



wwPDB EM Validation Summary Report ⓘ

Dec 26, 2024 – 10:08 AM EST

PDB ID : 6K33
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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.40

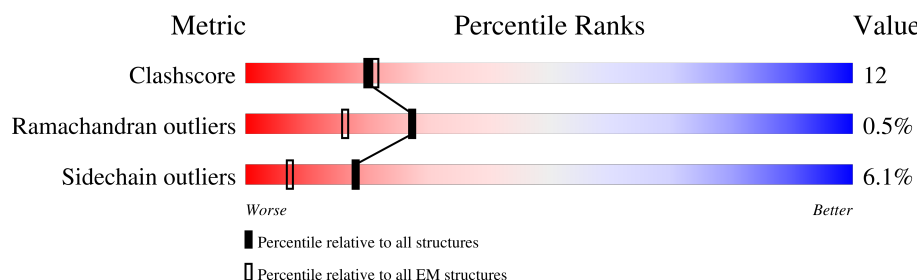
1 Overall quality at a glance

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.




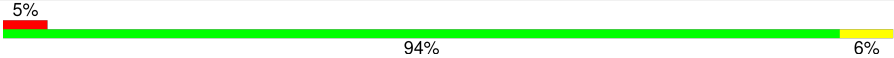
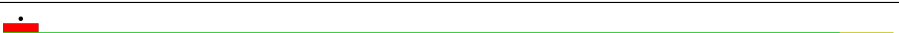
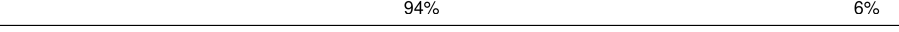
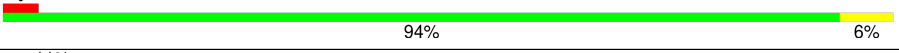






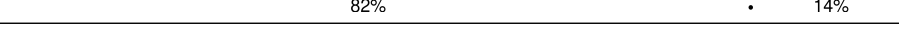
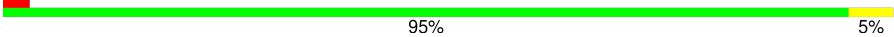

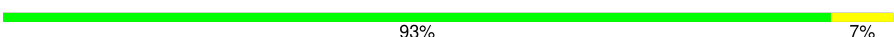
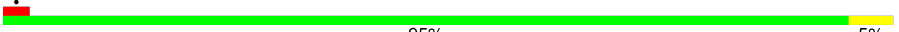



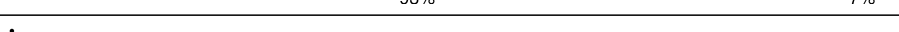





Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	bB	740	
2	cB	740	
3	aC	80	
3	bC	80	

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Mol	Chain	Length	Quality of chain
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	
10	cL	154	
11	aM	31	
11	bM	31	
11	cM	31	

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Mol	Chain	Length	Quality of chain
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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL0	aA	801	X	-	-	-
14	CL0	bA	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CL0	cA	801	X	-	-	-
15	CLA	a1	401	X	-	-	-
15	CLA	a1	402	X	-	-	-
15	CLA	a1	403	X	-	-	-
15	CLA	a1	404	X	-	-	-
15	CLA	a1	405	X	-	-	-
15	CLA	a1	406	X	-	-	-
15	CLA	a1	407	X	-	-	-
15	CLA	a1	408	X	-	-	-
15	CLA	a1	409	X	-	-	-
15	CLA	a1	410	X	-	-	-
15	CLA	a1	411	X	-	-	-
15	CLA	a1	412	X	-	-	-
15	CLA	a1	413	X	-	-	-
15	CLA	a1	415	X	-	-	-
15	CLA	a1	416	X	-	-	-
15	CLA	a1	422	X	-	-	-
15	CLA	a2	402	X	-	-	-
15	CLA	a2	403	X	-	-	-
15	CLA	a2	404	X	-	-	-
15	CLA	a2	405	X	-	-	-
15	CLA	a2	406	X	-	-	-
15	CLA	a2	407	X	-	-	-
15	CLA	a2	408	X	-	-	-
15	CLA	a2	409	X	-	-	-
15	CLA	a2	410	X	-	-	-
15	CLA	a2	411	X	-	-	-
15	CLA	a2	412	X	-	-	-
15	CLA	a2	413	X	-	-	-
15	CLA	a2	414	X	-	-	-
15	CLA	a2	415	X	-	-	-
15	CLA	a2	417	X	-	-	-
15	CLA	a2	418	X	-	-	-
15	CLA	a2	422	X	-	-	-
15	CLA	a3	402	X	-	-	-
15	CLA	a3	403	X	-	-	-
15	CLA	a3	404	X	-	-	-
15	CLA	a3	405	X	-	-	-
15	CLA	a3	406	X	-	-	-
15	CLA	a3	407	X	-	-	-
15	CLA	a3	408	X	-	-	-
15	CLA	a3	409	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a3	410	X	-	-	-
15	CLA	a3	411	X	-	-	-
15	CLA	a3	412	X	-	-	-
15	CLA	a3	413	X	-	-	-
15	CLA	a3	414	X	-	-	-
15	CLA	a3	416	X	-	-	-
15	CLA	a3	417	X	-	-	-
15	CLA	a3	421	X	-	-	-
15	CLA	a4	402	X	-	-	-
15	CLA	a4	403	X	-	-	-
15	CLA	a4	404	X	-	-	-
15	CLA	a4	405	X	-	-	-
15	CLA	a4	406	X	-	-	-
15	CLA	a4	407	X	-	-	-
15	CLA	a4	408	X	-	-	-
15	CLA	a4	409	X	-	-	-
15	CLA	a4	410	X	-	-	-
15	CLA	a4	411	X	-	-	-
15	CLA	a4	412	X	-	-	-
15	CLA	a4	413	X	-	-	-
15	CLA	a4	414	X	-	-	-
15	CLA	a4	416	X	-	-	-
15	CLA	a4	417	X	-	-	-
15	CLA	a4	421	X	-	-	-
15	CLA	a5	402	X	-	-	-
15	CLA	a5	403	X	-	-	-
15	CLA	a5	404	X	-	-	-
15	CLA	a5	405	X	-	-	-
15	CLA	a5	406	X	-	-	-
15	CLA	a5	407	X	-	-	-
15	CLA	a5	408	X	-	-	-
15	CLA	a5	409	X	-	-	-
15	CLA	a5	410	X	-	-	-
15	CLA	a5	411	X	-	-	-
15	CLA	a5	412	X	-	-	-
15	CLA	a5	413	X	-	-	-
15	CLA	a5	414	X	-	-	-
15	CLA	a5	416	X	-	-	-
15	CLA	a5	417	X	-	-	-
15	CLA	a5	420	X	-	-	-
15	CLA	a6	403	X	-	-	-
15	CLA	a6	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a6	405	X	-	-	-
15	CLA	a6	406	X	-	-	-
15	CLA	a6	407	X	-	-	-
15	CLA	a6	408	X	-	-	-
15	CLA	a6	409	X	-	-	-
15	CLA	a6	410	X	-	-	-
15	CLA	a6	411	X	-	-	-
15	CLA	a6	412	X	-	-	-
15	CLA	a6	413	X	-	-	-
15	CLA	a6	414	X	-	-	-
15	CLA	a6	415	X	-	-	-
15	CLA	a6	417	X	-	-	-
15	CLA	a6	418	X	-	-	-
15	CLA	a6	422	X	-	-	-
15	CLA	aA	802	X	-	-	-
15	CLA	aA	803	X	-	-	-
15	CLA	aA	804	X	-	-	-
15	CLA	aA	805	X	-	-	-
15	CLA	aA	806	X	-	-	-
15	CLA	aA	807	X	-	-	-
15	CLA	aA	809	X	-	-	-
15	CLA	aA	810	X	-	-	-
15	CLA	aA	811	X	-	-	-
15	CLA	aA	812	X	-	-	-
15	CLA	aA	813	X	-	-	-
15	CLA	aA	814	X	-	-	-
15	CLA	aA	815	X	-	-	-
15	CLA	aA	818	X	-	-	-
15	CLA	aA	819	X	-	-	-
15	CLA	aA	820	X	-	-	-
15	CLA	aA	821	X	-	-	-
15	CLA	aA	822	X	-	-	-
15	CLA	aA	823	X	-	-	-
15	CLA	aA	824	X	-	-	-
15	CLA	aA	825	X	-	-	-
15	CLA	aA	826	X	-	-	-
15	CLA	aA	827	X	-	-	-
15	CLA	aA	828	X	-	-	-
15	CLA	aA	829	X	-	-	-
15	CLA	aA	830	X	-	-	-
15	CLA	aA	831	X	-	-	-
15	CLA	aA	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	aA	833	X	-	-	-
15	CLA	aA	834	X	-	-	-
15	CLA	aA	835	X	-	-	-
15	CLA	aA	836	X	-	-	-
15	CLA	aA	838	X	-	-	-
15	CLA	aA	839	X	-	-	-
15	CLA	aA	840	X	-	-	-
15	CLA	aA	841	X	-	-	-
15	CLA	aA	842	X	-	-	-
15	CLA	aA	843	X	-	-	-
15	CLA	aA	844	X	-	-	-
15	CLA	aA	845	X	-	-	-
15	CLA	aB	801	X	-	-	-
15	CLA	aB	802	X	-	-	-
15	CLA	aB	803	X	-	-	-
15	CLA	aB	804	X	-	-	-
15	CLA	aB	805	X	-	-	-
15	CLA	aB	806	X	-	-	-
15	CLA	aB	807	X	-	-	-
15	CLA	aB	809	X	-	-	-
15	CLA	aB	810	X	-	-	-
15	CLA	aB	811	X	-	-	-
15	CLA	aB	812	X	-	-	-
15	CLA	aB	813	X	-	-	-
15	CLA	aB	814	X	-	-	-
15	CLA	aB	815	X	-	-	-
15	CLA	aB	816	X	-	-	-
15	CLA	aB	817	X	-	-	-
15	CLA	aB	818	X	-	-	-
15	CLA	aB	819	X	-	-	-
15	CLA	aB	820	X	-	-	-
15	CLA	aB	821	X	-	-	-
15	CLA	aB	822	X	-	-	-
15	CLA	aB	823	X	-	-	-
15	CLA	aB	824	X	-	-	-
15	CLA	aB	825	X	-	-	-
15	CLA	aB	826	X	-	-	-
15	CLA	aB	827	X	-	-	-
15	CLA	aB	828	X	-	-	-
15	CLA	aB	829	X	-	-	-
15	CLA	aB	830	X	-	-	-
15	CLA	aB	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	aB	832	X	-	-	-
15	CLA	aB	833	X	-	-	-
15	CLA	aB	834	X	-	-	-
15	CLA	aB	835	X	-	-	-
15	CLA	aB	836	X	-	-	-
15	CLA	aB	837	X	-	-	-
15	CLA	aB	838	X	-	-	-
15	CLA	aB	839	X	-	-	-
15	CLA	aB	840	X	-	-	-
15	CLA	aB	841	X	-	-	-
15	CLA	aJ	201	X	-	-	-
15	CLA	aJ	202	X	-	-	-
15	CLA	aJ	203	X	-	-	-
15	CLA	aK	102	X	-	-	-
15	CLA	aL	201	X	-	-	-
15	CLA	aL	202	X	-	-	-
15	CLA	aL	203	X	-	-	-
15	CLA	aX	102	X	-	-	-
15	CLA	b1	402	X	-	-	-
15	CLA	b1	403	X	-	-	-
15	CLA	b1	404	X	-	-	-
15	CLA	b1	405	X	-	-	-
15	CLA	b1	406	X	-	-	-
15	CLA	b1	407	X	-	-	-
15	CLA	b1	408	X	-	-	-
15	CLA	b1	409	X	-	-	-
15	CLA	b1	410	X	-	-	-
15	CLA	b1	411	X	-	-	-
15	CLA	b1	412	X	-	-	-
15	CLA	b1	413	X	-	-	-
15	CLA	b1	414	X	-	-	-
15	CLA	b1	416	X	-	-	-
15	CLA	b1	417	X	-	-	-
15	CLA	b2	402	X	-	-	-
15	CLA	b2	403	X	-	-	-
15	CLA	b2	404	X	-	-	-
15	CLA	b2	405	X	-	-	-
15	CLA	b2	406	X	-	-	-
15	CLA	b2	407	X	-	-	-
15	CLA	b2	408	X	-	-	-
15	CLA	b2	409	X	-	-	-
15	CLA	b2	410	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b2	411	X	-	-	-
15	CLA	b2	412	X	-	-	-
15	CLA	b2	413	X	-	-	-
15	CLA	b2	414	X	-	-	-
15	CLA	b2	415	X	-	-	-
15	CLA	b2	417	X	-	-	-
15	CLA	b2	418	X	-	-	-
15	CLA	b2	422	X	-	-	-
15	CLA	b3	402	X	-	-	-
15	CLA	b3	403	X	-	-	-
15	CLA	b3	404	X	-	-	-
15	CLA	b3	405	X	-	-	-
15	CLA	b3	406	X	-	-	-
15	CLA	b3	407	X	-	-	-
15	CLA	b3	408	X	-	-	-
15	CLA	b3	409	X	-	-	-
15	CLA	b3	410	X	-	-	-
15	CLA	b3	411	X	-	-	-
15	CLA	b3	412	X	-	-	-
15	CLA	b3	413	X	-	-	-
15	CLA	b3	414	X	-	-	-
15	CLA	b3	416	X	-	-	-
15	CLA	b3	417	X	-	-	-
15	CLA	b3	421	X	-	-	-
15	CLA	b4	402	X	-	-	-
15	CLA	b4	403	X	-	-	-
15	CLA	b4	404	X	-	-	-
15	CLA	b4	405	X	-	-	-
15	CLA	b4	406	X	-	-	-
15	CLA	b4	407	X	-	-	-
15	CLA	b4	408	X	-	-	-
15	CLA	b4	409	X	-	-	-
15	CLA	b4	410	X	-	-	-
15	CLA	b4	411	X	-	-	-
15	CLA	b4	412	X	-	-	-
15	CLA	b4	413	X	-	-	-
15	CLA	b4	414	X	-	-	-
15	CLA	b4	416	X	-	-	-
15	CLA	b4	417	X	-	-	-
15	CLA	b4	421	X	-	-	-
15	CLA	b5	402	X	-	-	-
15	CLA	b5	403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b5	404	X	-	-	-
15	CLA	b5	405	X	-	-	-
15	CLA	b5	406	X	-	-	-
15	CLA	b5	407	X	-	-	-
15	CLA	b5	408	X	-	-	-
15	CLA	b5	409	X	-	-	-
15	CLA	b5	410	X	-	-	-
15	CLA	b5	411	X	-	-	-
15	CLA	b5	412	X	-	-	-
15	CLA	b5	413	X	-	-	-
15	CLA	b5	414	X	-	-	-
15	CLA	b5	416	X	-	-	-
15	CLA	b5	417	X	-	-	-
15	CLA	b5	420	X	-	-	-
15	CLA	b6	403	X	-	-	-
15	CLA	b6	404	X	-	-	-
15	CLA	b6	405	X	-	-	-
15	CLA	b6	406	X	-	-	-
15	CLA	b6	407	X	-	-	-
15	CLA	b6	408	X	-	-	-
15	CLA	b6	409	X	-	-	-
15	CLA	b6	410	X	-	-	-
15	CLA	b6	411	X	-	-	-
15	CLA	b6	412	X	-	-	-
15	CLA	b6	413	X	-	-	-
15	CLA	b6	414	X	-	-	-
15	CLA	b6	415	X	-	-	-
15	CLA	b6	417	X	-	-	-
15	CLA	b6	418	X	-	-	-
15	CLA	b6	422	X	-	-	-
15	CLA	bA	802	X	-	-	-
15	CLA	bA	803	X	-	-	-
15	CLA	bA	804	X	-	-	-
15	CLA	bA	805	X	-	-	-
15	CLA	bA	806	X	-	-	-
15	CLA	bA	807	X	-	-	-
15	CLA	bA	809	X	-	-	-
15	CLA	bA	810	X	-	-	-
15	CLA	bA	811	X	-	-	-
15	CLA	bA	812	X	-	-	-
15	CLA	bA	813	X	-	-	-
15	CLA	bA	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	bA	815	X	-	-	-
15	CLA	bA	818	X	-	-	-
15	CLA	bA	819	X	-	-	-
15	CLA	bA	820	X	-	-	-
15	CLA	bA	821	X	-	-	-
15	CLA	bA	822	X	-	-	-
15	CLA	bA	823	X	-	-	-
15	CLA	bA	824	X	-	-	-
15	CLA	bA	825	X	-	-	-
15	CLA	bA	826	X	-	-	-
15	CLA	bA	827	X	-	-	-
15	CLA	bA	828	X	-	-	-
15	CLA	bA	829	X	-	-	-
15	CLA	bA	830	X	-	-	-
15	CLA	bA	831	X	-	-	-
15	CLA	bA	832	X	-	-	-
15	CLA	bA	833	X	-	-	-
15	CLA	bA	834	X	-	-	-
15	CLA	bA	835	X	-	-	-
15	CLA	bA	836	X	-	-	-
15	CLA	bA	838	X	-	-	-
15	CLA	bA	839	X	-	-	-
15	CLA	bA	840	X	-	-	-
15	CLA	bA	841	X	-	-	-
15	CLA	bA	842	X	-	-	-
15	CLA	bA	843	X	-	-	-
15	CLA	bA	844	X	-	-	-
15	CLA	bA	845	X	-	-	-
15	CLA	bB	801	X	-	-	-
15	CLA	bB	802	X	-	-	-
15	CLA	bB	803	X	-	-	-
15	CLA	bB	804	X	-	-	-
15	CLA	bB	805	X	-	-	-
15	CLA	bB	806	X	-	-	-
15	CLA	bB	807	X	-	-	-
15	CLA	bB	809	X	-	-	-
15	CLA	bB	810	X	-	-	-
15	CLA	bB	811	X	-	-	-
15	CLA	bB	812	X	-	-	-
15	CLA	bB	813	X	-	-	-
15	CLA	bB	814	X	-	-	-
15	CLA	bB	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	bB	816	X	-	-	-
15	CLA	bB	817	X	-	-	-
15	CLA	bB	818	X	-	-	-
15	CLA	bB	819	X	-	-	-
15	CLA	bB	820	X	-	-	-
15	CLA	bB	821	X	-	-	-
15	CLA	bB	822	X	-	-	-
15	CLA	bB	823	X	-	-	-
15	CLA	bB	824	X	-	-	-
15	CLA	bB	825	X	-	-	-
15	CLA	bB	826	X	-	-	-
15	CLA	bB	827	X	-	-	-
15	CLA	bB	828	X	-	-	-
15	CLA	bB	829	X	-	-	-
15	CLA	bB	830	X	-	-	-
15	CLA	bB	831	X	-	-	-
15	CLA	bB	832	X	-	-	-
15	CLA	bB	833	X	-	-	-
15	CLA	bB	834	X	-	-	-
15	CLA	bB	835	X	-	-	-
15	CLA	bB	836	X	-	-	-
15	CLA	bB	837	X	-	-	-
15	CLA	bB	838	X	-	-	-
15	CLA	bB	839	X	-	-	-
15	CLA	bB	840	X	-	-	-
15	CLA	bB	841	X	-	-	-
15	CLA	bF	201	X	-	-	-
15	CLA	bJ	101	X	-	-	-
15	CLA	bJ	102	X	-	-	-
15	CLA	bK	101	X	-	-	-
15	CLA	bL	202	X	-	-	-
15	CLA	bL	203	X	-	-	-
15	CLA	bL	204	X	-	-	-
15	CLA	bX	102	X	-	-	-
15	CLA	c1	402	X	-	-	-
15	CLA	c1	403	X	-	-	-
15	CLA	c1	404	X	-	-	-
15	CLA	c1	405	X	-	-	-
15	CLA	c1	406	X	-	-	-
15	CLA	c1	407	X	-	-	-
15	CLA	c1	408	X	-	-	-
15	CLA	c1	409	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c1	410	X	-	-	-
15	CLA	c1	411	X	-	-	-
15	CLA	c1	412	X	-	-	-
15	CLA	c1	413	X	-	-	-
15	CLA	c1	414	X	-	-	-
15	CLA	c1	416	X	-	-	-
15	CLA	c1	417	X	-	-	-
15	CLA	c2	402	X	-	-	-
15	CLA	c2	403	X	-	-	-
15	CLA	c2	404	X	-	-	-
15	CLA	c2	405	X	-	-	-
15	CLA	c2	406	X	-	-	-
15	CLA	c2	407	X	-	-	-
15	CLA	c2	408	X	-	-	-
15	CLA	c2	409	X	-	-	-
15	CLA	c2	410	X	-	-	-
15	CLA	c2	411	X	-	-	-
15	CLA	c2	412	X	-	-	-
15	CLA	c2	413	X	-	-	-
15	CLA	c2	414	X	-	-	-
15	CLA	c2	415	X	-	-	-
15	CLA	c2	417	X	-	-	-
15	CLA	c2	418	X	-	-	-
15	CLA	c2	422	X	-	-	-
15	CLA	c3	402	X	-	-	-
15	CLA	c3	403	X	-	-	-
15	CLA	c3	404	X	-	-	-
15	CLA	c3	405	X	-	-	-
15	CLA	c3	406	X	-	-	-
15	CLA	c3	407	X	-	-	-
15	CLA	c3	408	X	-	-	-
15	CLA	c3	410	X	-	-	-
15	CLA	c3	411	X	-	-	-
15	CLA	c3	412	X	-	-	-
15	CLA	c3	413	X	-	-	-
15	CLA	c3	414	X	-	-	-
15	CLA	c3	416	X	-	-	-
15	CLA	c3	417	X	-	-	-
15	CLA	c3	421	X	-	-	-
15	CLA	c4	402	X	-	-	-
15	CLA	c4	403	X	-	-	-
15	CLA	c4	404	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c4	405	X	-	-	-
15	CLA	c4	406	X	-	-	-
15	CLA	c4	407	X	-	-	-
15	CLA	c4	408	X	-	-	-
15	CLA	c4	409	X	-	-	-
15	CLA	c4	410	X	-	-	-
15	CLA	c4	411	X	-	-	-
15	CLA	c4	412	X	-	-	-
15	CLA	c4	413	X	-	-	-
15	CLA	c4	414	X	-	-	-
15	CLA	c4	416	X	-	-	-
15	CLA	c4	417	X	-	-	-
15	CLA	c4	421	X	-	-	-
15	CLA	c5	402	X	-	-	-
15	CLA	c5	403	X	-	-	-
15	CLA	c5	404	X	-	-	-
15	CLA	c5	405	X	-	-	-
15	CLA	c5	406	X	-	-	-
15	CLA	c5	407	X	-	-	-
15	CLA	c5	408	X	-	-	-
15	CLA	c5	409	X	-	-	-
15	CLA	c5	410	X	-	-	-
15	CLA	c5	411	X	-	-	-
15	CLA	c5	412	X	-	-	-
15	CLA	c5	413	X	-	-	-
15	CLA	c5	414	X	-	-	-
15	CLA	c5	416	X	-	-	-
15	CLA	c5	417	X	-	-	-
15	CLA	c5	420	X	-	-	-
15	CLA	c6	403	X	-	-	-
15	CLA	c6	404	X	-	-	-
15	CLA	c6	405	X	-	-	-
15	CLA	c6	406	X	-	-	-
15	CLA	c6	407	X	-	-	-
15	CLA	c6	408	X	-	-	-
15	CLA	c6	409	X	-	-	-
15	CLA	c6	410	X	-	-	-
15	CLA	c6	411	X	-	-	-
15	CLA	c6	412	X	-	-	-
15	CLA	c6	413	X	-	-	-
15	CLA	c6	414	X	-	-	-
15	CLA	c6	415	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	c6	417	X	-	-	-
15	CLA	c6	418	X	-	-	-
15	CLA	cA	802	X	-	-	-
15	CLA	cA	803	X	-	-	-
15	CLA	cA	804	X	-	-	-
15	CLA	cA	805	X	-	-	-
15	CLA	cA	806	X	-	-	-
15	CLA	cA	807	X	-	-	-
15	CLA	cA	809	X	-	-	-
15	CLA	cA	810	X	-	-	-
15	CLA	cA	811	X	-	-	-
15	CLA	cA	812	X	-	-	-
15	CLA	cA	813	X	-	-	-
15	CLA	cA	814	X	-	-	-
15	CLA	cA	815	X	-	-	-
15	CLA	cA	818	X	-	-	-
15	CLA	cA	819	X	-	-	-
15	CLA	cA	820	X	-	-	-
15	CLA	cA	821	X	-	-	-
15	CLA	cA	822	X	-	-	-
15	CLA	cA	823	X	-	-	-
15	CLA	cA	824	X	-	-	-
15	CLA	cA	825	X	-	-	-
15	CLA	cA	826	X	-	-	-
15	CLA	cA	827	X	-	-	-
15	CLA	cA	828	X	-	-	-
15	CLA	cA	829	X	-	-	-
15	CLA	cA	830	X	-	-	-
15	CLA	cA	831	X	-	-	-
15	CLA	cA	832	X	-	-	-
15	CLA	cA	833	X	-	-	-
15	CLA	cA	834	X	-	-	-
15	CLA	cA	835	X	-	-	-
15	CLA	cA	836	X	-	-	-
15	CLA	cA	838	X	-	-	-
15	CLA	cA	839	X	-	-	-
15	CLA	cA	840	X	-	-	-
15	CLA	cA	841	X	-	-	-
15	CLA	cA	842	X	-	-	-
15	CLA	cA	843	X	-	-	-
15	CLA	cA	844	X	-	-	-
15	CLA	cB	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	cB	802	X	-	-	-
15	CLA	cB	803	X	-	-	-
15	CLA	cB	804	X	-	-	-
15	CLA	cB	805	X	-	-	-
15	CLA	cB	806	X	-	-	-
15	CLA	cB	807	X	-	-	-
15	CLA	cB	809	X	-	-	-
15	CLA	cB	810	X	-	-	-
15	CLA	cB	811	X	-	-	-
15	CLA	cB	812	X	-	-	-
15	CLA	cB	813	X	-	-	-
15	CLA	cB	814	X	-	-	-
15	CLA	cB	815	X	-	-	-
15	CLA	cB	816	X	-	-	-
15	CLA	cB	817	X	-	-	-
15	CLA	cB	818	X	-	-	-
15	CLA	cB	819	X	-	-	-
15	CLA	cB	820	X	-	-	-
15	CLA	cB	821	X	-	-	-
15	CLA	cB	822	X	-	-	-
15	CLA	cB	823	X	-	-	-
15	CLA	cB	824	X	-	-	-
15	CLA	cB	825	X	-	-	-
15	CLA	cB	826	X	-	-	-
15	CLA	cB	827	X	-	-	-
15	CLA	cB	828	X	-	-	-
15	CLA	cB	829	X	-	-	-
15	CLA	cB	830	X	-	-	-
15	CLA	cB	831	X	-	-	-
15	CLA	cB	832	X	-	-	-
15	CLA	cB	833	X	-	-	-
15	CLA	cB	834	X	-	-	-
15	CLA	cB	835	X	-	-	-
15	CLA	cB	836	X	-	-	-
15	CLA	cB	837	X	-	-	-
15	CLA	cB	838	X	-	-	-
15	CLA	cB	839	X	-	-	-
15	CLA	cB	840	X	-	-	-
15	CLA	cB	841	X	-	-	-
15	CLA	cF	201	X	-	-	-
15	CLA	cF	203	X	-	-	-
15	CLA	cJ	101	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	cJ	102	X	-	-	-
15	CLA	cK	102	X	-	-	-
15	CLA	cL	201	X	-	-	-
15	CLA	cL	202	X	-	-	-
15	CLA	cL	203	X	-	-	-
15	CLA	cX	102	X	-	-	-

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		

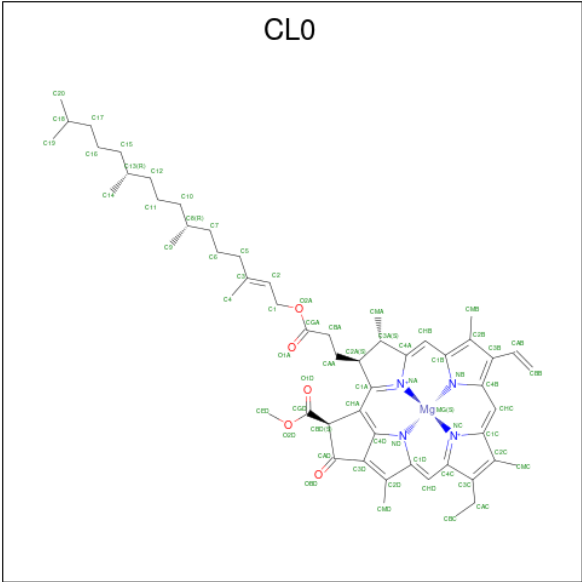
- Molecule 12 is a protein called Photosystem I reaction center subunit psaX.

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.

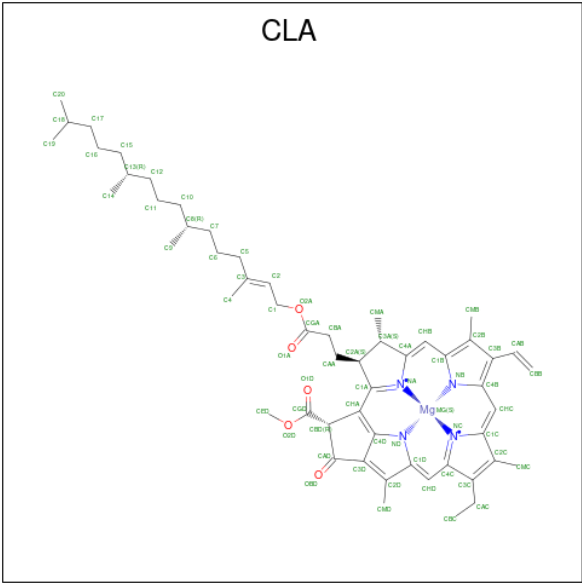
Mol	Chain	Residues	Atoms					AltConf	Trace
13	a1	329	Total	C	N	O	S	0	0
			2583	1727	426	426	4		
13	a2	327	Total	C	N	O	S	0	0
			2565	1716	422	423	4		
13	a3	332	Total	C	N	O	S	0	0
			2607	1742	429	432	4		
13	a4	336	Total	C	N	O	S	0	0
			2641	1766	434	437	4		
13	a5	332	Total	C	N	O	S	0	0
			2607	1742	429	432	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 (three-letter code: 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 (three-letter code: 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 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 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	C	Mg	N	O	0
			58	48	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bF	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bJ	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
15	bK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bL	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	bX	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
15	b1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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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 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 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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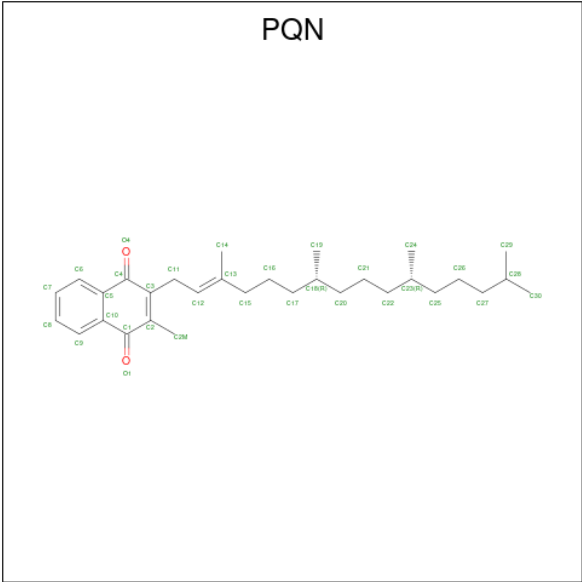
Mol	Chain	Residues	Atoms					AltConf
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 41	C 33	Mg 1	N 4	O 3	0
15	c4	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c4	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c4	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c4	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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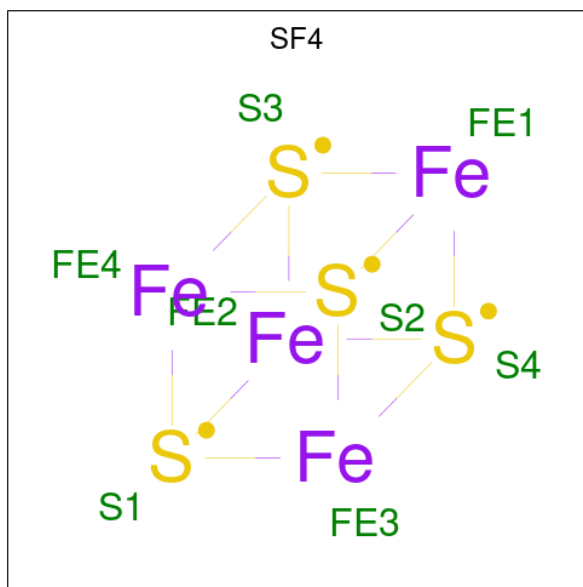
Mol	Chain	Residues	Atoms					AltConf
15	c5	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	c5	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	c5	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	c5	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	c6	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 (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



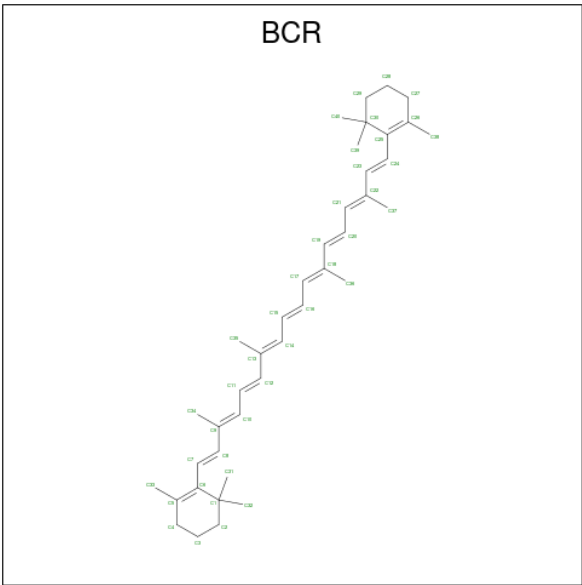
Mol	Chain	Residues	Atoms			AltConf
16	aA	1	Total	C	O	0
			33	31	2	
16	aB	1	Total	C	O	0
			33	31	2	
16	bA	1	Total	C	O	0
			33	31	2	
16	bB	1	Total	C	O	0
			33	31	2	
16	cA	1	Total	C	O	0
			33	31	2	
16	cB	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: 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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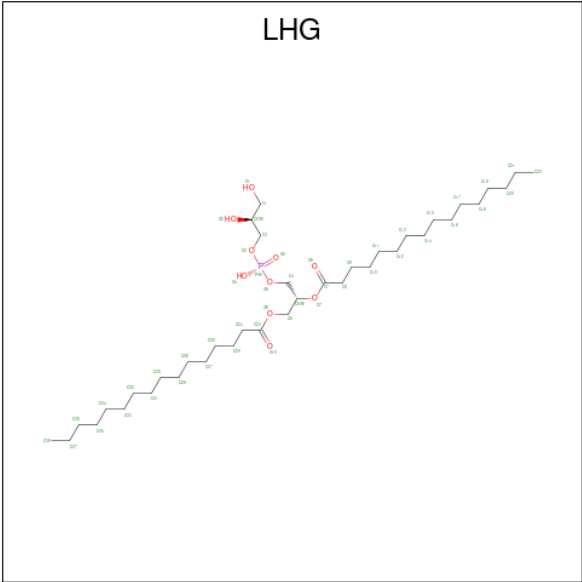
Mol	Chain	Residues	Atoms	AltConf
18	cA	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 25 25	0
18	cB	1	Total C 40 40	0
18	cB	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cF	1	Total C 40 40	0
18	cI	1	Total C 40 40	0
18	cI	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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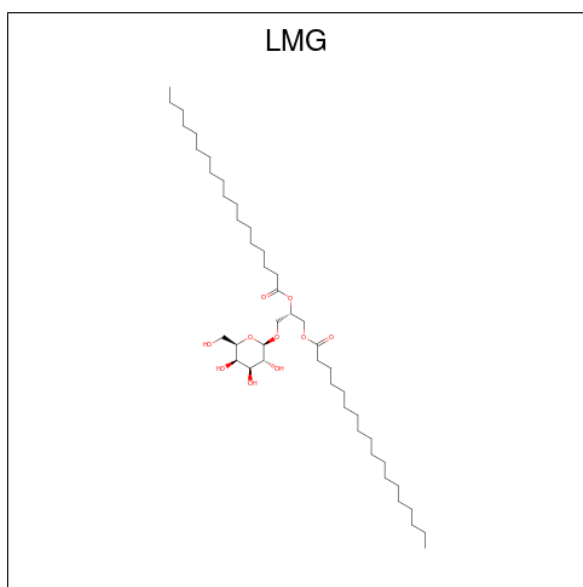
Mol	Chain	Residues	Atoms	AltConf
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c2	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c3	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	1	Total C 40 40	0
18	c4	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 (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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 (three-letter code: 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 (three-letter code: 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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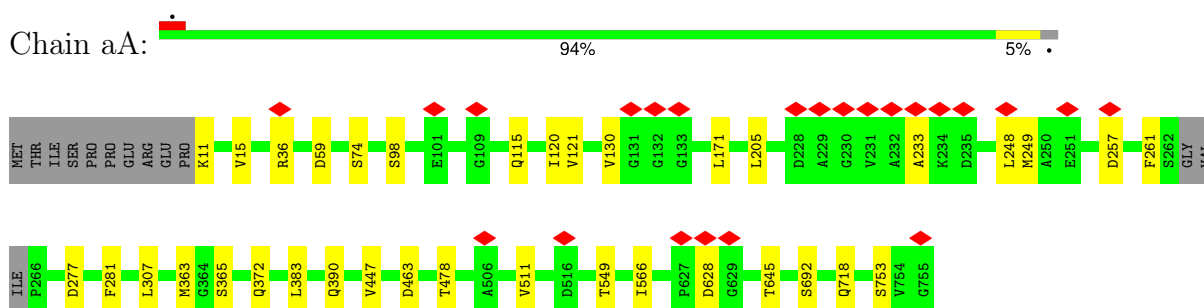
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Mol	Chain	Residues	Atoms		AltConf
22	bB	3	Total 3	O 3	0
22	bL	1	Total 1	O 1	0
22	cA	2	Total 2	O 2	0
22	cB	3	Total 3	O 3	0
22	cF	1	Total 1	O 1	0
22	cL	1	Total 1	O 1	0

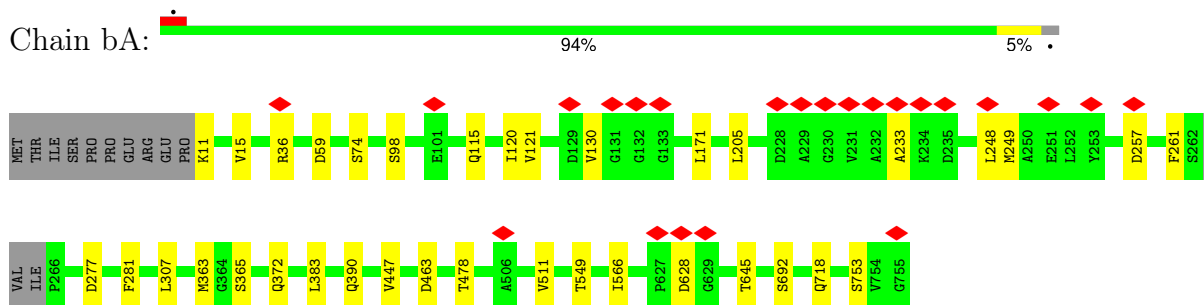
3 Residue-property plots [i](#)

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.

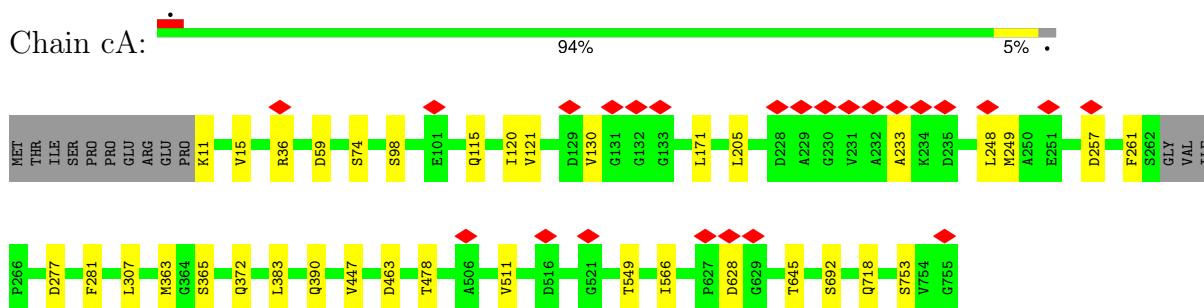
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

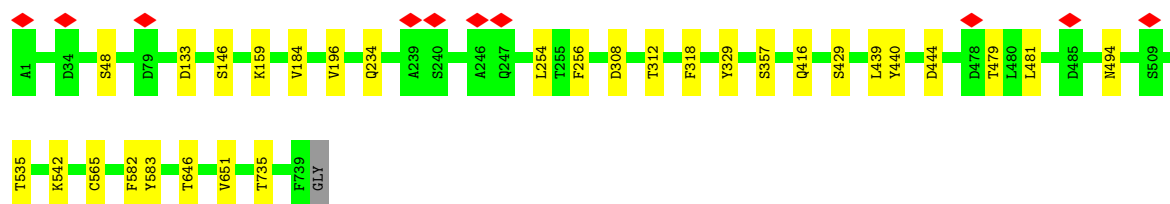


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



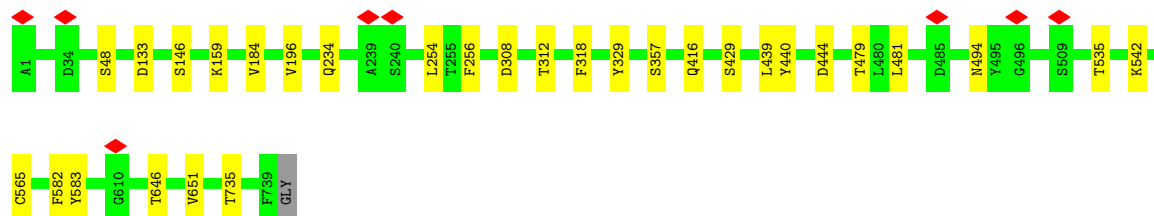
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2





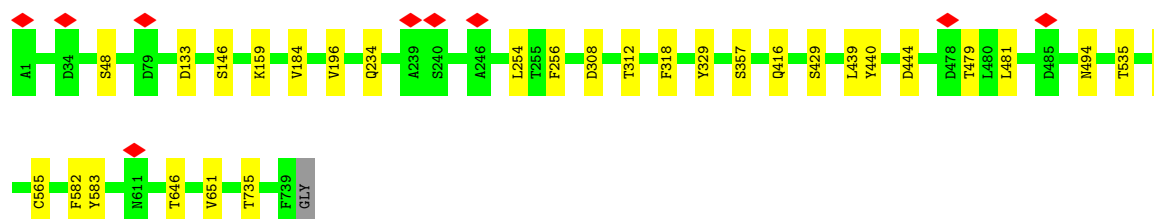
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain bB: 96%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain cB: 96%



- Molecule 3: Photosystem I iron-sulfur center

Chain aC: 90%



- Molecule 3: Photosystem I iron-sulfur center

Chain bC: 90%



- Molecule 3: Photosystem I iron-sulfur center

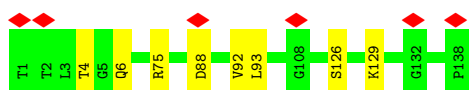
Chain cC: 90%



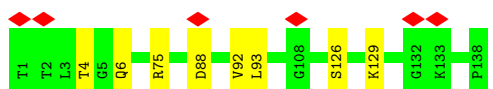
- Molecule 4: Photosystem I reaction center subunit II



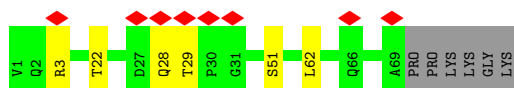
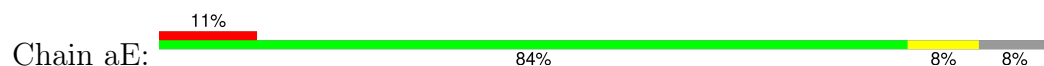
- Molecule 4: Photosystem I reaction center subunit II



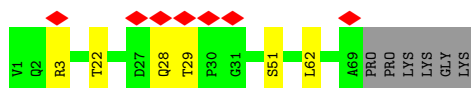
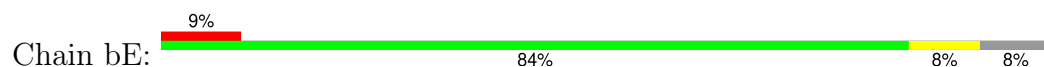
- Molecule 4: Photosystem I reaction center subunit II



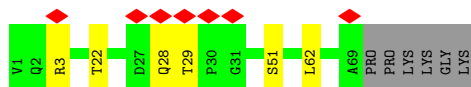
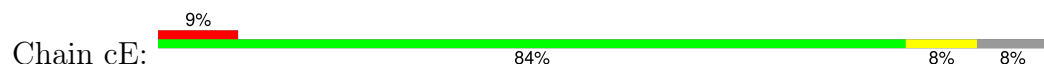
- Molecule 5: Photosystem I reaction center subunit IV



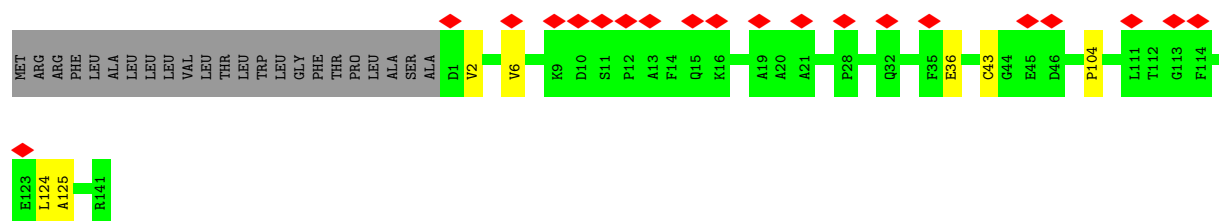
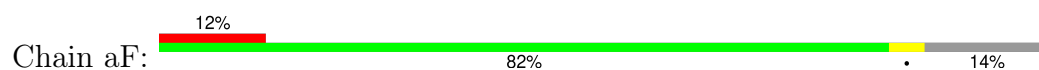
- Molecule 5: Photosystem I reaction center subunit IV



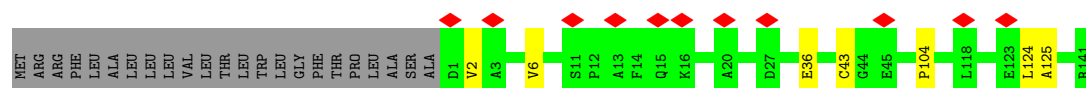
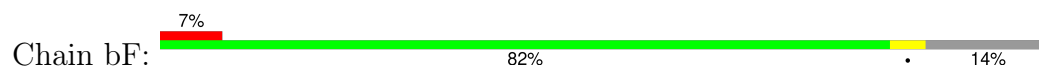
- Molecule 5: Photosystem I reaction center subunit IV



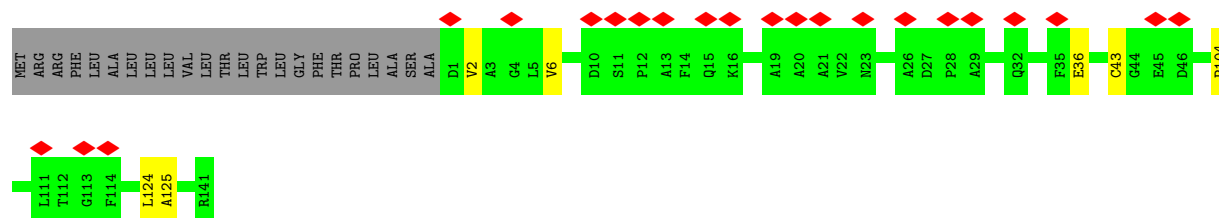
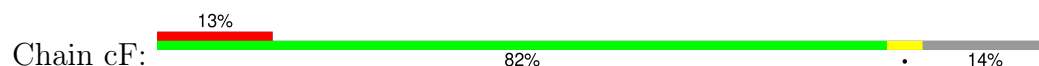
- Molecule 6: Photosystem I reaction center subunit III



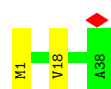
- Molecule 6: Photosystem I reaction center subunit III



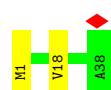
- Molecule 6: Photosystem I reaction center subunit III



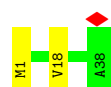
- Molecule 7: Photosystem I reaction center subunit VIII



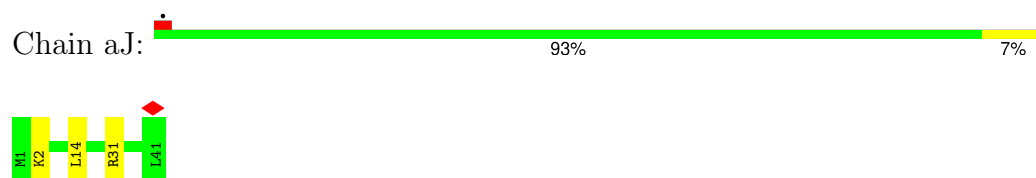
- Molecule 7: Photosystem I reaction center subunit VIII



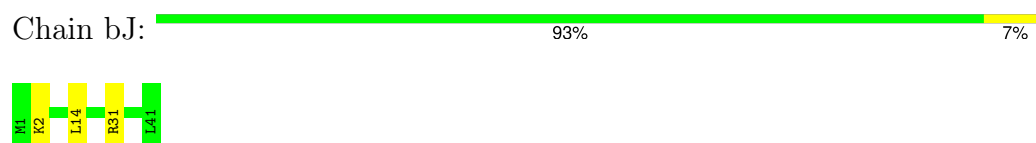
- Molecule 7: Photosystem I reaction center subunit VIII



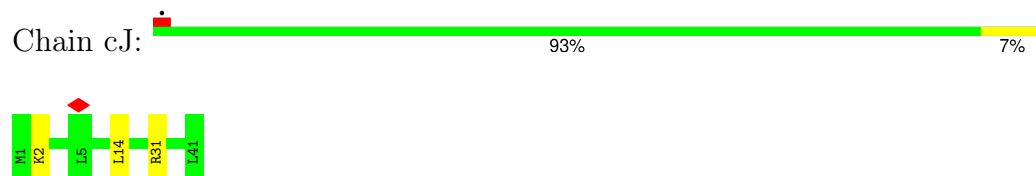
- Molecule 8: Photosystem I reaction center subunit IX



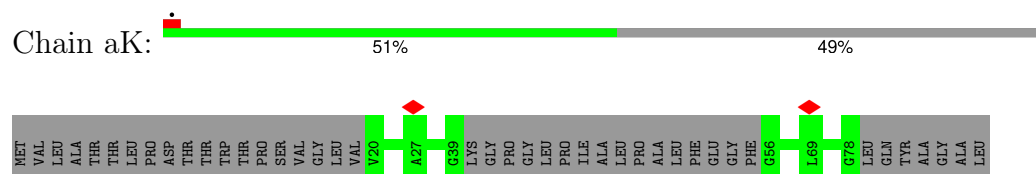
- Molecule 8: Photosystem I reaction center subunit IX



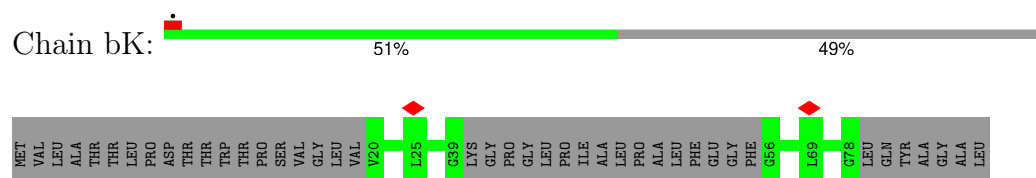
- Molecule 8: Photosystem I reaction center subunit IX



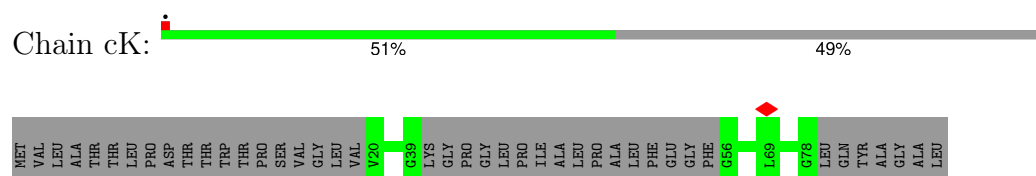
- Molecule 9: Photosystem I reaction center subunit Psak



- Molecule 9: Photosystem I reaction center subunit Psak

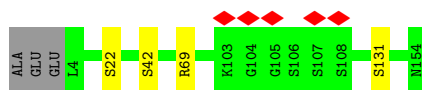


- Molecule 9: Photosystem I reaction center subunit Psak

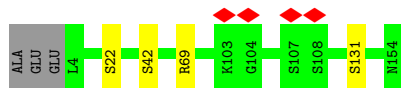


- Molecule 10: Photosystem I reaction center subunit XI

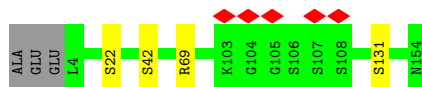




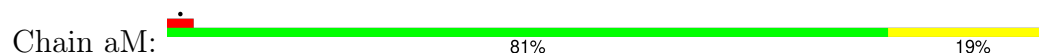
- Molecule 10: Photosystem I reaction center subunit XI



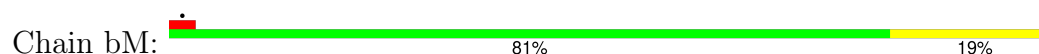
- Molecule 10: Photosystem I reaction center subunit XI



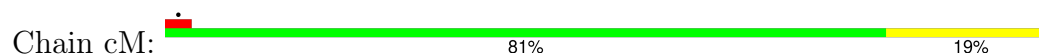
- Molecule 11: Photosystem I reaction center subunit XII



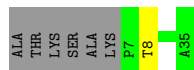
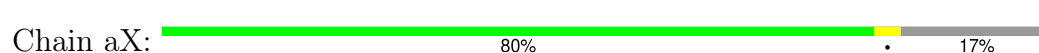
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I reaction center subunit psaX



- Molecule 12: Photosystem I reaction center subunit psaX

80% • 17%



Opinion	Percentage
Doing a good job	80%
Doing a bad job	17%

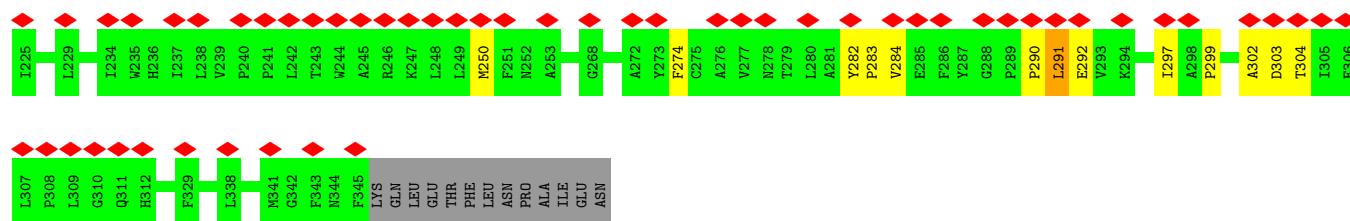


Response	Percentage
Yes	48%
No	84%
Other (Yellow)	7%
Other (Grey)	8%

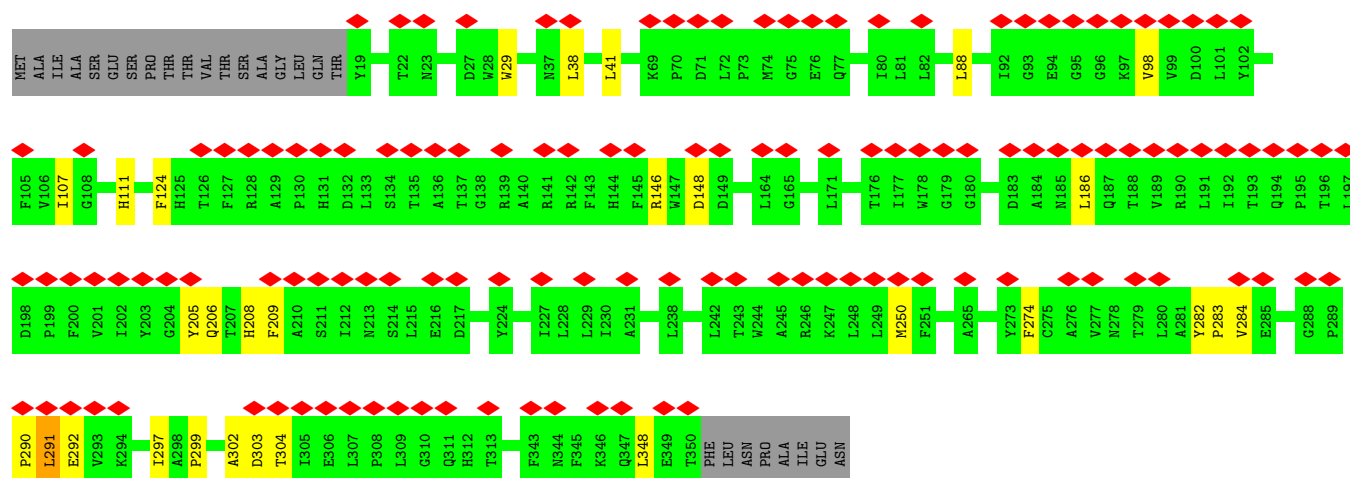
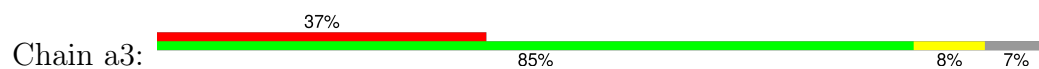


Category	Percentage
Current government is the best for the country	52%
Best government	84%
Worst government	7%
Best government	9%

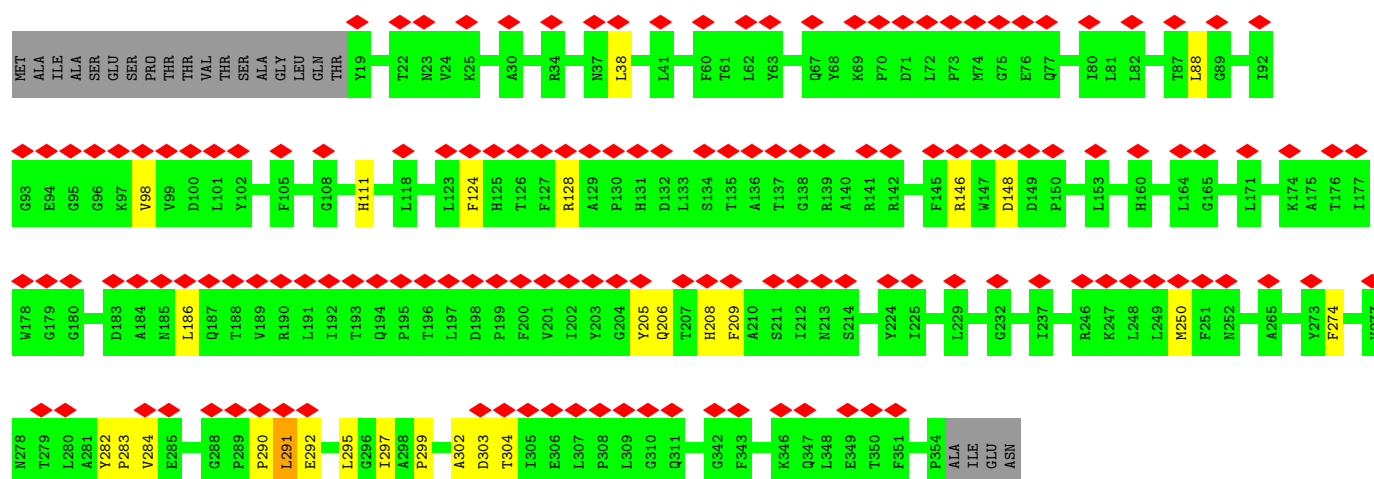
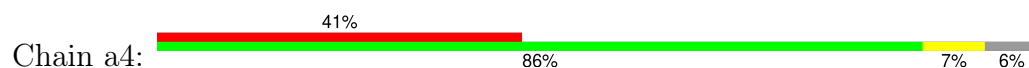




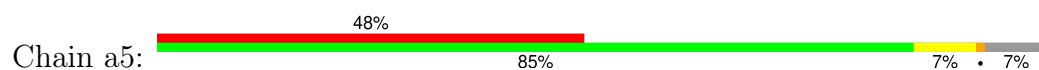
• Molecule 13: Iron stress in-duced protein A

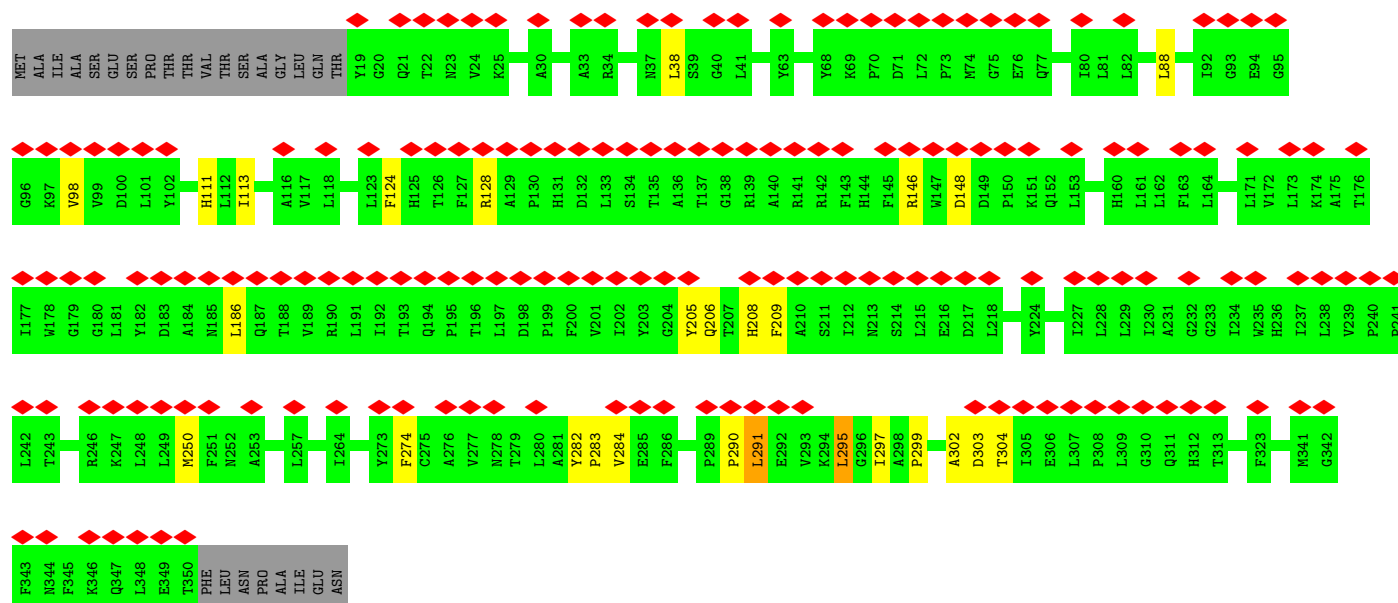


• Molecule 13: Iron stress in-duced protein A



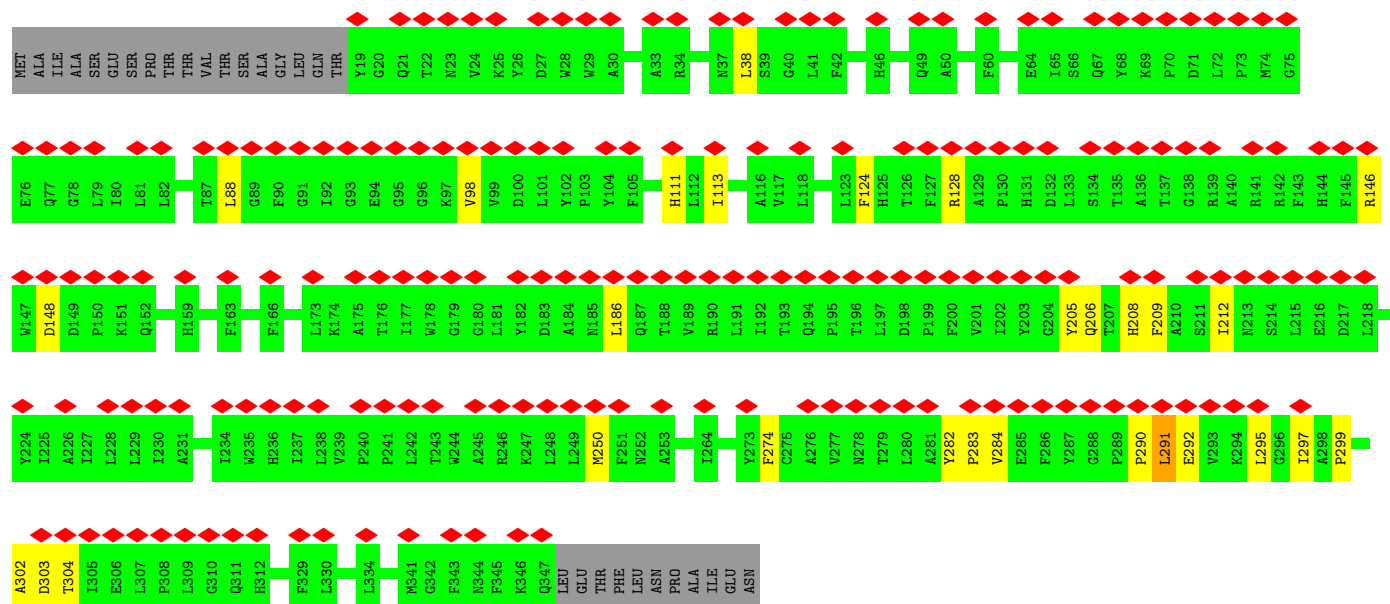
• Molecule 13: Iron stress in-duced protein A





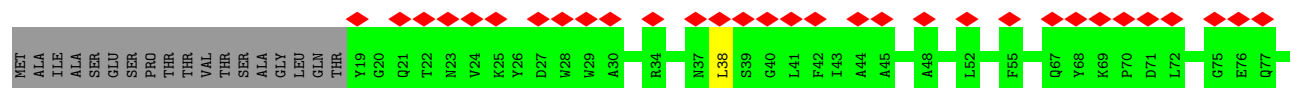
• Molecule 13: Iron stress in-duced protein A

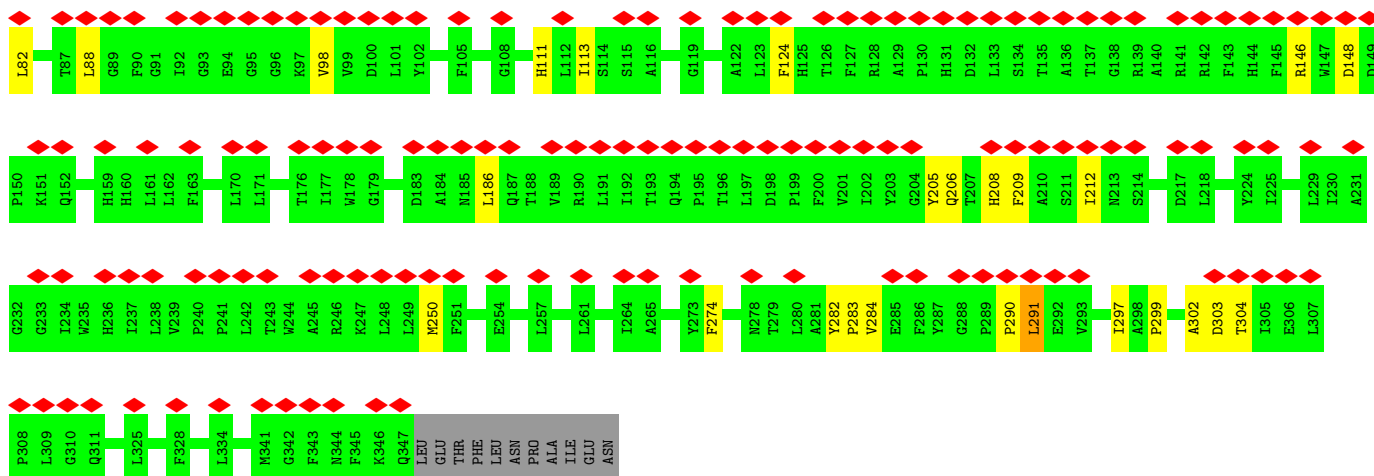
Chain a6: 54% 84% 8% 8%



• Molecule 13: Iron stress in-duced protein A

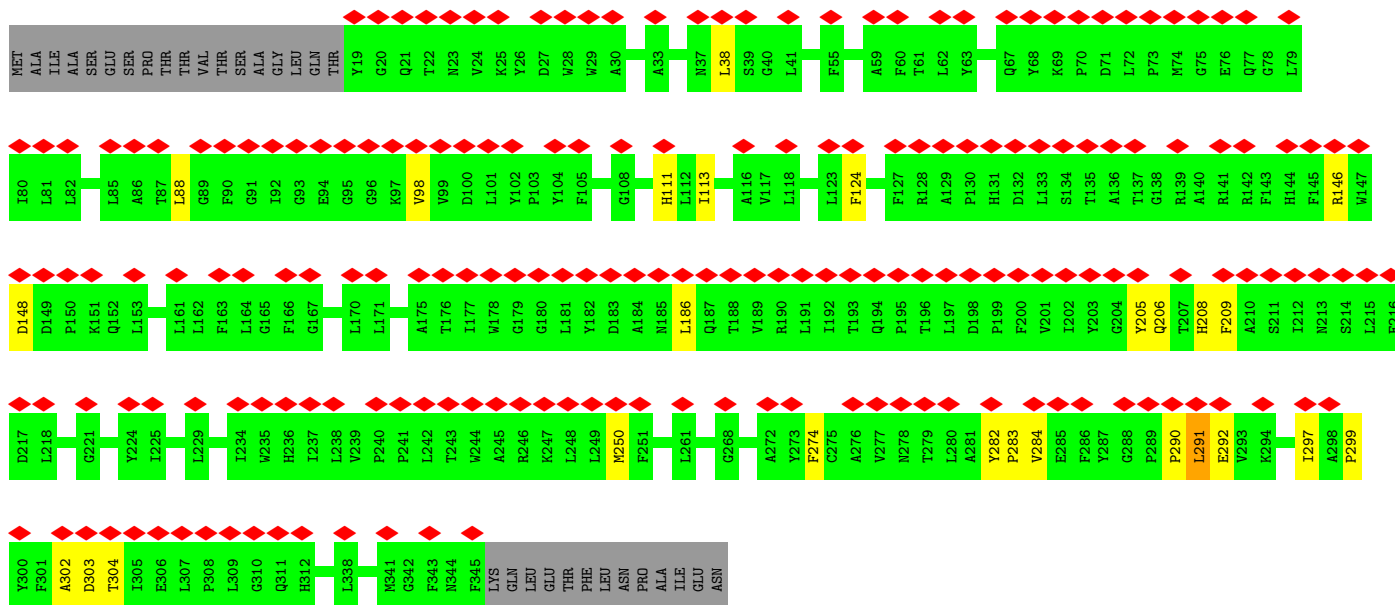
Chain b1: 49% 84% 7% 8%





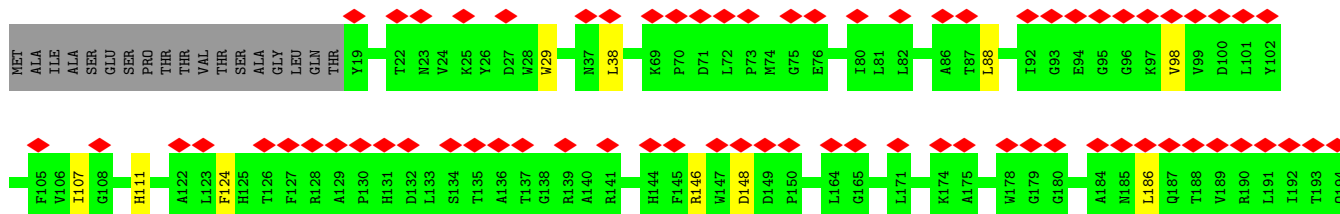
• Molecule 13: Iron stress in-duced protein A

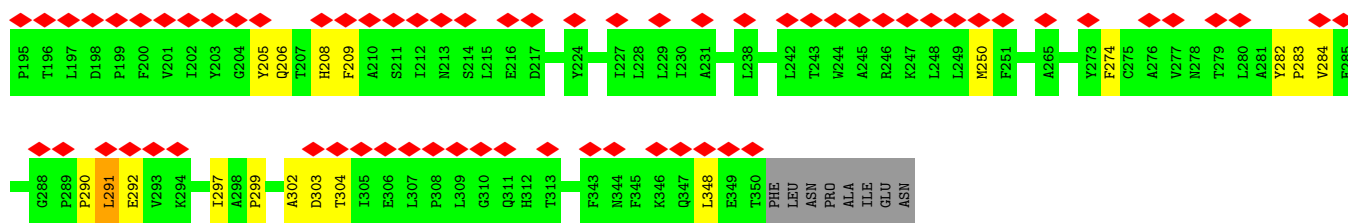
Chain b2:



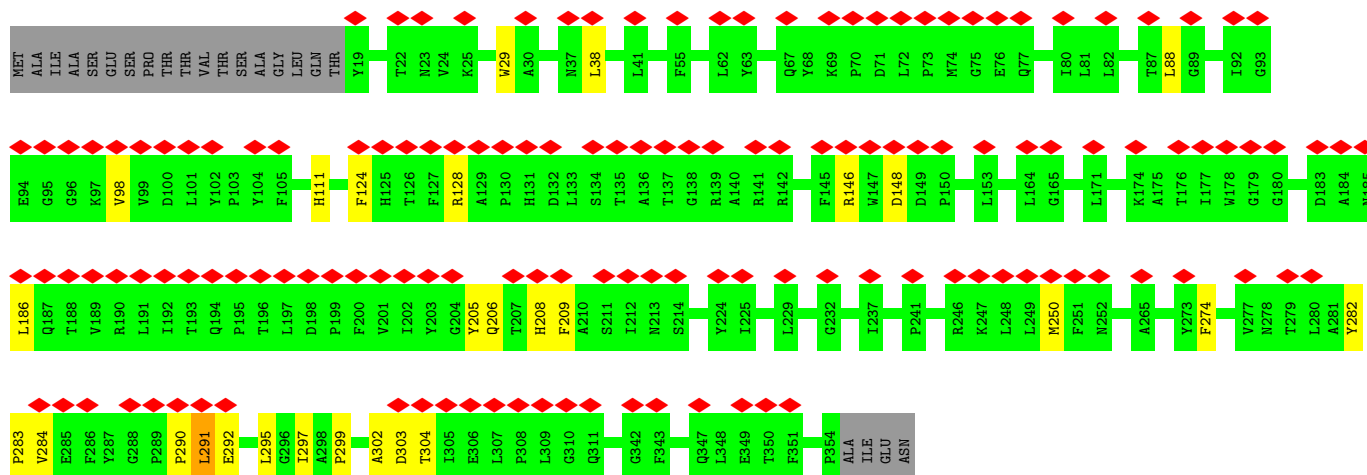
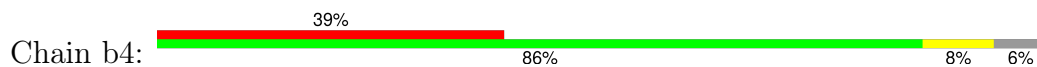
• Molecule 13: Iron stress in-duced protein A

Chain b3:

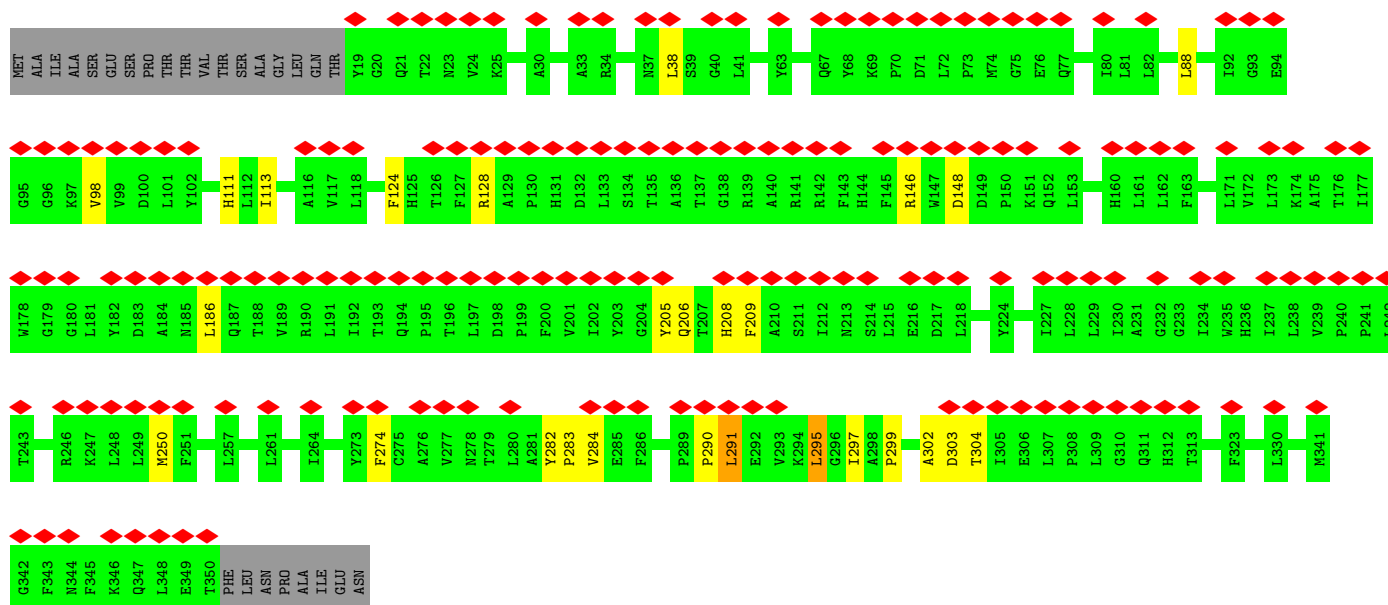
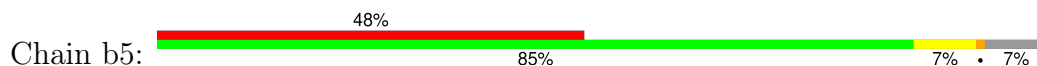





• Molecule 13: Iron stress in-duced protein A

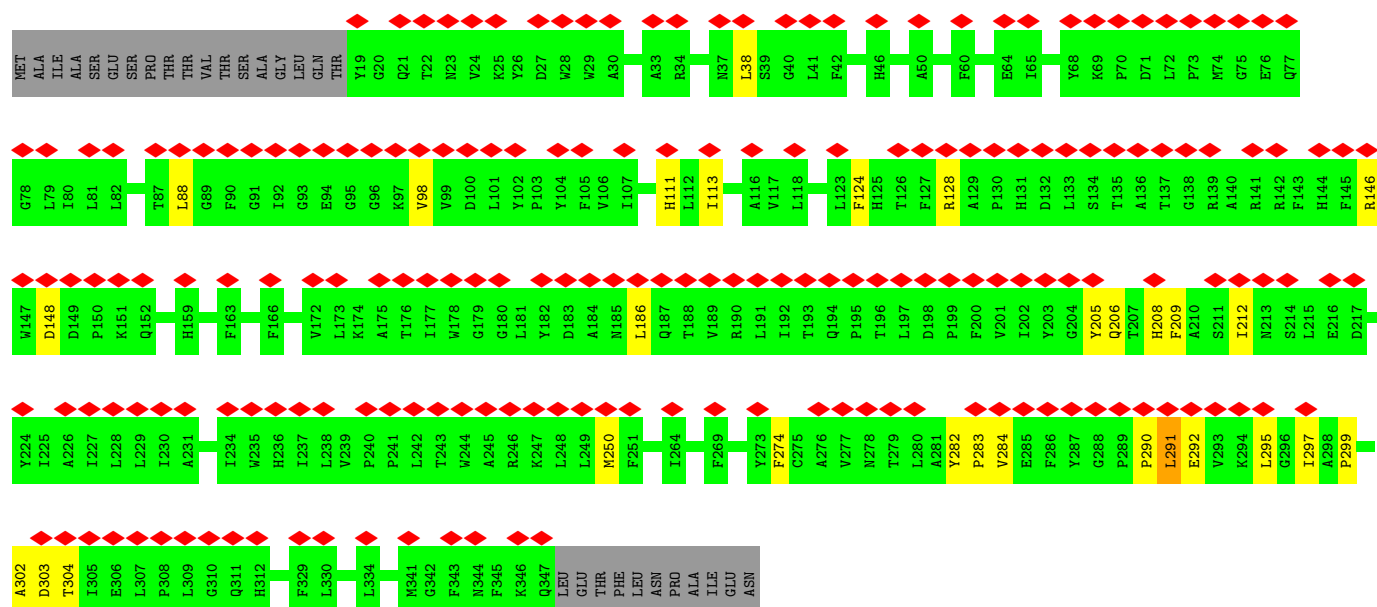


• Molecule 13: Iron stress in-duced protein A




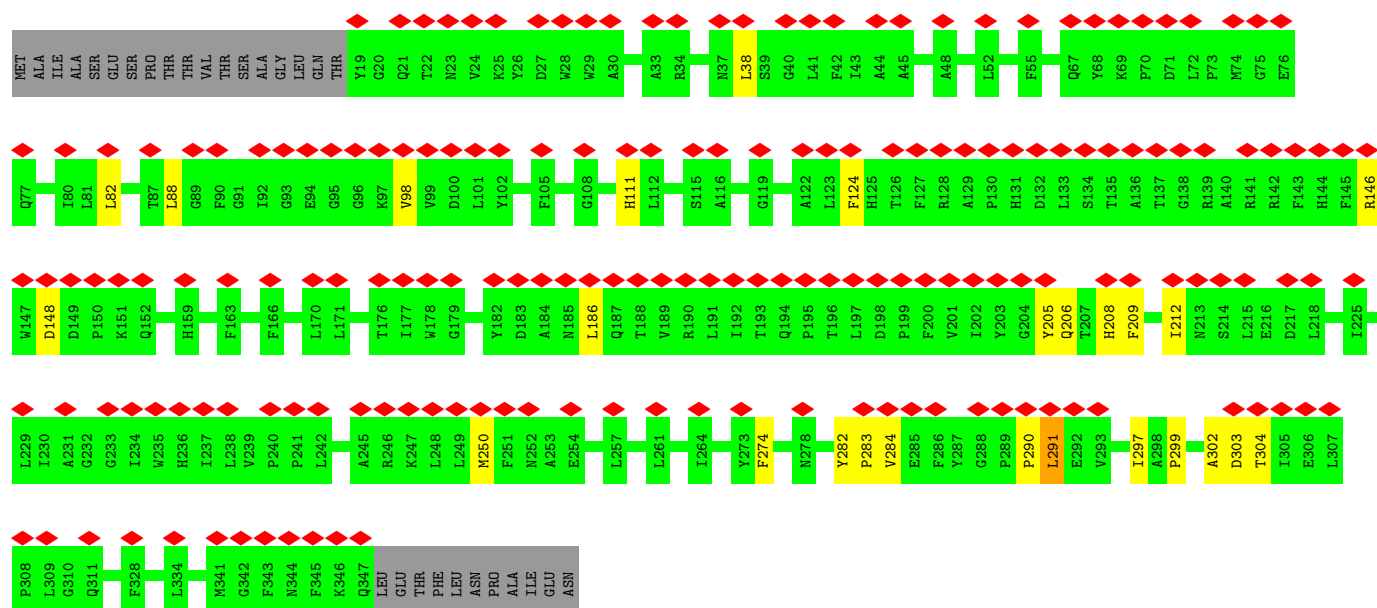
• Molecule 13: Iron stress in-duced protein A

Chain b6: 




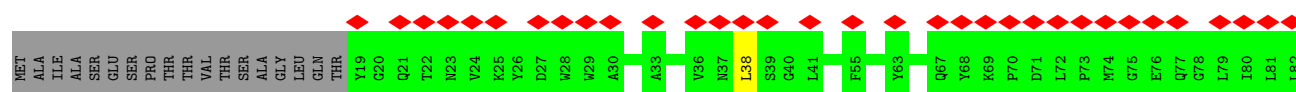
• Molecule 13: Iron stress in-duced protein A

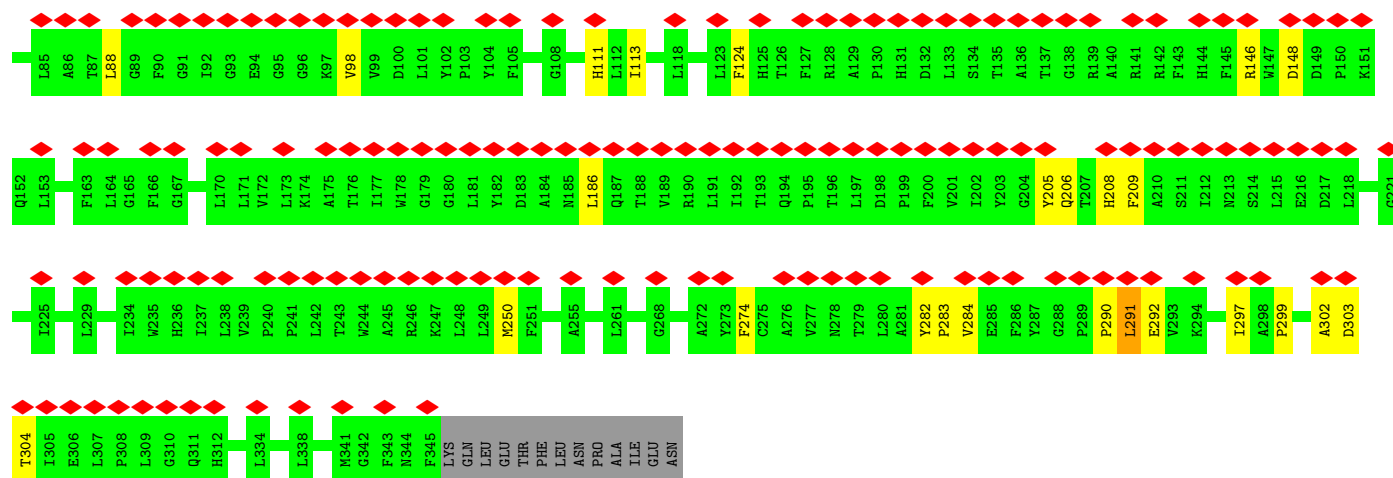
Chain c1: 



• Molecule 13: Iron stress in-duced protein A

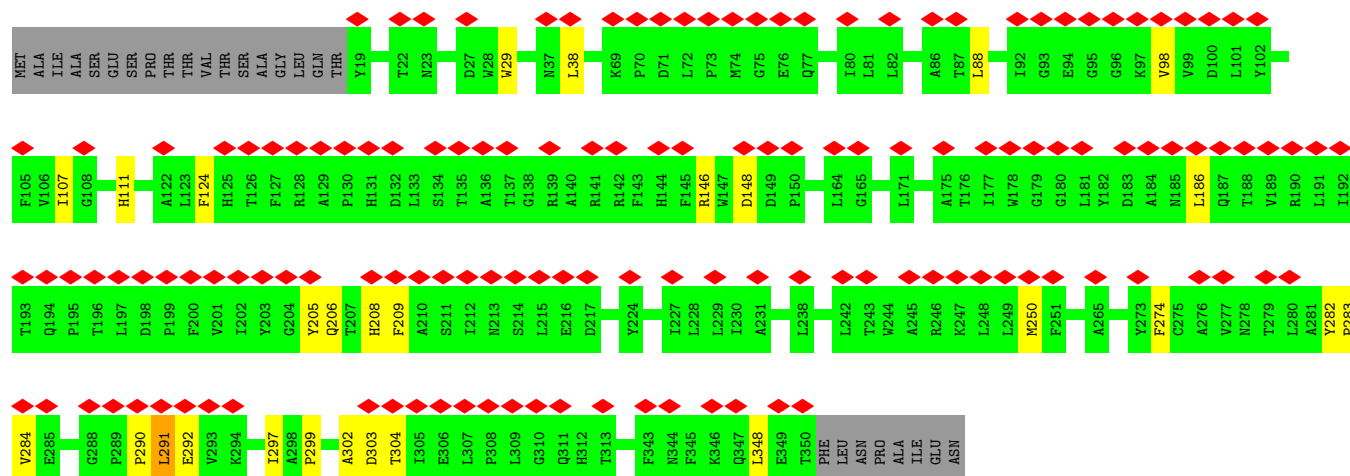
Chain c2: 





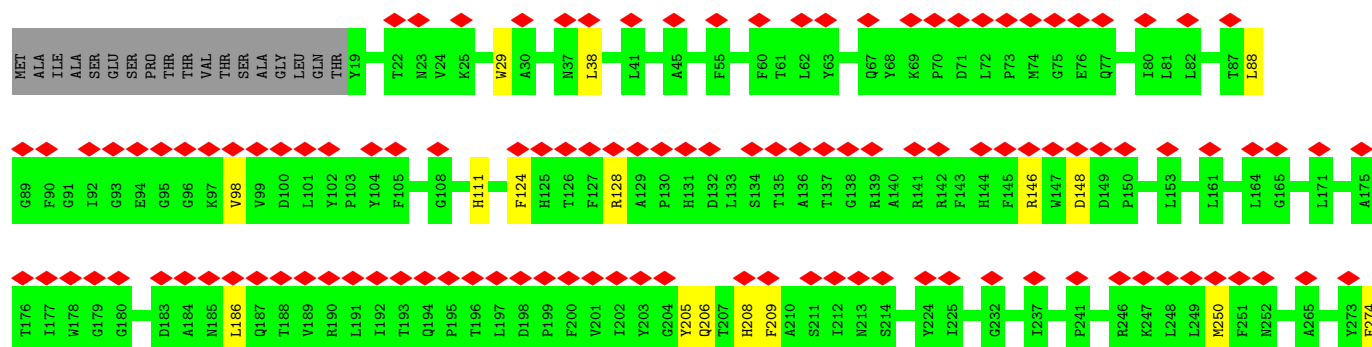
• Molecule 13: Iron stress in-duced protein A

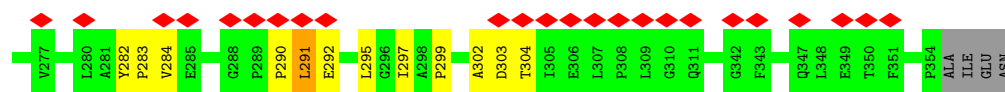
Chain c3:



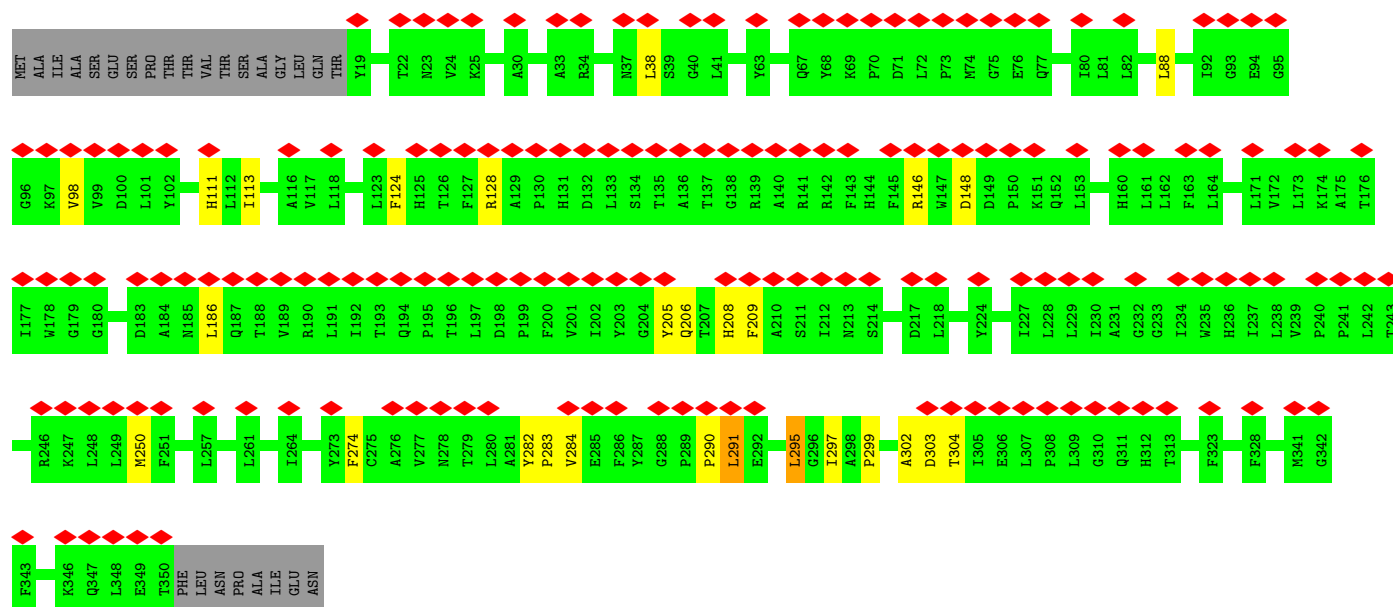
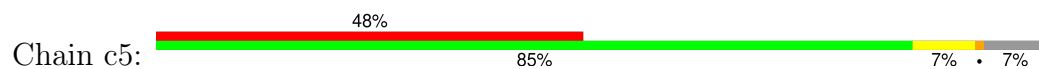
• Molecule 13: Iron stress in-duced protein A

Chain c4:

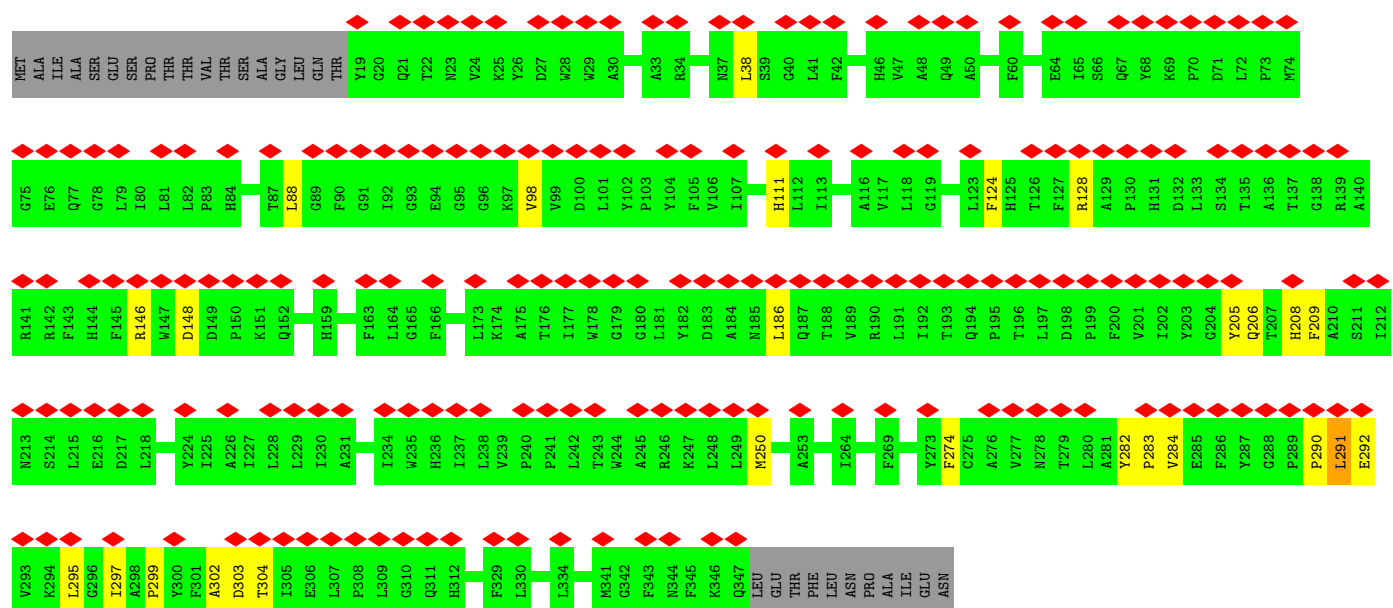
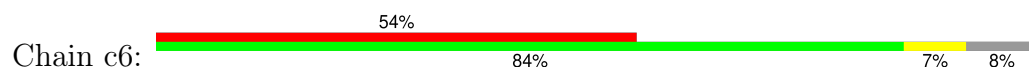




• Molecule 13: Iron stress in-duced protein A



• 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: PQN, SF4, LMG, CA, BCR, CL0, CLA, LHG

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	0.58	1/6000 (0.0%)	0.55	0/8180
1	bA	0.58	1/6000 (0.0%)	0.55	0/8180
1	cA	0.58	1/6000 (0.0%)	0.55	0/8180
2	aB	0.58	1/6096 (0.0%)	0.58	1/8332 (0.0%)
2	bB	0.58	1/6096 (0.0%)	0.57	1/8332 (0.0%)
2	cB	0.58	1/6096 (0.0%)	0.57	1/8332 (0.0%)
3	aC	0.60	0/608	0.65	0/824
3	bC	0.60	0/608	0.65	0/824
3	cC	0.60	0/608	0.65	0/824
4	aD	0.49	0/1101	0.53	0/1492
4	bD	0.49	0/1101	0.53	0/1492
4	cD	0.49	0/1101	0.53	0/1492
5	aE	0.47	0/551	0.51	0/750
5	bE	0.47	0/551	0.51	0/750
5	cE	0.47	0/551	0.51	0/750
6	aF	0.43	0/1087	0.57	0/1476
6	bF	0.43	0/1087	0.57	0/1476
6	cF	0.43	0/1087	0.57	0/1476
7	aI	0.63	0/312	0.68	0/425
7	bI	0.63	0/312	0.68	0/425
7	cI	0.63	0/312	0.68	0/425
8	aJ	0.50	0/350	0.64	0/477
8	bJ	0.50	0/350	0.64	0/477
8	cJ	0.50	0/350	0.64	0/477
9	aK	0.25	0/206	0.36	0/281
9	bK	0.25	0/206	0.36	0/281
9	cK	0.25	0/206	0.36	0/281
10	aL	0.57	0/1148	0.54	0/1558
10	bL	0.57	0/1148	0.54	0/1558
10	cL	0.57	0/1148	0.54	0/1558
11	aM	0.45	0/244	0.59	0/332
11	bM	0.46	0/244	0.59	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	cM	0.45	0/244	0.59	0/332
12	aX	0.53	0/242	0.45	0/332
12	bX	0.53	0/242	0.45	0/332
12	cX	0.53	0/242	0.45	0/332
13	a1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	a2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	a3	0.49	2/2695 (0.1%)	0.69	5/3680 (0.1%)
13	a4	0.48	1/2731 (0.0%)	0.71	6/3730 (0.2%)
13	a5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	a6	0.46	1/2671 (0.0%)	0.72	8/3647 (0.2%)
13	b1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	b2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	b3	0.48	2/2695 (0.1%)	0.68	4/3680 (0.1%)
13	b4	0.48	2/2731 (0.1%)	0.71	6/3730 (0.2%)
13	b5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	b6	0.46	1/2671 (0.0%)	0.72	8/3647 (0.2%)
13	c1	0.47	1/2671 (0.0%)	0.68	4/3647 (0.1%)
13	c2	0.46	1/2653 (0.0%)	0.69	4/3624 (0.1%)
13	c3	0.49	2/2695 (0.1%)	0.69	4/3680 (0.1%)
13	c4	0.48	2/2731 (0.1%)	0.71	6/3730 (0.2%)
13	c5	0.47	1/2695 (0.0%)	0.73	7/3680 (0.2%)
13	c6	0.46	1/2671 (0.0%)	0.71	8/3647 (0.2%)
All	All	0.52	29/102183 (0.0%)	0.63	103/139401 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
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 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a1	297	ILE	CB-CG2	-7.19	1.30	1.52
13	b1	297	ILE	CB-CG2	-7.19	1.30	1.52
13	c4	297	ILE	CB-CG2	-7.18	1.30	1.52
13	a4	297	ILE	CB-CG2	-7.16	1.30	1.52
13	b4	297	ILE	CB-CG2	-7.16	1.30	1.52

The worst 5 of 103 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a6	128	ARG	NE-CZ-NH1	-10.78	114.91	120.30
13	b6	128	ARG	NE-CZ-NH1	-10.05	115.28	120.30
13	c5	295	LEU	CA-CB-CG	9.71	137.64	115.30
13	b5	295	LEU	CA-CB-CG	9.67	137.54	115.30
13	a5	295	LEU	CA-CB-CG	9.58	137.32	115.30

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	0	0
1	bA	5801	0	5660	0	0
1	cA	5801	0	5660	0	0
2	aB	5879	0	5627	0	0
2	bB	5879	0	5627	0	0
2	cB	5879	0	5627	0	0
3	aC	598	0	580	0	0
3	bC	598	0	580	0	0
3	cC	598	0	580	0	0
4	aD	1075	0	1077	0	0
4	bD	1075	0	1077	0	0
4	cD	1075	0	1077	0	0
5	aE	539	0	528	0	0
5	bE	539	0	528	0	0
5	cE	539	0	528	0	0
6	aF	1065	0	1077	0	0
6	bF	1065	0	1077	0	0
6	cF	1065	0	1077	0	0
7	aI	301	0	306	0	0
7	bI	301	0	306	0	0
7	cI	301	0	306	0	0
8	aJ	338	0	347	0	0
8	bJ	338	0	347	0	0
8	cJ	338	0	347	0	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	0	0
10	bL	1119	0	1125	0	0
10	cL	1119	0	1125	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	aM	241	0	264	0	0
11	bM	241	0	264	0	0
11	cM	241	0	264	0	0
12	aX	233	0	231	0	0
12	bX	233	0	231	0	0
12	cX	233	0	231	0	0
13	a1	2583	0	2568	0	0
13	a2	2565	0	2545	0	0
13	a3	2607	0	2590	0	0
13	a4	2641	0	2624	0	0
13	a5	2607	0	2591	0	0
13	a6	2583	0	2567	0	0
13	b1	2583	0	2568	0	0
13	b2	2565	0	2545	0	0
13	b3	2607	0	2590	0	0
13	b4	2641	0	2624	0	0
13	b5	2607	0	2591	0	0
13	b6	2583	0	2567	0	0
13	c1	2583	0	2568	0	0
13	c2	2565	0	2545	0	0
13	c3	2607	0	2590	0	0
13	c4	2641	0	2624	0	0
13	c5	2607	0	2591	0	0
13	c6	2583	0	2567	0	0
14	aA	65	0	72	0	0
14	bA	65	0	72	0	0
14	cA	65	0	72	0	0
15	a1	895	0	790	0	0
15	a2	960	0	862	0	0
15	a3	895	0	790	0	0
15	a4	895	0	792	0	0
15	a5	895	0	792	0	0
15	a6	895	0	790	0	0
15	aA	2557	0	2532	0	0
15	aB	2414	0	2369	0	0
15	aJ	127	0	91	0	0
15	aK	45	0	33	0	0
15	aL	195	0	216	0	0
15	aX	45	0	33	0	0
15	b1	830	0	720	0	0
15	b2	960	0	862	0	0
15	b3	895	0	790	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	b4	895	0	792	0	0
15	b5	895	0	792	0	0
15	b6	895	0	790	0	0
15	bA	2557	0	2532	0	0
15	bB	2414	0	2369	0	0
15	bF	45	0	33	0	0
15	bJ	82	0	58	0	0
15	bK	45	0	33	0	0
15	bL	195	0	216	0	0
15	bX	45	0	33	0	0
15	c1	830	0	720	0	0
15	c2	960	0	862	0	0
15	c3	895	0	790	0	0
15	c4	895	0	792	0	0
15	c5	895	0	792	0	0
15	c6	830	0	720	0	0
15	cA	2506	0	2491	0	0
15	cB	2414	0	2369	0	0
15	cF	96	0	74	0	0
15	cJ	82	0	58	0	0
15	cK	45	0	33	0	0
15	cL	195	0	216	0	0
15	cX	45	0	33	0	0
16	aA	33	0	46	0	0
16	aB	33	0	46	0	0
16	bA	33	0	46	0	0
16	bB	33	0	46	0	0
16	cA	33	0	46	0	0
16	cB	33	0	46	0	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	0	0
18	a2	160	0	224	0	0
18	a3	160	0	224	0	0
18	a4	160	0	224	0	0
18	a5	120	0	168	0	0
18	a6	200	0	280	0	0
18	aA	200	0	278	0	0

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	cB	55	0	86	0	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	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	aA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	70
1	bA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	70
1	cA	738/755 (98%)	703 (95%)	34 (5%)	1 (0%)	48	70
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	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	bC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	7
3	cC	78/80 (98%)	72 (92%)	4 (5%)	2 (3%)	4	7
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
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%)	22	37
13	a2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	a3	330/358 (92%)	303 (92%)	24 (7%)	3 (1%)	14	27
13	a4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	27
13	a5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	22	37
13	a6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	27
13	b1	327/358 (91%)	299 (91%)	26 (8%)	2 (1%)	22	37
13	b2	325/358 (91%)	297 (91%)	25 (8%)	3 (1%)	14	27
13	b3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	27
13	b4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	27
13	b5	330/358 (92%)	303 (92%)	25 (8%)	2 (1%)	22	37
13	b6	327/358 (91%)	299 (91%)	25 (8%)	3 (1%)	14	27
13	c1	327/358 (91%)	300 (92%)	25 (8%)	2 (1%)	22	37
13	c2	325/358 (91%)	298 (92%)	24 (7%)	3 (1%)	14	27
13	c3	330/358 (92%)	301 (91%)	26 (8%)	3 (1%)	14	27
13	c4	334/358 (93%)	305 (91%)	26 (8%)	3 (1%)	14	27
13	c5	330/358 (92%)	302 (92%)	26 (8%)	2 (1%)	22	37
13	c6	327/358 (91%)	298 (91%)	26 (8%)	3 (1%)	14	27
All	All	12561/13452 (93%)	11740 (94%)	764 (6%)	57 (0%)	27	41

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%)	558 (94%)	34 (6%)	17	31
1	bA	592/604 (98%)	558 (94%)	34 (6%)	17	31
1	cA	592/604 (98%)	558 (94%)	34 (6%)	17	31
2	aB	595/597 (100%)	568 (96%)	27 (4%)	23	41
2	bB	595/597 (100%)	568 (96%)	27 (4%)	23	41
2	cB	595/597 (100%)	568 (96%)	27 (4%)	23	41
3	aC	67/67 (100%)	60 (90%)	7 (10%)	5	10
3	bC	67/67 (100%)	60 (90%)	7 (10%)	5	10
3	cC	67/67 (100%)	60 (90%)	7 (10%)	5	10
4	aD	115/115 (100%)	107 (93%)	8 (7%)	12	22
4	bD	115/115 (100%)	107 (93%)	8 (7%)	12	22
4	cD	115/115 (100%)	107 (93%)	8 (7%)	12	22
5	aE	59/64 (92%)	53 (90%)	6 (10%)	6	11
5	bE	59/64 (92%)	53 (90%)	6 (10%)	6	11
5	cE	59/64 (92%)	53 (90%)	6 (10%)	6	11
6	aF	109/128 (85%)	103 (94%)	6 (6%)	18	32
6	bF	109/128 (85%)	103 (94%)	6 (6%)	18	32
6	cF	109/128 (85%)	103 (94%)	6 (6%)	18	32
7	aI	32/32 (100%)	30 (94%)	2 (6%)	15	27
7	bI	32/32 (100%)	30 (94%)	2 (6%)	15	27
7	cI	32/32 (100%)	30 (94%)	2 (6%)	15	27
8	aJ	36/36 (100%)	33 (92%)	3 (8%)	9	17
8	bJ	36/36 (100%)	33 (92%)	3 (8%)	9	17
8	cJ	36/36 (100%)	33 (92%)	3 (8%)	9	17
10	aL	117/119 (98%)	113 (97%)	4 (3%)	32	53
10	bL	117/119 (98%)	113 (97%)	4 (3%)	32	53
10	cL	117/119 (98%)	113 (97%)	4 (3%)	32	53
11	aM	26/26 (100%)	21 (81%)	5 (19%)	1	1
11	bM	26/26 (100%)	21 (81%)	5 (19%)	1	1
11	cM	26/26 (100%)	21 (81%)	5 (19%)	1	1
12	aX	20/24 (83%)	19 (95%)	1 (5%)	20	37
12	bX	20/24 (83%)	19 (95%)	1 (5%)	20	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	cX	20/24 (83%)	19 (95%)	1 (5%)	20	37
13	a1	255/279 (91%)	237 (93%)	18 (7%)	12	22
13	a2	253/279 (91%)	237 (94%)	16 (6%)	15	27
13	a3	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	a4	262/279 (94%)	247 (94%)	15 (6%)	17	31
13	a5	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	a6	255/279 (91%)	238 (93%)	17 (7%)	13	24
13	b1	255/279 (91%)	237 (93%)	18 (7%)	12	22
13	b2	253/279 (91%)	237 (94%)	16 (6%)	15	27
13	b3	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	b4	262/279 (94%)	247 (94%)	15 (6%)	17	31
13	b5	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	b6	255/279 (91%)	238 (93%)	17 (7%)	13	24
13	c1	255/279 (91%)	238 (93%)	17 (7%)	13	24
13	c2	253/279 (91%)	237 (94%)	16 (6%)	15	27
13	c3	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	c4	262/279 (94%)	247 (94%)	15 (6%)	17	31
13	c5	258/279 (92%)	241 (93%)	17 (7%)	14	25
13	c6	255/279 (91%)	240 (94%)	15 (6%)	16	29
All	All	9927/10458 (95%)	9321 (94%)	606 (6%)	18	28

5 of 606 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	cB	583	TYR
13	c4	304	THR
4	cD	75	ARG
2	cB	582	PHE
13	c1	212	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
5	bE	18	ASN

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Mol	Chain	Res	Type
13	b6	320	ASN
13	c2	320	ASN
10	bL	16	HIS
13	b3	320	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	$\# Z > 2$
15	CLA	b6	405	-	63,73,73	1.34	7 (11%)	74,113,113	1.46	9 (12%)
18	BCR	b4	418	-	41,41,41	1.47	6 (14%)	56,56,56	1.60	8 (14%)
15	CLA	a5	406	-	43,53,73	1.56	6 (13%)	50,89,113	1.70	8 (16%)
15	CLA	c6	416	-	43,53,73	1.64	7 (16%)	50,89,113	2.07	10 (20%)
15	CLA	b3	412	-	43,53,73	1.55	9 (20%)	50,89,113	1.75	14 (28%)
15	CLA	a1	410	13	43,53,73	1.54	7 (16%)	50,89,113	1.90	8 (16%)
15	CLA	c5	420	-	63,73,73	1.38	9 (14%)	74,113,113	1.98	18 (24%)
18	BCR	b6	402	-	41,41,41	1.22	4 (9%)	56,56,56	1.72	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b2	410	-	63,73,73	1.35	5 (7%)	74,113,113	1.46	9 (12%)
18	BCR	c4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.42	8 (14%)
15	CLA	cB	801	-	63,73,73	1.33	9 (14%)	74,113,113	1.50	9 (12%)
15	CLA	aA	815	-	43,53,73	1.52	8 (18%)	50,89,113	1.64	8 (16%)
15	CLA	a5	415	-	43,53,73	1.60	8 (18%)	50,89,113	2.08	10 (20%)
15	CLA	cX	102	12	43,53,73	1.50	8 (18%)	50,89,113	1.84	12 (24%)
15	CLA	cA	824	-	49,59,73	1.39	8 (16%)	56,96,113	1.60	7 (12%)
15	CLA	a4	407	-	43,53,73	1.57	7 (16%)	50,89,113	1.72	8 (16%)
15	CLA	b6	403	-	63,73,73	1.35	6 (9%)	74,113,113	1.48	8 (10%)
18	BCR	a1	418	-	41,41,41	1.24	4 (9%)	56,56,56	1.64	12 (21%)
18	BCR	b6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	bA	810	1	63,73,73	1.34	8 (12%)	74,113,113	1.57	9 (12%)
15	CLA	c4	405	-	43,53,73	1.64	9 (20%)	50,89,113	2.13	21 (42%)
18	BCR	b1	420	-	41,41,41	1.21	4 (9%)	56,56,56	1.47	11 (19%)
15	CLA	cB	803	-	63,73,73	1.23	7 (11%)	74,113,113	1.69	14 (18%)
15	CLA	b4	409	-	63,73,73	1.34	6 (9%)	74,113,113	1.44	9 (12%)
18	BCR	bJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.46	7 (12%)
15	CLA	b5	408	-	43,53,73	1.49	7 (16%)	50,89,113	1.85	8 (16%)
15	CLA	b2	411	13	62,72,73	1.32	8 (12%)	72,111,113	1.70	14 (19%)
15	CLA	cA	813	-	52,62,73	1.36	8 (15%)	60,99,113	1.55	10 (16%)
15	CLA	aL	201	10	63,73,73	1.29	8 (12%)	74,113,113	1.34	8 (10%)
15	CLA	aA	835	-	63,73,73	1.33	9 (14%)	74,113,113	1.64	10 (13%)
15	CLA	b1	404	-	63,73,73	1.33	8 (12%)	74,113,113	1.47	9 (12%)
15	CLA	b4	402	-	63,73,73	1.31	6 (9%)	74,113,113	1.50	9 (12%)
15	CLA	b5	402	-	63,73,73	1.32	6 (9%)	74,113,113	1.50	7 (9%)
15	CLA	a6	411	13	62,72,73	1.32	7 (11%)	72,111,113	1.69	14 (19%)
15	CLA	cB	805	-	52,62,73	1.36	8 (15%)	60,99,113	1.67	7 (11%)
15	CLA	a6	408	-	43,53,73	1.58	6 (13%)	50,89,113	1.73	8 (16%)
15	CLA	c1	405	-	43,53,73	1.67	8 (18%)	50,89,113	2.06	20 (40%)
15	CLA	c5	406	-	43,53,73	1.57	6 (13%)	50,89,113	1.70	8 (16%)
15	CLA	c5	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.15	9 (14%)
15	CLA	bA	833	-	63,73,73	1.24	8 (12%)	74,113,113	1.49	7 (9%)
19	LHG	cA	852	-	48,48,48	0.98	2 (4%)	51,54,54	1.37	7 (13%)
15	CLA	cA	827	22	63,73,73	1.26	8 (12%)	74,113,113	1.62	11 (14%)
15	CLA	b4	414	-	39,49,73	1.64	8 (20%)	46,84,113	1.77	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b2	422	-	63,73,73	1.41	8 (12%)	74,113,113	1.90	18 (24%)
15	CLA	aA	819	-	52,62,73	1.39	8 (15%)	60,99,113	1.69	10 (16%)
15	CLA	b5	410	13	62,72,73	1.33	8 (12%)	72,111,113	1.73	14 (19%)
15	CLA	aB	804	-	63,73,73	1.34	7 (11%)	74,113,113	2.06	17 (22%)
15	CLA	b4	413	-	43,53,73	1.60	7 (16%)	50,89,113	1.60	4 (8%)
18	BCR	a2	421	-	41,41,41	1.18	2 (4%)	56,56,56	1.43	8 (14%)
15	CLA	aA	837	1	43,53,73	1.56	7 (16%)	50,89,113	1.75	9 (18%)
15	CLA	aB	824	-	43,53,73	1.52	7 (16%)	50,89,113	1.63	10 (20%)
15	CLA	a1	402	-	63,73,73	1.27	6 (9%)	74,113,113	1.58	9 (12%)
15	CLA	bA	816	-	43,53,73	1.54	7 (16%)	50,89,113	1.89	6 (12%)
15	CLA	bA	820	-	63,73,73	1.24	8 (12%)	74,113,113	1.69	10 (13%)
15	CLA	c5	405	-	43,53,73	1.66	7 (16%)	50,89,113	2.14	21 (42%)
15	CLA	c5	411	13	43,53,73	1.51	7 (16%)	50,89,113	1.90	8 (16%)
15	CLA	a4	416	-	48,58,73	1.51	8 (16%)	56,95,113	2.56	16 (28%)
18	BCR	a3	418	-	41,41,41	1.47	6 (14%)	56,56,56	1.59	9 (16%)
15	CLA	c5	415	-	43,53,73	1.60	7 (16%)	50,89,113	2.07	10 (20%)
15	CLA	a4	404	-	63,73,73	1.32	7 (11%)	74,113,113	1.44	8 (10%)
15	CLA	cB	815	-	63,73,73	1.30	7 (11%)	74,113,113	1.53	8 (10%)
15	CLA	c1	408	-	43,53,73	1.49	7 (16%)	50,89,113	1.82	8 (16%)
18	BCR	bA	853	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	6 (10%)
15	CLA	cB	804	-	63,73,73	1.35	7 (11%)	74,113,113	2.07	17 (22%)
15	CLA	c2	409	-	43,53,73	1.51	7 (16%)	50,89,113	1.80	9 (18%)
15	CLA	aB	815	-	63,73,73	1.31	7 (11%)	74,113,113	1.53	8 (10%)
15	CLA	a1	401	-	63,73,73	1.33	6 (9%)	74,113,113	1.48	7 (9%)
15	CLA	aA	825	-	57,67,73	1.32	8 (14%)	66,105,113	1.49	8 (12%)
15	CLA	cB	826	22	44,54,73	1.40	8 (18%)	51,90,113	1.98	11 (21%)
15	CLA	a6	409	-	43,53,73	1.52	7 (16%)	50,89,113	1.86	7 (14%)
18	BCR	c3	418	-	41,41,41	1.47	6 (14%)	56,56,56	1.58	9 (16%)
15	CLA	aA	803	-	63,73,73	1.34	8 (12%)	74,113,113	1.92	15 (20%)
15	CLA	c2	402	-	63,73,73	1.32	5 (7%)	74,113,113	1.49	7 (9%)
18	BCR	a1	419	-	41,41,41	1.20	3 (7%)	56,56,56	1.46	11 (19%)
15	CLA	aA	841	-	63,73,73	1.27	7 (11%)	74,113,113	1.46	8 (10%)
15	CLA	aA	842	22	49,59,73	1.57	8 (16%)	56,96,113	1.44	9 (16%)
15	CLA	aA	829	-	63,73,73	1.29	8 (12%)	74,113,113	1.66	12 (16%)
19	LHG	aX	101	-	22,22,48	0.90	1 (4%)	25,28,54	1.21	2 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c2	416	-	43,53,73	1.58	8 (18%)	50,89,113	2.05	10 (20%)
15	CLA	c1	404	-	63,73,73	1.32	7 (11%)	74,113,113	1.46	9 (12%)
15	CLA	b2	409	-	43,53,73	1.50	7 (16%)	50,89,113	1.81	9 (18%)
15	CLA	a3	421	-	63,73,73	1.48	9 (14%)	74,113,113	1.69	15 (20%)
15	CLA	b2	418	13	53,63,73	1.45	4 (7%)	62,101,113	2.12	11 (17%)
15	CLA	cA	834	-	63,73,73	1.29	10 (15%)	74,113,113	1.70	10 (13%)
18	BCR	aI	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.30	6 (10%)
15	CLA	bA	819	-	52,62,73	1.39	8 (15%)	60,99,113	1.69	10 (16%)
18	BCR	b3	418	-	41,41,41	1.46	6 (14%)	56,56,56	1.59	9 (16%)
15	CLA	a3	414	-	39,49,73	1.59	8 (20%)	46,84,113	1.80	7 (15%)
18	BCR	cA	850	-	41,41,41	1.37	5 (12%)	56,56,56	1.36	8 (14%)
15	CLA	bB	822	-	43,53,73	1.53	5 (11%)	50,89,113	1.83	6 (12%)
19	LHG	bA	855	15	26,26,48	1.00	2 (7%)	29,32,54	1.39	3 (10%)
15	CLA	aB	835	-	43,53,73	1.51	8 (18%)	50,89,113	1.87	8 (16%)
15	CLA	c2	414	-	43,53,73	1.60	8 (18%)	50,89,113	1.62	4 (8%)
18	BCR	aA	852	-	41,41,41	1.22	3 (7%)	56,56,56	1.40	6 (10%)
15	CLA	aB	836	-	58,68,73	1.33	8 (13%)	68,107,113	1.57	11 (16%)
15	CLA	aB	811	2	63,73,73	1.41	10 (15%)	74,113,113	1.71	11 (14%)
15	CLA	a6	414	-	43,53,73	1.63	9 (20%)	50,89,113	1.79	11 (22%)
15	CLA	a2	418	13	53,63,73	1.43	4 (7%)	62,101,113	2.12	11 (17%)
15	CLA	b4	408	-	43,53,73	1.47	7 (16%)	50,89,113	1.83	9 (18%)
15	CLA	c1	409	-	63,73,73	1.36	5 (7%)	74,113,113	1.41	7 (9%)
15	CLA	cA	820	-	63,73,73	1.24	8 (12%)	74,113,113	1.69	10 (13%)
15	CLA	a5	410	13	62,72,73	1.33	7 (11%)	72,111,113	1.74	14 (19%)
15	CLA	bA	804	-	63,73,73	1.29	8 (12%)	74,113,113	1.57	11 (14%)
18	BCR	cI	101	-	41,41,41	1.25	4 (9%)	56,56,56	1.29	6 (10%)
15	CLA	aB	819	-	58,68,73	1.27	9 (15%)	68,107,113	1.75	9 (13%)
18	BCR	c3	401	-	41,41,41	1.27	4 (9%)	56,56,56	1.68	10 (17%)
15	CLA	bA	817	-	47,57,73	1.47	6 (12%)	53,93,113	1.60	6 (11%)
15	CLA	a3	416	-	48,58,73	1.53	8 (16%)	56,95,113	2.53	18 (32%)
18	BCR	b3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.42	8 (14%)
15	CLA	c4	408	-	43,53,73	1.48	7 (16%)	50,89,113	1.82	8 (16%)
18	BCR	aM	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	9 (16%)
15	CLA	bA	845	19	50,60,73	1.48	8 (16%)	57,97,113	2.20	15 (26%)
15	CLA	c1	414	-	39,49,73	1.66	6 (15%)	46,84,113	1.78	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	a4	420	-	41,41,41	1.18	4 (9%)	56,56,56	1.45	10 (17%)
15	CLA	c2	413	-	43,53,73	1.57	9 (20%)	50,89,113	1.75	14 (28%)
15	CLA	bB	829	-	63,73,73	1.25	9 (14%)	74,113,113	1.51	8 (10%)
15	CLA	c2	418	13	53,63,73	1.43	4 (7%)	62,101,113	2.13	10 (16%)
15	CLA	a6	413	-	43,53,73	1.60	9 (20%)	50,89,113	1.74	13 (26%)
15	CLA	bF	201	-	43,53,73	1.52	9 (20%)	50,89,113	1.85	10 (20%)
18	BCR	a1	421	-	41,41,41	1.09	4 (9%)	56,56,56	1.61	9 (16%)
15	CLA	bB	827	-	63,73,73	1.33	8 (12%)	74,113,113	1.69	12 (16%)
15	CLA	aA	823	-	47,57,73	1.46	7 (14%)	53,93,113	1.60	7 (13%)
18	BCR	cB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.60	9 (27%)
15	CLA	b5	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.14	9 (14%)
15	CLA	aB	842	-	43,53,73	1.60	7 (16%)	50,89,113	1.57	5 (10%)
15	CLA	cA	819	-	52,62,73	1.39	8 (15%)	60,99,113	1.70	10 (16%)
15	CLA	a4	410	13	62,72,73	1.33	8 (12%)	72,111,113	1.71	14 (19%)
15	CLA	c5	402	-	63,73,73	1.32	6 (9%)	74,113,113	1.49	7 (9%)
18	BCR	a6	419	-	41,41,41	1.40	6 (14%)	56,56,56	1.56	10 (17%)
15	CLA	cB	813	-	43,53,73	1.55	8 (18%)	50,89,113	1.77	6 (12%)
18	BCR	aB	845	-	41,41,41	1.13	4 (9%)	56,56,56	1.30	6 (10%)
18	BCR	c2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.47	8 (14%)
15	CLA	aB	840	-	63,73,73	1.37	9 (14%)	74,113,113	1.75	11 (14%)
15	CLA	cB	832	-	47,57,73	1.43	9 (19%)	53,93,113	1.72	7 (13%)
18	BCR	b5	418	-	41,41,41	1.41	6 (14%)	56,56,56	1.58	10 (17%)
15	CLA	cK	102	-	43,53,73	1.51	7 (16%)	50,89,113	1.66	10 (20%)
15	CLA	c1	413	-	43,53,73	1.60	7 (16%)	50,89,113	1.56	4 (8%)
18	BCR	aB	844	-	41,41,41	1.20	4 (9%)	56,56,56	1.43	7 (12%)
15	CLA	c5	410	13	62,72,73	1.33	8 (12%)	72,111,113	1.75	14 (19%)
15	CLA	bB	813	-	43,53,73	1.55	8 (18%)	50,89,113	1.77	6 (12%)
15	CLA	b3	415	-	43,53,73	1.60	9 (20%)	50,89,113	2.06	9 (18%)
15	CLA	c5	408	-	43,53,73	1.49	7 (16%)	50,89,113	1.83	8 (16%)
18	BCR	bA	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.42	9 (16%)
18	BCR	aK	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	c4	407	-	43,53,73	1.58	7 (16%)	50,89,113	1.73	8 (16%)
15	CLA	bB	818	-	57,67,73	1.35	7 (12%)	66,105,113	1.66	11 (16%)
15	CLA	cA	841	-	63,73,73	1.28	7 (11%)	74,113,113	1.47	8 (10%)
15	CLA	aA	831	-	63,73,73	1.35	8 (12%)	74,113,113	1.65	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aA	820	-	63,73,73	1.25	8 (12%)	74,113,113	1.69	9 (12%)
15	CLA	aA	840	-	45,55,73	1.51	9 (20%)	52,91,113	2.04	9 (17%)
15	CLA	b4	412	-	43,53,73	1.58	9 (20%)	50,89,113	1.74	14 (28%)
15	CLA	a6	415	-	39,49,73	1.65	6 (15%)	46,84,113	1.76	7 (15%)
15	CLA	aB	822	-	43,53,73	1.54	5 (11%)	50,89,113	1.83	6 (12%)
18	BCR	b4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.53	11 (19%)
15	CLA	c1	416	-	48,58,73	1.52	9 (18%)	56,95,113	2.56	17 (30%)
18	BCR	b5	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.54	12 (21%)
18	BCR	cA	849	-	41,41,41	1.17	3 (7%)	56,56,56	1.45	9 (16%)
15	CLA	aA	818	-	52,62,73	1.36	7 (13%)	60,99,113	1.79	7 (11%)
15	CLA	bA	834	-	63,73,73	1.29	10 (15%)	74,113,113	1.70	10 (13%)
15	CLA	bA	809	1	63,73,73	1.30	8 (12%)	74,113,113	1.57	10 (13%)
15	CLA	cB	822	-	43,53,73	1.53	5 (11%)	50,89,113	1.83	6 (12%)
15	CLA	cB	828	-	63,73,73	1.31	9 (14%)	74,113,113	1.70	8 (10%)
15	CLA	aA	813	-	52,62,73	1.36	8 (15%)	60,99,113	1.55	10 (16%)
15	CLA	cL	202	-	63,73,73	1.21	8 (12%)	74,113,113	1.71	10 (13%)
15	CLA	b3	405	-	43,53,73	1.64	9 (20%)	50,89,113	2.09	20 (40%)
15	CLA	b1	413	-	43,53,73	1.61	7 (16%)	50,89,113	1.54	4 (8%)
15	CLA	a2	422	-	63,73,73	1.41	8 (12%)	74,113,113	1.90	18 (24%)
15	CLA	cA	831	-	63,73,73	1.35	8 (12%)	74,113,113	1.65	9 (12%)
18	BCR	c1	401	-	41,41,41	1.15	3 (7%)	56,56,56	1.56	9 (16%)
19	LHG	cA	853	15	26,26,48	1.00	2 (7%)	29,32,54	1.39	3 (10%)
15	CLA	a4	411	13	43,53,73	1.53	6 (13%)	50,89,113	1.90	7 (14%)
15	CLA	bB	831	-	43,53,73	1.62	9 (20%)	50,89,113	1.66	6 (12%)
18	BCR	cA	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.43	9 (16%)
18	BCR	aJ	205	-	41,41,41	1.32	4 (9%)	56,56,56	1.46	7 (12%)
18	BCR	c4	418	-	41,41,41	1.45	6 (14%)	56,56,56	1.60	9 (16%)
18	BCR	b1	419	-	41,41,41	1.24	4 (9%)	56,56,56	1.65	12 (21%)
18	BCR	cB	845	-	41,41,41	1.12	4 (9%)	56,56,56	1.31	7 (12%)
15	CLA	c2	408	-	43,53,73	1.58	7 (16%)	50,89,113	1.67	9 (18%)
18	BCR	bB	846	-	41,41,41	1.22	3 (7%)	56,56,56	1.38	8 (14%)
15	CLA	aB	833	-	63,73,73	1.22	7 (11%)	74,113,113	1.47	11 (14%)
15	CLA	aA	812	-	63,73,73	1.27	9 (14%)	74,113,113	1.44	8 (10%)
15	CLA	c3	416	-	48,58,73	1.52	8 (16%)	56,95,113	2.53	18 (32%)
15	CLA	cA	805	-	57,67,73	1.35	9 (15%)	66,105,113	1.72	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	c2	421	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	8 (14%)
18	BCR	bL	205	-	41,41,41	1.32	4 (9%)	56,56,56	1.47	9 (16%)
15	CLA	c6	412	13	43,53,73	1.52	7 (16%)	50,89,113	1.90	9 (18%)
15	CLA	cA	842	-	63,73,73	1.31	7 (11%)	74,113,113	1.59	9 (12%)
18	BCR	c2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.85	14 (25%)
15	CLA	b2	416	-	43,53,73	1.58	8 (18%)	50,89,113	2.04	10 (20%)
15	CLA	cA	830	-	63,73,73	1.24	9 (14%)	74,113,113	1.67	10 (13%)
15	CLA	c3	407	-	43,53,73	1.55	7 (16%)	50,89,113	1.73	8 (16%)
15	CLA	cB	816	-	43,53,73	1.53	8 (18%)	50,89,113	1.97	7 (14%)
15	CLA	cL	201	10	63,73,73	1.29	8 (12%)	74,113,113	1.34	8 (10%)
18	BCR	a6	402	-	41,41,41	1.23	4 (9%)	56,56,56	1.73	14 (25%)
18	BCR	c1	418	-	41,41,41	1.40	6 (14%)	56,56,56	1.58	11 (19%)
15	CLA	a2	403	-	63,73,73	1.28	6 (9%)	74,113,113	1.57	9 (12%)
15	CLA	cA	804	-	63,73,73	1.28	8 (12%)	74,113,113	1.57	11 (14%)
15	CLA	bA	832	-	48,58,73	1.46	9 (18%)	56,95,113	1.81	9 (16%)
15	CLA	a3	412	-	43,53,73	1.56	9 (20%)	50,89,113	1.76	14 (28%)
15	CLA	bB	842	-	43,53,73	1.61	7 (16%)	50,89,113	1.57	5 (10%)
15	CLA	bA	824	-	49,59,73	1.40	8 (16%)	56,96,113	1.61	7 (12%)
15	CLA	cF	201	22	49,59,73	1.56	8 (16%)	56,96,113	1.44	9 (16%)
15	CLA	a2	412	13	43,53,73	1.55	8 (18%)	50,89,113	1.92	8 (16%)
15	CLA	c6	406	-	43,53,73	1.70	6 (13%)	50,89,113	2.10	19 (38%)
15	CLA	b2	414	-	43,53,73	1.60	8 (18%)	50,89,113	1.63	4 (8%)
15	CLA	b2	408	-	43,53,73	1.56	7 (16%)	50,89,113	1.70	9 (18%)
15	CLA	b1	417	13	53,63,73	1.43	5 (9%)	62,101,113	2.15	10 (16%)
15	CLA	a2	410	-	63,73,73	1.34	5 (7%)	74,113,113	1.46	9 (12%)
15	CLA	a6	417	-	48,58,73	1.51	7 (14%)	56,95,113	2.57	18 (32%)
15	CLA	aB	828	-	63,73,73	1.30	9 (14%)	74,113,113	1.69	8 (10%)
18	BCR	aA	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.45	9 (16%)
18	BCR	bL	201	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	9 (16%)
18	BCR	b2	421	-	41,41,41	1.17	2 (4%)	56,56,56	1.42	8 (14%)
15	CLA	b2	402	-	63,73,73	1.33	5 (7%)	74,113,113	1.48	7 (9%)
15	CLA	c4	421	-	63,73,73	1.43	11 (17%)	74,113,113	1.78	16 (21%)
15	CLA	aA	839	-	63,73,73	1.29	9 (14%)	74,113,113	1.55	9 (12%)
18	BCR	cF	202	-	41,41,41	1.33	5 (12%)	56,56,56	1.41	10 (17%)
15	CLA	b5	413	-	43,53,73	1.61	8 (18%)	50,89,113	1.61	4 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c4	414	-	39,49,73	1.63	8 (20%)	46,84,113	1.77	7 (15%)
16	PQN	cA	845	-	34,34,34	1.43	2 (5%)	43,45,45	1.19	6 (13%)
15	CLA	aA	828	-	63,73,73	1.32	8 (12%)	74,113,113	1.41	8 (10%)
18	BCR	a3	420	-	41,41,41	1.20	3 (7%)	56,56,56	1.45	10 (17%)
18	BCR	a2	401	-	41,41,41	1.25	4 (9%)	56,56,56	1.85	13 (23%)
15	CLA	bB	810	2	63,73,73	1.41	10 (15%)	74,113,113	1.68	12 (16%)
15	CLA	cB	842	-	43,53,73	1.62	7 (16%)	50,89,113	1.56	5 (10%)
15	CLA	a4	403	-	63,73,73	1.28	6 (9%)	74,113,113	1.54	9 (12%)
15	CLA	bB	801	-	63,73,73	1.33	9 (14%)	74,113,113	1.50	9 (12%)
15	CLA	c3	404	-	63,73,73	1.32	8 (12%)	74,113,113	1.46	9 (12%)
18	BCR	c3	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	b5	409	-	63,73,73	1.34	6 (9%)	74,113,113	1.43	8 (10%)
15	CLA	b3	406	-	43,53,73	1.55	6 (13%)	50,89,113	1.69	7 (14%)
15	CLA	b1	408	-	43,53,73	1.48	6 (13%)	50,89,113	1.83	8 (16%)
18	BCR	aI	103	-	41,41,41	1.32	4 (9%)	56,56,56	1.47	9 (16%)
15	CLA	c5	403	-	63,73,73	1.26	6 (9%)	74,113,113	1.58	10 (13%)
18	BCR	cK	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.42	10 (17%)
18	BCR	c5	401	-	41,41,41	1.20	4 (9%)	56,56,56	1.55	12 (21%)
15	CLA	aB	830	-	63,73,73	1.33	8 (12%)	74,113,113	1.86	11 (14%)
15	CLA	b4	416	-	48,58,73	1.52	8 (16%)	56,95,113	2.56	16 (28%)
15	CLA	bB	821	-	45,55,73	1.48	8 (17%)	52,91,113	1.59	6 (11%)
15	CLA	b5	416	-	48,58,73	1.48	8 (16%)	56,95,113	2.56	17 (30%)
15	CLA	b3	408	-	43,53,73	1.46	7 (16%)	50,89,113	1.82	10 (20%)
15	CLA	bB	839	22	63,73,73	1.29	8 (12%)	74,113,113	1.54	10 (13%)
15	CLA	b5	404	-	63,73,73	1.32	7 (11%)	74,113,113	1.46	9 (12%)
15	CLA	c4	409	-	63,73,73	1.36	5 (7%)	74,113,113	1.45	9 (12%)
15	CLA	aA	808	-	49,59,73	1.44	7 (14%)	56,96,113	1.65	8 (14%)
15	CLA	a2	406	-	63,73,73	1.47	9 (14%)	74,113,113	2.02	19 (25%)
15	CLA	b4	407	-	43,53,73	1.57	7 (16%)	50,89,113	1.72	8 (16%)
15	CLA	b1	405	-	43,53,73	1.66	7 (16%)	50,89,113	2.07	22 (44%)
18	BCR	a6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.54	10 (17%)
15	CLA	c6	405	-	63,73,73	1.33	7 (11%)	74,113,113	1.47	9 (12%)
15	CLA	b5	407	-	43,53,73	1.59	6 (13%)	50,89,113	1.73	9 (18%)
15	CLA	b1	406	-	43,53,73	1.59	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	b1	415	-	43,53,73	1.62	8 (18%)	50,89,113	2.04	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b5	405	-	43,53,73	1.65	7 (16%)	50,89,113	2.14	21 (42%)
15	CLA	a1	404	-	43,53,73	1.65	7 (16%)	50,89,113	2.07	20 (40%)
15	CLA	a2	417	-	48,58,73	1.50	8 (16%)	56,95,113	2.66	20 (35%)
15	CLA	cA	826	-	63,73,73	1.27	7 (11%)	74,113,113	1.65	10 (13%)
15	CLA	aL	202	-	63,73,73	1.21	8 (12%)	74,113,113	1.72	10 (13%)
18	BCR	cB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.53	9 (16%)
18	BCR	c5	418	-	41,41,41	1.41	6 (14%)	56,56,56	1.57	9 (16%)
15	CLA	c4	402	-	63,73,73	1.30	6 (9%)	74,113,113	1.51	9 (12%)
15	CLA	bB	811	2	63,73,73	1.41	10 (15%)	74,113,113	1.72	11 (14%)
15	CLA	bB	806	-	63,73,73	1.26	10 (15%)	74,113,113	1.66	8 (10%)
15	CLA	c2	406	-	63,73,73	1.46	9 (14%)	74,113,113	2.01	19 (25%)
15	CLA	c6	407	-	43,53,73	1.58	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	bA	808	-	49,59,73	1.43	7 (14%)	56,96,113	1.65	8 (14%)
18	BCR	bJ	105	-	41,41,41	1.21	5 (12%)	56,56,56	1.37	10 (17%)
16	PQN	aA	846	-	34,34,34	1.44	2 (5%)	43,45,45	1.19	6 (13%)
15	CLA	aB	816	-	43,53,73	1.52	8 (18%)	50,89,113	1.98	7 (14%)
15	CLA	bA	821	-	59,69,73	1.31	9 (15%)	69,108,113	1.50	9 (13%)
15	CLA	c4	413	-	43,53,73	1.61	7 (16%)	50,89,113	1.61	4 (8%)
15	CLA	a4	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.17	9 (14%)
15	CLA	bA	839	-	63,73,73	1.29	9 (14%)	74,113,113	1.55	9 (12%)
15	CLA	c1	406	-	43,53,73	1.60	6 (13%)	50,89,113	1.65	7 (14%)
15	CLA	aB	808	-	63,73,73	1.22	8 (12%)	74,113,113	1.59	11 (14%)
15	CLA	cB	830	-	63,73,73	1.33	8 (12%)	74,113,113	1.87	11 (14%)
19	LHG	bA	854	-	48,48,48	0.98	2 (4%)	51,54,54	1.37	7 (13%)
15	CLA	a2	405	-	43,53,73	1.70	7 (16%)	50,89,113	2.11	19 (38%)
15	CLA	bA	828	-	63,73,73	1.33	8 (12%)	74,113,113	1.40	8 (10%)
15	CLA	aB	809	-	63,73,73	1.30	9 (14%)	74,113,113	1.64	10 (13%)
15	CLA	a6	407	-	43,53,73	1.58	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	b4	404	-	63,73,73	1.33	8 (12%)	74,113,113	1.43	8 (10%)
18	BCR	bI	101	-	41,41,41	1.26	3 (7%)	56,56,56	1.30	6 (10%)
18	BCR	bL	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.39	9 (16%)
15	CLA	b6	412	13	43,53,73	1.52	7 (16%)	50,89,113	1.89	9 (18%)
15	CLA	b1	403	-	63,73,73	1.27	6 (9%)	74,113,113	1.60	10 (13%)
15	CLA	a2	416	-	43,53,73	1.57	8 (18%)	50,89,113	2.04	11 (22%)
15	CLA	cA	807	-	63,73,73	1.30	9 (14%)	74,113,113	1.60	12 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	cA	806	-	63,73,73	1.27	9 (14%)	74,113,113	1.74	10 (13%)
15	CLA	a2	404	-	63,73,73	1.35	7 (11%)	74,113,113	1.48	9 (12%)
15	CLA	c4	416	-	48,58,73	1.51	8 (16%)	56,95,113	2.57	16 (28%)
15	CLA	aB	817	-	53,63,73	1.16	5 (9%)	62,101,113	1.74	12 (19%)
15	CLA	b2	405	-	43,53,73	1.70	6 (13%)	50,89,113	2.10	20 (40%)
15	CLA	aB	823	-	53,63,73	1.37	6 (11%)	62,101,113	1.69	8 (12%)
15	CLA	a4	402	-	63,73,73	1.31	6 (9%)	74,113,113	1.49	9 (12%)
15	CLA	bB	832	-	47,57,73	1.42	9 (19%)	53,93,113	1.71	7 (13%)
15	CLA	cB	817	-	53,63,73	1.17	5 (9%)	62,101,113	1.74	12 (19%)
18	BCR	aF	203	-	41,41,41	1.22	5 (12%)	56,56,56	1.37	9 (16%)
17	SF4	aC	101	3	0,12,12	-	-	-	-	-
18	BCR	c4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.52	12 (21%)
15	CLA	c6	411	13	62,72,73	1.31	7 (11%)	72,111,113	1.69	14 (19%)
15	CLA	c6	410	-	63,73,73	1.33	6 (9%)	74,113,113	1.44	8 (10%)
15	CLA	c6	408	-	43,53,73	1.59	6 (13%)	50,89,113	1.72	8 (16%)
18	BCR	c6	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	a5	408	-	43,53,73	1.50	7 (16%)	50,89,113	1.84	9 (18%)
15	CLA	aB	832	-	47,57,73	1.43	9 (19%)	53,93,113	1.72	6 (11%)
18	BCR	b2	401	-	41,41,41	1.24	4 (9%)	56,56,56	1.84	13 (23%)
15	CLA	cB	812	-	43,53,73	1.44	7 (16%)	50,89,113	1.63	7 (14%)
15	CLA	a4	406	-	43,53,73	1.55	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	a4	408	-	43,53,73	1.47	7 (16%)	50,89,113	1.81	8 (16%)
15	CLA	c2	404	-	63,73,73	1.35	7 (11%)	74,113,113	1.48	9 (12%)
18	BCR	aA	851	-	41,41,41	1.37	5 (12%)	56,56,56	1.36	8 (14%)
15	CLA	b5	412	-	43,53,73	1.57	9 (20%)	50,89,113	1.78	12 (24%)
15	CLA	b6	408	-	43,53,73	1.57	6 (13%)	50,89,113	1.74	8 (16%)
15	CLA	cA	825	-	57,67,73	1.32	8 (14%)	66,105,113	1.49	8 (12%)
15	CLA	a5	402	-	63,73,73	1.32	6 (9%)	74,113,113	1.51	7 (9%)
18	BCR	bB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	b1	410	13	62,72,73	1.32	8 (12%)	72,111,113	1.73	14 (19%)
15	CLA	aA	832	-	48,58,73	1.47	9 (18%)	56,95,113	1.81	9 (16%)
18	BCR	a4	401	-	41,41,41	1.18	3 (7%)	56,56,56	1.52	12 (21%)
18	BCR	a3	401	-	41,41,41	1.27	4 (9%)	56,56,56	1.69	10 (17%)
15	CLA	a1	414	-	43,53,73	1.61	8 (18%)	50,89,113	2.07	10 (20%)
15	CLA	bA	813	-	52,62,73	1.37	8 (15%)	60,99,113	1.55	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aJ	201	-	43,53,73	1.51	8 (18%)	50,89,113	1.85	10 (20%)
15	CLA	c2	417	-	48,58,73	1.52	8 (16%)	56,95,113	2.65	21 (37%)
15	CLA	cB	811	2	63,73,73	1.41	9 (14%)	74,113,113	1.72	11 (14%)
15	CLA	aA	810	1	63,73,73	1.34	8 (12%)	74,113,113	1.56	9 (12%)
15	CLA	cA	836	-	52,62,73	1.53	8 (15%)	60,99,113	1.50	6 (10%)
15	CLA	cB	806	-	63,73,73	1.26	10 (15%)	74,113,113	1.67	8 (10%)
15	CLA	cB	809	-	63,73,73	1.29	9 (14%)	74,113,113	1.64	10 (13%)
15	CLA	c6	409	-	43,53,73	1.52	7 (16%)	50,89,113	1.85	7 (14%)
15	CLA	a1	405	-	43,53,73	1.58	6 (13%)	50,89,113	1.67	7 (14%)
15	CLA	a5	412	-	43,53,73	1.56	9 (20%)	50,89,113	1.77	12 (24%)
15	CLA	b4	421	-	63,73,73	1.44	12 (19%)	74,113,113	1.78	16 (21%)
15	CLA	cB	820	22	63,73,73	1.25	7 (11%)	74,113,113	1.43	6 (8%)
18	BCR	a2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.46	8 (14%)
15	CLA	c2	410	-	63,73,73	1.35	5 (7%)	74,113,113	1.45	9 (12%)
15	CLA	bA	823	-	47,57,73	1.47	8 (17%)	53,93,113	1.59	7 (13%)
15	CLA	aL	203	22	63,73,73	1.29	8 (12%)	74,113,113	1.43	8 (10%)
15	CLA	a4	409	-	63,73,73	1.34	6 (9%)	74,113,113	1.44	9 (12%)
15	CLA	b1	411	13	43,53,73	1.53	6 (13%)	50,89,113	1.91	8 (16%)
18	BCR	a3	419	-	41,41,41	1.06	2 (4%)	56,56,56	1.41	8 (14%)
15	CLA	a6	410	-	63,73,73	1.32	6 (9%)	74,113,113	1.46	8 (10%)
18	BCR	c4	420	-	41,41,41	1.18	3 (7%)	56,56,56	1.45	10 (17%)
18	BCR	aA	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	7 (12%)
15	CLA	cB	827	-	63,73,73	1.33	7 (11%)	74,113,113	1.69	12 (16%)
15	CLA	aJ	203	-	35,45,73	1.67	9 (25%)	42,78,113	1.82	7 (16%)
18	BCR	bB	845	-	41,41,41	1.12	3 (7%)	56,56,56	1.31	7 (12%)
18	BCR	c1	420	-	41,41,41	1.21	4 (9%)	56,56,56	1.46	11 (19%)
15	CLA	a1	416	13	53,63,73	1.41	5 (9%)	62,101,113	2.16	11 (17%)
15	CLA	cB	821	-	45,55,73	1.49	8 (17%)	52,91,113	1.59	6 (11%)
15	CLA	c6	404	-	63,73,73	1.25	6 (9%)	74,113,113	1.58	10 (13%)
15	CLA	bA	818	-	52,62,73	1.36	8 (15%)	60,99,113	1.79	7 (11%)
18	BCR	aF	202	-	41,41,41	1.21	3 (7%)	56,56,56	1.42	11 (19%)
15	CLA	c5	409	-	63,73,73	1.33	6 (9%)	74,113,113	1.43	7 (9%)
15	CLA	a1	411	-	43,53,73	1.59	9 (20%)	50,89,113	1.83	14 (28%)
15	CLA	bB	838	-	45,55,73	1.44	8 (17%)	52,91,113	1.87	8 (15%)
15	CLA	a1	403	-	63,73,73	1.32	8 (12%)	74,113,113	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bA	827	22	63,73,73	1.25	8 (12%)	74,113,113	1.63	11 (14%)
15	CLA	bA	838	-	49,59,73	1.46	9 (18%)	56,96,113	1.90	9 (16%)
15	CLA	a5	409	-	63,73,73	1.34	6 (9%)	74,113,113	1.44	8 (10%)
15	CLA	a4	414	-	39,49,73	1.63	8 (20%)	46,84,113	1.77	7 (15%)
15	CLA	bL	203	-	63,73,73	1.21	8 (12%)	74,113,113	1.72	10 (13%)
19	LHG	bX	101	-	22,22,48	0.90	1 (4%)	25,28,54	1.21	2 (8%)
15	CLA	c1	410	13	62,72,73	1.31	8 (12%)	72,111,113	1.72	14 (19%)
15	CLA	c5	404	-	63,73,73	1.33	7 (11%)	74,113,113	1.47	9 (12%)
19	LHG	aA	854	15	26,26,48	0.99	2 (7%)	29,32,54	1.39	3 (10%)
15	CLA	a4	415	-	43,53,73	1.59	7 (16%)	50,89,113	2.10	11 (22%)
15	CLA	b3	409	-	63,73,73	1.35	6 (9%)	74,113,113	1.47	8 (10%)
15	CLA	aA	805	-	57,67,73	1.34	9 (15%)	66,105,113	1.72	10 (15%)
15	CLA	aB	803	-	63,73,73	1.23	7 (11%)	74,113,113	1.70	14 (18%)
15	CLA	bB	819	-	58,68,73	1.28	9 (15%)	68,107,113	1.76	9 (13%)
15	CLA	c5	414	-	39,49,73	1.64	6 (15%)	46,84,113	1.81	7 (15%)
15	CLA	a3	405	-	43,53,73	1.65	9 (20%)	50,89,113	2.09	20 (40%)
18	BCR	aJ	204	-	41,41,41	1.28	3 (7%)	56,56,56	1.47	10 (17%)
18	BCR	bF	202	-	41,41,41	1.21	3 (7%)	56,56,56	1.42	11 (19%)
15	CLA	aB	838	-	45,55,73	1.44	9 (20%)	52,91,113	1.88	8 (15%)
15	CLA	bB	816	-	43,53,73	1.52	8 (18%)	50,89,113	1.98	7 (14%)
15	CLA	c2	422	-	63,73,73	1.39	8 (12%)	74,113,113	1.90	18 (24%)
15	CLA	a3	415	-	43,53,73	1.60	9 (20%)	50,89,113	2.06	9 (18%)
15	CLA	bB	836	-	58,68,73	1.34	8 (13%)	68,107,113	1.57	11 (16%)
15	CLA	bB	837	-	63,73,73	1.22	8 (12%)	74,113,113	1.60	8 (10%)
15	CLA	cB	802	-	63,73,73	1.46	11 (17%)	74,113,113	1.54	9 (12%)
15	CLA	a3	407	-	43,53,73	1.55	7 (16%)	50,89,113	1.73	8 (16%)
15	CLA	aX	102	12	43,53,73	1.51	8 (18%)	50,89,113	1.84	12 (24%)
15	CLA	cB	841	-	43,53,73	1.59	8 (18%)	50,89,113	1.69	9 (18%)
15	CLA	a4	413	-	43,53,73	1.61	7 (16%)	50,89,113	1.60	4 (8%)
17	SF4	cA	846	2,1	0,12,12	-	-	-	-	-
15	CLA	b3	407	-	43,53,73	1.55	7 (16%)	50,89,113	1.74	8 (16%)
15	CLA	a3	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.14	12 (19%)
15	CLA	cB	814	-	63,73,73	1.28	7 (11%)	74,113,113	1.74	14 (18%)
19	LHG	aA	853	-	48,48,48	0.98	2 (4%)	51,54,54	1.37	7 (13%)
15	CLA	b5	411	13	43,53,73	1.52	7 (16%)	50,89,113	1.91	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c5	413	-	43,53,73	1.60	8 (18%)	50,89,113	1.63	4 (8%)
15	CLA	cA	815	-	43,53,73	1.52	8 (18%)	50,89,113	1.64	8 (16%)
15	CLA	c3	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.13	12 (19%)
15	CLA	bB	814	-	63,73,73	1.27	7 (11%)	74,113,113	1.74	14 (18%)
15	CLA	b1	402	-	63,73,73	1.34	6 (9%)	74,113,113	1.48	7 (9%)
15	CLA	b3	421	-	63,73,73	1.47	9 (14%)	74,113,113	1.68	15 (20%)
15	CLA	cB	834	-	56,66,73	1.38	8 (14%)	65,104,113	1.60	10 (15%)
15	CLA	c3	415	-	43,53,73	1.61	9 (20%)	50,89,113	2.05	9 (18%)
15	CLA	bA	814	-	58,68,73	1.37	9 (15%)	68,107,113	1.49	8 (11%)
15	CLA	b3	414	-	39,49,73	1.59	8 (20%)	46,84,113	1.80	7 (15%)
15	CLA	aB	825	2	52,62,73	1.43	8 (15%)	60,99,113	1.78	9 (15%)
15	CLA	aA	804	-	63,73,73	1.29	8 (12%)	74,113,113	1.57	11 (14%)
15	CLA	a3	408	-	43,53,73	1.46	7 (16%)	50,89,113	1.82	9 (18%)
15	CLA	cA	812	-	63,73,73	1.28	9 (14%)	74,113,113	1.45	8 (10%)
15	CLA	c2	412	13	43,53,73	1.56	8 (18%)	50,89,113	1.90	8 (16%)
15	CLA	bB	815	-	63,73,73	1.31	7 (11%)	74,113,113	1.53	8 (10%)
15	CLA	b2	407	-	43,53,73	1.57	6 (13%)	50,89,113	1.67	7 (14%)
18	BCR	bA	851	-	41,41,41	1.16	2 (4%)	56,56,56	1.45	9 (16%)
15	CLA	bA	803	-	63,73,73	1.35	8 (12%)	74,113,113	1.91	14 (18%)
15	CLA	b3	413	-	43,53,73	1.59	9 (20%)	50,89,113	1.63	4 (8%)
15	CLA	cA	835	-	63,73,73	1.32	8 (12%)	74,113,113	1.63	10 (13%)
18	BCR	a1	420	-	41,41,41	1.14	3 (7%)	56,56,56	1.53	10 (17%)
15	CLA	cA	844	19	50,60,73	1.48	8 (16%)	57,97,113	2.20	15 (26%)
14	CL0	bA	801	-	63,73,73	1.87	16 (25%)	74,113,113	2.74	33 (44%)
15	CLA	a3	404	-	63,73,73	1.32	8 (12%)	74,113,113	1.47	9 (12%)
15	CLA	bL	204	22	63,73,73	1.28	8 (12%)	74,113,113	1.42	8 (10%)
15	CLA	c6	403	-	63,73,73	1.35	6 (9%)	74,113,113	1.48	7 (9%)
18	BCR	bI	102	-	41,41,41	1.35	4 (9%)	56,56,56	1.42	9 (16%)
15	CLA	a5	405	-	43,53,73	1.66	7 (16%)	50,89,113	2.14	21 (42%)
18	BCR	bJ	103	-	41,41,41	1.28	3 (7%)	56,56,56	1.47	10 (17%)
15	CLA	b3	416	-	48,58,73	1.52	8 (16%)	56,95,113	2.53	18 (32%)
15	CLA	c2	411	13	62,72,73	1.33	8 (12%)	72,111,113	1.71	14 (19%)
15	CLA	a3	403	-	63,73,73	1.25	6 (9%)	74,113,113	1.59	9 (12%)
15	CLA	cB	807	-	63,73,73	1.40	10 (15%)	74,113,113	1.60	9 (12%)
15	CLA	aA	826	-	63,73,73	1.26	7 (11%)	74,113,113	1.65	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	c4	406	-	43,53,73	1.56	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	bB	805	-	52,62,73	1.36	8 (15%)	60,99,113	1.68	7 (11%)
15	CLA	aA	811	-	43,53,73	1.53	8 (18%)	50,89,113	1.63	7 (14%)
15	CLA	a1	412	-	43,53,73	1.60	7 (16%)	50,89,113	1.56	4 (8%)
15	CLA	b6	414	-	43,53,73	1.64	7 (16%)	50,89,113	1.81	12 (24%)
15	CLA	aA	806	-	63,73,73	1.28	9 (14%)	74,113,113	1.74	10 (13%)
15	CLA	cA	828	-	63,73,73	1.33	8 (12%)	74,113,113	1.41	8 (10%)
18	BCR	a5	401	-	41,41,41	1.20	4 (9%)	56,56,56	1.54	12 (21%)
15	CLA	cA	817	-	47,57,73	1.47	6 (12%)	53,93,113	1.60	6 (11%)
15	CLA	a6	416	-	43,53,73	1.64	8 (18%)	50,89,113	2.06	11 (22%)
15	CLA	a4	412	-	43,53,73	1.58	9 (20%)	50,89,113	1.74	13 (26%)
15	CLA	aA	827	22	63,73,73	1.26	7 (11%)	74,113,113	1.62	11 (14%)
15	CLA	c2	403	-	63,73,73	1.29	6 (9%)	74,113,113	1.56	9 (12%)
15	CLA	b4	403	-	63,73,73	1.28	6 (9%)	74,113,113	1.55	9 (12%)
18	BCR	b2	420	-	41,41,41	1.12	3 (7%)	56,56,56	1.47	8 (14%)
17	SF4	aA	847	2,1	0,12,12	-	-	-	-	-
18	BCR	bB	847	-	25,25,41	1.17	2 (8%)	33,33,56	1.61	9 (27%)
15	CLA	bB	828	-	63,73,73	1.31	10 (15%)	74,113,113	1.69	8 (10%)
15	CLA	cA	829	-	63,73,73	1.29	8 (12%)	74,113,113	1.66	12 (16%)
18	BCR	cM	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.35	9 (16%)
15	CLA	bB	834	-	56,66,73	1.38	8 (14%)	65,104,113	1.61	10 (15%)
15	CLA	cB	831	-	43,53,73	1.61	9 (20%)	50,89,113	1.67	6 (12%)
15	CLA	c3	411	13	43,53,73	1.53	7 (16%)	50,89,113	1.88	8 (16%)
18	BCR	a6	421	-	41,41,41	1.10	4 (9%)	56,56,56	1.57	10 (17%)
15	CLA	cB	840	-	63,73,73	1.36	9 (14%)	74,113,113	1.76	11 (14%)
15	CLA	cB	825	2	52,62,73	1.43	8 (15%)	60,99,113	1.77	9 (15%)
15	CLA	bB	826	22	44,54,73	1.40	8 (18%)	51,90,113	1.98	11 (21%)
15	CLA	b2	413	-	43,53,73	1.57	9 (20%)	50,89,113	1.78	14 (28%)
15	CLA	cA	843	-	39,49,73	1.58	6 (15%)	46,83,113	1.75	5 (10%)
14	CL0	aA	801	-	63,73,73	1.87	16 (25%)	74,113,113	2.73	33 (44%)
15	CLA	b6	409	-	43,53,73	1.51	7 (16%)	50,89,113	1.85	7 (14%)
15	CLA	bB	830	-	63,73,73	1.33	8 (12%)	74,113,113	1.88	11 (14%)
18	BCR	a5	418	-	41,41,41	1.42	6 (14%)	56,56,56	1.57	9 (16%)
15	CLA	bB	820	22	63,73,73	1.25	7 (11%)	74,113,113	1.43	6 (8%)
15	CLA	a5	420	-	63,73,73	1.38	9 (14%)	74,113,113	1.96	18 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bL	202	10	63,73,73	1.30	8 (12%)	74,113,113	1.34	8 (10%)
15	CLA	cA	833	-	63,73,73	1.24	9 (14%)	74,113,113	1.49	7 (9%)
15	CLA	c1	403	-	63,73,73	1.28	6 (9%)	74,113,113	1.58	9 (12%)
15	CLA	cA	839	-	63,73,73	1.30	9 (14%)	74,113,113	1.55	9 (12%)
18	BCR	b2	419	-	41,41,41	1.39	6 (14%)	56,56,56	1.59	9 (16%)
15	CLA	b6	416	-	43,53,73	1.64	7 (16%)	50,89,113	2.07	10 (20%)
15	CLA	a4	421	-	63,73,73	1.44	12 (19%)	74,113,113	1.77	16 (21%)
15	CLA	a6	422	-	63,73,73	1.54	12 (19%)	74,113,113	2.29	20 (27%)
15	CLA	bA	837	1	43,53,73	1.56	7 (16%)	50,89,113	1.75	9 (18%)
17	SF4	bA	847	2,1	0,12,12	-	-	-	-	-
15	CLA	b6	407	-	43,53,73	1.59	6 (13%)	50,89,113	1.69	7 (14%)
15	CLA	aB	812	-	43,53,73	1.45	6 (13%)	50,89,113	1.62	7 (14%)
15	CLA	bB	835	-	43,53,73	1.51	8 (18%)	50,89,113	1.88	8 (16%)
15	CLA	bB	823	-	53,63,73	1.37	6 (11%)	62,101,113	1.69	8 (12%)
15	CLA	a6	412	13	43,53,73	1.52	7 (16%)	50,89,113	1.89	9 (18%)
15	CLA	c3	406	-	43,53,73	1.54	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	c3	408	-	43,53,73	1.46	7 (16%)	50,89,113	1.82	10 (20%)
15	CLA	a5	414	-	39,49,73	1.63	6 (15%)	46,84,113	1.80	8 (17%)
15	CLA	aA	814	-	58,68,73	1.38	9 (15%)	68,107,113	1.50	8 (11%)
18	BCR	bB	849	-	41,41,41	1.33	5 (12%)	56,56,56	1.40	10 (17%)
15	CLA	aB	827	-	63,73,73	1.32	7 (11%)	74,113,113	1.70	12 (16%)
17	SF4	bC	102	3	0,12,12	-	-	-	-	-
19	LHG	cX	101	-	22,22,48	0.90	1 (4%)	25,28,54	1.21	2 (8%)
15	CLA	aB	821	-	45,55,73	1.48	8 (17%)	52,91,113	1.61	6 (11%)
15	CLA	c4	404	-	63,73,73	1.33	7 (11%)	74,113,113	1.43	8 (10%)
18	BCR	bB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.53	9 (16%)
15	CLA	b1	416	-	48,58,73	1.53	8 (16%)	56,95,113	2.54	17 (30%)
15	CLA	b4	406	-	43,53,73	1.57	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	a5	417	13	53,63,73	1.43	5 (9%)	62,101,113	2.15	9 (14%)
15	CLA	cA	808	-	49,59,73	1.44	7 (14%)	56,96,113	1.64	8 (14%)
15	CLA	c5	412	-	43,53,73	1.57	9 (20%)	50,89,113	1.76	12 (24%)
15	CLA	aA	844	-	39,49,73	1.57	6 (15%)	46,83,113	1.76	5 (10%)
15	CLA	aB	839	22	63,73,73	1.29	8 (12%)	74,113,113	1.53	10 (13%)
15	CLA	cB	837	-	63,73,73	1.22	8 (12%)	74,113,113	1.60	8 (10%)
15	CLA	c1	412	-	43,53,73	1.60	9 (20%)	50,89,113	1.80	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	aA	838	-	49,59,73	1.46	10 (20%)	56,96,113	1.89	9 (16%)
15	CLA	b2	404	-	63,73,73	1.34	7 (11%)	74,113,113	1.47	9 (12%)
15	CLA	b6	413	-	43,53,73	1.59	9 (20%)	50,89,113	1.72	12 (24%)
18	BCR	cB	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.43	7 (12%)
15	CLA	a6	403	-	63,73,73	1.35	6 (9%)	74,113,113	1.47	7 (9%)
15	CLA	cA	802	22	63,73,73	1.38	10 (15%)	74,113,113	1.61	10 (13%)
15	CLA	c3	403	-	63,73,73	1.25	6 (9%)	74,113,113	1.60	9 (12%)
15	CLA	b4	415	-	43,53,73	1.59	8 (18%)	50,89,113	2.11	11 (22%)
15	CLA	a1	406	-	43,53,73	1.58	6 (13%)	50,89,113	1.76	8 (16%)
15	CLA	bA	843	-	63,73,73	1.32	7 (11%)	74,113,113	1.59	8 (10%)
15	CLA	cA	838	-	49,59,73	1.46	10 (20%)	56,96,113	1.90	9 (16%)
15	CLA	c4	410	13	62,72,73	1.34	9 (14%)	72,111,113	1.70	14 (19%)
16	PQN	cB	843	-	34,34,34	1.46	3 (8%)	43,45,45	1.19	5 (11%)
18	BCR	b6	420	-	41,41,41	1.19	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	bA	802	22	63,73,73	1.38	10 (15%)	74,113,113	1.60	10 (13%)
15	CLA	a5	416	-	48,58,73	1.48	8 (16%)	56,95,113	2.56	16 (28%)
15	CLA	bA	806	-	63,73,73	1.28	9 (14%)	74,113,113	1.74	10 (13%)
15	CLA	a3	411	13	43,53,73	1.53	7 (16%)	50,89,113	1.89	8 (16%)
15	CLA	c4	417	13	53,63,73	1.41	5 (9%)	62,101,113	2.17	9 (14%)
15	CLA	c5	407	-	43,53,73	1.59	7 (16%)	50,89,113	1.72	9 (18%)
18	BCR	bA	848	-	41,41,41	1.21	3 (7%)	56,56,56	1.43	10 (17%)
15	CLA	c3	410	13	62,72,73	1.34	8 (12%)	72,111,113	1.74	14 (19%)
15	CLA	b6	404	-	63,73,73	1.25	6 (9%)	74,113,113	1.57	10 (13%)
15	CLA	a5	407	-	43,53,73	1.59	7 (16%)	50,89,113	1.73	9 (18%)
15	CLA	bA	805	-	57,67,73	1.34	9 (15%)	66,105,113	1.72	10 (15%)
15	CLA	c6	415	-	39,49,73	1.66	6 (15%)	46,84,113	1.76	7 (15%)
18	BCR	b6	421	-	41,41,41	1.10	4 (9%)	56,56,56	1.55	9 (16%)
15	CLA	b1	409	-	63,73,73	1.36	5 (7%)	74,113,113	1.42	7 (9%)
15	CLA	aK	102	-	43,53,73	1.51	7 (16%)	50,89,113	1.66	10 (20%)
15	CLA	b5	420	-	63,73,73	1.38	9 (14%)	74,113,113	1.96	18 (24%)
15	CLA	c6	417	-	48,58,73	1.50	7 (14%)	56,95,113	2.57	18 (32%)
18	BCR	cA	847	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	6 (10%)
15	CLA	aB	805	-	52,62,73	1.36	8 (15%)	60,99,113	1.67	7 (11%)
18	BCR	cI	102	-	41,41,41	1.35	5 (12%)	56,56,56	1.42	9 (16%)
15	CLA	cB	833	-	63,73,73	1.22	7 (11%)	74,113,113	1.47	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	cL	204	-	41,41,41	1.32	4 (9%)	56,56,56	1.47	9 (16%)
15	CLA	a1	409	13	62,72,73	1.32	8 (12%)	72,111,113	1.73	14 (19%)
15	CLA	a5	413	-	43,53,73	1.61	9 (20%)	50,89,113	1.62	4 (8%)
15	CLA	bB	804	-	63,73,73	1.34	7 (11%)	74,113,113	2.07	17 (22%)
15	CLA	cB	808	-	63,73,73	1.22	7 (11%)	74,113,113	1.59	11 (14%)
15	CLA	cJ	102	-	35,45,73	1.68	8 (22%)	42,78,113	1.83	7 (16%)
15	CLA	aA	816	-	43,53,73	1.53	7 (16%)	50,89,113	1.90	6 (12%)
15	CLA	aB	813	-	43,53,73	1.55	8 (18%)	50,89,113	1.76	6 (12%)
15	CLA	aA	836	-	52,62,73	1.52	8 (15%)	60,99,113	1.50	6 (10%)
15	CLA	bB	807	-	63,73,73	1.41	10 (15%)	74,113,113	1.60	9 (12%)
15	CLA	cA	814	-	58,68,73	1.36	8 (13%)	68,107,113	1.50	8 (11%)
15	CLA	cJ	101	8	43,53,73	1.54	8 (18%)	50,89,113	1.81	9 (18%)
15	CLA	bB	817	-	53,63,73	1.16	5 (9%)	62,101,113	1.75	12 (19%)
15	CLA	a6	405	-	63,73,73	1.33	7 (11%)	74,113,113	1.46	9 (12%)
15	CLA	c1	402	-	63,73,73	1.33	6 (9%)	74,113,113	1.48	7 (9%)
15	CLA	c4	411	13	43,53,73	1.53	6 (13%)	50,89,113	1.92	7 (14%)
15	CLA	c6	414	-	43,53,73	1.64	6 (13%)	50,89,113	1.75	10 (20%)
16	PQN	bA	846	-	34,34,34	1.44	2 (5%)	43,45,45	1.19	6 (13%)
15	CLA	cB	823	-	53,63,73	1.37	6 (11%)	62,101,113	1.69	8 (12%)
15	CLA	b2	403	-	63,73,73	1.27	6 (9%)	74,113,113	1.58	9 (12%)
15	CLA	b5	403	-	63,73,73	1.26	6 (9%)	74,113,113	1.58	10 (13%)
15	CLA	bB	812	-	43,53,73	1.45	6 (13%)	50,89,113	1.63	7 (14%)
18	BCR	c2	419	-	41,41,41	1.42	6 (14%)	56,56,56	1.57	9 (16%)
15	CLA	aJ	202	8	43,53,73	1.54	9 (20%)	50,89,113	1.82	9 (18%)
15	CLA	cL	203	22	63,73,73	1.29	8 (12%)	74,113,113	1.42	8 (10%)
18	BCR	a4	418	-	41,41,41	1.46	6 (14%)	56,56,56	1.60	8 (14%)
18	BCR	b4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.41	8 (14%)
15	CLA	bA	841	-	63,73,73	1.27	7 (11%)	74,113,113	1.46	8 (10%)
15	CLA	a2	413	-	43,53,73	1.57	9 (20%)	50,89,113	1.78	14 (28%)
15	CLA	bA	829	-	63,73,73	1.30	8 (12%)	74,113,113	1.66	12 (16%)
15	CLA	bB	802	-	63,73,73	1.46	10 (15%)	74,113,113	1.53	8 (10%)
18	BCR	aL	205	-	41,41,41	1.17	3 (7%)	56,56,56	1.39	9 (16%)
15	CLA	a3	402	-	63,73,73	1.30	6 (9%)	74,113,113	1.49	7 (9%)
15	CLA	a1	415	-	48,58,73	1.53	8 (16%)	56,95,113	2.57	18 (32%)
15	CLA	a5	404	-	63,73,73	1.32	7 (11%)	74,113,113	1.48	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bB	840	-	63,73,73	1.37	9 (14%)	74,113,113	1.75	11 (14%)
15	CLA	b4	410	13	62,72,73	1.34	8 (12%)	72,111,113	1.72	14 (19%)
18	BCR	a2	419	-	41,41,41	1.41	6 (14%)	56,56,56	1.57	9 (16%)
20	LMG	aB	850	-	55,55,55	1.12	3 (5%)	63,63,63	1.62	8 (12%)
15	CLA	bA	811	-	43,53,73	1.52	8 (18%)	50,89,113	1.62	7 (14%)
15	CLA	bB	809	-	63,73,73	1.30	9 (14%)	74,113,113	1.65	10 (13%)
15	CLA	c6	413	-	43,53,73	1.60	9 (20%)	50,89,113	1.72	13 (26%)
18	BCR	c6	401	-	41,41,41	1.19	4 (9%)	56,56,56	1.55	10 (17%)
15	CLA	a2	409	-	43,53,73	1.51	7 (16%)	50,89,113	1.79	9 (18%)
15	CLA	a6	406	-	43,53,73	1.70	6 (13%)	50,89,113	2.09	20 (40%)
15	CLA	aA	802	22	63,73,73	1.38	9 (14%)	74,113,113	1.61	10 (13%)
18	BCR	a4	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.41	8 (14%)
18	BCR	aI	102	-	41,41,41	1.35	4 (9%)	56,56,56	1.42	9 (16%)
15	CLA	aA	833	-	63,73,73	1.24	9 (14%)	74,113,113	1.48	7 (9%)
15	CLA	cB	818	-	57,67,73	1.35	7 (12%)	66,105,113	1.66	11 (16%)
15	CLA	a1	413	-	39,49,73	1.64	6 (15%)	46,84,113	1.77	8 (17%)
15	CLA	c3	421	-	63,73,73	1.48	9 (14%)	74,113,113	1.69	15 (20%)
15	CLA	c3	414	-	39,49,73	1.60	7 (17%)	46,84,113	1.80	7 (15%)
15	CLA	b4	405	-	43,53,73	1.64	8 (18%)	50,89,113	2.13	19 (38%)
15	CLA	bA	836	-	52,62,73	1.52	8 (15%)	60,99,113	1.49	6 (10%)
15	CLA	bA	807	-	63,73,73	1.29	9 (14%)	74,113,113	1.60	11 (14%)
15	CLA	b3	411	13	43,53,73	1.54	7 (16%)	50,89,113	1.88	8 (16%)
15	CLA	c2	415	-	39,49,73	1.61	6 (15%)	46,84,113	1.78	7 (15%)
18	BCR	c5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.44	12 (21%)
15	CLA	c6	418	13	53,63,73	1.46	4 (7%)	62,101,113	2.12	10 (16%)
18	BCR	a6	420	-	41,41,41	1.20	2 (4%)	56,56,56	1.44	10 (17%)
15	CLA	cB	835	-	43,53,73	1.51	7 (16%)	50,89,113	1.88	8 (16%)
15	CLA	a2	408	-	43,53,73	1.57	7 (16%)	50,89,113	1.69	9 (18%)
15	CLA	aB	837	-	63,73,73	1.22	8 (12%)	74,113,113	1.60	8 (10%)
17	SF4	bC	101	3	0,12,12	-	-	-	-	-
18	BCR	cB	849	-	41,41,41	1.41	5 (12%)	56,56,56	1.31	8 (14%)
15	CLA	aA	843	-	63,73,73	1.31	7 (11%)	74,113,113	1.60	9 (12%)
15	CLA	a6	404	-	63,73,73	1.25	6 (9%)	74,113,113	1.57	10 (13%)
15	CLA	b6	406	-	43,53,73	1.70	6 (13%)	50,89,113	2.10	19 (38%)
15	CLA	aB	818	-	57,67,73	1.35	7 (12%)	66,105,113	1.66	11 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	cA	810	1	63,73,73	1.34	8 (12%)	74,113,113	1.57	9 (12%)
20	LMG	bB	851	-	55,55,55	1.12	4 (7%)	63,63,63	1.62	8 (12%)
15	CLA	bA	812	-	63,73,73	1.28	9 (14%)	74,113,113	1.44	9 (12%)
15	CLA	c1	415	-	43,53,73	1.61	8 (18%)	50,89,113	2.08	10 (20%)
18	BCR	aB	847	-	25,25,41	1.18	2 (8%)	33,33,56	1.60	9 (27%)
15	CLA	cA	809	1	63,73,73	1.31	8 (12%)	74,113,113	1.57	10 (13%)
15	CLA	bA	815	-	43,53,73	1.52	8 (18%)	50,89,113	1.64	8 (16%)
15	CLA	b2	412	13	43,53,73	1.57	8 (18%)	50,89,113	1.91	8 (16%)
15	CLA	aB	807	-	63,73,73	1.41	10 (15%)	74,113,113	1.60	8 (10%)
15	CLA	bK	101	-	43,53,73	1.51	7 (16%)	50,89,113	1.66	10 (20%)
15	CLA	b4	417	13	53,63,73	1.41	5 (9%)	62,101,113	2.16	9 (14%)
15	CLA	a1	422	-	63,73,73	1.46	11 (17%)	74,113,113	2.10	20 (27%)
15	CLA	c2	405	-	43,53,73	1.70	6 (13%)	50,89,113	2.09	20 (40%)
15	CLA	cB	838	-	45,55,73	1.44	8 (17%)	52,91,113	1.88	8 (15%)
15	CLA	c1	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.15	11 (17%)
18	BCR	b1	401	-	41,41,41	1.15	4 (9%)	56,56,56	1.55	10 (17%)
15	CLA	bJ	101	8	43,53,73	1.54	9 (20%)	50,89,113	1.83	9 (18%)
15	CLA	cA	823	-	47,57,73	1.47	8 (17%)	53,93,113	1.60	7 (13%)
18	BCR	c6	419	-	41,41,41	1.40	6 (14%)	56,56,56	1.56	9 (16%)
15	CLA	c4	412	-	43,53,73	1.58	9 (20%)	50,89,113	1.72	14 (28%)
15	CLA	a3	413	-	43,53,73	1.59	9 (20%)	50,89,113	1.61	4 (8%)
15	CLA	aB	834	-	56,66,73	1.38	8 (14%)	65,104,113	1.60	10 (15%)
15	CLA	bA	844	-	39,49,73	1.58	6 (15%)	46,83,113	1.75	5 (10%)
15	CLA	c3	402	-	63,73,73	1.30	6 (9%)	74,113,113	1.47	7 (9%)
15	CLA	b4	411	13	43,53,73	1.54	6 (13%)	50,89,113	1.91	7 (14%)
15	CLA	a6	418	13	53,63,73	1.45	4 (7%)	62,101,113	2.10	10 (16%)
15	CLA	aA	817	-	47,57,73	1.48	7 (14%)	53,93,113	1.60	6 (11%)
18	BCR	c1	419	-	41,41,41	1.23	4 (9%)	56,56,56	1.65	12 (21%)
15	CLA	aB	820	22	63,73,73	1.24	7 (11%)	74,113,113	1.44	6 (8%)
15	CLA	a2	411	13	62,72,73	1.33	8 (12%)	72,111,113	1.71	14 (19%)
15	CLA	b3	402	-	63,73,73	1.30	6 (9%)	74,113,113	1.47	7 (9%)
15	CLA	b3	410	13	62,72,73	1.33	8 (12%)	72,111,113	1.74	14 (19%)
15	CLA	cA	822	-	63,73,73	1.25	9 (14%)	74,113,113	1.54	7 (9%)
18	BCR	aB	848	-	41,41,41	1.32	4 (9%)	56,56,56	1.53	9 (16%)
15	CLA	b2	415	-	39,49,73	1.61	6 (15%)	46,84,113	1.78	7 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	aF	201	-	41,41,41	1.34	5 (12%)	56,56,56	1.40	10 (17%)
18	BCR	cJ	103	-	41,41,41	1.28	3 (7%)	56,56,56	1.47	10 (17%)
15	CLA	cA	811	-	43,53,73	1.53	8 (18%)	50,89,113	1.62	7 (14%)
16	PQN	aB	843	-	34,34,34	1.47	3 (8%)	43,45,45	1.20	5 (11%)
18	BCR	b1	418	-	41,41,41	1.41	6 (14%)	56,56,56	1.57	9 (16%)
15	CLA	a1	408	-	63,73,73	1.36	5 (7%)	74,113,113	1.42	7 (9%)
15	CLA	c3	413	-	43,53,73	1.59	8 (18%)	50,89,113	1.62	4 (8%)
15	CLA	bA	822	-	63,73,73	1.26	9 (14%)	74,113,113	1.54	7 (9%)
18	BCR	cJ	104	-	41,41,41	1.31	4 (9%)	56,56,56	1.47	7 (12%)
15	CLA	b2	417	-	48,58,73	1.51	8 (16%)	56,95,113	2.62	19 (33%)
15	CLA	b1	412	-	43,53,73	1.59	9 (20%)	50,89,113	1.80	13 (26%)
15	CLA	b6	418	13	53,63,73	1.45	4 (7%)	62,101,113	2.11	10 (16%)
18	BCR	c3	419	-	41,41,41	1.07	2 (4%)	56,56,56	1.42	8 (14%)
15	CLA	bX	102	12	43,53,73	1.51	8 (18%)	50,89,113	1.85	12 (24%)
15	CLA	bB	833	-	63,73,73	1.22	7 (11%)	74,113,113	1.46	11 (14%)
15	CLA	bA	842	22	49,59,73	1.57	8 (16%)	56,96,113	1.44	9 (16%)
15	CLA	bB	808	-	63,73,73	1.22	8 (12%)	74,113,113	1.59	10 (13%)
15	CLA	a3	406	-	43,53,73	1.56	6 (13%)	50,89,113	1.68	7 (14%)
15	CLA	bA	840	-	45,55,73	1.51	9 (20%)	52,91,113	2.04	9 (17%)
18	BCR	c6	402	-	41,41,41	1.22	4 (9%)	56,56,56	1.72	14 (25%)
15	CLA	a5	411	13	43,53,73	1.51	7 (16%)	50,89,113	1.90	8 (16%)
18	BCR	b5	419	-	41,41,41	1.17	2 (4%)	56,56,56	1.43	11 (19%)
20	LMG	cB	850	-	55,55,55	1.12	4 (7%)	63,63,63	1.63	8 (12%)
15	CLA	aA	824	-	49,59,73	1.40	8 (16%)	56,96,113	1.60	7 (12%)
18	BCR	a1	417	-	41,41,41	1.42	6 (14%)	56,56,56	1.58	10 (17%)
15	CLA	b6	417	-	48,58,73	1.51	7 (14%)	56,95,113	2.57	18 (32%)
15	CLA	aB	801	-	63,73,73	1.33	9 (14%)	74,113,113	1.50	9 (12%)
15	CLA	bJ	102	-	35,45,73	1.67	9 (25%)	42,78,113	1.81	7 (16%)
15	CLA	aA	807	-	63,73,73	1.30	9 (14%)	74,113,113	1.60	11 (14%)
15	CLA	aB	810	2	63,73,73	1.41	10 (15%)	74,113,113	1.68	12 (16%)
18	BCR	b4	420	-	41,41,41	1.18	3 (7%)	56,56,56	1.46	10 (17%)
15	CLA	c3	405	-	43,53,73	1.64	9 (20%)	50,89,113	2.09	20 (40%)
15	CLA	b6	410	-	63,73,73	1.32	6 (9%)	74,113,113	1.45	8 (10%)
15	CLA	aB	841	-	43,53,73	1.59	7 (16%)	50,89,113	1.70	9 (18%)
15	CLA	aB	829	-	63,73,73	1.25	9 (14%)	74,113,113	1.50	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	bB	824	-	43,53,73	1.54	7 (16%)	50,89,113	1.63	10 (20%)
15	CLA	bB	825	2	52,62,73	1.43	8 (15%)	60,99,113	1.78	9 (15%)
15	CLA	aA	845	19	50,60,73	1.48	8 (16%)	57,97,113	2.20	15 (26%)
18	BCR	cA	851	-	41,41,41	1.21	3 (7%)	56,56,56	1.40	6 (10%)
15	CLA	bA	825	-	57,67,73	1.31	8 (14%)	66,105,113	1.49	8 (12%)
15	CLA	aA	830	-	63,73,73	1.24	9 (14%)	74,113,113	1.68	10 (13%)
15	CLA	b5	415	-	43,53,73	1.60	8 (18%)	50,89,113	2.08	10 (20%)
18	BCR	bB	850	-	41,41,41	1.42	5 (12%)	56,56,56	1.31	9 (16%)
15	CLA	aA	809	1	63,73,73	1.30	8 (12%)	74,113,113	1.56	10 (13%)
15	CLA	a2	402	-	63,73,73	1.31	5 (7%)	74,113,113	1.49	7 (9%)
15	CLA	bB	841	-	43,53,73	1.59	7 (16%)	50,89,113	1.70	9 (18%)
18	BCR	aA	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.42	9 (16%)
15	CLA	c4	403	-	63,73,73	1.28	6 (9%)	74,113,113	1.55	8 (10%)
15	CLA	b2	406	-	63,73,73	1.46	9 (14%)	74,113,113	2.01	20 (27%)
15	CLA	cA	832	-	48,58,73	1.46	9 (18%)	56,95,113	1.81	9 (16%)
17	SF4	cC	102	3	0,12,12	-	-	-	-	-
17	SF4	cC	101	3	0,12,12	-	-	-	-	-
15	CLA	b3	417	13	53,63,73	1.42	5 (9%)	62,101,113	2.14	12 (19%)
15	CLA	a2	414	-	43,53,73	1.61	8 (18%)	50,89,113	1.62	4 (8%)
15	CLA	a2	407	-	43,53,73	1.56	6 (13%)	50,89,113	1.67	7 (14%)
14	CL0	cA	801	-	63,73,73	1.87	16 (25%)	74,113,113	2.74	33 (44%)
15	CLA	a3	409	-	63,73,73	1.35	6 (9%)	74,113,113	1.46	8 (10%)
15	CLA	a1	407	-	43,53,73	1.49	7 (16%)	50,89,113	1.83	7 (14%)
18	BCR	b6	419	-	41,41,41	1.41	6 (14%)	56,56,56	1.56	10 (17%)
15	CLA	bA	826	-	63,73,73	1.25	7 (11%)	74,113,113	1.66	10 (13%)
15	CLA	cB	836	-	58,68,73	1.33	8 (13%)	68,107,113	1.58	11 (16%)
15	CLA	b1	414	-	39,49,73	1.65	6 (15%)	46,84,113	1.77	8 (17%)
15	CLA	cF	203	-	43,53,73	1.51	9 (20%)	50,89,113	1.86	10 (20%)
15	CLA	b1	407	-	43,53,73	1.58	7 (16%)	50,89,113	1.76	8 (16%)
15	CLA	c1	411	13	43,53,73	1.53	7 (16%)	50,89,113	1.89	8 (16%)
15	CLA	bB	803	-	63,73,73	1.23	7 (11%)	74,113,113	1.69	14 (18%)
15	CLA	cB	824	-	43,53,73	1.53	7 (16%)	50,89,113	1.64	10 (20%)
15	CLA	bA	835	-	63,73,73	1.33	9 (14%)	74,113,113	1.65	10 (13%)
15	CLA	cB	819	-	58,68,73	1.28	9 (15%)	68,107,113	1.75	9 (13%)
15	CLA	c5	416	-	48,58,73	1.50	8 (16%)	56,95,113	2.55	15 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	cF	205	-	41,41,41	1.22	5 (12%)	56,56,56	1.36	9 (16%)
15	CLA	cA	840	-	45,55,73	1.51	9 (20%)	52,91,113	2.04	9 (17%)
15	CLA	aA	822	-	63,73,73	1.26	9 (14%)	74,113,113	1.54	7 (9%)
15	CLA	aB	826	22	44,54,73	1.40	8 (18%)	51,90,113	1.98	10 (19%)
18	BCR	bA	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.40	7 (12%)
15	CLA	a5	403	-	63,73,73	1.26	6 (9%)	74,113,113	1.58	10 (13%)
15	CLA	c2	407	-	43,53,73	1.58	6 (13%)	50,89,113	1.67	7 (14%)
15	CLA	c3	409	-	63,73,73	1.35	6 (9%)	74,113,113	1.47	8 (10%)
15	CLA	aB	806	-	63,73,73	1.27	10 (15%)	74,113,113	1.65	8 (10%)
15	CLA	b3	404	-	63,73,73	1.33	8 (12%)	74,113,113	1.47	9 (12%)
18	BCR	b3	420	-	41,41,41	1.20	3 (7%)	56,56,56	1.45	10 (17%)
15	CLA	aA	834	-	63,73,73	1.28	9 (14%)	74,113,113	1.71	10 (13%)
15	CLA	b5	406	-	43,53,73	1.57	6 (13%)	50,89,113	1.70	8 (16%)
18	BCR	cF	204	-	41,41,41	1.20	3 (7%)	56,56,56	1.42	11 (19%)
15	CLA	b6	411	13	62,72,73	1.32	7 (11%)	72,111,113	1.69	14 (19%)
15	CLA	cB	810	2	63,73,73	1.41	10 (15%)	74,113,113	1.68	12 (16%)
15	CLA	b6	415	-	39,49,73	1.66	6 (15%)	46,84,113	1.77	7 (15%)
18	BCR	aB	846	-	41,41,41	1.22	3 (7%)	56,56,56	1.37	8 (14%)
15	CLA	bA	831	-	63,73,73	1.35	8 (12%)	74,113,113	1.65	9 (12%)
15	CLA	cA	821	-	59,69,73	1.32	9 (15%)	69,108,113	1.51	9 (13%)
15	CLA	cB	829	-	63,73,73	1.25	9 (14%)	74,113,113	1.51	8 (10%)
18	BCR	aB	849	-	41,41,41	1.41	5 (12%)	56,56,56	1.31	8 (14%)
15	CLA	b3	403	-	63,73,73	1.25	6 (9%)	74,113,113	1.61	10 (13%)
15	CLA	cA	818	-	52,62,73	1.35	7 (13%)	60,99,113	1.78	7 (11%)
18	BCR	a5	419	-	41,41,41	1.18	2 (4%)	56,56,56	1.42	11 (19%)
15	CLA	c1	407	-	43,53,73	1.59	7 (16%)	50,89,113	1.75	8 (16%)
18	BCR	cB	846	-	41,41,41	1.22	3 (7%)	56,56,56	1.38	8 (14%)
16	PQN	bB	843	-	34,34,34	1.46	3 (8%)	43,45,45	1.19	5 (11%)
15	CLA	b6	422	-	63,73,73	1.51	11 (17%)	74,113,113	2.11	20 (27%)
15	CLA	a3	410	13	62,72,73	1.34	8 (12%)	72,111,113	1.72	14 (19%)
15	CLA	cA	803	-	63,73,73	1.35	8 (12%)	74,113,113	1.91	15 (20%)
18	BCR	b3	401	-	41,41,41	1.27	4 (9%)	56,56,56	1.69	10 (17%)
15	CLA	a2	415	-	39,49,73	1.61	6 (15%)	46,84,113	1.78	7 (15%)
15	CLA	aB	831	-	43,53,73	1.61	9 (20%)	50,89,113	1.66	6 (12%)
15	CLA	cB	839	22	63,73,73	1.30	8 (12%)	74,113,113	1.54	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	SF4	aC	102	3	0,12,12	-	-	-		
15	CLA	c4	415	-	43,53,73	1.59	7 (16%)	50,89,113	2.09	11 (22%)
15	CLA	b5	414	-	39,49,73	1.64	6 (15%)	46,84,113	1.81	7 (15%)
18	BCR	bA	852	-	41,41,41	1.37	4 (9%)	56,56,56	1.36	8 (14%)
15	CLA	bA	830	-	63,73,73	1.24	8 (12%)	74,113,113	1.68	10 (13%)
15	CLA	aA	821	-	59,69,73	1.32	9 (15%)	69,108,113	1.50	8 (11%)
15	CLA	c3	412	-	43,53,73	1.55	9 (20%)	50,89,113	1.75	14 (28%)
15	CLA	aB	814	-	63,73,73	1.28	7 (11%)	74,113,113	1.74	14 (18%)
15	CLA	cA	816	-	43,53,73	1.54	7 (16%)	50,89,113	1.90	6 (12%)
15	CLA	cA	837	1	43,53,73	1.56	7 (16%)	50,89,113	1.75	9 (18%)
15	CLA	aB	802	-	63,73,73	1.46	10 (15%)	74,113,113	1.54	8 (10%)
15	CLA	a4	405	-	43,53,73	1.64	8 (18%)	50,89,113	2.13	20 (40%)
18	BCR	bM	101	-	41,41,41	1.17	3 (7%)	56,56,56	1.34	9 (16%)

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
15	CLA	b6	405	-	1/1/15/20	8/37/115/115	-
18	BCR	b4	418	-	-	9/29/63/63	0/2/2/2
15	CLA	a5	406	-	1/1/11/20	4/13/91/115	-
15	CLA	c6	416	-	-	4/13/91/115	-
15	CLA	b3	412	-	1/1/11/20	7/13/91/115	-
15	CLA	a1	410	13	1/1/11/20	4/13/91/115	-
15	CLA	c5	420	-	1/1/15/20	8/37/115/115	-
18	BCR	b6	402	-	-	13/29/63/63	0/2/2/2
15	CLA	b2	410	-	1/1/15/20	5/37/115/115	-
18	BCR	c4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	801	-	1/1/15/20	10/37/115/115	-
15	CLA	aA	815	-	1/1/11/20	0/13/91/115	-
15	CLA	cX	102	12	1/1/11/20	6/13/91/115	-
15	CLA	a5	415	-	-	5/13/91/115	-
15	CLA	cA	824	-	1/1/12/20	9/21/99/115	-
15	CLA	a4	407	-	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b6	403	-	1/1/15/20	12/37/115/115	-
18	BCR	a1	418	-	-	11/29/63/63	0/2/2/2
18	BCR	b6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	810	1	1/1/15/20	15/37/115/115	-
15	CLA	c4	405	-	1/1/11/20	3/13/91/115	-
18	BCR	b1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cB	803	-	1/1/15/20	12/37/115/115	-
15	CLA	b4	409	-	1/1/15/20	5/37/115/115	-
18	BCR	bJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	b5	408	-	1/1/11/20	5/13/91/115	-
15	CLA	b2	411	13	1/1/14/20	10/36/114/115	-
15	CLA	cA	813	-	1/1/12/20	6/24/102/115	-
15	CLA	aL	201	10	1/1/15/20	10/37/115/115	-
15	CLA	aA	835	-	1/1/15/20	12/37/115/115	-
15	CLA	b1	404	-	1/1/15/20	9/37/115/115	-
15	CLA	b4	402	-	1/1/15/20	14/37/115/115	-
15	CLA	b5	402	-	1/1/15/20	14/37/115/115	-
15	CLA	a6	411	13	1/1/14/20	10/36/114/115	-
15	CLA	cB	805	-	1/1/12/20	5/24/102/115	-
15	CLA	a6	408	-	1/1/11/20	4/13/91/115	-
15	CLA	c1	405	-	1/1/11/20	3/13/91/115	-
15	CLA	c5	406	-	1/1/11/20	4/13/91/115	-
15	CLA	c5	417	13	1/1/13/20	9/25/103/115	-
15	CLA	bA	833	-	1/1/15/20	12/37/115/115	-
19	LHG	cA	852	-	-	18/53/53/53	-
15	CLA	cA	827	22	1/1/15/20	8/37/115/115	-
15	CLA	b4	414	-	1/1/10/20	2/8/86/115	-
15	CLA	b2	422	-	1/1/15/20	10/37/115/115	-
15	CLA	aA	819	-	1/1/12/20	8/24/102/115	-
15	CLA	b5	410	13	1/1/14/20	12/36/114/115	-
15	CLA	aB	804	-	1/1/15/20	9/37/115/115	-
15	CLA	b4	413	-	1/1/11/20	1/13/91/115	-
18	BCR	a2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	837	1	-	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	824	-	1/1/11/20	3/13/91/115	-
15	CLA	a1	402	-	1/1/15/20	15/37/115/115	-
15	CLA	bA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	bA	816	-	-	3/13/91/115	-
15	CLA	c5	405	-	1/1/11/20	3/13/91/115	-
15	CLA	c5	411	13	1/1/11/20	3/13/91/115	-
15	CLA	a4	416	-	1/1/12/20	7/19/97/115	-
18	BCR	a3	418	-	-	10/29/63/63	0/2/2/2
15	CLA	c5	415	-	-	5/13/91/115	-
15	CLA	a4	404	-	1/1/15/20	8/37/115/115	-
15	CLA	cB	815	-	1/1/15/20	16/37/115/115	-
15	CLA	c1	408	-	1/1/11/20	5/13/91/115	-
18	BCR	bA	853	-	-	22/29/63/63	0/2/2/2
15	CLA	cB	804	-	1/1/15/20	9/37/115/115	-
15	CLA	c2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	aB	815	-	1/1/15/20	16/37/115/115	-
15	CLA	a1	401	-	1/1/15/20	13/37/115/115	-
15	CLA	aA	825	-	1/1/13/20	13/30/108/115	-
15	CLA	cB	826	22	1/1/11/20	8/15/93/115	-
15	CLA	a6	409	-	1/1/11/20	5/13/91/115	-
18	BCR	c3	418	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	803	-	1/1/15/20	12/37/115/115	-
15	CLA	c2	402	-	1/1/15/20	12/37/115/115	-
18	BCR	a1	419	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	aA	842	22	1/1/12/20	6/21/99/115	-
15	CLA	aA	829	-	1/1/15/20	18/37/115/115	-
19	LHG	aX	101	-	-	12/26/26/53	-
15	CLA	c2	416	-	-	4/13/91/115	-
15	CLA	c1	404	-	1/1/15/20	9/37/115/115	-
15	CLA	b2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	a3	421	-	1/1/15/20	7/37/115/115	-
15	CLA	b2	418	13	1/1/13/20	10/25/103/115	-
15	CLA	cA	834	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	aI	101	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	819	-	1/1/12/20	8/24/102/115	-
18	BCR	b3	418	-	-	10/29/63/63	0/2/2/2
15	CLA	a3	414	-	1/1/10/20	2/8/86/115	-
18	BCR	cA	850	-	-	8/29/63/63	0/2/2/2
15	CLA	bB	822	-	1/1/11/20	3/13/91/115	-
19	LHG	bA	855	15	-	14/31/31/53	-
15	CLA	aB	835	-	1/1/11/20	9/13/91/115	-
15	CLA	c2	414	-	1/1/11/20	1/13/91/115	-
18	BCR	aA	852	-	-	22/29/63/63	0/2/2/2
15	CLA	aB	836	-	1/1/14/20	8/31/109/115	-
15	CLA	aB	811	2	1/1/15/20	9/37/115/115	-
15	CLA	a6	414	-	1/1/11/20	1/13/91/115	-
15	CLA	a2	418	13	1/1/13/20	10/25/103/115	-
15	CLA	b4	408	-	1/1/11/20	5/13/91/115	-
15	CLA	c1	409	-	1/1/15/20	5/37/115/115	-
15	CLA	cA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	a5	410	13	1/1/14/20	12/36/114/115	-
15	CLA	bA	804	-	1/1/15/20	10/37/115/115	-
18	BCR	cI	101	-	-	10/29/63/63	0/2/2/2
15	CLA	aB	819	-	1/1/14/20	11/31/109/115	-
18	BCR	c3	401	-	-	13/29/63/63	0/2/2/2
15	CLA	bA	817	-	-	4/18/96/115	-
15	CLA	a3	416	-	1/1/12/20	7/19/97/115	-
18	BCR	b3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c4	408	-	1/1/11/20	5/13/91/115	-
18	BCR	aM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	845	19	1/1/12/20	11/22/100/115	-
15	CLA	c1	414	-	1/1/10/20	2/8/86/115	-
18	BCR	a4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	c2	413	-	1/1/11/20	7/13/91/115	-
15	CLA	bB	829	-	1/1/15/20	13/37/115/115	-
15	CLA	c2	418	13	1/1/13/20	10/25/103/115	-
15	CLA	a6	413	-	1/1/11/20	8/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bF	201	-	1/1/11/20	5/13/91/115	-
18	BCR	a1	421	-	-	14/29/63/63	0/2/2/2
15	CLA	bB	827	-	1/1/15/20	12/37/115/115	-
15	CLA	aA	823	-	1/1/11/20	3/18/96/115	-
18	BCR	cB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	b5	417	13	1/1/13/20	9/25/103/115	-
15	CLA	aB	842	-	-	0/13/91/115	-
15	CLA	cA	819	-	1/1/12/20	8/24/102/115	-
15	CLA	a4	410	13	1/1/14/20	10/36/114/115	-
15	CLA	c5	402	-	1/1/15/20	14/37/115/115	-
18	BCR	a6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	cB	813	-	1/1/11/20	4/13/91/115	-
18	BCR	aB	845	-	-	11/29/63/63	0/2/2/2
18	BCR	c2	420	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	840	-	1/1/15/20	13/37/115/115	-
15	CLA	cB	832	-	1/1/11/20	7/18/96/115	-
18	BCR	b5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	cK	102	-	1/1/11/20	5/13/91/115	-
15	CLA	c1	413	-	1/1/11/20	1/13/91/115	-
18	BCR	aB	844	-	-	10/29/63/63	0/2/2/2
15	CLA	c5	410	13	1/1/14/20	12/36/114/115	-
15	CLA	bB	813	-	1/1/11/20	4/13/91/115	-
15	CLA	b3	415	-	-	4/13/91/115	-
15	CLA	c5	408	-	1/1/11/20	5/13/91/115	-
18	BCR	bA	850	-	-	11/29/63/63	0/2/2/2
18	BCR	aK	101	-	-	7/29/63/63	0/2/2/2
15	CLA	c4	407	-	1/1/11/20	4/13/91/115	-
15	CLA	bB	818	-	1/1/13/20	10/30/108/115	-
15	CLA	cA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	aA	831	-	1/1/15/20	8/37/115/115	-
15	CLA	aA	820	-	1/1/15/20	18/37/115/115	-
15	CLA	aA	840	-	1/1/11/20	5/16/94/115	-
15	CLA	b4	412	-	1/1/11/20	8/13/91/115	-
15	CLA	a6	415	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	822	-	1/1/11/20	3/13/91/115	-
18	BCR	b4	401	-	-	13/29/63/63	0/2/2/2
15	CLA	c1	416	-	1/1/12/20	7/19/97/115	-
18	BCR	b5	401	-	-	14/29/63/63	0/2/2/2
18	BCR	cA	849	-	-	14/29/63/63	0/2/2/2
15	CLA	aA	818	-	1/1/12/20	5/24/102/115	-
15	CLA	bA	834	-	1/1/15/20	12/37/115/115	-
15	CLA	bA	809	1	1/1/15/20	19/37/115/115	-
15	CLA	cB	822	-	1/1/11/20	3/13/91/115	-
15	CLA	cB	828	-	1/1/15/20	20/37/115/115	-
15	CLA	aA	813	-	1/1/12/20	6/24/102/115	-
15	CLA	cL	202	-	1/1/15/20	7/37/115/115	-
15	CLA	b3	405	-	1/1/11/20	3/13/91/115	-
15	CLA	b1	413	-	1/1/11/20	1/13/91/115	-
15	CLA	a2	422	-	1/1/15/20	9/37/115/115	-
15	CLA	cA	831	-	1/1/15/20	8/37/115/115	-
18	BCR	c1	401	-	-	12/29/63/63	0/2/2/2
19	LHG	cA	853	15	-	14/31/31/53	-
15	CLA	a4	411	13	1/1/11/20	4/13/91/115	-
15	CLA	bB	831	-	1/1/11/20	7/13/91/115	-
18	BCR	cA	848	-	-	11/29/63/63	0/2/2/2
18	BCR	aJ	205	-	-	10/29/63/63	0/2/2/2
18	BCR	c4	418	-	-	9/29/63/63	0/2/2/2
18	BCR	b1	419	-	-	11/29/63/63	0/2/2/2
18	BCR	cB	845	-	-	11/29/63/63	0/2/2/2
15	CLA	c2	408	-	1/1/11/20	4/13/91/115	-
18	BCR	bB	846	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	833	-	1/1/15/20	17/37/115/115	-
15	CLA	aA	812	-	1/1/15/20	11/37/115/115	-
15	CLA	c3	416	-	1/1/12/20	7/19/97/115	-
15	CLA	cA	805	-	1/1/13/20	11/30/108/115	-
18	BCR	c2	421	-	-	12/29/63/63	0/2/2/2
18	BCR	bL	205	-	-	9/29/63/63	0/2/2/2
15	CLA	c6	412	13	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cA	842	-	1/1/15/20	14/37/115/115	-
18	BCR	c2	401	-	-	11/29/63/63	0/2/2/2
15	CLA	b2	416	-	-	4/13/91/115	-
15	CLA	cA	830	-	1/1/15/20	10/37/115/115	-
15	CLA	c3	407	-	1/1/11/20	4/13/91/115	-
15	CLA	cB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	cL	201	10	1/1/15/20	10/37/115/115	-
18	BCR	a6	402	-	-	13/29/63/63	0/2/2/2
18	BCR	c1	418	-	-	8/29/63/63	0/2/2/2
15	CLA	a2	403	-	1/1/15/20	15/37/115/115	-
15	CLA	cA	804	-	1/1/15/20	10/37/115/115	-
15	CLA	bA	832	-	1/1/12/20	6/19/97/115	-
15	CLA	a3	412	-	1/1/11/20	7/13/91/115	-
15	CLA	cF	201	22	1/1/12/20	6/21/99/115	-
15	CLA	bA	824	-	1/1/12/20	9/21/99/115	-
15	CLA	bB	842	-	-	0/13/91/115	-
15	CLA	a2	412	13	1/1/11/20	3/13/91/115	-
15	CLA	c6	406	-	1/1/11/20	3/13/91/115	-
15	CLA	b2	414	-	1/1/11/20	1/13/91/115	-
15	CLA	b2	408	-	1/1/11/20	4/13/91/115	-
15	CLA	b1	417	13	1/1/13/20	10/25/103/115	-
15	CLA	a2	410	-	1/1/15/20	4/37/115/115	-
15	CLA	a6	417	-	1/1/12/20	7/19/97/115	-
15	CLA	aB	828	-	1/1/15/20	20/37/115/115	-
18	BCR	aA	850	-	-	14/29/63/63	0/2/2/2
18	BCR	bL	201	-	-	12/29/63/63	0/2/2/2
18	BCR	b2	421	-	-	12/29/63/63	0/2/2/2
15	CLA	b2	402	-	1/1/15/20	12/37/115/115	-
15	CLA	c4	421	-	1/1/15/20	7/37/115/115	-
15	CLA	aA	839	-	1/1/15/20	13/37/115/115	-
18	BCR	cF	202	-	-	12/29/63/63	0/2/2/2
15	CLA	b5	413	-	1/1/11/20	1/13/91/115	-
15	CLA	c4	414	-	1/1/10/20	2/8/86/115	-
16	PQN	cA	845	-	-	6/23/43/43	0/2/2/2
15	CLA	aA	828	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	a3	420	-	-	12/29/63/63	0/2/2/2
18	BCR	a2	401	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	810	2	1/1/15/20	12/37/115/115	-
15	CLA	cB	842	-	-	0/13/91/115	-
15	CLA	a4	403	-	1/1/15/20	15/37/115/115	-
15	CLA	bB	801	-	1/1/15/20	10/37/115/115	-
15	CLA	c3	404	-	1/1/15/20	10/37/115/115	-
18	BCR	c3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	b5	409	-	1/1/15/20	5/37/115/115	-
15	CLA	b3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	b1	408	-	1/1/11/20	5/13/91/115	-
18	BCR	aI	103	-	-	9/29/63/63	0/2/2/2
15	CLA	c5	403	-	1/1/15/20	15/37/115/115	-
18	BCR	cK	101	-	-	7/29/63/63	0/2/2/2
18	BCR	c5	401	-	-	14/29/63/63	0/2/2/2
15	CLA	aB	830	-	1/1/15/20	5/37/115/115	-
15	CLA	b4	416	-	1/1/12/20	7/19/97/115	-
15	CLA	bB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	b5	416	-	1/1/12/20	7/19/97/115	-
15	CLA	b3	408	-	1/1/11/20	5/13/91/115	-
15	CLA	bB	839	22	1/1/15/20	8/37/115/115	-
15	CLA	b5	404	-	1/1/15/20	7/37/115/115	-
15	CLA	c4	409	-	1/1/15/20	5/37/115/115	-
15	CLA	a2	406	-	1/1/15/20	8/37/115/115	-
15	CLA	aA	808	-	-	2/21/99/115	-
15	CLA	b4	407	-	1/1/11/20	4/13/91/115	-
15	CLA	b1	405	-	1/1/11/20	3/13/91/115	-
18	BCR	a6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	c6	405	-	1/1/15/20	7/37/115/115	-
15	CLA	b5	407	-	1/1/11/20	4/13/91/115	-
15	CLA	b1	406	-	1/1/11/20	4/13/91/115	-
15	CLA	b1	415	-	-	4/13/91/115	-
15	CLA	b5	405	-	1/1/11/20	3/13/91/115	-
15	CLA	a1	404	-	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a2	417	-	1/1/12/20	7/19/97/115	-
15	CLA	cA	826	-	1/1/15/20	10/37/115/115	-
15	CLA	aL	202	-	1/1/15/20	7/37/115/115	-
18	BCR	cB	848	-	-	13/29/63/63	0/2/2/2
18	BCR	c5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	402	-	1/1/15/20	14/37/115/115	-
15	CLA	bB	811	2	1/1/15/20	9/37/115/115	-
15	CLA	bB	806	-	1/1/15/20	19/37/115/115	-
15	CLA	c2	406	-	1/1/15/20	8/37/115/115	-
15	CLA	c6	407	-	1/1/11/20	4/13/91/115	-
15	CLA	bA	808	-	-	2/21/99/115	-
18	BCR	bJ	105	-	-	10/29/63/63	0/2/2/2
16	PQN	aA	846	-	-	6/23/43/43	0/2/2/2
15	CLA	aB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	bA	821	-	1/1/14/20	14/33/111/115	-
15	CLA	c4	413	-	1/1/11/20	1/13/91/115	-
15	CLA	a4	417	13	1/1/13/20	8/25/103/115	-
15	CLA	bA	839	-	1/1/15/20	13/37/115/115	-
15	CLA	c1	406	-	1/1/11/20	4/13/91/115	-
15	CLA	aB	808	-	-	9/37/115/115	-
15	CLA	cB	830	-	1/1/15/20	5/37/115/115	-
19	LHG	bA	854	-	-	18/53/53/53	-
15	CLA	a2	405	-	1/1/11/20	3/13/91/115	-
15	CLA	bA	828	-	1/1/15/20	9/37/115/115	-
15	CLA	aB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	a6	407	-	1/1/11/20	4/13/91/115	-
15	CLA	b4	404	-	1/1/15/20	8/37/115/115	-
18	BCR	bI	101	-	-	10/29/63/63	0/2/2/2
18	BCR	bL	206	-	-	12/29/63/63	0/2/2/2
15	CLA	b6	412	13	1/1/11/20	4/13/91/115	-
15	CLA	b1	403	-	1/1/15/20	15/37/115/115	-
15	CLA	a2	416	-	-	4/13/91/115	-
15	CLA	cA	807	-	1/1/15/20	9/37/115/115	-
15	CLA	cA	806	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a2	404	-	1/1/15/20	8/37/115/115	-
15	CLA	c4	416	-	1/1/12/20	7/19/97/115	-
15	CLA	aB	817	-	1/1/13/20	9/25/103/115	-
15	CLA	b2	405	-	1/1/11/20	3/13/91/115	-
15	CLA	aB	823	-	1/1/13/20	4/25/103/115	-
15	CLA	a4	402	-	1/1/15/20	14/37/115/115	-
15	CLA	bB	832	-	1/1/11/20	7/18/96/115	-
15	CLA	cB	817	-	1/1/13/20	9/25/103/115	-
18	BCR	aF	203	-	-	10/29/63/63	0/2/2/2
18	BCR	c4	401	-	-	13/29/63/63	0/2/2/2
17	SF4	aC	101	3	-	-	0/6/5/5
15	CLA	c6	411	13	1/1/14/20	10/36/114/115	-
15	CLA	c6	410	-	1/1/15/20	5/37/115/115	-
15	CLA	c6	408	-	1/1/11/20	4/13/91/115	-
18	BCR	c6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a5	408	-	1/1/11/20	5/13/91/115	-
15	CLA	aB	832	-	1/1/11/20	7/18/96/115	-
18	BCR	b2	401	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	812	-	1/1/11/20	3/13/91/115	-
15	CLA	a4	406	-	1/1/11/20	4/13/91/115	-
15	CLA	a4	408	-	1/1/11/20	5/13/91/115	-
15	CLA	c2	404	-	1/1/15/20	7/37/115/115	-
18	BCR	aA	851	-	-	8/29/63/63	0/2/2/2
15	CLA	b5	412	-	1/1/11/20	7/13/91/115	-
15	CLA	b6	408	-	1/1/11/20	4/13/91/115	-
15	CLA	cA	825	-	1/1/13/20	13/30/108/115	-
15	CLA	a5	402	-	1/1/15/20	14/37/115/115	-
18	BCR	bB	844	-	-	10/29/63/63	0/2/2/2
15	CLA	b1	410	13	1/1/14/20	11/36/114/115	-
15	CLA	aA	832	-	1/1/12/20	6/19/97/115	-
18	BCR	a4	401	-	-	13/29/63/63	0/2/2/2
18	BCR	a3	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a1	414	-	-	4/13/91/115	-
15	CLA	bA	813	-	1/1/12/20	6/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aJ	201	-	1/1/11/20	5/13/91/115	-
15	CLA	c2	417	-	1/1/12/20	7/19/97/115	-
15	CLA	cB	811	2	1/1/15/20	9/37/115/115	-
15	CLA	aA	810	1	1/1/15/20	15/37/115/115	-
15	CLA	cA	836	-	1/1/12/20	6/24/102/115	-
15	CLA	cB	806	-	1/1/15/20	19/37/115/115	-
15	CLA	cB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	c6	409	-	1/1/11/20	5/13/91/115	-
15	CLA	a1	405	-	1/1/11/20	4/13/91/115	-
15	CLA	a5	412	-	1/1/11/20	8/13/91/115	-
15	CLA	b4	421	-	1/1/15/20	7/37/115/115	-
15	CLA	cB	820	22	1/1/15/20	8/37/115/115	-
18	BCR	a2	420	-	-	10/29/63/63	0/2/2/2
15	CLA	c2	410	-	1/1/15/20	5/37/115/115	-
15	CLA	bA	823	-	1/1/11/20	3/18/96/115	-
15	CLA	aL	203	22	1/1/15/20	10/37/115/115	-
15	CLA	a4	409	-	1/1/15/20	5/37/115/115	-
15	CLA	b1	411	13	1/1/11/20	4/13/91/115	-
18	BCR	a3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	a6	410	-	1/1/15/20	5/37/115/115	-
18	BCR	c4	420	-	-	12/29/63/63	0/2/2/2
18	BCR	aA	848	-	-	11/29/63/63	0/2/2/2
15	CLA	cB	827	-	1/1/15/20	12/37/115/115	-
15	CLA	aJ	203	-	1/1/8/20	0/2/76/115	-
18	BCR	bB	845	-	-	11/29/63/63	0/2/2/2
18	BCR	c1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	a1	416	13	1/1/13/20	9/25/103/115	-
15	CLA	cB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	c6	404	-	1/1/15/20	15/37/115/115	-
15	CLA	bA	818	-	1/1/12/20	6/24/102/115	-
18	BCR	aF	202	-	-	10/29/63/63	0/2/2/2
15	CLA	c5	409	-	1/1/15/20	5/37/115/115	-
15	CLA	a1	411	-	1/1/11/20	8/13/91/115	-
15	CLA	bB	838	-	1/1/11/20	1/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a1	403	-	1/1/15/20	9/37/115/115	-
15	CLA	bA	827	22	1/1/15/20	8/37/115/115	-
15	CLA	bA	838	-	1/1/12/20	6/21/99/115	-
15	CLA	a5	409	-	1/1/15/20	5/37/115/115	-
15	CLA	a4	414	-	1/1/10/20	2/8/86/115	-
15	CLA	bL	203	-	1/1/15/20	7/37/115/115	-
19	LHG	bX	101	-	-	12/26/26/53	-
15	CLA	c1	410	13	1/1/14/20	11/36/114/115	-
15	CLA	c5	404	-	1/1/15/20	7/37/115/115	-
19	LHG	aA	854	15	-	14/31/31/53	-
15	CLA	a4	415	-	-	4/13/91/115	-
15	CLA	b3	409	-	1/1/15/20	6/37/115/115	-
15	CLA	aA	805	-	1/1/13/20	11/30/108/115	-
15	CLA	aB	803	-	1/1/15/20	12/37/115/115	-
15	CLA	bB	819	-	1/1/14/20	11/31/109/115	-
15	CLA	c5	414	-	1/1/10/20	2/8/86/115	-
15	CLA	a3	405	-	1/1/11/20	3/13/91/115	-
18	BCR	aJ	204	-	-	12/29/63/63	0/2/2/2
18	BCR	bF	202	-	-	10/29/63/63	0/2/2/2
15	CLA	aB	838	-	1/1/11/20	1/16/94/115	-
15	CLA	bB	816	-	1/1/11/20	6/13/91/115	-
15	CLA	c2	422	-	1/1/15/20	9/37/115/115	-
15	CLA	cB	802	-	1/1/15/20	7/37/115/115	-
15	CLA	bB	836	-	1/1/14/20	8/31/109/115	-
15	CLA	bB	837	-	1/1/15/20	13/37/115/115	-
15	CLA	a3	415	-	-	4/13/91/115	-
15	CLA	a3	407	-	1/1/11/20	4/13/91/115	-
15	CLA	aX	102	12	1/1/11/20	6/13/91/115	-
15	CLA	cB	841	-	1/1/11/20	2/13/91/115	-
15	CLA	a4	413	-	1/1/11/20	1/13/91/115	-
17	SF4	cA	846	2,1	-	-	0/6/5/5
15	CLA	b3	407	-	1/1/11/20	4/13/91/115	-
15	CLA	a3	417	13	1/1/13/20	11/25/103/115	-
15	CLA	cB	814	-	1/1/15/20	24/37/115/115	-
19	LHG	aA	853	-	-	18/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b5	411	13	1/1/11/20	3/13/91/115	-
15	CLA	c5	413	-	1/1/11/20	1/13/91/115	-
15	CLA	cA	815	-	1/1/11/20	1/13/91/115	-
15	CLA	c3	417	13	1/1/13/20	11/25/103/115	-
15	CLA	bB	814	-	1/1/15/20	24/37/115/115	-
15	CLA	b1	402	-	1/1/15/20	13/37/115/115	-
15	CLA	b3	421	-	1/1/15/20	7/37/115/115	-
15	CLA	cB	834	-	1/1/13/20	10/29/107/115	-
15	CLA	c3	415	-	-	4/13/91/115	-
15	CLA	bA	814	-	1/1/14/20	13/31/109/115	-
15	CLA	b3	414	-	1/1/10/20	2/8/86/115	-
15	CLA	aB	825	2	1/1/12/20	9/24/102/115	-
15	CLA	aA	804	-	1/1/15/20	10/37/115/115	-
15	CLA	a3	408	-	1/1/11/20	5/13/91/115	-
15	CLA	cA	812	-	1/1/15/20	11/37/115/115	-
15	CLA	c2	412	13	1/1/11/20	3/13/91/115	-
15	CLA	bB	815	-	1/1/15/20	16/37/115/115	-
15	CLA	b2	407	-	1/1/11/20	4/13/91/115	-
18	BCR	bA	851	-	-	14/29/63/63	0/2/2/2
15	CLA	bA	803	-	1/1/15/20	12/37/115/115	-
15	CLA	b3	413	-	1/1/11/20	1/13/91/115	-
15	CLA	cA	835	-	1/1/15/20	12/37/115/115	-
18	BCR	a1	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	844	19	1/1/12/20	11/22/100/115	-
14	CL0	bA	801	-	3/3/20/25	4/37/135/135	-
15	CLA	a3	404	-	1/1/15/20	9/37/115/115	-
15	CLA	bL	204	22	1/1/15/20	10/37/115/115	-
15	CLA	c6	403	-	1/1/15/20	12/37/115/115	-
18	BCR	bI	102	-	-	9/29/63/63	0/2/2/2
15	CLA	a5	405	-	1/1/11/20	3/13/91/115	-
18	BCR	bJ	103	-	-	12/29/63/63	0/2/2/2
15	CLA	b3	416	-	1/1/12/20	7/19/97/115	-
15	CLA	c2	411	13	1/1/14/20	9/36/114/115	-
15	CLA	a3	403	-	1/1/15/20	15/37/115/115	-
15	CLA	cB	807	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	826	-	1/1/15/20	10/37/115/115	-
15	CLA	c4	406	-	1/1/11/20	4/13/91/115	-
15	CLA	bB	805	-	1/1/12/20	5/24/102/115	-
15	CLA	aA	811	-	1/1/11/20	6/13/91/115	-
15	CLA	a1	412	-	1/1/11/20	1/13/91/115	-
15	CLA	b6	414	-	1/1/11/20	1/13/91/115	-
15	CLA	aA	806	-	1/1/15/20	19/37/115/115	-
15	CLA	cA	828	-	1/1/15/20	9/37/115/115	-
18	BCR	a5	401	-	-	13/29/63/63	0/2/2/2
15	CLA	cA	817	-	-	4/18/96/115	-
15	CLA	a6	416	-	-	4/13/91/115	-
15	CLA	a4	412	-	1/1/11/20	8/13/91/115	-
15	CLA	aA	827	22	1/1/15/20	8/37/115/115	-
15	CLA	c2	403	-	1/1/15/20	15/37/115/115	-
15	CLA	b4	403	-	1/1/15/20	15/37/115/115	-
18	BCR	b2	420	-	-	9/29/63/63	0/2/2/2
18	BCR	bB	847	-	-	9/18/35/63	0/1/1/2
17	SF4	aA	847	2,1	-	-	0/6/5/5
15	CLA	bB	828	-	1/1/15/20	20/37/115/115	-
15	CLA	cA	829	-	1/1/15/20	18/37/115/115	-
18	BCR	cM	101	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	834	-	1/1/13/20	10/29/107/115	-
15	CLA	cB	831	-	1/1/11/20	7/13/91/115	-
15	CLA	c3	411	13	1/1/11/20	4/13/91/115	-
18	BCR	a6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	cB	840	-	1/1/15/20	13/37/115/115	-
15	CLA	cB	825	2	1/1/12/20	9/24/102/115	-
15	CLA	bB	826	22	1/1/11/20	8/15/93/115	-
15	CLA	b2	413	-	1/1/11/20	8/13/91/115	-
15	CLA	cA	843	-	1/1/9/20	5/7/81/115	-
14	CL0	aA	801	-	3/3/20/25	4/37/135/135	-
15	CLA	b6	409	-	1/1/11/20	5/13/91/115	-
15	CLA	bB	830	-	1/1/15/20	5/37/115/115	-
18	BCR	a5	418	-	-	11/29/63/63	0/2/2/2
15	CLA	bB	820	22	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a5	420	-	1/1/15/20	8/37/115/115	-
15	CLA	bL	202	10	1/1/15/20	10/37/115/115	-
15	CLA	cA	833	-	1/1/15/20	12/37/115/115	-
15	CLA	c1	403	-	1/1/15/20	15/37/115/115	-
15	CLA	cA	839	-	1/1/15/20	13/37/115/115	-
18	BCR	b2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	b6	416	-	-	4/13/91/115	-
15	CLA	a4	421	-	1/1/15/20	7/37/115/115	-
15	CLA	a6	422	-	1/1/15/20	13/37/115/115	-
15	CLA	bA	837	1	-	5/13/91/115	-
17	SF4	bA	847	2,1	-	-	0/6/5/5
15	CLA	b6	407	-	1/1/11/20	4/13/91/115	-
15	CLA	aB	812	-	1/1/11/20	3/13/91/115	-
15	CLA	bB	835	-	1/1/11/20	9/13/91/115	-
15	CLA	bB	823	-	1/1/13/20	4/25/103/115	-
15	CLA	a6	412	13	1/1/11/20	4/13/91/115	-
15	CLA	c3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	c3	408	-	1/1/11/20	5/13/91/115	-
15	CLA	a5	414	-	1/1/10/20	2/8/86/115	-
15	CLA	aA	814	-	1/1/14/20	13/31/109/115	-
18	BCR	bB	849	-	-	12/29/63/63	0/2/2/2
15	CLA	aB	827	-	1/1/15/20	12/37/115/115	-
17	SF4	bC	102	3	-	-	0/6/5/5
19	LHG	cX	101	-	-	12/26/26/53	-
15	CLA	aB	821	-	1/1/11/20	11/16/94/115	-
15	CLA	c4	404	-	1/1/15/20	8/37/115/115	-
18	BCR	bB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	b1	416	-	1/1/12/20	7/19/97/115	-
15	CLA	b4	406	-	1/1/11/20	4/13/91/115	-
15	CLA	a5	417	13	1/1/13/20	9/25/103/115	-
15	CLA	cA	808	-	-	2/21/99/115	-
15	CLA	c5	412	-	1/1/11/20	8/13/91/115	-
15	CLA	aA	844	-	1/1/9/20	5/7/81/115	-
15	CLA	aB	839	22	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	cB	837	-	1/1/15/20	13/37/115/115	-
15	CLA	c1	412	-	1/1/11/20	8/13/91/115	-
15	CLA	aA	838	-	1/1/12/20	6/21/99/115	-
15	CLA	b2	404	-	1/1/15/20	7/37/115/115	-
15	CLA	b6	413	-	1/1/11/20	8/13/91/115	-
18	BCR	cB	844	-	-	10/29/63/63	0/2/2/2
15	CLA	a6	403	-	1/1/15/20	12/37/115/115	-
15	CLA	cA	802	22	1/1/15/20	15/37/115/115	-
15	CLA	c3	403	-	1/1/15/20	15/37/115/115	-
15	CLA	b4	415	-	-	4/13/91/115	-
15	CLA	a1	406	-	1/1/11/20	4/13/91/115	-
15	CLA	bA	843	-	1/1/15/20	14/37/115/115	-
15	CLA	cA	838	-	1/1/12/20	6/21/99/115	-
15	CLA	c4	410	13	1/1/14/20	10/36/114/115	-
16	PQN	cB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	b6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	802	22	1/1/15/20	15/37/115/115	-
15	CLA	a5	416	-	1/1/12/20	7/19/97/115	-
15	CLA	bA	806	-	1/1/15/20	19/37/115/115	-
15	CLA	a3	411	13	1/1/11/20	4/13/91/115	-
15	CLA	c4	417	13	1/1/13/20	8/25/103/115	-
15	CLA	c5	407	-	1/1/11/20	4/13/91/115	-
18	BCR	bA	848	-	-	7/29/63/63	0/2/2/2
15	CLA	c3	410	13	1/1/14/20	9/36/114/115	-
15	CLA	b6	404	-	1/1/15/20	15/37/115/115	-
15	CLA	a5	407	-	1/1/11/20	4/13/91/115	-
15	CLA	bA	805	-	1/1/13/20	11/30/108/115	-
15	CLA	c6	415	-	1/1/10/20	2/8/86/115	-
18	BCR	b6	421	-	-	13/29/63/63	0/2/2/2
15	CLA	b1	409	-	1/1/15/20	5/37/115/115	-
15	CLA	aK	102	-	1/1/11/20	5/13/91/115	-
15	CLA	b5	420	-	1/1/15/20	8/37/115/115	-
15	CLA	c6	417	-	1/1/12/20	7/19/97/115	-
18	BCR	cA	847	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aB	805	-	1/1/12/20	5/24/102/115	-
18	BCR	cI	102	-	-	9/29/63/63	0/2/2/2
15	CLA	cB	833	-	1/1/15/20	17/37/115/115	-
18	BCR	cL	204	-	-	9/29/63/63	0/2/2/2
15	CLA	a1	409	13	1/1/14/20	11/36/114/115	-
15	CLA	a5	413	-	1/1/11/20	1/13/91/115	-
15	CLA	bB	804	-	1/1/15/20	9/37/115/115	-
15	CLA	cJ	102	-	1/1/8/20	0/2/76/115	-
15	CLA	cB	808	-	-	9/37/115/115	-
15	CLA	aA	816	-	-	3/13/91/115	-
15	CLA	aB	813	-	1/1/11/20	4/13/91/115	-
15	CLA	aA	836	-	1/1/12/20	6/24/102/115	-
15	CLA	bB	807	-	1/1/15/20	15/37/115/115	-
15	CLA	cA	814	-	1/1/14/20	13/31/109/115	-
15	CLA	cJ	101	8	1/1/11/20	4/13/91/115	-
15	CLA	bB	817	-	1/1/13/20	10/25/103/115	-
15	CLA	a6	405	-	1/1/15/20	9/37/115/115	-
15	CLA	c1	402	-	1/1/15/20	13/37/115/115	-
15	CLA	c4	411	13	1/1/11/20	4/13/91/115	-
15	CLA	c6	414	-	1/1/11/20	1/13/91/115	-
16	PQN	bA	846	-	-	6/23/43/43	0/2/2/2
15	CLA	cB	823	-	1/1/13/20	4/25/103/115	-
15	CLA	b2	403	-	1/1/15/20	15/37/115/115	-
15	CLA	b5	403	-	1/1/15/20	15/37/115/115	-
15	CLA	bB	812	-	1/1/11/20	3/13/91/115	-
18	BCR	c2	419	-	-	10/29/63/63	0/2/2/2
15	CLA	aJ	202	8	1/1/11/20	4/13/91/115	-
15	CLA	cL	203	22	1/1/15/20	10/37/115/115	-
18	BCR	a4	418	-	-	10/29/63/63	0/2/2/2
18	BCR	b4	419	-	-	11/29/63/63	0/2/2/2
15	CLA	bA	841	-	1/1/15/20	15/37/115/115	-
15	CLA	a2	413	-	1/1/11/20	8/13/91/115	-
15	CLA	bA	829	-	1/1/15/20	18/37/115/115	-
15	CLA	bB	802	-	1/1/15/20	7/37/115/115	-
18	BCR	aL	205	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a3	402	-	1/1/15/20	14/37/115/115	-
15	CLA	a1	415	-	1/1/12/20	7/19/97/115	-
15	CLA	a5	404	-	1/1/15/20	7/37/115/115	-
15	CLA	bB	840	-	1/1/15/20	13/37/115/115	-
15	CLA	b4	410	13	1/1/14/20	10/36/114/115	-
18	BCR	a2	419	-	-	10/29/63/63	0/2/2/2
20	LMG	aB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	bA	811	-	1/1/11/20	6/13/91/115	-
15	CLA	bB	809	-	1/1/15/20	11/37/115/115	-
15	CLA	c6	413	-	1/1/11/20	8/13/91/115	-
18	BCR	c6	401	-	-	11/29/63/63	0/2/2/2
15	CLA	a2	409	-	1/1/11/20	5/13/91/115	-
15	CLA	a6	406	-	1/1/11/20	3/13/91/115	-
15	CLA	aA	802	22	1/1/15/20	15/37/115/115	-
18	BCR	a4	419	-	-	11/29/63/63	0/2/2/2
18	BCR	aI	102	-	-	9/29/63/63	0/2/2/2
15	CLA	aA	833	-	1/1/15/20	12/37/115/115	-
15	CLA	cB	818	-	1/1/13/20	10/30/108/115	-
15	CLA	a1	413	-	1/1/10/20	2/8/86/115	-
15	CLA	c3	421	-	1/1/15/20	7/37/115/115	-
15	CLA	c3	414	-	1/1/10/20	2/8/86/115	-
15	CLA	b4	405	-	1/1/11/20	3/13/91/115	-
15	CLA	bA	836	-	1/1/12/20	6/24/102/115	-
15	CLA	bA	807	-	1/1/15/20	9/37/115/115	-
15	CLA	b3	411	13	1/1/11/20	5/13/91/115	-
15	CLA	c2	415	-	1/1/10/20	2/8/86/115	-
18	BCR	c5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	c6	418	13	1/1/13/20	10/25/103/115	-
18	BCR	a6	420	-	-	12/29/63/63	0/2/2/2
15	CLA	cB	835	-	1/1/11/20	9/13/91/115	-
15	CLA	a2	408	-	1/1/11/20	4/13/91/115	-
15	CLA	aB	837	-	1/1/15/20	13/37/115/115	-
17	SF4	bC	101	3	-	-	0/6/5/5
18	BCR	cB	849	-	-	11/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	aA	843	-	1/1/15/20	14/37/115/115	-
15	CLA	a6	404	-	1/1/15/20	15/37/115/115	-
15	CLA	b6	406	-	1/1/11/20	3/13/91/115	-
15	CLA	aB	818	-	1/1/13/20	10/30/108/115	-
15	CLA	cA	810	1	1/1/15/20	15/37/115/115	-
20	LMG	bB	851	-	-	26/50/70/70	0/1/1/1
15	CLA	bA	812	-	1/1/15/20	11/37/115/115	-
15	CLA	c1	415	-	-	4/13/91/115	-
18	BCR	aB	847	-	-	9/18/35/63	0/1/1/2
15	CLA	cA	809	1	1/1/15/20	19/37/115/115	-
15	CLA	bA	815	-	1/1/11/20	0/13/91/115	-
15	CLA	b2	412	13	1/1/11/20	3/13/91/115	-
15	CLA	aB	807	-	1/1/15/20	15/37/115/115	-
15	CLA	bK	101	-	1/1/11/20	5/13/91/115	-
15	CLA	b4	417	13	1/1/13/20	9/25/103/115	-
15	CLA	a1	422	-	1/1/15/20	12/37/115/115	-
15	CLA	c2	405	-	1/1/11/20	3/13/91/115	-
15	CLA	cB	838	-	1/1/11/20	1/16/94/115	-
15	CLA	c1	417	13	1/1/13/20	9/25/103/115	-
18	BCR	b1	401	-	-	12/29/63/63	0/2/2/2
15	CLA	bJ	101	8	1/1/11/20	4/13/91/115	-
15	CLA	cA	823	-	1/1/11/20	3/18/96/115	-
18	BCR	c6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	c4	412	-	1/1/11/20	8/13/91/115	-
15	CLA	a3	413	-	1/1/11/20	1/13/91/115	-
15	CLA	aB	834	-	1/1/13/20	10/29/107/115	-
15	CLA	bA	844	-	1/1/9/20	5/7/81/115	-
15	CLA	c3	402	-	1/1/15/20	14/37/115/115	-
15	CLA	b4	411	13	1/1/11/20	4/13/91/115	-
15	CLA	a6	418	13	1/1/13/20	10/25/103/115	-
15	CLA	aA	817	-	-	4/18/96/115	-
18	BCR	c1	419	-	-	11/29/63/63	0/2/2/2
15	CLA	aB	820	22	1/1/15/20	8/37/115/115	-
15	CLA	a2	411	13	1/1/14/20	10/36/114/115	-
15	CLA	b3	402	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b3	410	13	1/1/14/20	9/36/114/115	-
15	CLA	cA	822	-	1/1/15/20	15/37/115/115	-
18	BCR	aB	848	-	-	13/29/63/63	0/2/2/2
15	CLA	b2	415	-	1/1/10/20	2/8/86/115	-
18	BCR	aF	201	-	-	12/29/63/63	0/2/2/2
18	BCR	cJ	103	-	-	12/29/63/63	0/2/2/2
15	CLA	cA	811	-	1/1/11/20	6/13/91/115	-
16	PQN	aB	843	-	-	10/23/43/43	0/2/2/2
18	BCR	b1	418	-	-	9/29/63/63	0/2/2/2
15	CLA	a1	408	-	1/1/15/20	5/37/115/115	-
15	CLA	c3	413	-	1/1/11/20	1/13/91/115	-
15	CLA	bA	822	-	1/1/15/20	15/37/115/115	-
18	BCR	cJ	104	-	-	10/29/63/63	0/2/2/2
15	CLA	b2	417	-	1/1/12/20	7/19/97/115	-
15	CLA	b1	412	-	1/1/11/20	8/13/91/115	-
15	CLA	b6	418	13	1/1/13/20	10/25/103/115	-
18	BCR	c3	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bX	102	12	1/1/11/20	6/13/91/115	-
15	CLA	bB	833	-	1/1/15/20	17/37/115/115	-
15	CLA	bA	842	22	1/1/12/20	6/21/99/115	-
15	CLA	bB	808	-	-	9/37/115/115	-
15	CLA	a3	406	-	1/1/11/20	4/13/91/115	-
15	CLA	bA	840	-	1/1/11/20	5/16/94/115	-
18	BCR	c6	402	-	-	13/29/63/63	0/2/2/2
15	CLA	a5	411	13	1/1/11/20	3/13/91/115	-
18	BCR	b5	419	-	-	12/29/63/63	0/2/2/2
20	LMG	cB	850	-	-	26/50/70/70	0/1/1/1
15	CLA	aA	824	-	1/1/12/20	9/21/99/115	-
18	BCR	a1	417	-	-	9/29/63/63	0/2/2/2
15	CLA	b6	417	-	1/1/12/20	7/19/97/115	-
15	CLA	aB	801	-	1/1/15/20	10/37/115/115	-
15	CLA	bJ	102	-	1/1/8/20	0/2/76/115	-
15	CLA	aA	807	-	1/1/15/20	9/37/115/115	-
15	CLA	aB	810	2	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	b4	420	-	-	12/29/63/63	0/2/2/2
15	CLA	c3	405	-	1/1/11/20	3/13/91/115	-
15	CLA	b6	410	-	1/1/15/20	5/37/115/115	-
15	CLA	aB	841	-	1/1/11/20	2/13/91/115	-
15	CLA	aB	829	-	1/1/15/20	13/37/115/115	-
15	CLA	bB	824	-	1/1/11/20	3/13/91/115	-
15	CLA	bB	825	2	1/1/12/20	9/24/102/115	-
15	CLA	aA	845	19	1/1/12/20	11/22/100/115	-
18	BCR	cA	851	-	-	22/29/63/63	0/2/2/2
15	CLA	bA	825	-	1/1/13/20	13/30/108/115	-
15	CLA	aA	830	-	1/1/15/20	10/37/115/115	-
15	CLA	b5	415	-	-	5/13/91/115	-
18	BCR	bB	850	-	-	11/29/63/63	0/2/2/2
15	CLA	aA	809	1	1/1/15/20	19/37/115/115	-
15	CLA	a2	402	-	1/1/15/20	12/37/115/115	-
15	CLA	bB	841	-	1/1/11/20	2/13/91/115	-
18	BCR	aA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	c4	403	-	1/1/15/20	15/37/115/115	-
15	CLA	b2	406	-	1/1/15/20	8/37/115/115	-
15	CLA	cA	832	-	1/1/12/20	6/19/97/115	-
17	SF4	cC	102	3	-	-	0/6/5/5
17	SF4	cC	101	3	-	-	0/6/5/5
15	CLA	b3	417	13	1/1/13/20	11/25/103/115	-
15	CLA	a2	414	-	1/1/11/20	0/13/91/115	-
15	CLA	a2	407	-	1/1/11/20	4/13/91/115	-
14	CL0	cA	801	-	3/3/20/25	4/37/135/135	-
15	CLA	a3	409	-	1/1/15/20	4/37/115/115	-
15	CLA	a1	407	-	1/1/11/20	5/13/91/115	-
18	BCR	b6	419	-	-	10/29/63/63	0/2/2/2
15	CLA	bA	826	-	1/1/15/20	10/37/115/115	-
15	CLA	cB	836	-	1/1/14/20	8/31/109/115	-
15	CLA	b1	414	-	1/1/10/20	2/8/86/115	-
15	CLA	cF	203	-	1/1/11/20	5/13/91/115	-
15	CLA	b1	407	-	1/1/11/20	4/13/91/115	-
15	CLA	c1	411	13	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	bB	803	-	1/1/15/20	12/37/115/115	-
15	CLA	cB	824	-	1/1/11/20	3/13/91/115	-
15	CLA	bA	835	-	1/1/15/20	12/37/115/115	-
15	CLA	cB	819	-	1/1/14/20	11/31/109/115	-
15	CLA	c5	416	-	1/1/12/20	7/19/97/115	-
18	BCR	cF	205	-	-	10/29/63/63	0/2/2/2
15	CLA	cA	840	-	1/1/11/20	5/16/94/115	-
15	CLA	aA	822	-	1/1/15/20	15/37/115/115	-
15	CLA	aB	826	22	1/1/11/20	8/15/93/115	-
18	BCR	bA	849	-	-	11/29/63/63	0/2/2/2
15	CLA	a5	403	-	1/1/15/20	15/37/115/115	-
15	CLA	c2	407	-	1/1/11/20	4/13/91/115	-
15	CLA	c3	409	-	-	5/37/115/115	-
15	CLA	aB	806	-	1/1/15/20	19/37/115/115	-
15	CLA	b3	404	-	1/1/15/20	10/37/115/115	-
18	BCR	b3	420	-	-	12/29/63/63	0/2/2/2
15	CLA	aA	834	-	1/1/15/20	12/37/115/115	-
15	CLA	b5	406	-	1/1/11/20	4/13/91/115	-
18	BCR	cF	204	-	-	10/29/63/63	0/2/2/2
15	CLA	b6	411	13	1/1/14/20	10/36/114/115	-
15	CLA	cB	810	2	1/1/15/20	12/37/115/115	-
15	CLA	b6	415	-	1/1/10/20	2/8/86/115	-
18	BCR	aB	846	-	-	12/29/63/63	0/2/2/2
15	CLA	bA	831	-	1/1/15/20	8/37/115/115	-
15	CLA	cA	821	-	1/1/14/20	14/33/111/115	-
15	CLA	cB	829	-	1/1/15/20	13/37/115/115	-
18	BCR	aB	849	-	-	11/29/63/63	0/2/2/2
15	CLA	b3	403	-	1/1/15/20	15/37/115/115	-
15	CLA	cA	818	-	1/1/12/20	6/24/102/115	-
18	BCR	a5	419	-	-	12/29/63/63	0/2/2/2
15	CLA	c1	407	-	1/1/11/20	4/13/91/115	-
18	BCR	cB	846	-	-	12/29/63/63	0/2/2/2
16	PQN	bB	843	-	-	10/23/43/43	0/2/2/2
15	CLA	b6	422	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a3	410	13	1/1/14/20	9/36/114/115	-
15	CLA	cA	803	-	1/1/15/20	12/37/115/115	-
18	BCR	b3	401	-	-	12/29/63/63	0/2/2/2
15	CLA	a2	415	-	1/1/10/20	2/8/86/115	-
15	CLA	aB	831	-	1/1/11/20	7/13/91/115	-
15	CLA	cB	839	22	1/1/15/20	8/37/115/115	-
17	SF4	aC	102	3	-	-	0/6/5/5
15	CLA	c4	415	-	-	4/13/91/115	-
15	CLA	b5	414	-	1/1/10/20	2/8/86/115	-
18	BCR	bA	852	-	-	8/29/63/63	0/2/2/2
15	CLA	bA	830	-	1/1/15/20	10/37/115/115	-
15	CLA	aA	821	-	1/1/14/20	14/33/111/115	-
15	CLA	c3	412	-	1/1/11/20	7/13/91/115	-
15	CLA	aB	814	-	1/1/15/20	24/37/115/115	-
15	CLA	cA	816	-	-	3/13/91/115	-
15	CLA	cA	837	1	-	5/13/91/115	-
15	CLA	aB	802	-	1/1/15/20	7/37/115/115	-
15	CLA	a4	405	-	1/1/11/20	3/13/91/115	-
18	BCR	bM	101	-	-	11/29/63/63	0/2/2/2

The worst 5 of 5028 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	aA	846	PQN	C3-C2	7.05	1.47	1.35
16	bA	846	PQN	C3-C2	7.01	1.47	1.35
16	cA	845	PQN	C3-C2	6.99	1.47	1.35
16	cB	843	PQN	C3-C2	6.91	1.47	1.35
16	aB	843	PQN	C3-C2	6.90	1.47	1.35

The worst 5 of 7305 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	cB	804	CLA	C4A-NA-C1A	10.42	111.43	106.68
15	bB	804	CLA	C4A-NA-C1A	10.41	111.43	106.68
15	aB	804	CLA	C4A-NA-C1A	10.35	111.40	106.68
15	aA	803	CLA	C4A-NA-C1A	9.88	111.19	106.68
15	cA	803	CLA	C4A-NA-C1A	9.83	111.16	106.68

5 of 560 chirality outliers are listed below:

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

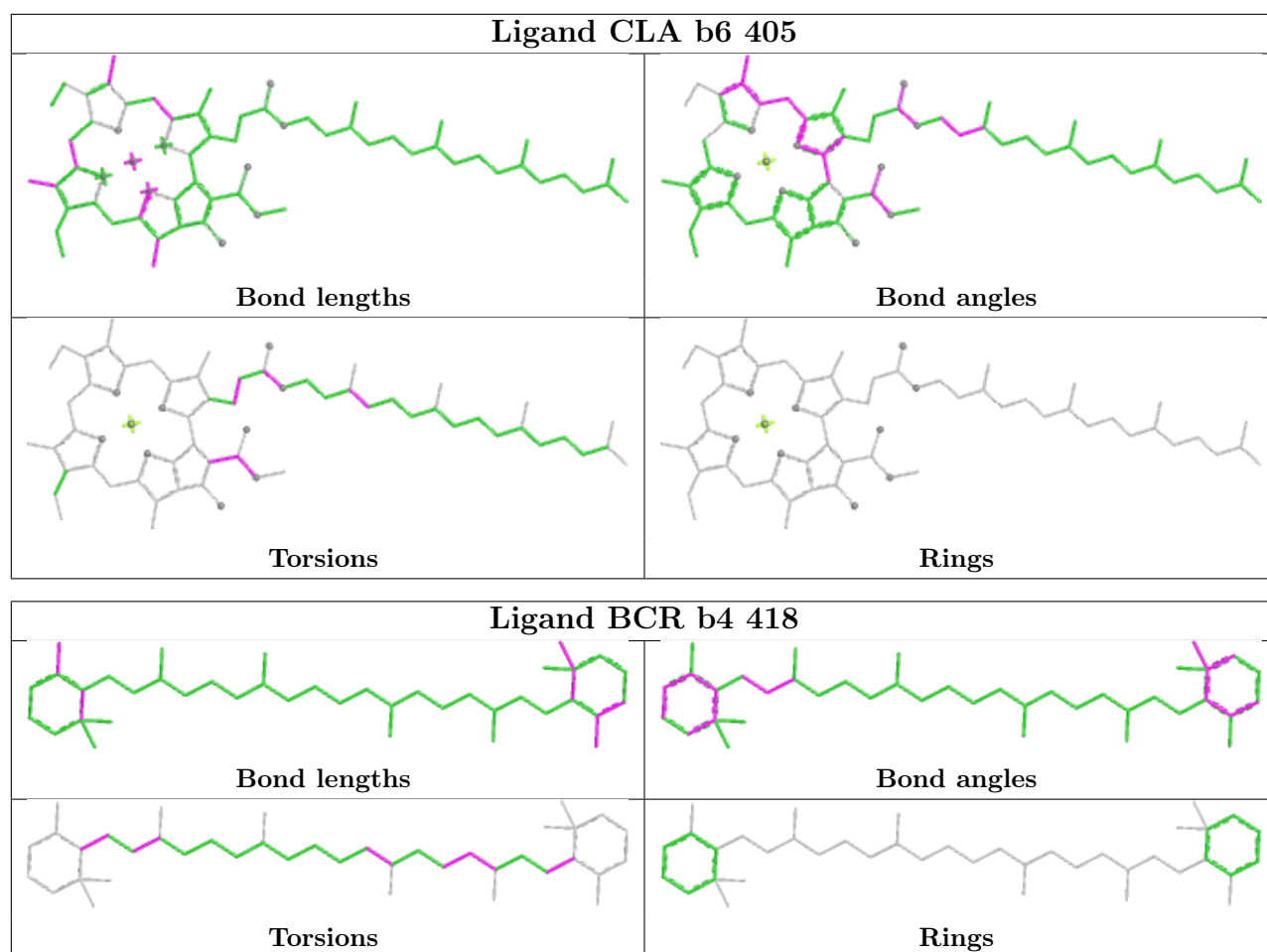
5 of 6439 torsion outliers are listed below:

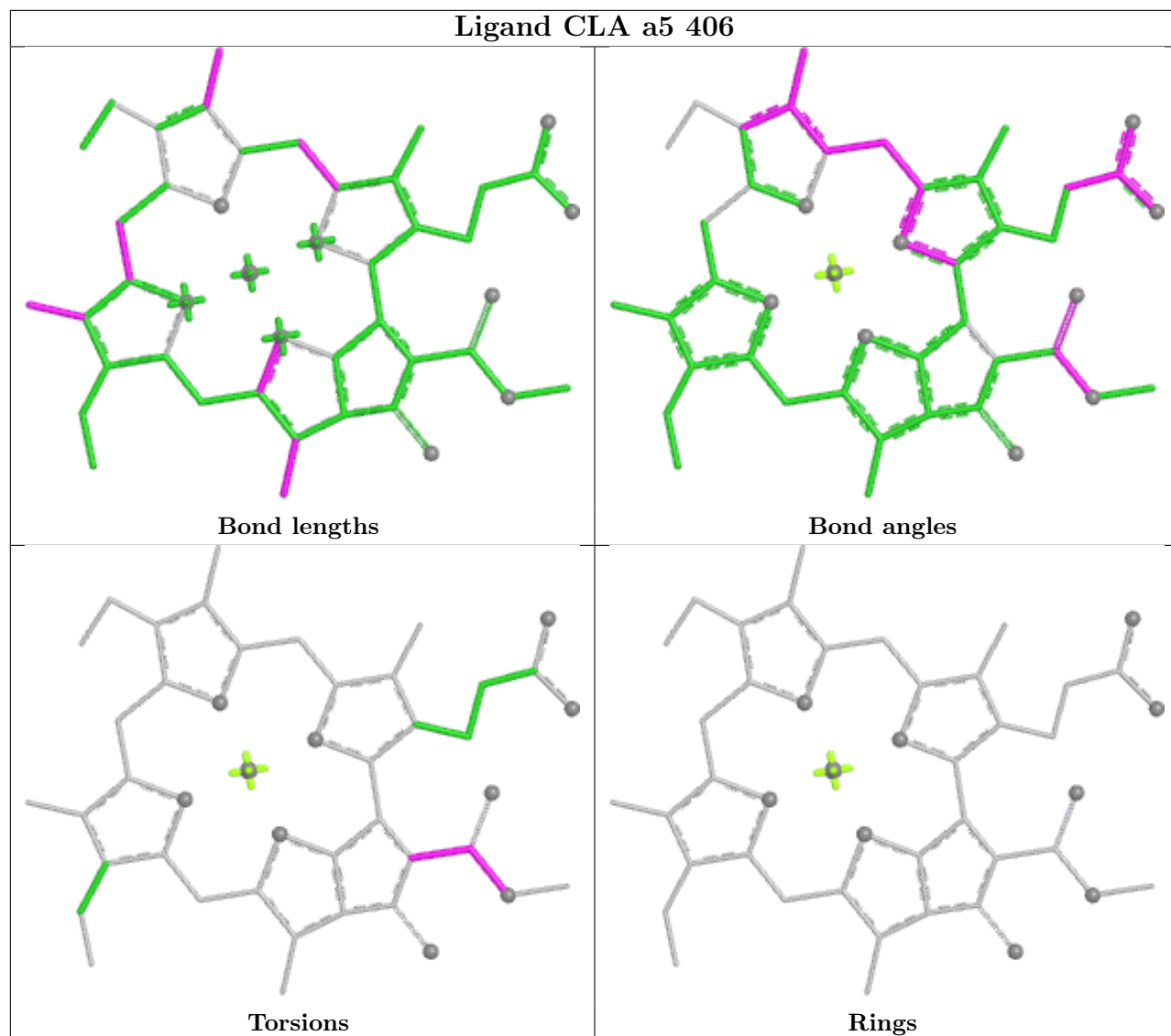
Mol	Chain	Res	Type	Atoms
15	aA	803	CLA	CBA-CGA-O2A-C1
15	aA	803	CLA	O1A-CGA-O2A-C1
15	aA	804	CLA	C1A-C2A-CAA-CBA
15	aA	804	CLA	CHA-CBD-CGD-O1D
15	aA	804	CLA	CHA-CBD-CGD-O2D

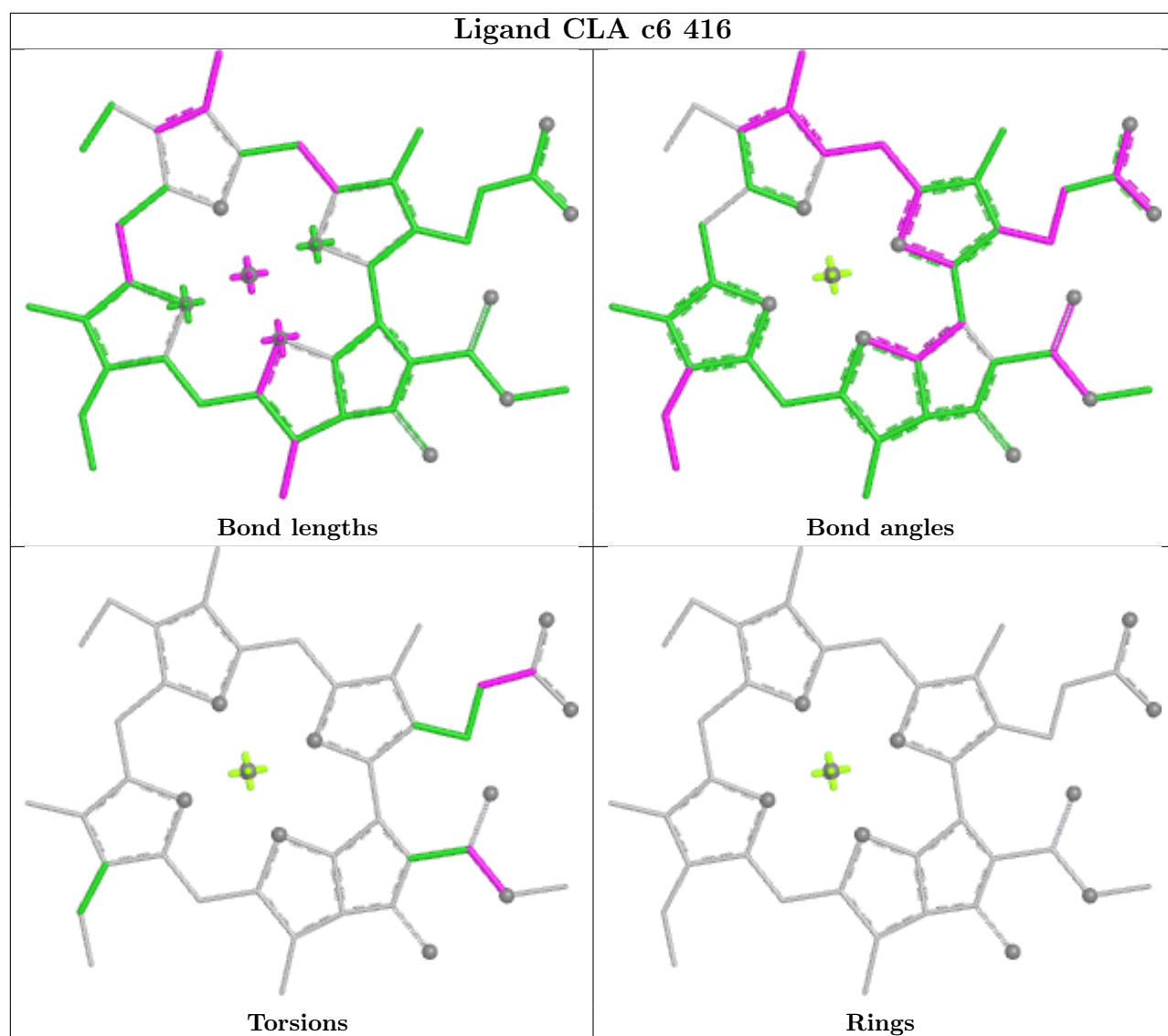
There are no ring outliers.

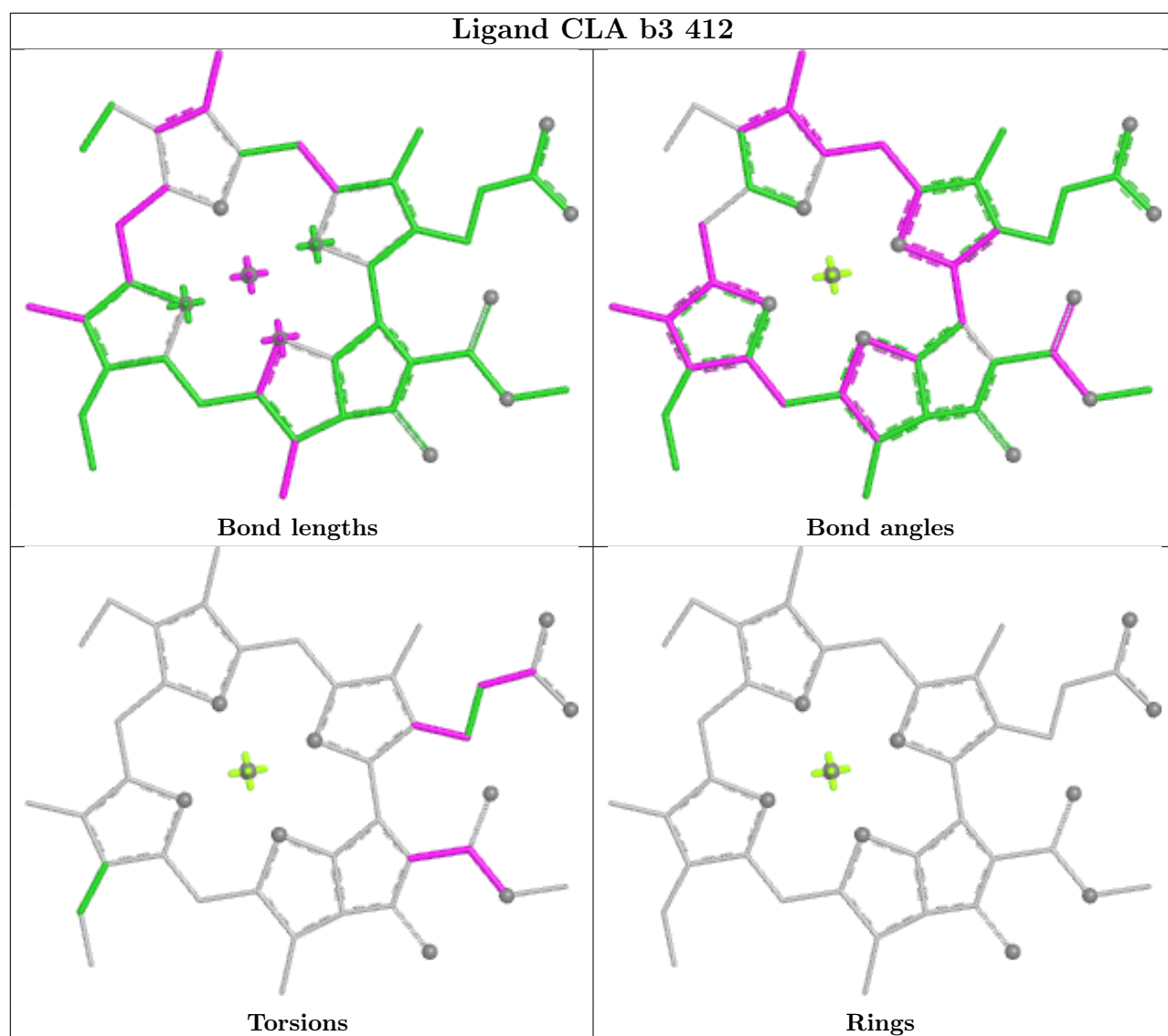
No monomer is involved in short contacts.

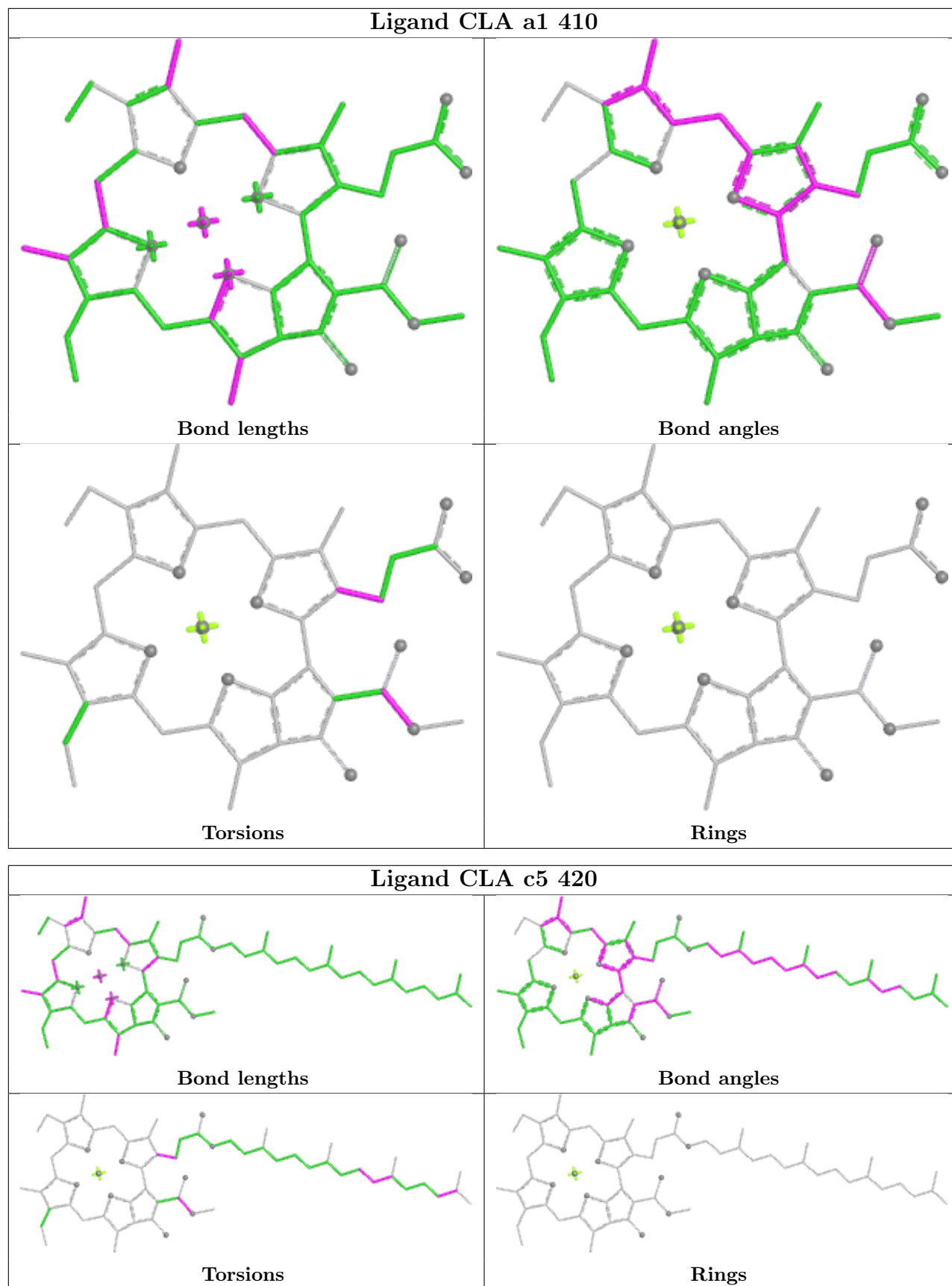
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

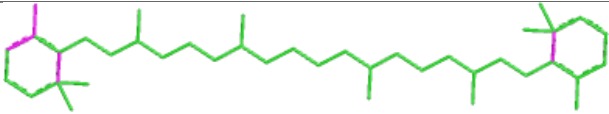
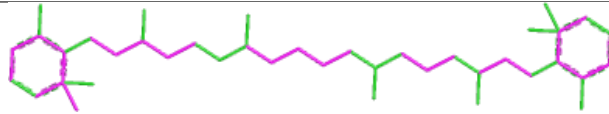
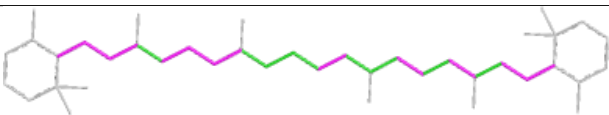
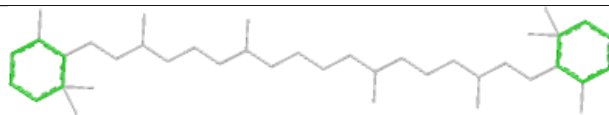


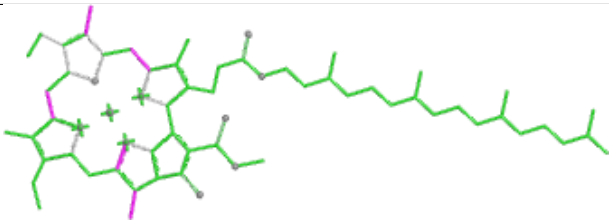
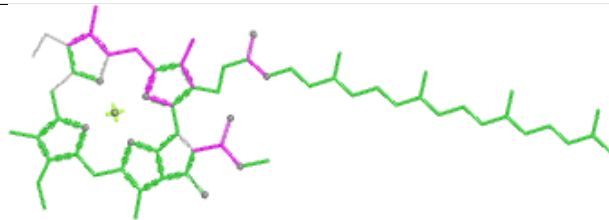
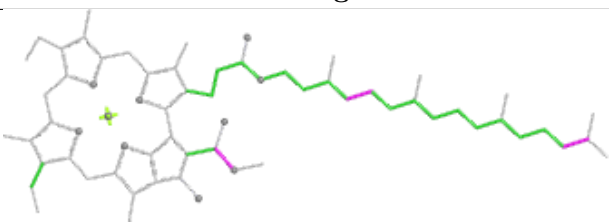
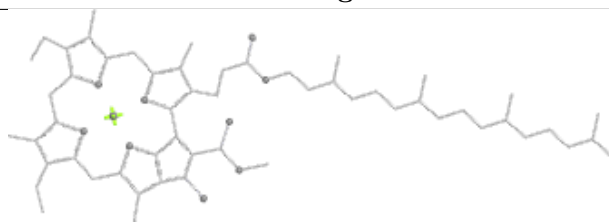


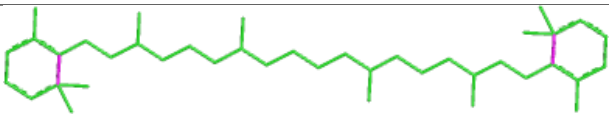
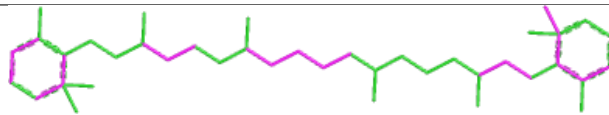
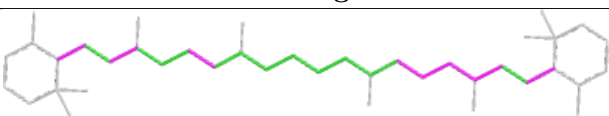
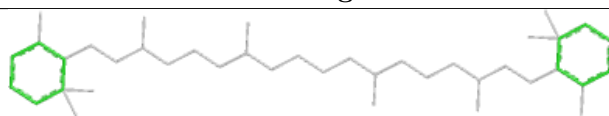


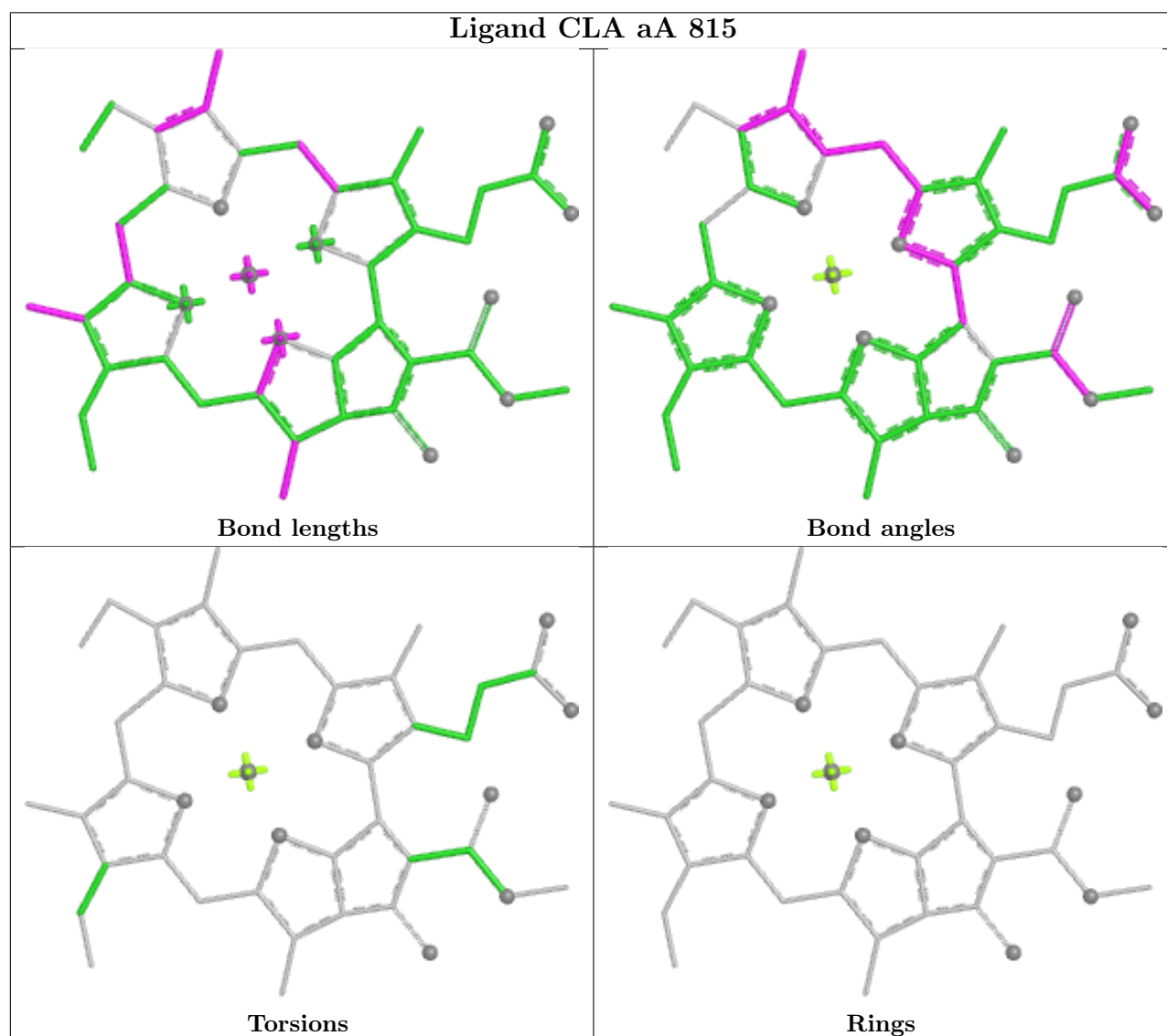
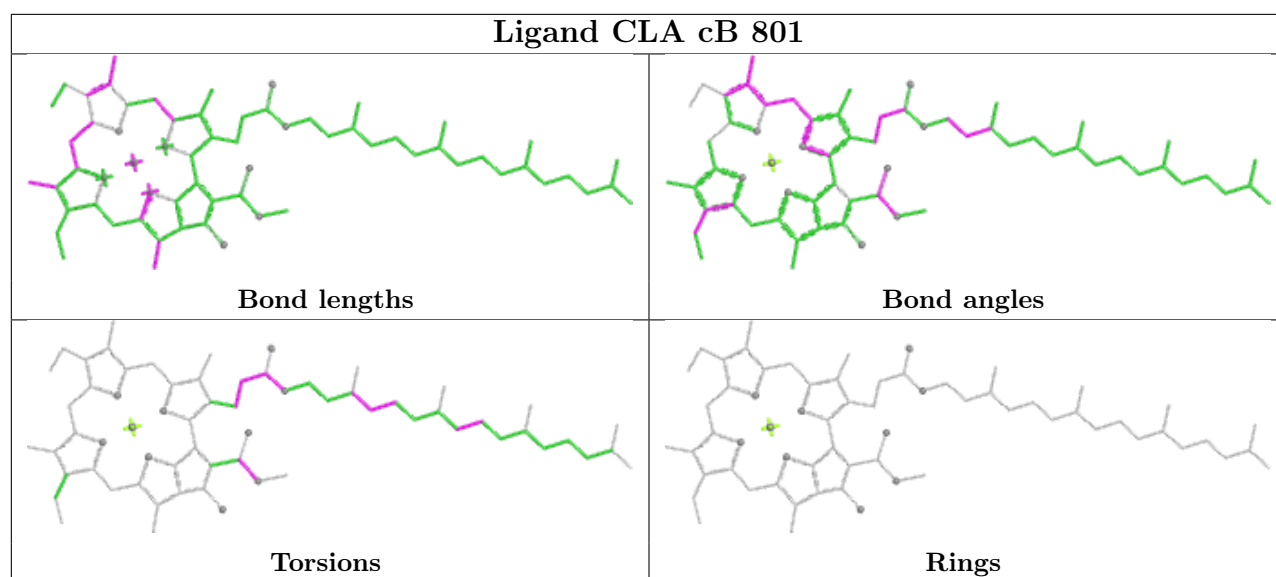


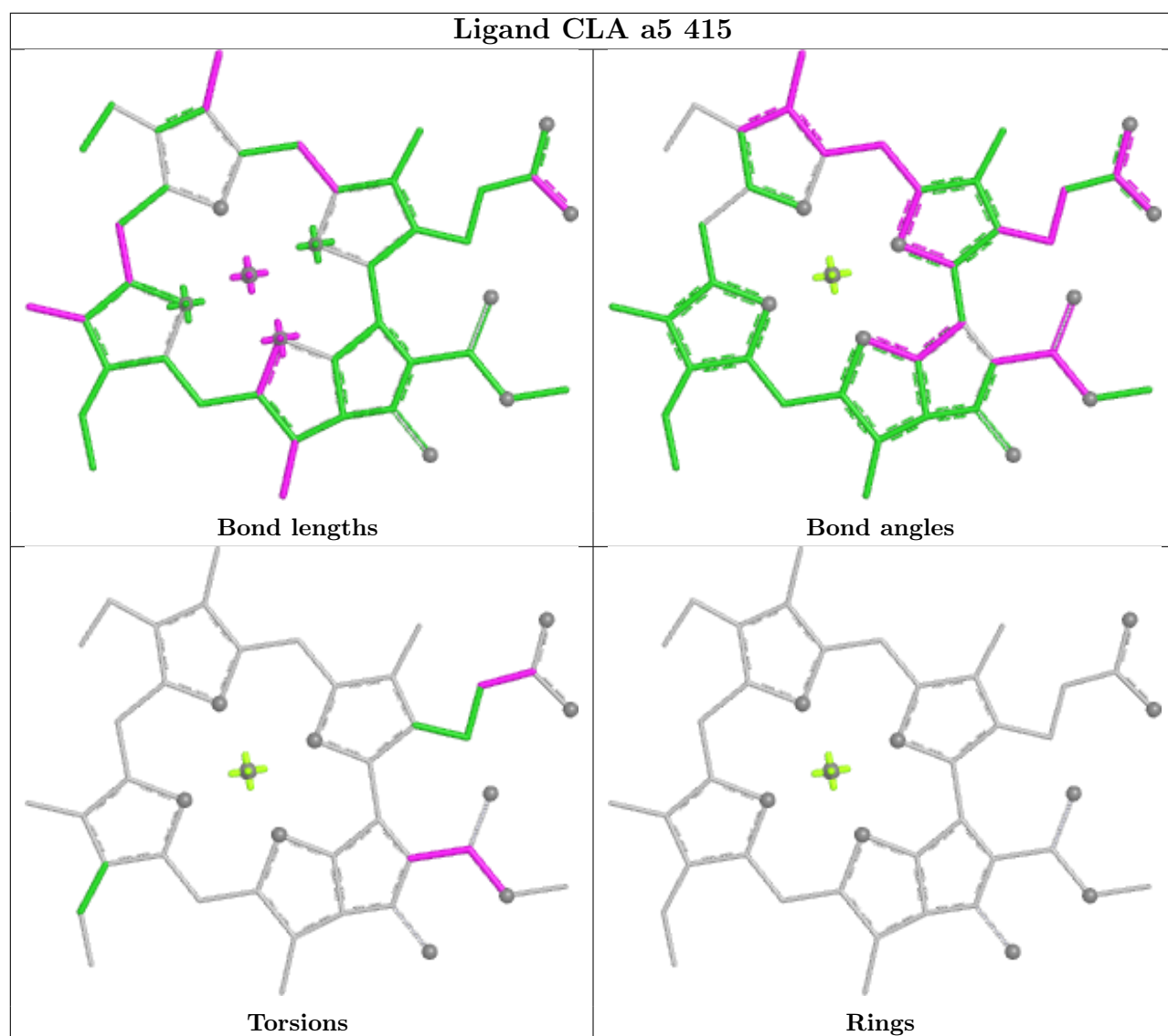


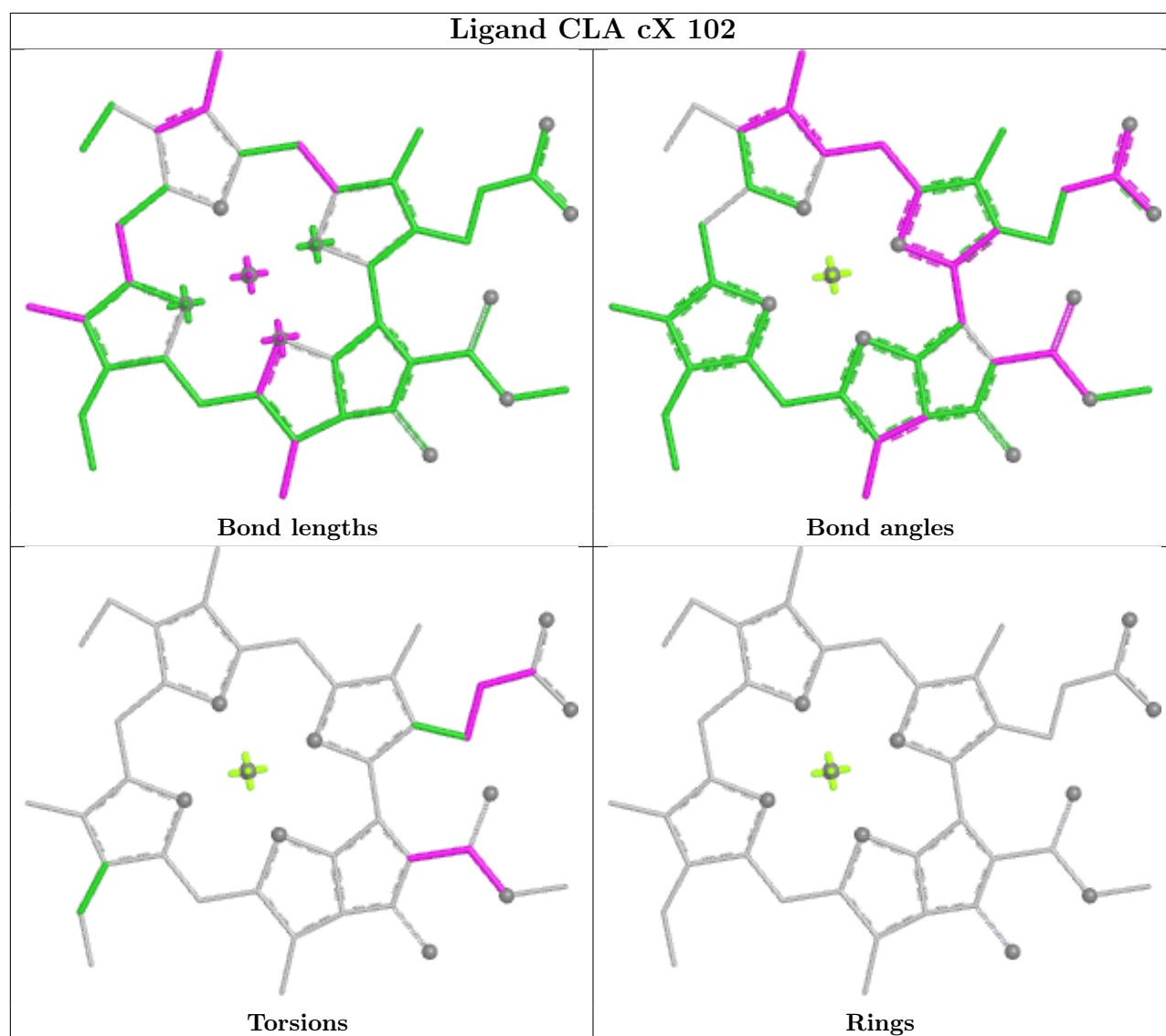
Ligand BCR b6 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

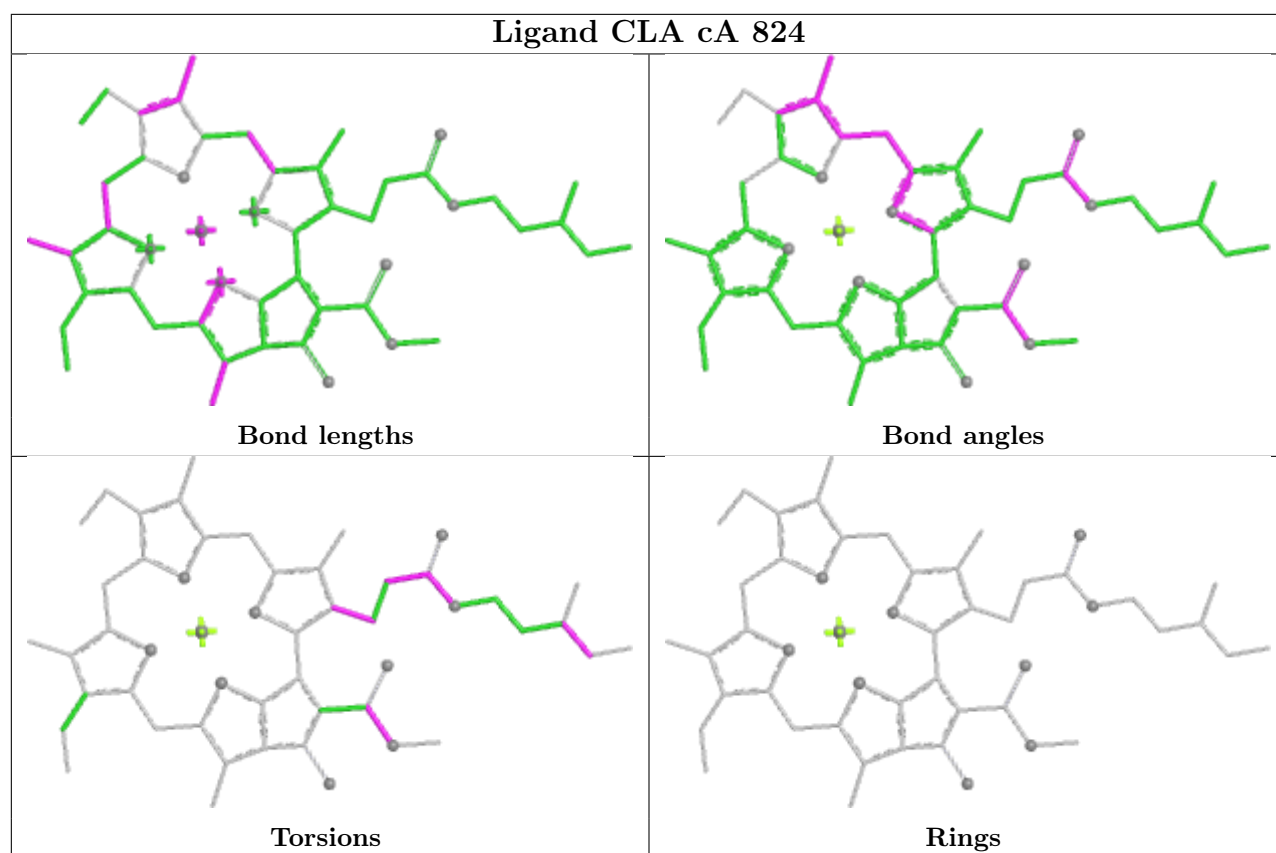
Ligand CLA b2 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

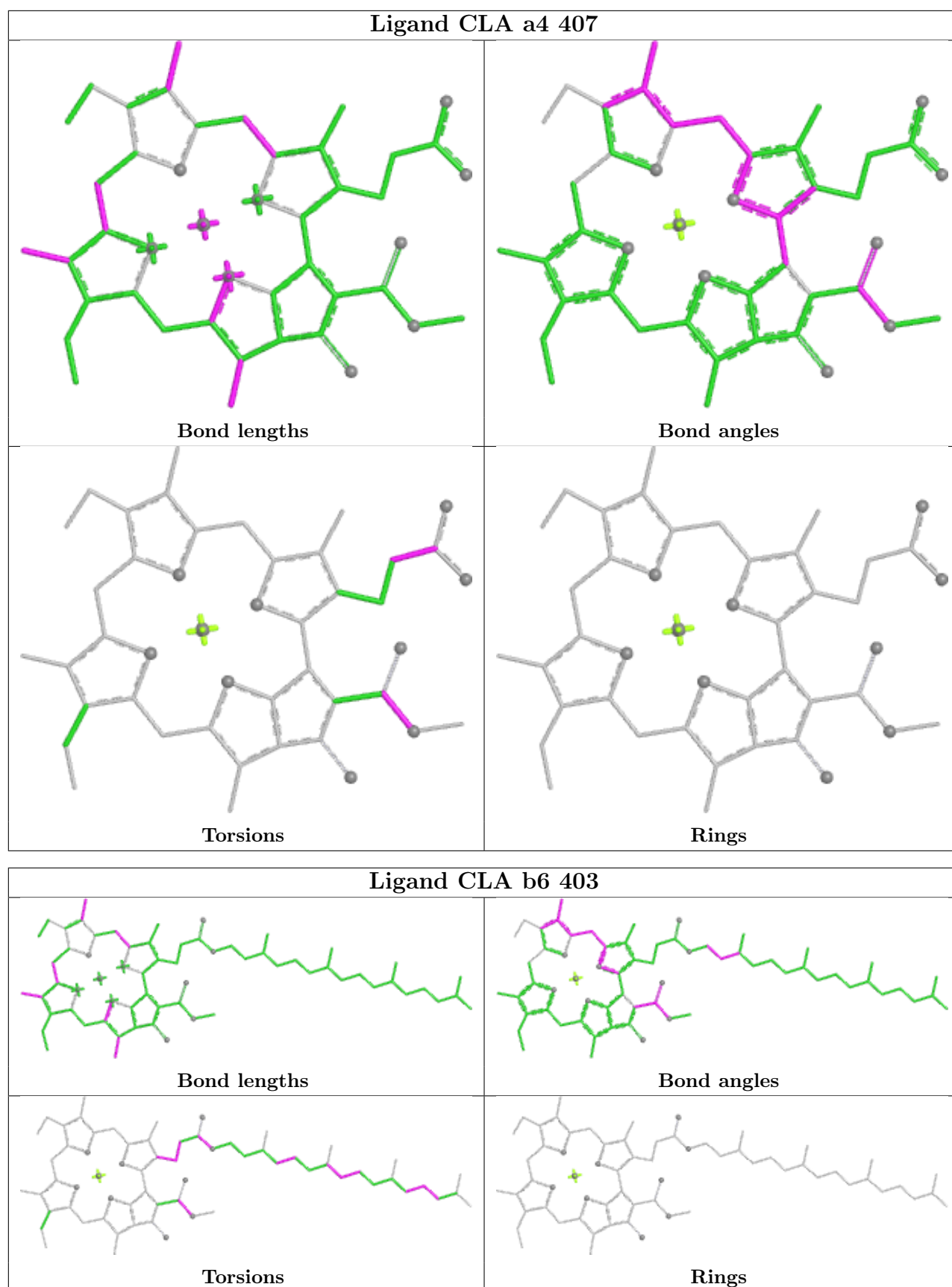
Ligand BCR c4 419	
	
Bond lengths	Bond angles
	
Torsions	Rings

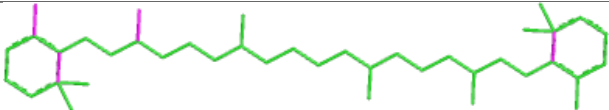
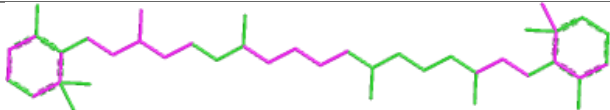
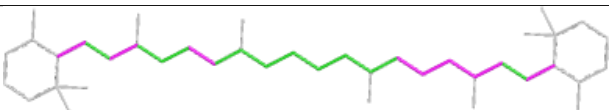
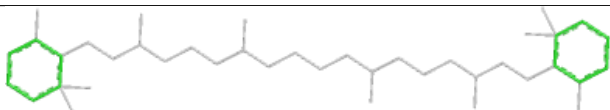



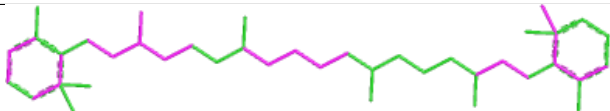
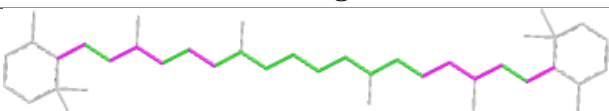
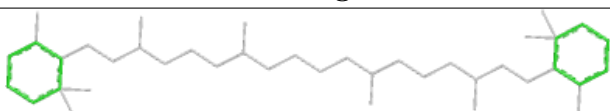


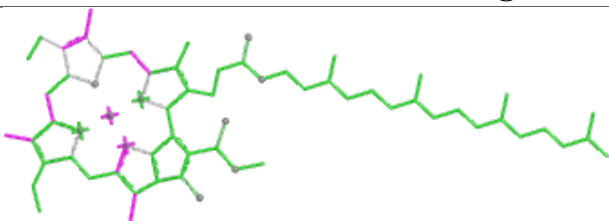
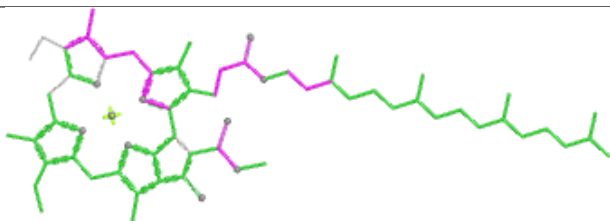
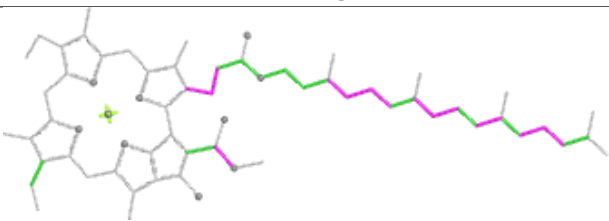
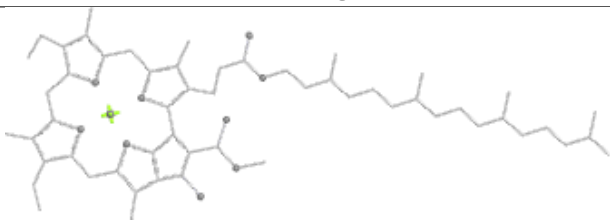


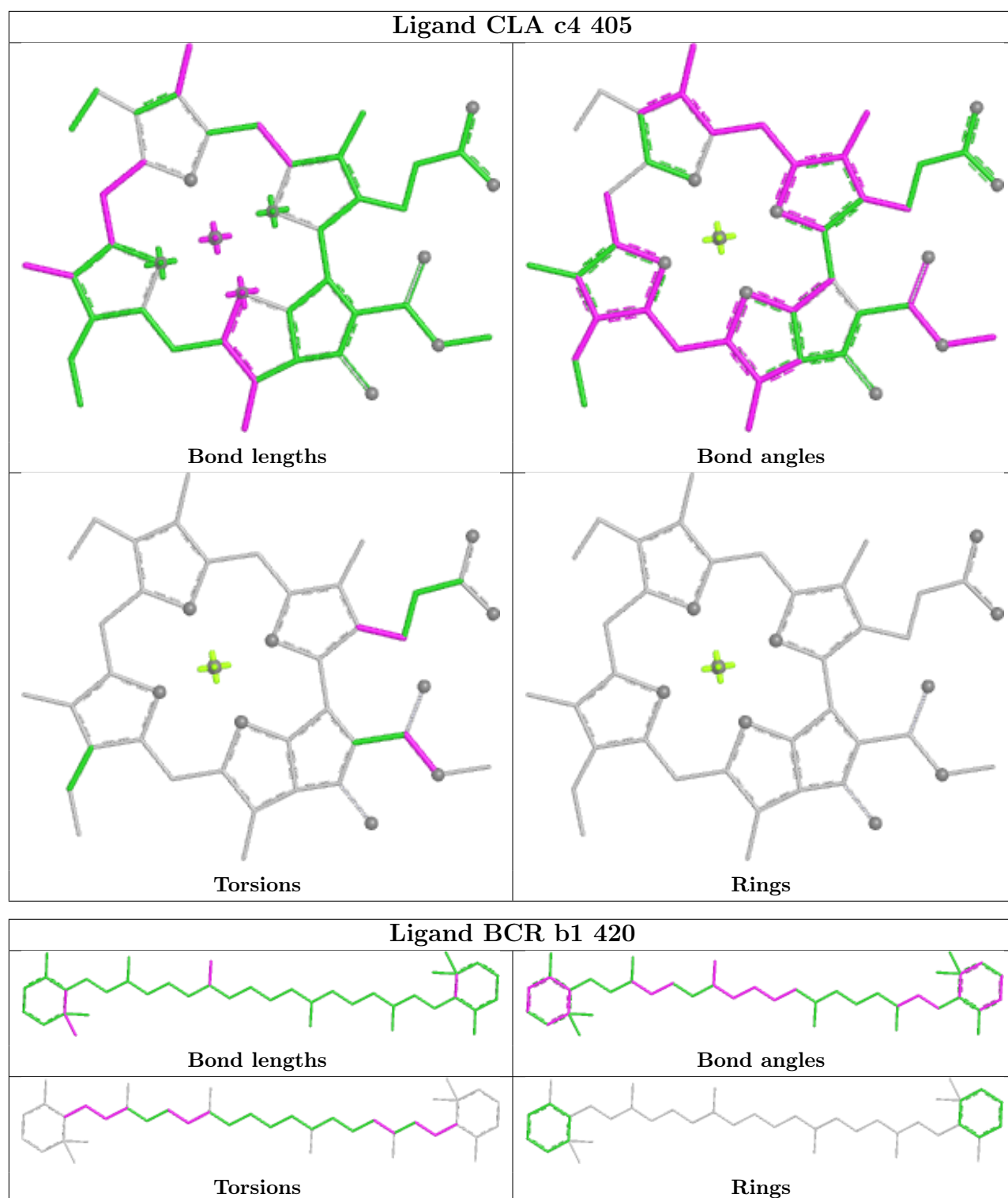


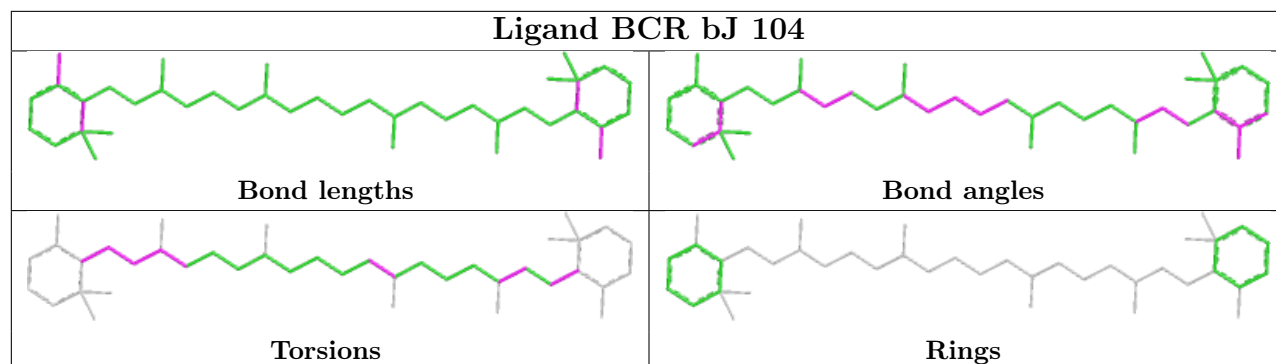
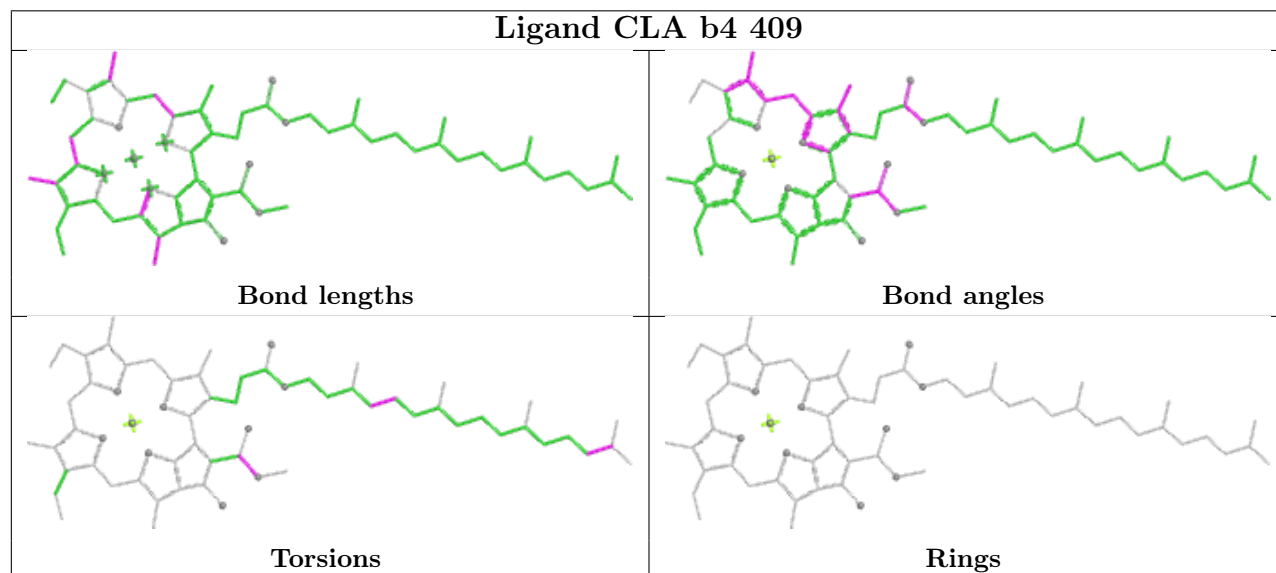
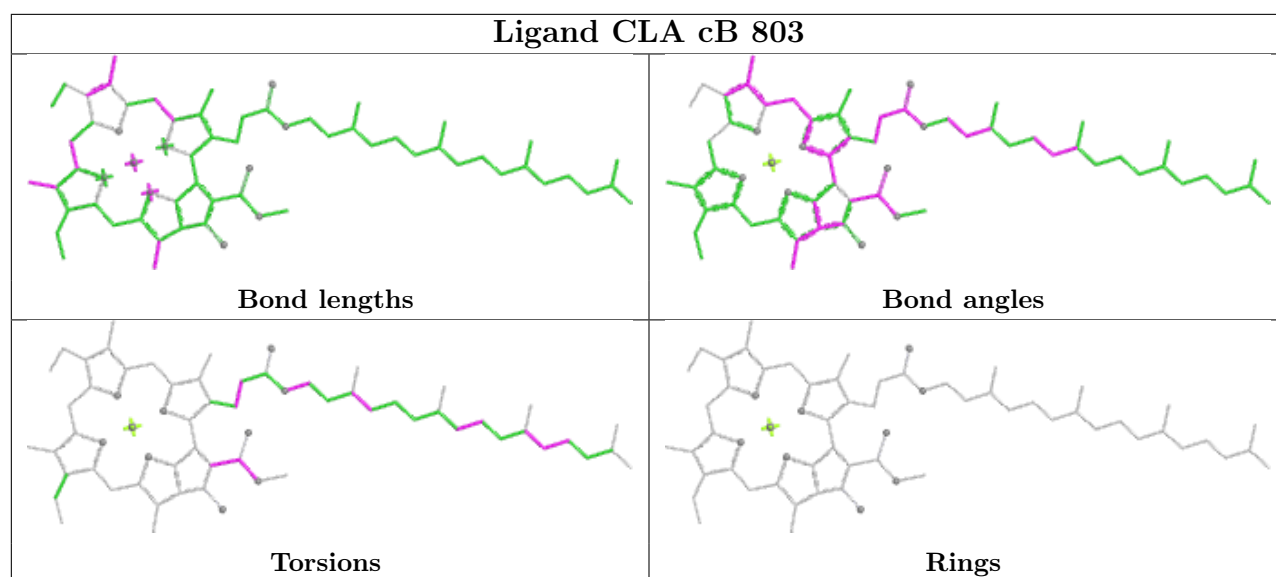


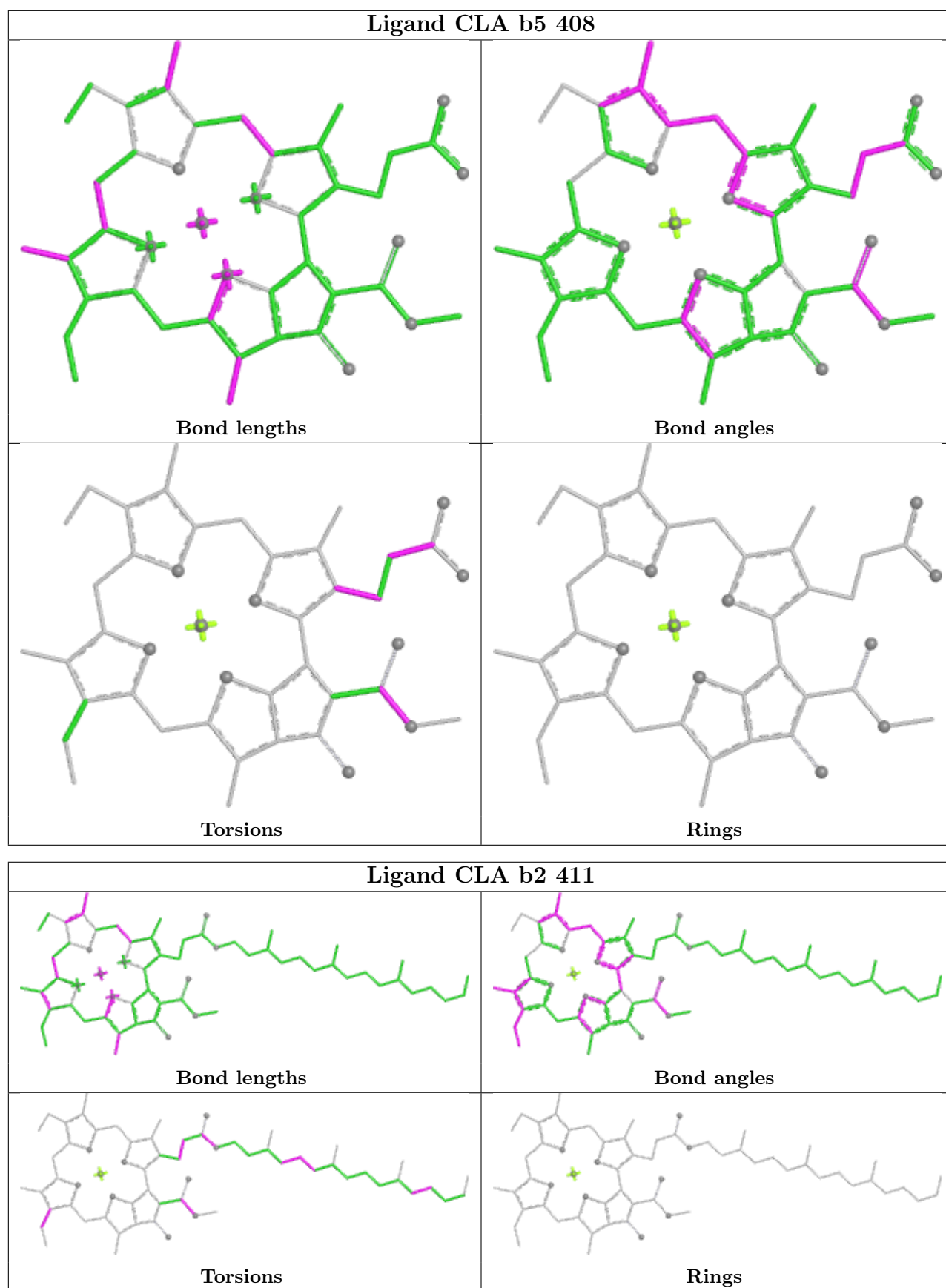
Ligand BCR a1 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

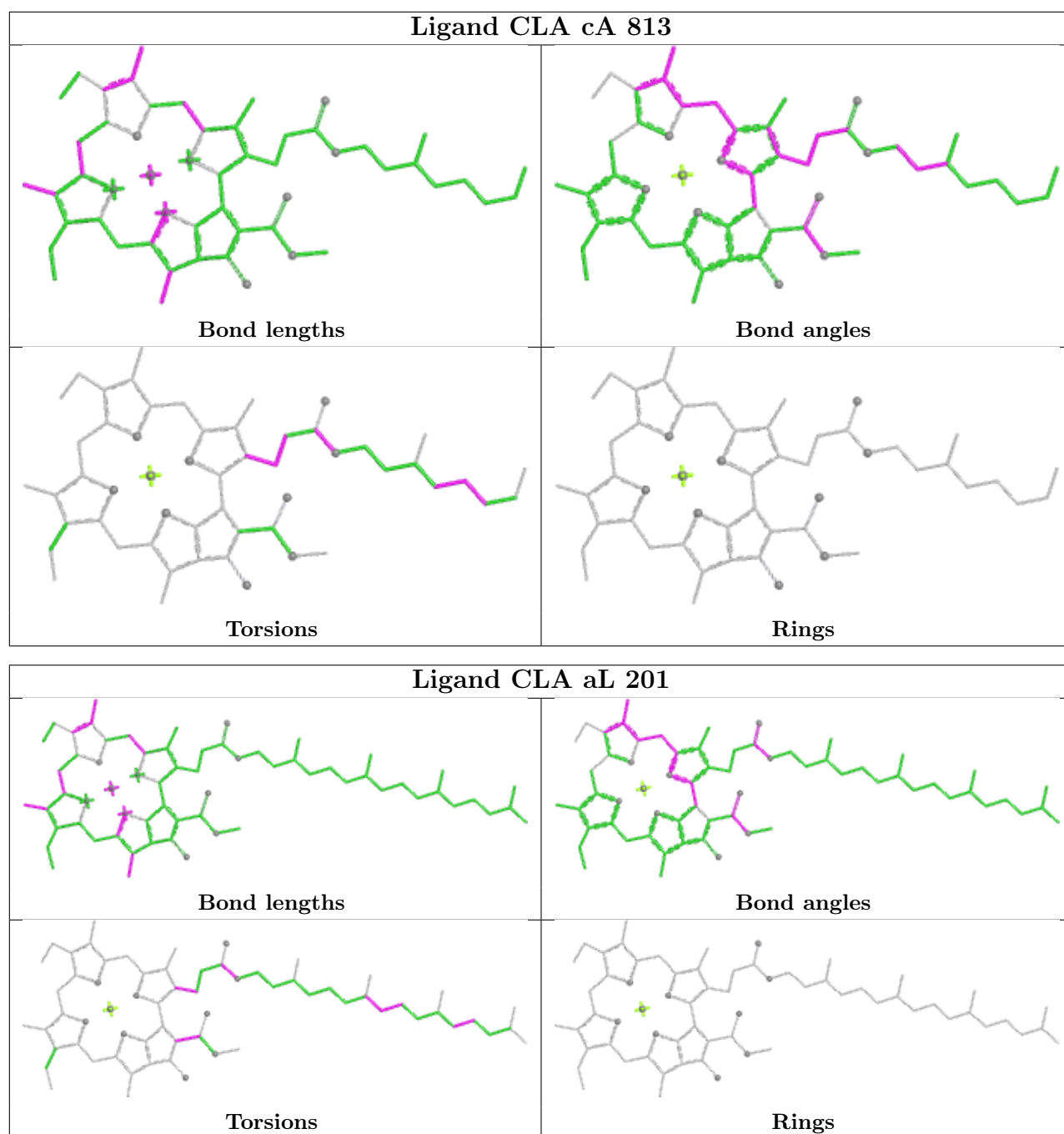
Ligand BCR b6 401	
	
Bond lengths	Bond angles
	
Torsions	Rings

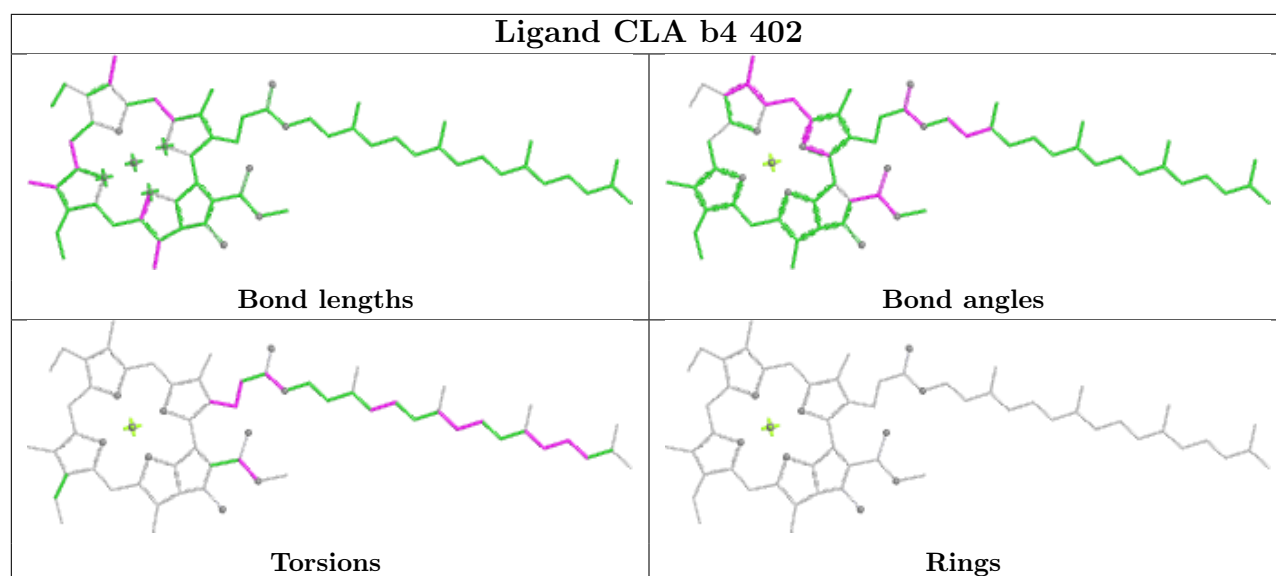
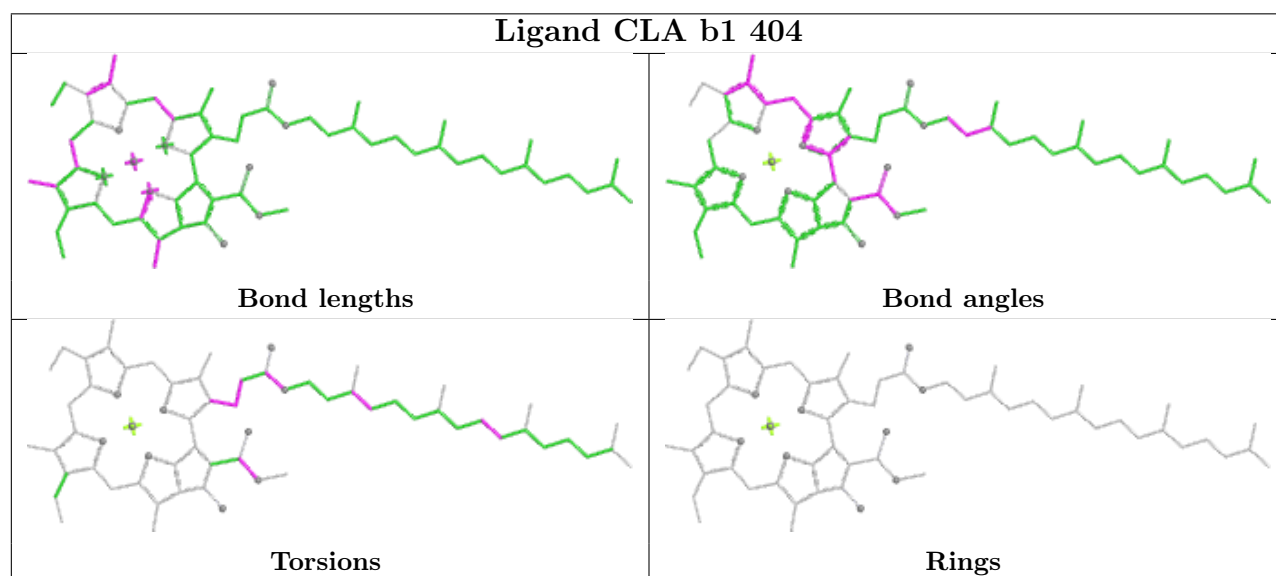
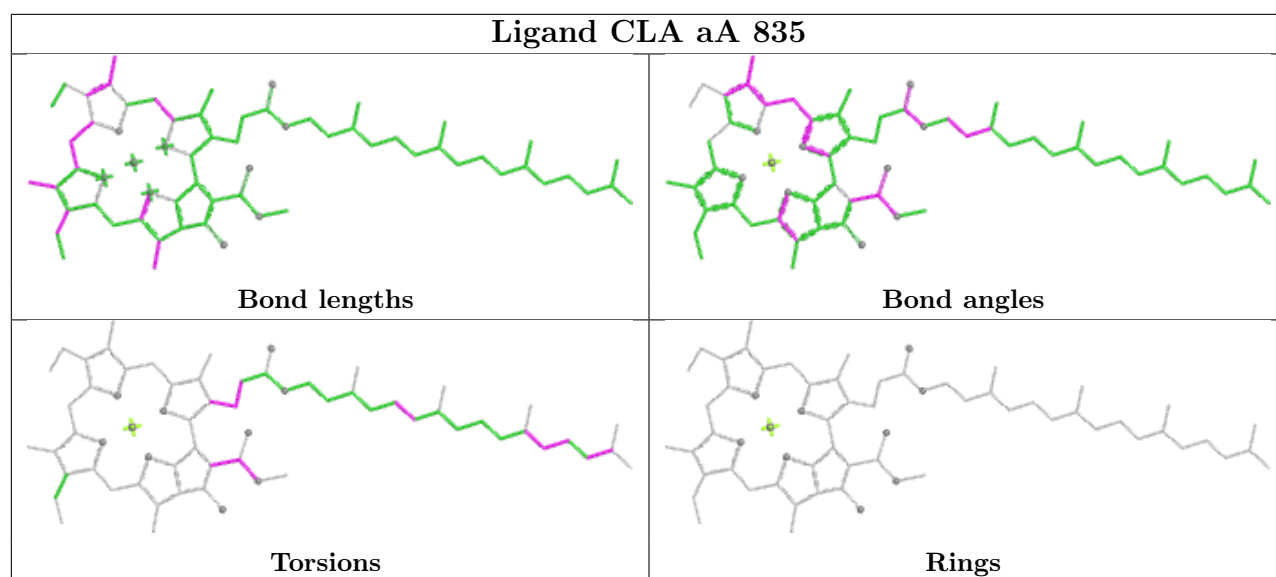
Ligand CLA bA 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

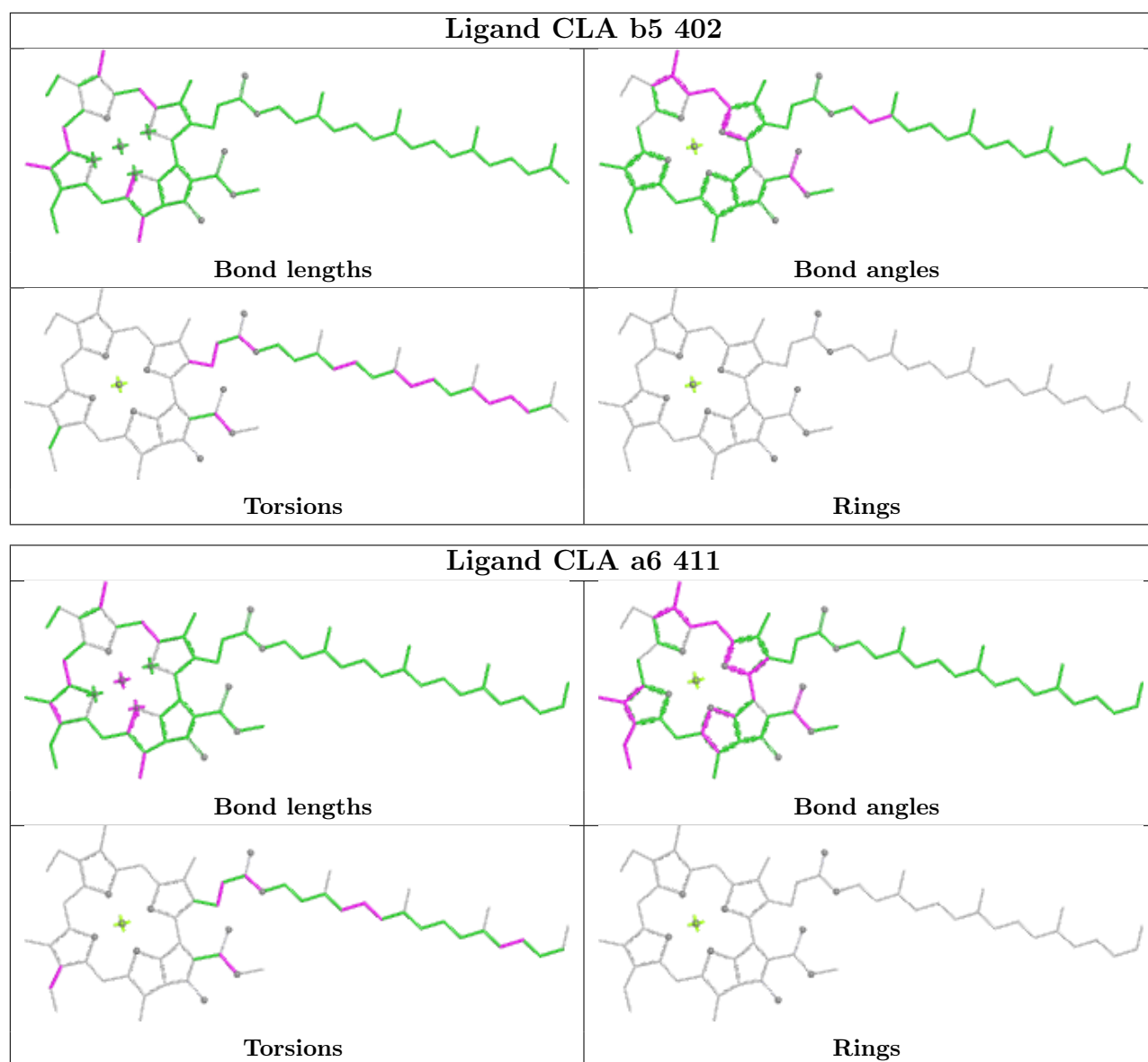


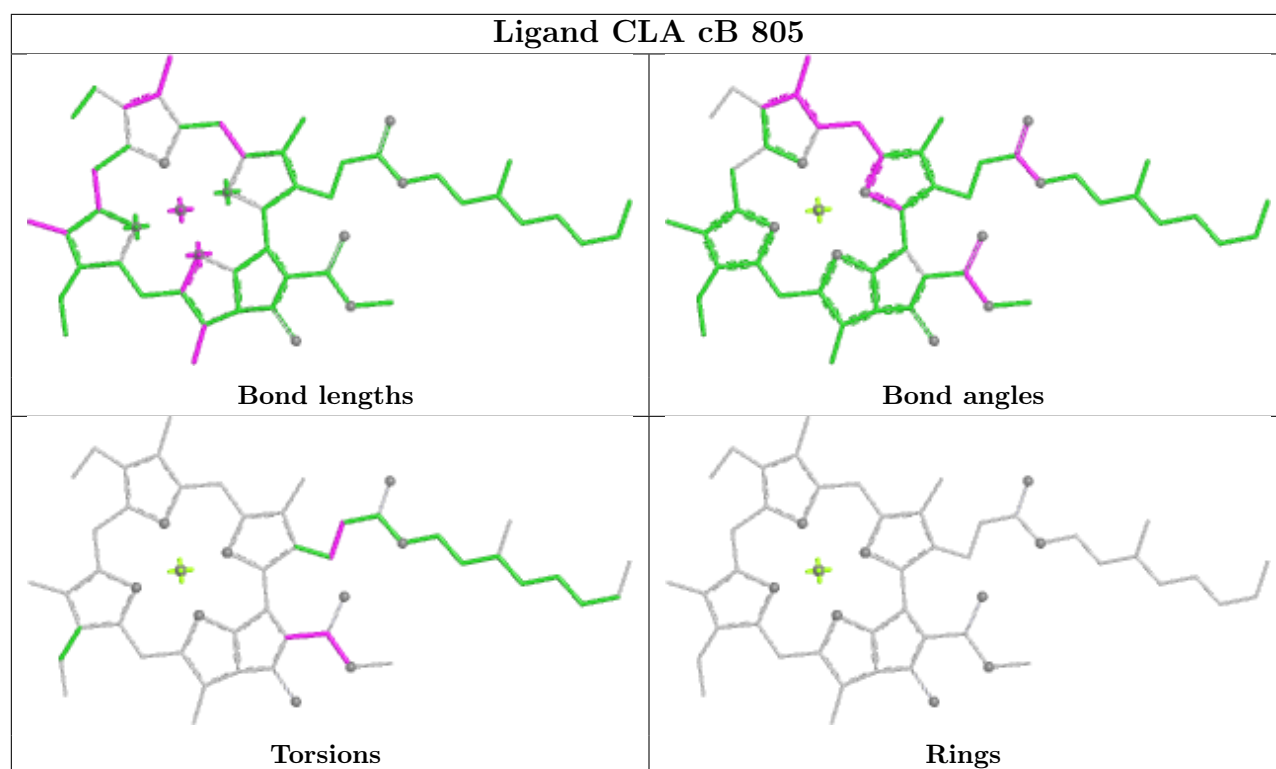


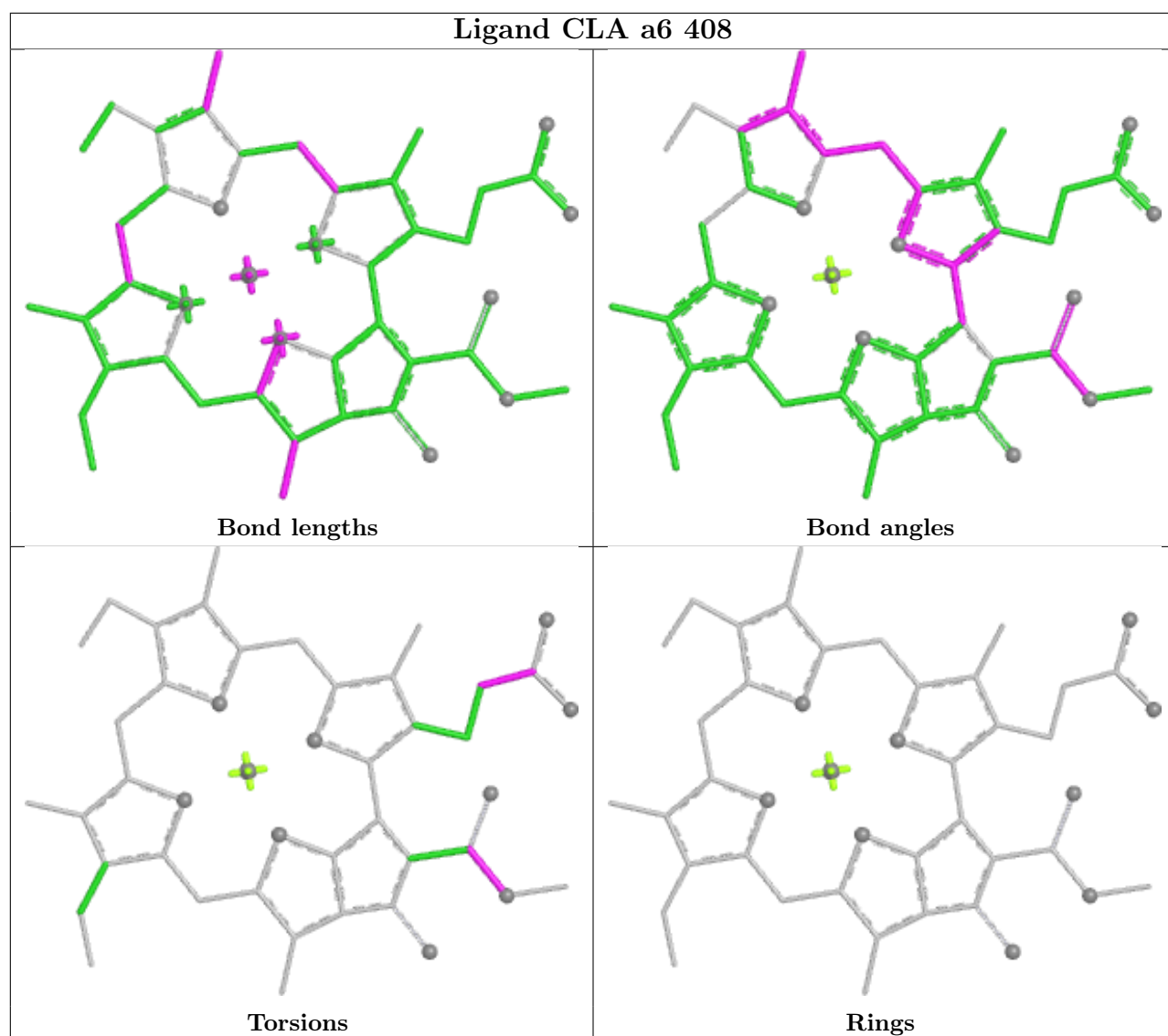


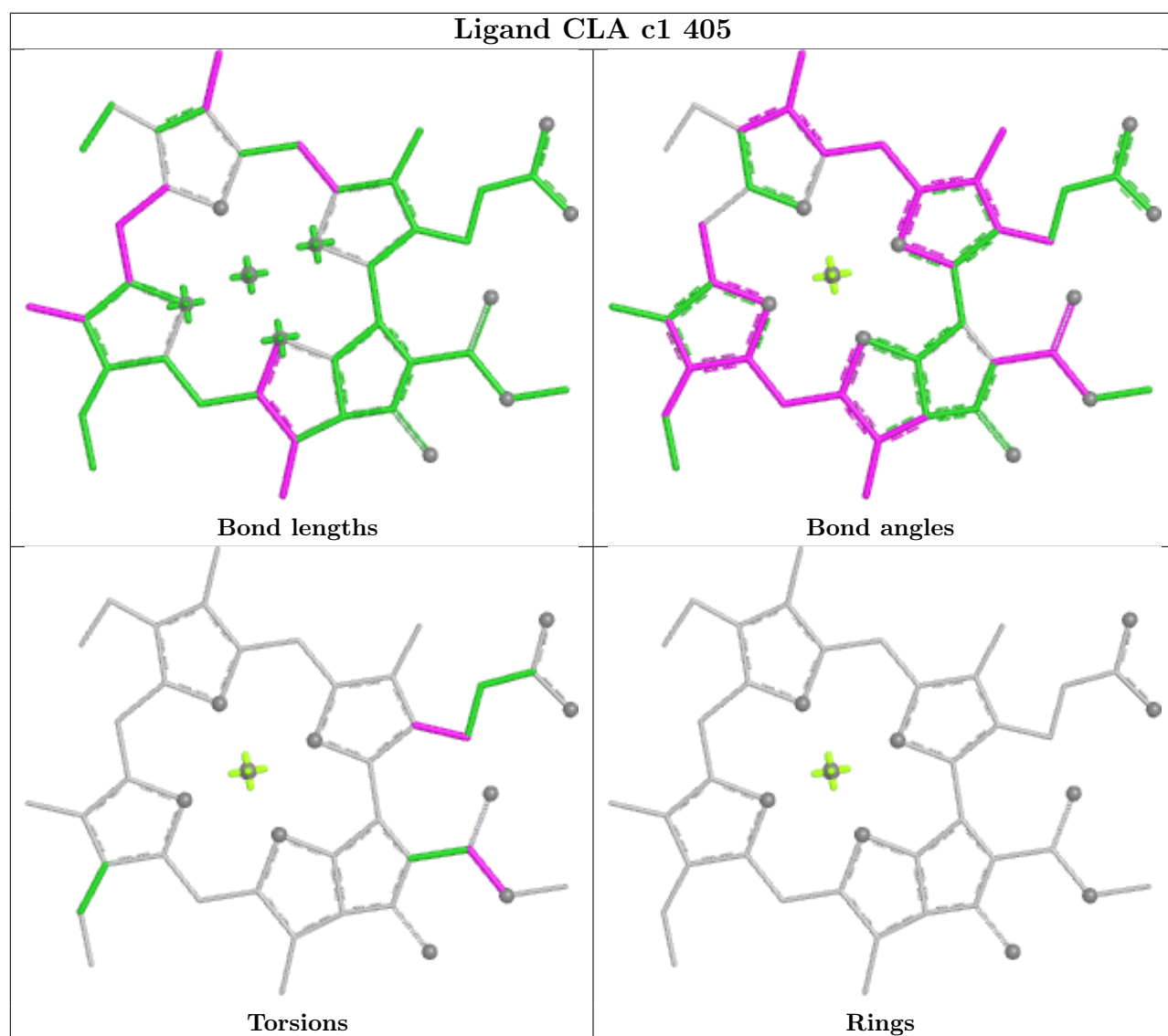


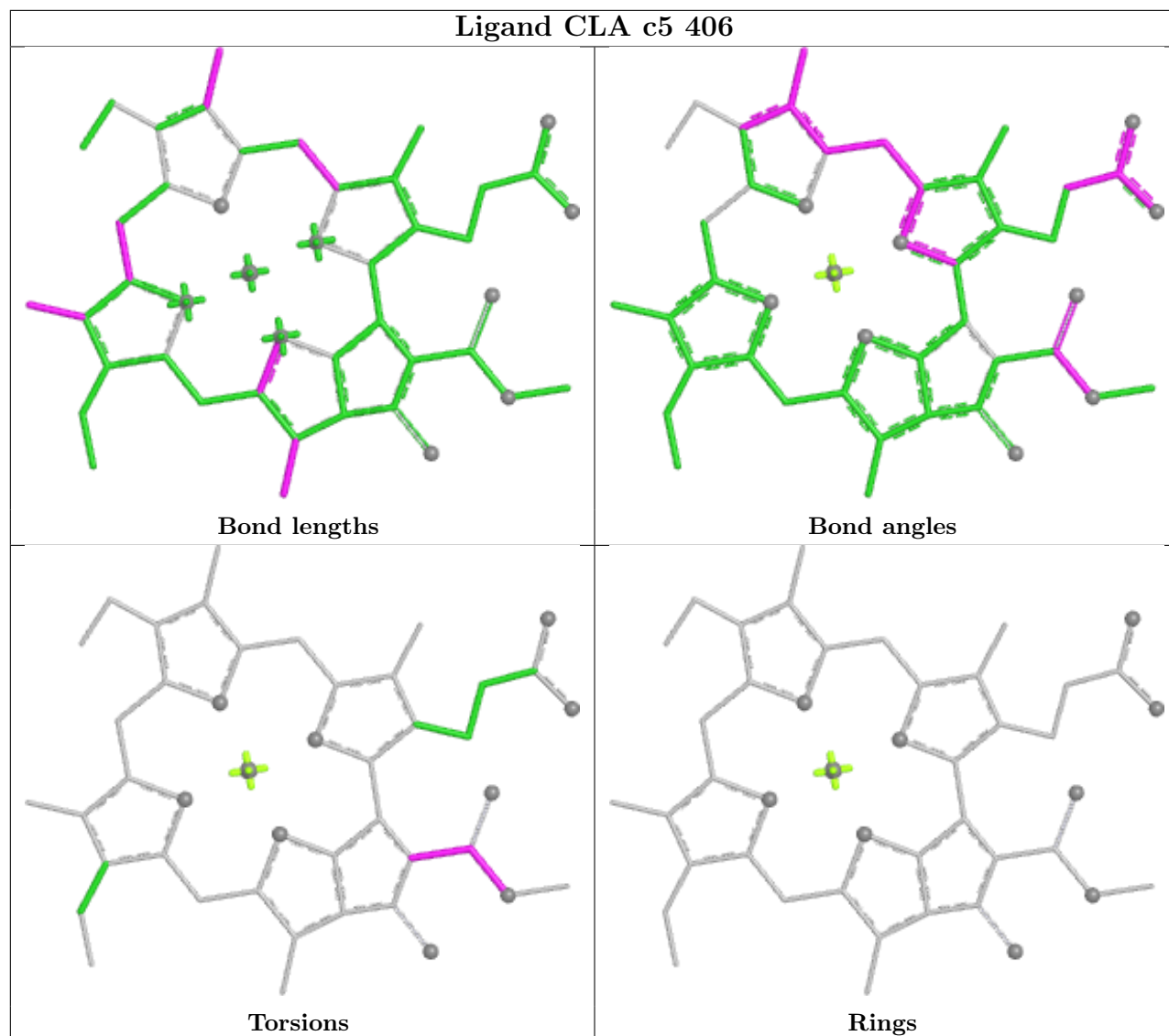


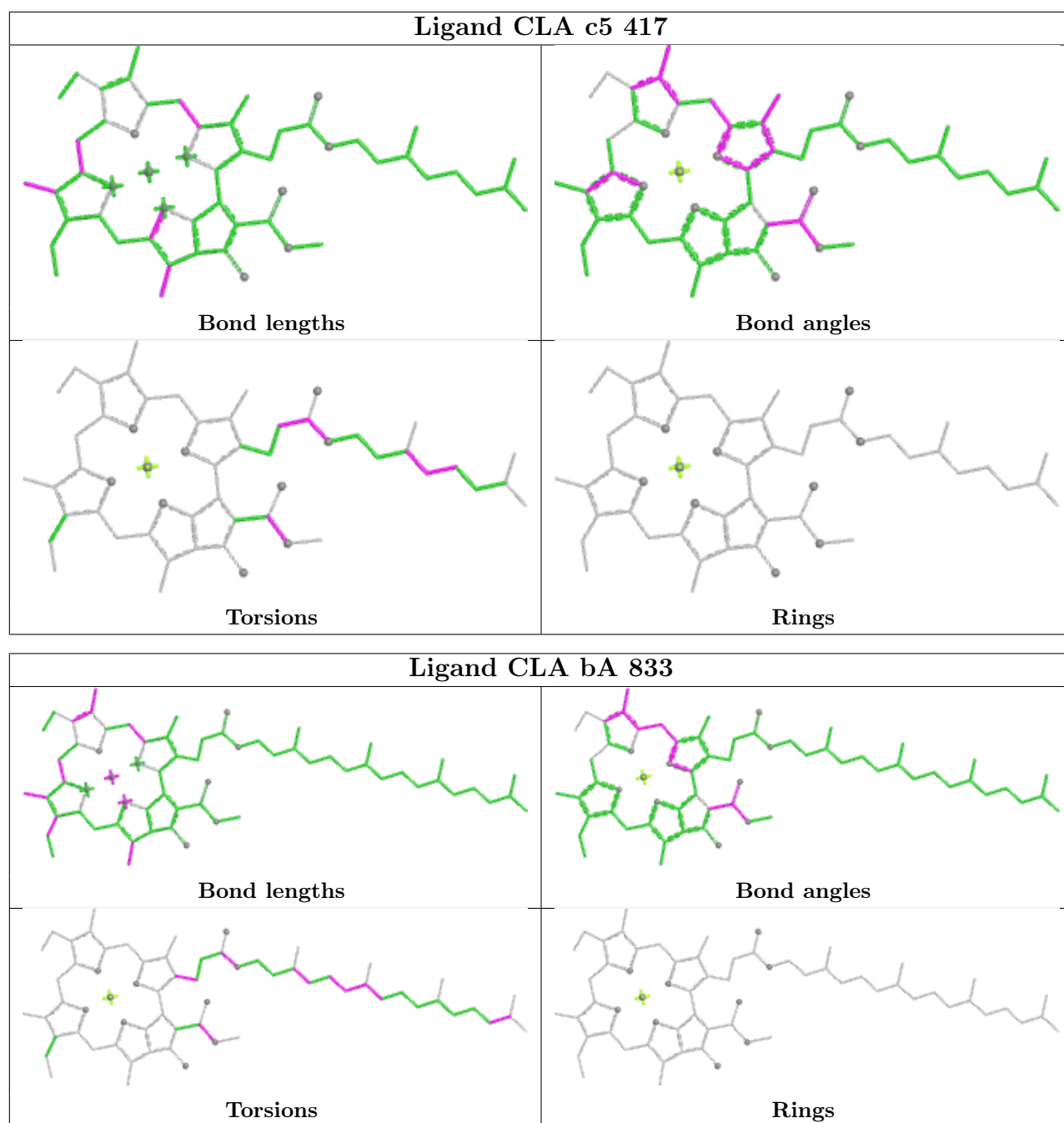


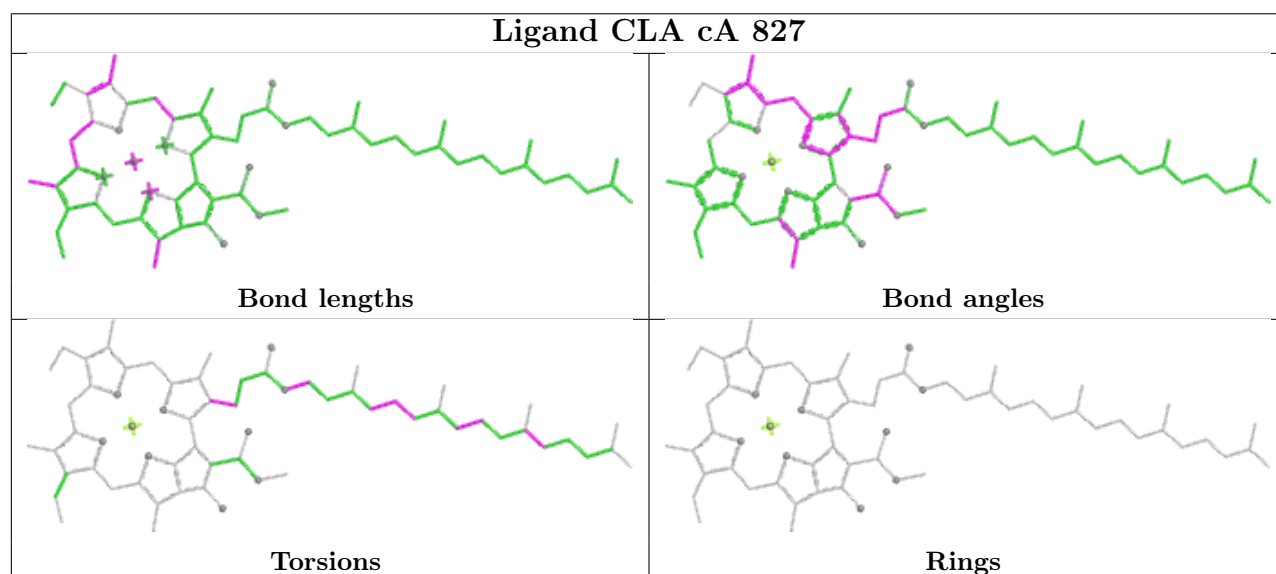
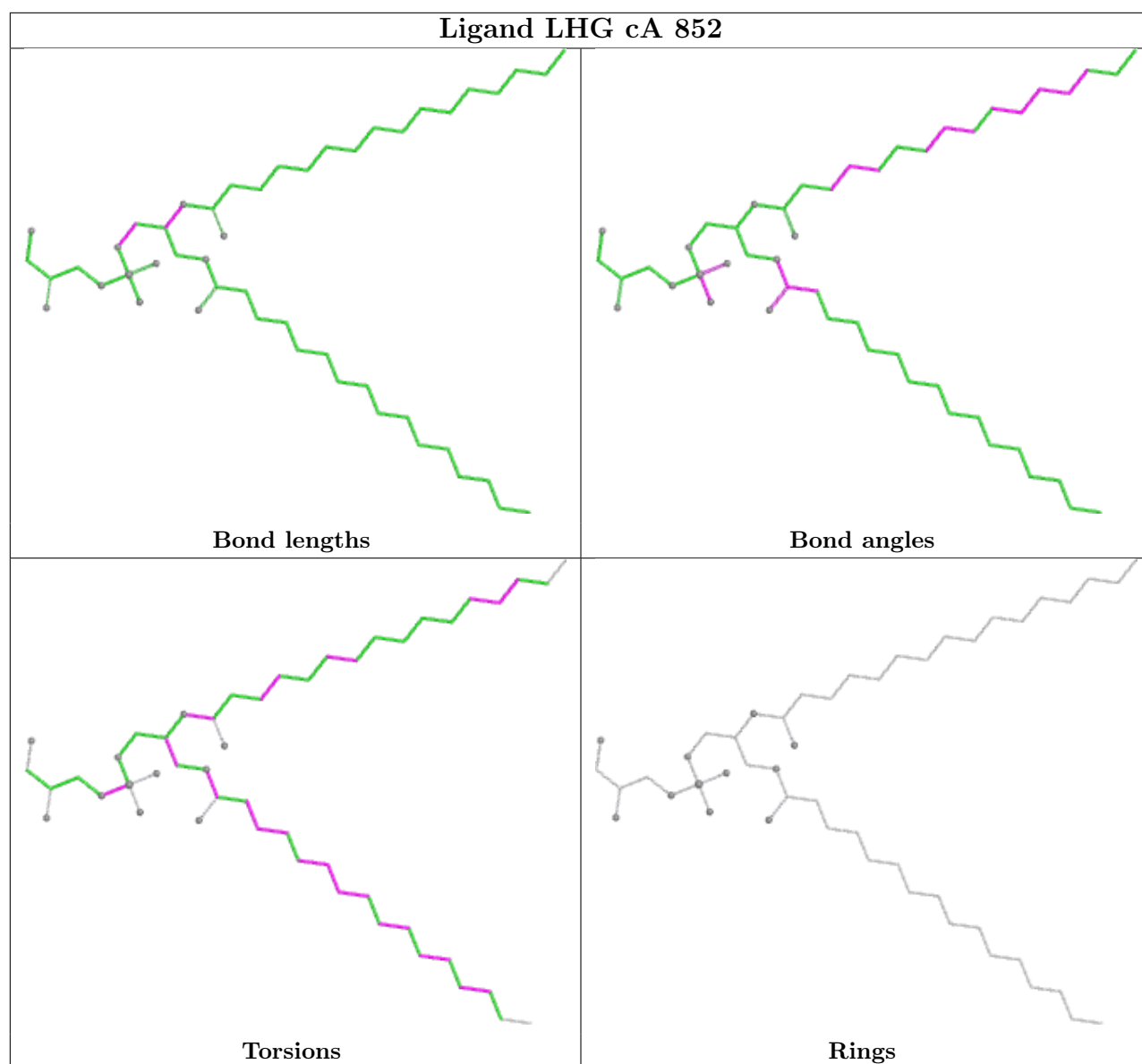


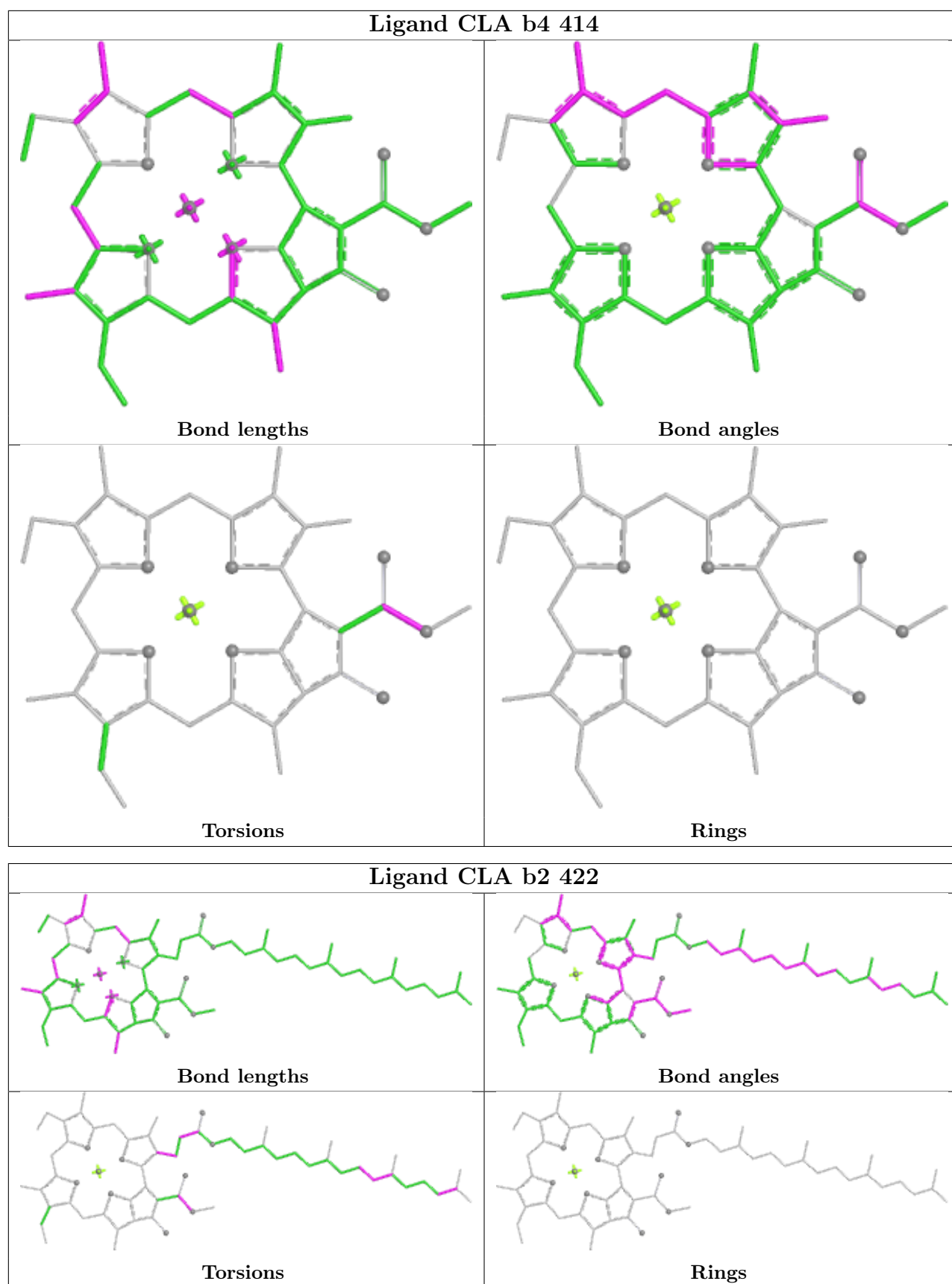


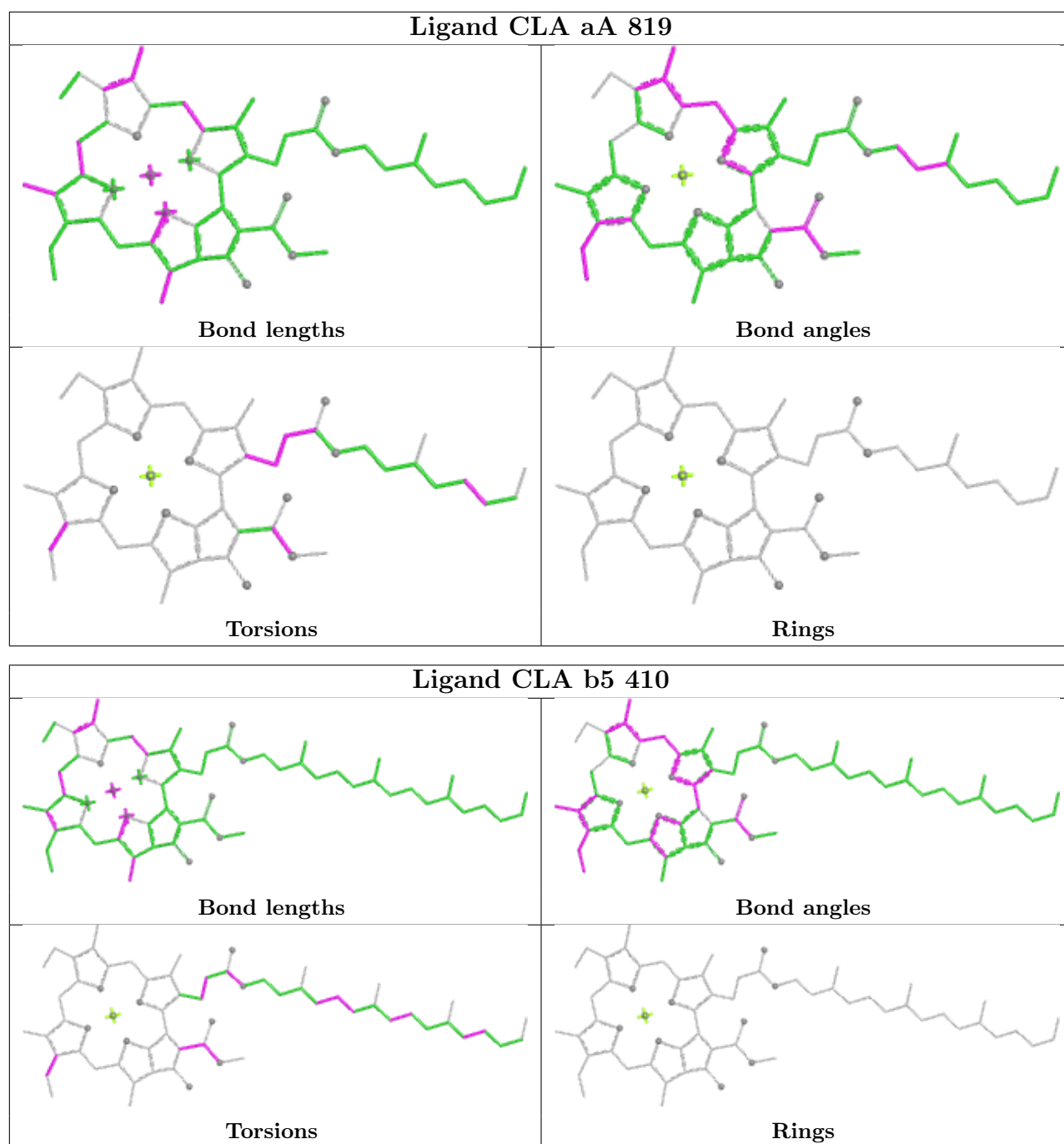


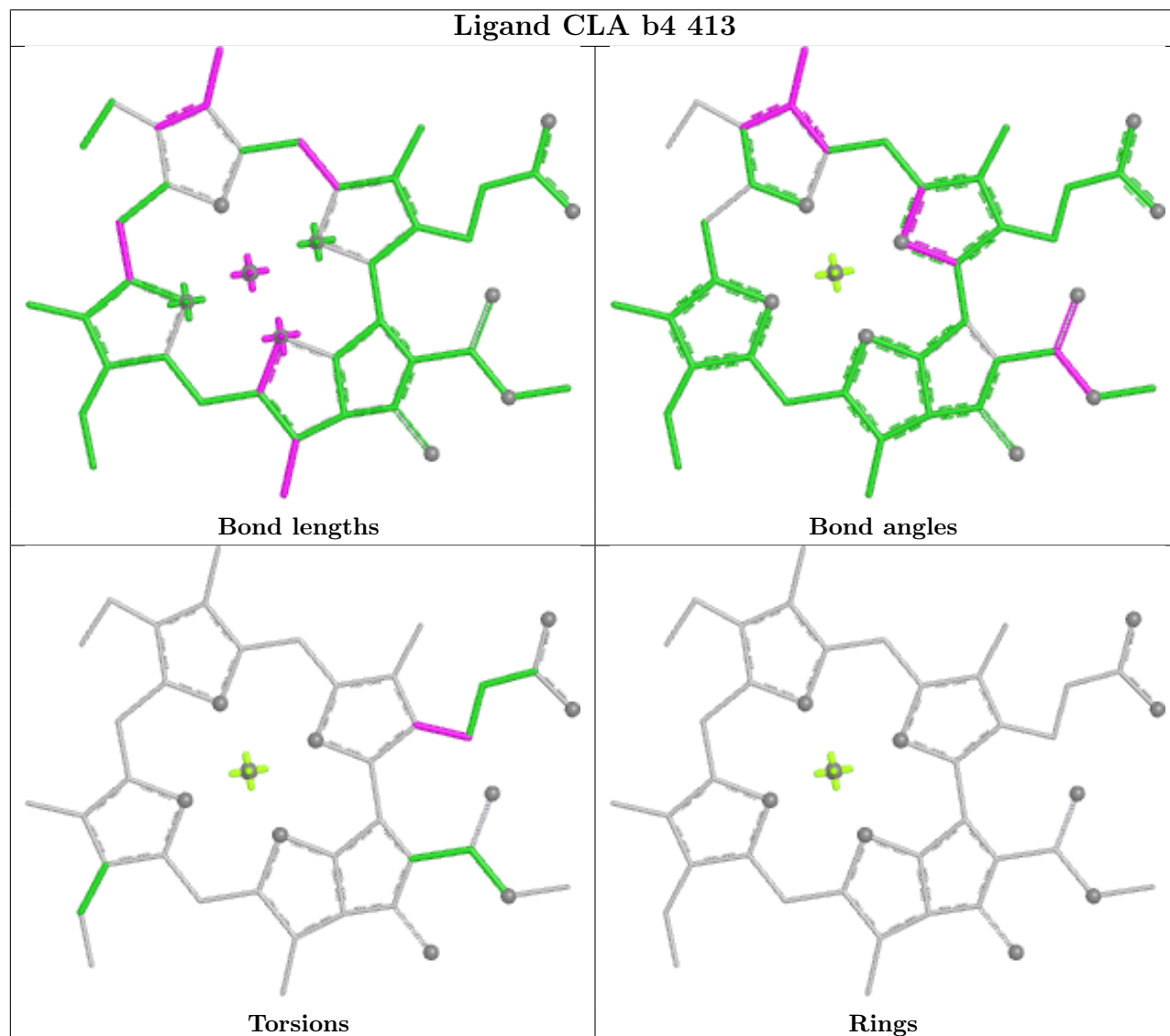
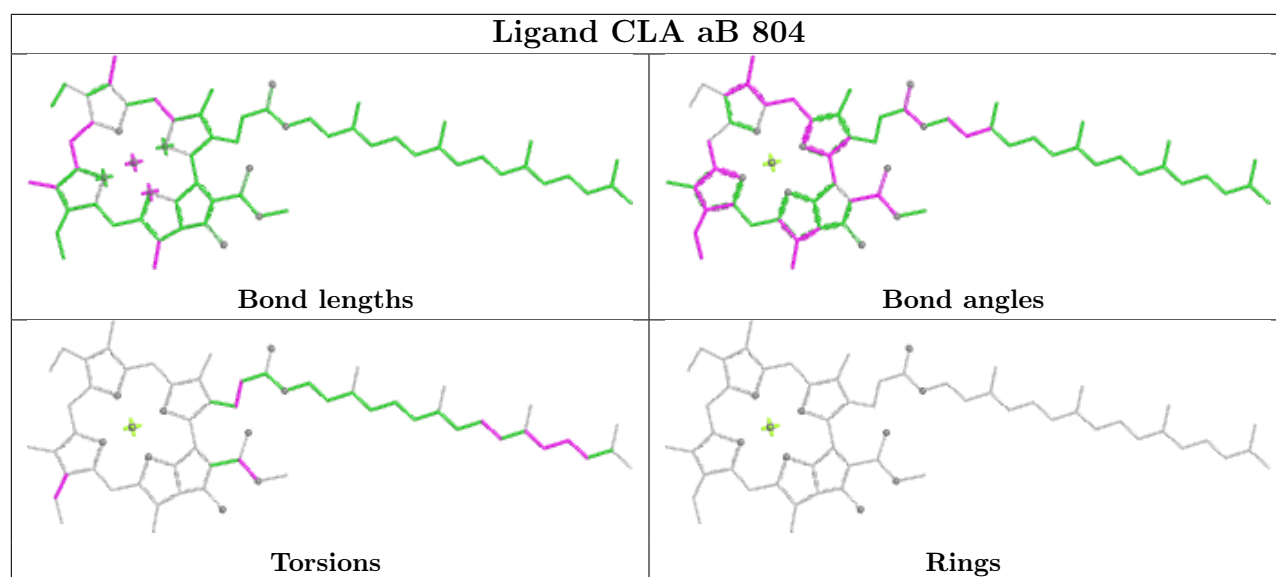


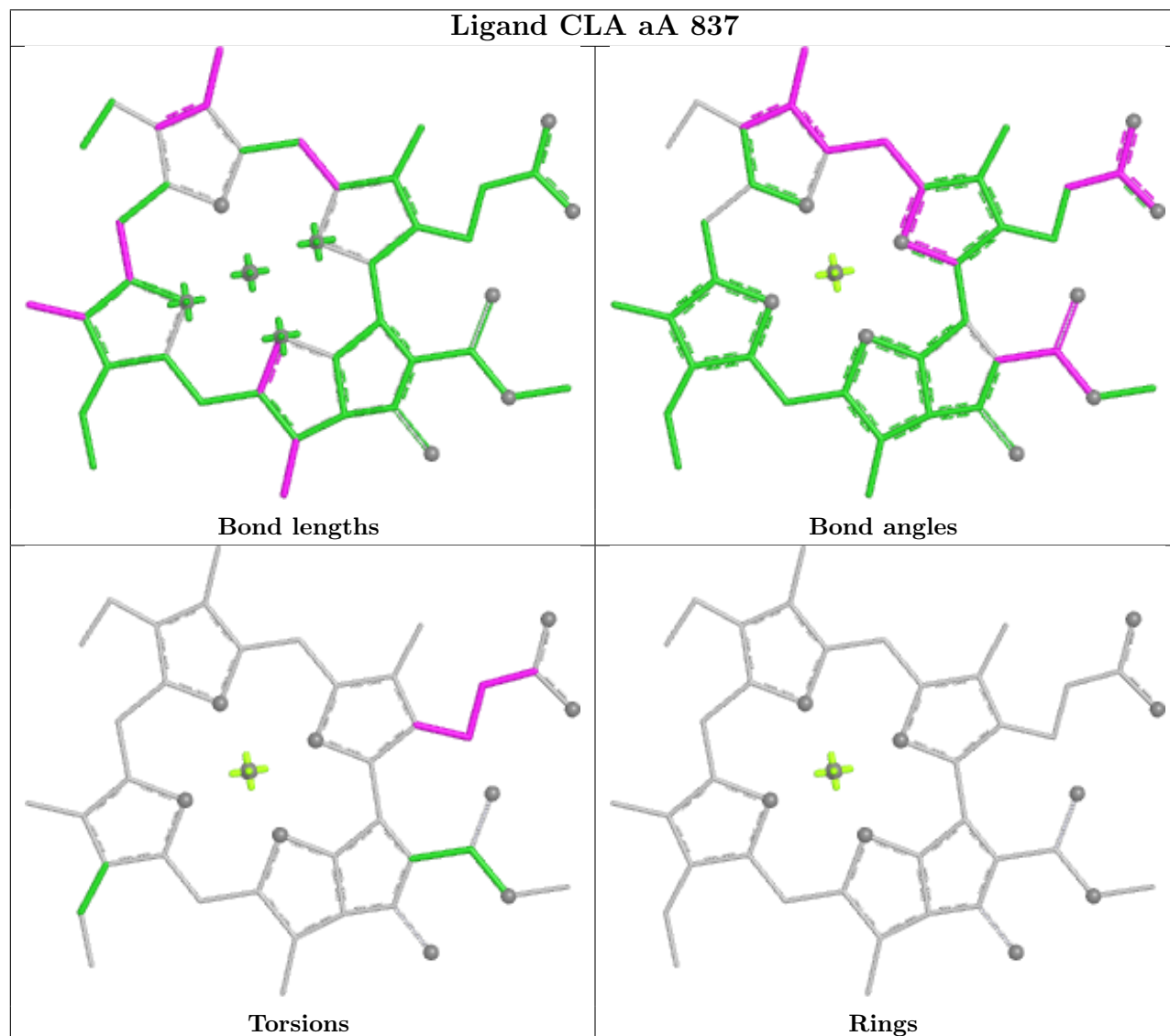
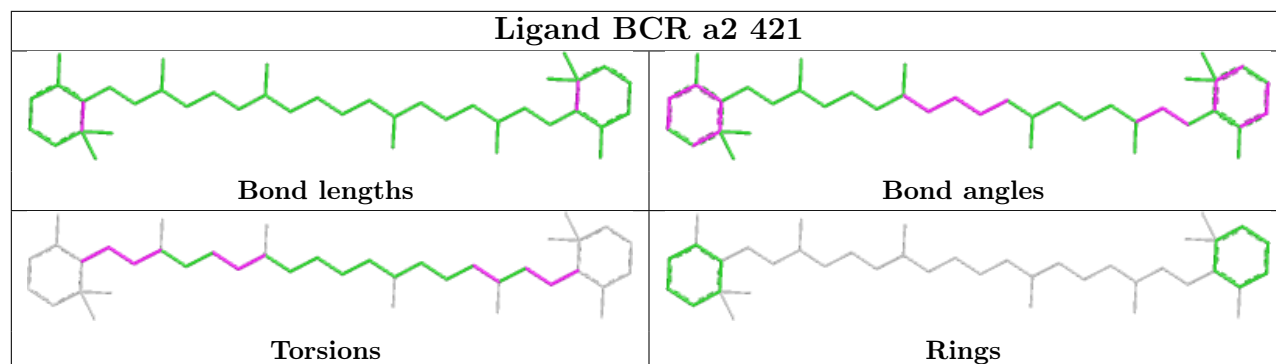


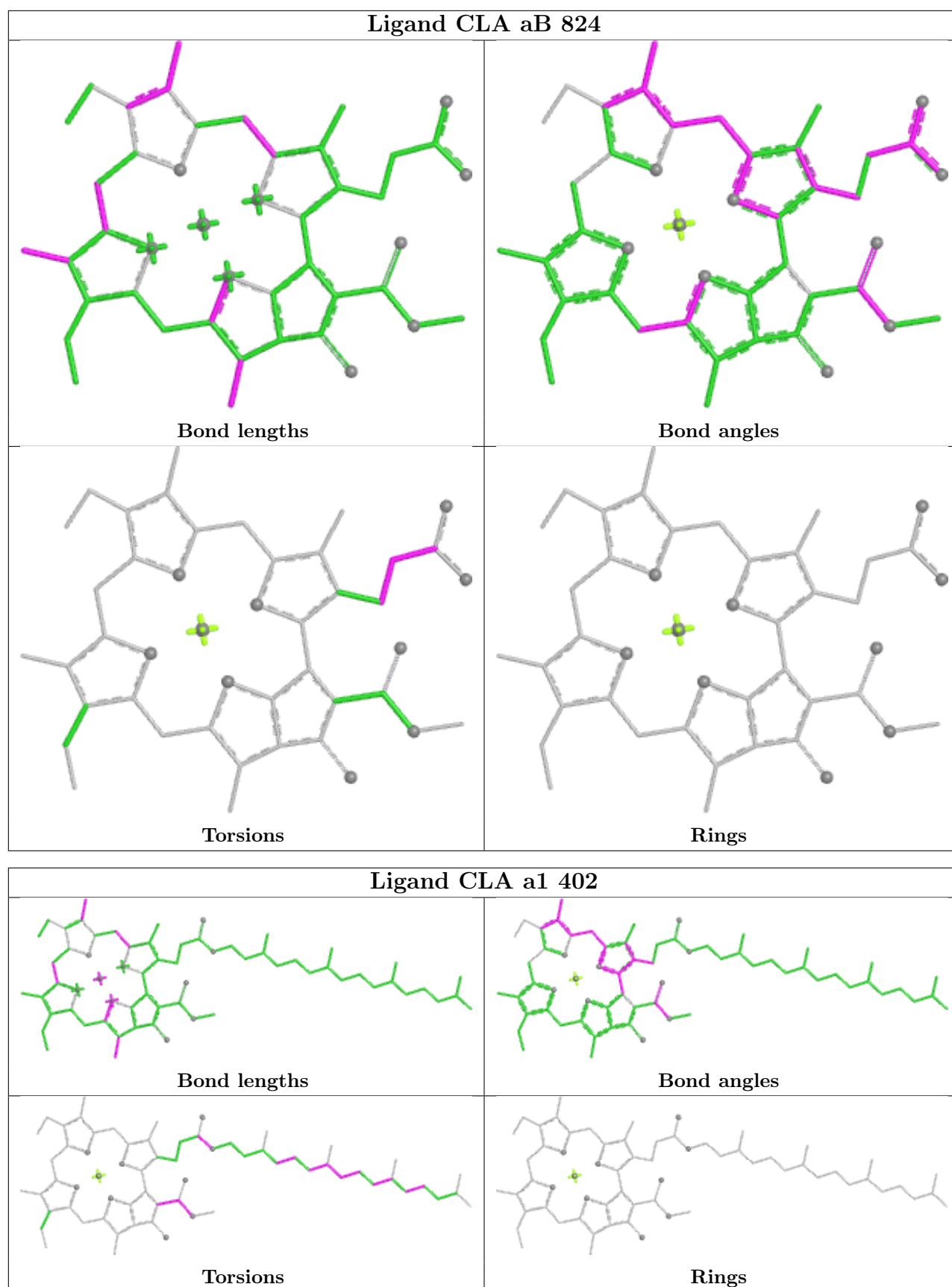




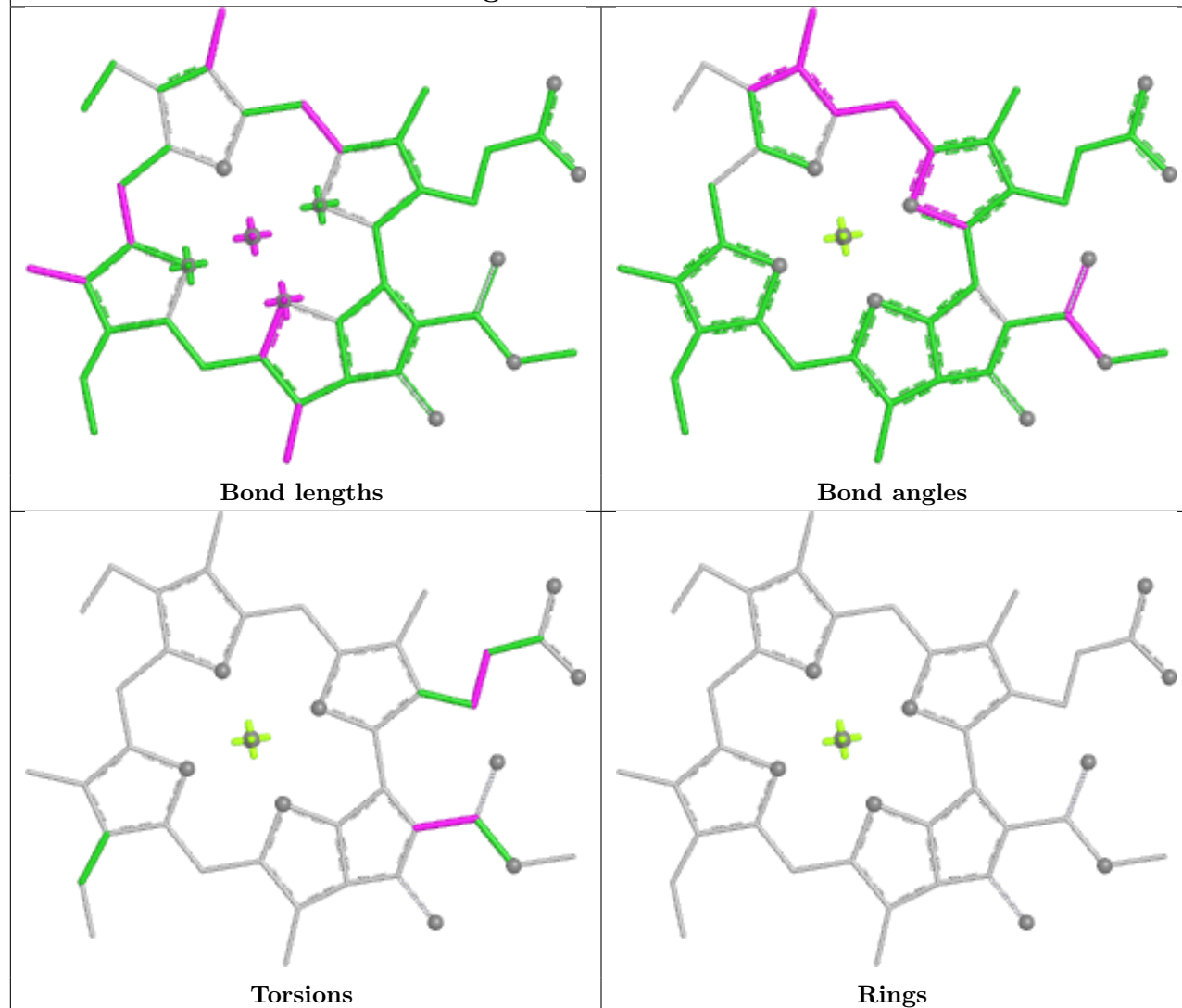




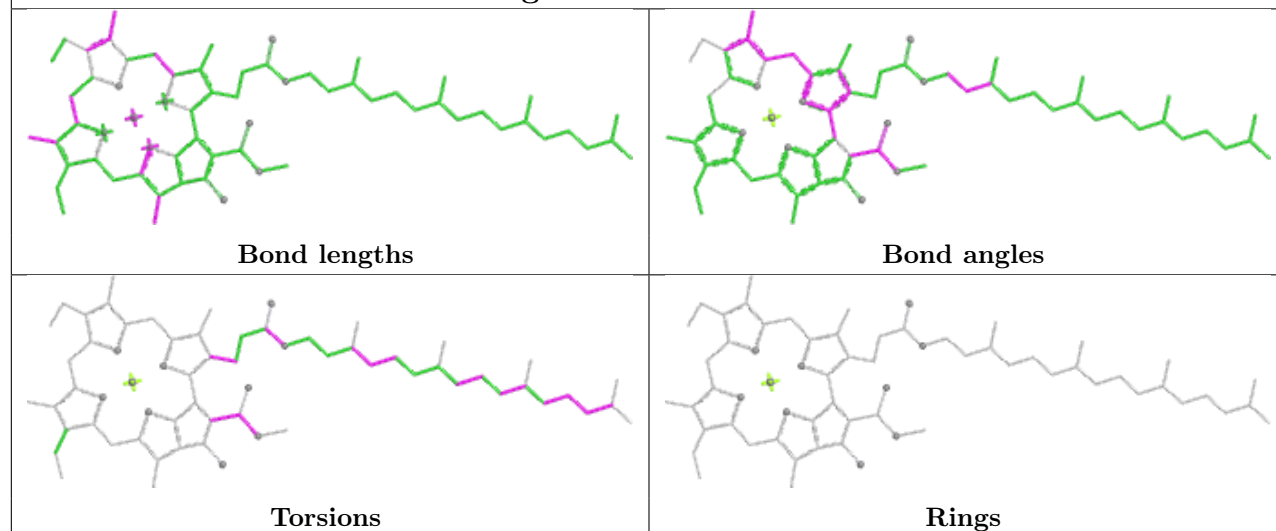


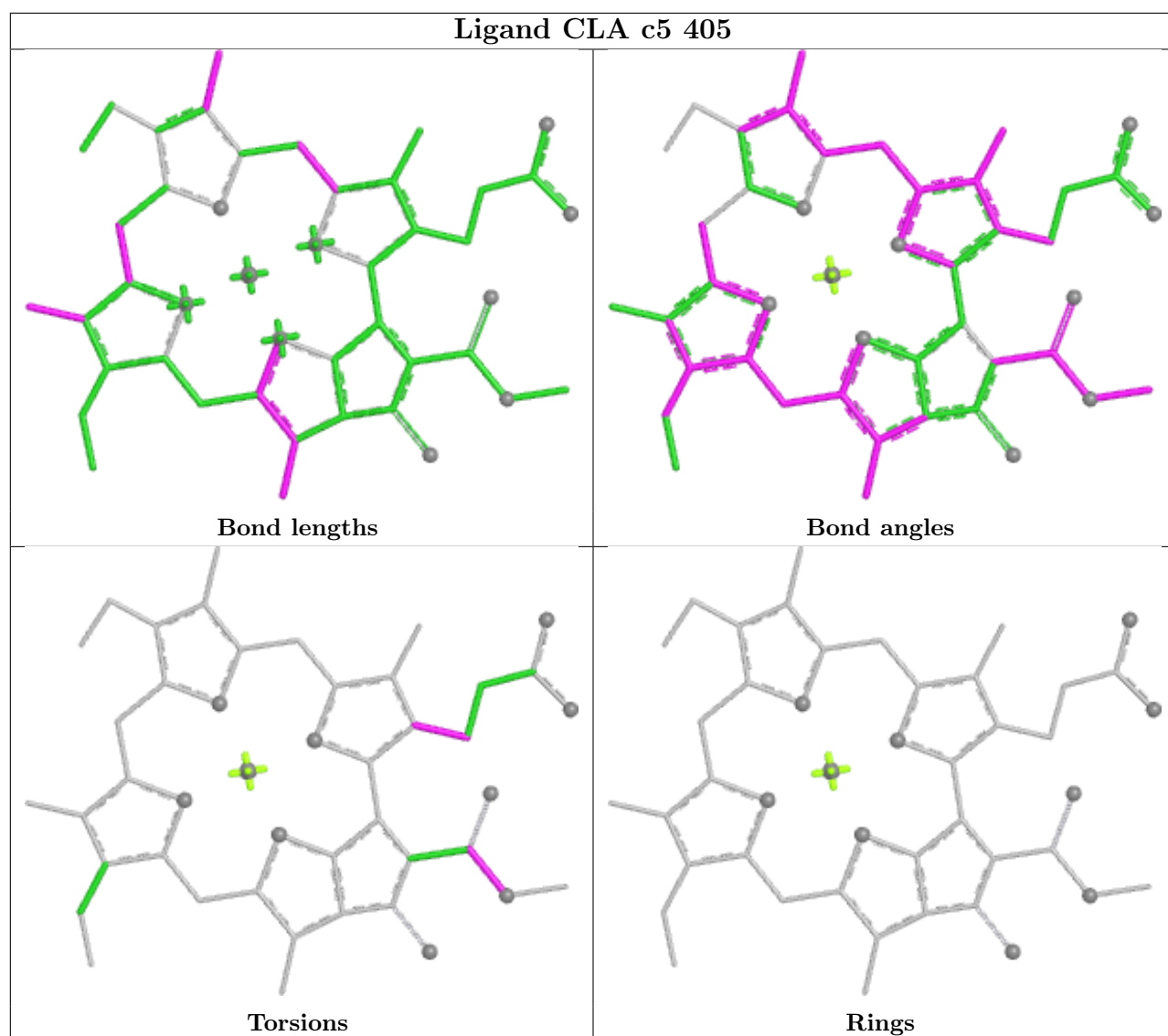


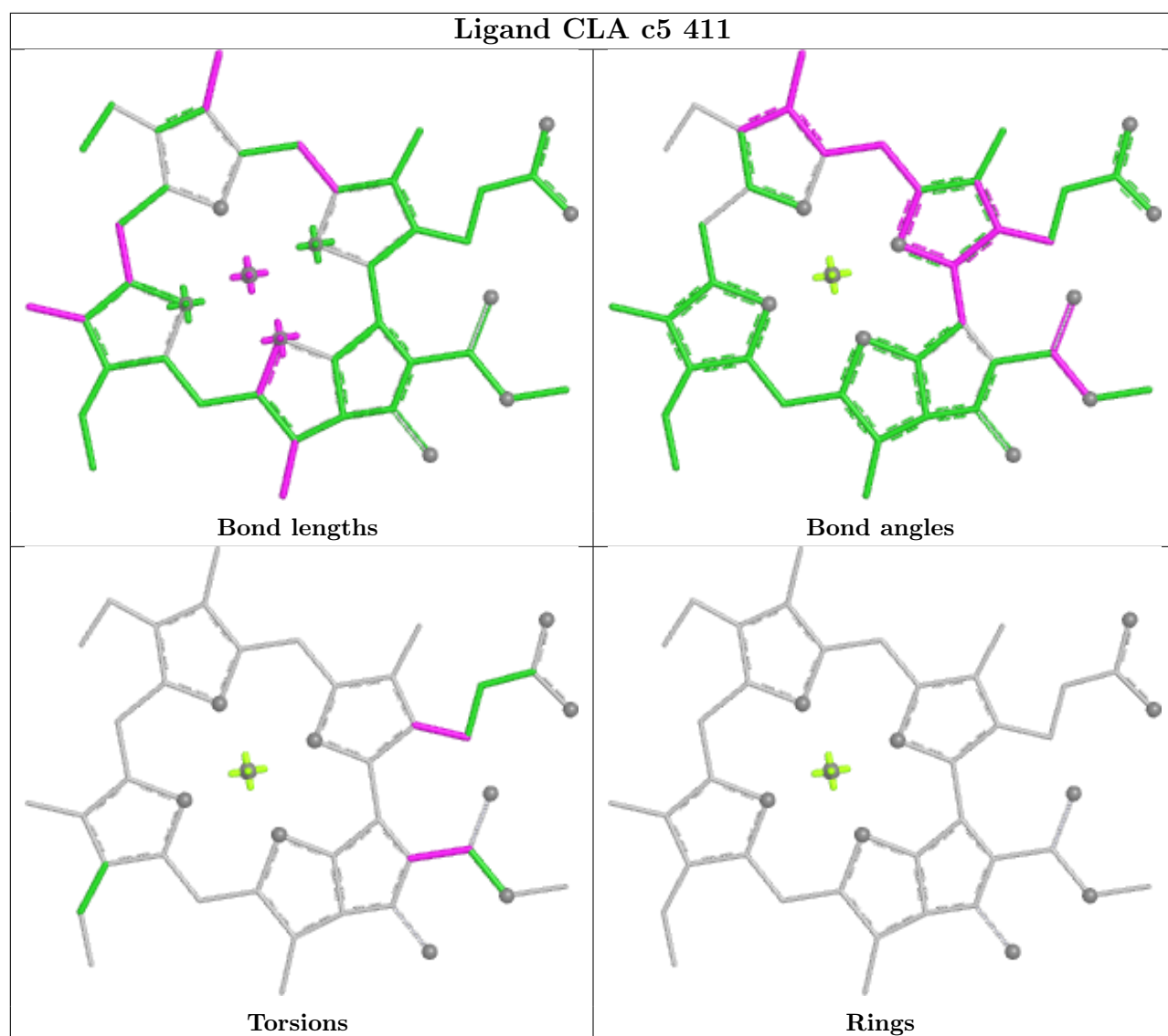
Ligand CLA bA 816

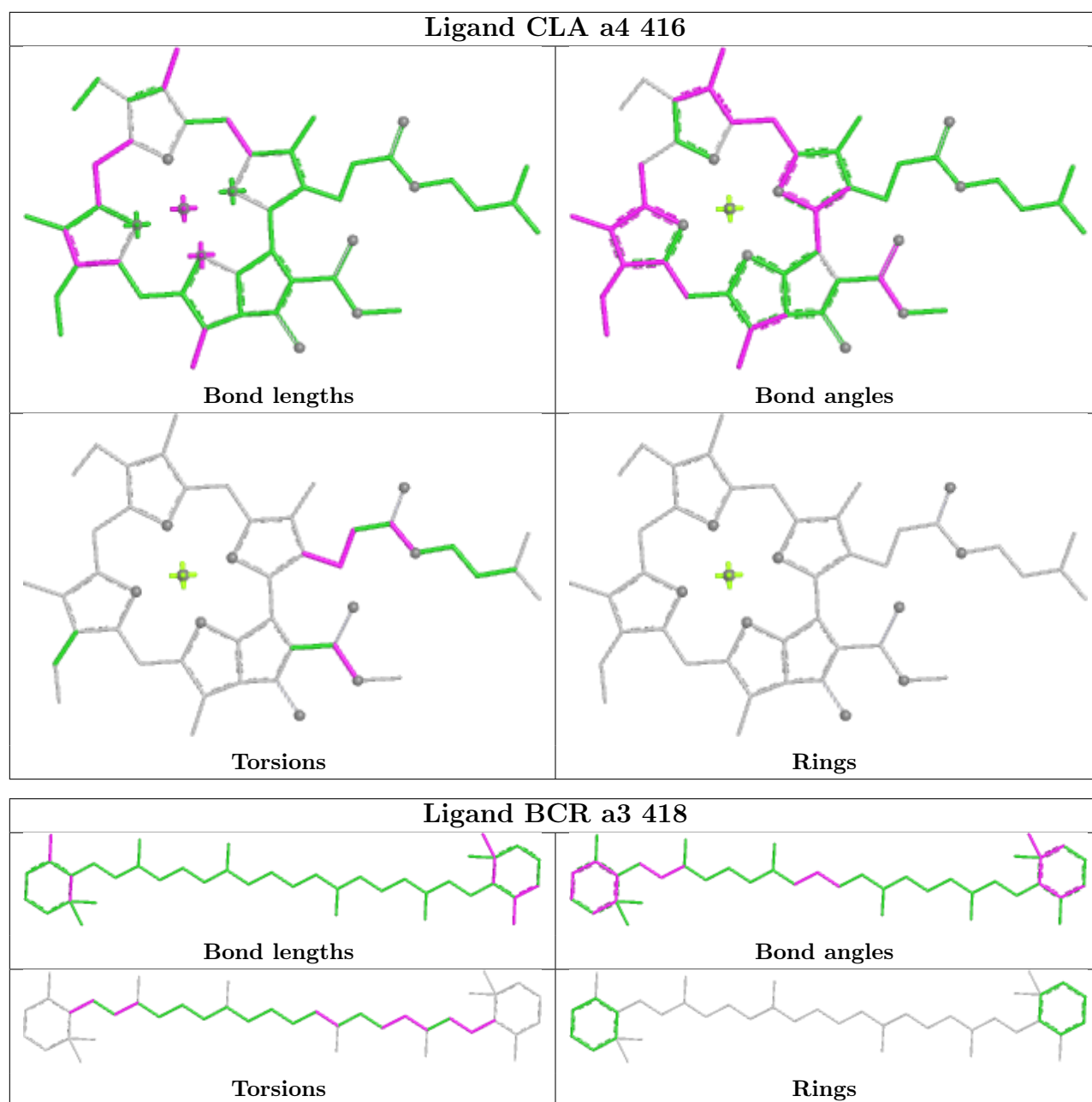


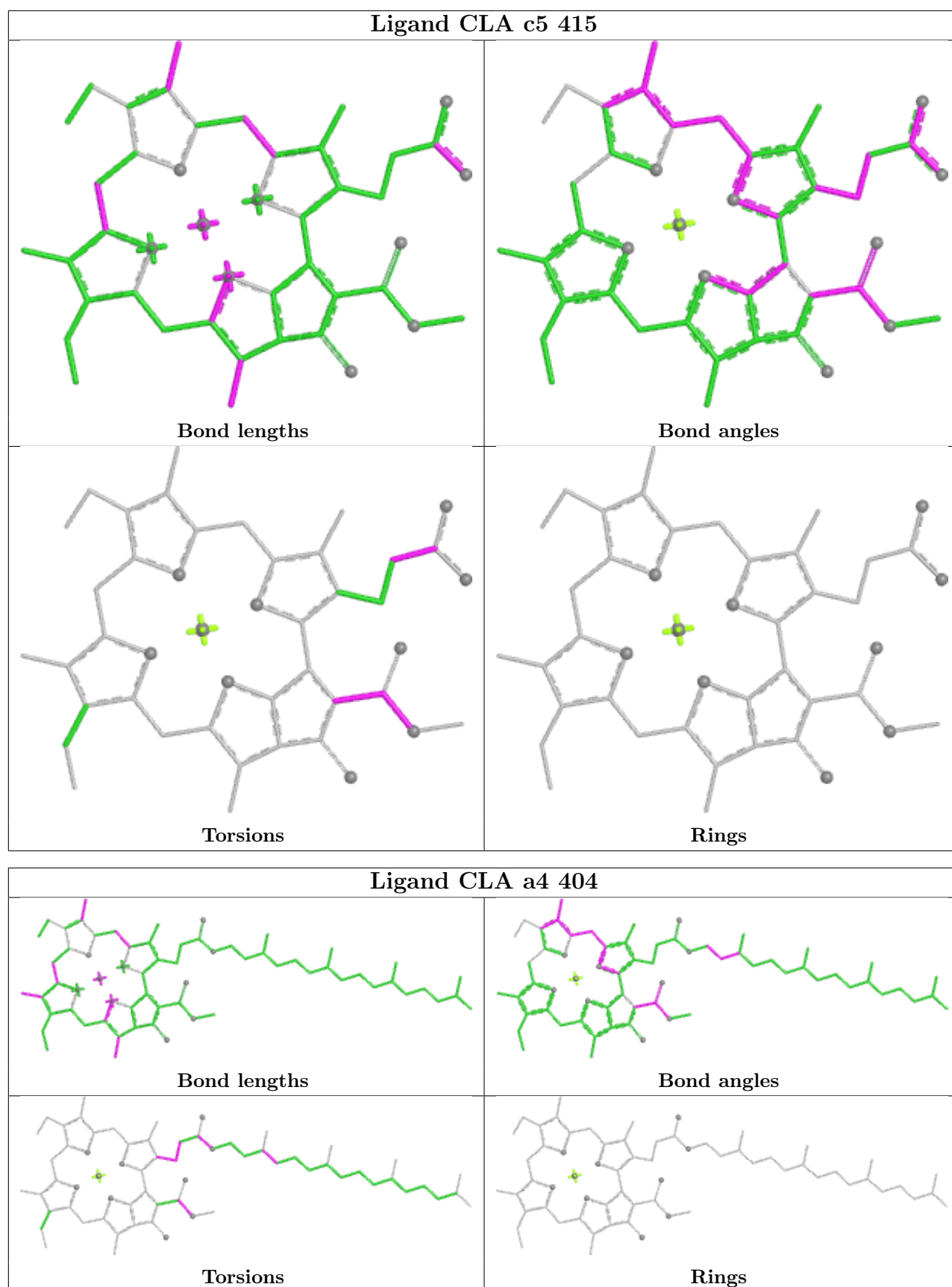
Ligand CLA bA 820

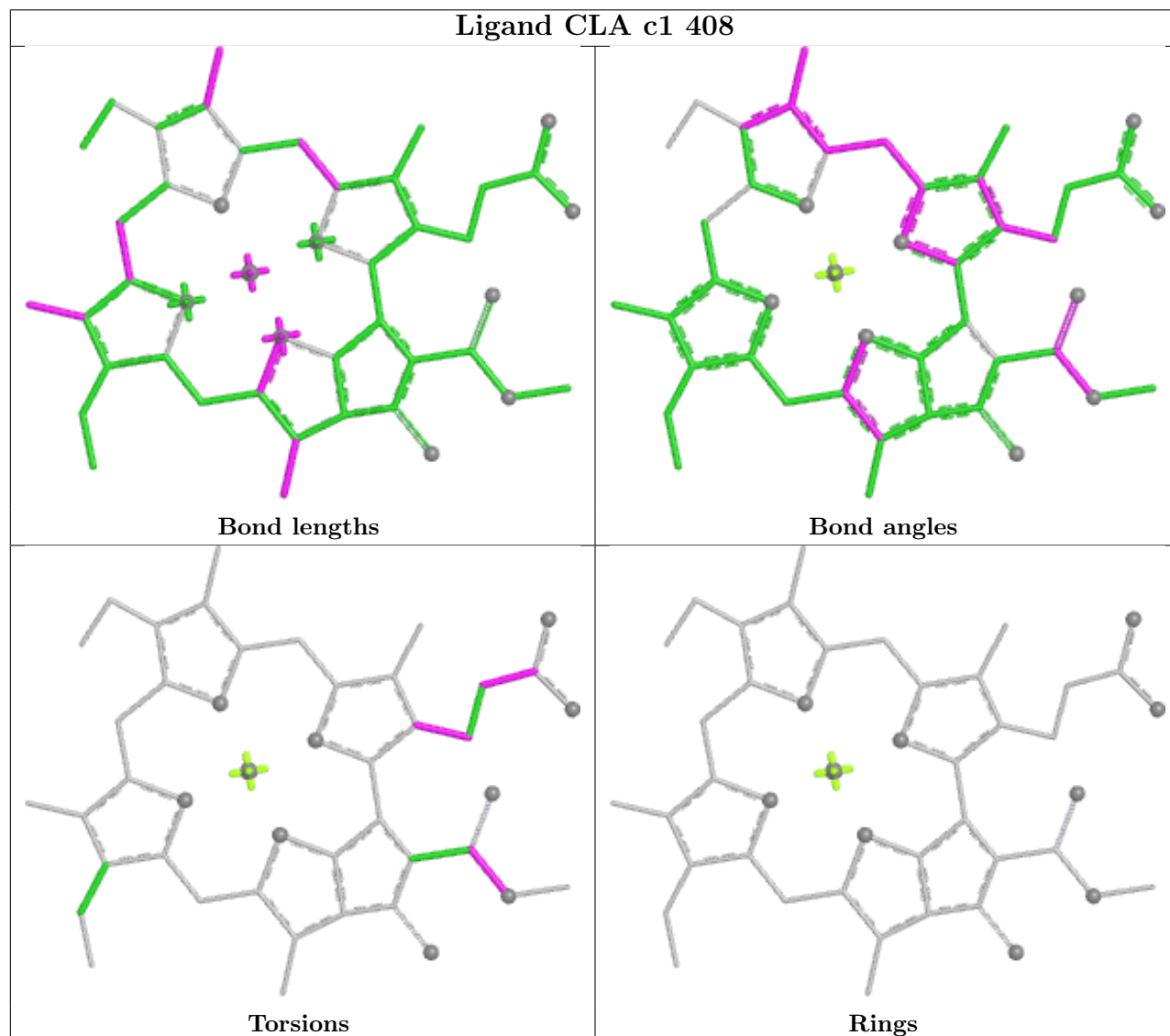
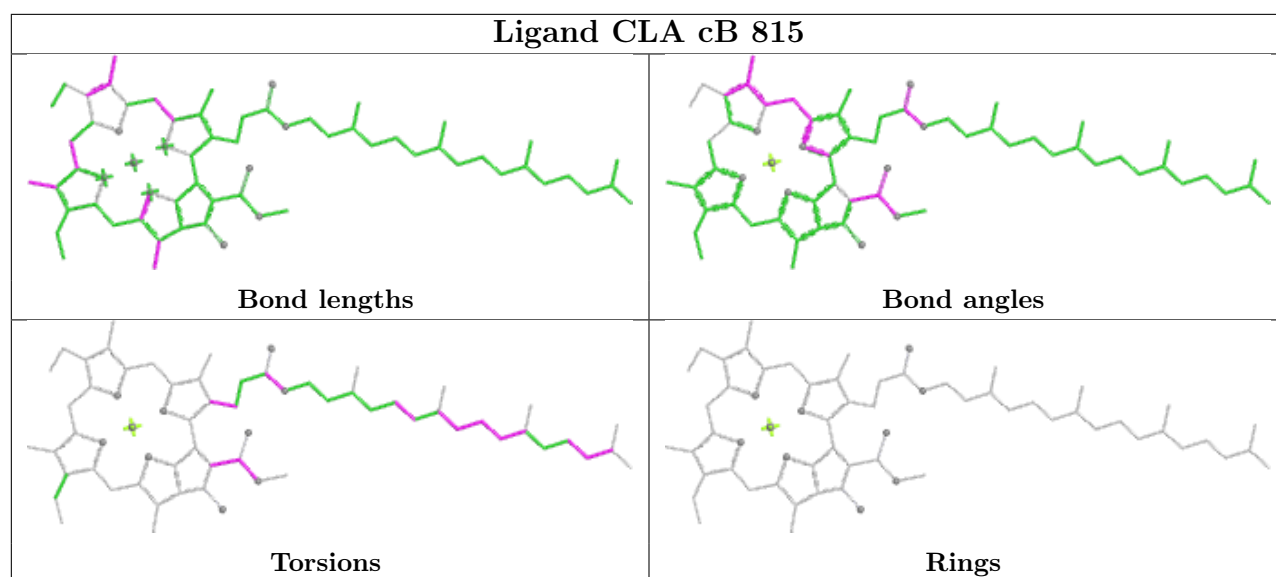


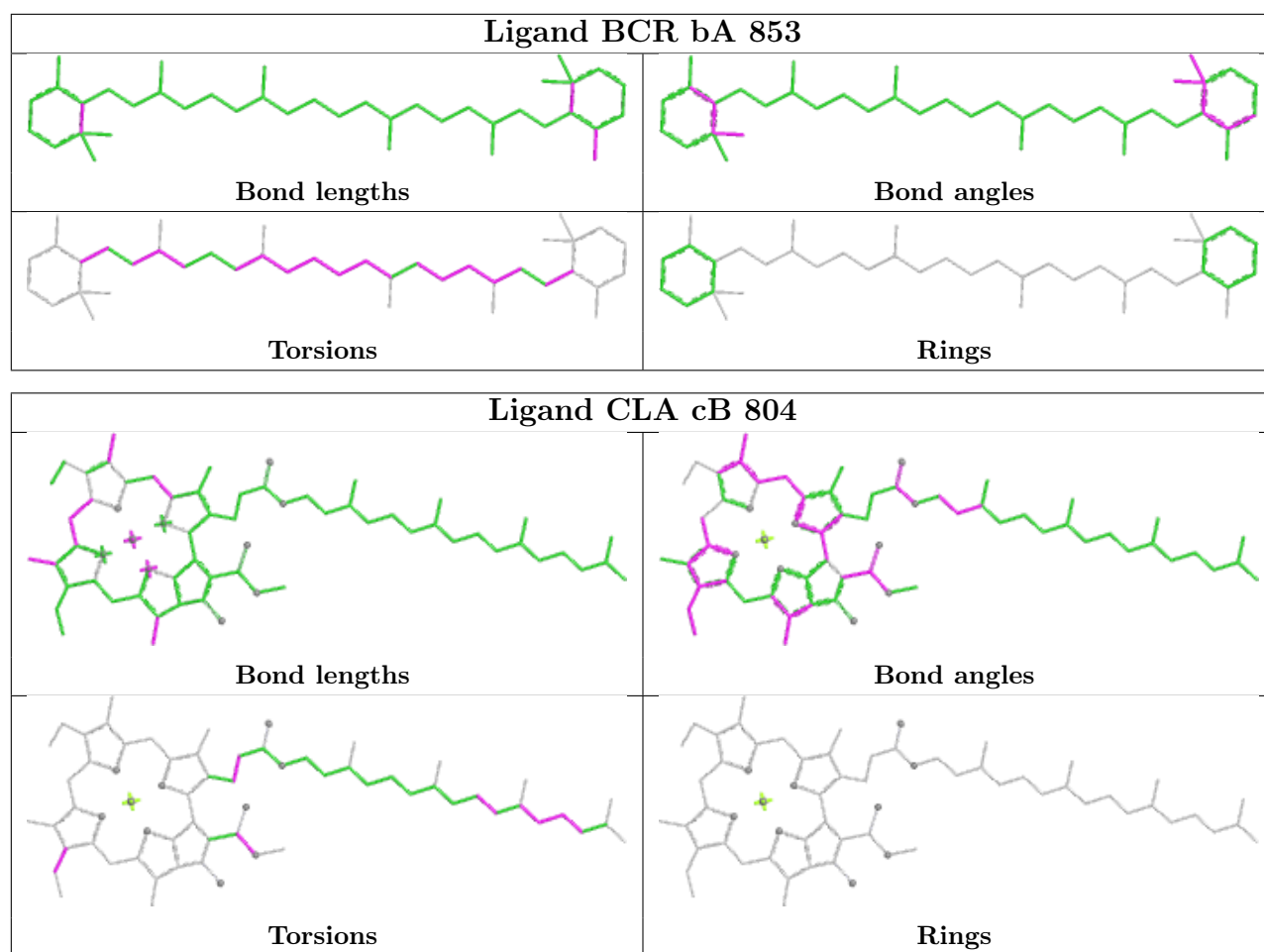


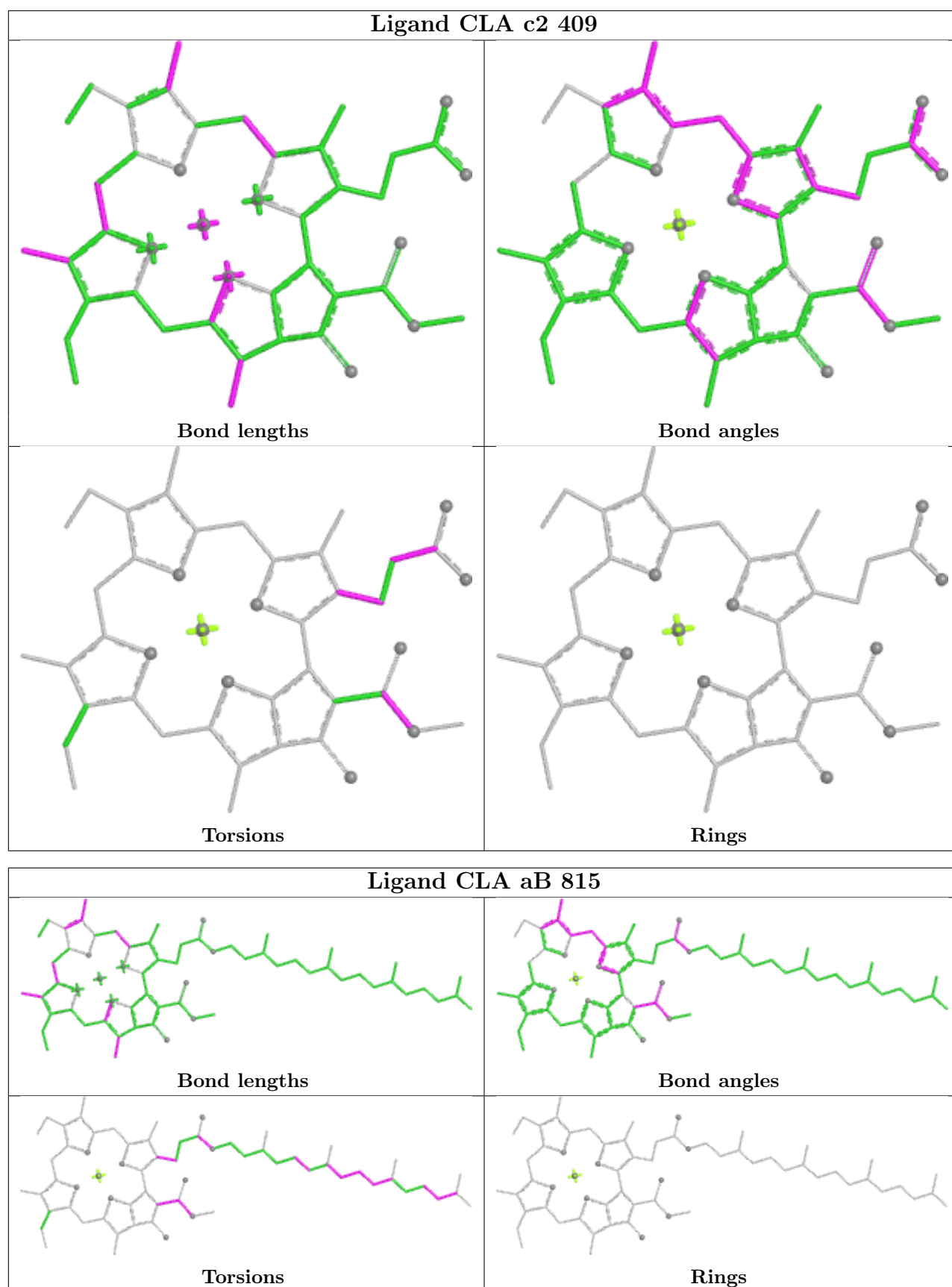


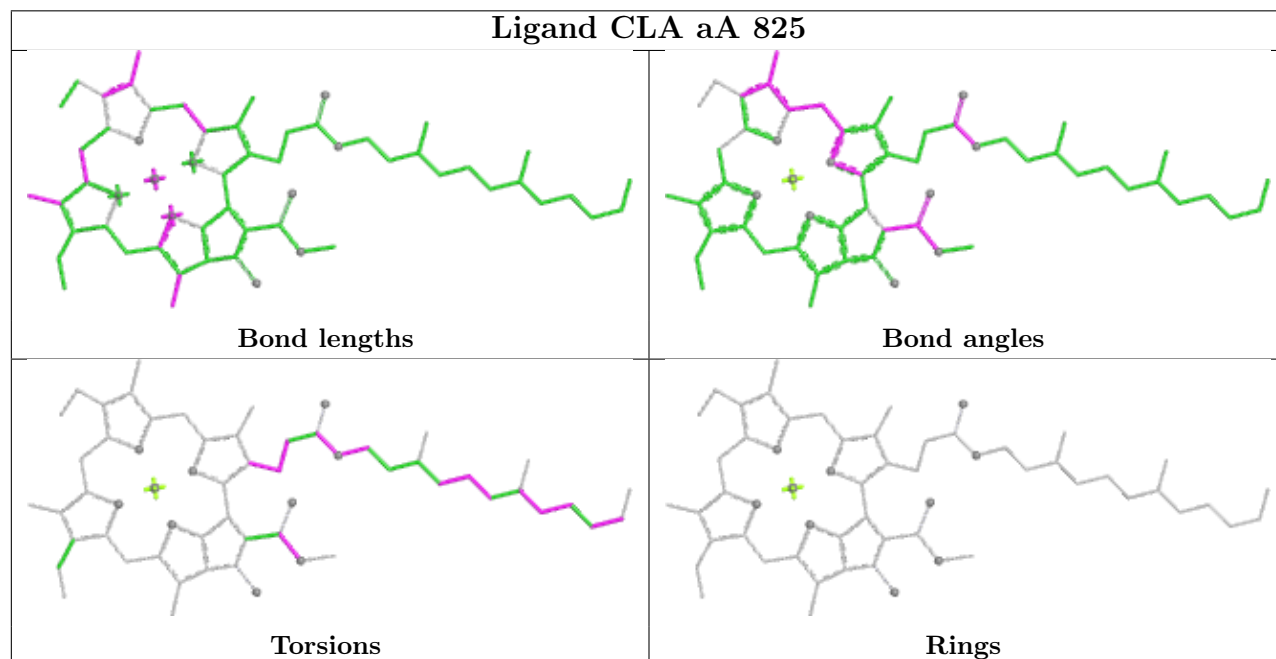
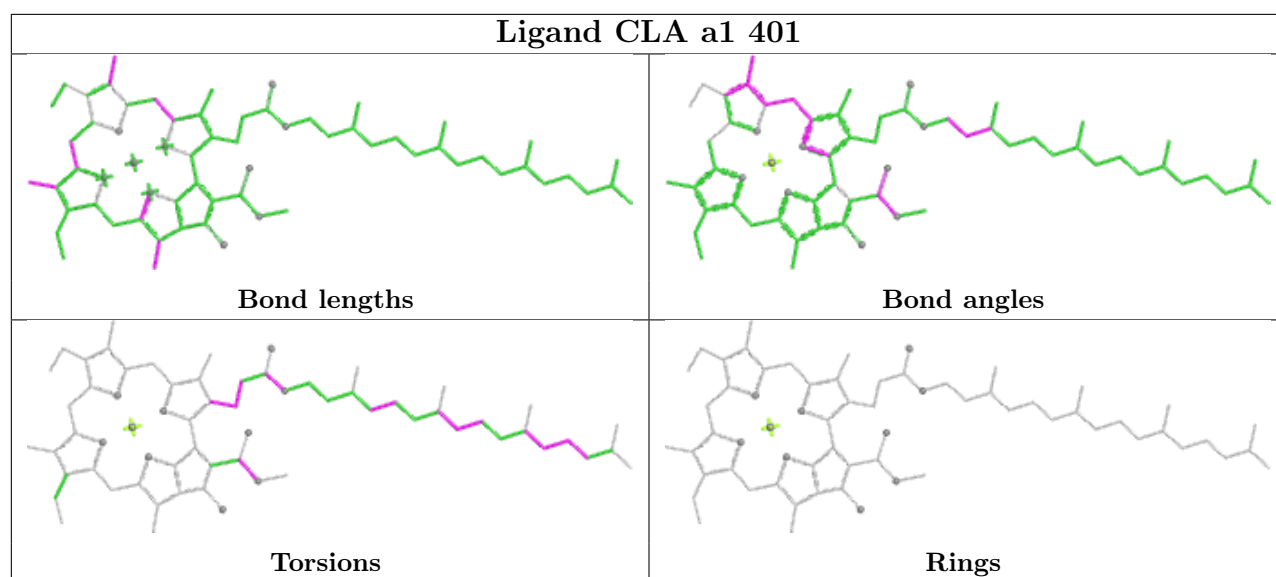


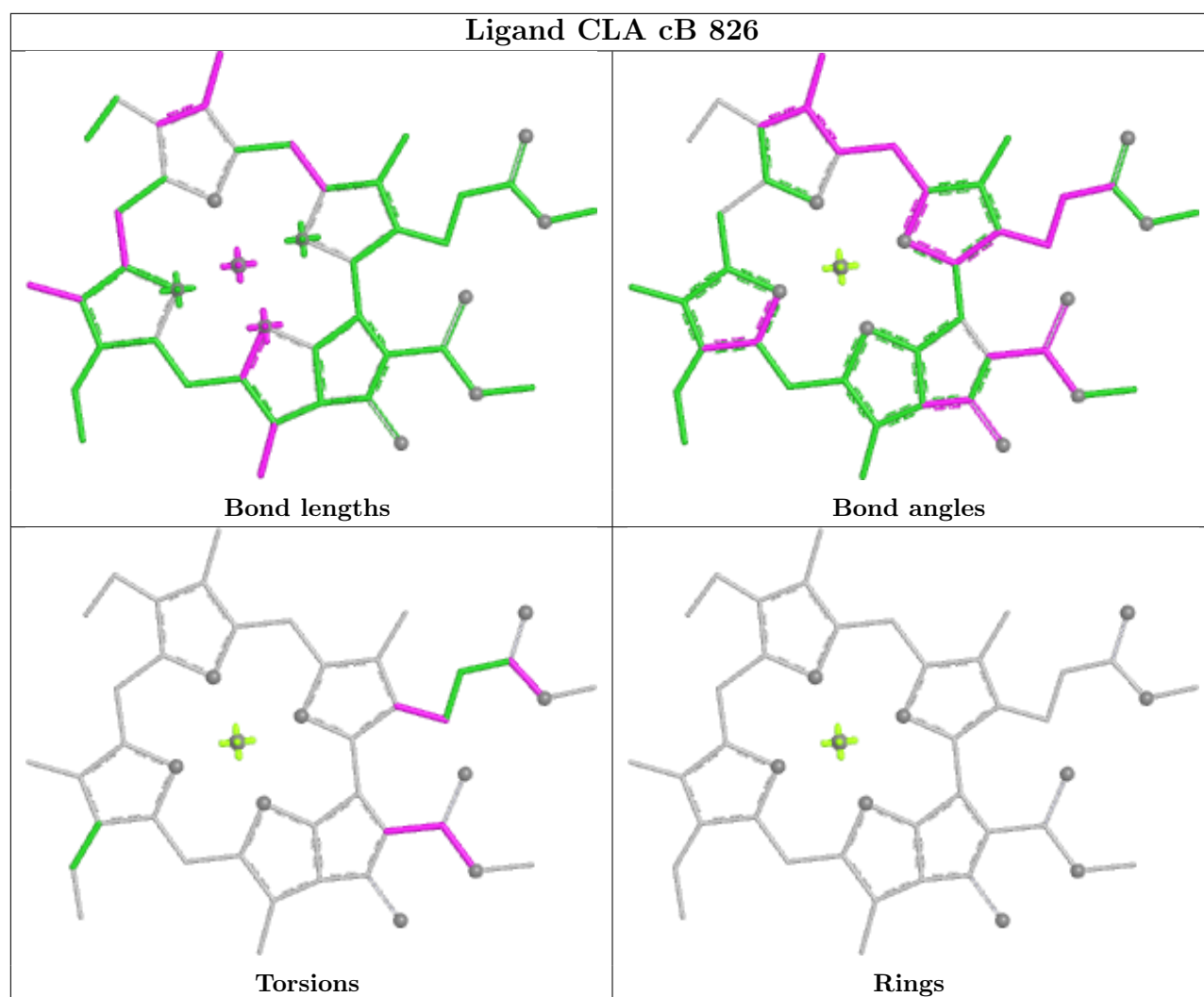


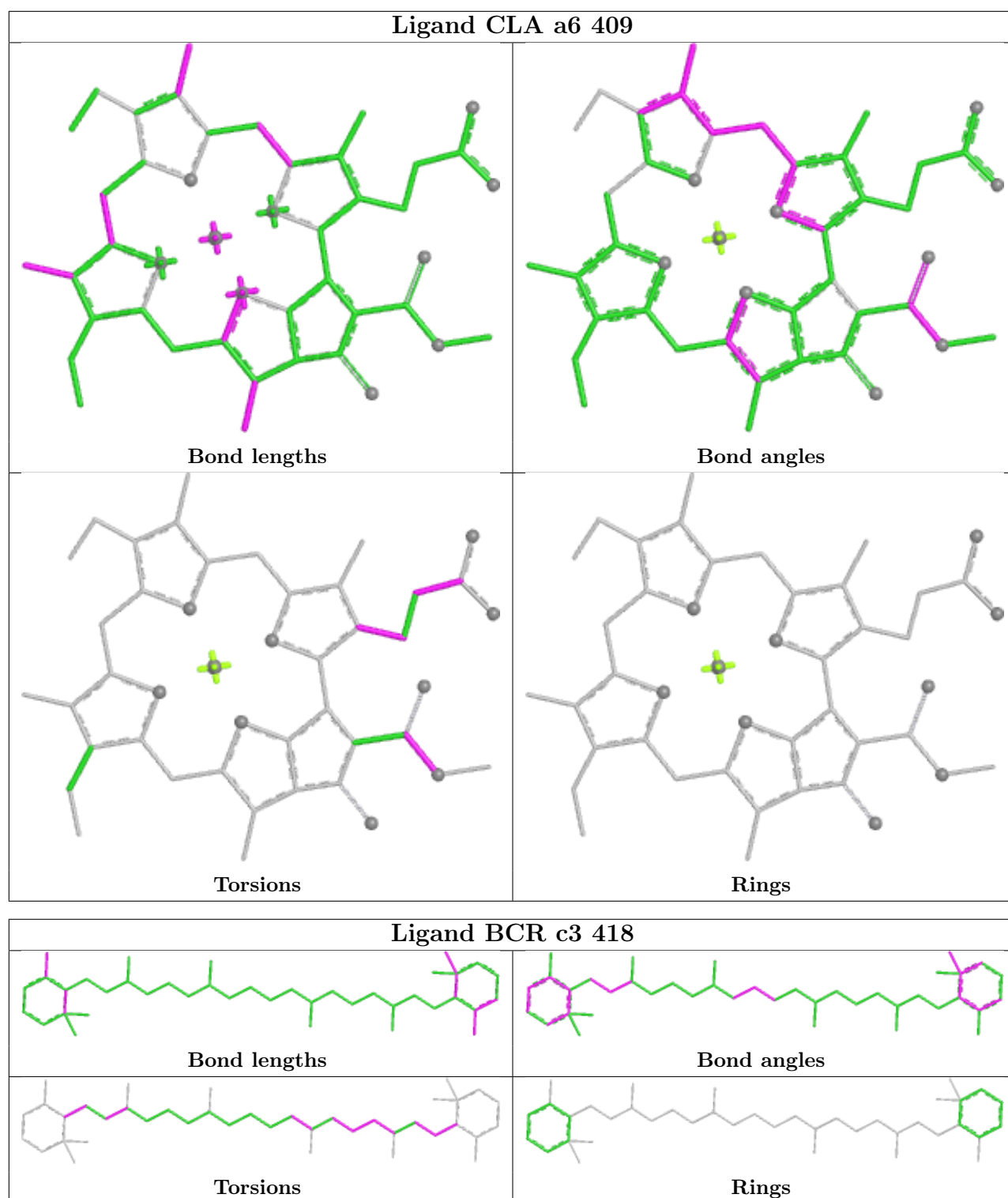


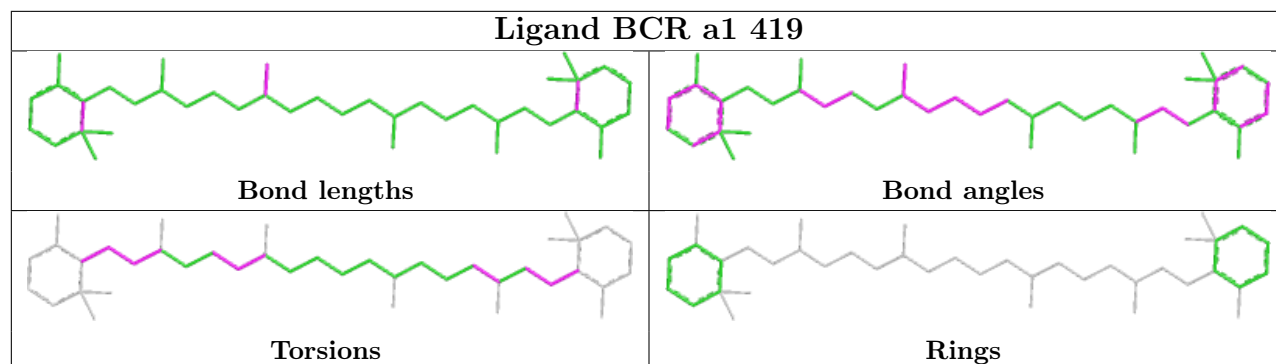
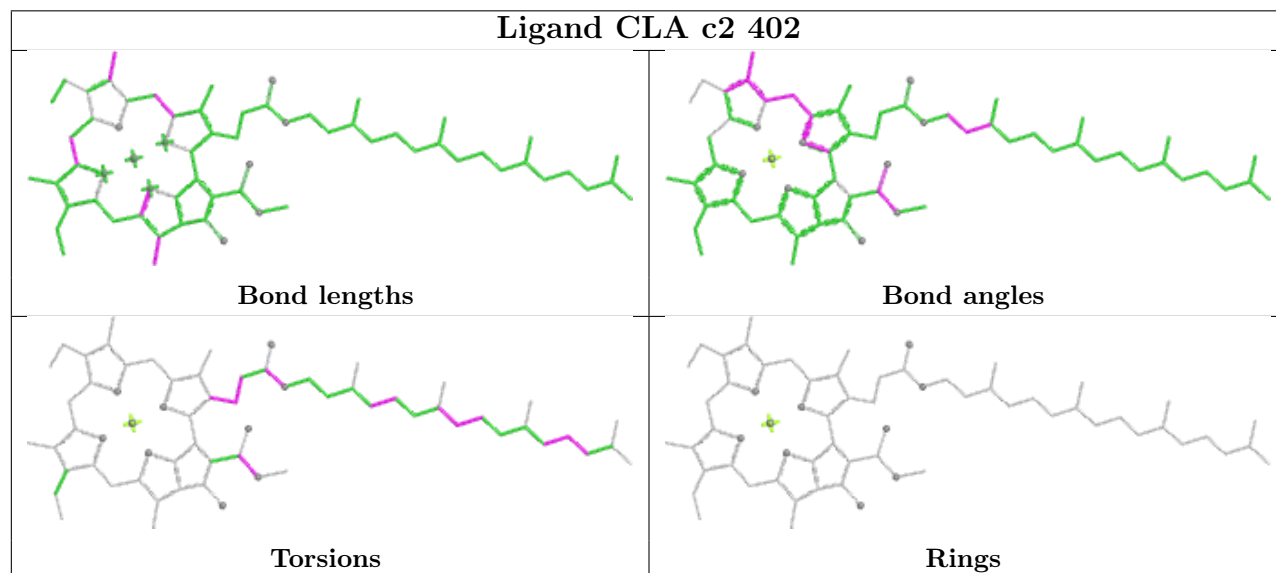
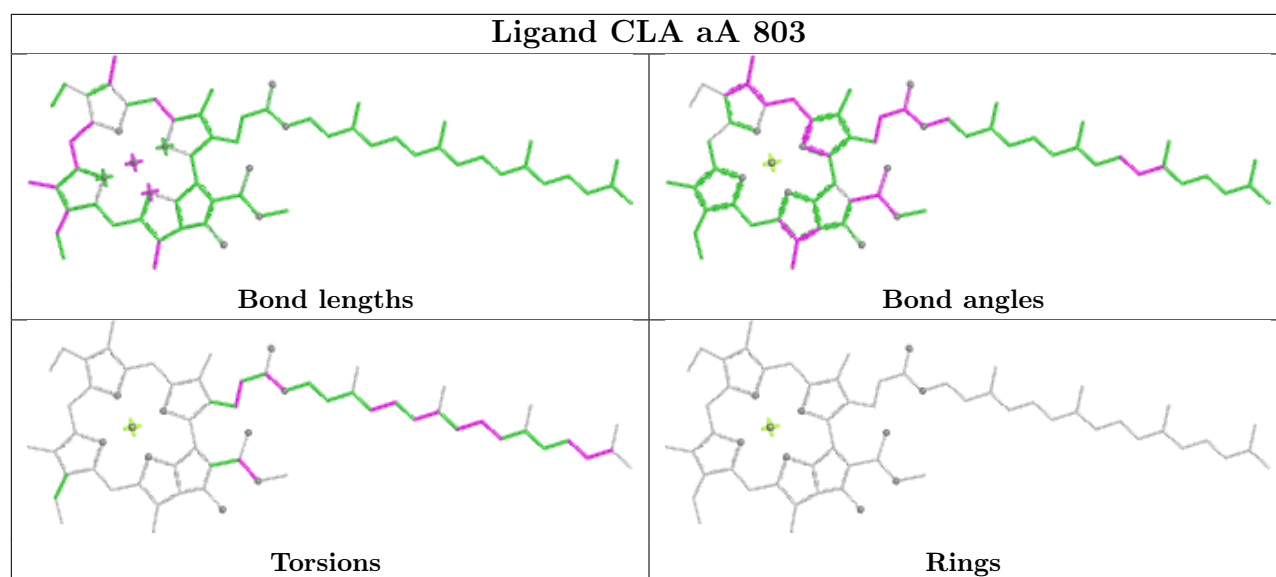


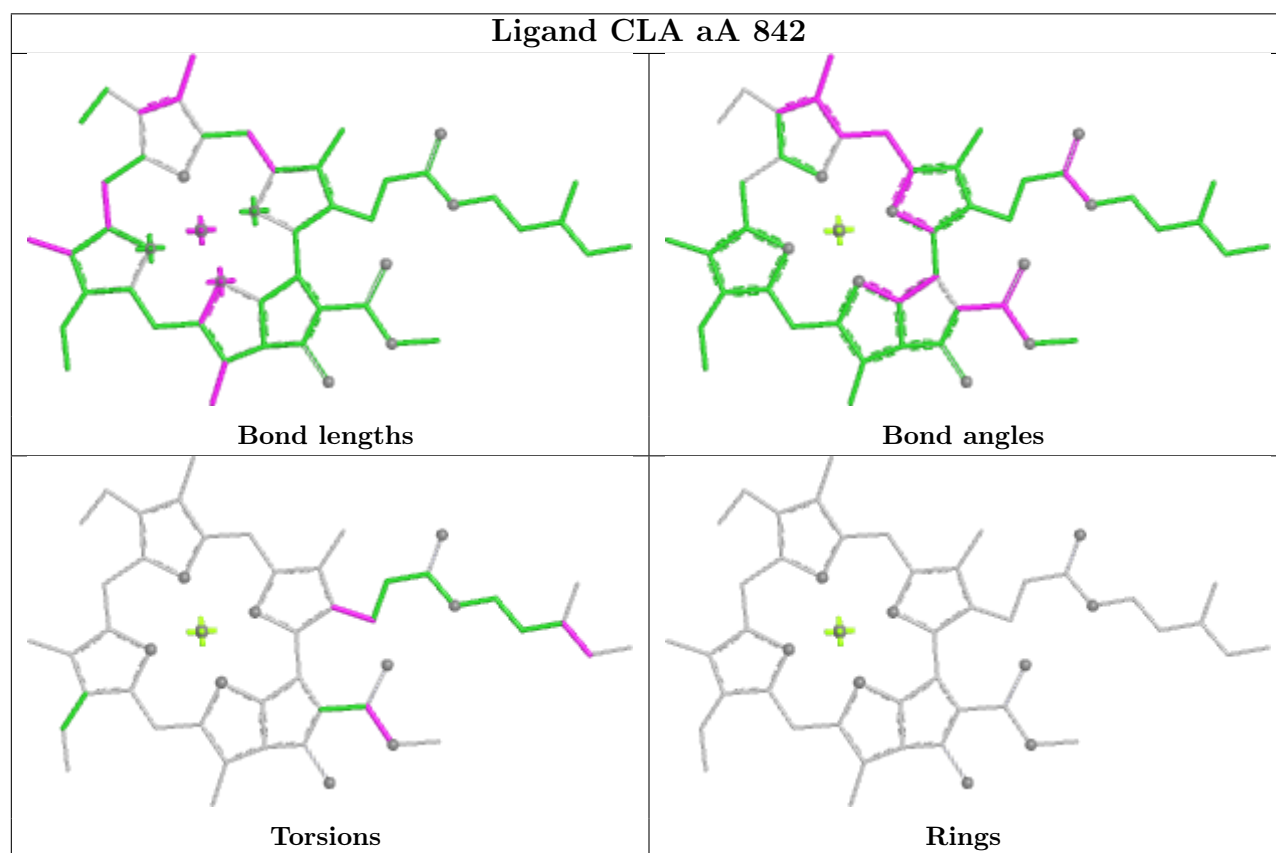
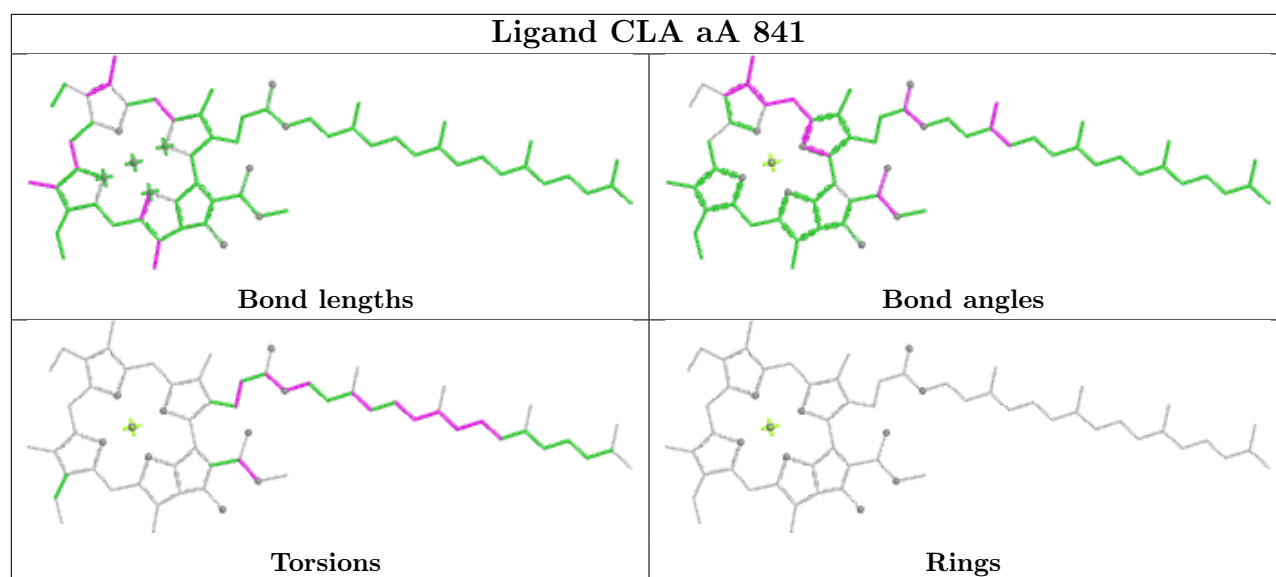


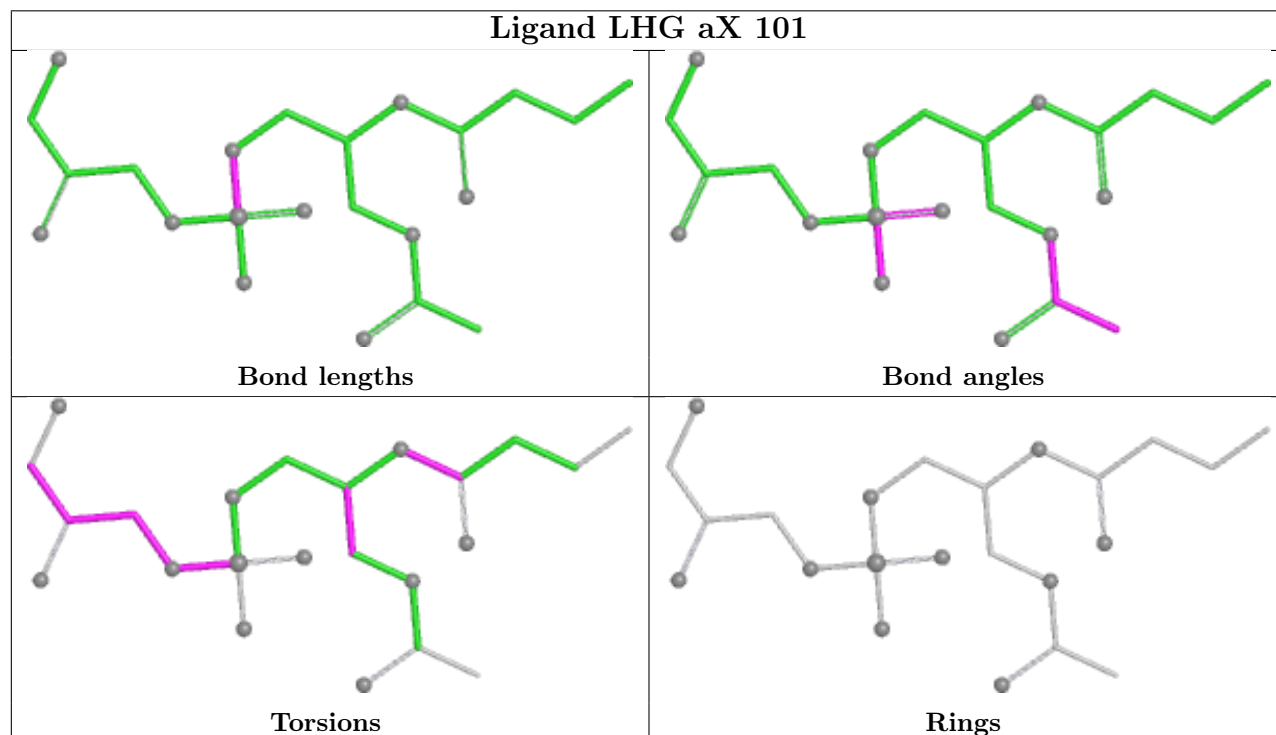
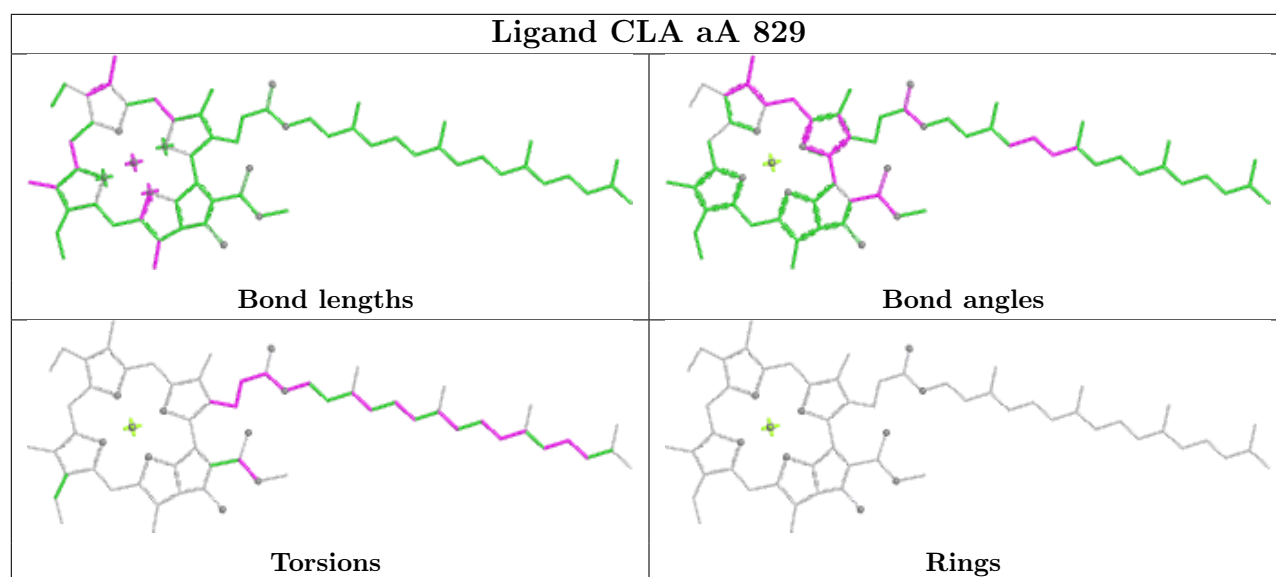


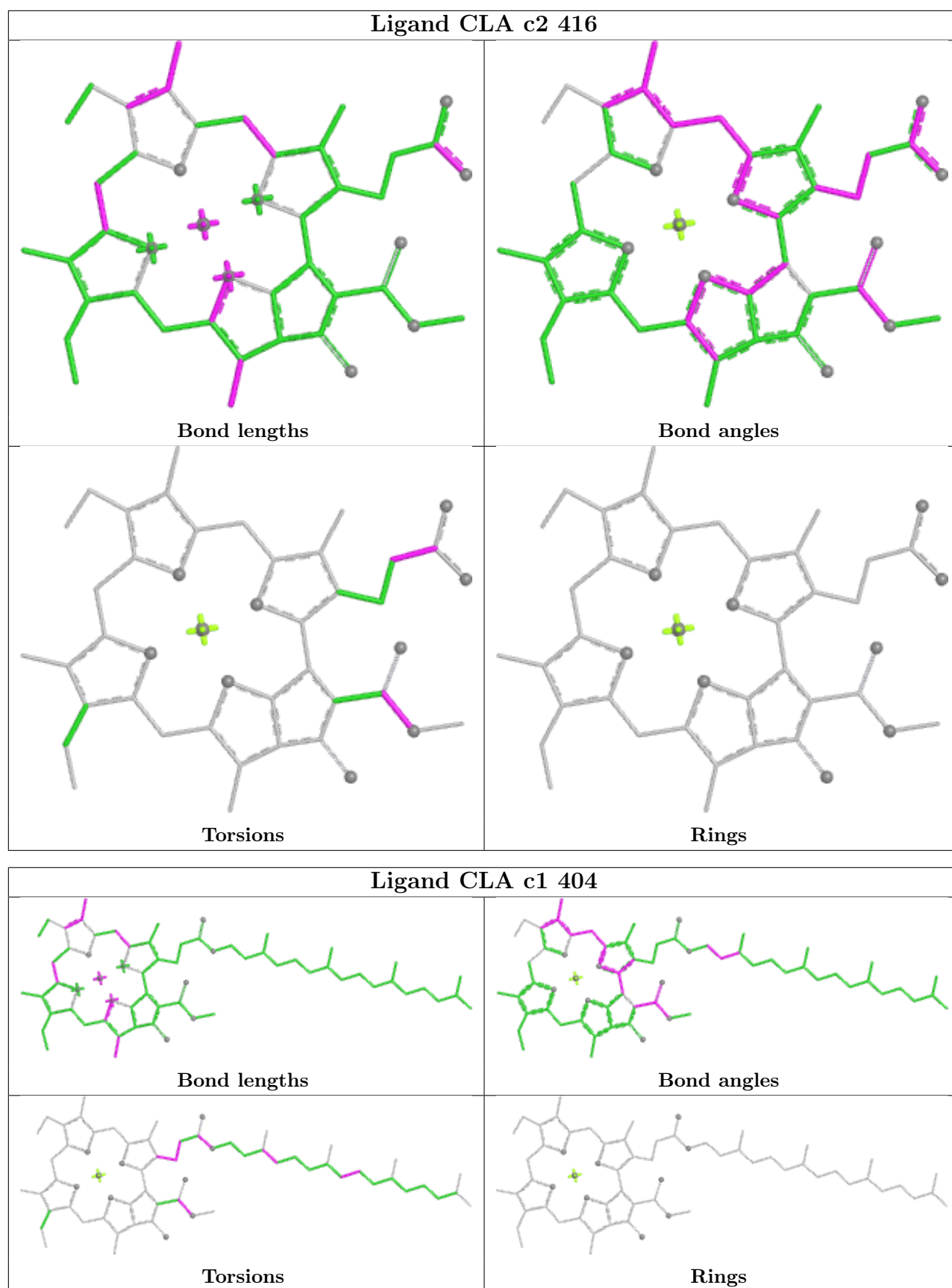


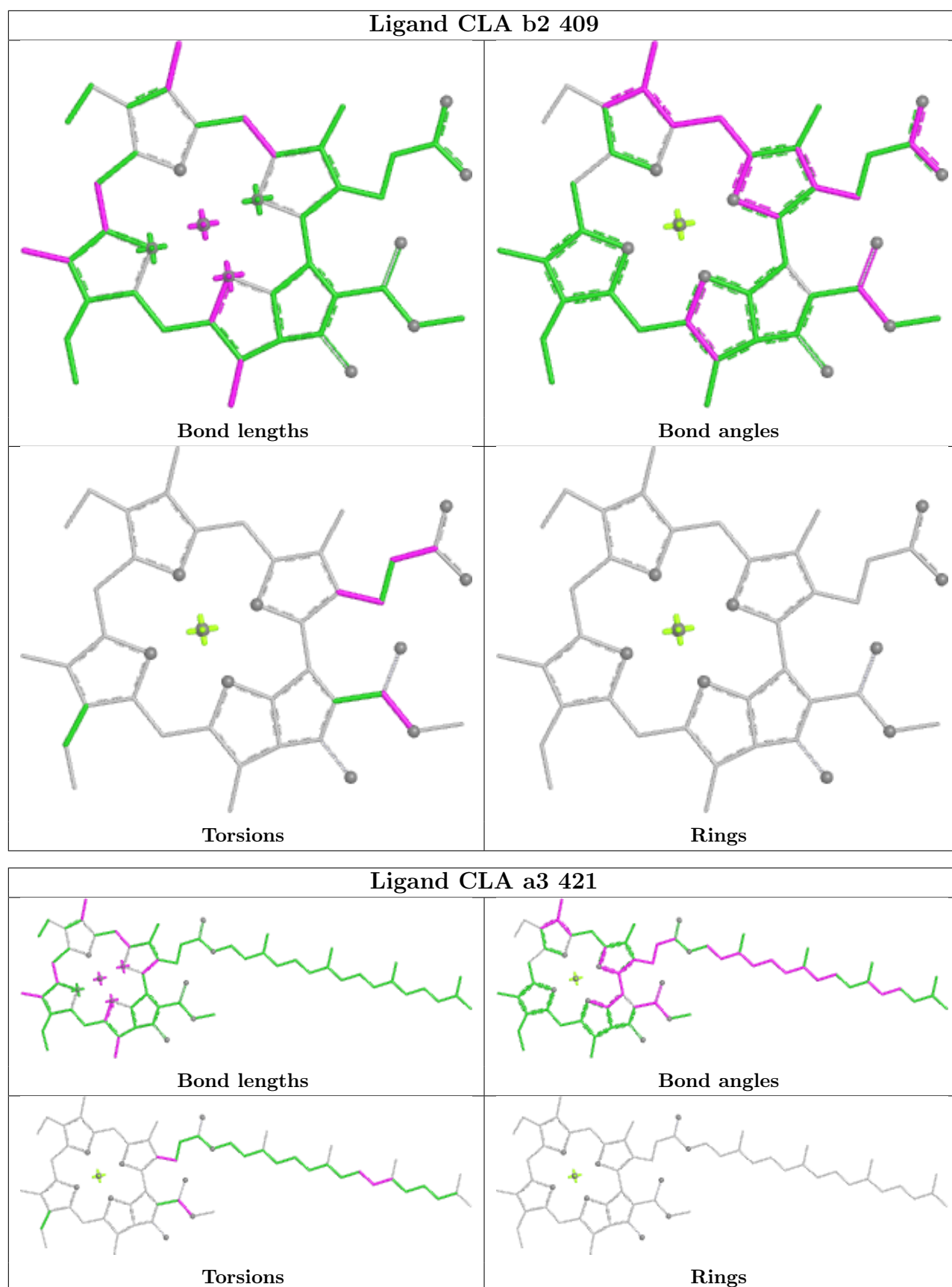


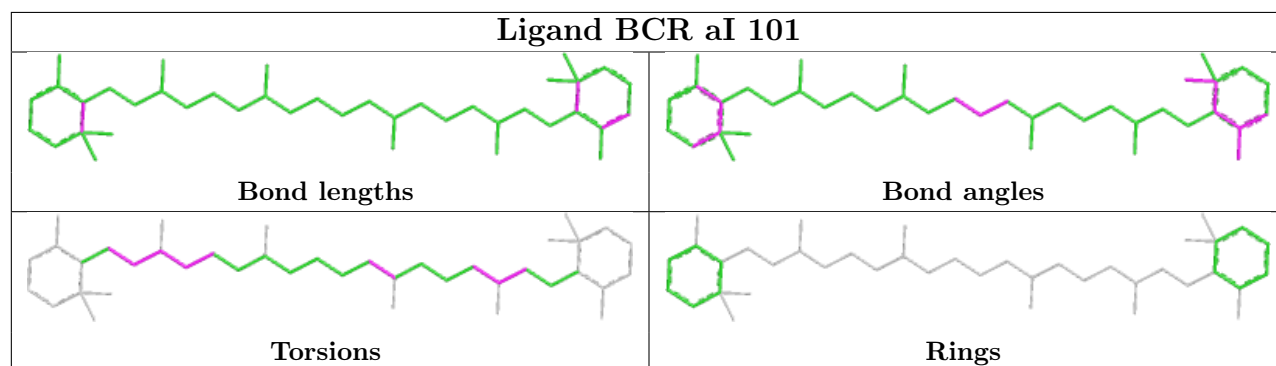
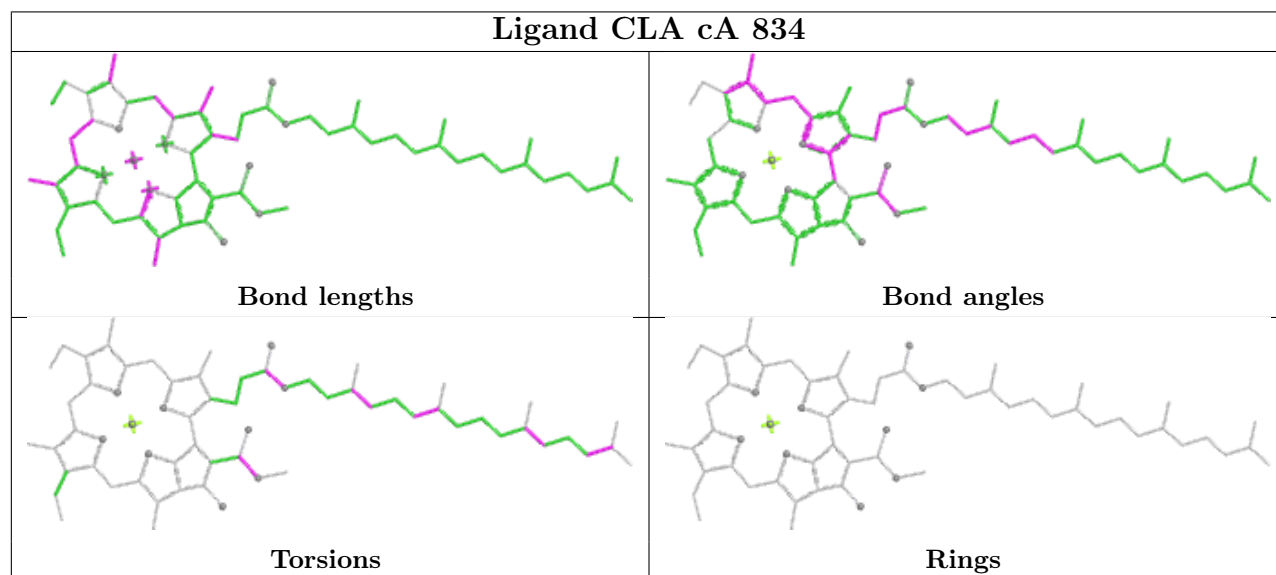
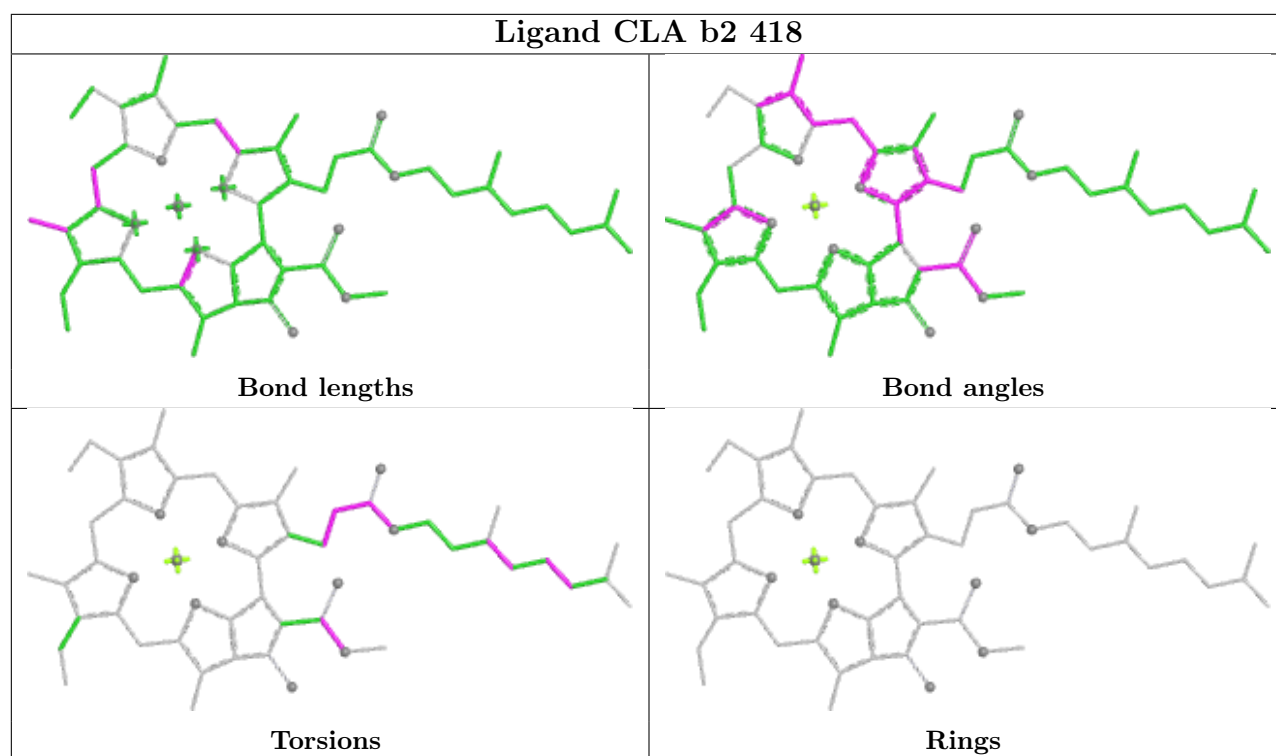


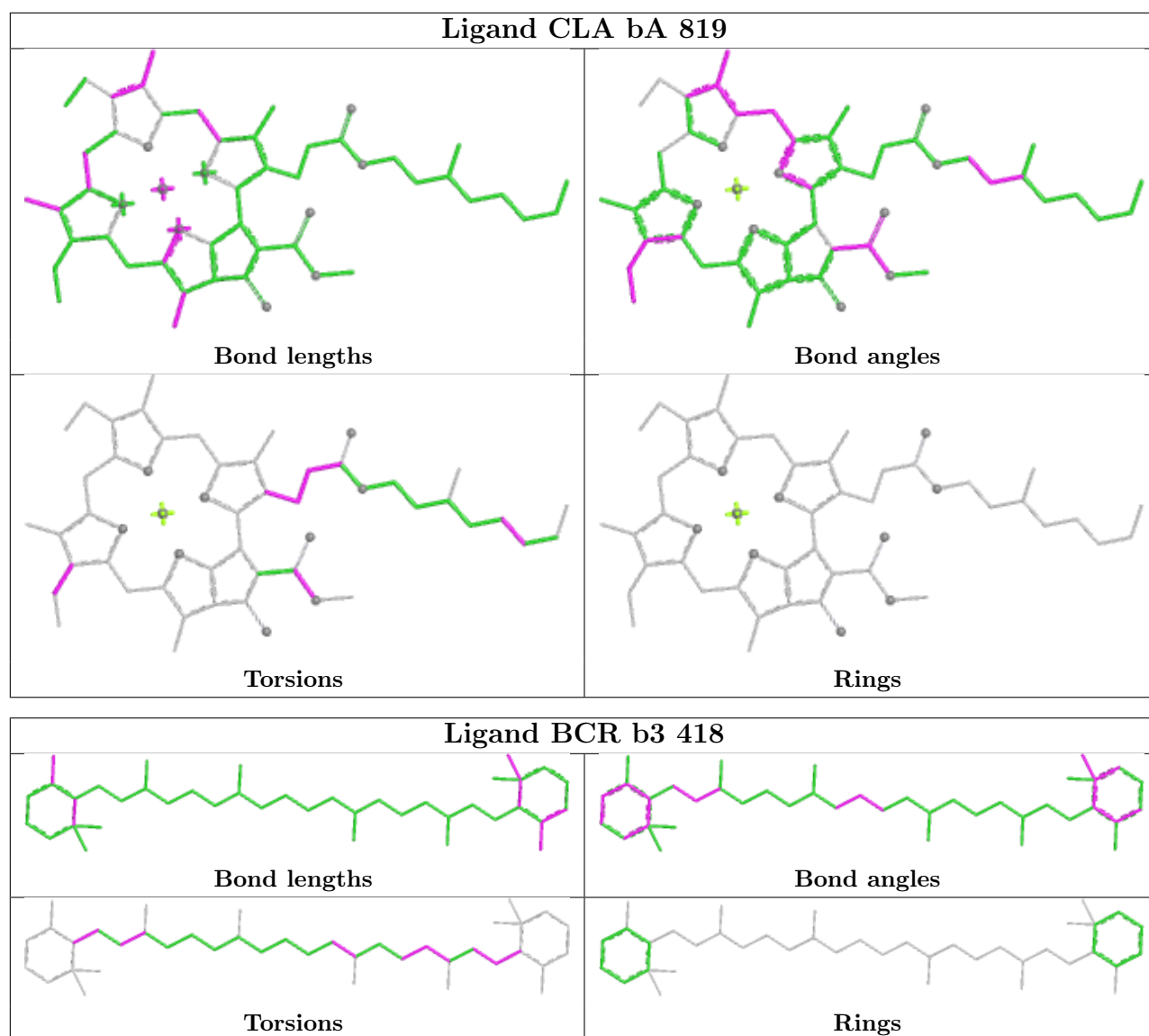


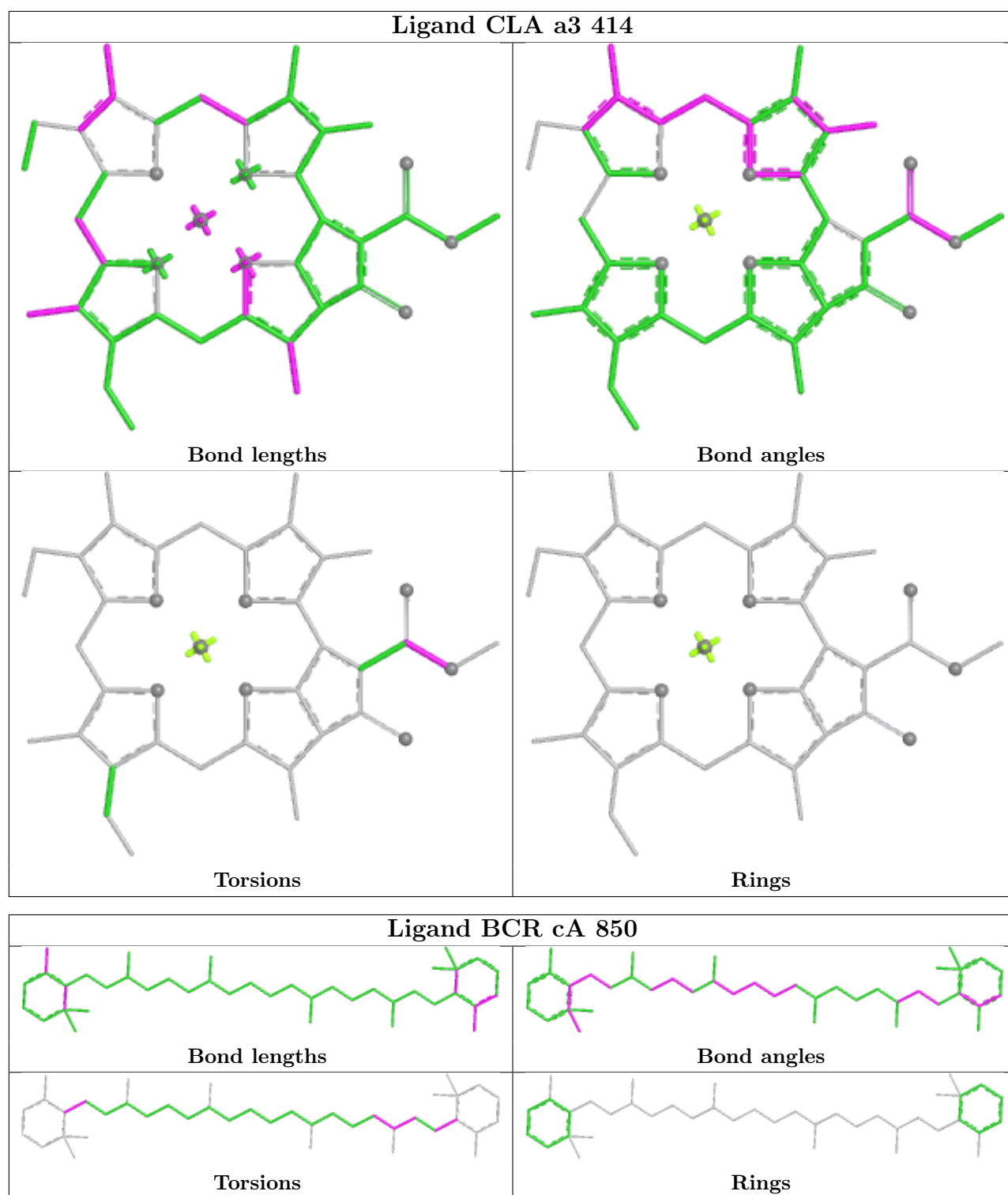




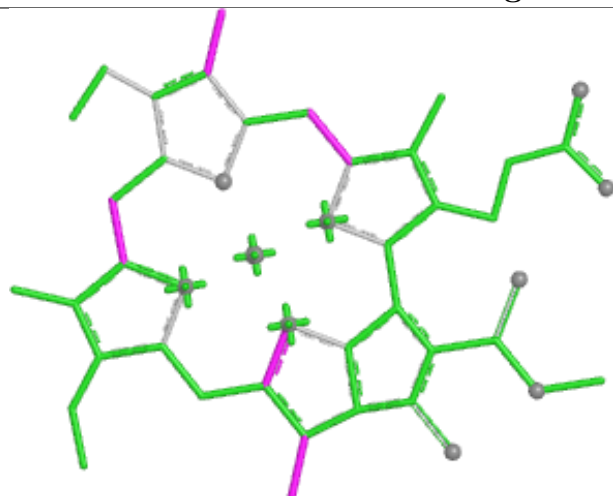




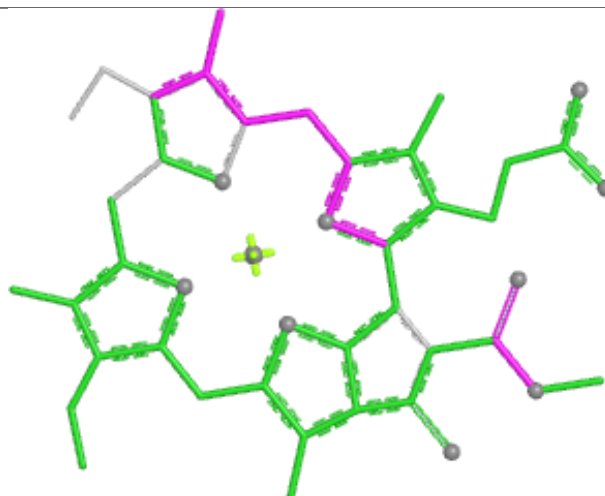




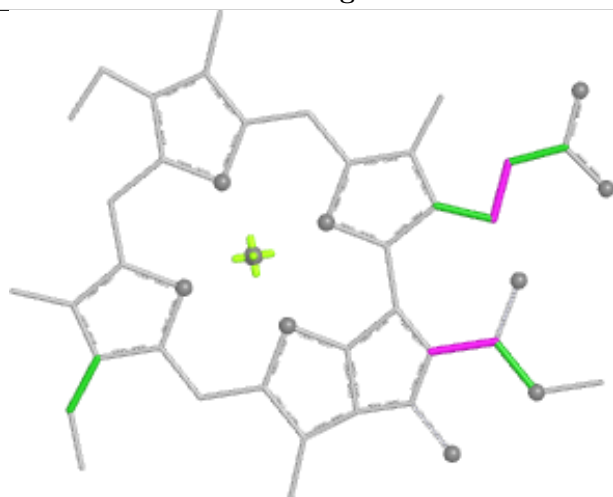
Ligand CLA bB 822



Bond lengths



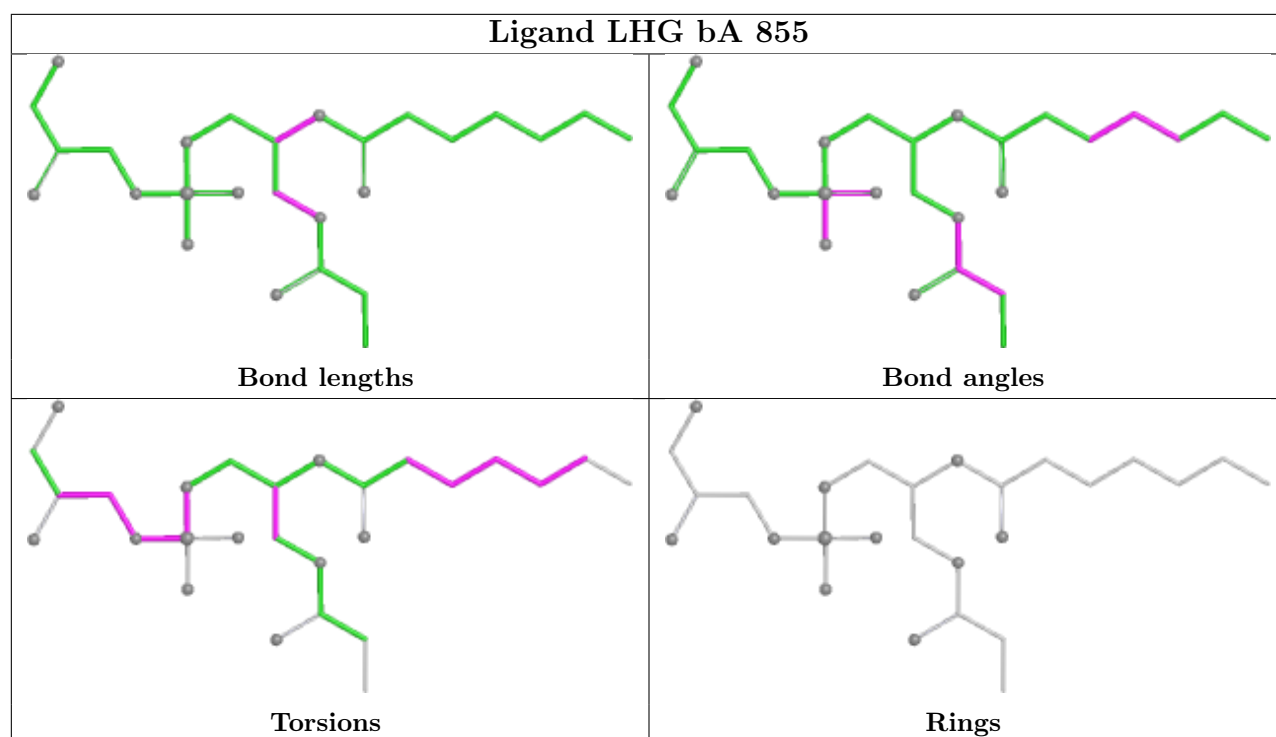
Bond angles

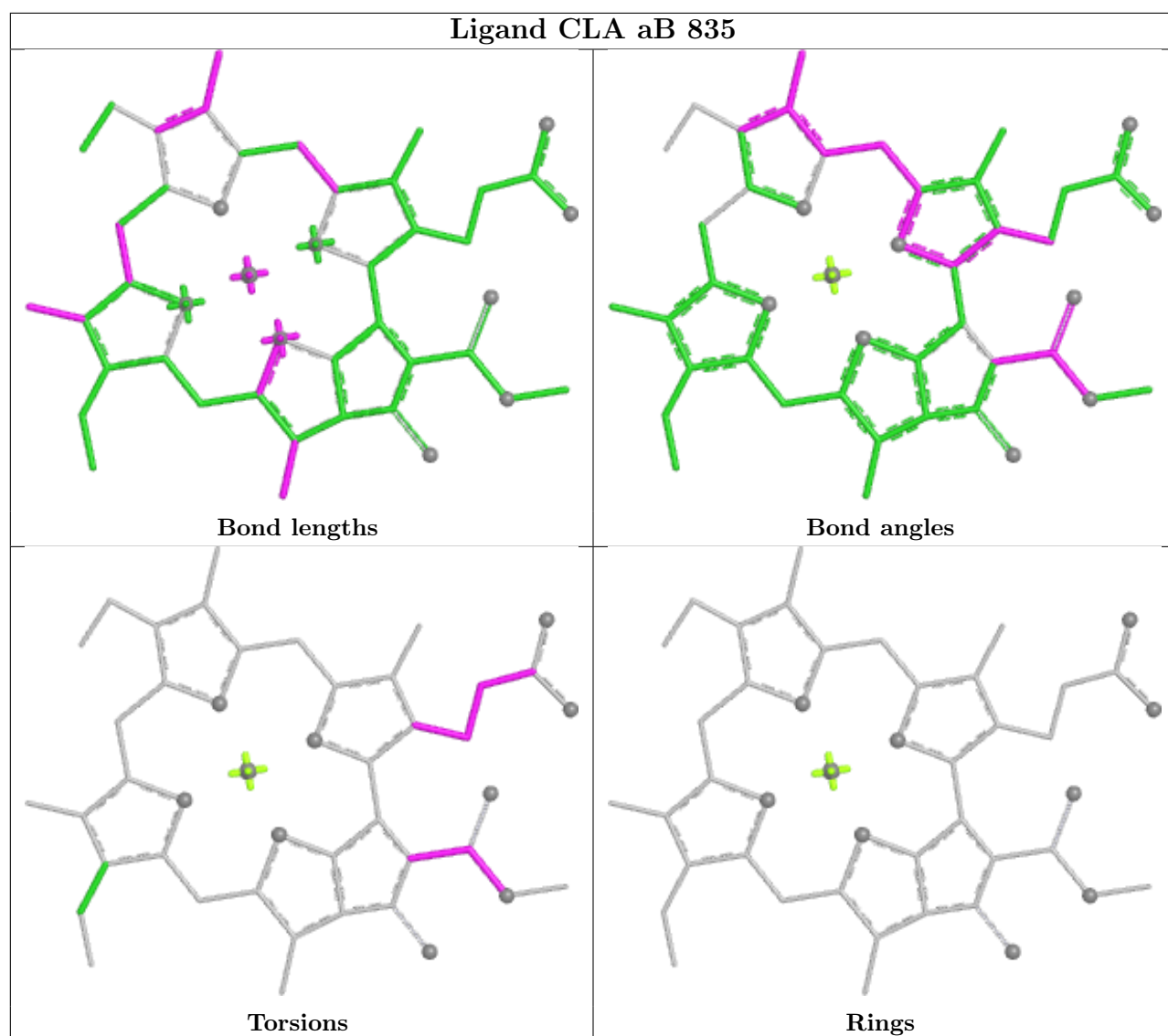


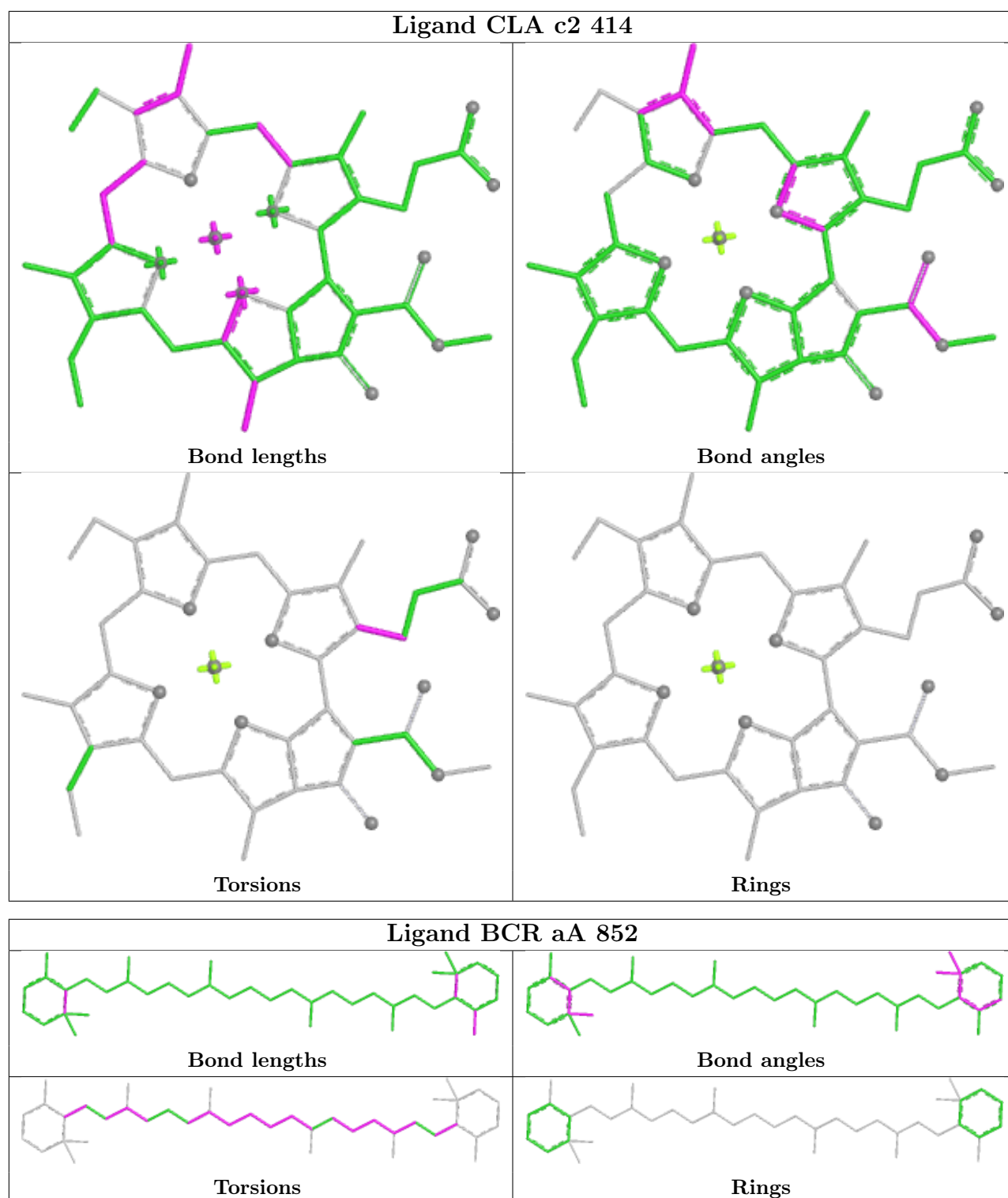
Torsions

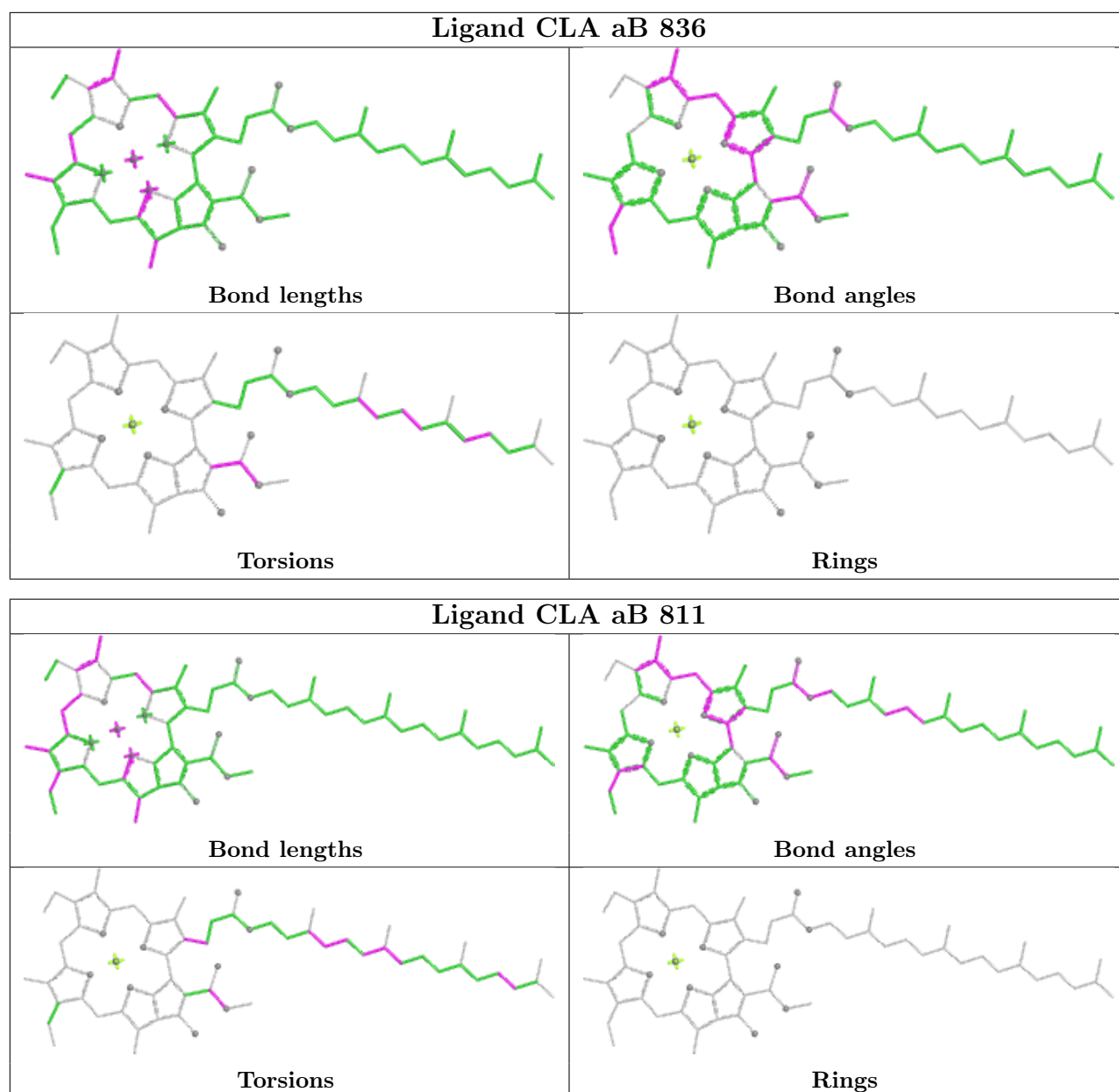


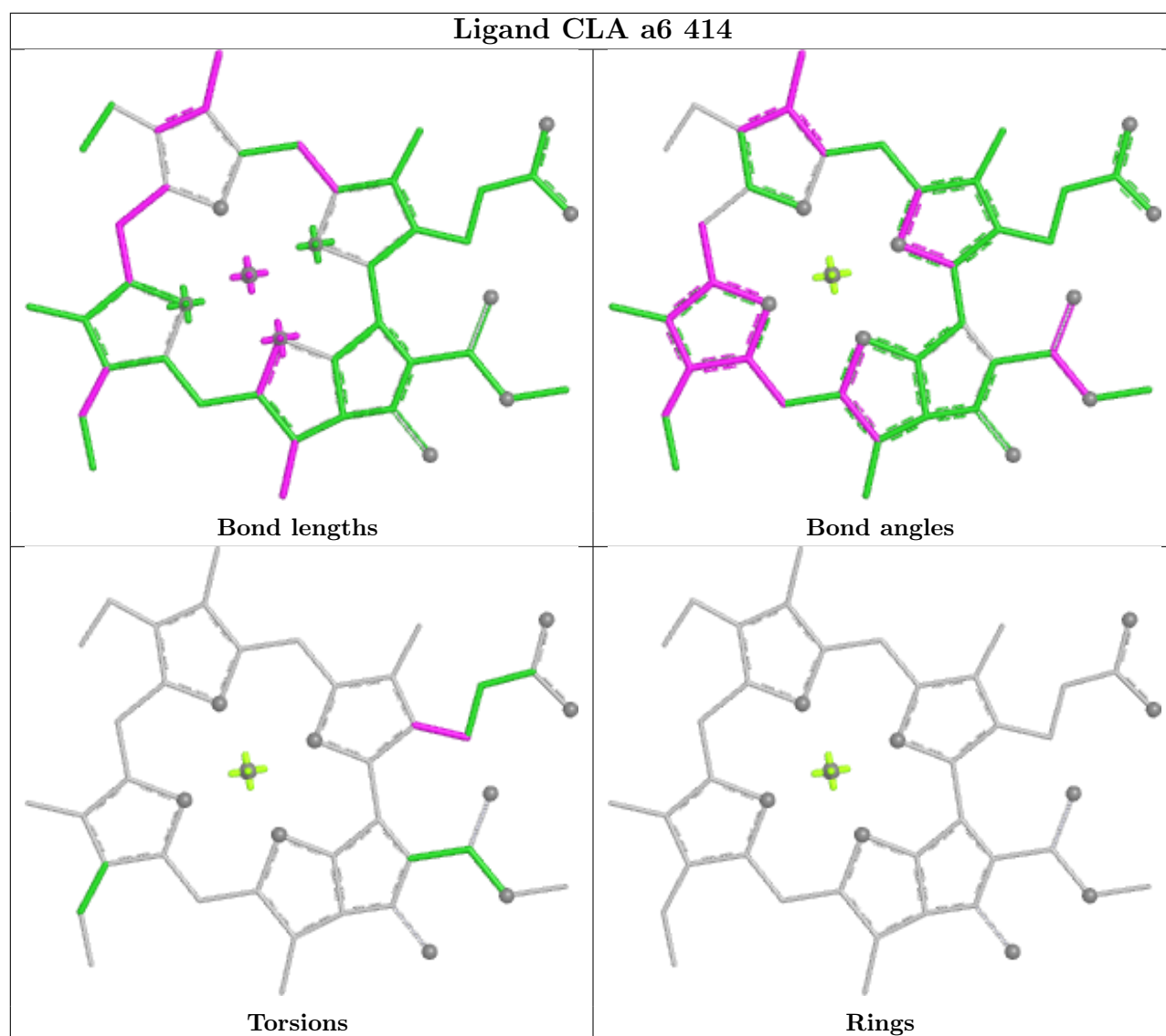
Rings

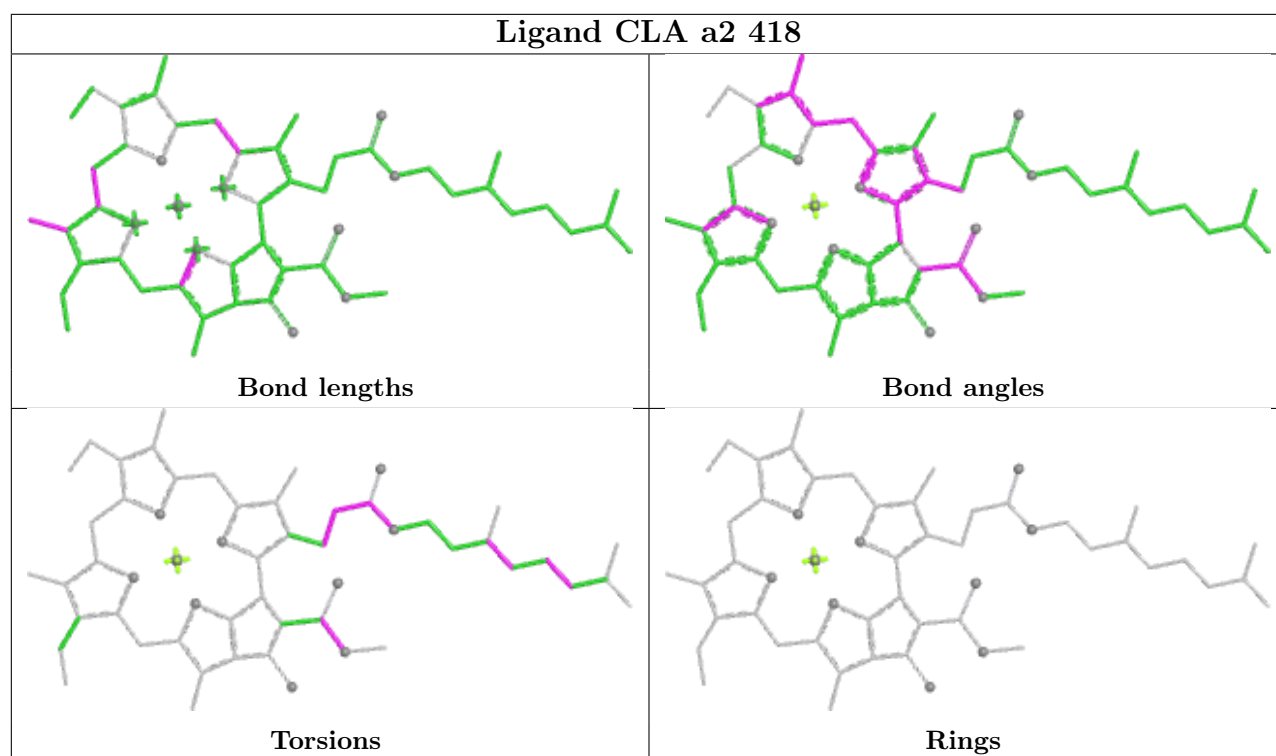


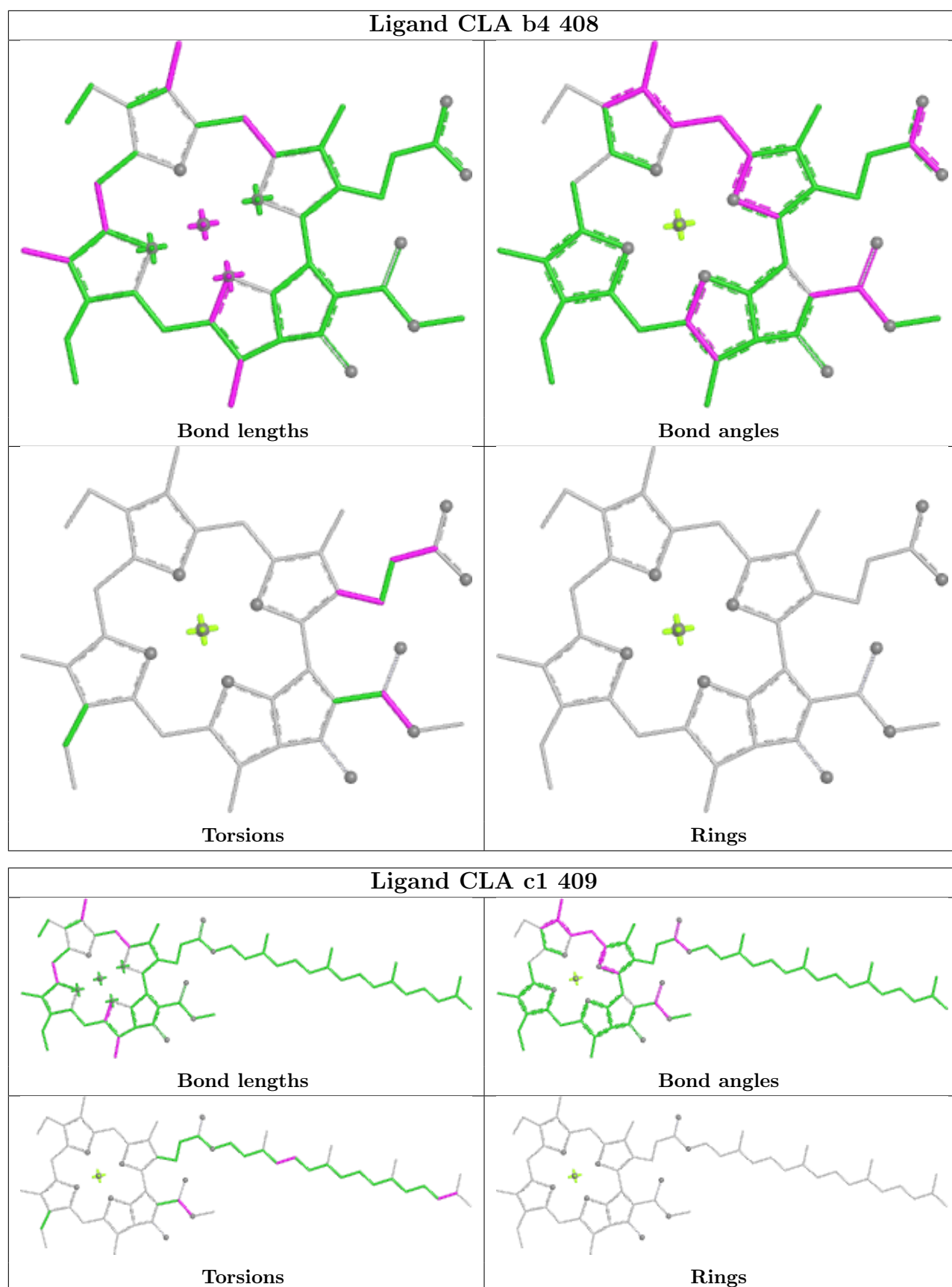


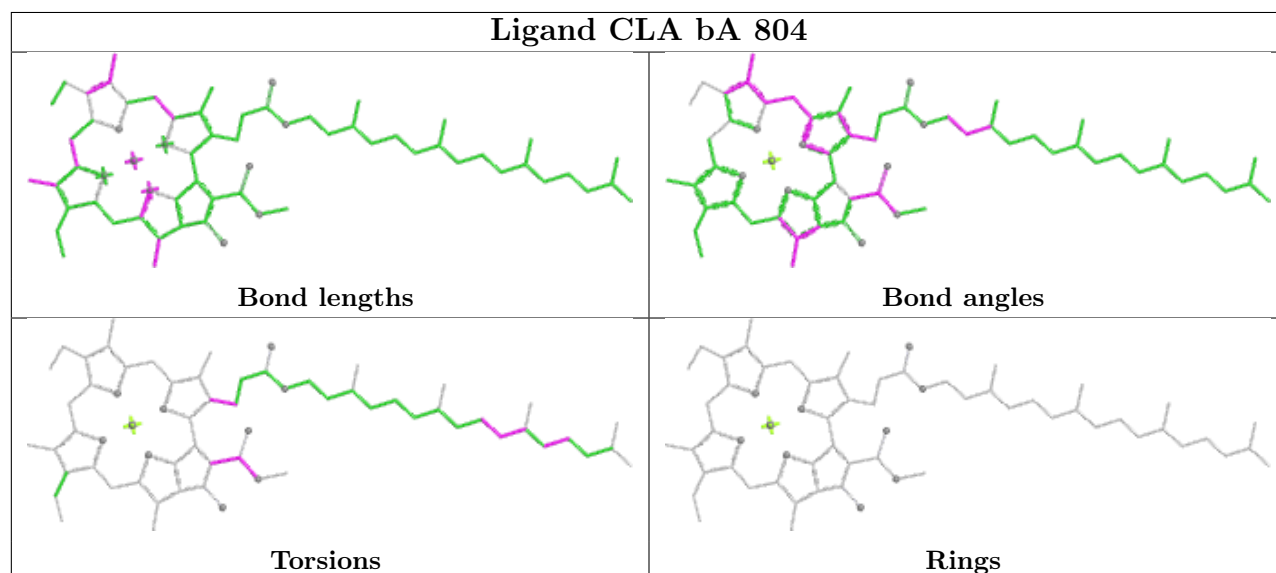
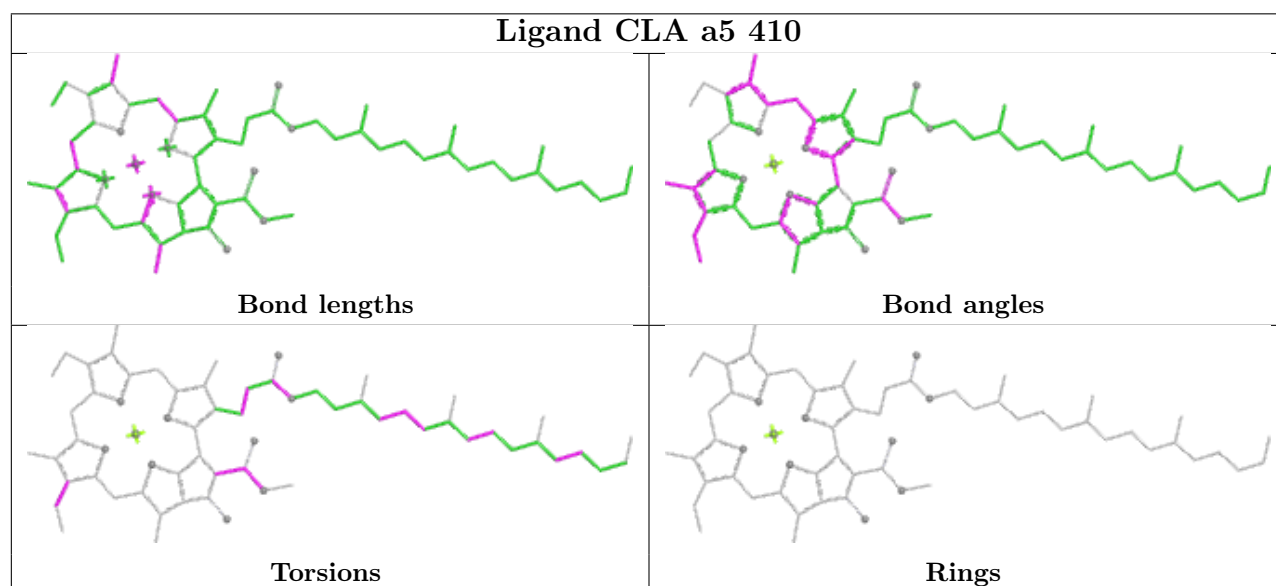
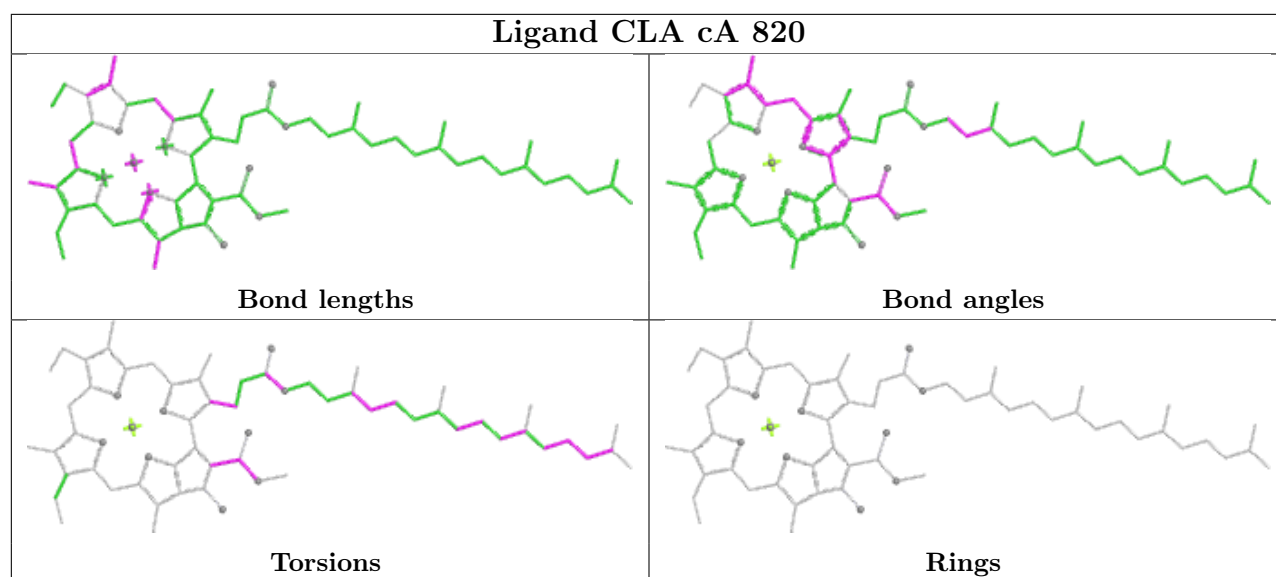


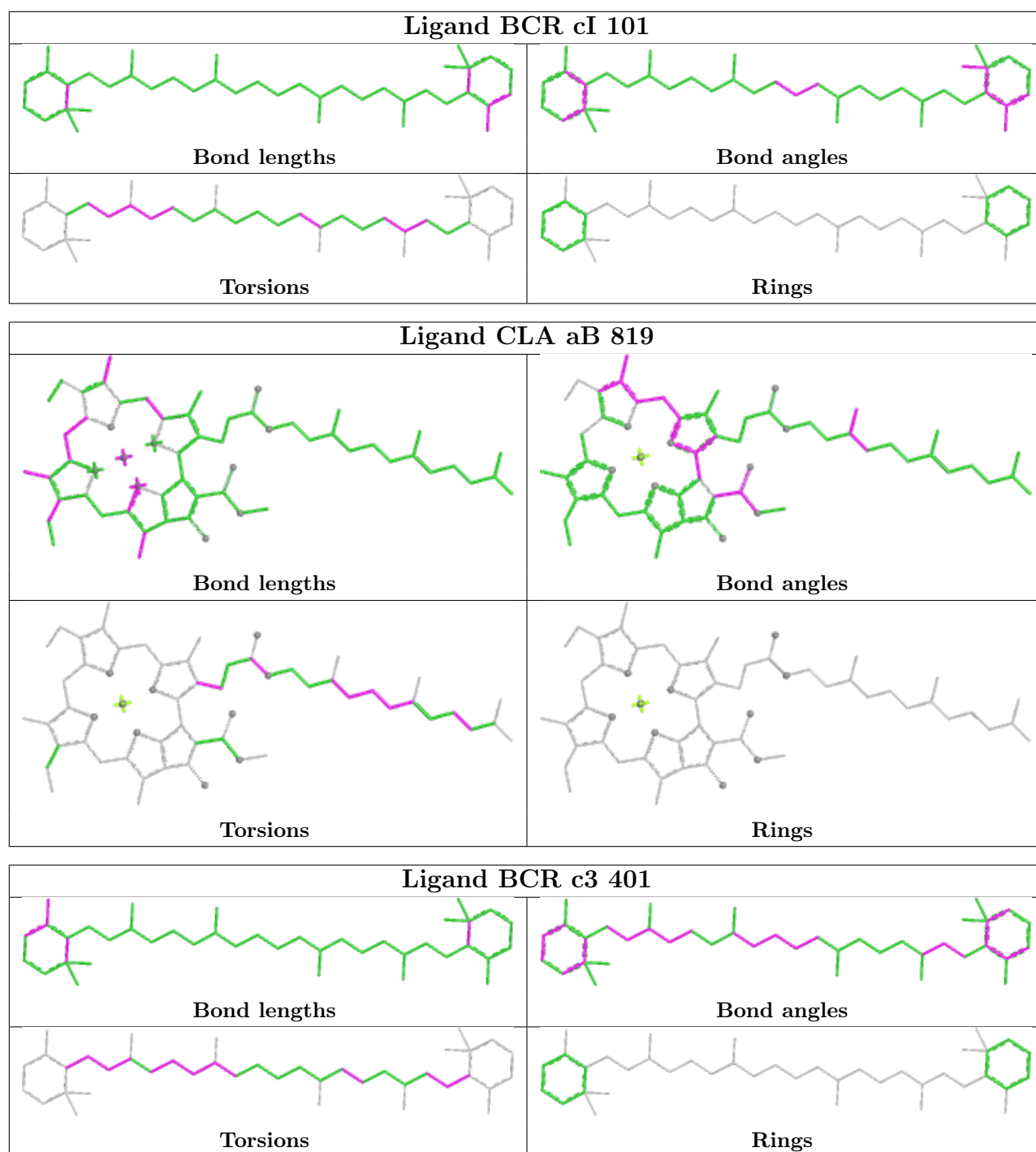


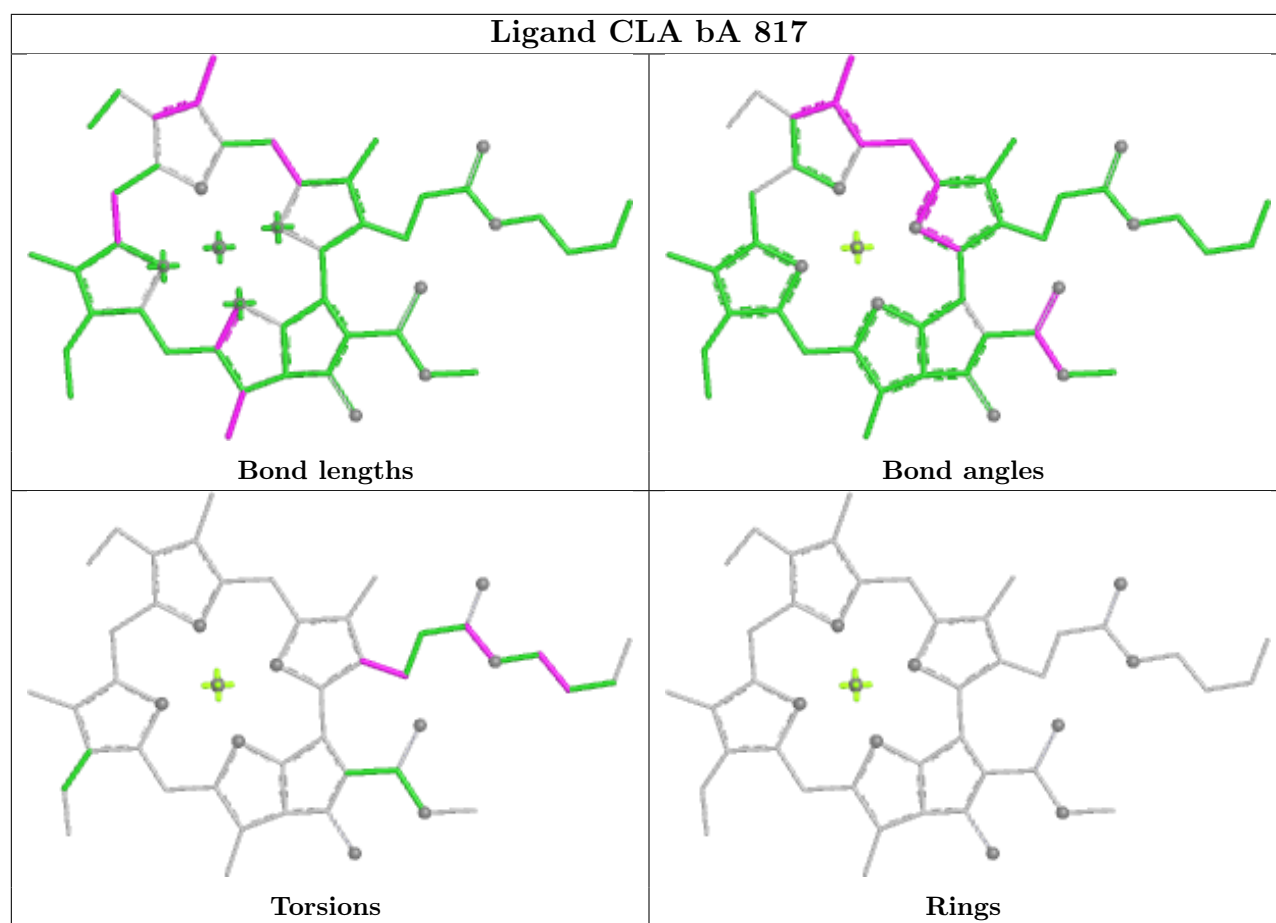


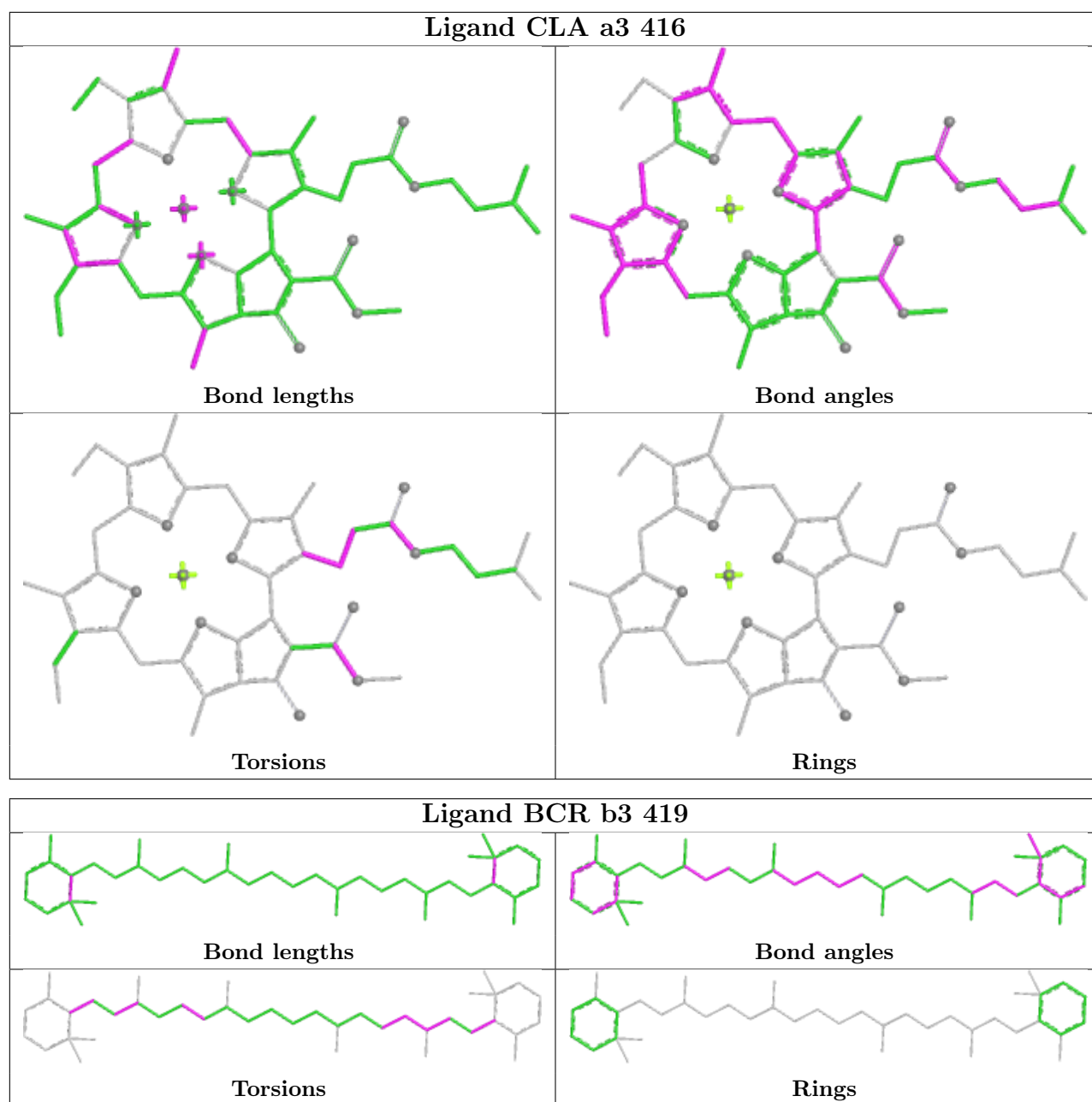


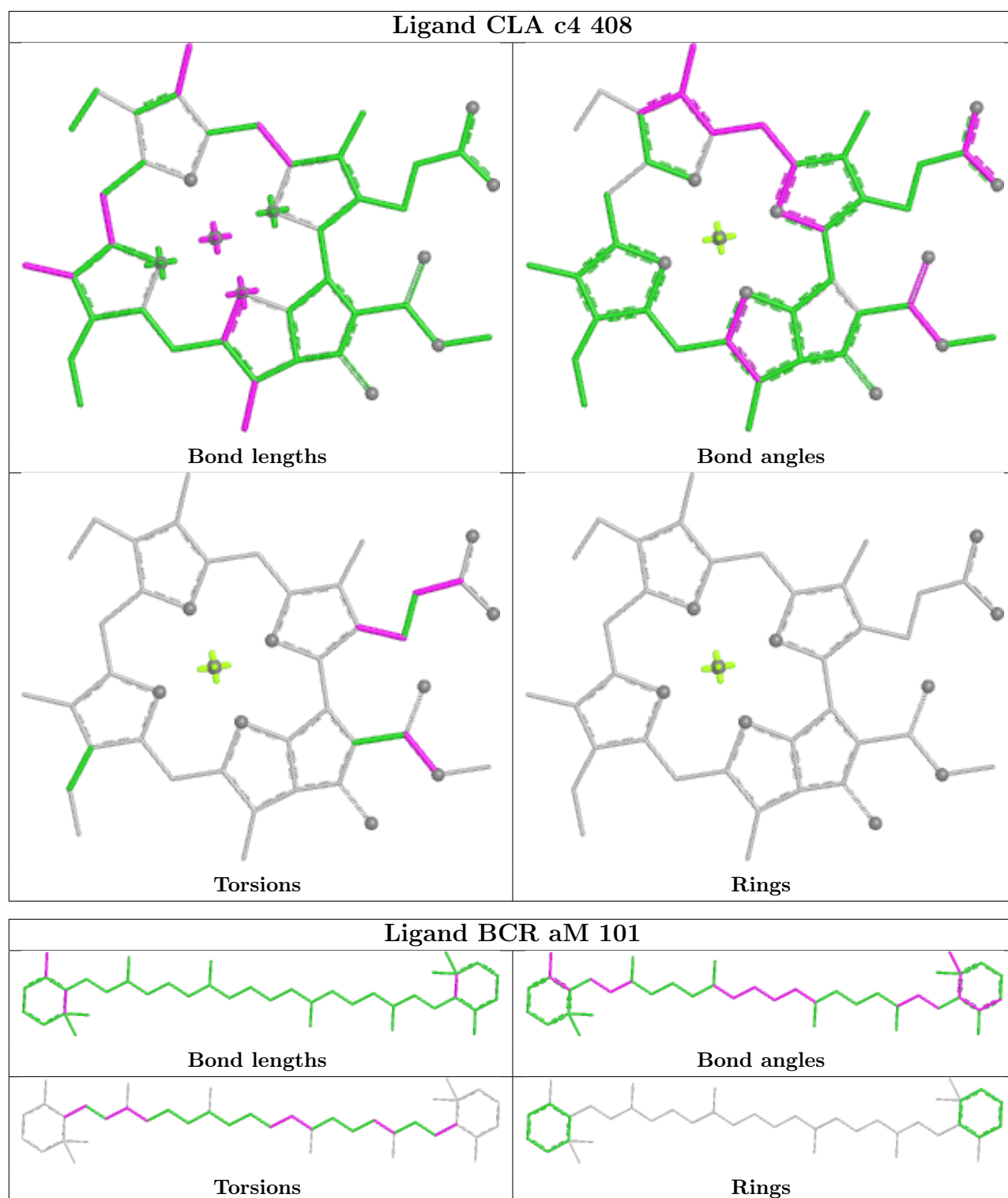


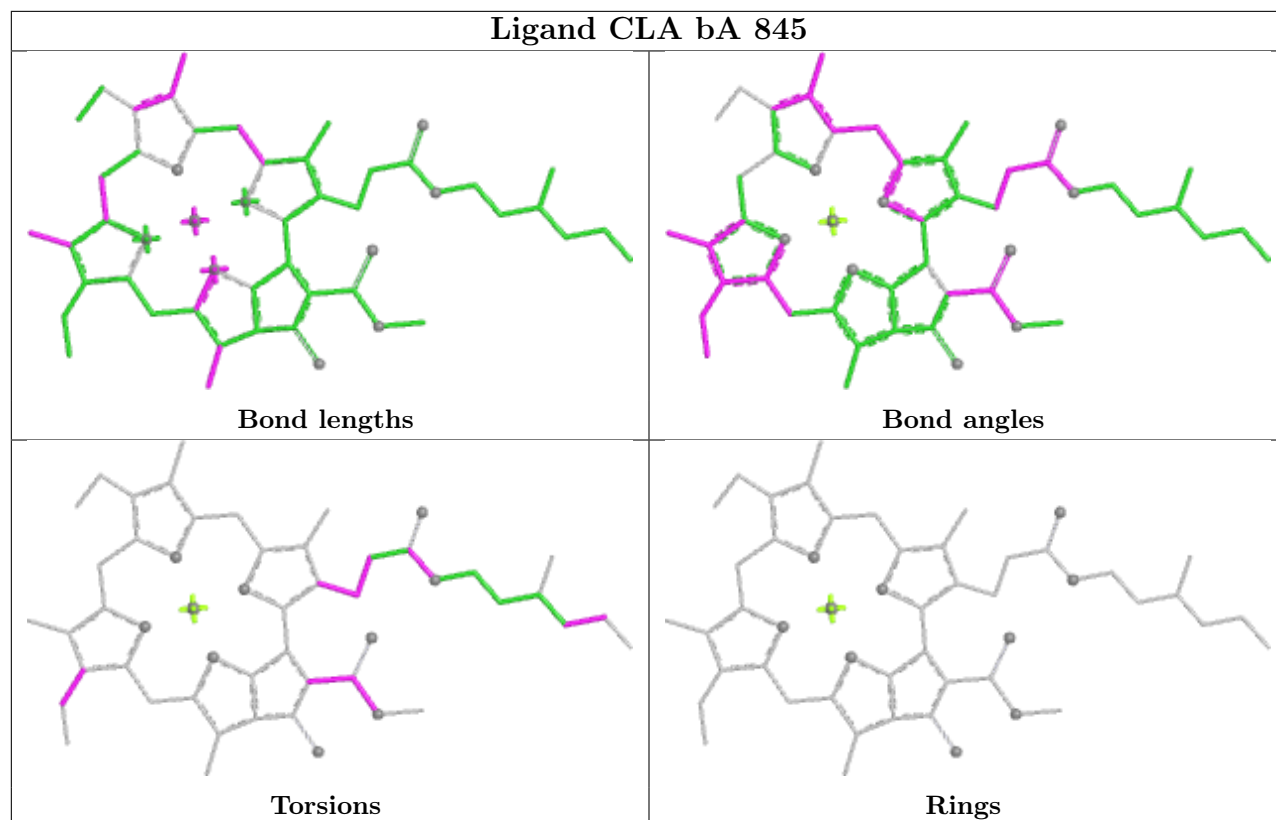


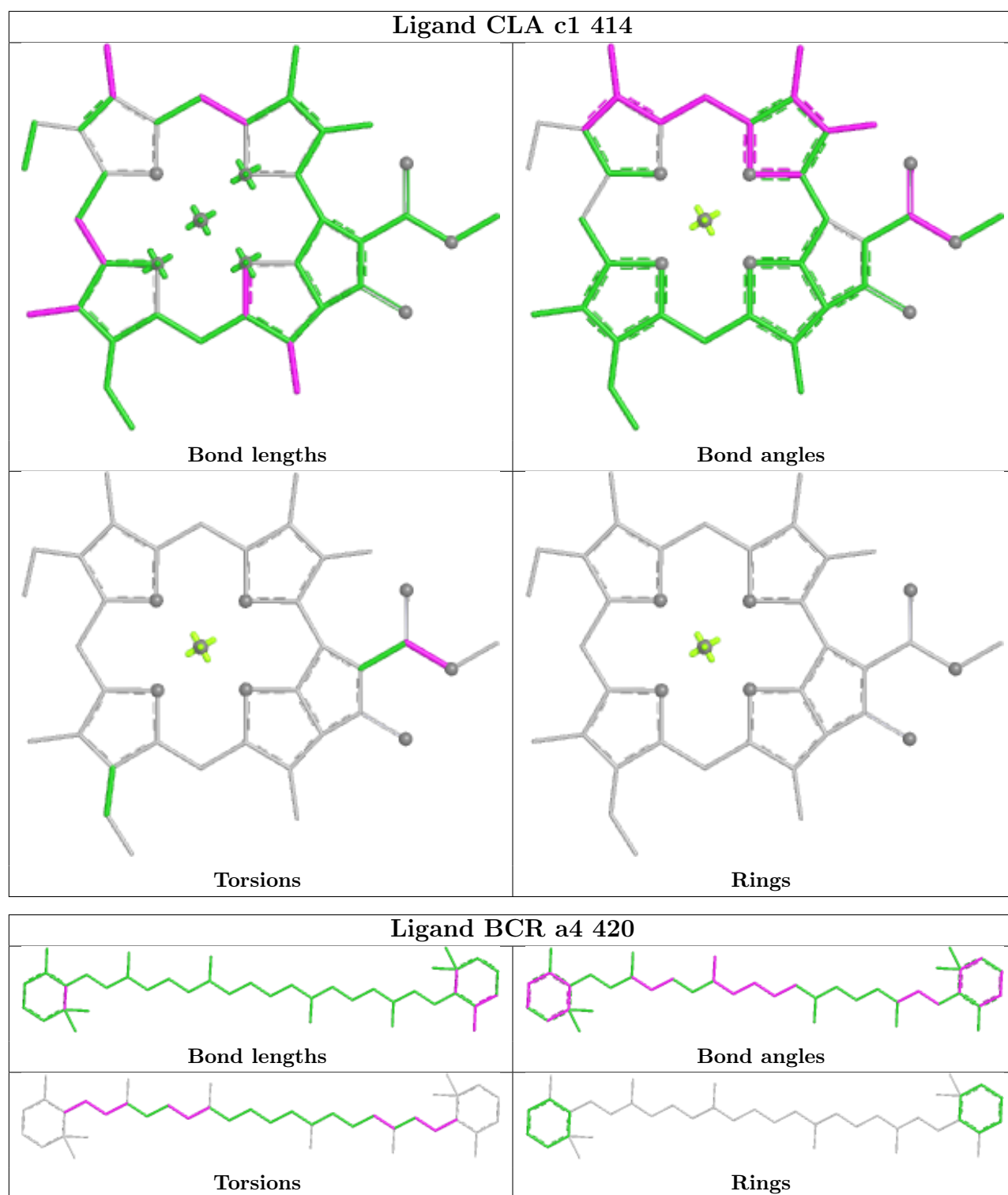


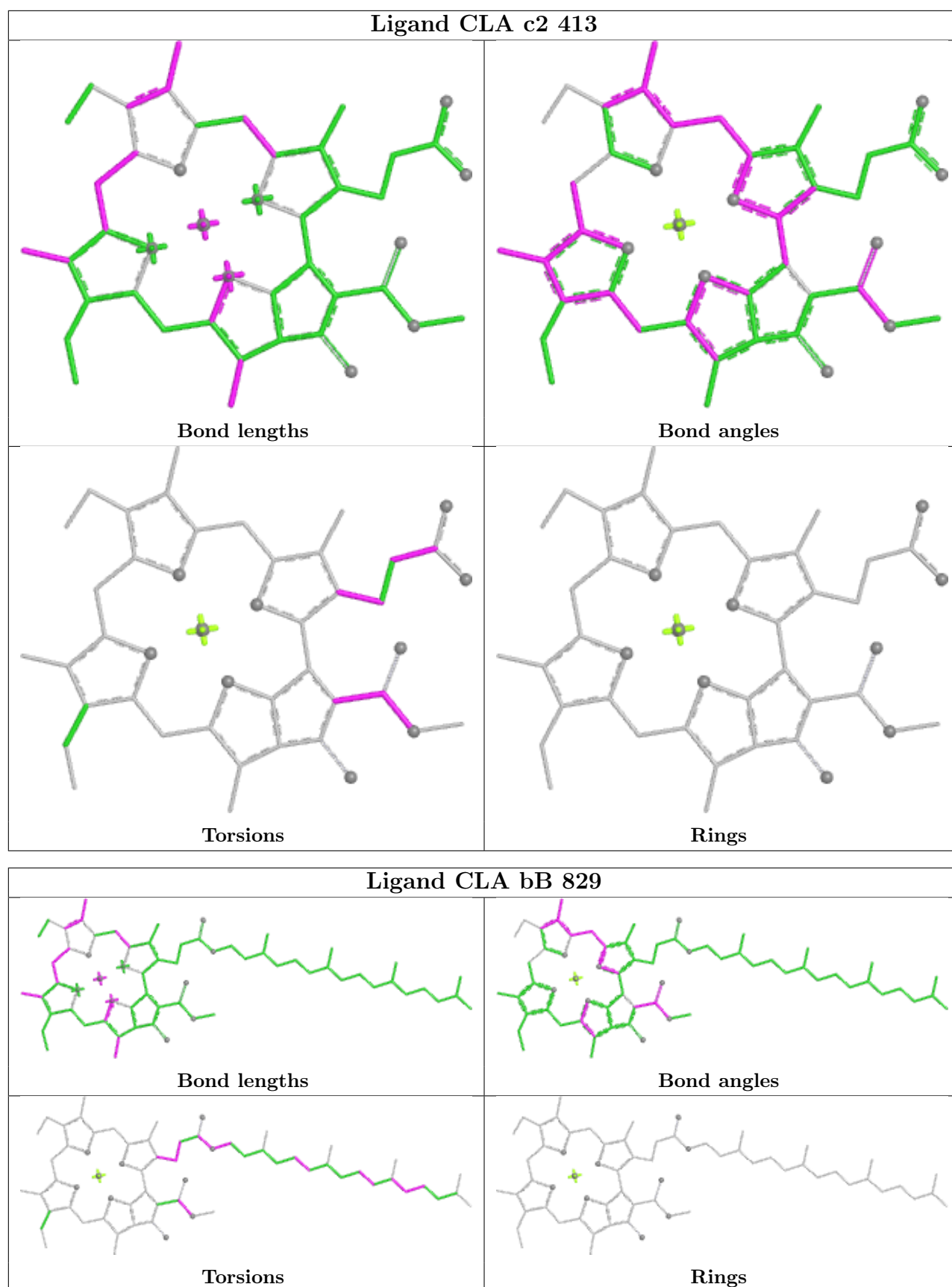


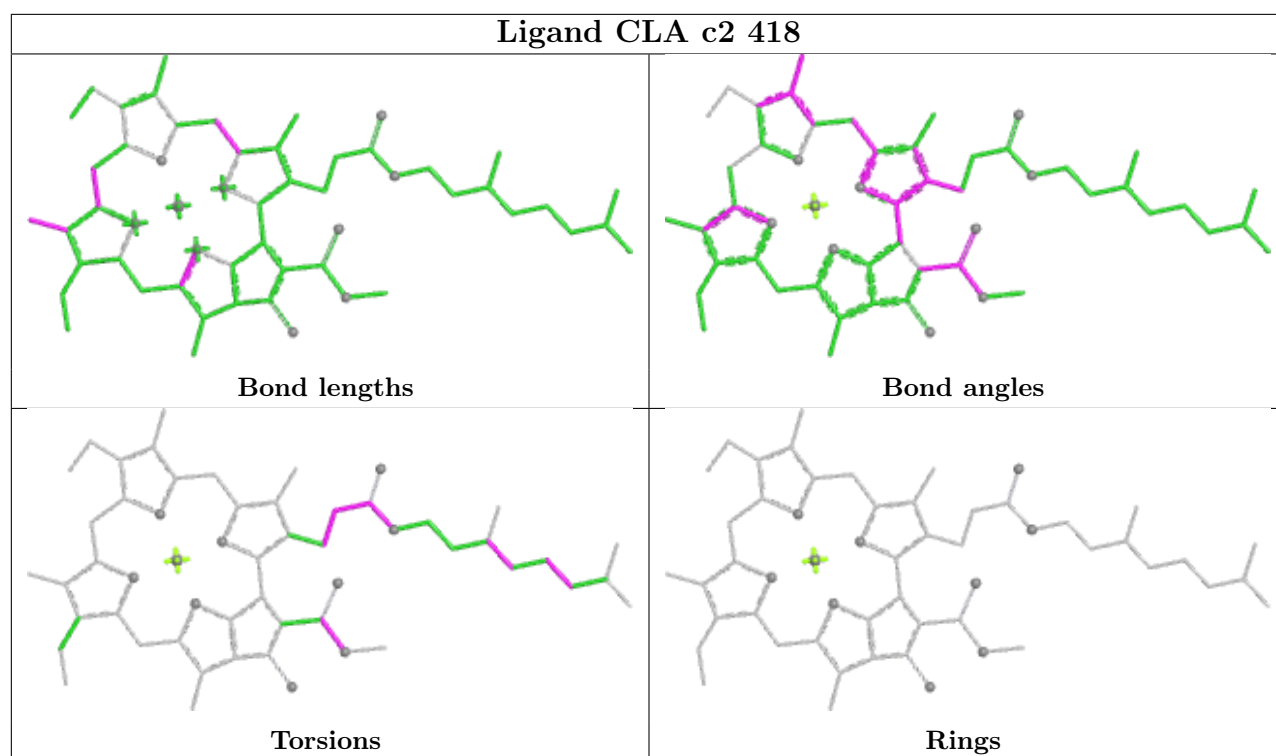


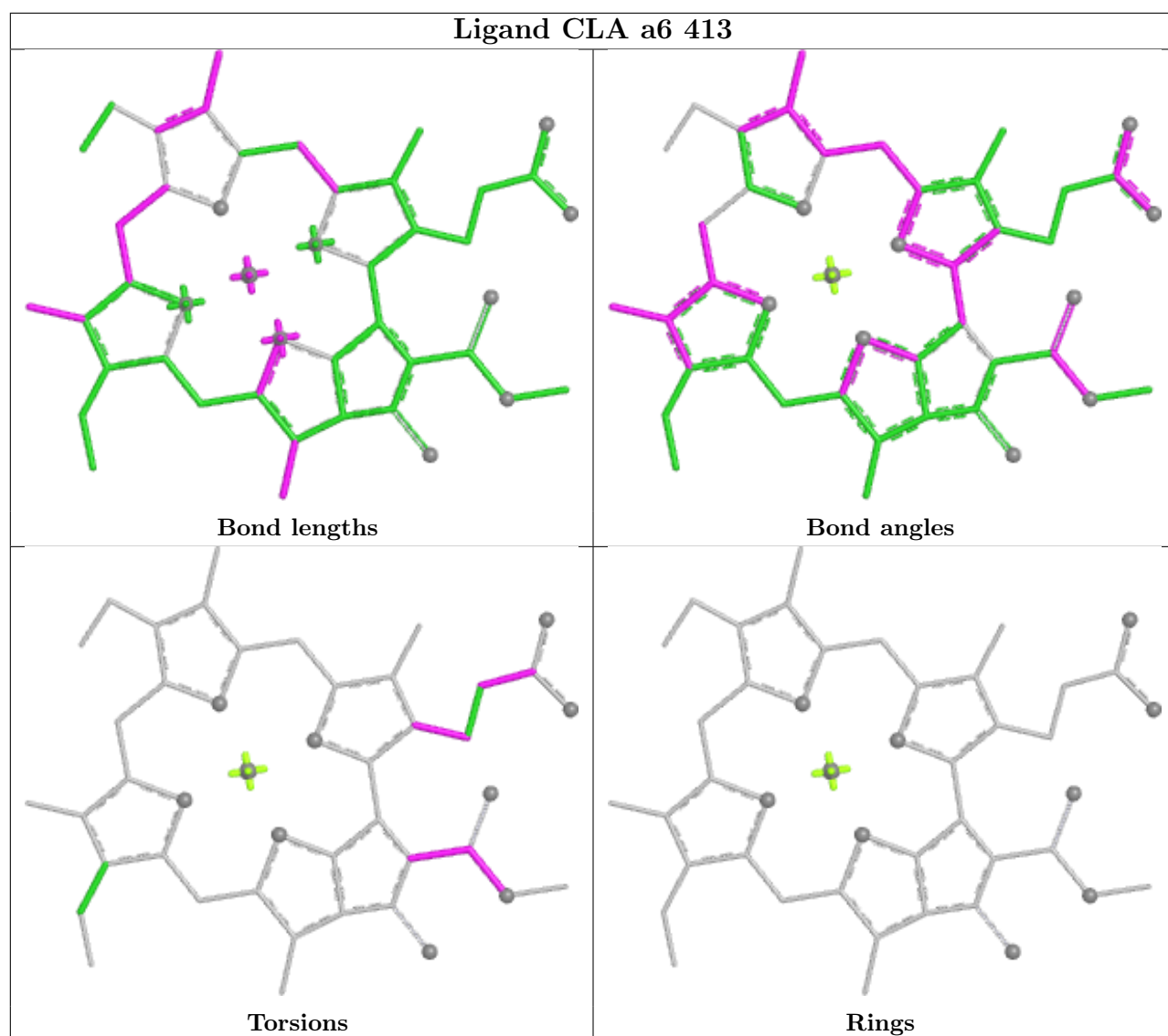


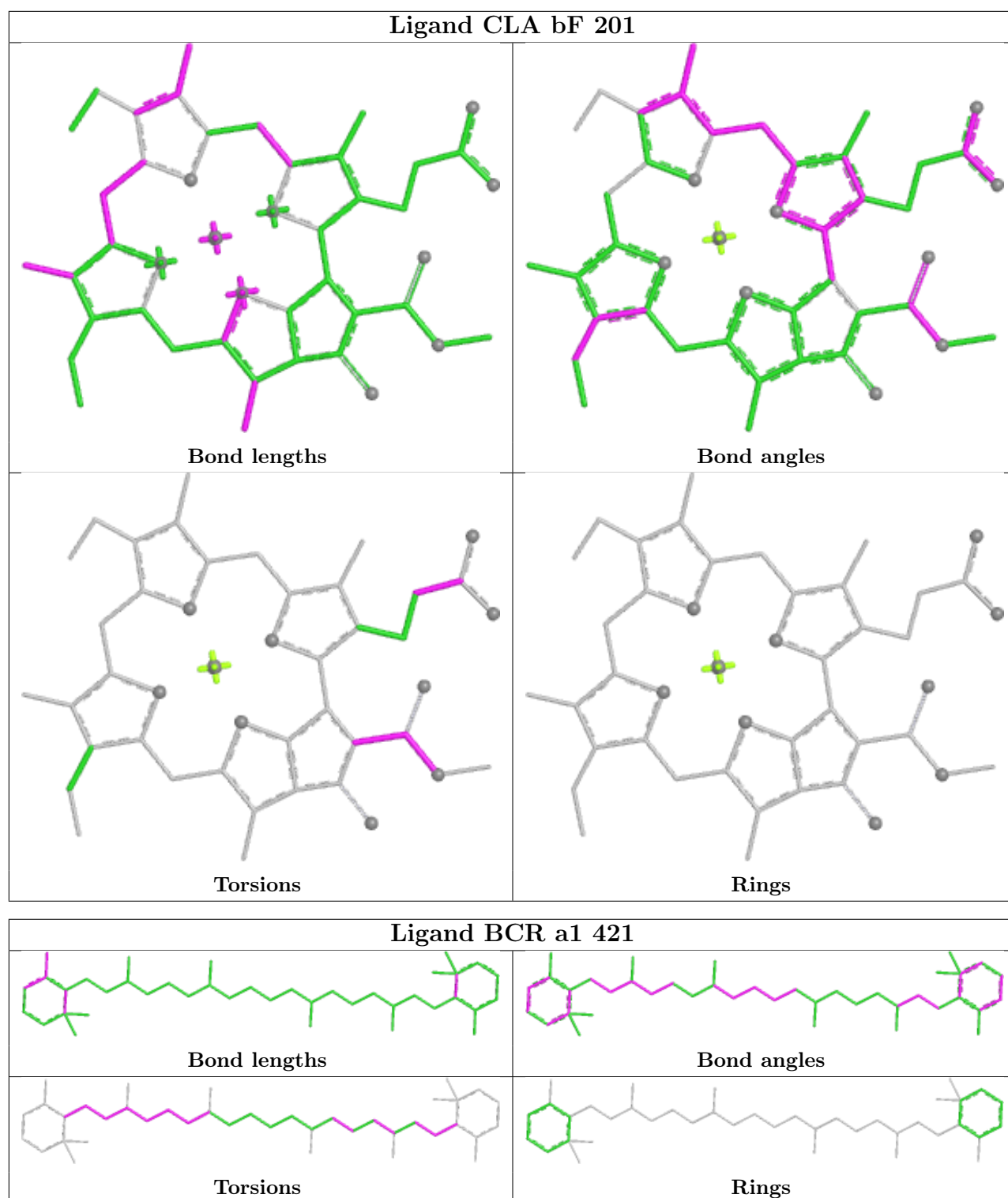


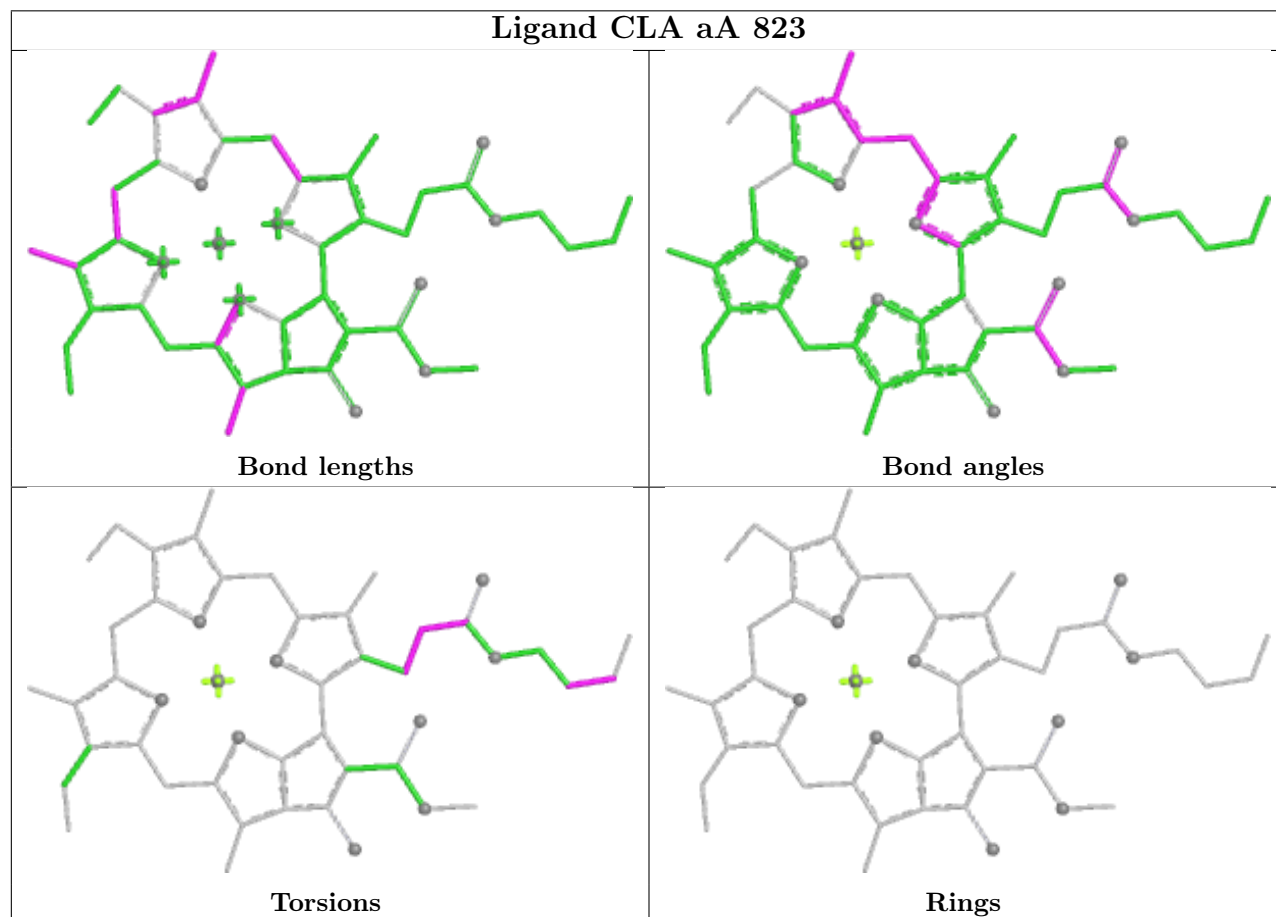
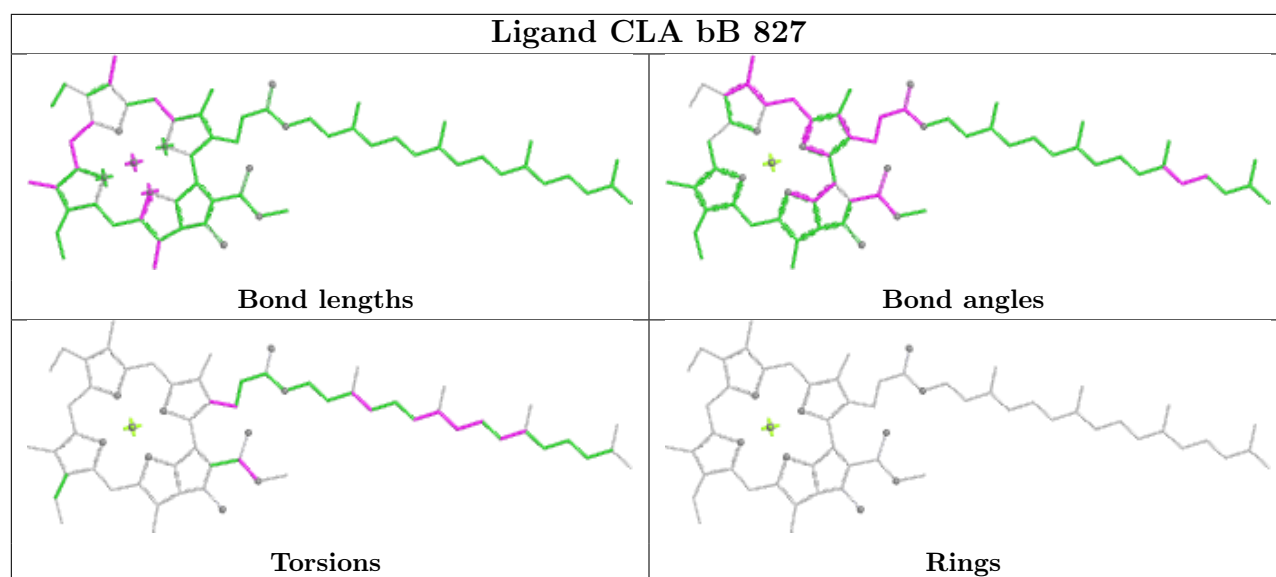


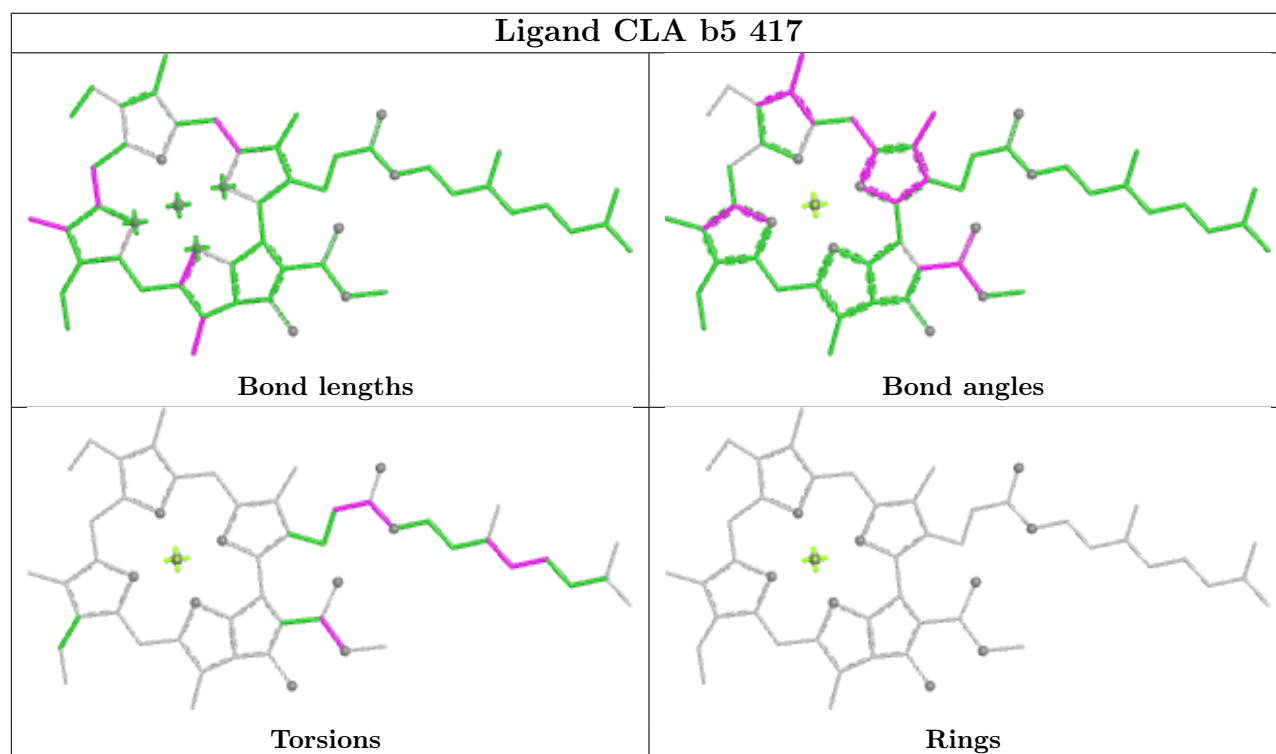
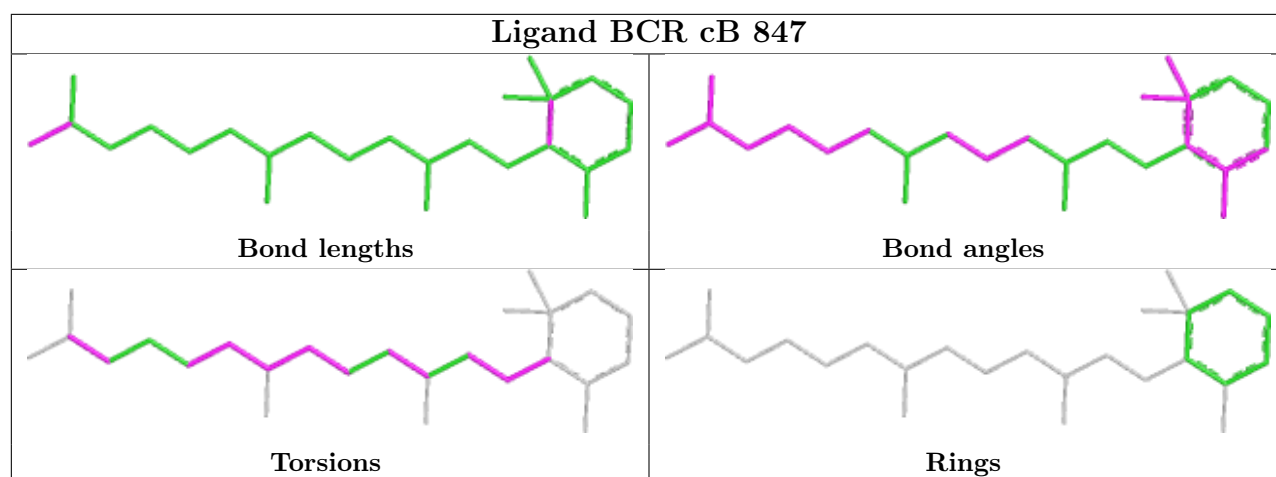


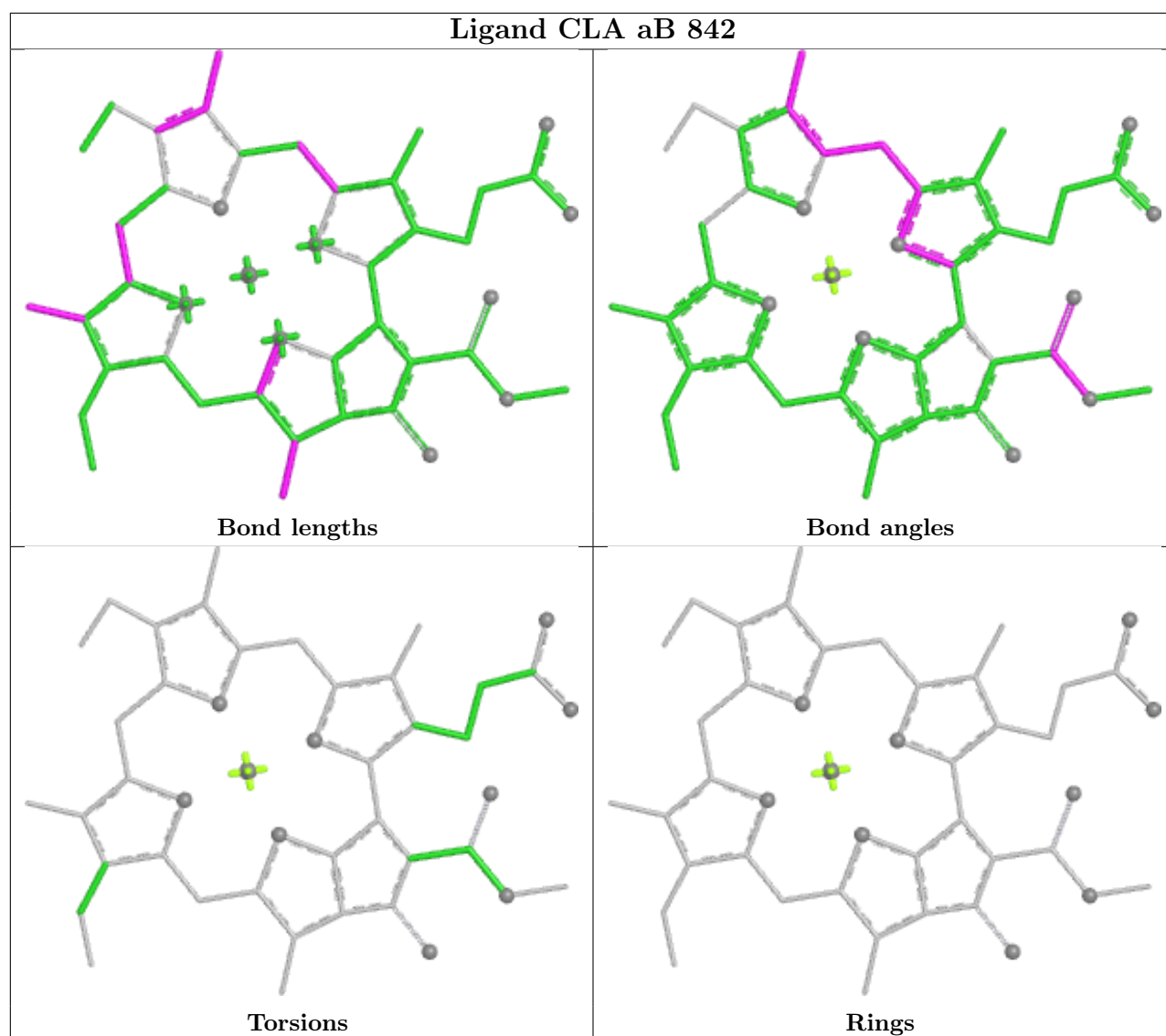


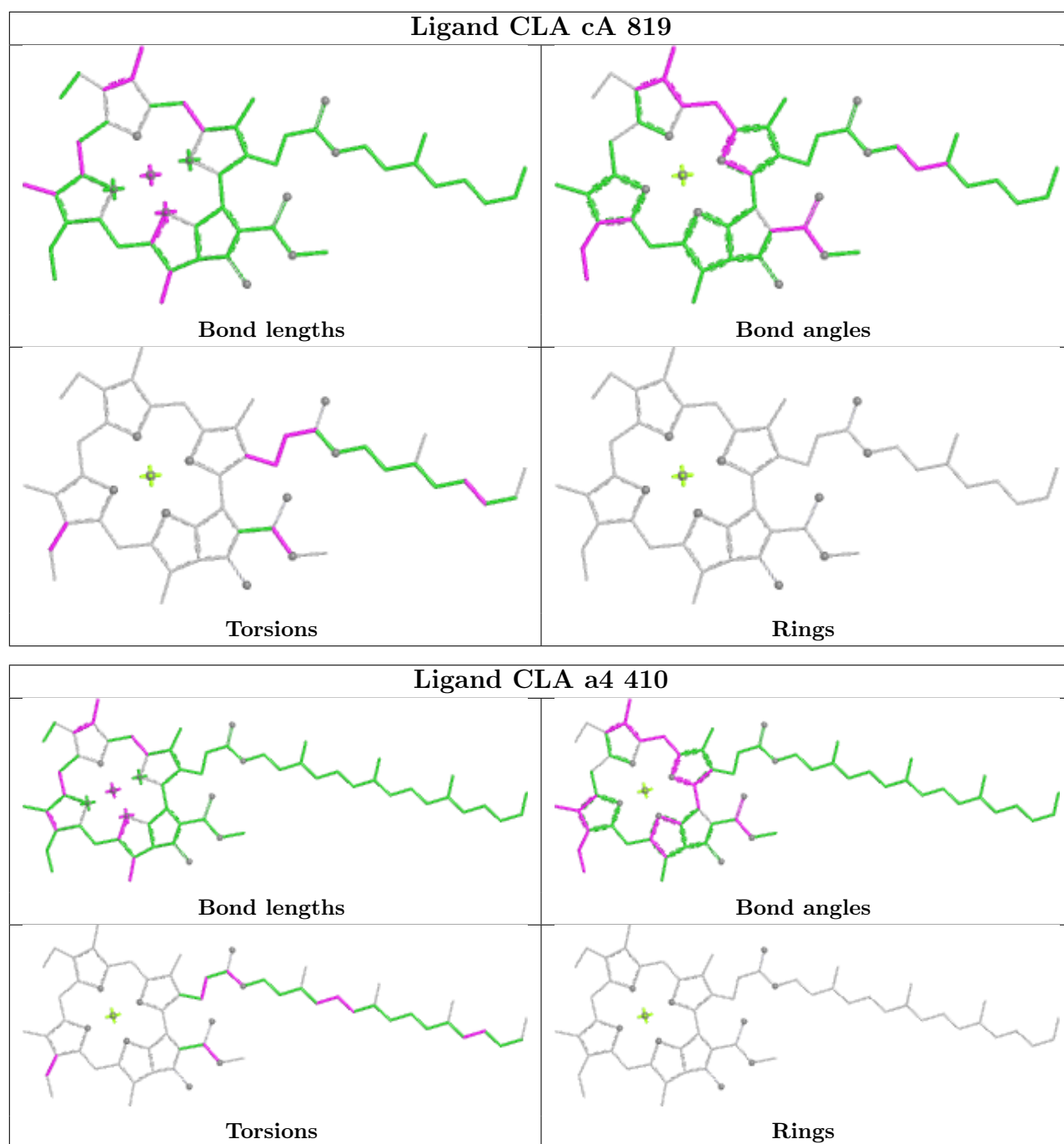


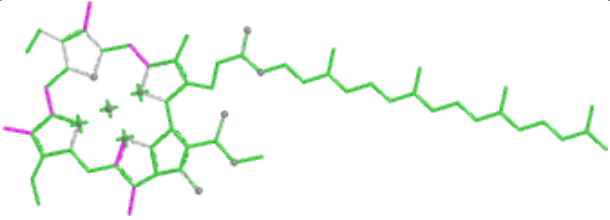
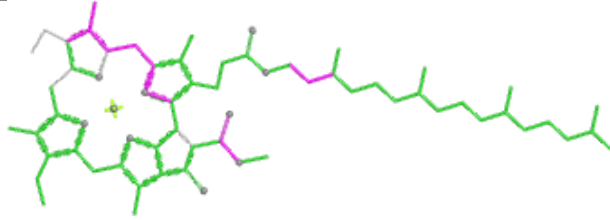
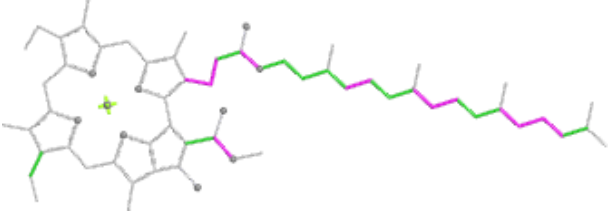
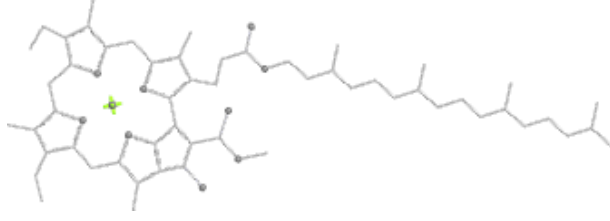
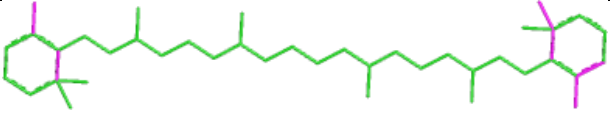
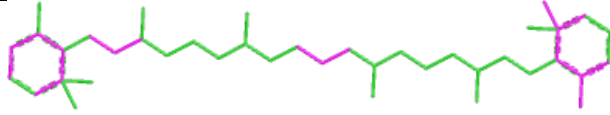
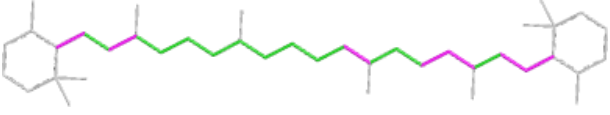
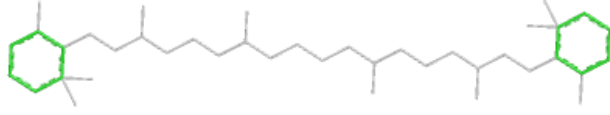


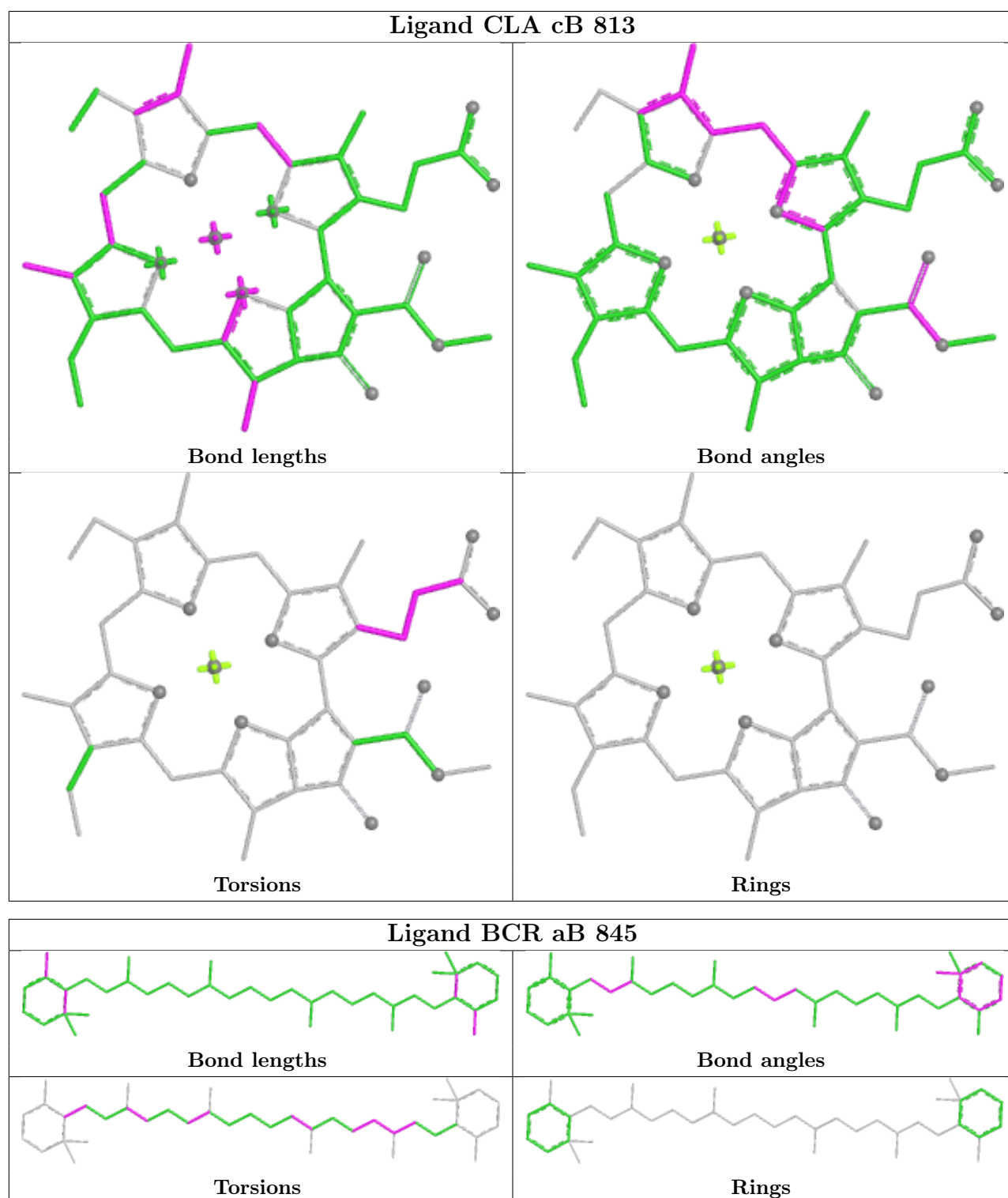


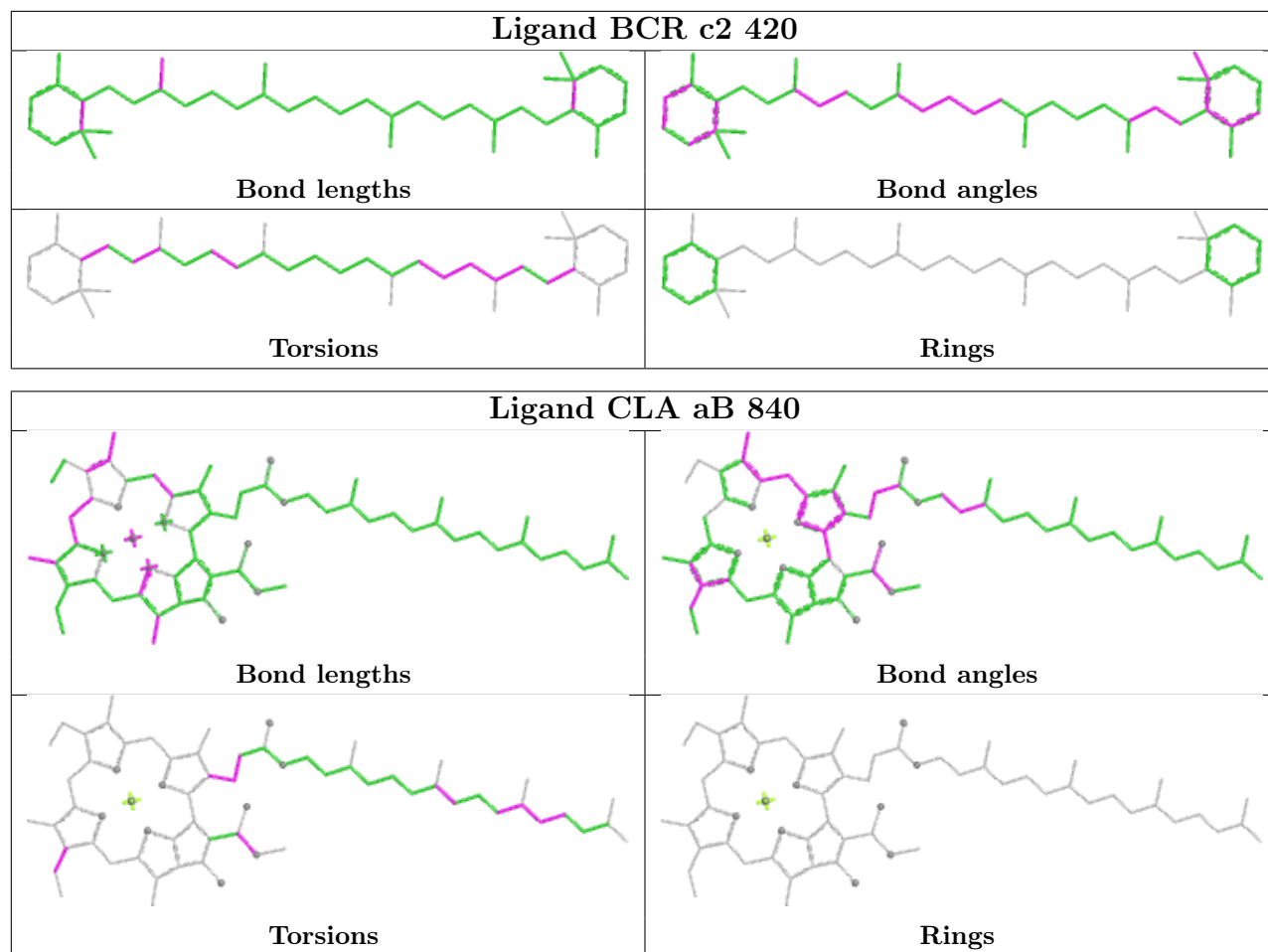


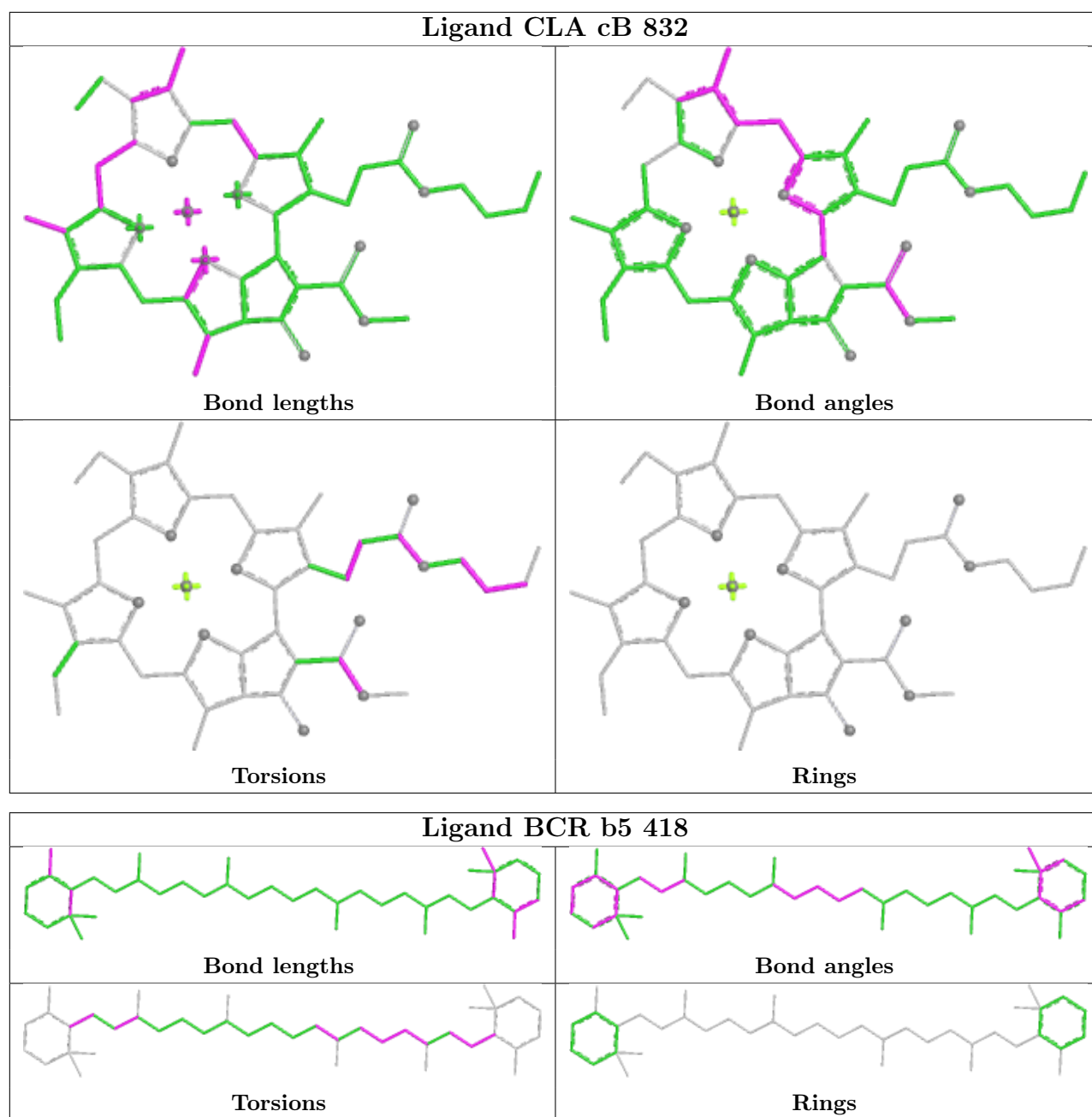


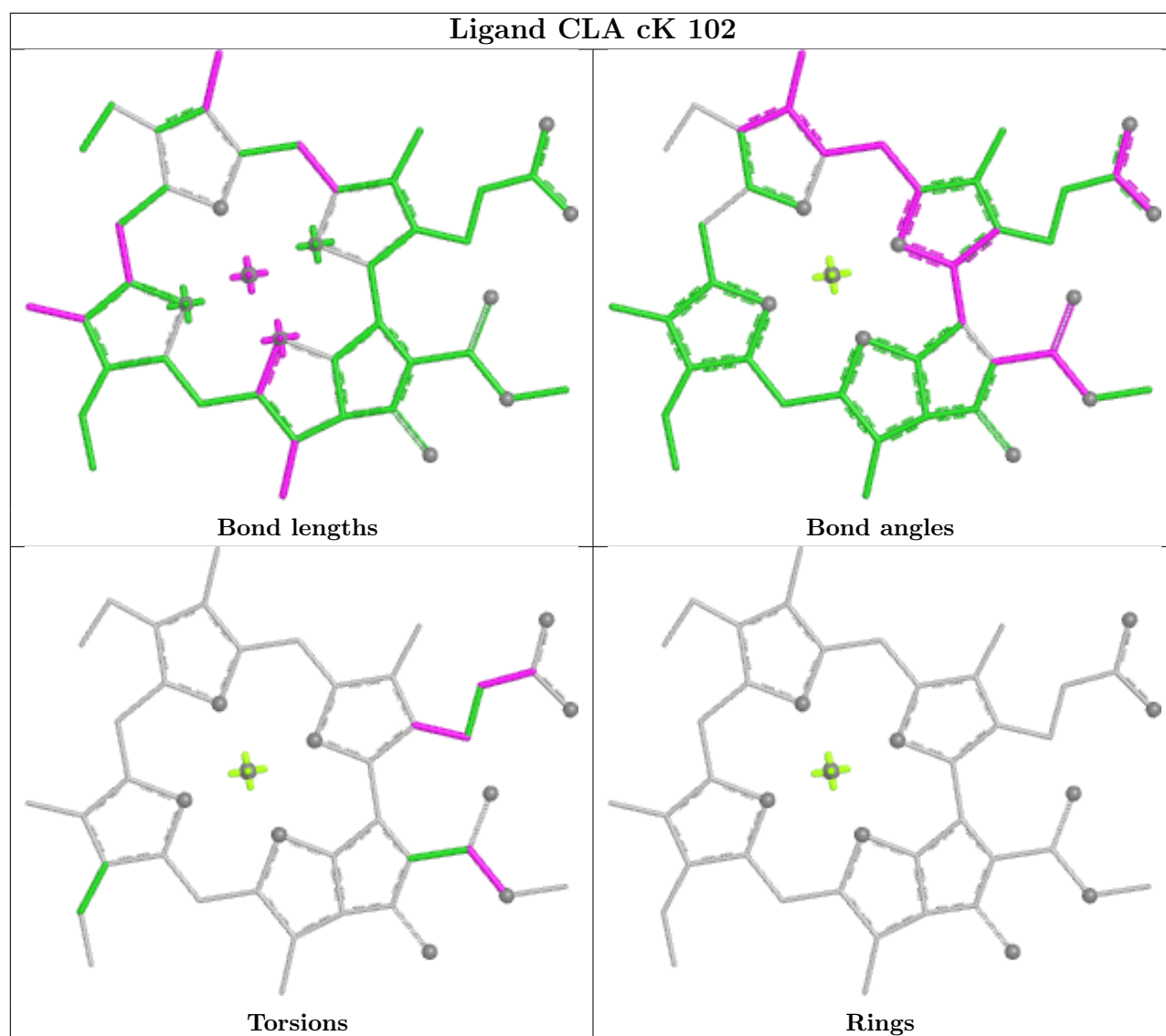


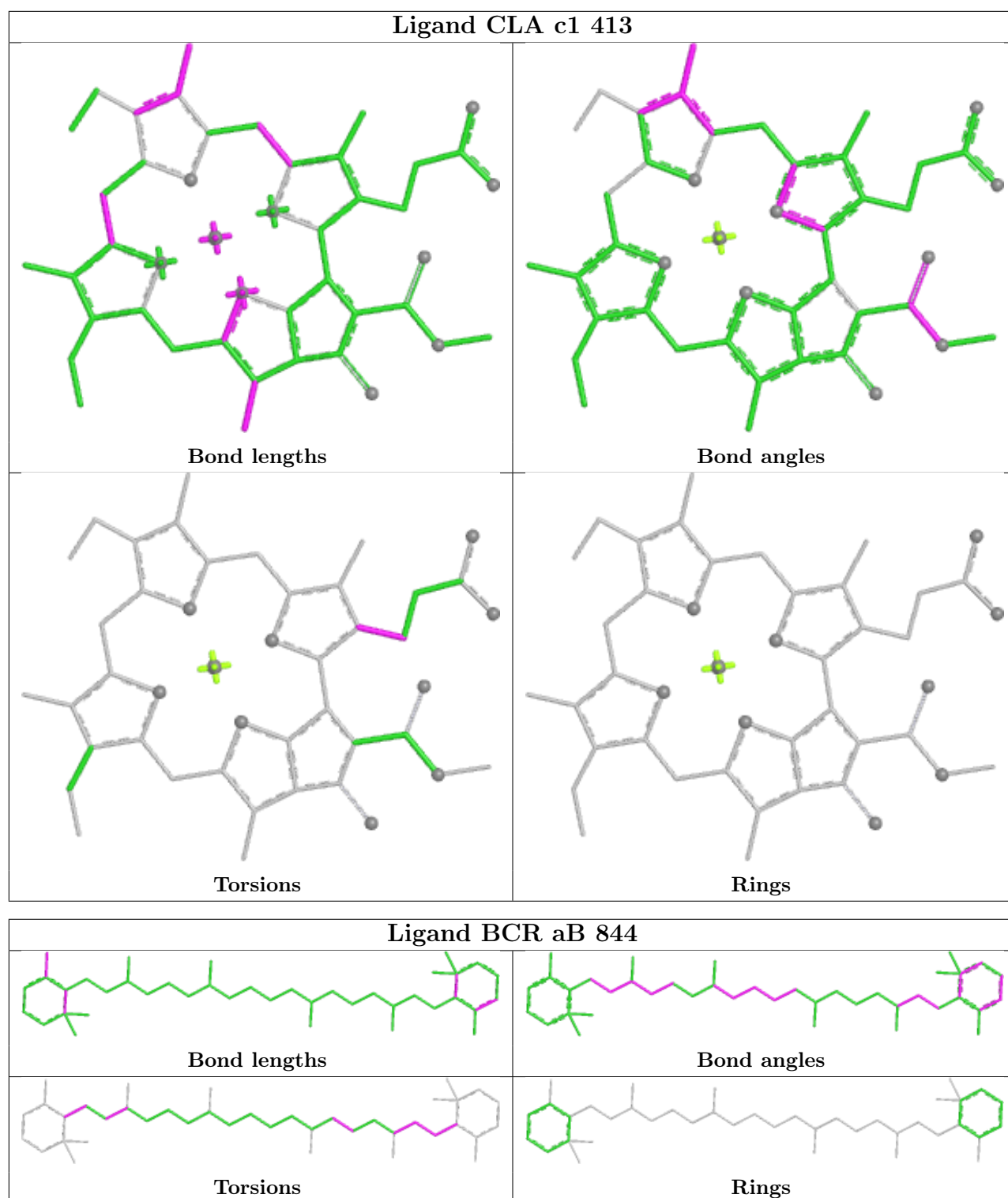
Ligand CLA c5 402	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR a6 419	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

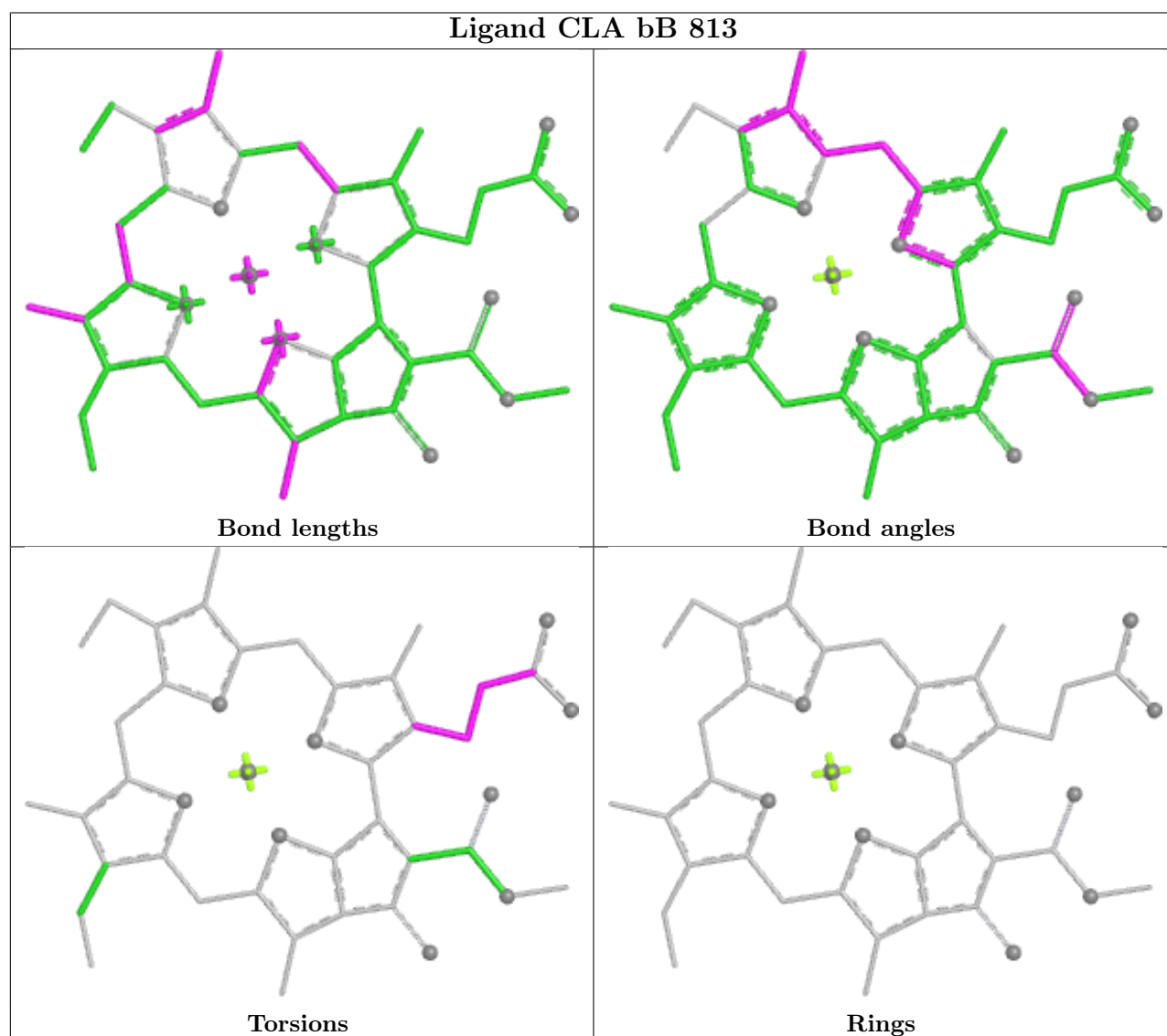
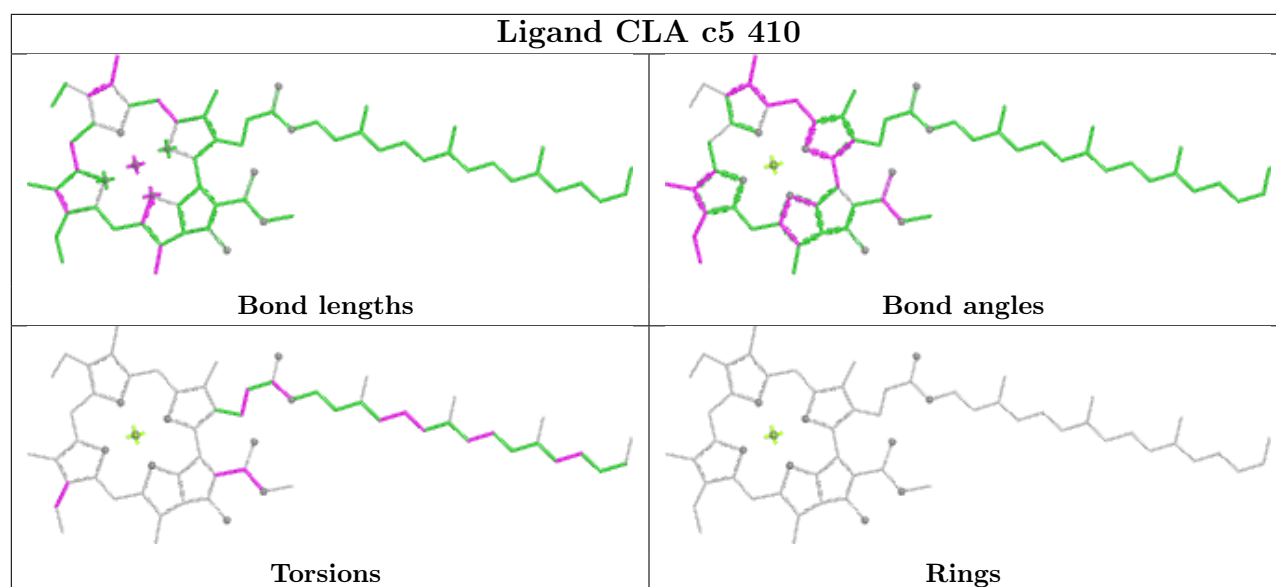


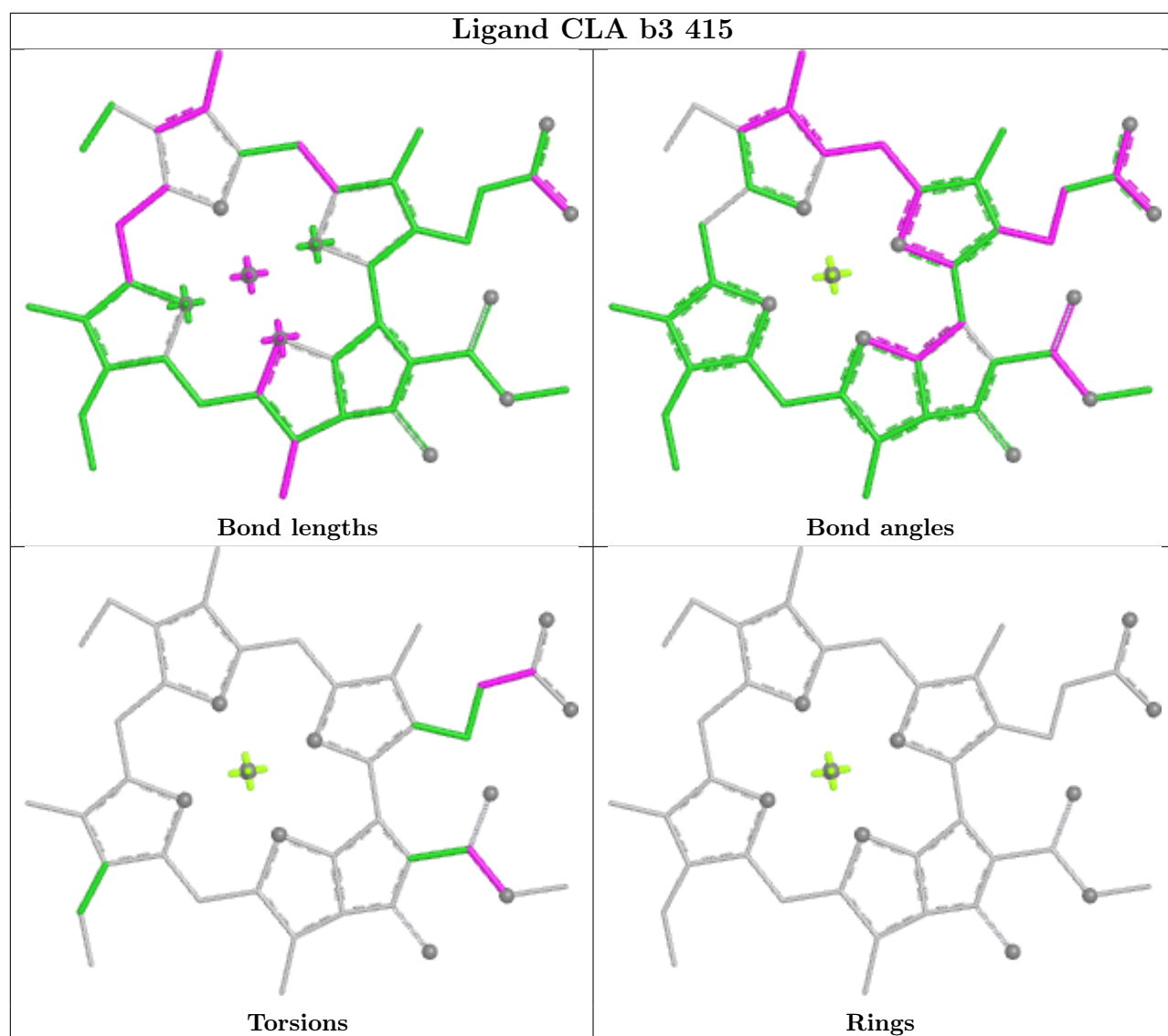


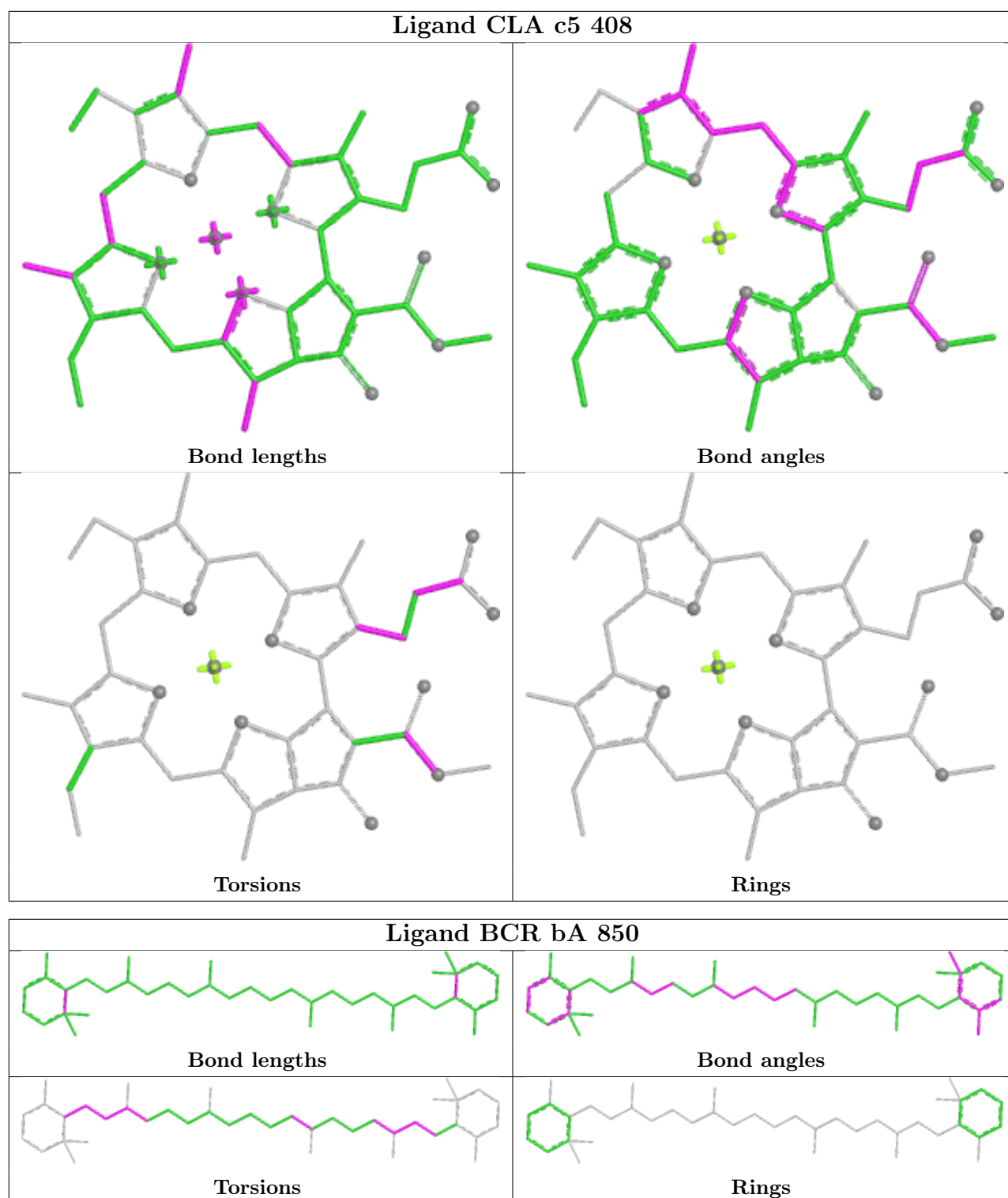


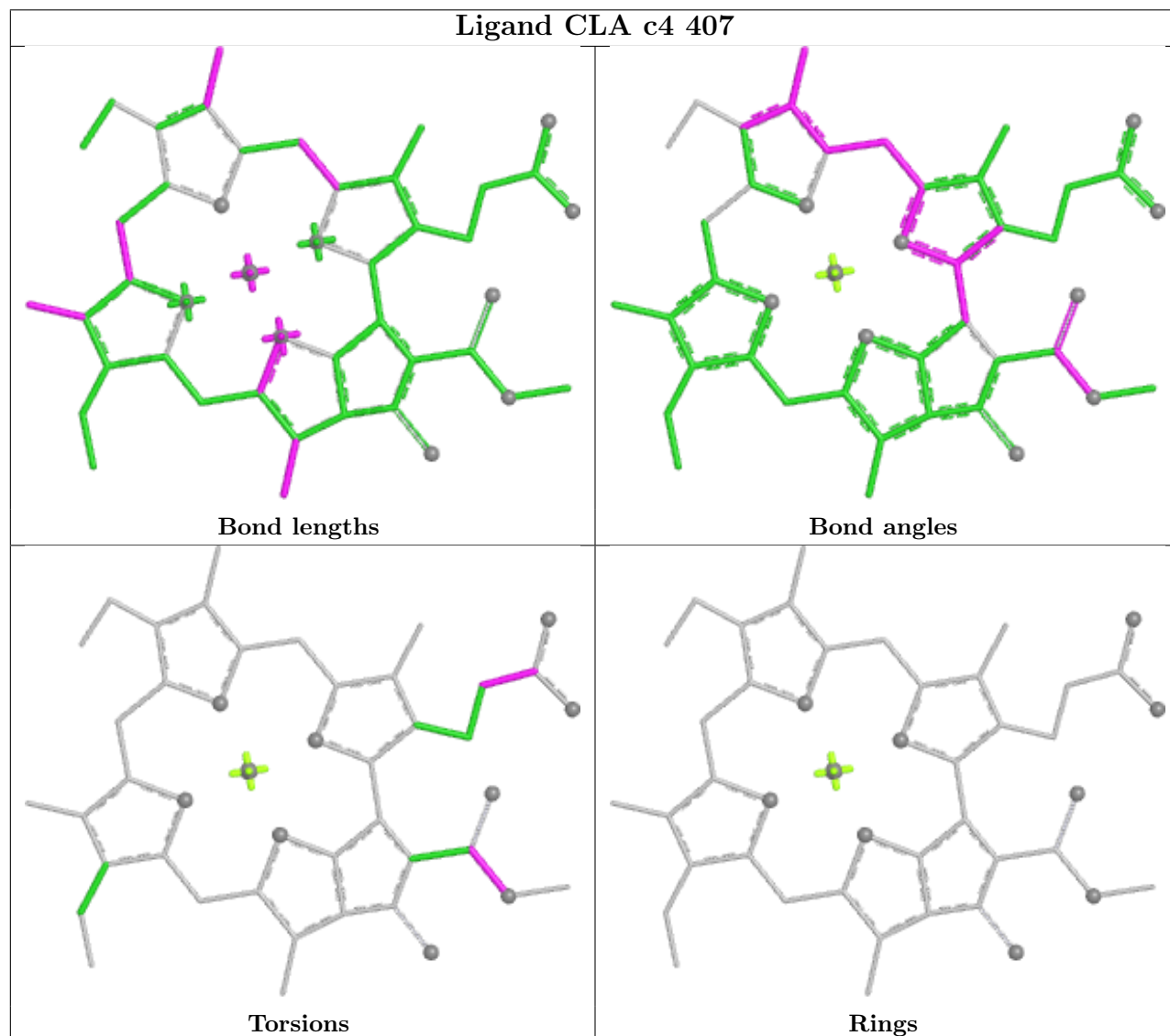
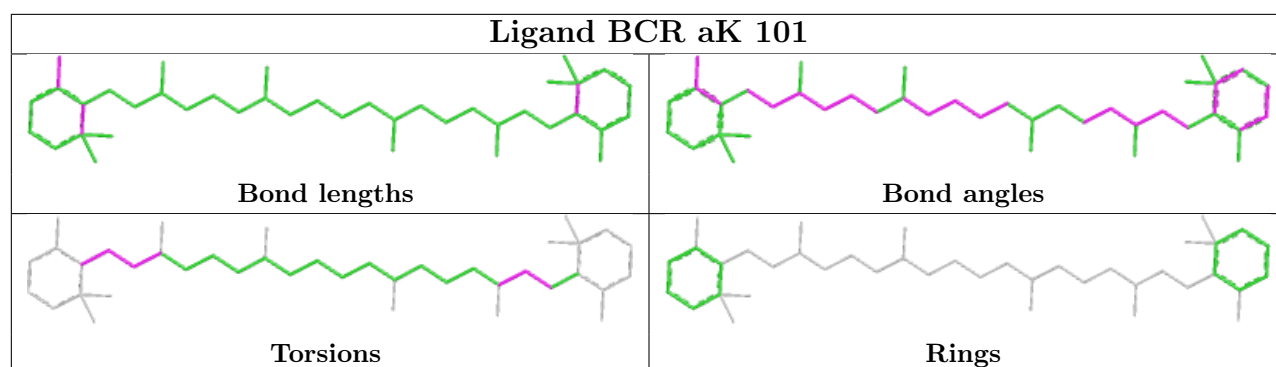




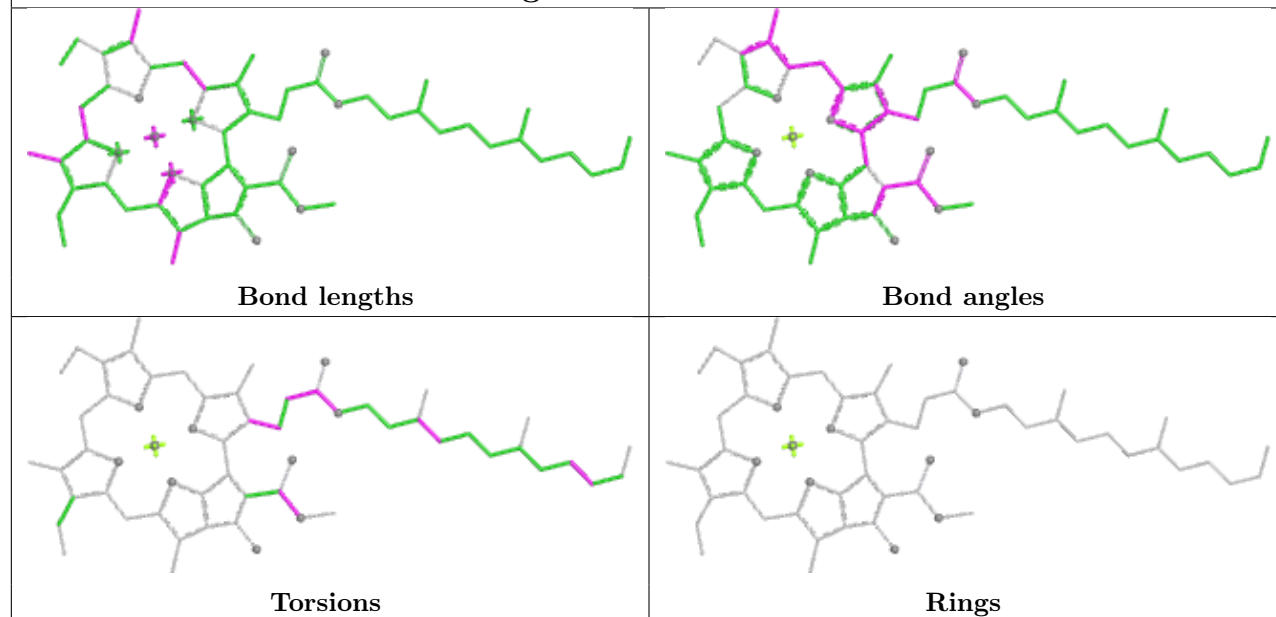




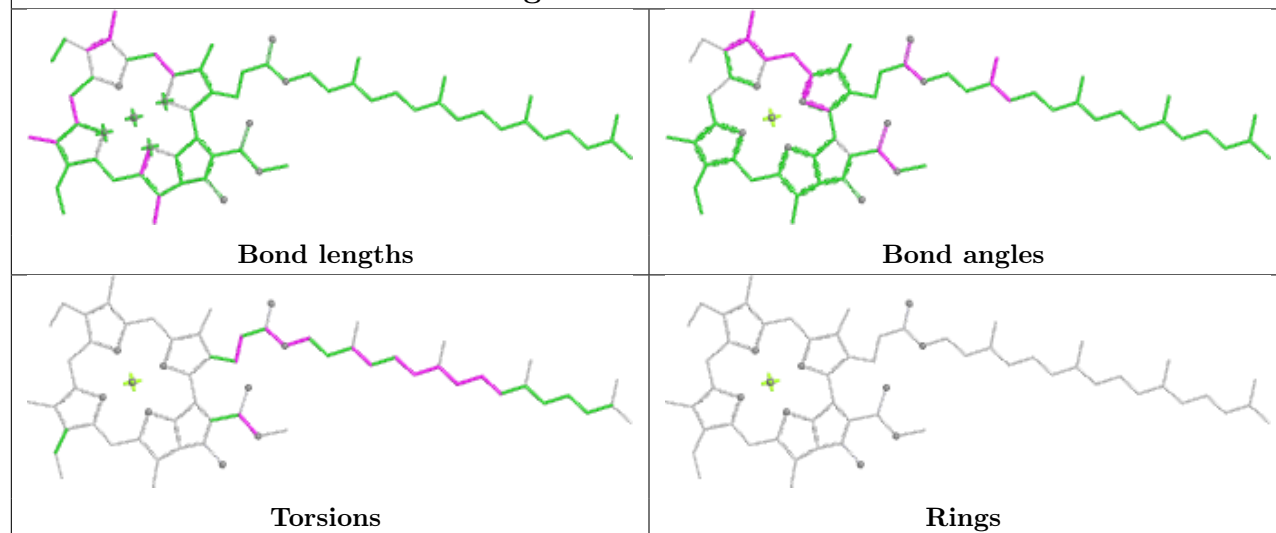


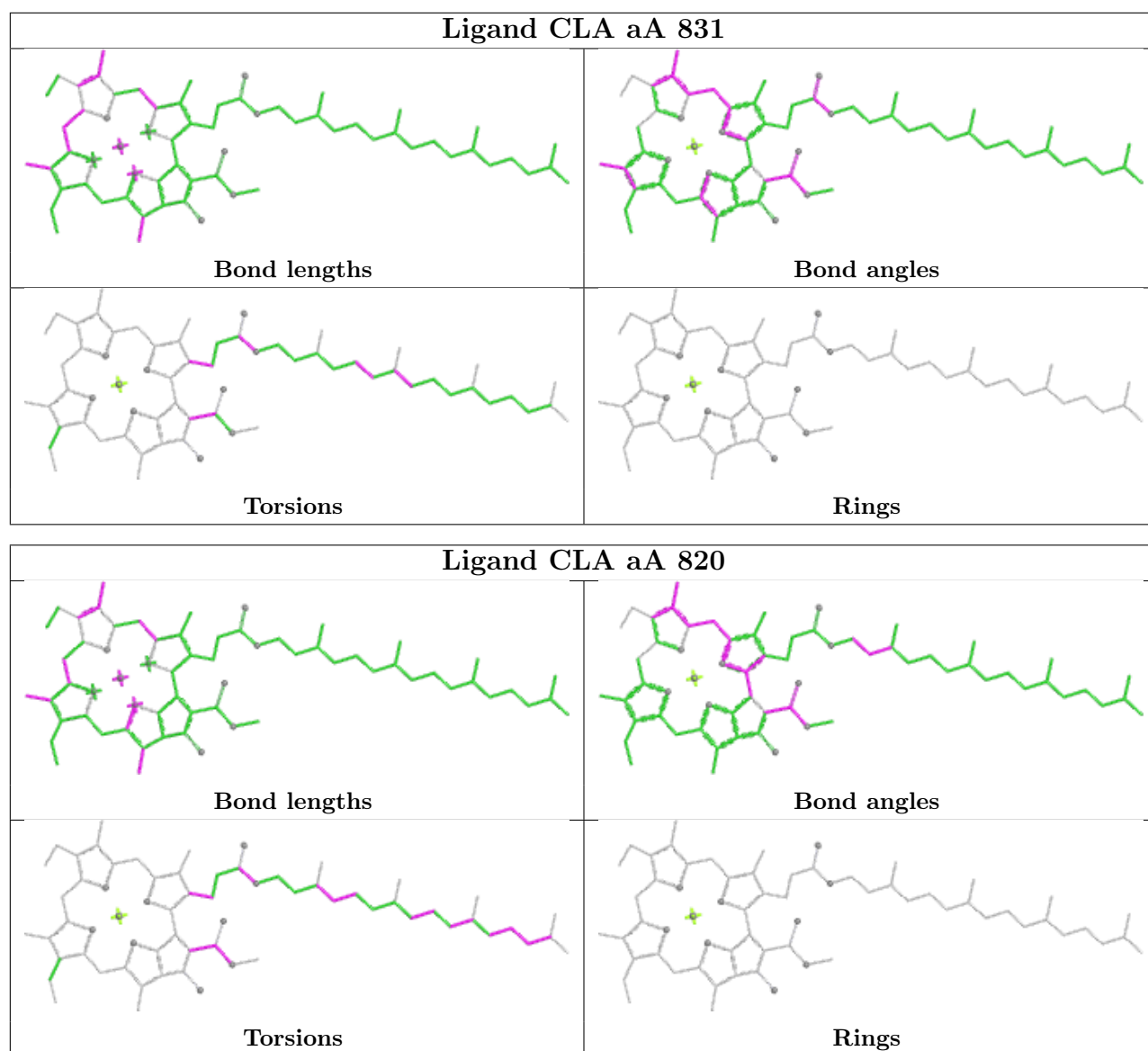


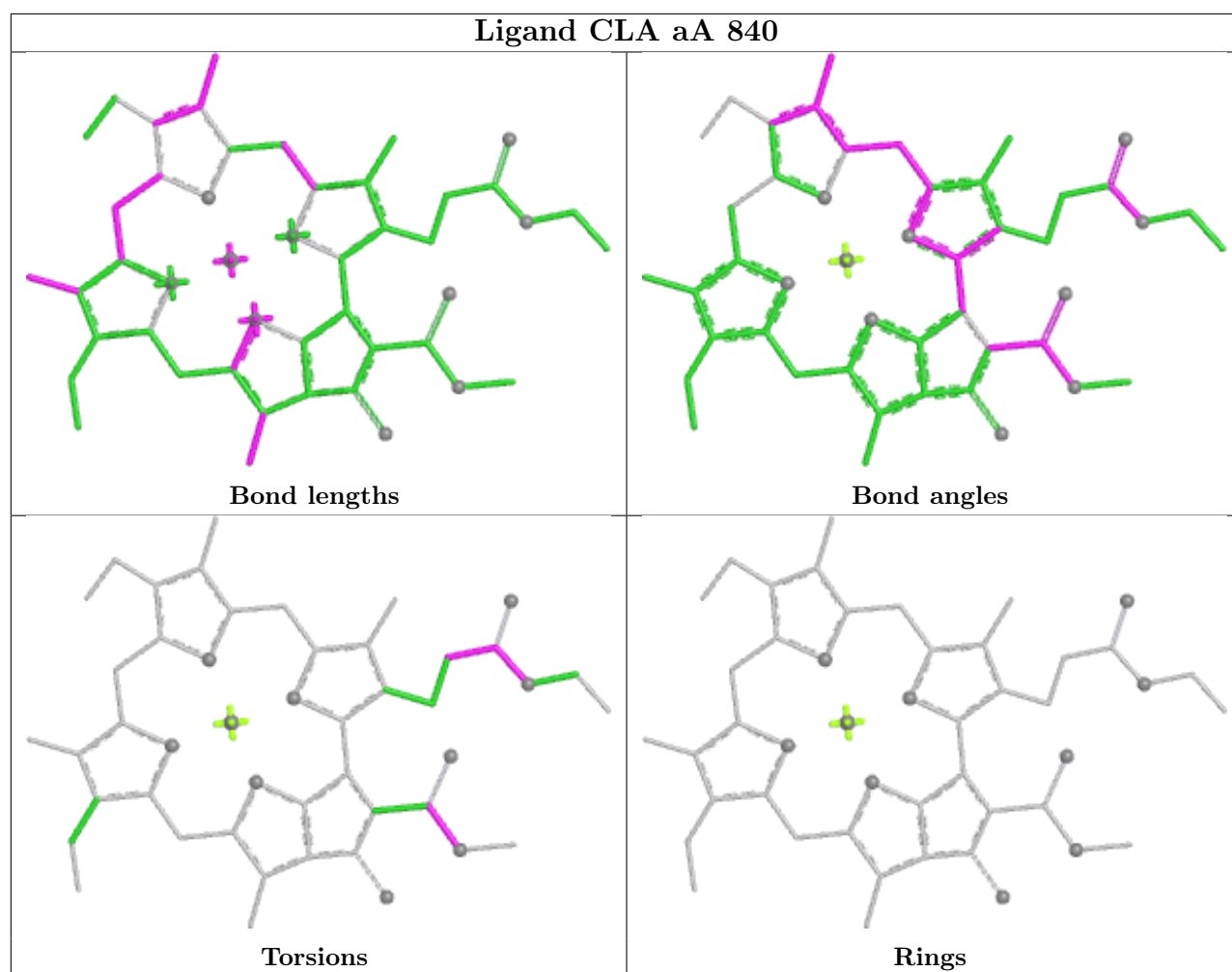
Ligand CLA bB 818

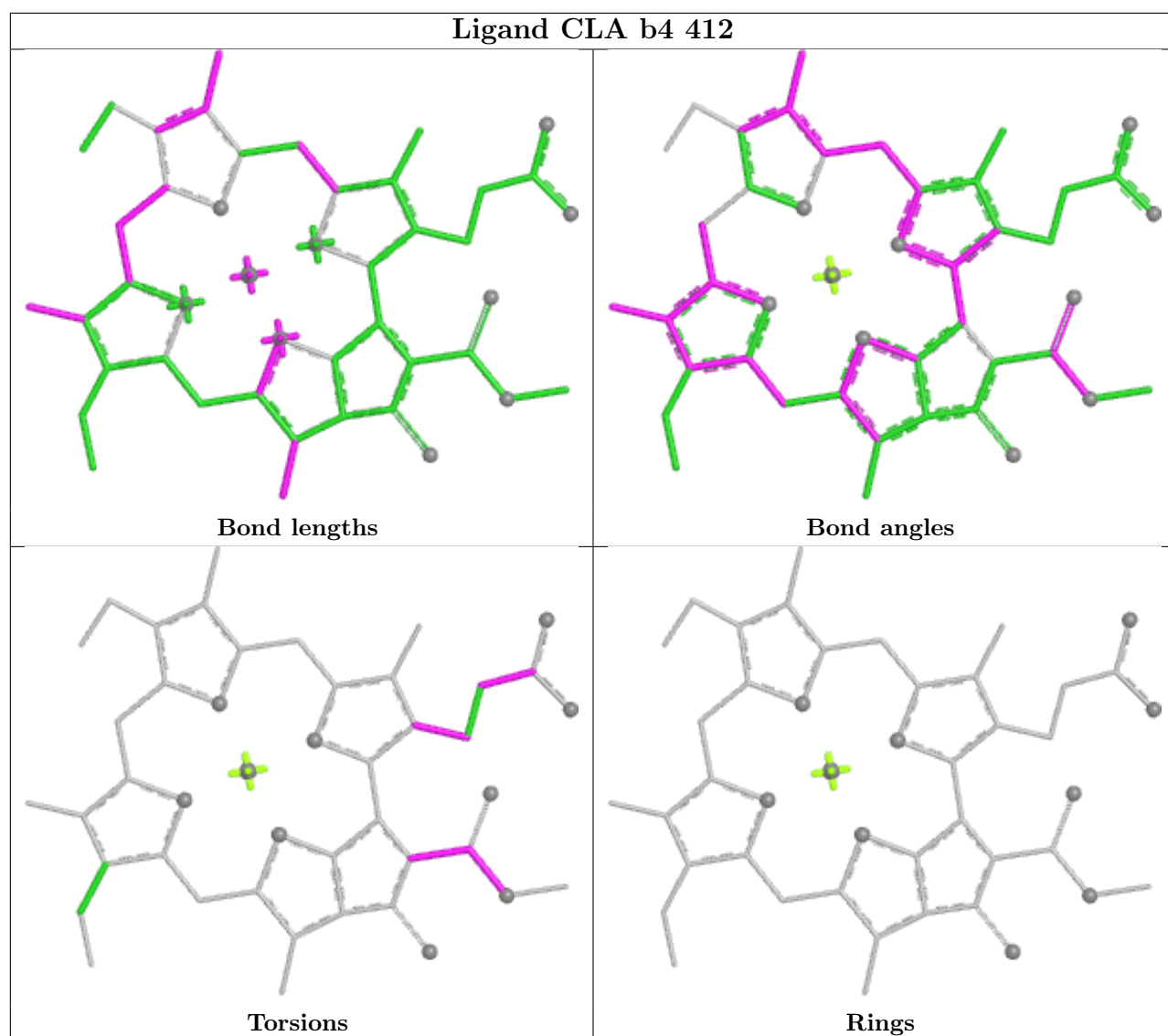


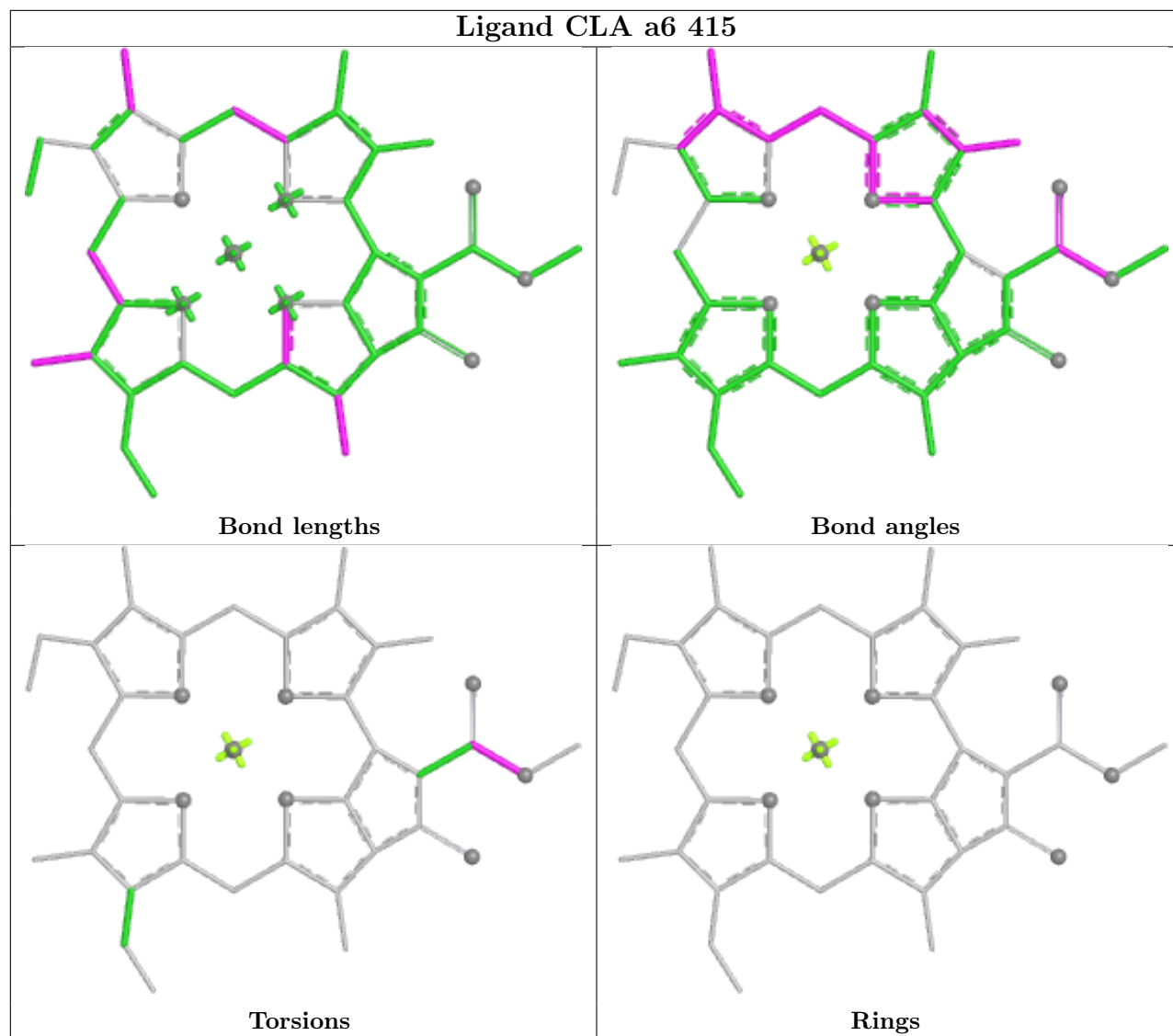
Ligand CLA cA 841

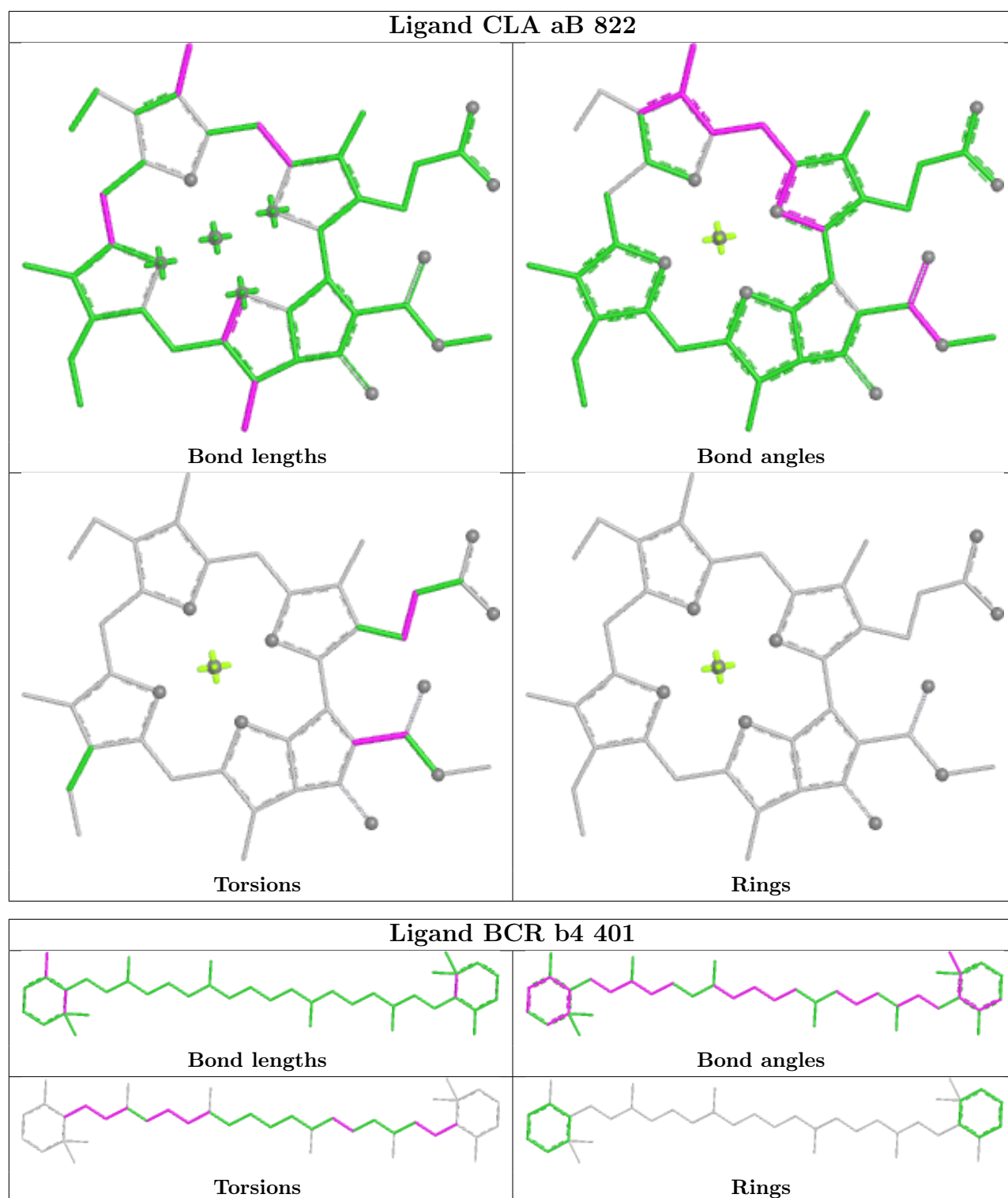


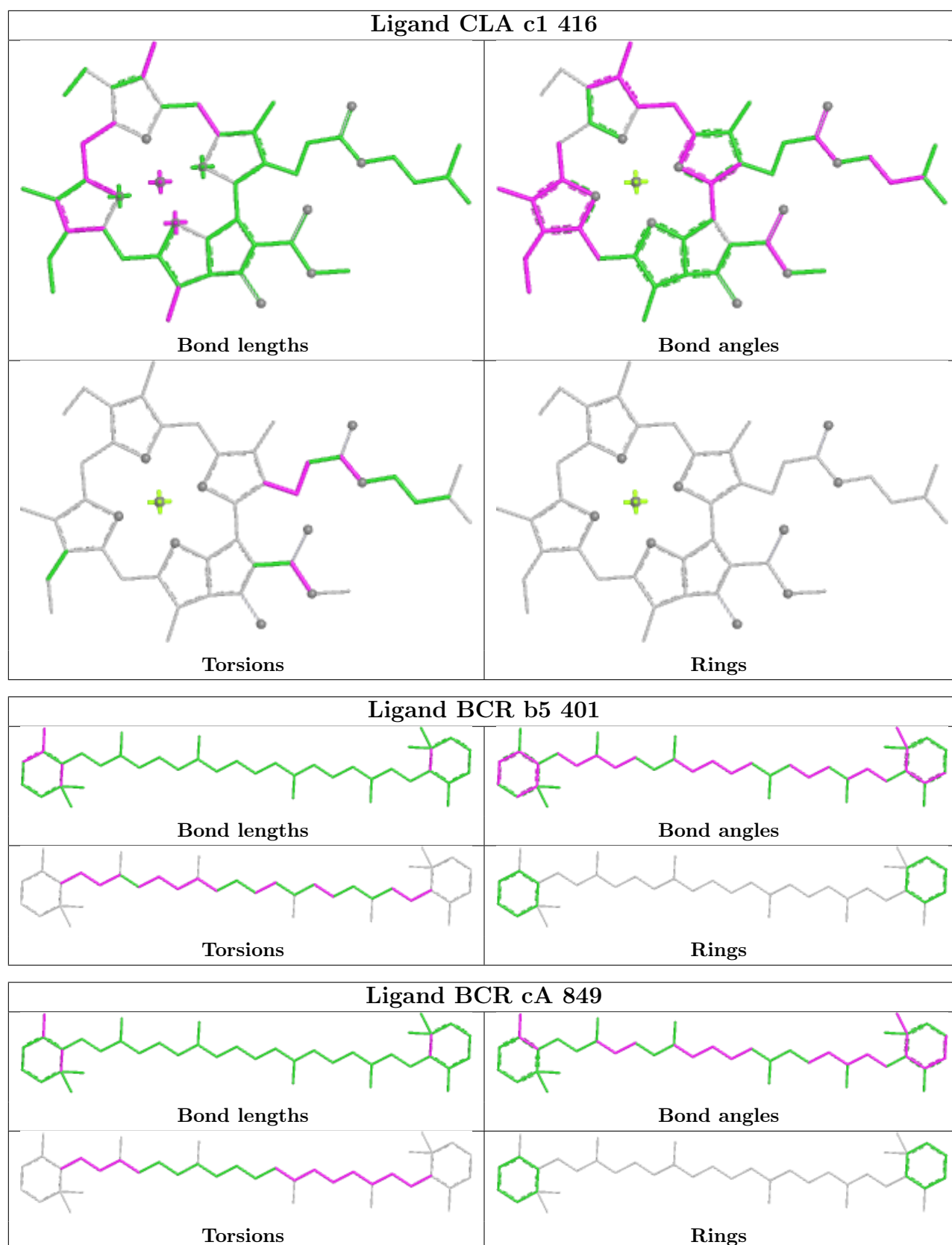


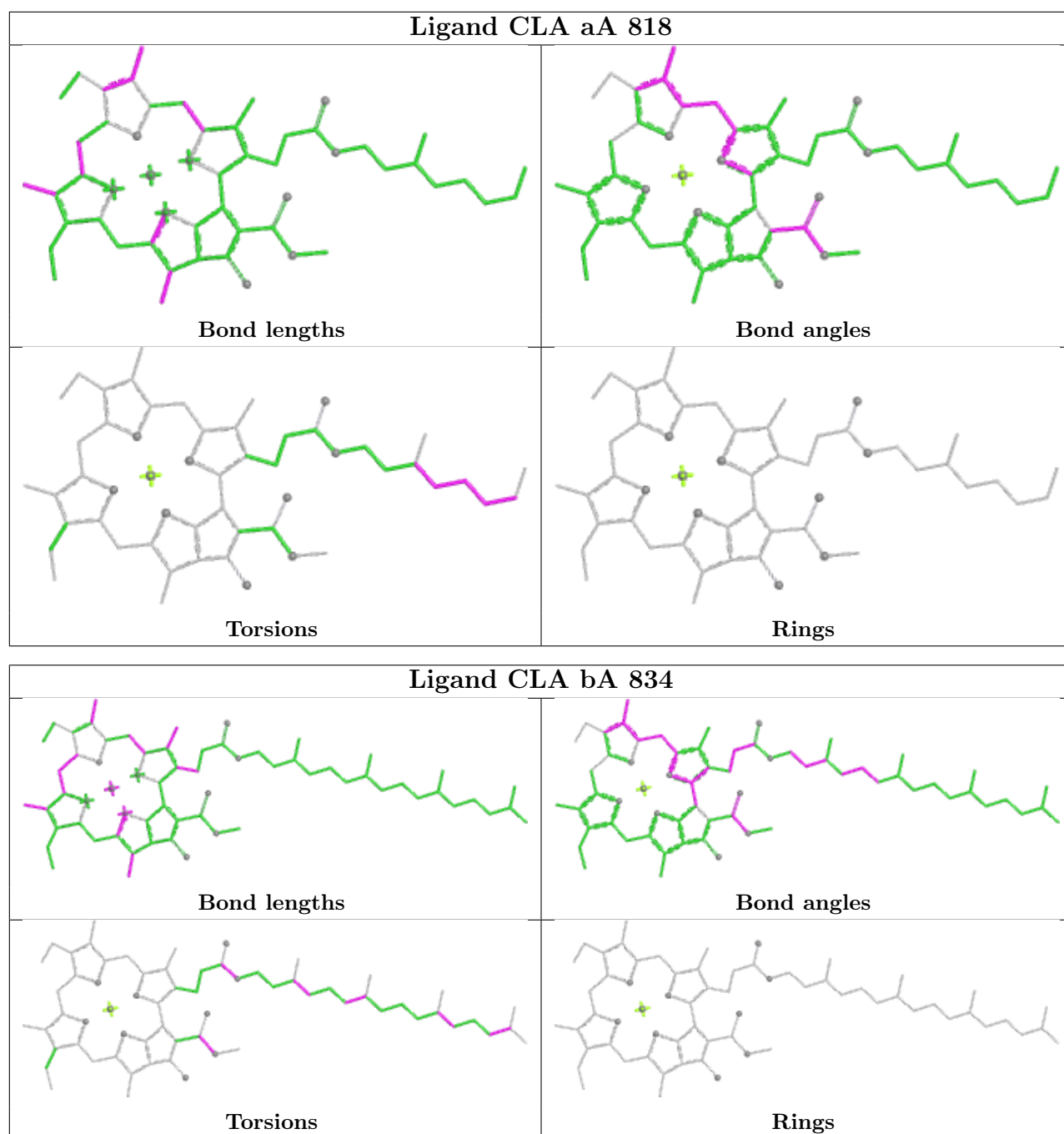


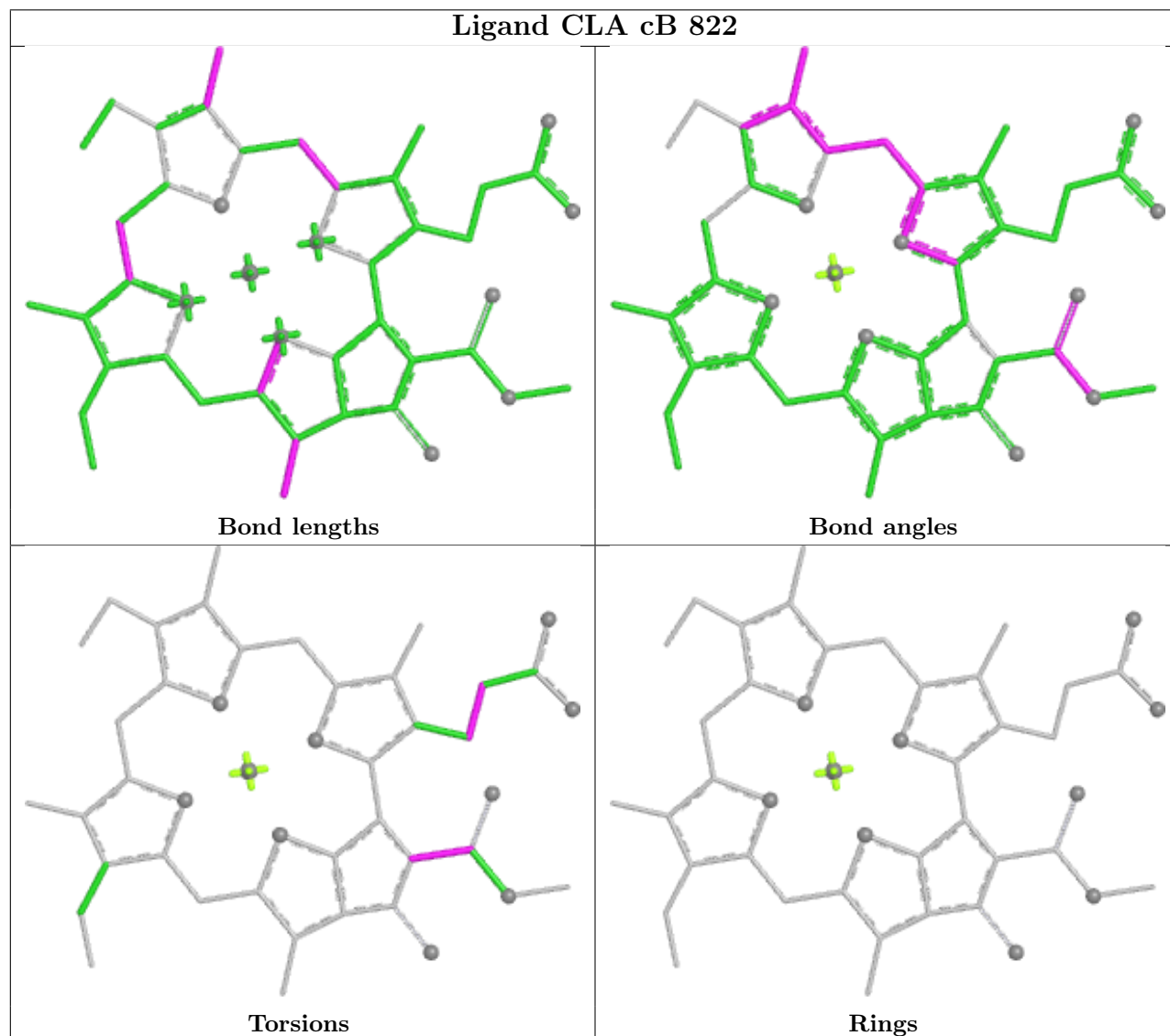
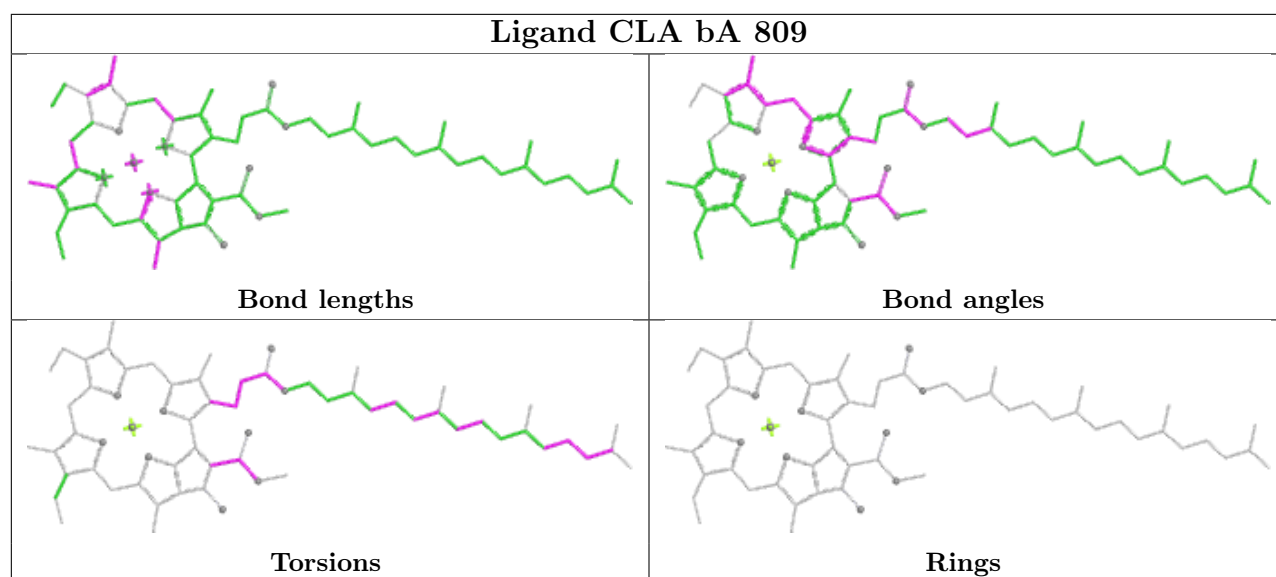


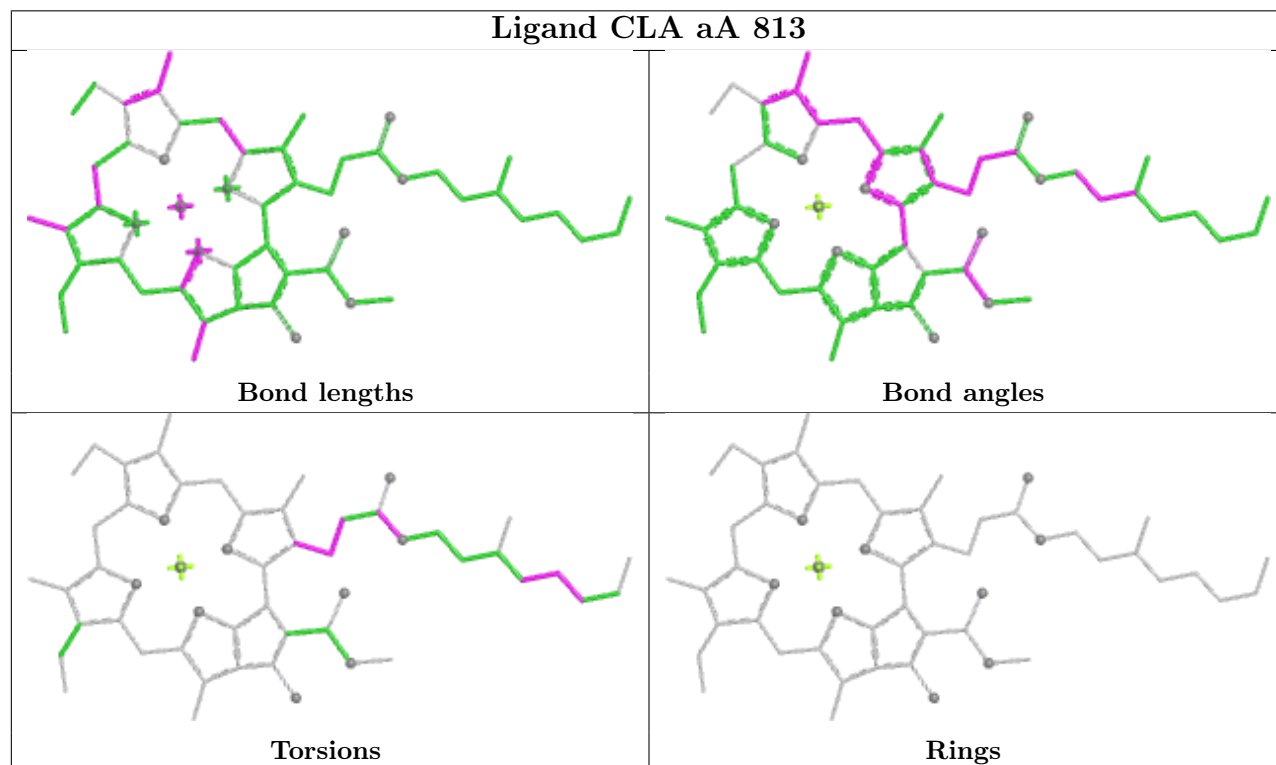
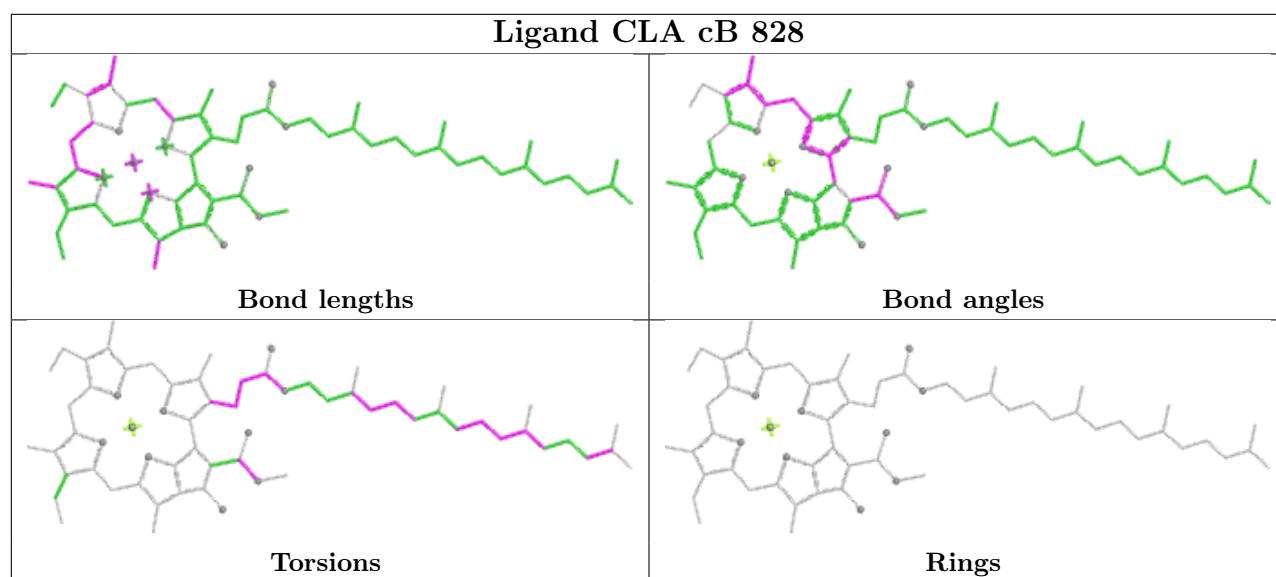


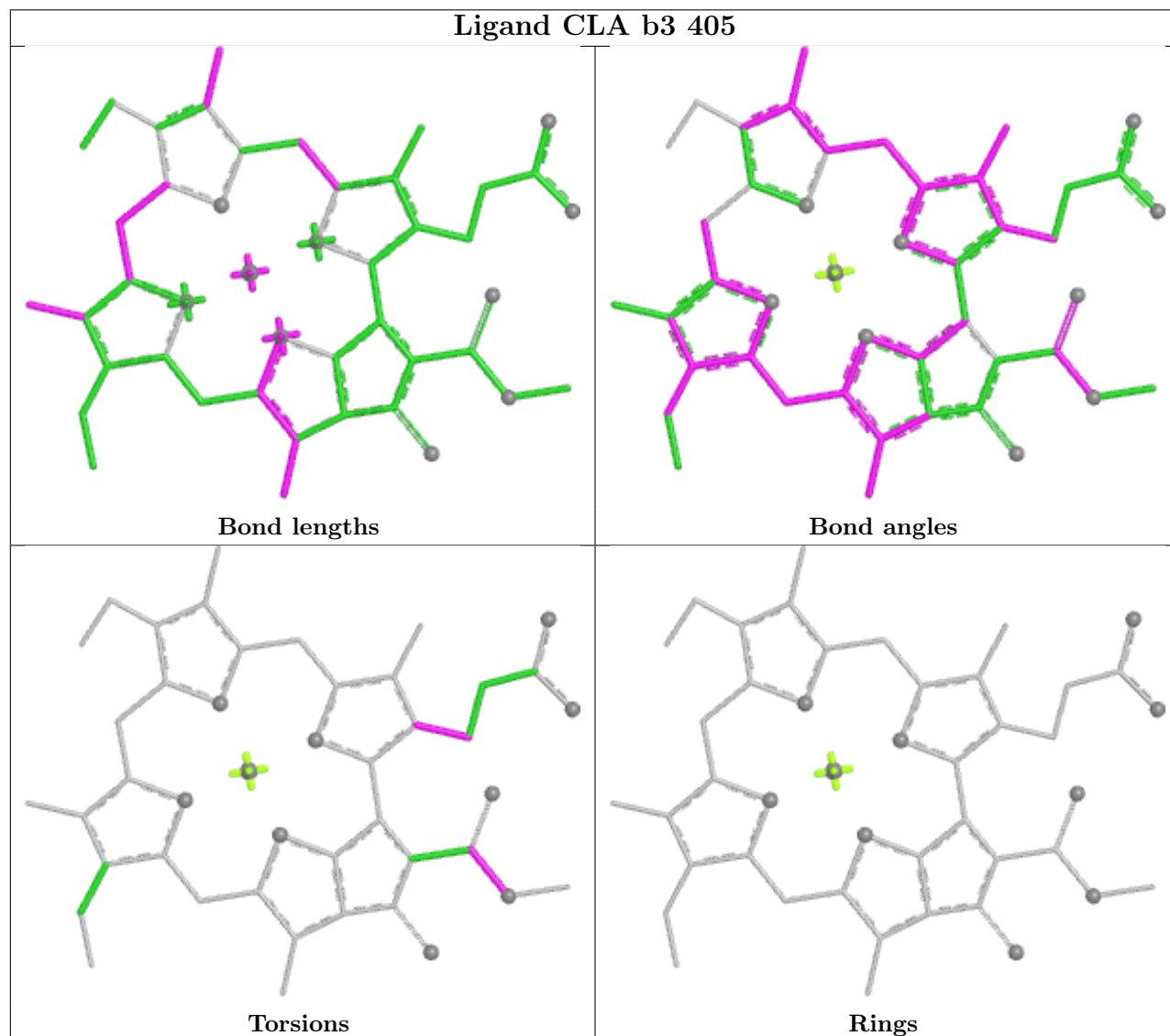
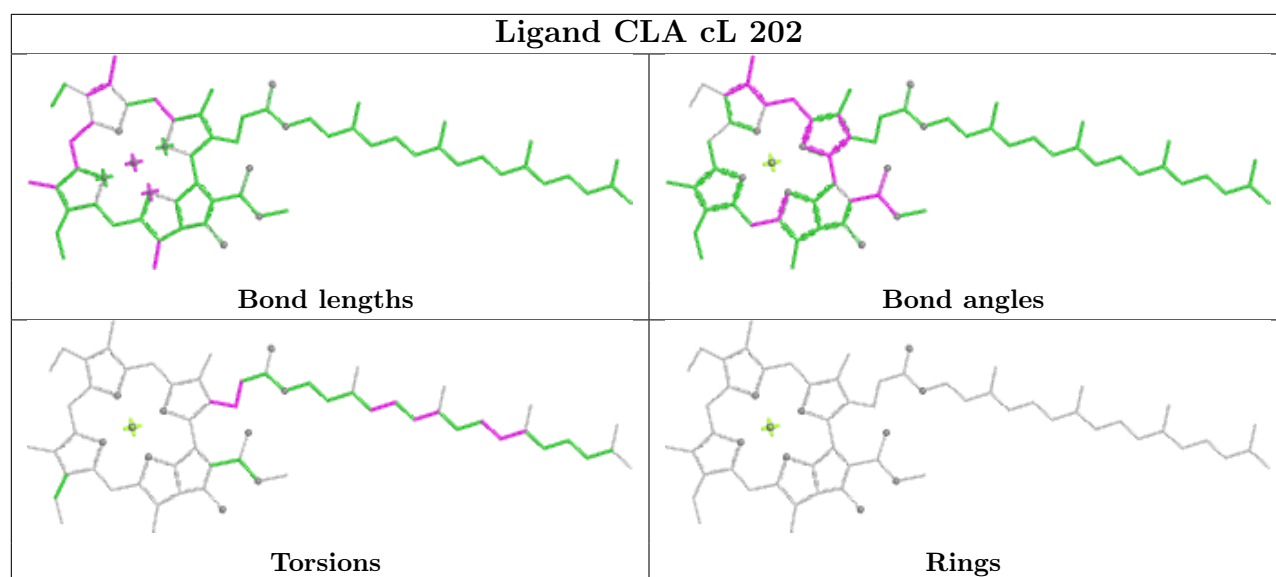


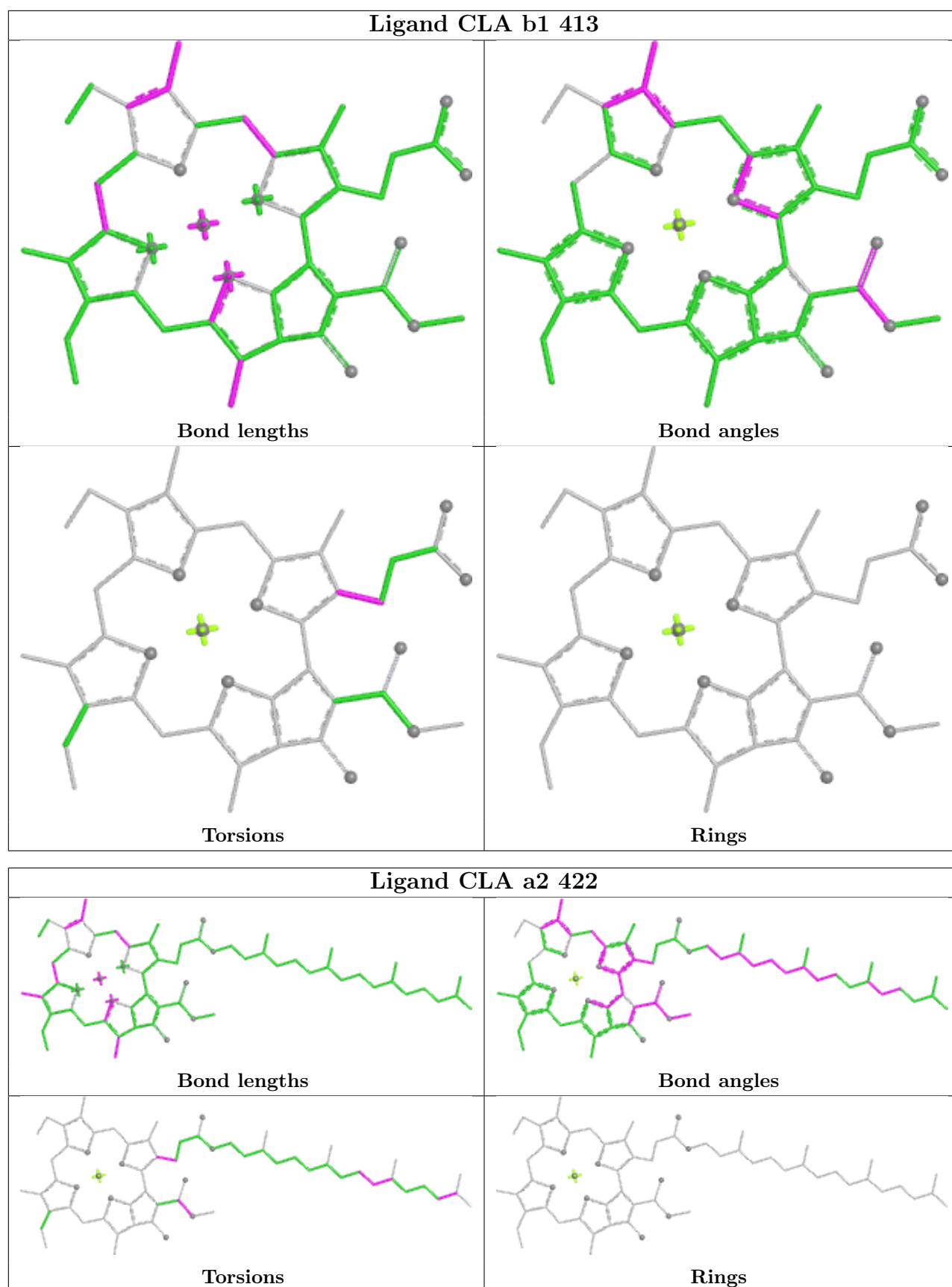


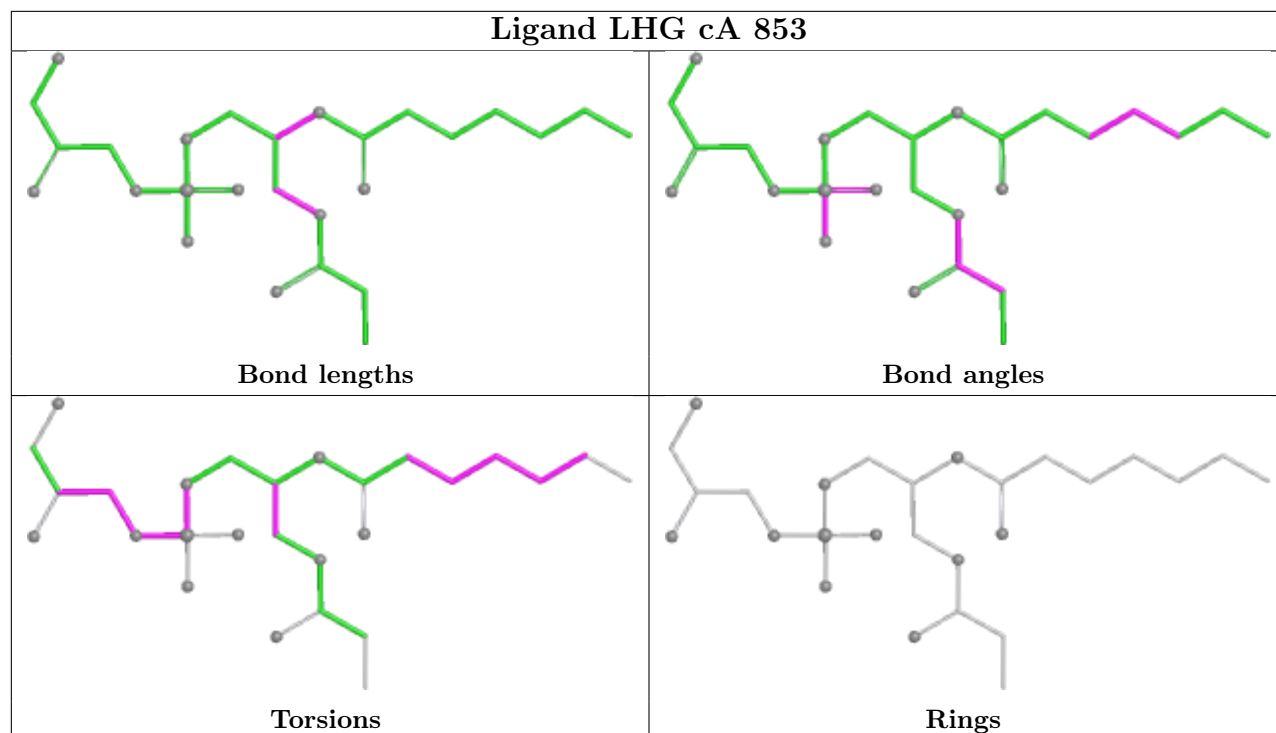
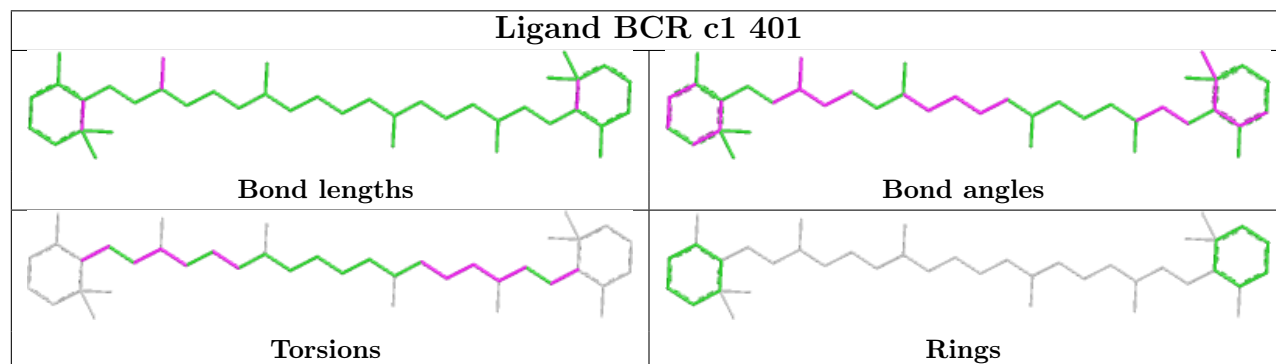
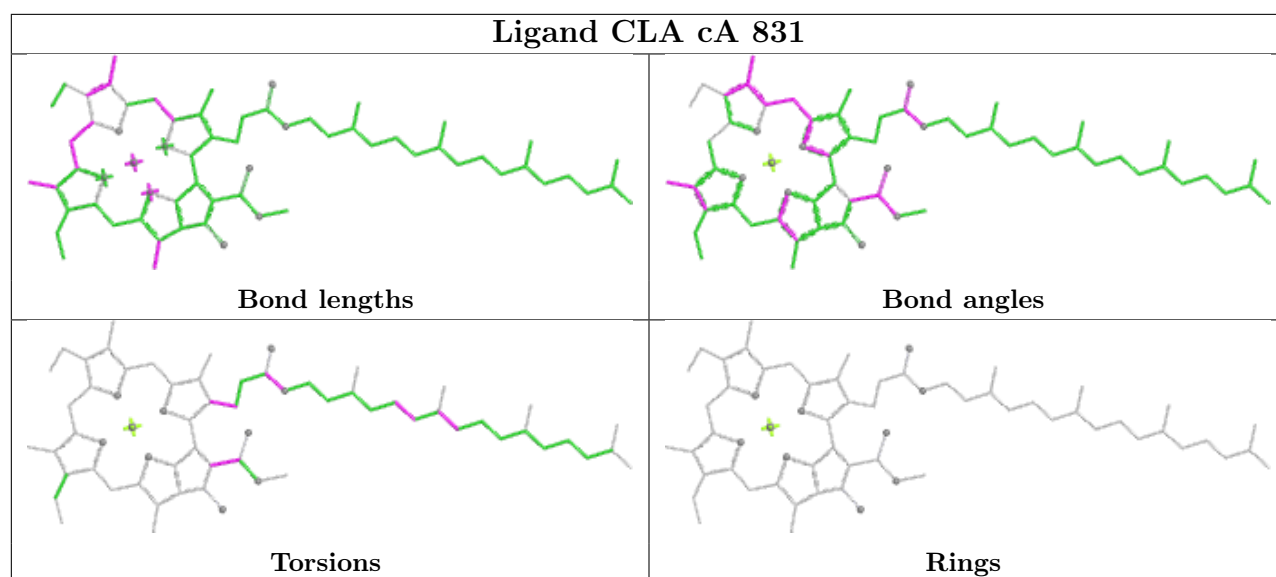


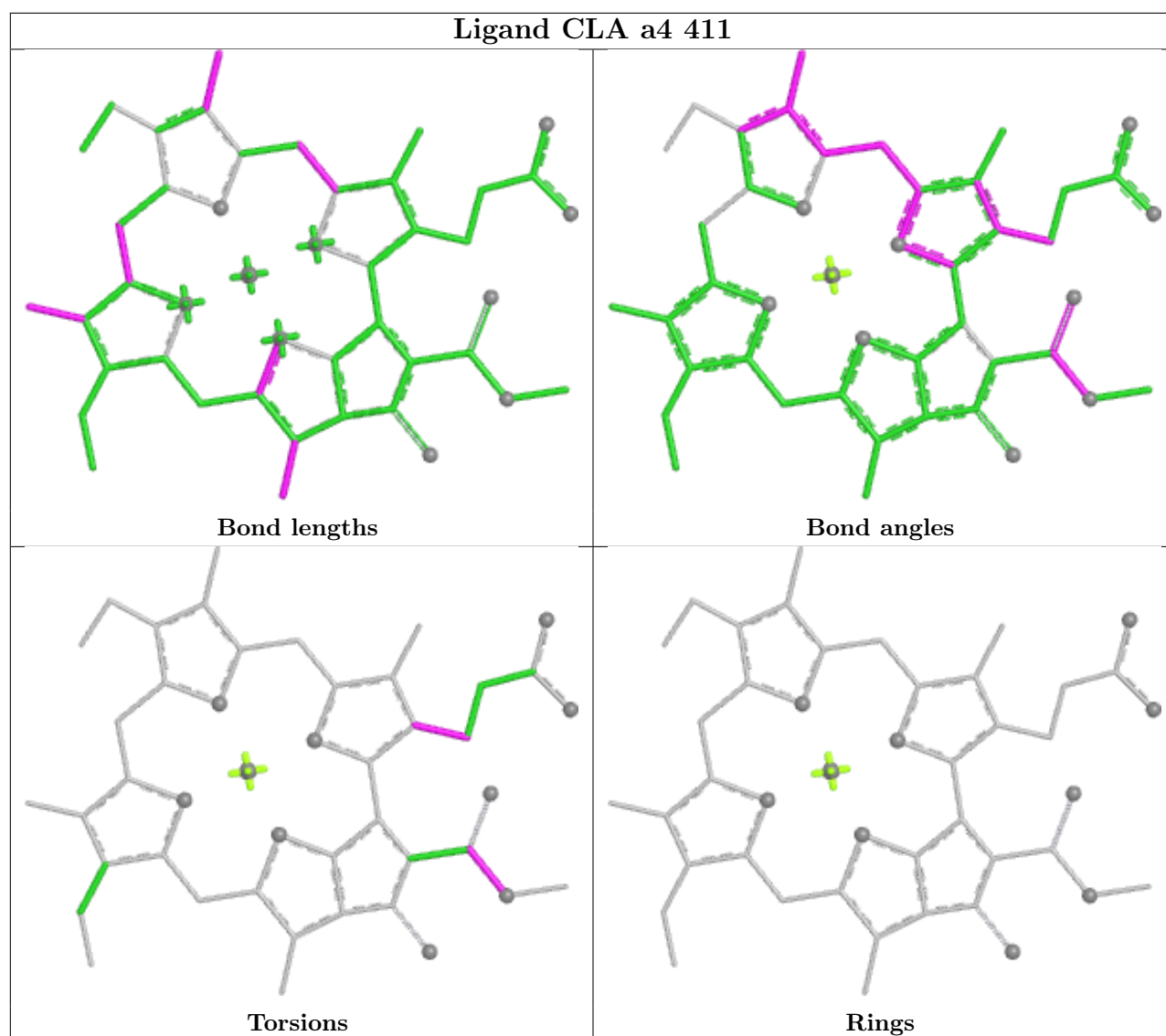


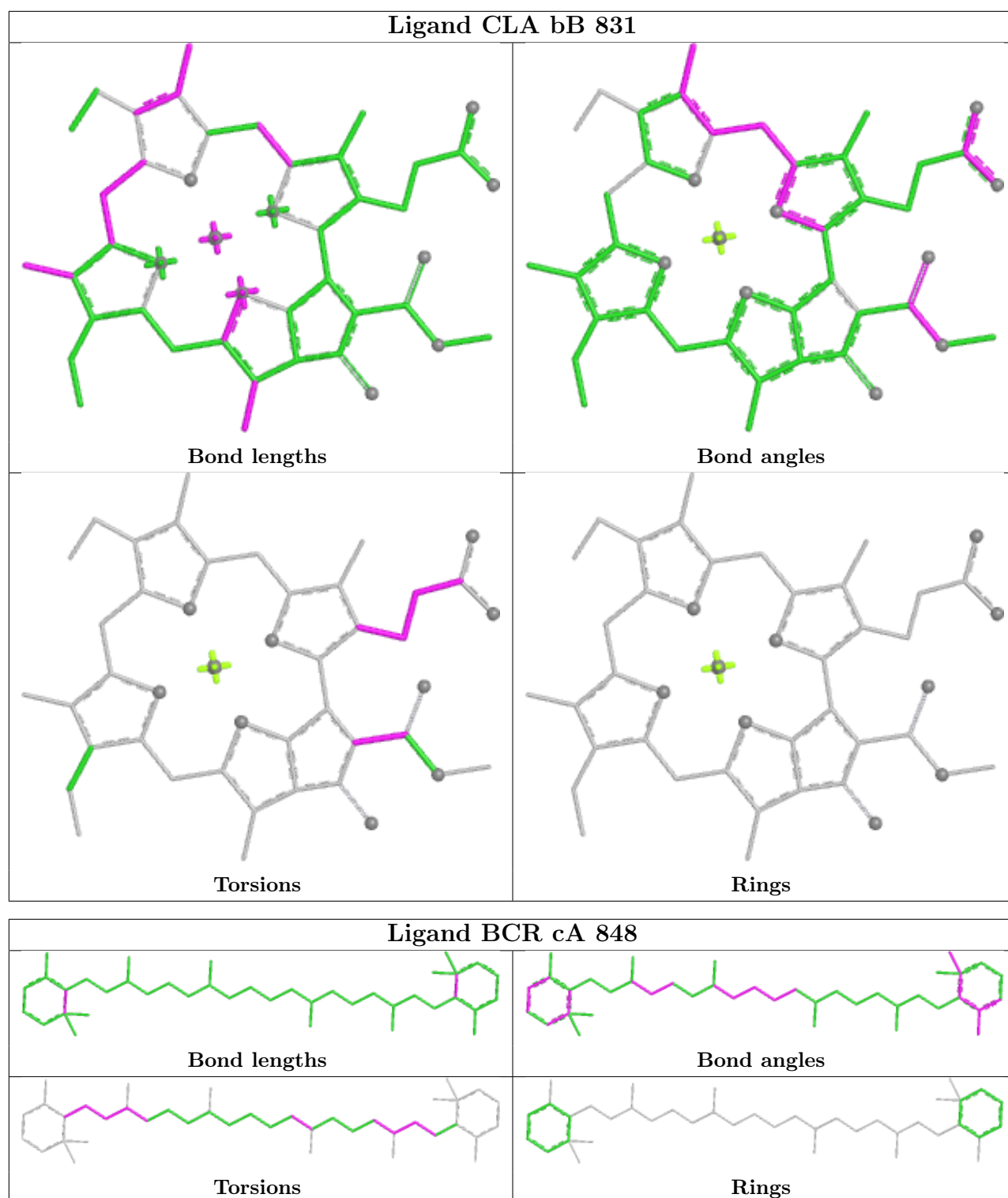


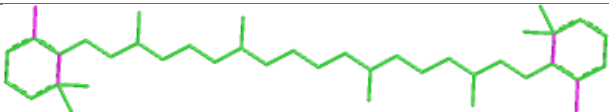
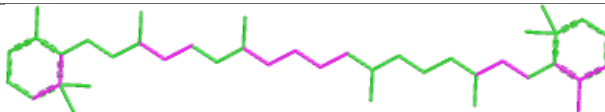
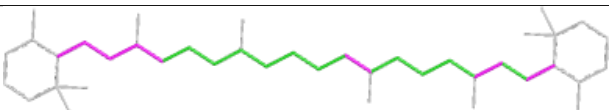
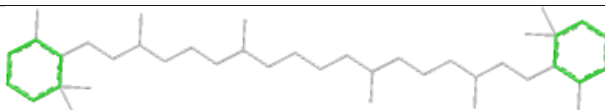




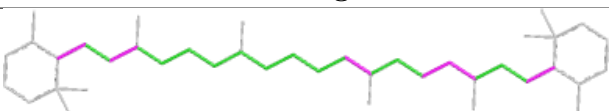
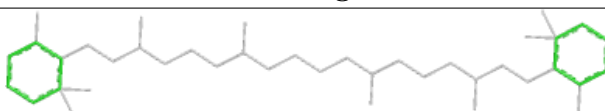


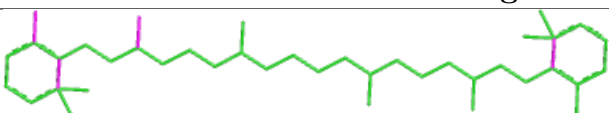
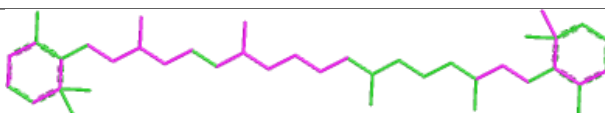
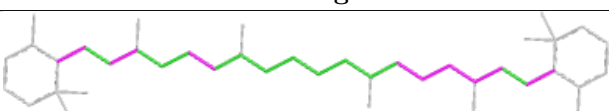
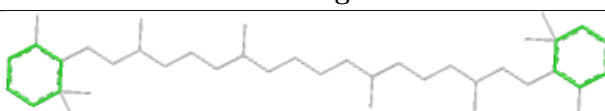




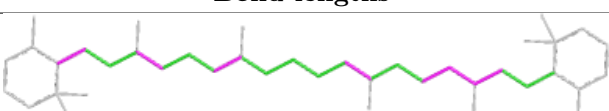
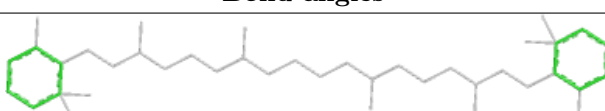


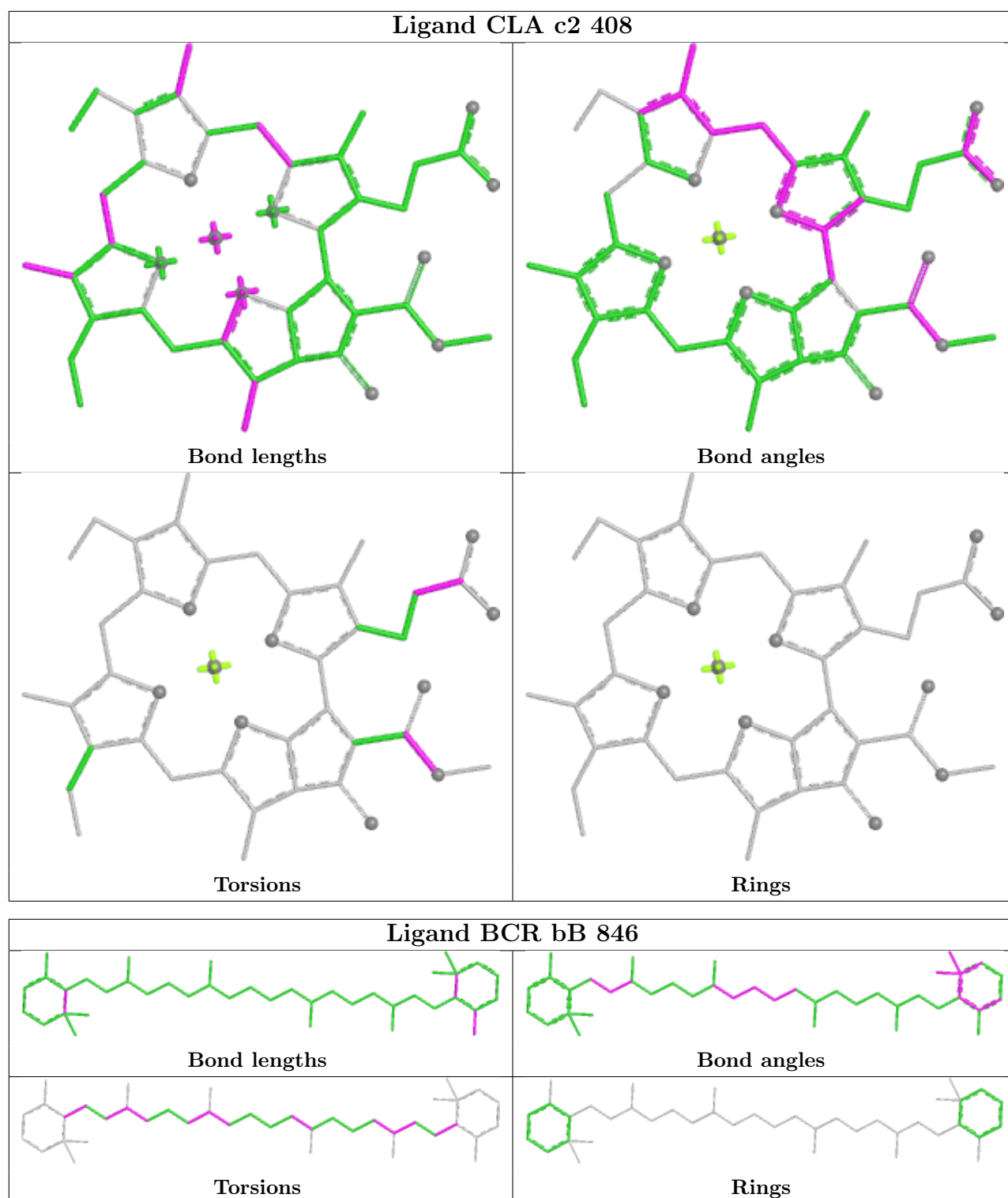


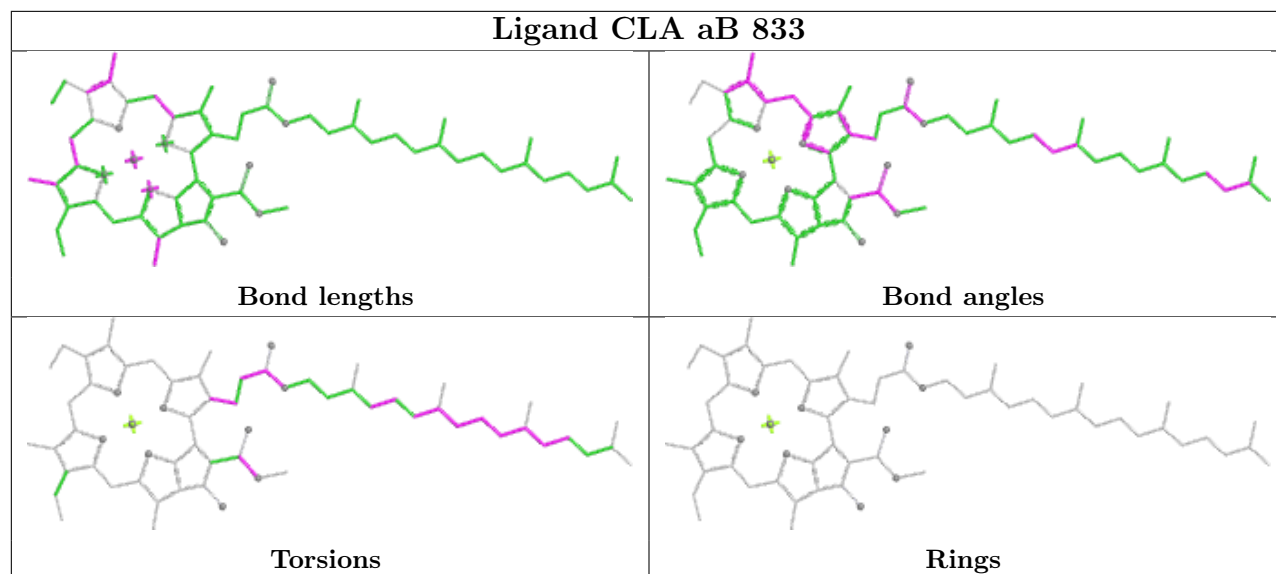
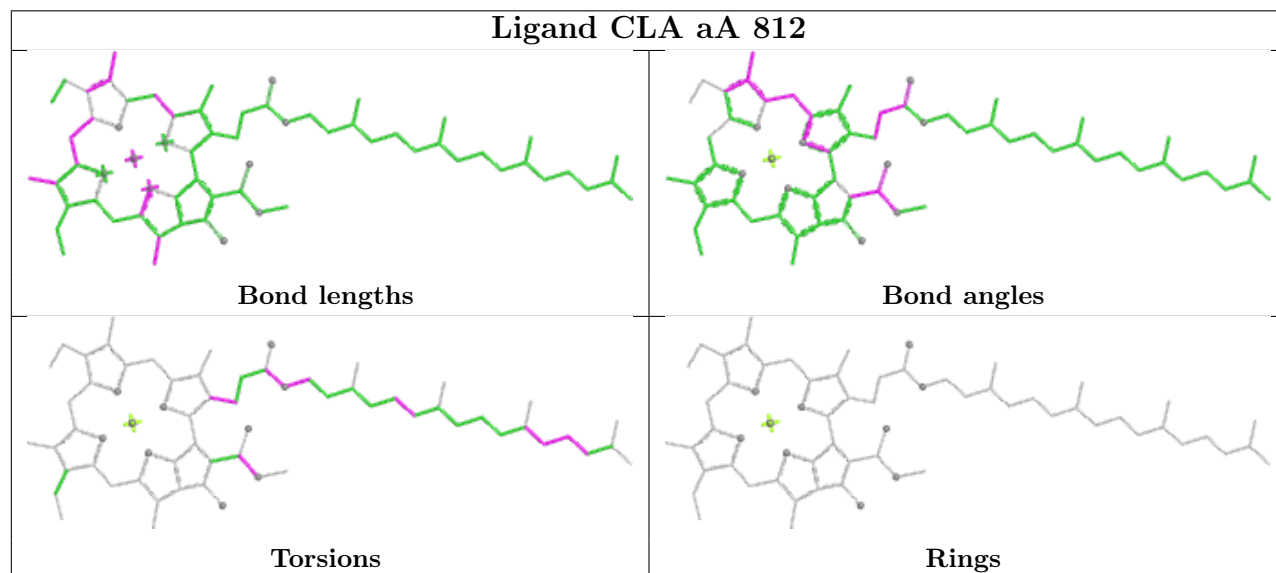
Ligand BCR aJ 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

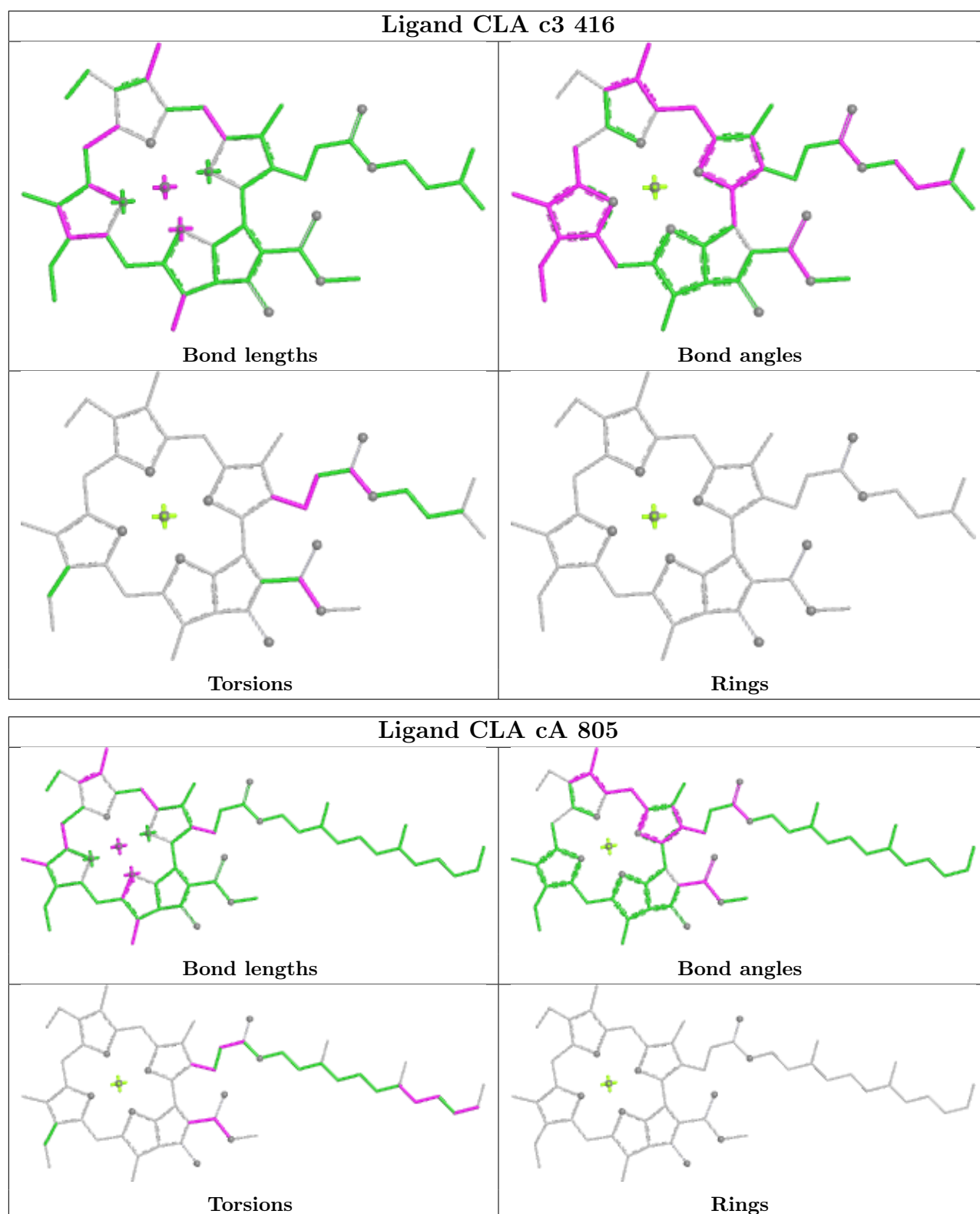
Ligand BCR c4 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

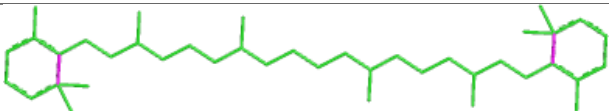
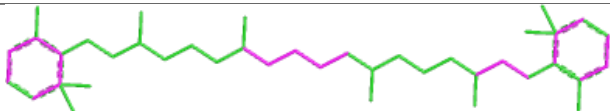
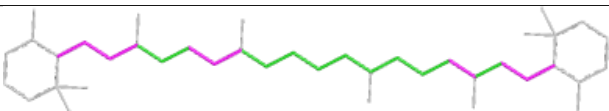
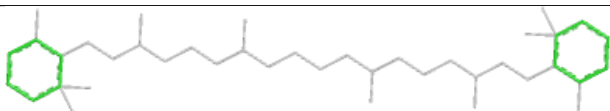
Ligand BCR b1 419	
	
Bond lengths	Bond angles
	
Torsions	Rings


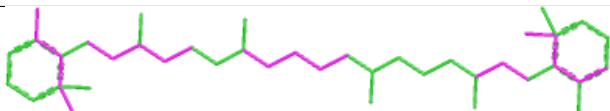
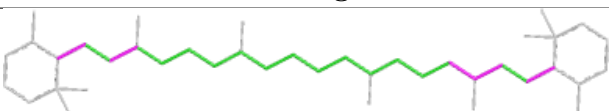
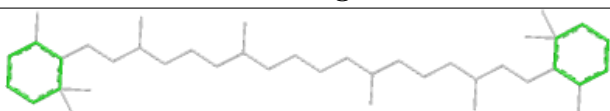
Ligand BCR cB 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

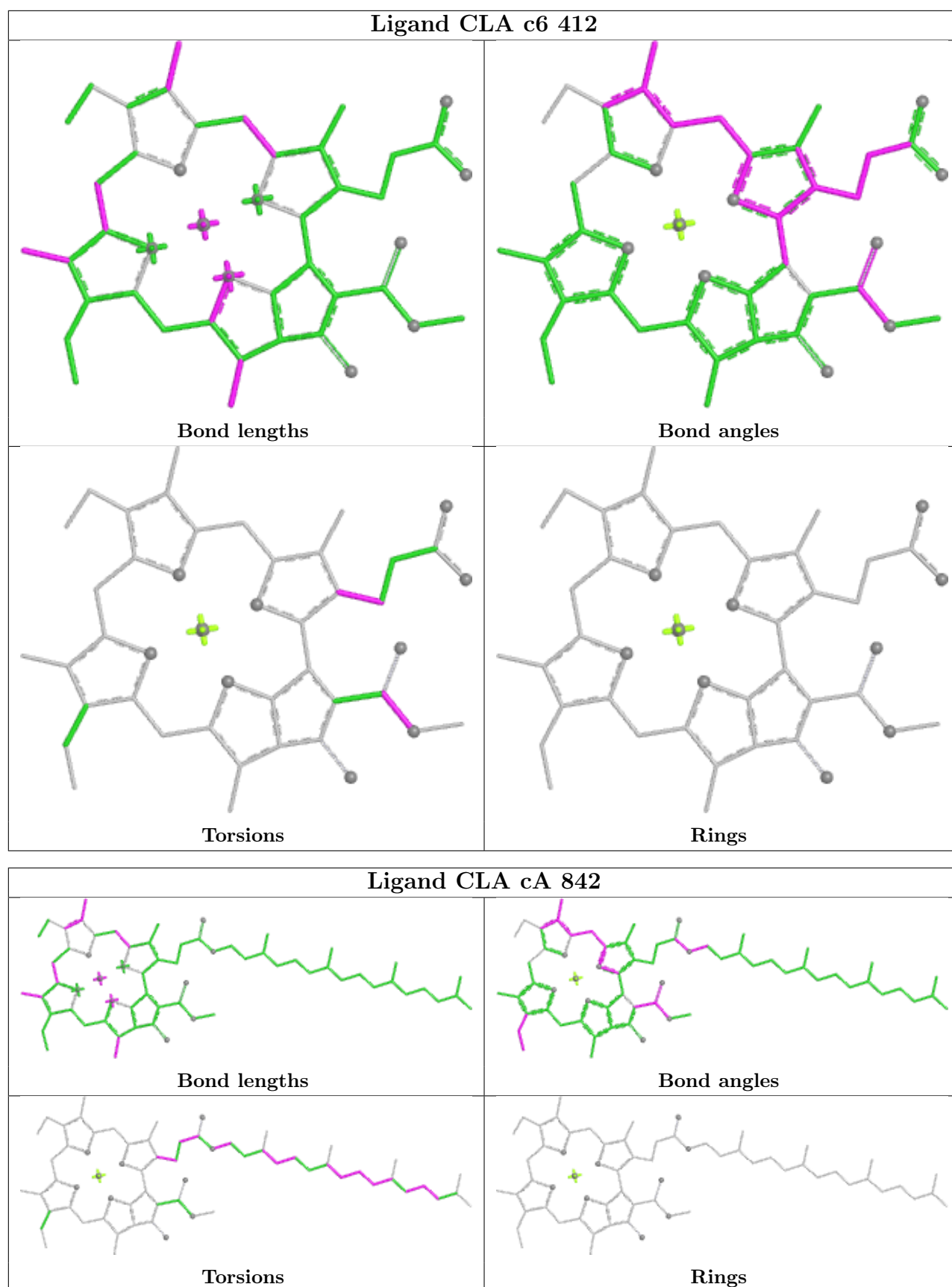


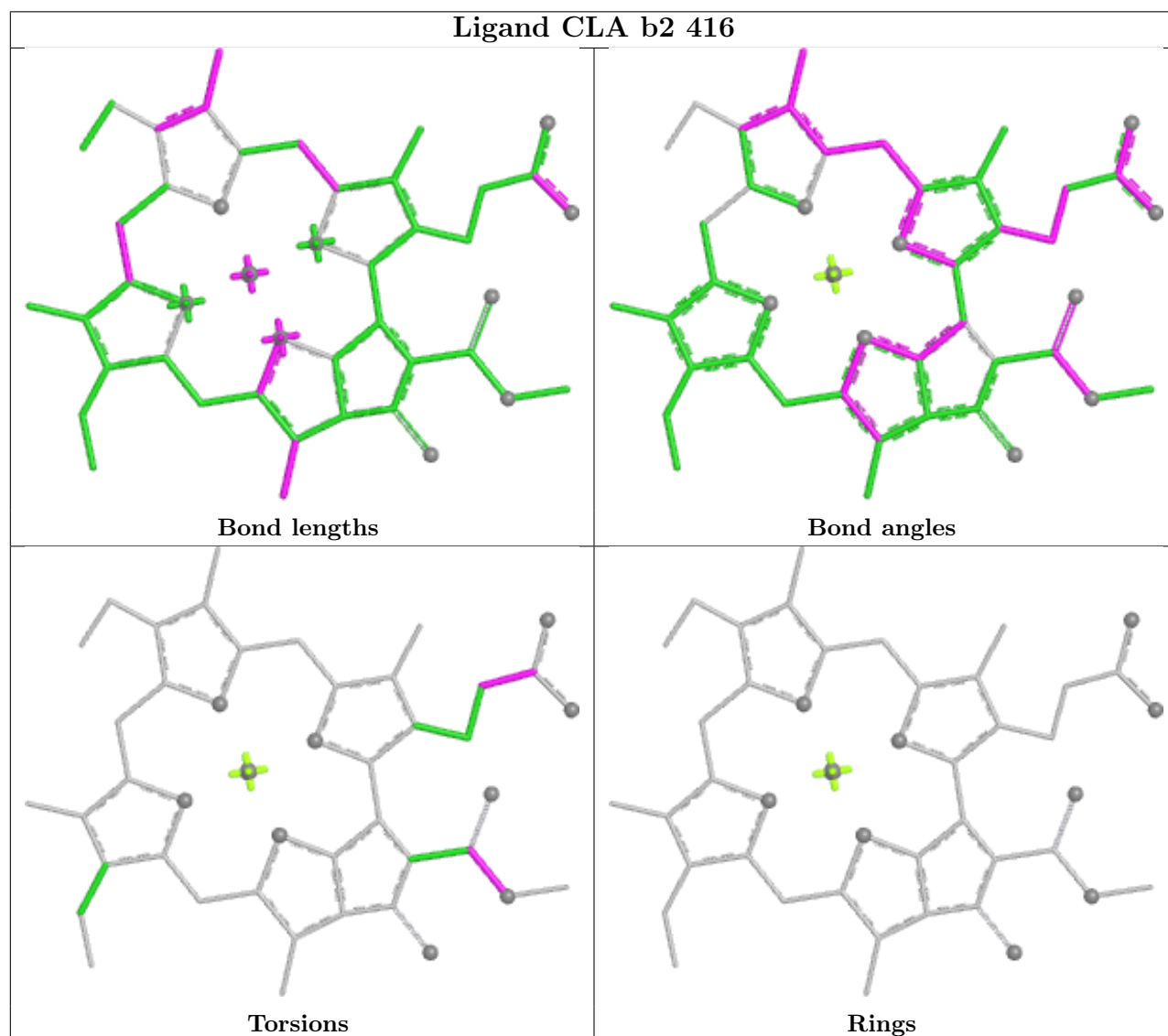
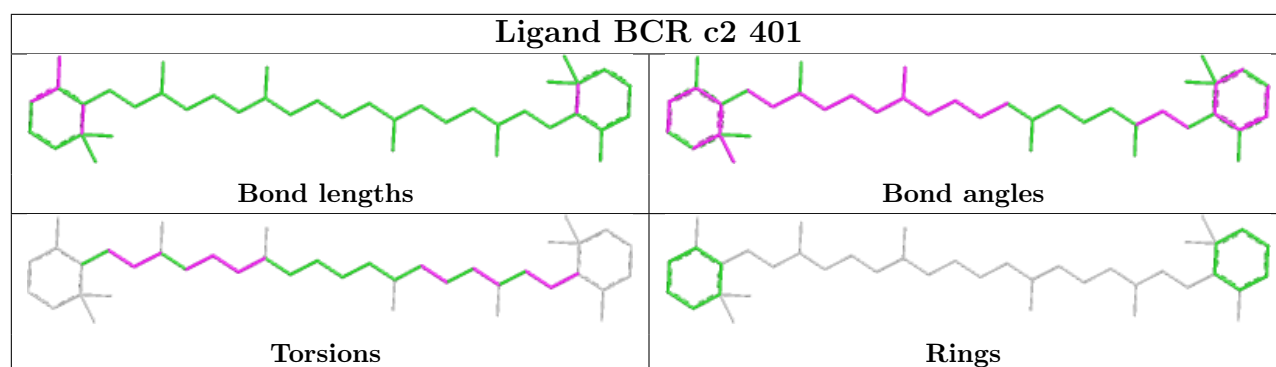
Ligand CLA aB 833**Ligand CLA aA 812**

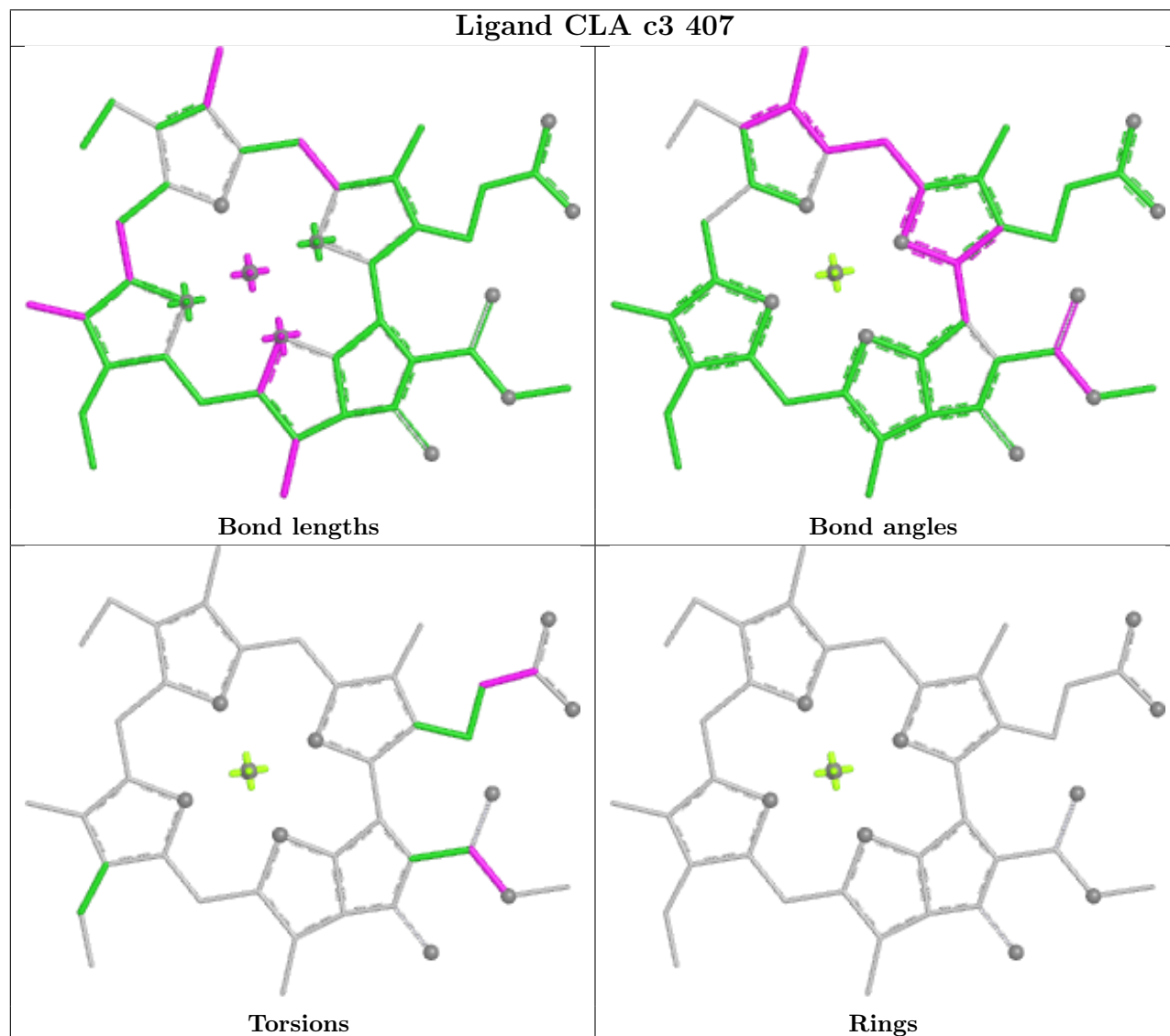
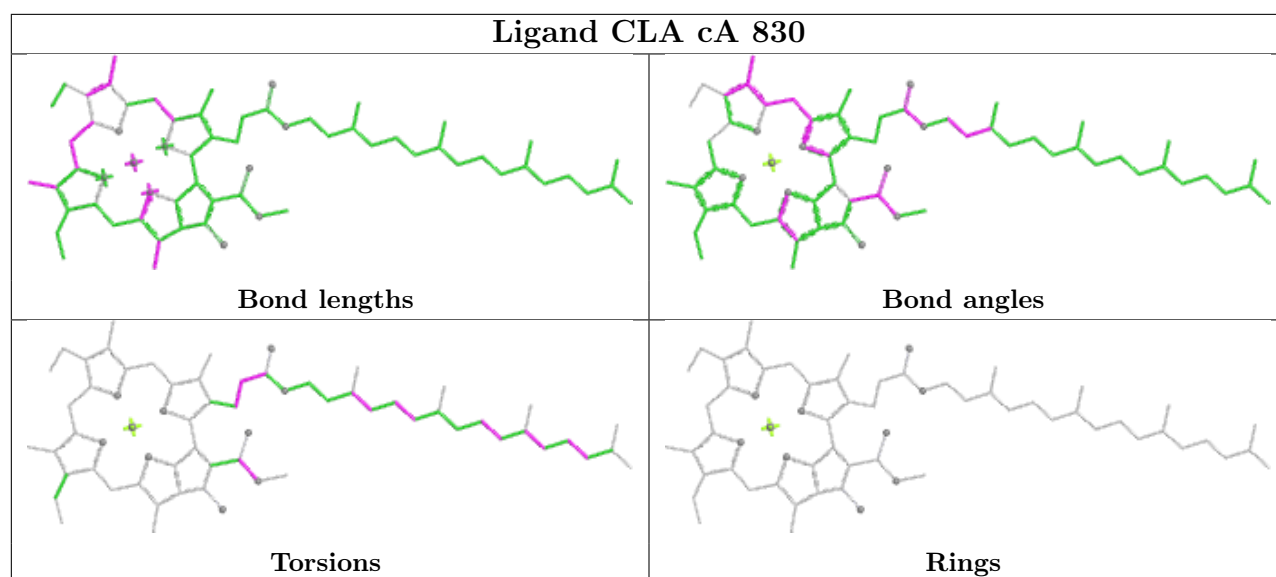


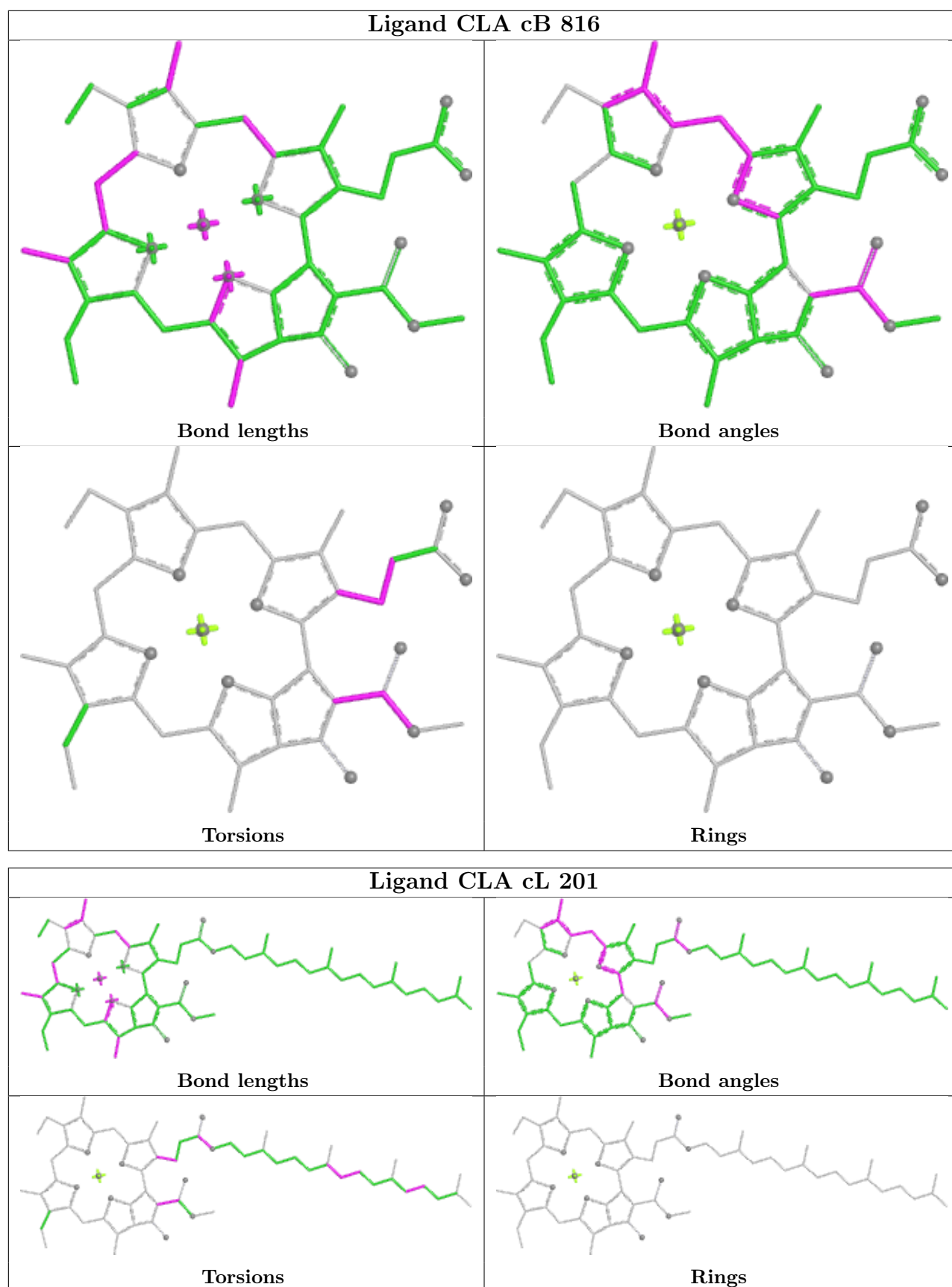
Ligand BCR c2 421	
	
Bond lengths	Bond angles
	
Torsions	Rings

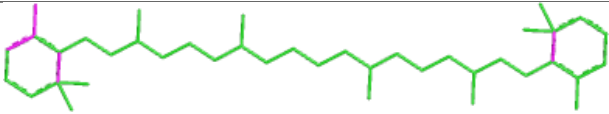
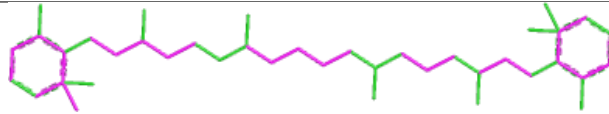
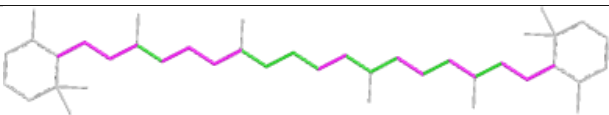
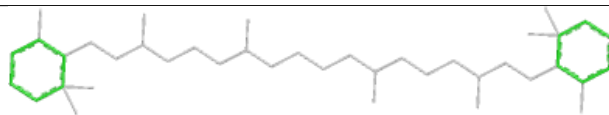
Ligand BCR bL 205	
	
Bond lengths	Bond angles
	
Torsions	Rings


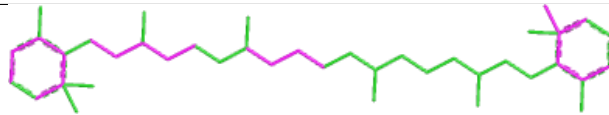
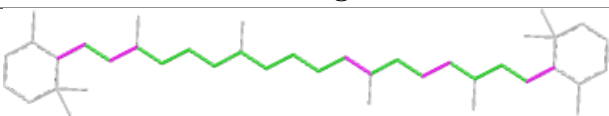
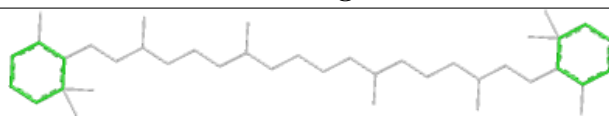


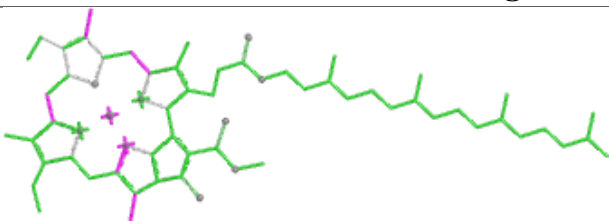
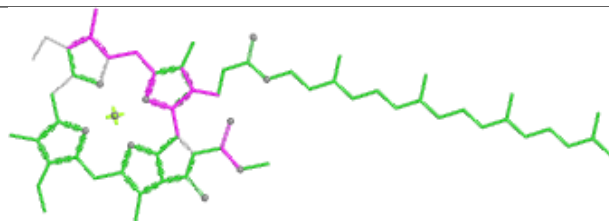
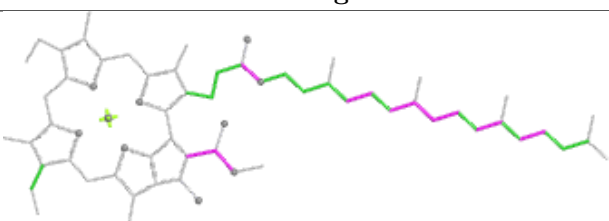
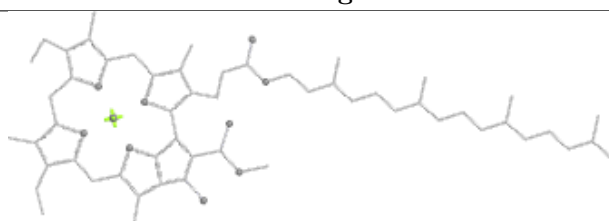




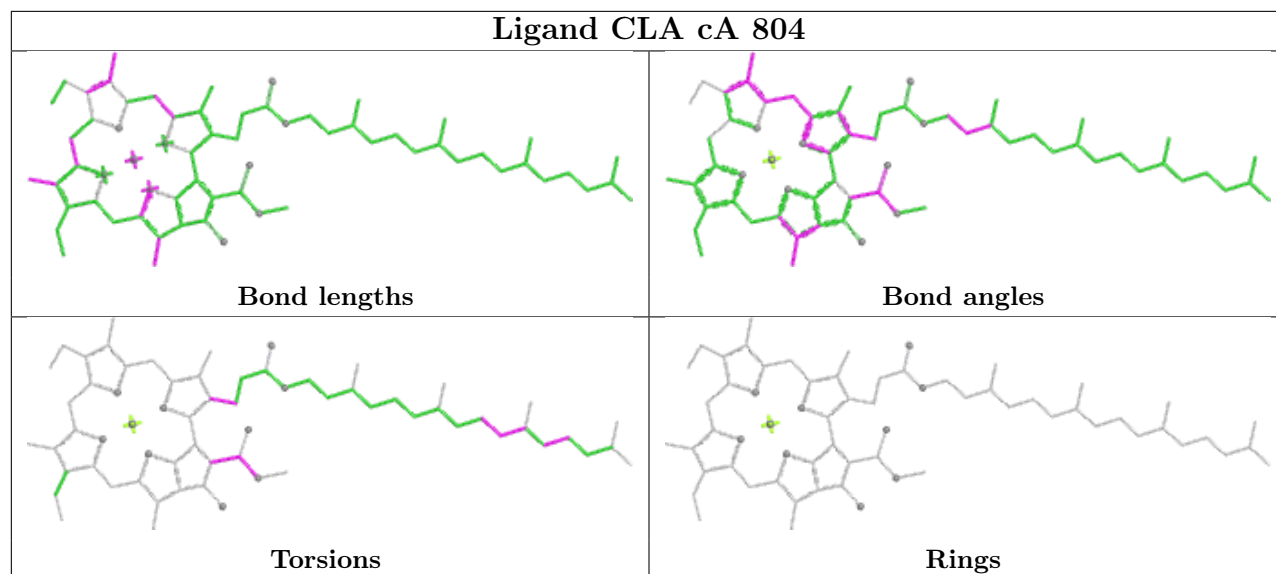


Ligand BCR a6 402	
	
Bond lengths	Bond angles
	
Torsions	Rings

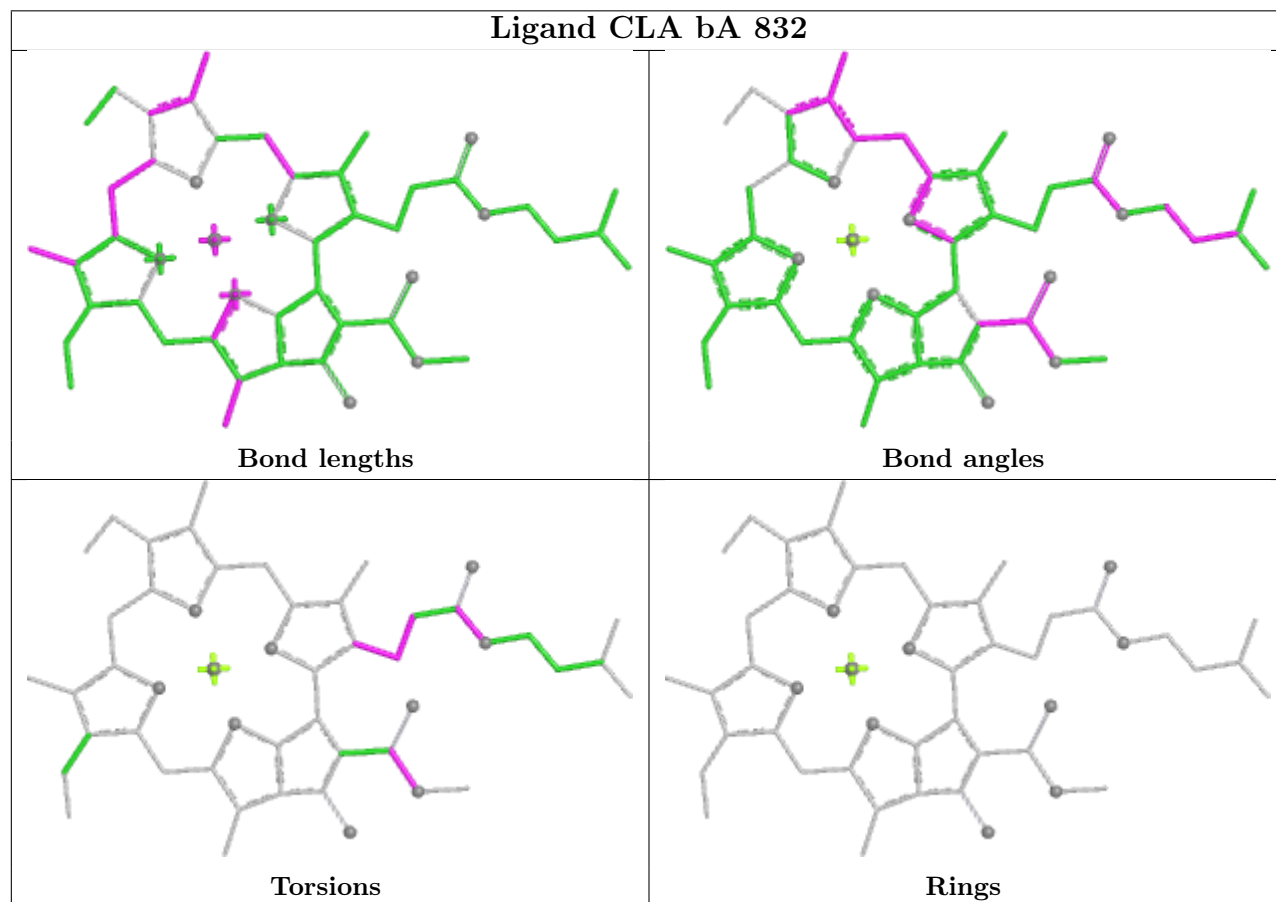
Ligand BCR c1 418	
	
Bond lengths	Bond angles
	
Torsions	Rings

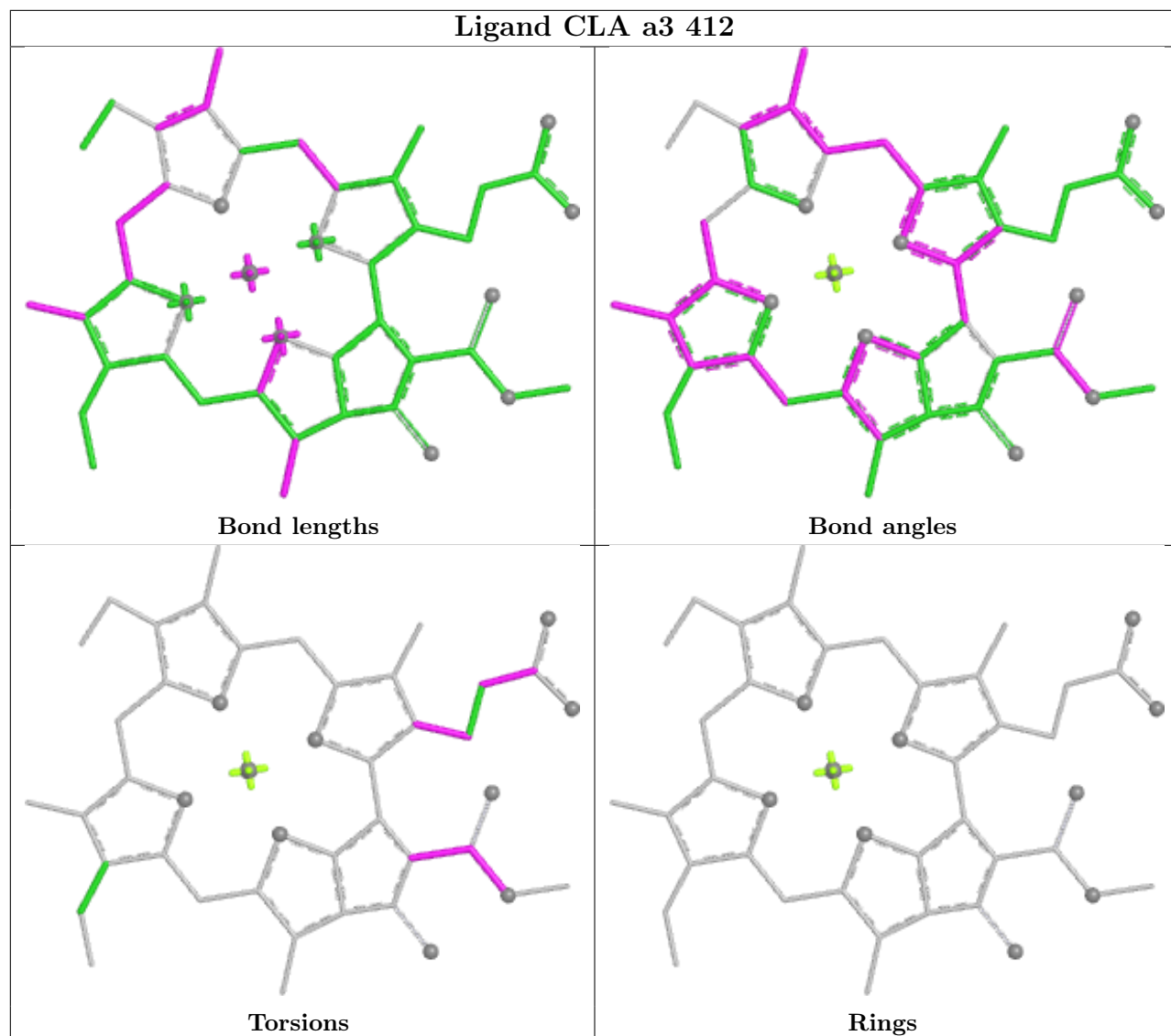
Ligand CLA a2 403	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA cA 804

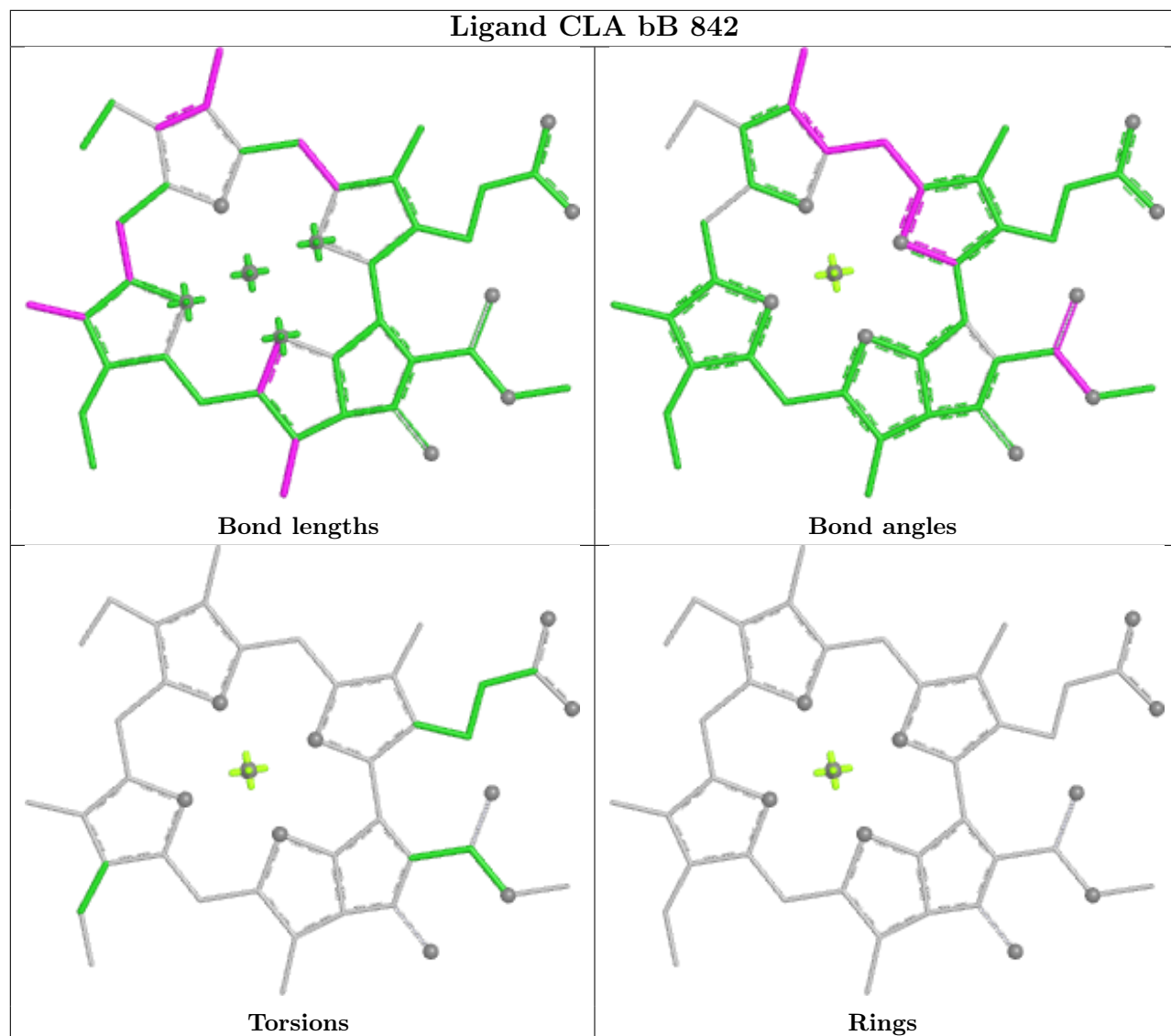


Ligand CLA bA 832

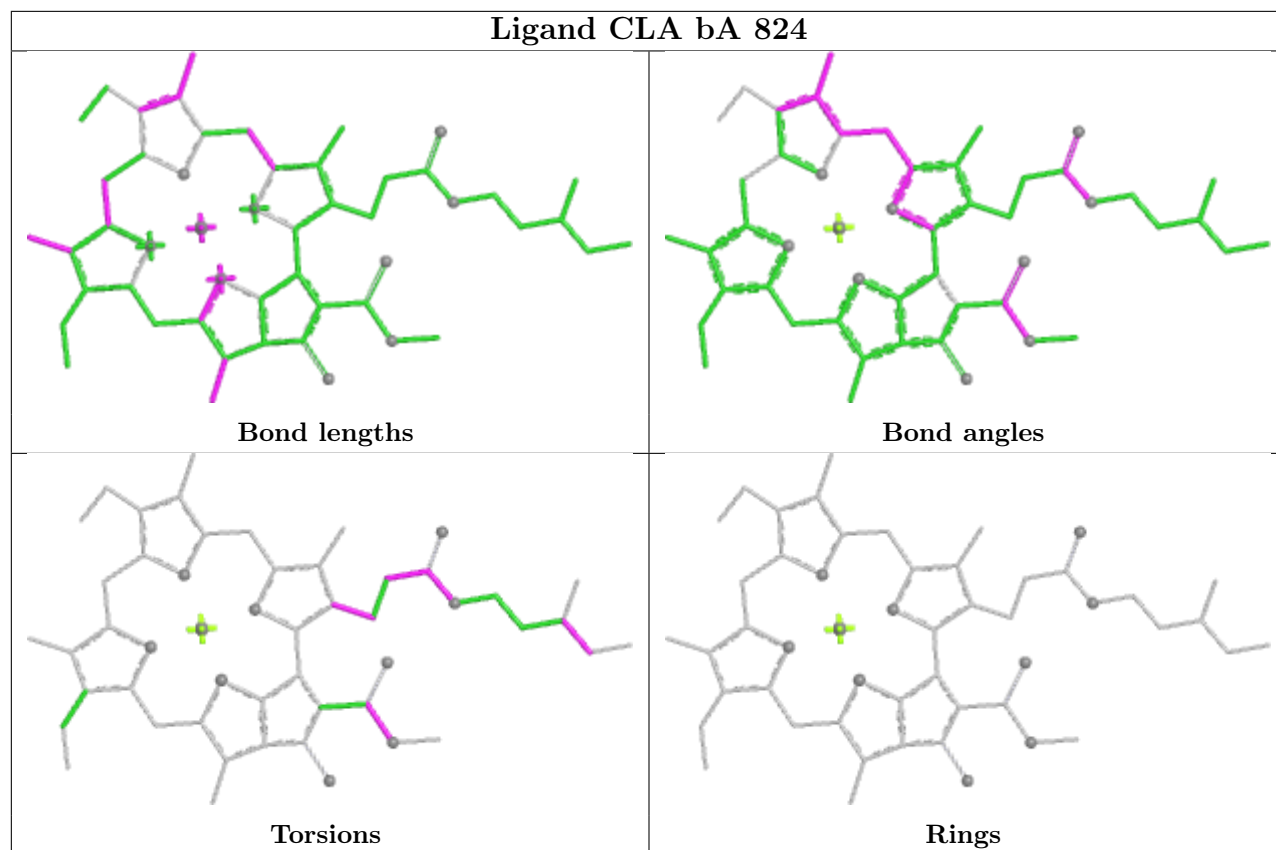




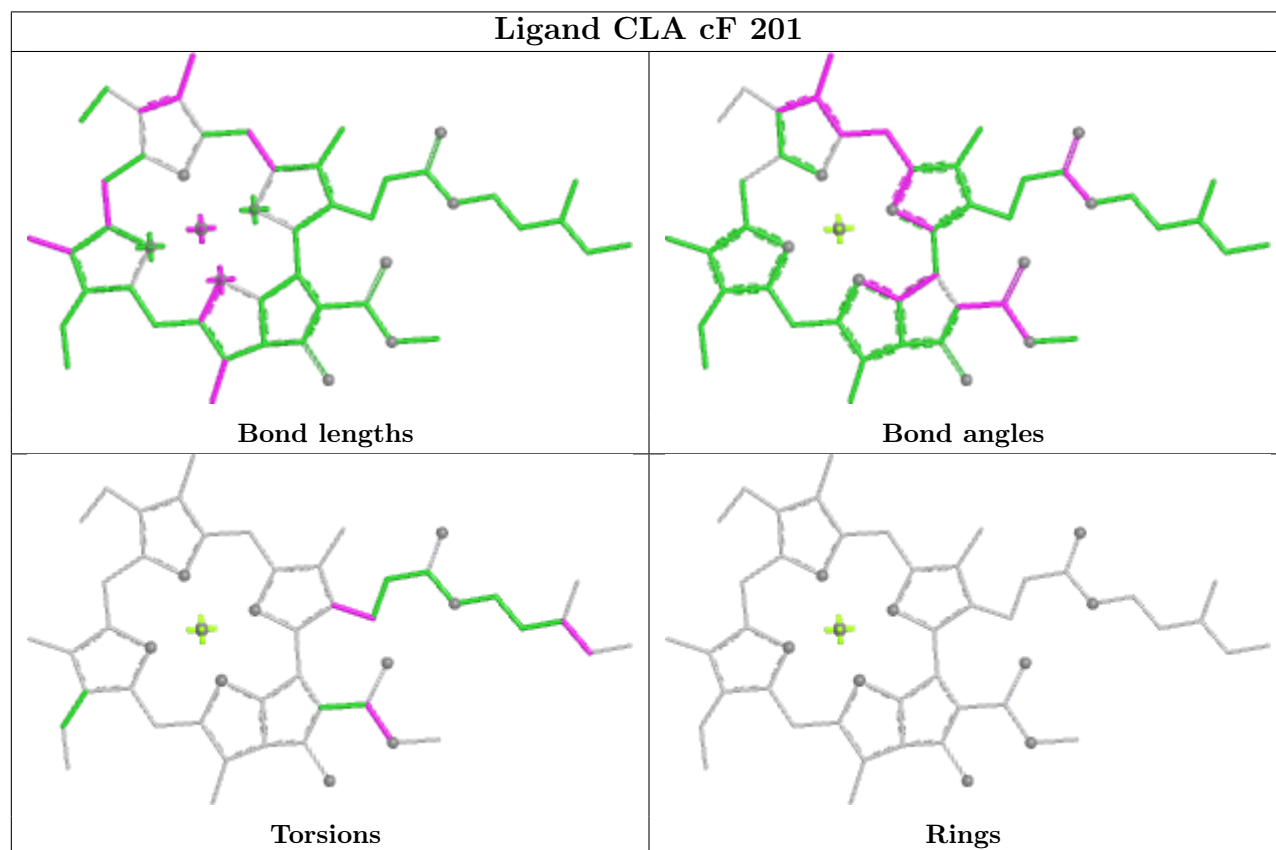
Ligand CLA bB 842

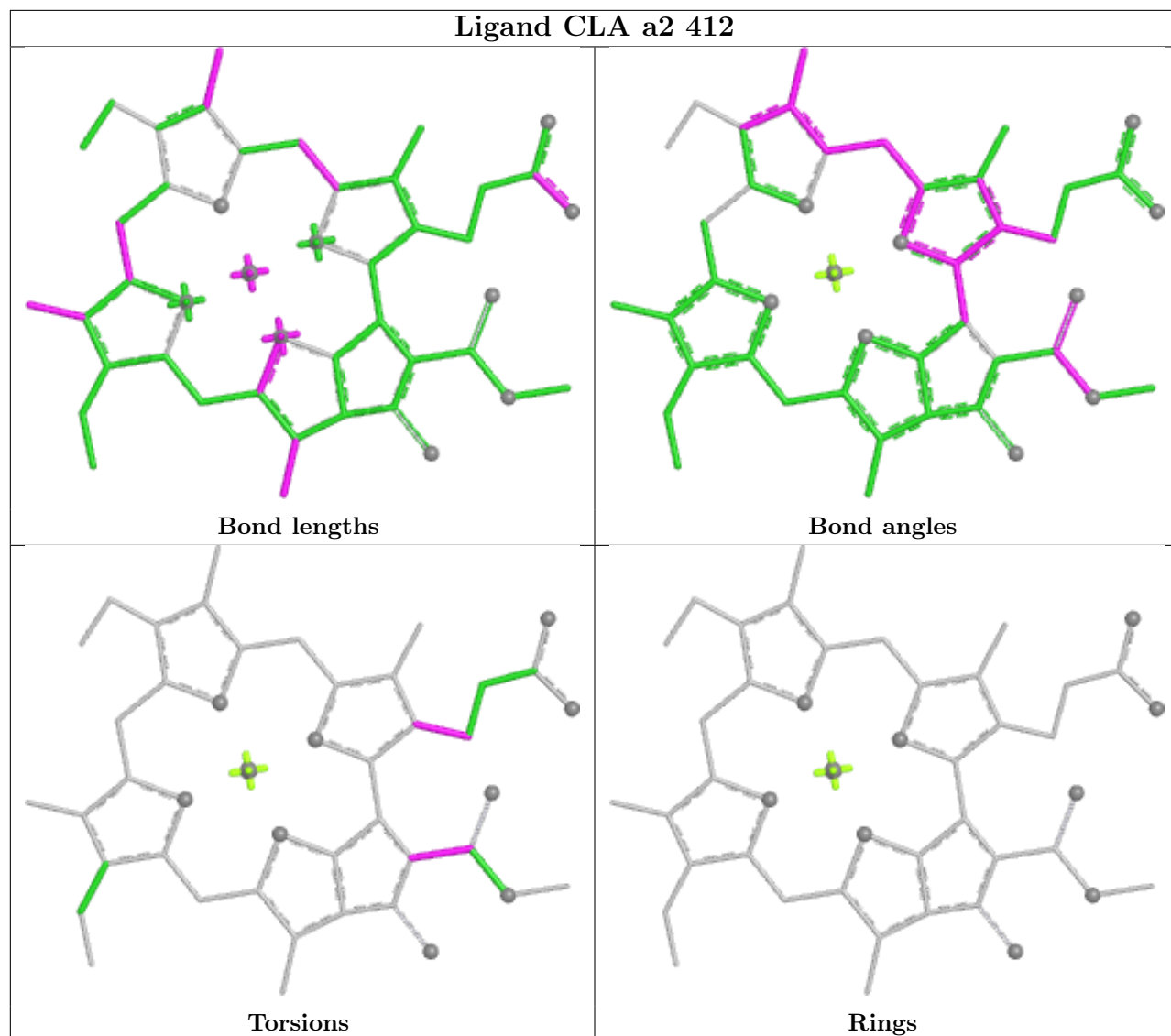


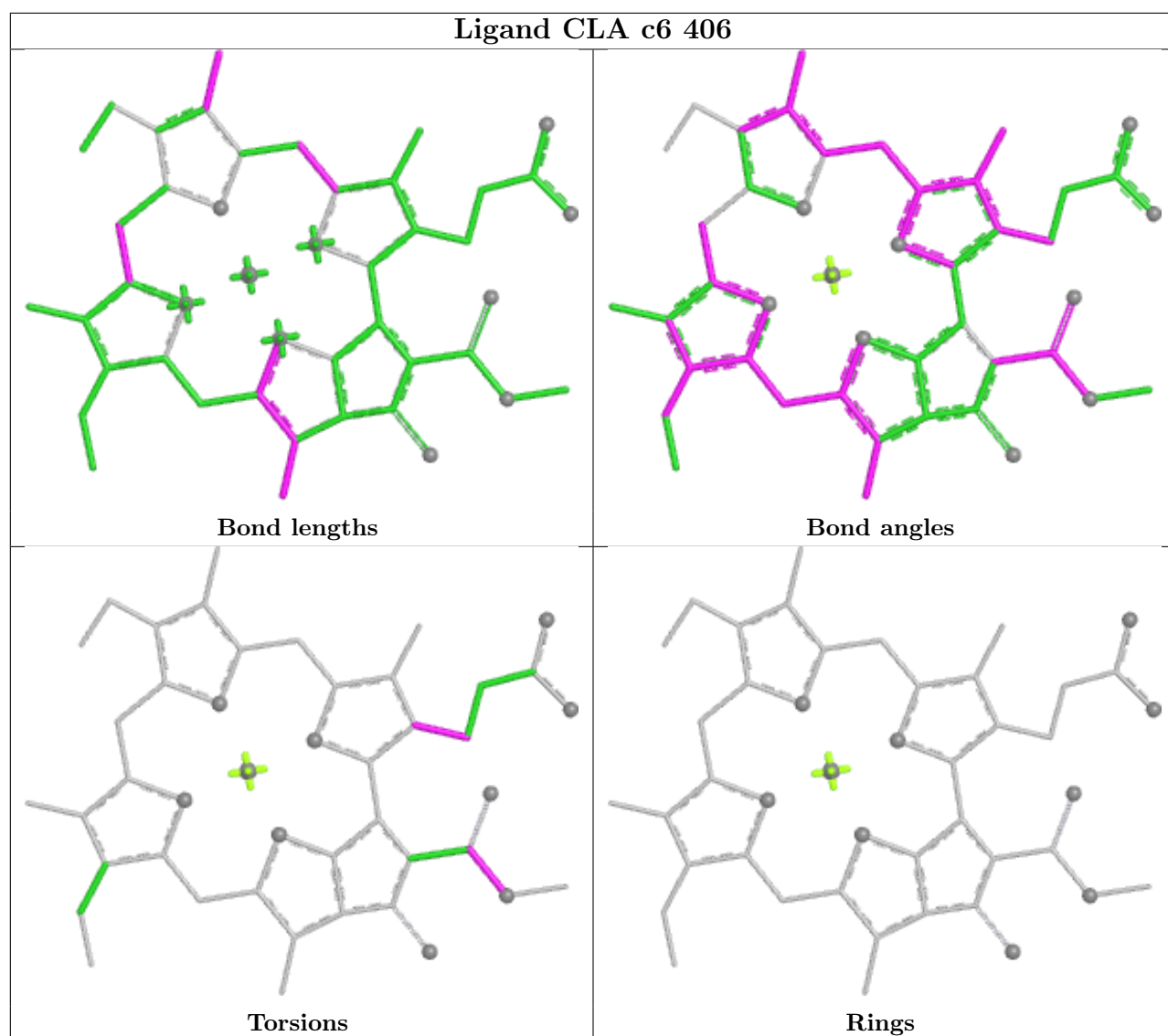
Ligand CLA bA 824

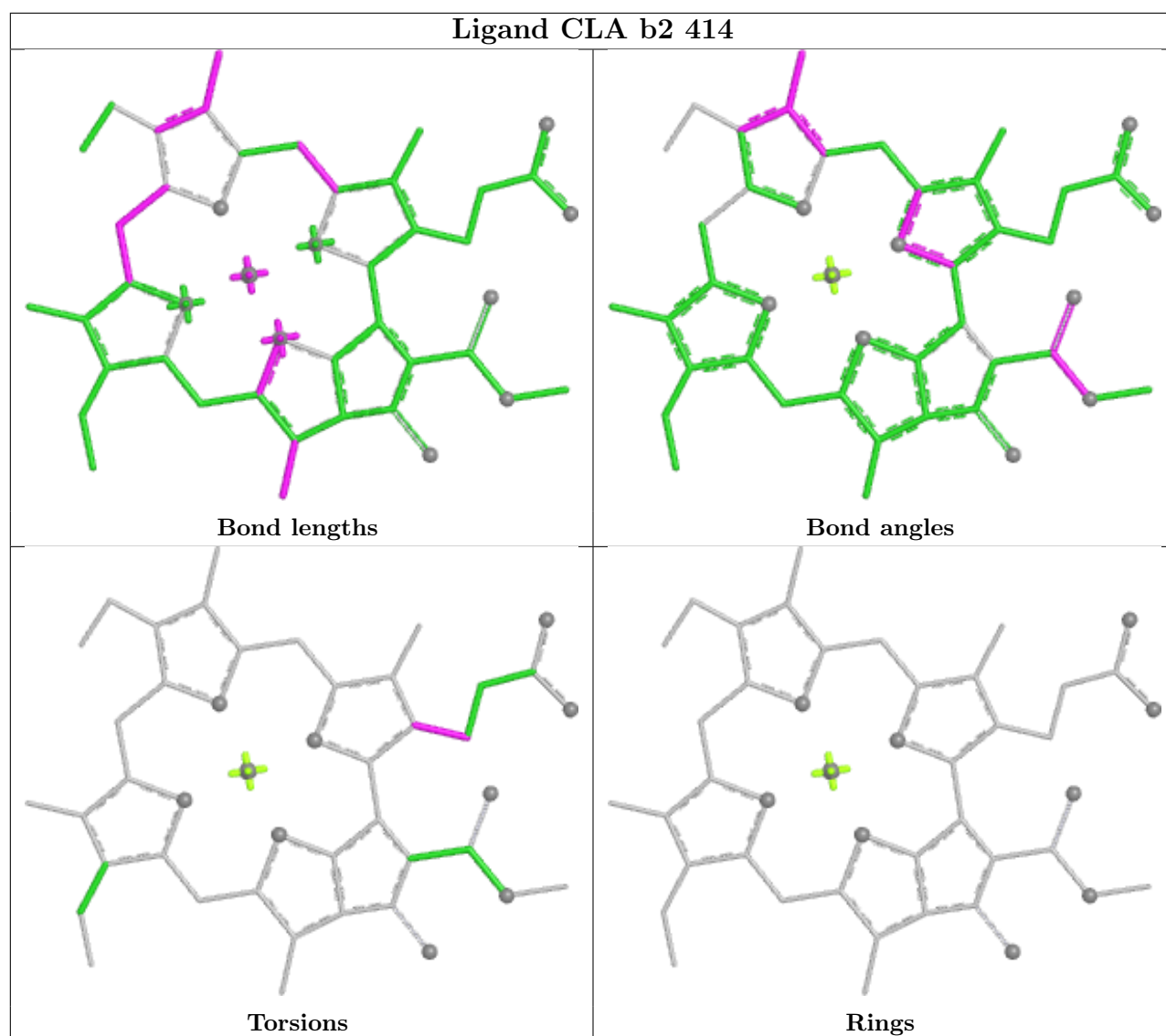


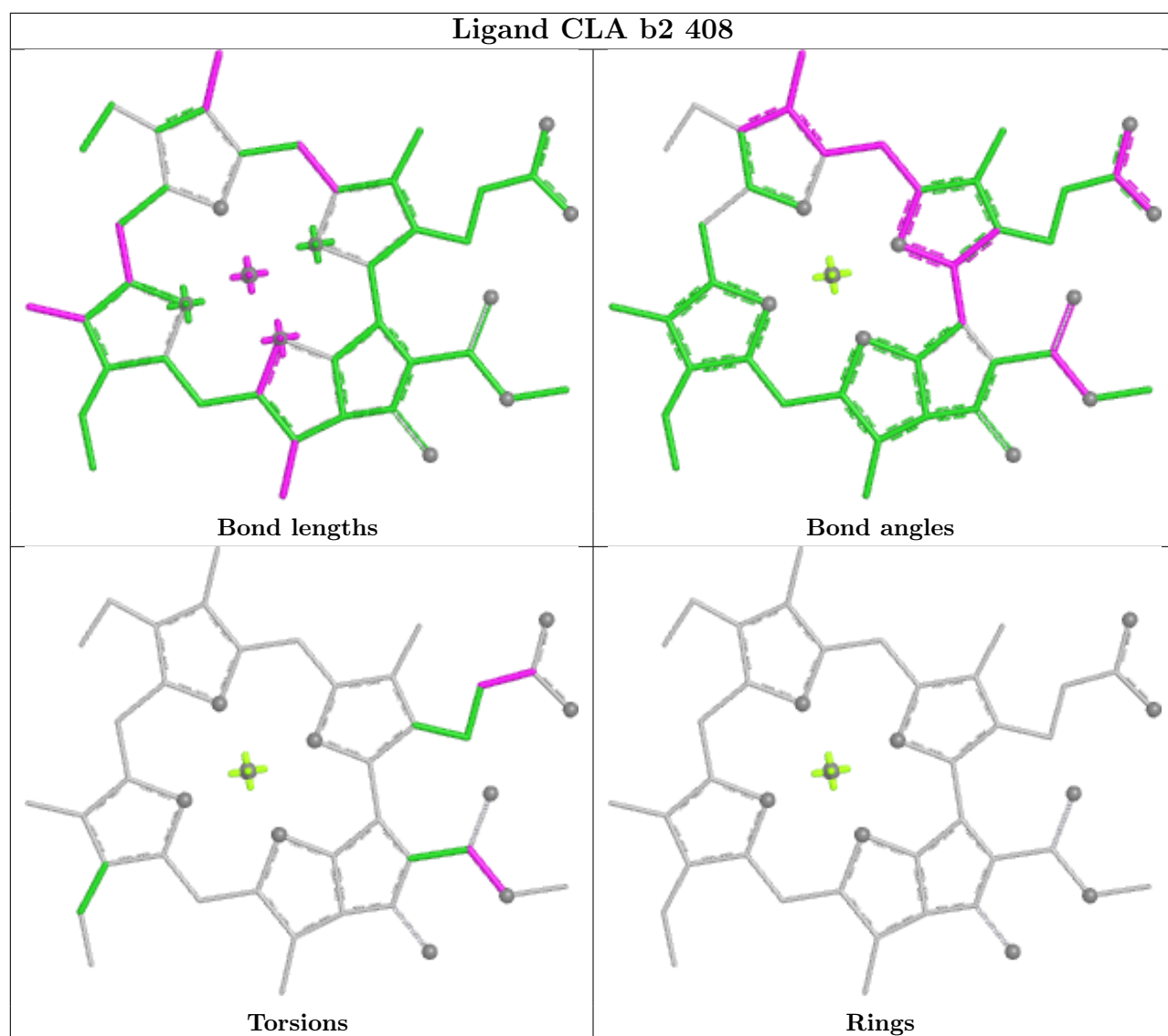
Ligand CLA cF 201

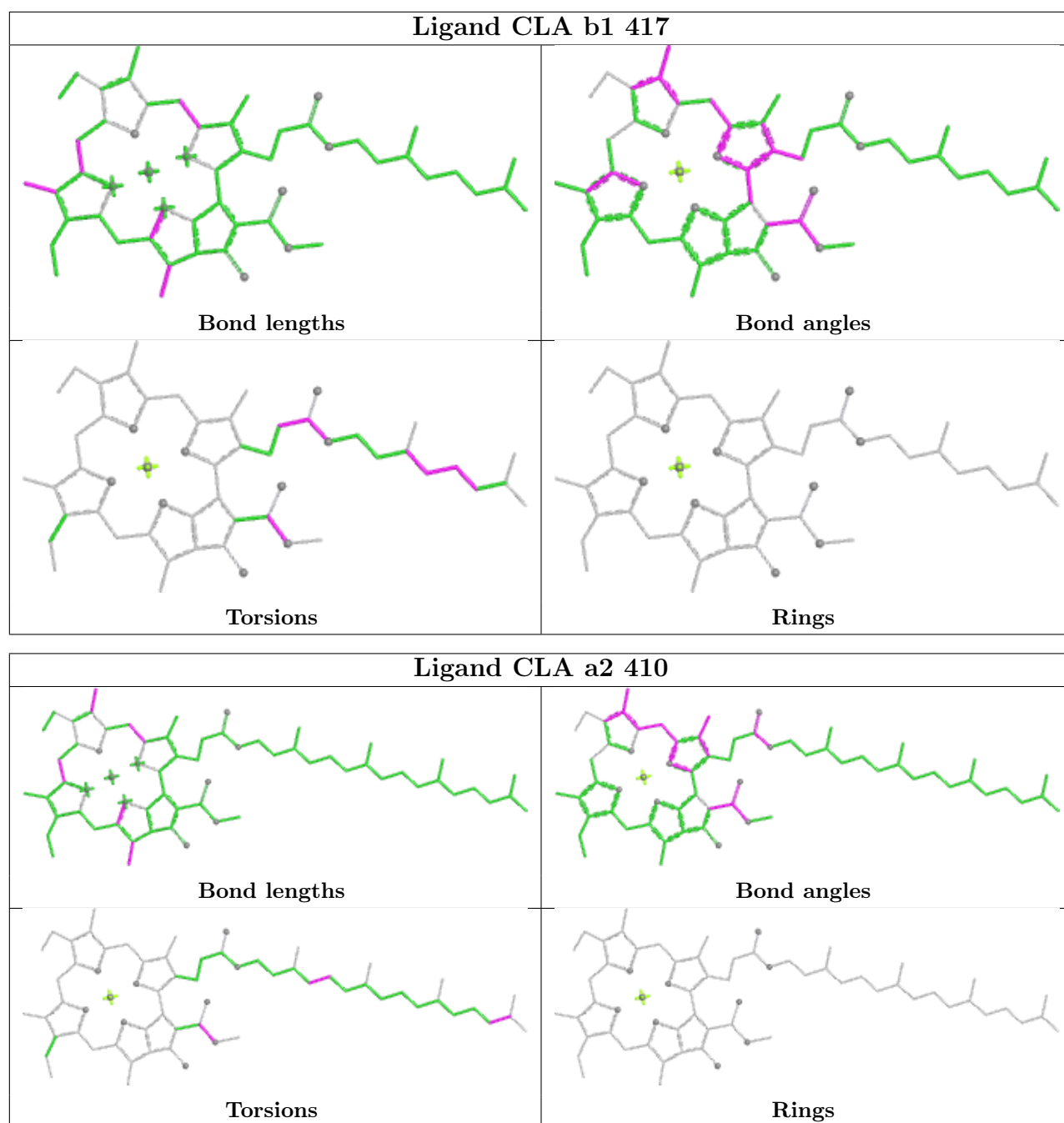


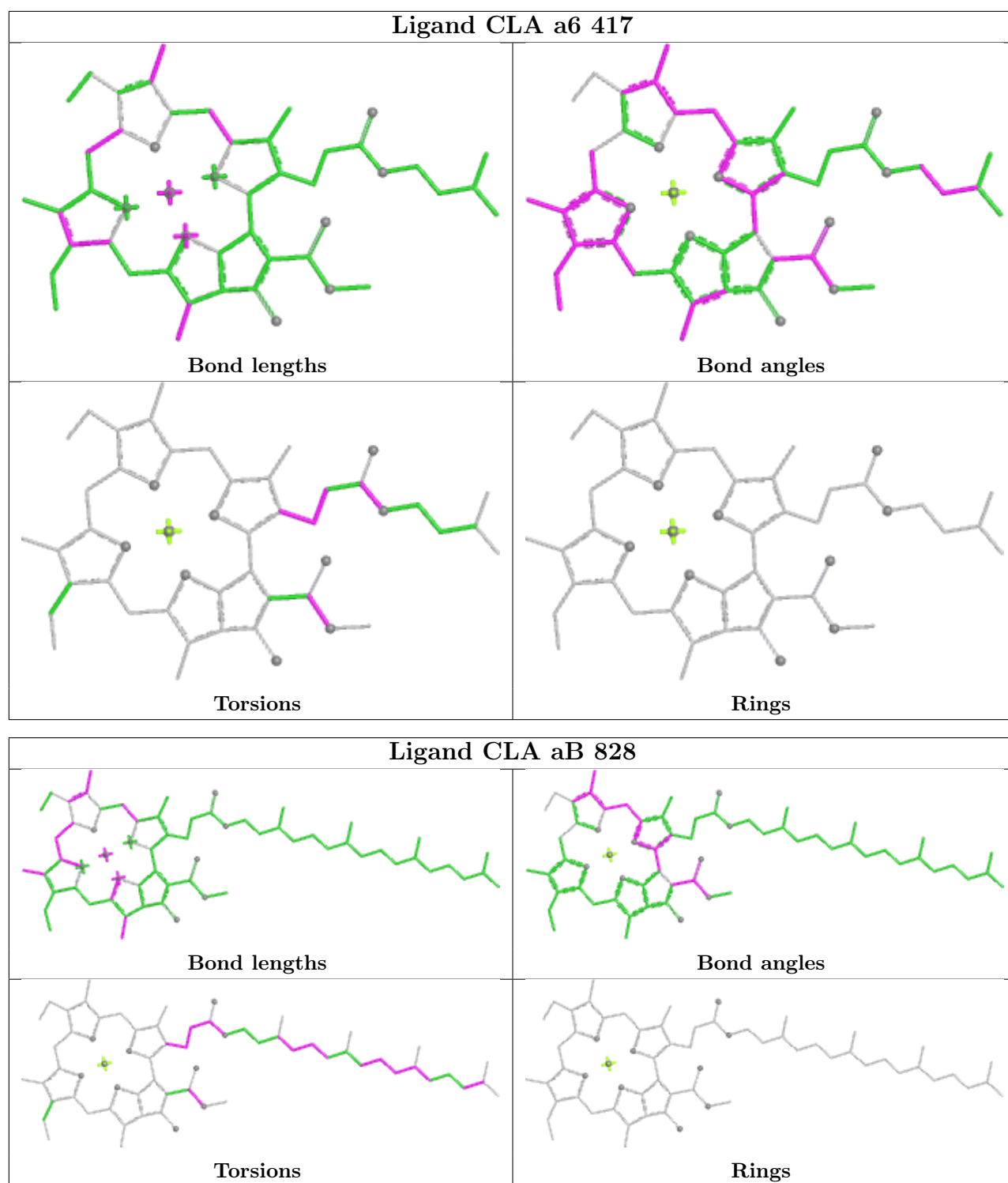


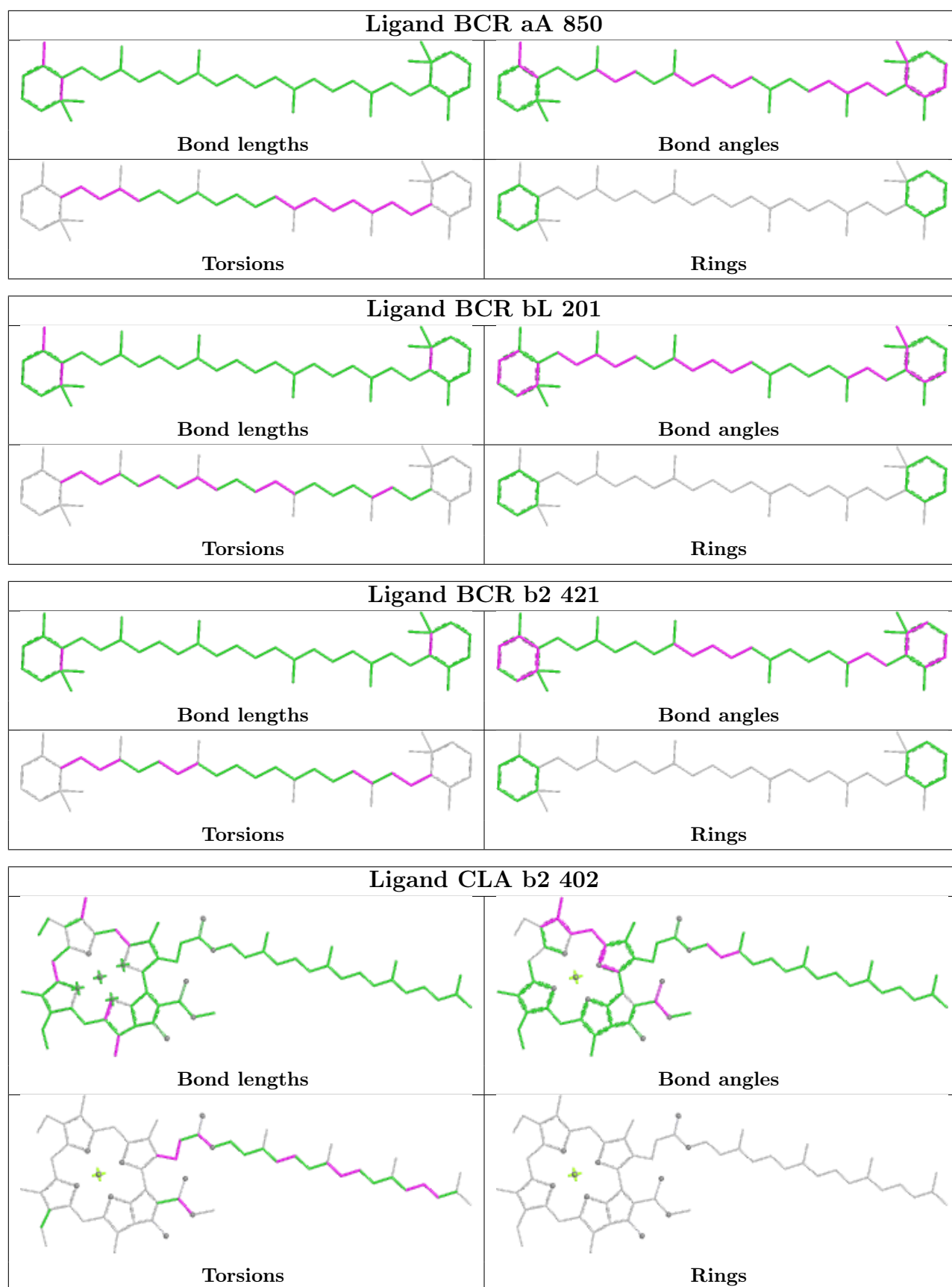


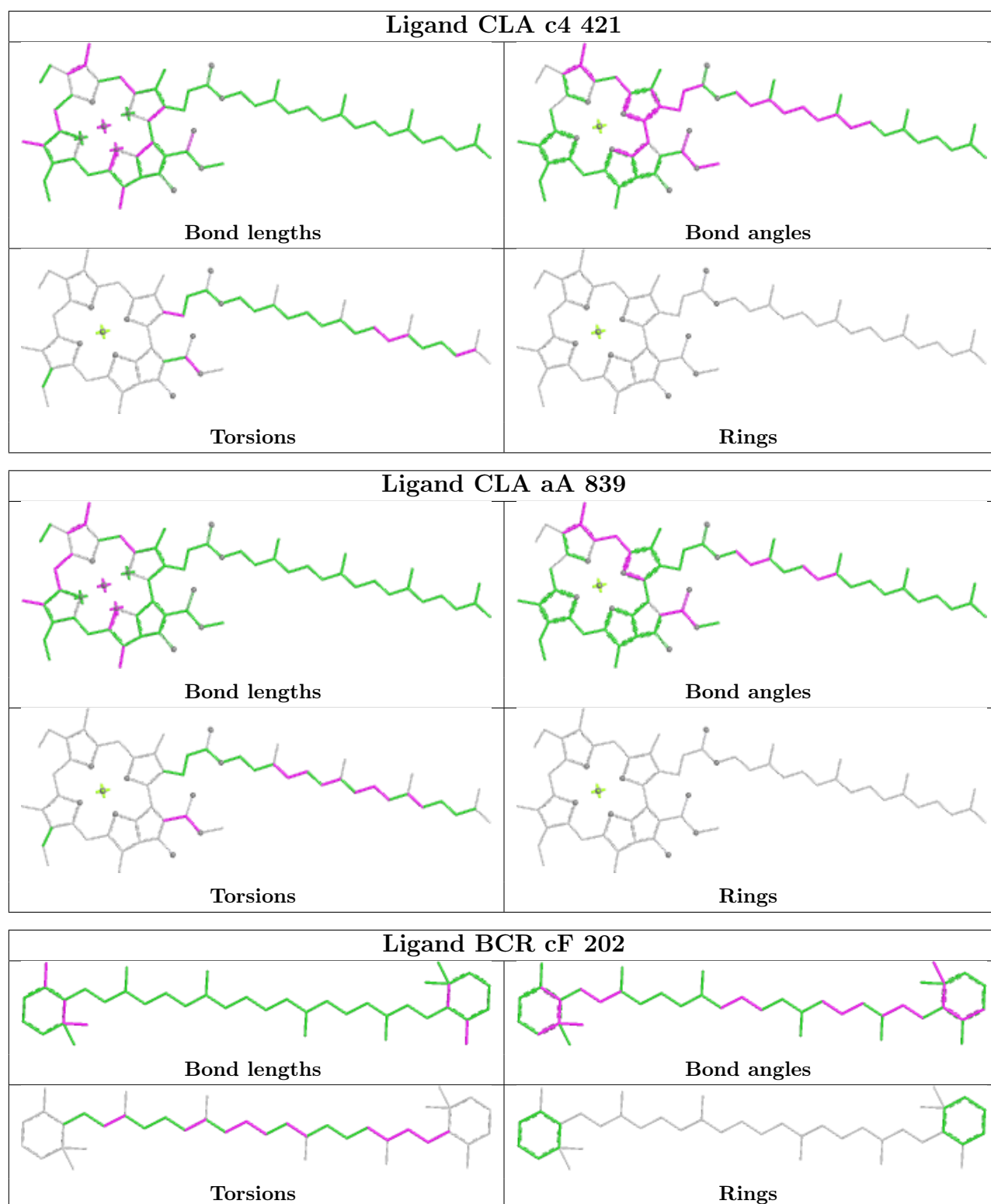


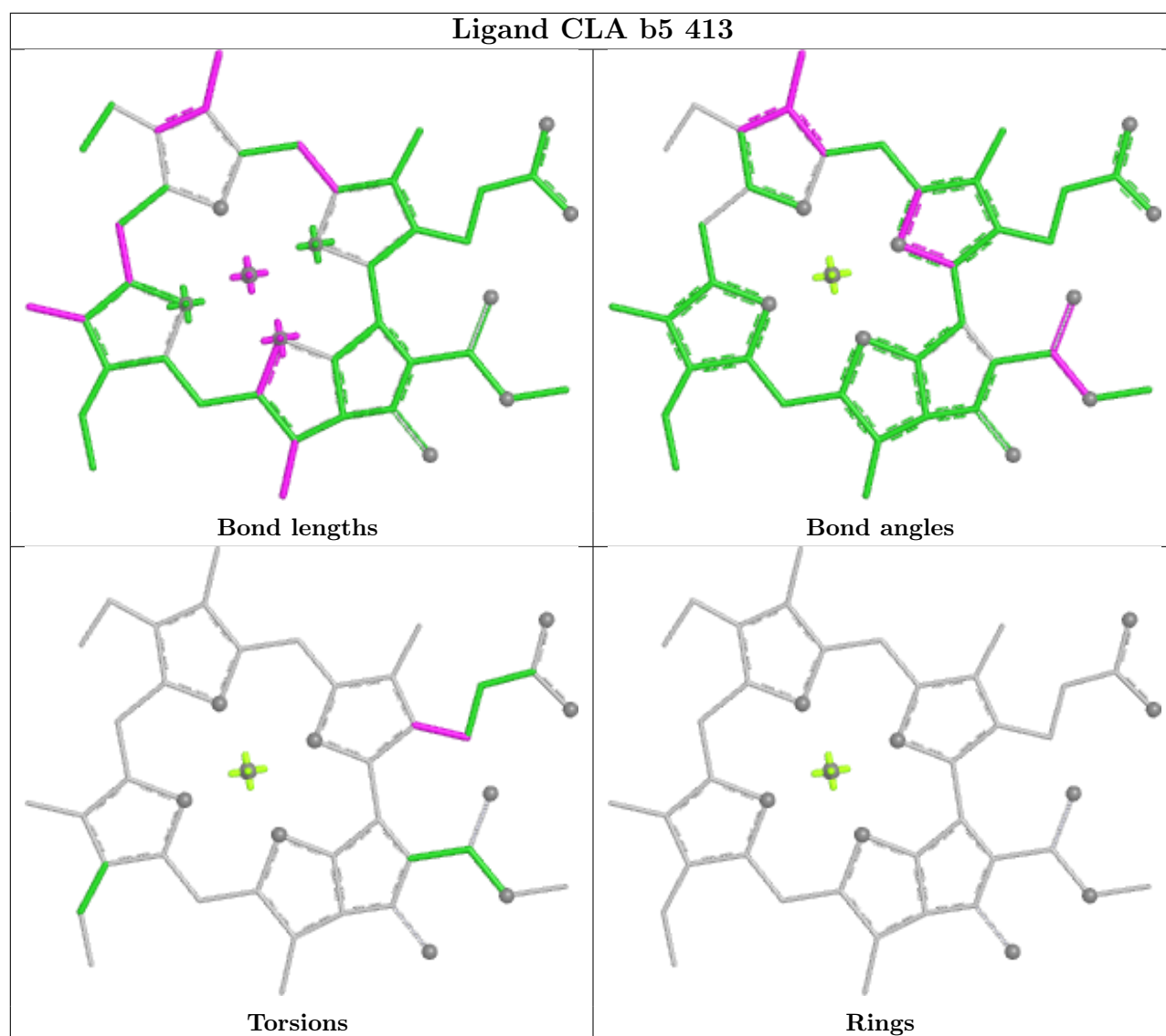


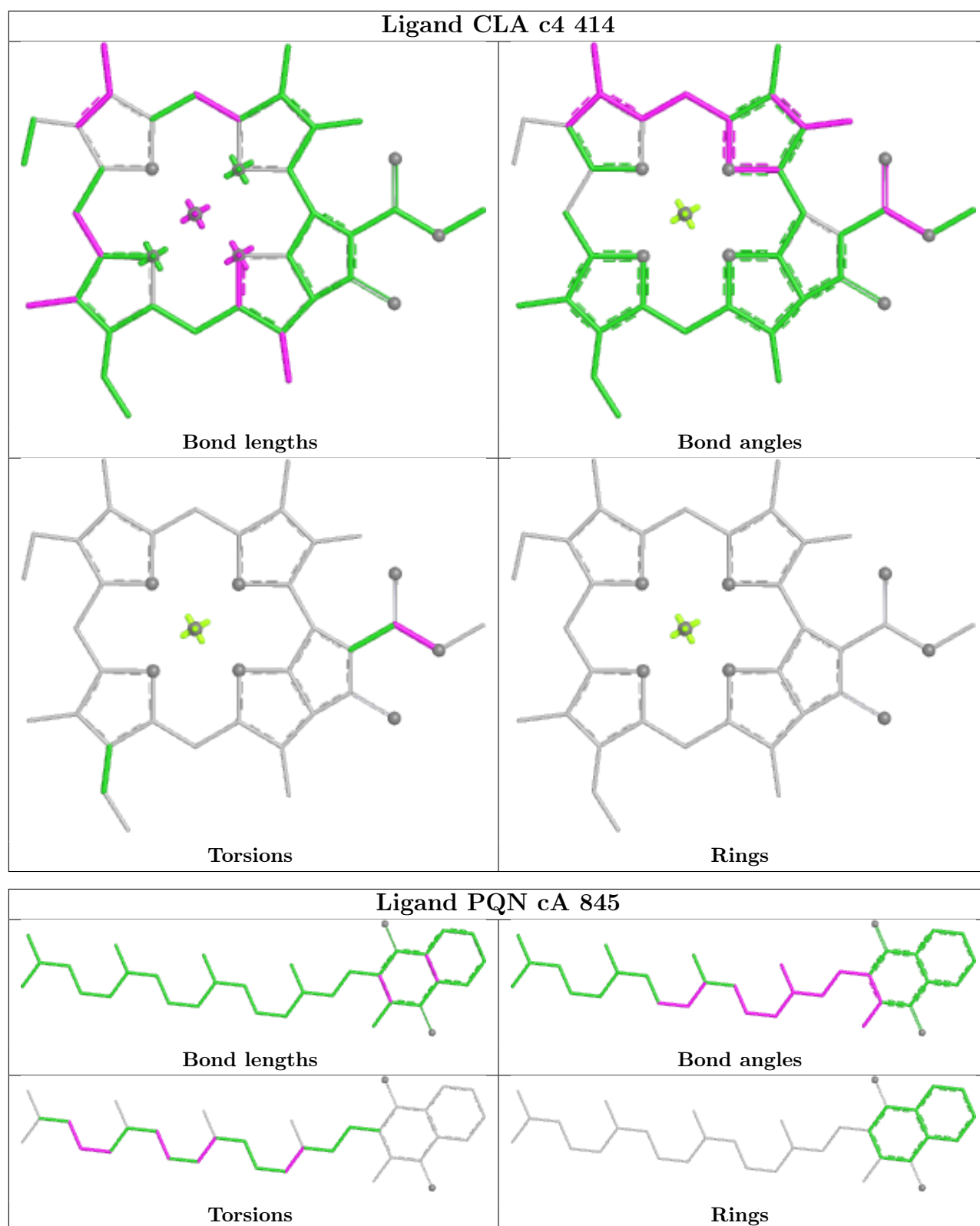


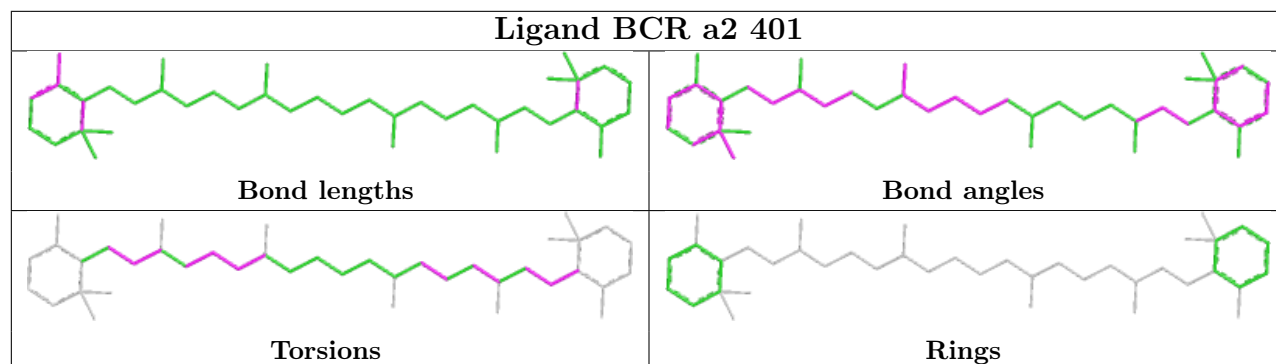
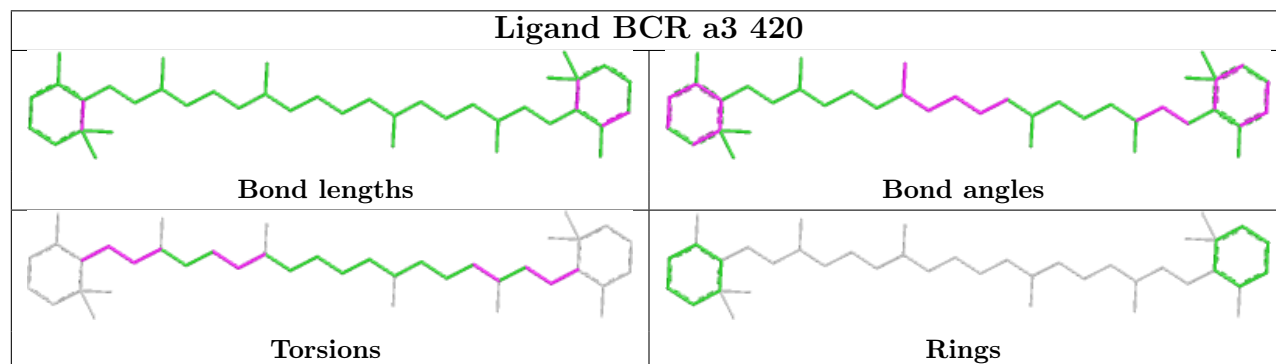
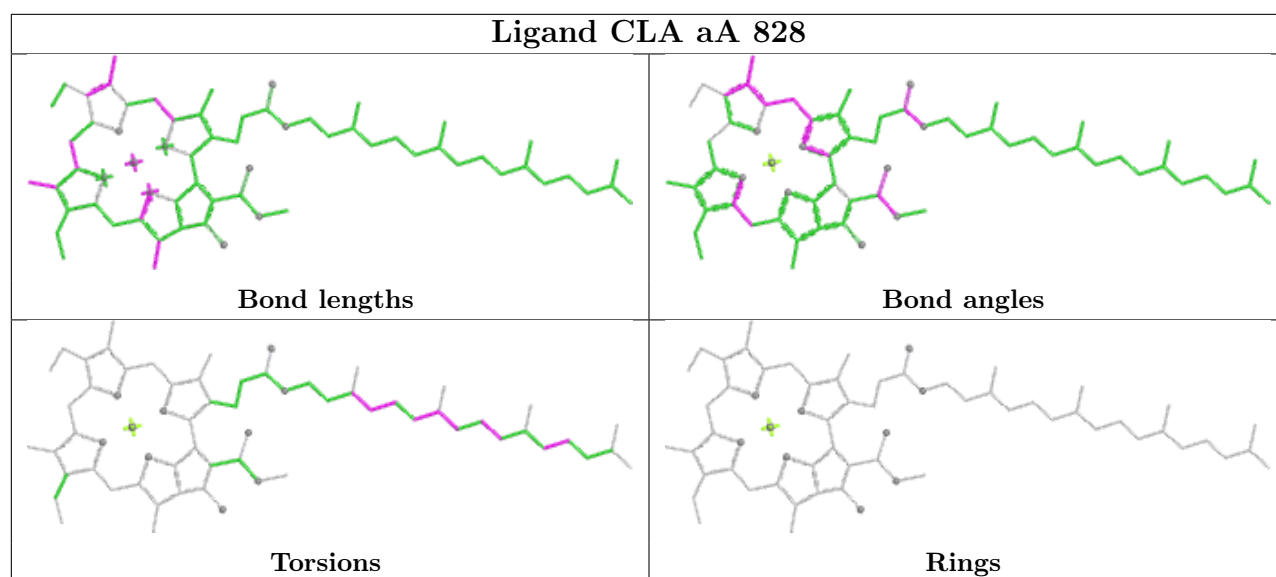




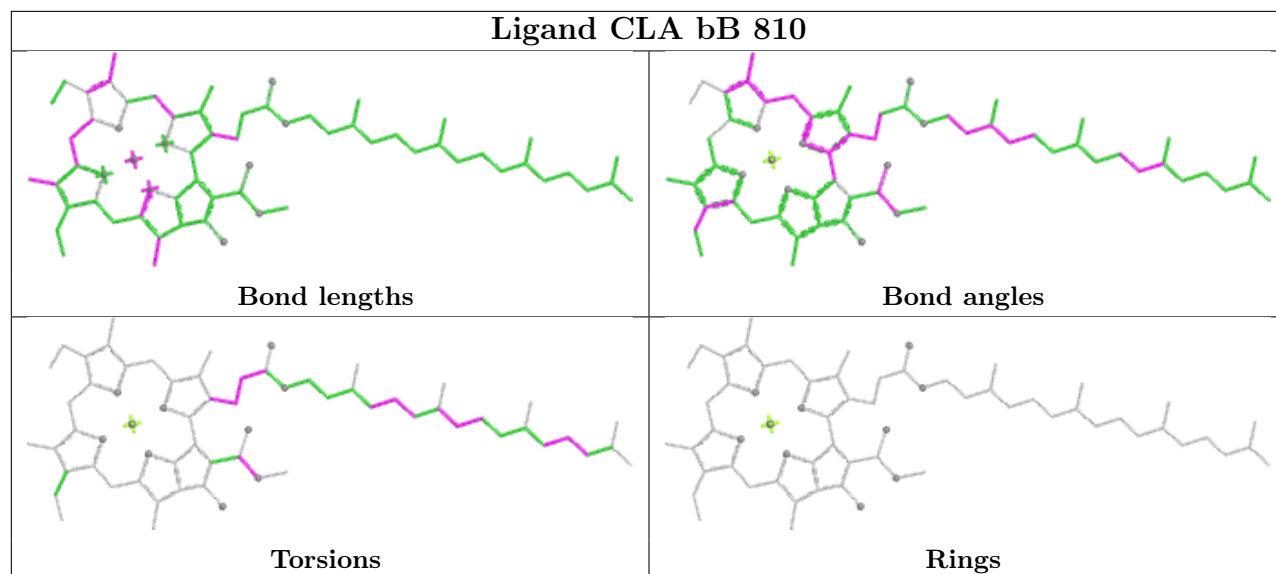




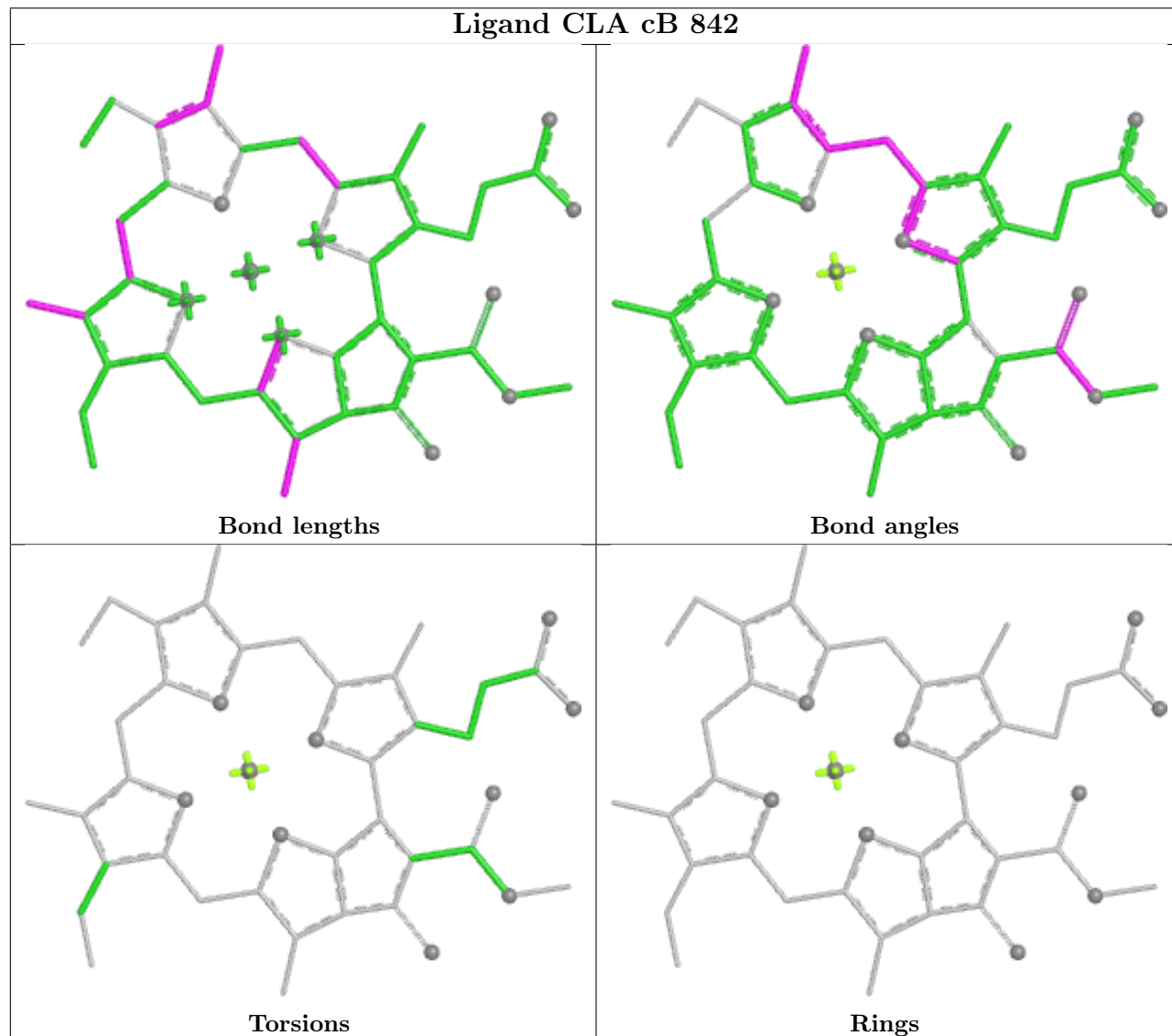


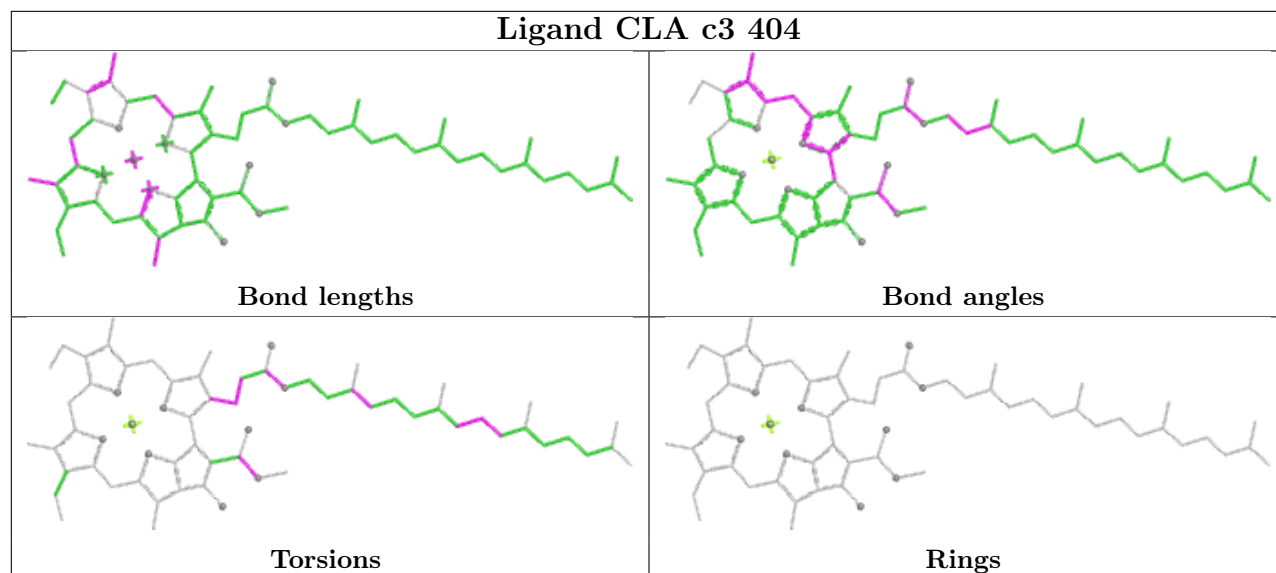
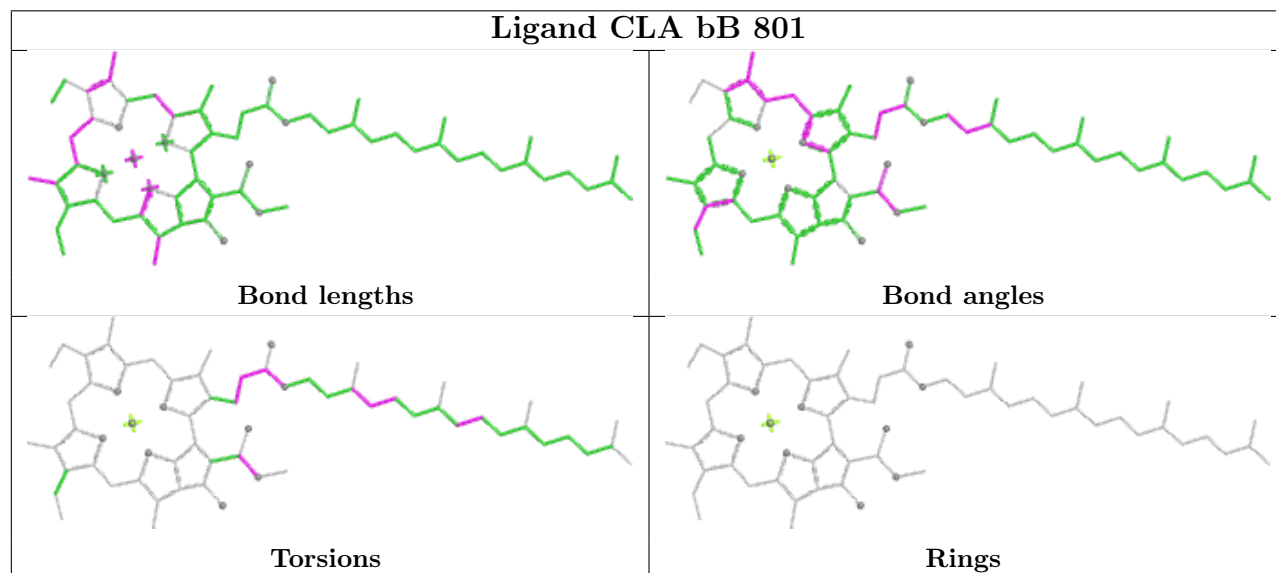
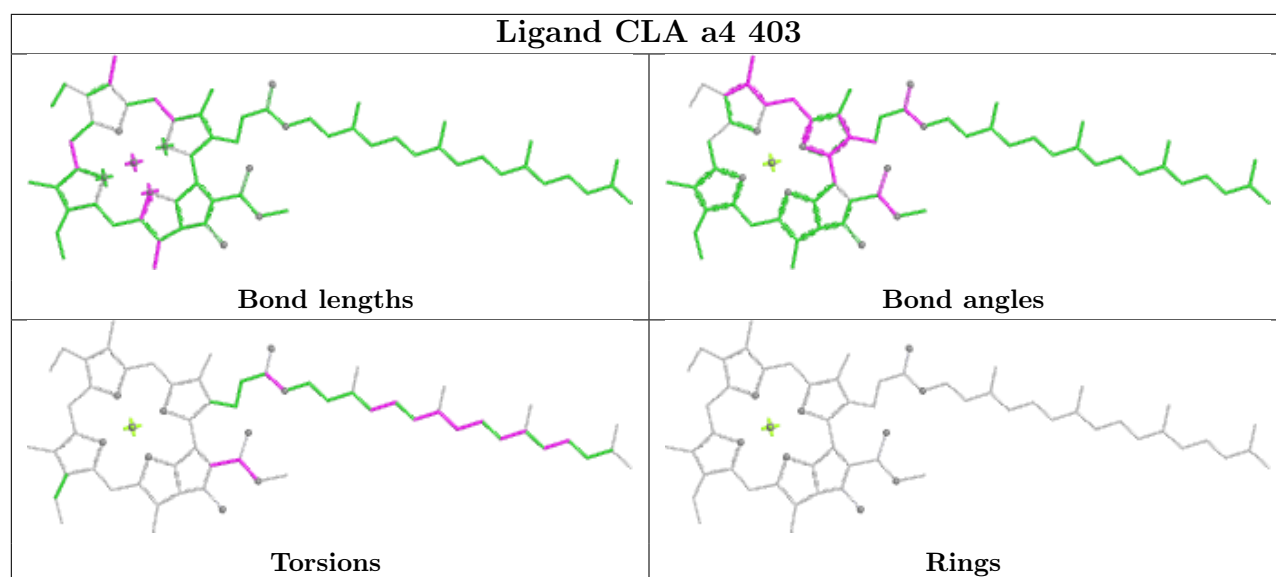


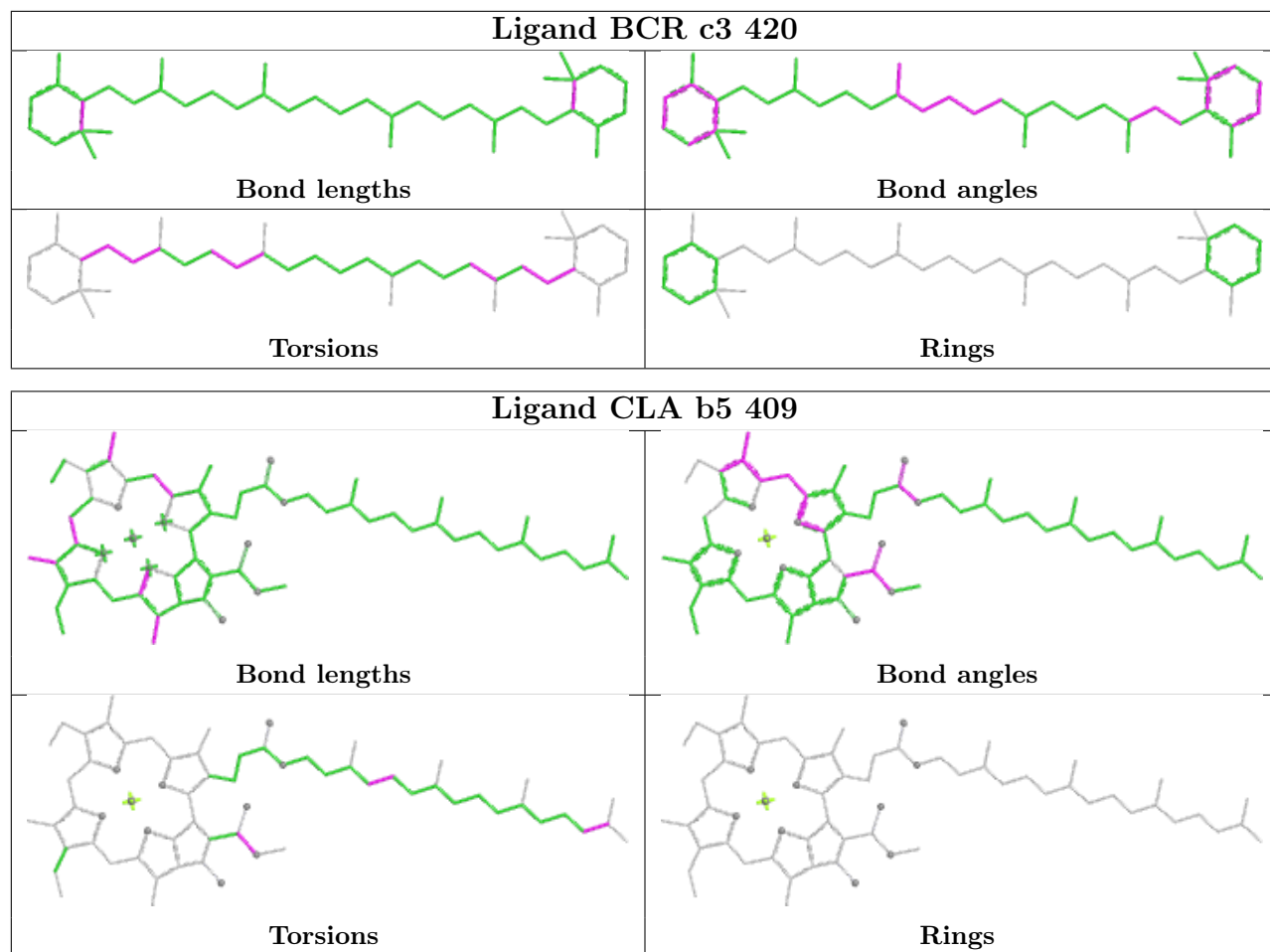
Ligand CLA bB 810

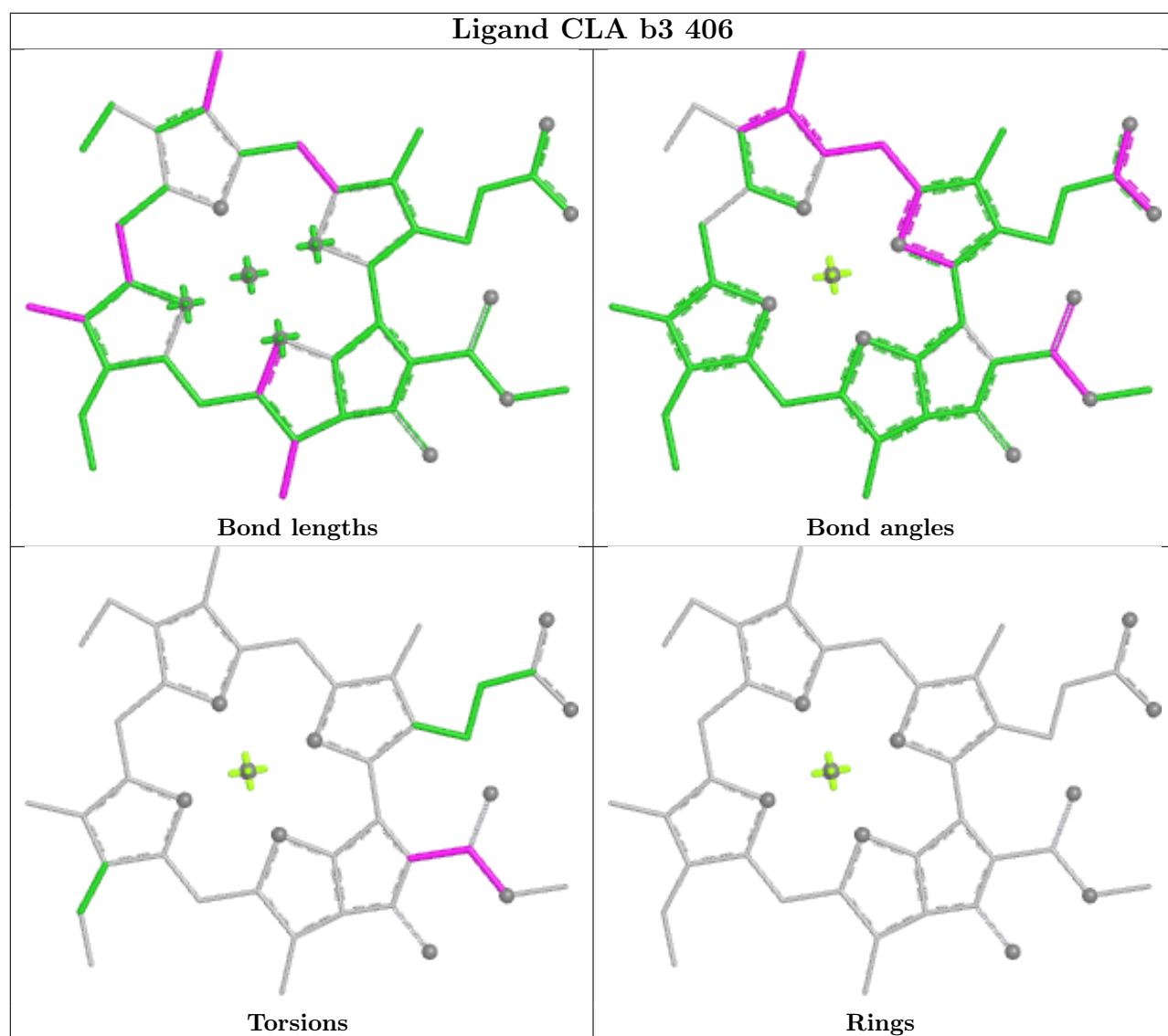


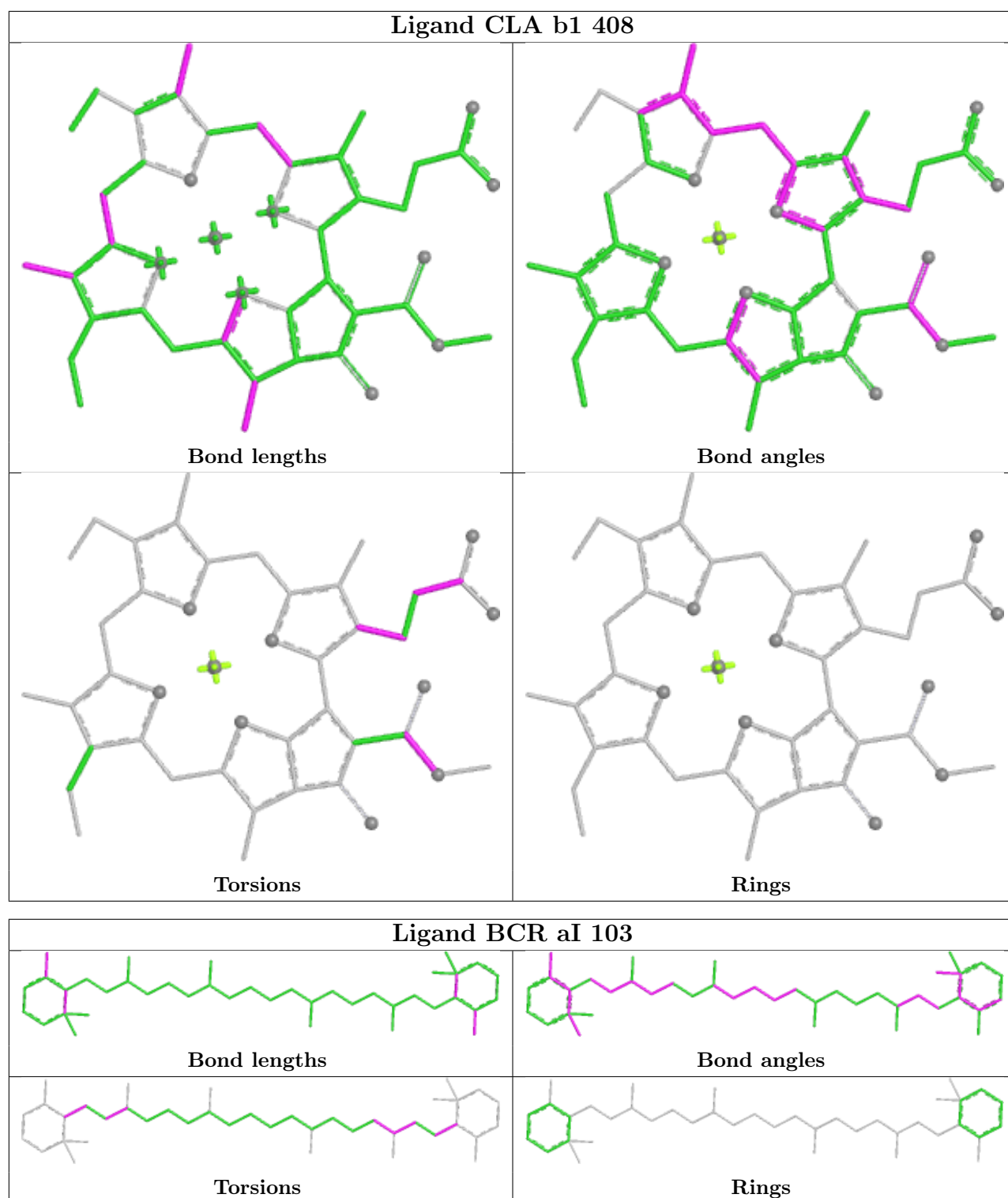
Ligand CLA cB 842

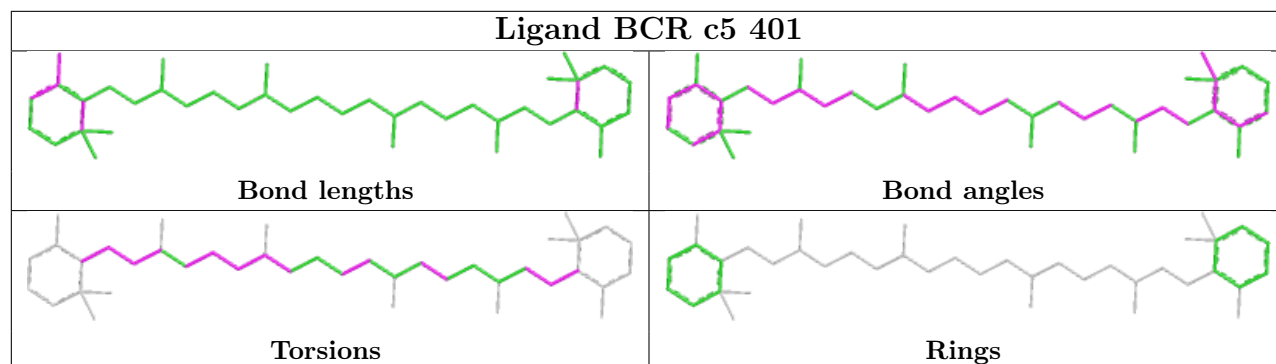
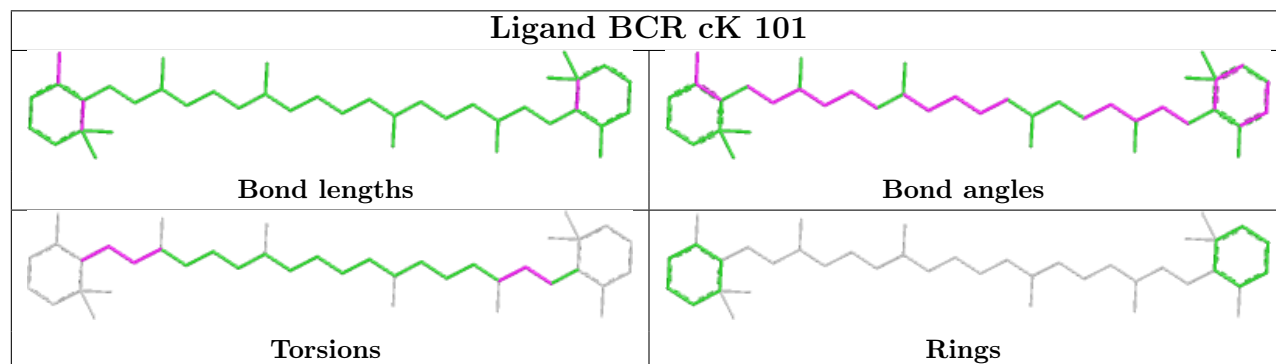
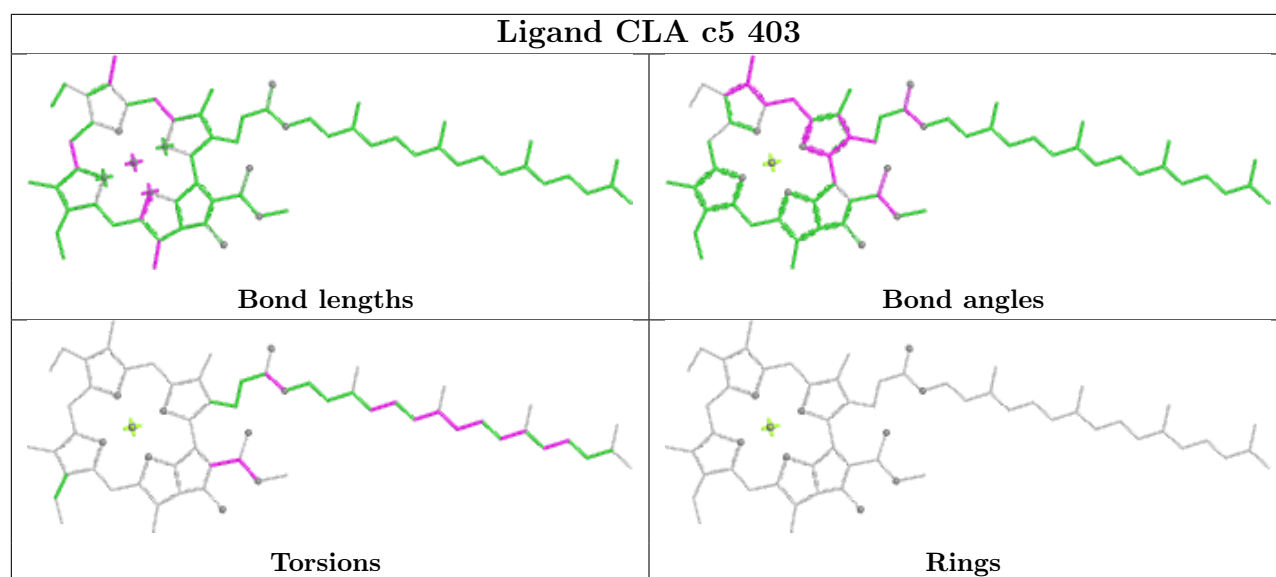




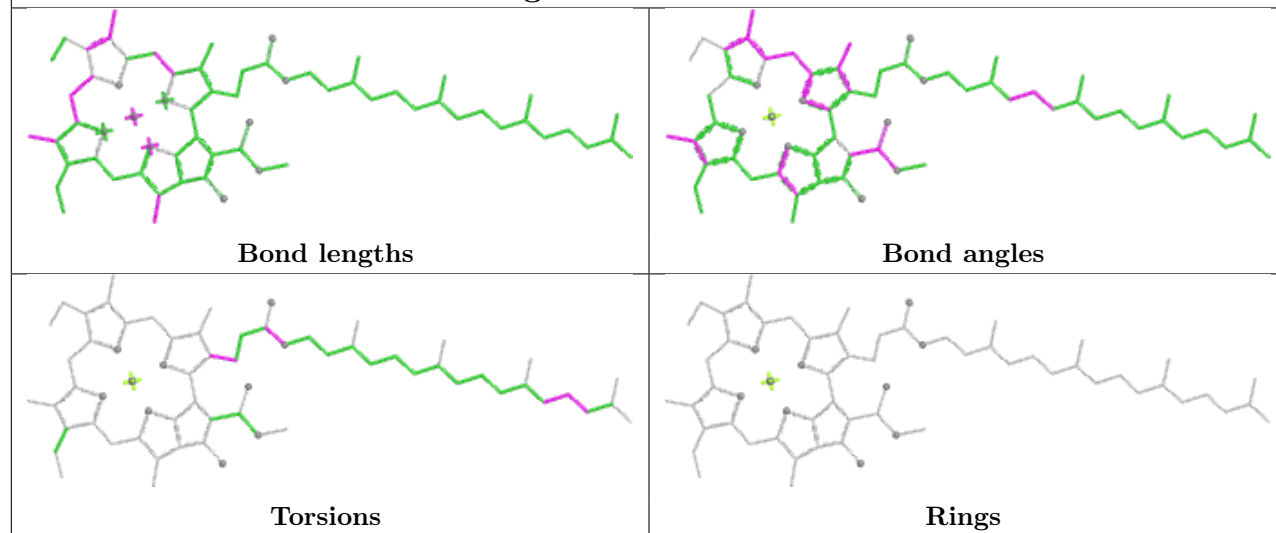




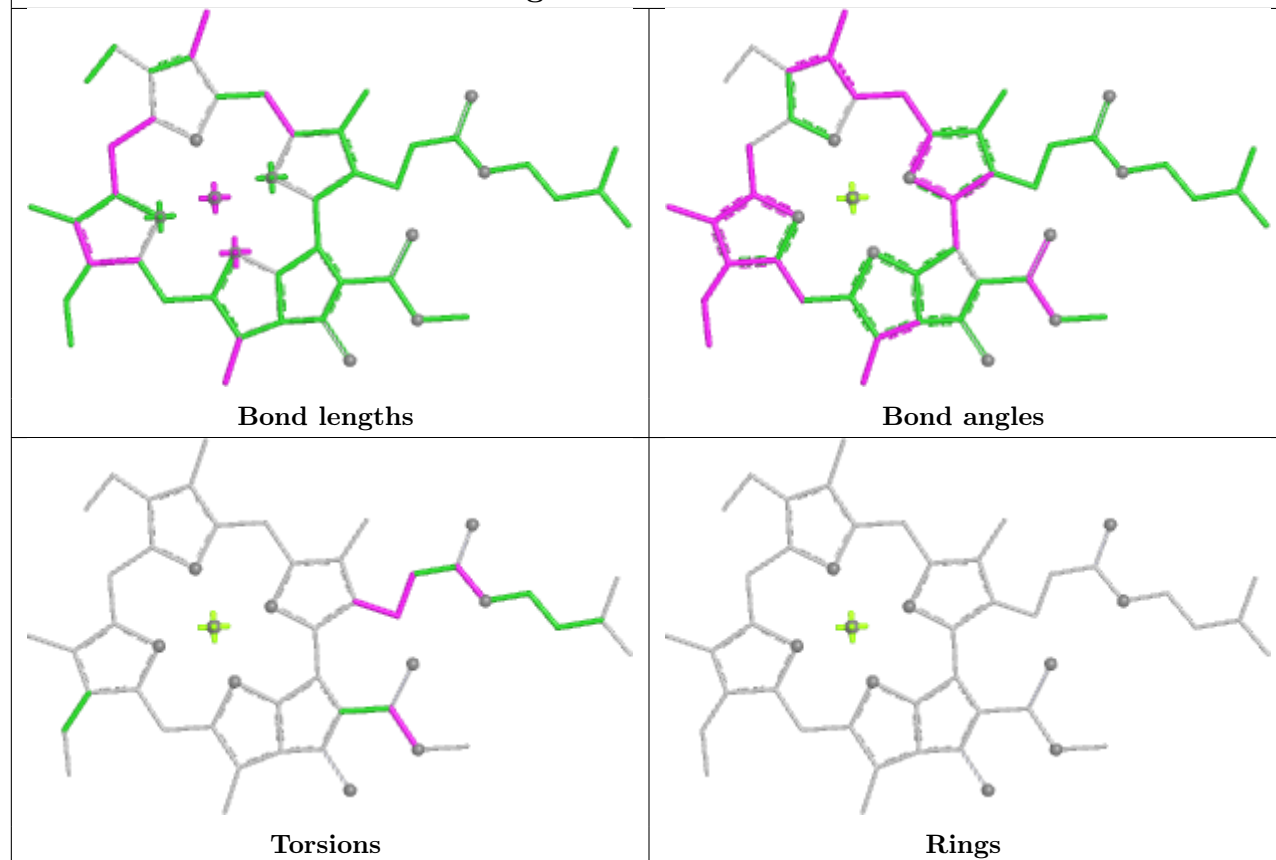




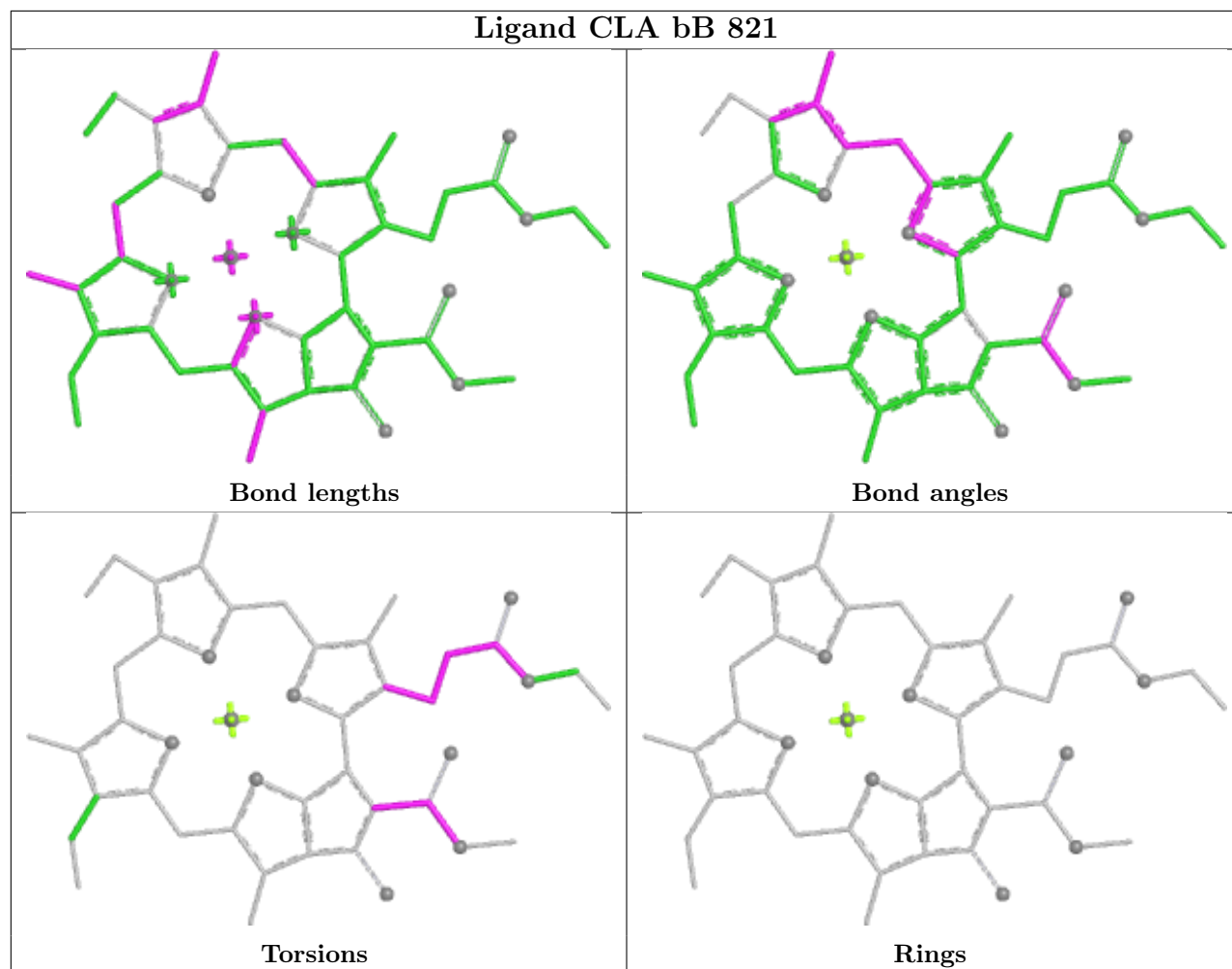
Ligand CLA aB 830

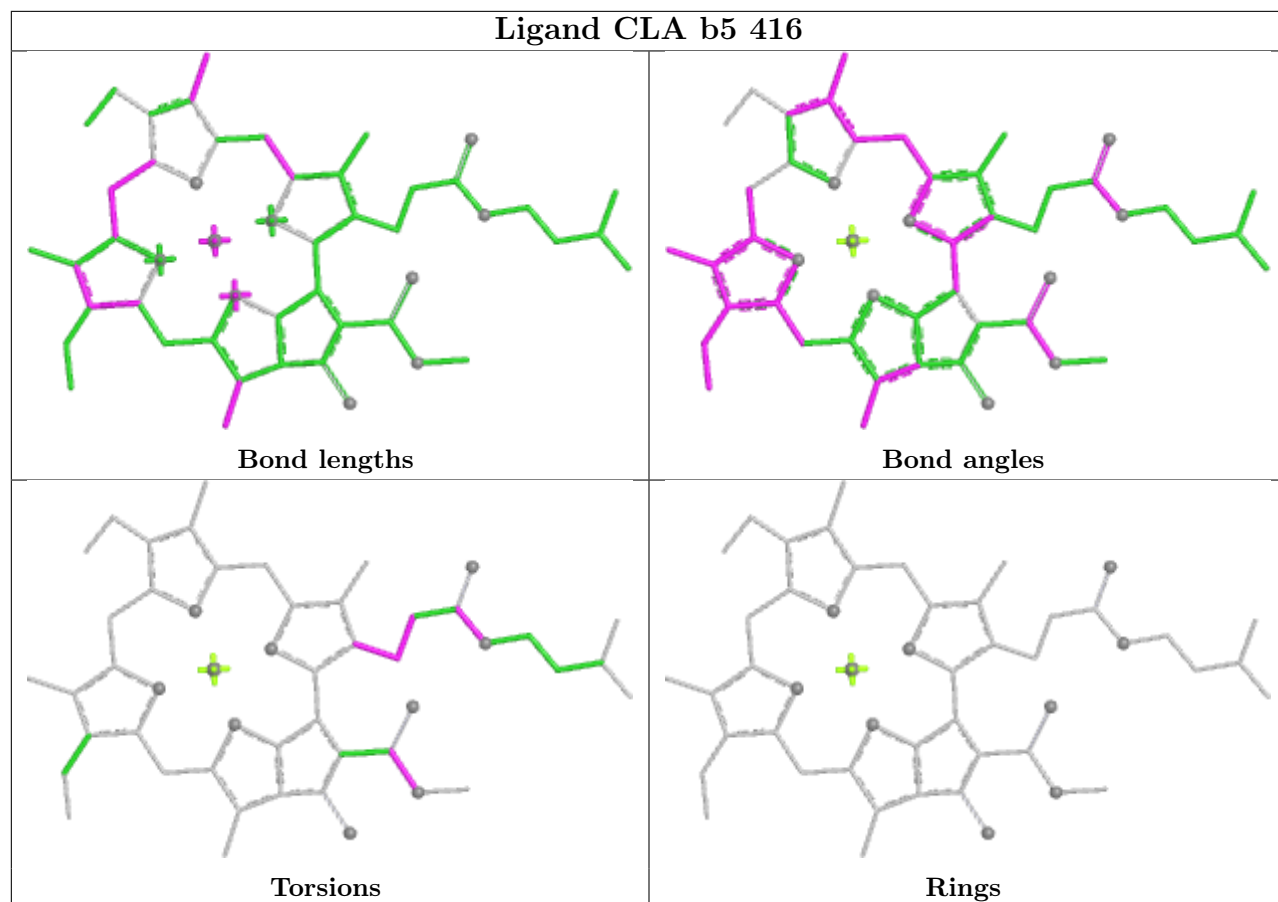


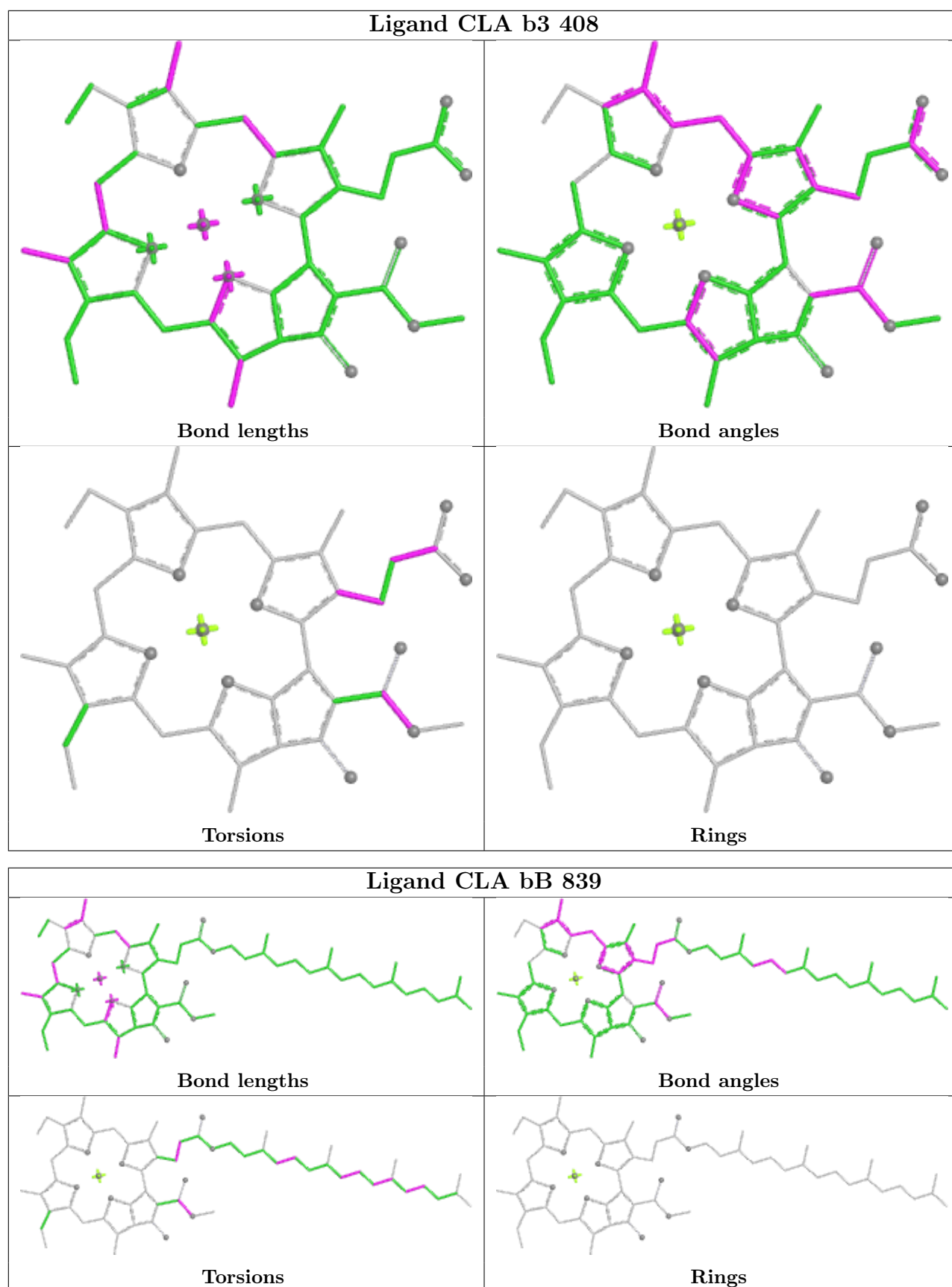
Ligand CLA b4 416

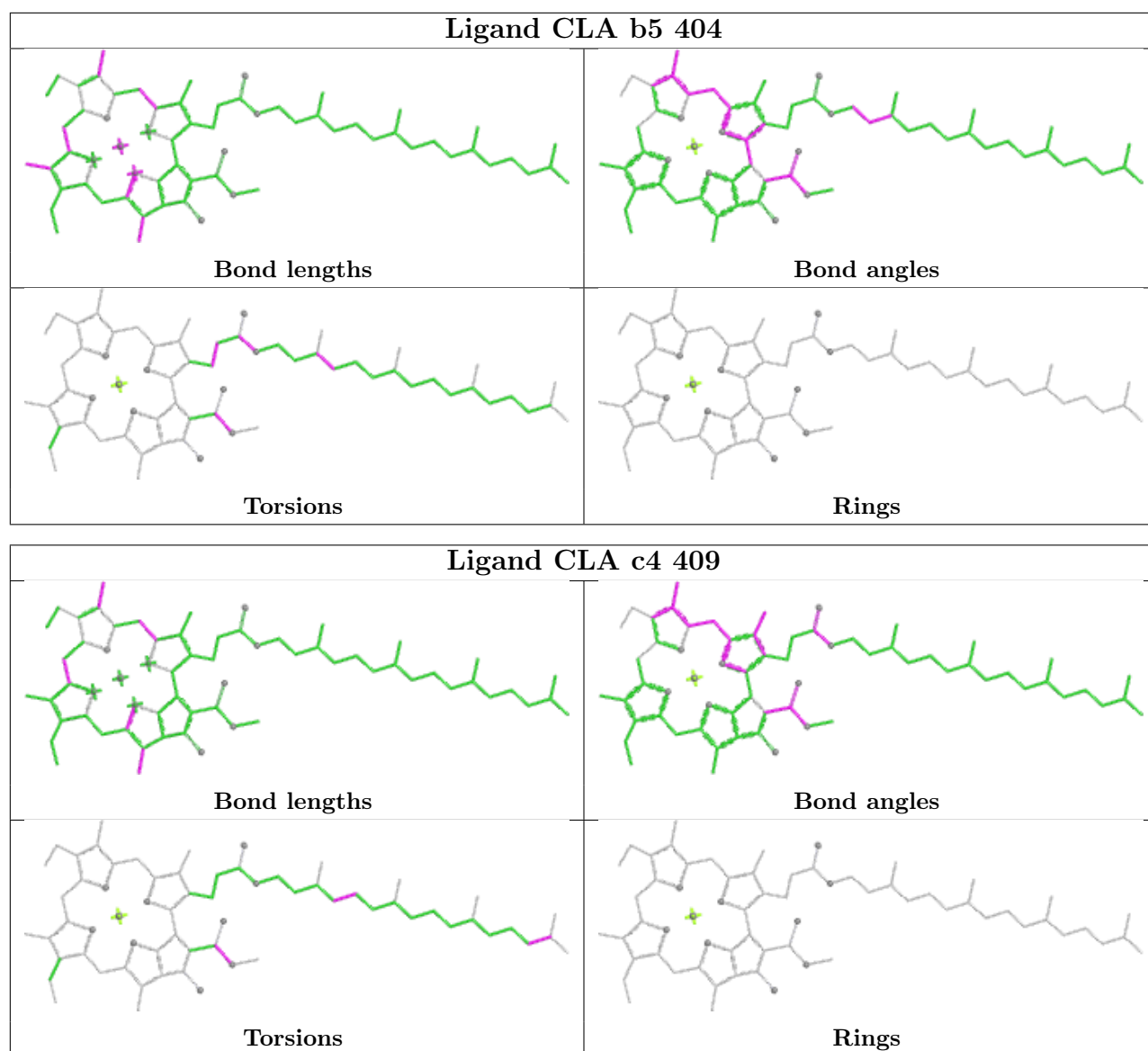


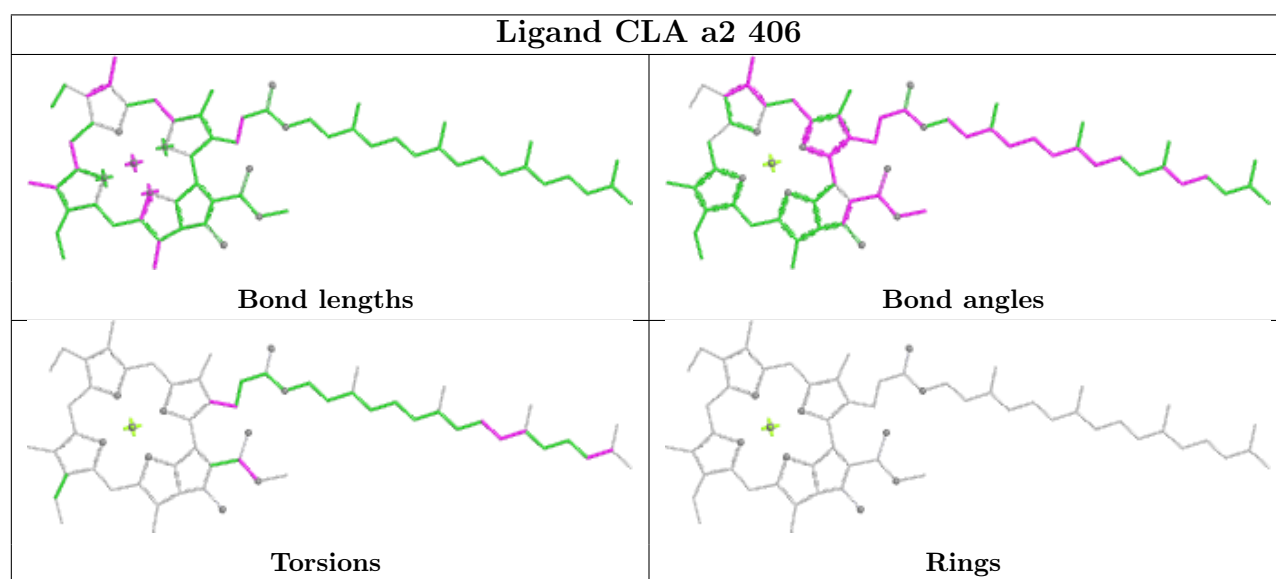
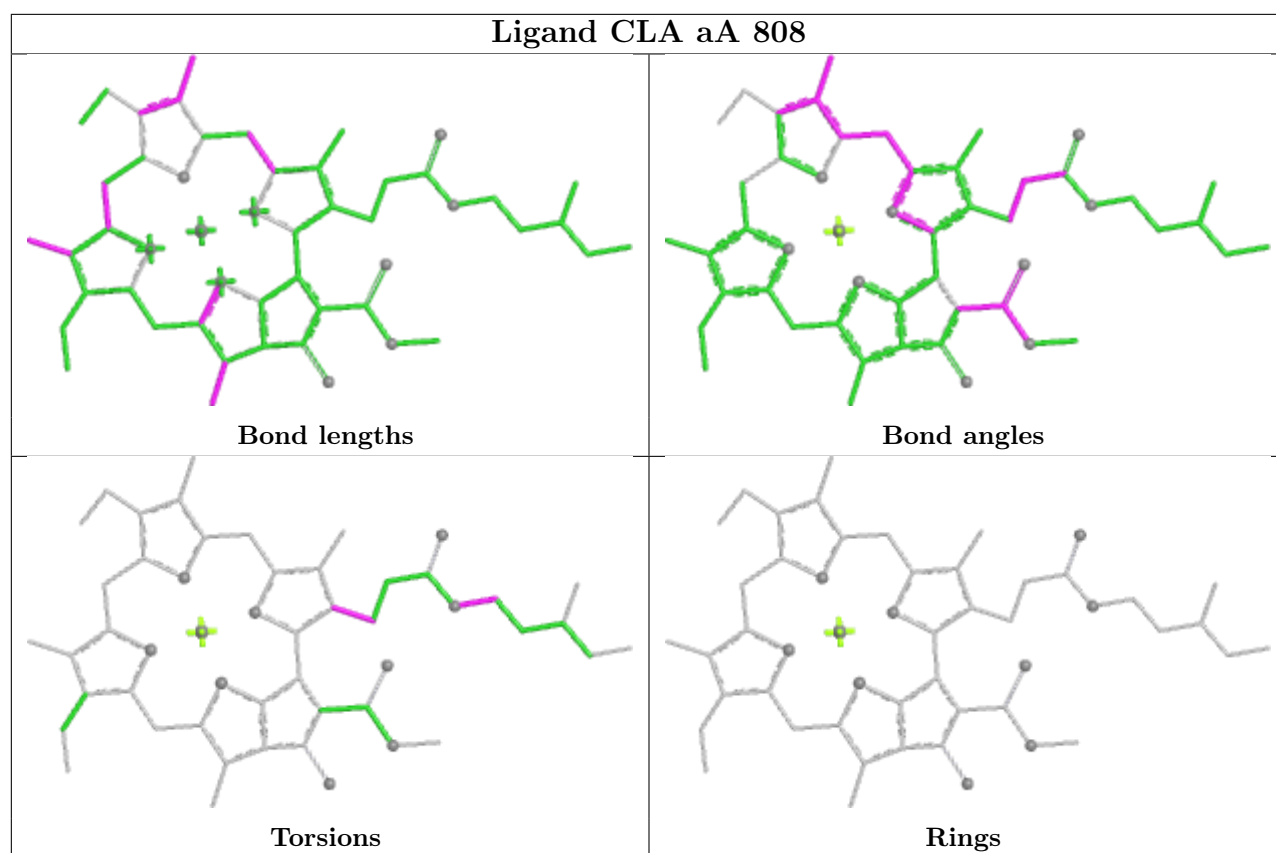
Ligand CLA bB 821

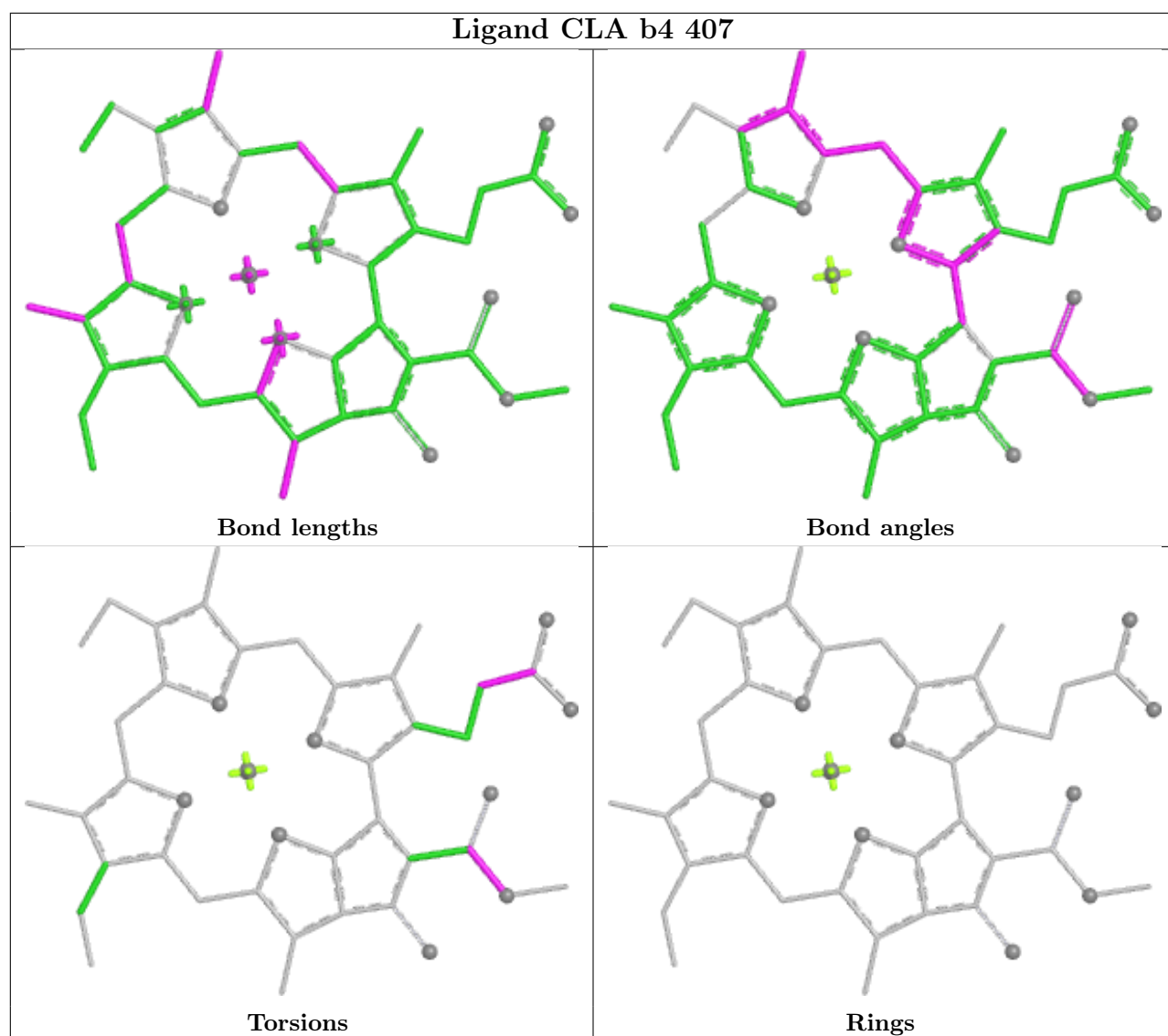


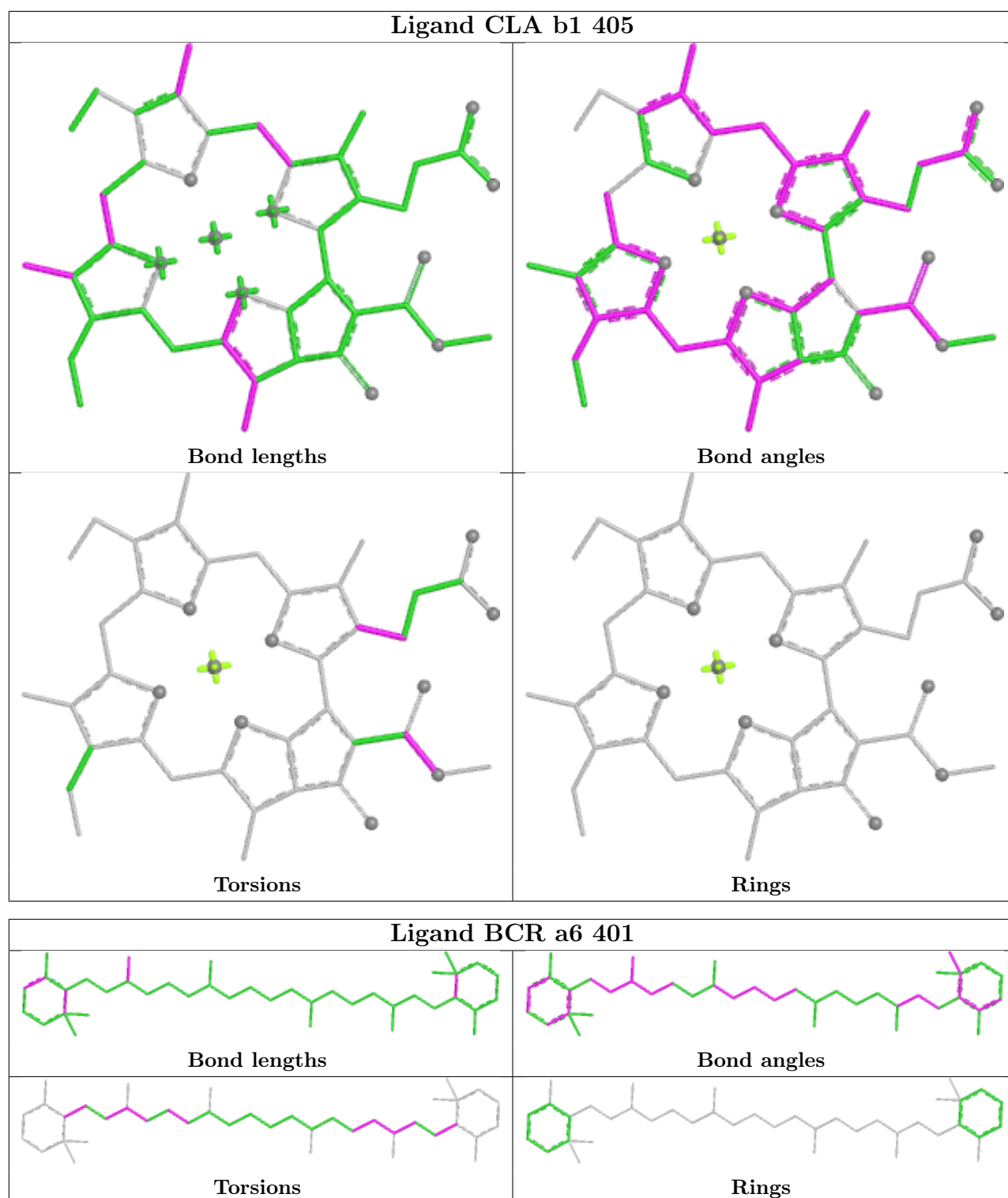


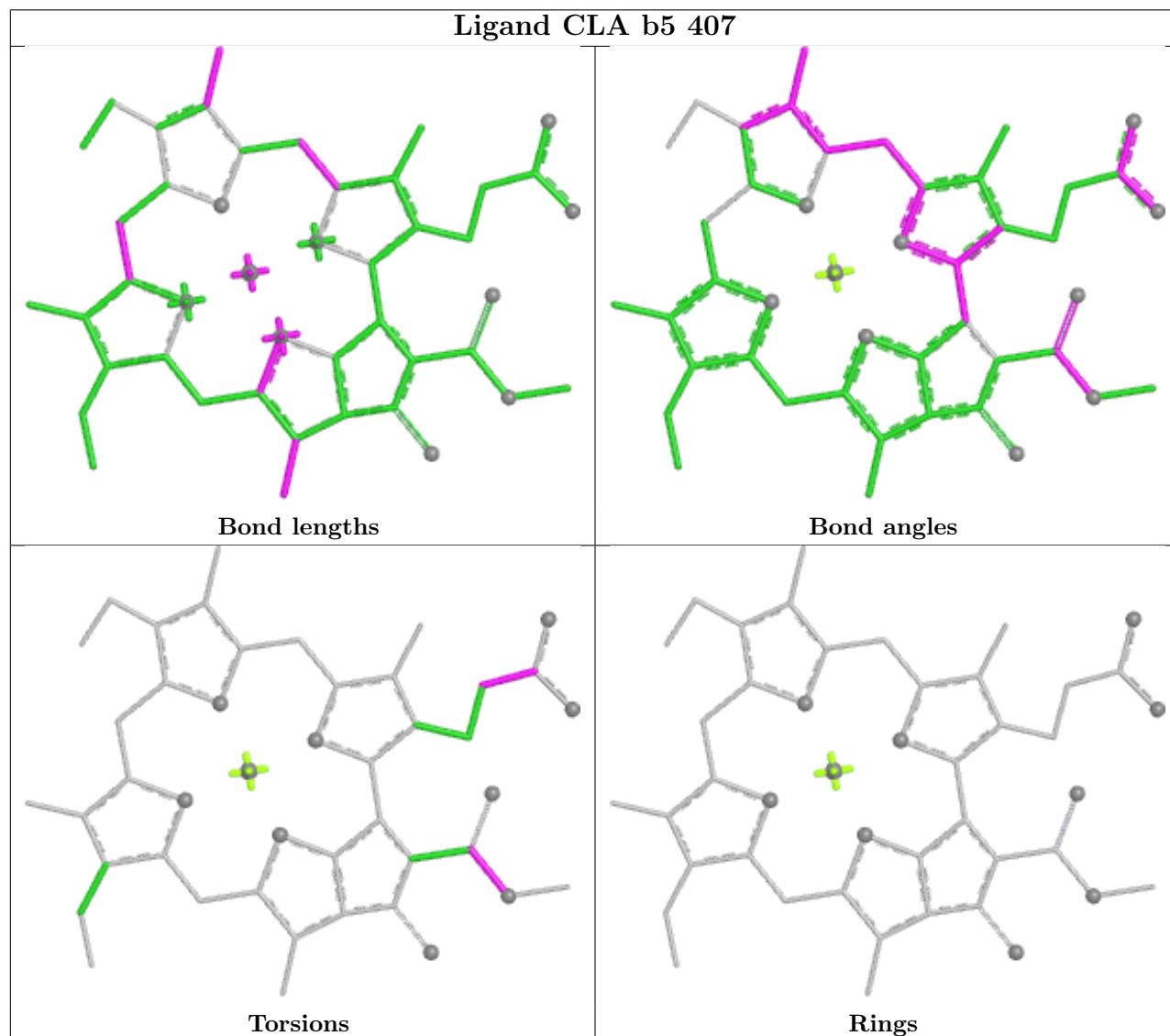
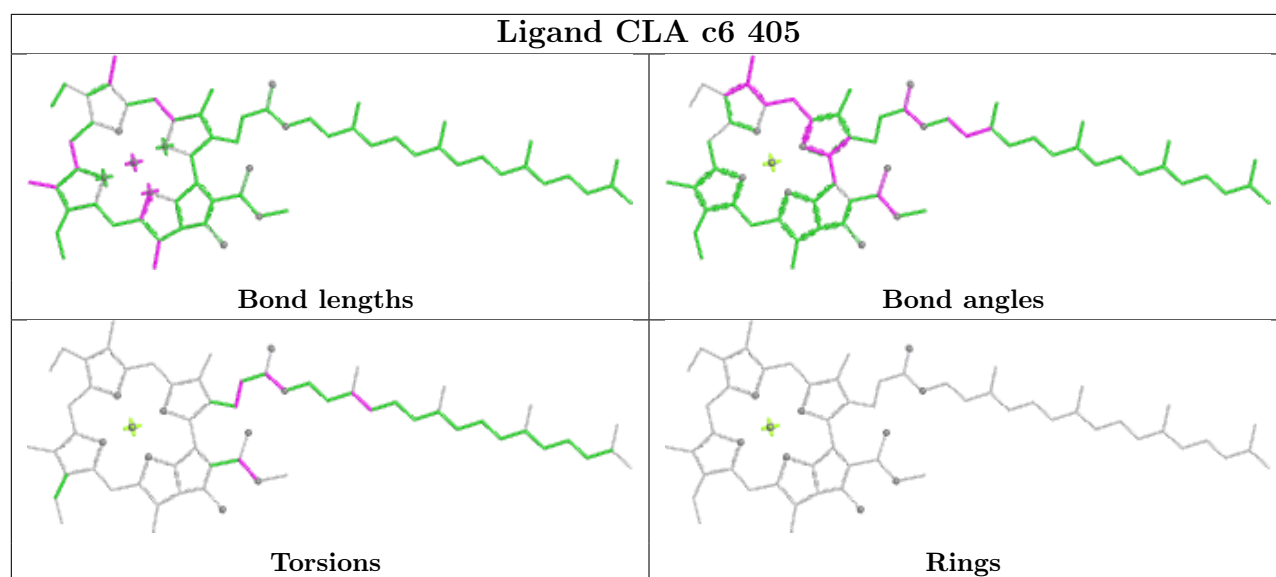


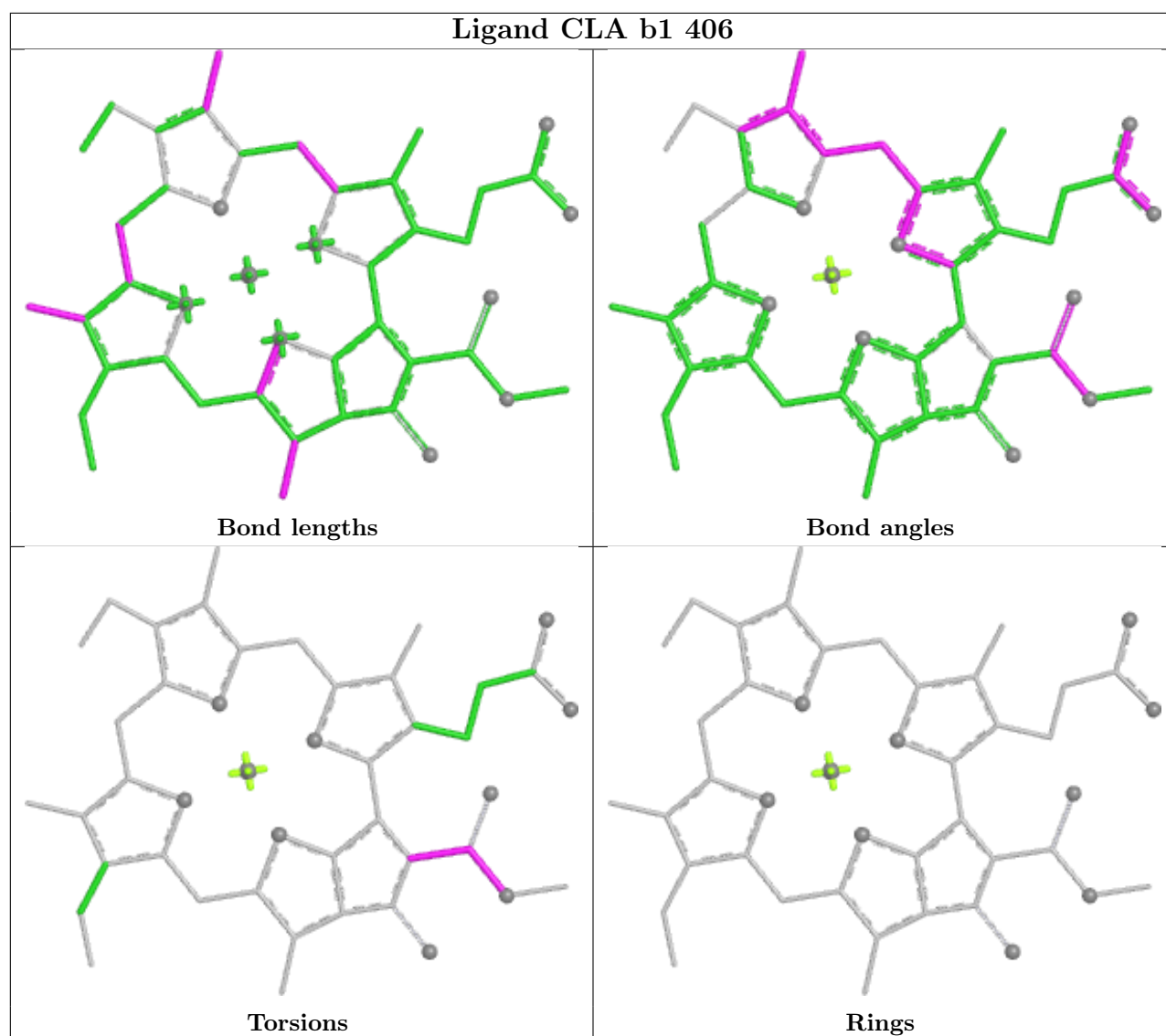


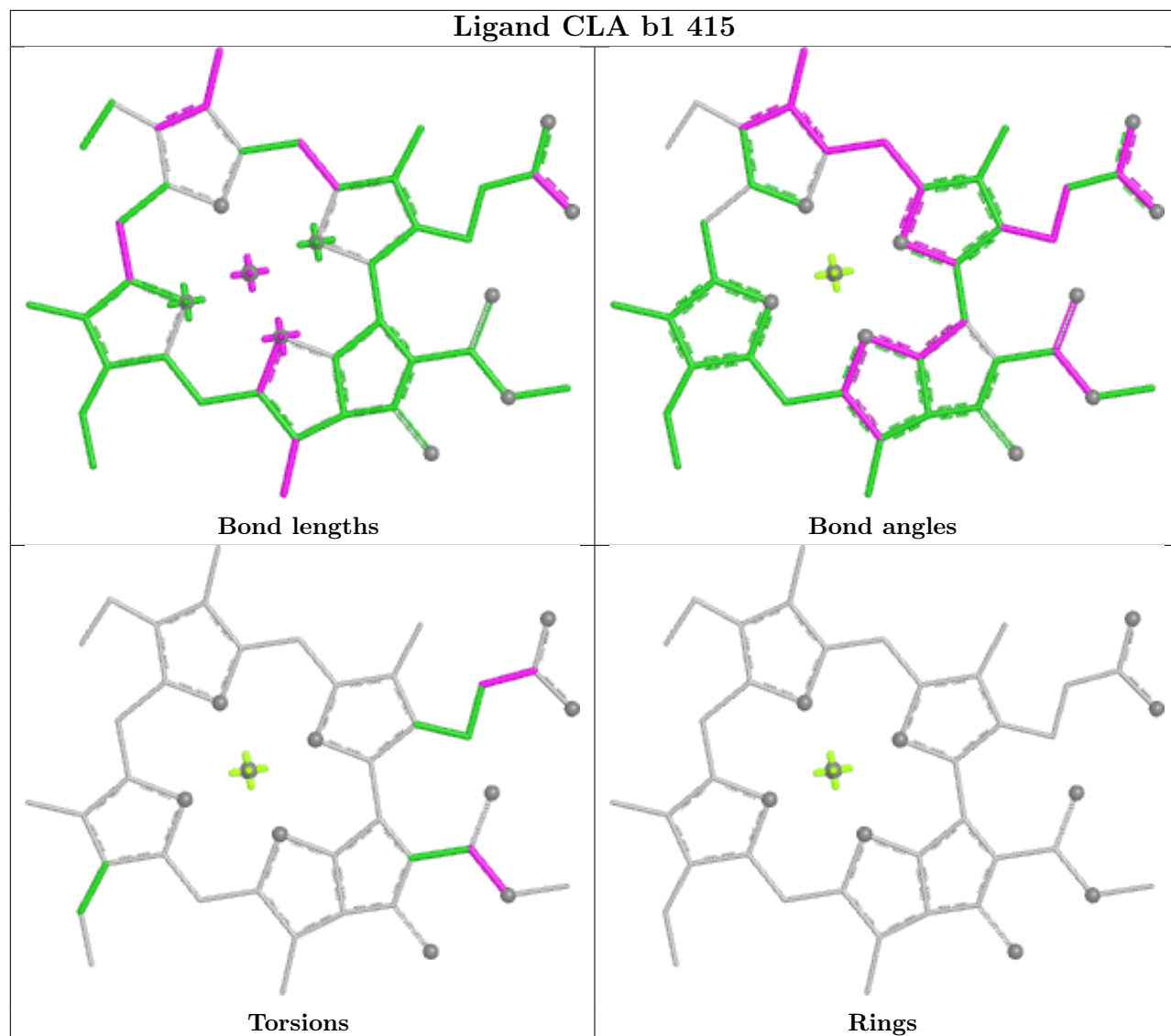


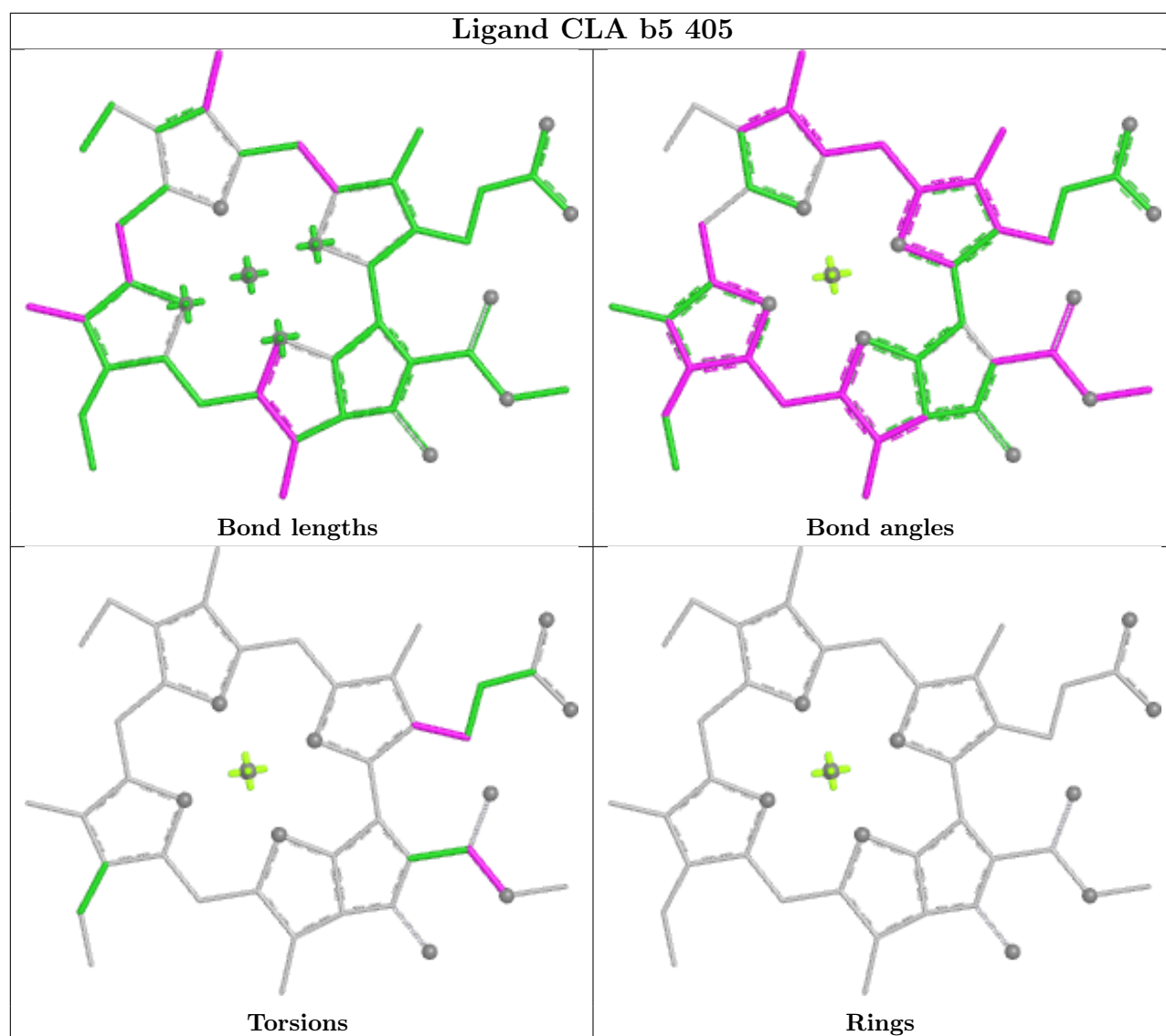


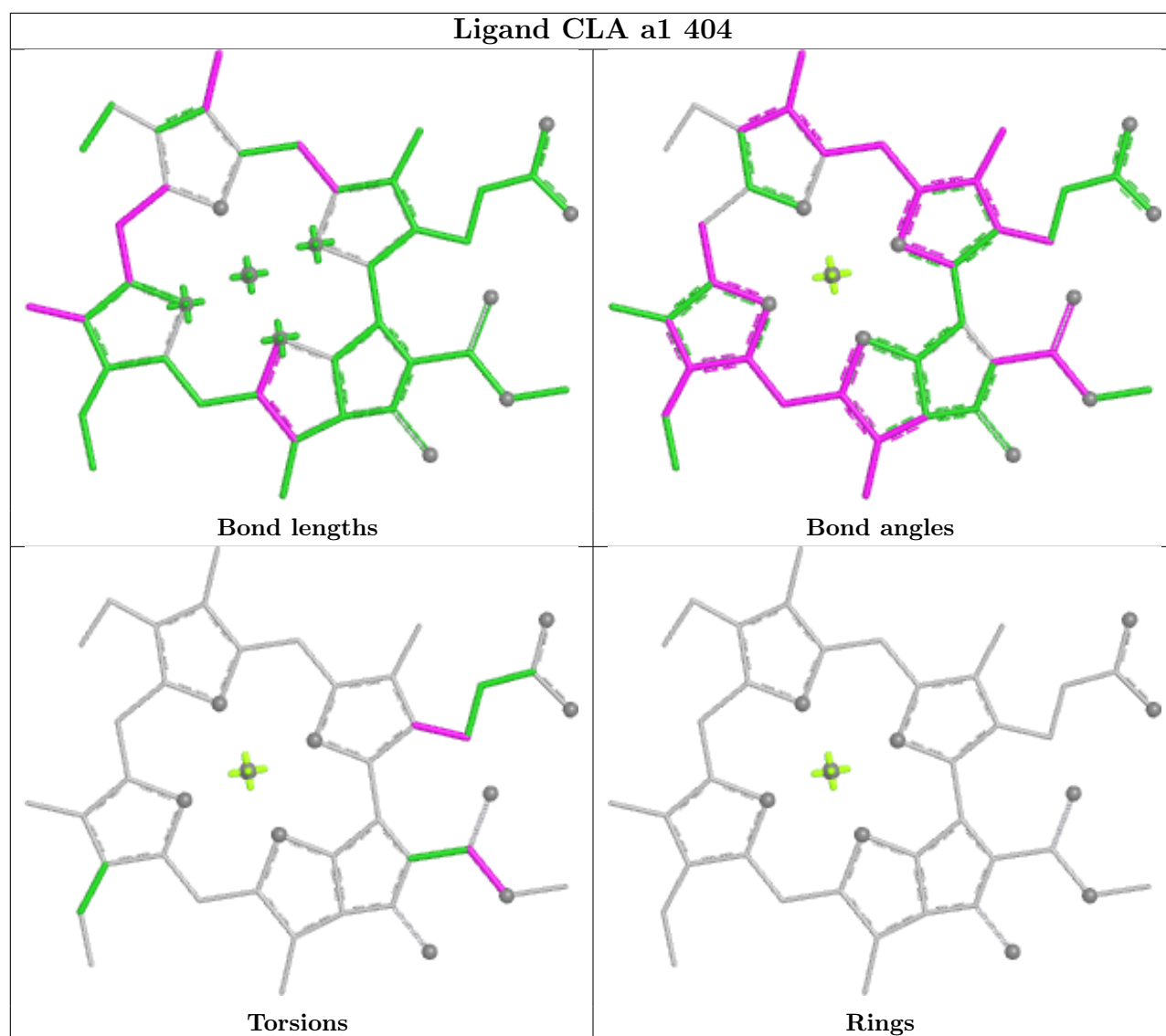


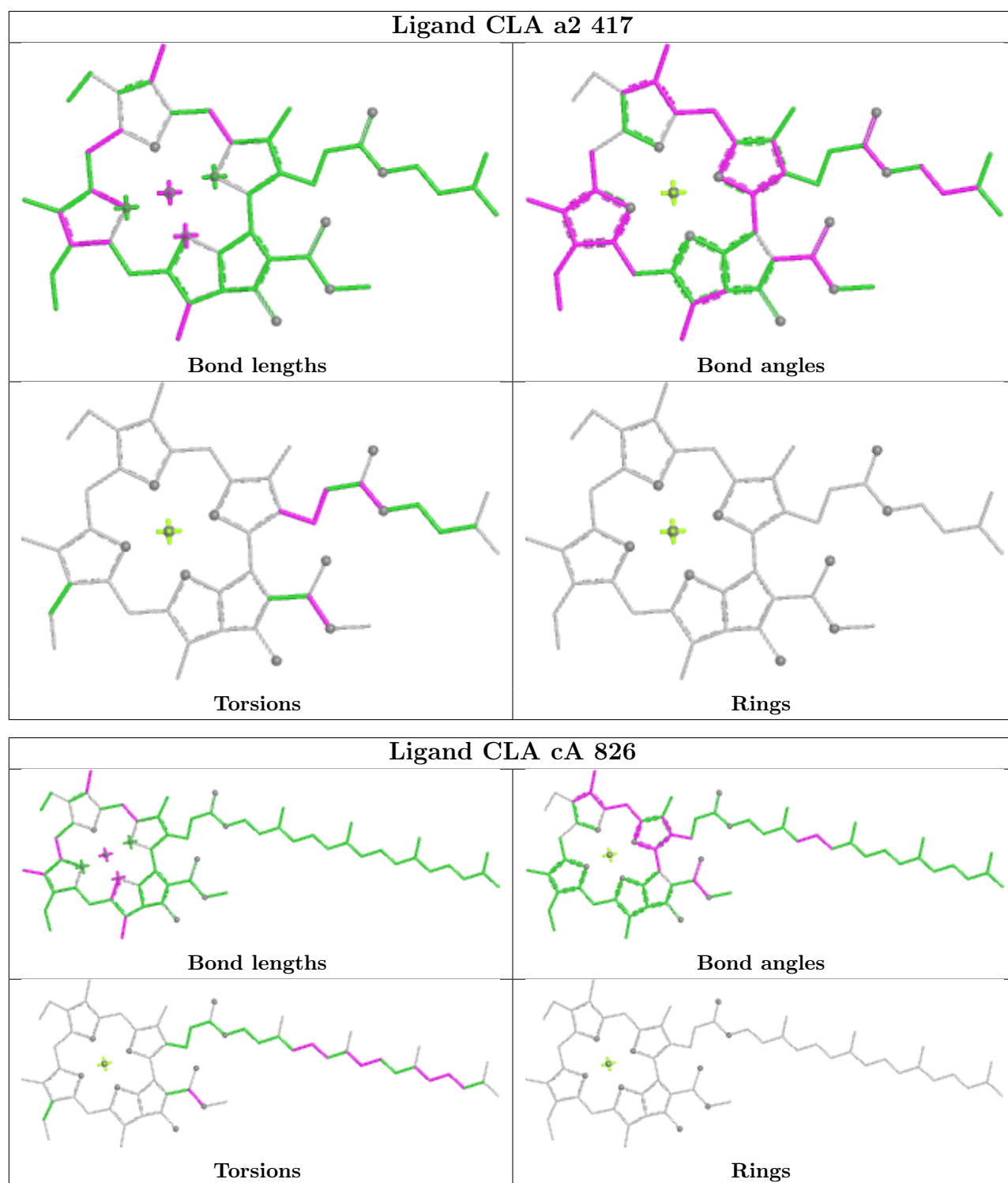


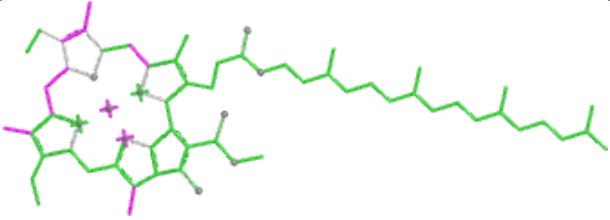
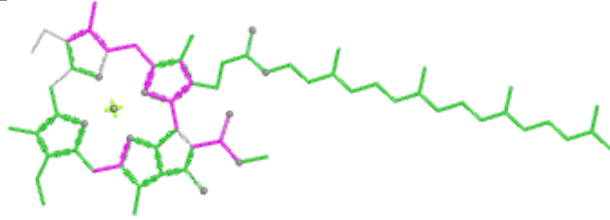
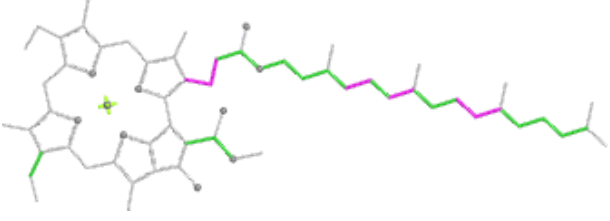
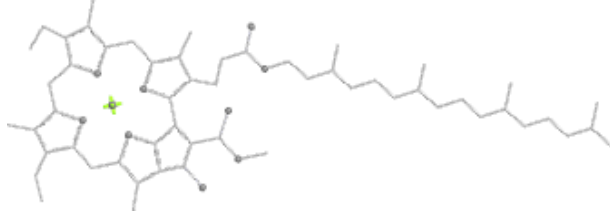
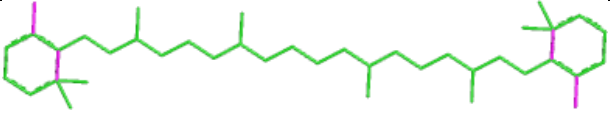
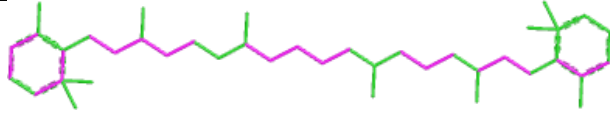
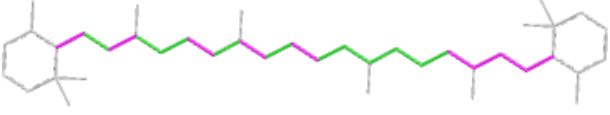
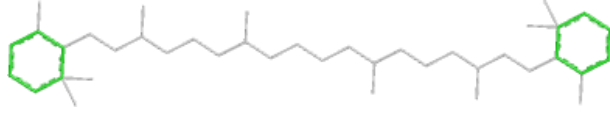
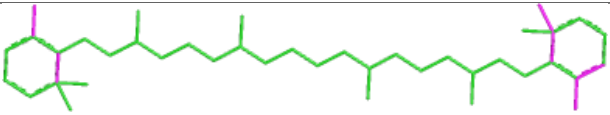
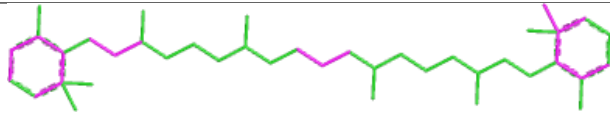
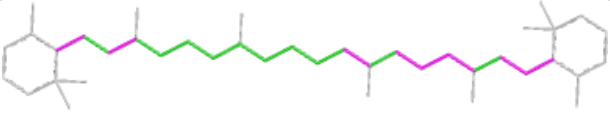
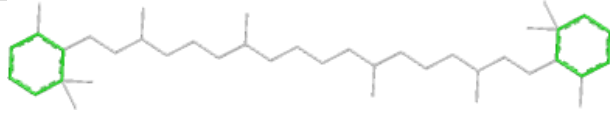


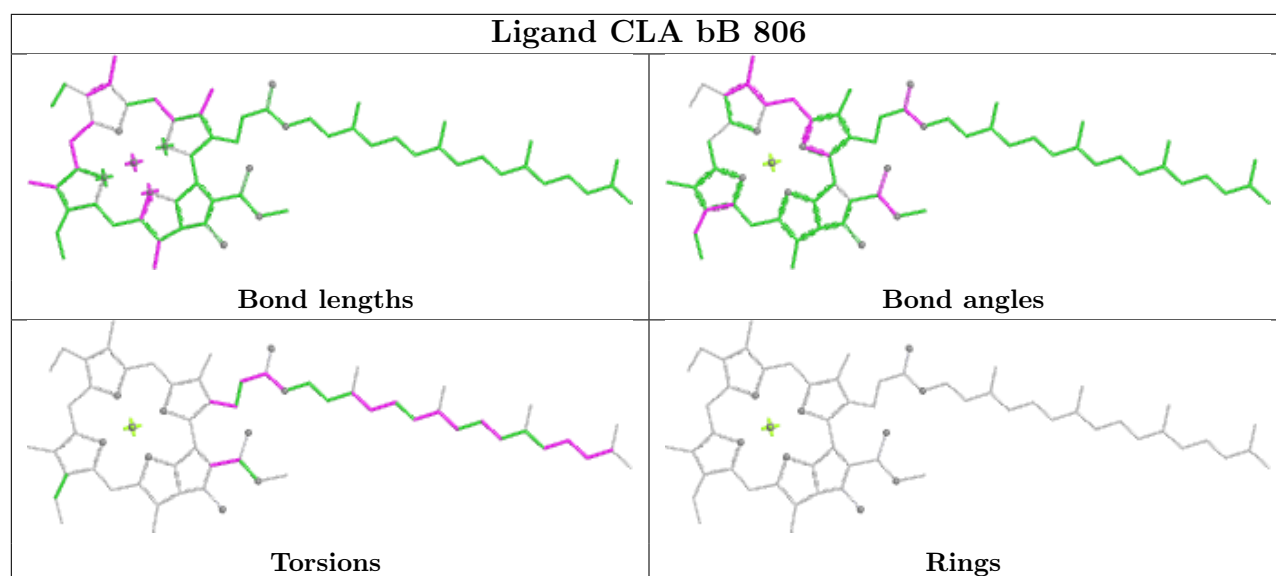
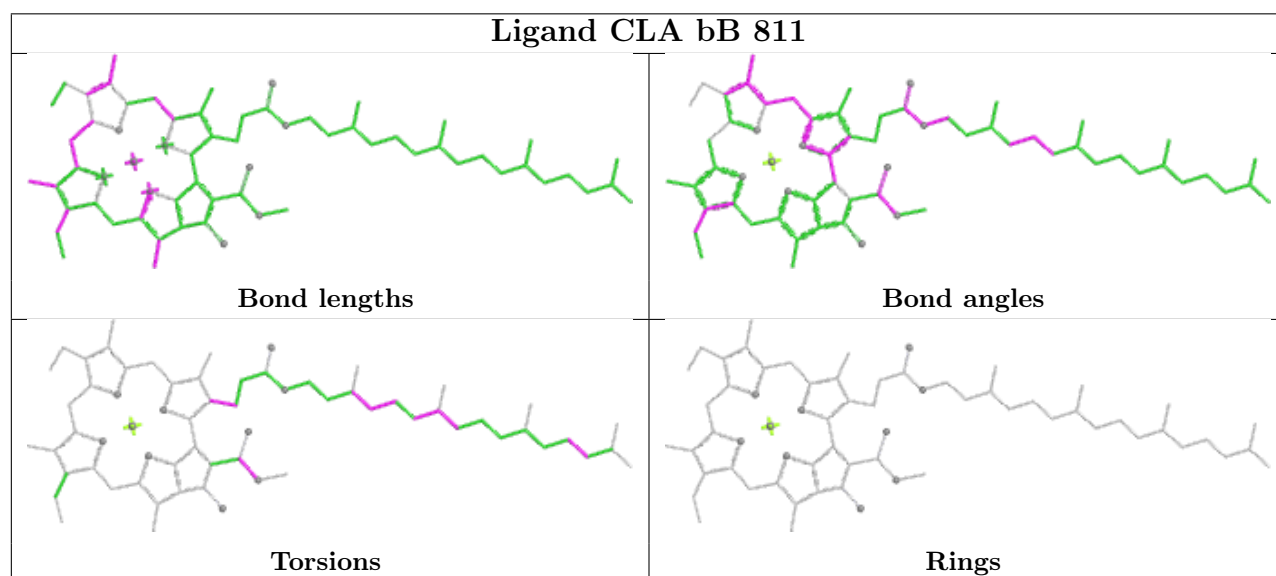
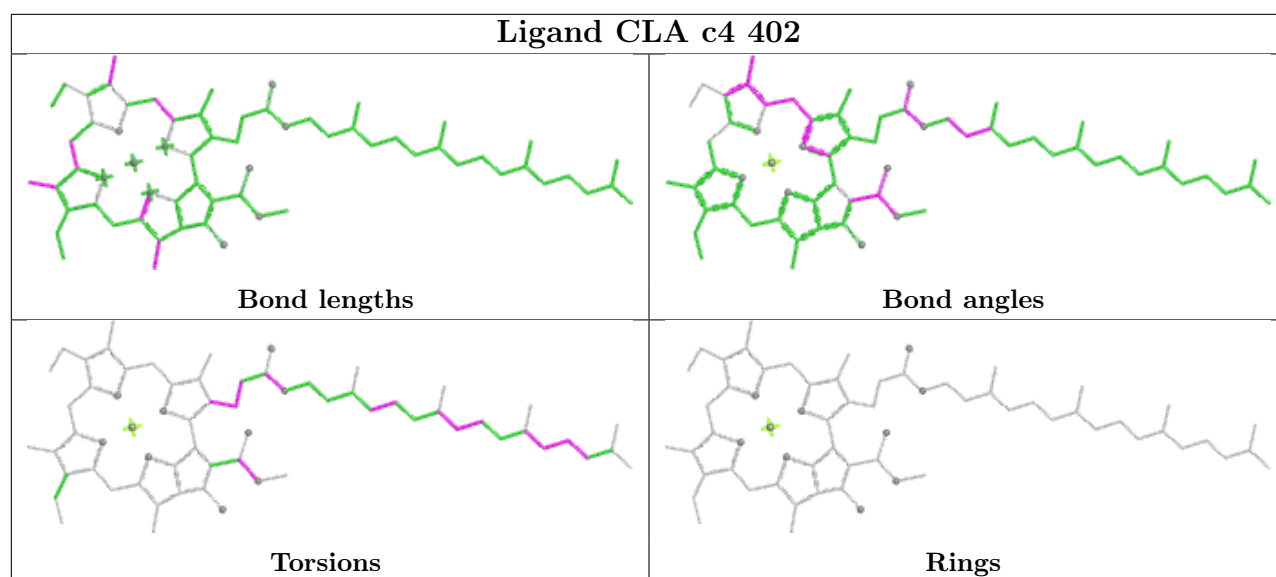


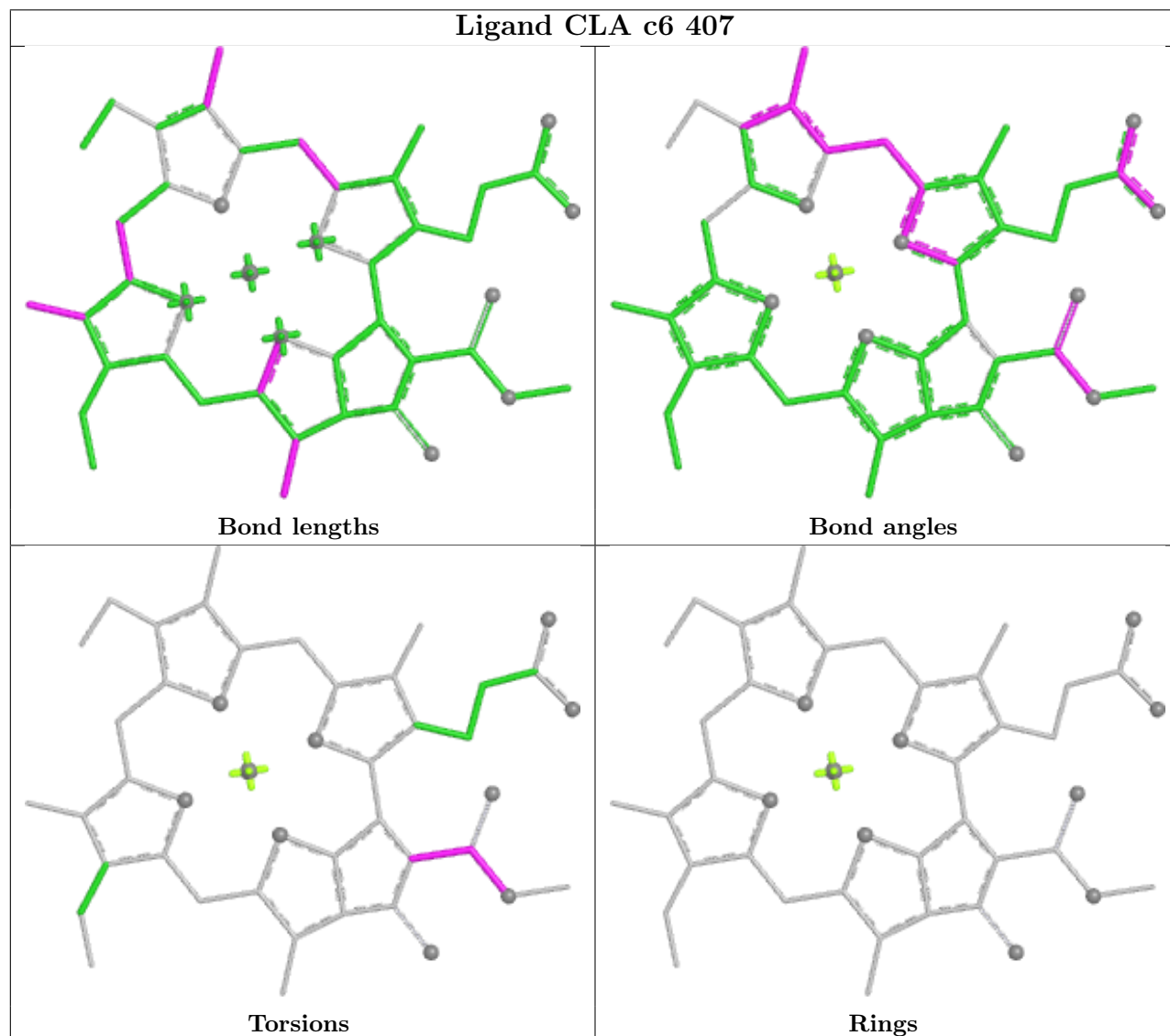
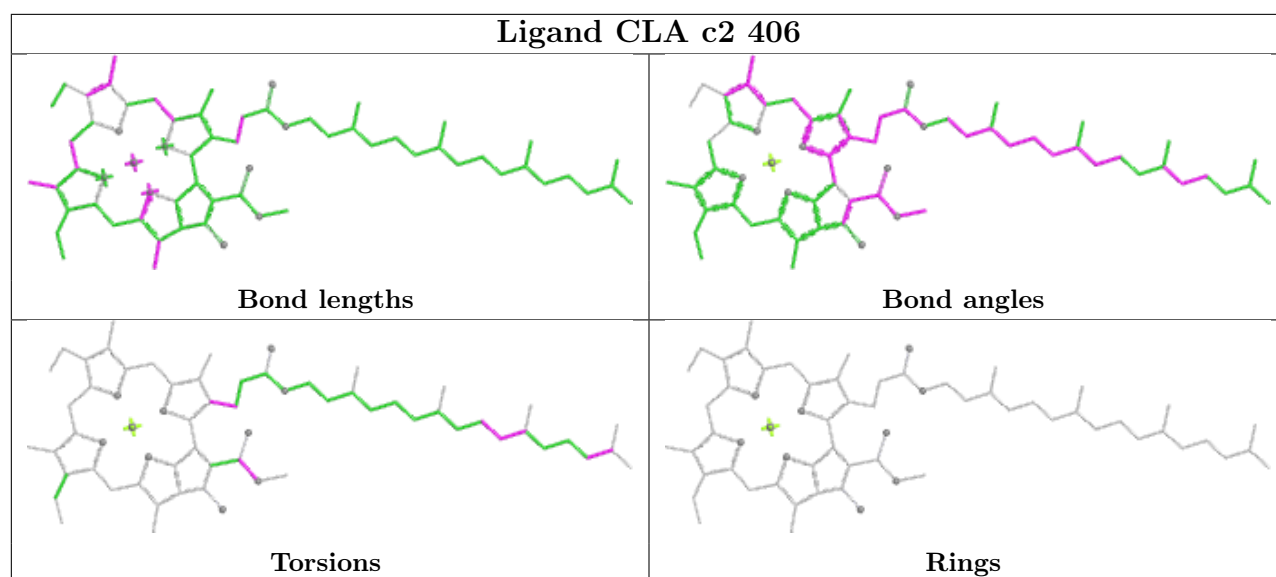


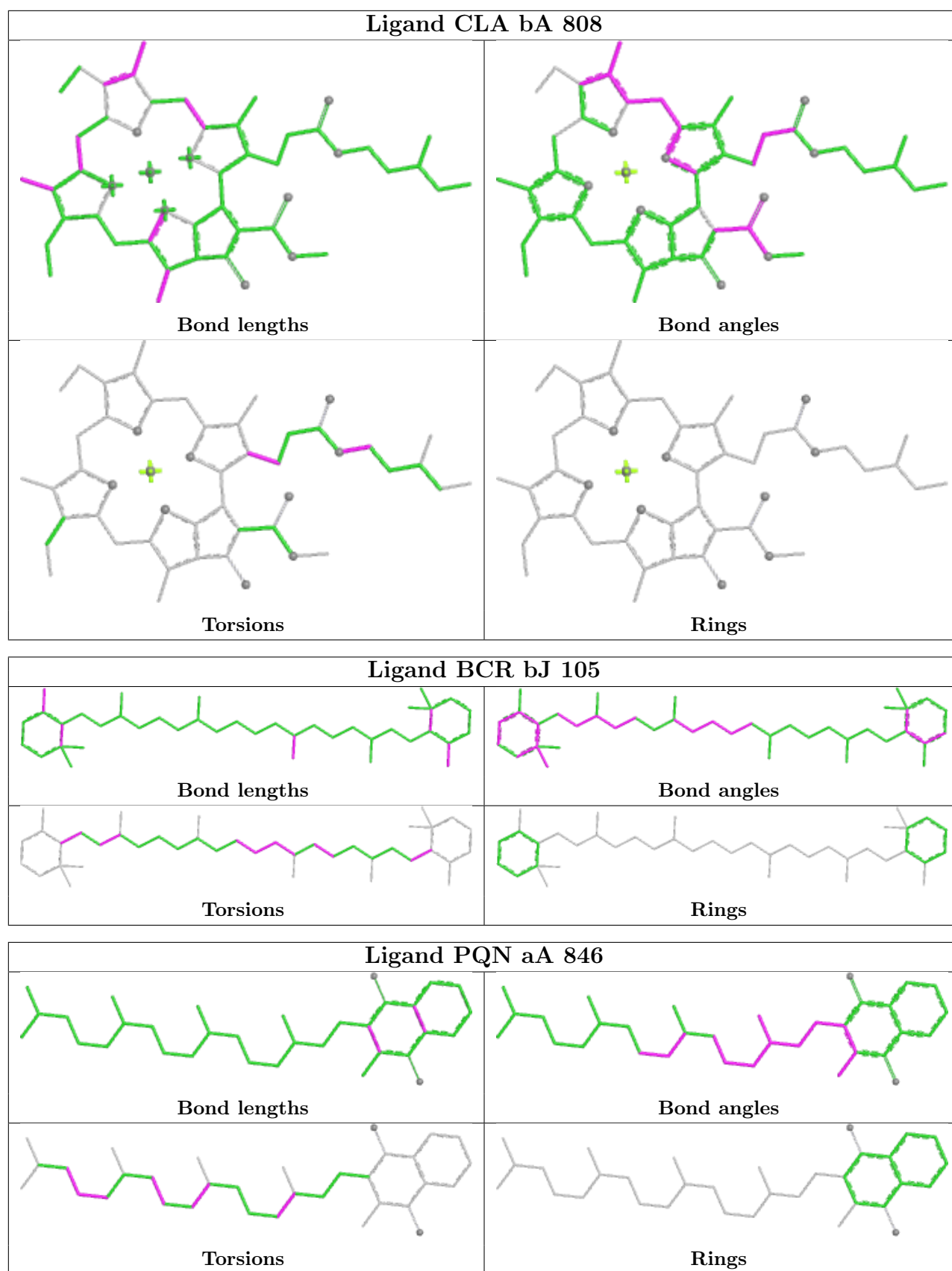




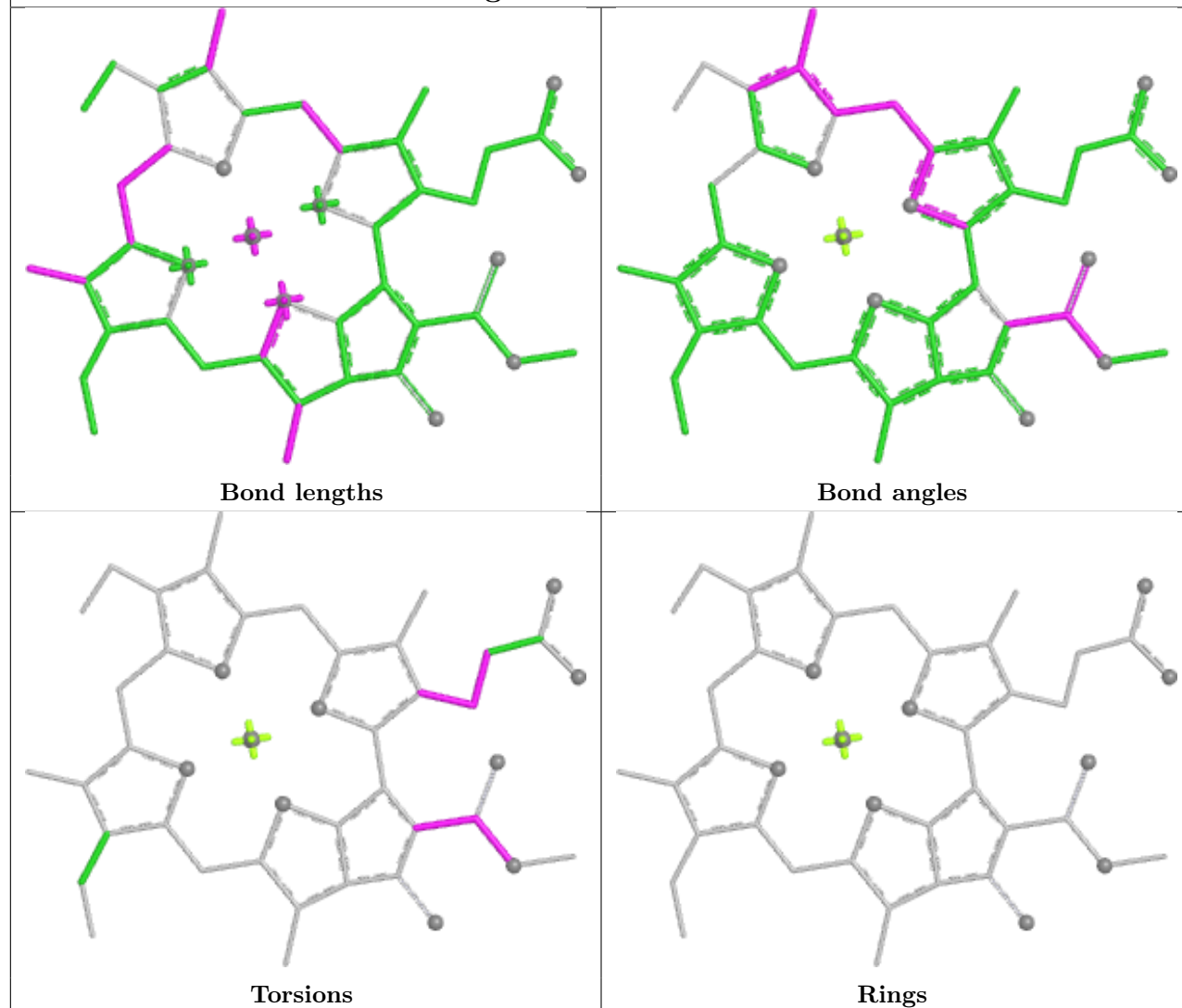
Ligand CLA aL 202	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR cB 848	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR c5 418	
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 <p>Torsions</p>	 <p>Rings</p>



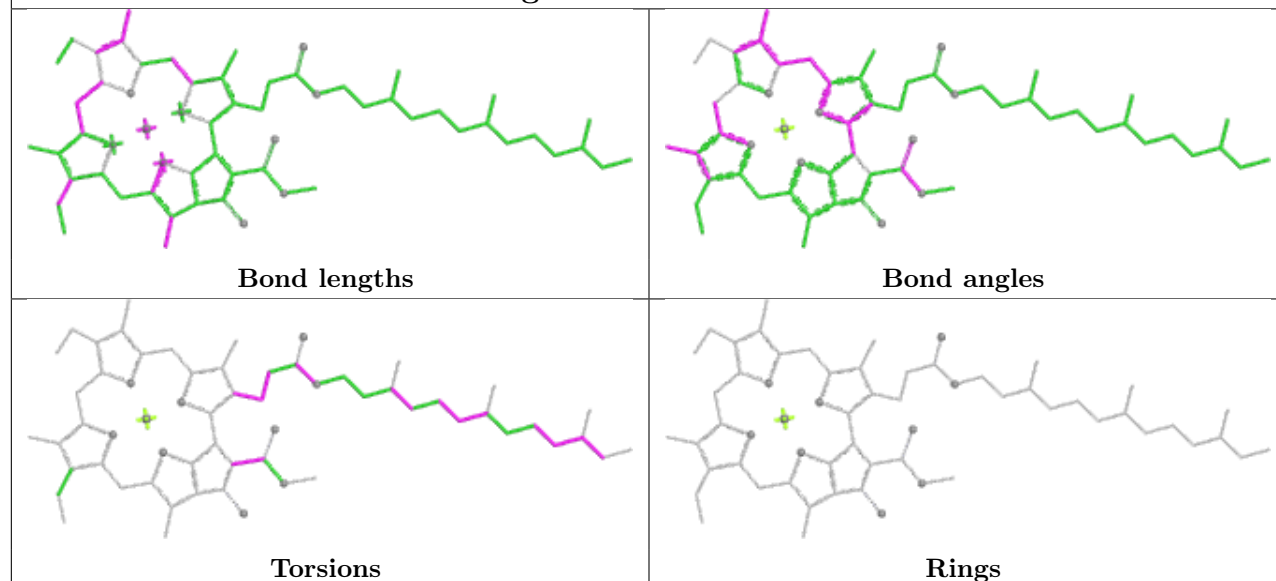


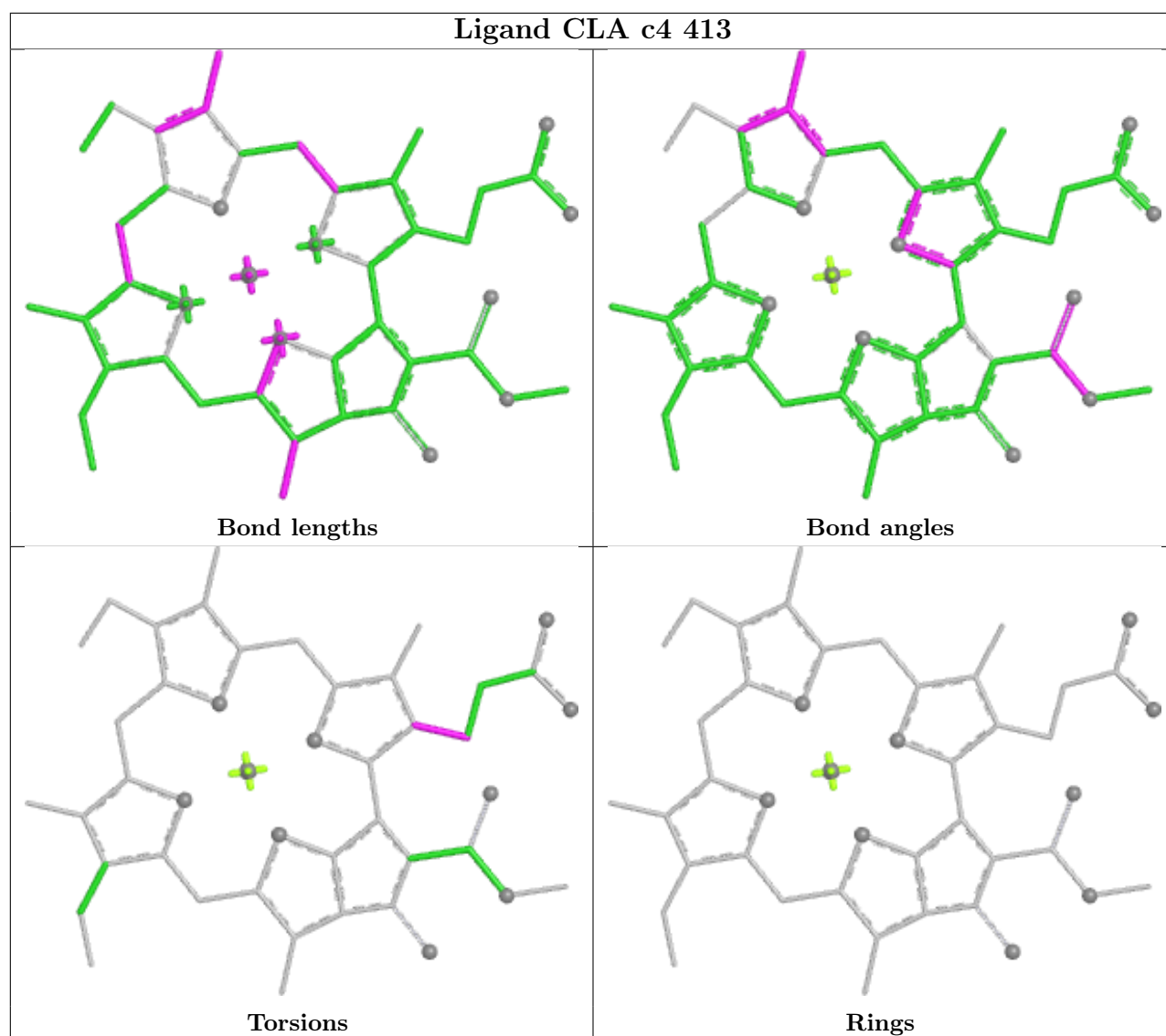


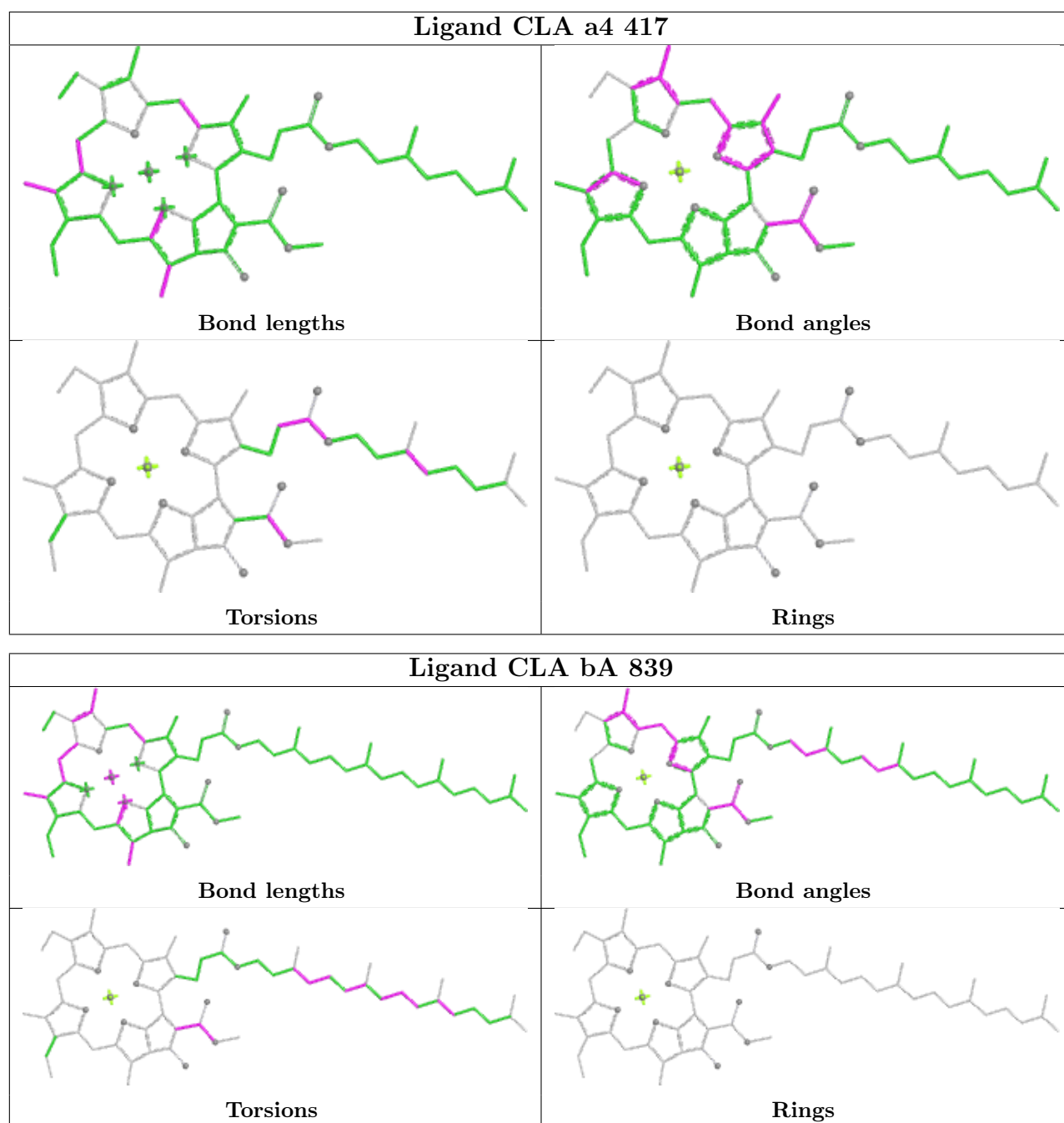
Ligand CLA aB 816

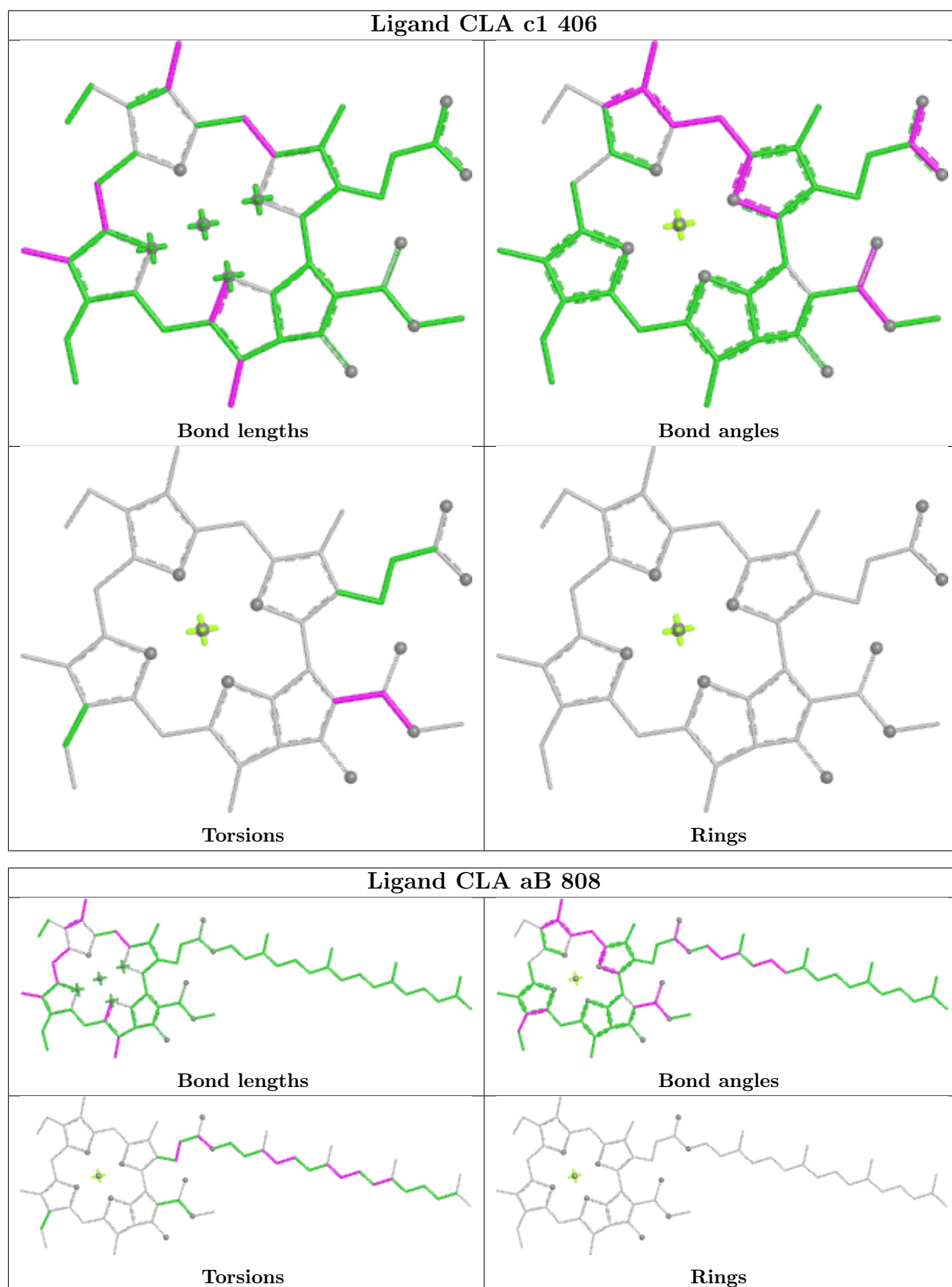


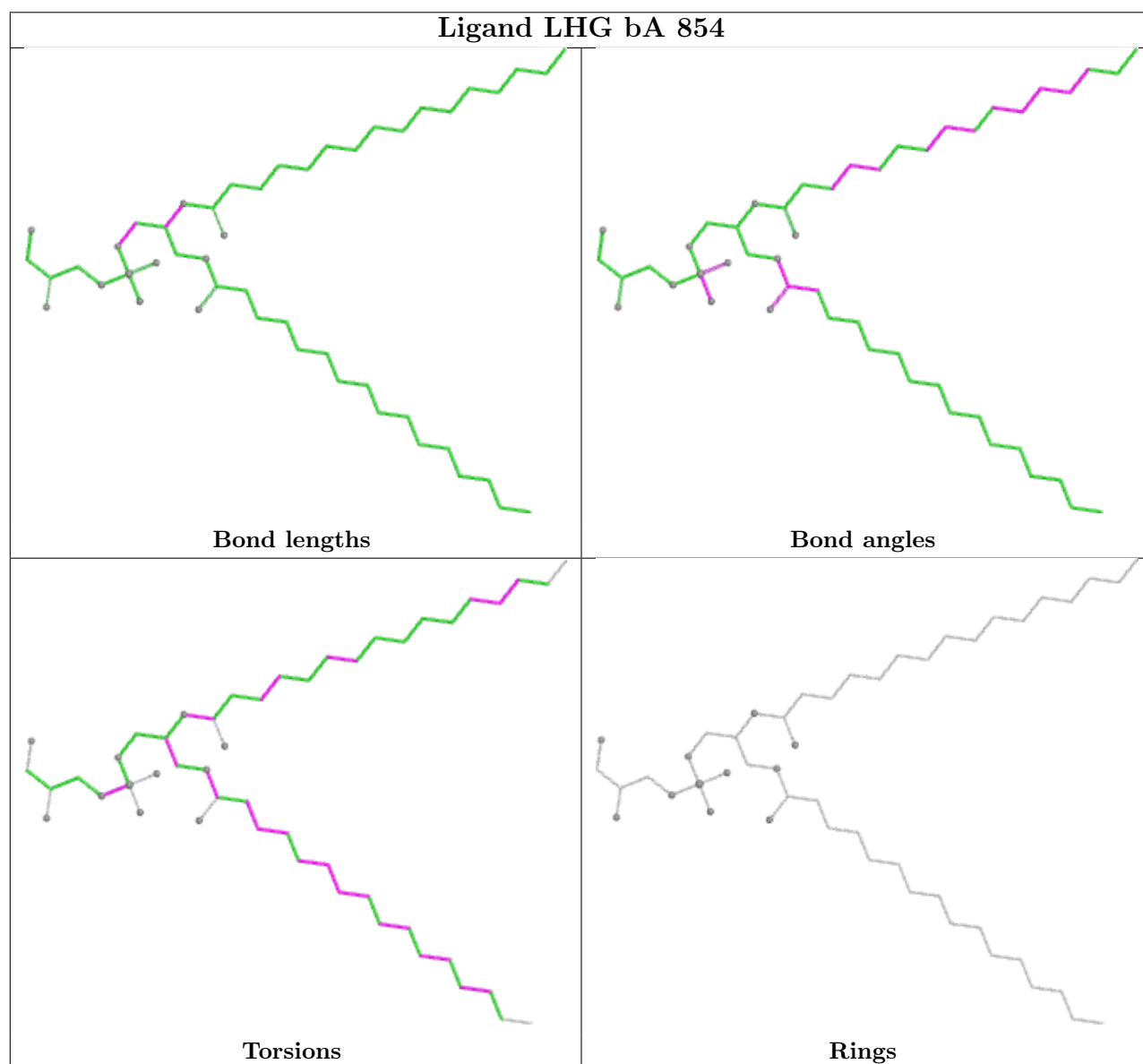
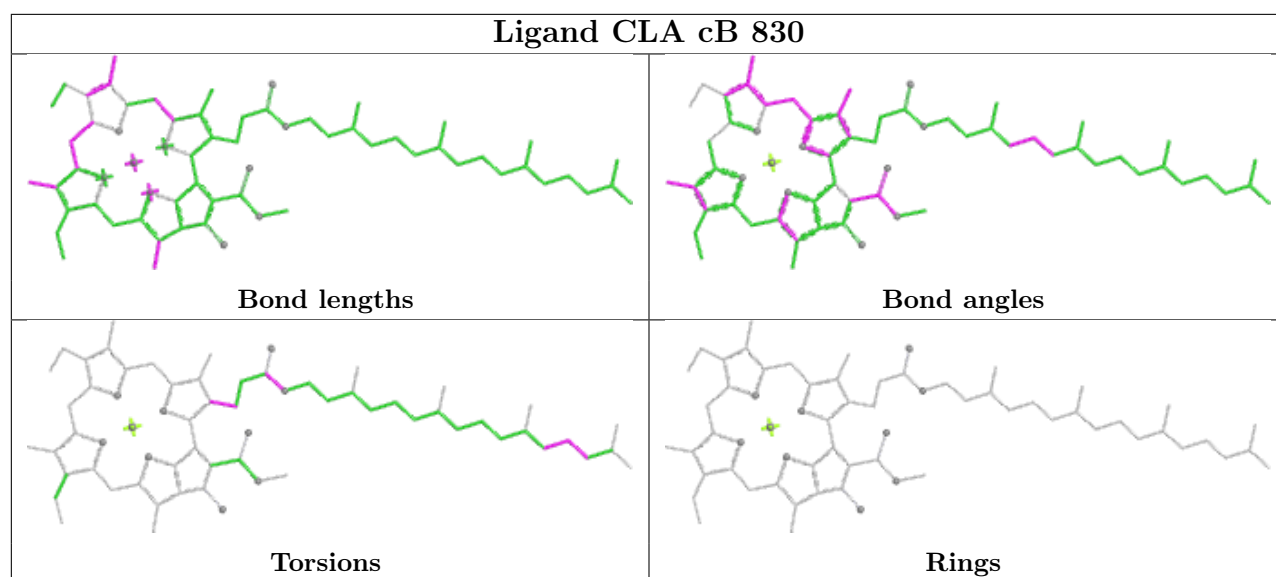
Ligand CLA bA 821

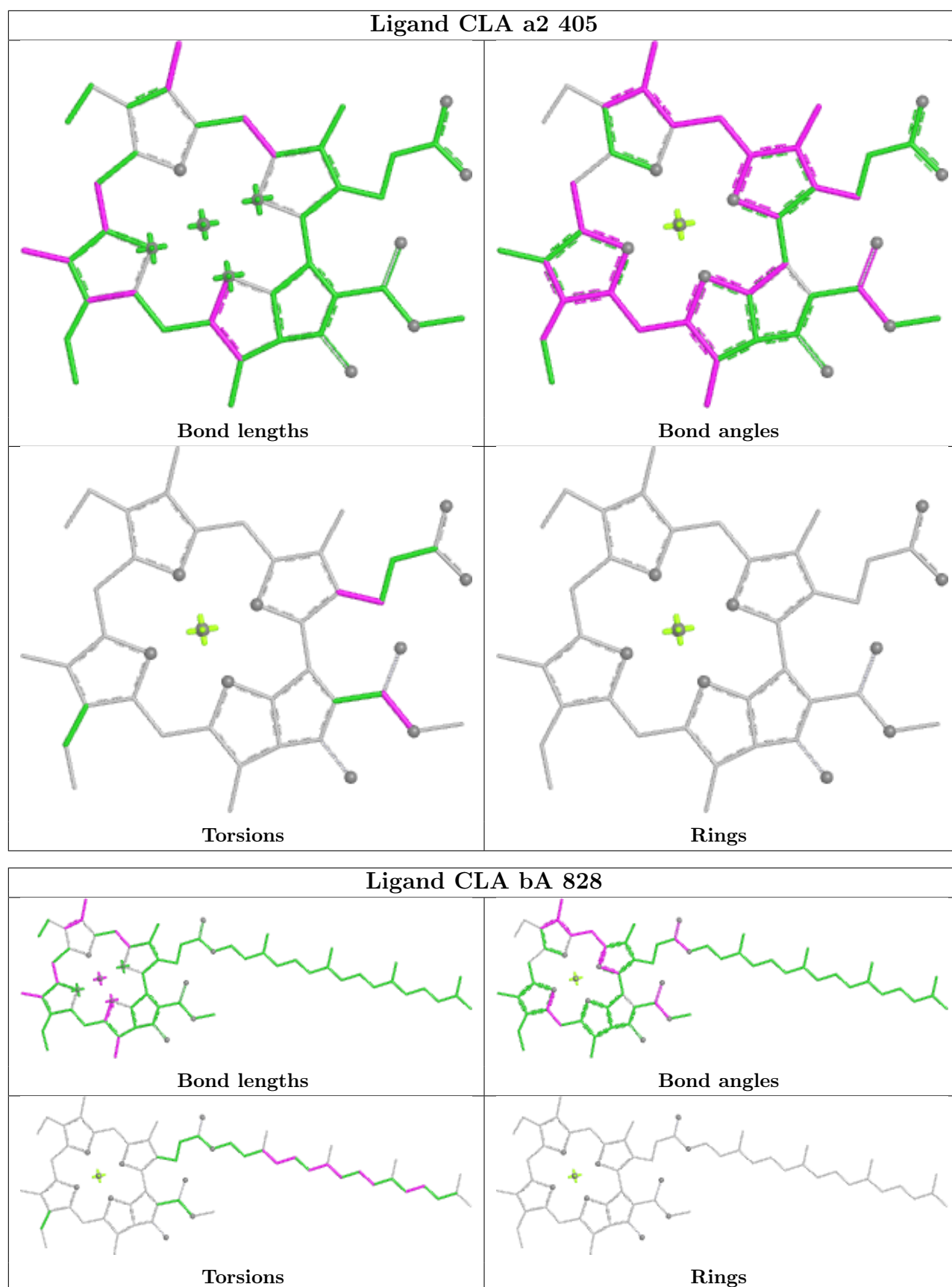


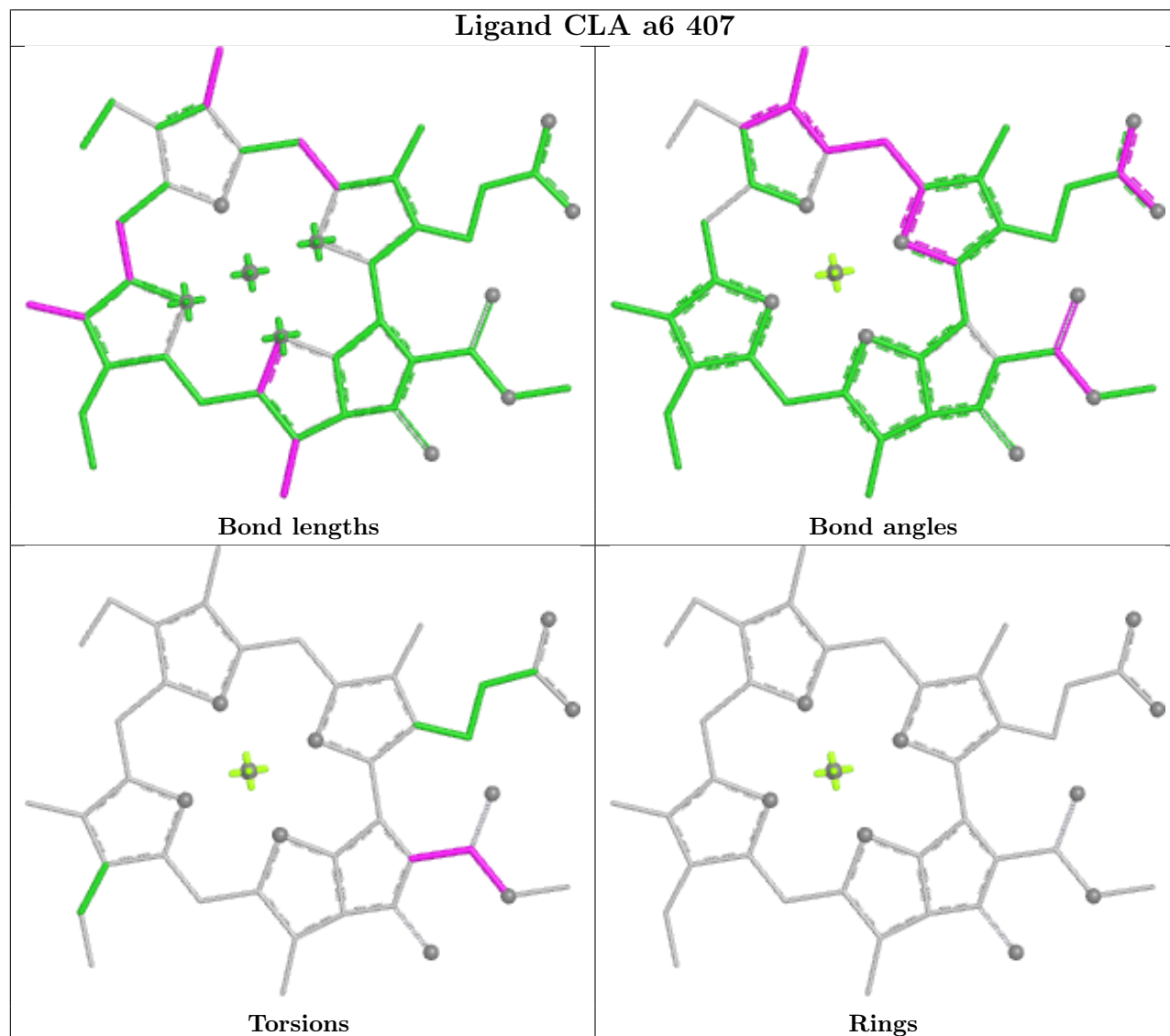
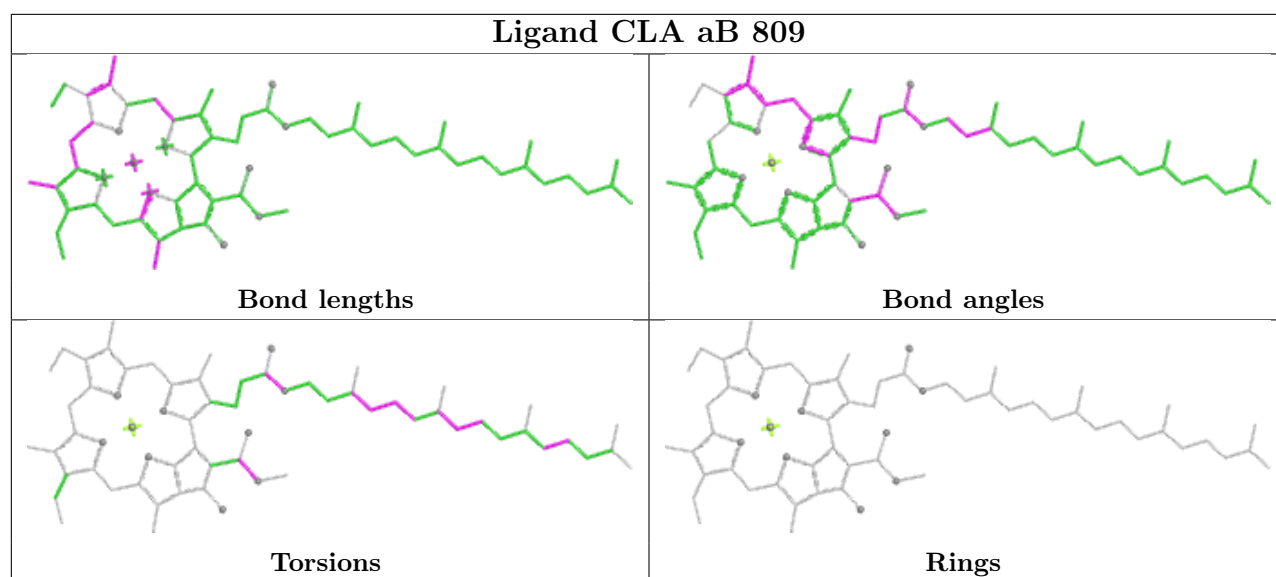


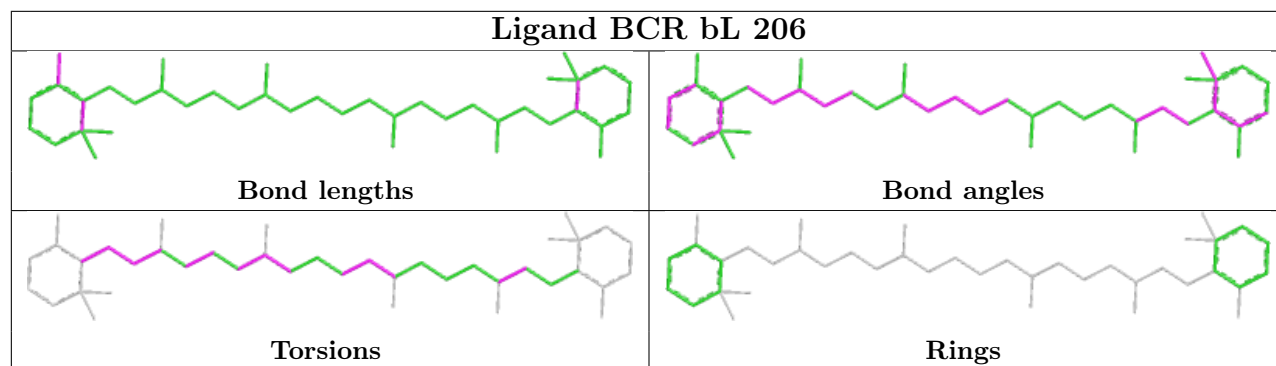
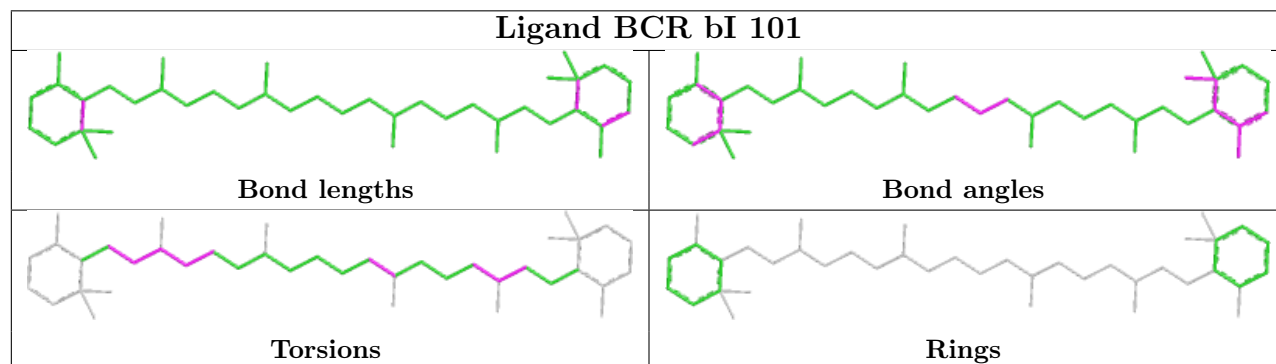
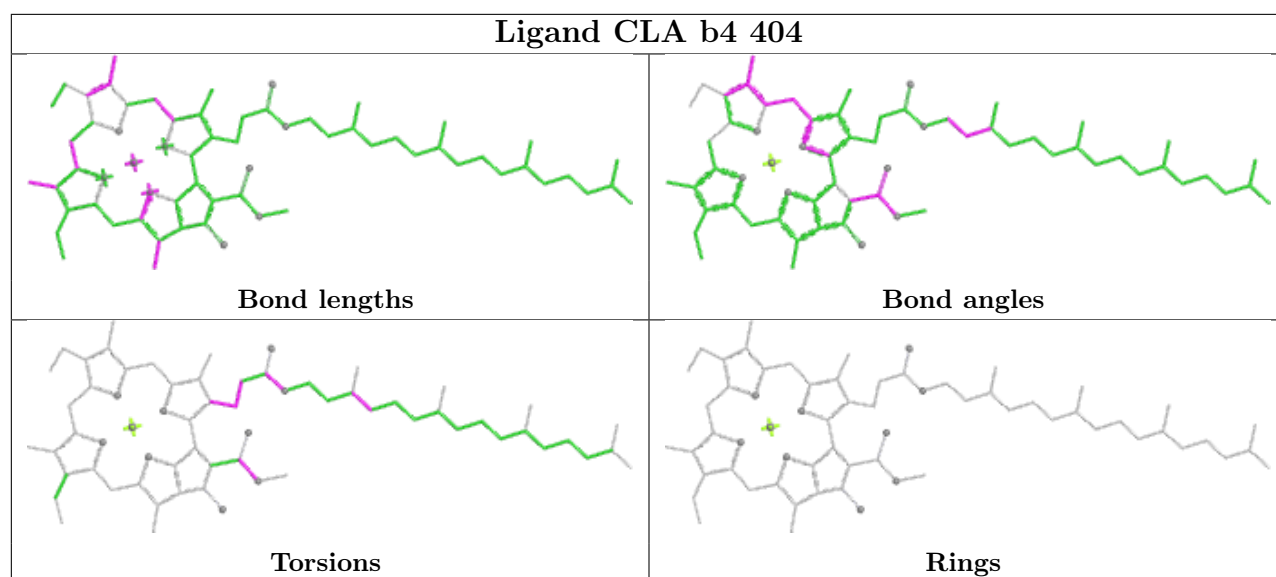


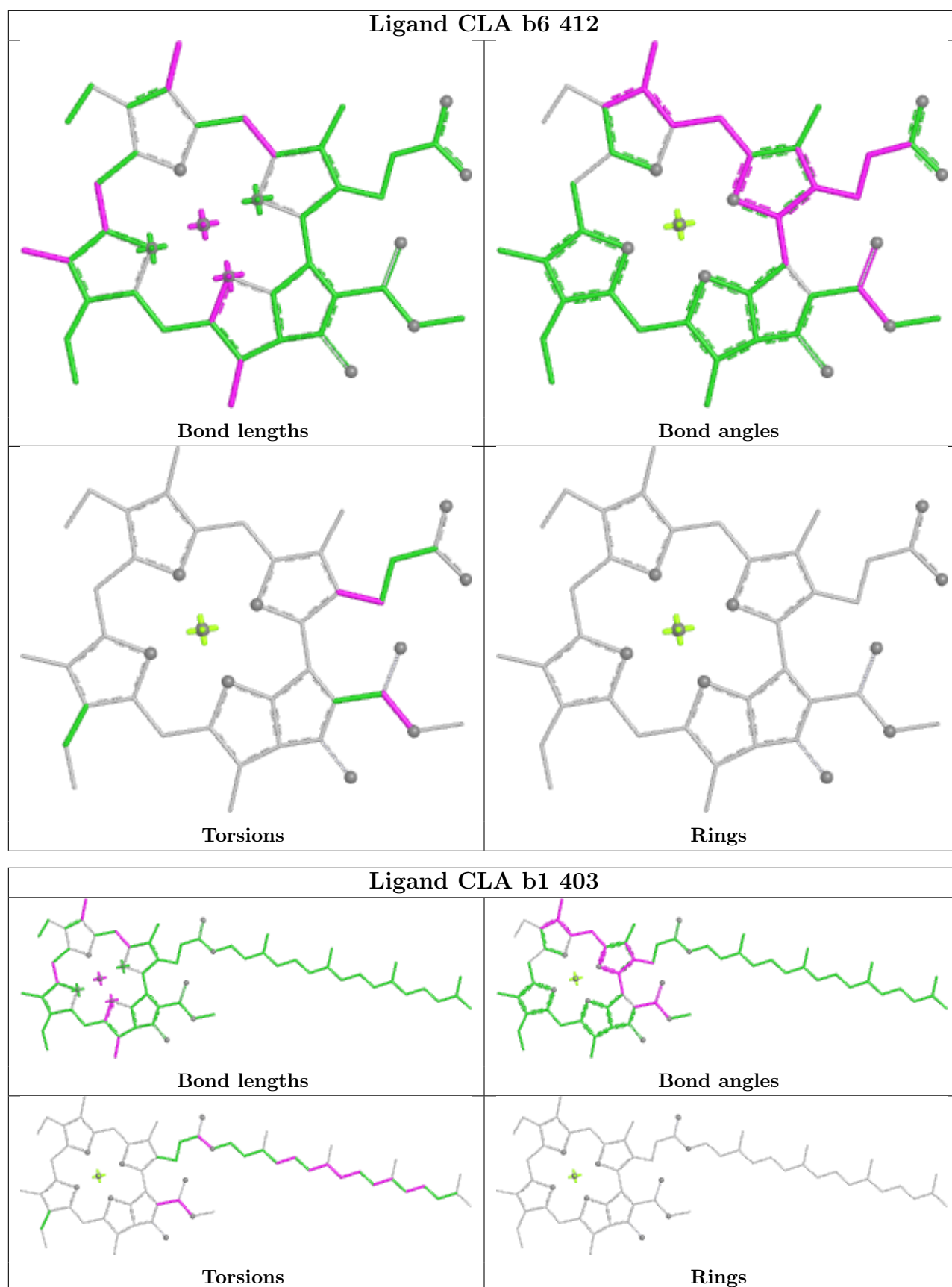


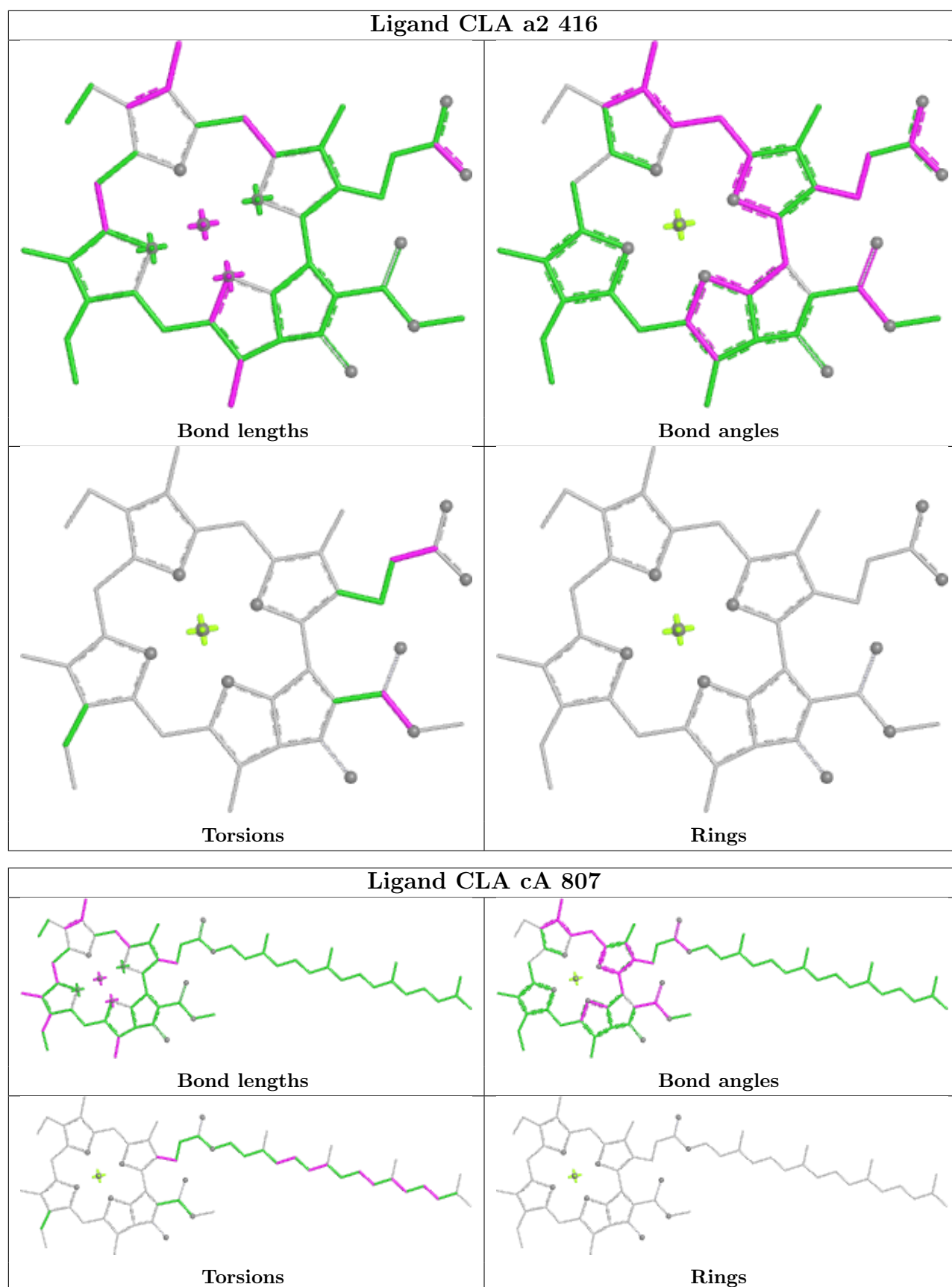


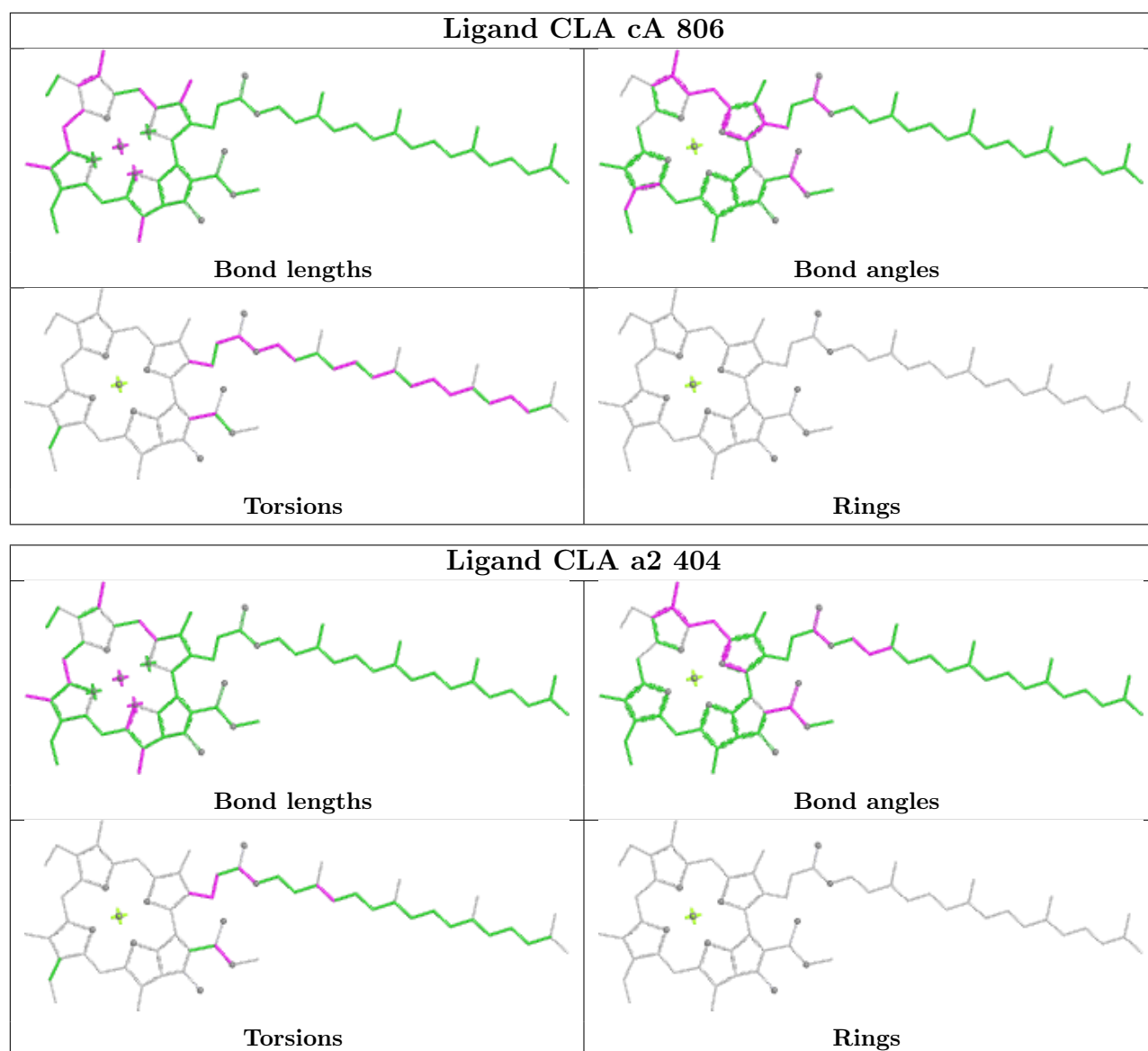


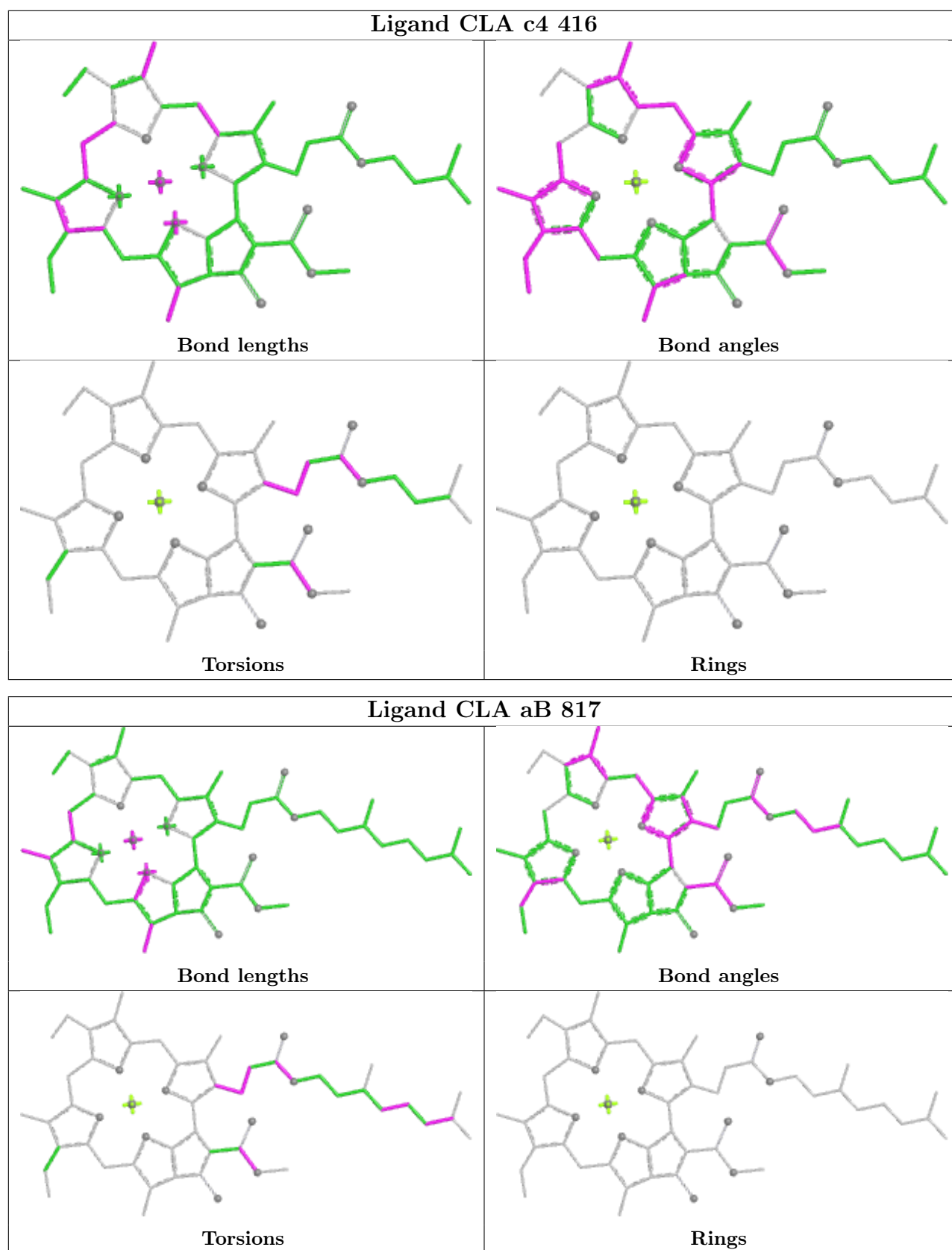


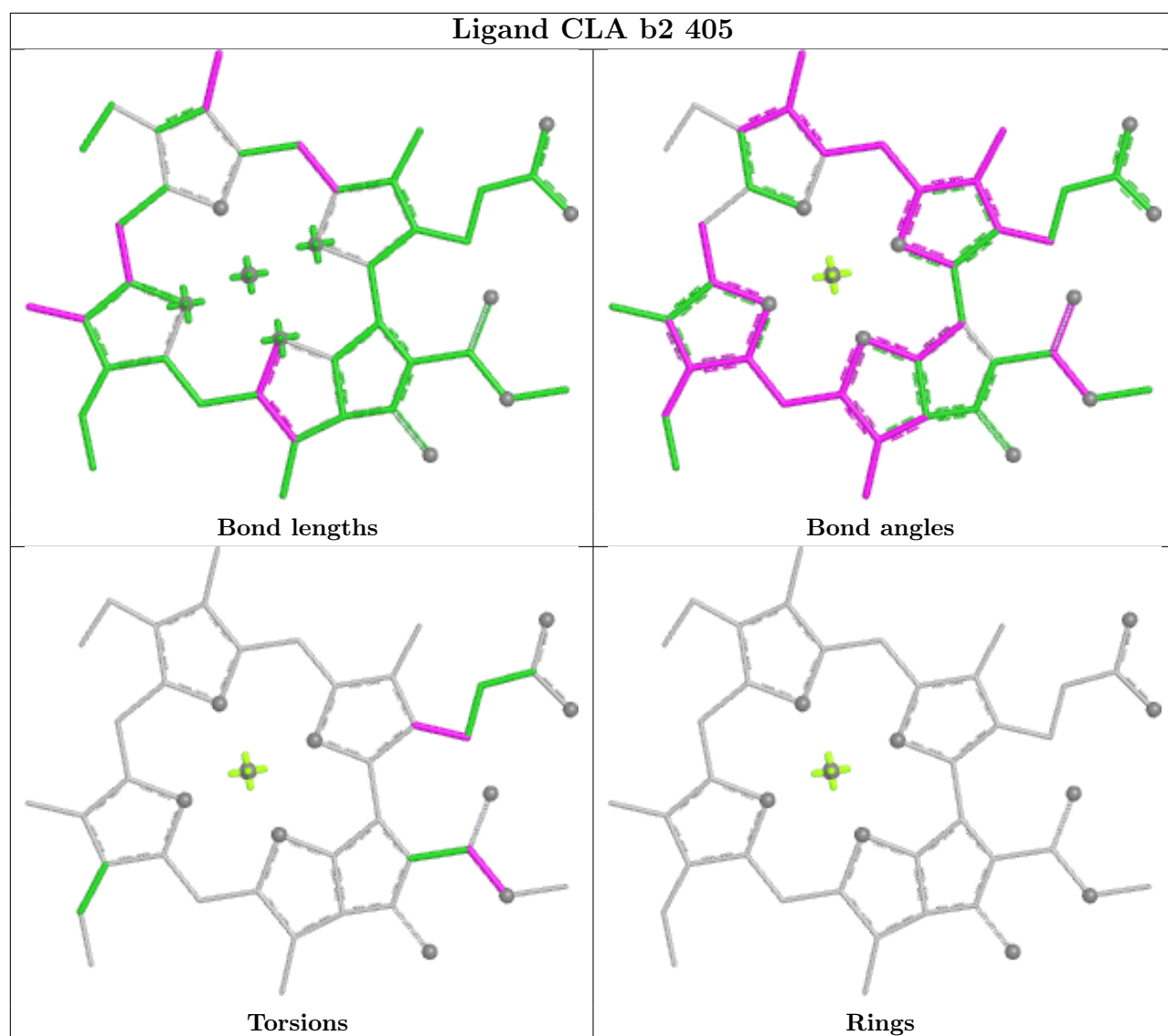


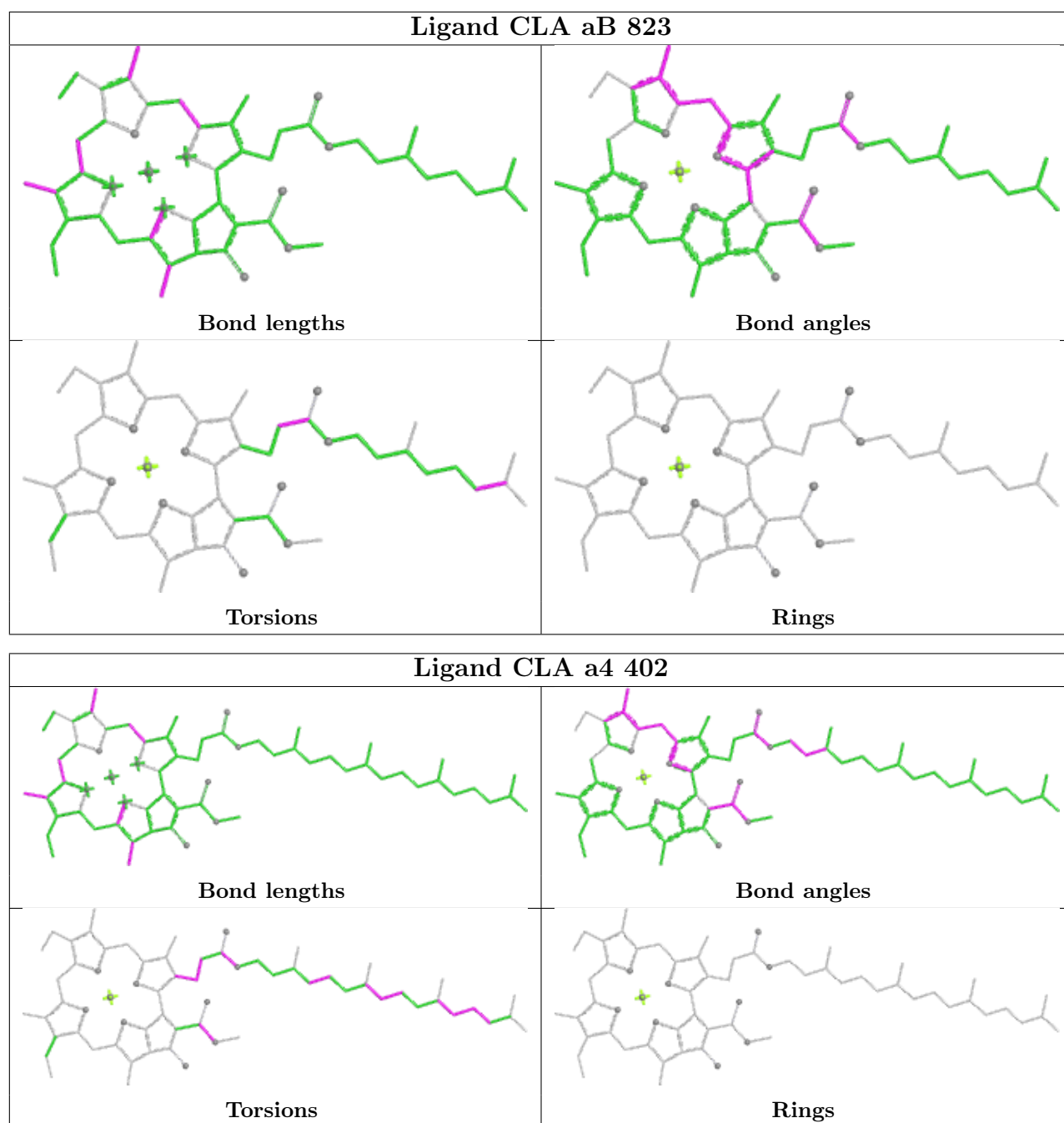




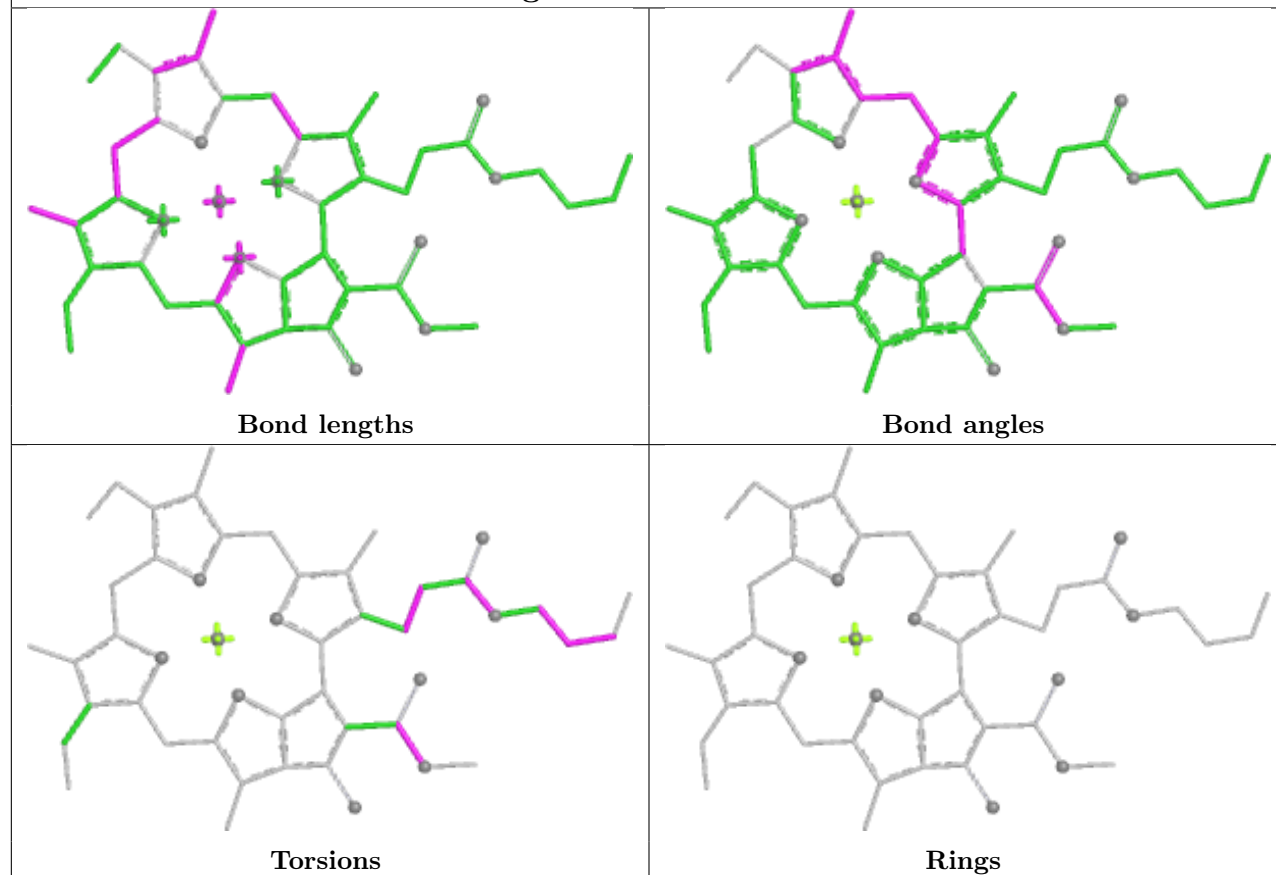




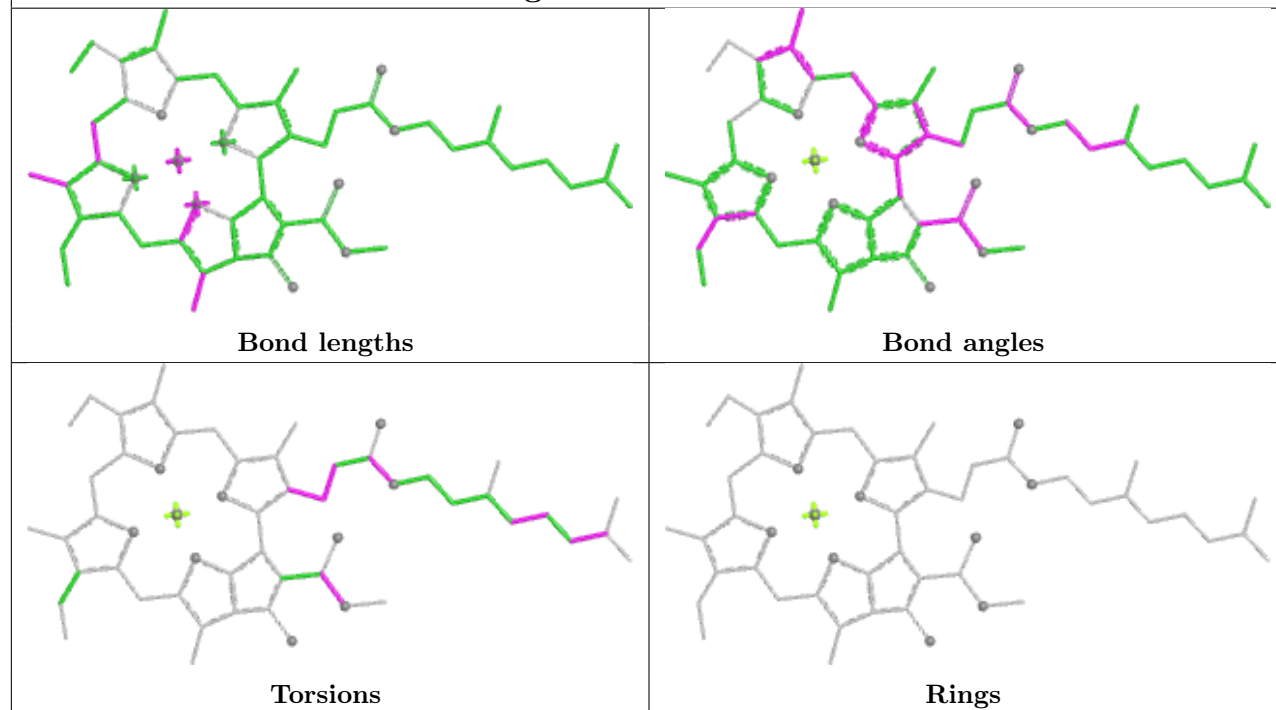


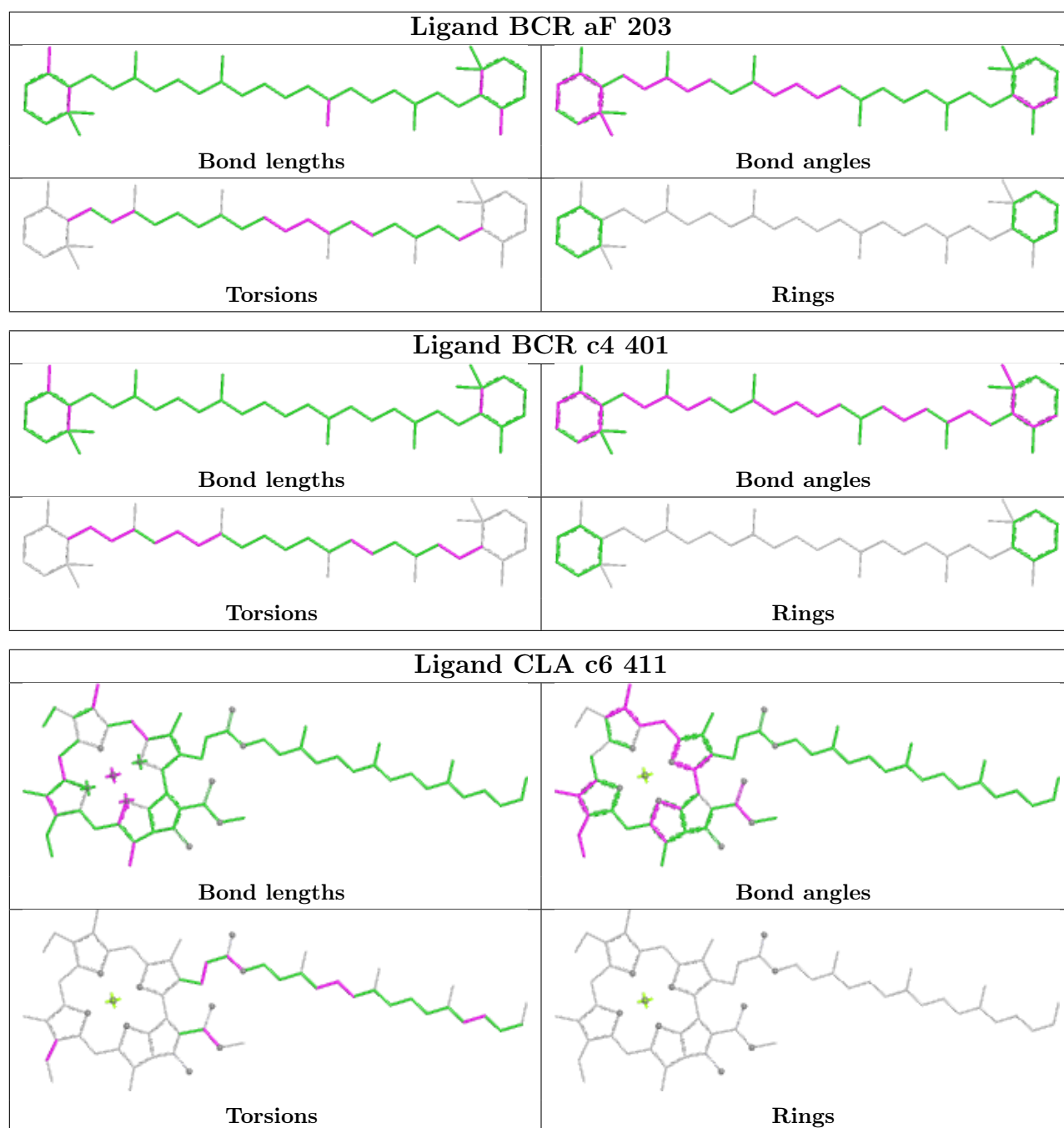


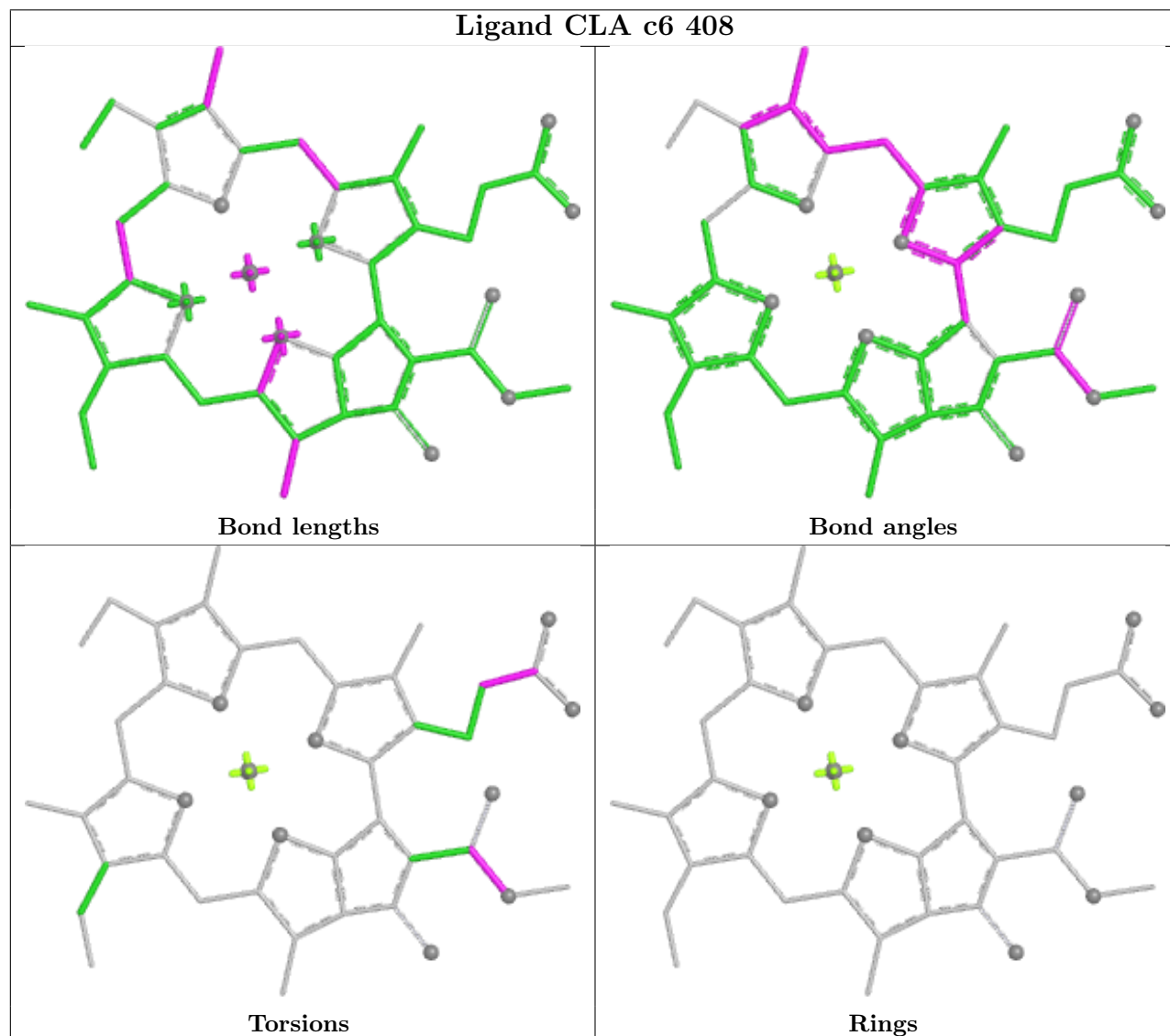
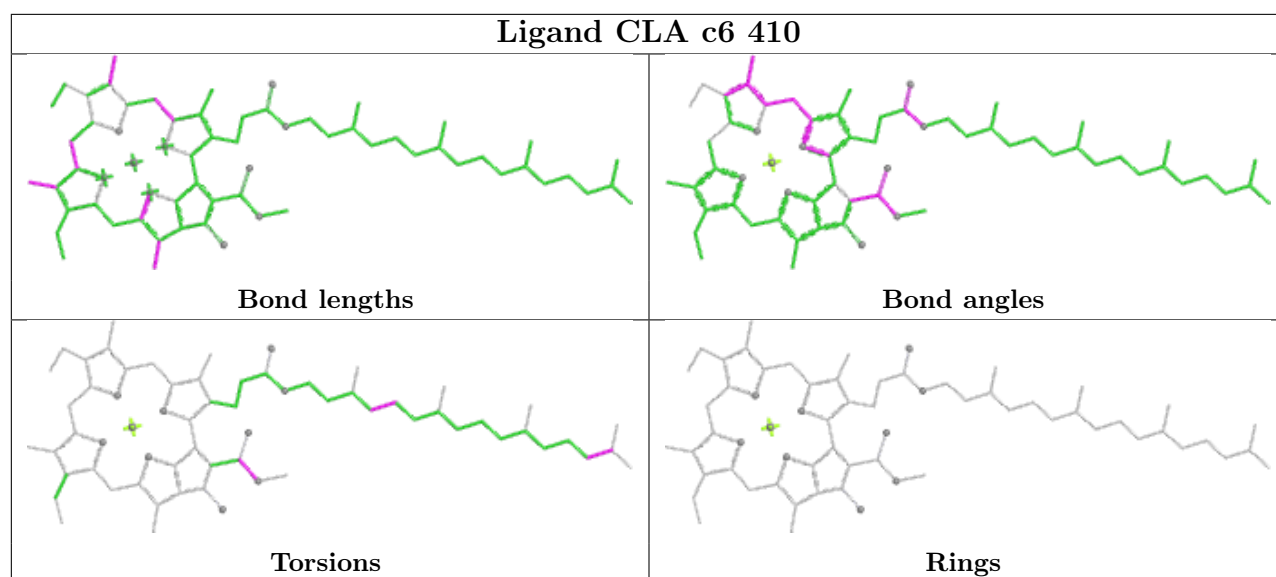
Ligand CLA bB 832

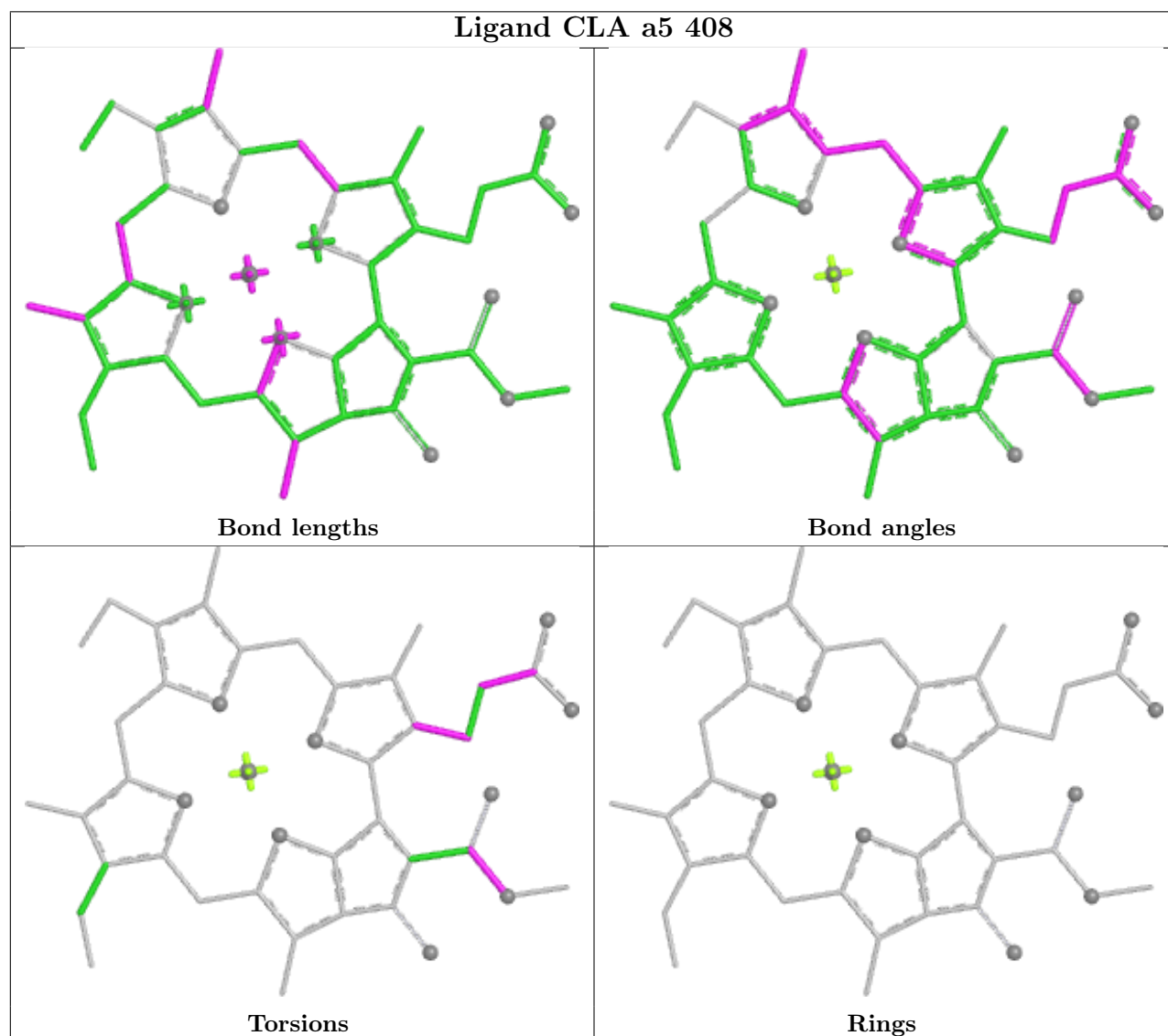
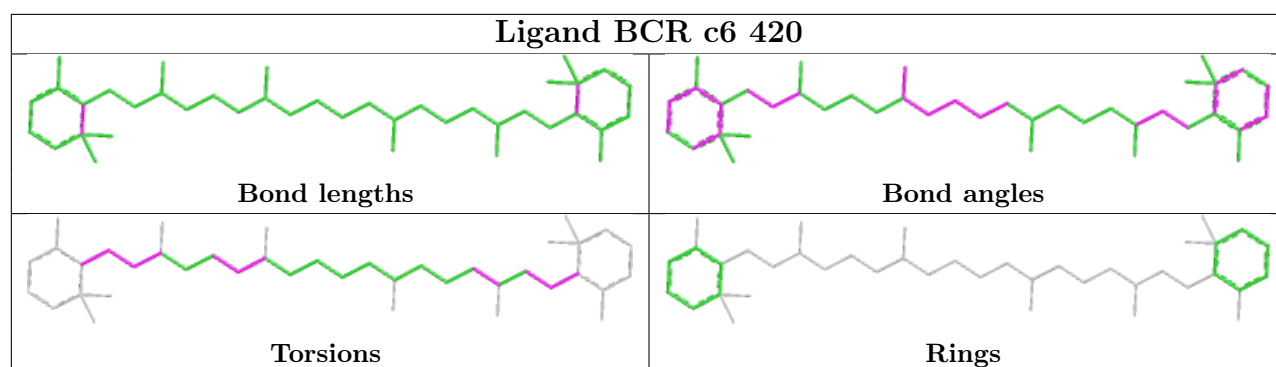


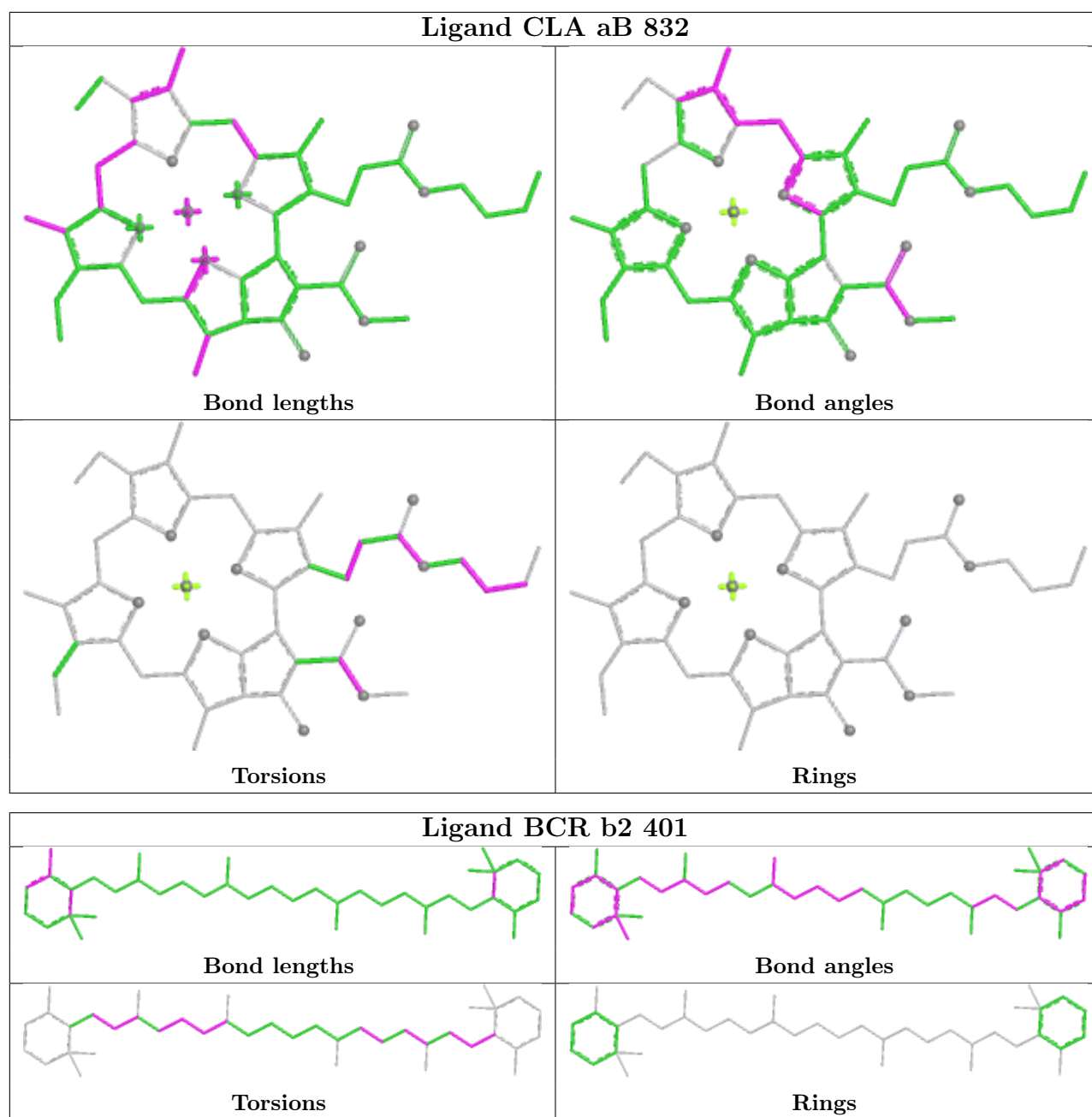
Ligand CLA cB 817

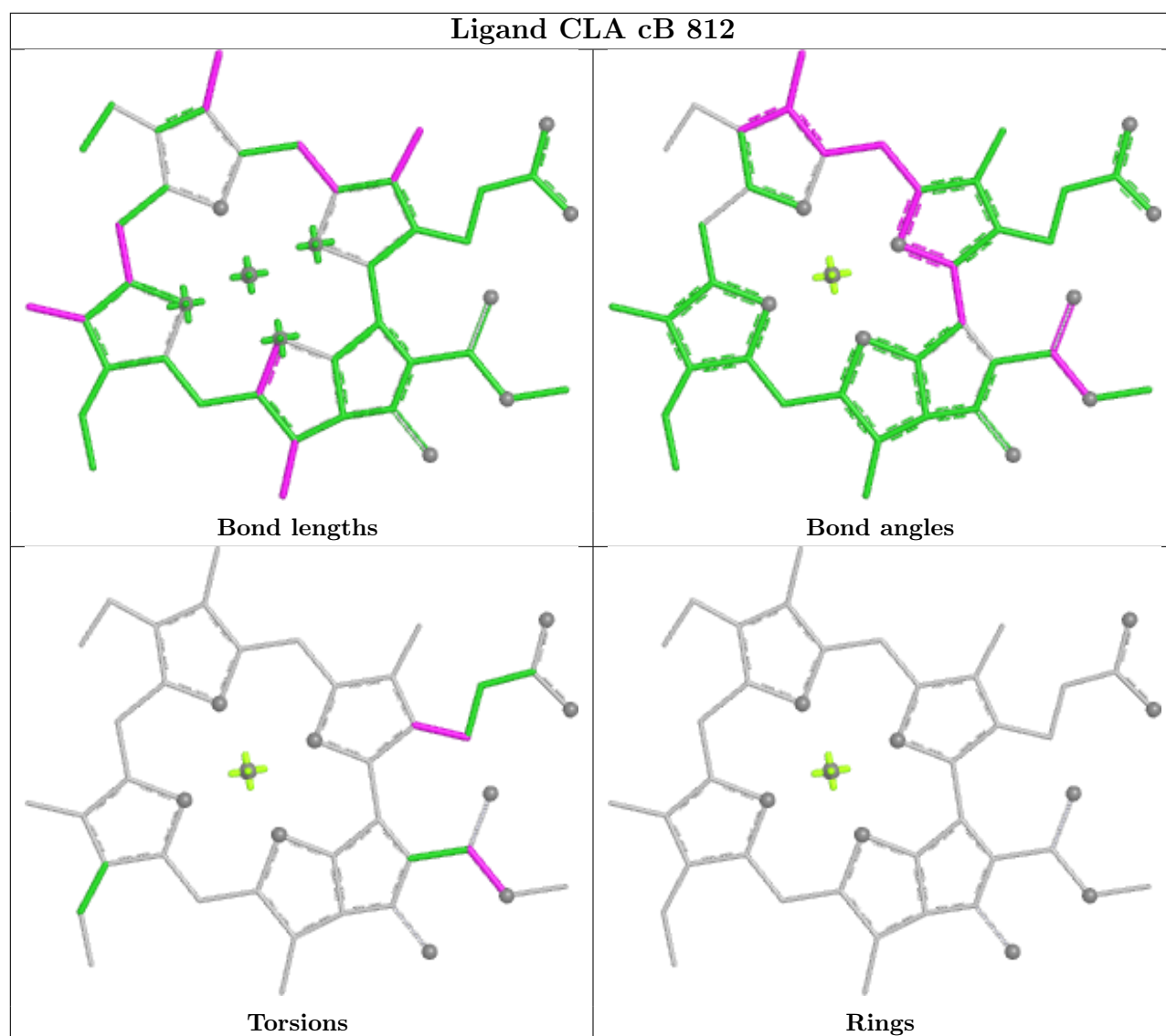


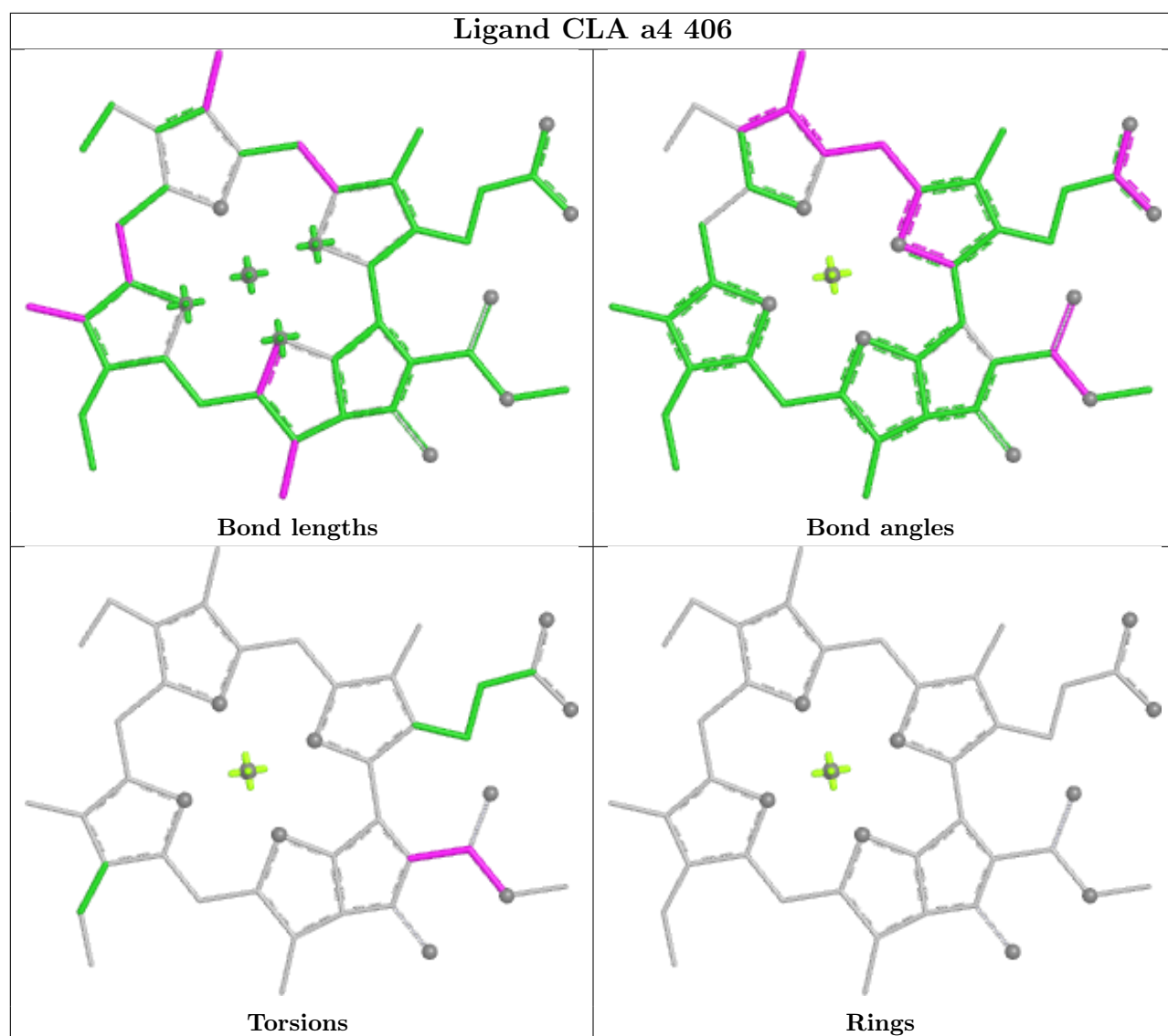


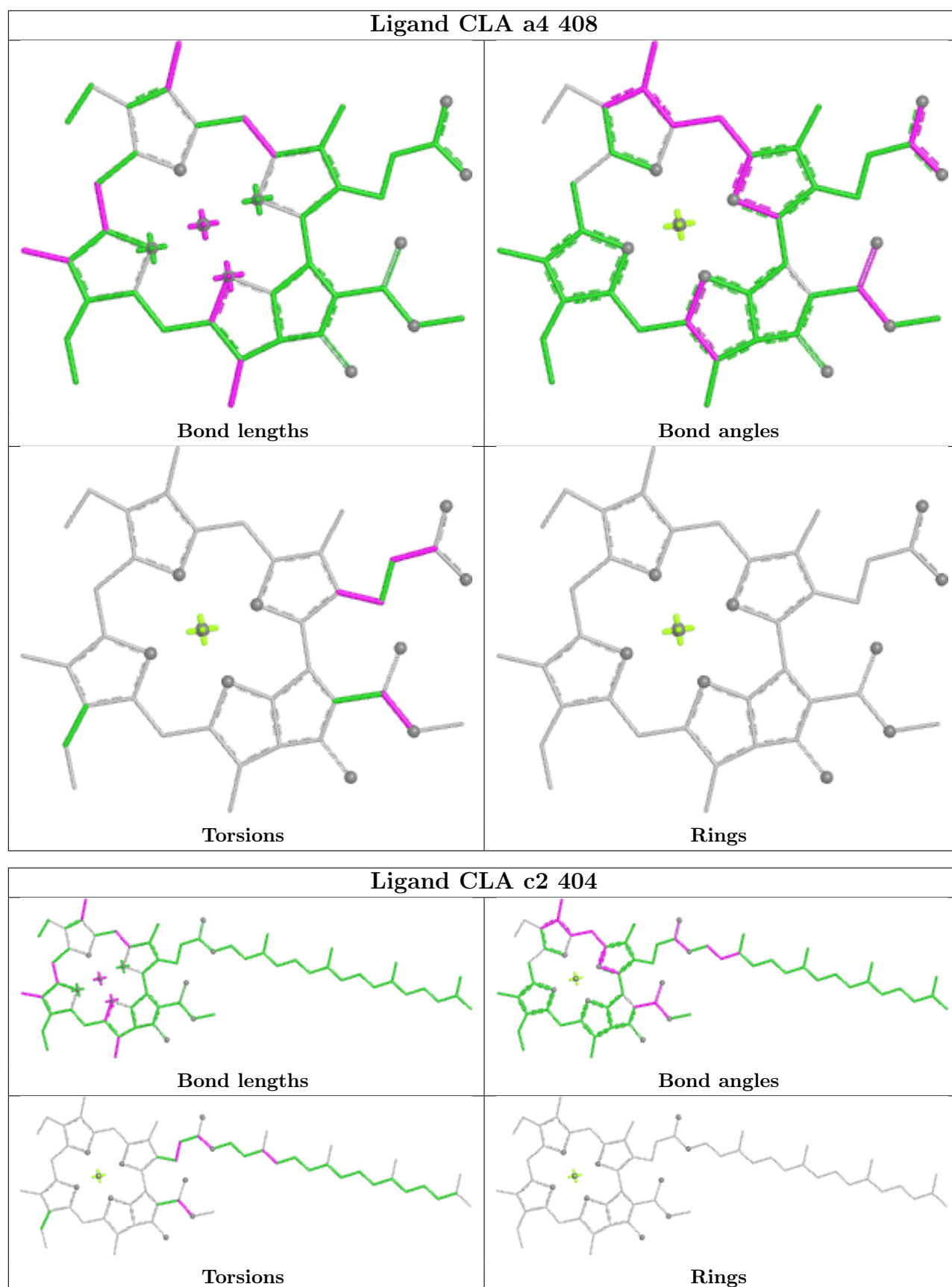


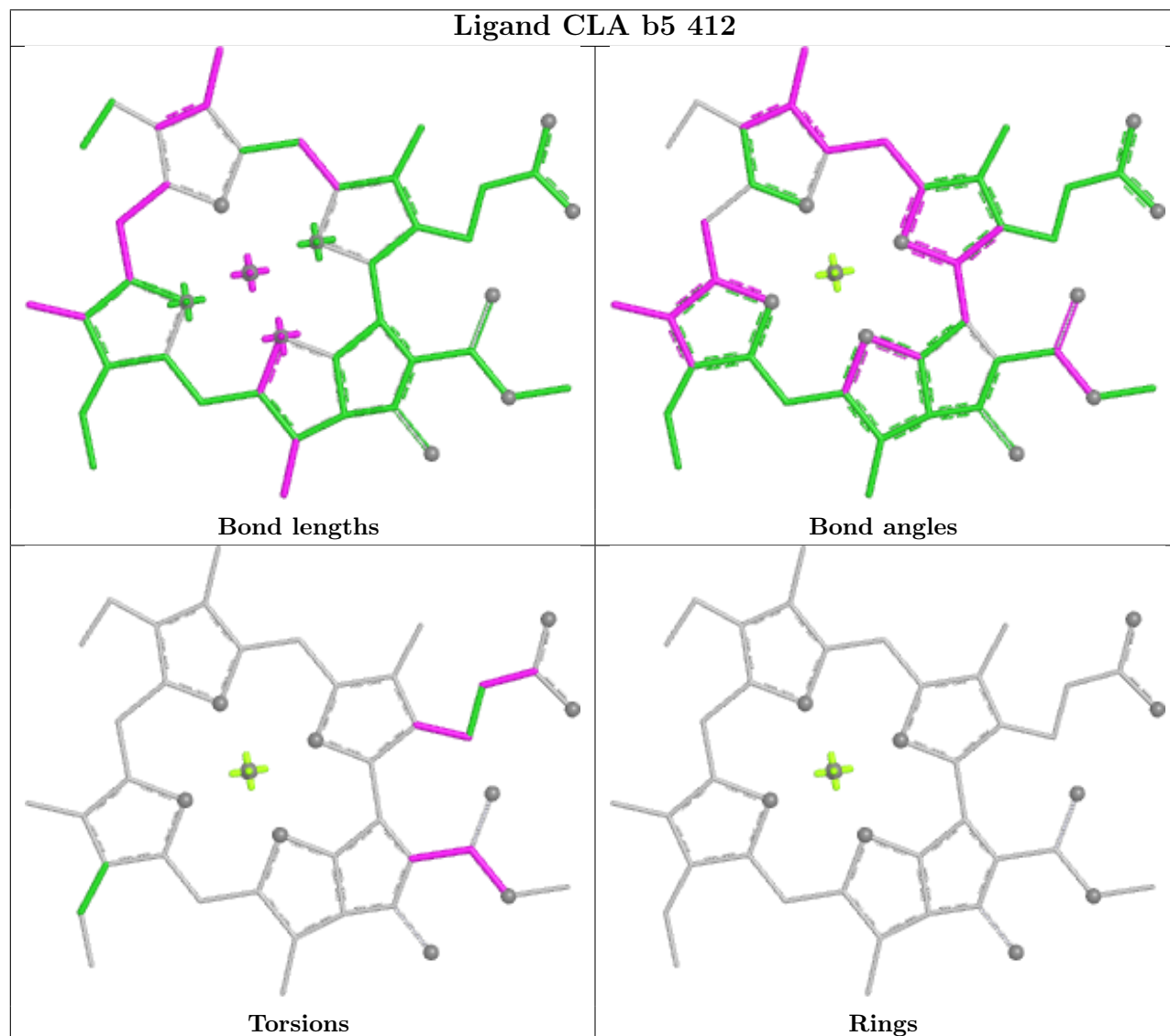
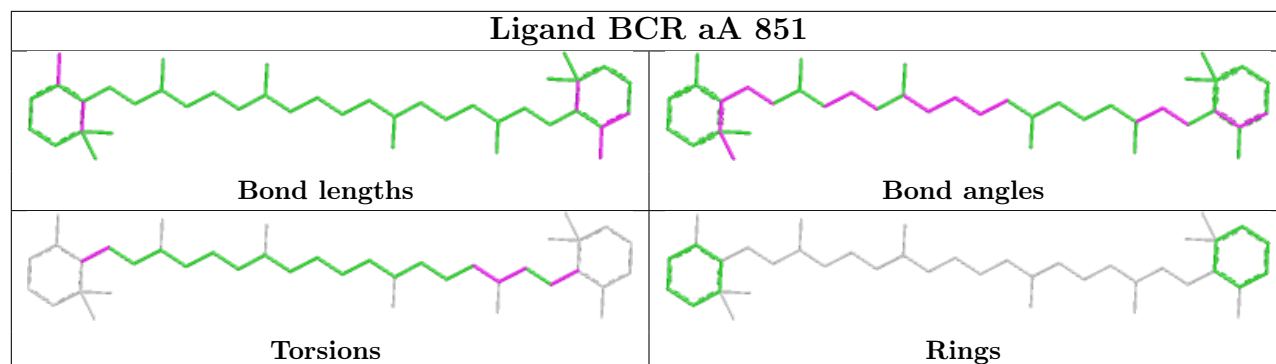


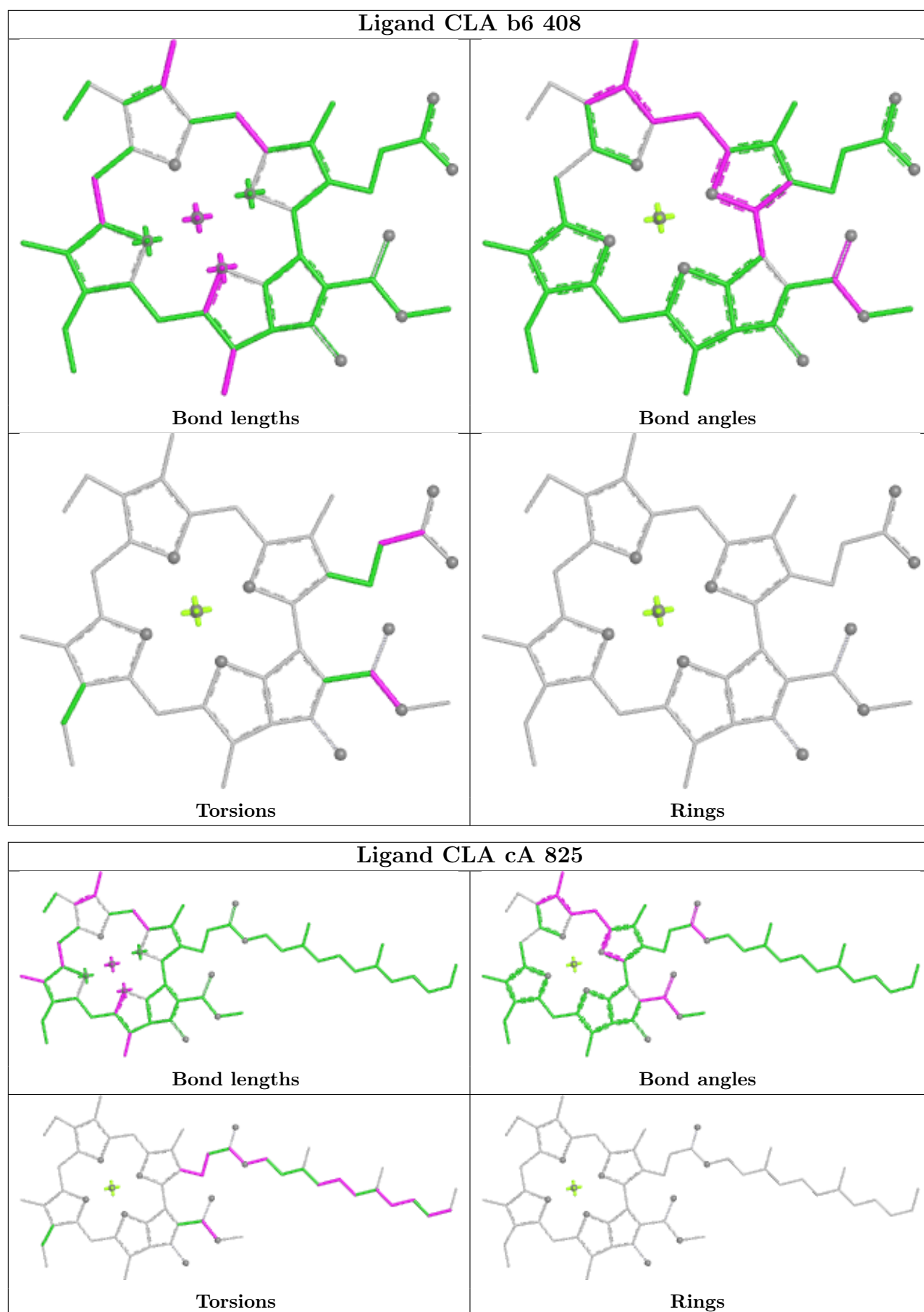


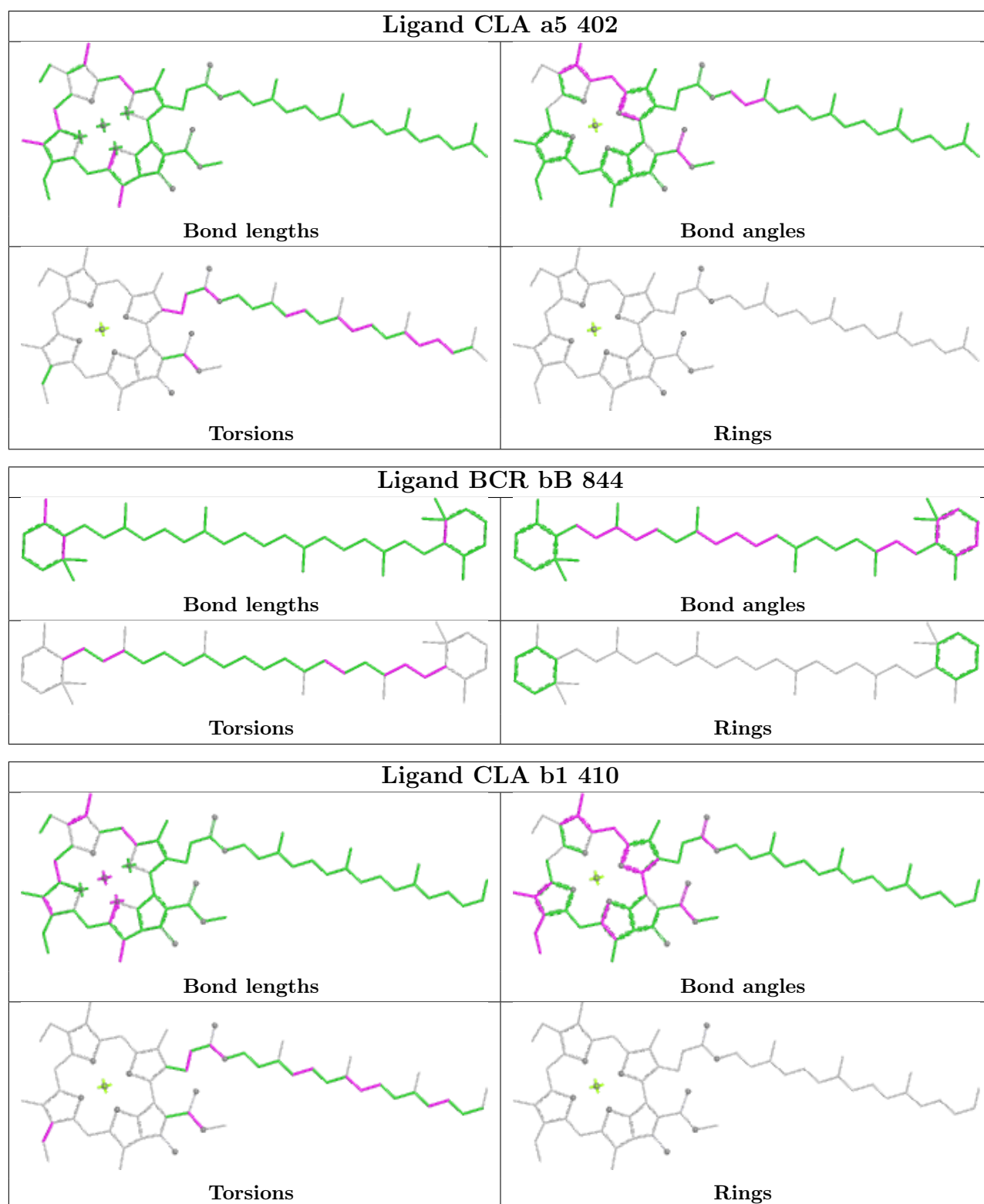


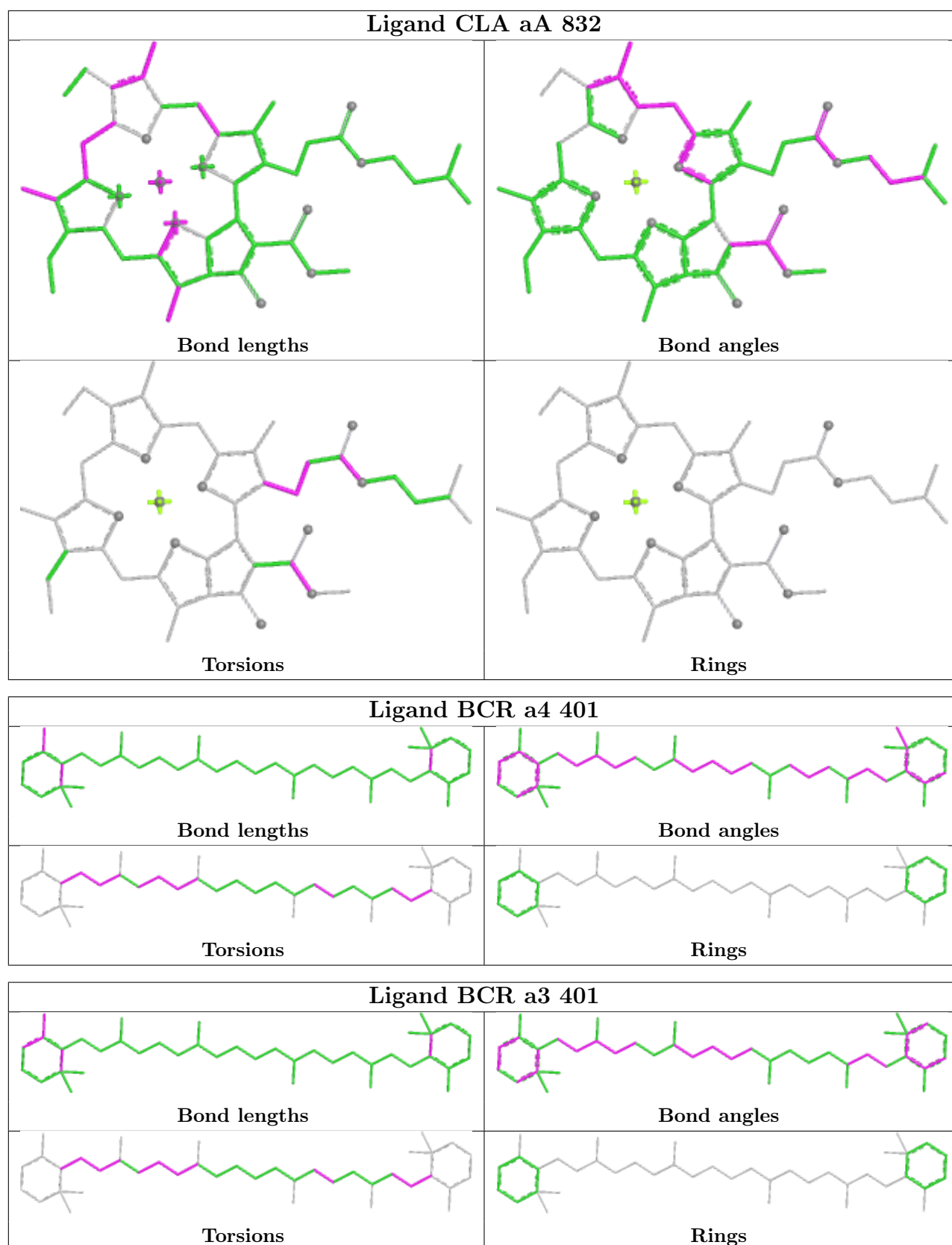


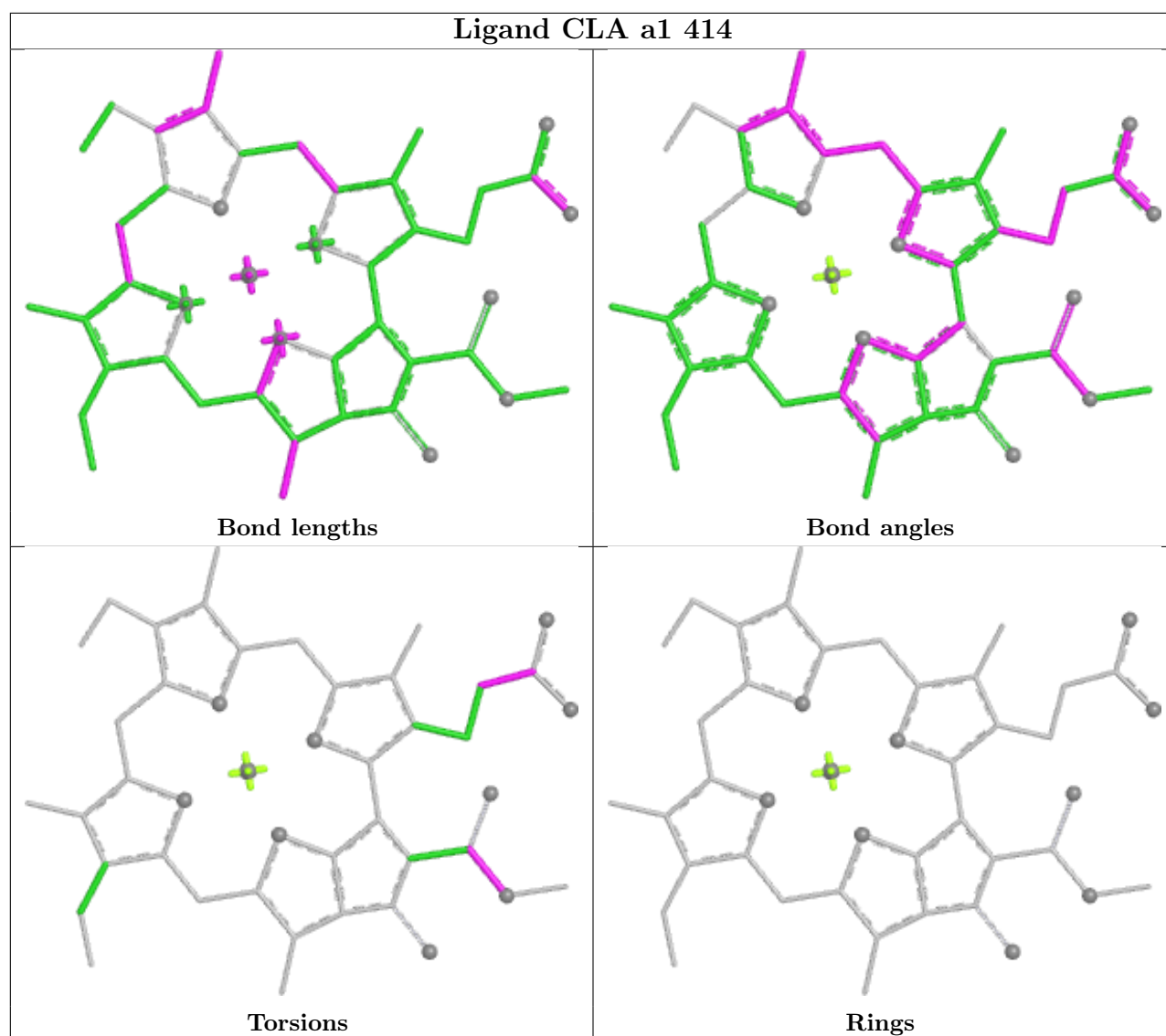


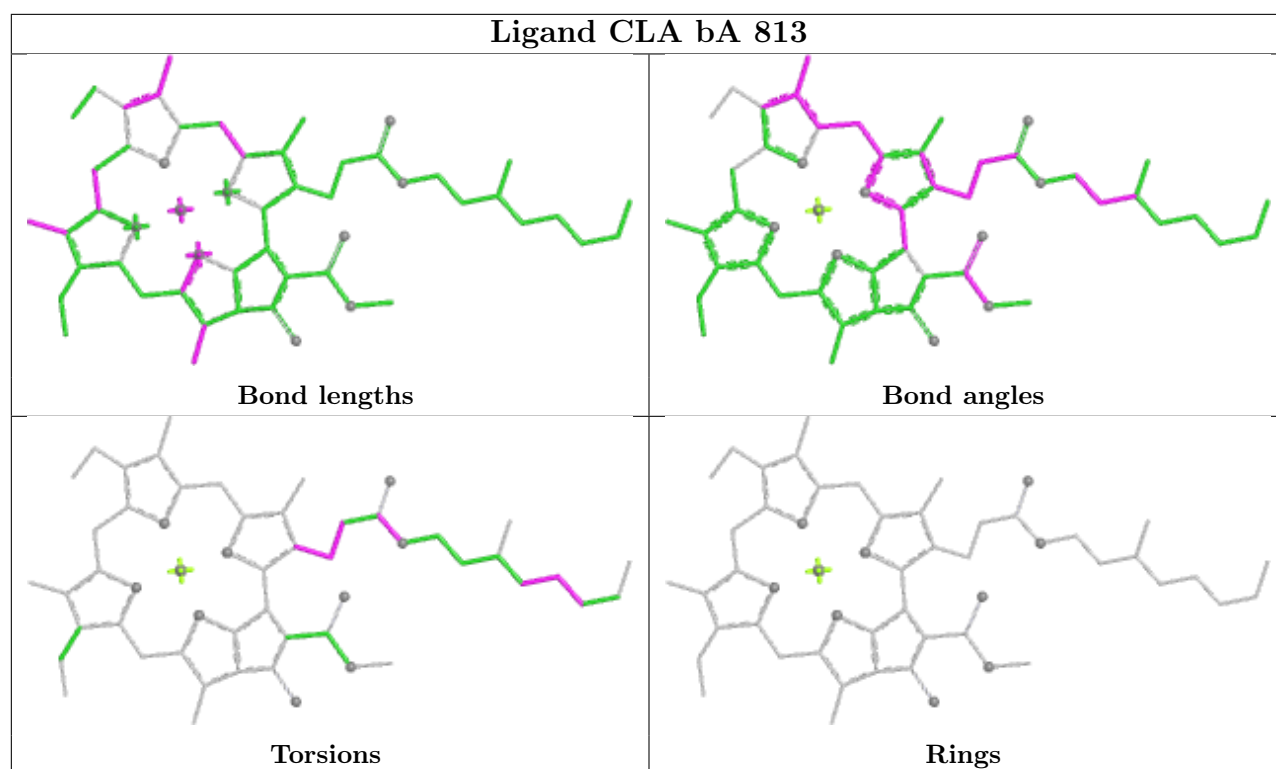


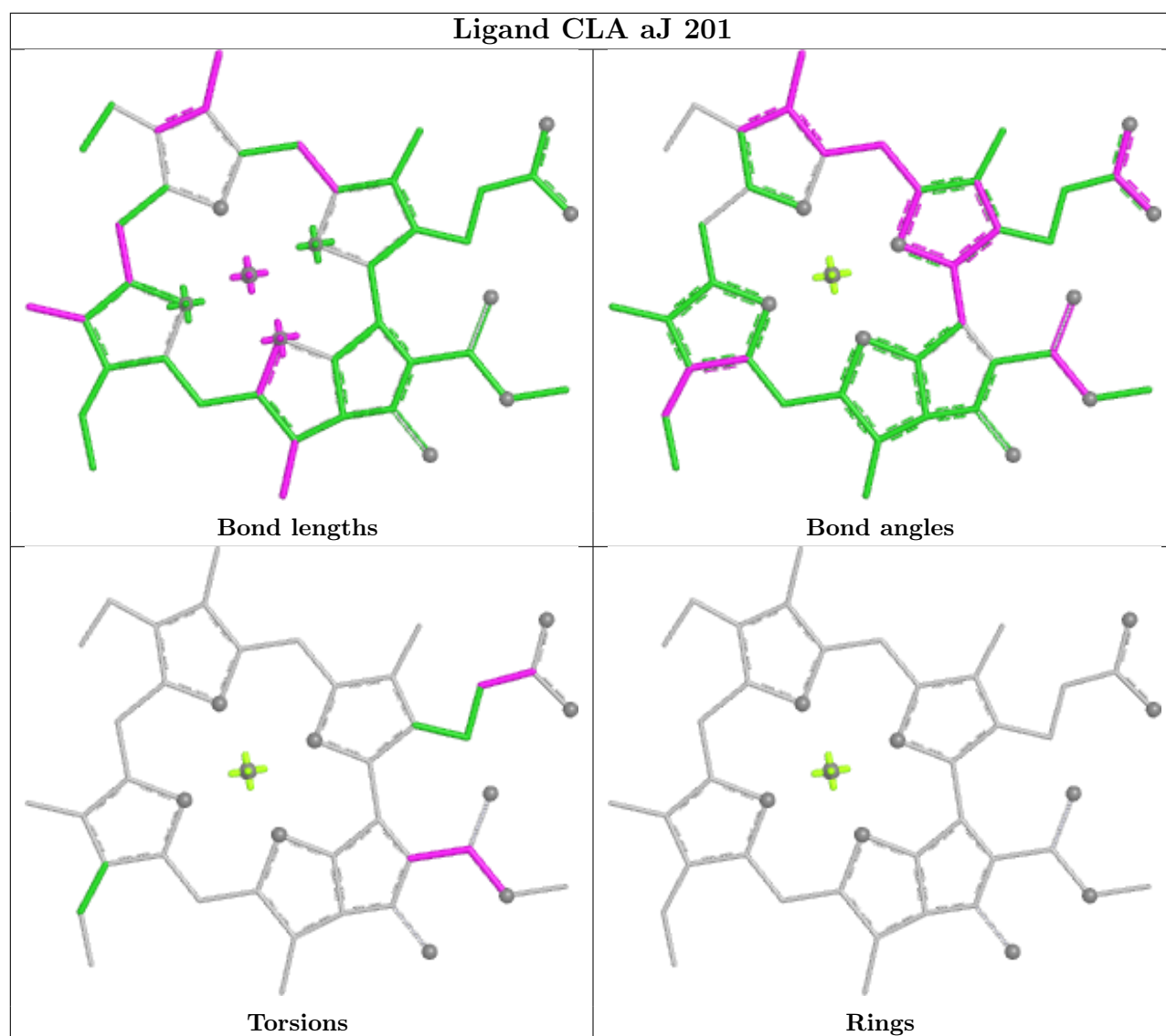


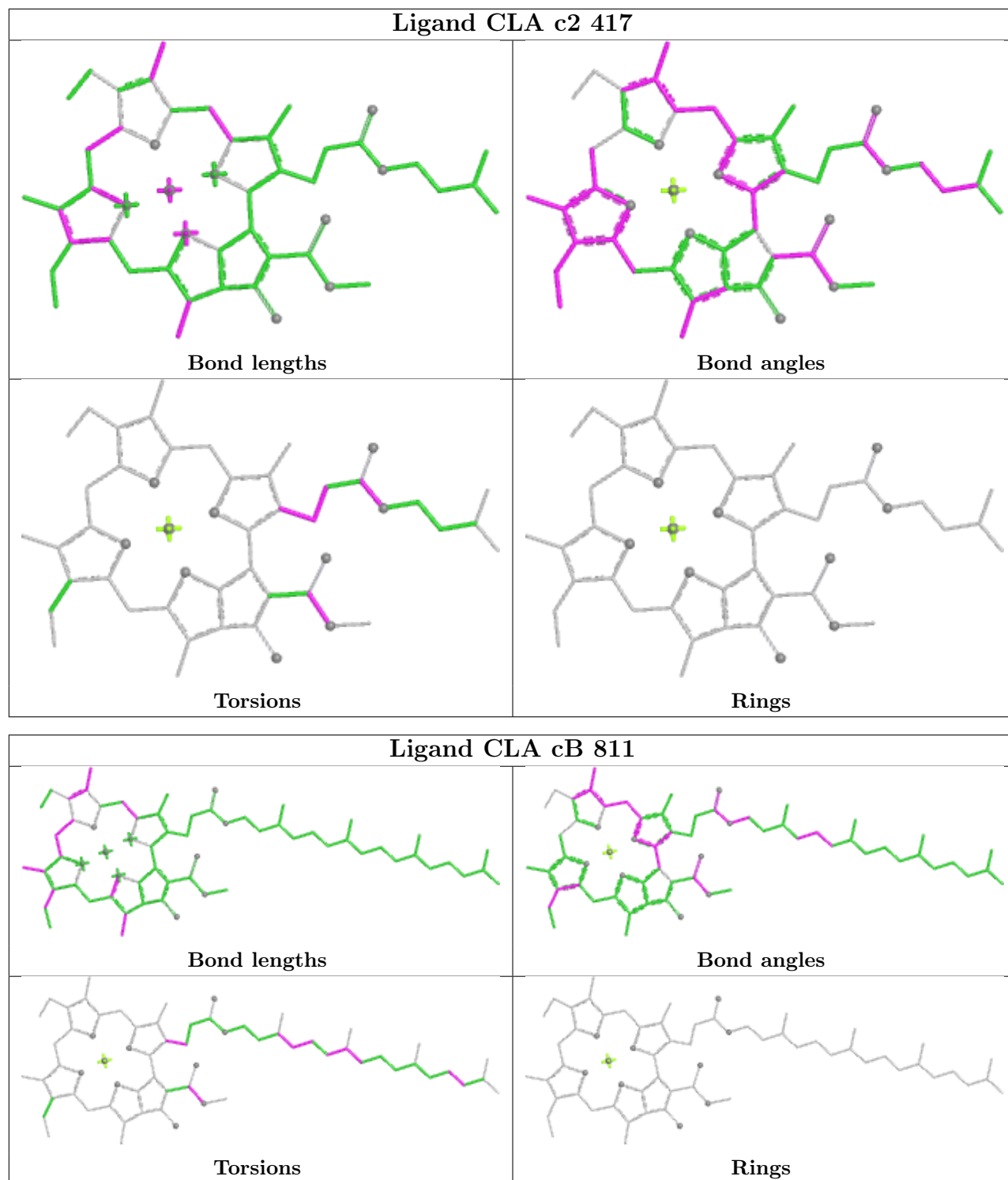


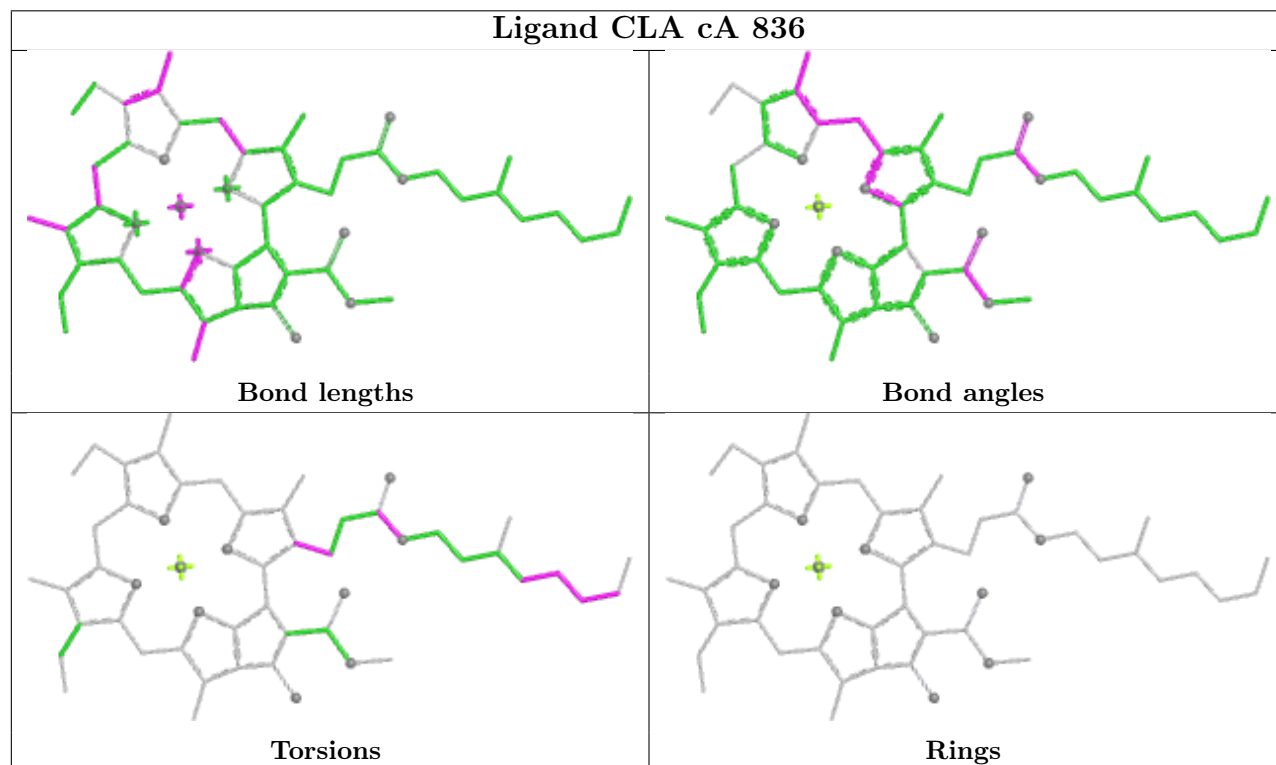
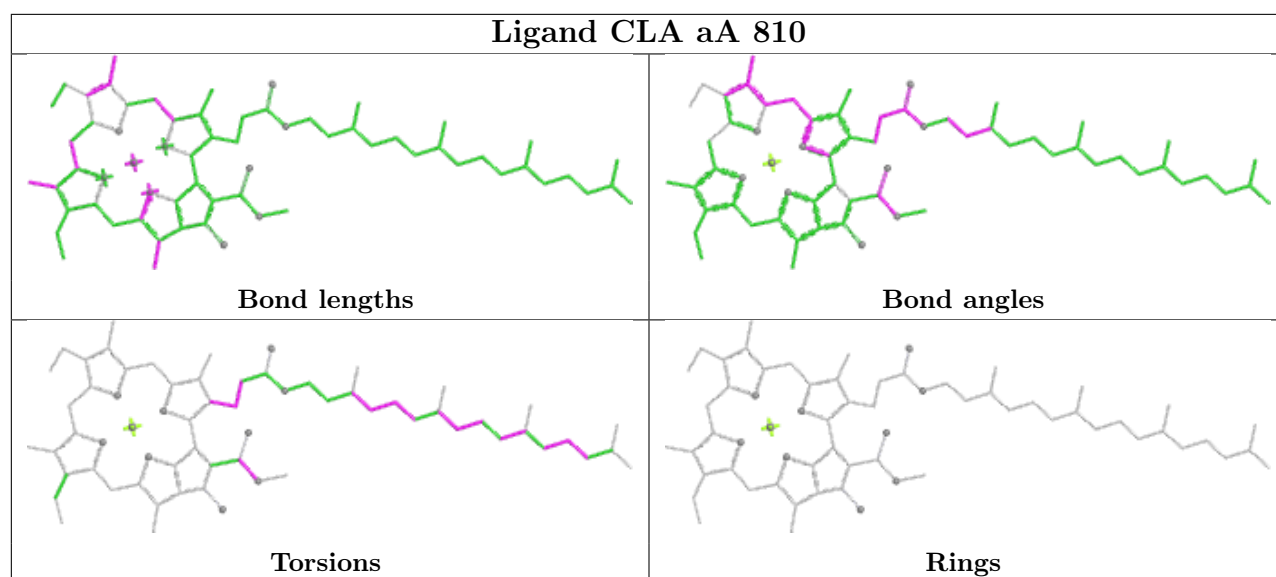


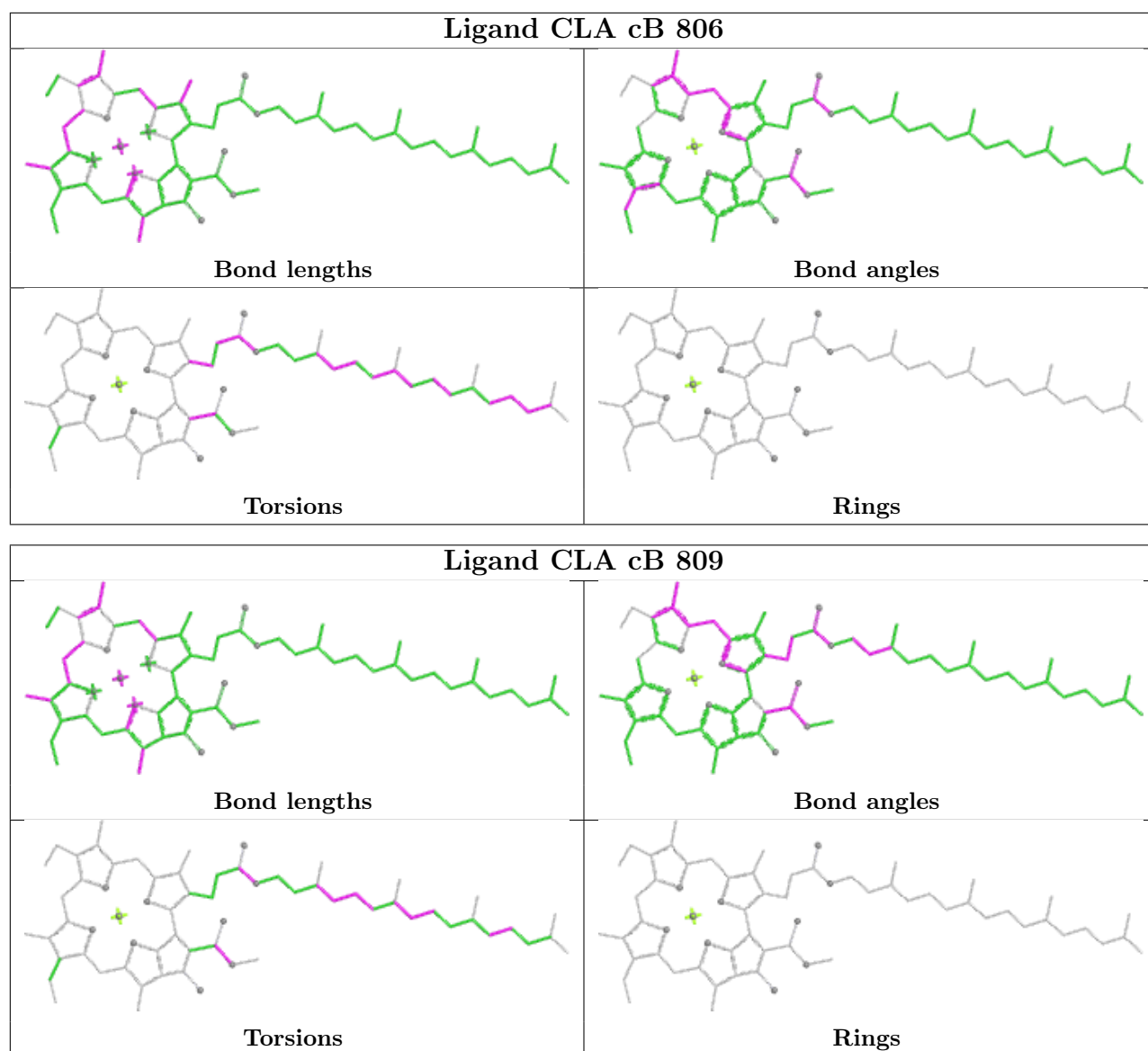


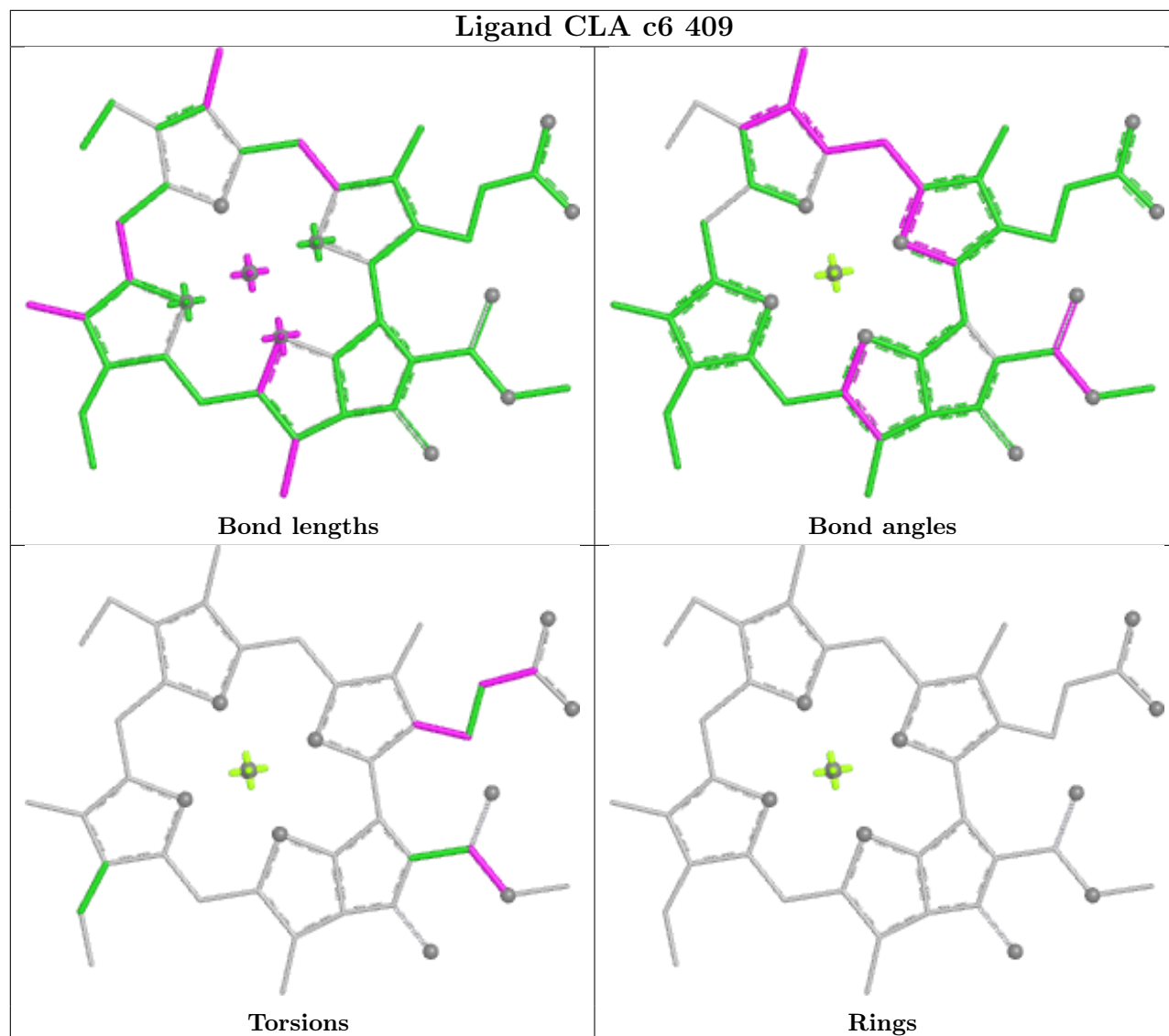


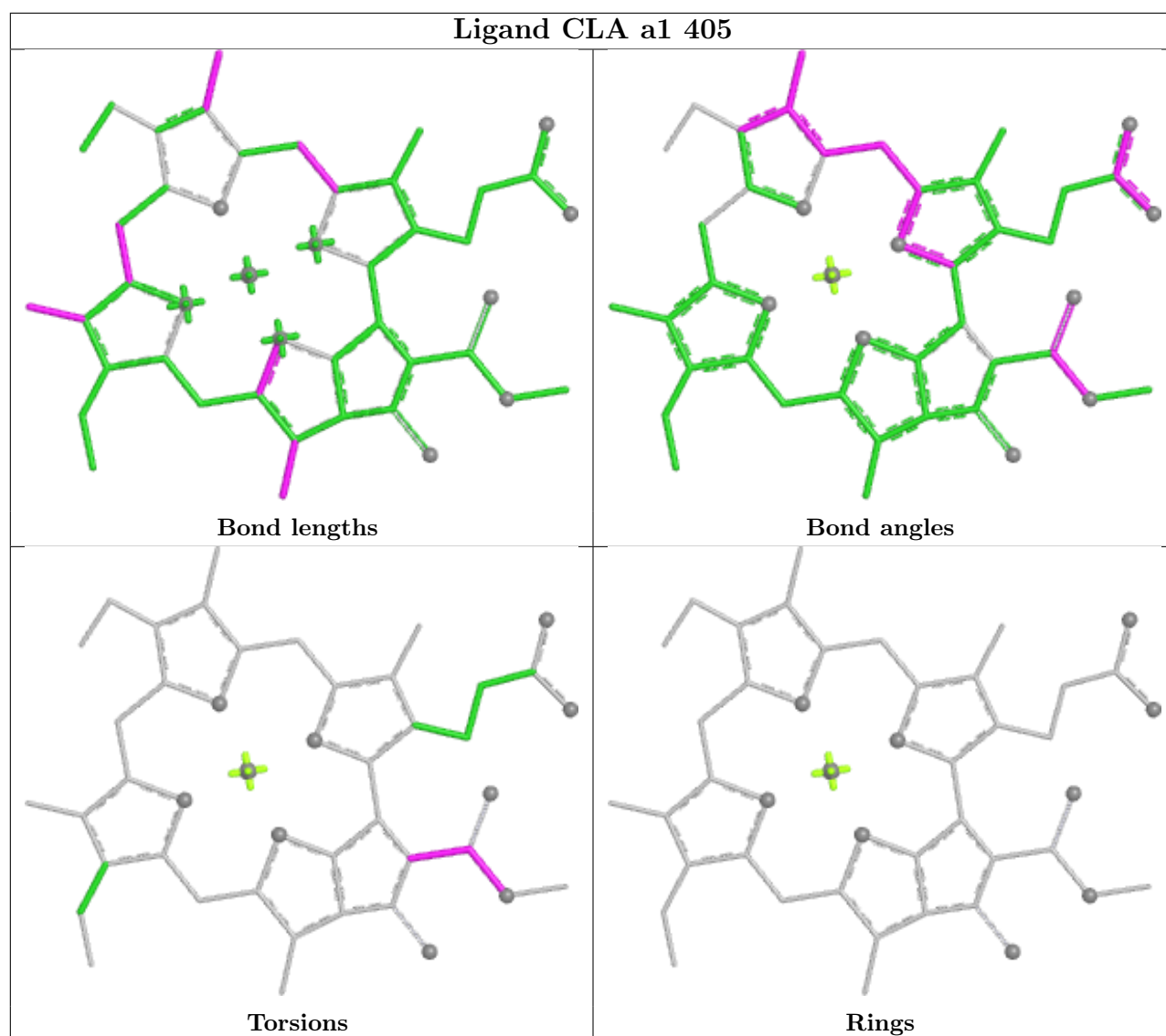


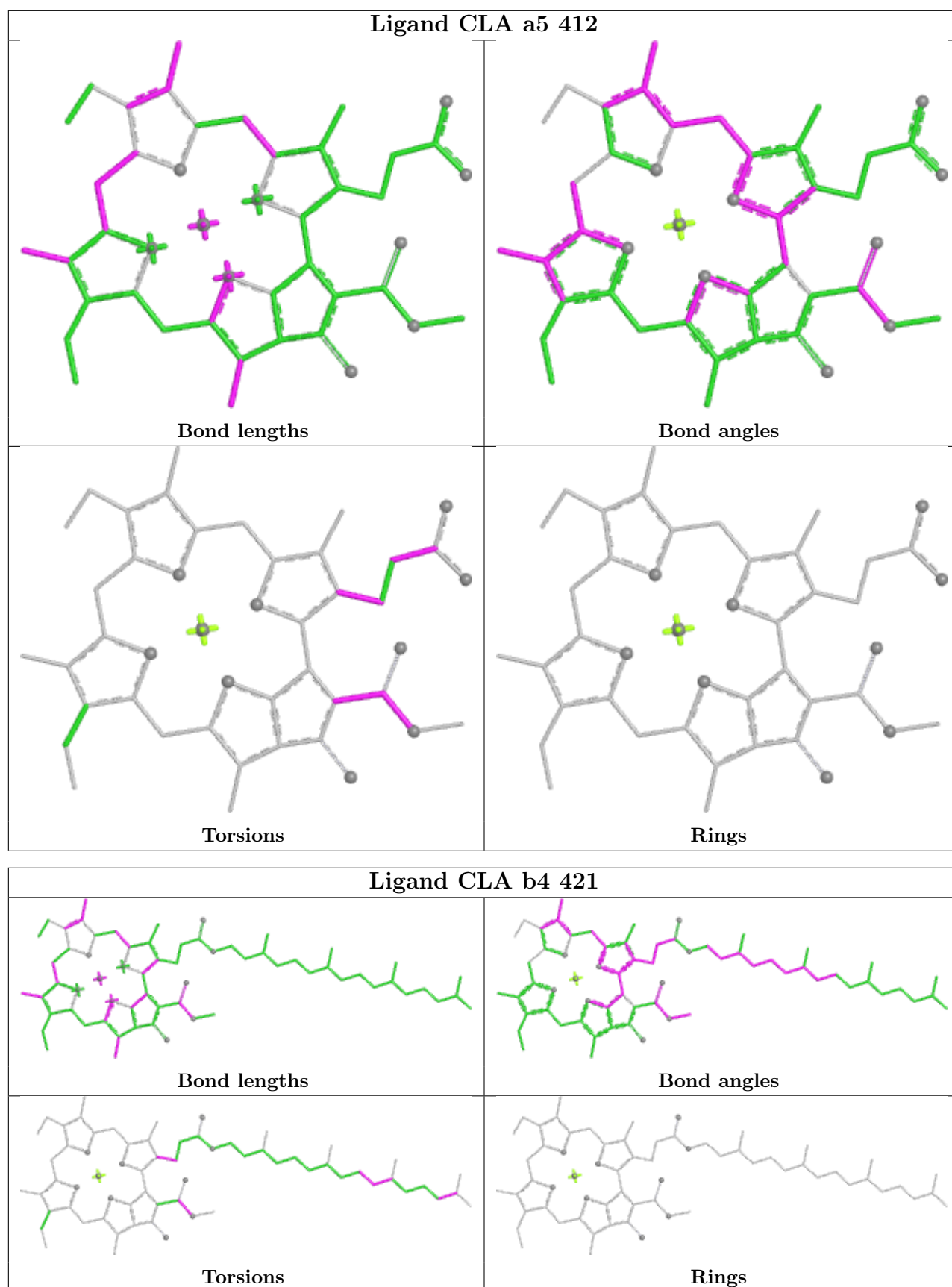


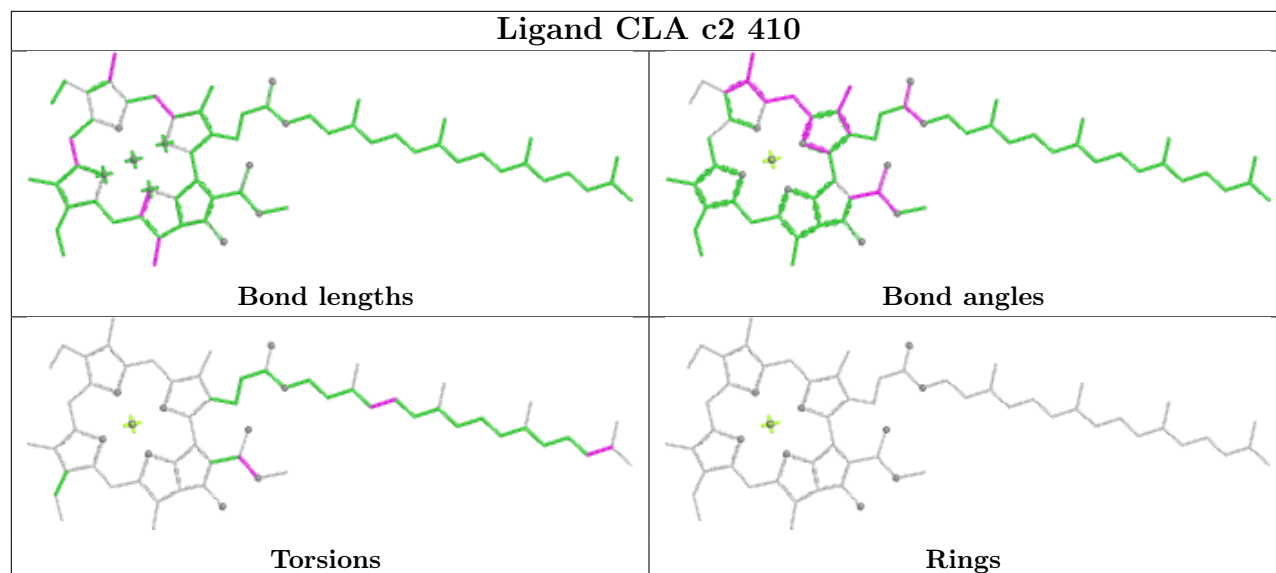
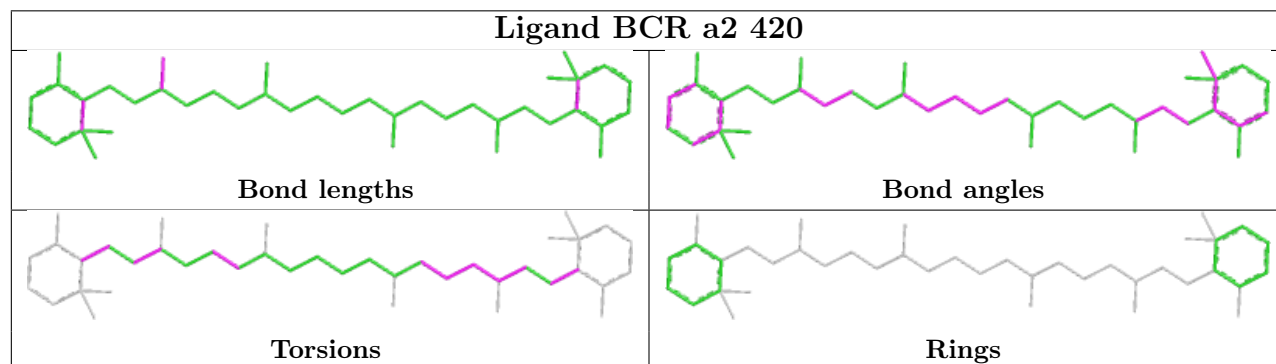
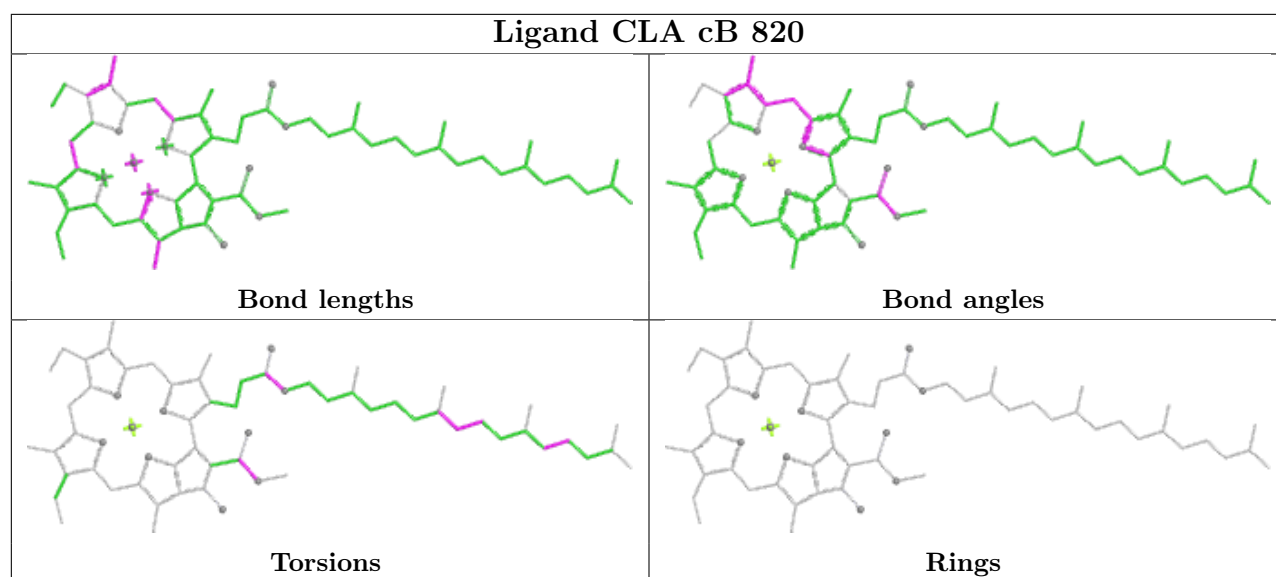




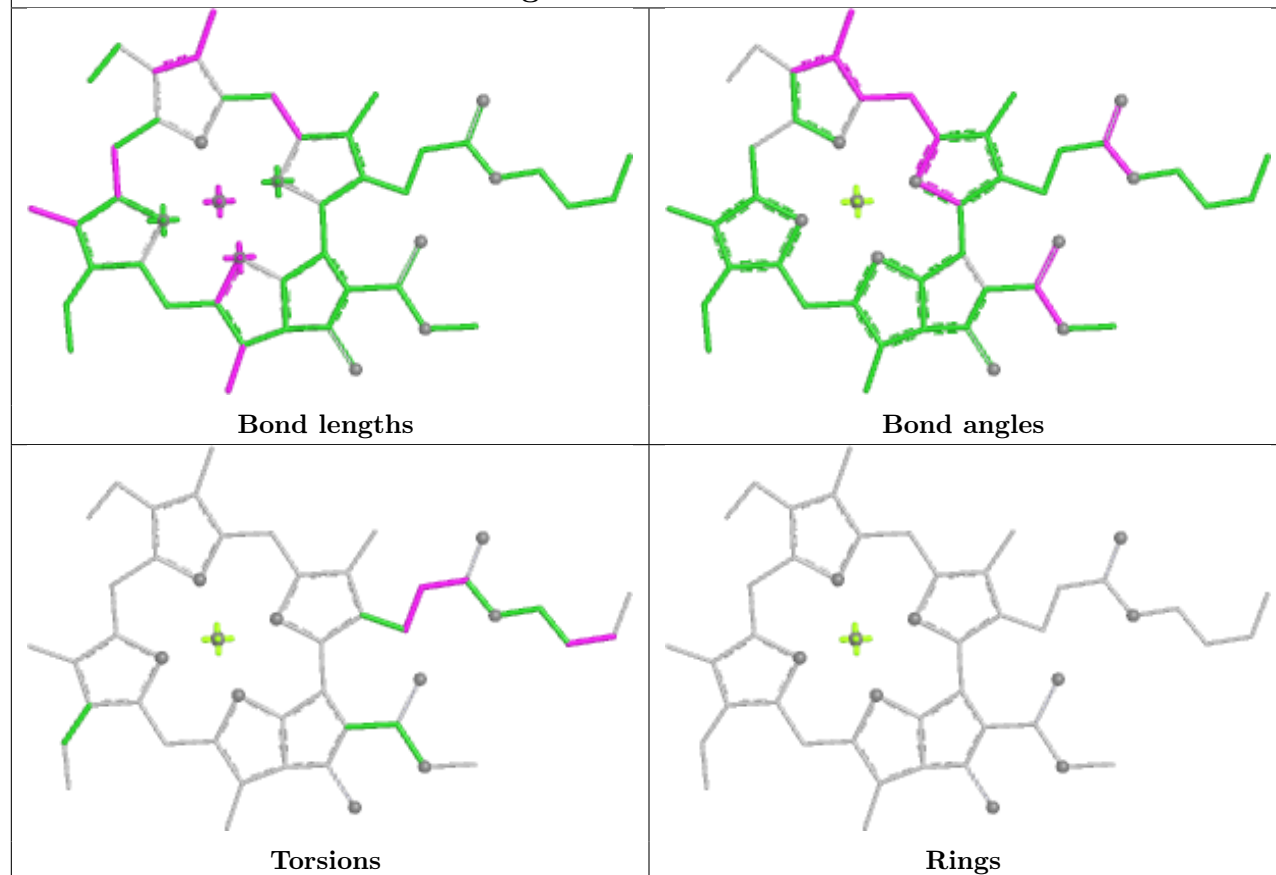




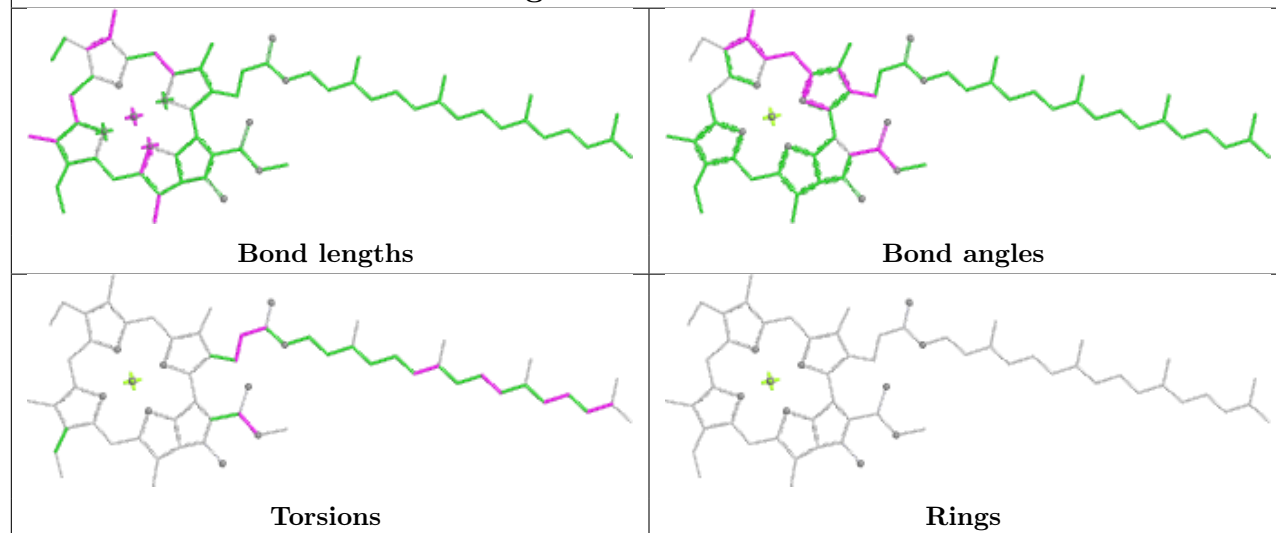


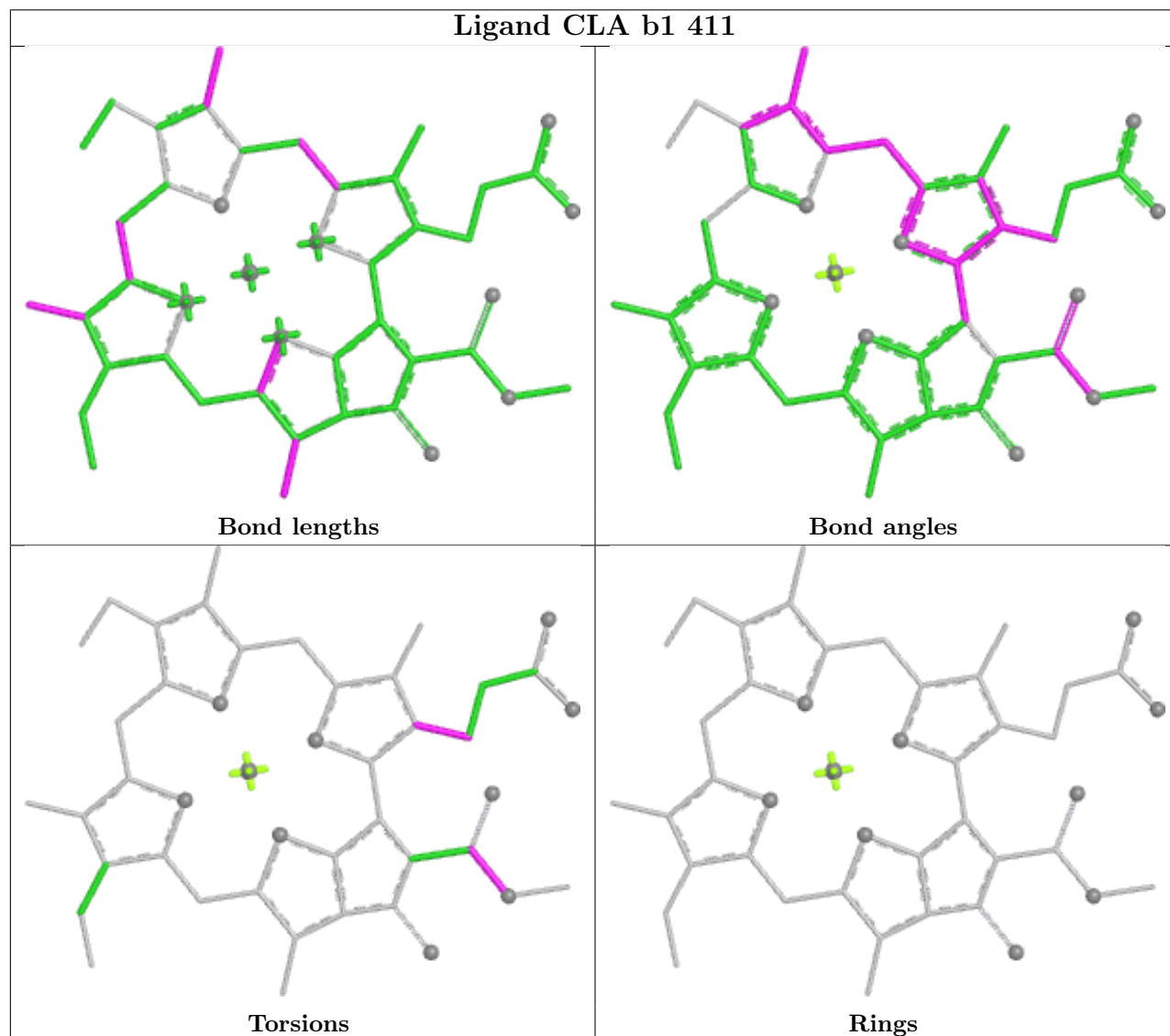
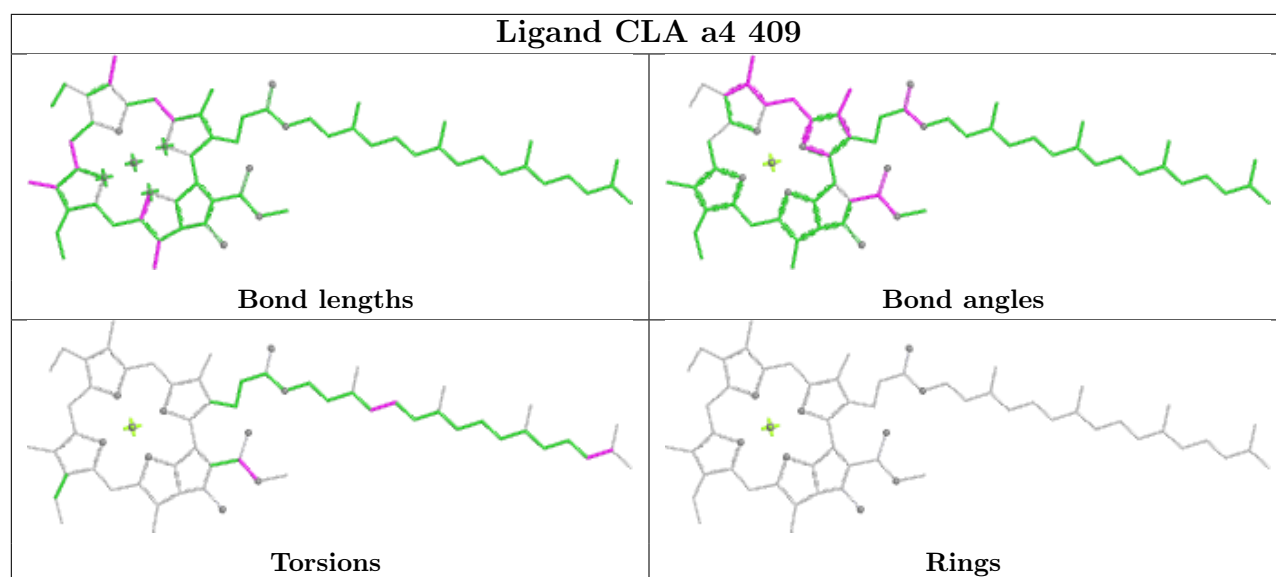


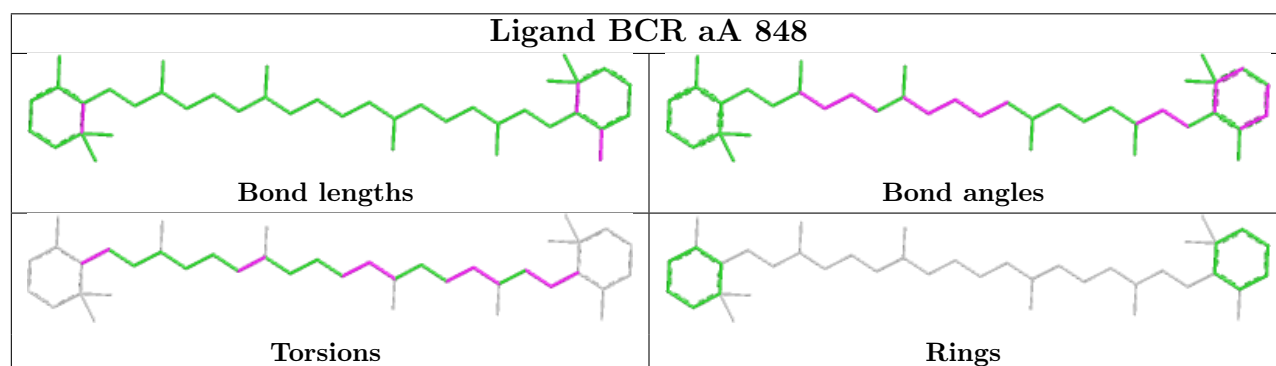
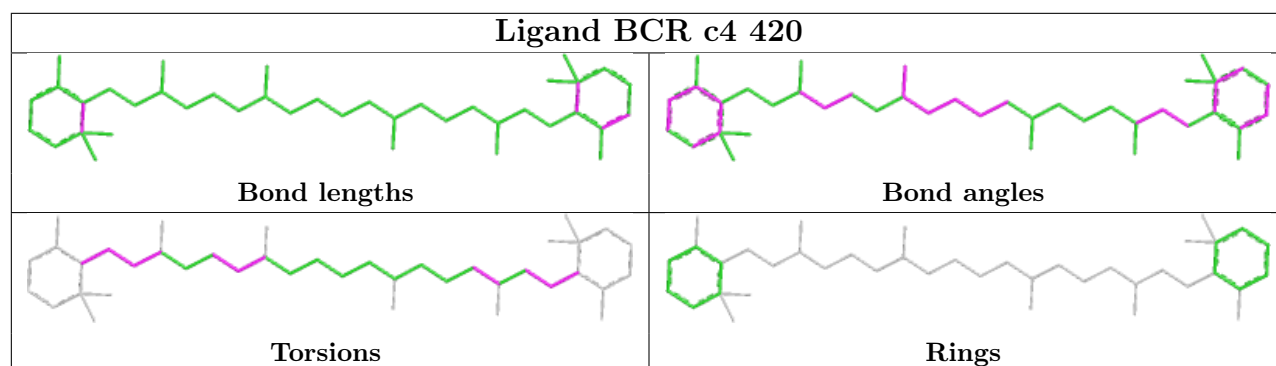
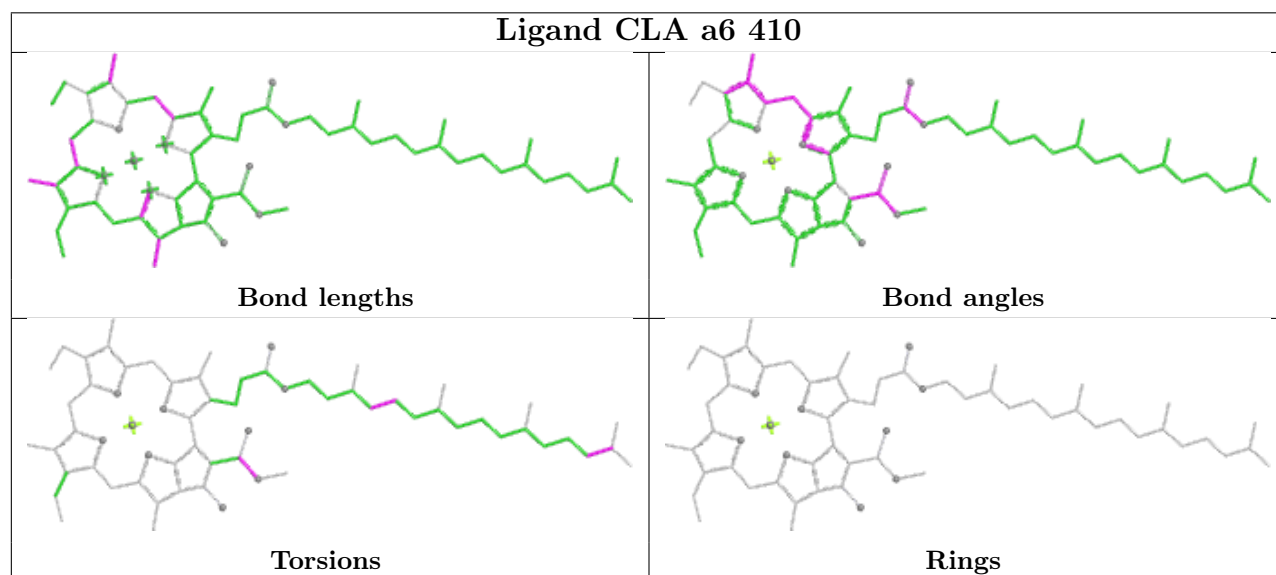
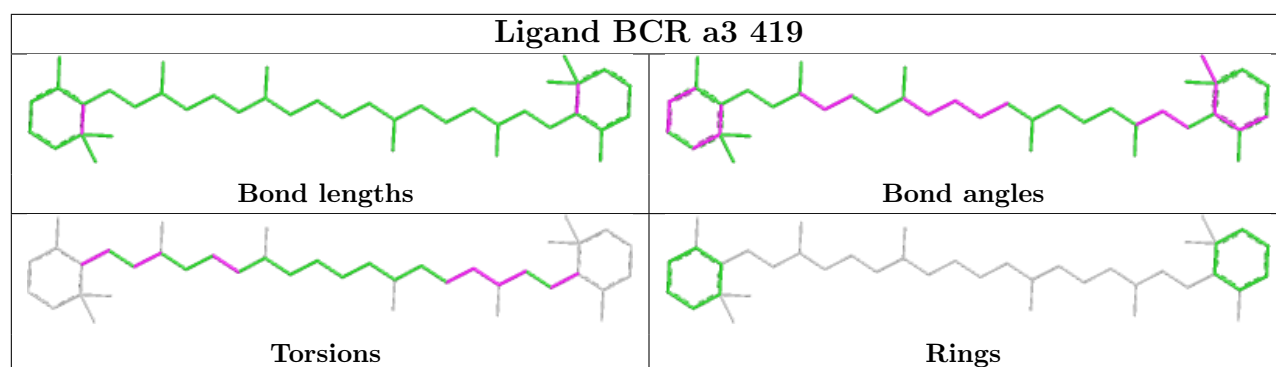
Ligand CLA bA 823

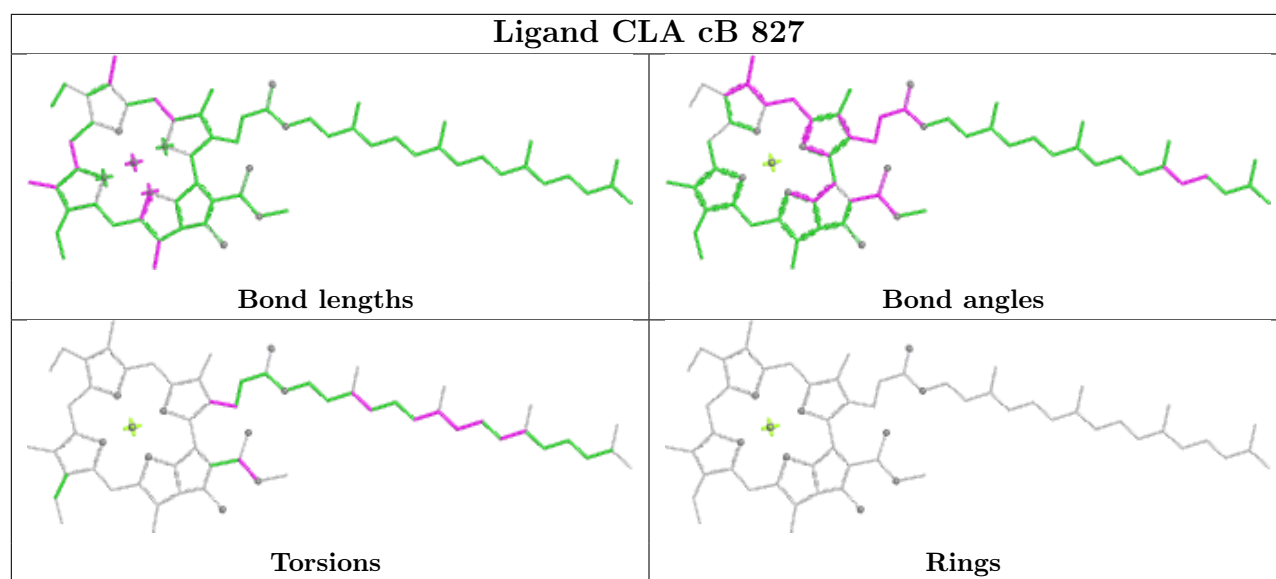


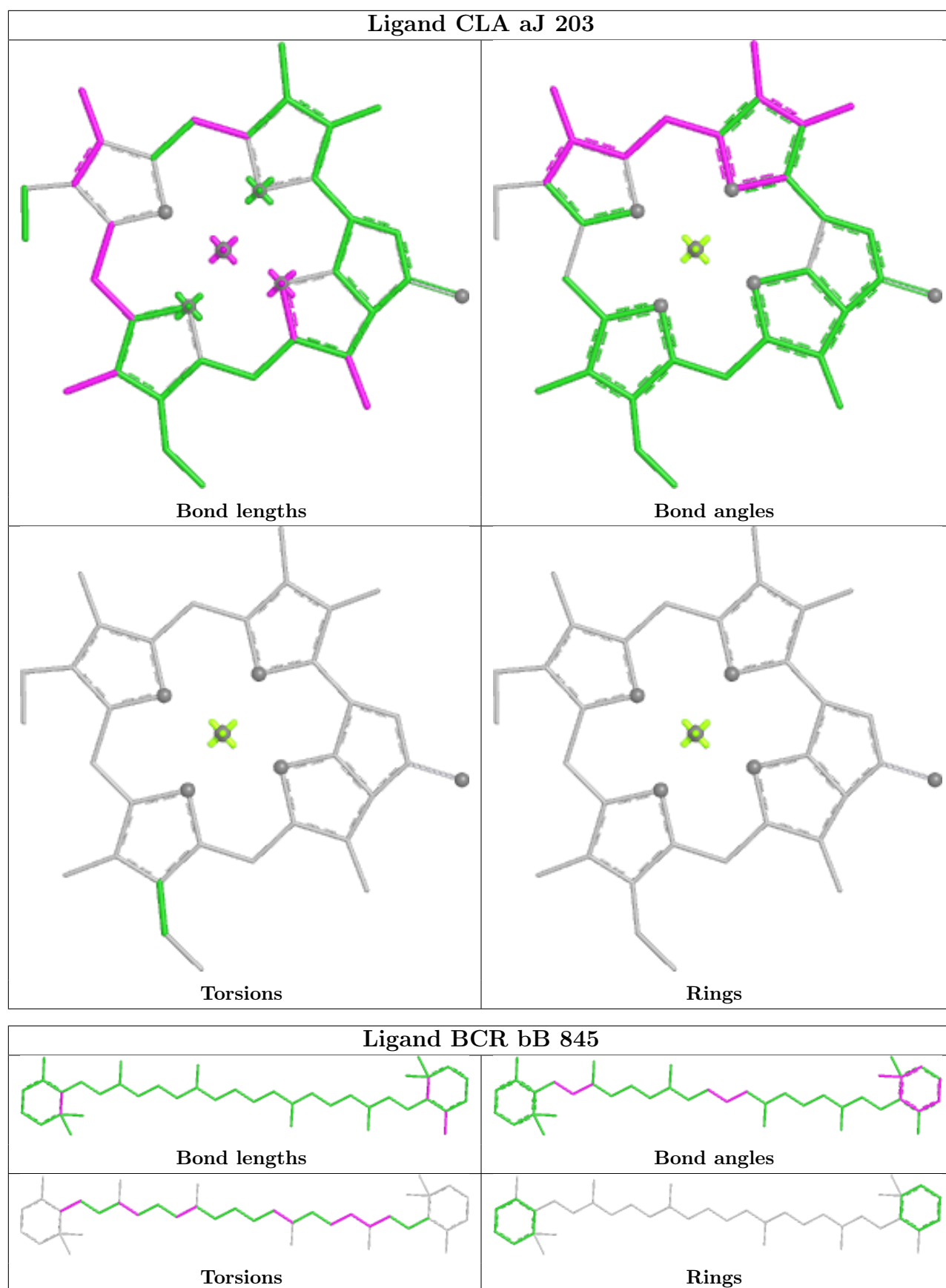
Ligand CLA aL 203

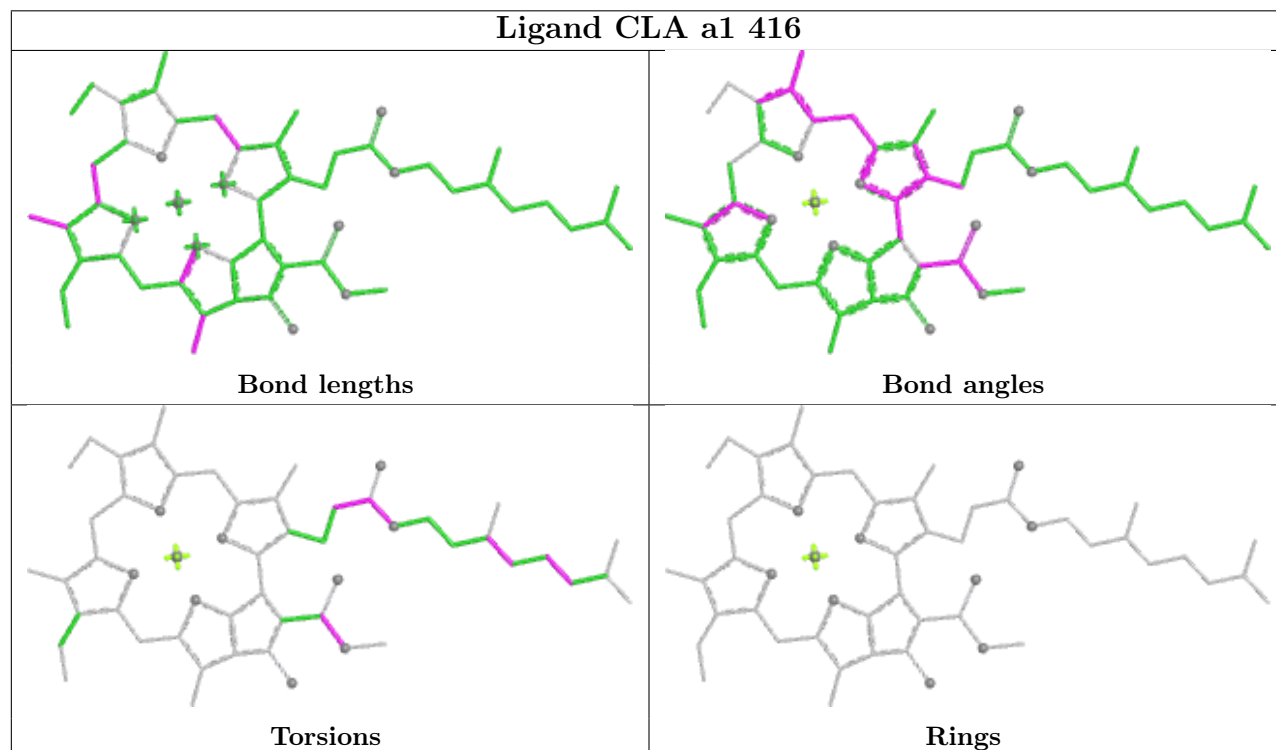
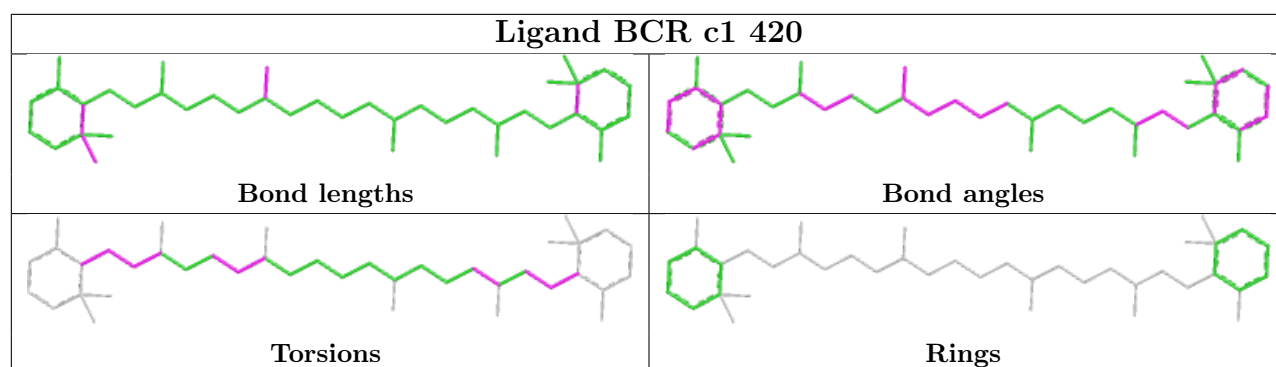




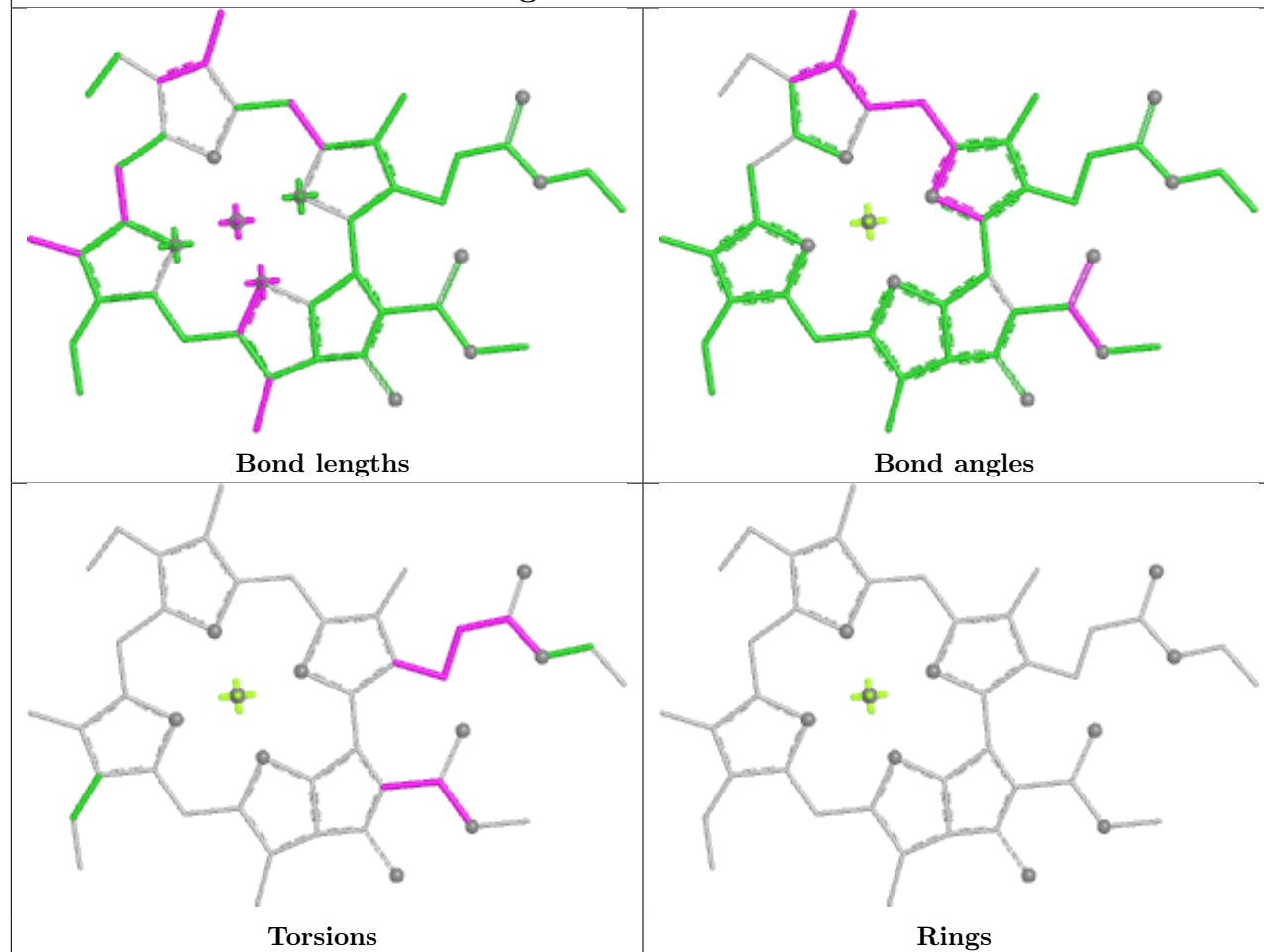




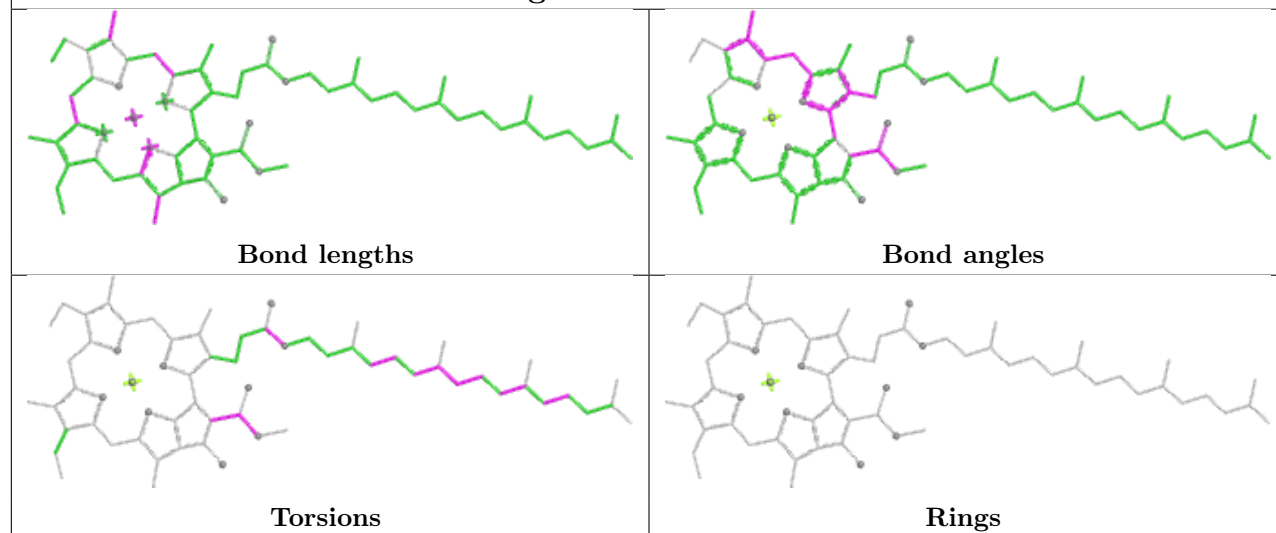


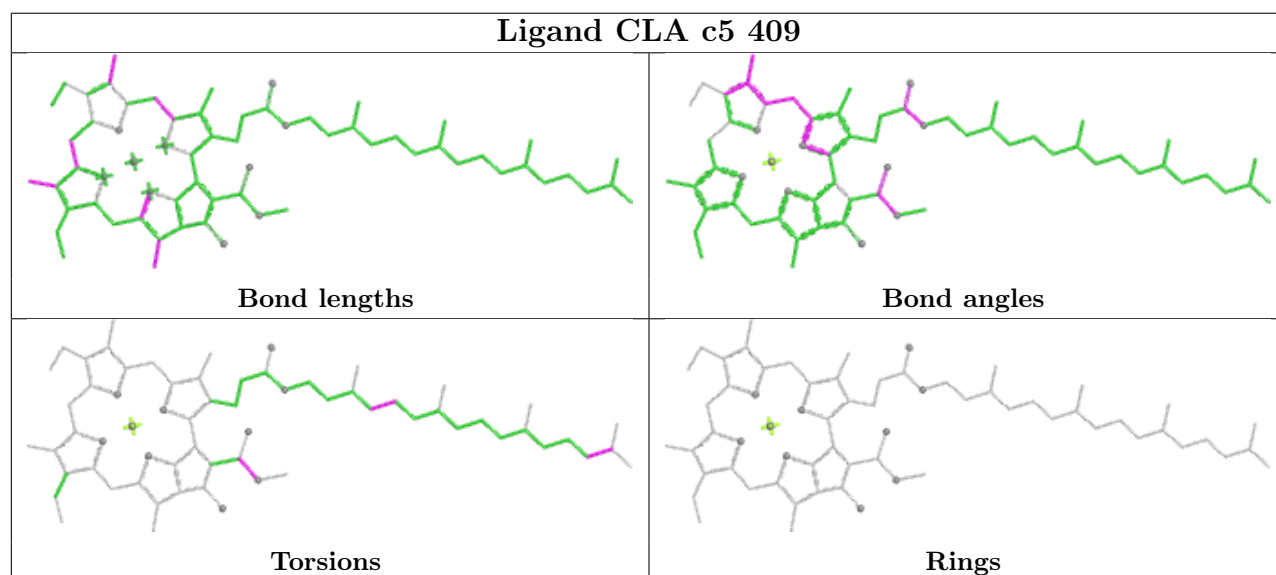
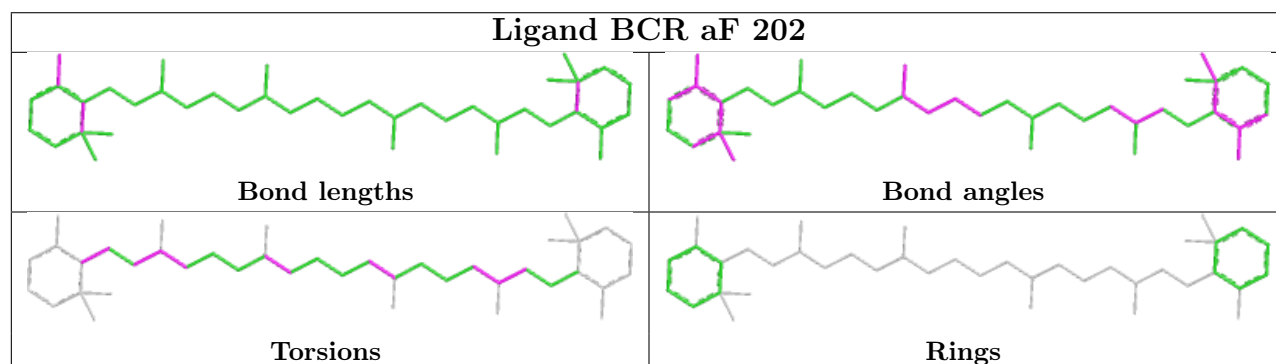
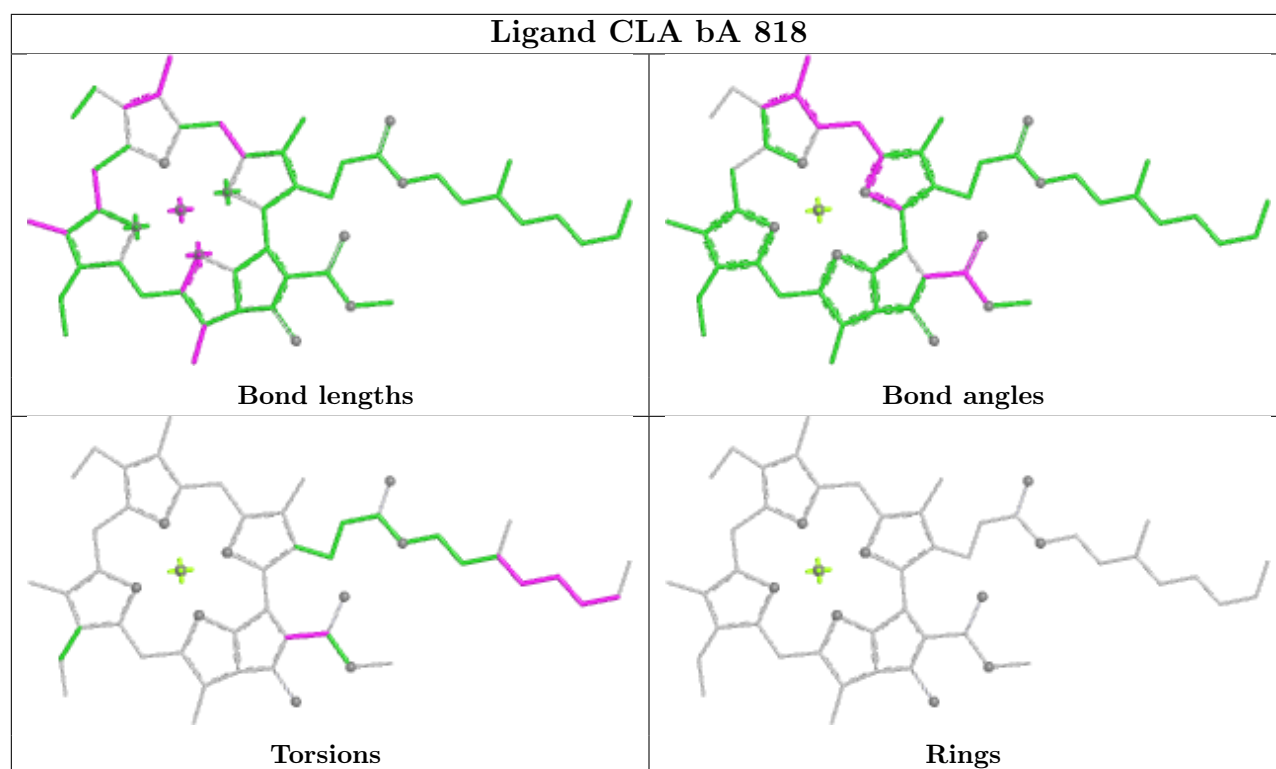


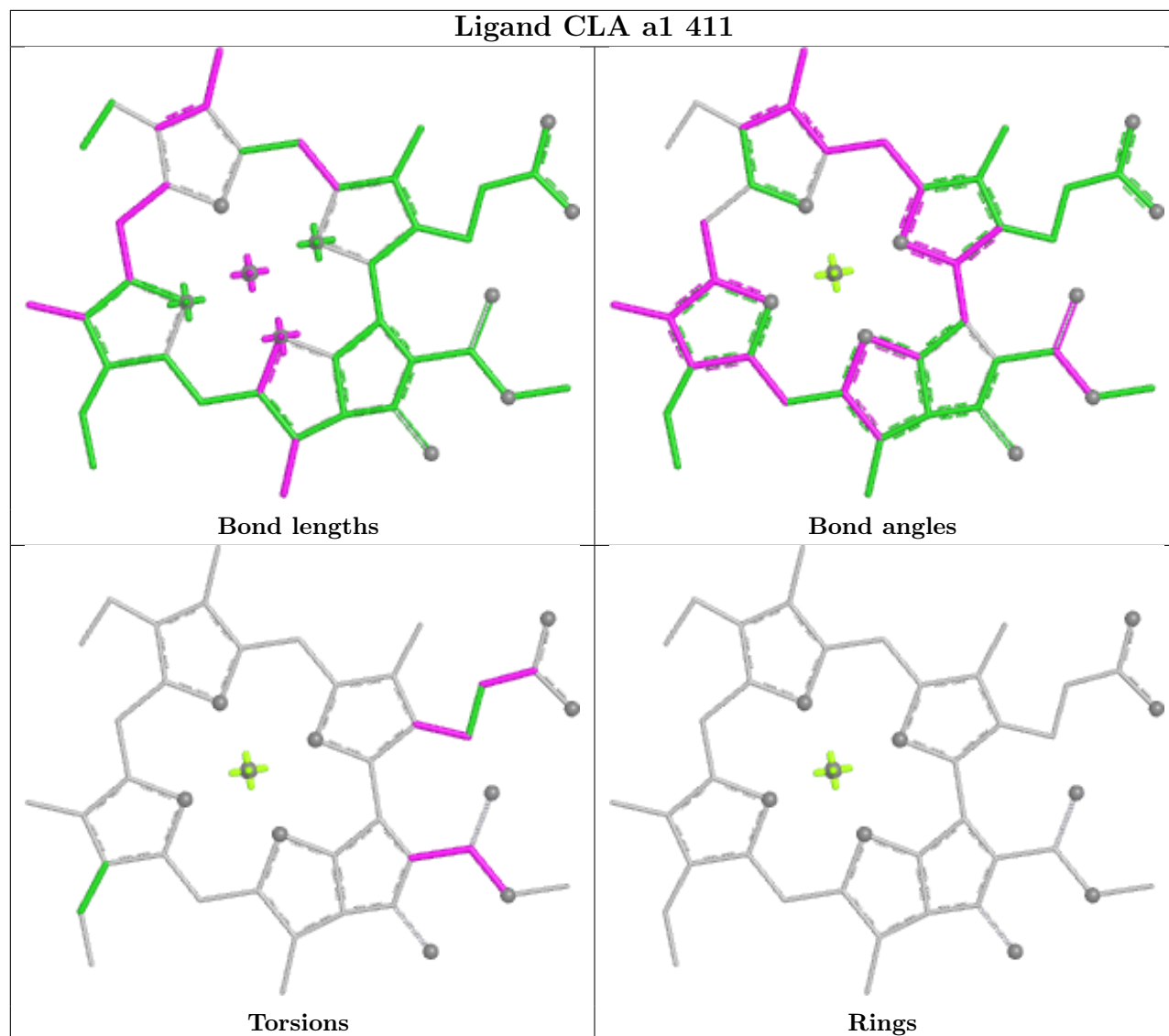
Ligand CLA cB 821



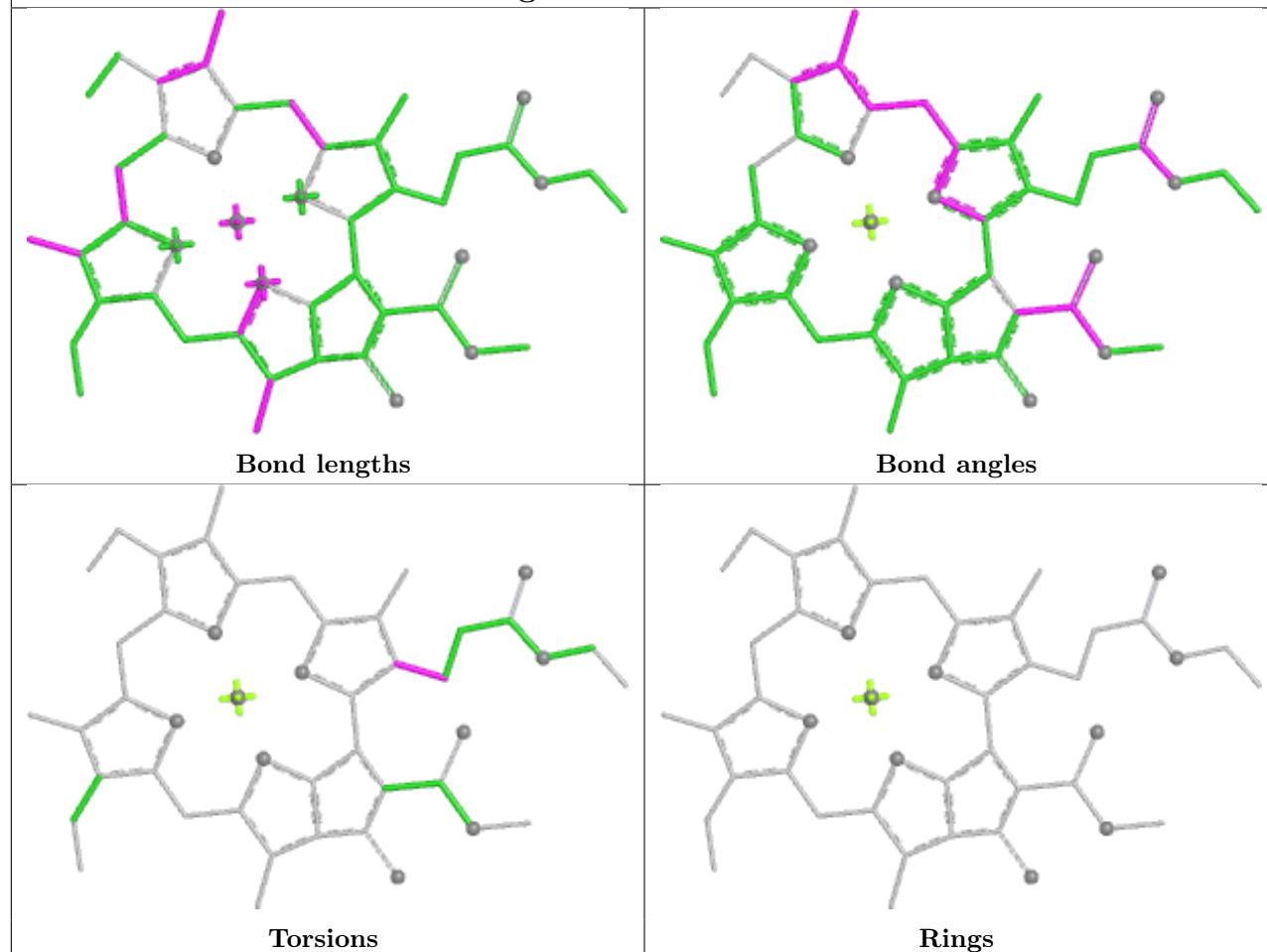
Ligand CLA c6 404



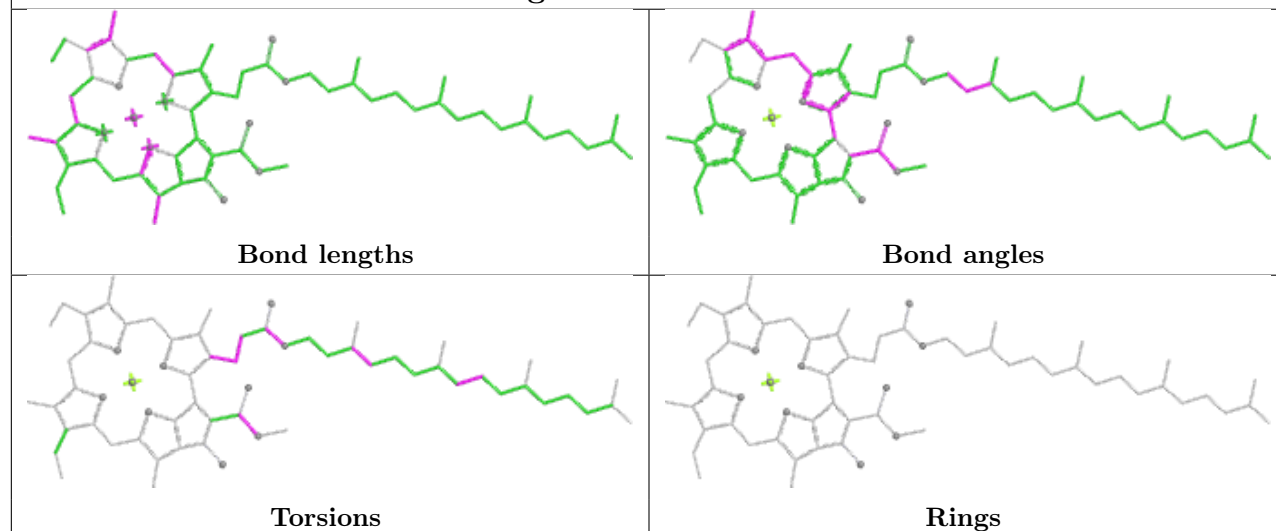




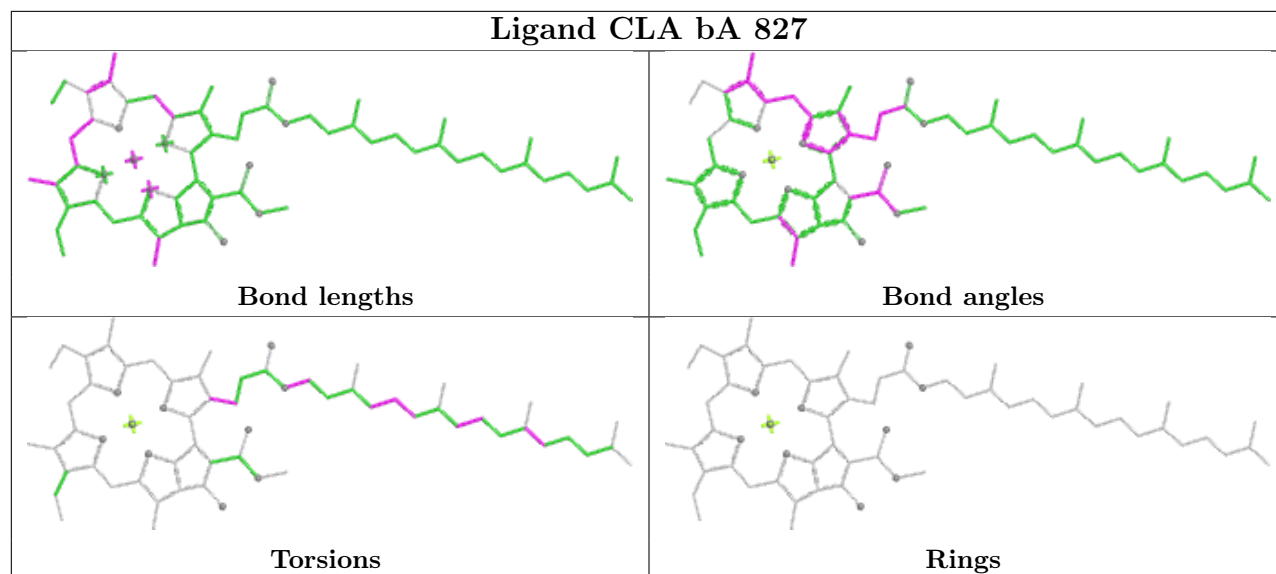
Ligand CLA bB 838



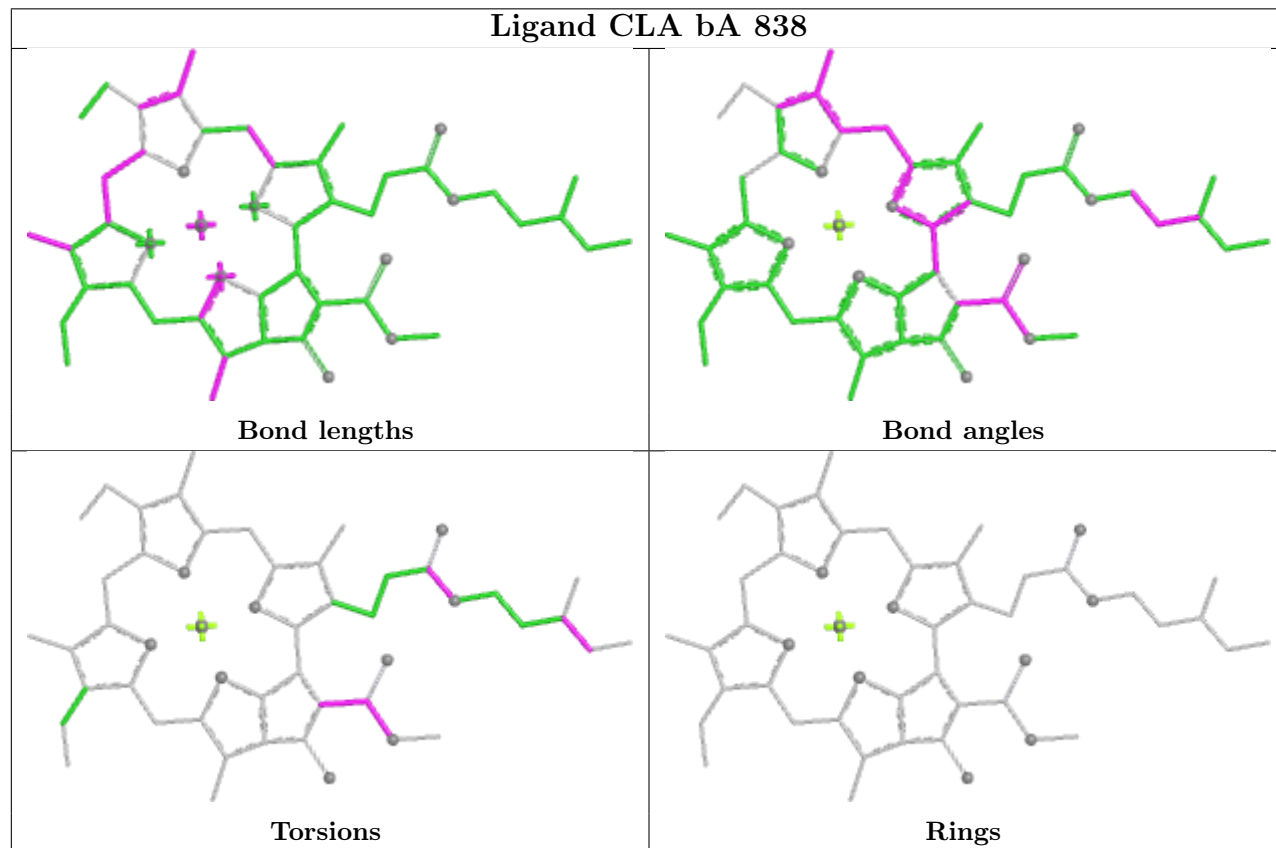
Ligand CLA a1 403

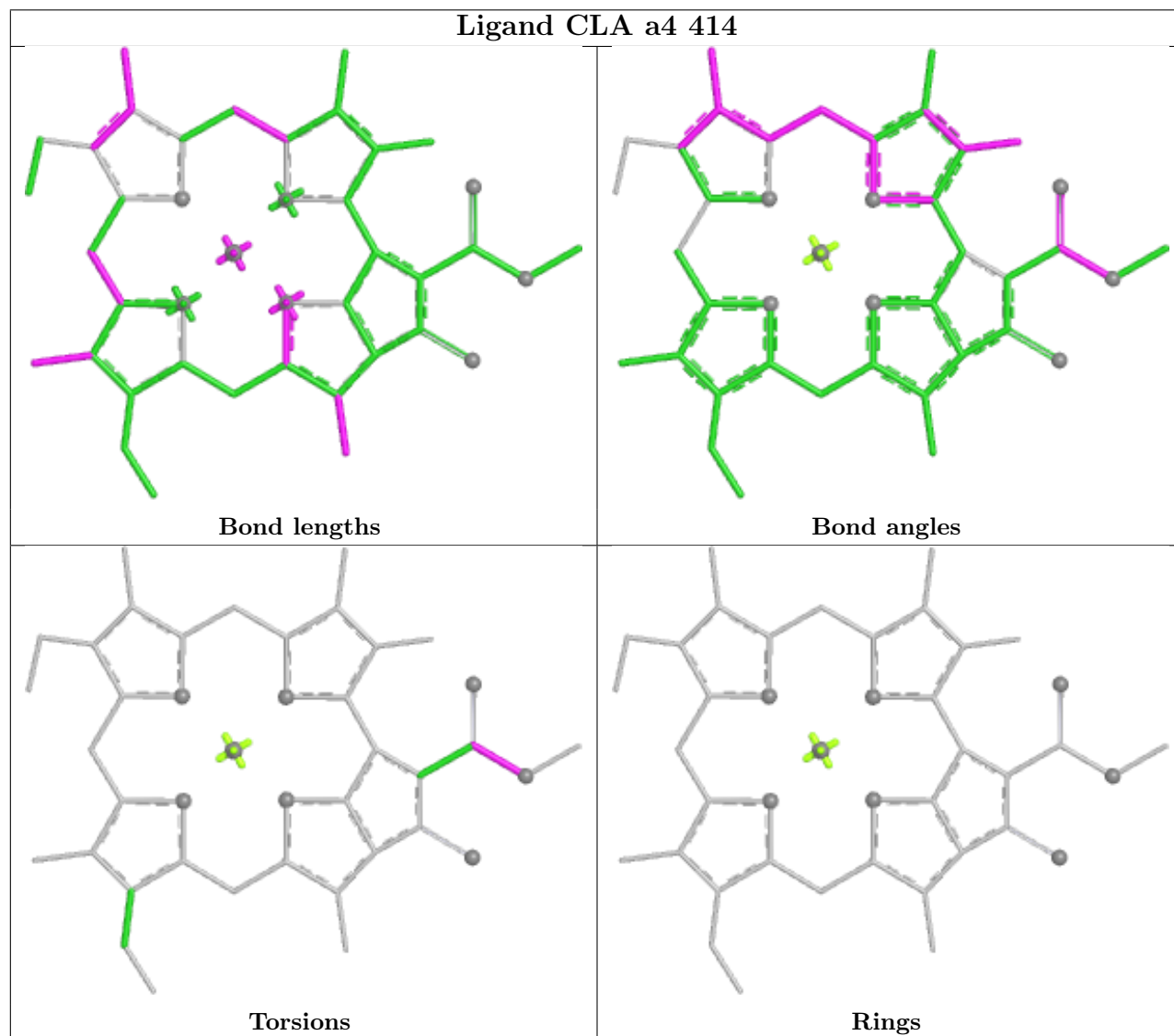
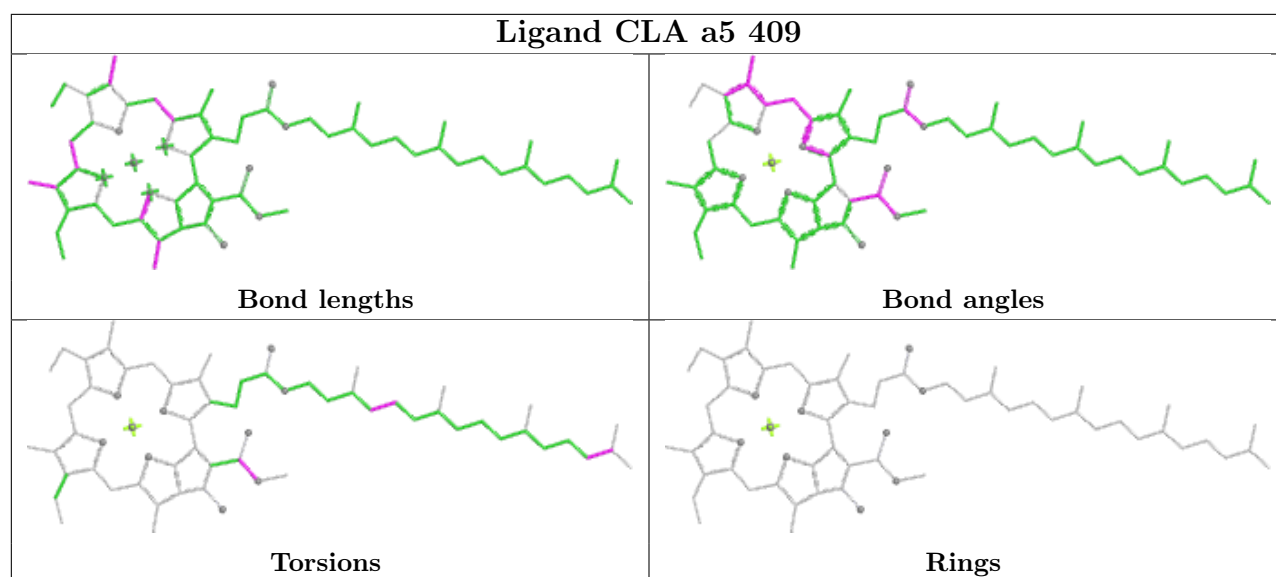


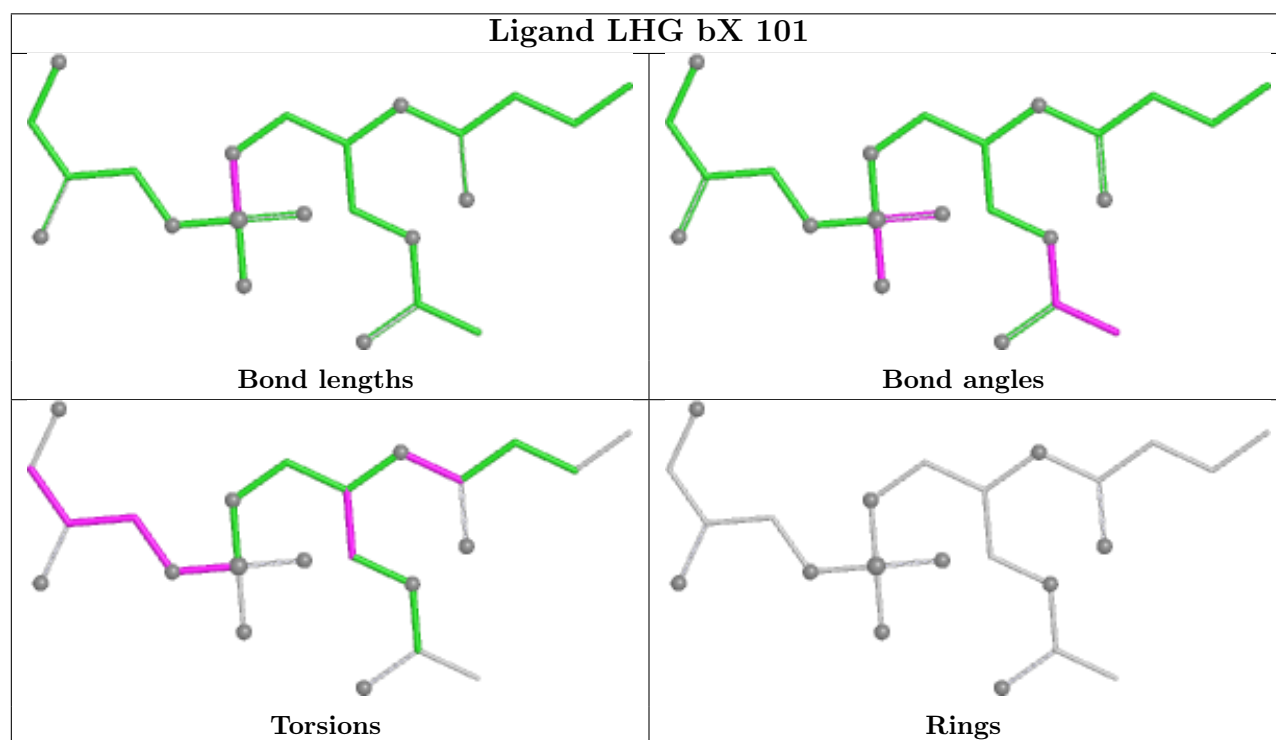
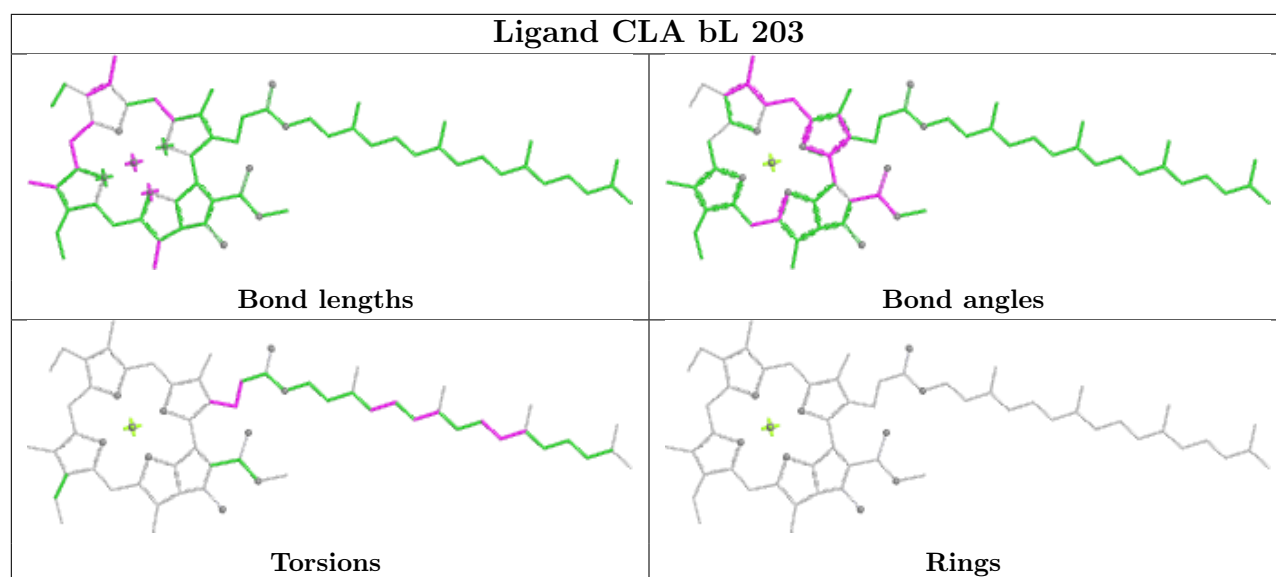
Ligand CLA bA 827

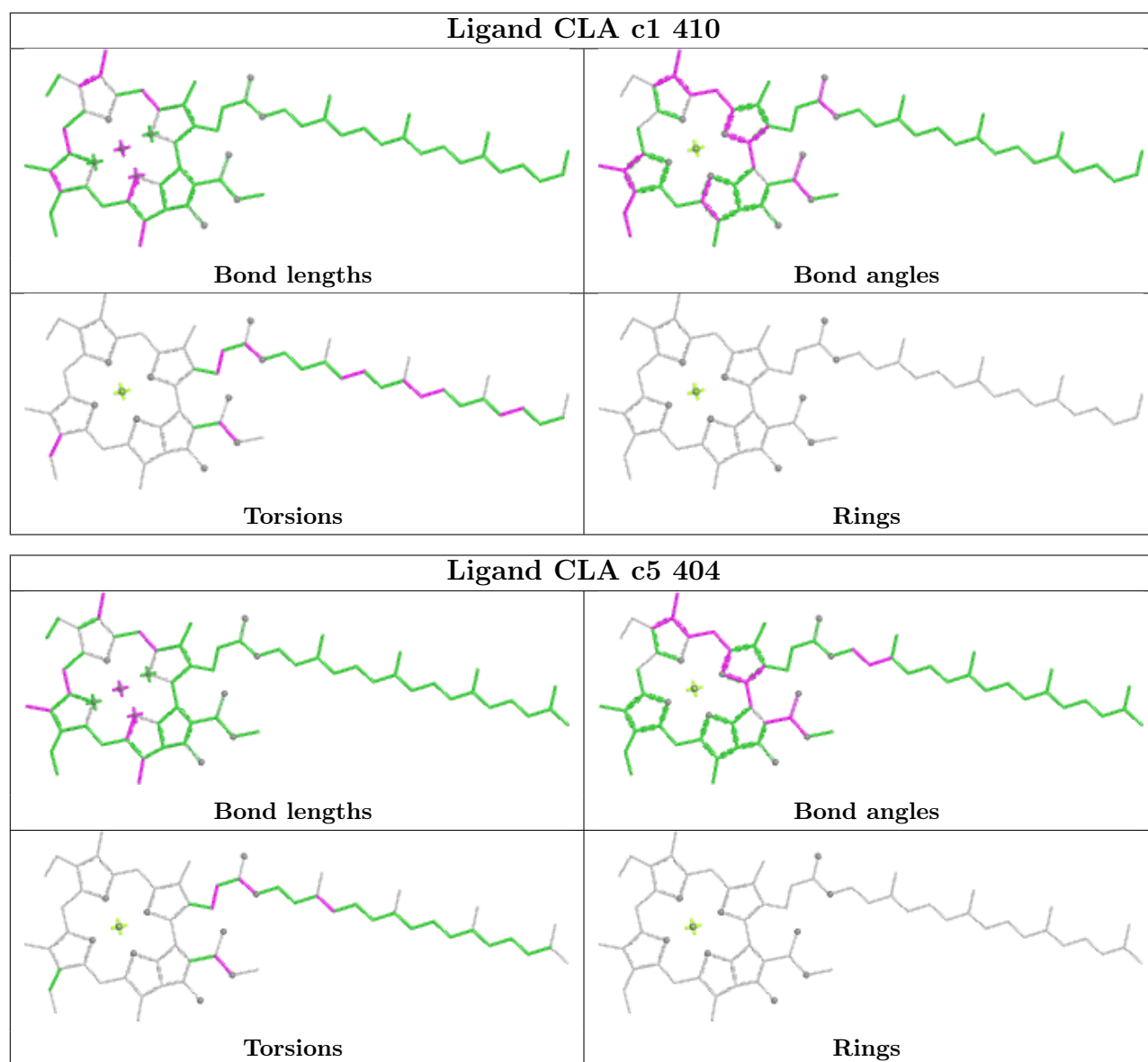


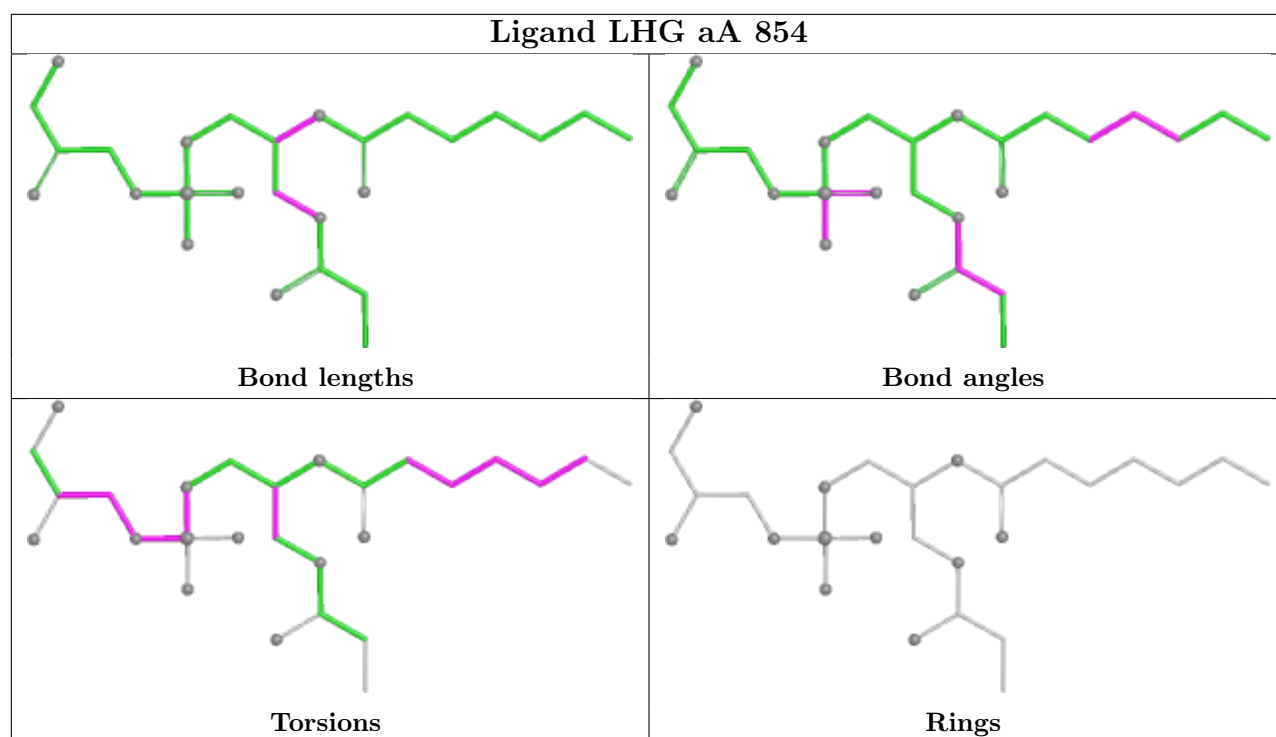
Ligand CLA bA 838

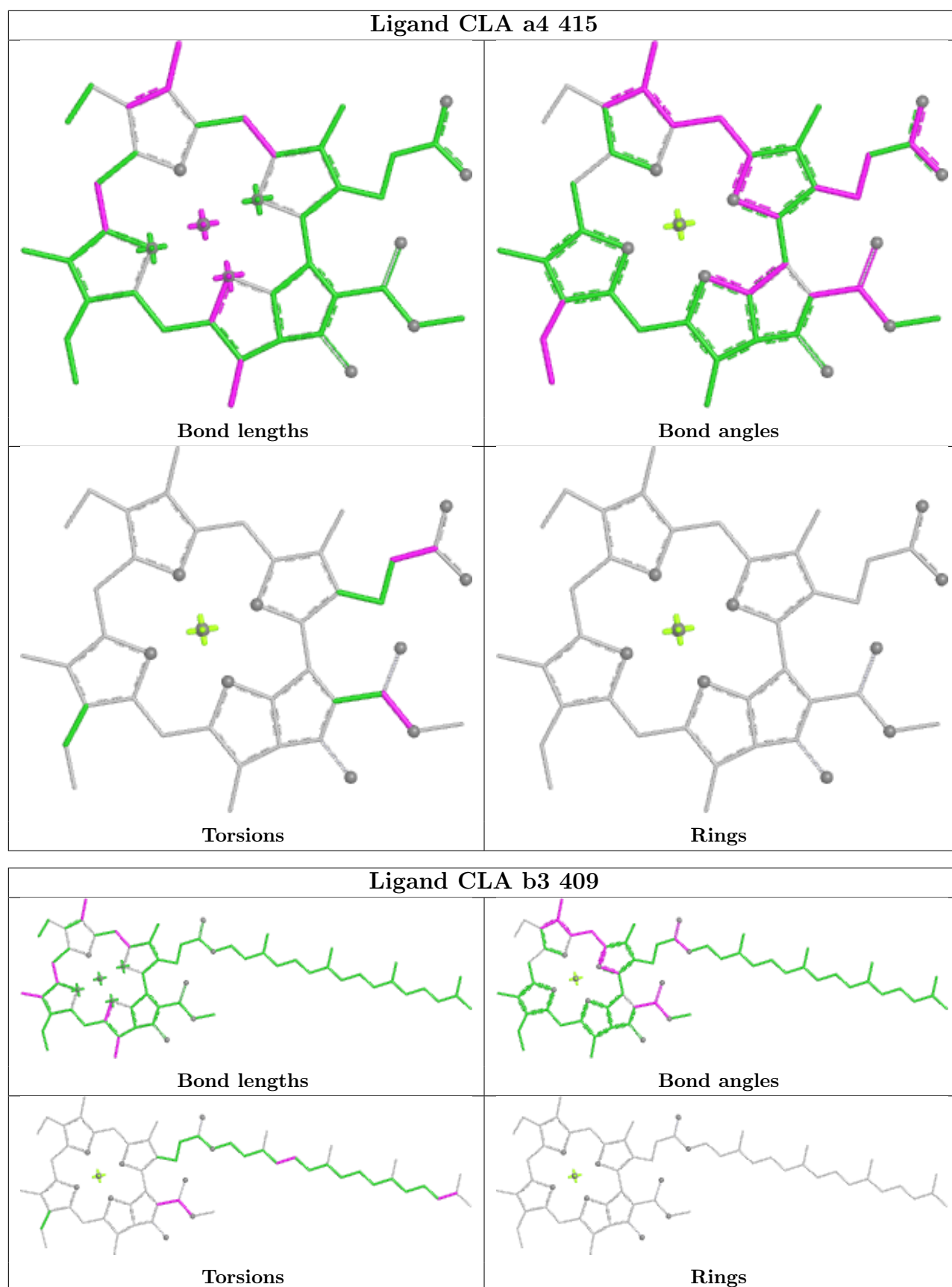


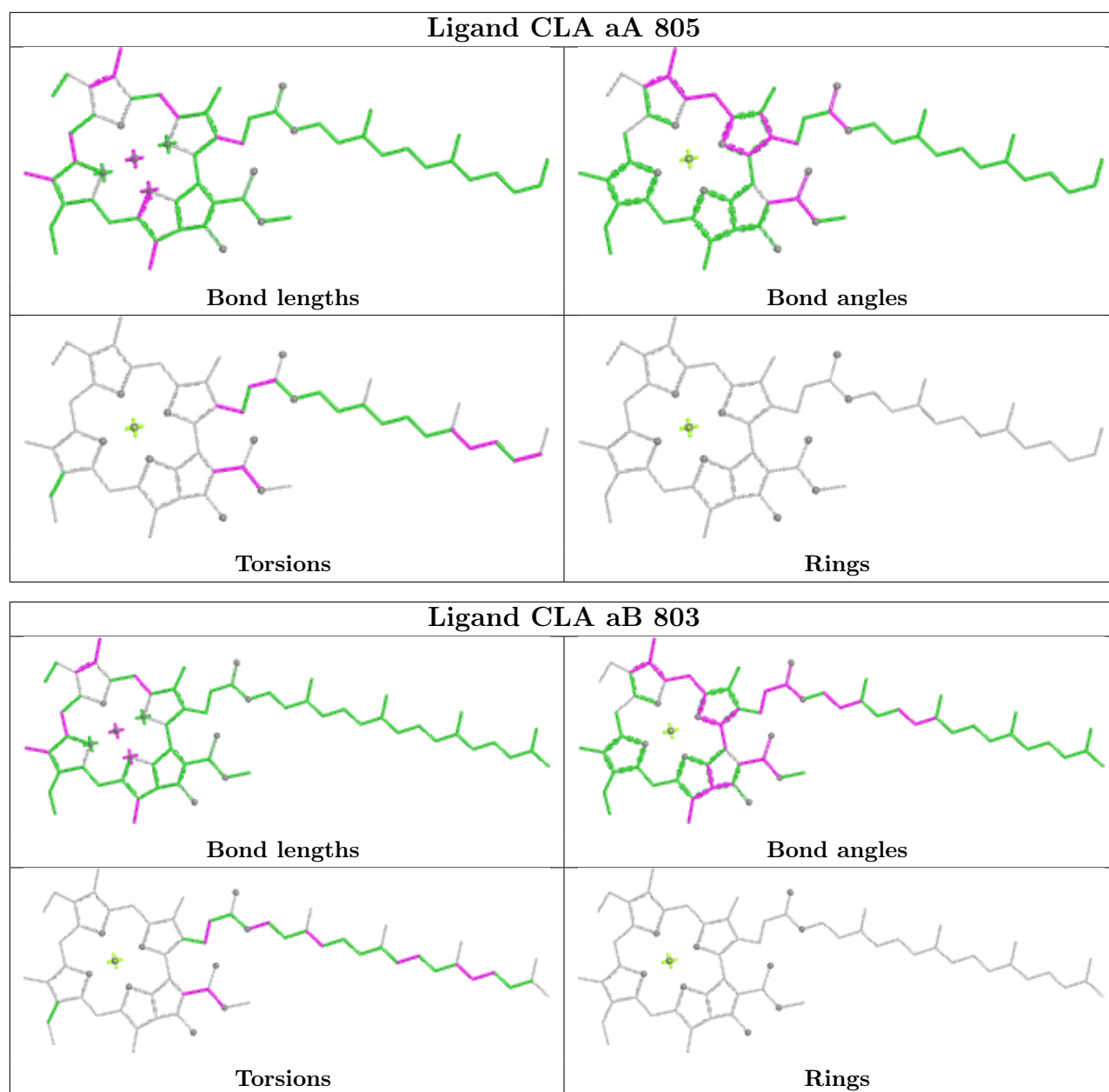




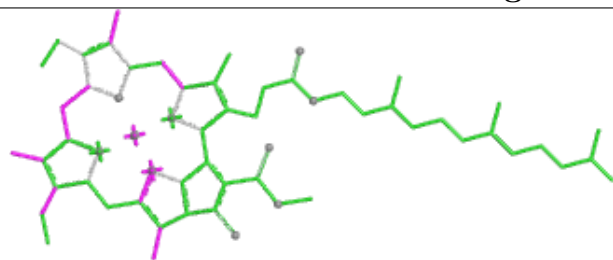




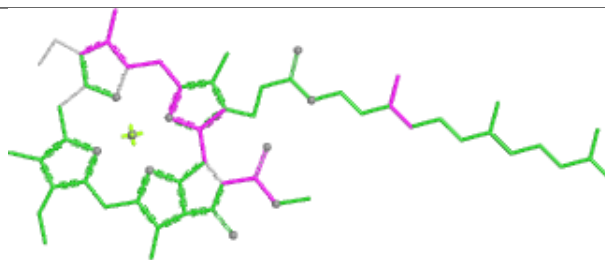




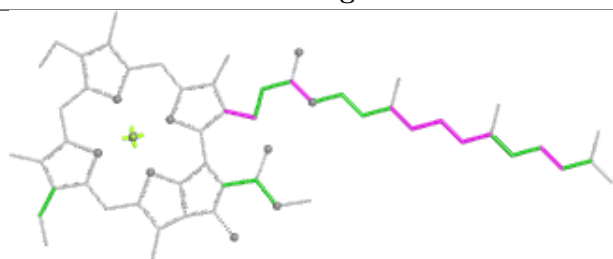
Ligand CLA bB 819



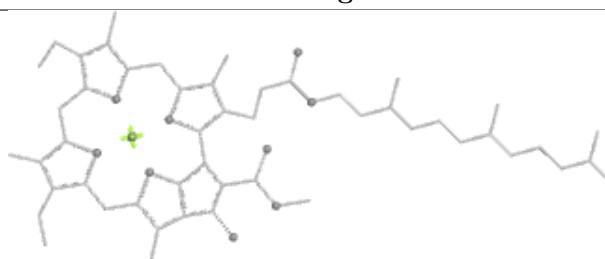
Bond lengths



Bond angles

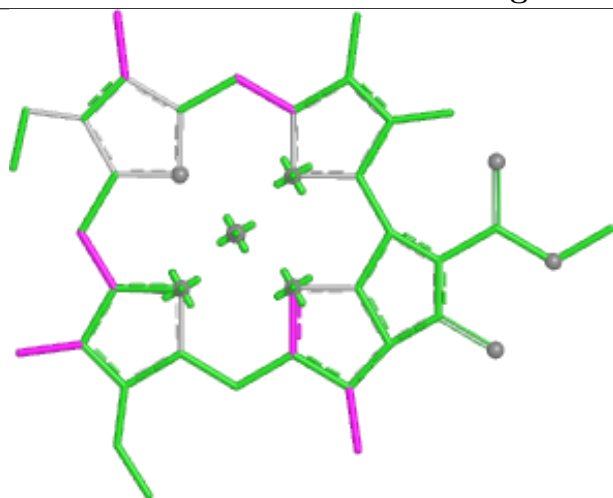


Torsions

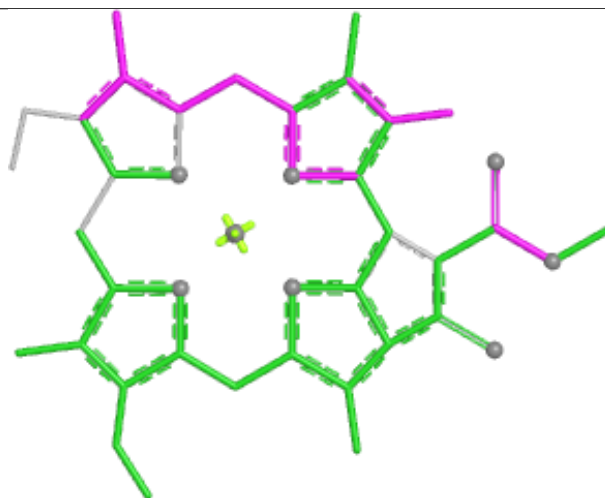


Rings

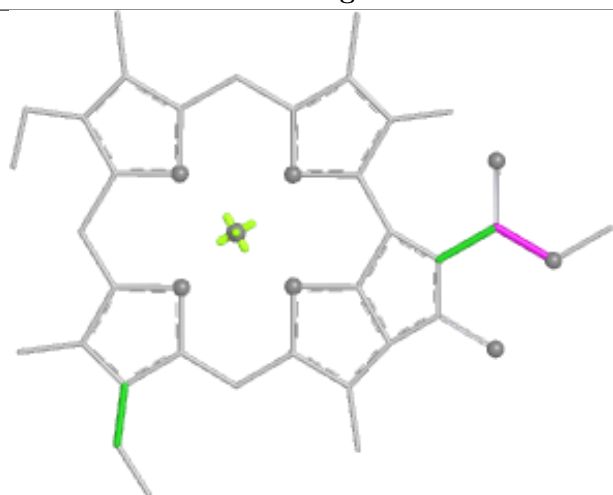
Ligand CLA c5 414



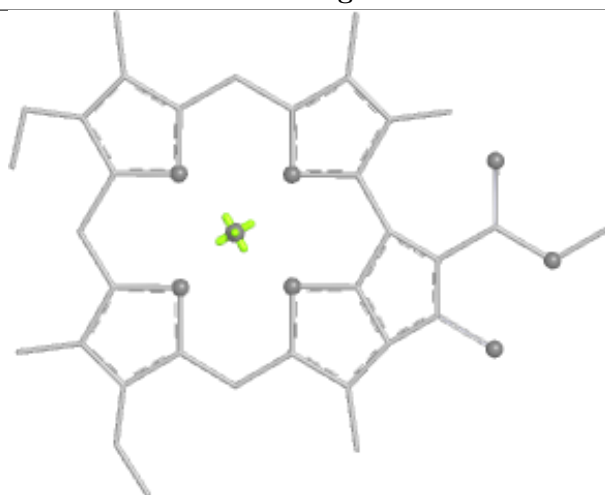
Bond lengths



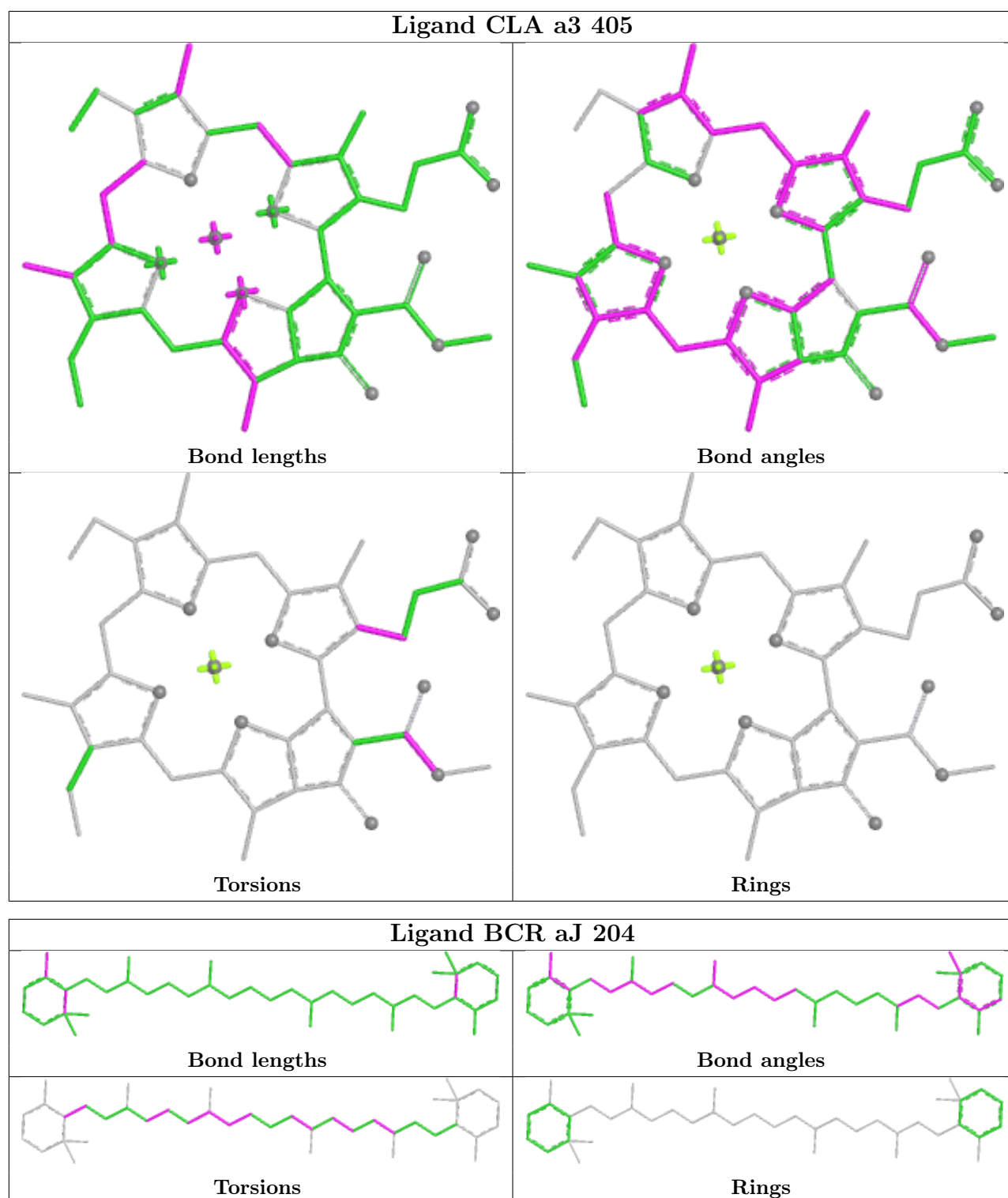
Bond angles

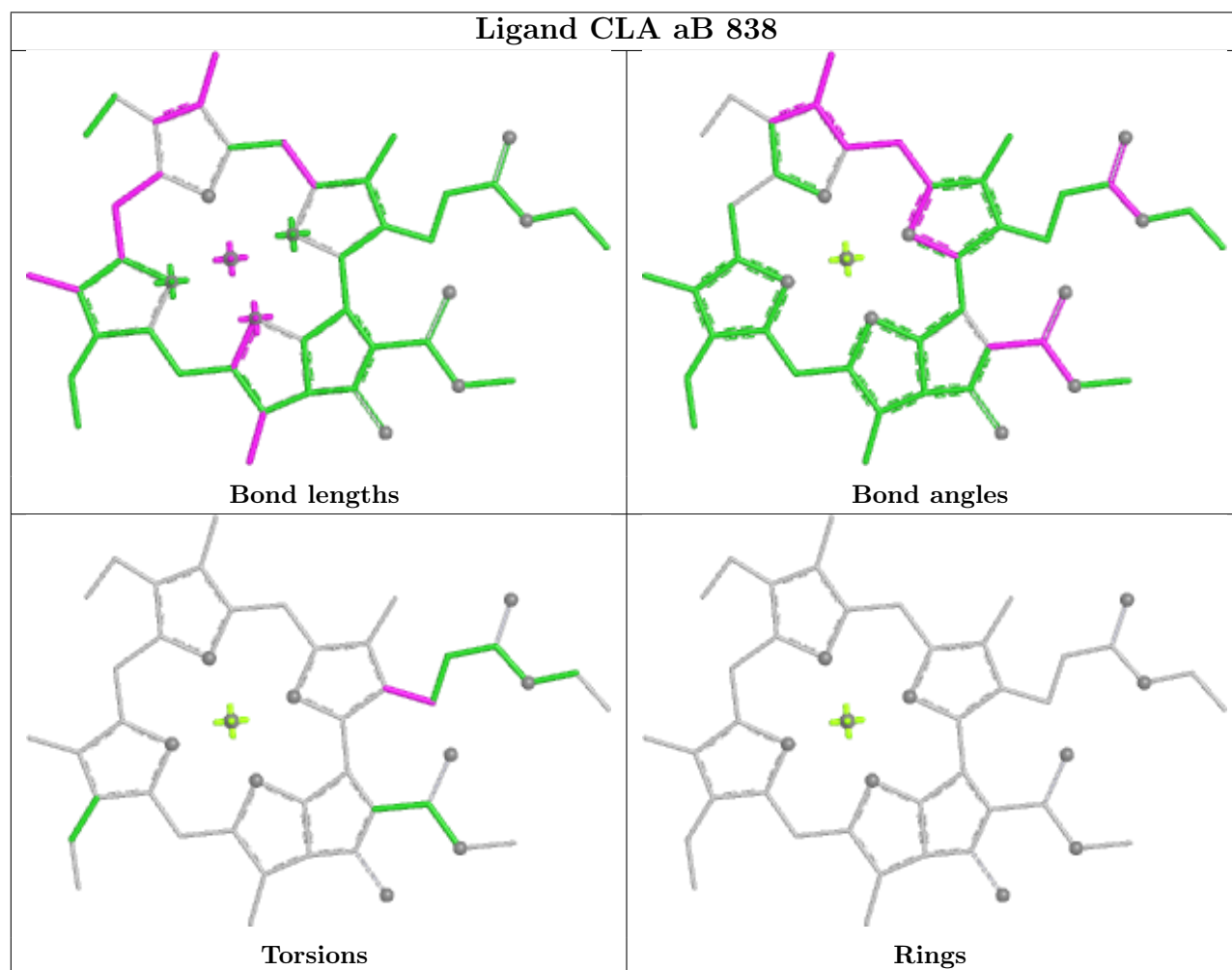
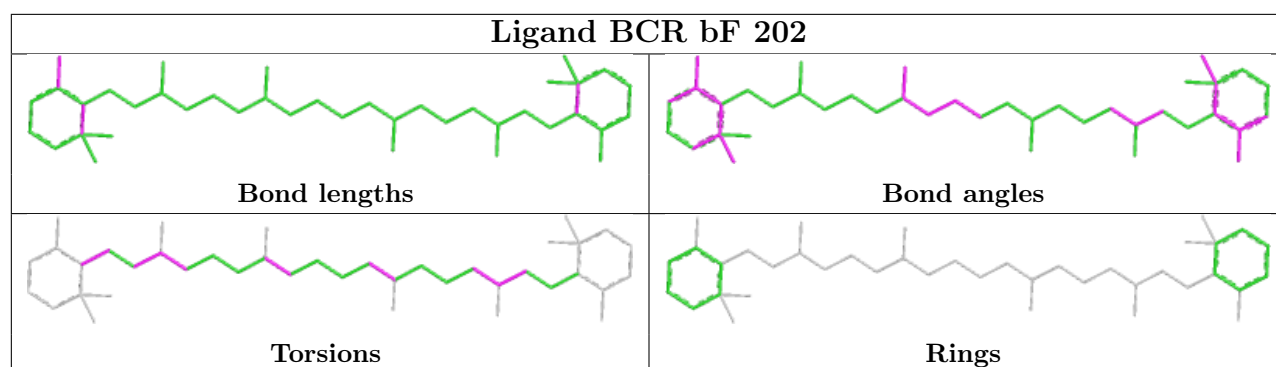


Torsions

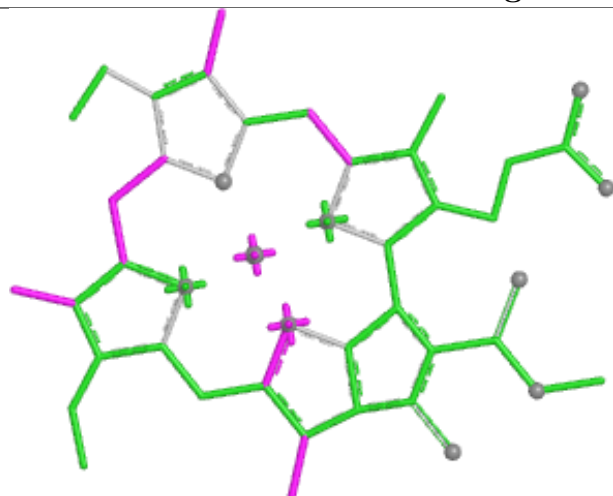


Rings

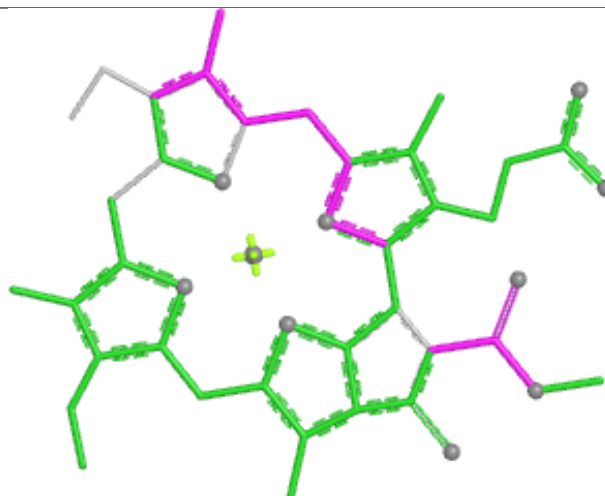




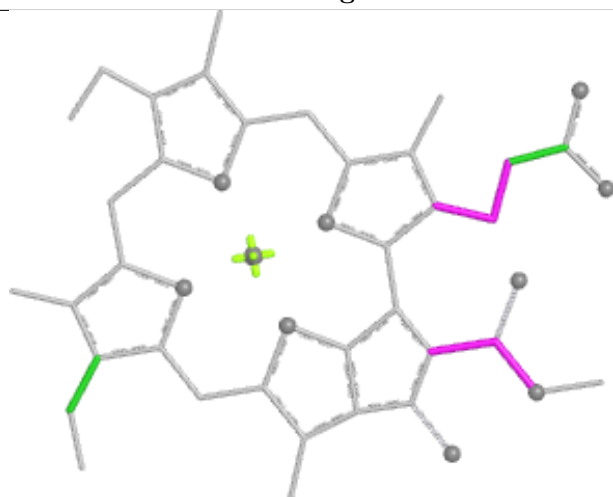
Ligand CLA bB 816



Bond lengths



Bond angles

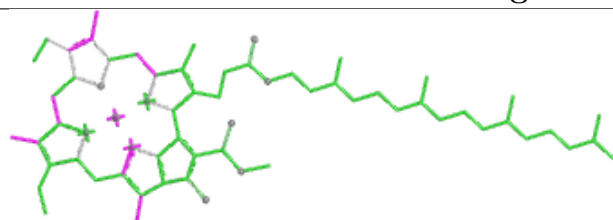


Torsions

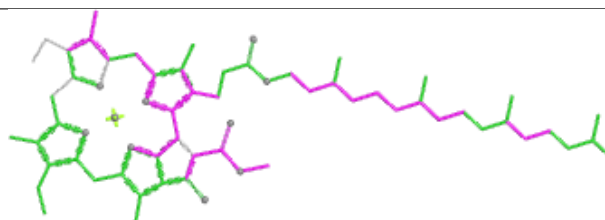


Rings

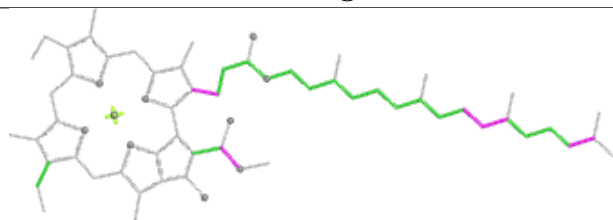
Ligand CLA c2 422



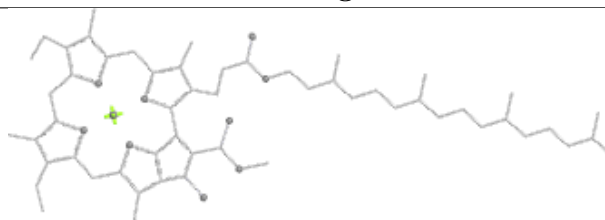
Bond lengths



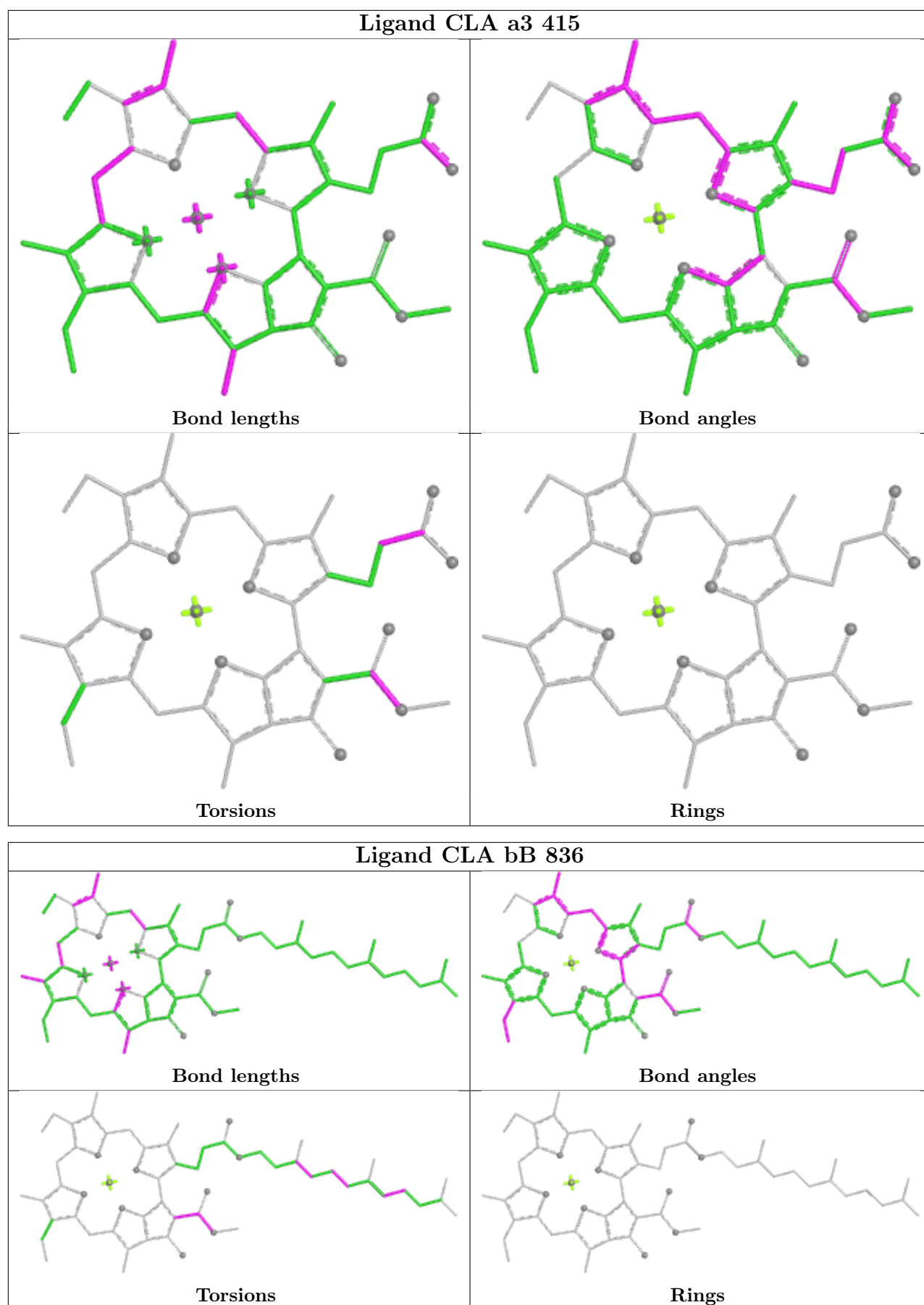
Bond angles

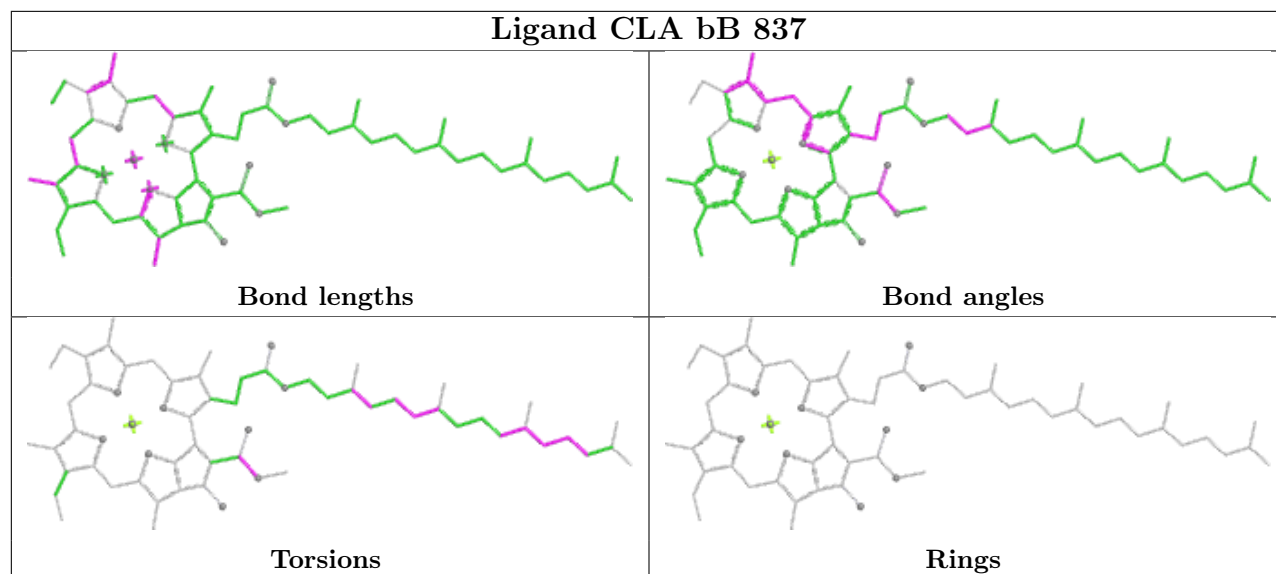
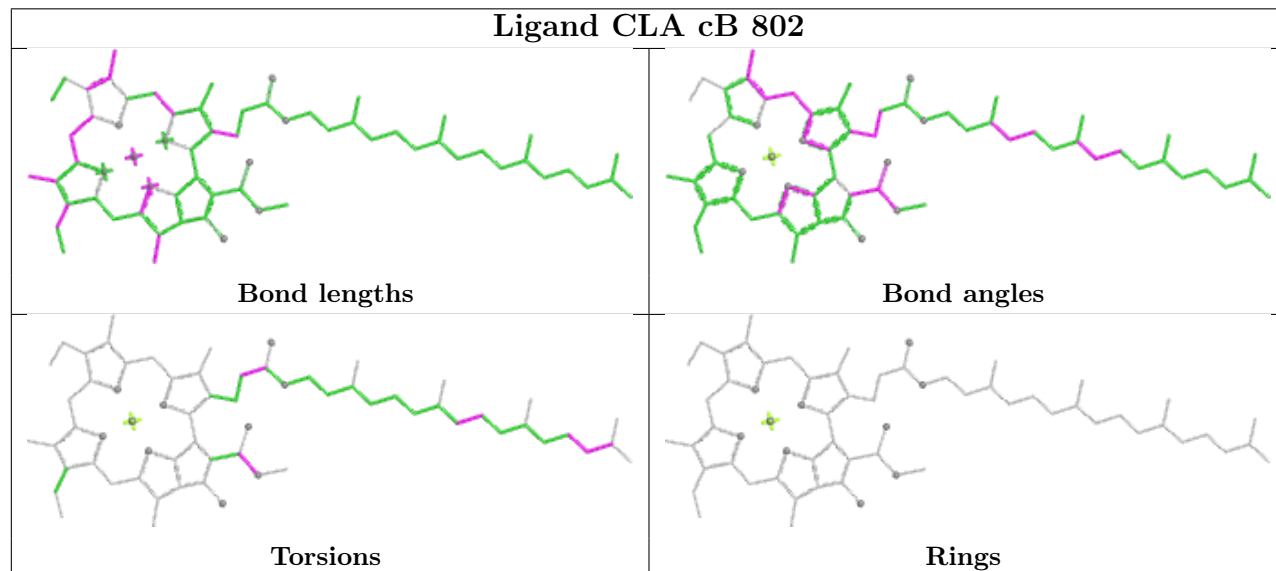


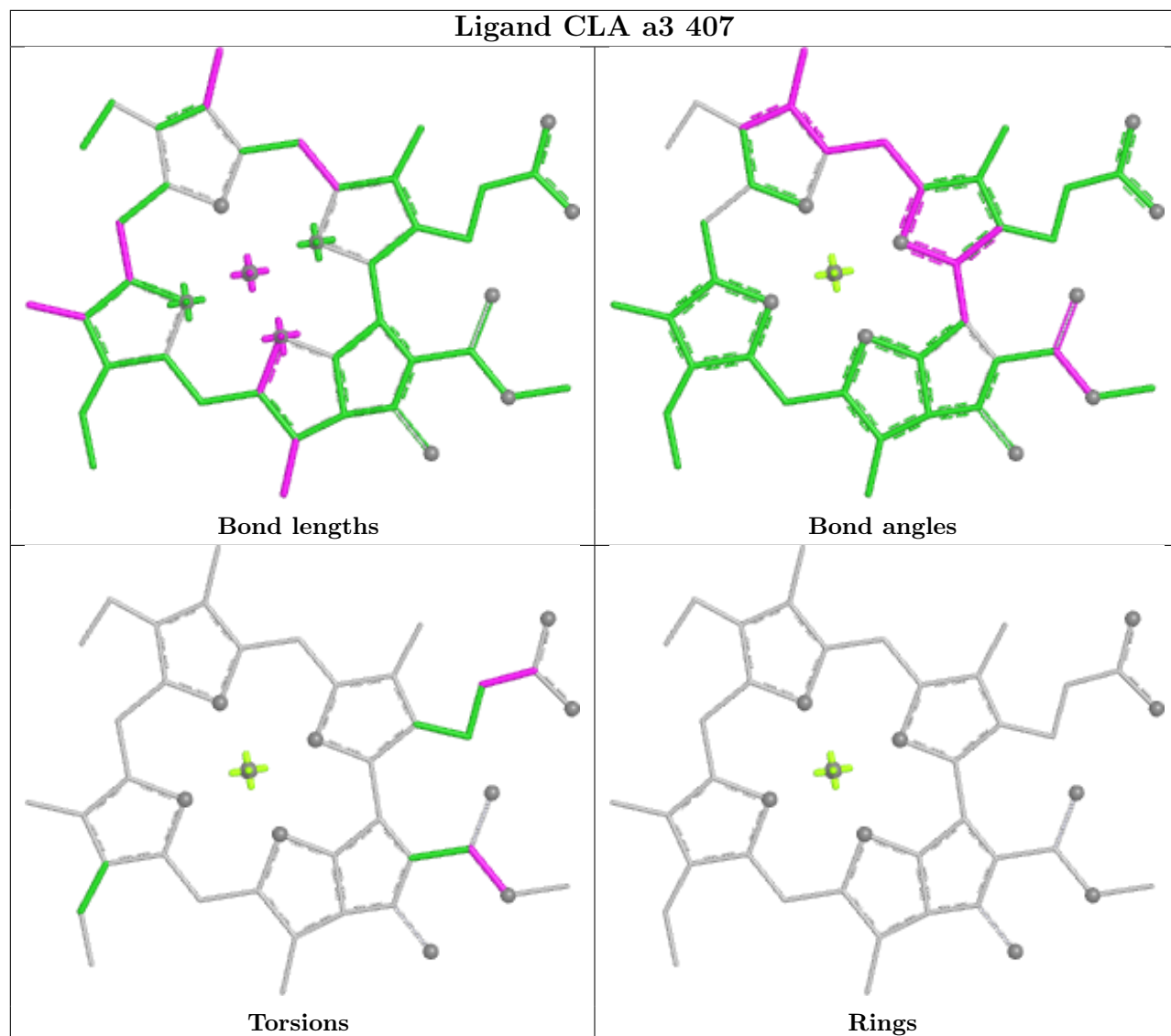
Torsions

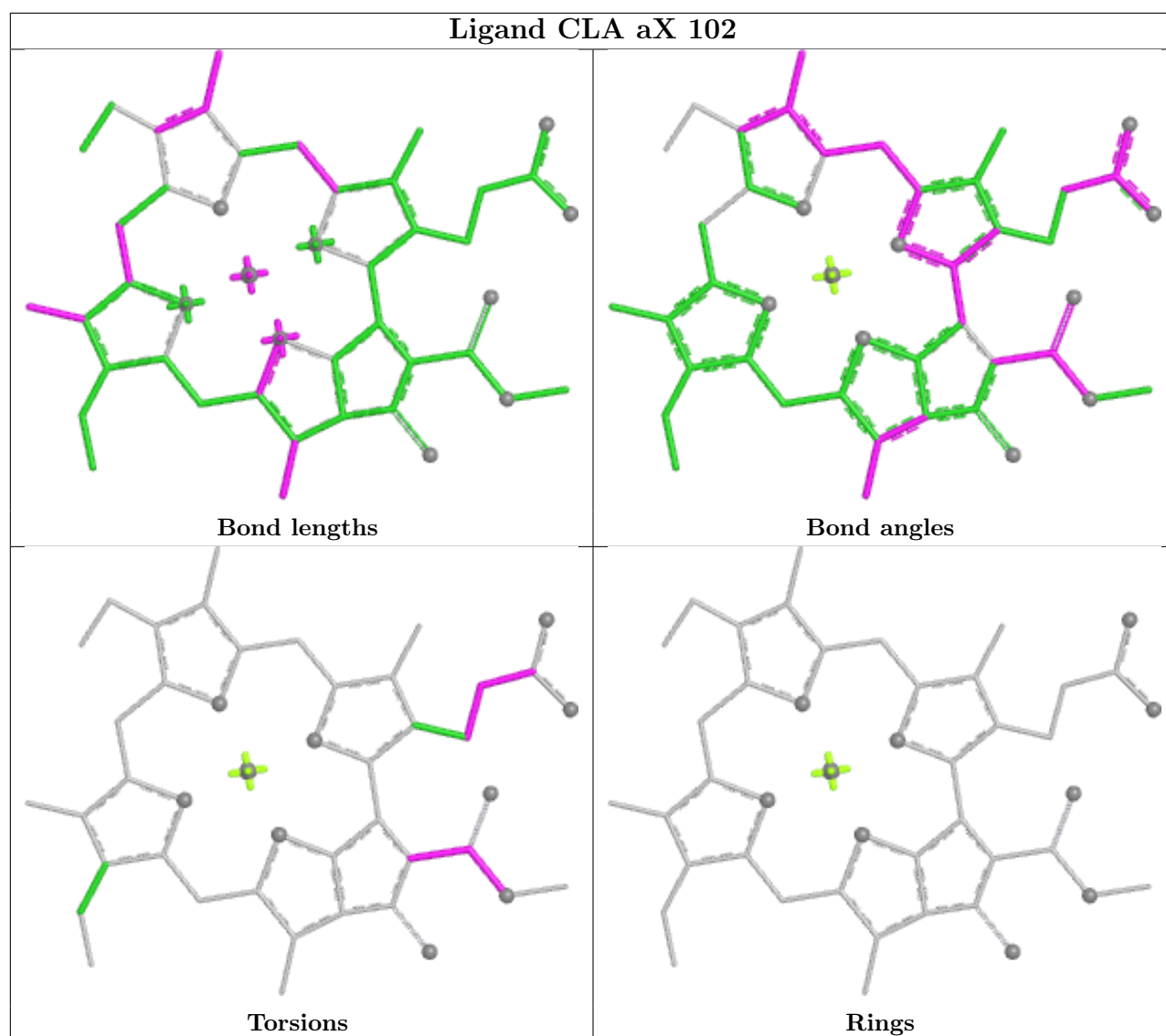


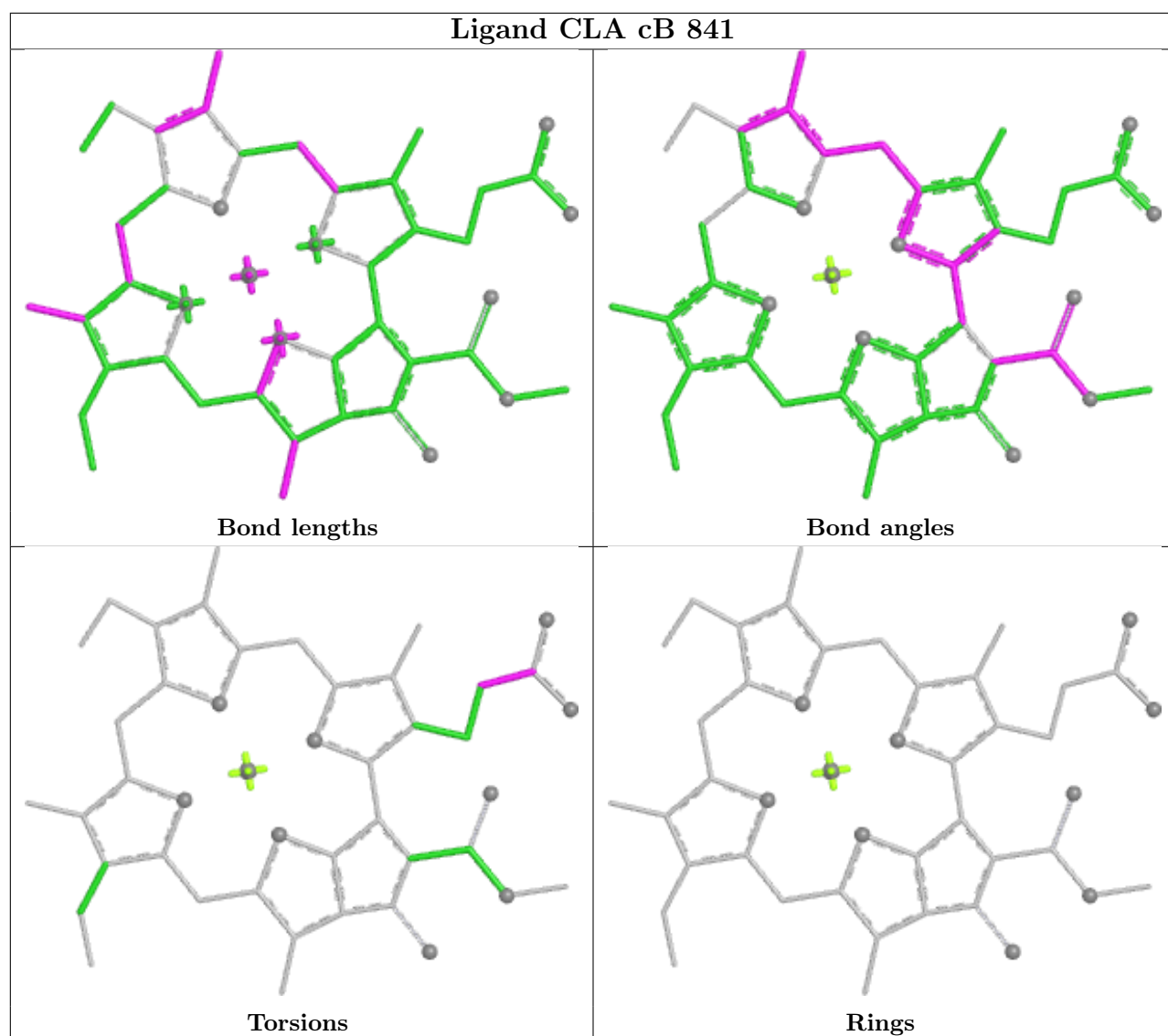
Rings

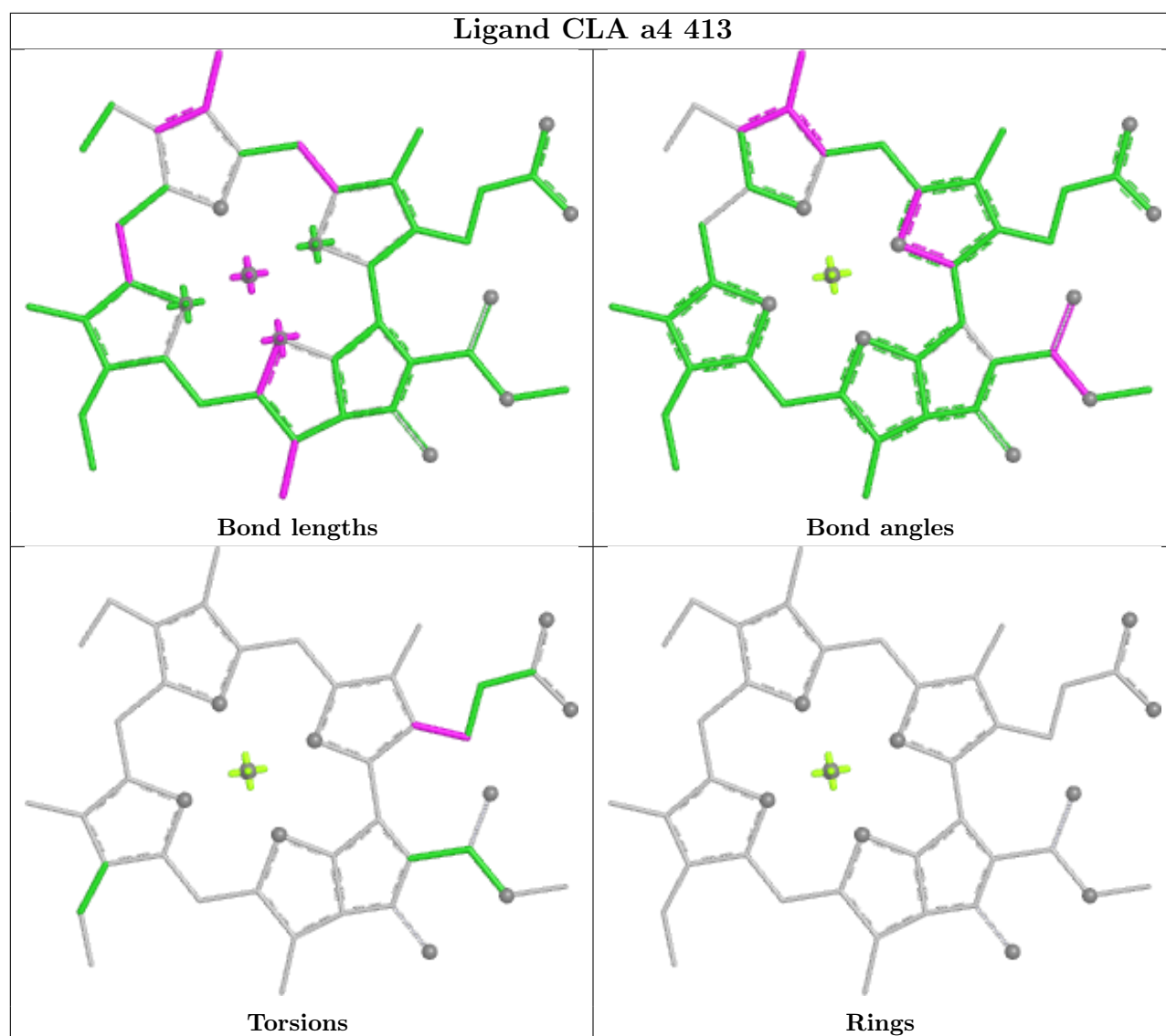


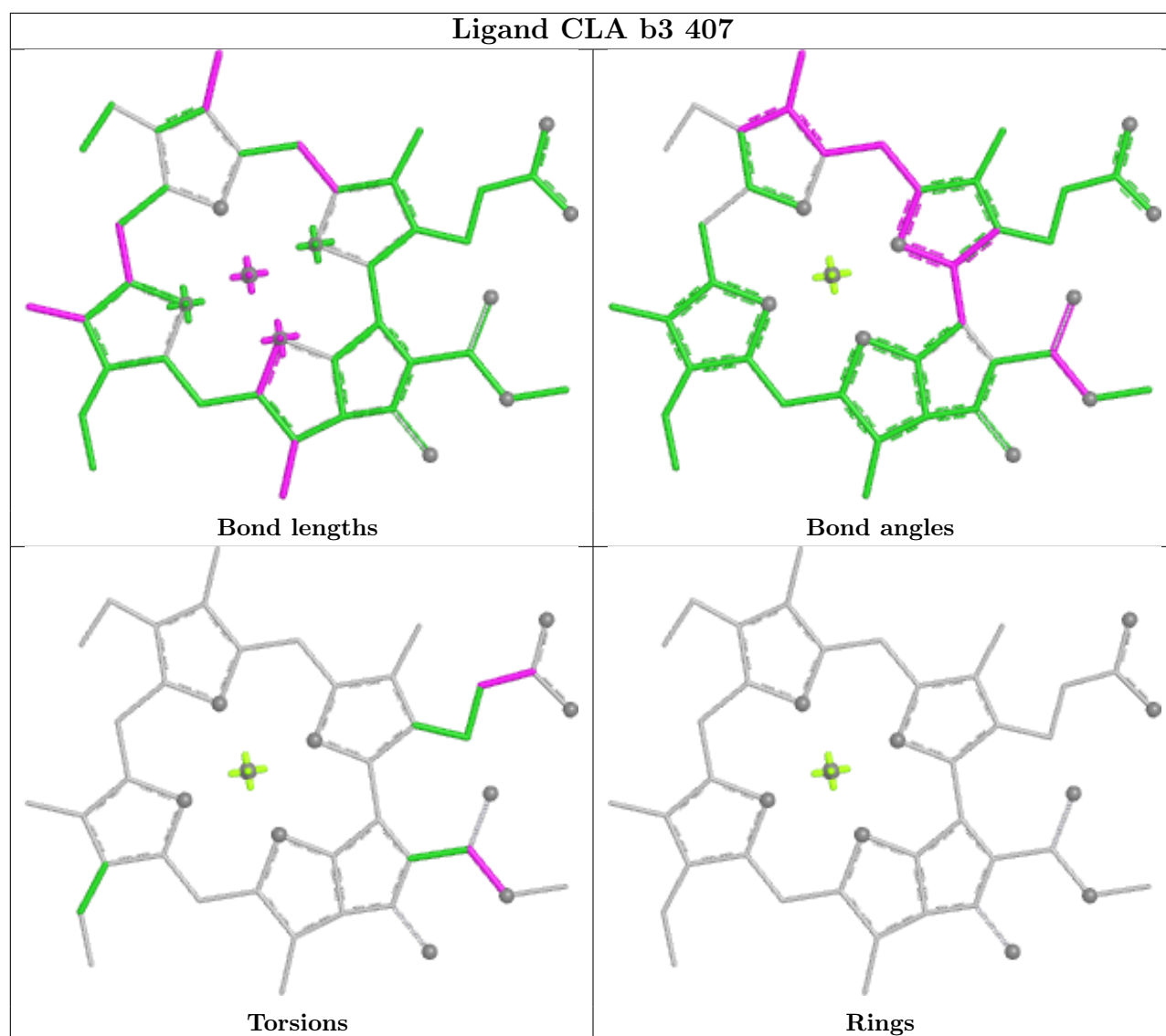
Ligand CLA bB 837**Ligand CLA cB 802**

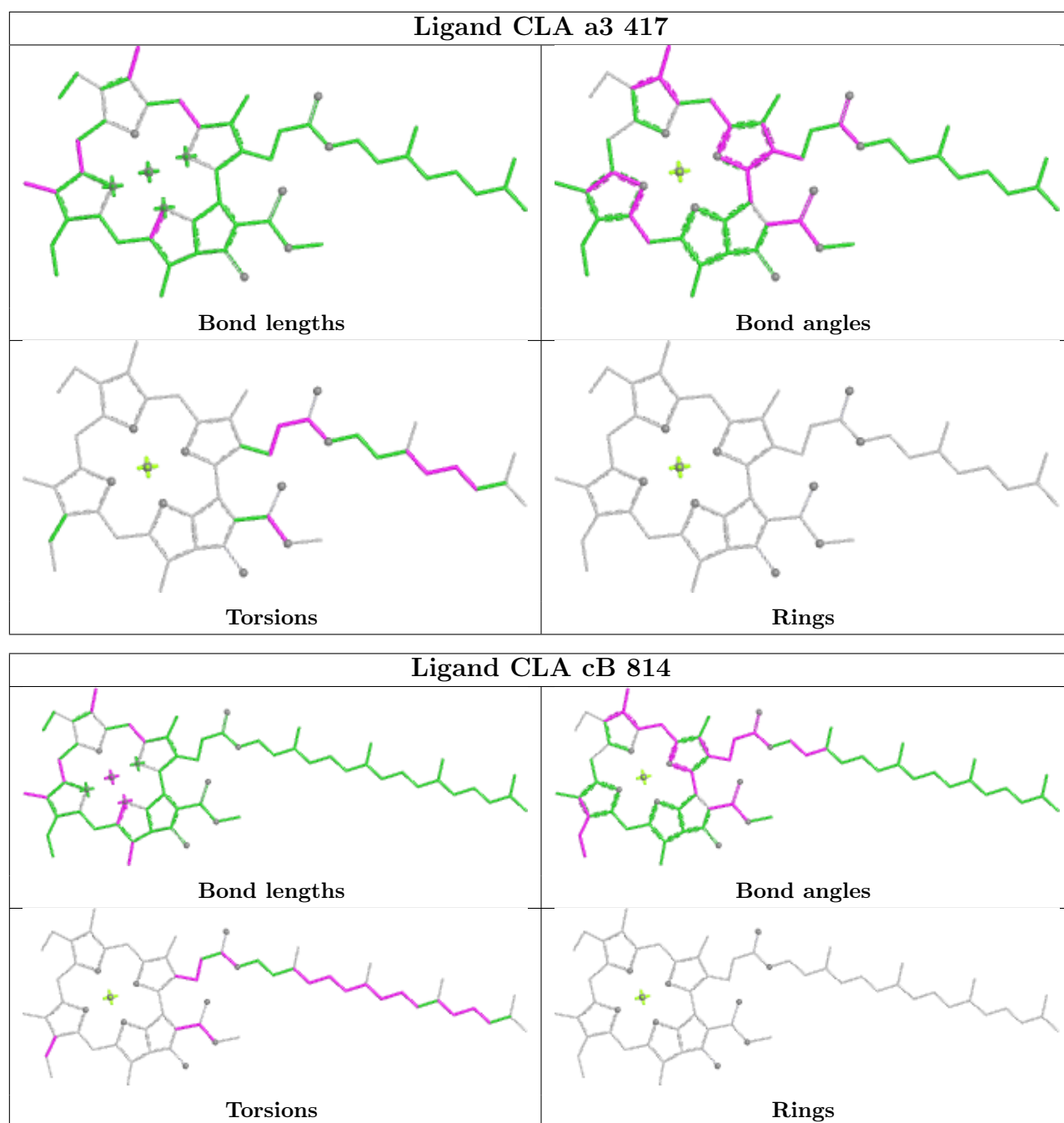


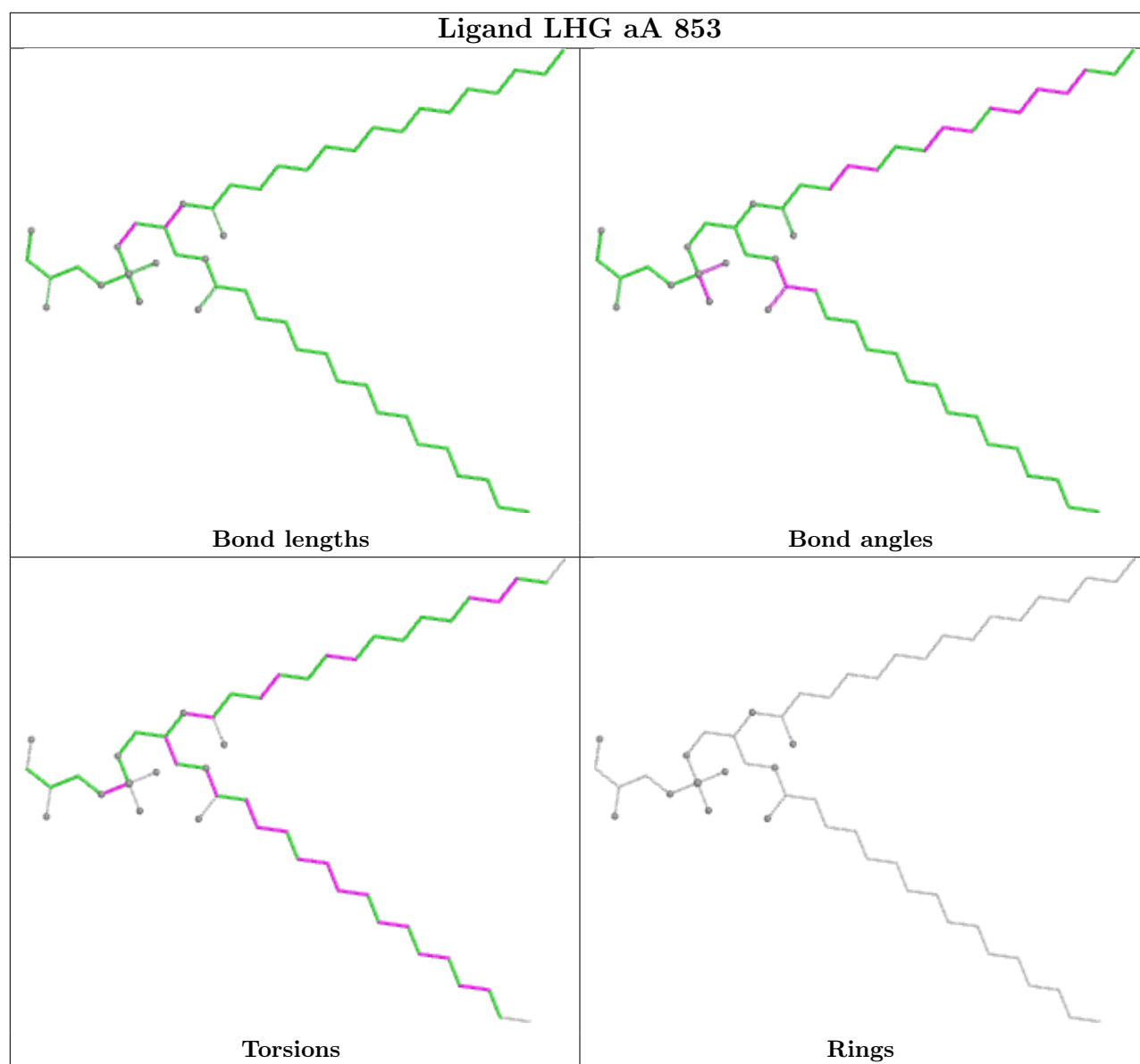


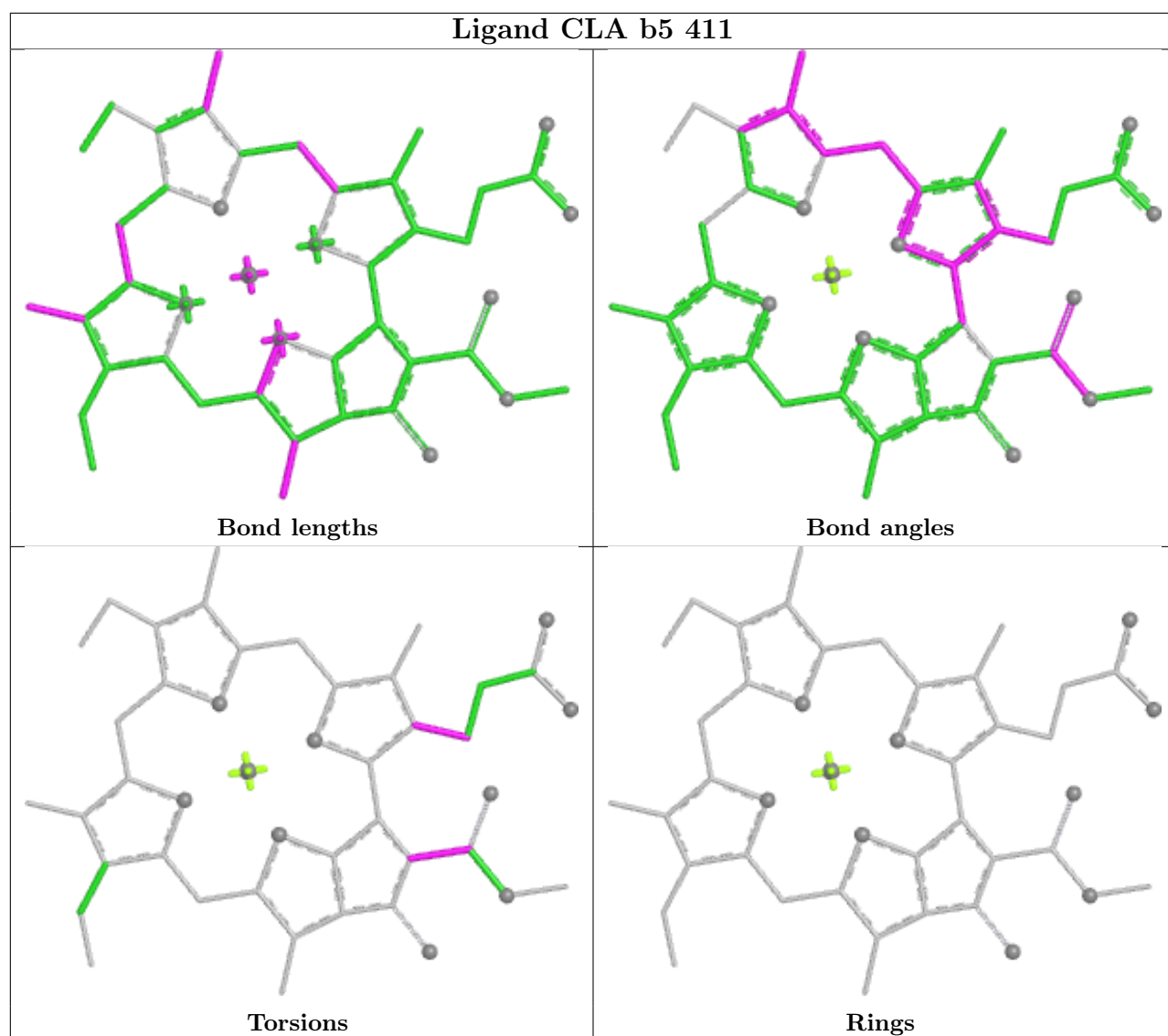


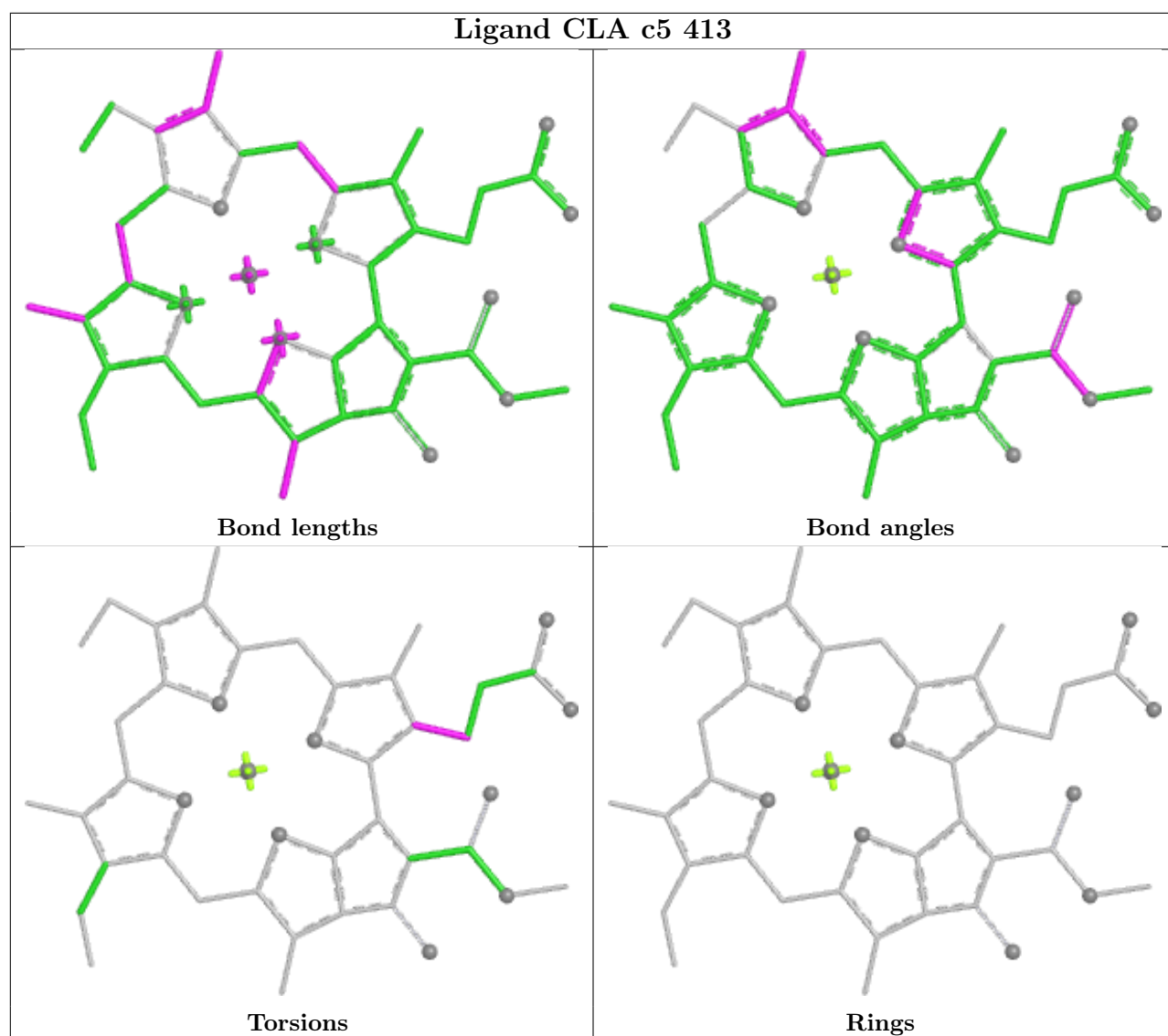


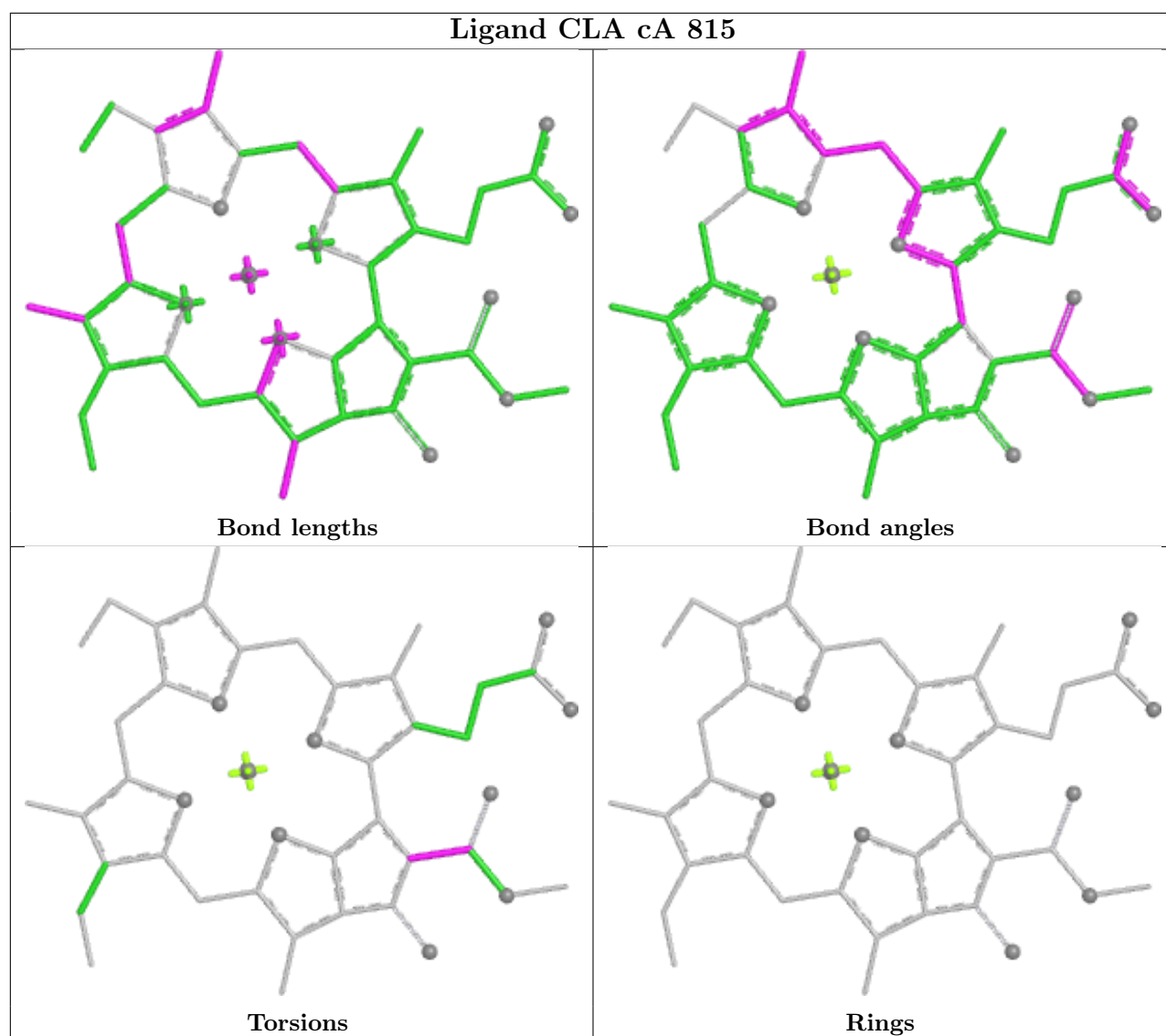


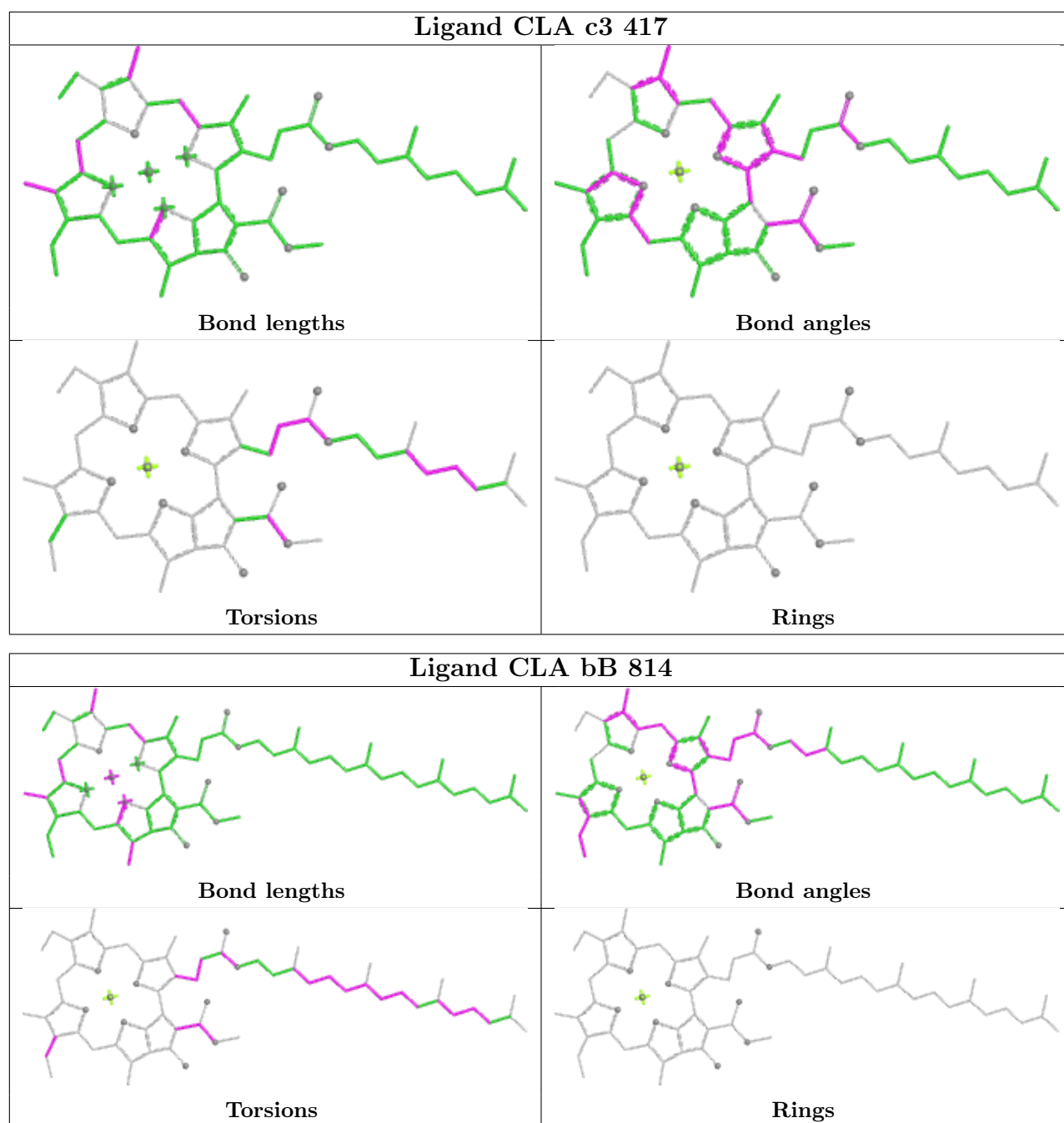


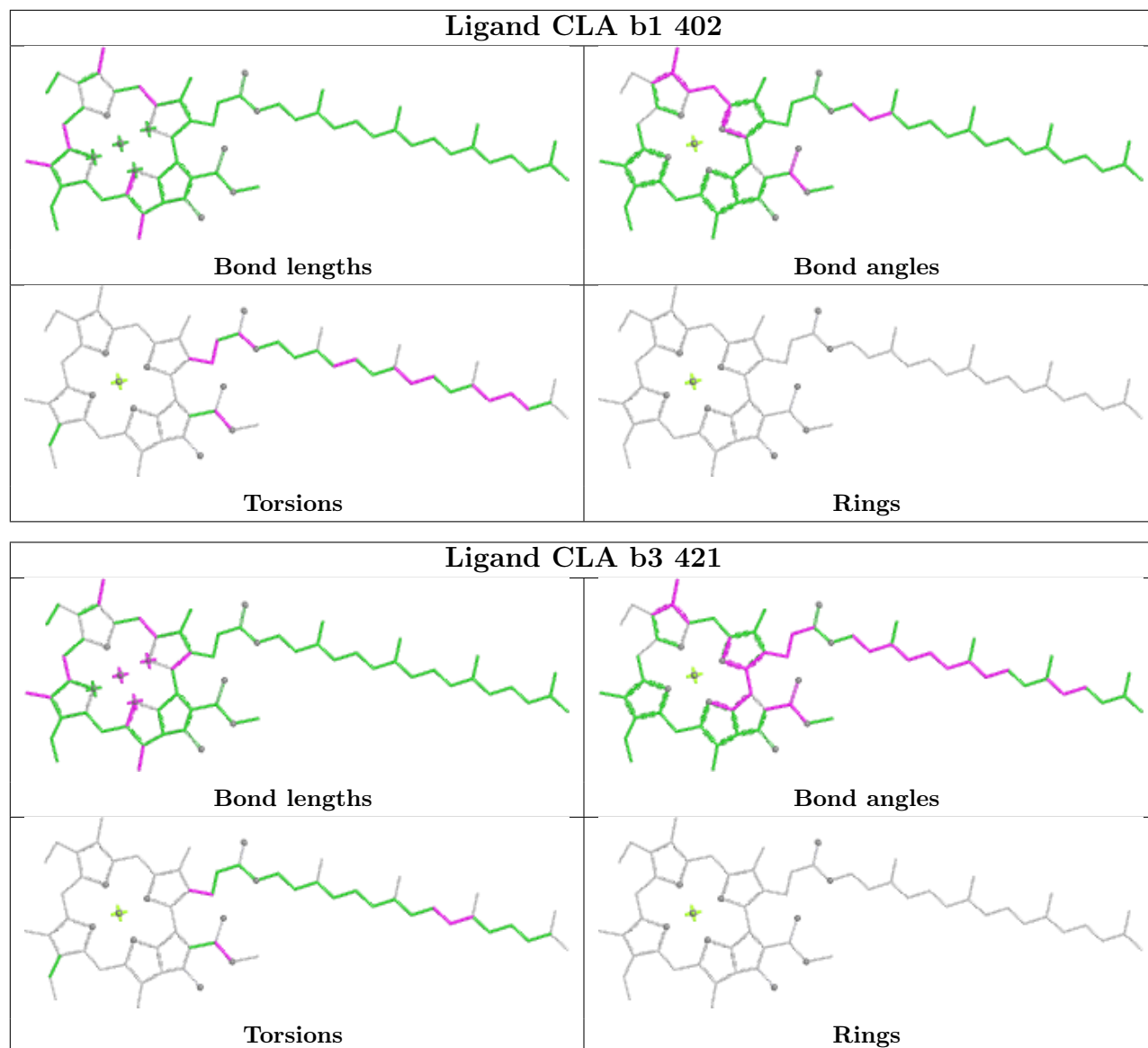




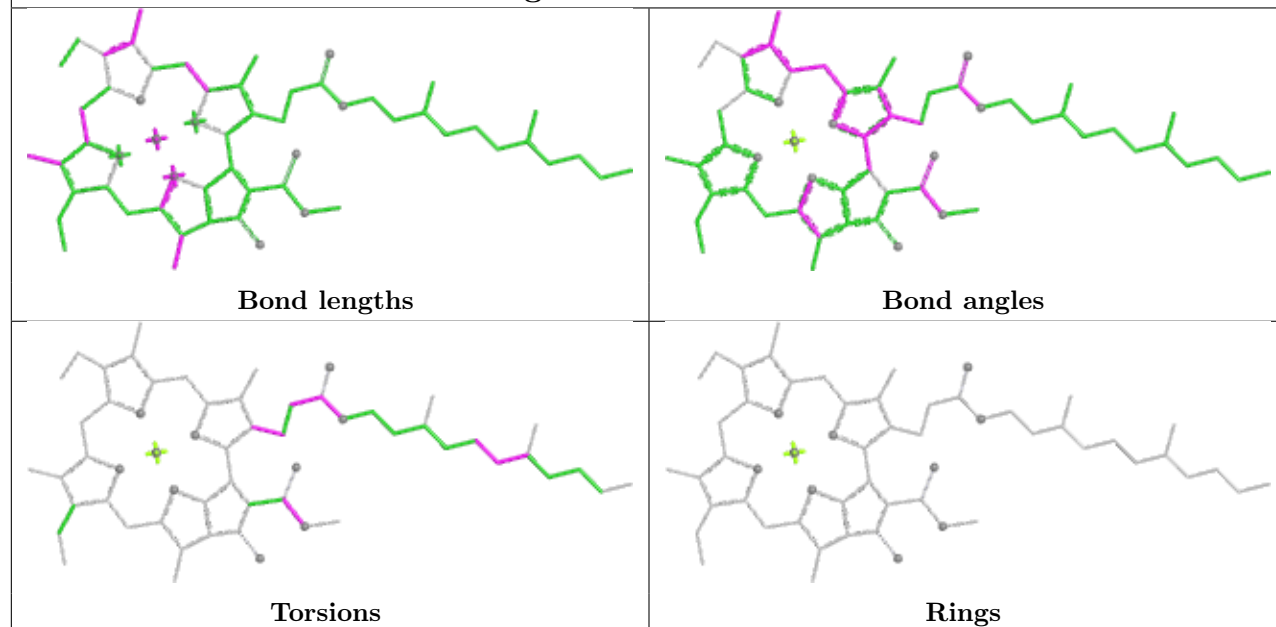




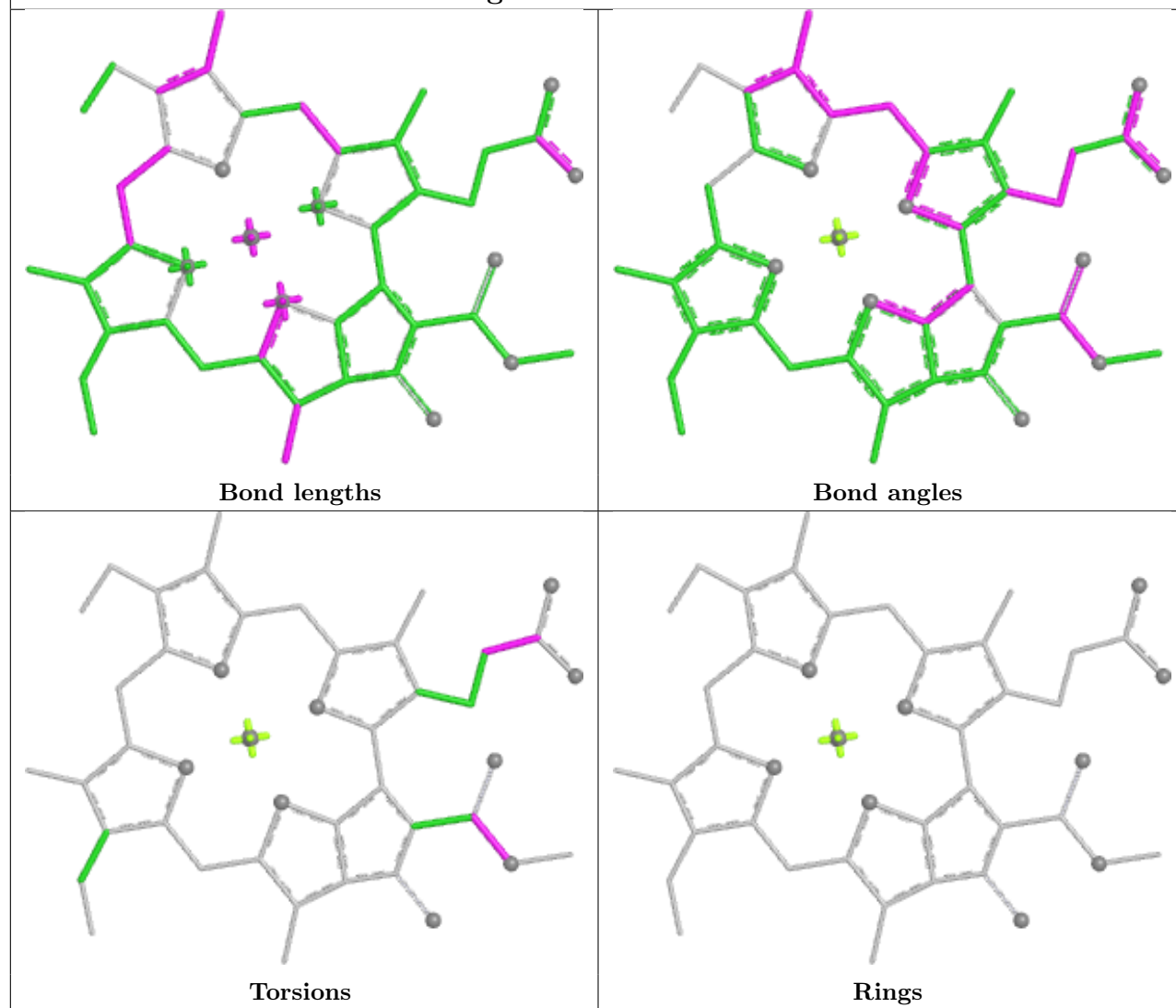


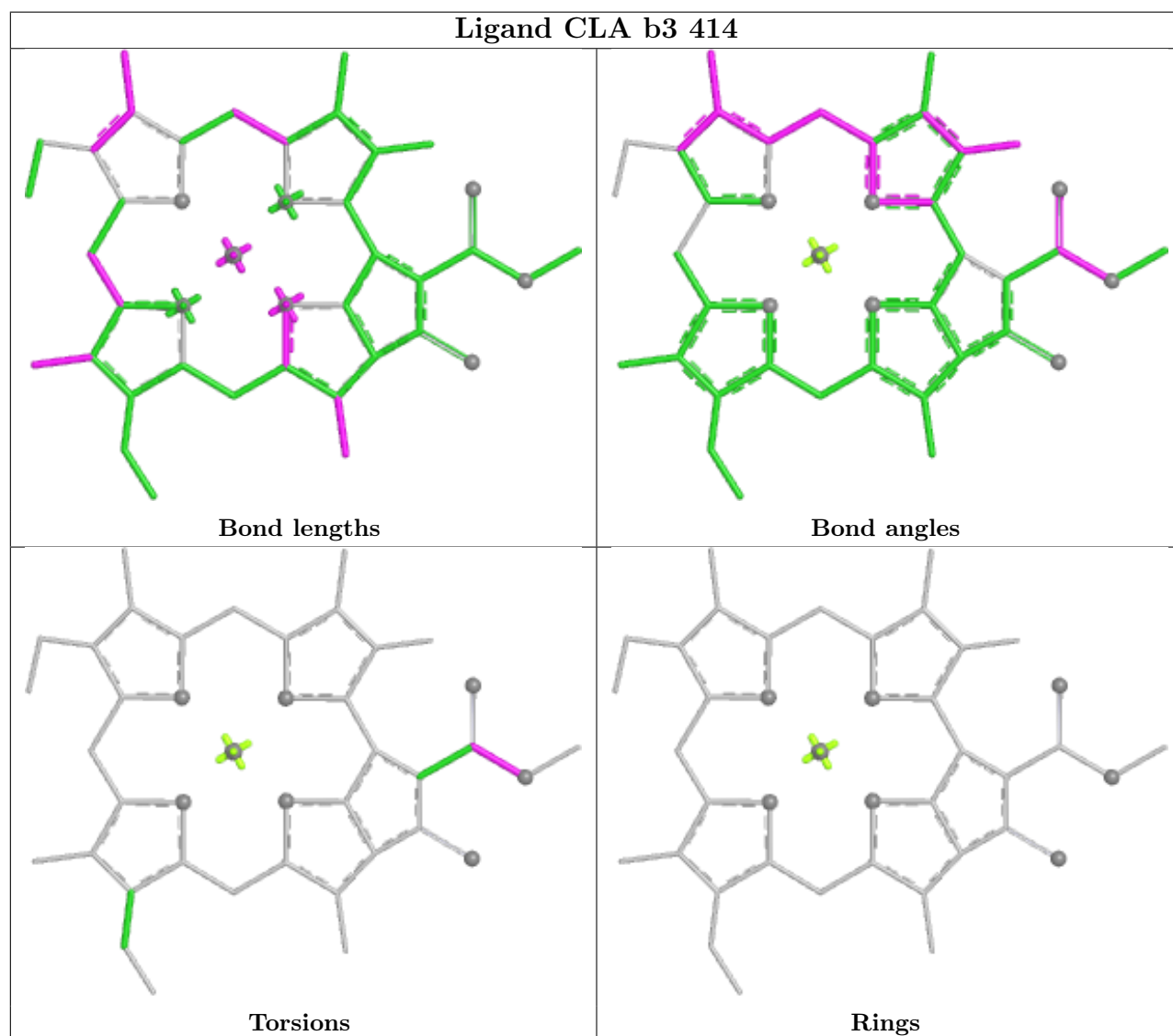
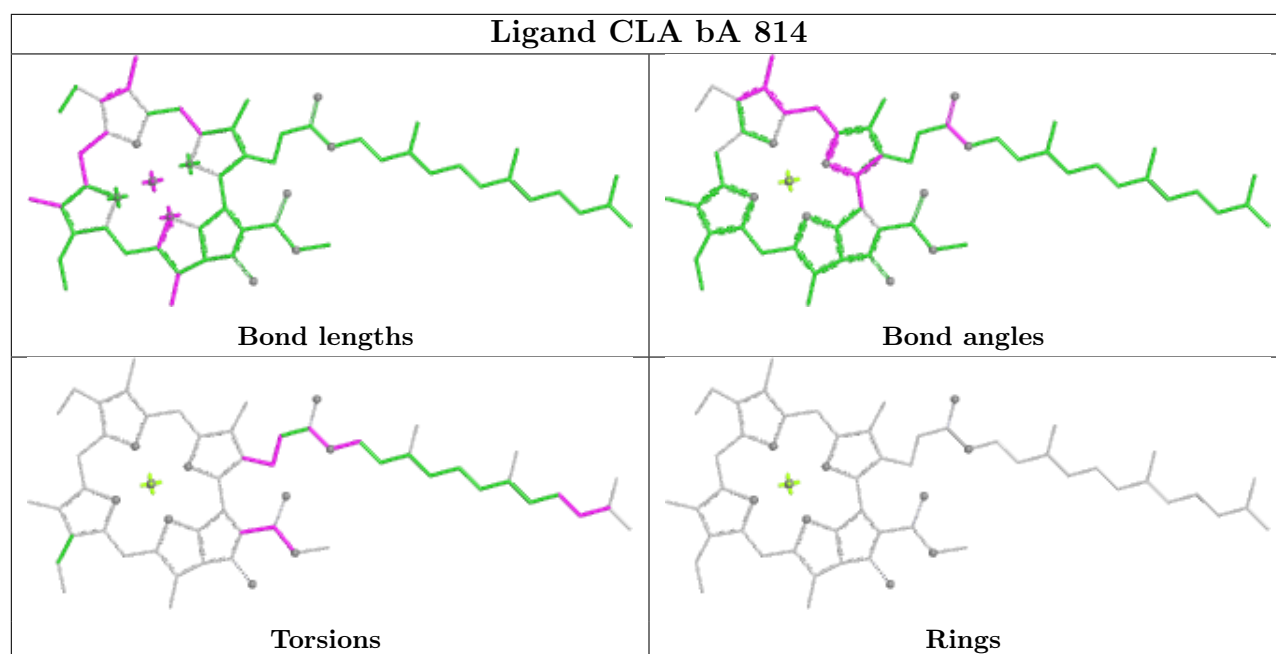


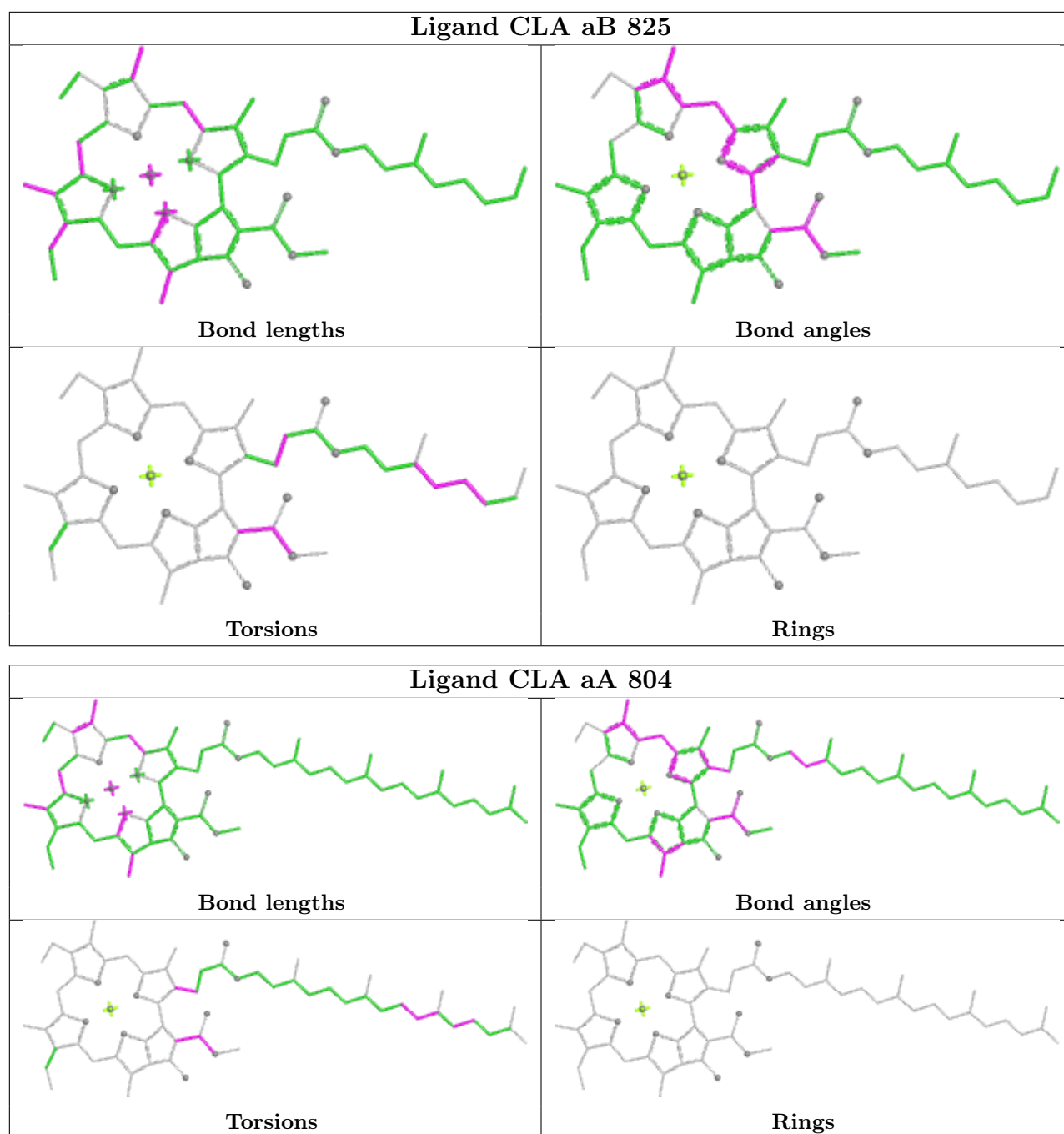
Ligand CLA cB 834

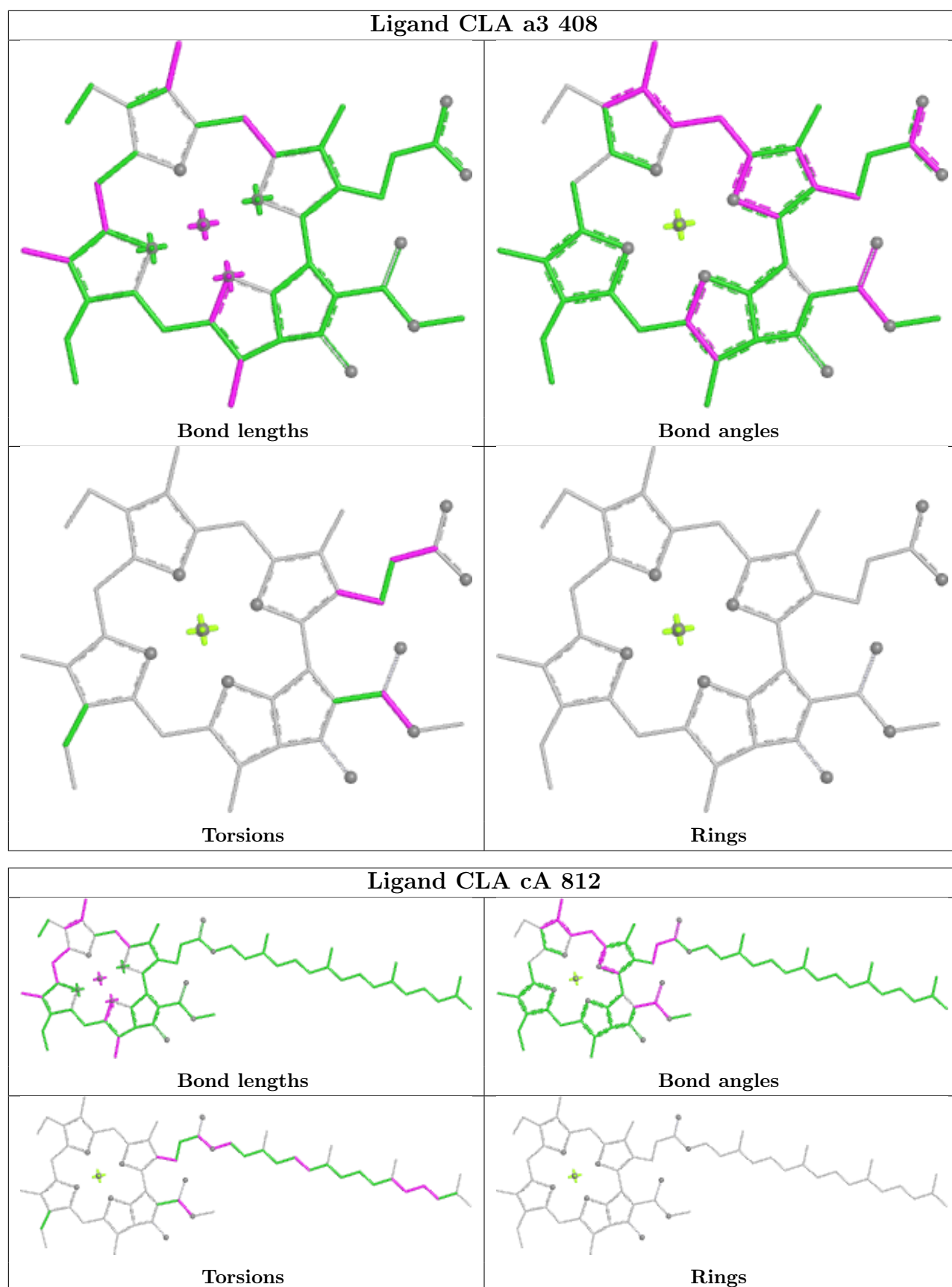


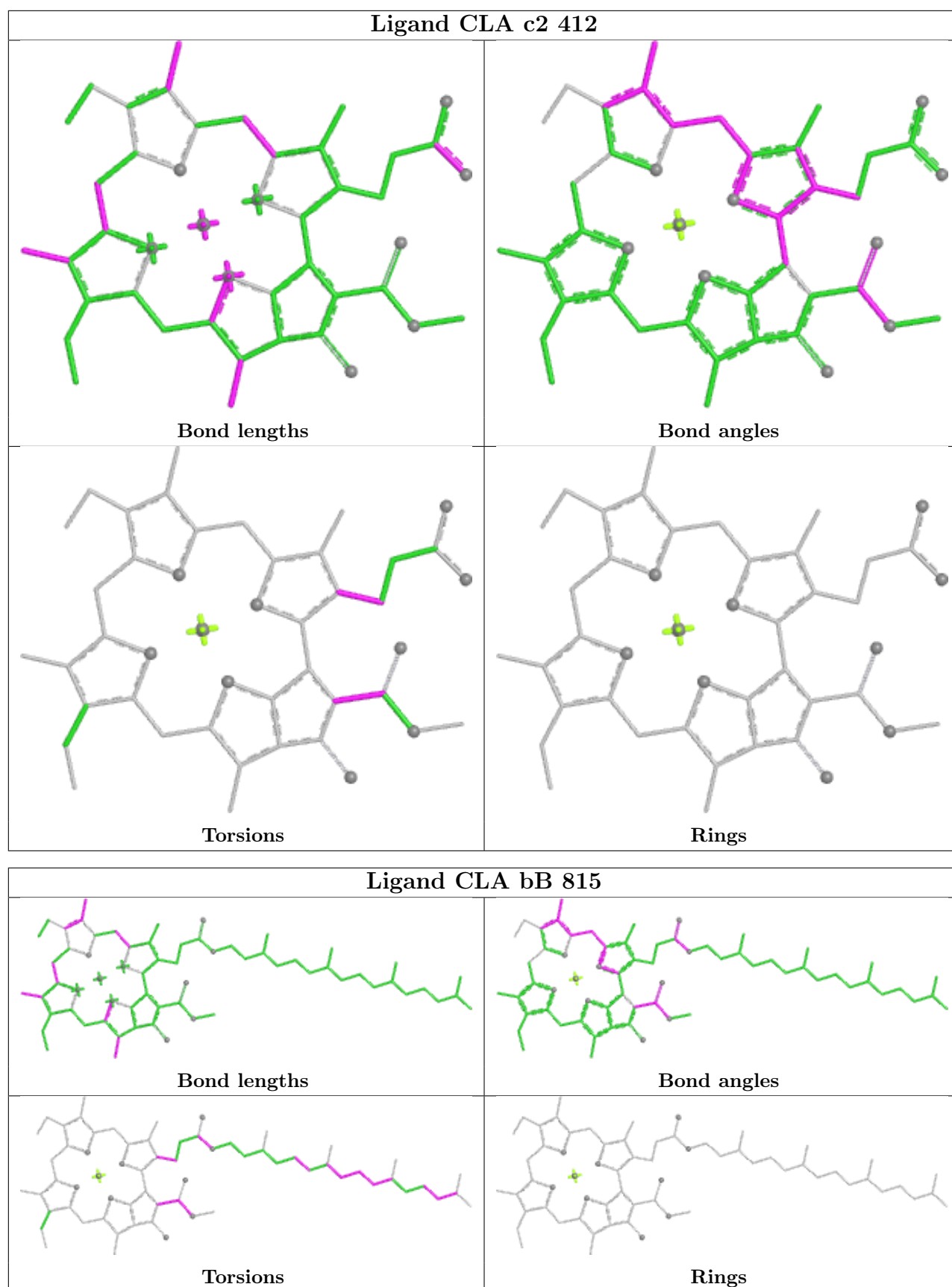
Ligand CLA c3 415

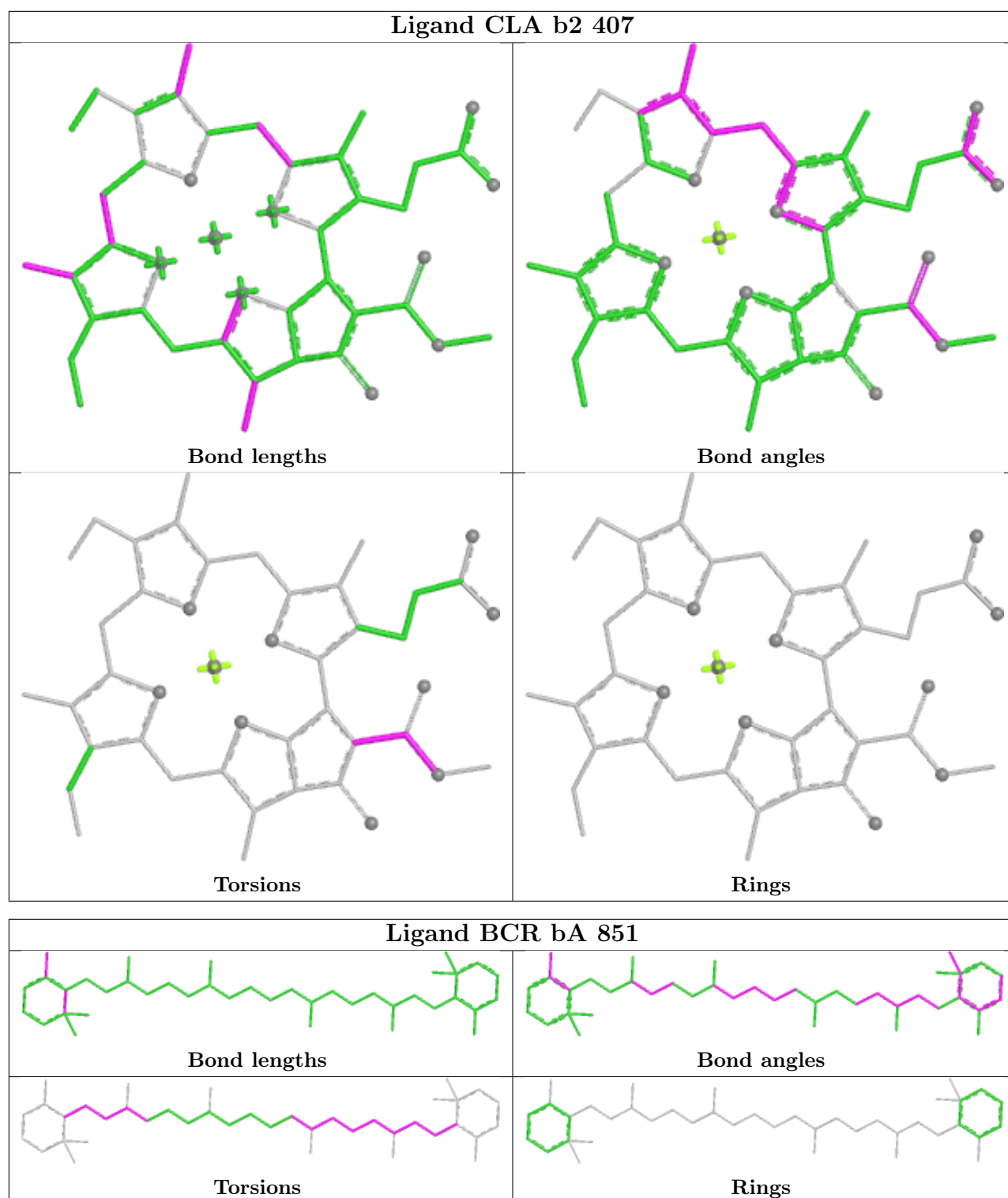




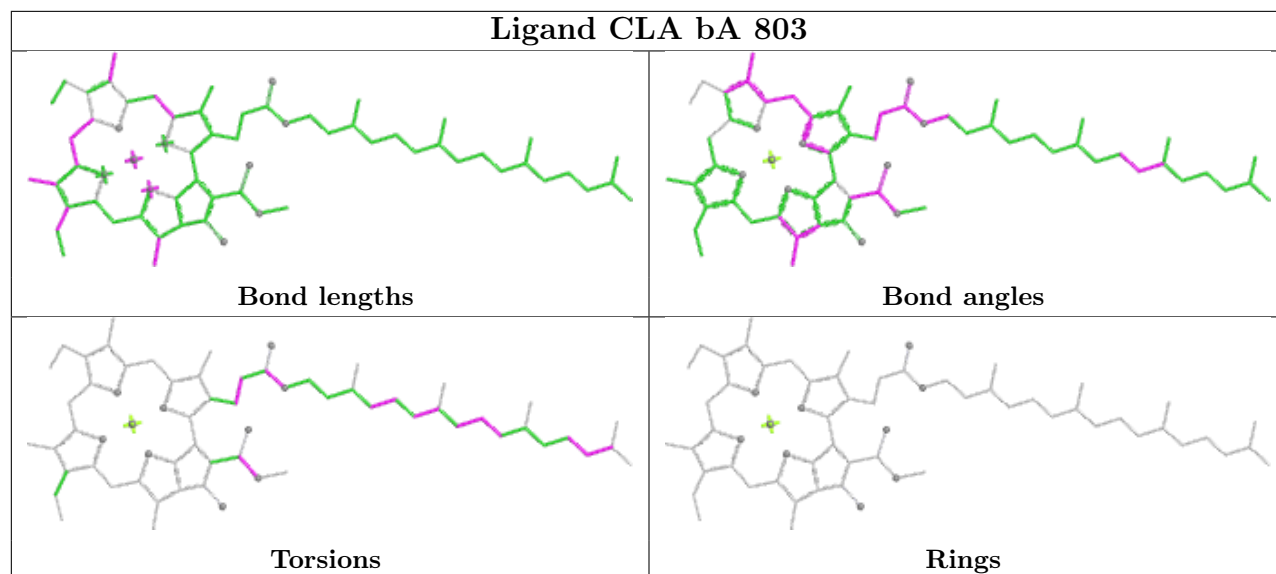




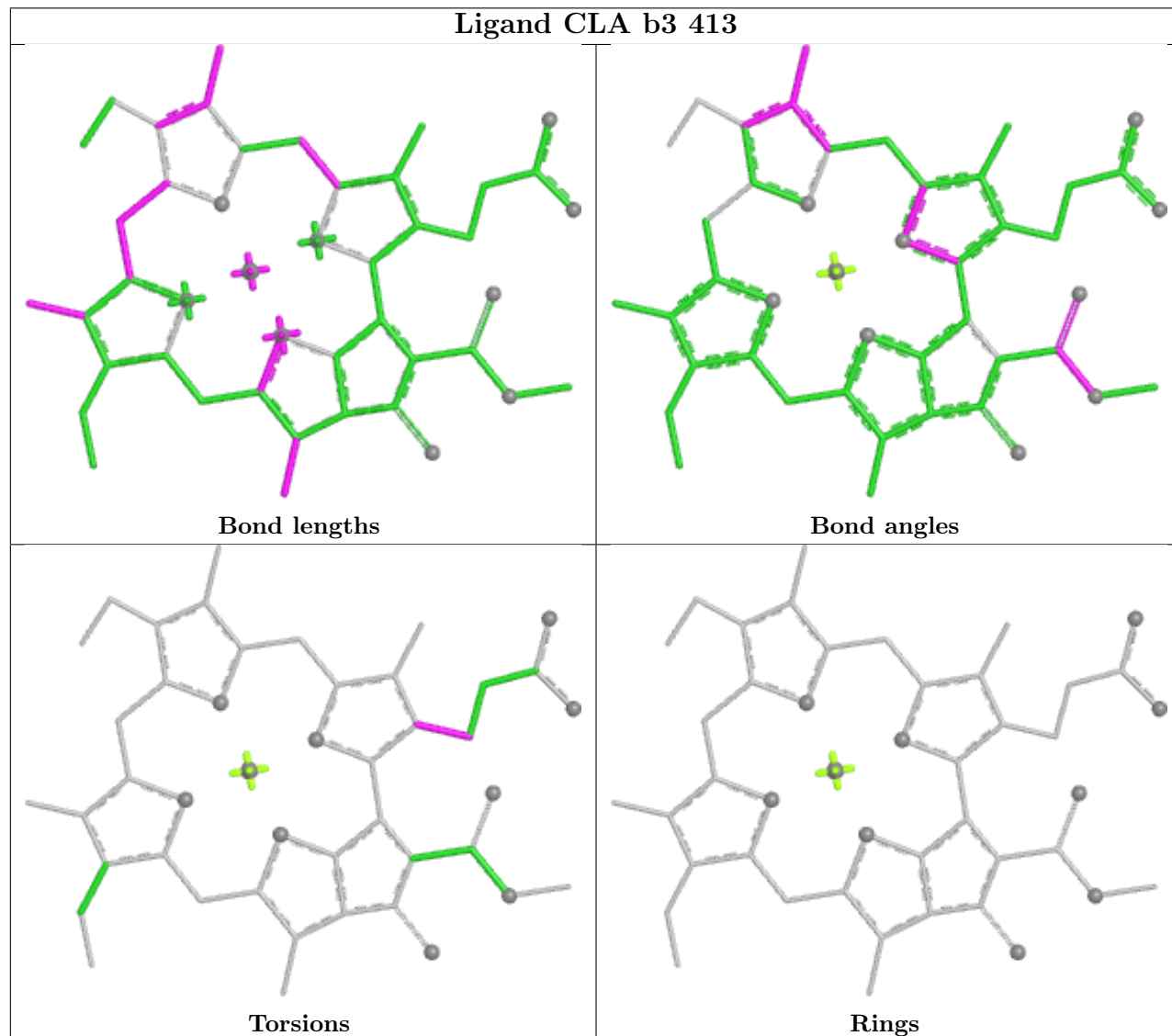


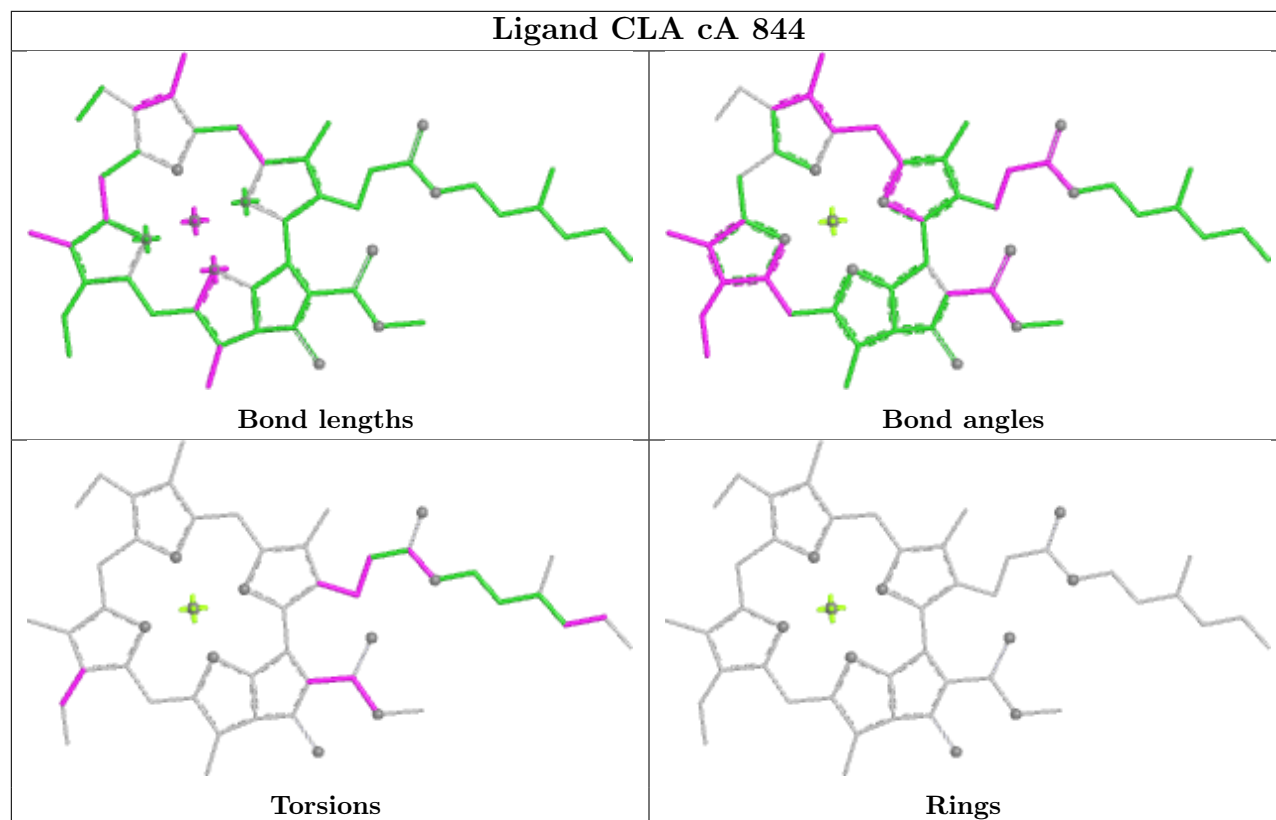
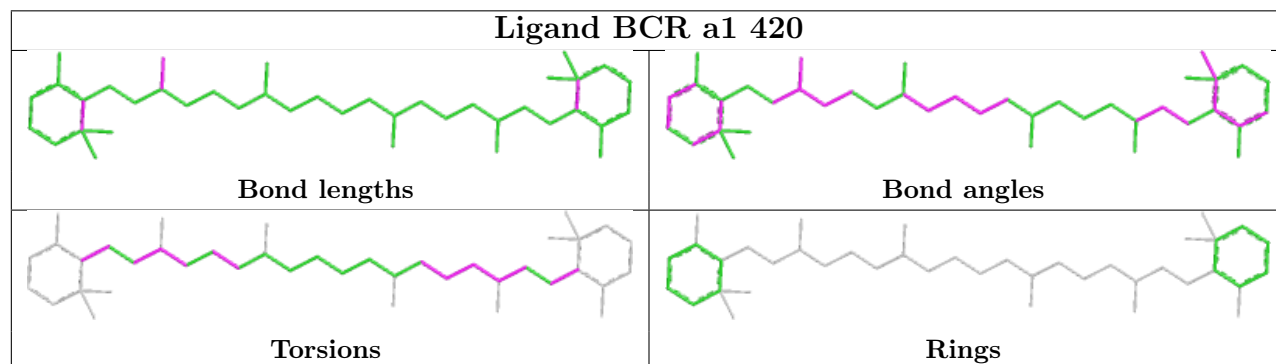
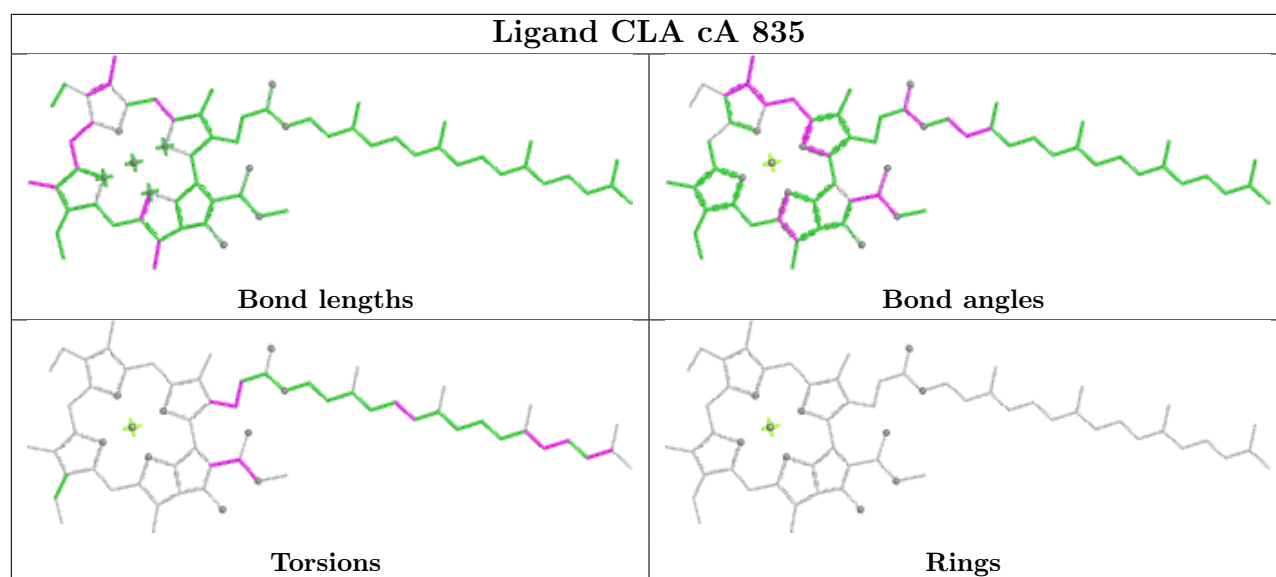


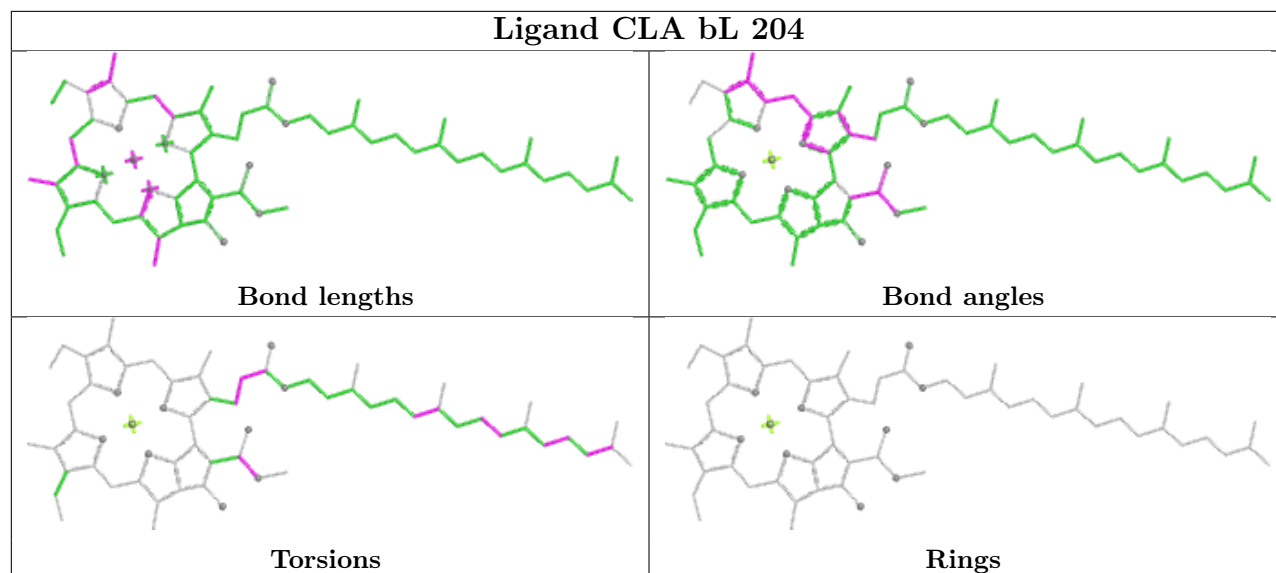
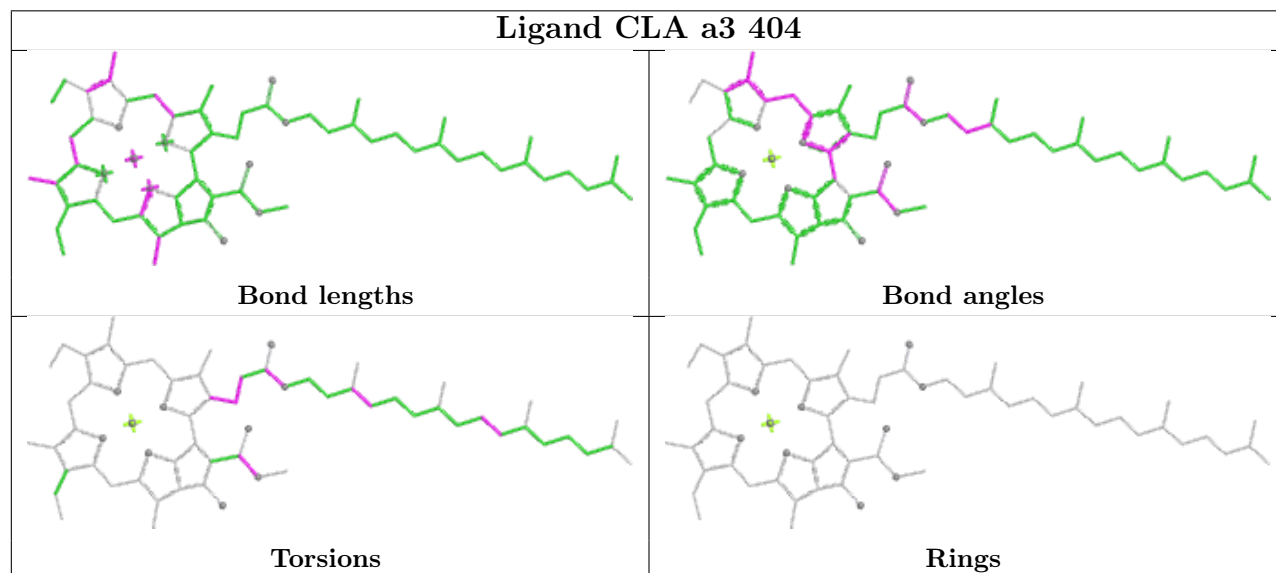
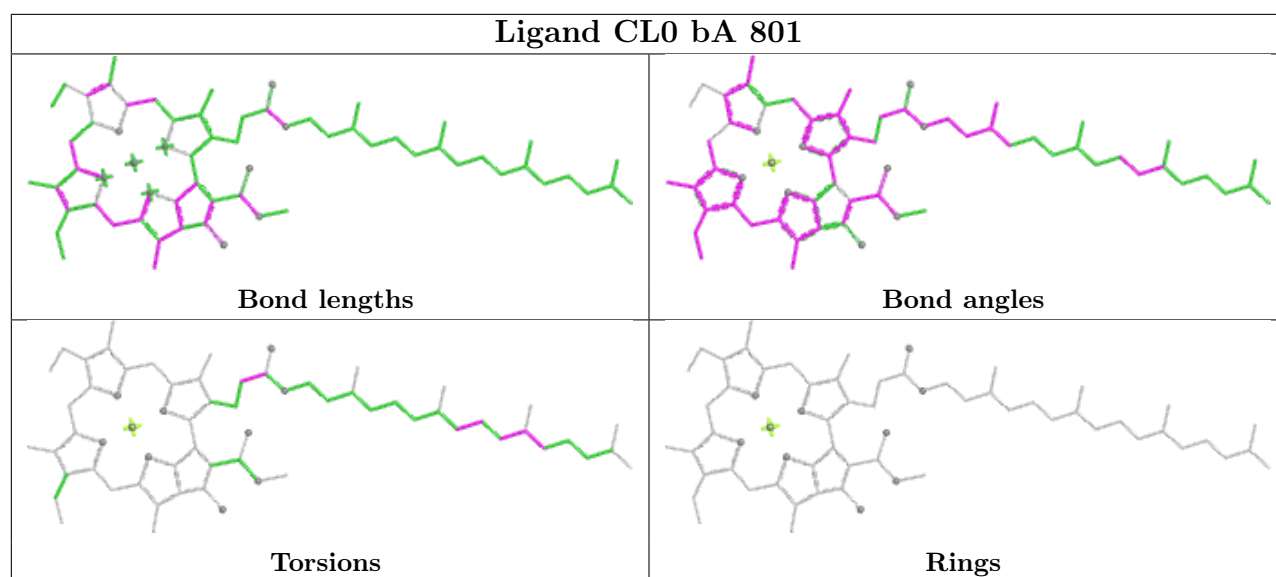
Ligand CLA bA 803

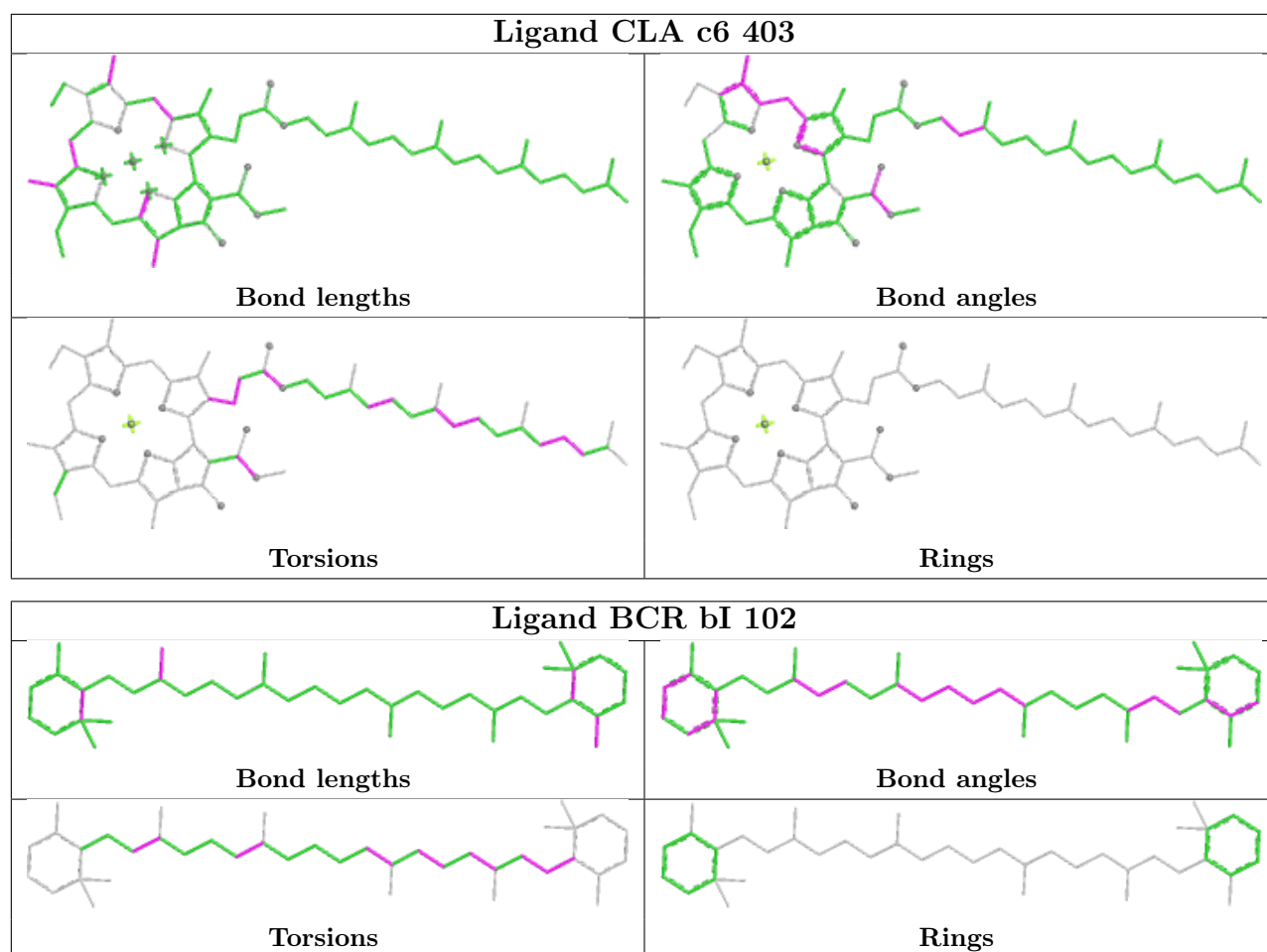


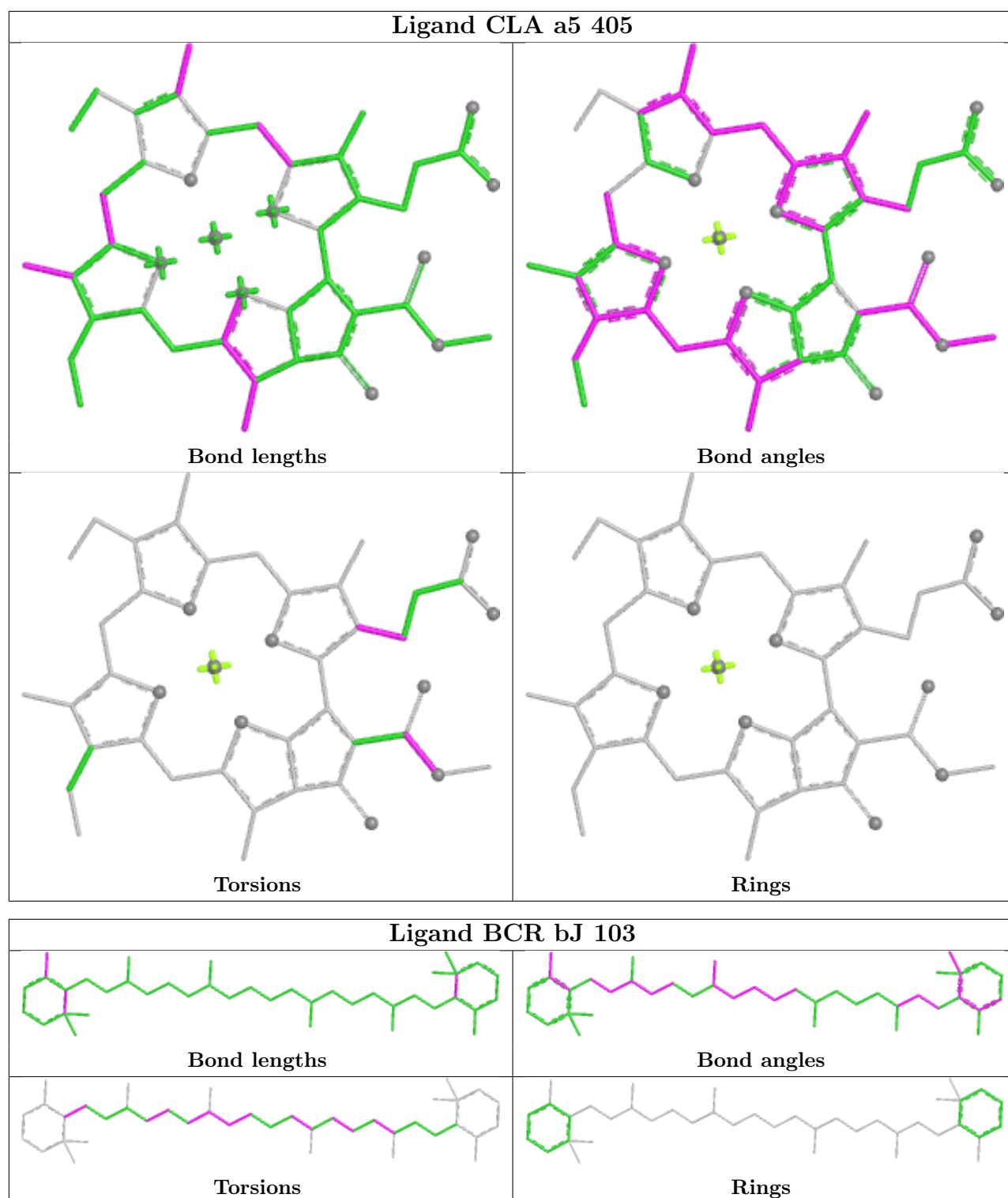
Ligand CLA b3 413

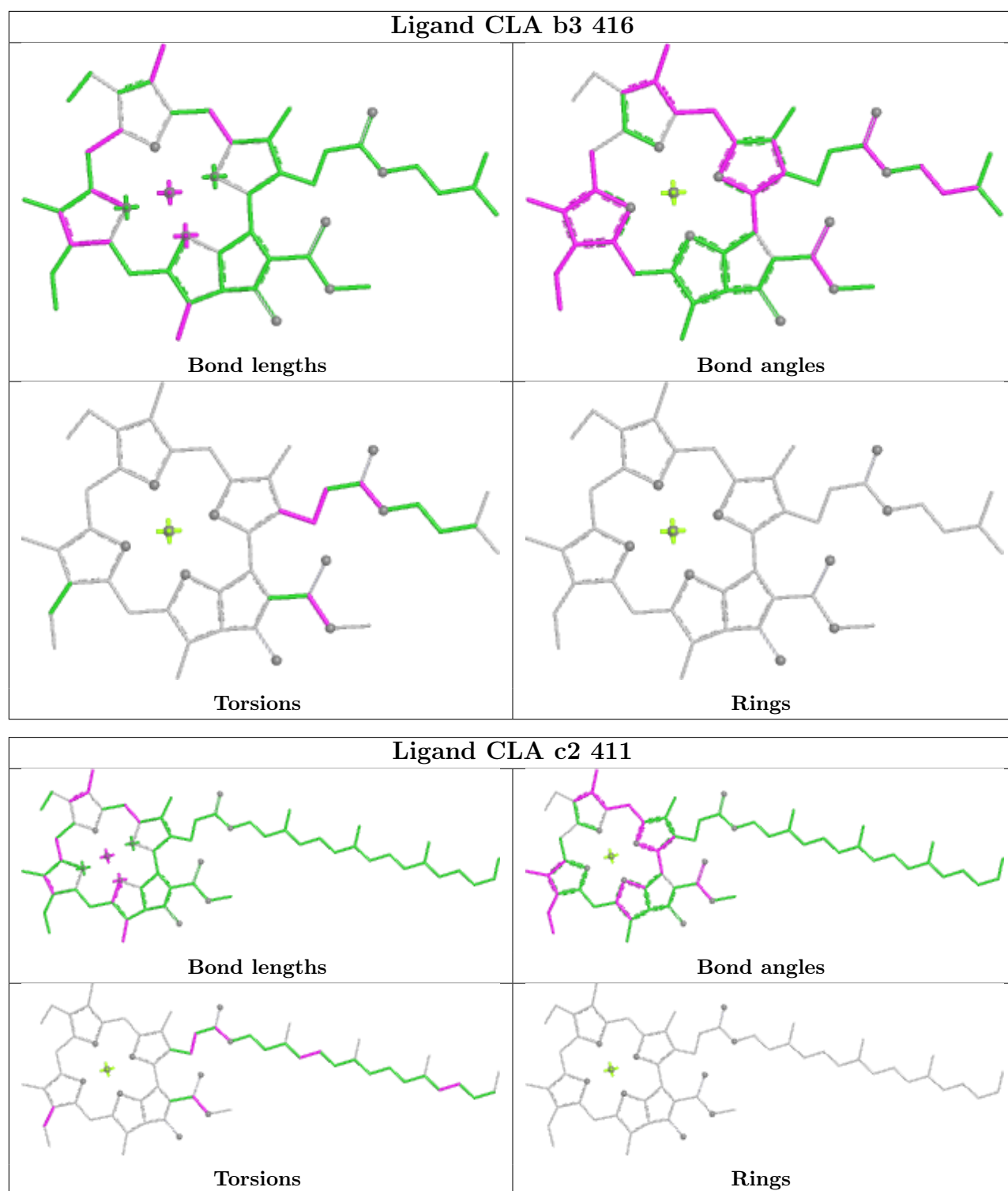


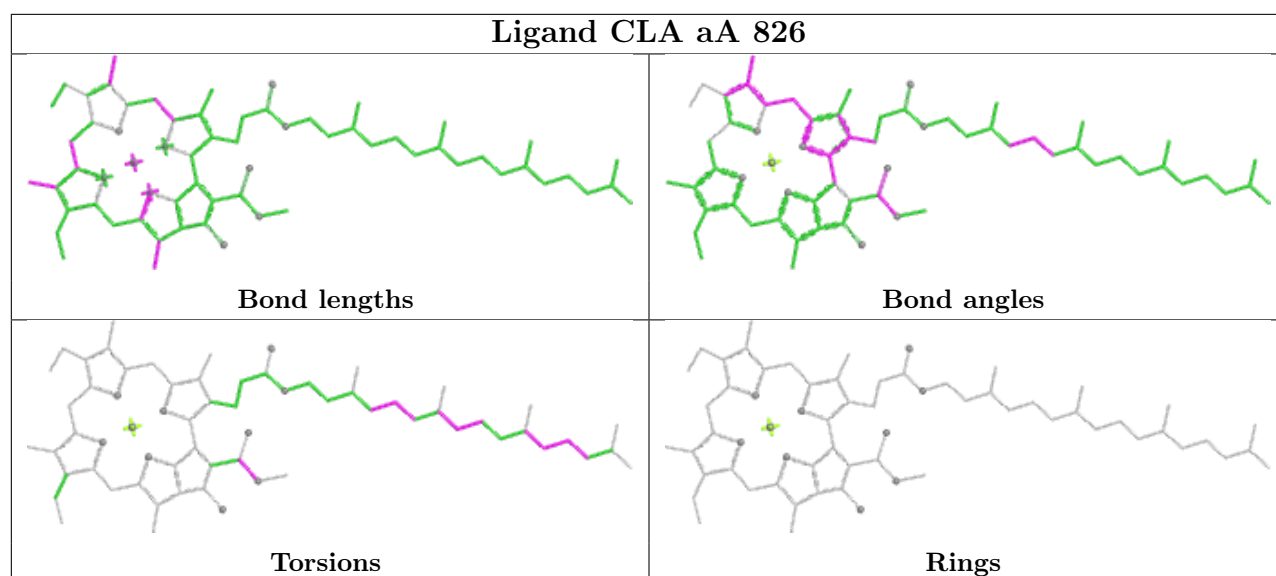
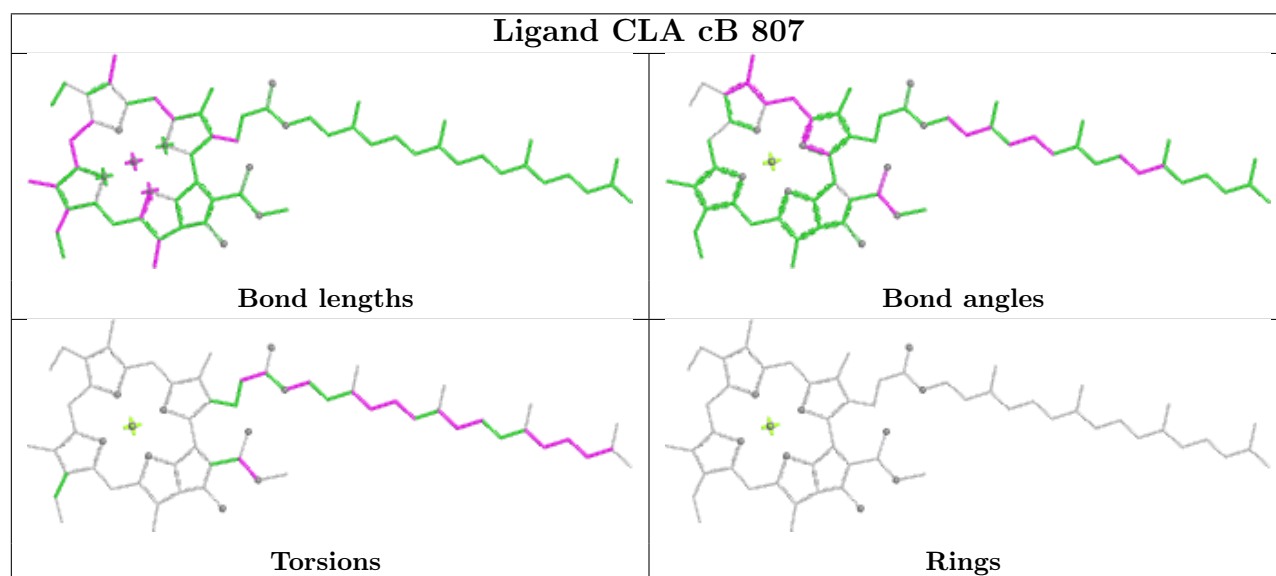
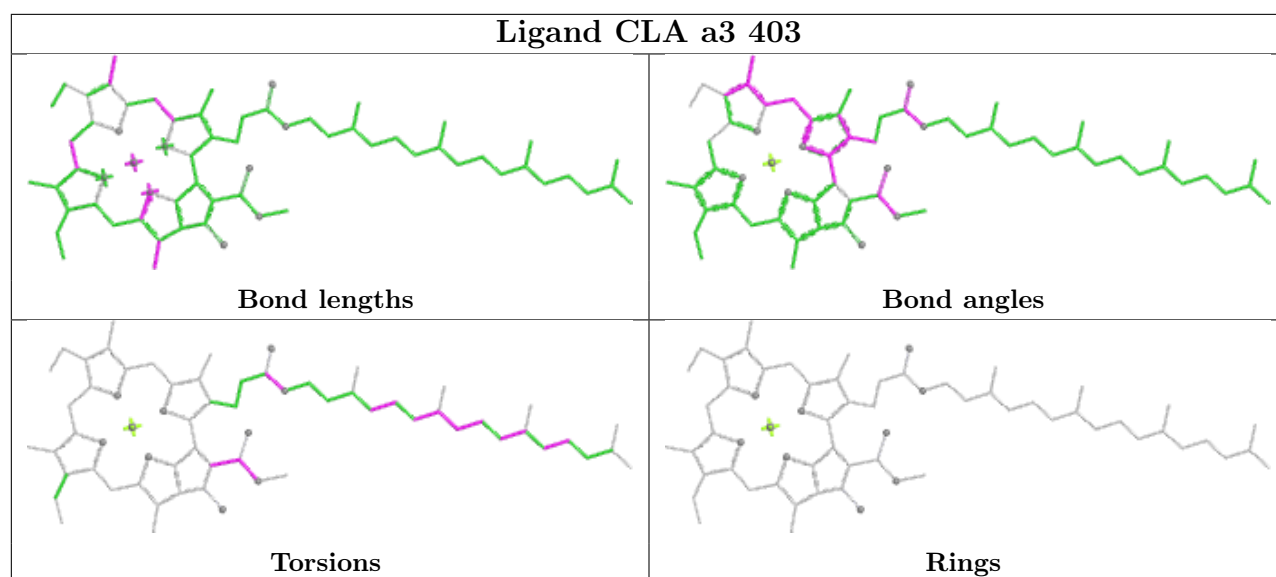


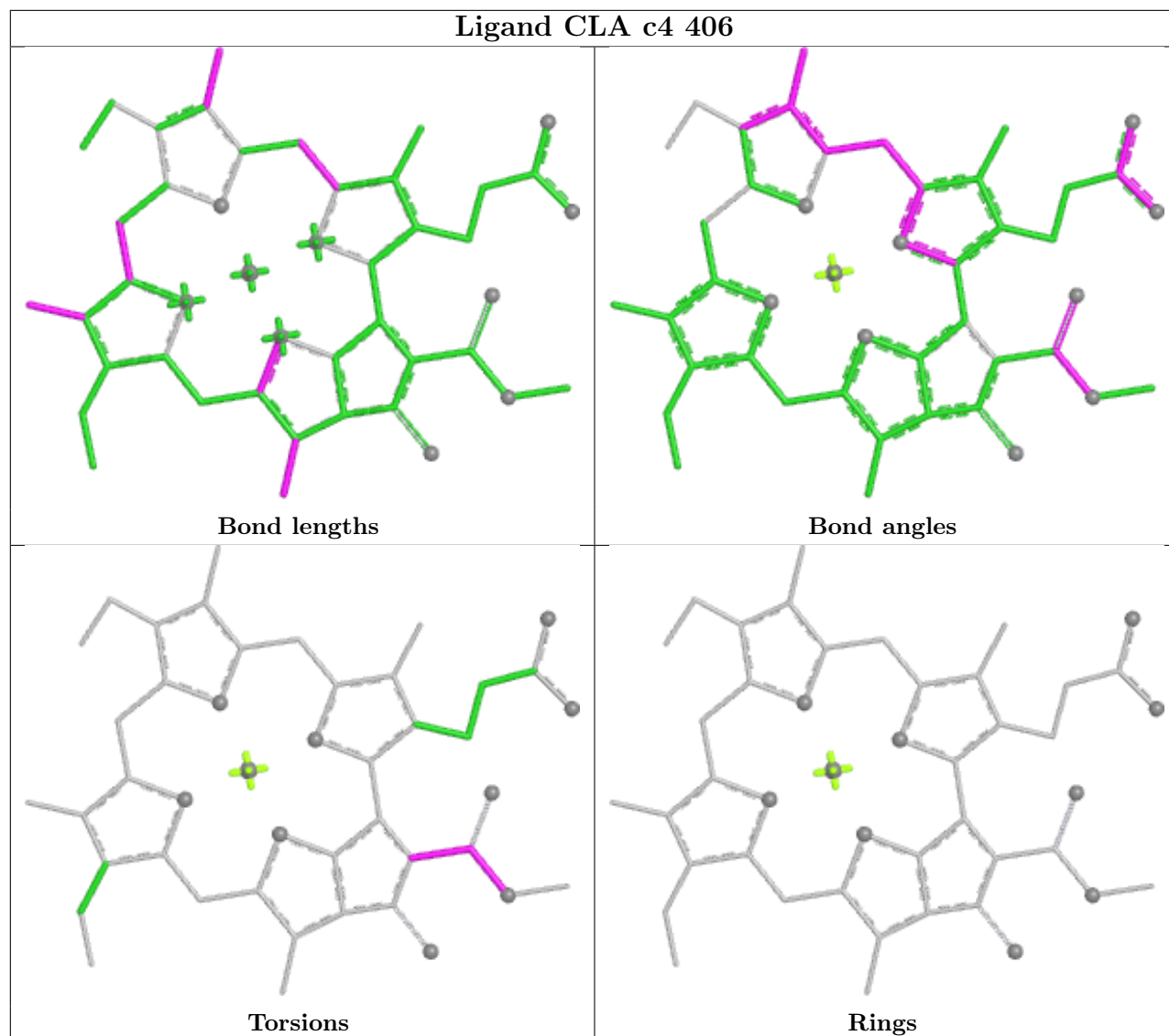


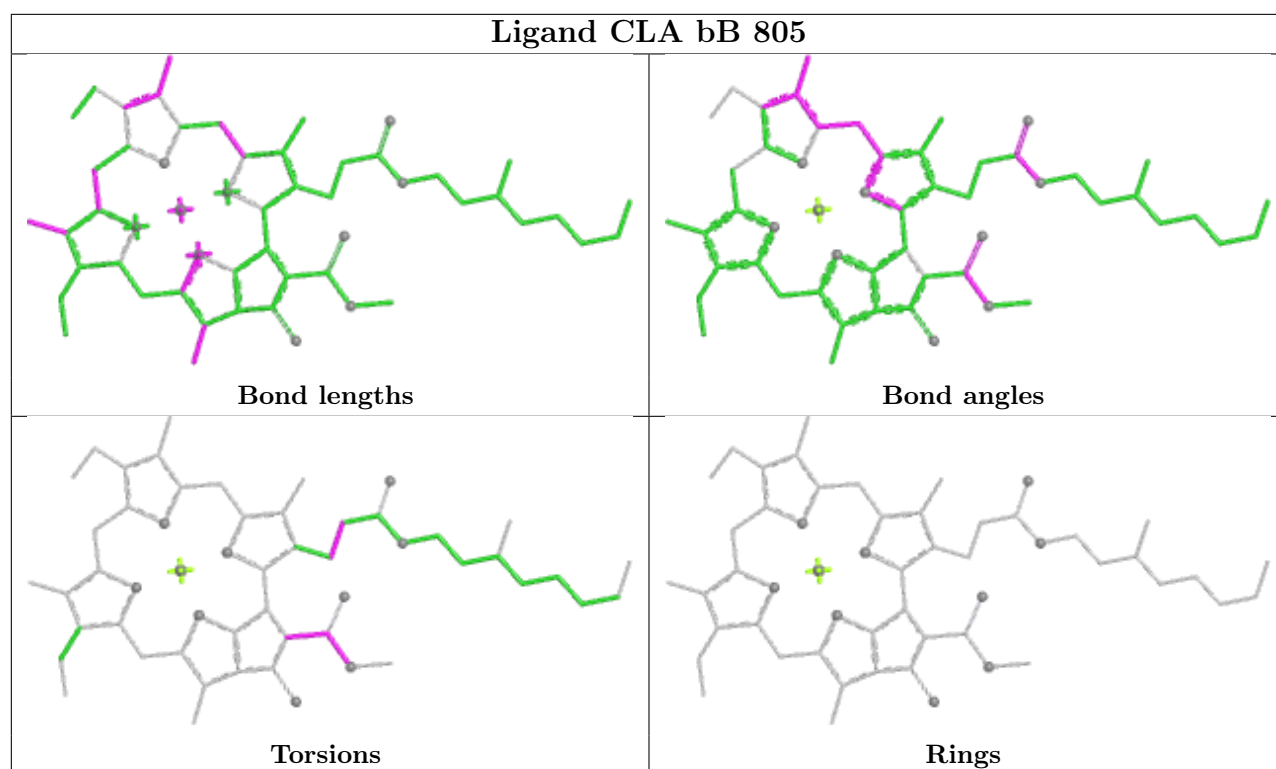


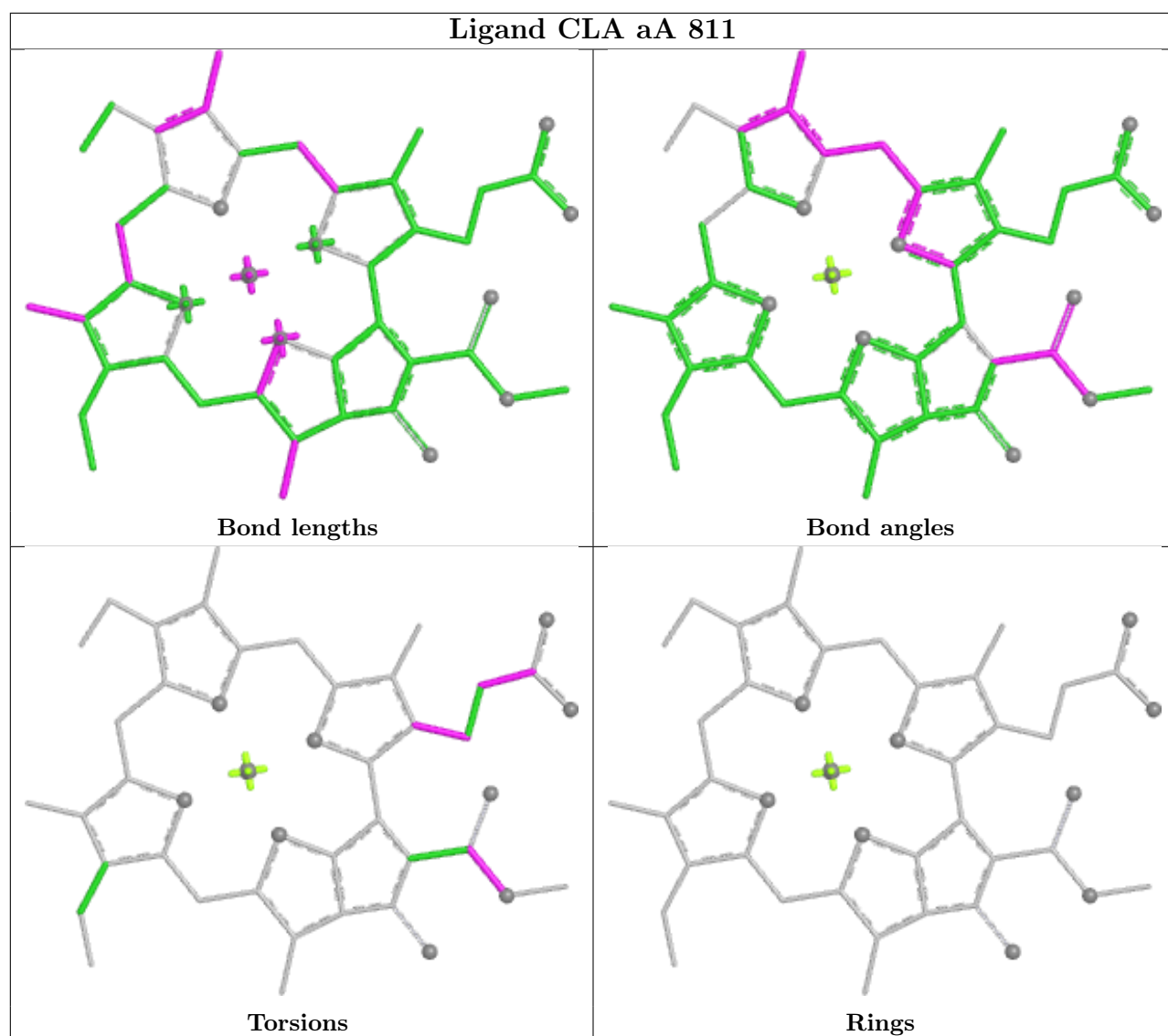


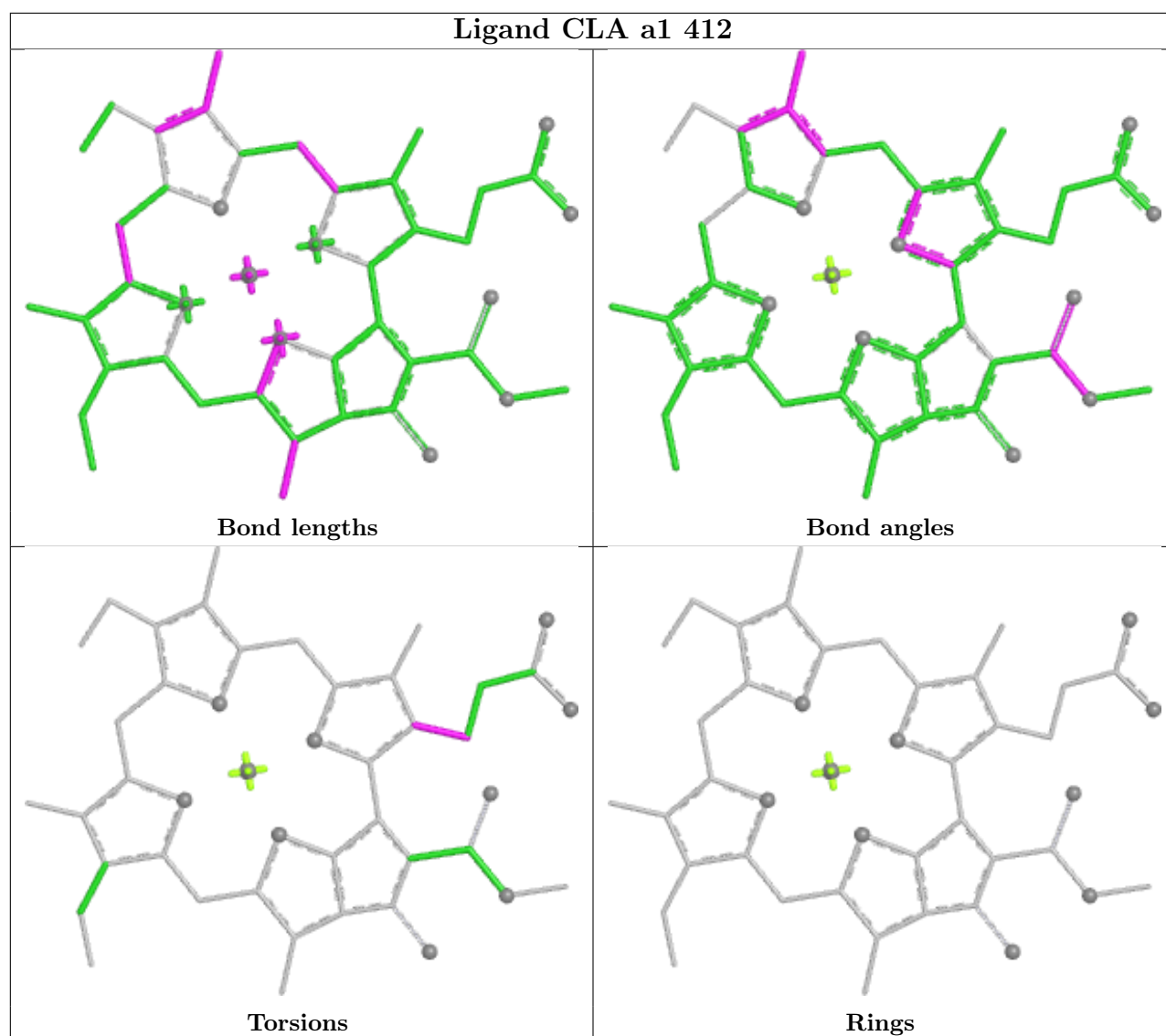


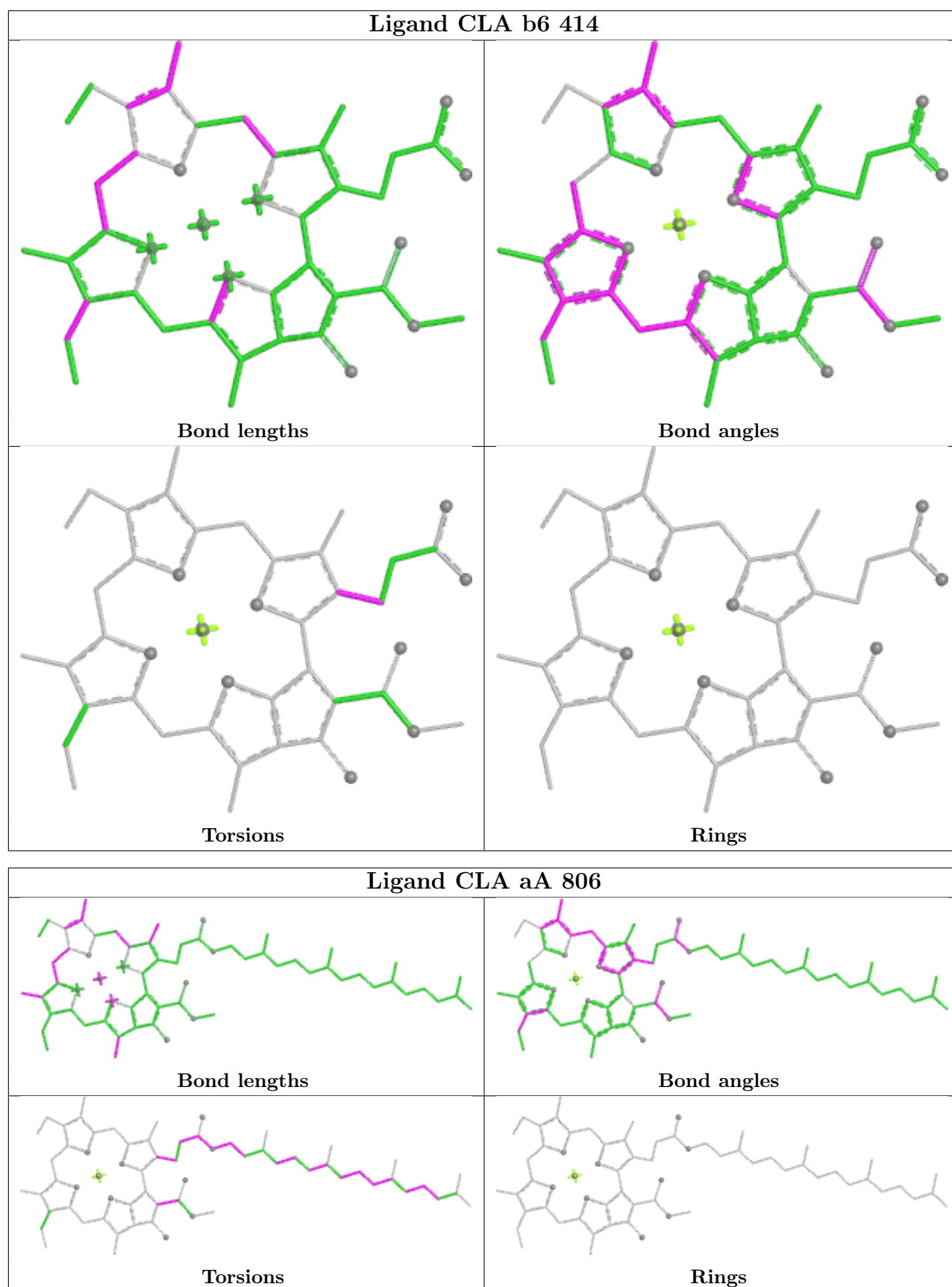


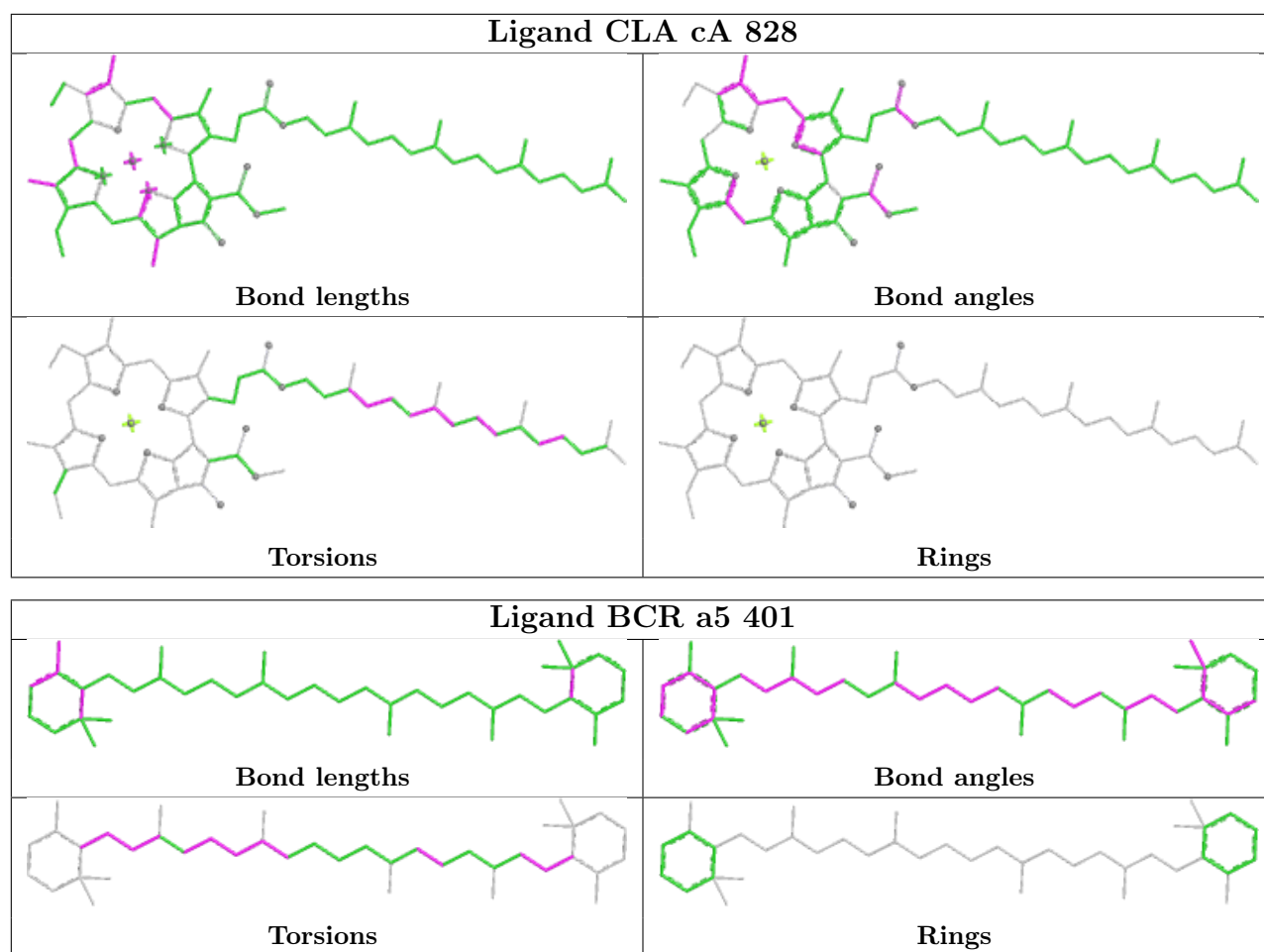


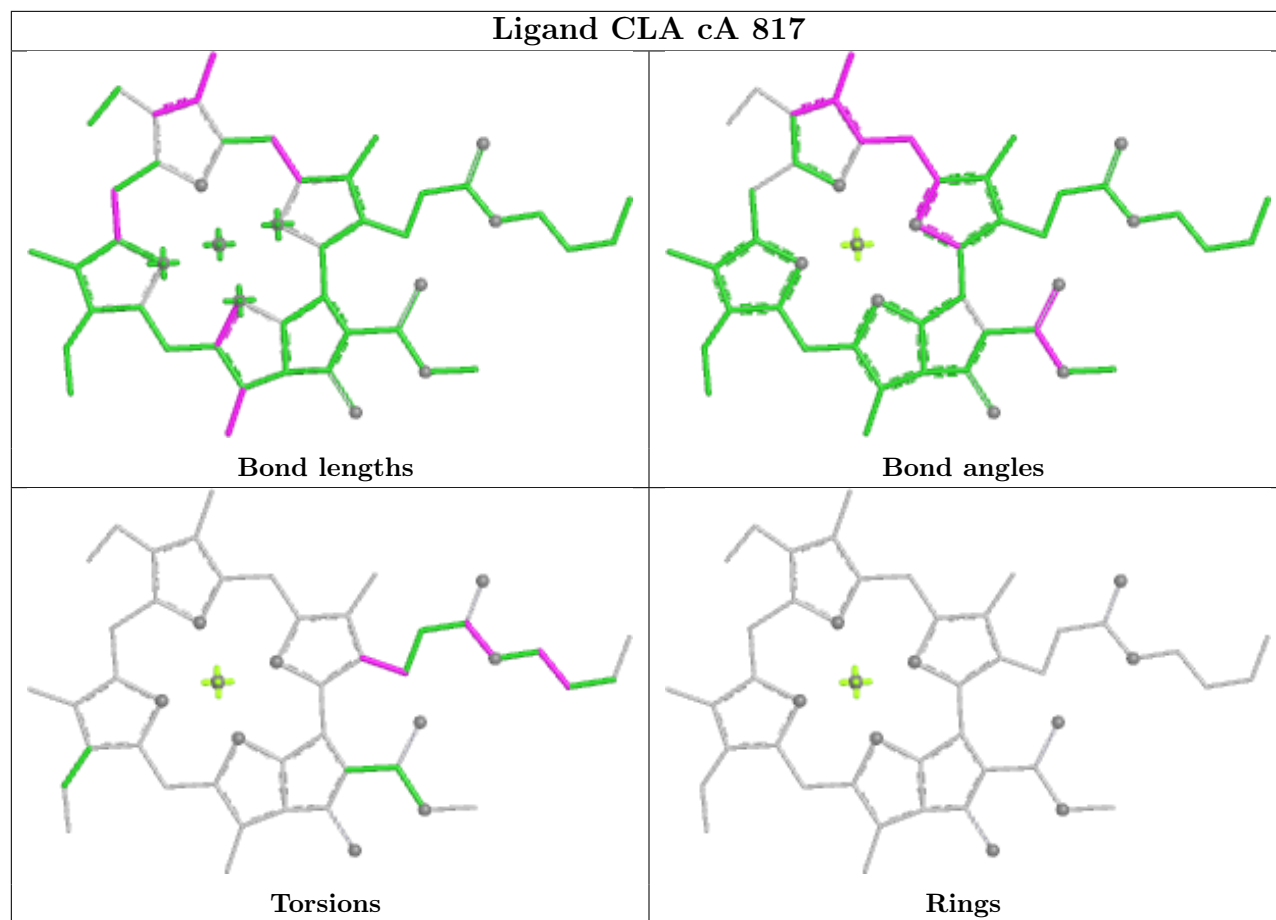


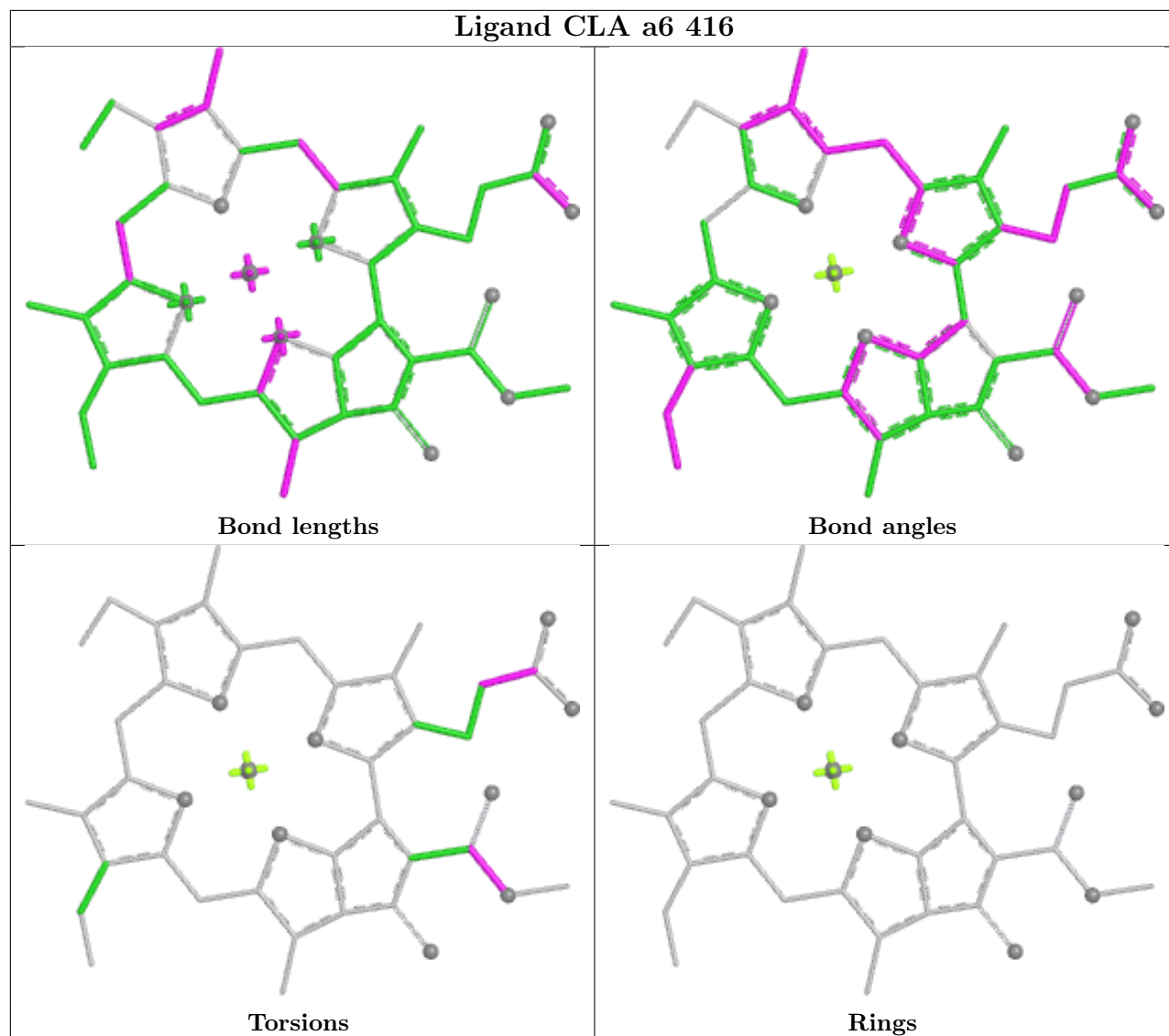


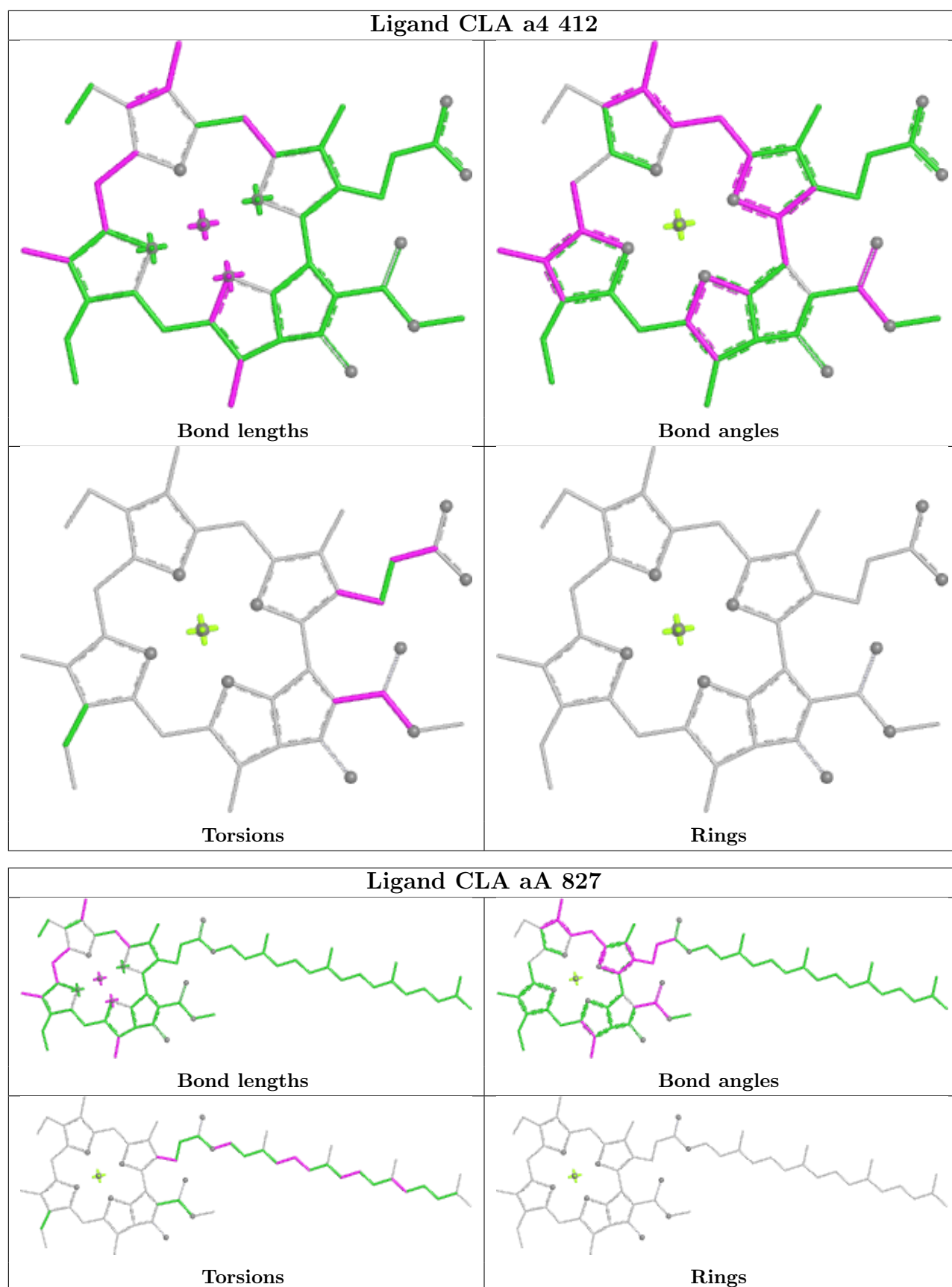


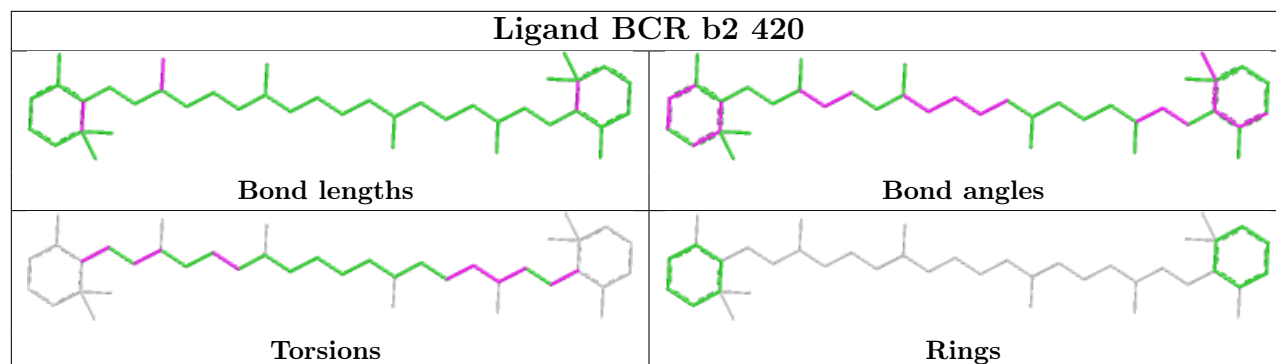
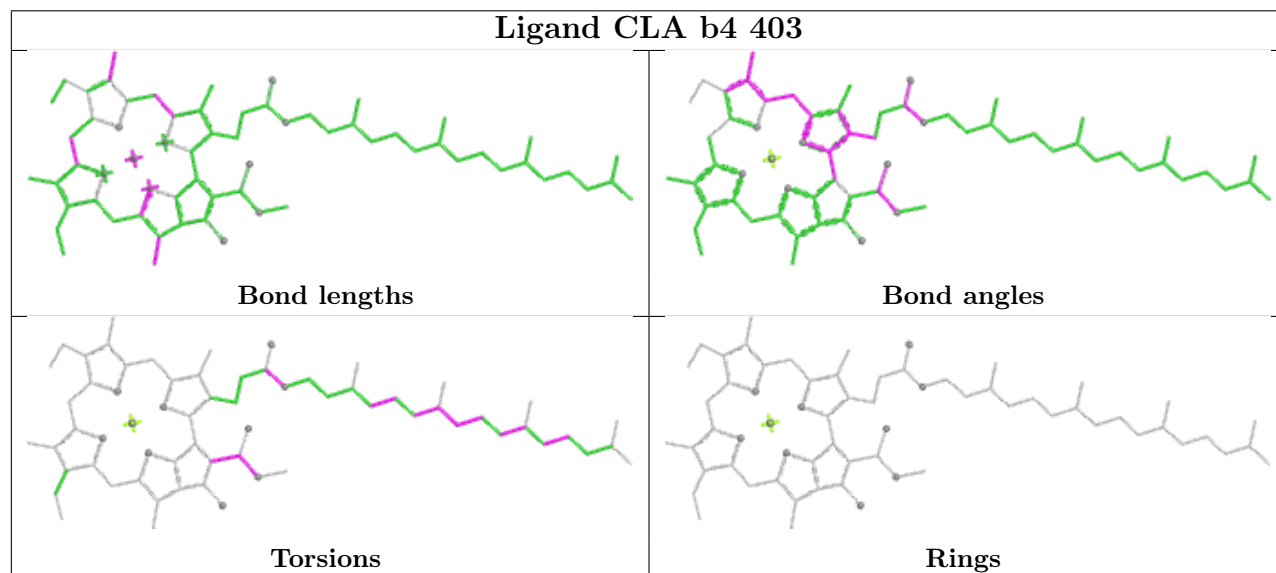
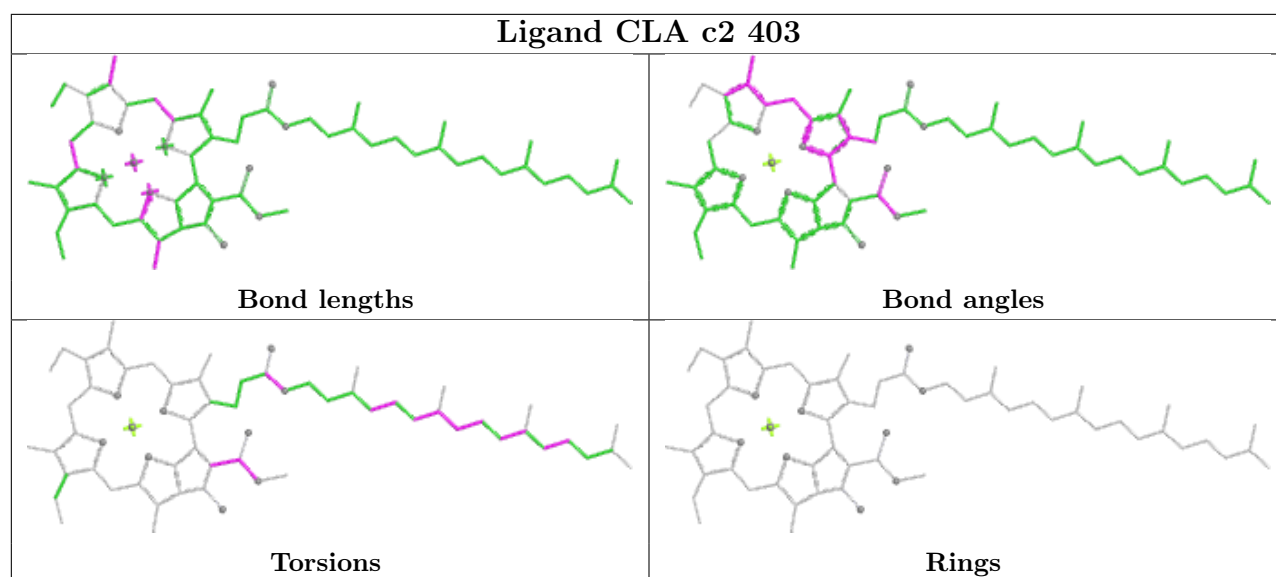


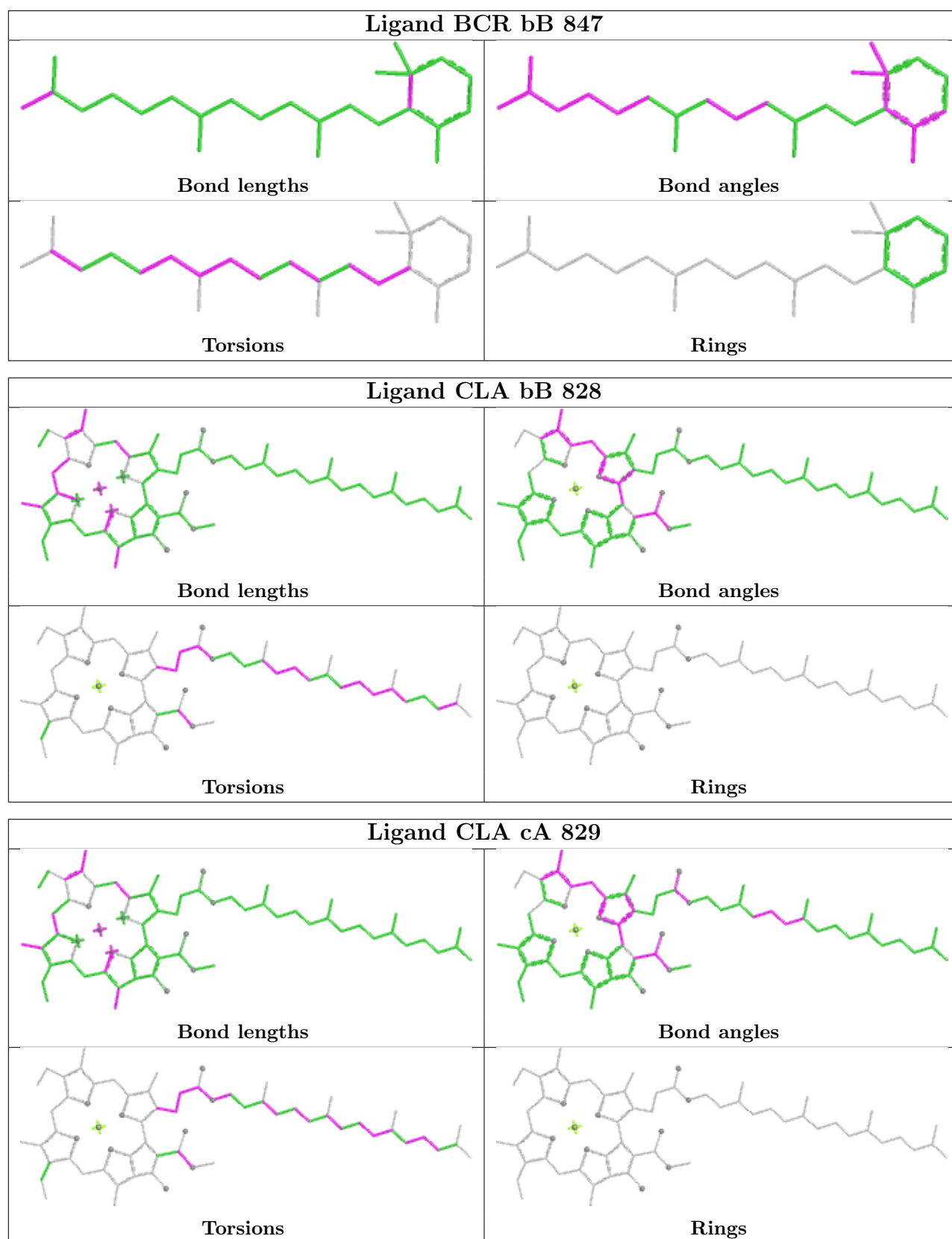


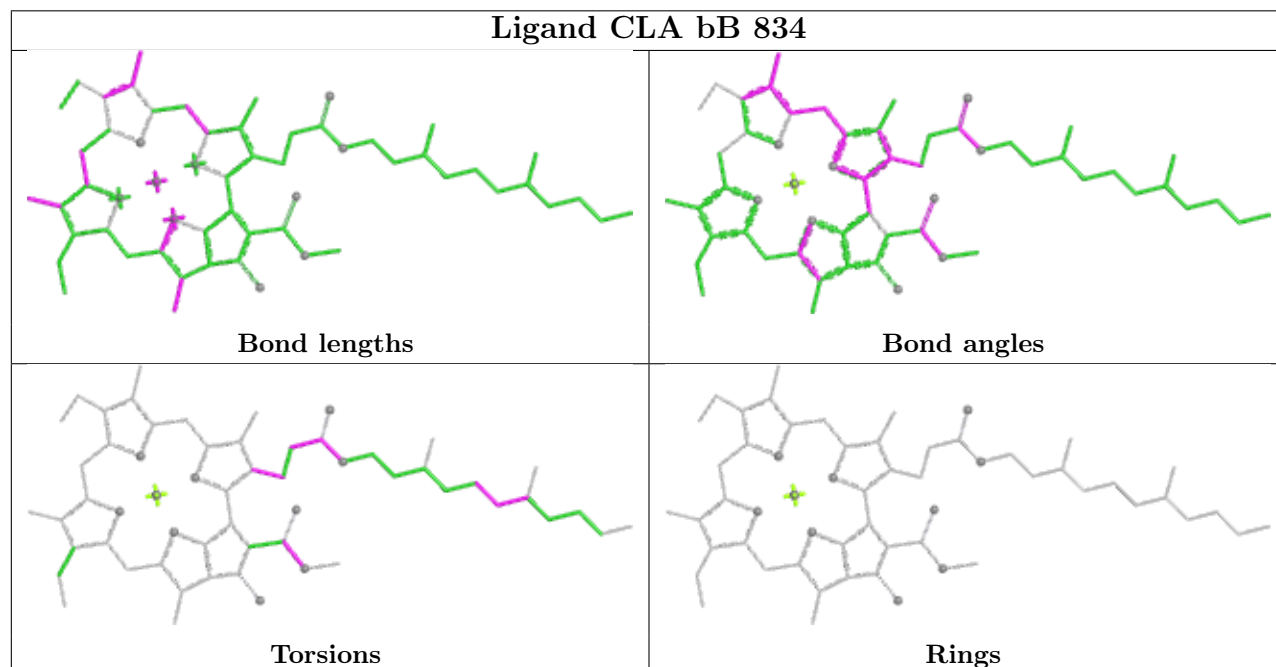
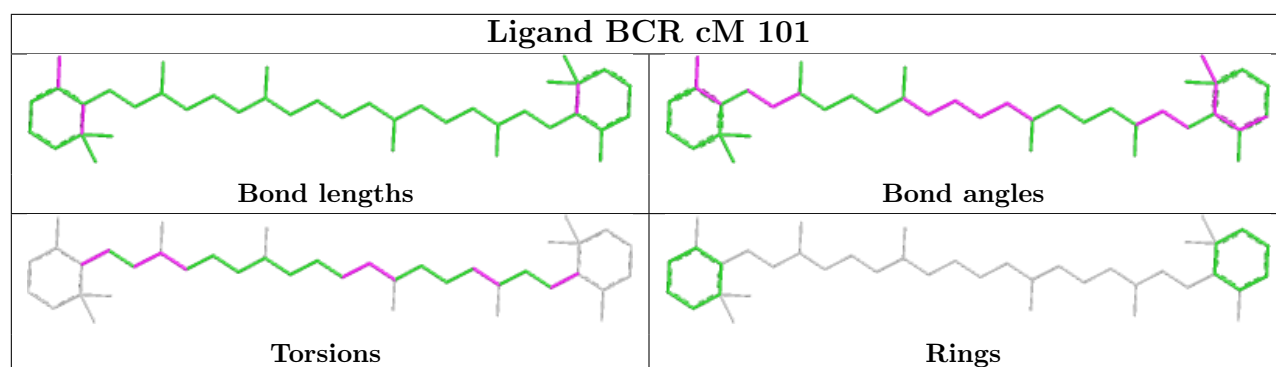


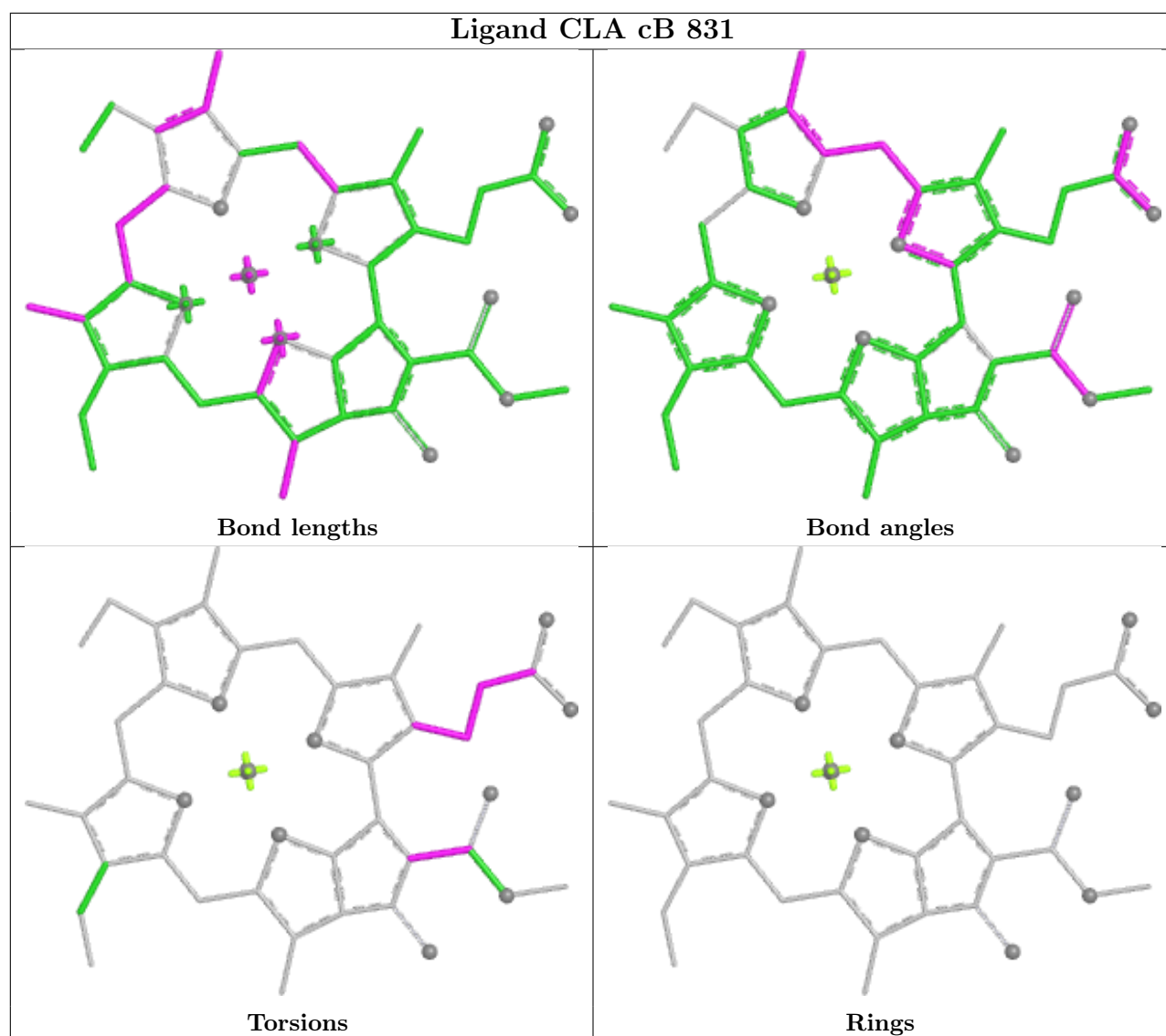


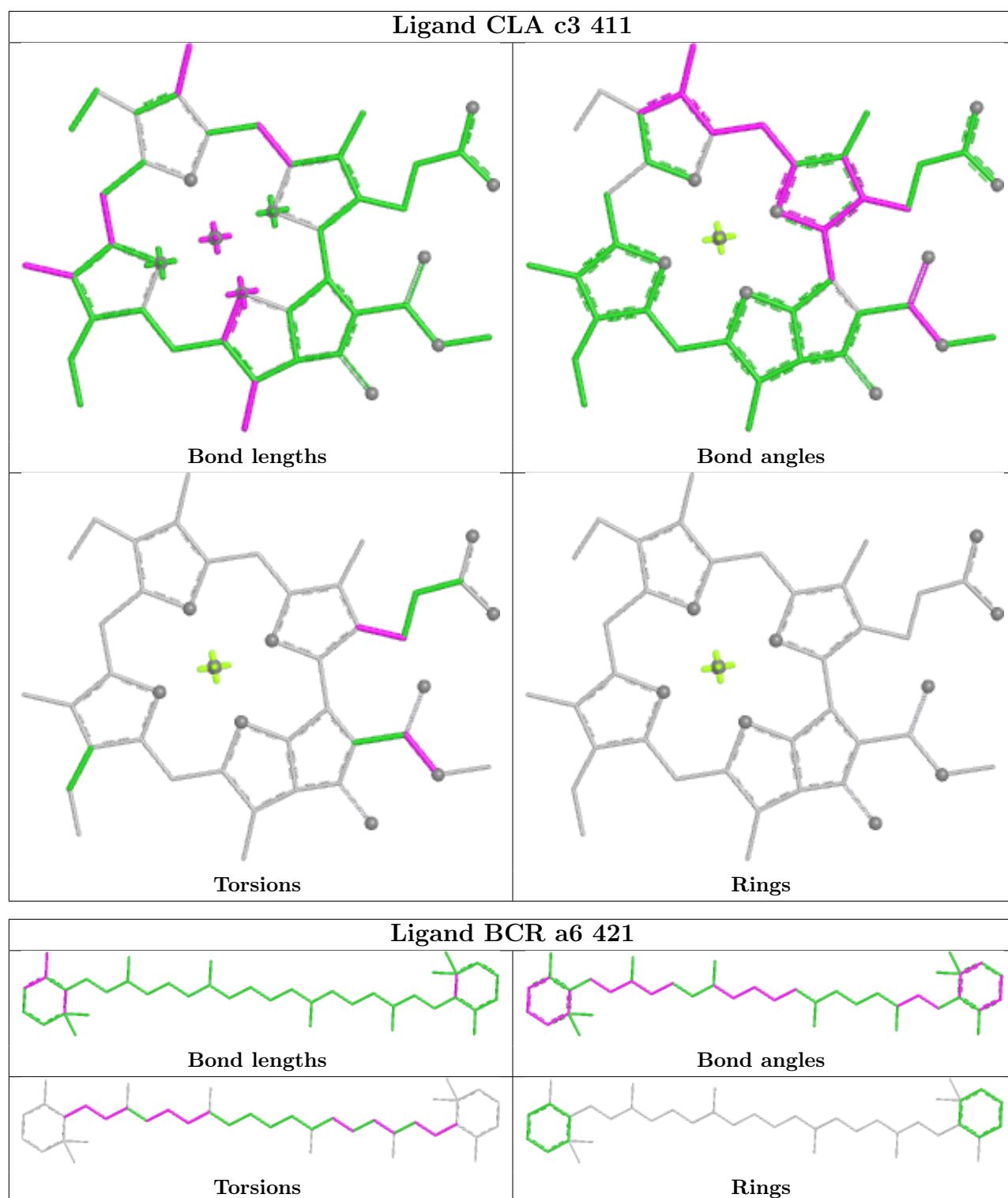


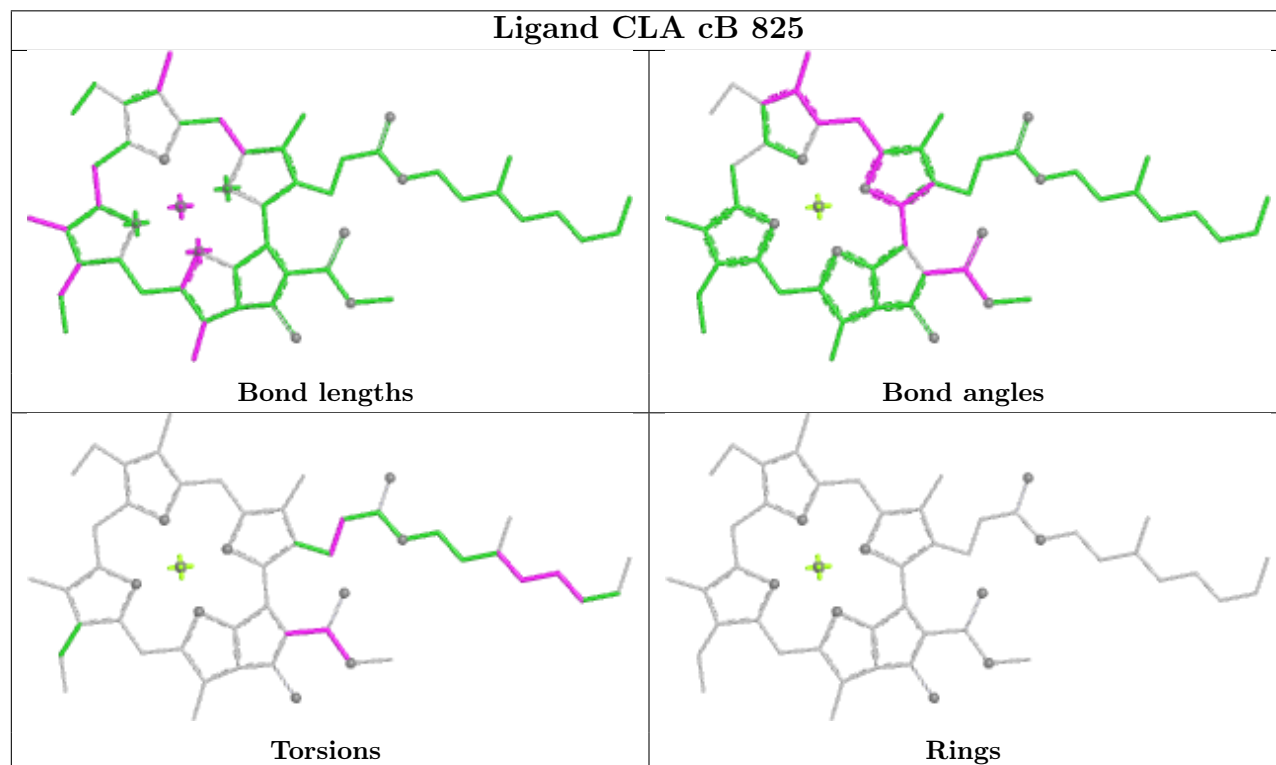
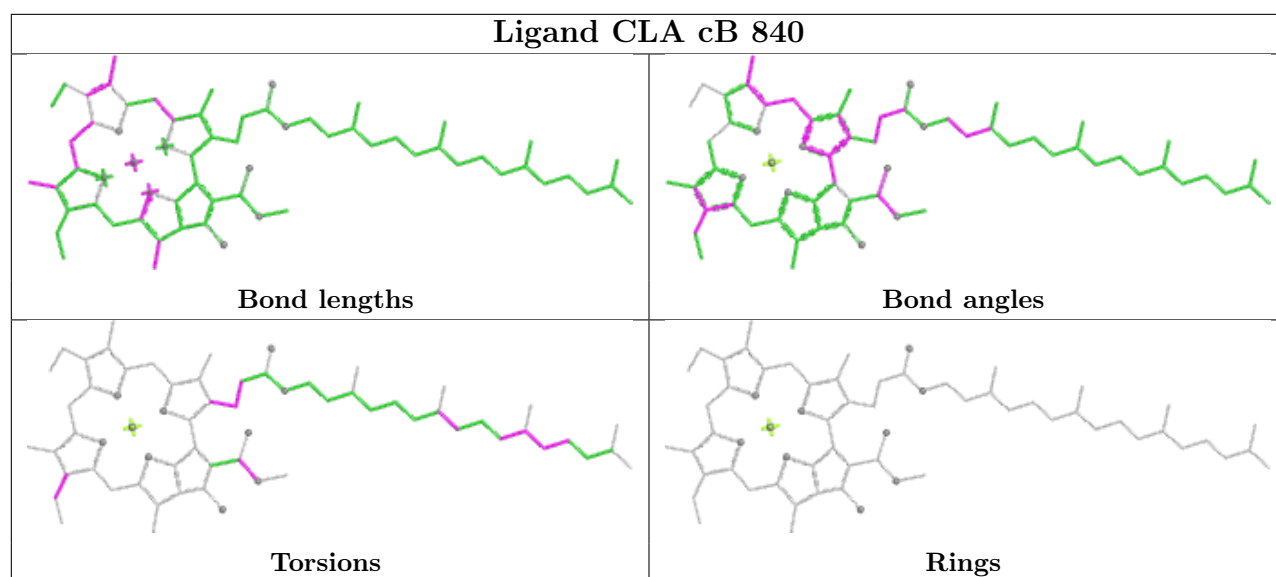




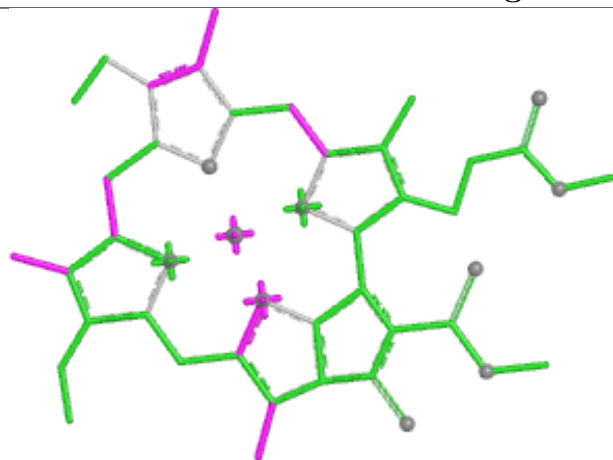




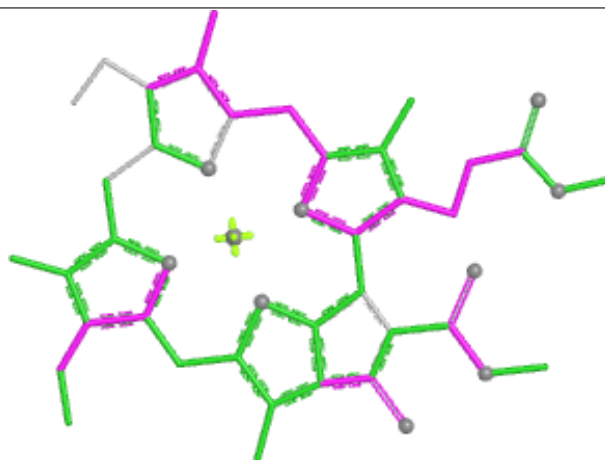




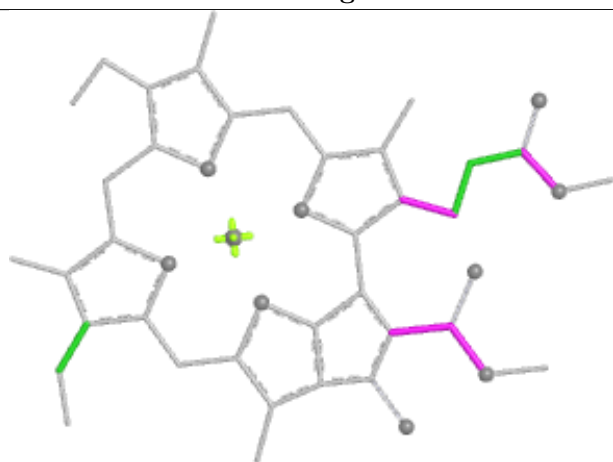
Ligand CLA bB 826



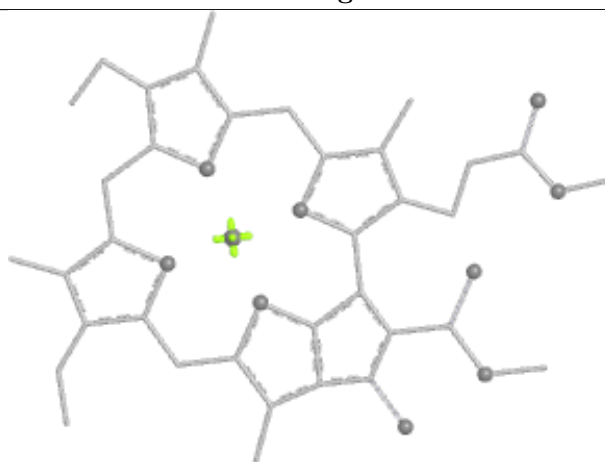
Bond lengths



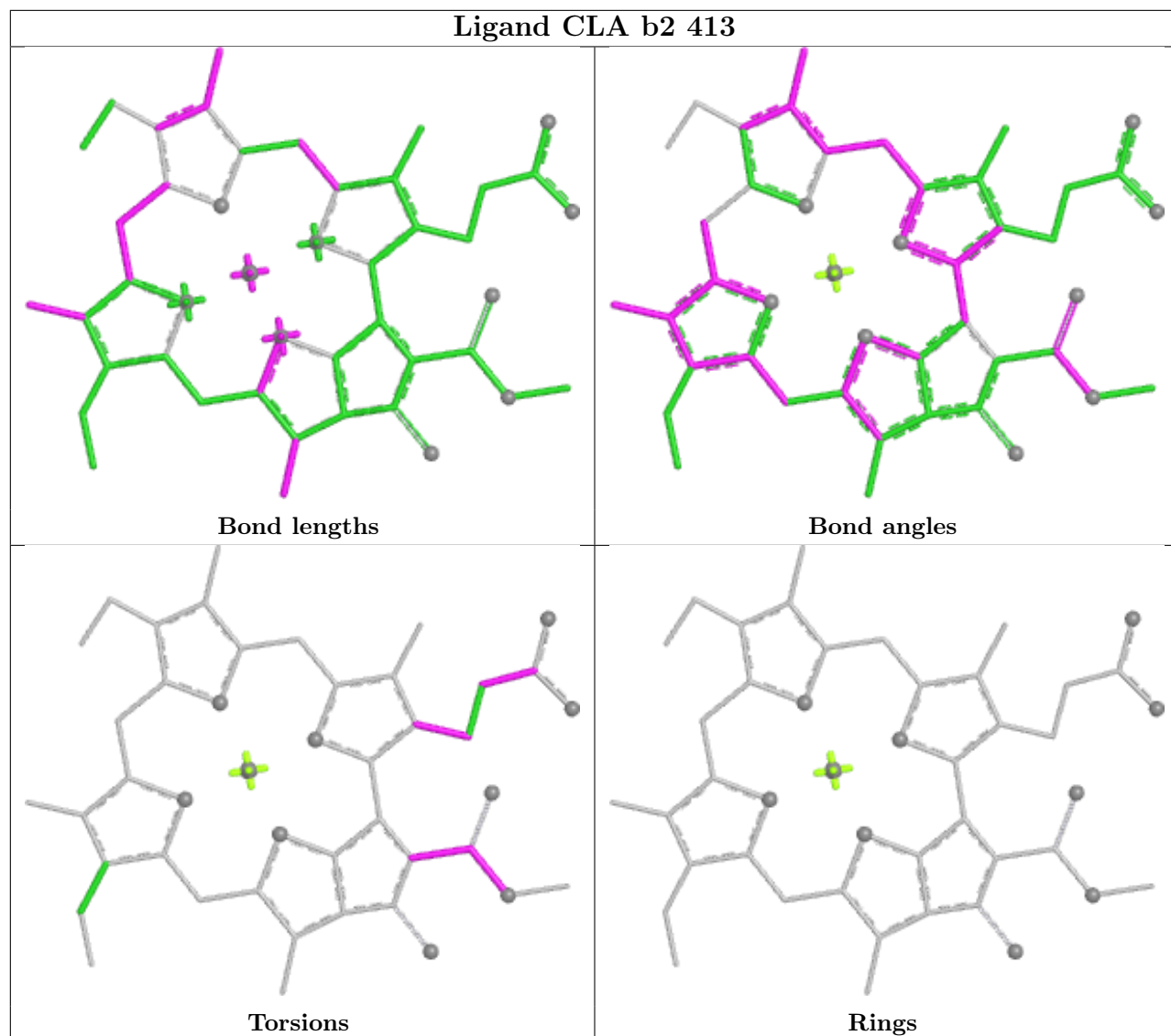
Bond angles

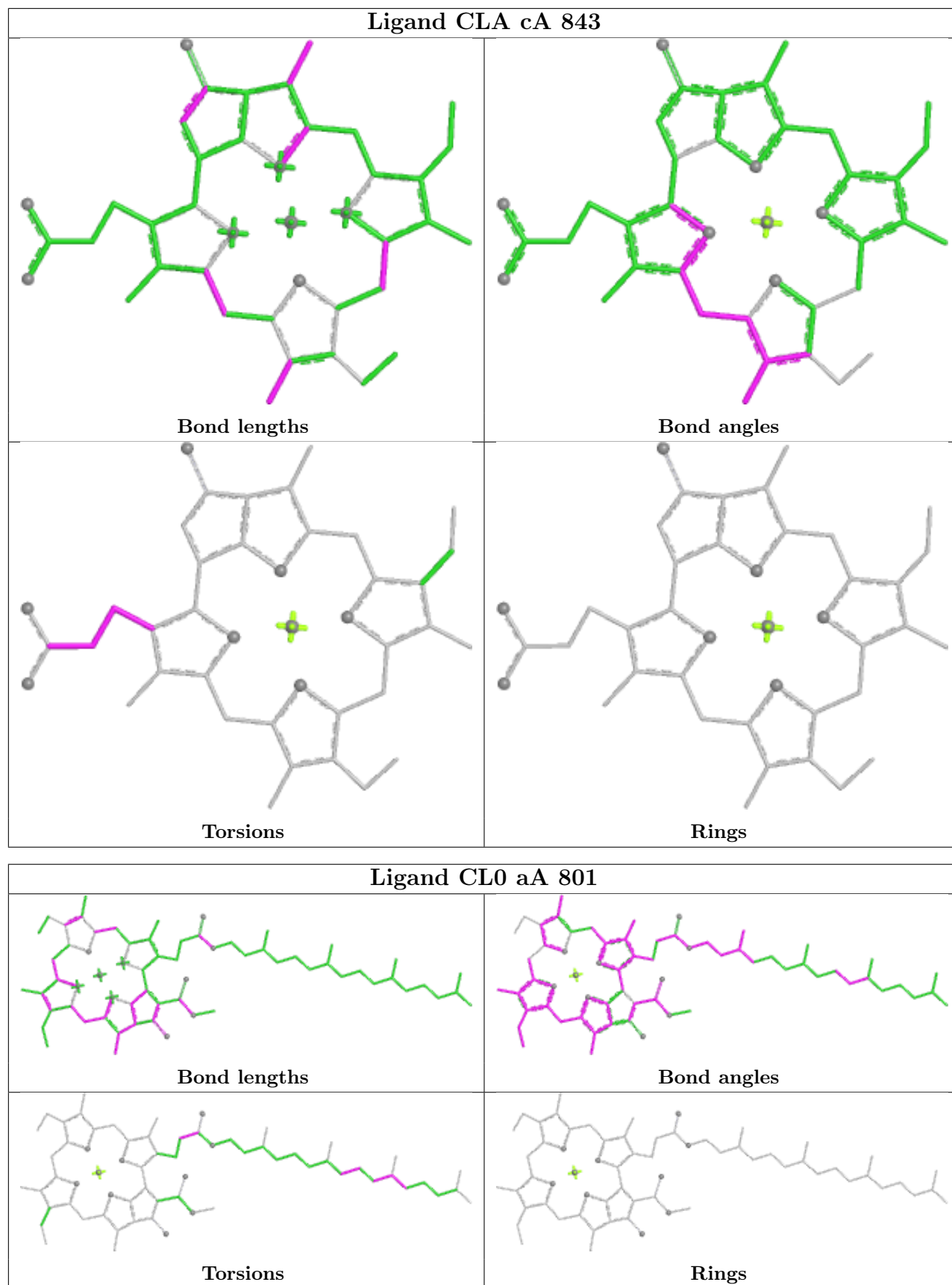


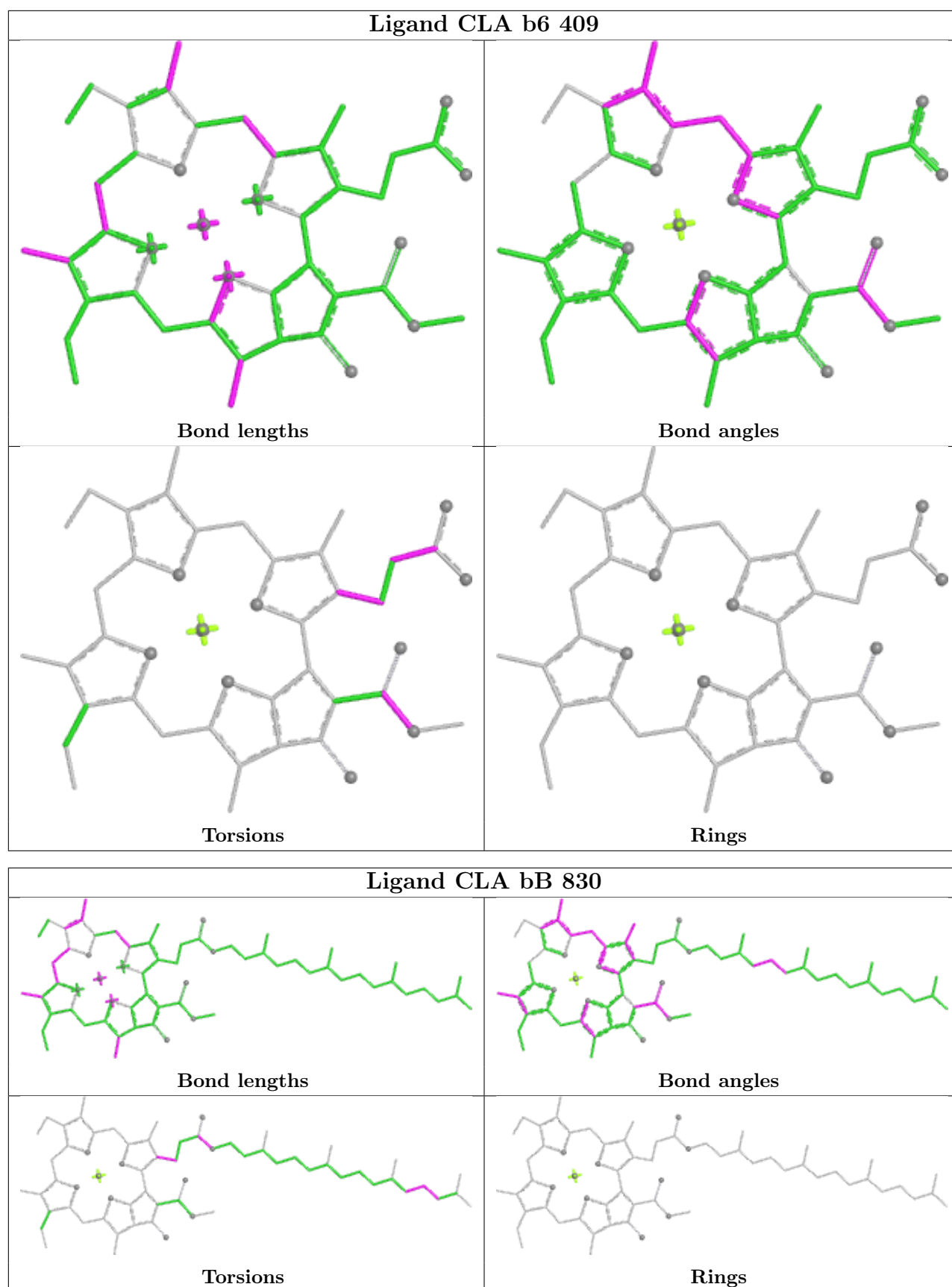
Torsions

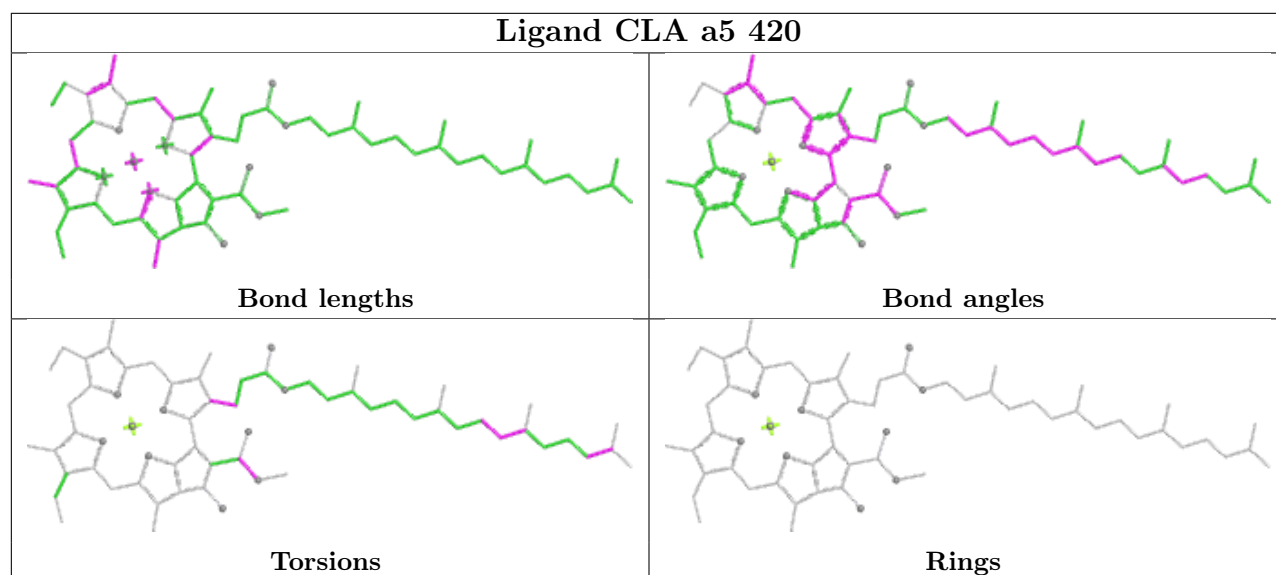
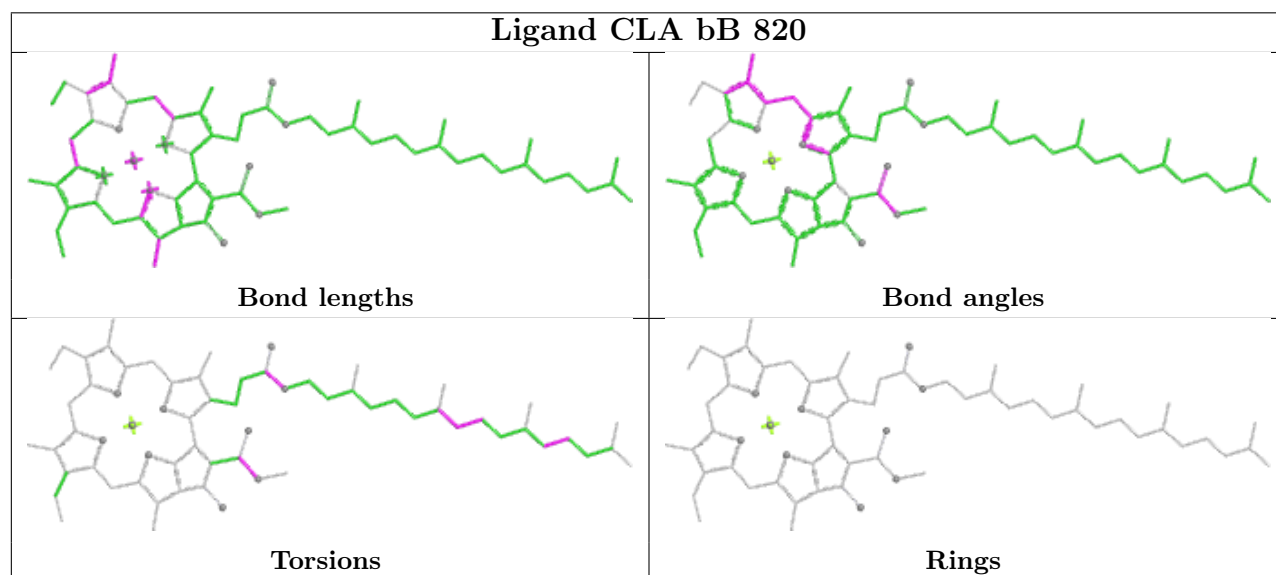
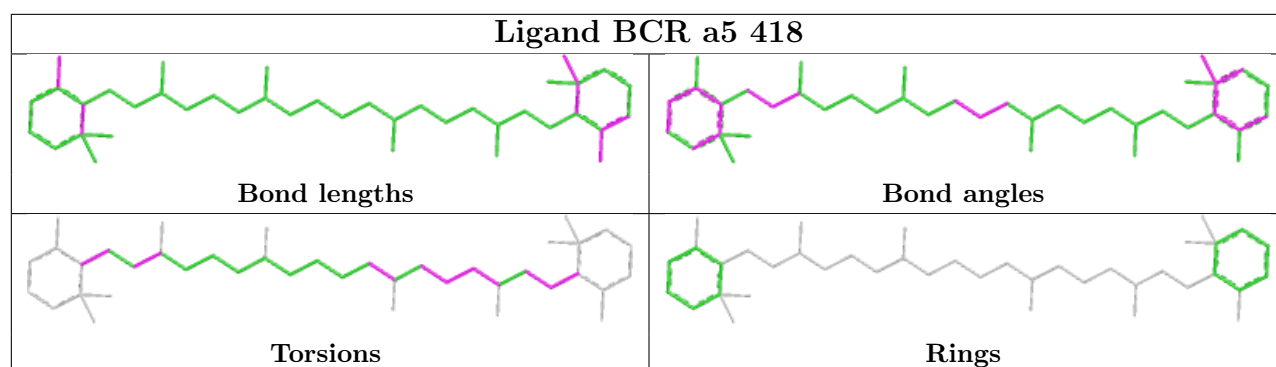


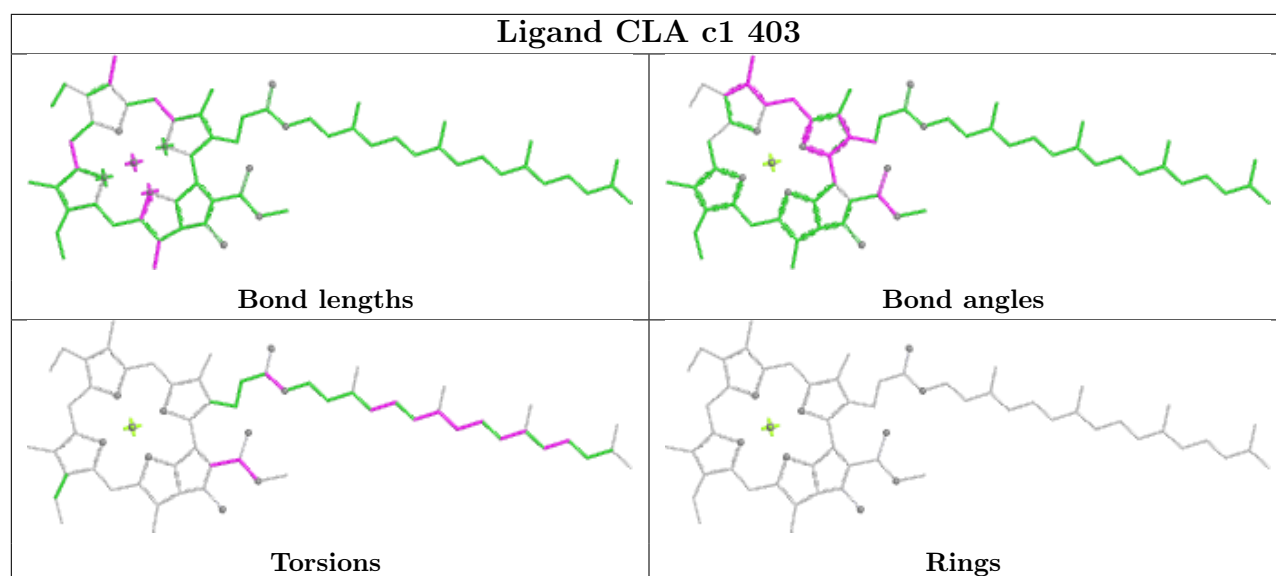
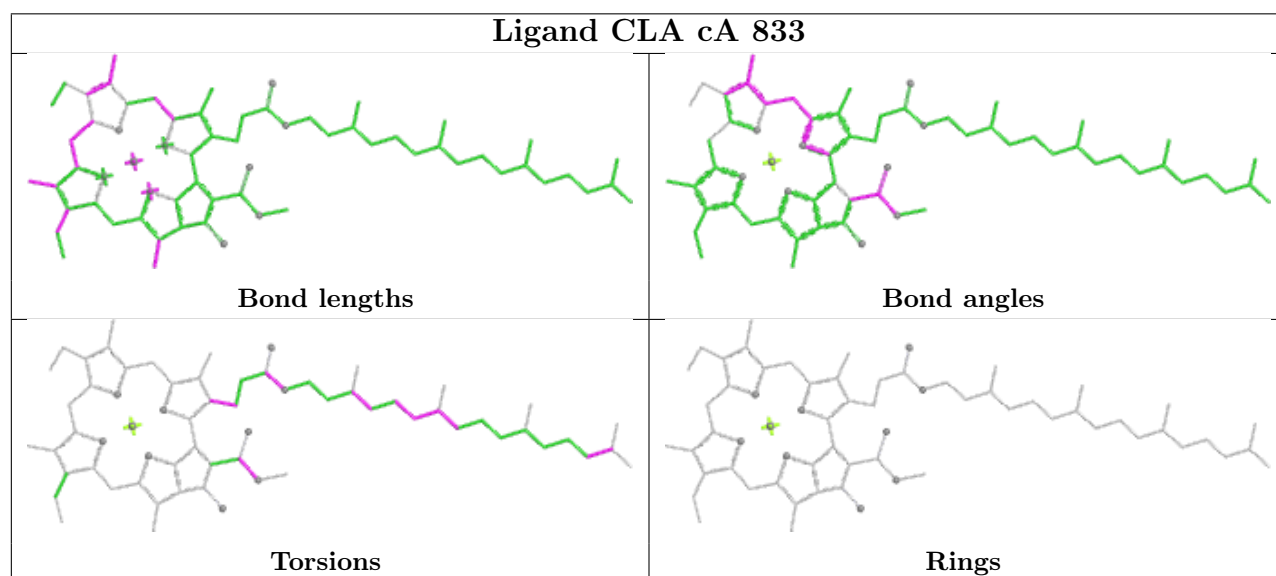
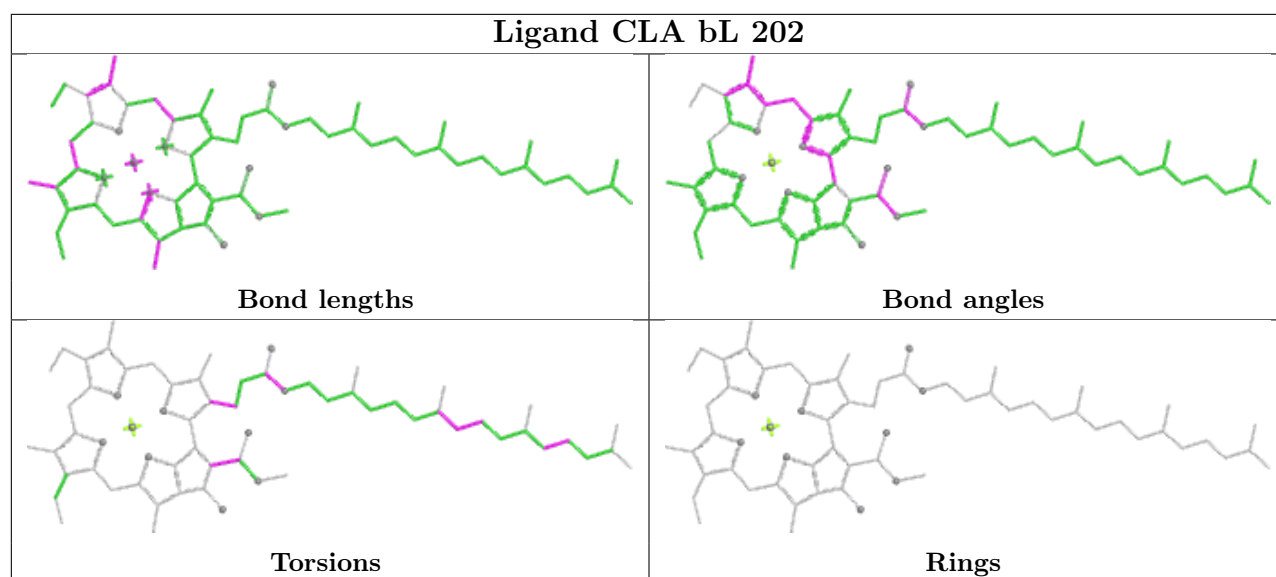
Rings

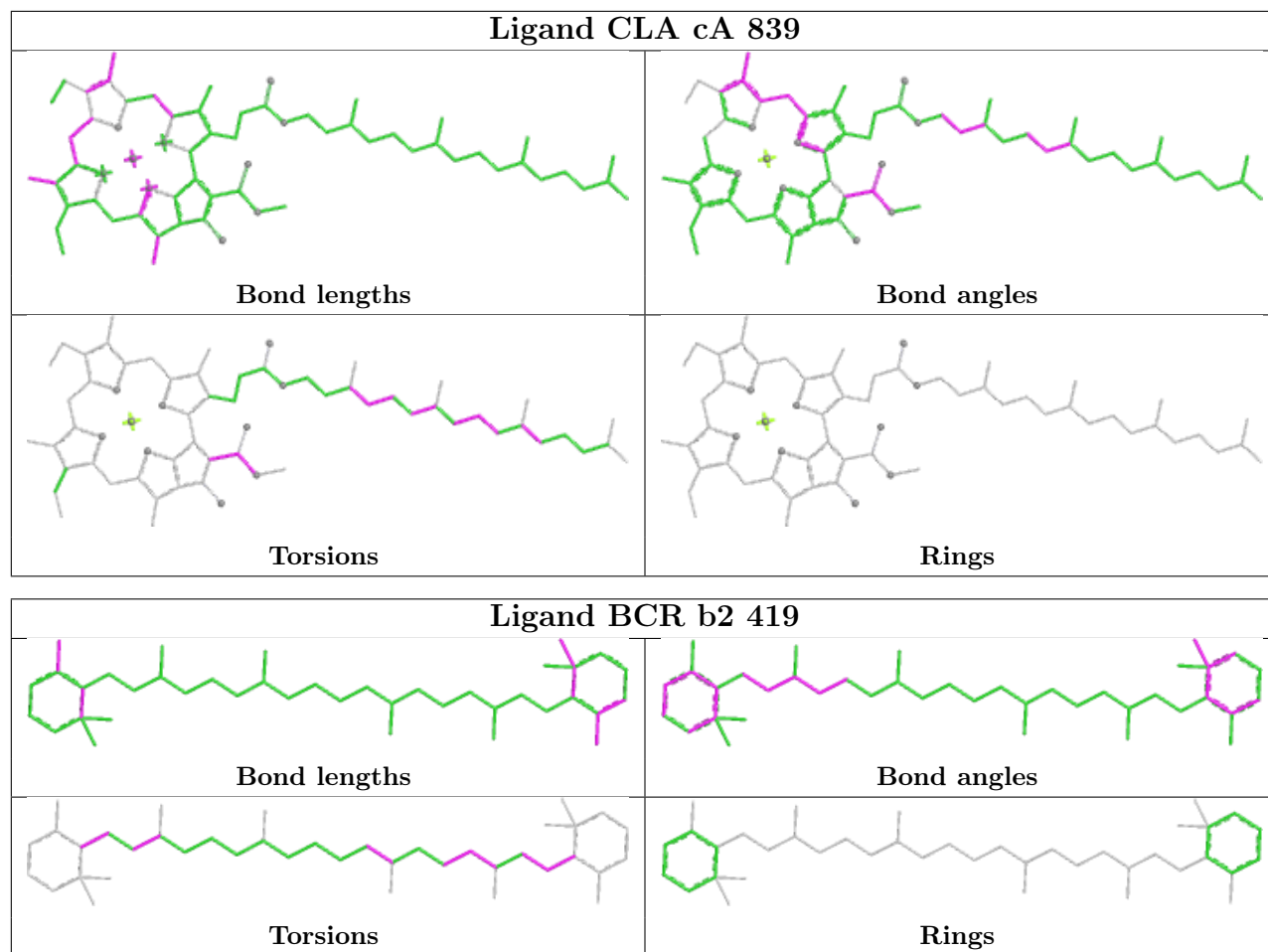


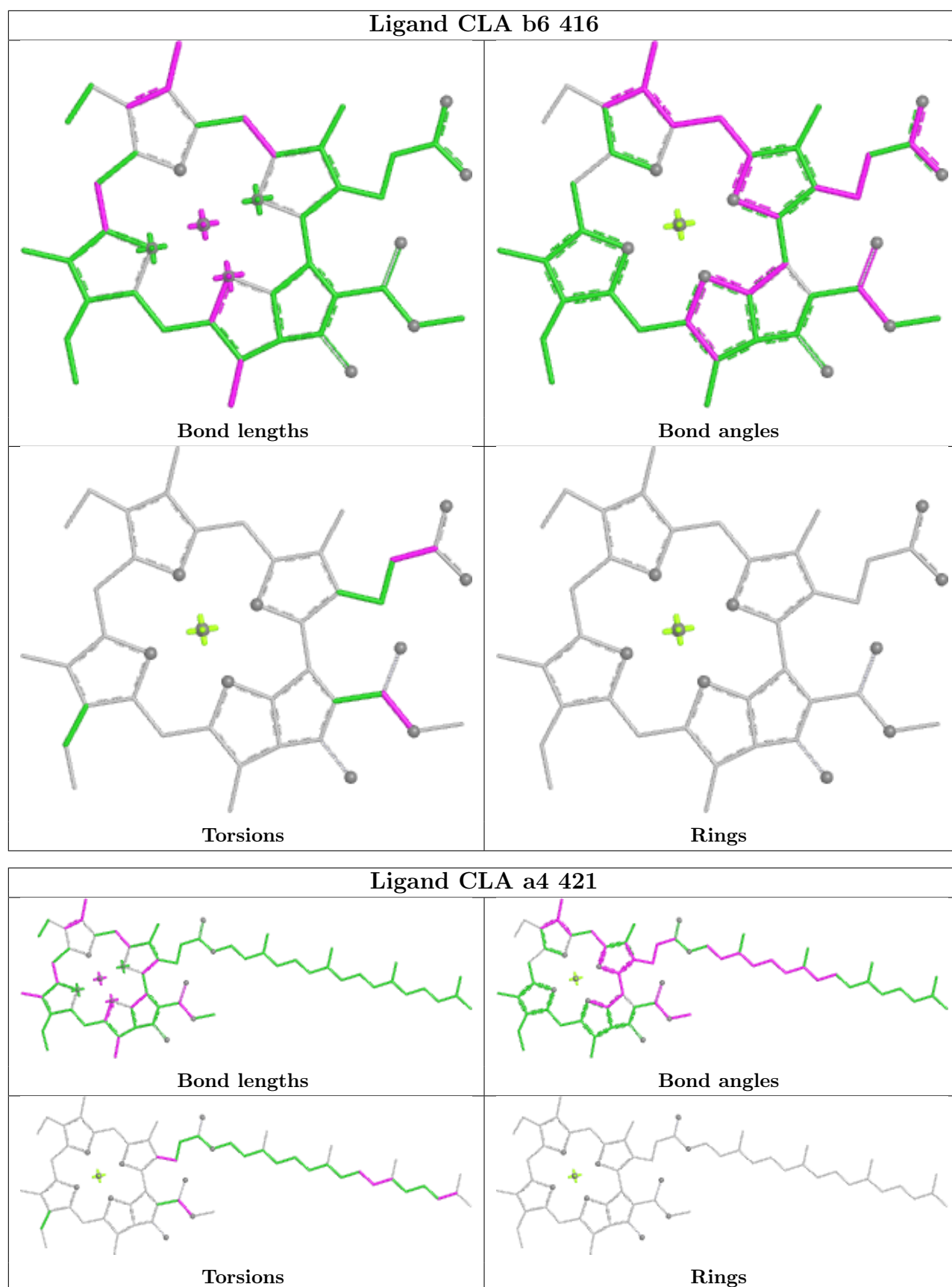


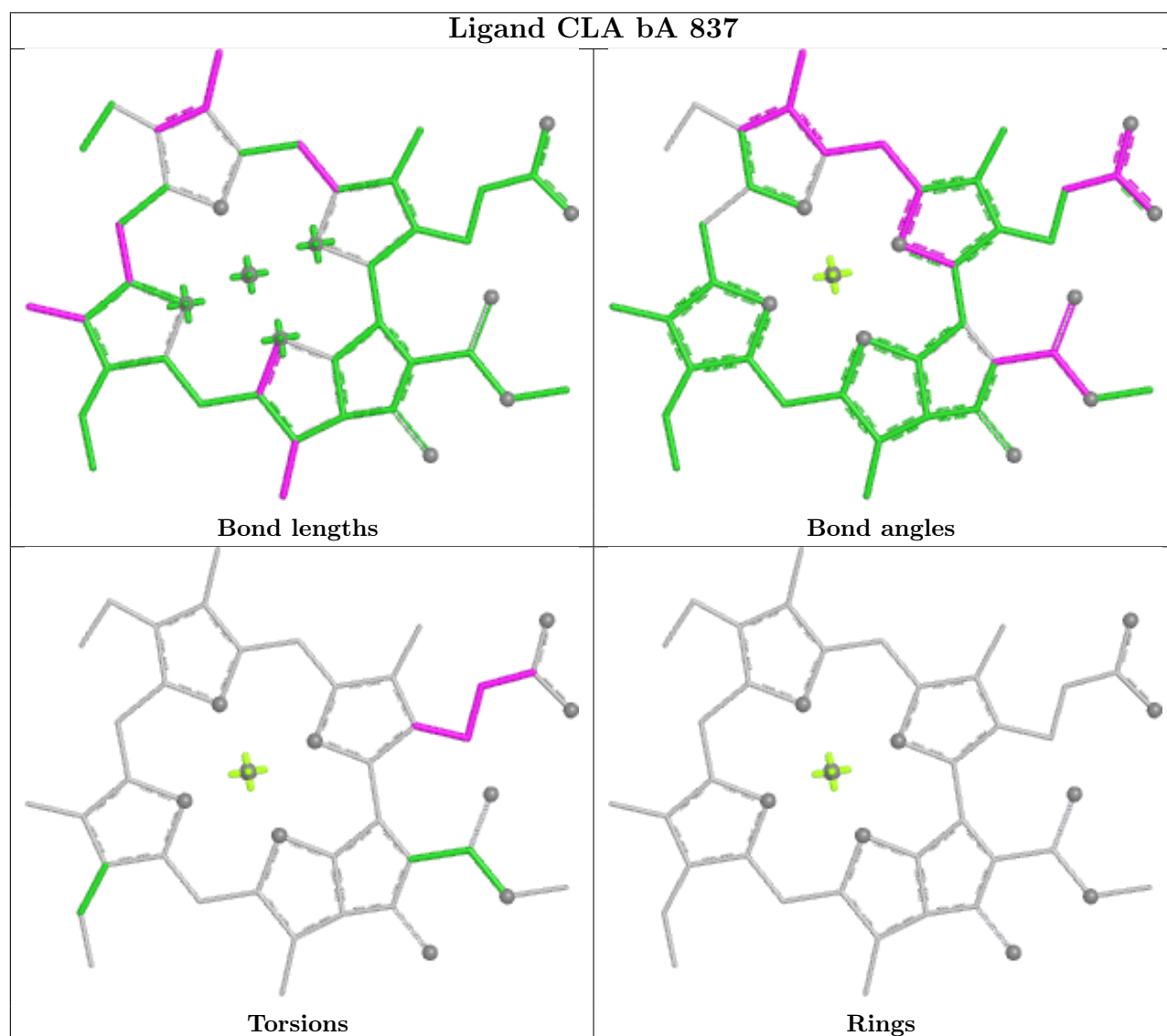
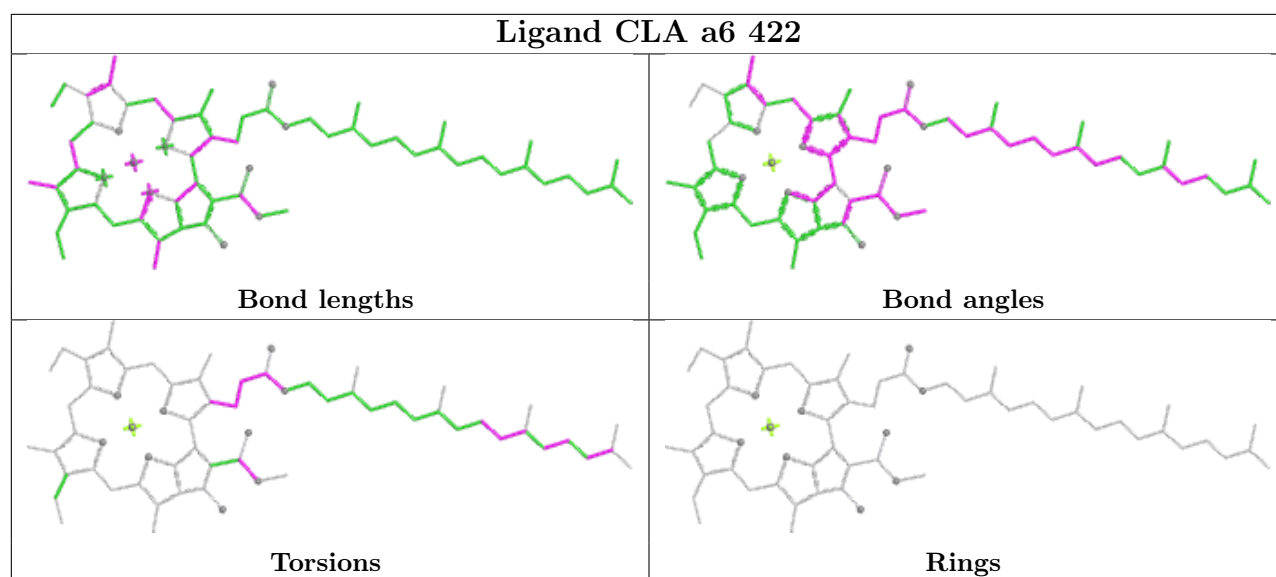


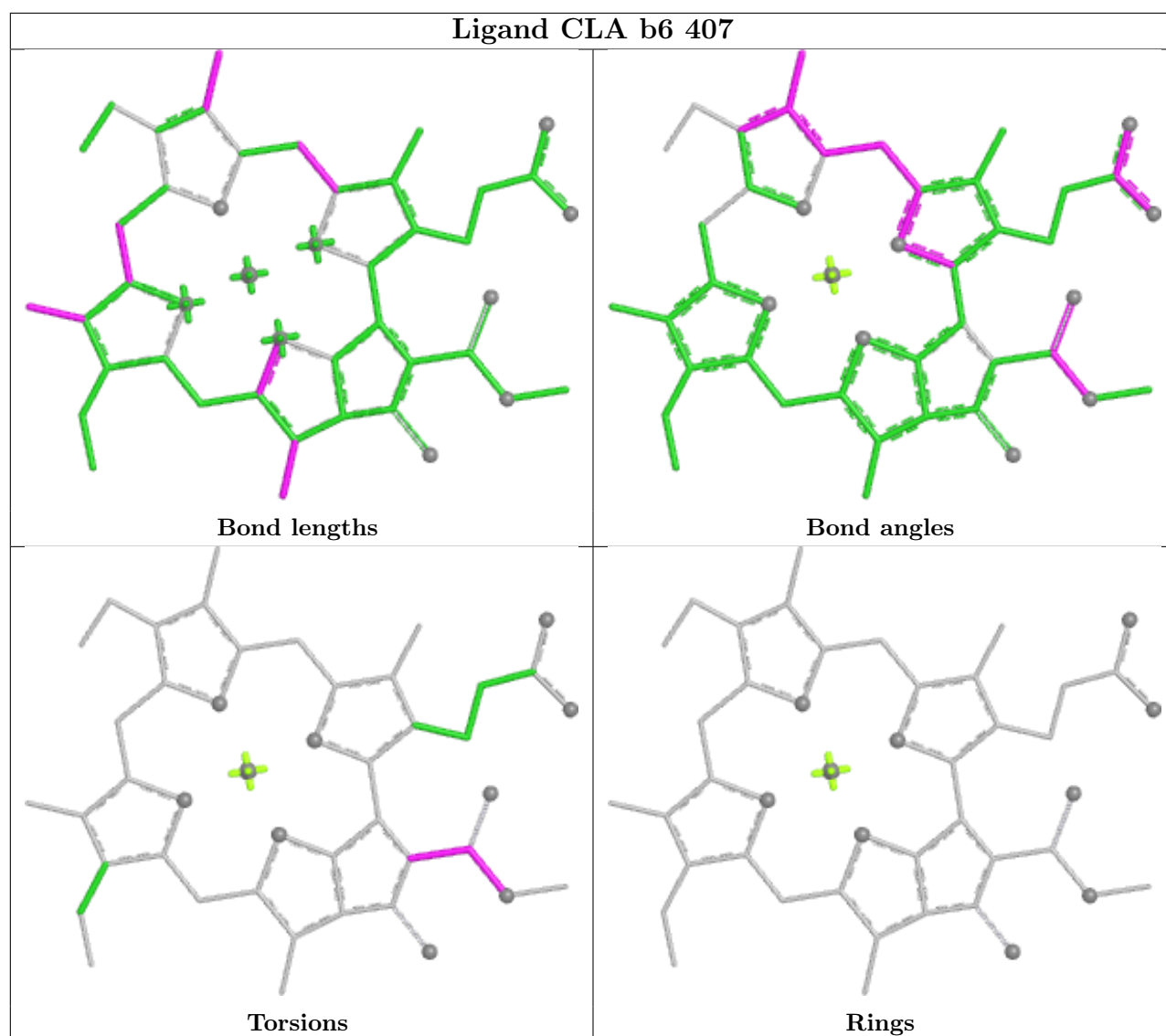


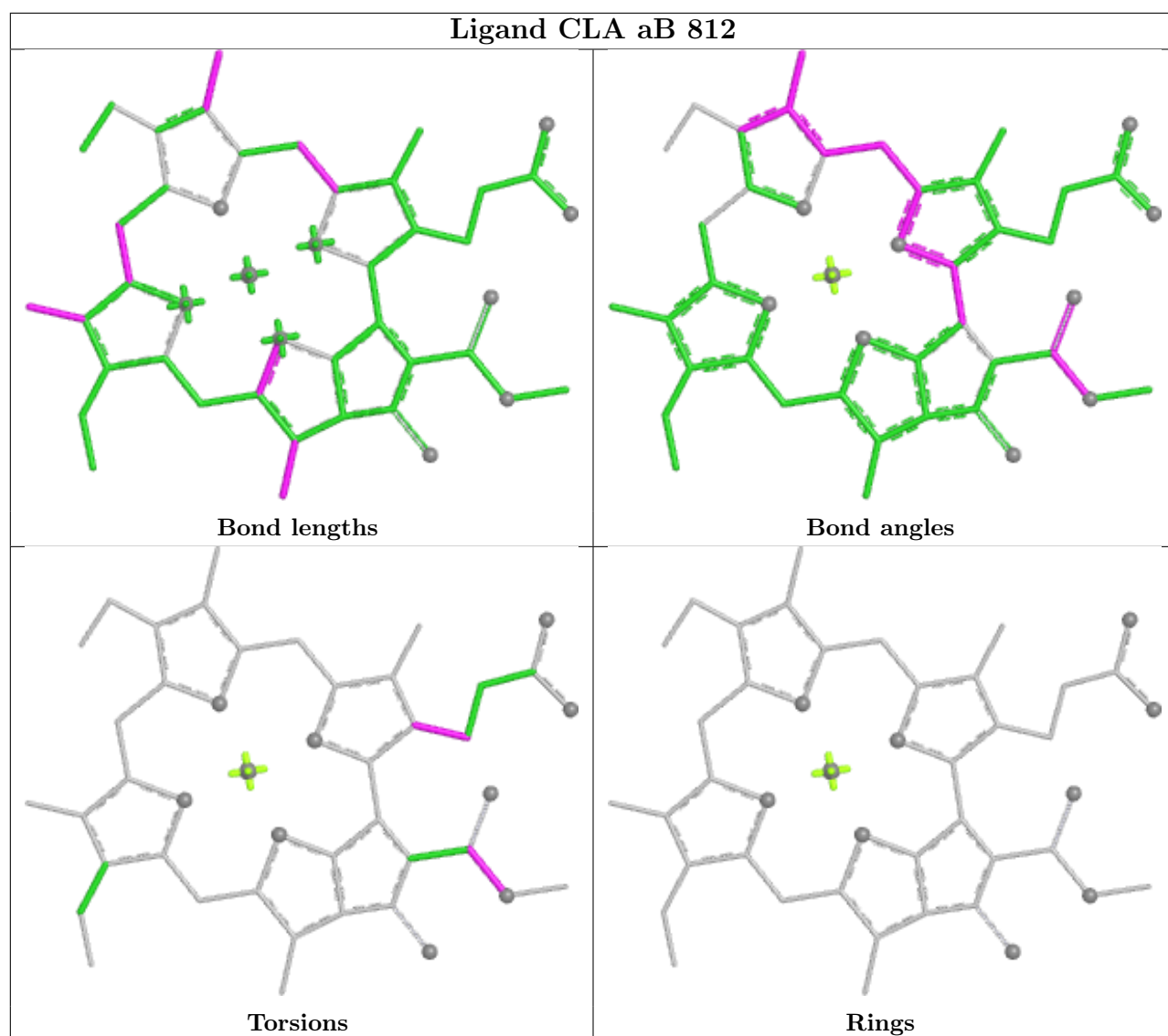


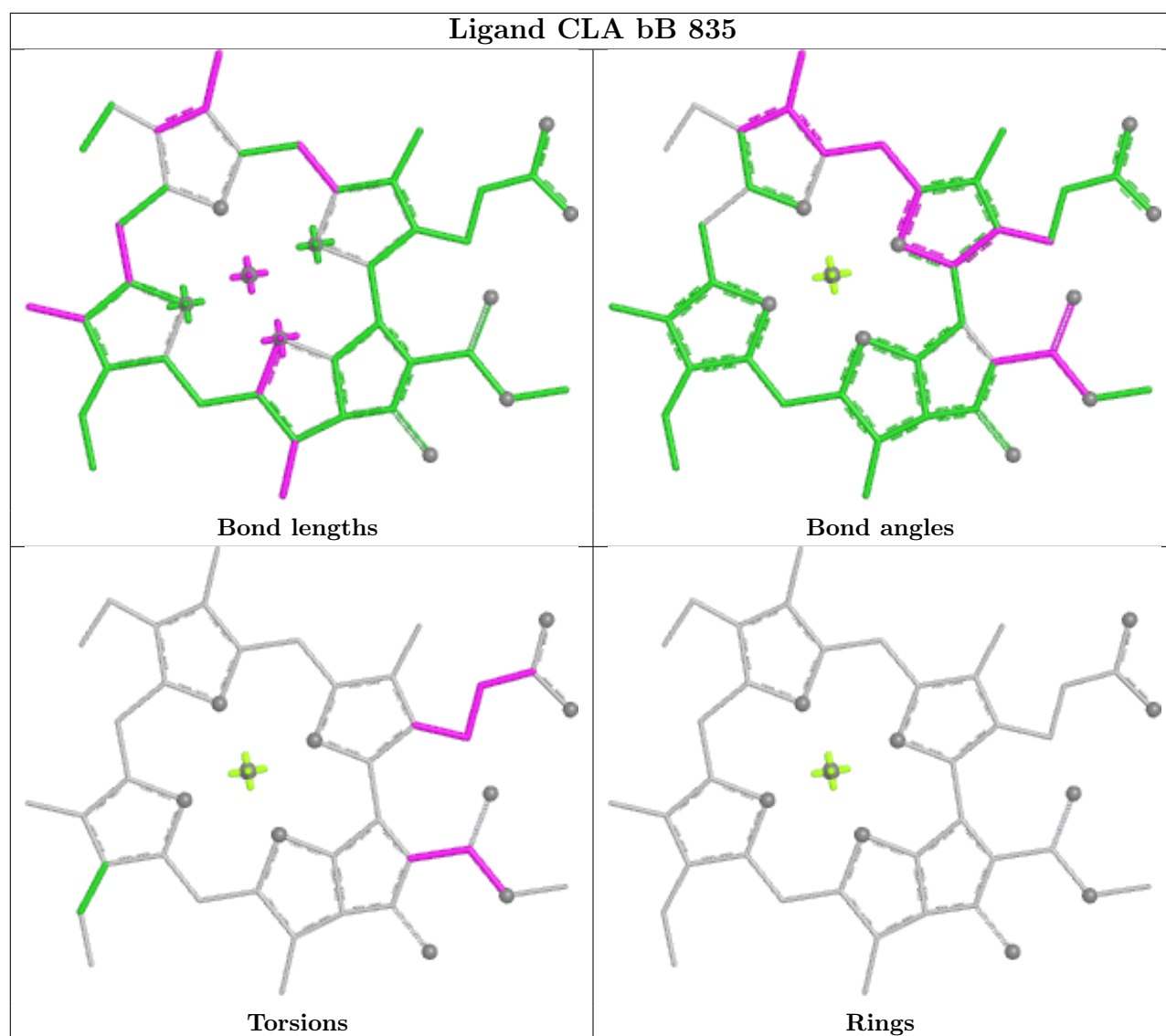


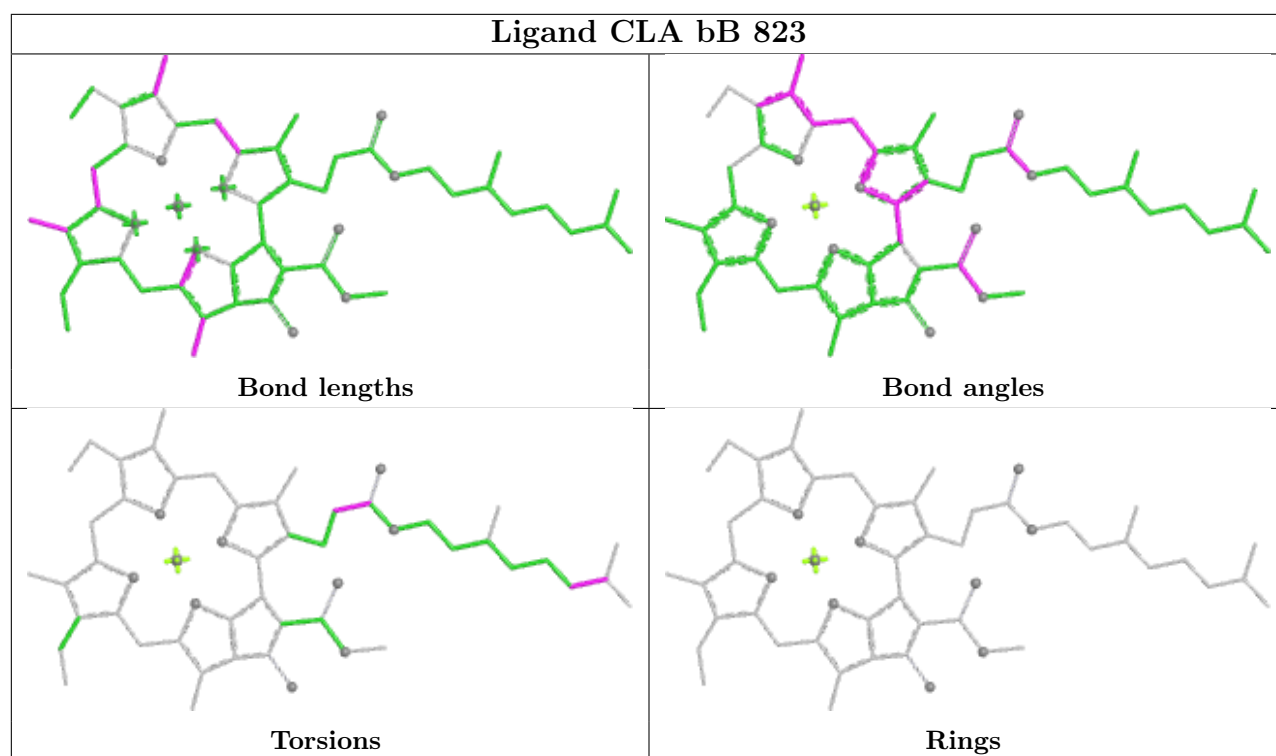


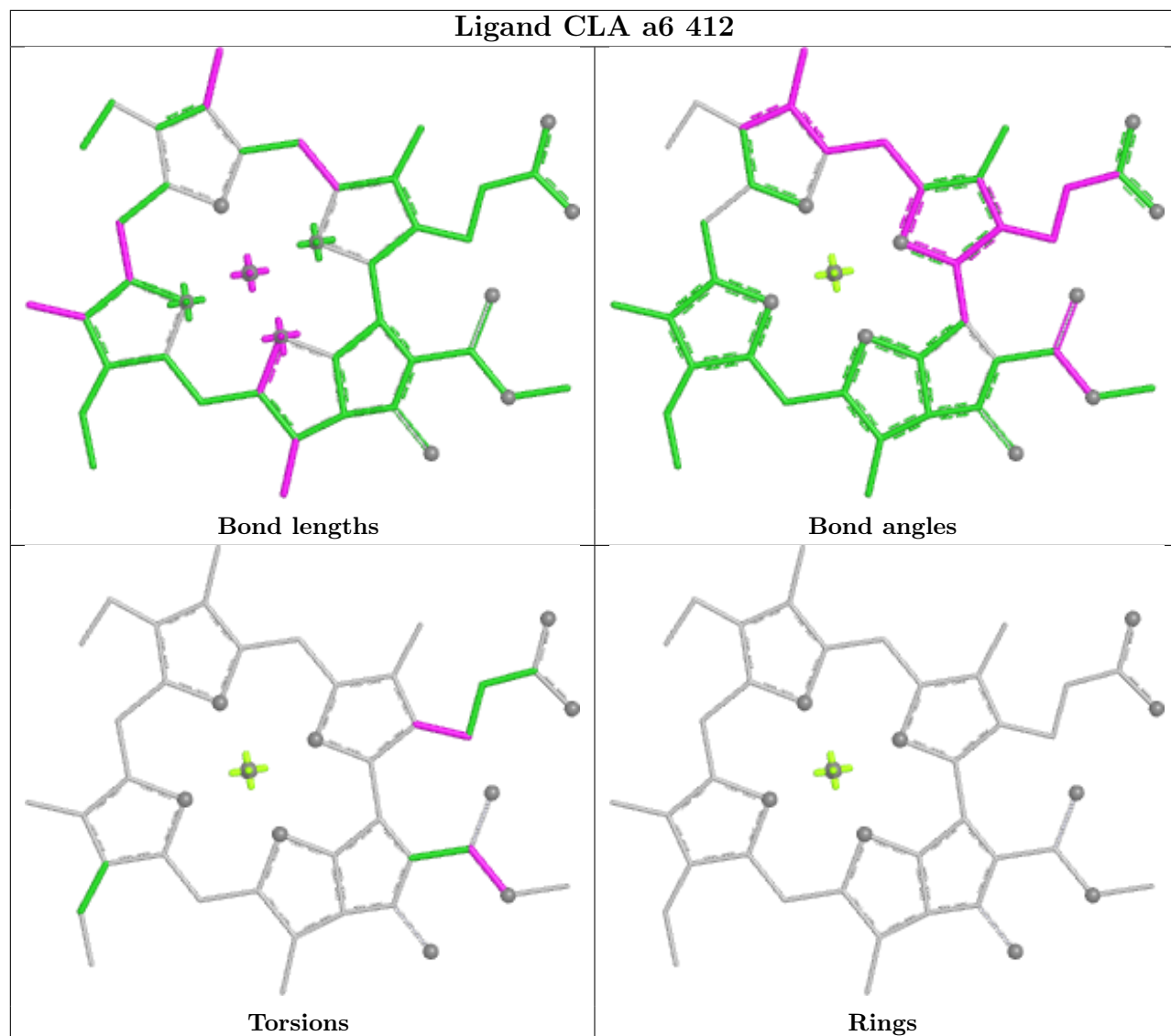


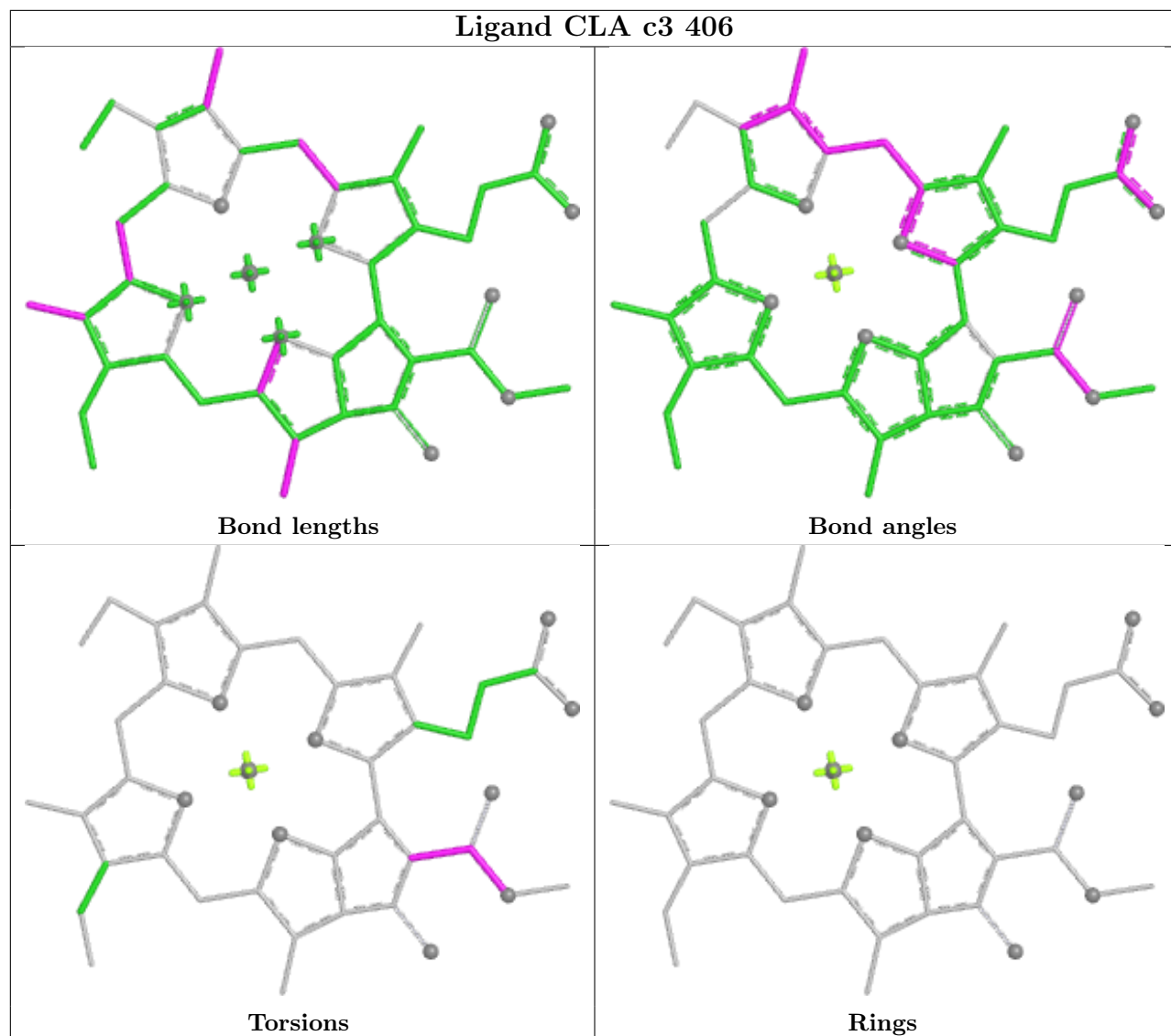


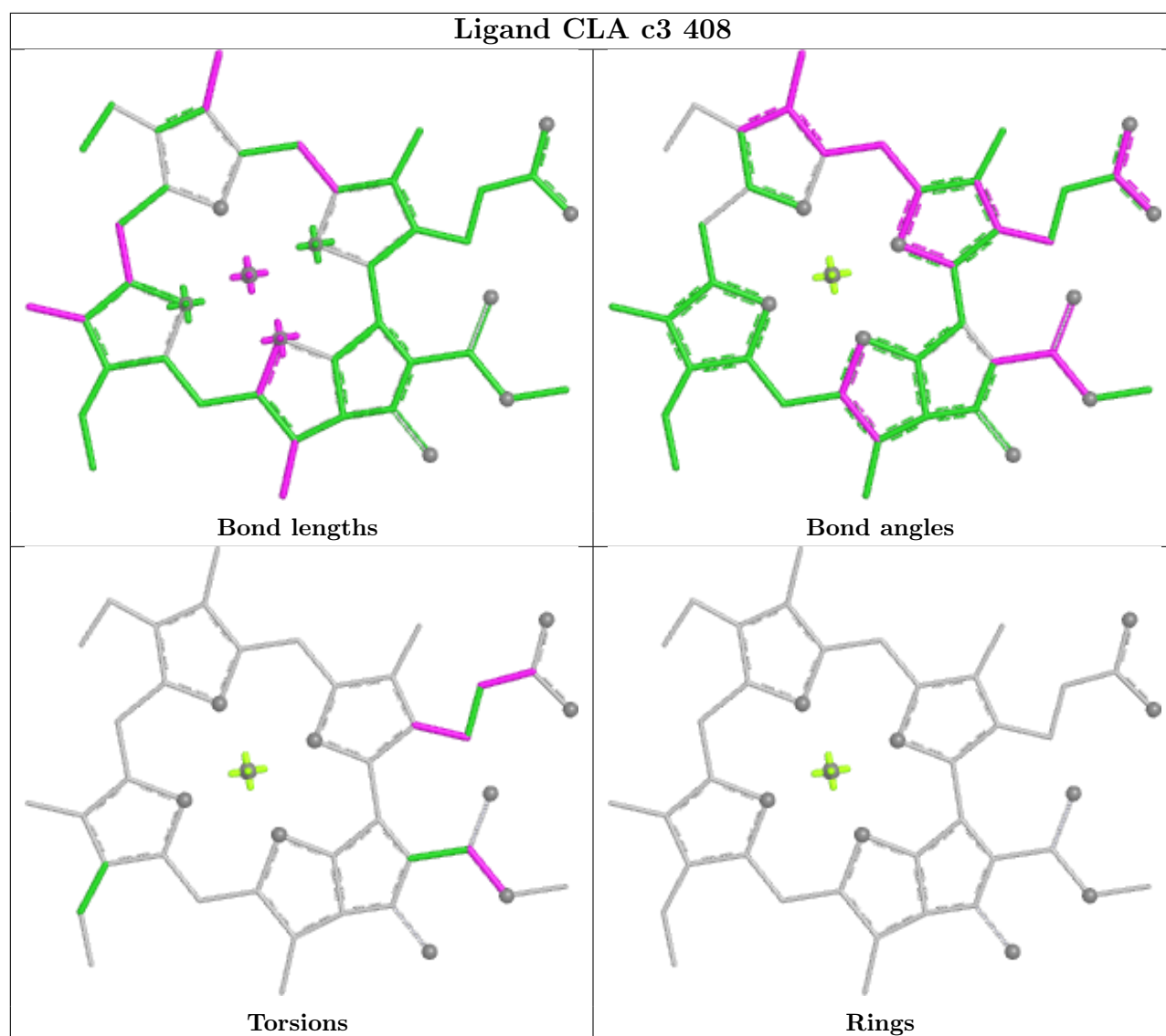


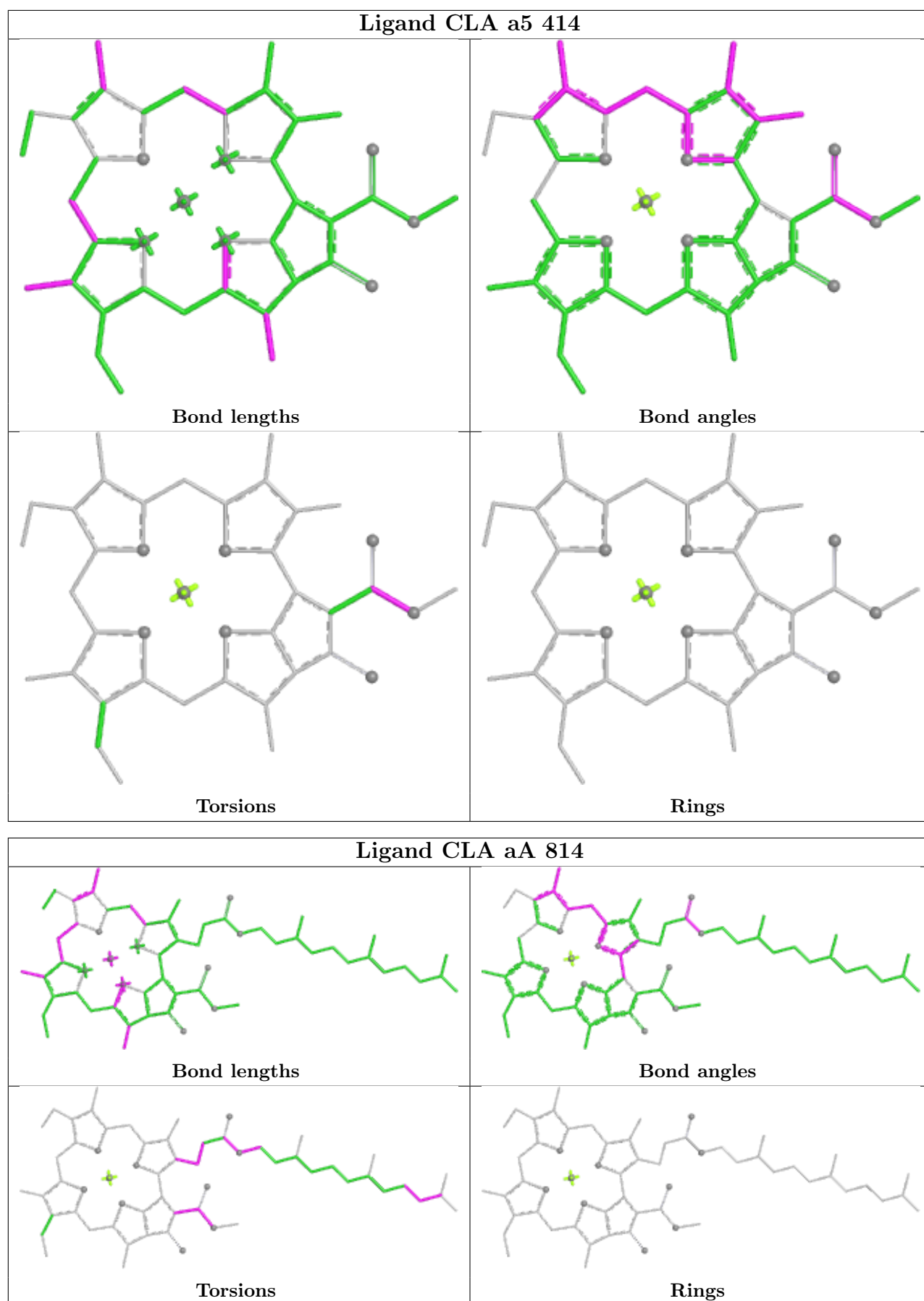


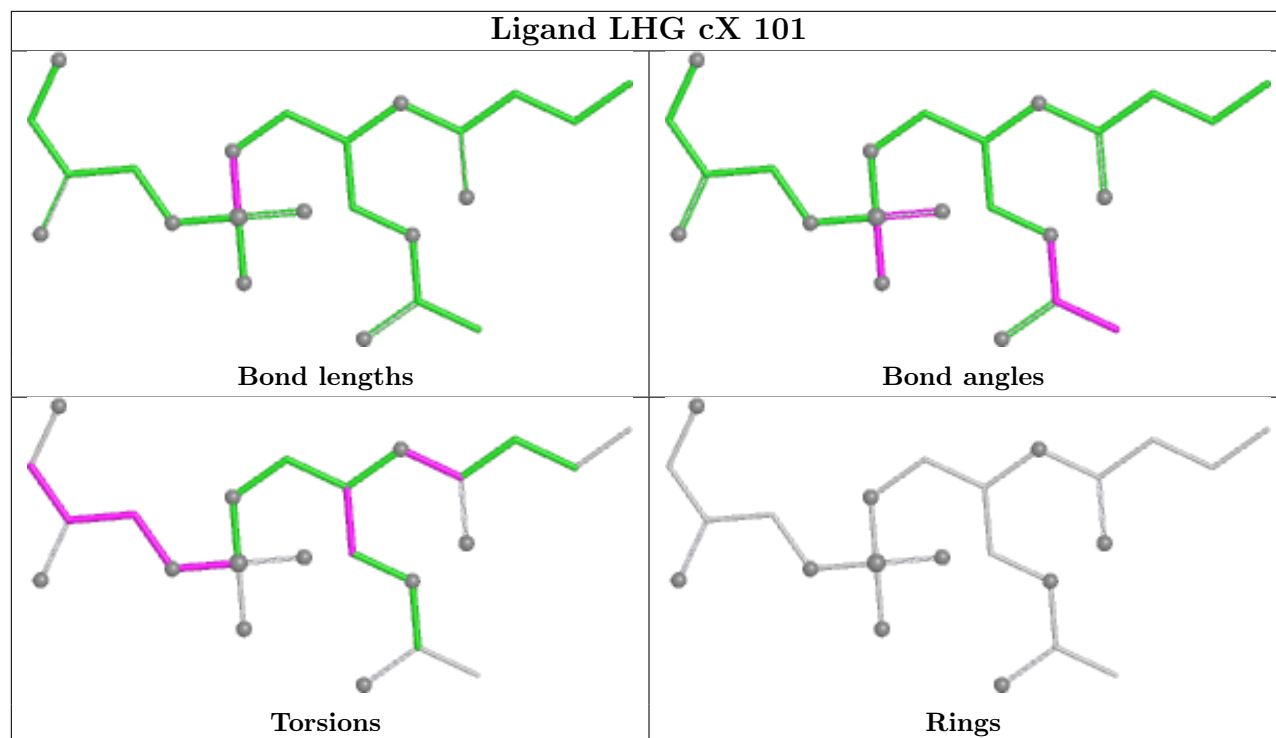
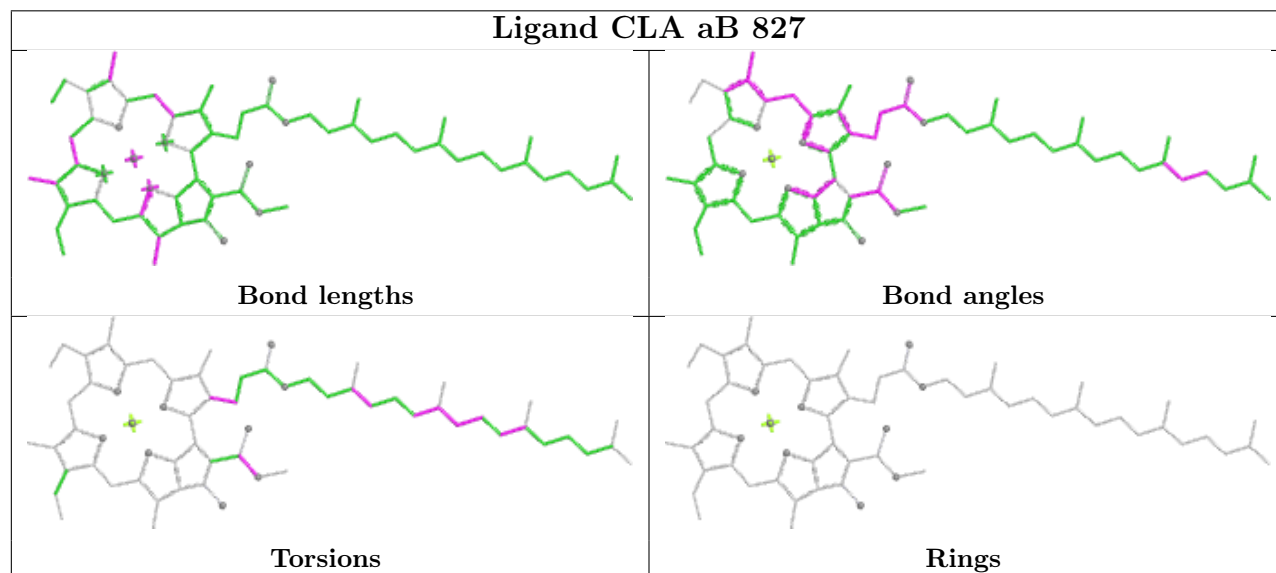
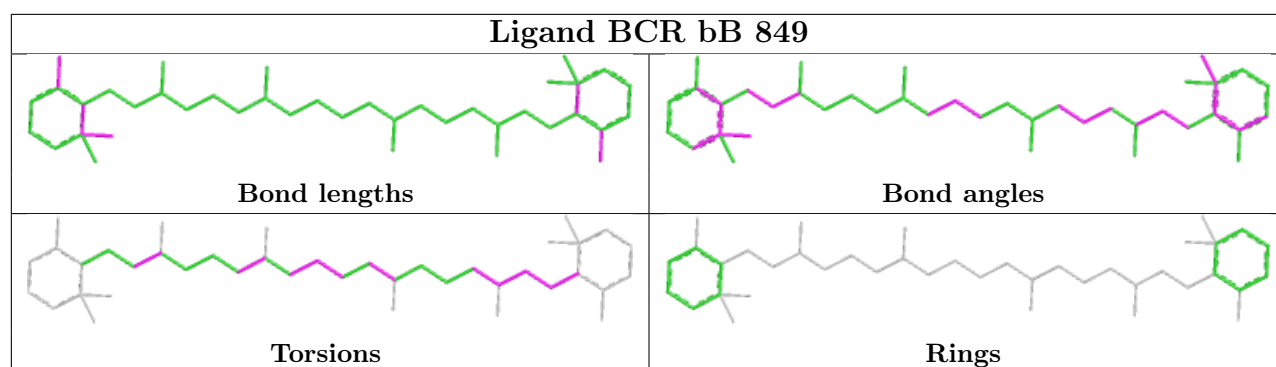




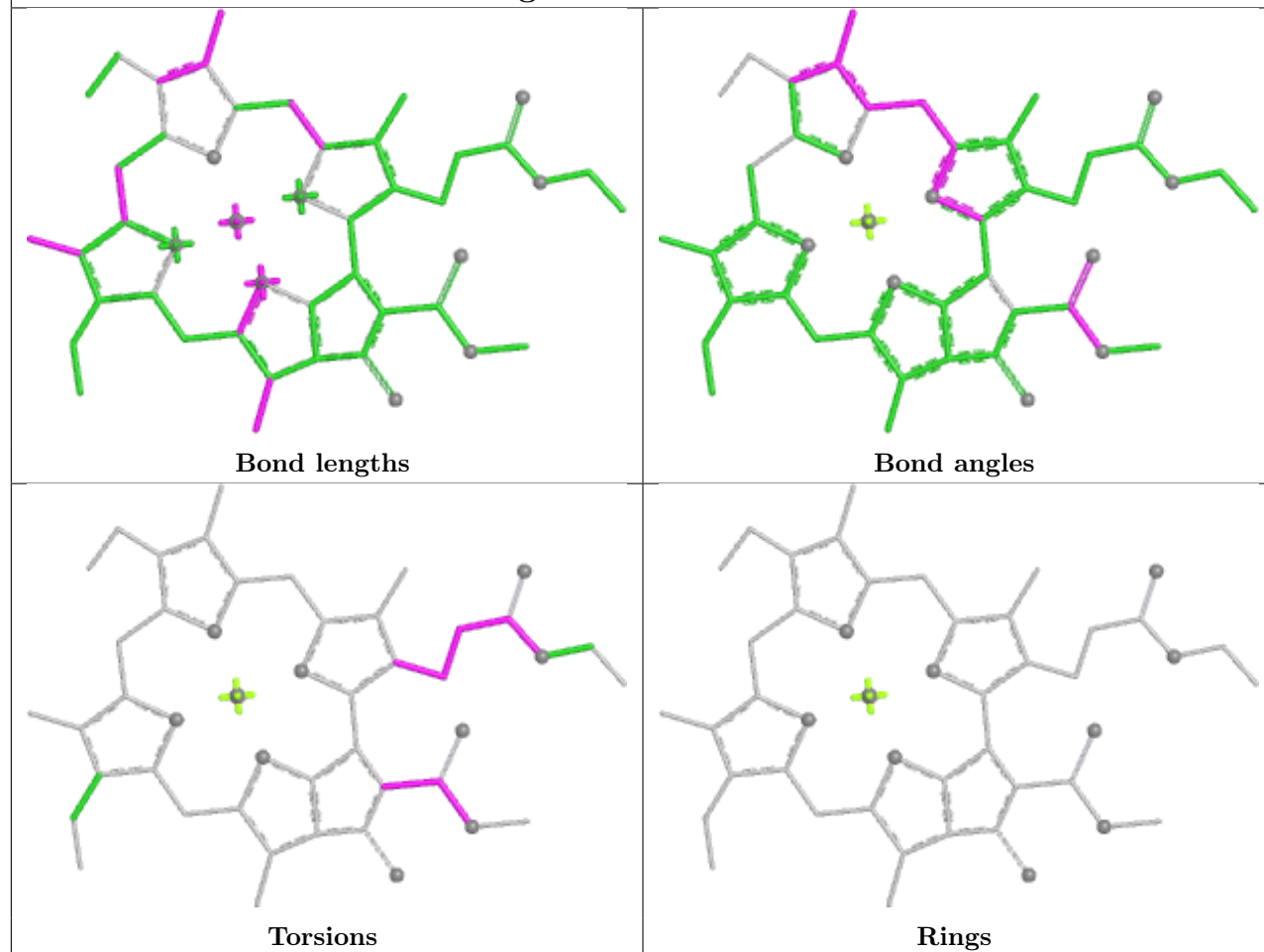




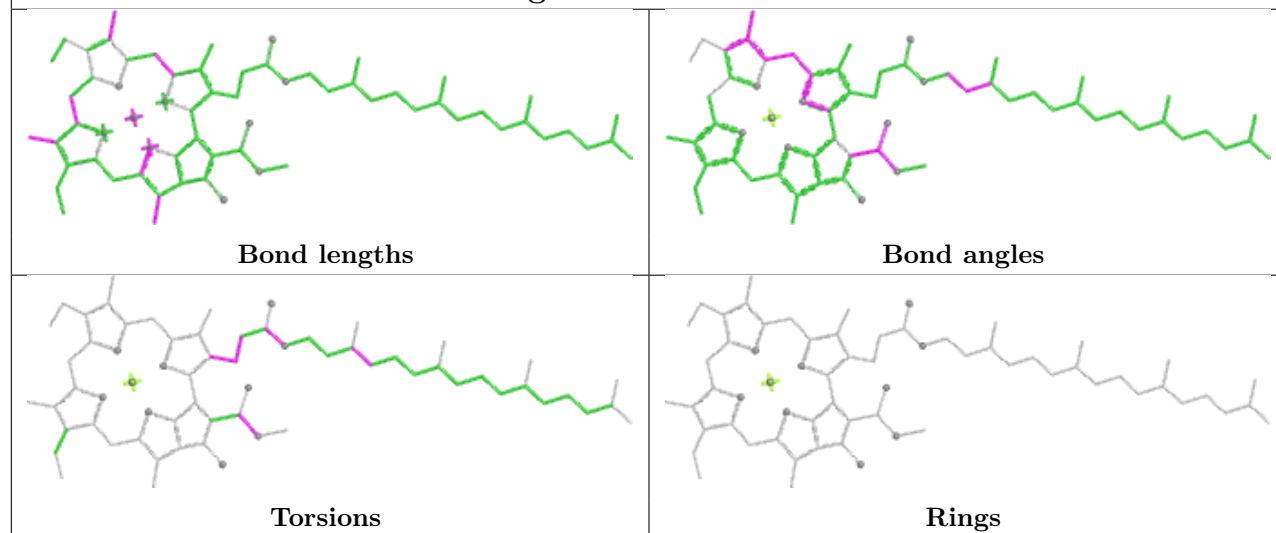


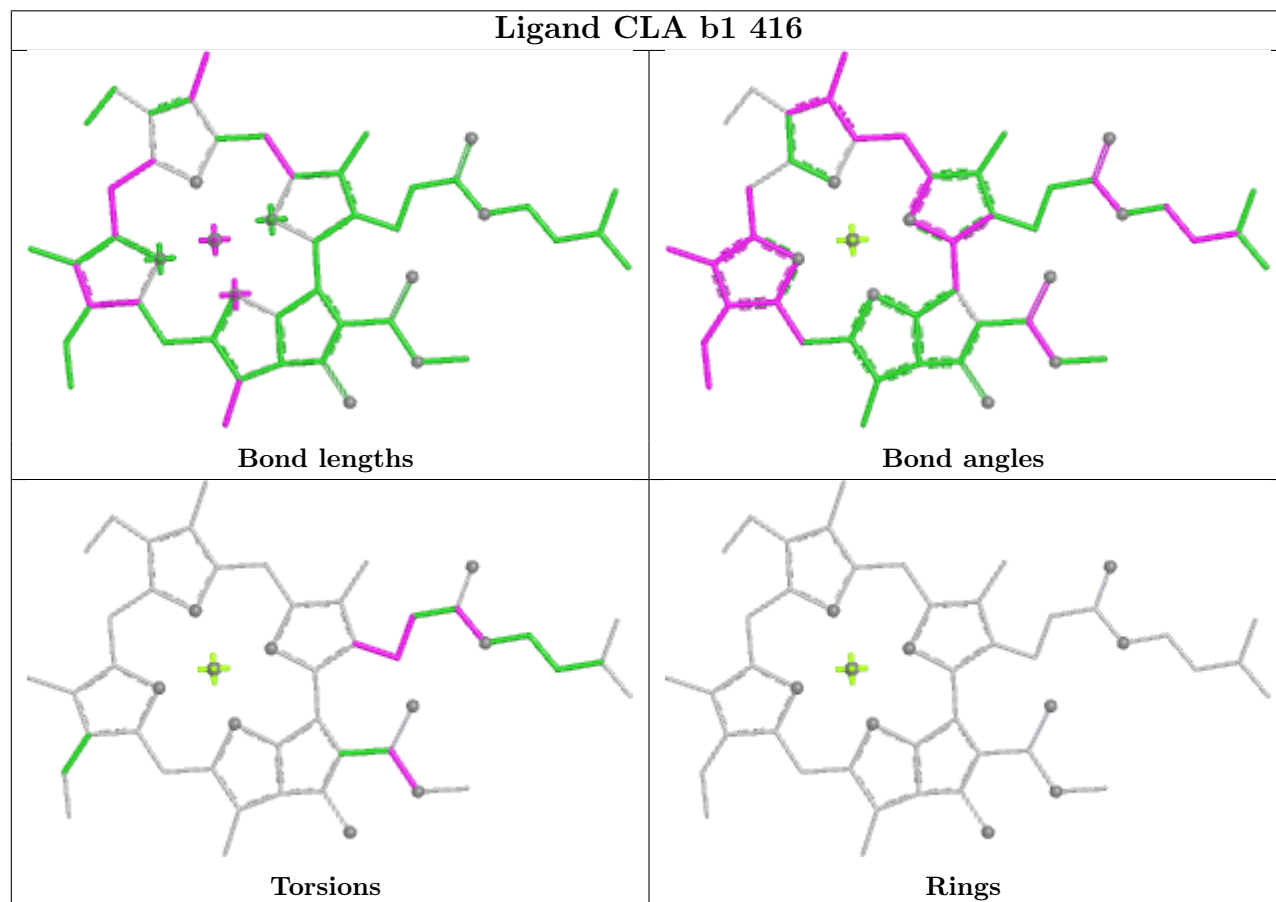
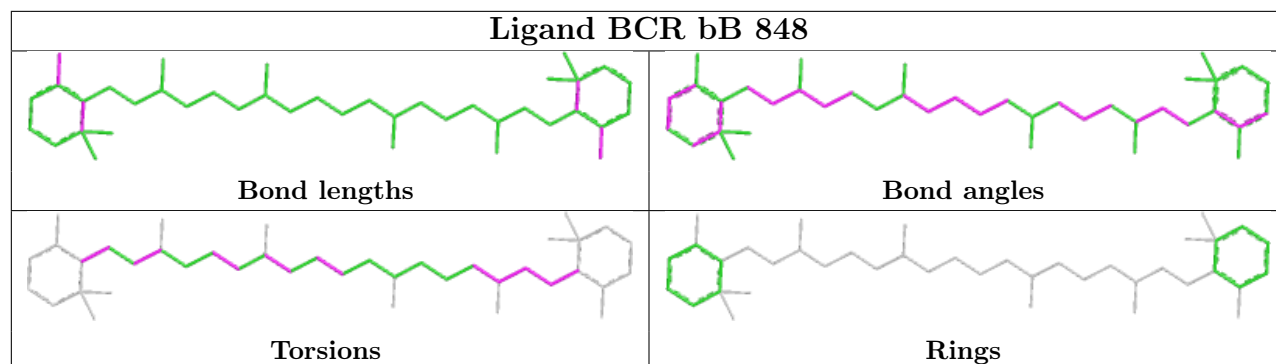


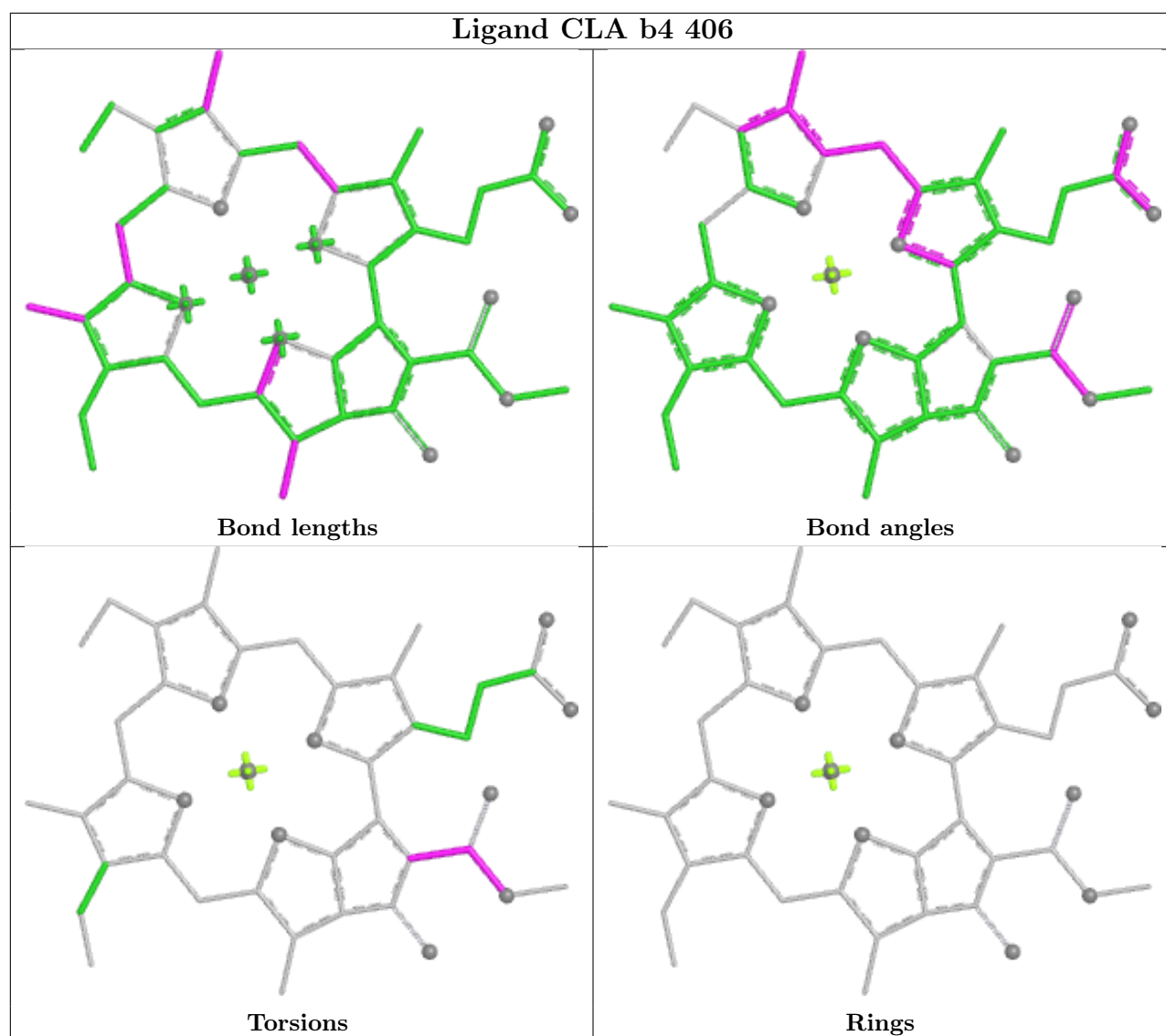
Ligand CLA aB 821

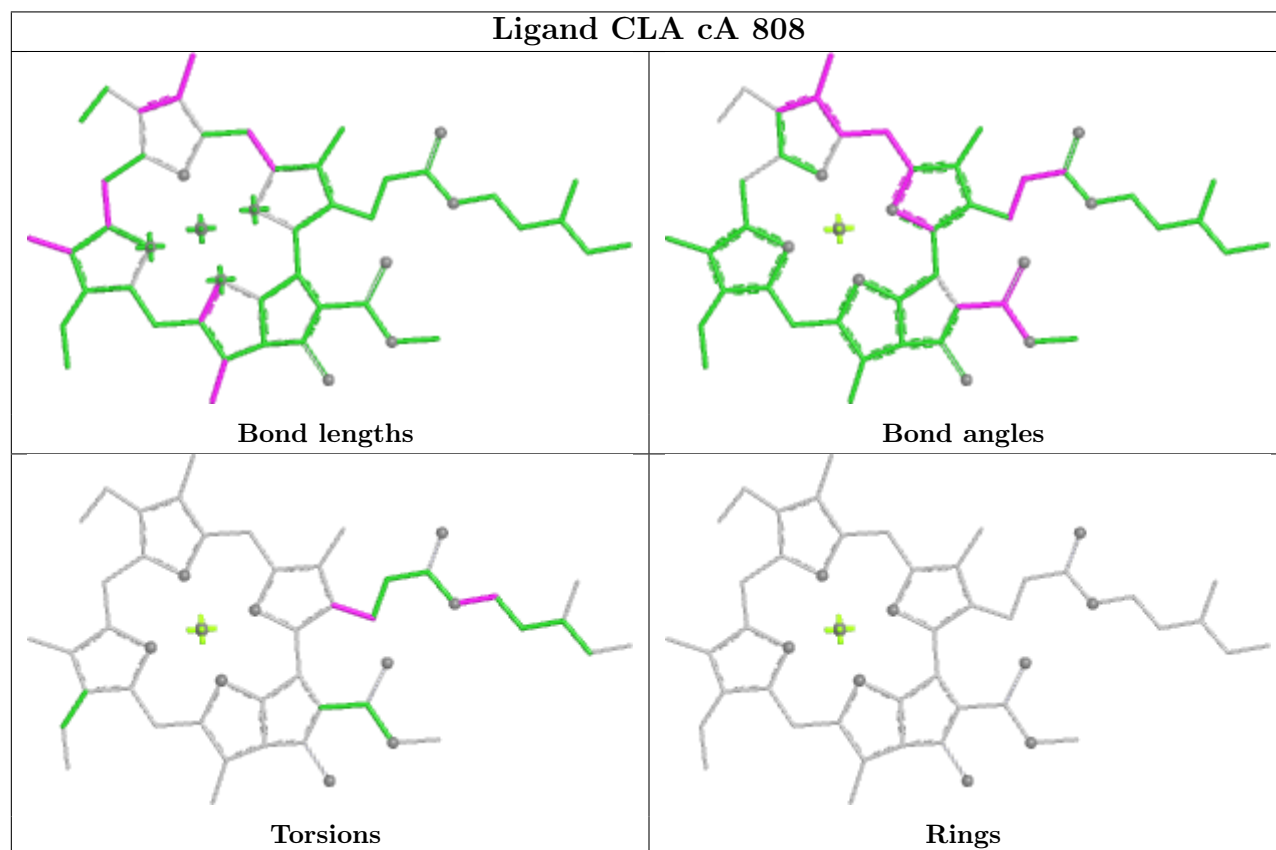
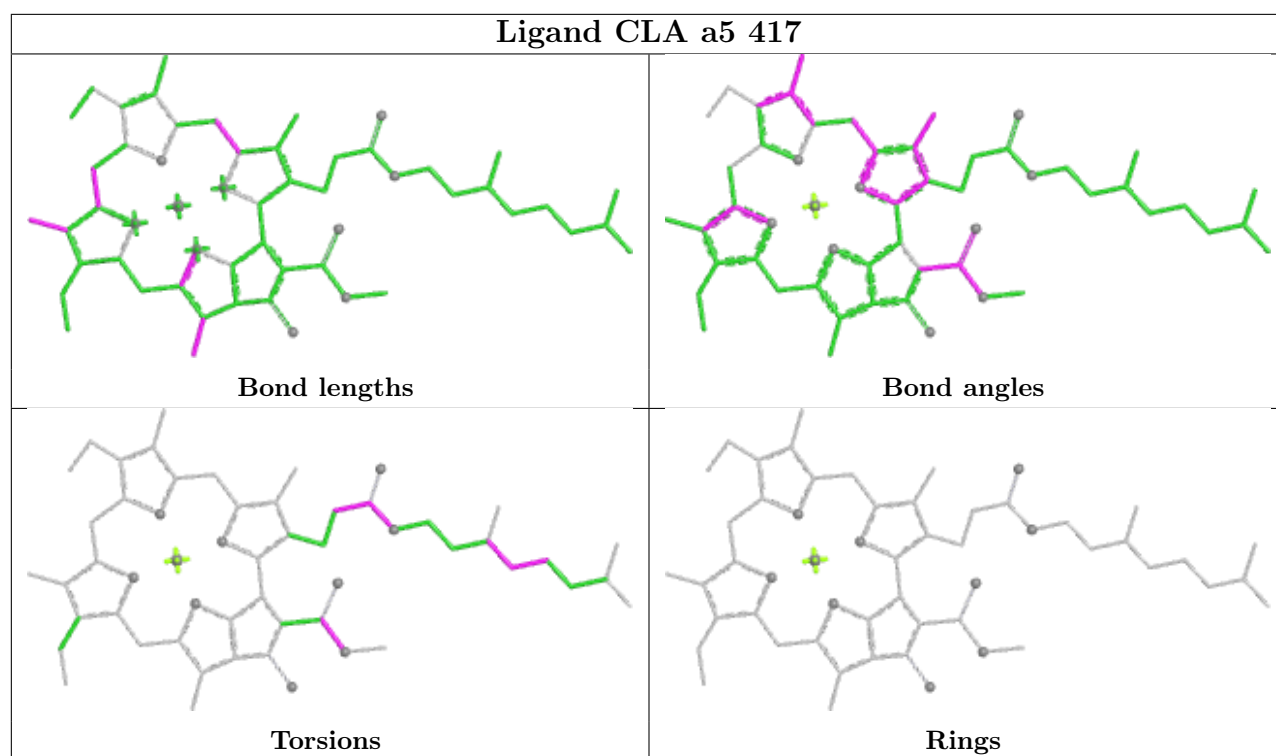


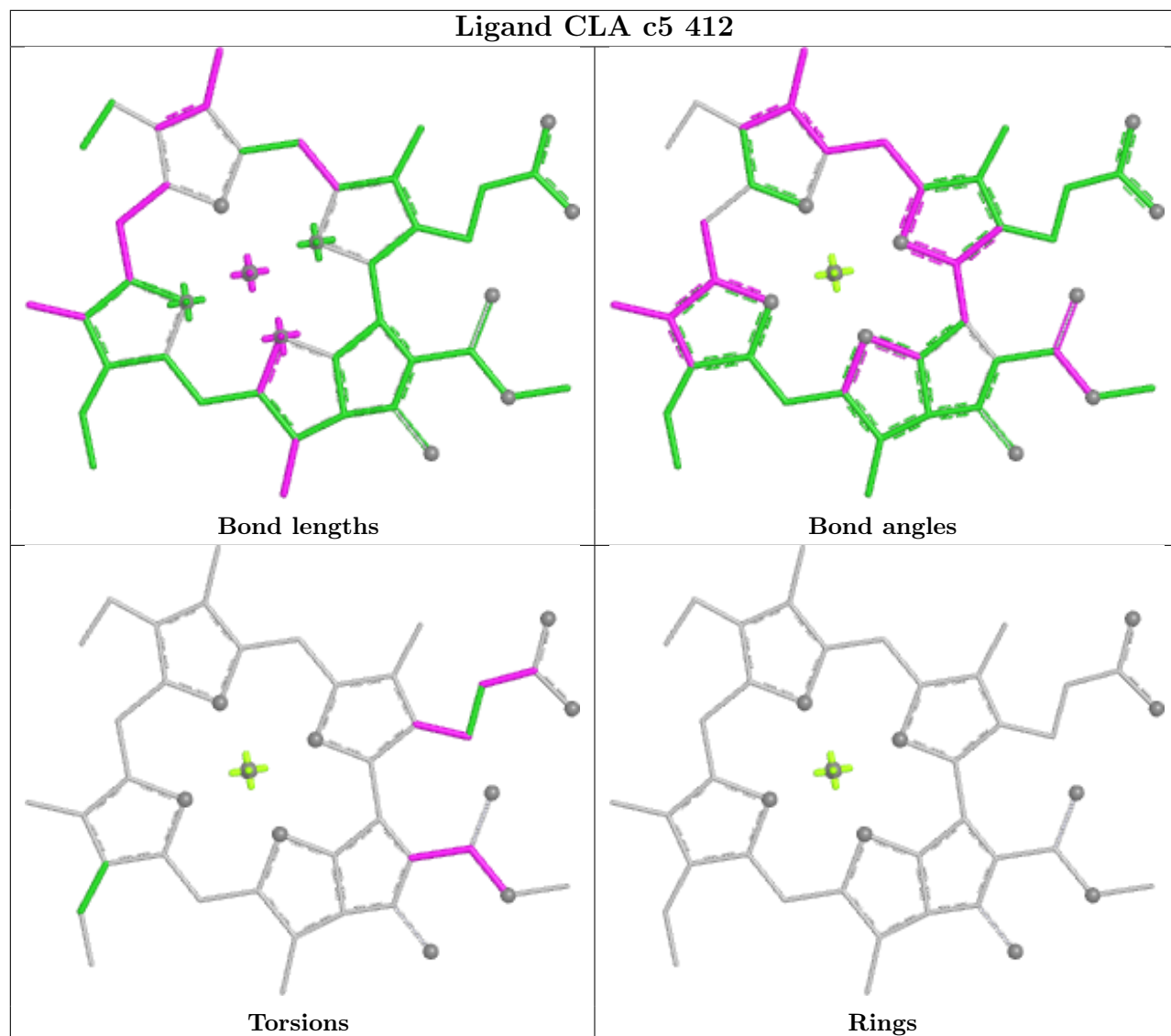
Ligand CLA c4 404

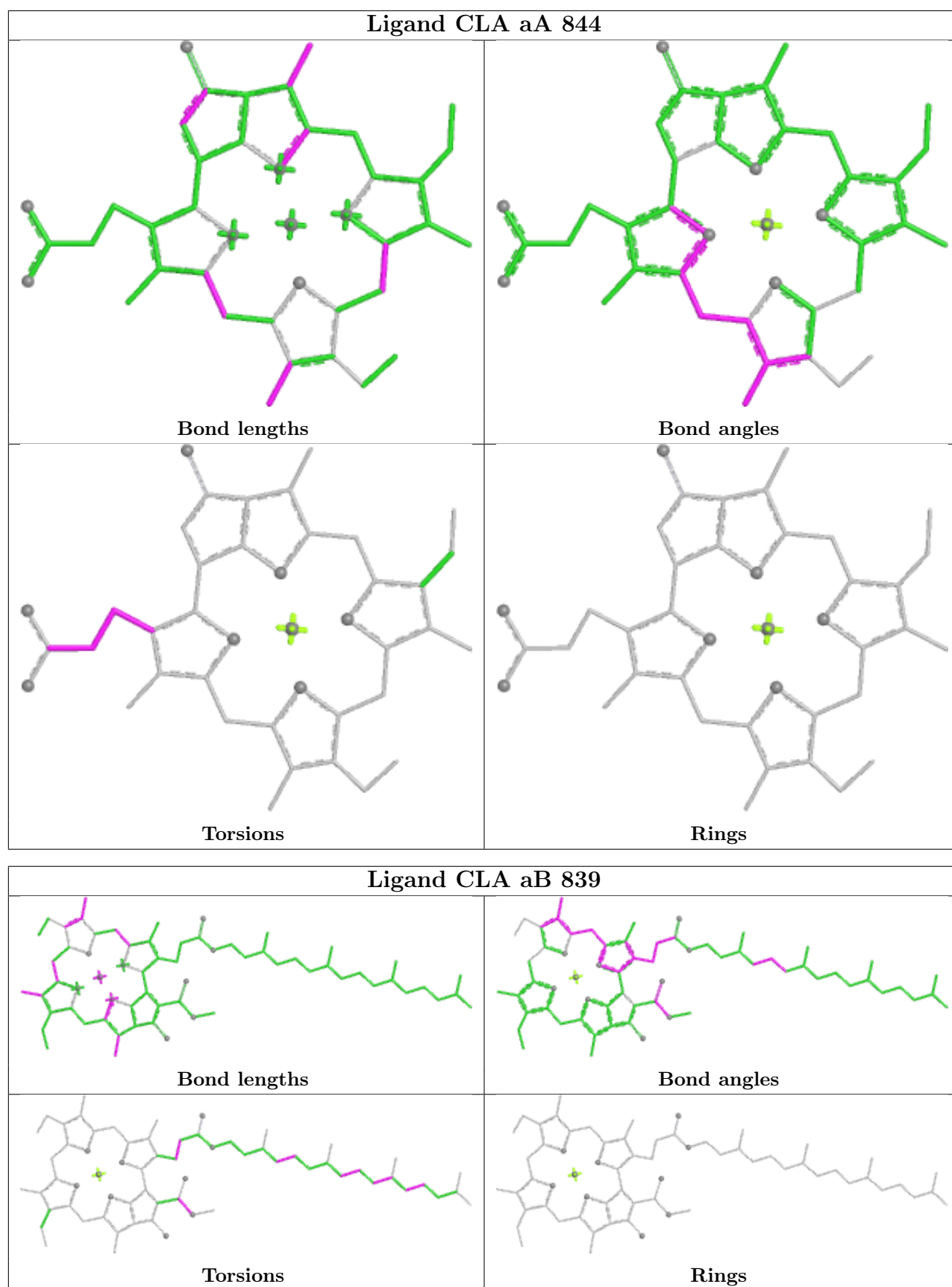


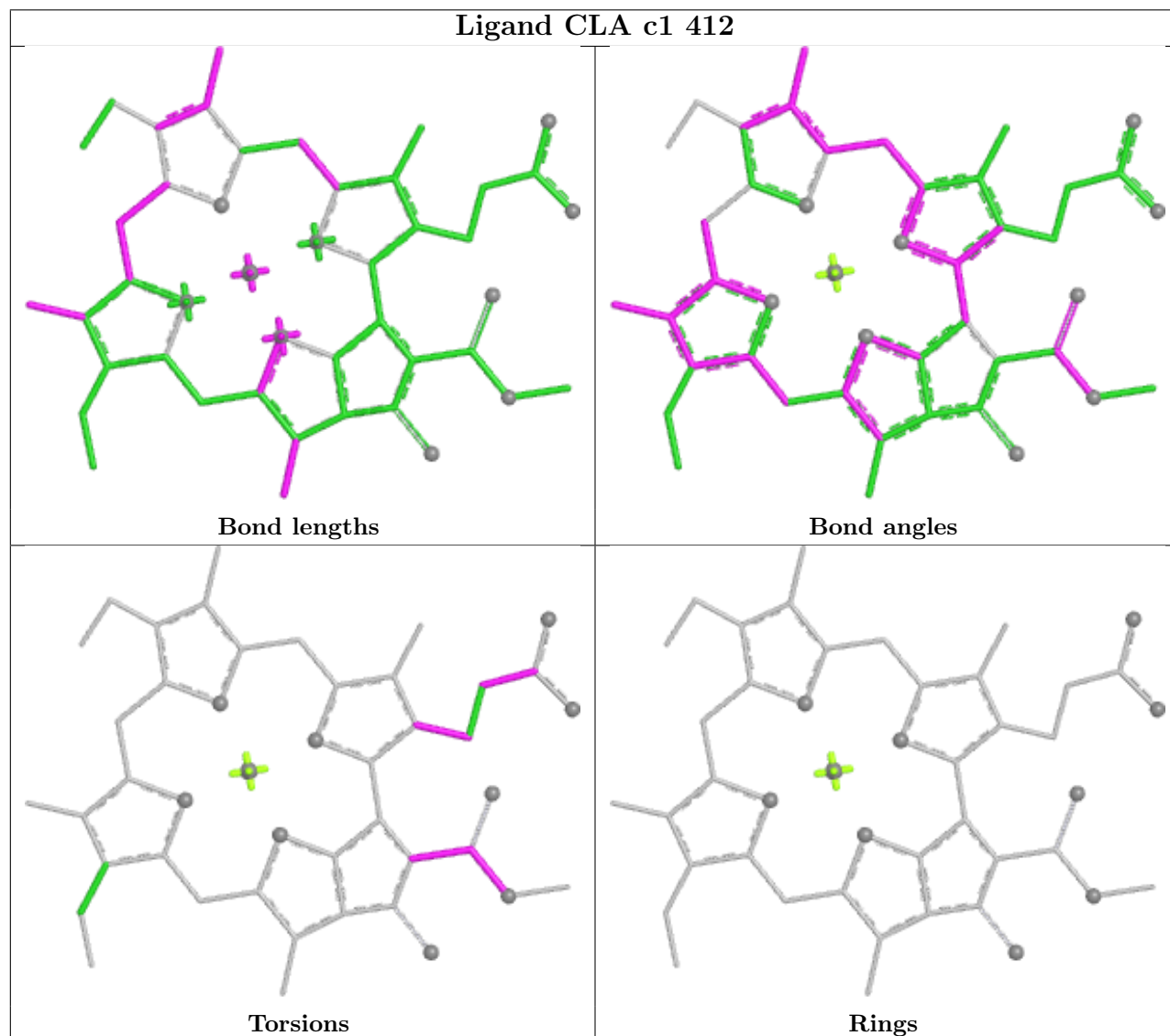
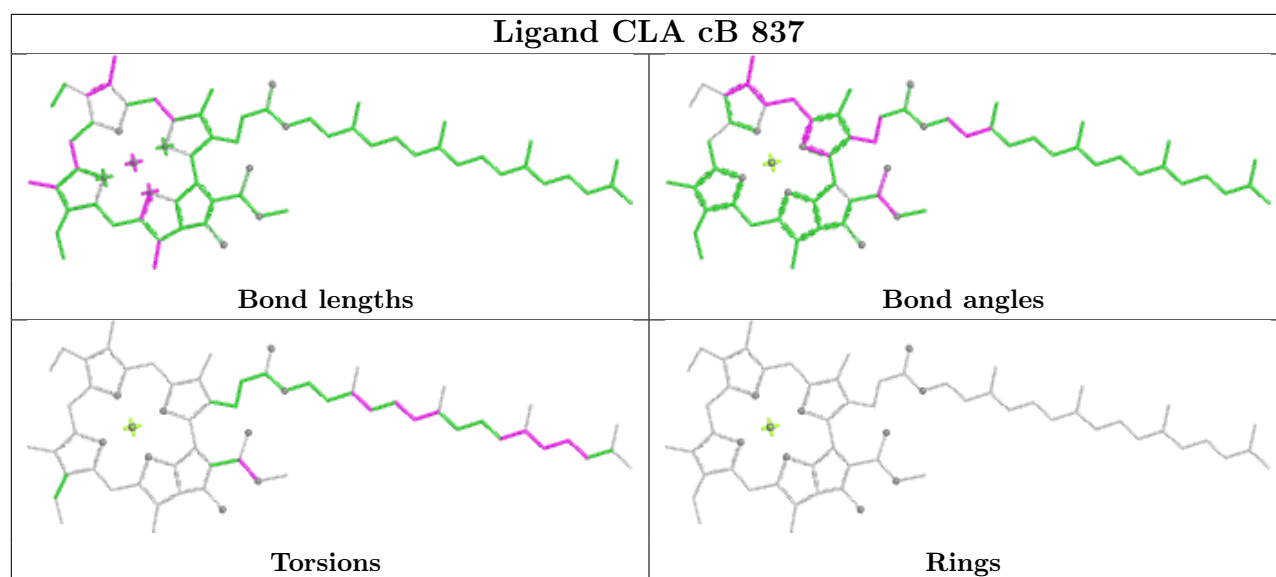


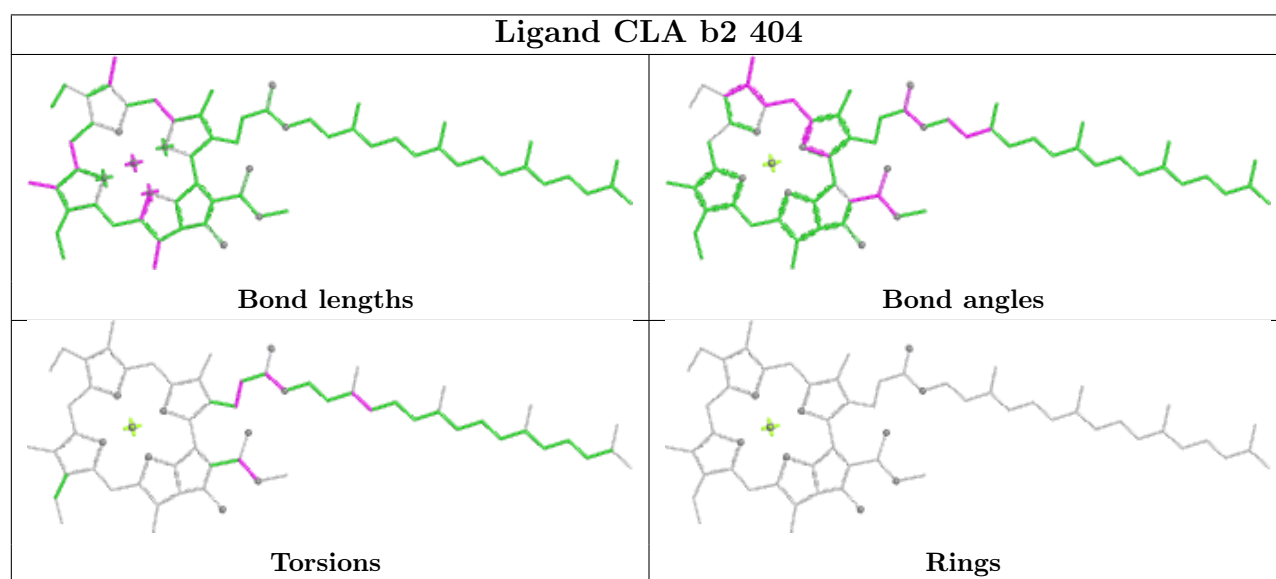
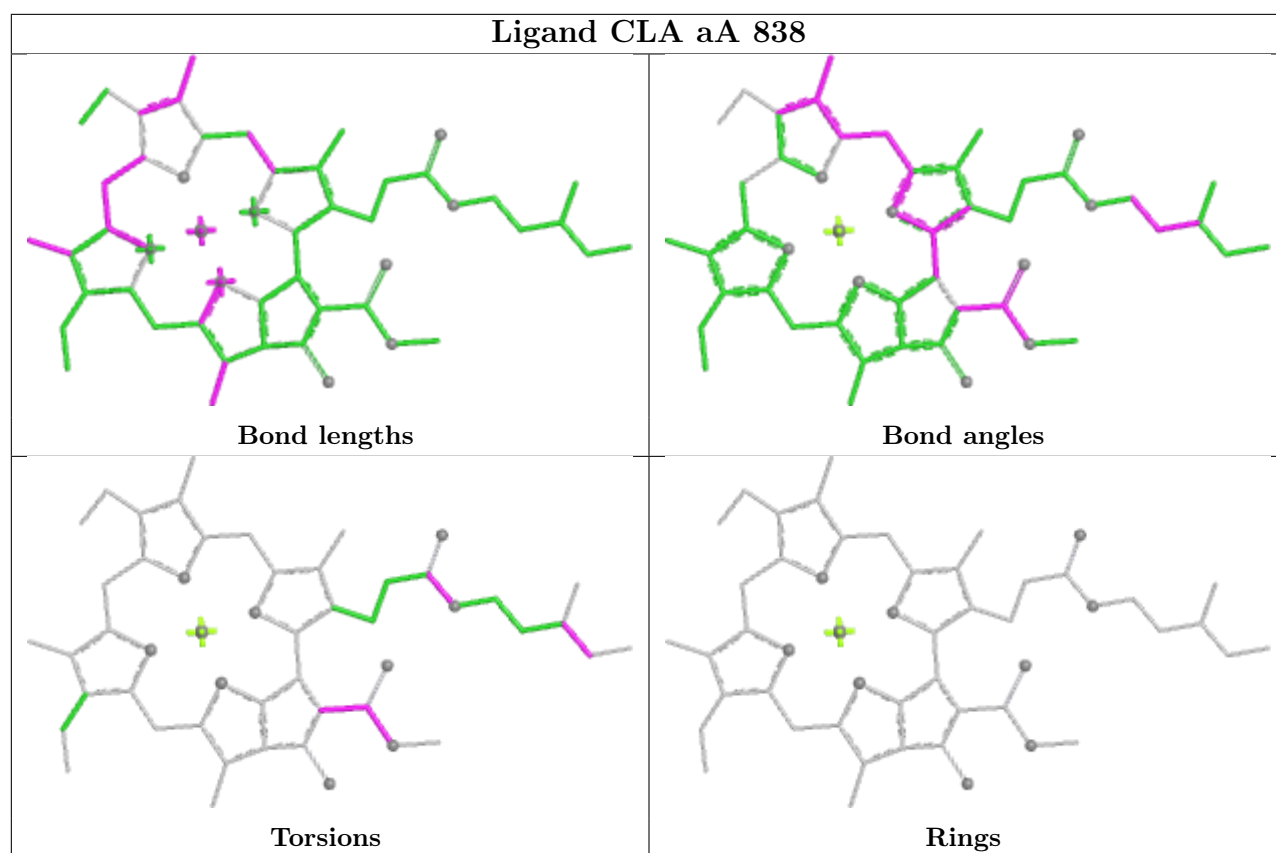


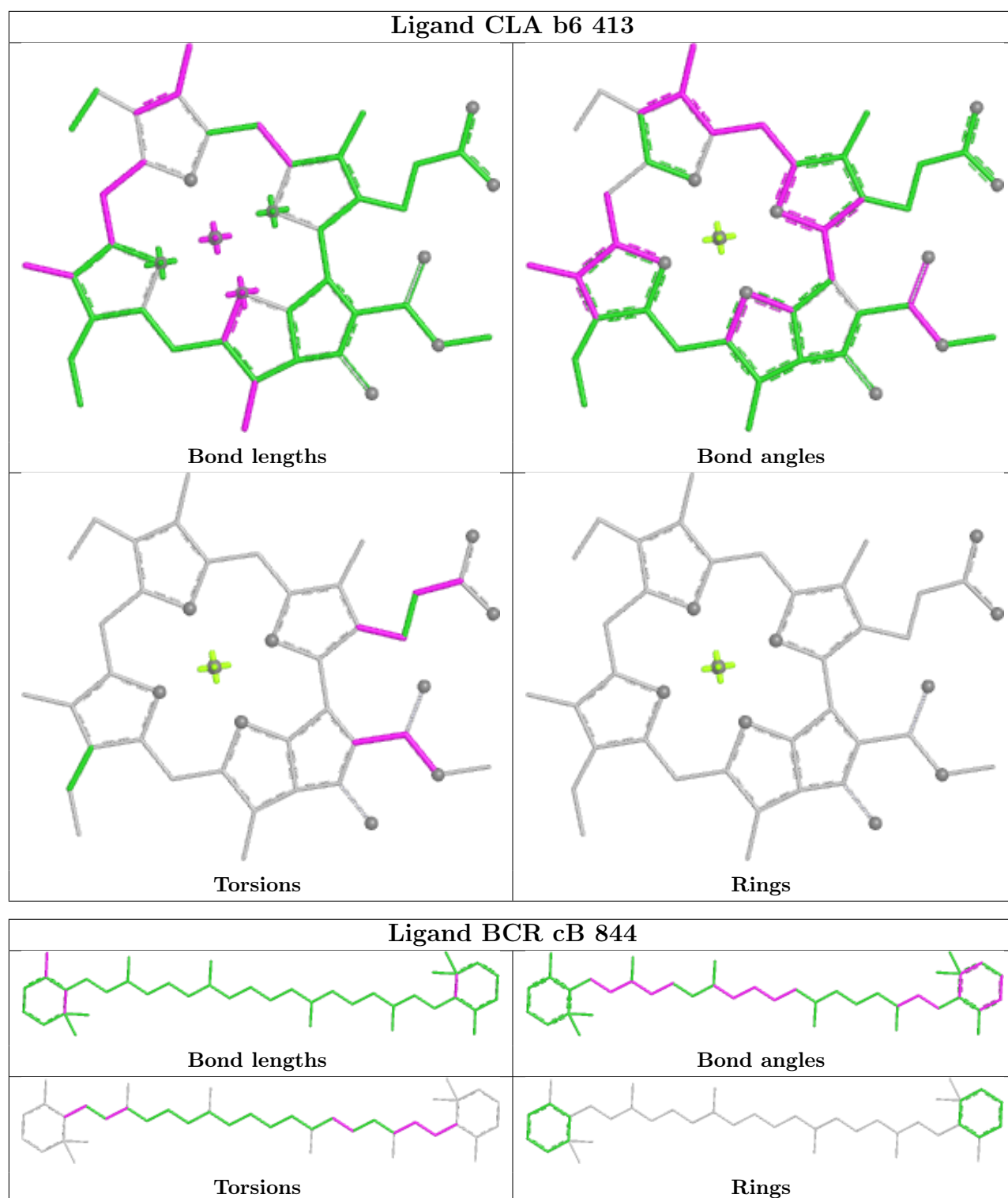


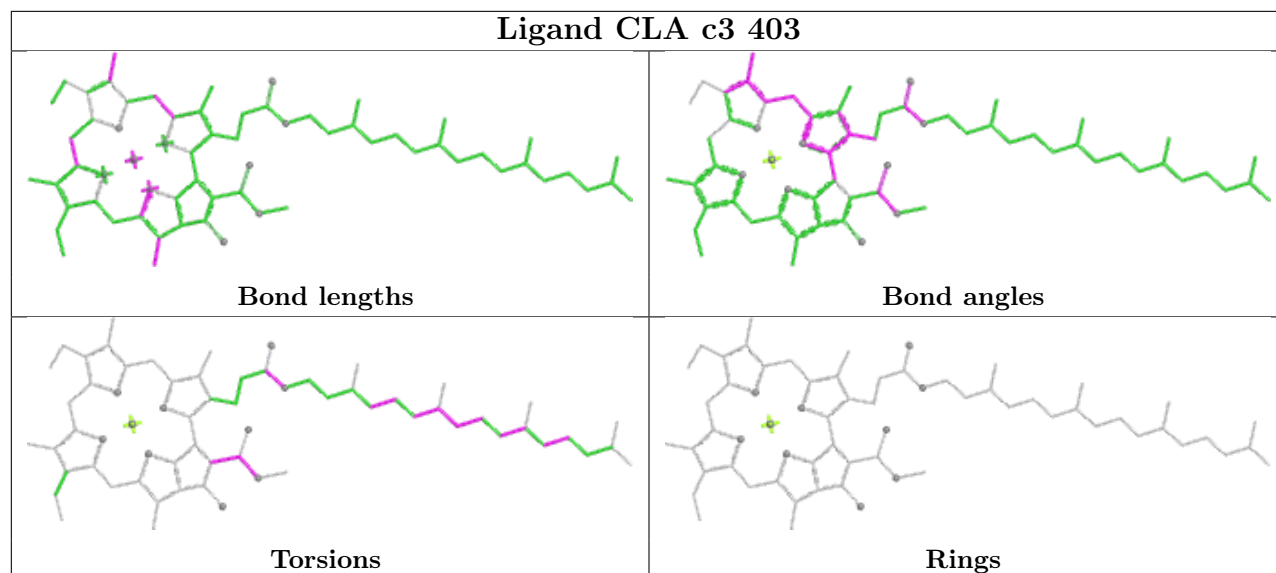
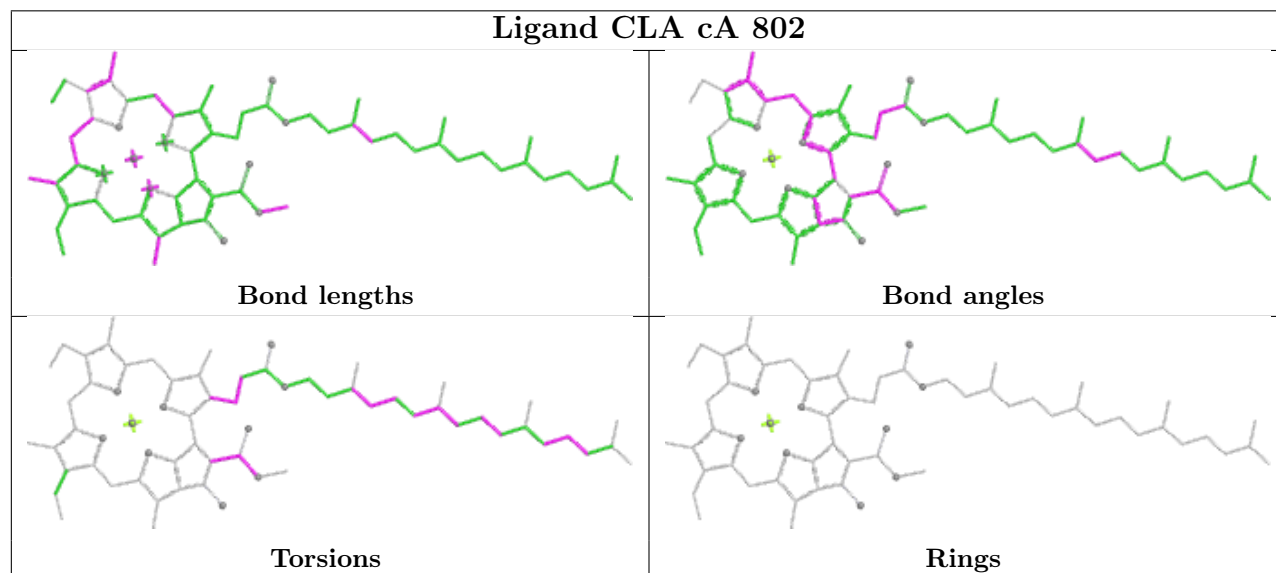
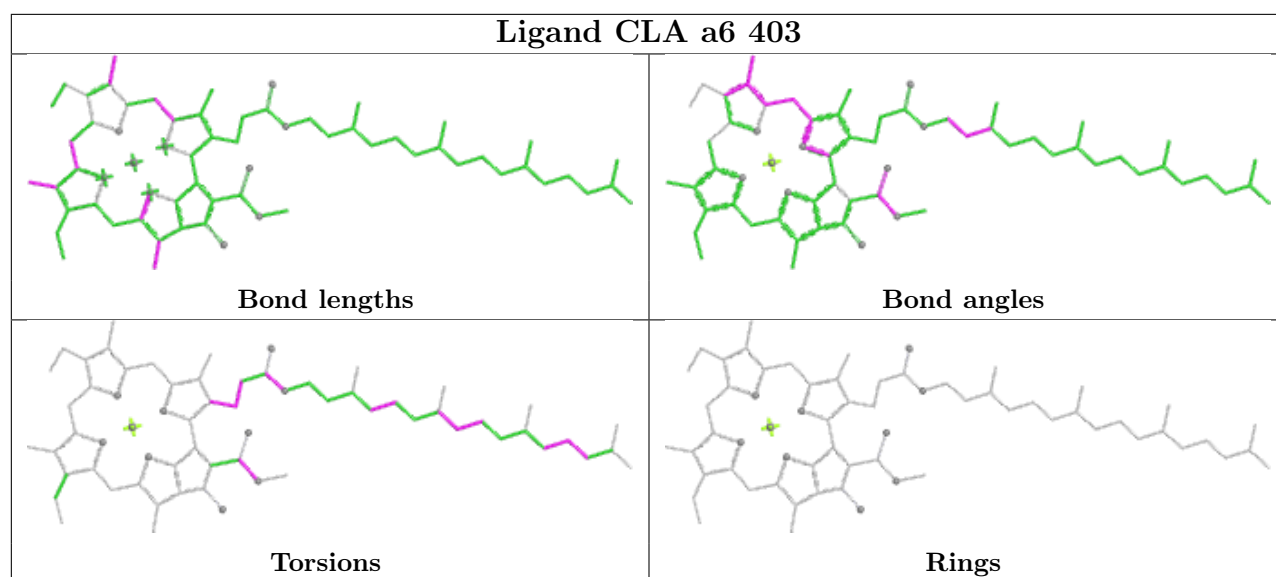


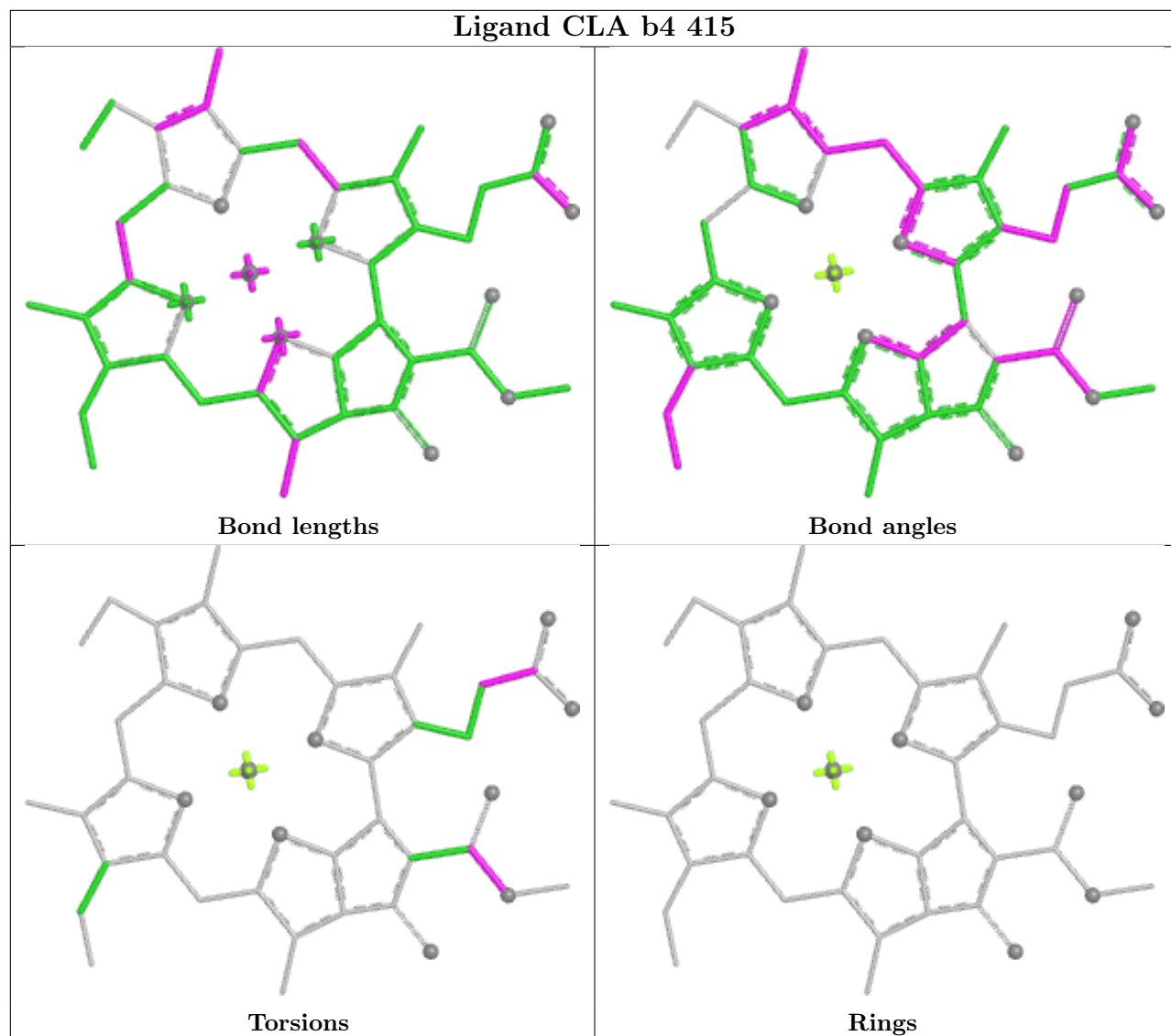


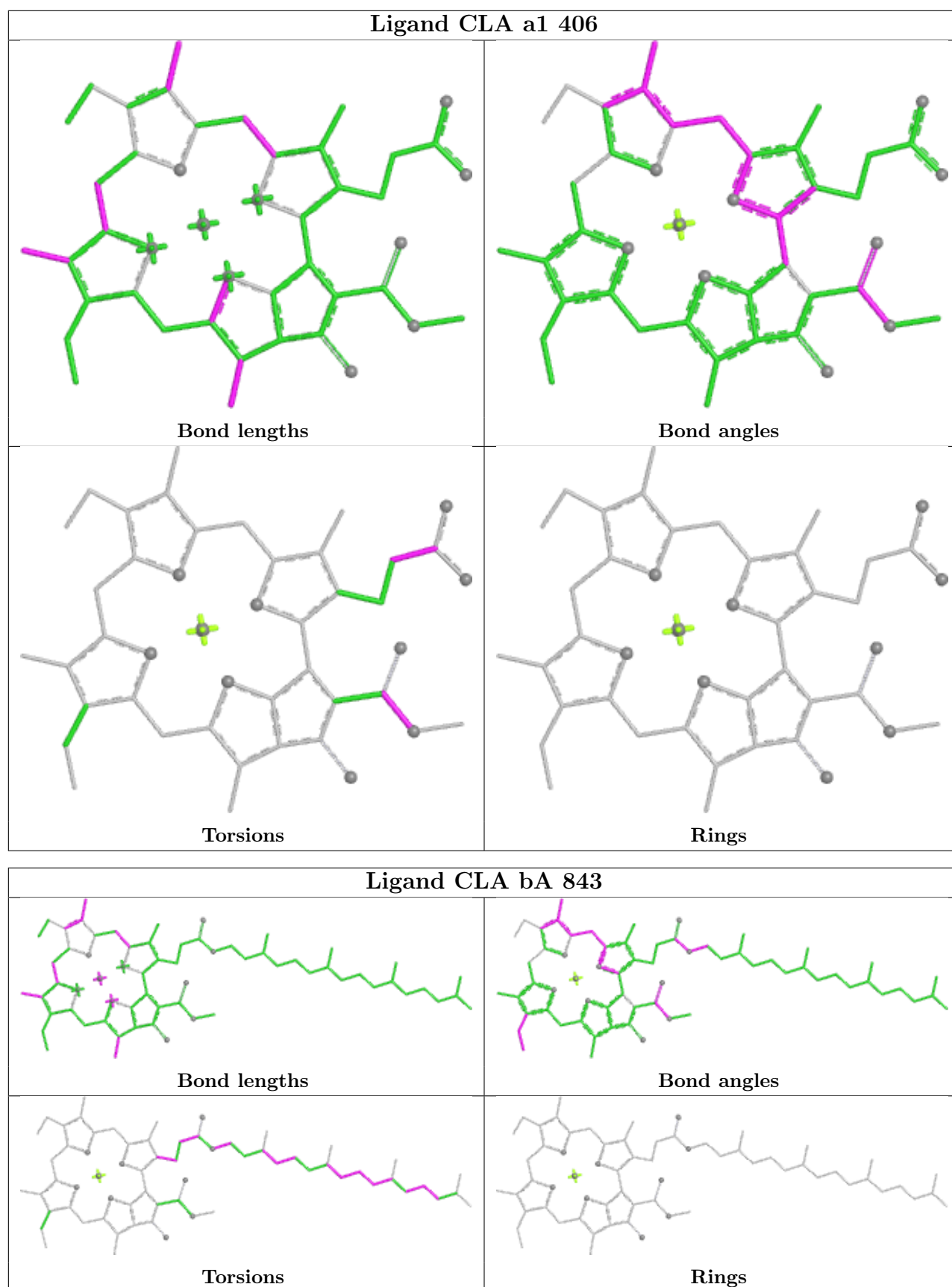


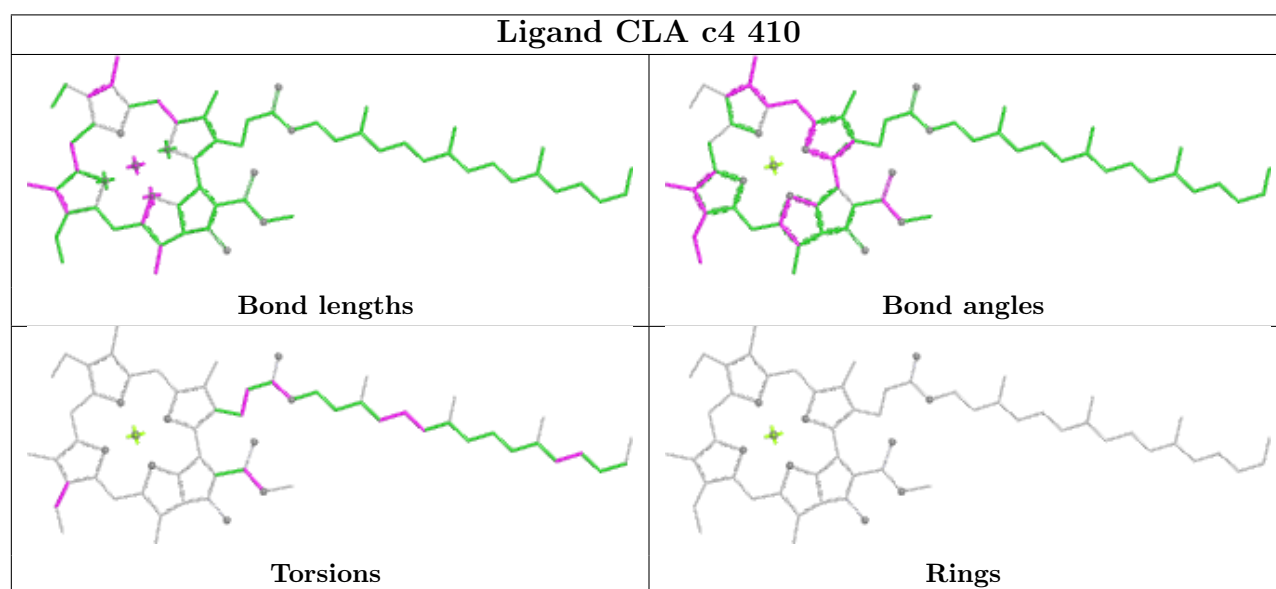
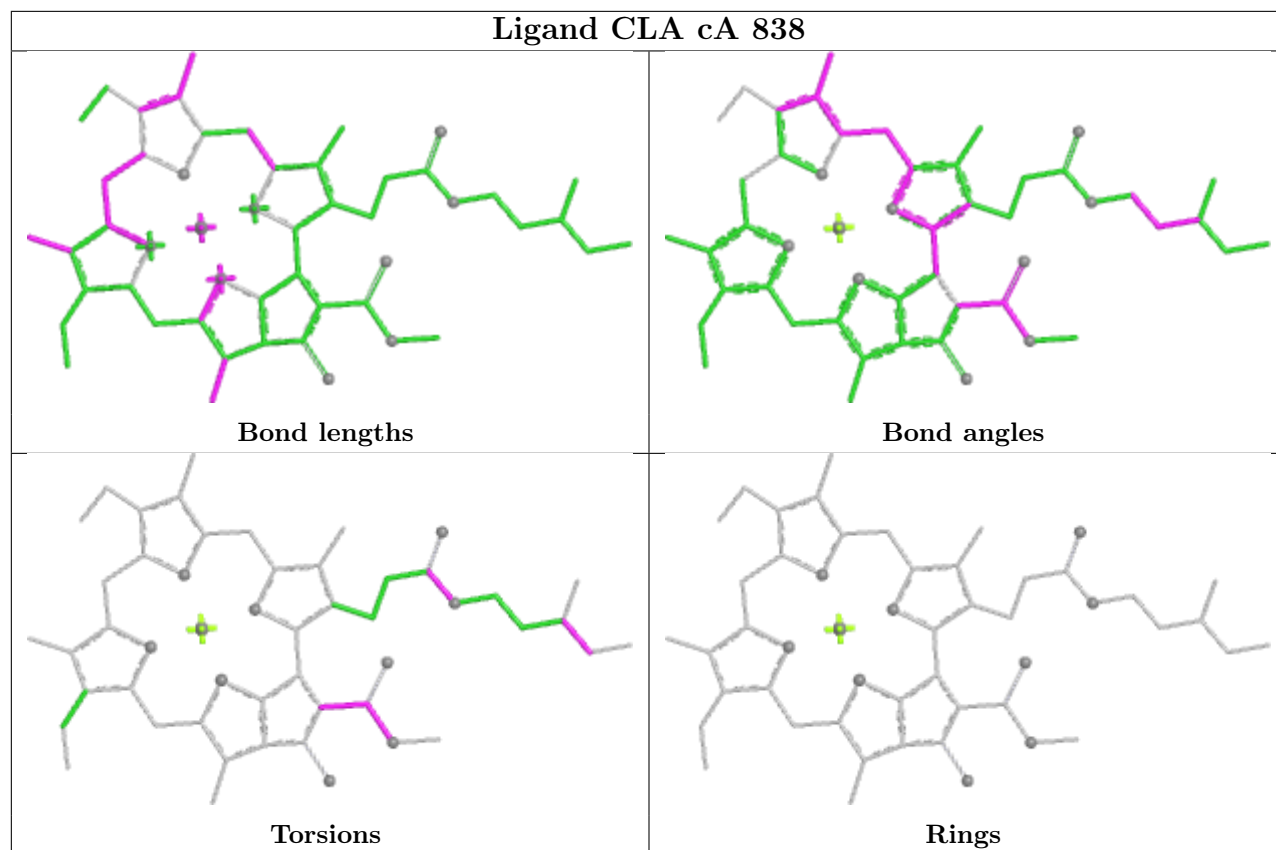


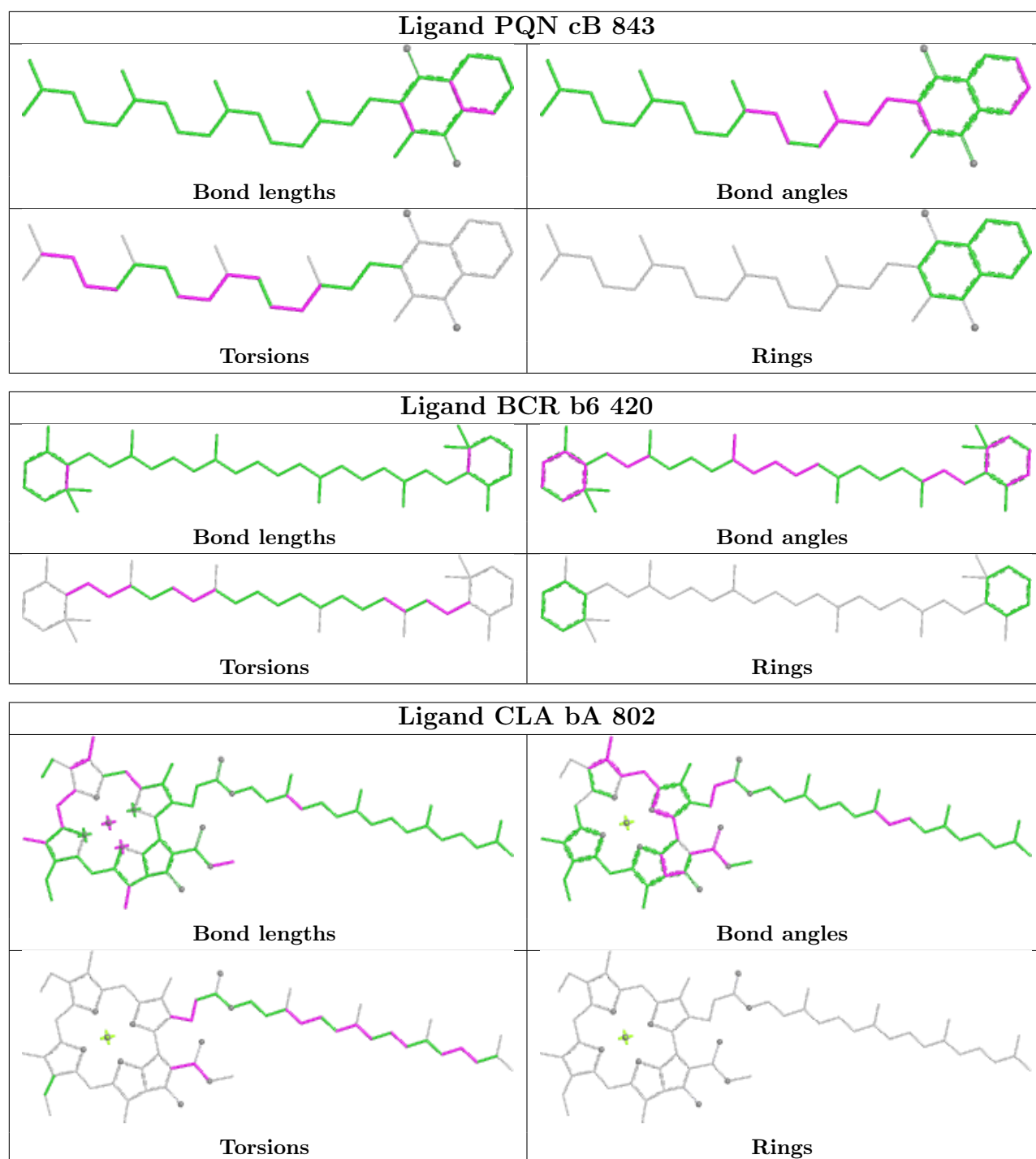


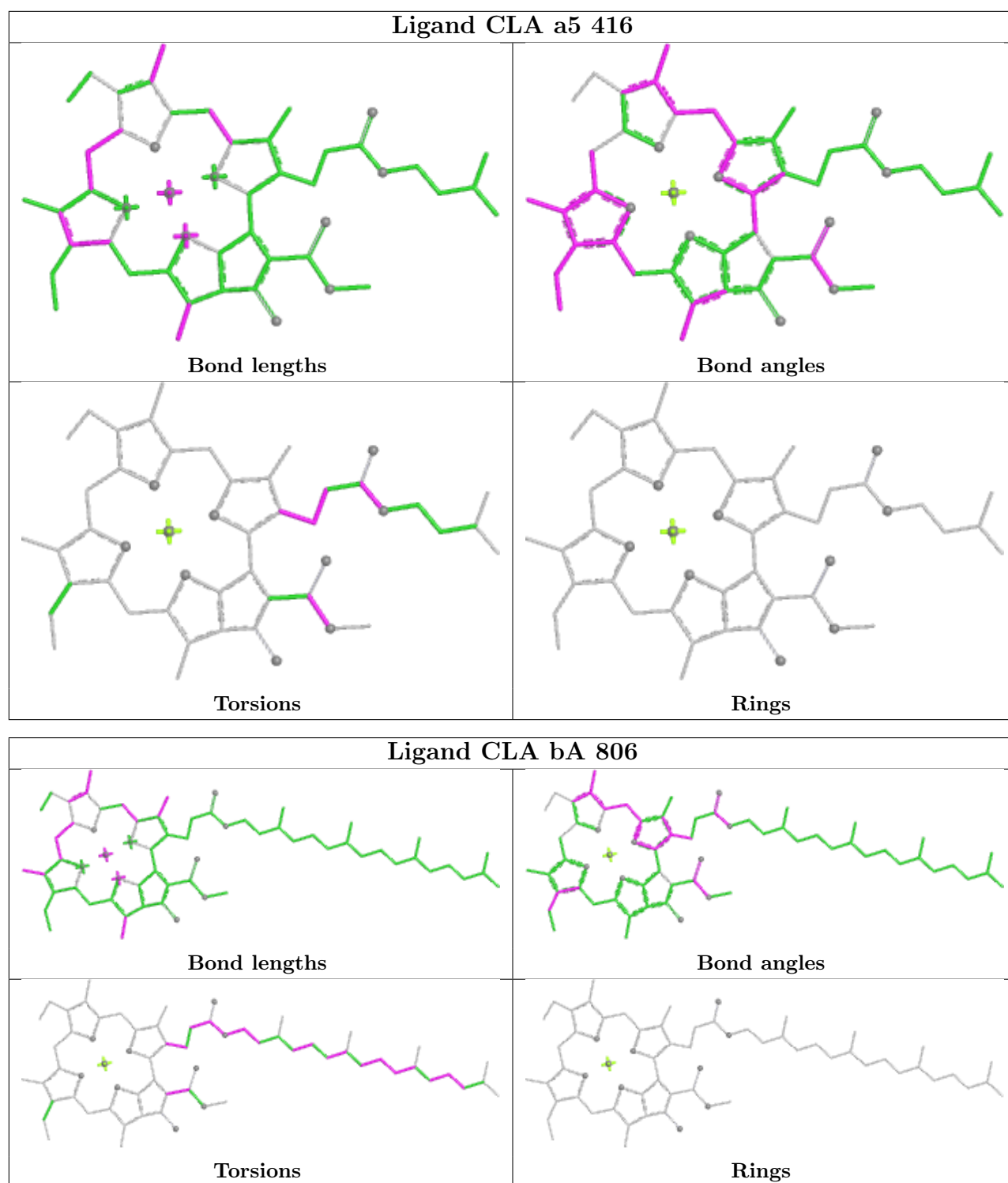


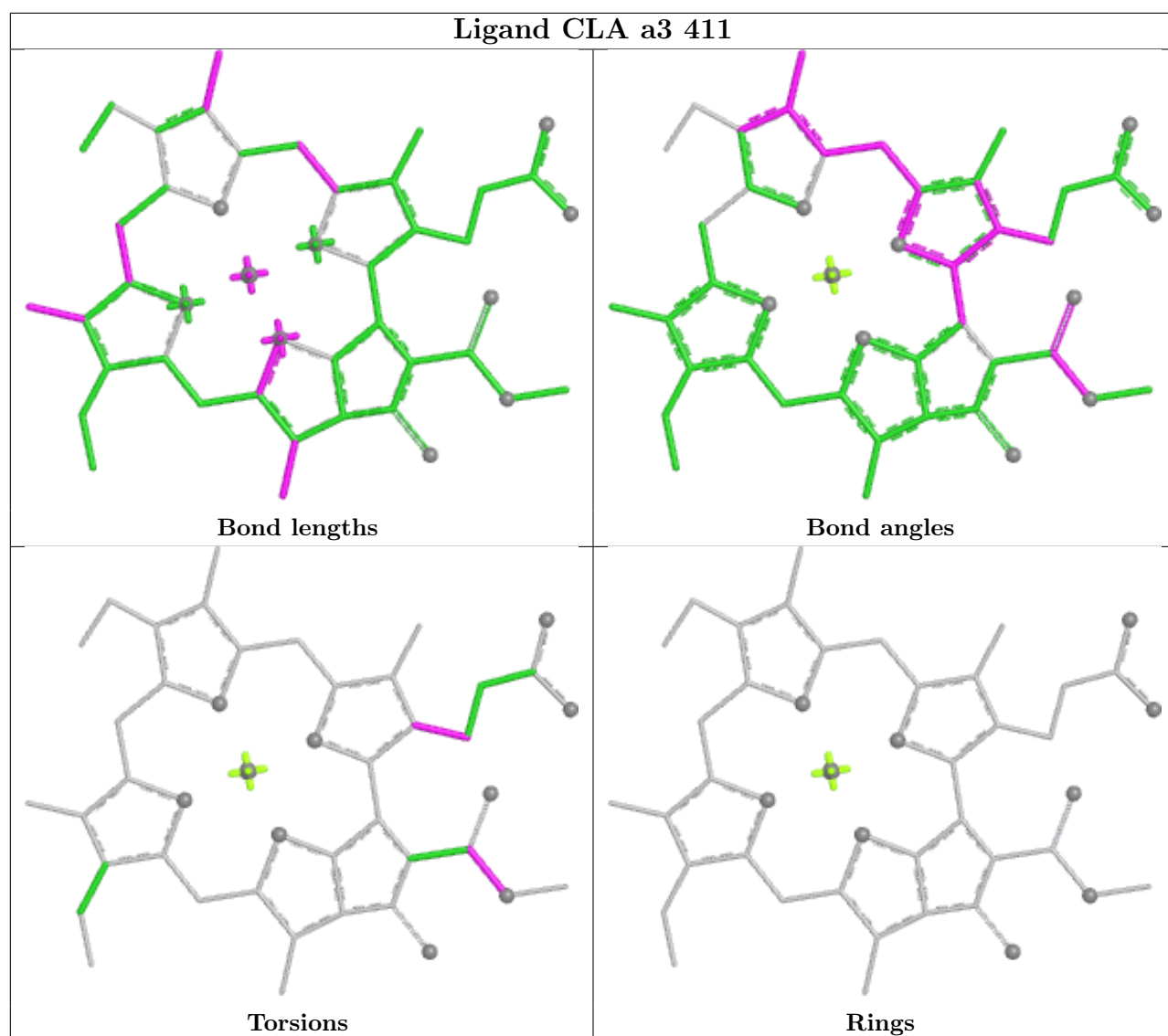


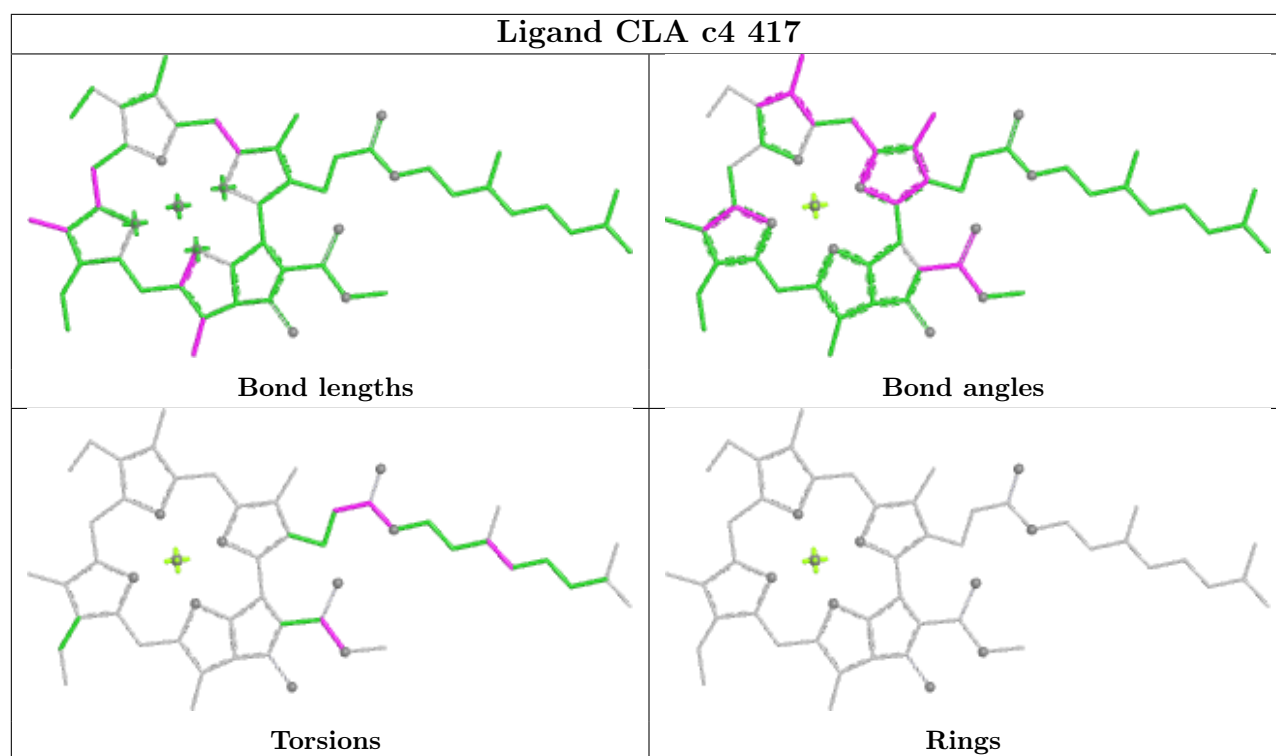


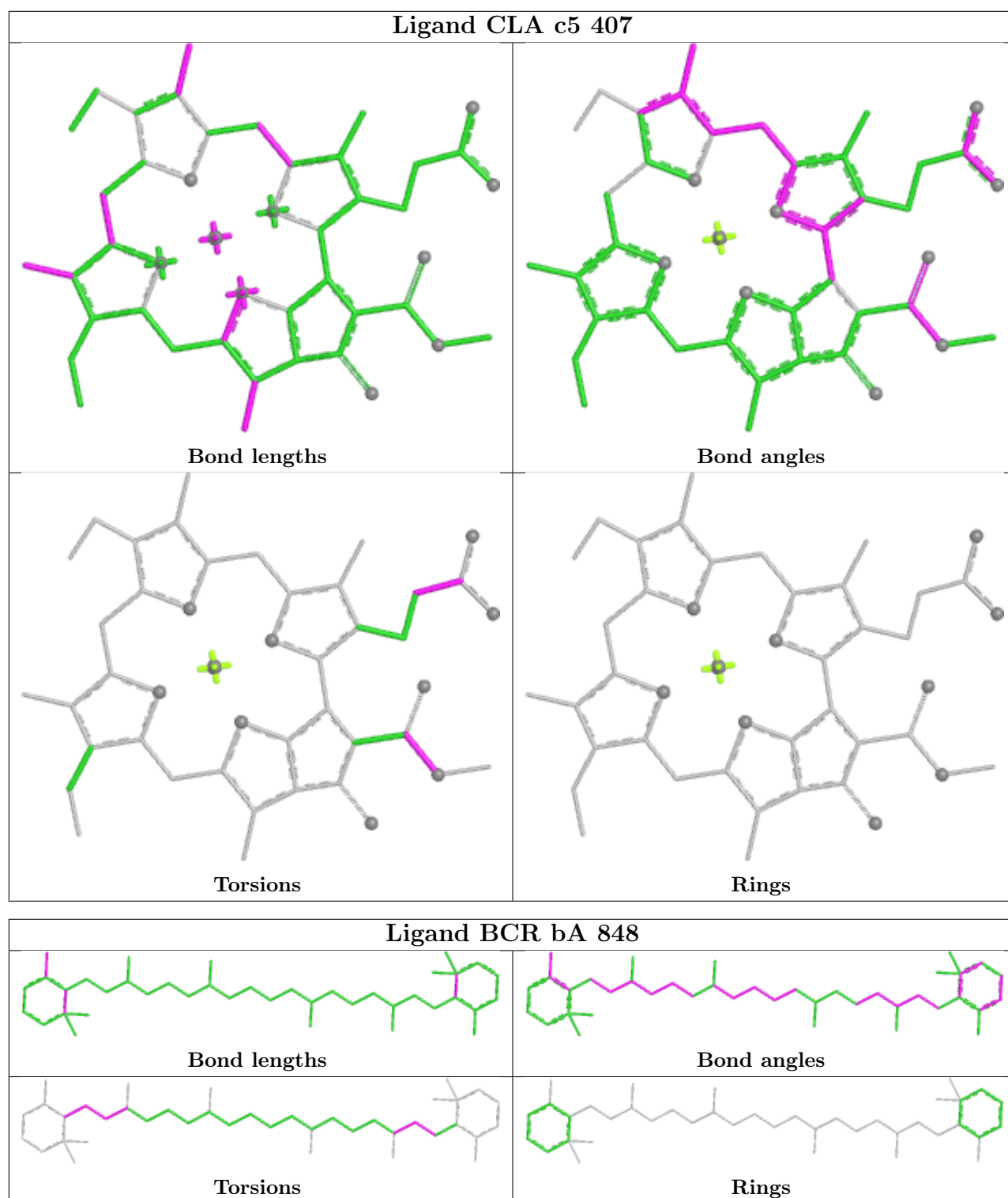


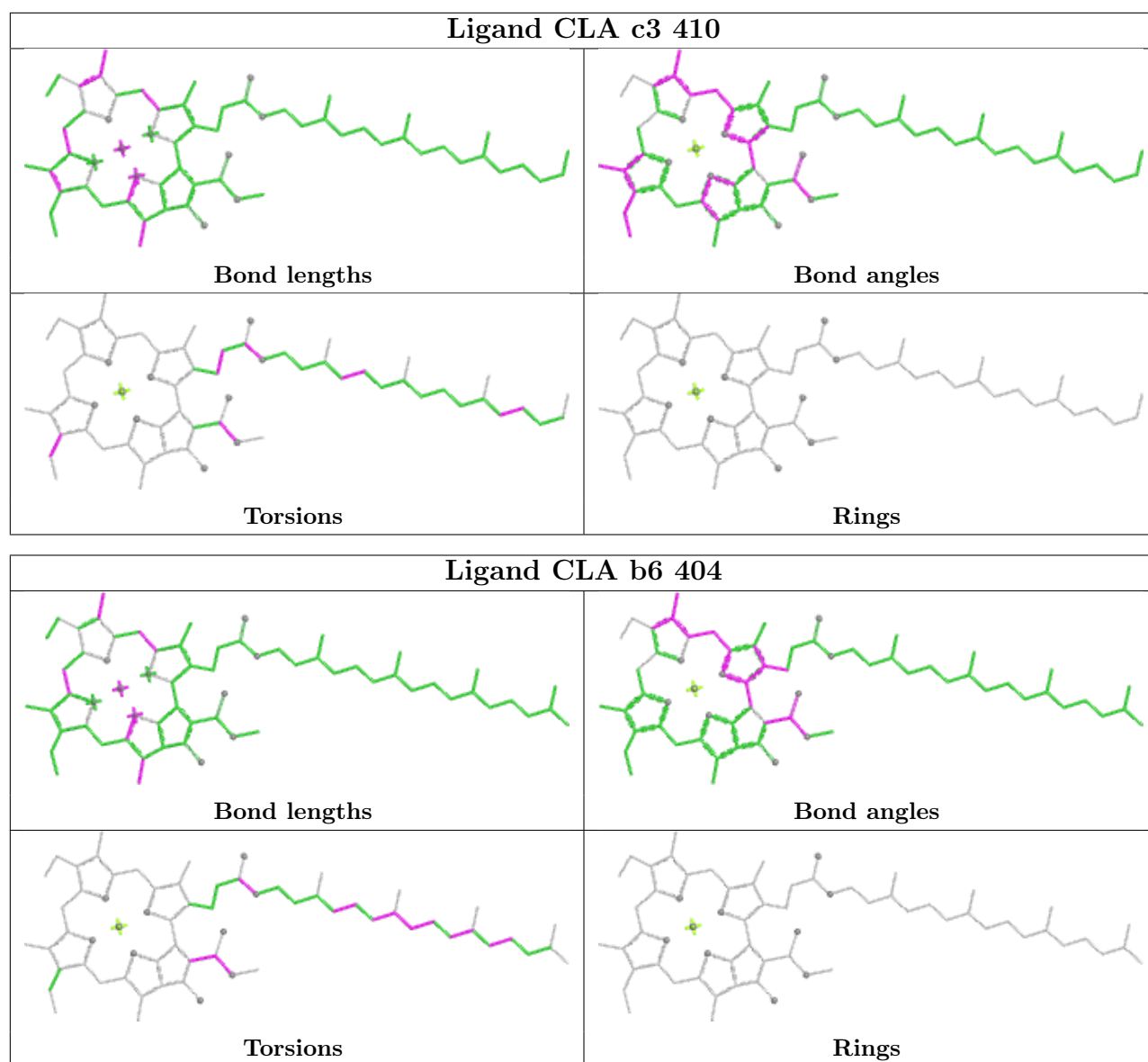


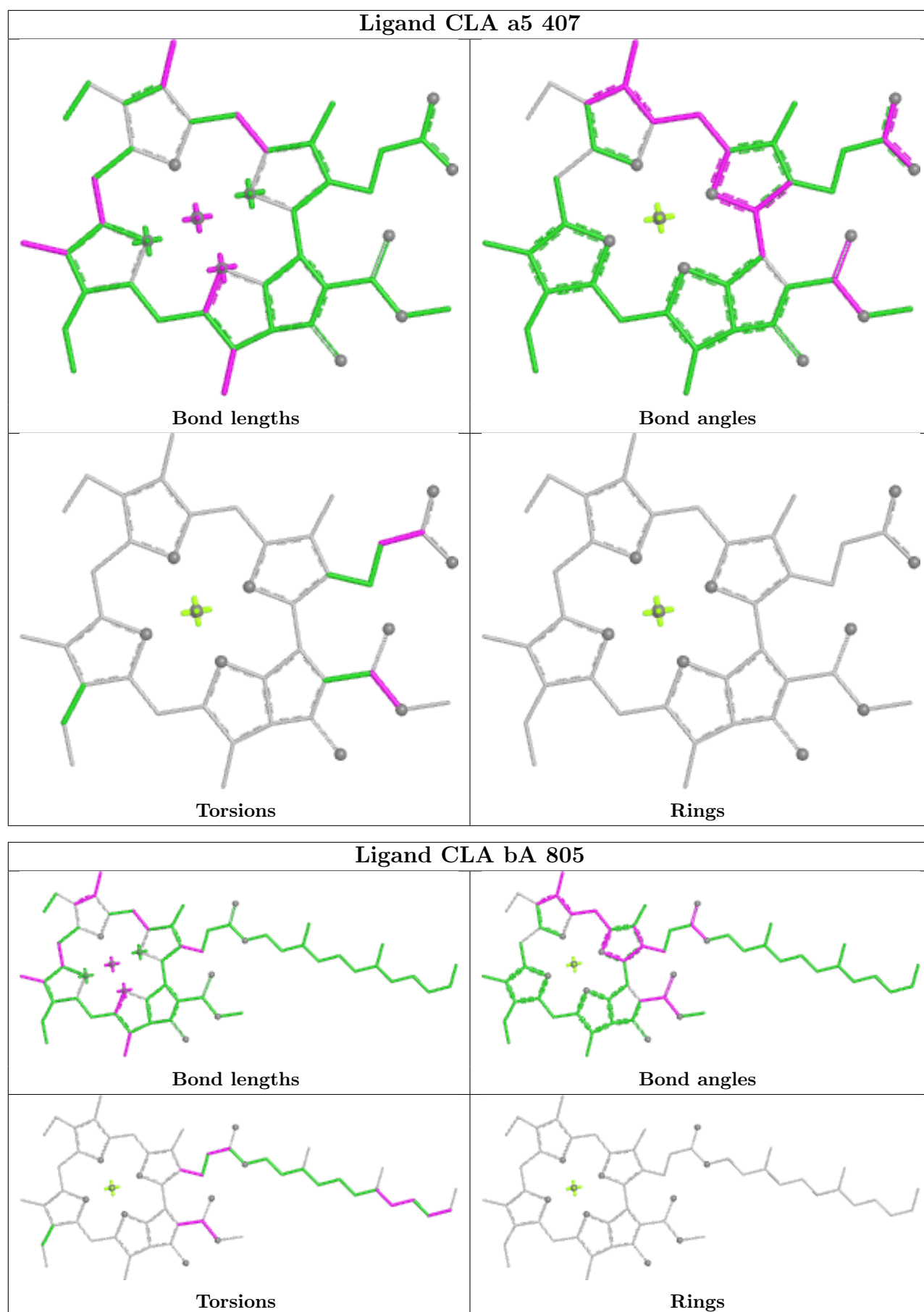


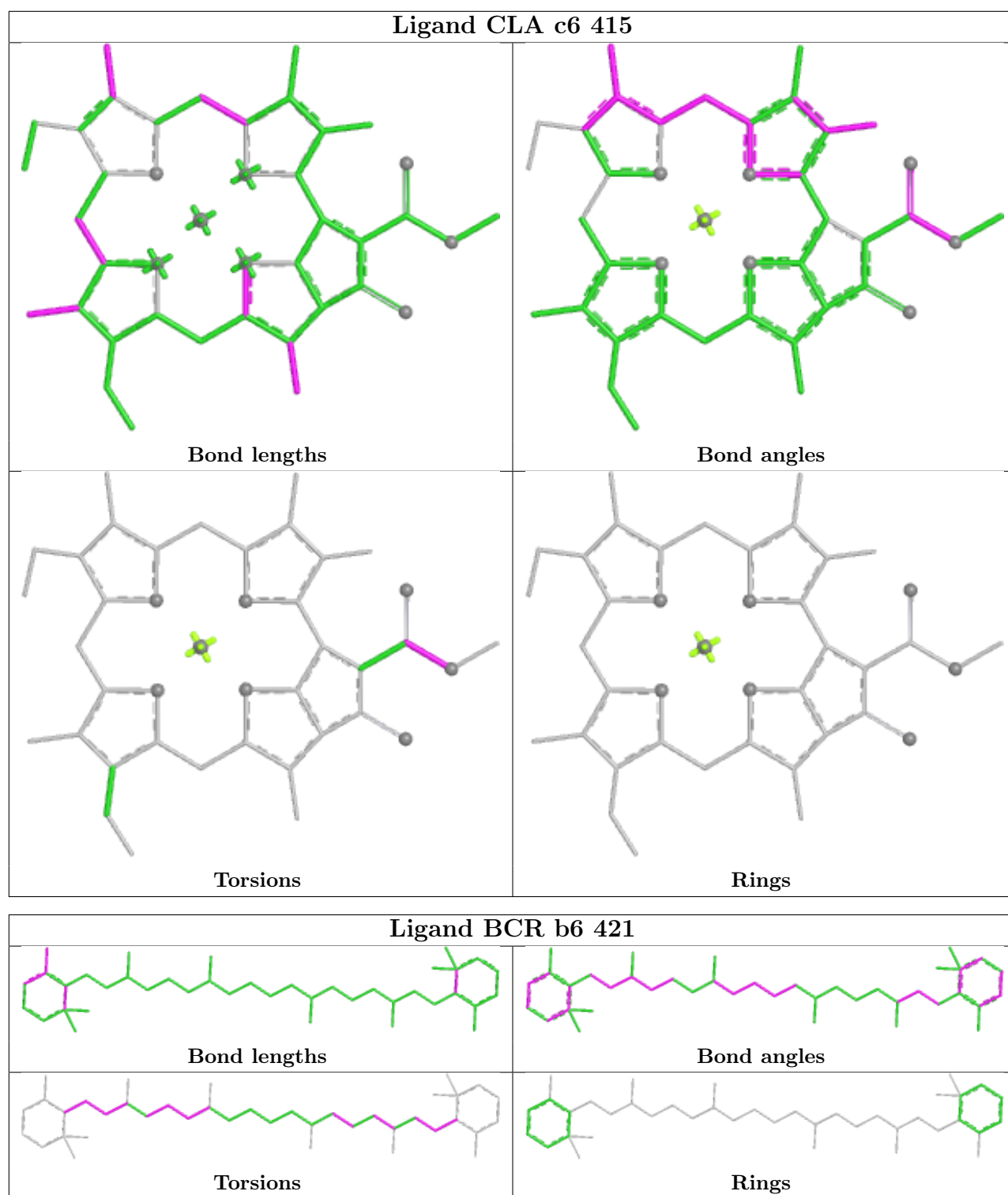


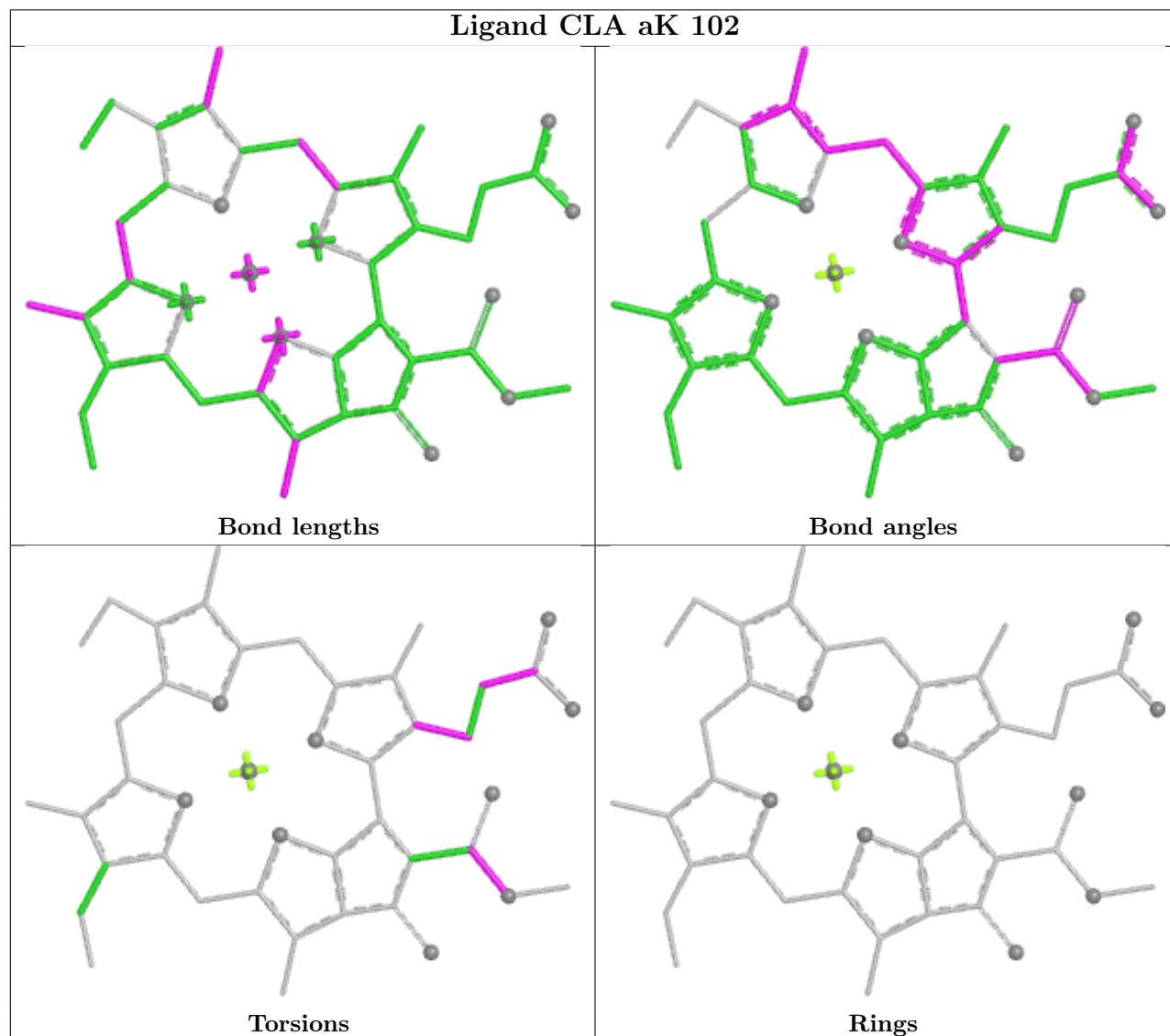
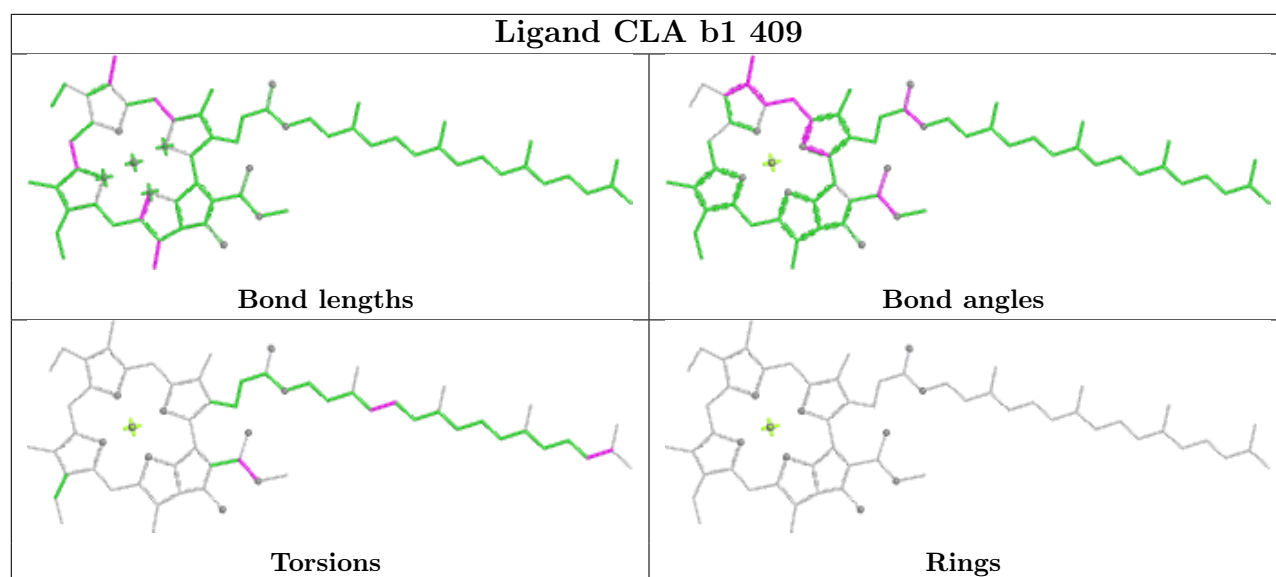


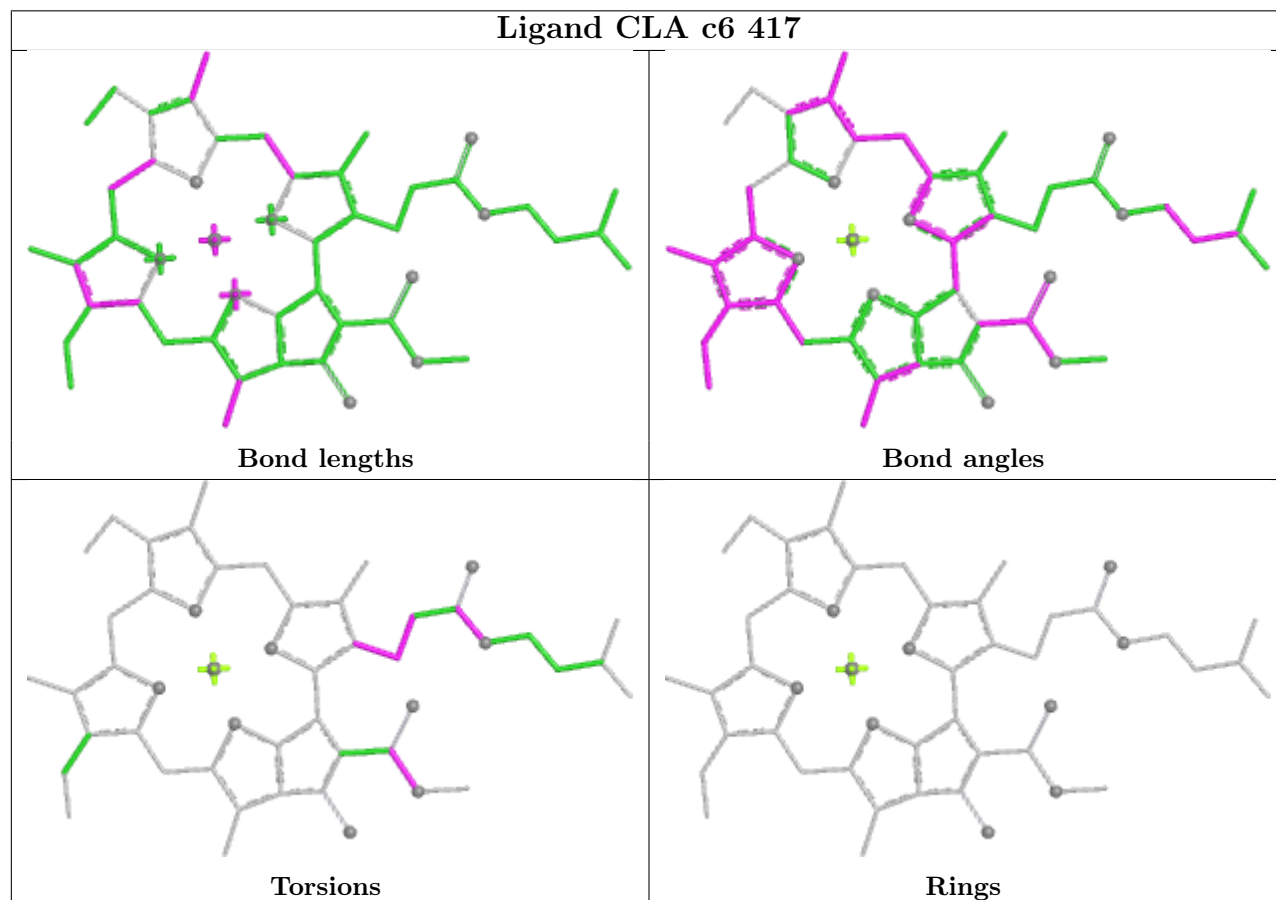
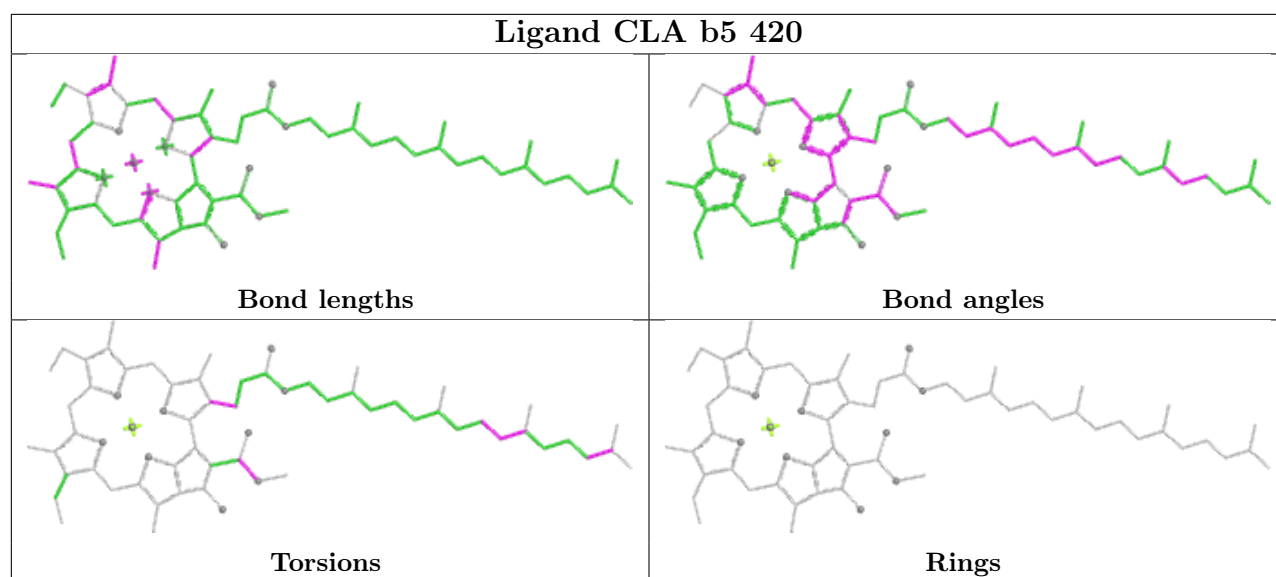


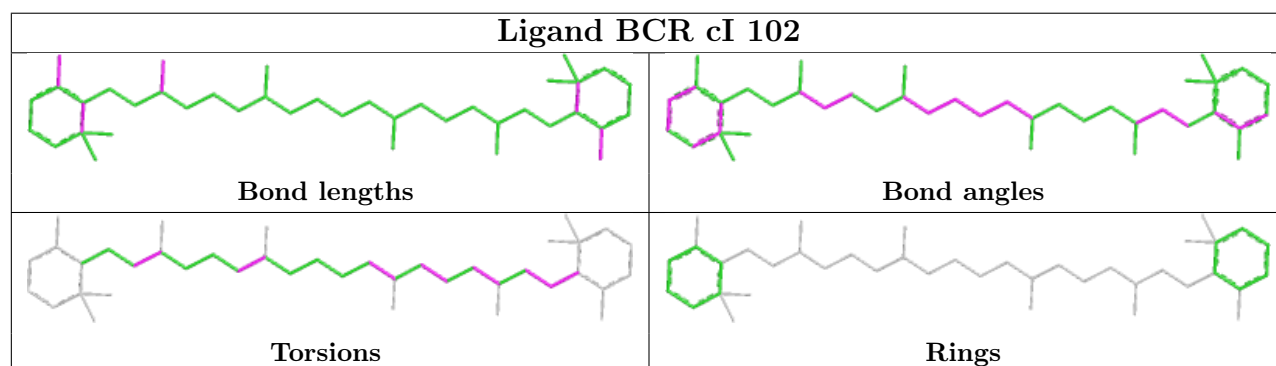
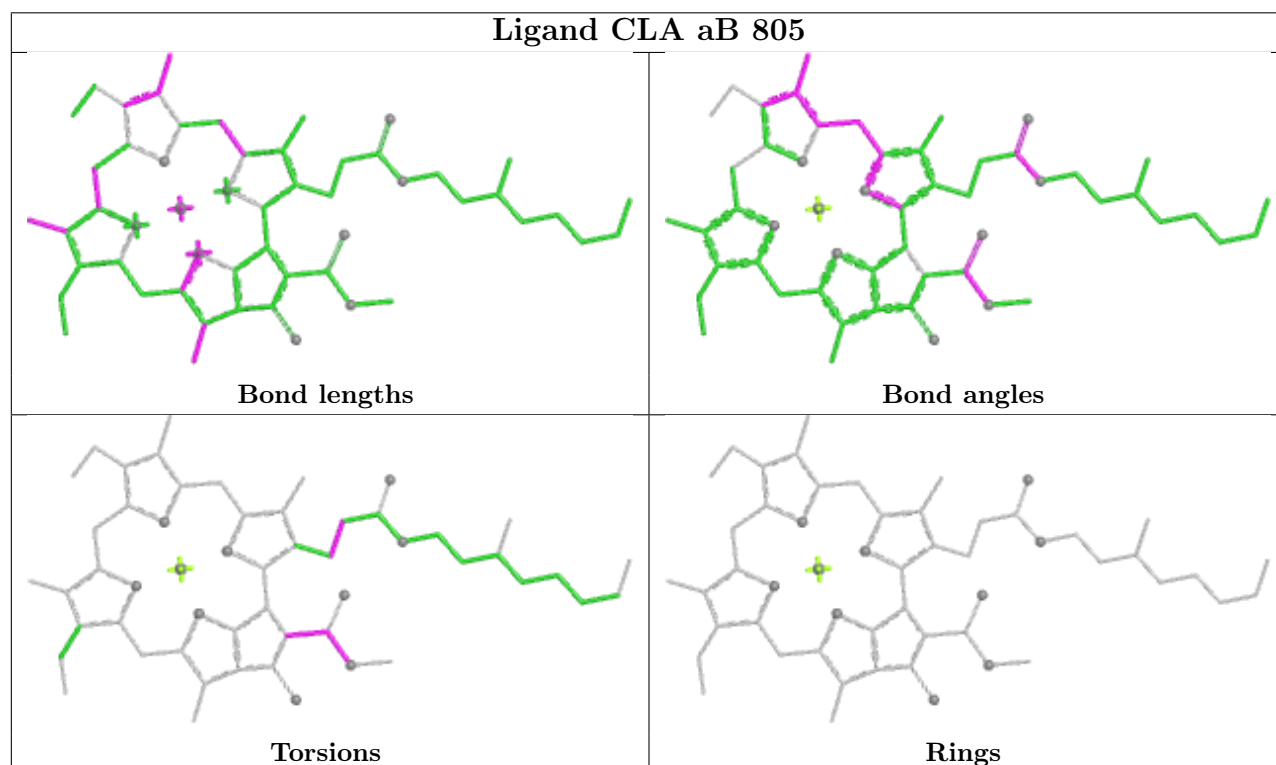
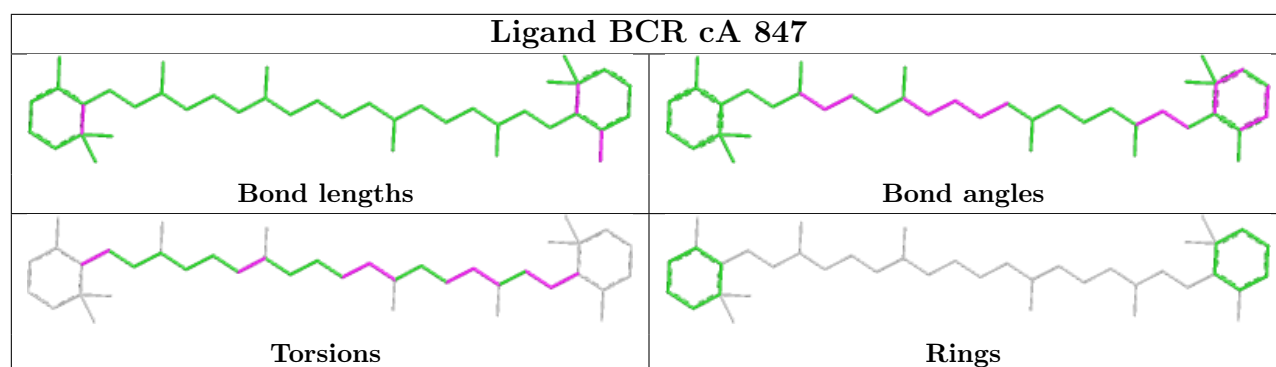


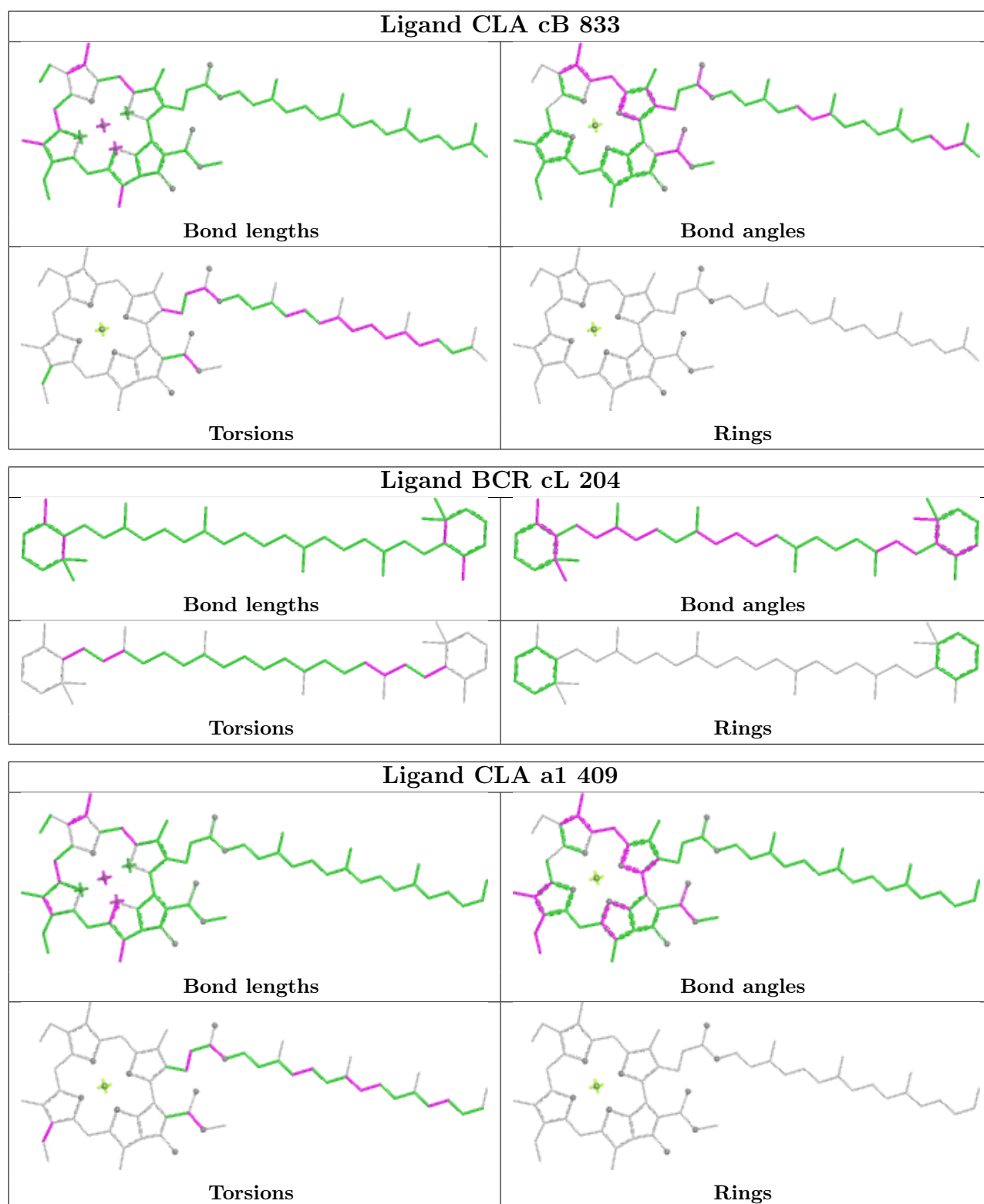


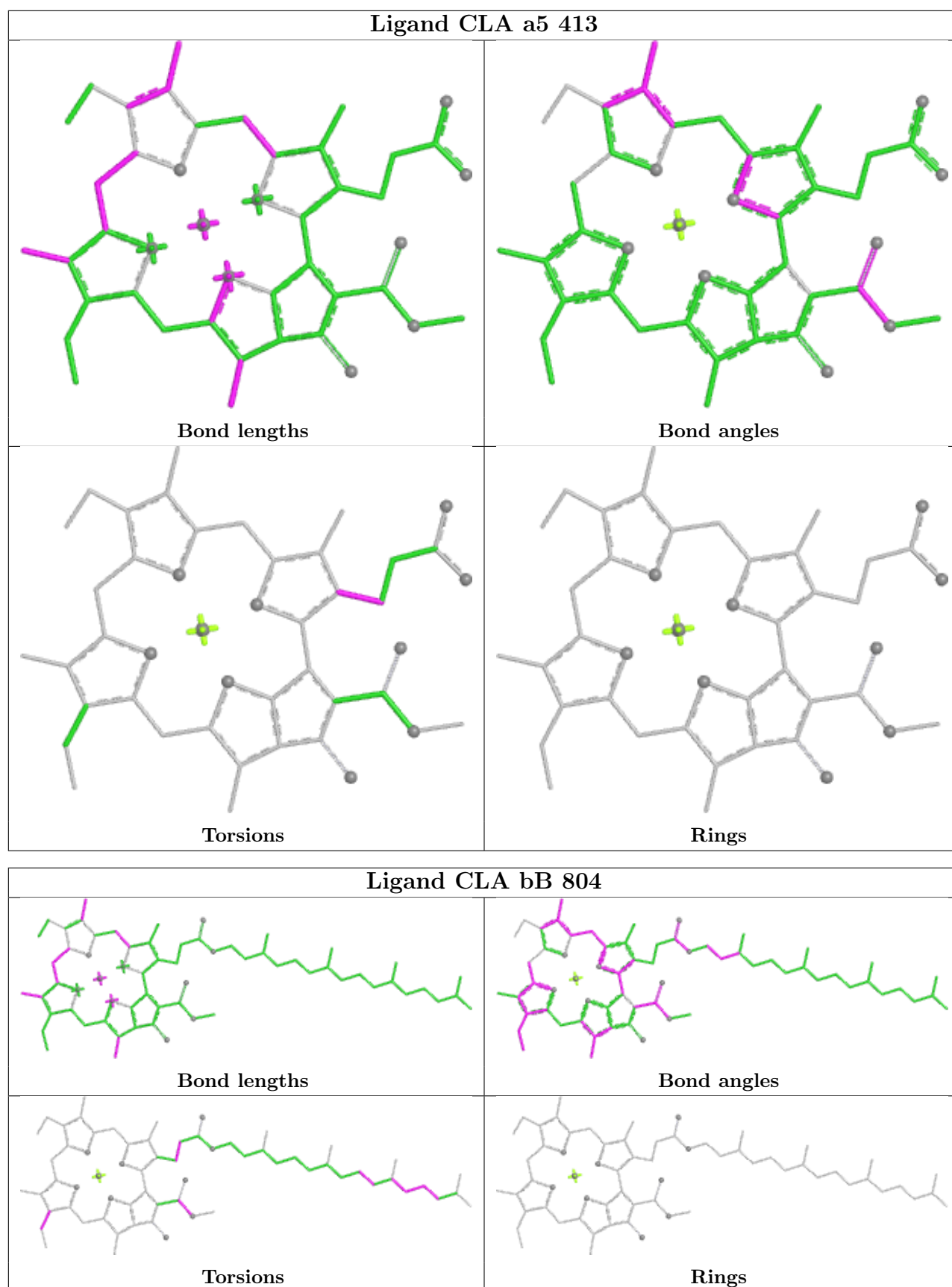


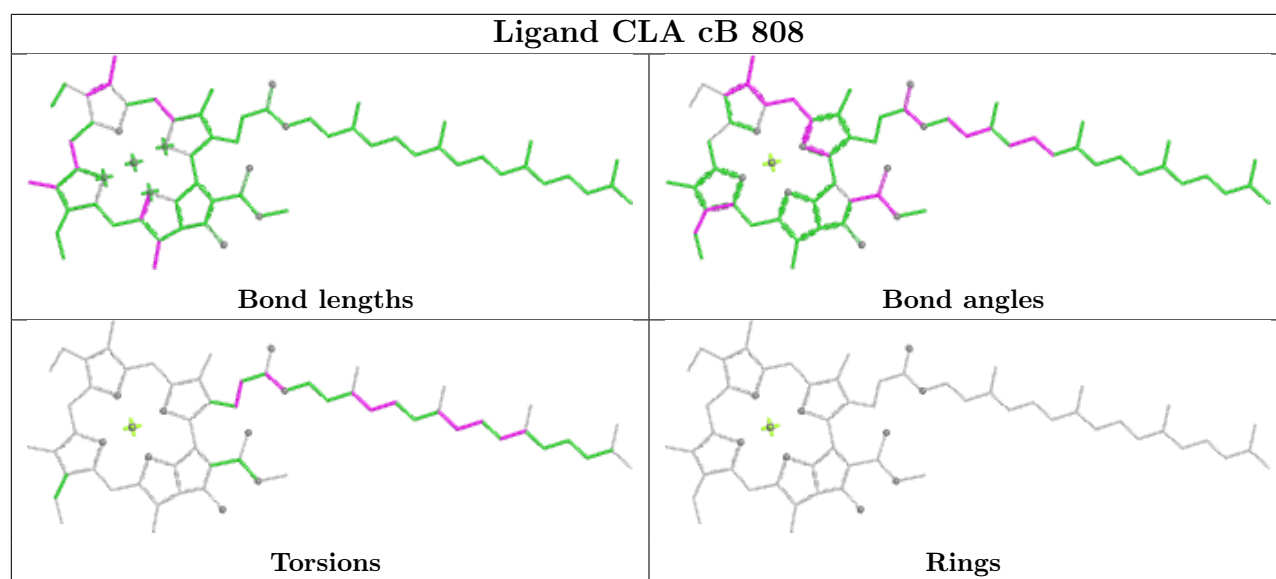


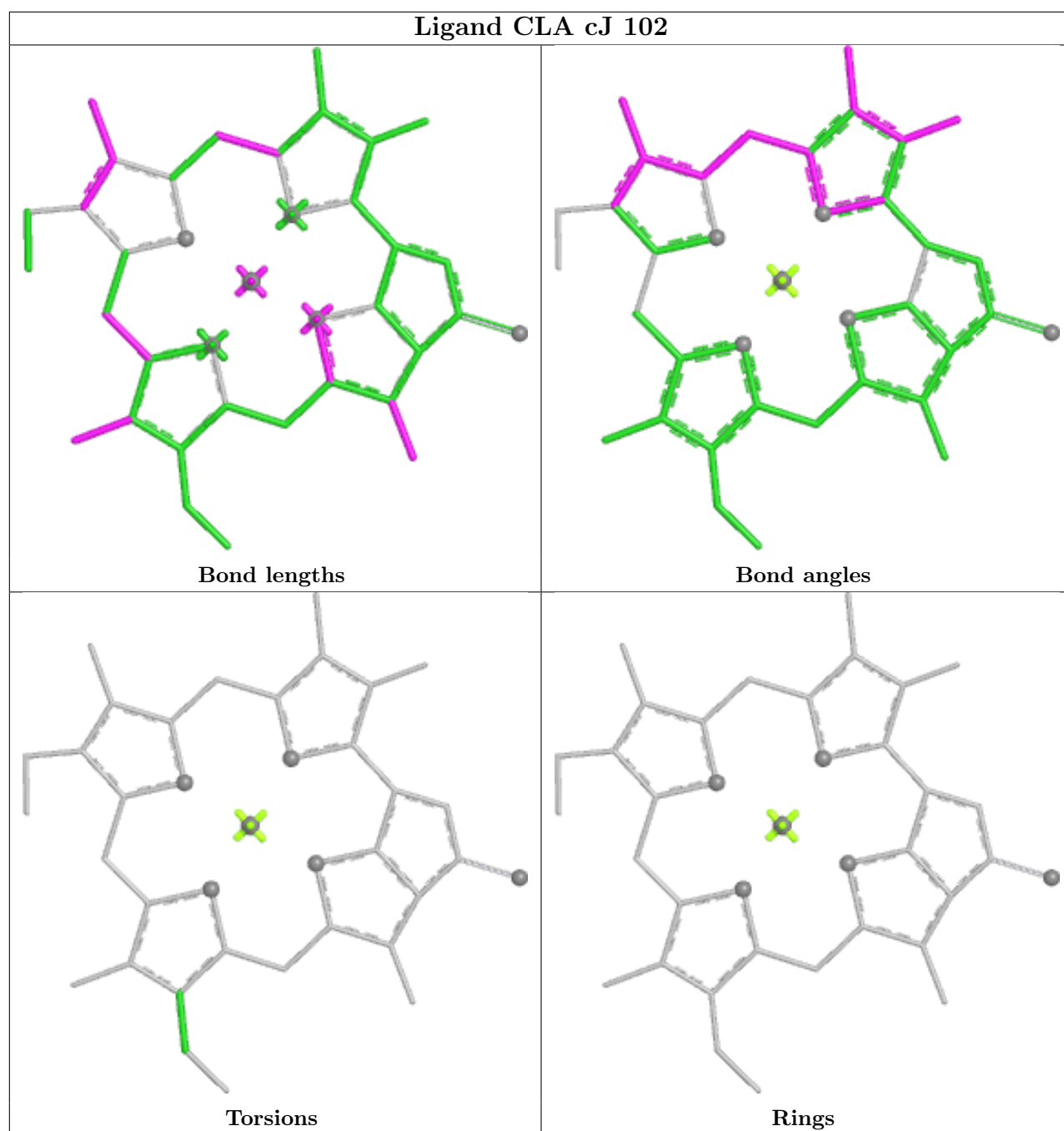


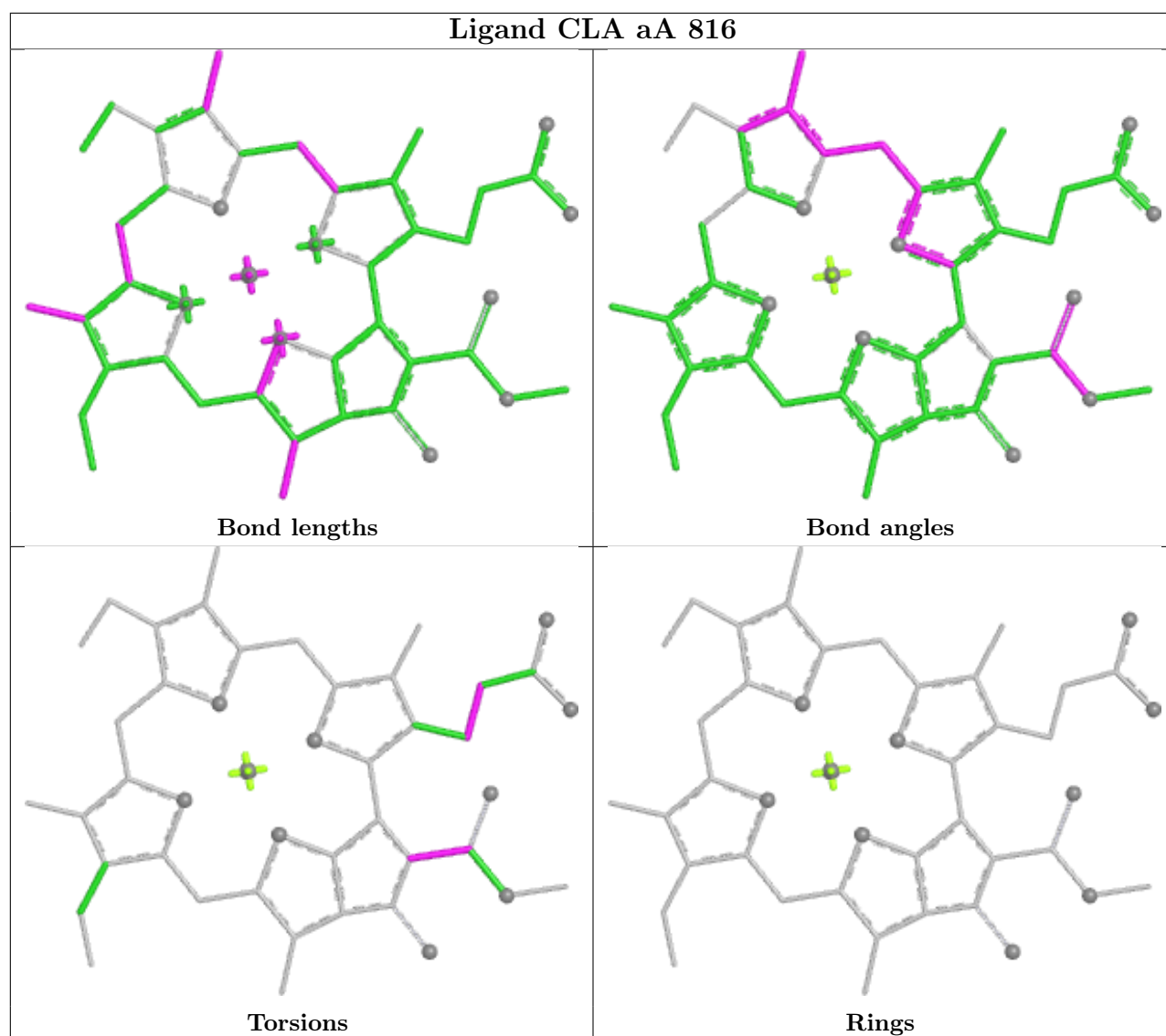


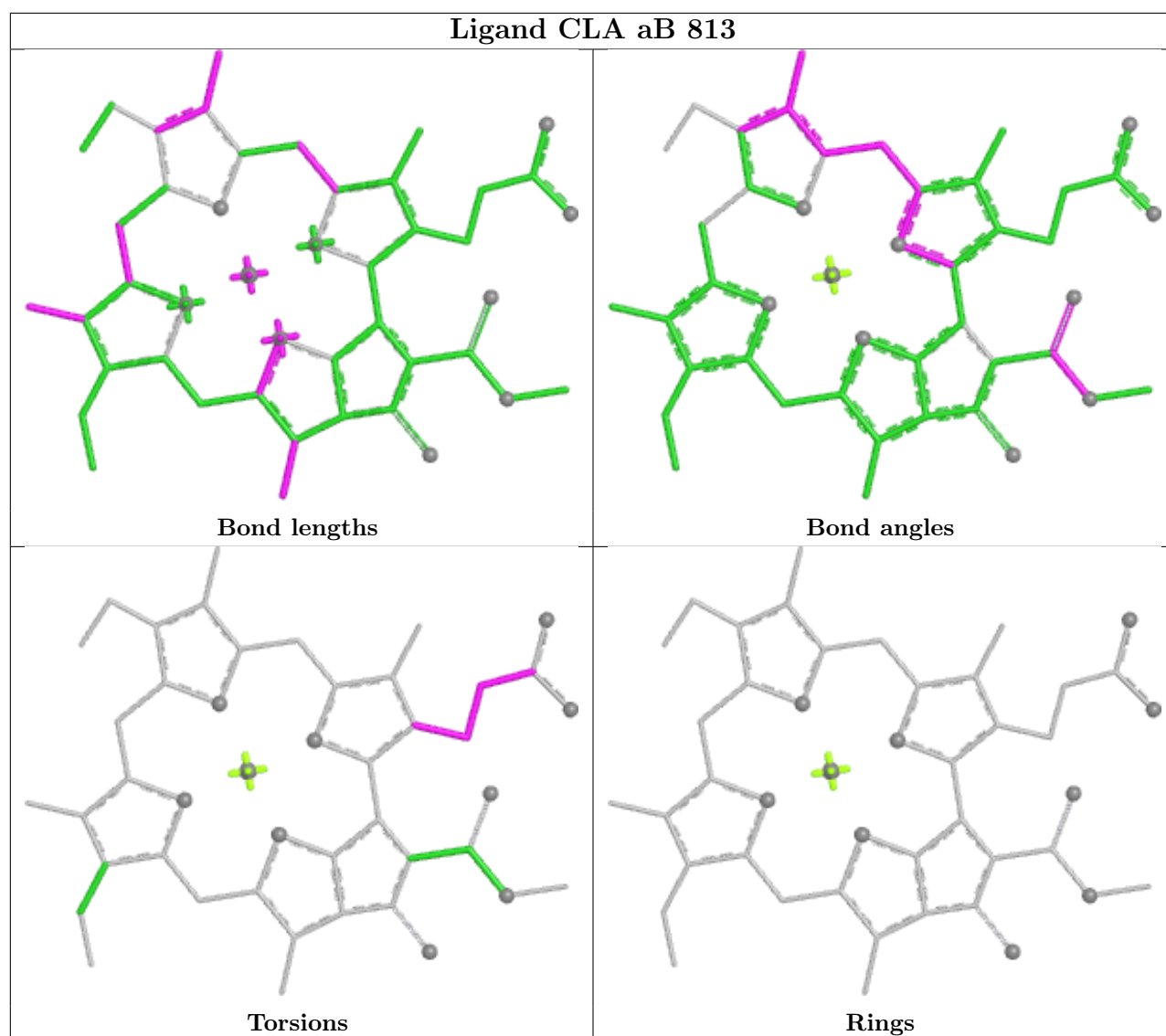


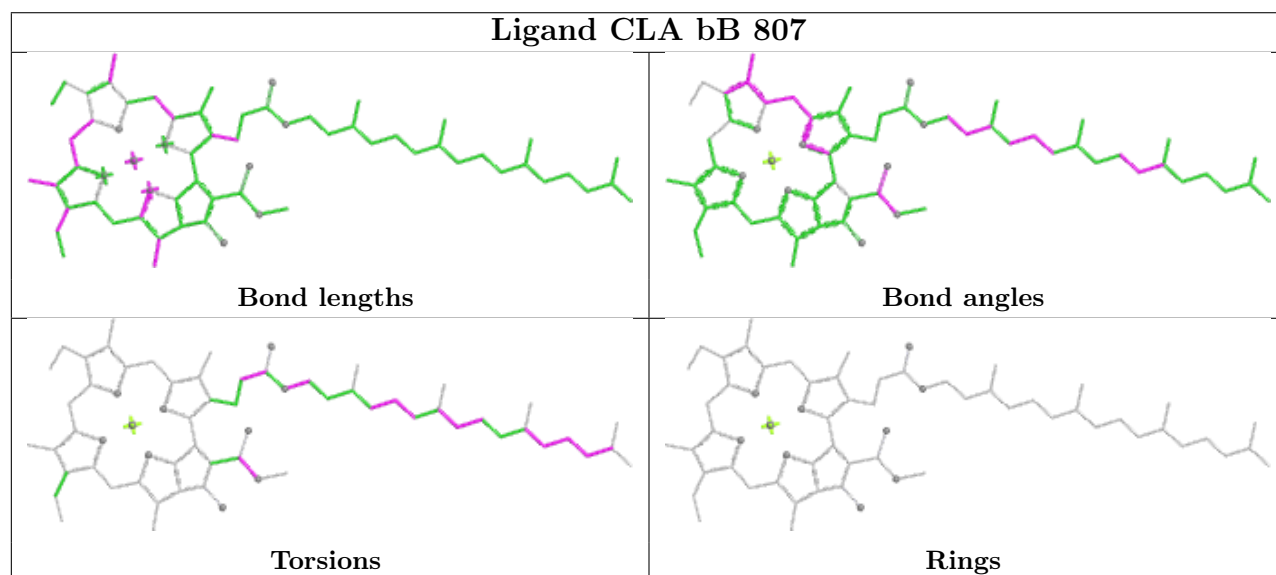
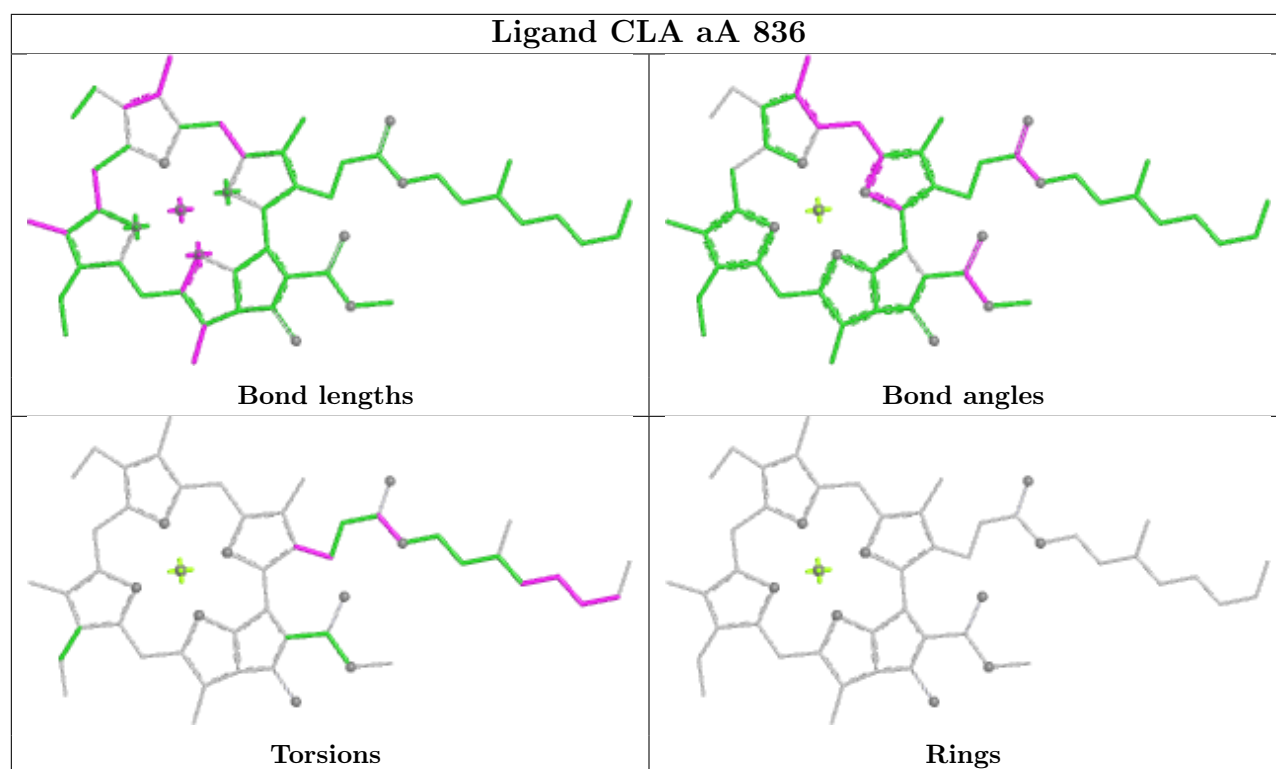


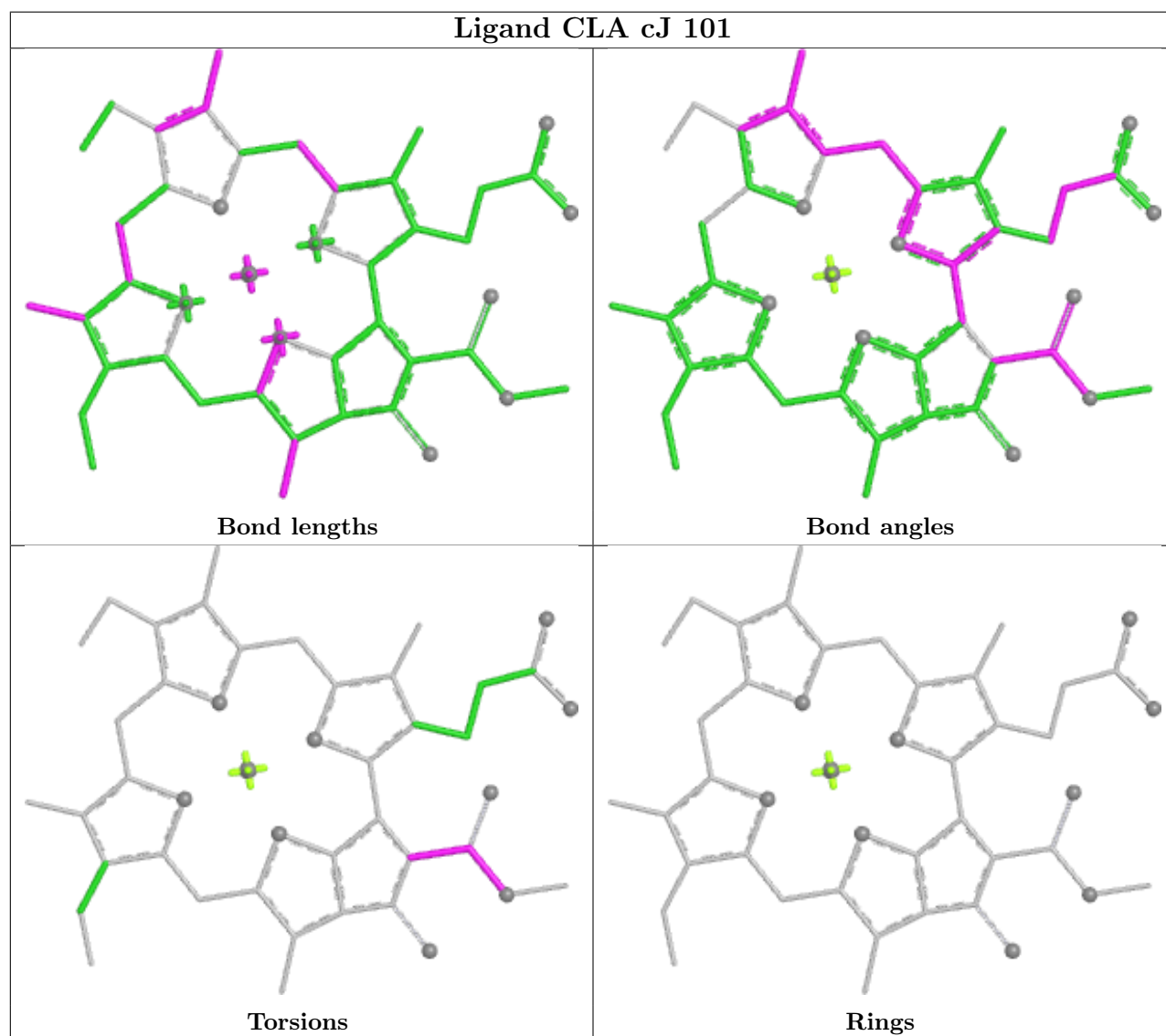
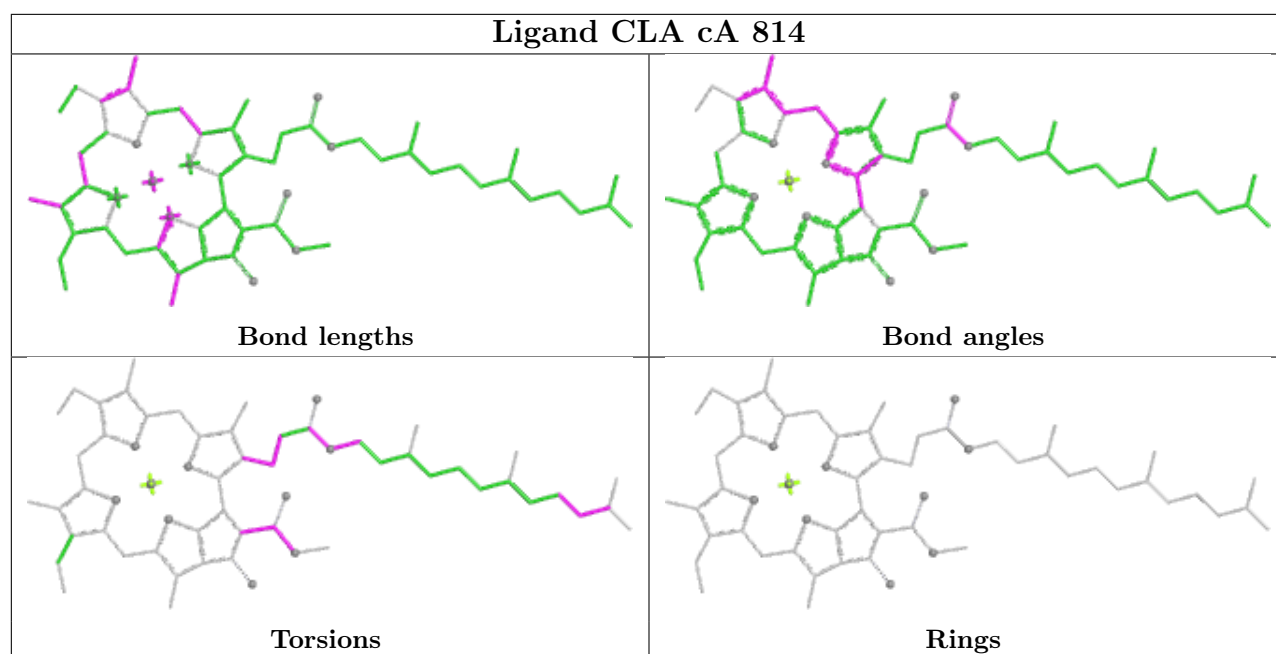


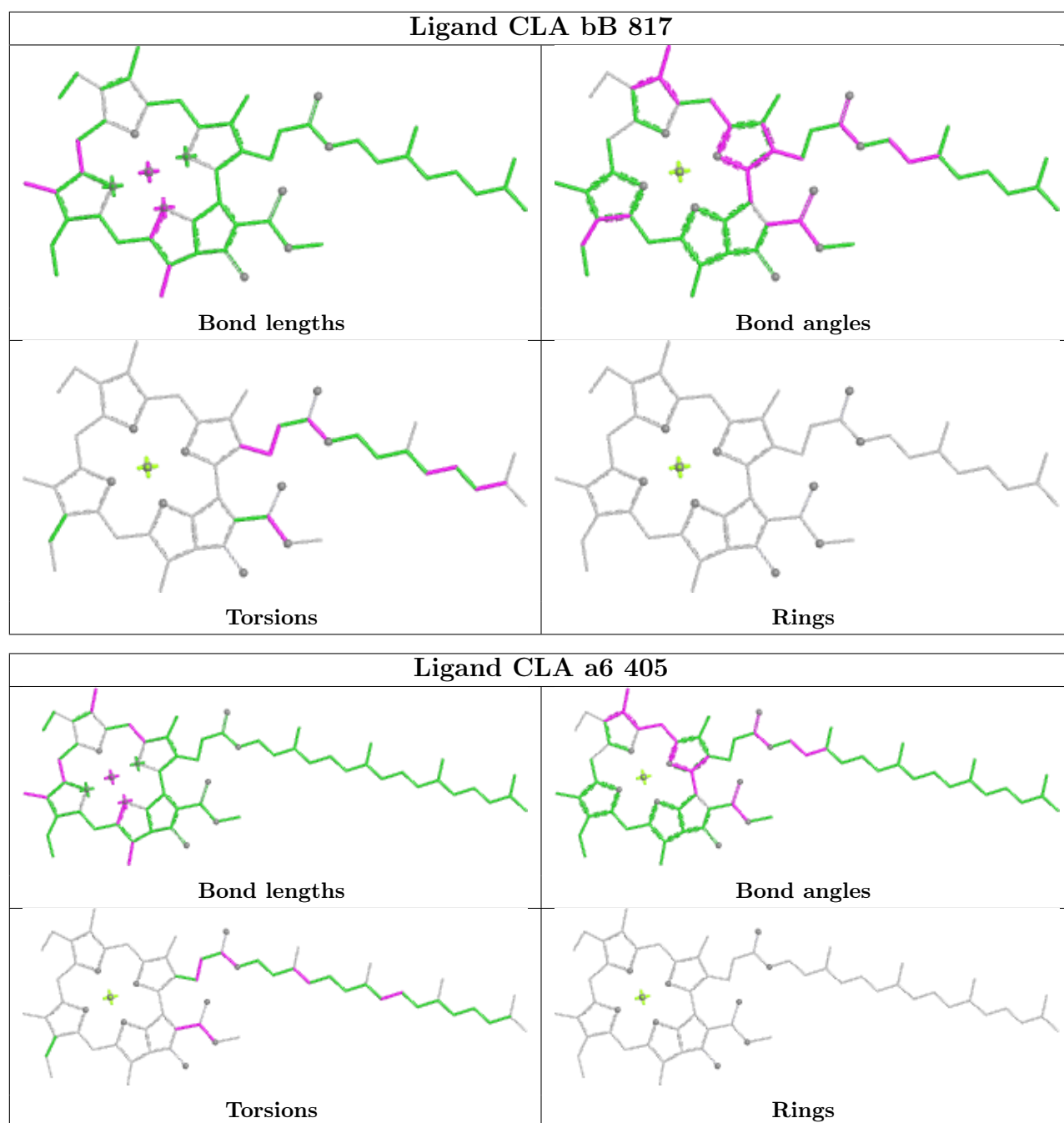


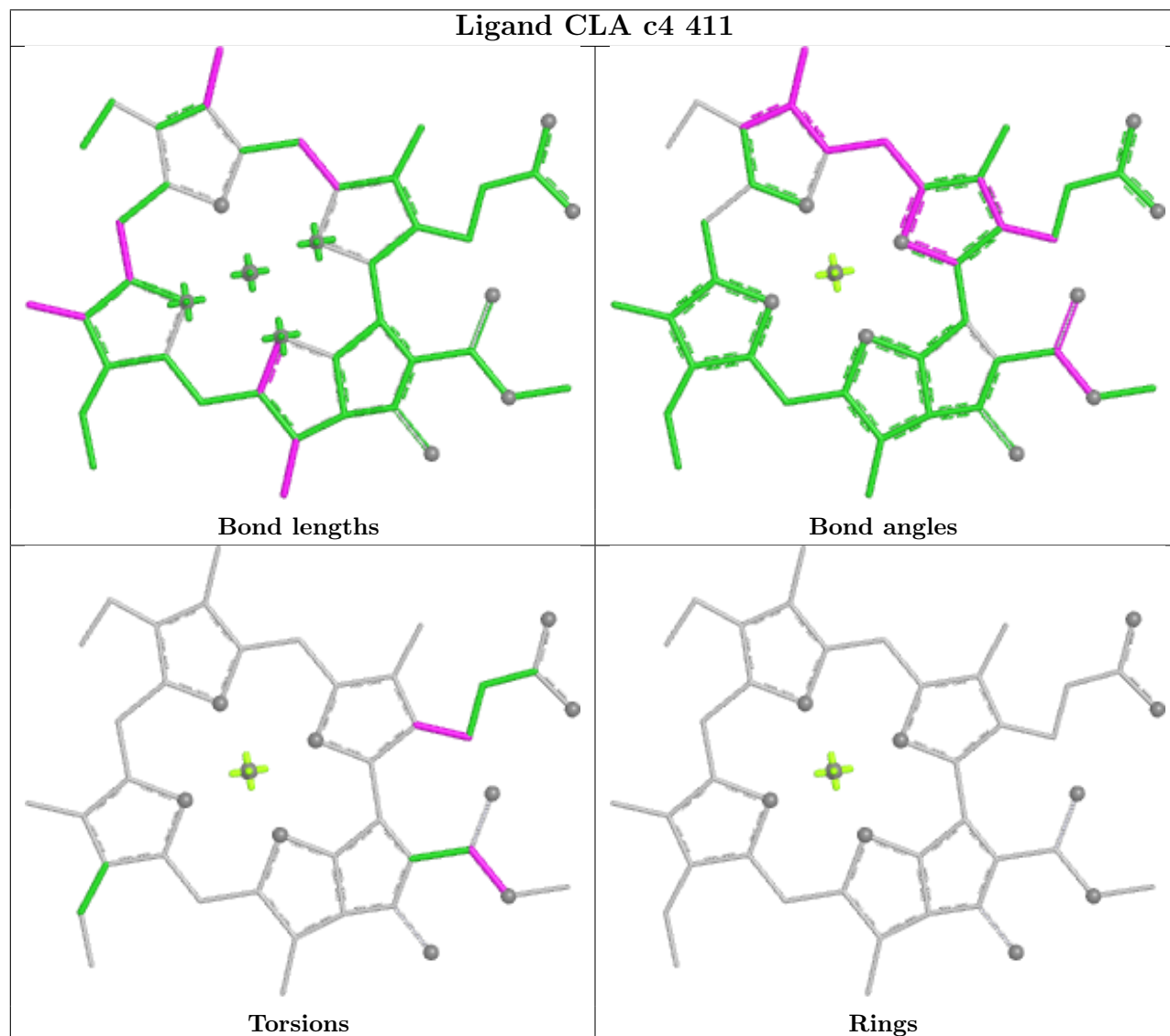
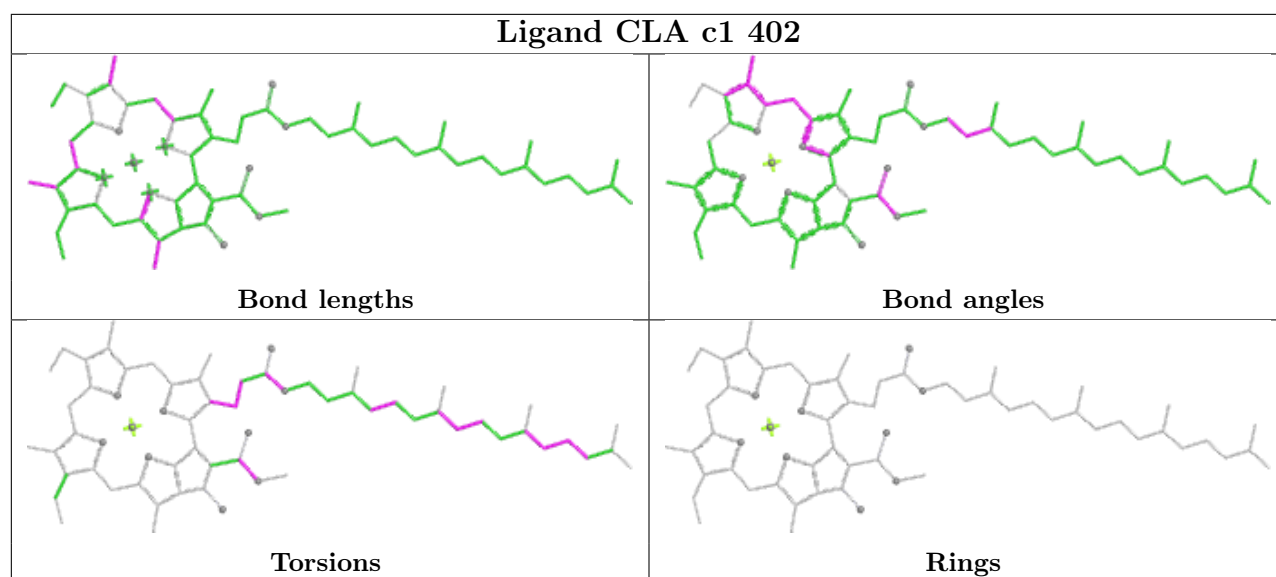


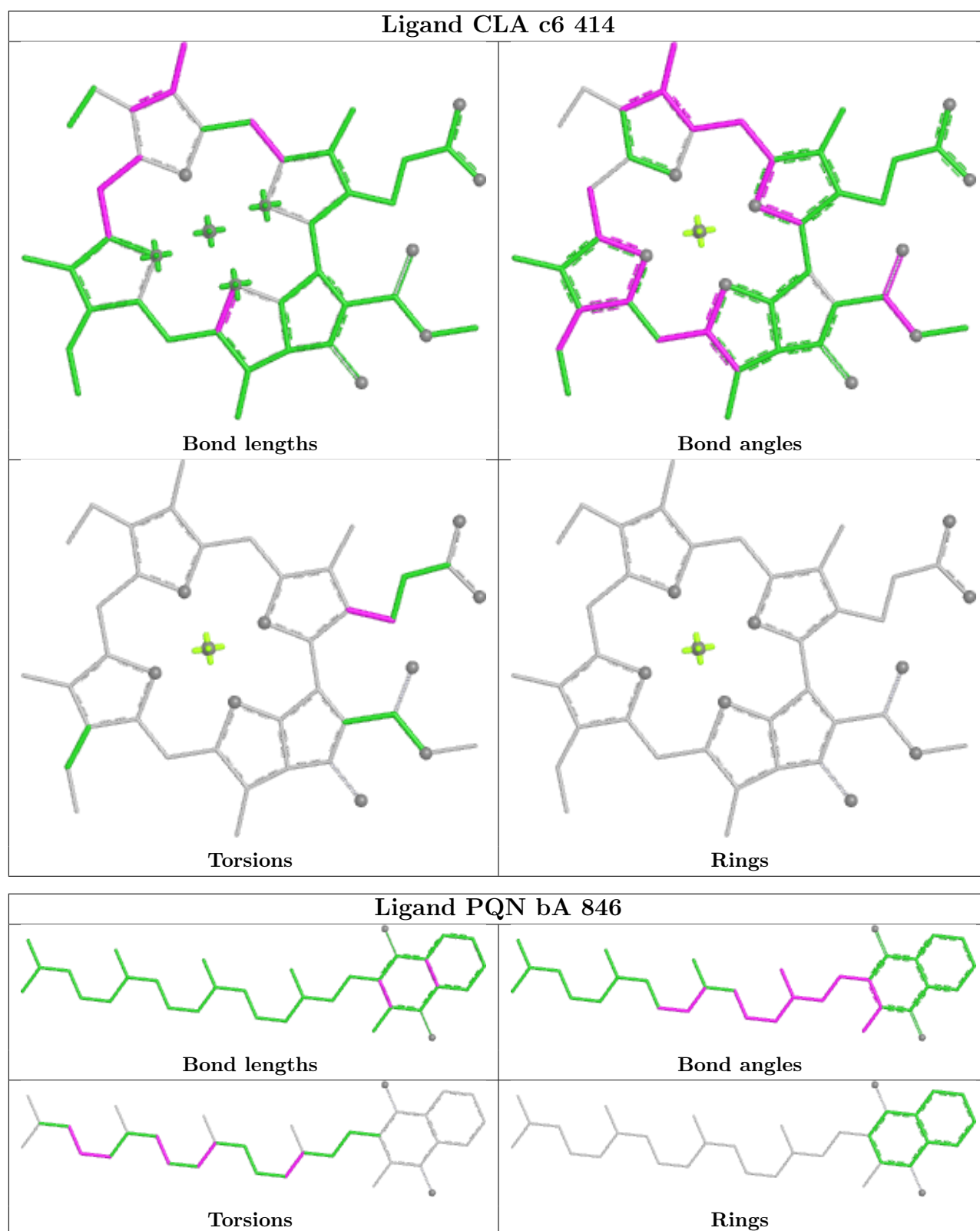


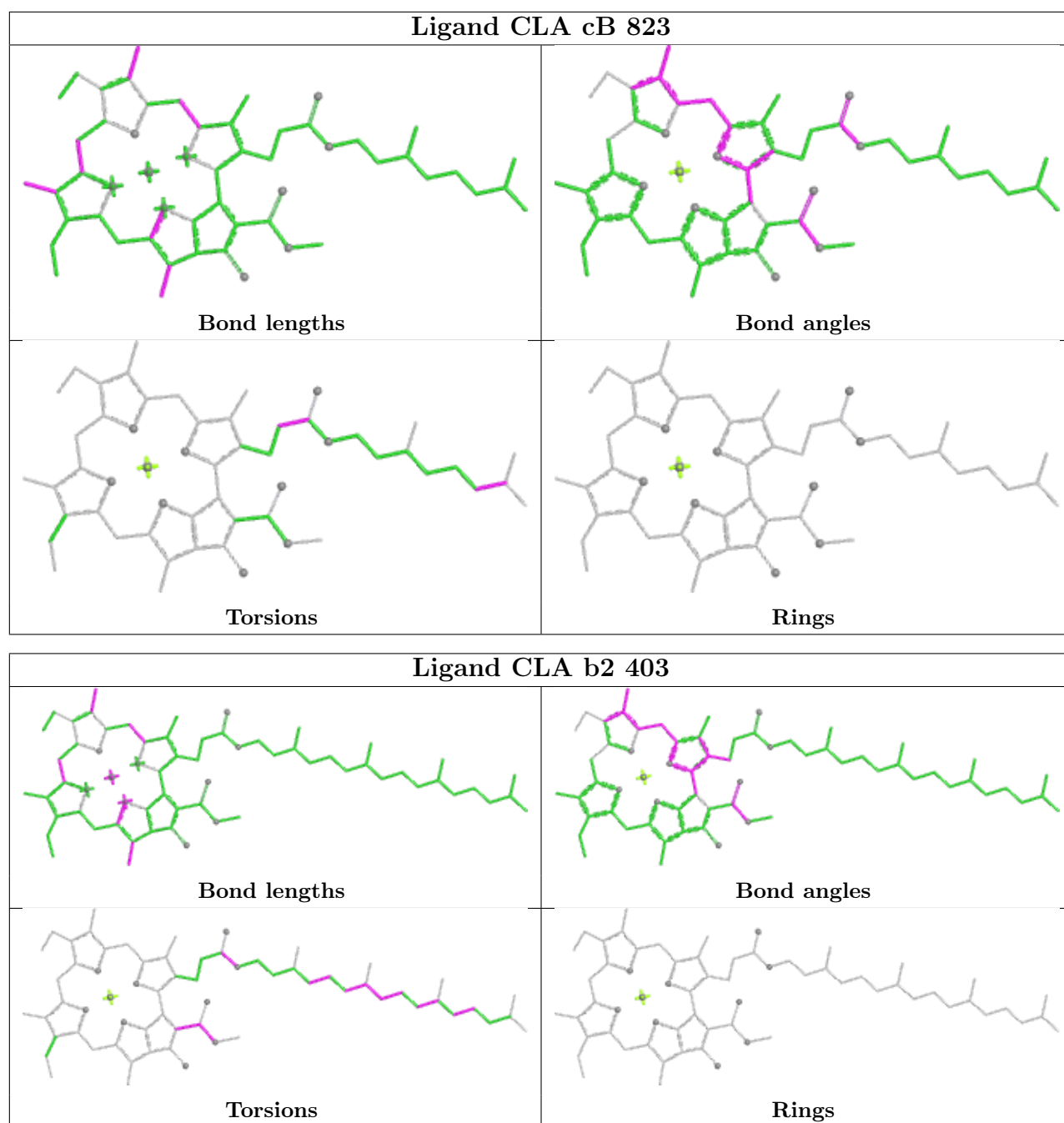


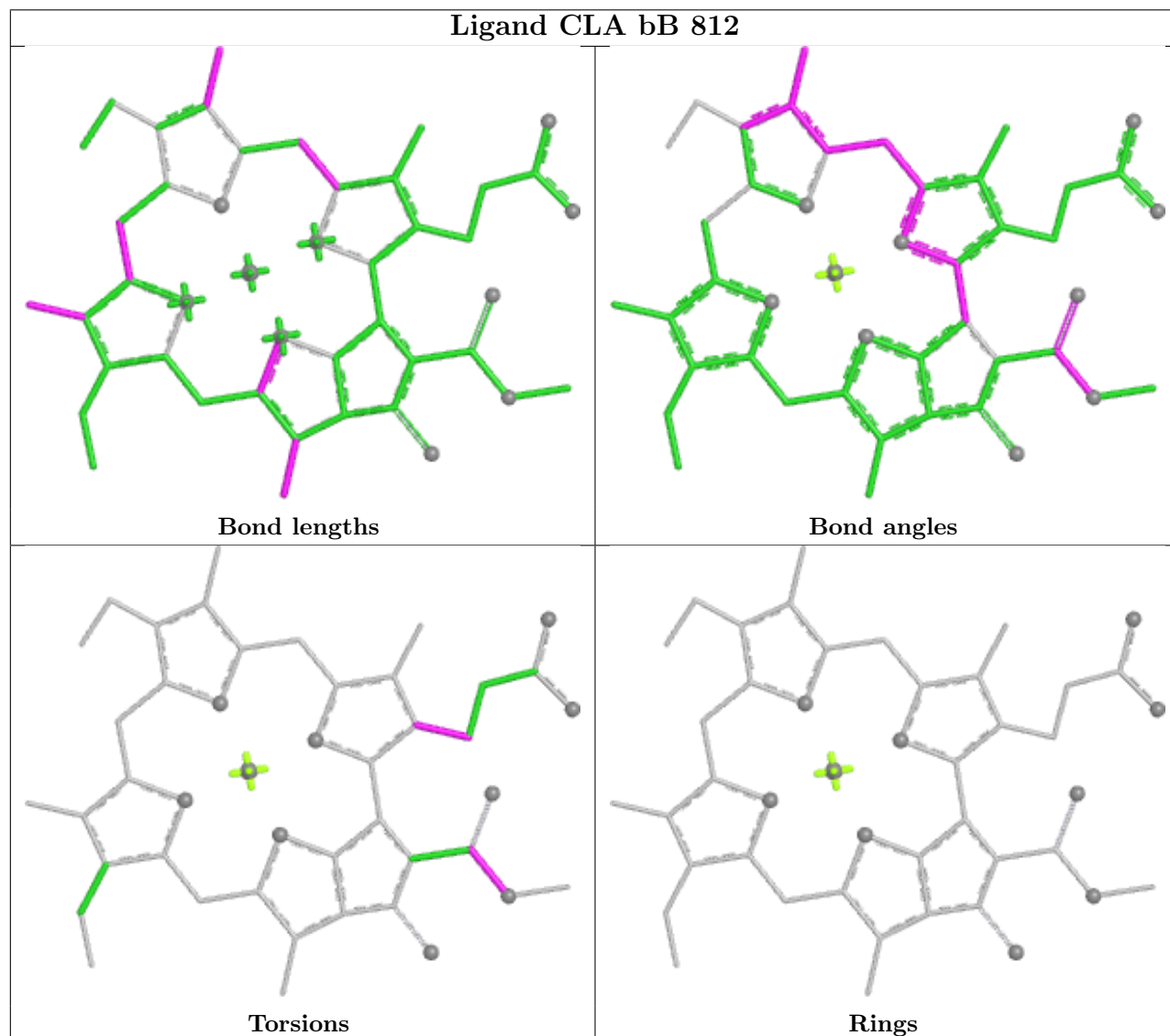
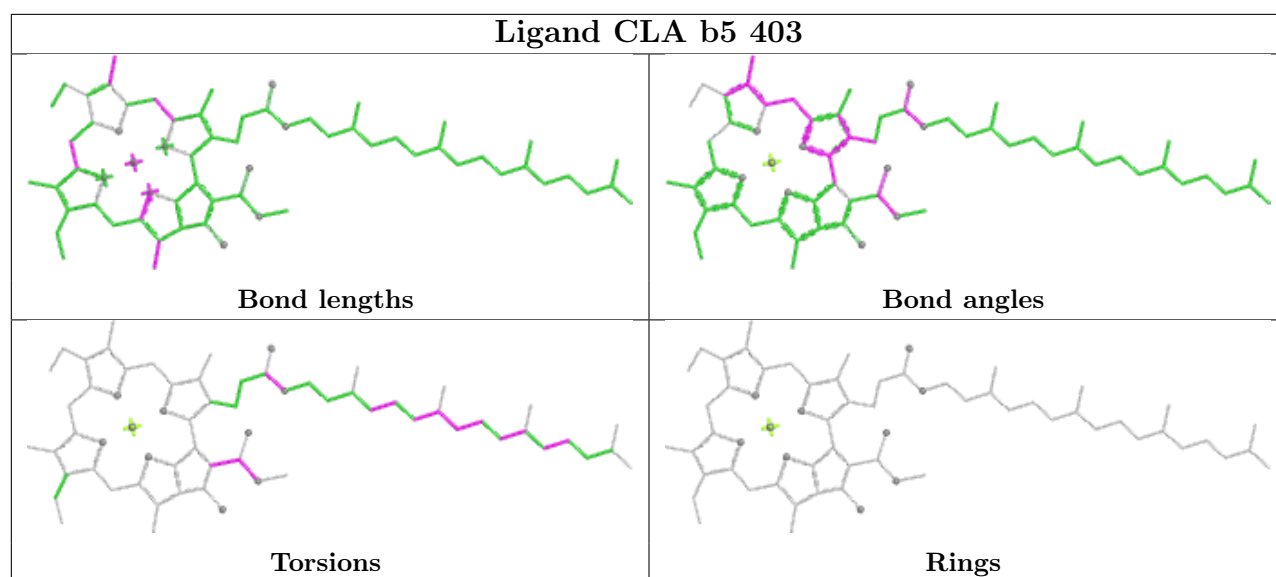


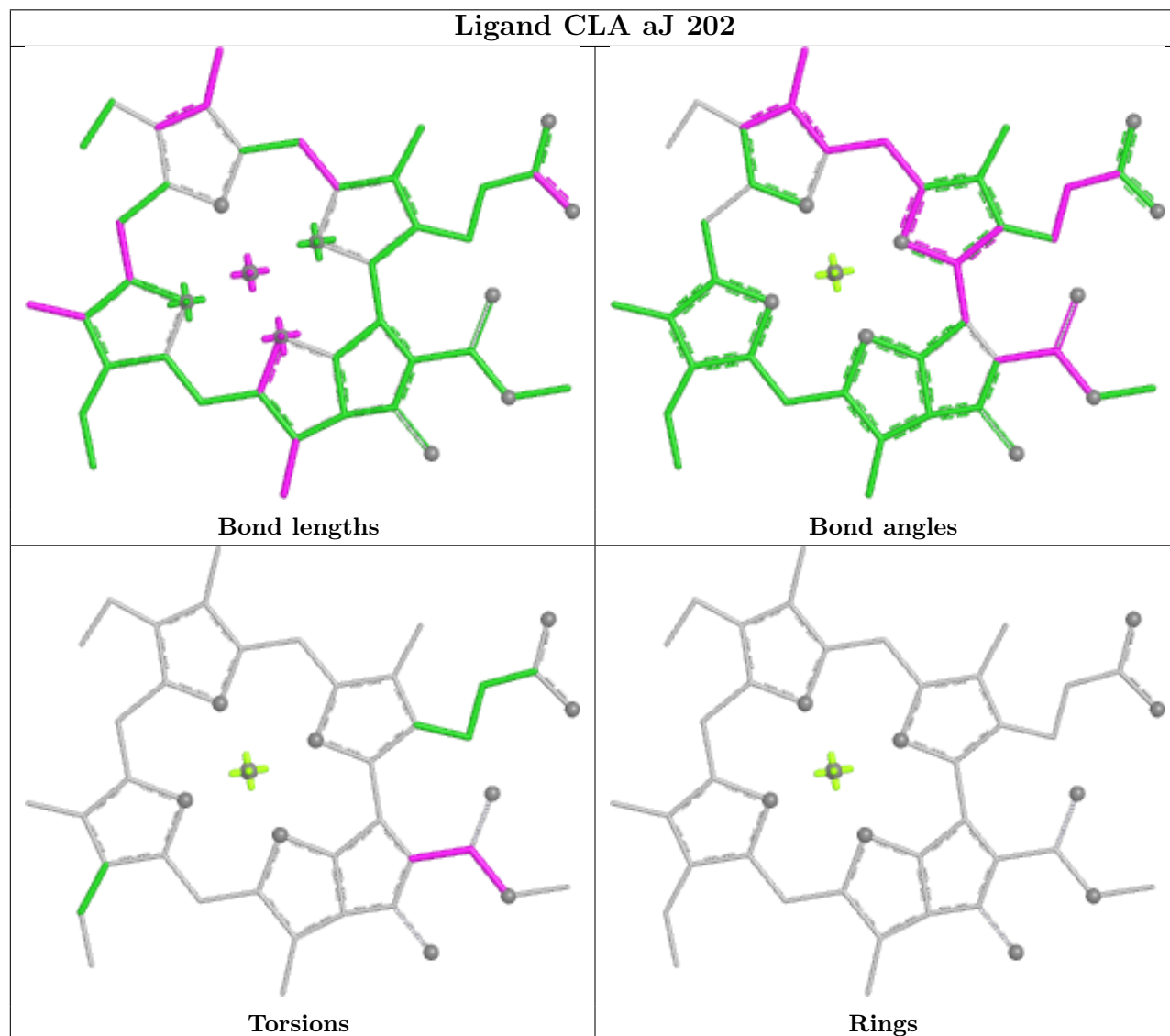
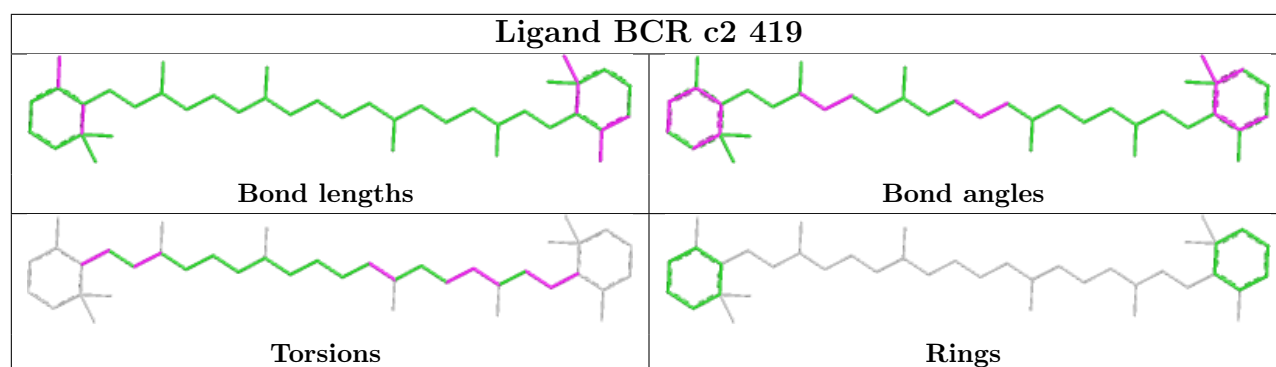


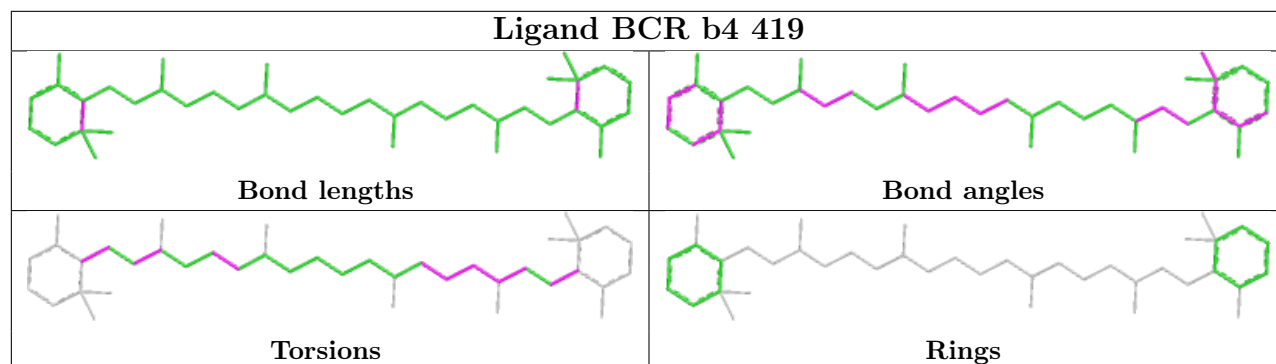
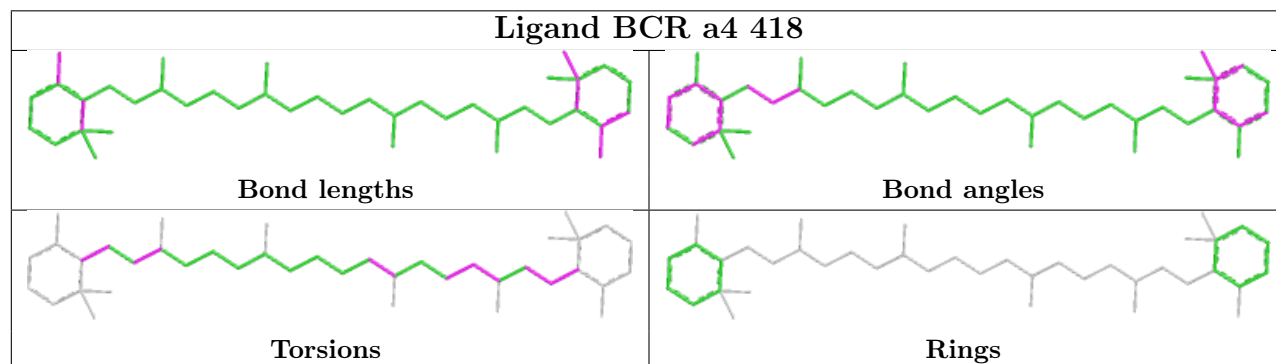
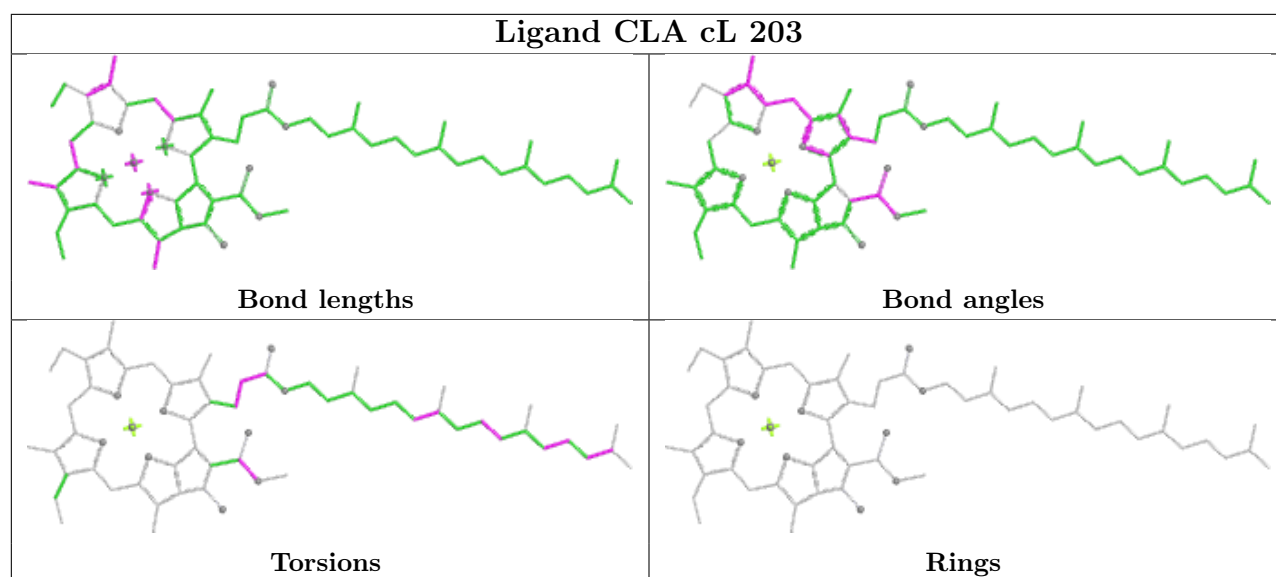




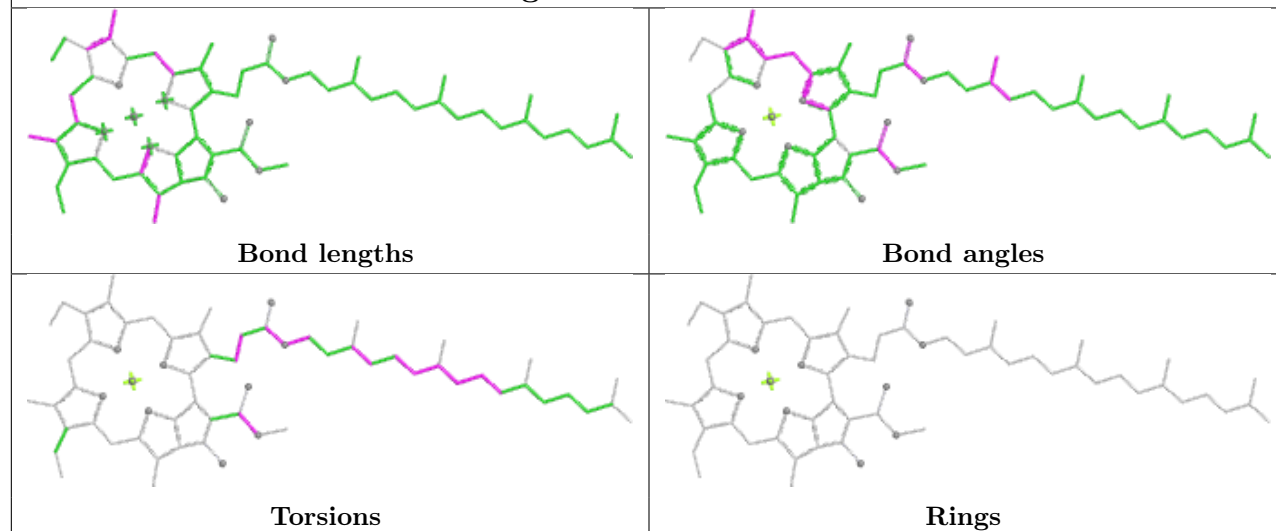




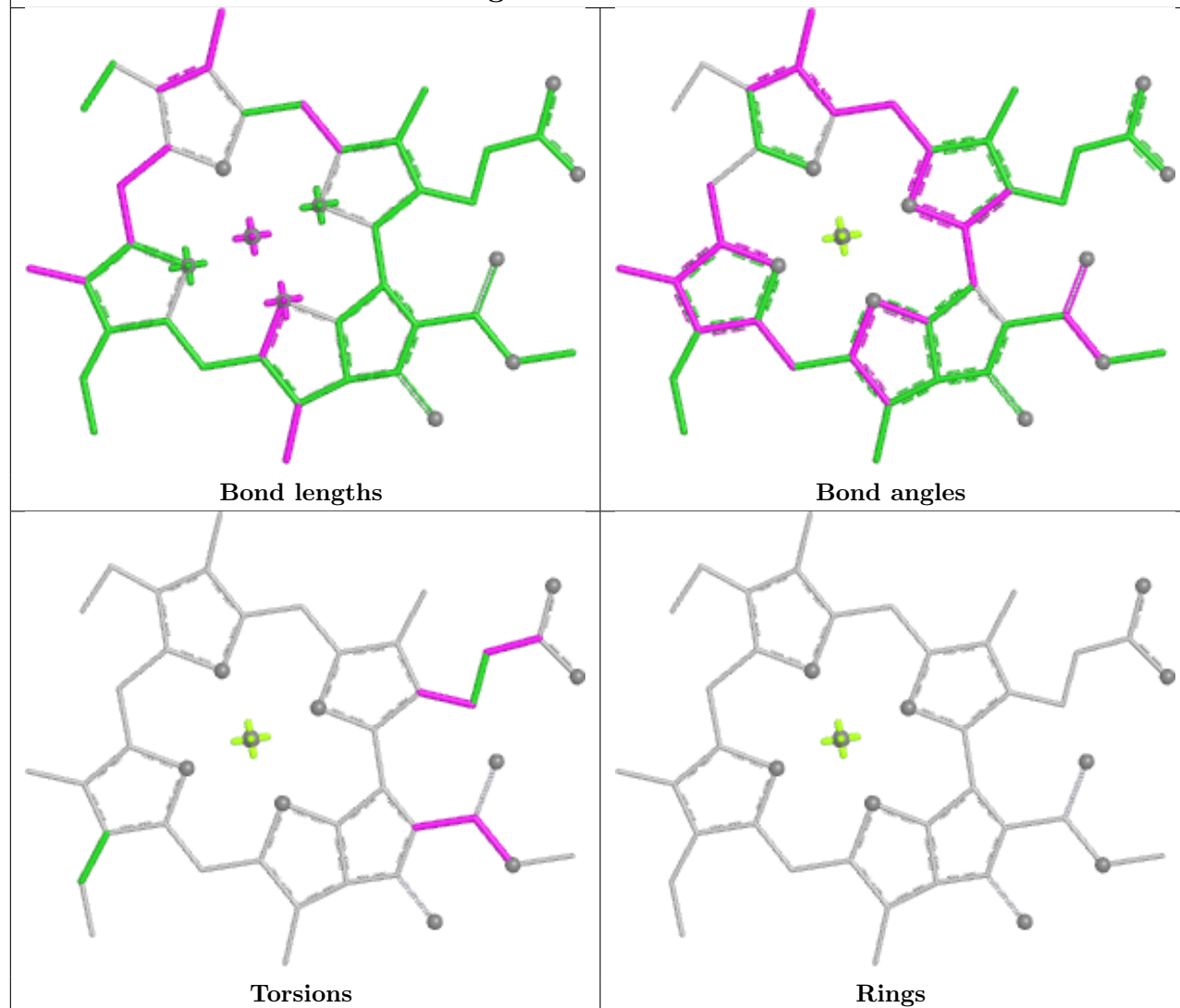


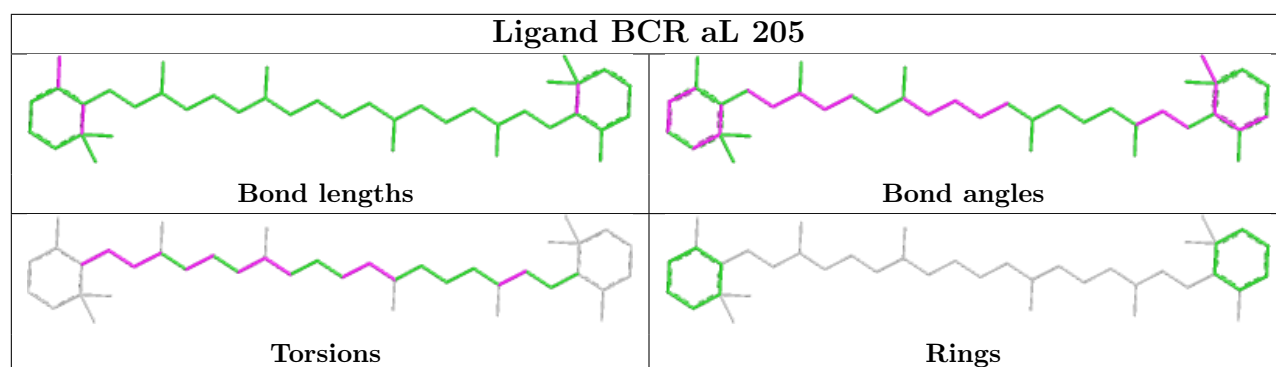
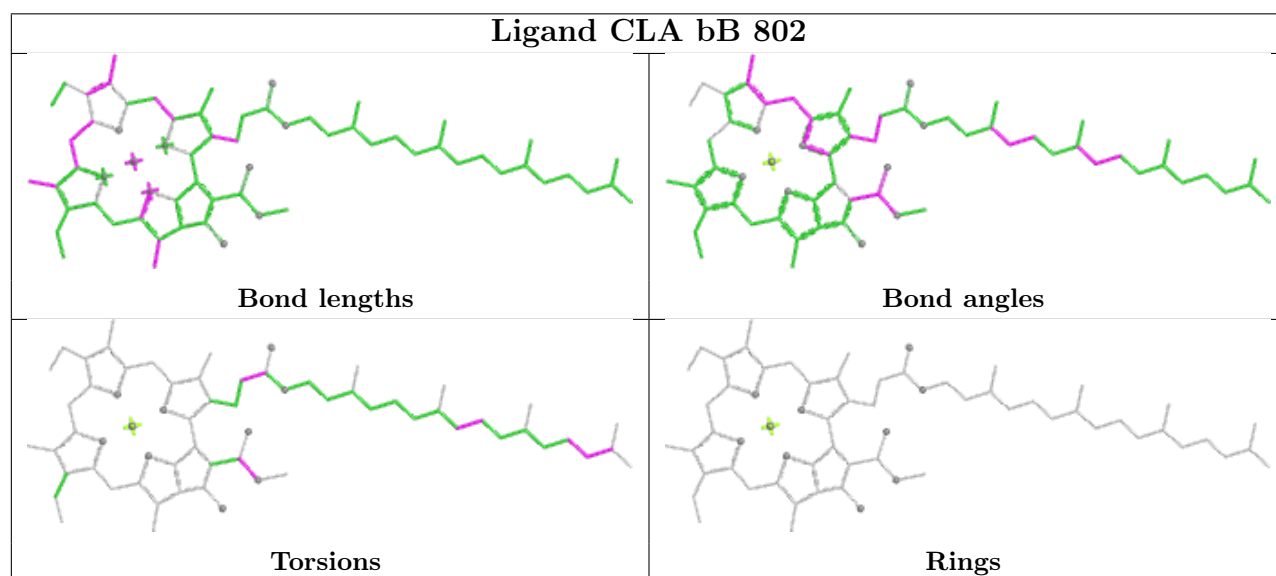
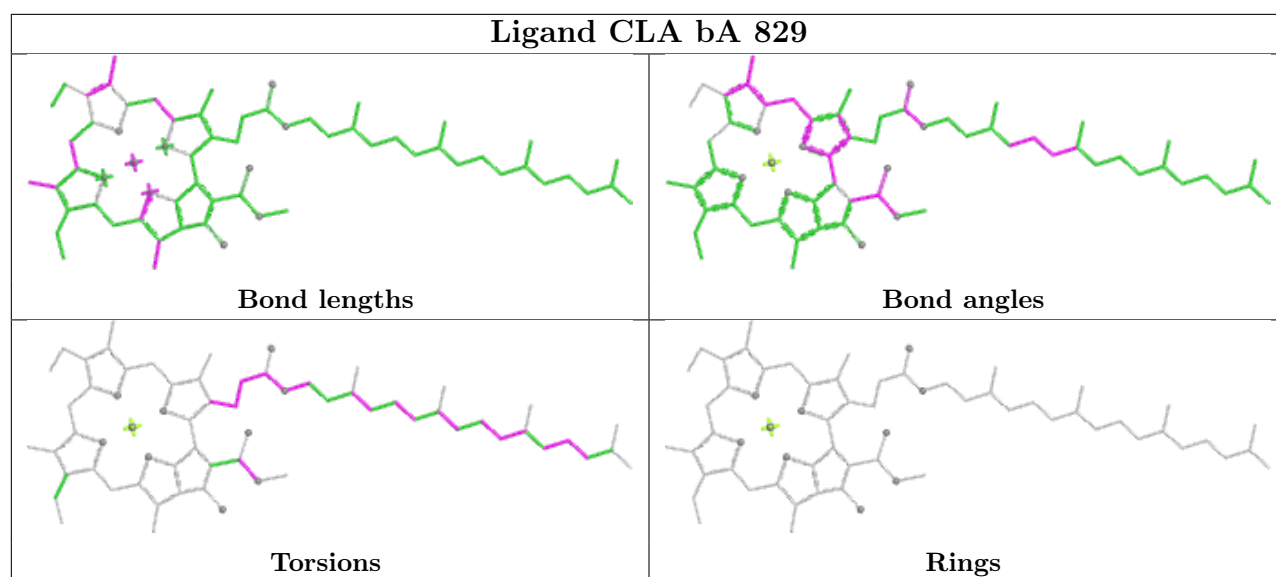


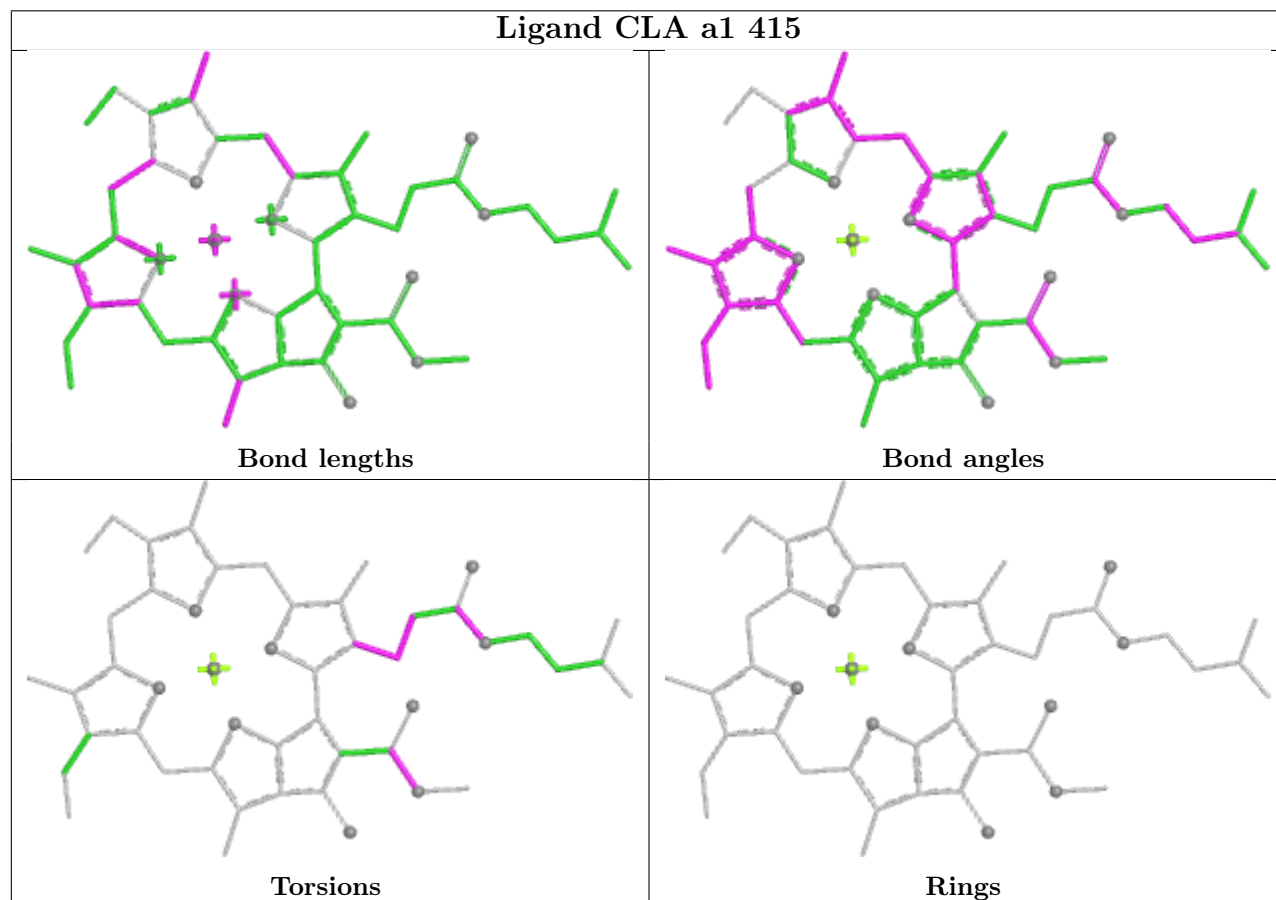
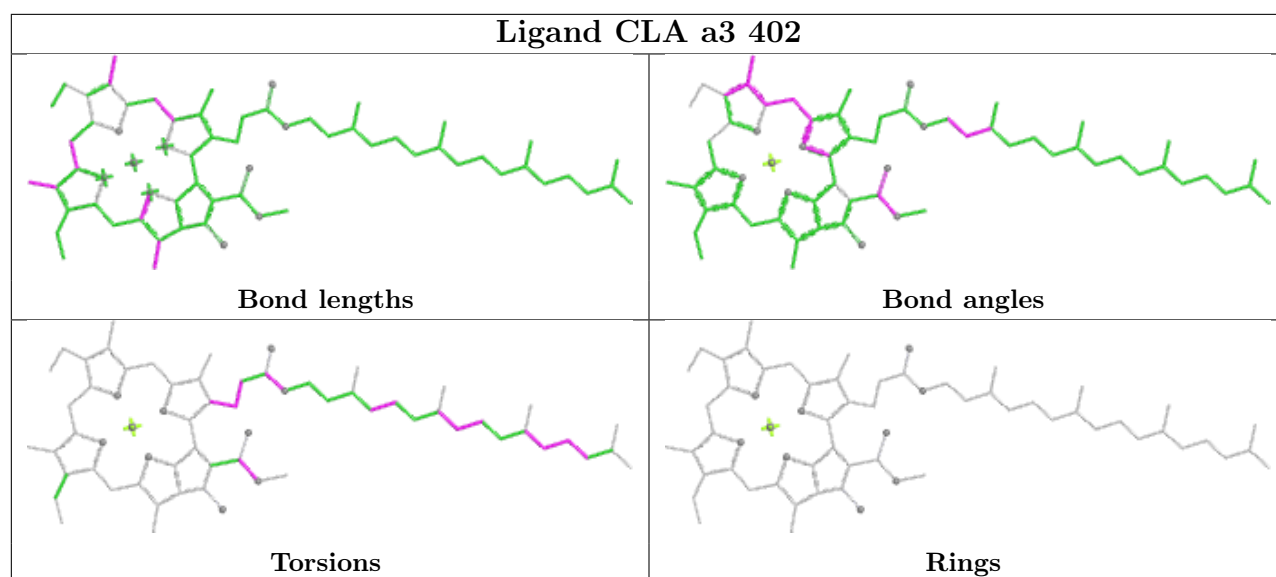
Ligand CLA bA 841

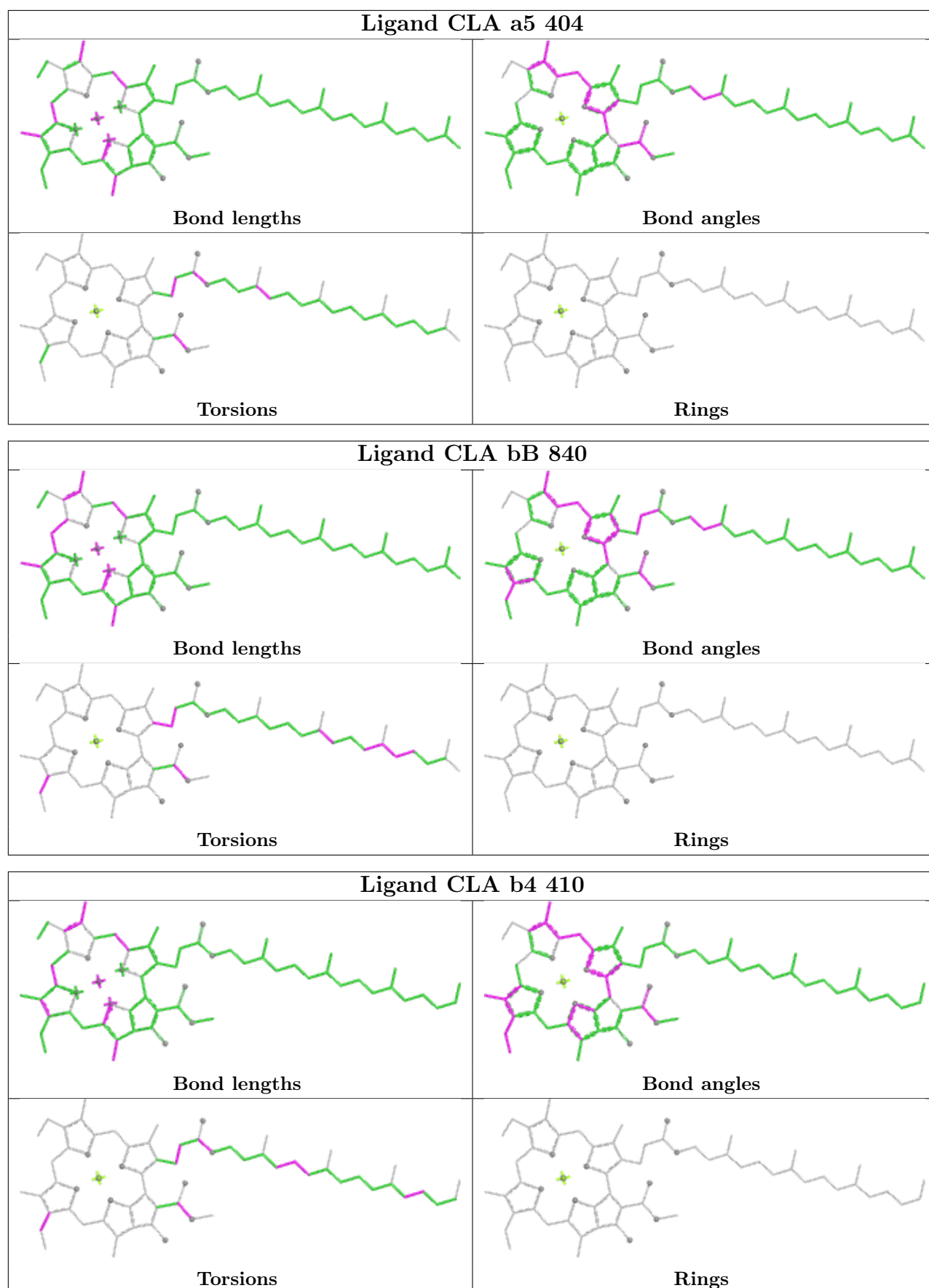


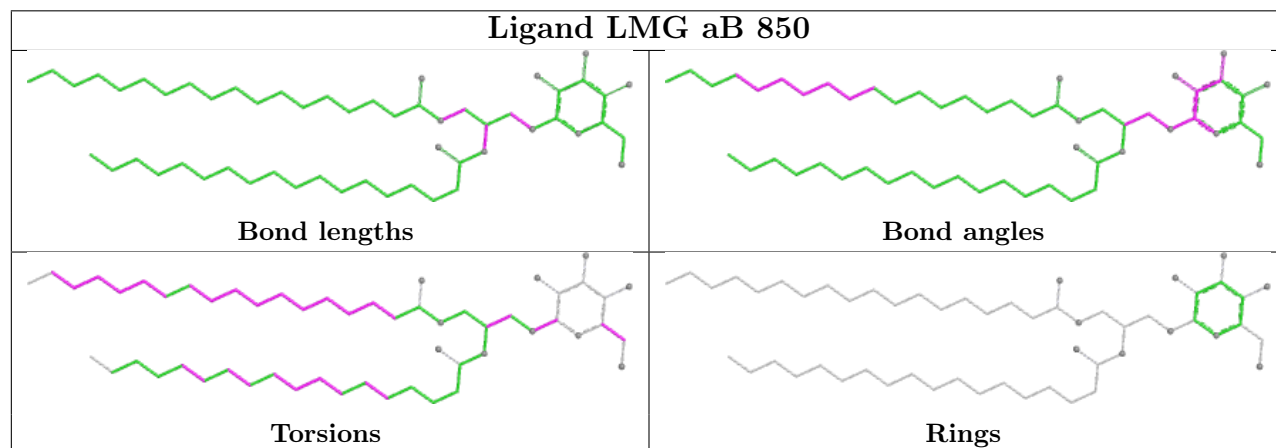
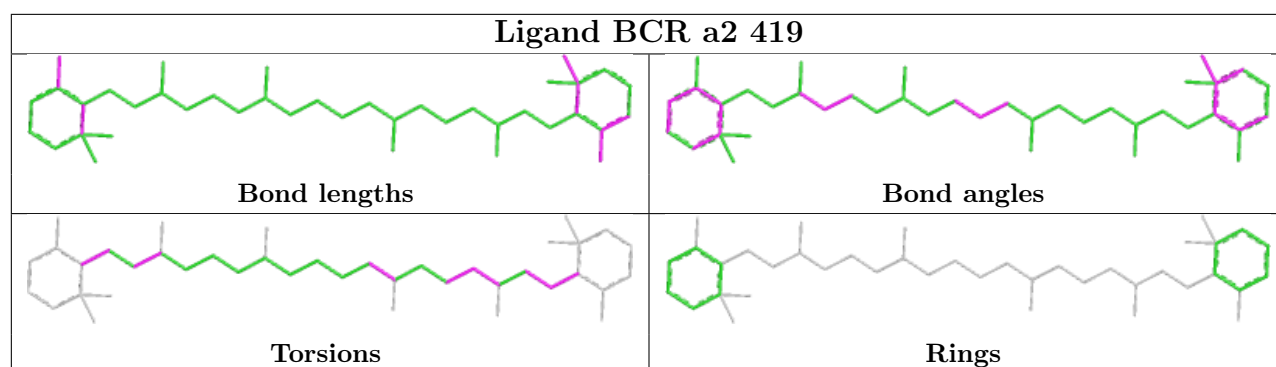
Ligand CLA a2 413



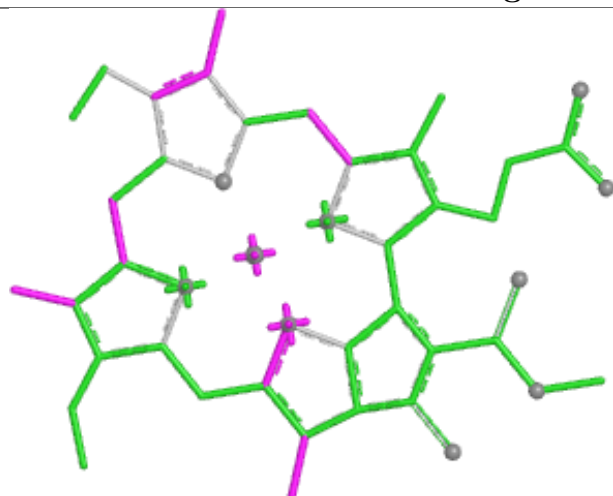




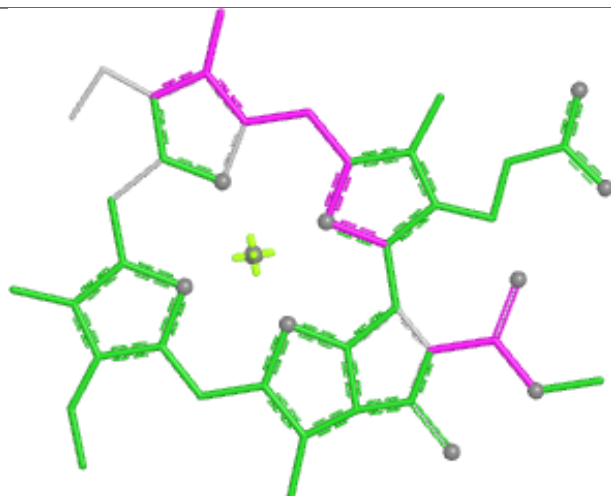




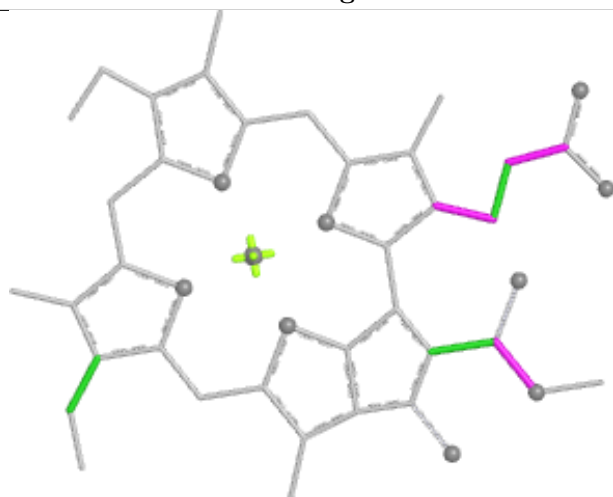
Ligand CLA bA 811



Bond lengths



Bond angles

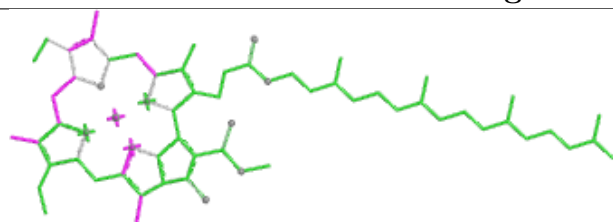


Torsions

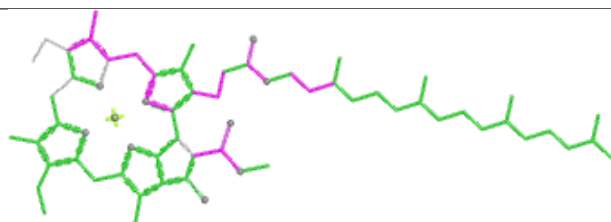


Rings

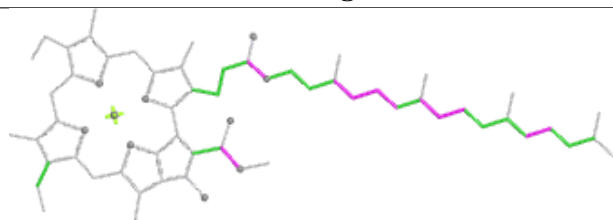
Ligand CLA bB 809



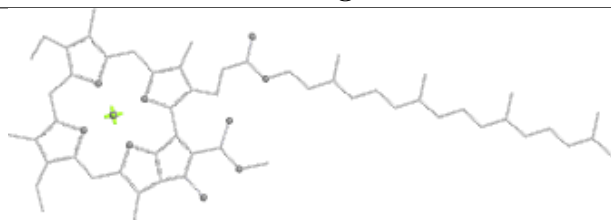
Bond lengths



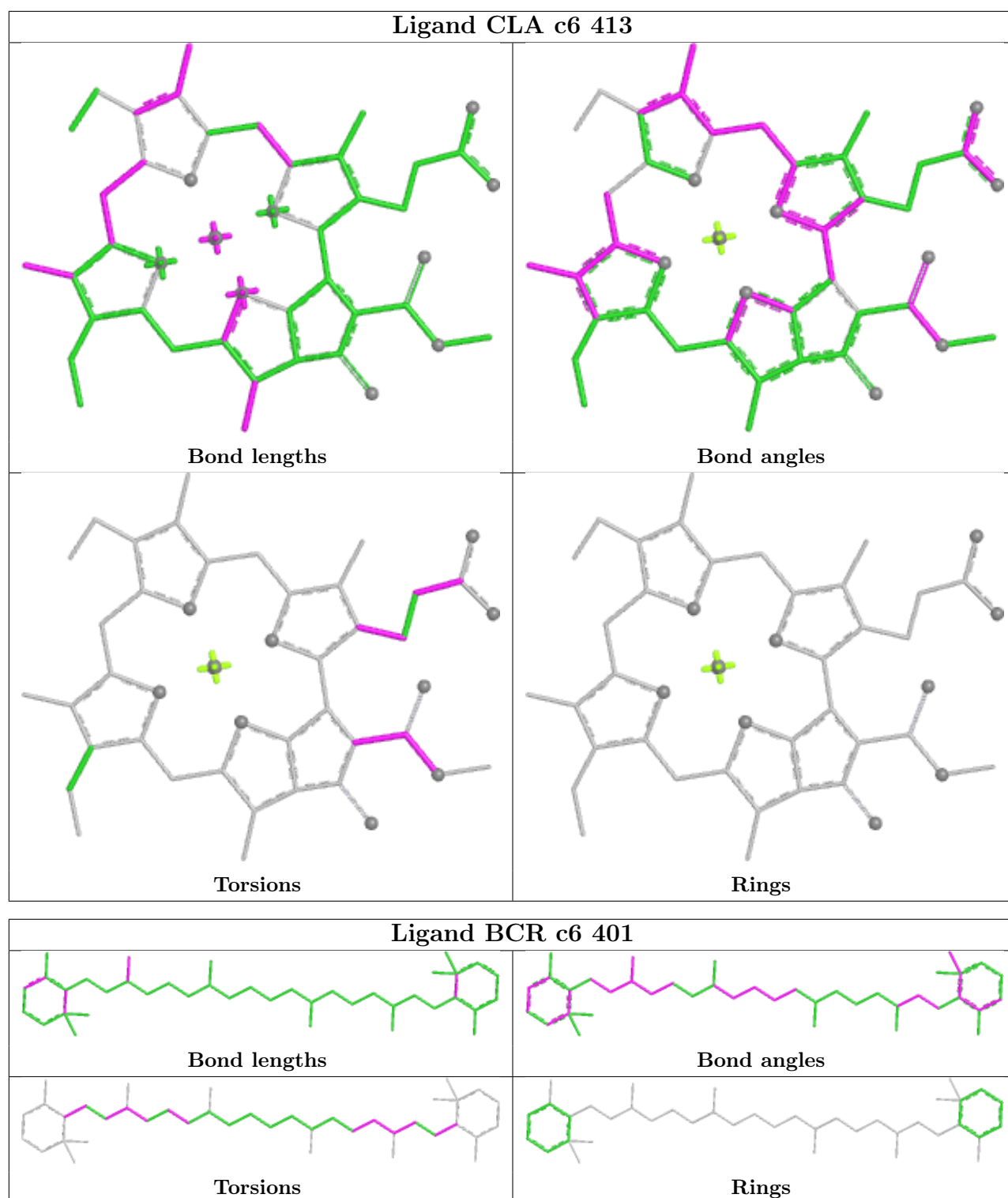
Bond angles

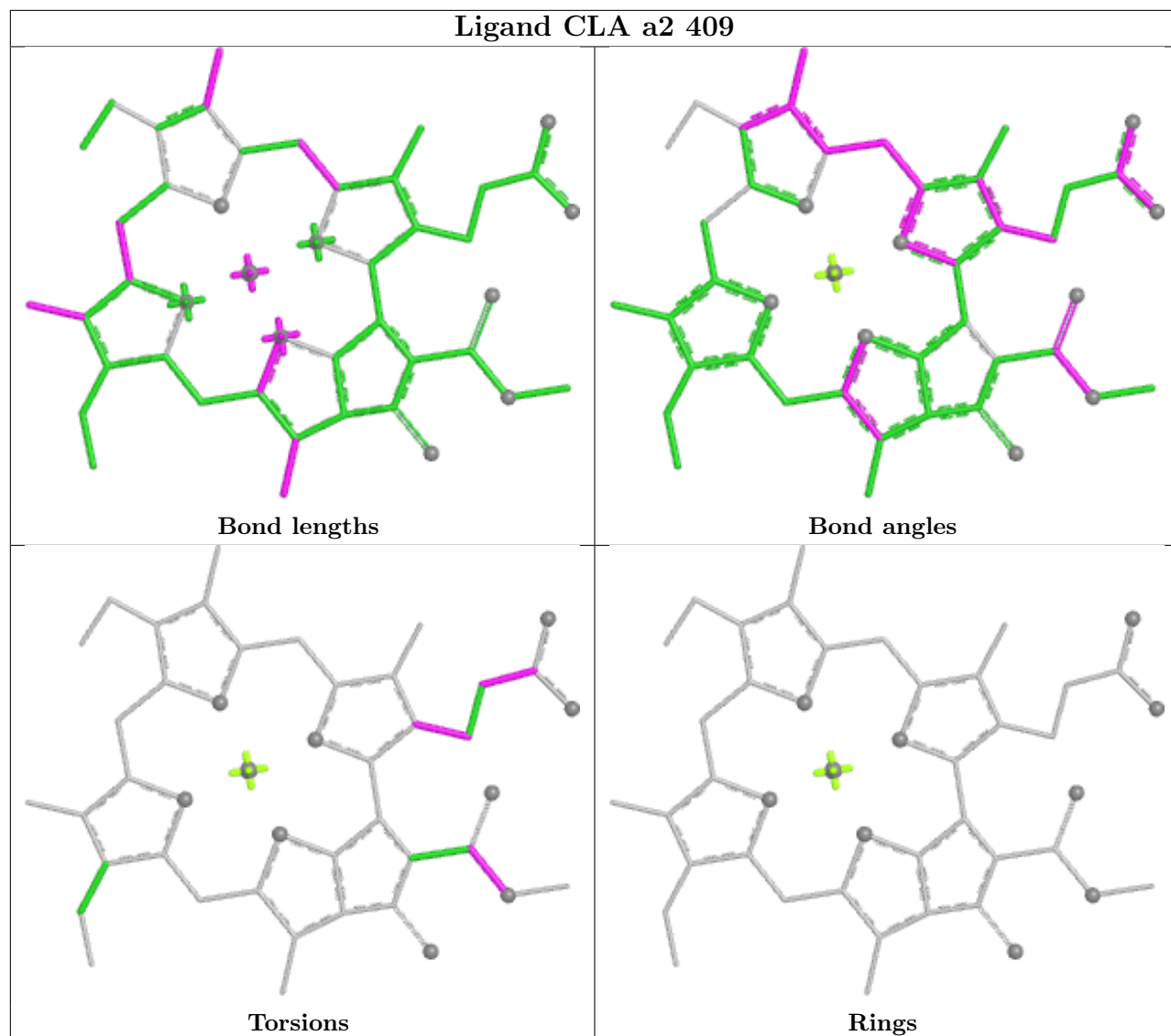


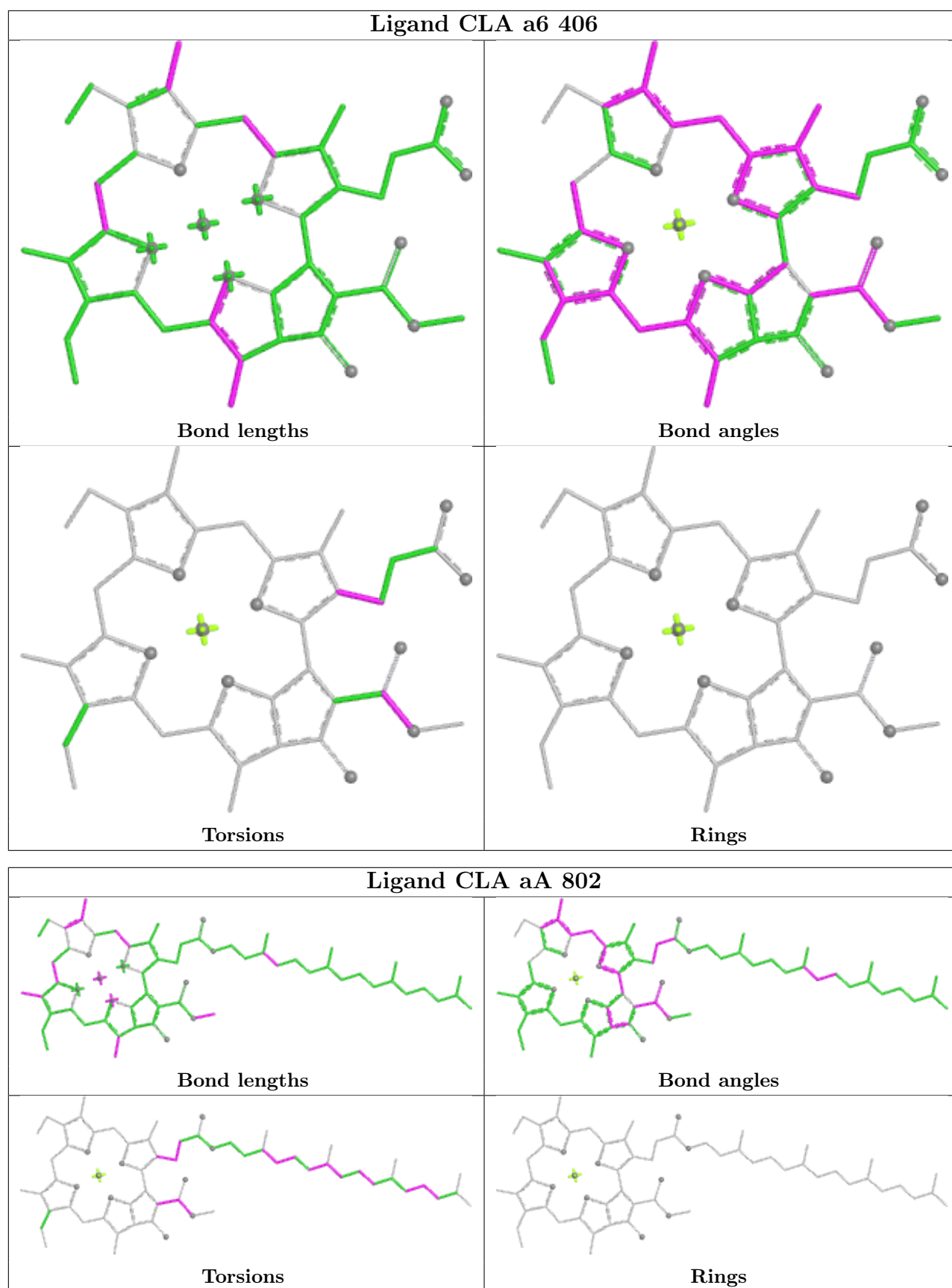
Torsions

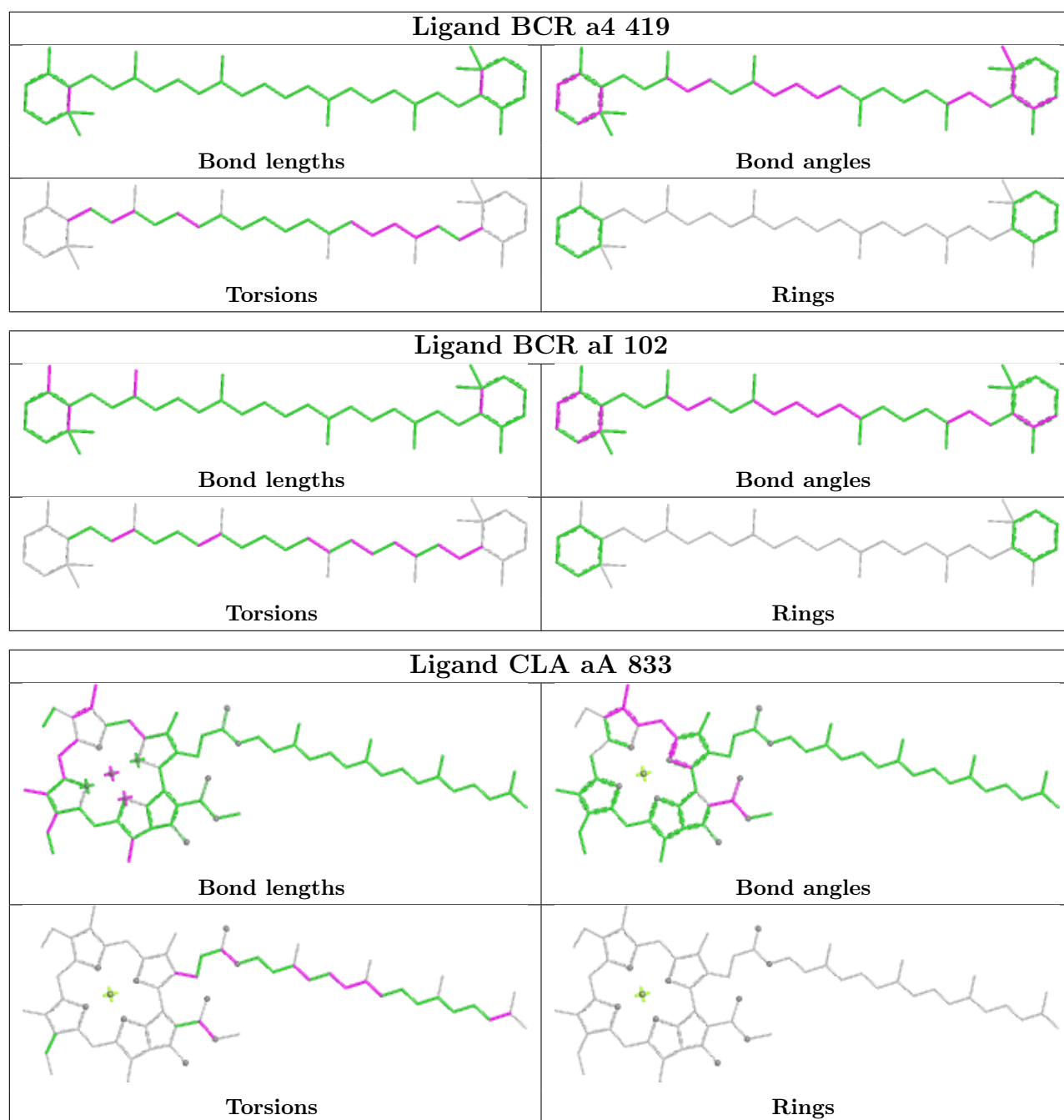


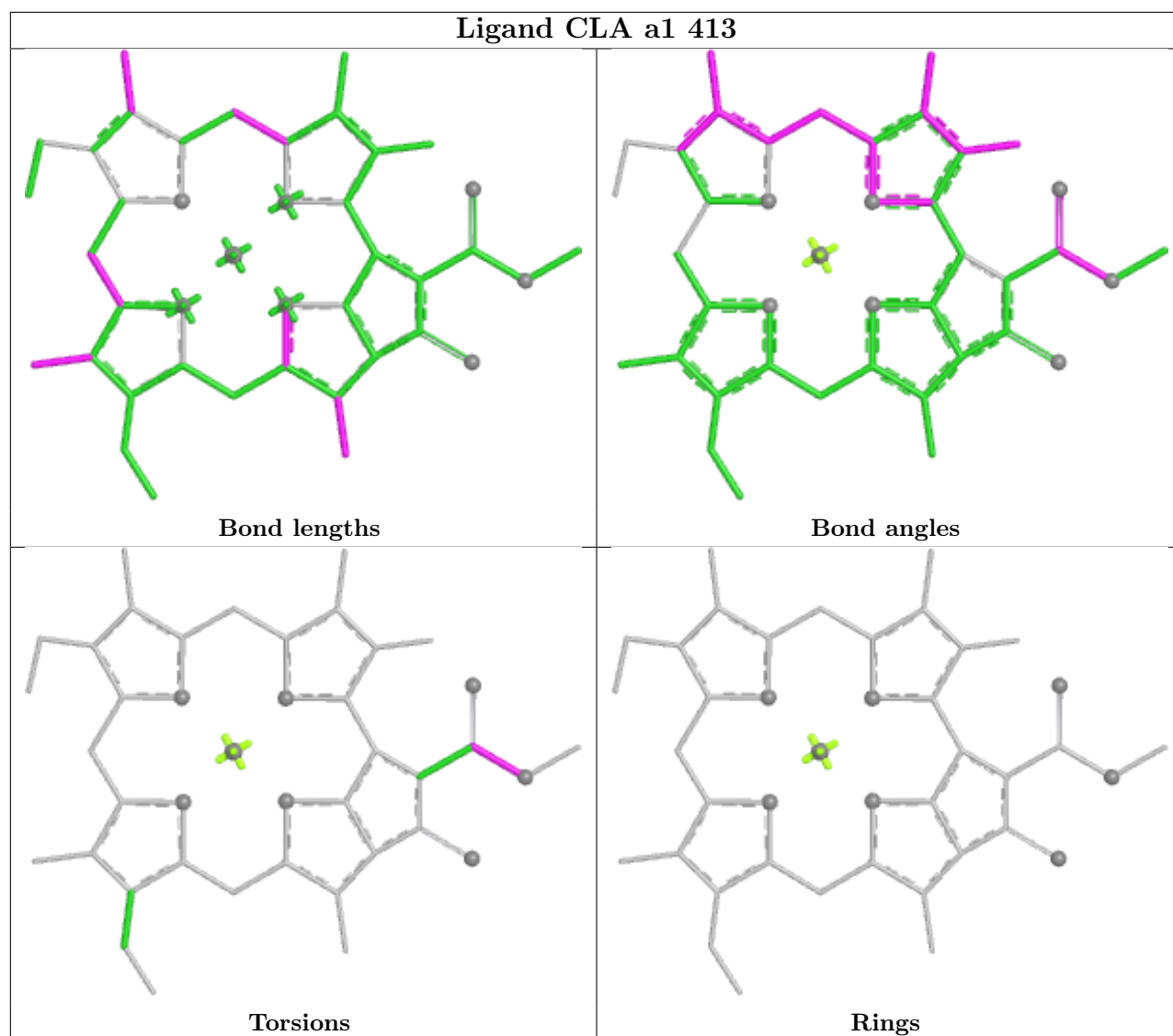
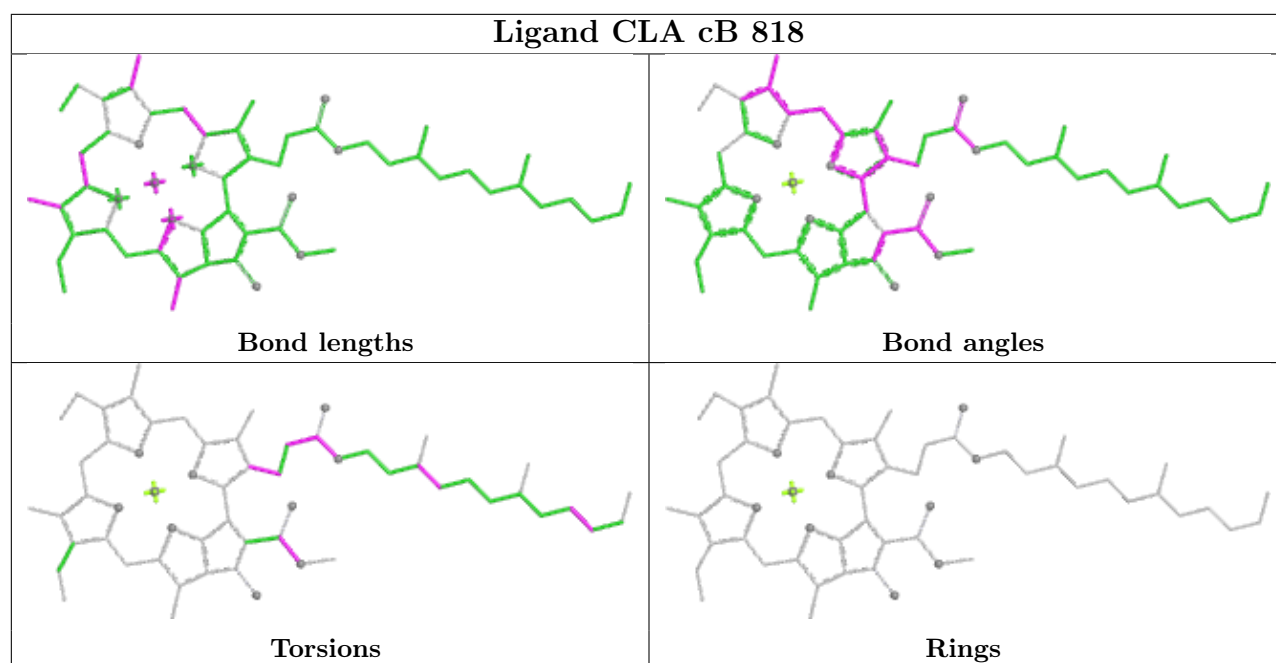
Rings

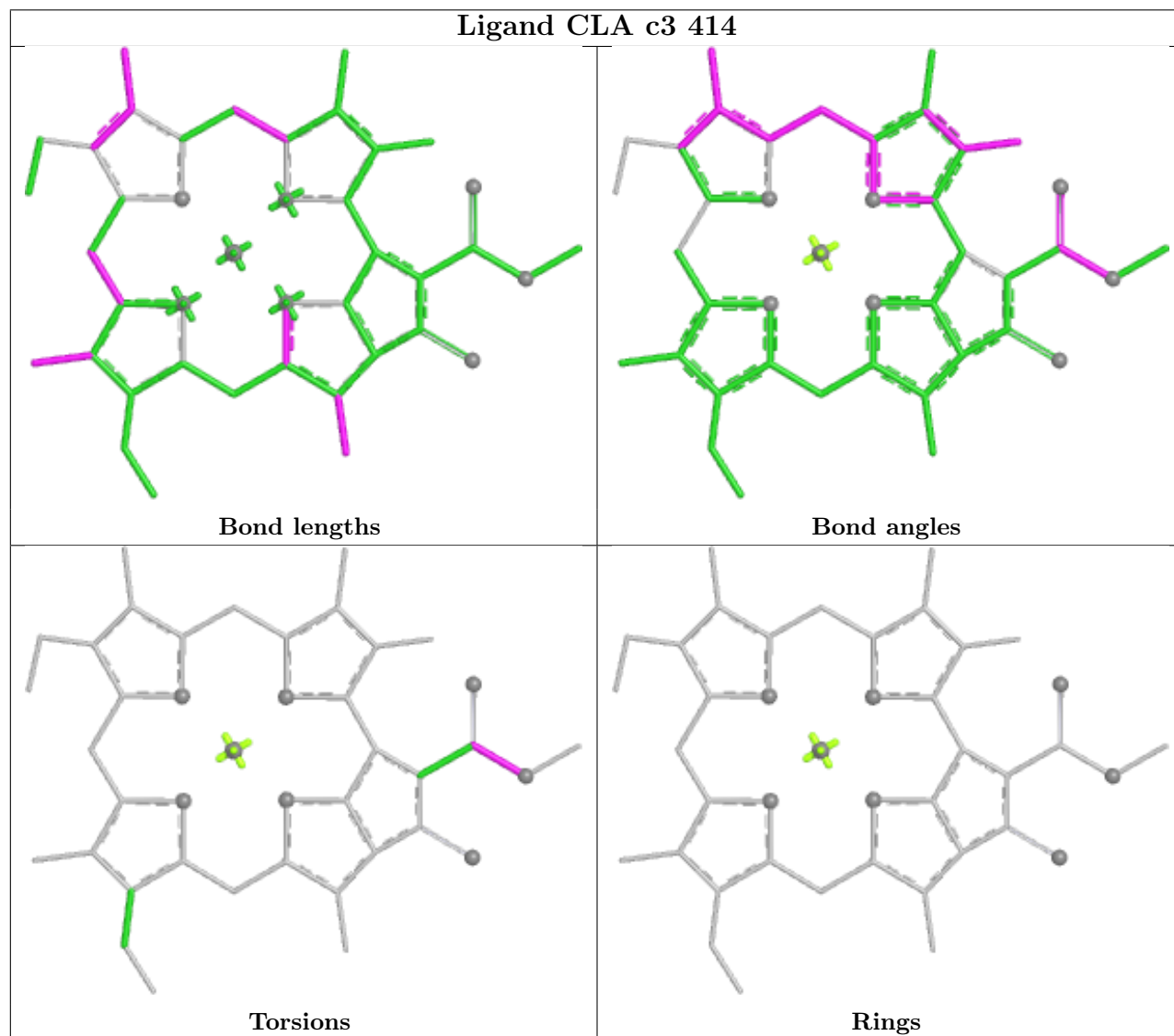
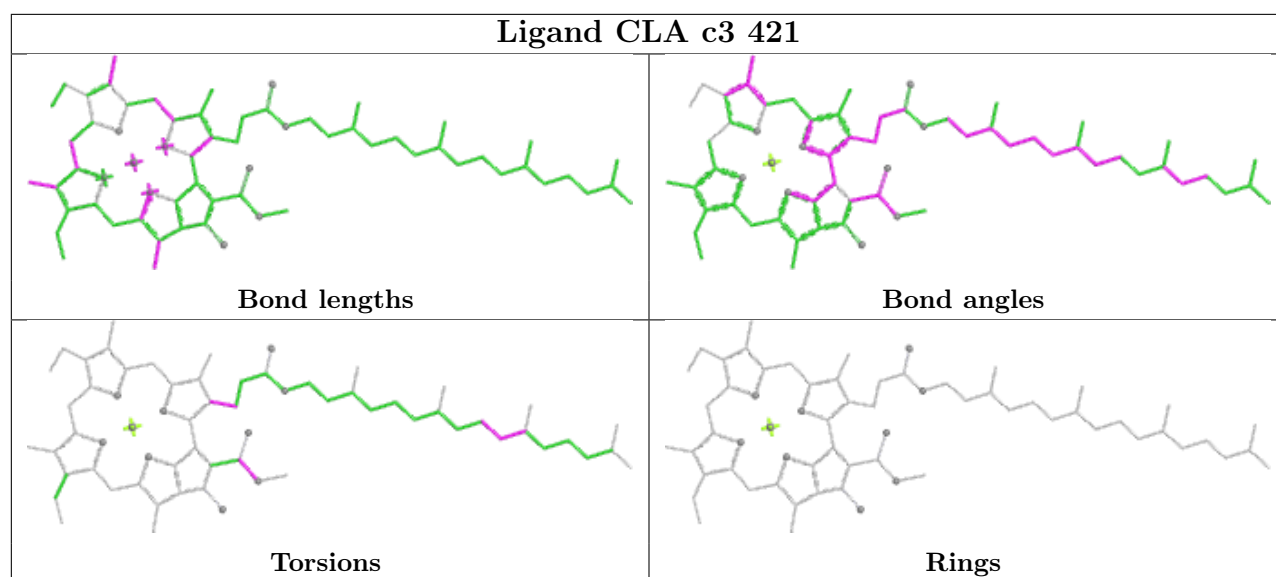


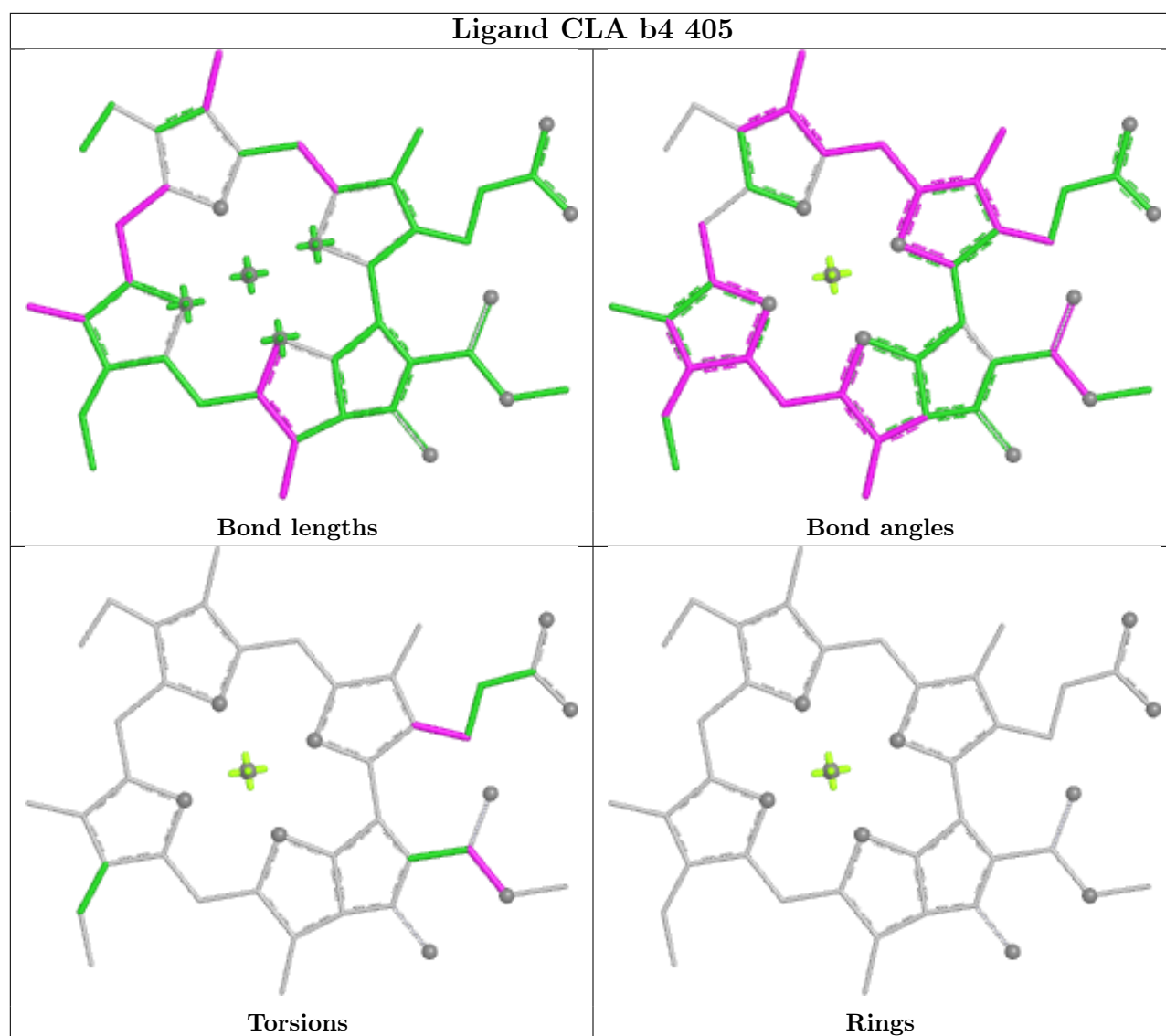


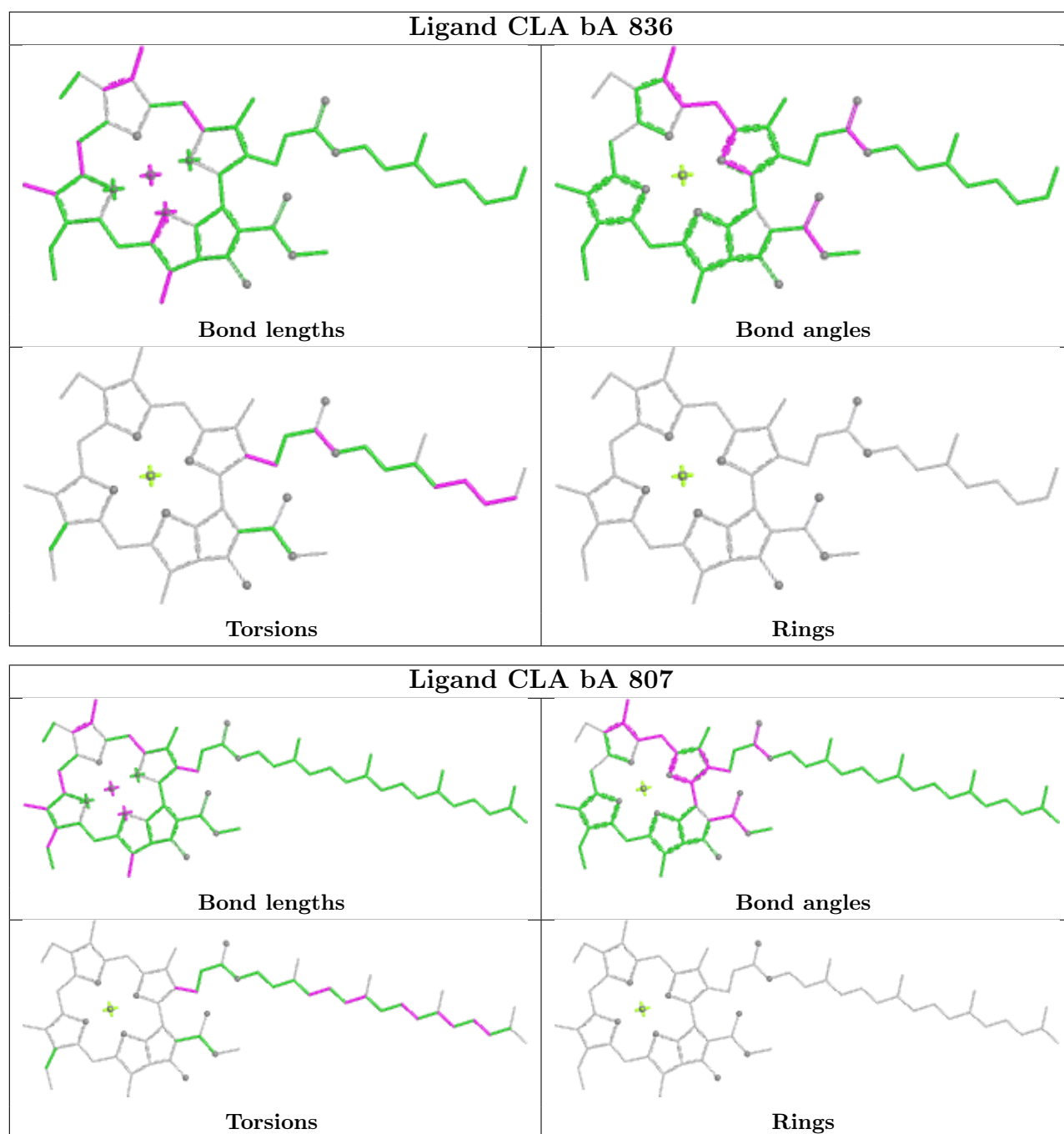


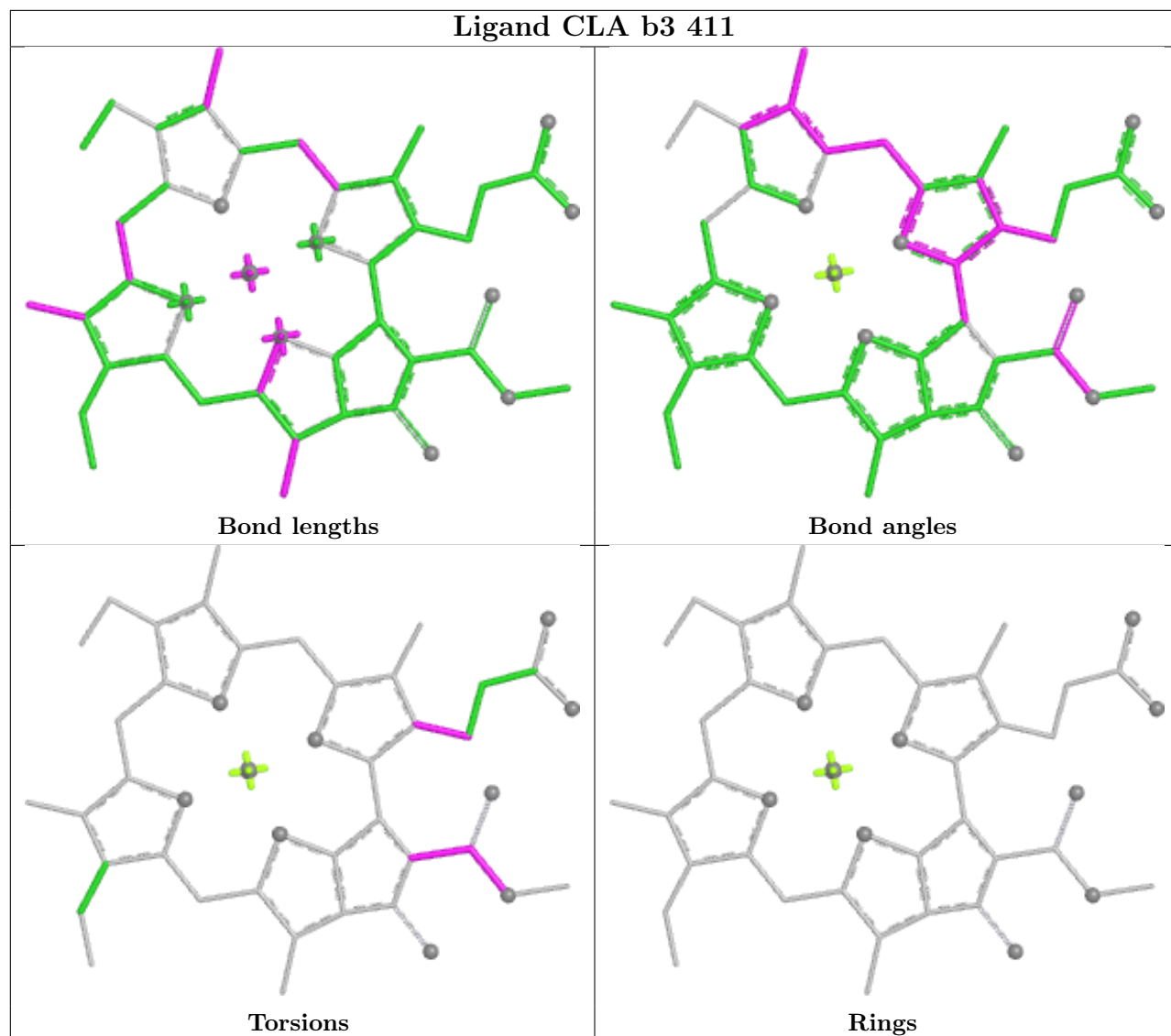


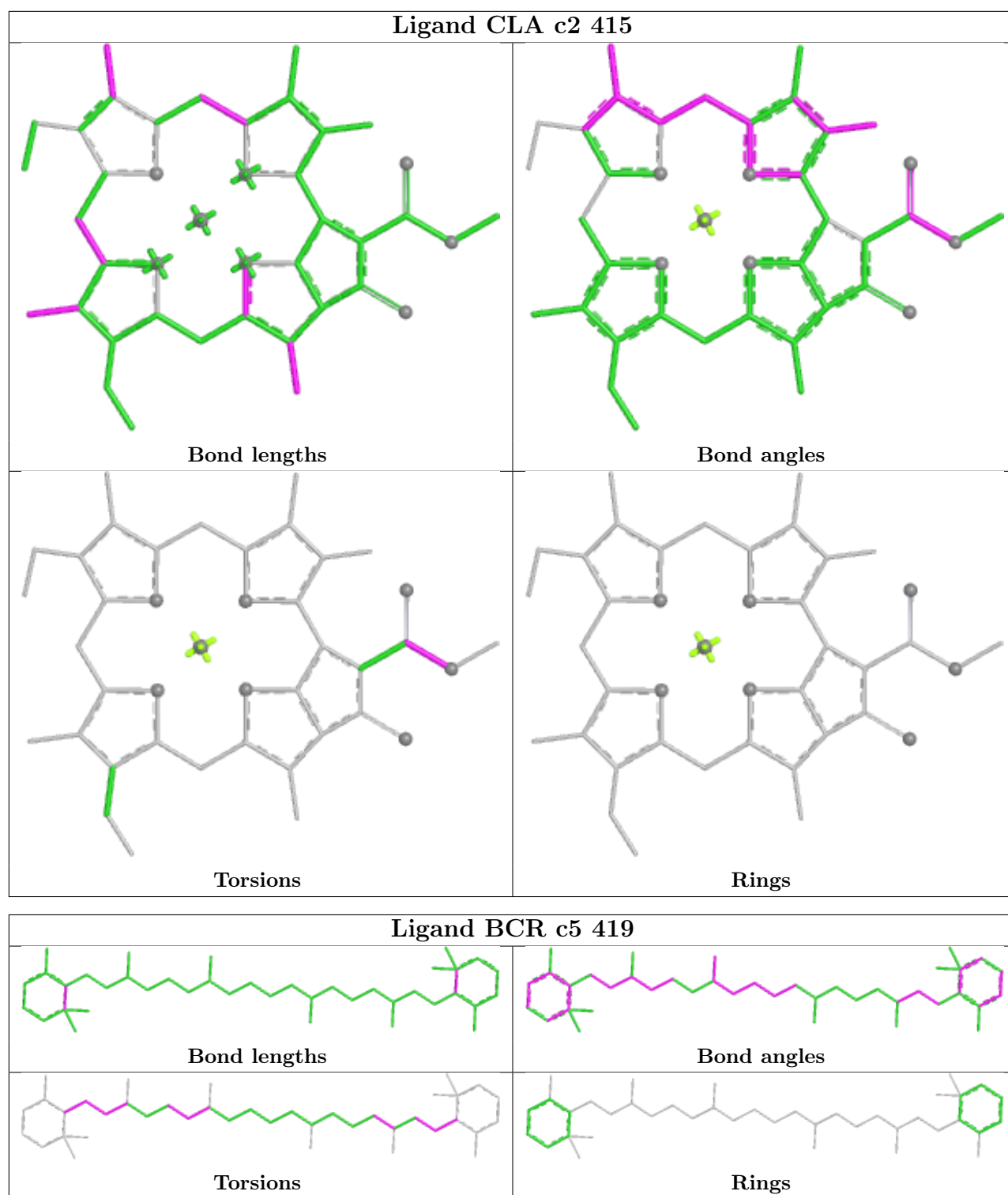


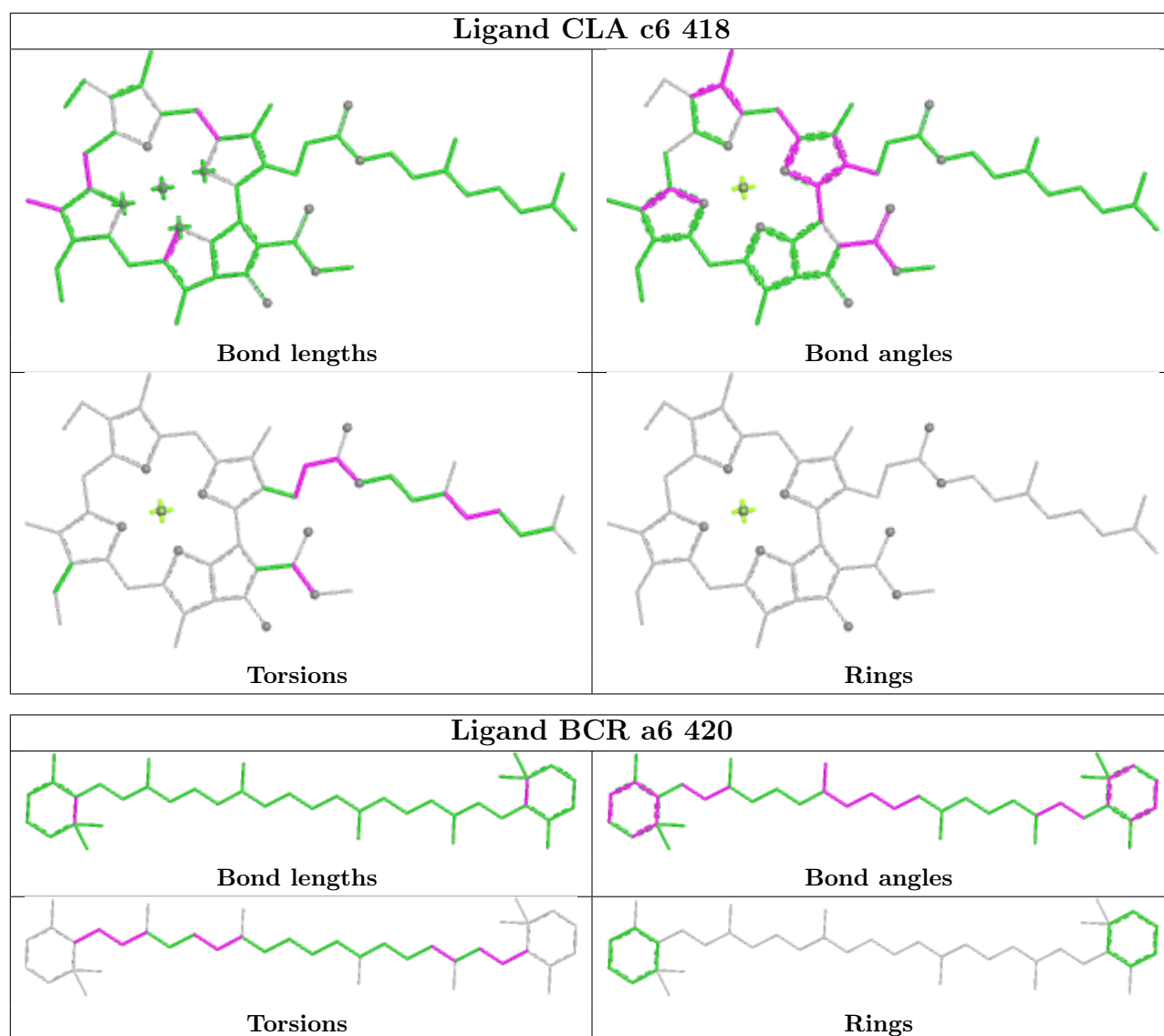


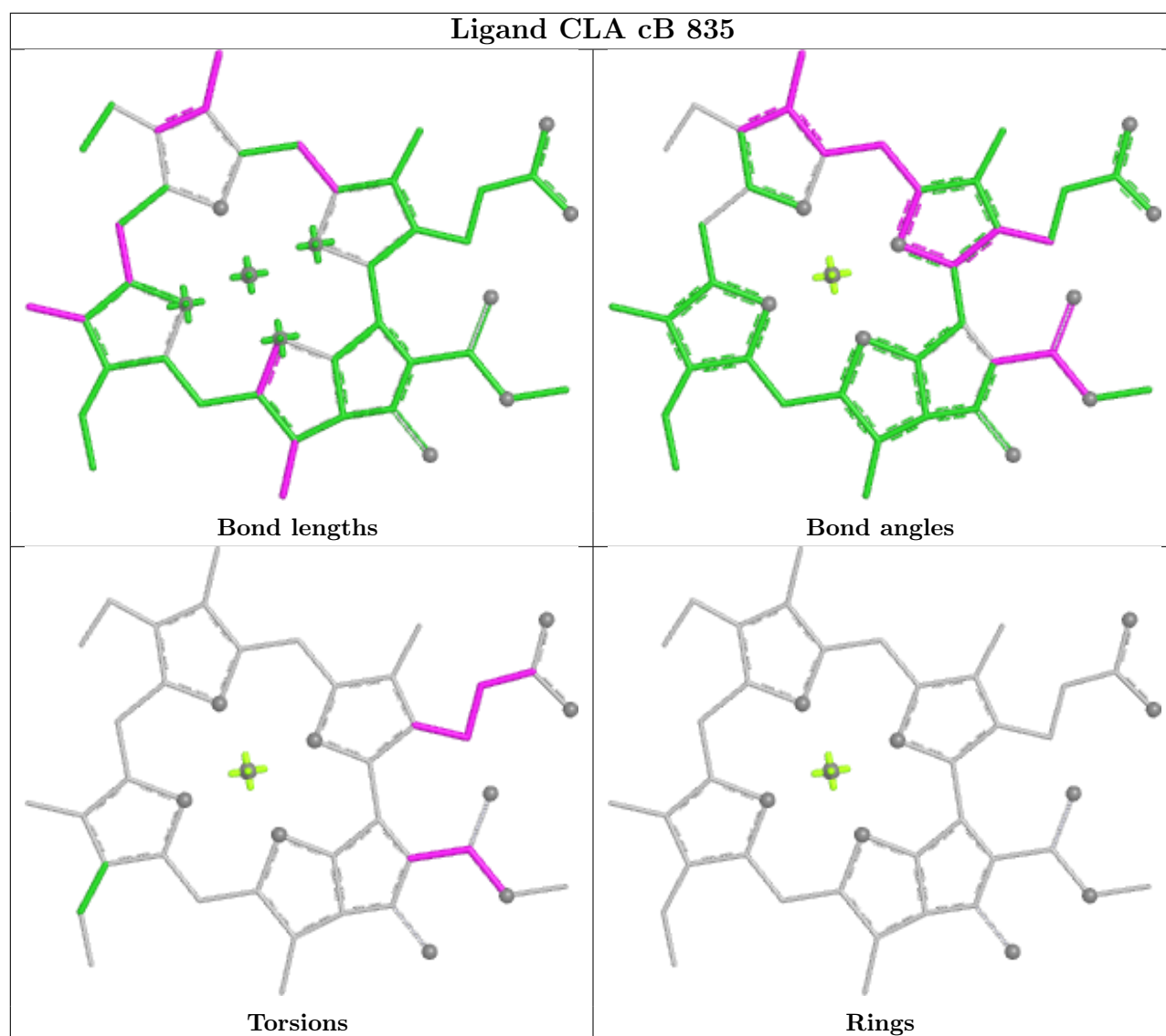


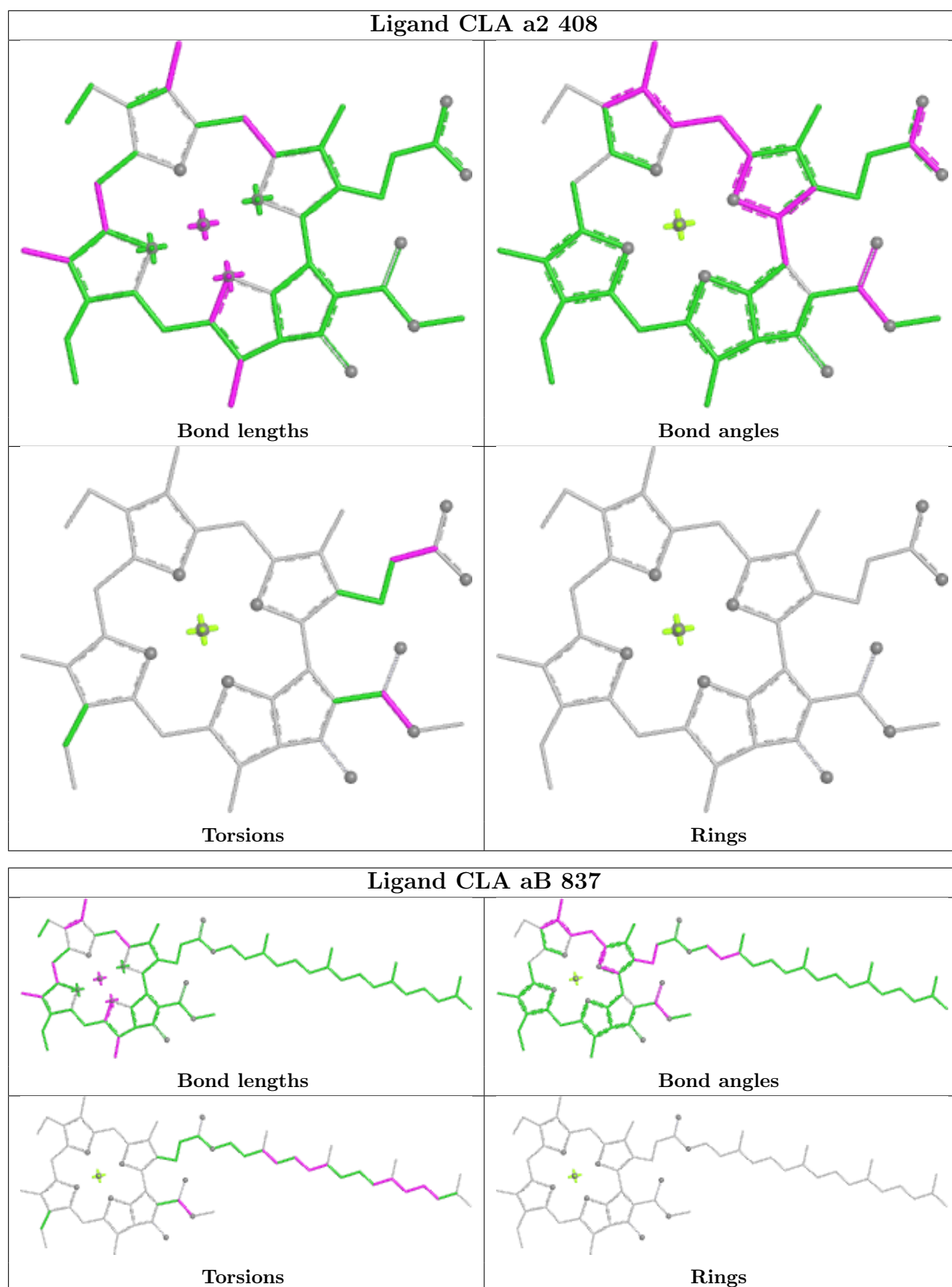


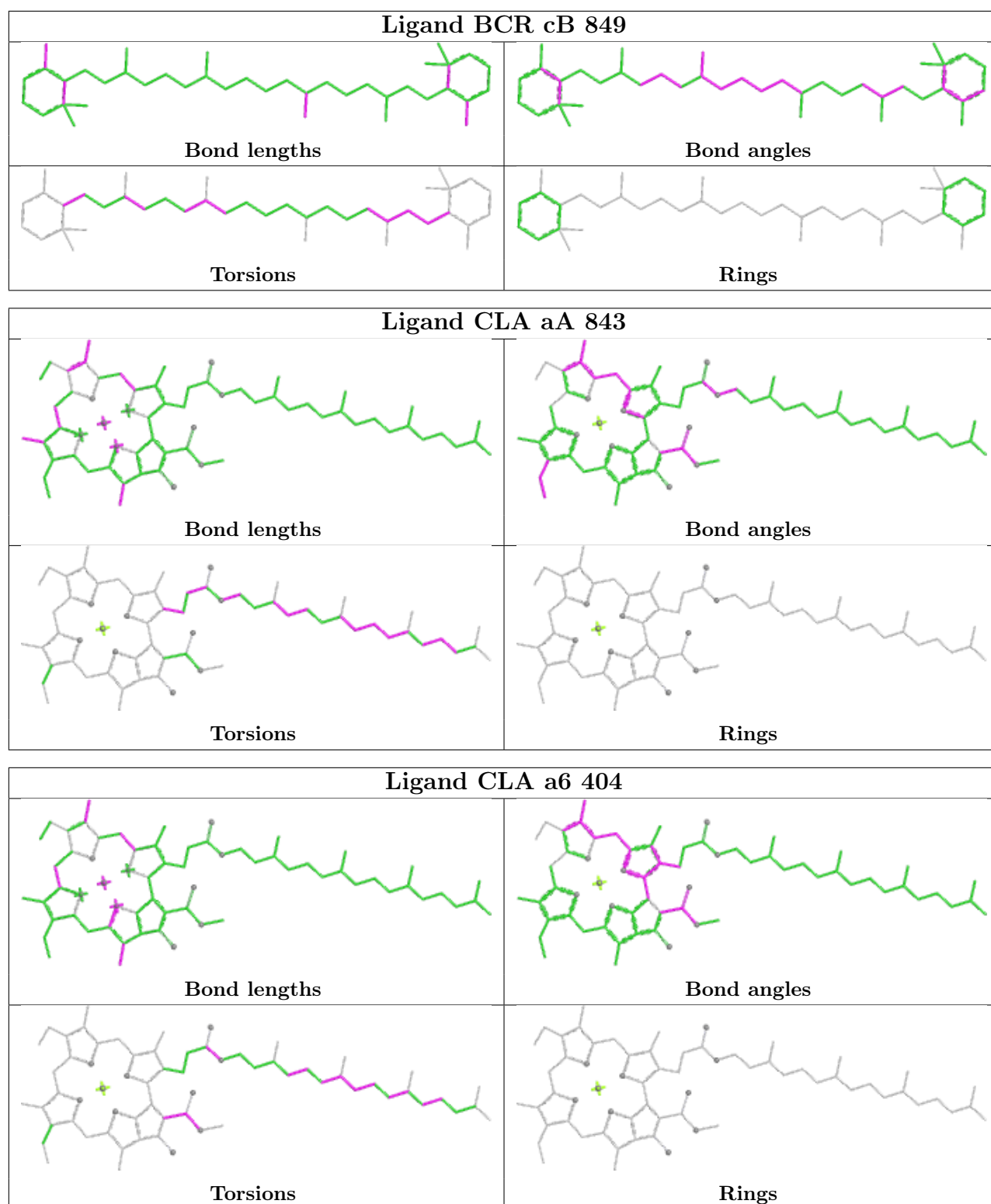


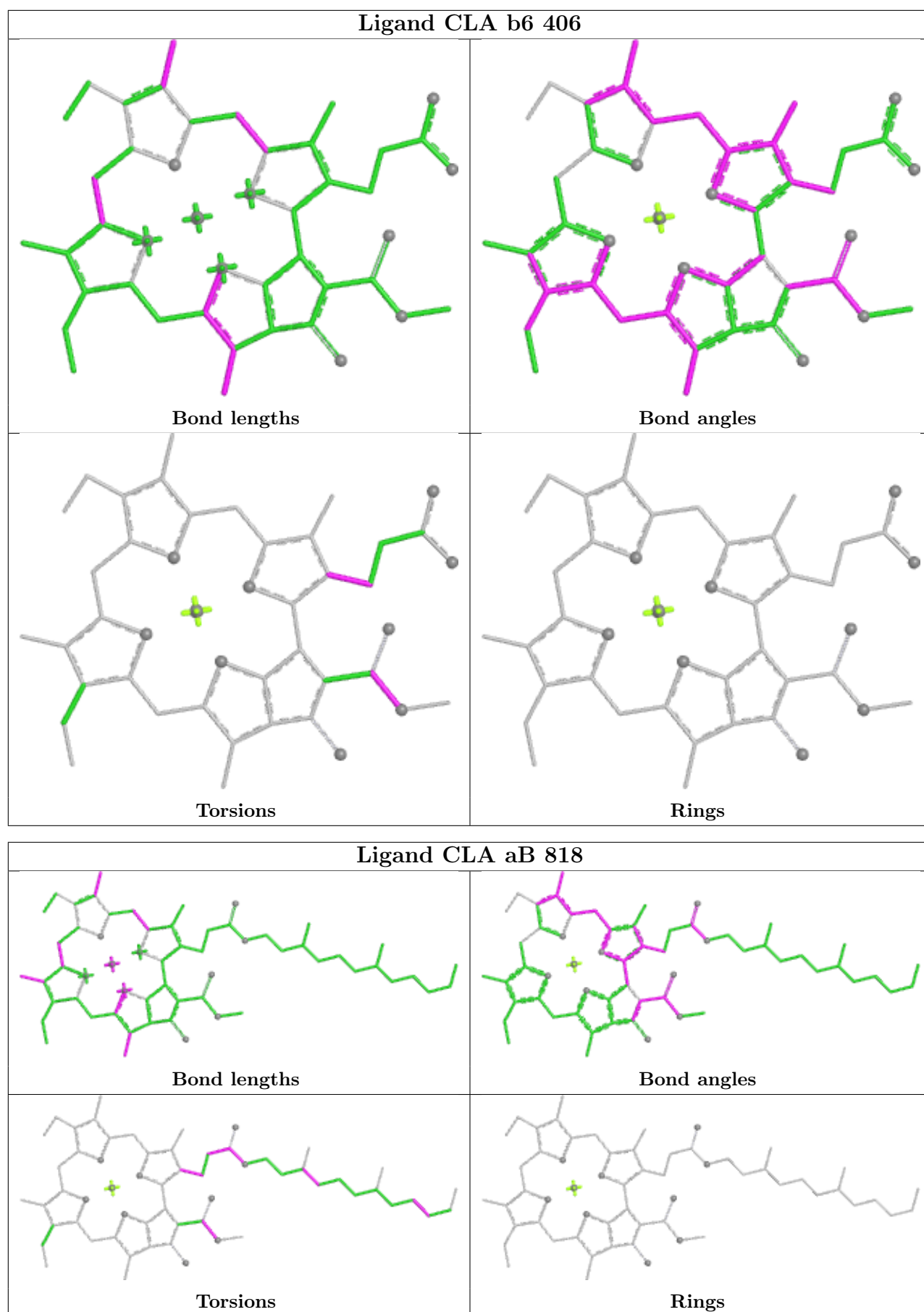


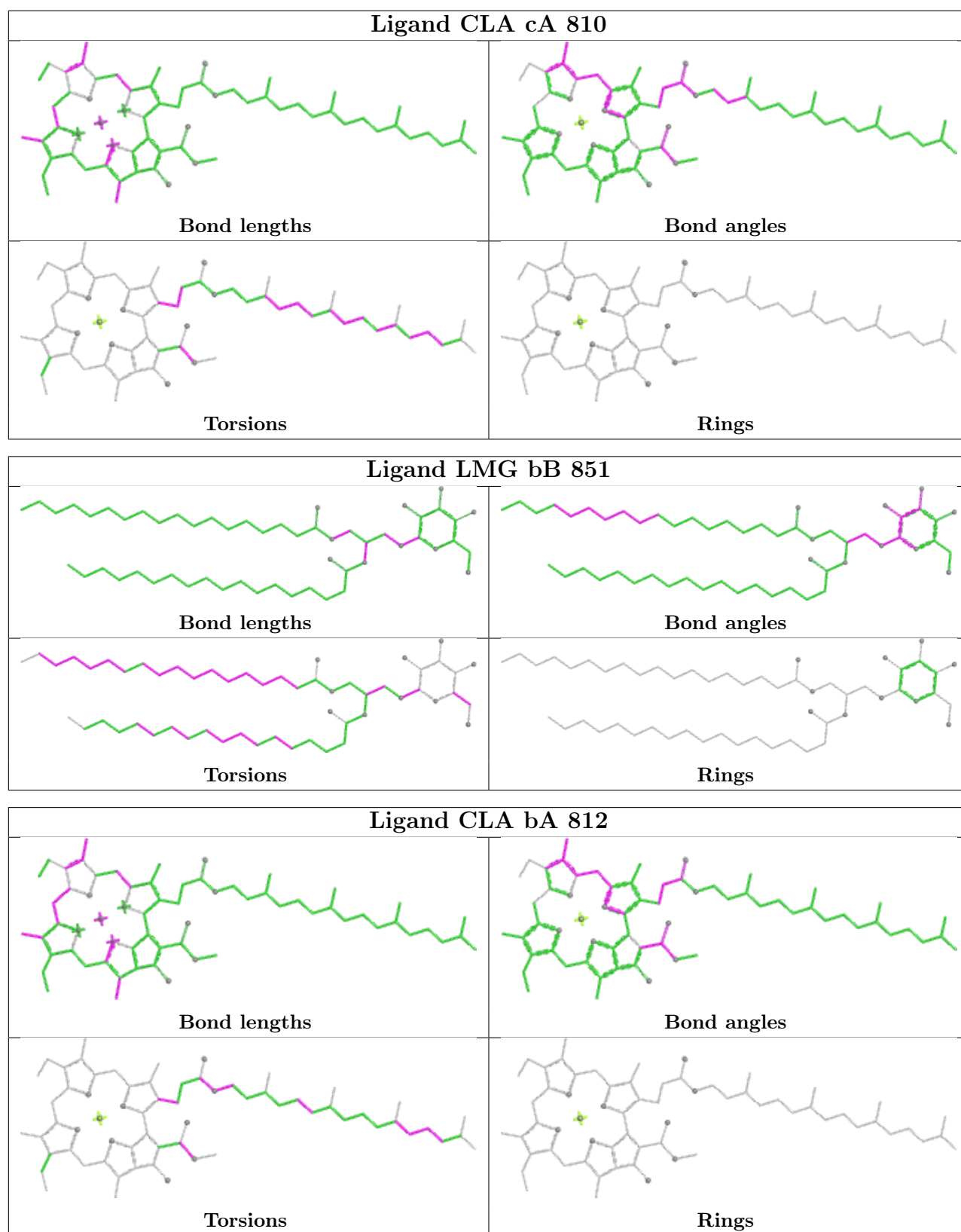


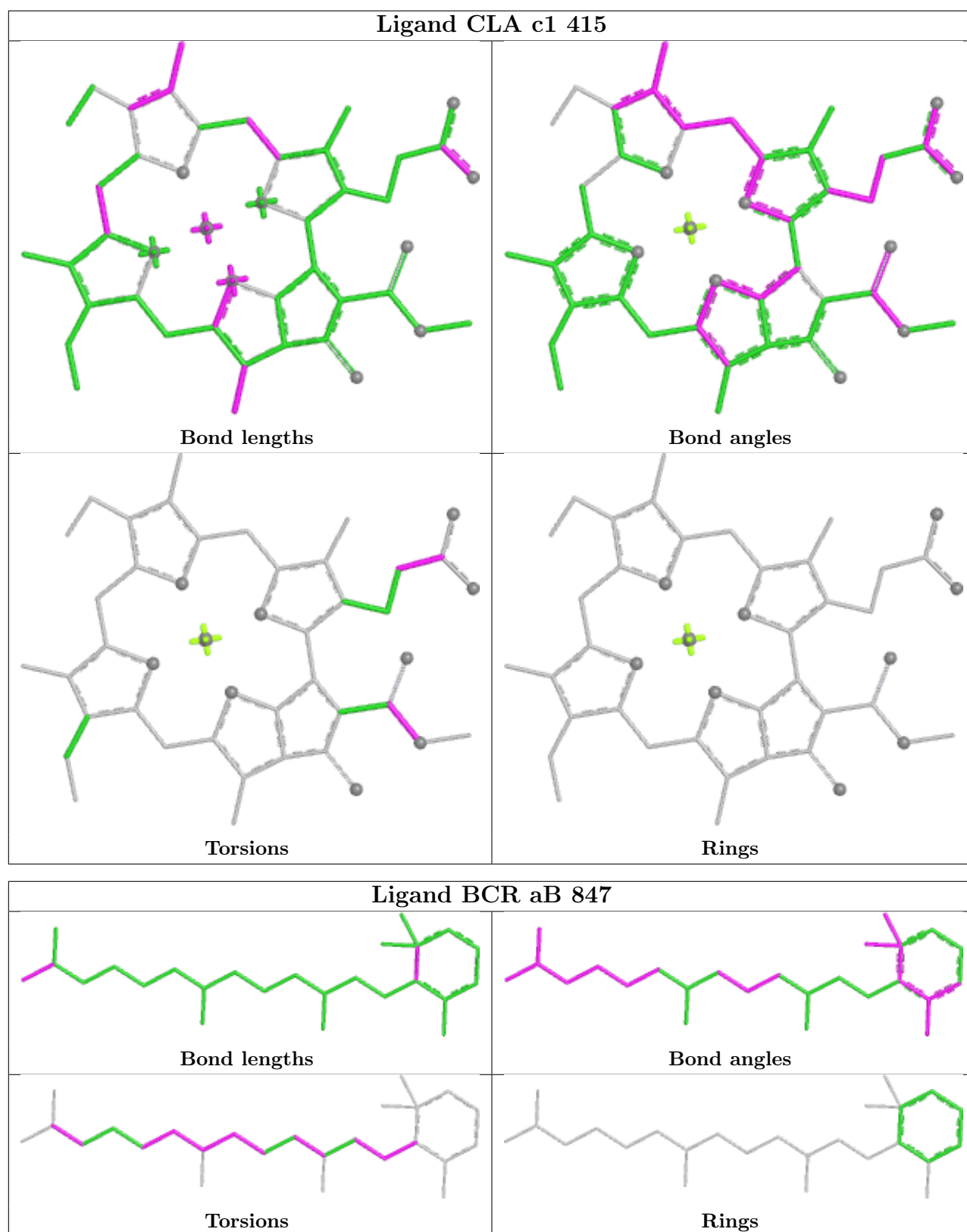


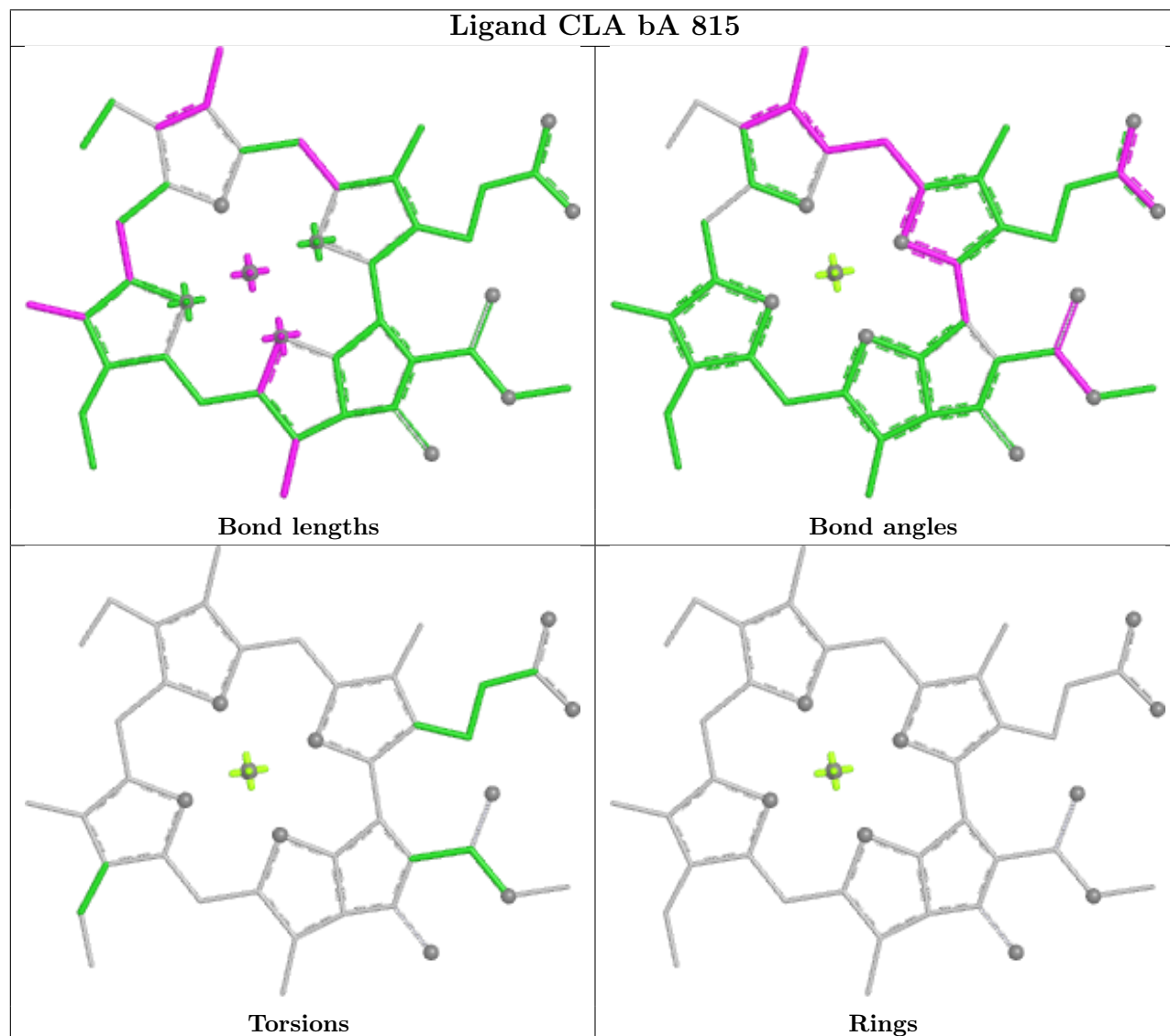
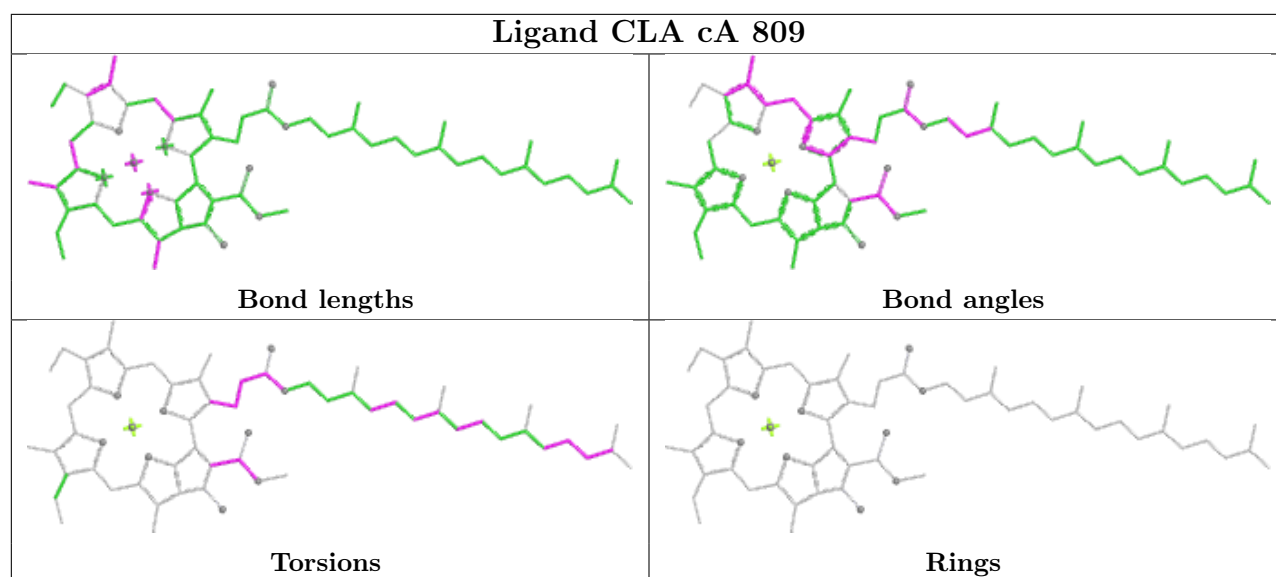


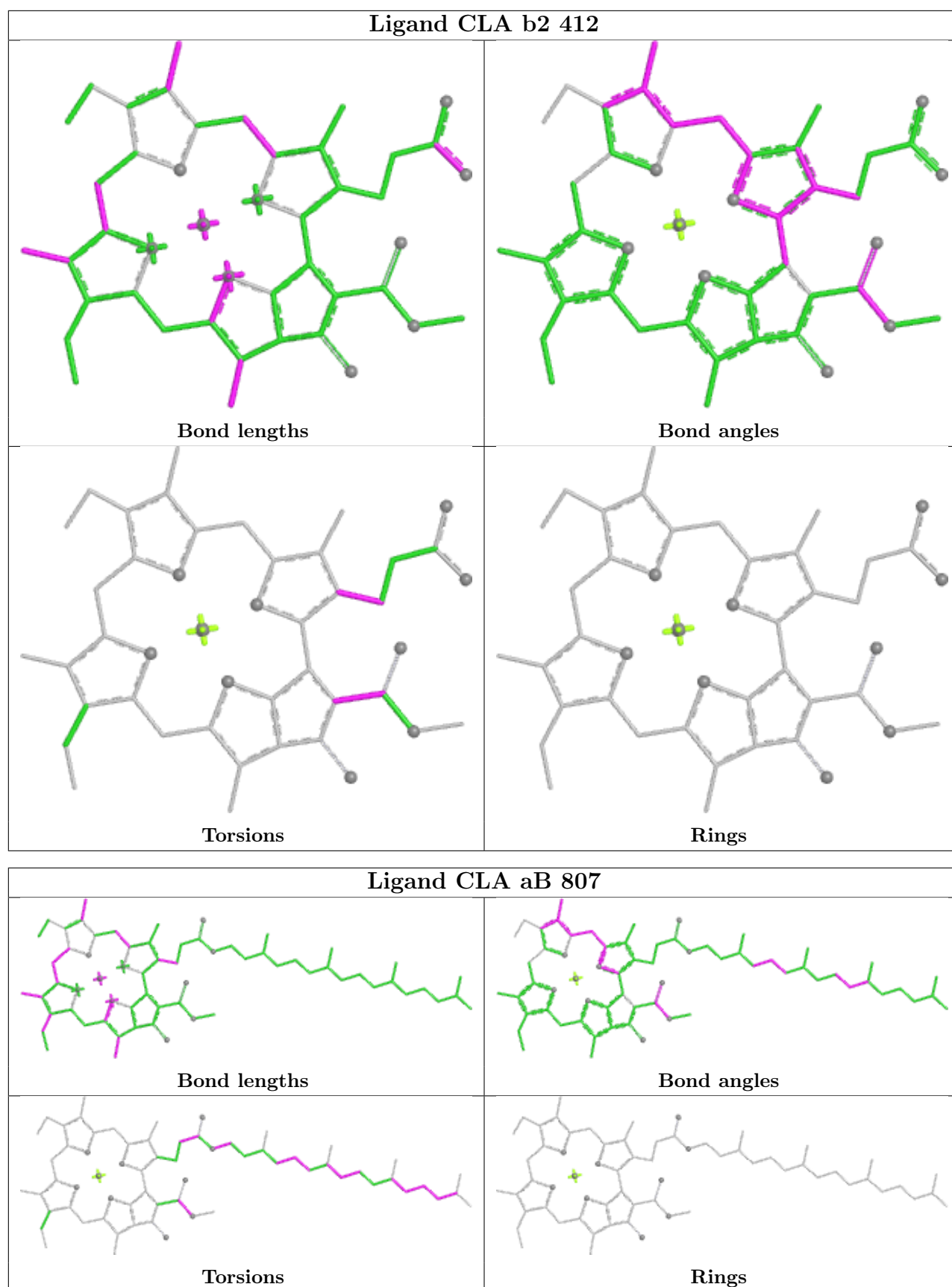




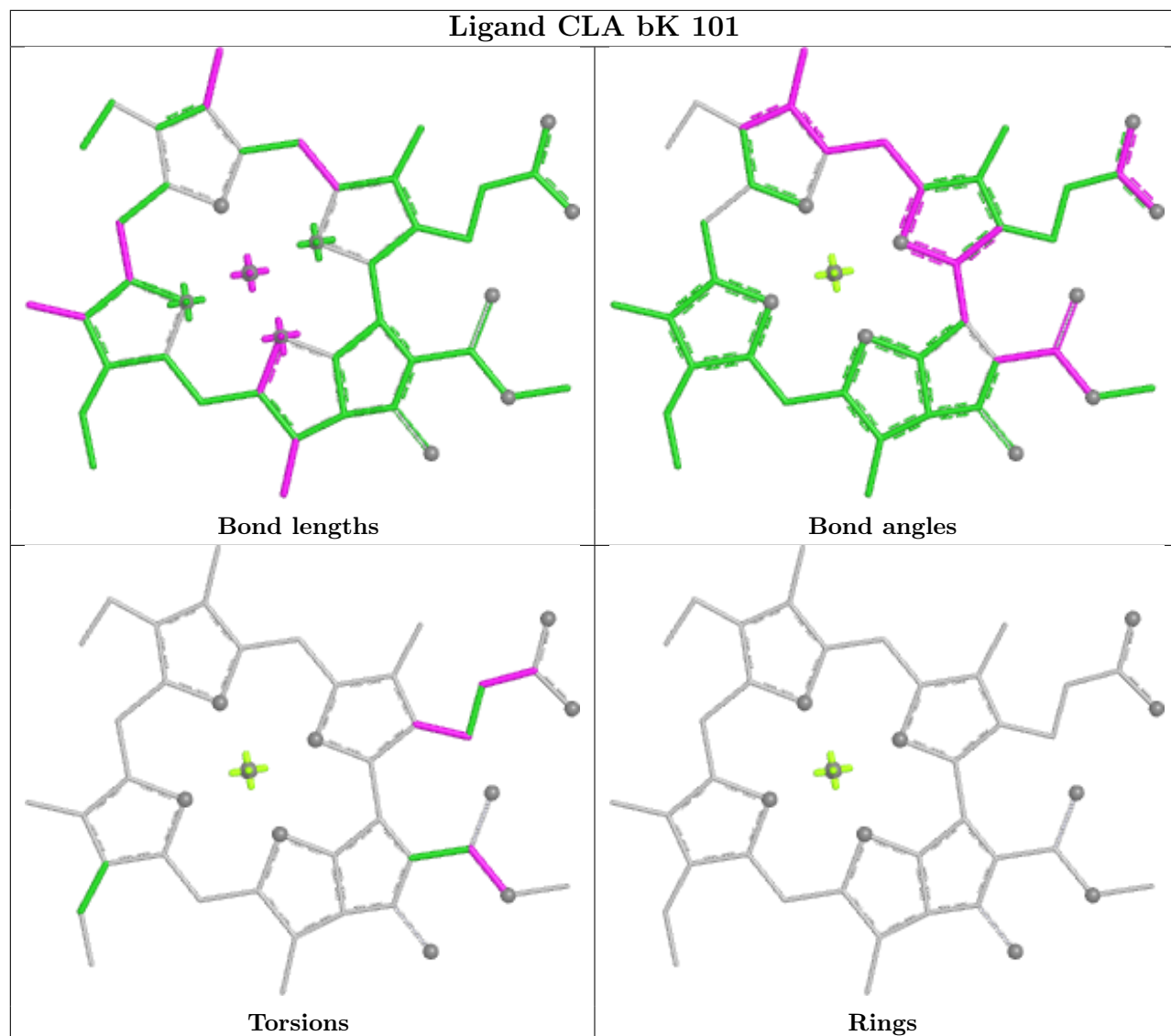


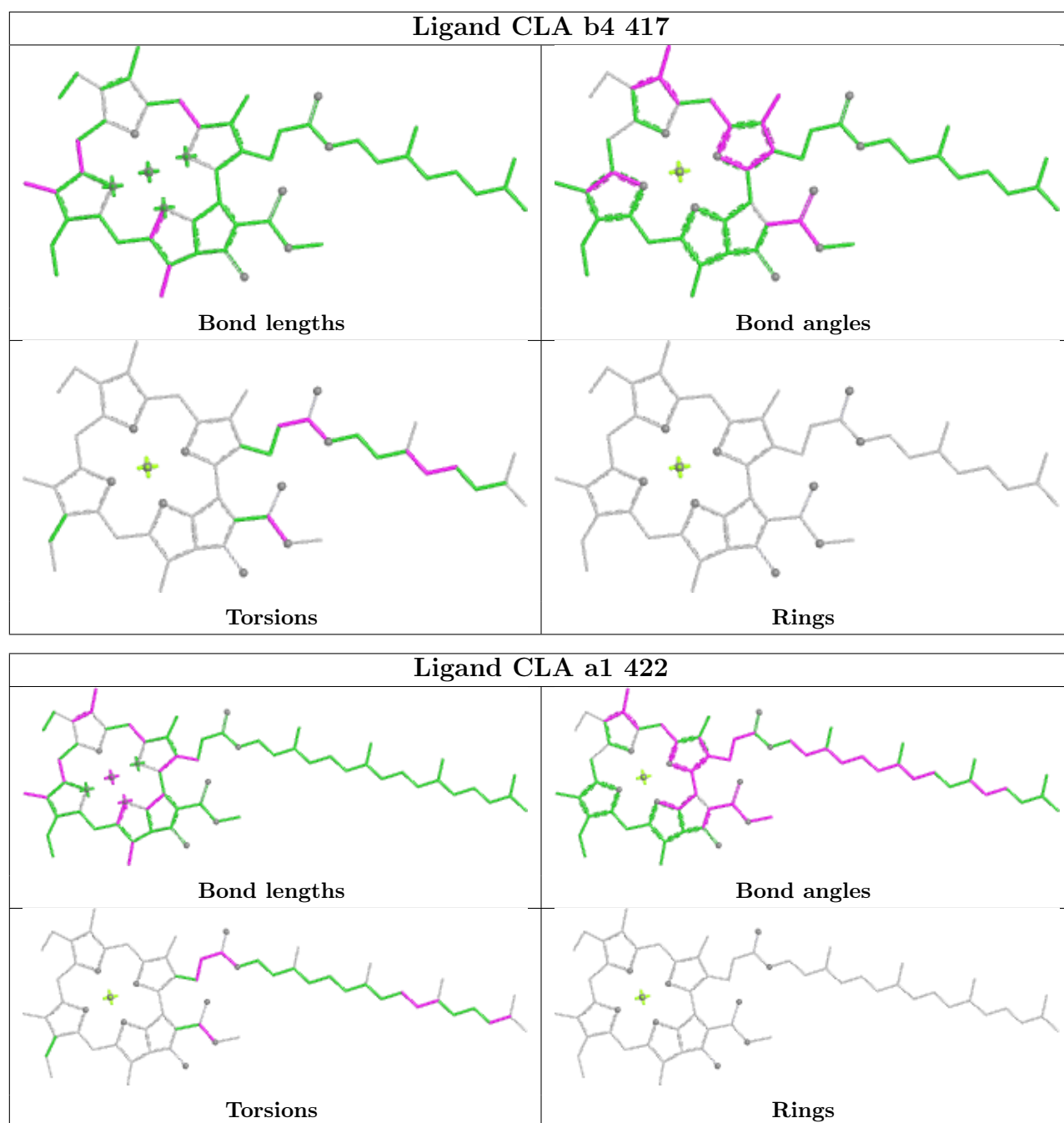


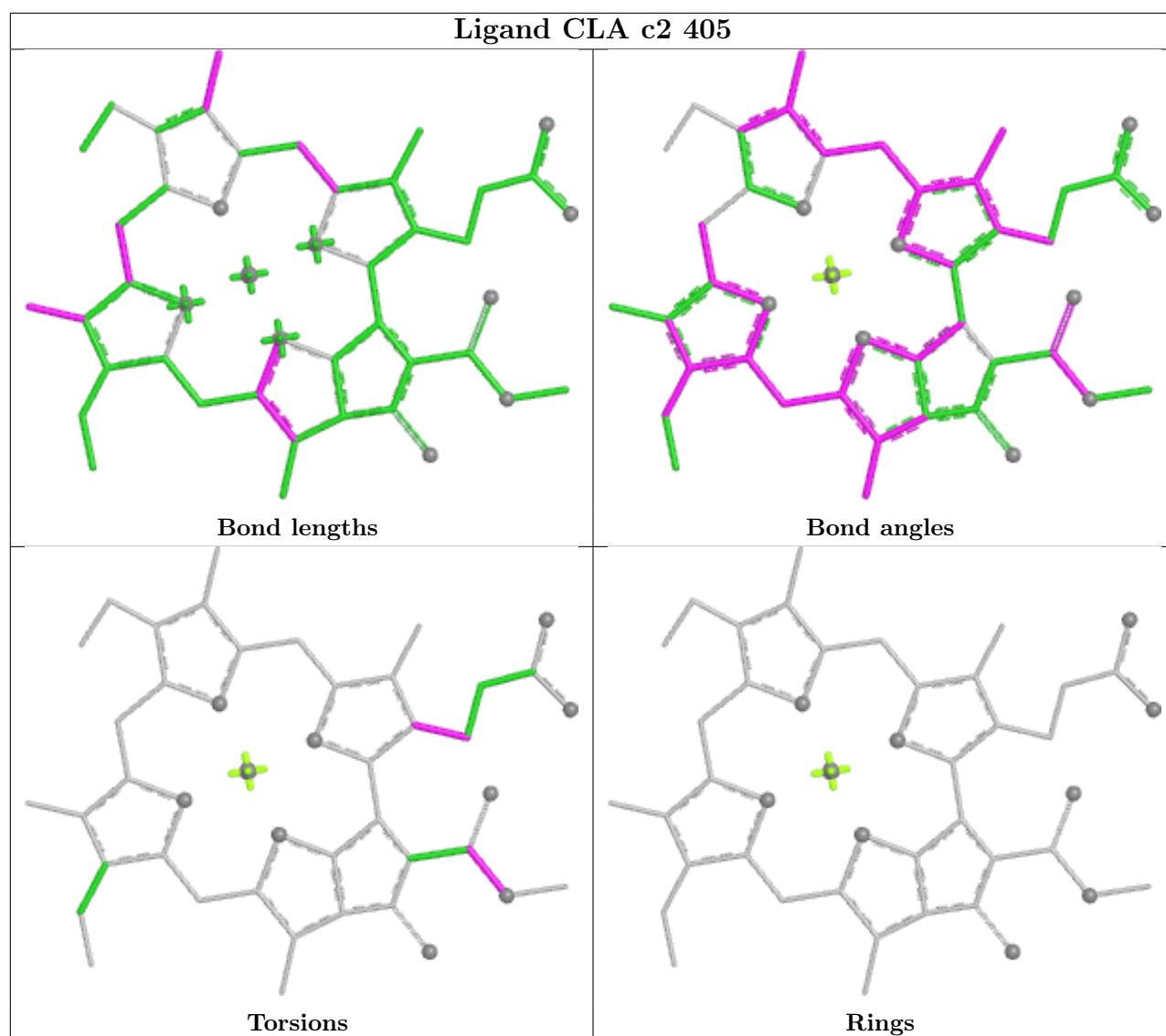




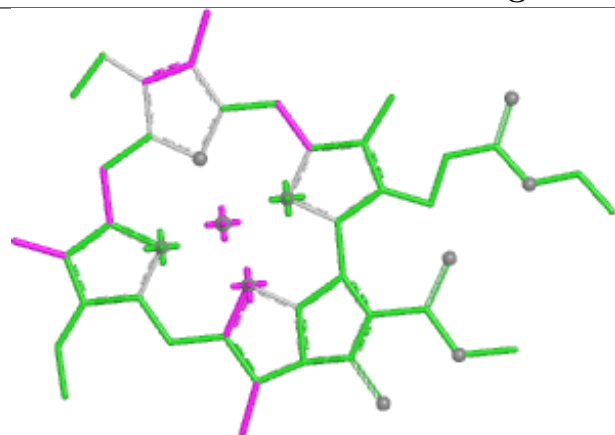
Ligand CLA bK 101



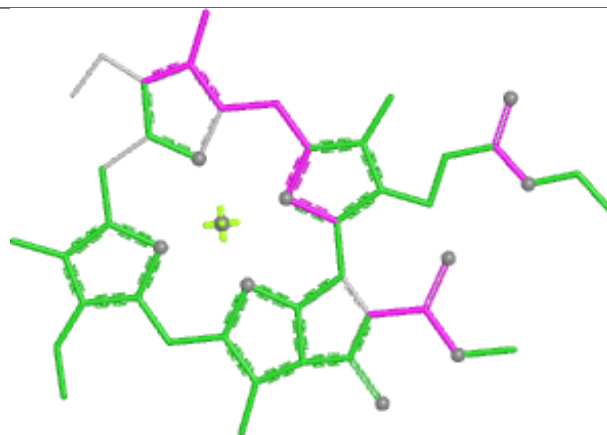




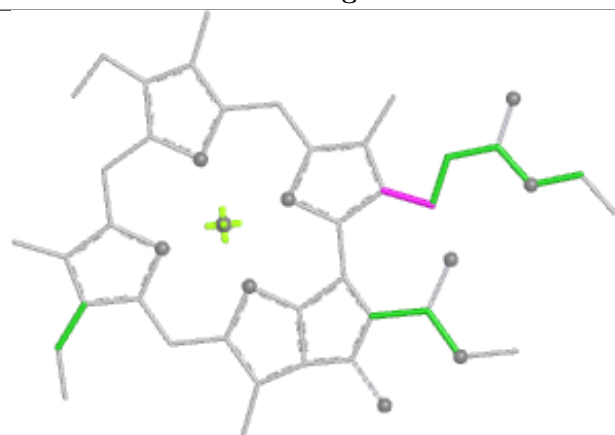
Ligand CLA cB 838



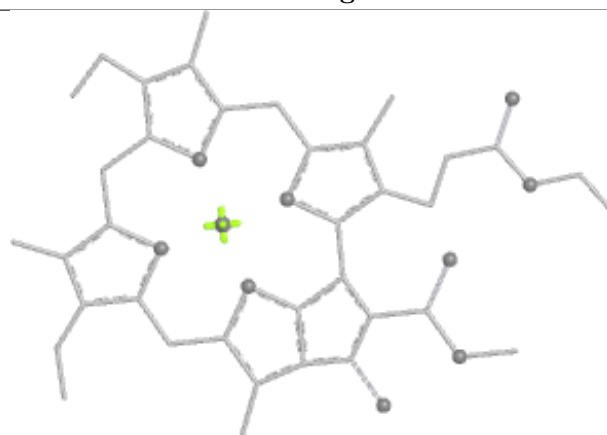
Bond lengths



Bond angles

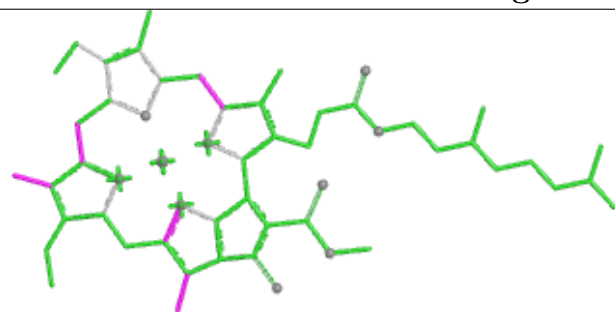


Torsions

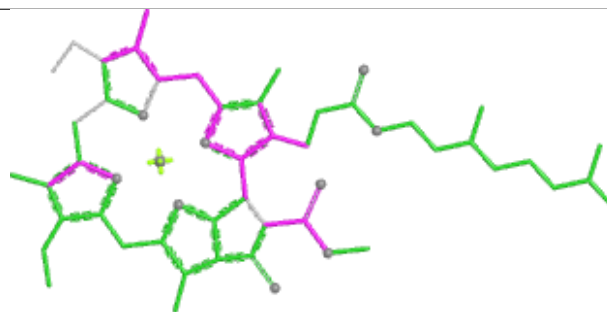


Rings

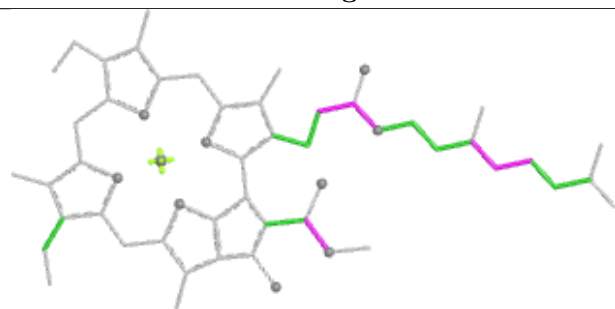
Ligand CLA c1 417



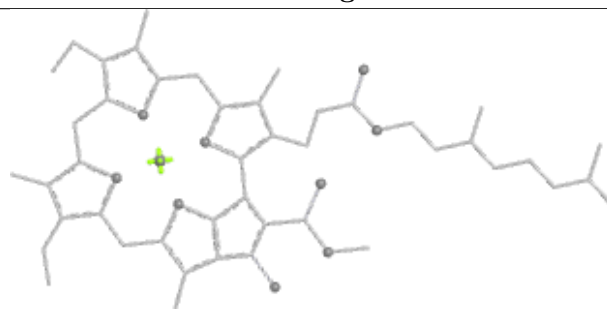
Bond lengths



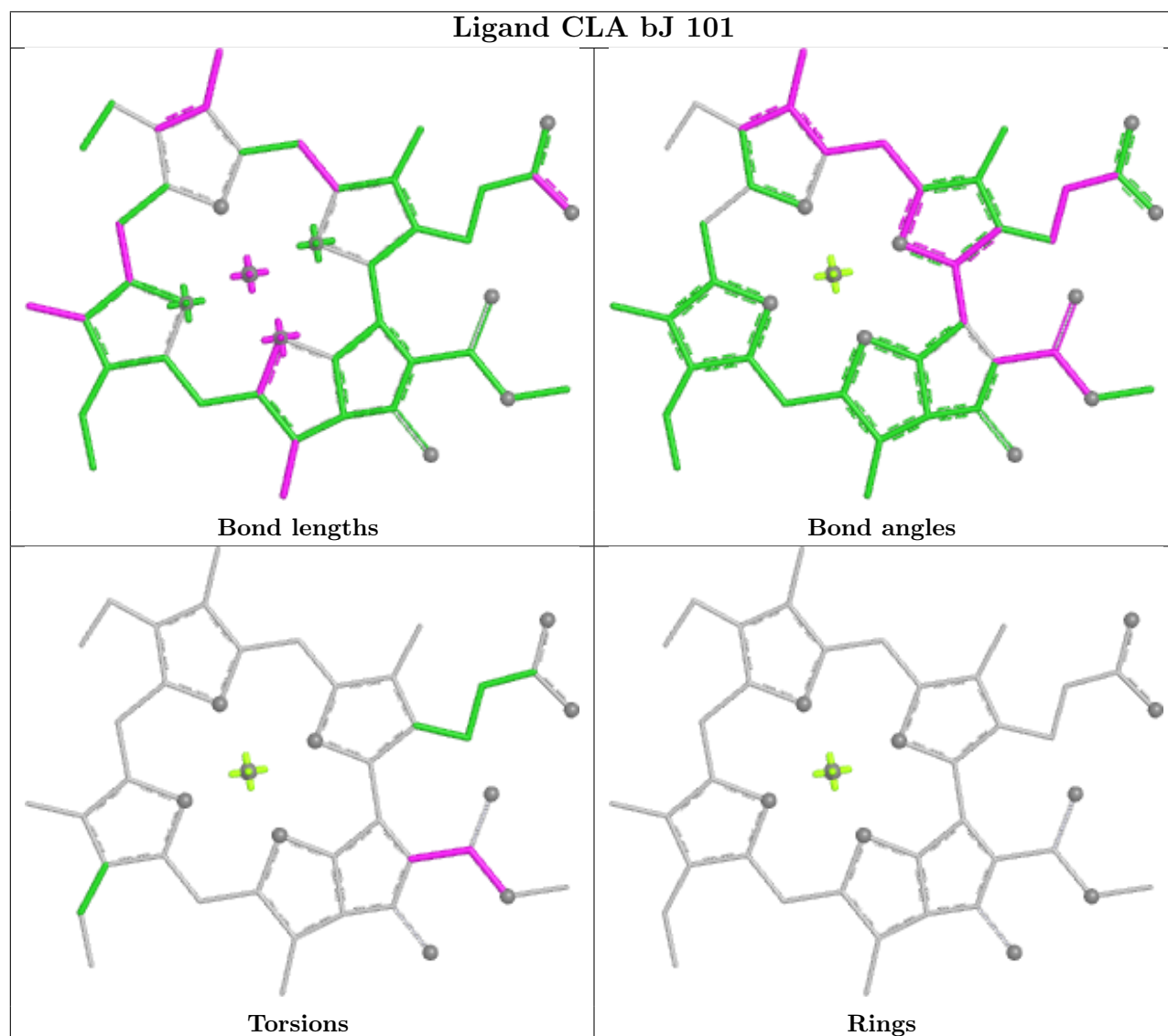
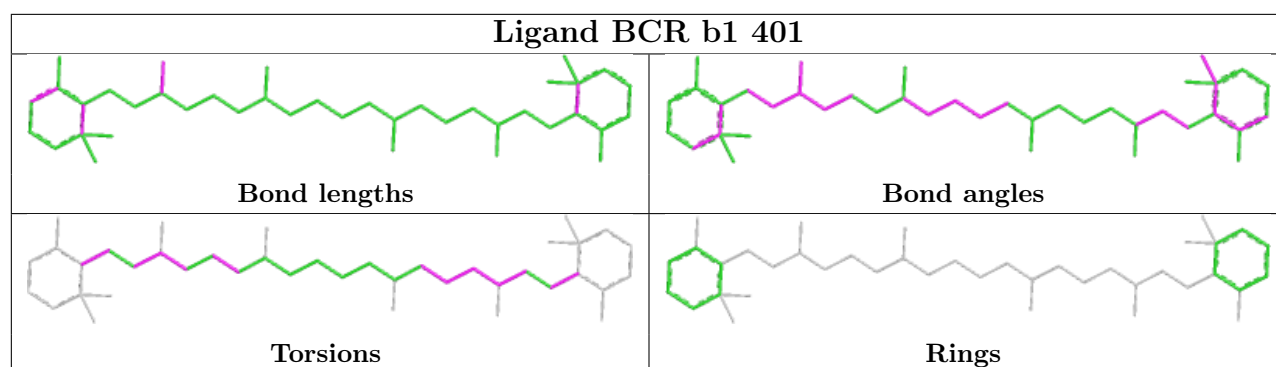
Bond angles

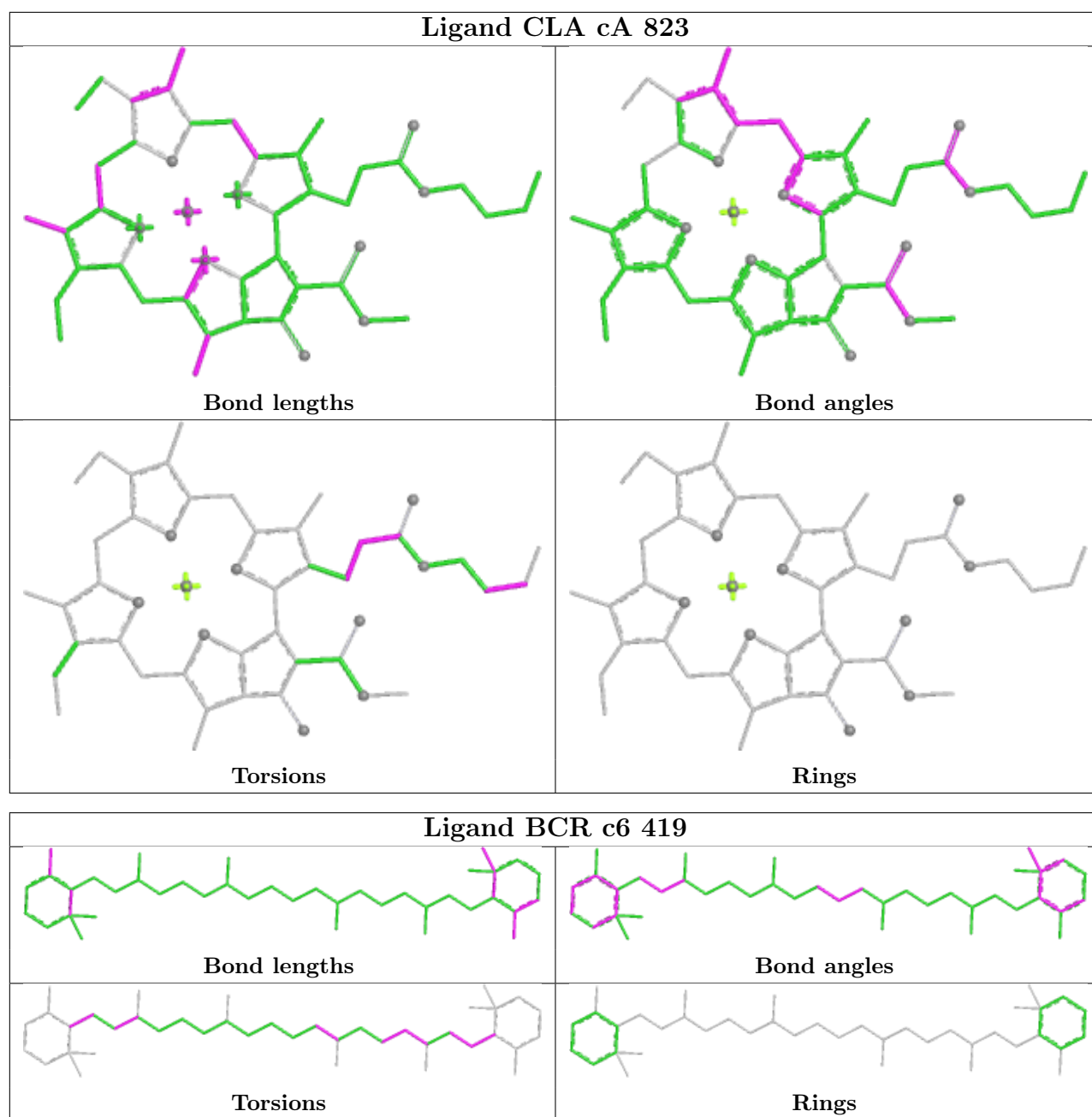


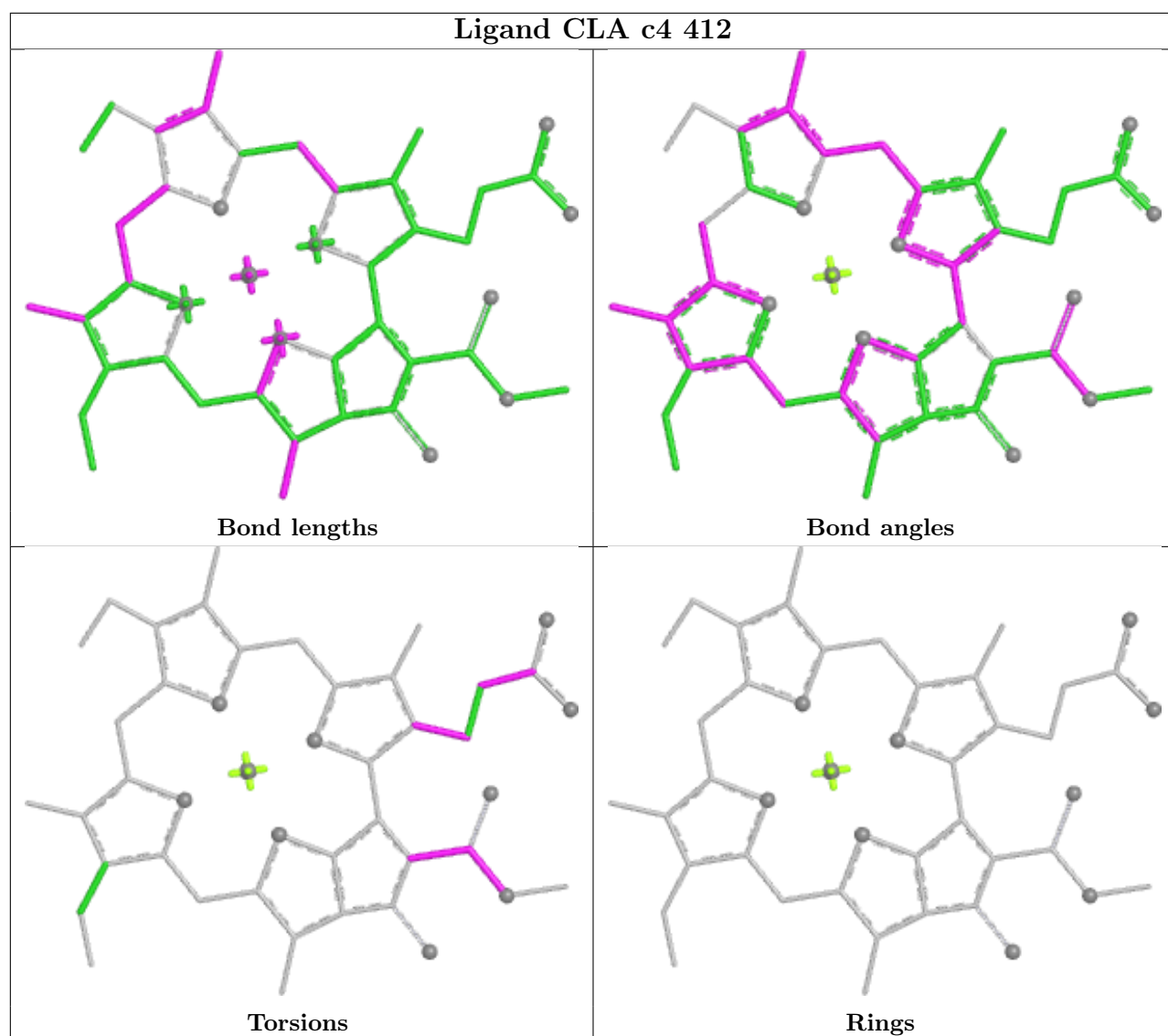
Torsions

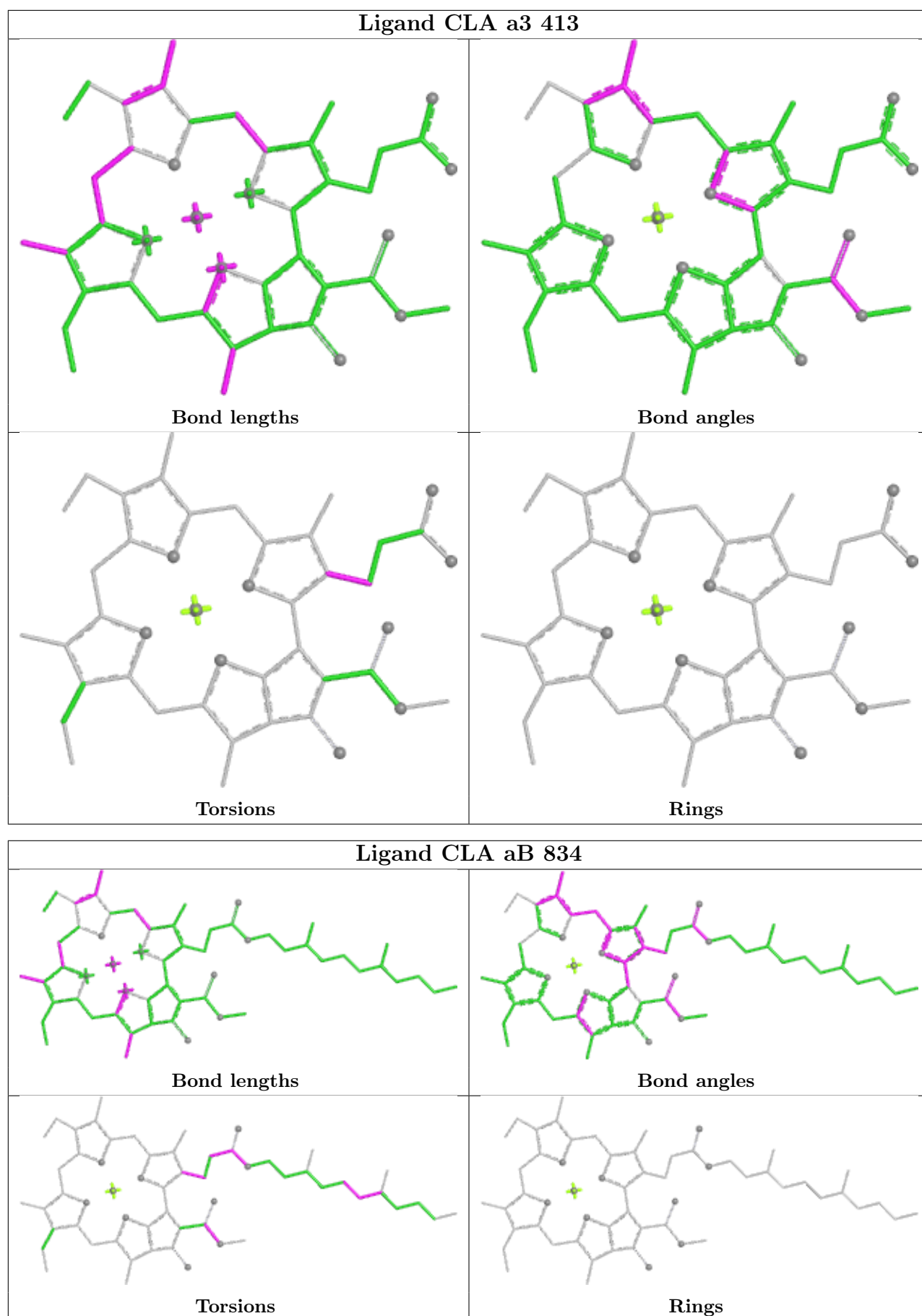


Rings

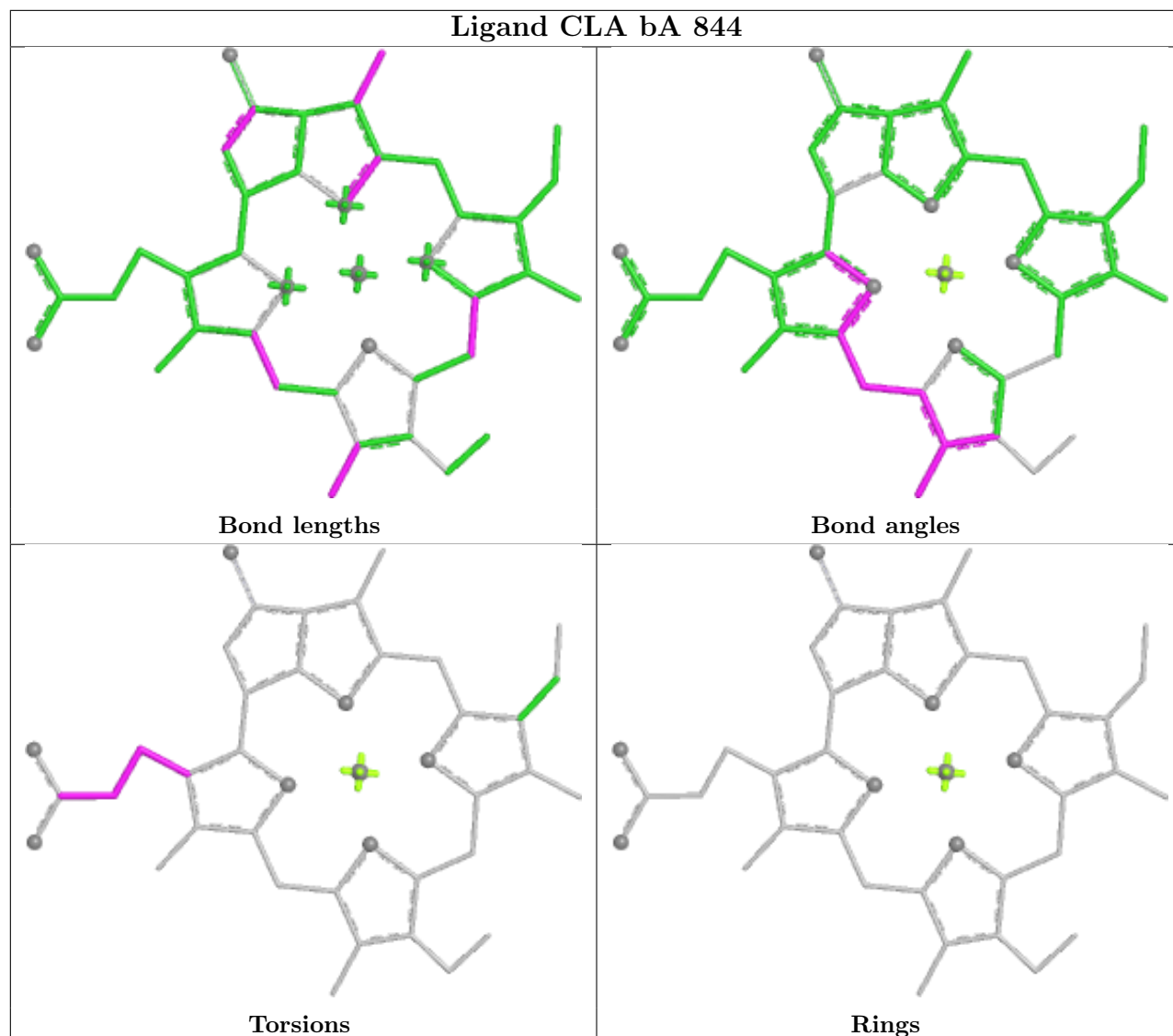




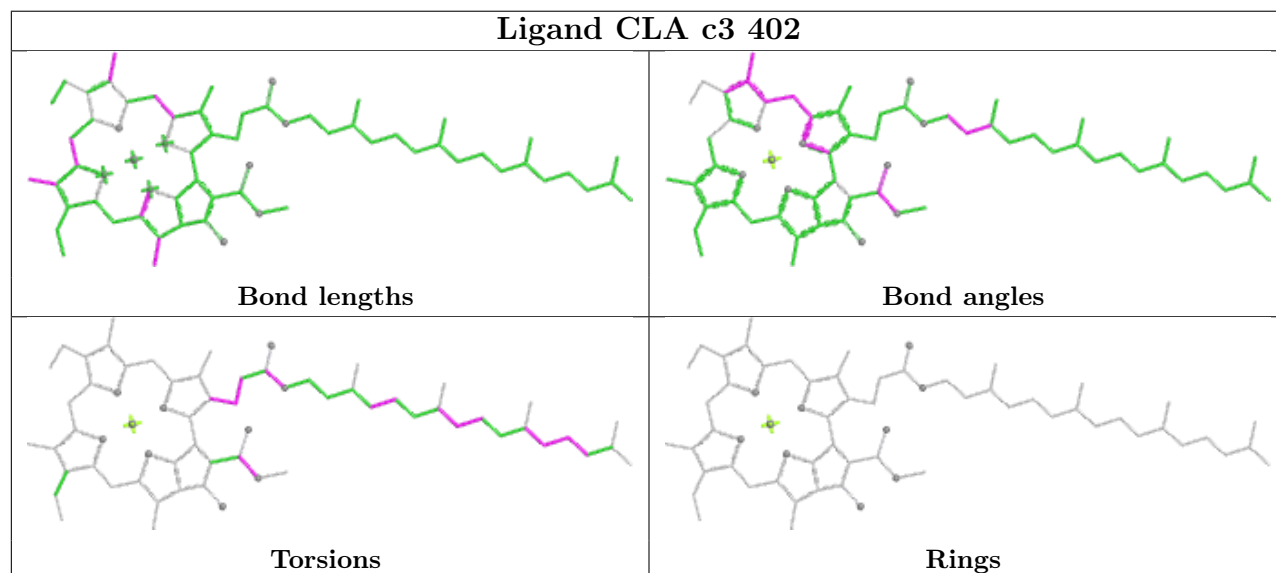


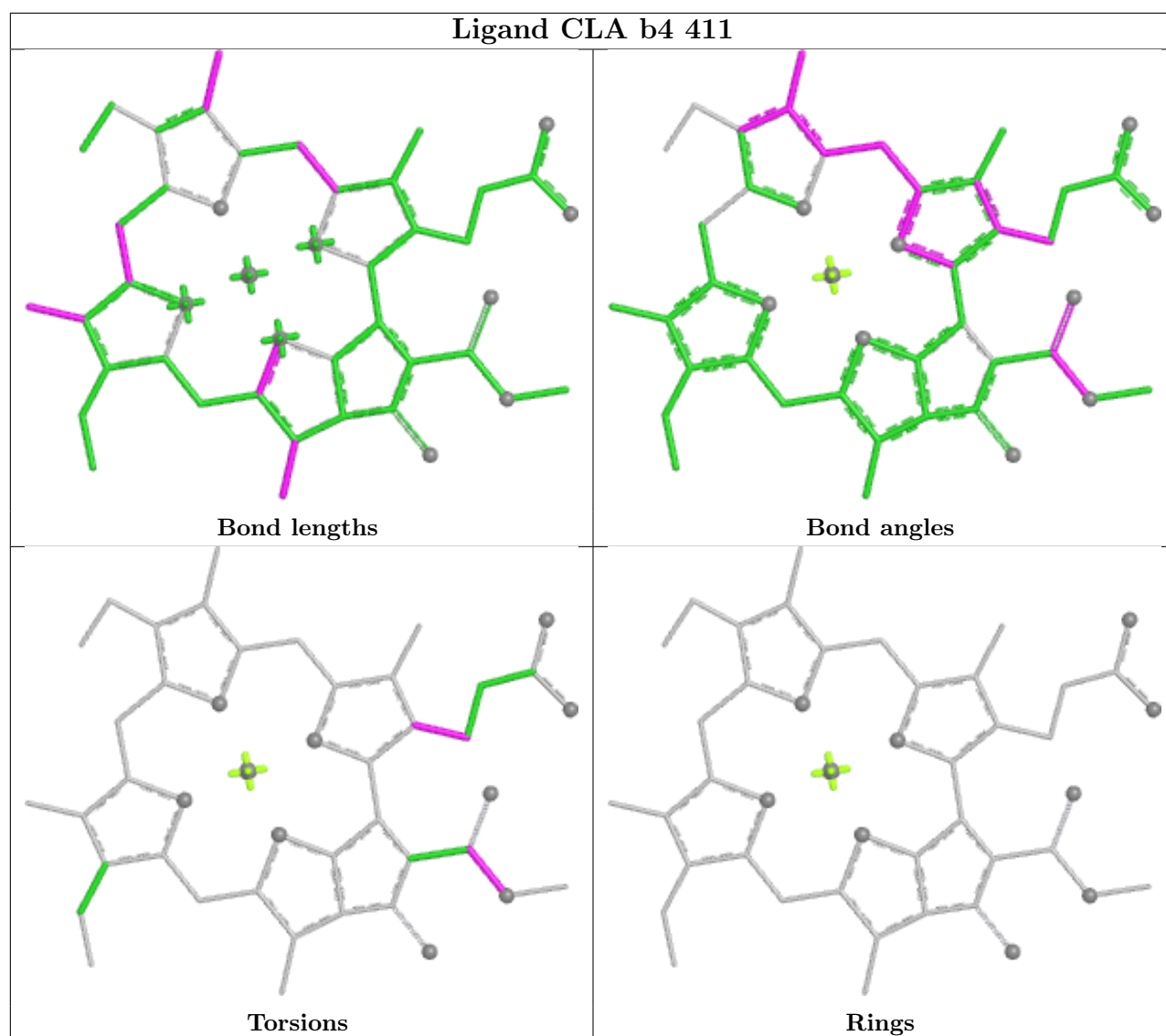


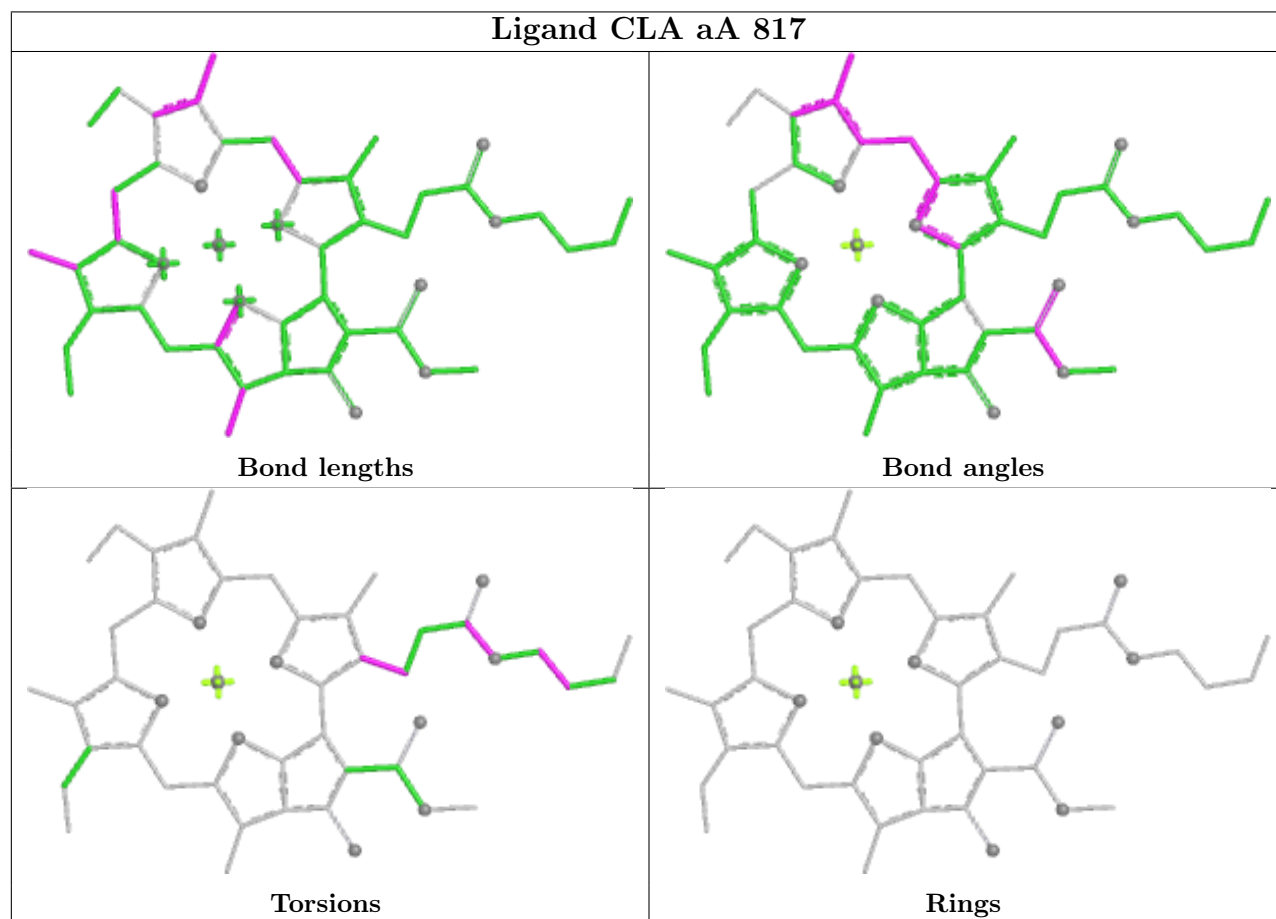
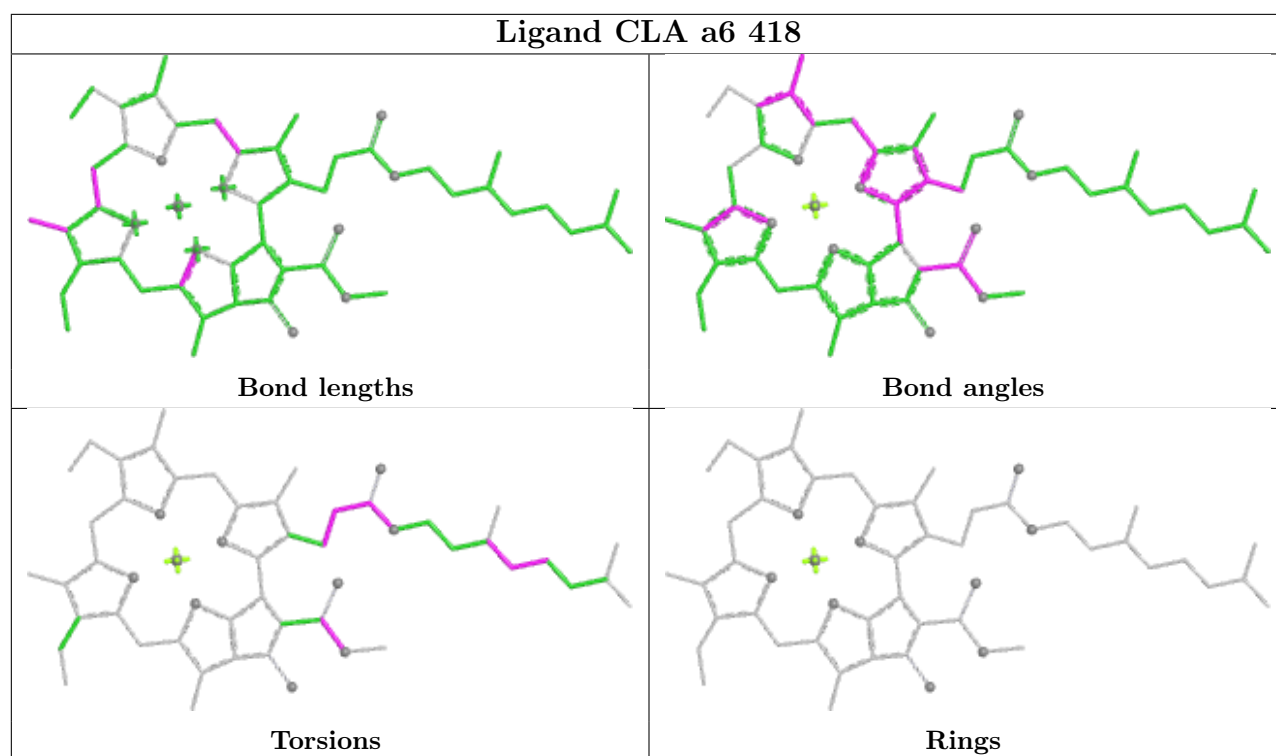
Ligand CLA bA 844

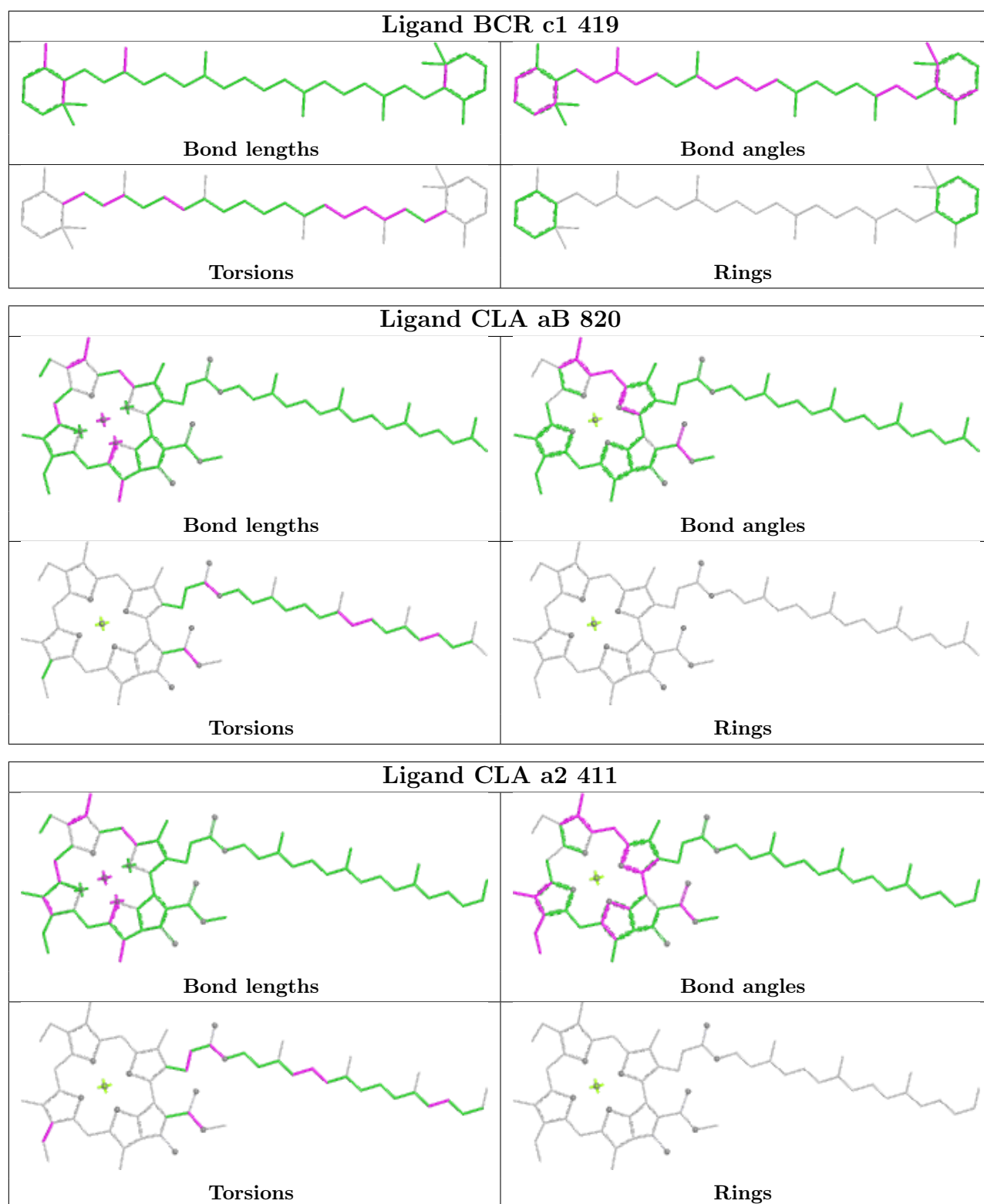


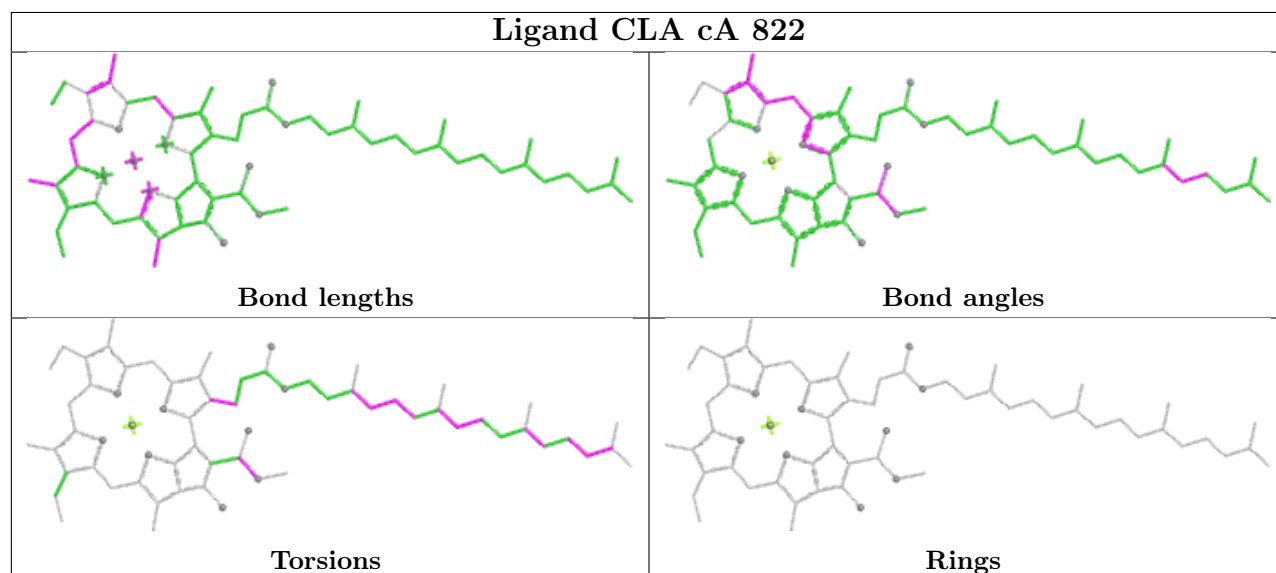
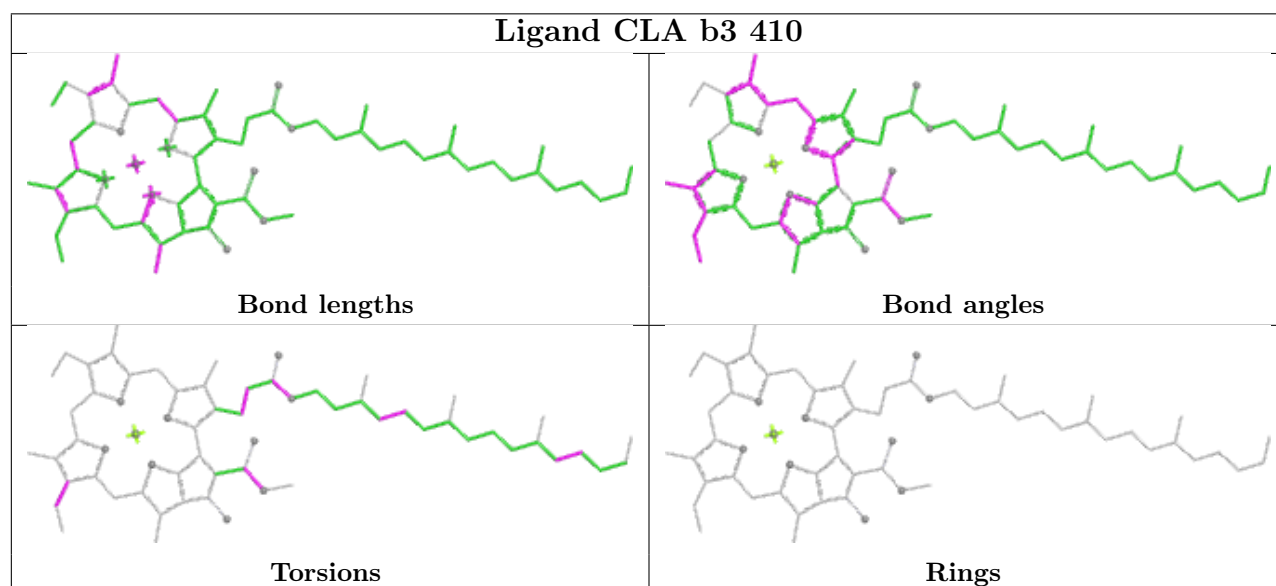
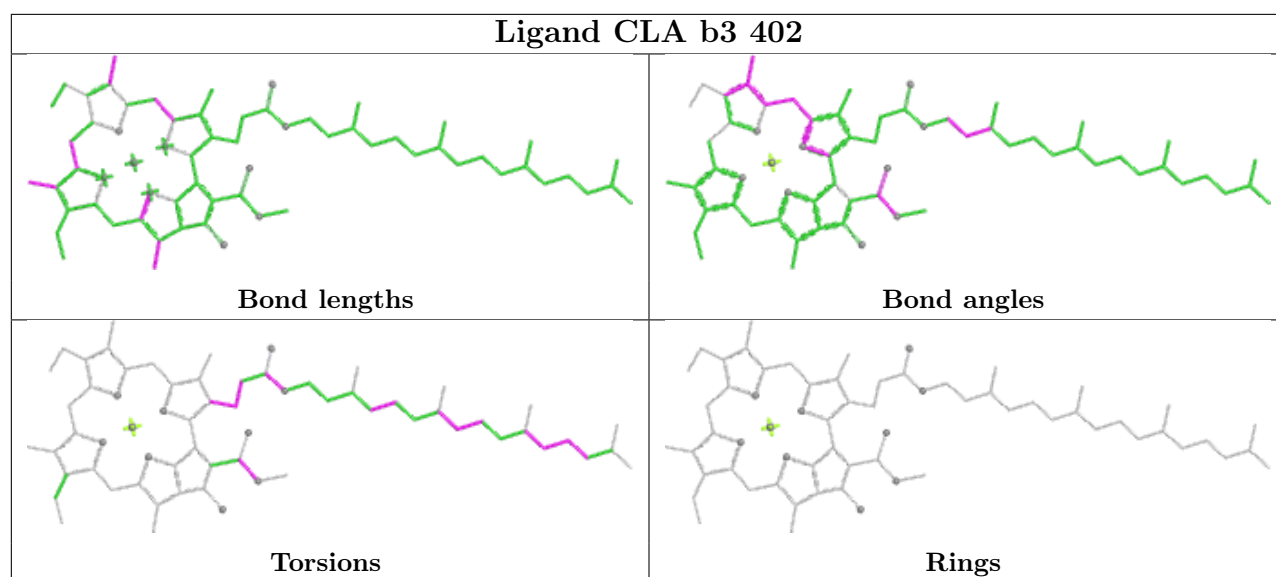
Ligand CLA c3 402

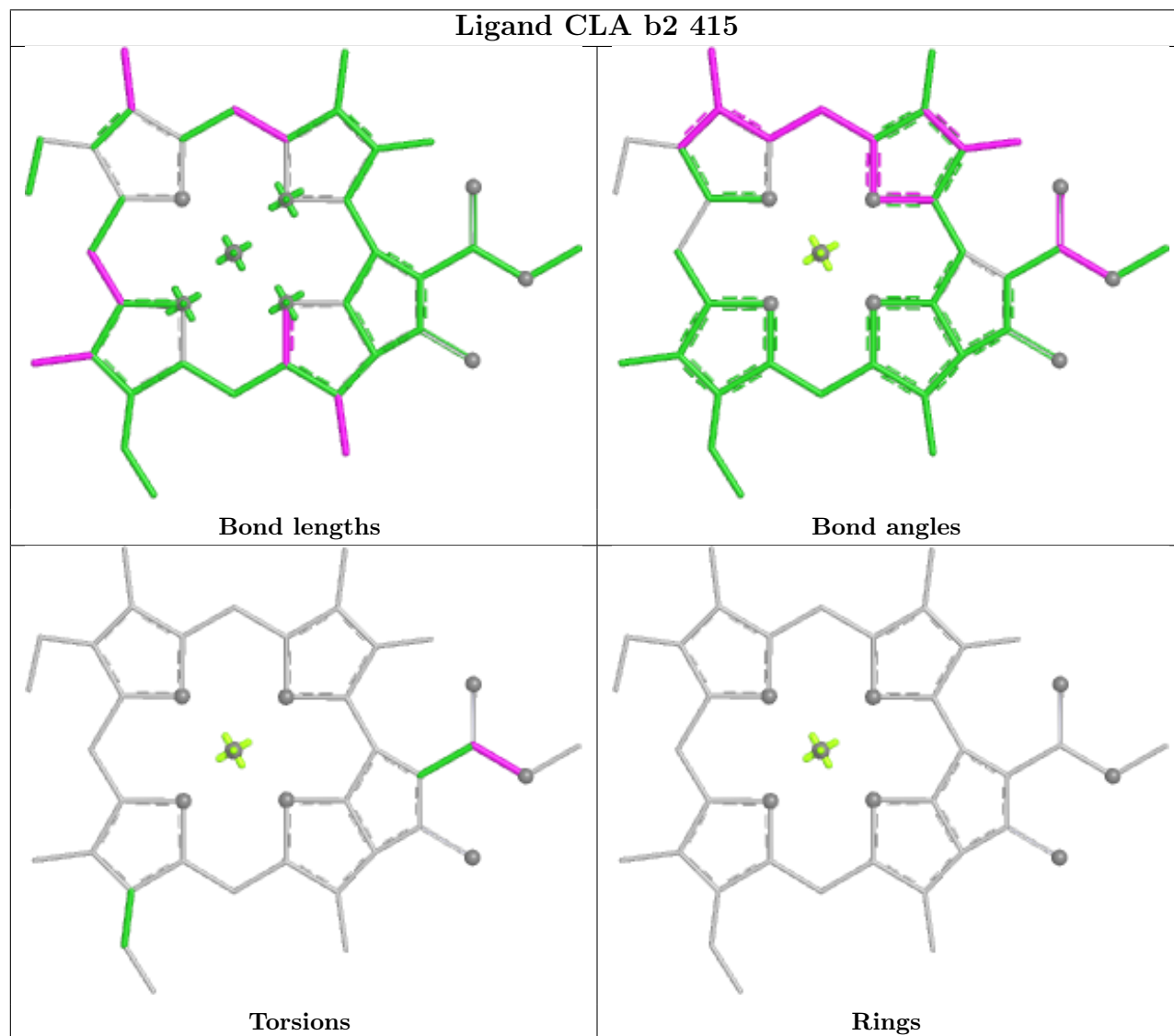
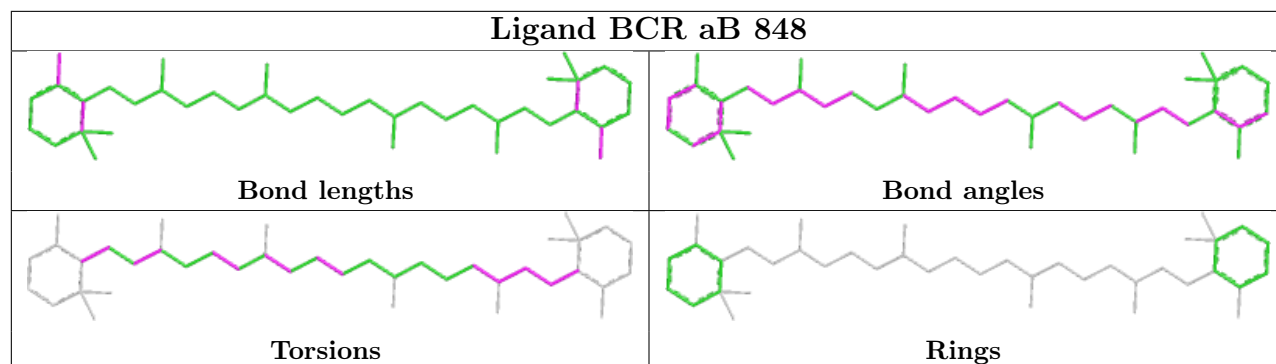


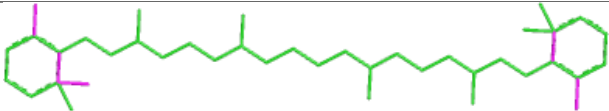
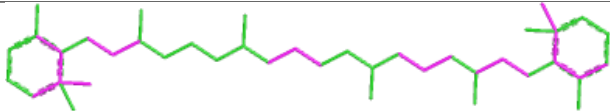
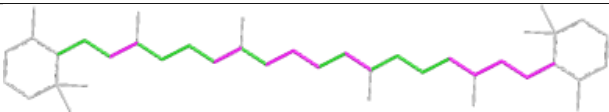
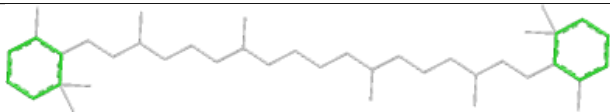

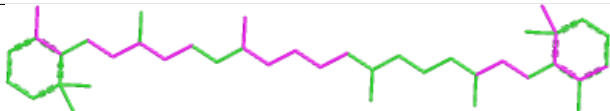
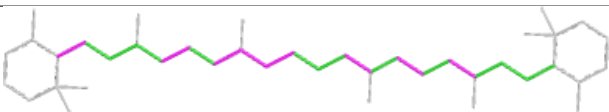
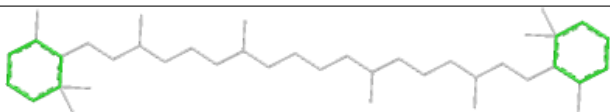


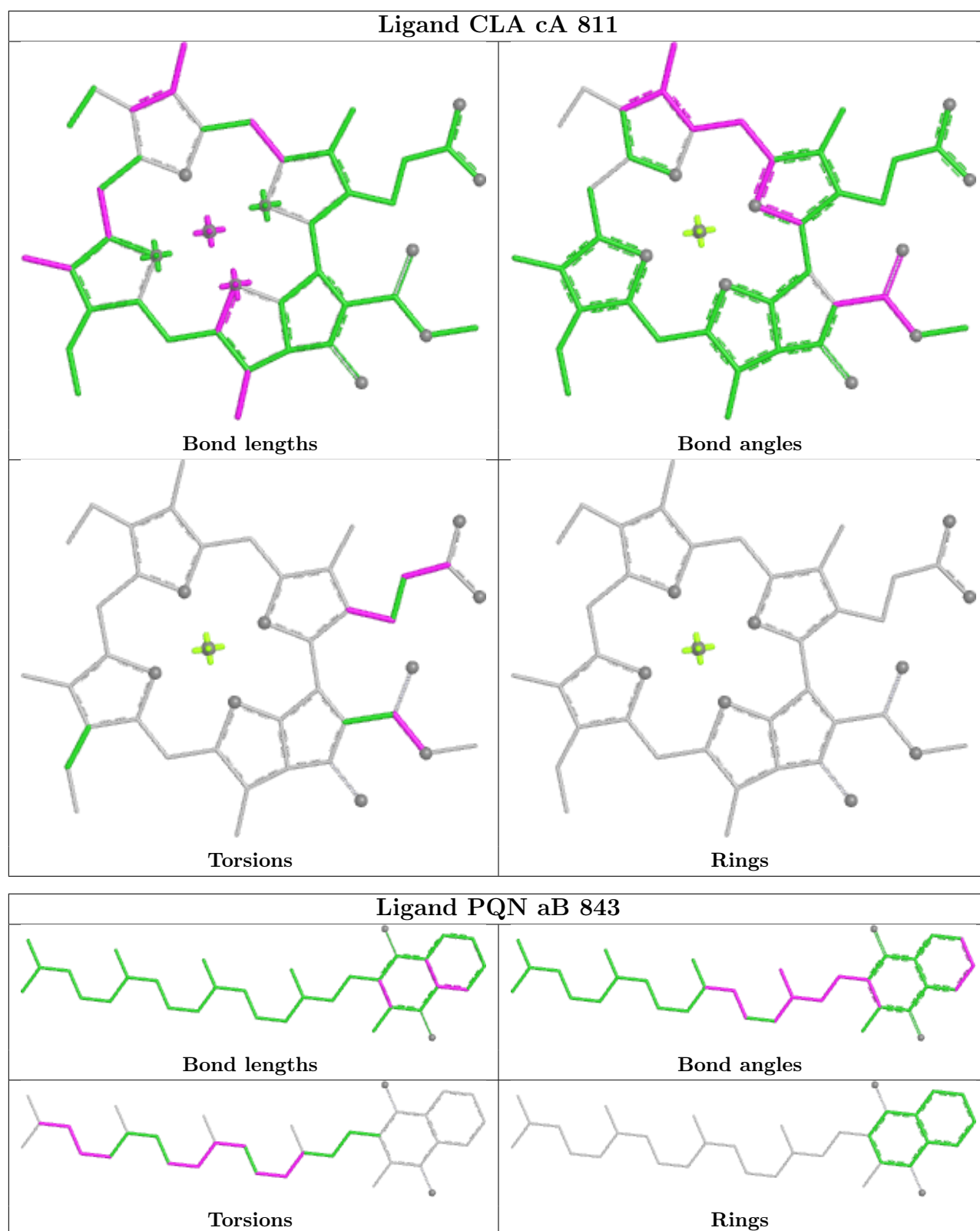


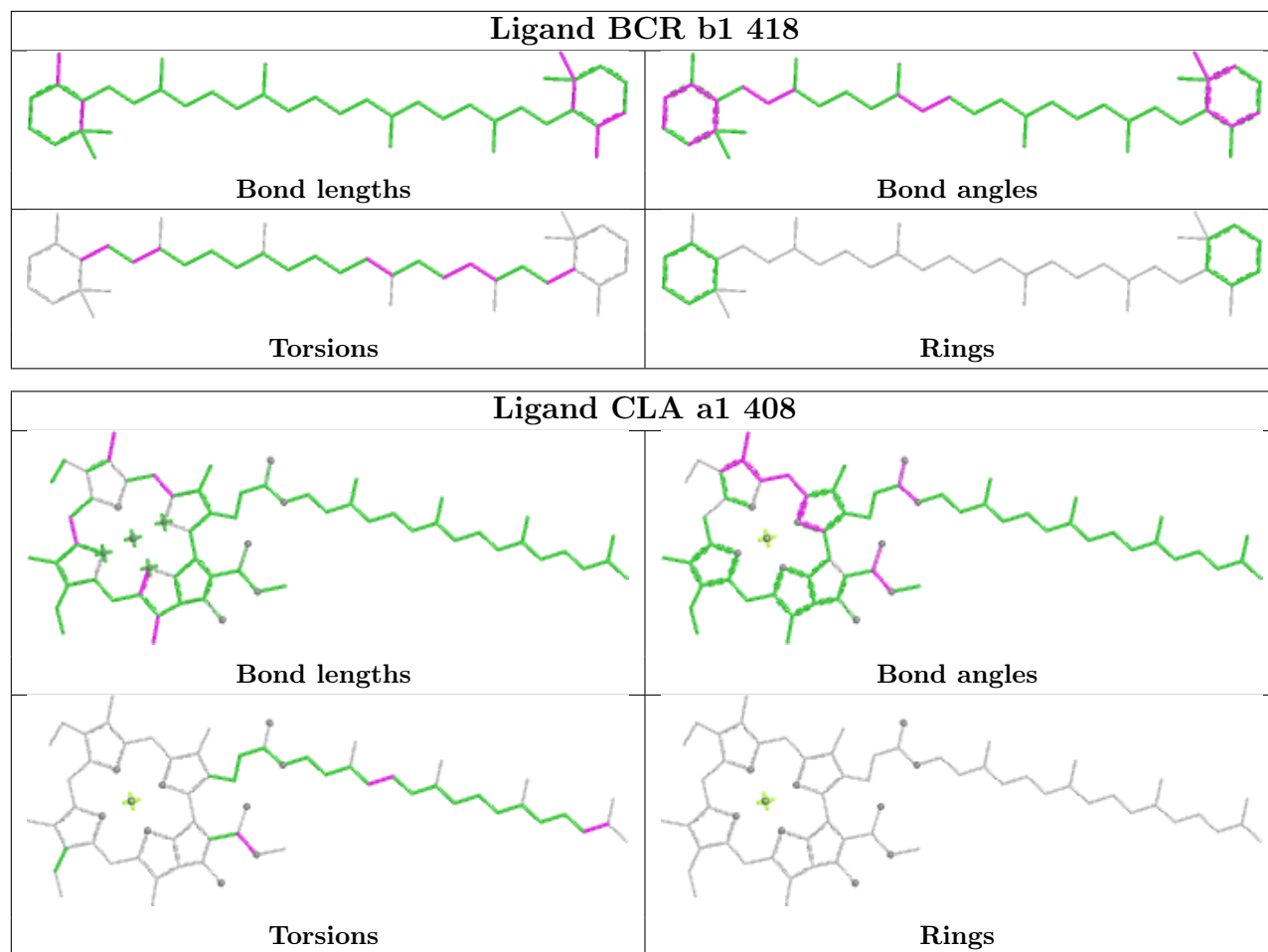


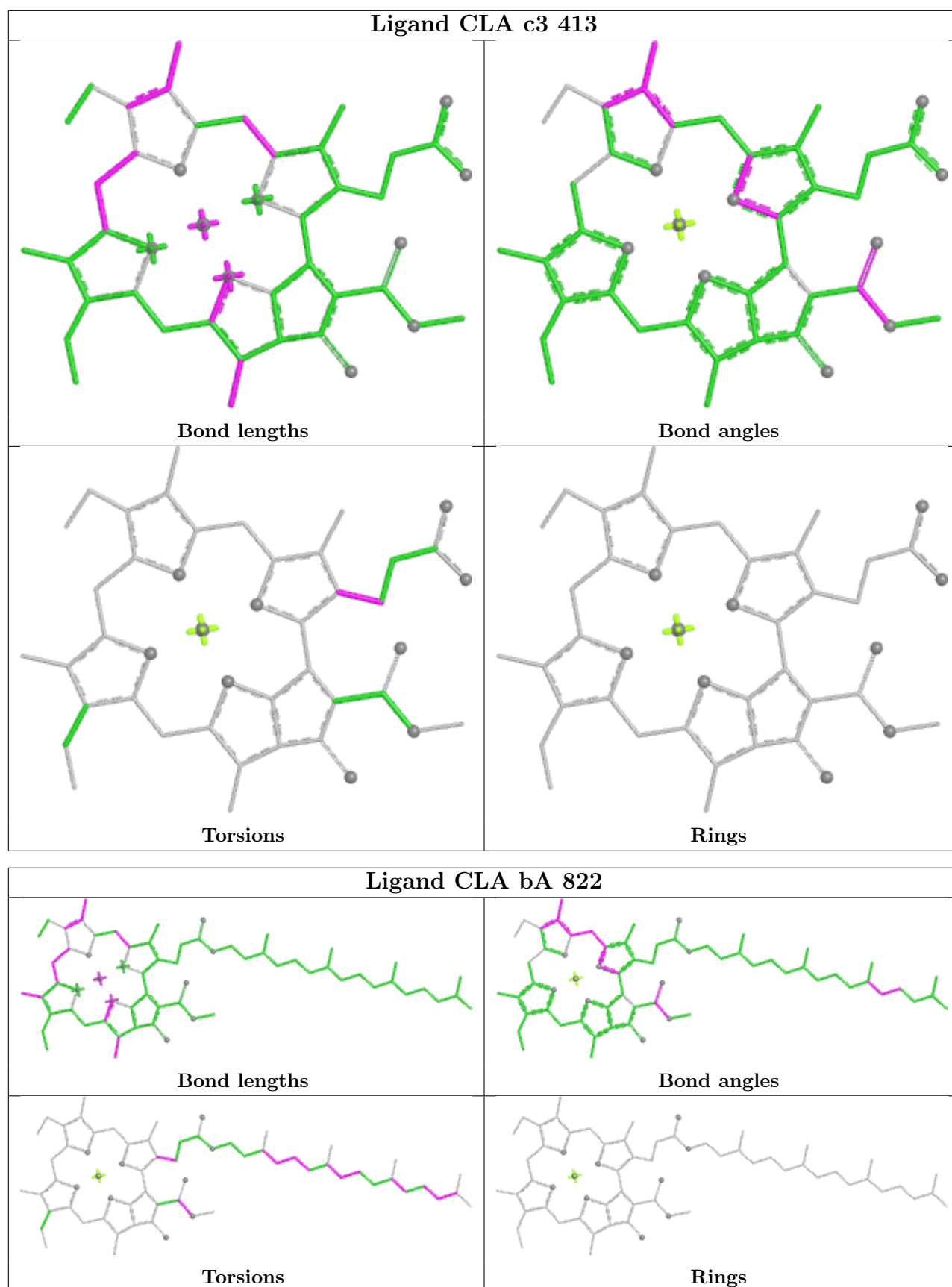


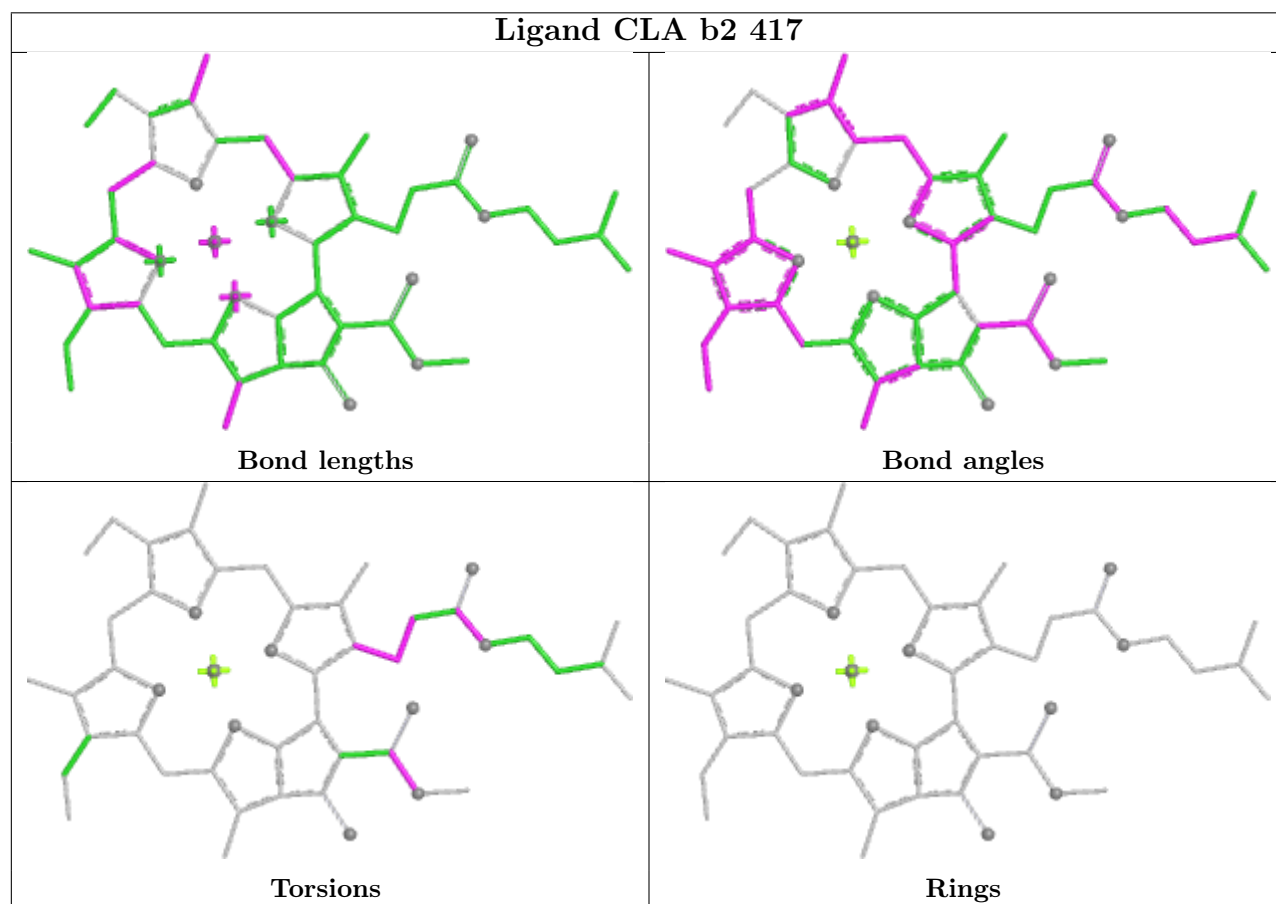
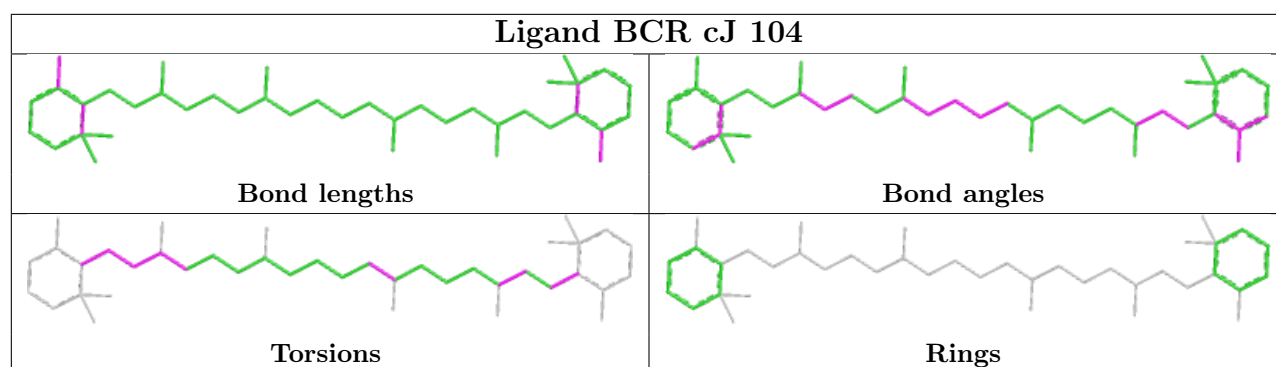


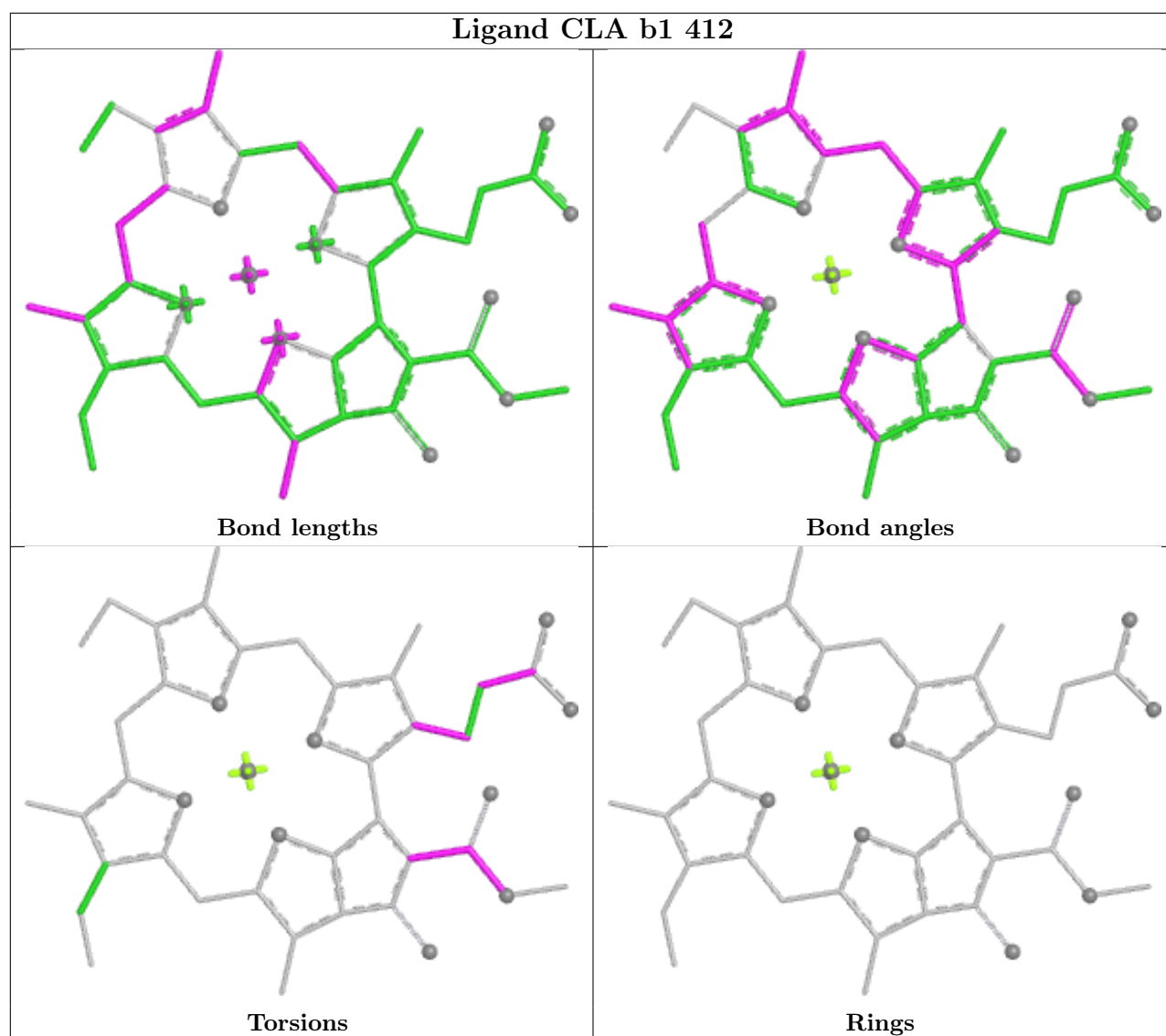
Ligand BCR aF 201					
	Bond lengths				
	Torsions				
Rings					
Ligand BCR cJ 103					
	Bond lengths				
	Torsions				
Rings					

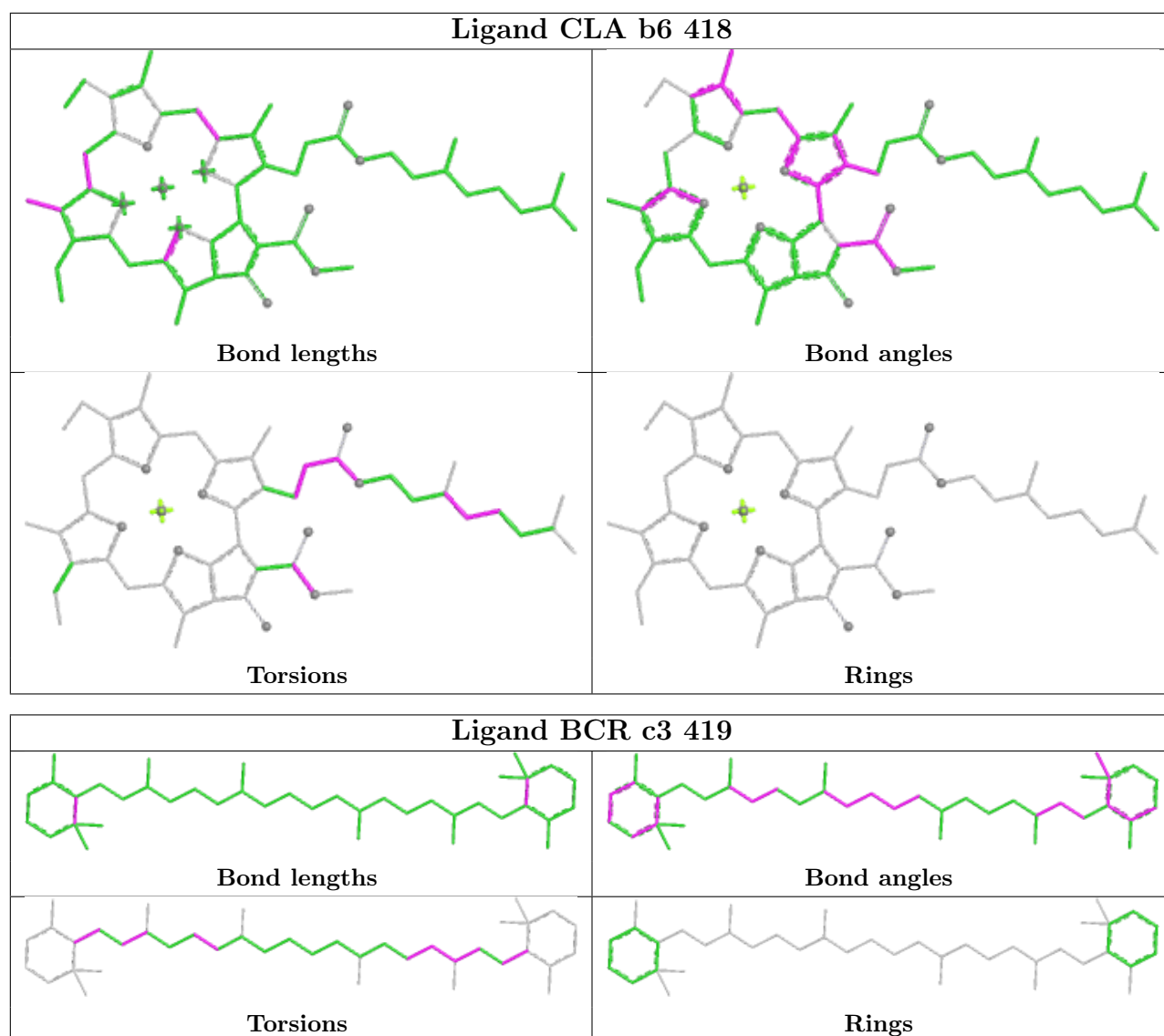




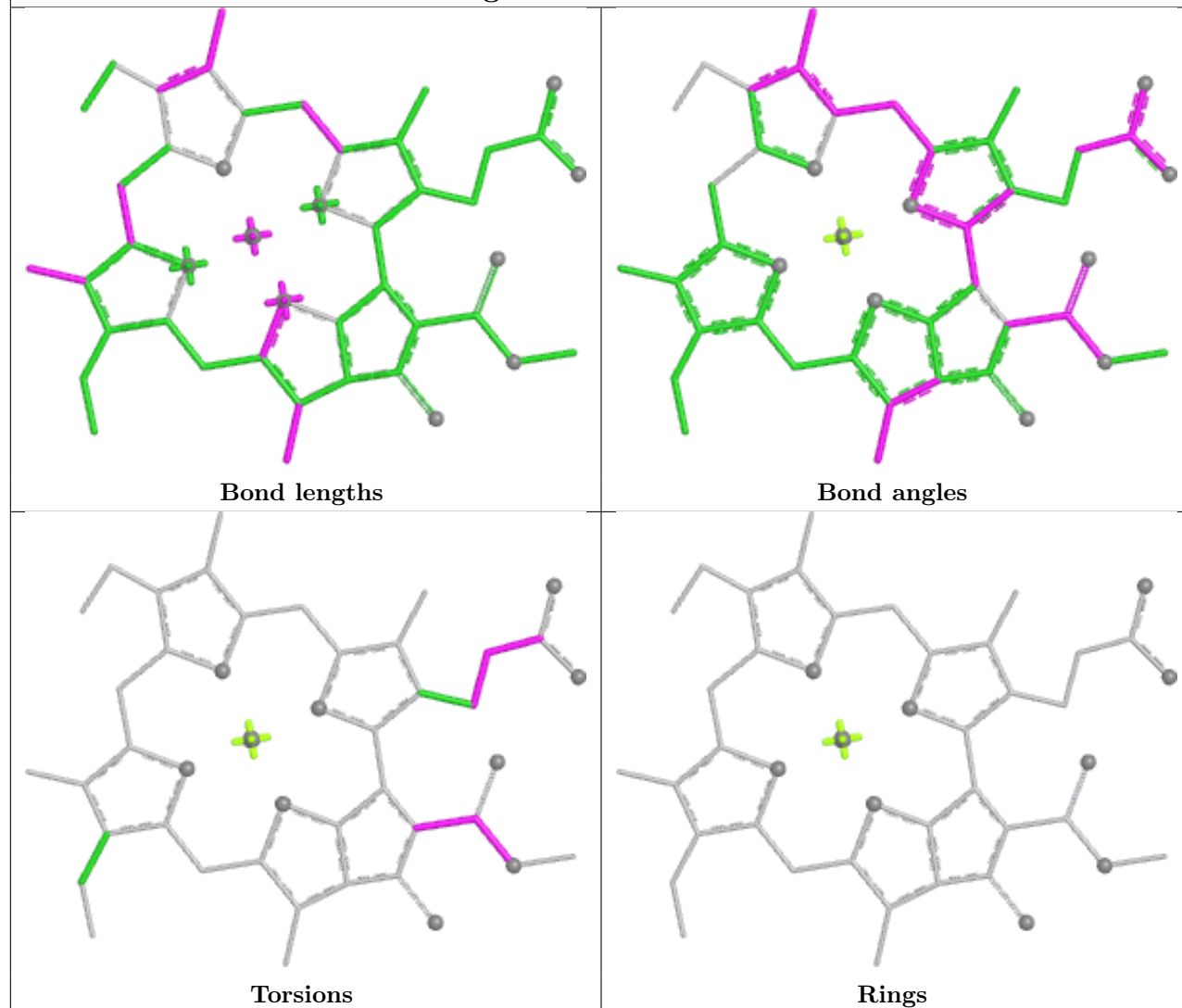




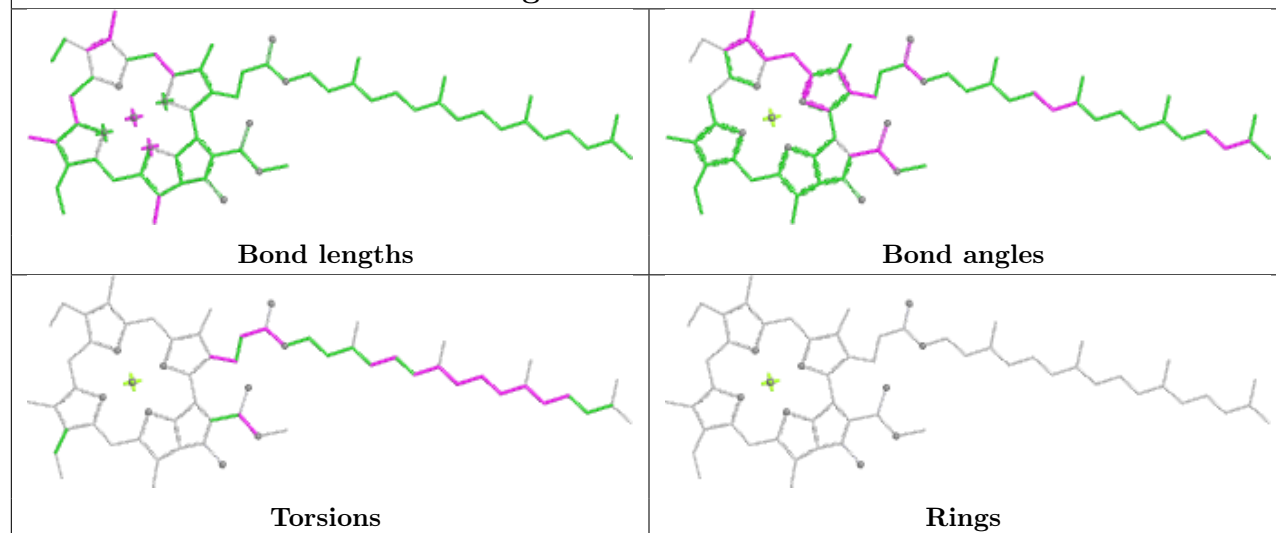




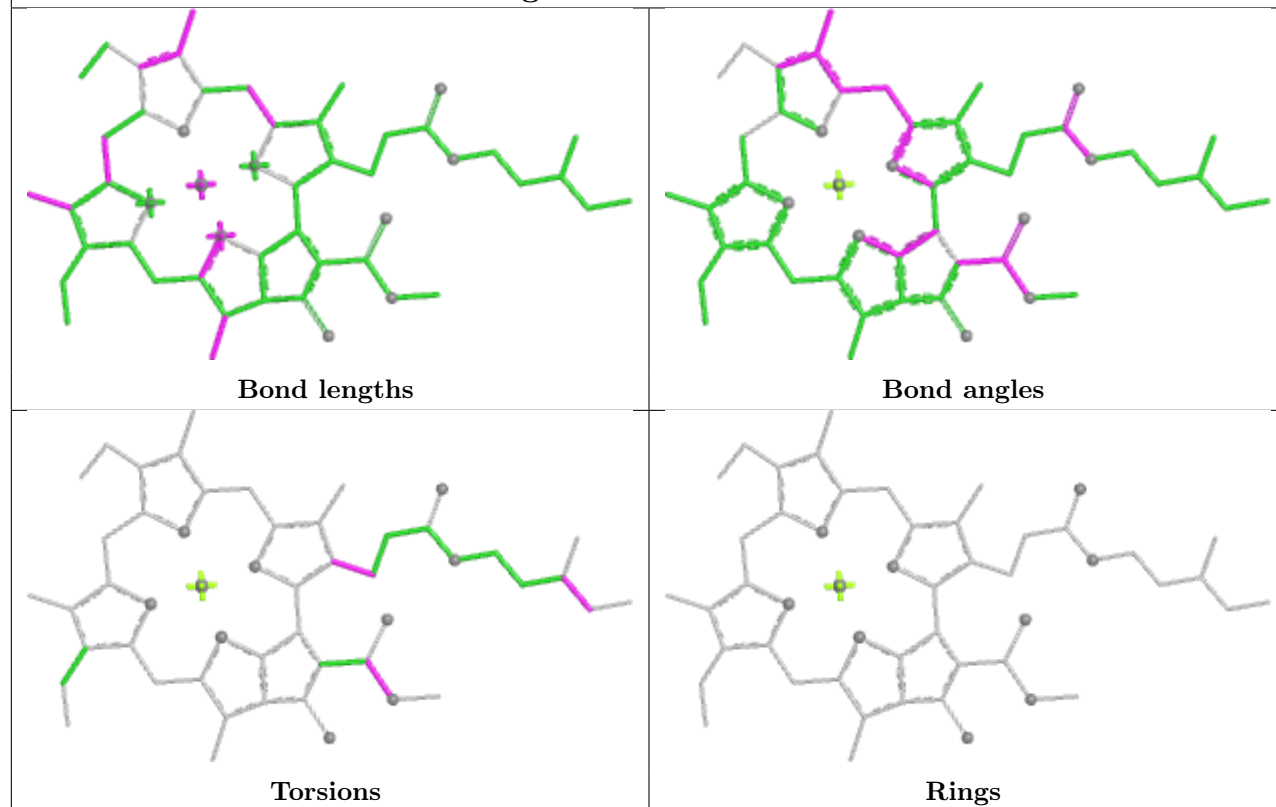
Ligand CLA bX 102



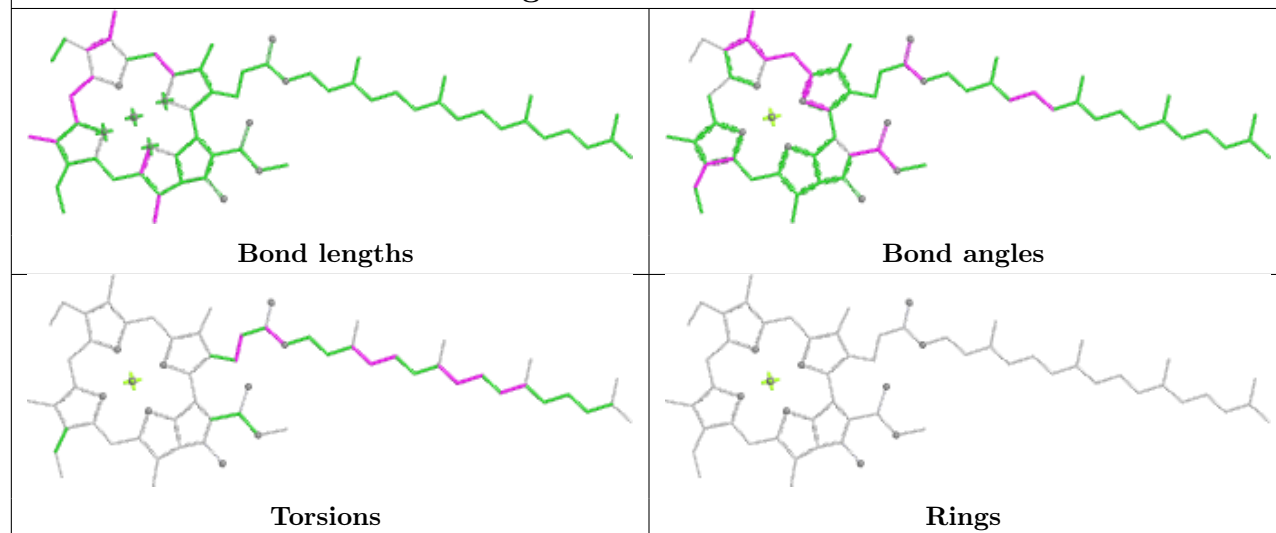
Ligand CLA bB 833

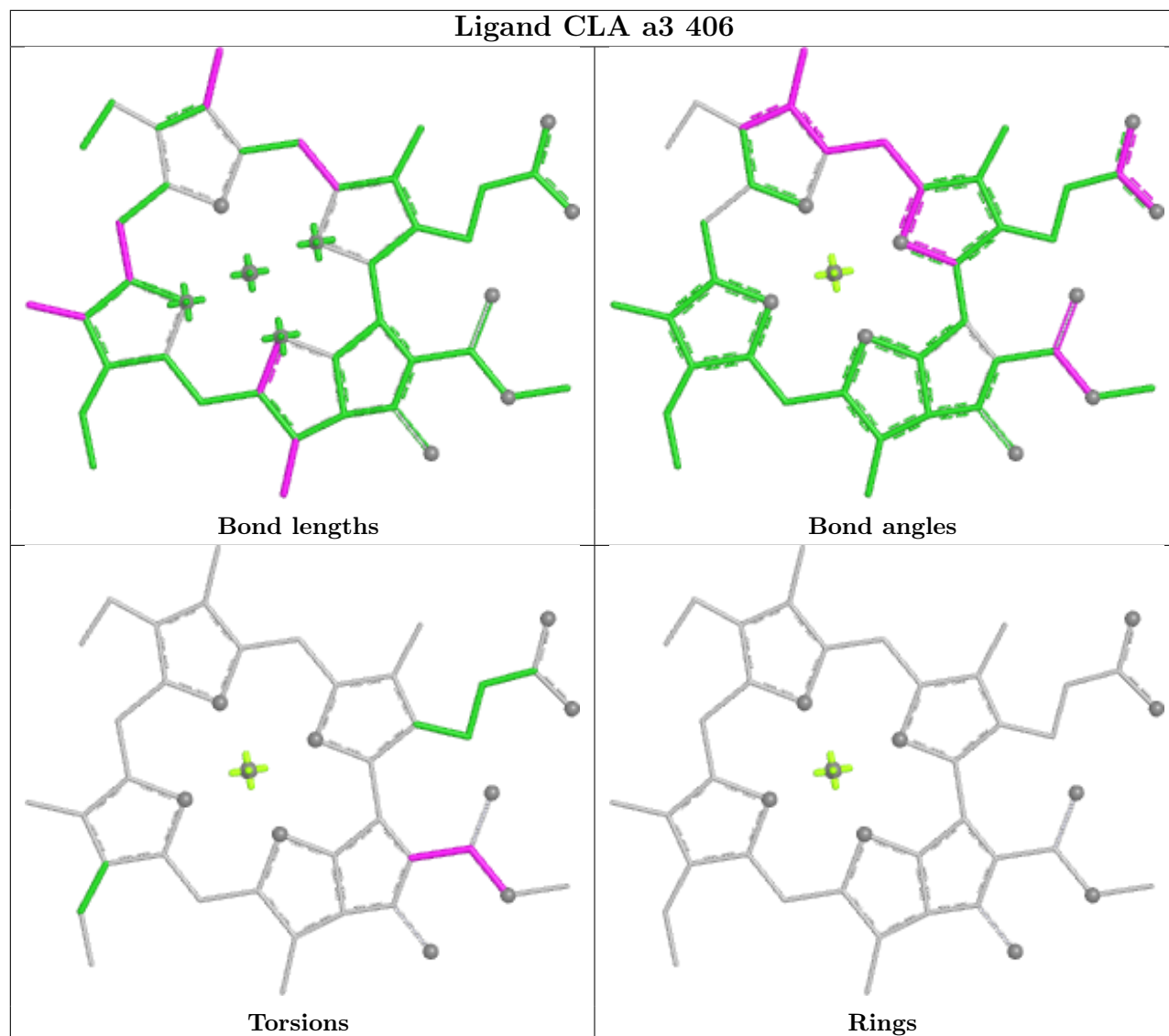


Ligand CLA bA 842

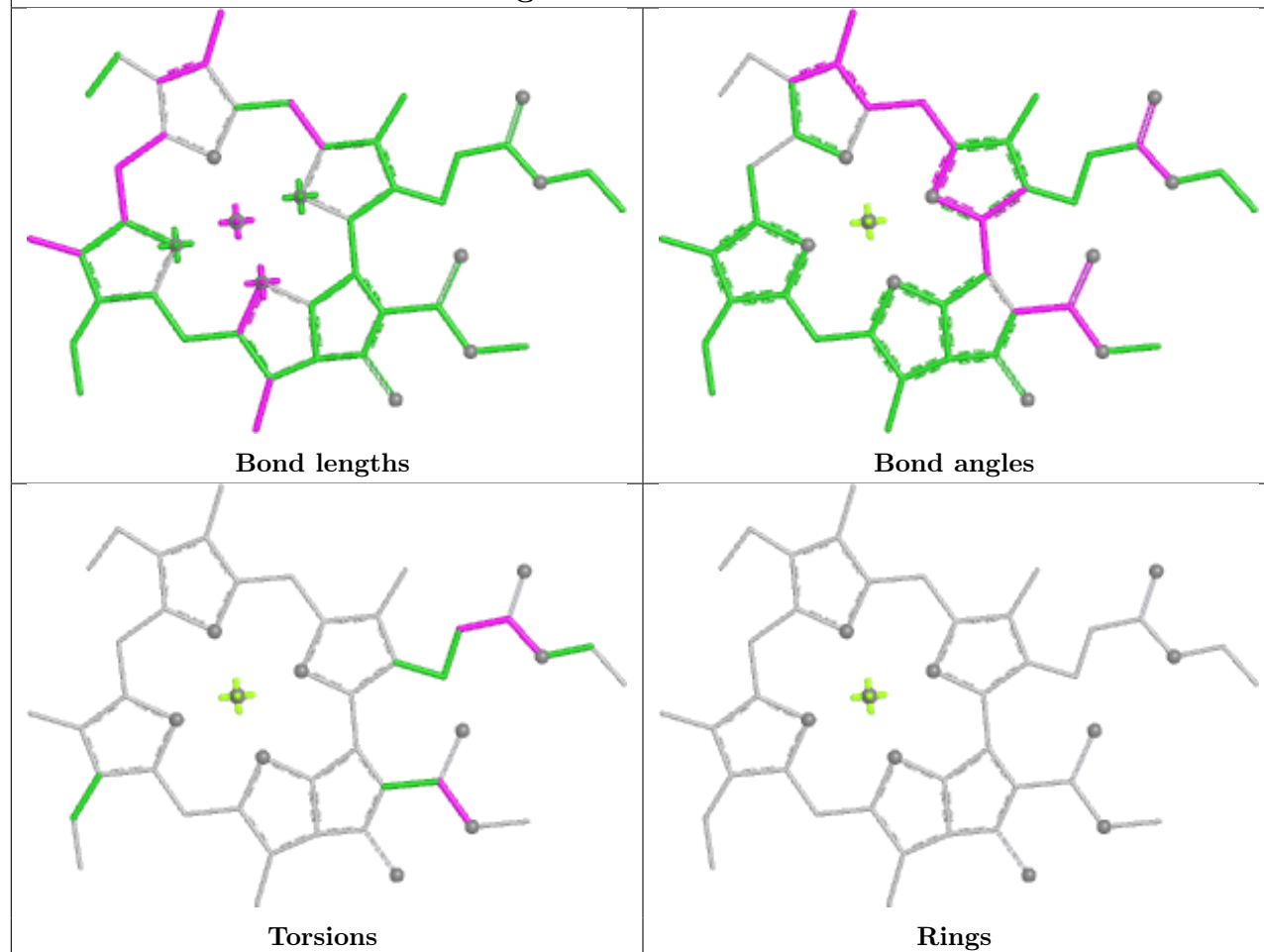


Ligand CLA bB 808

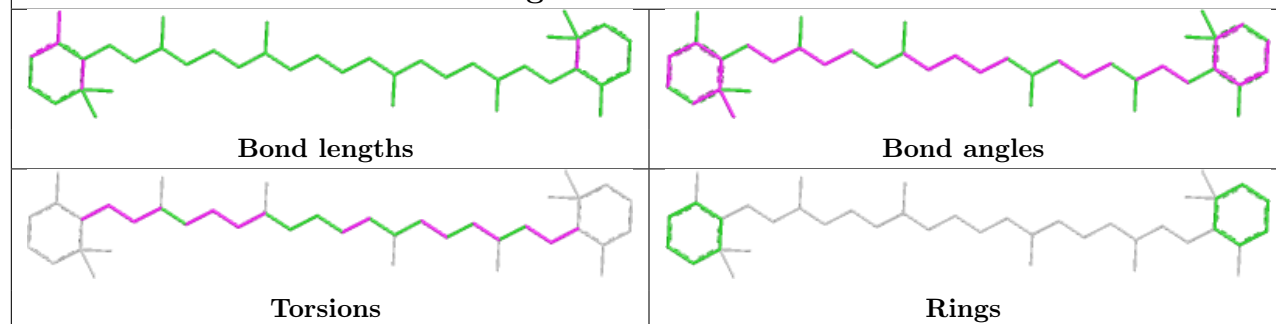


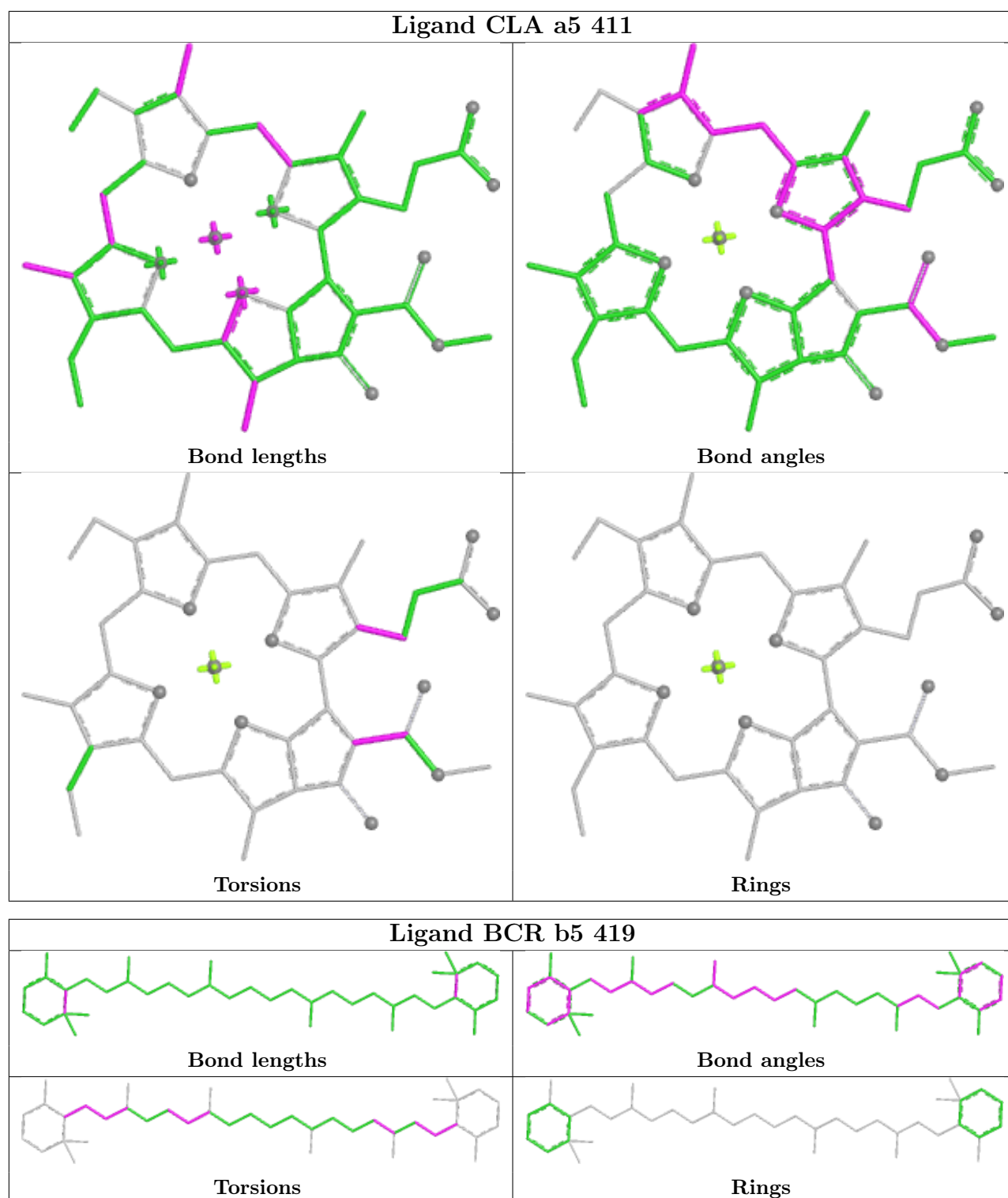


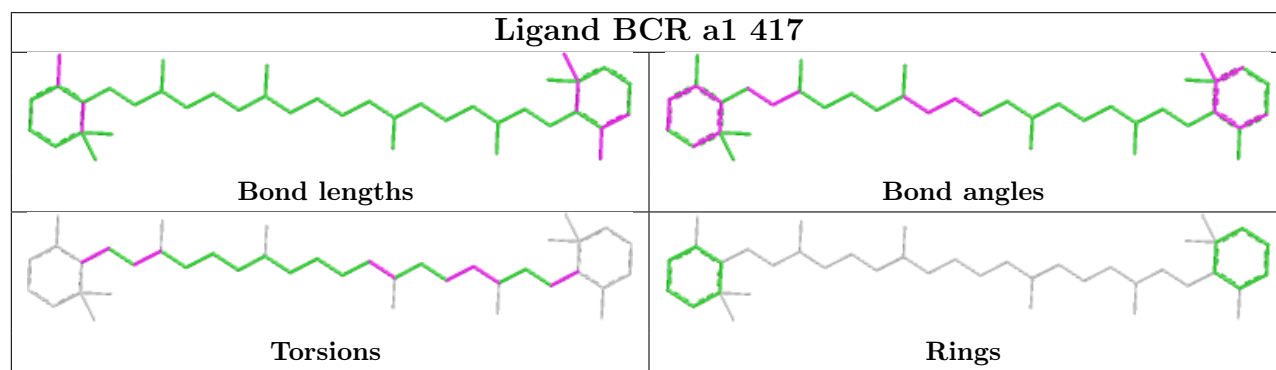
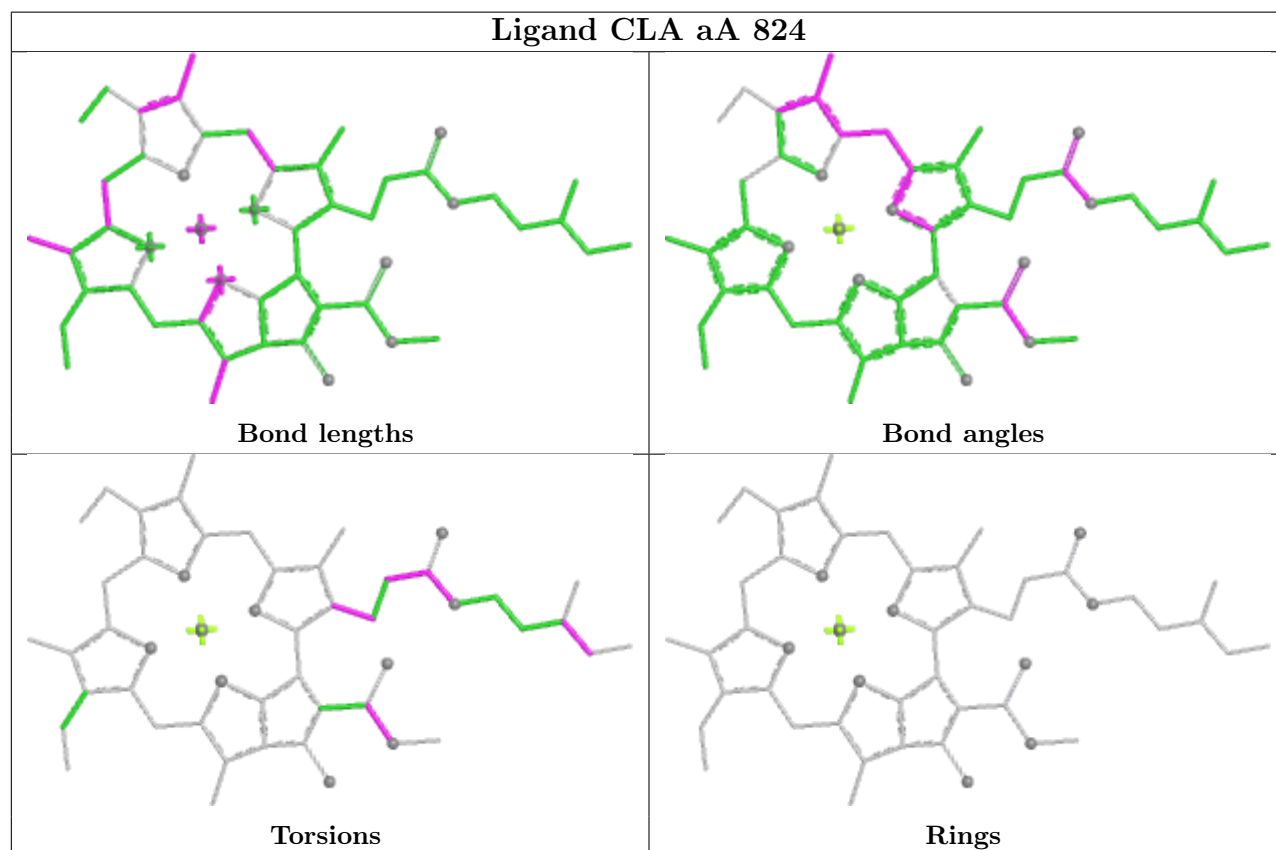
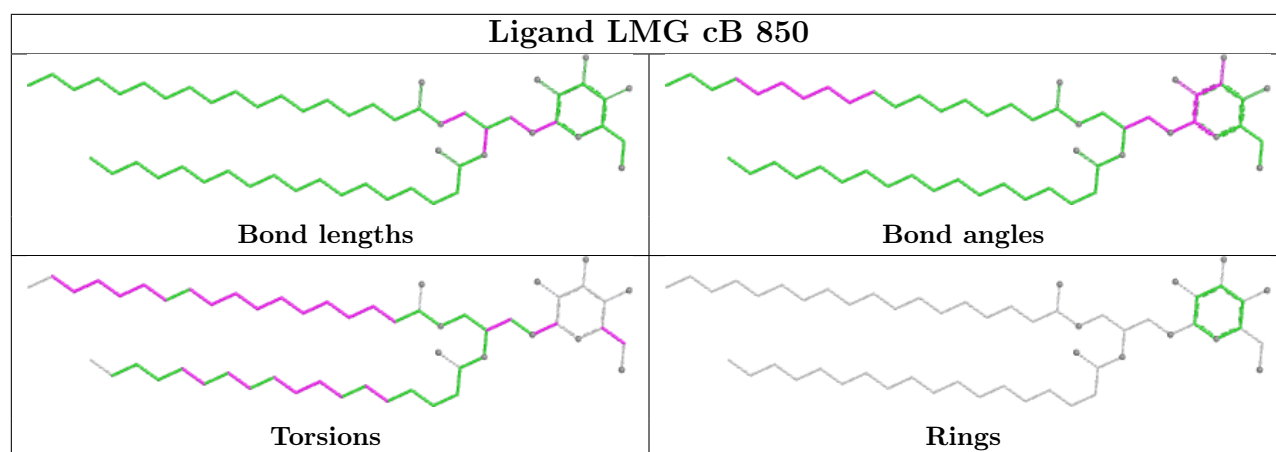
Ligand CLA bA 840

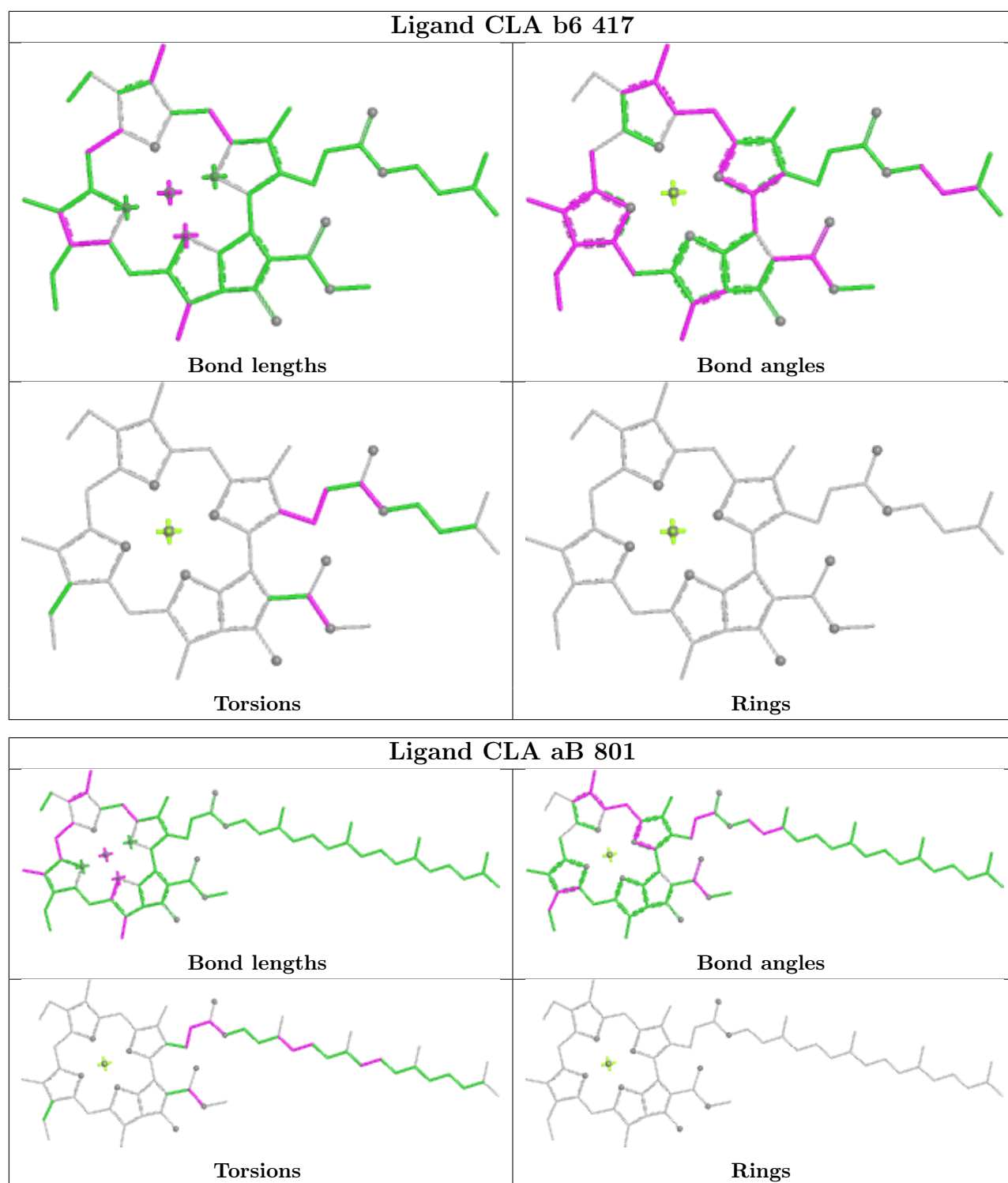


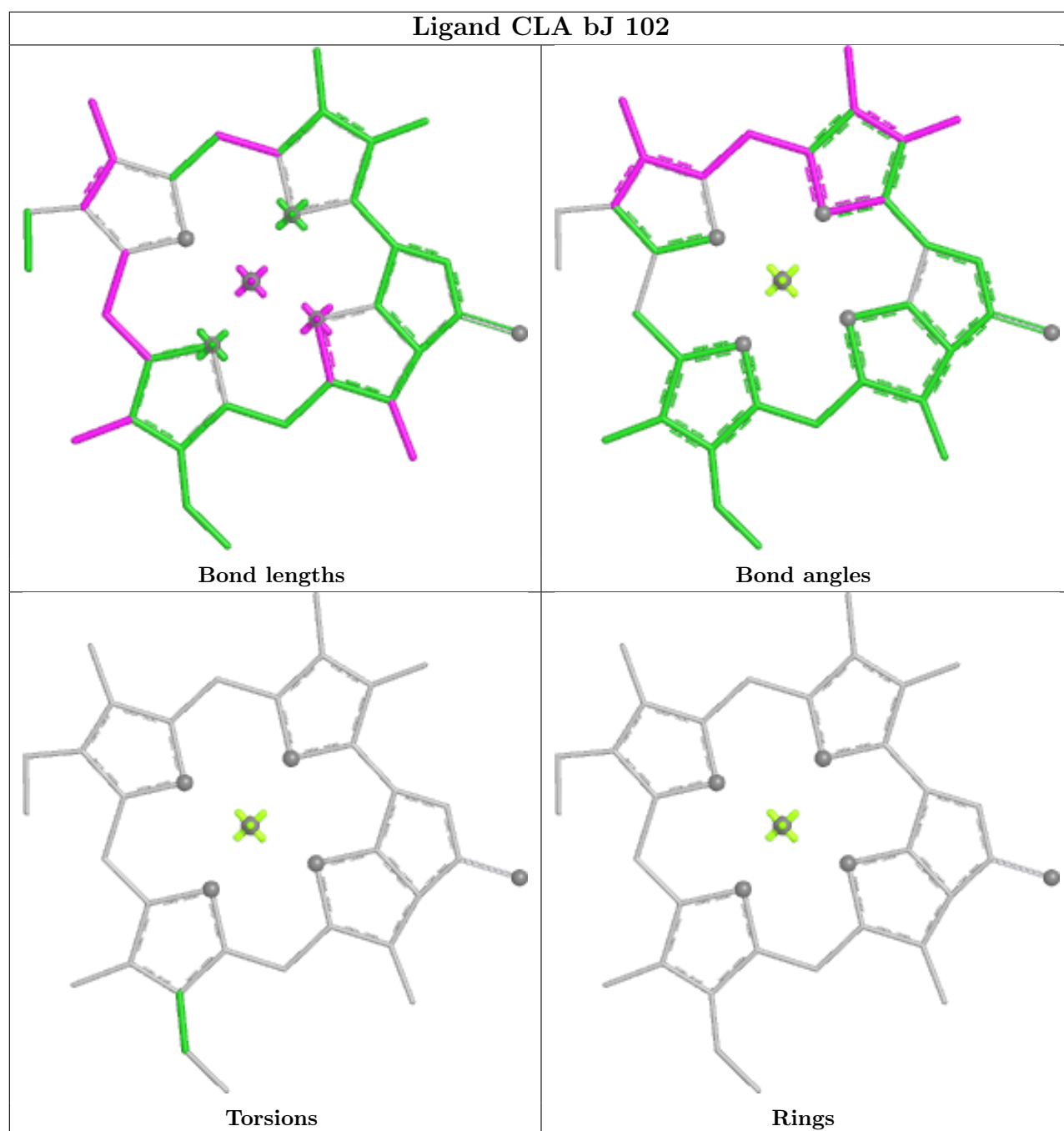
Ligand BCR c6 402

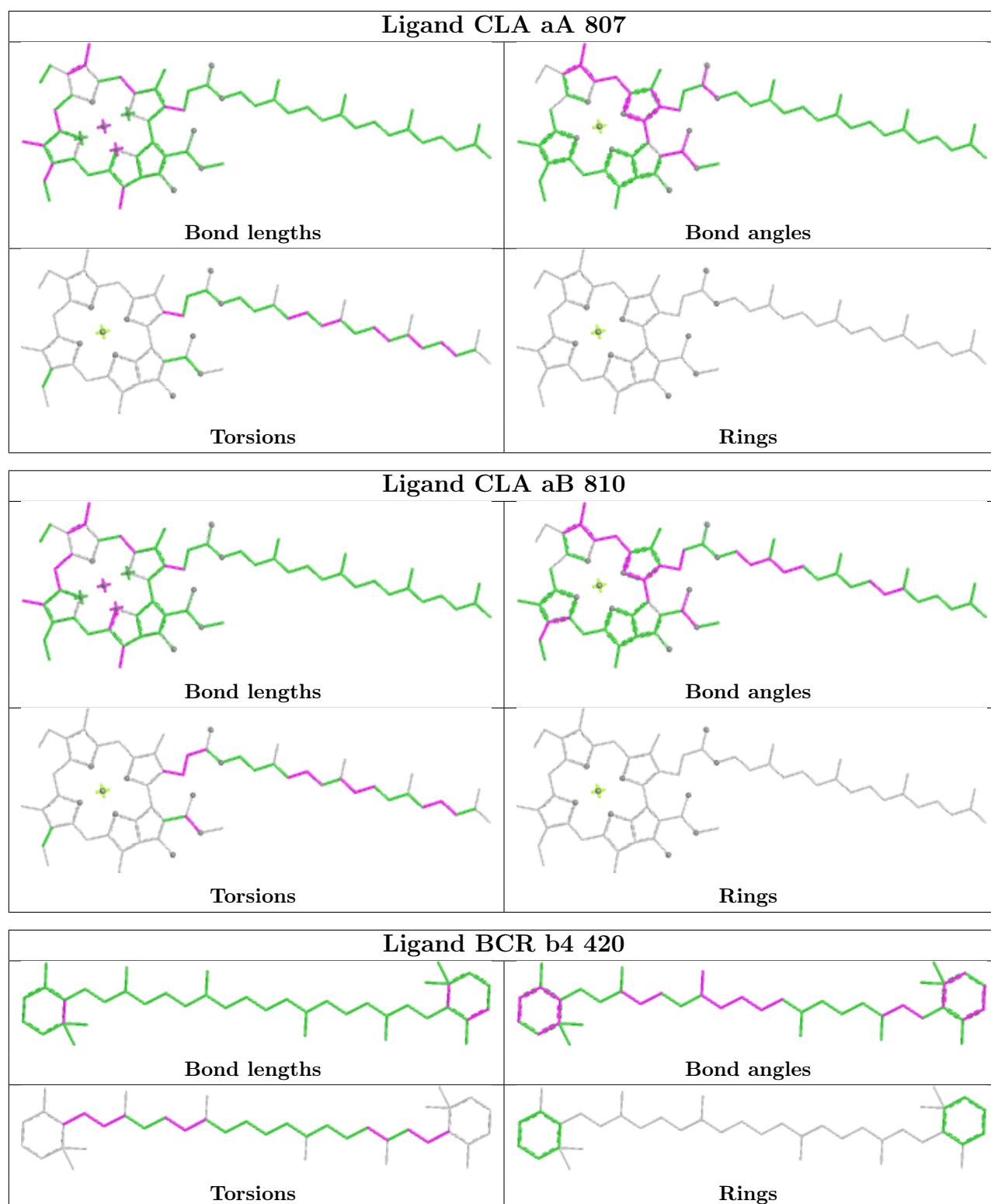


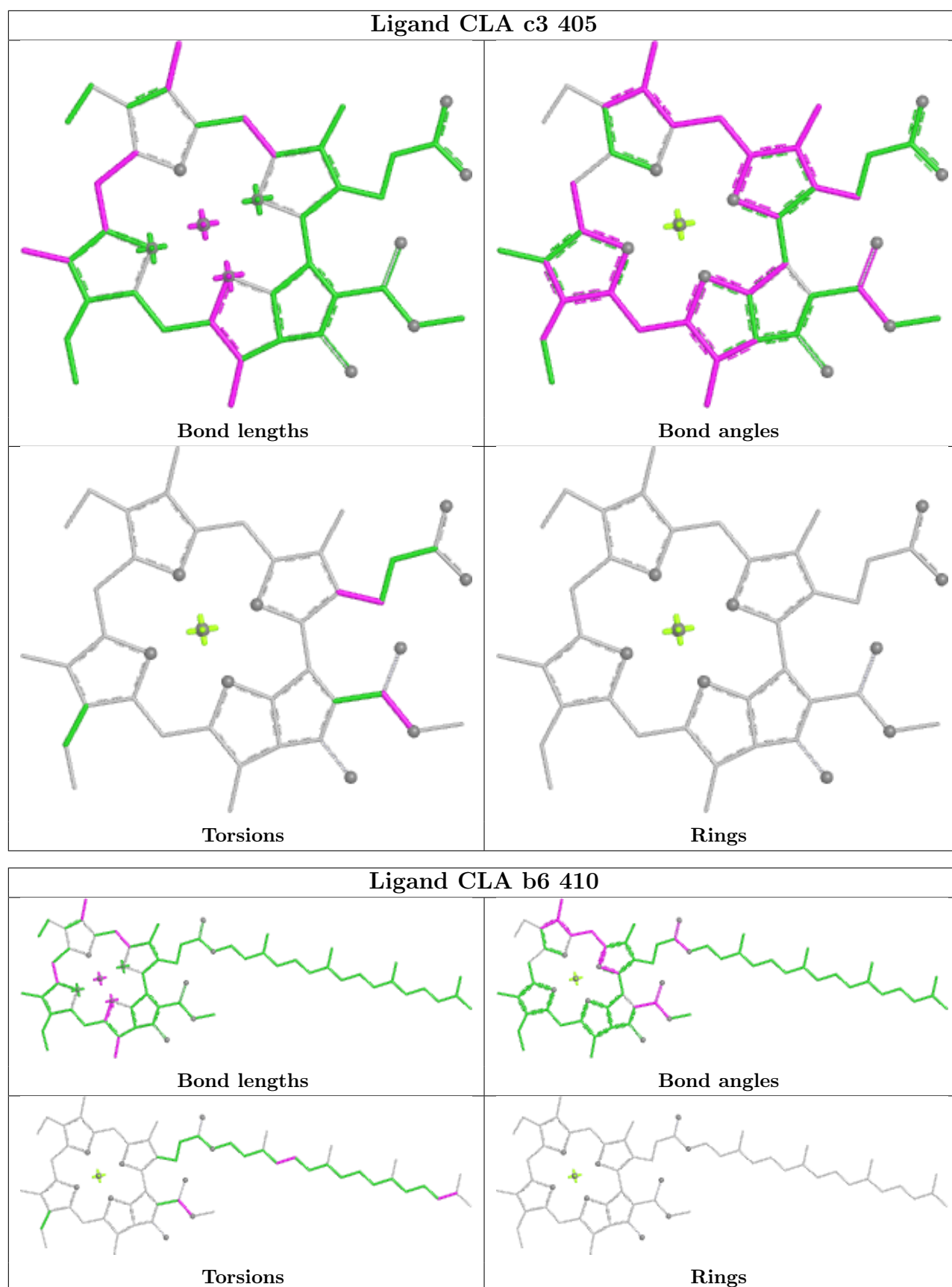




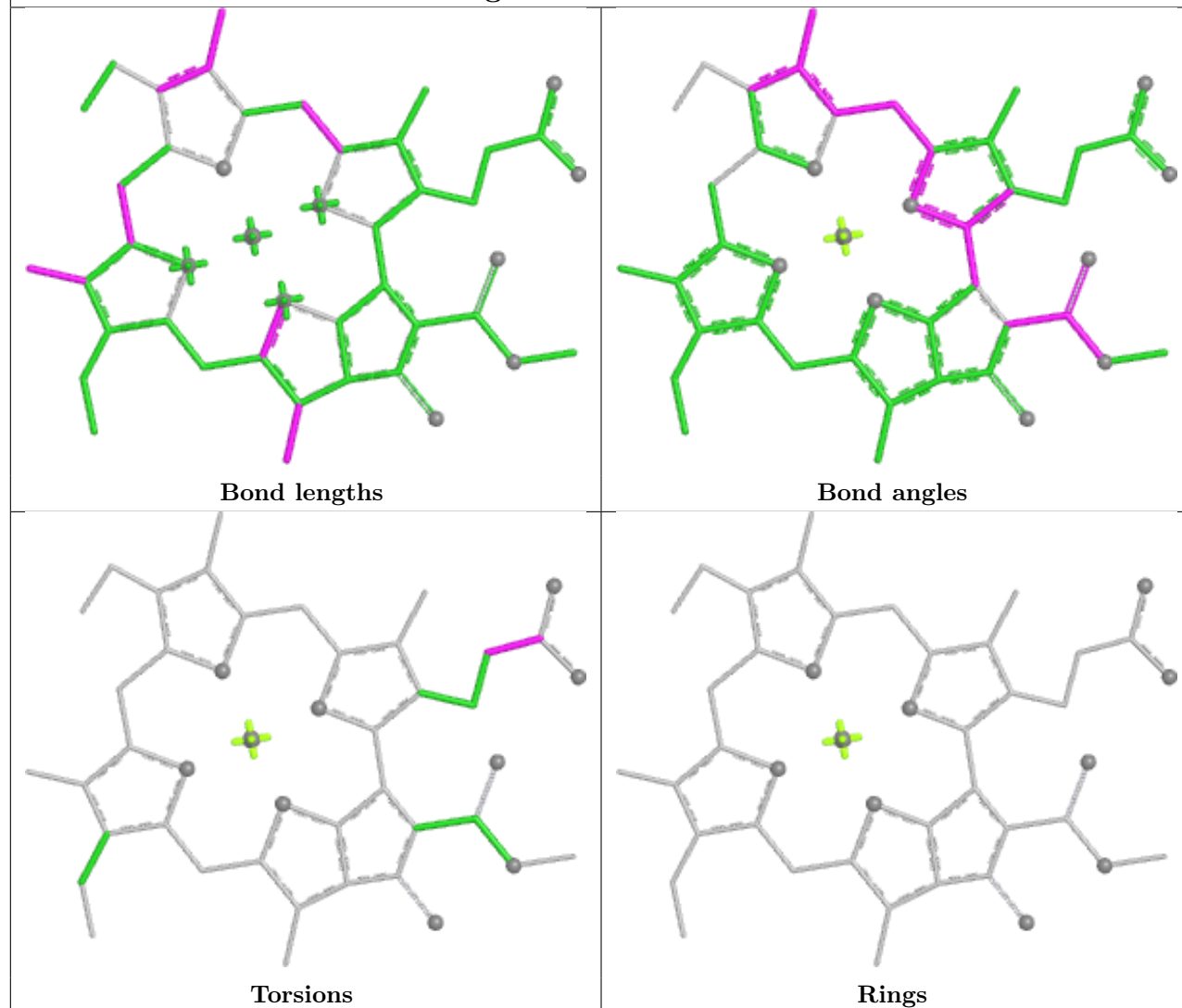




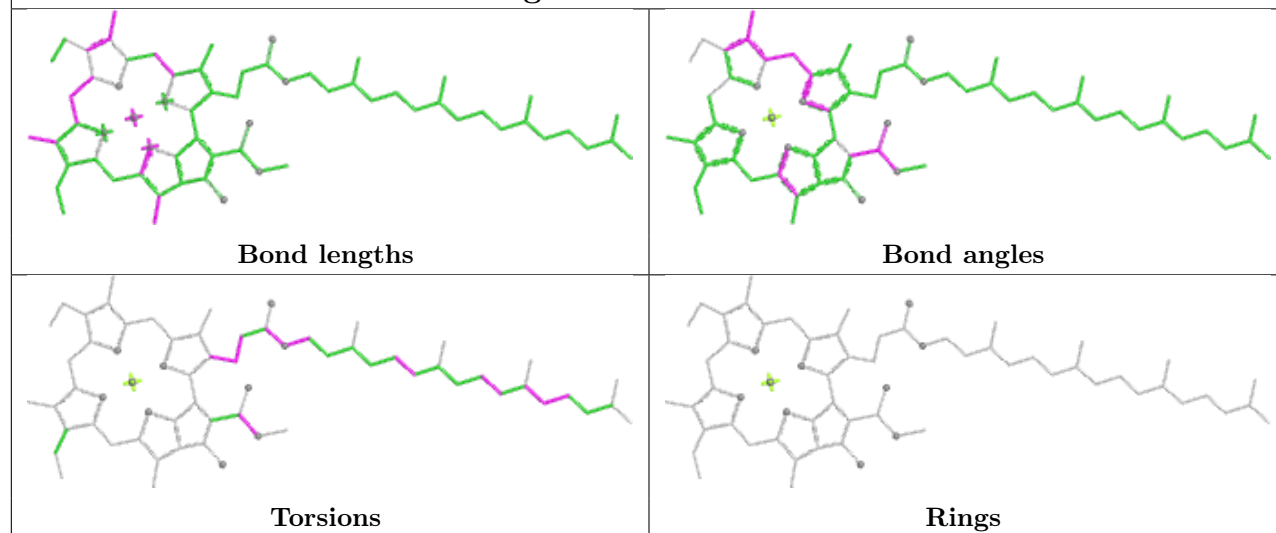




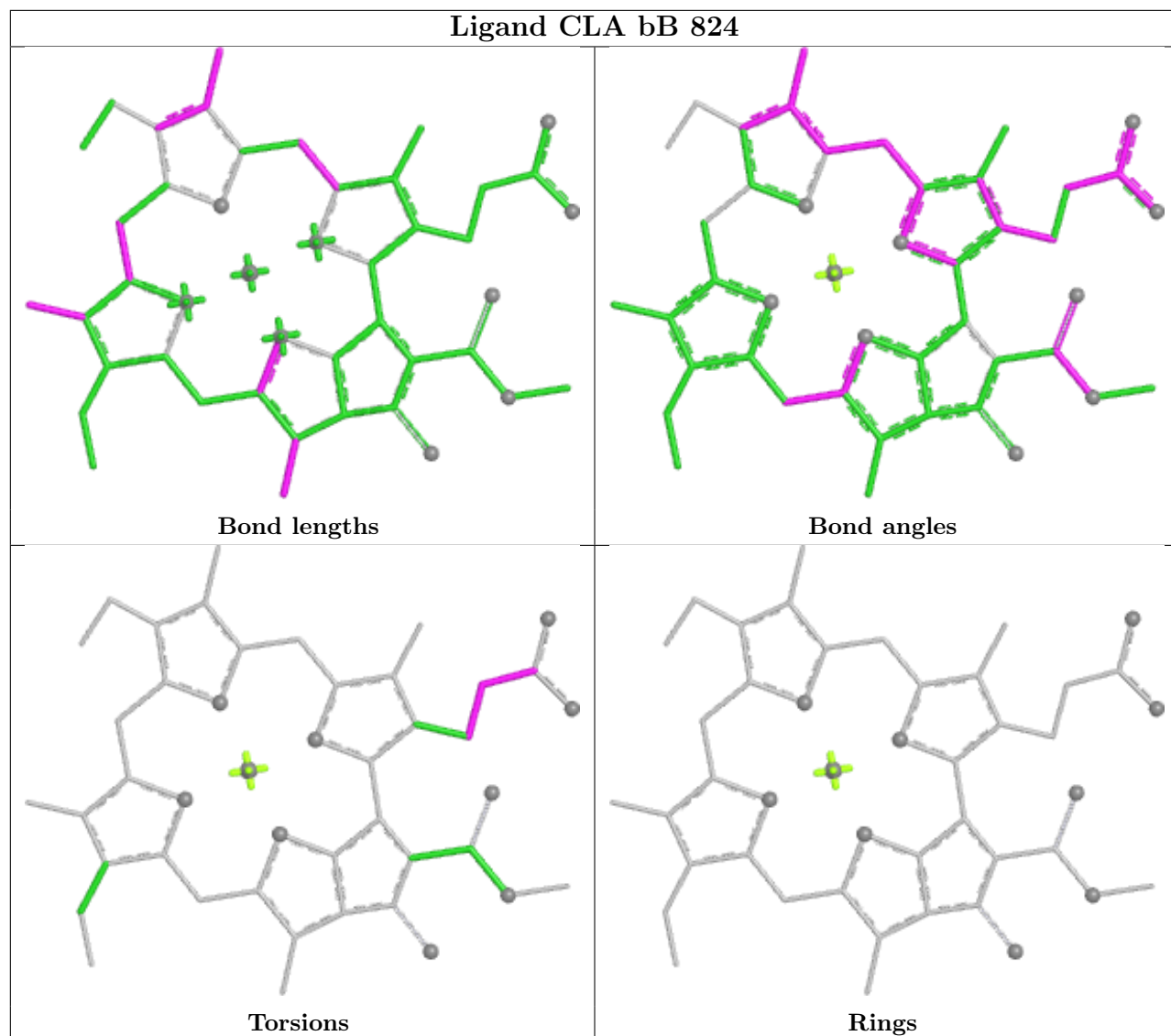
Ligand CLA aB 841



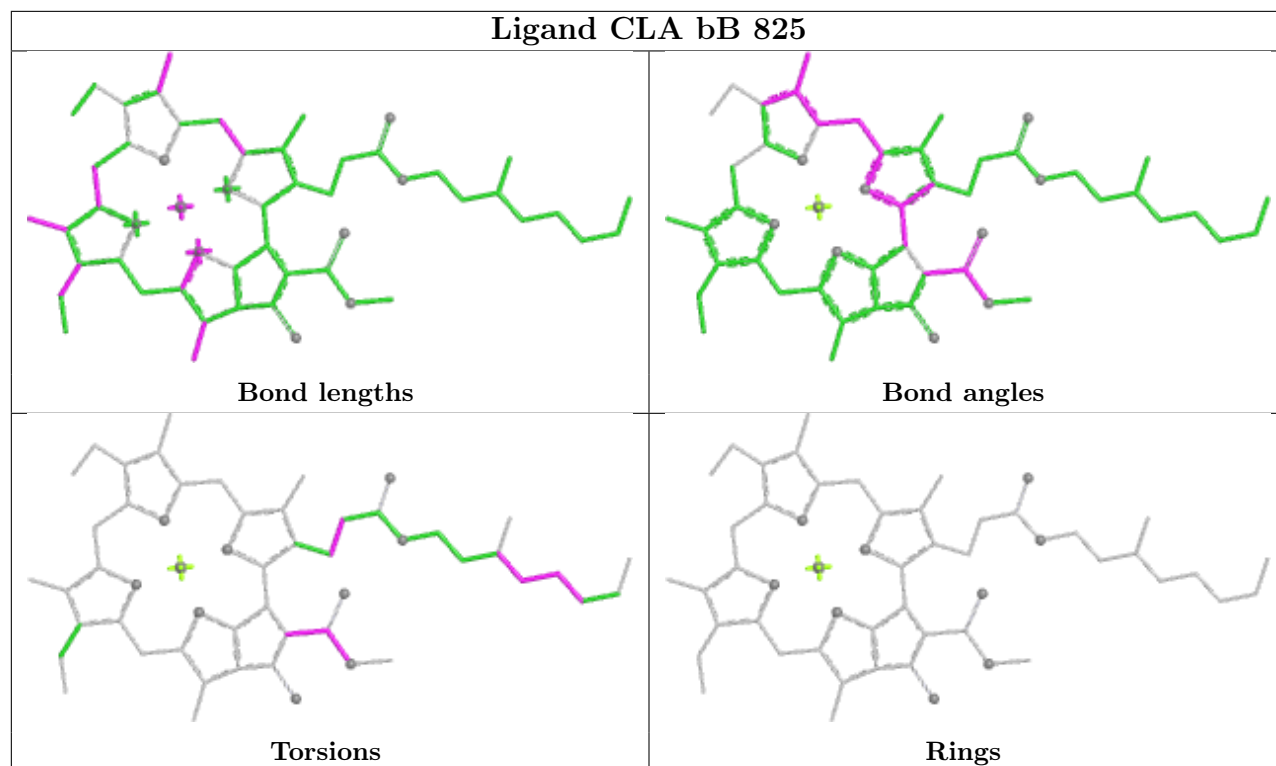
Ligand CLA aB 829



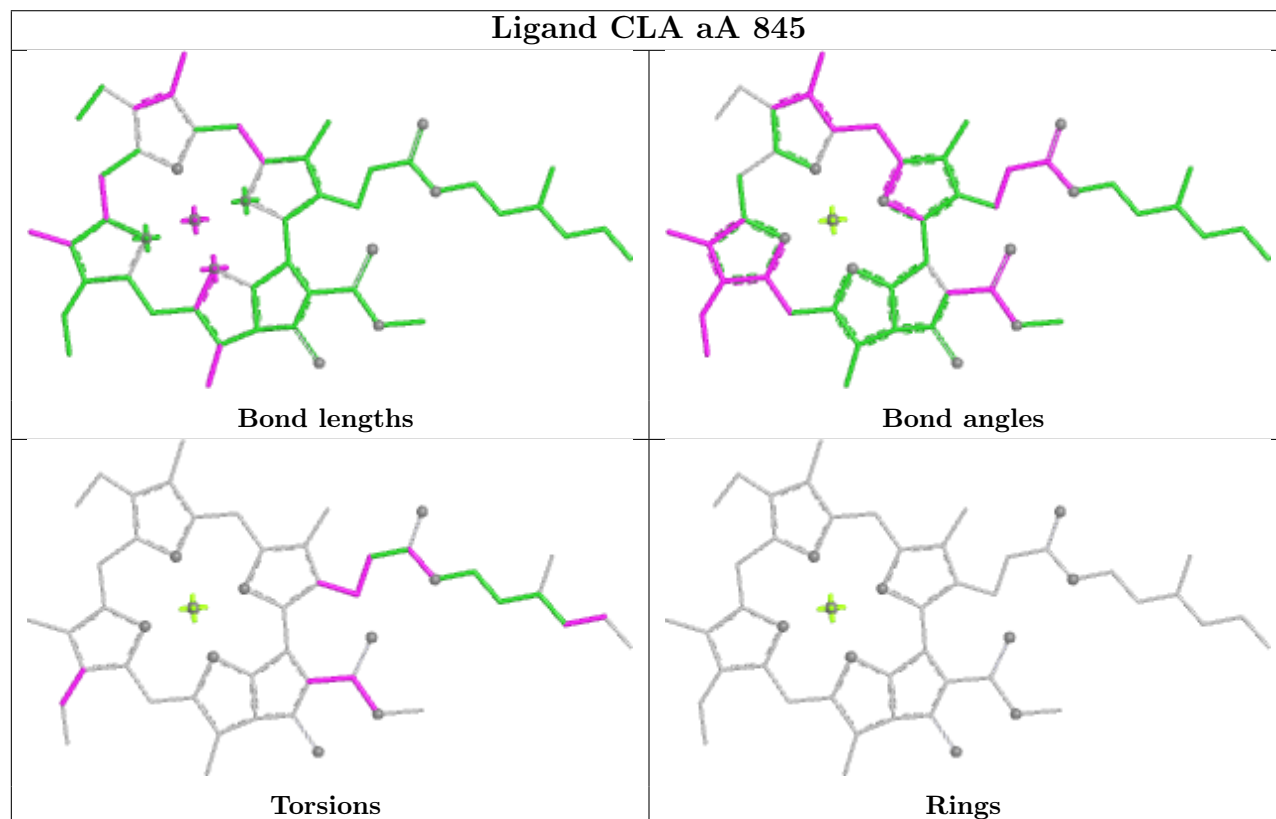
Ligand CLA bB 824

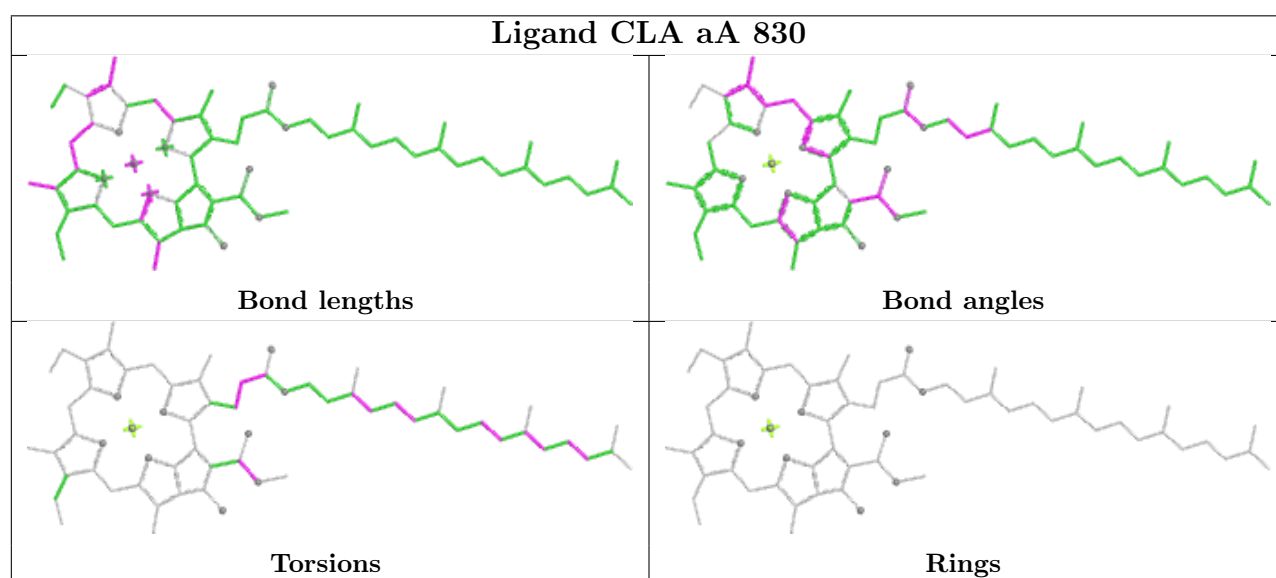
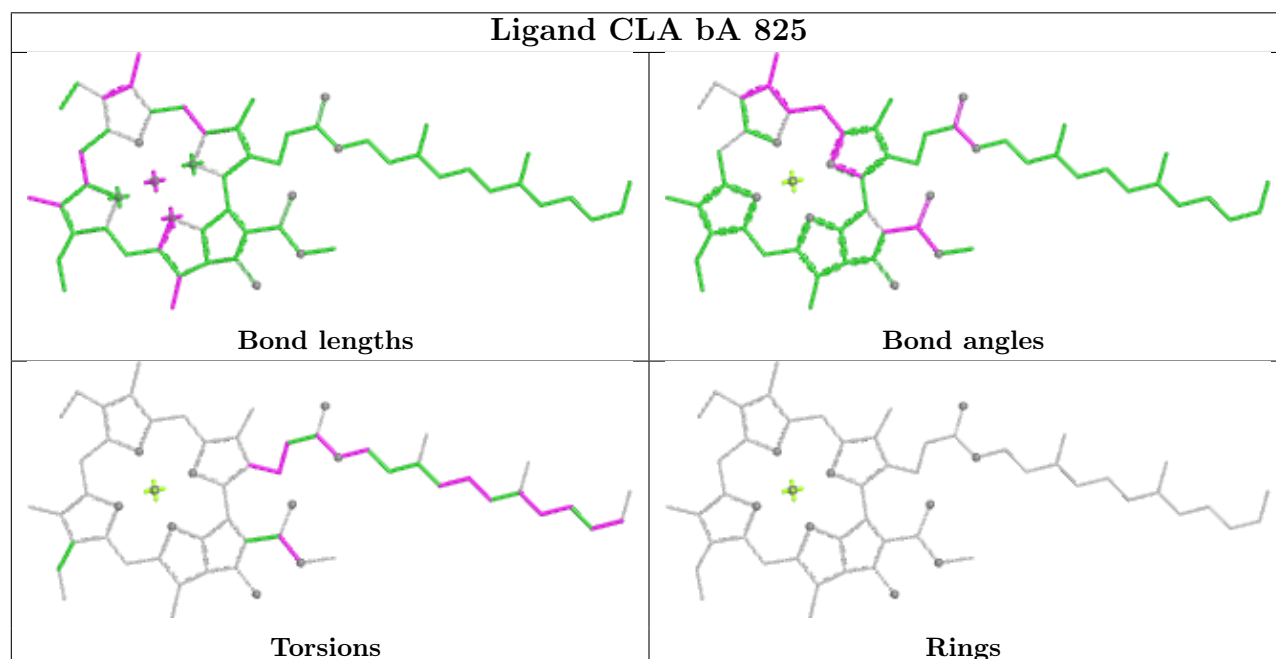
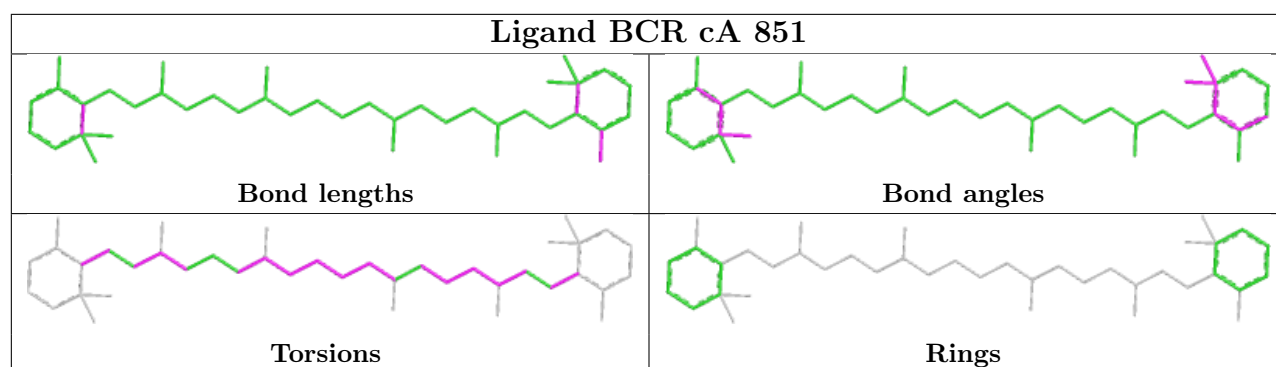


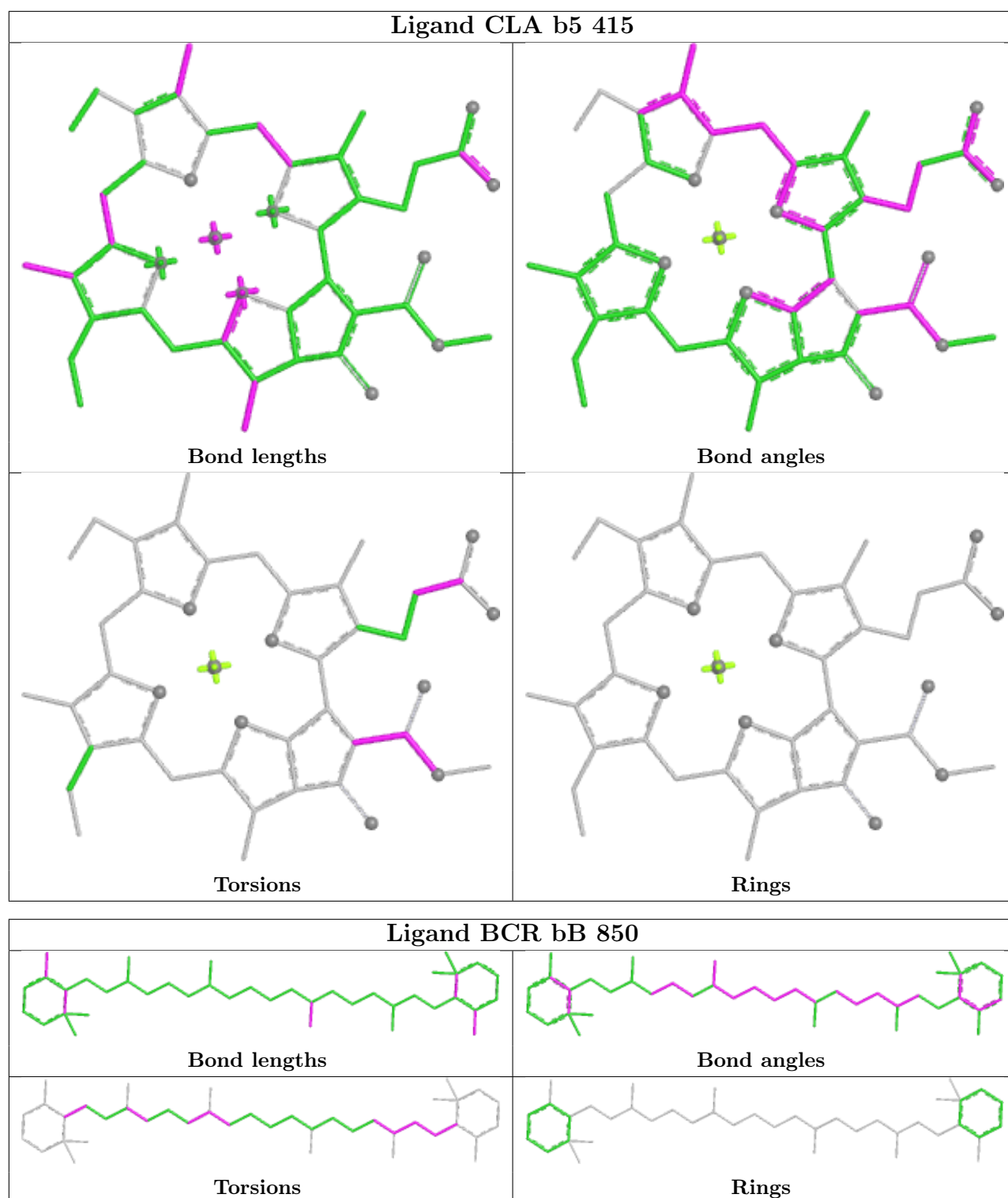
Ligand CLA bB 825

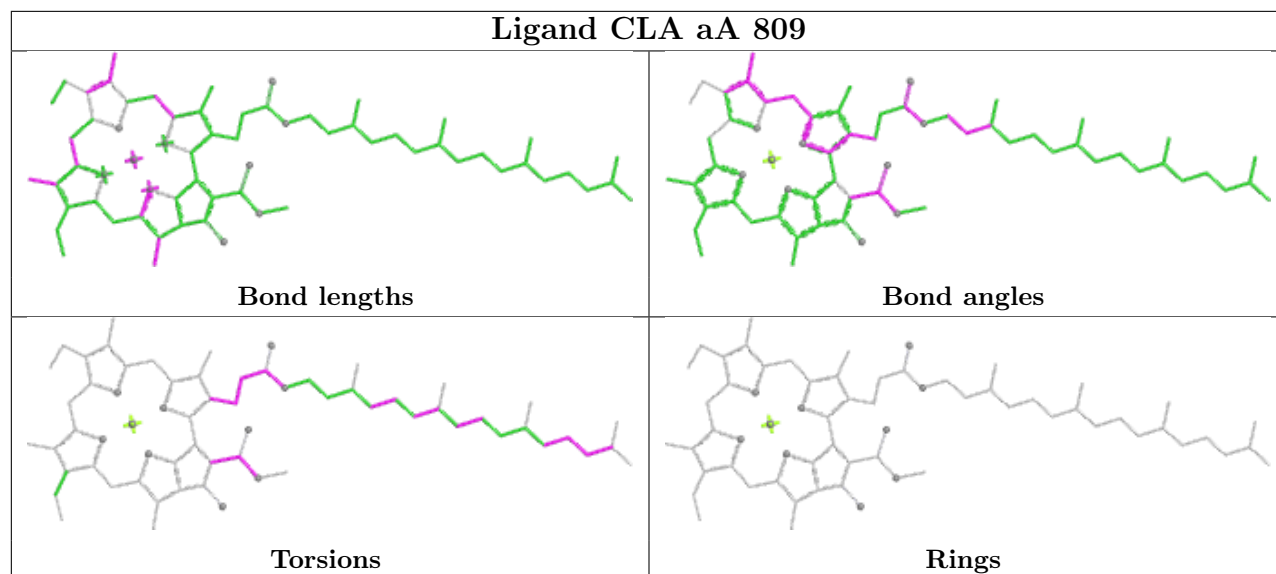
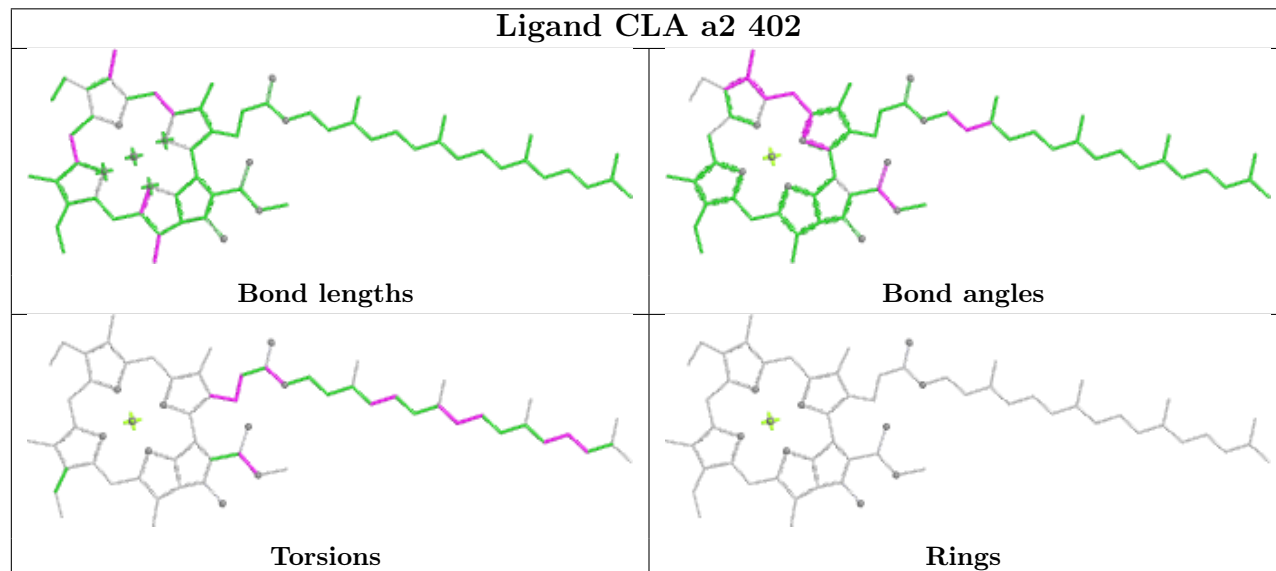


Ligand CLA aA 845

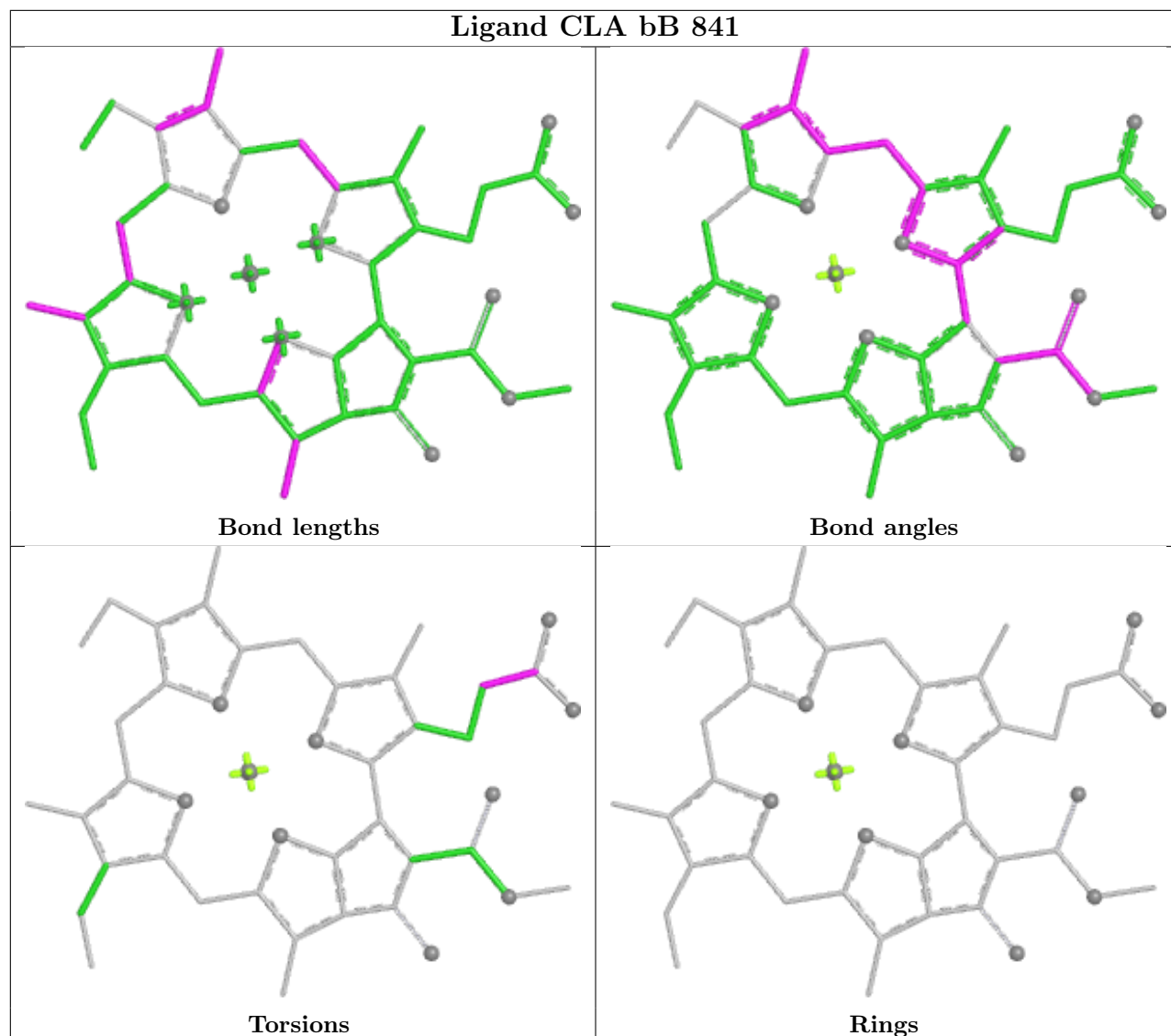




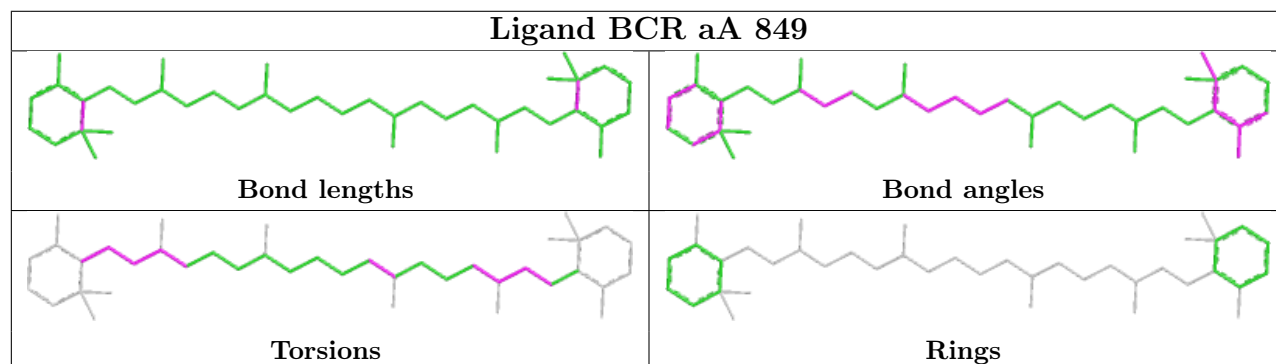


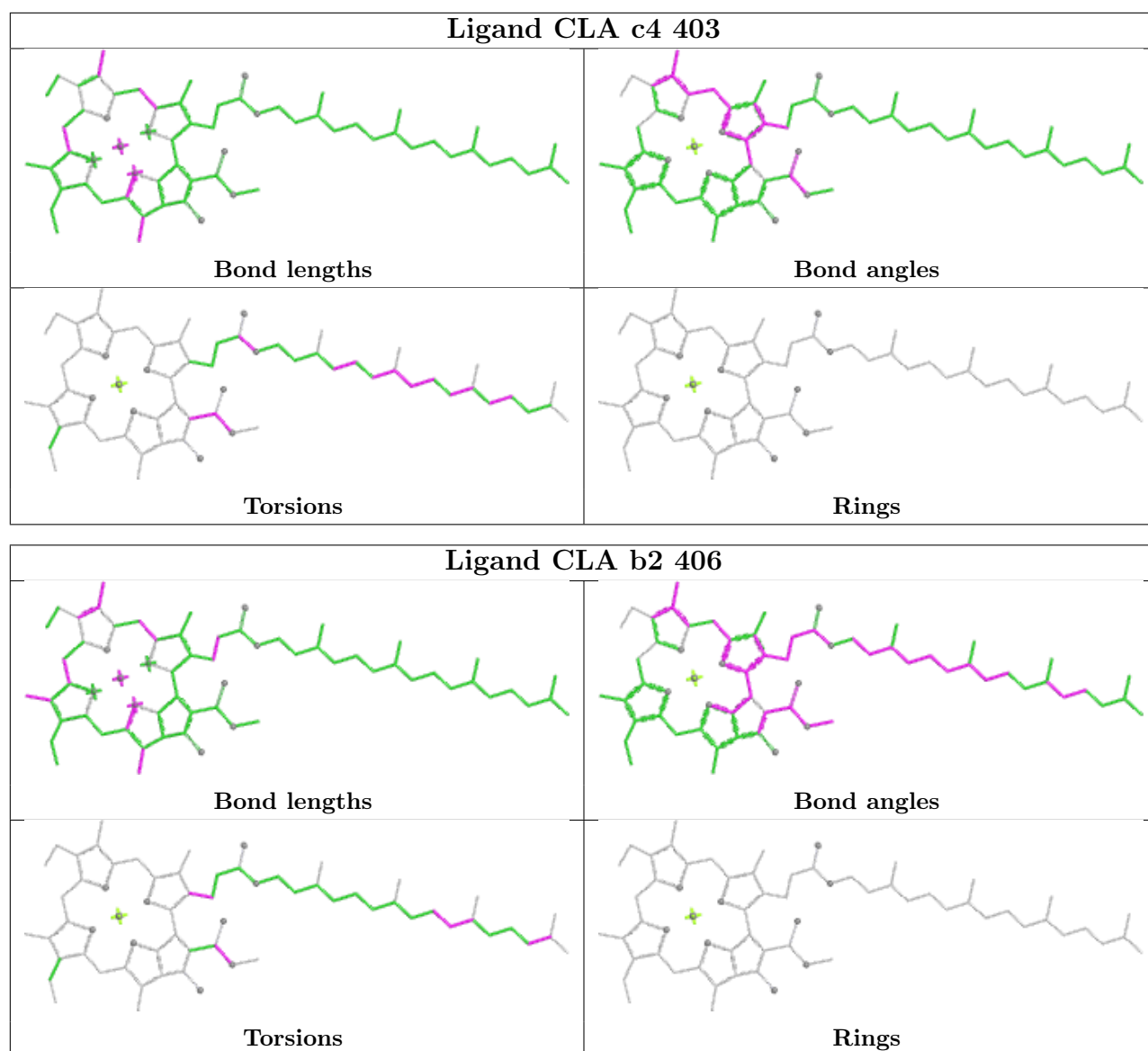
Ligand CLA aA 809**Ligand CLA a2 402**

Ligand CLA bB 841

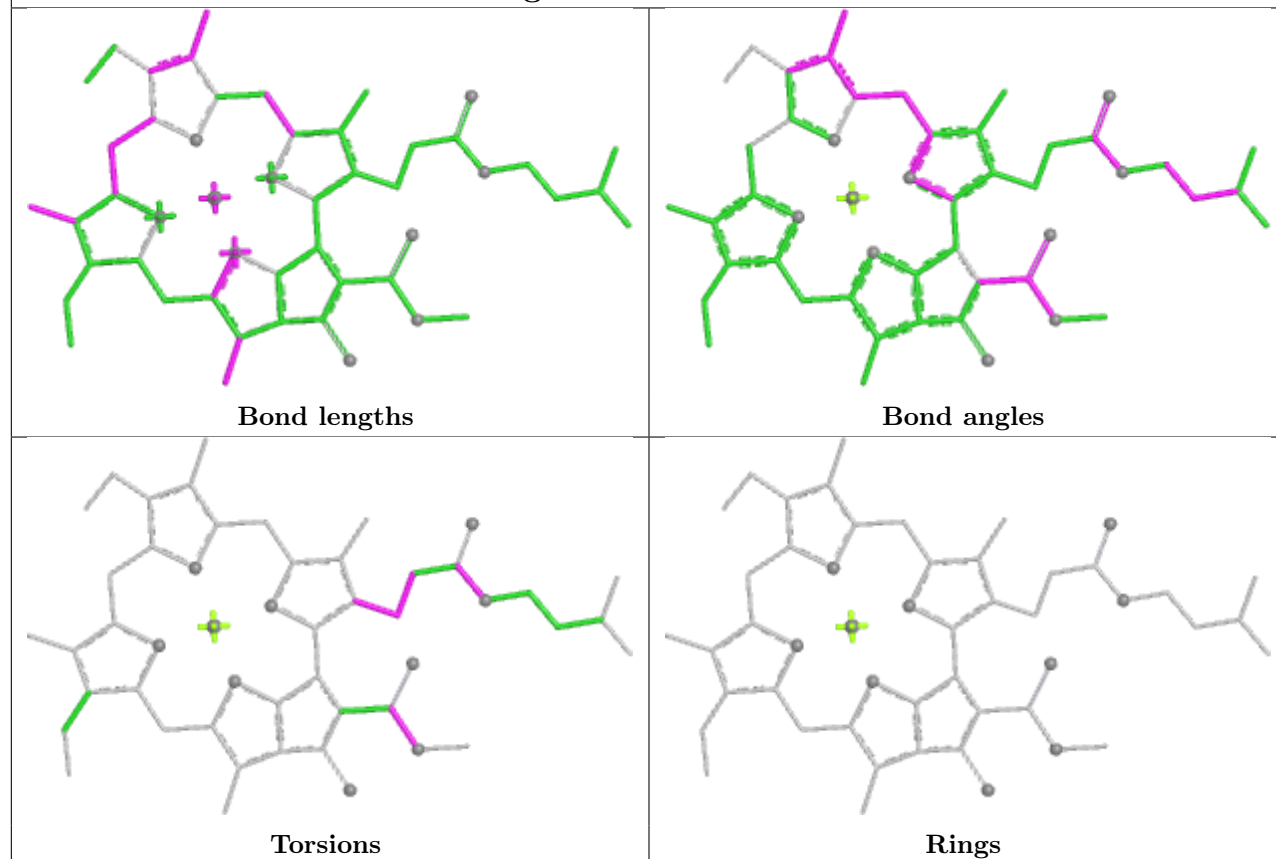


Ligand BCR aA 849

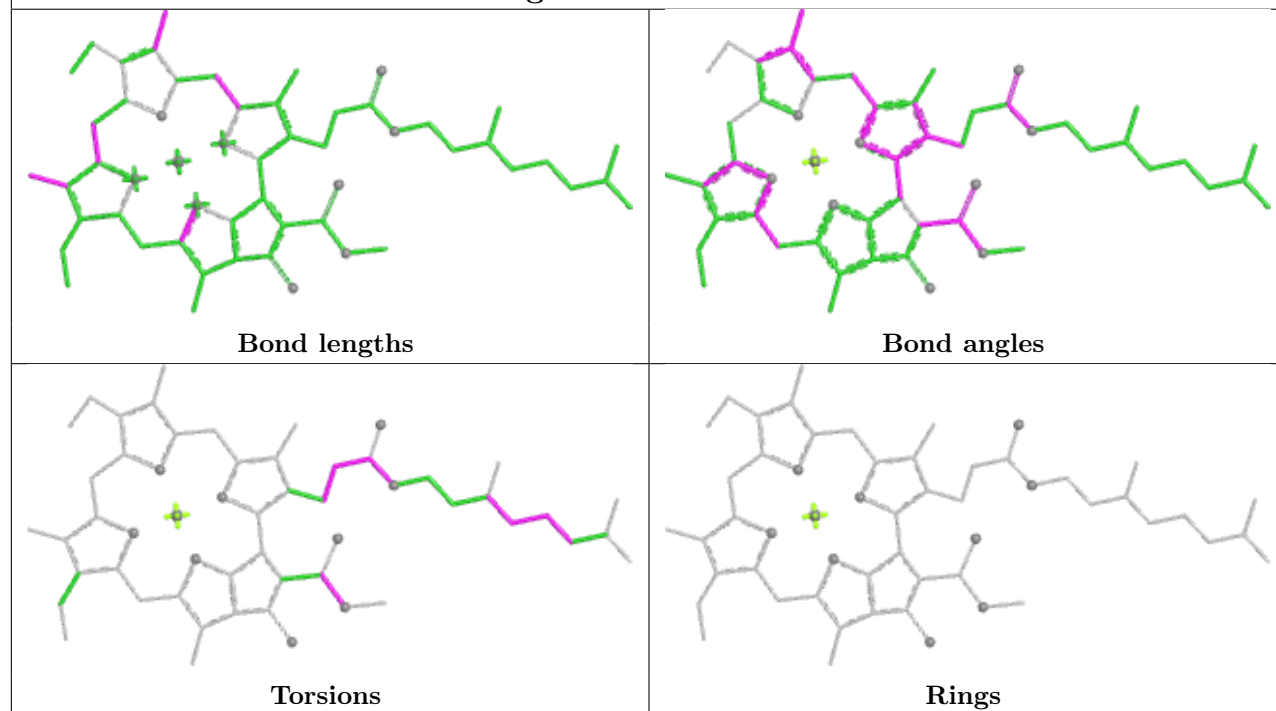


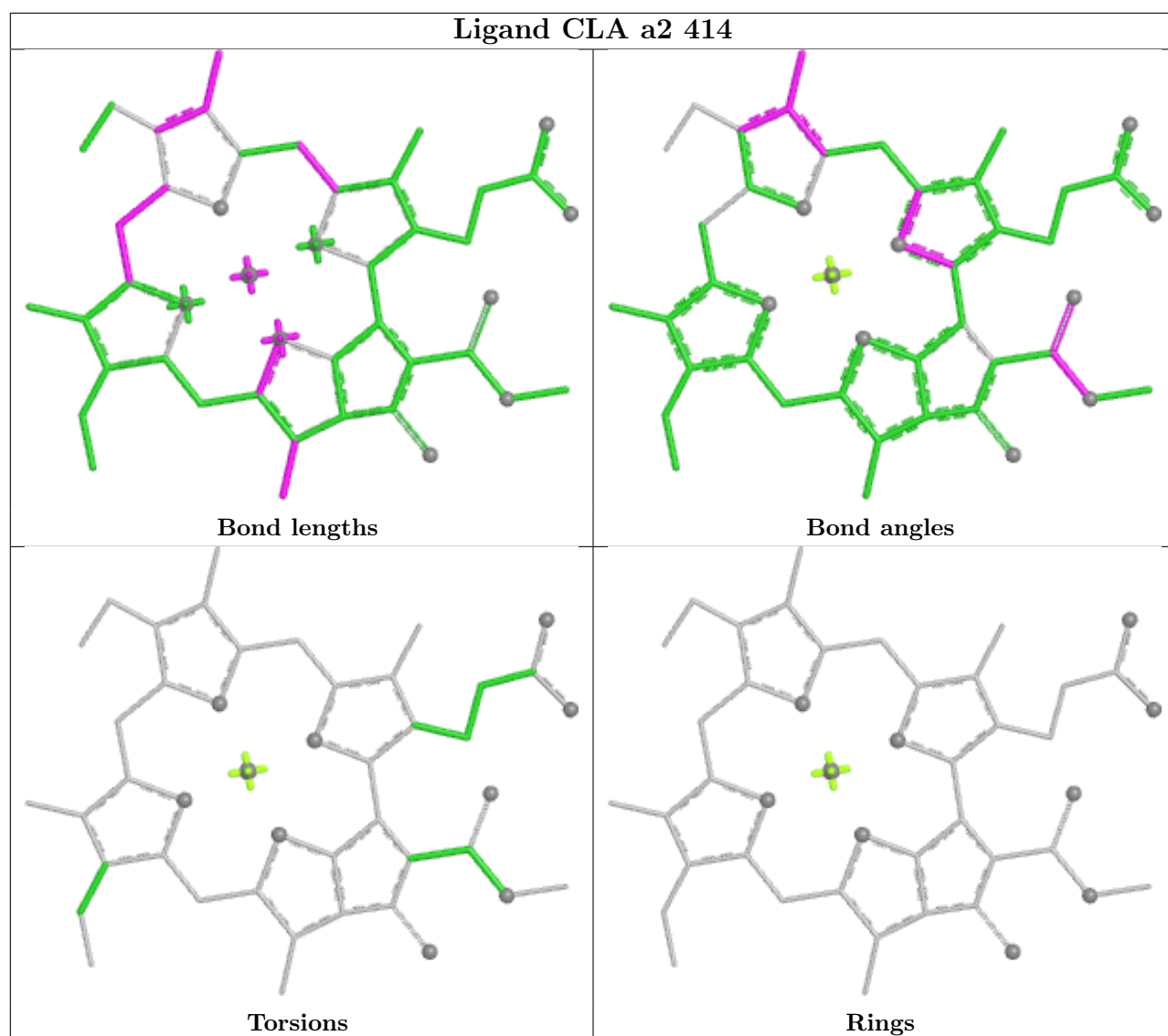


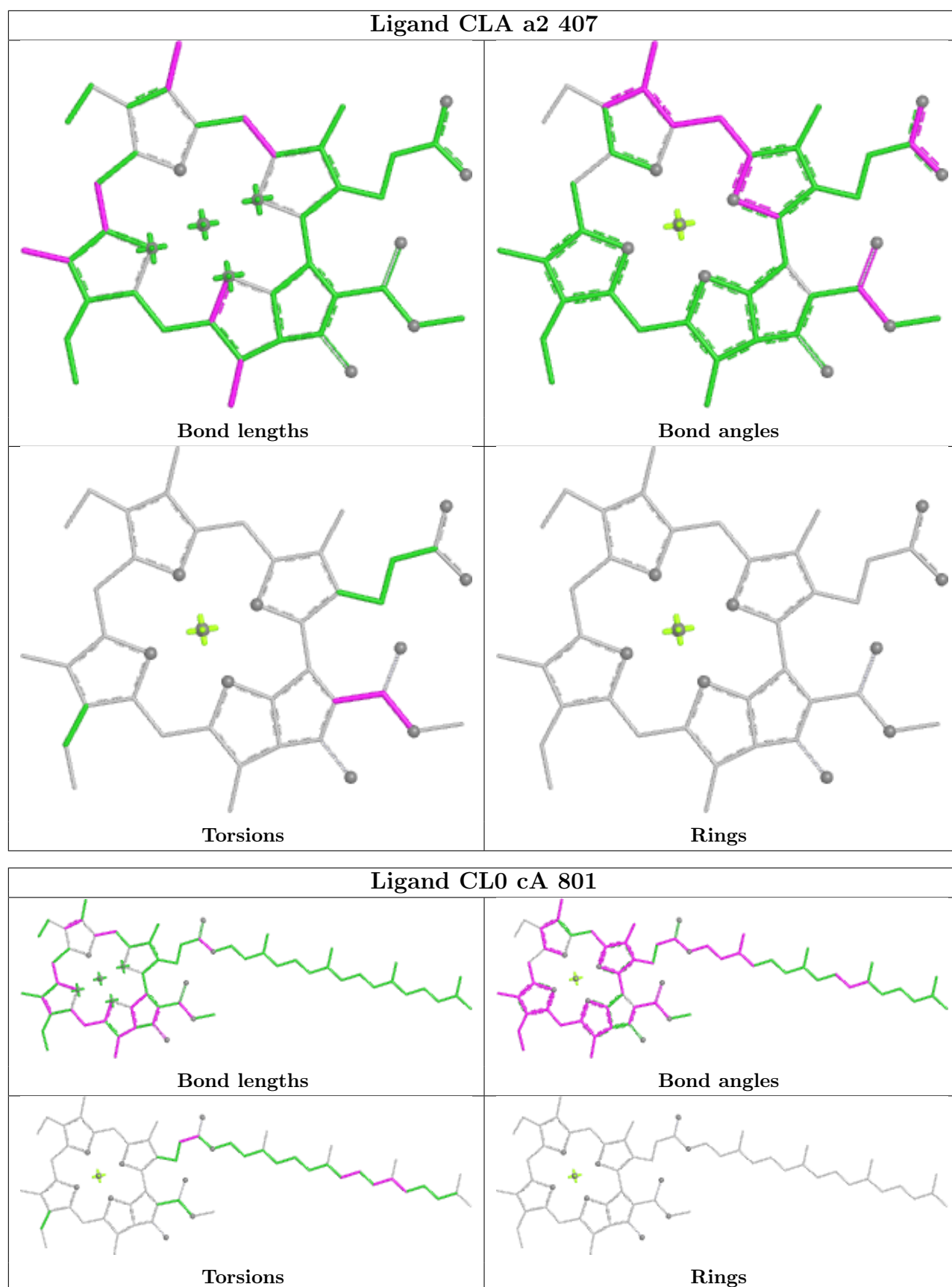
Ligand CLA cA 832

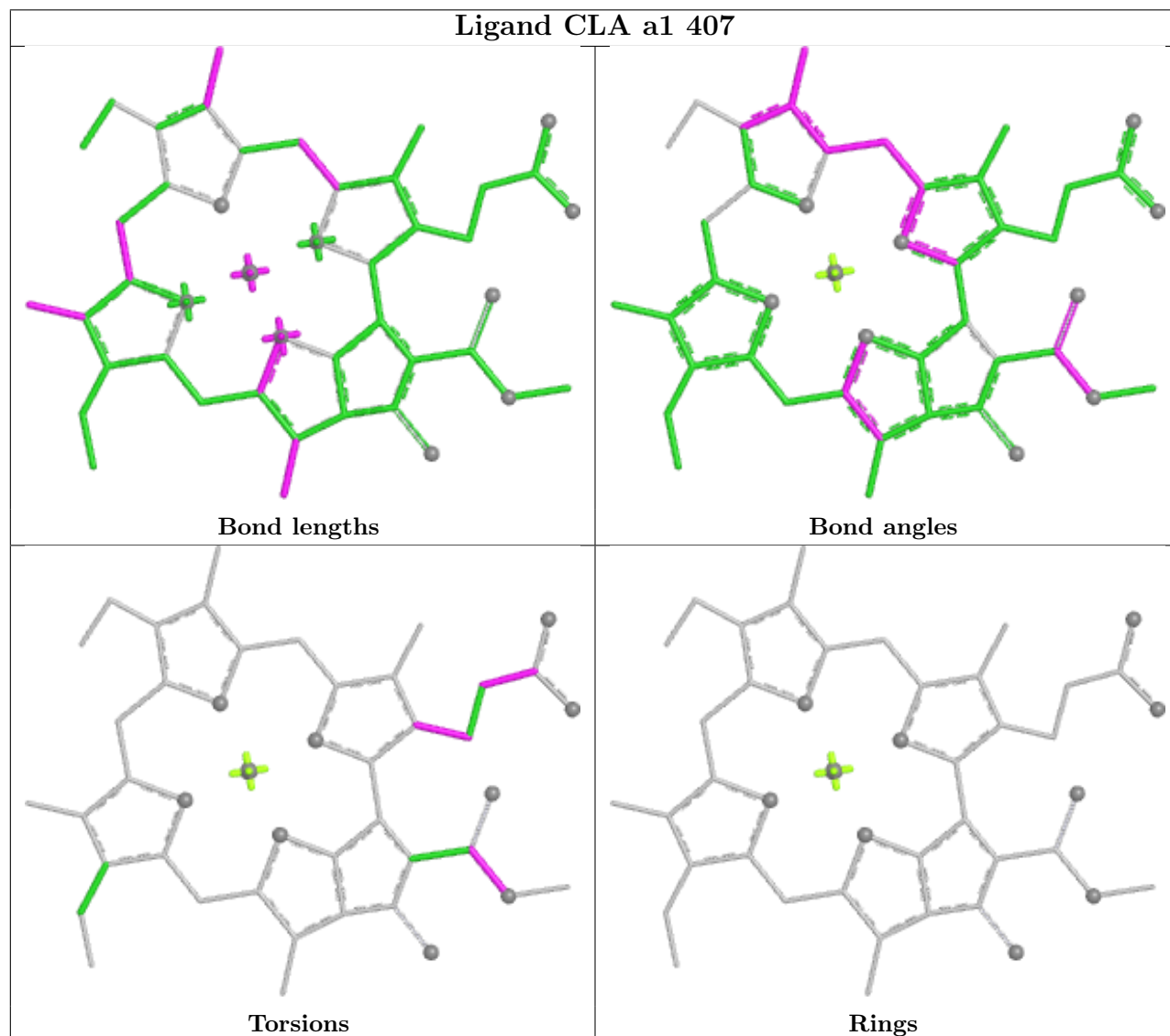
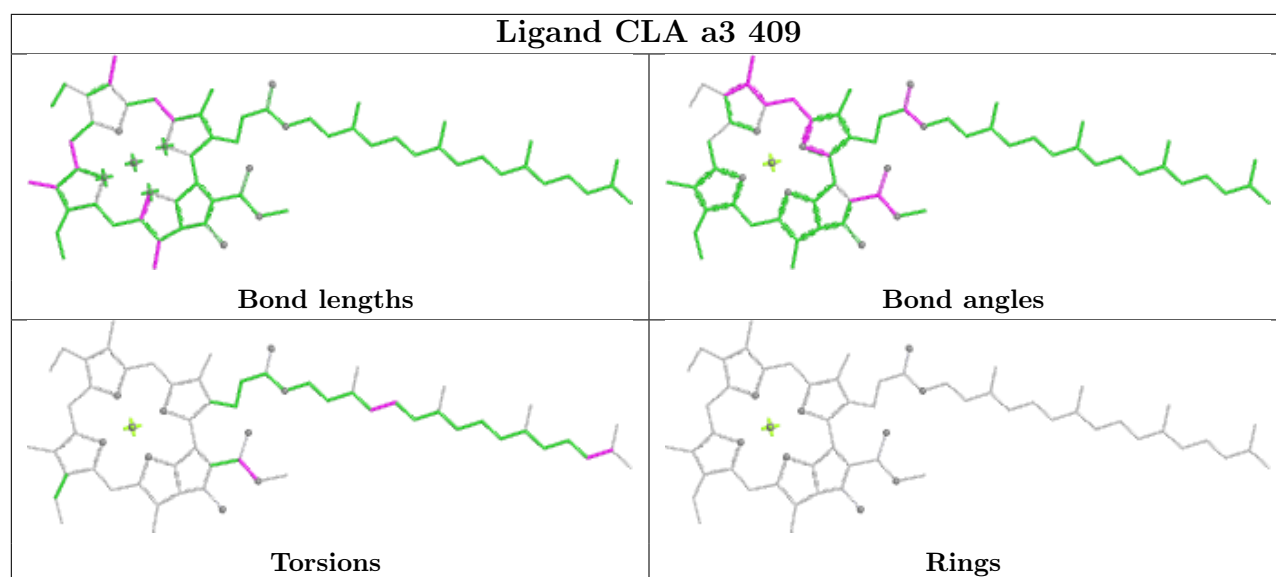


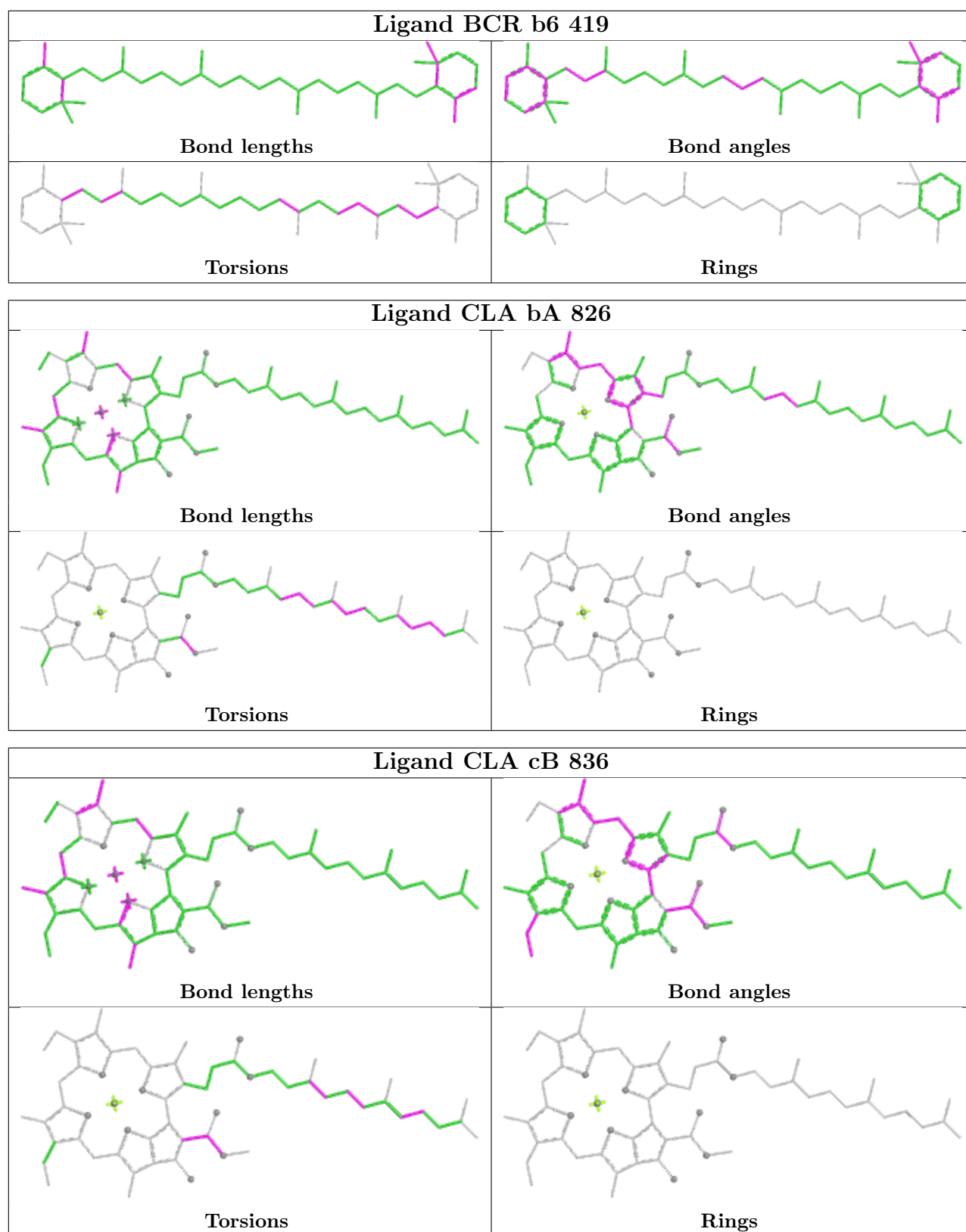
Ligand CLA b3 417

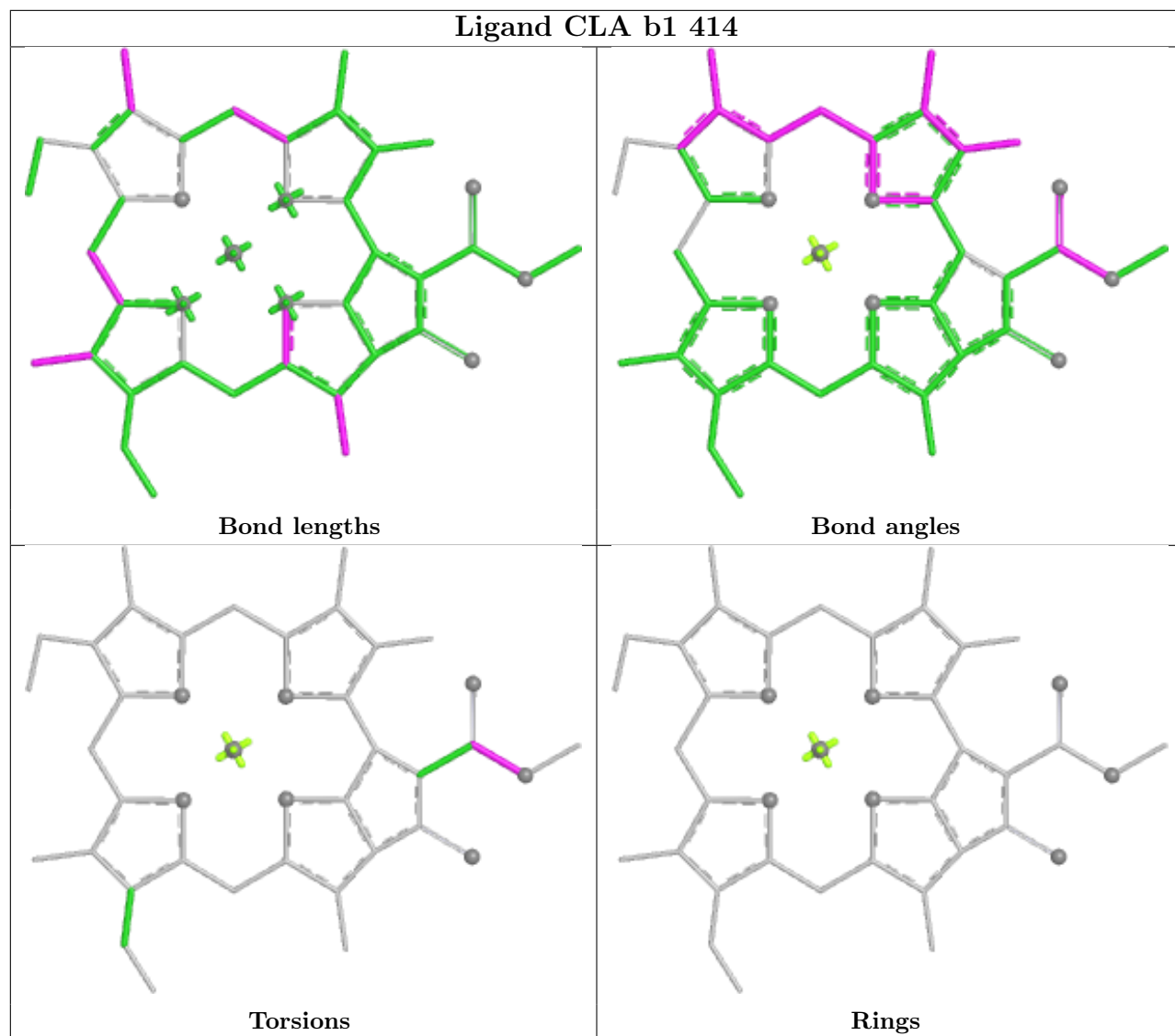


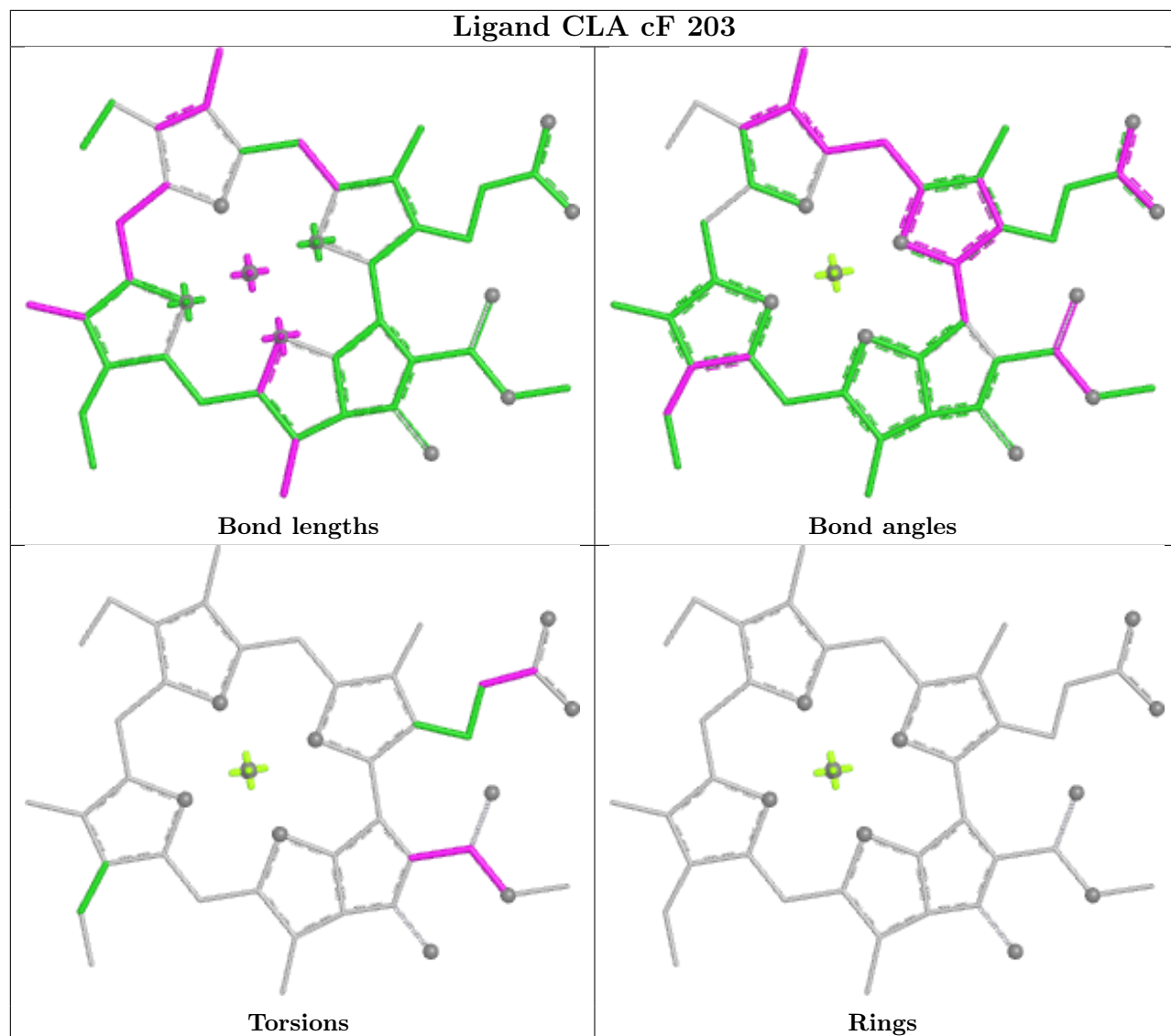


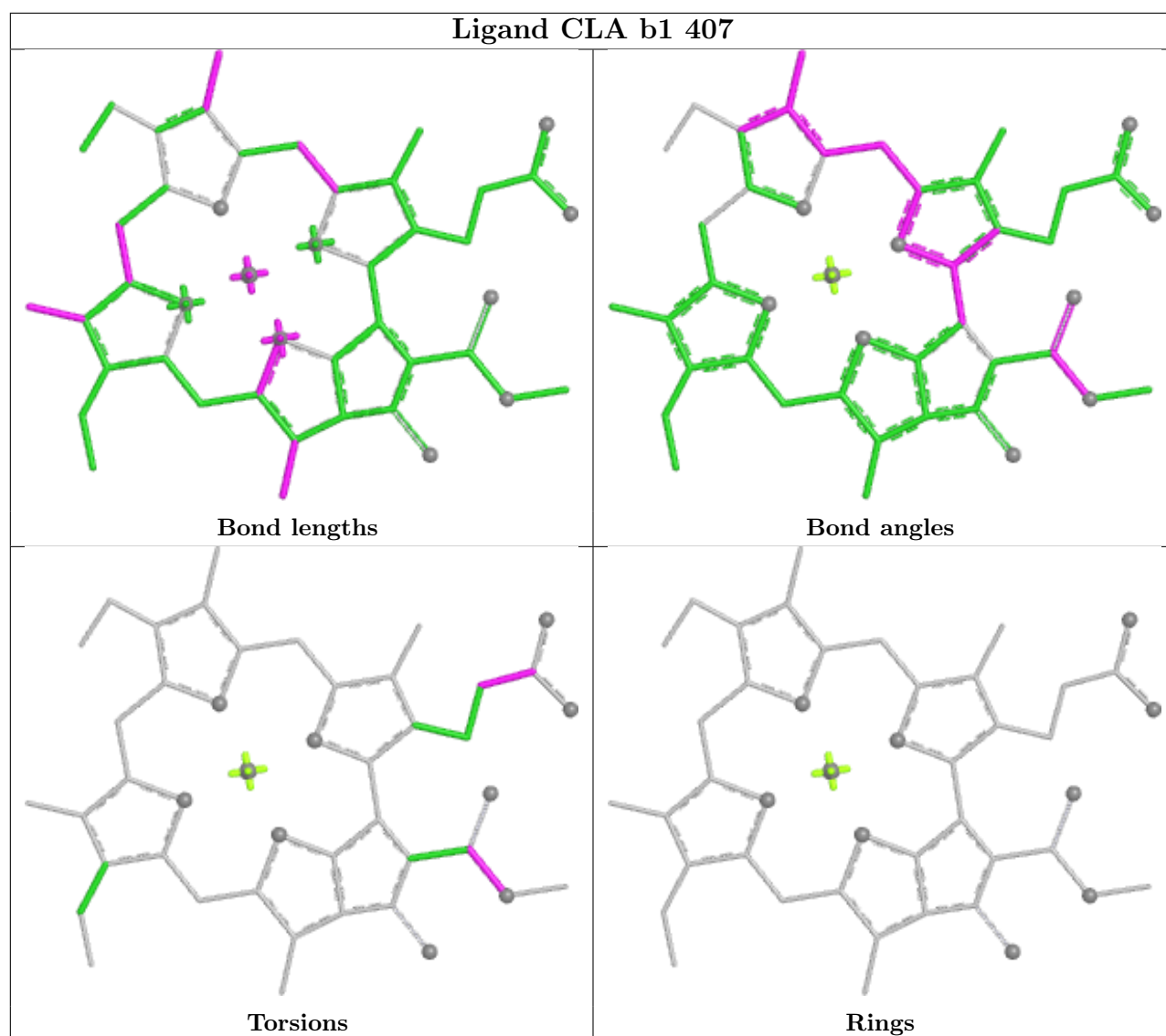


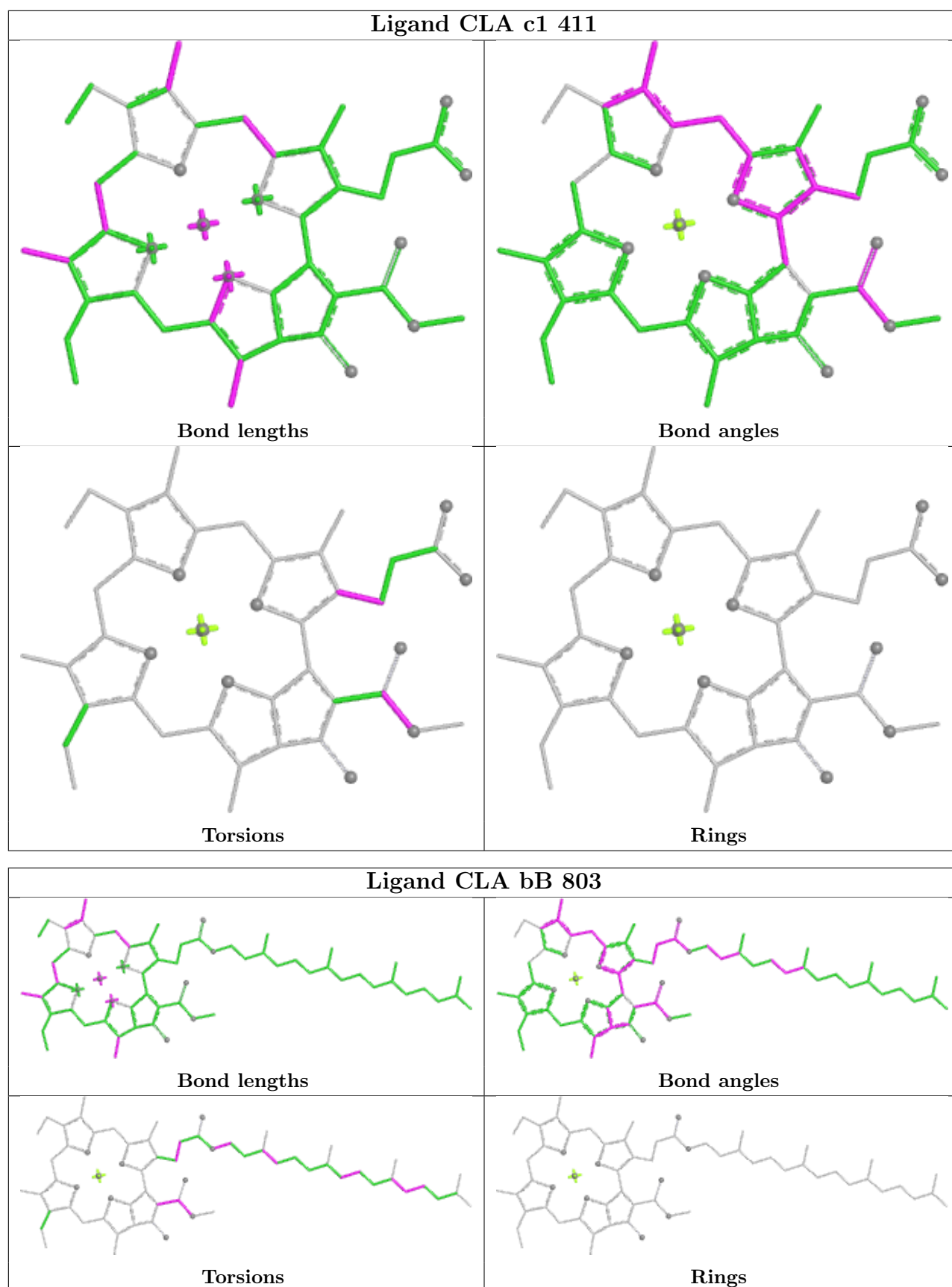


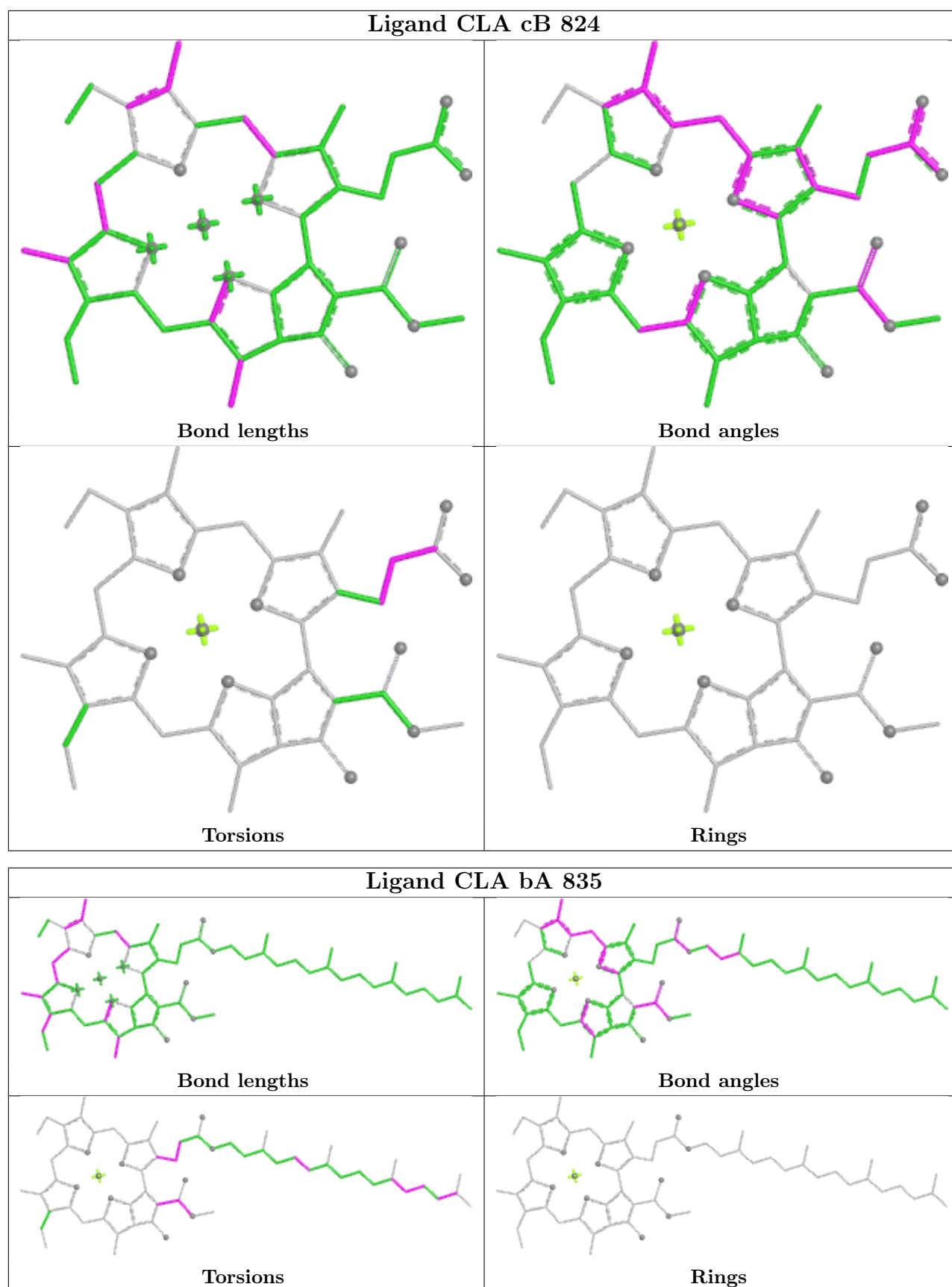


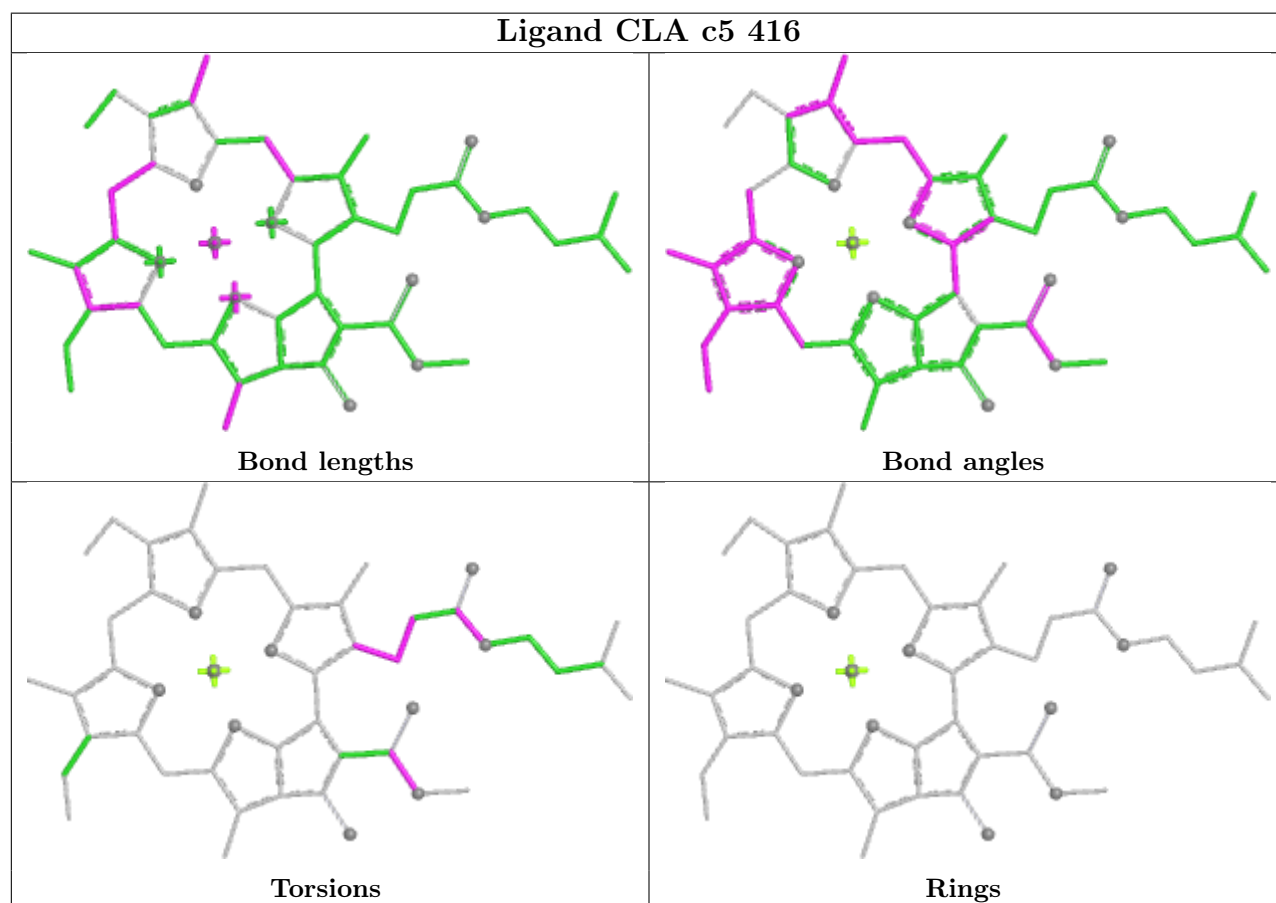
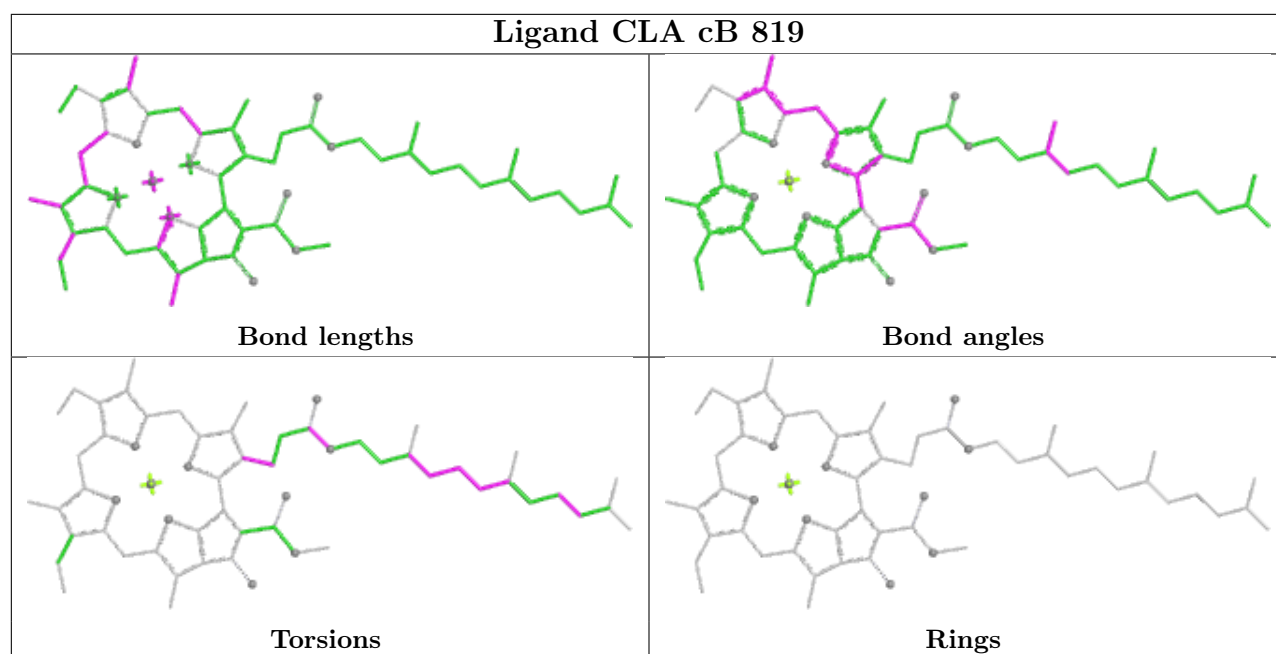


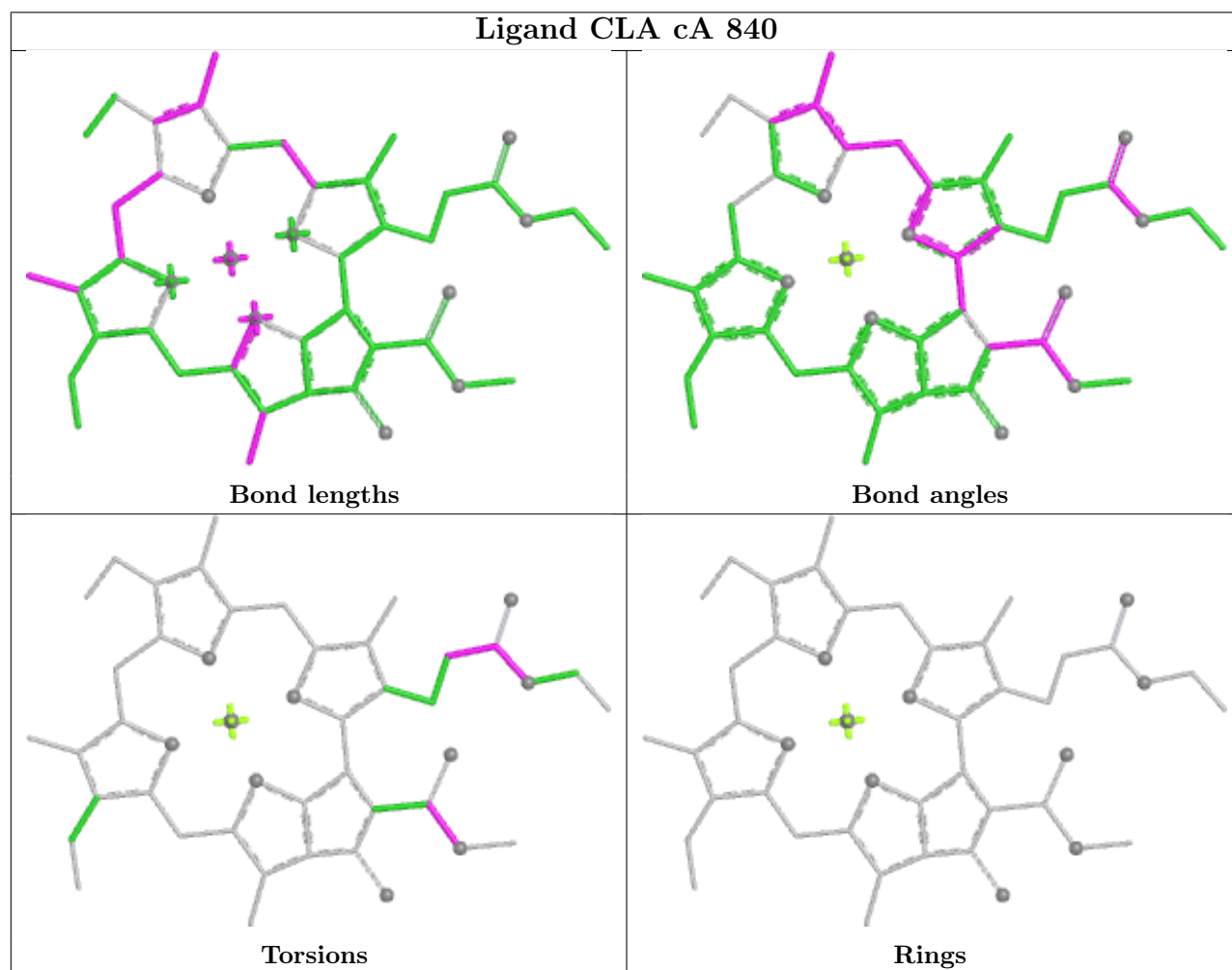
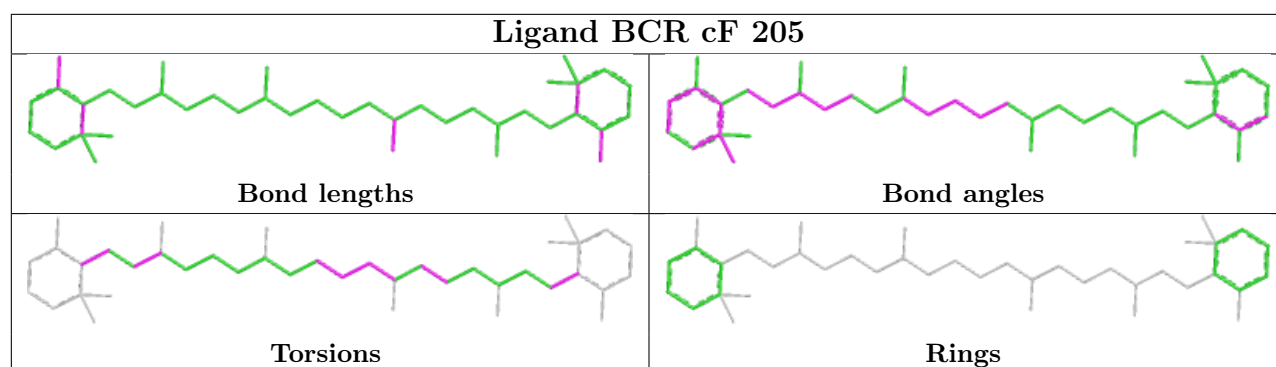




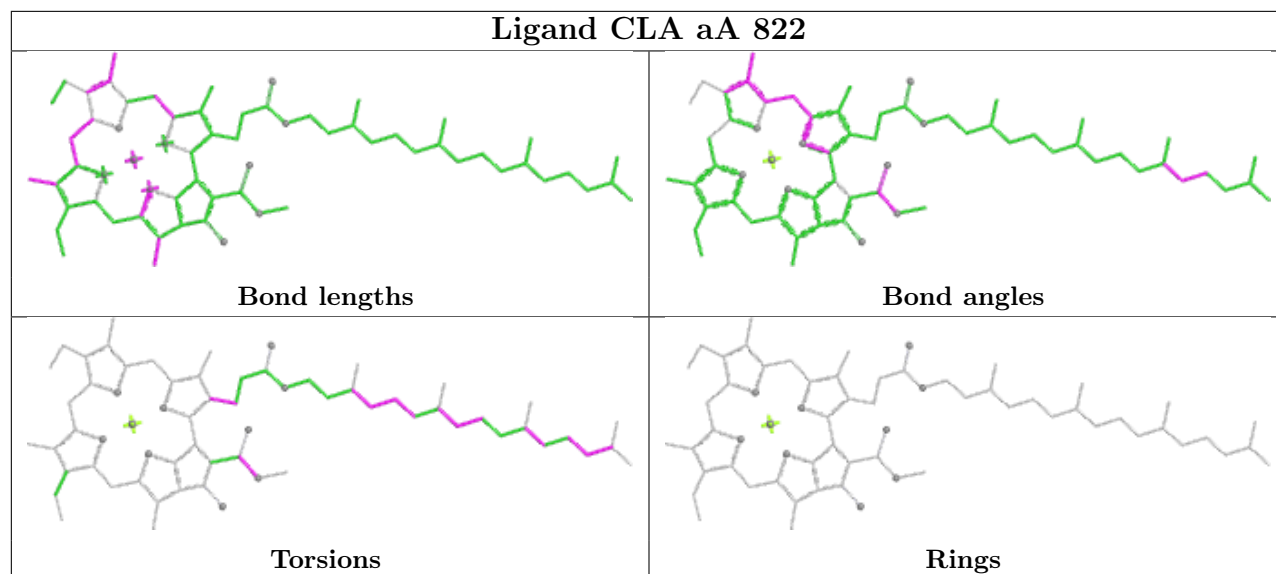




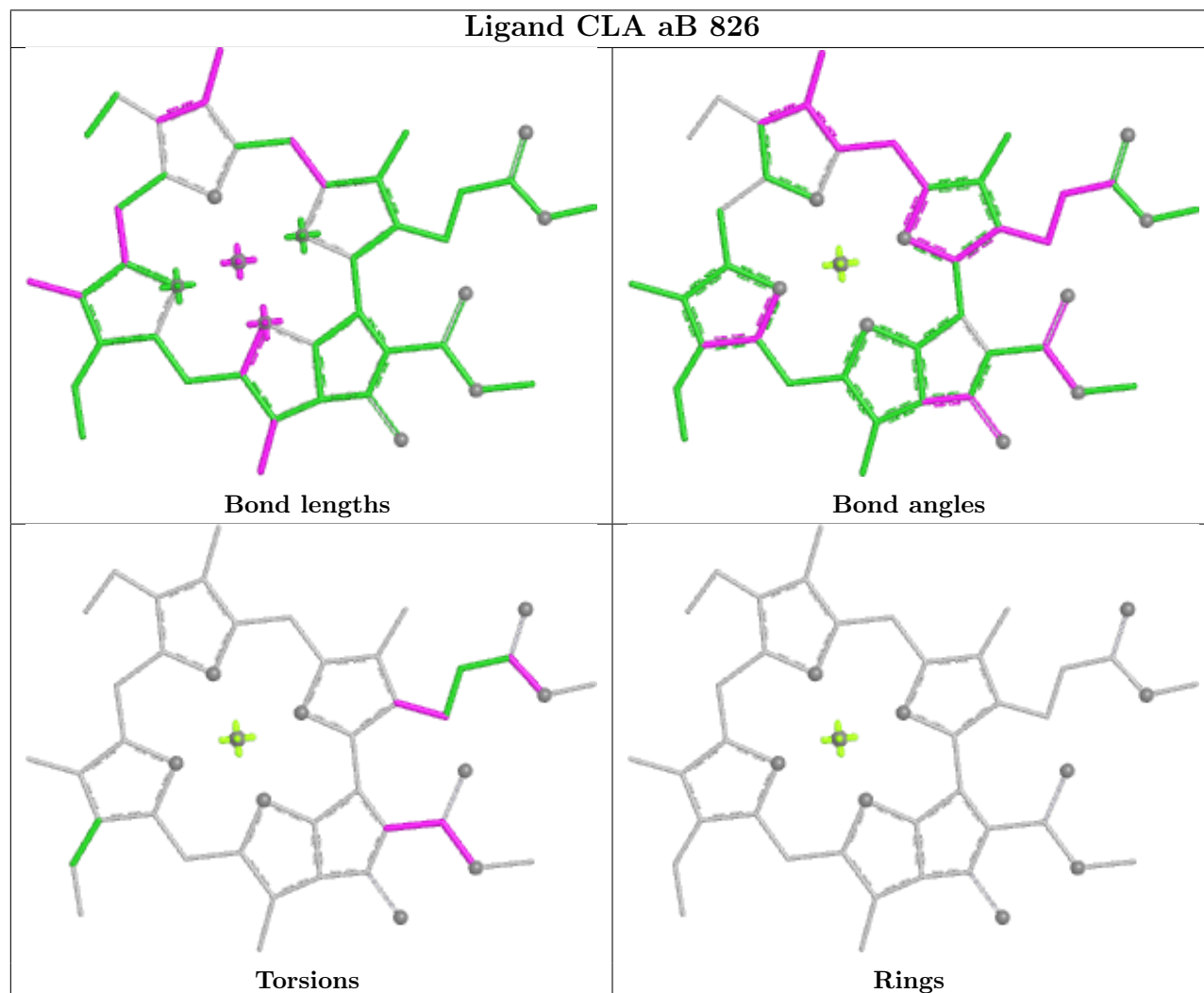


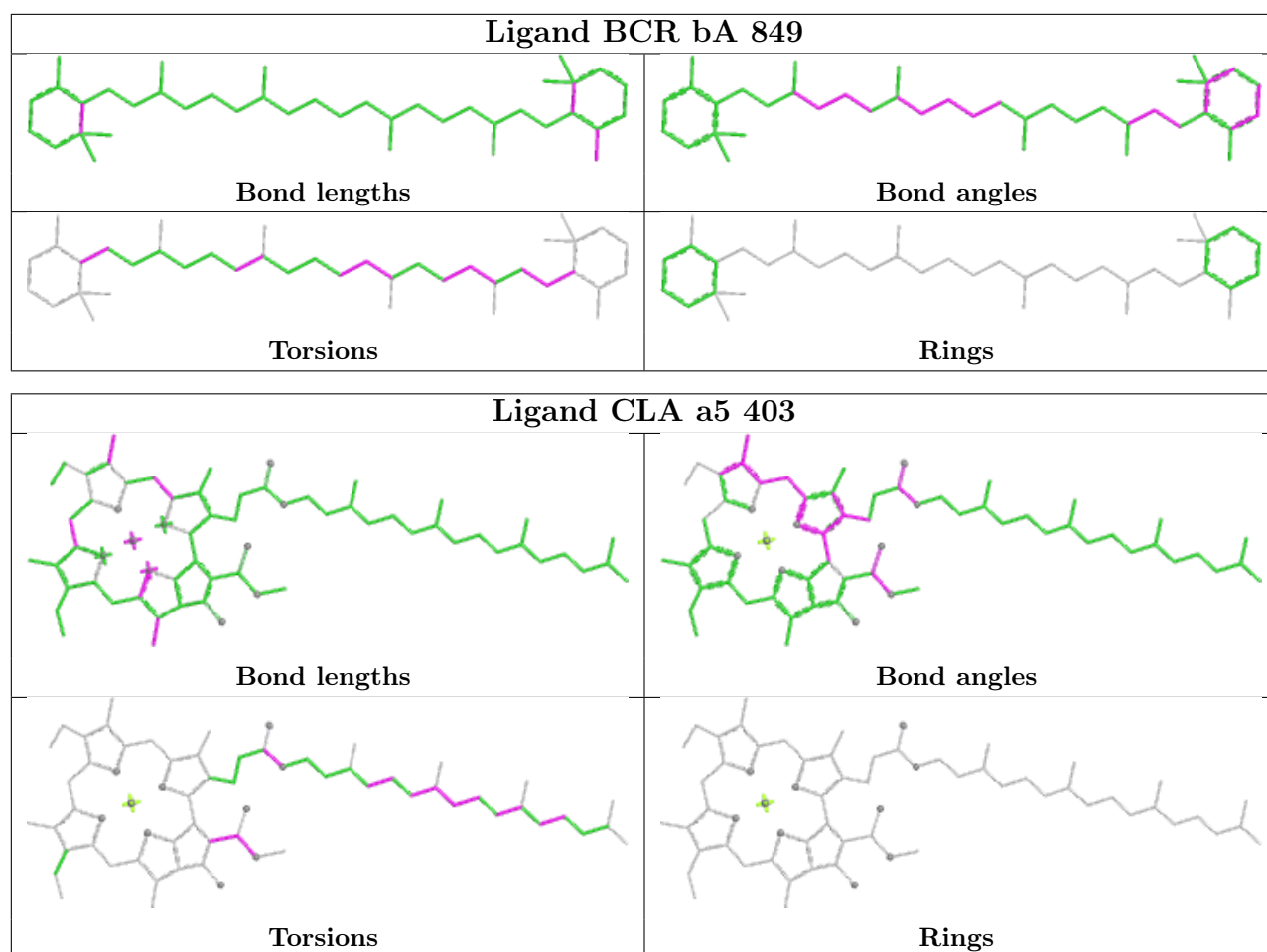


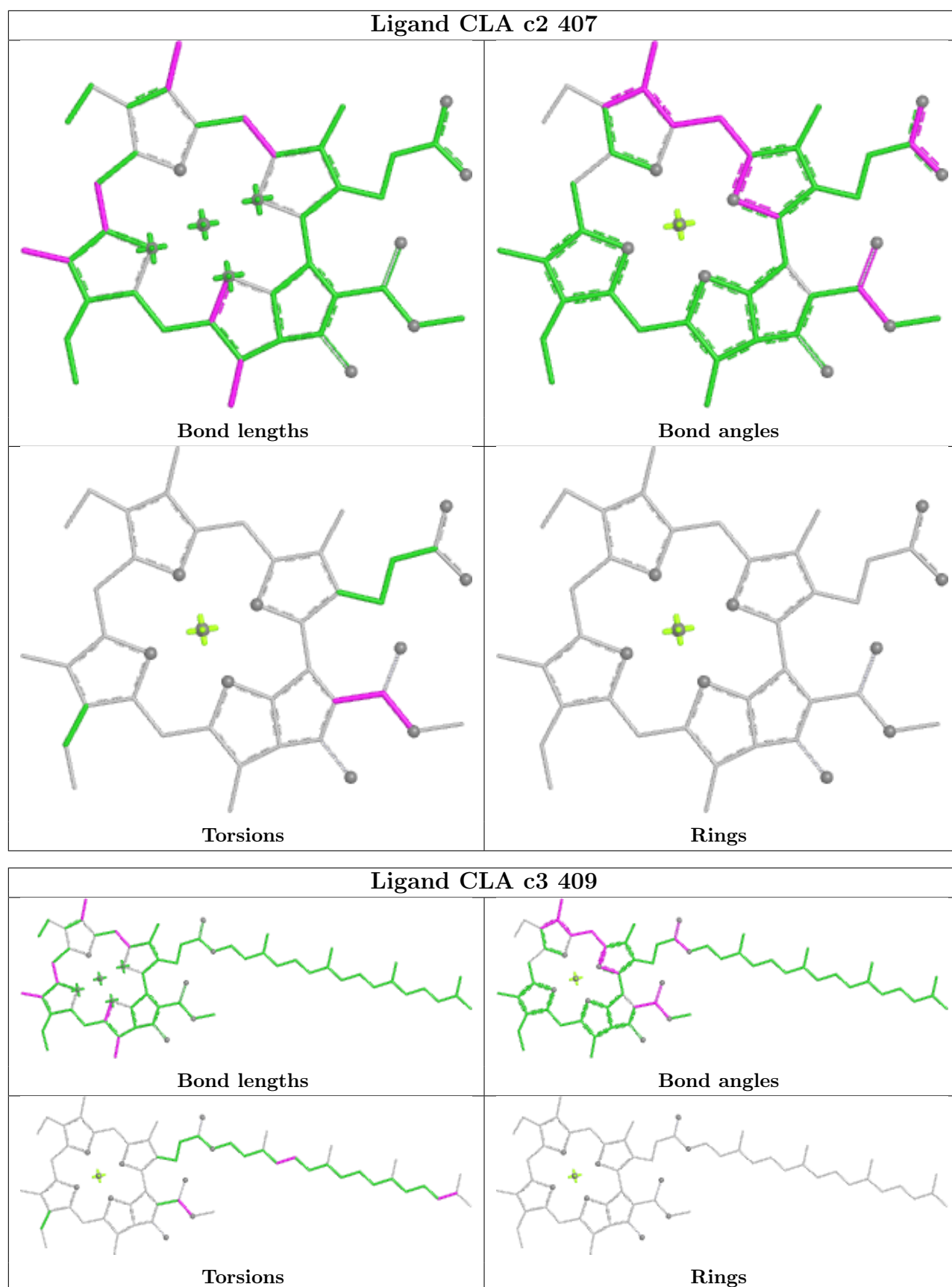
Ligand CLA aA 822

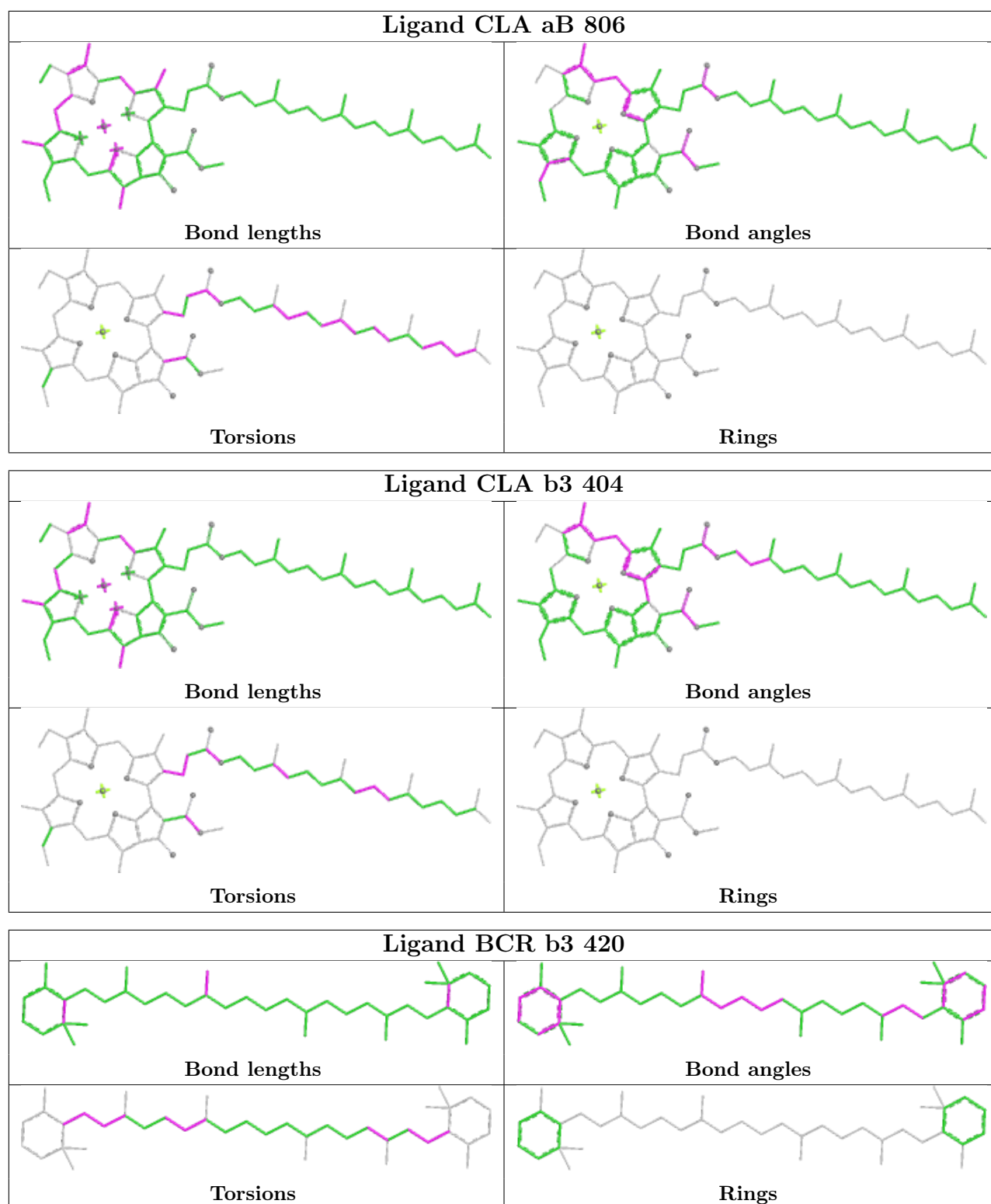


Ligand CLA aB 826

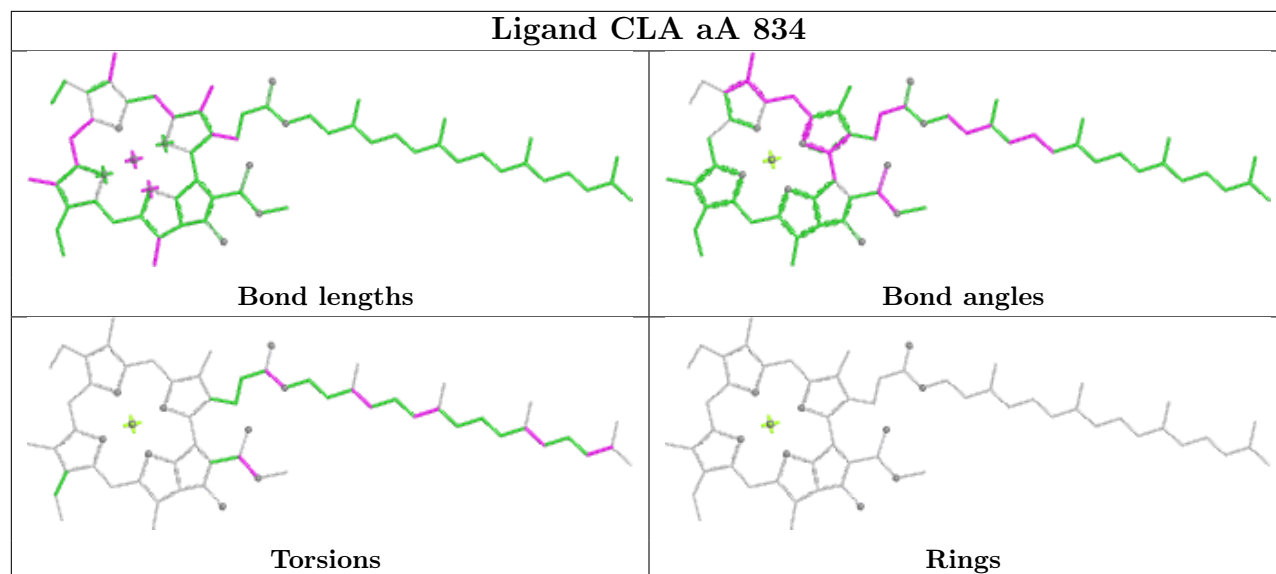




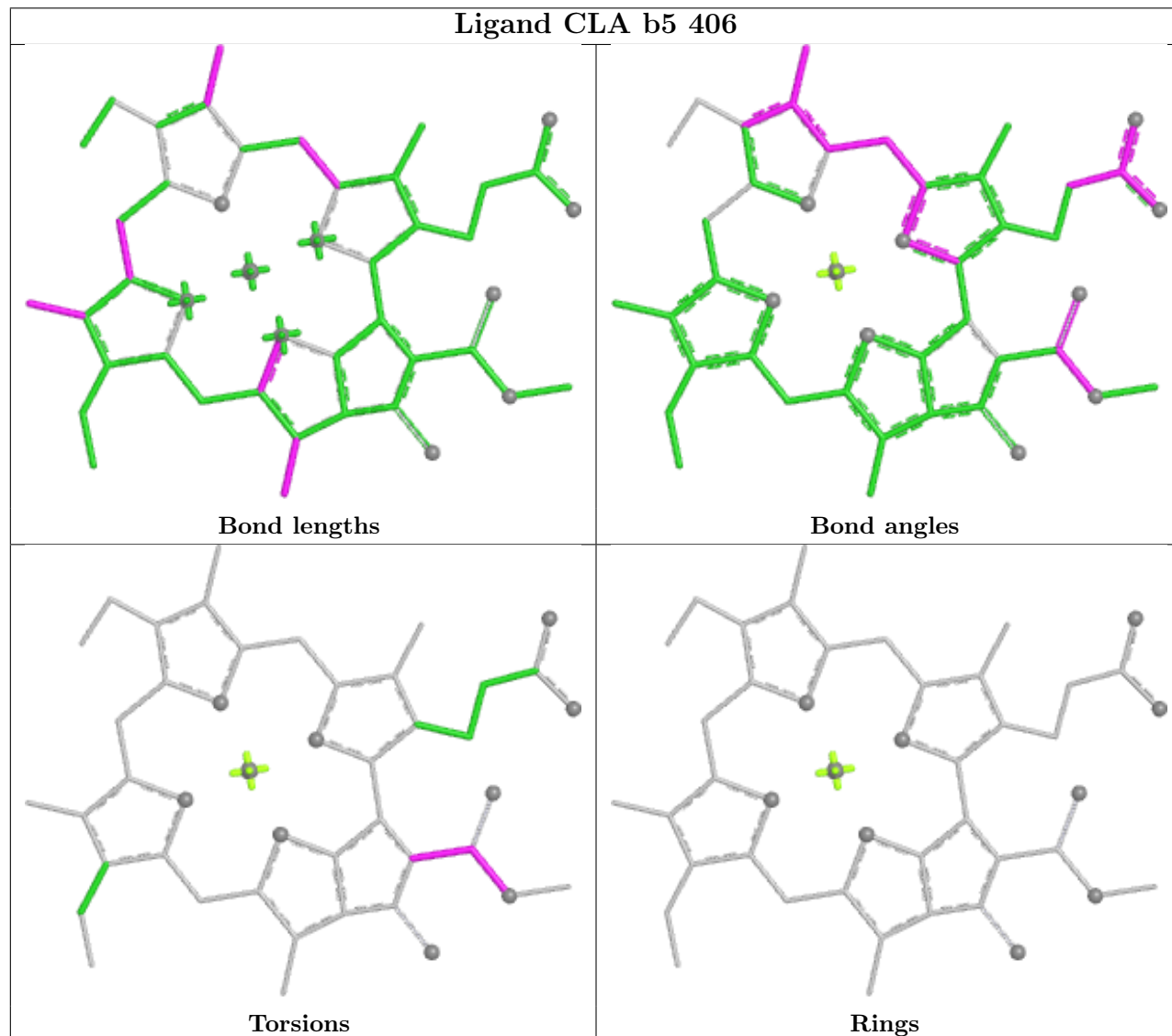


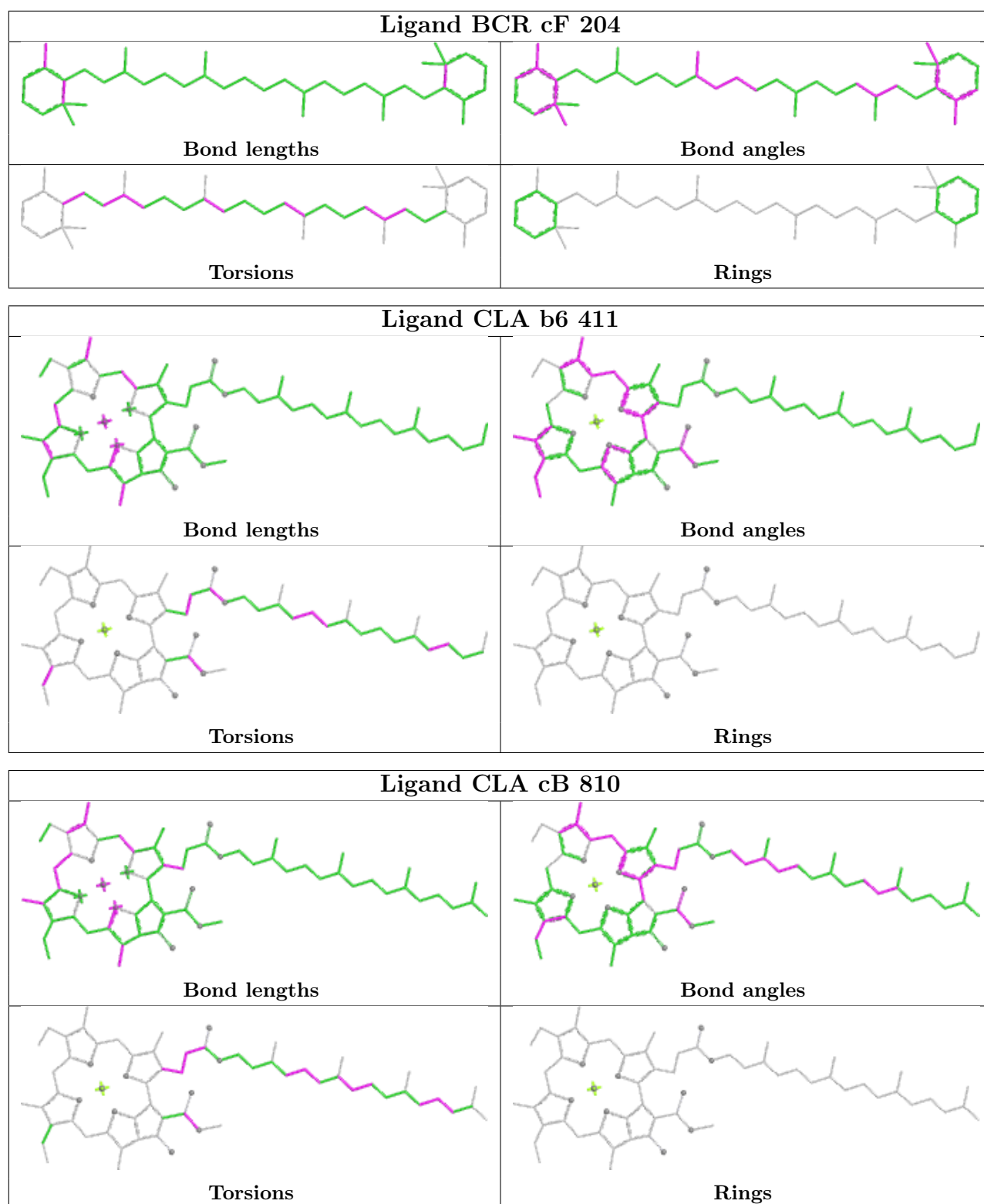


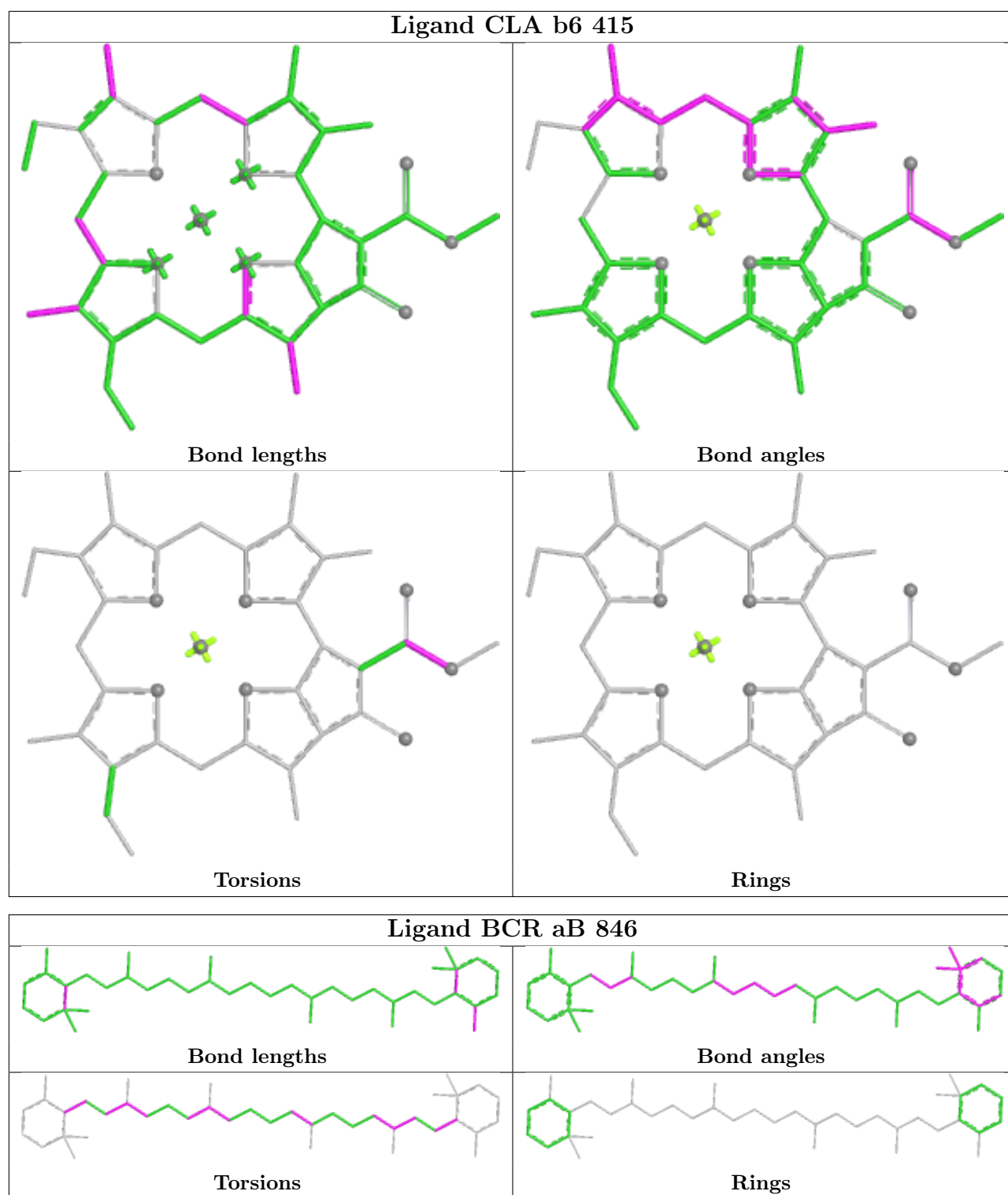
Ligand CLA aA 834

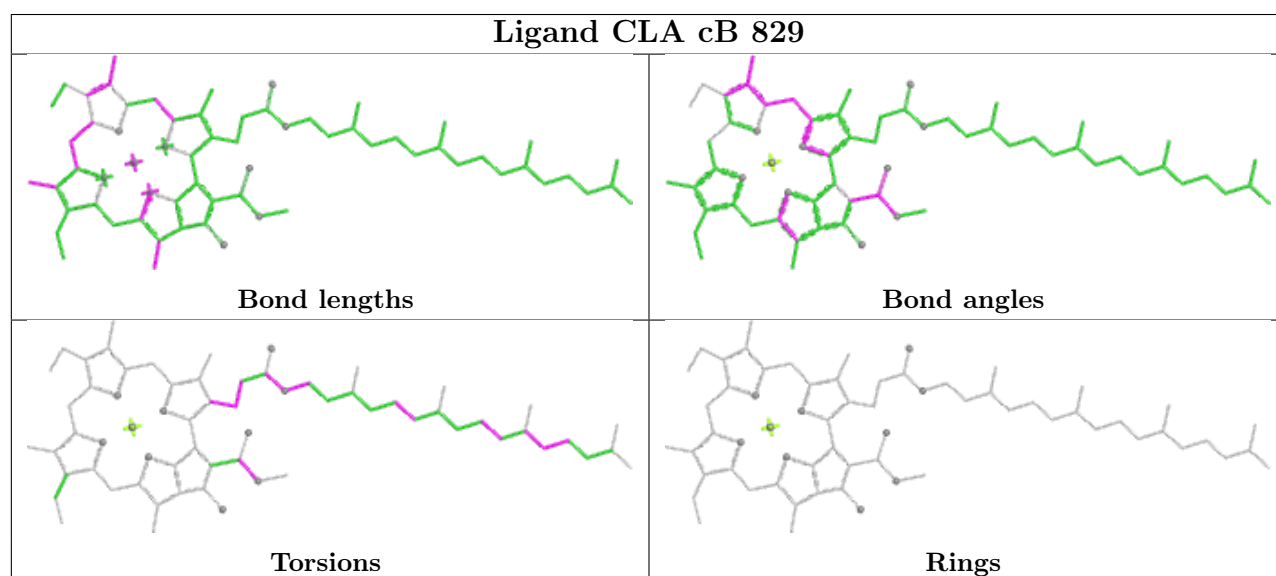
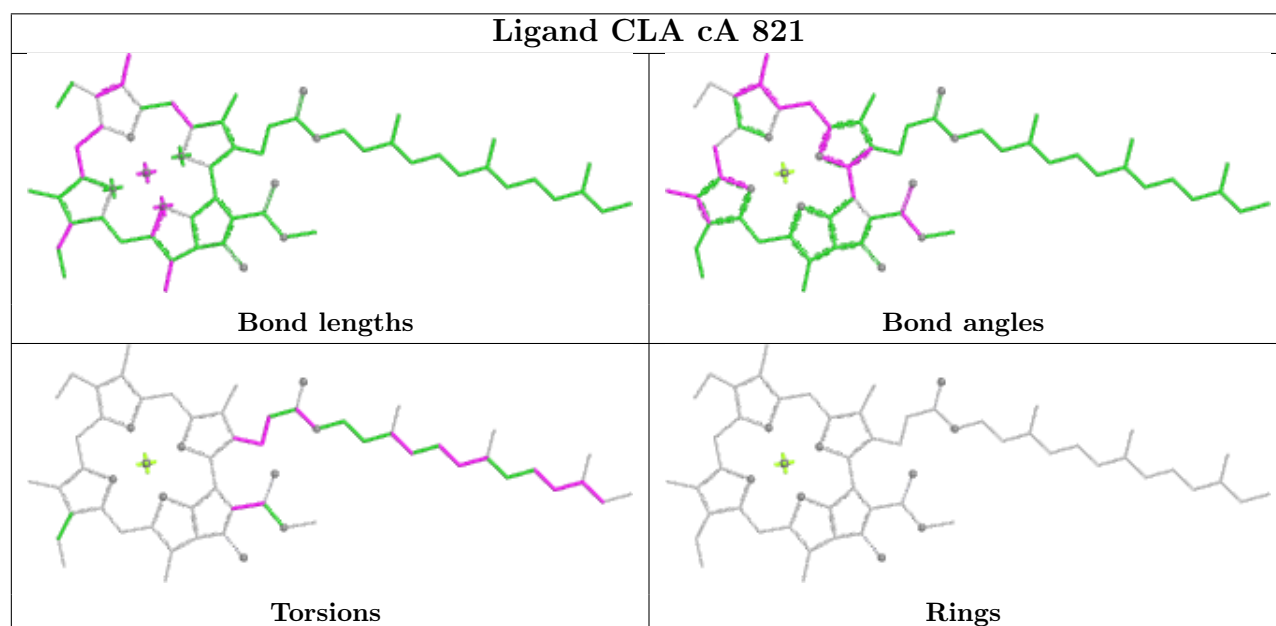
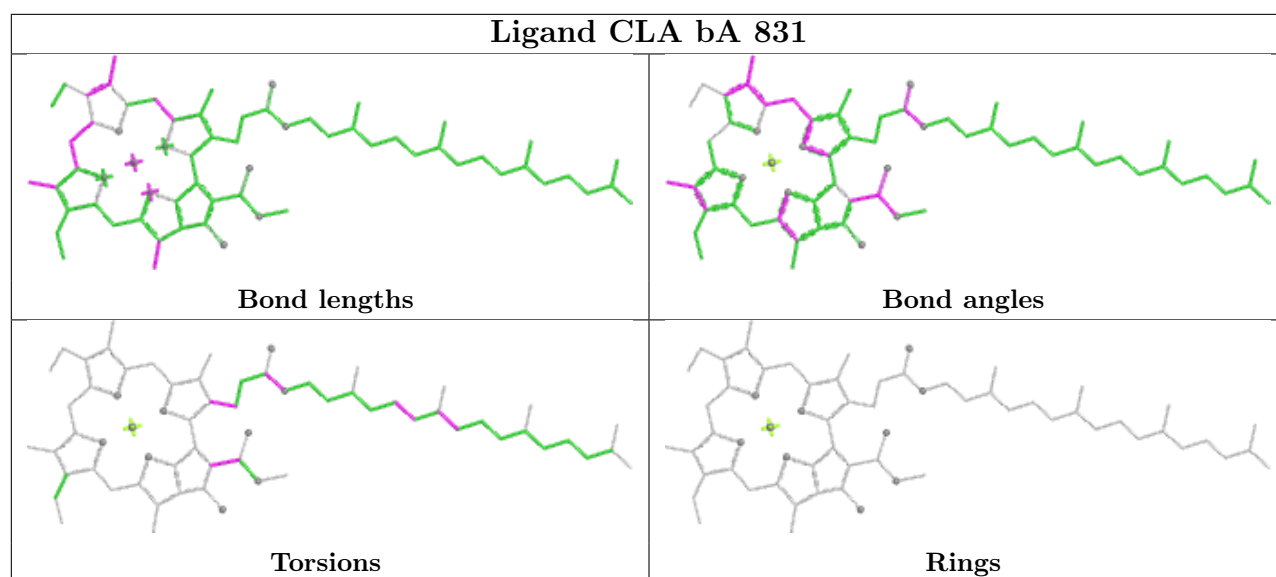


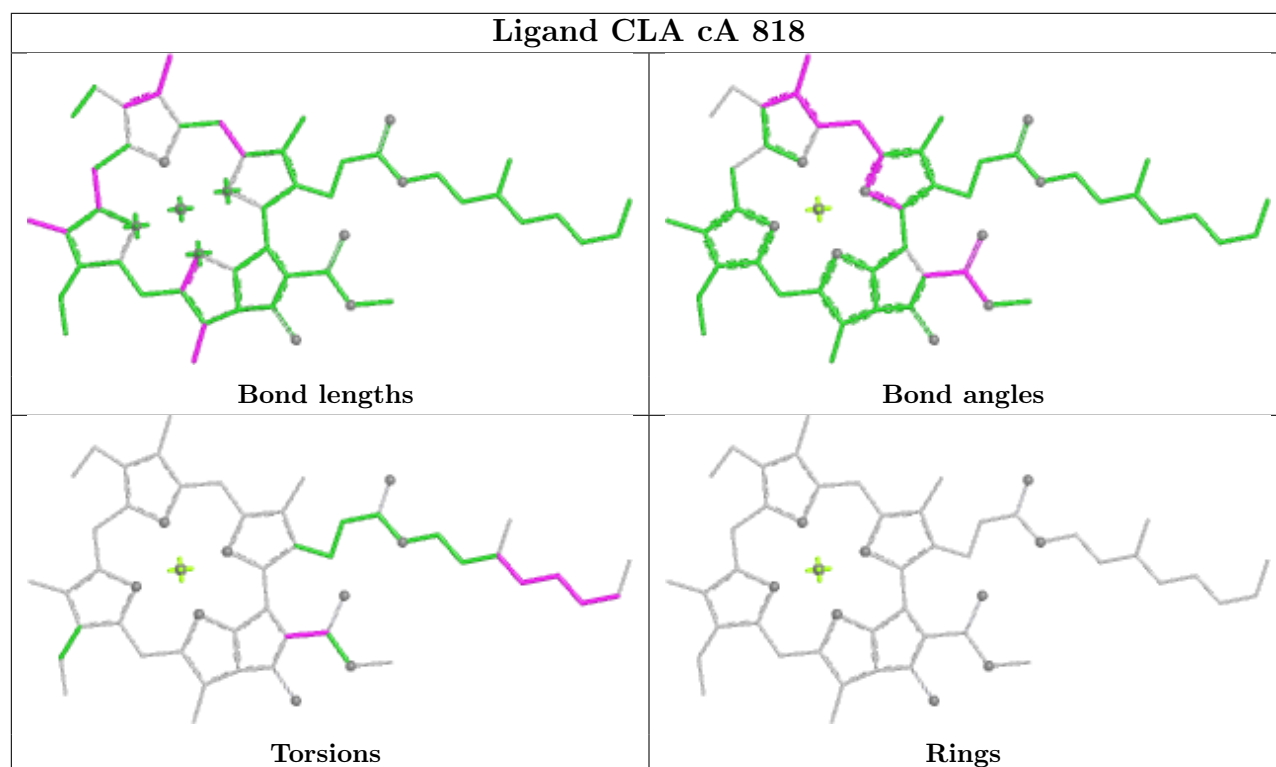
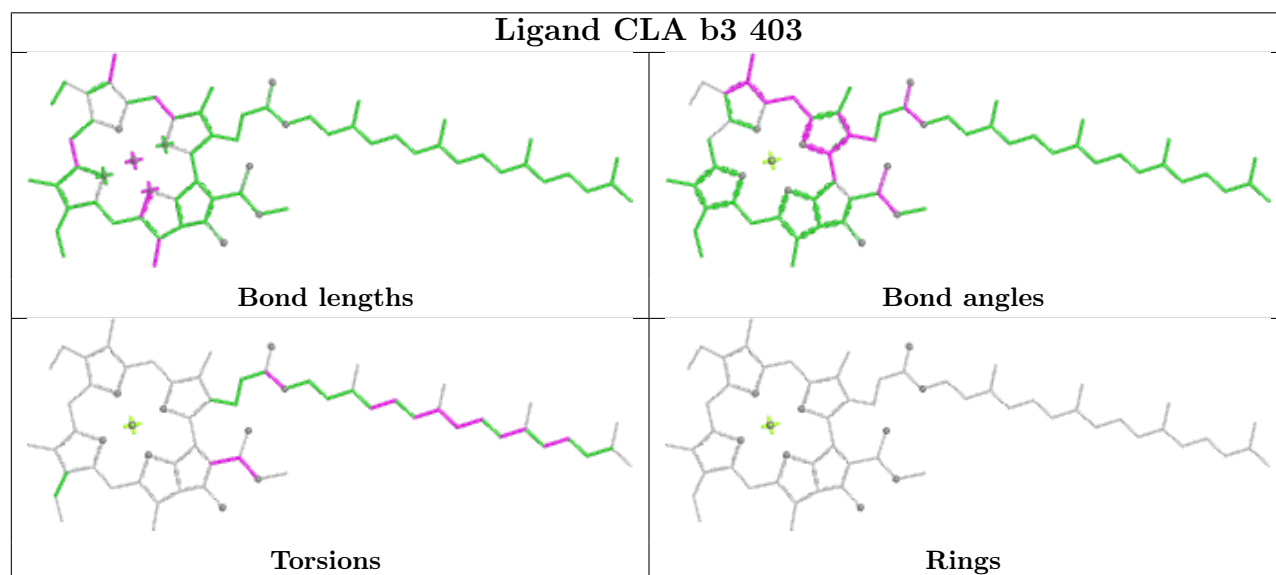
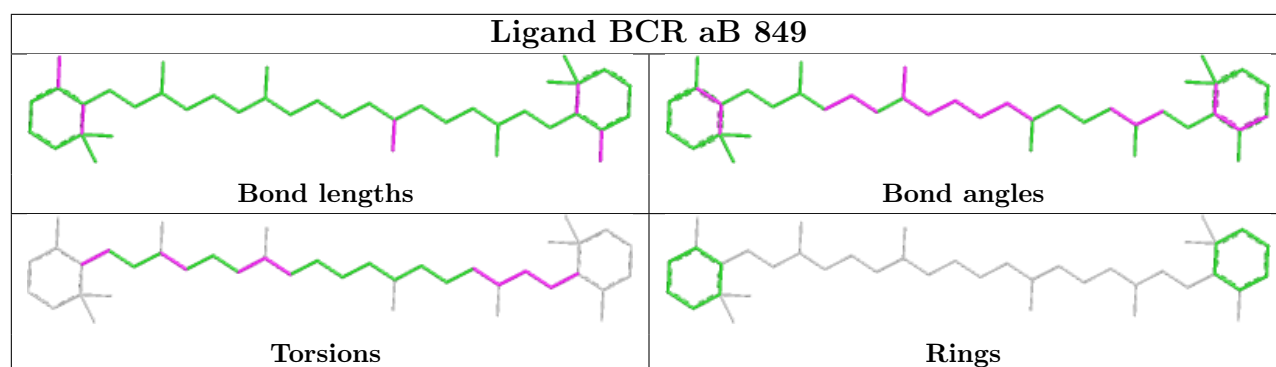
Ligand CLA b5 406

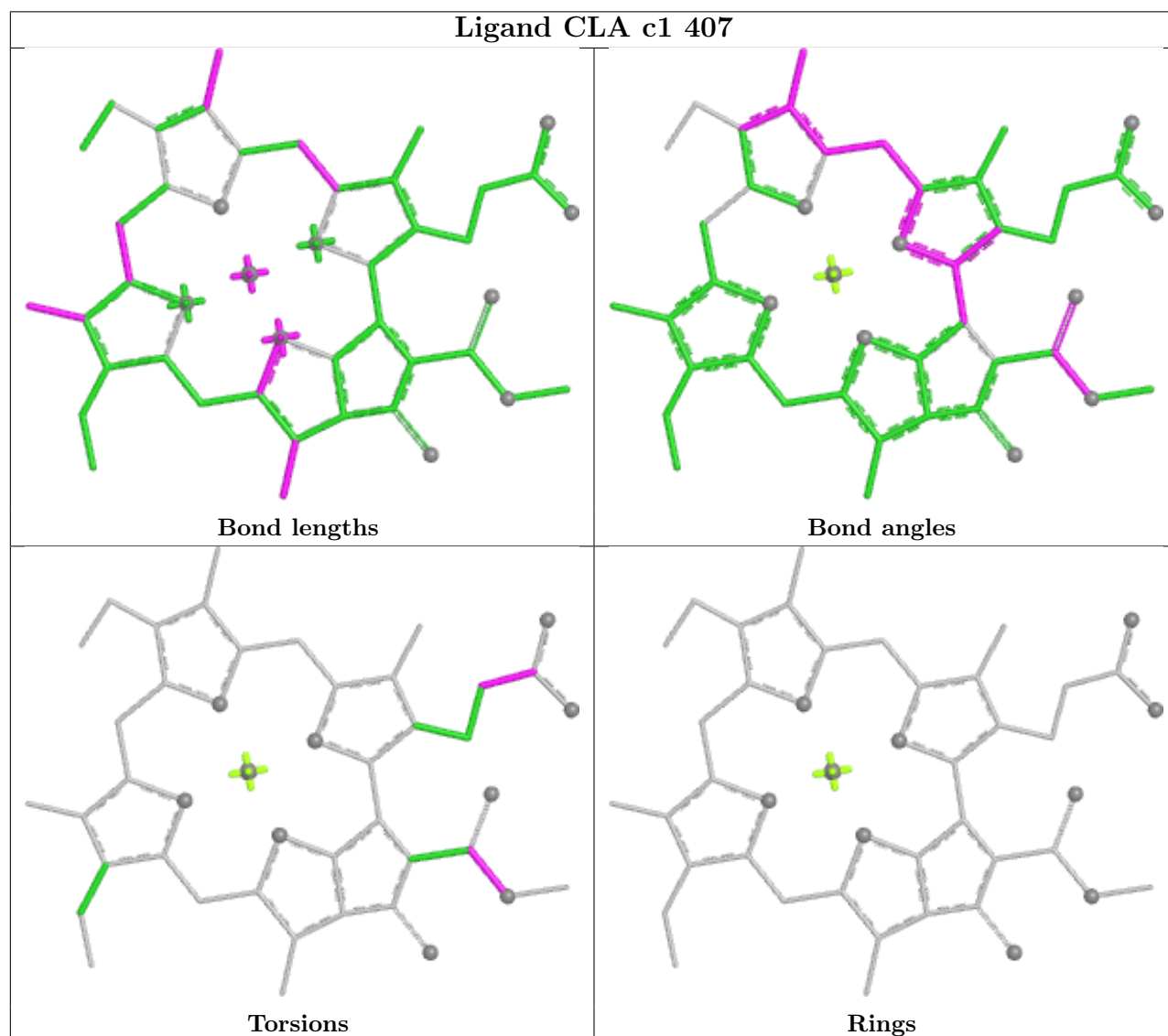
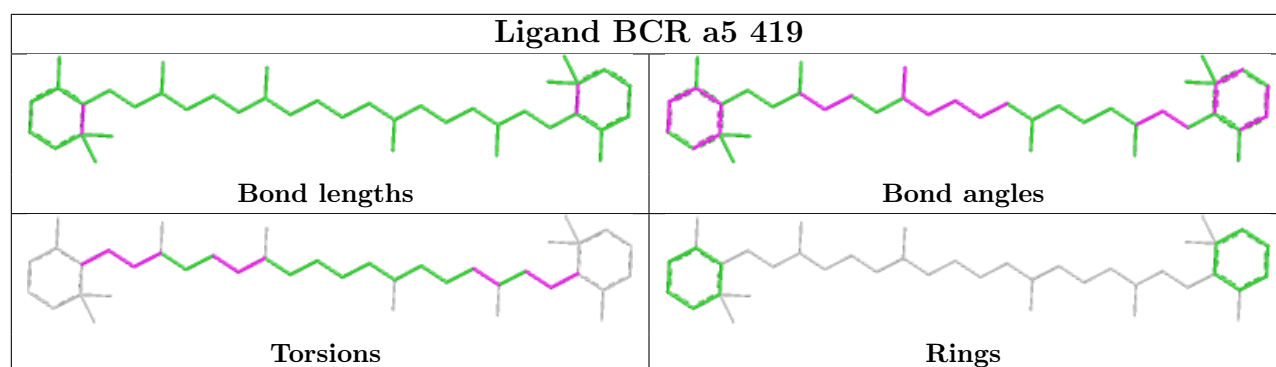


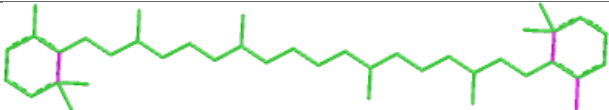
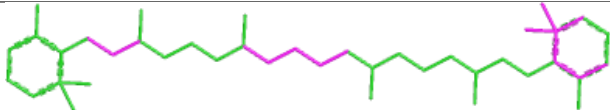
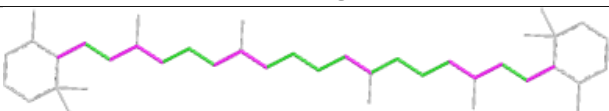
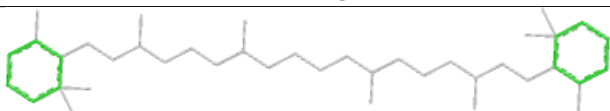


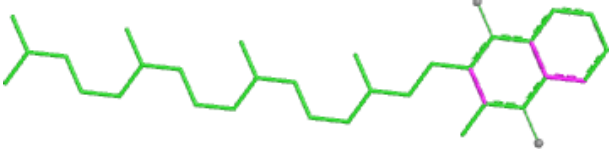
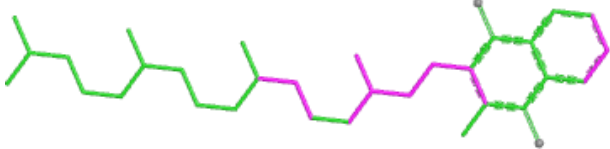
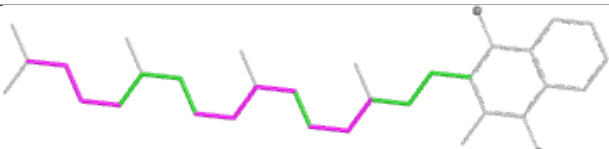
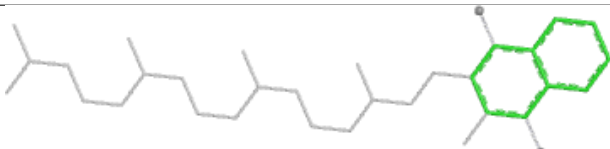


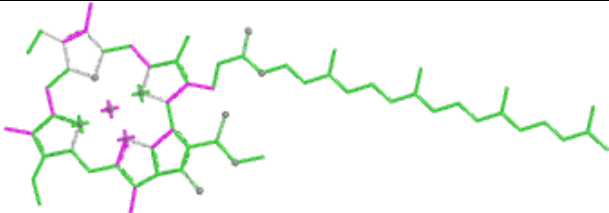
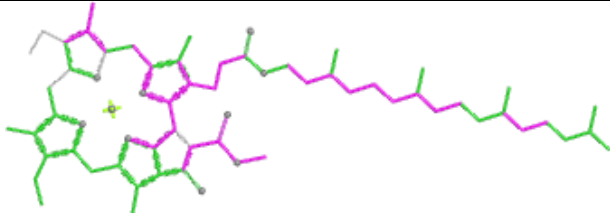
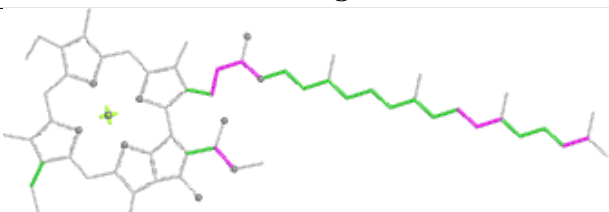
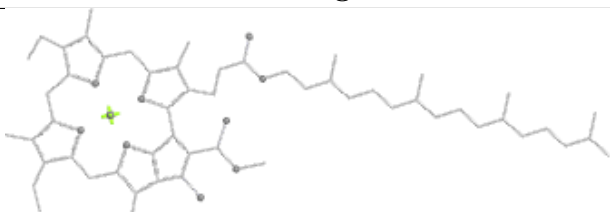


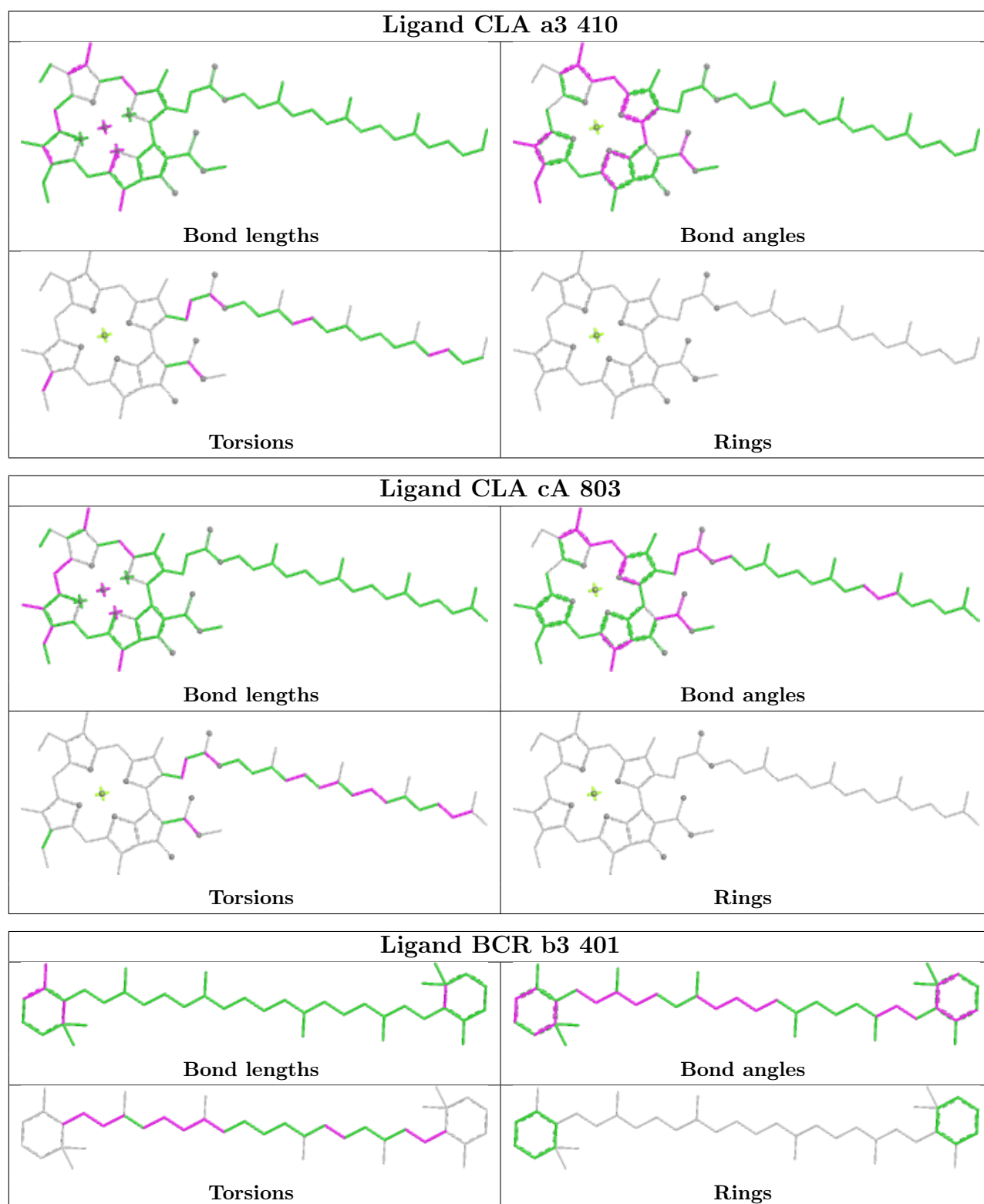


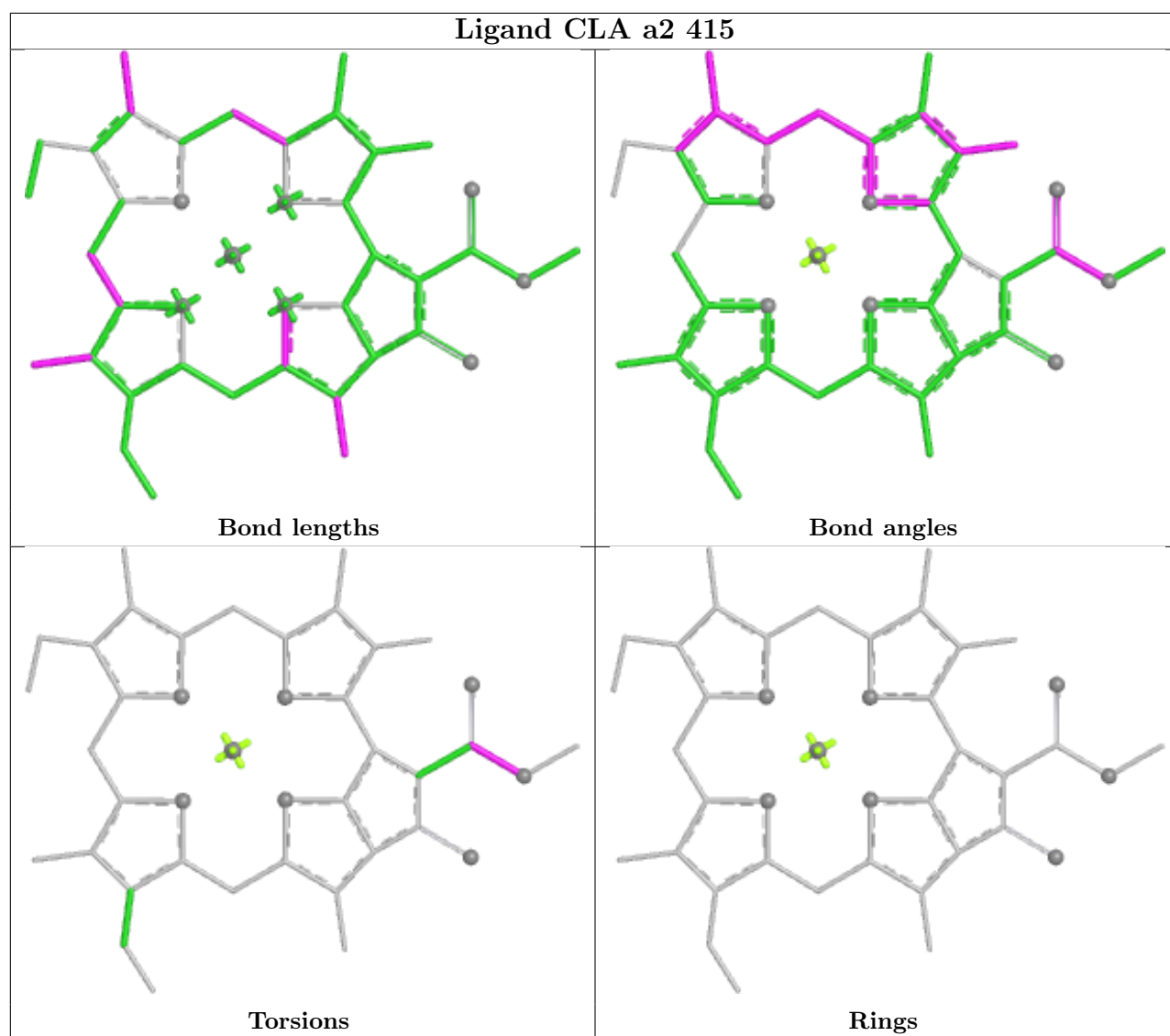


Ligand BCR cB 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

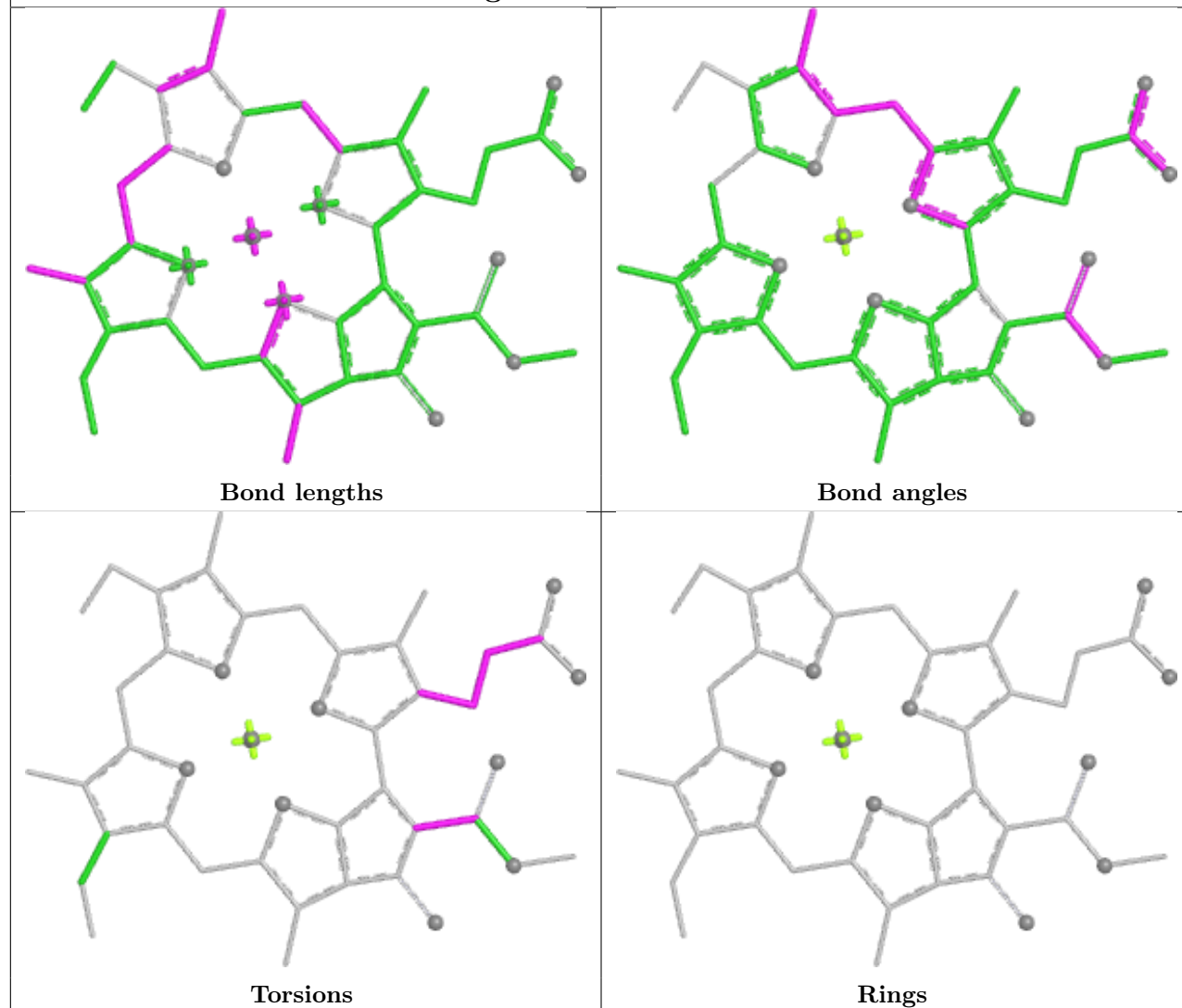
Ligand PQN bB 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b6 422	
	
Bond lengths	Bond angles
	
Torsions	Rings

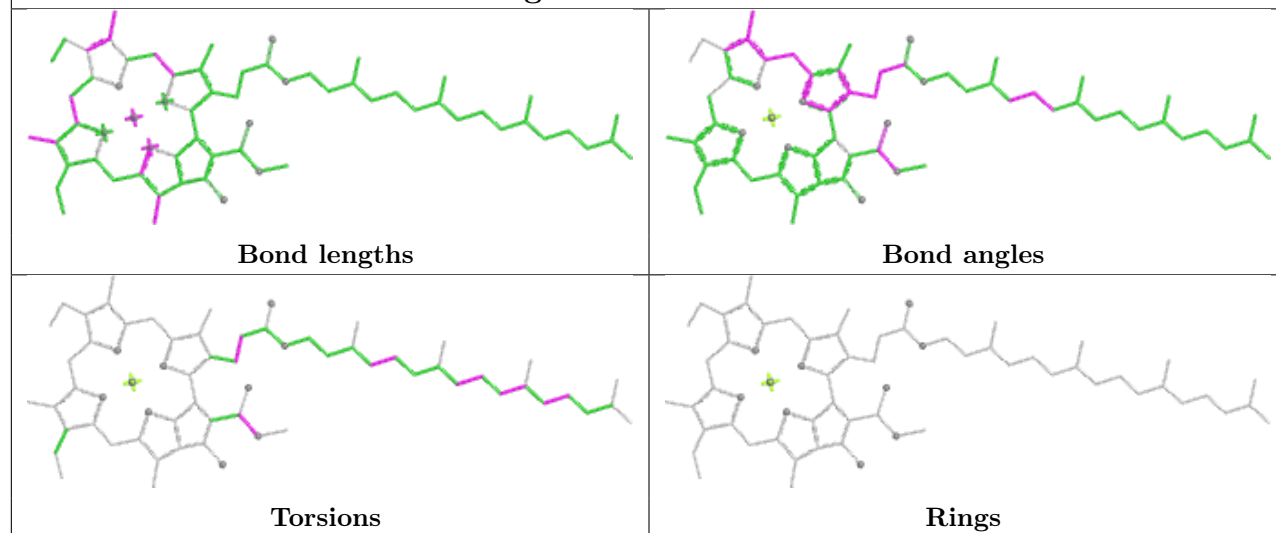


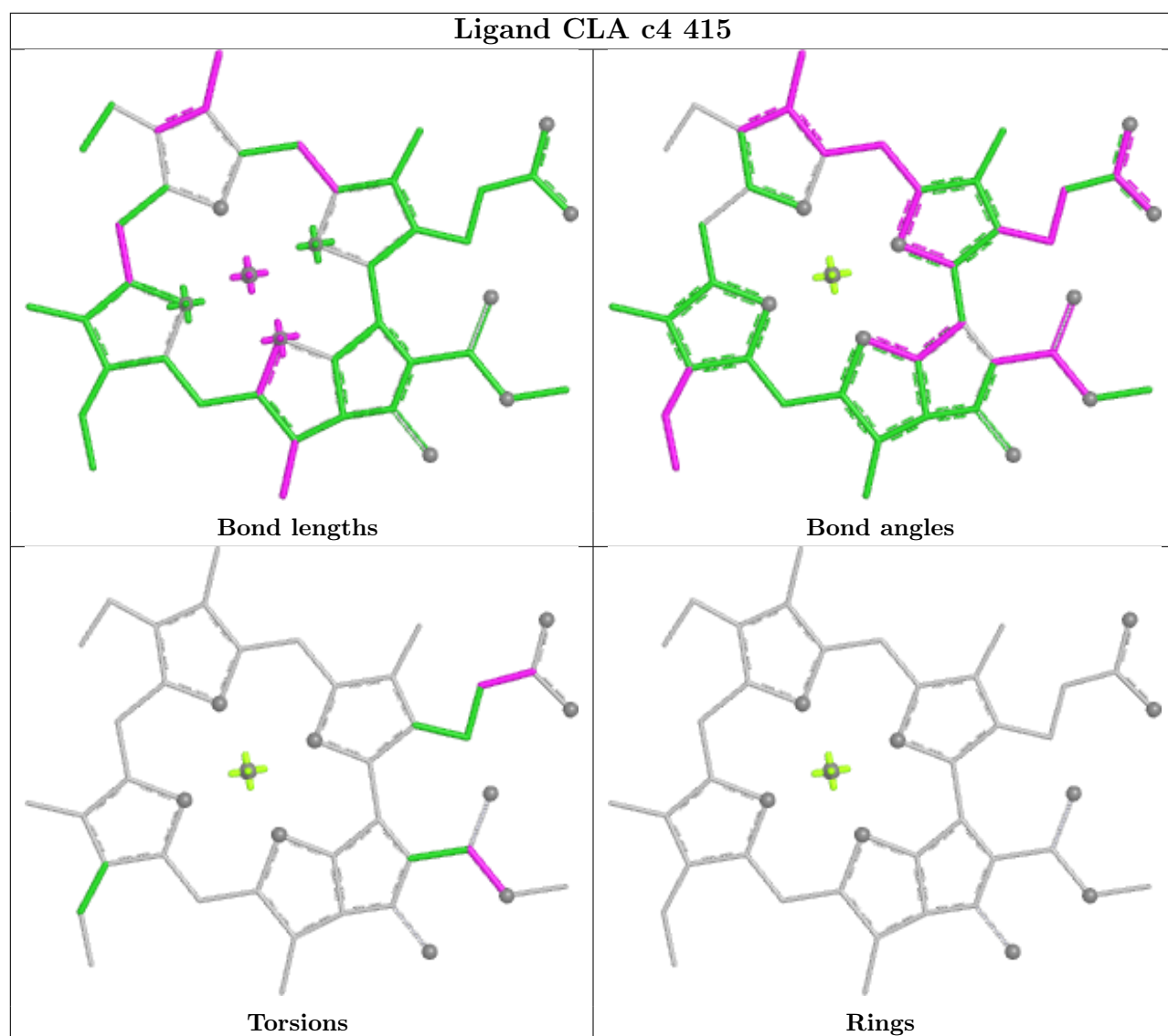


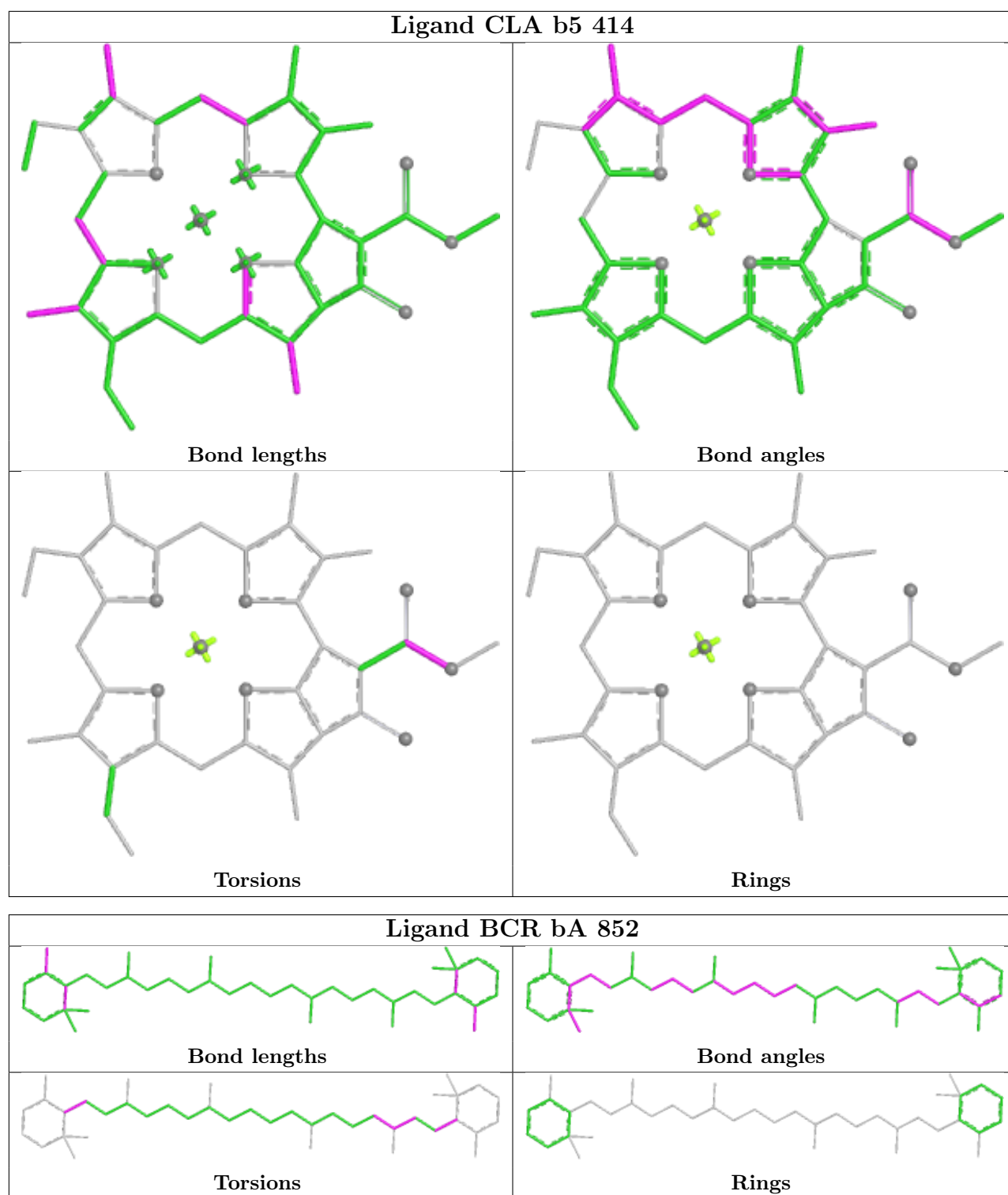
Ligand CLA aB 831

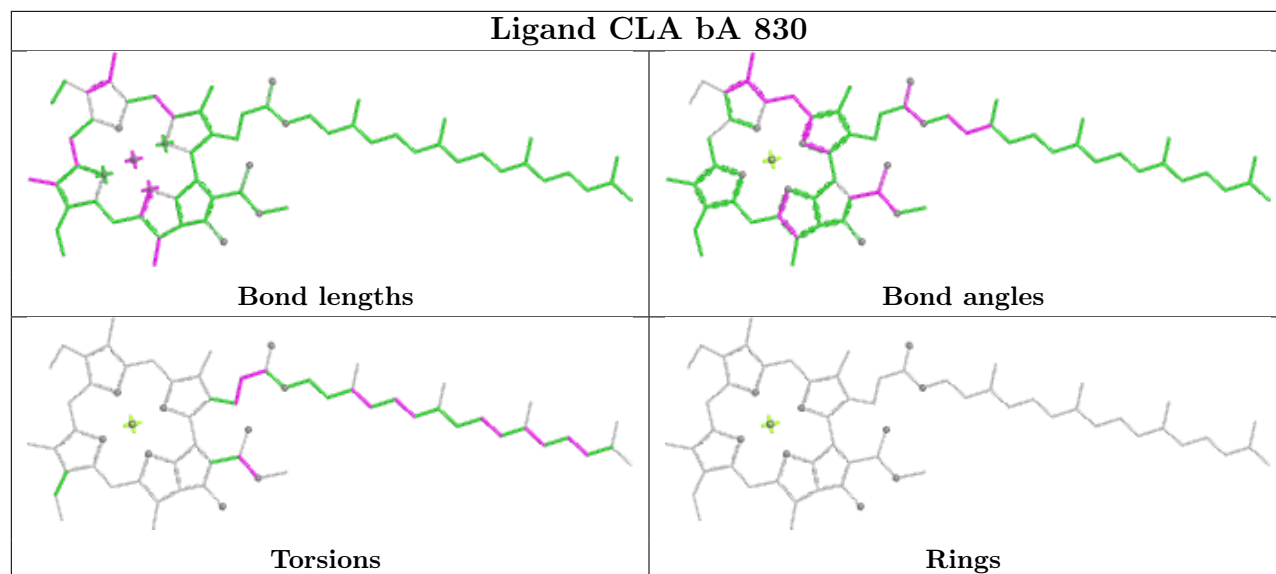
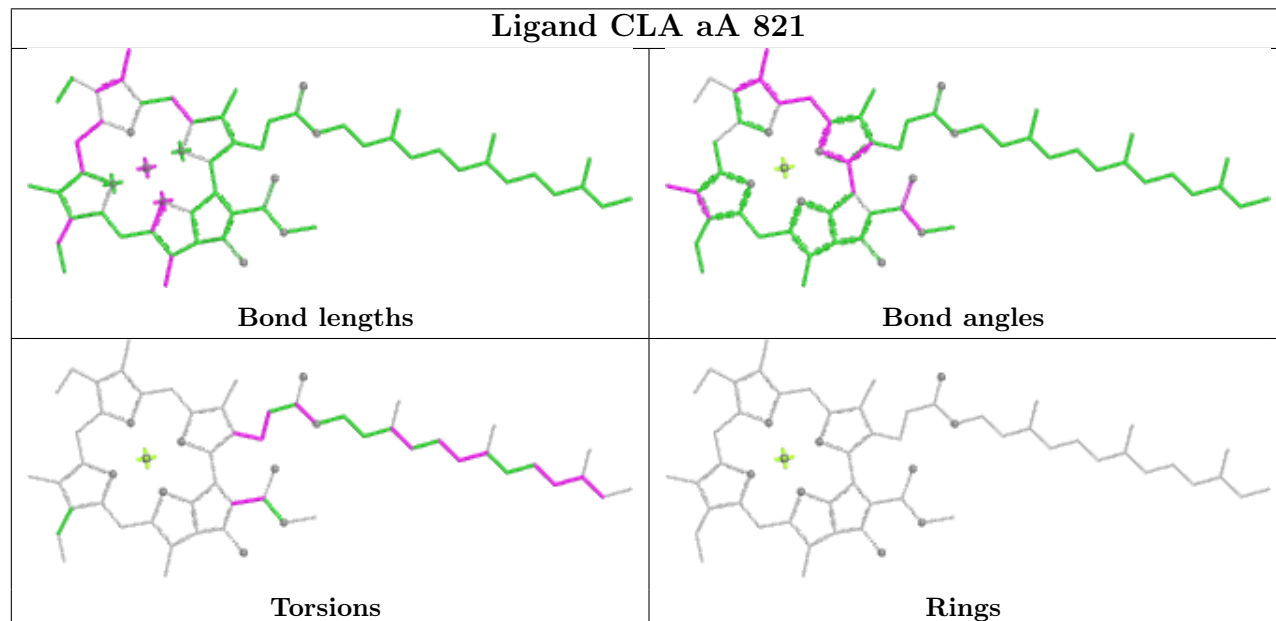


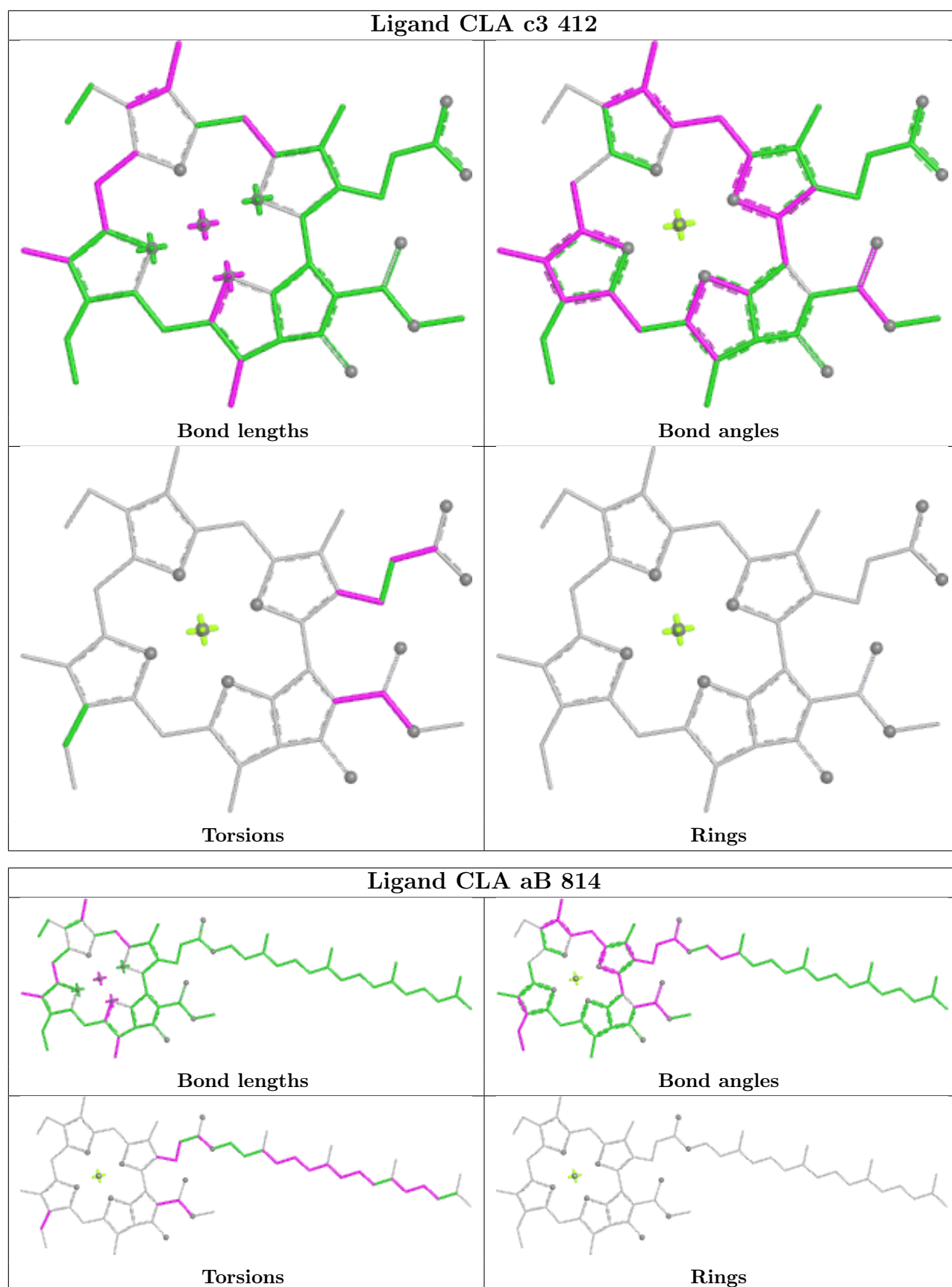
Ligand CLA cB 839

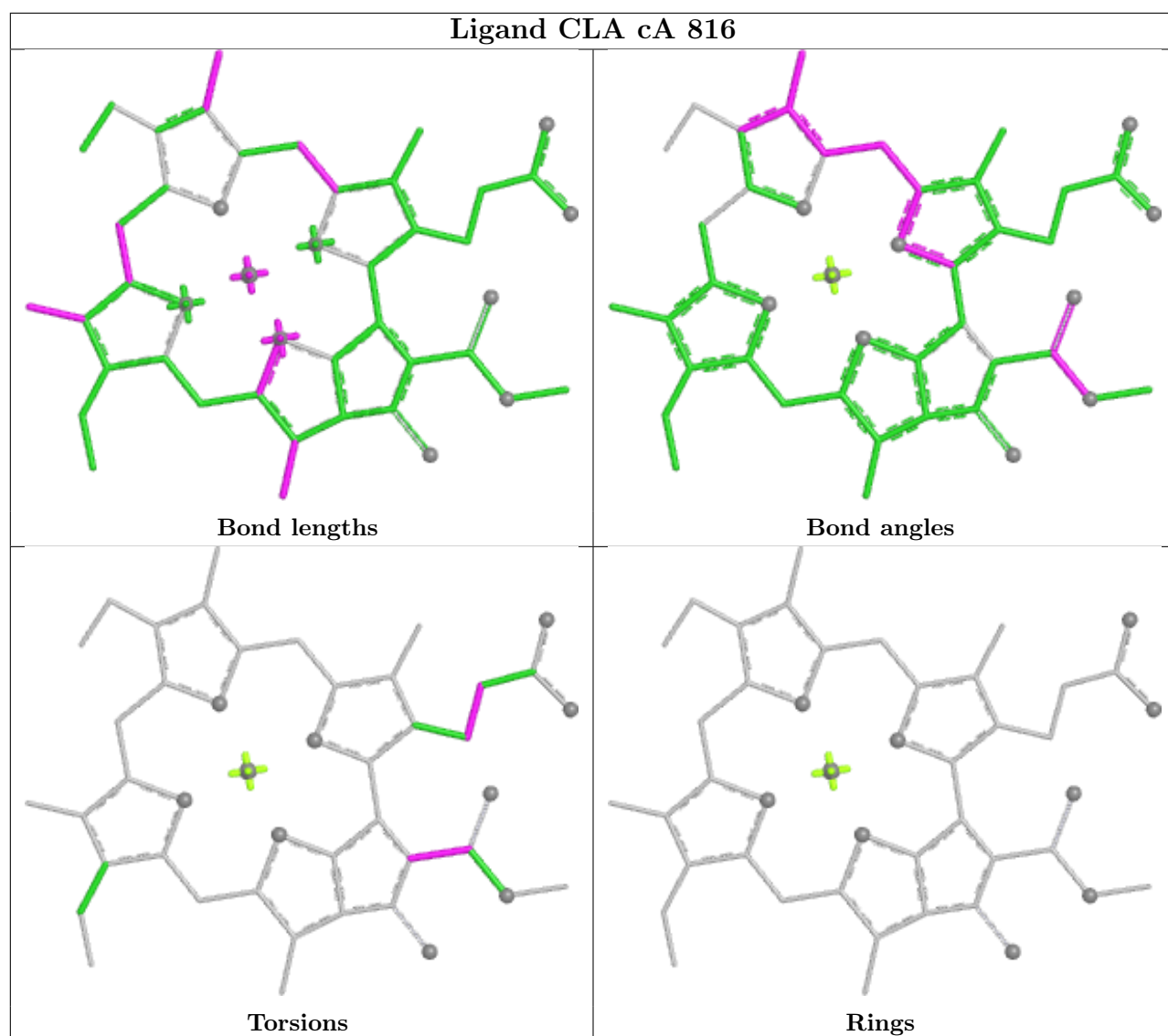




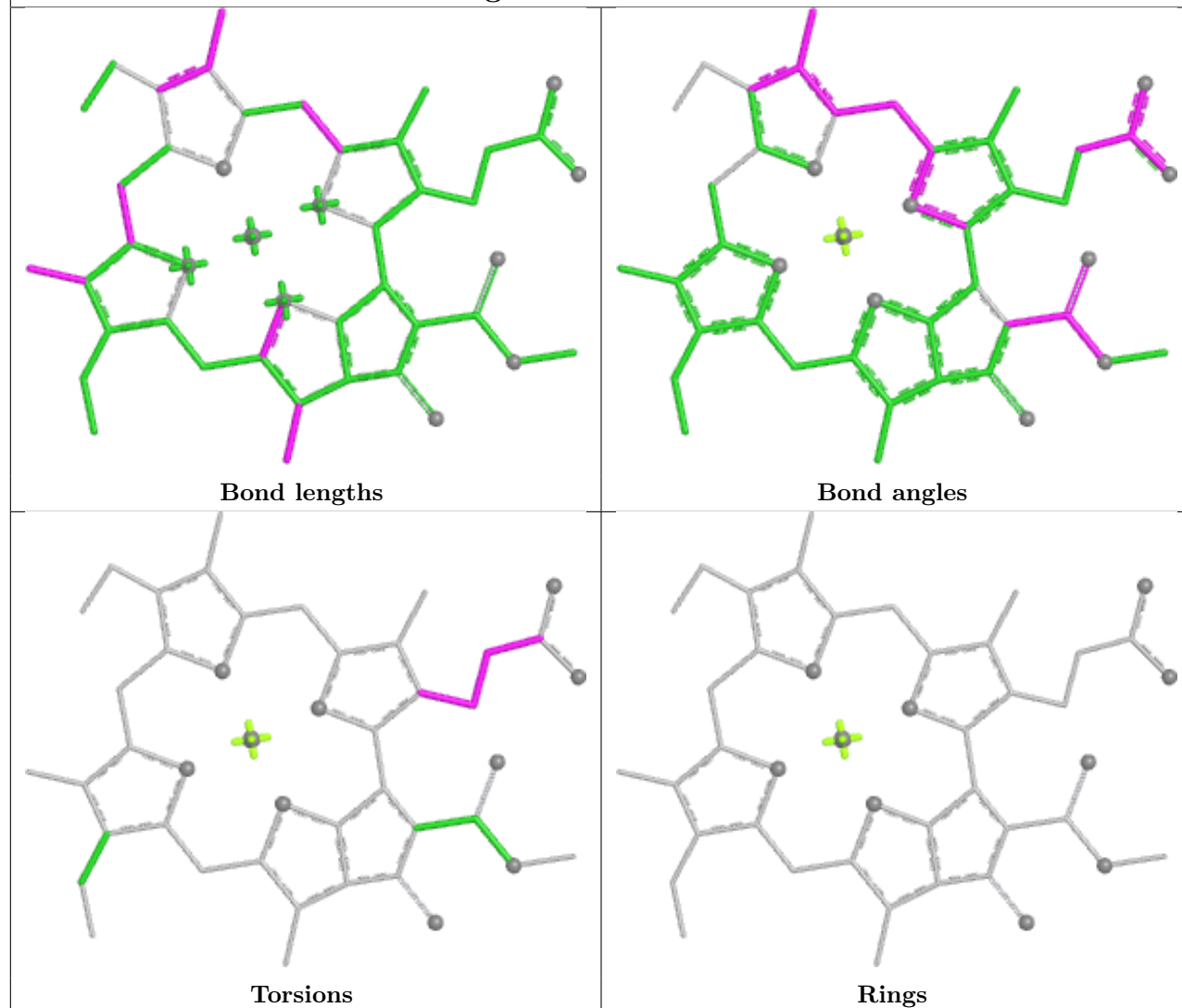


Ligand CLA bA 830**Ligand CLA aA 821**

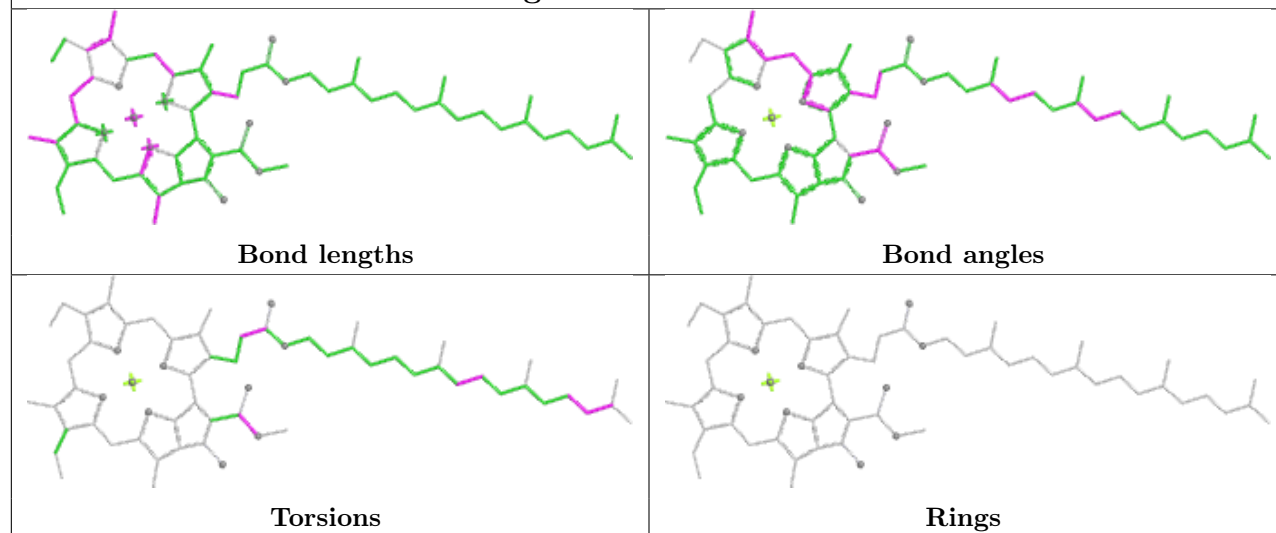


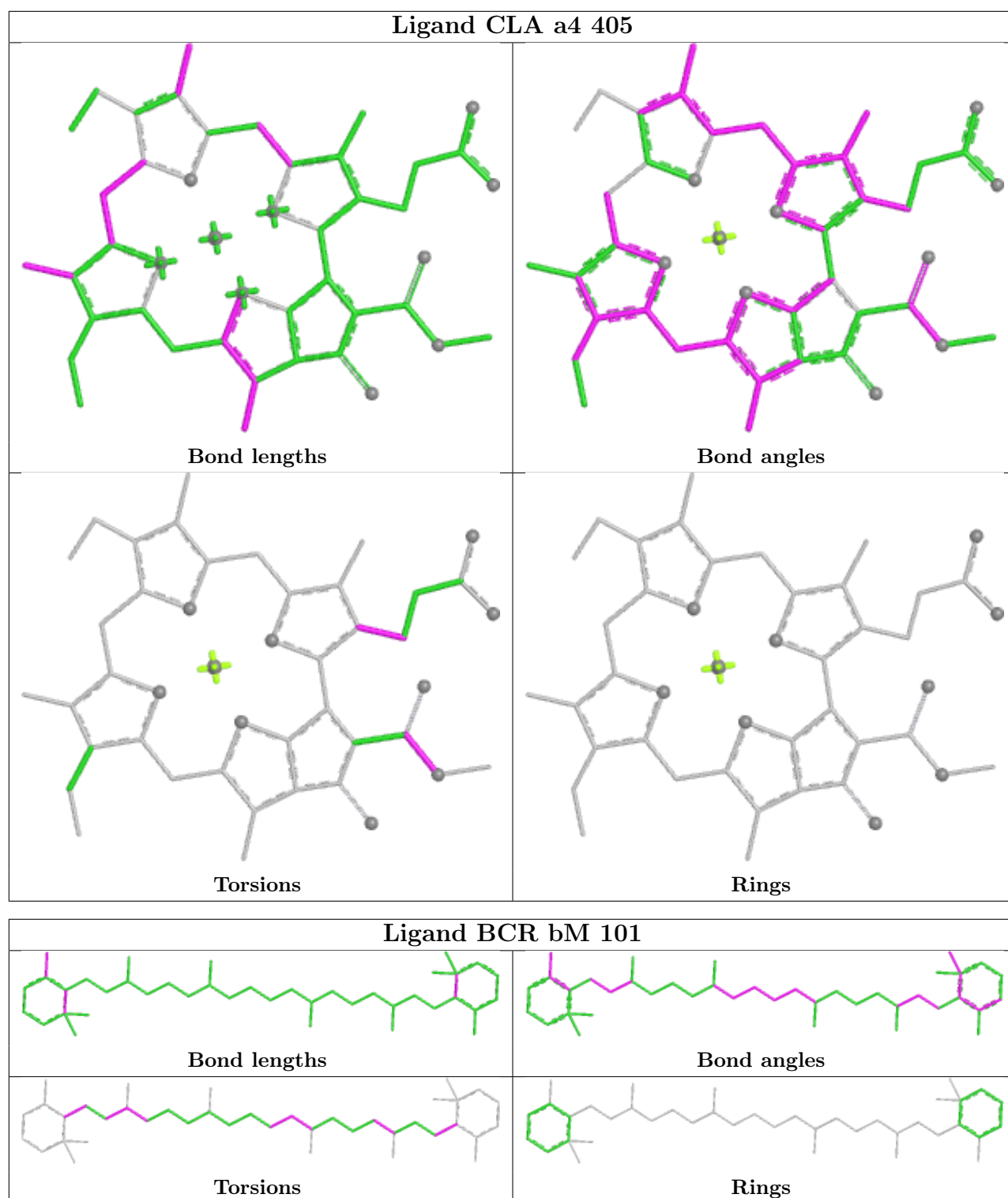


Ligand CLA cA 837



Ligand CLA aB 802





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

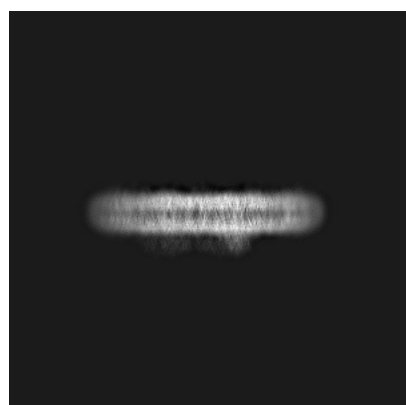
6 Map visualisation [i](#)

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

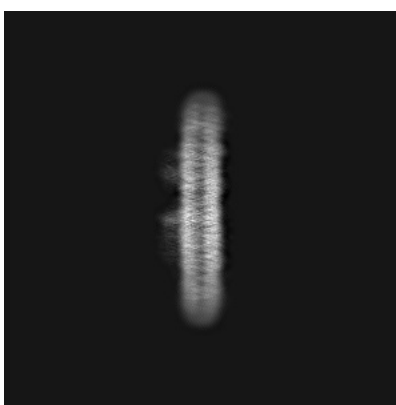
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

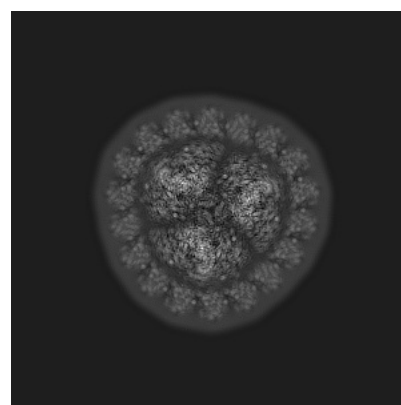
6.1.1 Primary map



X



Y

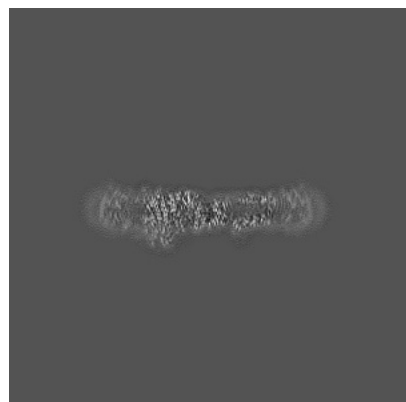


Z

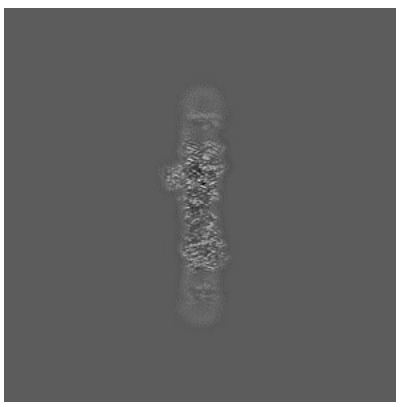
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

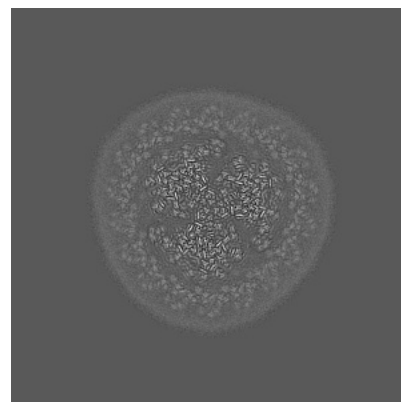
6.2.1 Primary map



X Index: 240



Y Index: 240

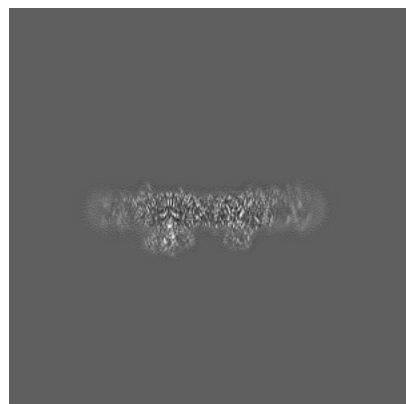


Z Index: 240

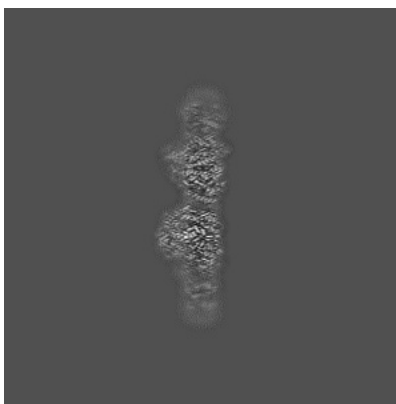
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

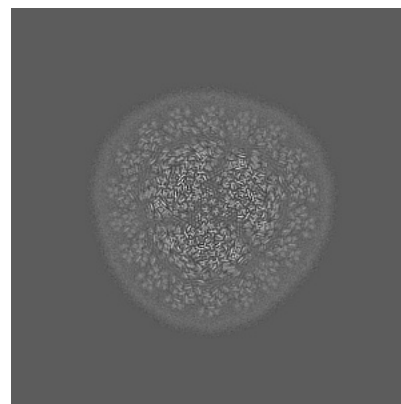
6.3.1 Primary map



X Index: 229



Y Index: 273

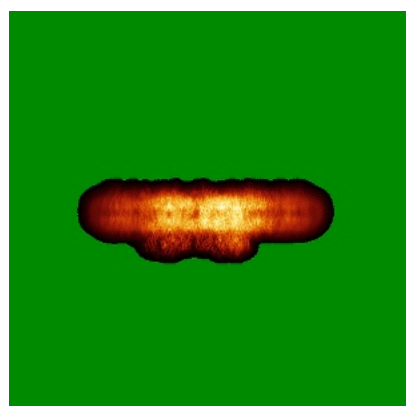


Z Index: 245

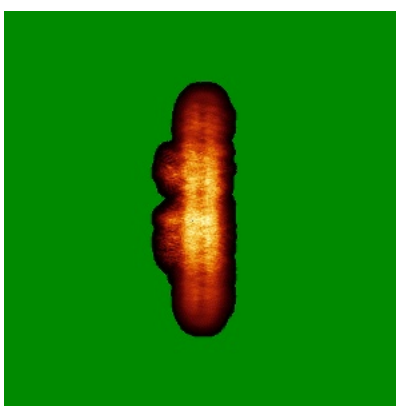
The images above show the largest variance slices of the map in three orthogonal directions.

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

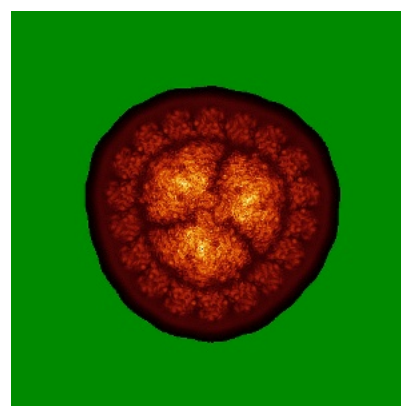
6.4.1 Primary map



X



Y

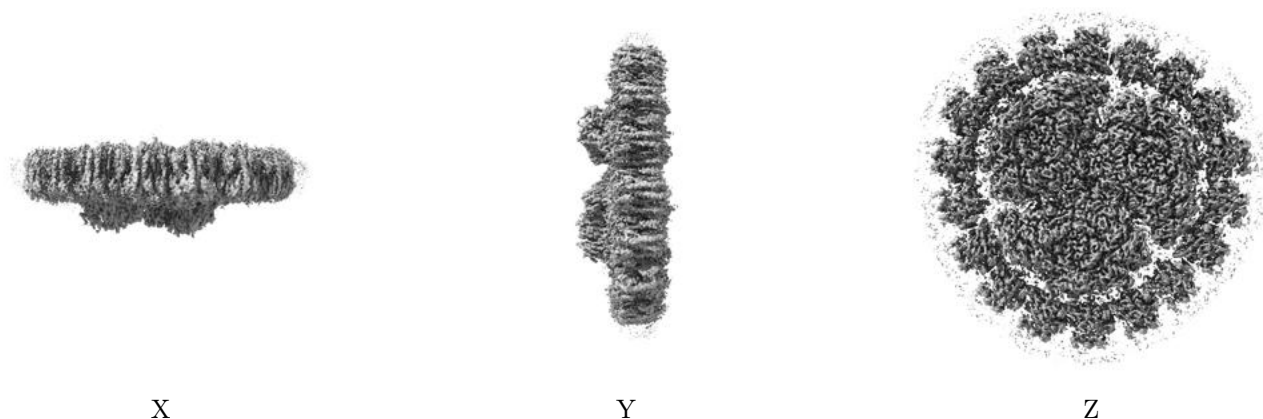


Z

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.

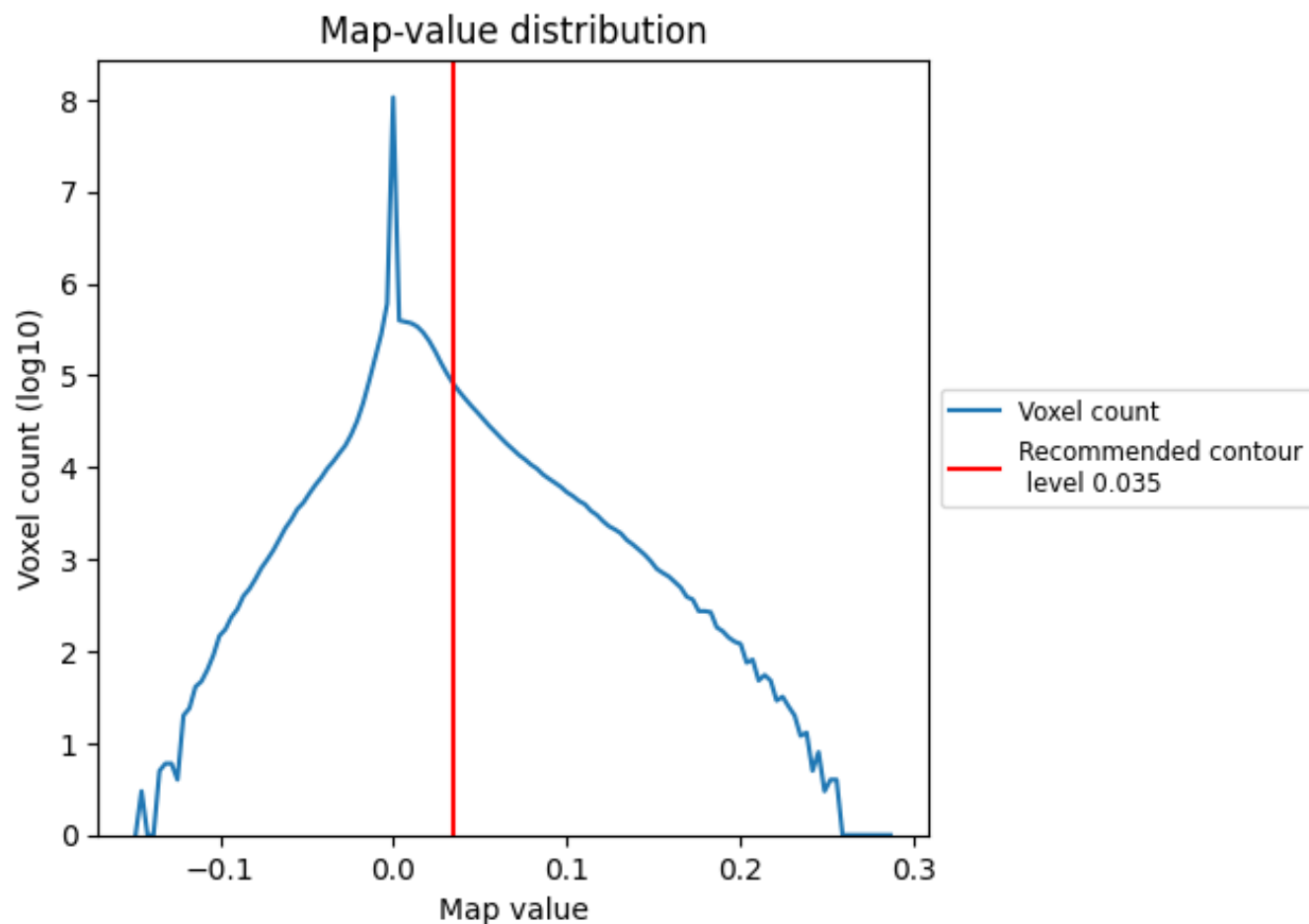
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

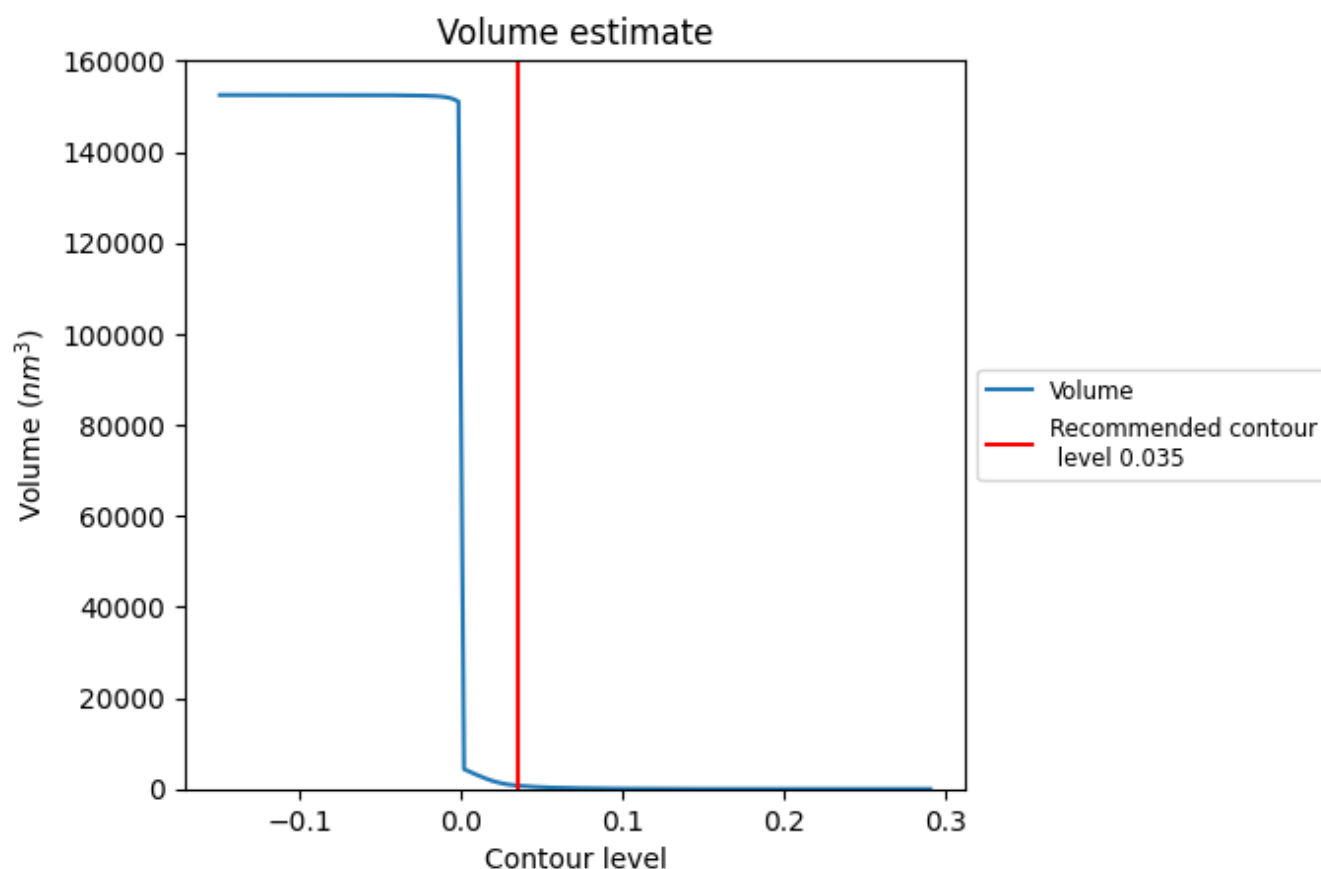
This section contains the results of statistical analysis of the map.

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.

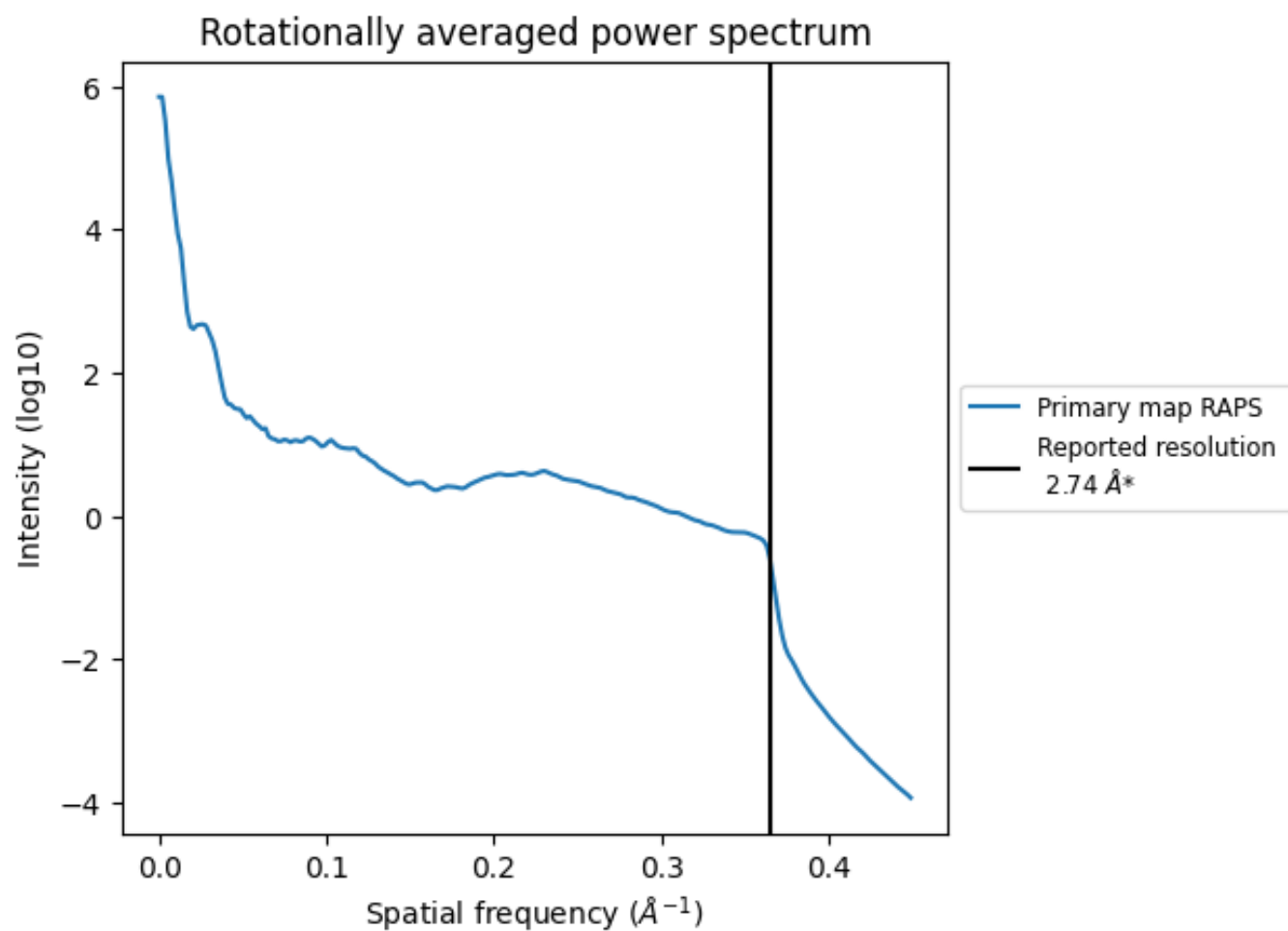
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 747 nm^3 ; 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 ⓘ

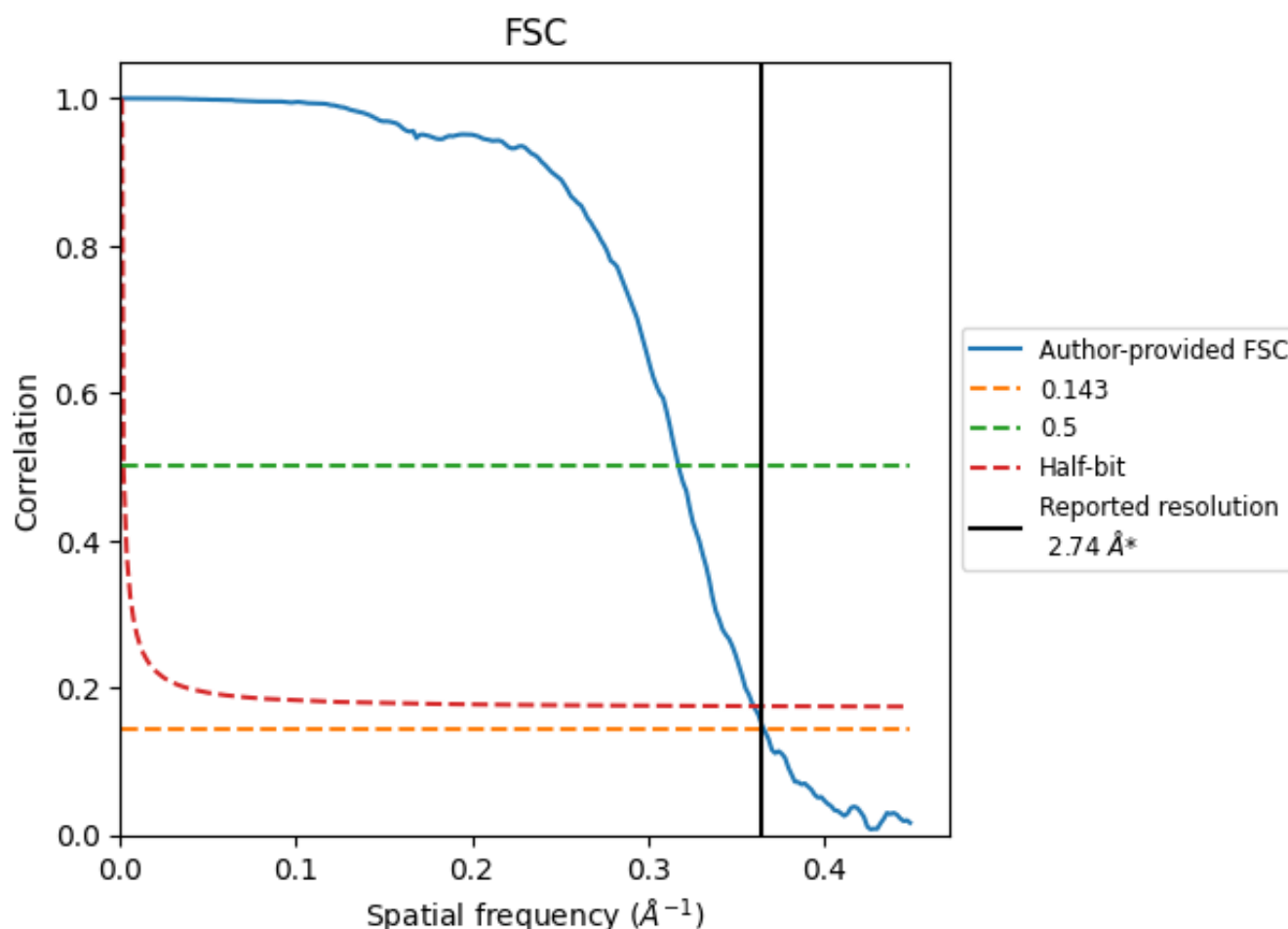


*Reported resolution corresponds to spatial frequency of 0.365 Å⁻¹

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](#)

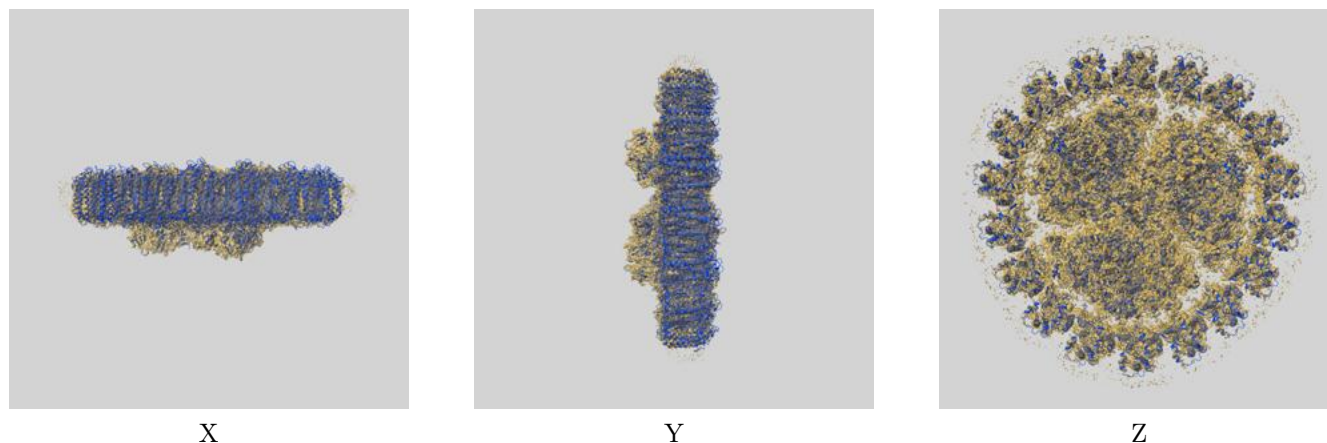
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.15	2.78
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

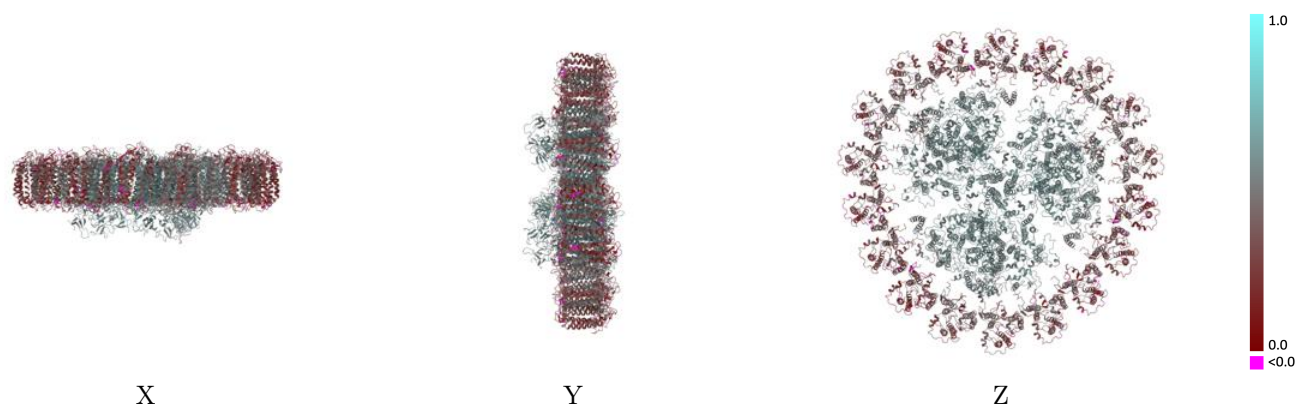
This section contains information regarding the fit between EMDB map EMD-9908 and PDB model 6K33. Per-residue inclusion information can be found in [section 3](#) on [page 64](#).

9.1 Map-model overlay [i](#)



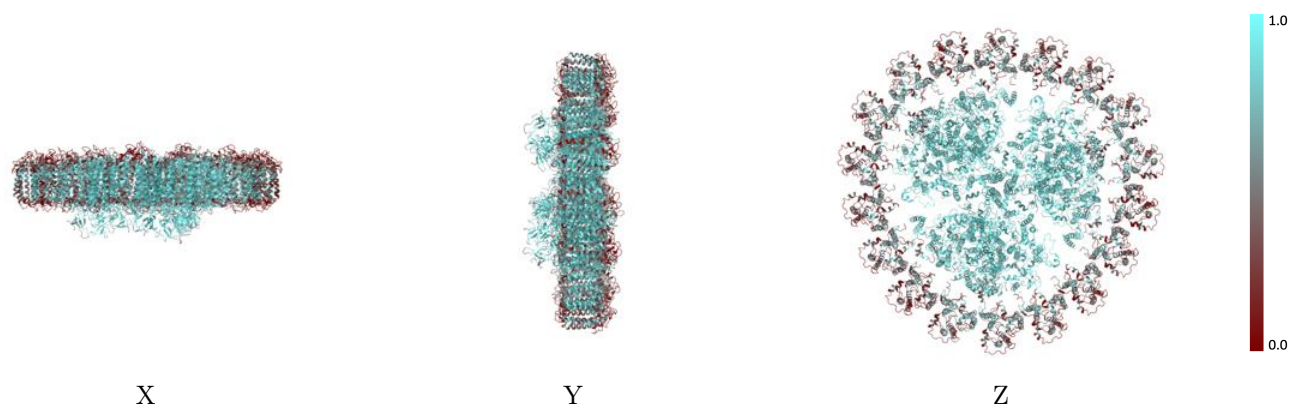
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



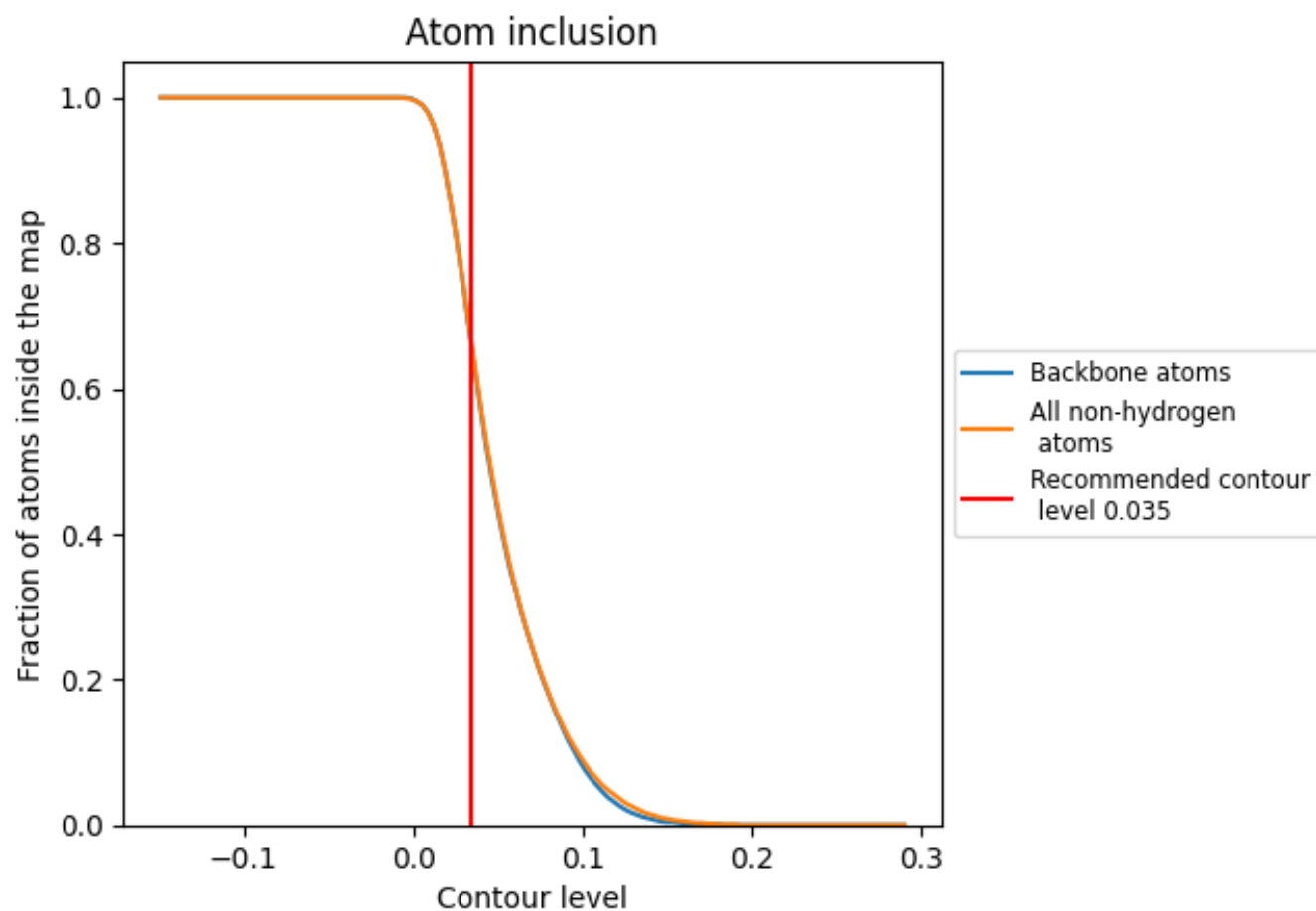
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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







































































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