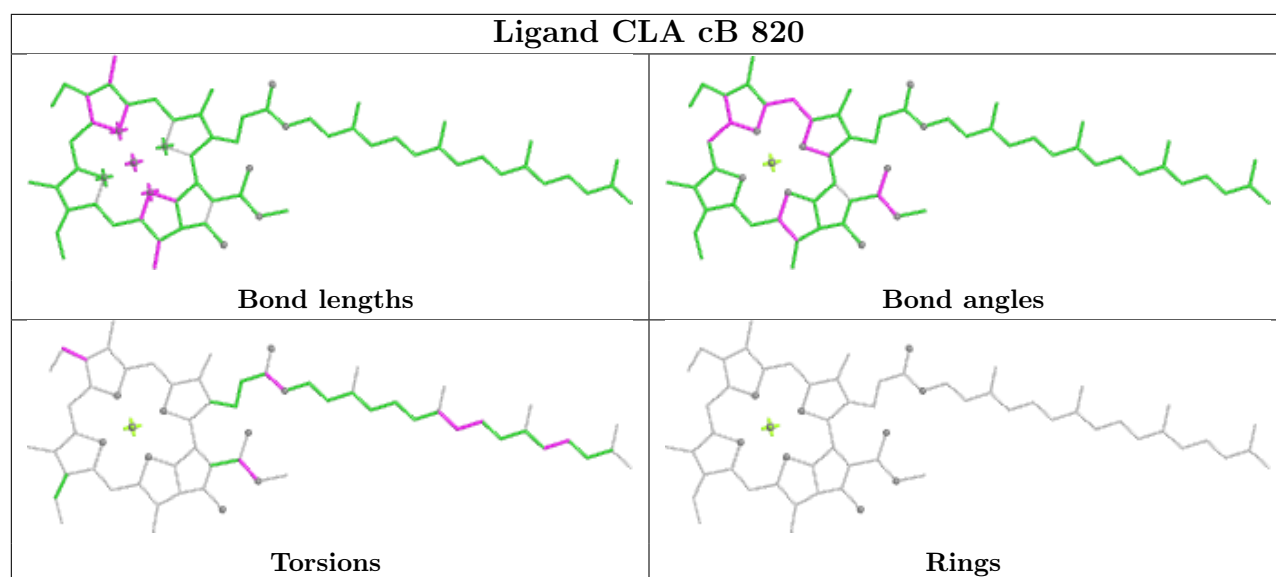
Bond angles

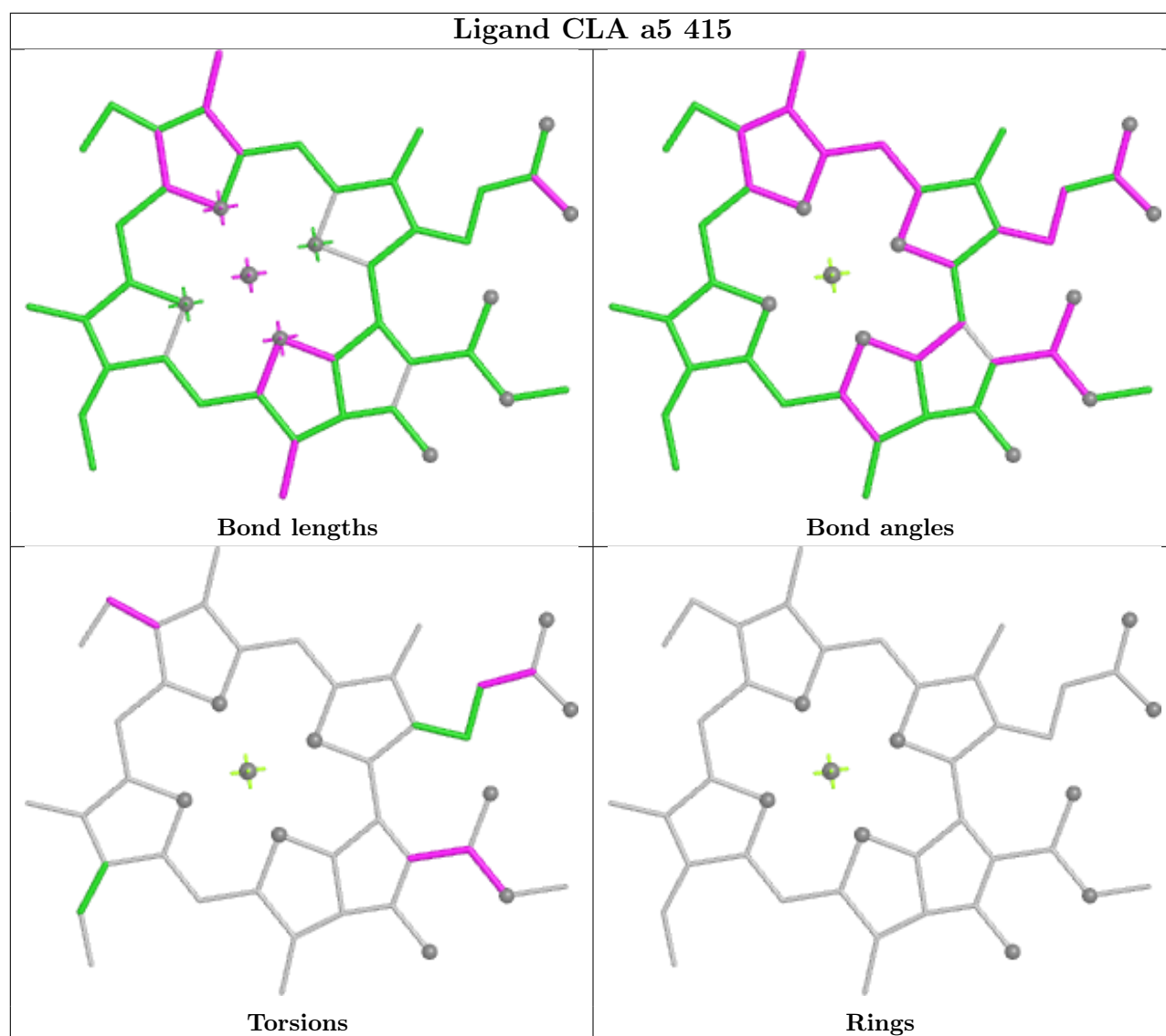


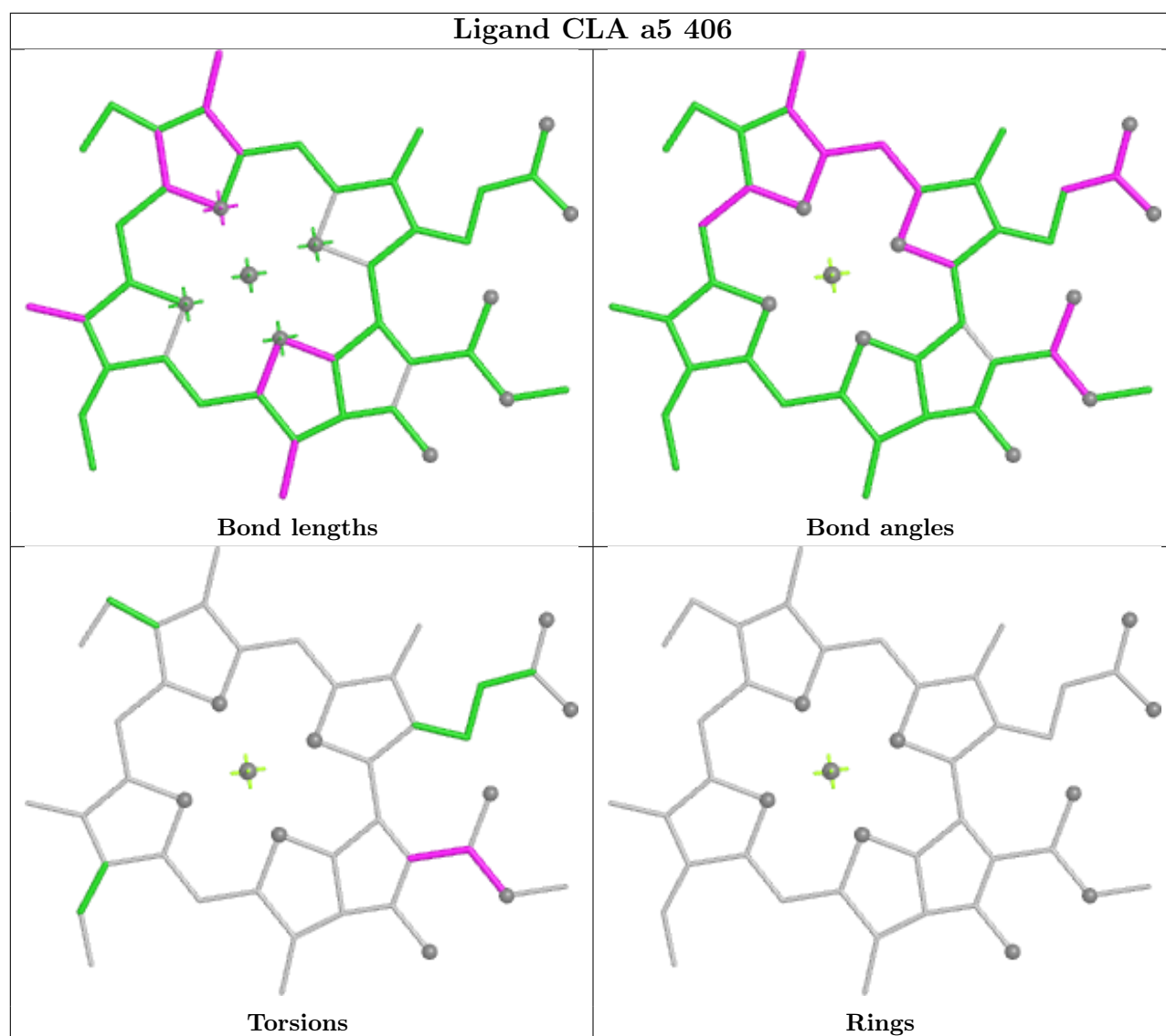
Torsions

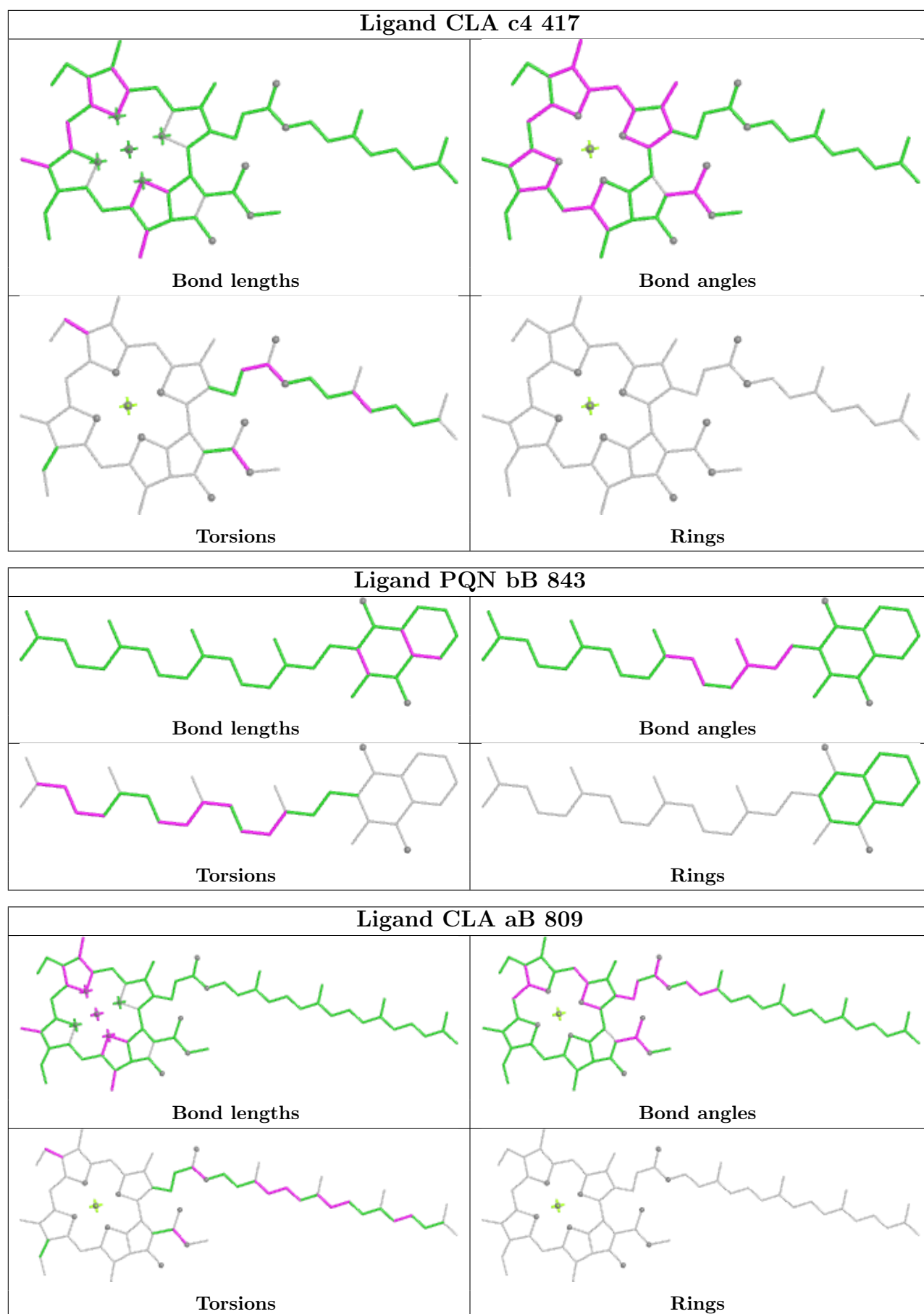


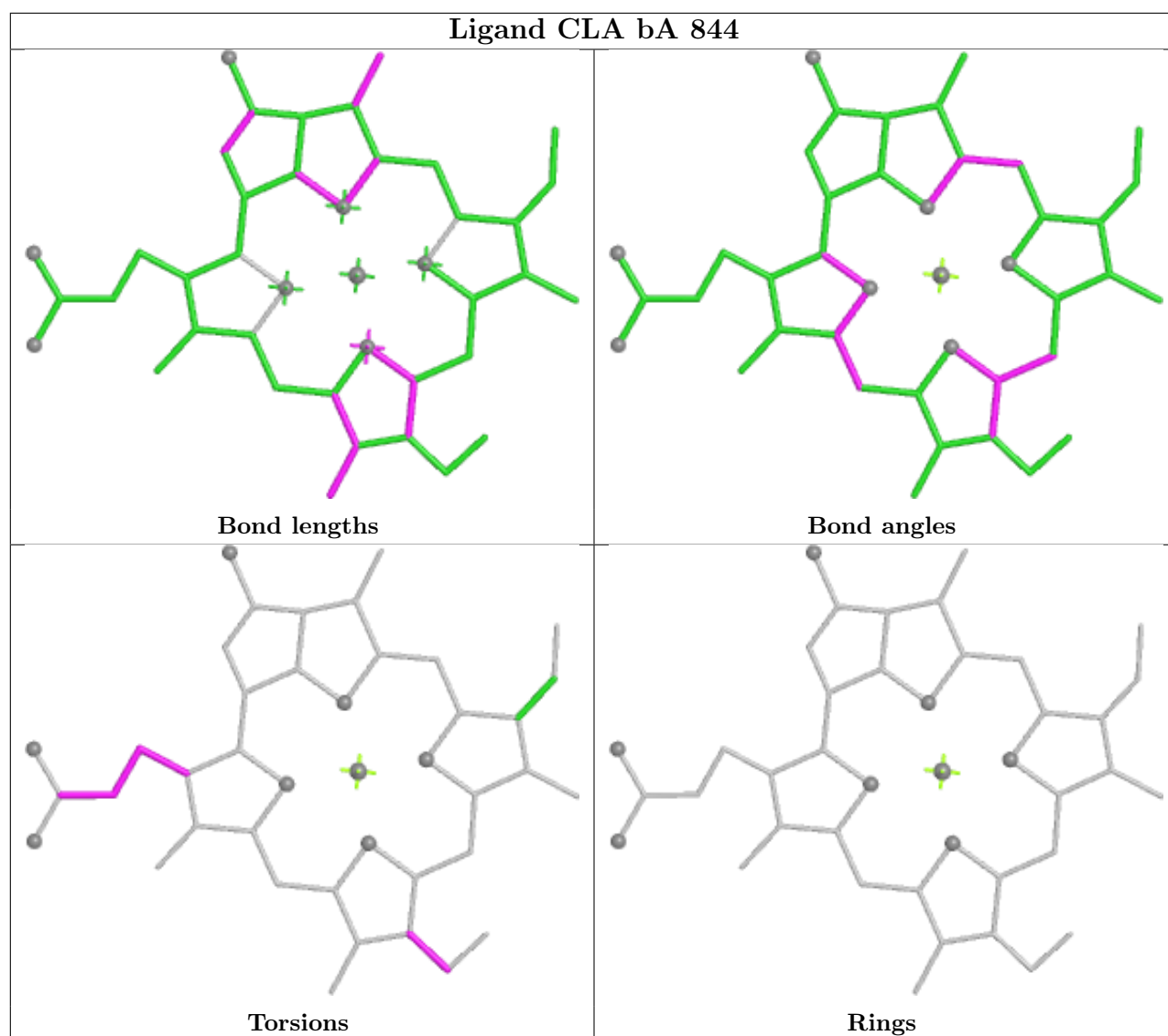
Rings

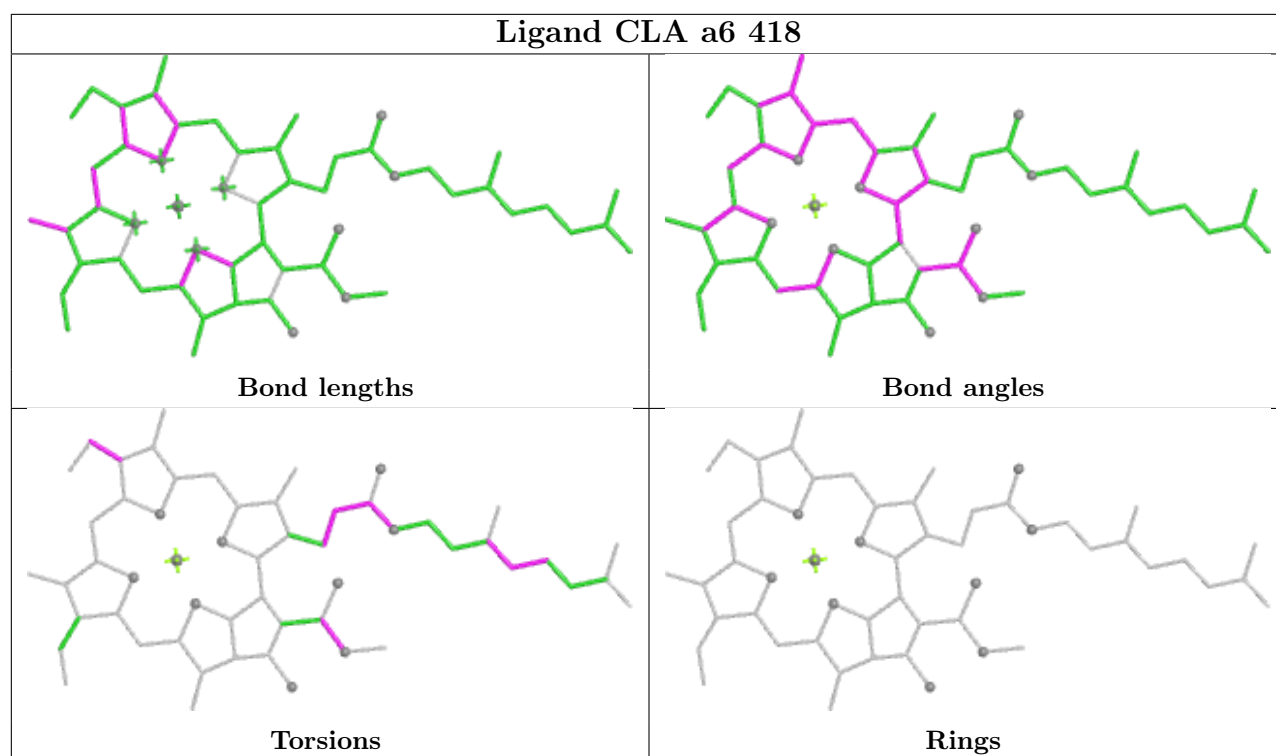


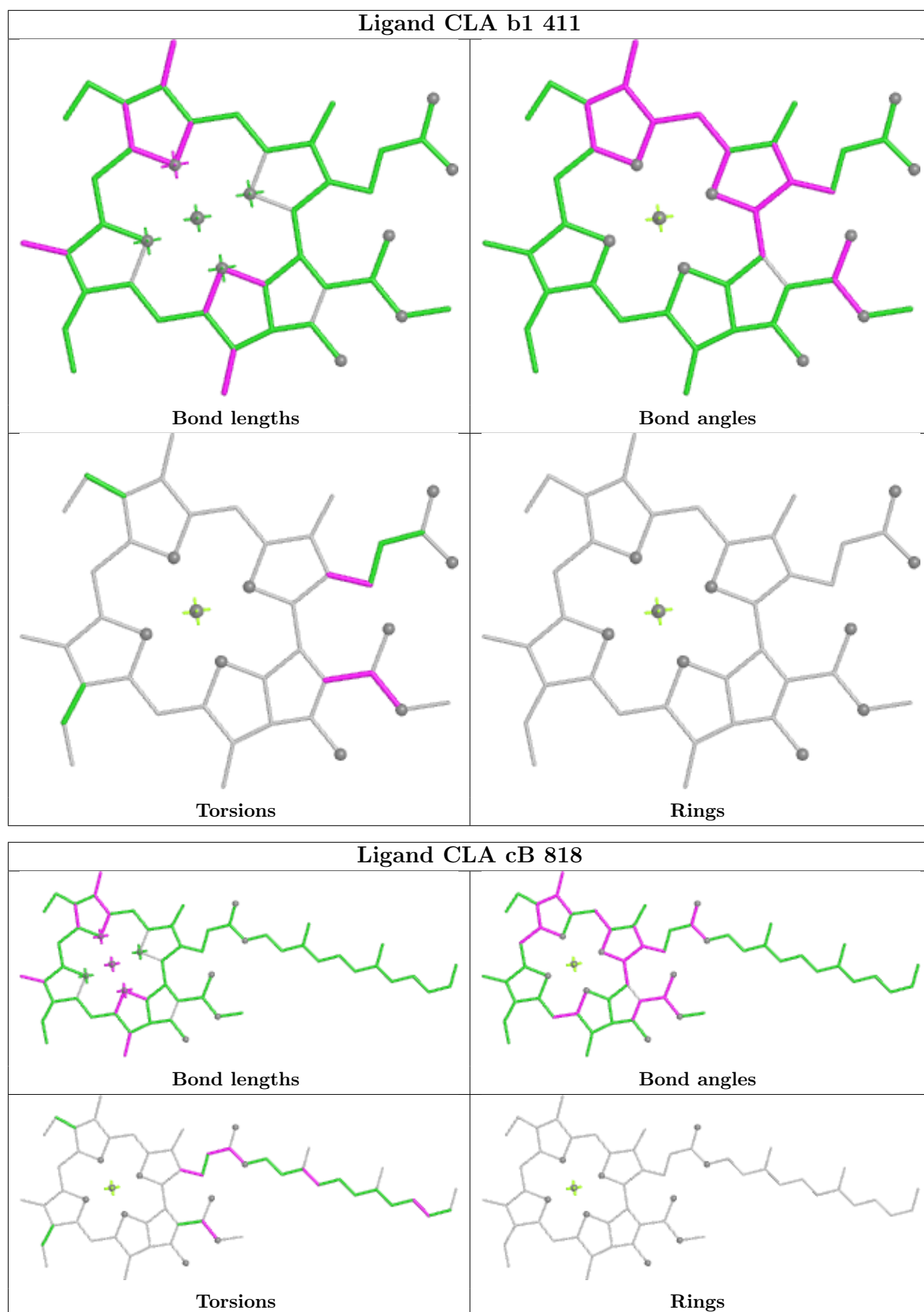


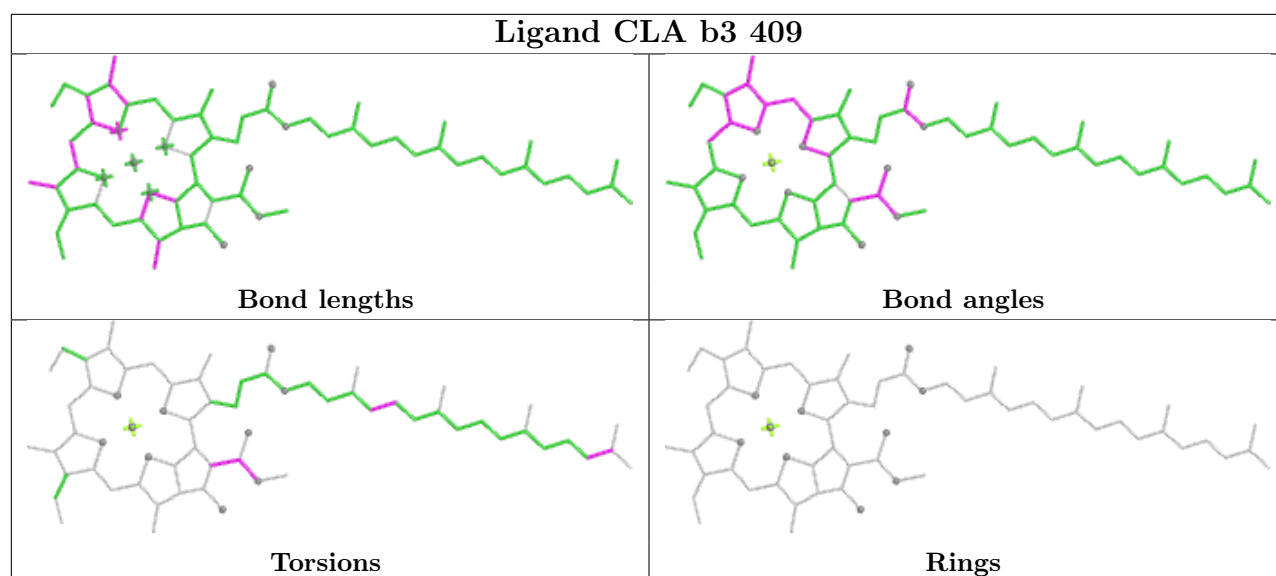
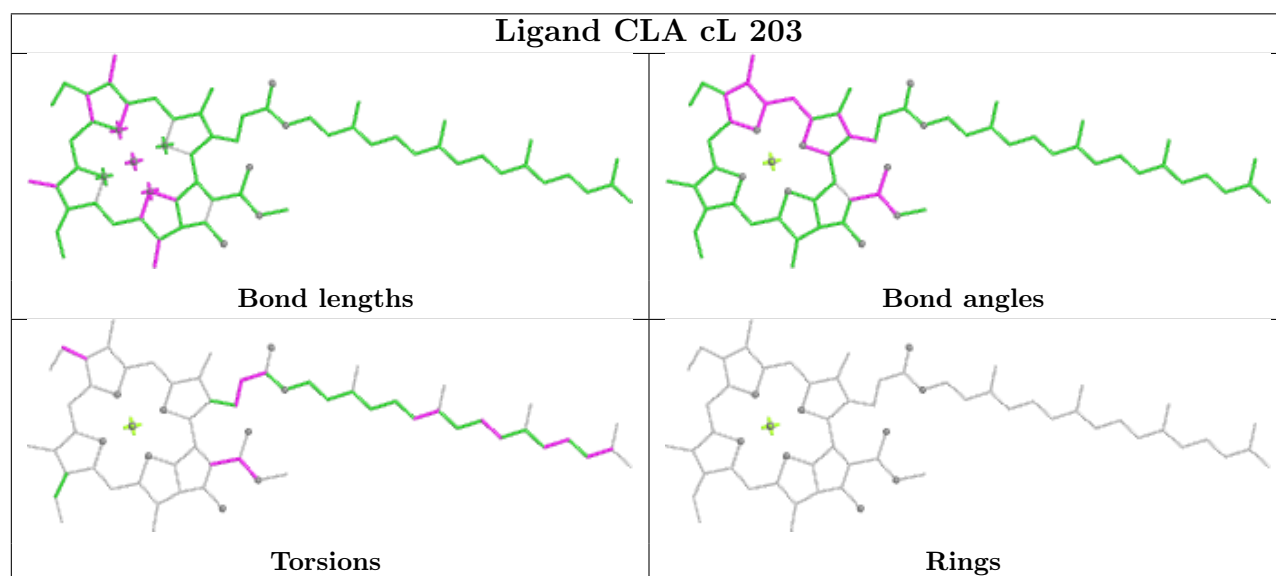
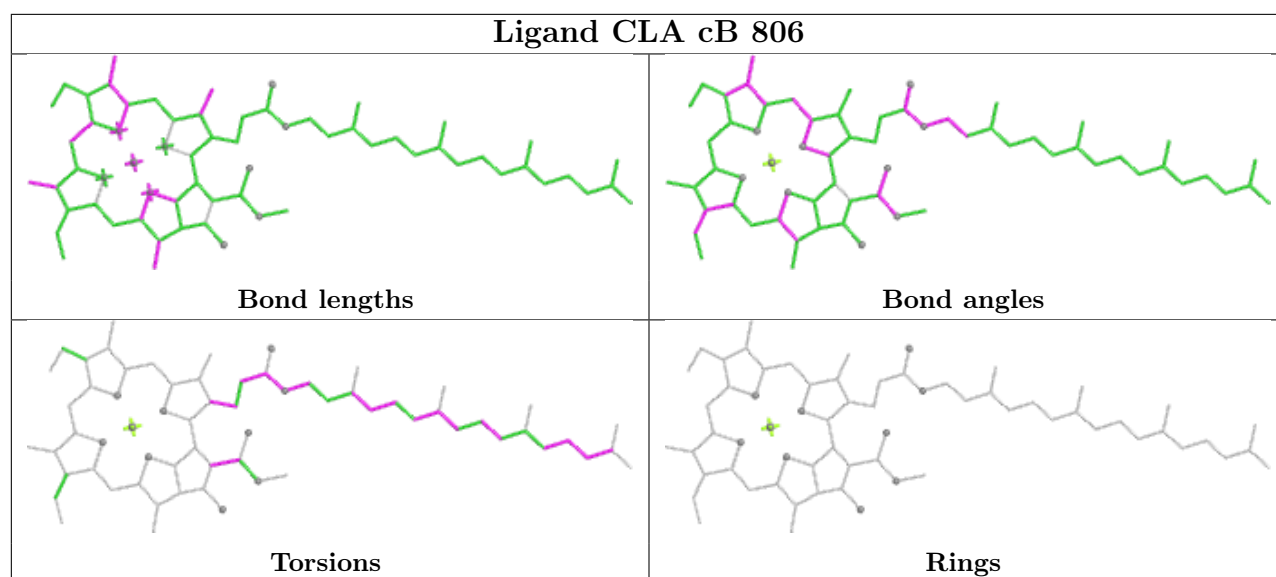


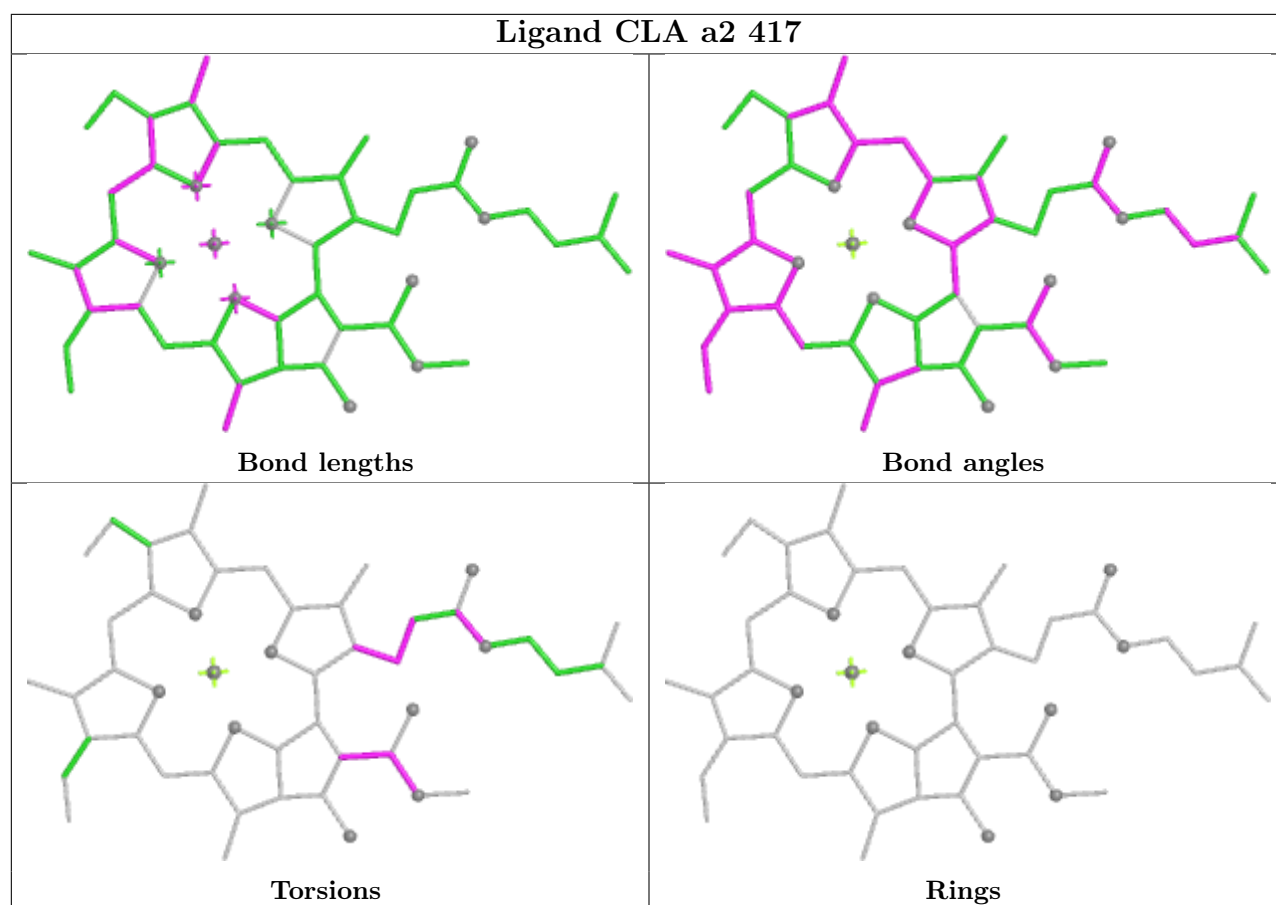


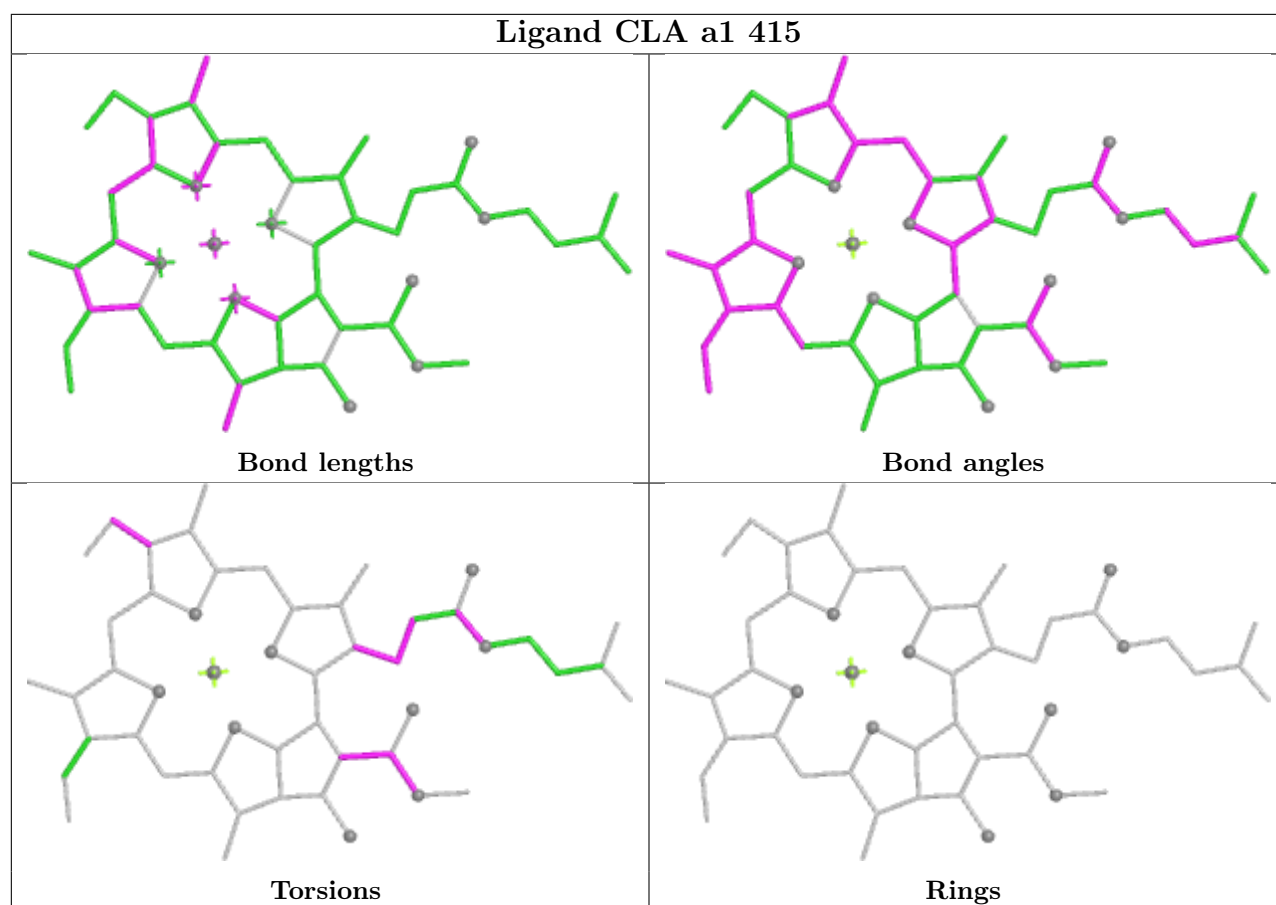


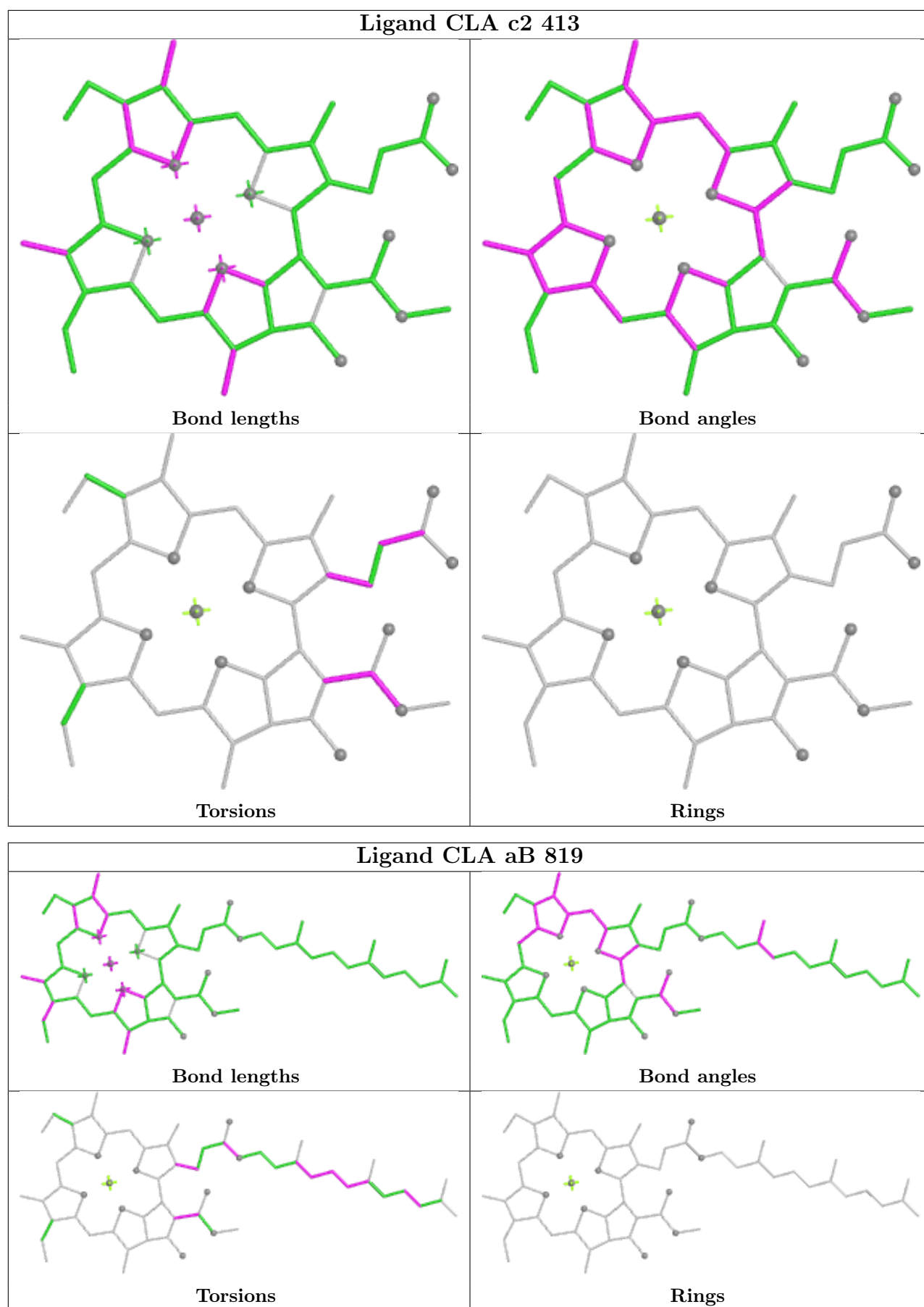


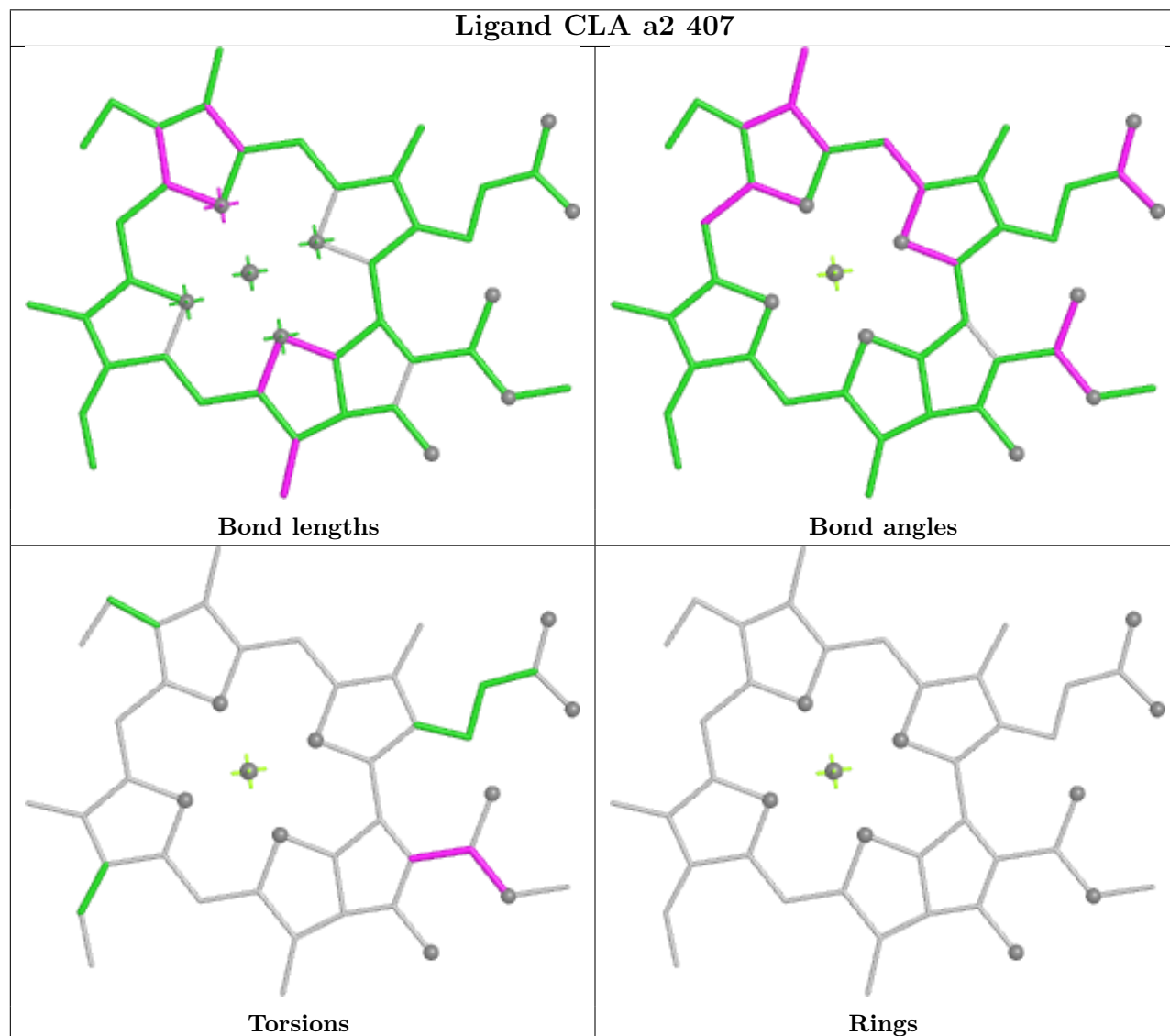
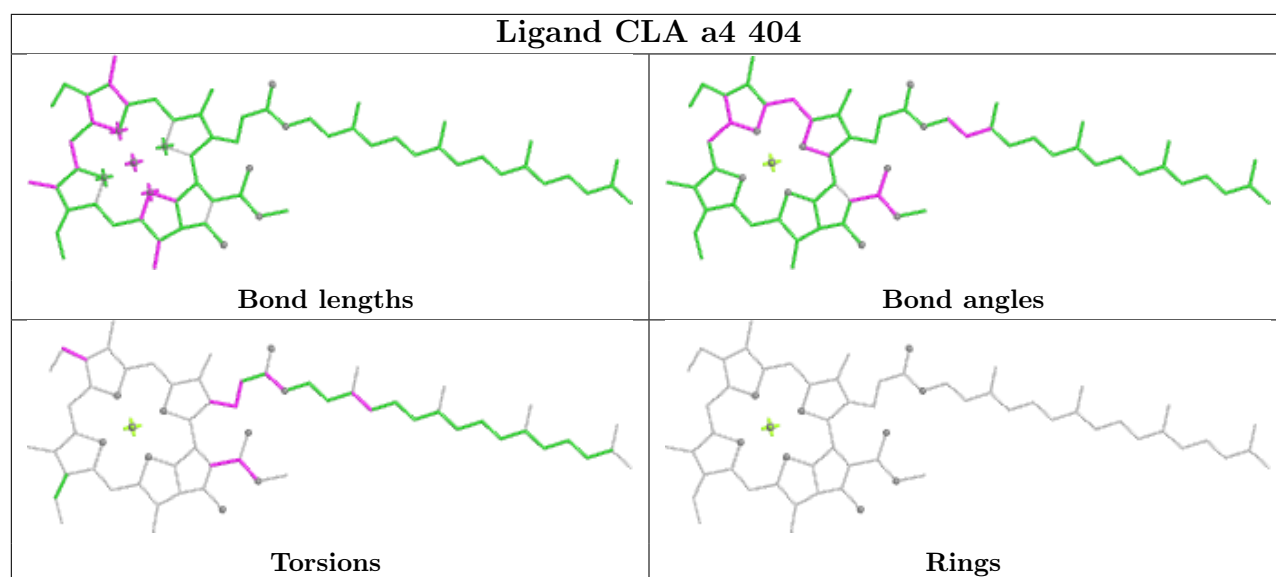


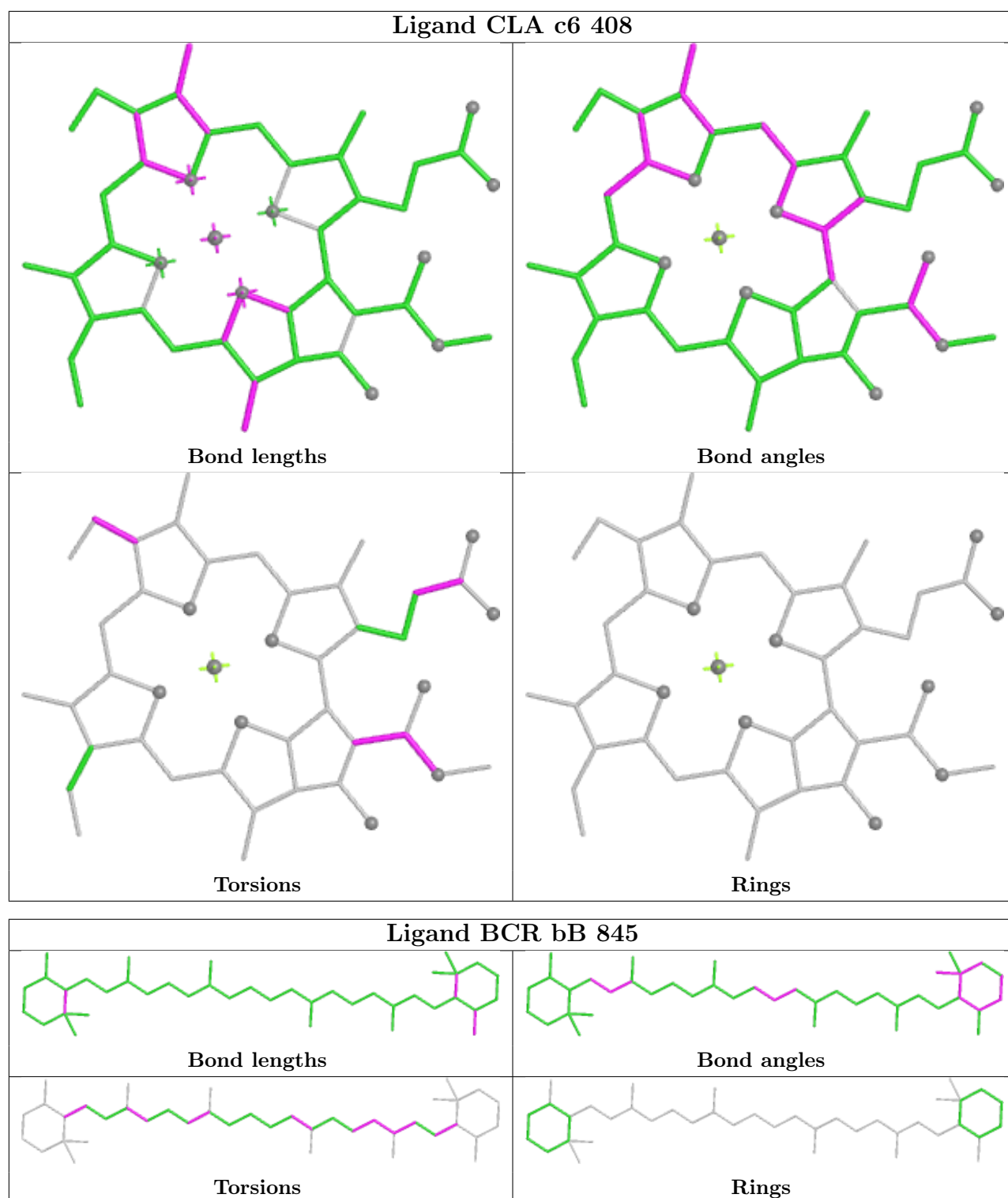


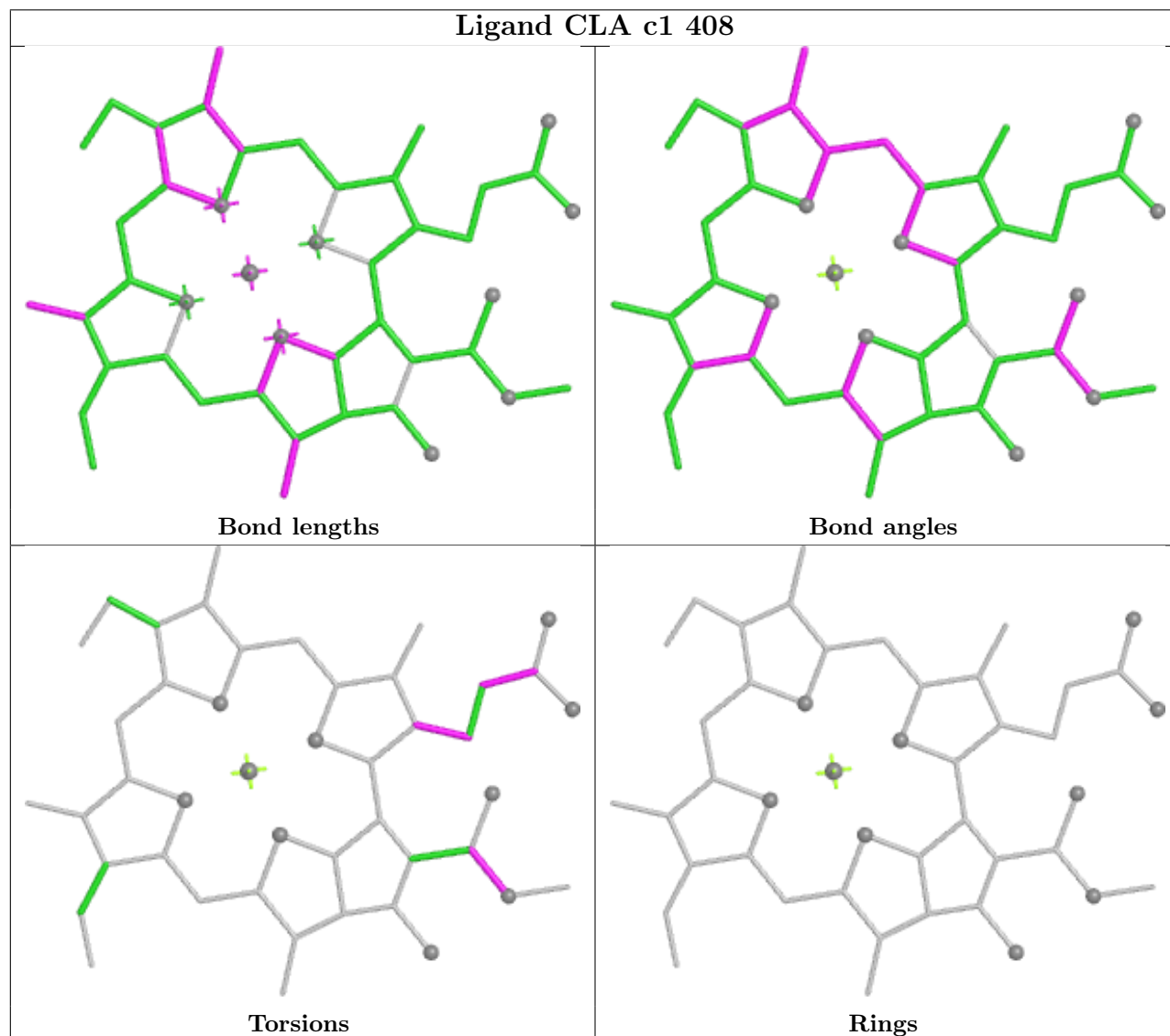
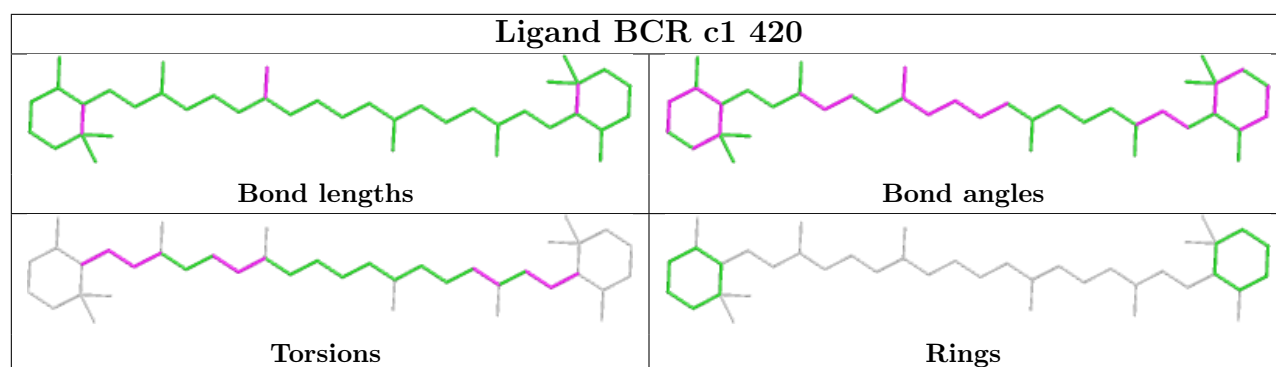


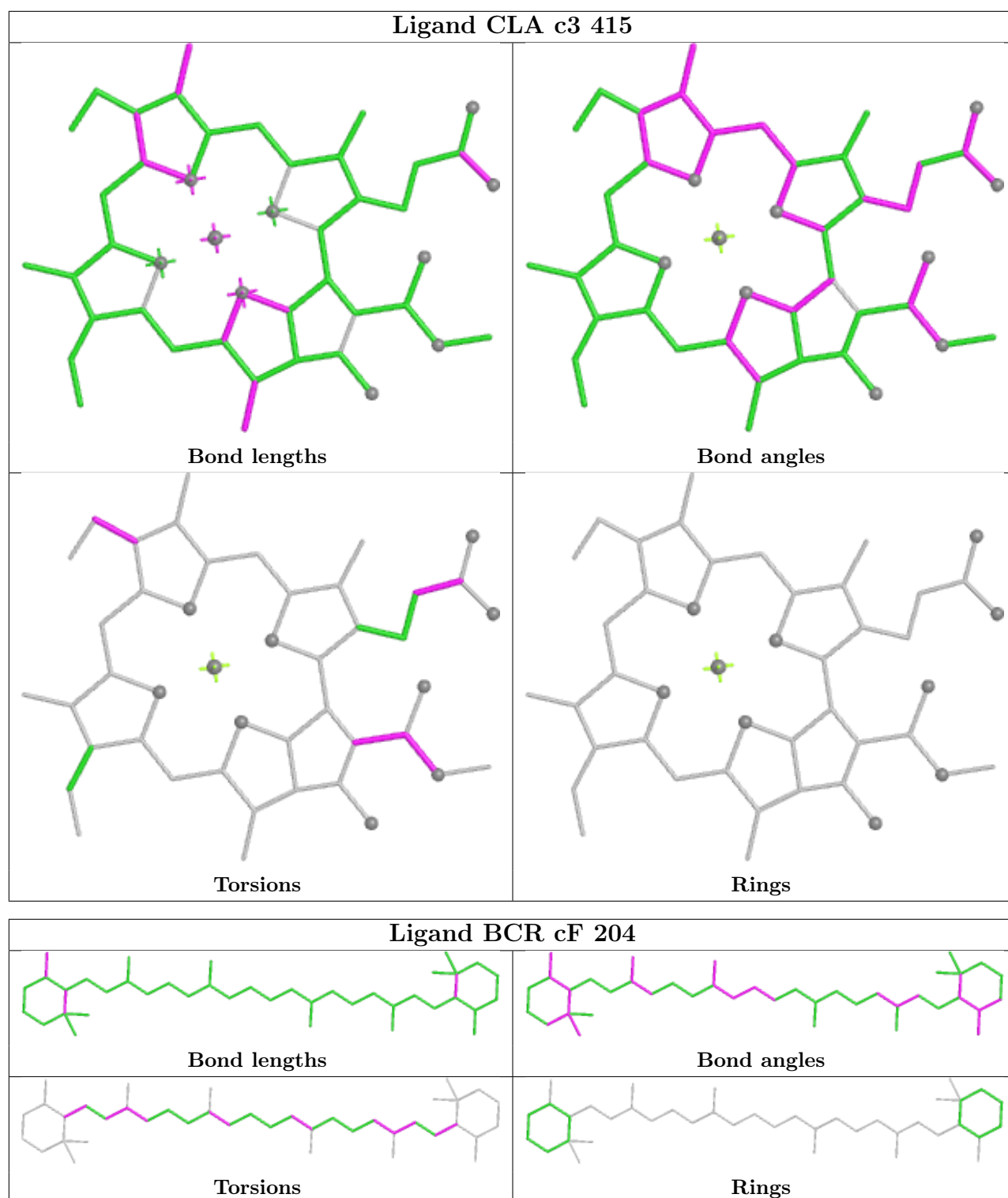


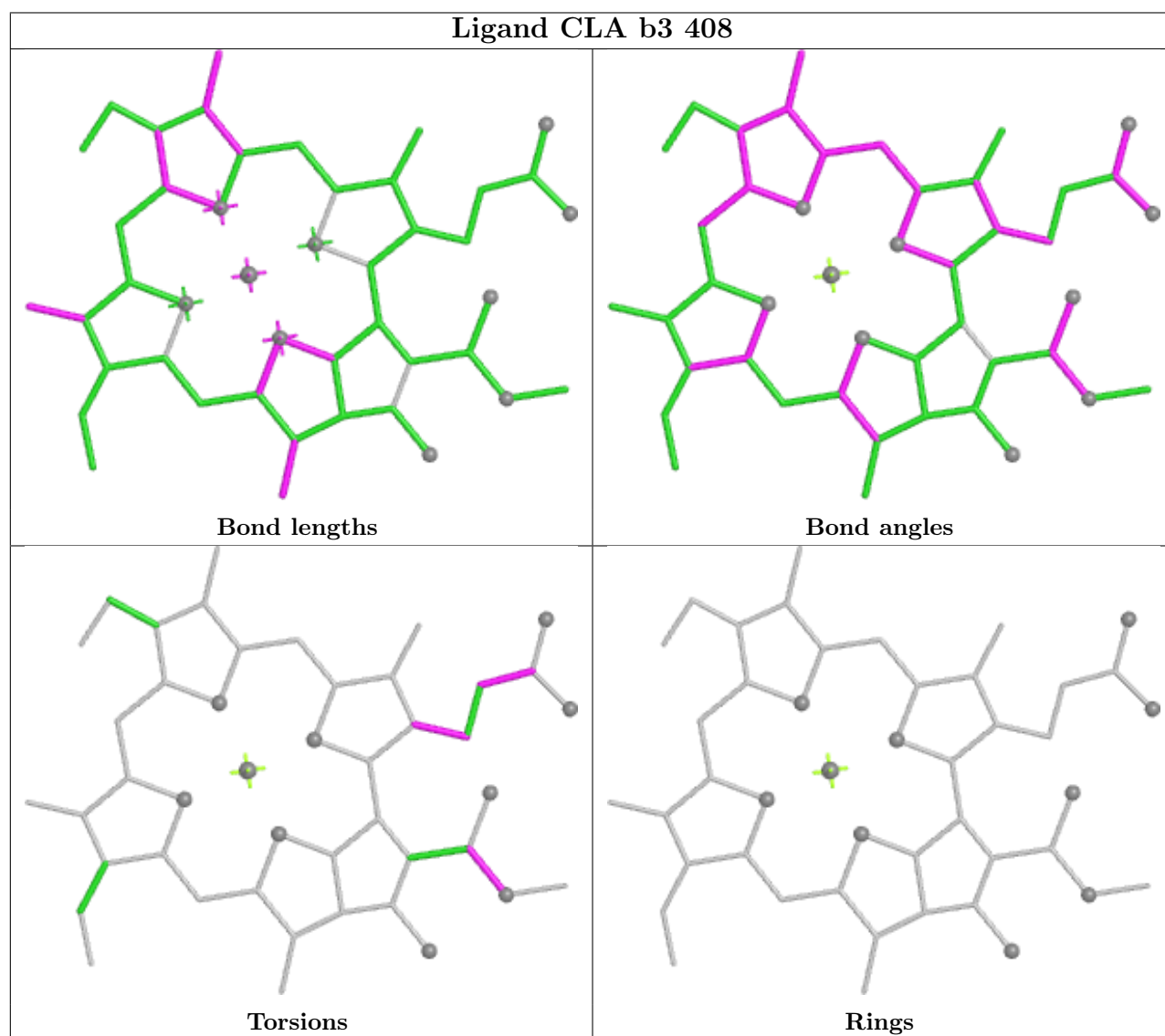
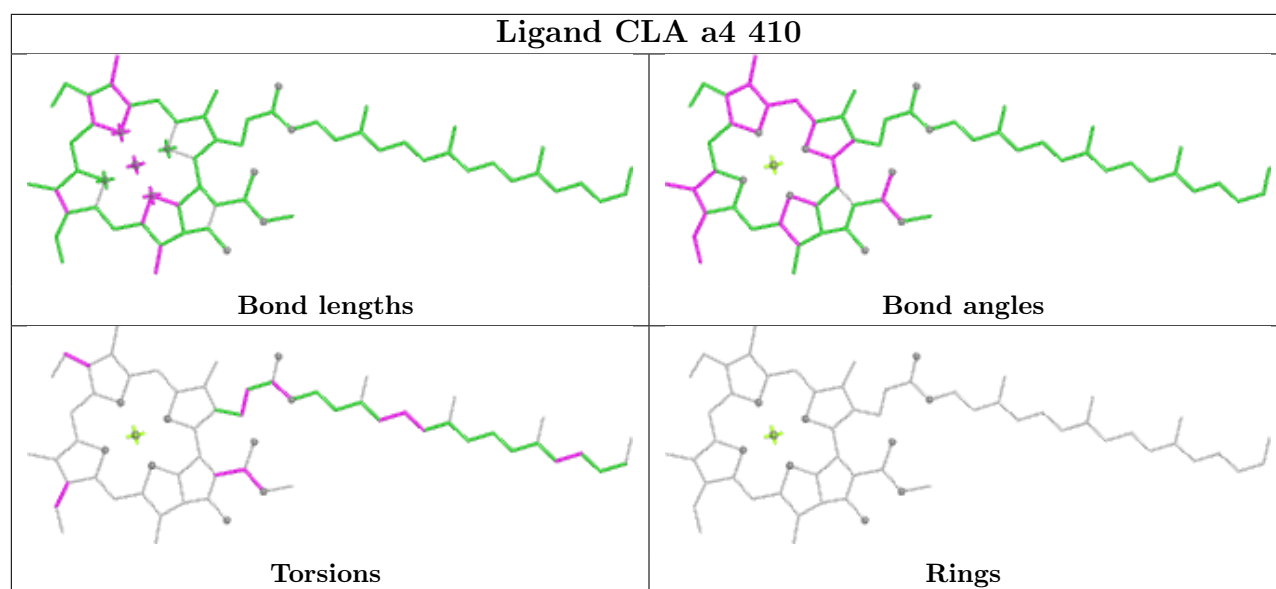


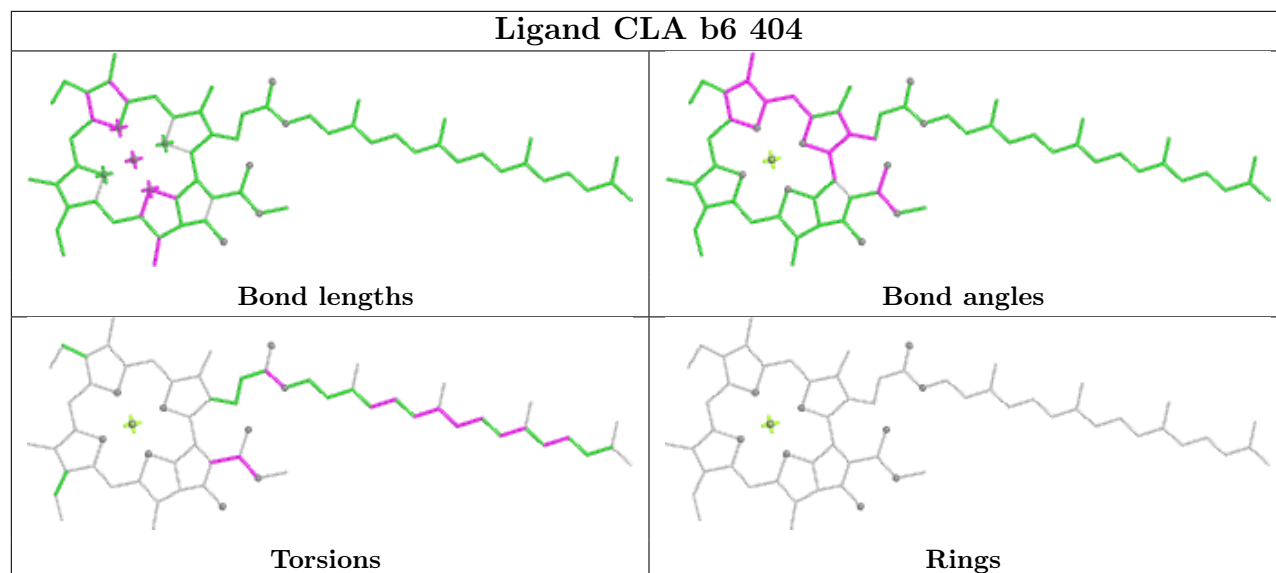
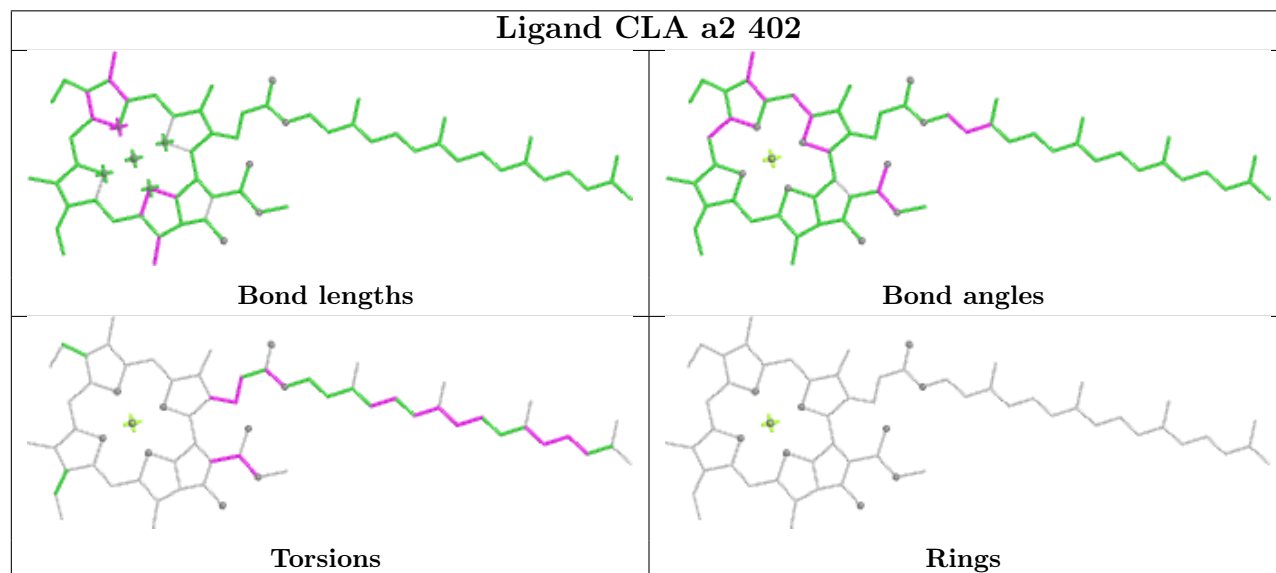
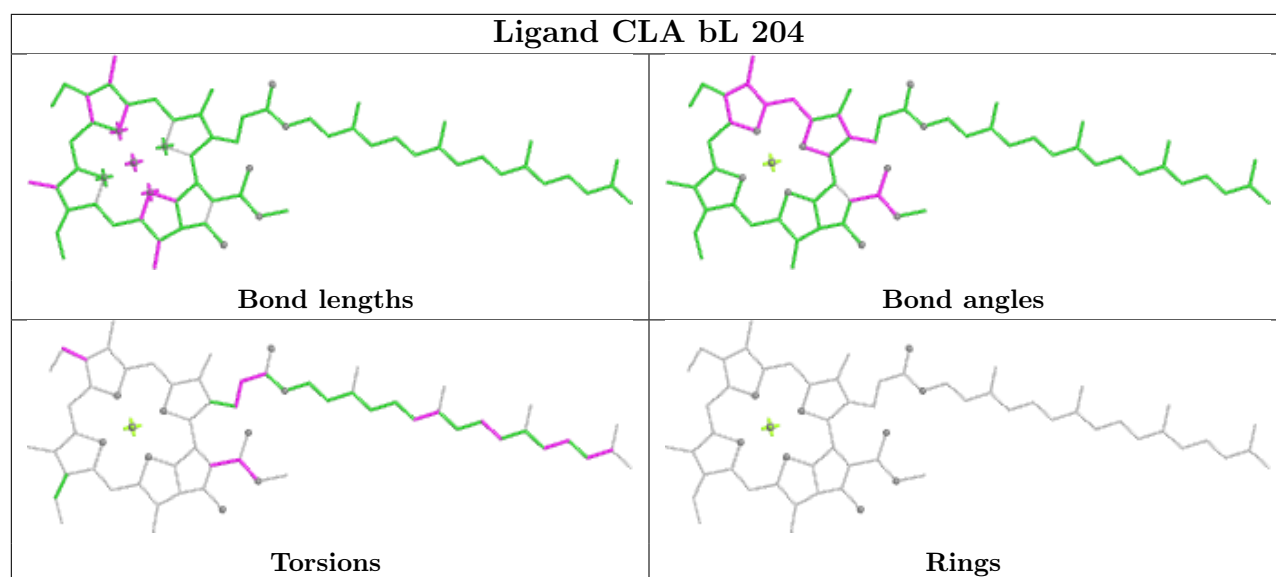


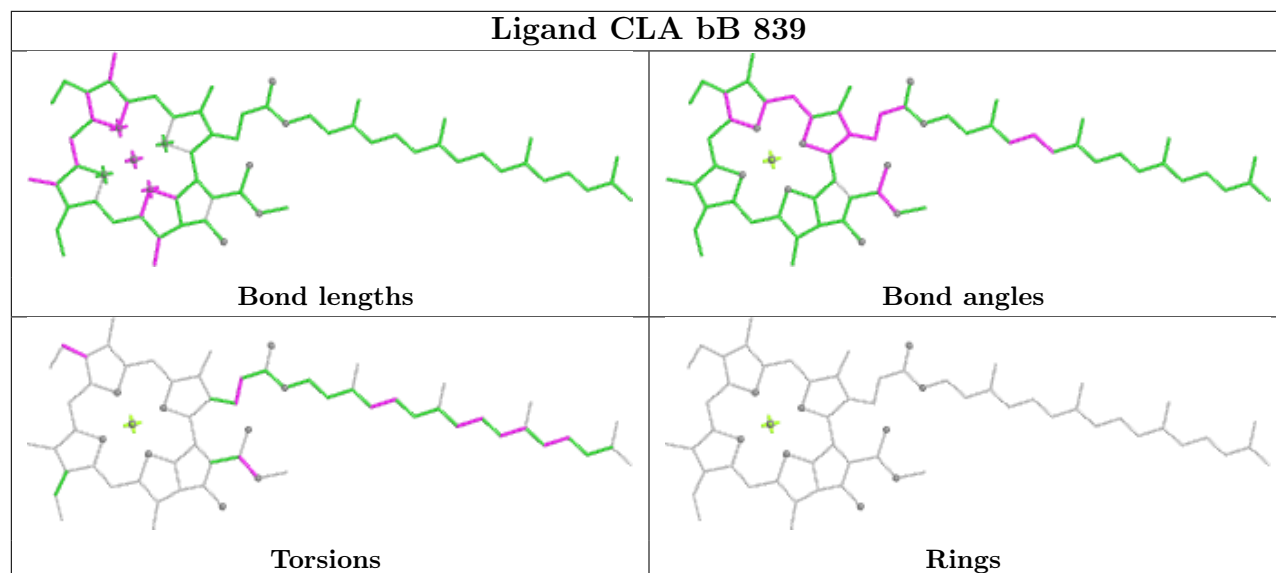
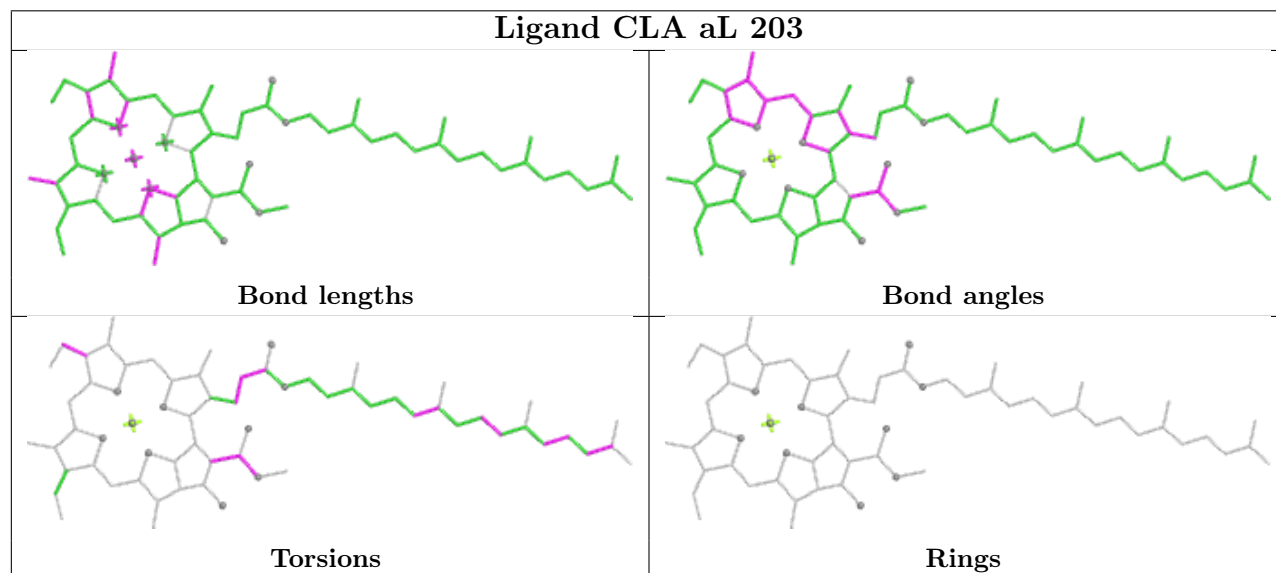
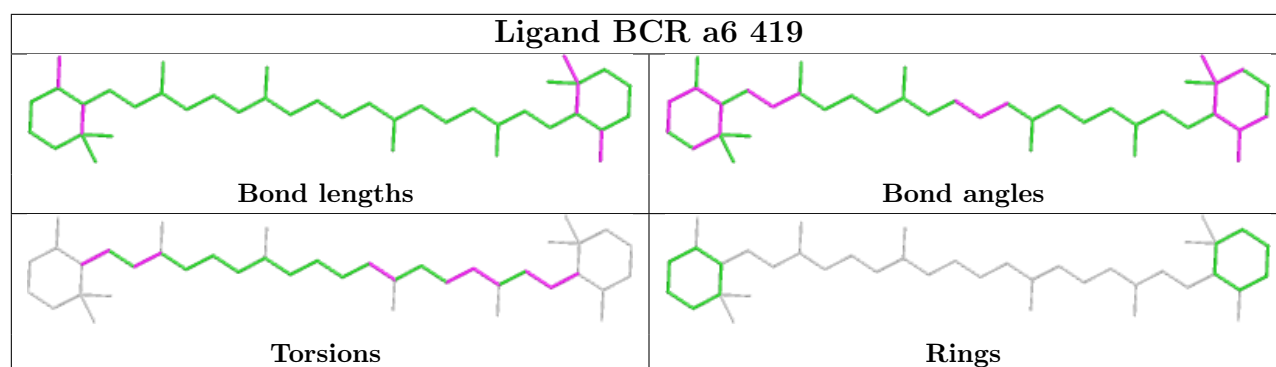


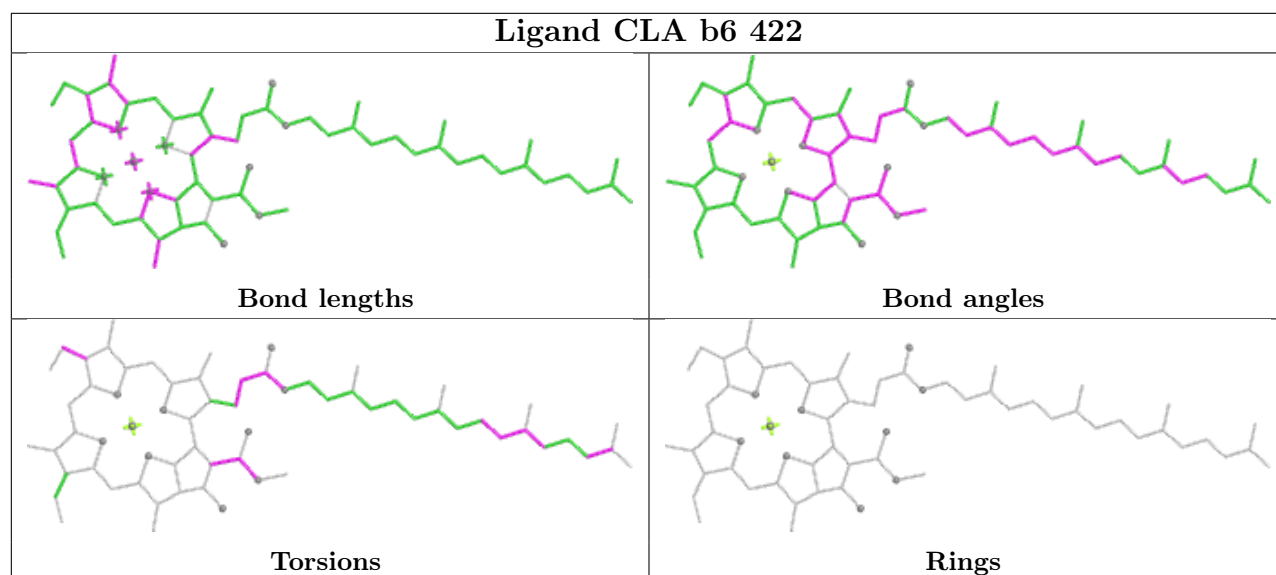
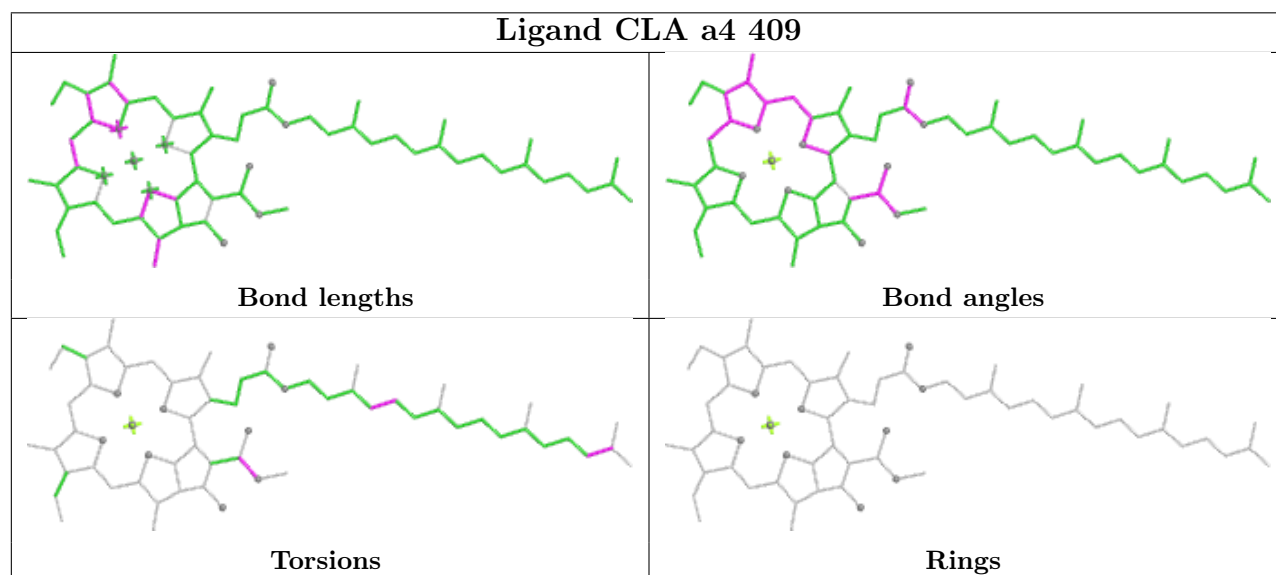
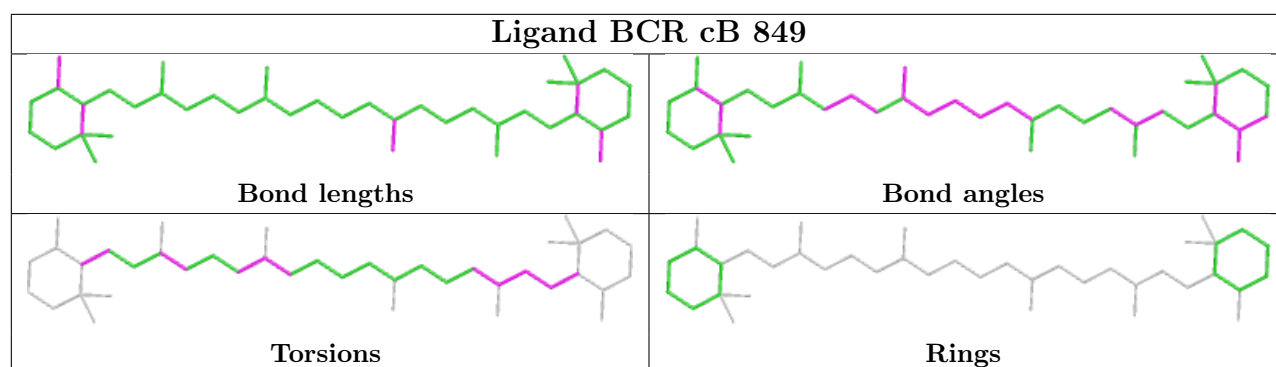


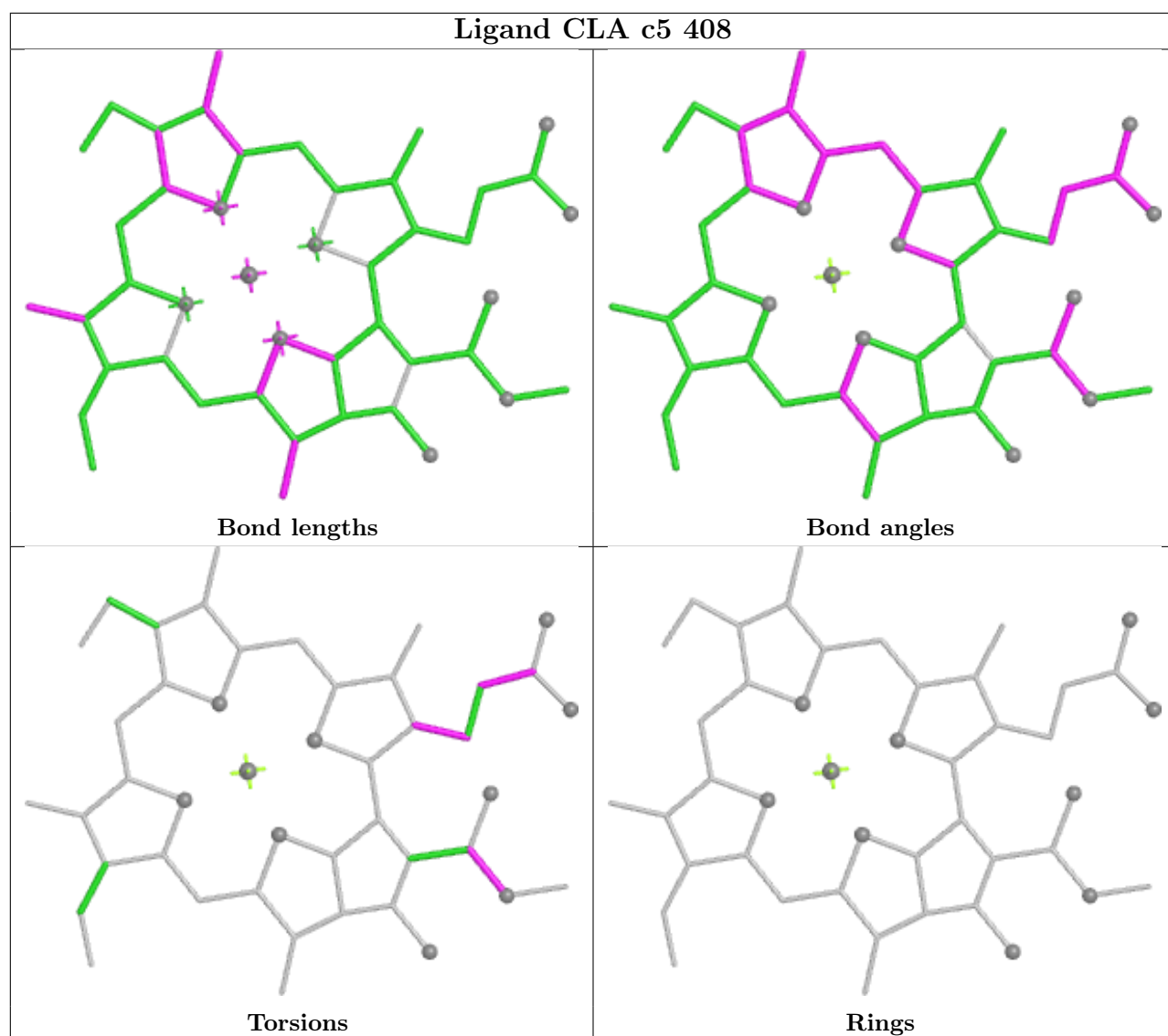


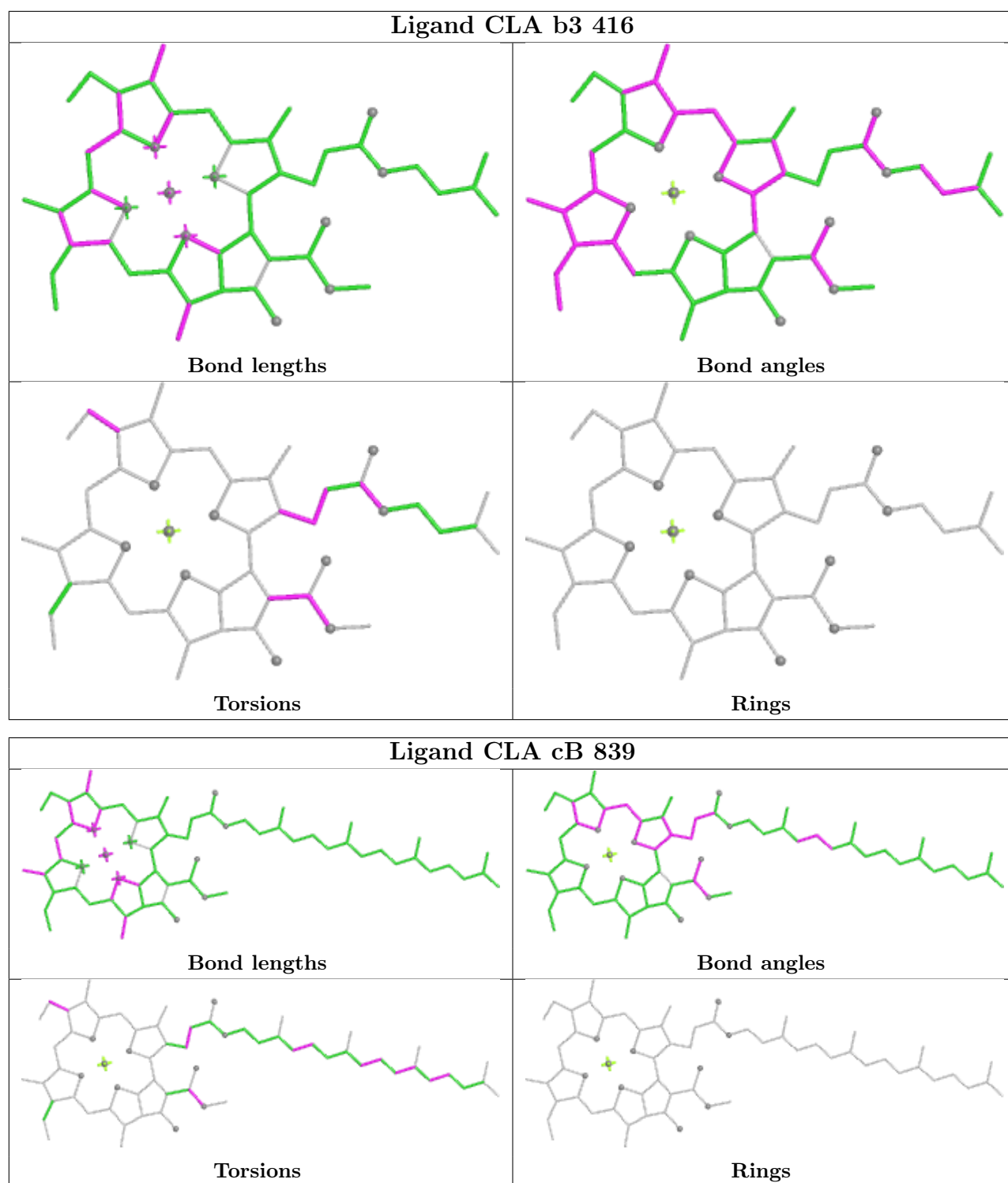


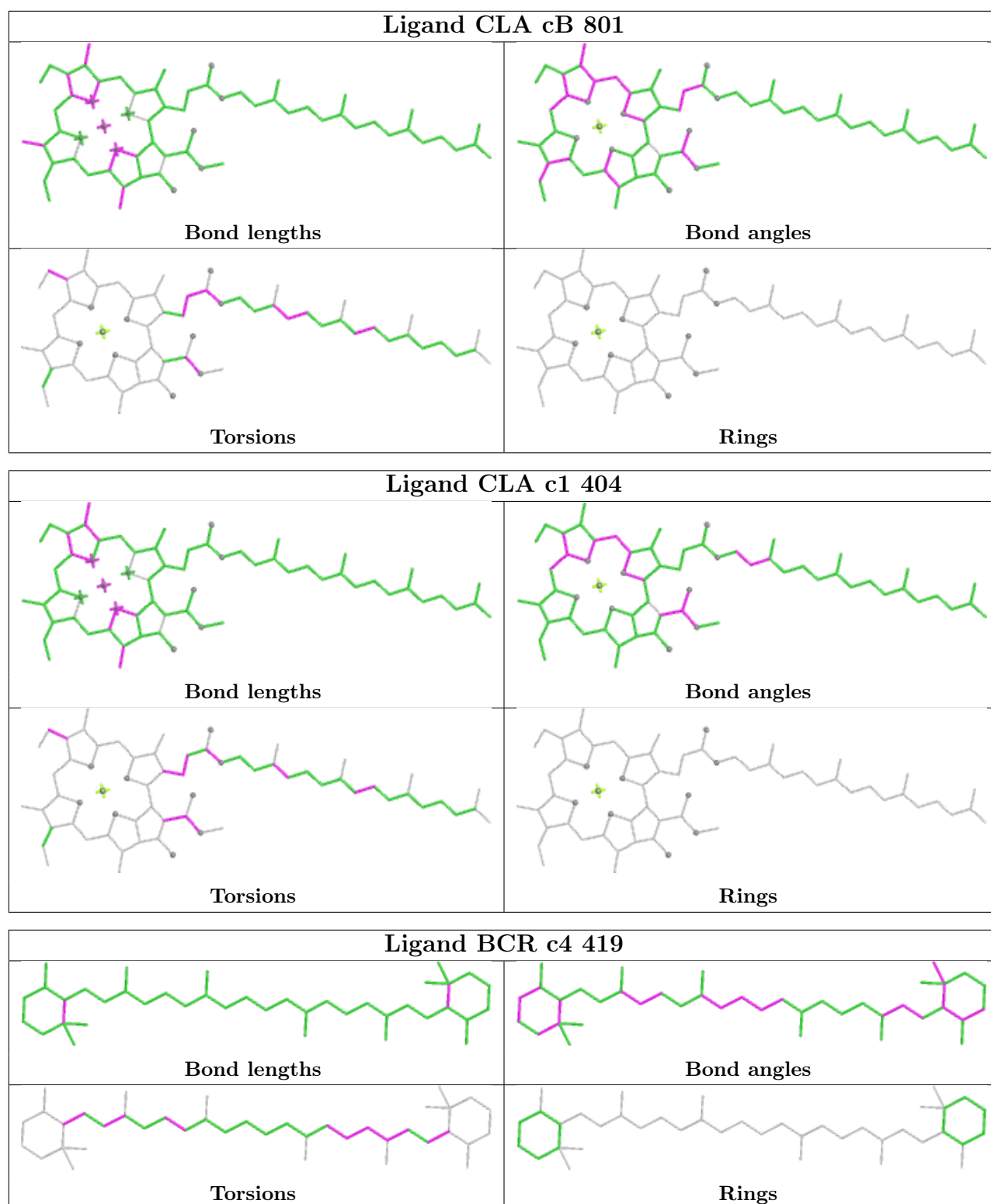


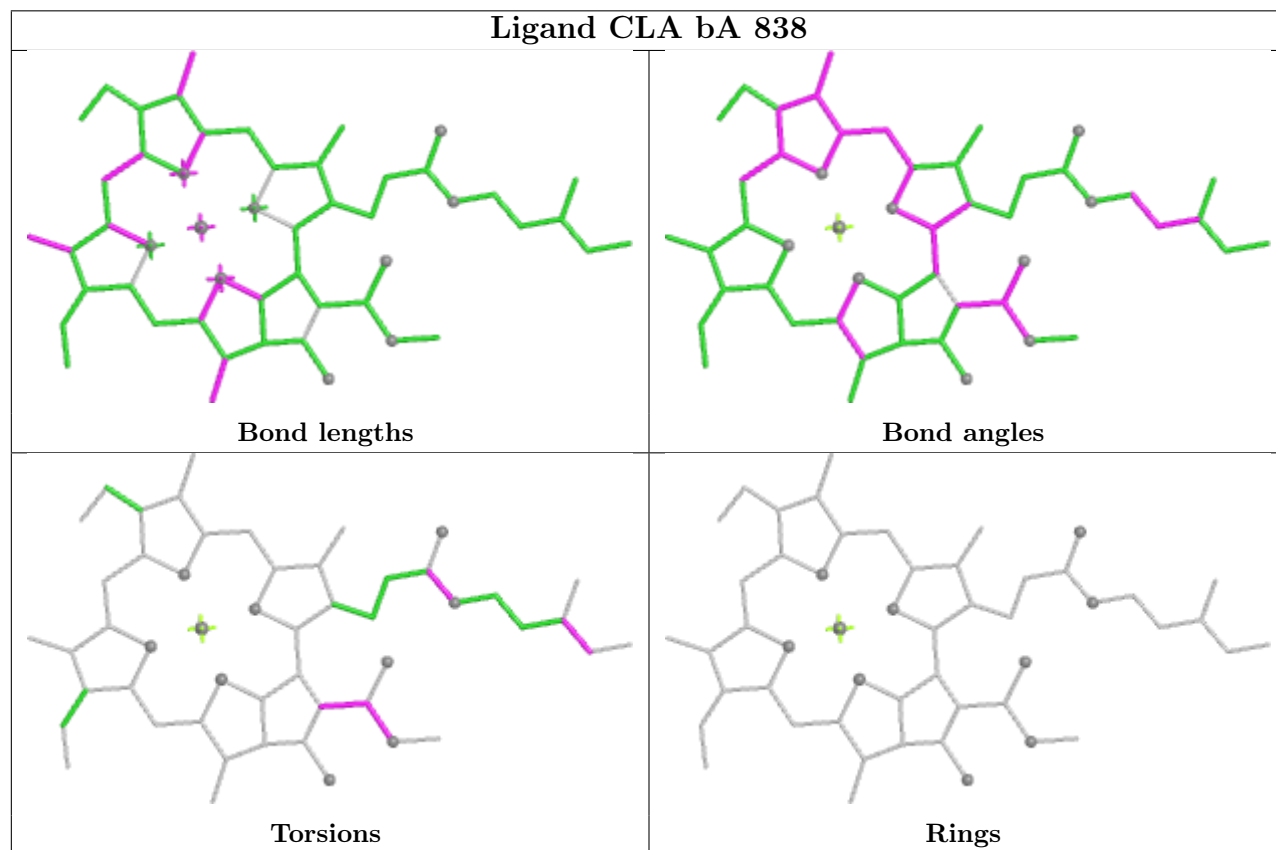
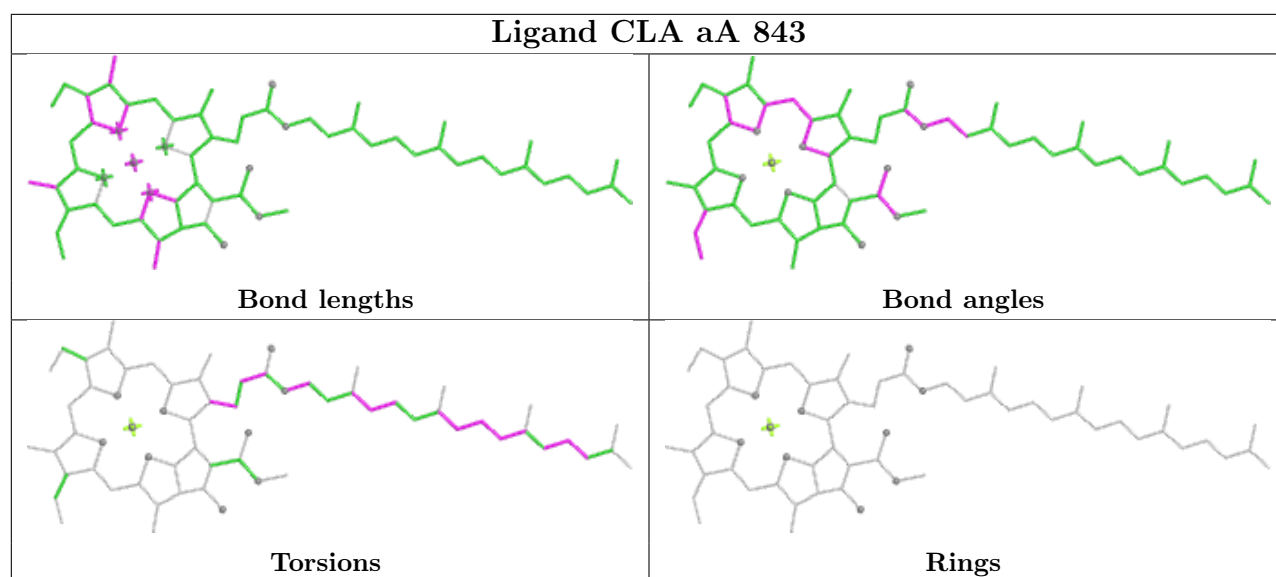


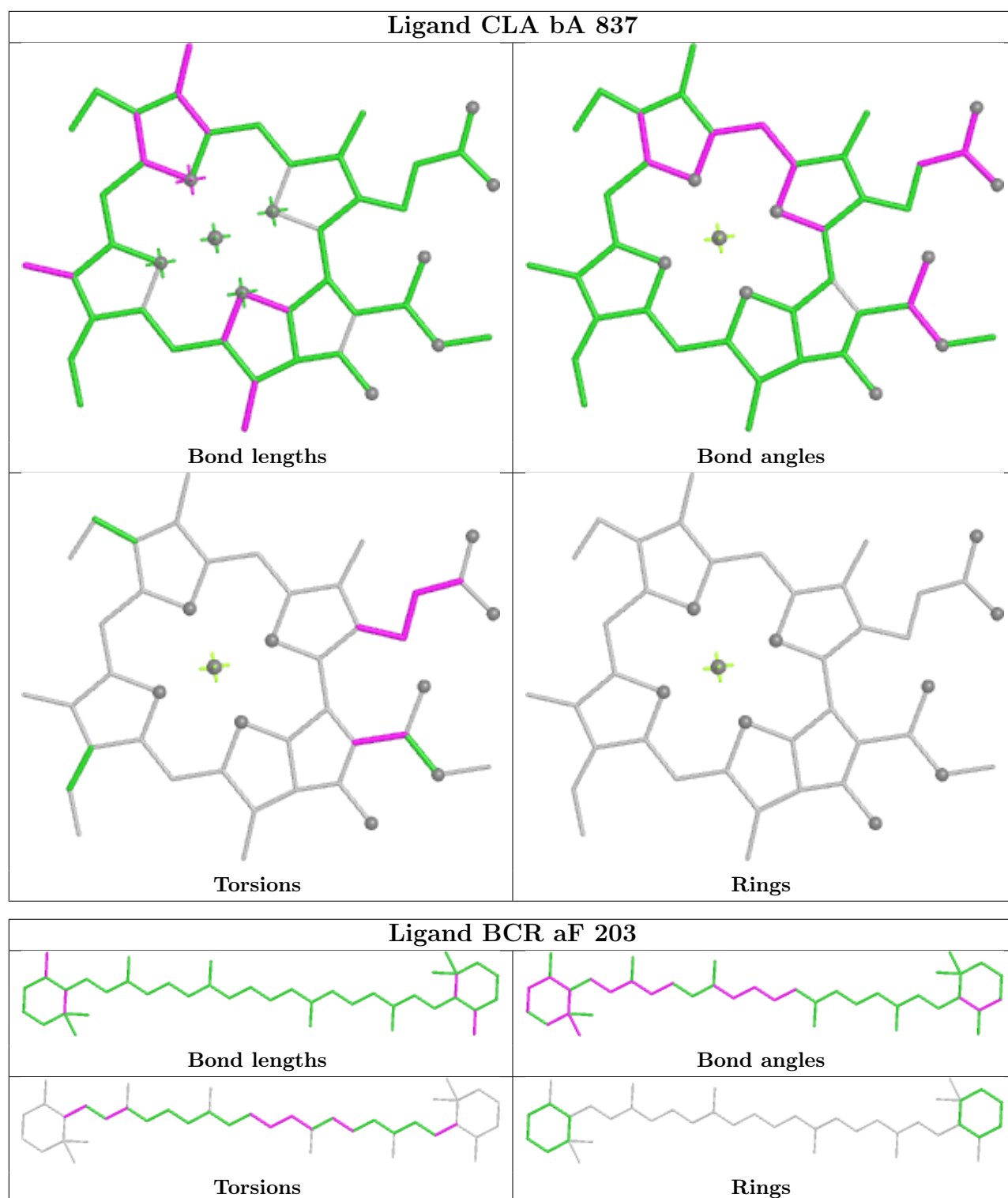


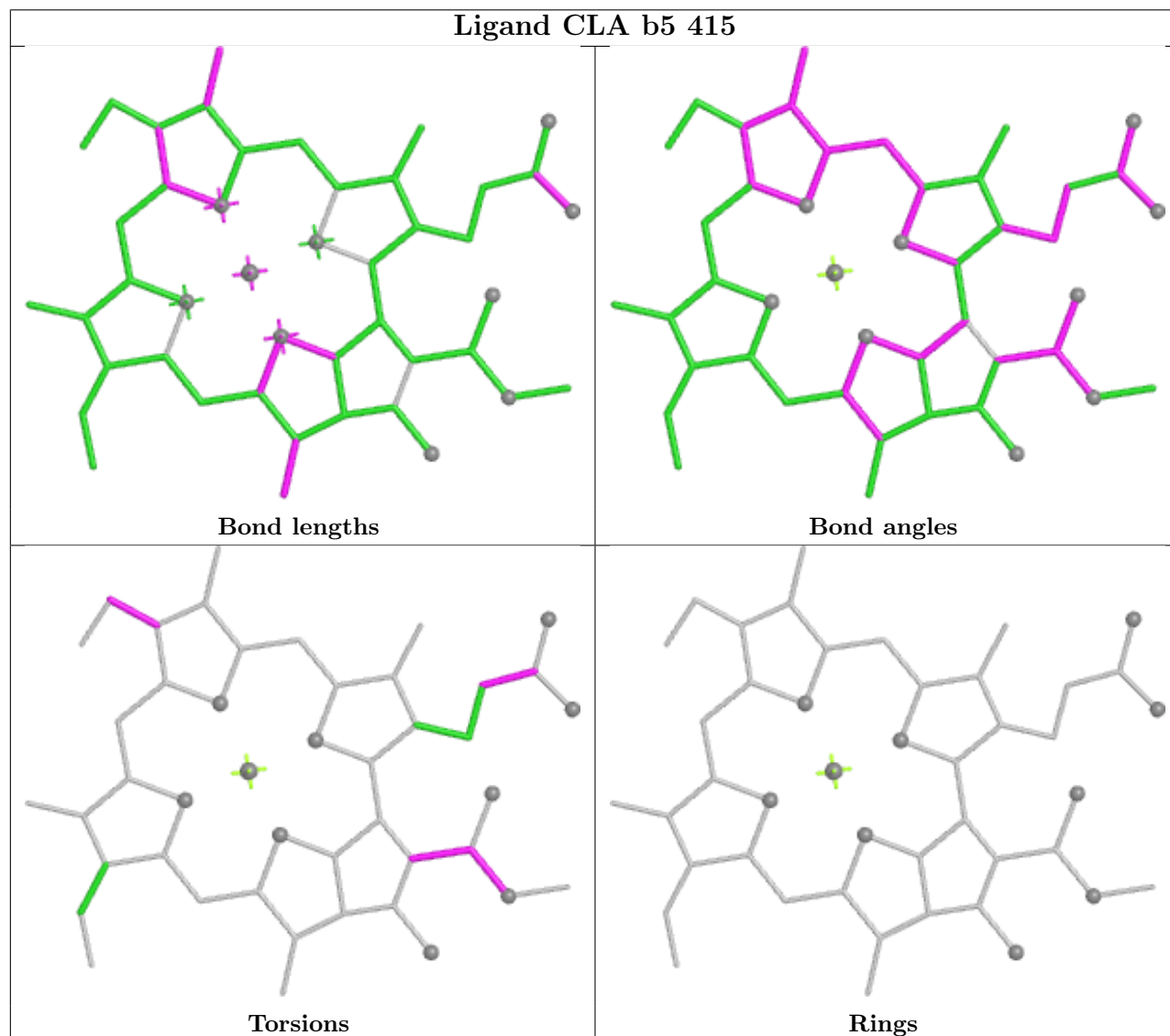
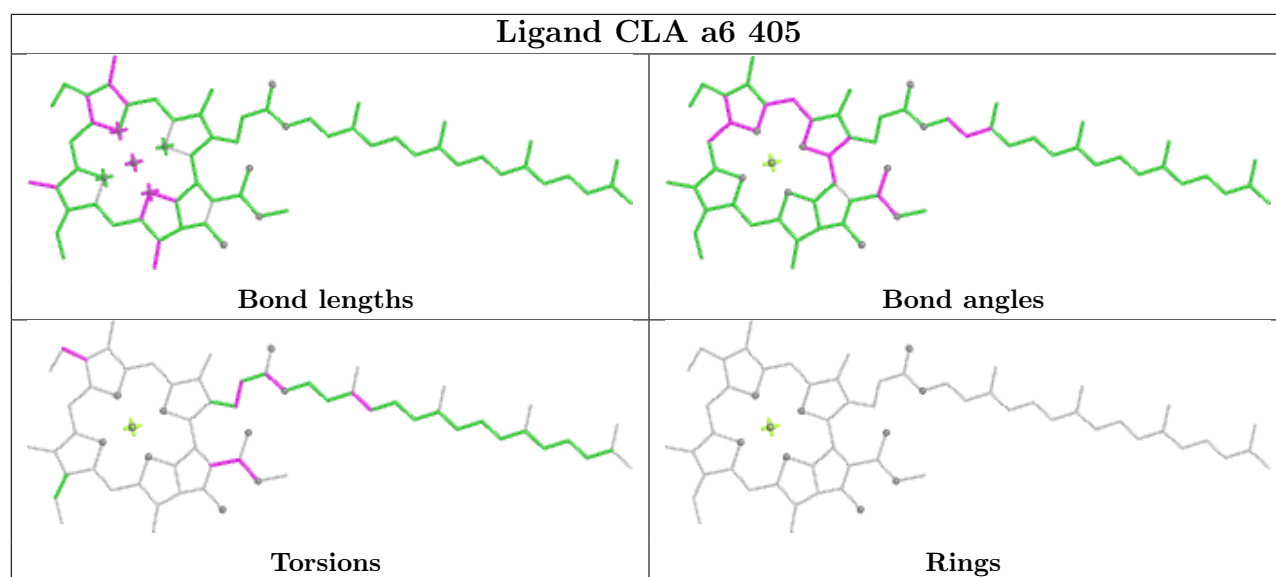


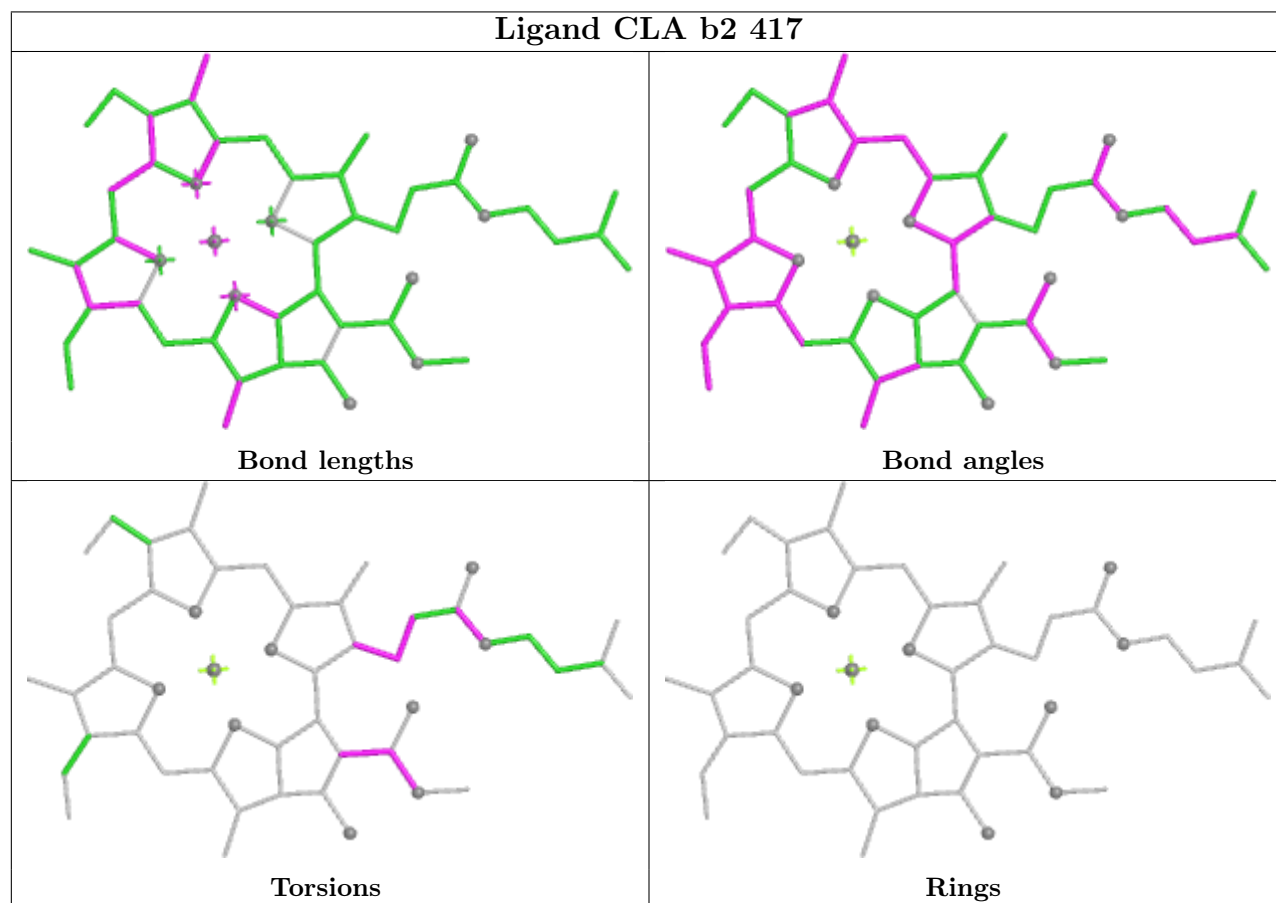
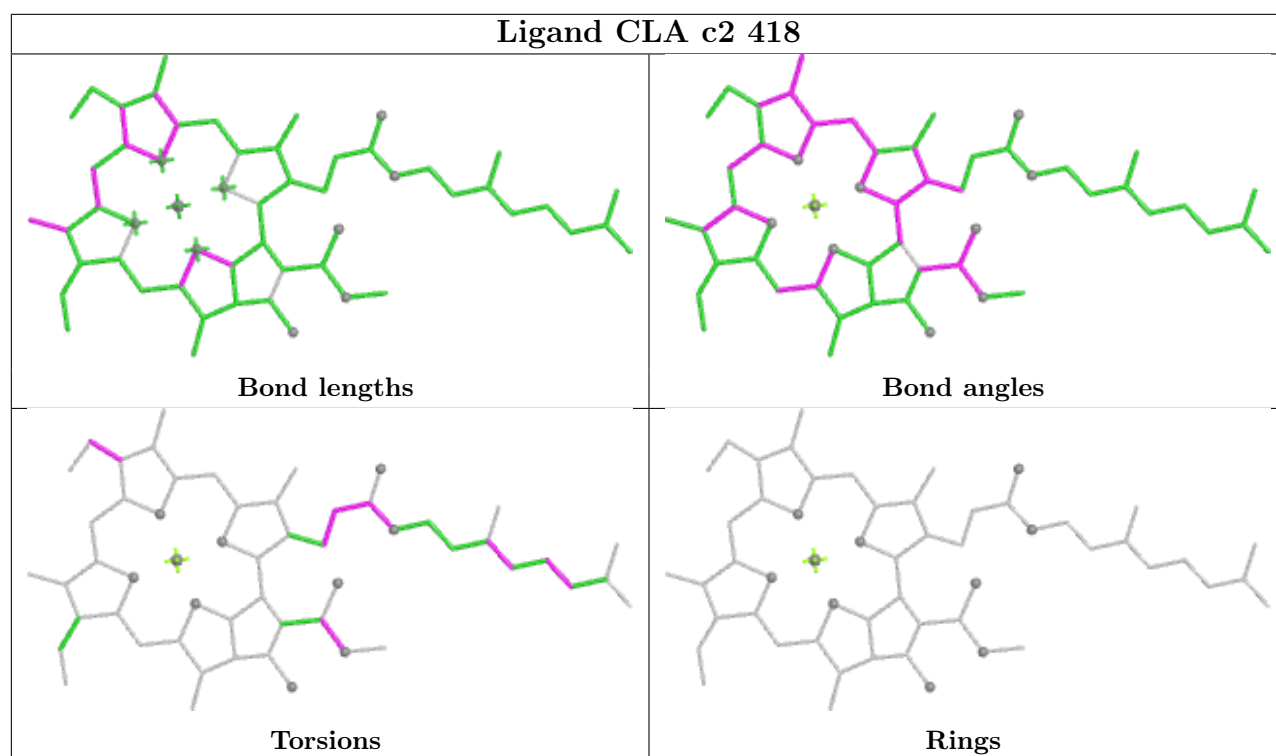


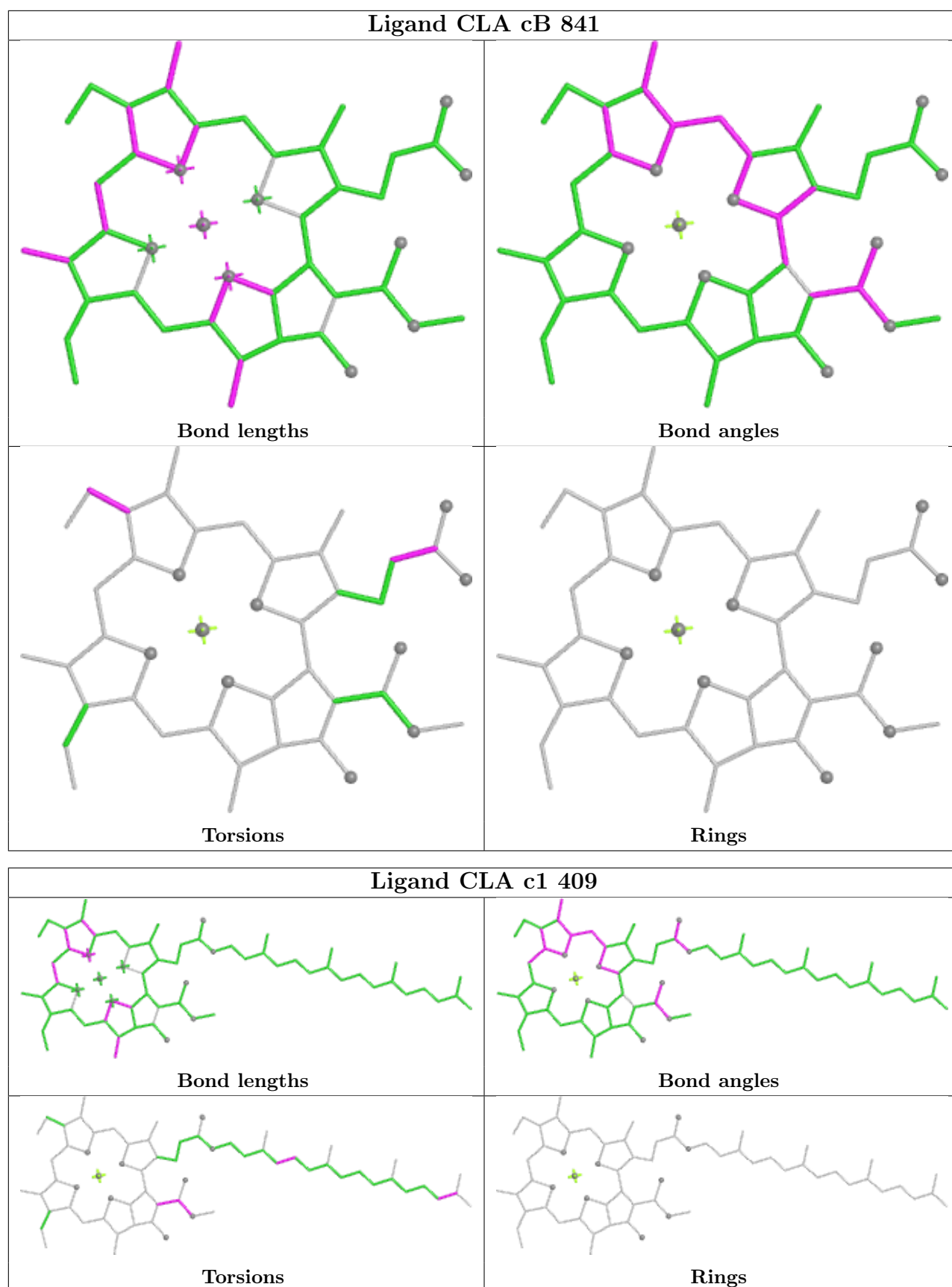


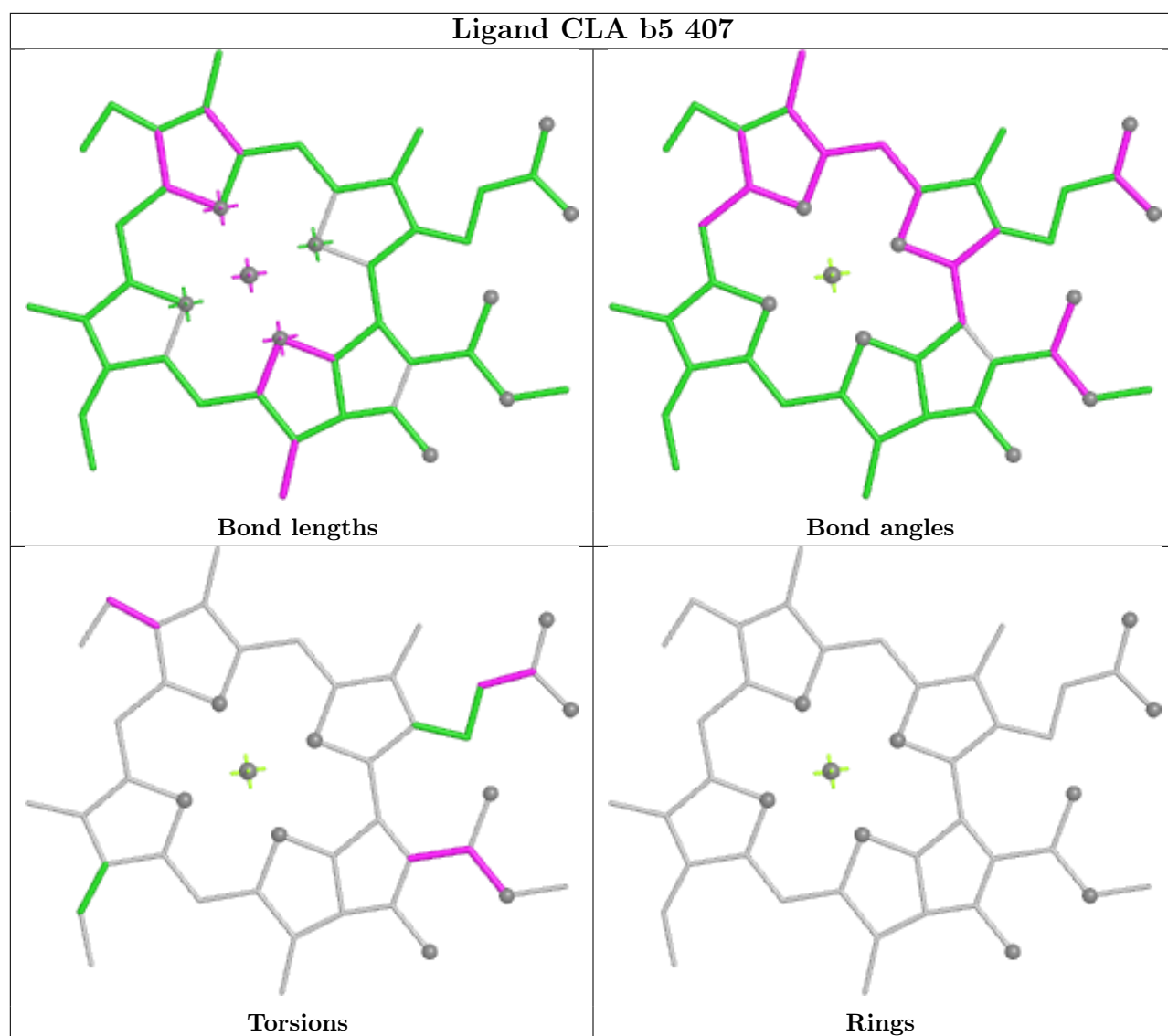




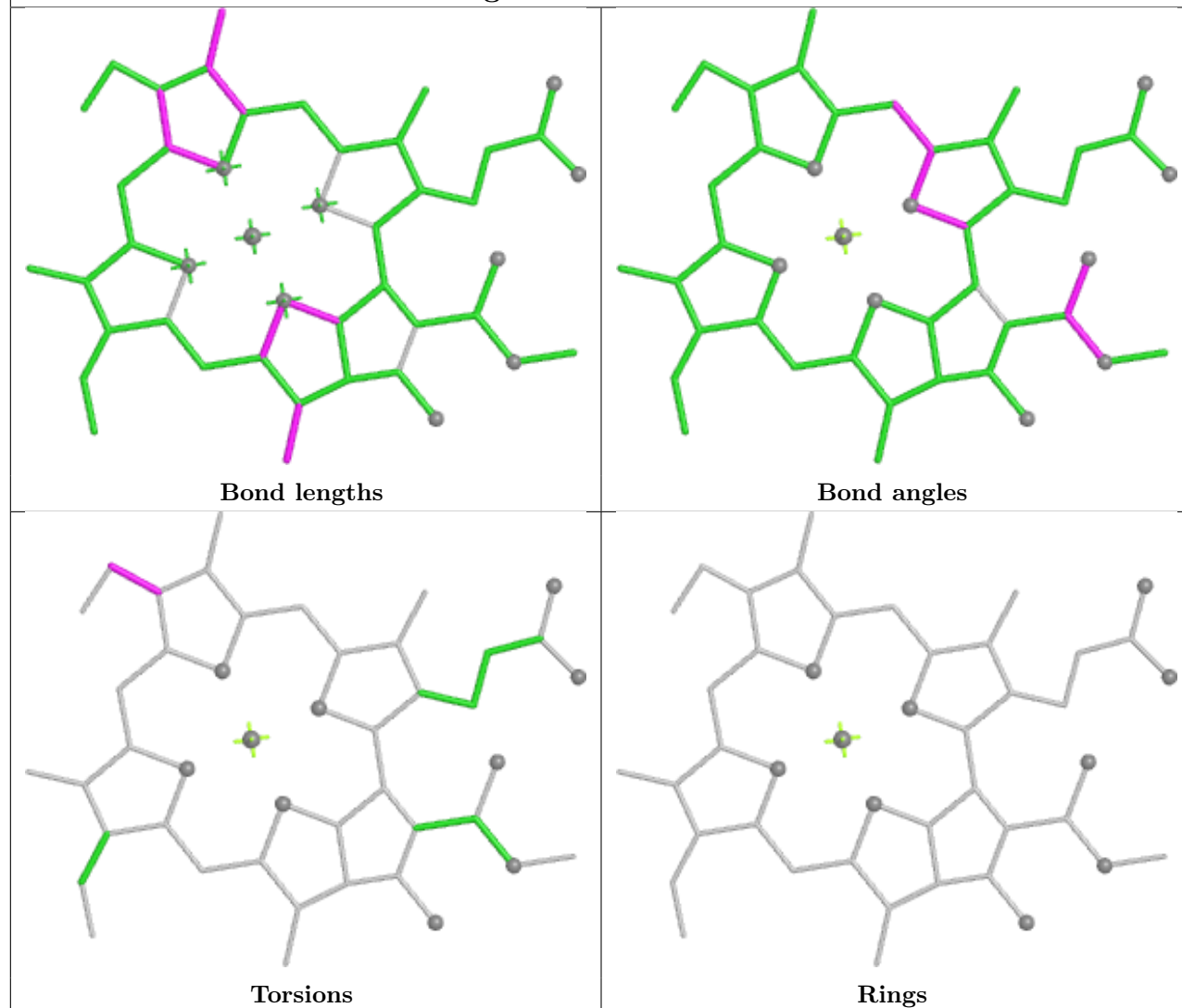




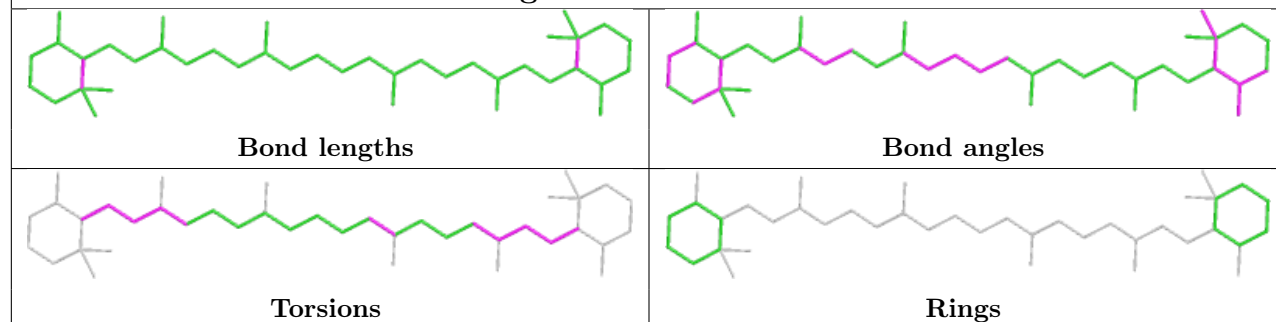


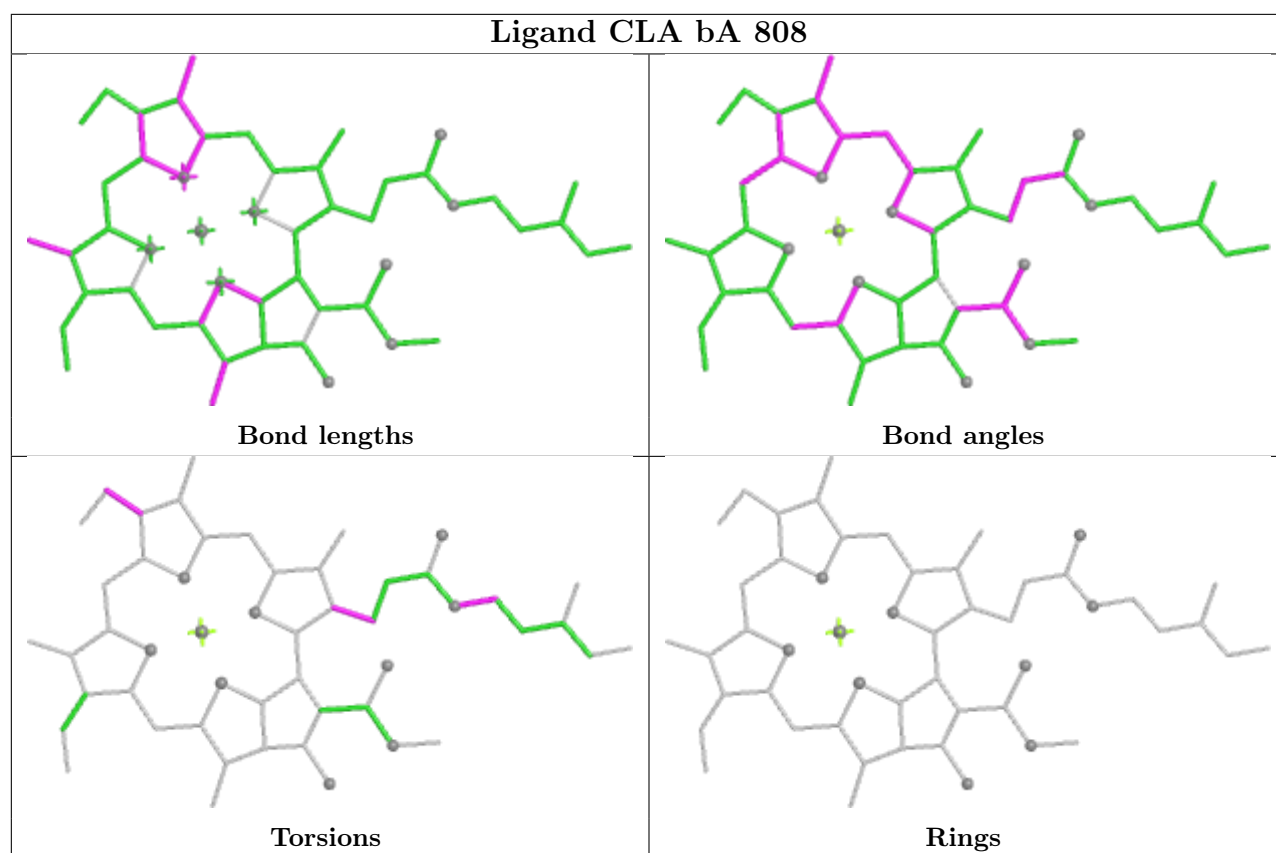


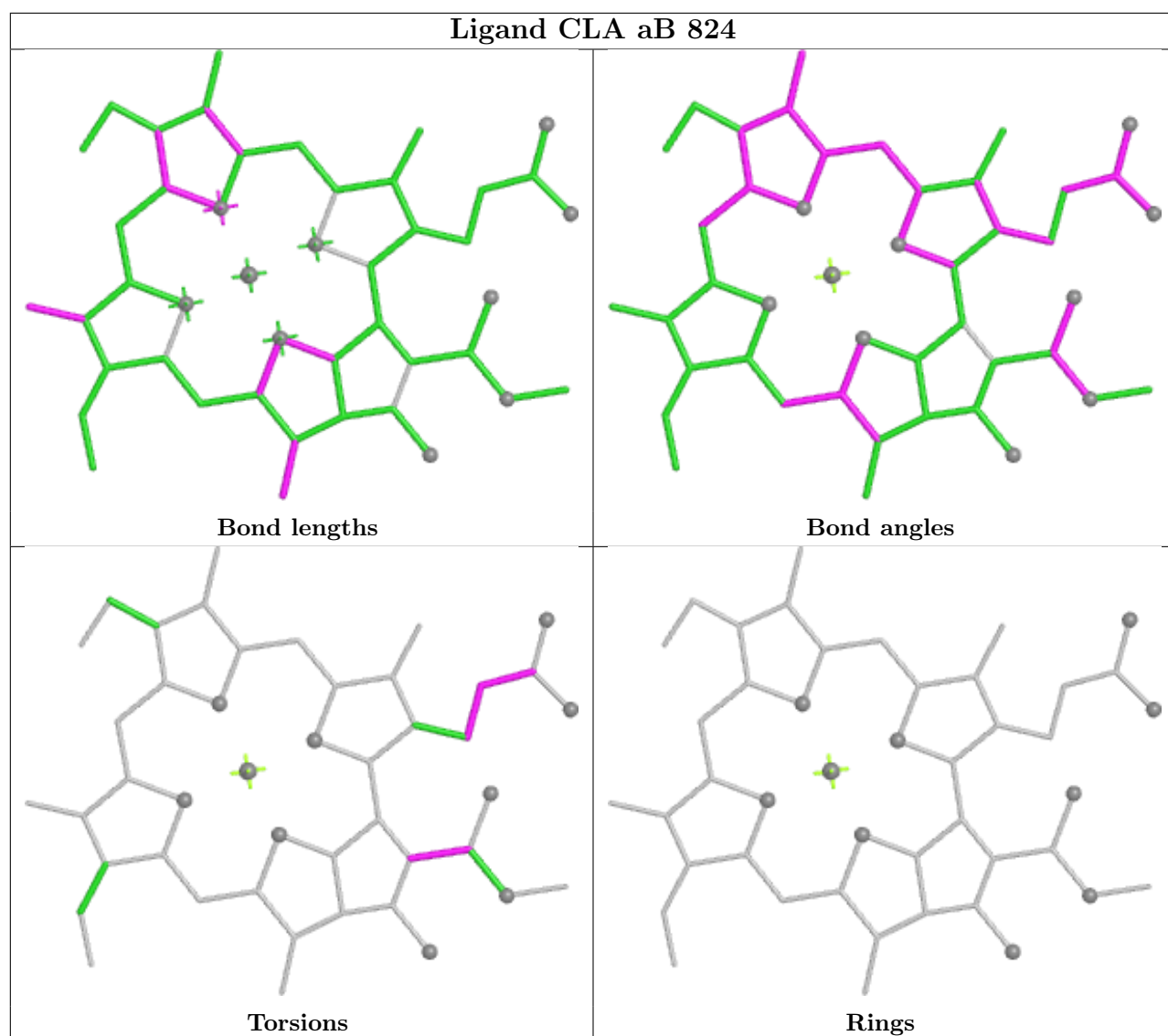
Ligand CLA bB 842

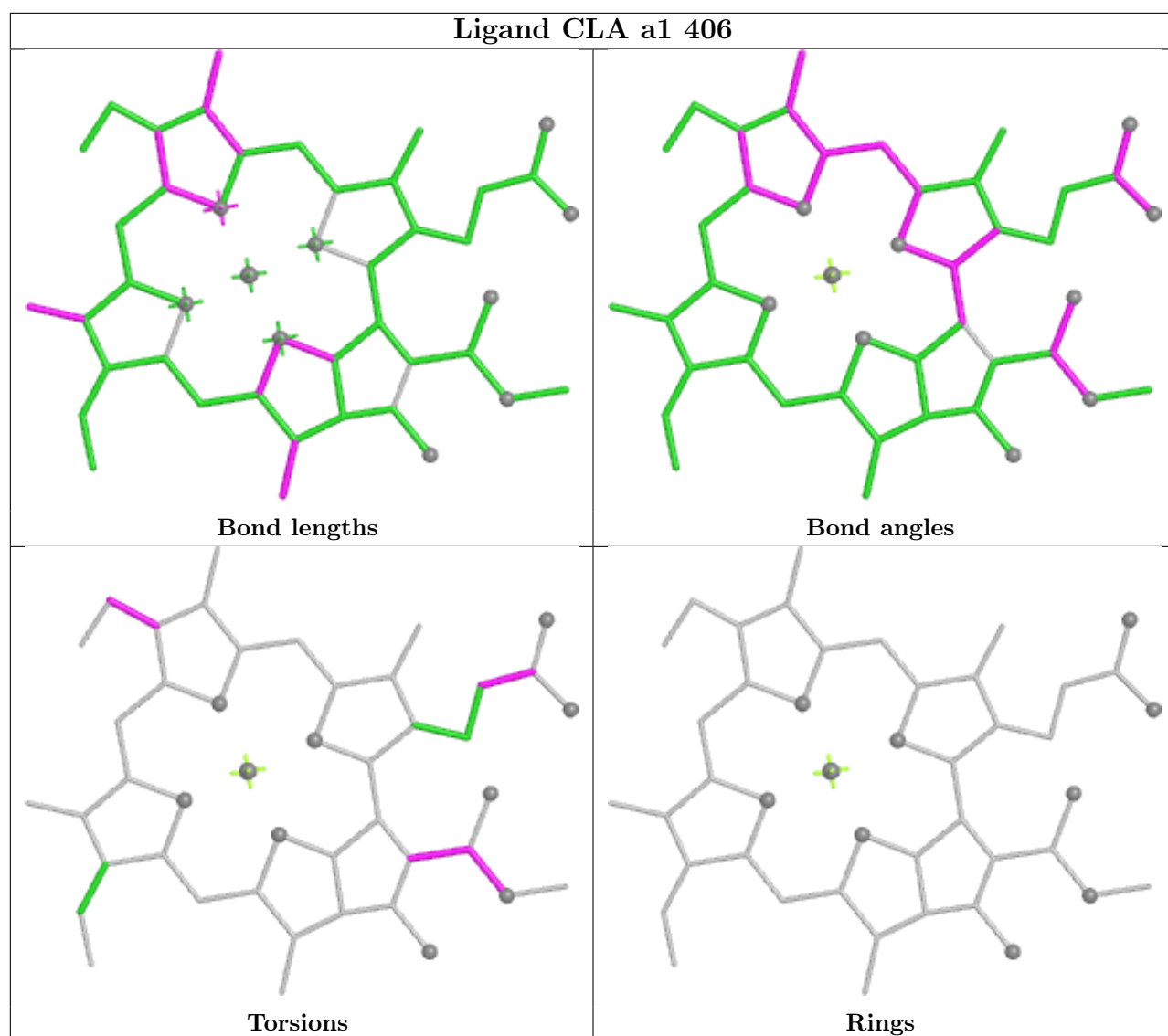


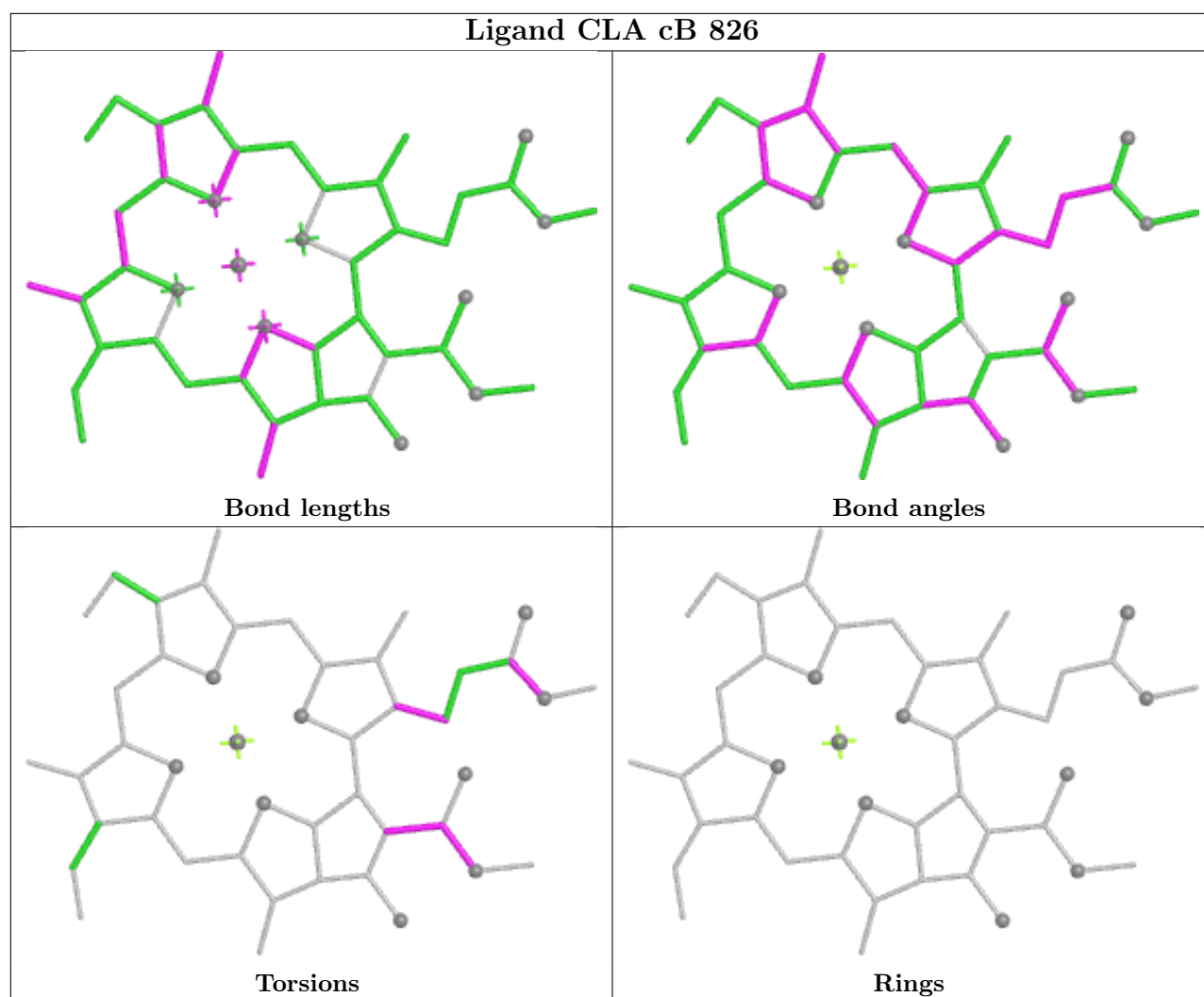
Ligand BCR bA 850

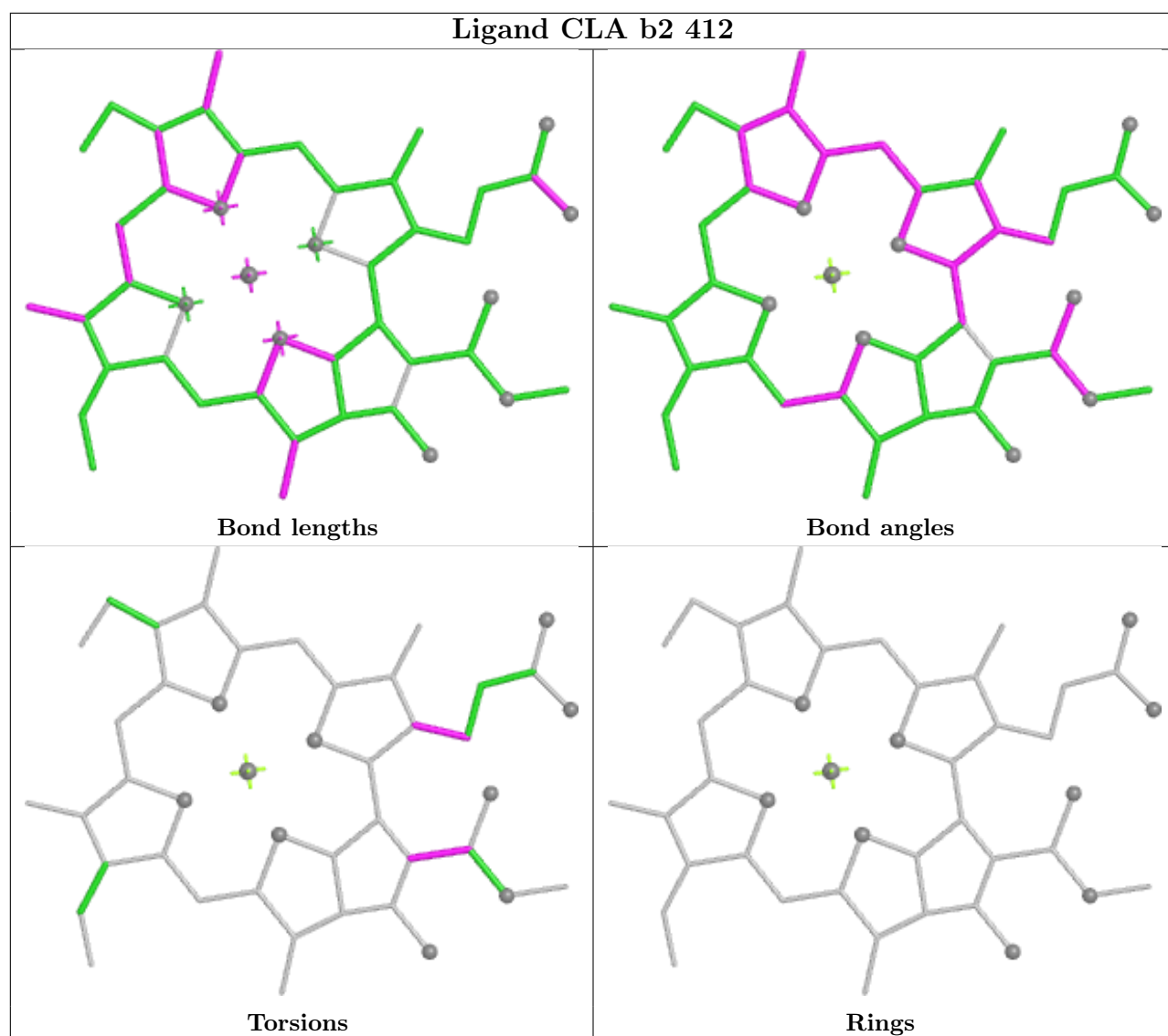


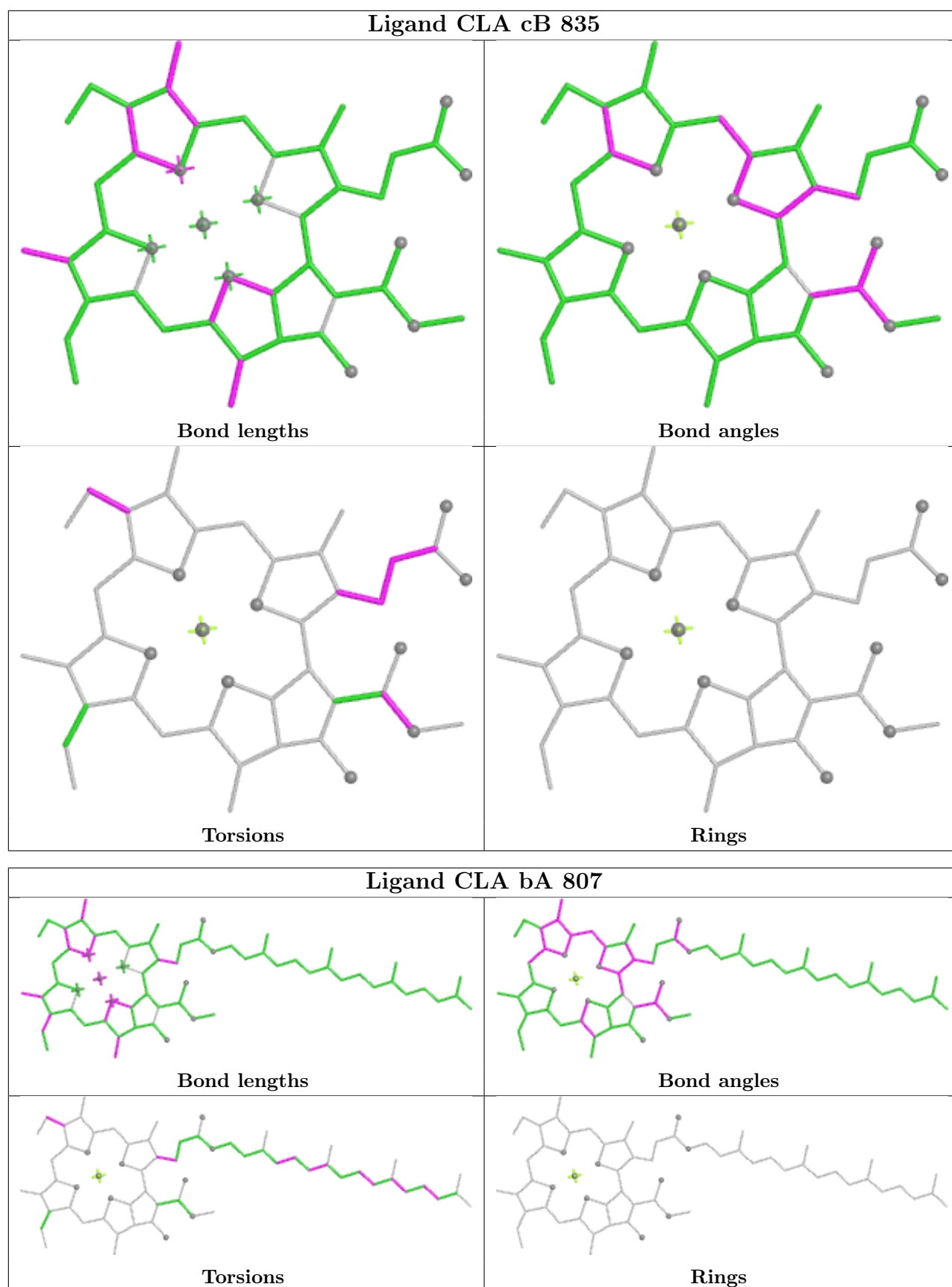


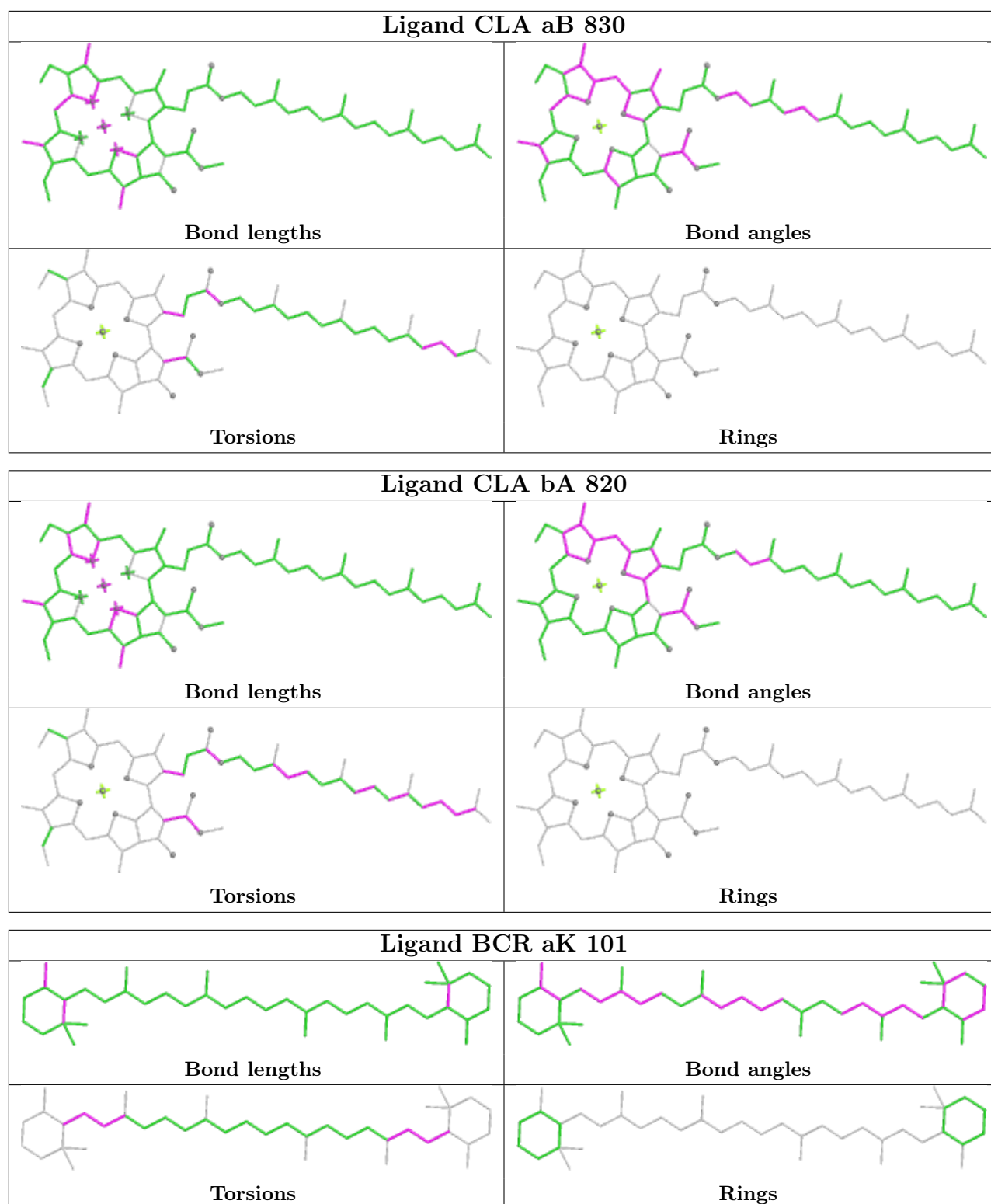


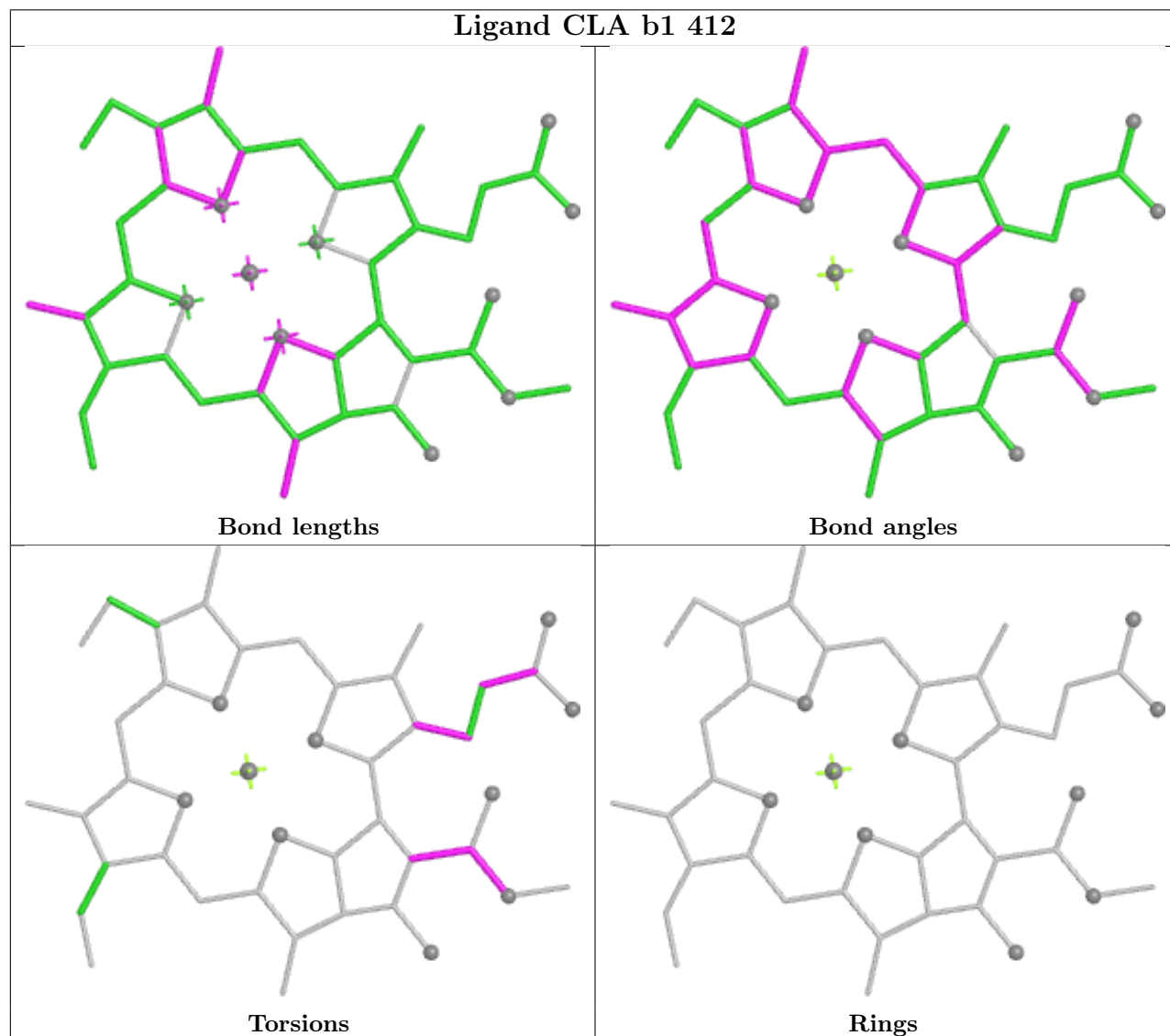
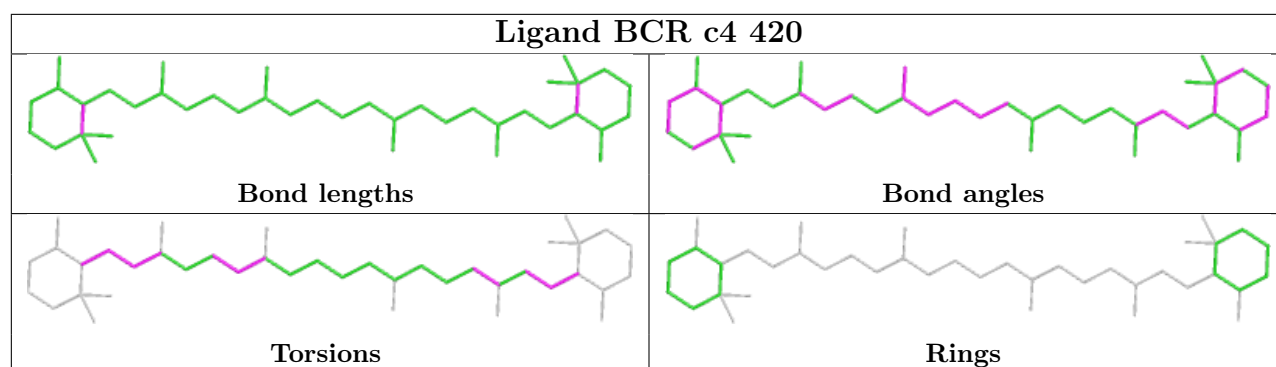


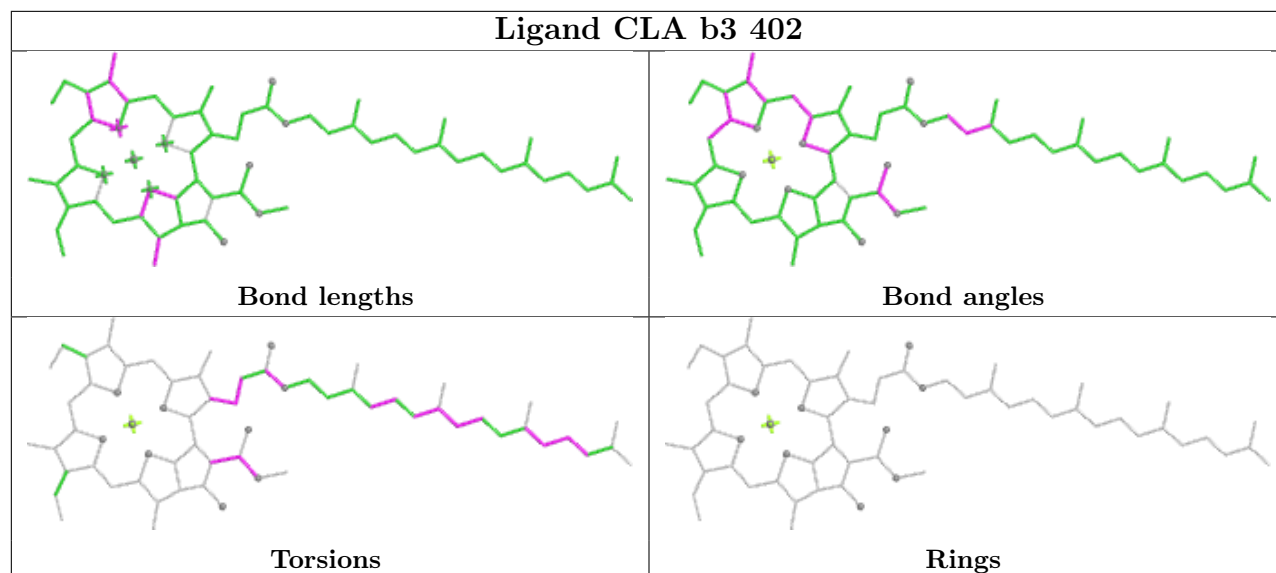
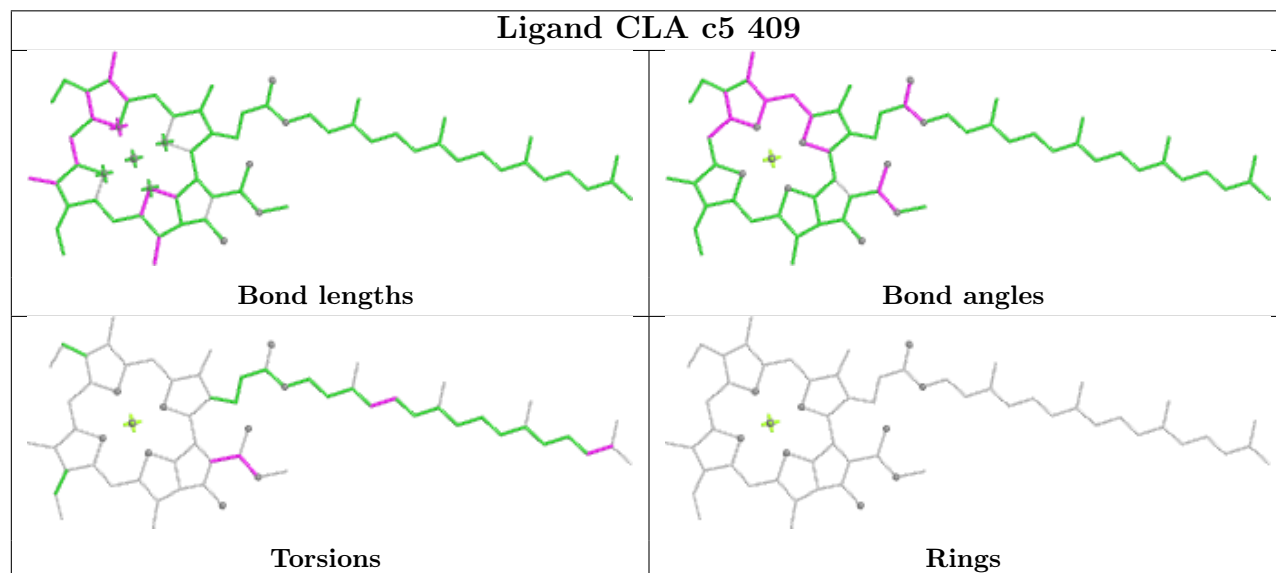
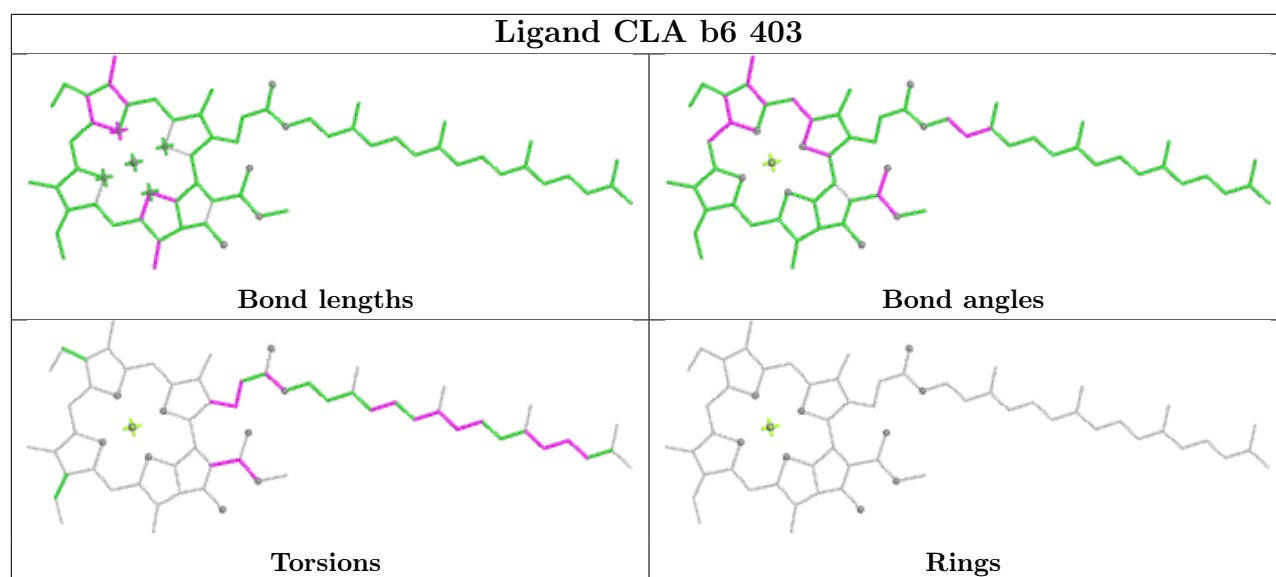


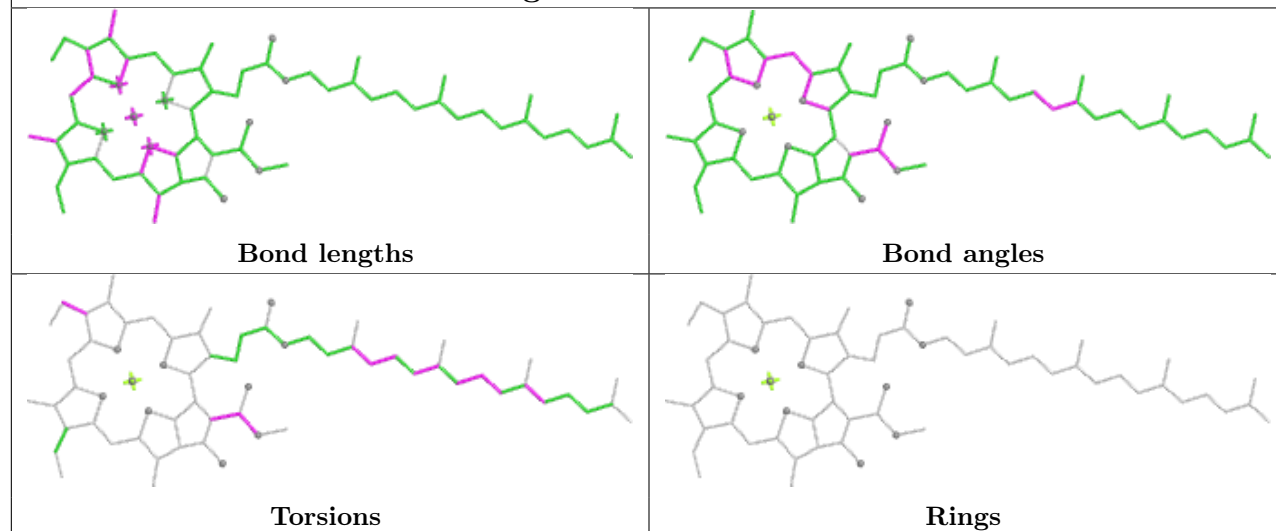
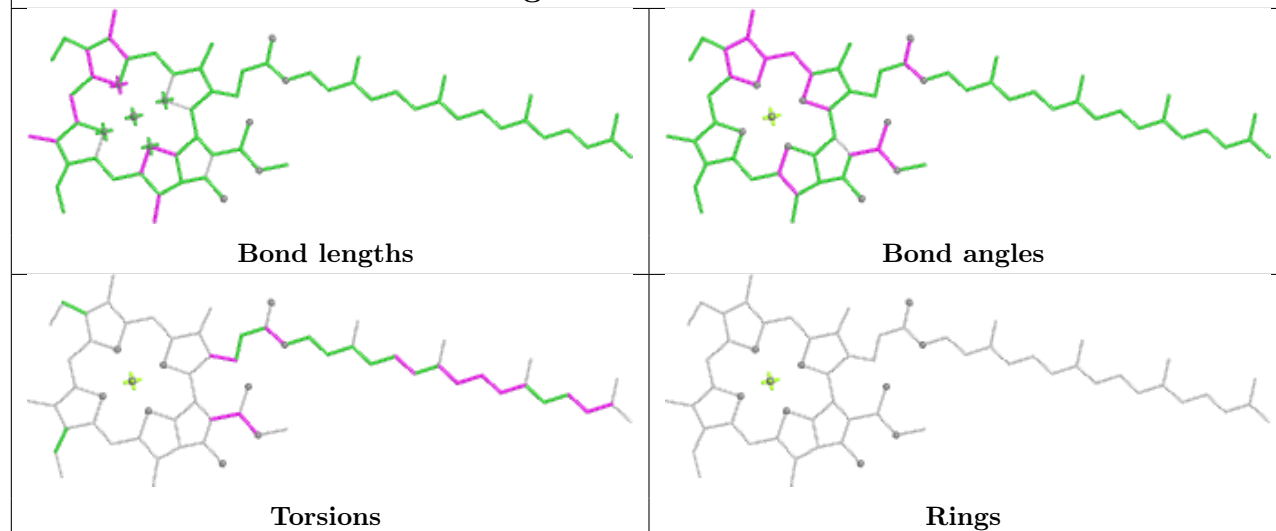


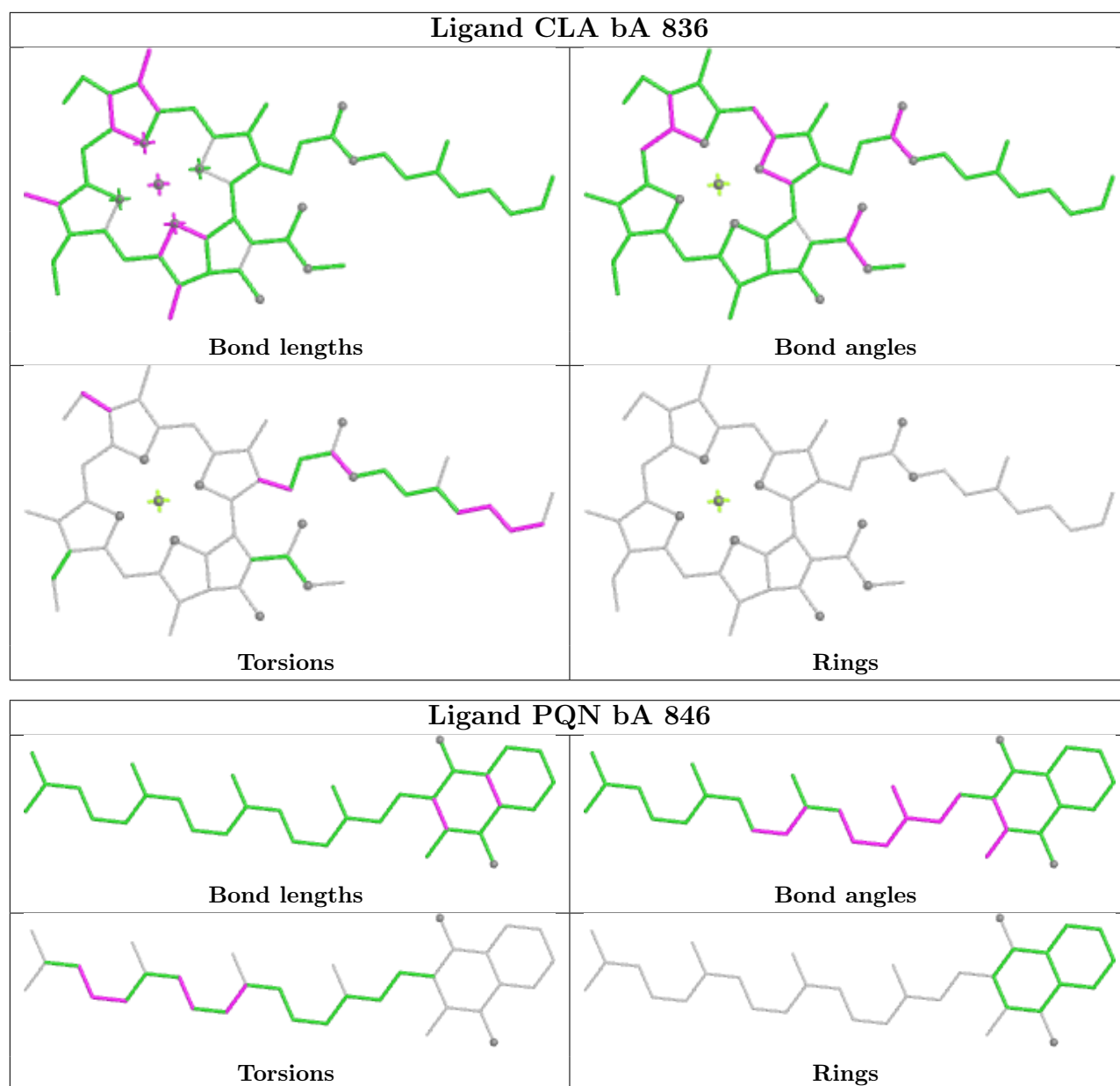


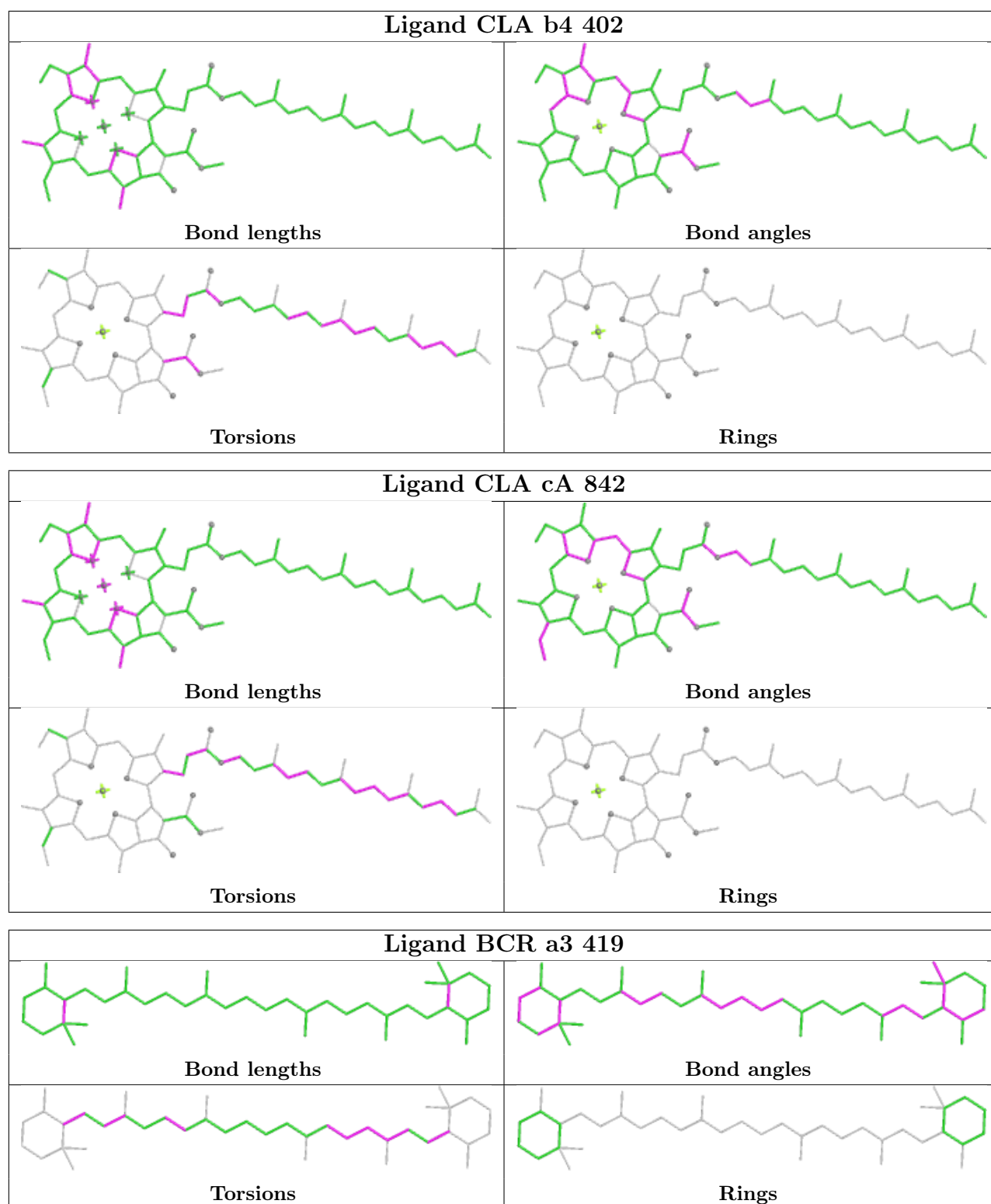


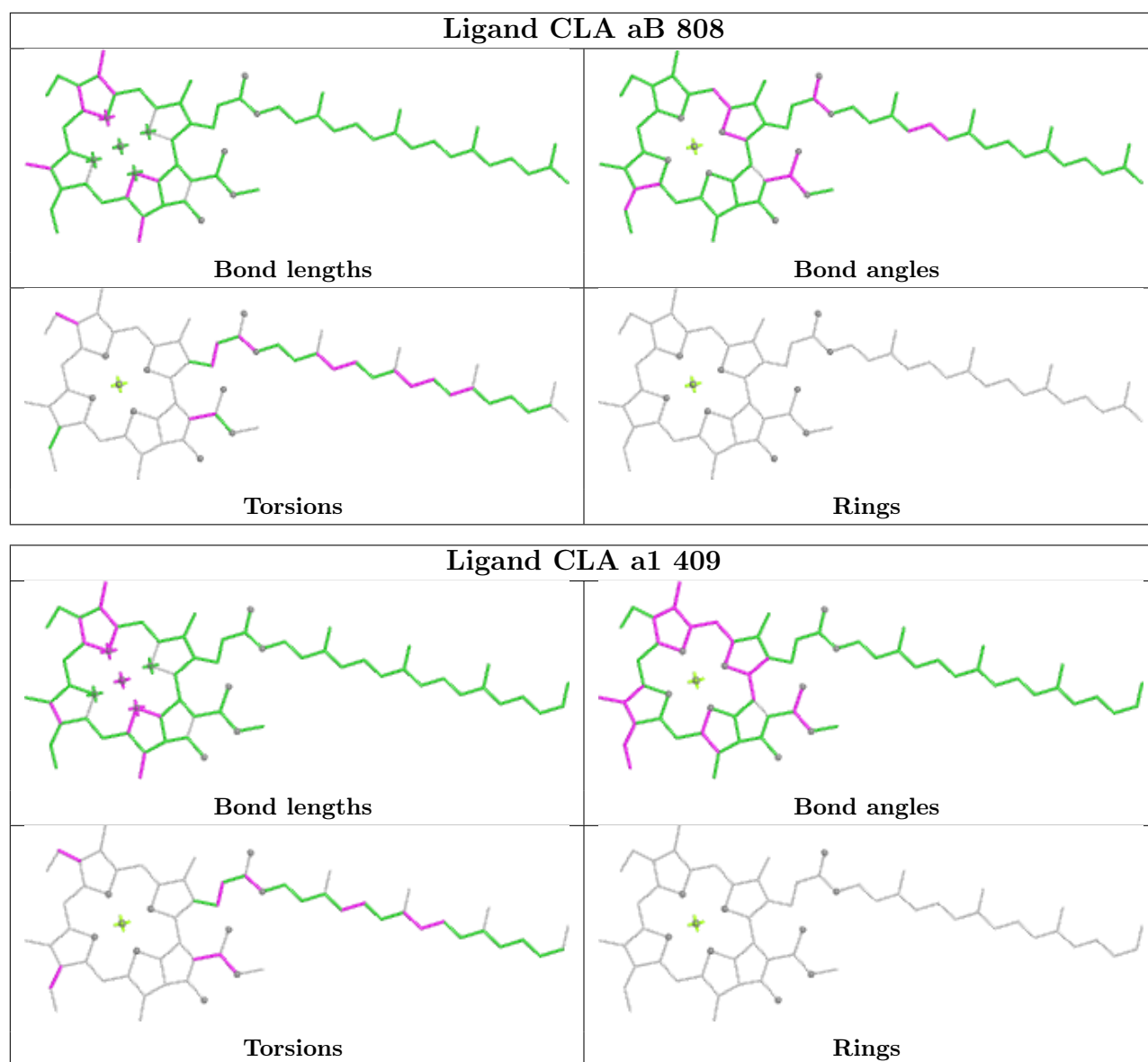


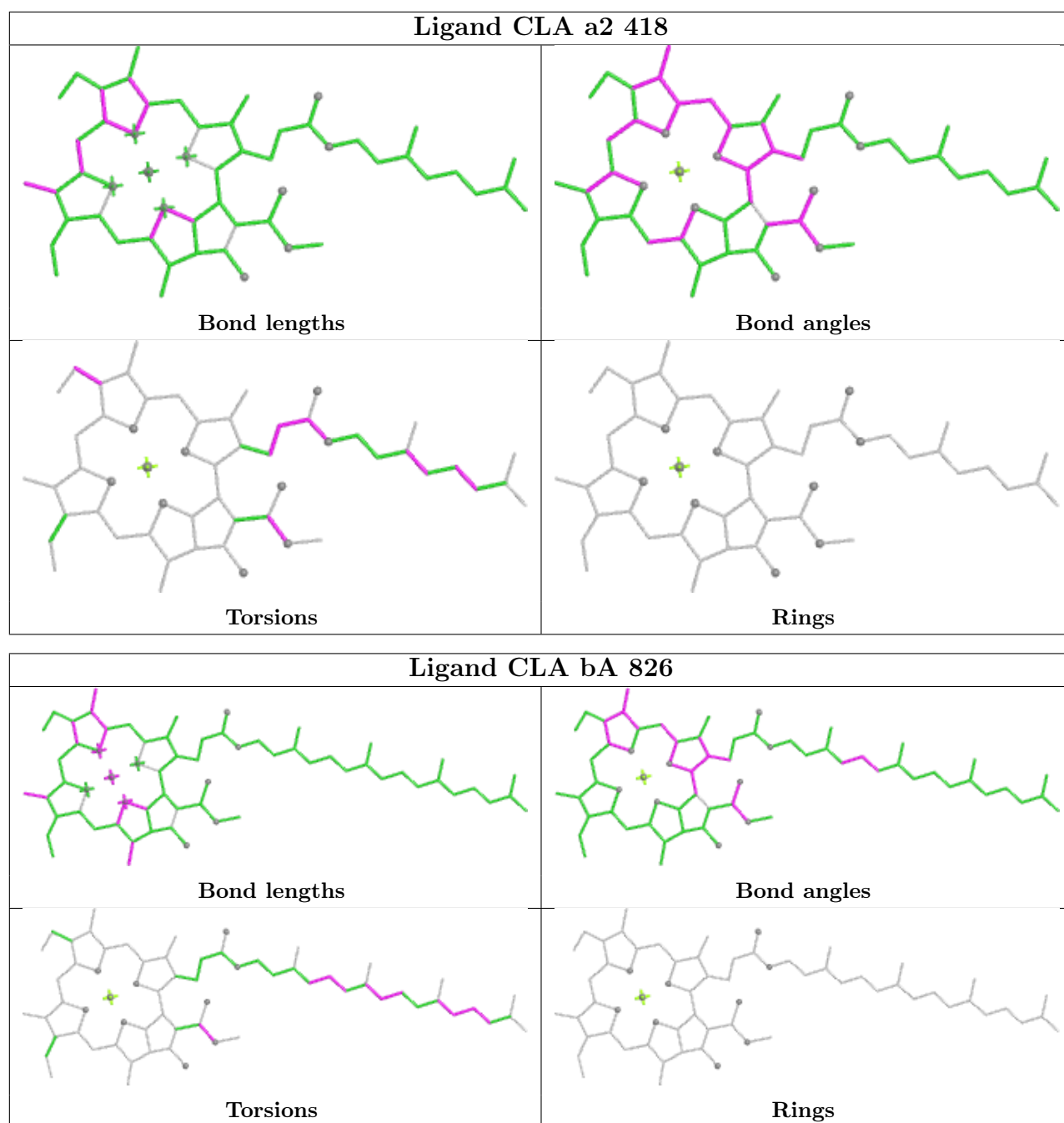


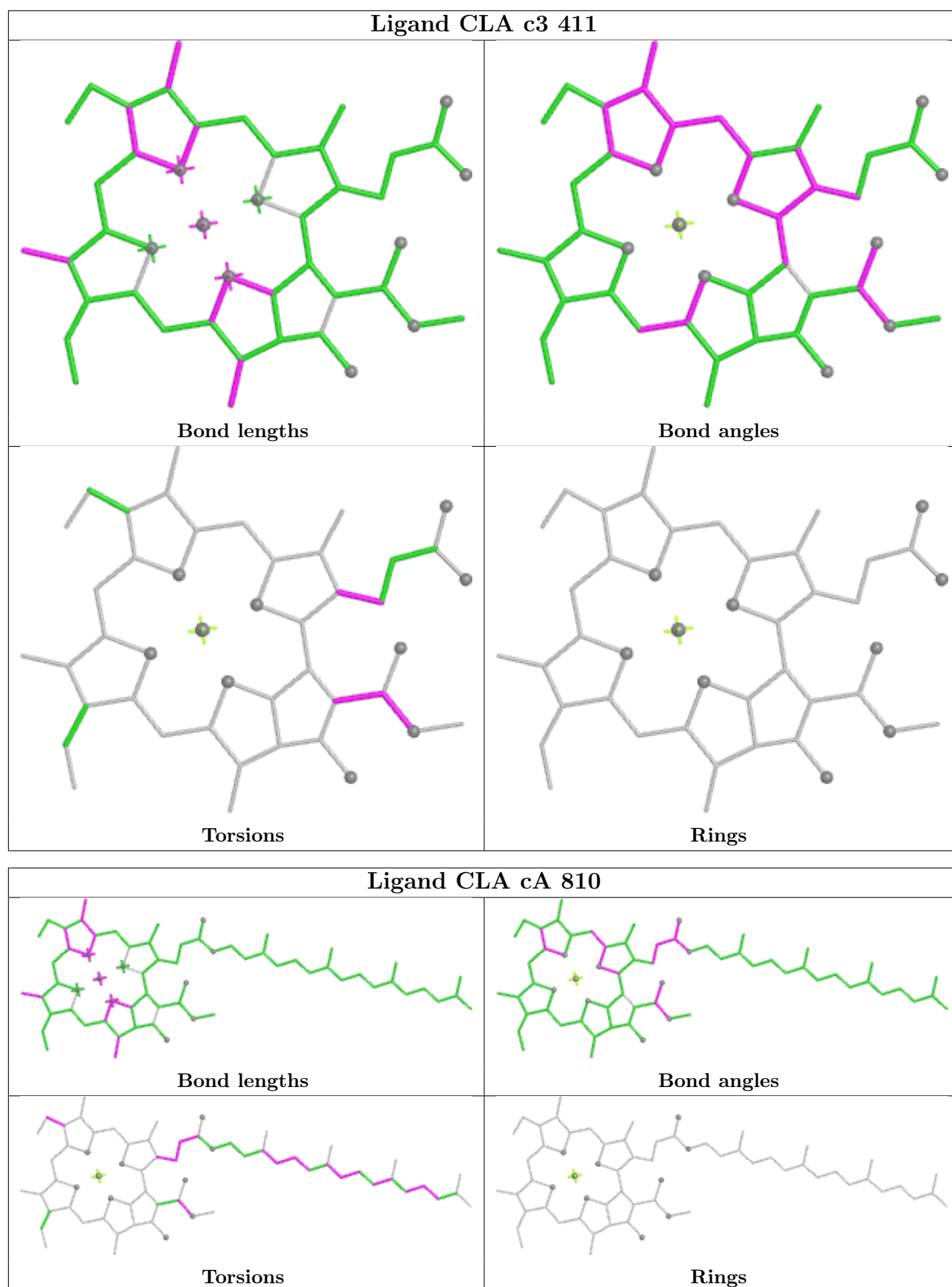
Ligand CLA aA 839**Ligand CLA aB 815**

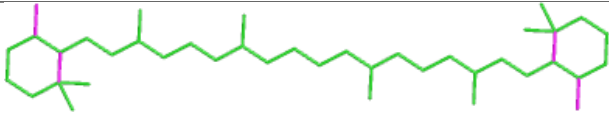
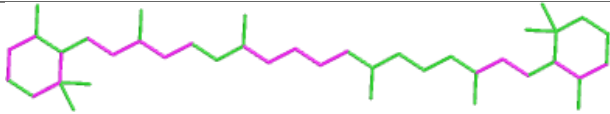
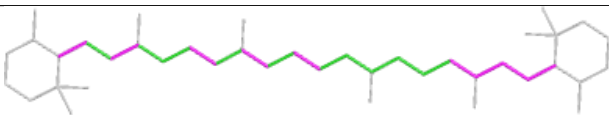
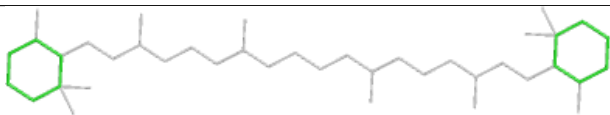


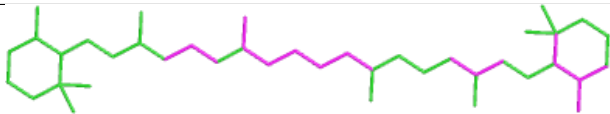
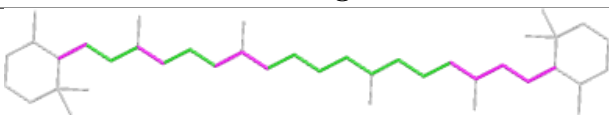
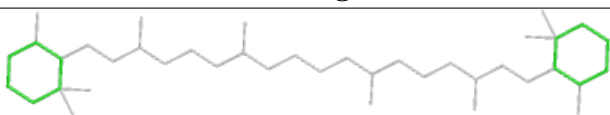


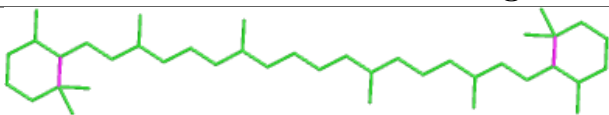
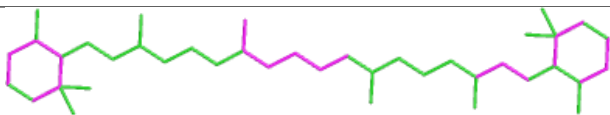
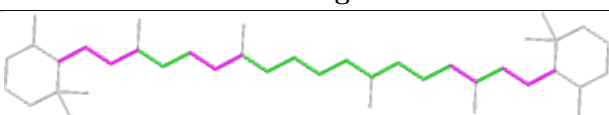
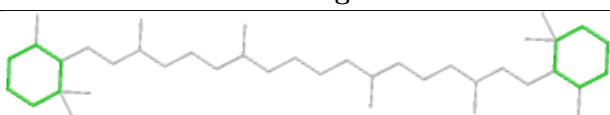




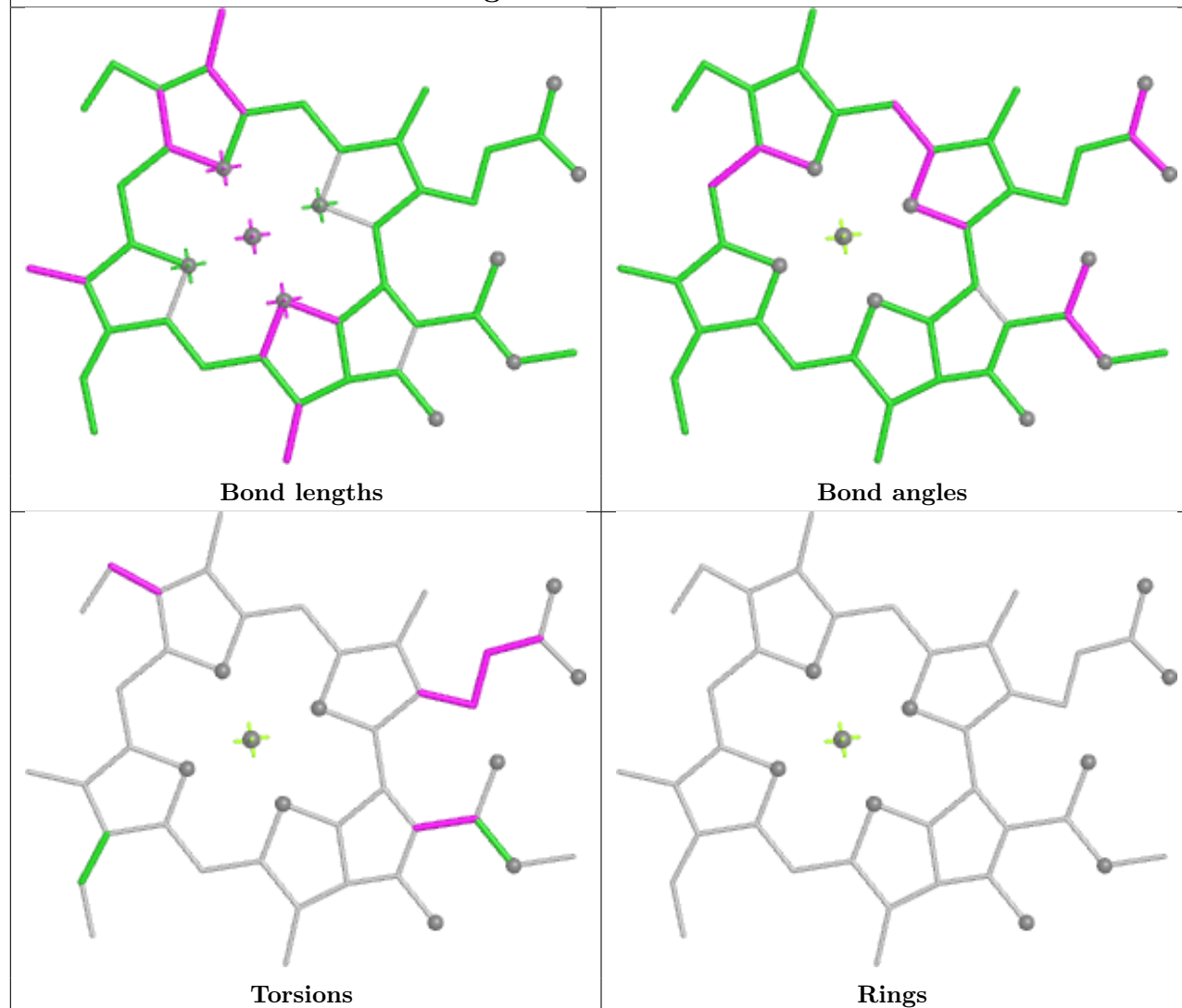


Ligand BCR aB 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

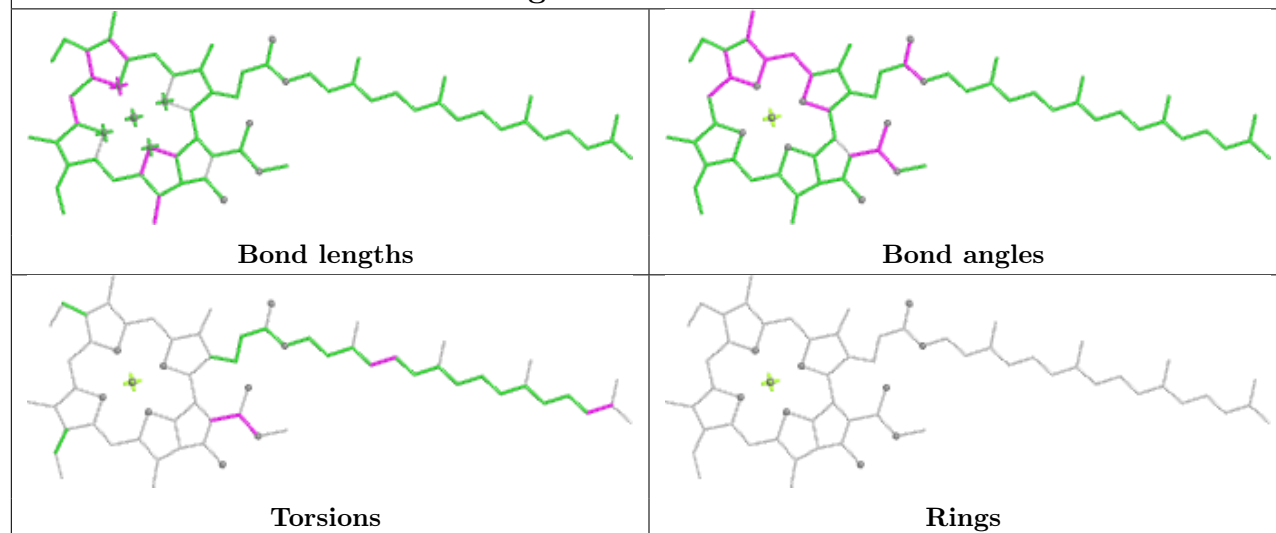
Ligand BCR aB 849	
	
Bond lengths	Bond angles
	
Torsions	Rings

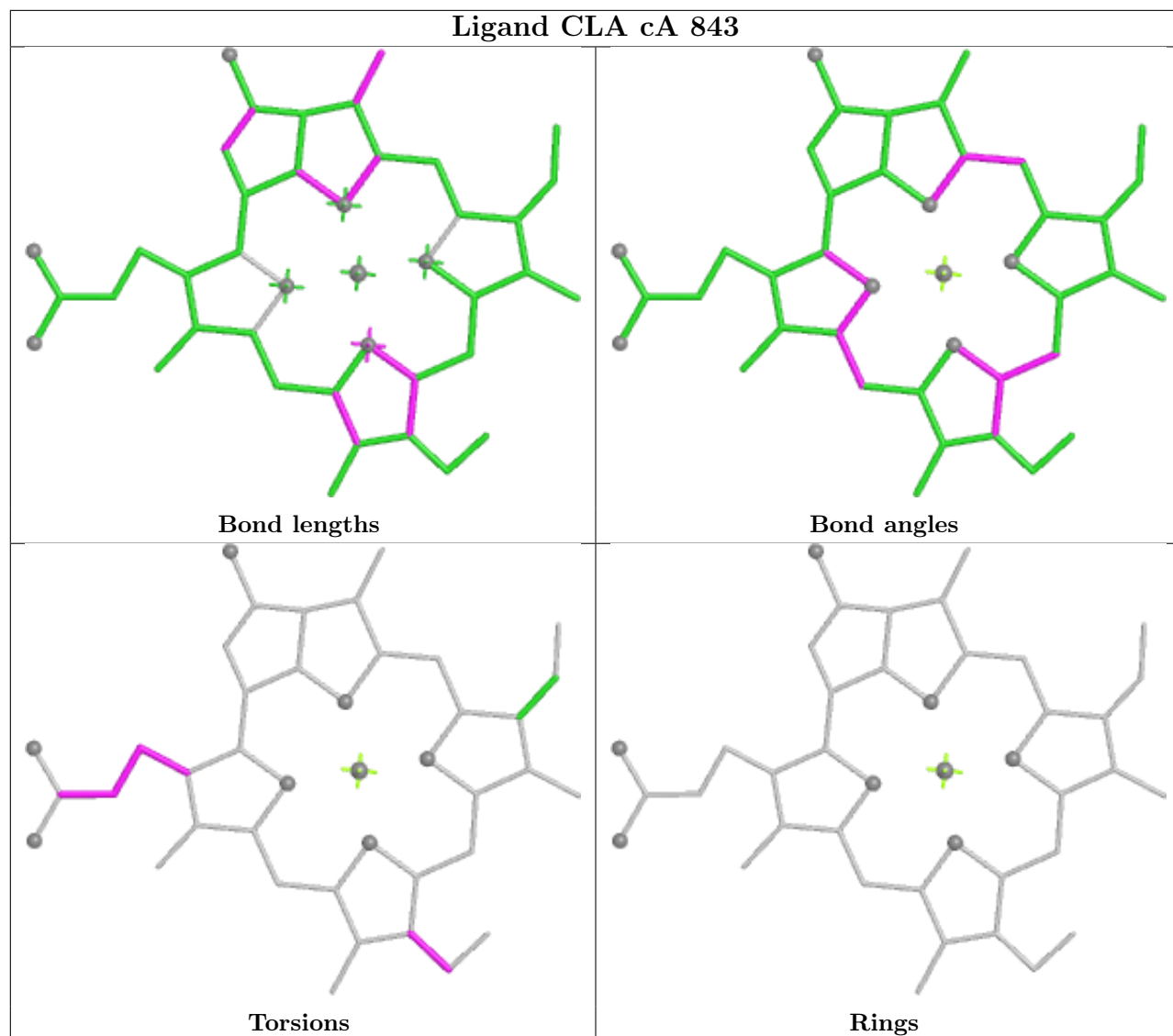
Ligand BCR a3 420	
	
Bond lengths	Bond angles
	
Torsions	Rings

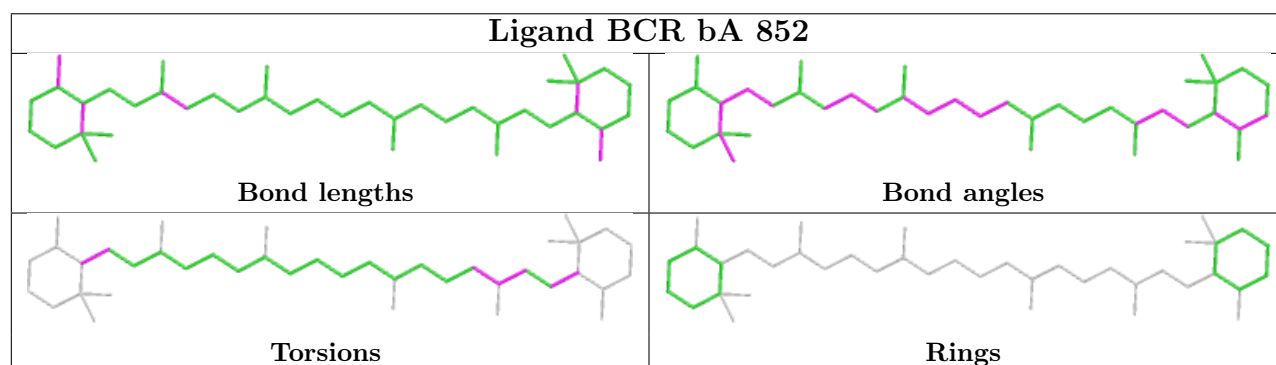
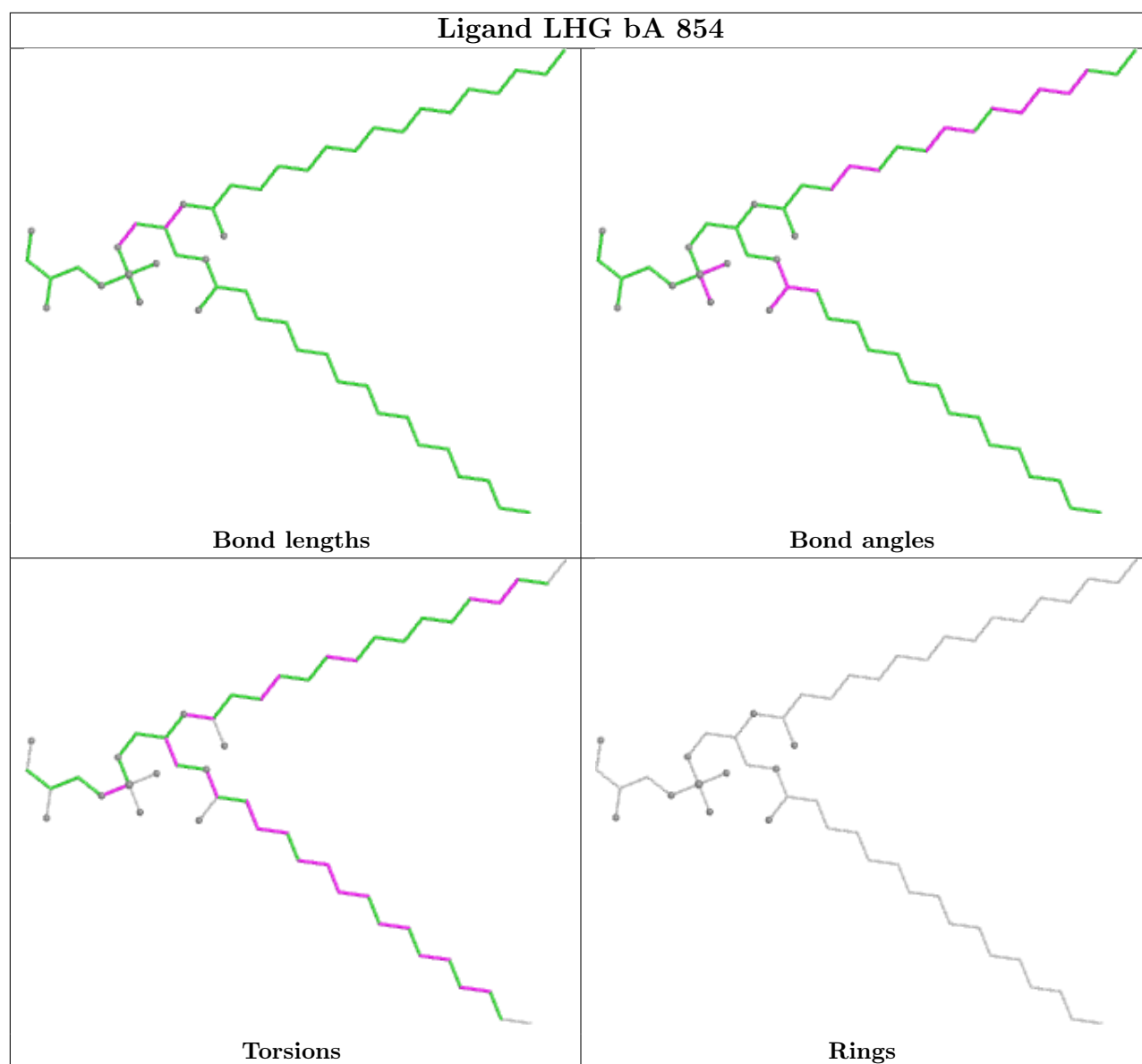
Ligand CLA bB 831

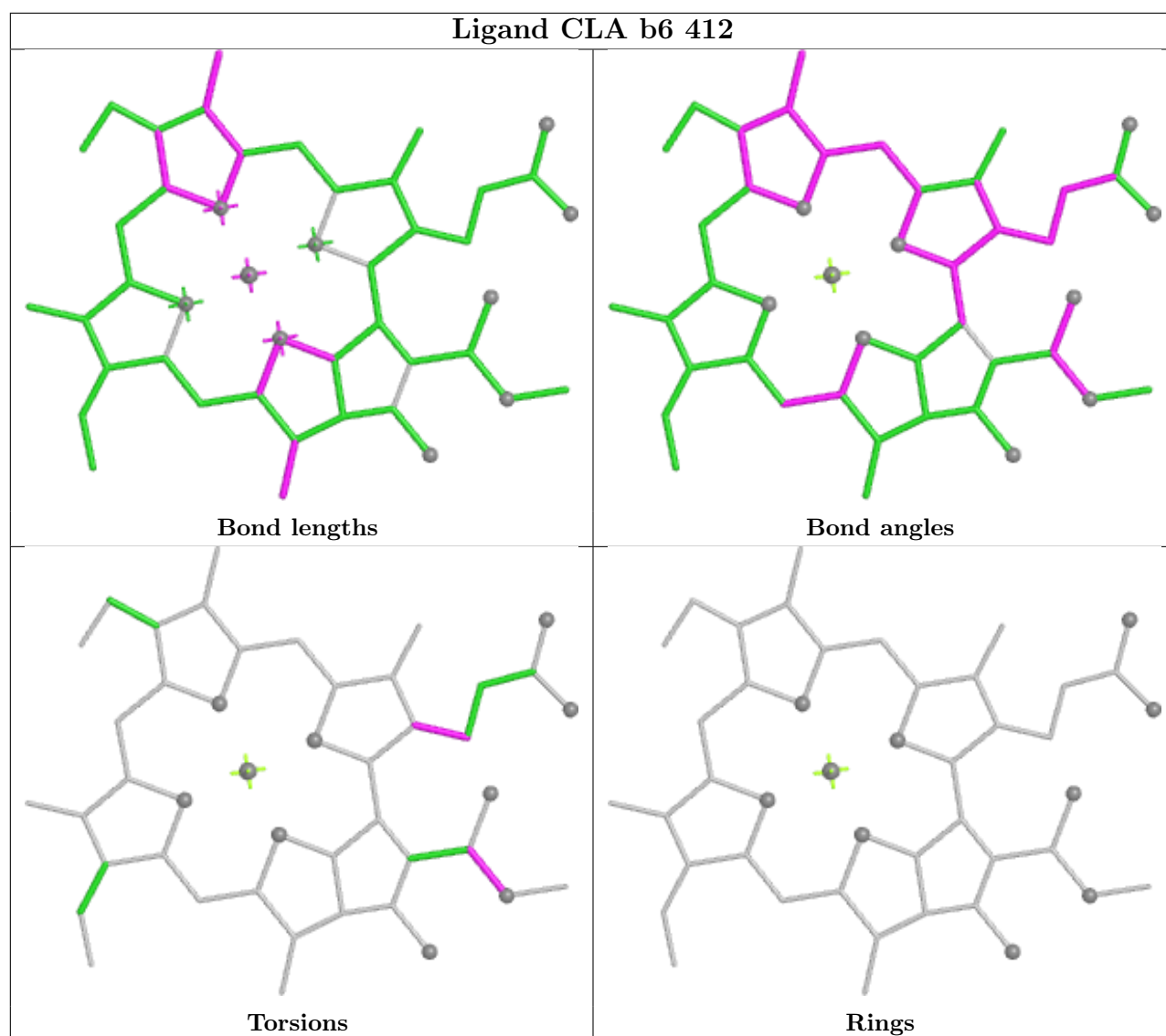


Ligand CLA c6 410

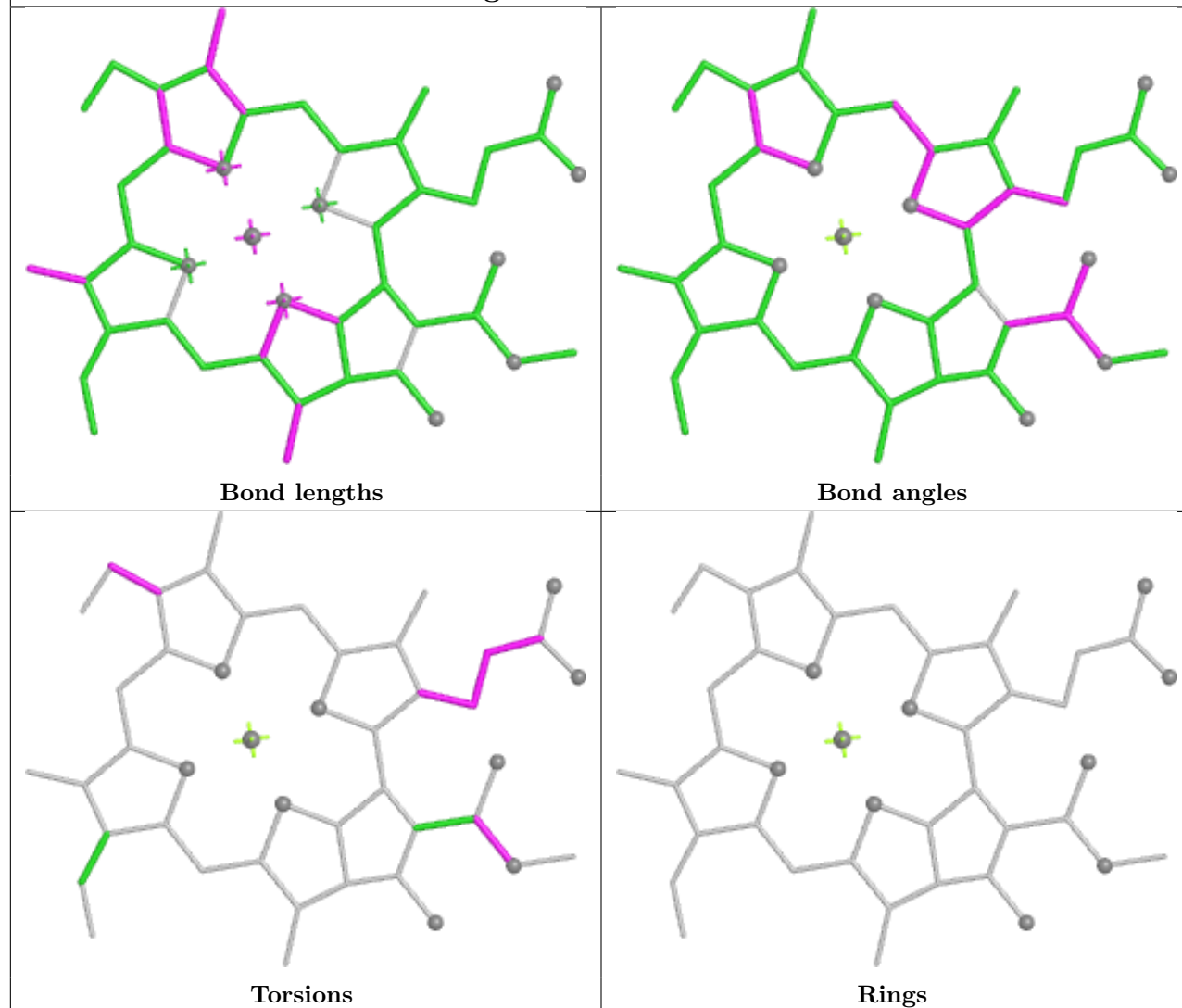




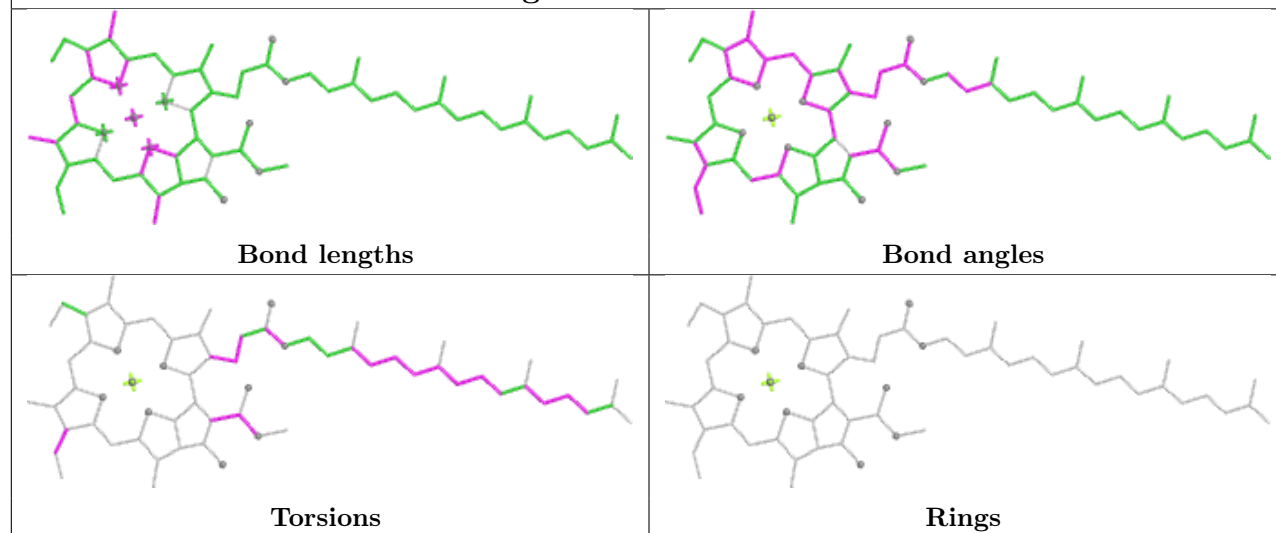


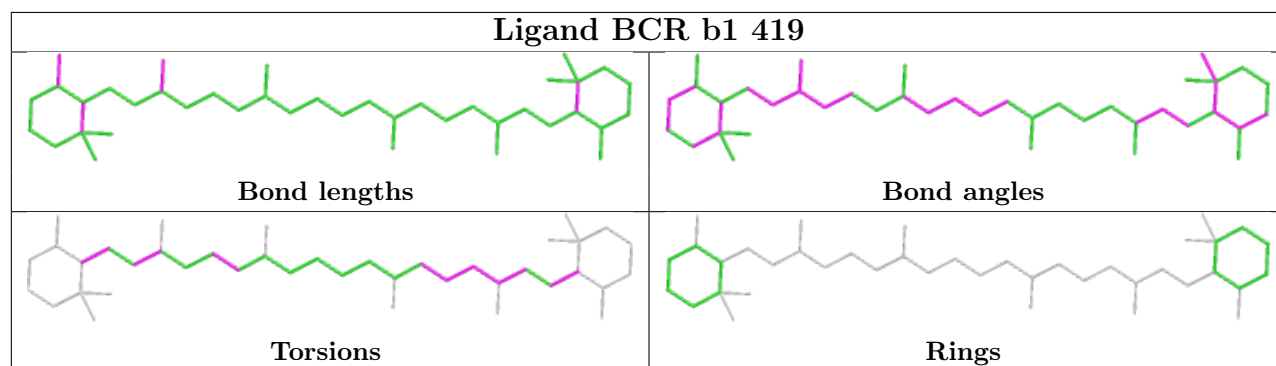
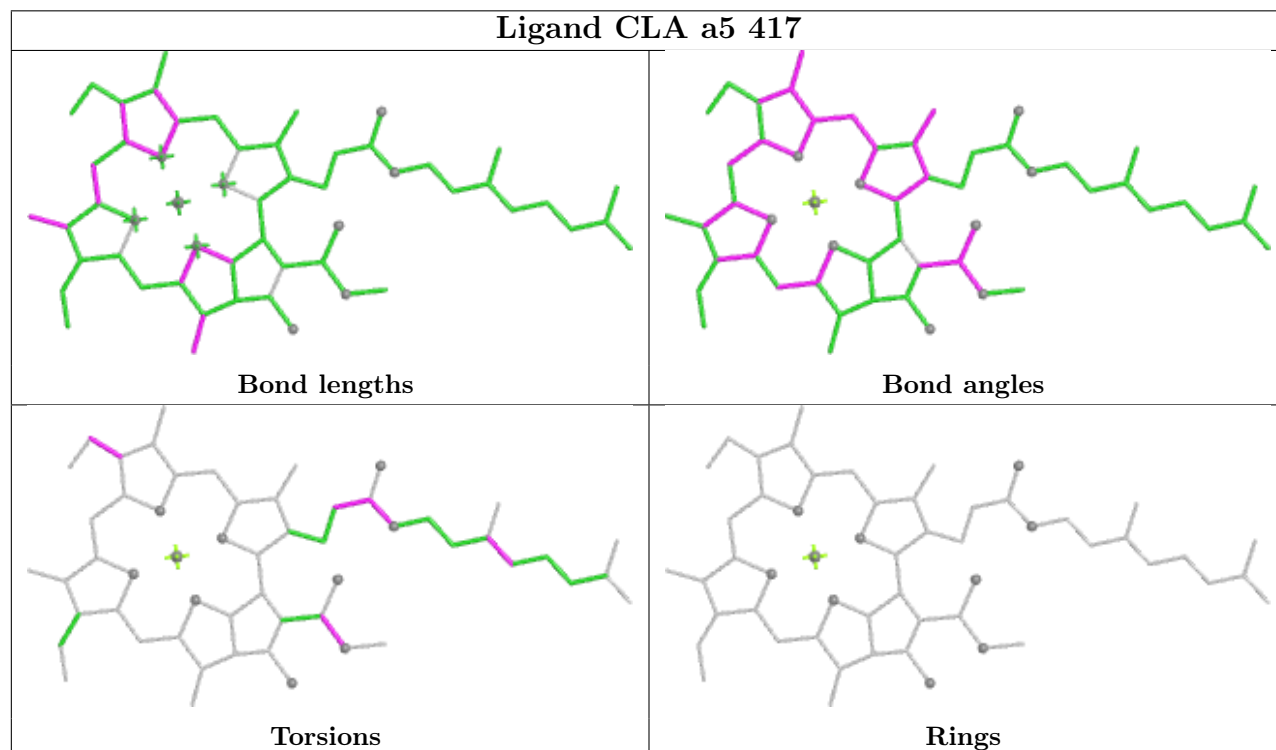
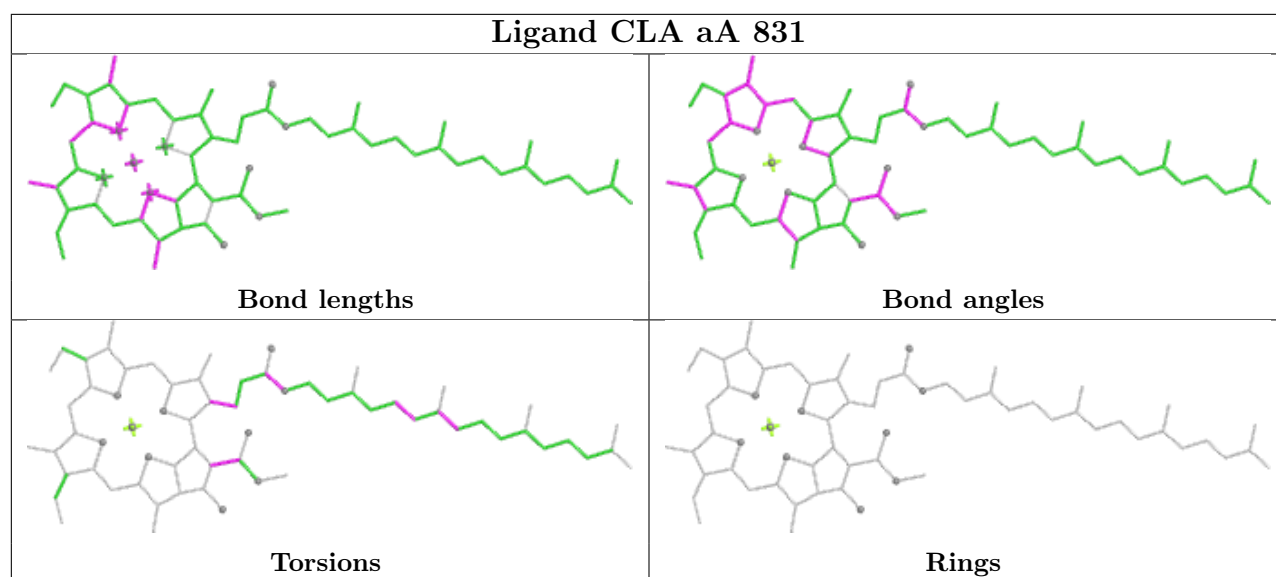


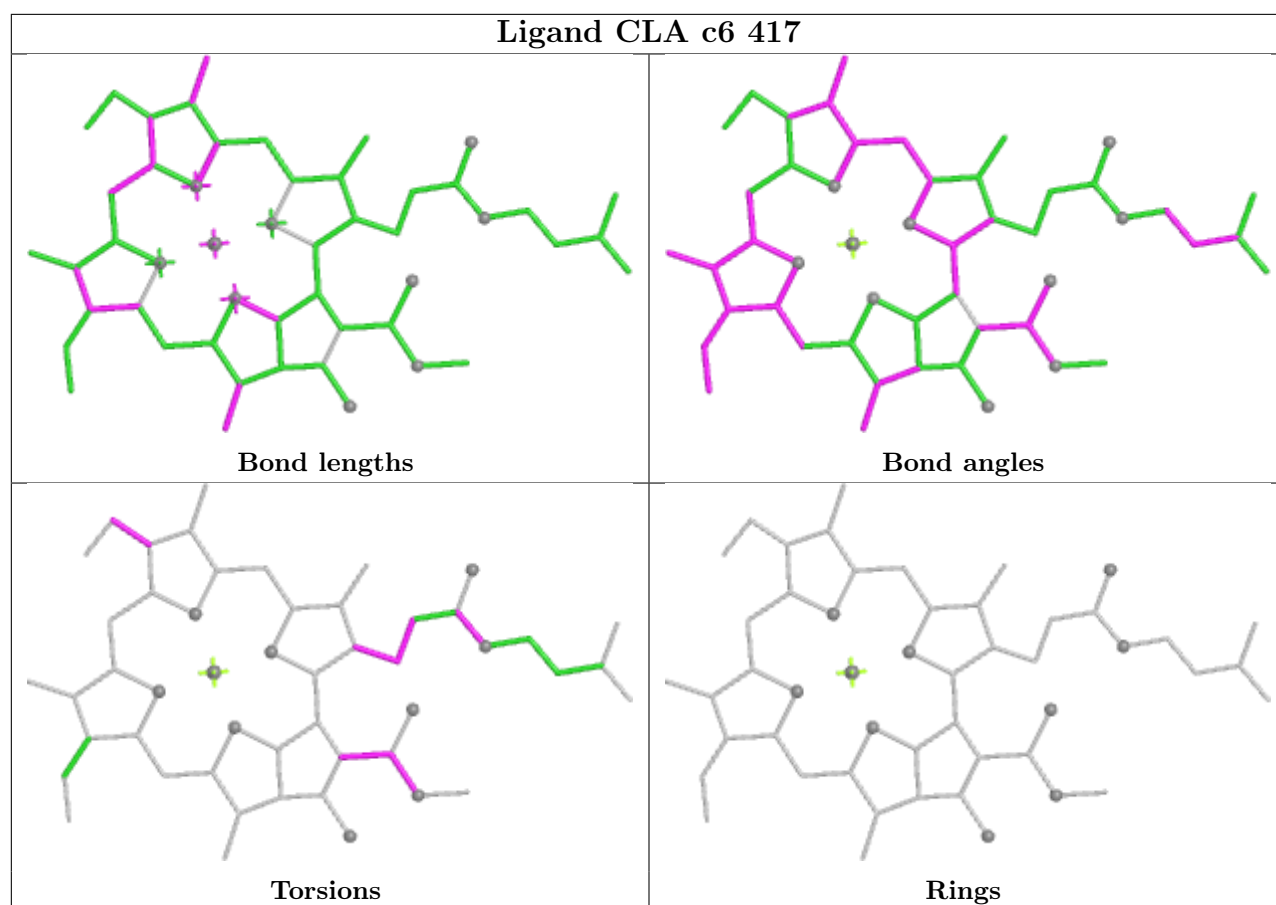
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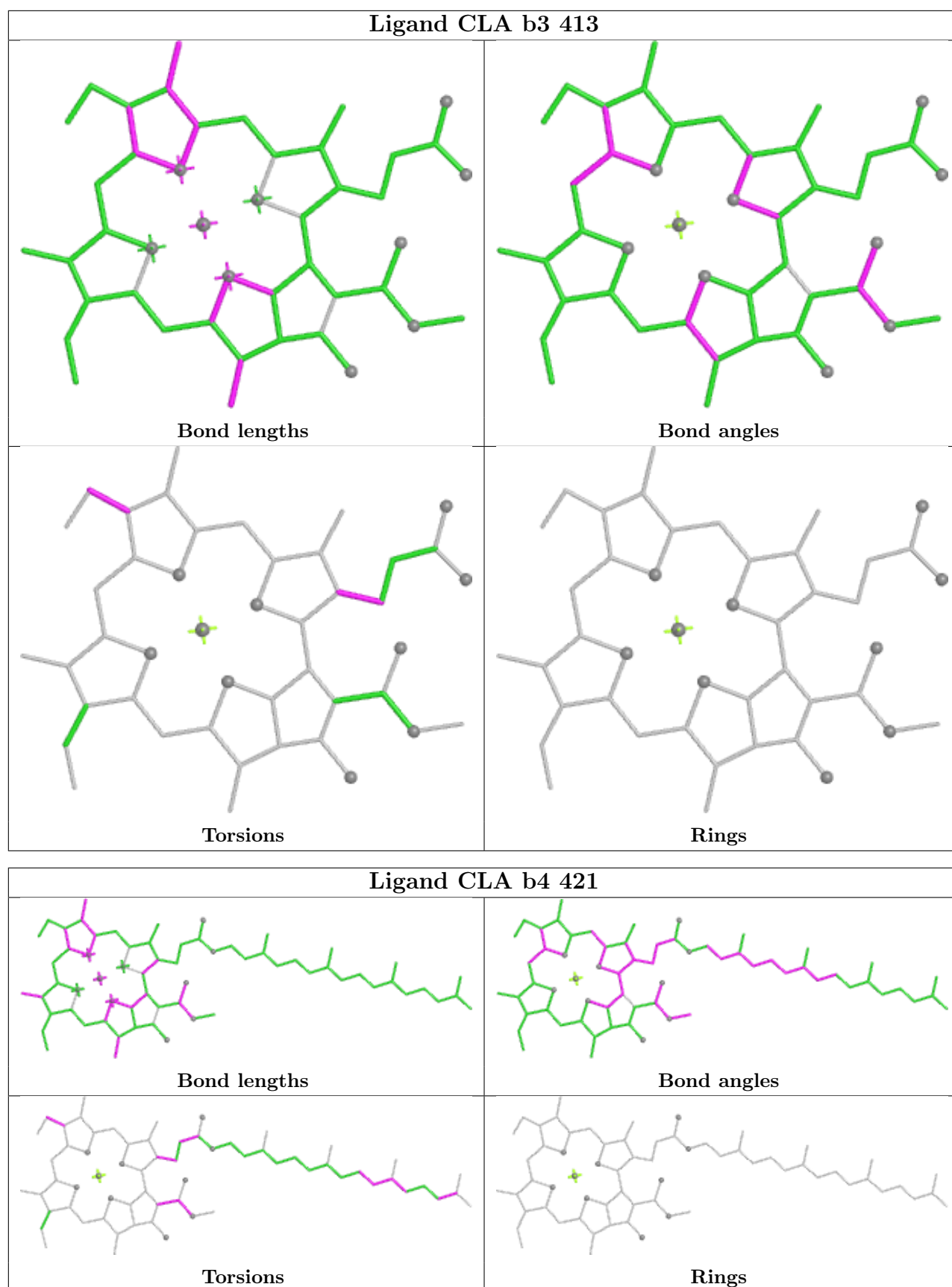


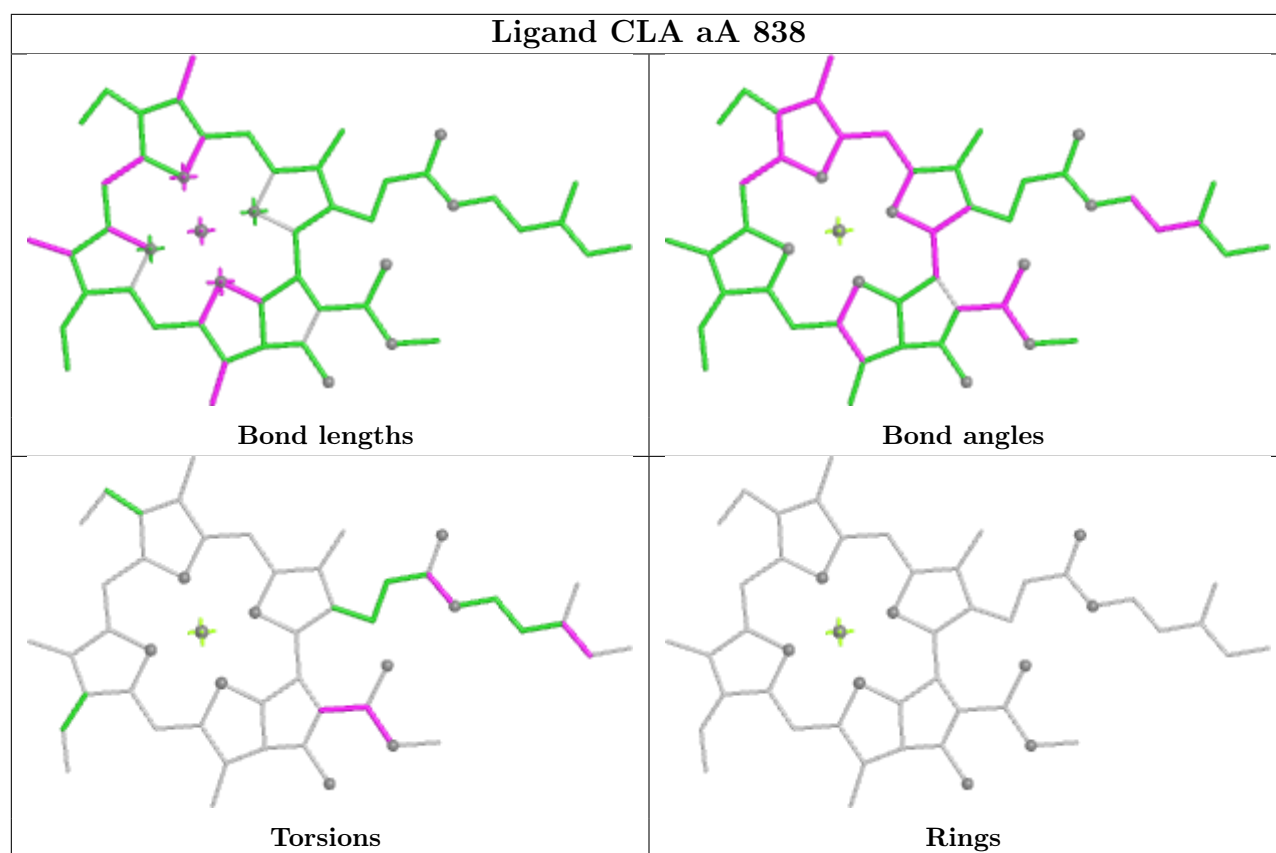
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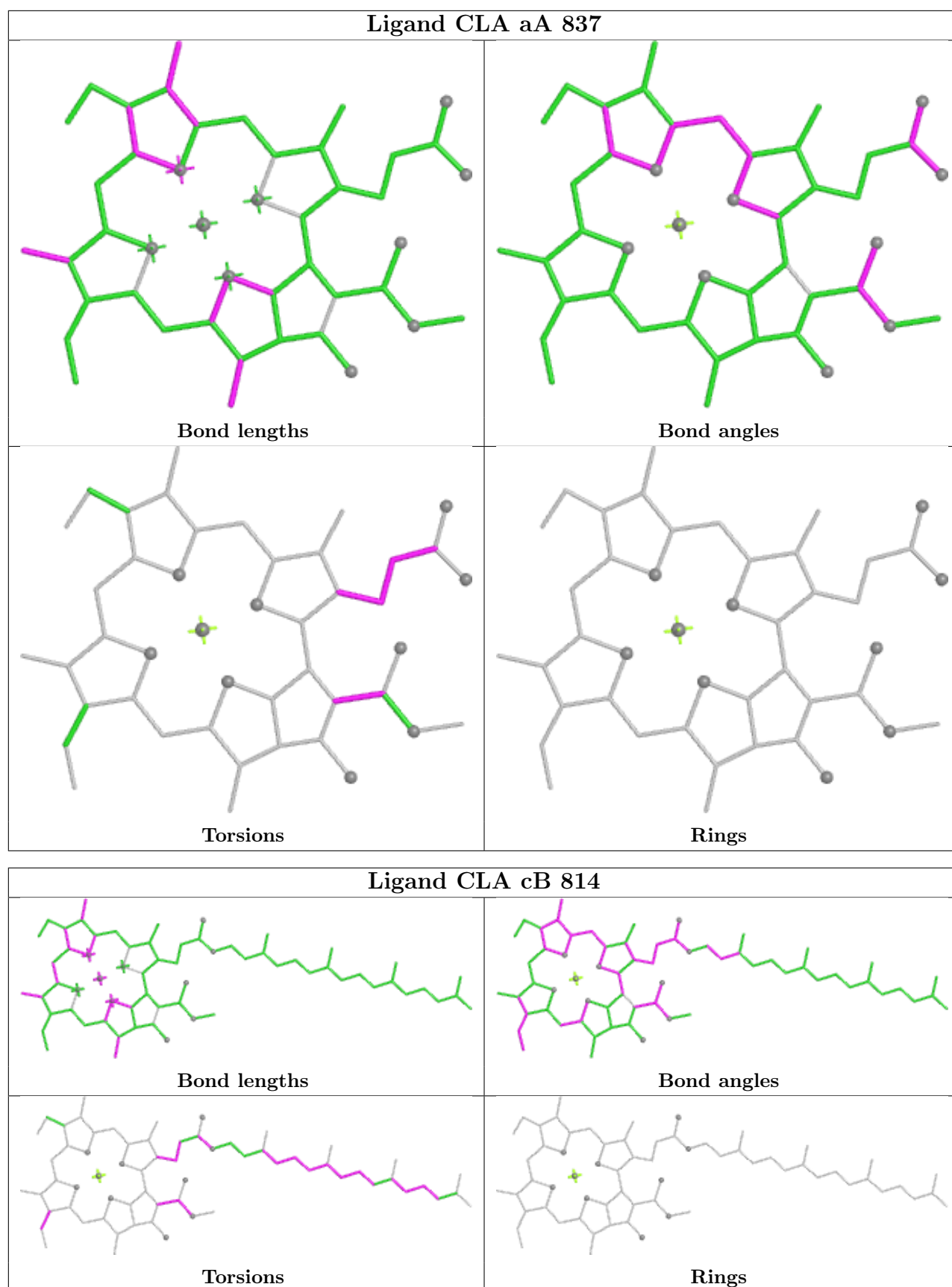


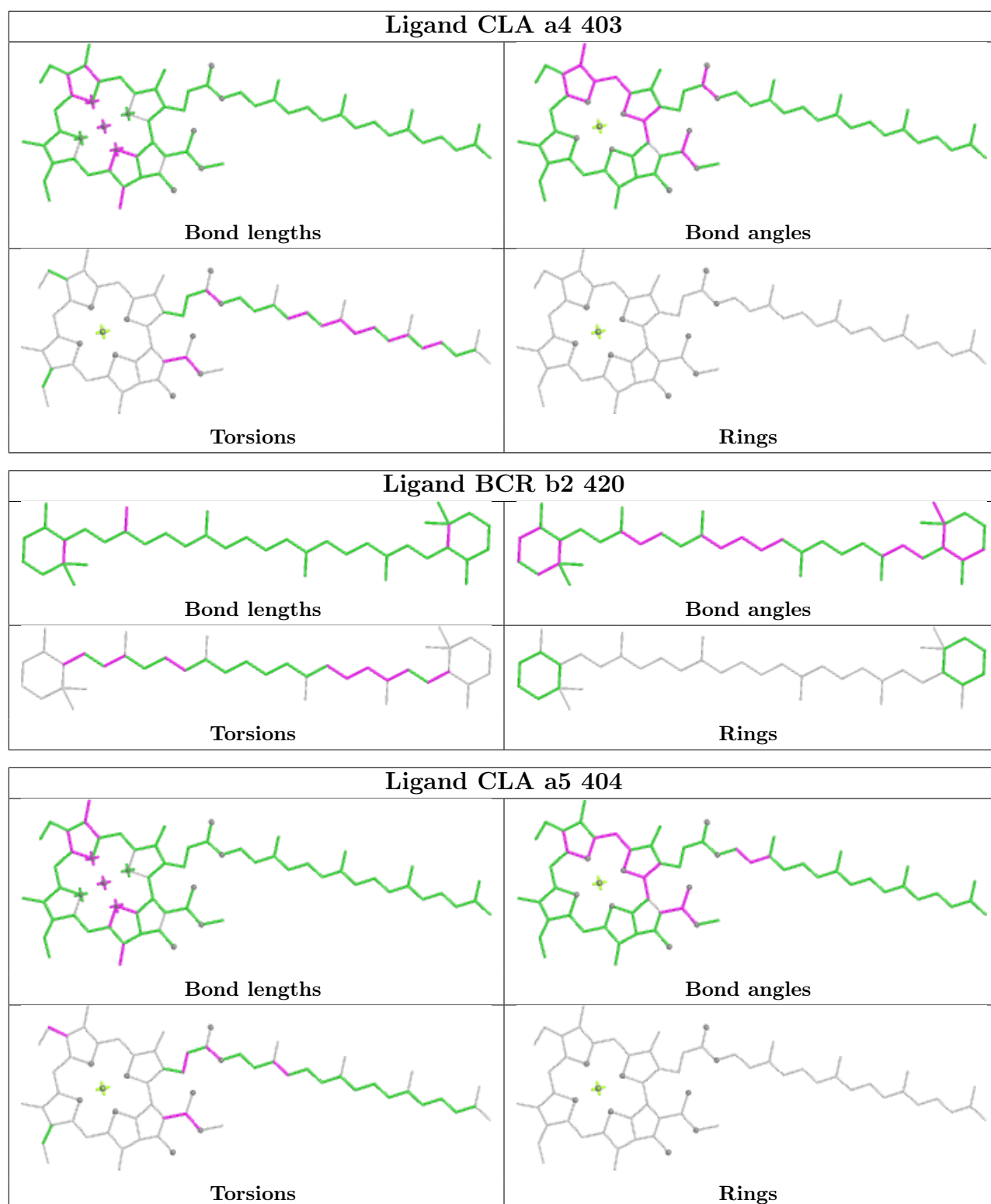


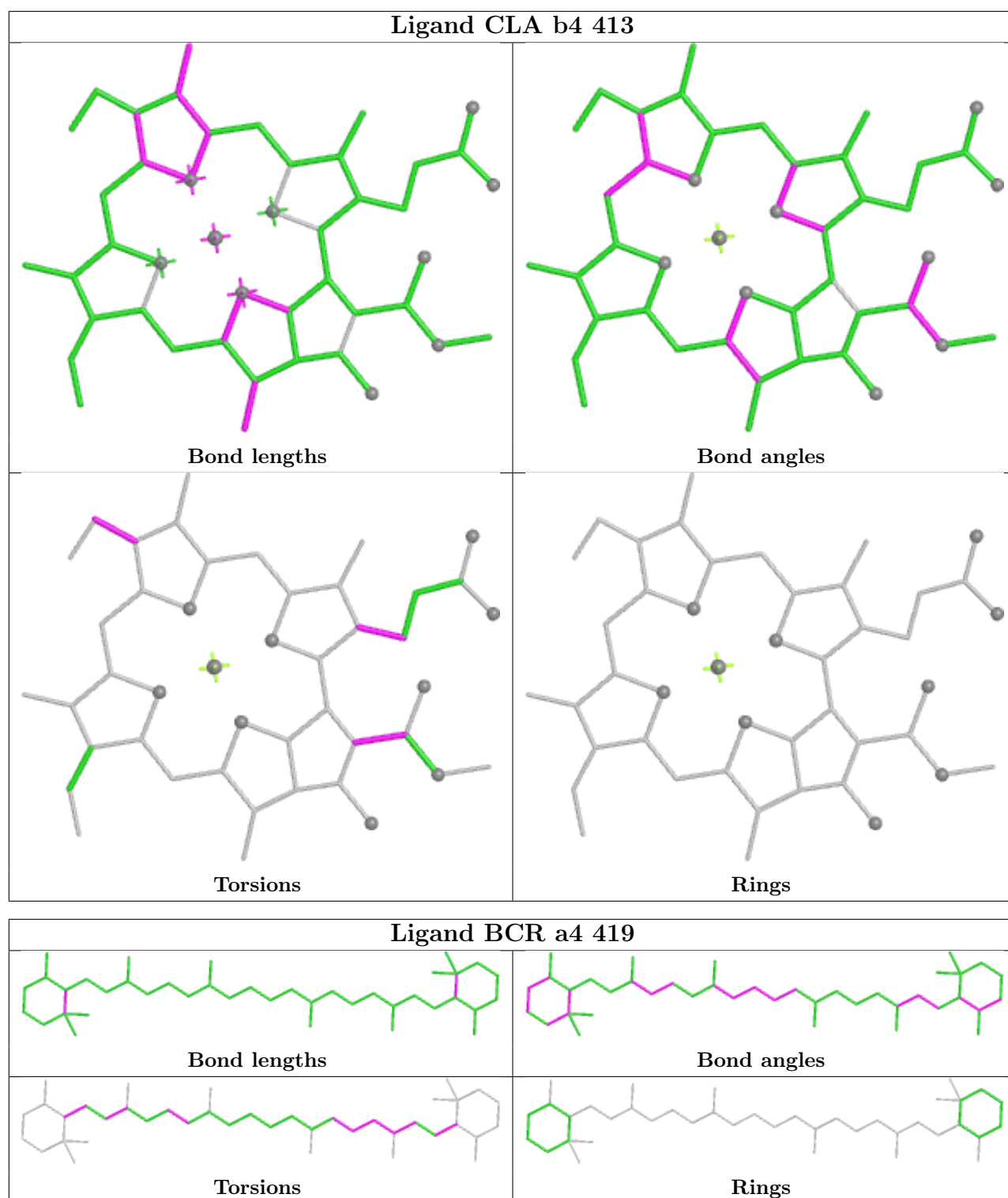


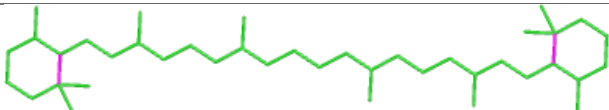
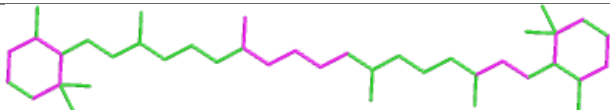
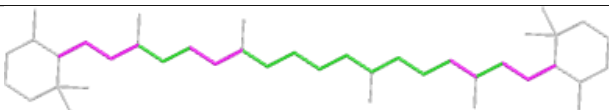
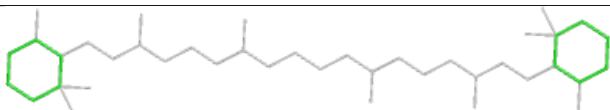


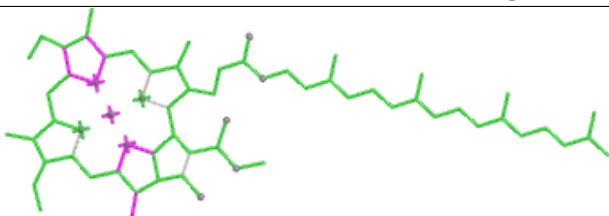
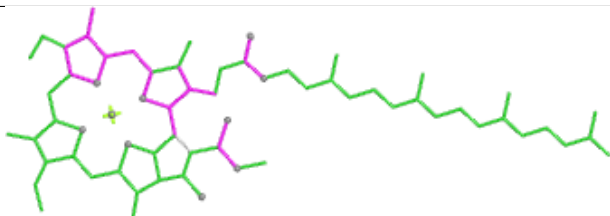
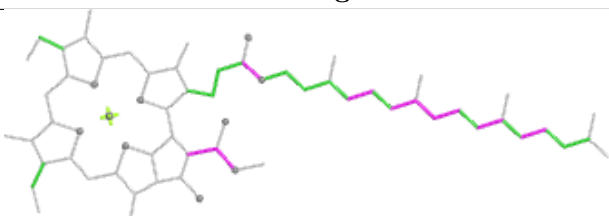
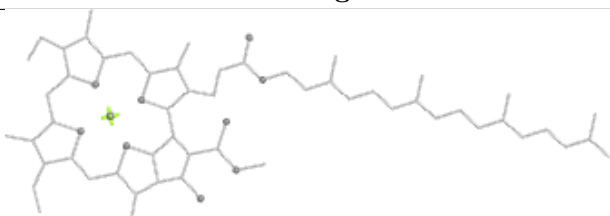


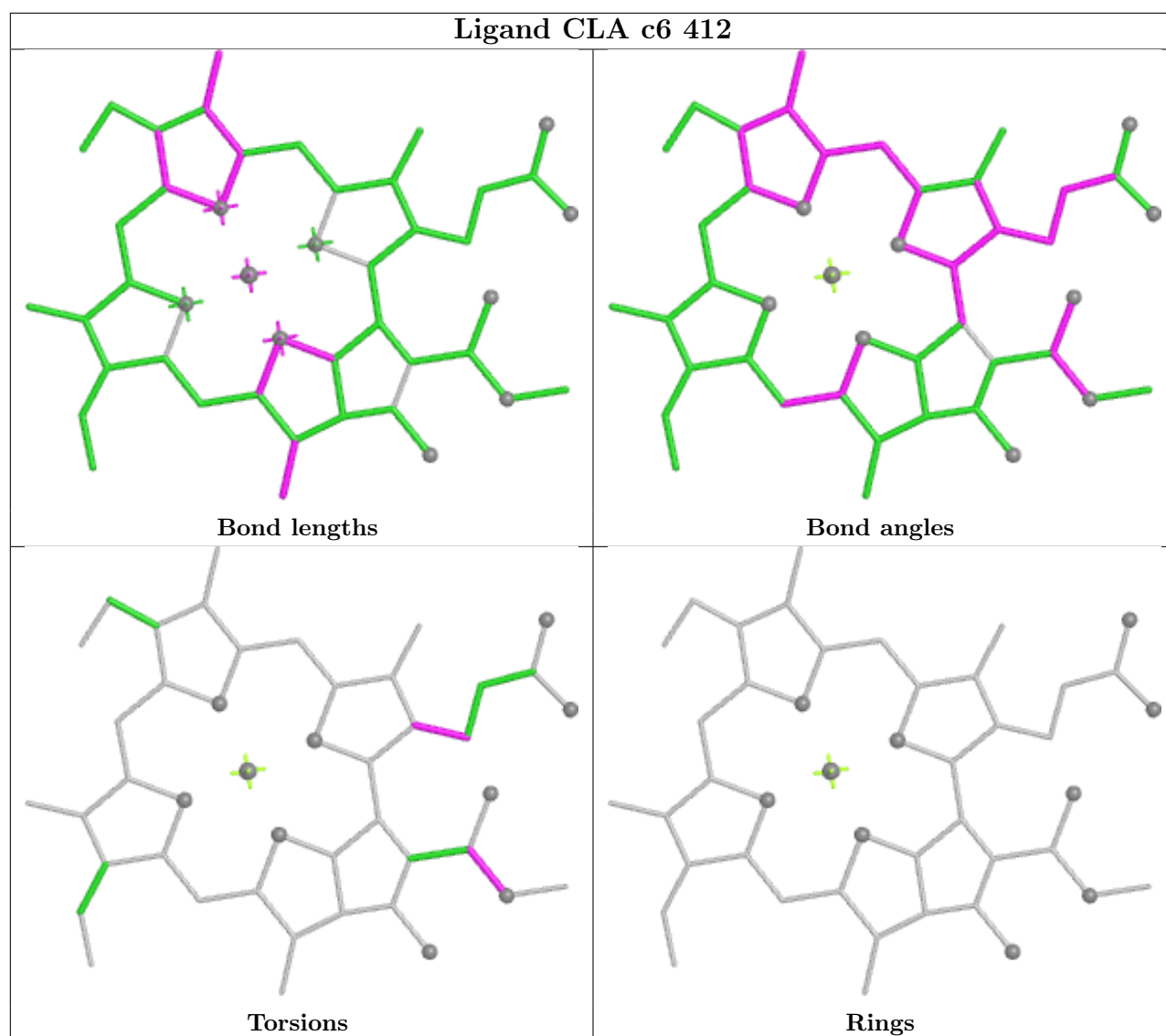


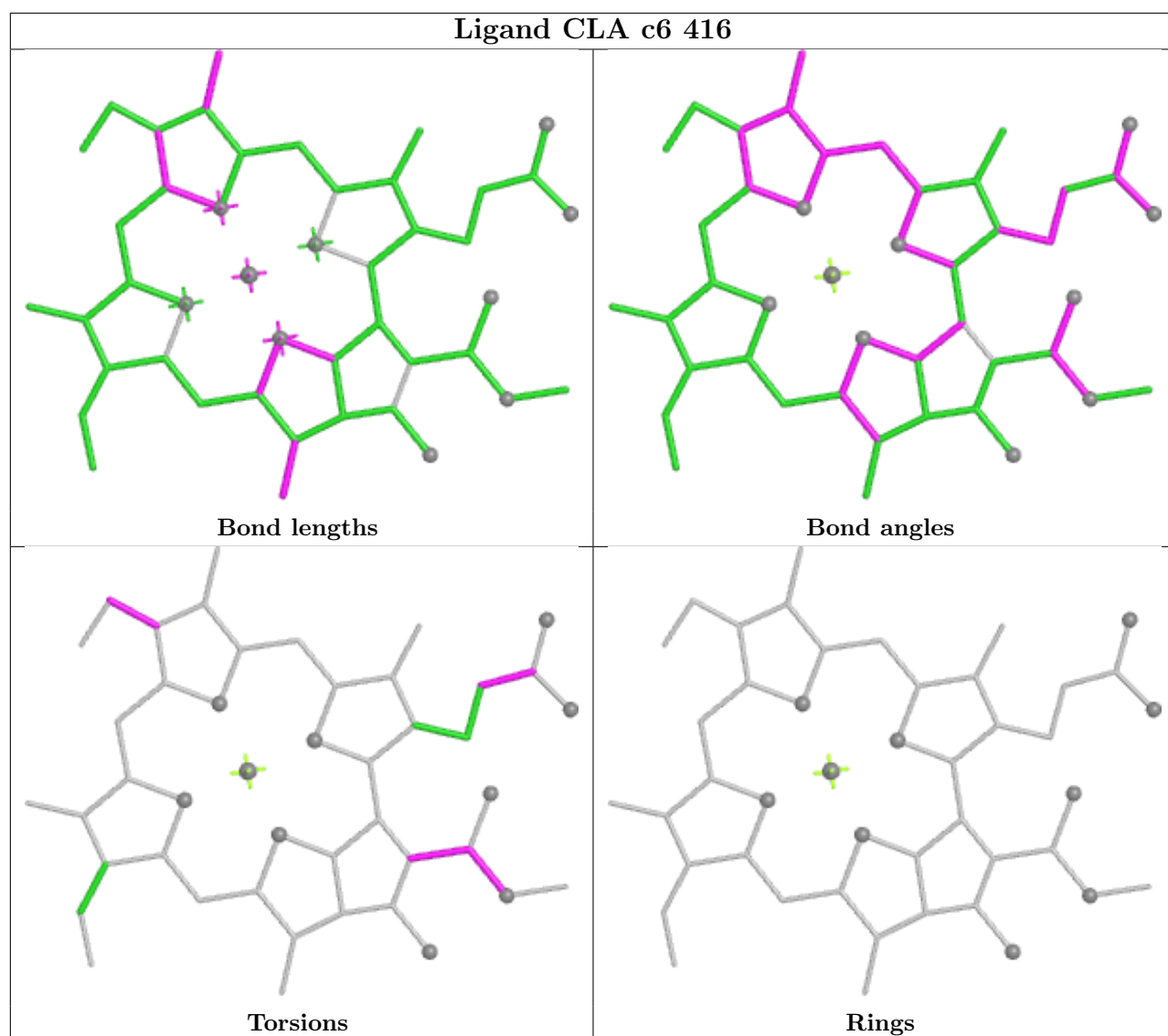


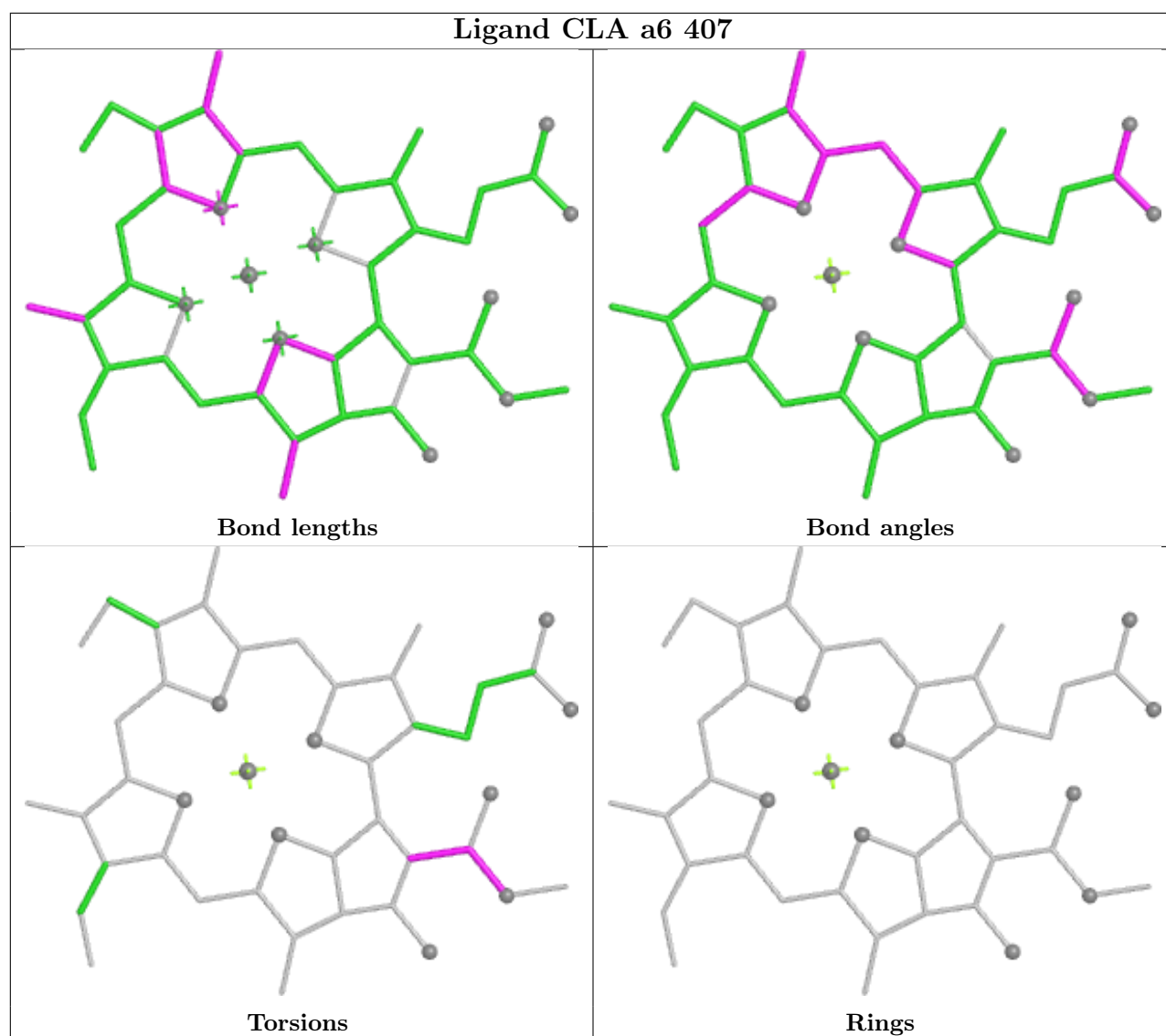


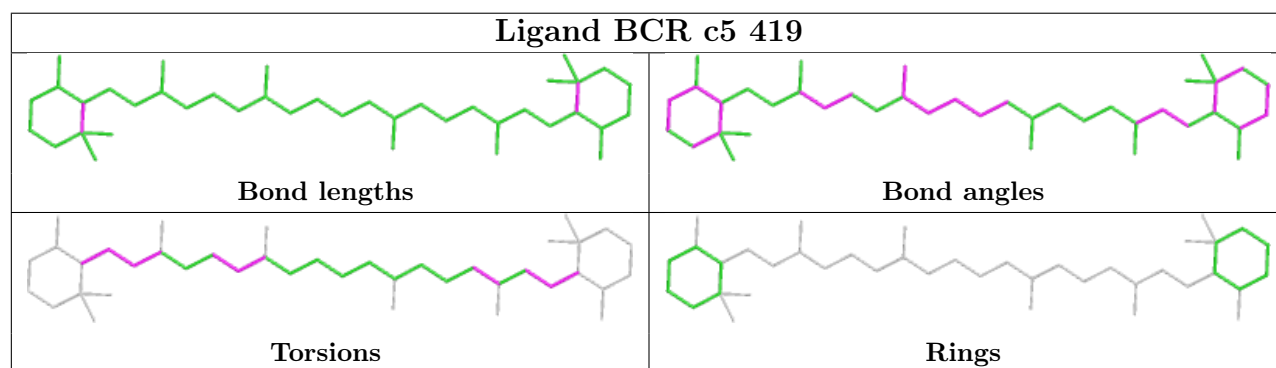
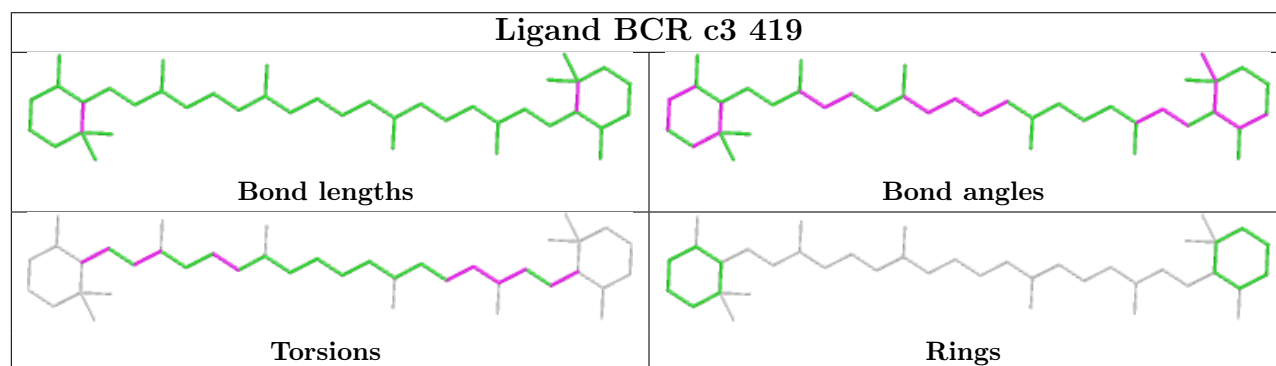
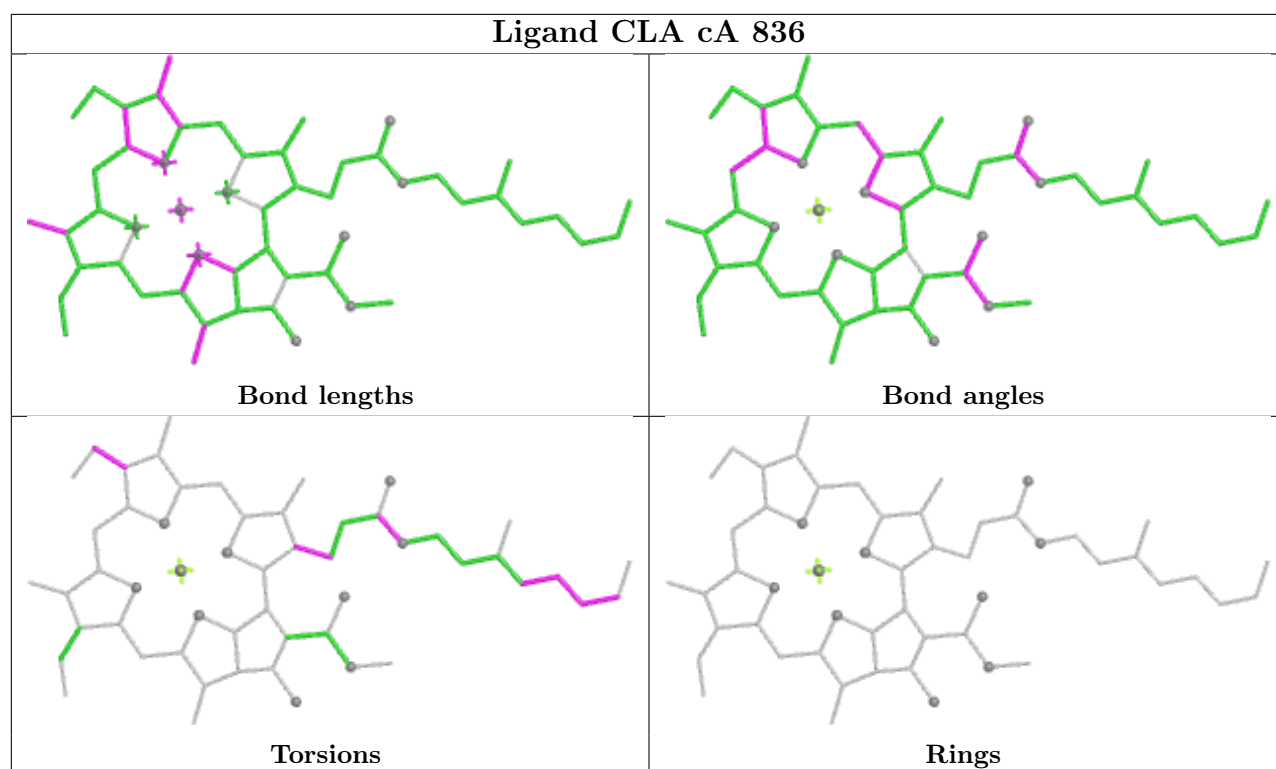
Ligand BCR c2 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

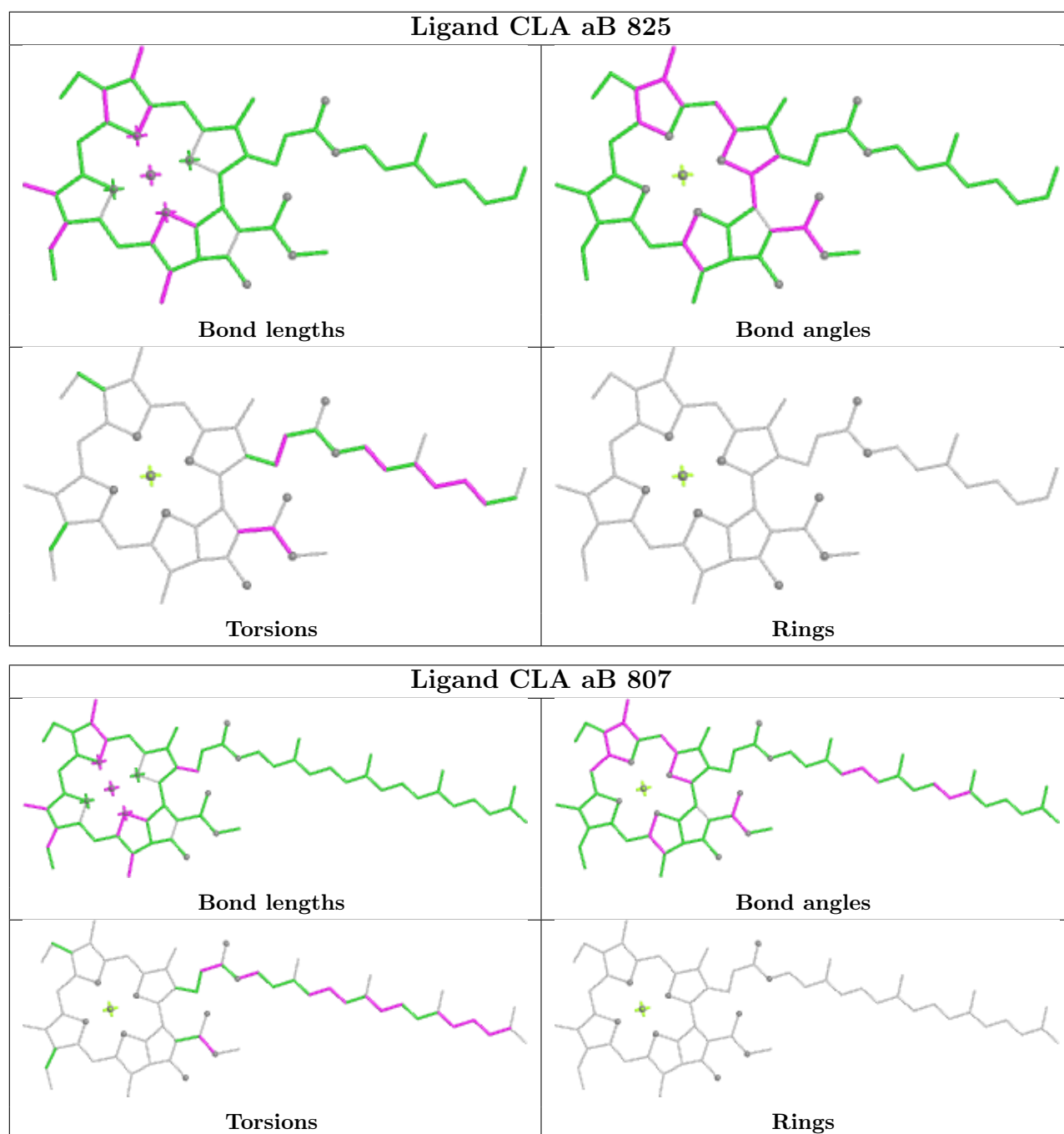
Ligand CLA b5 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

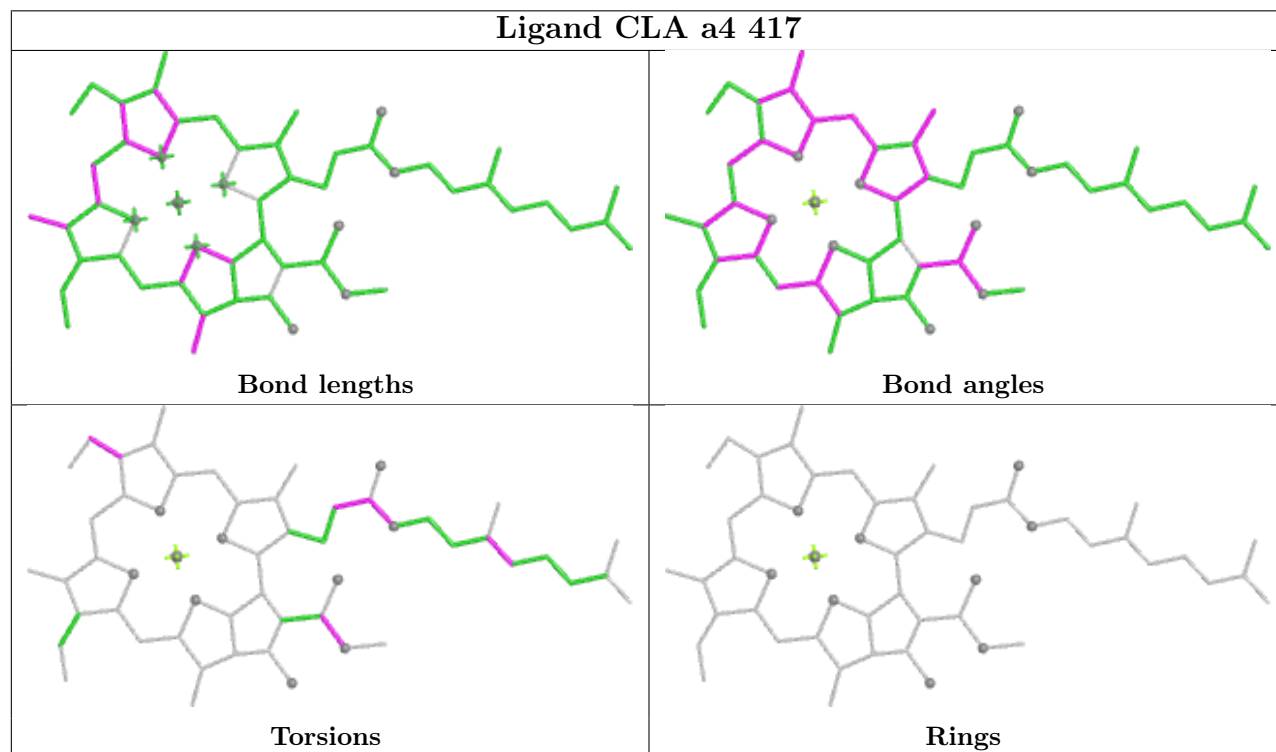
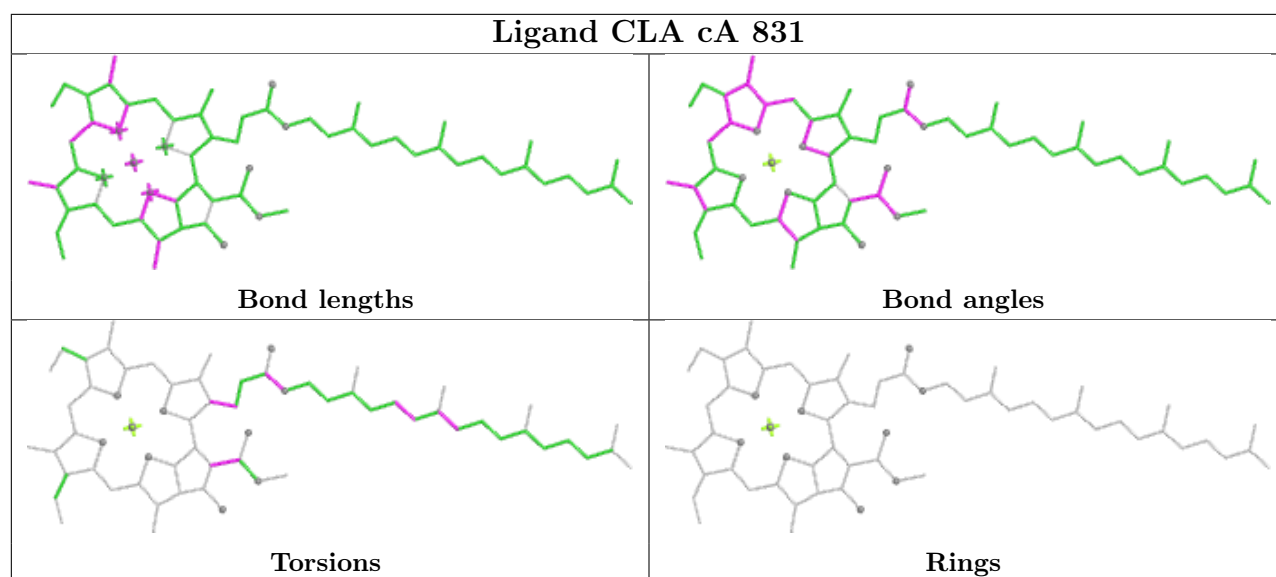


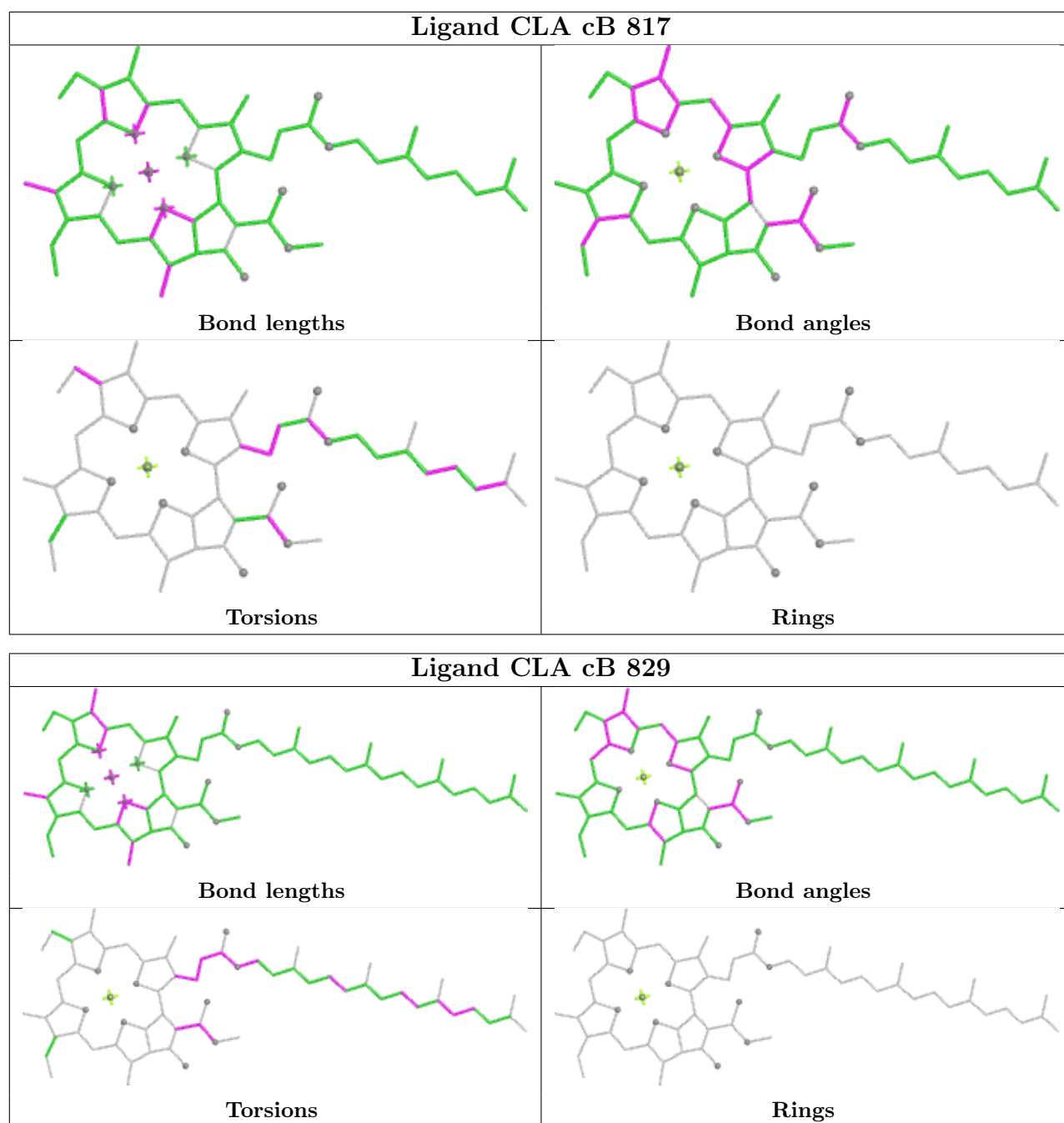


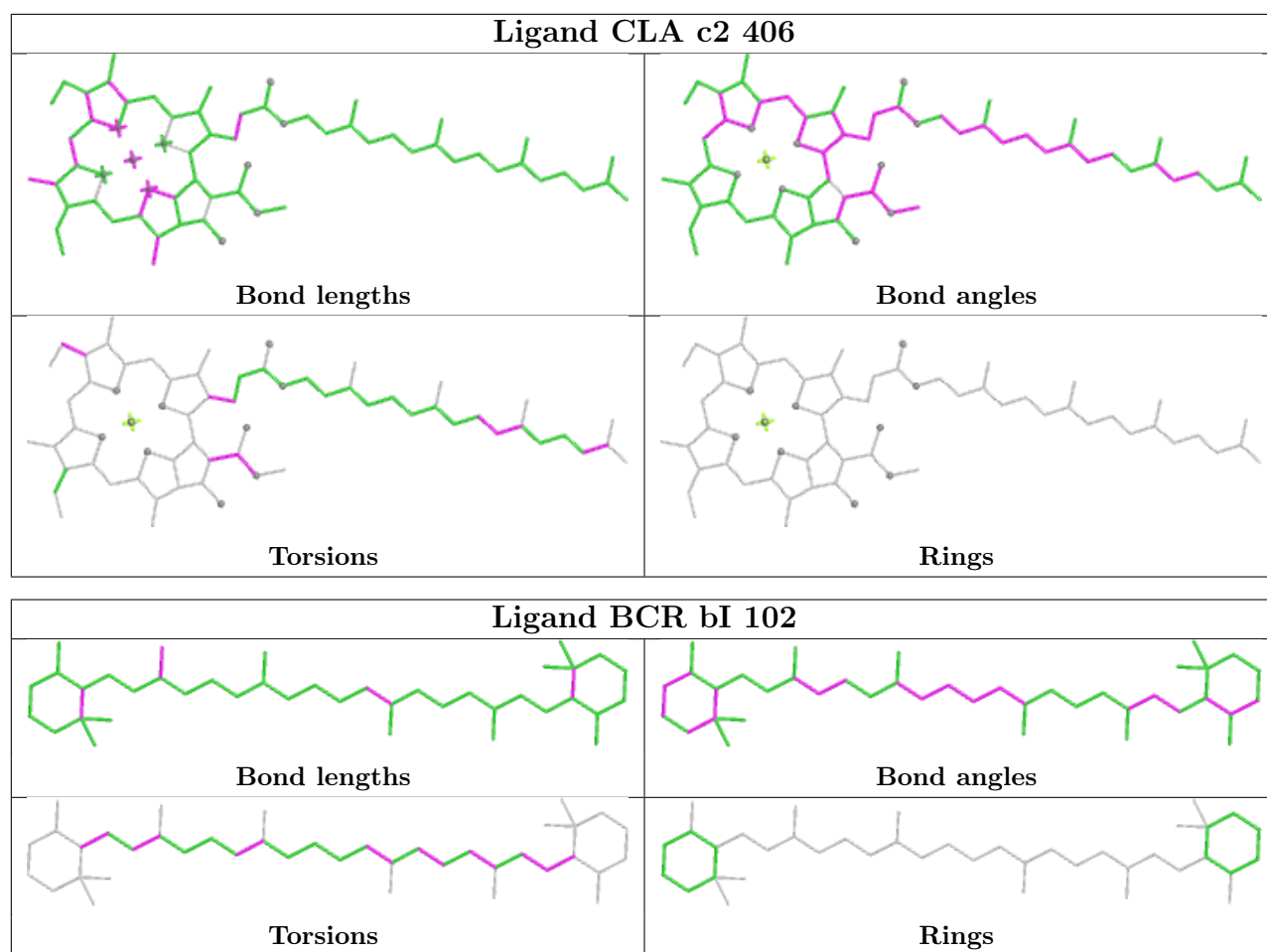


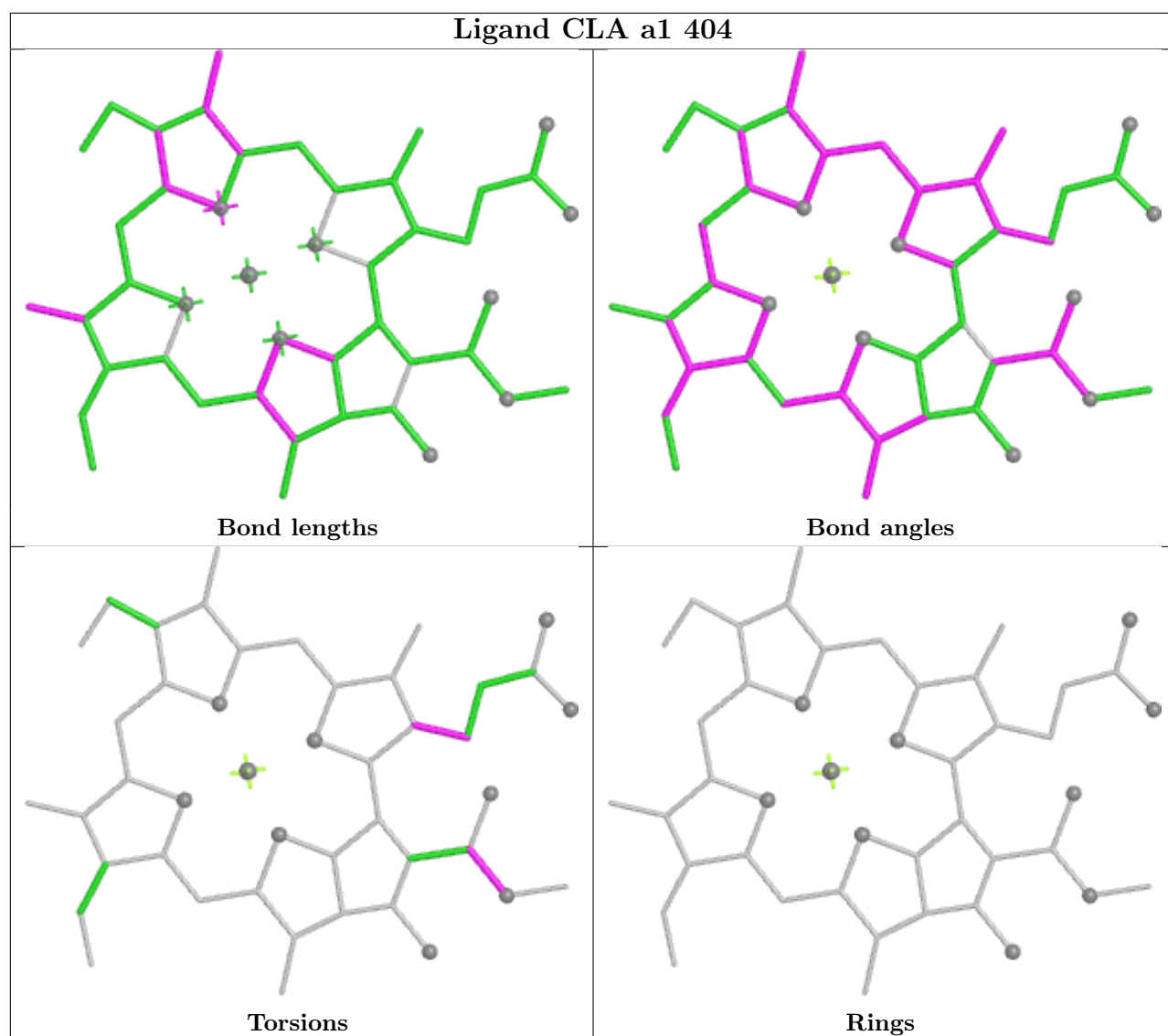


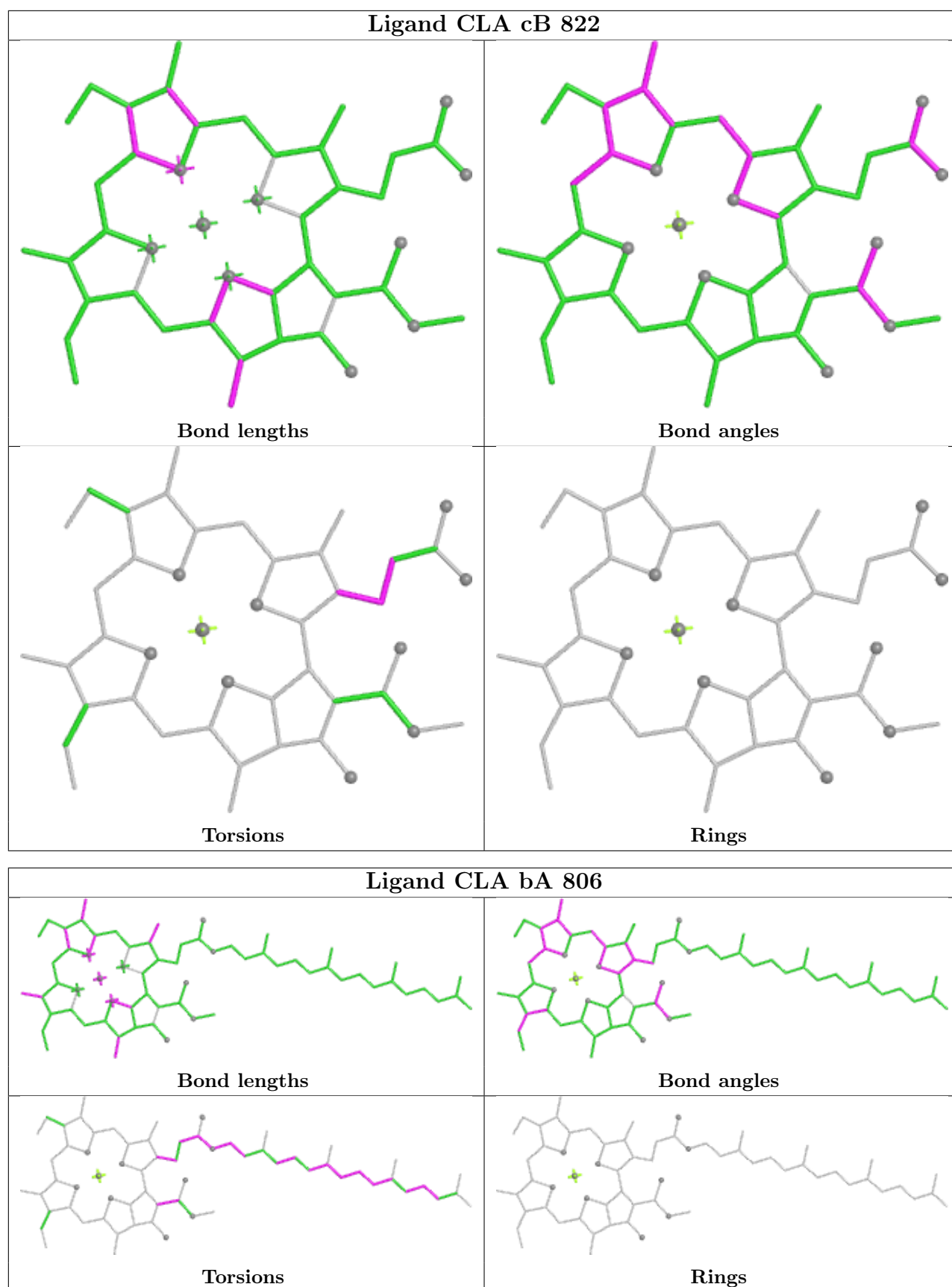


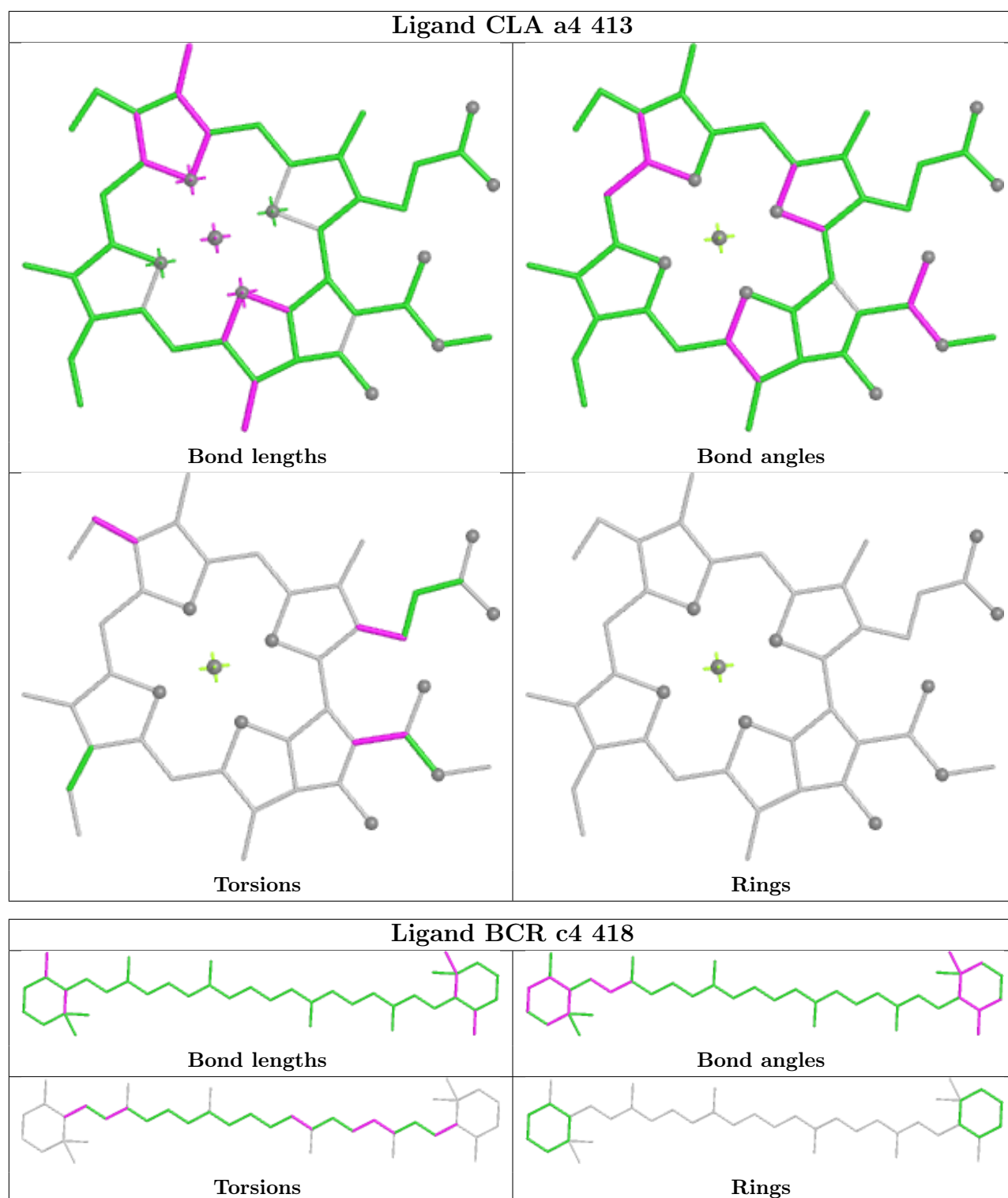


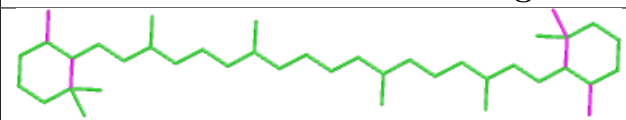
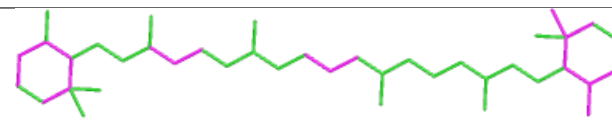
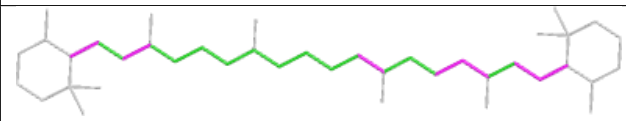
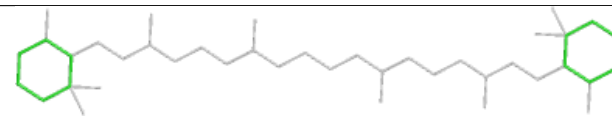


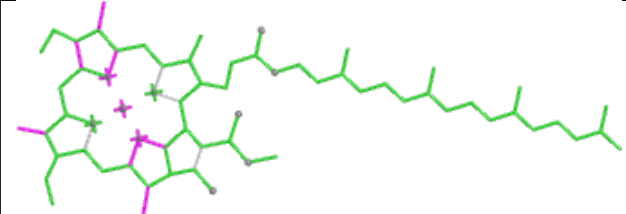
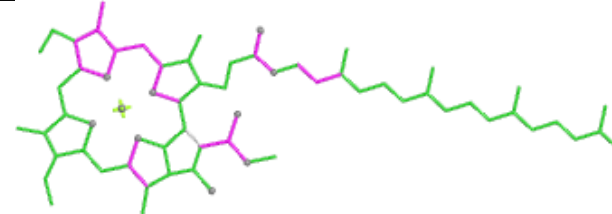
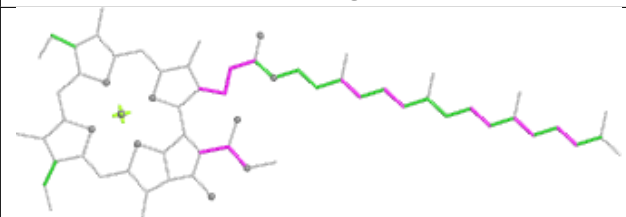
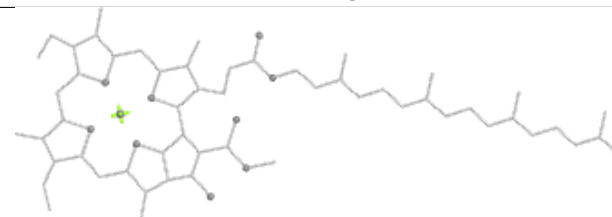


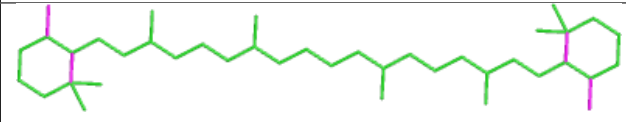
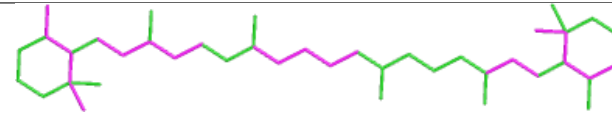
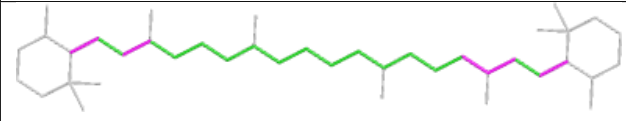
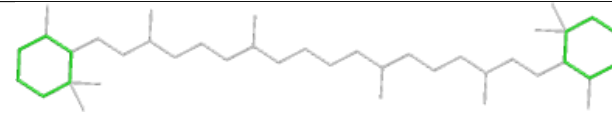


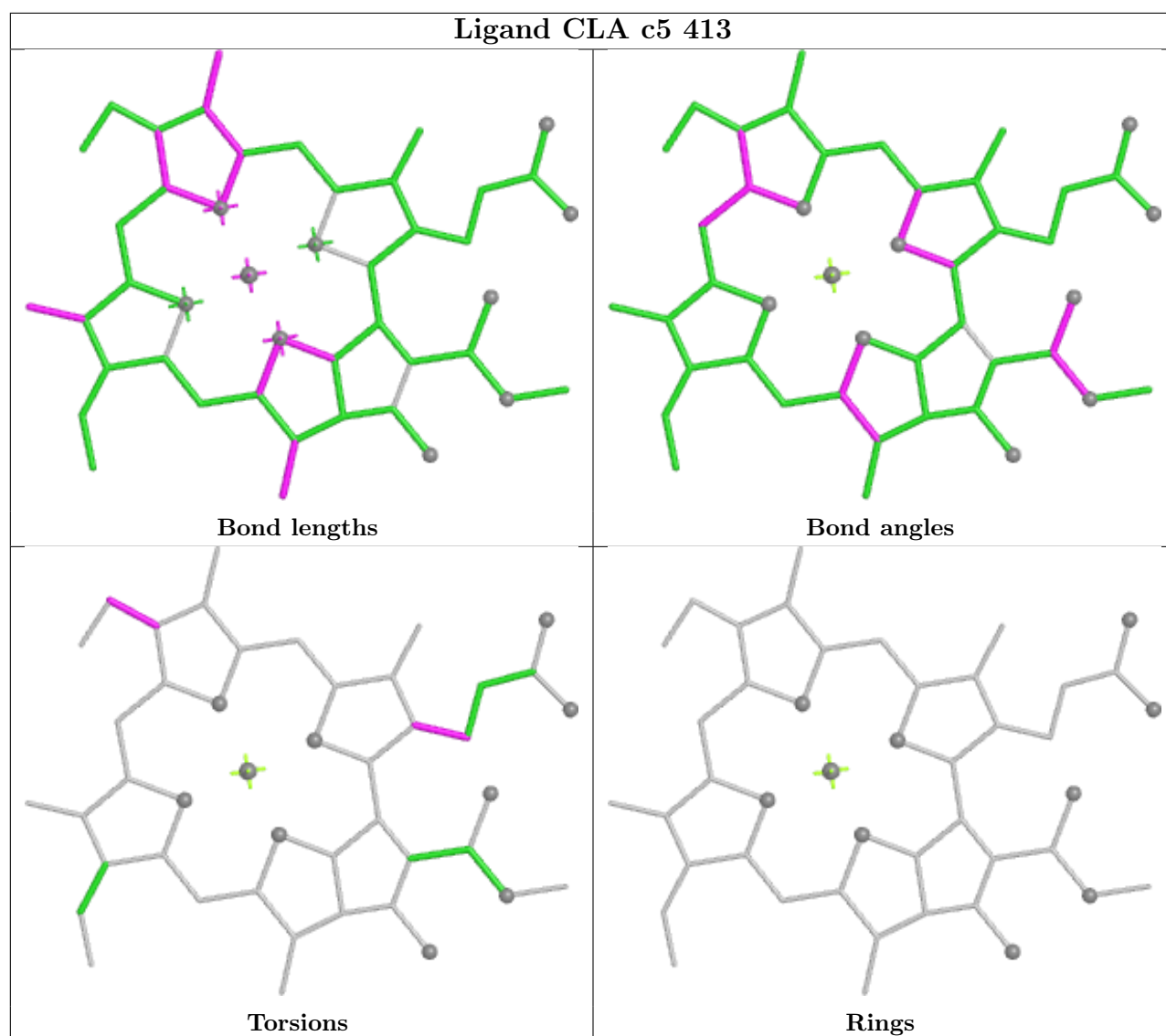


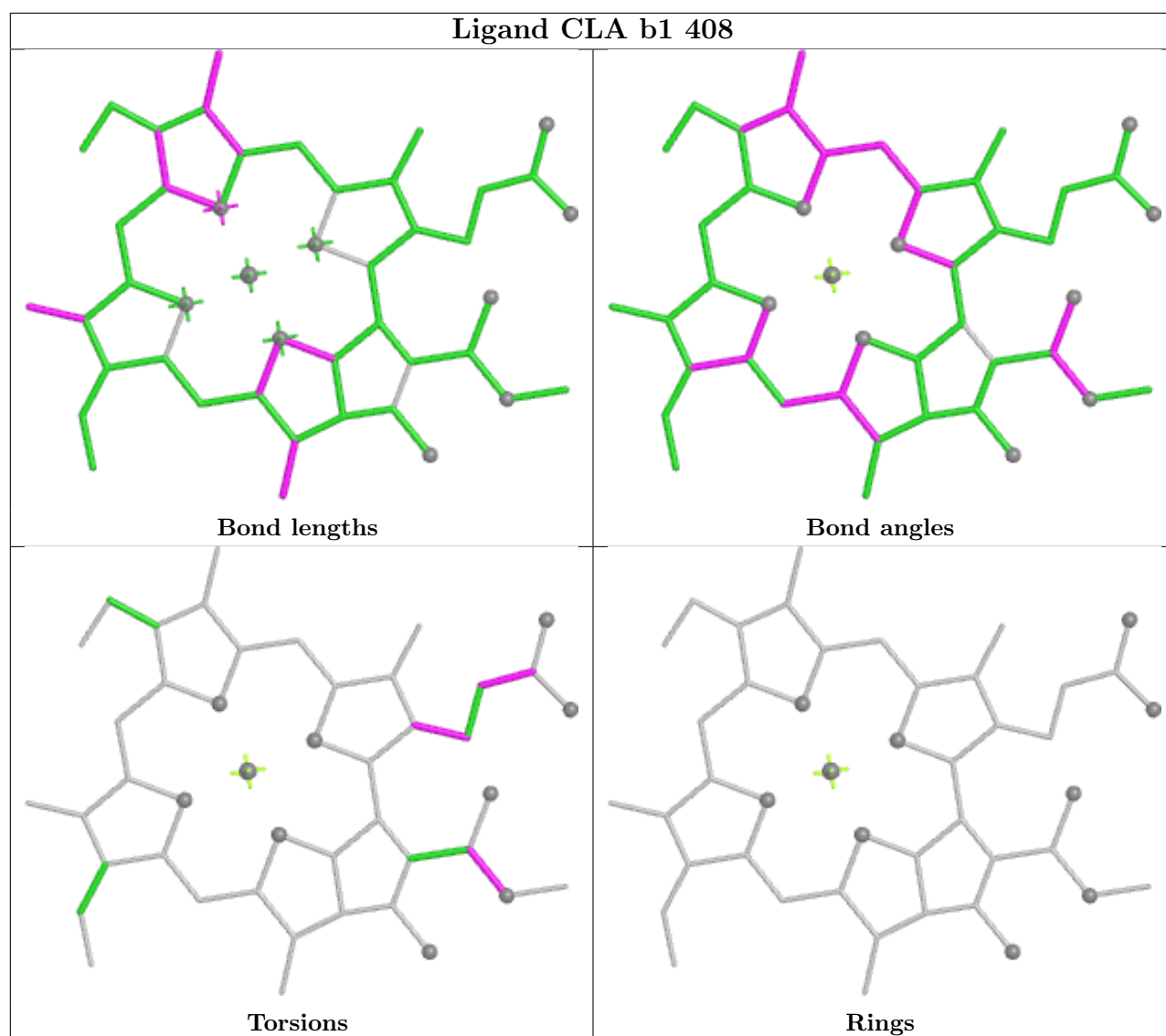


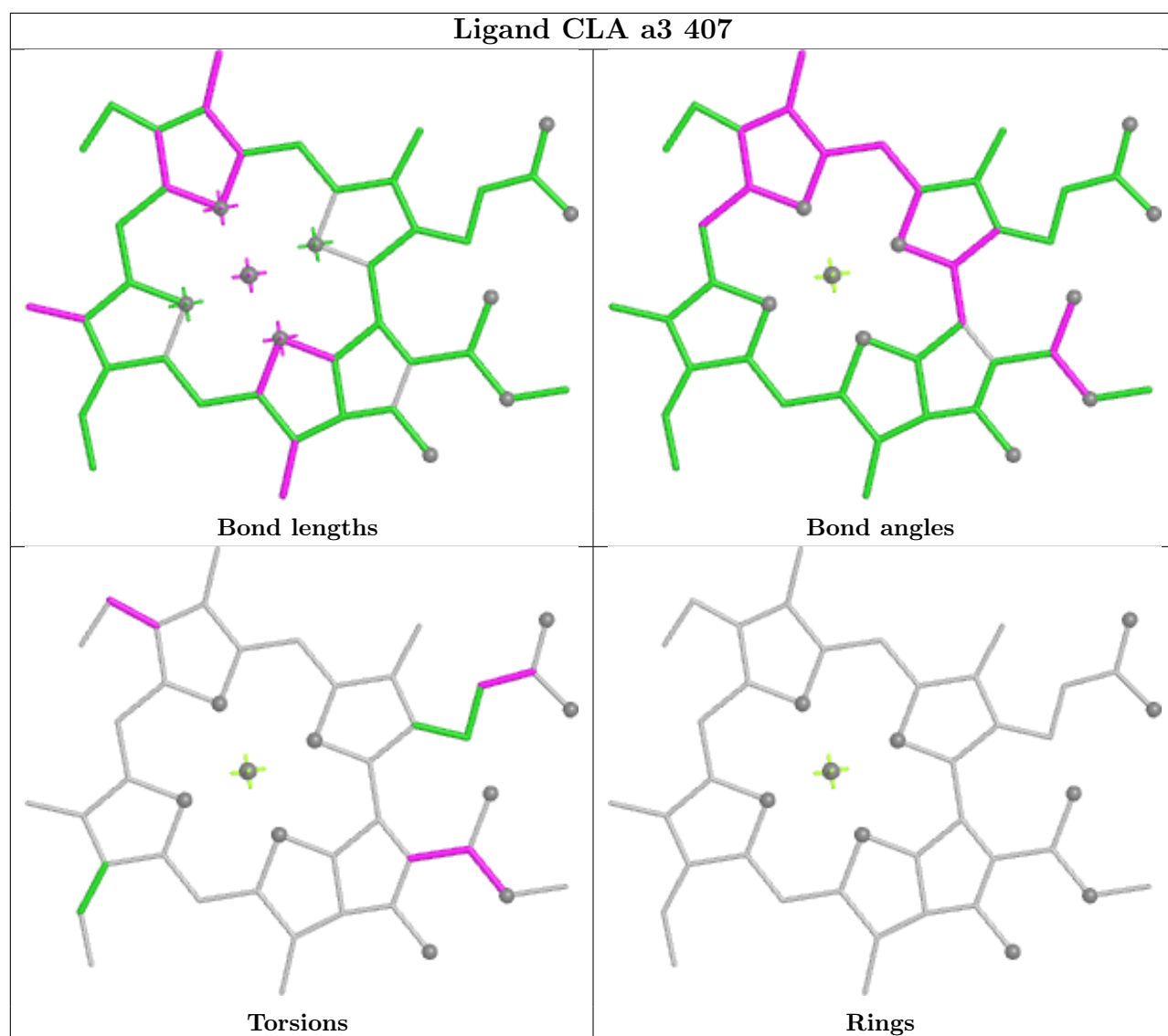
Ligand BCR a2 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

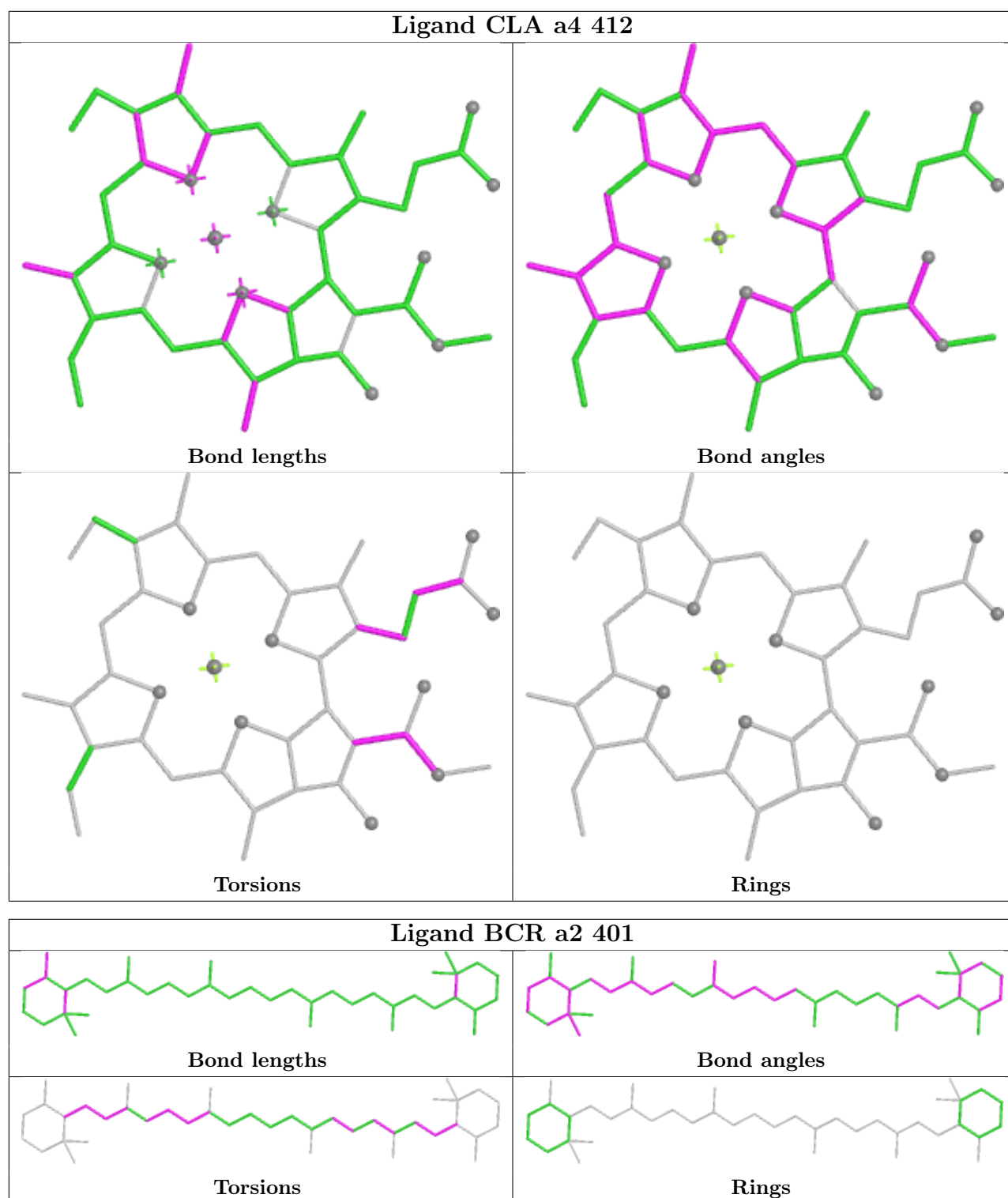
Ligand CLA cA 830	
	
Bond lengths	Bond angles
	
Torsions	Rings

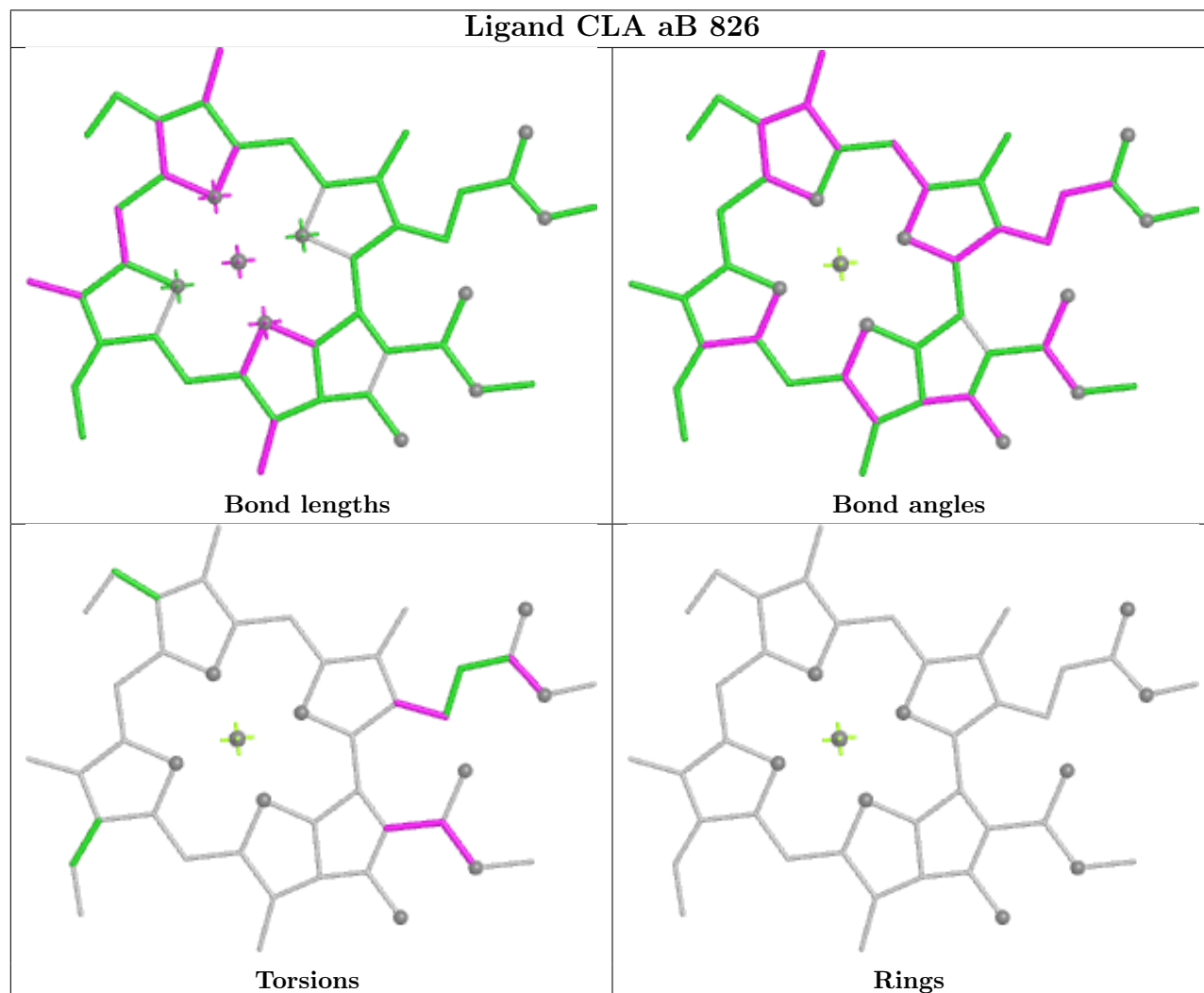
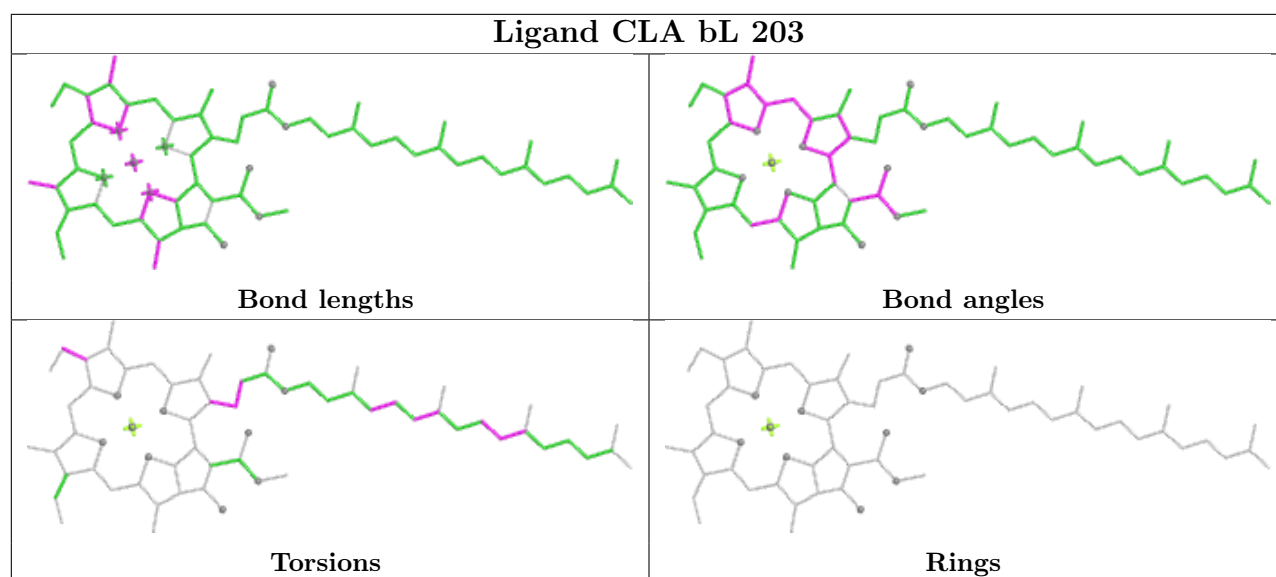
Ligand BCR cL 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

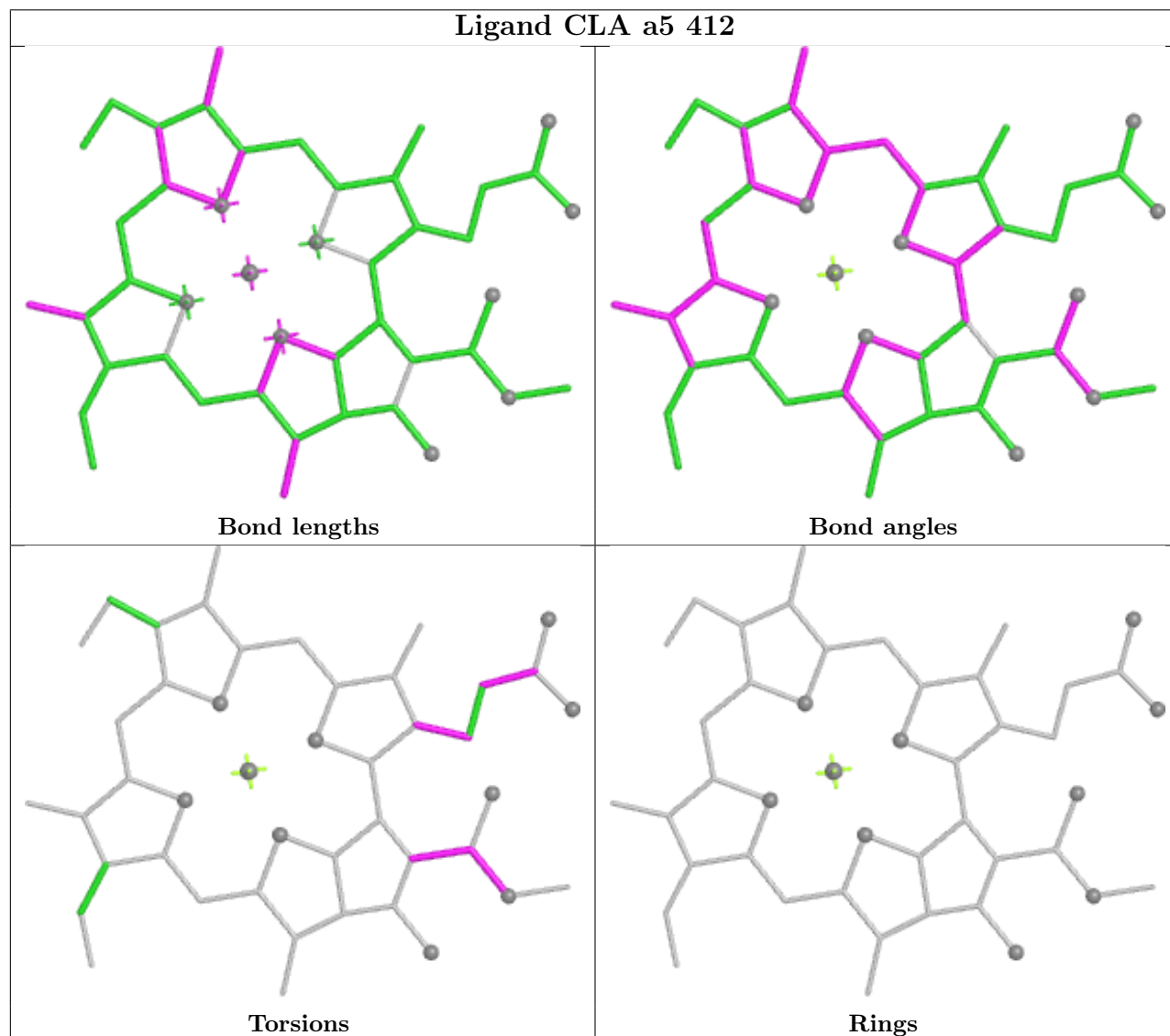
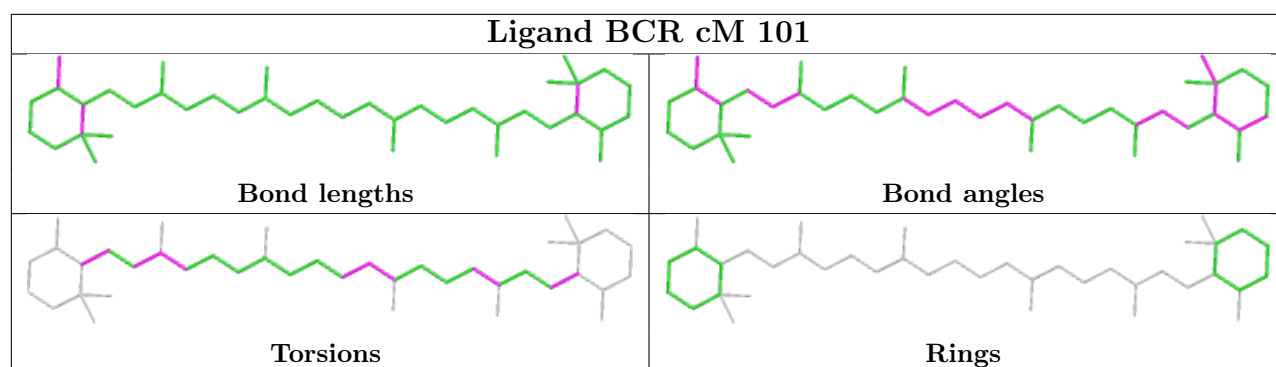


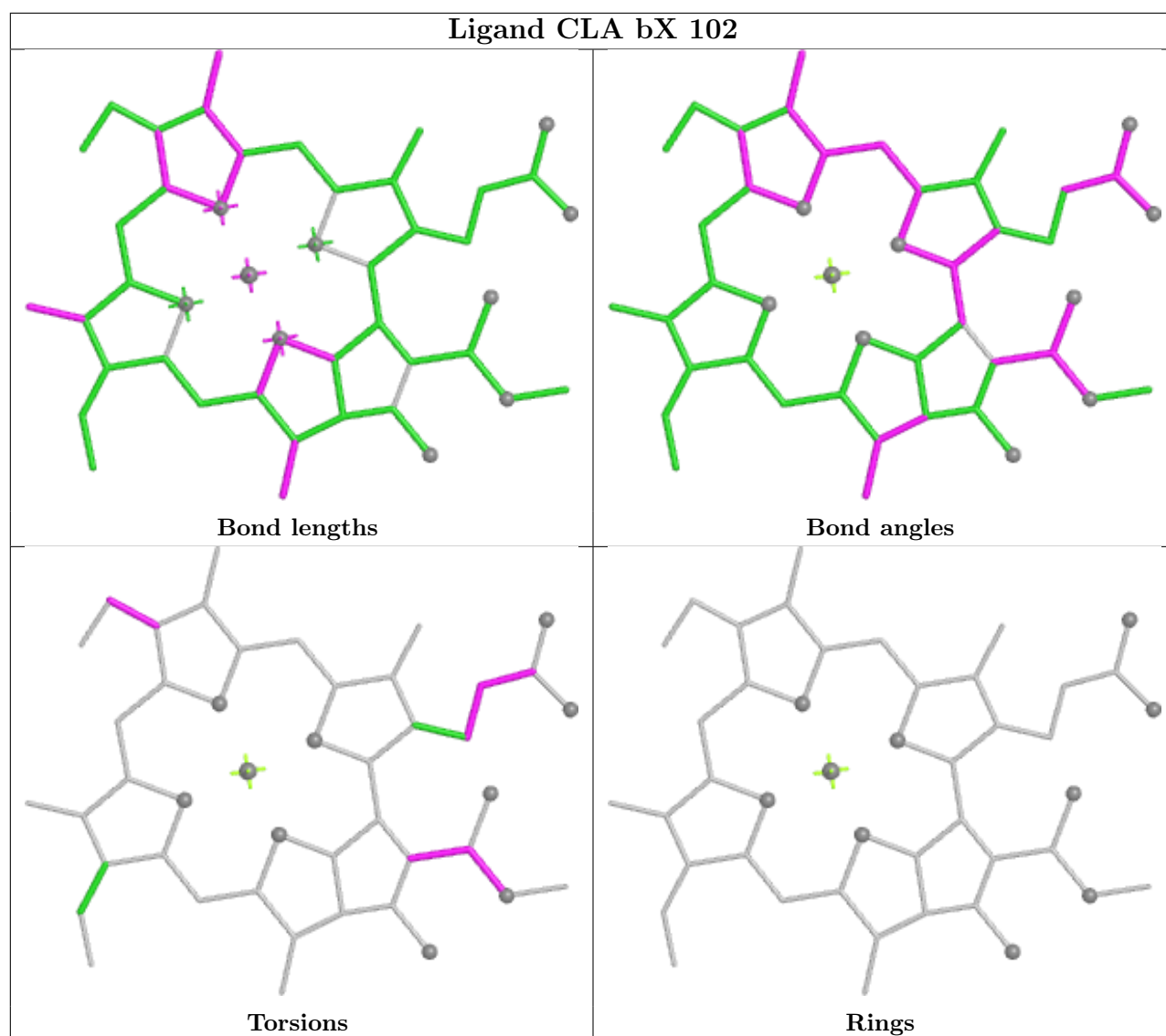


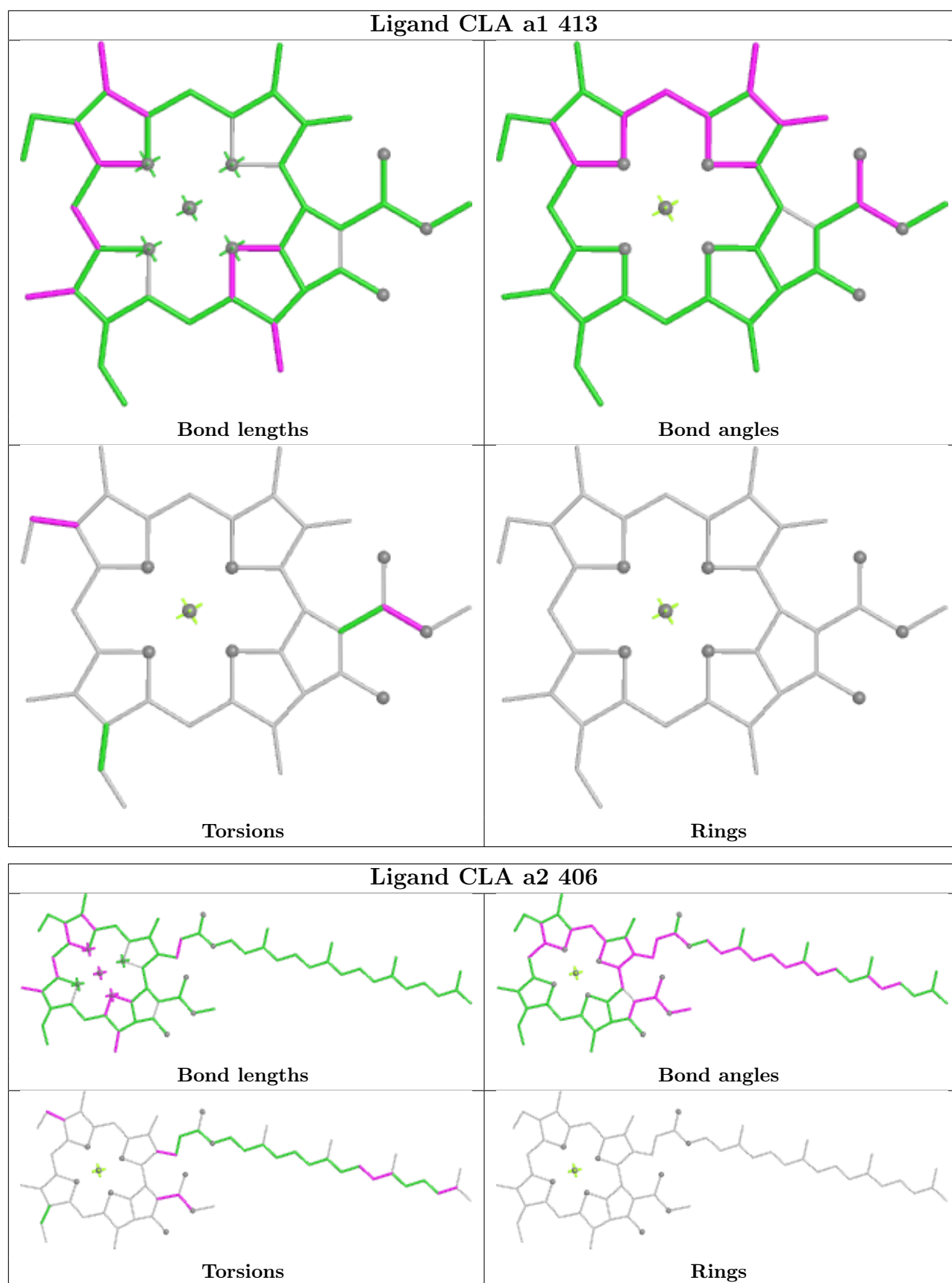


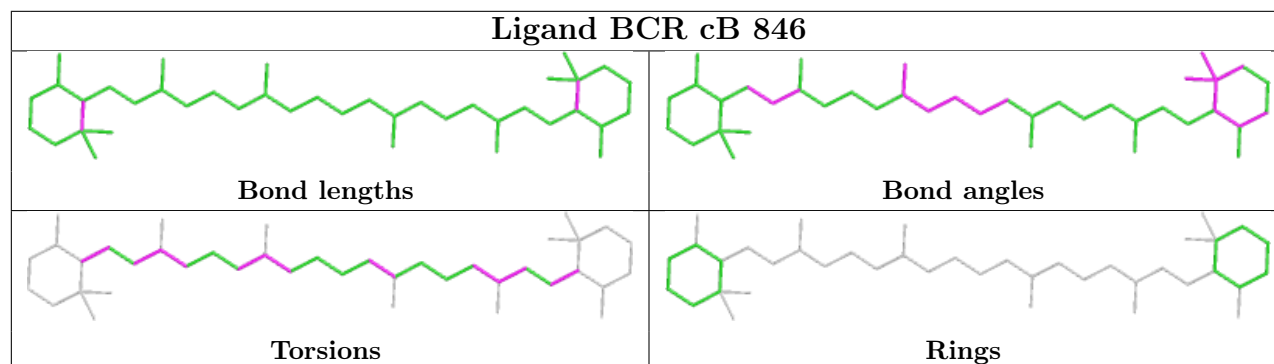
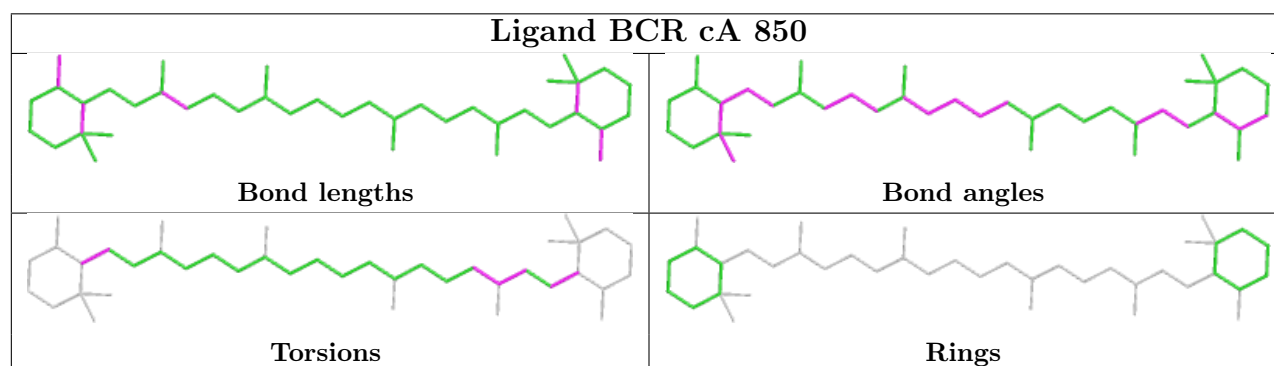
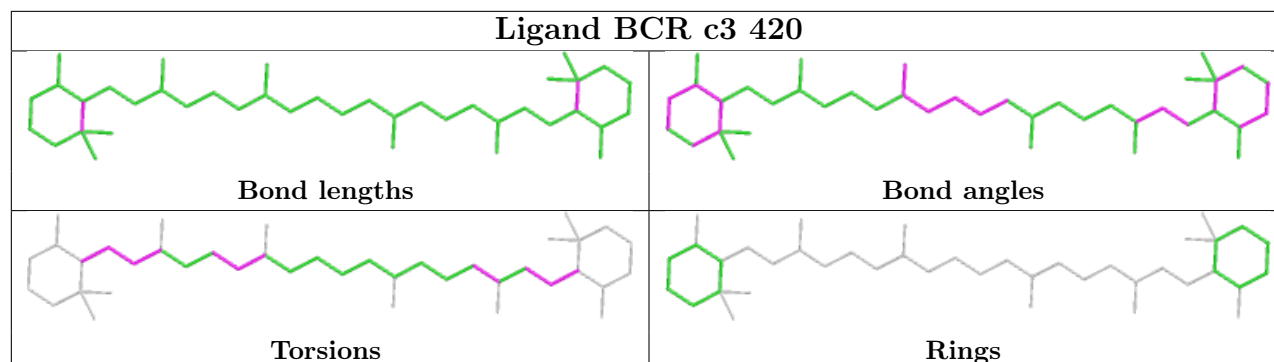
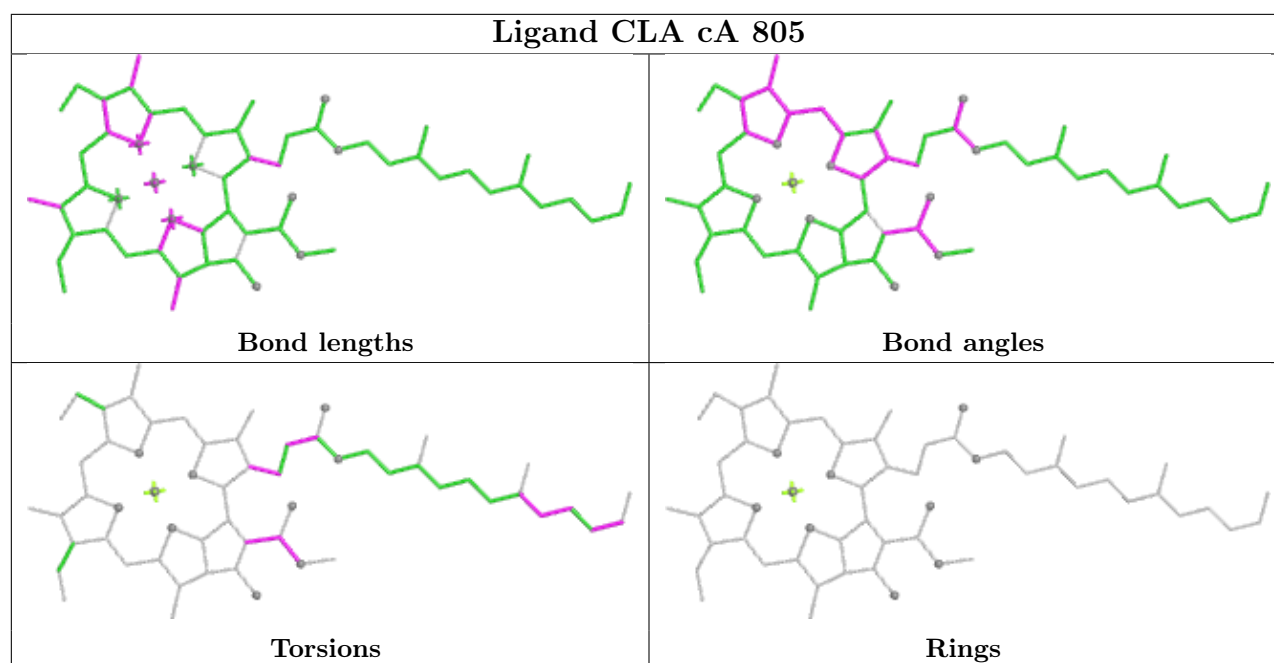


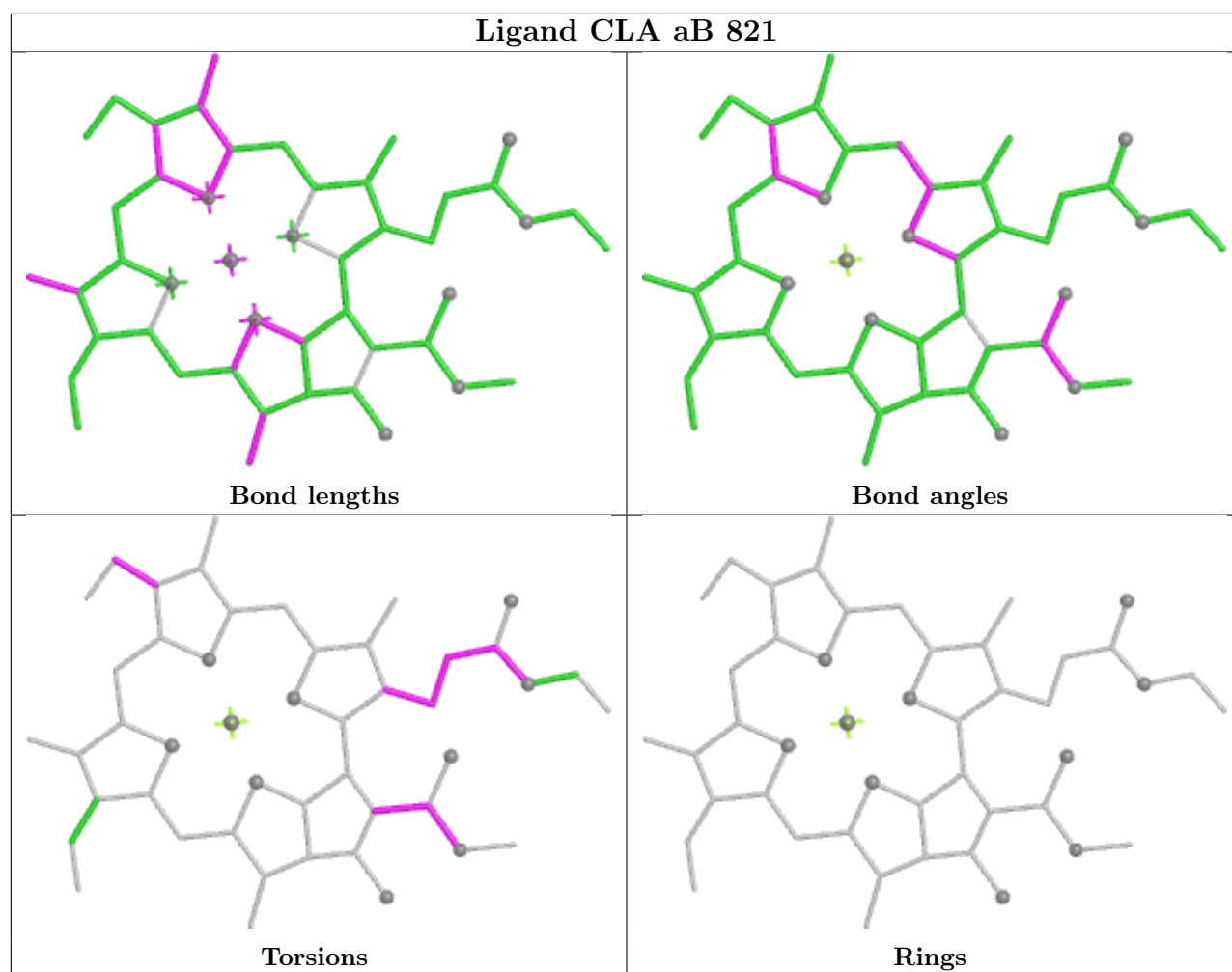


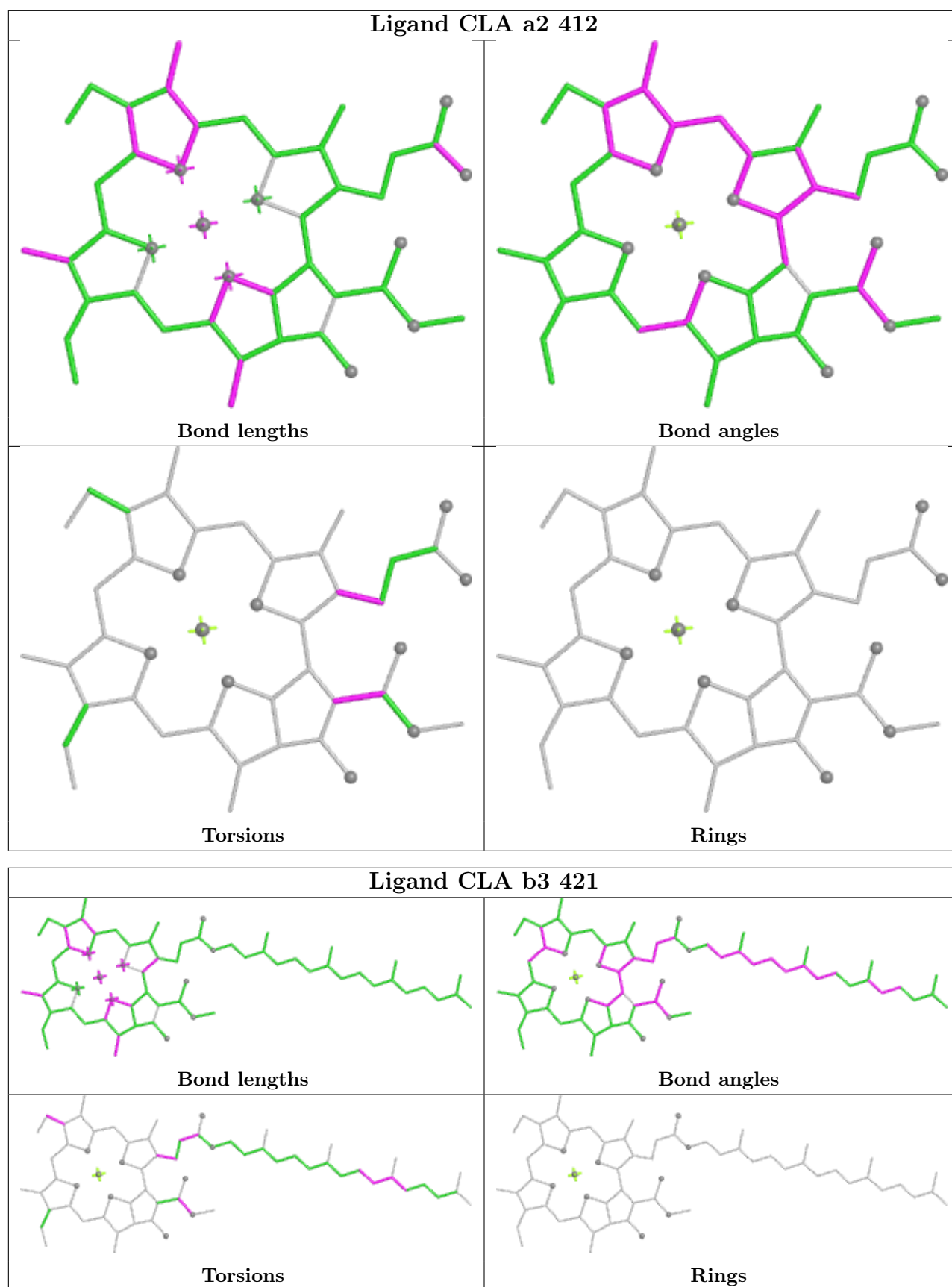


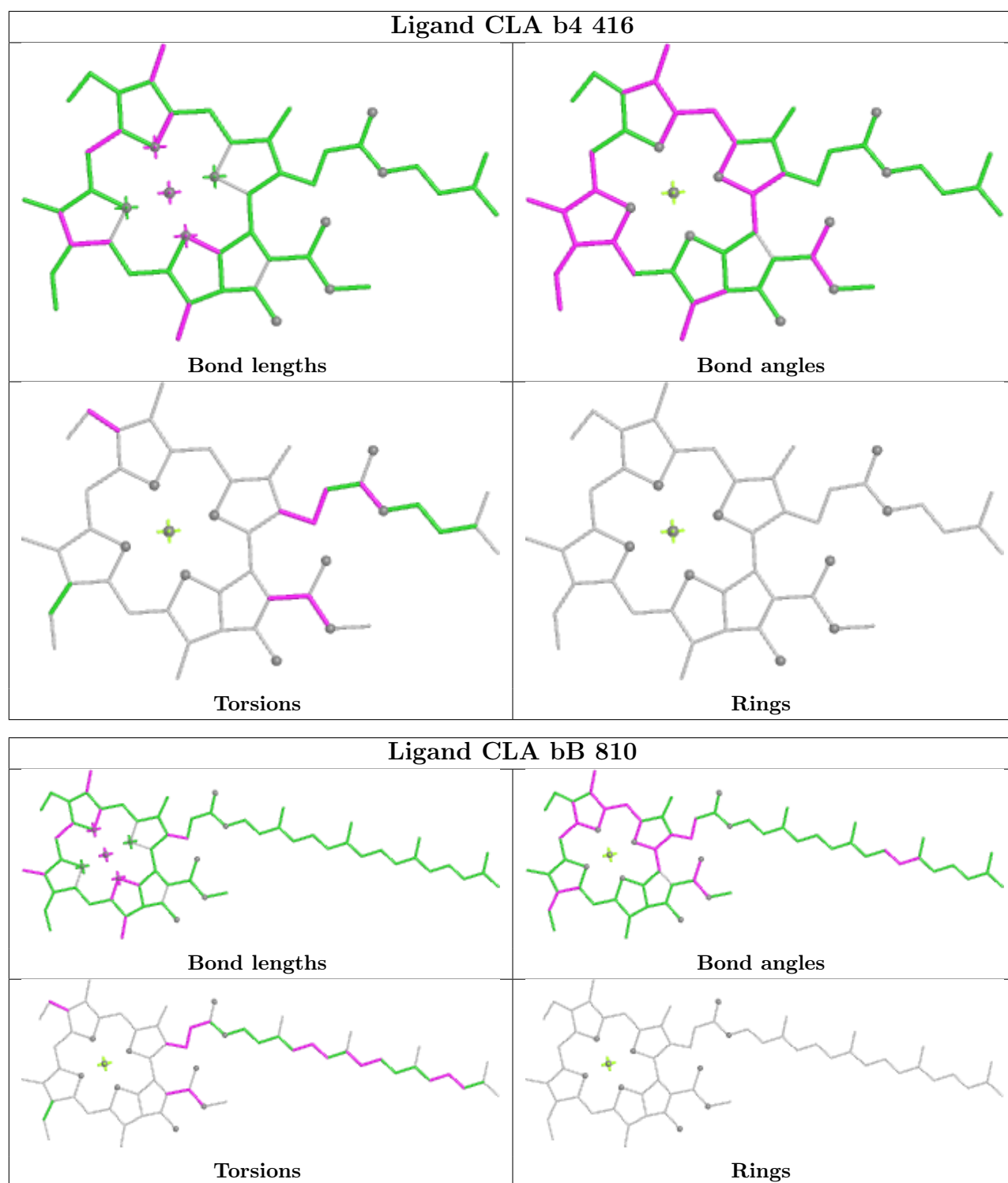


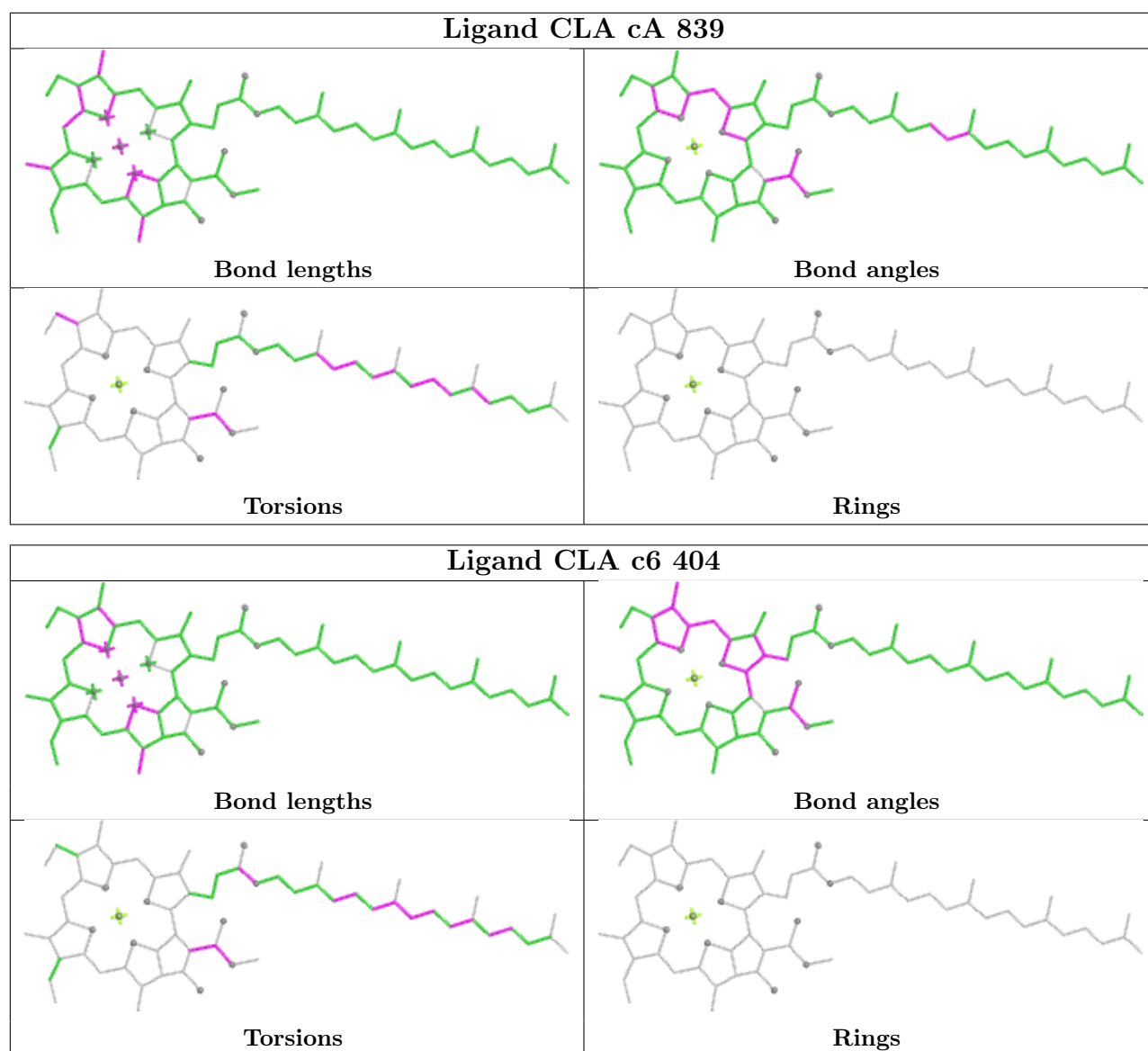


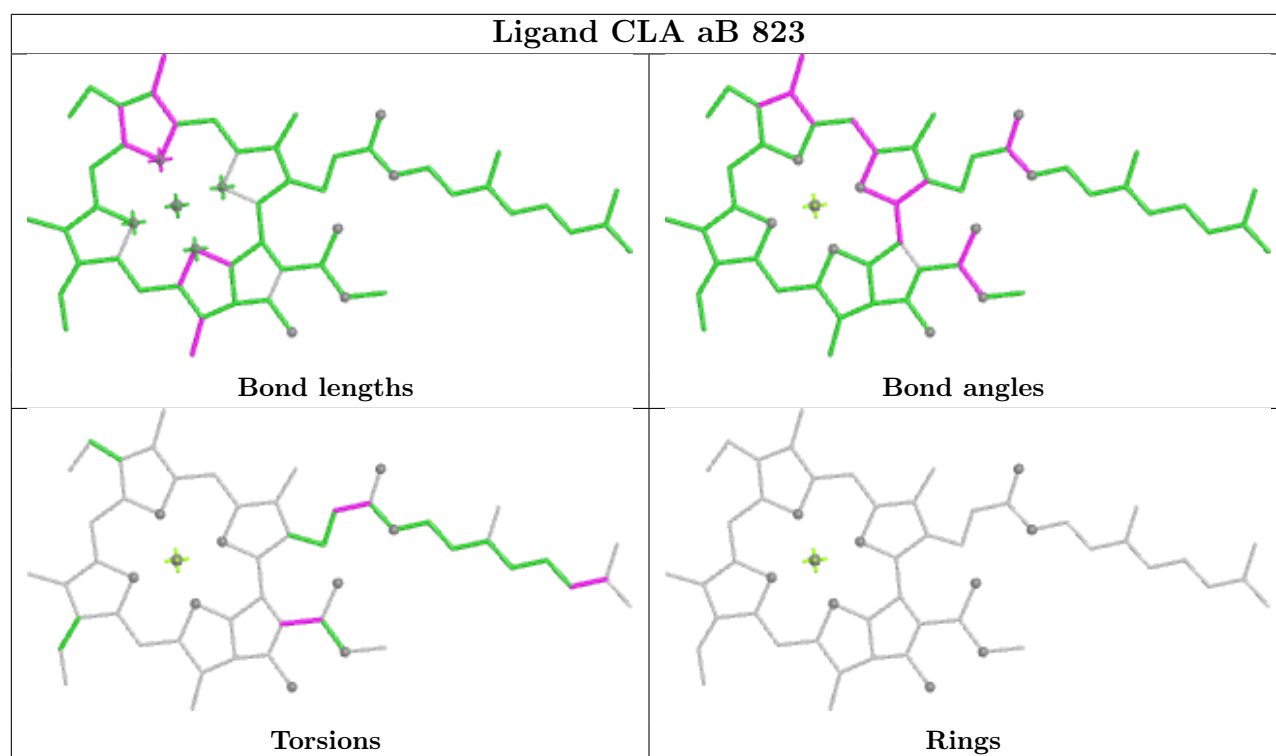


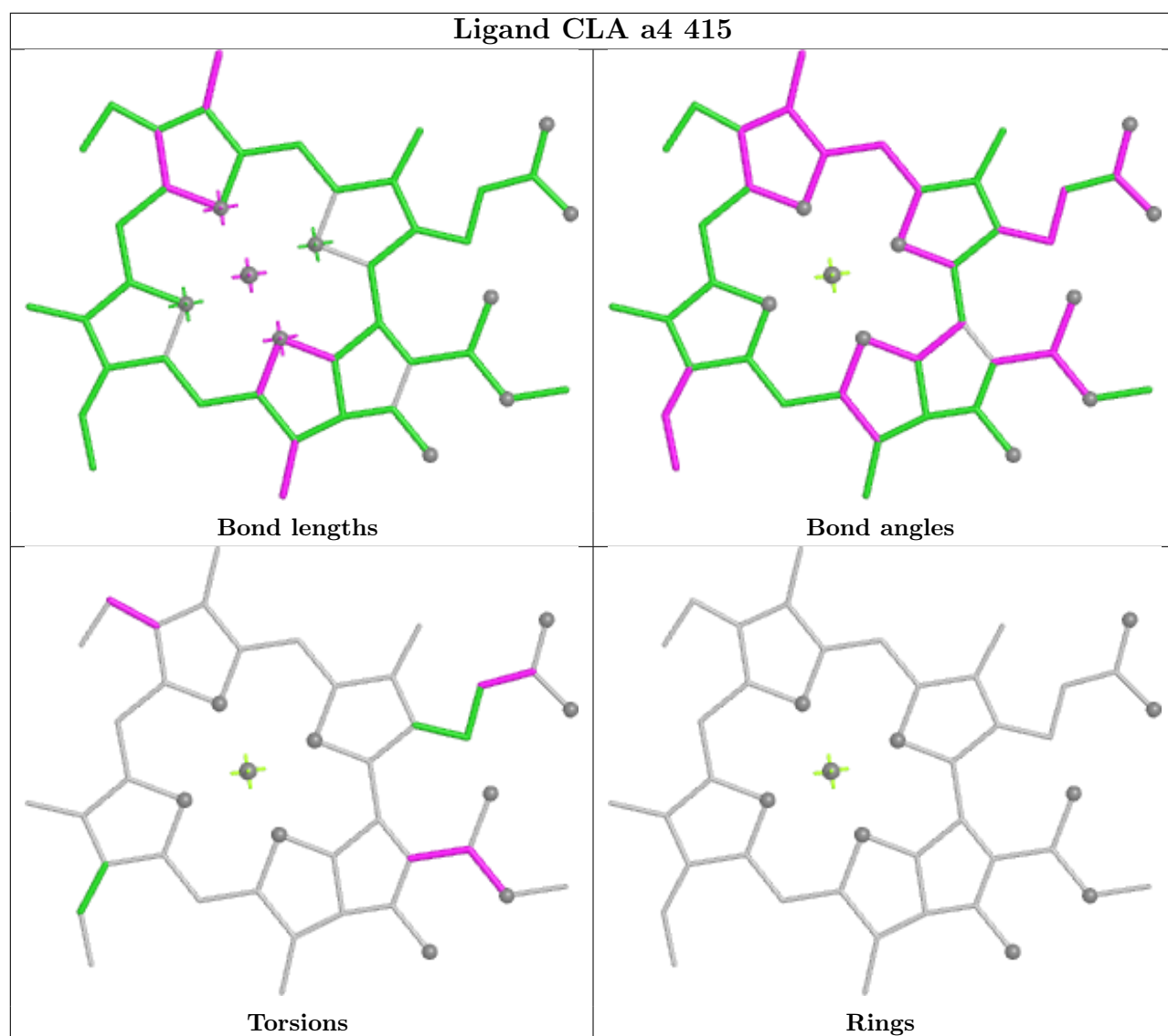


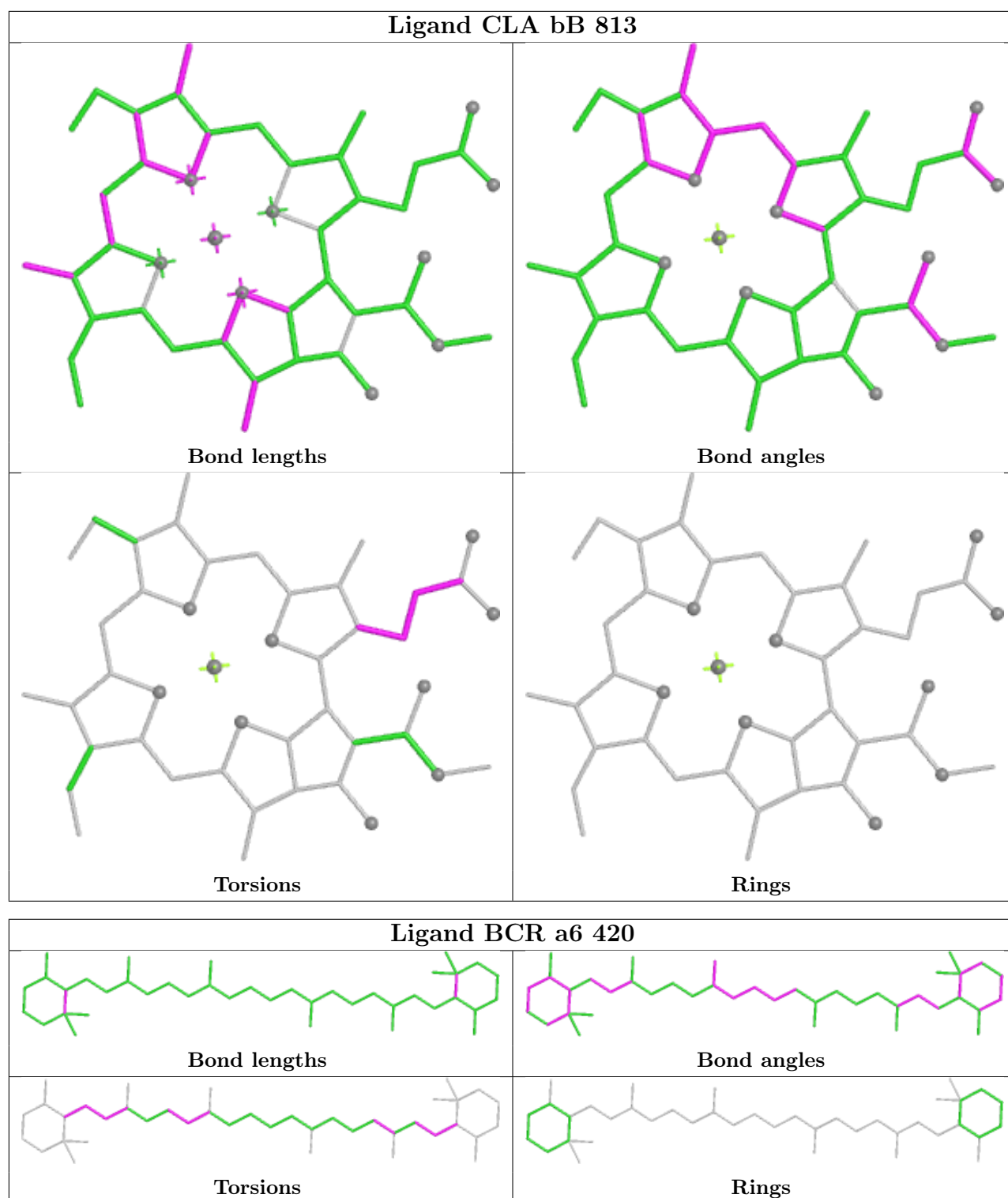


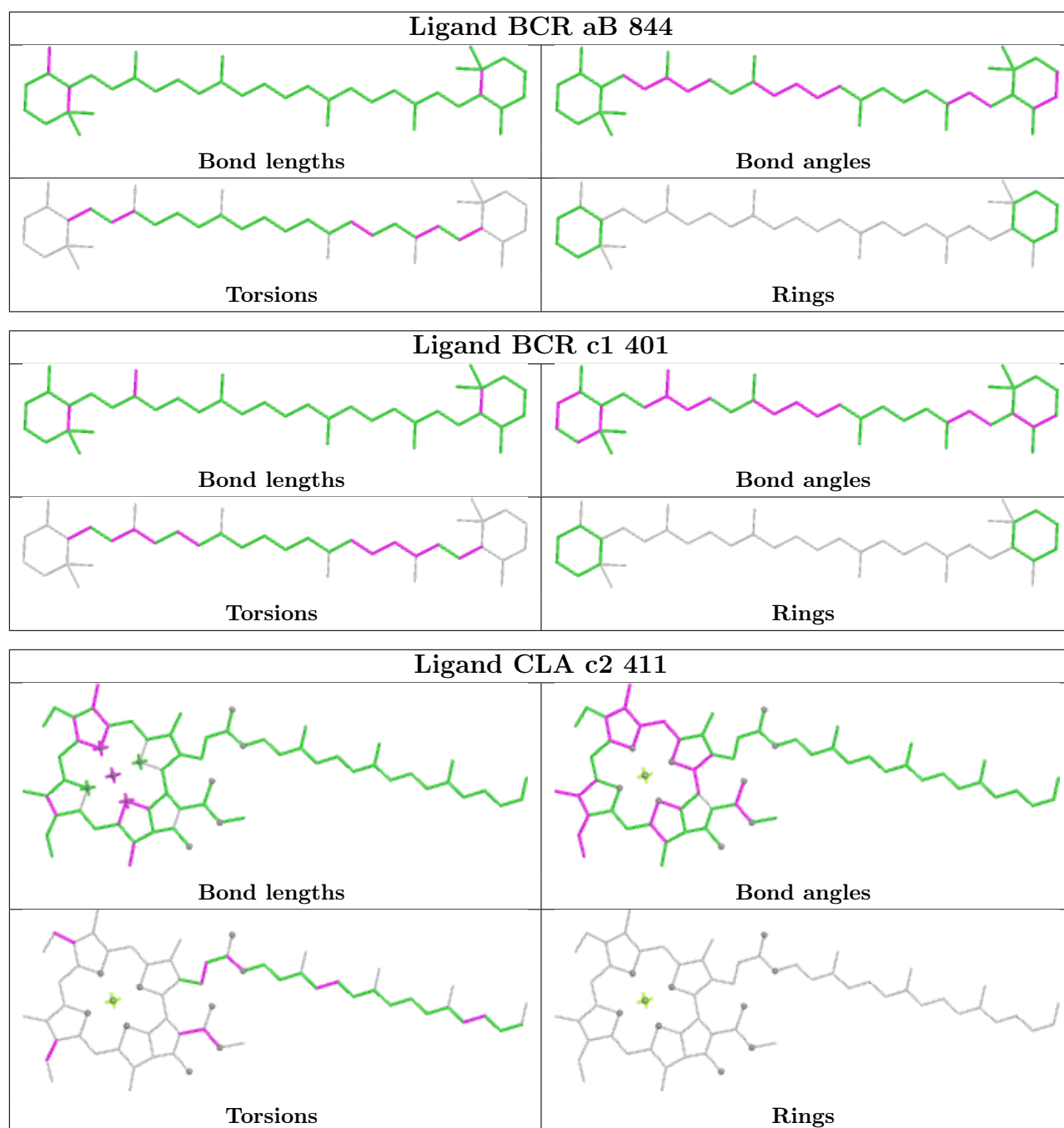


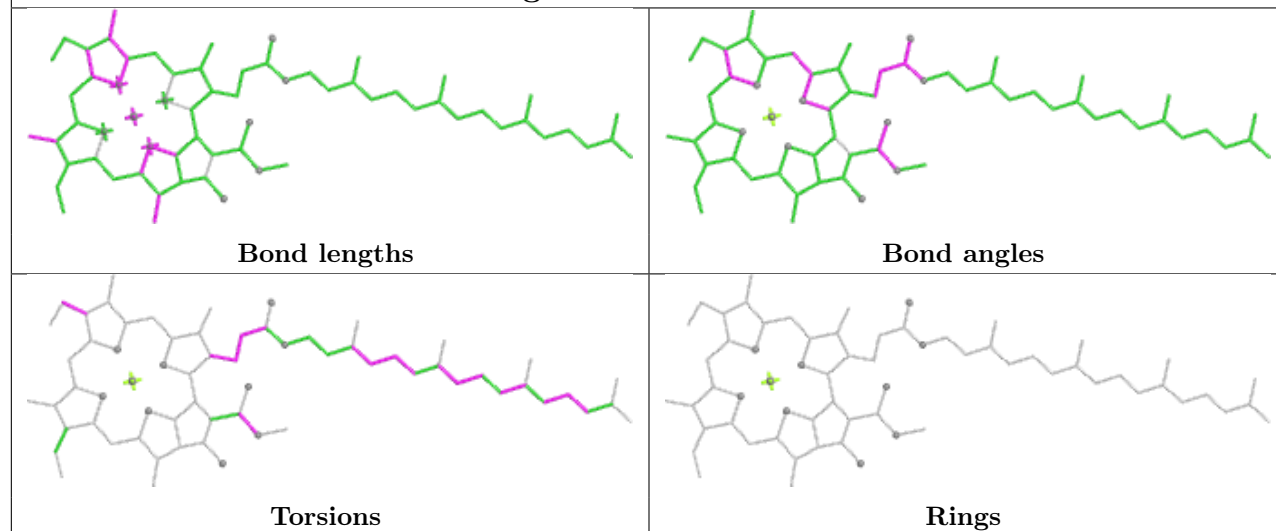
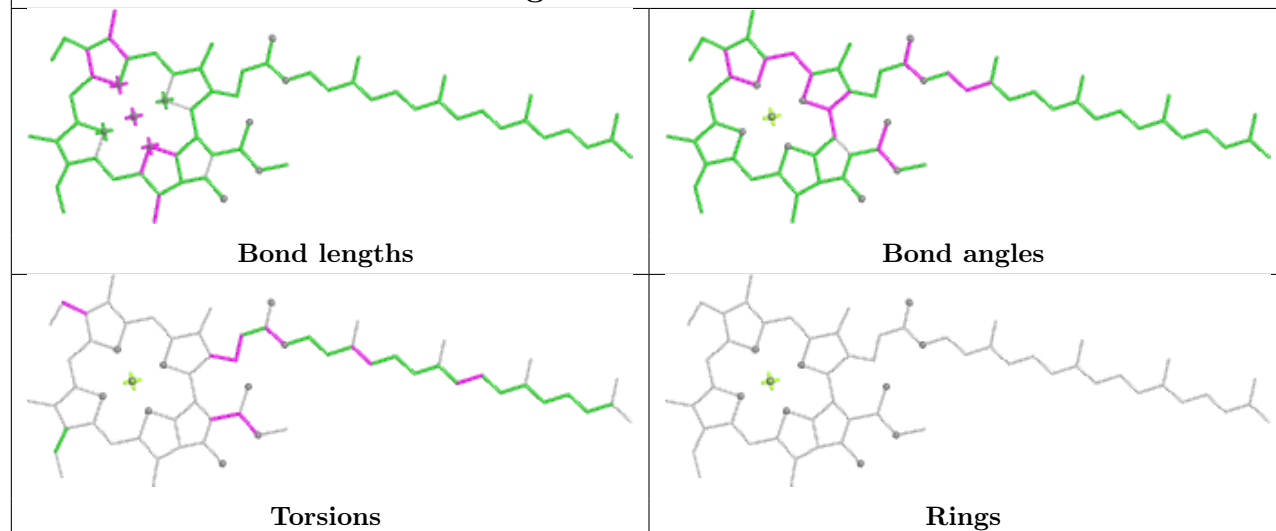


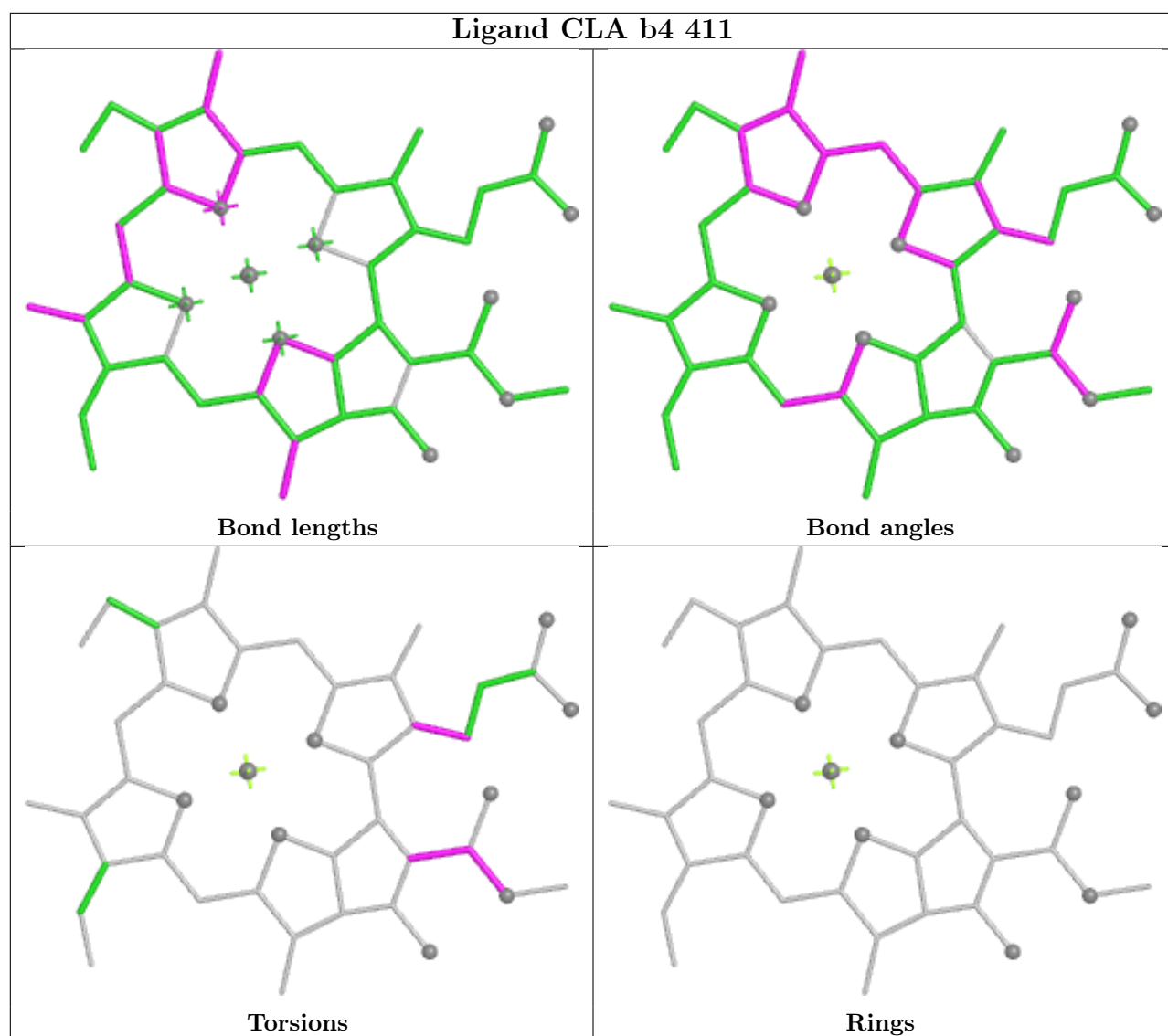


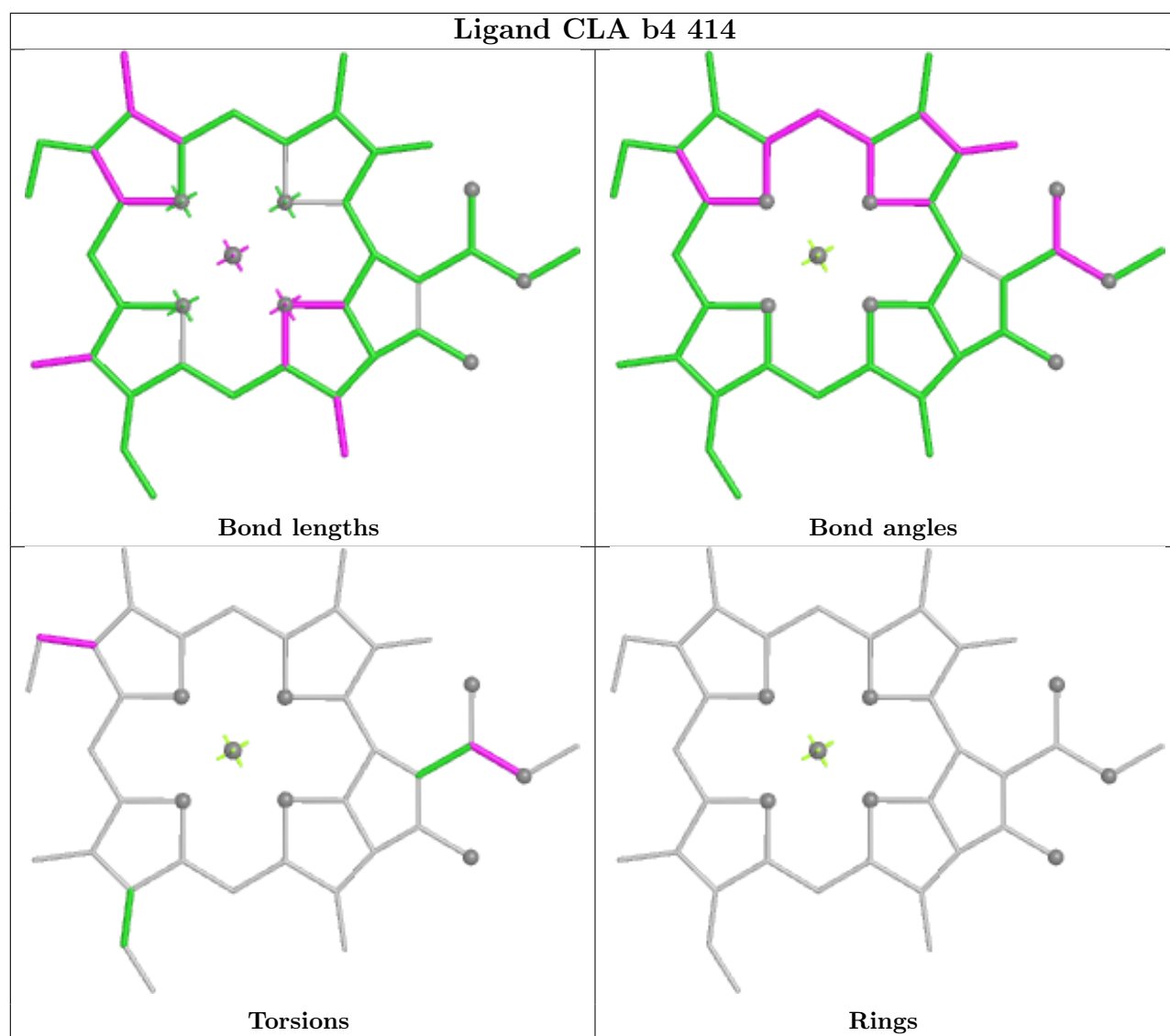




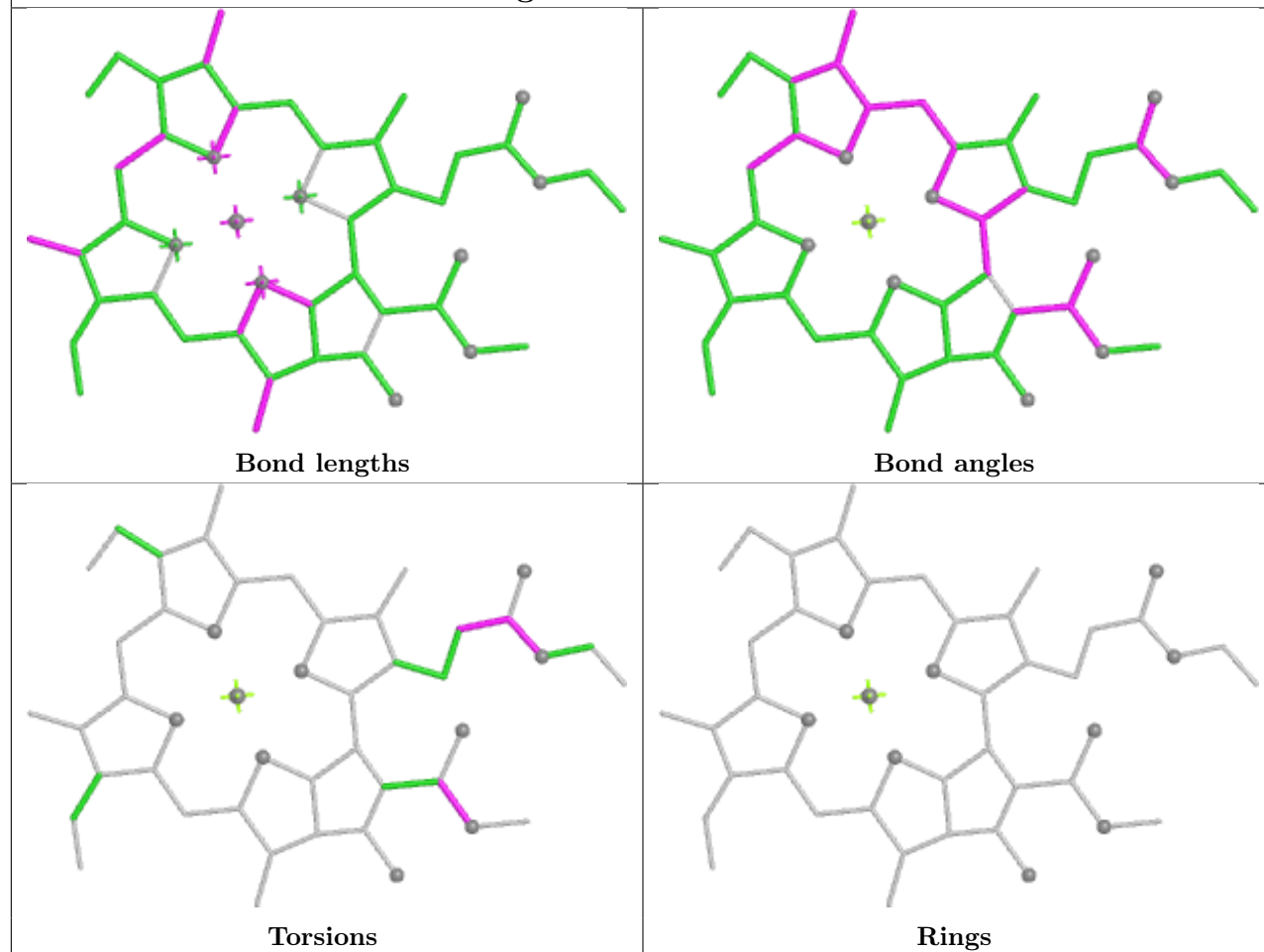


Ligand CLA aA 810**Ligand CLA b3 404**

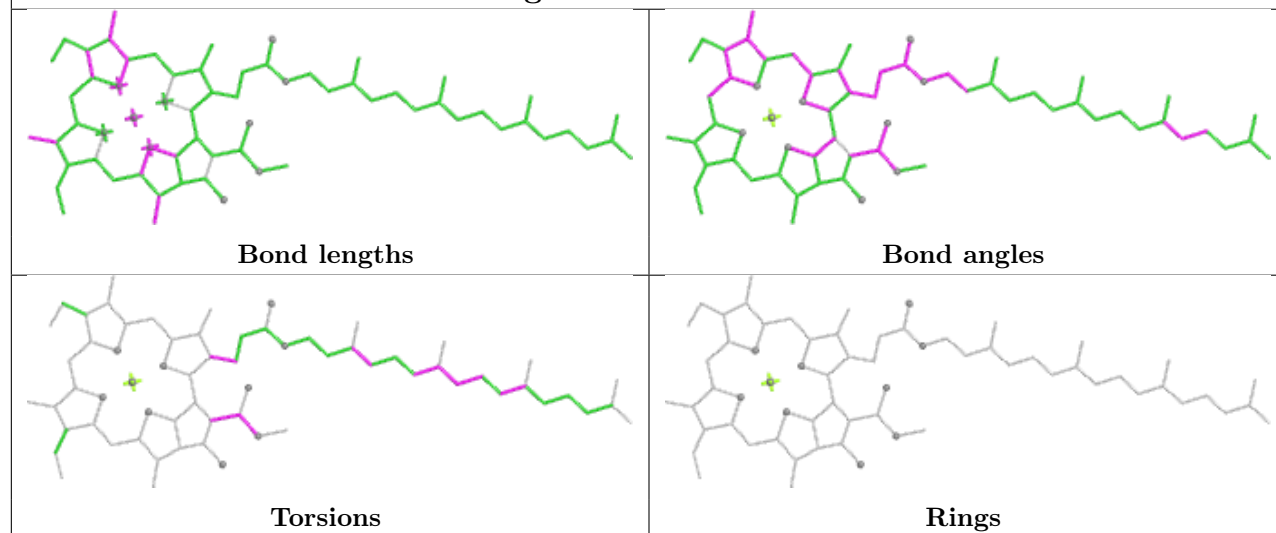


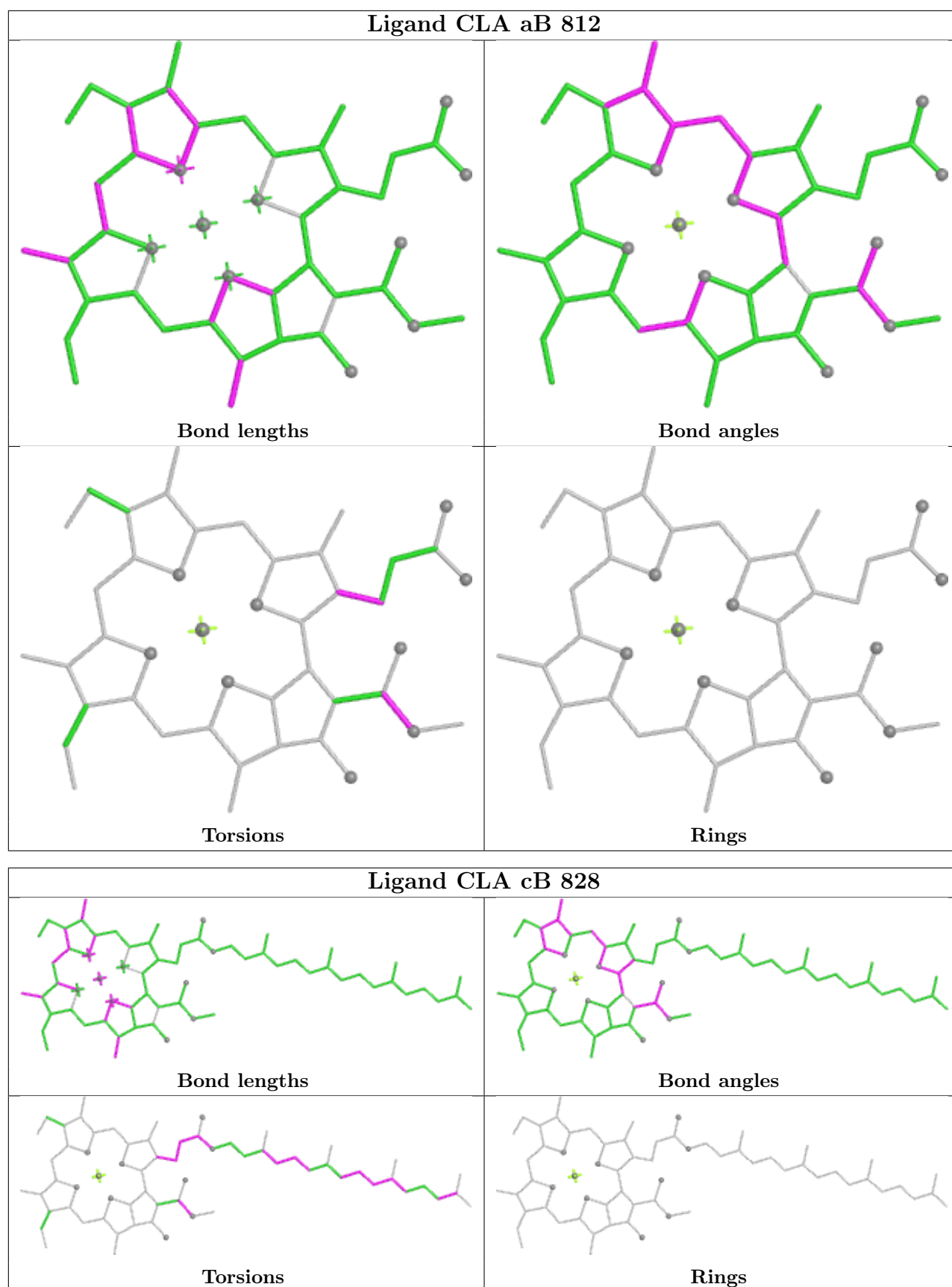


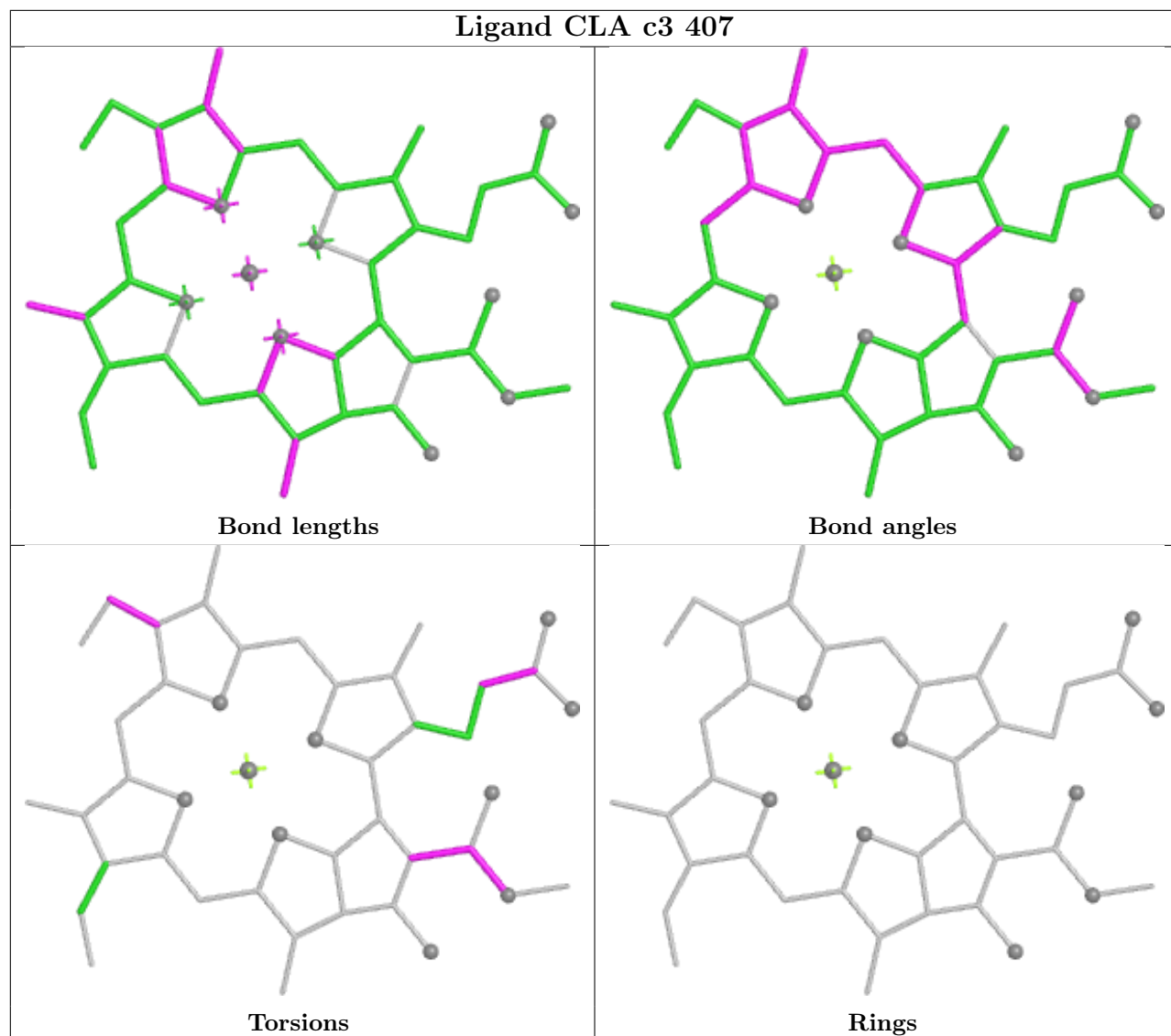
Ligand CLA bA 840

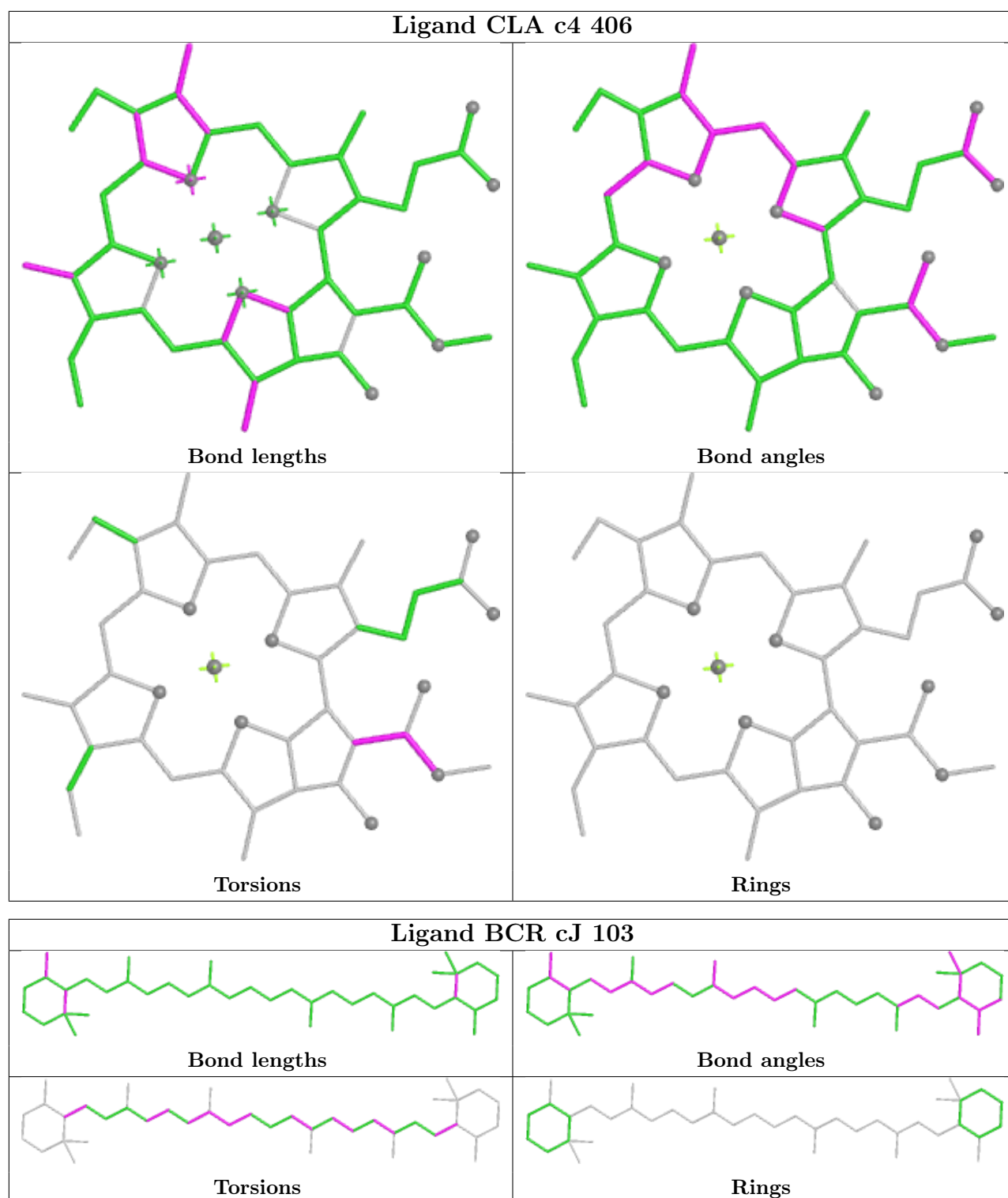


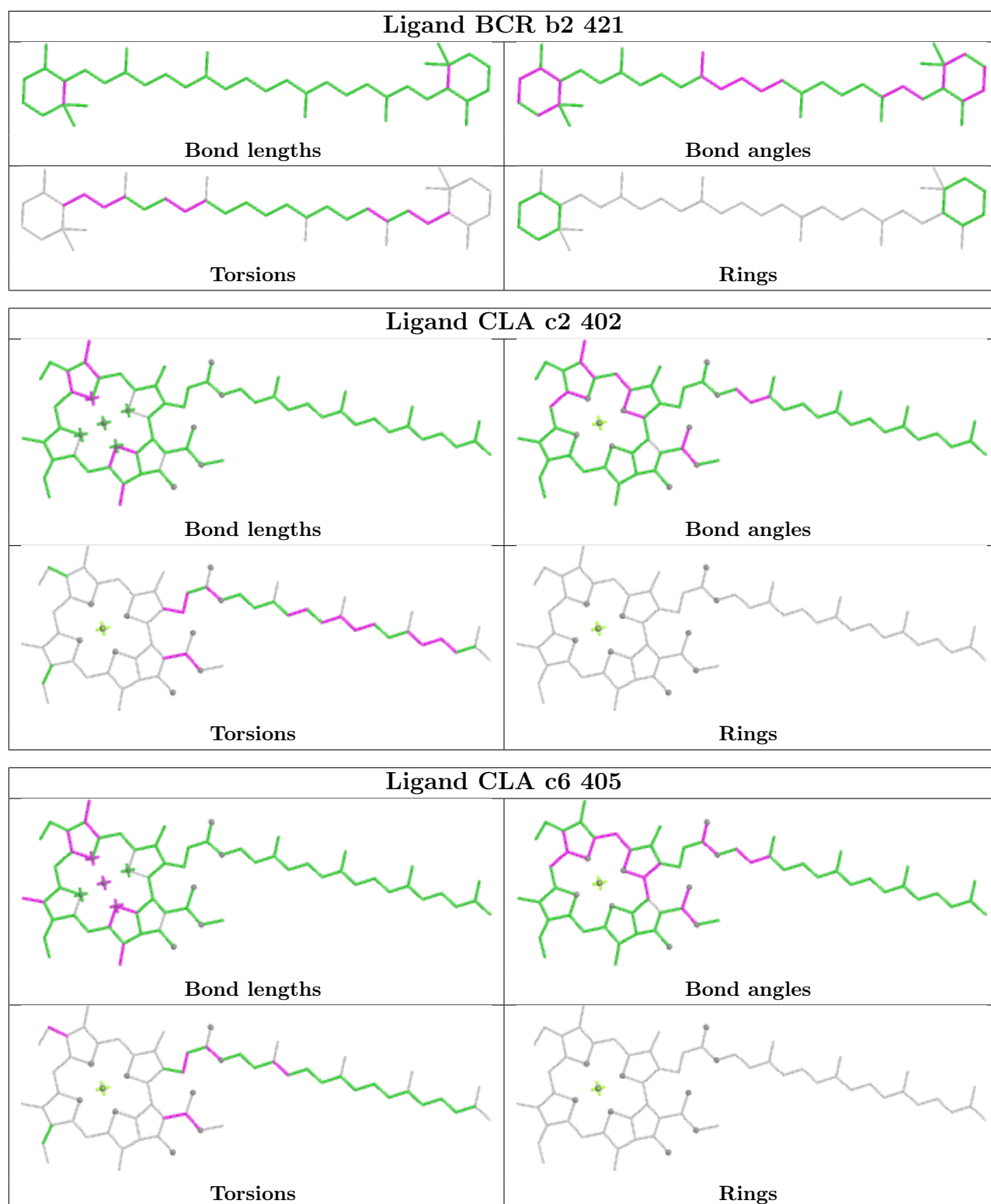
Ligand CLA cB 827

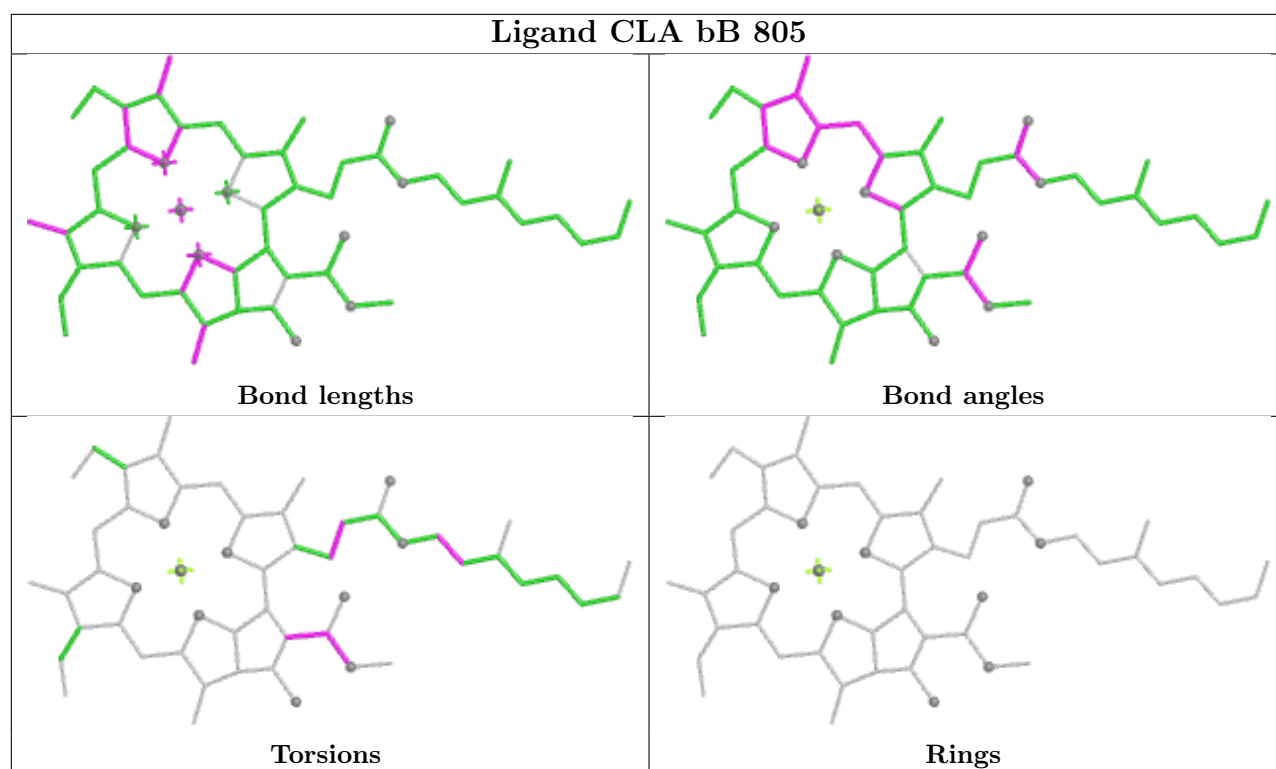


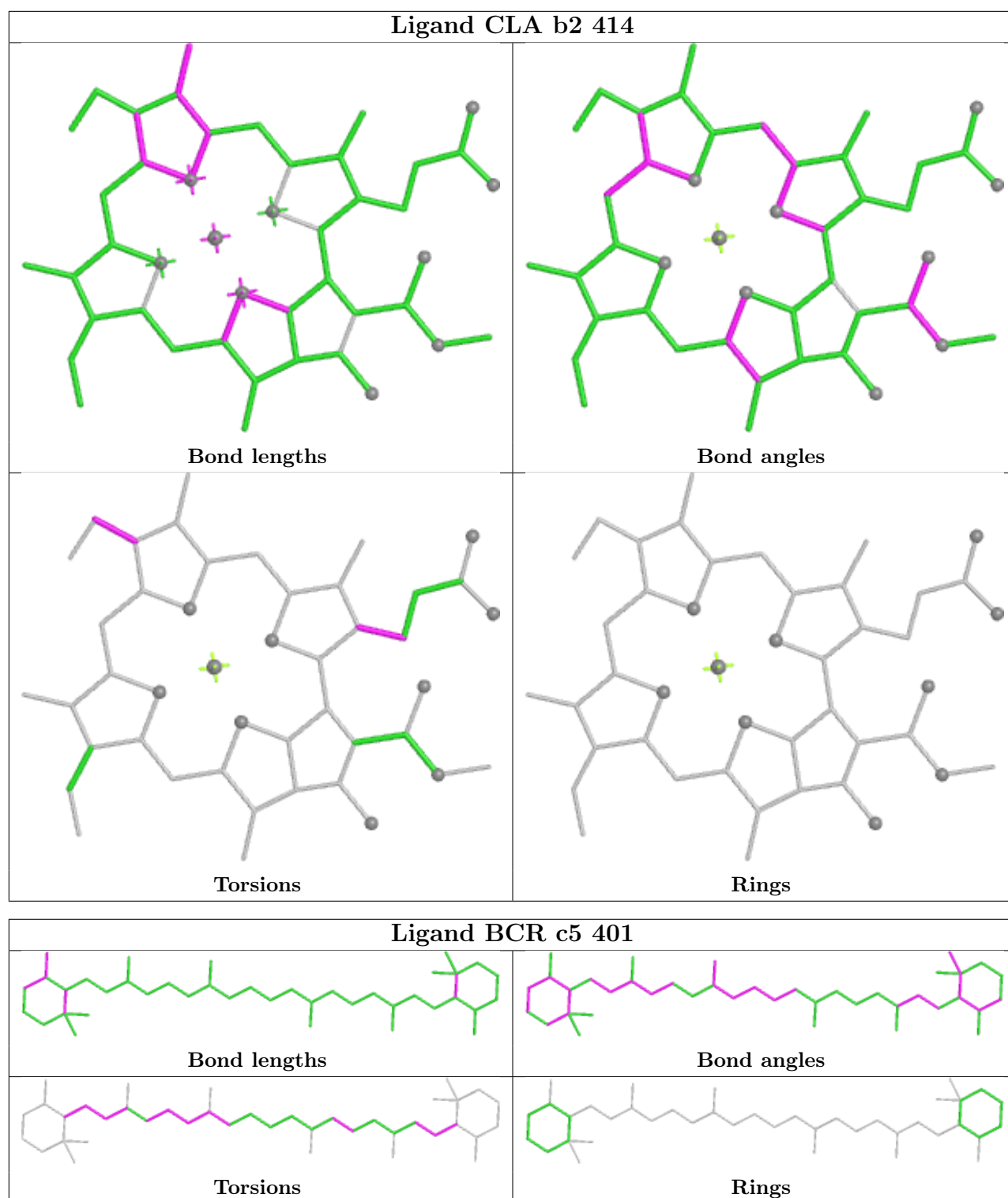


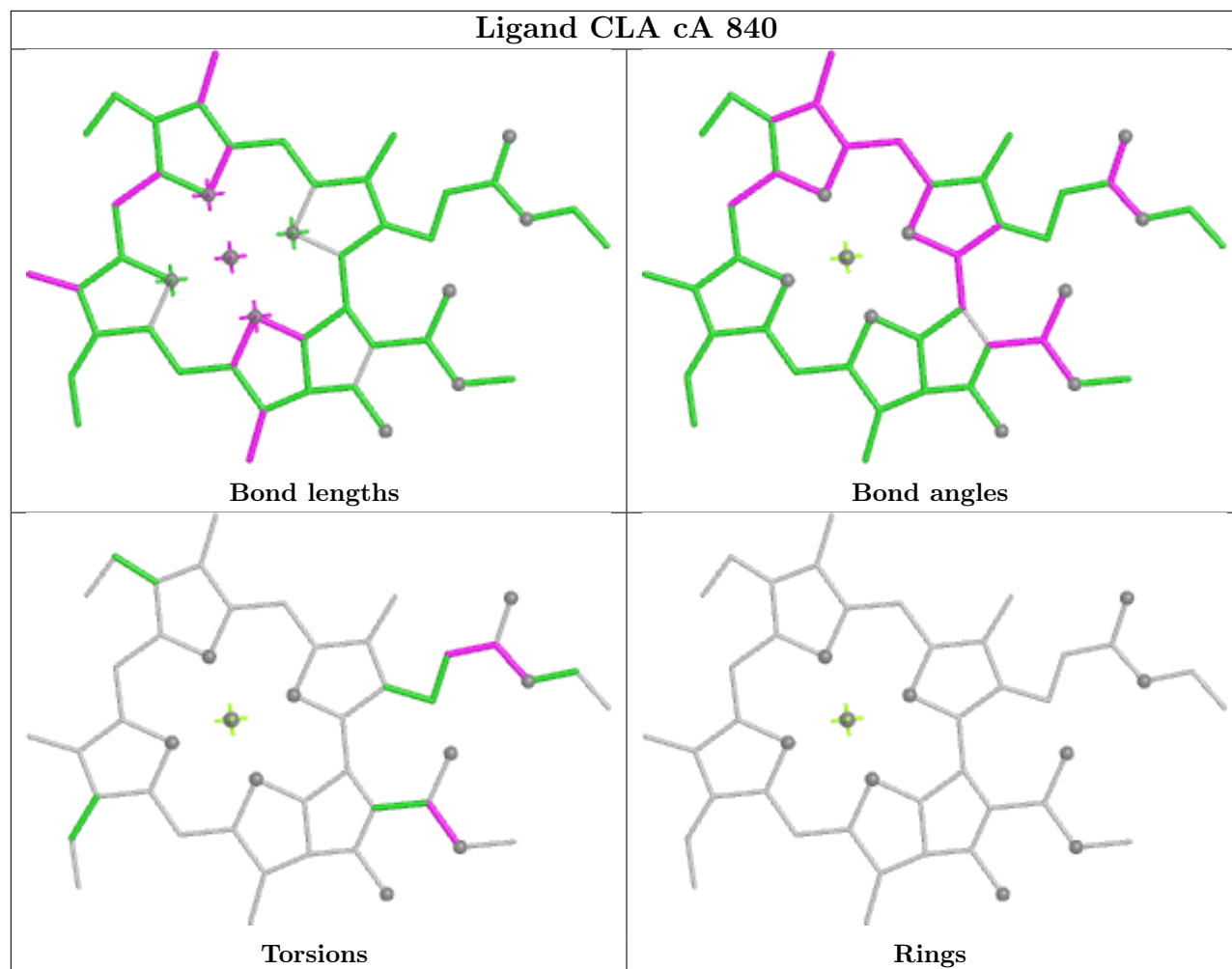


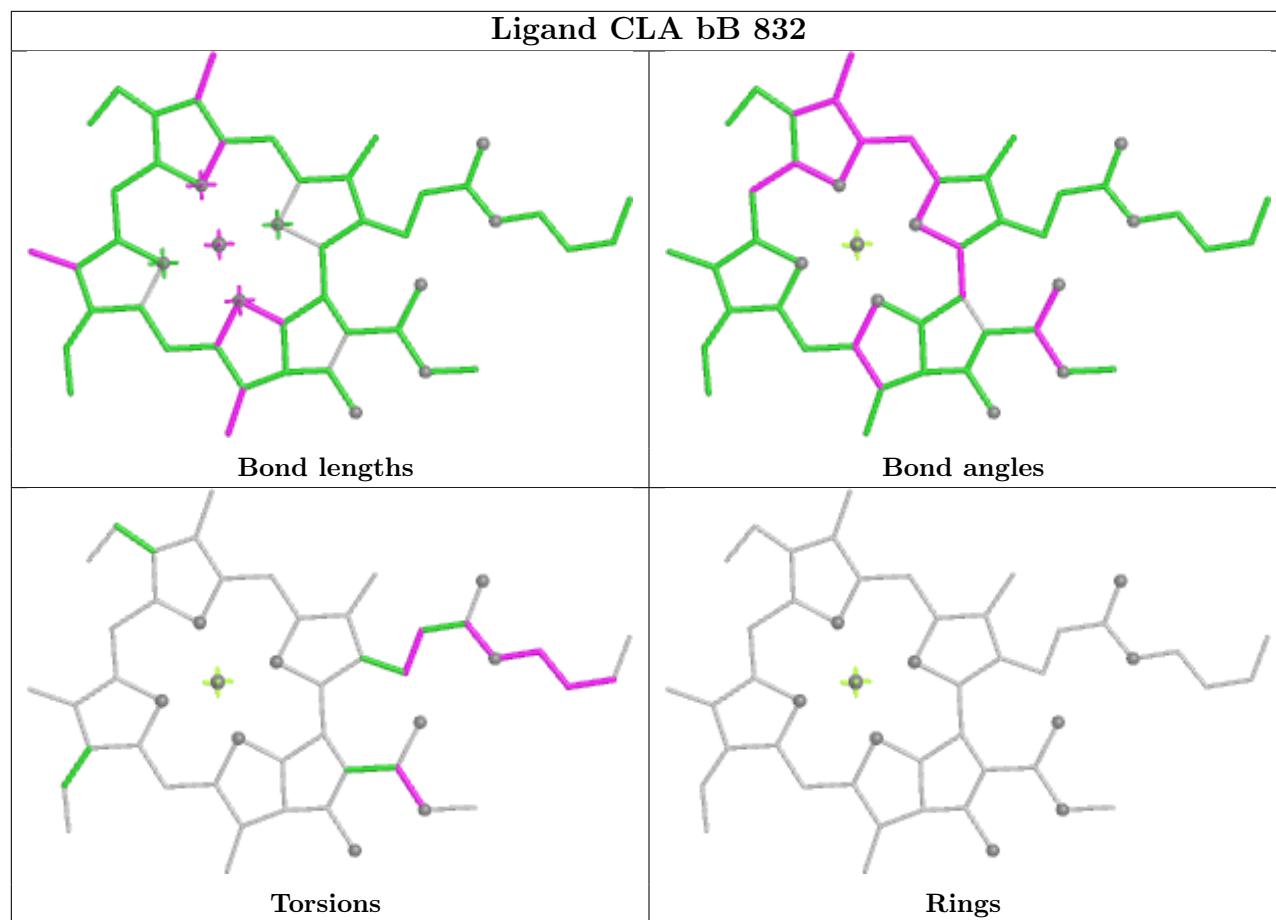


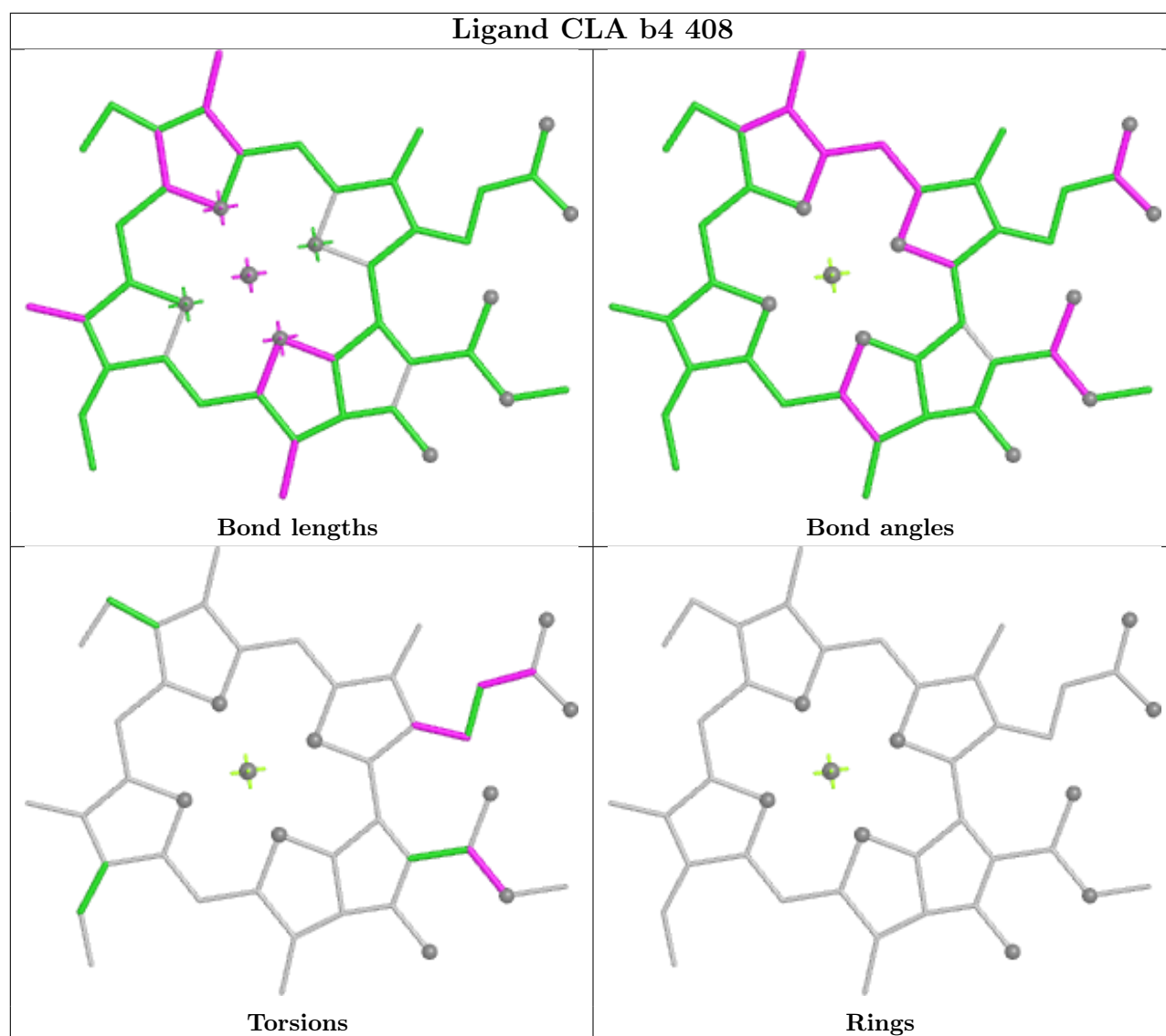


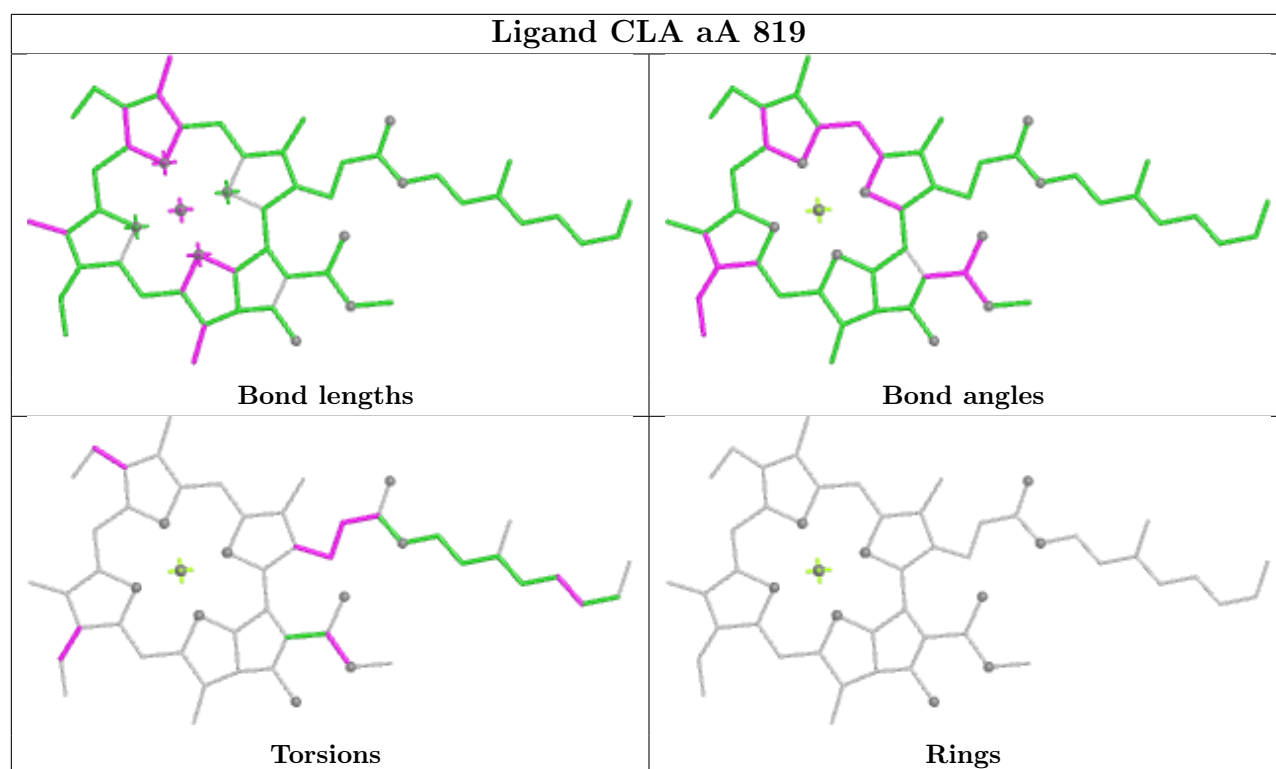


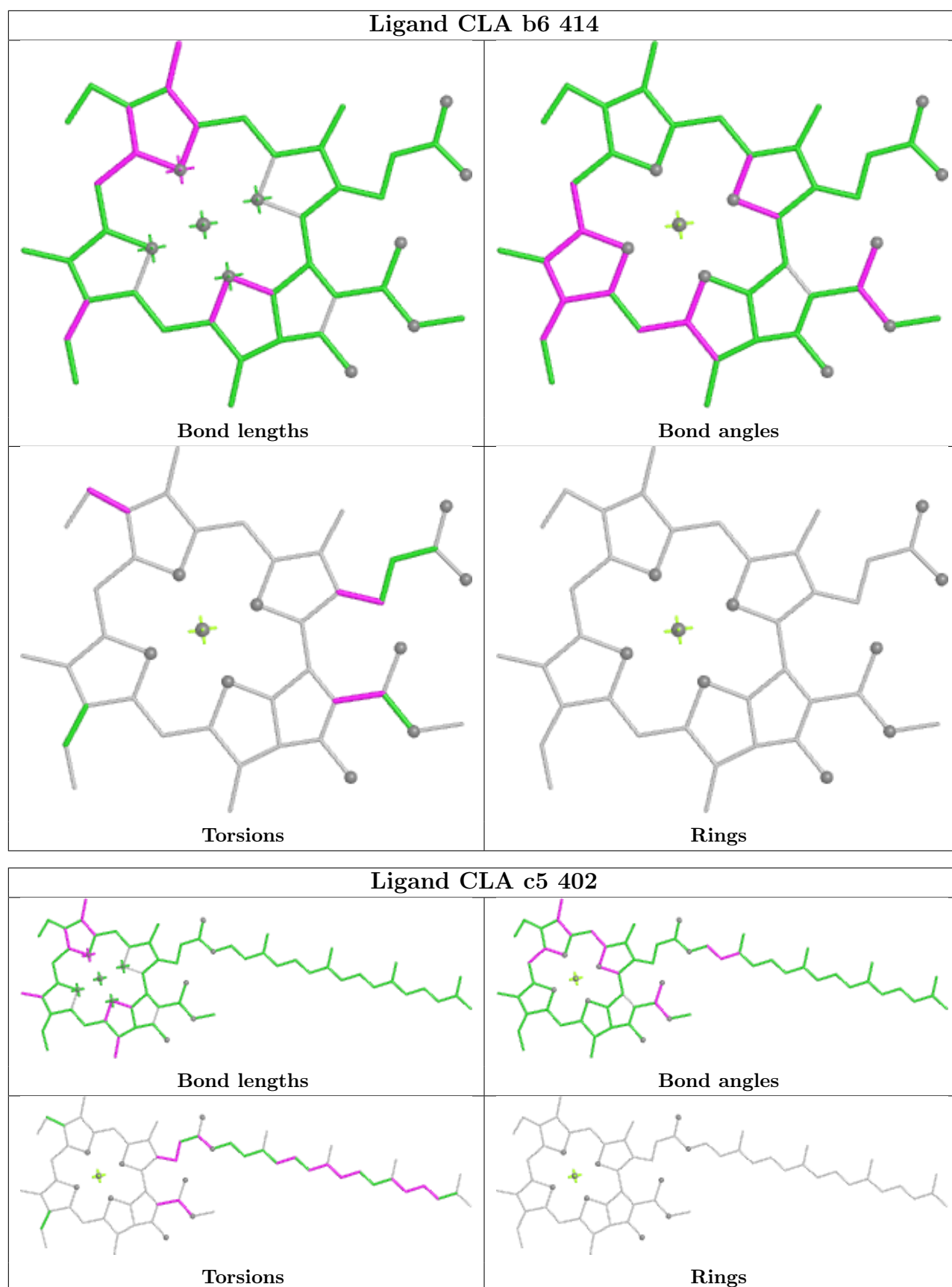


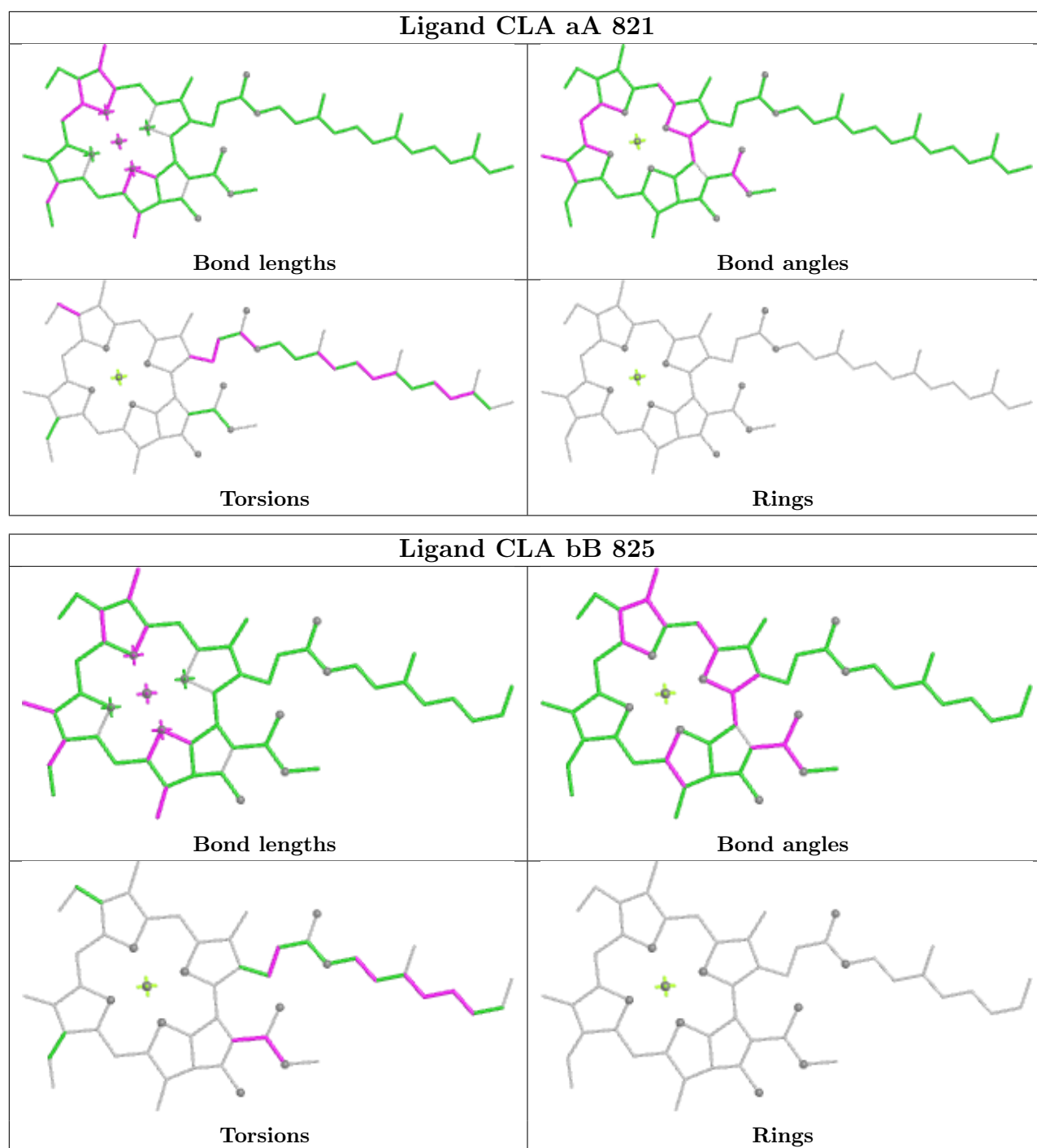


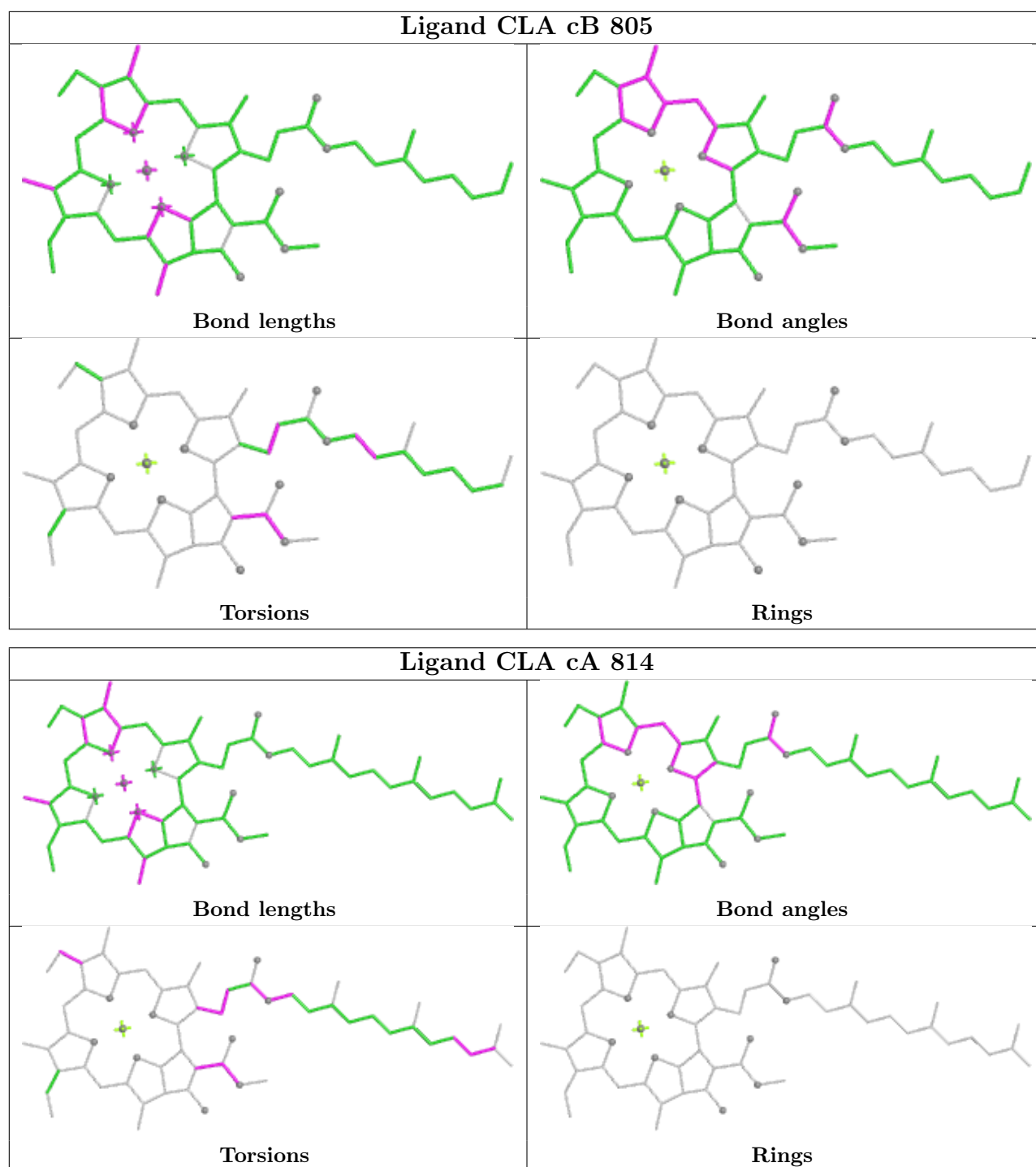


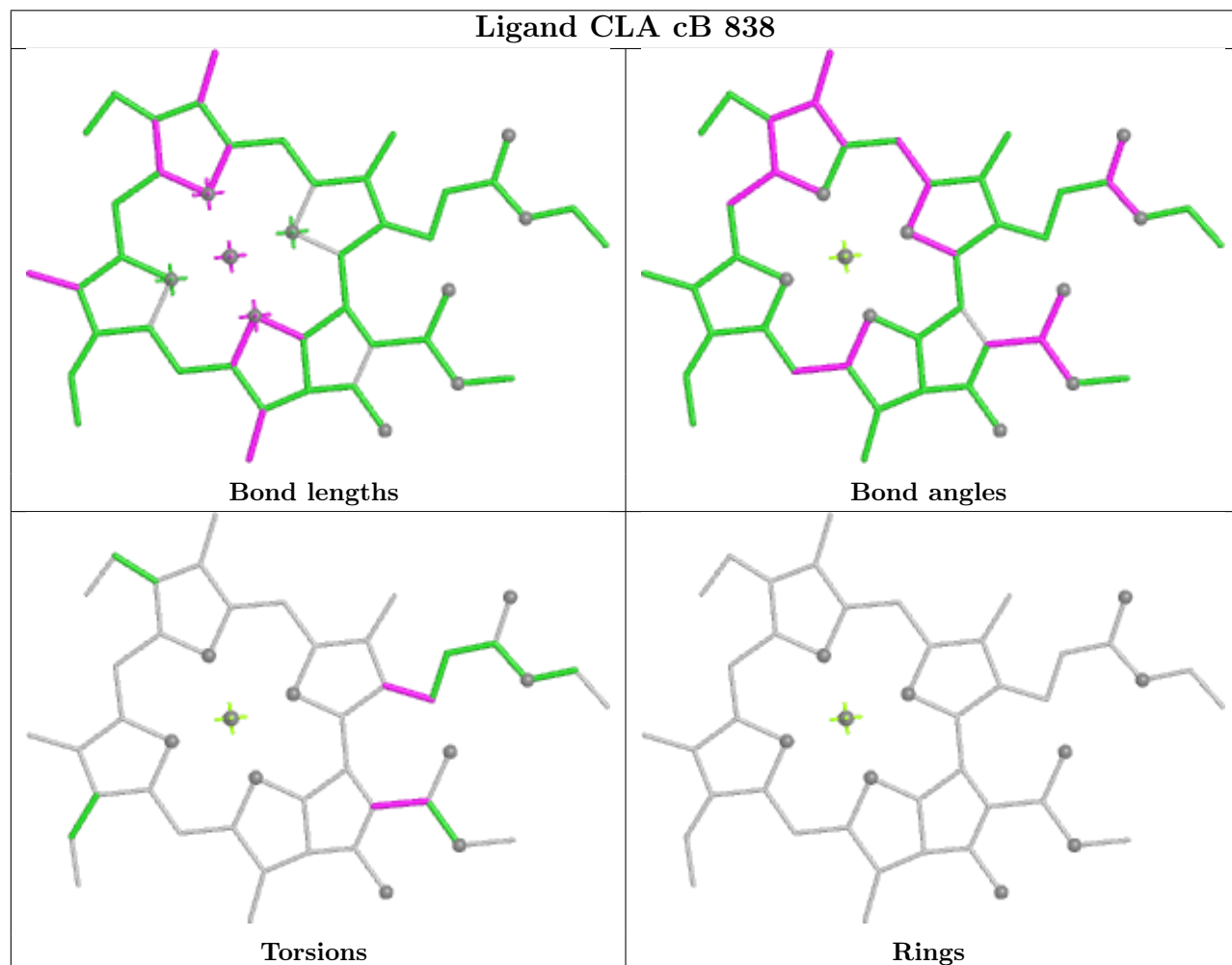
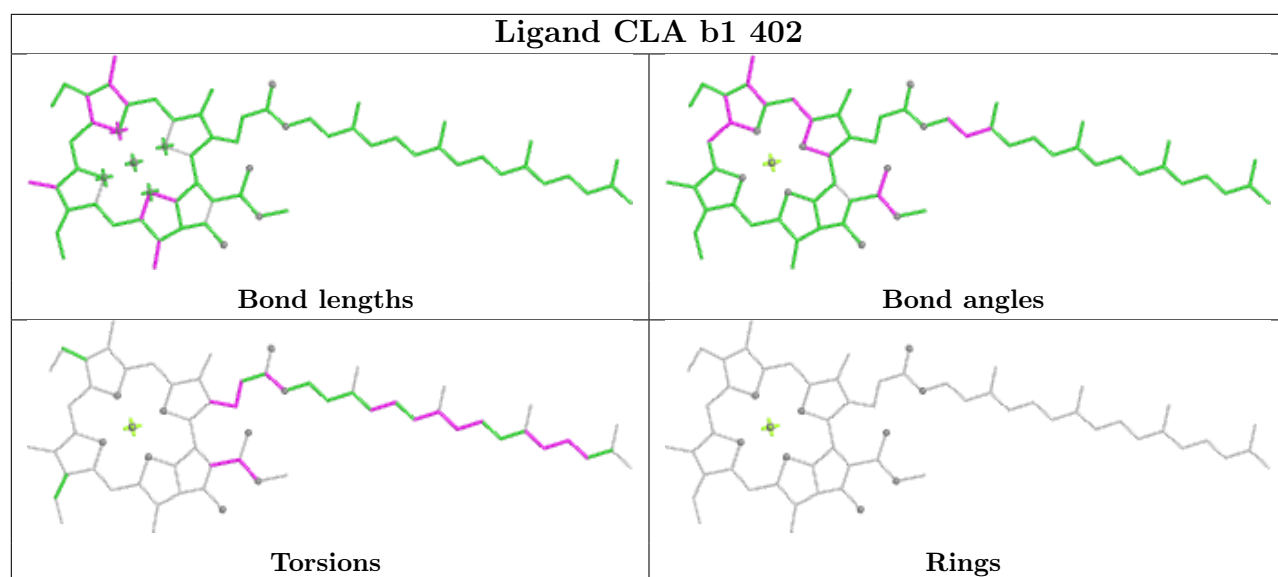


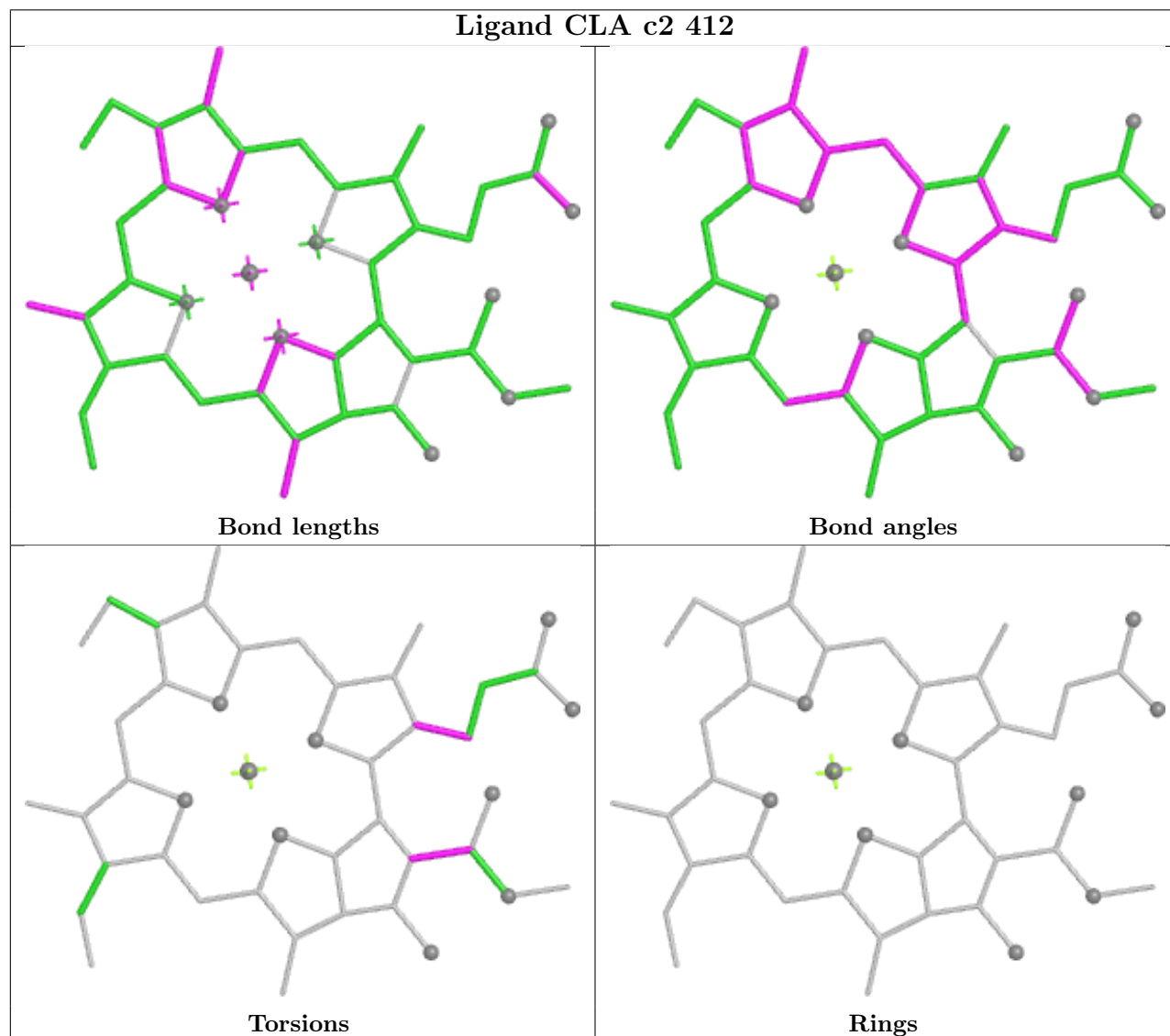
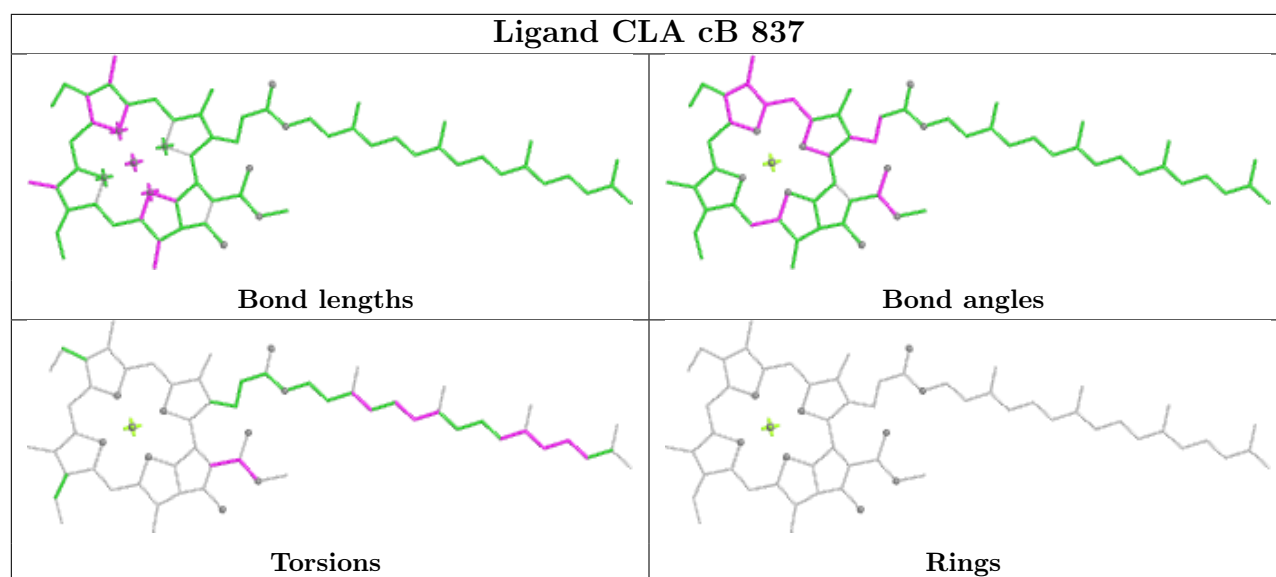


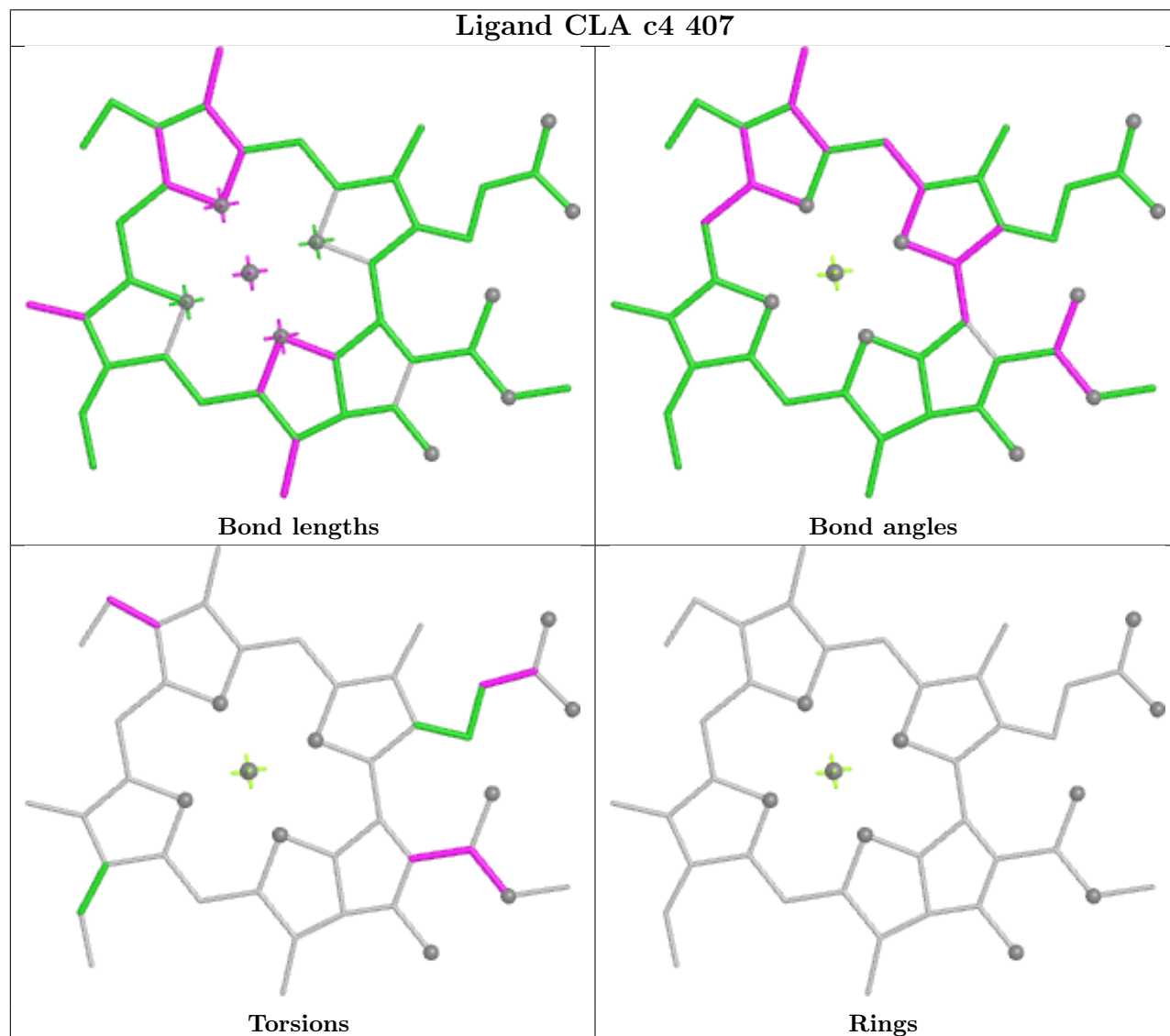
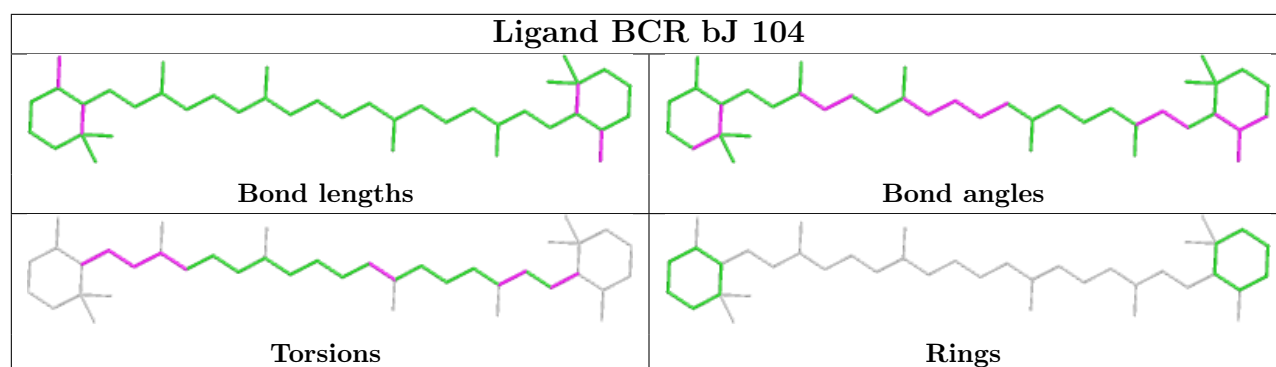


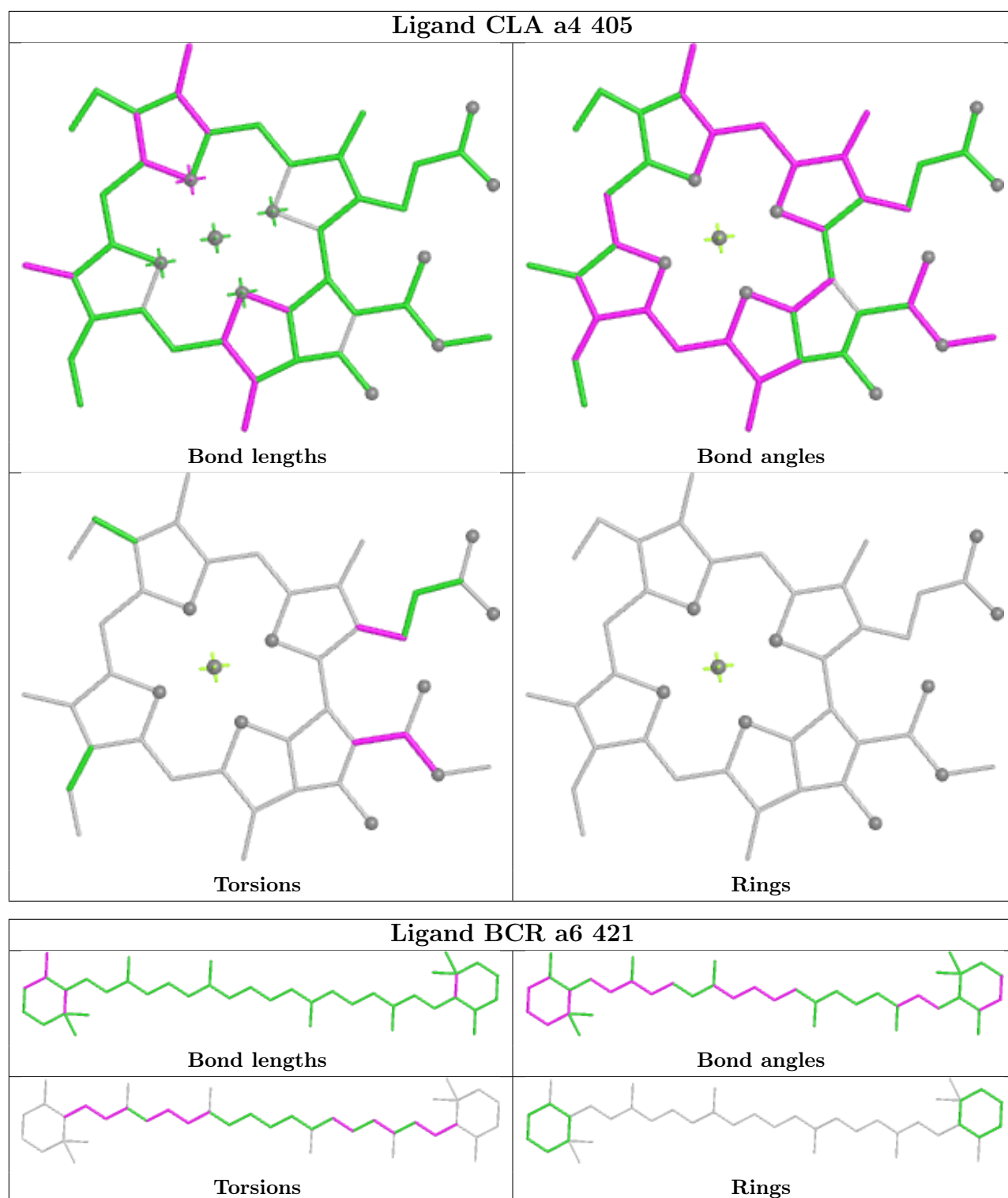


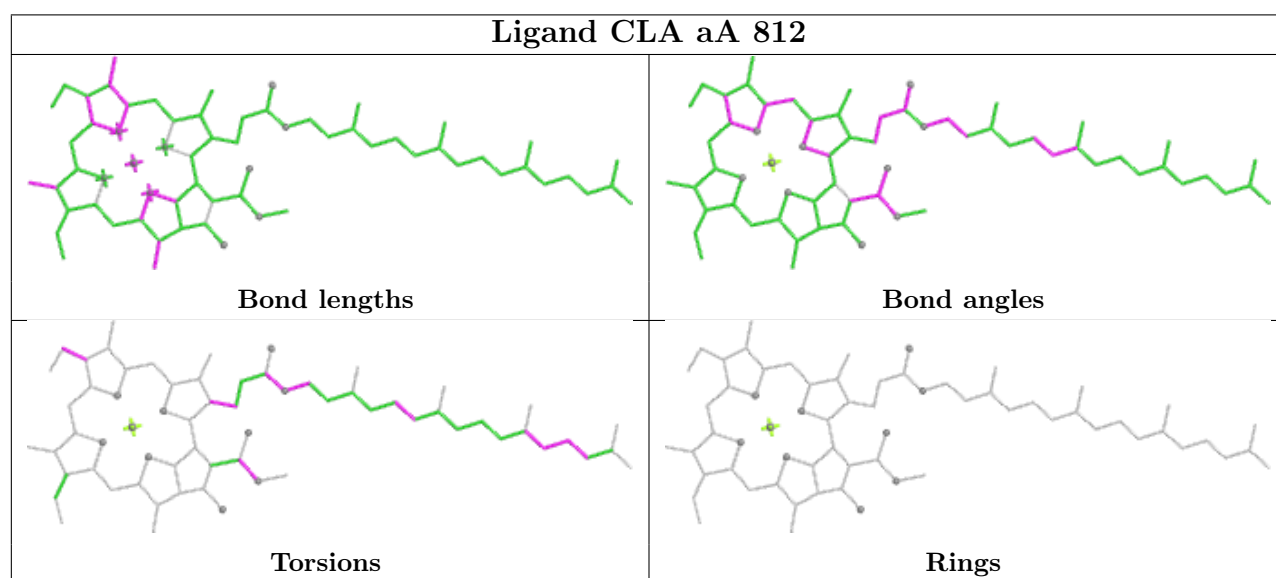
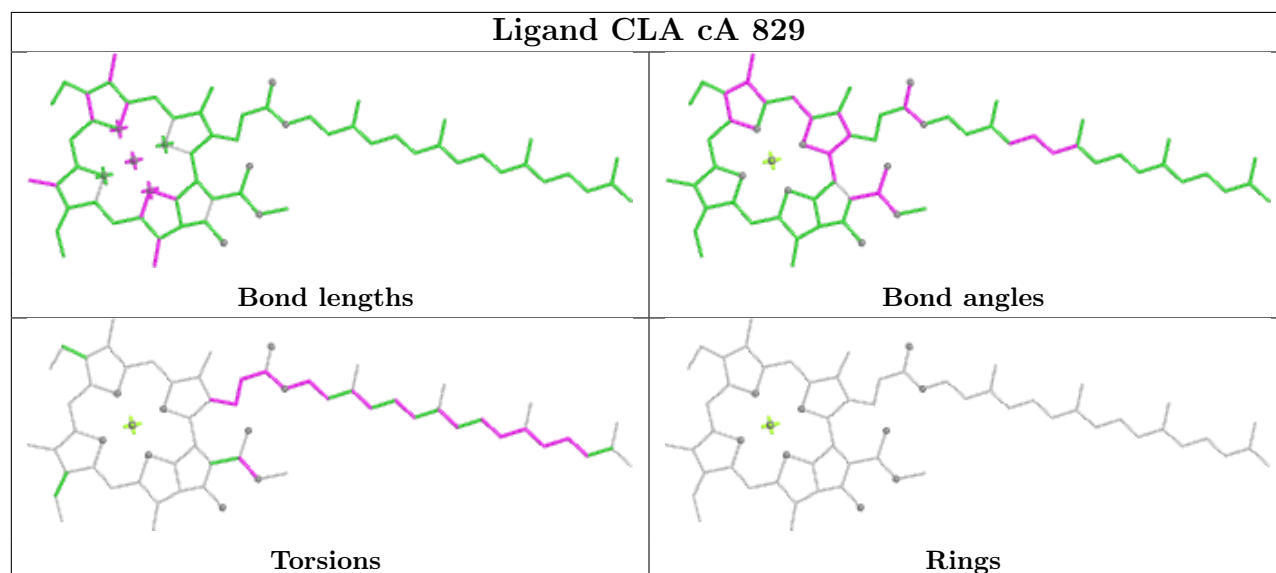
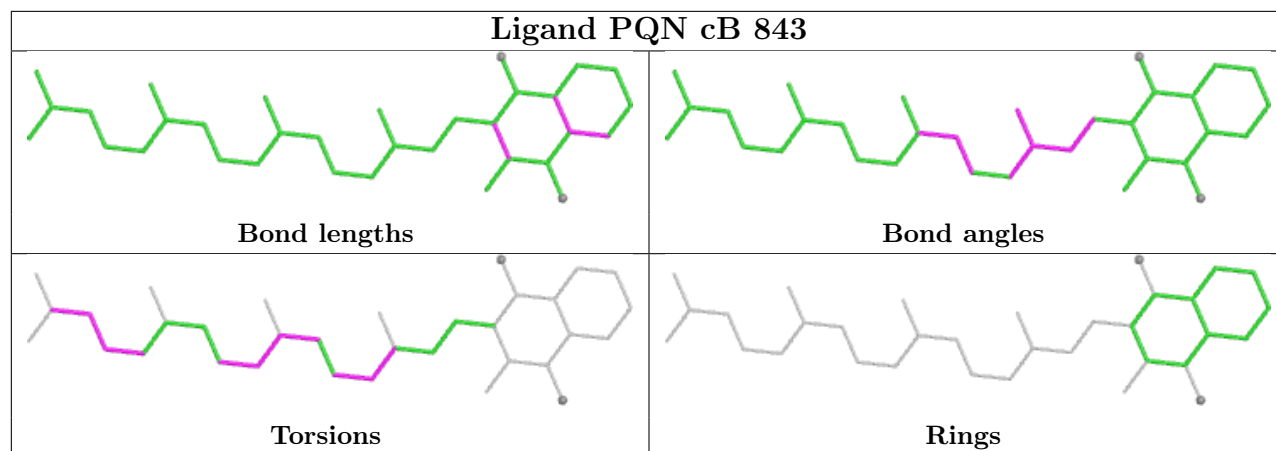


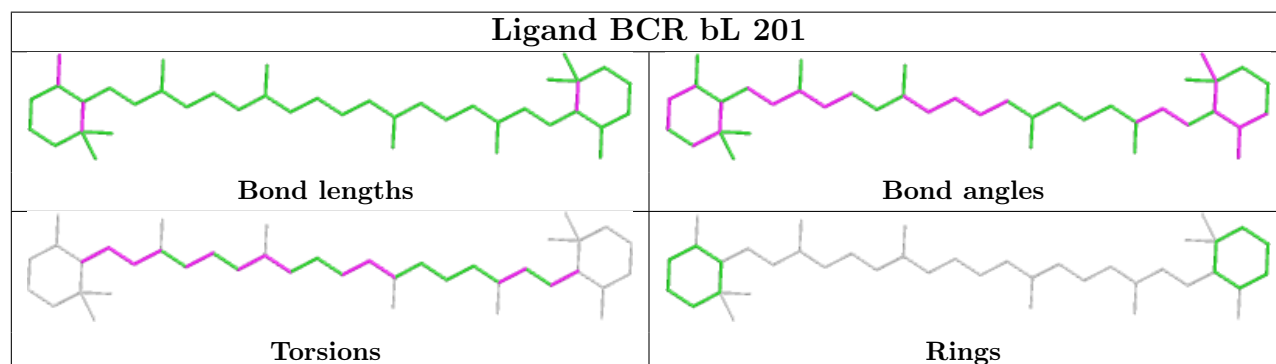
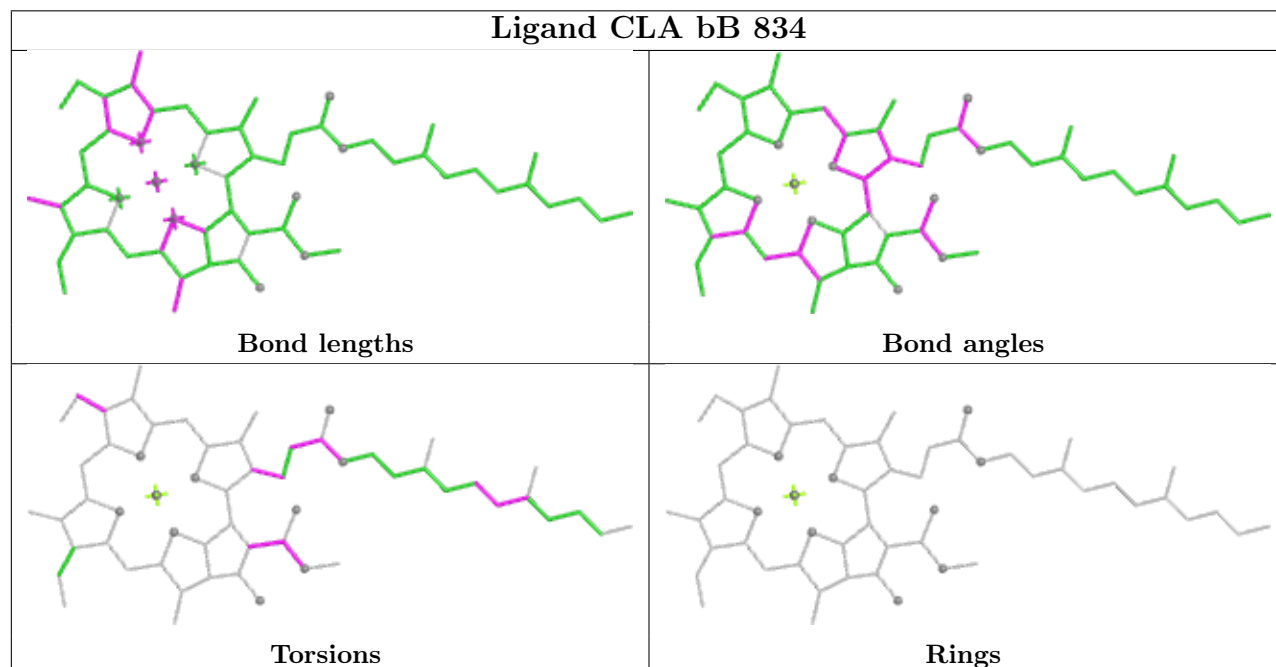
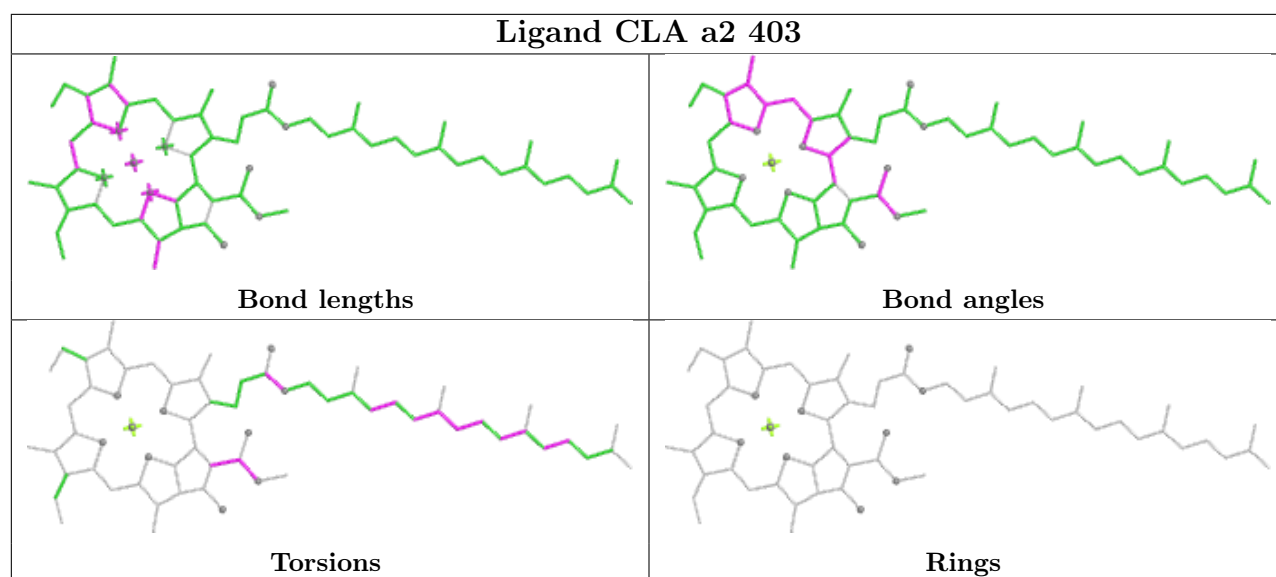


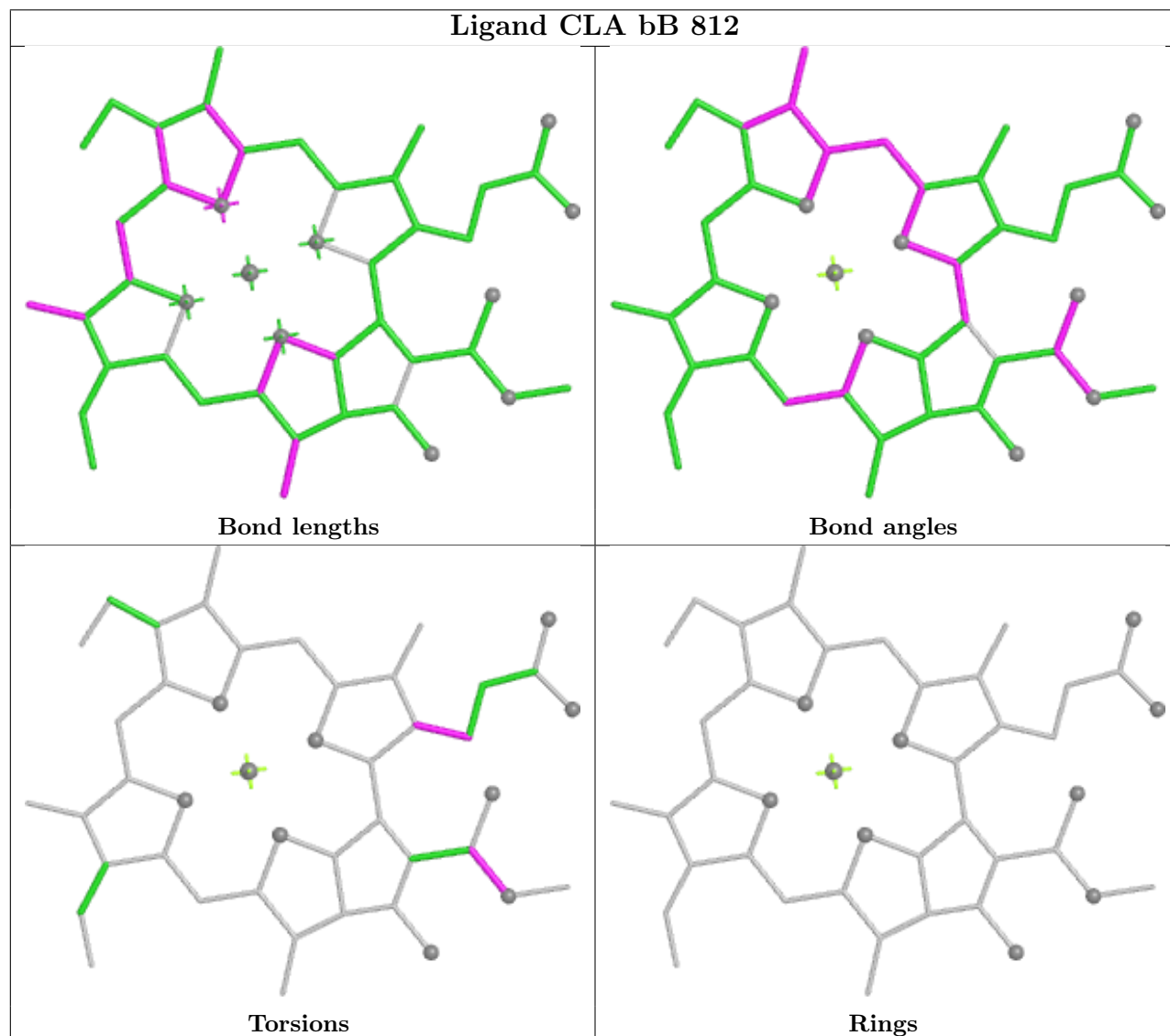
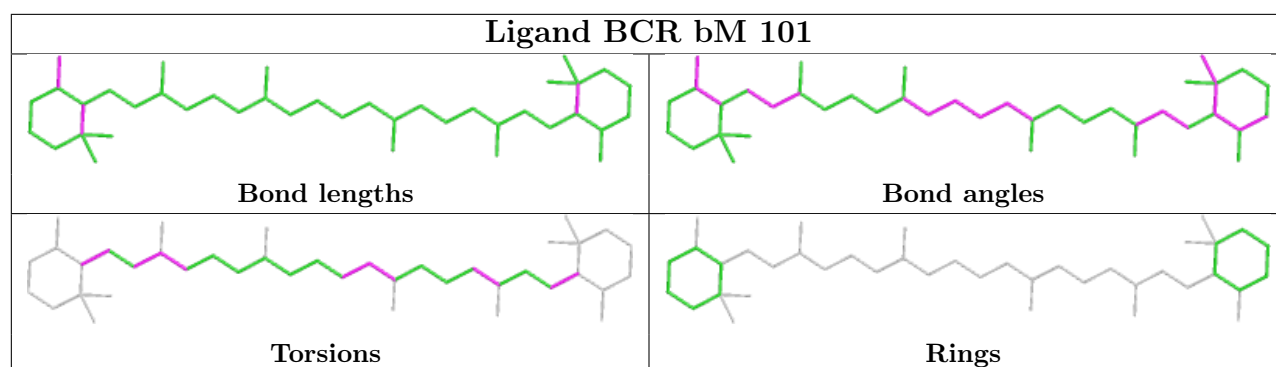


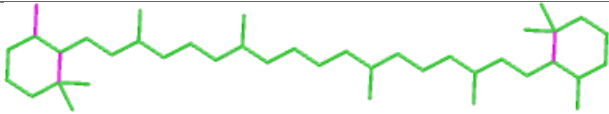
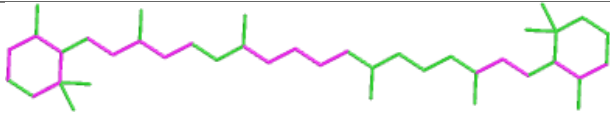
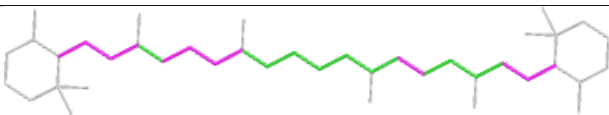
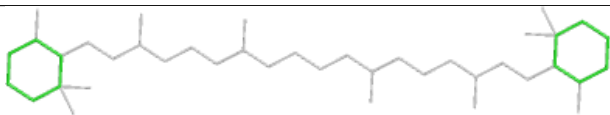


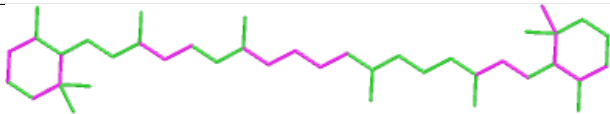
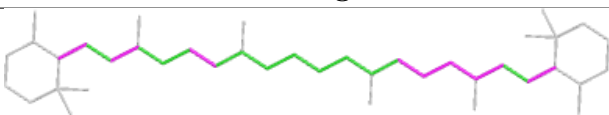
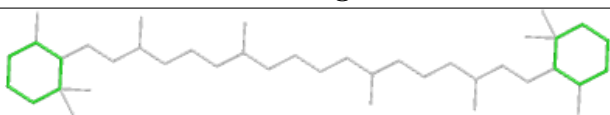


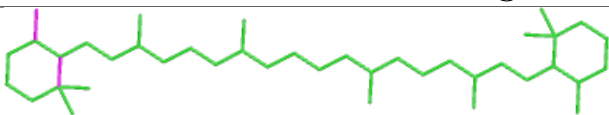
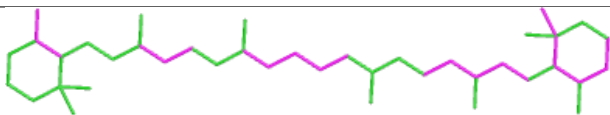
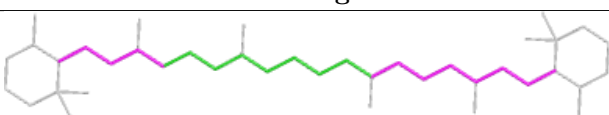
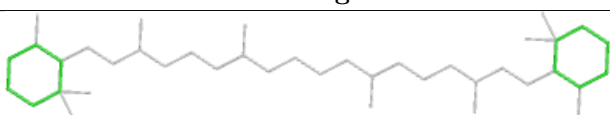


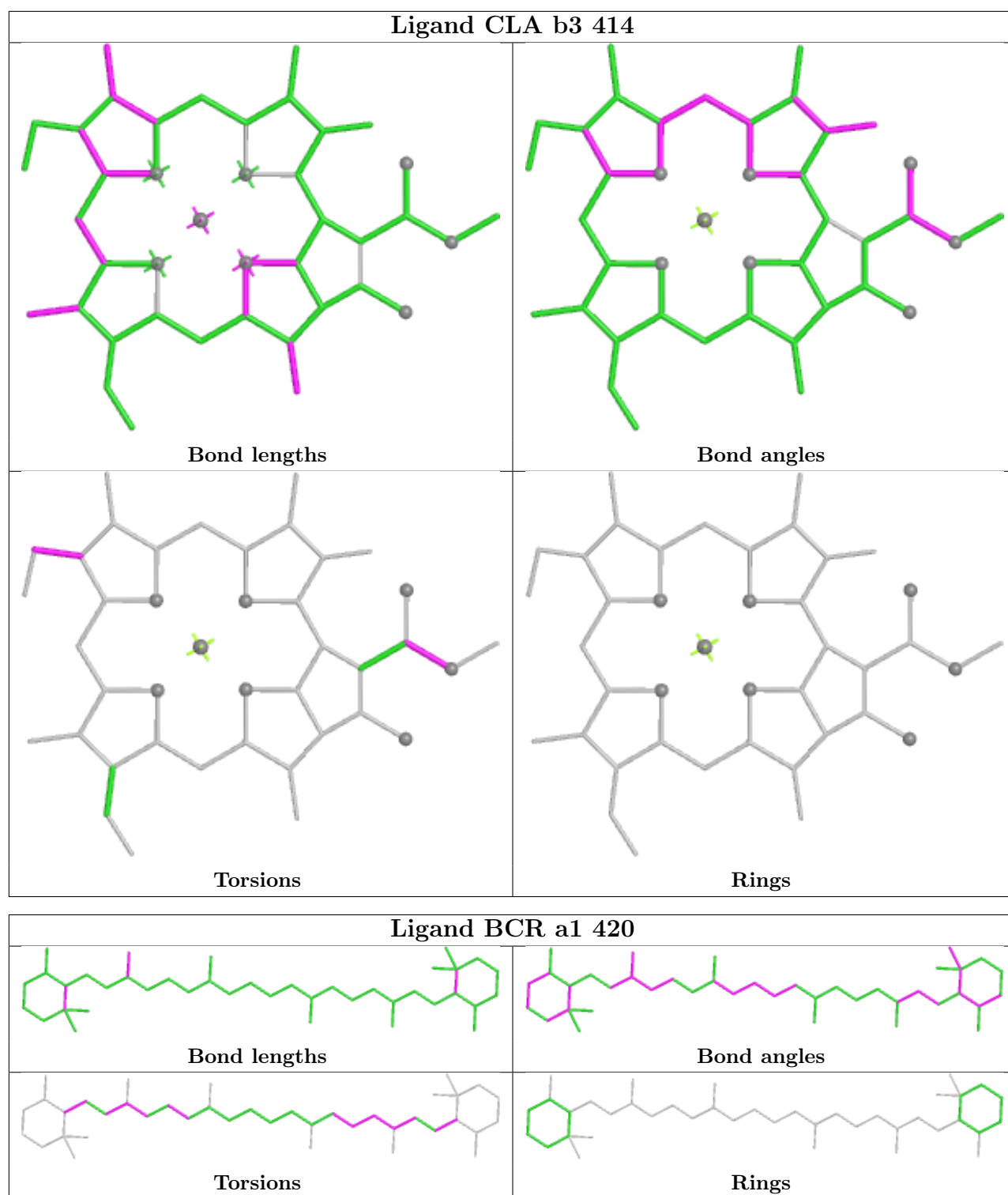


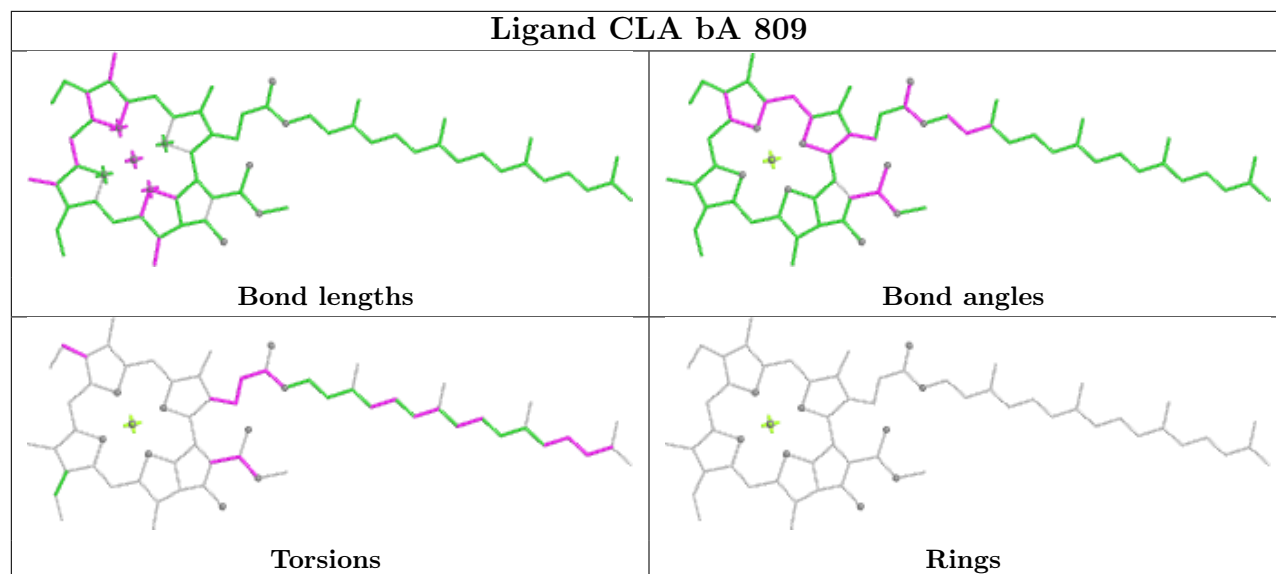
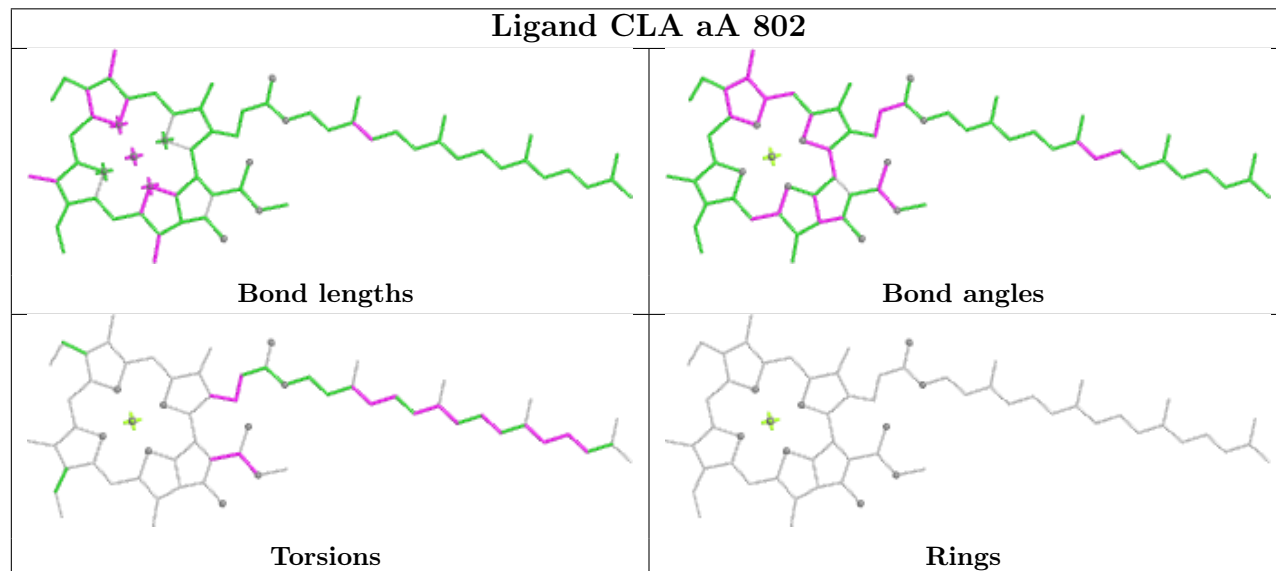


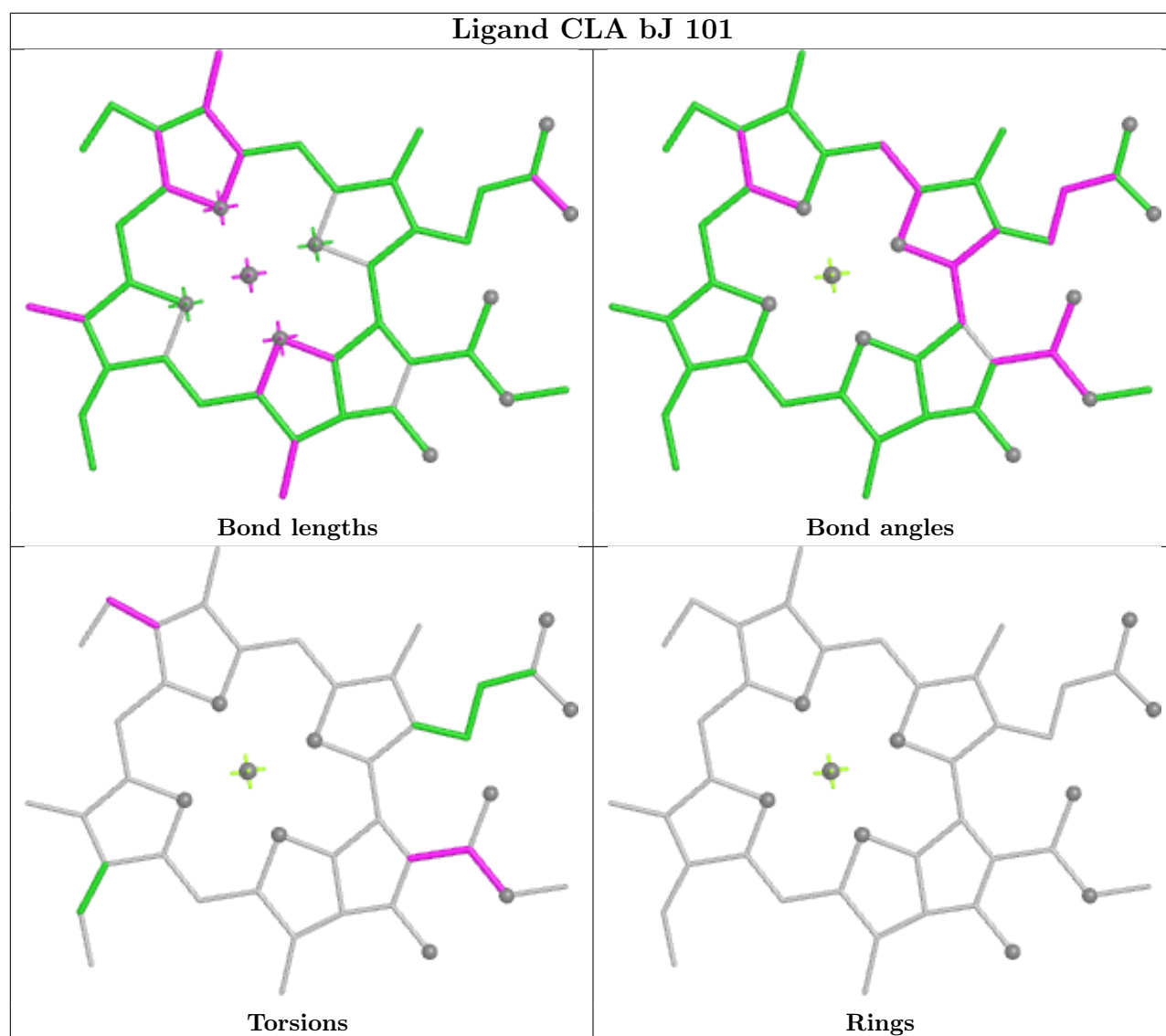
Ligand BCR c4 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

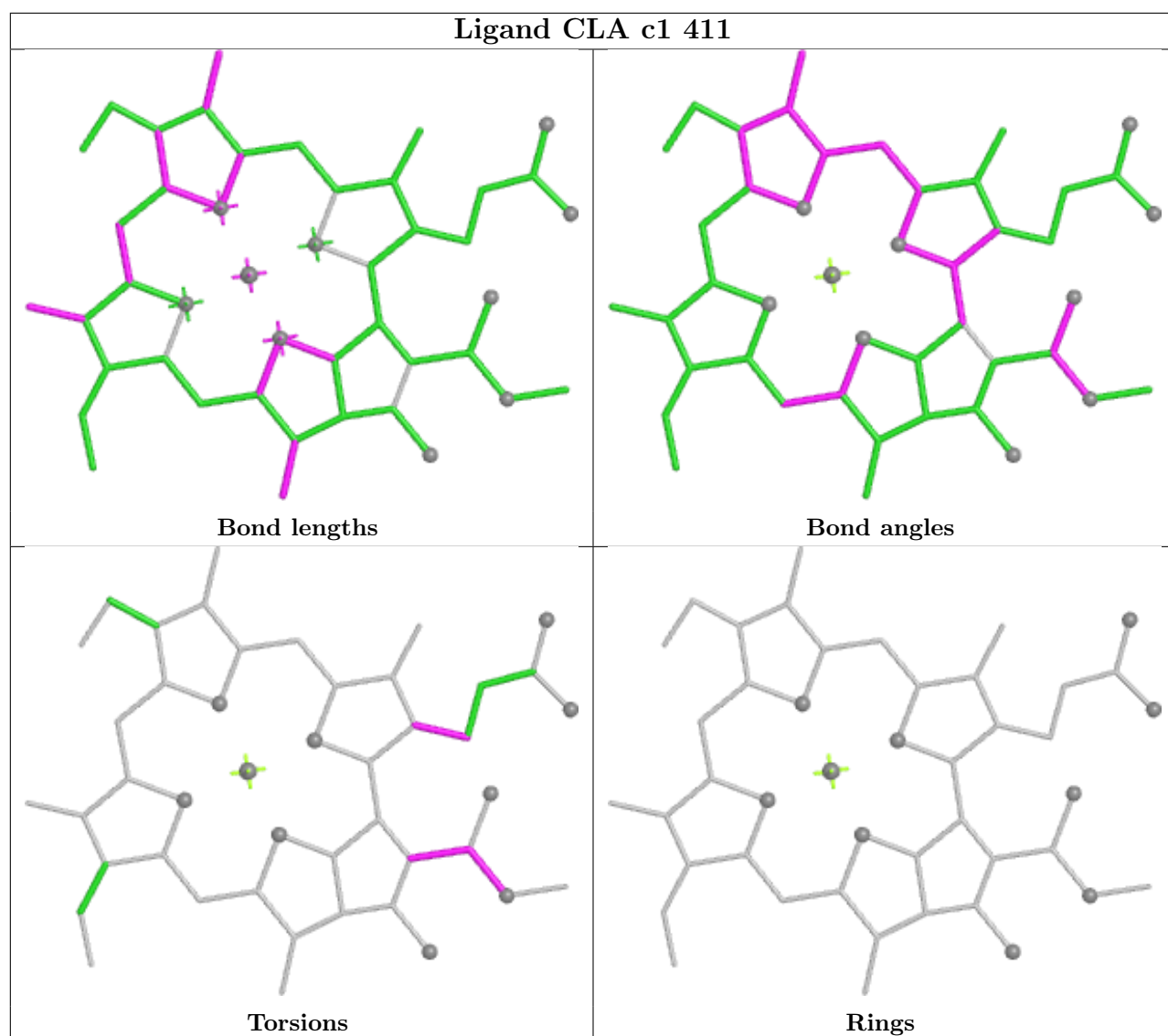
Ligand BCR b3 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

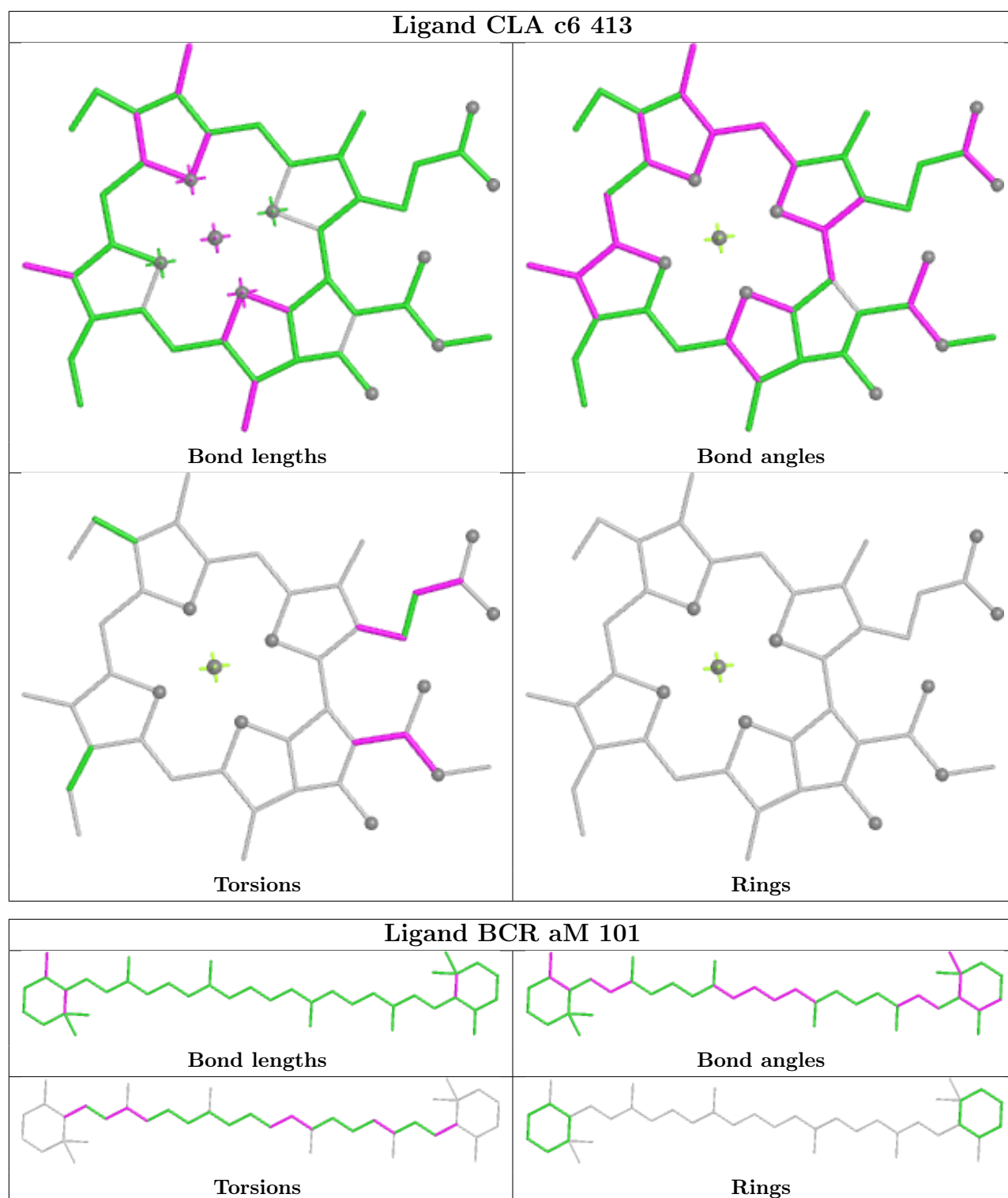
Ligand BCR aA 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

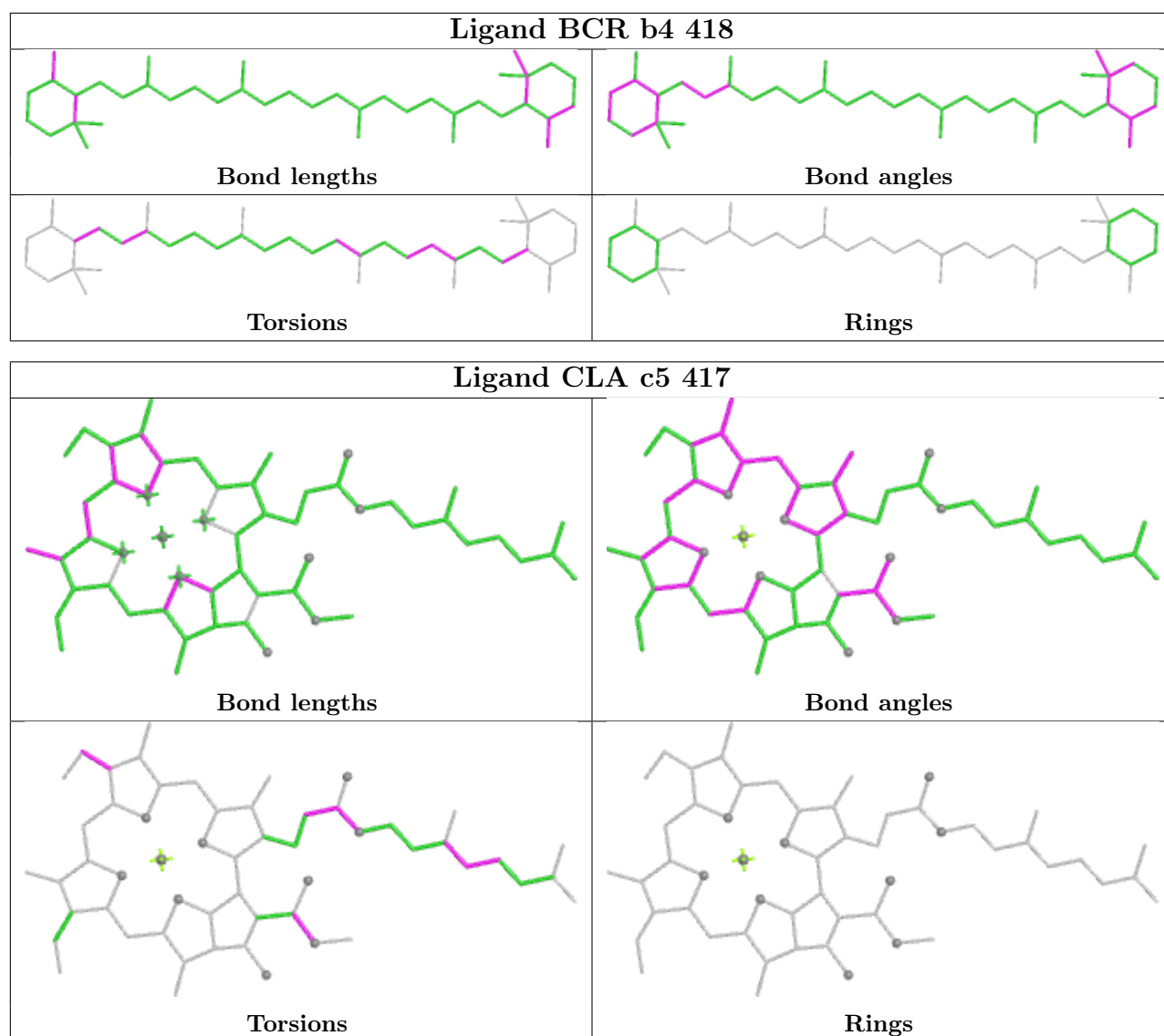


Ligand CLA bA 809**Ligand CLA aA 802**









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.

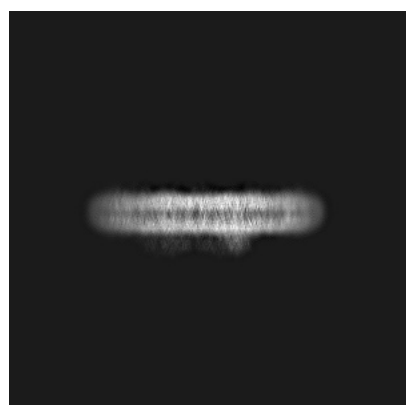
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9908. These allow visual inspection of the internal detail of the map and identification of artifacts.

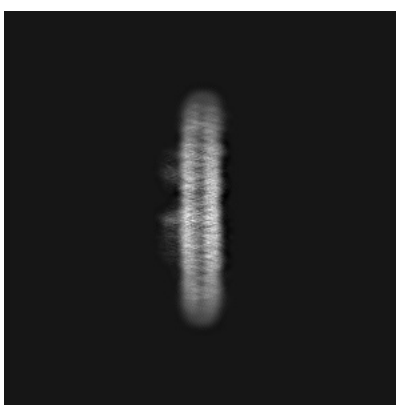
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

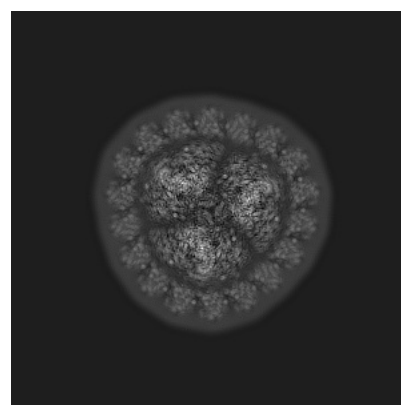
6.1.1 Primary map



X



Y

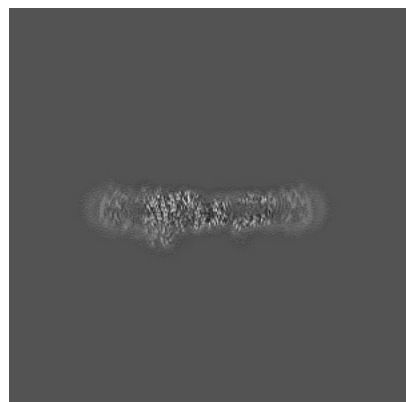


Z

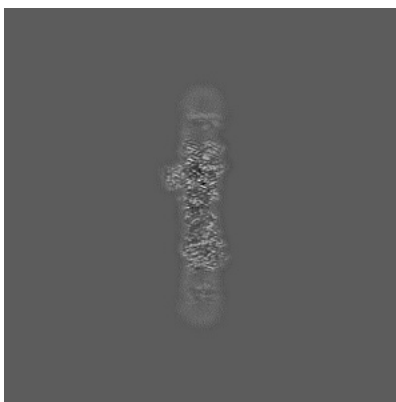
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

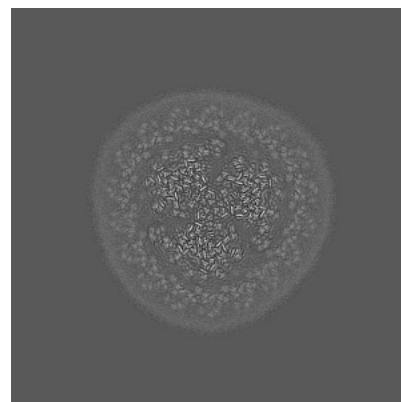
6.2.1 Primary map



X Index: 240



Y Index: 240

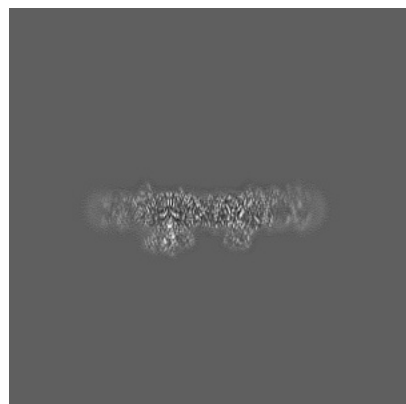


Z Index: 240

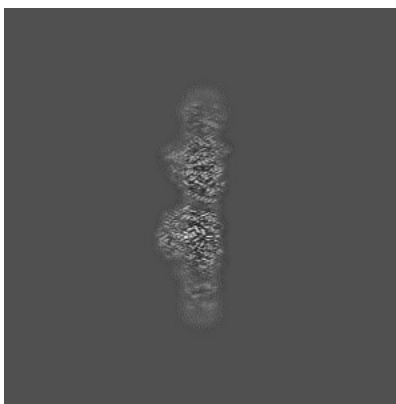
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

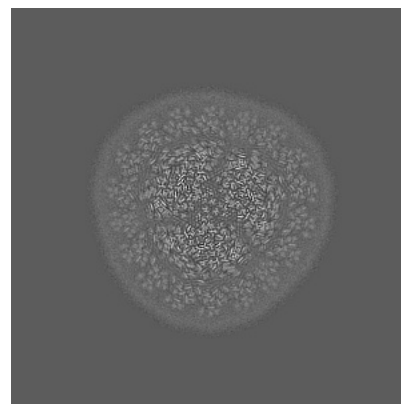
6.3.1 Primary map



X Index: 229



Y Index: 273

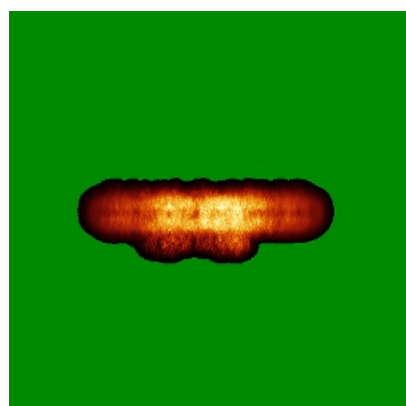


Z Index: 245

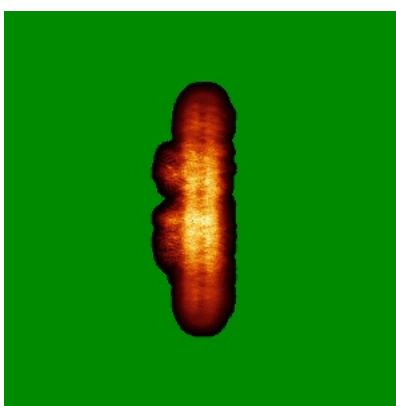
The images above show the largest variance slices of the map in three orthogonal directions.

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

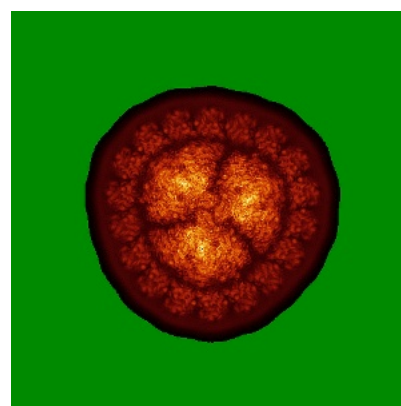
6.4.1 Primary map



X



Y

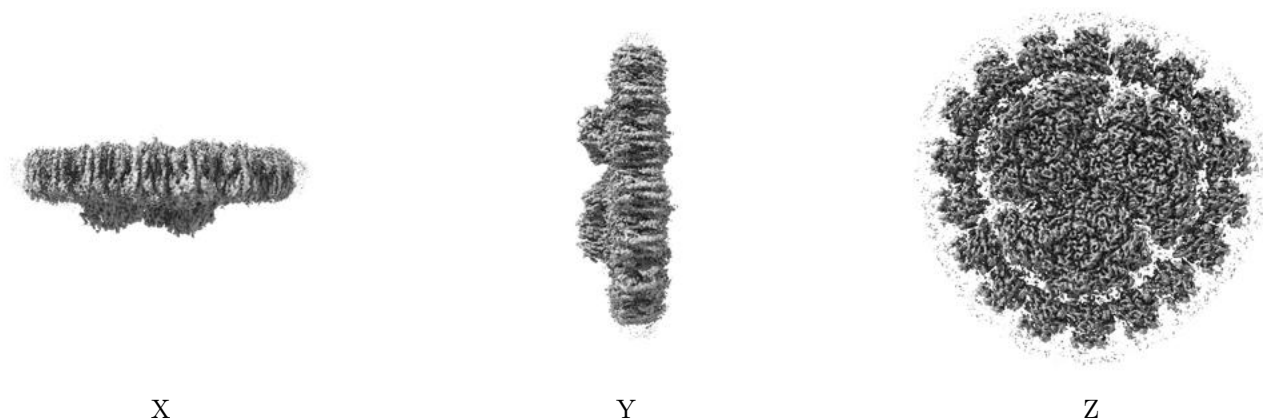


Z

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

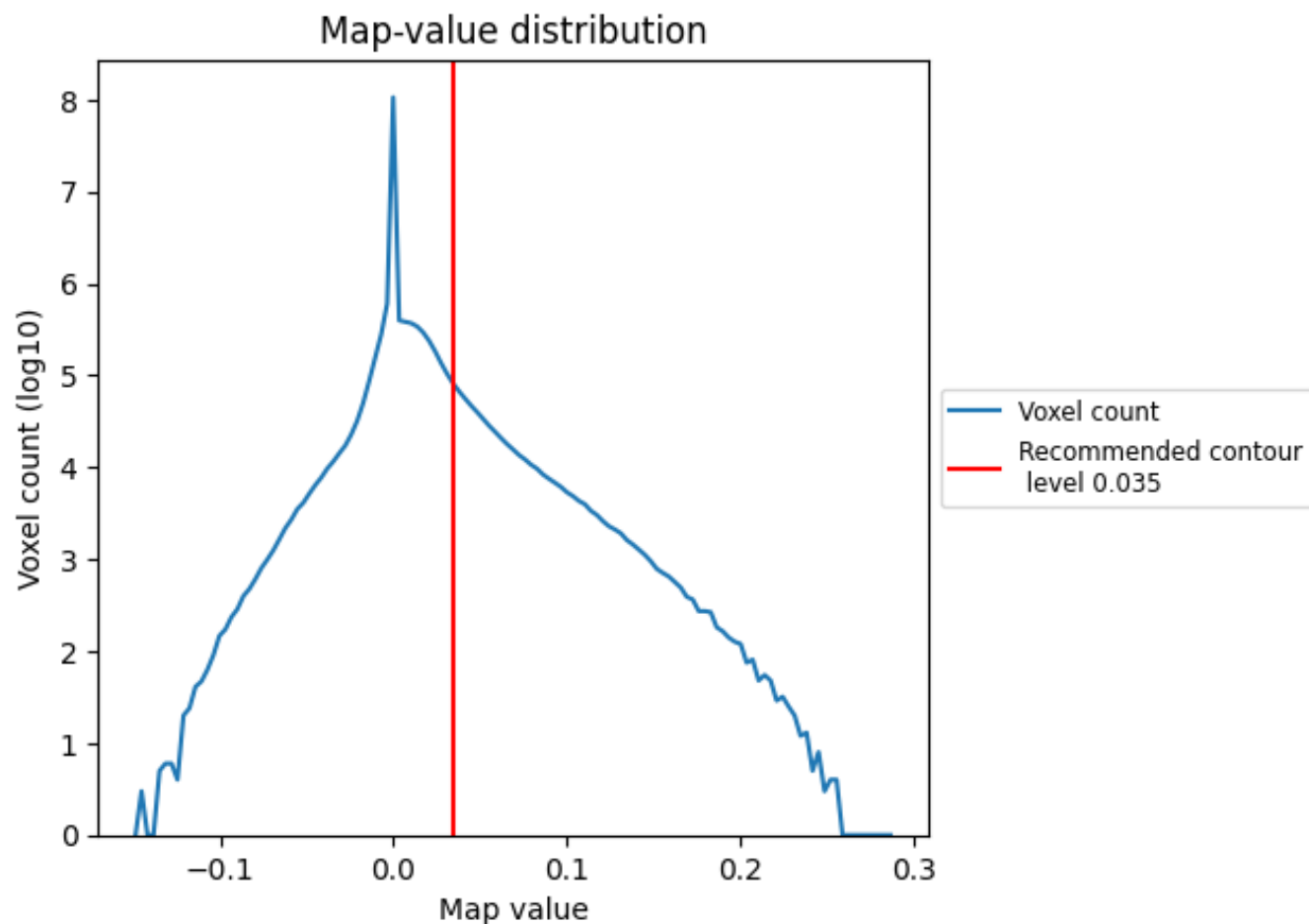
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

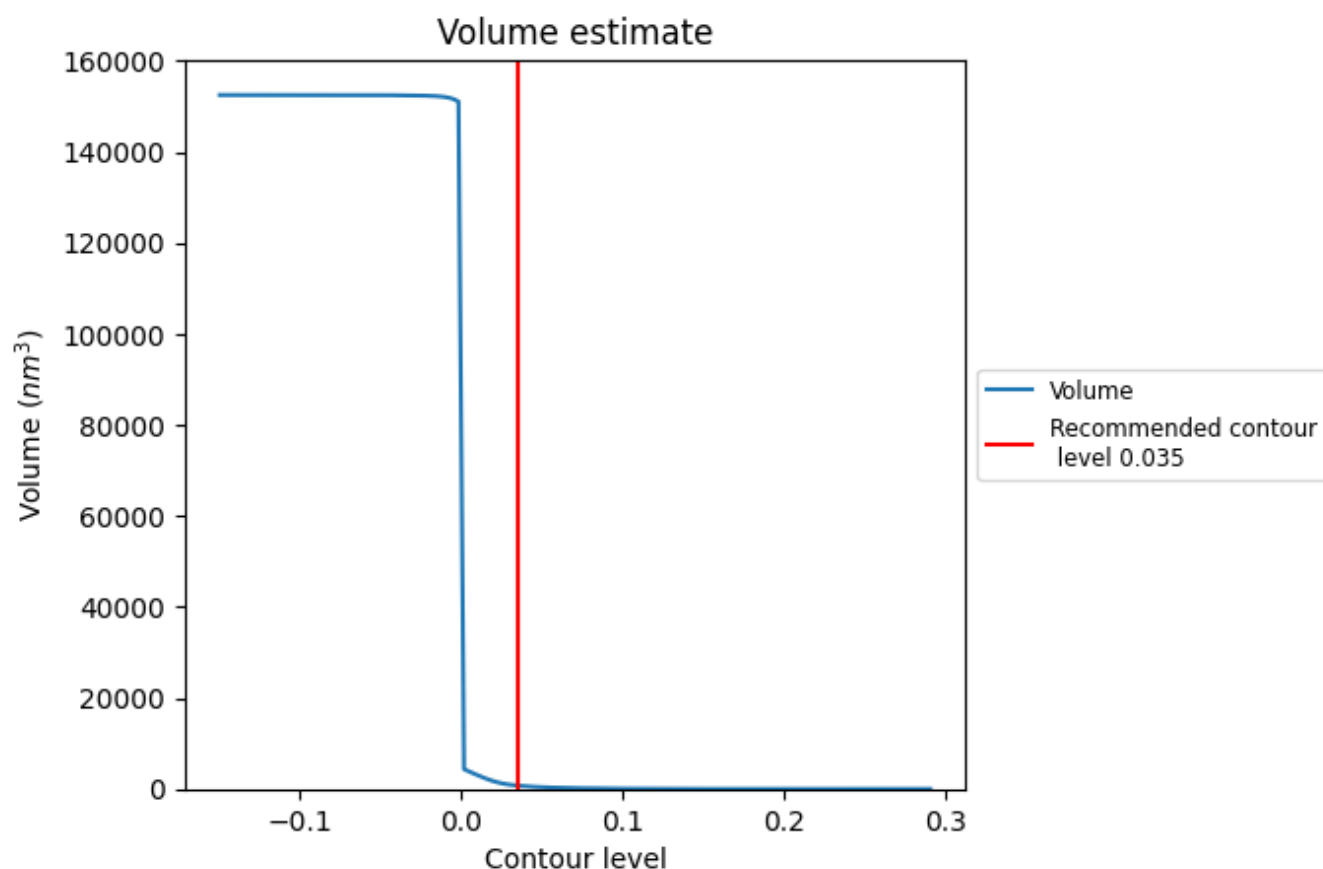
This section contains the results of statistical analysis of the map.

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.

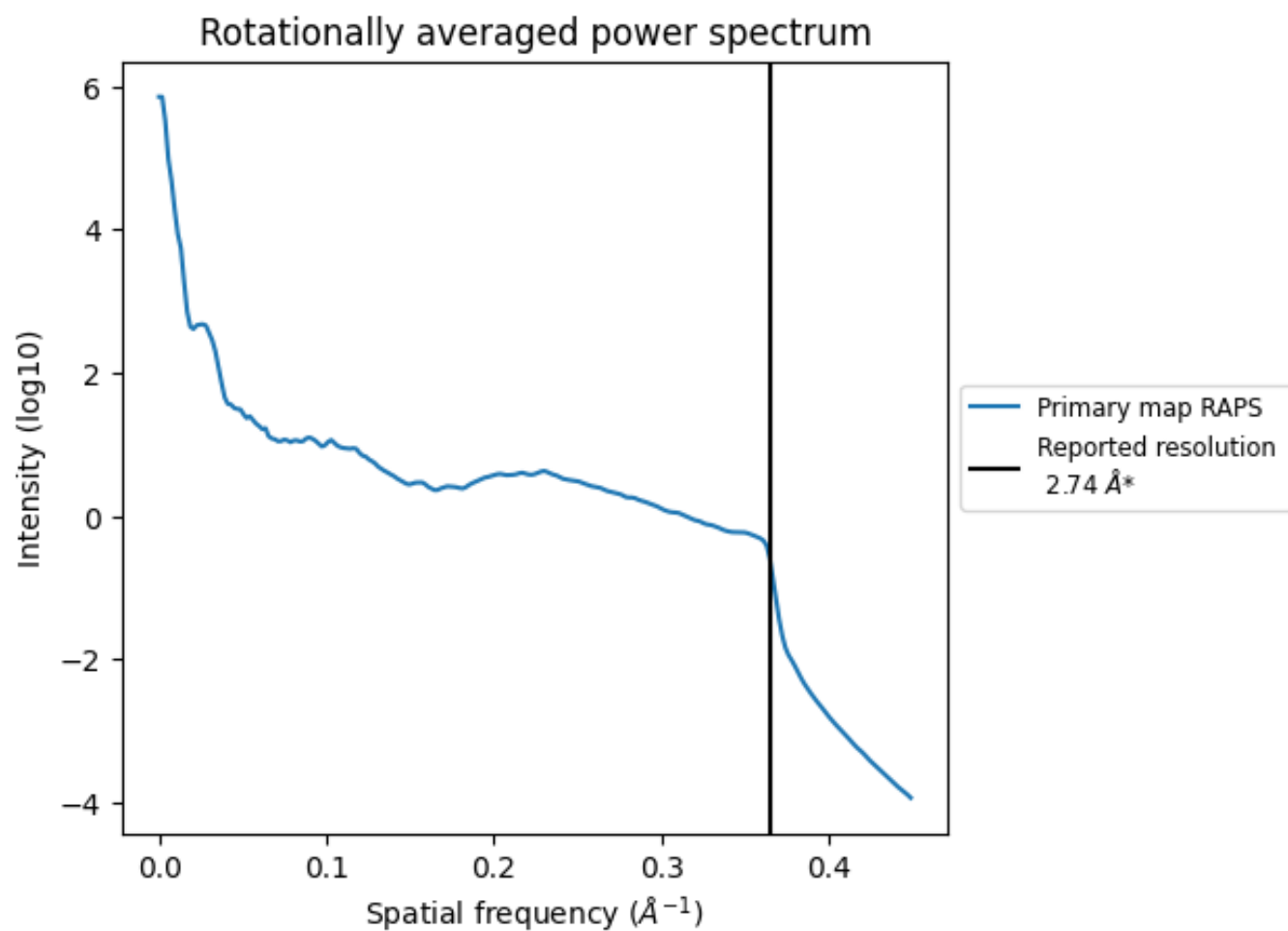
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm³; this corresponds to an approximate mass of 675 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 ⓘ

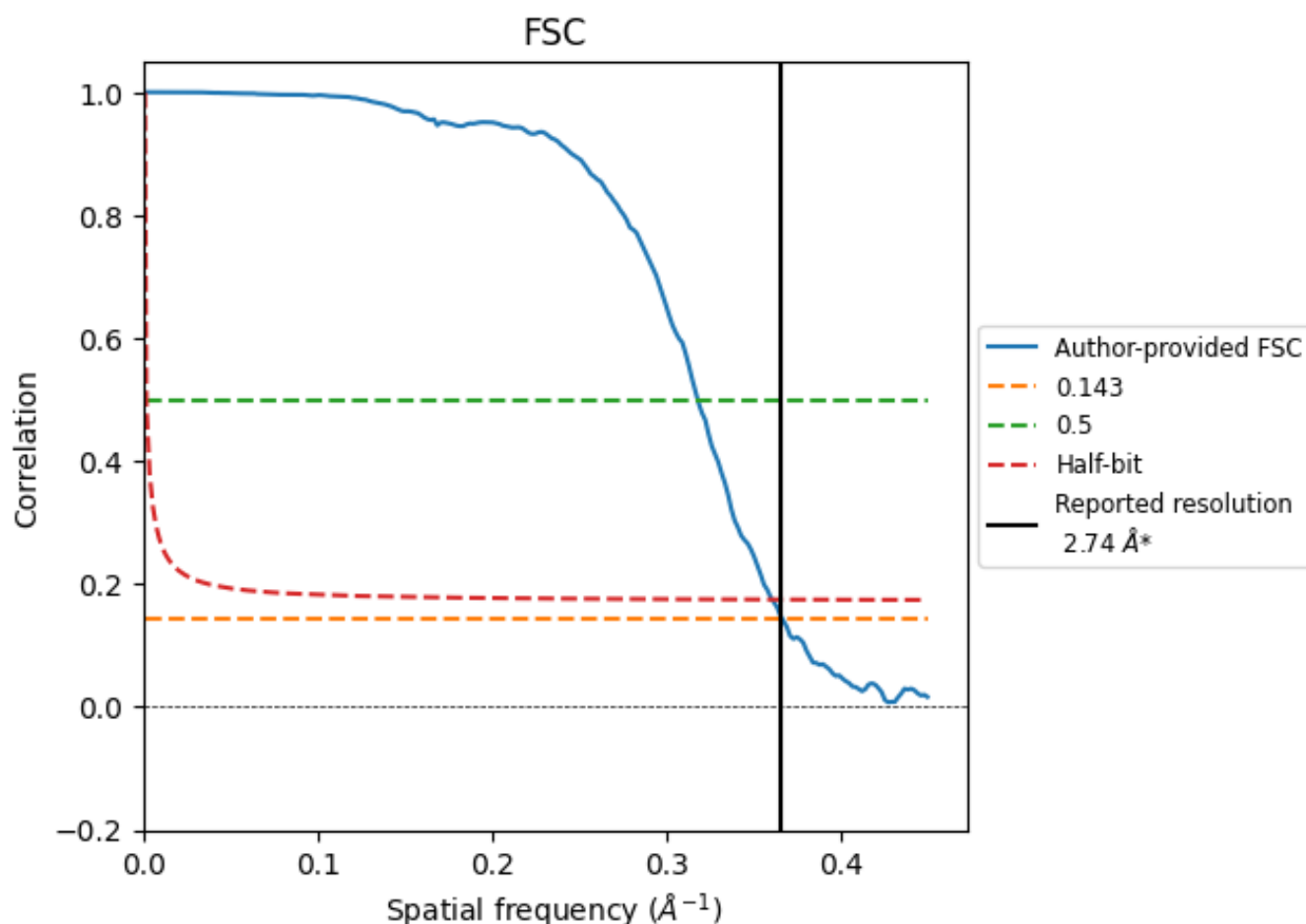


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

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 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

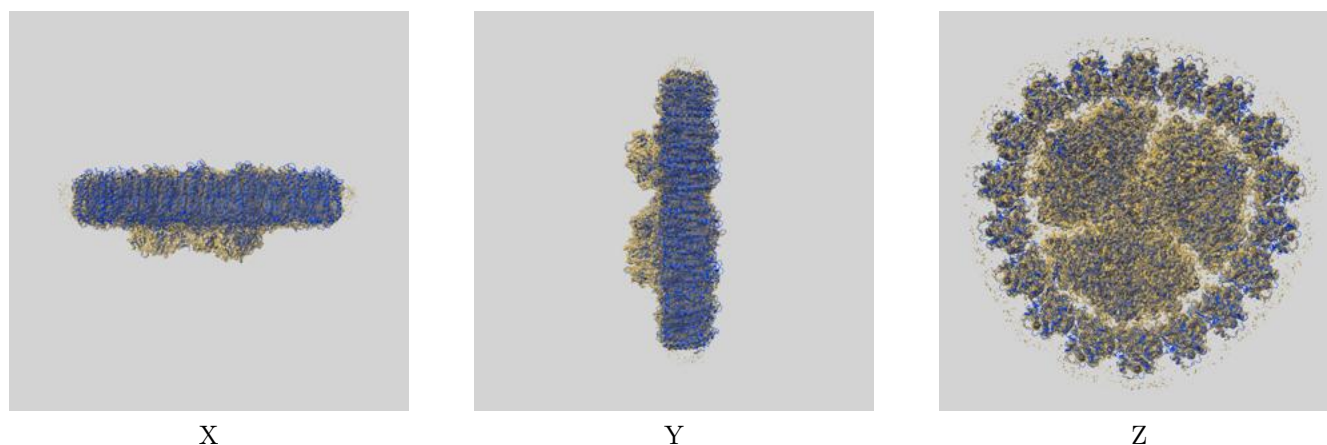
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.15	2.78
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

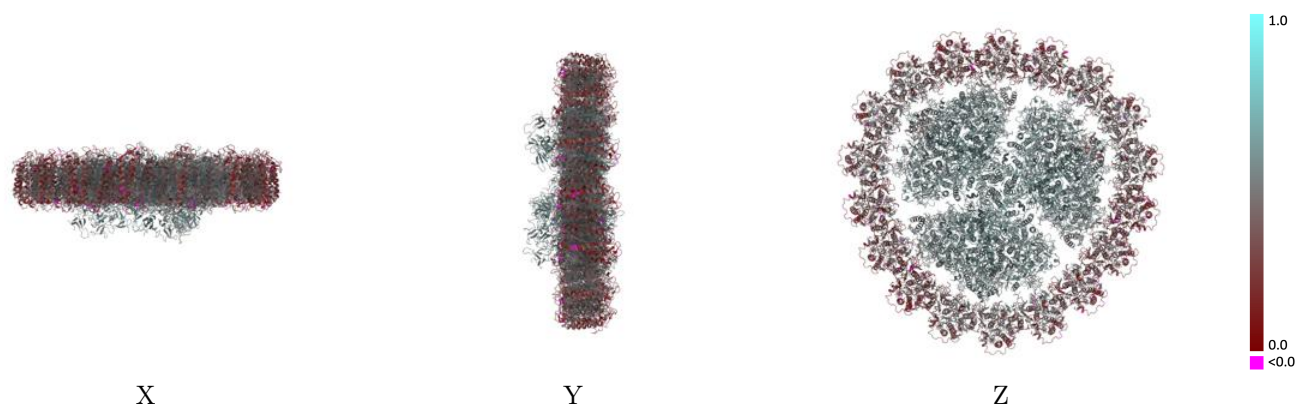
This section contains information regarding the fit between EMDB map EMD-9908 and PDB model 6K33. Per-residue inclusion information can be found in [section 3](#) on [page 50](#).

9.1 Map-model overlay [i](#)



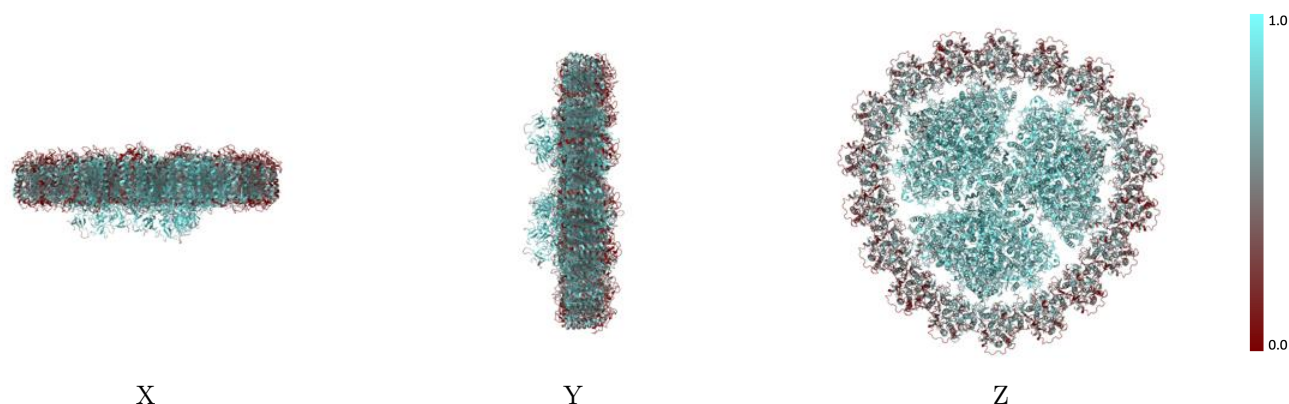
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



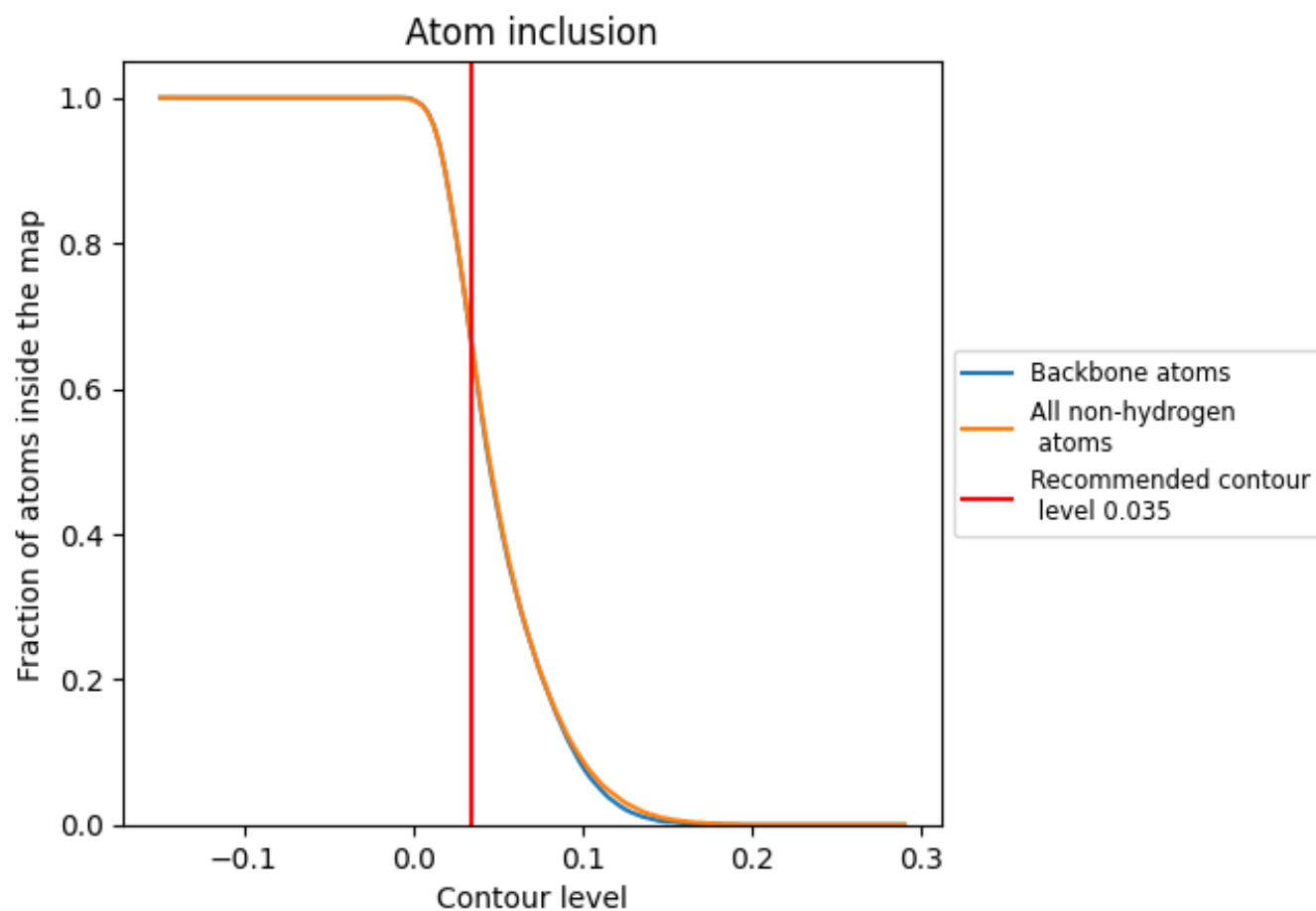
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 66% 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 (0.035) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6560	 0.4450
a1	 0.4050	 0.2890
a2	 0.3810	 0.2690
a3	 0.5040	 0.3620
a4	 0.4840	 0.3610
a5	 0.4290	 0.3390
a6	 0.3750	 0.2970
aA	 0.8720	 0.5710
aB	 0.8890	 0.5690
aC	 0.9200	 0.5550
aD	 0.8210	 0.5560
aE	 0.7720	 0.5160
aF	 0.7100	 0.4700
aI	 0.8900	 0.5860
aJ	 0.8030	 0.5310
aK	 0.8060	 0.4710
aL	 0.8840	 0.5870
aM	 0.8010	 0.5490
aX	 0.8250	 0.5250
b1	 0.4030	 0.2870
b2	 0.3720	 0.2590
b3	 0.4950	 0.3600
b4	 0.4810	 0.3600
b5	 0.4320	 0.3380
b6	 0.3710	 0.2950
bA	 0.8710	 0.5680
bB	 0.8900	 0.5680
bC	 0.9150	 0.5500
bD	 0.8220	 0.5470
bE	 0.7650	 0.5100
bF	 0.7370	 0.5110
bI	 0.9020	 0.5940
bJ	 0.8310	 0.5420
bK	 0.8190	 0.4930
bL	 0.8760	 0.5850



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Chain	Atom inclusion	Q-score
bM	 0.7910	 0.5420
bX	 0.8250	 0.5140
c1	 0.4120	 0.2890
c2	 0.3680	 0.2650
c3	 0.4980	 0.3590
c4	 0.4880	 0.3590
c5	 0.4310	 0.3390
c6	 0.3710	 0.2990
cA	 0.8720	 0.5700
cB	 0.8870	 0.5670
cC	 0.9170	 0.5510
cD	 0.8250	 0.5510
cE	 0.7820	 0.5150
cF	 0.6930	 0.4520
cI	 0.8940	 0.5930
cJ	 0.8190	 0.5400
cK	 0.8300	 0.4940
cL	 0.8880	 0.5900
cM	 0.8090	 0.5490
cX	 0.8350	 0.5280