



wwPDB EM Validation Summary Report ⓘ

Dec 13, 2022 – 05:04 PM JST

PDB ID : 6LU1
EMDB ID : EMD-0977
Title : Cyanobacterial PSI Monomer from *T. elongatus* by Single Particle CRYO-EM at 3.2 Å Resolution
Authors : Kurisu, G.; Coruh, O.; Tanaka, H.; Gerle, C.; Kawamoto, A.; Kato, T.; Namba, K.; Nowaczyk, M.M.; Rogner, M.; Misumi, Y.; Frank, A.; Eithar, E.M.
Deposited on : 2020-01-24
Resolution : 3.20 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

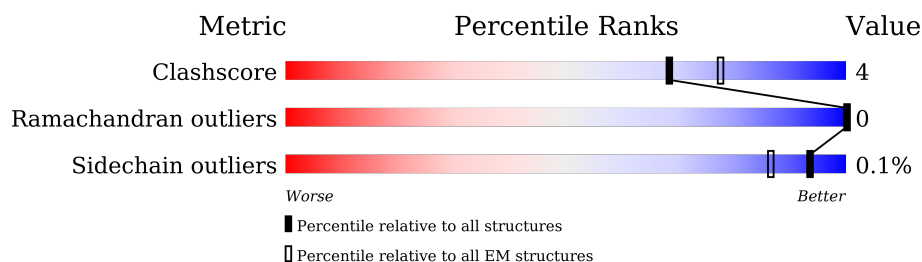
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.




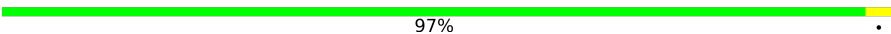
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	755	95% . .
2	B	741	92% . .
3	C	81	91% 7% .
4	D	139	94% 5% .
5	E	76	86% 5% 9%
6	F	164	16% . 82%
7	I	38	89% 11%
8	J	41	20% 80%

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Mol	Chain	Length	Quality of chain
9	L	155	 83% 13%
10	M	31	 97%

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
11	CLA	A	801	X	-	-	-
11	CLA	A	802	X	-	-	-
11	CLA	A	803	X	-	-	-
11	CLA	A	804	X	-	-	-
11	CLA	A	805	X	-	-	-
11	CLA	A	806	X	-	-	-
11	CLA	A	807	X	-	-	-
11	CLA	A	808	X	-	-	-
11	CLA	A	809	X	-	-	-
11	CLA	A	810	X	-	-	-
11	CLA	A	811	X	-	-	-
11	CLA	A	812	X	-	-	-
11	CLA	A	813	X	-	-	-
11	CLA	A	814	X	-	-	-
11	CLA	A	815	X	-	-	-
11	CLA	A	816	X	-	-	-
11	CLA	A	817	X	-	-	-
11	CLA	A	818	X	-	-	-
11	CLA	A	819	X	-	-	-
11	CLA	A	820	X	-	-	-
11	CLA	A	821	X	-	-	-
11	CLA	A	822	X	-	-	-
11	CLA	A	823	X	-	-	-
11	CLA	A	824	X	-	-	-
11	CLA	A	825	X	-	-	-
11	CLA	A	826	X	-	-	-
11	CLA	A	827	X	-	-	-
11	CLA	A	828	X	-	-	-
11	CLA	A	829	X	-	-	-
11	CLA	A	830	X	-	-	-
11	CLA	A	831	X	-	-	-
11	CLA	A	832	X	-	-	-
11	CLA	A	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	A	834	X	-	-	-
11	CLA	A	835	X	-	-	-
11	CLA	A	836	X	-	-	-
11	CLA	A	837	X	-	-	-
11	CLA	A	838	X	-	-	-
11	CLA	A	839	X	-	-	-
11	CLA	A	840	X	-	-	-
11	CLA	A	841	X	-	-	-
11	CLA	A	842	X	-	-	-
11	CLA	A	859	X	-	-	-
11	CLA	A	860	X	-	-	-
11	CLA	B	801	X	-	-	-
11	CLA	B	802	X	-	-	-
11	CLA	B	803	X	-	-	-
11	CLA	B	805	X	-	-	-
11	CLA	B	806	X	-	-	-
11	CLA	B	807	X	-	-	-
11	CLA	B	808	X	-	-	-
11	CLA	B	809	X	-	-	-
11	CLA	B	810	X	-	-	-
11	CLA	B	811	X	-	-	-
11	CLA	B	812	X	-	-	-
11	CLA	B	813	X	-	-	-
11	CLA	B	814	X	-	-	-
11	CLA	B	815	X	-	-	-
11	CLA	B	816	X	-	-	-
11	CLA	B	817	X	-	-	-
11	CLA	B	818	X	-	-	-
11	CLA	B	819	X	-	-	-
11	CLA	B	820	X	-	-	-
11	CLA	B	821	X	-	-	-
11	CLA	B	822	X	-	-	-
11	CLA	B	823	X	-	-	-
11	CLA	B	824	X	-	-	-
11	CLA	B	825	X	-	-	-
11	CLA	B	826	X	-	-	-
11	CLA	B	827	X	-	-	-
11	CLA	B	828	X	-	-	-
11	CLA	B	829	X	-	-	-
11	CLA	B	830	X	-	-	-
11	CLA	B	831	X	-	-	-
11	CLA	B	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CLA	B	833	X	-	-	-
11	CLA	B	834	X	-	-	-
11	CLA	B	835	X	-	-	-
11	CLA	B	836	X	-	-	-
11	CLA	L	1501	X	-	-	-
11	CLA	L	1502	X	-	-	-
11	CLA	L	1503	X	-	-	-

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 21198 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	A	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	713	Total	C	N	O	S	0	0
			5685	3747	952	967	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	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	D	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	E	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	F	29	Total	C	N	O	0	0
			231	160	37	34		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	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	J	8	Total	C	N	O	0	0
			67	44	12	11		

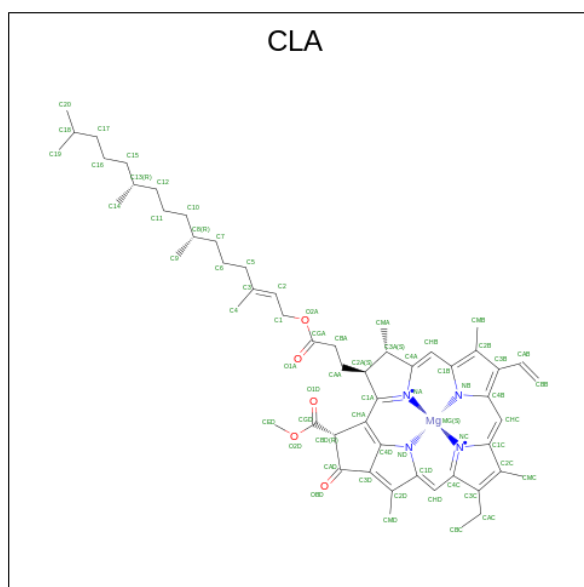
- Molecule 9 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	135	Total	C	N	O	S	0	0
			994	653	161	177	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 11 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0

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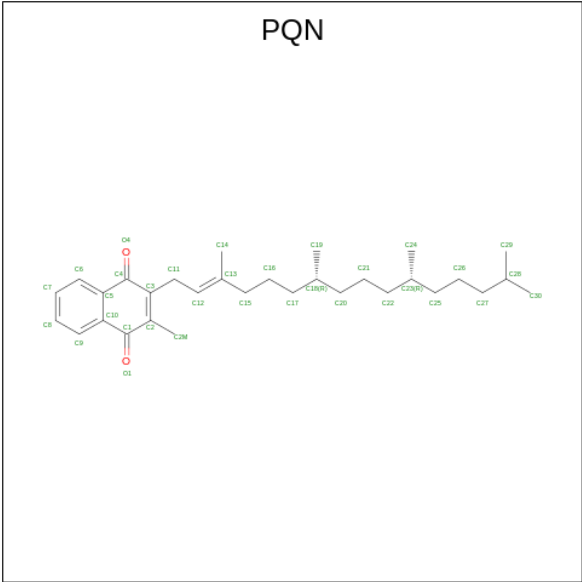
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total 2422	C 1999	Mg 44	N 176	O 203	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0

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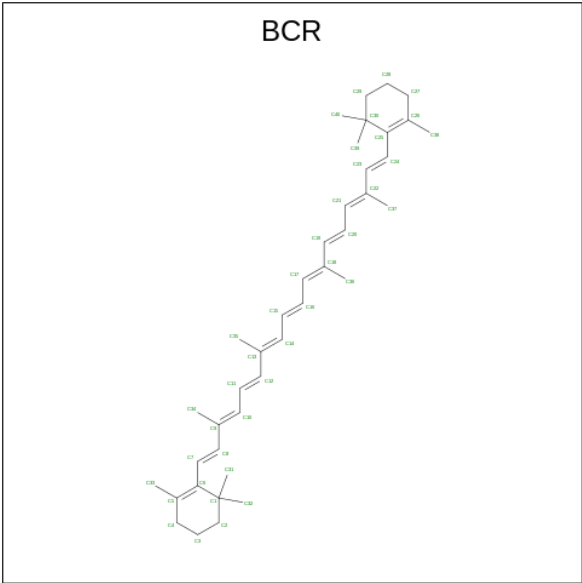
Mol	Chain	Residues	Atoms					AltConf
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	B	1	Total 1932	C 1595	Mg 35	N 140	O 162	0
11	L	1	Total 136	C 112	Mg 3	N 12	O 9	0
11	L	1	Total 136	C 112	Mg 3	N 12	O 9	0
11	L	1	Total 136	C 112	Mg 3	N 12	O 9	0

- Molecule 12 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 13 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total	C	0
			462	462	
13	A	1	Total	C	0
			462	462	

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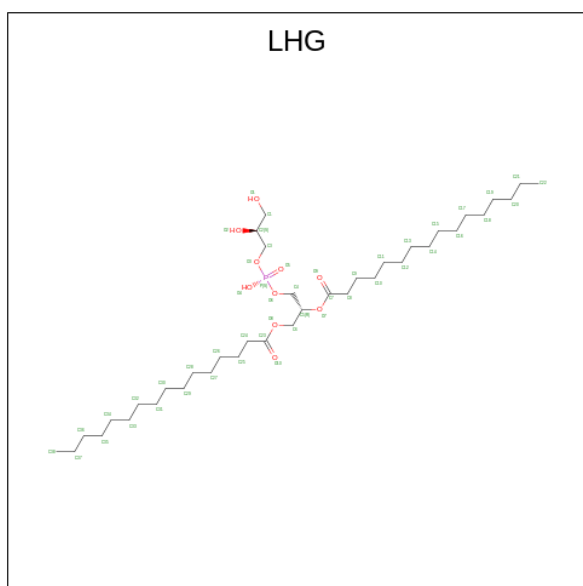
Mol	Chain	Residues	Atoms		AltConf
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	A	1	Total 462	C 462	0
13	B	1	Total 230	C 230	0
13	B	1	Total 230	C 230	0
13	B	1	Total 230	C 230	0
13	B	1	Total 230	C 230	0
13	B	1	Total 230	C 230	0
13	B	1	Total 230	C 230	0
13	F	1	Total 80	C 80	0
13	F	1	Total 80	C 80	0
13	I	1	Total 80	C 80	0

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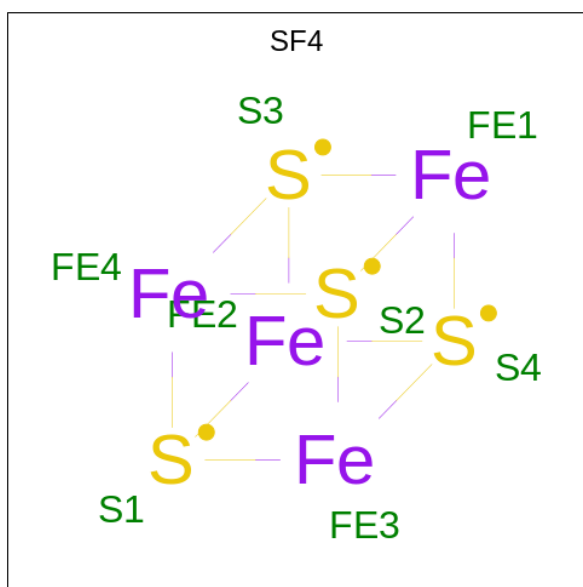
Mol	Chain	Residues	Atoms		AltConf
13	I	1	Total	C	0
			80	80	
13	L	1	Total	C	0
			40	40	
13	M	1	Total	C	0
			40	40	

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



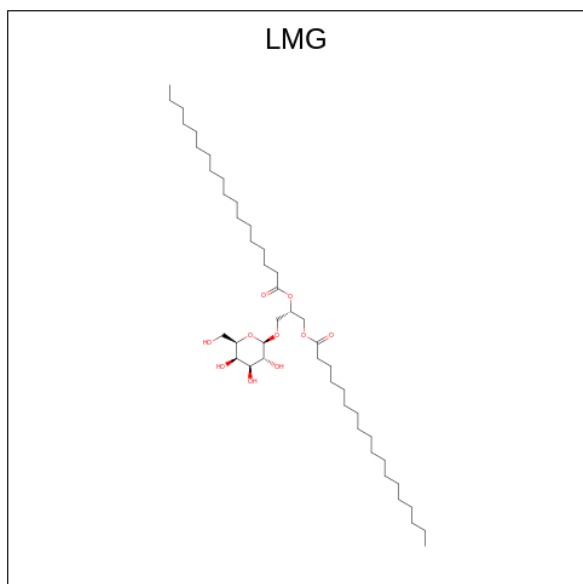
Mol	Chain	Residues	Atoms				AltConf
14	A	1	Total	C	O	P	0
			76	54	20	2	
14	A	1	Total	C	O	P	0
			76	54	20	2	

- Molecule 15 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			16	8	8	
15	C	1	Total	Fe	S	0
			16	8	8	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
16	B	1	Total	C	O	0
			55	45	10	

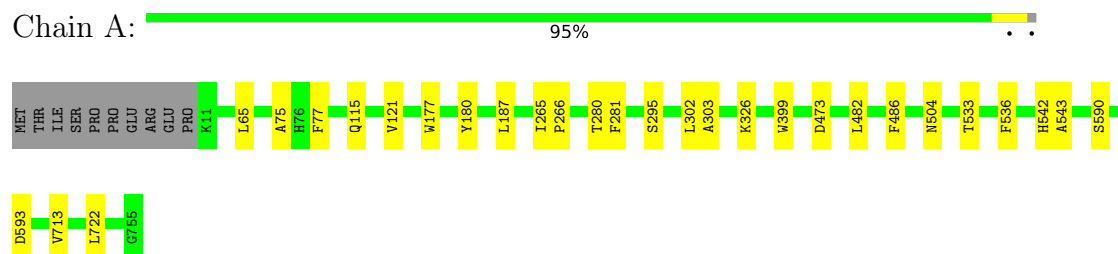
- Molecule 17 is water.

Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	O	0
			1	1	
17	B	2	Total	O	0
			2	2	
17	C	1	Total	O	0
			1	1	
17	D	1	Total	O	0
			1	1	

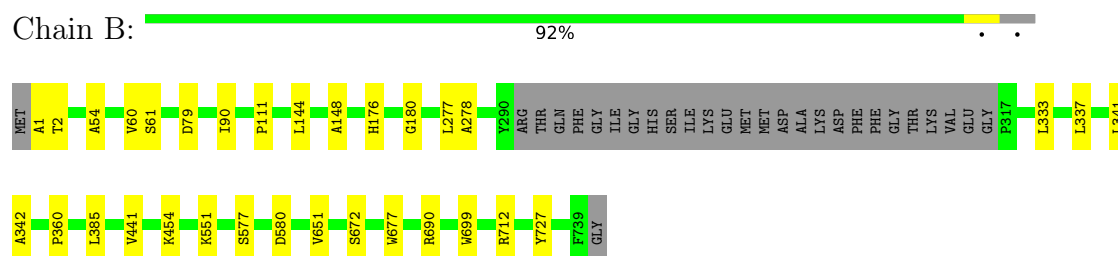
3 Residue-property plots

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.

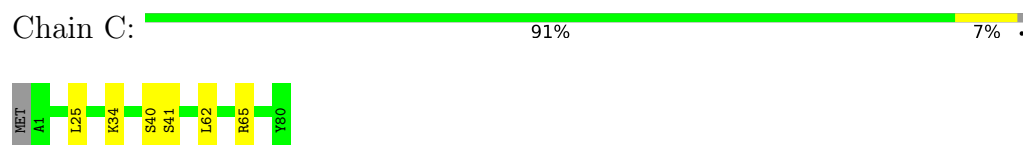
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



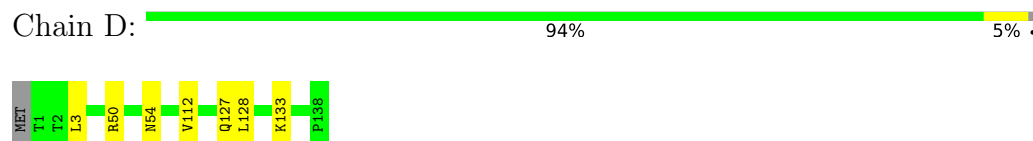
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



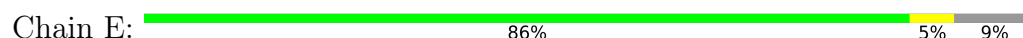
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



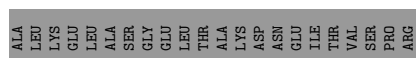
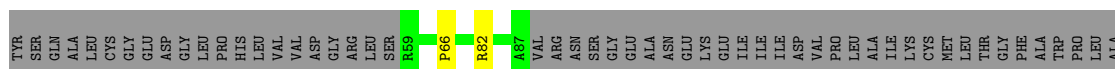
- Molecule 5: Photosystem I reaction center subunit IV





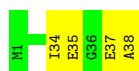
- Molecule 6: Photosystem I reaction center subunit III

Chain F: 16% 82%



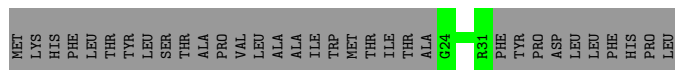
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I: 89% 11%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 20% 80%



- Molecule 9: Photosystem I reaction center subunit XI

Chain L: 83% 13%



- Molecule 10: Photosystem I reaction center subunit XII

Chain M: 97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46105	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL CRYO ARM 200	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.34	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	56497	Depositor
Image detector	GATAN K2 SUMMIT (4k 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: SF4, CLA, LMG, BCR, LHG, PQN

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	0.31	0/6019	0.49	0/8209
2	B	0.31	0/5898	0.50	0/8066
3	C	0.34	0/608	0.55	0/824
4	D	0.30	0/1101	0.53	0/1492
5	E	0.29	0/551	0.48	0/750
6	F	0.29	0/239	0.63	0/326
7	I	0.31	0/312	0.60	0/425
8	J	0.28	0/67	0.49	0/88
9	L	0.28	0/1021	0.48	0/1387
10	M	0.25	0/244	0.51	0/332
All	All	0.31	0/16060	0.50	0/21899

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	5819	0	5686	26	0
2	B	5685	0	5453	27	0
3	C	598	0	588	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1075	0	1077	5	0
5	E	539	0	528	3	0
6	F	231	0	235	1	0
7	I	301	0	306	3	0
8	J	67	0	69	0	0
9	L	994	0	1001	4	0
10	M	241	0	264	0	0
11	A	2422	0	2293	50	0
11	B	1932	0	1849	34	0
11	L	136	0	106	1	0
12	A	33	0	46	20	0
12	B	33	0	46	9	0
13	A	462	0	630	16	0
13	B	230	0	319	7	0
13	F	80	0	112	15	0
13	I	80	0	112	2	0
13	L	40	0	56	0	0
13	M	40	0	56	0	0
14	A	76	0	98	2	0
15	B	8	0	0	0	0
15	C	16	0	0	0	0
16	B	55	0	86	0	0
17	A	1	0	0	0	0
17	B	2	0	0	0	0
17	C	1	0	0	0	0
17	D	1	0	0	0	0
All	All	21198	0	21016	159	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 159 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)
12:A:843:PQN:H303	13:F:201:BCR:C19	1.72	1.20
12:A:843:PQN:H292	13:F:201:BCR:H17C	1.22	1.14
12:B:837:PQN:H242	12:B:837:PQN:H201	1.41	1.02
12:A:843:PQN:H303	13:F:201:BCR:C20	1.92	0.99
12:B:837:PQN:H272	12:B:837:PQN:H241	1.43	0.99

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	A	743/755 (98%)	712 (96%)	31 (4%)	0	100	100
2	B	709/741 (96%)	671 (95%)	38 (5%)	0	100	100
3	C	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
4	D	136/139 (98%)	122 (90%)	14 (10%)	0	100	100
5	E	67/76 (88%)	62 (92%)	5 (8%)	0	100	100
6	F	27/164 (16%)	26 (96%)	1 (4%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	J	6/41 (15%)	6 (100%)	0	0	100	100
9	L	133/155 (86%)	128 (96%)	5 (4%)	0	100	100
10	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
All	All	1964/2221 (88%)	1859 (95%)	105 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	A	593/603 (98%)	593 (100%)	0	100	100
2	B	576/598 (96%)	576 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	E	59/65 (91%)	59 (100%)	0	100	100
6	F	21/128 (16%)	20 (95%)	1 (5%)	25	61
7	I	32/32 (100%)	32 (100%)	0	100	100
8	J	7/36 (19%)	7 (100%)	0	100	100
9	L	103/120 (86%)	103 (100%)	0	100	100
10	M	26/26 (100%)	25 (96%)	1 (4%)	33	67
All	All	1599/1792 (89%)	1597 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	F	82	ARG
10	M	30	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
4	D	71	GLN
9	L	16	HIS
1	A	461	HIS
1	A	542	HIS
1	A	718	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

116 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$
11	CLA	B	805	-	65,73,73	2.09	9 (13%)	76,113,113	1.08	8 (10%)
14	LHG	A	851	-	26,26,48	0.88	1 (3%)	29,32,54	1.34	3 (10%)
11	CLA	A	830	-	65,73,73	2.25	8 (12%)	76,113,113	1.07	8 (10%)
11	CLA	B	829	-	42,50,73	2.85	7 (16%)	48,85,113	1.37	8 (16%)
13	BCR	A	848	-	41,41,41	0.30	0	56,56,56	0.44	0
11	CLA	B	819	-	59,67,73	2.41	8 (13%)	68,105,113	1.32	10 (14%)
11	CLA	A	824	-	64,72,73	2.25	9 (14%)	75,112,113	1.09	8 (10%)
11	CLA	B	825	-	65,73,73	2.30	8 (12%)	76,113,113	1.06	8 (10%)
11	CLA	A	801	-	62,69,73	2.18	10 (16%)	72,107,113	1.18	8 (11%)
13	BCR	A	857	-	26,26,41	0.35	0	34,34,56	0.42	0
11	CLA	B	812	-	43,51,73	2.81	8 (18%)	49,86,113	1.47	7 (14%)
13	BCR	M	101	-	41,41,41	0.32	0	56,56,56	0.39	0
11	CLA	A	828	-	65,73,73	2.09	9 (13%)	76,113,113	1.20	8 (10%)
11	CLA	A	808	-	54,62,73	2.48	8 (14%)	62,99,113	1.34	9 (14%)
11	CLA	A	840	-	41,49,73	2.90	9 (21%)	44,83,113	1.48	6 (13%)
11	CLA	A	821	-	65,73,73	2.18	8 (12%)	76,113,113	1.10	9 (11%)
11	CLA	A	804	-	59,67,73	2.36	8 (13%)	68,105,113	1.26	8 (11%)
11	CLA	B	836	-	43,51,73	2.67	8 (18%)	49,86,113	1.56	8 (16%)
15	SF4	C	102	-	0,12,12	-	-	-	-	-
11	CLA	B	815	-	65,73,73	2.25	8 (12%)	76,113,113	1.23	8 (10%)
13	BCR	A	844	-	41,41,41	0.35	0	56,56,56	0.51	0
11	CLA	A	814	-	41,49,73	2.95	9 (21%)	47,84,113	1.47	8 (17%)
11	CLA	B	827	-	41,49,73	2.85	9 (21%)	47,84,113	1.53	8 (17%)
11	CLA	L	1501	-	34,44,73	3.20	7 (20%)	40,77,113	1.78	10 (25%)
12	PQN	B	837	-	34,34,34	0.37	0	42,45,45	0.38	0
13	BCR	A	853	-	22,22,41	0.53	0	29,29,56	0.42	0
11	CLA	B	820	-	60,68,73	2.28	8 (13%)	70,107,113	1.32	10 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	B	818	-	55,63,73	2.51	9 (16%)	64,101,113	1.24	7 (10%)
11	CLA	B	811	-	65,73,73	2.19	9 (13%)	76,113,113	1.14	9 (11%)
11	CLA	B	830	-	41,49,73	2.89	9 (21%)	47,84,113	1.51	9 (19%)
11	CLA	A	832	-	51,59,73	2.56	8 (15%)	59,96,113	1.36	8 (13%)
11	CLA	A	827	-	65,73,73	2.23	8 (12%)	76,113,113	1.12	9 (11%)
13	BCR	A	861	-	41,41,41	0.28	0	56,56,56	0.56	0
11	CLA	A	860	-	65,73,73	2.20	8 (12%)	76,113,113	1.03	7 (9%)
11	CLA	A	834	-	65,73,73	2.14	8 (12%)	76,113,113	1.12	8 (10%)
11	CLA	A	822	-	49,57,73	2.65	7 (14%)	55,93,113	1.37	8 (14%)
11	CLA	A	815	-	45,53,73	2.70	9 (20%)	52,89,113	1.29	7 (13%)
12	PQN	A	843	-	34,34,34	0.36	0	42,45,45	0.40	0
11	CLA	A	816	-	47,54,73	2.74	10 (21%)	54,89,113	1.46	11 (20%)
11	CLA	A	813	-	65,73,73	2.23	8 (12%)	76,113,113	1.24	8 (10%)
11	CLA	A	837	-	51,59,73	2.54	9 (17%)	59,96,113	1.34	8 (13%)
13	BCR	A	845	-	41,41,41	0.34	0	56,56,56	0.60	0
11	CLA	B	807	-	65,73,73	2.17	8 (12%)	76,113,113	1.18	9 (11%)
11	CLA	B	808	-	62,70,73	2.21	8 (12%)	72,109,113	1.10	7 (9%)
11	CLA	A	836	-	45,53,73	2.68	8 (17%)	52,89,113	1.42	9 (17%)
11	CLA	A	833	-	65,73,73	2.17	9 (13%)	76,113,113	1.12	8 (10%)
11	CLA	A	842	-	39,48,73	2.98	8 (20%)	45,82,113	1.51	11 (24%)
11	CLA	B	828	-	65,73,73	2.27	7 (10%)	76,113,113	1.17	7 (9%)
13	BCR	B	841	-	41,41,41	0.26	0	56,56,56	0.45	0
11	CLA	B	801	-	65,73,73	2.18	8 (12%)	76,113,113	1.18	10 (13%)
11	CLA	A	805	-	65,73,73	2.16	8 (12%)	76,113,113	1.29	10 (13%)
11	CLA	B	835	-	65,73,73	2.22	8 (12%)	76,113,113	1.05	8 (10%)
11	CLA	B	821	-	46,54,73	2.59	9 (19%)	53,90,113	1.35	8 (15%)
11	CLA	B	810	-	65,73,73	2.15	8 (12%)	76,113,113	1.08	9 (11%)
13	BCR	A	847	-	41,41,41	0.28	0	56,56,56	0.32	0
11	CLA	B	802	-	65,73,73	2.19	8 (12%)	76,113,113	1.10	8 (10%)
16	LMG	B	843	-	55,55,55	0.78	2 (3%)	63,63,63	1.36	8 (12%)
11	CLA	A	803	-	42,50,73	2.82	8 (19%)	48,85,113	1.42	8 (16%)
13	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.49	0
11	CLA	B	816	-	65,73,73	2.25	8 (12%)	76,113,113	1.11	9 (11%)
13	BCR	A	852	-	39,40,41	0.32	0	52,53,56	0.98	4 (7%)
11	CLA	B	806	-	46,54,73	2.73	8 (17%)	53,90,113	1.33	7 (13%)
11	CLA	A	807	-	51,59,73	2.49	8 (15%)	59,96,113	1.27	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	841	-	49,57,73	2.58	8 (16%)	55,93,113	1.23	7 (12%)
11	CLA	B	831	-	45,53,73	2.69	7 (15%)	52,89,113	1.31	9 (17%)
11	CLA	B	826	-	45,53,73	2.69	8 (17%)	52,89,113	1.34	7 (13%)
11	CLA	B	814	-	45,53,73	2.76	8 (17%)	52,89,113	1.52	10 (19%)
11	CLA	A	859	-	56,64,73	2.28	9 (16%)	65,102,113	1.22	9 (13%)
11	CLA	B	822	-	43,52,73	2.68	8 (18%)	49,88,113	1.47	8 (16%)
11	CLA	B	833	-	65,73,73	2.27	8 (12%)	76,113,113	1.13	7 (9%)
11	CLA	L	1503	-	42,50,73	2.85	7 (16%)	48,85,113	1.64	9 (18%)
11	CLA	A	838	-	55,63,73	2.44	8 (14%)	64,101,113	1.22	9 (14%)
11	CLA	A	835	-	54,62,73	2.39	8 (14%)	62,99,113	1.19	8 (12%)
11	CLA	B	817	-	43,51,73	2.68	9 (20%)	47,86,113	1.60	10 (21%)
13	BCR	B	839	-	41,41,41	0.28	0	56,56,56	0.50	0
11	CLA	A	823	-	43,51,73	2.71	8 (18%)	49,86,113	1.51	8 (16%)
13	BCR	B	844	-	30,30,41	0.41	0	39,39,56	0.78	2 (5%)
11	CLA	A	817	-	54,62,73	2.45	8 (14%)	62,99,113	1.22	7 (11%)
11	CLA	A	802	-	65,73,73	2.10	8 (12%)	76,113,113	1.12	8 (10%)
13	BCR	A	846	-	41,41,41	0.31	0	56,56,56	0.39	0
11	CLA	B	809	-	65,73,73	2.18	8 (12%)	76,113,113	1.18	7 (9%)
11	CLA	A	809	-	45,53,73	2.74	8 (17%)	52,89,113	1.31	8 (15%)
11	CLA	A	825	-	65,73,73	2.26	8 (12%)	76,113,113	1.14	9 (11%)
13	BCR	A	856	-	29,29,41	0.40	0	37,37,56	1.14	3 (8%)
13	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.33	0
11	CLA	A	818	-	54,62,73	2.42	8 (14%)	62,99,113	1.29	10 (16%)
11	CLA	A	811	-	65,73,73	2.21	8 (12%)	76,113,113	1.28	9 (11%)
11	CLA	A	819	-	65,73,73	2.20	8 (12%)	76,113,113	1.33	12 (15%)
11	CLA	B	834	-	47,55,73	2.55	8 (17%)	54,91,113	1.35	7 (12%)
15	SF4	C	101	-	0,12,12	-	-	-	-	-
11	CLA	B	813	-	43,51,73	2.75	8 (18%)	49,86,113	1.42	7 (14%)
11	CLA	L	1502	-	58,66,73	2.47	9 (15%)	67,104,113	1.48	11 (16%)
13	BCR	B	842	-	41,41,41	0.21	0	56,56,56	0.39	0
11	CLA	A	831	-	49,57,73	2.46	9 (18%)	55,93,113	1.33	7 (12%)
11	CLA	B	823	-	57,65,73	2.33	8 (14%)	66,103,113	1.26	9 (13%)
11	CLA	A	839	-	49,57,73	2.49	9 (18%)	55,93,113	1.32	8 (14%)
15	SF4	B	804	-	0,12,12	-	-	-	-	-
13	BCR	B	840	-	41,41,41	0.25	0	56,56,56	0.70	2 (3%)
11	CLA	B	803	-	65,73,73	2.22	9 (13%)	76,113,113	1.29	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	CLA	A	812	-	53,61,73	2.61	8 (15%)	61,98,113	1.26	8 (13%)
11	CLA	A	806	-	65,73,73	2.20	9 (13%)	76,113,113	1.13	7 (9%)
13	BCR	B	838	-	41,41,41	0.32	0	56,56,56	0.53	1 (1%)
11	CLA	B	824	-	65,73,73	2.14	8 (12%)	76,113,113	1.32	11 (14%)
11	CLA	A	810	-	45,53,73	2.59	7 (15%)	52,89,113	1.26	7 (13%)
13	BCR	F	201	-	41,41,41	0.52	0	56,56,56	1.58	10 (17%)
11	CLA	A	829	-	65,73,73	2.15	9 (13%)	76,113,113	1.12	8 (10%)
11	CLA	A	820	-	41,49,73	2.94	9 (21%)	47,84,113	1.53	8 (17%)
13	BCR	A	858	-	21,21,41	0.31	0	28,28,56	0.62	1 (3%)
13	BCR	A	854	-	21,21,41	0.40	0	28,28,56	0.49	0
14	LHG	A	850	-	48,48,48	0.68	1 (2%)	51,54,54	1.26	6 (11%)
13	BCR	A	855	-	23,24,41	0.49	0	29,30,56	0.94	2 (6%)
11	CLA	A	826	-	60,68,73	2.27	9 (15%)	70,107,113	1.25	8 (11%)
13	BCR	A	849	-	41,41,41	0.44	1 (2%)	56,56,56	1.12	6 (10%)
13	BCR	L	1504	-	41,41,41	0.30	0	56,56,56	0.68	1 (1%)
11	CLA	B	832	-	50,58,73	2.59	8 (16%)	58,95,113	1.33	9 (15%)
13	BCR	F	202	-	41,41,41	0.28	0	56,56,56	1.07	3 (5%)

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
11	CLA	B	805	-	1/1/15/20	4/37/115/115	-
14	LHG	A	851	-	-	14/31/31/53	-
11	CLA	A	830	-	1/1/15/20	5/37/115/115	-
11	CLA	B	829	-	1/1/10/20	1/10/88/115	-
13	BCR	A	848	-	-	2/29/63/63	0/2/2/2
11	CLA	B	819	-	1/1/13/20	3/30/108/115	-
11	CLA	A	824	-	1/1/15/20	7/35/113/115	-
11	CLA	B	825	-	1/1/15/20	3/37/115/115	-
11	CLA	A	801	-	1/1/13/20	2/31/105/115	-
13	BCR	A	857	-	-	0/20/37/63	0/1/1/2
11	CLA	B	812	-	1/1/10/20	1/11/89/115	-
13	BCR	M	101	-	-	2/29/63/63	0/2/2/2
11	CLA	A	828	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	CLA	A	808	-	1/1/12/20	6/24/102/115	-
11	CLA	A	840	-	1/1/9/20	0/5/85/115	-
11	CLA	A	821	-	1/1/15/20	3/37/115/115	-
11	CLA	A	804	-	1/1/13/20	6/30/108/115	-
11	CLA	B	836	-	1/1/10/20	6/11/89/115	-
15	SF4	C	102	-	-	-	0/6/5/5
11	CLA	B	815	-	1/1/15/20	9/37/115/115	-
13	BCR	A	844	-	-	0/29/63/63	0/2/2/2
11	CLA	A	814	-	1/1/10/20	1/8/86/115	-
11	CLA	B	827	-	1/1/10/20	0/8/86/115	-
11	CLA	L	1501	-	1/1/8/20	0/0/74/115	-
12	PQN	B	837	-	-	10/23/43/43	0/2/2/2
13	BCR	A	853	-	-	0/15/32/63	0/1/1/2
11	CLA	B	820	-	1/1/14/20	4/31/109/115	-
11	CLA	B	818	-	1/1/13/20	2/25/103/115	-
11	CLA	B	811	-	1/1/15/20	9/37/115/115	-
11	CLA	B	830	-	1/1/10/20	3/8/86/115	-
11	CLA	A	832	-	1/1/12/20	3/21/99/115	-
11	CLA	A	827	-	1/1/15/20	10/37/115/115	-
13	BCR	A	861	-	-	3/29/63/63	0/2/2/2
11	CLA	A	860	-	1/1/15/20	6/37/115/115	-
11	CLA	A	834	-	1/1/15/20	8/37/115/115	-
11	CLA	A	822	-	1/1/11/20	3/18/96/115	-
11	CLA	A	815	-	1/1/11/20	4/13/91/115	-
12	PQN	A	843	-	-	15/23/43/43	0/2/2/2
11	CLA	A	816	-	1/1/10/20	2/13/87/115	-
11	CLA	A	813	-	1/1/15/20	11/37/115/115	-
11	CLA	A	837	-	1/1/12/20	4/21/99/115	-
13	BCR	A	845	-	-	2/29/63/63	0/2/2/2
11	CLA	B	807	-	1/1/15/20	10/37/115/115	-
11	CLA	B	808	-	1/1/14/20	4/34/112/115	-
11	CLA	A	836	-	1/1/11/20	4/13/91/115	-
11	CLA	A	833	-	1/1/15/20	4/37/115/115	-
11	CLA	A	842	-	1/1/9/20	2/8/82/115	-
11	CLA	B	828	-	1/1/15/20	6/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	B	841	-	-	2/29/63/63	0/2/2/2
11	CLA	B	801	-	1/1/15/20	4/37/115/115	-
11	CLA	A	805	-	1/1/15/20	12/37/115/115	-
11	CLA	B	835	-	1/1/15/20	3/37/115/115	-
11	CLA	B	821	-	1/1/11/20	2/15/93/115	-
11	CLA	B	810	-	1/1/15/20	5/37/115/115	-
13	BCR	A	847	-	-	4/29/63/63	0/2/2/2
11	CLA	B	802	-	1/1/15/20	6/37/115/115	-
16	LMG	B	843	-	-	24/50/70/70	0/1/1/1
11	CLA	A	803	-	1/1/10/20	4/10/88/115	-
13	BCR	I	101	-	-	0/29/63/63	0/2/2/2
11	CLA	B	816	-	1/1/15/20	6/37/115/115	-
13	BCR	A	852	-	-	14/29/60/63	0/2/2/2
11	CLA	B	806	-	1/1/11/20	2/15/93/115	-
11	CLA	A	807	-	1/1/12/20	2/21/99/115	-
11	CLA	A	841	-	1/1/11/20	5/18/96/115	-
11	CLA	B	831	-	1/1/11/20	3/13/91/115	-
11	CLA	B	826	-	1/1/11/20	1/13/91/115	-
11	CLA	B	814	-	1/1/11/20	5/13/91/115	-
11	CLA	A	859	-	1/1/13/20	6/27/105/115	-
11	CLA	B	822	-	1/1/11/20	7/11/89/115	-
11	CLA	B	833	-	1/1/15/20	2/37/115/115	-
11	CLA	L	1503	-	1/1/10/20	0/10/88/115	-
11	CLA	A	838	-	1/1/13/20	2/25/103/115	-
11	CLA	A	835	-	1/1/12/20	2/24/102/115	-
11	CLA	B	817	-	1/1/10/20	4/7/87/115	-
13	BCR	B	839	-	-	4/29/63/63	0/2/2/2
11	CLA	A	823	-	1/1/10/20	2/11/89/115	-
13	BCR	B	844	-	-	0/24/41/63	0/1/1/2
11	CLA	A	817	-	1/1/12/20	6/24/102/115	-
11	CLA	A	802	-	1/1/15/20	2/37/115/115	-
13	BCR	A	846	-	-	0/29/63/63	0/2/2/2
11	CLA	B	809	-	1/1/15/20	3/37/115/115	-
11	CLA	A	809	-	1/1/11/20	0/13/91/115	-
11	CLA	A	825	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	BCR	A	856	-	-	9/23/40/63	0/1/1/2
13	BCR	I	102	-	-	4/29/63/63	0/2/2/2
11	CLA	A	818	-	1/1/12/20	6/24/102/115	-
11	CLA	A	811	-	1/1/15/20	11/37/115/115	-
11	CLA	A	819	-	1/1/15/20	12/37/115/115	-
11	CLA	B	834	-	1/1/11/20	2/16/94/115	-
15	SF4	C	101	-	-	-	0/6/5/5
11	CLA	B	813	-	1/1/10/20	0/11/89/115	-
11	CLA	L	1502	-	1/1/13/20	2/29/107/115	-
13	BCR	B	842	-	-	4/29/63/63	0/2/2/2
11	CLA	A	831	-	1/1/11/20	4/18/96/115	-
11	CLA	B	823	-	1/1/13/20	7/28/106/115	-
11	CLA	A	839	-	1/1/11/20	2/18/96/115	-
15	SF4	B	804	-	-	-	0/6/5/5
13	BCR	B	840	-	-	6/29/63/63	0/2/2/2
11	CLA	B	803	-	1/1/15/20	7/37/115/115	-
11	CLA	A	812	-	1/1/12/20	2/22/100/115	-
11	CLA	A	806	-	1/1/15/20	7/37/115/115	-
13	BCR	B	838	-	-	0/29/63/63	0/2/2/2
11	CLA	B	824	-	1/1/15/20	4/37/115/115	-
11	CLA	A	810	-	1/1/11/20	4/13/91/115	-
13	BCR	F	201	-	-	12/29/63/63	0/2/2/2
11	CLA	A	829	-	1/1/15/20	5/37/115/115	-
11	CLA	A	820	-	1/1/10/20	2/8/86/115	-
13	BCR	A	858	-	-	2/14/31/63	0/1/1/2
13	BCR	A	854	-	-	0/14/31/63	0/1/1/2
14	LHG	A	850	-	-	22/53/53/53	-
13	BCR	A	855	-	-	1/18/32/63	0/1/1/2
11	CLA	A	826	-	1/1/14/20	4/31/109/115	-
13	BCR	A	849	-	-	12/29/63/63	0/2/2/2
13	BCR	L	1504	-	-	3/29/63/63	0/2/2/2
11	CLA	B	832	-	1/1/12/20	2/19/97/115	-
13	BCR	F	202	-	-	0/29/63/63	0/2/2/2

The worst 5 of 681 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	812	CLA	C4B-NB	14.92	1.48	1.35
11	A	816	CLA	C4B-NB	14.56	1.48	1.35
11	B	825	CLA	C4B-NB	14.49	1.48	1.35
11	B	832	CLA	C4B-NB	14.47	1.48	1.35
11	A	814	CLA	C4B-NB	14.46	1.48	1.35

The worst 5 of 740 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	L	1502	CLA	C4A-NA-C1A	-7.42	103.37	106.71
11	A	805	CLA	C4A-NA-C1A	-6.85	103.63	106.71
11	B	824	CLA	C4A-NA-C1A	-6.80	103.65	106.71
11	L	1503	CLA	C4A-NA-C1A	-6.75	103.67	106.71
11	B	803	CLA	C4A-NA-C1A	-6.74	103.67	106.71

5 of 82 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	A	801	CLA	ND
11	A	802	CLA	ND
11	A	803	CLA	ND
11	A	804	CLA	ND
11	A	805	CLA	ND

5 of 522 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	803	CLA	CAD-CBD-CGD-O1D
11	A	803	CLA	CAD-CBD-CGD-O2D
11	A	806	CLA	C1A-C2A-CAA-CBA
11	A	808	CLA	CHA-CBD-CGD-O1D
11	A	808	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

75 monomers are involved in 127 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	805	CLA	3	0
14	A	851	LHG	2	0
11	A	830	CLA	1	0
11	B	829	CLA	1	0
13	A	848	BCR	1	0

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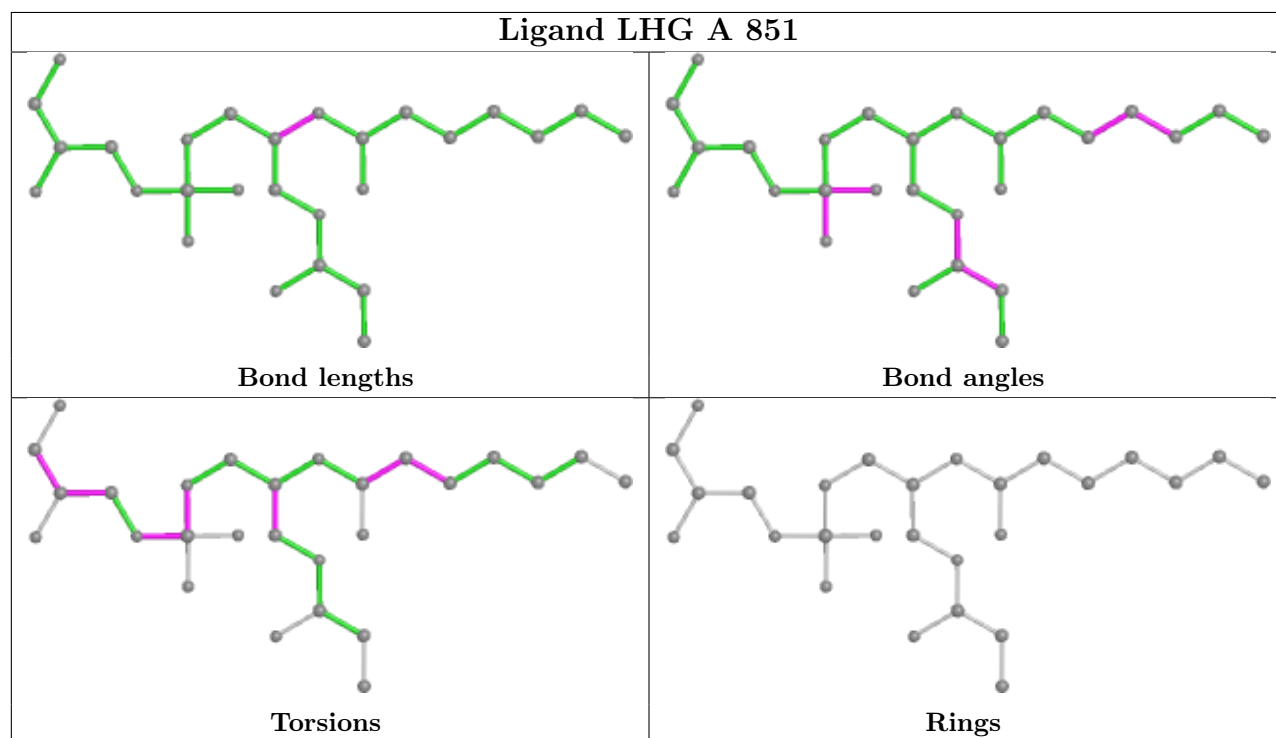
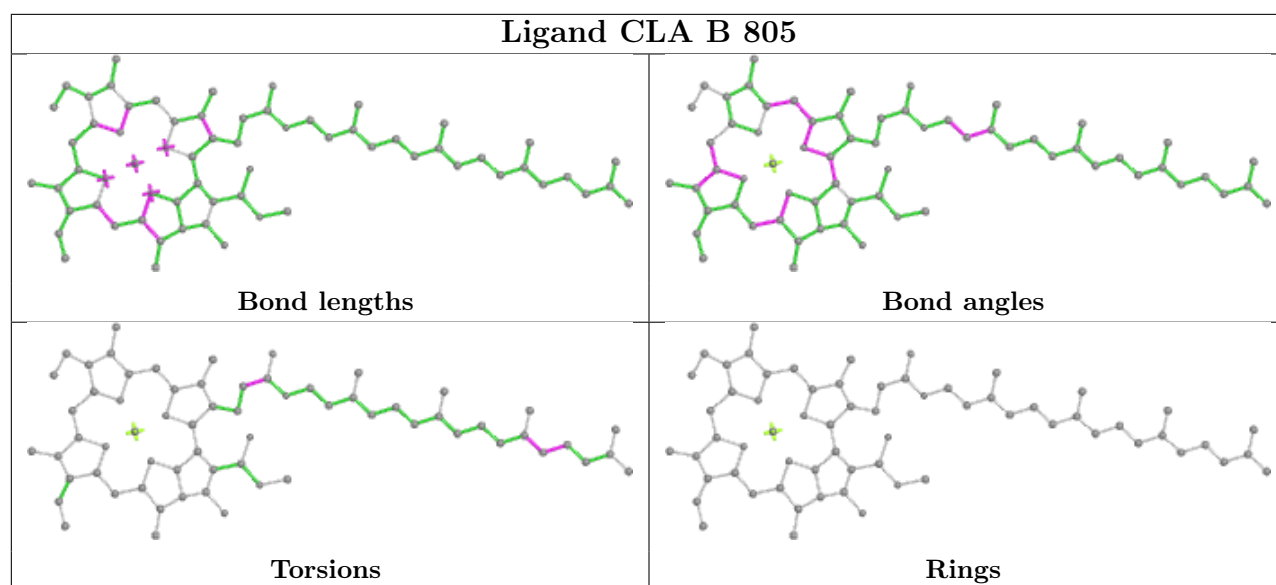
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	824	CLA	2	0
11	B	825	CLA	1	0
13	A	857	BCR	2	0
11	B	812	CLA	1	0
11	A	828	CLA	2	0
11	A	808	CLA	3	0
11	A	840	CLA	1	0
11	A	821	CLA	4	0
11	B	836	CLA	1	0
11	B	815	CLA	4	0
13	A	844	BCR	2	0
12	B	837	PQN	9	0
11	B	820	CLA	1	0
11	B	818	CLA	2	0
11	B	811	CLA	2	0
11	A	860	CLA	1	0
11	A	815	CLA	1	0
12	A	843	PQN	20	0
11	A	813	CLA	2	0
11	A	837	CLA	3	0
13	A	845	BCR	2	0
11	B	807	CLA	2	0
11	B	808	CLA	2	0
11	A	836	CLA	2	0
11	A	842	CLA	1	0
11	B	828	CLA	2	0
13	B	841	BCR	2	0
11	A	805	CLA	3	0
11	B	835	CLA	2	0
11	B	821	CLA	1	0
11	B	802	CLA	4	0
13	I	101	BCR	2	0
11	B	816	CLA	2	0
13	A	852	BCR	2	0
11	A	841	CLA	2	0
11	A	859	CLA	2	0
11	L	1503	CLA	1	0
11	A	838	CLA	2	0
11	A	835	CLA	2	0
11	B	817	CLA	1	0
13	B	844	BCR	2	0
11	A	817	CLA	4	0

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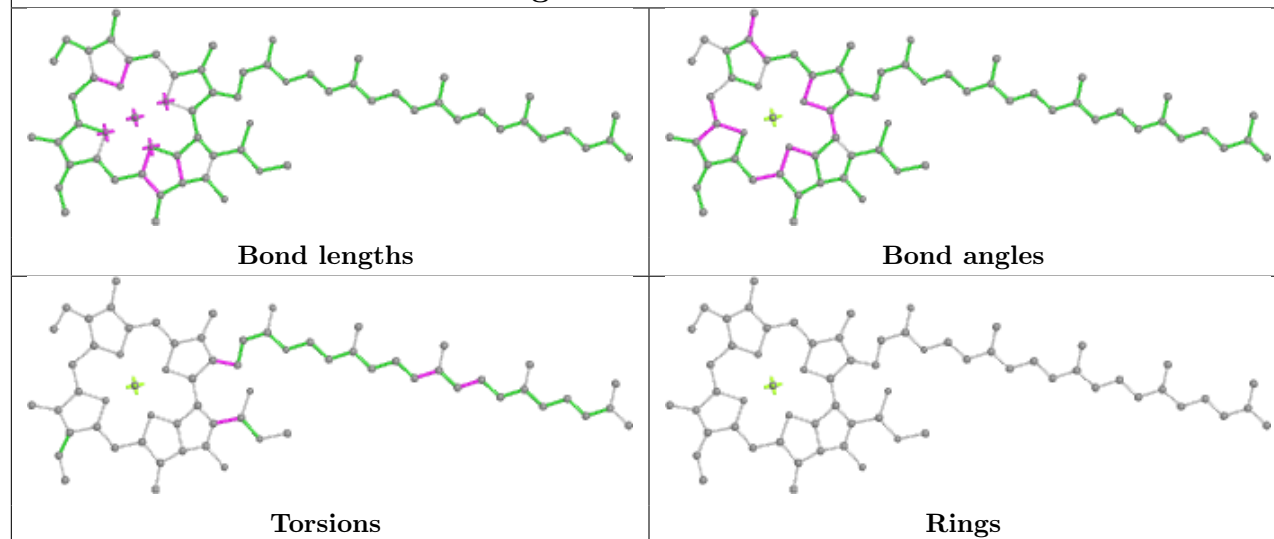
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	802	CLA	1	0
13	A	846	BCR	1	0
11	B	809	CLA	1	0
11	A	809	CLA	3	0
11	A	825	CLA	2	0
11	A	818	CLA	3	0
11	A	811	CLA	3	0
11	A	819	CLA	1	0
11	B	834	CLA	1	0
11	B	813	CLA	1	0
13	B	842	BCR	1	0
11	A	831	CLA	1	0
13	B	840	BCR	1	0
11	B	803	CLA	1	0
11	A	812	CLA	1	0
11	A	806	CLA	2	0
13	B	838	BCR	1	0
11	B	824	CLA	3	0
11	A	810	CLA	2	0
13	F	201	BCR	13	0
11	A	829	CLA	1	0
11	A	820	CLA	1	0
13	A	858	BCR	2	0
13	A	854	BCR	1	0
13	A	855	BCR	2	0
11	A	826	CLA	1	0
13	A	849	BCR	2	0
13	F	202	BCR	2	0

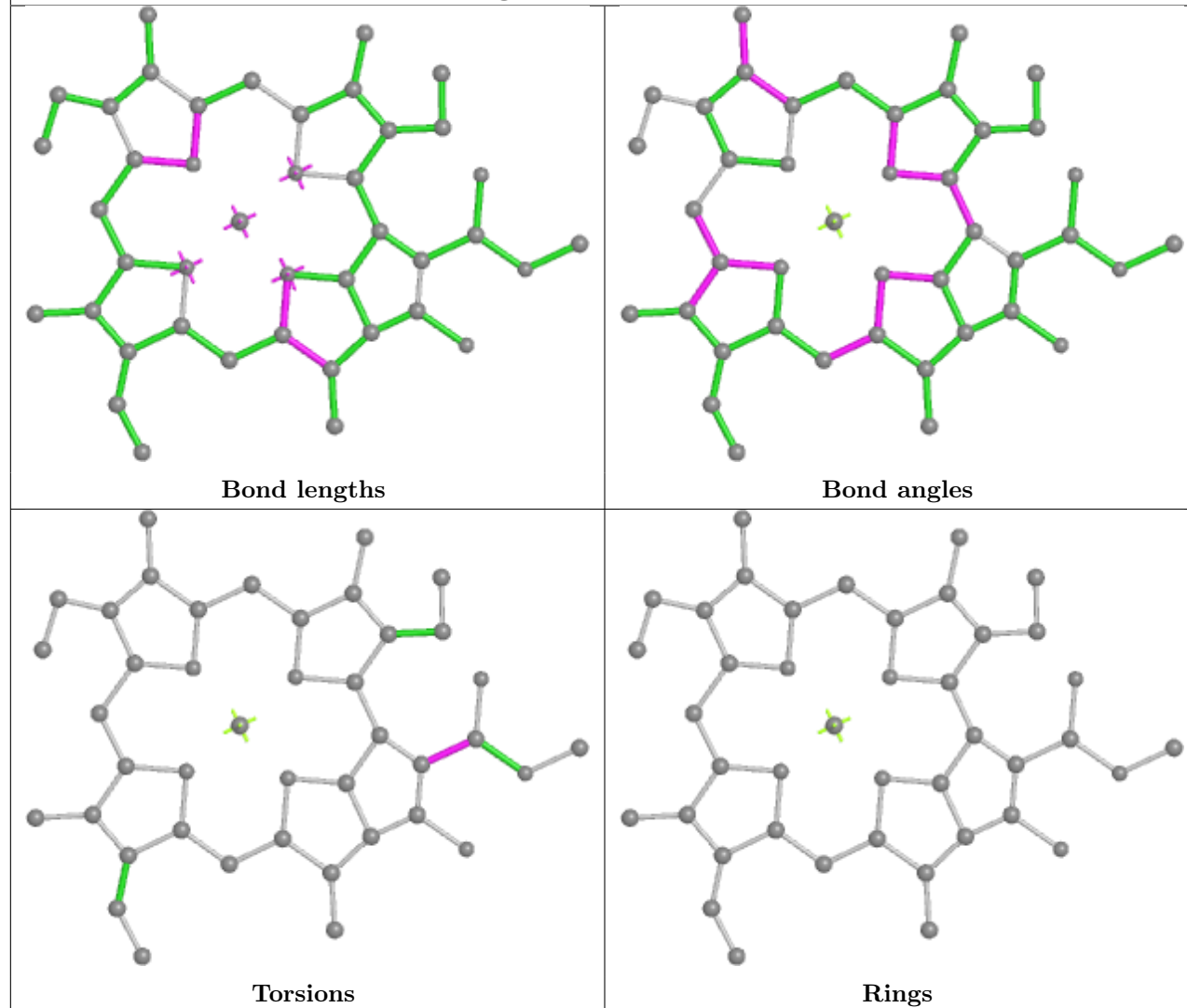
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

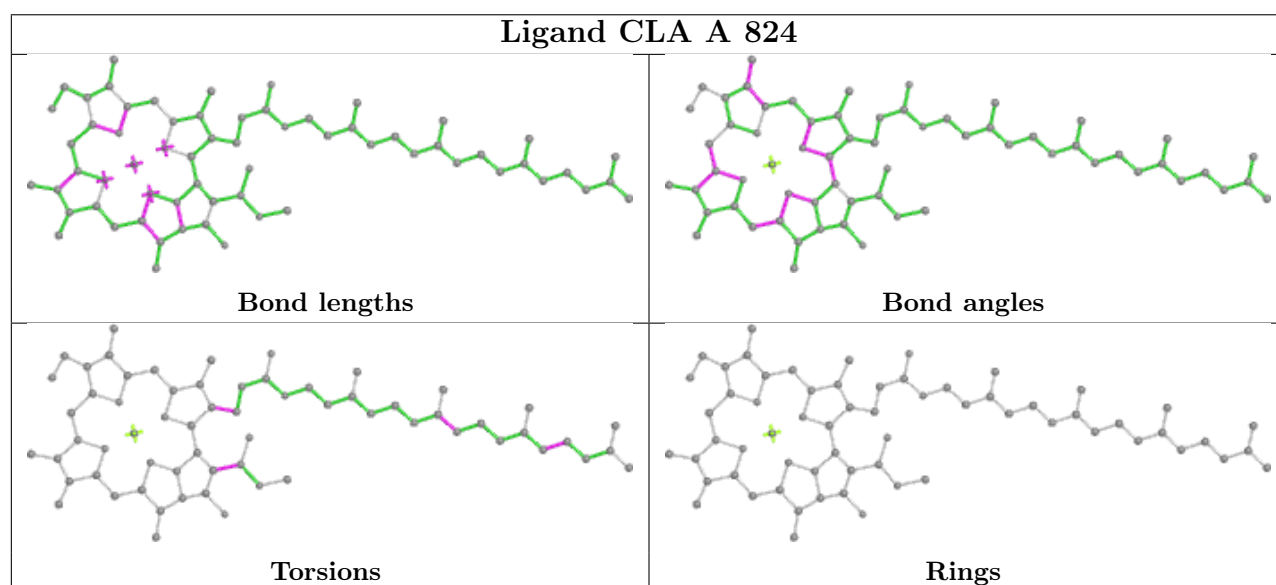
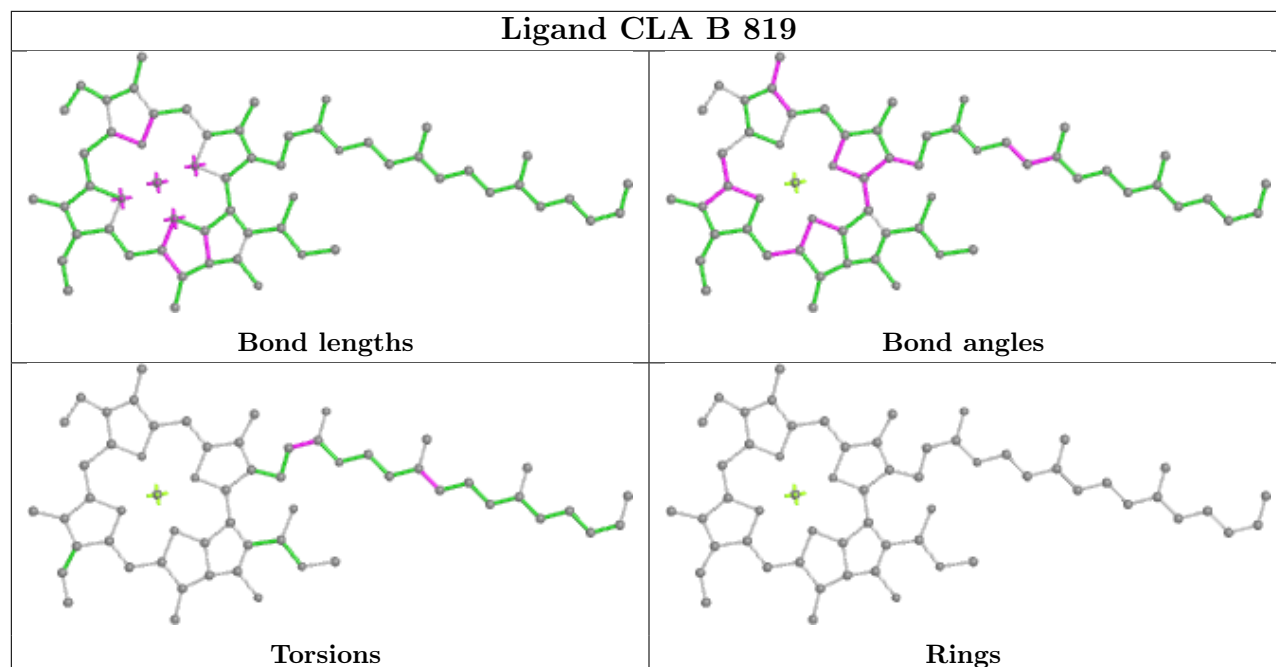
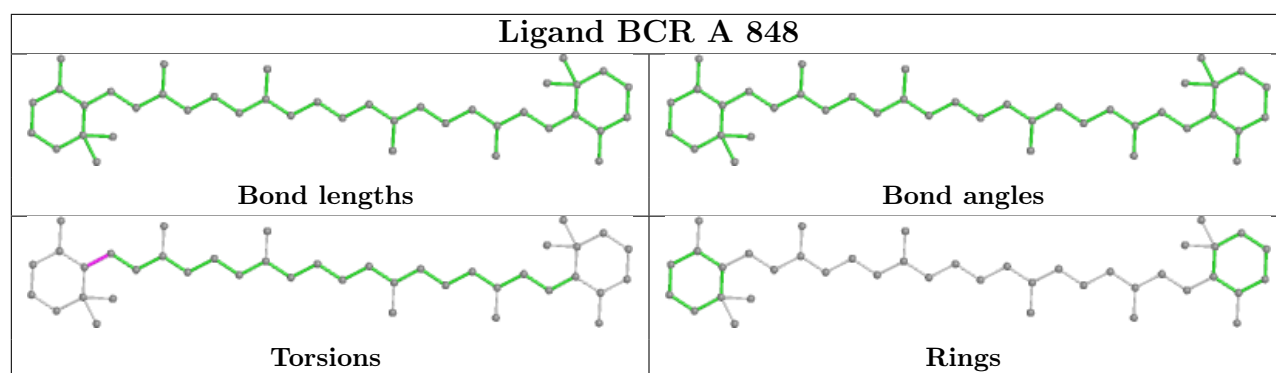


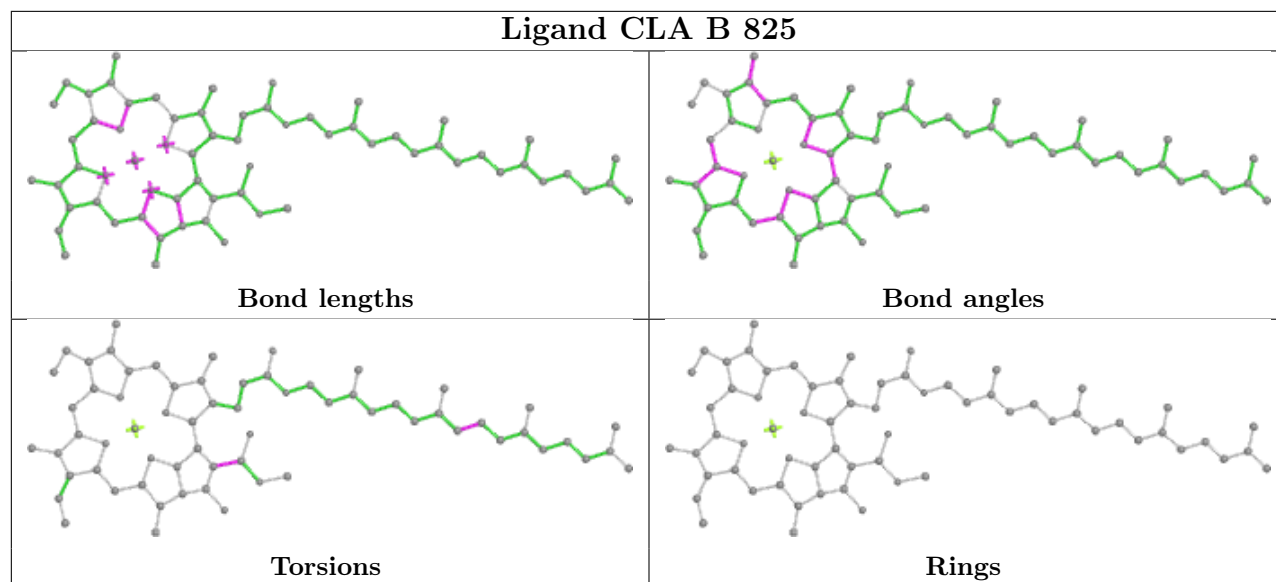
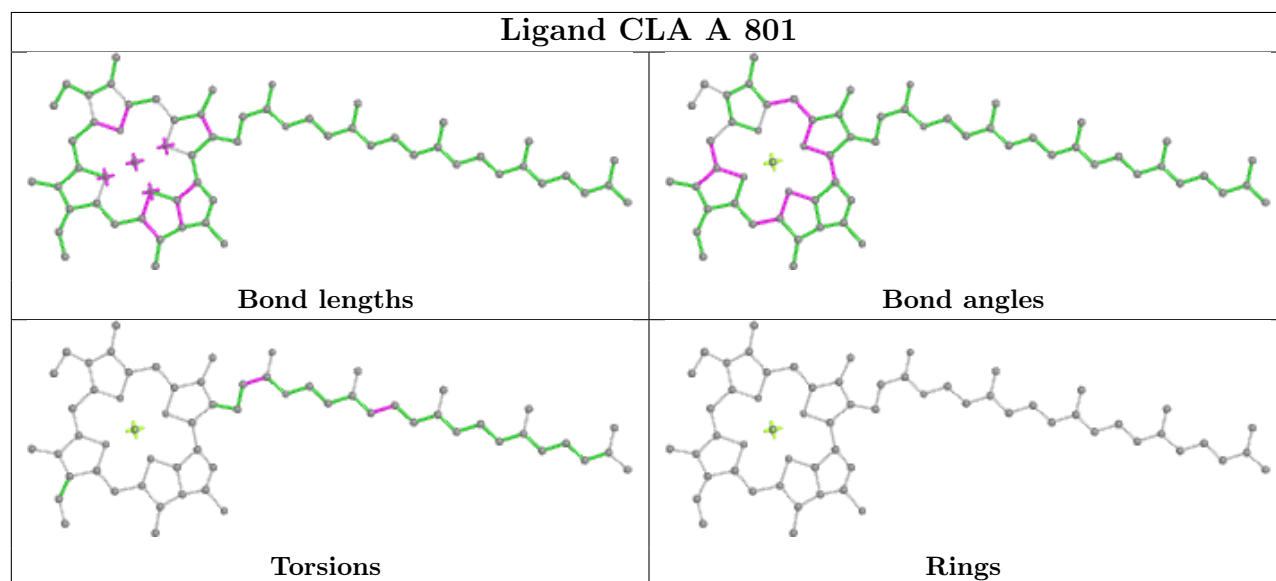
Ligand CLA A 830



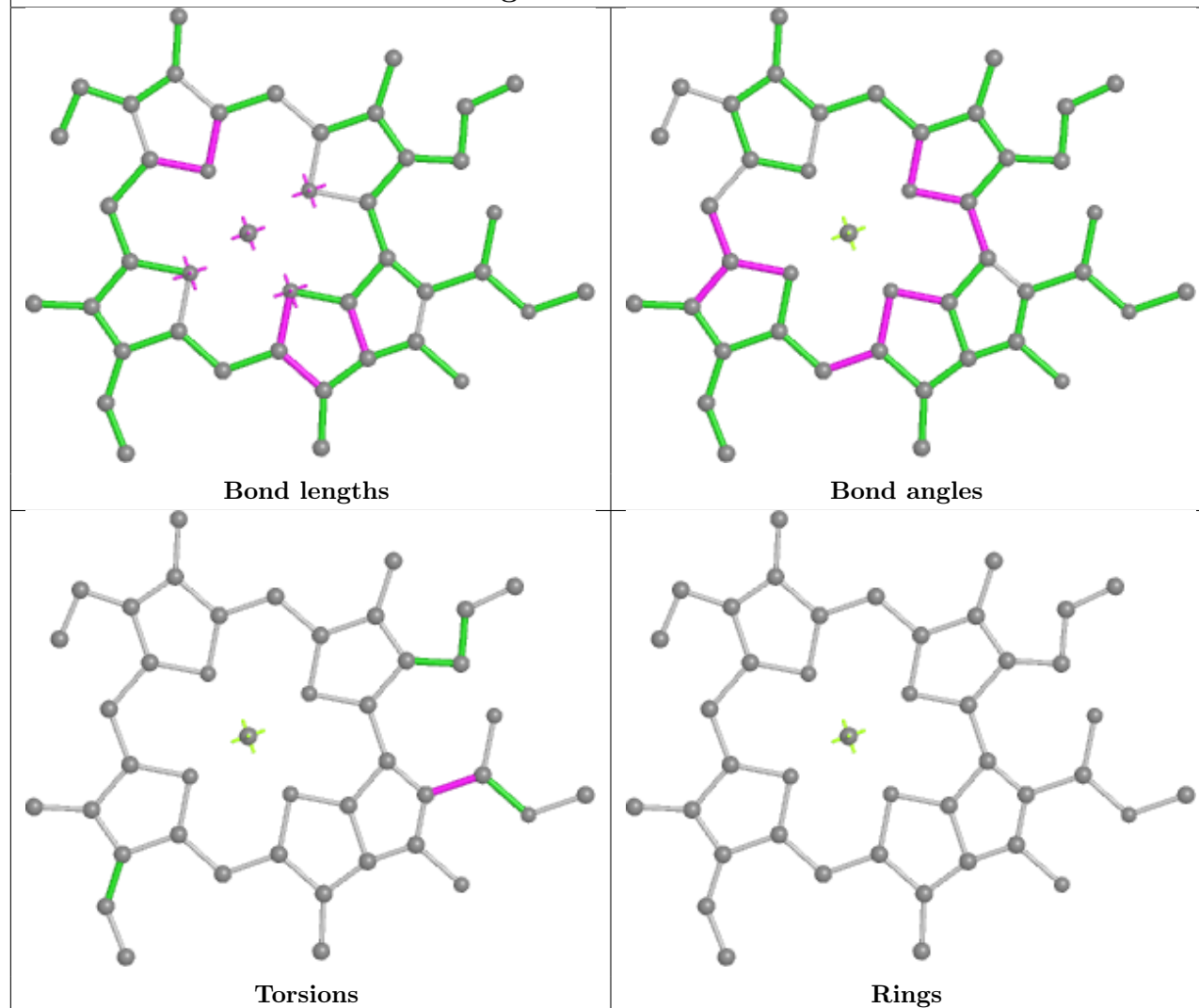
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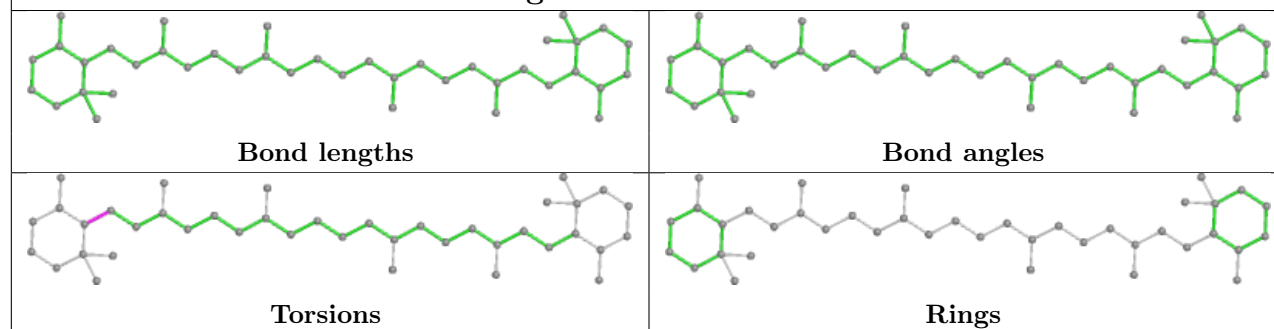


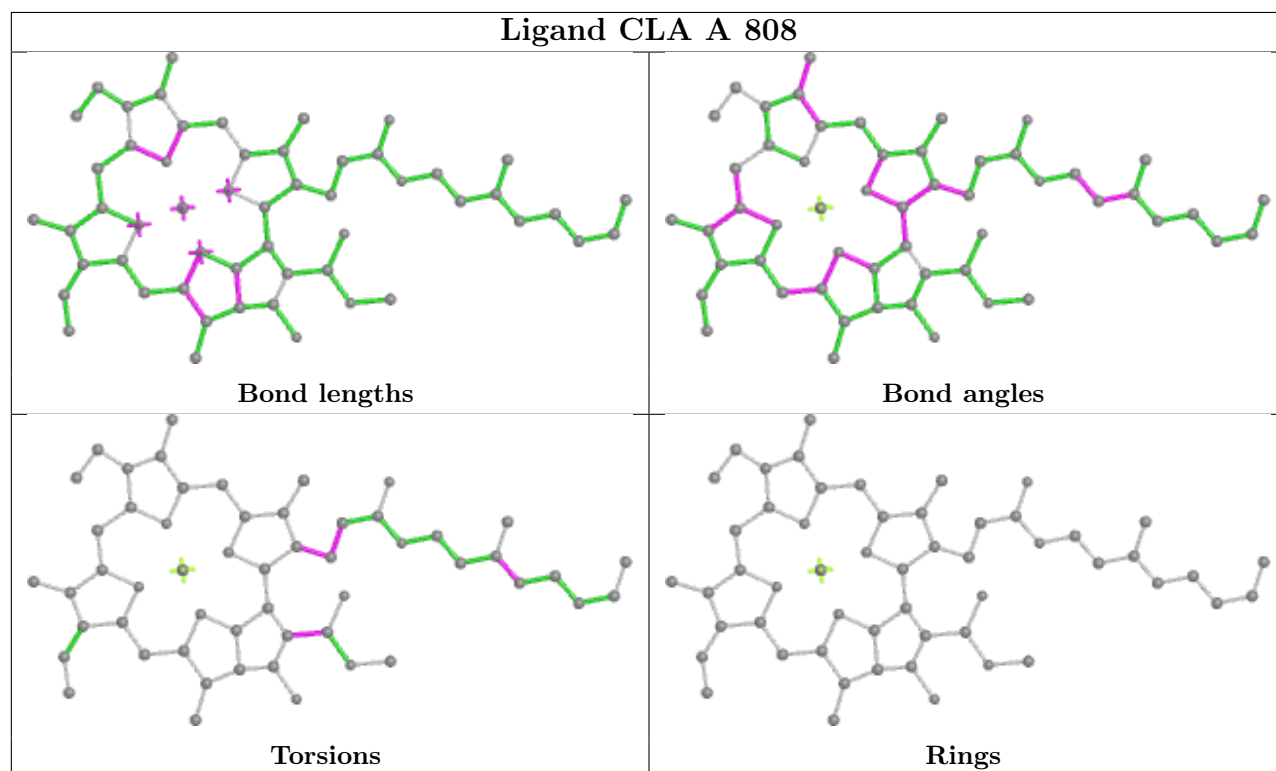
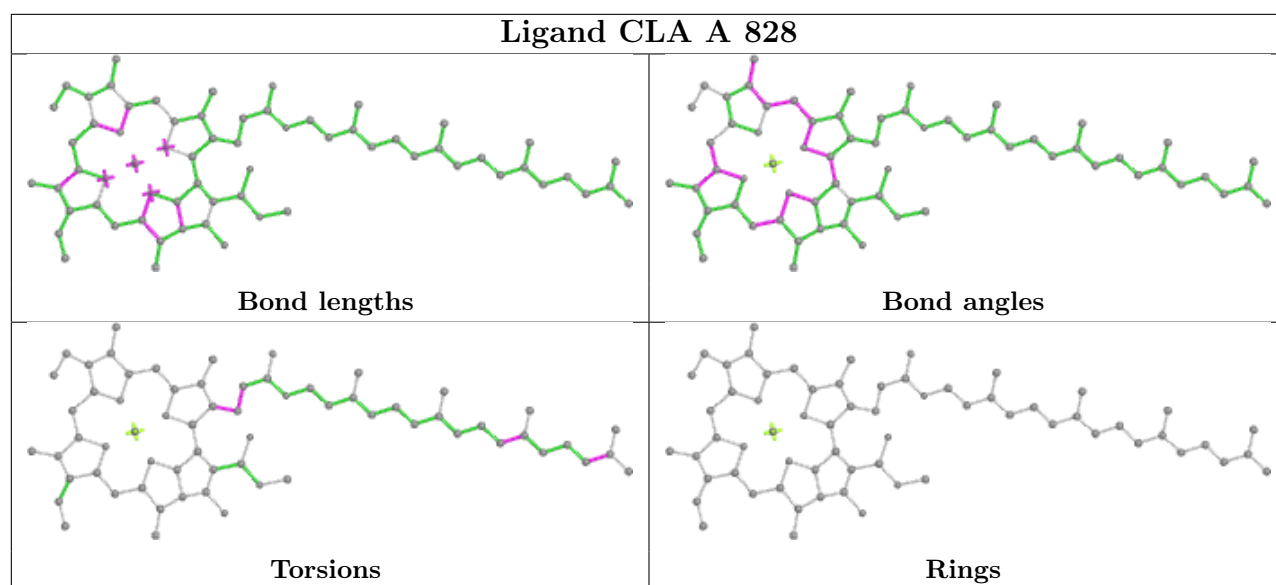
Ligand CLA B 825**Ligand CLA A 801**

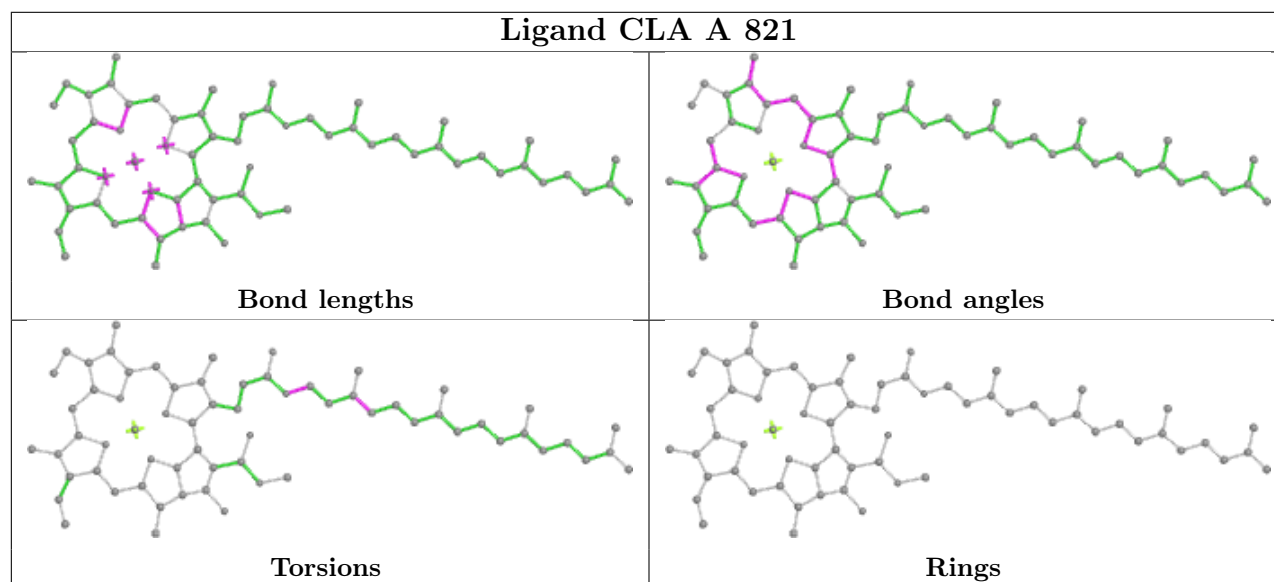
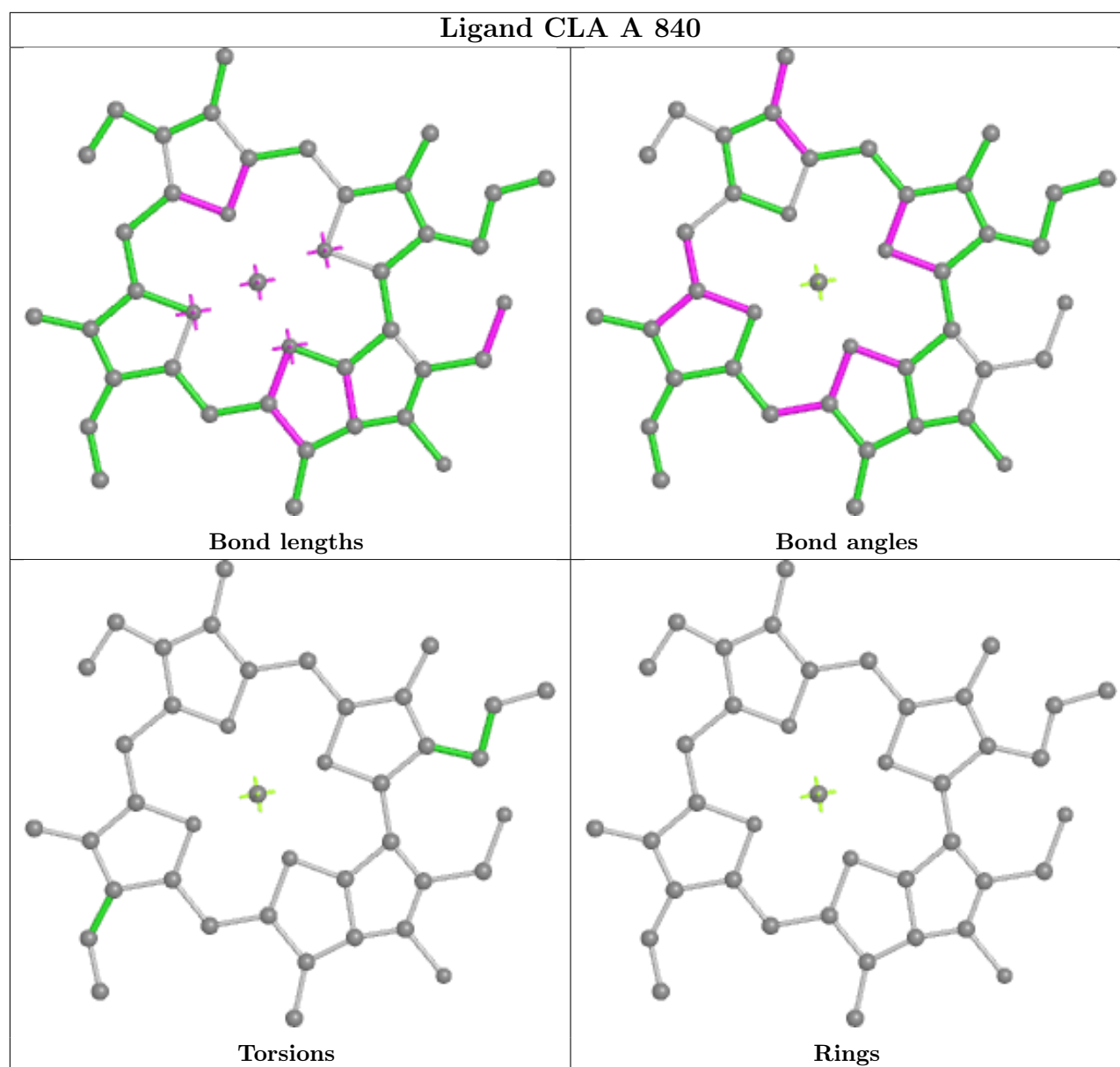
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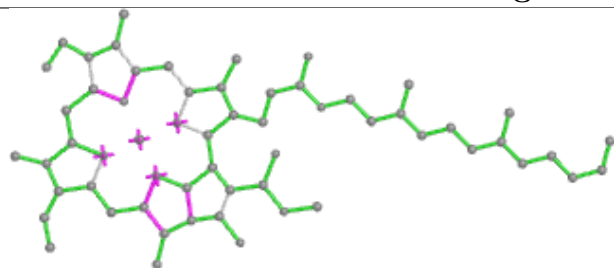
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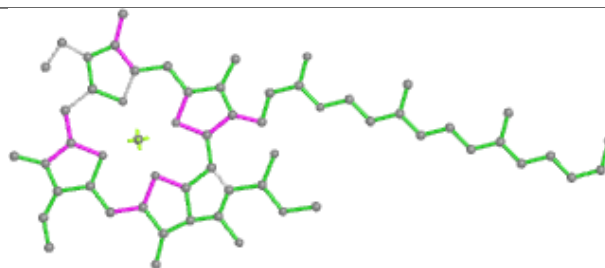




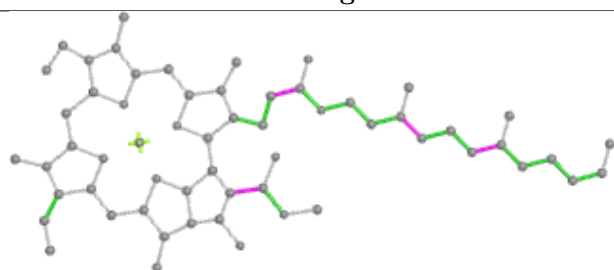
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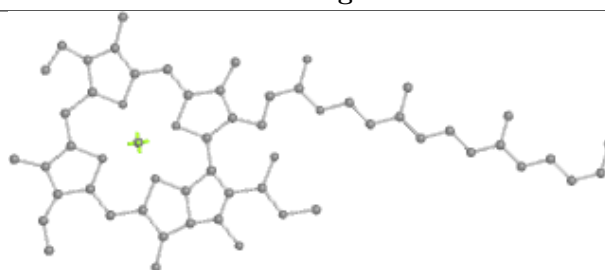
Bond lengths



Bond angles

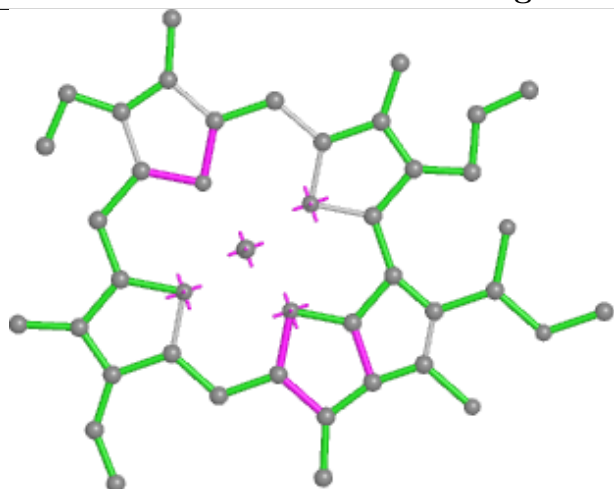


Torsions

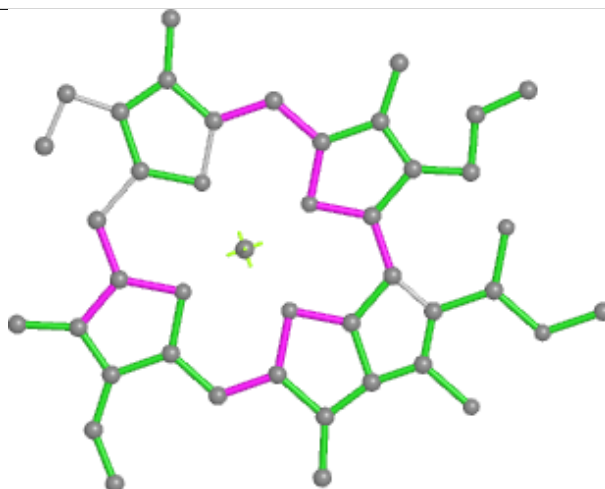


Rings

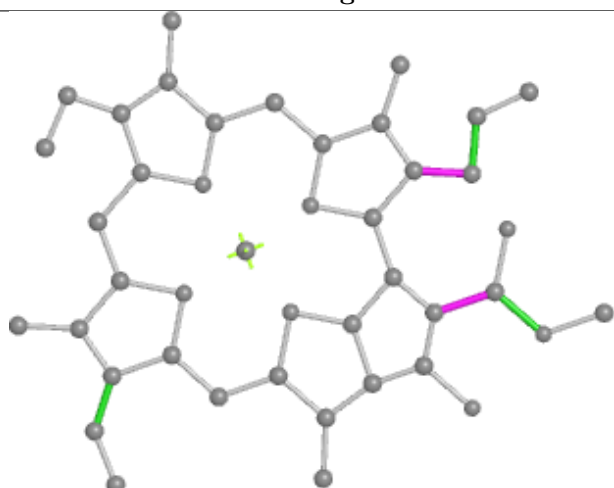
Ligand CLA B 836



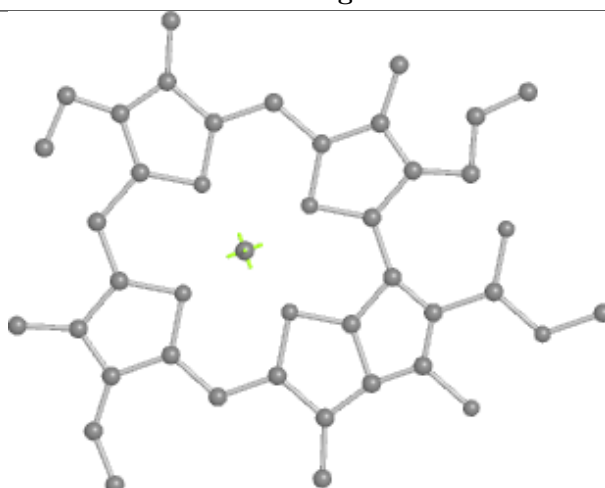
Bond lengths



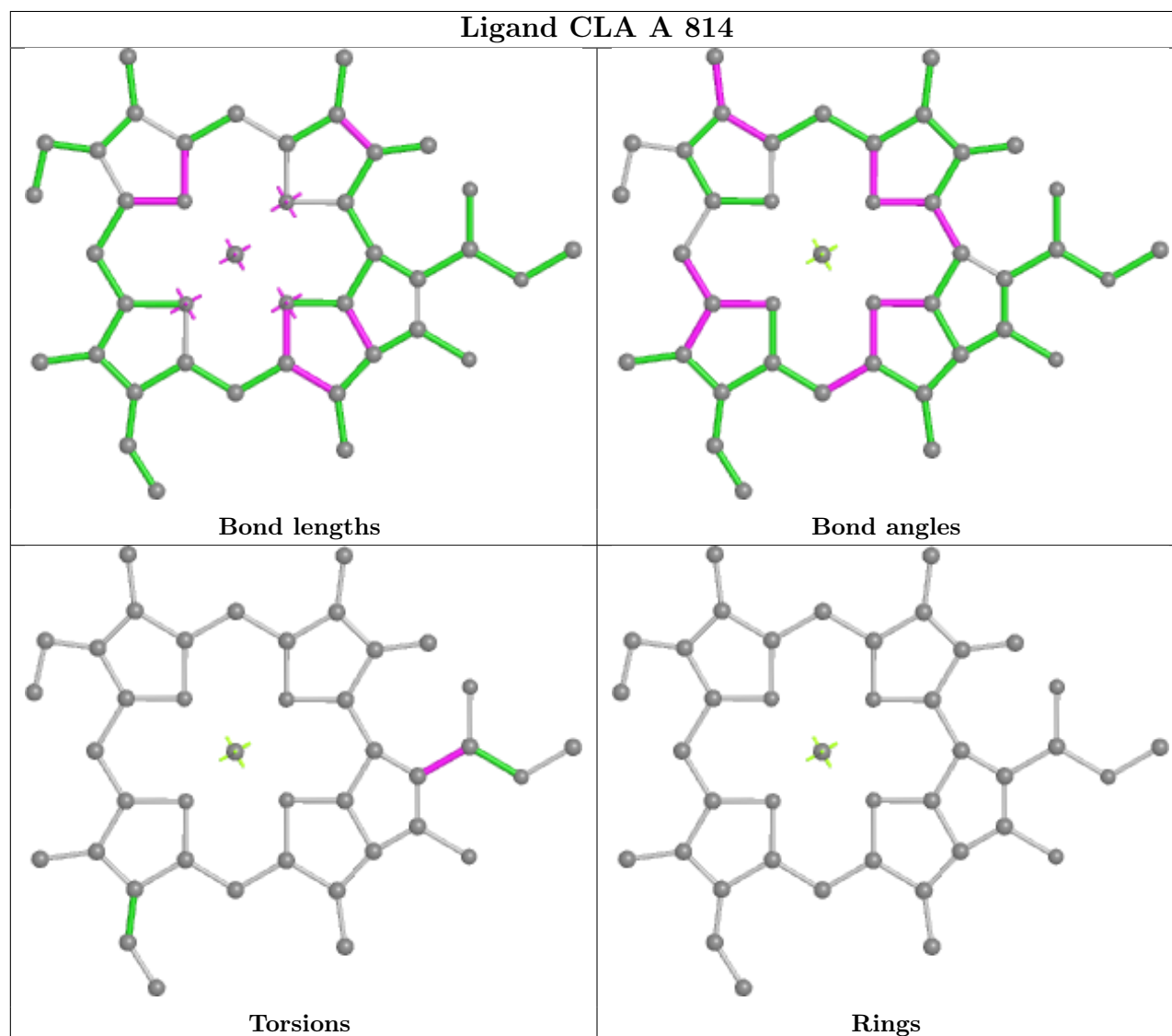
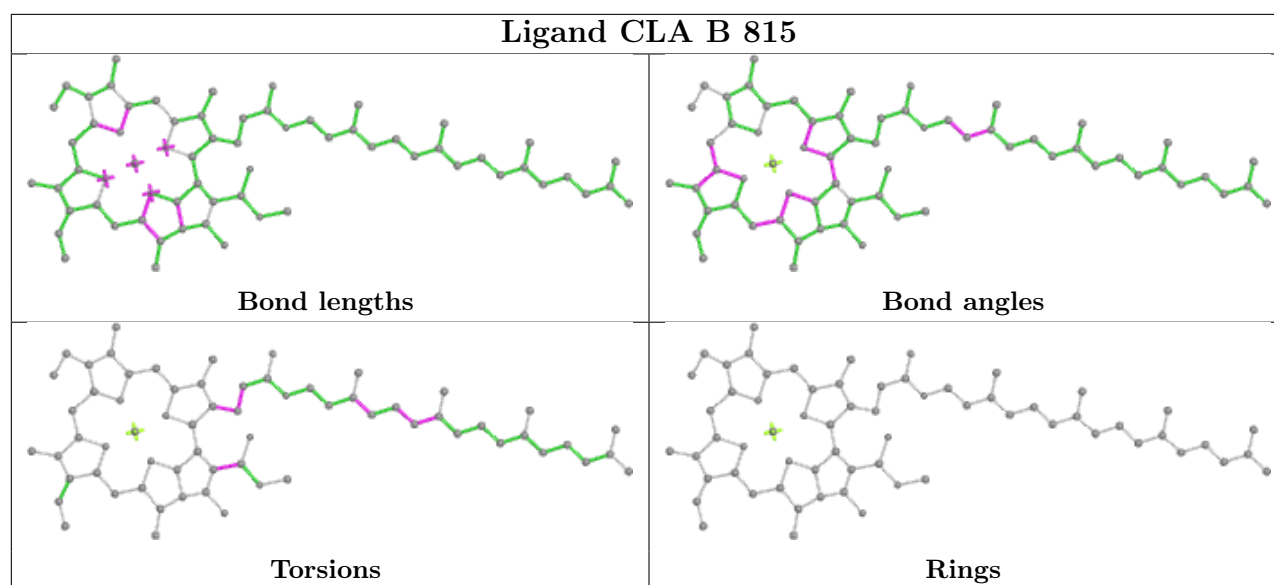
Bond angles

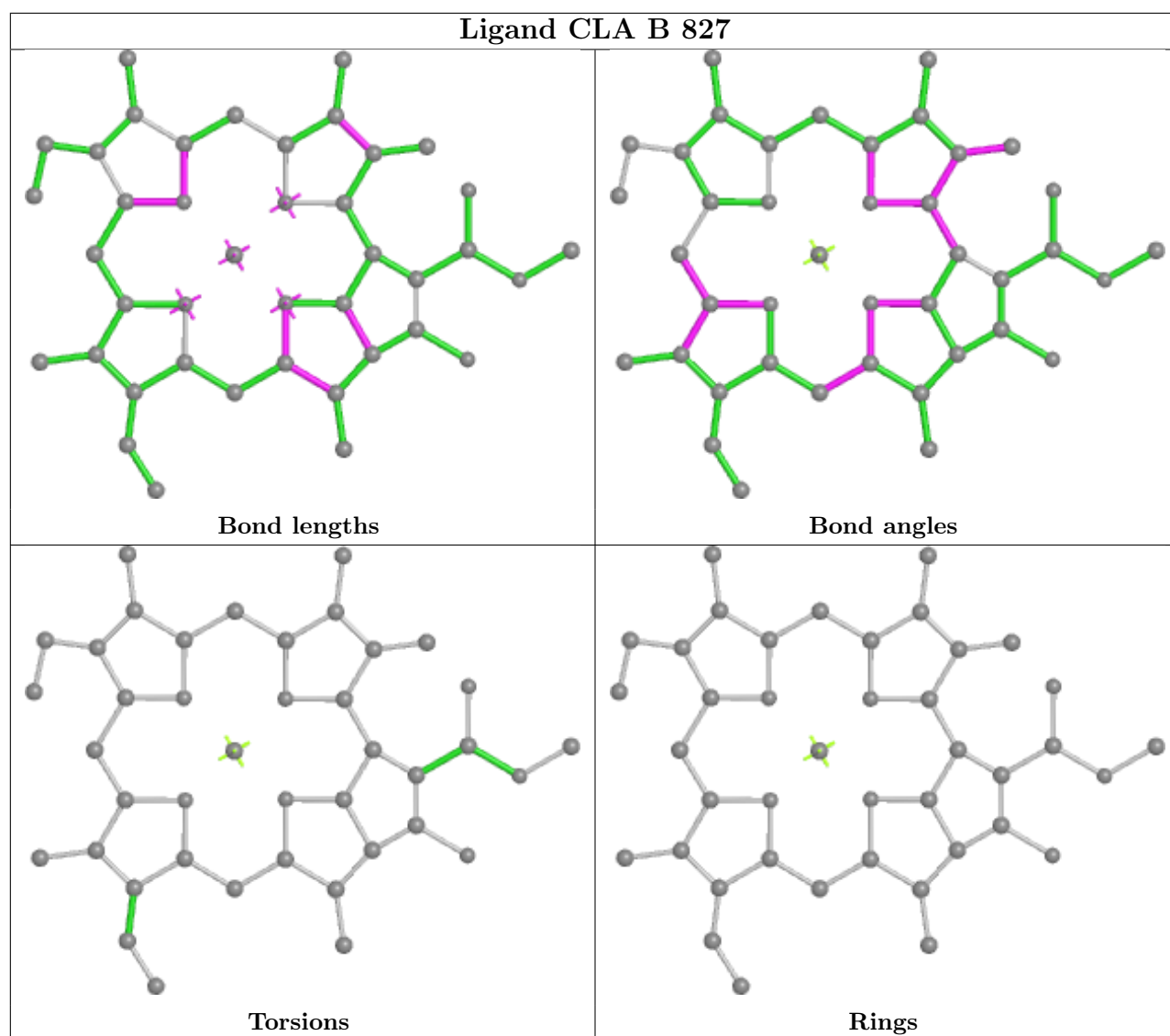


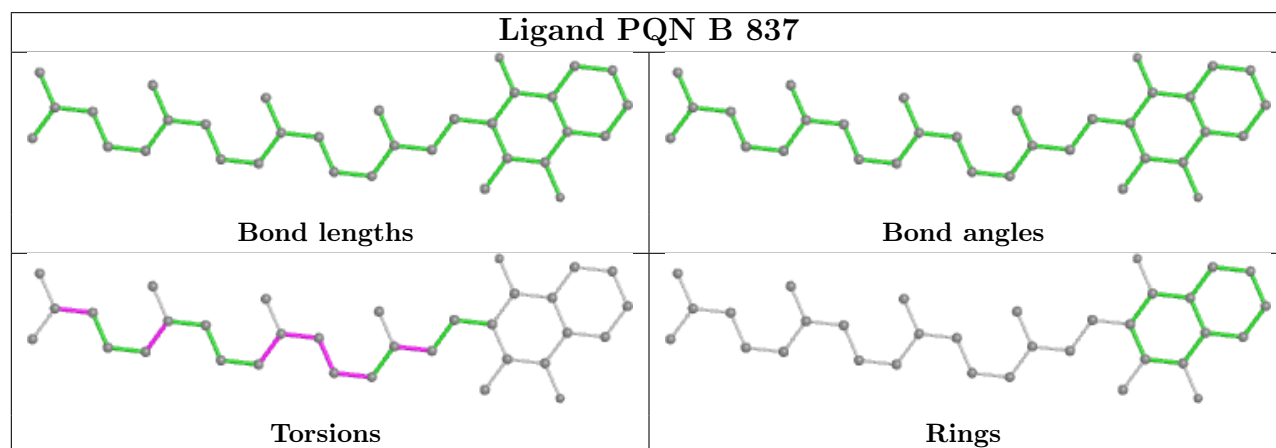
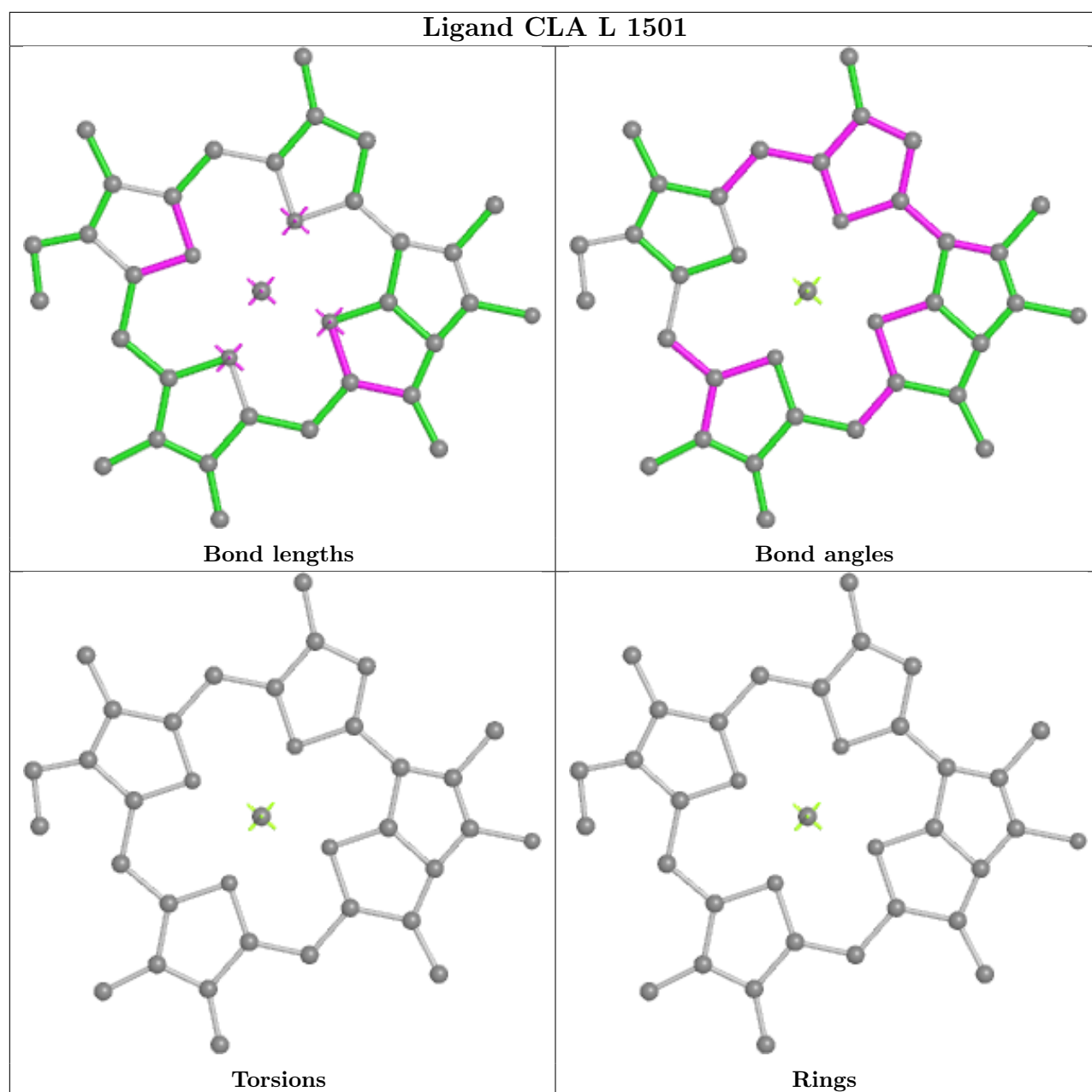
Torsions



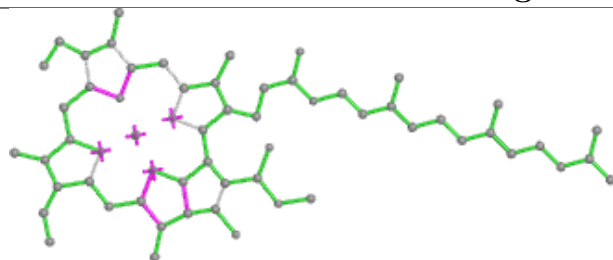
Rings



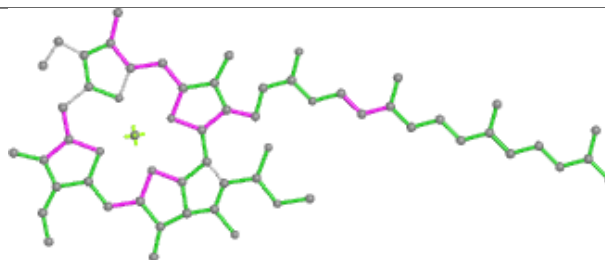




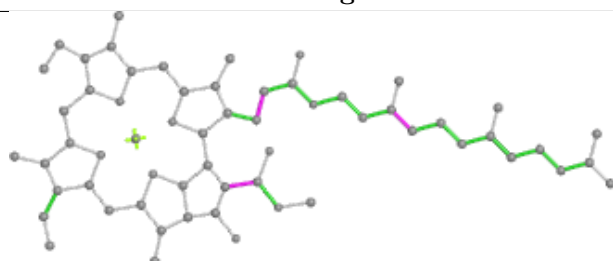
Ligand CLA B 820



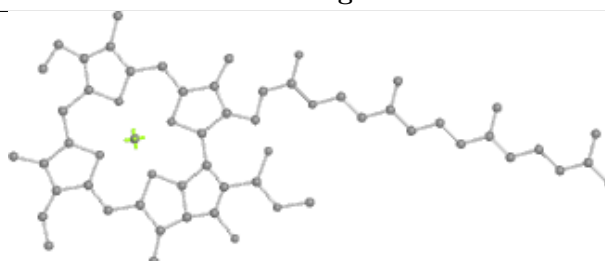
Bond lengths



Bond angles

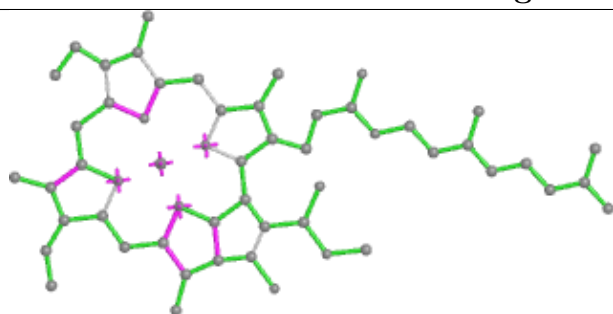


Torsions

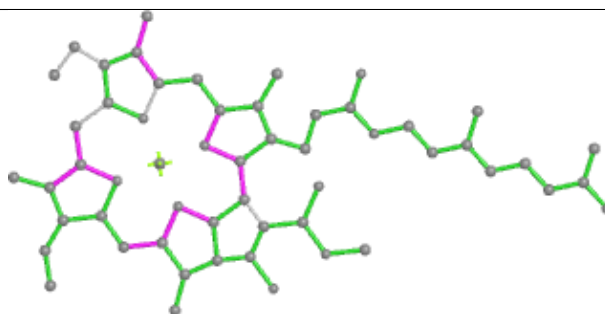


Rings

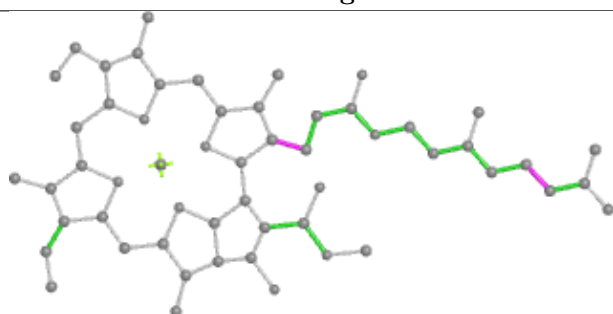
Ligand CLA B 818



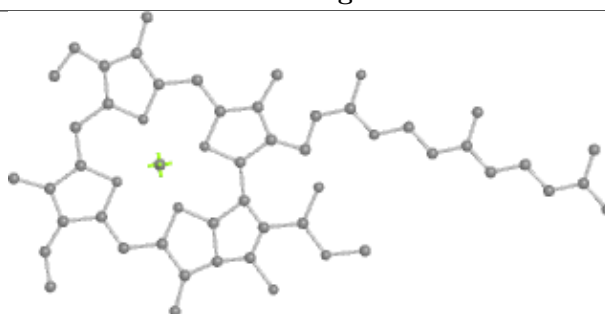
Bond lengths



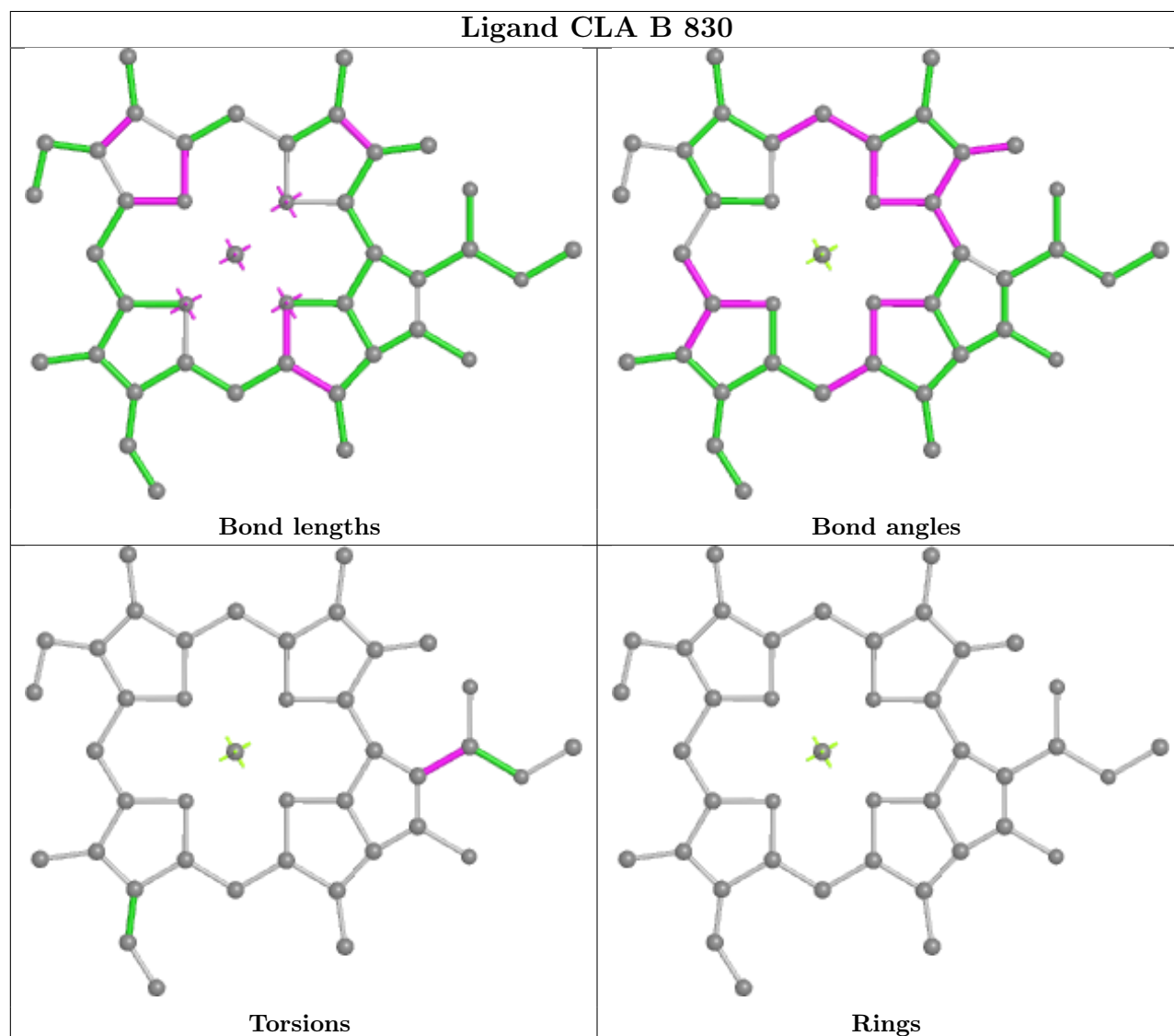
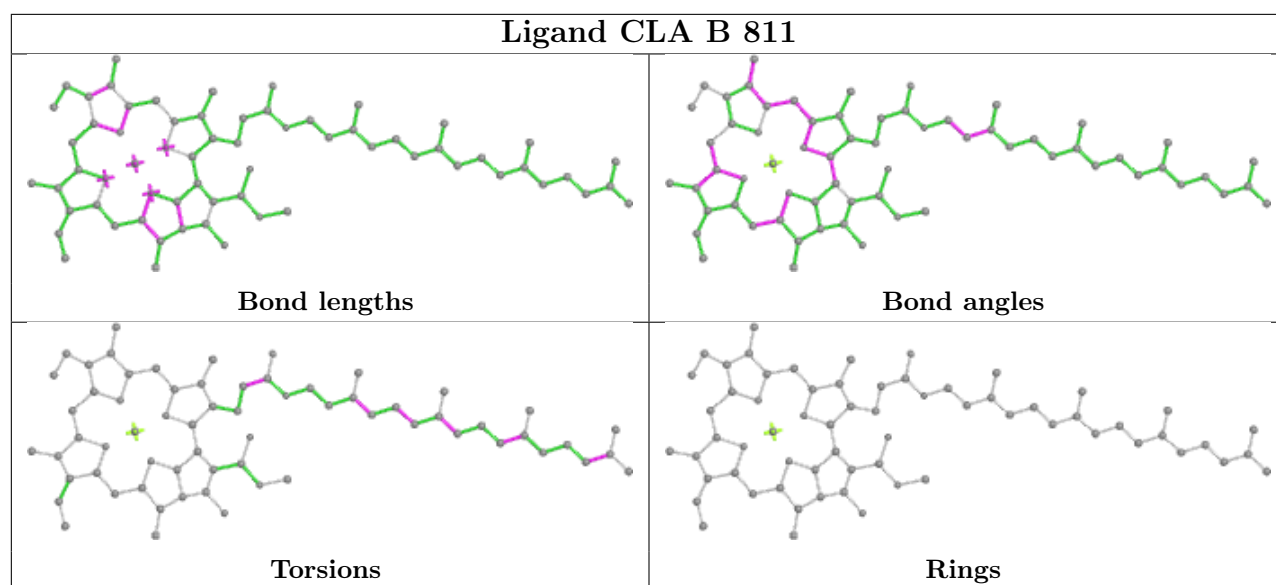
Bond angles

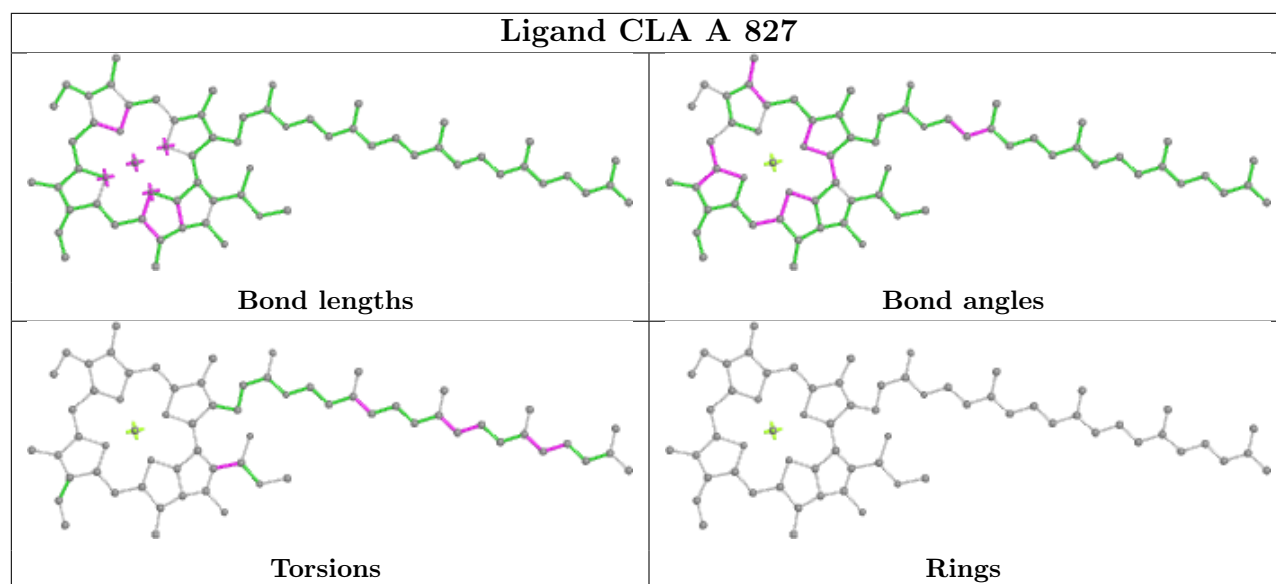
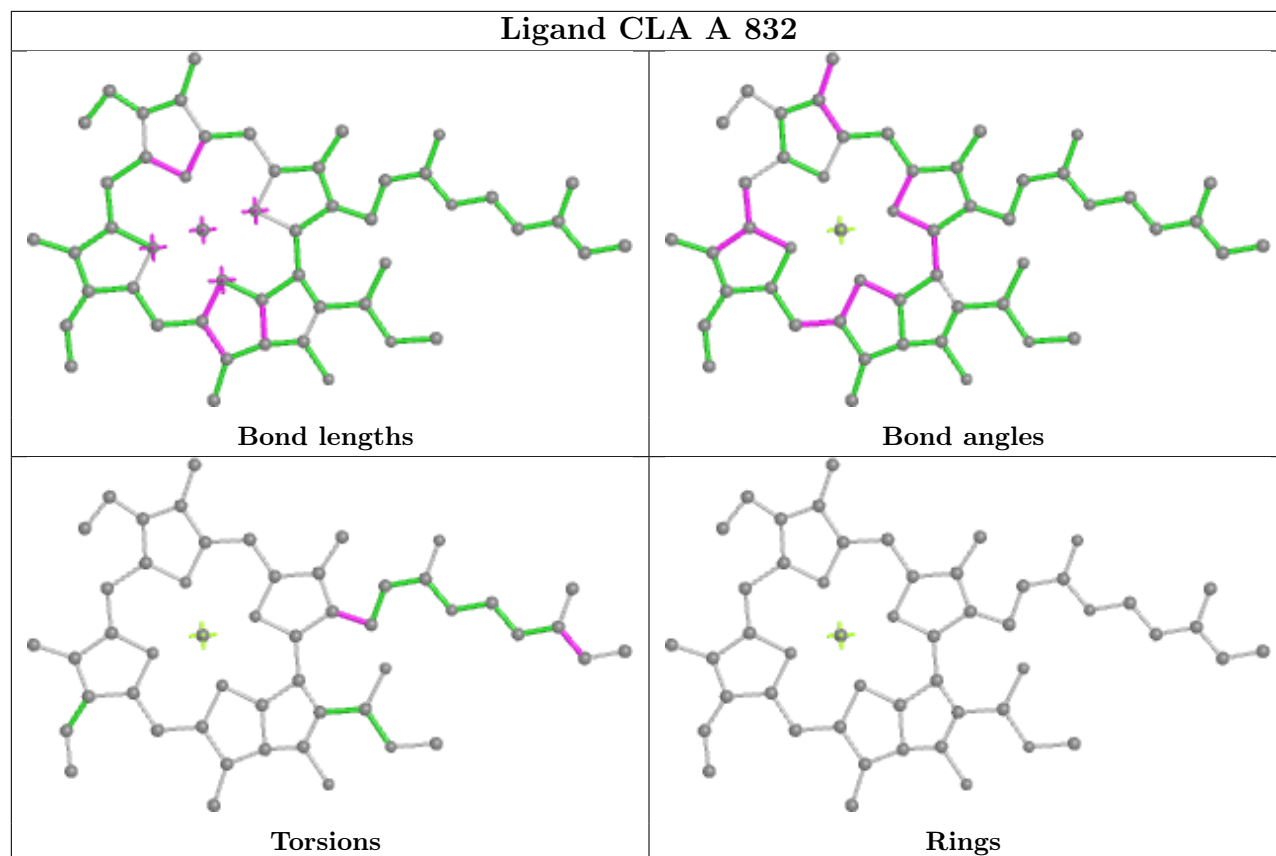


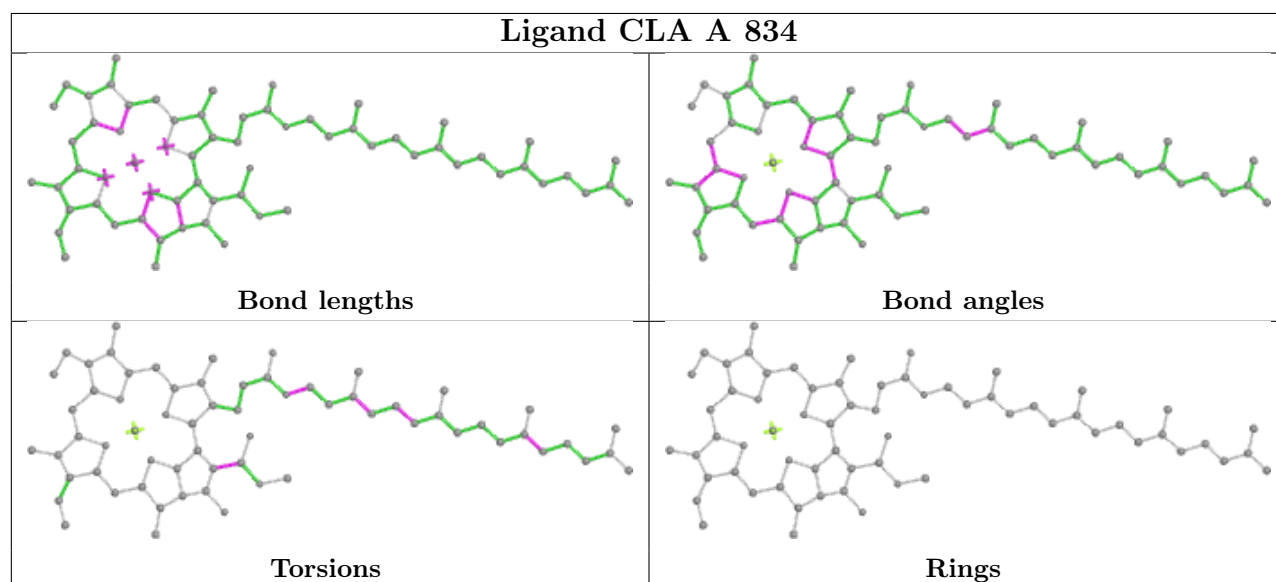
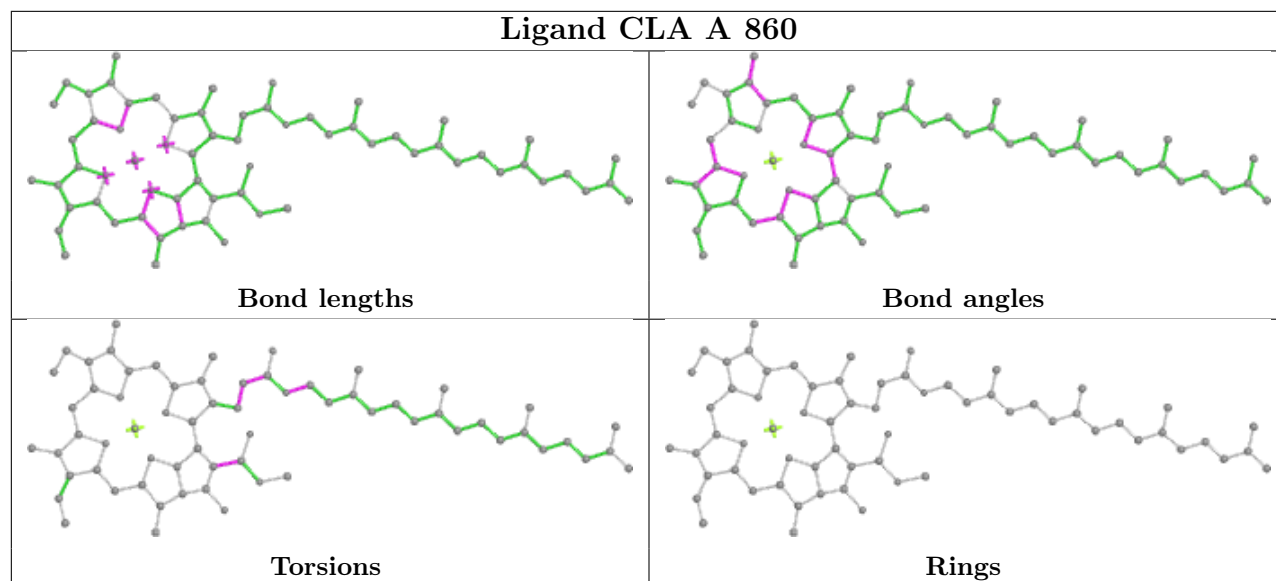
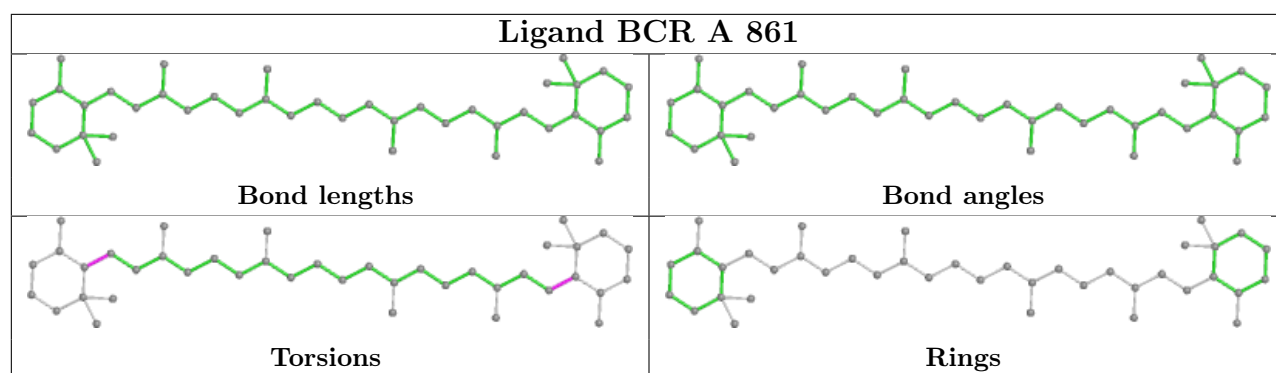
Torsions

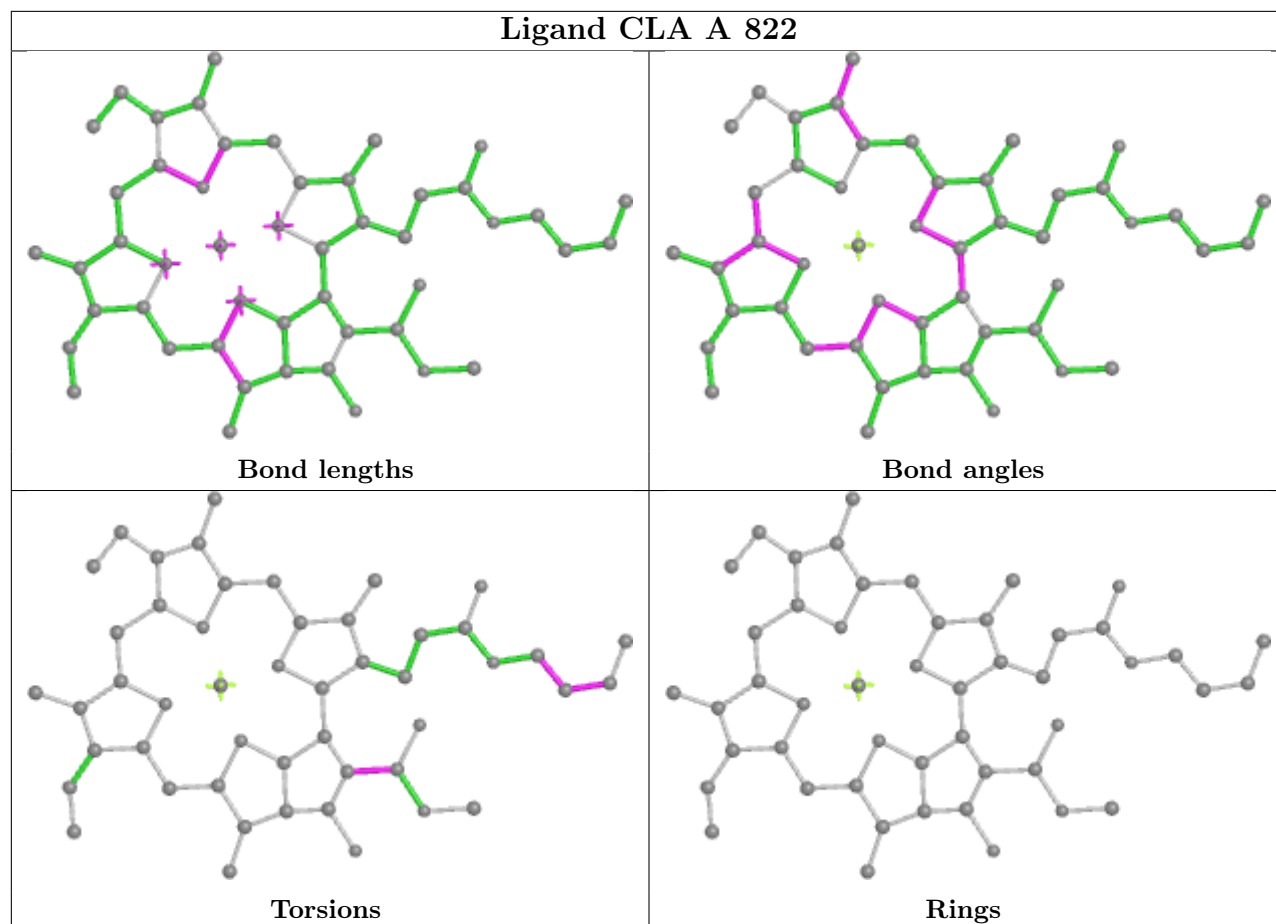


Rings

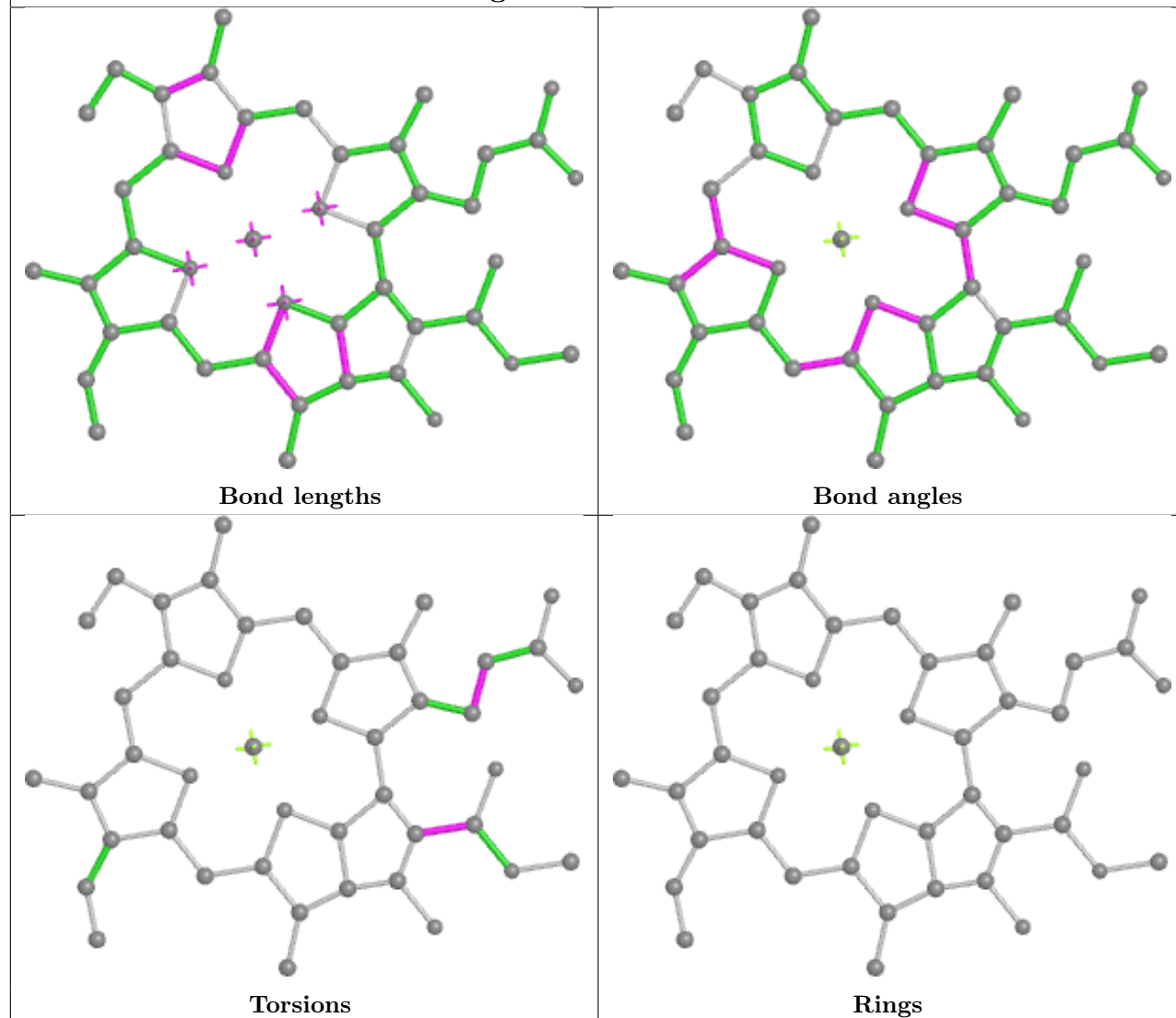




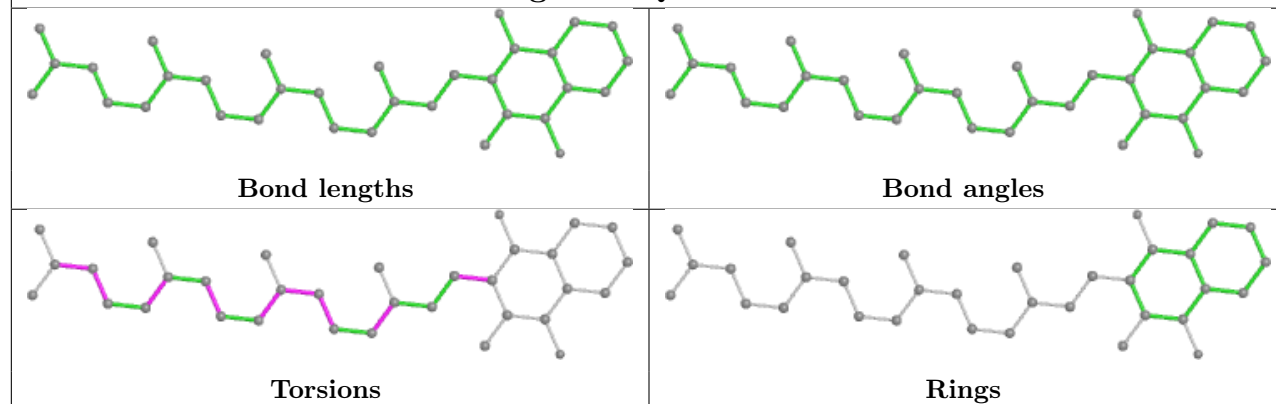


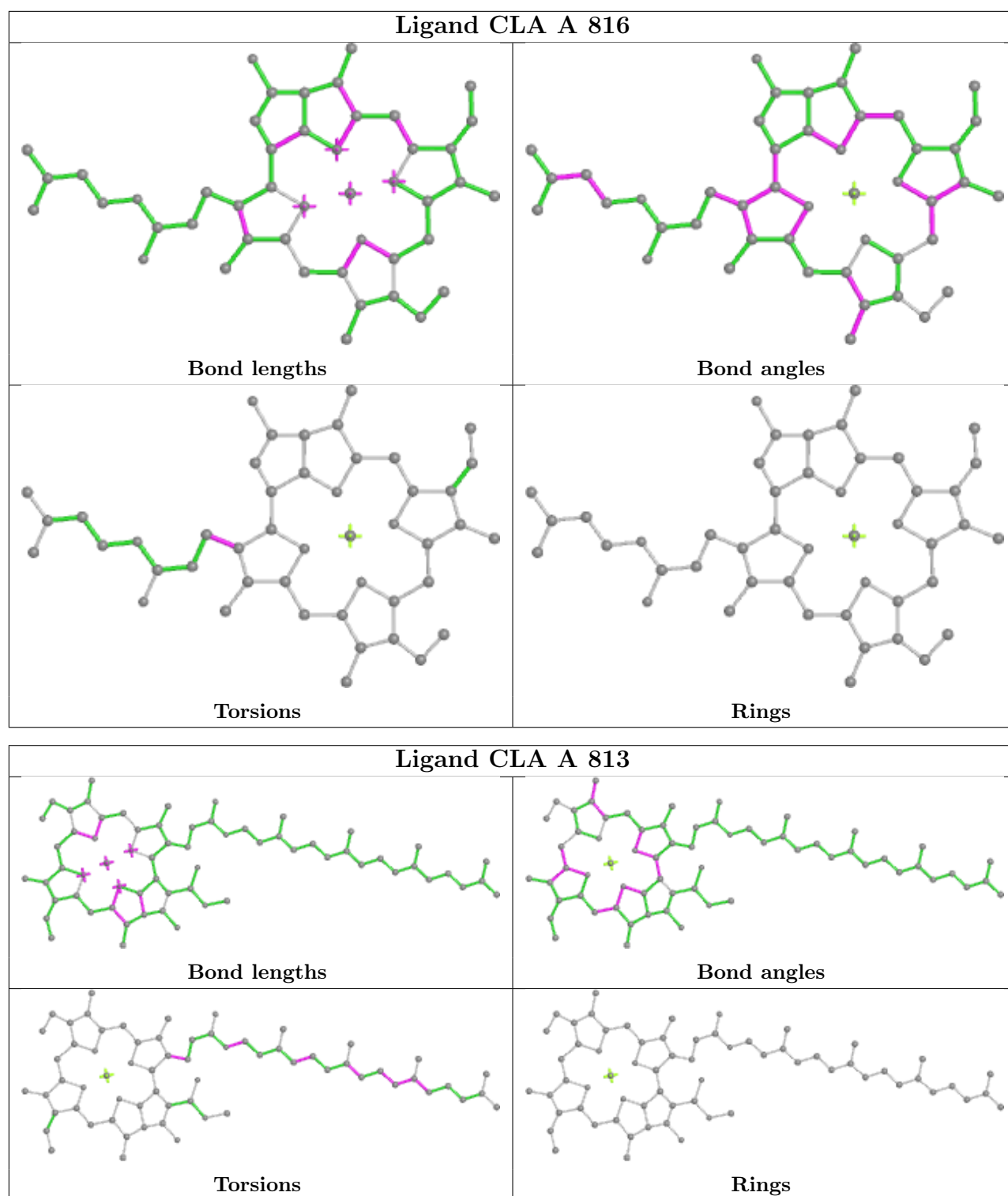


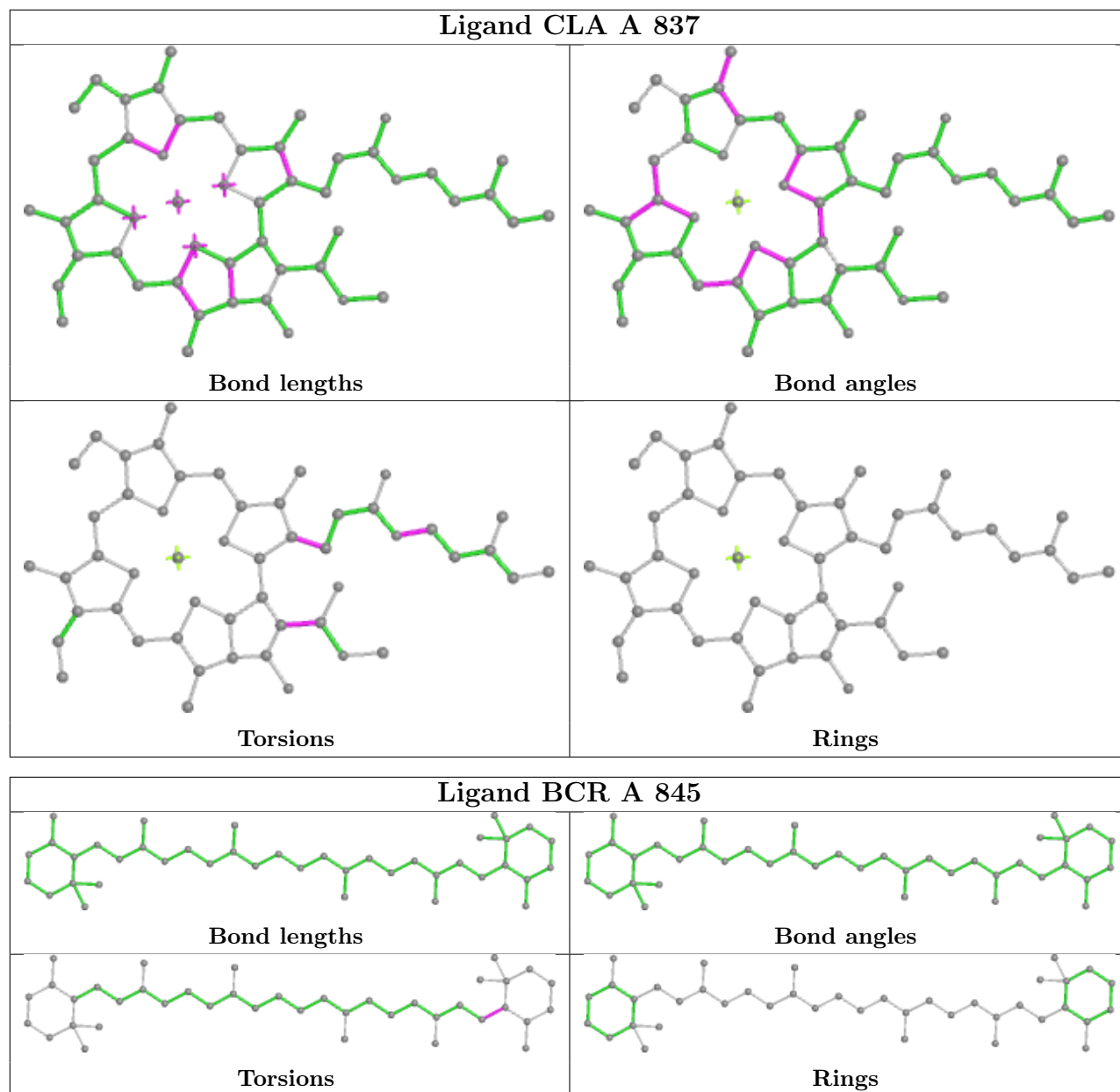
Ligand CLA A 815



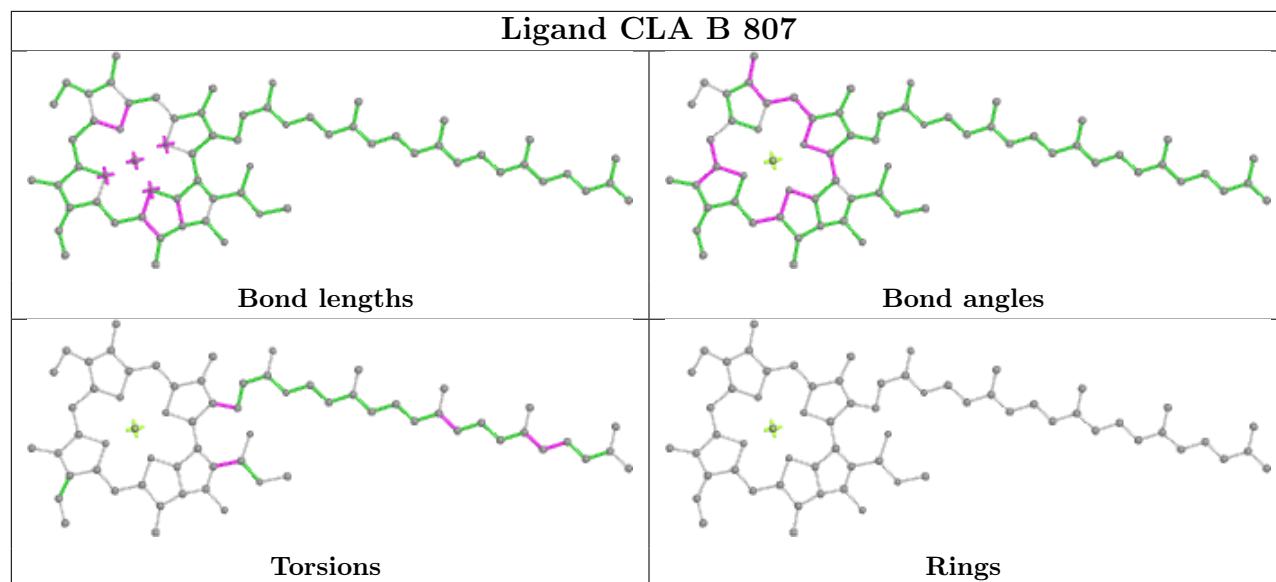
Ligand PQN A 843



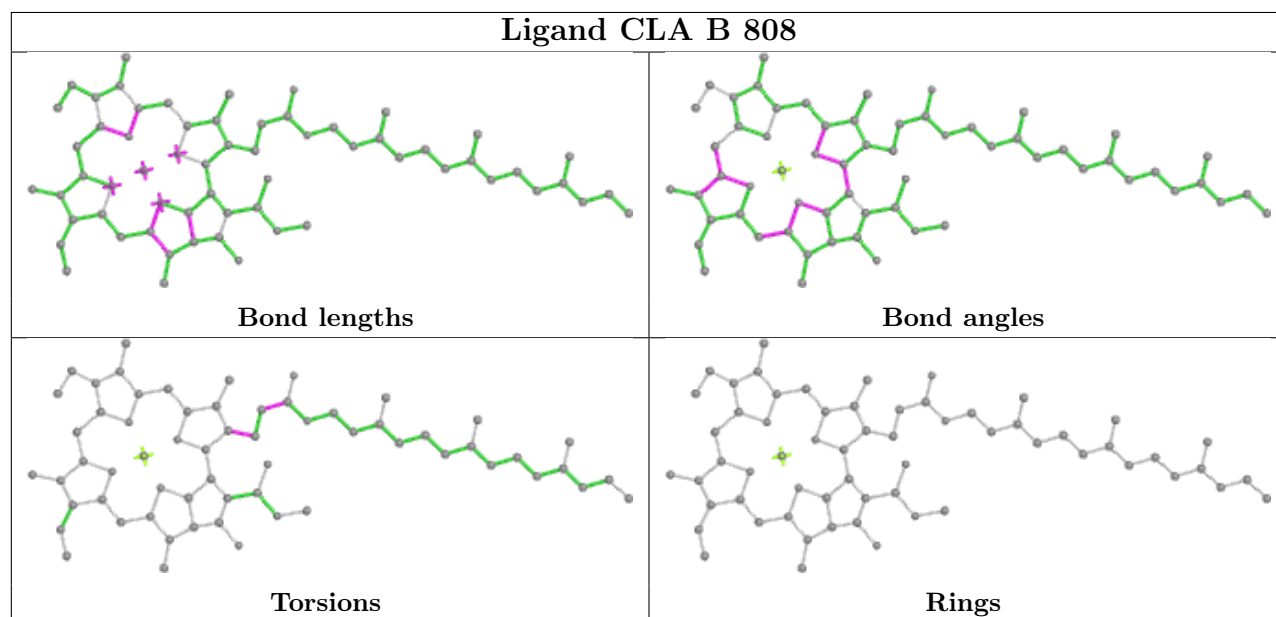




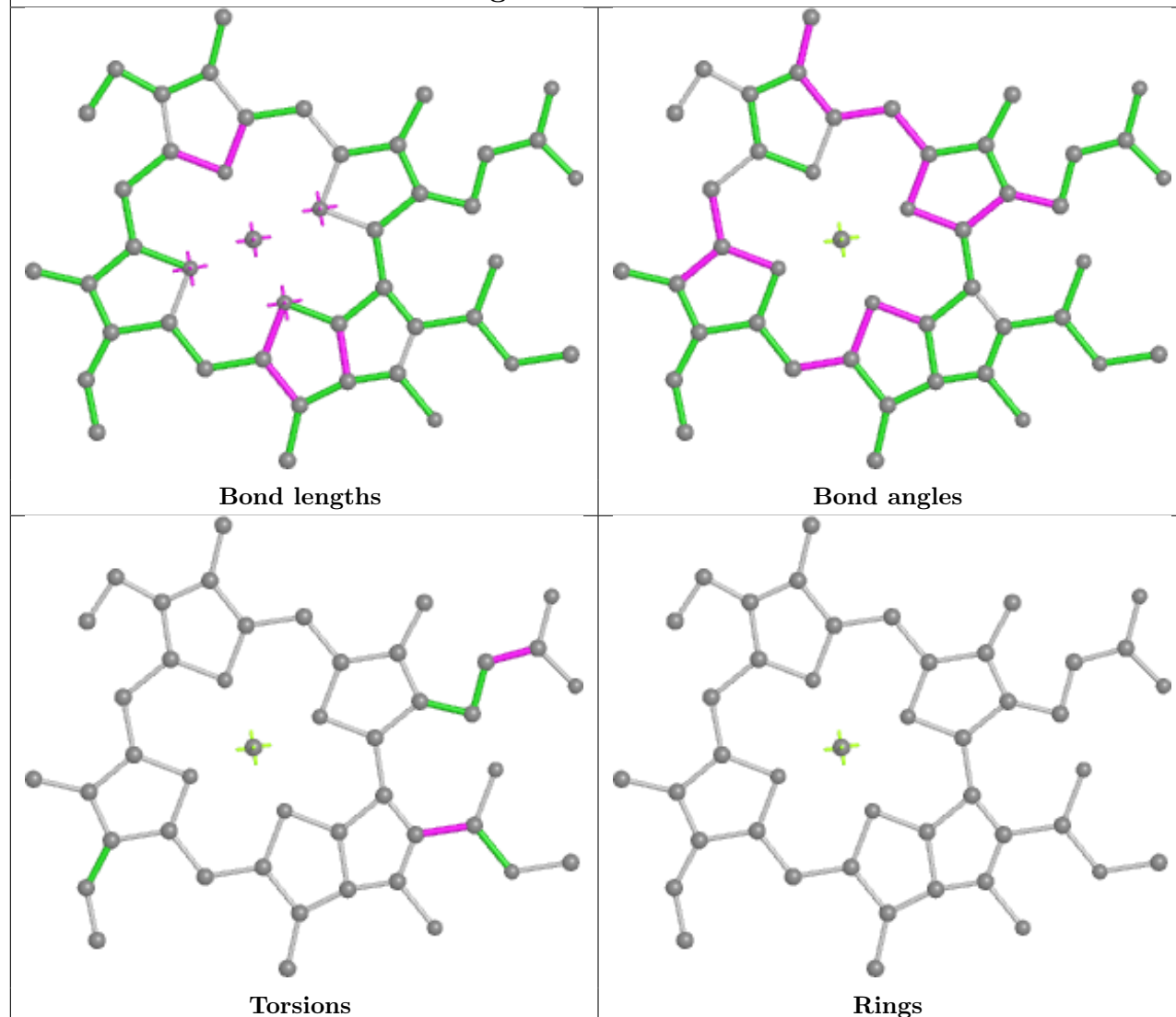
Ligand CLA B 807



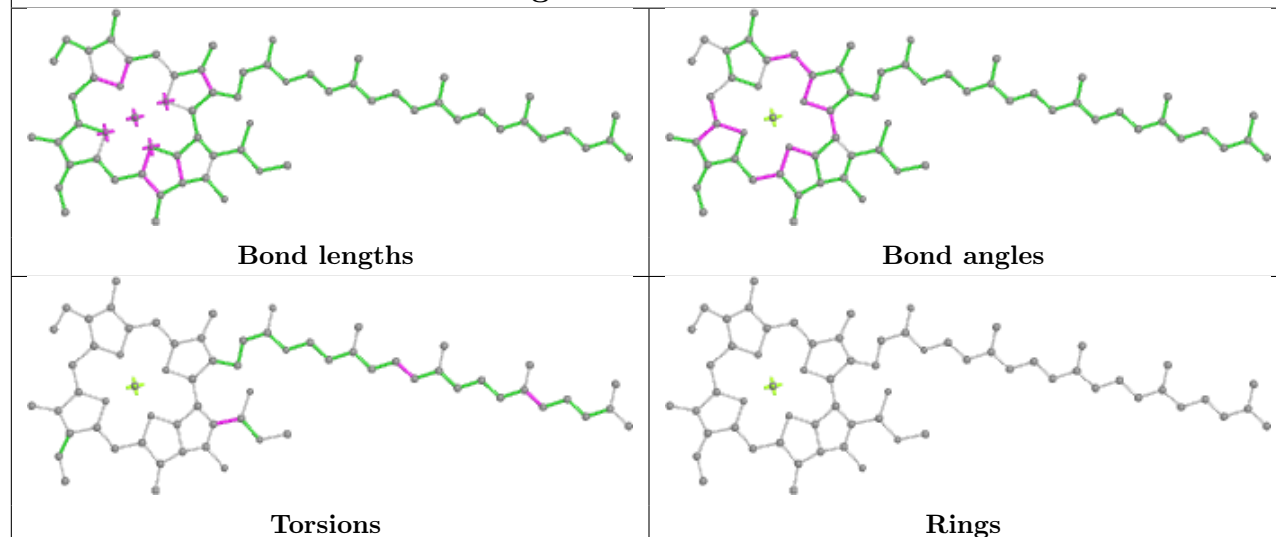
Ligand CLA B 808



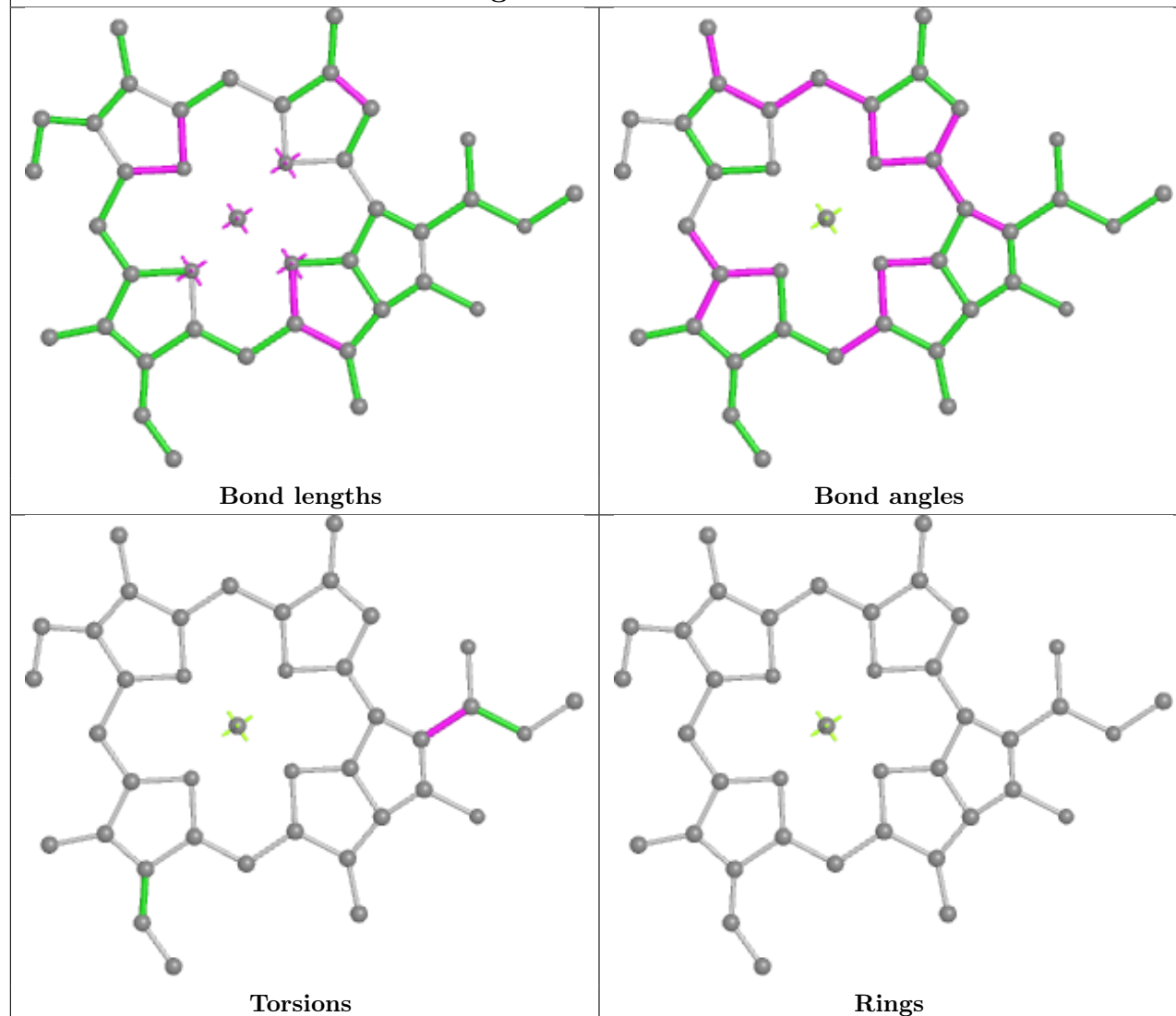
Ligand CLA A 836



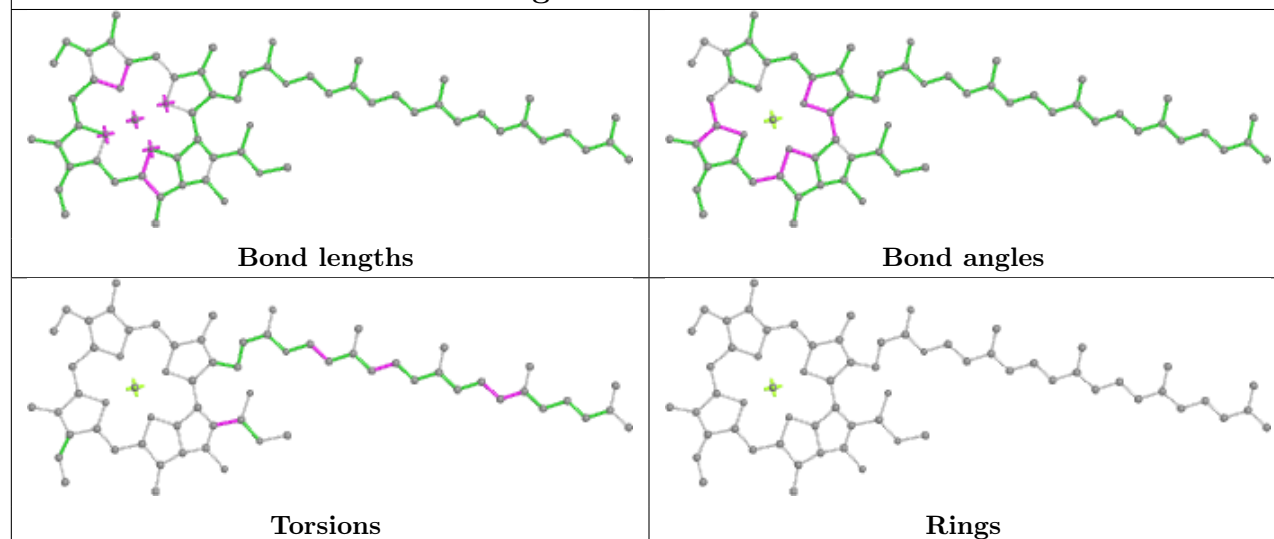
Ligand CLA A 833

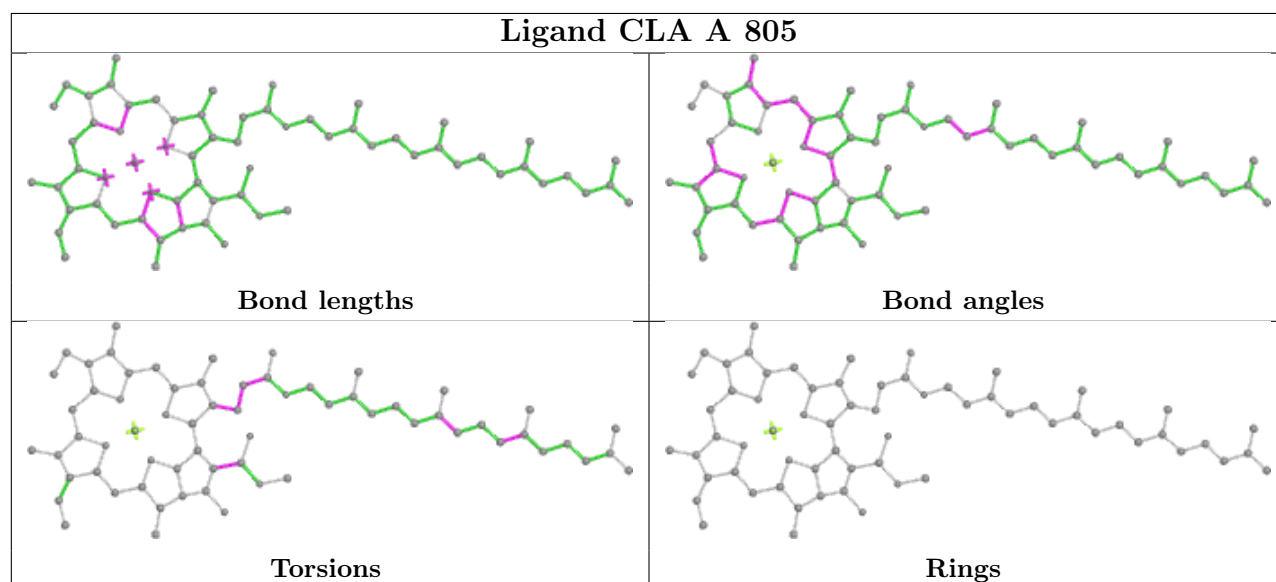
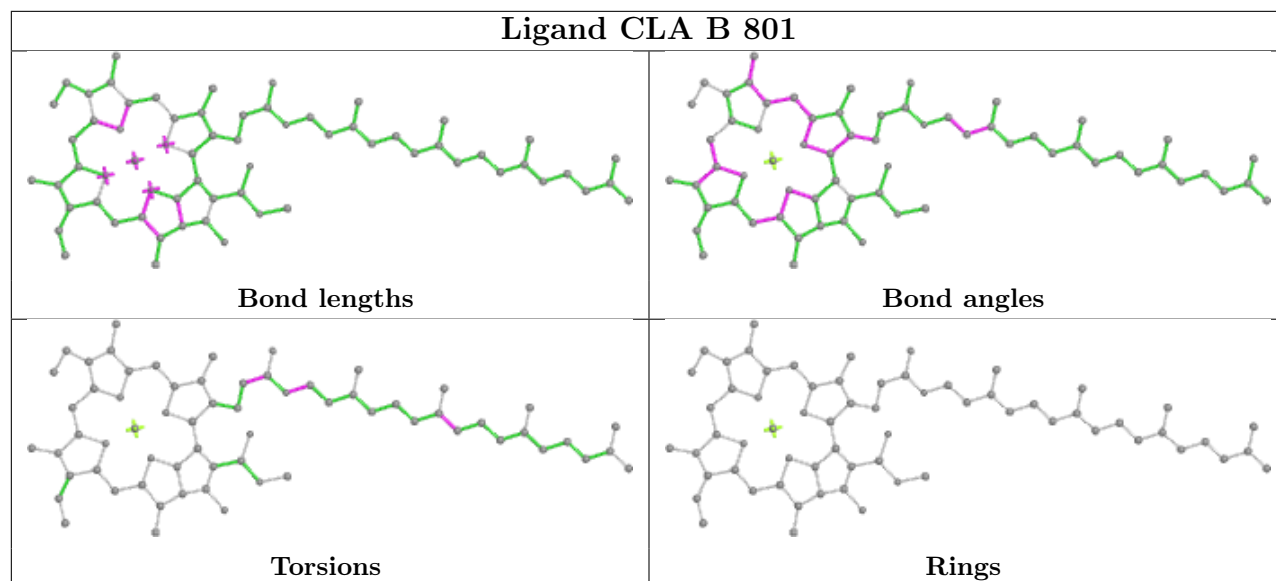
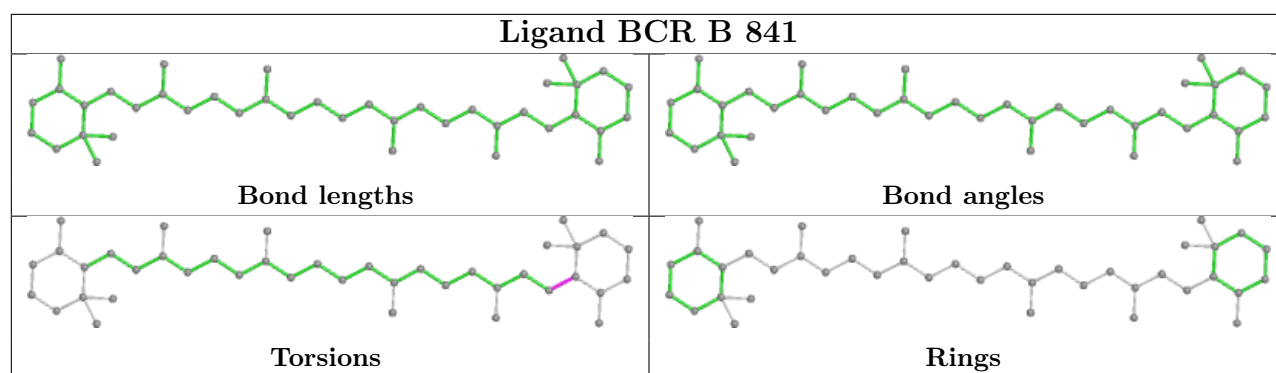


Ligand CLA A 842

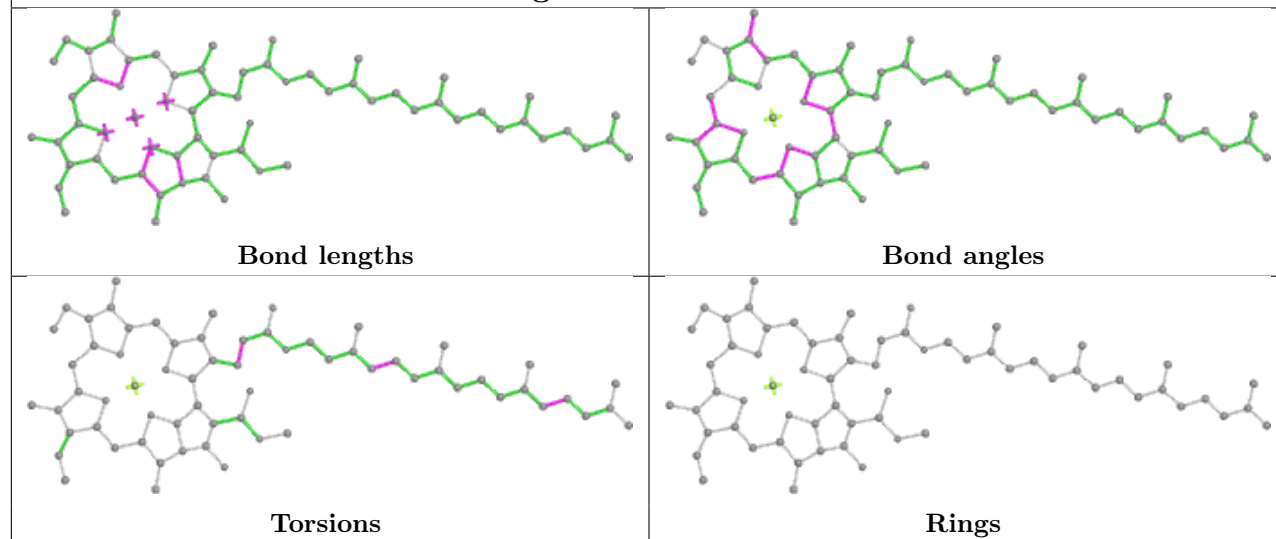


Ligand CLA B 828

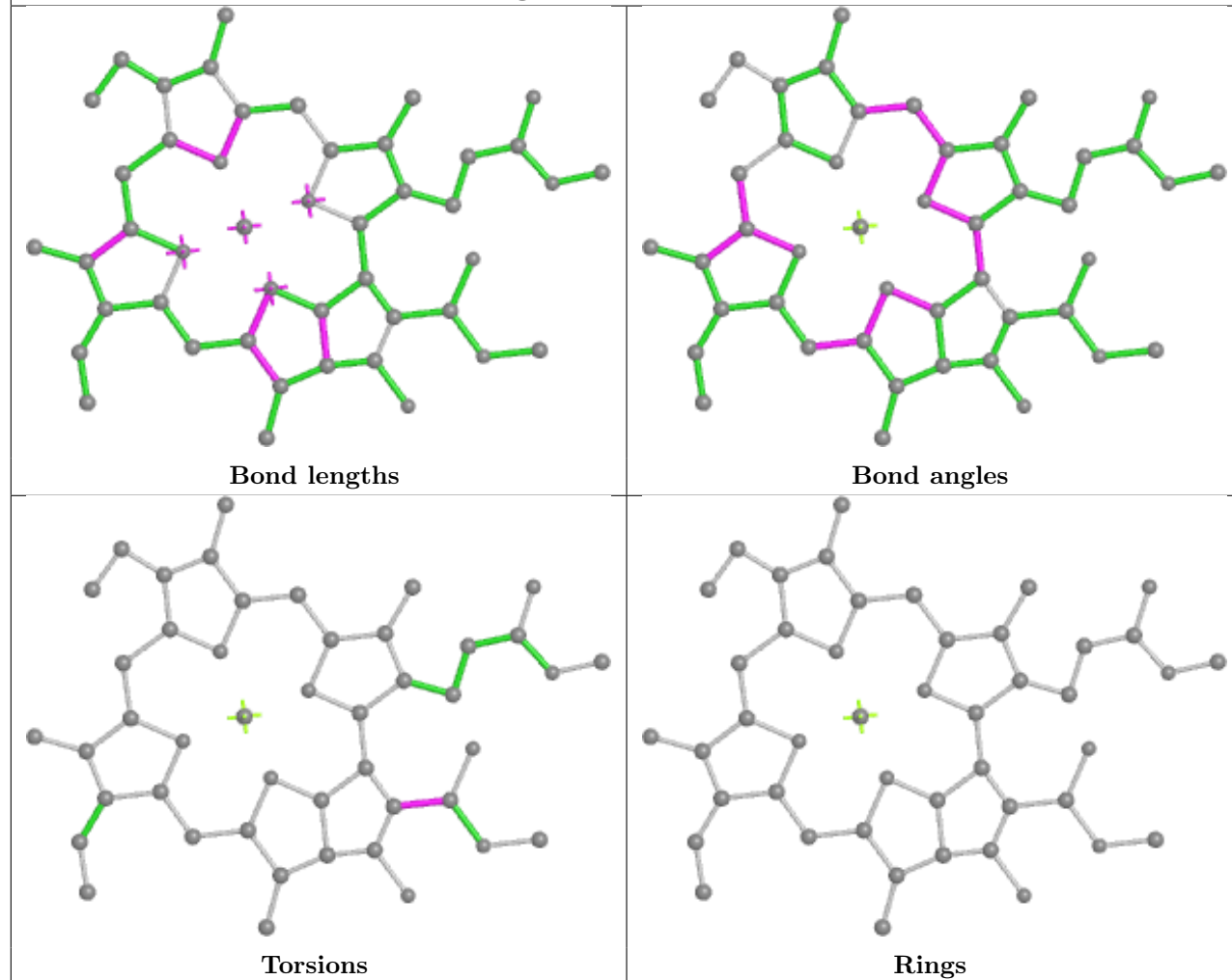


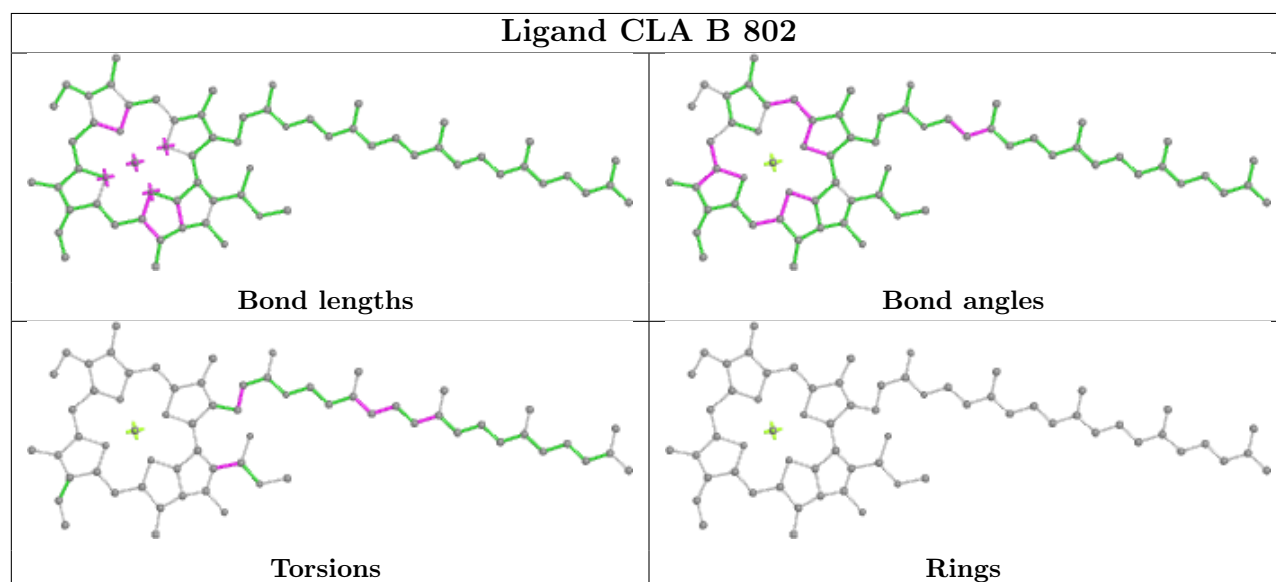
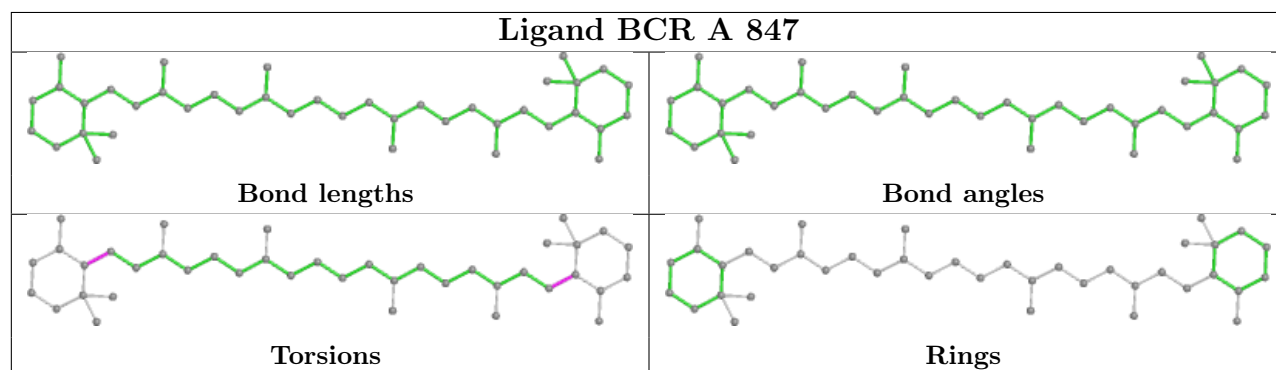
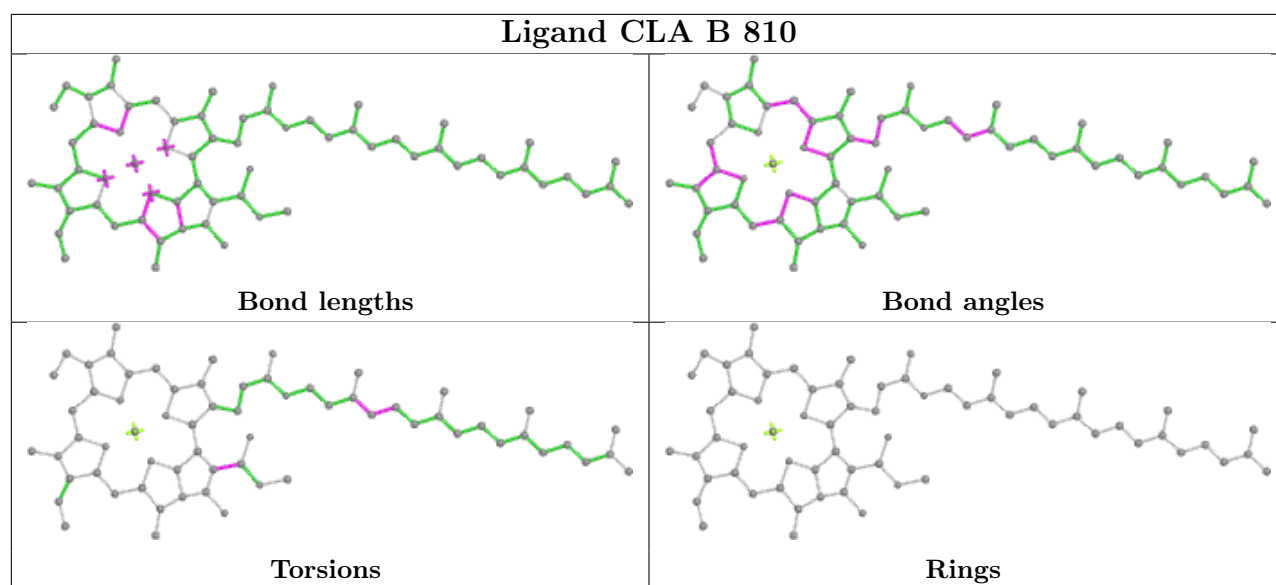


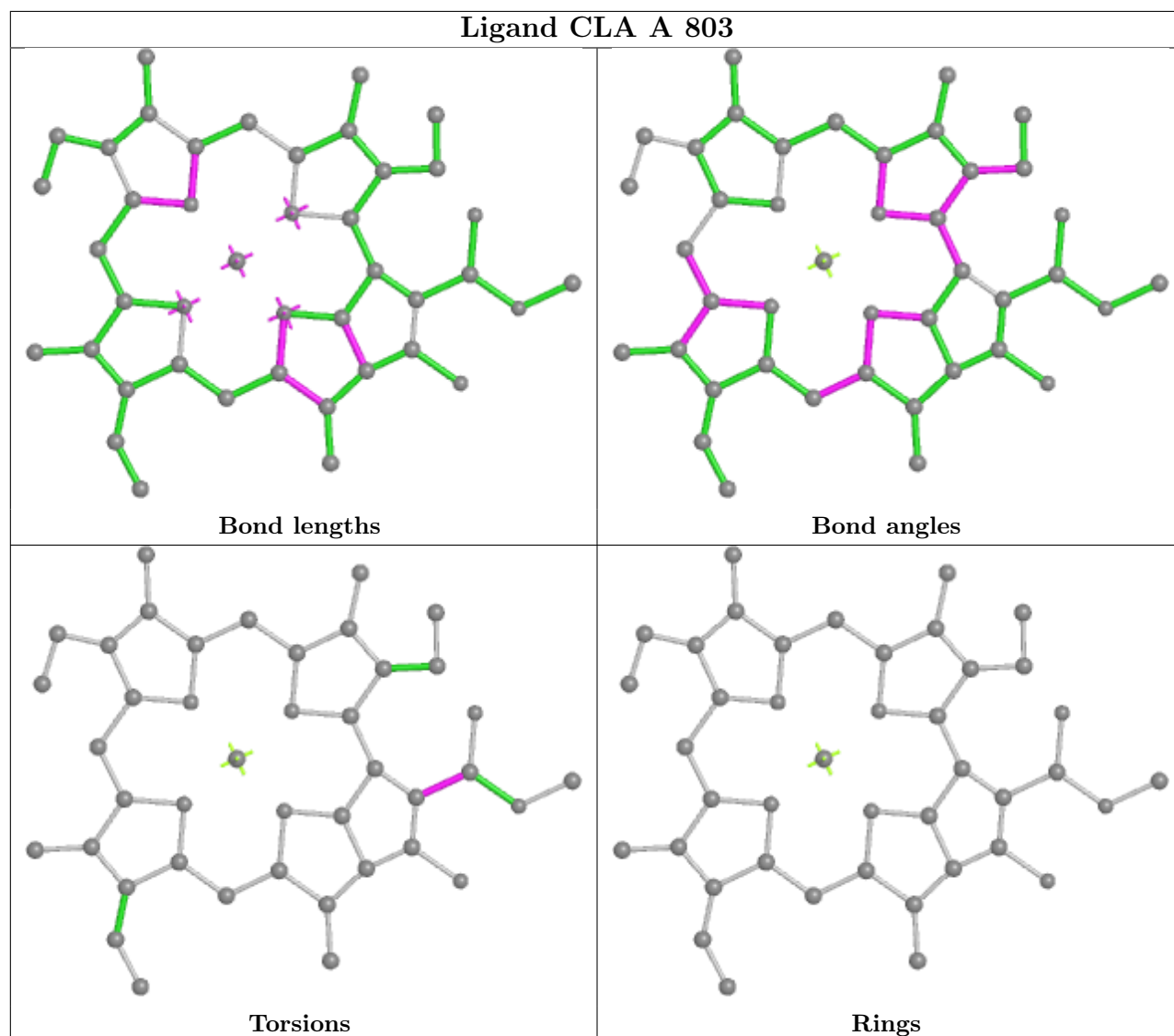
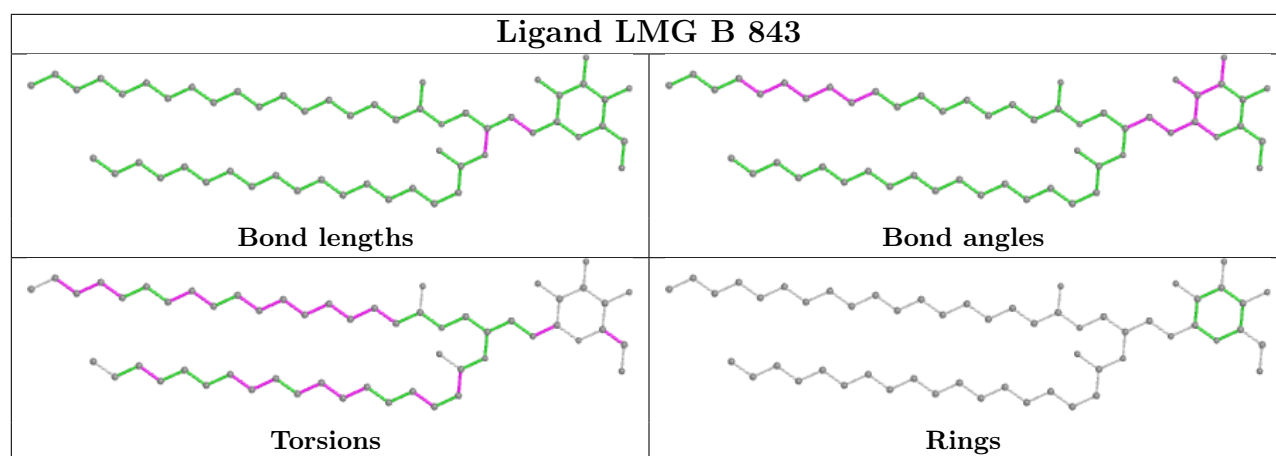
Ligand CLA B 835

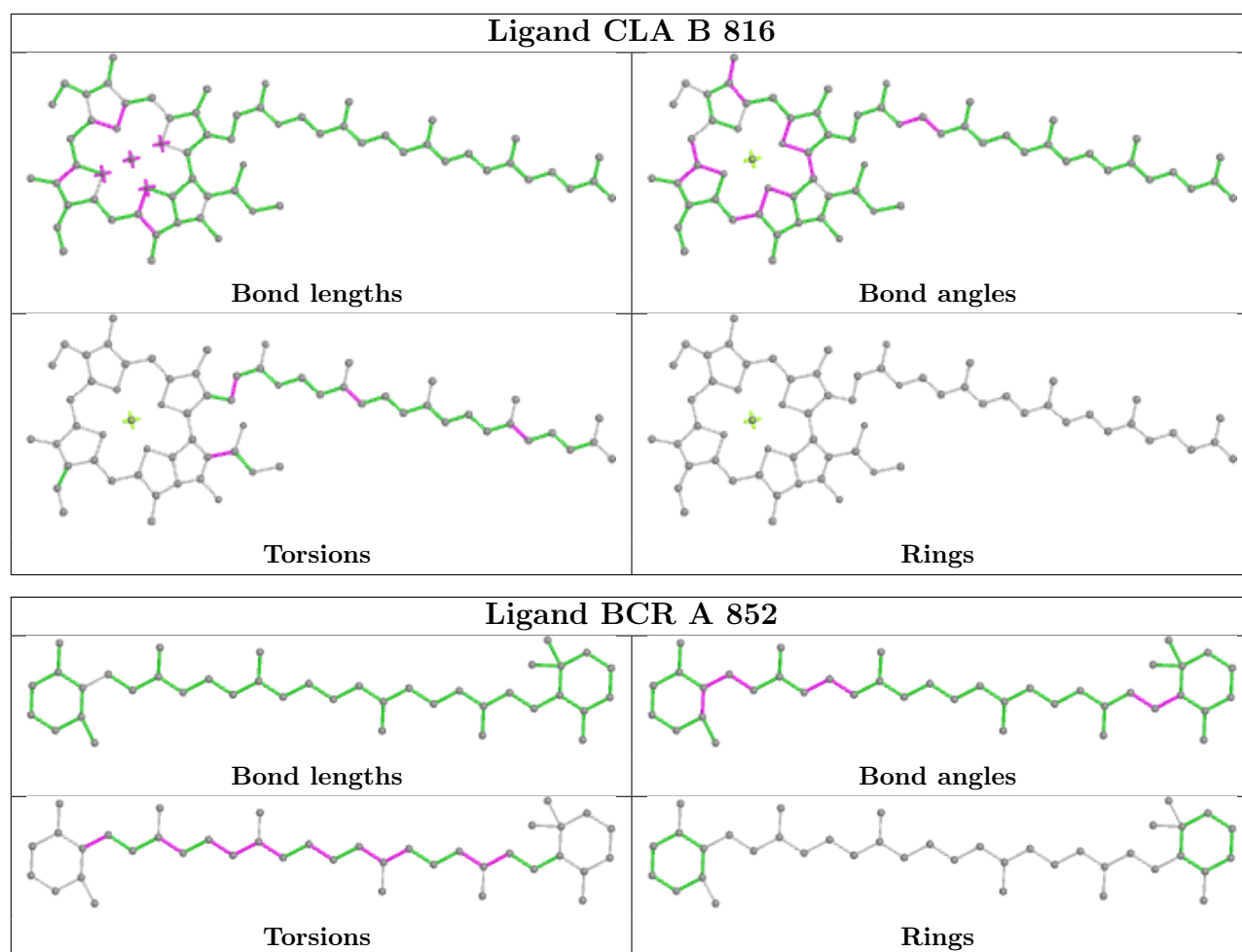


Ligand CLA B 821

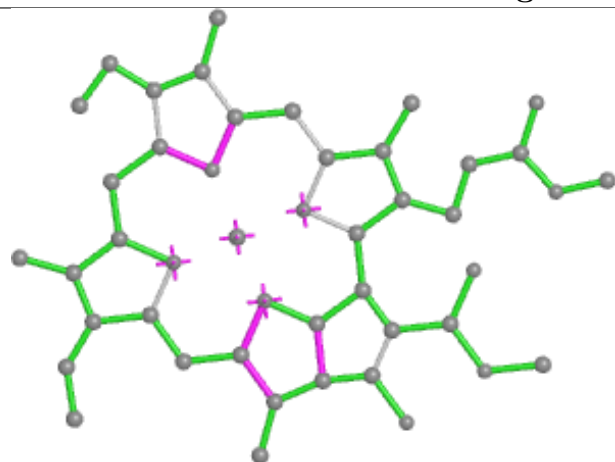




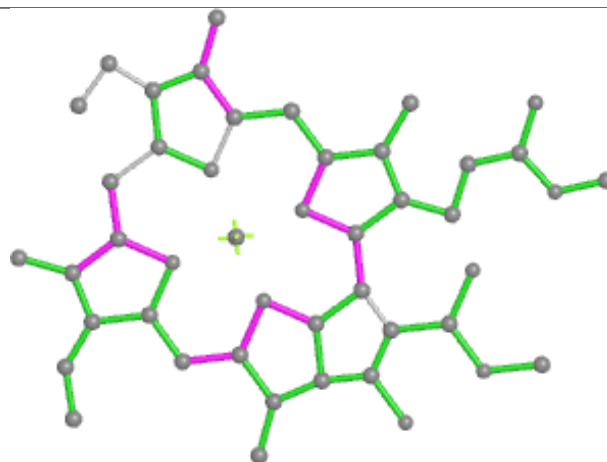




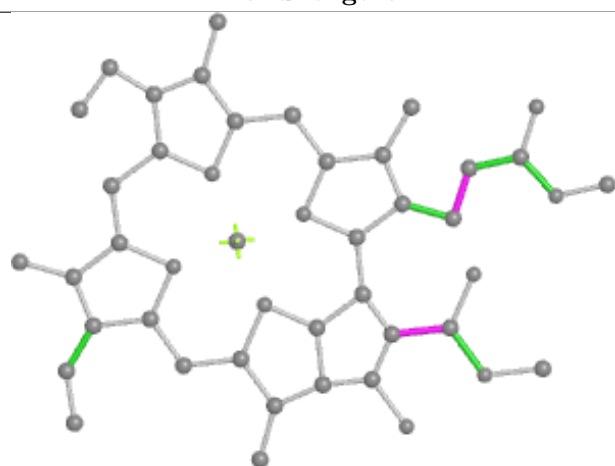
Ligand CLA B 806



Bond lengths



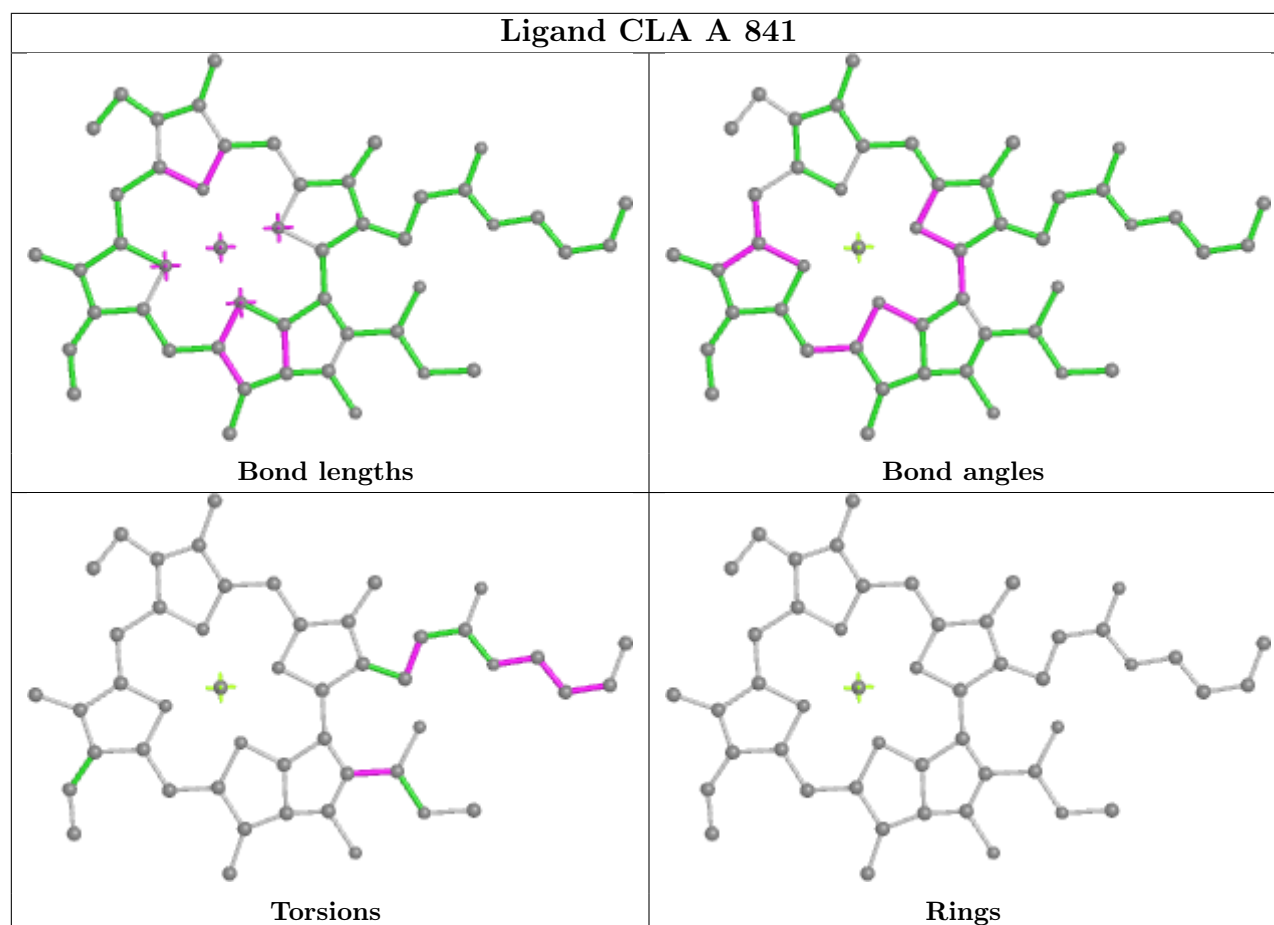
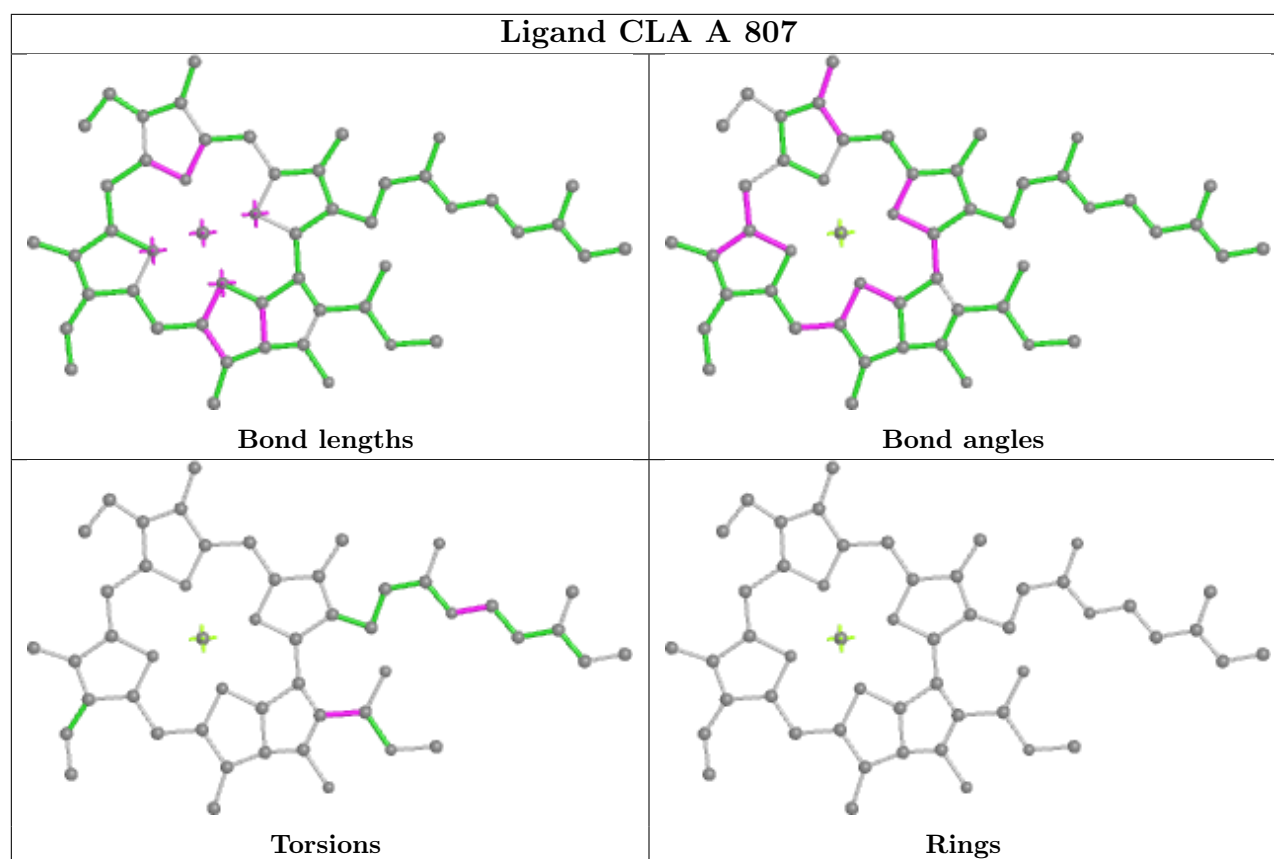
Bond angles



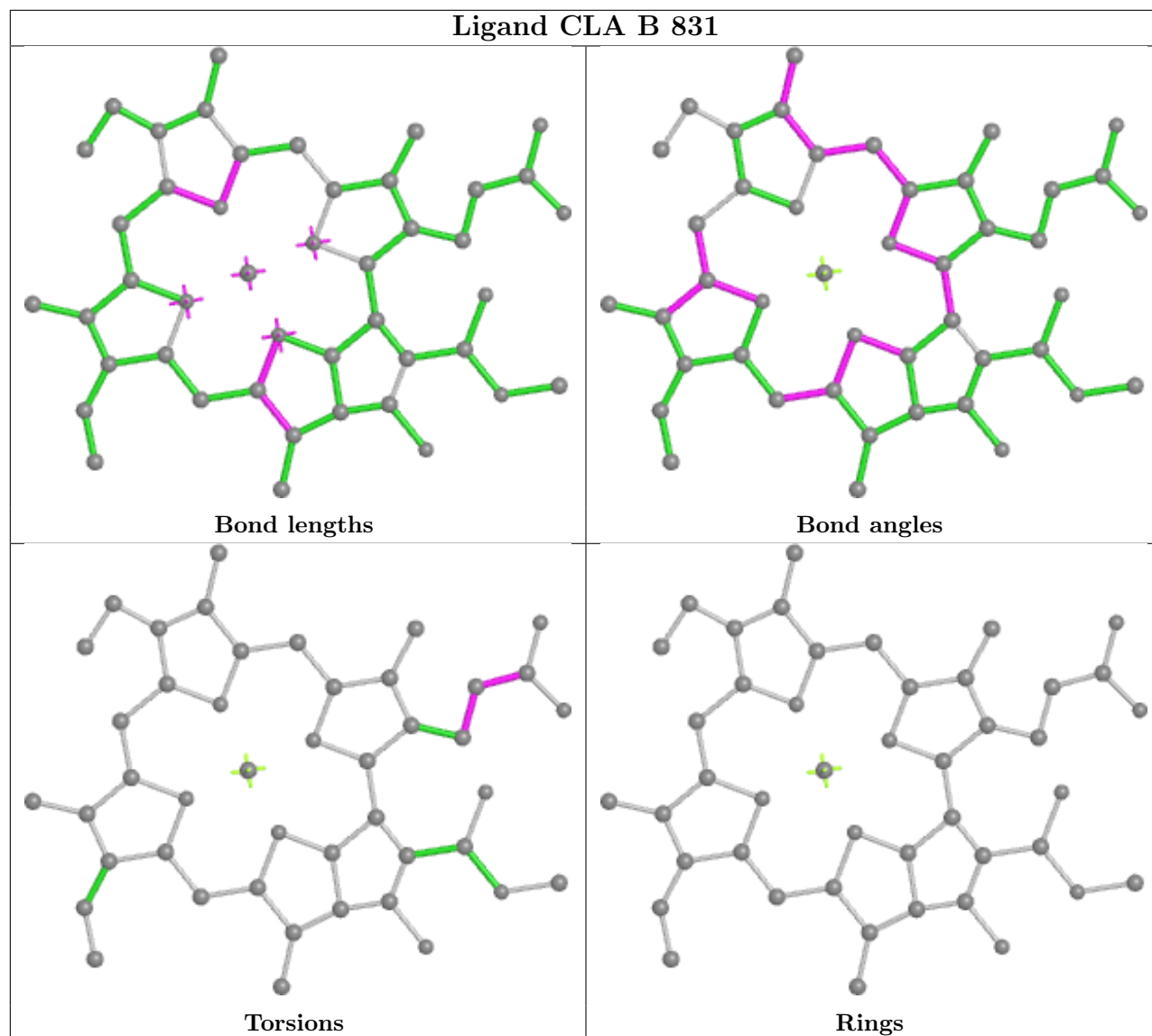
Torsions

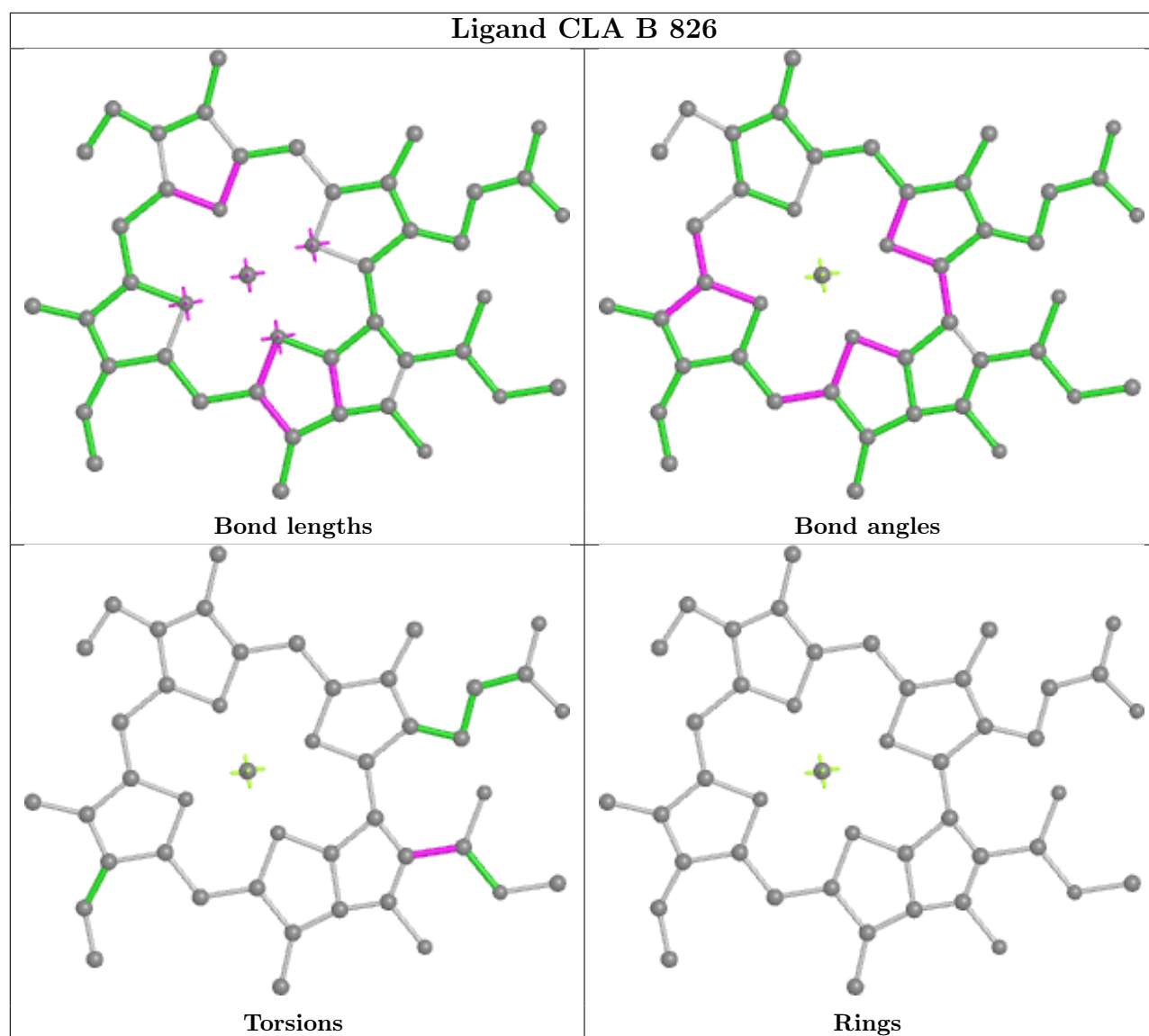


Rings

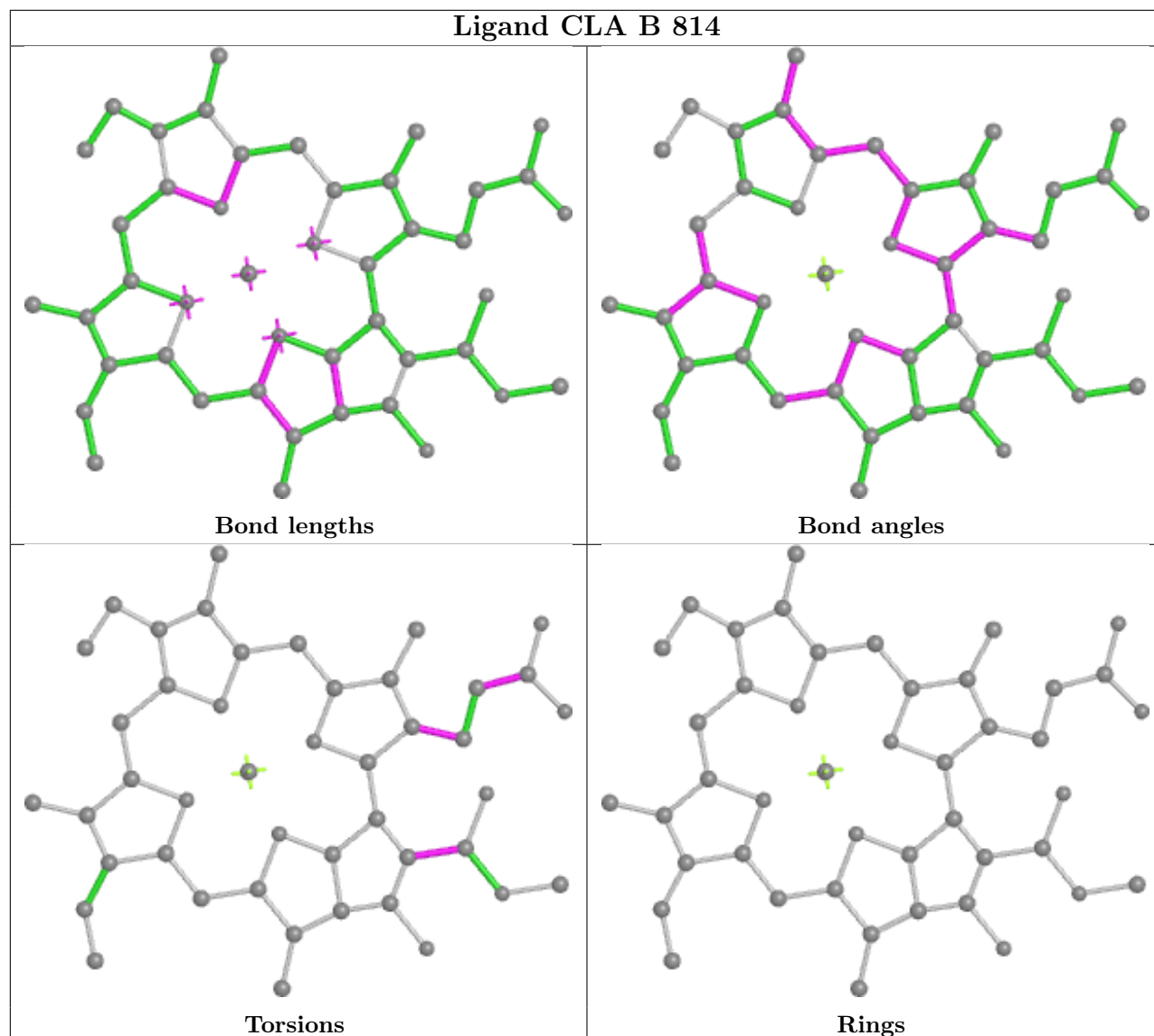


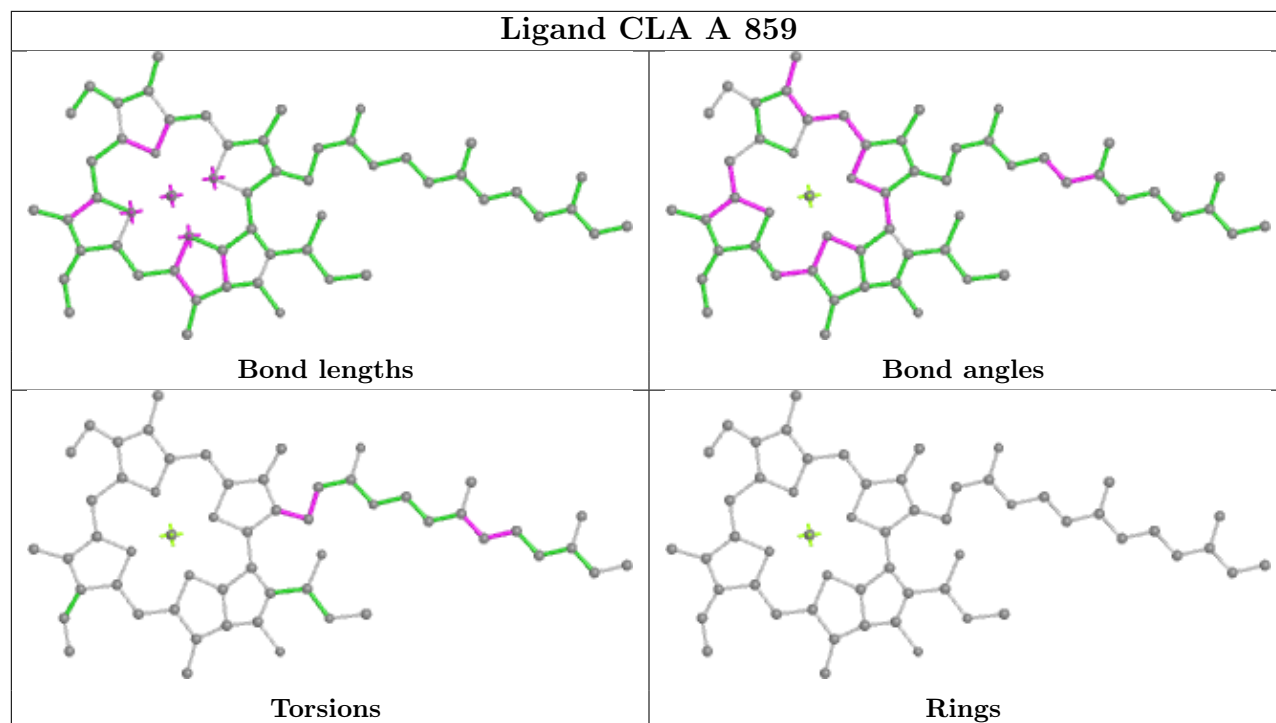
Ligand CLA B 831



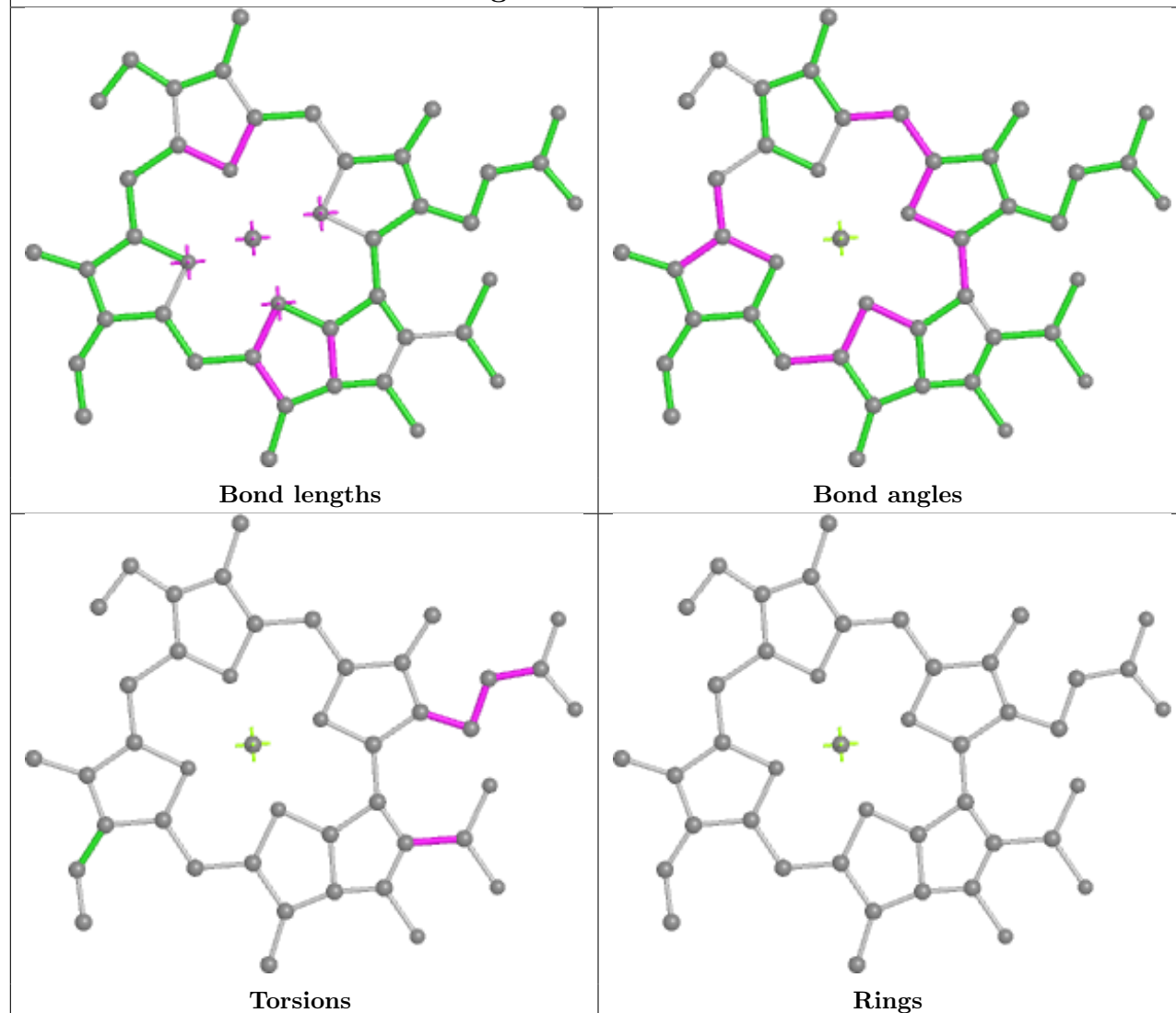


Ligand CLA B 814

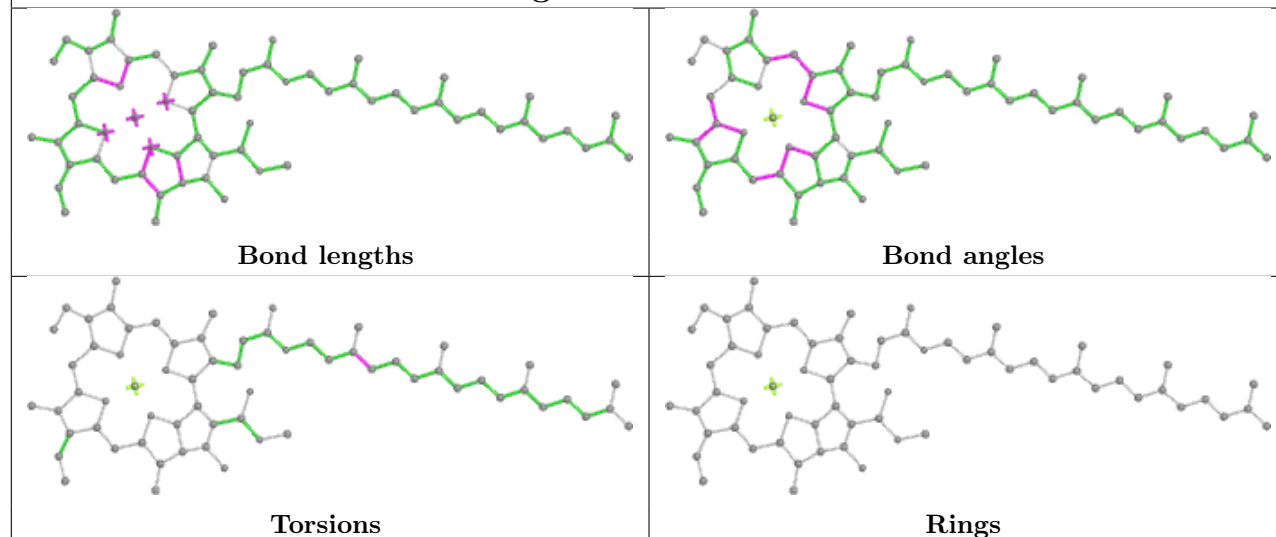


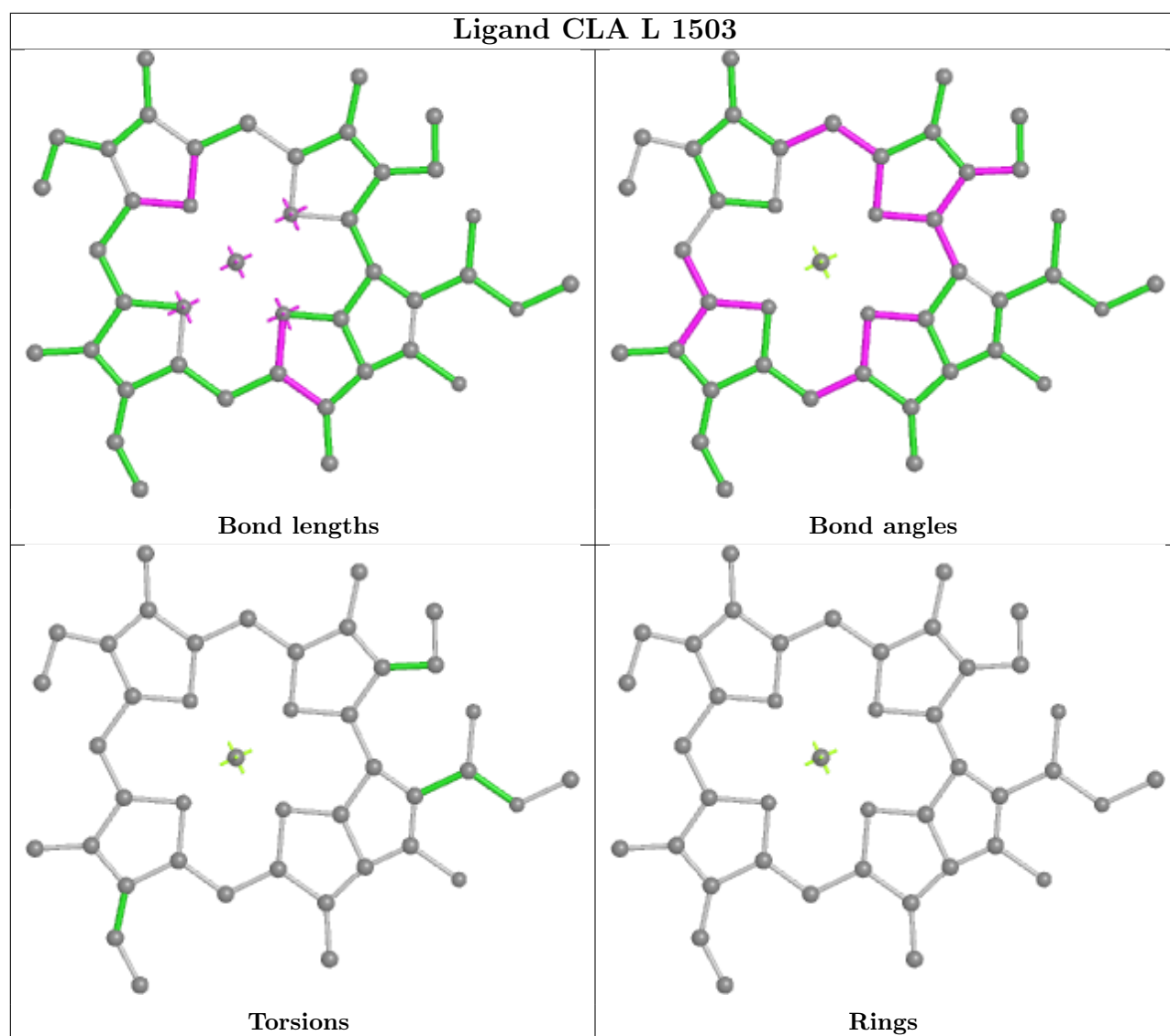


Ligand CLA B 822

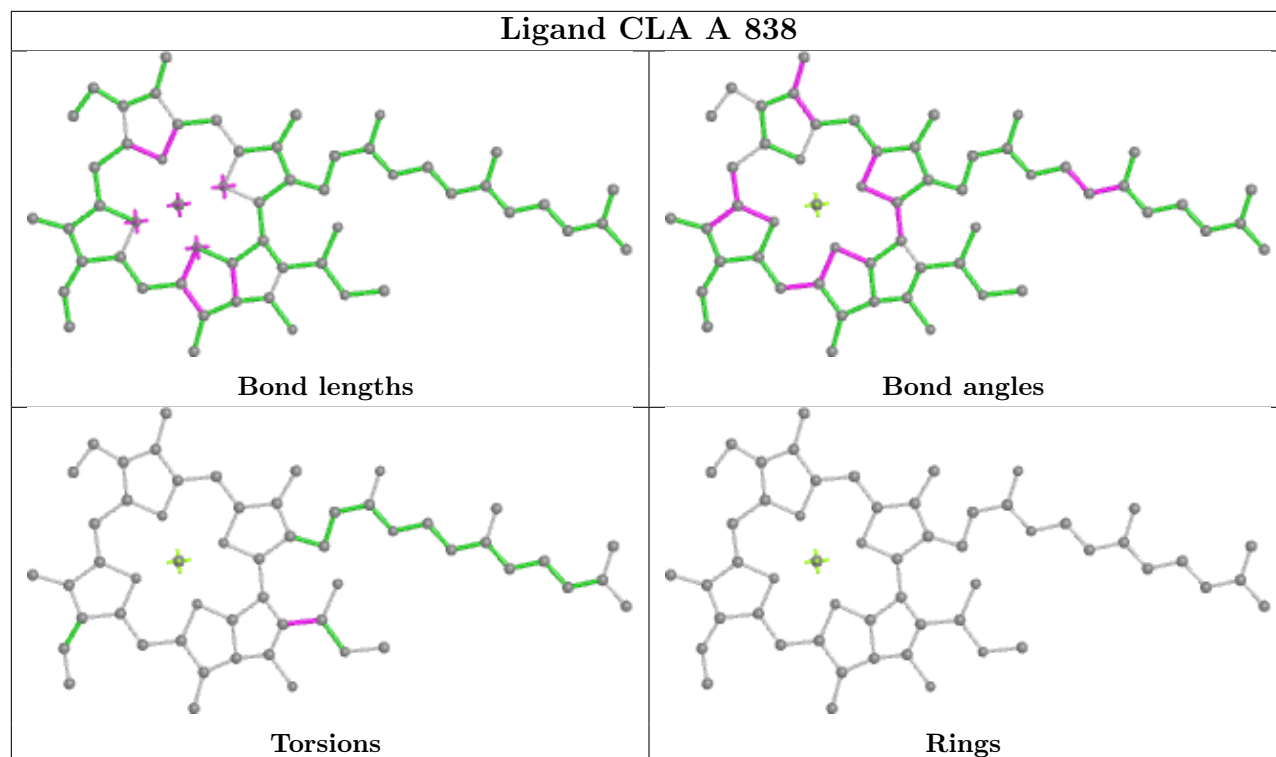


Ligand CLA B 833

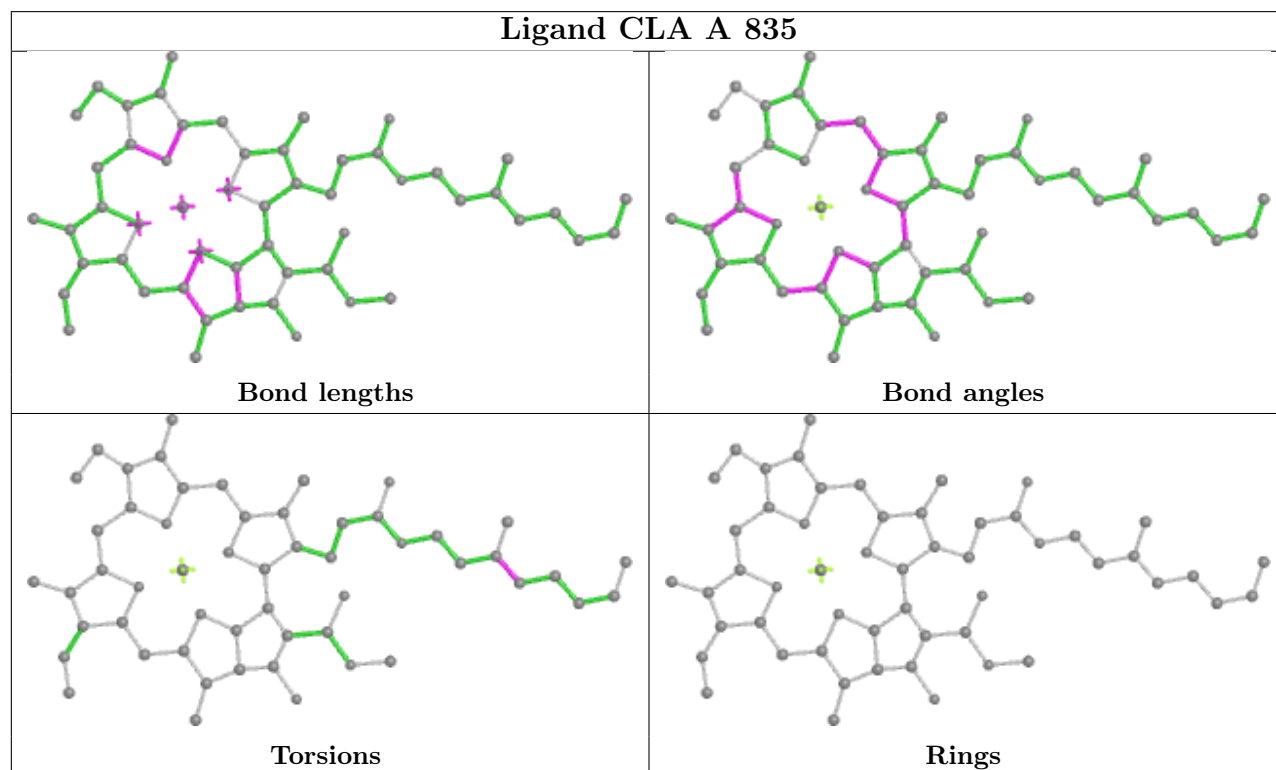




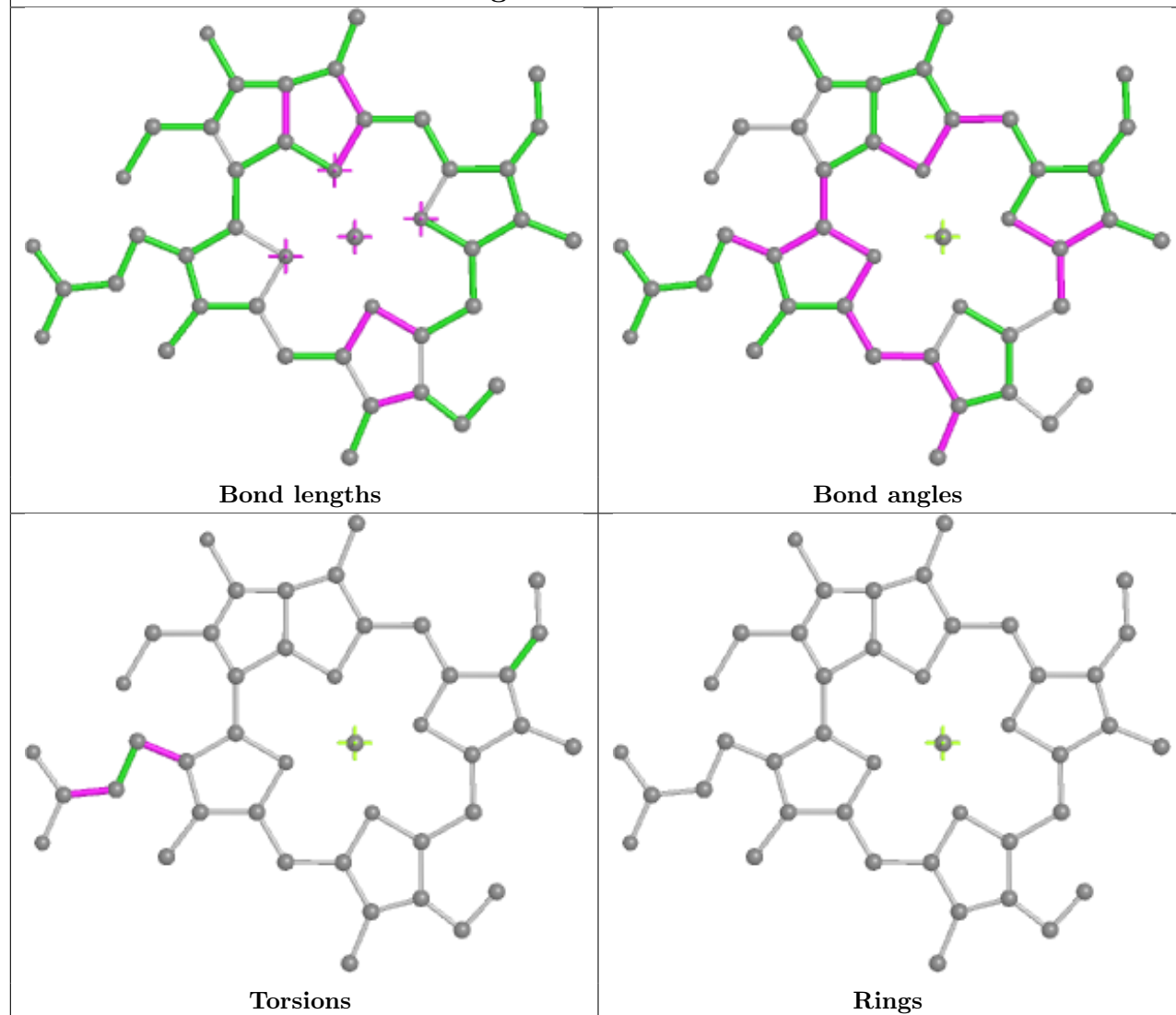
Ligand CLA A 838



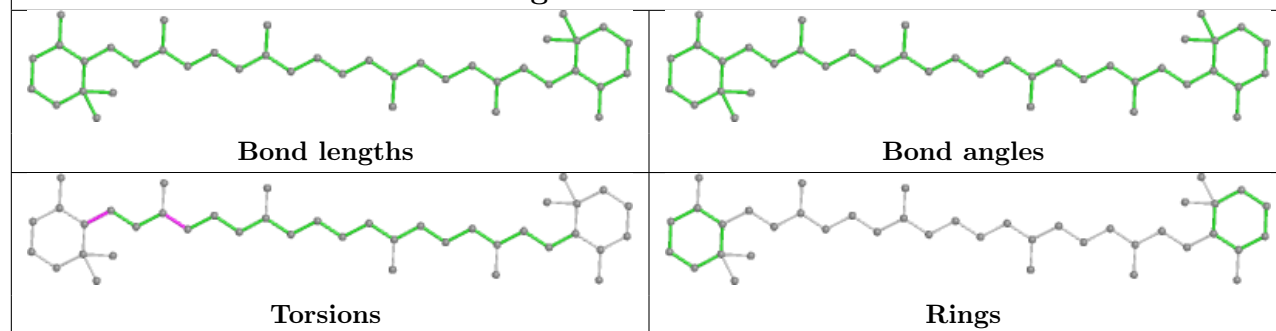
Ligand CLA A 835



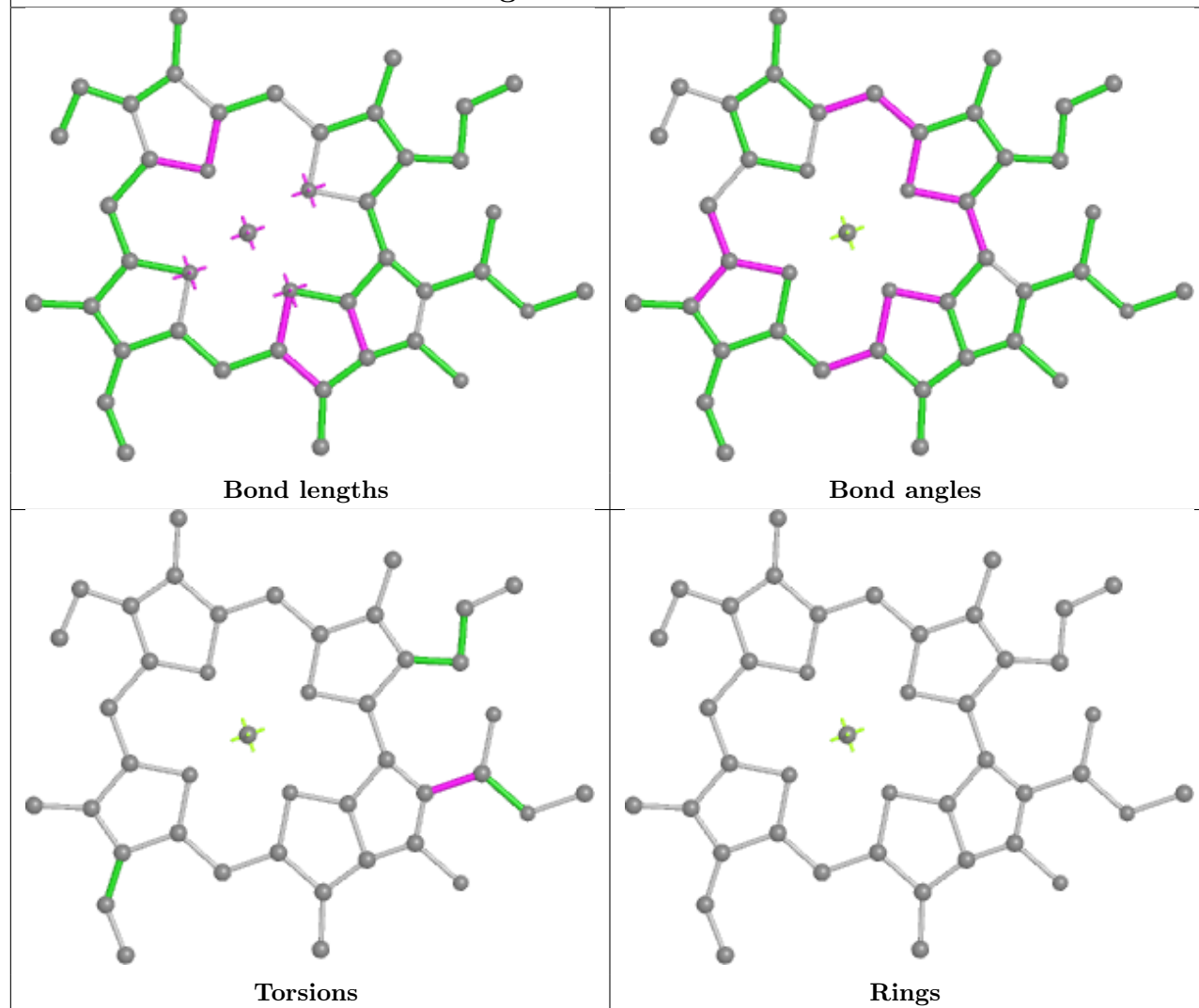
Ligand CLA B 817



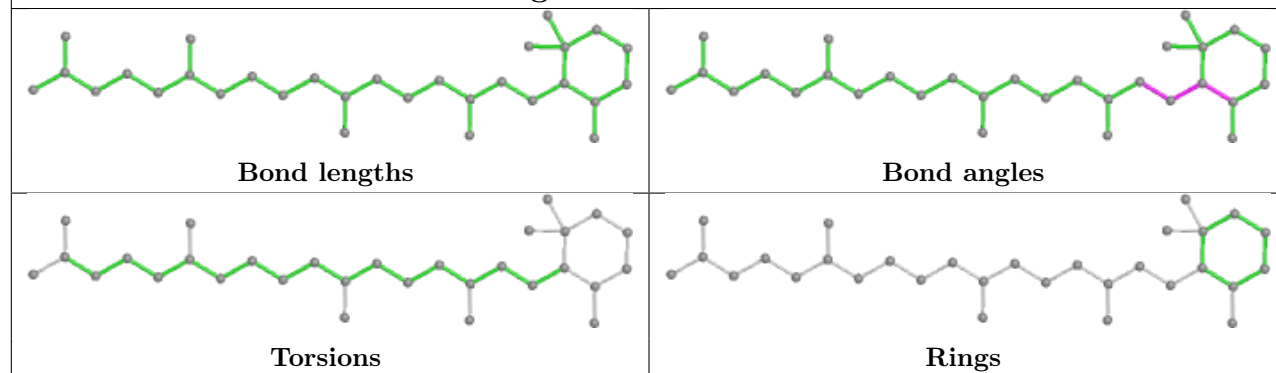
Ligand BCR B 839

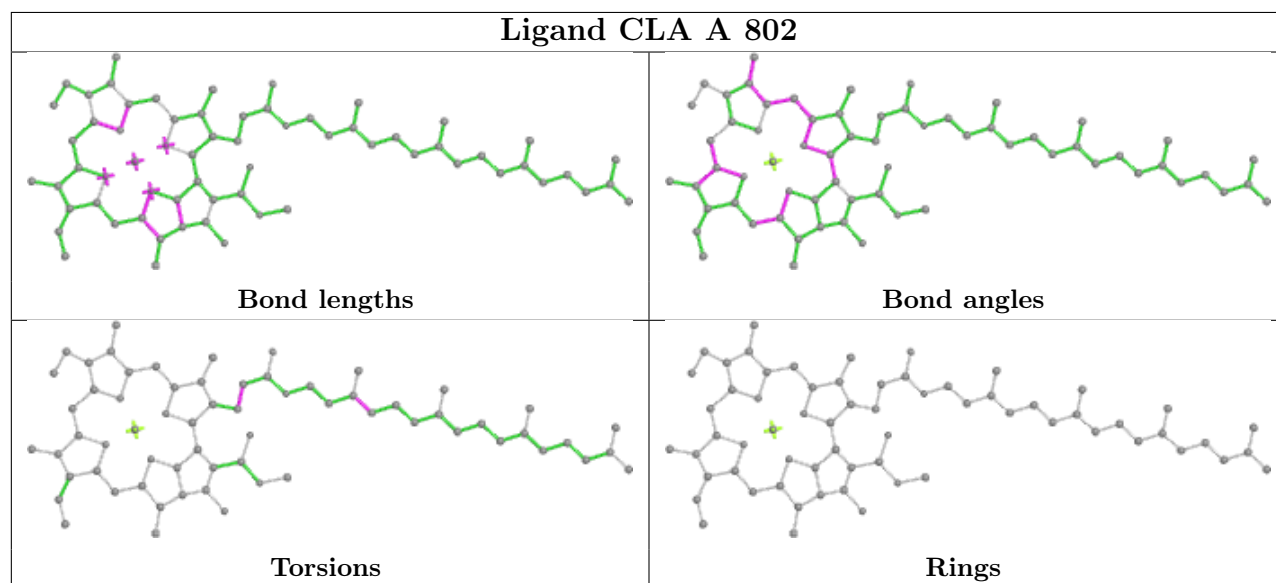
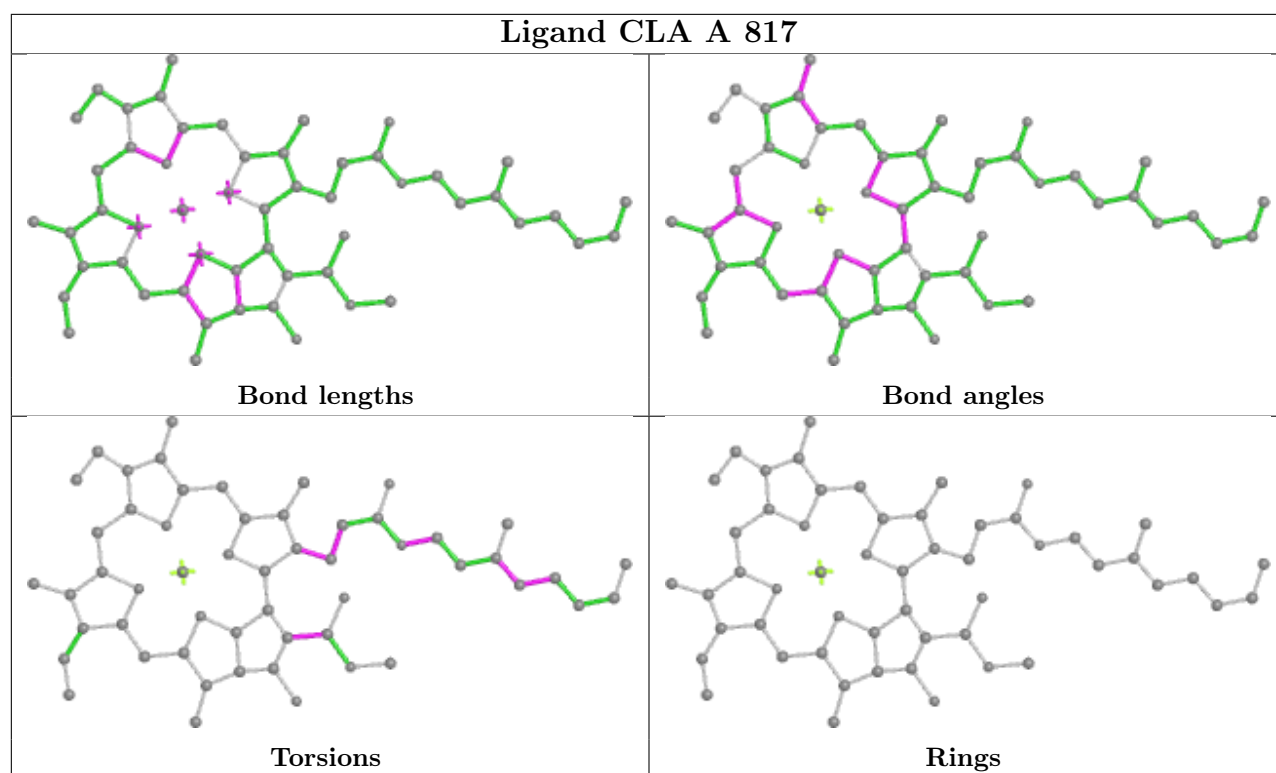


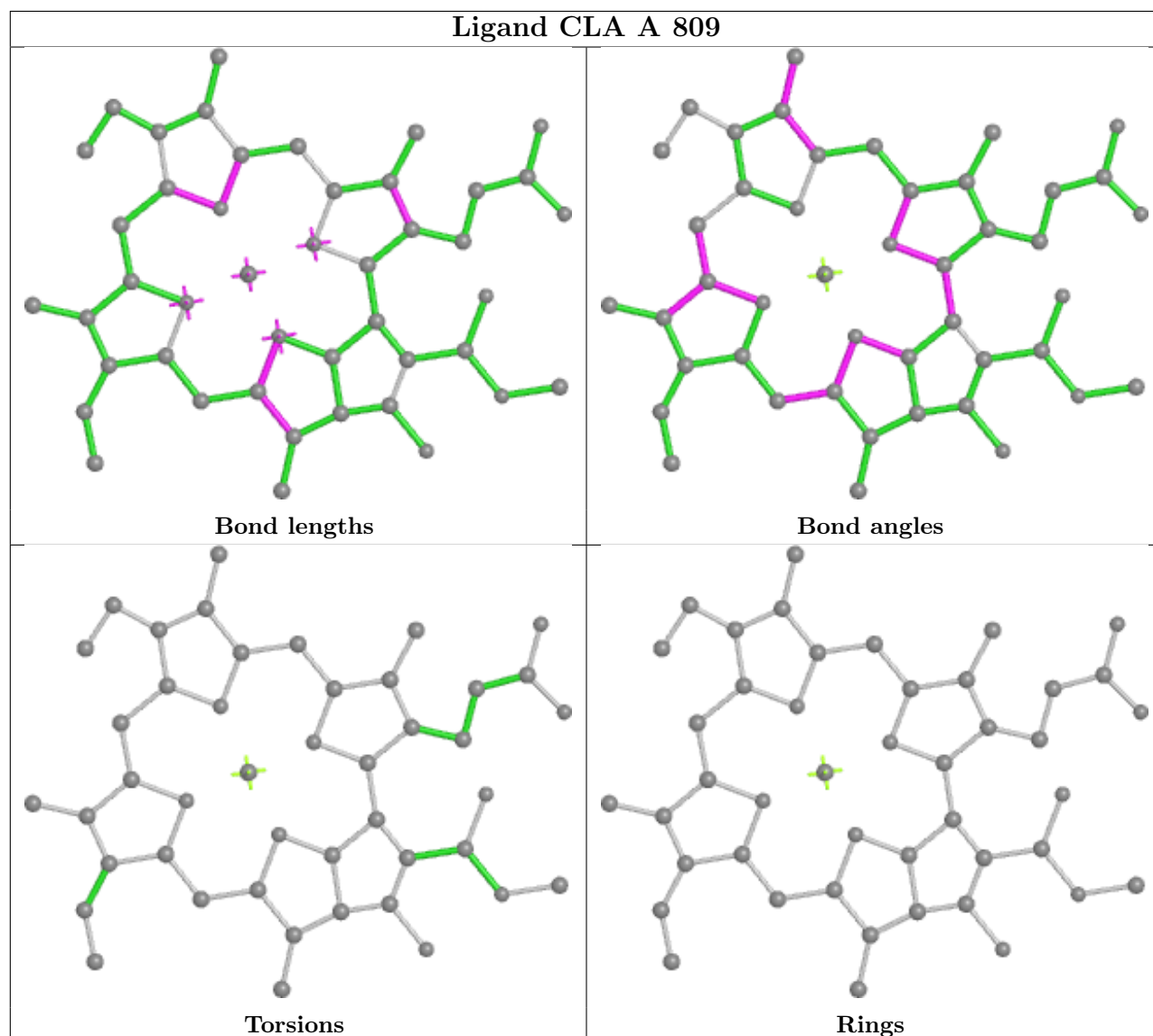
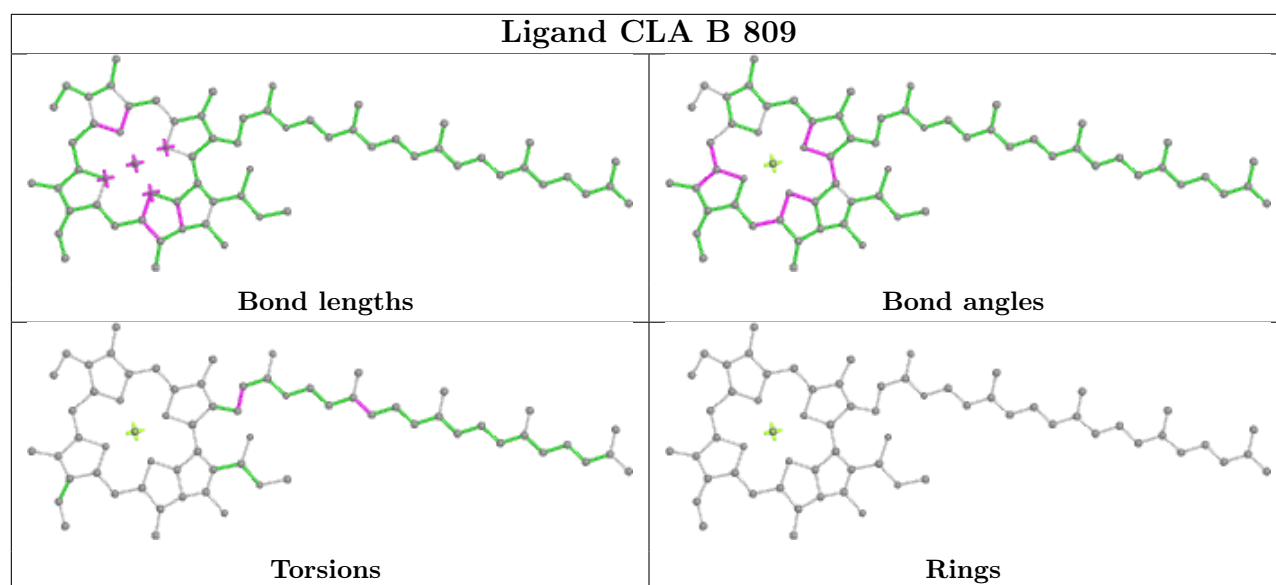
Ligand CLA A 823

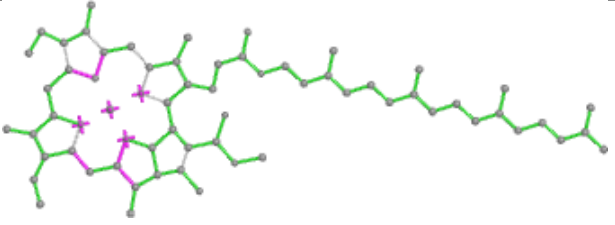
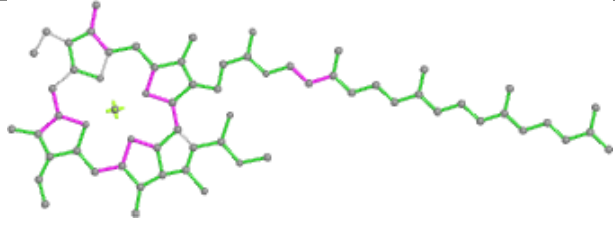
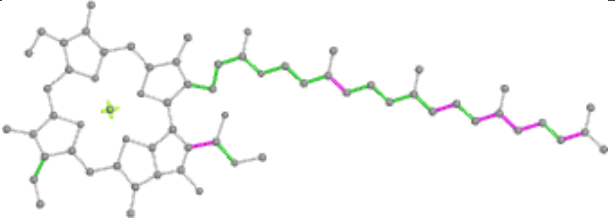
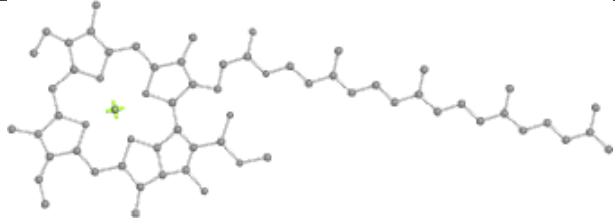
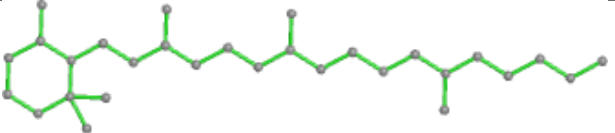
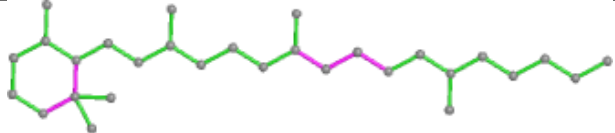
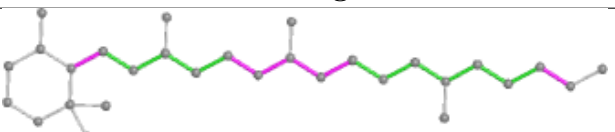
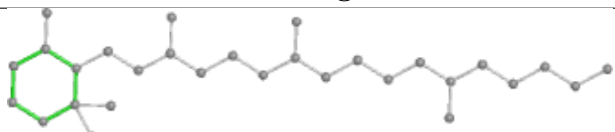
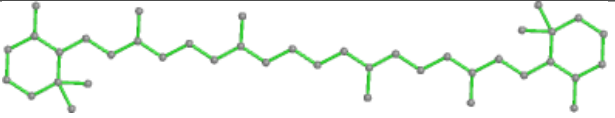
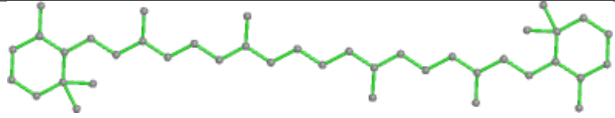
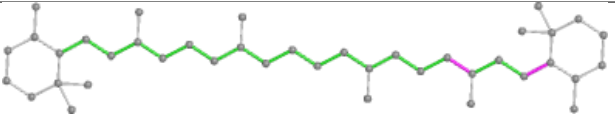
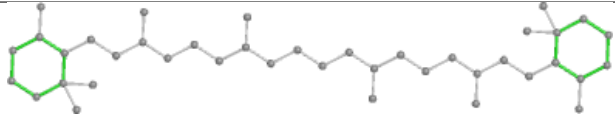


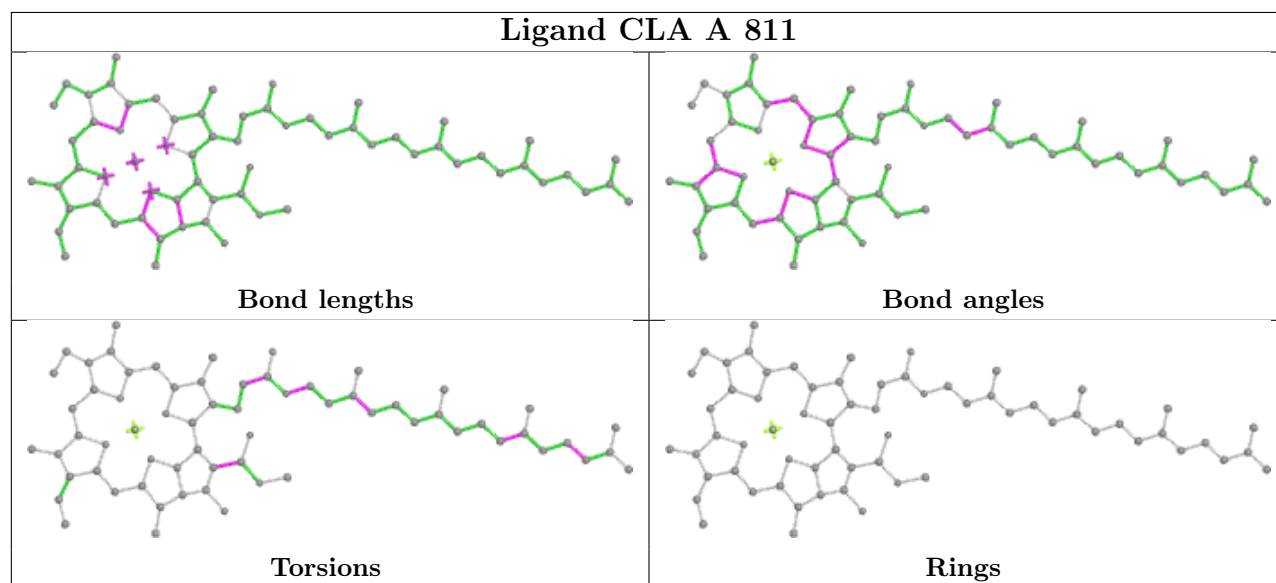
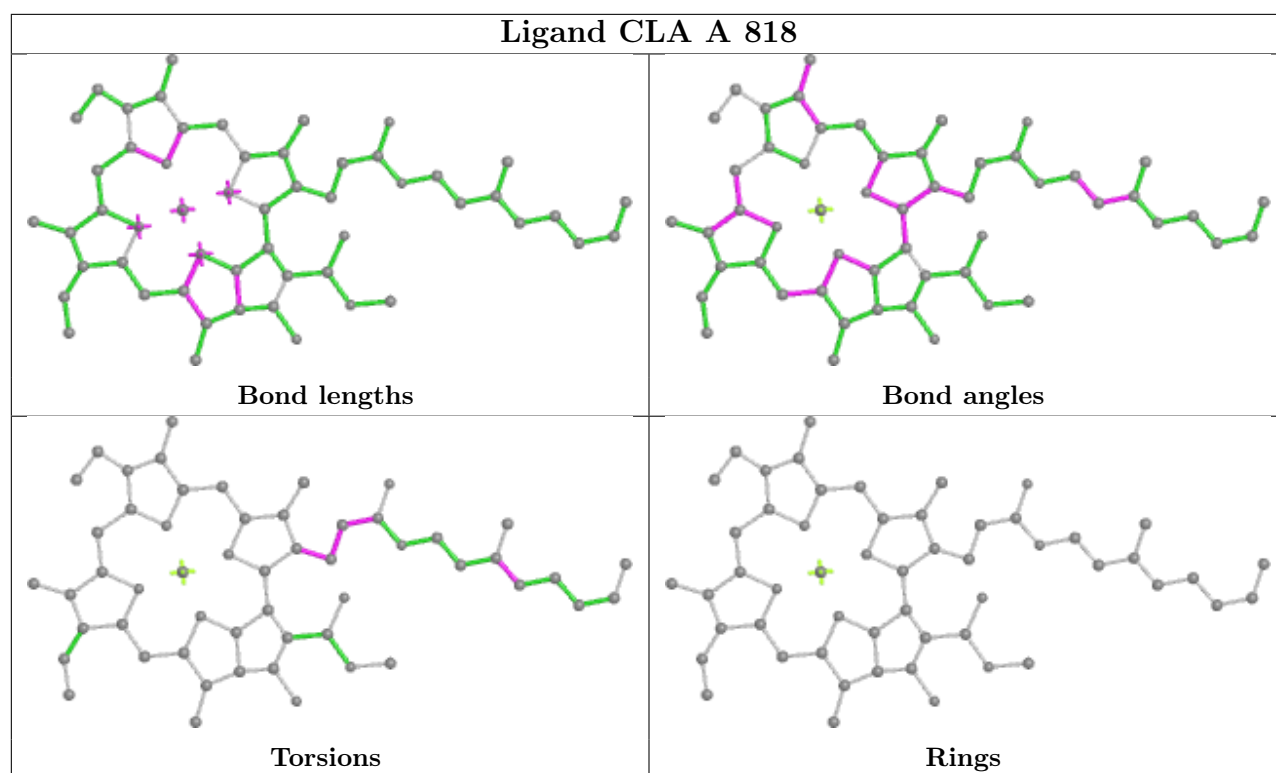
Ligand BCR B 844



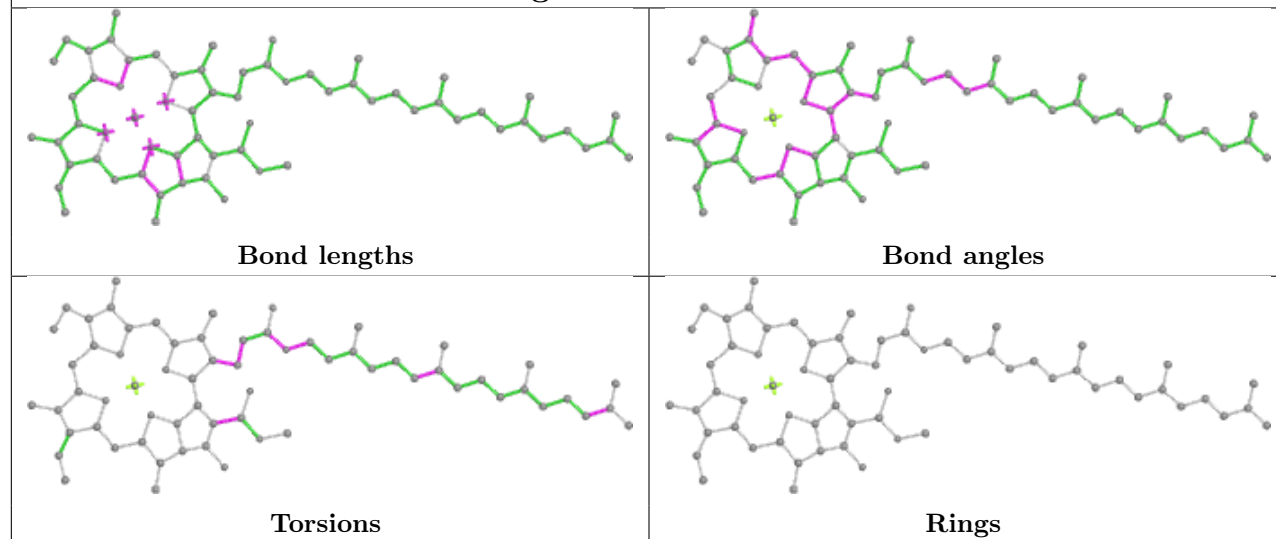




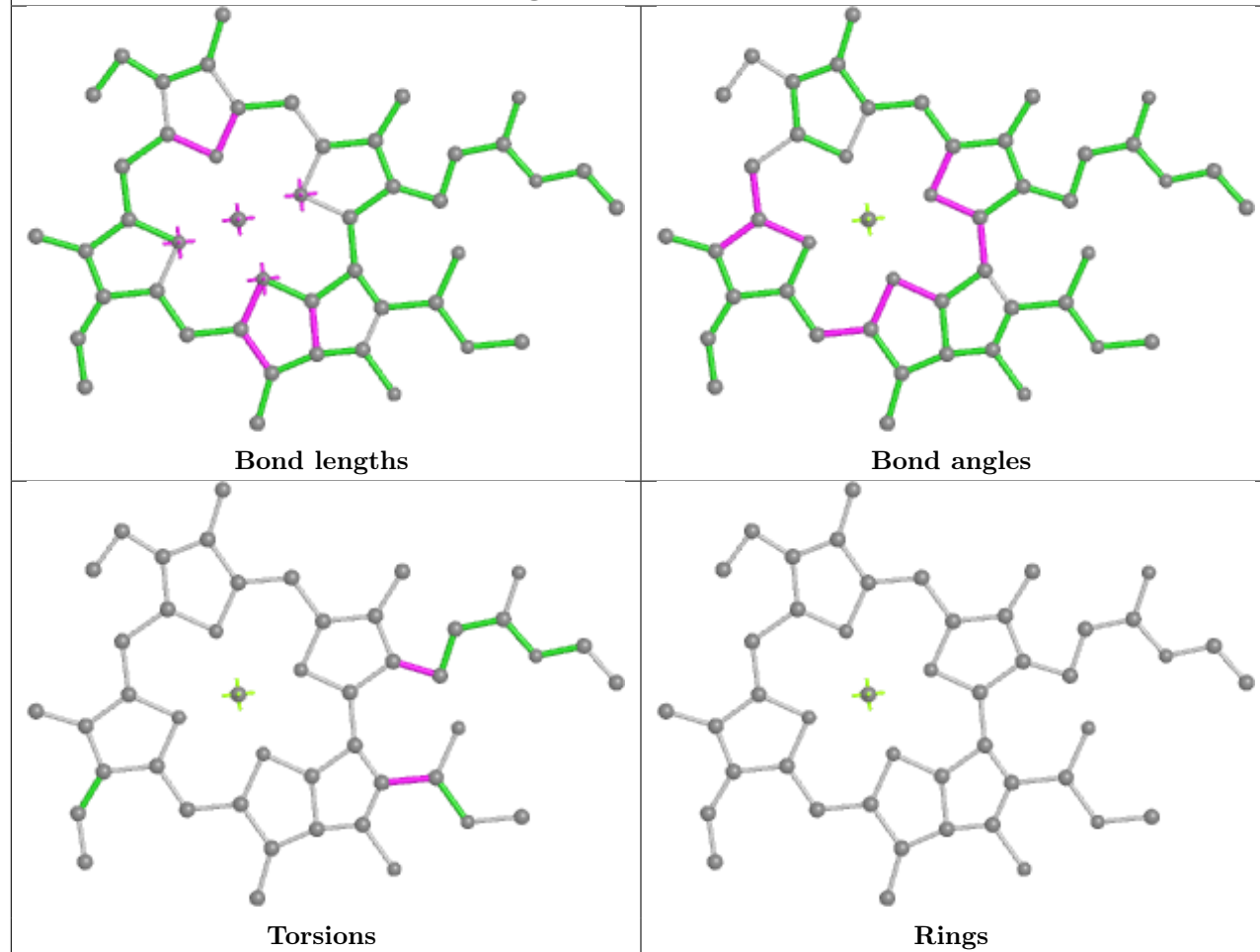
Ligand CLA A 825	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 856	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR I 102	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



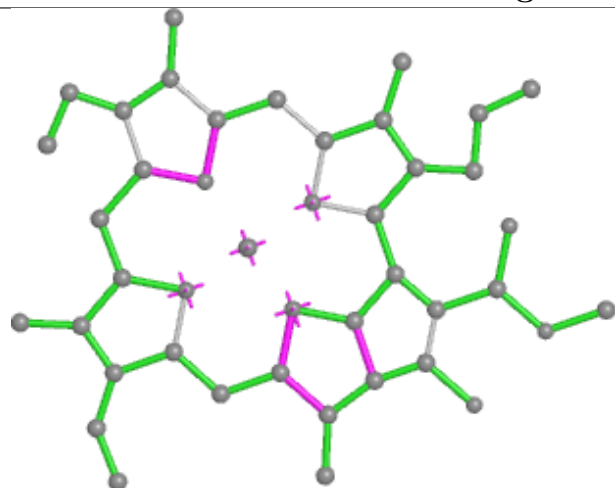
Ligand CLA A 819



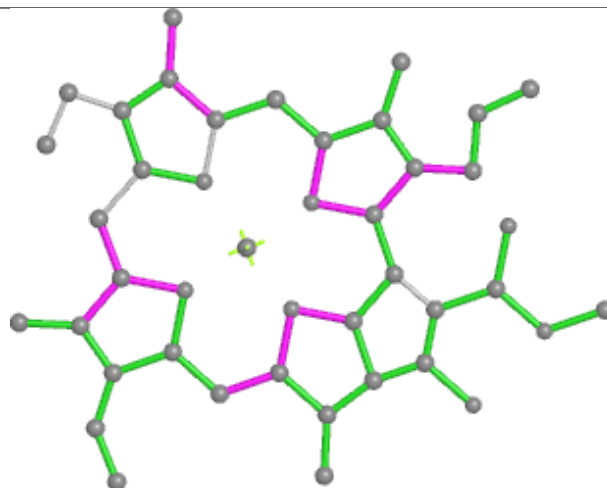
Ligand CLA B 834



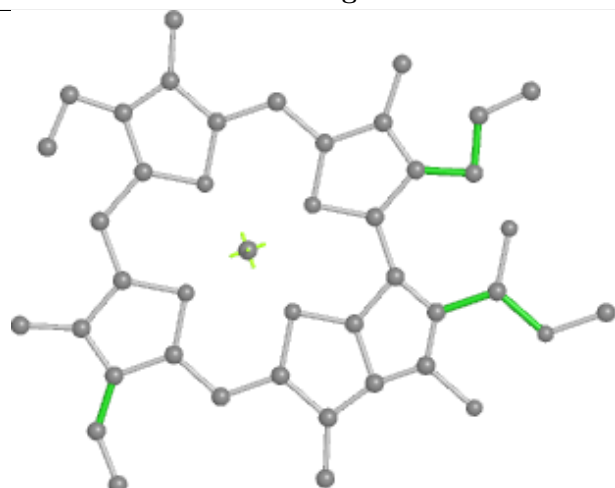
Ligand CLA B 813



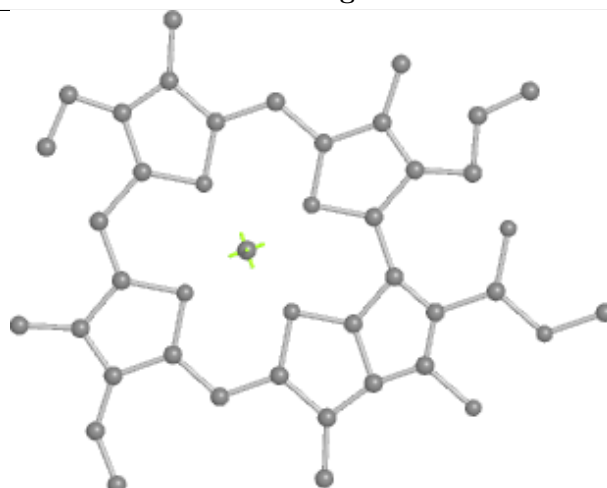
Bond lengths



Bond angles

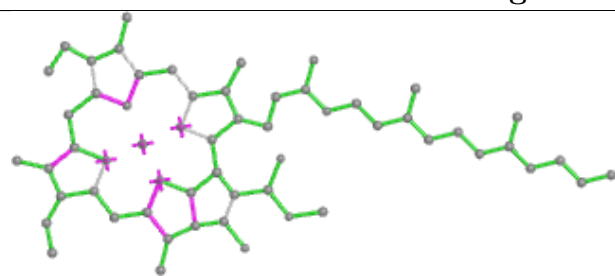


Torsions

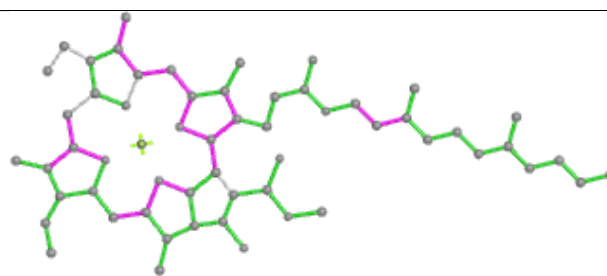


Rings

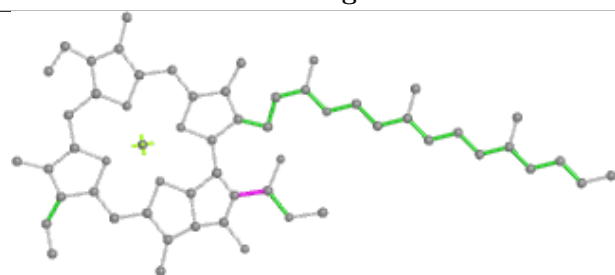
Ligand CLA L 1502



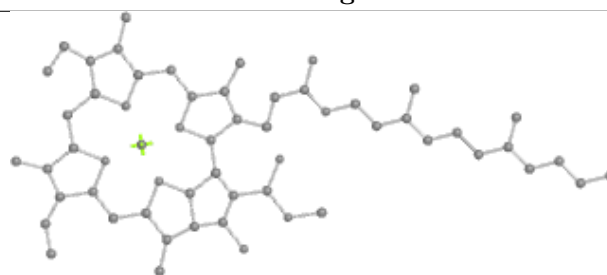
Bond lengths



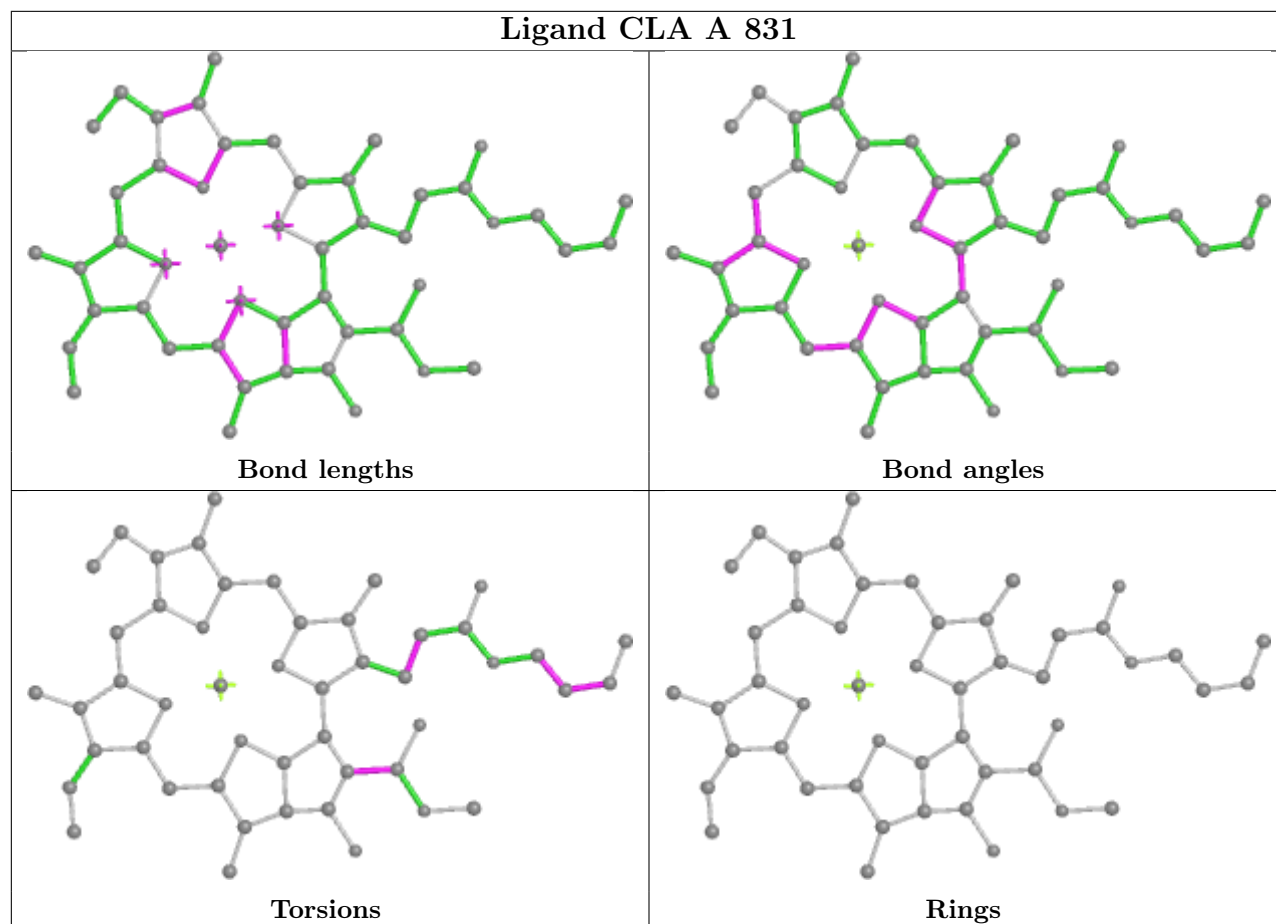
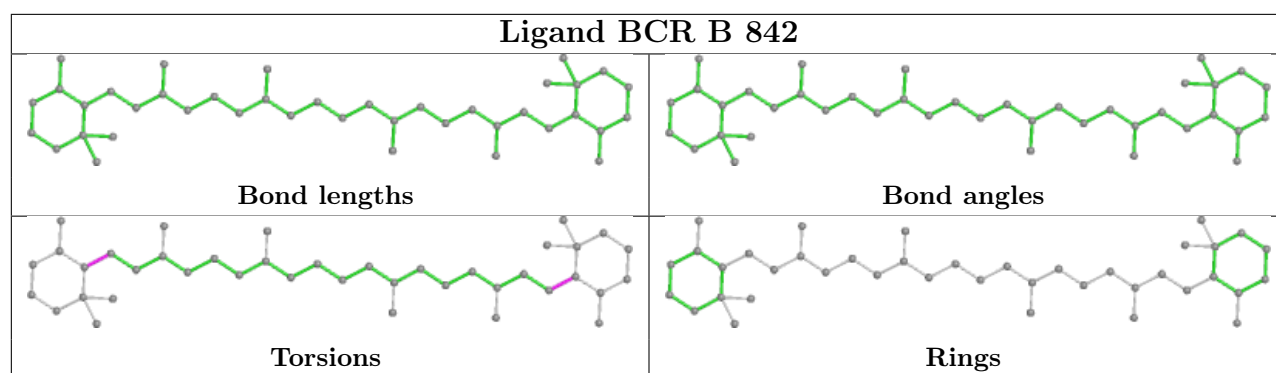
Bond angles



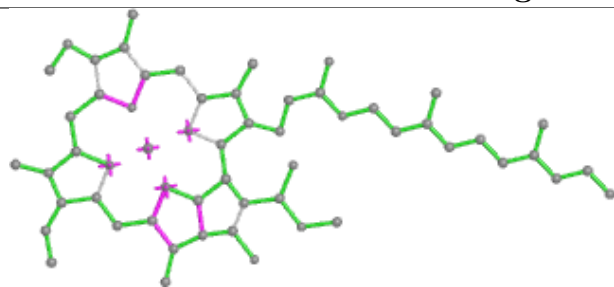
Torsions



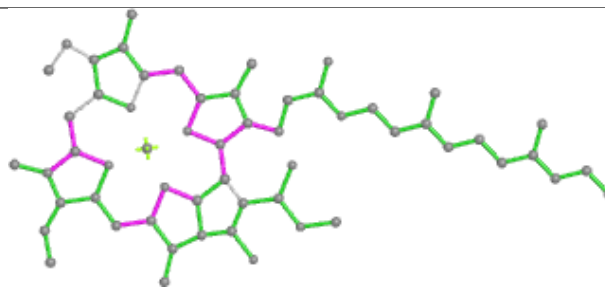
Rings



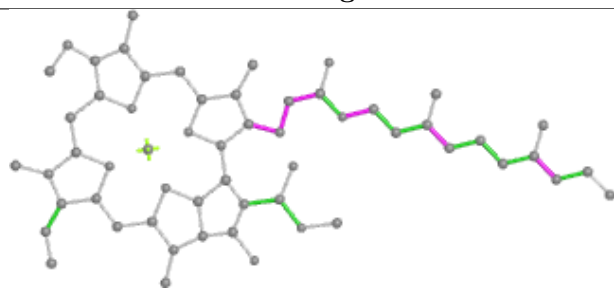
Ligand CLA B 823



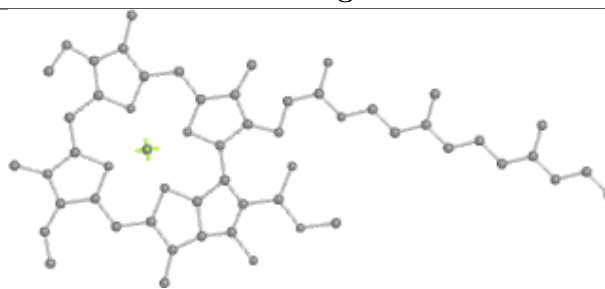
Bond lengths



Bond angles

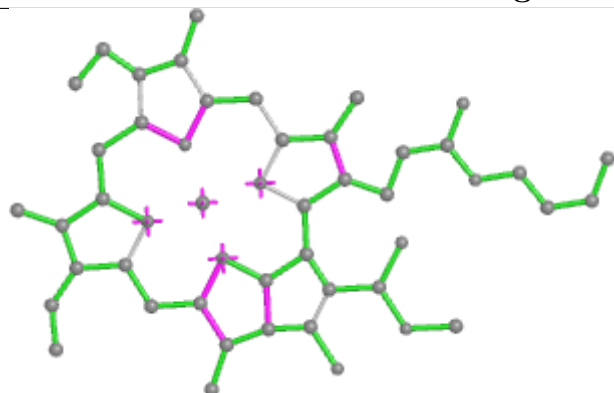


Torsions

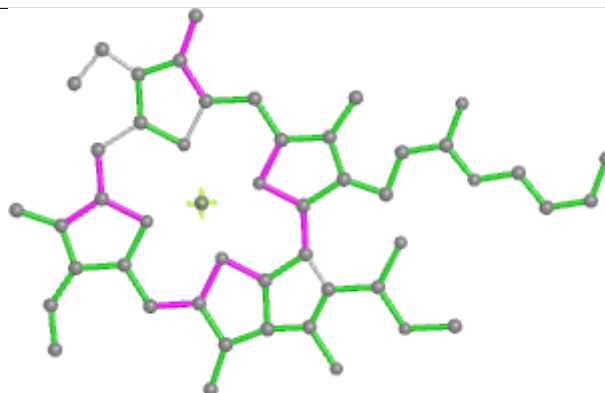


Rings

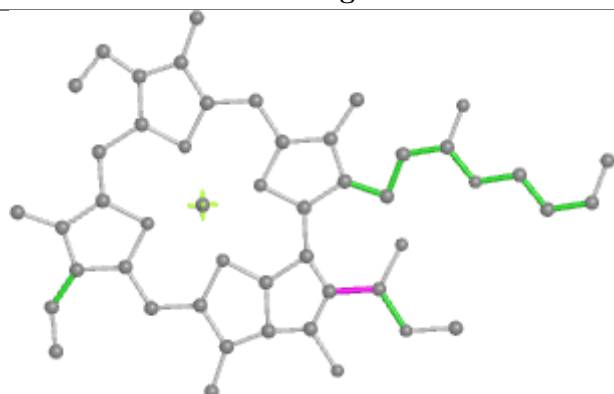
Ligand CLA A 839



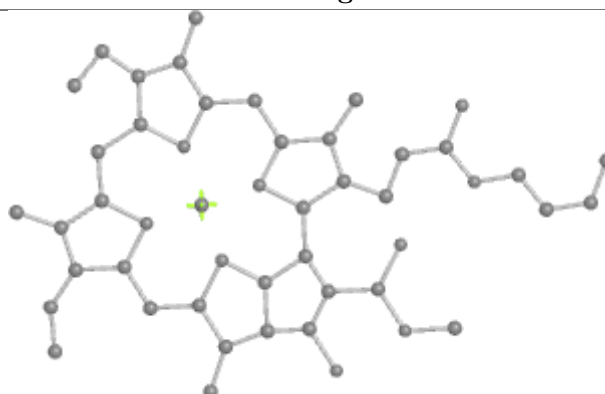
Bond lengths



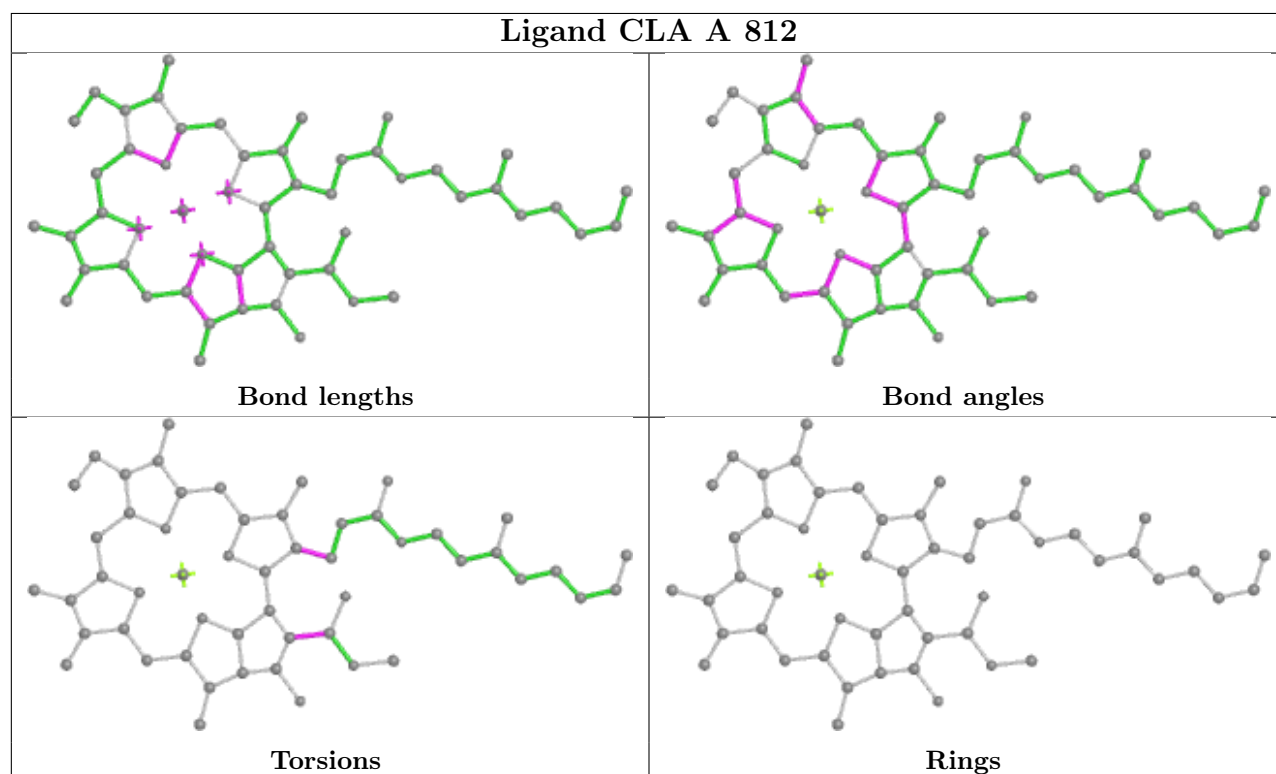
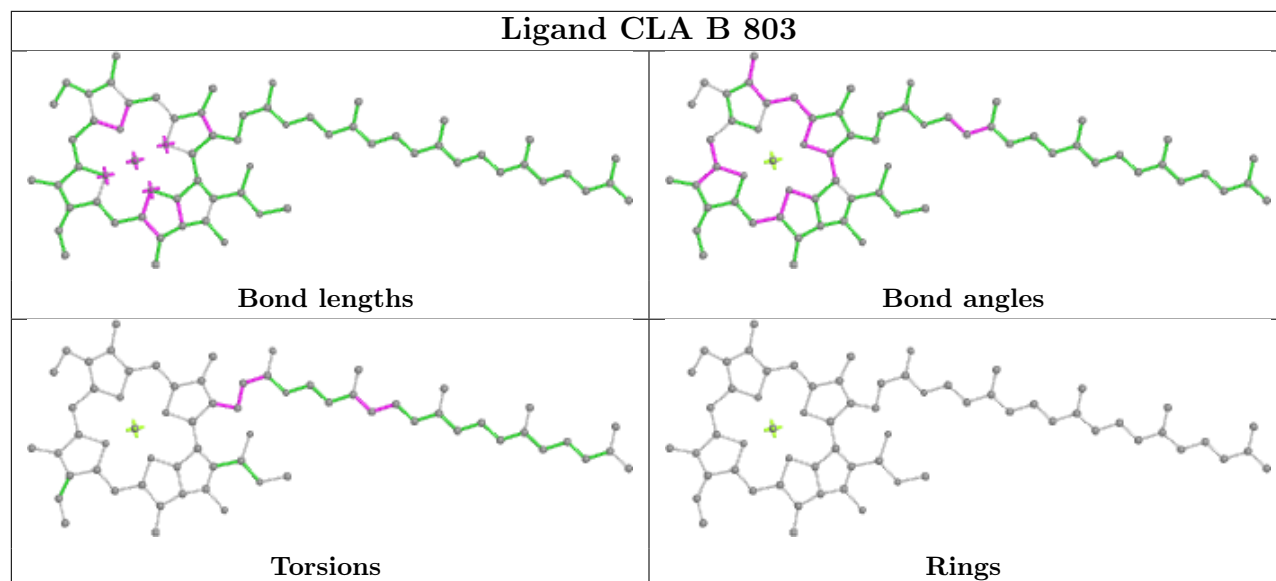
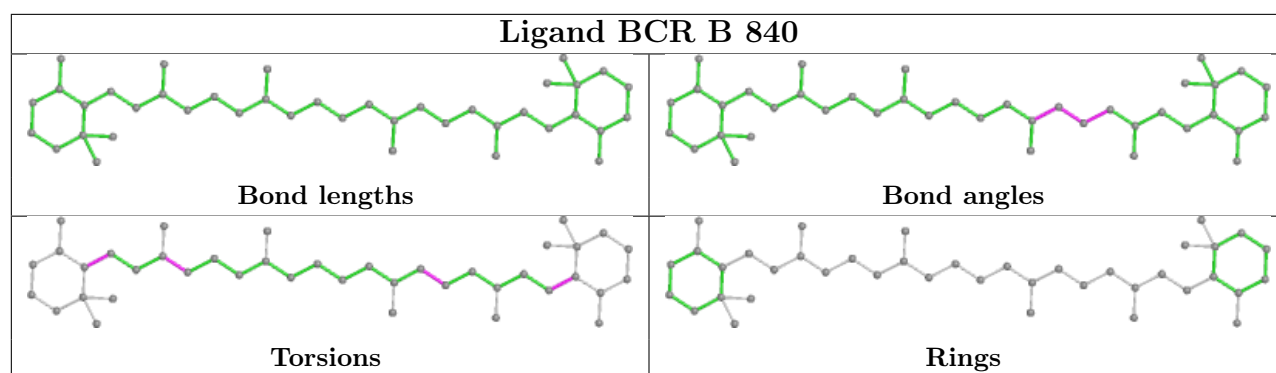
Bond angles

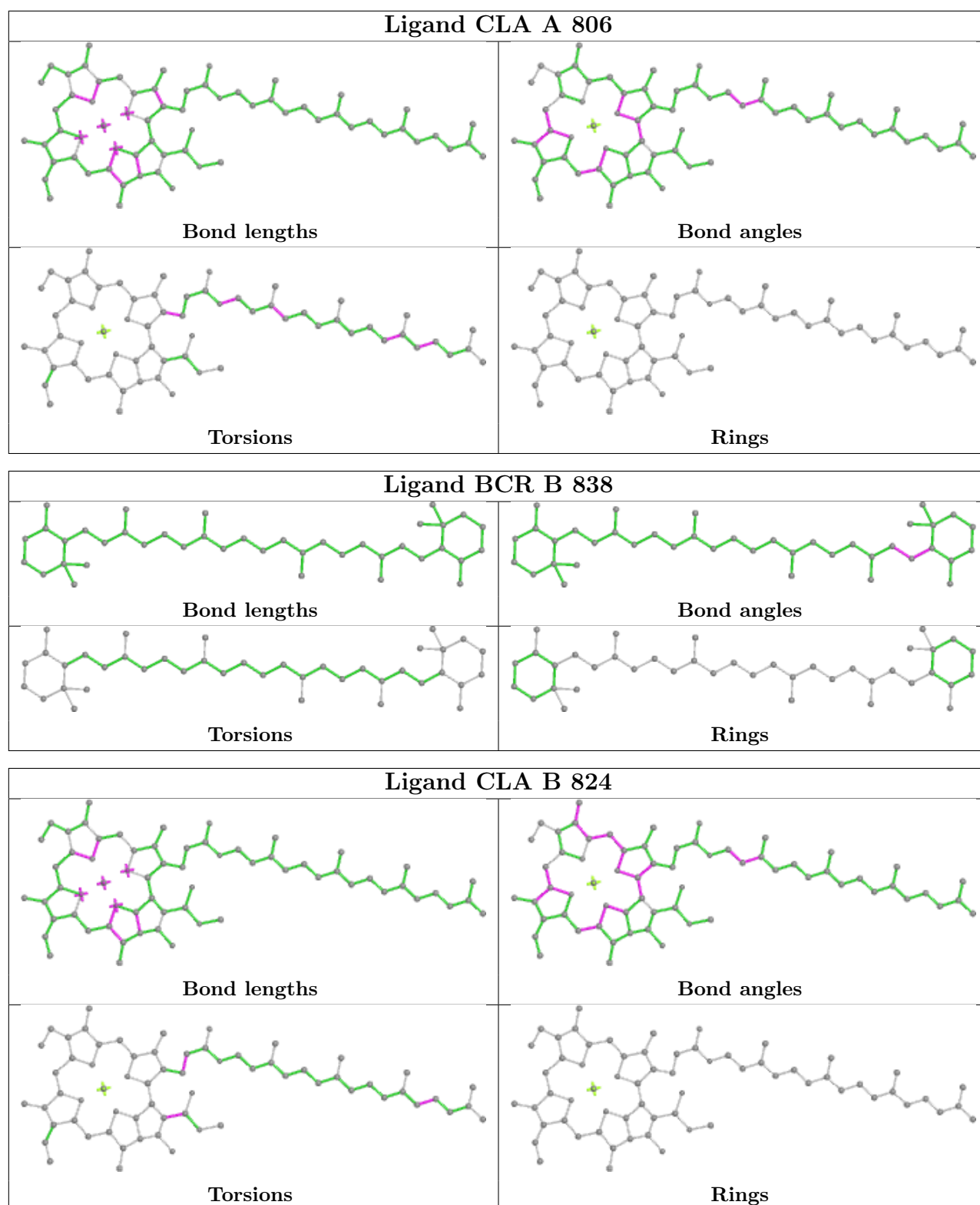


Torsions

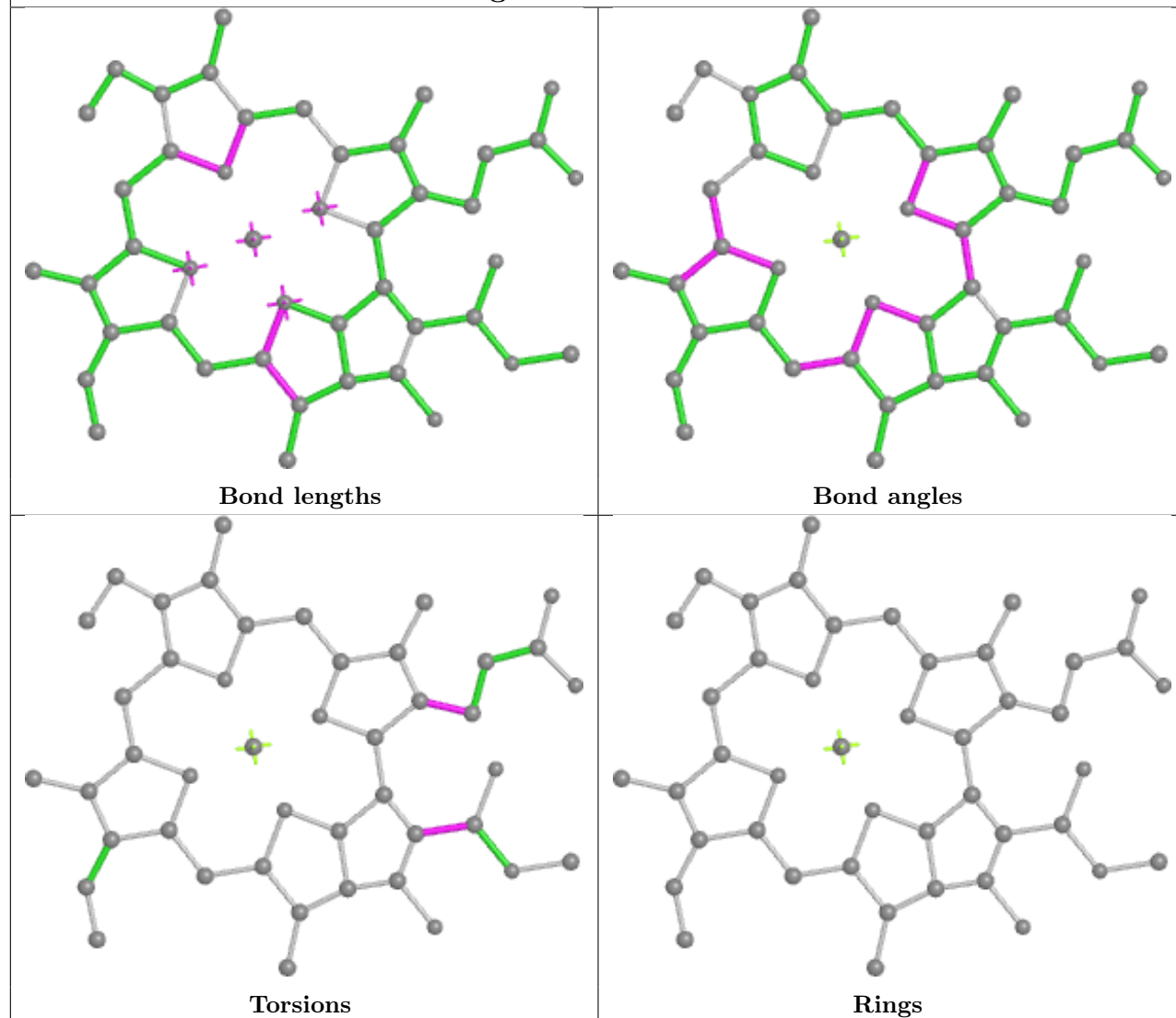


Rings

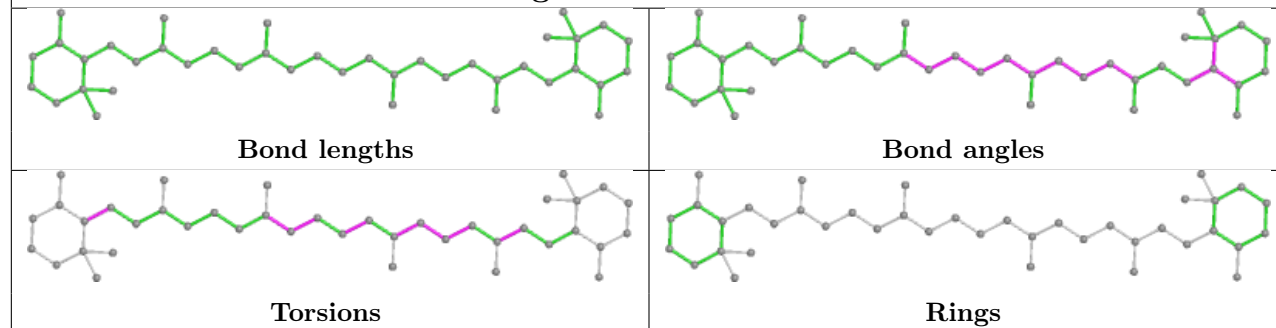


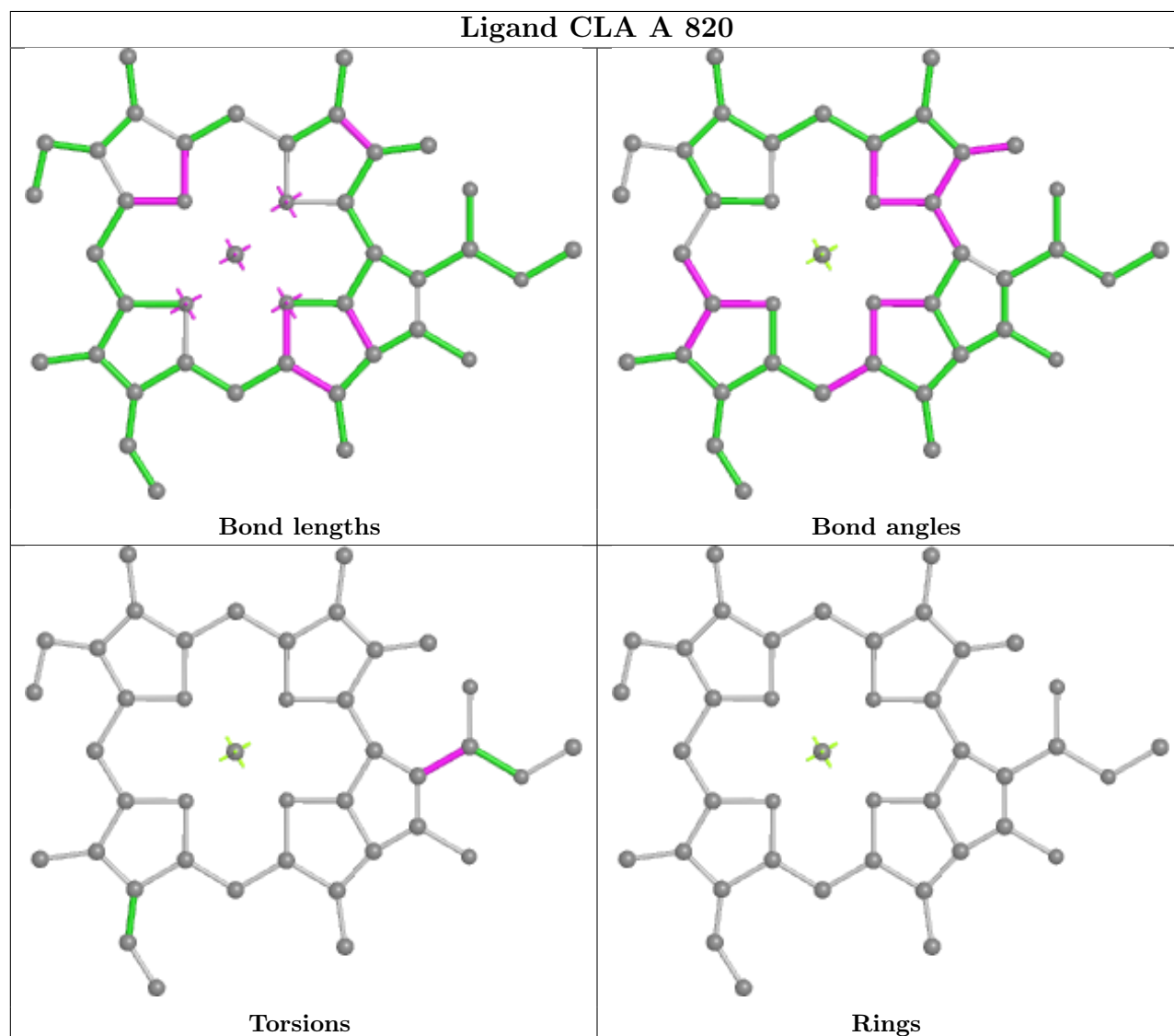
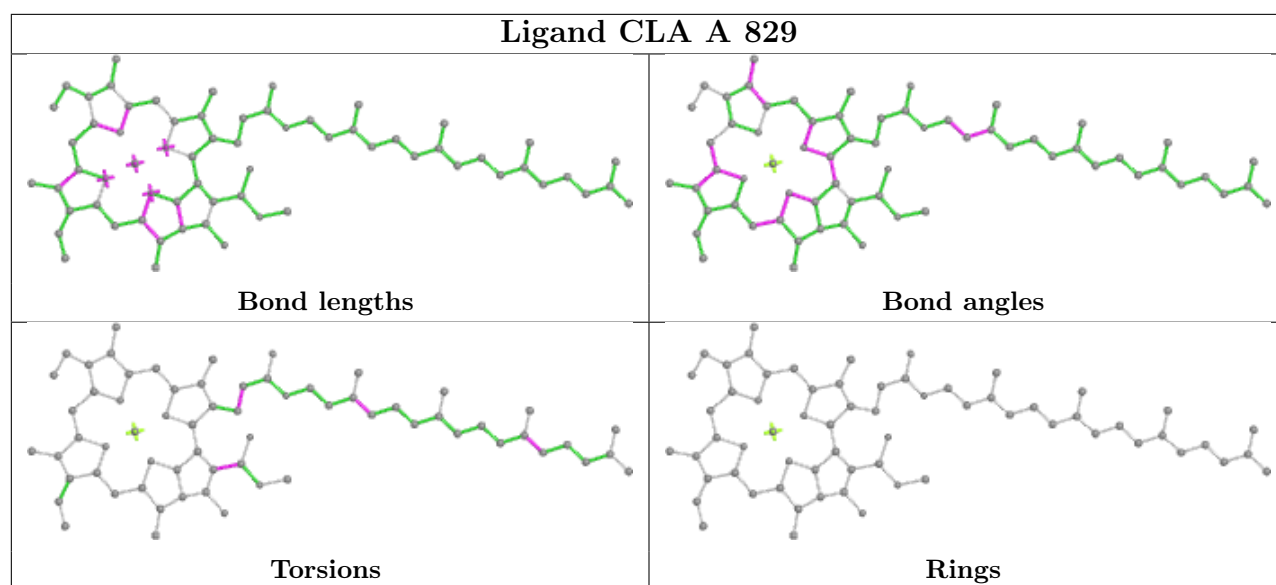


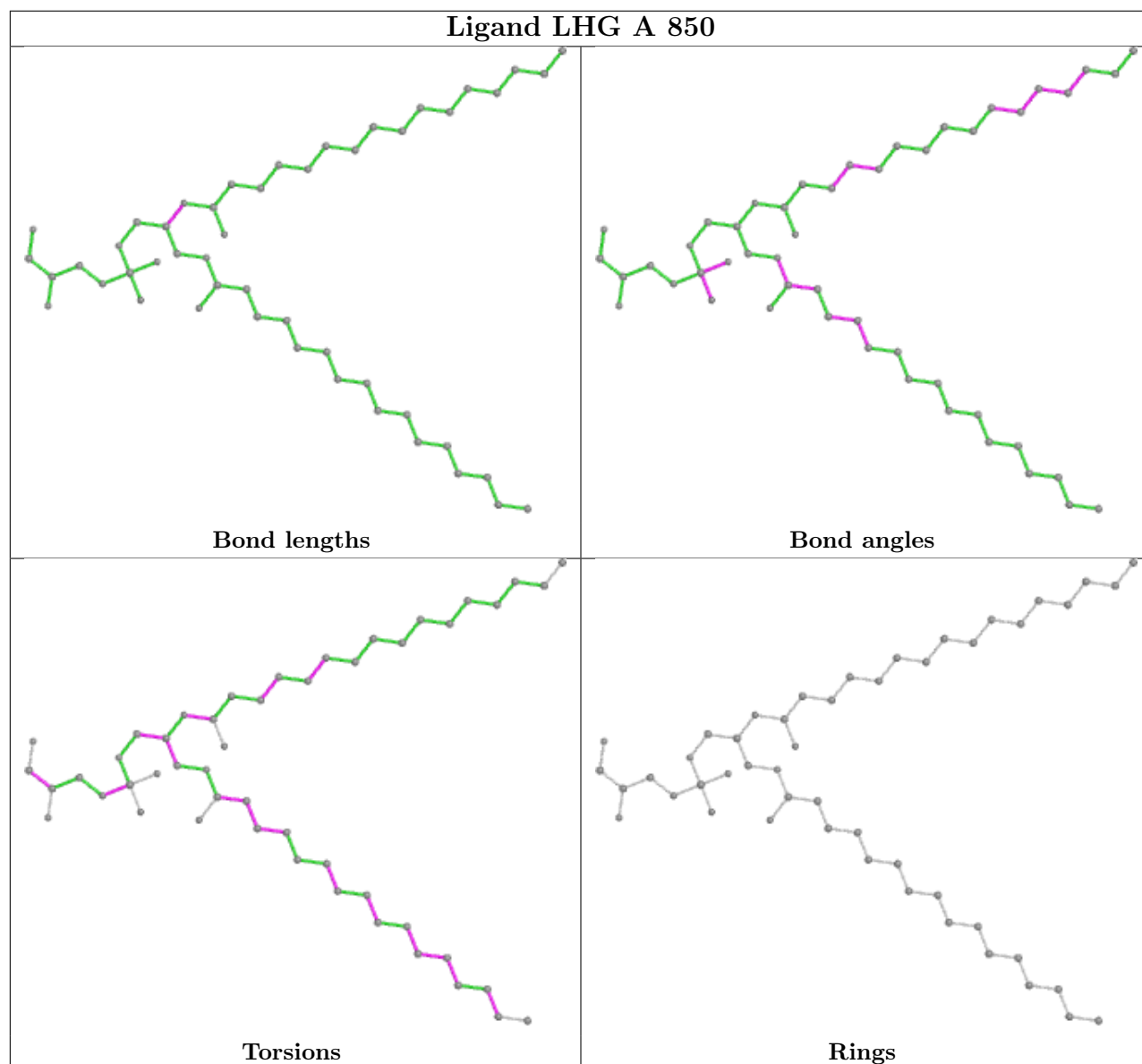
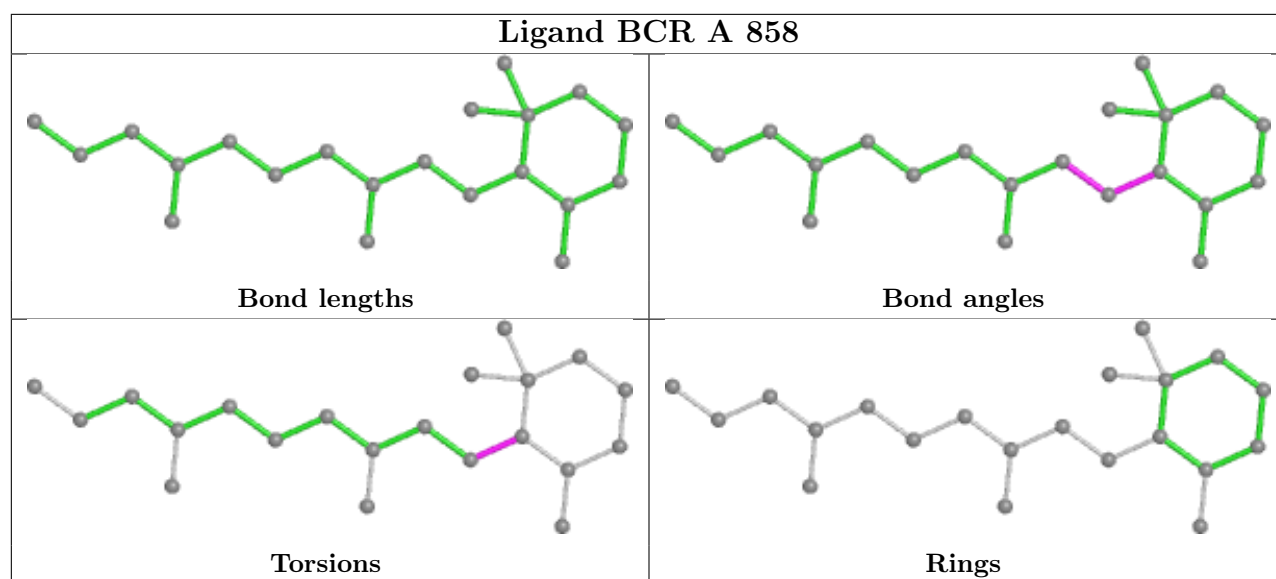
Ligand CLA A 810

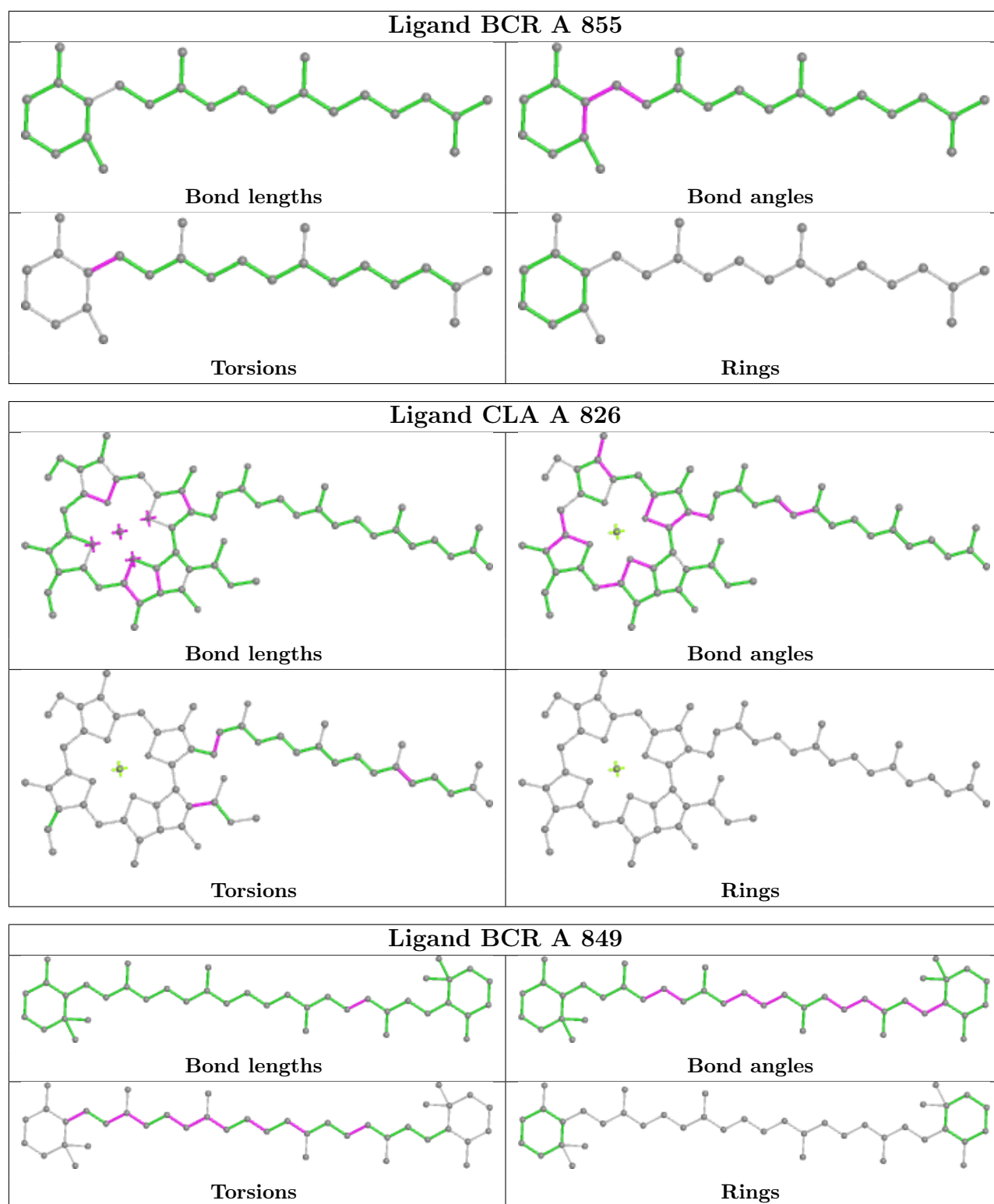


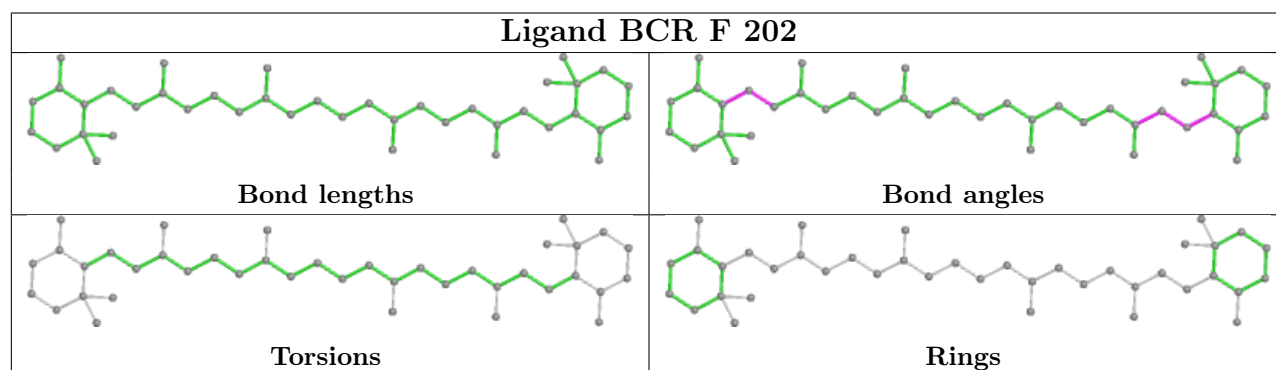
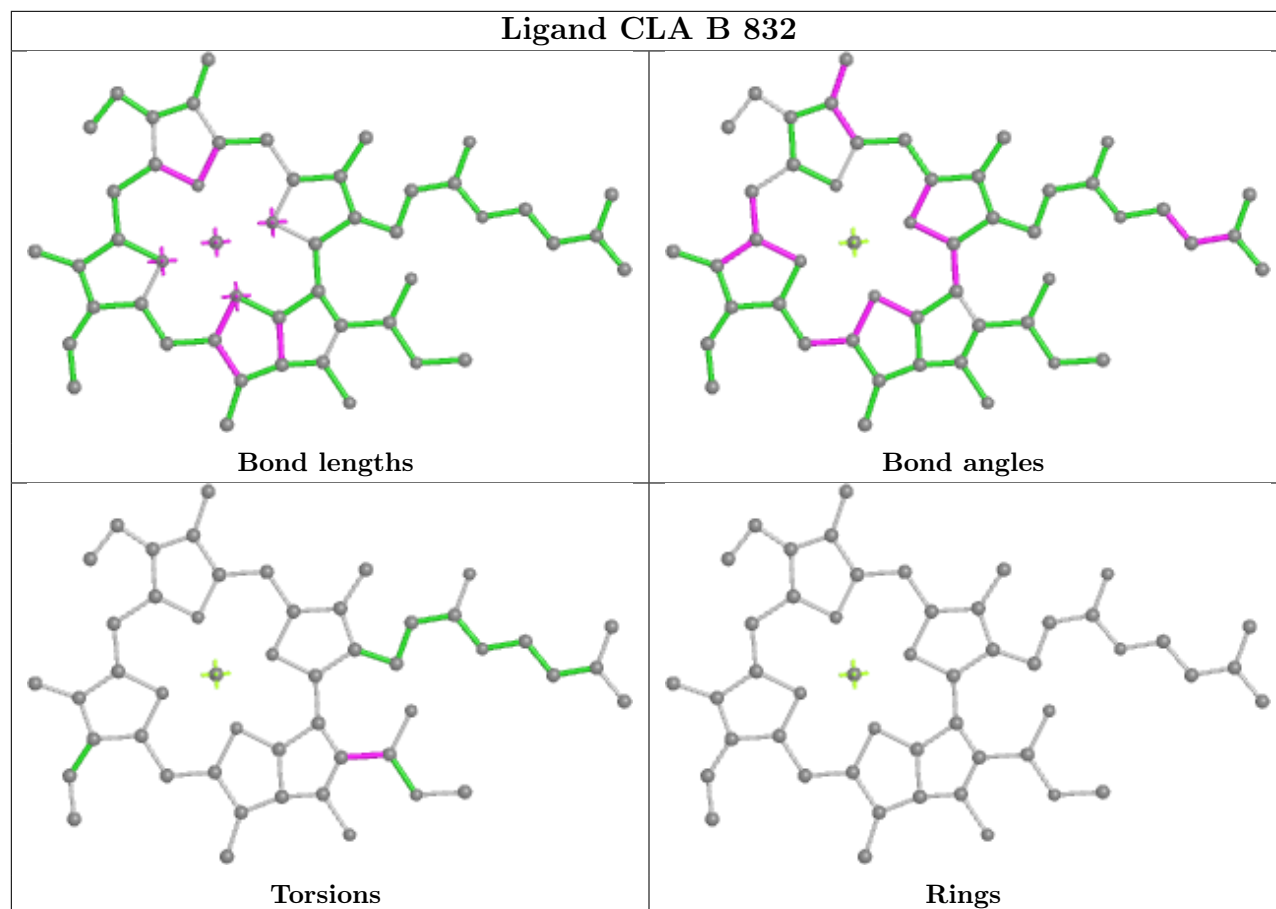
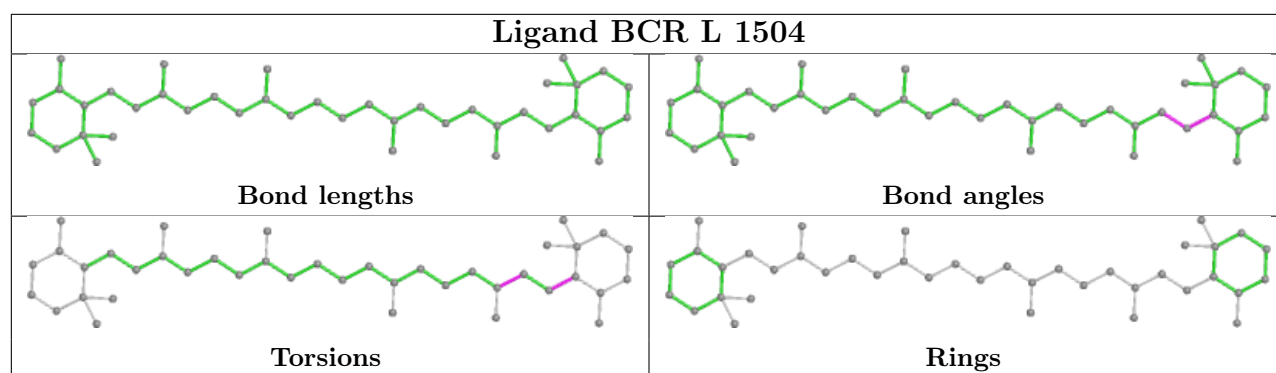
Ligand BCR F 201











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.