



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:36 AM UTC

PDB ID : 8BCW / pdb_00008bcw
EMDB ID : EMD-15970
Title : Photosystem I assembly intermediate of Avena sativa
Authors : Naschberger, A.; Amunts, A.; Nelson, N.
Deposited on : 2022-10-17
Resolution : 2.11 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

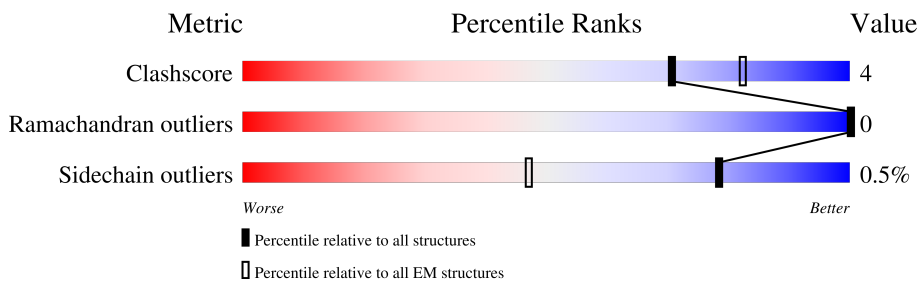
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 2.11 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	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

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

Mol	Chain	Length	Quality of chain
1	A	750	
2	B	734	
3	C	81	
4	D	206	
5	E	143	
6	H	94	
7	I	33	
8	L	213	

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
10	CLA	A	802	X	-	-	-
10	CLA	A	803	X	-	-	-
10	CLA	A	804	X	-	-	-
10	CLA	A	805	X	-	-	-
10	CLA	A	806	X	-	-	-
10	CLA	A	807	X	-	-	-
10	CLA	A	808	X	-	-	-
10	CLA	A	809	X	-	-	-
10	CLA	A	810	X	-	-	-
10	CLA	A	811	X	-	-	-
10	CLA	A	812	X	-	-	-
10	CLA	A	813	X	-	-	-
10	CLA	A	814	X	-	-	-
10	CLA	A	815	X	-	-	-
10	CLA	A	816	X	-	-	-
10	CLA	A	817	X	-	-	-
10	CLA	A	818	X	-	-	-
10	CLA	A	819	X	-	-	-
10	CLA	A	820	X	-	-	-
10	CLA	A	821	X	-	-	-
10	CLA	A	822	X	-	-	-
10	CLA	A	823	X	-	-	-
10	CLA	A	824	X	-	-	-
10	CLA	A	825	X	-	-	-
10	CLA	A	826	X	-	-	-
10	CLA	A	827	X	-	-	-
10	CLA	A	828	X	-	-	-
10	CLA	A	829	X	-	-	-
10	CLA	A	830	X	-	-	-
10	CLA	A	831	X	-	-	-
10	CLA	A	832	X	-	-	-
10	CLA	A	833	X	-	-	-
10	CLA	A	834	X	-	-	-
10	CLA	A	835	X	-	-	-
10	CLA	A	836	X	-	-	-
10	CLA	A	837	X	-	-	-
10	CLA	A	838	X	-	-	-
10	CLA	A	839	X	-	-	-
10	CLA	A	840	X	-	-	-
10	CLA	A	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	A	842	X	-	-	-
10	CLA	A	843	X	-	-	-
10	CLA	A	845	X	-	-	-
10	CLA	A	854	X	-	-	-
10	CLA	A	856	X	-	-	-
10	CLA	B	801	X	-	-	-
10	CLA	B	802	X	-	-	-
10	CLA	B	803	X	-	-	-
10	CLA	B	804	X	-	-	-
10	CLA	B	805	X	-	-	-
10	CLA	B	806	X	-	-	-
10	CLA	B	807	X	-	-	-
10	CLA	B	808	X	-	-	-
10	CLA	B	809	X	-	-	-
10	CLA	B	810	X	-	-	-
10	CLA	B	811	X	-	-	-
10	CLA	B	812	X	-	-	-
10	CLA	B	813	X	-	-	-
10	CLA	B	814	X	-	-	-
10	CLA	B	815	X	-	-	-
10	CLA	B	816	X	-	-	-
10	CLA	B	817	X	-	-	-
10	CLA	B	818	X	-	-	-
10	CLA	B	819	X	-	-	-
10	CLA	B	820	X	-	-	-
10	CLA	B	821	X	-	-	-
10	CLA	B	822	X	-	-	-
10	CLA	B	823	X	-	-	-
10	CLA	B	824	X	-	-	-
10	CLA	B	825	X	-	-	-
10	CLA	B	826	X	-	-	-
10	CLA	B	827	X	-	-	-
10	CLA	B	828	X	-	-	-
10	CLA	B	829	X	-	-	-
10	CLA	B	830	X	-	-	-
10	CLA	B	831	X	-	-	-
10	CLA	B	832	X	-	-	-
10	CLA	B	833	X	-	-	-
10	CLA	B	834	X	-	-	-
10	CLA	B	835	X	-	-	-
10	CLA	B	836	X	-	-	-
10	CLA	B	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	CLA	B	838	X	-	-	-
10	CLA	L	302	X	-	-	-
10	CLA	L	303	X	-	-	-
10	CLA	L	304	X	-	-	-
9	CL0	A	801	X	-	-	-
9	CL0	H	201	X	-	-	-

2 Entry composition [i](#)

There are 18 unique types of molecules in this entry. The entry contains 22313 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
			Total	C	N	O	S		
1	A	720	5660	3711	961	969	19	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	733	5864	3848	996	1007	13	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	80	605	372	104	118	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	143	1124	722	196	203	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	E	67	533	340	94	99	0	0

- Molecule 6 is a protein called Photosystem I reaction center subunit VI, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
6	H	94	715	469	114	132	0	0

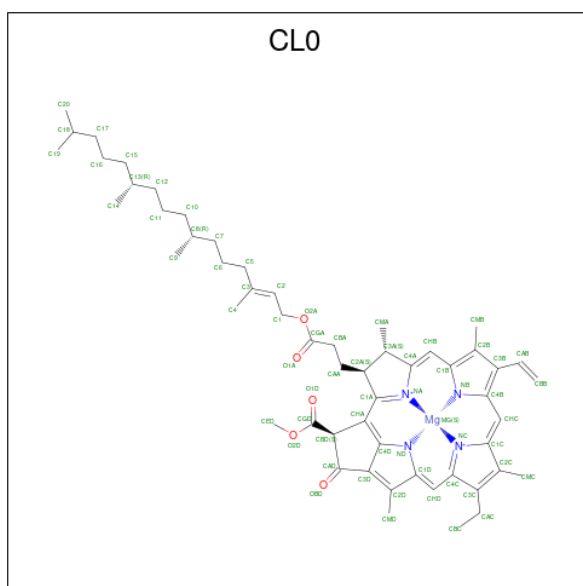
- Molecule 7 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	I	33	258	178	38	41	1	0	0

- Molecule 8 is a protein called PSI subunit V.

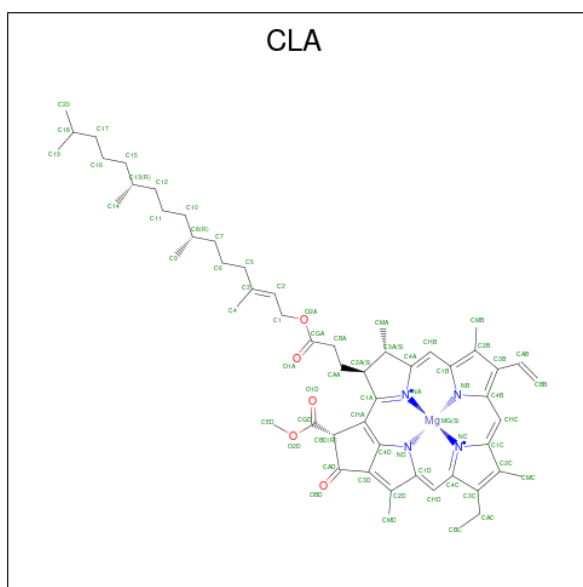
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	L	159	1192	788	189	214	1	0	0

- Molecule 9 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
9	A	1	65	55	1	4	5	0
9	H	1	55	45	1	4	5	0

- Molecule 10 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
10	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
10	A	1	60	50	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	56	46	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	52	42	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	60	50	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	55	45	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	60	50	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	55	45	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
10	A	1	45	35	1	4	5	0
10	A	1	51	41	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	55	45	1	4	5	0
10	A	1	55	45	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	65	55	1	4	5	0
10	A	1	45	35	1	4	5	0
10	A	1	55	45	1	4	5	0
10	A	1	50	40	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	60	50	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	56	46	1	4	5	0
10	B	1	45	35	1	4	5	0

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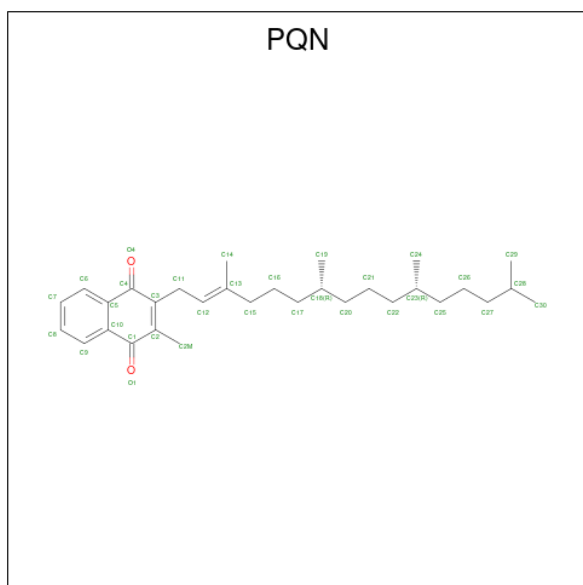
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	55	45	1	4	5	0
10	B	1	57	47	1	4	5	0
10	B	1	60	50	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	55	45	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	56	46	1	4	5	0
10	B	1	50	40	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	65	55	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0
10	B	1	45	35	1	4	5	0

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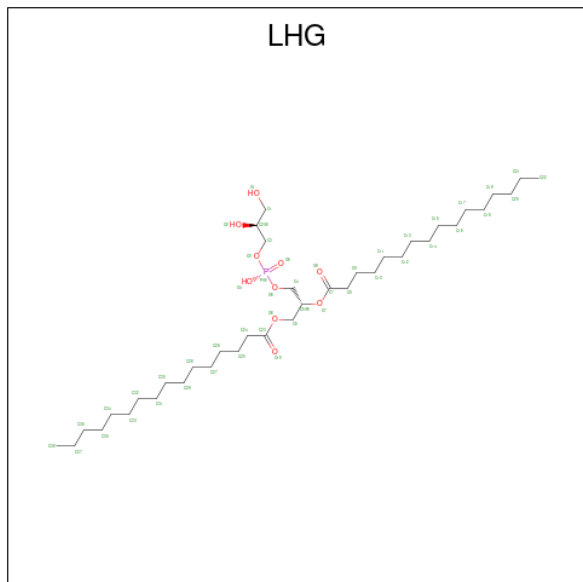
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
10	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	B	1	Total 51	C 41	Mg 1	N 4	O 5	0
10	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
10	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
10	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
10	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
10	L	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 11 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



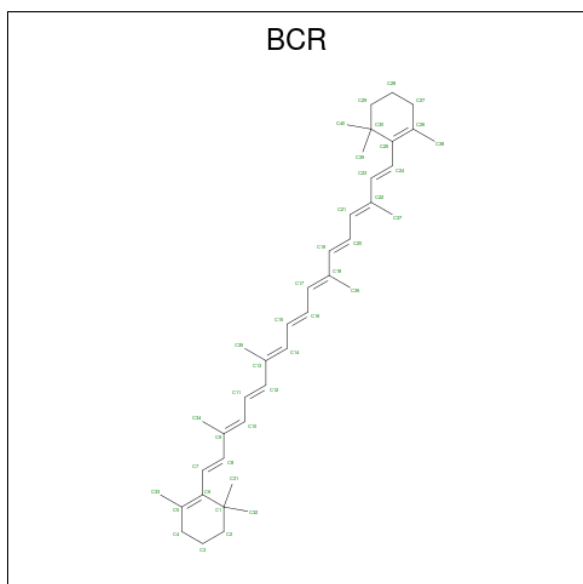
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
11	A	1	Total 33	C 31	O 2	0
11	B	1	Total 33	C 31	O 2	0

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



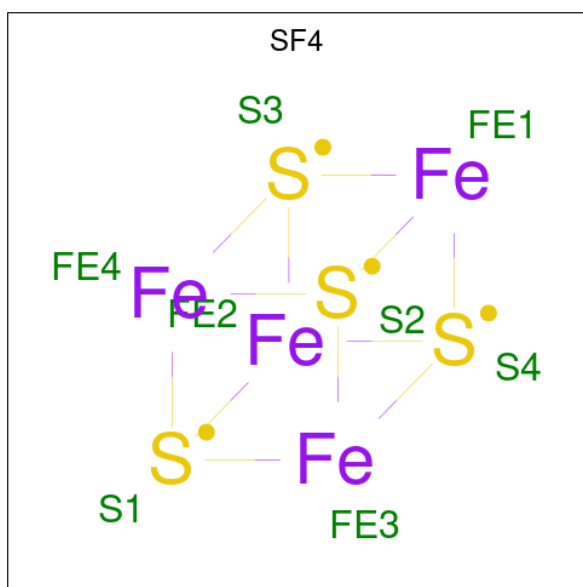
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
12	A	1	41	30	10	1	0
12	A	1	31	20	10	1	0
12	B	1	49	38	10	1	0

- Molecule 13 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



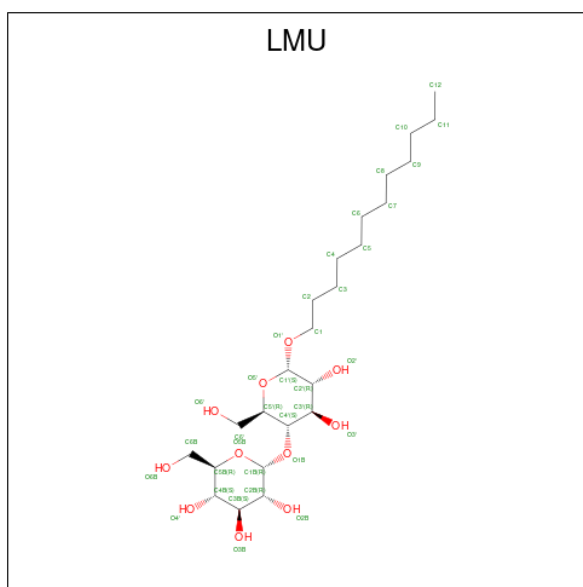
Mol	Chain	Residues	Atoms	AltConf
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	A	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	B	1	Total C 40 40	0
13	I	1	Total C 40 40	0
13	L	1	Total C 40 40	0
13	L	1	Total C 40 40	0
13	L	1	Total C 40 40	0

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
14	A	1	Total	Fe S	0
			8	4 4	
14	C	1	Total	Fe S	0
			8	4 4	
14	C	1	Total	Fe S	0
			8	4 4	

- Molecule 15 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



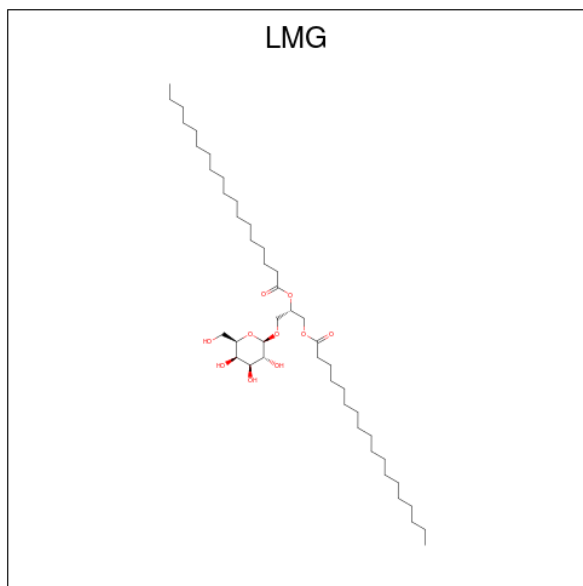
Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C O	0
			35	24 11	

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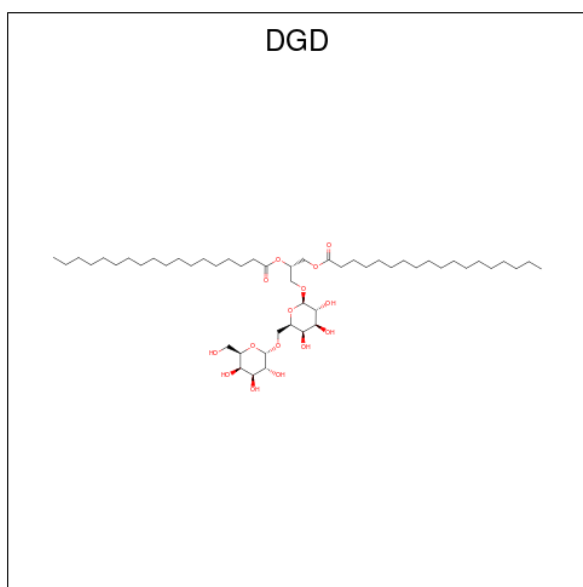
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
15	A	1	24	18	6	0
15	A	1	21	15	6	0

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
16	A	1	43	33	10	0

- Molecule 17 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
17	B	1	61	46	15	0

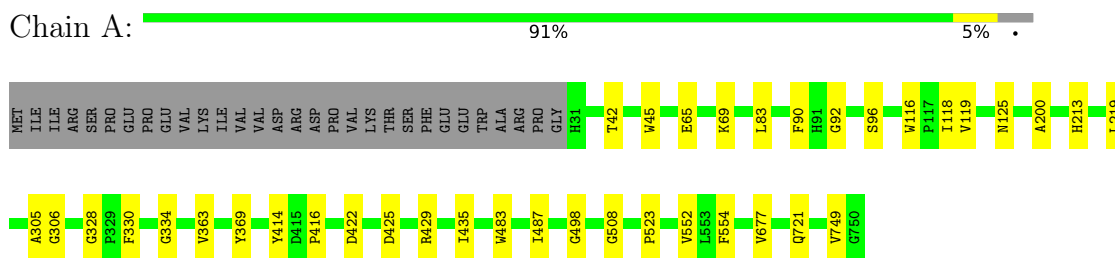
- Molecule 18 is water.

Mol	Chain	Residues	Atoms		AltConf
			Total	O	
18	A	155	155	155	0
18	B	203	203	203	0
18	C	62	62	62	0
18	D	47	47	47	0
18	E	13	13	13	0
18	H	9	9	9	0
18	I	4	4	4	0
18	L	24	24	24	0

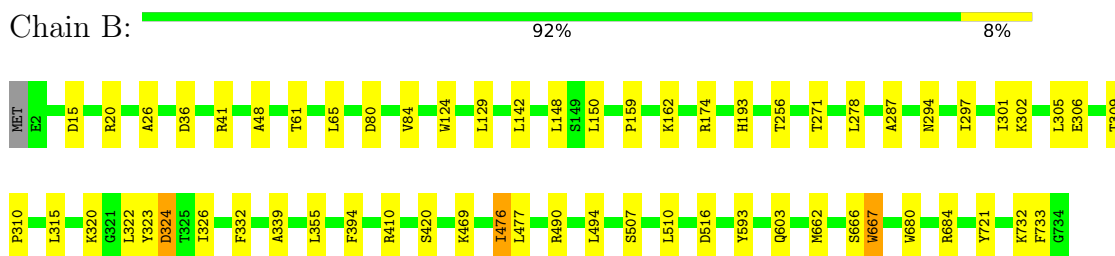
3 Residue-property plots

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

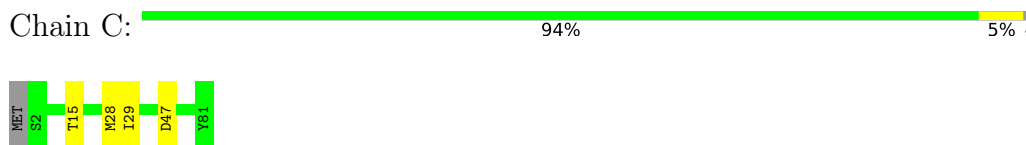
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



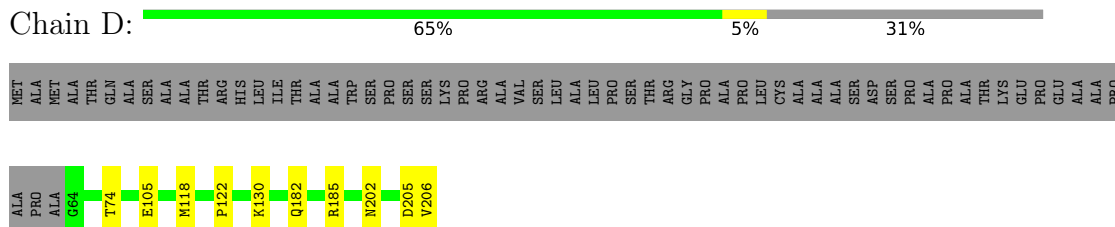
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



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



- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	169213	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 ($e^-/\text{\AA}^2$)	51.346	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	2100	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.15	0/5853	0.30	0/7985
2	B	0.15	0/6075	0.31	0/8297
3	C	0.13	0/616	0.33	0/834
4	D	0.11	0/1153	0.34	0/1557
5	E	0.09	0/546	0.24	0/743
6	H	0.11	0/737	0.27	0/1002
7	I	0.13	0/264	0.28	0/359
8	L	0.12	0/1228	0.27	0/1681
All	All	0.14	0/16472	0.30	0/22458

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	667	TRP	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	A	5660	0	5513	27	0
2	B	5864	0	5642	44	0
3	C	605	0	587	3	0
4	D	1124	0	1128	6	0
5	E	533	0	538	1	0
6	H	715	0	715	4	0
7	I	258	0	285	2	0
8	L	1192	0	1197	9	0
9	A	65	0	72	0	0
9	H	55	0	49	1	0
10	A	2520	0	2393	35	0
10	B	2140	0	2054	36	0
10	L	150	0	125	3	0
11	A	33	0	46	1	0
11	B	33	0	46	1	0
12	A	72	0	87	3	0
12	B	49	0	74	6	0
13	A	200	0	280	15	0
13	B	160	0	224	8	0
13	I	40	0	56	2	0
13	L	120	0	168	3	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
15	A	80	0	107	3	0
16	A	43	0	56	1	0
17	B	61	0	83	1	0
18	A	155	0	0	1	0
18	B	203	0	0	1	0
18	C	62	0	0	0	0
18	D	47	0	0	0	0
18	E	13	0	0	0	0
18	H	9	0	0	0	0
18	I	4	0	0	0	0
18	L	24	0	0	1	0
All	All	22313	0	21525	153	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 4.

The worst 5 of 153 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125:ASN:ND2	15:A:855:LMU:O6'	2.24	0.70
2:B:490:ARG:HA	2:B:494:LEU:HD12	1.76	0.68
10:B:802:CLA:H143	13:B:843:BCR:H362	1.76	0.66
2:B:150:LEU:HD11	12:B:845:LHG:H382	1.80	0.63
8:L:59:ILE:HA	8:L:69:GLU:HG3	1.79	0.63

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	A	718/750 (96%)	703 (98%)	15 (2%)	0	100	100
2	B	731/734 (100%)	716 (98%)	15 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	141/206 (68%)	138 (98%)	3 (2%)	0	100	100
5	E	65/143 (46%)	65 (100%)	0	0	100	100
6	H	92/94 (98%)	91 (99%)	1 (1%)	0	100	100
7	I	31/33 (94%)	31 (100%)	0	0	100	100
8	L	157/213 (74%)	154 (98%)	3 (2%)	0	100	100
All	All	2013/2254 (89%)	1974 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	A	580/608 (95%)	577 (100%)	3 (0%)	81	87
2	B	598/599 (100%)	594 (99%)	4 (1%)	76	83
3	C	70/71 (99%)	70 (100%)	0	100	100
4	D	120/163 (74%)	120 (100%)	0	100	100
5	E	59/115 (51%)	59 (100%)	0	100	100
6	H	76/76 (100%)	75 (99%)	1 (1%)	61	69
7	I	30/30 (100%)	30 (100%)	0	100	100
8	L	123/168 (73%)	122 (99%)	1 (1%)	73	80
All	All	1656/1830 (90%)	1647 (100%)	9 (0%)	78	87

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	50	GLU
8	L	143	VAL
2	B	297	ILE
2	B	324	ASP
2	B	394	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	38	GLN
6	H	66	GLN
8	L	121	ASN
6	H	79	ASN
1	A	486	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](#)

114 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	B	843	-	41,41,41	0.14	0	56,56,56	0.42	0
10	CLA	B	828	-	69,73,73	1.07	5 (7%)	82,113,113	0.81	2 (2%)
13	BCR	A	852	-	41,41,41	0.27	0	56,56,56	0.86	2 (3%)
10	CLA	A	838	-	55,59,73	1.26	4 (7%)	64,96,113	0.92	2 (3%)
10	CLA	B	807	-	69,73,73	1.11	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	823	18	60,64,73	1.26	4 (6%)	71,102,113	0.86	2 (2%)
10	CLA	A	806	-	69,73,73	1.13	4 (5%)	82,113,113	0.81	2 (2%)
13	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.34	0
10	CLA	A	820	-	69,73,73	1.13	4 (5%)	82,113,113	0.84	3 (3%)
10	CLA	A	843	18	69,73,73	1.15	4 (5%)	82,113,113	0.83	2 (2%)
10	CLA	A	856	18	54,58,73	1.30	4 (7%)	64,95,113	0.92	2 (3%)
10	CLA	A	830	-	69,73,73	1.13	4 (5%)	82,113,113	0.78	2 (2%)
10	CLA	A	807	1	69,73,73	1.14	4 (5%)	82,113,113	0.81	2 (2%)
10	CLA	A	831	-	69,73,73	1.11	4 (5%)	82,113,113	0.79	2 (2%)
9	CL0	A	801	-	58,73,73	1.33	7 (12%)	60,113,113	1.69	5 (8%)
10	CLA	A	833	-	59,63,73	1.21	4 (6%)	70,101,113	0.85	2 (2%)
10	CLA	A	839	-	69,73,73	1.15	4 (5%)	82,113,113	0.82	2 (2%)
10	CLA	A	824	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	B	812	-	69,73,73	1.16	4 (5%)	82,113,113	0.82	2 (2%)
10	CLA	A	808	-	51,55,73	1.32	4 (7%)	60,91,113	0.95	2 (3%)
10	CLA	A	805	10	54,58,73	1.29	4 (7%)	64,95,113	0.88	2 (3%)
13	BCR	B	840	-	41,41,41	0.20	0	56,56,56	0.45	0
14	SF4	C	102	3	0,12,12	-	-	-		
10	CLA	B	832	-	49,53,73	1.34	4 (8%)	58,89,113	0.97	2 (3%)
13	BCR	B	842	-	41,41,41	0.13	0	56,56,56	0.41	0
10	CLA	A	842	-	49,53,73	1.38	4 (8%)	58,89,113	0.99	3 (5%)
10	CLA	B	815	-	61,65,73	1.22	4 (6%)	72,103,113	0.88	2 (2%)
17	DGD	B	844	-	62,62,67	0.18	0	76,76,81	0.30	0
10	CLA	A	803	18	69,73,73	1.22	4 (5%)	82,113,113	0.85	3 (3%)
14	SF4	A	853	1,2	0,12,12	-	-	-		
10	CLA	B	826	-	69,73,73	1.14	4 (5%)	82,113,113	0.84	2 (2%)
10	CLA	A	821	-	49,53,73	1.37	4 (8%)	58,89,113	0.96	2 (3%)
10	CLA	B	829	-	49,53,73	1.37	4 (8%)	58,89,113	0.97	2 (3%)
12	LHG	B	845	-	48,48,48	0.22	0	51,54,54	0.24	0
10	CLA	A	854	18	59,63,73	1.24	5 (8%)	70,101,113	0.95	3 (4%)
10	CLA	B	809	-	69,73,73	1.15	4 (5%)	82,113,113	0.79	2 (2%)
10	CLA	B	817	-	69,73,73	1.16	4 (5%)	82,113,113	0.84	3 (3%)
10	CLA	A	809	1	59,63,73	1.22	4 (6%)	70,101,113	0.86	2 (2%)
10	CLA	B	803	-	49,53,73	1.34	4 (8%)	58,89,113	0.95	2 (3%)
10	CLA	B	801	-	69,73,73	1.10	4 (5%)	82,113,113	0.78	2 (2%)
10	CLA	B	811	-	49,53,73	1.38	4 (8%)	58,89,113	0.98	2 (3%)
10	CLA	A	812	10	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
15	LMU	A	859	-	21,21,36	0.12	0	26,26,47	0.28	0
10	CLA	A	815	-	58,62,73	1.29	4 (6%)	68,99,113	0.89	2 (2%)
10	CLA	A	825	-	64,68,73	1.19	4 (6%)	76,107,113	0.83	2 (2%)
10	CLA	B	806	-	64,68,73	1.16	4 (6%)	76,107,113	0.83	2 (2%)
15	LMU	A	855	-	36,36,36	0.11	0	47,47,47	0.26	0
13	BCR	A	851	-	41,41,41	0.19	0	56,56,56	0.36	0
10	CLA	A	818	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	2 (3%)
10	CLA	B	837	18	69,73,73	1.10	4 (5%)	82,113,113	0.81	2 (2%)
10	CLA	B	822	-	49,53,73	1.36	4 (8%)	58,89,113	0.97	2 (3%)
13	BCR	L	305	-	41,41,41	0.28	0	56,56,56	0.49	1 (1%)
10	CLA	B	813	-	69,73,73	1.16	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	A	816	-	64,68,73	1.18	4 (6%)	76,107,113	0.84	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	CLA	A	810	1	54,58,73	1.30	4 (7%)	64,95,113	0.92	2 (3%)
10	CLA	B	825	-	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
10	CLA	A	832	-	49,53,73	1.36	4 (8%)	58,89,113	0.96	2 (3%)
10	CLA	B	804	-	69,73,73	1.11	4 (5%)	82,113,113	0.81	3 (3%)
10	CLA	A	829	-	64,68,73	1.22	4 (6%)	76,107,113	0.84	2 (2%)
10	CLA	B	819	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
10	CLA	A	819	-	60,64,73	1.27	4 (6%)	71,102,113	0.88	2 (2%)
10	CLA	B	835	-	59,63,73	1.20	4 (6%)	70,101,113	0.88	3 (4%)
13	BCR	I	101	-	41,41,41	0.16	0	56,56,56	0.45	0
11	PQN	A	844	-	34,34,34	0.34	0	43,45,45	0.43	0
10	CLA	B	838	-	69,73,73	1.08	4 (5%)	82,113,113	0.83	2 (2%)
10	CLA	A	813	-	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	A	828	-	69,73,73	1.14	4 (5%)	82,113,113	0.83	2 (2%)
12	LHG	A	847	10	30,30,48	0.29	0	33,36,54	0.32	0
16	LMG	A	858	-	43,43,55	0.18	0	51,51,63	0.17	0
10	CLA	B	818	18	59,63,73	1.26	4 (6%)	70,101,113	0.89	3 (4%)
10	CLA	A	817	18	49,53,73	1.40	4 (8%)	58,89,113	0.97	2 (3%)
12	LHG	A	846	-	40,40,48	0.25	0	43,46,54	0.29	0
13	BCR	A	848	-	41,41,41	0.13	0	56,56,56	0.26	0
10	CLA	A	835	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	A	836	-	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	A	837	1	49,53,73	1.38	4 (8%)	58,89,113	0.97	3 (5%)
10	CLA	B	816	-	64,68,73	1.22	4 (6%)	76,107,113	0.84	2 (2%)
10	CLA	A	823	-	56,60,73	1.27	4 (7%)	65,97,113	0.92	2 (3%)
10	CLA	B	830	-	49,53,73	1.36	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	B	802	-	69,73,73	1.13	4 (5%)	82,113,113	0.78	3 (3%)
9	CL0	H	201	6	48,63,73	1.50	7 (14%)	48,101,113	1.93	5 (10%)
10	CLA	B	827	-	69,73,73	1.08	4 (5%)	82,113,113	0.84	2 (2%)
10	CLA	B	824	18	54,58,73	1.26	4 (7%)	64,95,113	0.89	2 (3%)
10	CLA	A	811	-	49,53,73	1.37	4 (8%)	58,89,113	0.96	3 (5%)
10	CLA	B	821	-	49,53,73	1.37	4 (8%)	58,89,113	0.97	2 (3%)
10	CLA	A	814	-	69,73,73	1.14	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	834	-	55,59,73	1.26	4 (7%)	64,96,113	0.92	2 (3%)
10	CLA	A	826	18	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
10	CLA	B	836	-	54,58,73	1.30	4 (7%)	64,95,113	0.91	2 (3%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	BCR	L	306	-	41,41,41	0.12	0	56,56,56	0.23	0
11	PQN	B	839	-	34,34,34	0.33	0	43,45,45	0.39	0
10	CLA	A	802	-	69,73,73	1.09	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	833	-	49,53,73	1.34	4 (8%)	58,89,113	0.98	3 (5%)
10	CLA	L	303	-	64,68,73	1.16	4 (6%)	76,107,113	0.85	3 (3%)
13	BCR	L	301	-	41,41,41	0.14	0	56,56,56	0.32	0
10	CLA	A	804	-	49,53,73	1.39	4 (8%)	58,89,113	0.99	3 (5%)
10	CLA	L	304	18	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
10	CLA	A	841	-	59,63,73	1.24	4 (6%)	70,101,113	0.87	2 (2%)
10	CLA	B	820	-	49,53,73	1.37	4 (8%)	58,89,113	0.98	3 (5%)
10	CLA	L	302	8	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
13	BCR	A	849	-	41,41,41	0.13	0	56,56,56	0.29	0
10	CLA	A	834	-	69,73,73	1.11	4 (5%)	82,113,113	0.86	2 (2%)
10	CLA	B	814	-	59,63,73	1.23	4 (6%)	70,101,113	0.87	2 (2%)
10	CLA	B	810	-	60,64,73	1.25	4 (6%)	71,102,113	0.86	2 (2%)
10	CLA	A	840	-	59,63,73	1.18	4 (6%)	70,101,113	0.88	2 (2%)
13	BCR	B	841	-	41,41,41	0.14	0	56,56,56	0.30	0
10	CLA	A	845	12	49,53,73	1.38	4 (8%)	58,89,113	0.98	3 (5%)
15	LMU	A	857	-	24,24,36	0.12	0	29,29,47	0.28	0
10	CLA	B	808	2	69,73,73	1.13	4 (5%)	82,113,113	0.80	2 (2%)
10	CLA	B	831	-	49,53,73	1.34	5 (10%)	58,89,113	0.99	3 (5%)
10	CLA	A	827	18	59,63,73	1.21	4 (6%)	70,101,113	0.85	2 (2%)
10	CLA	A	822	18	69,73,73	1.14	4 (5%)	82,113,113	0.83	3 (3%)
10	CLA	B	805	2	69,73,73	1.14	4 (5%)	82,113,113	0.78	2 (2%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	B	843	-	-	1/29/63/63	0/2/2/2
10	CLA	B	828	-	1/1/15/20	6/39/115/115	-
13	BCR	A	852	-	-	4/29/63/63	0/2/2/2
10	CLA	A	838	-	1/1/12/20	0/23/99/115	-
10	CLA	B	807	-	1/1/15/20	7/39/115/115	-
10	CLA	B	823	18	1/1/13/20	4/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	806	-	1/1/15/20	2/39/115/115	-
13	BCR	A	850	-	-	2/29/63/63	0/2/2/2
10	CLA	A	820	-	1/1/15/20	6/39/115/115	-
10	CLA	A	843	18	1/1/15/20	7/39/115/115	-
10	CLA	A	856	18	1/1/12/20	2/21/97/115	-
10	CLA	A	830	-	1/1/15/20	1/39/115/115	-
10	CLA	A	807	1	1/1/15/20	5/39/115/115	-
10	CLA	A	831	-	1/1/15/20	2/39/115/115	-
9	CL0	A	801	-	3/3/20/25	3/37/135/135	-
10	CLA	A	833	-	1/1/13/20	1/27/103/115	-
10	CLA	A	839	-	1/1/15/20	3/39/115/115	-
10	CLA	A	824	-	1/1/11/20	5/15/91/115	-
10	CLA	B	812	-	1/1/15/20	8/39/115/115	-
10	CLA	A	808	-	1/1/11/20	2/18/94/115	-
10	CLA	A	805	10	1/1/12/20	1/21/97/115	-
13	BCR	B	840	-	-	0/29/63/63	0/2/2/2
14	SF4	C	102	3	-	-	0/6/5/5
10	CLA	B	832	-	1/1/11/20	4/15/91/115	-
13	BCR	B	842	-	-	2/29/63/63	0/2/2/2
10	CLA	A	842	-	1/1/11/20	4/15/91/115	-
10	CLA	B	815	-	1/1/13/20	5/30/106/115	-
17	DGD	B	844	-	-	11/50/90/95	0/2/2/2
10	CLA	A	803	18	1/1/15/20	2/39/115/115	-
14	SF4	A	853	1,2	-	-	0/6/5/5
10	CLA	B	826	-	1/1/15/20	6/39/115/115	-
10	CLA	A	821	-	1/1/11/20	5/15/91/115	-
10	CLA	B	829	-	1/1/11/20	6/15/91/115	-
12	LHG	B	845	-	-	15/53/53/53	-
10	CLA	A	854	18	1/1/13/20	3/27/103/115	-
10	CLA	B	809	-	1/1/15/20	4/39/115/115	-
10	CLA	B	817	-	1/1/15/20	5/39/115/115	-
10	CLA	A	809	1	1/1/13/20	8/27/103/115	-
10	CLA	B	803	-	1/1/11/20	5/15/91/115	-
10	CLA	B	801	-	1/1/15/20	4/39/115/115	-
10	CLA	B	811	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	812	10	1/1/15/20	7/39/115/115	-
15	LMU	A	859	-	-	4/12/32/61	0/1/1/2
10	CLA	A	815	-	1/1/12/20	2/26/102/115	-
10	CLA	A	825	-	1/1/14/20	2/33/109/115	-
10	CLA	B	806	-	1/1/14/20	4/33/109/115	-
15	LMU	A	855	-	-	4/21/61/61	0/2/2/2
13	BCR	A	851	-	-	2/29/63/63	0/2/2/2
10	CLA	A	818	-	1/1/11/20	4/15/91/115	-
10	CLA	B	837	18	1/1/15/20	5/39/115/115	-
10	CLA	B	822	-	1/1/11/20	3/15/91/115	-
13	BCR	L	305	-	-	2/29/63/63	0/2/2/2
10	CLA	B	813	-	1/1/15/20	4/39/115/115	-
10	CLA	A	816	-	1/1/14/20	3/33/109/115	-
10	CLA	A	810	1	1/1/12/20	4/21/97/115	-
10	CLA	B	825	-	1/1/15/20	2/39/115/115	-
10	CLA	A	832	-	1/1/11/20	2/15/91/115	-
10	CLA	B	804	-	1/1/15/20	5/39/115/115	-
10	CLA	A	829	-	1/1/14/20	2/33/109/115	-
10	CLA	B	819	-	1/1/11/20	3/15/91/115	-
10	CLA	A	819	-	1/1/13/20	7/29/105/115	-
10	CLA	B	835	-	1/1/13/20	2/27/103/115	-
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
11	PQN	A	844	-	-	0/23/43/43	0/2/2/2
10	CLA	B	838	-	1/1/15/20	4/39/115/115	-
10	CLA	A	813	-	1/1/11/20	2/15/91/115	-
10	CLA	A	828	-	1/1/15/20	2/39/115/115	-
12	LHG	A	847	10	-	8/35/35/53	-
16	LMG	A	858	-	-	3/38/58/70	0/1/1/1
10	CLA	B	818	18	1/1/13/20	2/27/103/115	-
10	CLA	A	817	18	1/1/11/20	2/15/91/115	-
12	LHG	A	846	-	-	7/45/45/53	-
13	BCR	A	848	-	-	4/29/63/63	0/2/2/2
10	CLA	A	835	-	1/1/15/20	2/39/115/115	-
10	CLA	A	836	-	1/1/15/20	7/39/115/115	-
10	CLA	A	837	1	1/1/11/20	0/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	B	816	-	1/1/14/20	2/33/109/115	-
10	CLA	A	823	-	1/1/12/20	6/24/100/115	-
10	CLA	B	830	-	1/1/11/20	4/15/91/115	-
10	CLA	B	802	-	1/1/15/20	1/39/115/115	-
9	CL0	H	201	6	3/3/18/25	3/25/123/135	-
10	CLA	B	827	-	1/1/15/20	8/39/115/115	-
10	CLA	B	824	18	1/1/12/20	2/21/97/115	-
10	CLA	A	811	-	1/1/11/20	1/15/91/115	-
10	CLA	B	821	-	1/1/11/20	5/15/91/115	-
10	CLA	A	814	-	1/1/15/20	5/39/115/115	-
10	CLA	B	834	-	1/1/12/20	2/23/99/115	-
10	CLA	A	826	18	1/1/15/20	8/39/115/115	-
10	CLA	B	836	-	1/1/12/20	0/21/97/115	-
14	SF4	C	101	3	-	-	0/6/5/5
13	BCR	L	306	-	-	0/29/63/63	0/2/2/2
11	PQN	B	839	-	-	3/23/43/43	0/2/2/2
10	CLA	A	802	-	1/1/15/20	0/39/115/115	-
10	CLA	B	833	-	1/1/11/20	4/15/91/115	-
10	CLA	L	303	-	1/1/14/20	3/33/109/115	-
13	BCR	L	301	-	-	4/29/63/63	0/2/2/2
10	CLA	A	804	-	1/1/11/20	4/15/91/115	-
10	CLA	L	304	18	1/1/11/20	0/15/91/115	-
10	CLA	A	841	-	1/1/13/20	2/27/103/115	-
10	CLA	B	820	-	1/1/11/20	4/15/91/115	-
10	CLA	L	302	8	1/1/11/20	2/15/91/115	-
13	BCR	A	849	-	-	2/29/63/63	0/2/2/2
10	CLA	A	834	-	1/1/15/20	4/39/115/115	-
10	CLA	B	814	-	1/1/13/20	7/27/103/115	-
10	CLA	B	810	-	1/1/13/20	4/29/105/115	-
10	CLA	A	840	-	1/1/13/20	0/27/103/115	-
13	BCR	B	841	-	-	6/29/63/63	0/2/2/2
10	CLA	A	845	12	1/1/11/20	6/15/91/115	-
15	LMU	A	857	-	-	3/15/35/61	0/1/1/2
10	CLA	B	808	2	1/1/15/20	5/39/115/115	-
10	CLA	B	831	-	1/1/11/20	2/15/91/115	-
10	CLA	A	827	18	1/1/13/20	0/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	CLA	A	822	18	1/1/15/20	0/39/115/115	-
10	CLA	B	805	2	1/1/15/20	2/39/115/115	-

The worst 5 of 361 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	823	CLA	C1D-ND	5.47	1.45	1.37
10	A	803	CLA	MG-NB	-5.47	1.94	2.05
10	A	803	CLA	C1D-ND	5.44	1.45	1.37
10	A	838	CLA	C1D-ND	5.44	1.45	1.37
10	B	825	CLA	MG-NB	-5.44	1.95	2.05

The worst 5 of 207 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	H	201	CL0	C1B-CHB-C4A	11.30	128.59	121.32
9	A	801	CL0	C1B-CHB-C4A	10.98	128.38	121.32
10	B	831	CLA	C1D-ND-C4D	-4.29	103.30	106.31
10	A	820	CLA	C1D-ND-C4D	-4.27	103.31	106.31
10	A	828	CLA	C1D-ND-C4D	-4.23	103.34	106.31

5 of 92 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	801	CL0	NA
9	A	801	CL0	NC
9	A	801	CL0	ND
9	H	201	CL0	NA
9	H	201	CL0	NC

5 of 395 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	A	809	CLA	CHA-CBD-CGD-O1D
10	A	809	CLA	CHA-CBD-CGD-O2D
10	A	812	CLA	C2B-C3B-CAB-CBB
10	A	812	CLA	C4B-C3B-CAB-CBB
10	A	812	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

72 monomers are involved in 98 short contacts:

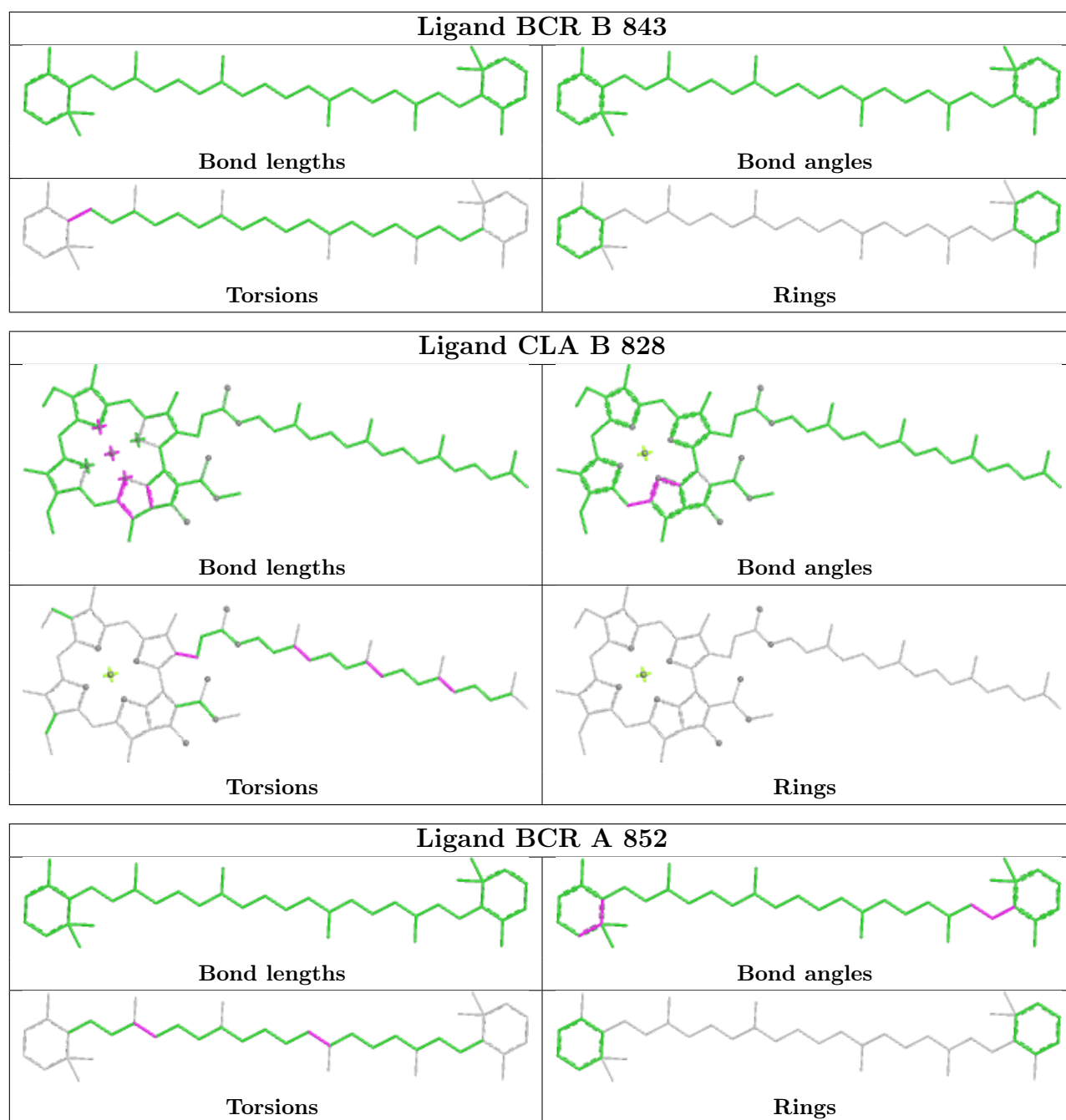
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	843	BCR	1	0
10	B	828	CLA	1	0
13	A	852	BCR	7	0
10	B	807	CLA	2	0
10	B	823	CLA	1	0
13	A	850	BCR	3	0
10	A	820	CLA	1	0
10	A	843	CLA	3	0
10	A	830	CLA	1	0
10	B	812	CLA	1	0
10	A	808	CLA	1	0
10	A	805	CLA	1	0
13	B	840	BCR	1	0
13	B	842	BCR	5	0
10	A	842	CLA	1	0
17	B	844	DGD	1	0
10	A	803	CLA	1	0
10	B	826	CLA	1	0
10	B	829	CLA	2	0
12	B	845	LHG	6	0
10	A	854	CLA	2	0
10	A	809	CLA	2	0
10	B	803	CLA	1	0
10	B	801	CLA	1	0
10	A	812	CLA	2	0
15	A	859	LMU	1	0
10	A	815	CLA	3	0
10	A	825	CLA	1	0
10	B	806	CLA	3	0
15	A	855	LMU	2	0
13	A	851	BCR	2	0
10	B	837	CLA	1	0
10	B	822	CLA	1	0
13	L	305	BCR	1	0
10	B	813	CLA	4	0
10	A	810	CLA	1	0
10	B	825	CLA	3	0
10	A	832	CLA	1	0
10	A	819	CLA	2	0
13	I	101	BCR	2	0
11	A	844	PQN	1	0
10	A	828	CLA	2	0
12	A	847	LHG	3	0

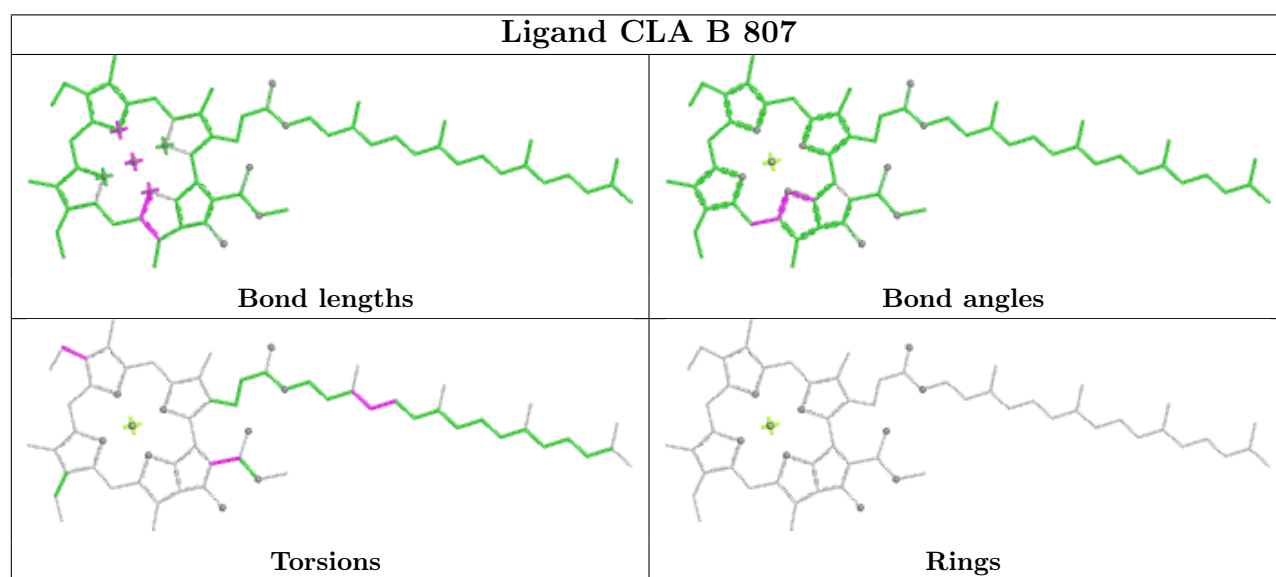
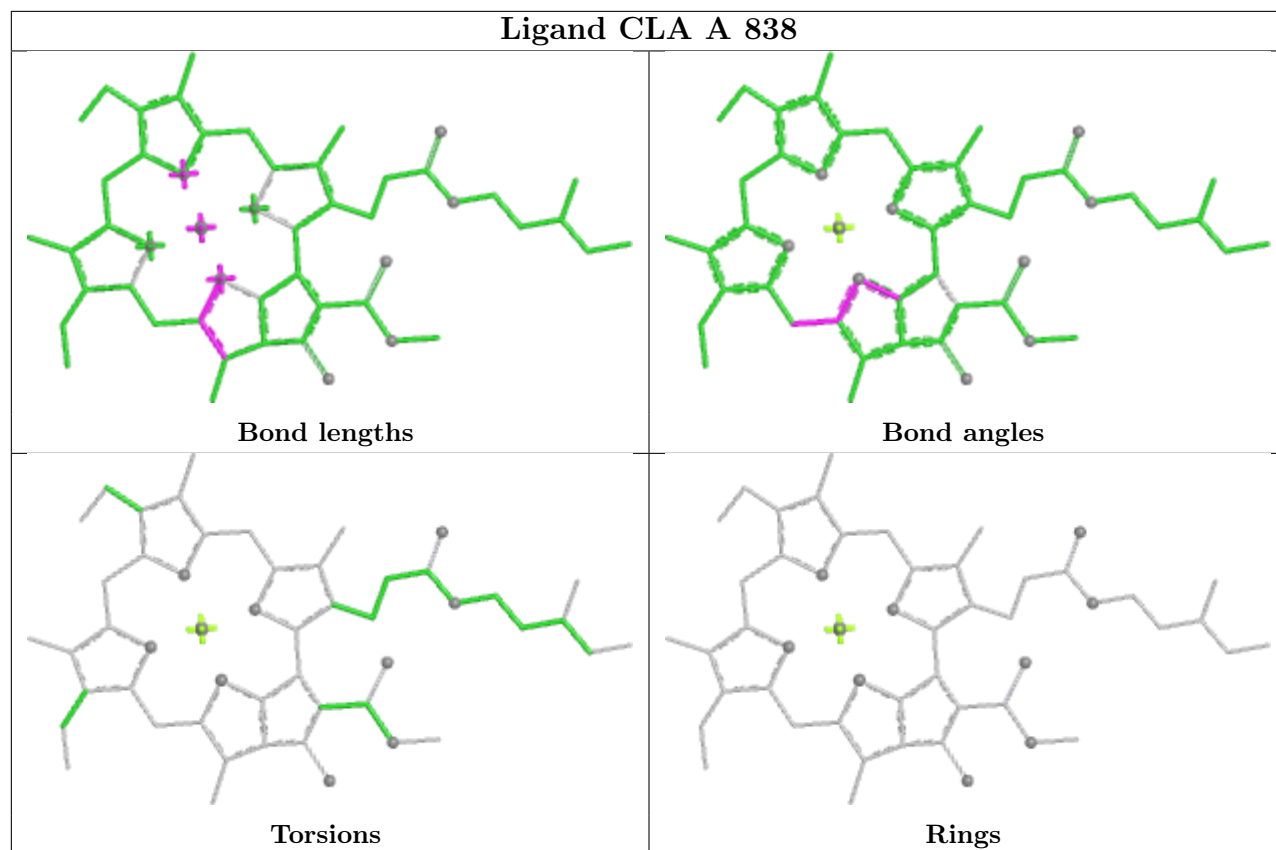
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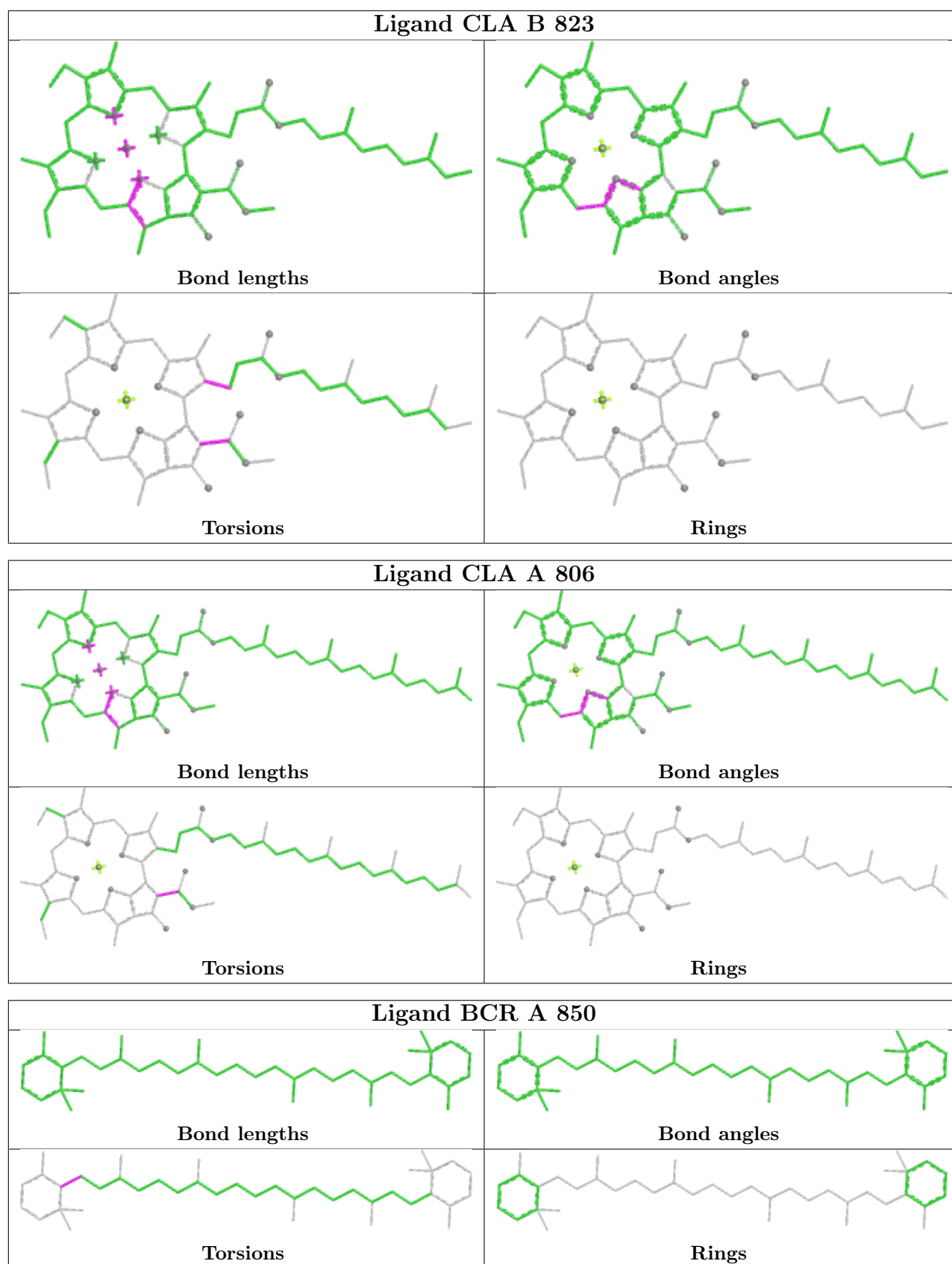
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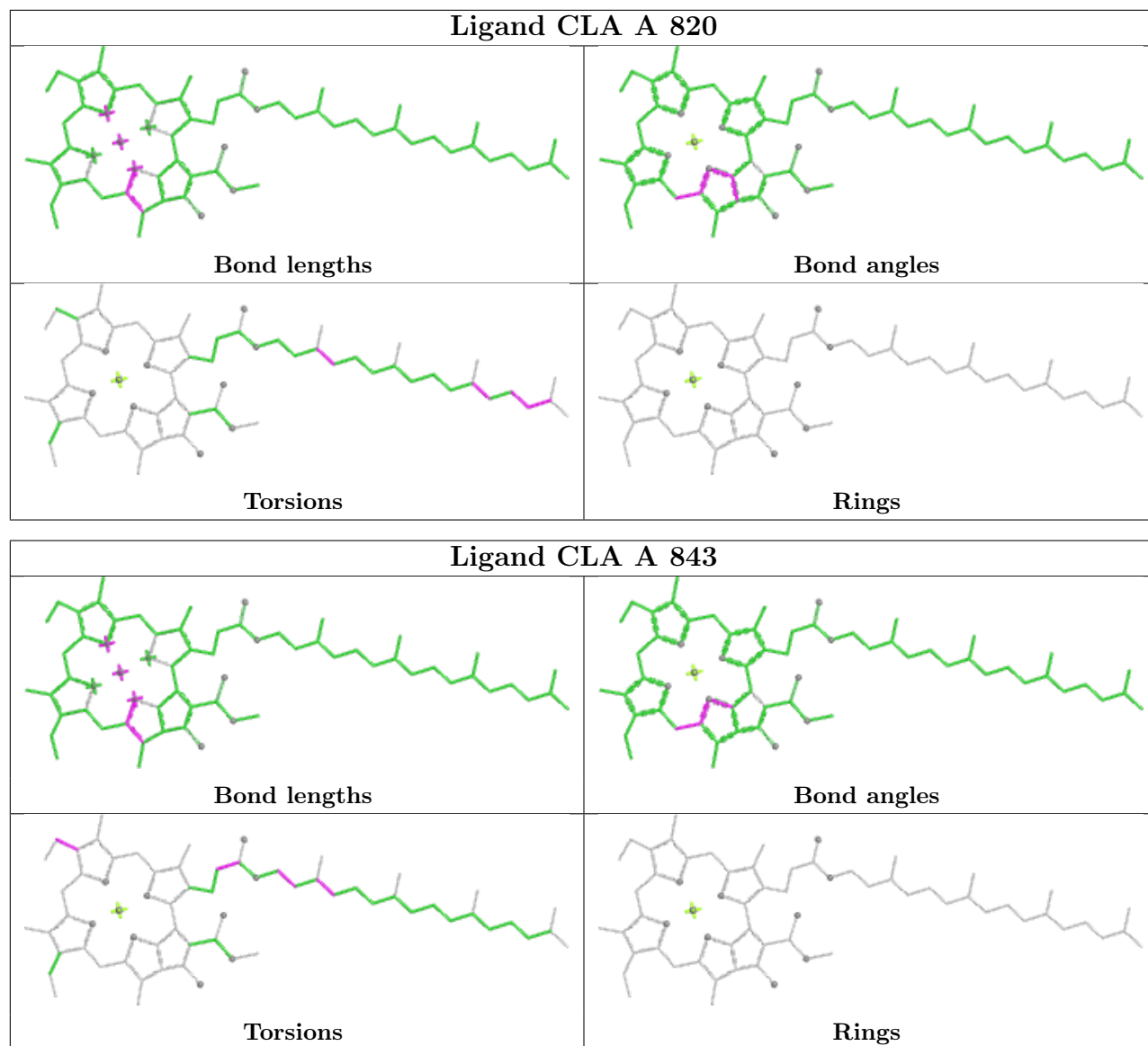
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	A	858	LMG	1	0
10	B	818	CLA	3	0
10	A	817	CLA	1	0
13	A	848	BCR	2	0
10	A	836	CLA	2	0
10	A	837	CLA	1	0
10	B	816	CLA	2	0
10	B	802	CLA	2	0
9	H	201	CL0	1	0
10	B	827	CLA	2	0
10	B	824	CLA	2	0
10	B	821	CLA	1	0
10	A	814	CLA	2	0
10	A	826	CLA	3	0
13	L	306	BCR	1	0
11	B	839	PQN	1	0
10	A	802	CLA	2	0
10	B	833	CLA	3	0
13	L	301	BCR	1	0
10	A	804	CLA	1	0
10	L	304	CLA	2	0
10	A	841	CLA	1	0
10	L	302	CLA	1	0
13	A	849	BCR	2	0
10	B	814	CLA	1	0
13	B	841	BCR	1	0
10	B	808	CLA	1	0
10	B	831	CLA	1	0
10	A	822	CLA	4	0

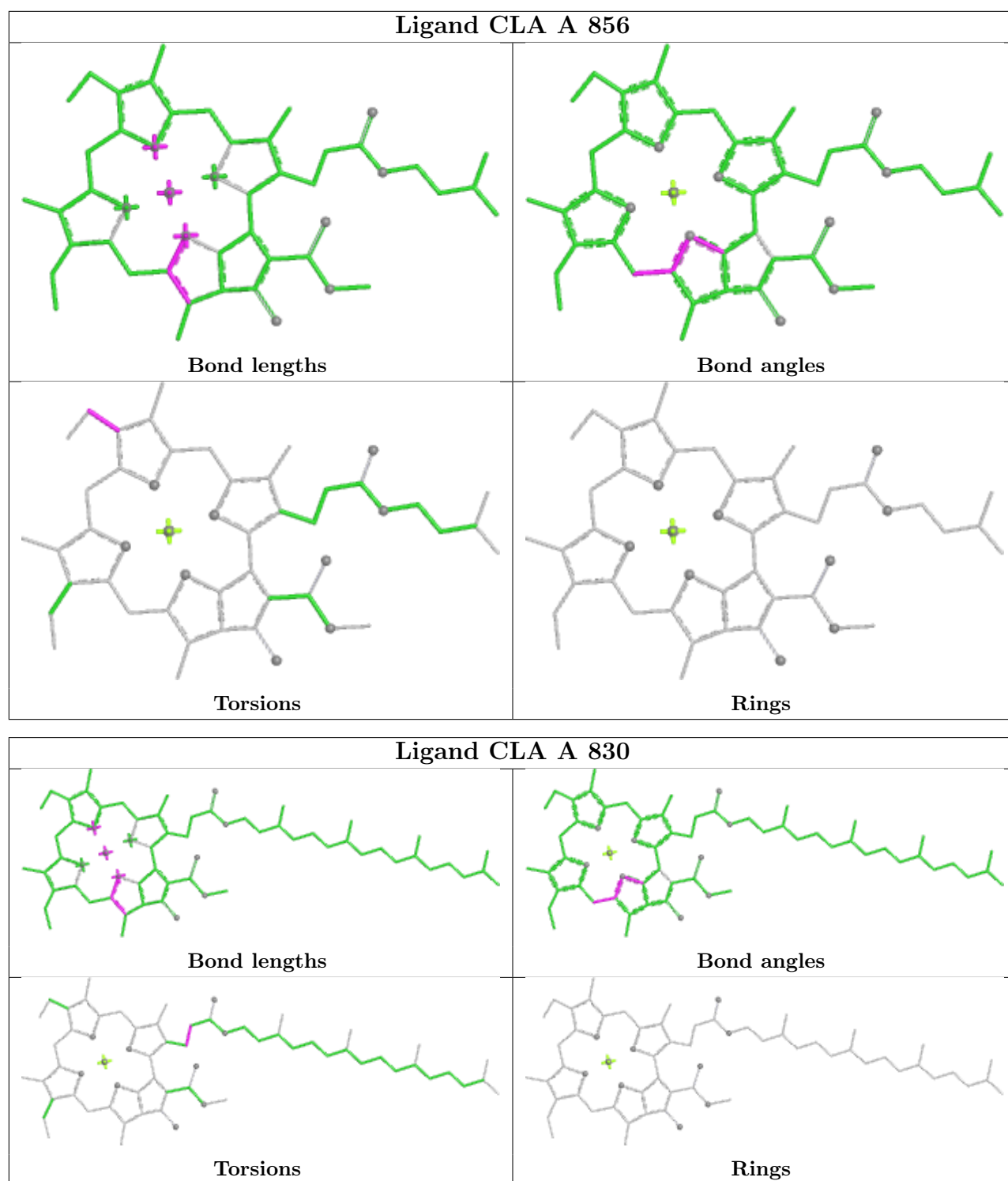
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

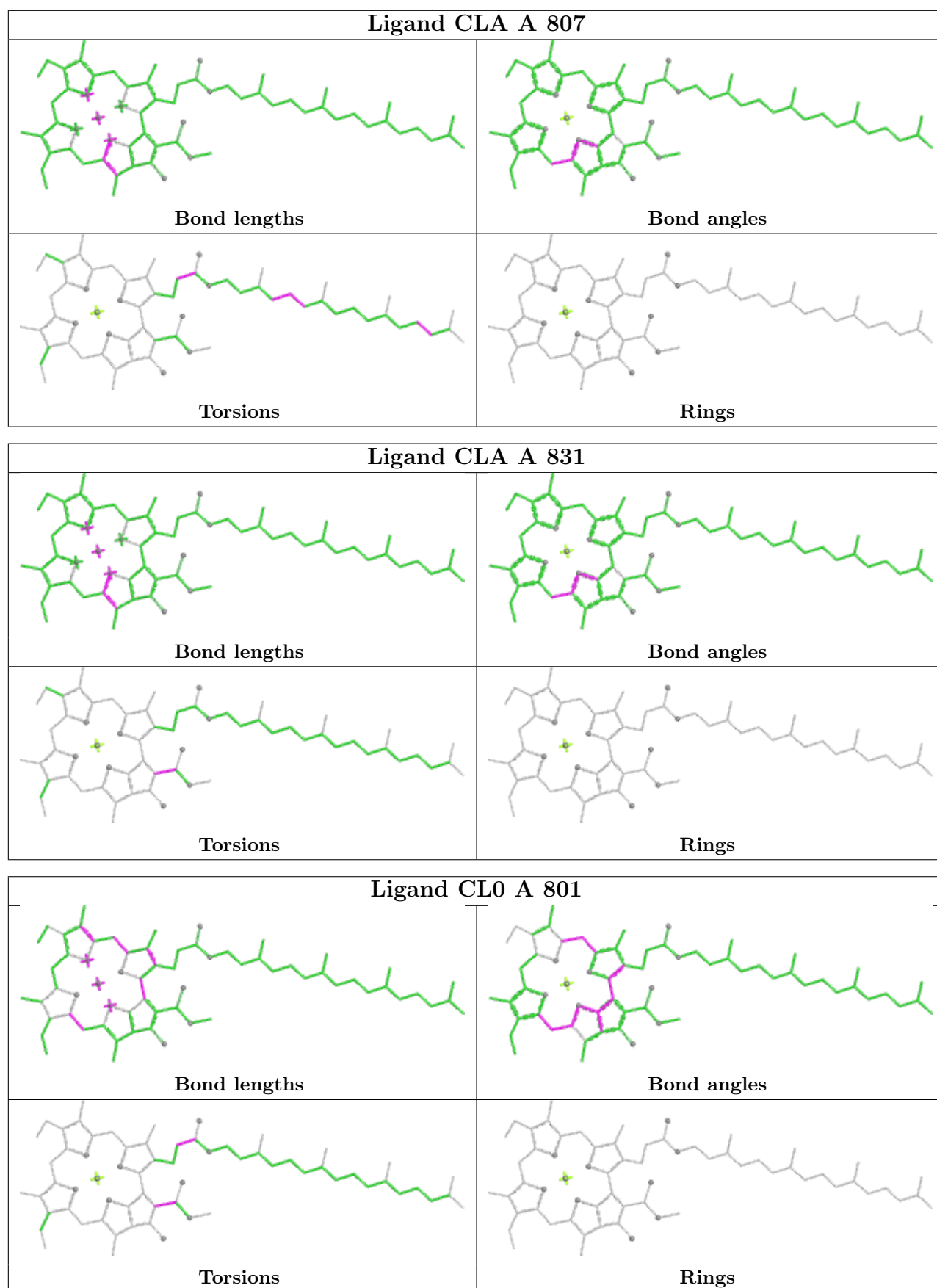


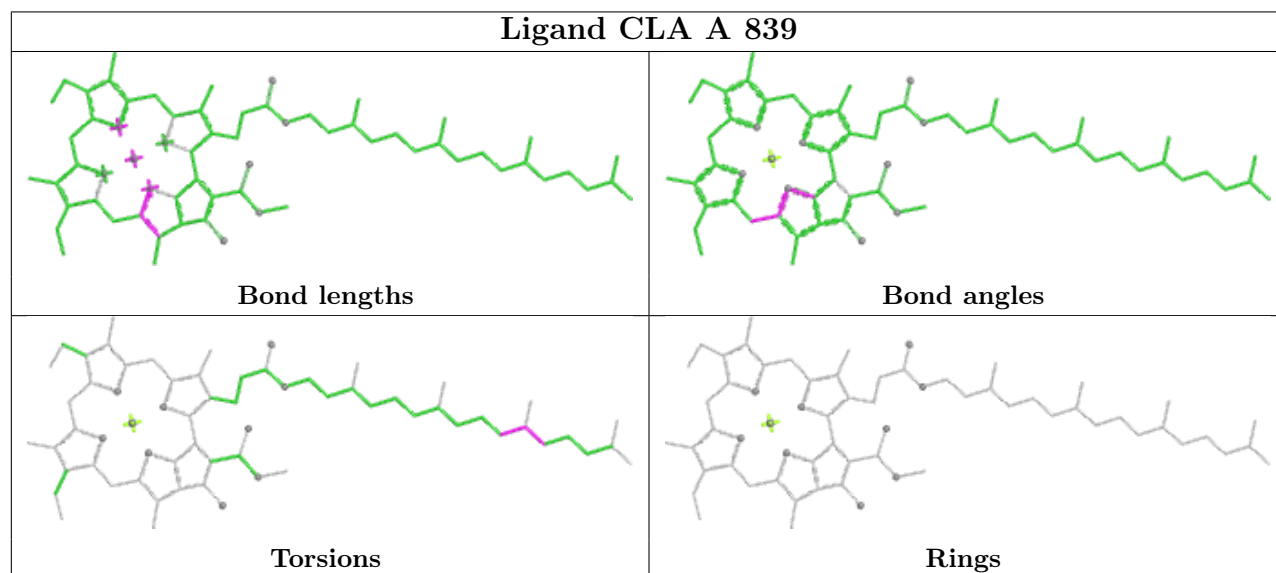
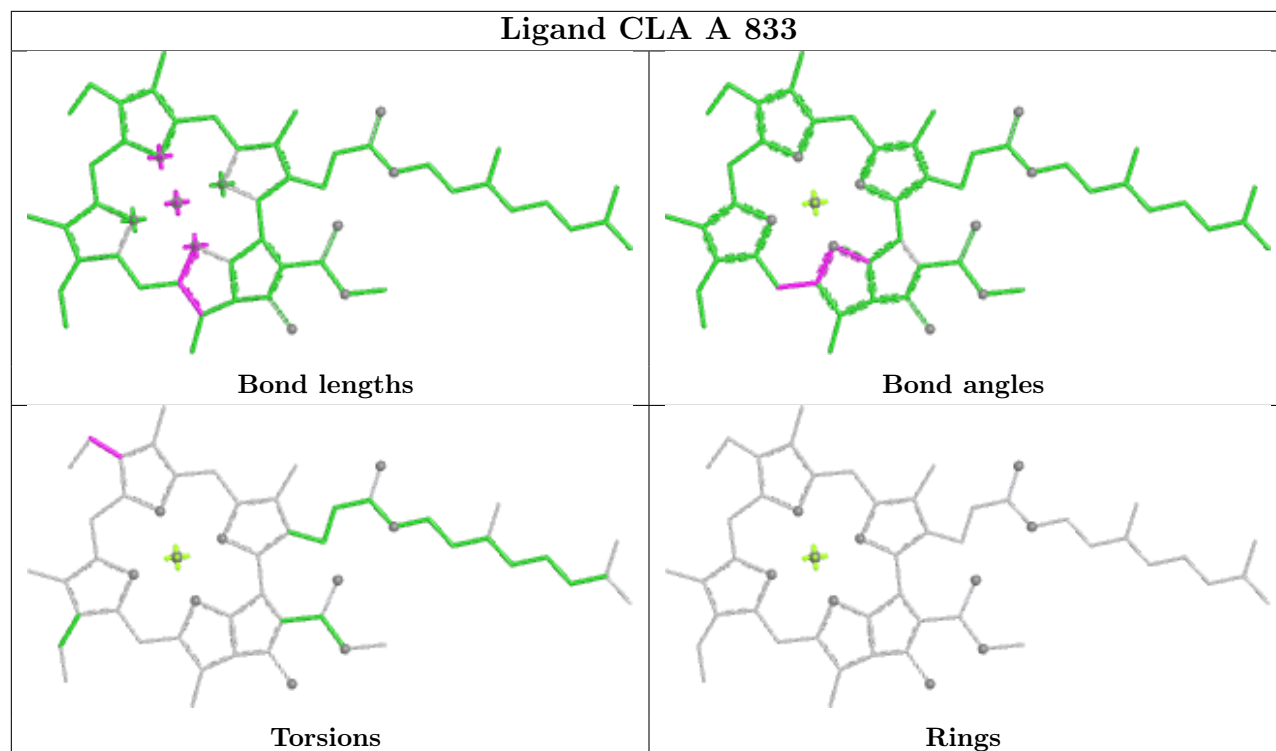


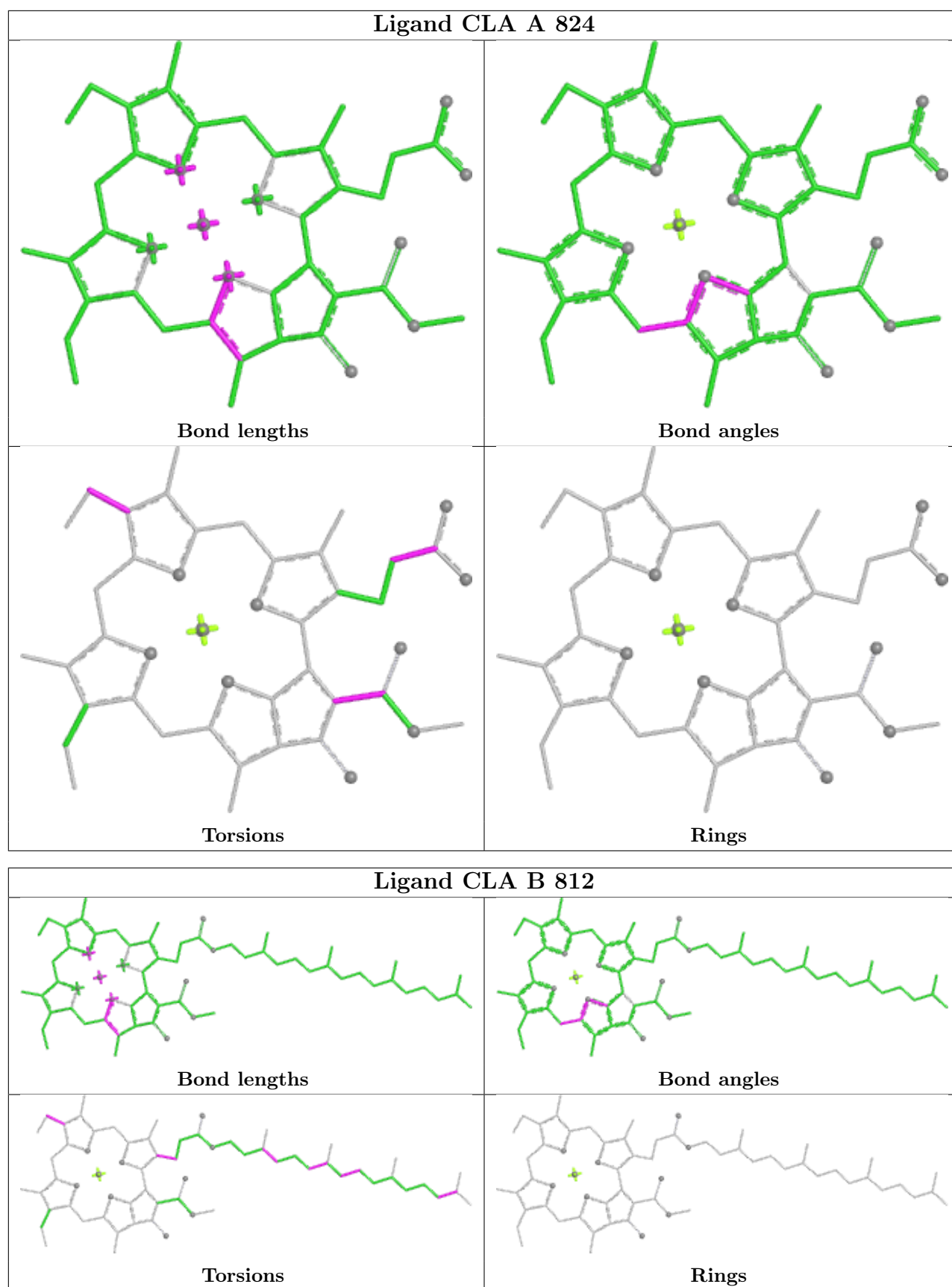


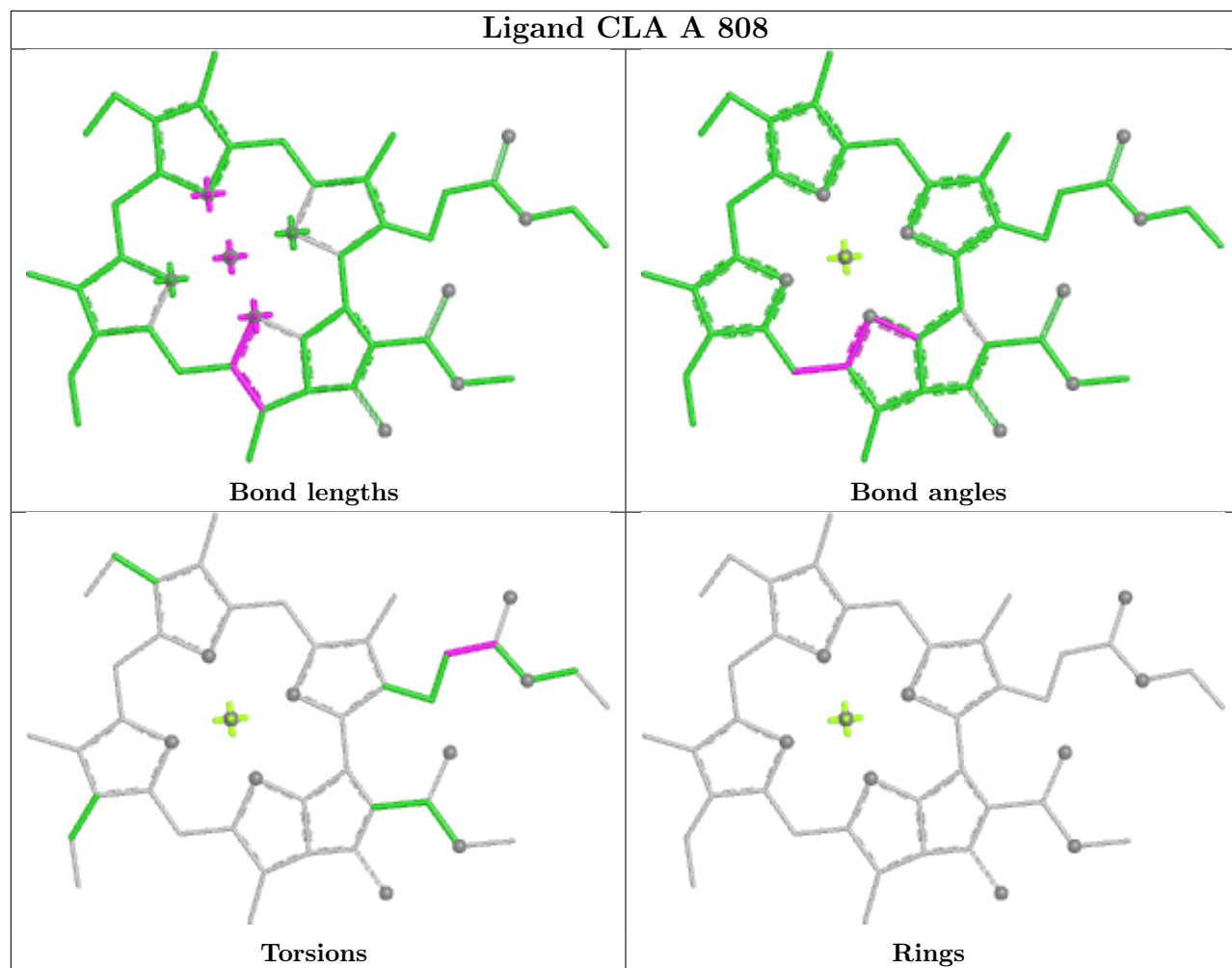


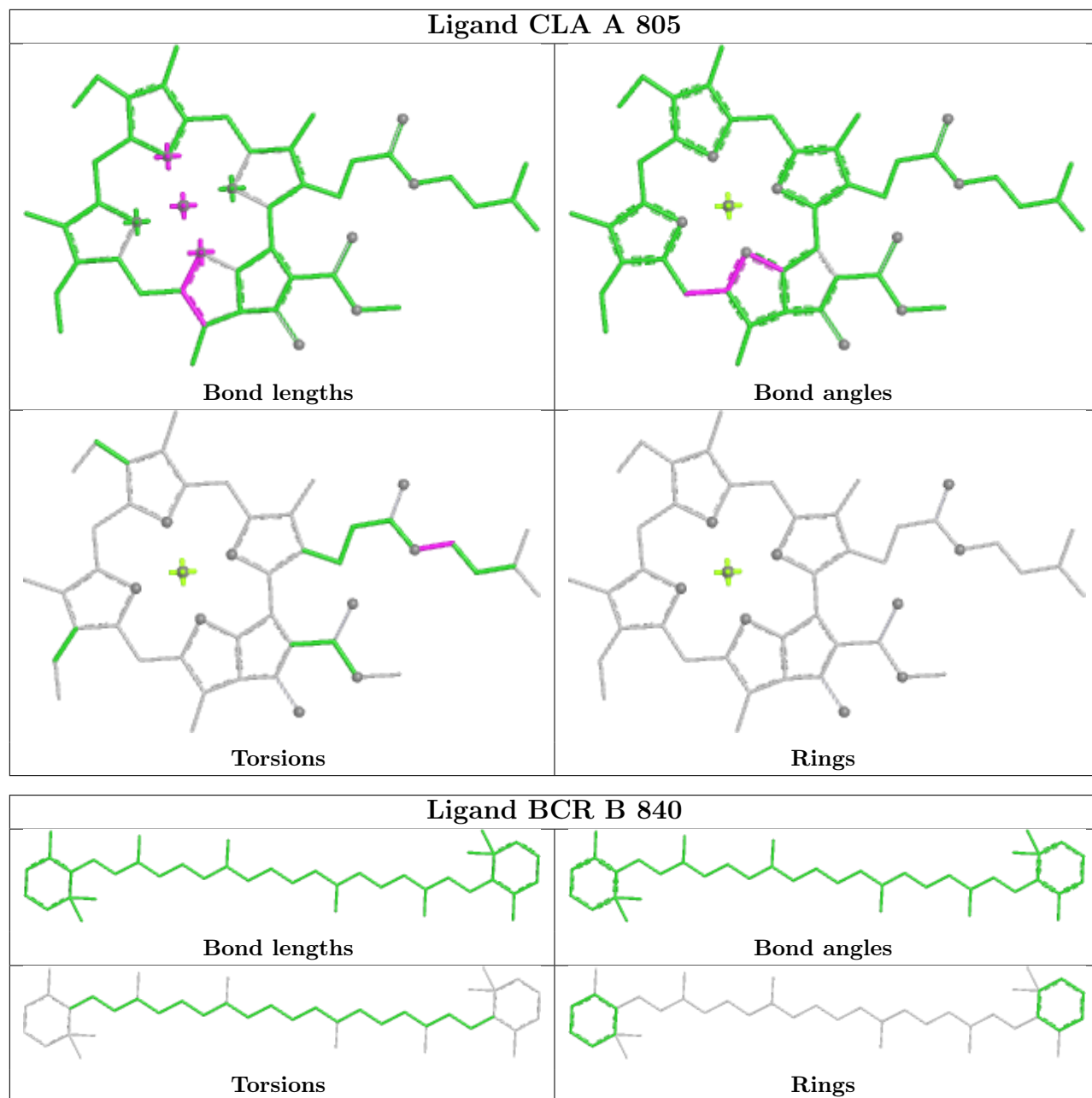


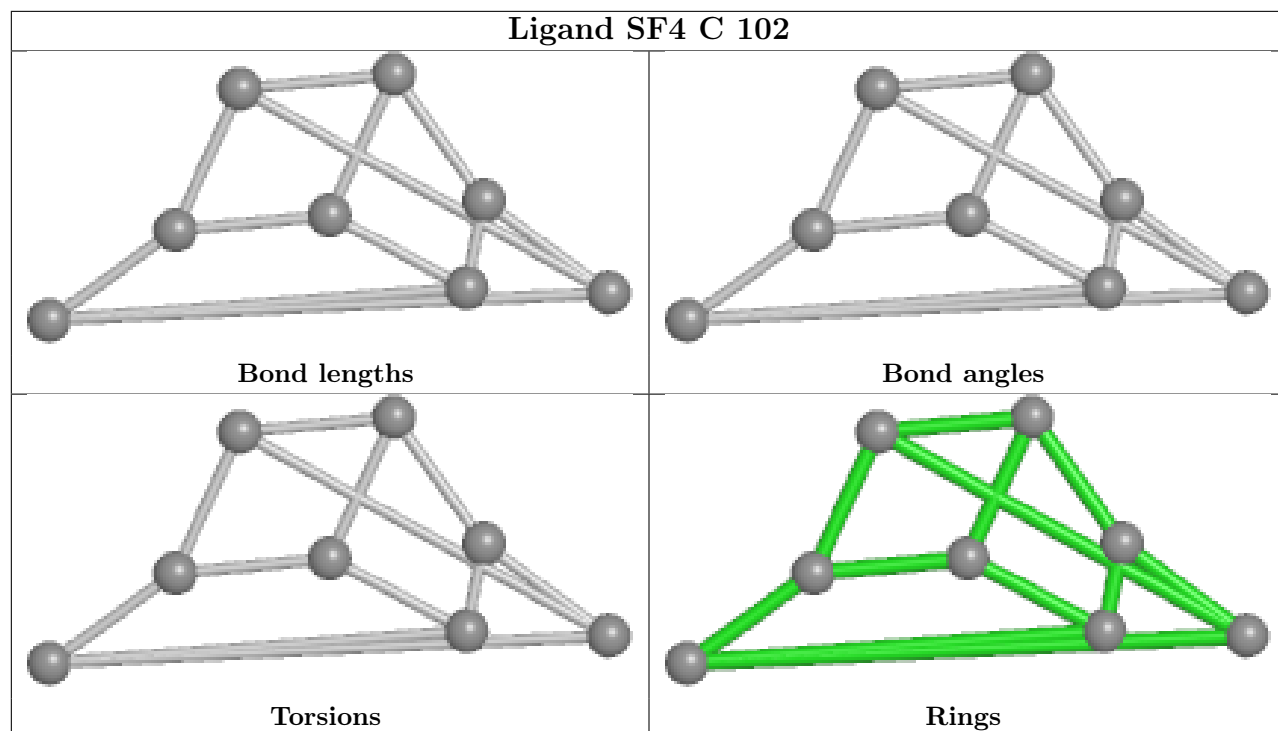


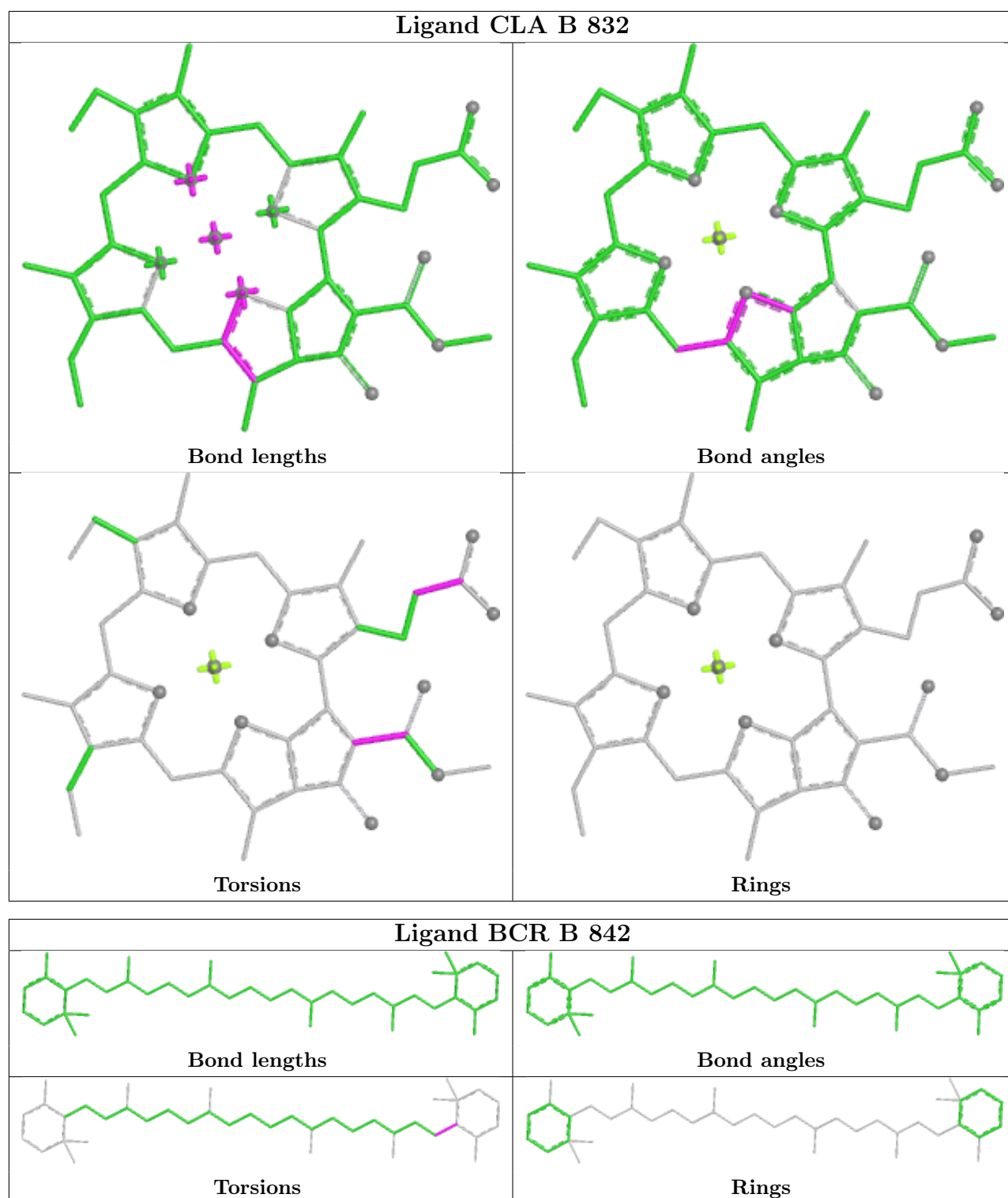


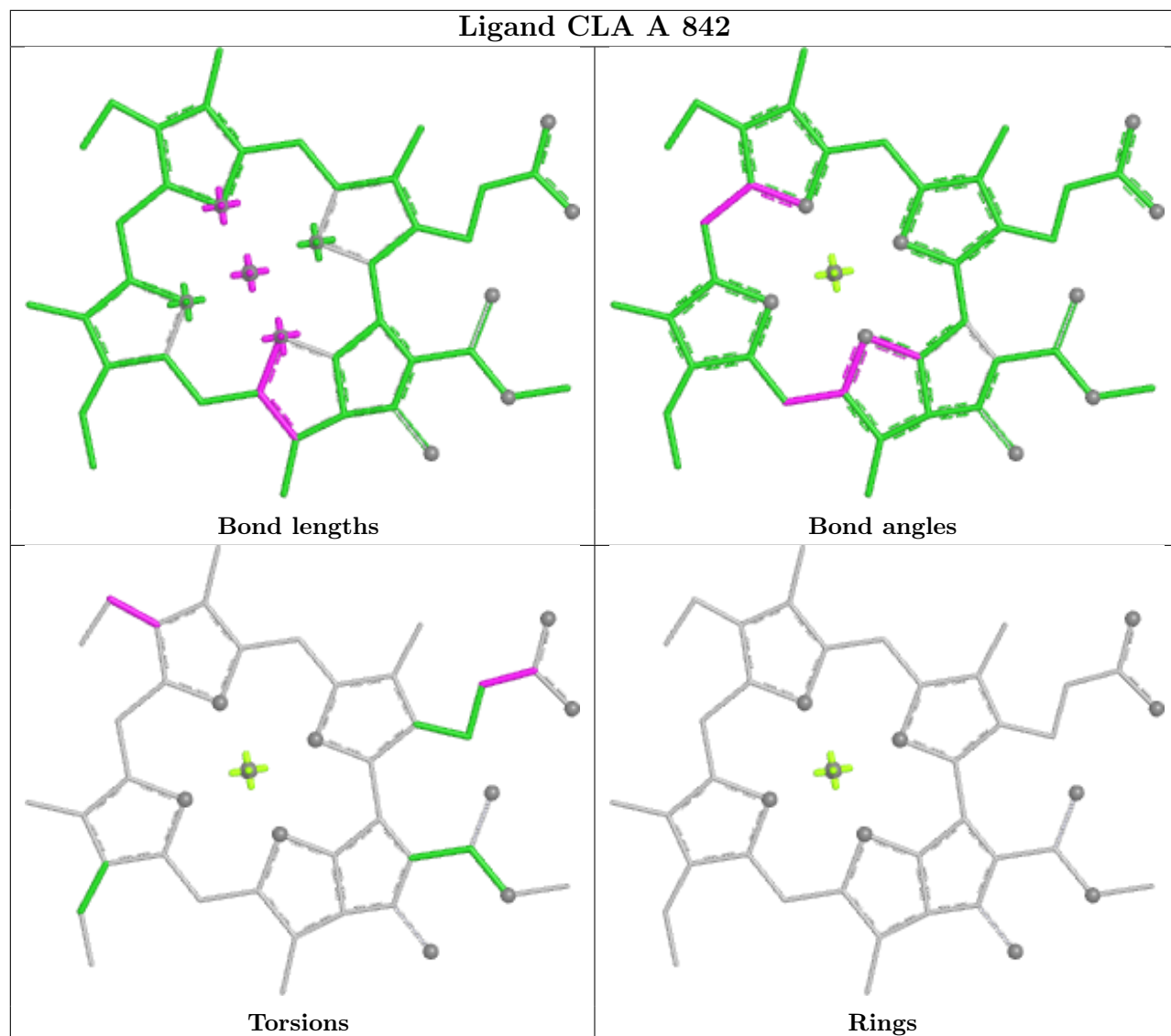


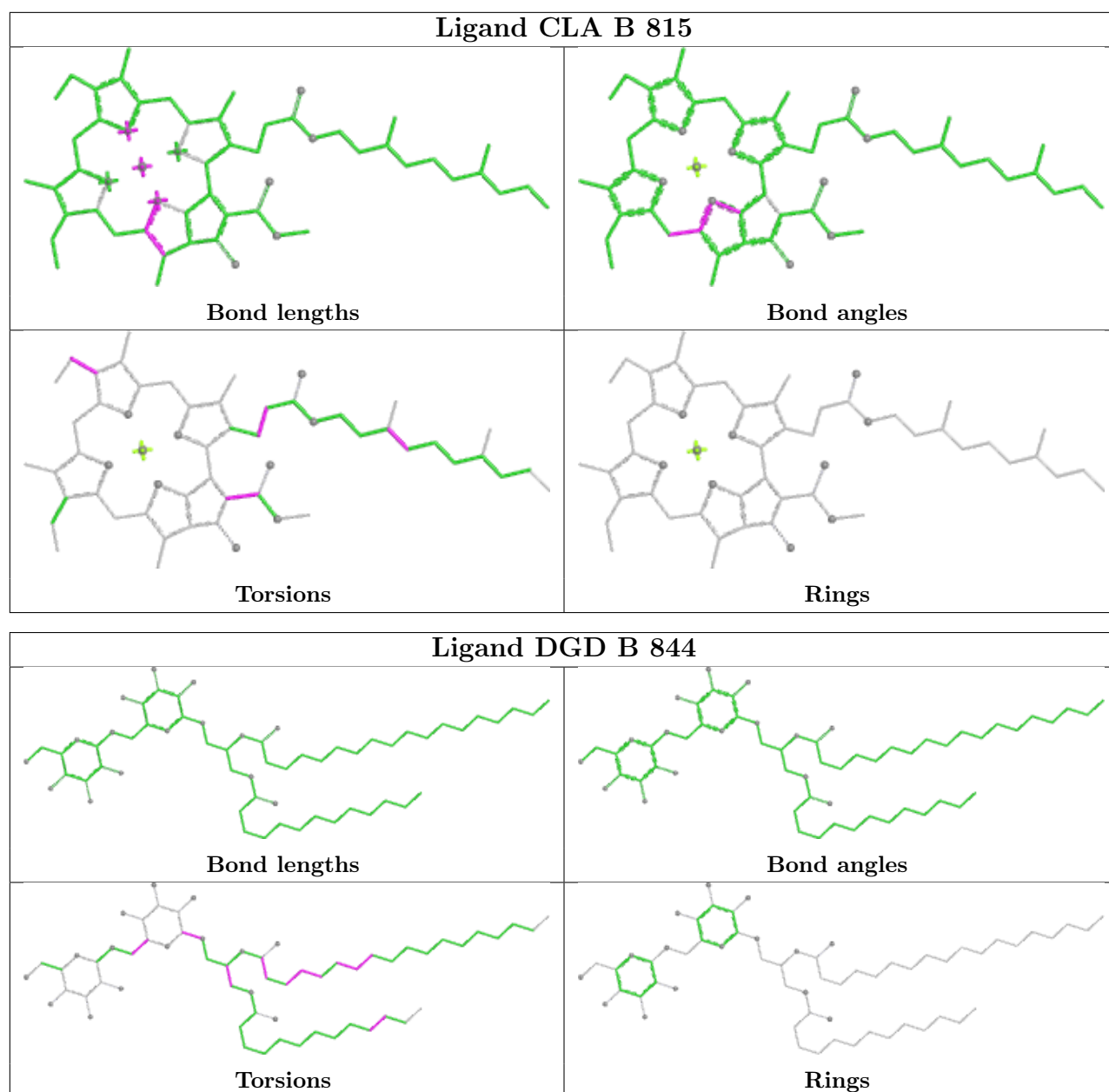


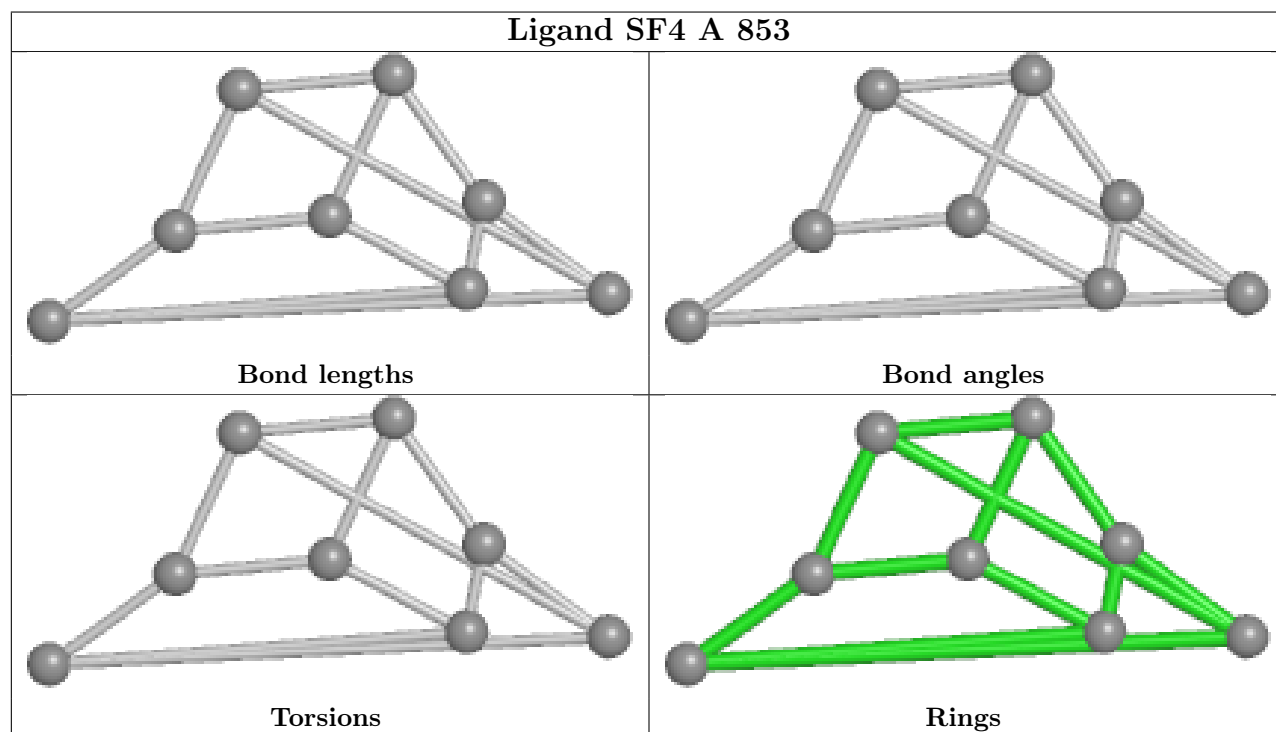
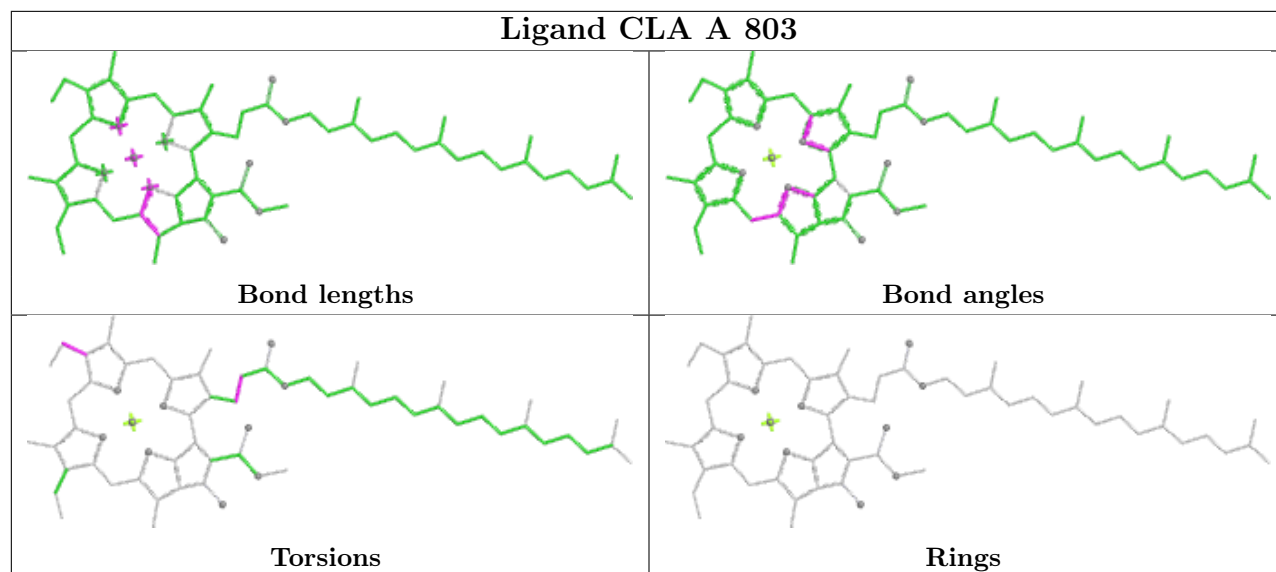


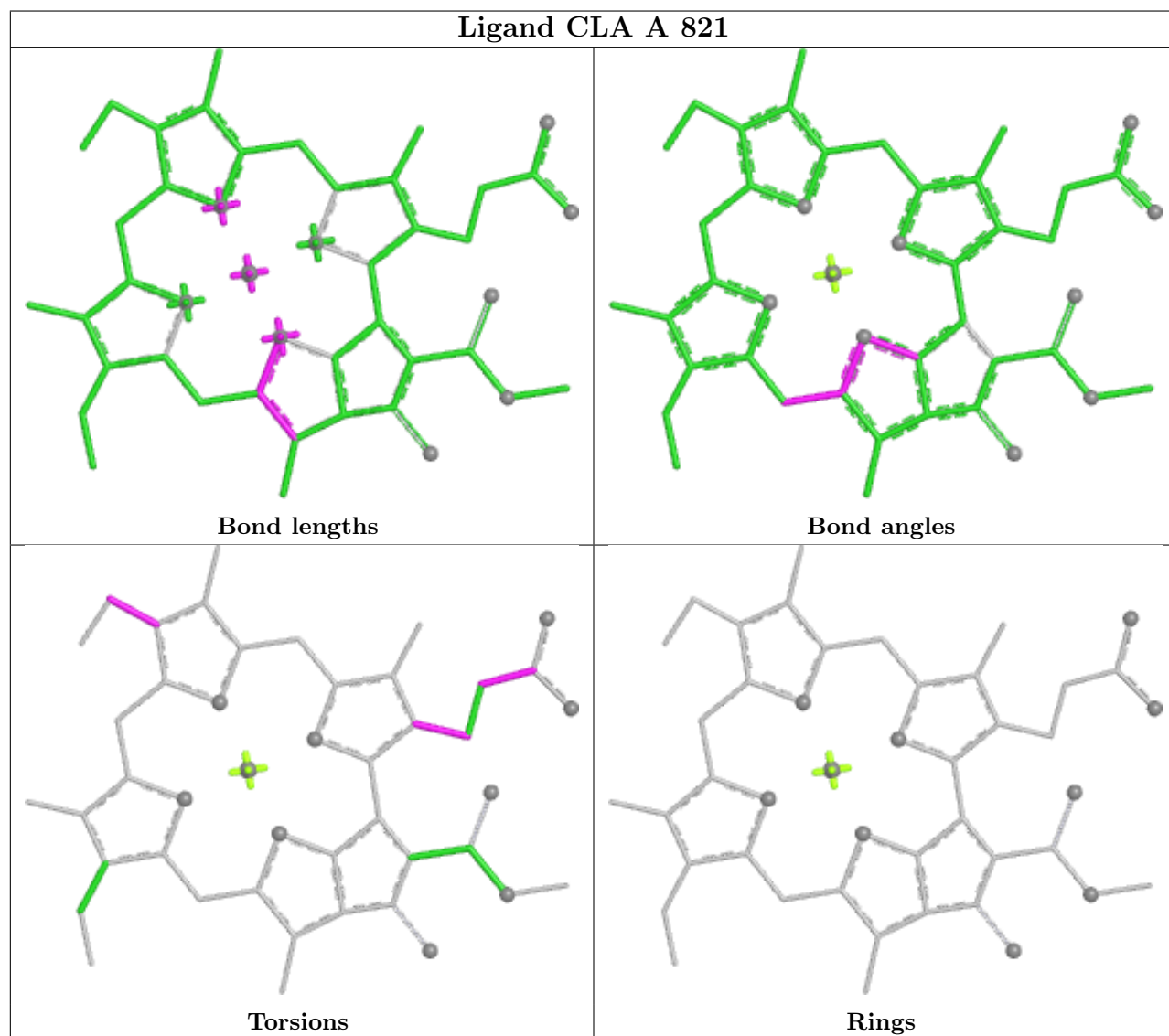
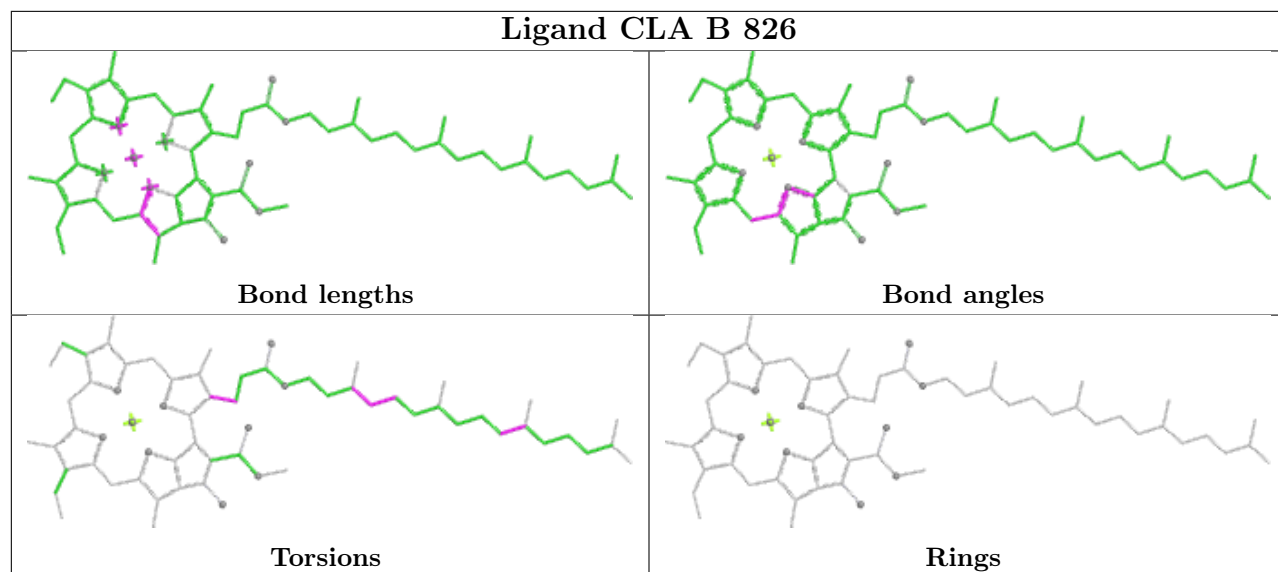


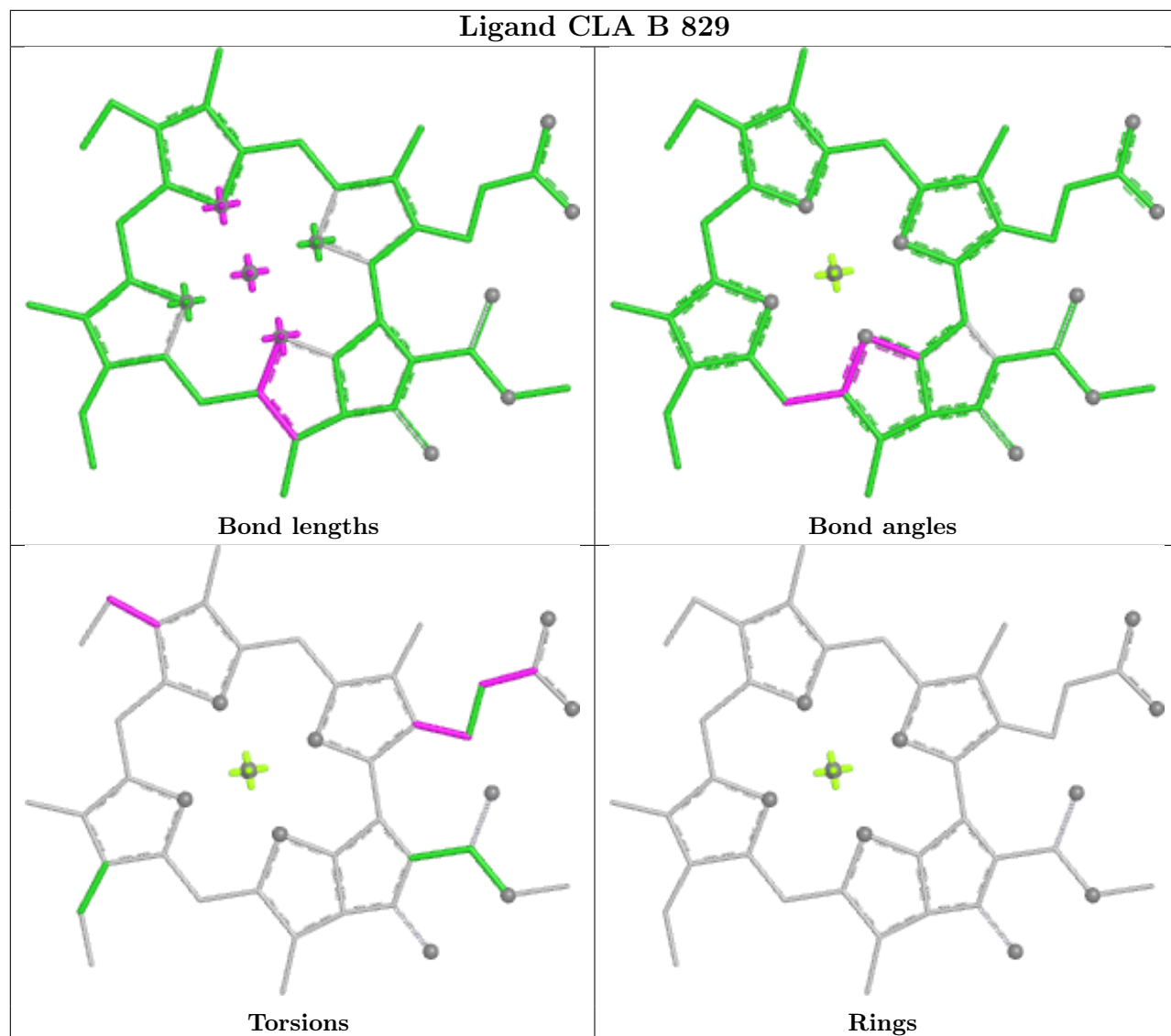


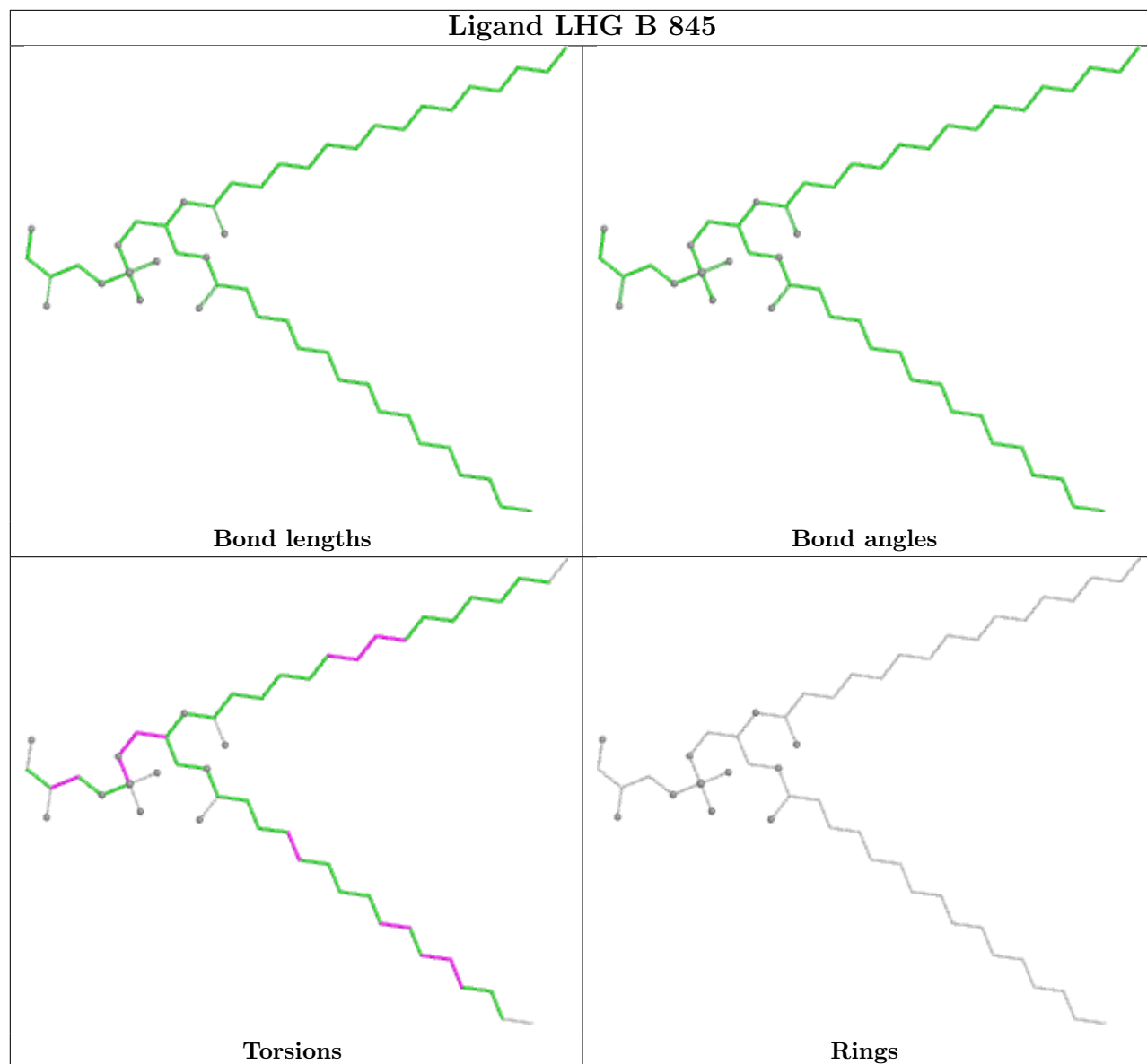


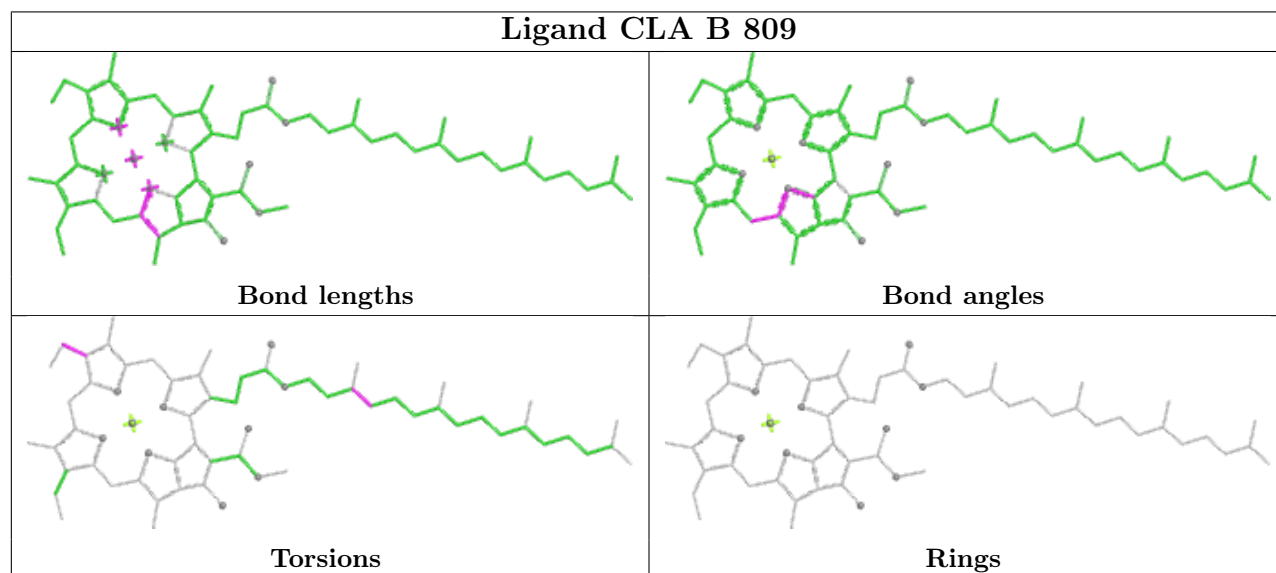
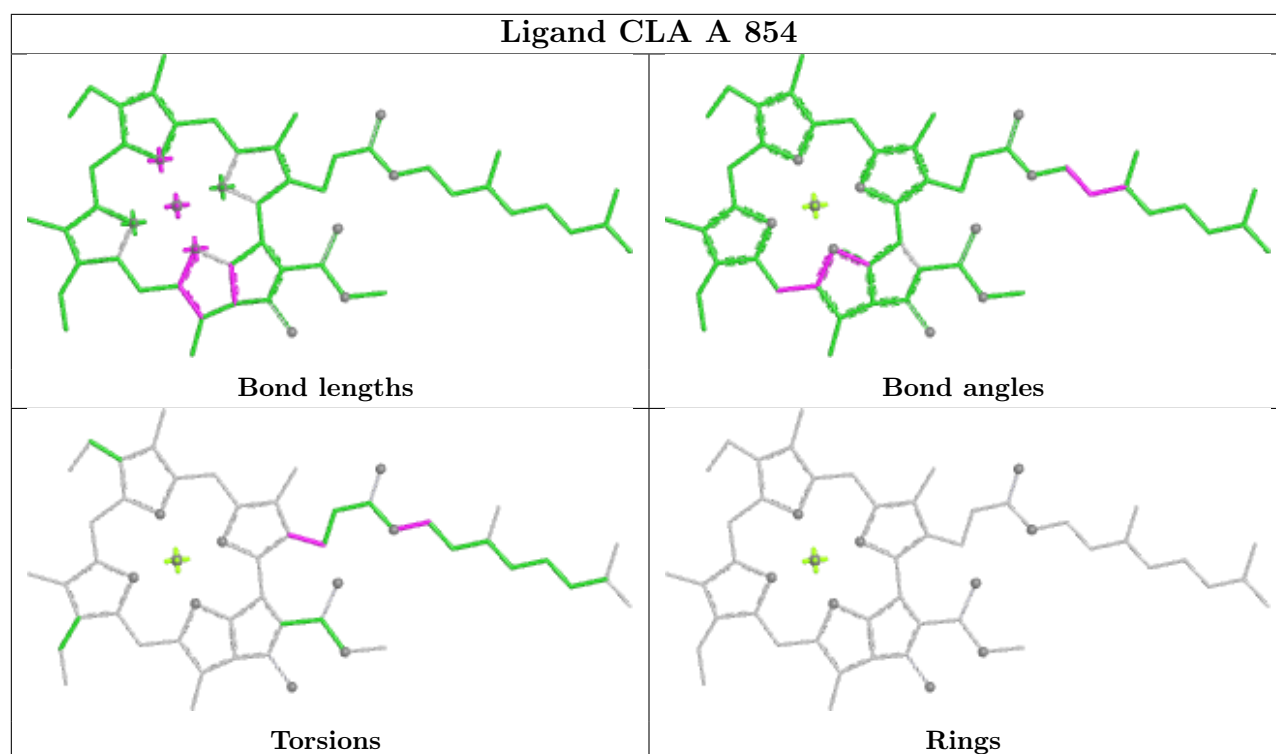


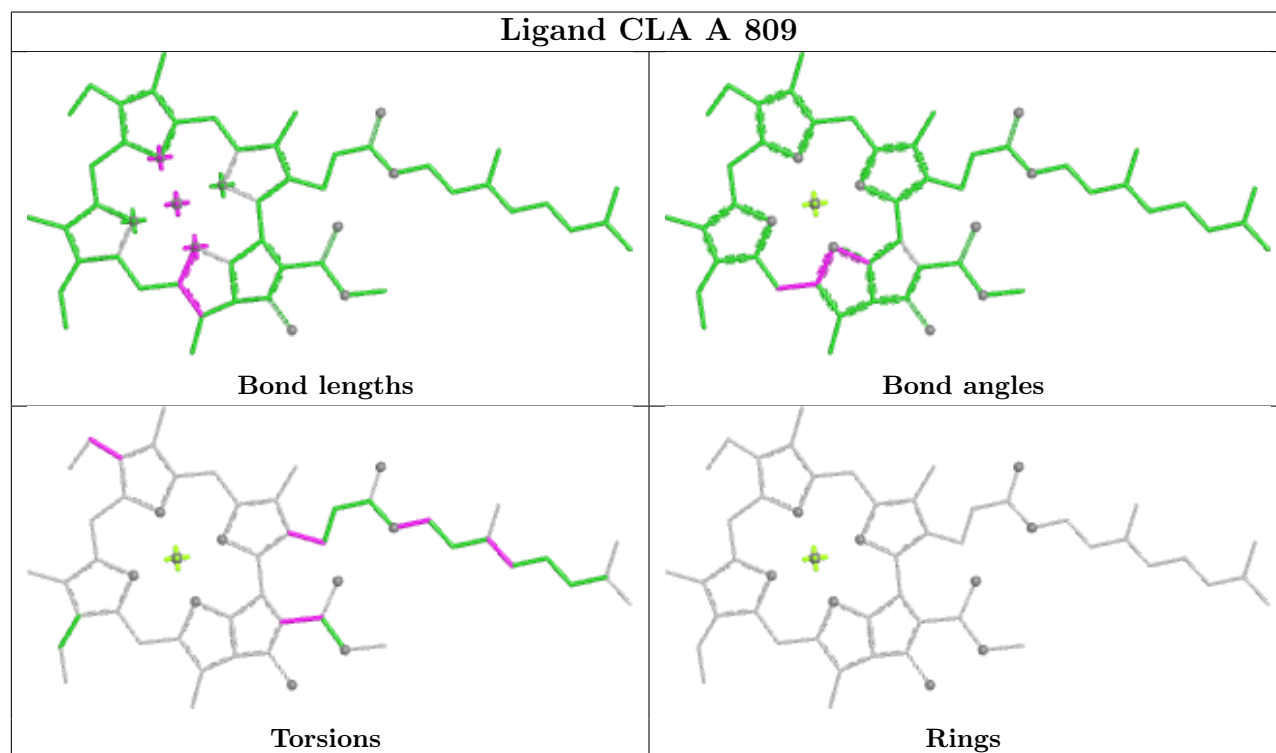
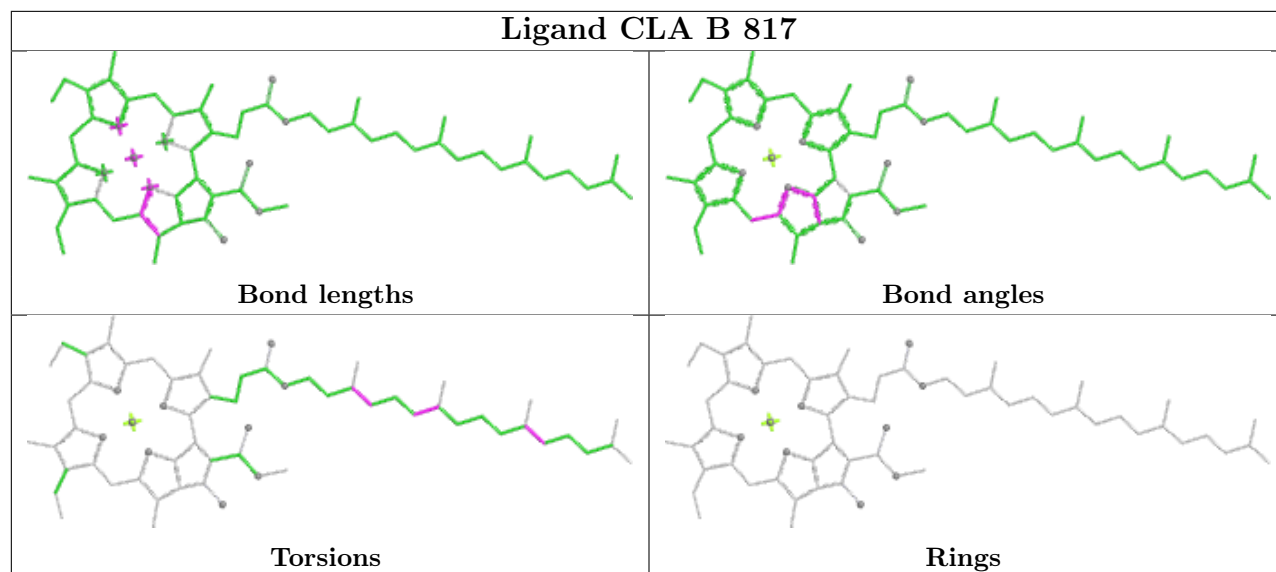


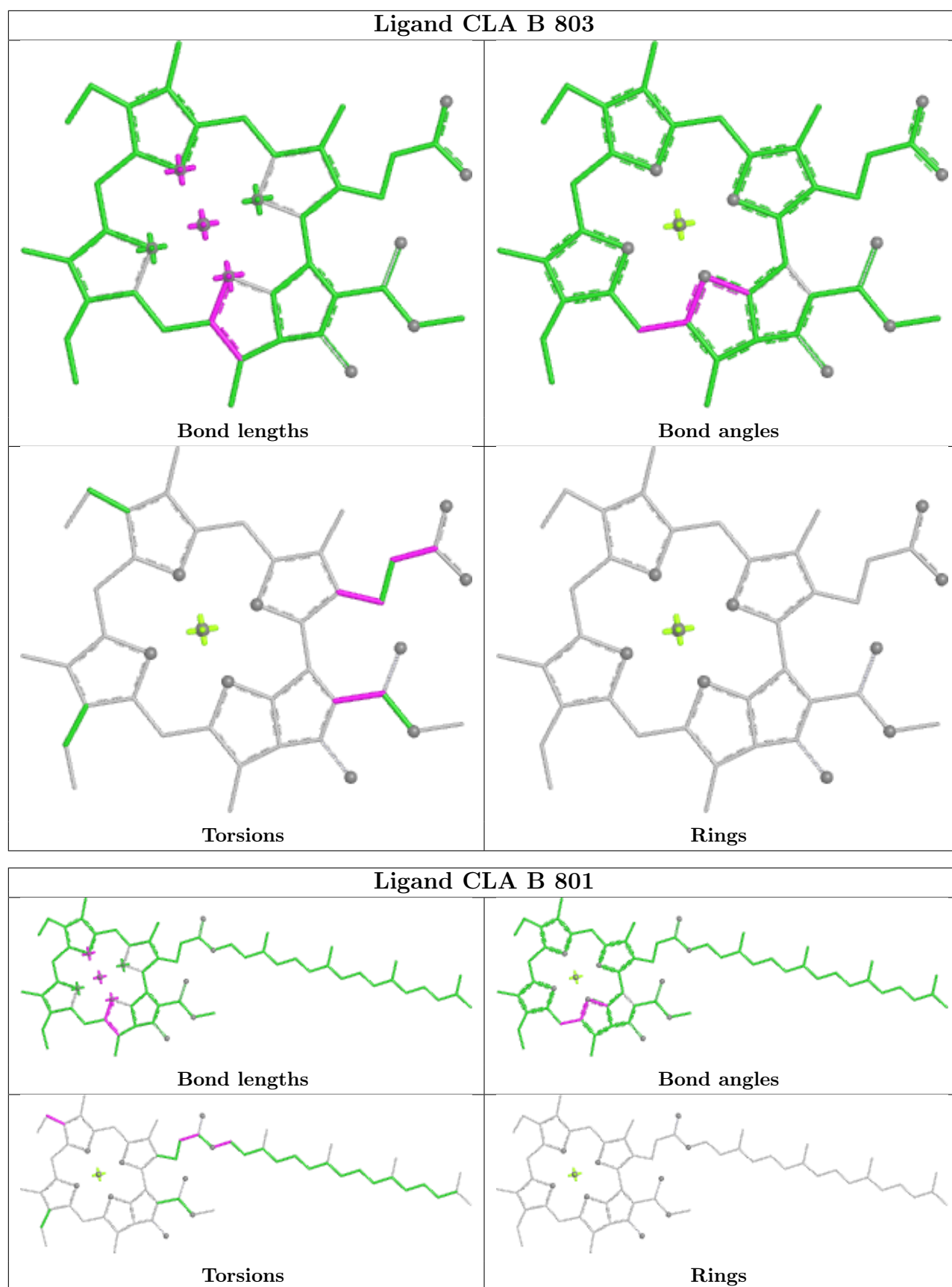


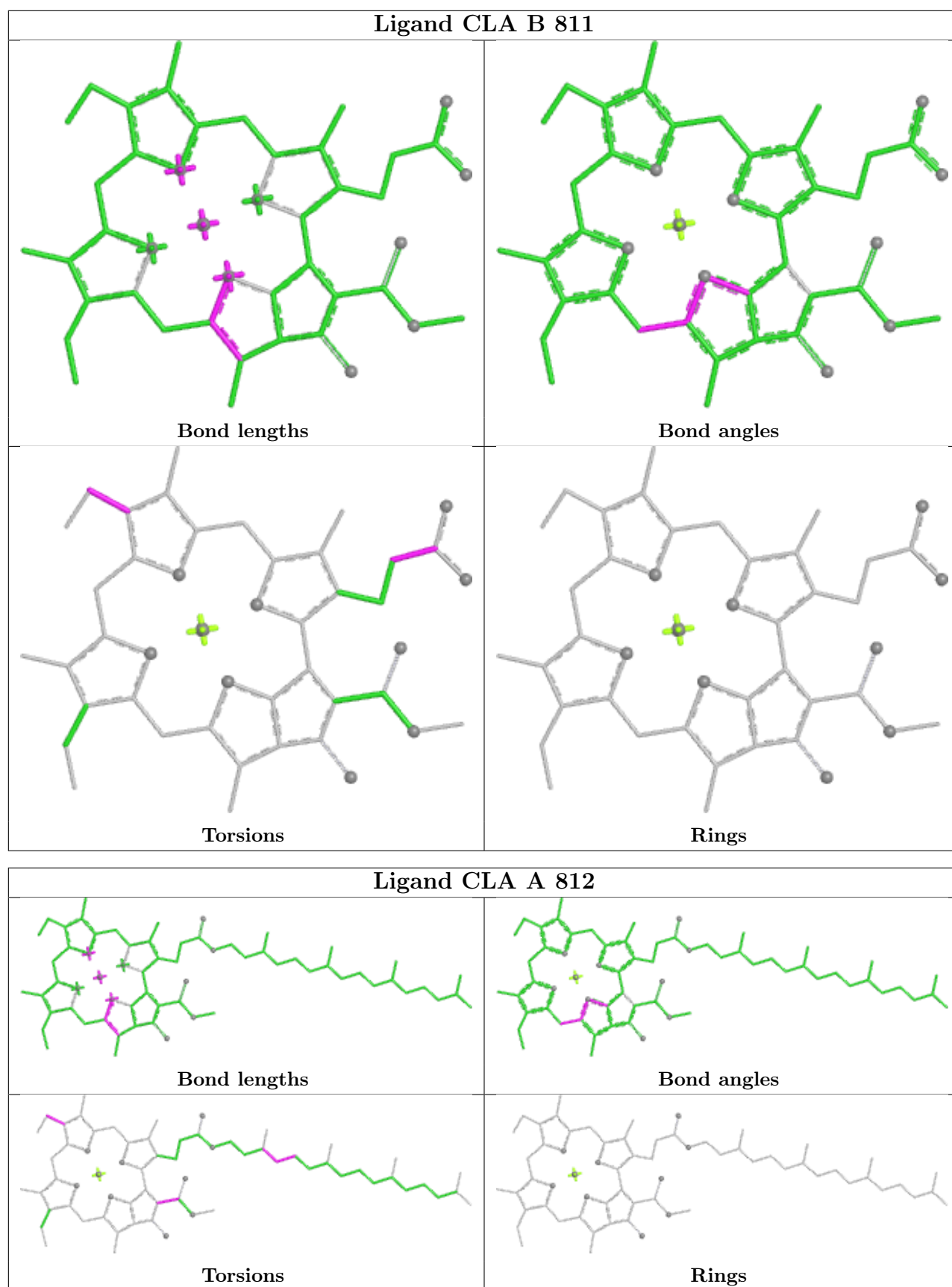


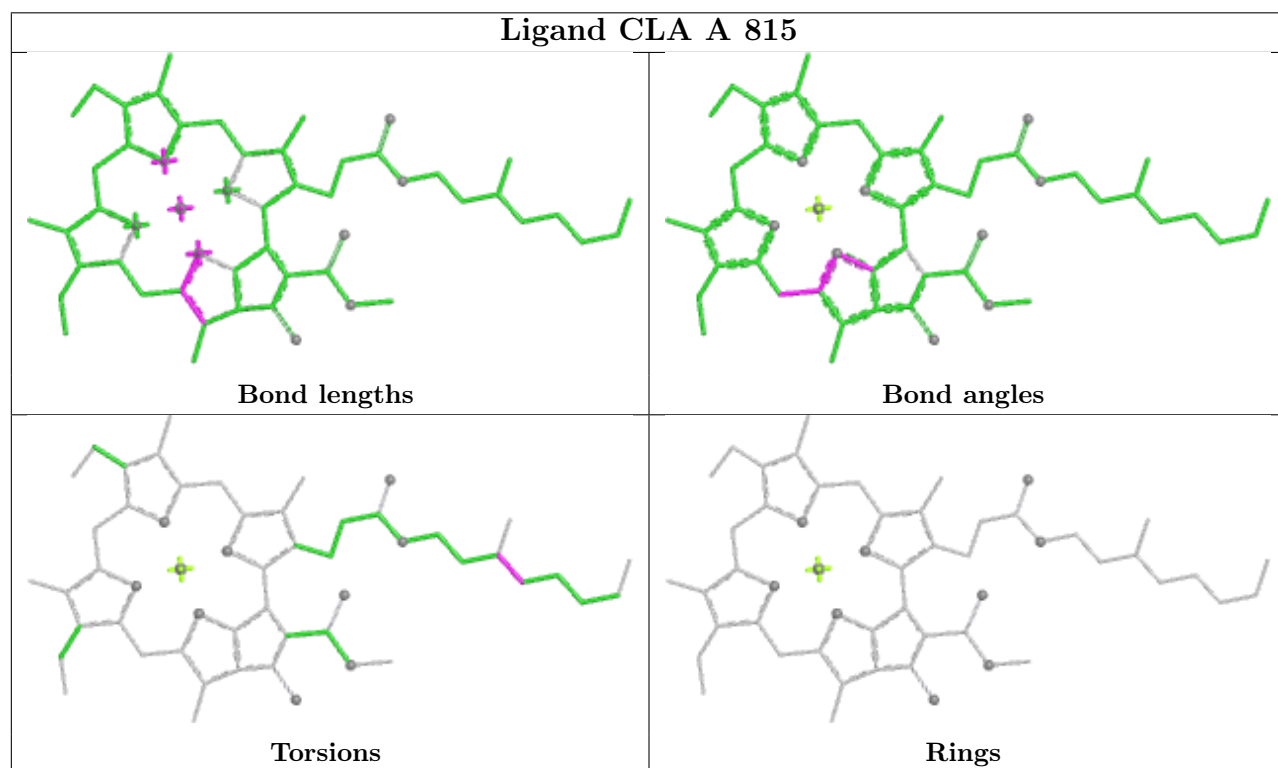
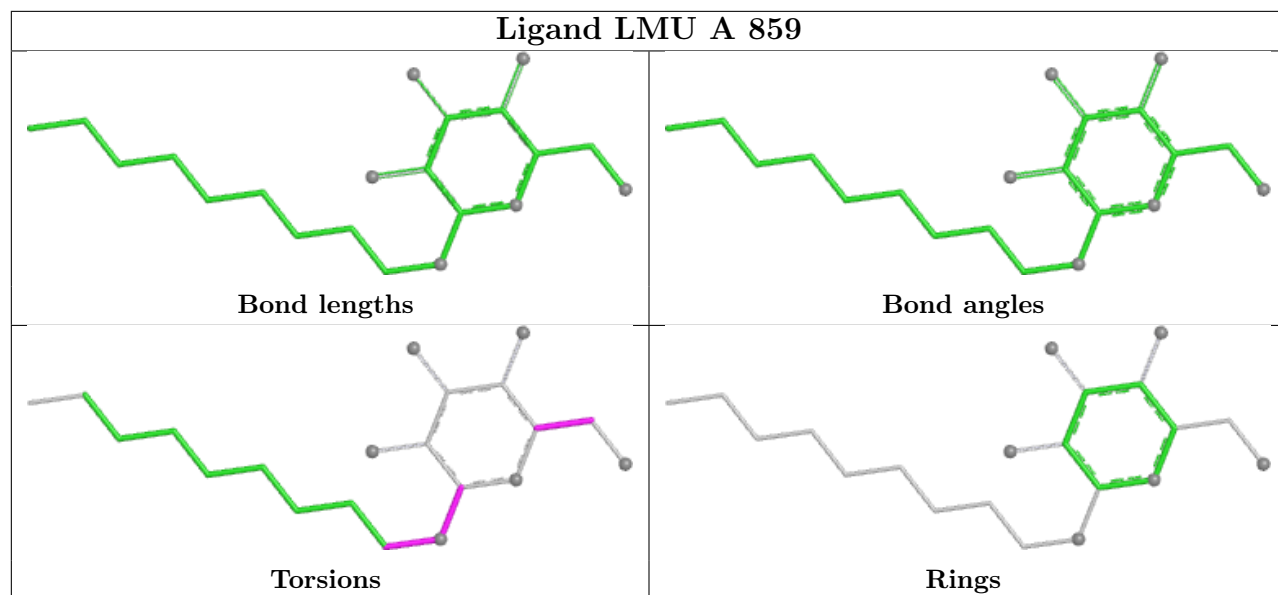


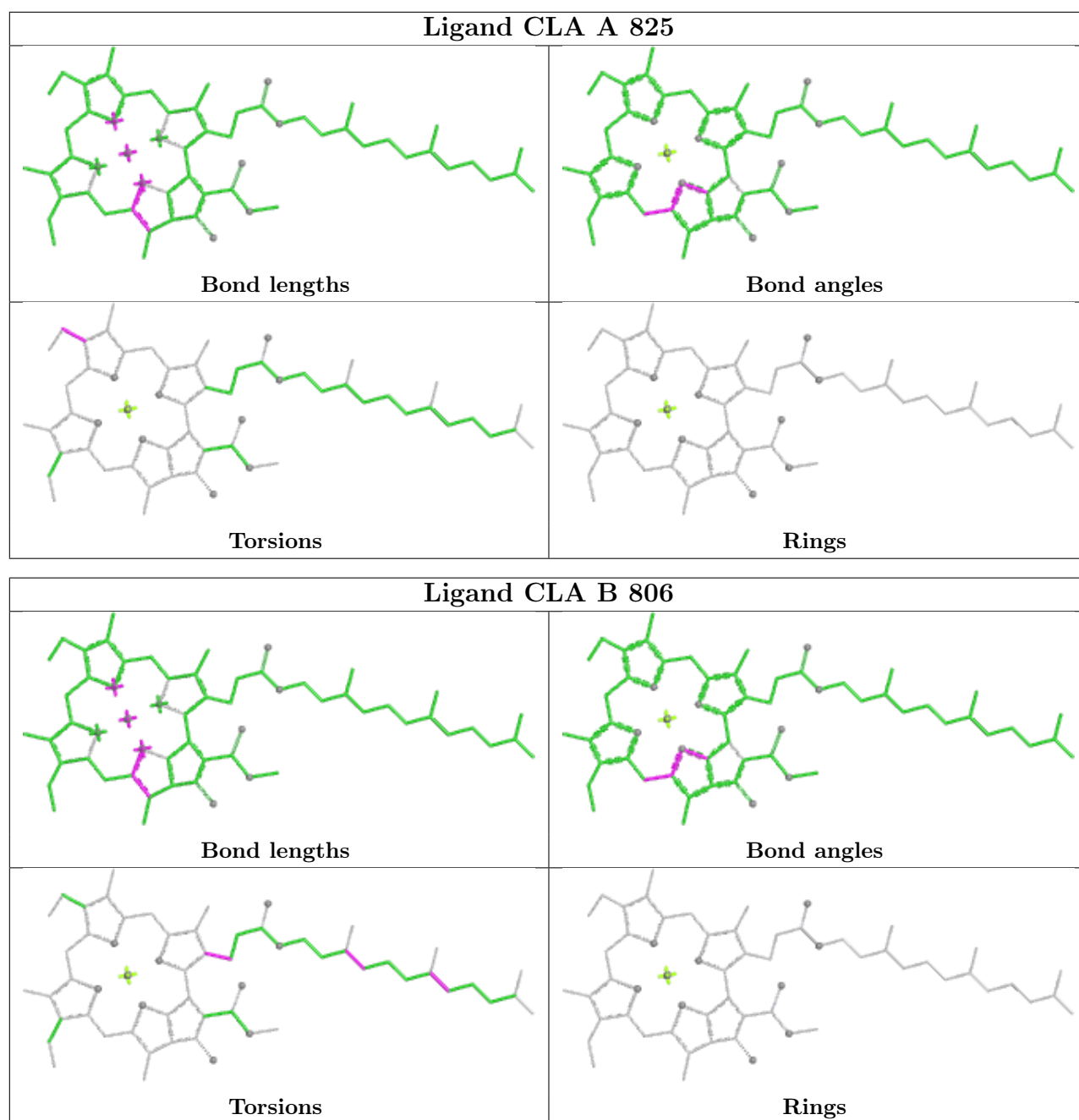


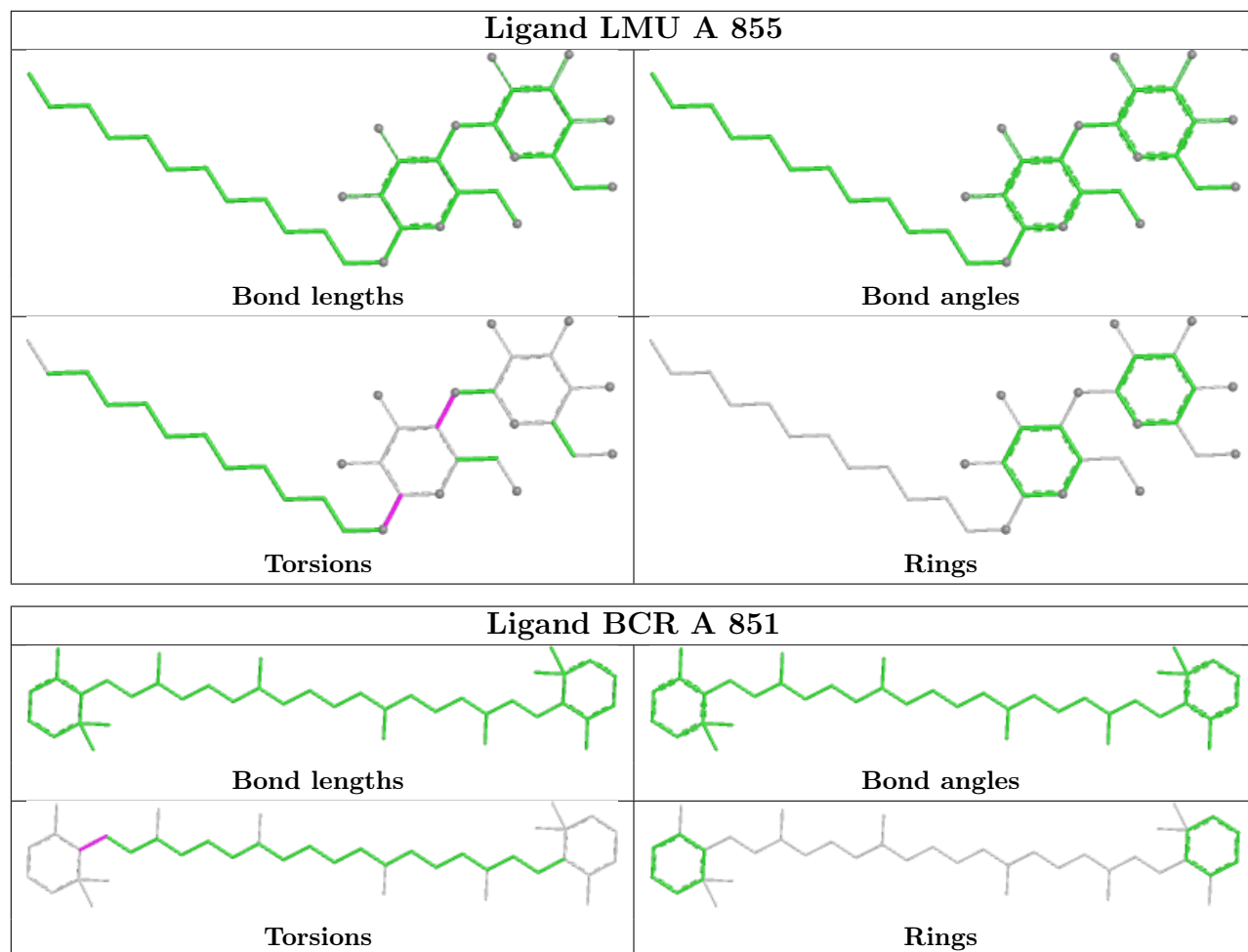


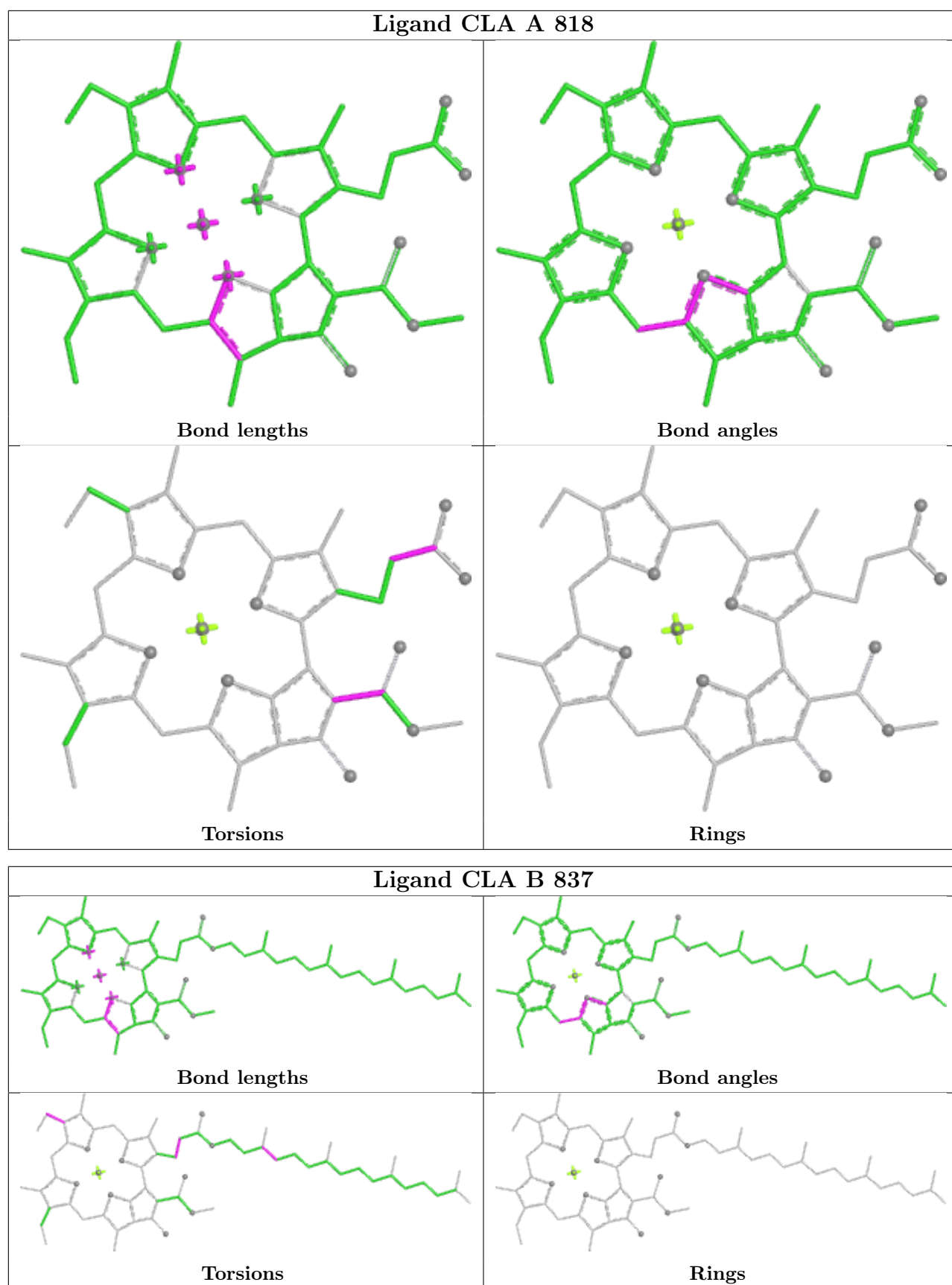


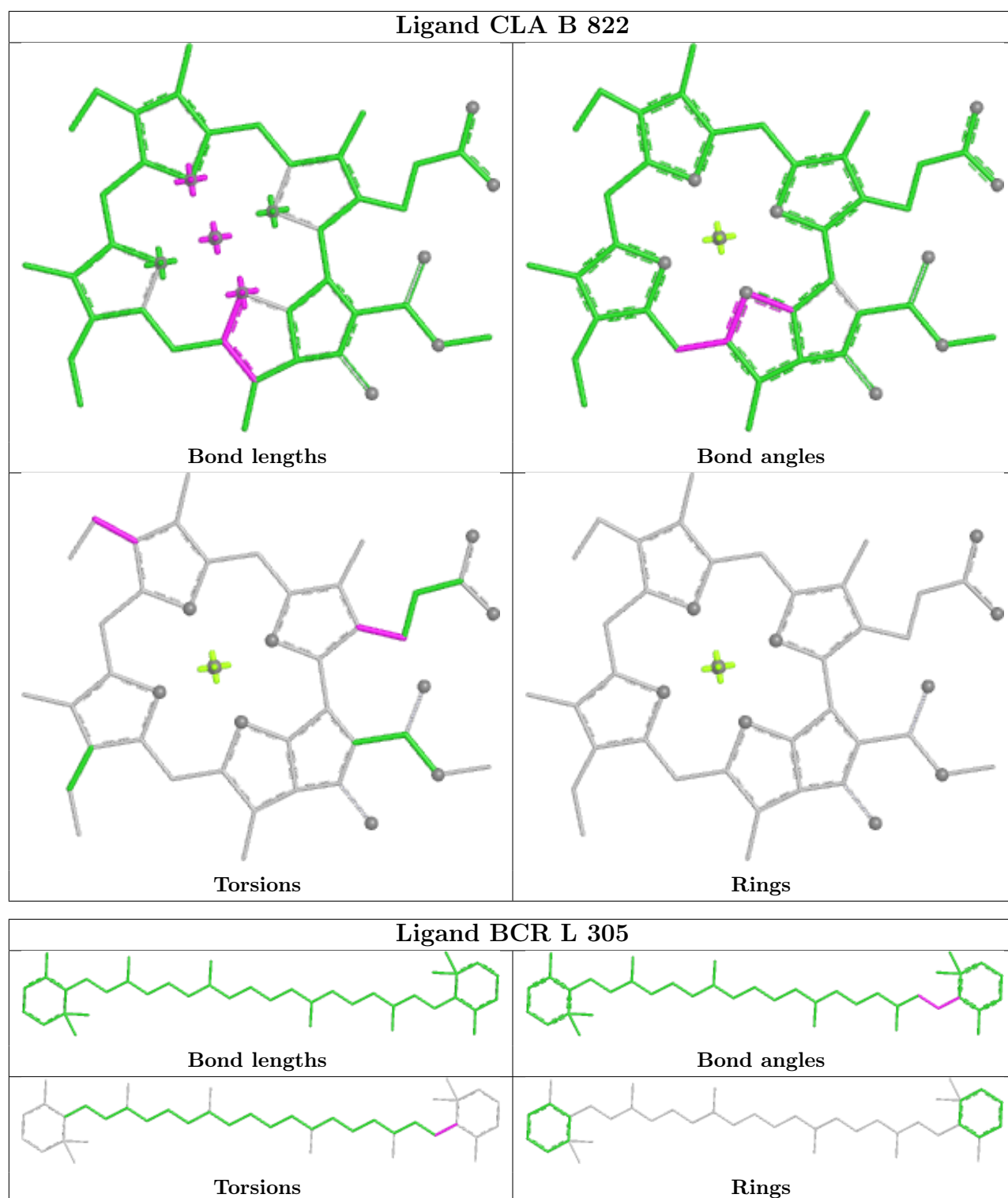


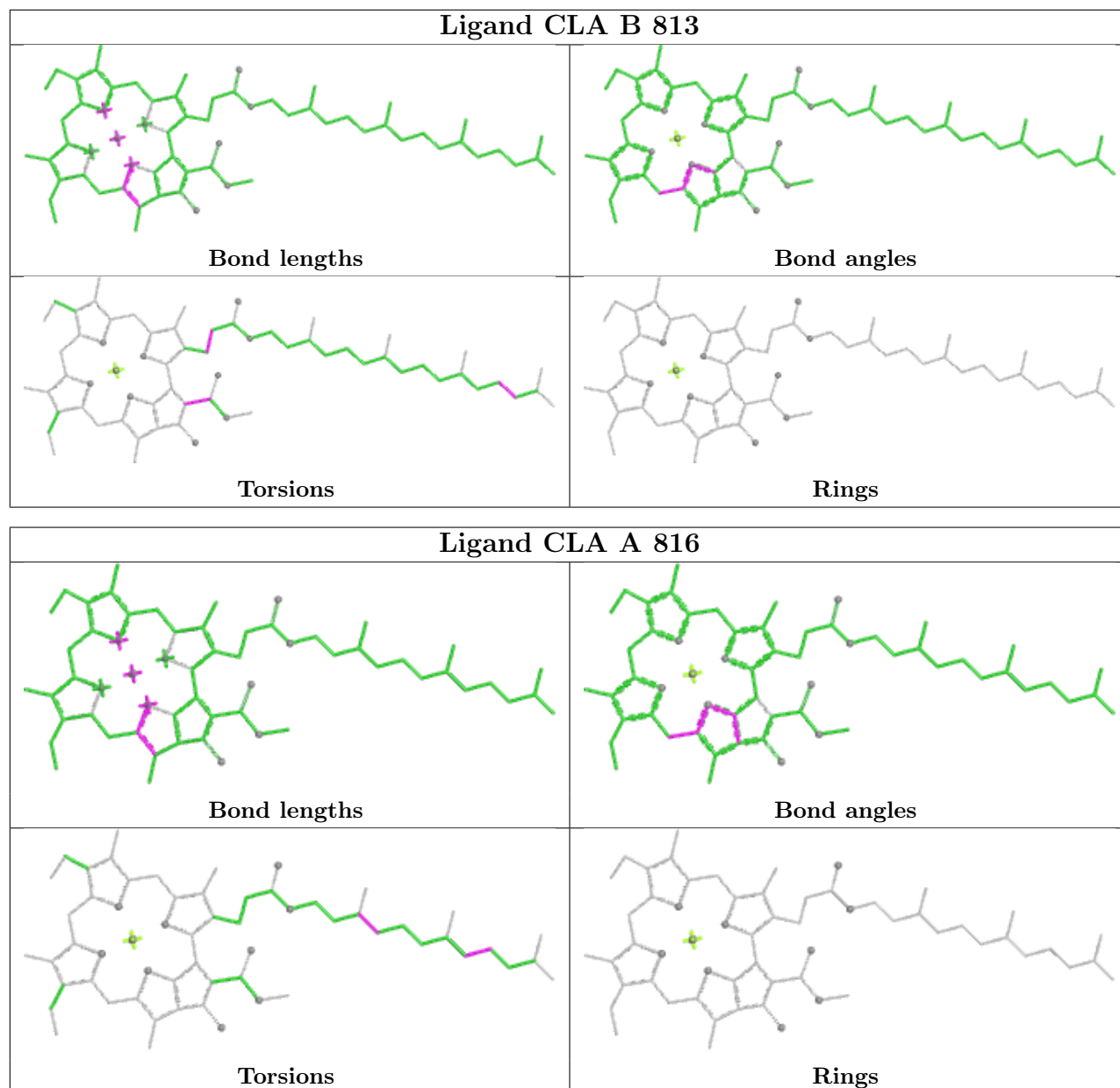


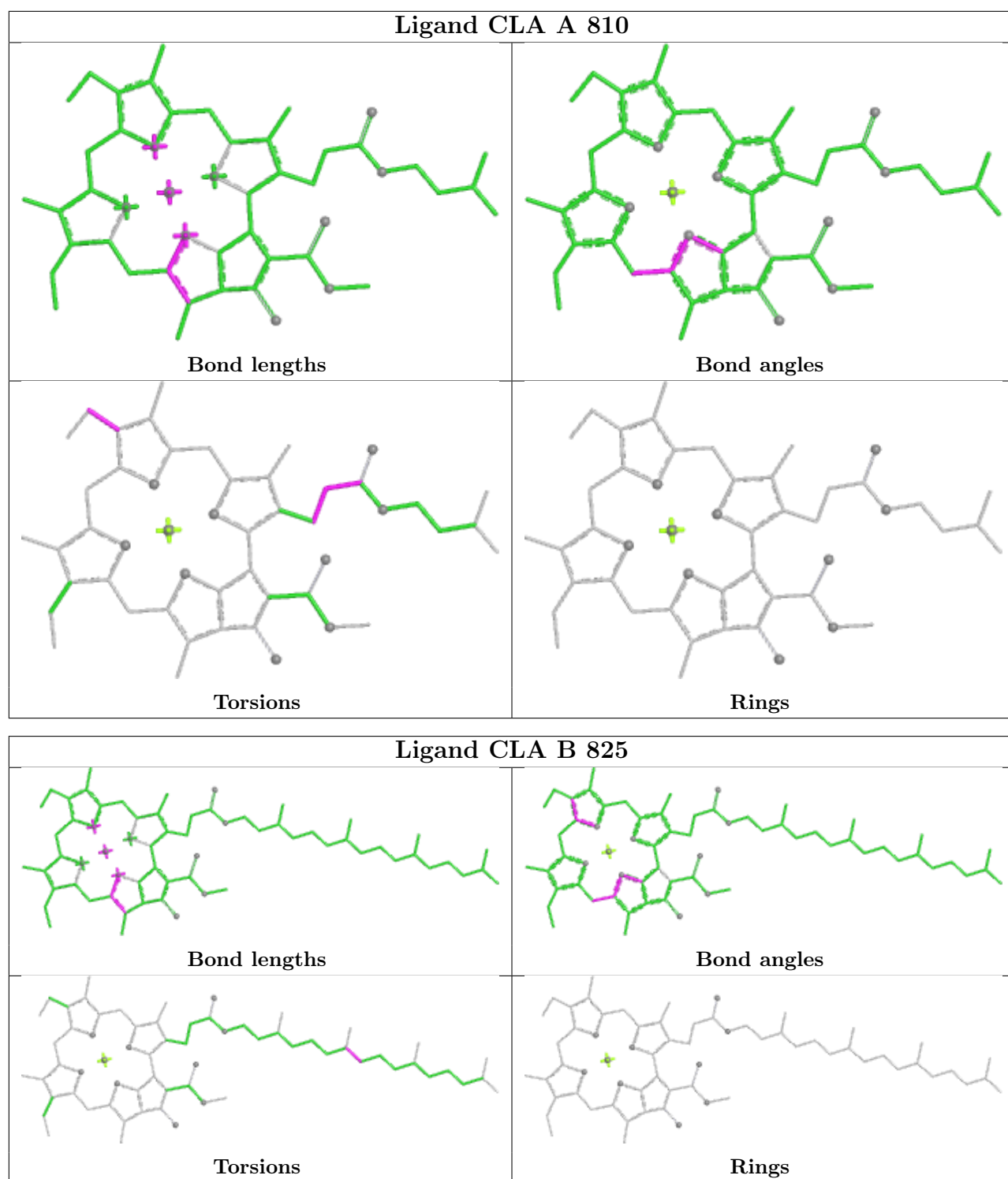


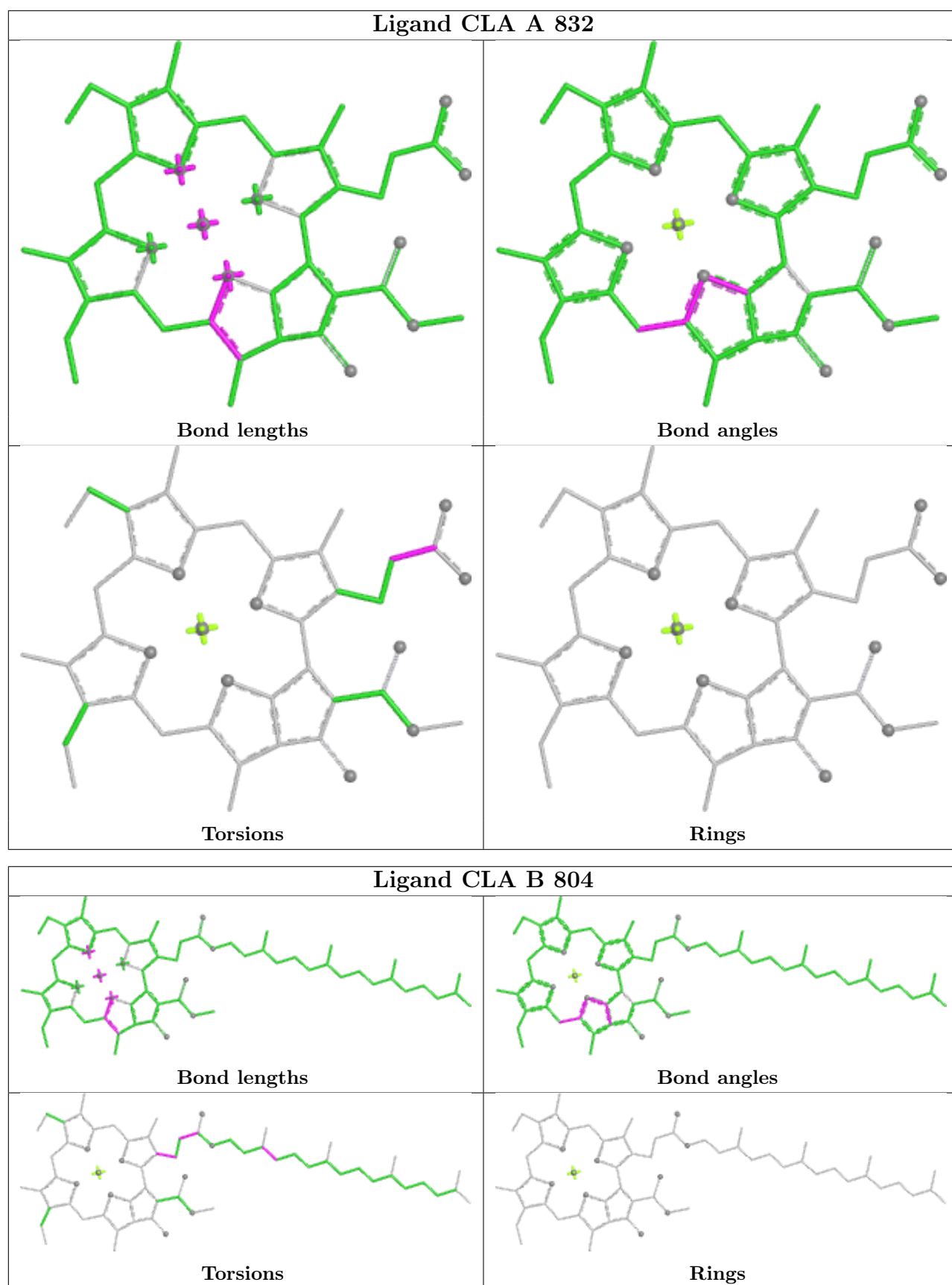


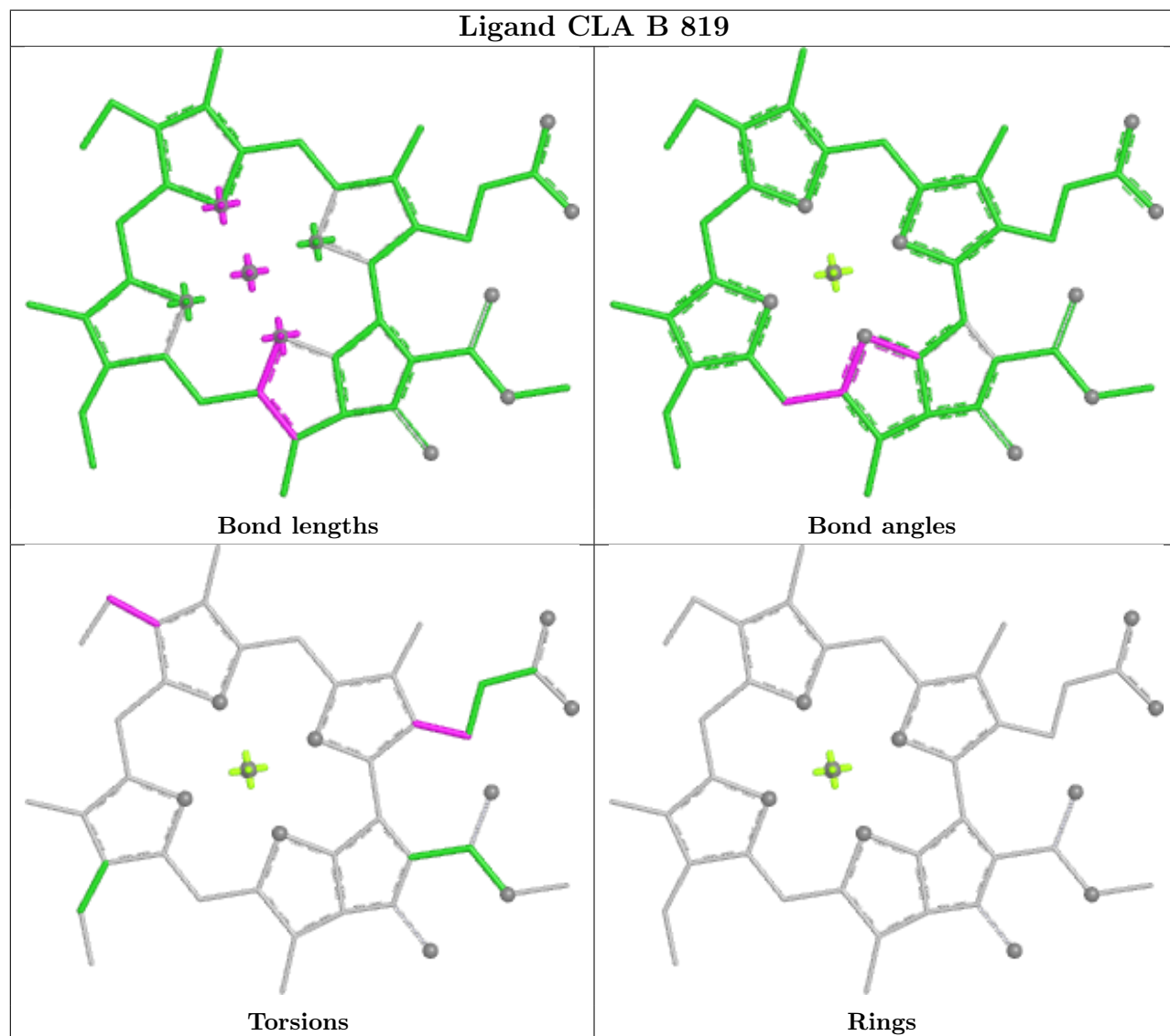
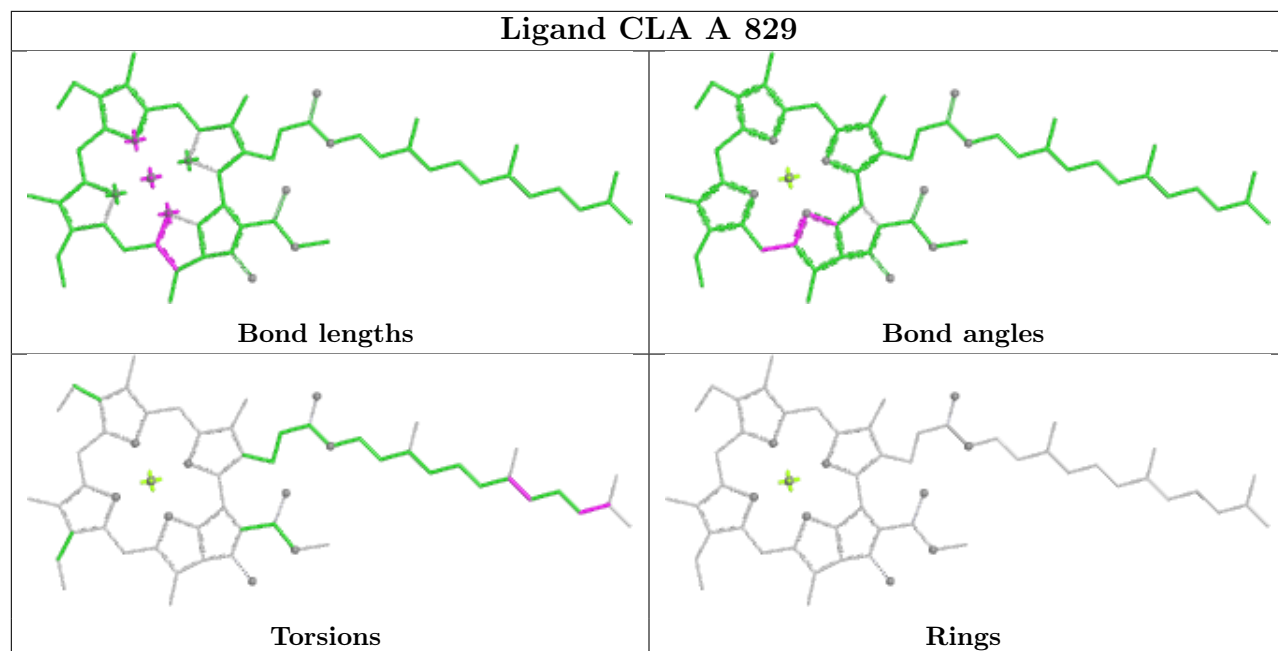


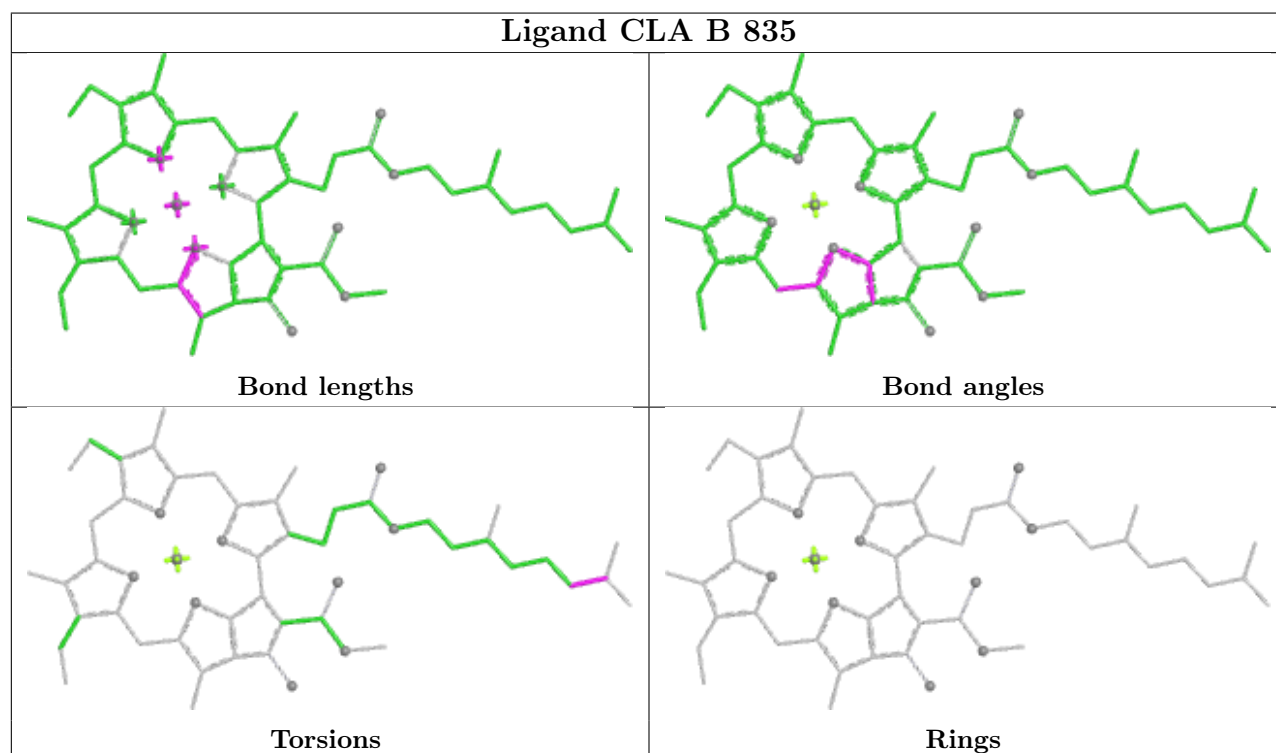
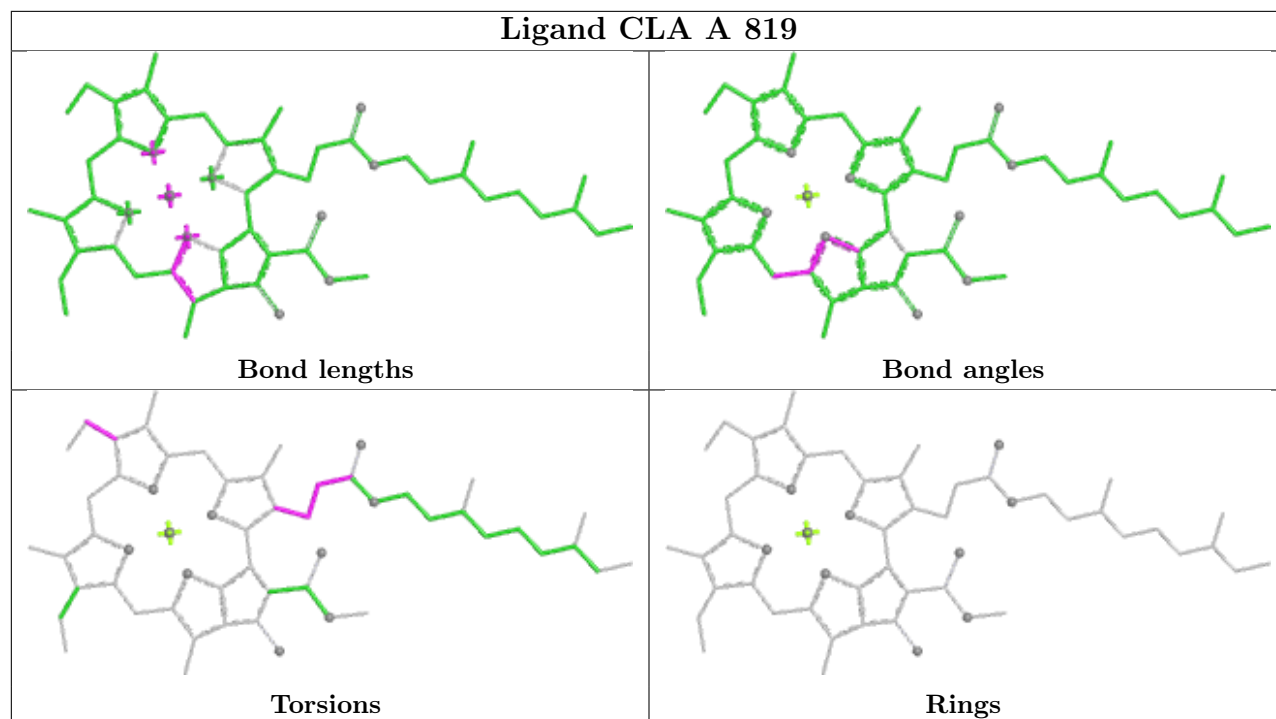


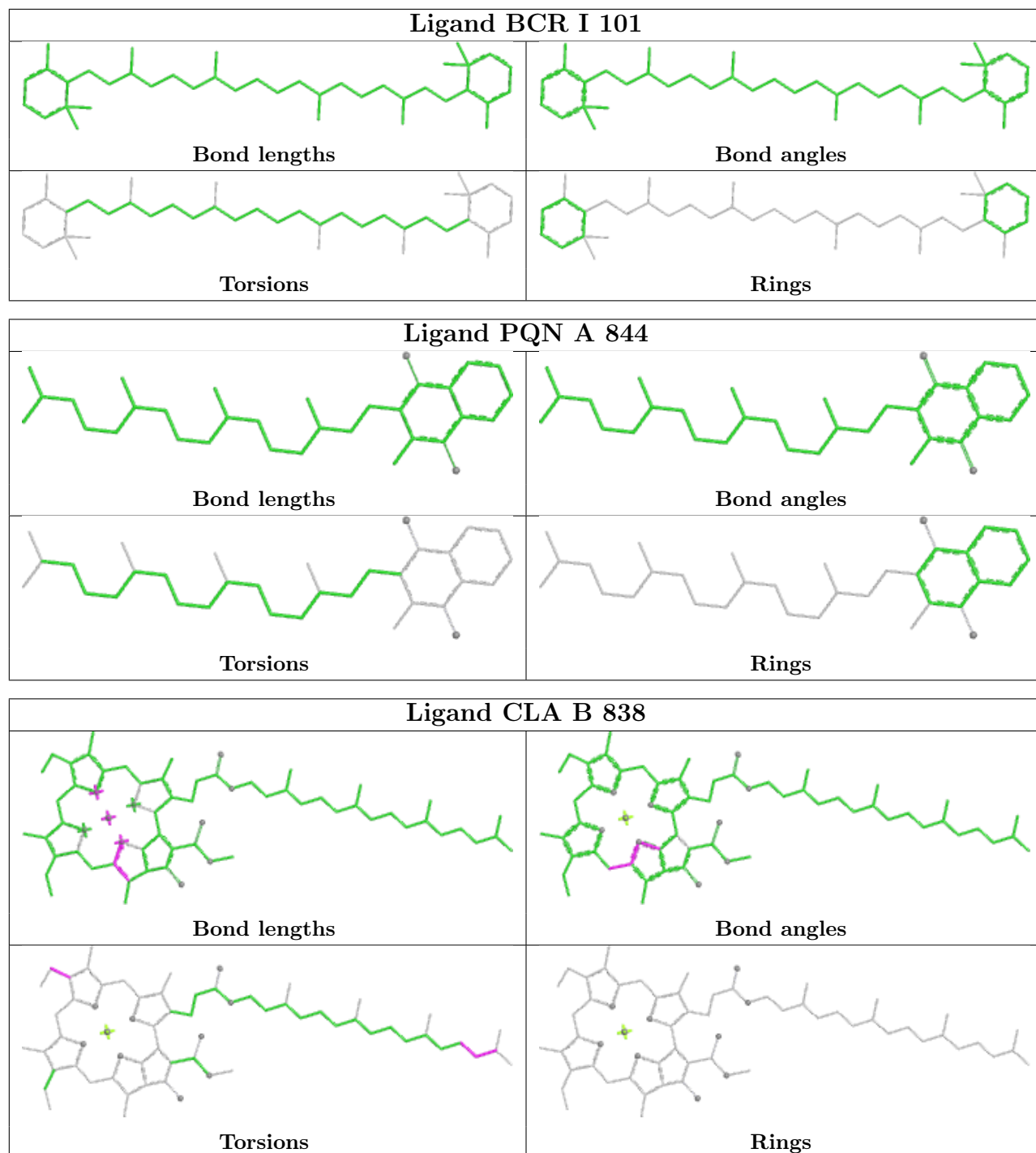


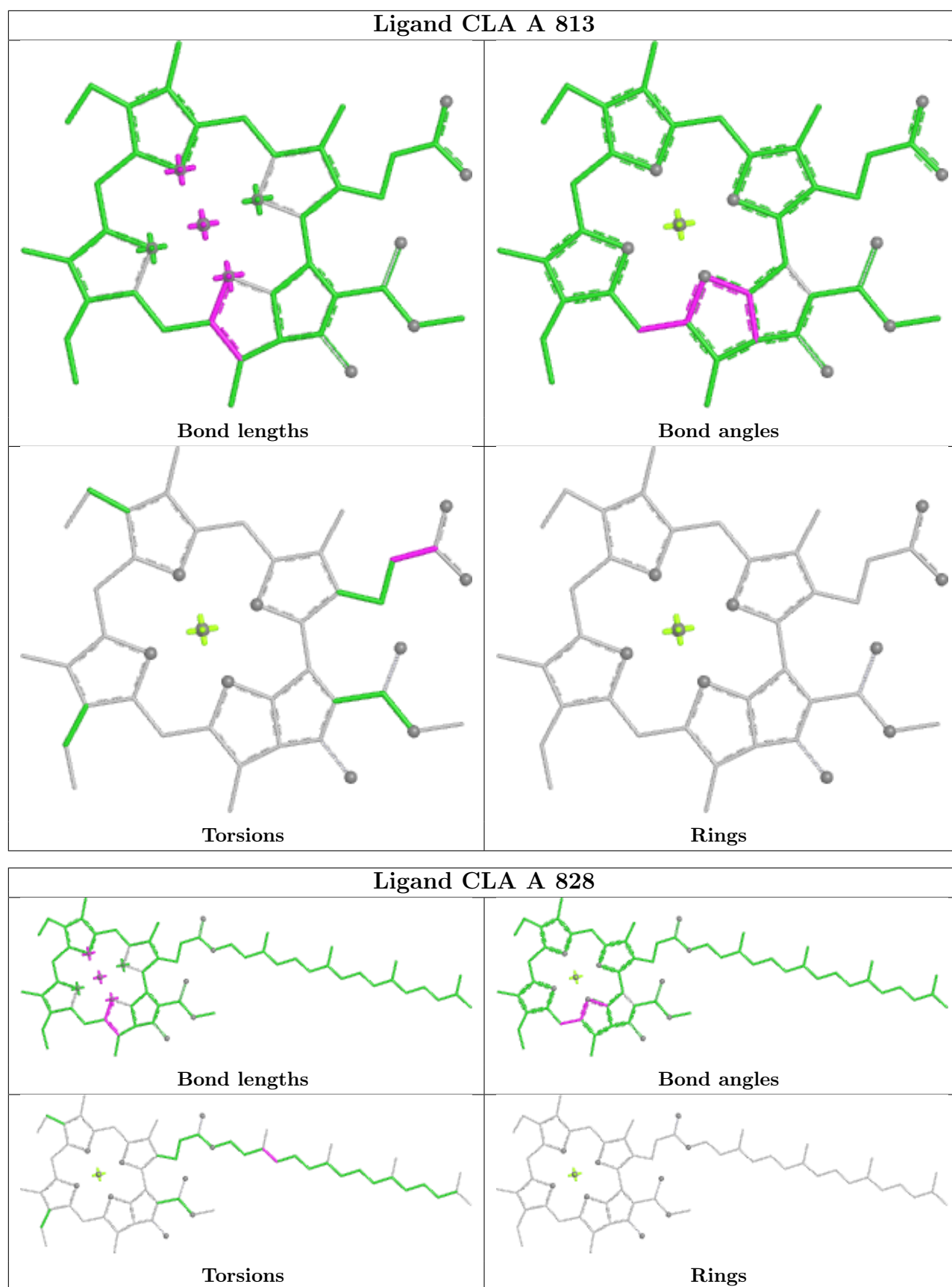


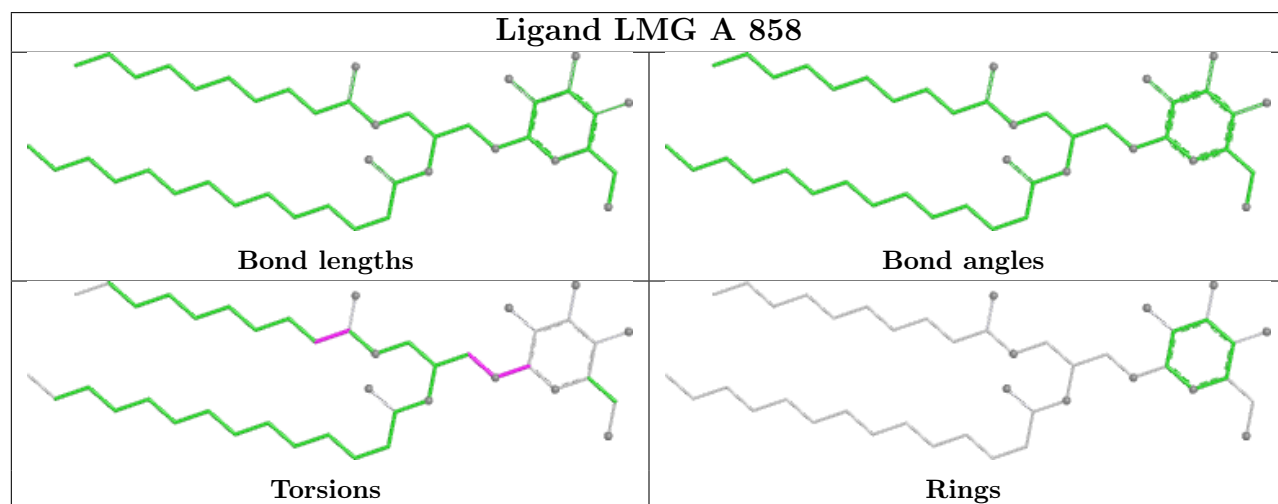
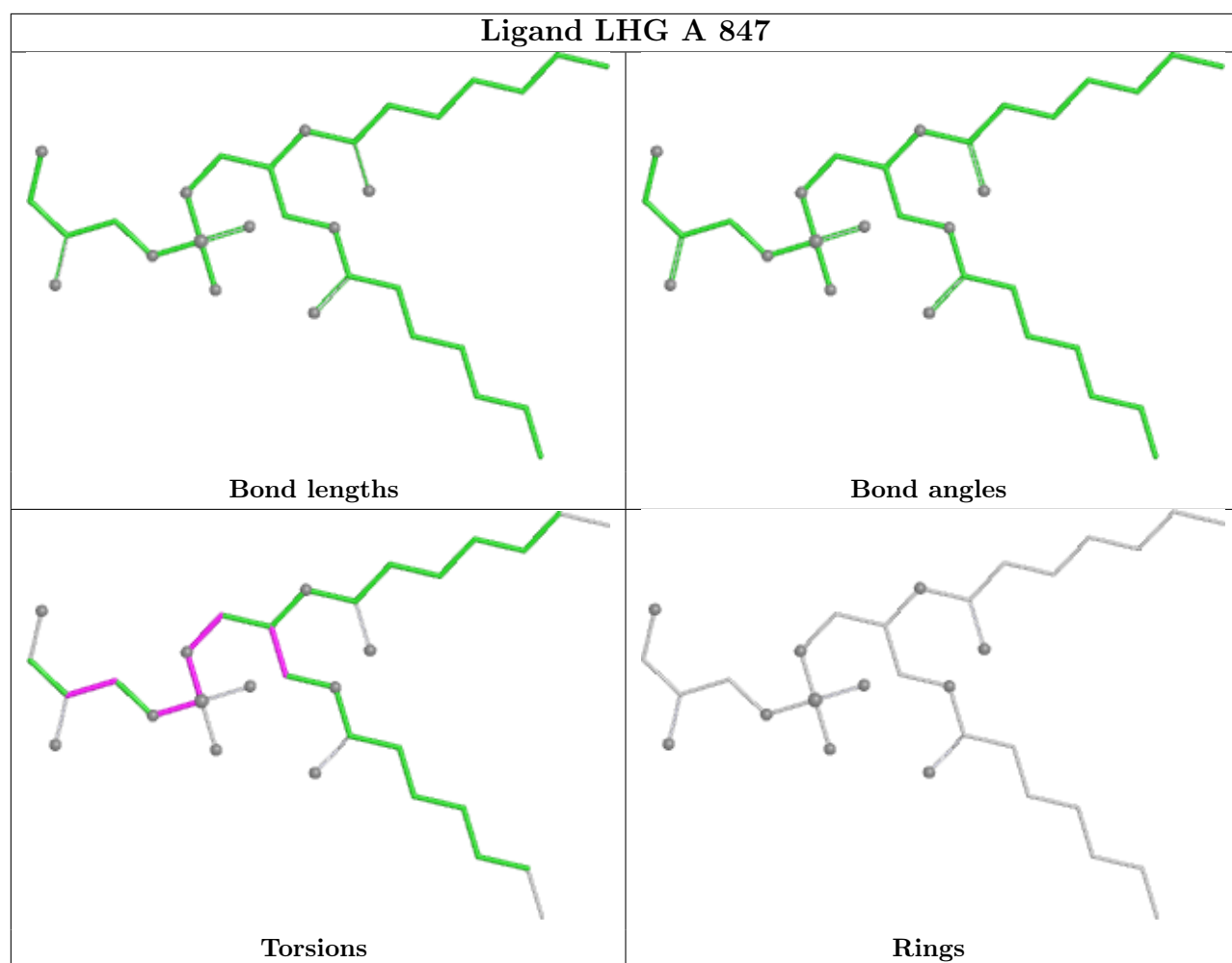


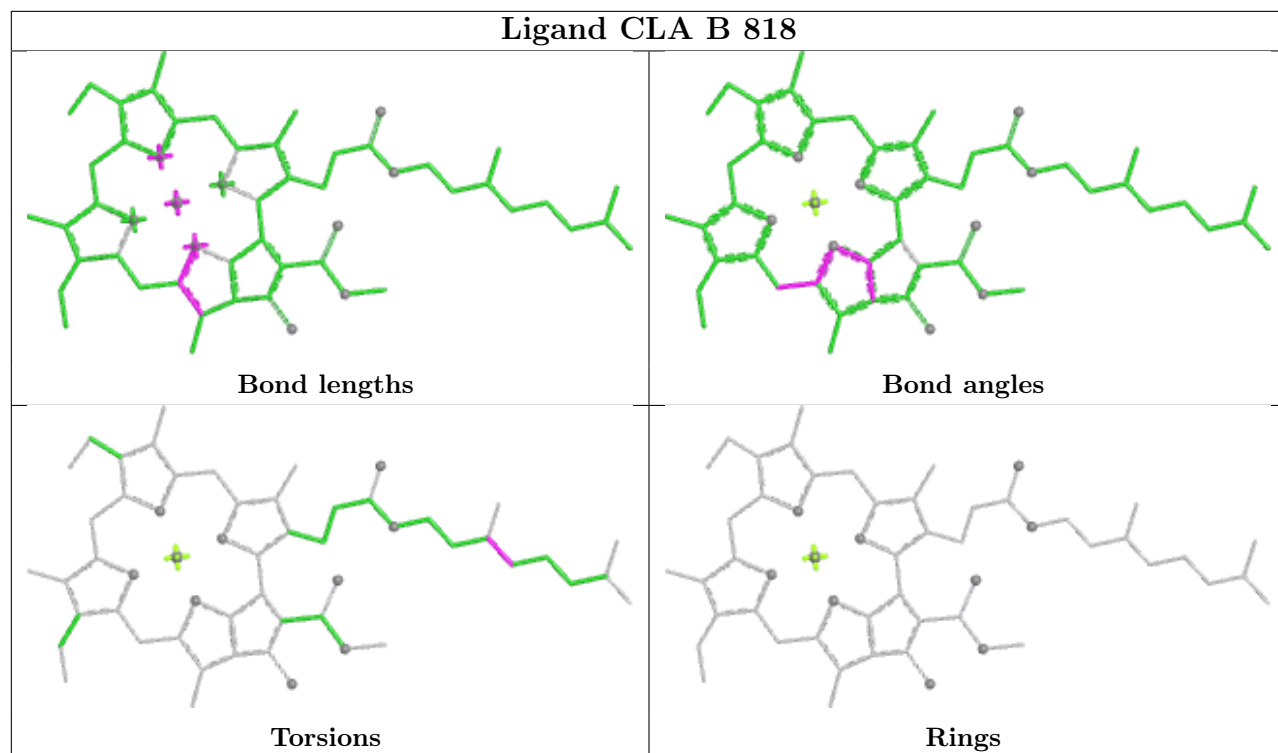


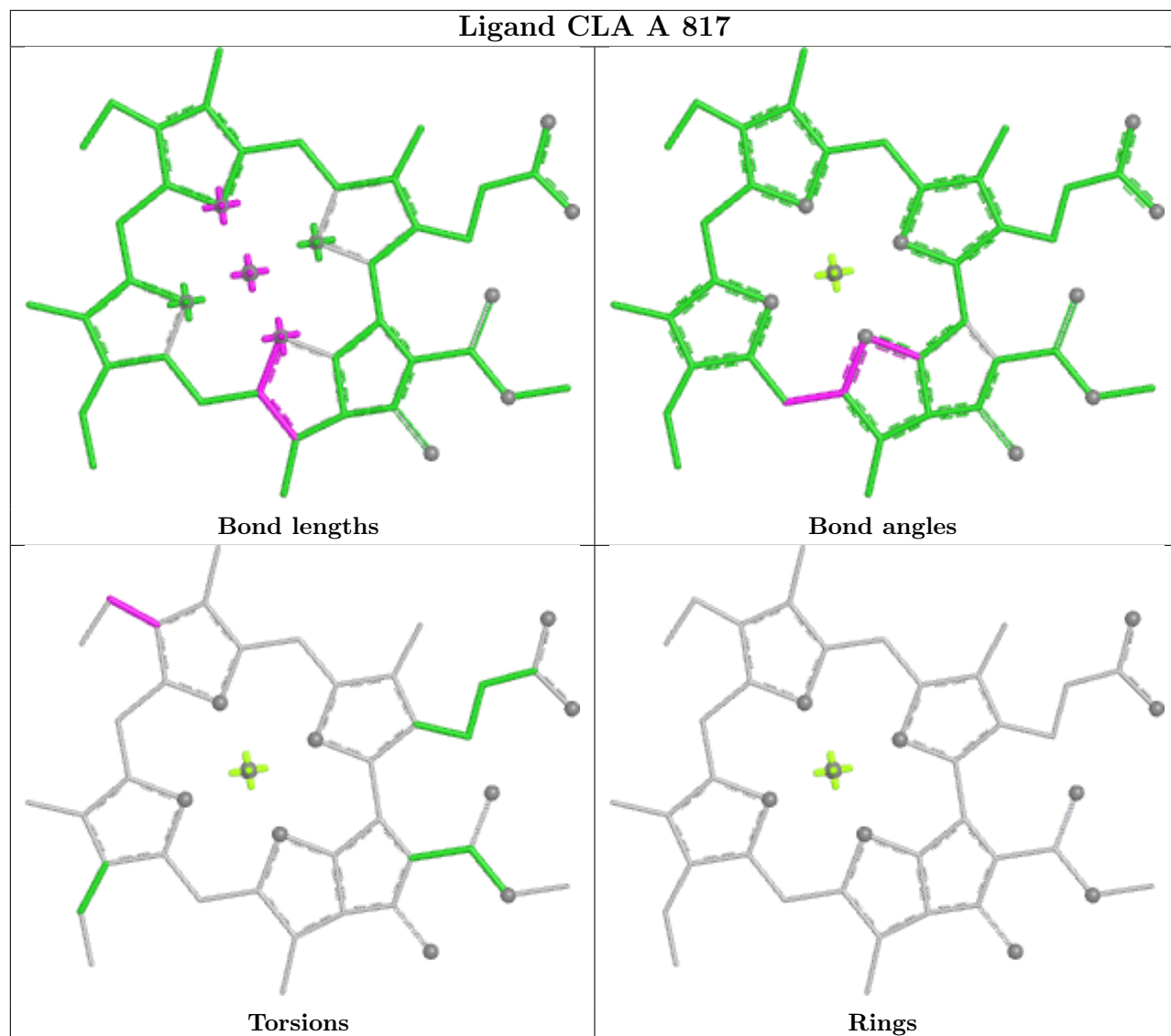


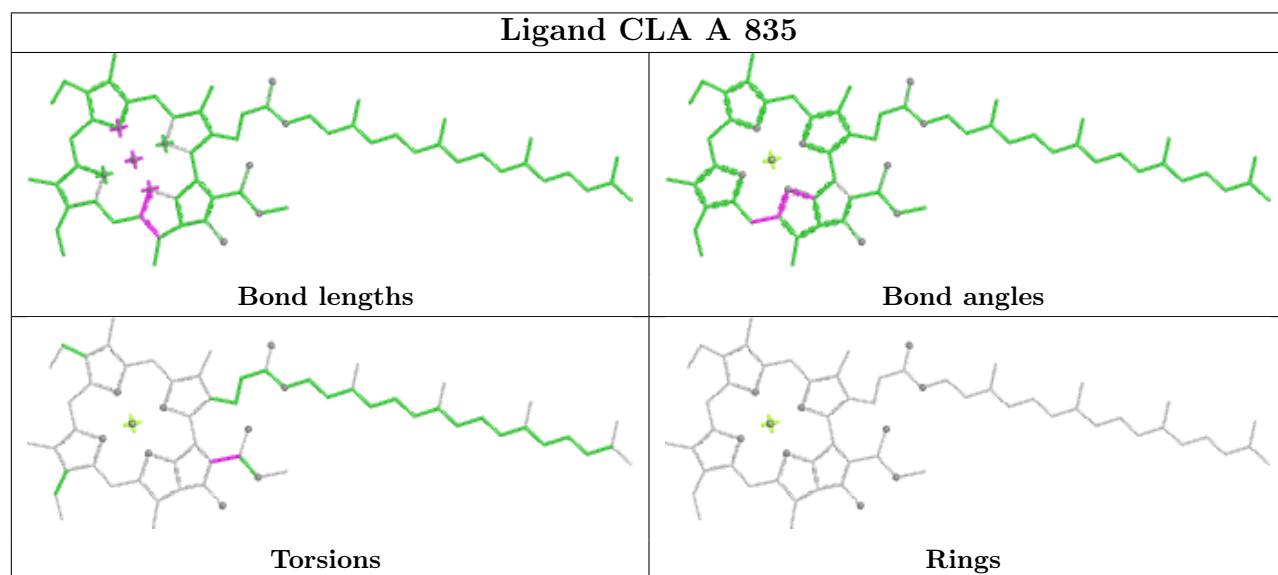
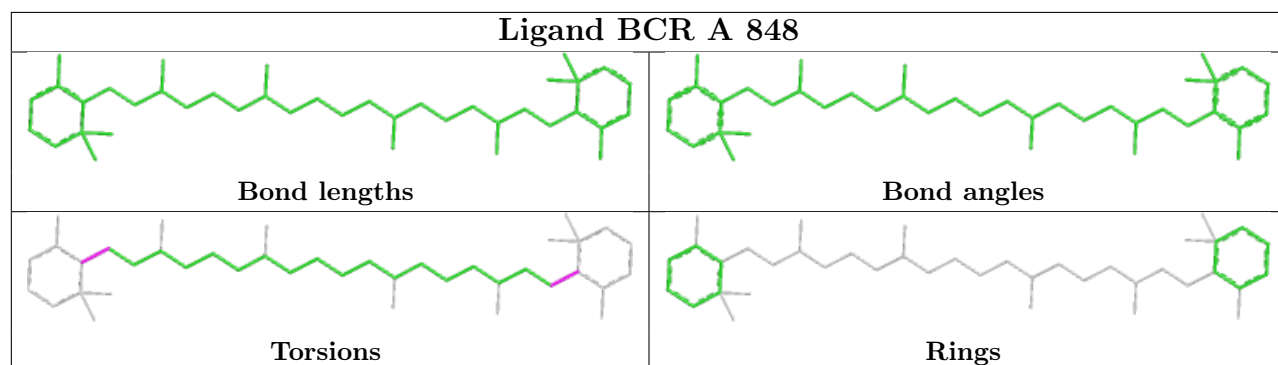
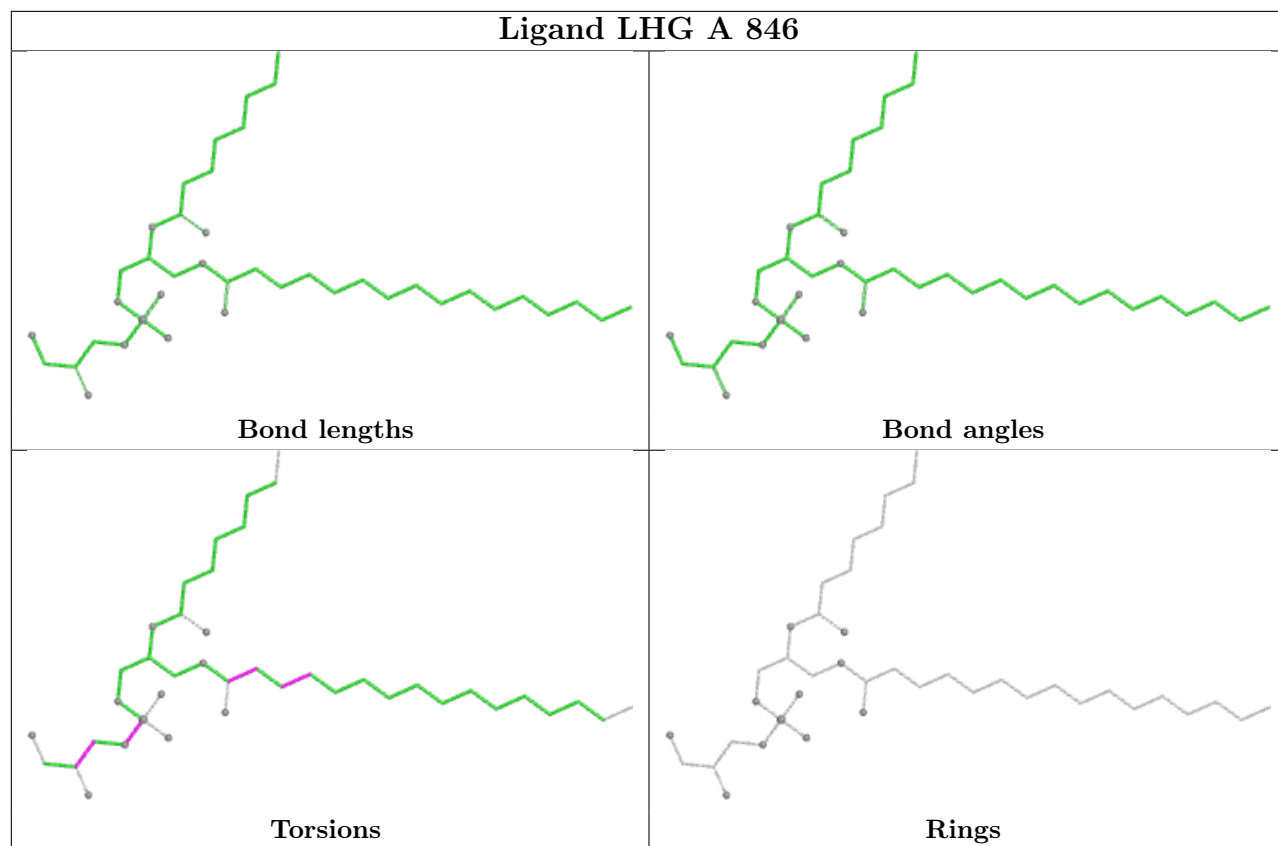


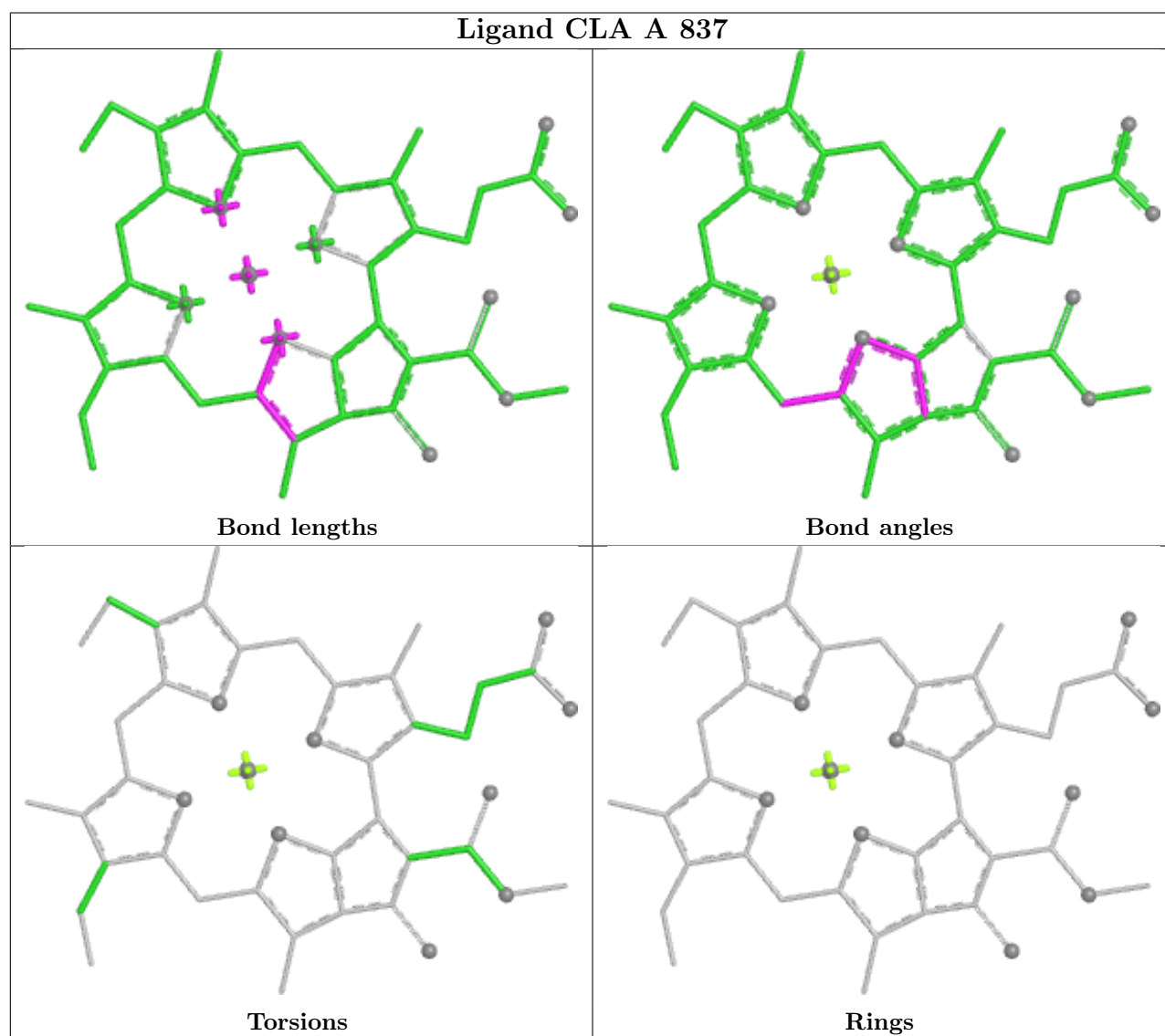
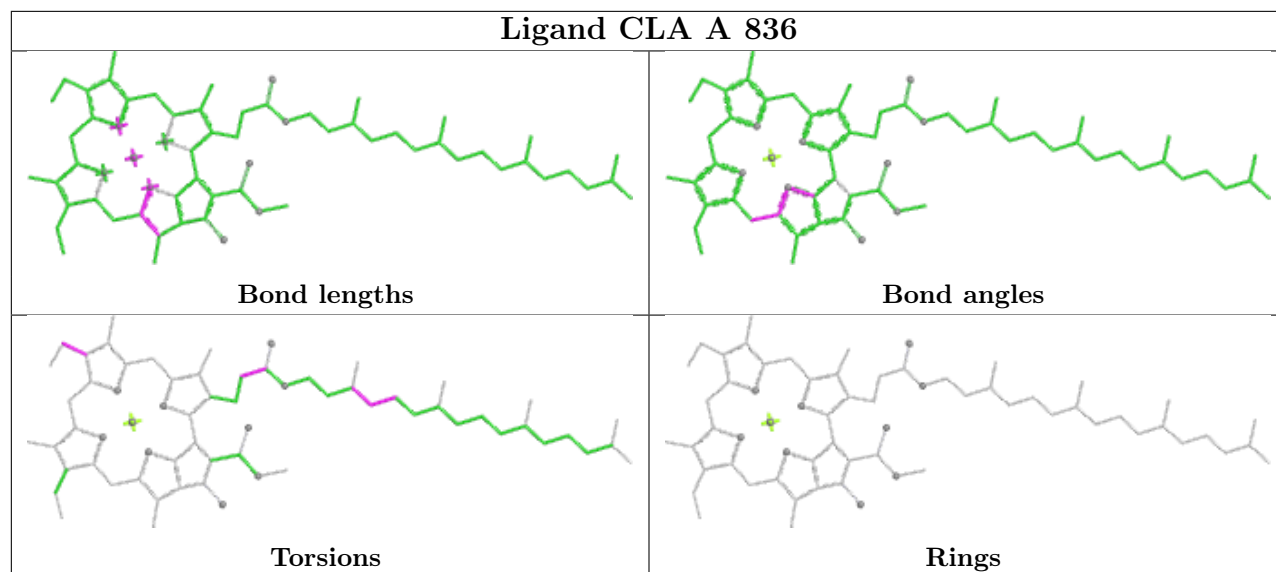


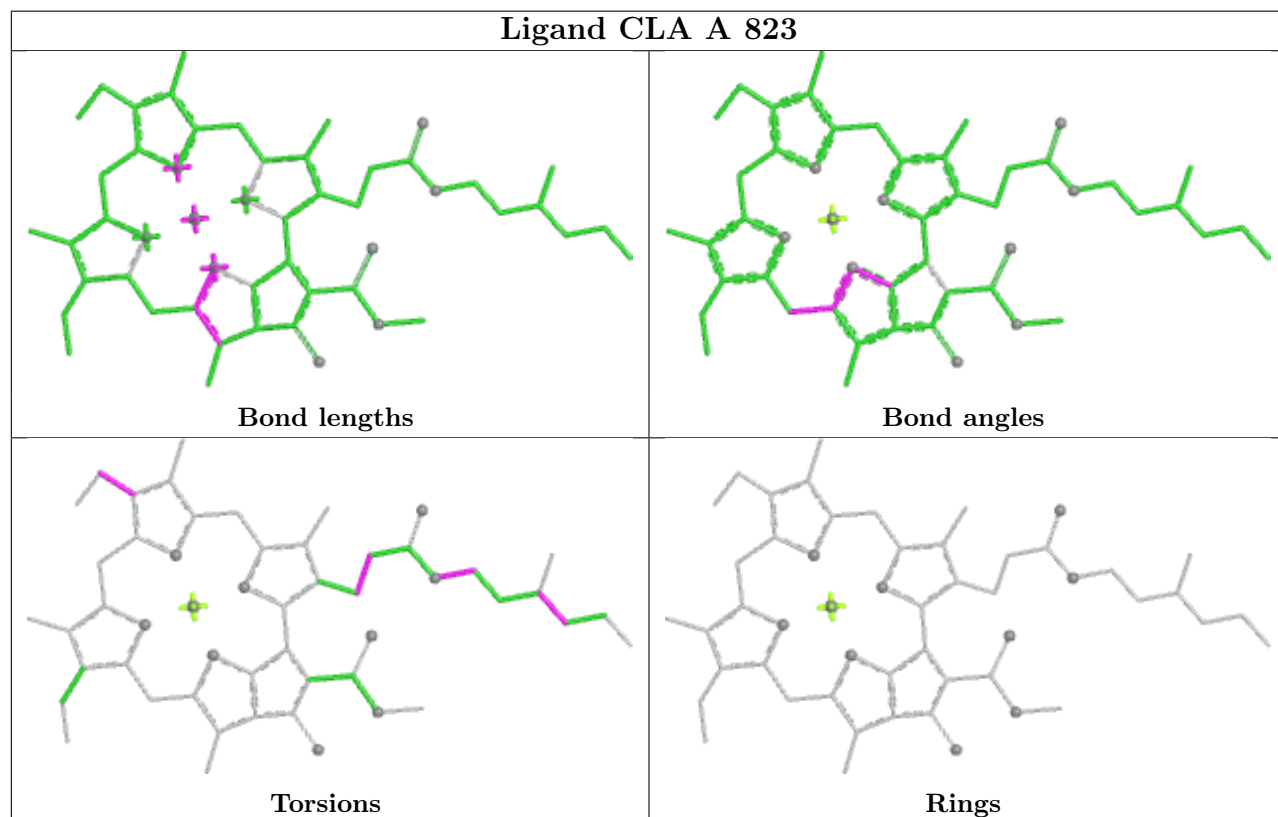
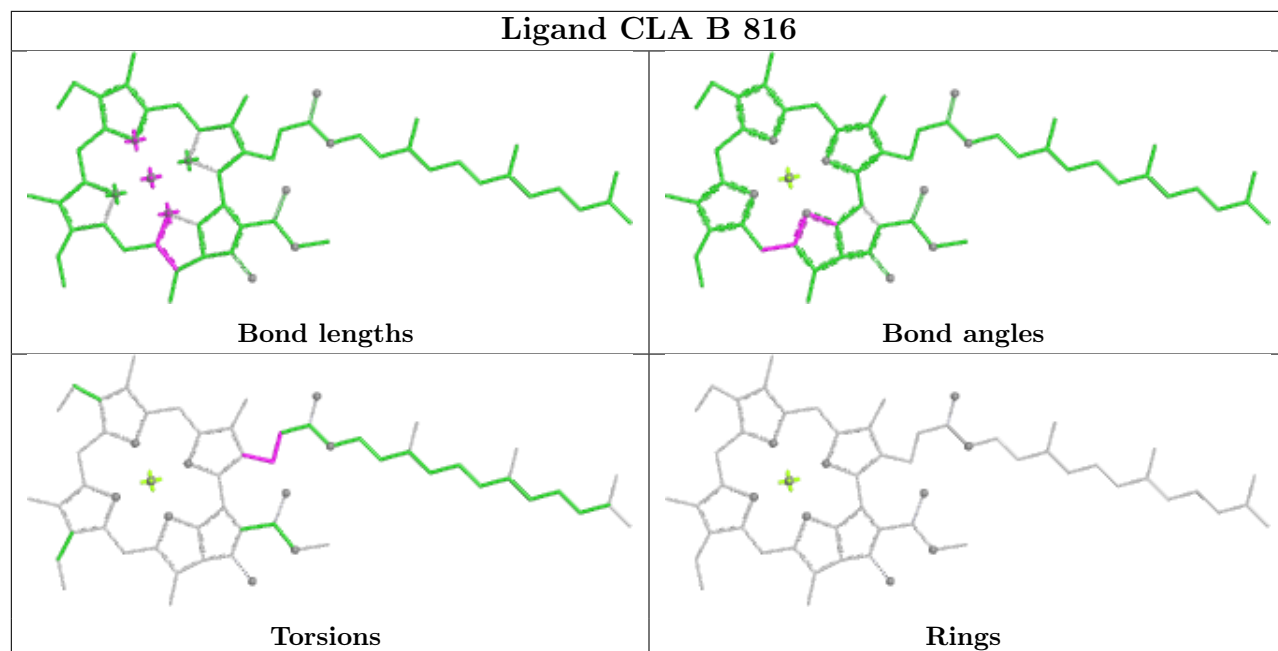


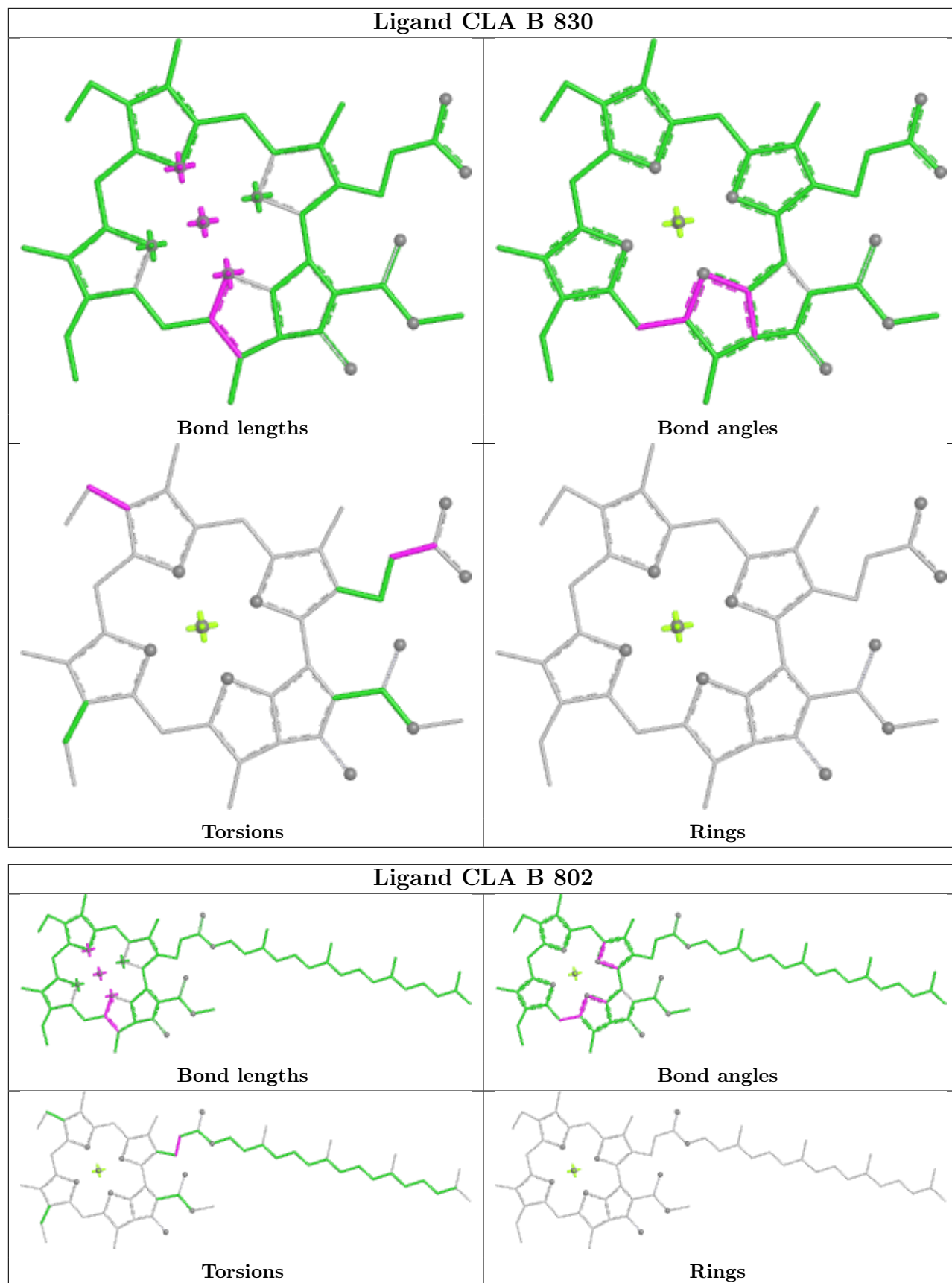


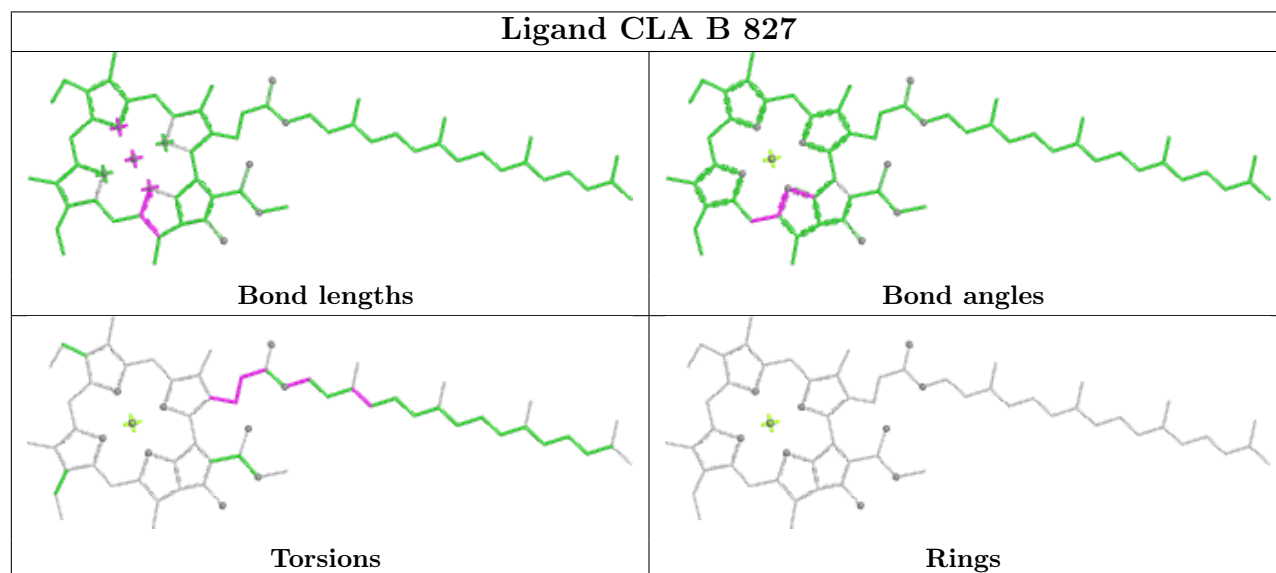
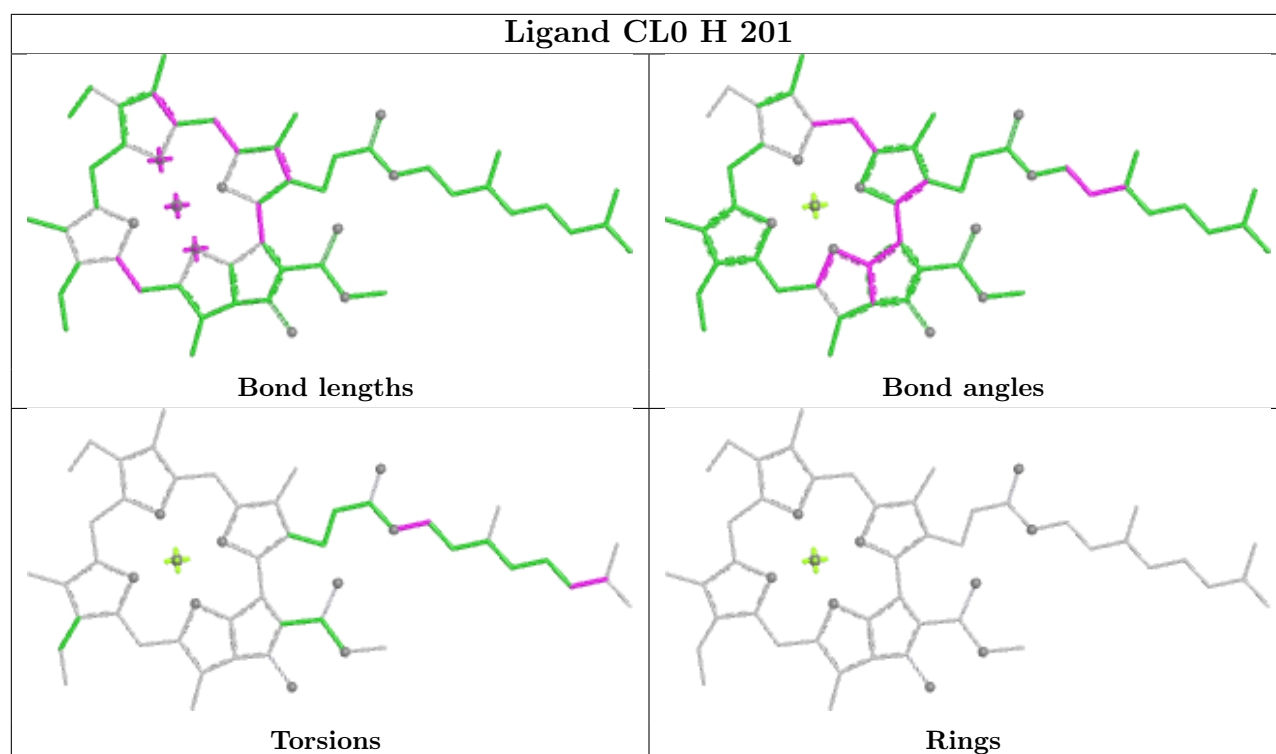


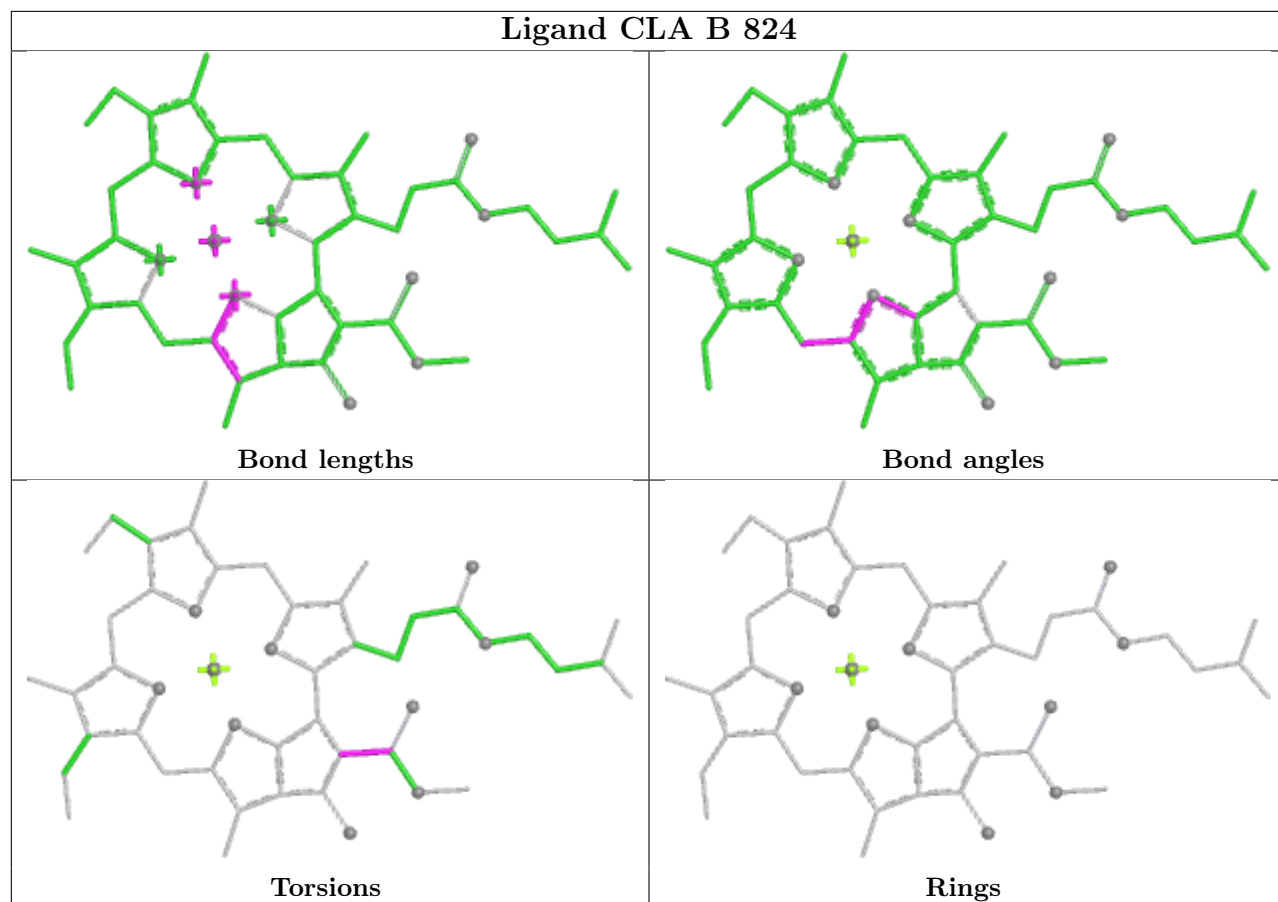


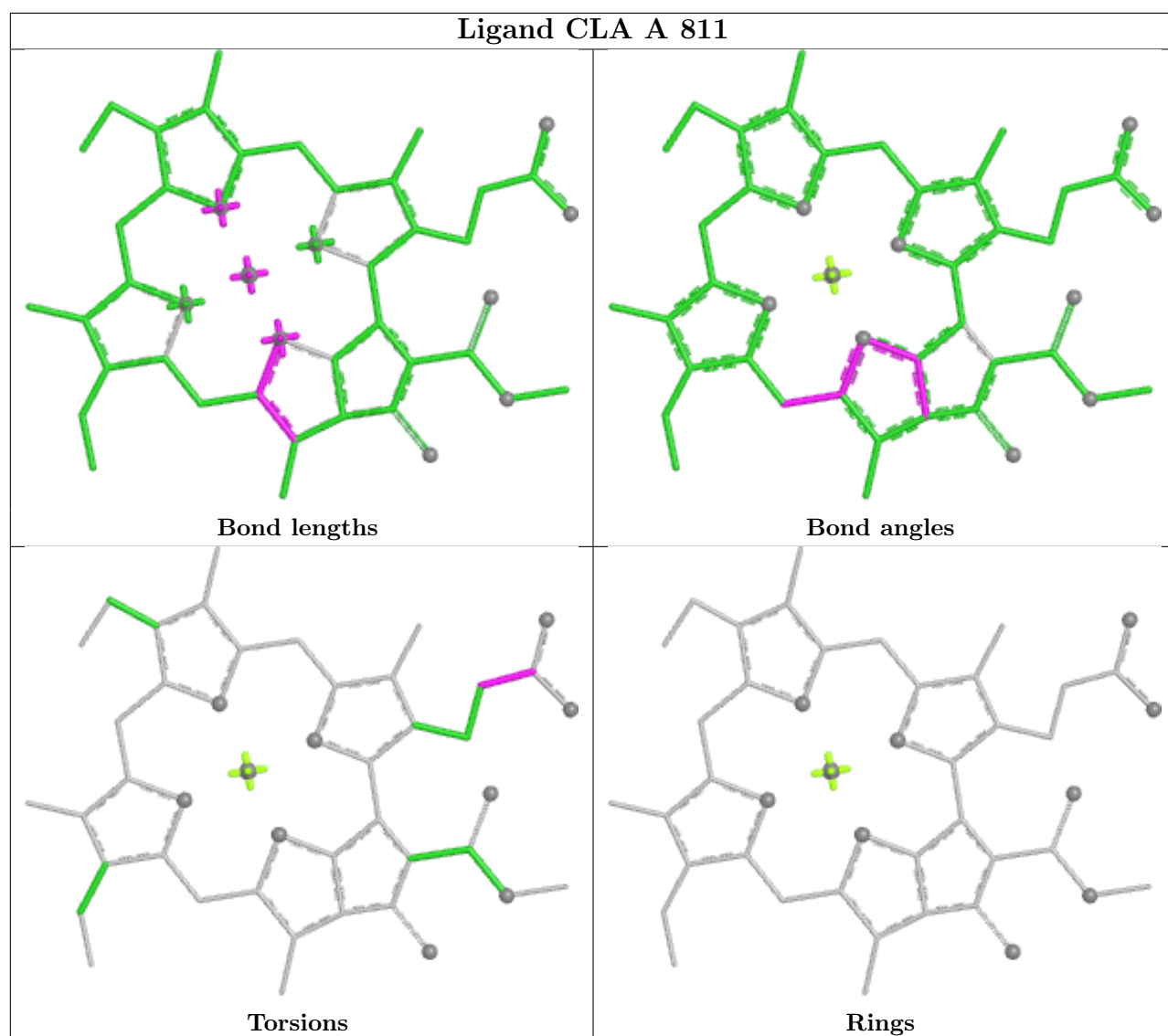


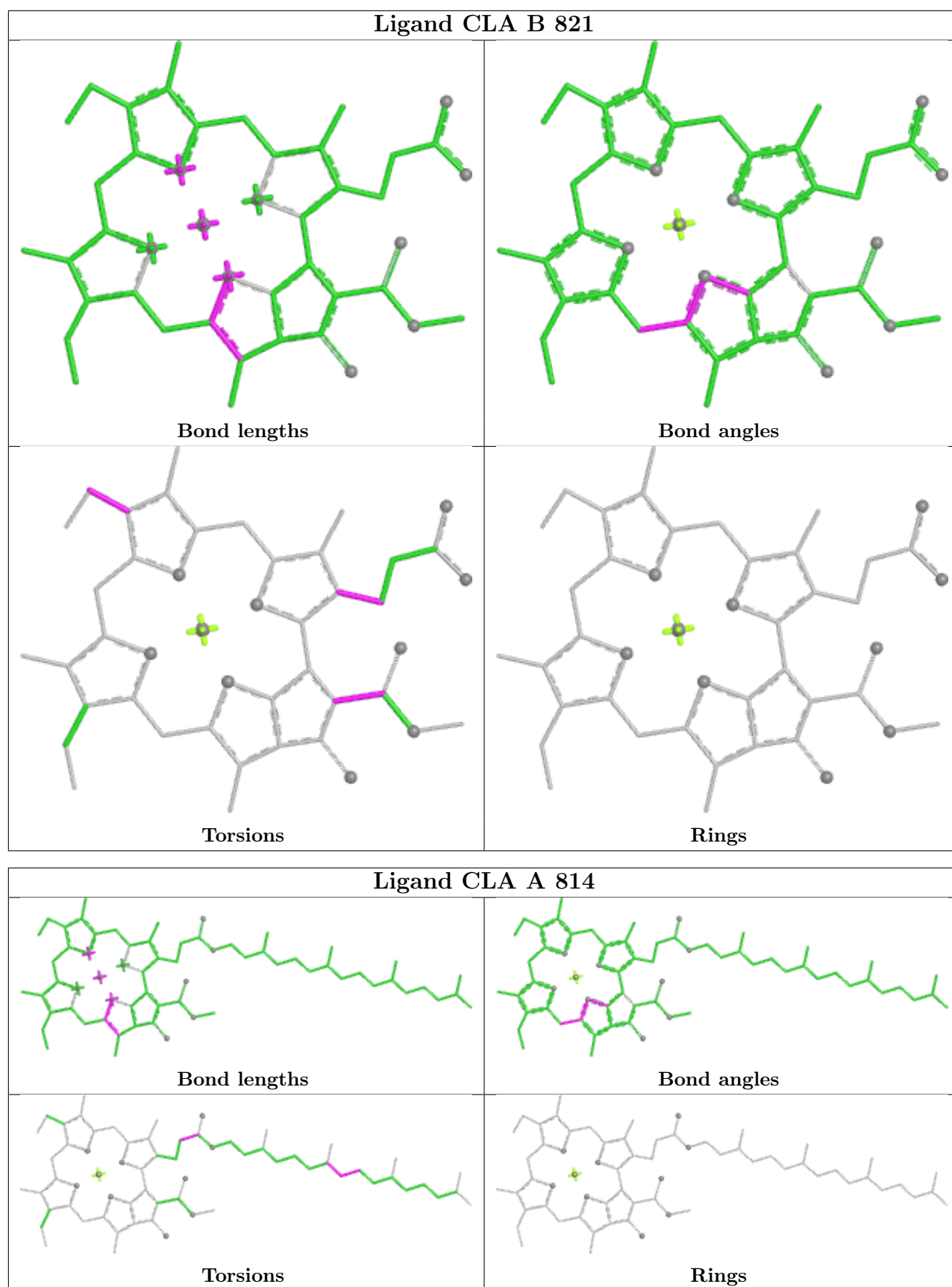


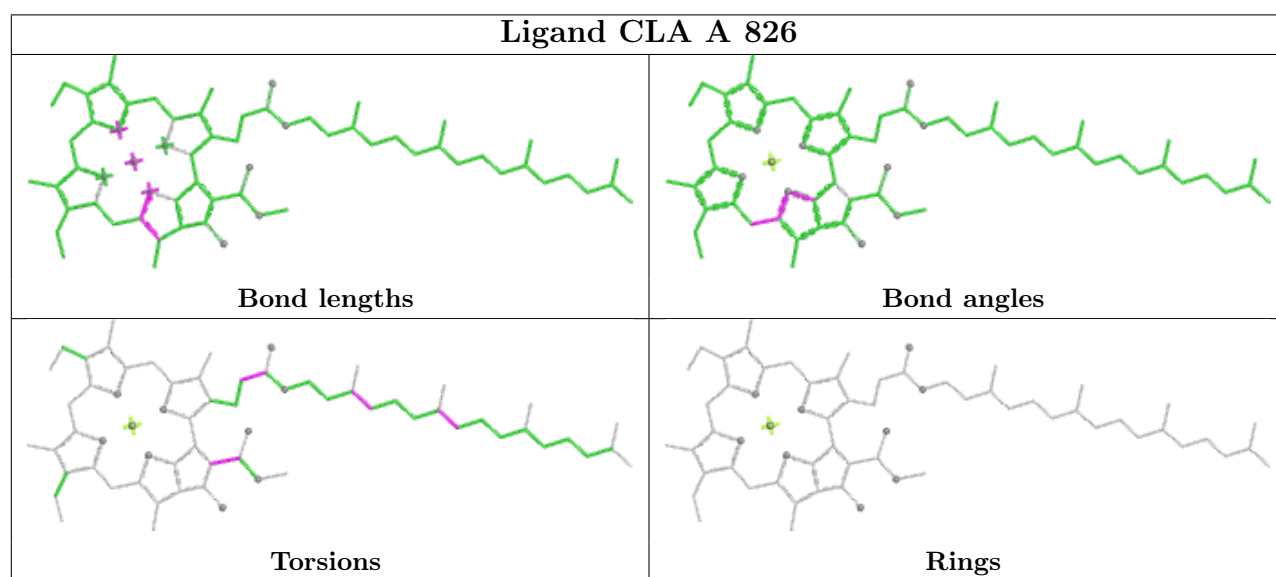
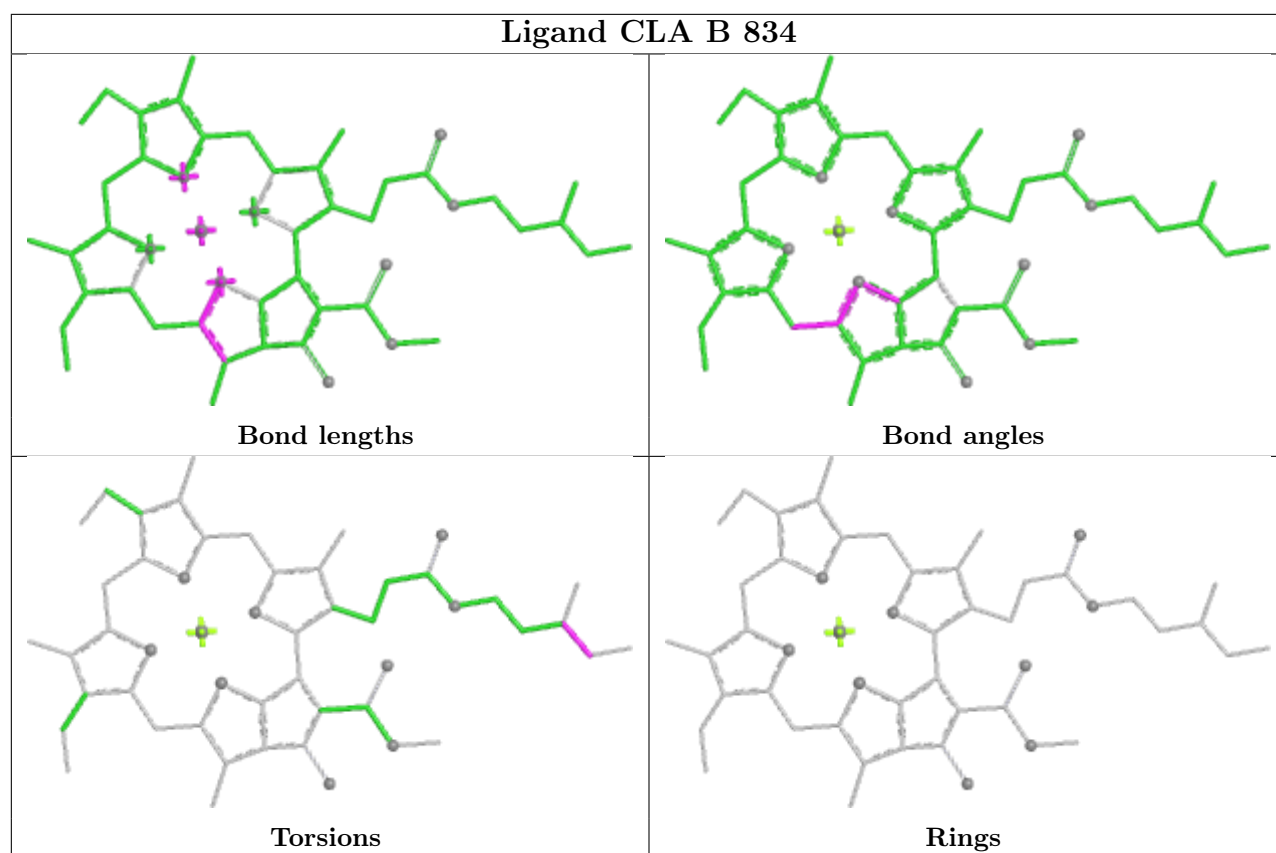


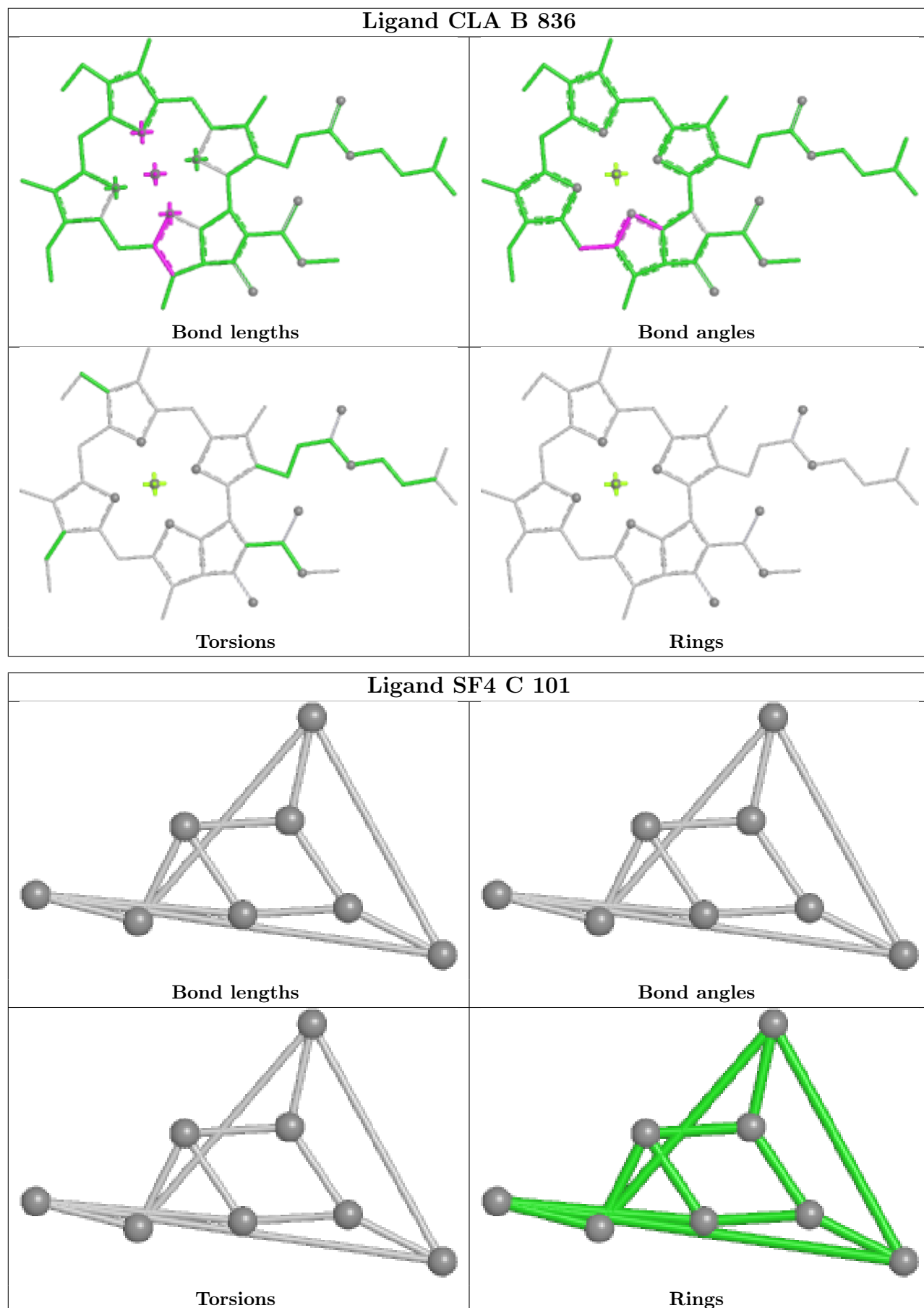


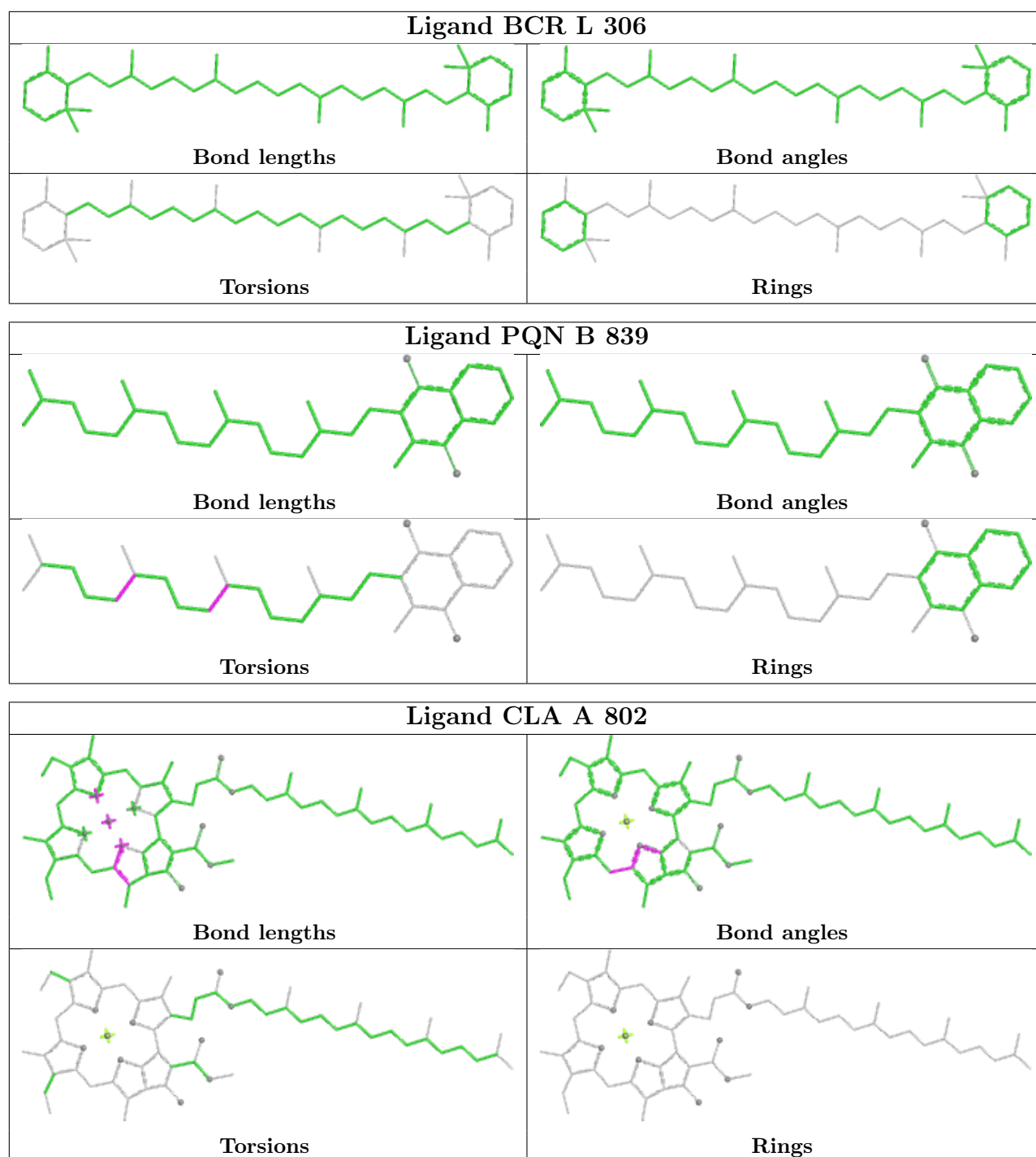


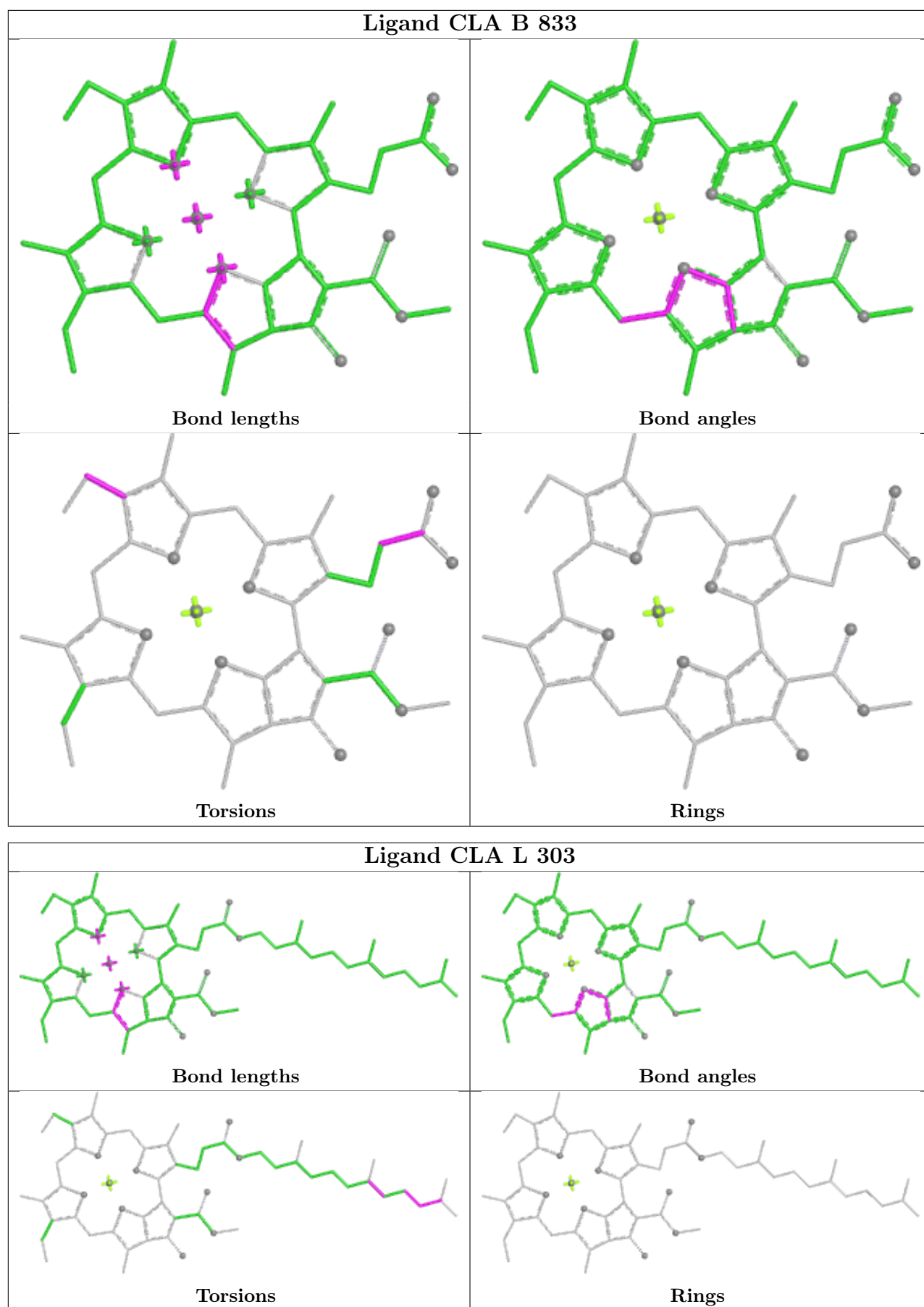


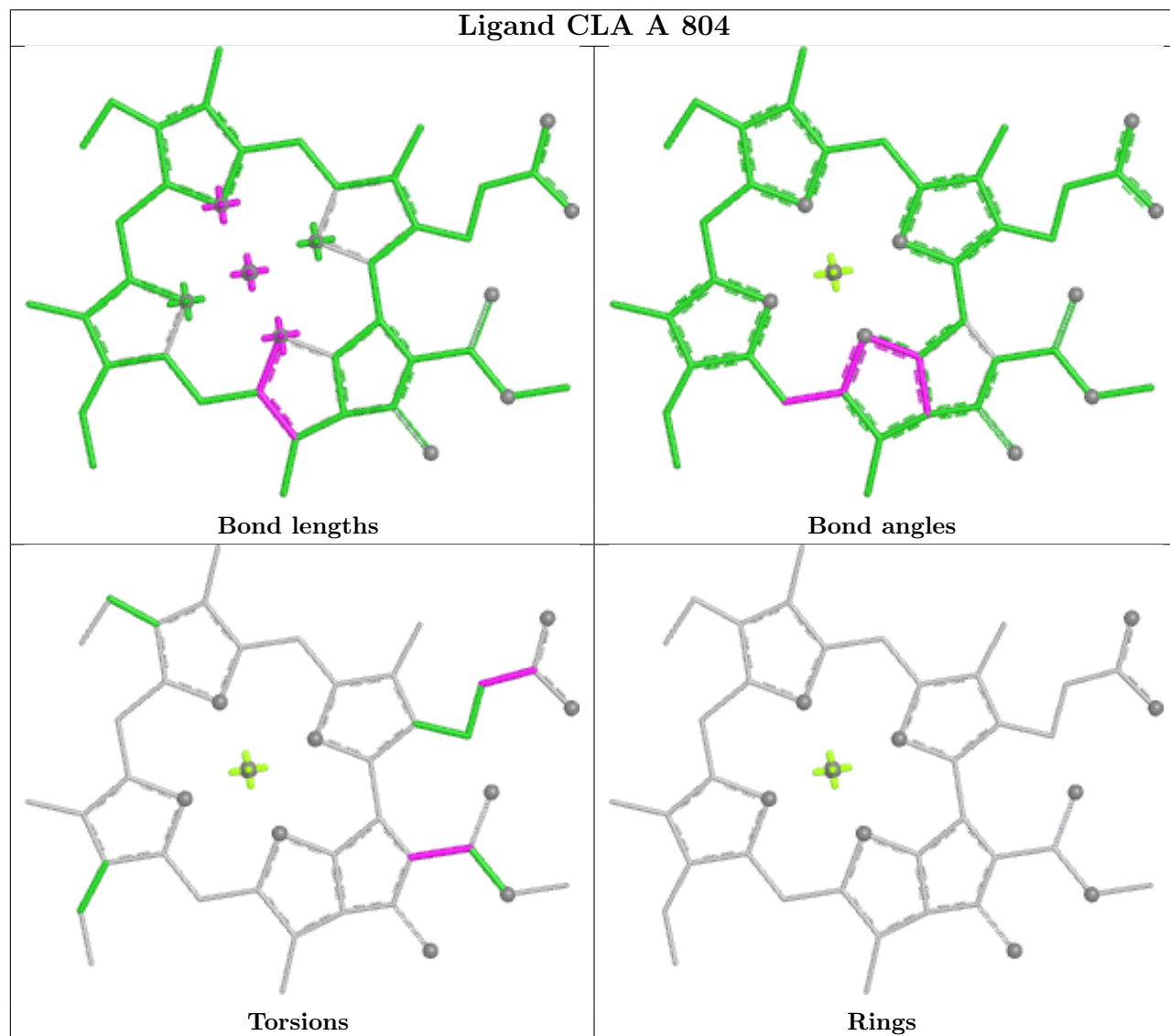
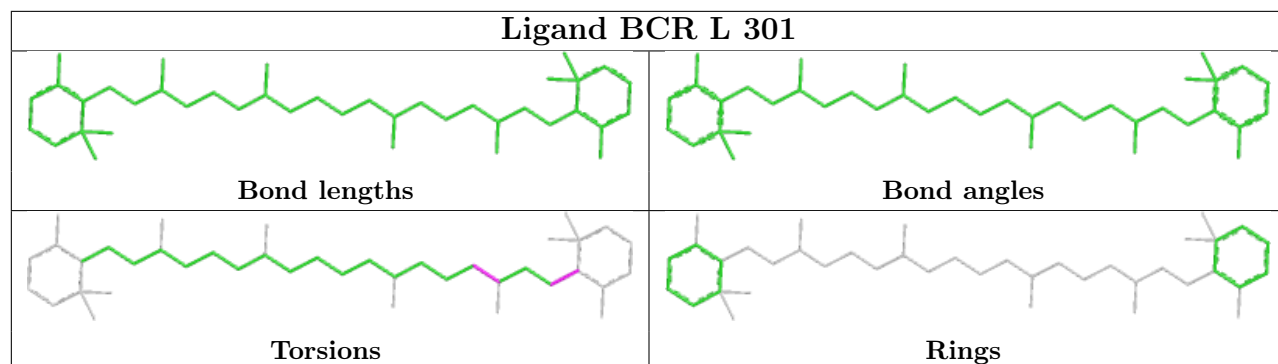


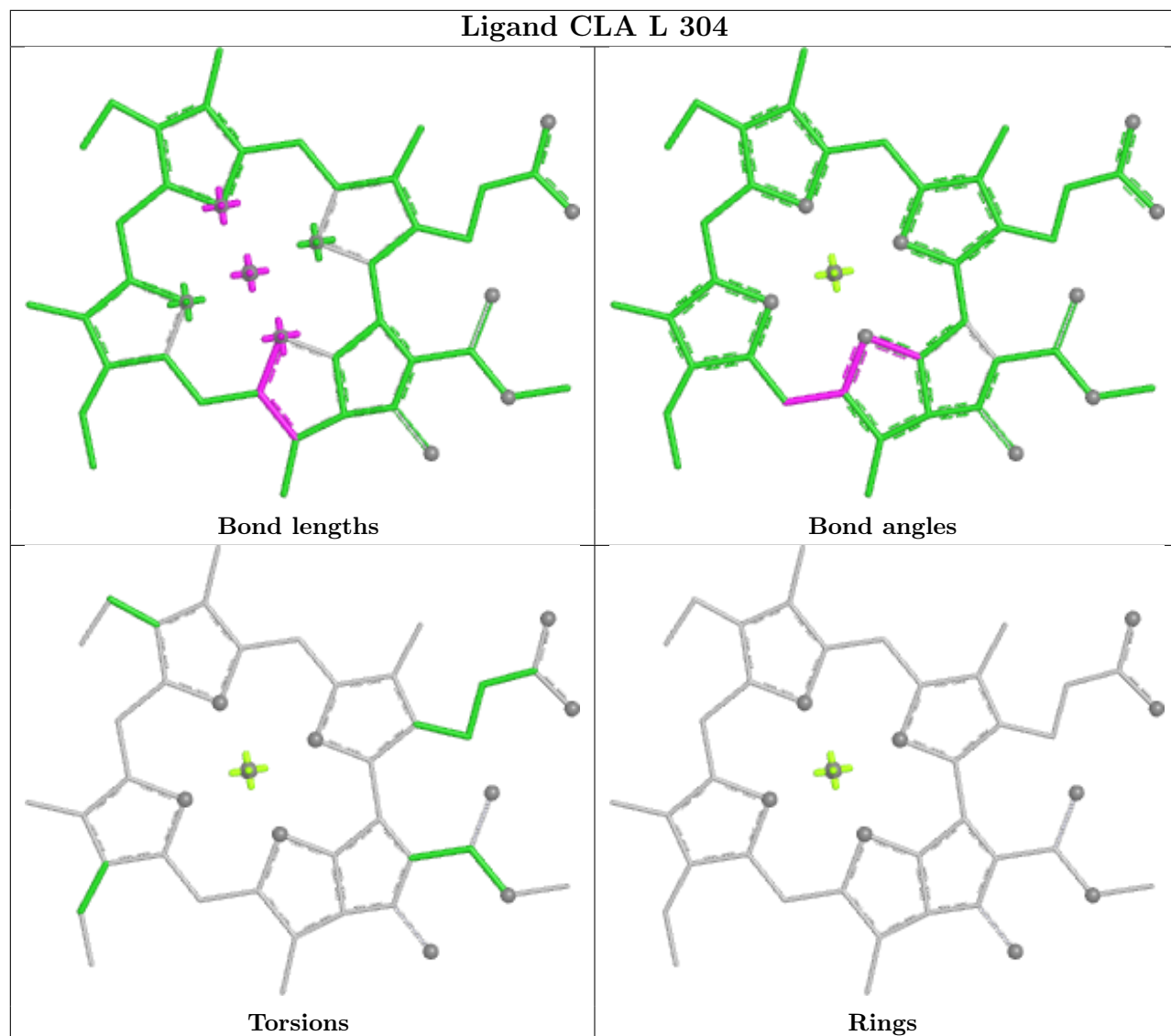


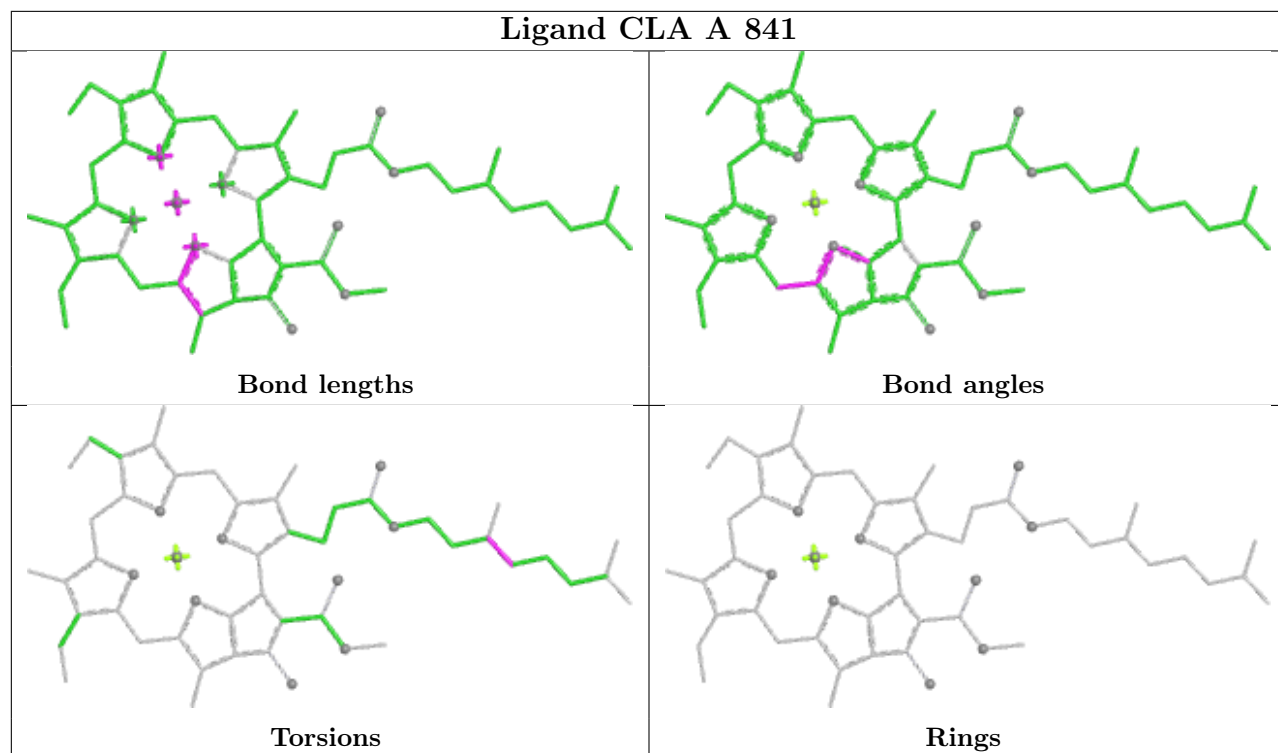


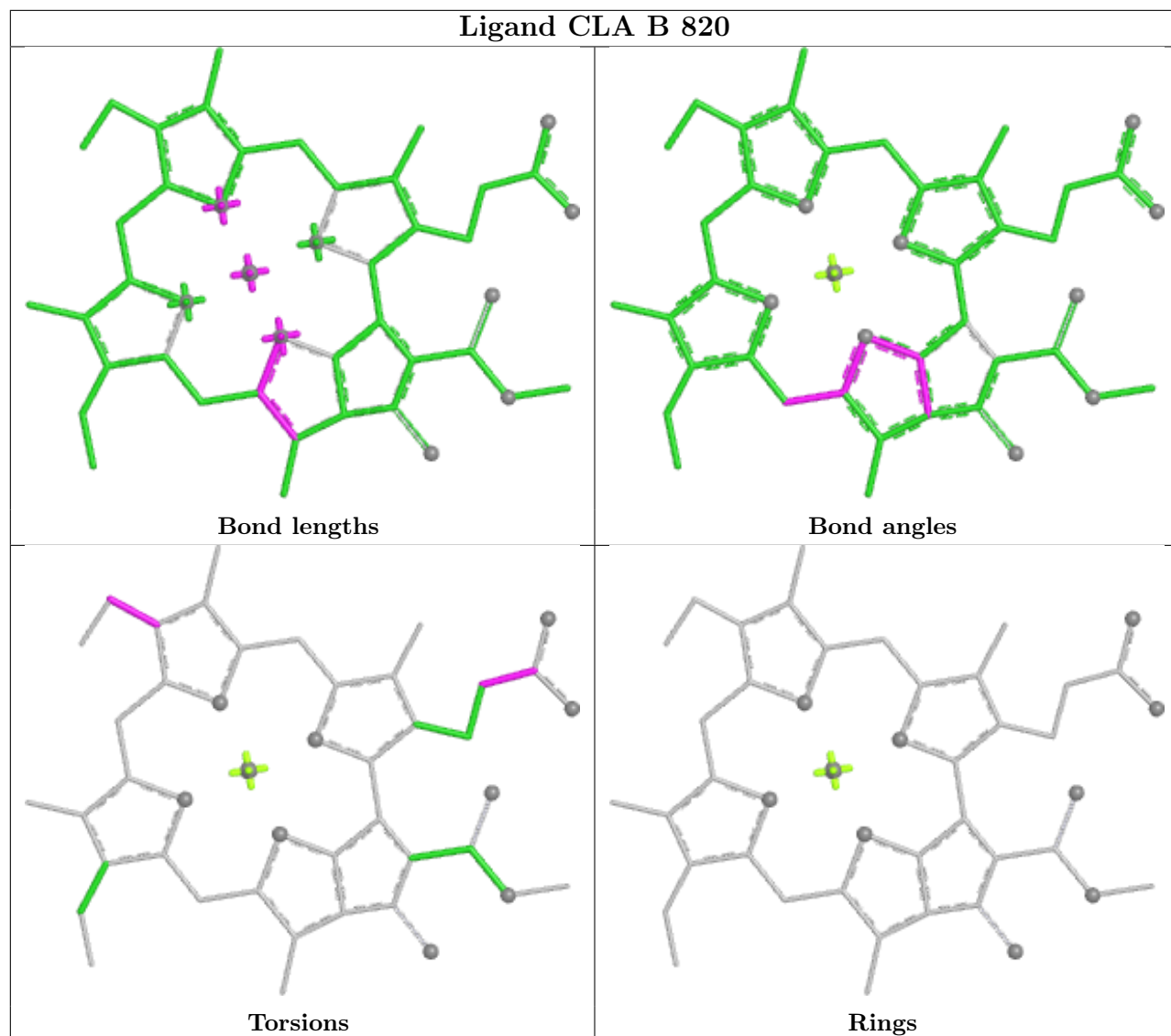


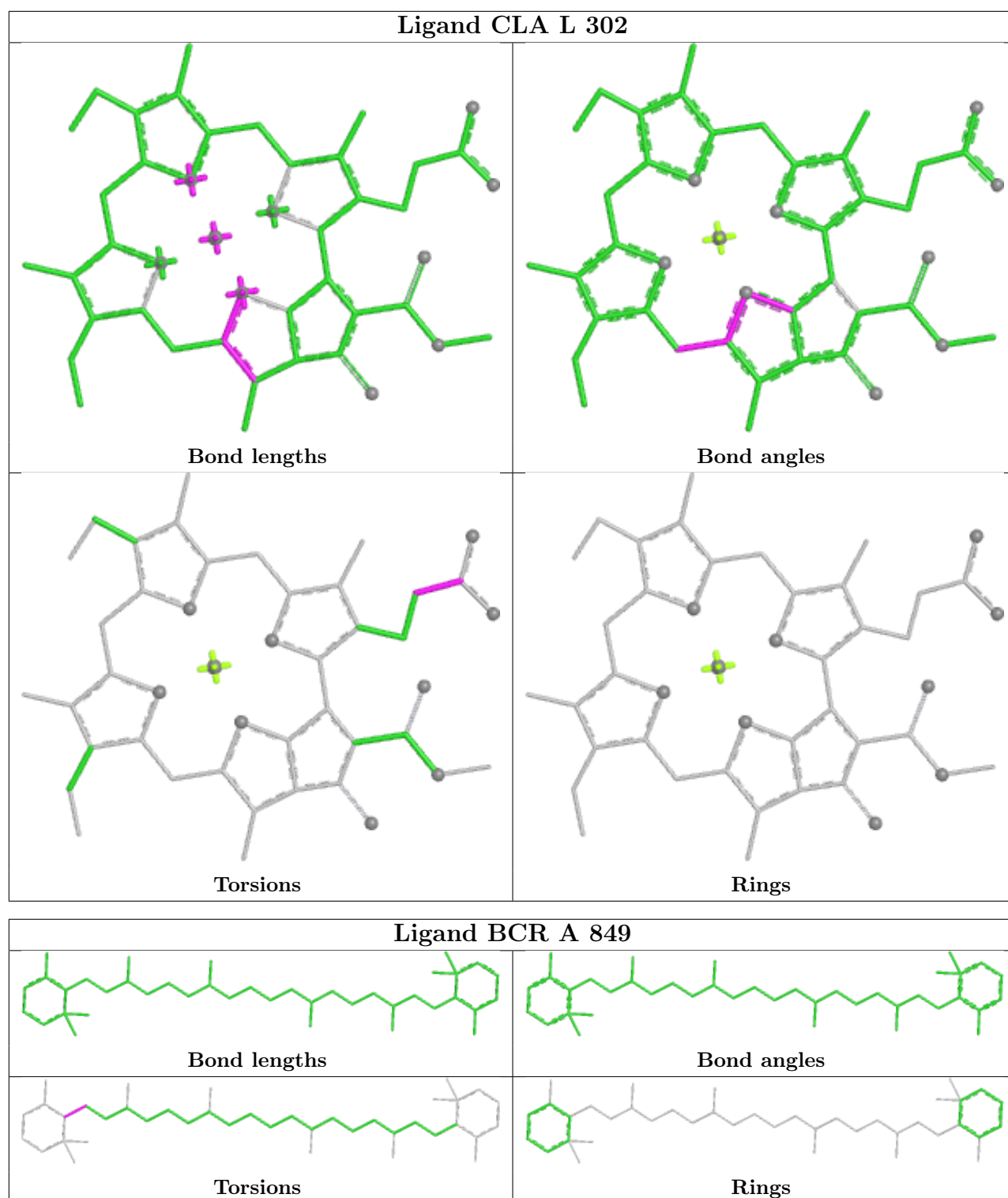


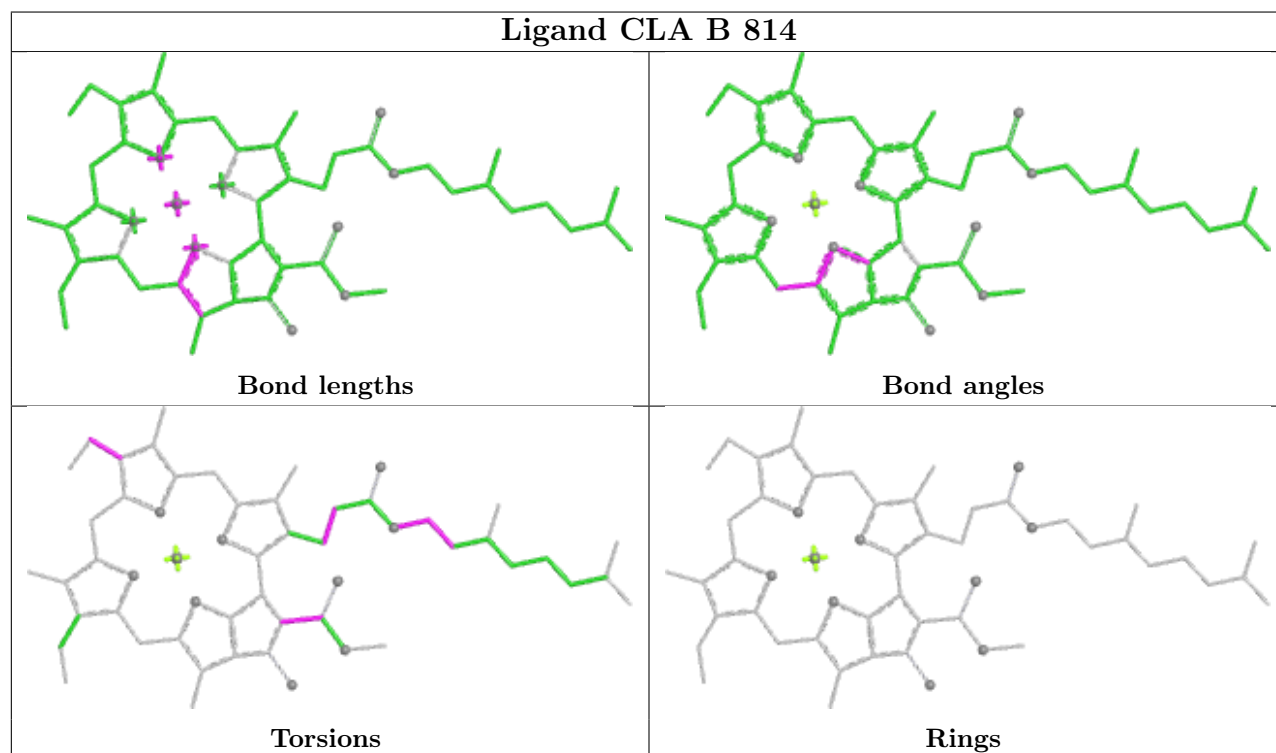
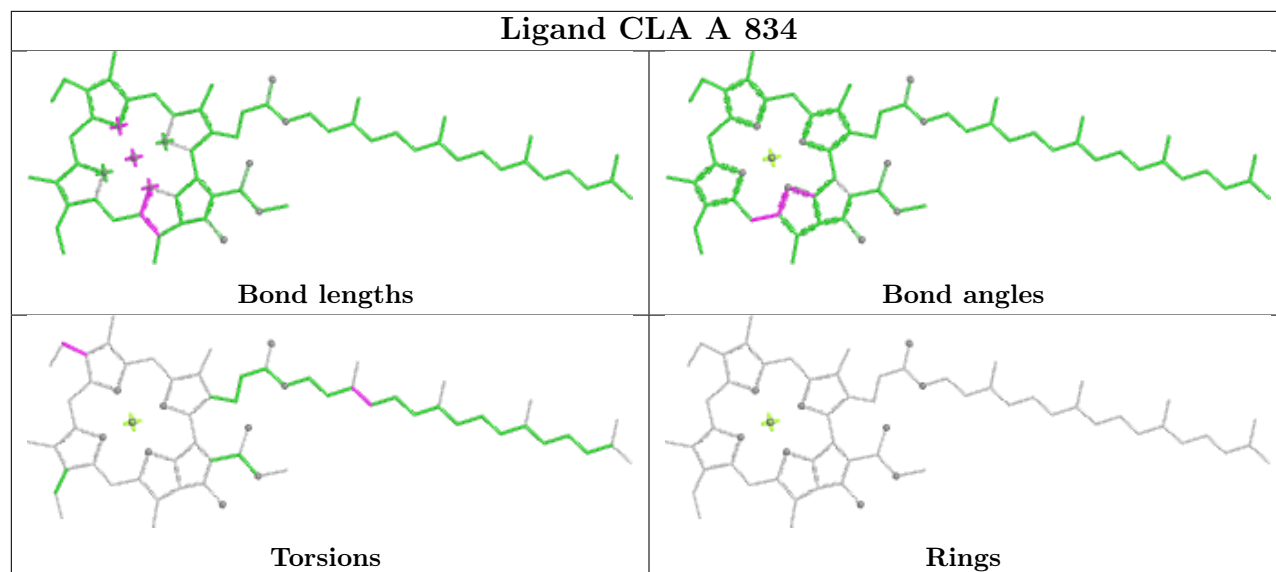


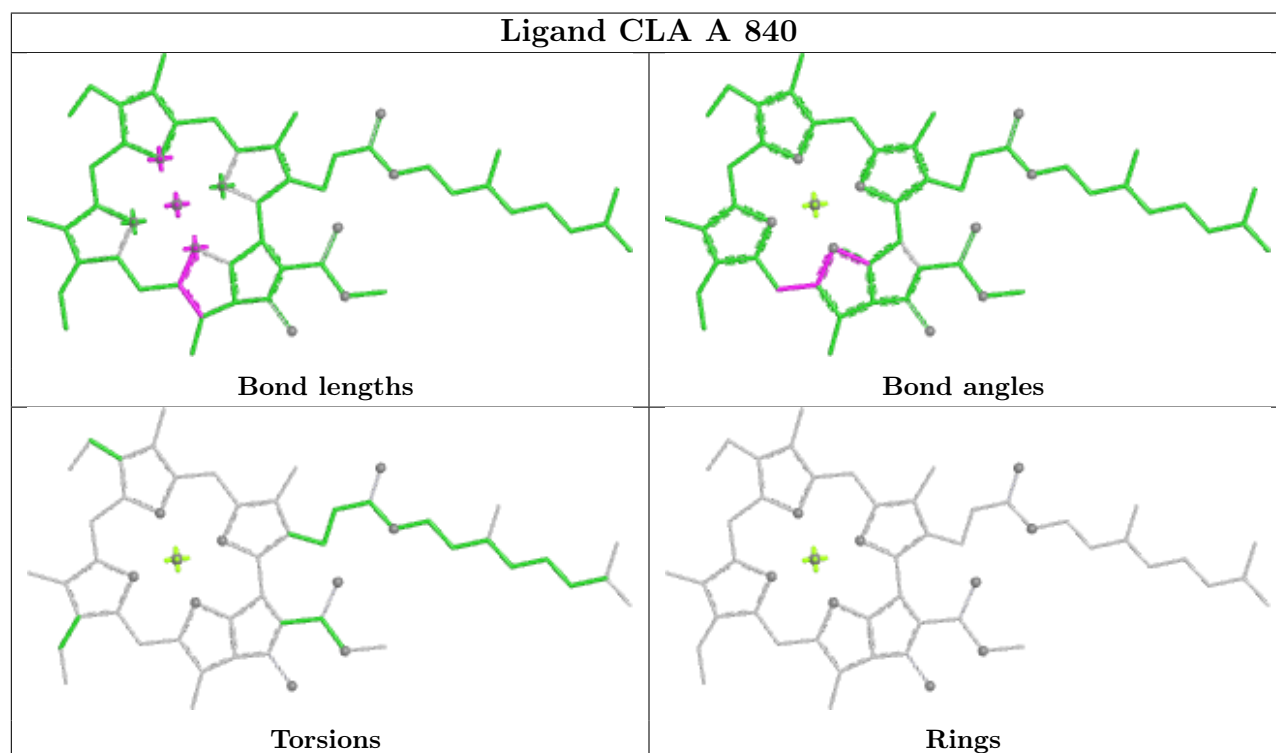
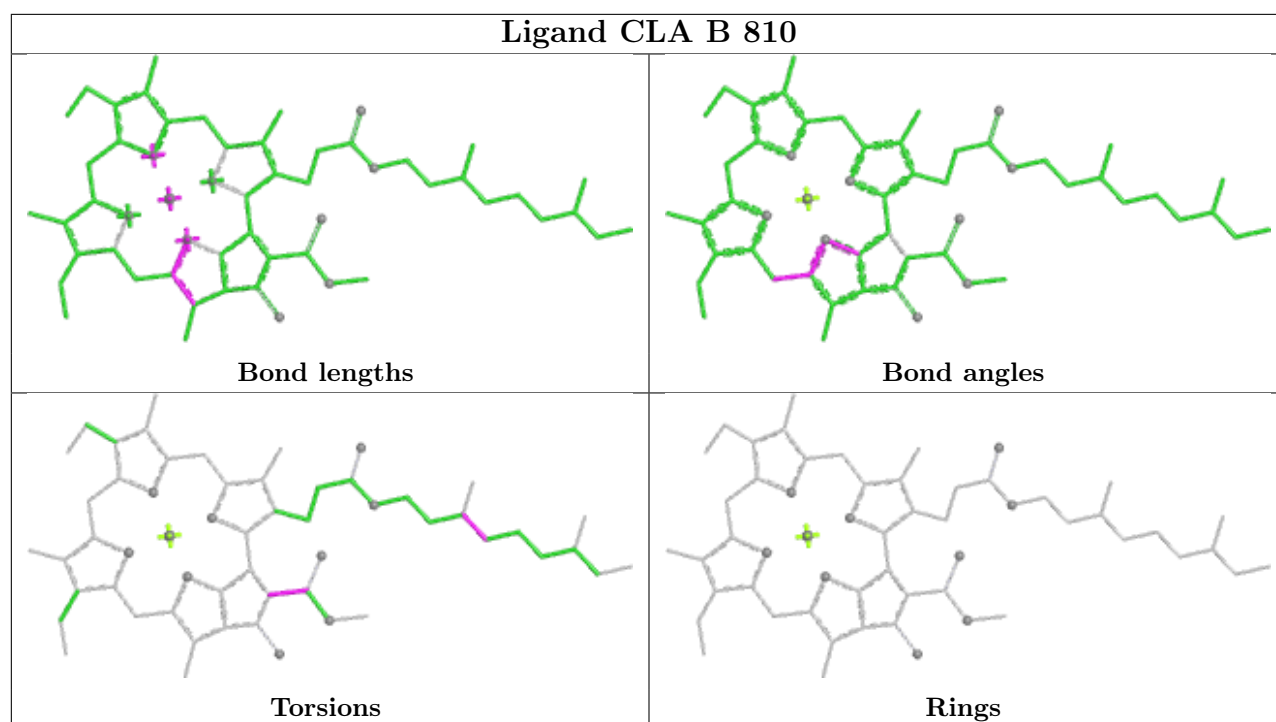


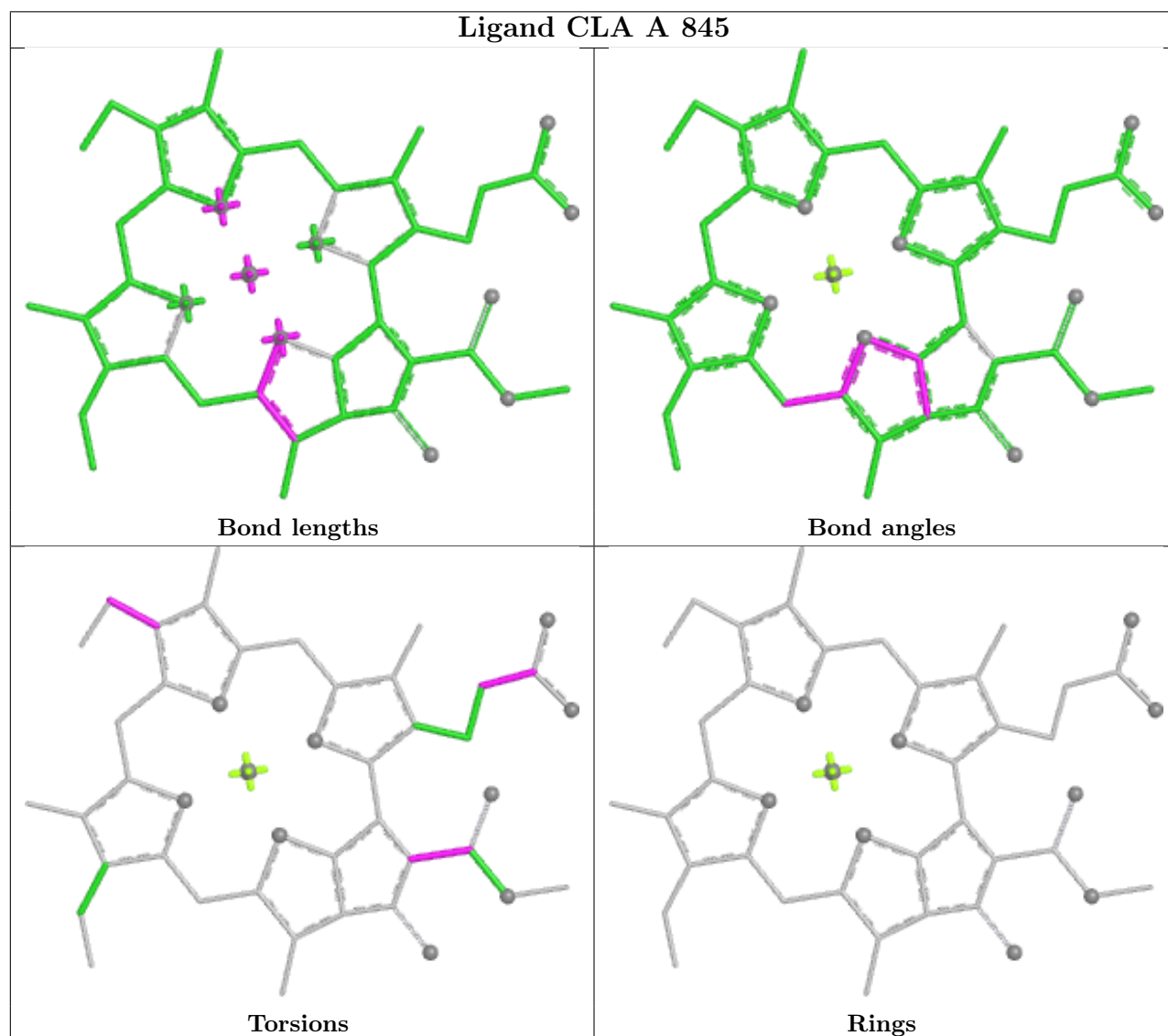
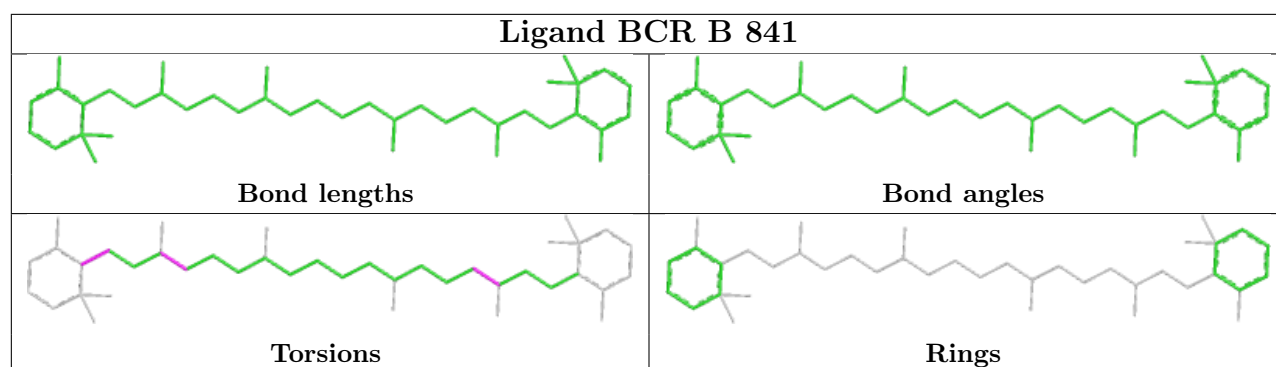


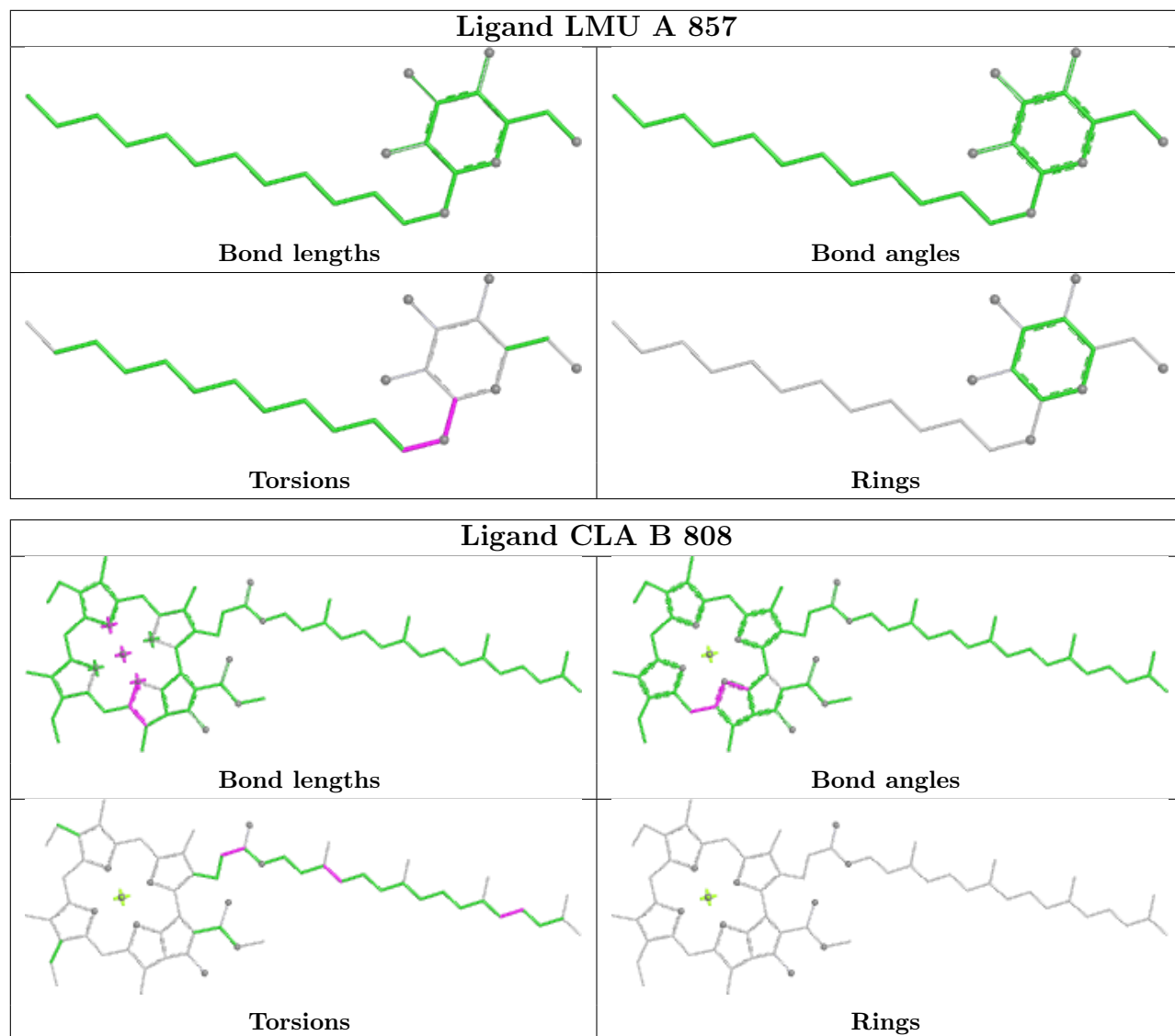


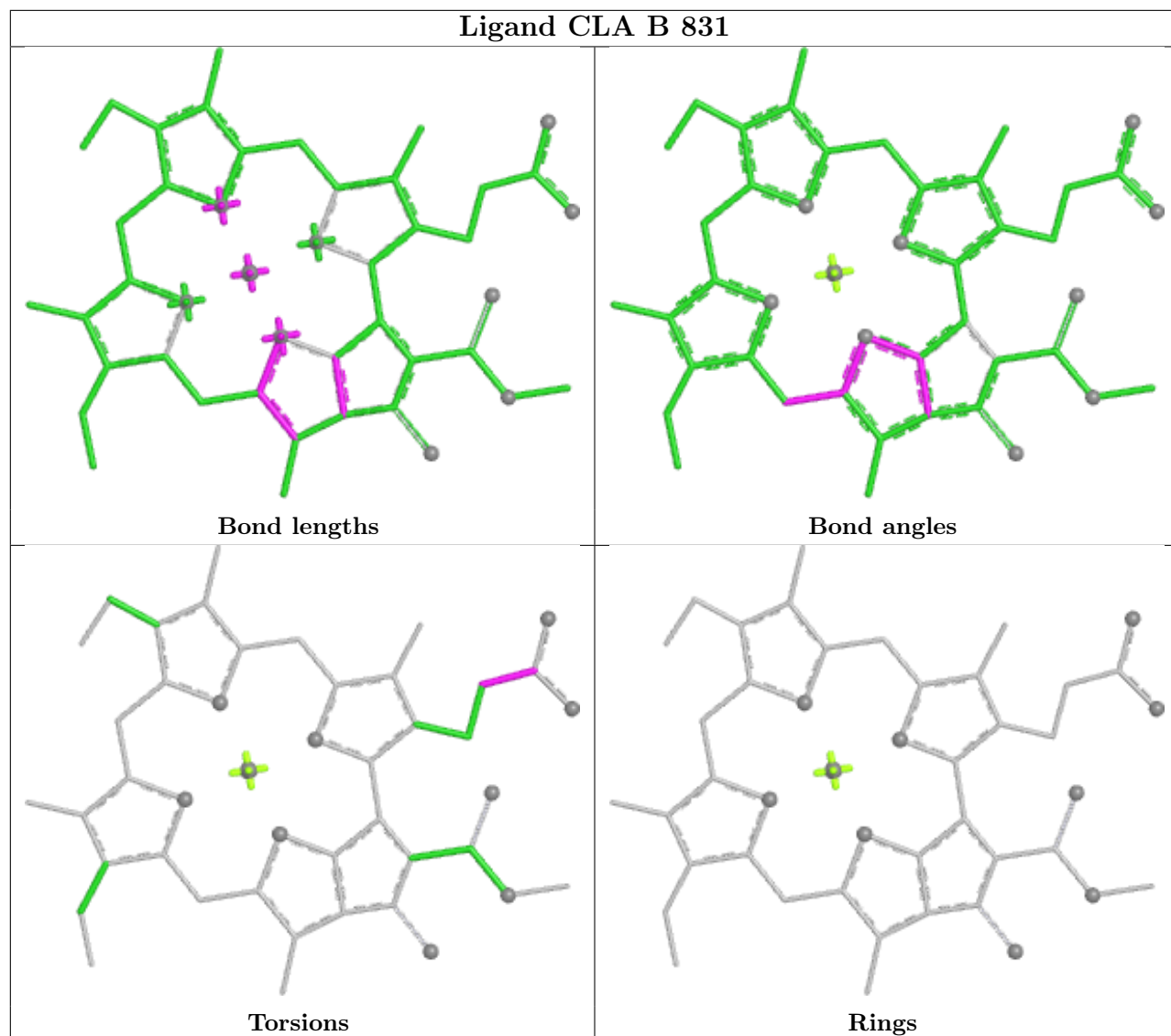


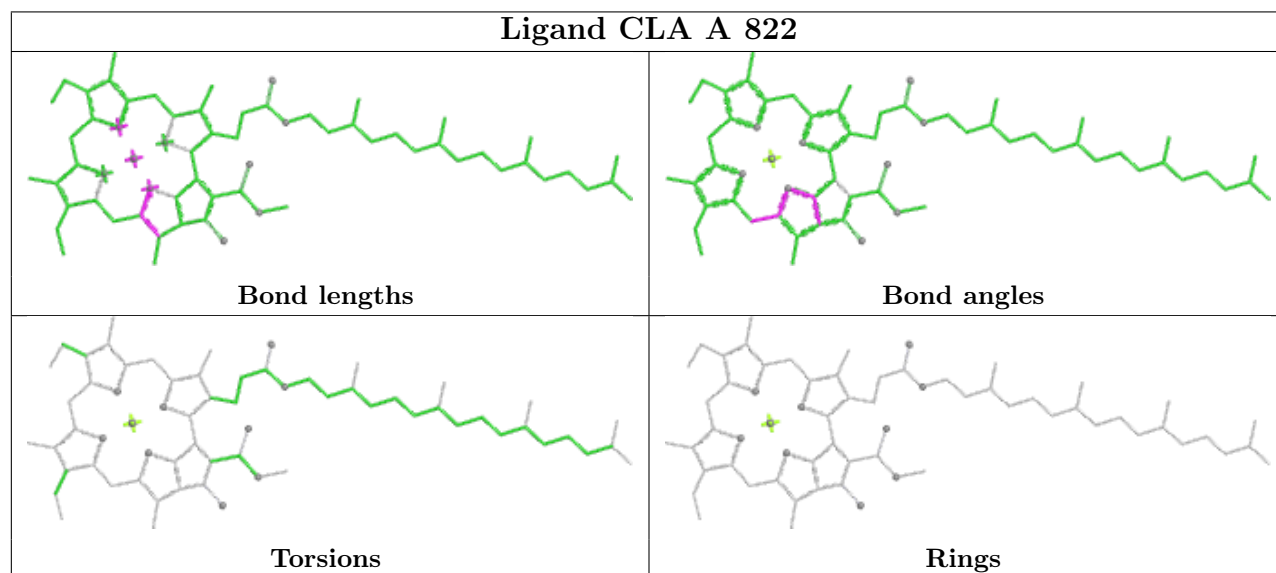
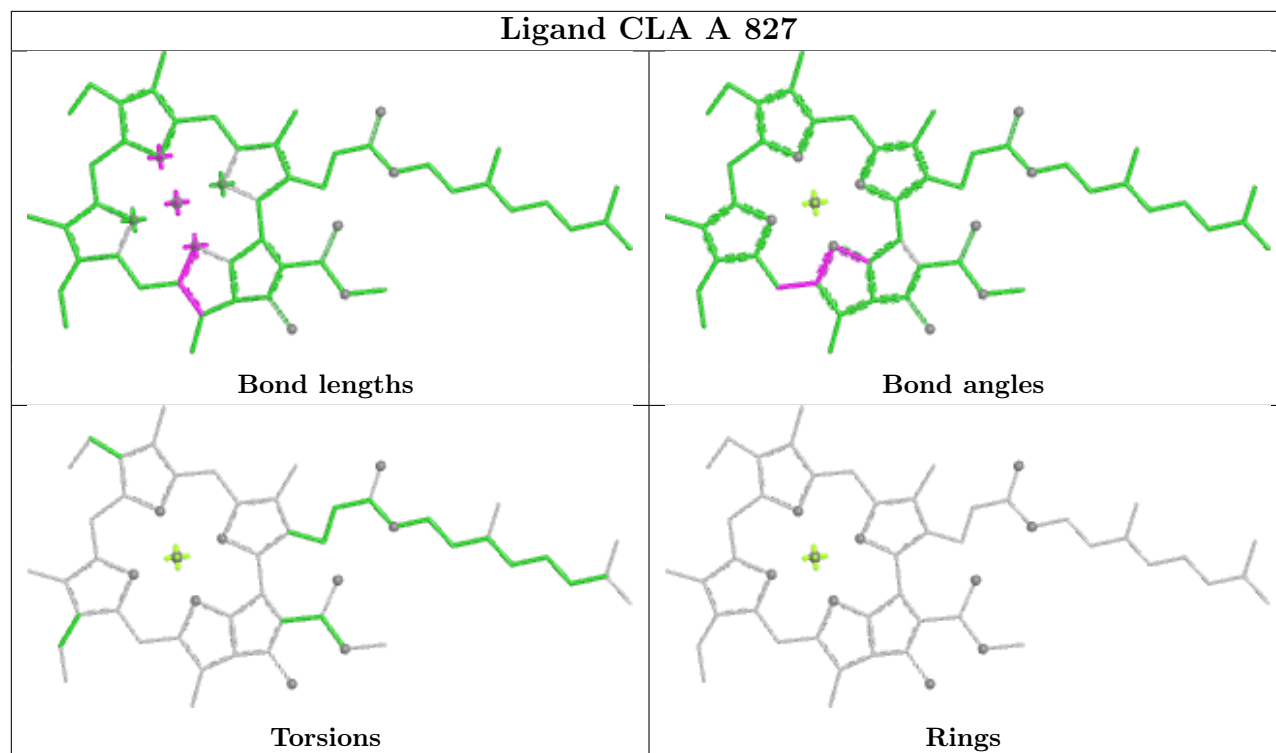


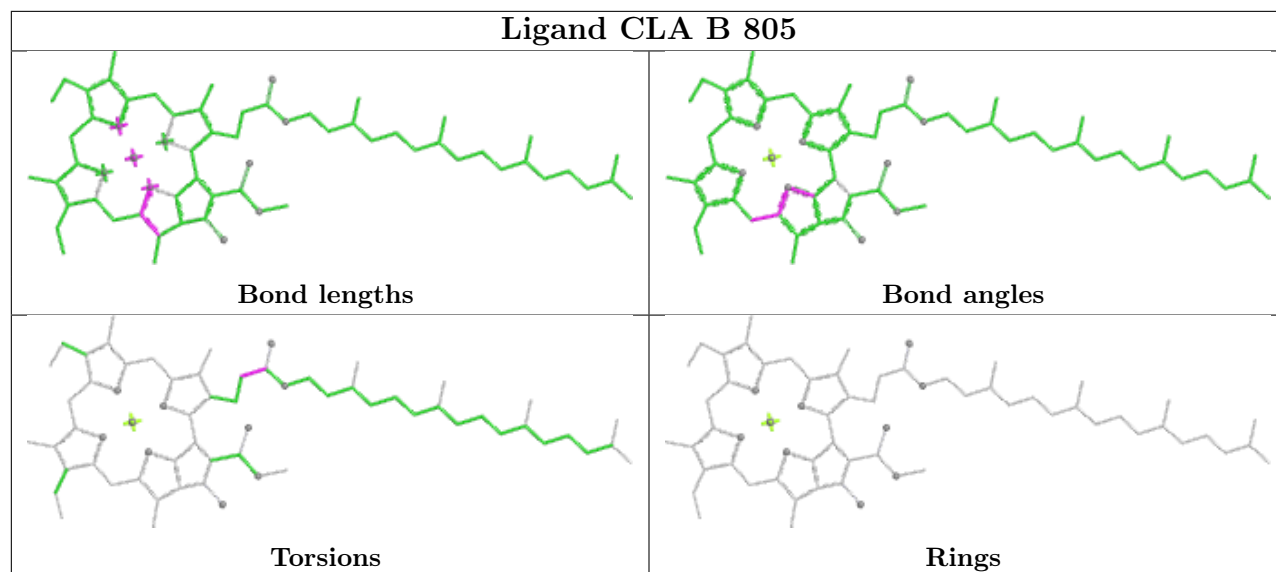












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-15970. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis

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

7.1 Map-value distribution

This section was not generated.

7.2 Volume estimate versus contour level

This section was not generated.

7.3 Rotationally averaged power spectrum

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

8 Fourier-Shell correlation

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

9 Map-model fit

This section was not generated.