



## wwPDB EM Validation Summary Report ⓘ

Oct 13, 2025 – 02:25 pm BST

PDB ID : 9I9L / pdb\_00009i9l  
EMDB ID : EMD-52762  
Title : Structure of Far-Red Photosystem I from *C. thermalis* PCC 7203  
Authors : Consoli, G.; Tufail, F.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.  
Deposited on : 2025-02-06  
Resolution : 1.89 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev129  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

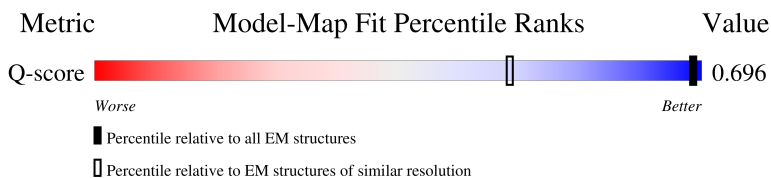
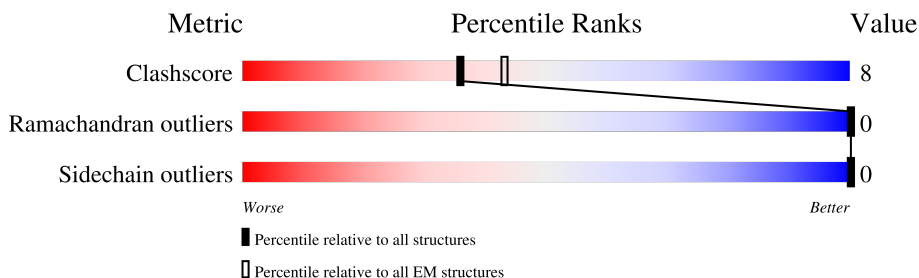
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 1.89 Å.

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






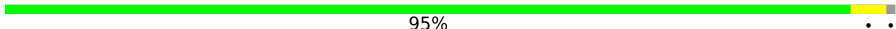





















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	1004 ( 1.39 - 2.38 )

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	782	 81% 15% .
1	N	782	 84% 12% .
1	a	782	 83% 13% .
2	B	740	 86% 14%





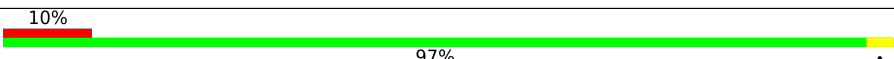
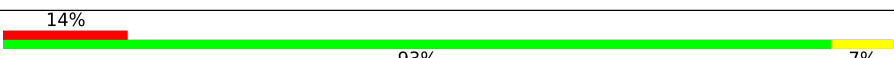
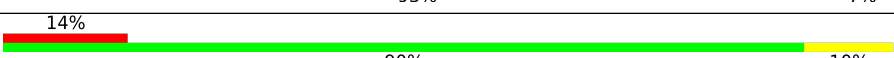
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Mol	Chain	Length	Quality of chain
2	O	740	 88% 12%
2	b	740	 89% 11%
3	C	81	 90% 9% .
3	P	81	 95% . .
3	c	81	 90% 9% .
4	D	142	 87% 11% .
4	Q	142	 84% 14% .
4	d	142	 91% 7% .
5	E	66	 89% 9% .
5	R	66	 89% 9% .
5	e	66	 92% 6% .
6	F	161	 73% 12% 15%
6	S	161	 74% 11% 15%
6	f	161	 75% 10% 15%
7	I	51	 57% 25% 18%
7	T	51	 63% 20% 18%
7	g	51	 65% 18% 18%
8	J	46	 83% 17%
8	U	46	 80% 20%
8	h	46	 85% 15%
9	K	80	 12% 84% 10% 6%
9	V	80	 11% 84% 10% 6%
9	i	80	 10% 80% 14% 6%
10	L	183	 84% 10% 6%
10	W	183	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
10	j	183	
11	M	32	
11	Y	32	
11	k	32	
12	X	29	
12	Z	29	
12	l	29	

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
13	CL0	A	801	X	-	-	-
13	CL0	N	801	X	-	-	-
13	CL0	a	801	X	-	-	-
15	CLA	A	803	X	-	-	-
15	CLA	A	804	X	-	-	-
15	CLA	A	805	X	-	-	-
15	CLA	A	806	X	-	-	-
15	CLA	A	807	X	-	-	-
15	CLA	A	808	X	-	-	-
15	CLA	A	809	X	-	-	-
15	CLA	A	810	X	-	-	-
15	CLA	A	811	X	-	-	-
15	CLA	A	812	X	-	-	-
15	CLA	A	813	X	-	-	-
15	CLA	A	814	X	-	-	-
15	CLA	A	815	X	-	-	-
15	CLA	A	816	X	-	-	-
15	CLA	A	817	X	-	-	-
15	CLA	A	818	X	-	-	-
15	CLA	A	819	X	-	-	-
15	CLA	A	820	X	-	-	-
15	CLA	A	821	X	-	-	-
15	CLA	A	822	X	-	-	-
15	CLA	A	823	X	-	-	-
15	CLA	A	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	A	827	X	-	-	-
15	CLA	A	828	X	-	-	-
15	CLA	A	829	X	-	-	-
15	CLA	A	830	X	-	-	-
15	CLA	A	831	X	-	-	-
15	CLA	A	832	X	-	-	-
15	CLA	A	833	X	-	-	-
15	CLA	A	834	X	-	-	-
15	CLA	A	835	X	-	-	-
15	CLA	A	836	X	-	-	-
15	CLA	A	837	X	-	-	-
15	CLA	A	838	X	-	-	-
15	CLA	A	839	X	-	-	-
15	CLA	A	840	X	-	-	-
15	CLA	A	841	X	-	-	-
15	CLA	A	842	X	-	-	-
15	CLA	B	801	X	-	-	-
15	CLA	B	802	X	-	-	-
15	CLA	B	803	X	-	-	-
15	CLA	B	804	X	-	-	-
15	CLA	B	805	X	-	-	-
15	CLA	B	806	X	-	-	-
15	CLA	B	807	X	-	-	-
15	CLA	B	808	X	-	-	-
15	CLA	B	809	X	-	-	-
15	CLA	B	810	X	-	-	-
15	CLA	B	811	X	-	-	-
15	CLA	B	813	X	-	-	-
15	CLA	B	814	X	-	-	-
15	CLA	B	815	X	-	-	-
15	CLA	B	816	X	-	-	-
15	CLA	B	817	X	-	-	-
15	CLA	B	818	X	-	-	-
15	CLA	B	819	X	-	-	-
15	CLA	B	820	X	-	-	-
15	CLA	B	821	X	-	-	-
15	CLA	B	822	X	-	-	-
15	CLA	B	823	X	-	-	-
15	CLA	B	824	X	-	-	-
15	CLA	B	825	X	-	-	-
15	CLA	B	826	X	-	-	-
15	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	828	X	-	-	-
15	CLA	B	829	X	-	-	-
15	CLA	B	830	X	-	-	-
15	CLA	B	831	X	-	-	-
15	CLA	B	833	X	-	-	-
15	CLA	B	834	X	-	-	-
15	CLA	B	835	X	-	-	-
15	CLA	B	836	X	-	-	-
15	CLA	B	837	X	-	-	-
15	CLA	B	838	X	-	-	-
15	CLA	B	840	X	-	-	-
15	CLA	F	201	X	-	-	-
15	CLA	K	102	X	-	-	-
15	CLA	K	103	X	-	-	-
15	CLA	L	202	X	-	-	-
15	CLA	L	203	X	-	-	-
15	CLA	N	803	X	-	-	-
15	CLA	N	804	X	-	-	-
15	CLA	N	805	X	-	-	-
15	CLA	N	806	X	-	-	-
15	CLA	N	807	X	-	-	-
15	CLA	N	808	X	-	-	-
15	CLA	N	809	X	-	-	-
15	CLA	N	810	X	-	-	-
15	CLA	N	811	X	-	-	-
15	CLA	N	812	X	-	-	-
15	CLA	N	813	X	-	-	-
15	CLA	N	814	X	-	-	-
15	CLA	N	815	X	-	-	-
15	CLA	N	816	X	-	-	-
15	CLA	N	817	X	-	-	-
15	CLA	N	818	X	-	-	-
15	CLA	N	819	X	-	-	-
15	CLA	N	820	X	-	-	-
15	CLA	N	821	X	-	-	-
15	CLA	N	822	X	-	-	-
15	CLA	N	823	X	-	-	-
15	CLA	N	825	X	-	-	-
15	CLA	N	827	X	-	-	-
15	CLA	N	828	X	-	-	-
15	CLA	N	829	X	-	-	-
15	CLA	N	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	N	831	X	-	-	-
15	CLA	N	832	X	-	-	-
15	CLA	N	833	X	-	-	-
15	CLA	N	834	X	-	-	-
15	CLA	N	835	X	-	-	-
15	CLA	N	836	X	-	-	-
15	CLA	N	837	X	-	-	-
15	CLA	N	838	X	-	-	-
15	CLA	N	839	X	-	-	-
15	CLA	N	840	X	-	-	-
15	CLA	N	841	X	-	-	-
15	CLA	N	842	X	-	-	-
15	CLA	O	801	X	-	-	-
15	CLA	O	802	X	-	-	-
15	CLA	O	803	X	-	-	-
15	CLA	O	804	X	-	-	-
15	CLA	O	805	X	-	-	-
15	CLA	O	806	X	-	-	-
15	CLA	O	807	X	-	-	-
15	CLA	O	808	X	-	-	-
15	CLA	O	809	X	-	-	-
15	CLA	O	810	X	-	-	-
15	CLA	O	811	X	-	-	-
15	CLA	O	813	X	-	-	-
15	CLA	O	814	X	-	-	-
15	CLA	O	815	X	-	-	-
15	CLA	O	816	X	-	-	-
15	CLA	O	817	X	-	-	-
15	CLA	O	818	X	-	-	-
15	CLA	O	819	X	-	-	-
15	CLA	O	820	X	-	-	-
15	CLA	O	821	X	-	-	-
15	CLA	O	822	X	-	-	-
15	CLA	O	823	X	-	-	-
15	CLA	O	824	X	-	-	-
15	CLA	O	825	X	-	-	-
15	CLA	O	826	X	-	-	-
15	CLA	O	827	X	-	-	-
15	CLA	O	828	X	-	-	-
15	CLA	O	829	X	-	-	-
15	CLA	O	830	X	-	-	-
15	CLA	O	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	O	833	X	-	-	-
15	CLA	O	834	X	-	-	-
15	CLA	O	835	X	-	-	-
15	CLA	O	836	X	-	-	-
15	CLA	O	837	X	-	-	-
15	CLA	O	838	X	-	-	-
15	CLA	O	840	X	-	-	-
15	CLA	S	201	X	-	-	-
15	CLA	V	102	X	-	-	-
15	CLA	V	103	X	-	-	-
15	CLA	W	202	X	-	-	-
15	CLA	W	203	X	-	-	-
15	CLA	X	102	X	-	-	-
15	CLA	Z	102	X	-	-	-
15	CLA	a	803	X	-	-	-
15	CLA	a	804	X	-	-	-
15	CLA	a	805	X	-	-	-
15	CLA	a	806	X	-	-	-
15	CLA	a	807	X	-	-	-
15	CLA	a	808	X	-	-	-
15	CLA	a	809	X	-	-	-
15	CLA	a	810	X	-	-	-
15	CLA	a	811	X	-	-	-
15	CLA	a	812	X	-	-	-
15	CLA	a	813	X	-	-	-
15	CLA	a	814	X	-	-	-
15	CLA	a	815	X	-	-	-
15	CLA	a	816	X	-	-	-
15	CLA	a	817	X	-	-	-
15	CLA	a	818	X	-	-	-
15	CLA	a	819	X	-	-	-
15	CLA	a	820	X	-	-	-
15	CLA	a	821	X	-	-	-
15	CLA	a	822	X	-	-	-
15	CLA	a	823	X	-	-	-
15	CLA	a	825	X	-	-	-
15	CLA	a	827	X	-	-	-
15	CLA	a	828	X	-	-	-
15	CLA	a	829	X	-	-	-
15	CLA	a	830	X	-	-	-
15	CLA	a	831	X	-	-	-
15	CLA	a	832	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a	833	X	-	-	-
15	CLA	a	834	X	-	-	-
15	CLA	a	835	X	-	-	-
15	CLA	a	836	X	-	-	-
15	CLA	a	837	X	-	-	-
15	CLA	a	838	X	-	-	-
15	CLA	a	839	X	-	-	-
15	CLA	a	840	X	-	-	-
15	CLA	a	841	X	-	-	-
15	CLA	a	842	X	-	-	-
15	CLA	b	801	X	-	-	-
15	CLA	b	802	X	-	-	-
15	CLA	b	803	X	-	-	-
15	CLA	b	804	X	-	-	-
15	CLA	b	805	X	-	-	-
15	CLA	b	806	X	-	-	-
15	CLA	b	807	X	-	-	-
15	CLA	b	808	X	-	-	-
15	CLA	b	809	X	-	-	-
15	CLA	b	810	X	-	-	-
15	CLA	b	811	X	-	-	-
15	CLA	b	813	X	-	-	-
15	CLA	b	814	X	-	-	-
15	CLA	b	815	X	-	-	-
15	CLA	b	816	X	-	-	-
15	CLA	b	817	X	-	-	-
15	CLA	b	818	X	-	-	-
15	CLA	b	819	X	-	-	-
15	CLA	b	820	X	-	-	-
15	CLA	b	821	X	-	-	-
15	CLA	b	822	X	-	-	-
15	CLA	b	823	X	-	-	-
15	CLA	b	824	X	-	-	-
15	CLA	b	825	X	-	-	-
15	CLA	b	826	X	-	-	-
15	CLA	b	827	X	-	-	-
15	CLA	b	828	X	-	-	-
15	CLA	b	829	X	-	-	-
15	CLA	b	830	X	-	-	-
15	CLA	b	831	X	-	-	-
15	CLA	b	833	X	-	-	-
15	CLA	b	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b	835	X	-	-	-
15	CLA	b	836	X	-	-	-
15	CLA	b	837	X	-	-	-
15	CLA	b	838	X	-	-	-
15	CLA	b	840	X	-	-	-
15	CLA	f	201	X	-	-	-
15	CLA	i	102	X	-	-	-
15	CLA	i	103	X	-	-	-
15	CLA	j	202	X	-	-	-
15	CLA	j	203	X	-	-	-
15	CLA	l	102	X	-	-	-

## 2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 75954 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	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	N	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	a	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	O	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		

- 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
			600	368	103	118	11		
3	P	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	c	80	Total	C	N	O	S	0	0
			600	368	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		
4	d	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O		0	0
			530	341	92	97			
5	R	65	Total	C	N	O		0	0
			530	341	92	97			
5	e	65	Total	C	N	O		0	0
			530	341	92	97			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	S	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	f	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	T	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	g	42	Total	C	N	O	S	0	0
			351	247	47	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	46	Total	C	N	O	S	0	0
			373	256	54	59	4		
8	U	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	V	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	i	75	Total	C	N	O	S	0	0
			539	356	88	94	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	12	MET	-	initiating methionine	UNP K9TX25
V	12	MET	-	initiating methionine	UNP K9TX25
i	12	MET	-	initiating methionine	UNP K9TX25

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	W	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	j	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	Y	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	k	31	Total	C	N	O	S	0	0
			240	160	37	42	1		

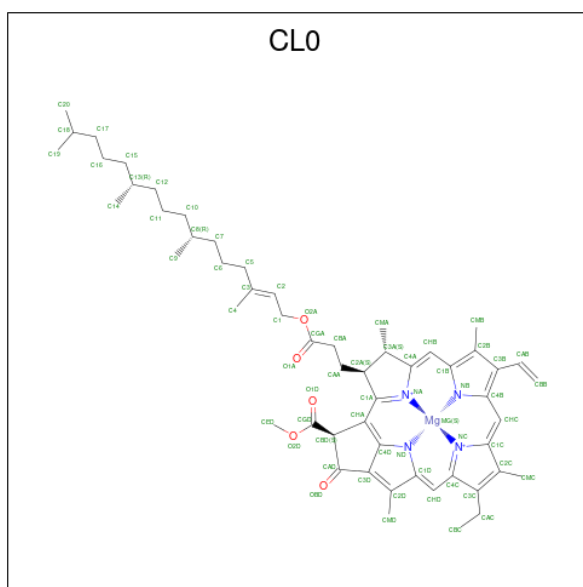
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	initiating methionine	UNP K9TSY6
Y	0	MET	-	initiating methionine	UNP K9TSY6
k	0	MET	-	initiating methionine	UNP K9TSY6

- Molecule 12 is a protein called Photosystem one Psax.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			227	157	36	34		
12	Z	29	Total	C	N	O	0	0
			227	157	36	34		
12	l	29	Total	C	N	O	0	0
			227	157	36	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	Mg	N	O
			65	55	1	4	5
13	N	1	Total	C	Mg	N	O
			65	55	1	4	5
13	a	1	Total	C	Mg	N	O
			65	55	1	4	5

- Molecule 14 is Chlorophyll F (CCD ID: F6C) (formula:  $C_{55}H_{68}MgN_4O_6$ ) (labeled as "Ligand of Interest" by depositor).

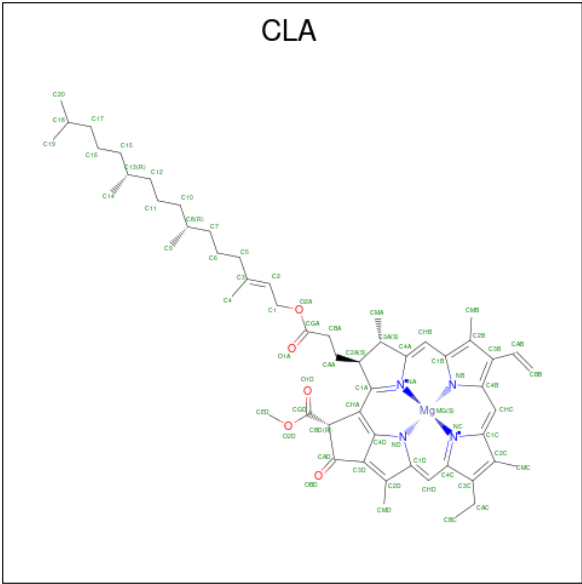


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Mol	Chain	Residues	Atoms					AltConf
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



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

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

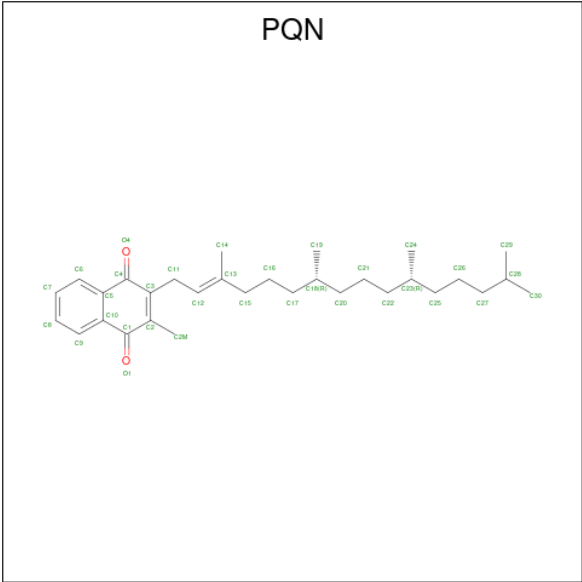
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Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	l	1	Total 55	C 45	Mg 1	N 4	O 5	0

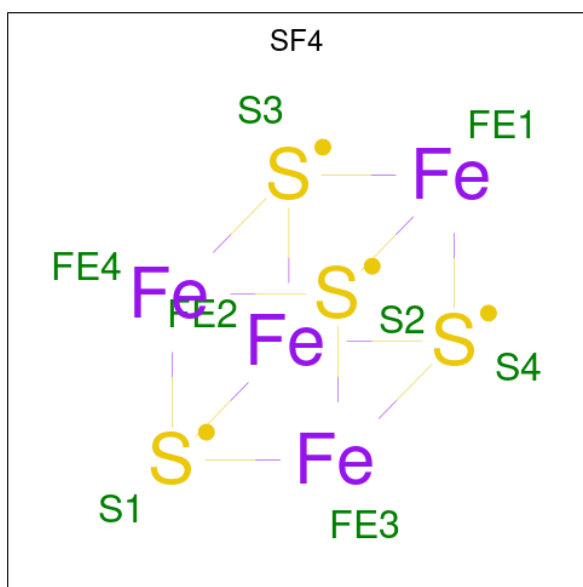
- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).





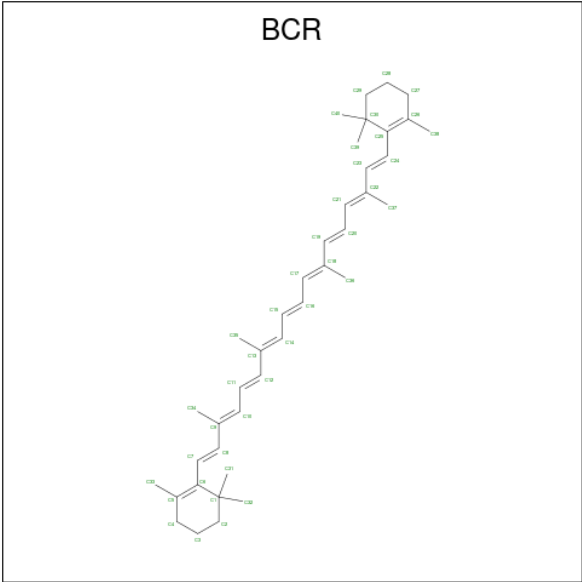
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	N	1	Total	C	O	0
			33	31	2	
16	O	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms			AltConf
17	A	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	C	1	Total	Fe	S	0
			8	4	4	
17	N	1	Total	Fe	S	0
			8	4	4	
17	P	1	Total	Fe	S	0
			8	4	4	
17	P	1	Total	Fe	S	0
			8	4	4	
17	a	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	
17	c	1	Total	Fe	S	0
			8	4	4	

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	F	1	Total	C	0
			40	40	
18	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 25 25	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

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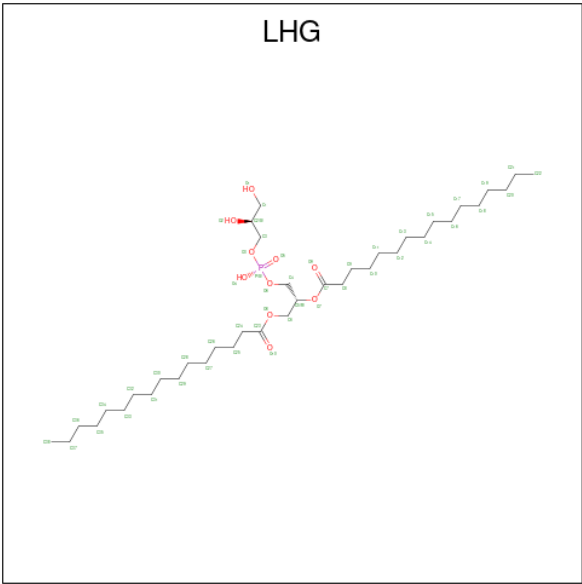
Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total C 40 40	0
18	S	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 25 25	0
18	W	1	Total C 40 40	0
18	W	1	Total C 40 40	0
18	Y	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total	C	0
			40	40	
18	b	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	i	1	Total	C	0
			25	25	
18	j	1	Total	C	0
			40	40	
18	k	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



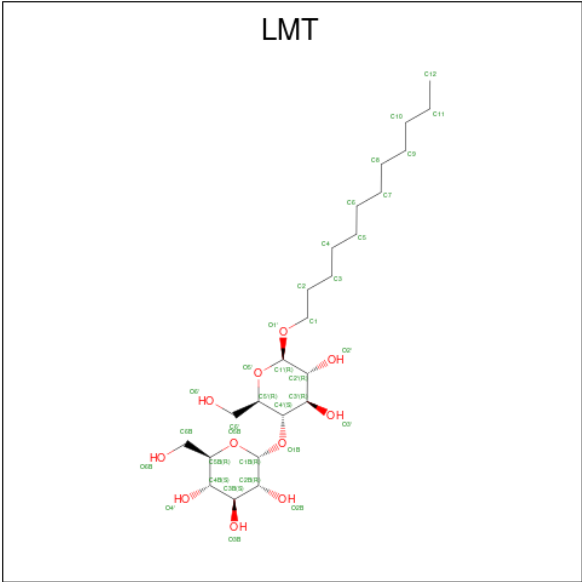
Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	

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Mol	Chain	Residues	Atoms				AltConf
19	B	1	Total 49	C 38	O 10	P 1	0
19	F	1	Total 49	C 38	O 10	P 1	0
19	L	1	Total 49	C 38	O 10	P 1	0
19	X	1	Total 44	C 33	O 10	P 1	0
19	N	1	Total 42	C 31	O 10	P 1	0
19	N	1	Total 49	C 38	O 10	P 1	0
19	W	1	Total 49	C 38	O 10	P 1	0
19	Y	1	Total 49	C 38	O 10	P 1	0
19	Z	1	Total 44	C 33	O 10	P 1	0
19	a	1	Total 42	C 31	O 10	P 1	0
19	f	1	Total 49	C 38	O 10	P 1	0
19	j	1	Total 49	C 38	O 10	P 1	0
19	k	1	Total 49	C 38	O 10	P 1	0
19	l	1	Total 44	C 33	O 10	P 1	0

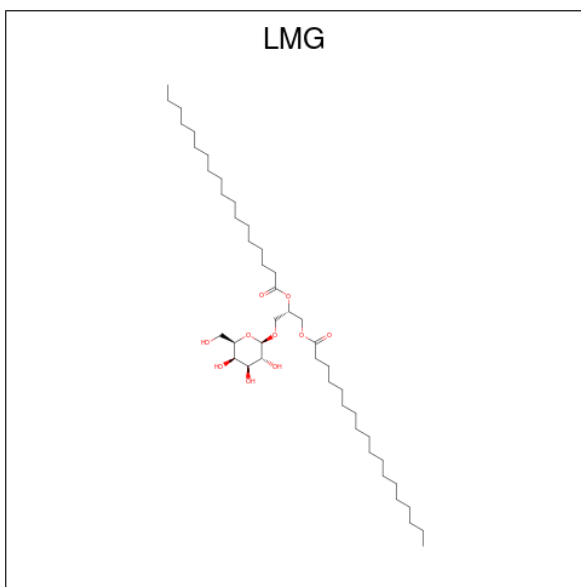
- Molecule 20 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			31	20	11	
20	A	1	Total	C	O	0
			28	17	11	
20	A	1	Total	C	O	0
			35	24	11	
20	N	1	Total	C	O	0
			31	20	11	
20	N	1	Total	C	O	0
			28	17	11	
20	N	1	Total	C	O	0
			35	24	11	
20	a	1	Total	C	O	0
			31	20	11	
20	a	1	Total	C	O	0
			28	17	11	
20	a	1	Total	C	O	0
			35	24	11	

- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).





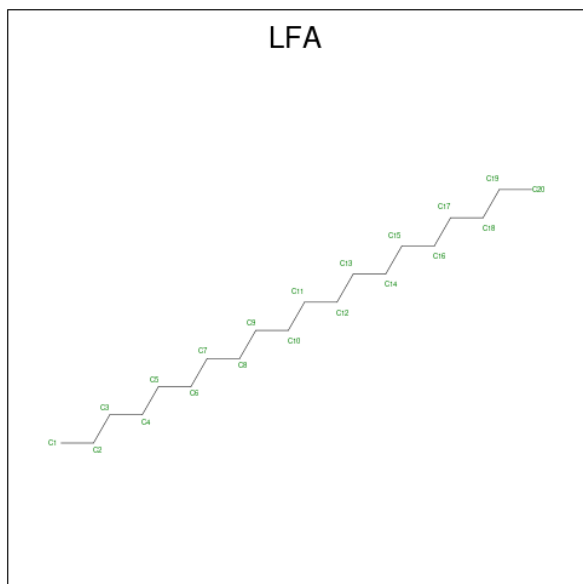
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			44	34	10	
21	B	1	Total	C	O	0
			55	45	10	
21	B	1	Total	C	O	0
			44	34	10	
21	I	1	Total	C	O	0
			37	27	10	
21	J	1	Total	C	O	0
			55	45	10	
21	L	1	Total	C	O	0
			50	40	10	
21	N	1	Total	C	O	0
			44	34	10	
21	O	1	Total	C	O	0
			55	45	10	
21	T	1	Total	C	O	0
			37	27	10	
21	U	1	Total	C	O	0
			55	45	10	
21	W	1	Total	C	O	0
			50	40	10	
21	b	1	Total	C	O	0
			55	45	10	
21	g	1	Total	C	O	0
			37	27	10	
21	h	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
21	j	1	Total	C	O	0
			50	40	10	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula:  $C_{20}H_{42}$ ).



Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			16	16	
22	L	1	Total	C	0
			15	15	
22	O	1	Total	C	0
			16	16	
22	W	1	Total	C	0
			15	15	
22	b	1	Total	C	0
			16	16	
22	j	1	Total	C	0
			15	15	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	W	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	j	1	Total 1	Ca 1	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	50	Total 50	O 50	0
24	B	55	Total 55	O 55	0
24	C	4	Total 4	O 4	0
24	D	10	Total 10	O 10	0
24	E	2	Total 2	O 2	0
24	F	2	Total 2	O 2	0
24	I	2	Total 2	O 2	0
24	K	1	Total 1	O 1	0
24	L	9	Total 9	O 9	0
24	N	51	Total 51	O 51	0
24	O	51	Total 51	O 51	0
24	P	3	Total 3	O 3	0
24	Q	12	Total 12	O 12	0
24	R	2	Total 2	O 2	0
24	S	2	Total 2	O 2	0
24	T	2	Total 2	O 2	0
24	V	1	Total 1	O 1	0
24	W	12	Total 12	O 12	0

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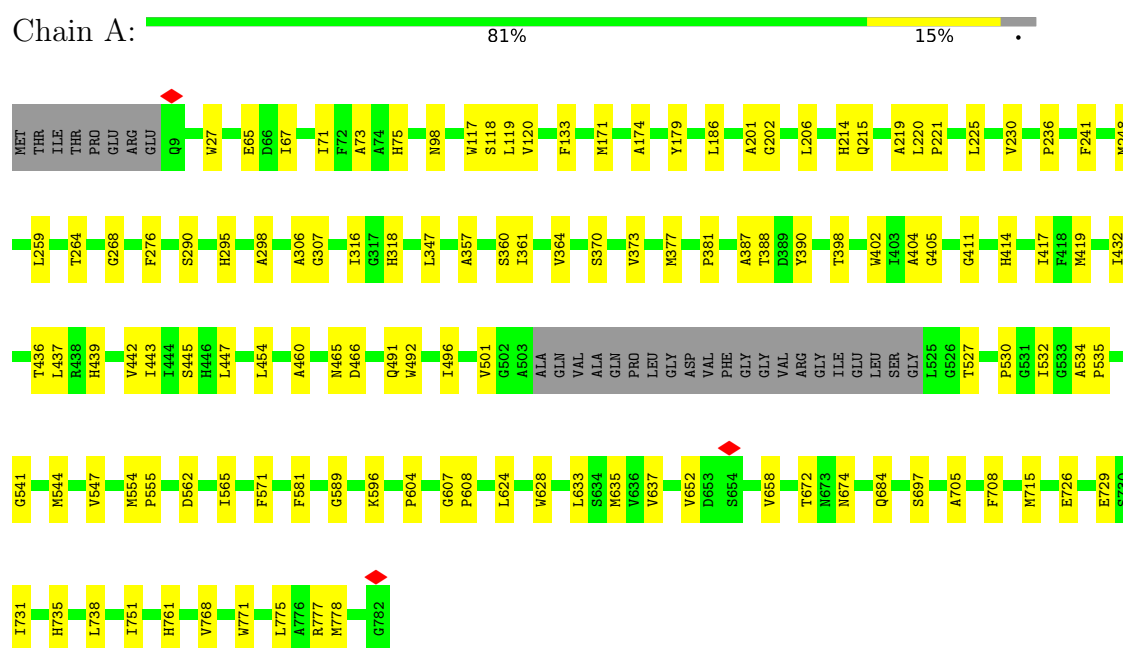
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Mol	Chain	Residues	Atoms		AltConf
24	a	51	Total 51	O 51	0
24	b	54	Total 54	O 54	0
24	c	2	Total 2	O 2	0
24	d	12	Total 12	O 12	0
24	e	2	Total 2	O 2	0
24	f	2	Total 2	O 2	0
24	g	2	Total 2	O 2	0
24	i	1	Total 1	O 1	0
24	j	8	Total 8	O 8	0

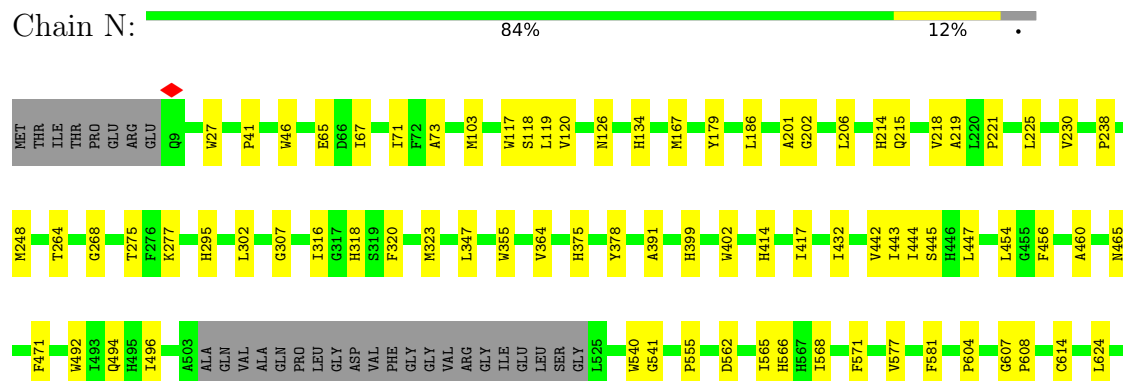
### 3 Residue-property plots

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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



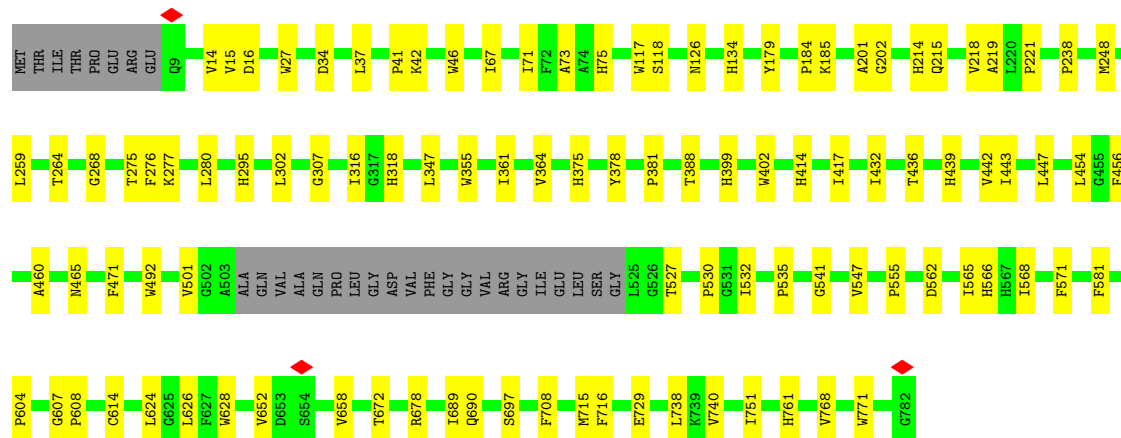
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 83% 13%



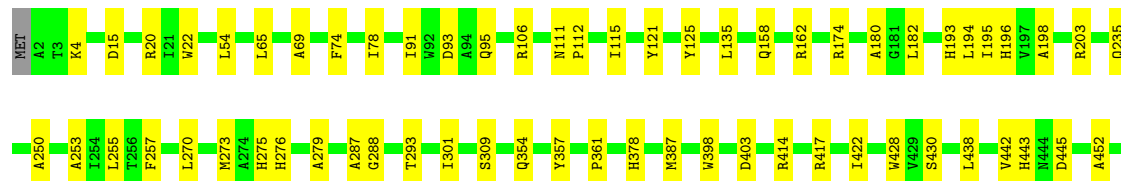
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

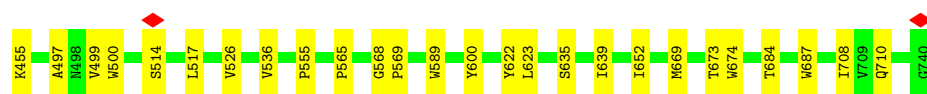
Chain B: 86% 14%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

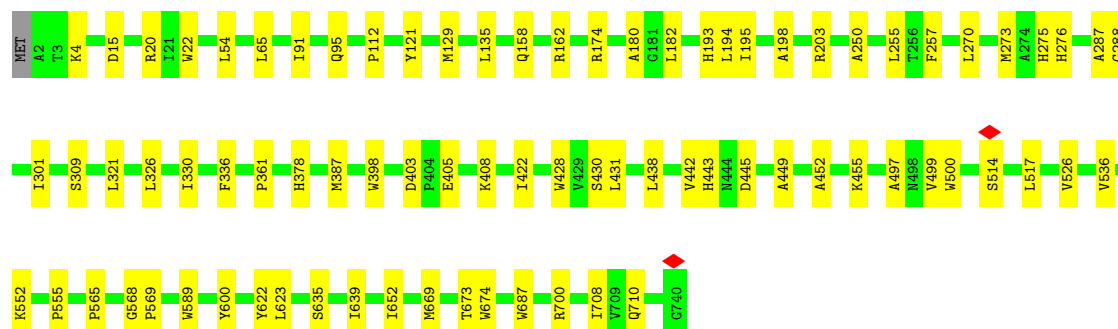
Chain O: 88% 12%





- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 89% 11%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 90% 9%



- Molecule 3: Photosystem I iron-sulfur center

Chain P: 95%



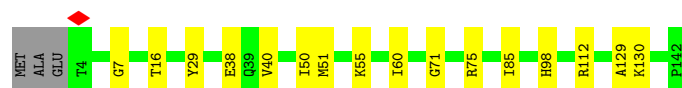
- Molecule 3: Photosystem I iron-sulfur center

Chain c: 90% 9%



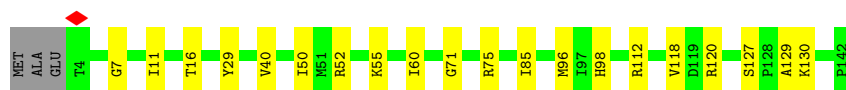
- Molecule 4: Photosystem I reaction center subunit II

Chain D: 87% 11%

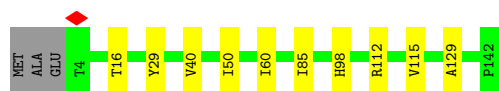
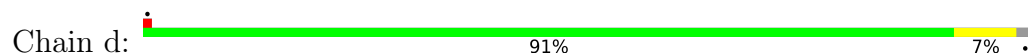


- Molecule 4: Photosystem I reaction center subunit II

Chain Q: 84% 14%



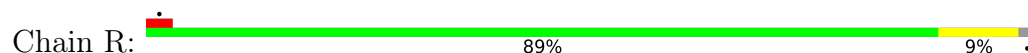
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 5: Photosystem I reaction center subunit IV



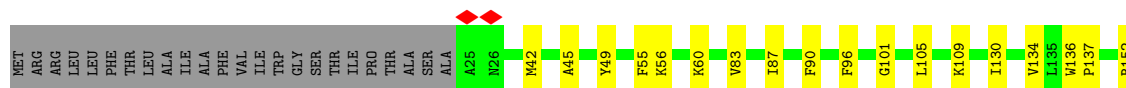
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV



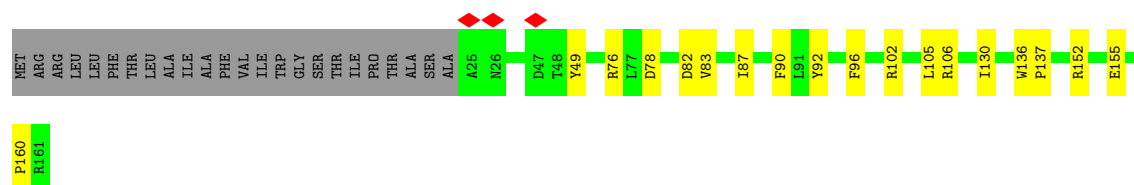
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



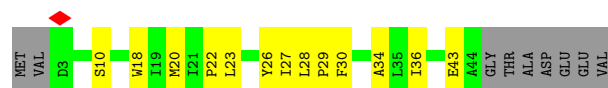




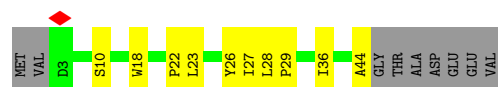
- Molecule 6: Photosystem I reaction center subunit III



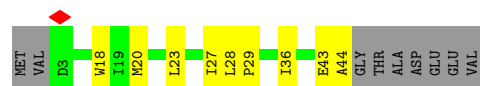
- Molecule 7: Photosystem I reaction center subunit VIII



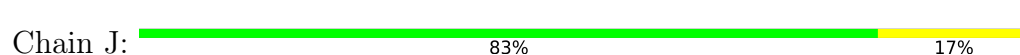
- Molecule 7: Photosystem I reaction center subunit VIII



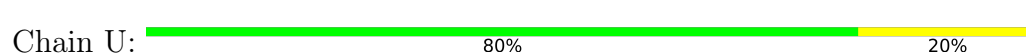
- Molecule 7: Photosystem I reaction center subunit VIII




- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX




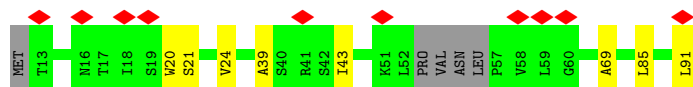
- Molecule 8: Photosystem I reaction center subunit IX

Chain h:  85% 15%




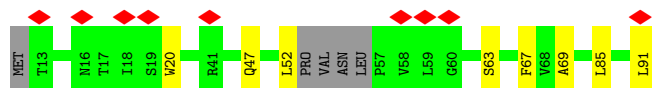
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  12% 84% 10% 6%




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain V:  11% 84% 10% 6%




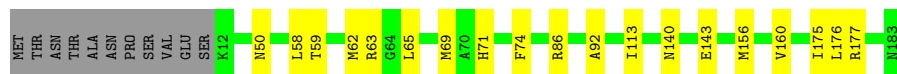
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain i:  10% 80% 14% 6%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  84% 10% 6%




- Molecule 10: Photosystem I reaction center subunit XI

Chain W:  87% 7% 6%




- Molecule 10: Photosystem I reaction center subunit XI

Chain j:  85% 9% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 12%




- Molecule 11: Photosystem I reaction center subunit XII

Chain Y:  91% 6%



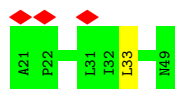
- Molecule 11: Photosystem I reaction center subunit XII

Chain k:  88% 9%



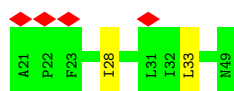
- Molecule 12: Photosystem one PsaX

Chain X:  10% 97%

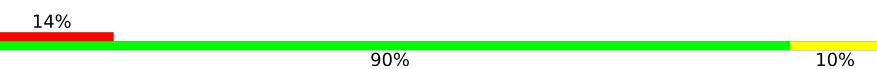


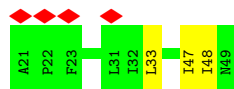
- Molecule 12: Photosystem one PsaX

Chain Z:  14% 93% 7%



- Molecule 12: Photosystem one PsaX

Chain l:  14% 90% 10%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.172	Depositor
Minimum map value	-0.295	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.13	Depositor
Map size (Å)	469.96, 469.96, 469.96	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.78326666, 0.78326666, 0.78326666	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, LMT, SF4, F6C, LFA, CL0, LHG, BCR, CLA, PQN, 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	0.12	0/6106	0.28	0/8323
1	N	0.09	0/6106	0.24	0/8323
1	a	0.09	0/6106	0.24	0/8323
2	B	0.12	0/6139	0.29	0/8394
2	O	0.10	0/6139	0.24	0/8394
2	b	0.10	0/6139	0.25	0/8394
3	C	0.10	0/610	0.27	0/827
3	P	0.09	0/610	0.27	0/827
3	c	0.10	0/610	0.28	0/827
4	D	0.10	0/1115	0.30	0/1501
4	Q	0.09	0/1115	0.26	0/1501
4	d	0.08	0/1115	0.26	0/1501
5	E	0.08	0/540	0.23	0/728
5	R	0.08	0/540	0.23	0/728
5	e	0.08	0/540	0.26	0/728
6	F	0.13	0/1104	0.32	0/1501
6	S	0.10	0/1104	0.28	0/1501
6	f	0.10	0/1104	0.28	0/1501
7	I	0.14	0/366	0.45	0/503
7	T	0.13	0/366	0.36	0/503
7	g	0.13	0/366	0.35	0/503
8	J	0.11	0/386	0.29	0/526
8	U	0.08	0/386	0.25	0/526
8	h	0.08	0/386	0.24	0/526
9	K	0.11	0/550	0.31	0/751
9	V	0.08	0/550	0.27	0/751
9	i	0.08	0/550	0.25	0/751
10	L	0.12	0/1340	0.32	0/1821
10	W	0.09	0/1340	0.24	0/1821
10	j	0.09	0/1340	0.24	0/1821
11	M	0.10	0/243	0.20	0/329
11	Y	0.07	0/243	0.17	0/329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	k	0.07	0/243	0.16	0/329
12	X	0.12	0/233	0.29	0/319
12	Z	0.07	0/233	0.23	0/319
12	l	0.07	0/233	0.22	0/319
All	All	0.10	0/56196	0.26	0/76569

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5900	0	5735	94	0
1	N	5900	0	5735	78	0
1	a	5900	0	5735	81	0
2	B	5913	0	5649	90	0
2	O	5913	0	5649	71	0
2	b	5913	0	5649	68	0
3	C	600	0	579	4	0
3	P	600	0	579	2	0
3	c	600	0	579	5	0
4	D	1090	0	1097	11	0
4	Q	1090	0	1097	13	0
4	d	1090	0	1097	8	0
5	E	530	0	535	3	0
5	R	530	0	535	3	0
5	e	530	0	535	2	0
6	F	1075	0	1081	18	0
6	S	1075	0	1081	15	0
6	f	1075	0	1081	13	0
7	I	351	0	354	10	0
7	T	351	0	354	8	0
7	g	351	0	354	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	373	0	390	10	0
8	U	373	0	390	8	0
8	h	373	0	390	6	0
9	K	539	0	578	6	0
9	V	539	0	578	6	0
9	i	539	0	578	7	0
10	L	1309	0	1289	14	0
10	W	1309	0	1289	12	0
10	j	1309	0	1289	14	0
11	M	240	0	261	4	0
11	Y	240	0	261	2	0
11	k	240	0	261	3	0
12	X	227	0	244	1	0
12	Z	227	0	244	2	0
12	l	227	0	244	2	0
13	A	65	0	72	3	0
13	N	65	0	72	2	0
13	a	65	0	72	2	0
14	A	250	0	0	0	0
14	B	132	0	0	1	0
14	L	132	0	0	2	0
14	N	250	0	0	0	0
14	O	132	0	0	1	0
14	W	132	0	0	1	0
14	a	250	0	0	0	0
14	b	132	0	0	1	0
14	j	132	0	0	1	0
15	A	2259	0	2271	100	0
15	B	2303	0	2383	108	0
15	F	65	0	72	0	0
15	K	95	0	72	1	0
15	L	125	0	131	3	0
15	N	2259	0	2271	94	0
15	O	2303	0	2383	98	0
15	S	65	0	72	1	0
15	V	95	0	72	1	0
15	W	125	0	131	3	0
15	X	55	0	49	1	0
15	Z	55	0	49	1	0
15	a	2259	0	2271	85	0
15	b	2303	0	2383	98	0
15	f	65	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	i	95	0	72	1	0
15	j	125	0	131	3	0
15	l	55	0	49	1	0
16	A	33	0	46	1	0
16	B	33	0	46	3	0
16	N	33	0	46	2	0
16	O	33	0	46	4	0
16	a	33	0	46	2	0
16	b	33	0	46	4	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	N	8	0	0	0	0
17	P	16	0	0	0	0
17	a	8	0	0	0	0
17	c	16	0	0	1	0
18	A	240	0	336	19	0
18	B	240	0	336	21	0
18	F	80	0	112	5	0
18	I	80	0	112	4	0
18	J	80	0	112	7	0
18	K	25	0	33	0	0
18	L	120	0	168	7	0
18	M	40	0	56	4	0
18	N	240	0	336	17	0
18	O	280	0	392	17	0
18	S	40	0	56	3	0
18	T	80	0	112	6	0
18	U	80	0	112	6	0
18	V	25	0	33	0	0
18	W	80	0	112	7	0
18	Y	40	0	56	3	0
18	a	240	0	336	16	0
18	b	280	0	392	20	0
18	f	40	0	56	4	0
18	g	80	0	112	5	0
18	h	80	0	112	7	0
18	i	25	0	33	0	0
18	j	40	0	56	1	0
18	k	40	0	56	4	0
19	A	42	0	54	0	0
19	B	49	0	74	4	0
19	F	49	0	74	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	L	49	0	74	6	0
19	N	91	0	128	2	0
19	W	49	0	74	8	0
19	X	44	0	61	3	0
19	Y	49	0	74	4	0
19	Z	44	0	61	1	0
19	a	42	0	54	0	0
19	f	49	0	74	2	0
19	j	49	0	74	7	0
19	k	49	0	74	5	0
19	l	44	0	61	3	0
20	A	94	0	110	5	0
20	N	94	0	110	3	0
20	a	94	0	110	3	0
21	A	44	0	61	1	0
21	B	99	0	147	4	0
21	I	37	0	44	4	0
21	J	55	0	86	0	0
21	L	50	0	70	4	0
21	N	44	0	61	0	0
21	O	55	0	86	6	0
21	T	37	0	44	2	0
21	U	55	0	86	1	0
21	W	50	0	70	4	0
21	b	55	0	86	5	0
21	g	37	0	44	3	0
21	h	55	0	86	2	0
21	j	50	0	70	3	0
22	B	16	0	28	1	0
22	L	15	0	29	2	0
22	O	16	0	28	1	0
22	W	15	0	29	1	0
22	b	16	0	28	2	0
22	j	15	0	29	1	0
23	L	1	0	0	0	0
23	W	1	0	0	0	0
23	j	1	0	0	0	0
24	A	50	0	0	0	0
24	B	55	0	0	1	0
24	C	4	0	0	0	0
24	D	10	0	0	0	0
24	E	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	F	2	0	0	0	0
24	I	2	0	0	0	0
24	K	1	0	0	0	0
24	L	9	0	0	0	0
24	N	51	0	0	0	0
24	O	51	0	0	1	0
24	P	3	0	0	0	0
24	Q	12	0	0	0	0
24	R	2	0	0	0	0
24	S	2	0	0	0	0
24	T	2	0	0	0	0
24	V	1	0	0	0	0
24	W	12	0	0	0	0
24	a	51	0	0	0	0
24	b	54	0	0	1	0
24	c	2	0	0	0	0
24	d	12	0	0	0	0
24	e	2	0	0	0	0
24	f	2	0	0	0	0
24	g	2	0	0	0	0
24	i	1	0	0	0	0
24	j	8	0	0	0	0
All	All	75954	0	74982	1150	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 8.

The worst 5 of 1150 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)
8:U:37:GLN:HE21	8:U:38:TYR:H	1.13	0.91
8:J:37:GLN:HE21	8:J:38:TYR:H	1.20	0.85
8:h:37:GLN:HE21	8:h:38:TYR:H	1.27	0.83
18:N:850:BCR:H362	15:O:802:CLA:H42	1.67	0.76
18:A:850:BCR:H362	15:B:802:CLA:H42	1.67	0.75

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	749/782 (96%)	732 (98%)	17 (2%)	0	100	100
1	N	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
1	a	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
2	B	737/740 (100%)	722 (98%)	15 (2%)	0	100	100
2	O	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	b	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	P	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	Q	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	d	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
5	E	63/66 (96%)	63 (100%)	0	0	100	100
5	R	63/66 (96%)	63 (100%)	0	0	100	100
5	e	63/66 (96%)	63 (100%)	0	0	100	100
6	F	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	S	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	f	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
7	I	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	T	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	g	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
8	J	44/46 (96%)	44 (100%)	0	0	100	100
8	U	44/46 (96%)	44 (100%)	0	0	100	100
8	h	44/46 (96%)	44 (100%)	0	0	100	100
9	K	71/80 (89%)	68 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	71/80 (89%)	69 (97%)	2 (3%)	0	100	100
9	i	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
10	L	170/183 (93%)	169 (99%)	1 (1%)	0	100	100
10	W	170/183 (93%)	170 (100%)	0	0	100	100
10	j	170/183 (93%)	170 (100%)	0	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	Y	29/32 (91%)	29 (100%)	0	0	100	100
11	k	29/32 (91%)	29 (100%)	0	0	100	100
12	X	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	Z	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
12	l	27/29 (93%)	26 (96%)	1 (4%)	0	100	100
All	All	6840/7179 (95%)	6716 (98%)	124 (2%)	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	600/623 (96%)	600 (100%)	0	100	100
1	N	600/623 (96%)	600 (100%)	0	100	100
1	a	600/623 (96%)	600 (100%)	0	100	100
2	B	594/595 (100%)	594 (100%)	0	100	100
2	O	594/595 (100%)	594 (100%)	0	100	100
2	b	594/595 (100%)	594 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	P	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	114/116 (98%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100
5	E	57/58 (98%)	57 (100%)	0	100	100
5	R	57/58 (98%)	57 (100%)	0	100	100
5	e	57/58 (98%)	57 (100%)	0	100	100
6	F	116/135 (86%)	116 (100%)	0	100	100
6	S	116/135 (86%)	116 (100%)	0	100	100
6	f	116/135 (86%)	116 (100%)	0	100	100
7	I	37/44 (84%)	37 (100%)	0	100	100
7	T	37/44 (84%)	37 (100%)	0	100	100
7	g	37/44 (84%)	37 (100%)	0	100	100
8	J	41/41 (100%)	41 (100%)	0	100	100
8	U	41/41 (100%)	41 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	K	60/65 (92%)	60 (100%)	0	100	100
9	V	60/65 (92%)	60 (100%)	0	100	100
9	i	60/65 (92%)	60 (100%)	0	100	100
10	L	135/146 (92%)	135 (100%)	0	100	100
10	W	135/146 (92%)	135 (100%)	0	100	100
10	j	135/146 (92%)	135 (100%)	0	100	100
11	M	26/27 (96%)	26 (100%)	0	100	100
11	Y	26/27 (96%)	26 (100%)	0	100	100
11	k	26/27 (96%)	26 (100%)	0	100	100
12	X	24/24 (100%)	24 (100%)	0	100	100
12	Z	24/24 (100%)	24 (100%)	0	100	100
12	l	24/24 (100%)	24 (100%)	0	100	100
All	All	5616/5829 (96%)	5616 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	496	HIS
2	b	637	GLN
1	N	215	GLN
1	N	114	GLN
4	d	110	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 3 are monoatomic - leaving 399 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
15	CLA	B	824	24	65,73,73	1.48	5 (7%)	76,113,113	1.43	9 (11%)
15	CLA	a	842	1	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
14	F6C	A	802	24	69,74,74	1.78	12 (17%)	70,114,114	2.19	15 (21%)
14	F6C	B	839	24	69,74,74	1.78	13 (18%)	70,114,114	2.27	16 (22%)
15	CLA	N	805	15,1	60,68,73	1.55	5 (8%)	70,107,113	1.42	7 (10%)
14	F6C	b	832	2	69,74,74	1.80	14 (20%)	70,114,114	2.21	15 (21%)
21	LMG	b	849	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	B	834	24	45,53,73	1.77	6 (13%)	52,89,113	1.64	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	N	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)
20	LMT	A	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	O	808	2	65,73,73	1.46	6 (9%)	76,113,113	1.43	9 (11%)
18	BCR	W	205	-	41,41,41	0.33	0	56,56,56	0.58	0
15	CLA	b	825	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	O	810	2	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
13	CL0	a	801	1	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
15	CLA	O	812	2	56,64,73	1.59	5 (8%)	65,102,113	1.51	8 (12%)
15	CLA	b	814	2	45,53,73	1.76	5 (11%)	52,89,113	1.65	7 (13%)
15	CLA	O	801	2	65,73,73	1.48	6 (9%)	76,113,113	1.31	7 (9%)
15	CLA	N	811	1	57,65,73	1.57	5 (8%)	66,103,113	1.45	7 (10%)
15	CLA	O	828	2	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
18	BCR	B	842	-	41,41,41	0.31	0	56,56,56	0.55	0
18	BCR	M	101	-	41,41,41	0.33	0	56,56,56	0.64	1 (1%)
21	LMG	N	855	-	44,44,55	0.52	0	52,52,63	0.64	0
15	CLA	A	804	1	65,73,73	1.50	5 (7%)	76,113,113	1.37	7 (9%)
15	CLA	j	202	10	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	a	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.40	7 (10%)
18	BCR	A	846	-	41,41,41	0.33	0	56,56,56	0.65	1 (1%)
13	CL0	A	801	1	65,73,73	1.47	6 (9%)	76,113,113	1.36	7 (9%)
15	CLA	B	817	2	60,68,73	1.55	5 (8%)	70,107,113	1.39	7 (10%)
15	CLA	a	835	1	65,73,73	1.50	6 (9%)	76,113,113	1.34	9 (11%)
15	CLA	O	824	24	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
16	PQN	b	841	-	34,34,34	0.34	0	42,45,45	0.57	1 (2%)
18	BCR	O	847	-	41,41,41	0.32	0	56,56,56	0.93	1 (1%)
15	CLA	B	840	2	65,73,73	1.49	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	O	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.38	9 (11%)
18	BCR	b	845	-	41,41,41	0.32	0	56,56,56	0.55	0
15	CLA	a	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.48	7 (10%)
15	CLA	A	810	1	57,65,73	1.57	6 (10%)	66,103,113	1.51	7 (10%)
15	CLA	A	805	15,1	60,68,73	1.55	5 (8%)	70,107,113	1.42	7 (10%)
15	CLA	O	831	2	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
18	BCR	A	850	-	41,41,41	0.33	0	56,56,56	0.81	0
19	LHG	f	203	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	b	821	24	53,61,73	1.63	5 (9%)	61,98,113	1.55	8 (13%)
15	CLA	A	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
22	LFA	b	850	-	15,15,19	0.24	0	14,14,18	0.20	0
15	CLA	b	838	2	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
18	BCR	L	206	-	41,41,41	0.30	0	56,56,56	0.67	0
19	LHG	Y	101	-	48,48,48	0.49	0	51,54,54	0.48	0
15	CLA	B	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.38	8 (10%)
15	CLA	b	809	2	65,73,73	1.48	6 (9%)	76,113,113	1.34	8 (10%)
16	PQN	B	841	-	34,34,34	0.34	0	42,45,45	0.58	1 (2%)
15	CLA	B	836	2	65,73,73	1.47	5 (7%)	76,113,113	1.41	8 (10%)
20	LMT	N	852	-	32,32,36	0.57	0	43,43,47	0.67	0
15	CLA	A	811	1	57,65,73	1.57	5 (8%)	66,103,113	1.45	7 (10%)
15	CLA	A	808	1	45,53,73	1.76	5 (11%)	52,89,113	1.63	8 (15%)
21	LMG	A	855	-	44,44,55	0.52	0	52,52,63	0.64	0
15	CLA	A	838	1	55,63,73	1.58	6 (10%)	64,101,113	1.48	7 (10%)
15	CLA	O	815	2	57,65,73	1.57	5 (8%)	66,103,113	1.48	7 (10%)
19	LHG	k	101	-	48,48,48	0.49	0	51,54,54	0.48	0
15	CLA	N	818	1	65,73,73	1.47	6 (9%)	76,113,113	1.42	7 (9%)
20	LMT	a	854	-	36,36,36	0.55	0	47,47,47	0.63	0
22	LFA	j	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	B	810	2	65,73,73	1.48	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	N	816	1	45,53,73	1.81	5 (11%)	52,89,113	1.56	7 (13%)
15	CLA	L	202	10	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
14	F6C	L	201	2	69,74,74	1.80	11 (15%)	70,114,114	2.13	14 (20%)
15	CLA	b	804	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	B	833	2	55,63,73	1.61	5 (9%)	64,101,113	1.48	8 (12%)
15	CLA	i	103	24	50,58,73	1.71	6 (12%)	58,95,113	1.52	8 (13%)
14	F6C	N	802	24	69,74,74	1.78	12 (17%)	70,114,114	2.17	14 (20%)
15	CLA	N	837	1	51,59,73	1.67	5 (9%)	59,96,113	1.51	8 (13%)
14	F6C	A	824	24	55,60,74	2.02	13 (23%)	53,97,114	2.48	14 (26%)
14	F6C	a	824	24	55,60,74	2.02	12 (21%)	53,97,114	2.48	14 (26%)
15	CLA	N	820	1	65,73,73	1.47	5 (7%)	76,113,113	1.46	9 (11%)
15	CLA	a	841	1	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	a	822	24	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
15	CLA	B	835	24	45,53,73	1.81	5 (11%)	52,89,113	1.55	6 (11%)
15	CLA	A	822	24	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
15	CLA	b	828	2	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
15	CLA	a	825	1	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	b	805	2	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
15	CLA	O	818	24	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
14	F6C	W	201	2	69,74,74	1.81	11 (15%)	70,114,114	2.13	14 (20%)
15	CLA	O	820	2	45,53,73	1.78	5 (11%)	52,89,113	1.61	7 (13%)
21	LMG	O	849	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	B	811	2	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
15	CLA	A	812	15,1	65,73,73	1.50	6 (9%)	76,113,113	1.35	8 (10%)
15	CLA	a	834	1	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
18	BCR	a	848	-	41,41,41	0.32	0	56,56,56	0.50	0
15	CLA	B	802	24	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
15	CLA	A	816	1	45,53,73	1.81	5 (11%)	52,89,113	1.56	7 (13%)
15	CLA	i	102	9	45,53,73	1.79	6 (13%)	52,89,113	1.57	6 (11%)
15	CLA	A	832	1	50,58,73	1.68	6 (12%)	58,95,113	1.53	8 (13%)
15	CLA	a	828	1	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)
17	SF4	c	102	3	0,12,12	-	-	-	-	-
15	CLA	a	805	15,1	60,68,73	1.55	5 (8%)	70,107,113	1.42	7 (10%)
15	CLA	b	833	2	55,63,73	1.61	6 (10%)	64,101,113	1.47	8 (12%)
18	BCR	j	205	-	41,41,41	0.34	0	56,56,56	0.62	0
15	CLA	b	819	2	55,63,73	1.63	5 (9%)	64,101,113	1.43	7 (10%)
15	CLA	b	836	2	65,73,73	1.47	5 (7%)	76,113,113	1.41	7 (9%)
15	CLA	A	814	1	65,73,73	1.47	5 (7%)	76,113,113	1.38	7 (9%)
18	BCR	g	101	-	41,41,41	0.34	0	56,56,56	0.72	0
15	CLA	N	830	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
15	CLA	O	802	24	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
14	F6C	b	839	24	69,74,74	1.78	13 (18%)	70,114,114	2.27	16 (22%)
18	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.58	0
15	CLA	j	203	10	60,68,73	1.55	5 (8%)	70,107,113	1.42	9 (12%)
15	CLA	O	814	2	45,53,73	1.76	6 (13%)	52,89,113	1.66	7 (13%)
15	CLA	b	837	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	9 (11%)
18	BCR	F	202	-	41,41,41	0.33	0	56,56,56	0.94	2 (3%)
15	CLA	N	841	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
15	CLA	B	801	2	65,73,73	1.47	6 (9%)	76,113,113	1.31	7 (9%)
15	CLA	B	822	2	55,63,73	1.65	7 (12%)	64,101,113	1.32	7 (10%)
18	BCR	b	843	-	41,41,41	0.31	0	56,56,56	0.61	0
15	CLA	B	813	2	65,73,73	1.49	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	B	818	24	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMT	N	853	-	29,29,36	0.57	0	40,40,47	1.39	4 (10%)
18	BCR	N	850	-	41,41,41	0.33	0	56,56,56	0.82	0
15	CLA	N	819	1	65,73,73	1.50	6 (9%)	76,113,113	1.34	8 (10%)
18	BCR	L	205	-	41,41,41	0.33	0	56,56,56	0.63	0
19	LHG	N	851	-	41,41,48	0.53	0	44,47,54	0.49	0
14	F6C	a	855	24	69,74,74	1.77	14 (20%)	70,114,114	2.26	16 (22%)
15	CLA	a	837	1	51,59,73	1.68	5 (9%)	59,96,113	1.52	9 (15%)
21	LMG	j	206	-	50,50,55	0.50	0	58,58,63	0.61	0
18	BCR	O	842	-	41,41,41	0.31	0	56,56,56	0.56	0
15	CLA	N	814	1	65,73,73	1.47	5 (7%)	76,113,113	1.38	7 (9%)
19	LHG	W	207	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	b	826	2	62,70,73	1.52	5 (8%)	72,109,113	1.39	7 (9%)
15	CLA	A	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.41	7 (10%)
15	CLA	b	840	2	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
16	PQN	A	843	-	34,34,34	0.33	0	42,45,45	0.55	1 (2%)
15	CLA	A	830	1	65,73,73	1.47	6 (9%)	76,113,113	1.39	6 (7%)
15	CLA	N	804	1	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)
13	CL0	N	801	1	65,73,73	1.46	6 (9%)	76,113,113	1.37	7 (9%)
15	CLA	O	804	2	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
15	CLA	a	816	1	45,53,73	1.81	5 (11%)	52,89,113	1.57	7 (13%)
18	BCR	N	846	-	41,41,41	0.33	0	56,56,56	0.67	1 (1%)
14	F6C	W	204	24	69,74,74	1.79	13 (18%)	70,114,114	2.24	17 (24%)
21	LMG	T	103	-	37,37,55	0.56	0	45,45,63	0.65	0
15	CLA	N	808	1	45,53,73	1.76	5 (11%)	52,89,113	1.64	8 (15%)
15	CLA	N	806	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	a	818	1	65,73,73	1.46	6 (9%)	76,113,113	1.43	7 (9%)
15	CLA	L	203	10	60,68,73	1.55	5 (8%)	70,107,113	1.41	9 (12%)
14	F6C	a	826	24	69,74,74	1.80	12 (17%)	70,114,114	2.29	19 (27%)
15	CLA	a	820	1	65,73,73	1.47	6 (9%)	76,113,113	1.50	10 (13%)
15	CLA	N	817	24	45,53,73	1.80	5 (11%)	52,89,113	1.59	6 (11%)
17	SF4	c	101	3	0,12,12	-	-	-	-	-
18	BCR	U	101	-	41,41,41	0.32	0	56,56,56	0.48	0
15	CLA	O	823	24	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
15	CLA	A	806	1	65,73,73	1.46	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	a	804	1	65,73,73	1.51	5 (7%)	76,113,113	1.36	7 (9%)
14	F6C	a	802	24	69,74,74	1.78	12 (17%)	70,114,114	2.18	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	B	821	24	53,61,73	1.63	5 (9%)	61,98,113	1.56	8 (13%)
15	CLA	A	820	1	65,73,73	1.47	5 (7%)	76,113,113	1.48	10 (13%)
15	CLA	a	833	1	55,63,73	1.60	6 (10%)	64,101,113	1.52	7 (10%)
15	CLA	B	825	2	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	b	817	2	60,68,73	1.55	5 (8%)	70,107,113	1.40	7 (10%)
15	CLA	V	103	24	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
15	CLA	O	835	24	45,53,73	1.81	5 (11%)	52,89,113	1.55	6 (11%)
15	CLA	N	840	1	50,58,73	1.69	5 (10%)	58,95,113	1.54	8 (13%)
18	BCR	B	844	-	41,41,41	0.31	0	56,56,56	0.47	0
15	CLA	A	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.48	7 (10%)
14	F6C	N	856	24	69,74,74	1.77	13 (18%)	70,114,114	2.26	16 (22%)
18	BCR	a	845	-	41,41,41	0.35	0	56,56,56	0.91	2 (3%)
15	CLA	O	806	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	l	102	12	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
15	CLA	A	819	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	8 (10%)
19	LHG	A	851	-	41,41,48	0.53	0	44,47,54	0.49	0
21	LMG	L	207	-	50,50,55	0.50	0	58,58,63	0.61	0
19	LHG	l	101	-	43,43,48	0.52	0	46,49,54	0.48	0
15	CLA	Z	102	12	55,63,73	1.62	6 (10%)	64,101,113	1.45	7 (10%)
15	CLA	A	817	24	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
15	CLA	a	838	1	55,63,73	1.59	6 (10%)	64,101,113	1.47	7 (10%)
22	LFA	W	208	-	14,14,19	0.24	0	13,13,18	0.24	0
15	CLA	A	841	1	65,73,73	1.47	5 (7%)	76,113,113	1.39	7 (9%)
15	CLA	N	836	1	54,62,73	1.61	5 (9%)	62,99,113	1.51	8 (12%)
15	CLA	a	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.41	6 (8%)
19	LHG	Z	101	-	43,43,48	0.52	0	46,49,54	0.48	0
15	CLA	b	824	24	65,73,73	1.48	5 (7%)	76,113,113	1.42	9 (11%)
16	PQN	a	843	-	34,34,34	0.33	0	42,45,45	0.56	1 (2%)
18	BCR	B	847	-	41,41,41	0.33	0	56,56,56	0.77	1 (1%)
15	CLA	A	815	1	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
15	CLA	O	838	2	65,73,73	1.48	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	O	811	2	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
15	CLA	b	810	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	A	818	1	65,73,73	1.46	7 (10%)	76,113,113	1.43	7 (9%)
15	CLA	B	816	2	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)
15	CLA	N	831	1	65,73,73	1.48	5 (7%)	76,113,113	1.40	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	O	803	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
15	CLA	B	805	2	65,73,73	1.47	6 (9%)	76,113,113	1.41	7 (9%)
18	BCR	b	844	-	41,41,41	0.30	0	56,56,56	0.49	0
15	CLA	b	834	24	45,53,73	1.77	5 (11%)	52,89,113	1.63	8 (15%)
18	BCR	F	203	-	41,41,41	0.31	0	56,56,56	0.53	0
15	CLA	B	828	2	65,73,73	1.47	5 (7%)	76,113,113	1.44	8 (10%)
18	BCR	b	848	-	41,41,41	0.30	0	56,56,56	0.63	0
15	CLA	a	808	1	45,53,73	1.76	5 (11%)	52,89,113	1.63	8 (15%)
15	CLA	A	837	1	51,59,73	1.68	5 (9%)	59,96,113	1.52	9 (15%)
15	CLA	N	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
15	CLA	B	809	2	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
19	LHG	N	857	-	48,48,48	0.50	0	51,54,54	0.46	0
18	BCR	N	849	-	41,41,41	0.32	0	56,56,56	0.59	0
15	CLA	b	815	2	57,65,73	1.56	5 (8%)	66,103,113	1.49	7 (10%)
21	LMG	g	103	-	37,37,55	0.55	0	45,45,63	0.65	0
15	CLA	O	822	2	55,63,73	1.61	7 (12%)	64,101,113	1.50	7 (10%)
15	CLA	b	807	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	O	813	2	65,73,73	1.48	6 (9%)	76,113,113	1.37	8 (10%)
14	F6C	O	832	2	69,74,74	1.80	14 (20%)	70,114,114	2.21	16 (22%)
15	CLA	O	825	2	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
15	CLA	B	808	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	8 (10%)
15	CLA	A	825	1	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	a	829	1	60,68,73	1.54	6 (10%)	70,107,113	1.41	7 (10%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
15	CLA	a	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
18	BCR	b	846	-	41,41,41	0.31	0	56,56,56	0.86	2 (3%)
18	BCR	a	850	-	41,41,41	0.33	0	56,56,56	0.83	0
15	CLA	a	819	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	8 (10%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
19	LHG	a	851	-	41,41,48	0.54	0	44,47,54	0.49	0
19	LHG	F	204	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	N	815	1	55,63,73	1.62	5 (9%)	64,101,113	1.48	8 (12%)
18	BCR	O	843	-	41,41,41	0.31	0	56,56,56	0.60	0
18	BCR	J	101	-	41,41,41	0.32	0	56,56,56	0.49	0
15	CLA	B	823	24	65,73,73	1.48	6 (9%)	76,113,113	1.41	7 (9%)
15	CLA	a	814	1	65,73,73	1.47	5 (7%)	76,113,113	1.38	7 (9%)
15	CLA	O	816	2	65,73,73	1.52	6 (9%)	76,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	A	807	1	65,73,73	1.48	6 (9%)	76,113,113	1.38	6 (7%)
15	CLA	N	809	1	60,68,73	1.53	5 (8%)	70,107,113	1.40	7 (10%)
16	PQN	N	843	-	34,34,34	0.33	0	42,45,45	0.54	1 (2%)
15	CLA	A	827	24	55,63,73	1.60	5 (9%)	64,101,113	1.52	8 (12%)
20	LMT	N	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	a	806	1	65,73,73	1.47	5 (7%)	76,113,113	1.38	7 (9%)
15	CLA	O	826	2	62,70,73	1.52	5 (8%)	72,109,113	1.39	7 (9%)
18	BCR	W	209	-	41,41,41	0.30	0	56,56,56	0.65	0
15	CLA	b	829	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	7 (9%)
21	LMG	U	103	-	55,55,55	0.49	0	63,63,63	0.60	0
18	BCR	O	846	-	41,41,41	0.32	0	56,56,56	0.80	2 (3%)
18	BCR	h	101	-	41,41,41	0.32	0	56,56,56	0.48	0
15	CLA	a	836	1	54,62,73	1.61	5 (9%)	62,99,113	1.52	8 (12%)
19	LHG	B	851	-	48,48,48	0.49	0	51,54,54	0.48	0
18	BCR	T	102	-	41,41,41	0.29	0	56,56,56	0.44	0
17	SF4	N	844	2,1	0,12,12	-	-	-	-	-
18	BCR	g	102	-	41,41,41	0.29	0	56,56,56	0.44	0
15	CLA	O	821	24	53,61,73	1.63	5 (9%)	61,98,113	1.57	8 (13%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.43	0
15	CLA	B	812	2	56,64,73	1.59	5 (8%)	65,102,113	1.50	8 (12%)
15	CLA	K	102	9	45,53,73	1.79	6 (13%)	52,89,113	1.57	6 (11%)
21	LMG	W	206	-	50,50,55	0.50	0	58,58,63	0.61	0
15	CLA	N	812	15,1	65,73,73	1.49	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	A	840	1	50,58,73	1.69	5 (10%)	58,95,113	1.54	8 (13%)
15	CLA	N	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.40	7 (10%)
18	BCR	f	202	-	41,41,41	0.31	0	56,56,56	0.52	0
19	LHG	j	207	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	F	201	24	65,73,73	1.50	6 (9%)	76,113,113	1.33	8 (10%)
15	CLA	B	806	2	65,73,73	1.46	6 (9%)	76,113,113	1.41	6 (7%)
15	CLA	N	834	1	65,73,73	1.50	6 (9%)	76,113,113	1.34	7 (9%)
15	CLA	N	833	1	55,63,73	1.59	6 (10%)	64,101,113	1.52	7 (10%)
18	BCR	i	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.52	0
15	CLA	W	202	10	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	b	818	24	65,73,73	1.50	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	V	102	9	45,53,73	1.79	6 (13%)	52,89,113	1.57	6 (11%)
15	CLA	A	835	1	65,73,73	1.49	5 (7%)	76,113,113	1.35	8 (10%)
15	CLA	B	837	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	b	820	2	45,53,73	1.78	5 (11%)	52,89,113	1.61	7 (13%)
18	BCR	N	848	-	41,41,41	0.32	0	56,56,56	0.51	0
15	CLA	X	102	12	55,63,73	1.61	6 (10%)	64,101,113	1.46	7 (10%)
15	CLA	B	819	2	55,63,73	1.63	5 (9%)	64,101,113	1.43	7 (10%)
16	PQN	O	841	-	34,34,34	0.34	0	42,45,45	0.57	1 (2%)
17	SF4	P	101	3	0,12,12	-	-	-	-	-
21	LMG	I	103	-	37,37,55	0.56	0	45,45,63	0.66	0
15	CLA	N	839	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
18	BCR	O	845	-	41,41,41	0.32	0	56,56,56	0.55	0
15	CLA	a	807	1	65,73,73	1.48	5 (7%)	76,113,113	1.37	7 (9%)
14	F6C	j	204	24	69,74,74	1.79	13 (18%)	70,114,114	2.23	17 (24%)
15	CLA	b	802	24	65,73,73	1.48	5 (7%)	76,113,113	1.38	7 (9%)
18	BCR	N	845	-	41,41,41	0.35	0	56,56,56	0.92	2 (3%)
15	CLA	B	814	2	45,53,73	1.76	5 (11%)	52,89,113	1.65	7 (13%)
15	CLA	A	836	1	54,62,73	1.62	5 (9%)	62,99,113	1.51	8 (12%)
15	CLA	b	831	2	65,73,73	1.48	5 (7%)	76,113,113	1.40	8 (10%)
15	CLA	K	103	24	50,58,73	1.71	5 (10%)	58,95,113	1.54	9 (15%)
15	CLA	N	829	1	60,68,73	1.53	6 (10%)	70,107,113	1.41	7 (10%)
17	SF4	A	844	2,1	0,12,12	-	-	-	-	-
15	CLA	a	840	1	50,58,73	1.69	5 (10%)	58,95,113	1.56	8 (13%)
18	BCR	O	844	-	41,41,41	0.30	0	56,56,56	0.49	0
19	LHG	X	101	-	43,43,48	0.52	0	46,49,54	0.48	0
15	CLA	a	827	24	55,63,73	1.60	5 (9%)	64,101,113	1.51	9 (14%)
18	BCR	a	846	-	41,41,41	0.33	0	56,56,56	0.67	1 (1%)
15	CLA	O	809	2	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
15	CLA	b	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.39	8 (10%)
18	BCR	a	847	-	41,41,41	0.33	0	56,56,56	0.63	1 (1%)
22	LFA	B	849	-	15,15,19	0.24	0	14,14,18	0.20	0
15	CLA	a	810	1	57,65,73	1.57	6 (10%)	66,103,113	1.51	7 (10%)
18	BCR	Y	102	-	41,41,41	0.32	0	56,56,56	0.64	1 (1%)
15	CLA	a	831	1	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
15	CLA	O	805	2	65,73,73	1.46	6 (9%)	76,113,113	1.42	7 (9%)
15	CLA	W	203	10	60,68,73	1.54	6 (10%)	70,107,113	1.41	9 (12%)
15	CLA	B	827	2	65,73,73	1.47	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	b	830	2	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
17	SF4	P	102	3	0,12,12	-	-	-	-	-
18	BCR	A	847	-	41,41,41	0.33	0	56,56,56	0.61	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	B	829	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	9 (11%)
22	LFA	L	209	-	14,14,19	0.23	0	13,13,18	0.22	0
14	F6C	j	201	2	69,74,74	1.80	13 (18%)	70,114,114	2.17	14 (20%)
18	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.55	0
18	BCR	a	849	-	41,41,41	0.32	0	56,56,56	0.58	0
14	F6C	L	204	24	69,74,74	1.79	13 (18%)	70,114,114	2.21	17 (24%)
15	CLA	b	827	2	65,73,73	1.46	6 (9%)	76,113,113	1.37	8 (10%)
15	CLA	N	842	1	65,73,73	1.51	6 (9%)	76,113,113	1.34	8 (10%)
15	CLA	a	811	1	57,65,73	1.57	5 (8%)	66,103,113	1.45	7 (10%)
15	CLA	b	835	24	45,53,73	1.81	5 (11%)	52,89,113	1.55	6 (11%)
18	BCR	O	848	-	41,41,41	0.30	0	56,56,56	0.62	0
15	CLA	B	830	2	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
14	F6C	B	832	2	69,74,74	1.79	12 (17%)	70,114,114	2.21	15 (21%)
15	CLA	b	823	24	65,73,73	1.49	6 (9%)	76,113,113	1.41	7 (9%)
18	BCR	S	202	-	41,41,41	0.31	0	56,56,56	0.52	0
20	LMT	A	853	-	29,29,36	0.57	0	40,40,47	1.39	4 (10%)
18	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.91	2 (3%)
15	CLA	A	831	1	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
15	CLA	O	833	2	55,63,73	1.61	5 (9%)	64,101,113	1.47	8 (12%)
18	BCR	U	102	-	41,41,41	0.41	0	56,56,56	1.29	8 (14%)
21	LMG	B	850	-	44,44,55	0.52	0	52,52,63	0.64	0
15	CLA	b	801	2	65,73,73	1.48	6 (9%)	76,113,113	1.31	7 (9%)
19	LHG	L	208	-	48,48,48	0.50	0	51,54,54	0.46	0
15	CLA	B	831	2	65,73,73	1.48	5 (7%)	76,113,113	1.39	8 (10%)
15	CLA	O	829	2	65,73,73	1.48	6 (9%)	76,113,113	1.36	7 (9%)
20	LMT	a	853	-	29,29,36	0.57	0	40,40,47	1.39	4 (10%)
18	BCR	b	842	-	41,41,41	0.32	0	56,56,56	0.54	0
21	LMG	J	103	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	S	201	24	65,73,73	1.50	6 (9%)	76,113,113	1.33	8 (10%)
15	CLA	B	803	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	N	813	1	54,62,73	1.62	5 (9%)	62,99,113	1.51	9 (14%)
14	F6C	O	839	24	69,74,74	1.78	13 (18%)	70,114,114	2.27	16 (22%)
15	CLA	B	826	2	62,70,73	1.52	5 (8%)	72,109,113	1.39	7 (9%)
17	SF4	a	844	2,1	0,12,12	-	-	-	-	-
15	CLA	N	832	1	50,58,73	1.68	6 (12%)	58,95,113	1.54	9 (15%)
18	BCR	h	102	-	41,41,41	0.41	0	56,56,56	1.30	8 (14%)
15	CLA	b	808	2	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
18	BCR	J	102	-	41,41,41	0.41	0	56,56,56	1.27	8 (14%)
14	F6C	N	826	24	69,74,74	1.80	12 (17%)	70,114,114	2.24	16 (22%)
15	CLA	N	807	1	65,73,73	1.49	6 (9%)	76,113,113	1.36	7 (9%)
15	CLA	A	833	1	55,63,73	1.59	6 (10%)	64,101,113	1.51	7 (10%)
18	BCR	b	847	-	41,41,41	0.33	0	56,56,56	0.92	1 (1%)
15	CLA	b	812	2	56,64,73	1.59	6 (10%)	65,102,113	1.50	8 (12%)
18	BCR	I	101	-	41,41,41	0.34	0	56,56,56	0.72	0
15	CLA	A	813	1	54,62,73	1.62	5 (9%)	62,99,113	1.51	9 (14%)
15	CLA	a	812	15,1	65,73,73	1.50	5 (7%)	76,113,113	1.34	8 (10%)
18	BCR	B	846	-	41,41,41	0.31	0	56,56,56	0.87	1 (1%)
15	CLA	O	819	2	55,63,73	1.63	5 (9%)	64,101,113	1.43	7 (10%)
15	CLA	B	820	2	45,53,73	1.78	5 (11%)	52,89,113	1.61	6 (11%)
18	BCR	B	845	-	41,41,41	0.32	0	56,56,56	0.56	0
15	CLA	N	810	1	57,65,73	1.57	6 (10%)	66,103,113	1.51	7 (10%)
15	CLA	O	836	2	65,73,73	1.47	5 (7%)	76,113,113	1.40	7 (9%)
21	LMG	h	103	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	A	834	1	65,73,73	1.50	6 (9%)	76,113,113	1.33	7 (9%)
15	CLA	B	838	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
18	BCR	K	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.53	0
20	LMT	A	852	-	32,32,36	0.57	0	43,43,47	0.69	0
15	CLA	A	842	1	65,73,73	1.51	5 (7%)	76,113,113	1.34	8 (10%)
15	CLA	B	804	2	65,73,73	1.48	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	a	832	1	50,58,73	1.68	6 (12%)	58,95,113	1.54	8 (13%)
15	CLA	b	822	2	55,63,73	1.64	7 (12%)	64,101,113	1.31	7 (10%)
15	CLA	O	840	2	65,73,73	1.49	5 (7%)	76,113,113	1.36	8 (10%)
15	CLA	a	815	1	55,63,73	1.61	5 (9%)	64,101,113	1.48	7 (10%)
15	CLA	b	806	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
15	CLA	O	834	24	45,53,73	1.76	6 (13%)	52,89,113	1.64	7 (13%)
15	CLA	O	837	2	65,73,73	1.47	6 (9%)	76,113,113	1.40	9 (11%)
14	F6C	A	826	24	69,74,74	1.80	12 (17%)	70,114,114	2.25	17 (24%)
15	CLA	N	838	1	55,63,73	1.59	6 (10%)	64,101,113	1.47	7 (10%)
15	CLA	B	815	2	57,65,73	1.57	5 (8%)	66,103,113	1.48	7 (10%)
15	CLA	N	835	1	65,73,73	1.49	5 (7%)	76,113,113	1.33	9 (11%)
21	LMG	B	848	-	55,55,55	0.49	0	63,63,63	0.59	0
15	CLA	a	817	24	45,53,73	1.81	5 (11%)	52,89,113	1.59	6 (11%)
15	CLA	N	827	24	55,63,73	1.60	5 (9%)	64,101,113	1.52	9 (14%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	CLA	N	823	1	56,64,73	1.59	5 (8%)	65,102,113	1.47	6 (9%)
18	BCR	V	101	-	25,25,41	0.51	1 (4%)	33,33,56	0.51	0
14	F6C	A	856	24	69,74,74	1.76	14 (20%)	70,114,114	2.27	16 (22%)
15	CLA	a	830	1	65,73,73	1.47	6 (9%)	76,113,113	1.38	6 (7%)
15	CLA	N	825	1	65,73,73	1.49	5 (7%)	76,113,113	1.33	8 (10%)
18	BCR	T	101	-	41,41,41	0.34	0	56,56,56	0.72	0
15	CLA	b	813	2	65,73,73	1.49	6 (9%)	76,113,113	1.38	9 (11%)
15	CLA	A	821	1	60,68,73	1.54	6 (10%)	70,107,113	1.40	7 (10%)
14	F6C	N	824	24	55,60,74	2.02	13 (23%)	53,97,114	2.48	14 (26%)
22	LFA	O	850	-	15,15,19	0.24	0	14,14,18	0.20	0
15	CLA	O	817	2	60,68,73	1.55	5 (8%)	70,107,113	1.39	7 (10%)
15	CLA	N	822	24	65,73,73	1.49	6 (9%)	76,113,113	1.35	7 (9%)
15	CLA	b	811	2	45,53,73	1.79	5 (11%)	52,89,113	1.56	7 (13%)
18	BCR	B	843	-	41,41,41	0.32	0	56,56,56	0.60	0
15	CLA	O	827	2	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
15	CLA	a	839	1	65,73,73	1.49	5 (7%)	76,113,113	1.37	8 (10%)
18	BCR	L	210	-	41,41,41	0.30	0	56,56,56	0.66	0
18	BCR	k	102	-	41,41,41	0.33	0	56,56,56	0.64	1 (1%)
15	CLA	A	829	1	60,68,73	1.53	6 (10%)	70,107,113	1.41	7 (10%)
15	CLA	a	813	1	54,62,73	1.62	5 (9%)	62,99,113	1.51	8 (12%)
15	CLA	A	803	-	65,73,73	1.45	7 (10%)	76,113,113	1.41	7 (9%)
15	CLA	b	816	2	65,73,73	1.52	6 (9%)	76,113,113	1.35	6 (7%)
18	BCR	N	847	-	41,41,41	0.32	0	56,56,56	0.61	1 (1%)
15	CLA	A	839	1	65,73,73	1.49	5 (7%)	76,113,113	1.38	8 (10%)
15	CLA	O	830	2	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
15	CLA	f	201	24	65,73,73	1.50	6 (9%)	76,113,113	1.33	8 (10%)
20	LMT	a	852	-	32,32,36	0.57	0	43,43,47	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	824	24	1/1/15/20	14/37/115/115	-
15	CLA	a	842	1	1/1/15/20	13/37/115/115	-
14	F6C	A	802	24	-	7/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	F6C	B	839	24	-	14/41/97/97	-
15	CLA	N	805	15,1	1/1/14/20	10/31/109/115	-
14	F6C	b	832	2	-	5/41/97/97	-
21	LMG	b	849	-	-	6/50/70/70	0/1/1/1
15	CLA	B	834	24	1/1/11/20	6/13/91/115	-
15	CLA	N	828	1	1/1/15/20	9/37/115/115	-
20	LMT	A	854	-	-	4/21/61/61	0/2/2/2
15	CLA	O	808	2	1/1/15/20	9/37/115/115	-
18	BCR	W	205	-	-	4/29/63/63	0/2/2/2
15	CLA	b	825	2	1/1/15/20	4/37/115/115	-
15	CLA	O	810	2	1/1/15/20	11/37/115/115	-
13	CL0	a	801	1	3/3/20/25	7/37/135/135	-
15	CLA	O	812	2	-	12/27/105/115	-
15	CLA	b	814	2	1/1/11/20	6/13/91/115	-
15	CLA	O	801	2	1/1/15/20	10/37/115/115	-
15	CLA	N	811	1	1/1/13/20	15/28/106/115	-
15	CLA	O	828	2	1/1/15/20	13/37/115/115	-
18	BCR	B	842	-	-	4/29/63/63	0/2/2/2
18	BCR	M	101	-	-	6/29/63/63	0/2/2/2
21	LMG	N	855	-	-	10/39/59/70	0/1/1/1
15	CLA	A	804	1	1/1/15/20	5/37/115/115	-
15	CLA	j	202	10	1/1/15/20	4/37/115/115	-
15	CLA	a	821	1	1/1/14/20	5/31/109/115	-
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
13	CL0	A	801	1	3/3/20/25	3/37/135/135	-
15	CLA	B	817	2	1/1/14/20	13/31/109/115	-
15	CLA	a	835	1	1/1/15/20	9/37/115/115	-
15	CLA	O	824	24	1/1/15/20	14/37/115/115	-
16	PQN	b	841	-	-	0/23/43/43	0/2/2/2
18	BCR	O	847	-	-	7/29/63/63	0/2/2/2
15	CLA	B	840	2	1/1/15/20	11/37/115/115	-
15	CLA	O	807	2	1/1/15/20	4/37/115/115	-
18	BCR	b	845	-	-	8/29/63/63	0/2/2/2
15	CLA	a	823	1	1/1/13/20	6/27/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	810	1	1/1/13/20	10/28/106/115	-
15	CLA	A	805	15,1	1/1/14/20	10/31/109/115	-
15	CLA	O	831	2	1/1/15/20	10/37/115/115	-
18	BCR	A	850	-	-	13/29/63/63	0/2/2/2
19	LHG	f	203	-	-	25/53/53/53	-
15	CLA	b	821	24	1/1/12/20	8/23/101/115	-
15	CLA	A	828	1	1/1/15/20	9/37/115/115	-
22	LFA	b	850	-	-	5/13/13/17	-
15	CLA	b	838	2	1/1/15/20	10/37/115/115	-
18	BCR	L	206	-	-	2/29/63/63	0/2/2/2
19	LHG	Y	101	-	-	18/53/53/53	-
15	CLA	B	807	2	1/1/15/20	5/37/115/115	-
15	CLA	b	809	2	1/1/15/20	15/37/115/115	-
16	PQN	B	841	-	-	0/23/43/43	0/2/2/2
15	CLA	B	836	2	1/1/15/20	8/37/115/115	-
20	LMT	N	852	-	-	2/17/57/61	0/2/2/2
15	CLA	A	811	1	1/1/13/20	14/28/106/115	-
15	CLA	A	808	1	1/1/11/20	3/13/91/115	-
21	LMG	A	855	-	-	11/39/59/70	0/1/1/1
15	CLA	A	838	1	1/1/13/20	11/25/103/115	-
15	CLA	O	815	2	1/1/13/20	8/28/106/115	-
19	LHG	k	101	-	-	16/53/53/53	-
15	CLA	N	818	1	1/1/15/20	20/37/115/115	-
20	LMT	a	854	-	-	4/21/61/61	0/2/2/2
22	LFA	j	208	-	-	0/12/12/17	-
15	CLA	B	810	2	1/1/15/20	12/37/115/115	-
15	CLA	N	816	1	1/1/11/20	7/13/91/115	-
15	CLA	L	202	10	1/1/15/20	5/37/115/115	-
14	F6C	L	201	2	-	8/41/97/97	-
15	CLA	b	804	2	1/1/15/20	9/37/115/115	-
15	CLA	B	833	2	1/1/13/20	6/25/103/115	-
15	CLA	i	103	24	1/1/12/20	3/19/97/115	-
14	F6C	N	802	24	-	9/41/97/97	-
15	CLA	N	837	1	1/1/12/20	7/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	F6C	A	824	24	-	10/25/81/97	-
14	F6C	a	824	24	-	8/25/81/97	-
15	CLA	N	820	1	1/1/15/20	26/37/115/115	-
15	CLA	a	841	1	1/1/15/20	13/37/115/115	-
15	CLA	a	822	24	1/1/15/20	15/37/115/115	-
15	CLA	B	835	24	1/1/11/20	10/13/91/115	-
15	CLA	A	822	24	1/1/15/20	14/37/115/115	-
15	CLA	b	828	2	1/1/15/20	15/37/115/115	-
15	CLA	a	825	1	1/1/15/20	8/37/115/115	-
15	CLA	b	805	2	1/1/15/20	10/37/115/115	-
15	CLA	O	818	24	1/1/15/20	8/37/115/115	-
14	F6C	W	201	2	-	8/41/97/97	-
15	CLA	O	820	2	1/1/11/20	3/13/91/115	-
21	LMG	O	849	-	-	5/50/70/70	0/1/1/1
15	CLA	B	811	2	1/1/11/20	2/13/91/115	-
15	CLA	A	812	15,1	1/1/15/20	19/37/115/115	-
15	CLA	a	834	1	1/1/15/20	4/37/115/115	-
18	BCR	a	848	-	-	6/29/63/63	0/2/2/2
15	CLA	B	802	24	1/1/15/20	15/37/115/115	-
15	CLA	A	816	1	1/1/11/20	7/13/91/115	-
15	CLA	i	102	9	1/1/11/20	6/13/91/115	-
15	CLA	A	832	1	1/1/12/20	3/19/97/115	-
15	CLA	a	828	1	1/1/15/20	10/37/115/115	-
17	SF4	c	102	3	-	-	0/6/5/5
15	CLA	a	805	15,1	1/1/14/20	11/31/109/115	-
15	CLA	b	833	2	1/1/13/20	8/25/103/115	-
18	BCR	j	205	-	-	2/29/63/63	0/2/2/2
15	CLA	b	819	2	1/1/13/20	10/25/103/115	-
15	CLA	b	836	2	1/1/15/20	8/37/115/115	-
15	CLA	A	814	1	1/1/15/20	9/37/115/115	-
18	BCR	g	101	-	-	8/29/63/63	0/2/2/2
15	CLA	N	830	1	1/1/15/20	5/37/115/115	-
15	CLA	O	802	24	1/1/15/20	14/37/115/115	-
14	F6C	b	839	24	-	14/41/97/97	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	A	849	-	-	3/29/63/63	0/2/2/2
15	CLA	j	203	10	1/1/14/20	9/31/109/115	-
15	CLA	O	814	2	1/1/11/20	6/13/91/115	-
15	CLA	b	837	2	1/1/15/20	11/37/115/115	-
18	BCR	F	202	-	-	7/29/63/63	0/2/2/2
15	CLA	N	841	1	1/1/15/20	13/37/115/115	-
15	CLA	B	801	2	1/1/15/20	10/37/115/115	-
15	CLA	B	822	2	1/1/13/20	11/25/103/115	-
18	BCR	b	843	-	-	5/29/63/63	0/2/2/2
15	CLA	B	813	2	1/1/15/20	15/37/115/115	-
15	CLA	B	818	24	1/1/15/20	8/37/115/115	-
20	LMT	N	853	-	-	8/14/54/61	0/2/2/2
18	BCR	N	850	-	-	13/29/63/63	0/2/2/2
15	CLA	N	819	1	1/1/15/20	11/37/115/115	-
18	BCR	L	205	-	-	4/29/63/63	0/2/2/2
19	LHG	N	851	-	-	13/46/46/53	-
14	F6C	a	855	24	-	17/41/97/97	-
15	CLA	a	837	1	1/1/12/20	11/21/99/115	-
21	LMG	j	206	-	-	10/45/65/70	0/1/1/1
18	BCR	O	842	-	-	3/29/63/63	0/2/2/2
15	CLA	N	814	1	1/1/15/20	9/37/115/115	-
19	LHG	W	207	-	-	14/53/53/53	-
15	CLA	b	826	2	1/1/14/20	13/34/112/115	-
15	CLA	A	809	1	1/1/14/20	15/31/109/115	-
15	CLA	b	840	2	1/1/15/20	11/37/115/115	-
16	PQN	A	843	-	-	0/23/43/43	0/2/2/2
15	CLA	A	830	1	1/1/15/20	8/37/115/115	-
15	CLA	N	804	1	1/1/15/20	5/37/115/115	-
13	CL0	N	801	1	3/3/20/25	6/37/135/135	-
15	CLA	O	804	2	1/1/15/20	8/37/115/115	-
15	CLA	a	816	1	1/1/11/20	7/13/91/115	-
18	BCR	N	846	-	-	8/29/63/63	0/2/2/2
14	F6C	W	204	24	-	10/41/97/97	-
21	LMG	T	103	-	-	16/32/52/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	808	1	1/1/11/20	1/13/91/115	-
15	CLA	N	806	1	1/1/15/20	19/37/115/115	-
15	CLA	a	818	1	1/1/15/20	19/37/115/115	-
15	CLA	L	203	10	1/1/14/20	9/31/109/115	-
15	CLA	a	820	1	1/1/15/20	21/37/115/115	-
14	F6C	a	826	24	-	17/41/97/97	-
15	CLA	N	817	24	1/1/11/20	3/13/91/115	-
17	SF4	c	101	3	-	-	0/6/5/5
18	BCR	U	101	-	-	7/29/63/63	0/2/2/2
15	CLA	O	823	24	1/1/15/20	9/37/115/115	-
15	CLA	A	806	1	1/1/15/20	19/37/115/115	-
15	CLA	a	804	1	1/1/15/20	5/37/115/115	-
14	F6C	a	802	24	-	7/41/97/97	-
15	CLA	B	821	24	1/1/12/20	10/23/101/115	-
15	CLA	A	820	1	1/1/15/20	21/37/115/115	-
15	CLA	a	833	1	1/1/13/20	4/25/103/115	-
15	CLA	B	825	2	1/1/15/20	3/37/115/115	-
15	CLA	b	817	2	1/1/14/20	13/31/109/115	-
15	CLA	V	103	24	1/1/12/20	5/19/97/115	-
15	CLA	O	835	24	1/1/11/20	10/13/91/115	-
15	CLA	N	840	1	1/1/12/20	4/19/97/115	-
18	BCR	B	844	-	-	4/29/63/63	0/2/2/2
15	CLA	A	823	1	1/1/13/20	6/27/105/115	-
14	F6C	N	856	24	-	16/41/97/97	-
18	BCR	a	845	-	-	3/29/63/63	0/2/2/2
15	CLA	O	806	2	1/1/15/20	19/37/115/115	-
15	CLA	l	102	12	1/1/13/20	2/25/103/115	-
15	CLA	A	819	1	1/1/15/20	12/37/115/115	-
19	LHG	A	851	-	-	13/46/46/53	-
21	LMG	L	207	-	-	10/45/65/70	0/1/1/1
19	LHG	l	101	-	-	23/48/48/53	-
15	CLA	Z	102	12	1/1/13/20	2/25/103/115	-
15	CLA	A	817	24	1/1/11/20	3/13/91/115	-
15	CLA	a	838	1	1/1/13/20	11/25/103/115	-
22	LFA	W	208	-	-	0/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	841	1	1/1/15/20	14/37/115/115	-
15	CLA	N	836	1	1/1/12/20	8/24/102/115	-
15	CLA	a	809	1	1/1/14/20	12/31/109/115	-
19	LHG	Z	101	-	-	23/48/48/53	-
15	CLA	b	824	24	1/1/15/20	14/37/115/115	-
16	PQN	a	843	-	-	0/23/43/43	0/2/2/2
18	BCR	B	847	-	-	3/29/63/63	0/2/2/2
15	CLA	A	815	1	1/1/13/20	4/25/103/115	-
15	CLA	O	838	2	1/1/15/20	7/37/115/115	-
15	CLA	O	811	2	1/1/11/20	2/13/91/115	-
15	CLA	b	810	2	1/1/15/20	13/37/115/115	-
15	CLA	A	818	1	1/1/15/20	21/37/115/115	-
15	CLA	B	816	2	1/1/15/20	10/37/115/115	-
15	CLA	N	831	1	1/1/15/20	12/37/115/115	-
15	CLA	O	803	-	1/1/15/20	4/37/115/115	-
15	CLA	B	805	2	1/1/15/20	14/37/115/115	-
18	BCR	b	844	-	-	4/29/63/63	0/2/2/2
15	CLA	b	834	24	1/1/11/20	4/13/91/115	-
18	BCR	F	203	-	-	2/29/63/63	0/2/2/2
15	CLA	B	828	2	1/1/15/20	12/37/115/115	-
18	BCR	b	848	-	-	3/29/63/63	0/2/2/2
15	CLA	a	808	1	1/1/11/20	3/13/91/115	-
15	CLA	A	837	1	1/1/12/20	10/21/99/115	-
15	CLA	N	803	-	1/1/15/20	10/37/115/115	-
15	CLA	B	809	2	1/1/15/20	14/37/115/115	-
19	LHG	N	857	-	-	23/53/53/53	-
18	BCR	N	849	-	-	3/29/63/63	0/2/2/2
15	CLA	b	815	2	1/1/13/20	4/28/106/115	-
21	LMG	g	103	-	-	16/32/52/70	0/1/1/1
15	CLA	O	822	2	1/1/13/20	11/25/103/115	-
15	CLA	b	807	2	1/1/15/20	8/37/115/115	-
15	CLA	O	813	2	1/1/15/20	14/37/115/115	-
14	F6C	O	832	2	-	7/41/97/97	-
15	CLA	O	825	2	1/1/15/20	3/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	808	2	1/1/15/20	8/37/115/115	-
15	CLA	A	825	1	1/1/15/20	8/37/115/115	-
15	CLA	a	829	1	1/1/14/20	15/31/109/115	-
17	SF4	C	101	3	-	-	0/6/5/5
15	CLA	a	803	-	1/1/15/20	10/37/115/115	-
18	BCR	b	846	-	-	0/29/63/63	0/2/2/2
18	BCR	a	850	-	-	13/29/63/63	0/2/2/2
15	CLA	a	819	1	1/1/15/20	10/37/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
19	LHG	a	851	-	-	13/46/46/53	-
19	LHG	F	204	-	-	24/53/53/53	-
15	CLA	N	815	1	1/1/13/20	4/25/103/115	-
18	BCR	O	843	-	-	5/29/63/63	0/2/2/2
18	BCR	J	101	-	-	7/29/63/63	0/2/2/2
15	CLA	B	823	24	1/1/15/20	9/37/115/115	-
15	CLA	a	814	1	1/1/15/20	8/37/115/115	-
15	CLA	O	816	2	1/1/15/20	9/37/115/115	-
15	CLA	A	807	1	1/1/15/20	16/37/115/115	-
15	CLA	N	809	1	1/1/14/20	14/31/109/115	-
16	PQN	N	843	-	-	0/23/43/43	0/2/2/2
15	CLA	A	827	24	1/1/13/20	2/25/103/115	-
20	LMT	N	854	-	-	4/21/61/61	0/2/2/2
15	CLA	a	806	1	1/1/15/20	19/37/115/115	-
15	CLA	O	826	2	1/1/14/20	14/34/112/115	-
18	BCR	W	209	-	-	2/29/63/63	0/2/2/2
15	CLA	b	829	2	1/1/15/20	16/37/115/115	-
21	LMG	U	103	-	-	15/50/70/70	0/1/1/1
18	BCR	O	846	-	-	1/29/63/63	0/2/2/2
18	BCR	h	101	-	-	7/29/63/63	0/2/2/2
15	CLA	a	836	1	1/1/12/20	8/24/102/115	-
19	LHG	B	851	-	-	18/53/53/53	-
18	BCR	T	102	-	-	5/29/63/63	0/2/2/2
18	BCR	g	102	-	-	5/29/63/63	0/2/2/2
17	SF4	N	844	2,1	-	-	0/6/5/5
15	CLA	O	821	24	1/1/12/20	9/23/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	I	102	-	-	4/29/63/63	0/2/2/2
15	CLA	B	812	2	-	12/27/105/115	-
15	CLA	K	102	9	1/1/11/20	6/13/91/115	-
21	LMG	W	206	-	-	10/45/65/70	0/1/1/1
15	CLA	N	812	15,1	1/1/15/20	17/37/115/115	-
15	CLA	A	840	1	1/1/12/20	4/19/97/115	-
15	CLA	N	821	1	1/1/14/20	6/31/109/115	-
18	BCR	f	202	-	-	2/29/63/63	0/2/2/2
19	LHG	j	207	-	-	13/53/53/53	-
15	CLA	F	201	24	1/1/15/20	8/37/115/115	-
15	CLA	B	806	2	1/1/15/20	20/37/115/115	-
15	CLA	N	834	1	1/1/15/20	5/37/115/115	-
15	CLA	N	833	1	1/1/13/20	3/25/103/115	-
18	BCR	i	101	-	-	0/18/35/63	0/1/1/2
15	CLA	W	202	10	1/1/15/20	5/37/115/115	-
15	CLA	b	818	24	1/1/15/20	8/37/115/115	-
15	CLA	V	102	9	1/1/11/20	7/13/91/115	-
15	CLA	A	835	1	1/1/15/20	11/37/115/115	-
15	CLA	B	837	2	1/1/15/20	13/37/115/115	-
15	CLA	b	820	2	1/1/11/20	4/13/91/115	-
18	BCR	N	848	-	-	6/29/63/63	0/2/2/2
15	CLA	X	102	12	1/1/13/20	2/25/103/115	-
15	CLA	B	819	2	1/1/13/20	10/25/103/115	-
16	PQN	O	841	-	-	0/23/43/43	0/2/2/2
17	SF4	P	101	3	-	-	0/6/5/5
21	LMG	I	103	-	-	15/32/52/70	0/1/1/1
15	CLA	N	839	1	1/1/15/20	15/37/115/115	-
18	BCR	O	845	-	-	8/29/63/63	0/2/2/2
15	CLA	a	807	1	1/1/15/20	16/37/115/115	-
14	F6C	j	204	24	-	9/41/97/97	-
15	CLA	b	802	24	1/1/15/20	14/37/115/115	-
18	BCR	N	845	-	-	3/29/63/63	0/2/2/2
15	CLA	B	814	2	1/1/11/20	4/13/91/115	-
15	CLA	A	836	1	1/1/12/20	8/24/102/115	-
15	CLA	b	831	2	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	K	103	24	1/1/12/20	2/19/97/115	-
15	CLA	N	829	1	1/1/14/20	15/31/109/115	-
17	SF4	A	844	2,1	-	-	0/6/5/5
15	CLA	a	840	1	1/1/12/20	2/19/97/115	-
18	BCR	O	844	-	-	4/29/63/63	0/2/2/2
19	LHG	X	101	-	-	21/48/48/53	-
15	CLA	a	827	24	1/1/13/20	2/25/103/115	-
18	BCR	a	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	809	2	1/1/15/20	13/37/115/115	-
15	CLA	b	803	-	1/1/15/20	5/37/115/115	-
18	BCR	a	847	-	-	5/29/63/63	0/2/2/2
22	LFA	B	849	-	-	5/13/13/17	-
15	CLA	a	810	1	1/1/13/20	11/28/106/115	-
18	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
15	CLA	a	831	1	1/1/15/20	12/37/115/115	-
15	CLA	O	805	2	1/1/15/20	14/37/115/115	-
15	CLA	W	203	10	1/1/14/20	9/31/109/115	-
15	CLA	B	827	2	1/1/15/20	7/37/115/115	-
15	CLA	b	830	2	1/1/15/20	11/37/115/115	-
17	SF4	P	102	3	-	-	0/6/5/5
18	BCR	A	847	-	-	4/29/63/63	0/2/2/2
15	CLA	B	829	2	1/1/15/20	16/37/115/115	-
22	LFA	L	209	-	-	0/12/12/17	-
14	F6C	j	201	2	-	10/41/97/97	-
18	BCR	A	848	-	-	6/29/63/63	0/2/2/2
18	BCR	a	849	-	-	3/29/63/63	0/2/2/2
14	F6C	L	204	24	-	11/41/97/97	-
15	CLA	b	827	2	1/1/15/20	7/37/115/115	-
15	CLA	N	842	1	1/1/15/20	13/37/115/115	-
15	CLA	a	811	1	1/1/13/20	14/28/106/115	-
15	CLA	b	835	24	1/1/11/20	10/13/91/115	-
18	BCR	O	848	-	-	3/29/63/63	0/2/2/2
15	CLA	B	830	2	1/1/15/20	11/37/115/115	-
14	F6C	B	832	2	-	5/41/97/97	-
15	CLA	b	823	24	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	BCR	S	202	-	-	2/29/63/63	0/2/2/2
20	LMT	A	853	-	-	8/14/54/61	0/2/2/2
18	BCR	A	845	-	-	3/29/63/63	0/2/2/2
15	CLA	A	831	1	1/1/15/20	12/37/115/115	-
15	CLA	O	833	2	1/1/13/20	8/25/103/115	-
18	BCR	U	102	-	-	8/29/63/63	0/2/2/2
21	LMG	B	850	-	-	8/39/59/70	0/1/1/1
15	CLA	b	801	2	1/1/15/20	9/37/115/115	-
19	LHG	L	208	-	-	13/53/53/53	-
15	CLA	B	831	2	1/1/15/20	10/37/115/115	-
15	CLA	O	829	2	1/1/15/20	16/37/115/115	-
20	LMT	a	853	-	-	8/14/54/61	0/2/2/2
18	BCR	b	842	-	-	4/29/63/63	0/2/2/2
21	LMG	J	103	-	-	17/50/70/70	0/1/1/1
15	CLA	S	201	24	1/1/15/20	7/37/115/115	-
15	CLA	B	803	-	1/1/15/20	9/37/115/115	-
15	CLA	N	813	1	1/1/12/20	9/24/102/115	-
14	F6C	O	839	24	-	14/41/97/97	-
15	CLA	B	826	2	1/1/14/20	15/34/112/115	-
17	SF4	a	844	2,1	-	-	0/6/5/5
15	CLA	N	832	1	1/1/12/20	3/19/97/115	-
18	BCR	h	102	-	-	8/29/63/63	0/2/2/2
15	CLA	b	808	2	1/1/15/20	7/37/115/115	-
18	BCR	J	102	-	-	8/29/63/63	0/2/2/2
14	F6C	N	826	24	-	12/41/97/97	-
15	CLA	N	807	1	1/1/15/20	16/37/115/115	-
15	CLA	A	833	1	1/1/13/20	3/25/103/115	-
18	BCR	b	847	-	-	7/29/63/63	0/2/2/2
15	CLA	b	812	2	-	13/27/105/115	-
18	BCR	I	101	-	-	8/29/63/63	0/2/2/2
15	CLA	A	813	1	1/1/12/20	9/24/102/115	-
15	CLA	a	812	15,1	1/1/15/20	16/37/115/115	-
18	BCR	B	846	-	-	0/29/63/63	0/2/2/2
15	CLA	O	819	2	1/1/13/20	10/25/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	B	820	2	1/1/11/20	5/13/91/115	-
18	BCR	B	845	-	-	8/29/63/63	0/2/2/2
15	CLA	N	810	1	1/1/13/20	10/28/106/115	-
15	CLA	O	836	2	1/1/15/20	7/37/115/115	-
21	LMG	h	103	-	-	15/50/70/70	0/1/1/1
15	CLA	A	834	1	1/1/15/20	5/37/115/115	-
15	CLA	B	838	2	1/1/15/20	12/37/115/115	-
18	BCR	K	101	-	-	0/18/35/63	0/1/1/2
20	LMT	A	852	-	-	1/17/57/61	0/2/2/2
15	CLA	A	842	1	1/1/15/20	13/37/115/115	-
15	CLA	B	804	2	1/1/15/20	9/37/115/115	-
15	CLA	a	832	1	1/1/12/20	3/19/97/115	-
15	CLA	b	822	2	1/1/13/20	9/25/103/115	-
15	CLA	O	840	2	1/1/15/20	10/37/115/115	-
15	CLA	a	815	1	1/1/13/20	4/25/103/115	-
15	CLA	b	806	2	1/1/15/20	19/37/115/115	-
15	CLA	O	834	24	1/1/11/20	6/13/91/115	-
15	CLA	O	837	2	1/1/15/20	11/37/115/115	-
14	F6C	A	826	24	-	14/41/97/97	-
15	CLA	N	838	1	1/1/13/20	11/25/103/115	-
15	CLA	B	815	2	1/1/13/20	6/28/106/115	-
15	CLA	N	835	1	1/1/15/20	10/37/115/115	-
21	LMG	B	848	-	-	4/50/70/70	0/1/1/1
15	CLA	a	817	24	1/1/11/20	3/13/91/115	-
15	CLA	N	827	24	1/1/13/20	2/25/103/115	-
15	CLA	N	823	1	1/1/13/20	6/27/105/115	-
18	BCR	V	101	-	-	0/18/35/63	0/1/1/2
14	F6C	A	856	24	-	17/41/97/97	-
15	CLA	a	830	1	1/1/15/20	5/37/115/115	-
15	CLA	N	825	1	1/1/15/20	11/37/115/115	-
18	BCR	T	101	-	-	8/29/63/63	0/2/2/2
15	CLA	b	813	2	1/1/15/20	11/37/115/115	-
15	CLA	A	821	1	1/1/14/20	7/31/109/115	-
14	F6C	N	824	24	-	9/25/81/97	-
22	LFA	O	850	-	-	7/13/13/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	817	2	1/1/14/20	13/31/109/115	-
15	CLA	N	822	24	1/1/15/20	15/37/115/115	-
15	CLA	b	811	2	1/1/11/20	2/13/91/115	-
18	BCR	B	843	-	-	5/29/63/63	0/2/2/2
15	CLA	O	827	2	1/1/15/20	7/37/115/115	-
15	CLA	a	839	1	1/1/15/20	13/37/115/115	-
18	BCR	L	210	-	-	2/29/63/63	0/2/2/2
18	BCR	k	102	-	-	6/29/63/63	0/2/2/2
15	CLA	A	829	1	1/1/14/20	17/31/109/115	-
15	CLA	a	813	1	1/1/12/20	9/24/102/115	-
15	CLA	A	803	-	1/1/15/20	12/37/115/115	-
15	CLA	b	816	2	1/1/15/20	10/37/115/115	-
18	BCR	N	847	-	-	5/29/63/63	0/2/2/2
15	CLA	A	839	1	1/1/15/20	16/37/115/115	-
15	CLA	O	830	2	1/1/15/20	11/37/115/115	-
15	CLA	f	201	24	1/1/15/20	8/37/115/115	-
20	LMT	a	852	-	-	0/17/57/61	0/2/2/2

The worst 5 of 1680 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	j	201	F6C	C2A-C3A	8.78	1.55	1.36
14	W	201	F6C	C2A-C3A	8.74	1.55	1.36
14	L	201	F6C	C2A-C3A	8.74	1.55	1.36
14	A	826	F6C	C2A-C3A	8.74	1.55	1.36
14	N	826	F6C	C2A-C3A	8.73	1.55	1.36

The worst 5 of 2301 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	839	F6C	CAA-C2A-C3A	-9.91	109.43	127.88
14	O	839	F6C	CAA-C2A-C3A	-9.89	109.45	127.88
14	B	839	F6C	CAA-C2A-C3A	-9.89	109.46	127.88
14	a	826	F6C	CAA-C2A-C3A	-9.83	109.56	127.88
14	W	204	F6C	CAA-C2A-C3A	-9.70	109.81	127.88

5 of 252 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NA
13	A	801	CL0	NC
13	A	801	CL0	ND
13	N	801	CL0	NA
13	N	801	CL0	NC

5 of 3453 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	F6C	C1B-C2B-CMB-OMB
14	A	802	F6C	C3B-C2B-CMB-OMB
14	A	824	F6C	C1B-C2B-CMB-OMB
14	A	824	F6C	C3B-C2B-CMB-OMB
14	A	826	F6C	C2C-C3C-CAC-CBC

There are no ring outliers.

331 monomers are involved in 769 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	824	CLA	6	0
15	a	842	CLA	2	0
14	b	832	F6C	1	0
21	b	849	LMG	5	0
15	B	834	CLA	2	0
20	A	854	LMT	2	0
15	O	808	CLA	5	0
18	W	205	BCR	1	0
15	b	825	CLA	1	0
15	O	810	CLA	1	0
13	a	801	CL0	2	0
15	O	812	CLA	5	0
15	O	801	CLA	1	0
15	N	811	CLA	2	0
15	O	828	CLA	2	0
18	B	842	BCR	3	0
18	M	101	BCR	4	0
15	A	804	CLA	3	0
15	j	202	CLA	2	0
15	a	821	CLA	1	0
18	A	846	BCR	2	0
13	A	801	CL0	3	0
15	B	817	CLA	3	0
15	O	824	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	b	841	PQN	4	0
18	O	847	BCR	1	0
15	B	840	CLA	3	0
15	O	807	CLA	1	0
15	a	823	CLA	1	0
15	A	810	CLA	4	0
15	A	805	CLA	1	0
15	O	831	CLA	4	0
18	A	850	BCR	8	0
19	f	203	LHG	2	0
15	b	821	CLA	1	0
22	b	850	LFA	2	0
15	b	838	CLA	8	0
18	L	206	BCR	3	0
19	Y	101	LHG	4	0
15	B	807	CLA	3	0
15	b	809	CLA	6	0
16	B	841	PQN	3	0
15	B	836	CLA	3	0
20	N	852	LMT	1	0
15	A	811	CLA	3	0
21	A	855	LMG	1	0
15	A	838	CLA	2	0
15	O	815	CLA	1	0
19	k	101	LHG	5	0
15	N	818	CLA	7	0
20	a	854	LMT	1	0
22	j	208	LFA	1	0
15	B	810	CLA	2	0
15	N	816	CLA	2	0
15	L	202	CLA	2	0
14	L	201	F6C	1	0
15	b	804	CLA	6	0
15	N	837	CLA	3	0
15	N	820	CLA	7	0
15	a	841	CLA	5	0
15	a	822	CLA	2	0
15	A	822	CLA	3	0
15	b	828	CLA	4	0
15	a	825	CLA	1	0
15	b	805	CLA	2	0
15	O	818	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	W	201	F6C	1	0
15	O	820	CLA	2	0
21	O	849	LMG	6	0
15	B	811	CLA	1	0
15	A	812	CLA	3	0
15	a	834	CLA	2	0
18	a	848	BCR	1	0
15	B	802	CLA	5	0
15	A	816	CLA	3	0
15	i	102	CLA	1	0
17	c	102	SF4	1	0
15	a	805	CLA	1	0
15	b	833	CLA	1	0
18	j	205	BCR	1	0
15	b	819	CLA	1	0
15	b	836	CLA	2	0
15	A	814	CLA	8	0
18	g	101	BCR	5	0
15	N	830	CLA	2	0
15	O	802	CLA	4	0
18	A	849	BCR	1	0
15	j	203	CLA	1	0
15	O	814	CLA	1	0
15	b	837	CLA	7	0
18	F	202	BCR	2	0
15	N	841	CLA	3	0
15	B	801	CLA	1	0
15	B	822	CLA	1	0
18	b	843	BCR	3	0
15	B	813	CLA	2	0
15	B	818	CLA	2	0
20	N	853	LMT	1	0
18	N	850	BCR	7	0
15	N	819	CLA	5	0
18	L	205	BCR	1	0
15	a	837	CLA	1	0
21	j	206	LMG	3	0
18	O	842	BCR	3	0
15	N	814	CLA	6	0
19	W	207	LHG	8	0
15	b	826	CLA	5	0
15	A	809	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	840	CLA	1	0
16	A	843	PQN	1	0
15	A	830	CLA	3	0
15	N	804	CLA	4	0
13	N	801	CL0	2	0
15	O	804	CLA	5	0
15	a	816	CLA	1	0
18	N	846	BCR	3	0
21	T	103	LMG	2	0
15	N	808	CLA	1	0
15	N	806	CLA	7	0
15	a	818	CLA	5	0
15	L	203	CLA	1	0
15	a	820	CLA	6	0
18	U	101	BCR	1	0
15	O	823	CLA	3	0
15	A	806	CLA	7	0
15	a	804	CLA	5	0
15	B	821	CLA	1	0
15	A	820	CLA	7	0
15	a	833	CLA	1	0
15	B	825	CLA	2	0
15	b	817	CLA	3	0
15	N	840	CLA	1	0
18	B	844	BCR	2	0
15	A	823	CLA	2	0
18	a	845	BCR	3	0
15	O	806	CLA	4	0
15	l	102	CLA	1	0
15	A	819	CLA	6	0
21	L	207	LMG	4	0
19	l	101	LHG	3	0
15	Z	102	CLA	1	0
15	a	838	CLA	1	0
22	W	208	LFA	1	0
15	A	841	CLA	6	0
15	N	836	CLA	1	0
15	a	809	CLA	1	0
19	Z	101	LHG	1	0
15	b	824	CLA	4	0
16	a	843	PQN	2	0
18	B	847	BCR	10	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	815	CLA	3	0
15	O	838	CLA	8	0
15	O	811	CLA	1	0
15	b	810	CLA	1	0
15	A	818	CLA	6	0
15	B	816	CLA	4	0
15	N	831	CLA	2	0
15	O	803	CLA	8	0
15	B	805	CLA	3	0
18	b	844	BCR	3	0
15	b	834	CLA	3	0
18	F	203	BCR	3	0
15	B	828	CLA	1	0
18	b	848	BCR	5	0
15	A	837	CLA	2	0
15	N	803	CLA	7	0
15	B	809	CLA	7	0
19	N	857	LHG	2	0
18	N	849	BCR	2	0
15	b	815	CLA	1	0
21	g	103	LMG	3	0
15	O	822	CLA	1	0
15	b	807	CLA	4	0
15	O	813	CLA	2	0
14	O	832	F6C	1	0
15	O	825	CLA	1	0
15	B	808	CLA	4	0
15	A	825	CLA	1	0
15	a	829	CLA	4	0
15	a	803	CLA	8	0
18	b	846	BCR	5	0
18	a	850	BCR	7	0
15	a	819	CLA	6	0
19	F	204	LHG	2	0
15	N	815	CLA	2	0
18	O	843	BCR	1	0
18	J	101	BCR	1	0
15	B	823	CLA	2	0
15	a	814	CLA	7	0
15	O	816	CLA	2	0
15	A	807	CLA	4	0
15	N	809	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	N	843	PQN	2	0
15	A	827	CLA	1	0
20	N	854	LMT	1	0
15	a	806	CLA	8	0
15	O	826	CLA	4	0
18	W	209	BCR	6	0
15	b	829	CLA	5	0
21	U	103	LMG	1	0
18	O	846	BCR	4	0
15	a	836	CLA	1	0
19	B	851	LHG	4	0
15	O	821	CLA	1	0
15	B	812	CLA	6	0
15	K	102	CLA	1	0
21	W	206	LMG	4	0
15	N	812	CLA	3	0
15	A	840	CLA	1	0
15	N	821	CLA	1	0
18	f	202	BCR	4	0
19	j	207	LHG	7	0
15	B	806	CLA	5	0
15	N	834	CLA	2	0
15	N	833	CLA	2	0
15	W	202	CLA	2	0
15	b	818	CLA	1	0
15	V	102	CLA	1	0
15	A	835	CLA	2	0
15	B	837	CLA	6	0
15	b	820	CLA	2	0
15	X	102	CLA	1	0
15	B	819	CLA	1	0
16	O	841	PQN	4	0
21	I	103	LMG	4	0
15	N	839	CLA	3	0
18	O	845	BCR	1	0
15	a	807	CLA	3	0
15	b	802	CLA	4	0
18	N	845	BCR	3	0
15	B	814	CLA	1	0
15	A	836	CLA	1	0
15	b	831	CLA	3	0
15	N	829	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	a	840	CLA	1	0
18	O	844	BCR	3	0
19	X	101	LHG	3	0
18	a	846	BCR	2	0
15	O	809	CLA	6	0
15	b	803	CLA	8	0
18	a	847	BCR	2	0
22	B	849	LFA	1	0
15	a	810	CLA	4	0
18	Y	102	BCR	3	0
15	a	831	CLA	3	0
15	O	805	CLA	2	0
15	W	203	CLA	1	0
15	B	827	CLA	1	0
15	b	830	CLA	3	0
18	A	847	BCR	2	0
15	B	829	CLA	6	0
22	L	209	LFA	2	0
14	j	201	F6C	1	0
18	A	848	BCR	2	0
18	a	849	BCR	1	0
14	L	204	F6C	1	0
15	N	842	CLA	1	0
15	a	811	CLA	2	0
18	O	848	BCR	4	0
15	B	830	CLA	3	0
14	B	832	F6C	1	0
15	b	823	CLA	3	0
18	S	202	BCR	3	0
20	A	853	LMT	1	0
18	A	845	BCR	4	0
15	A	831	CLA	4	0
15	O	833	CLA	1	0
18	U	102	BCR	5	0
19	L	208	LHG	6	0
15	B	831	CLA	3	0
15	O	829	CLA	7	0
20	a	853	LMT	1	0
18	b	842	BCR	2	0
15	S	201	CLA	1	0
15	B	803	CLA	8	0
15	N	813	CLA	3	0

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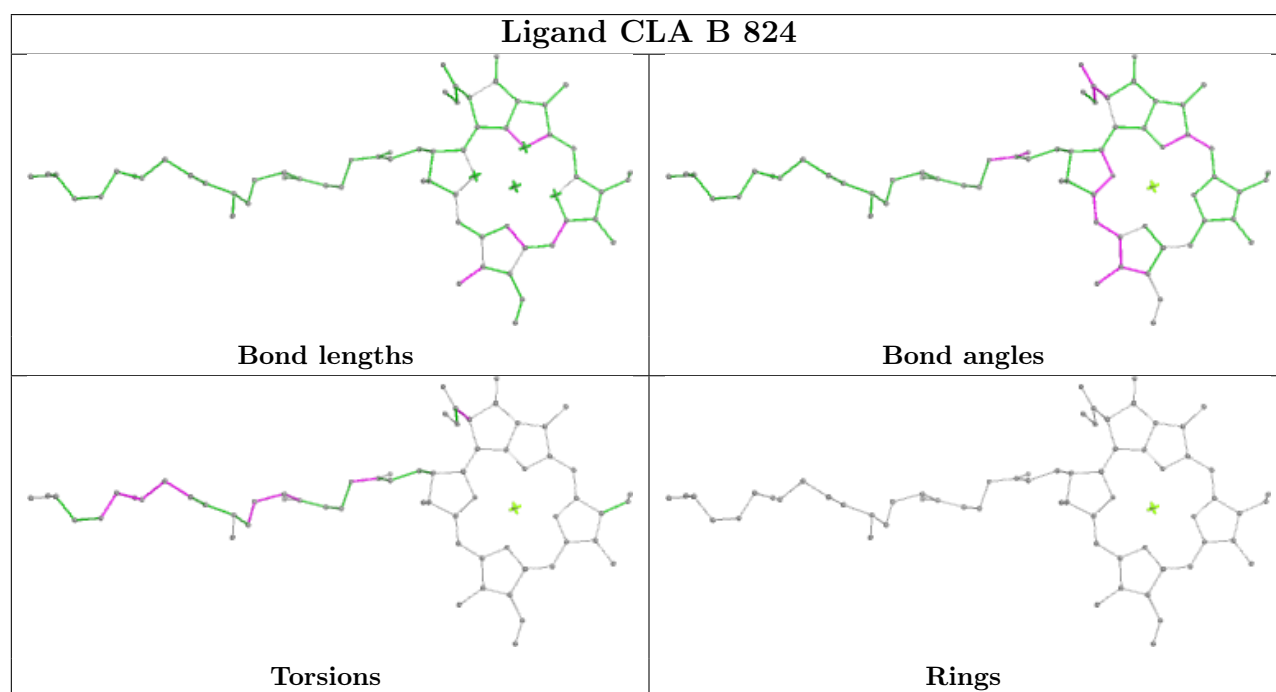
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	826	CLA	5	0
18	h	102	BCR	7	0
15	b	808	CLA	6	0
18	J	102	BCR	6	0
15	N	807	CLA	4	0
15	A	833	CLA	2	0
18	b	847	BCR	2	0
15	b	812	CLA	4	0
18	I	101	BCR	4	0
15	A	813	CLA	3	0
15	a	812	CLA	4	0
18	B	846	BCR	5	0
15	O	819	CLA	2	0
15	B	820	CLA	3	0
15	N	810	CLA	4	0
15	O	836	CLA	3	0
21	h	103	LMG	2	0
15	A	834	CLA	2	0
15	B	838	CLA	7	0
20	A	852	LMT	2	0
15	A	842	CLA	2	0
15	B	804	CLA	6	0
15	b	822	CLA	1	0
15	O	840	CLA	1	0
15	a	815	CLA	3	0
15	b	806	CLA	6	0
15	O	834	CLA	2	0
15	O	837	CLA	4	0
15	N	838	CLA	3	0
21	B	848	LMG	4	0
15	N	827	CLA	1	0
15	N	823	CLA	3	0
15	a	830	CLA	2	0
15	N	825	CLA	2	0
18	T	101	BCR	6	0
15	b	813	CLA	1	0
15	A	821	CLA	1	0
22	O	850	LFA	1	0
15	O	817	CLA	3	0
15	N	822	CLA	5	0
15	b	811	CLA	1	0
18	B	843	BCR	1	0

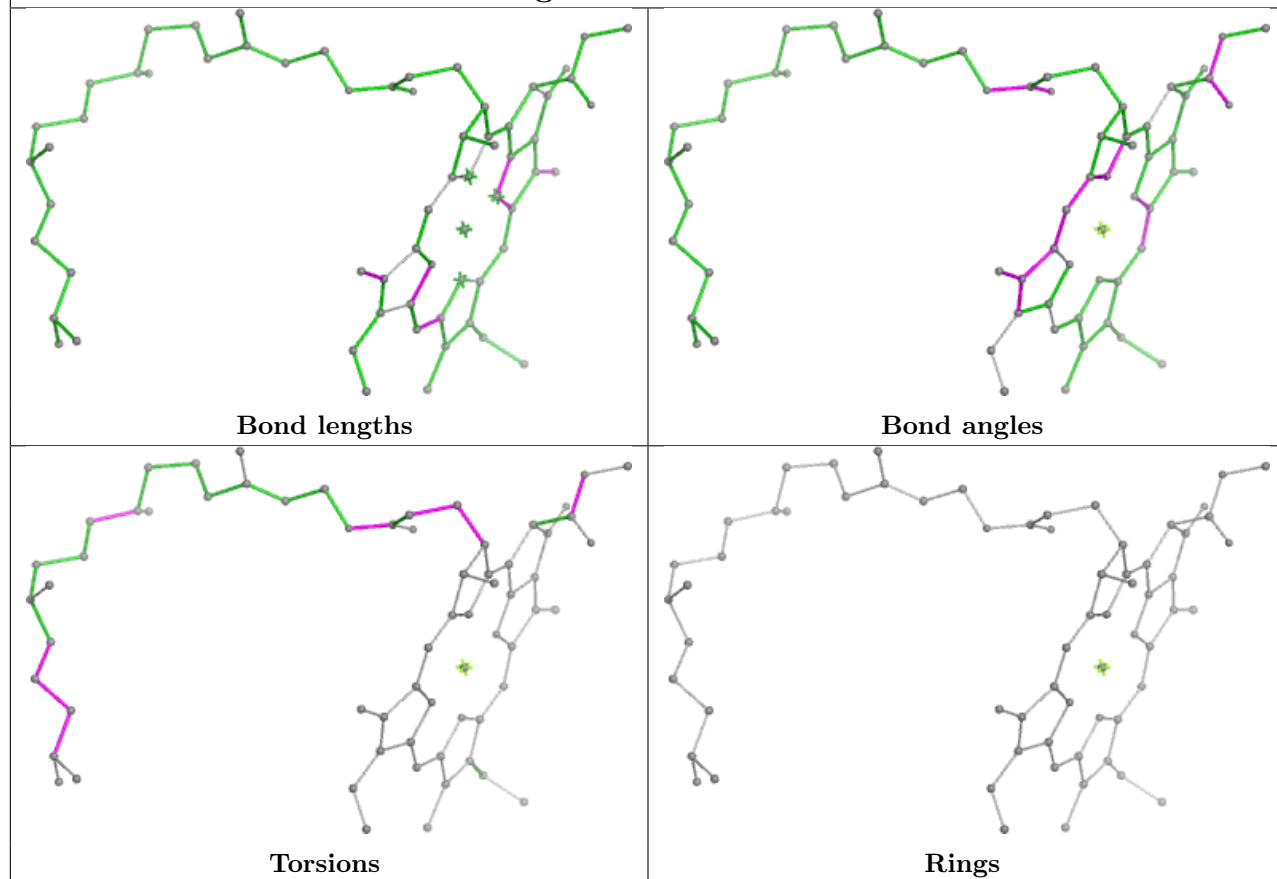
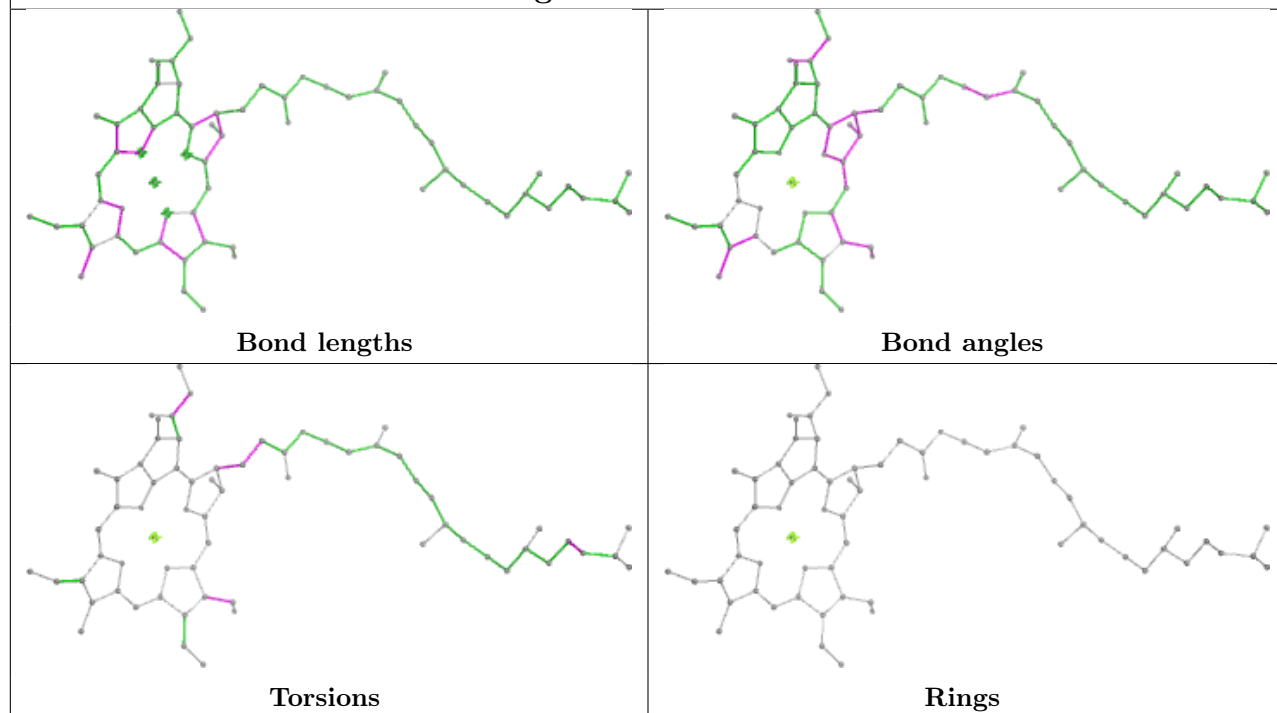
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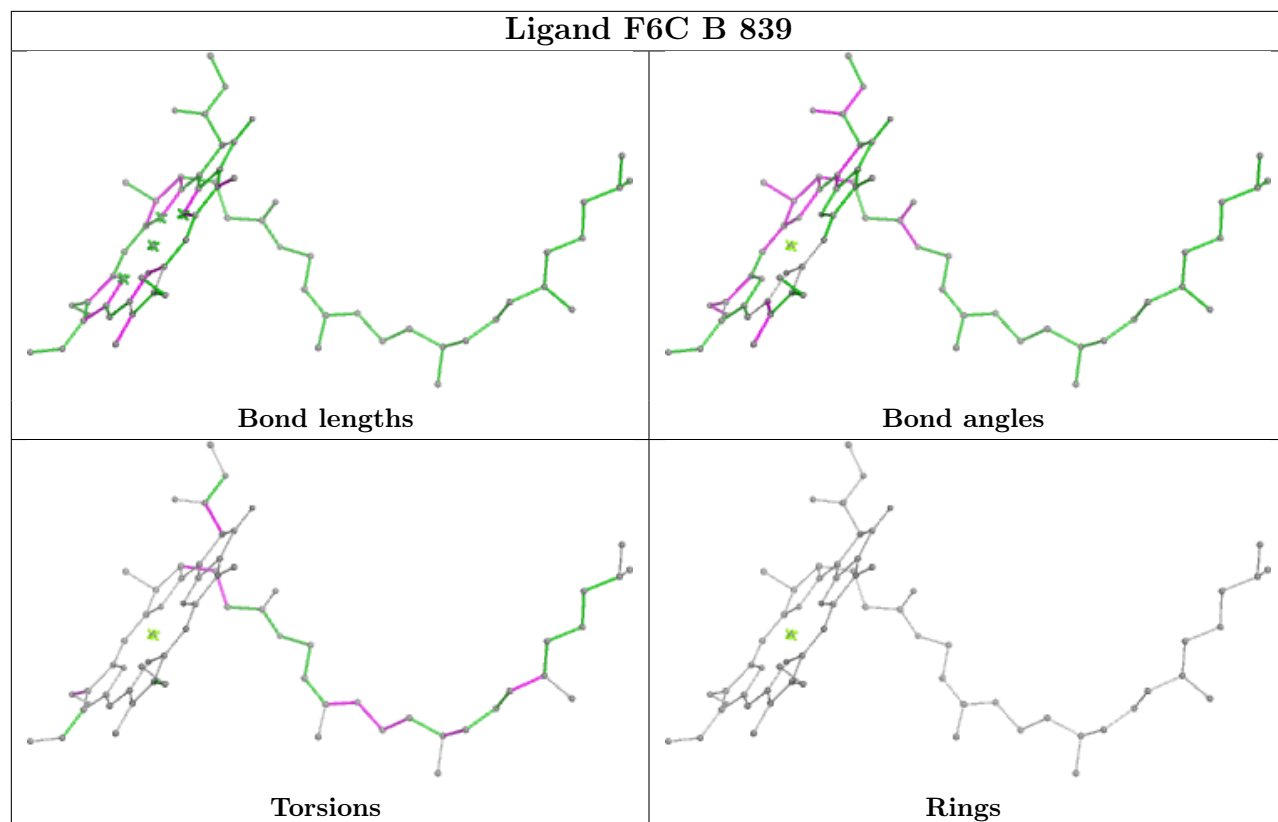
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	O	827	CLA	1	0
15	a	839	CLA	2	0
18	L	210	BCR	3	0
18	k	102	BCR	4	0
15	A	829	CLA	3	0
15	a	813	CLA	2	0
15	A	803	CLA	7	0
15	b	816	CLA	3	0
18	N	847	BCR	2	0
15	A	839	CLA	2	0
15	O	830	CLA	5	0
15	f	201	CLA	2	0
20	a	852	LMT	1	0

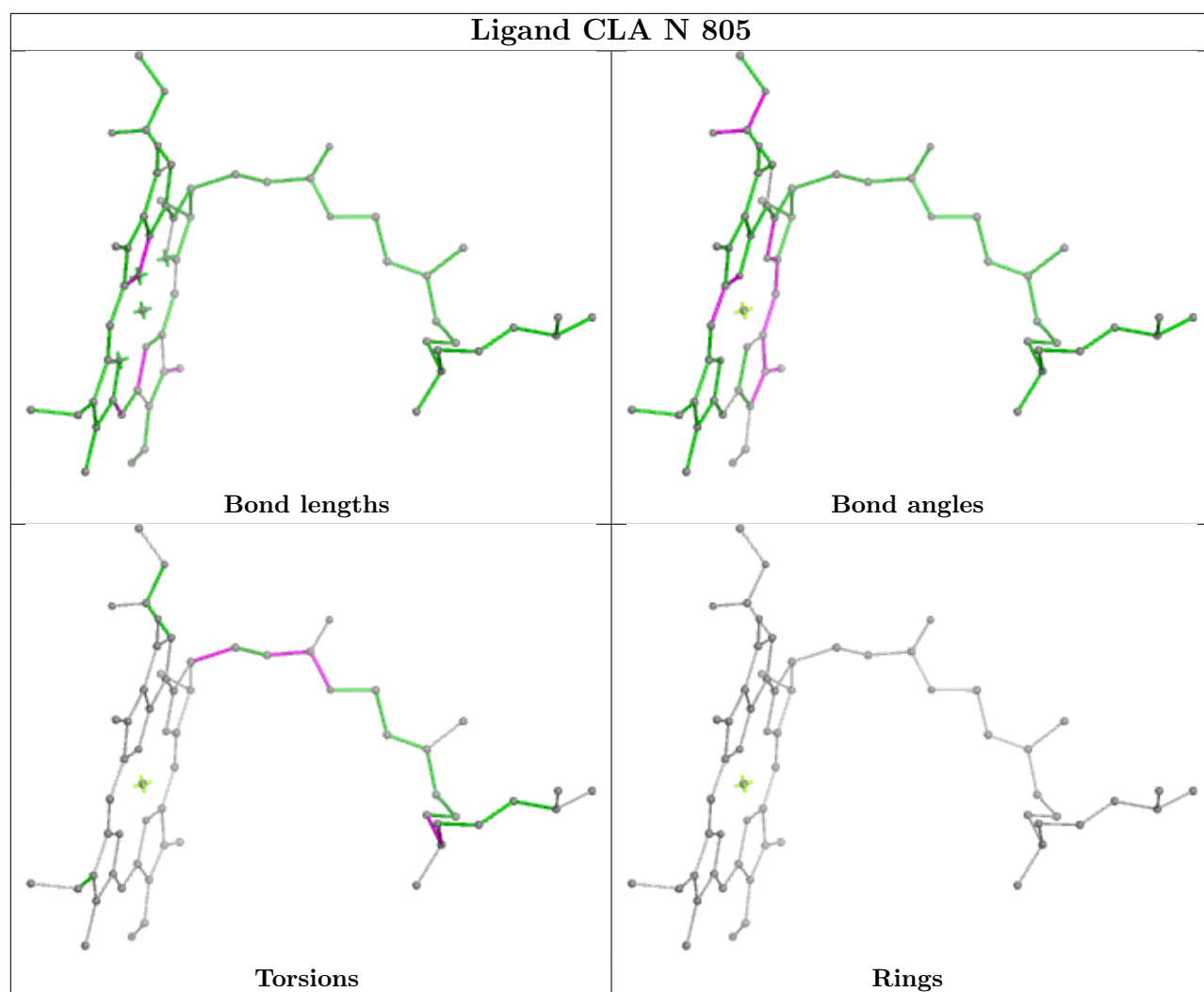
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



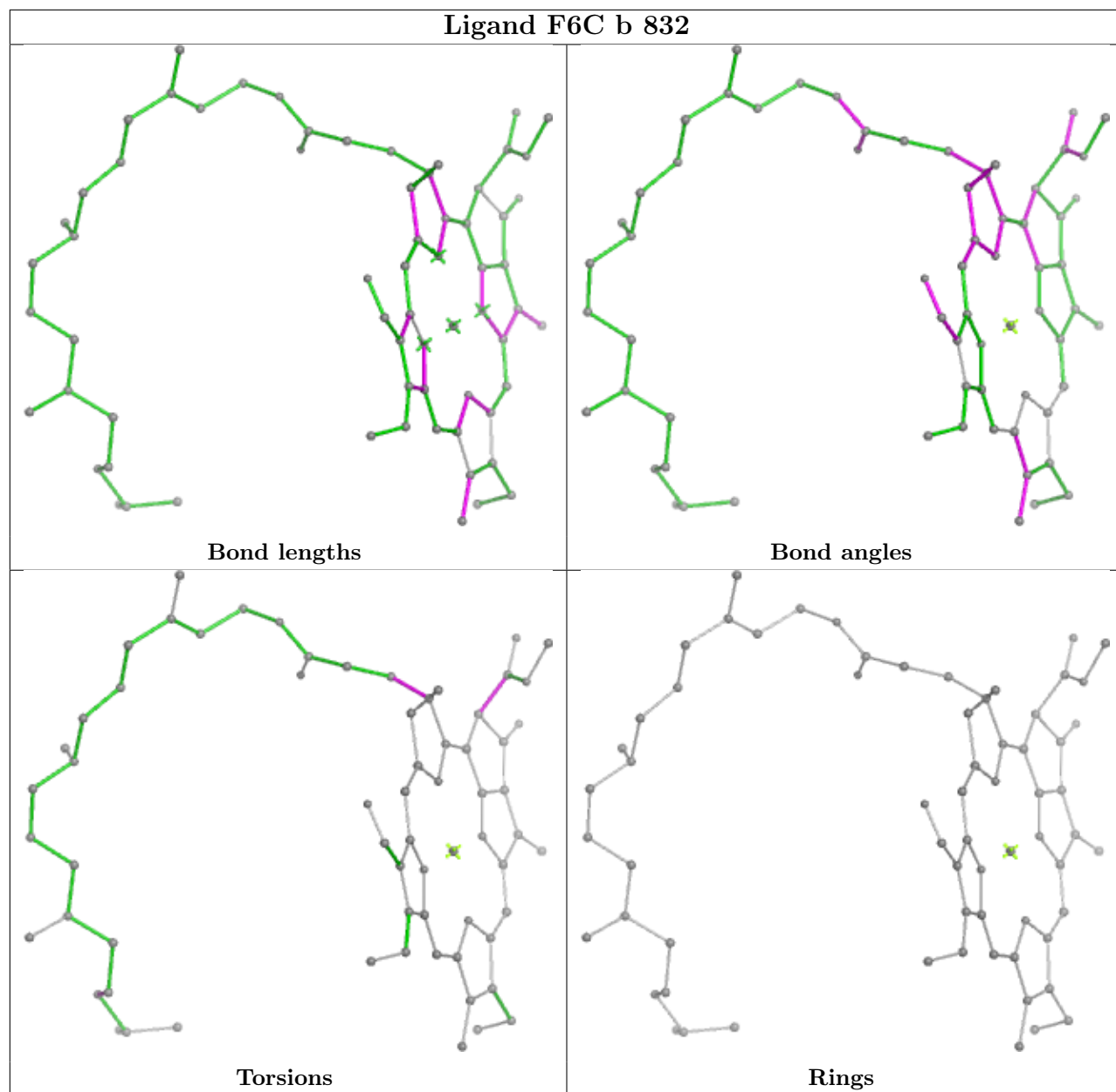
**Ligand CLA a 842****Ligand F6C A 802**

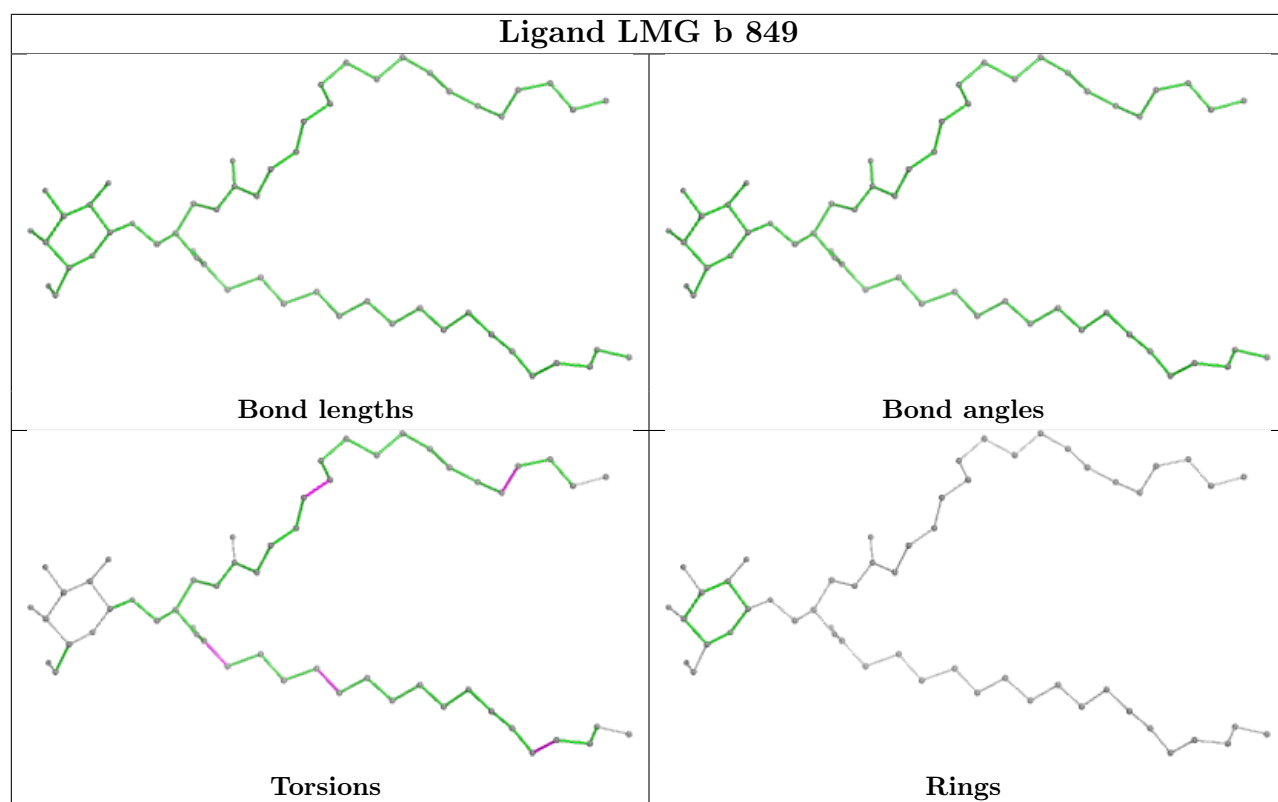




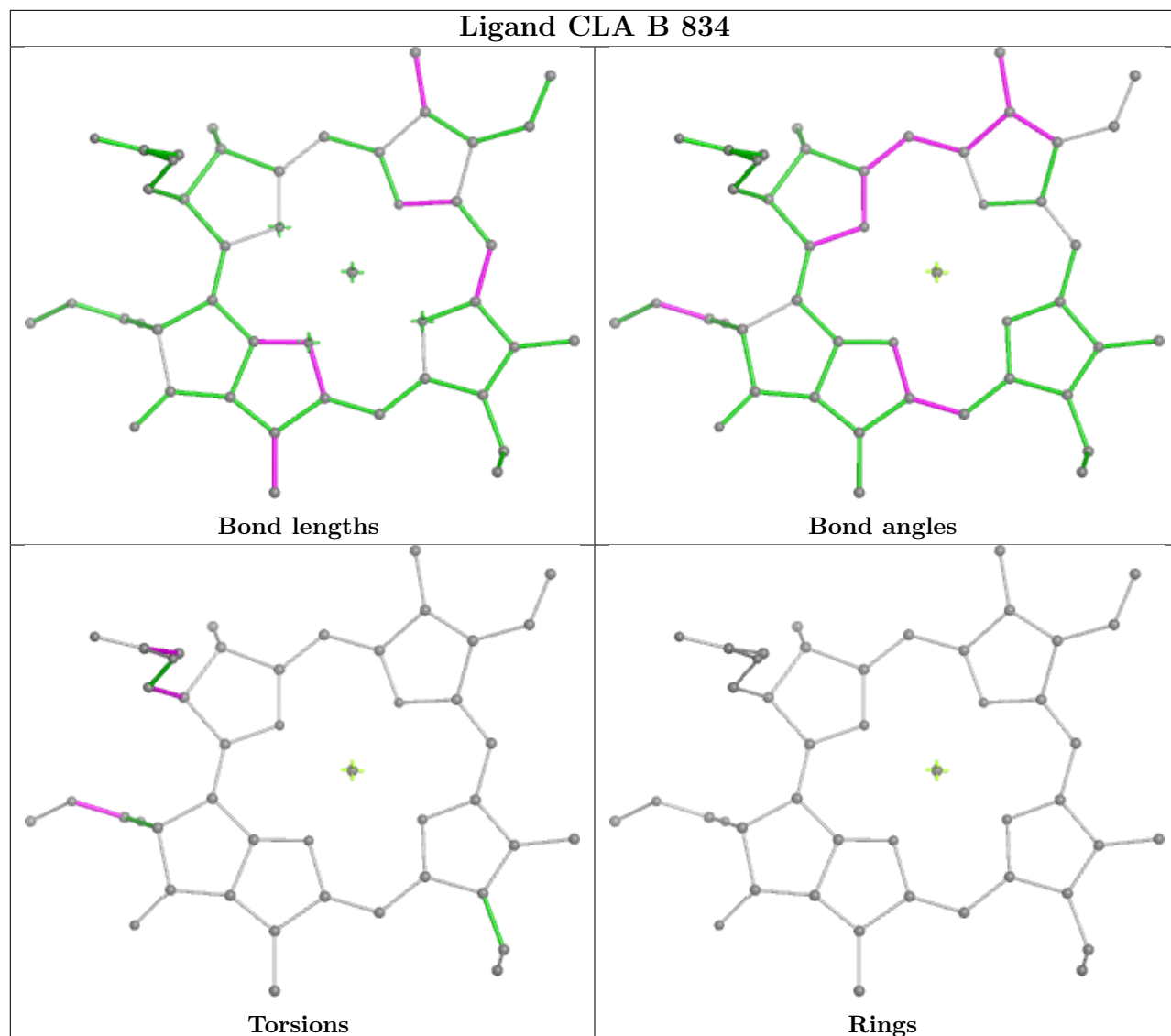


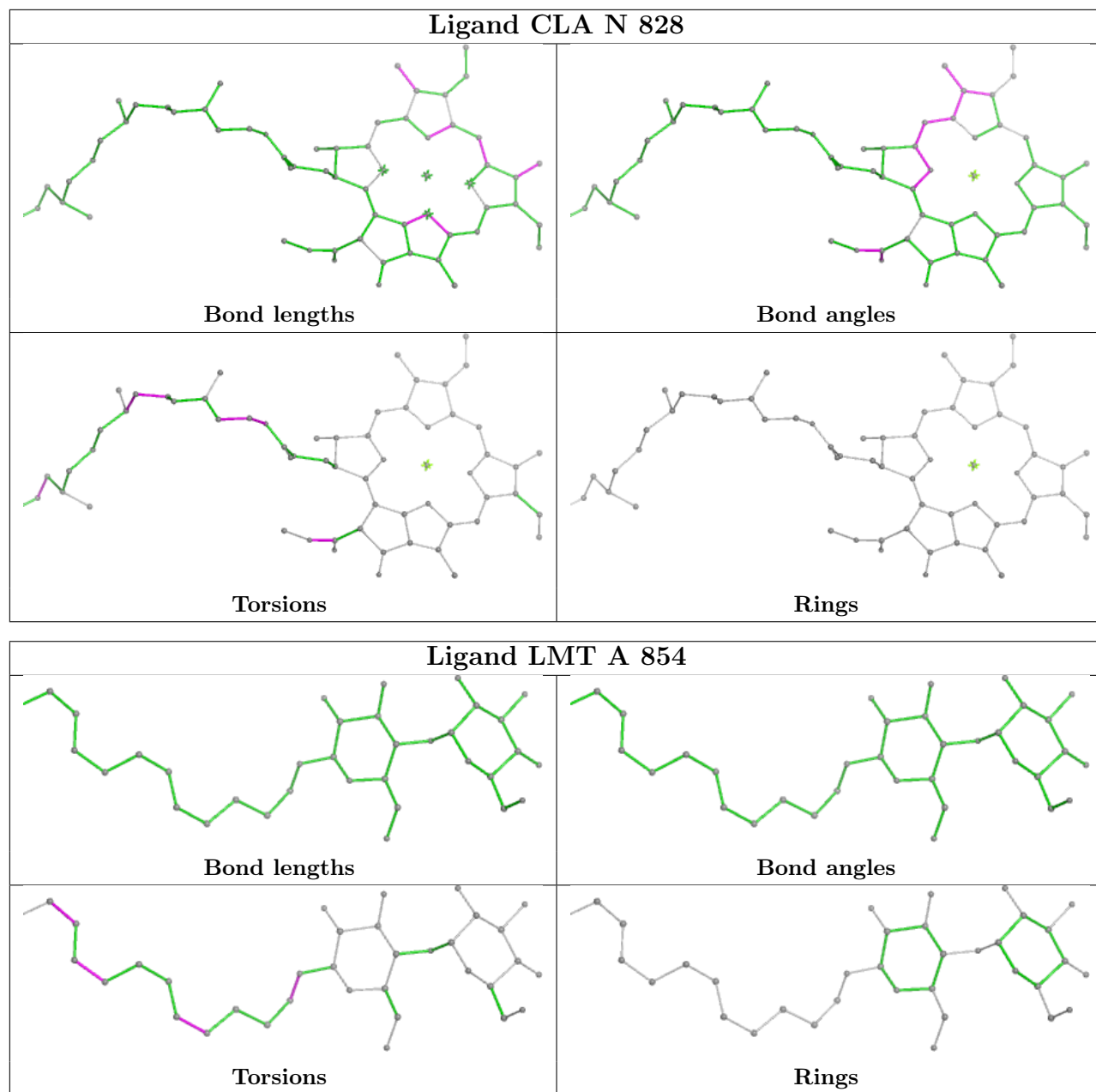
## Ligand F6C b 832



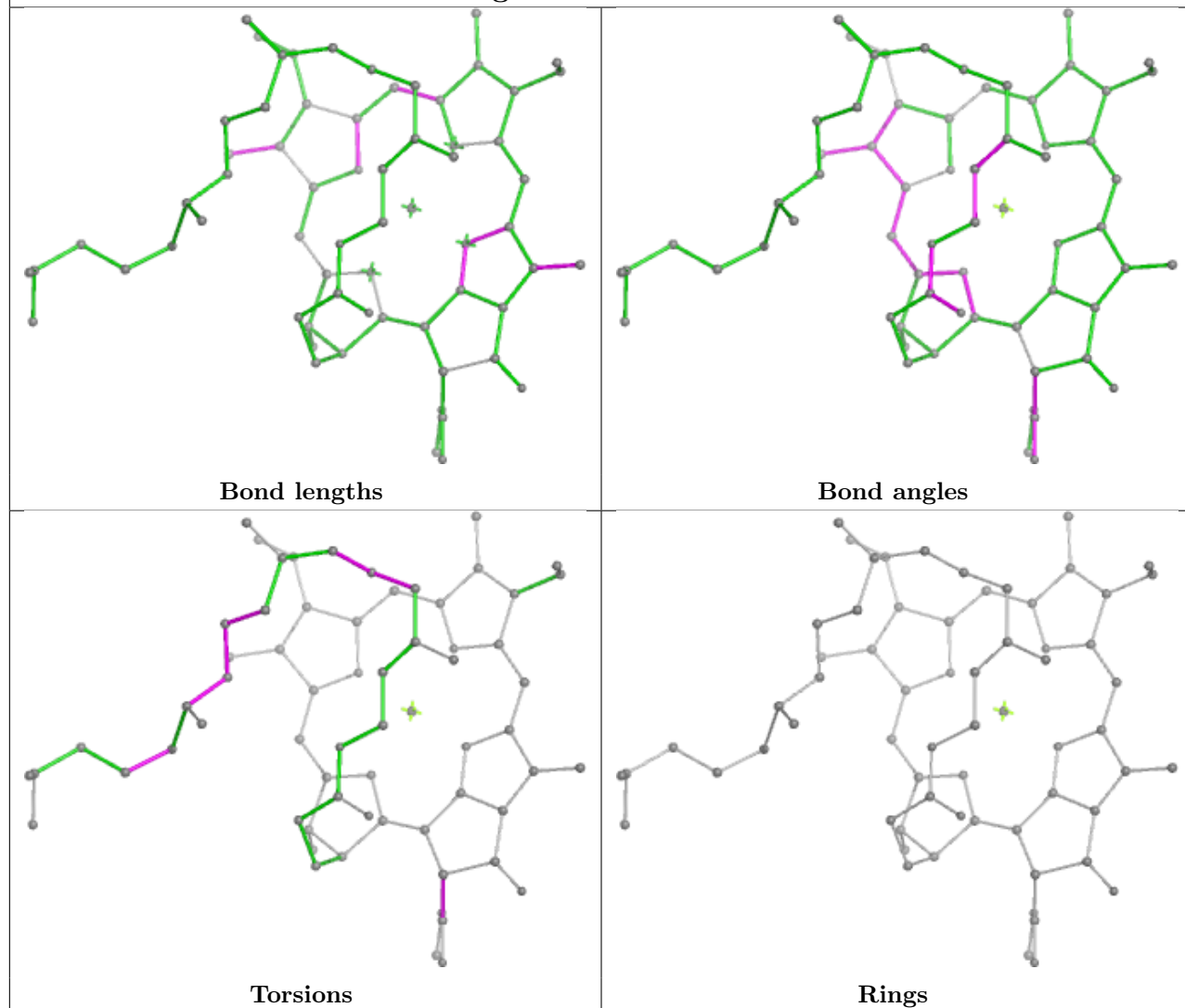


## Ligand CLA B 834

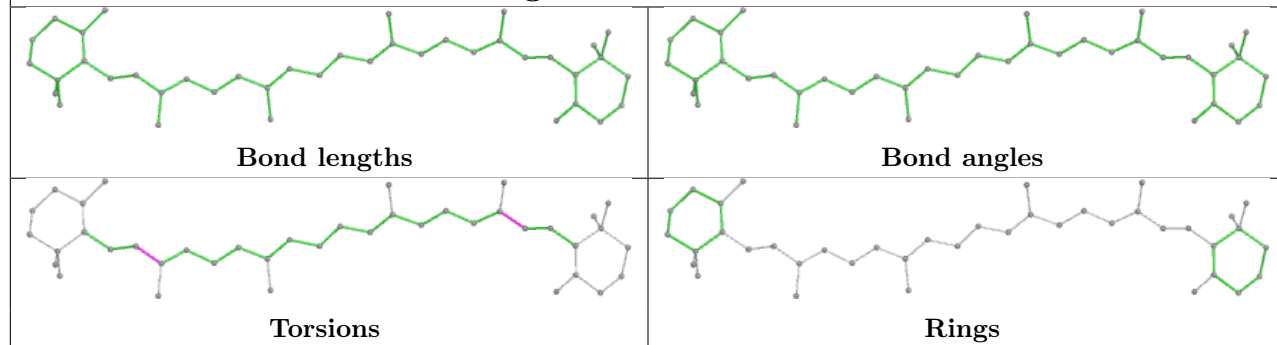


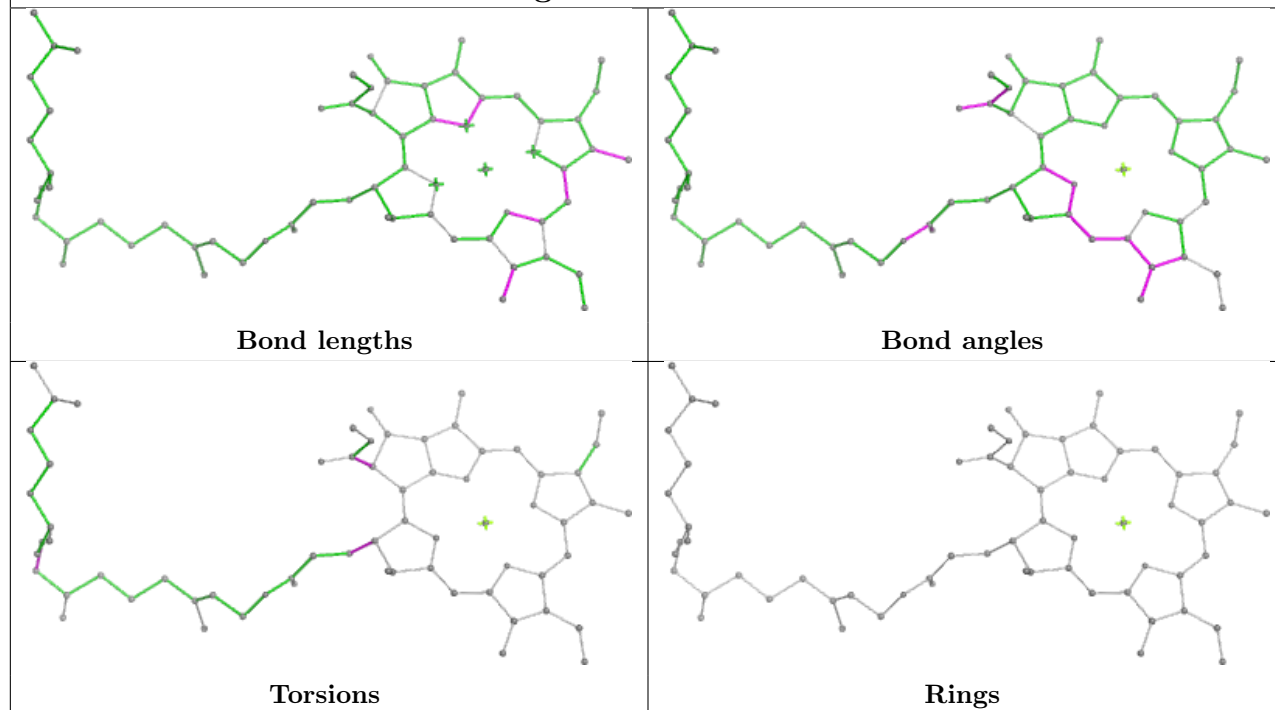
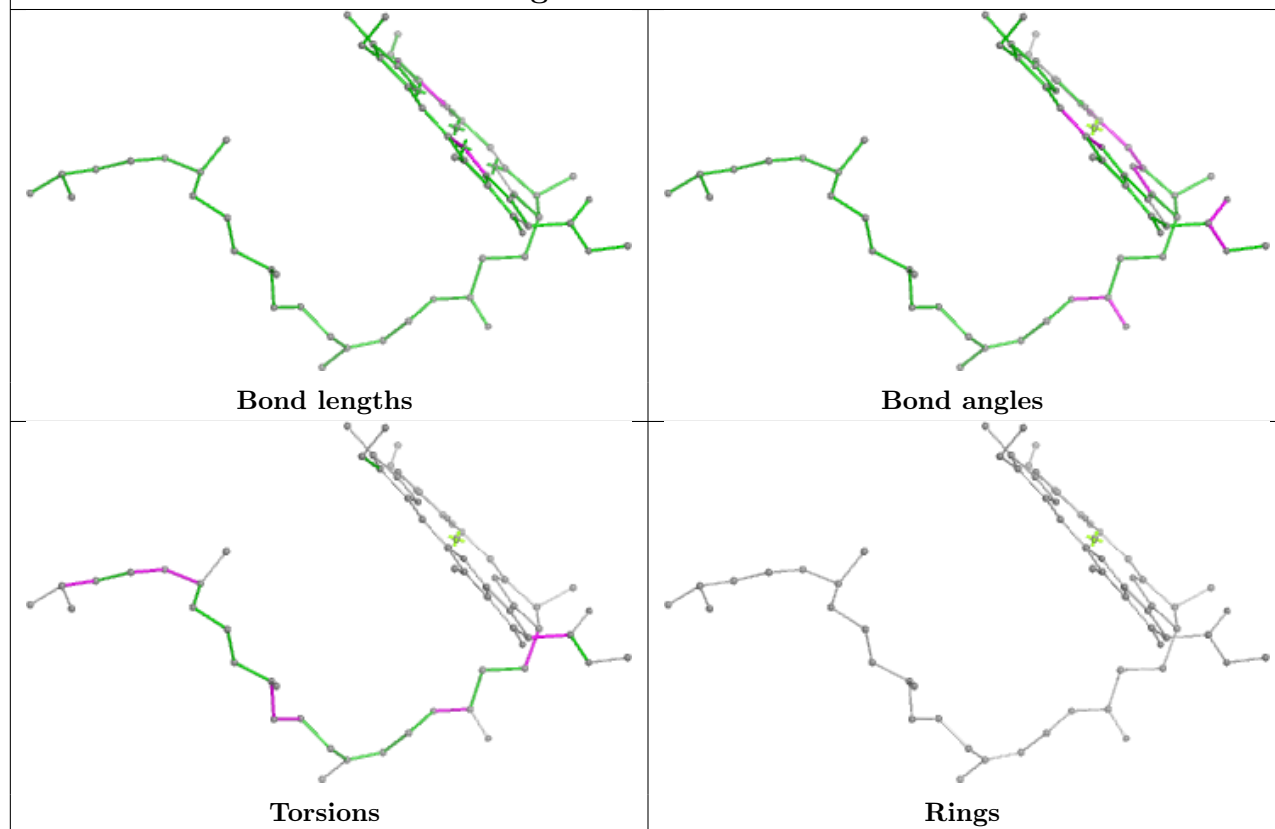


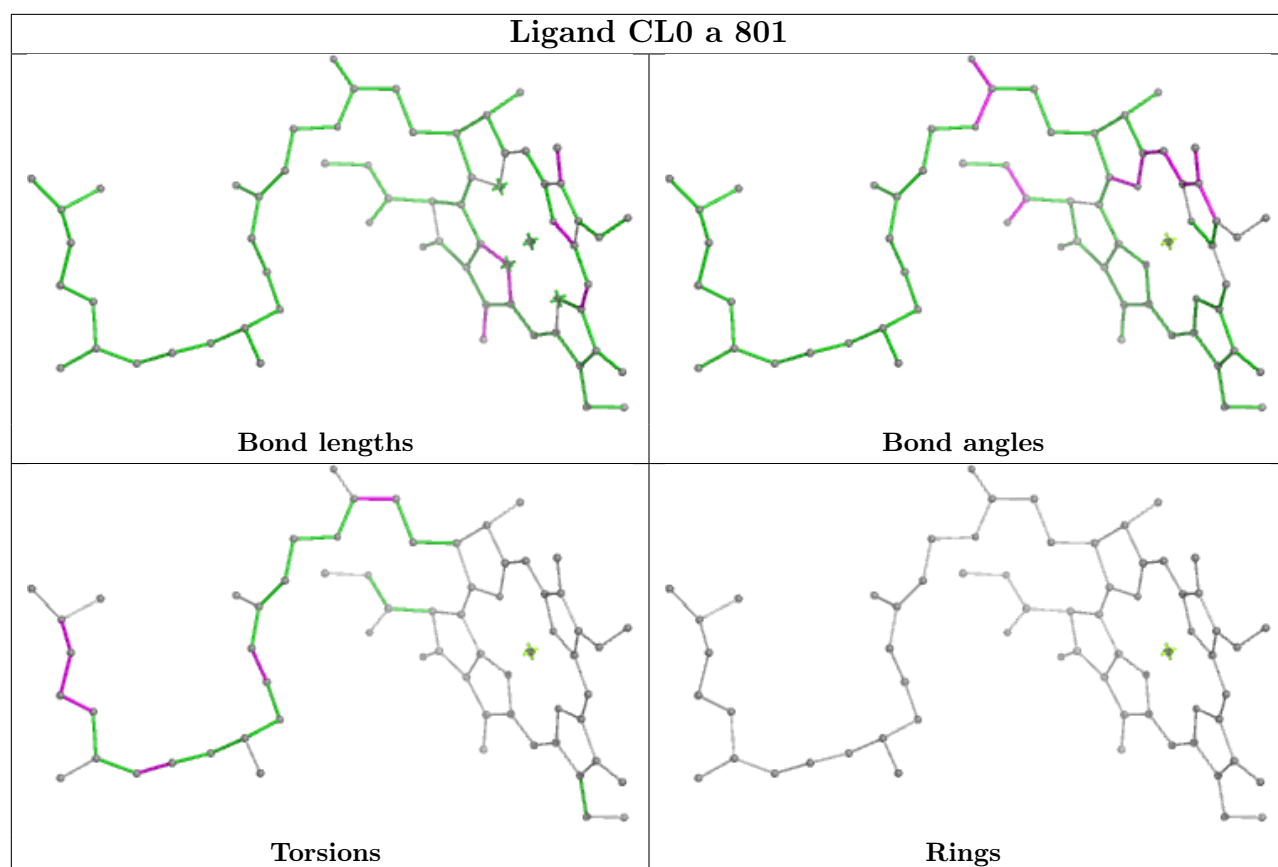
## Ligand CLA O 808



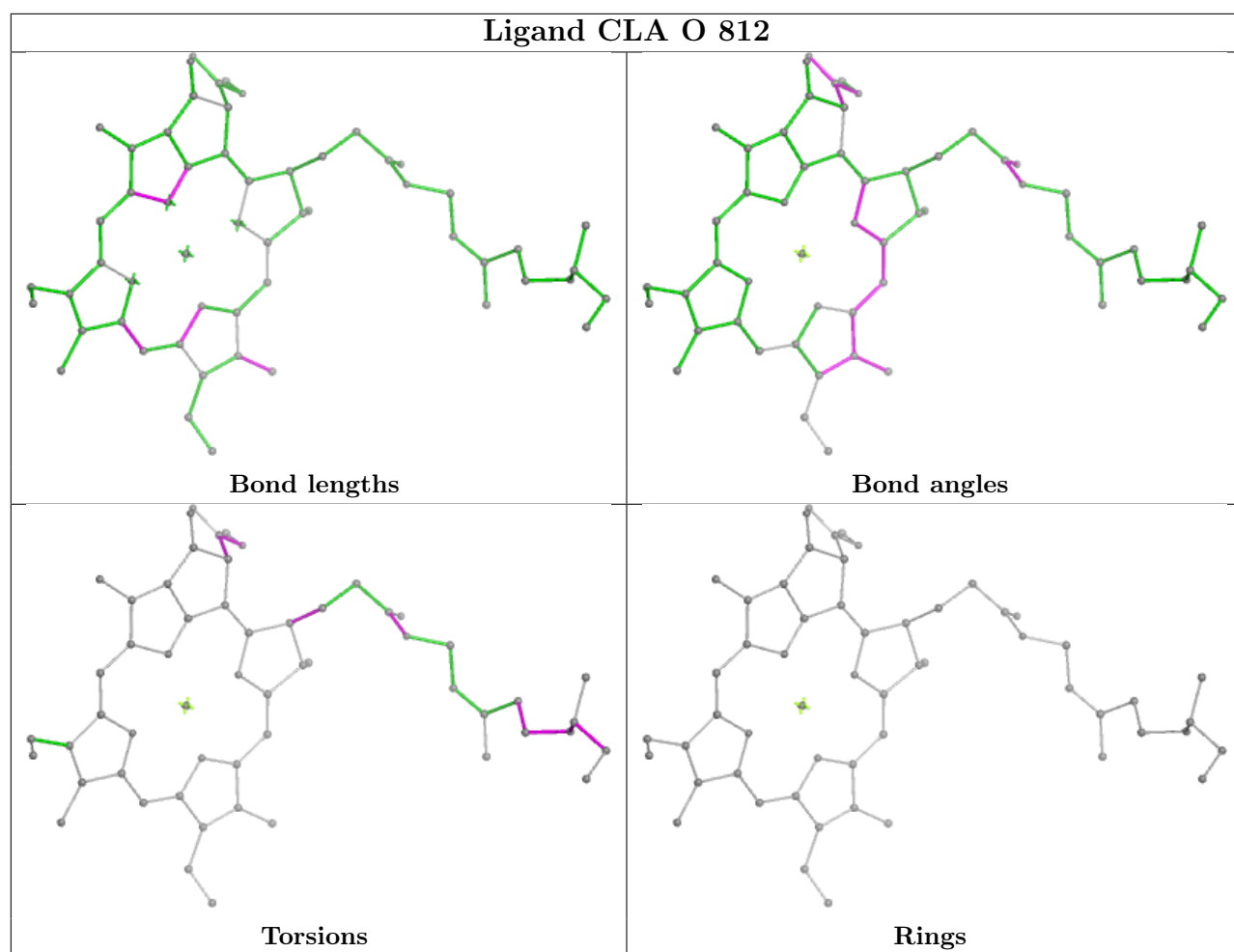
## Ligand BCR W 205



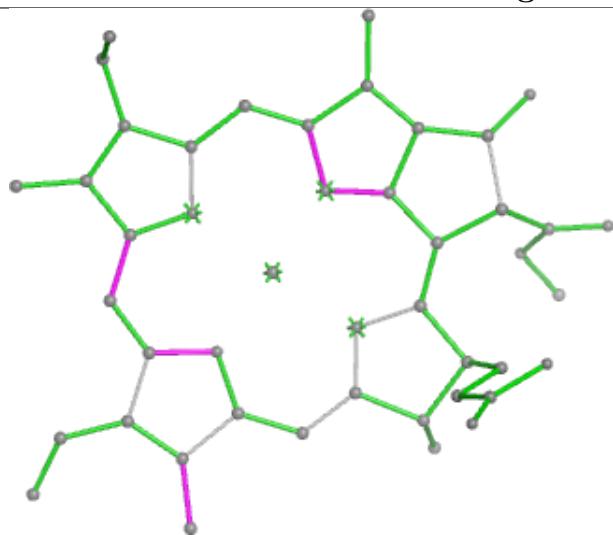
**Ligand CLA b 825****Ligand CLA O 810**



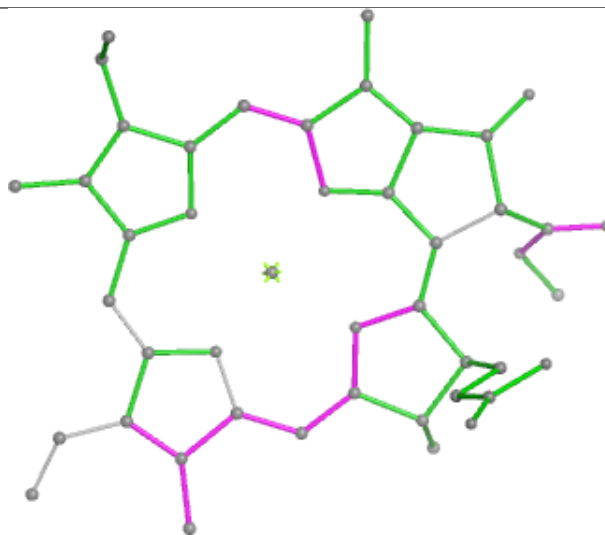




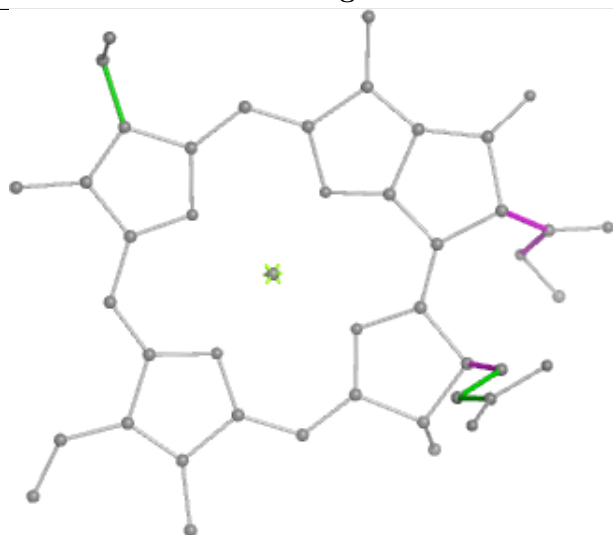
## Ligand CLA b 814



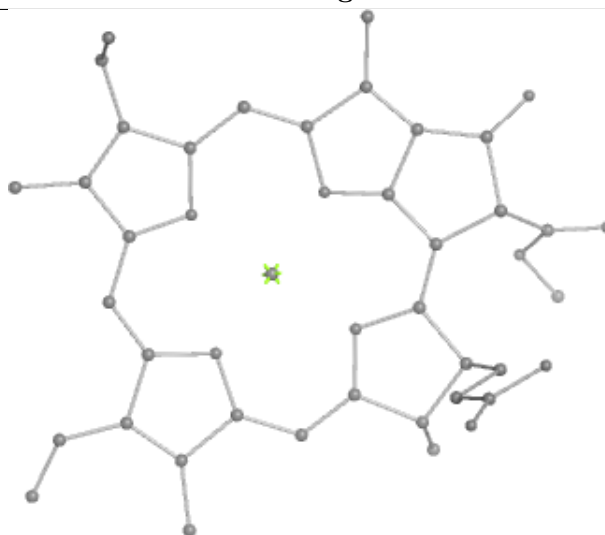
Bond lengths



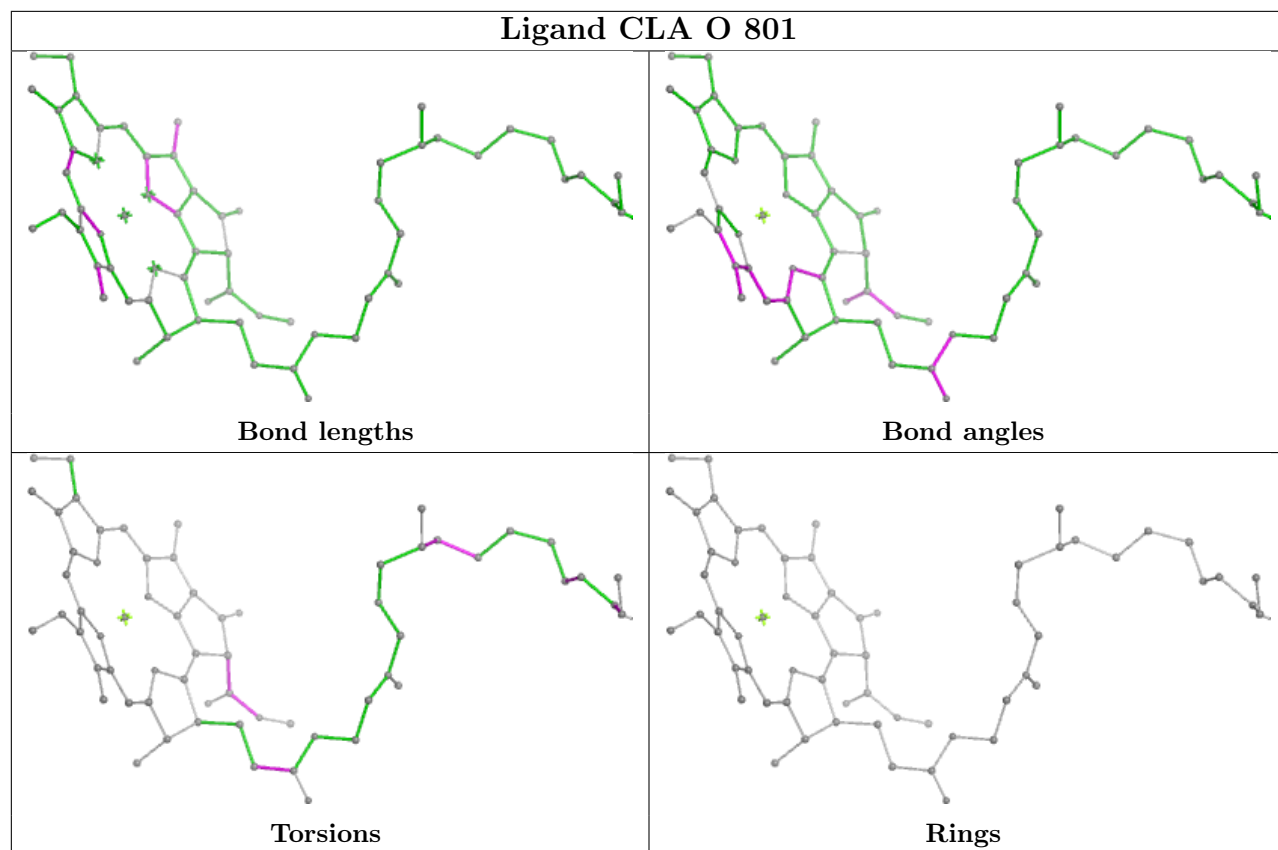
Bond angles

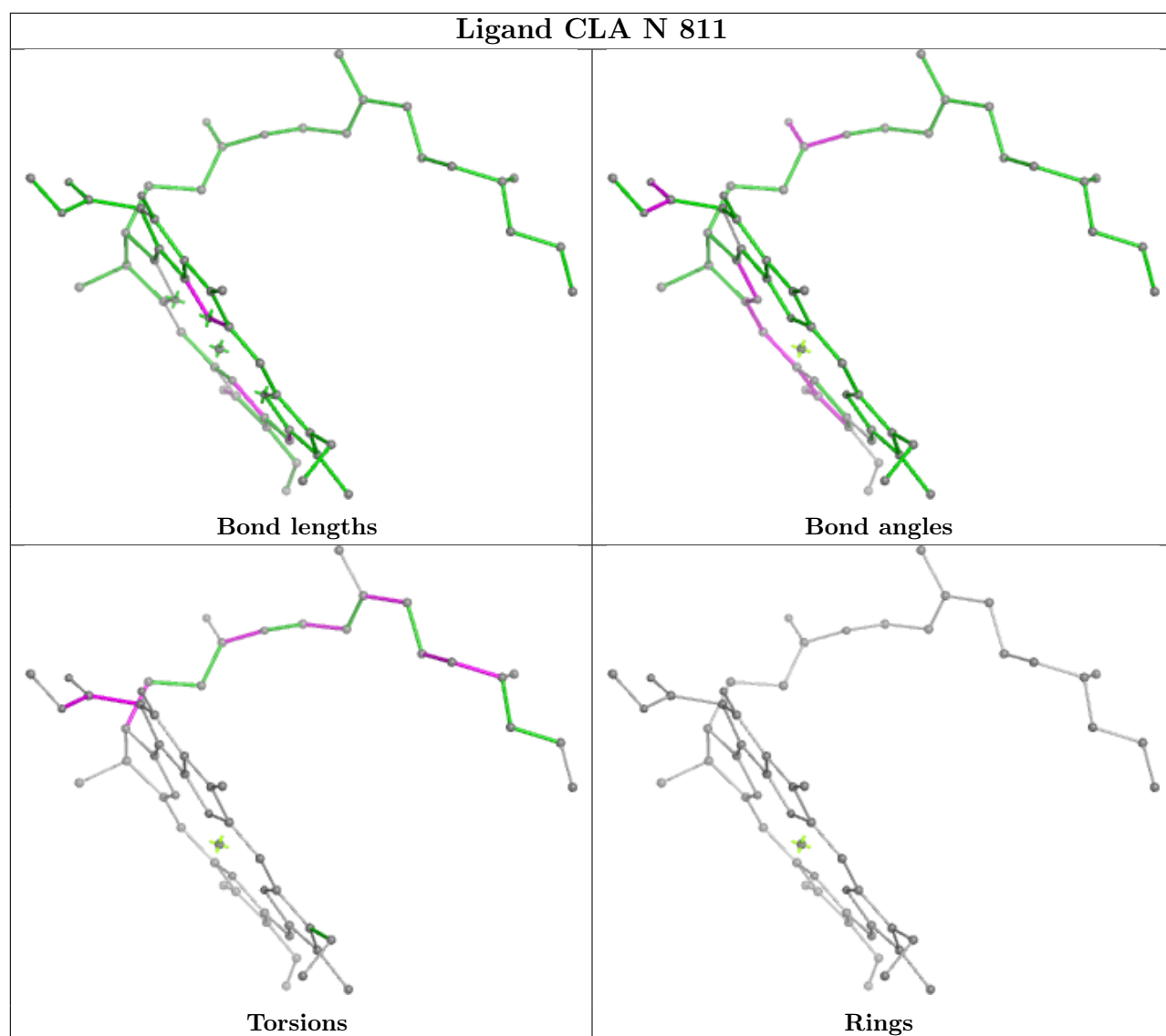


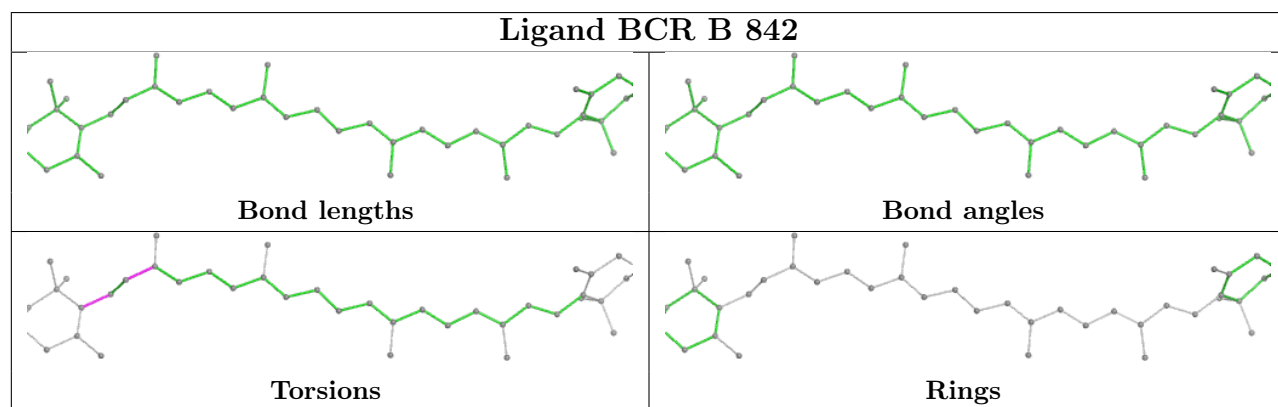
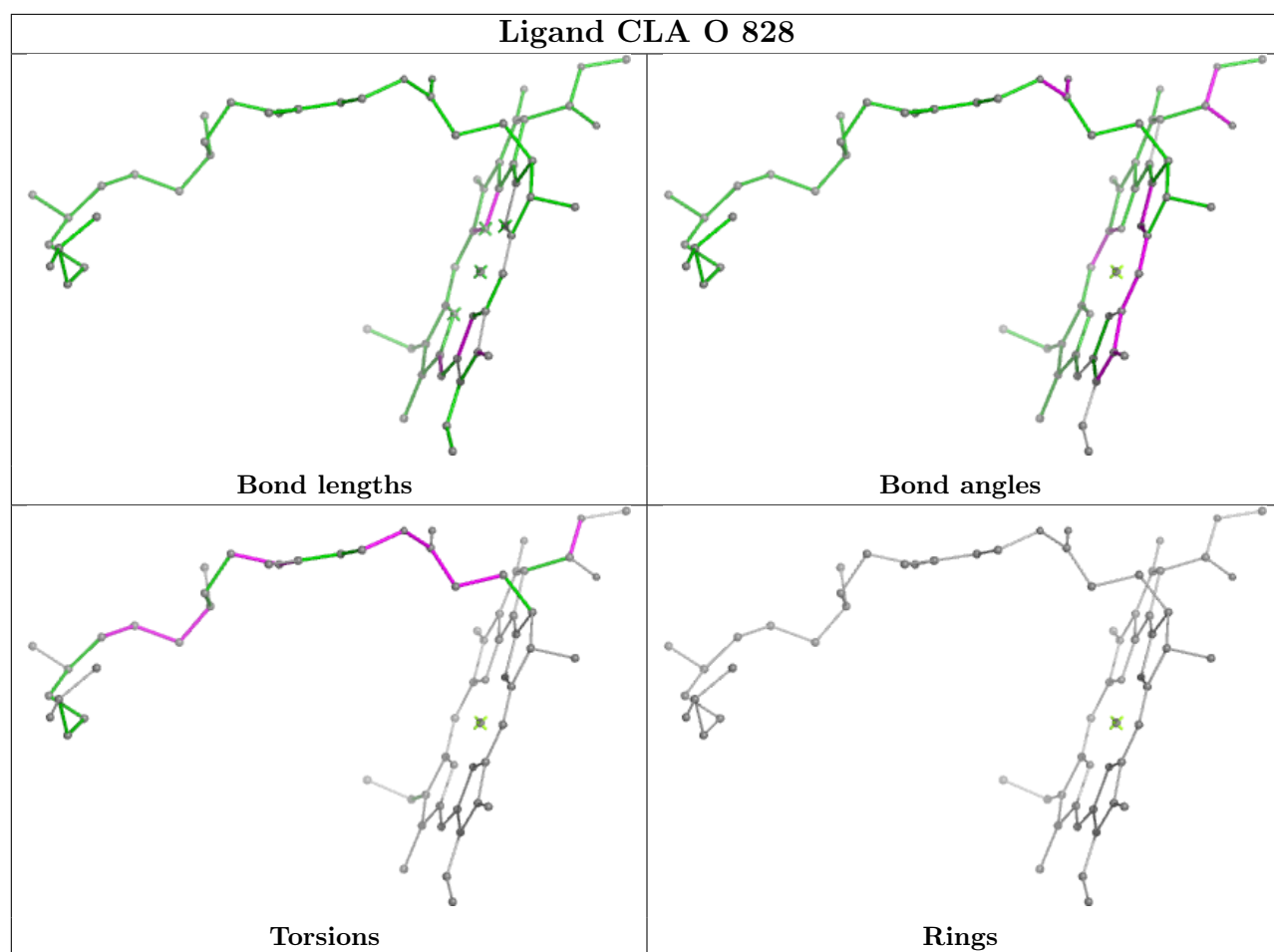
Torsions

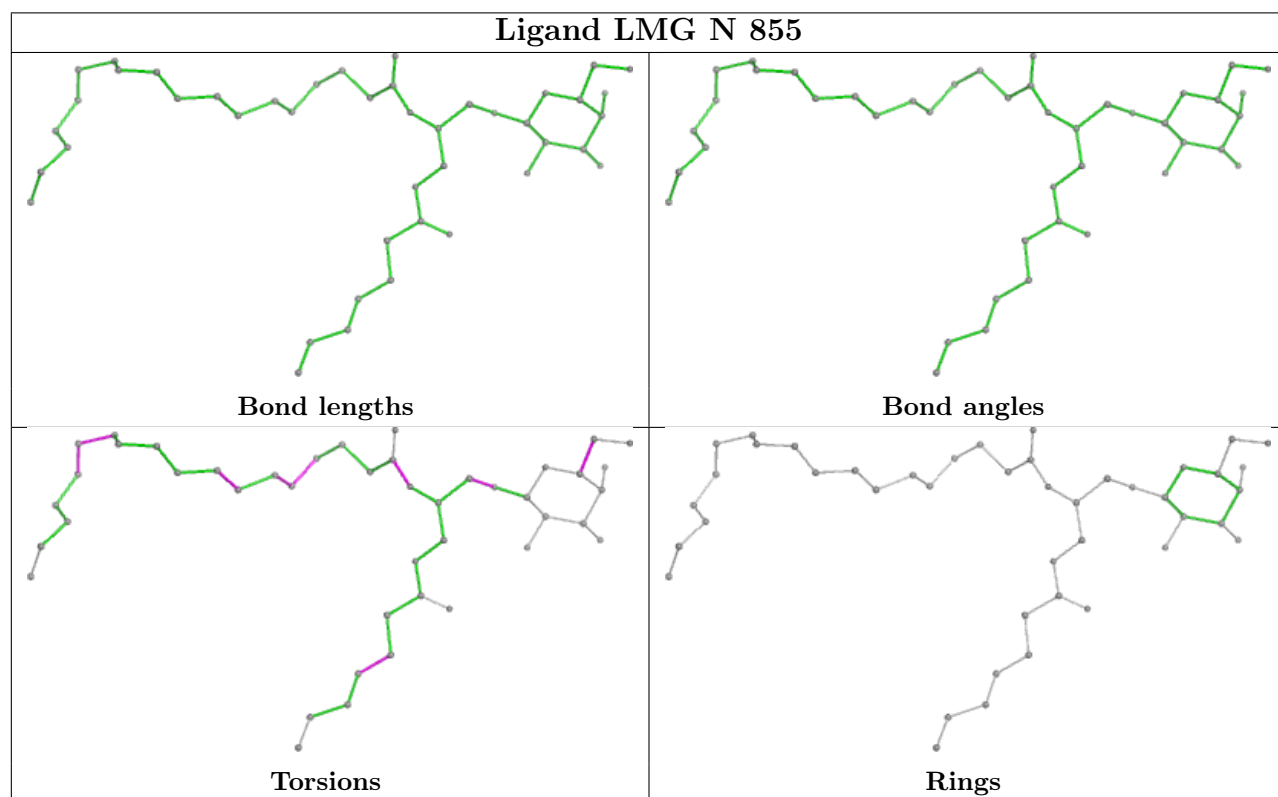
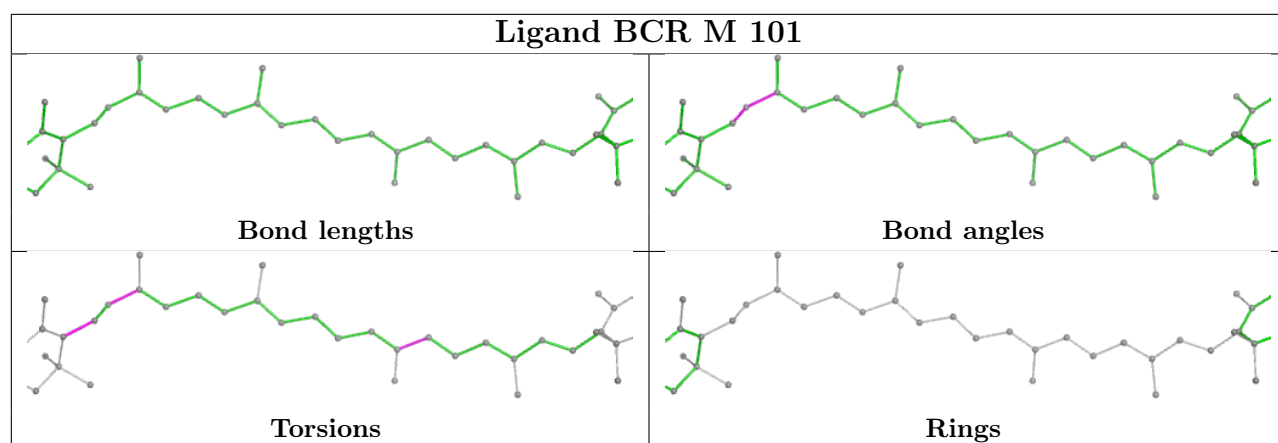


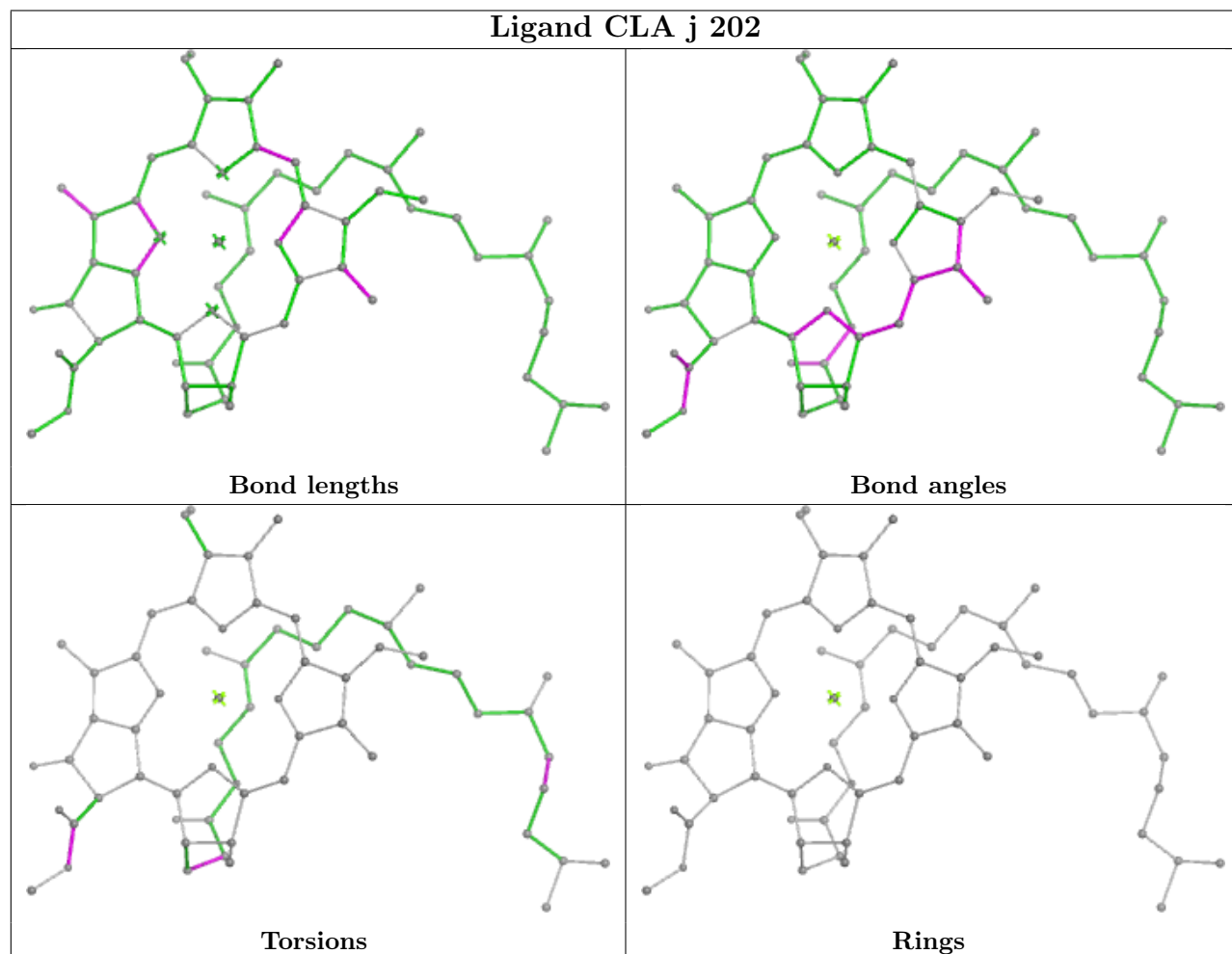
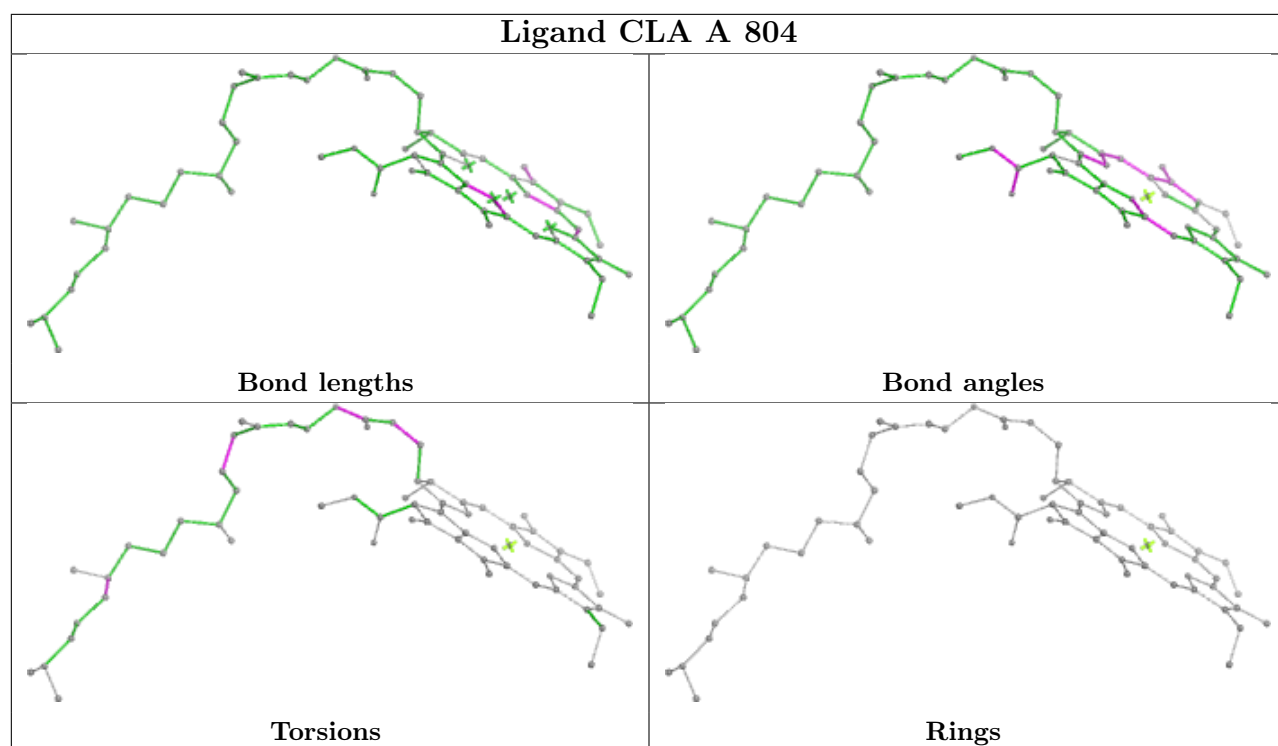
Rings



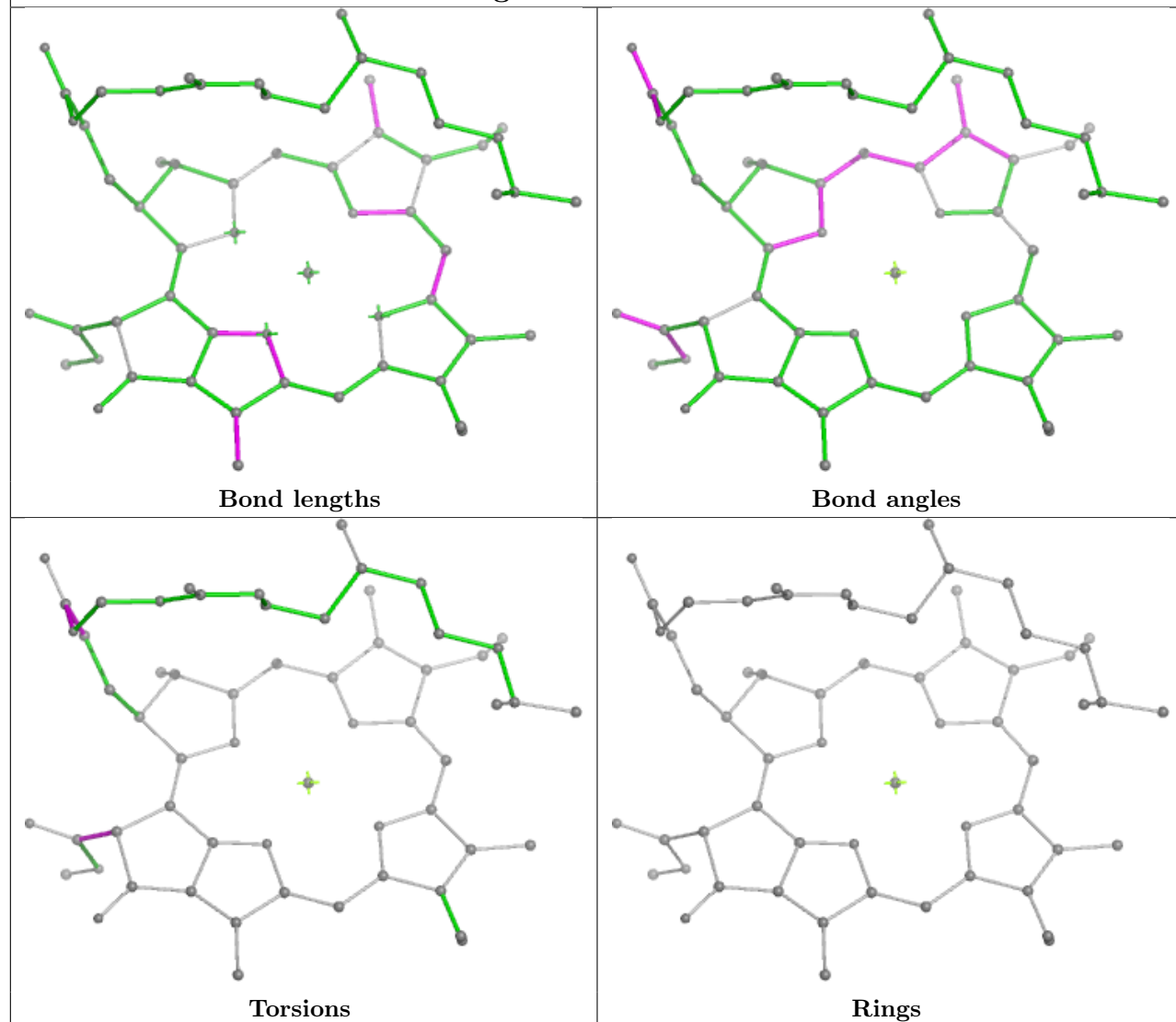




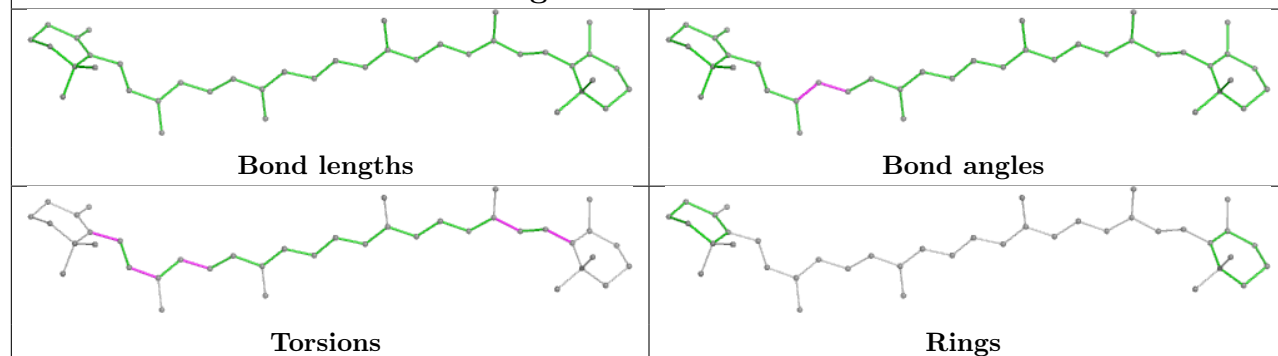




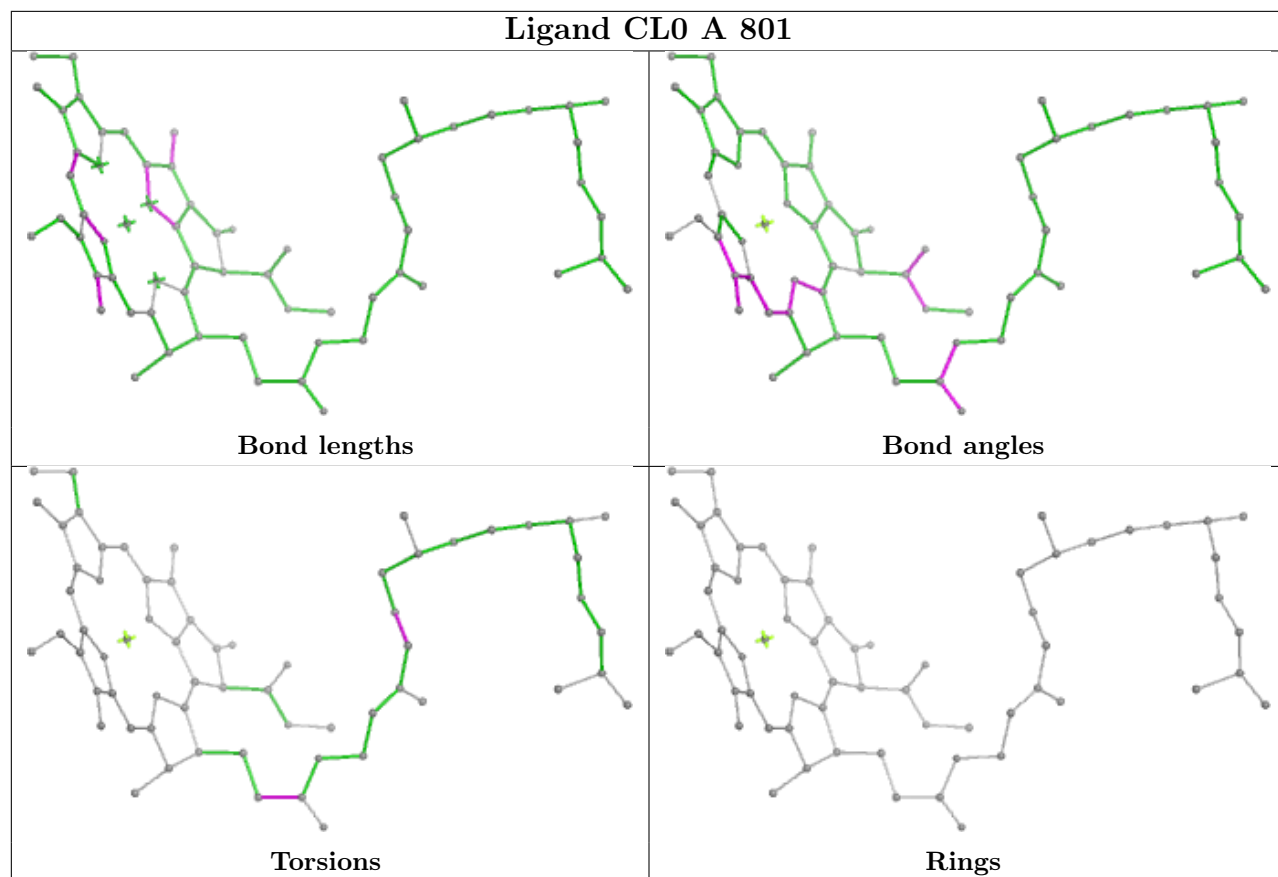
## Ligand CLA a 821



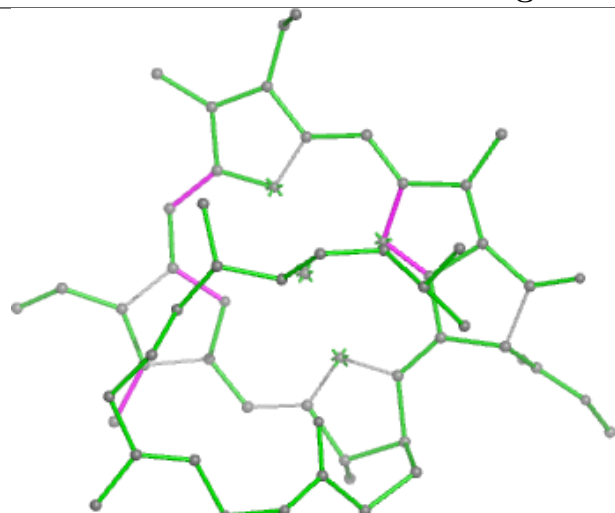
## Ligand BCR A 846



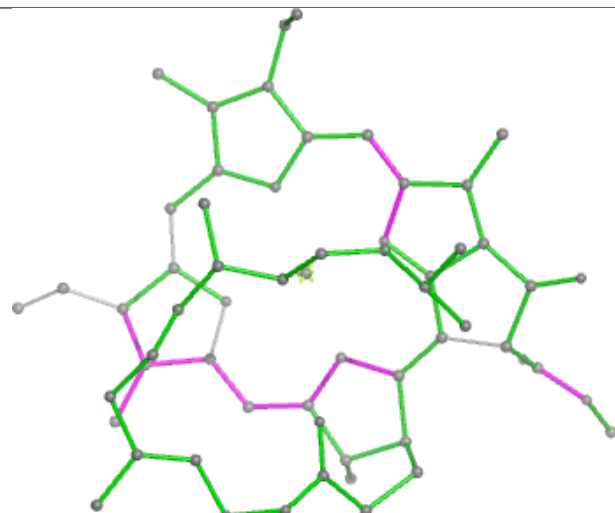




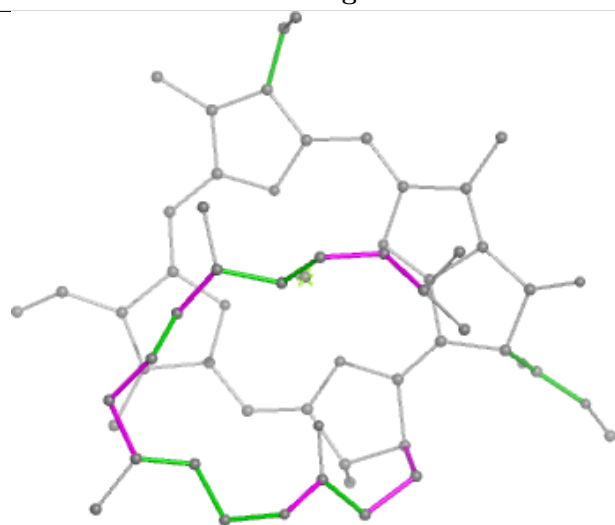
## Ligand CLA B 817



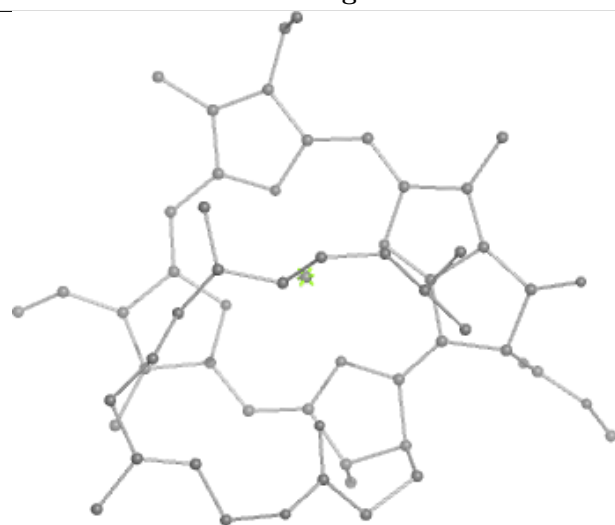
Bond lengths



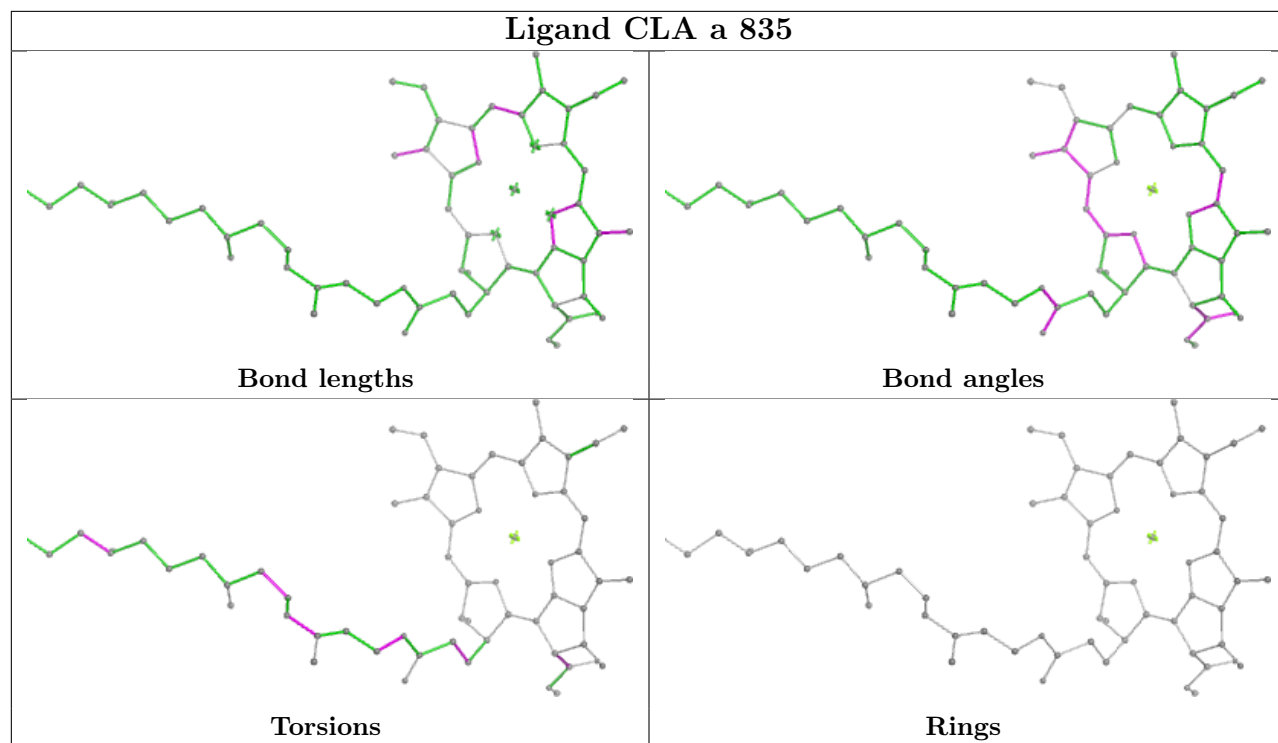
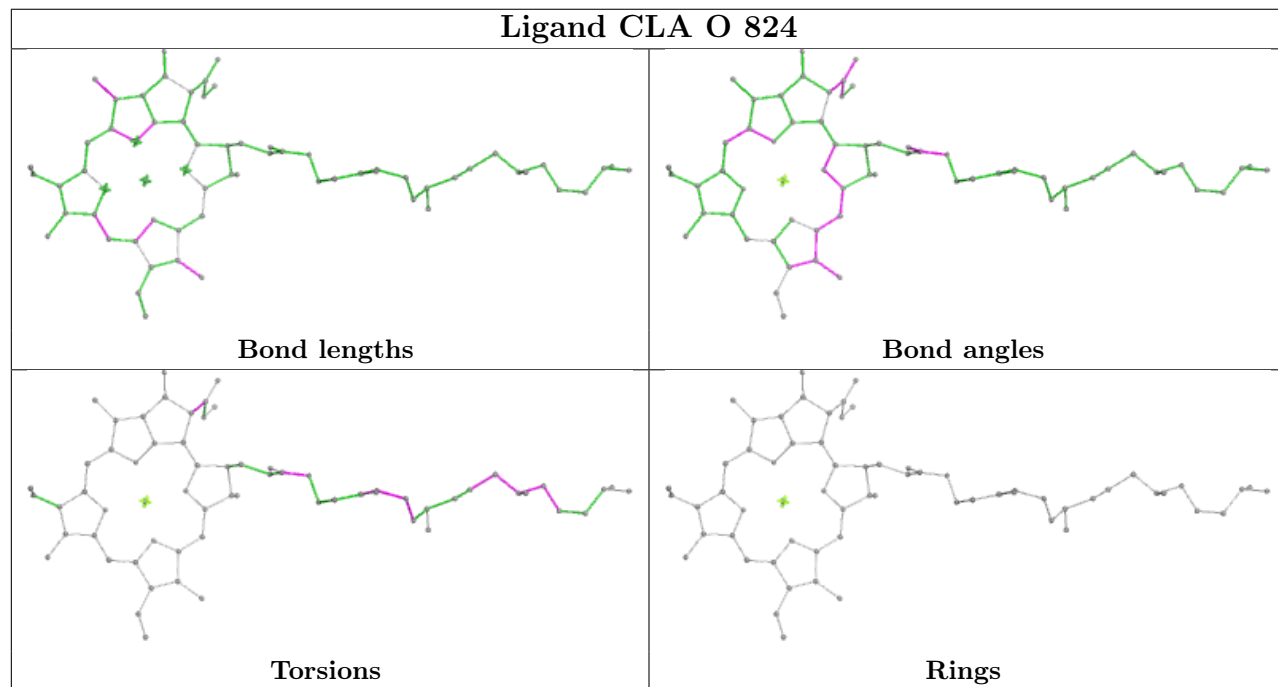
Bond angles

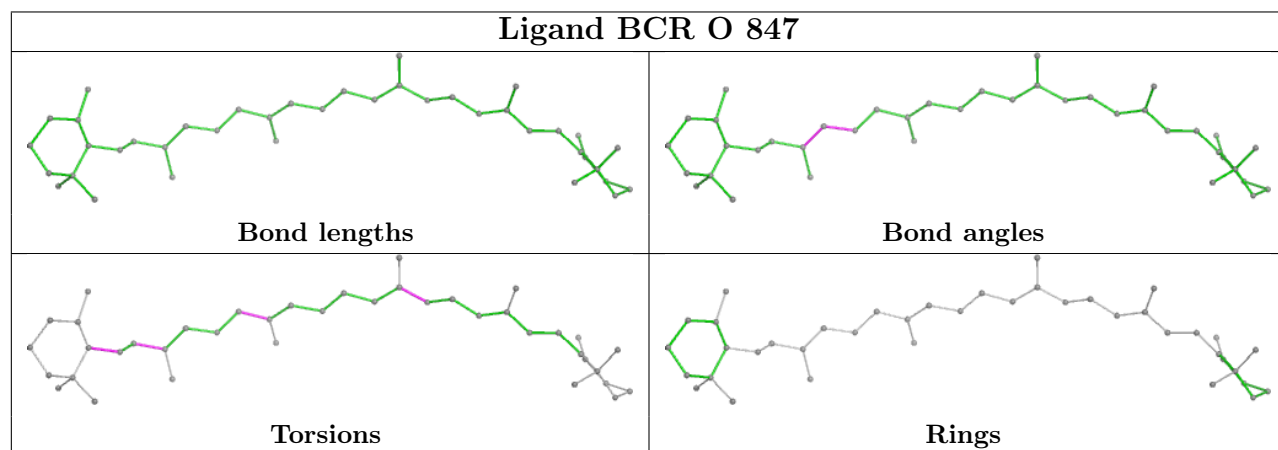
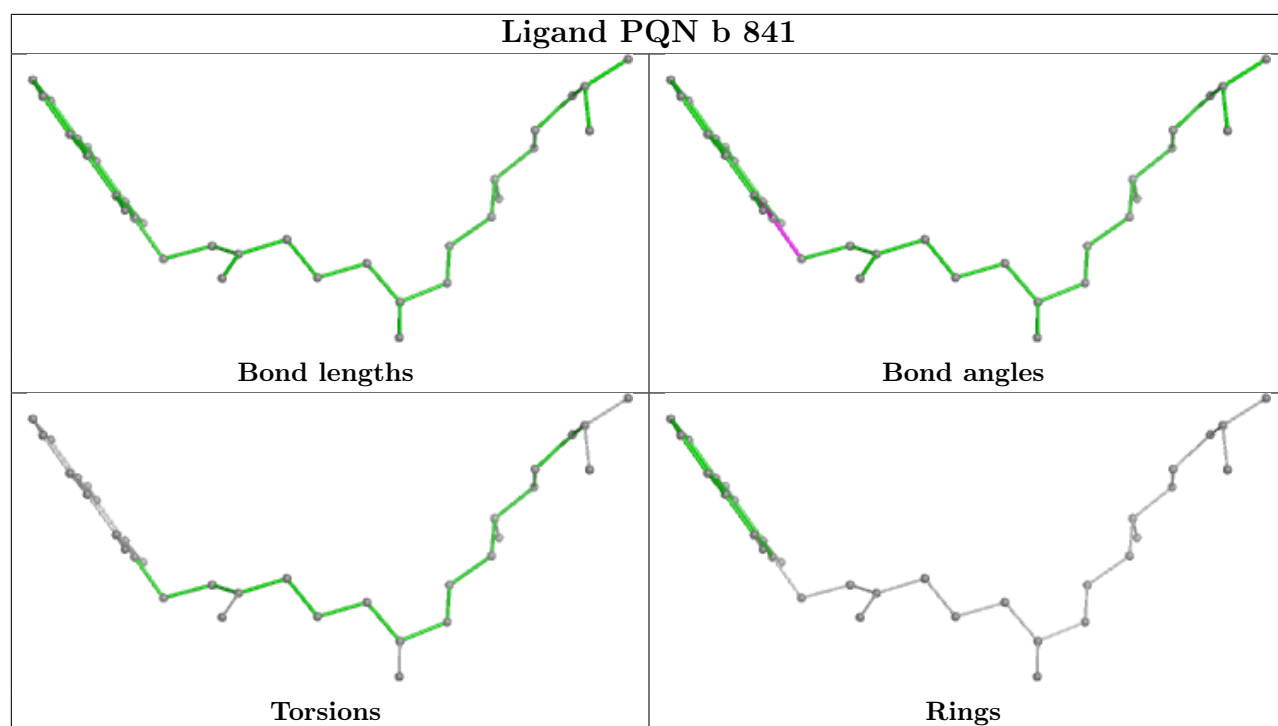


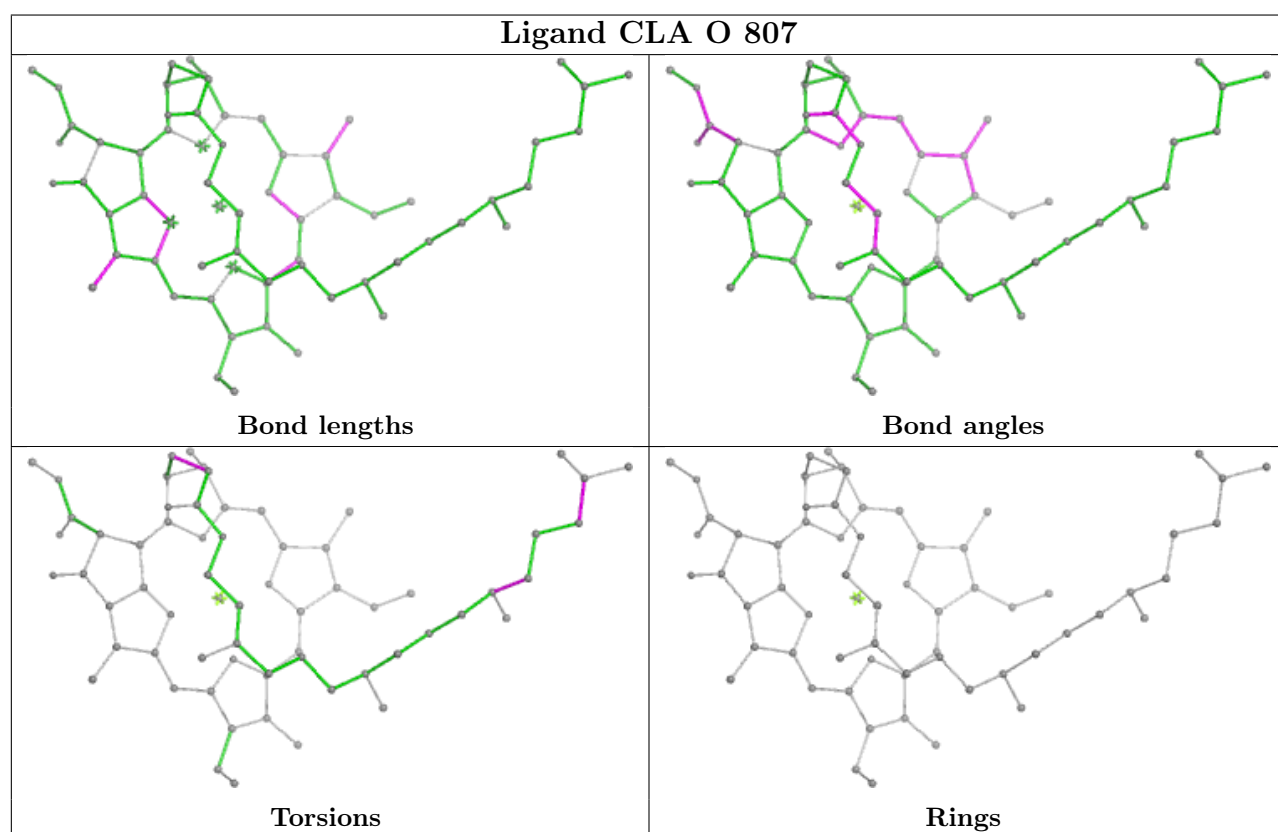
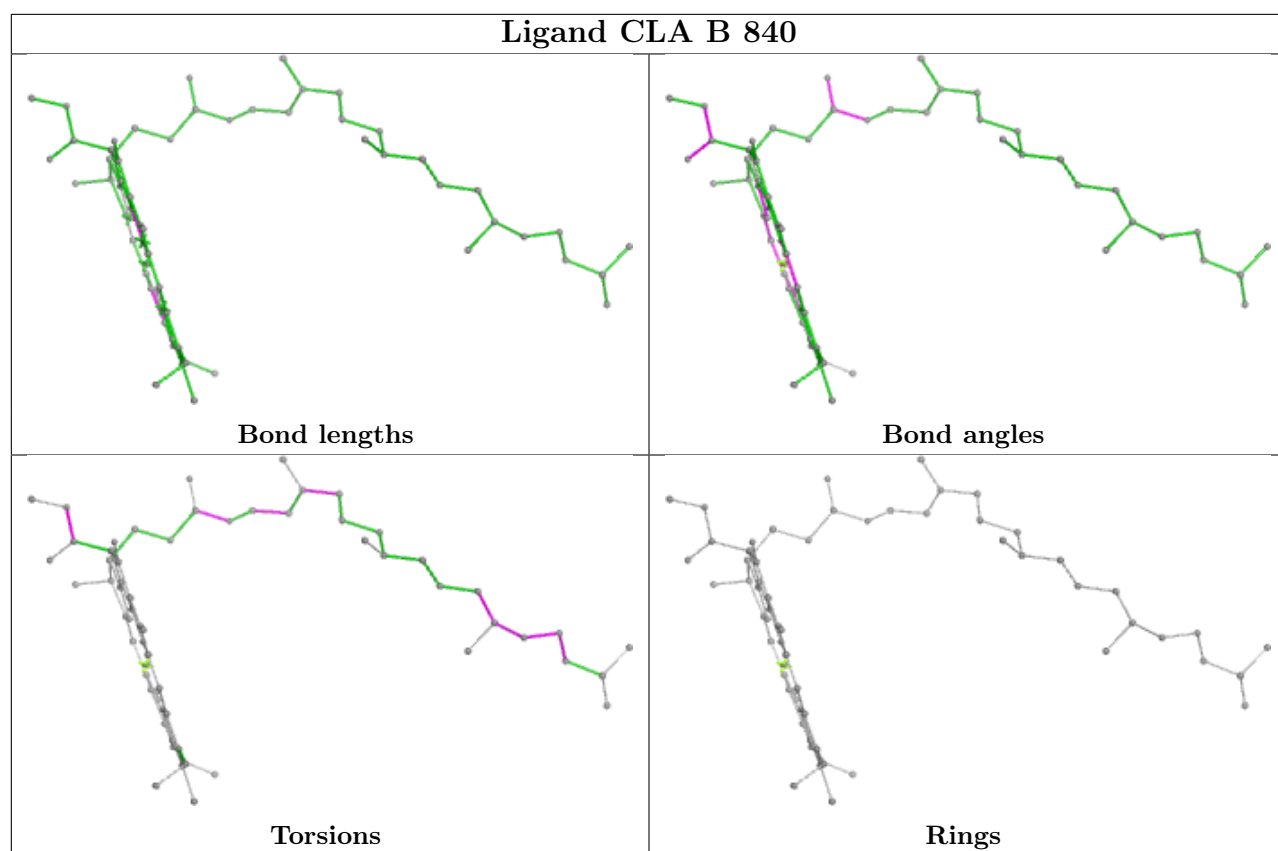
Torsions

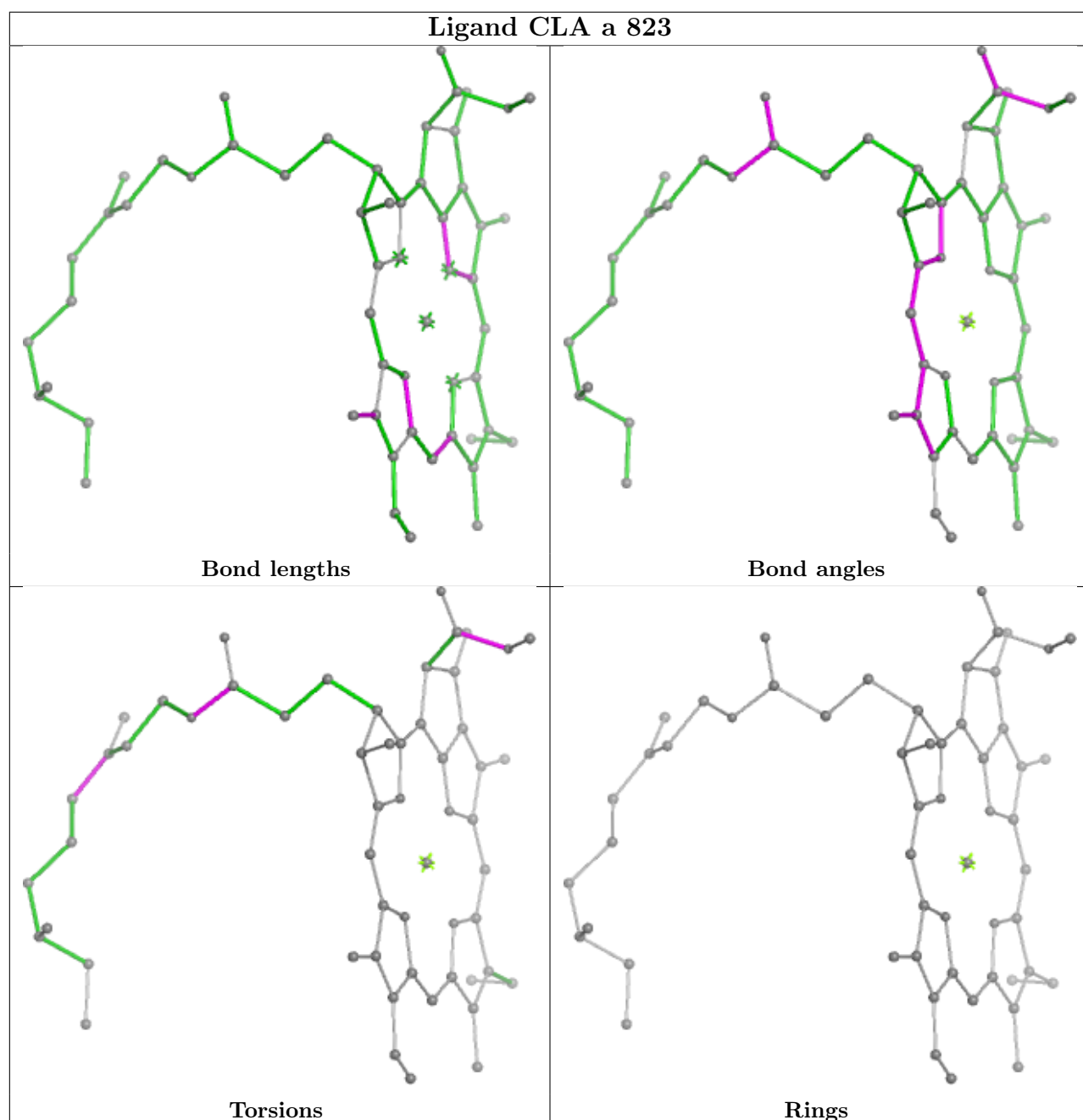
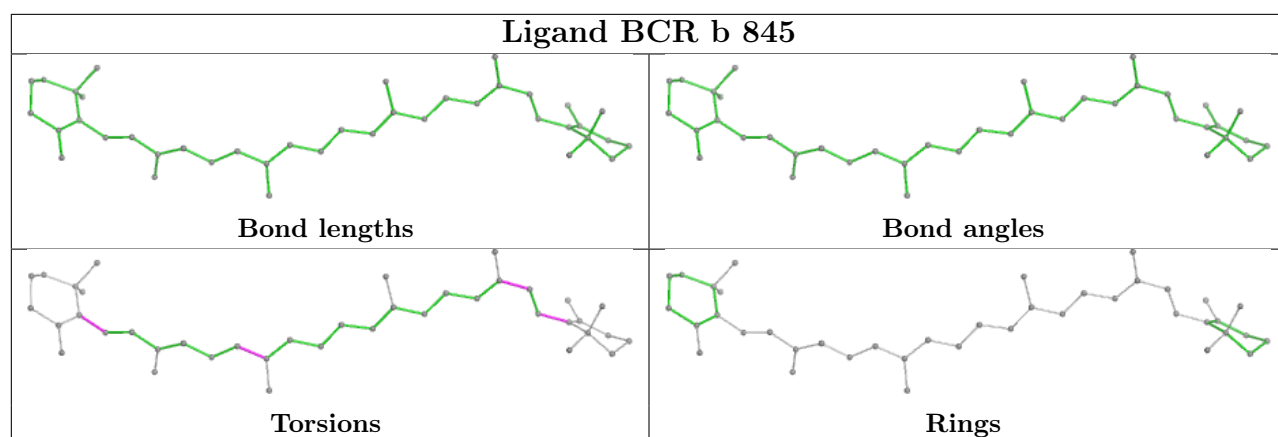


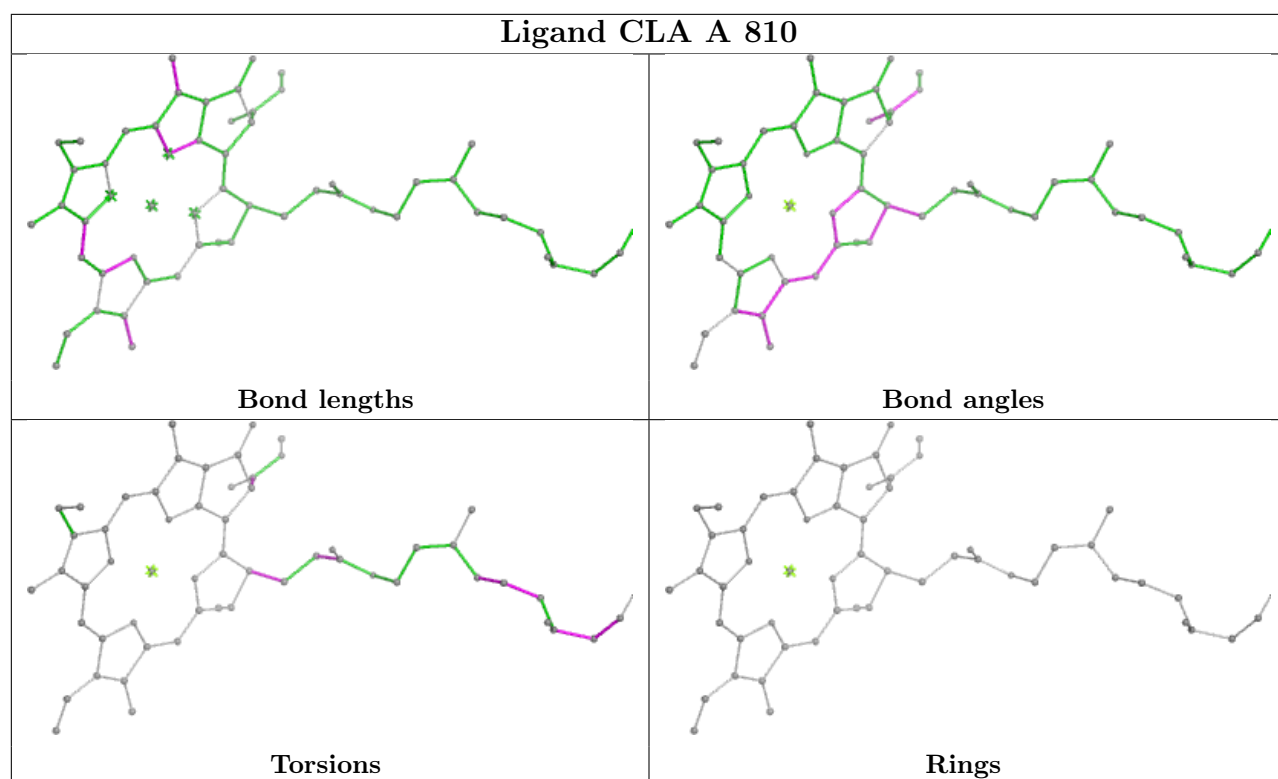
Rings

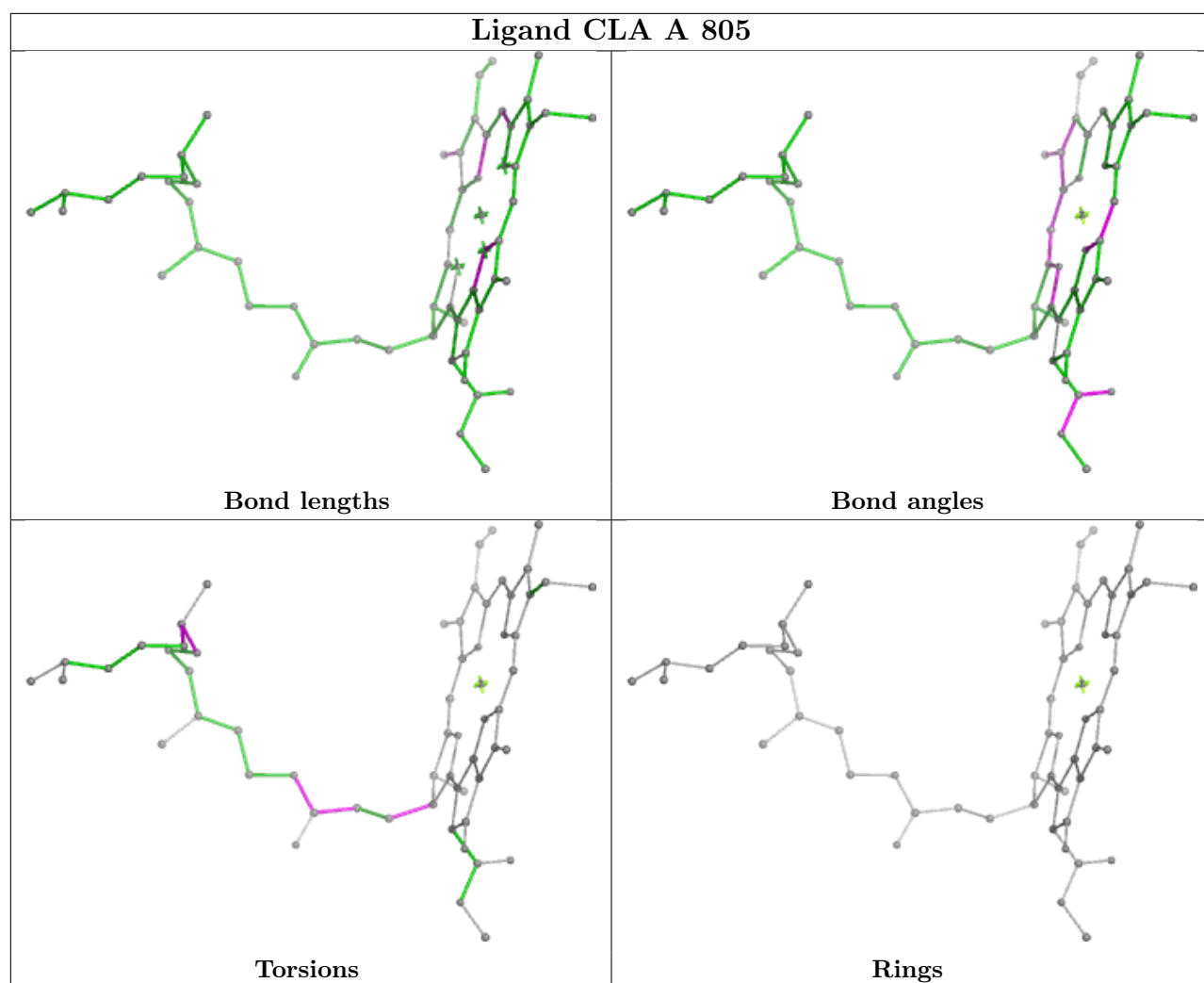
**Ligand CLA a 835****Ligand CLA O 824**





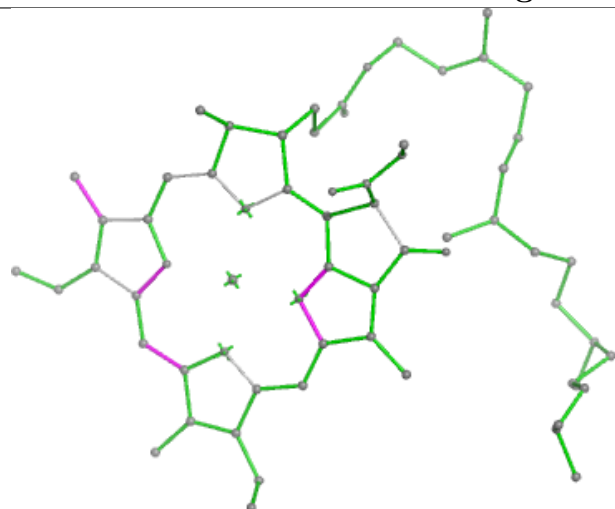




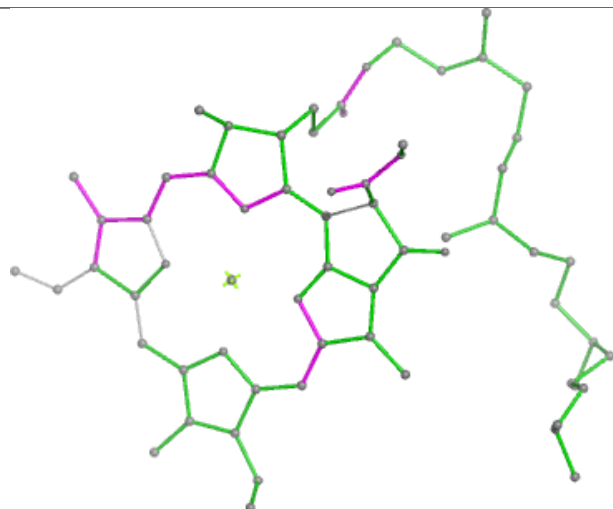




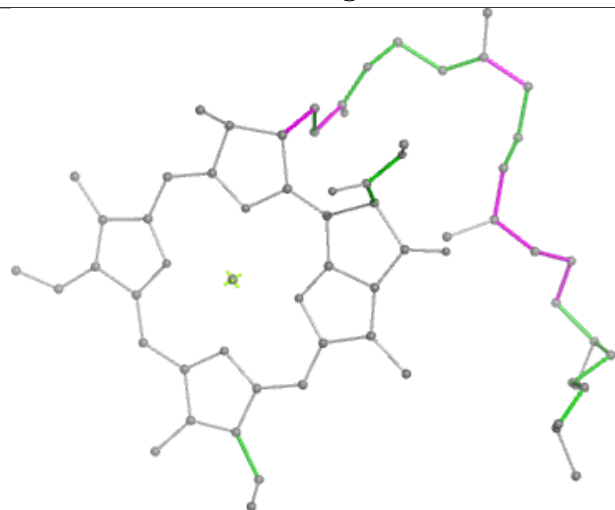
## Ligand CLA O 831



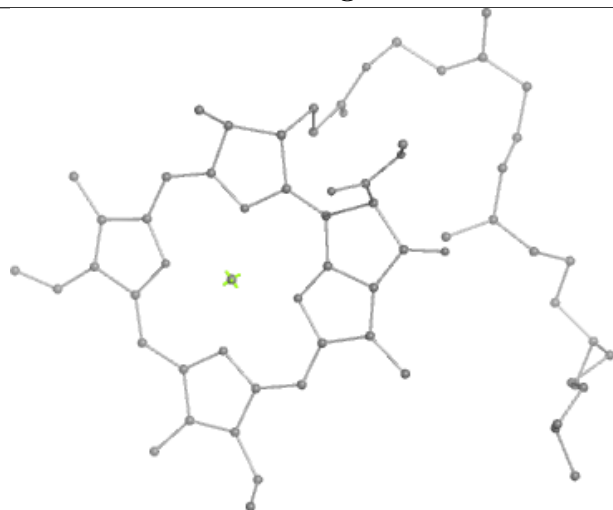
Bond lengths



Bond angles

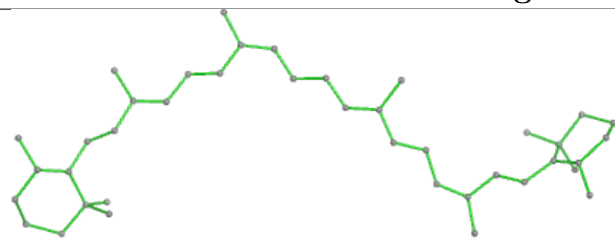


Torsions

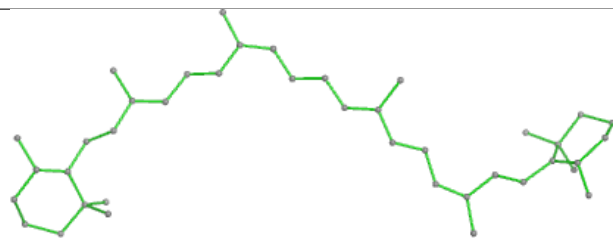


Rings

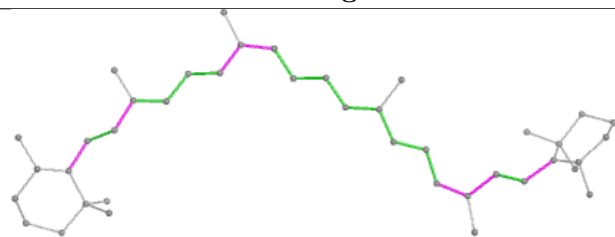
## Ligand BCR A 850



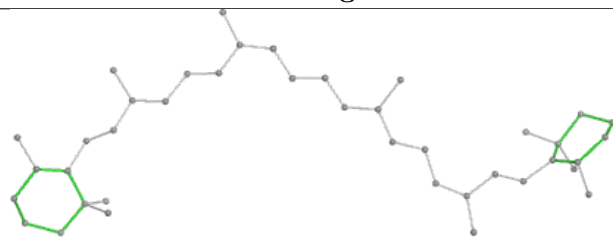
Bond lengths



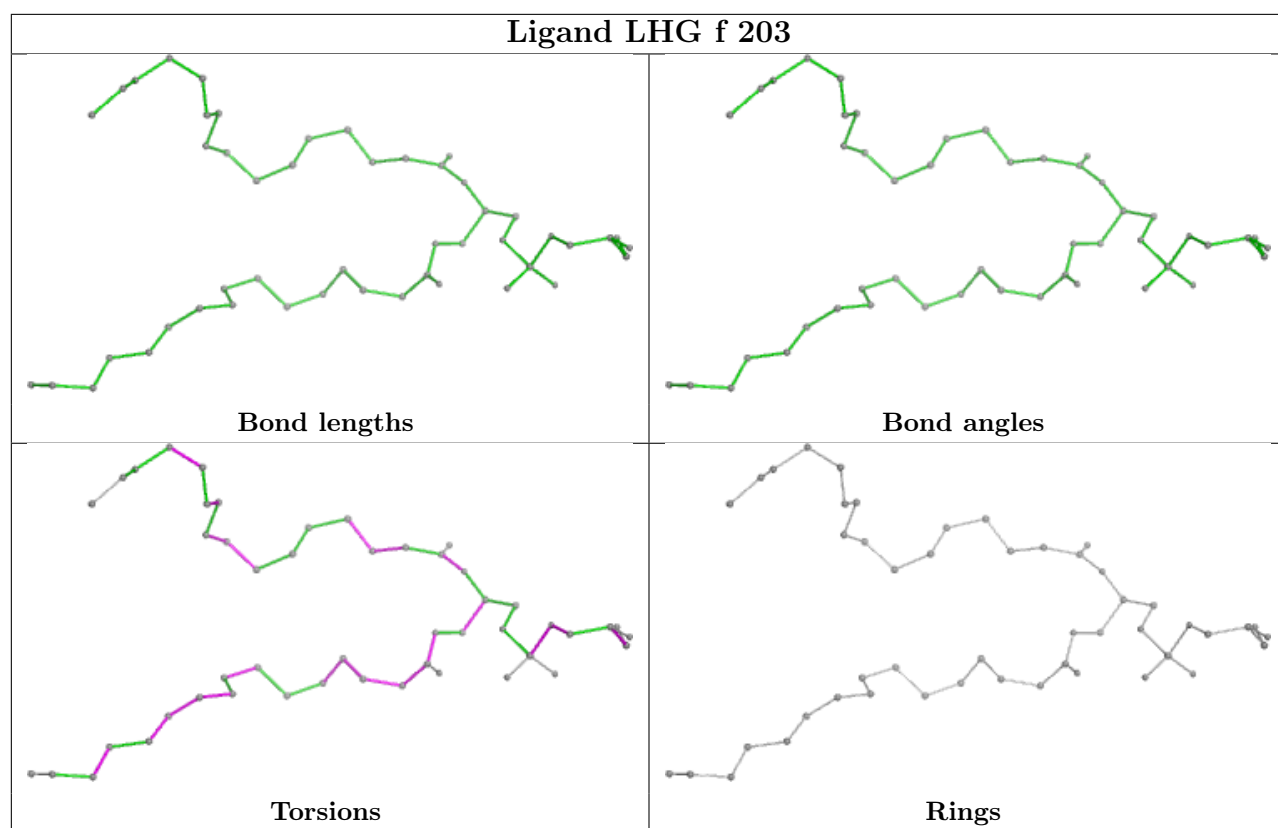
Bond angles



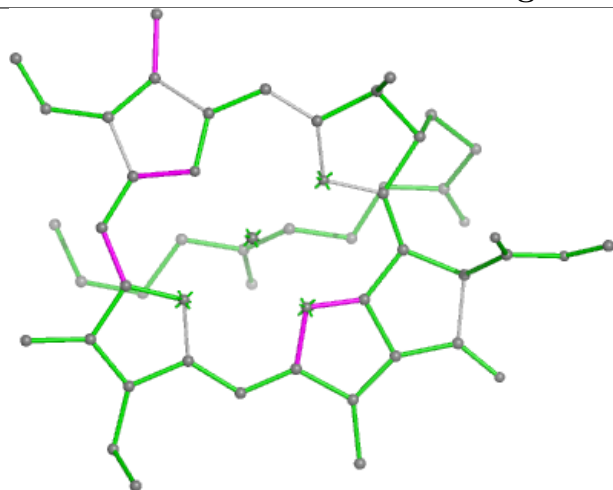
Torsions



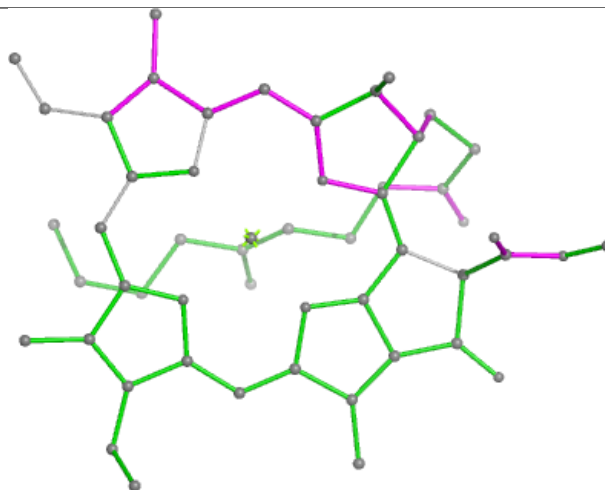
Rings



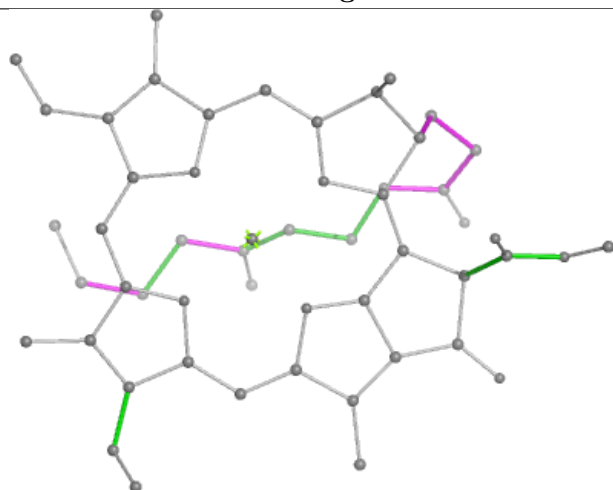
## Ligand CLA b 821



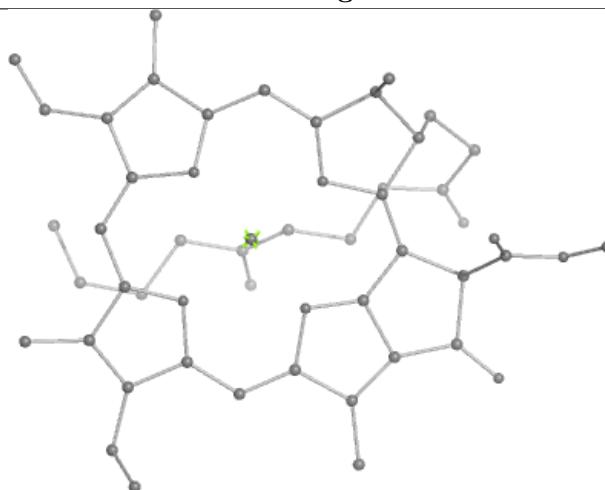
Bond lengths



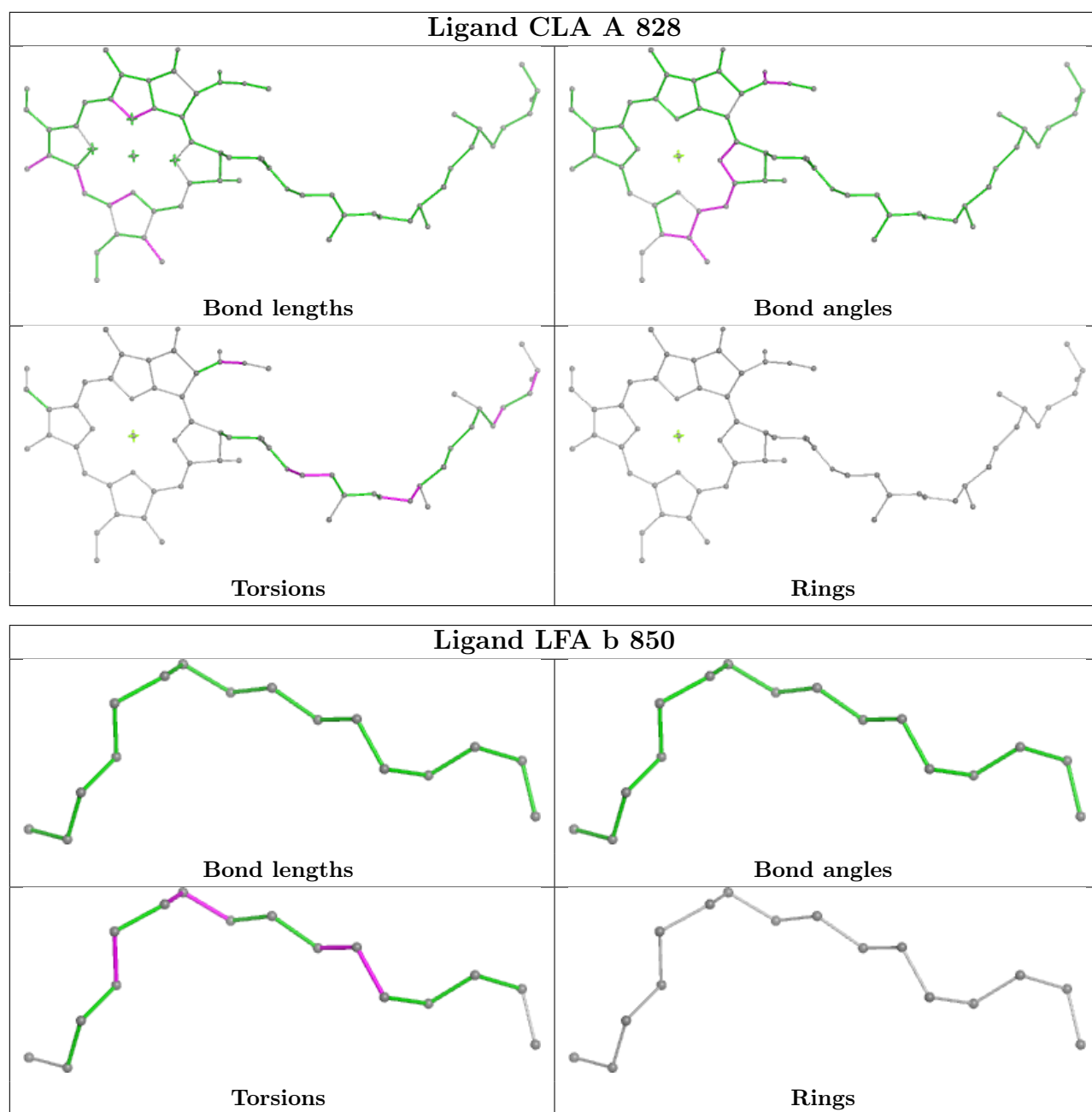
Bond angles



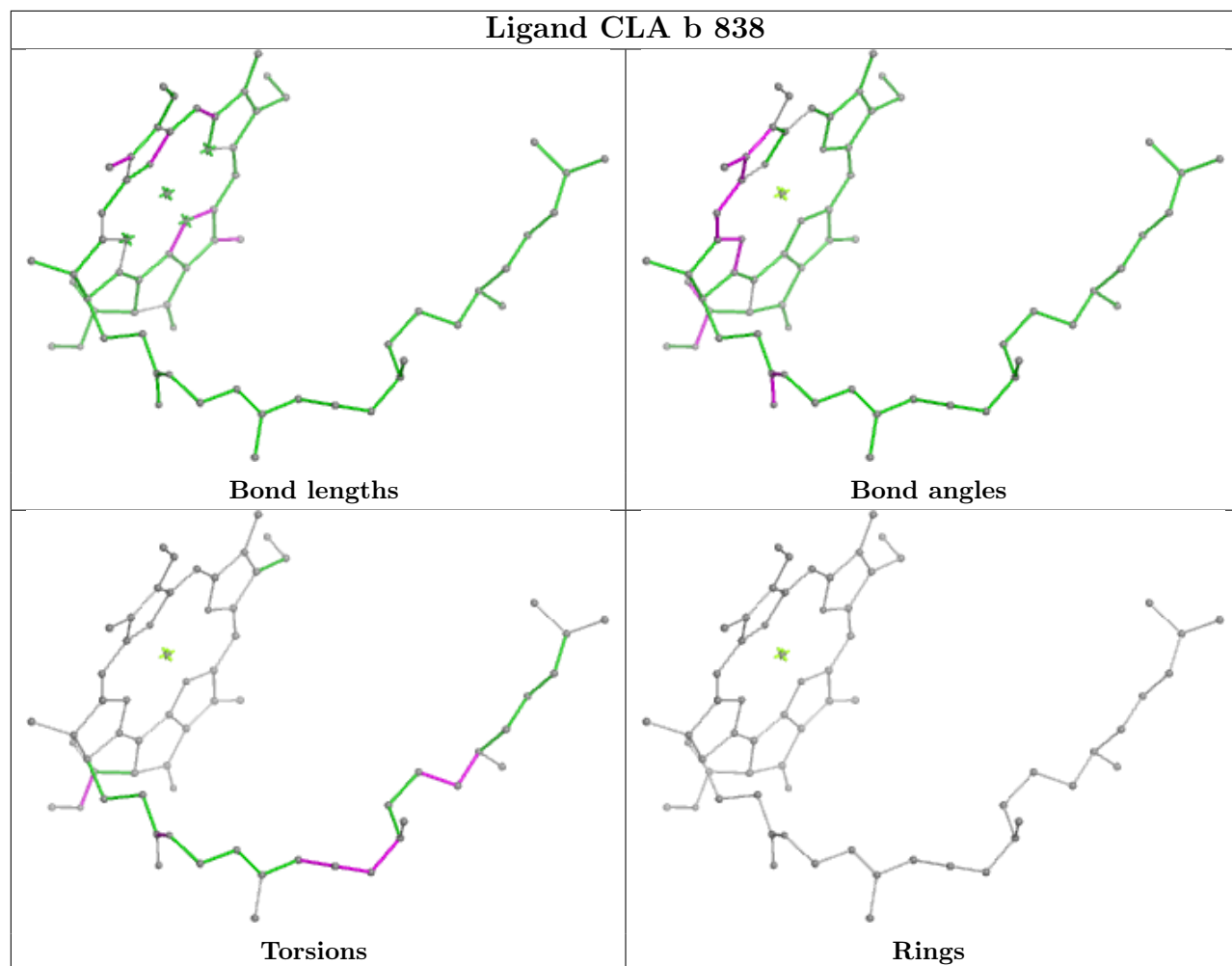
Torsions



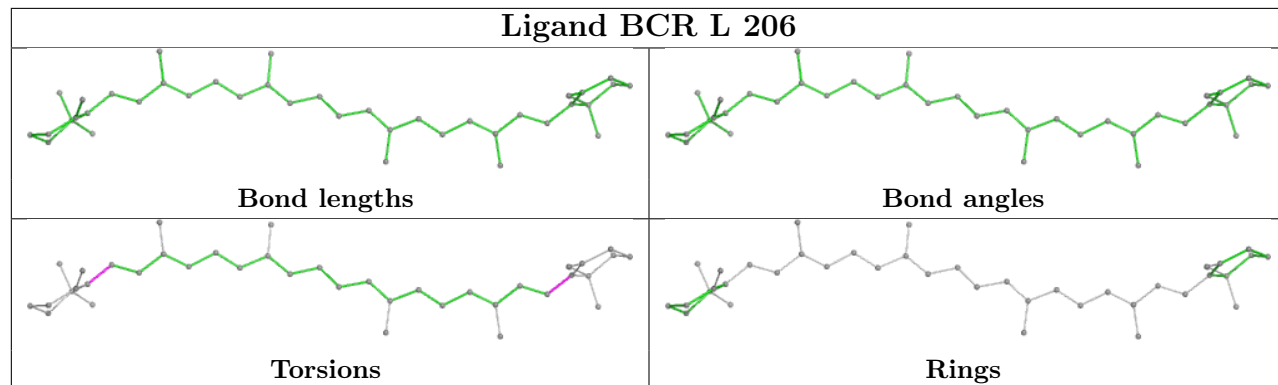
Rings

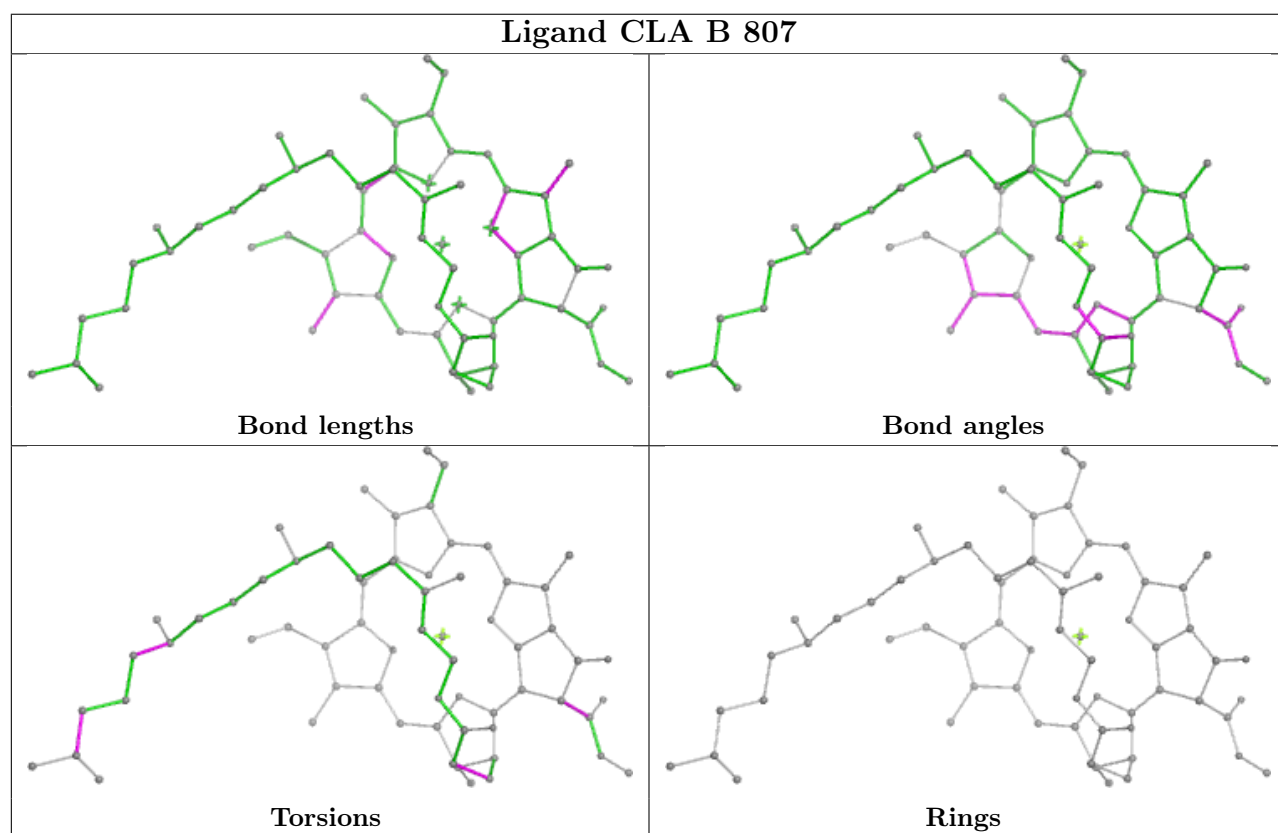
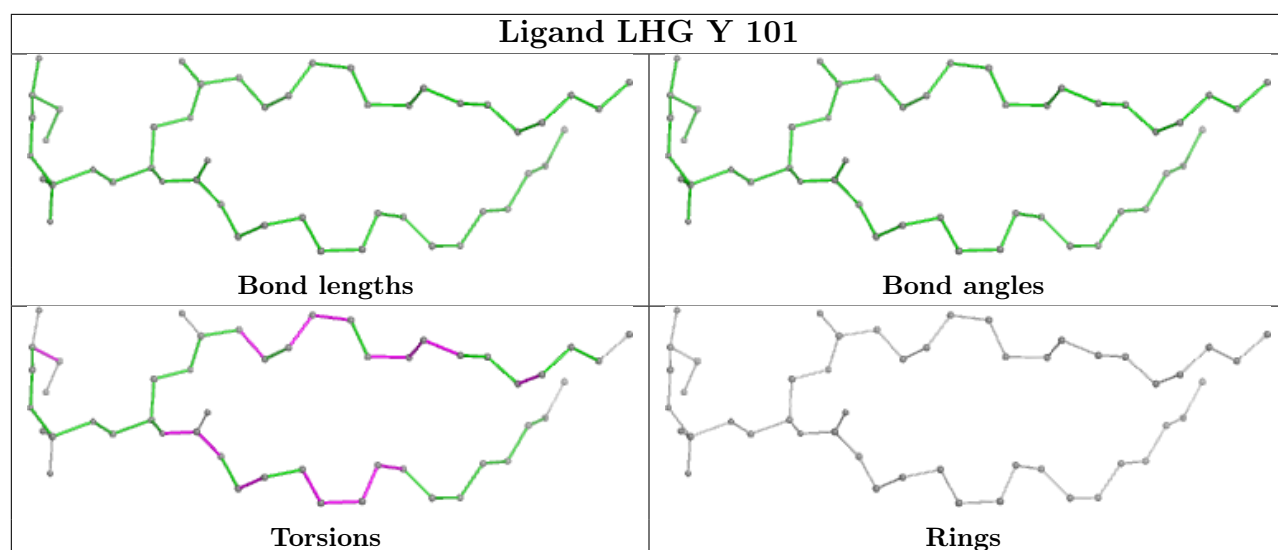


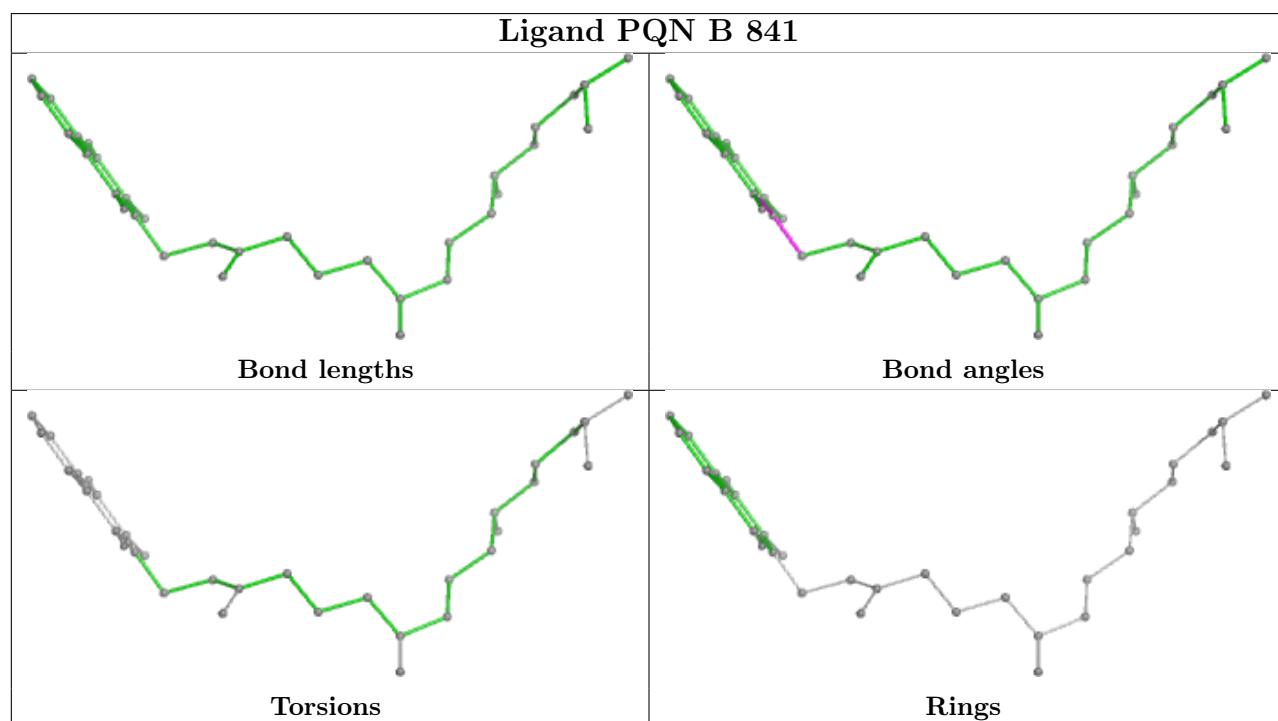
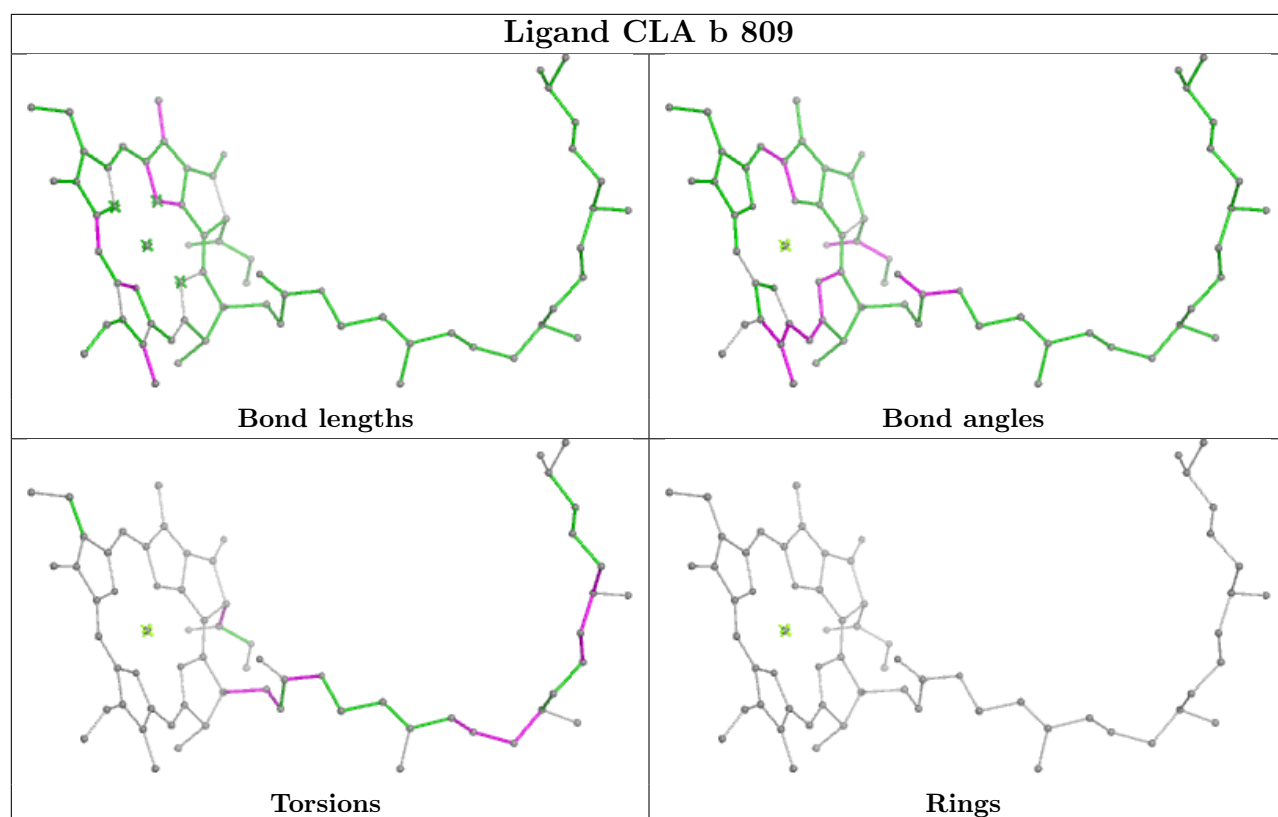
## Ligand CLA b 838

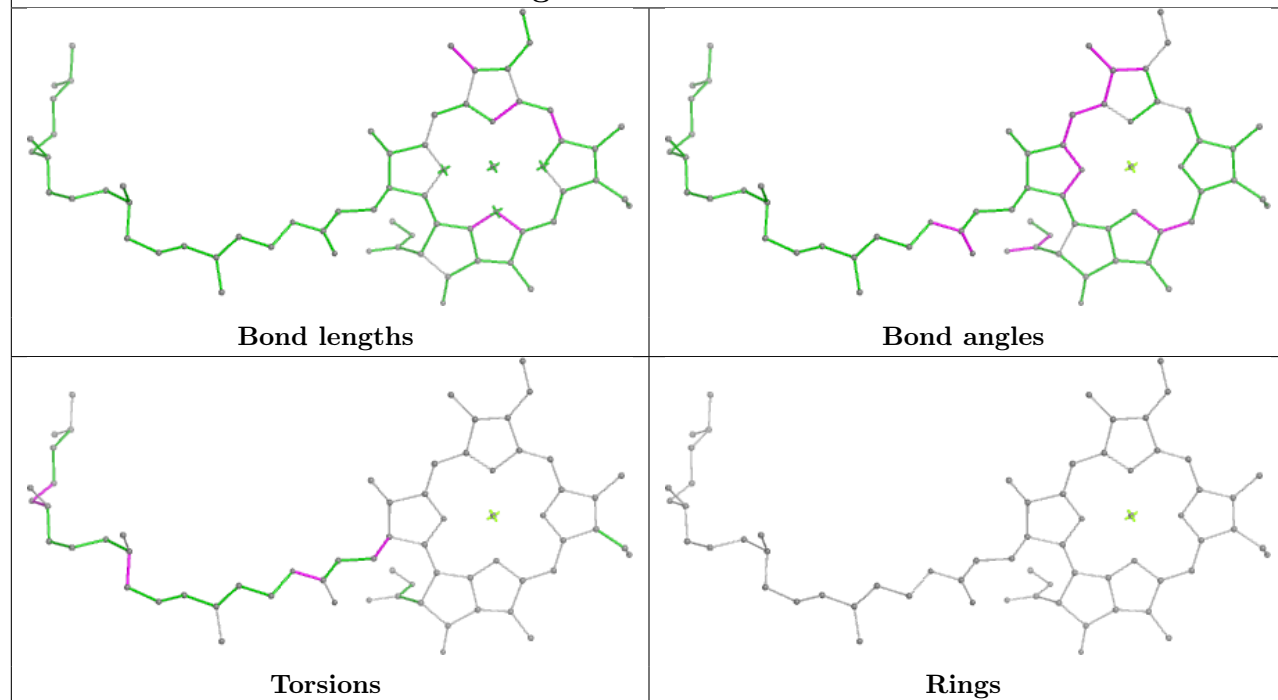
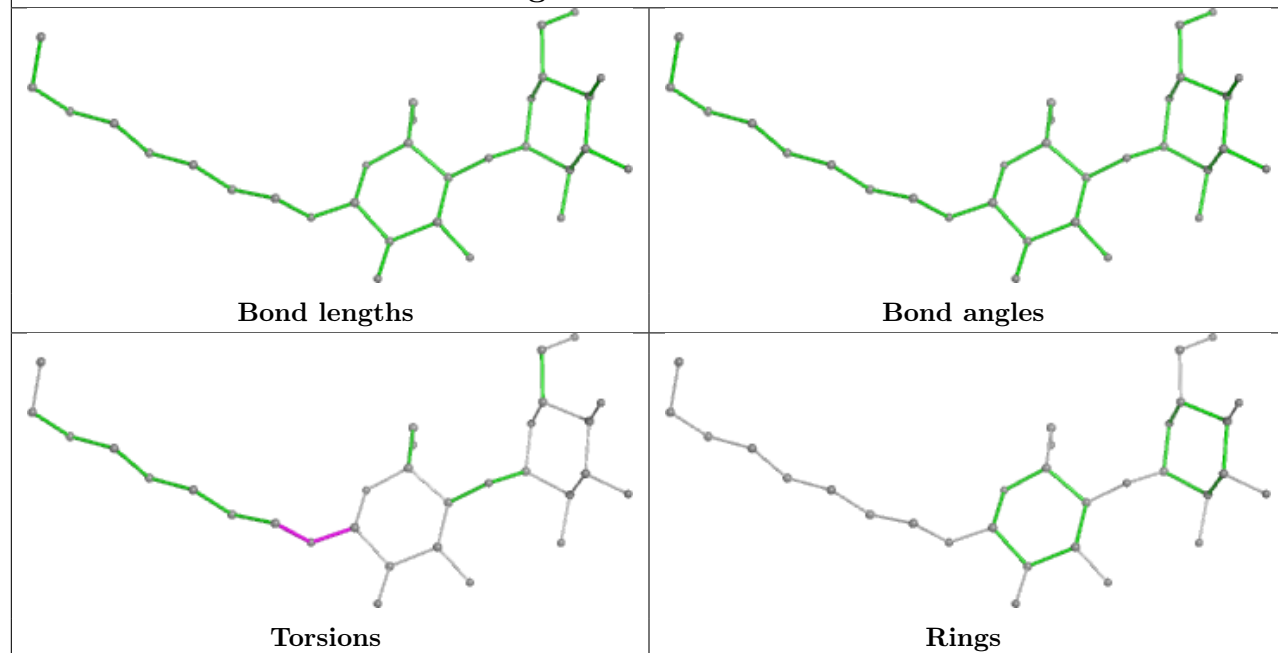


## Ligand BCR L 206

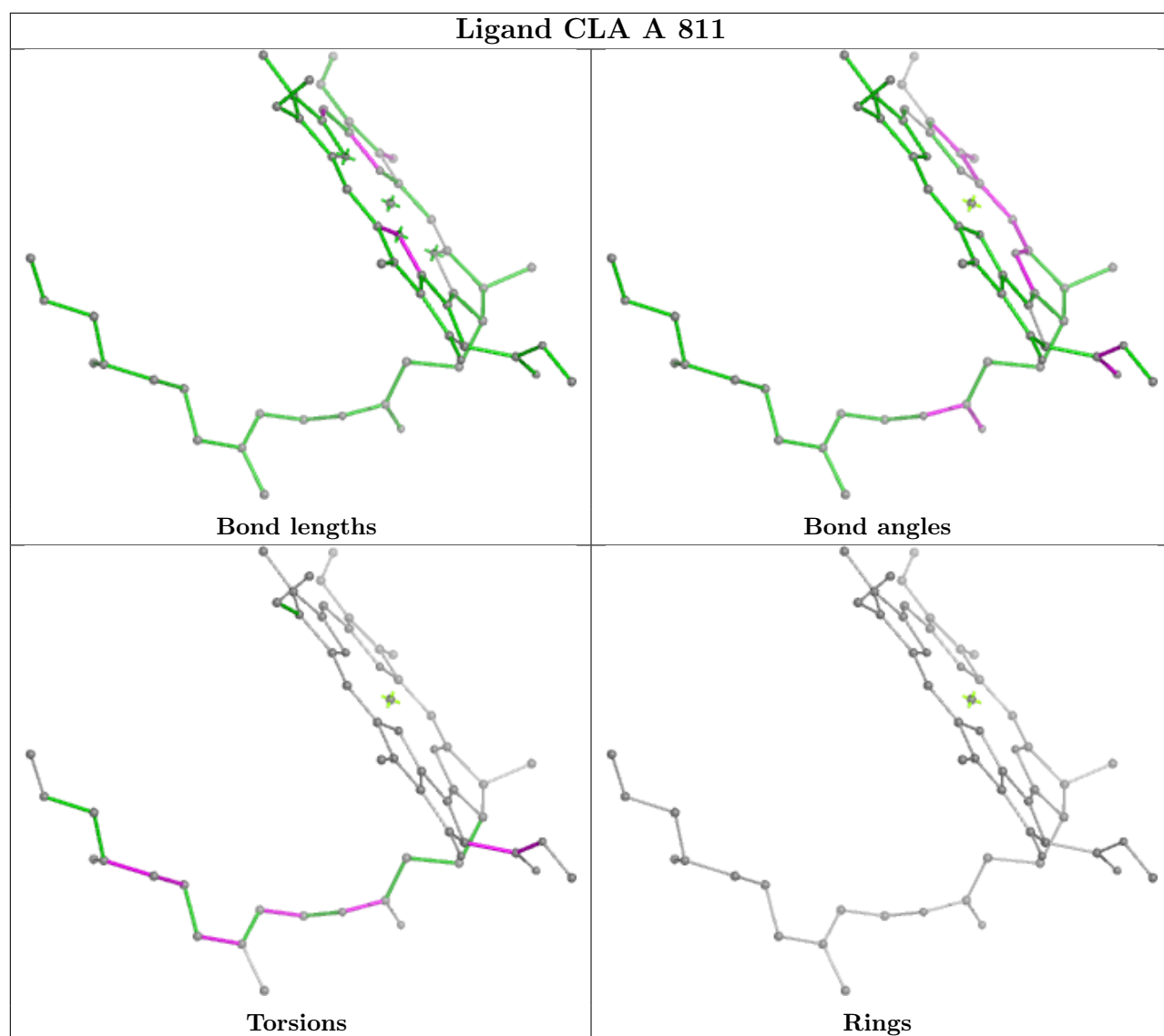




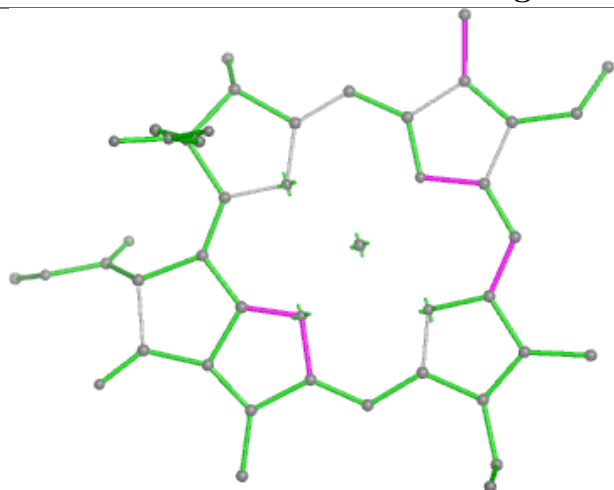


**Ligand CLA B 836****Ligand LMT N 852**

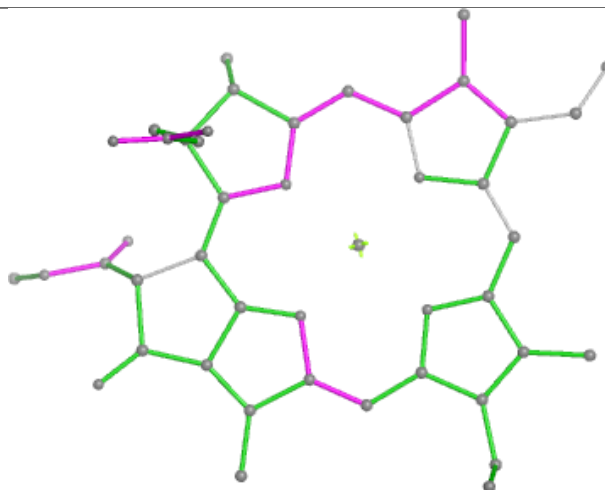




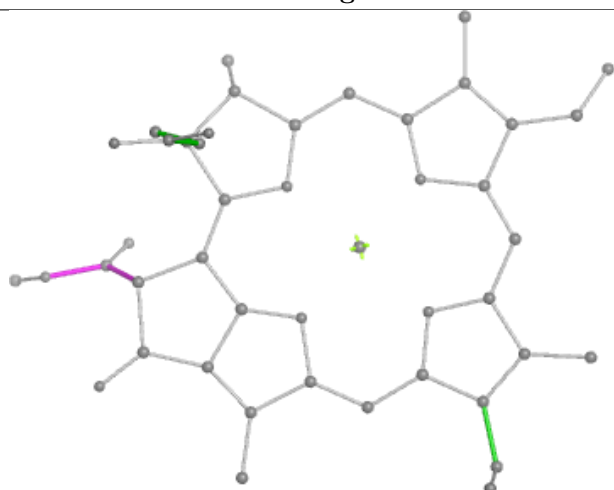
## Ligand CLA A 808



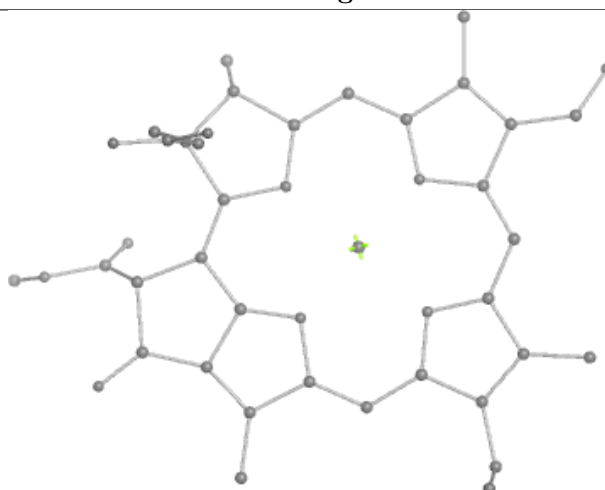
Bond lengths



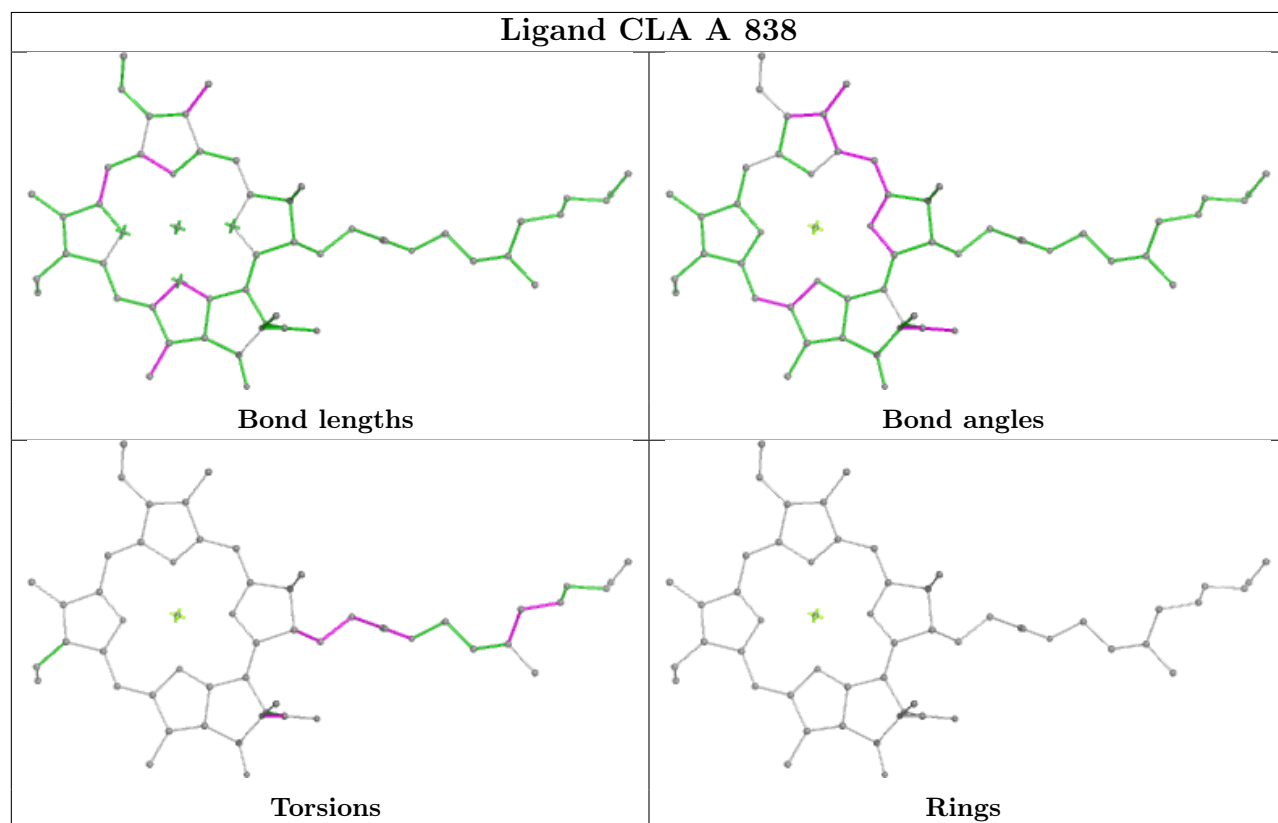
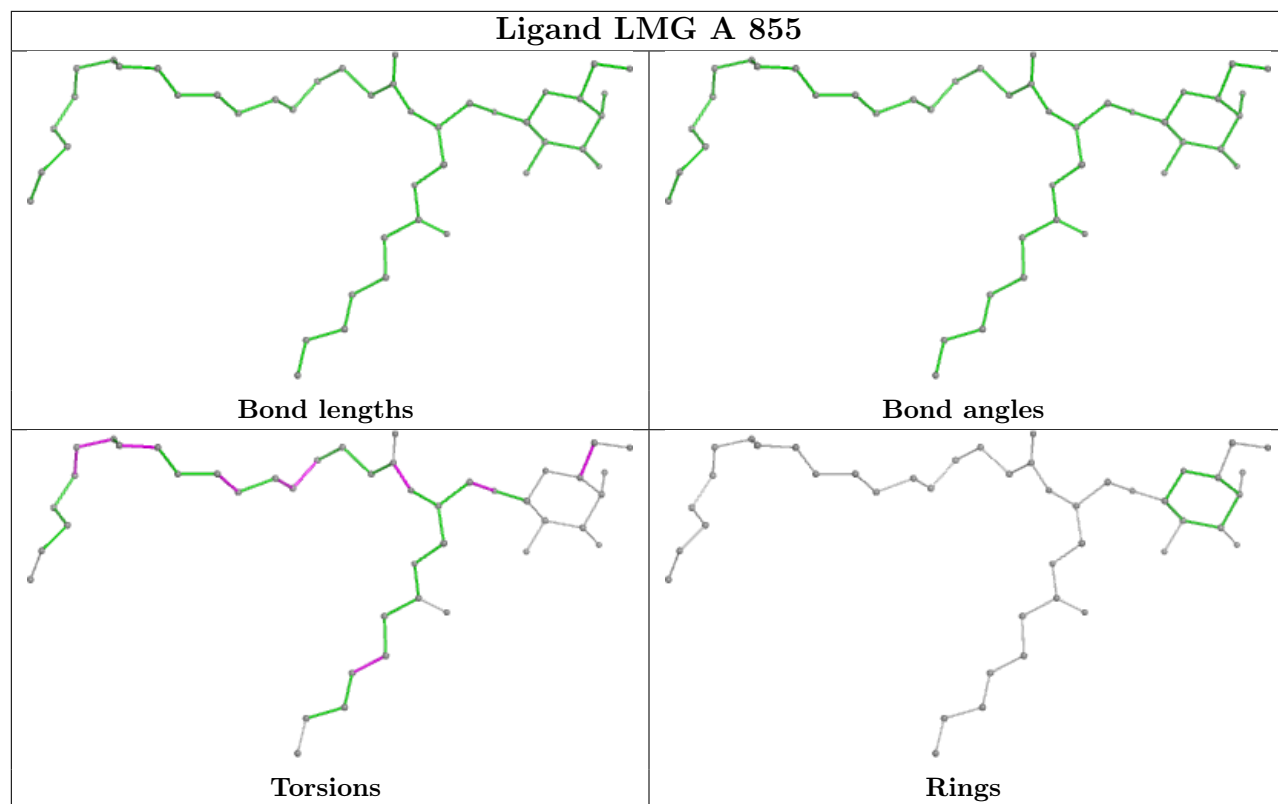
Bond angles



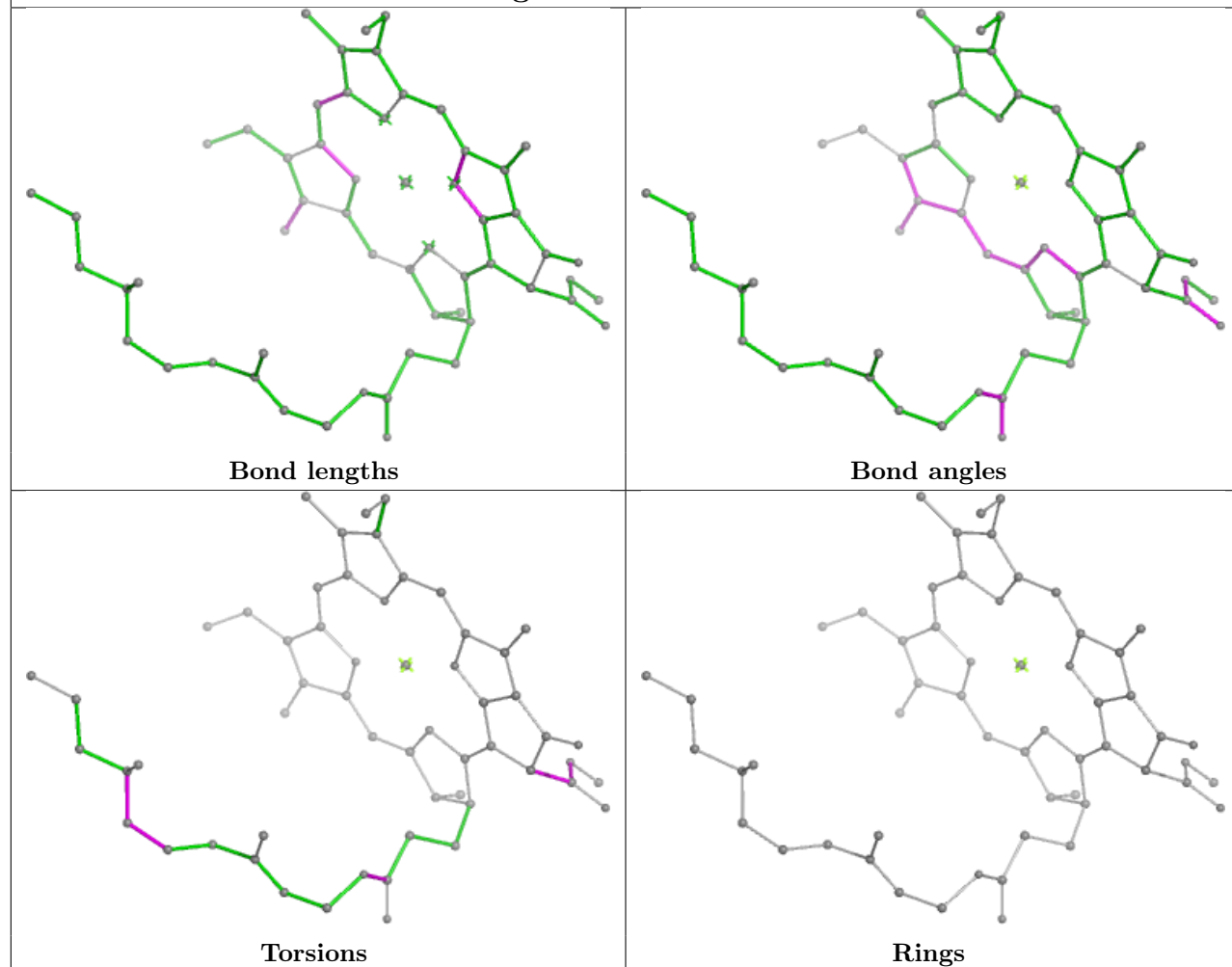
Torsions



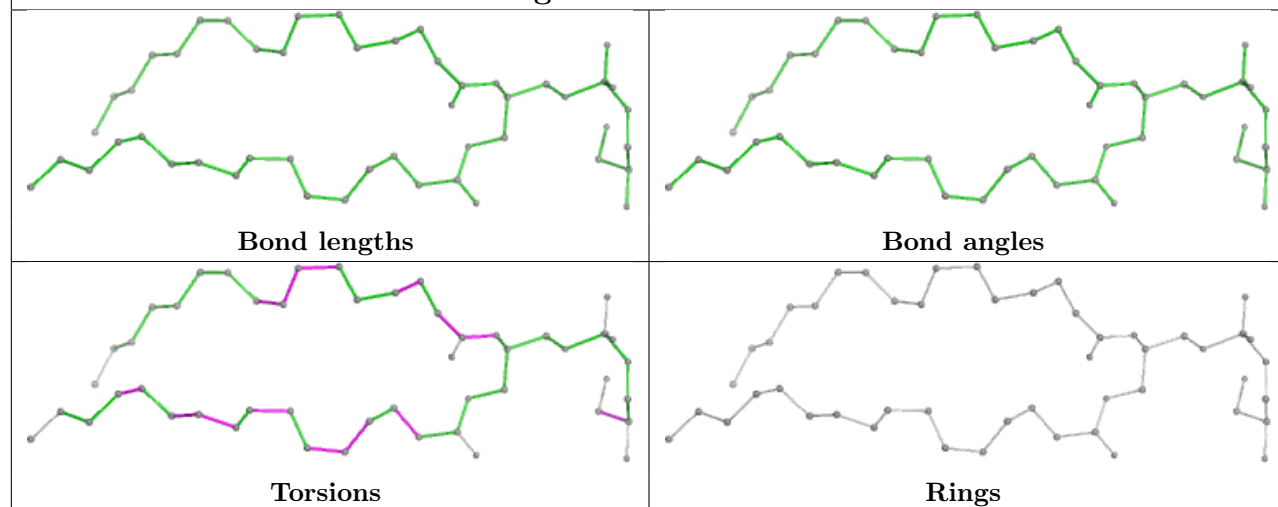
Rings

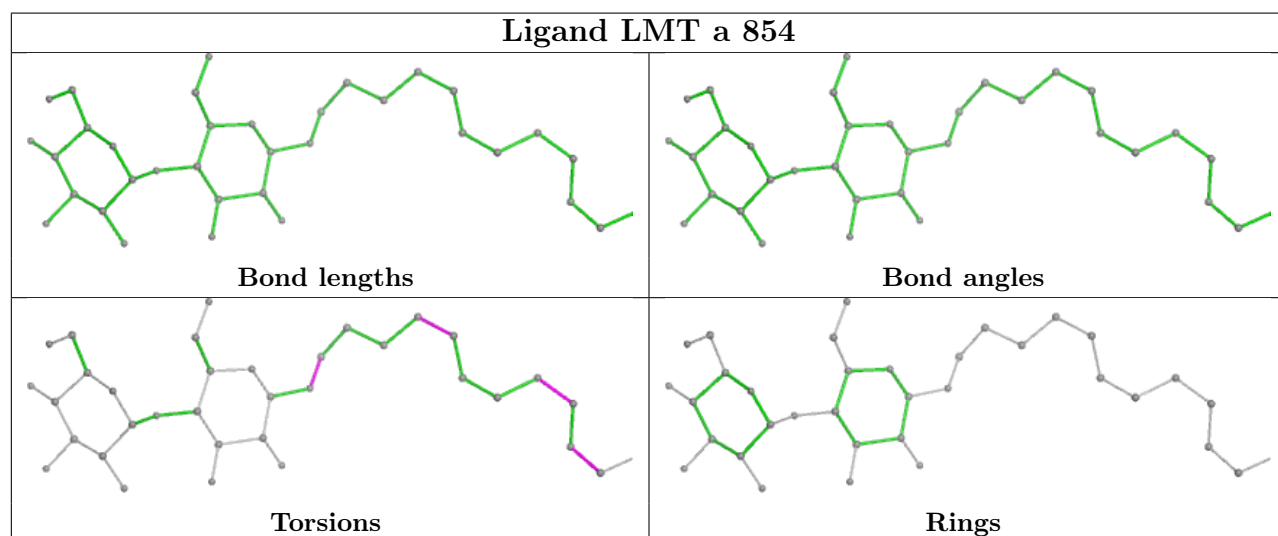
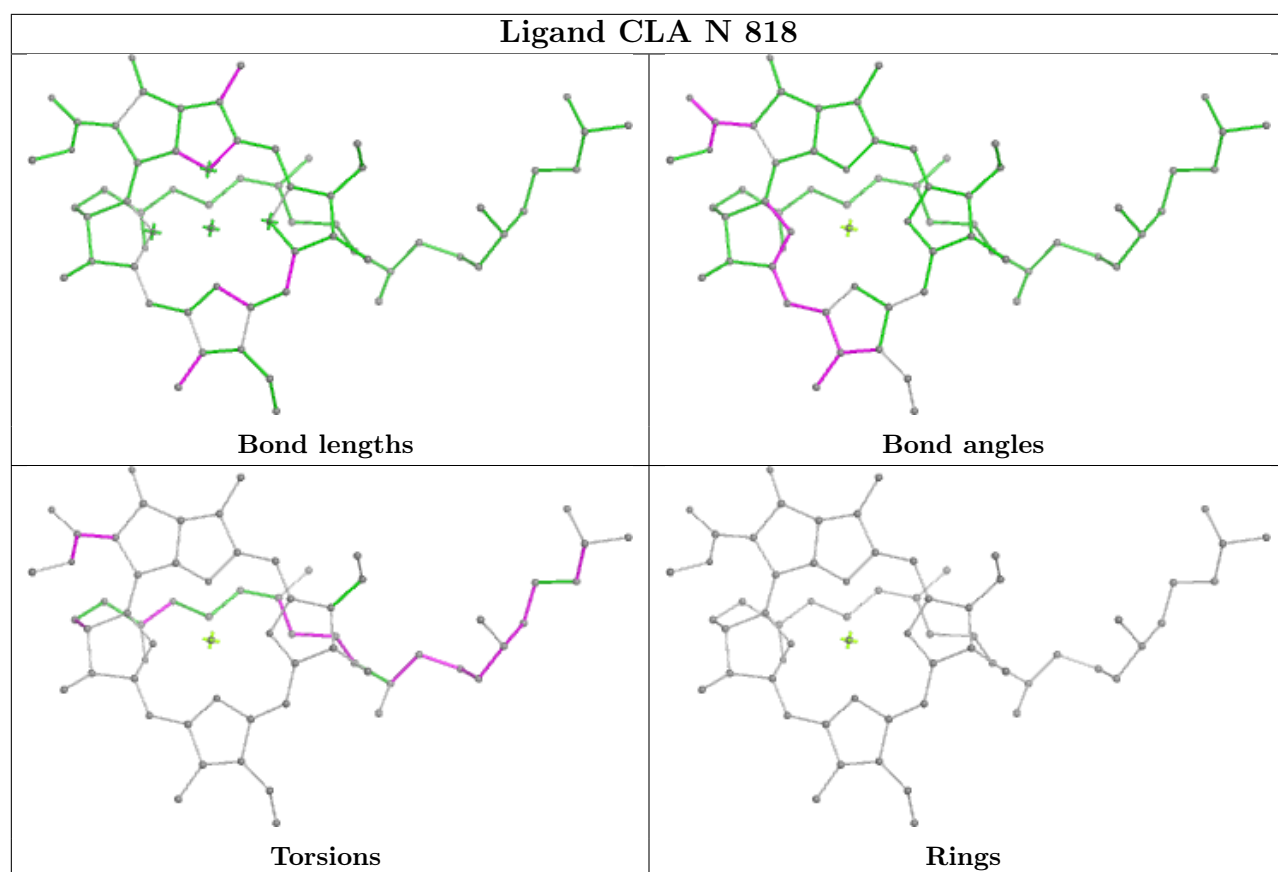


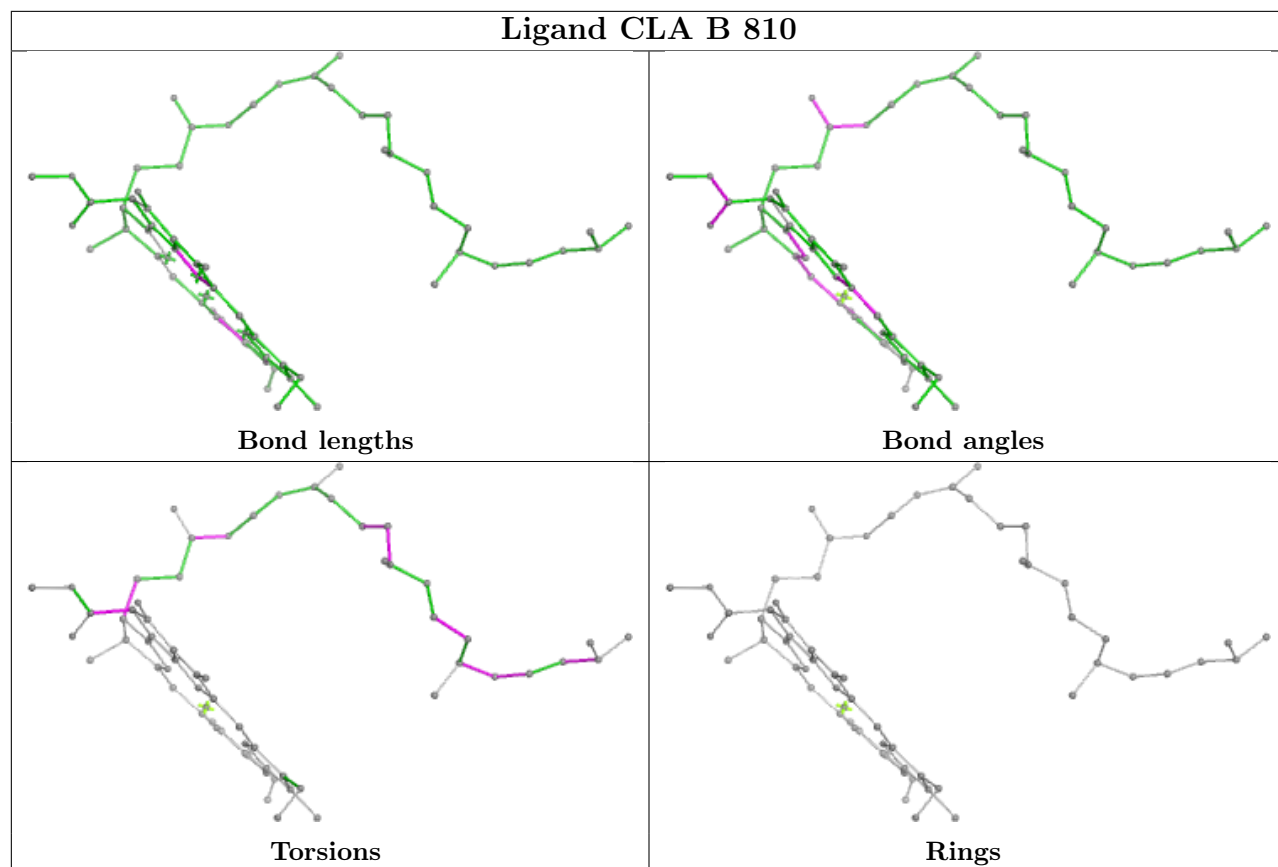
## Ligand CLA O 815



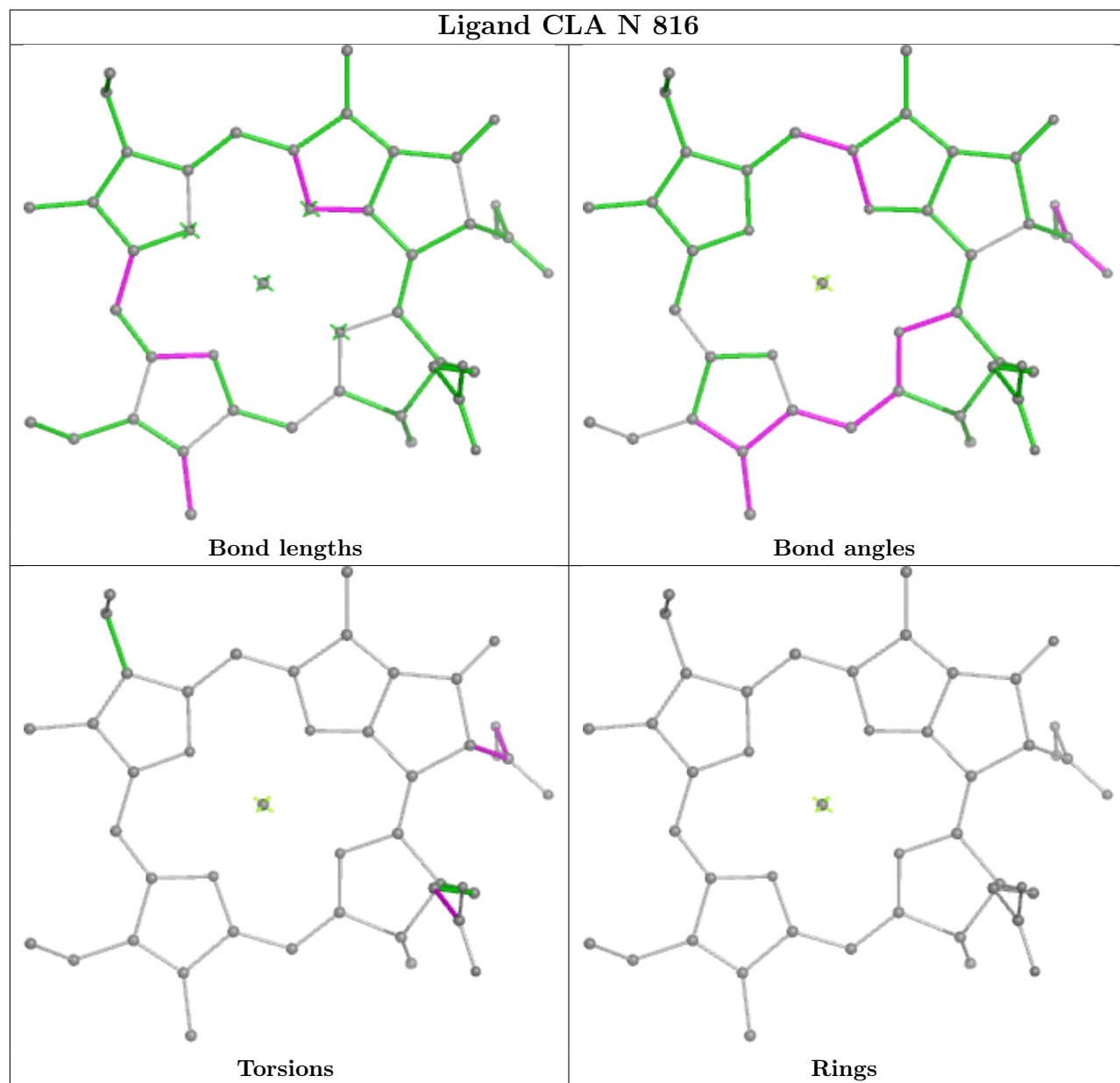
## Ligand LHG k 101

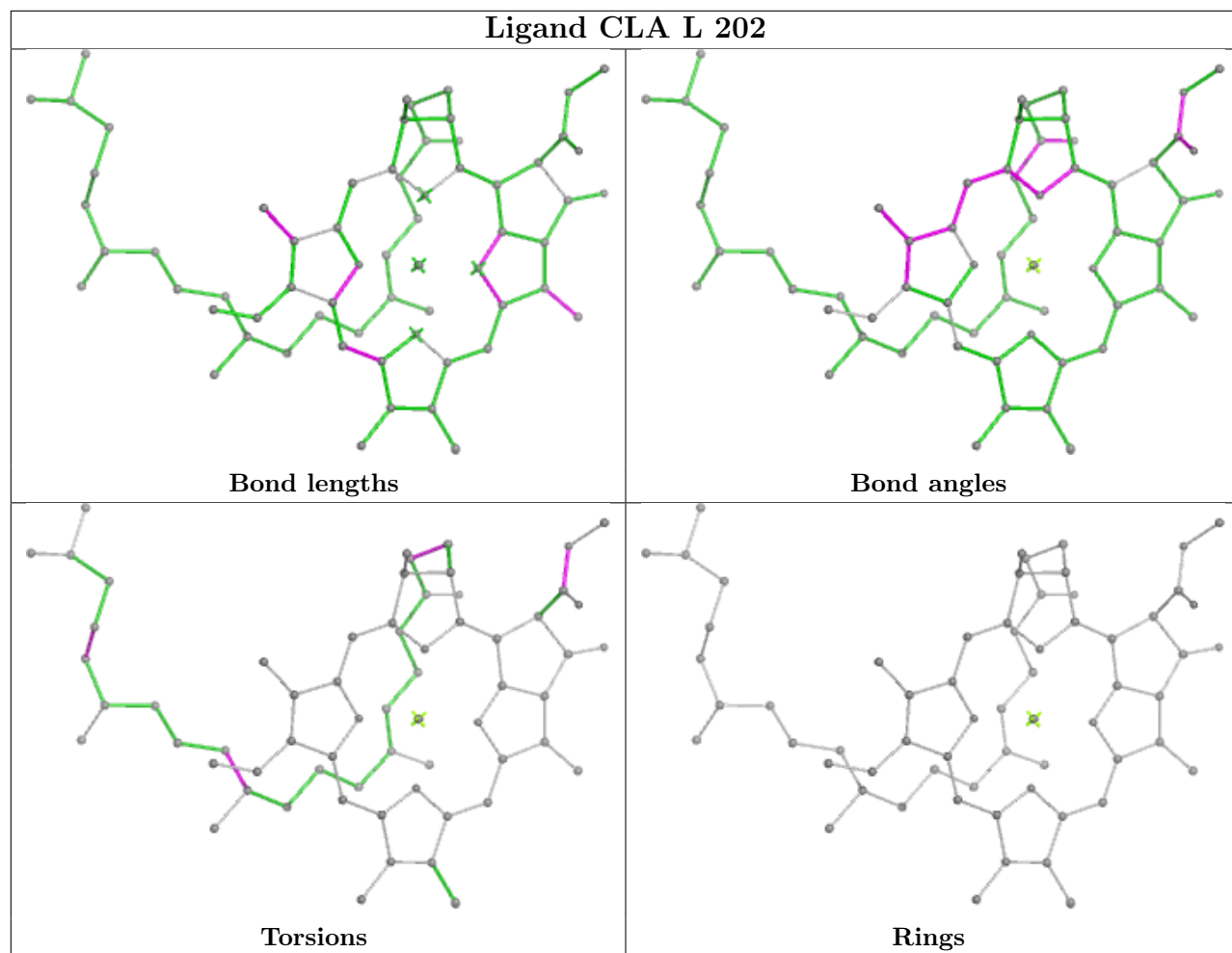




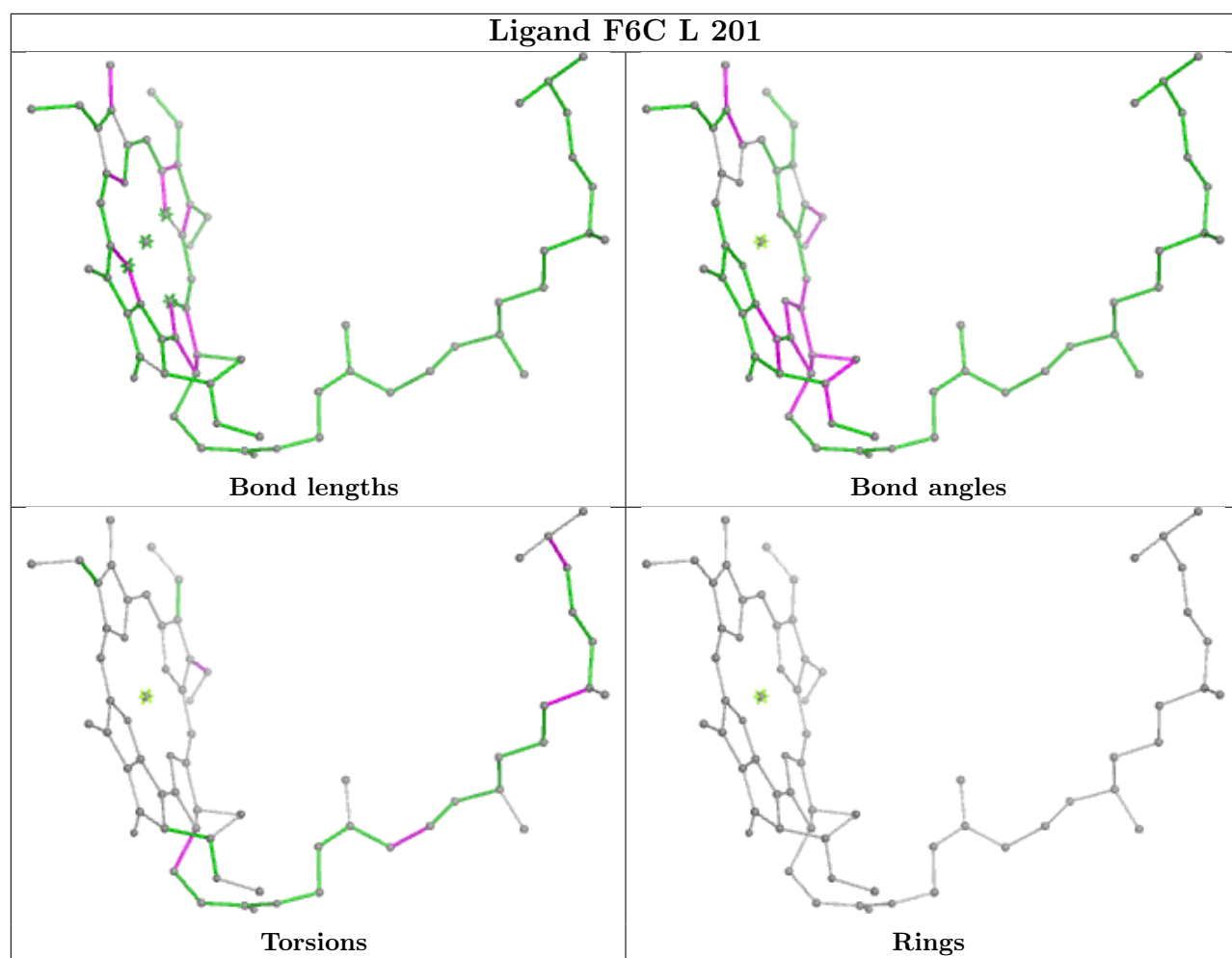


## Ligand CLA N 816

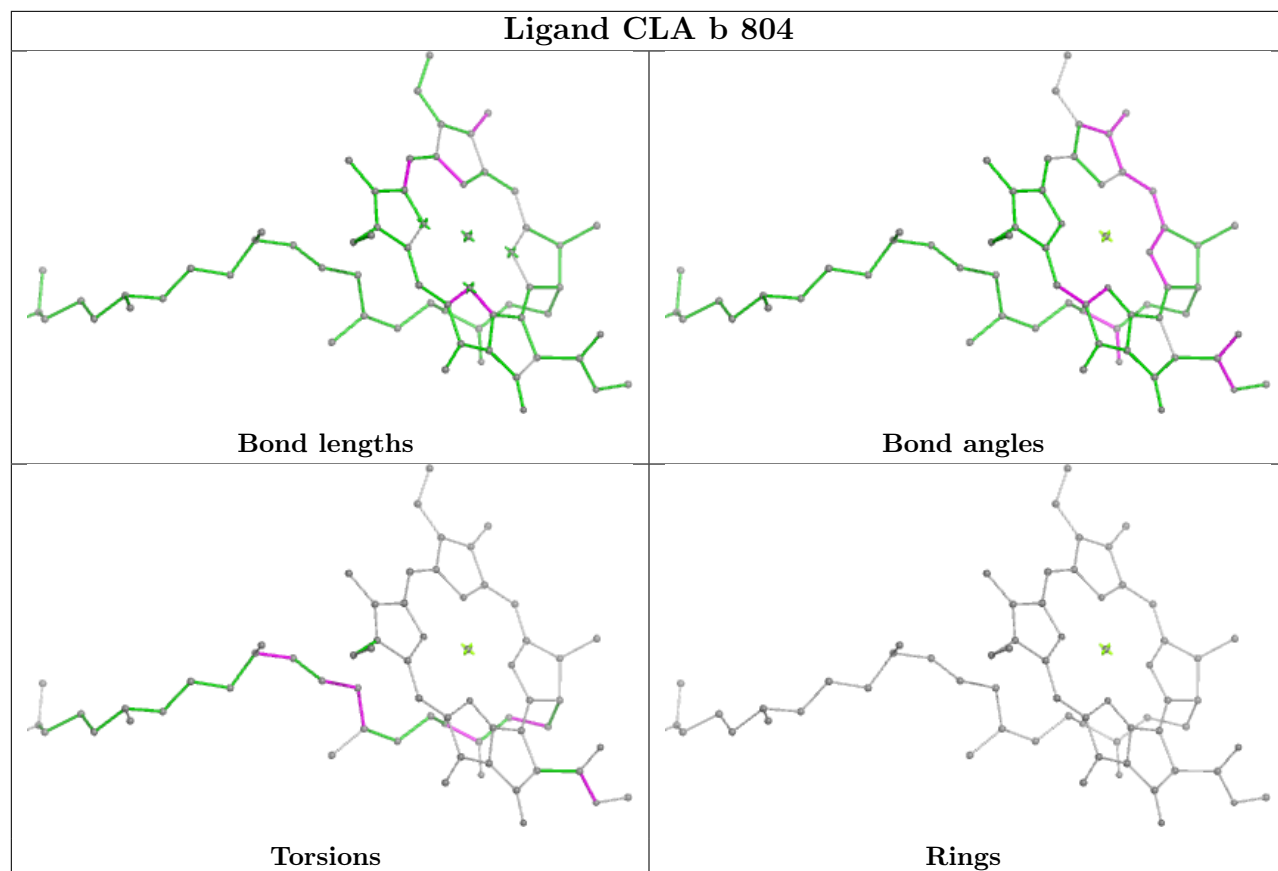




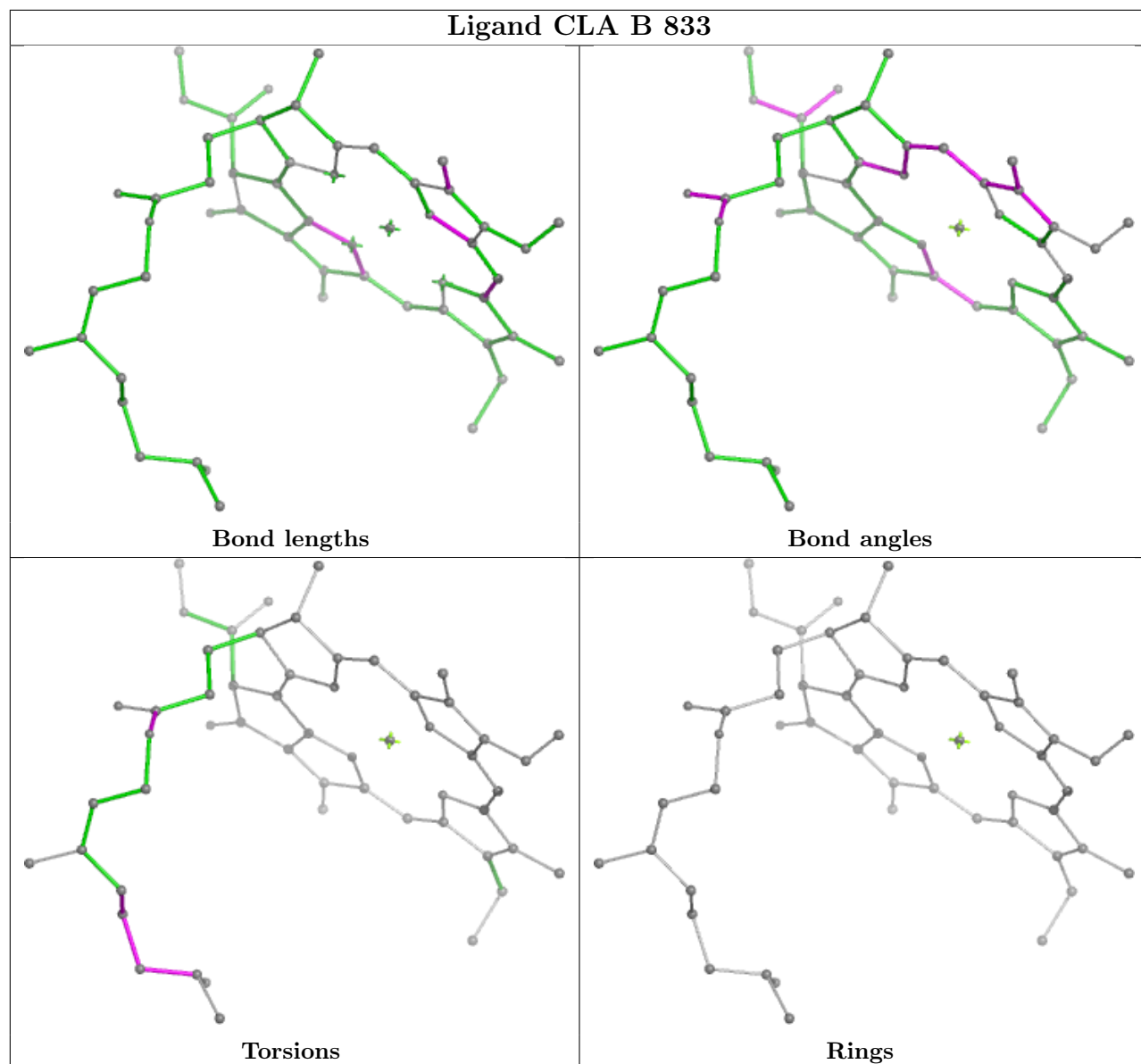




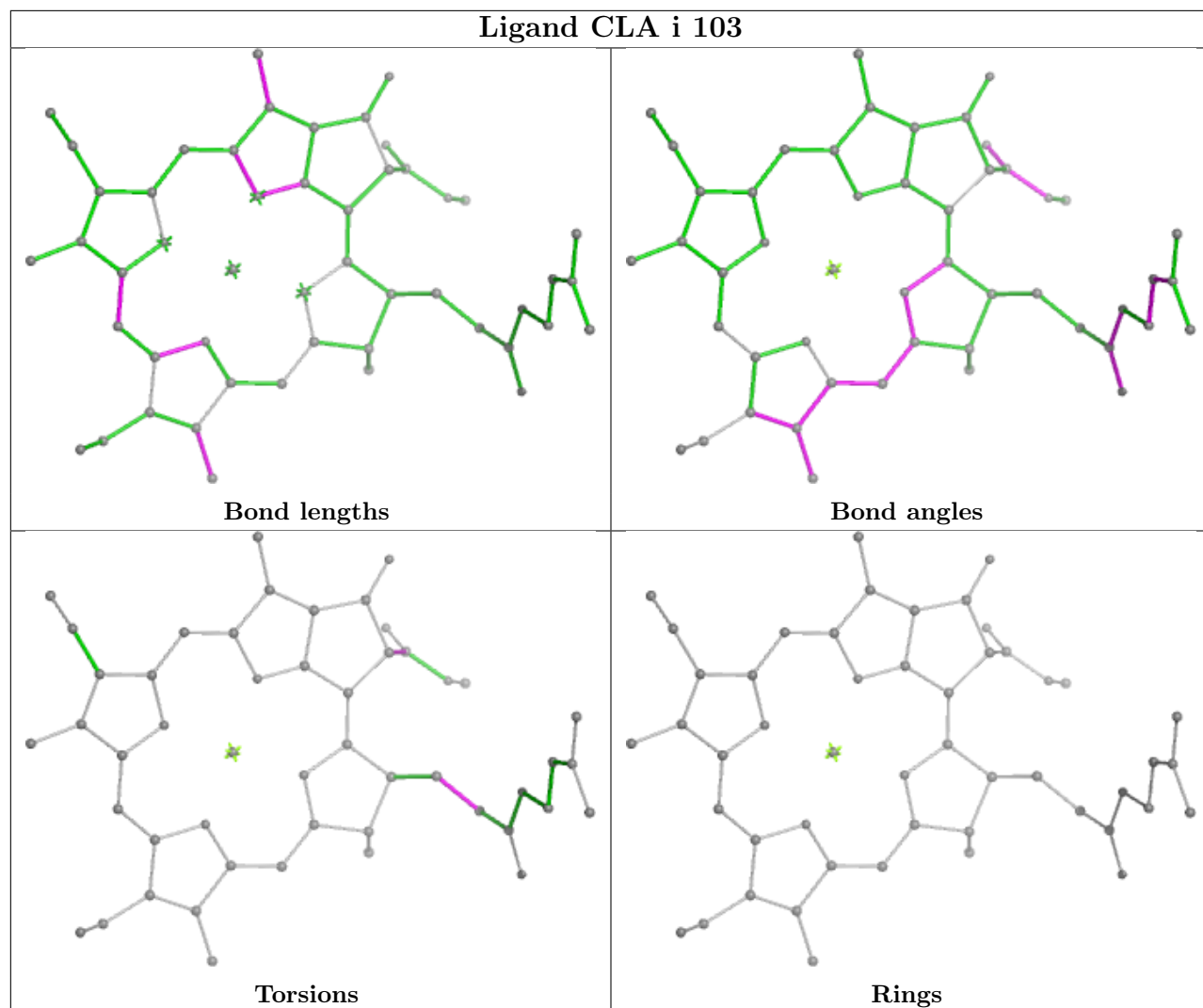
## Ligand CLA b 804

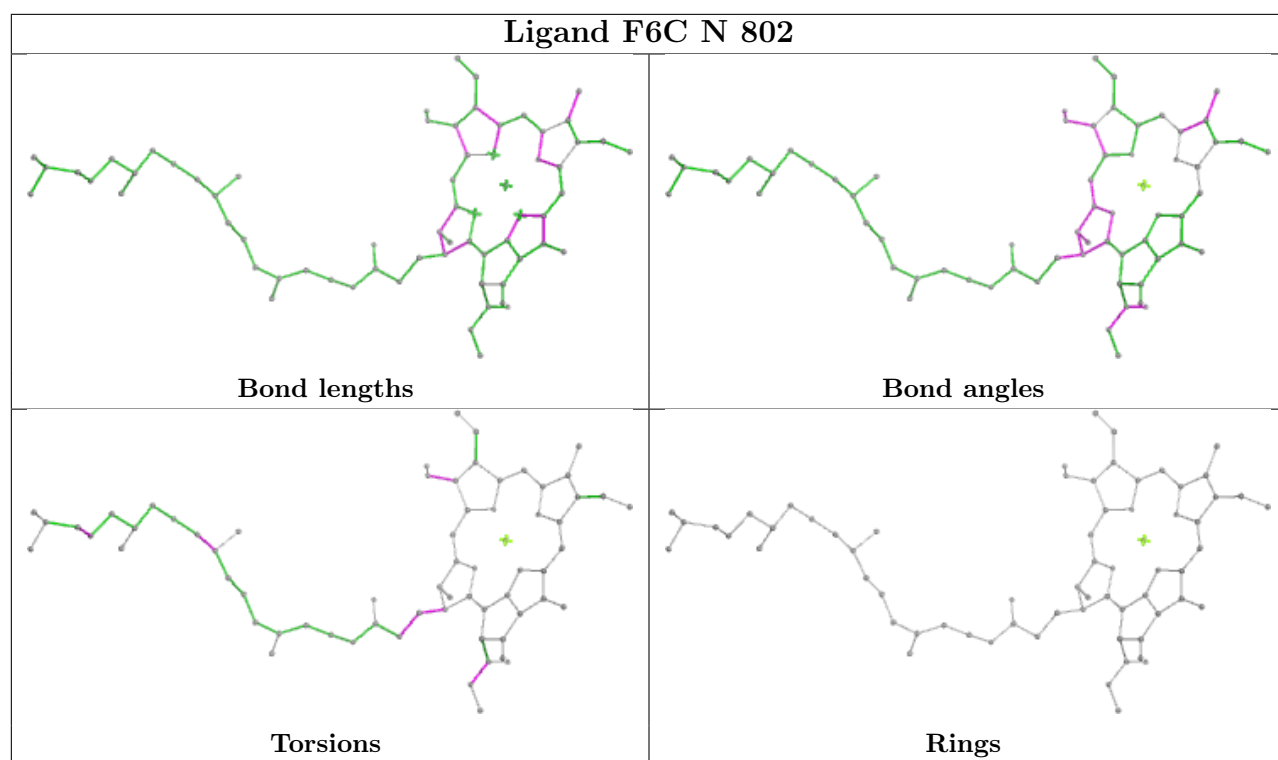


## Ligand CLA B 833

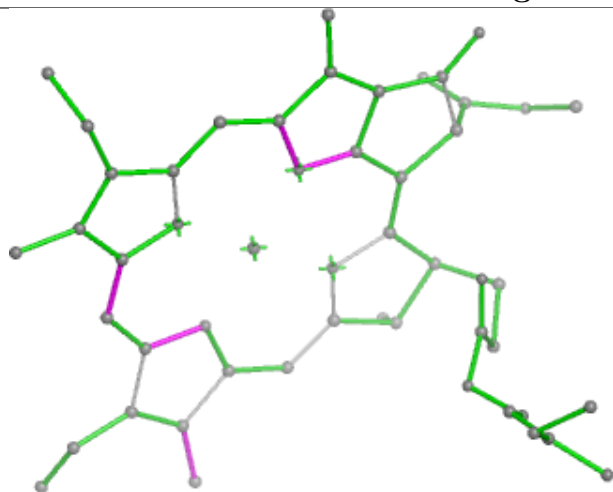


## Ligand CLA i 103

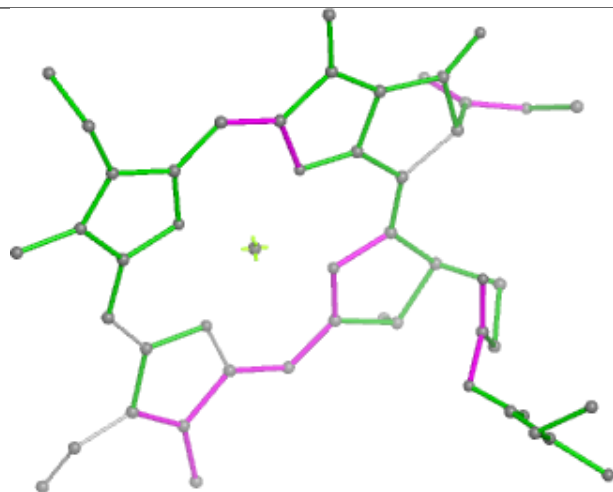




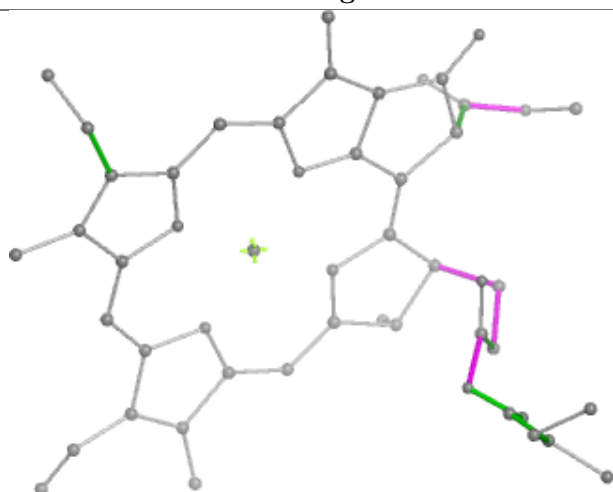
## Ligand CLA N 837



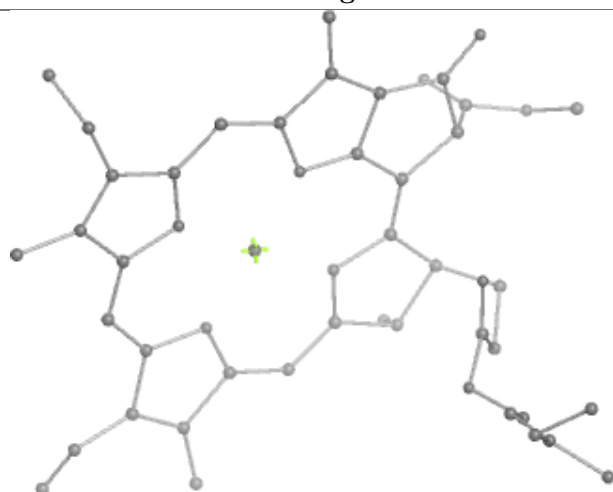
Bond lengths



Bond angles

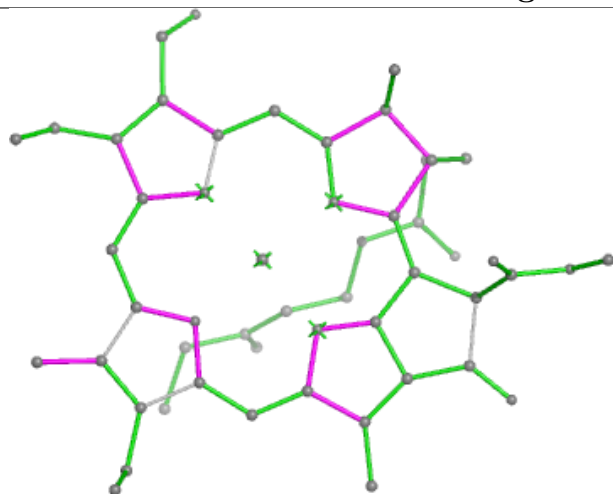


Torsions

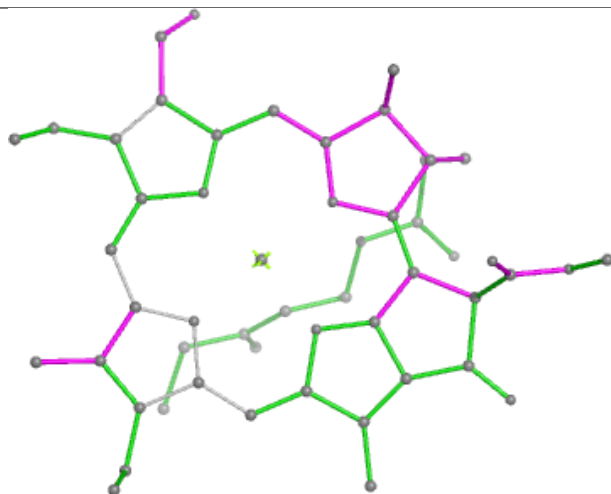


Rings

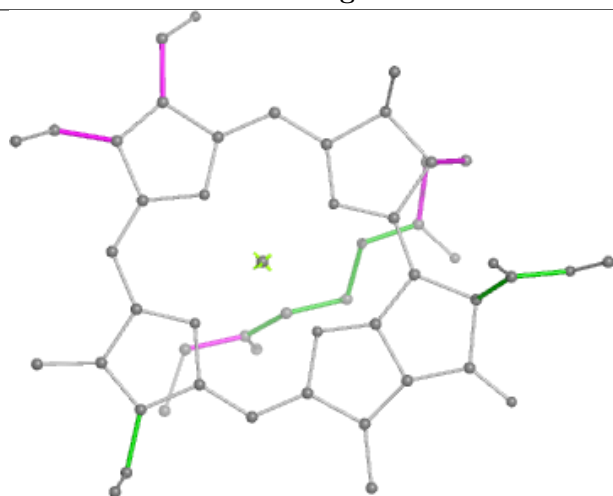
## Ligand F6C A 824



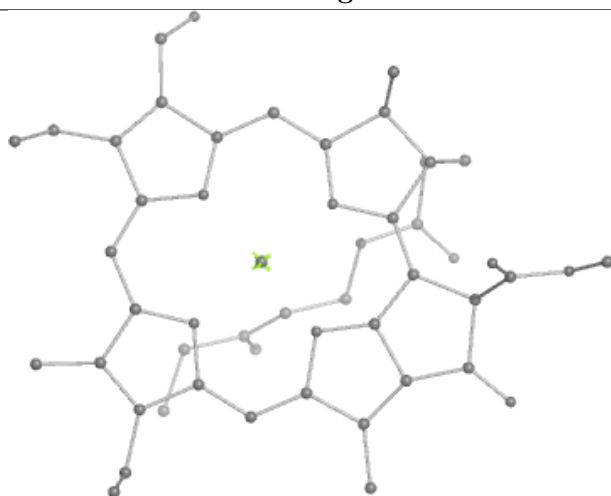
Bond lengths



Bond angles

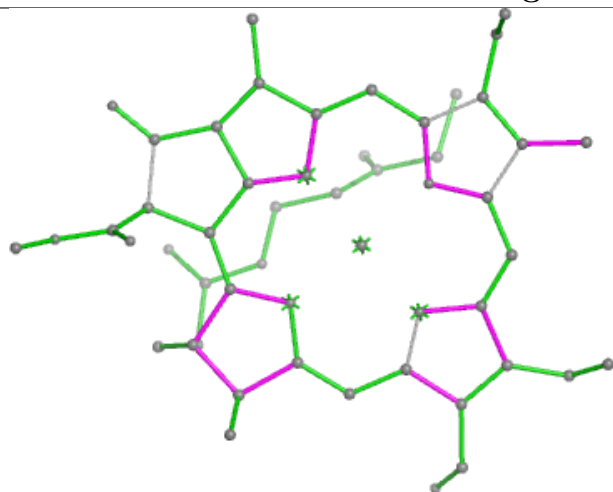


Torsions

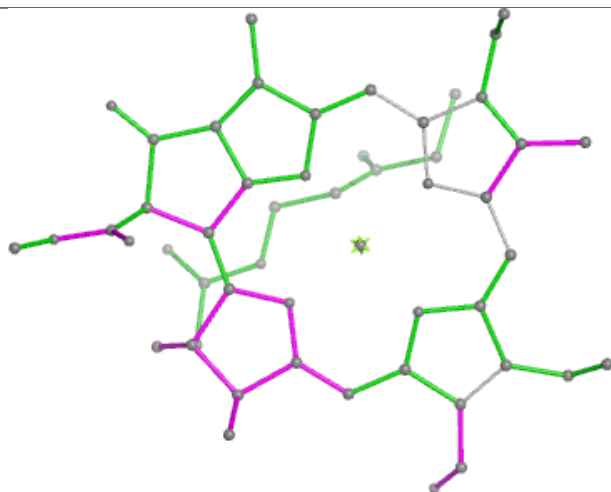


Rings

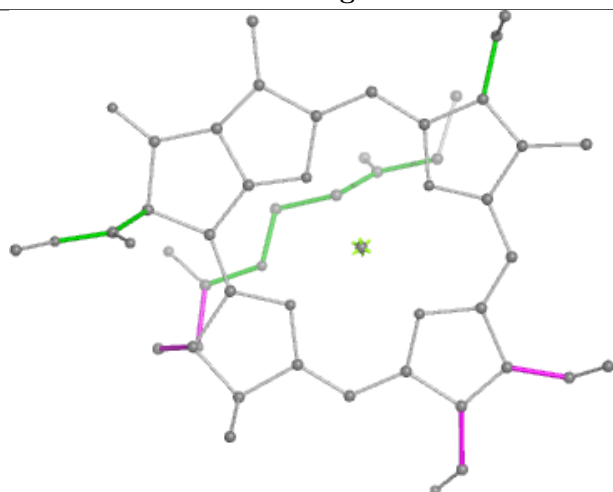
## Ligand F6C a 824



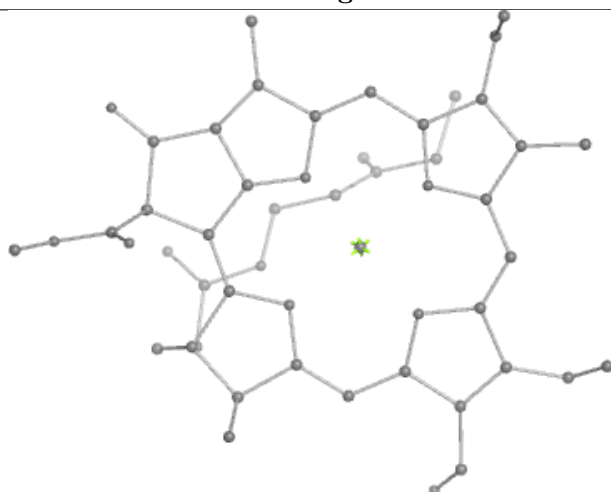
Bond lengths



Bond angles

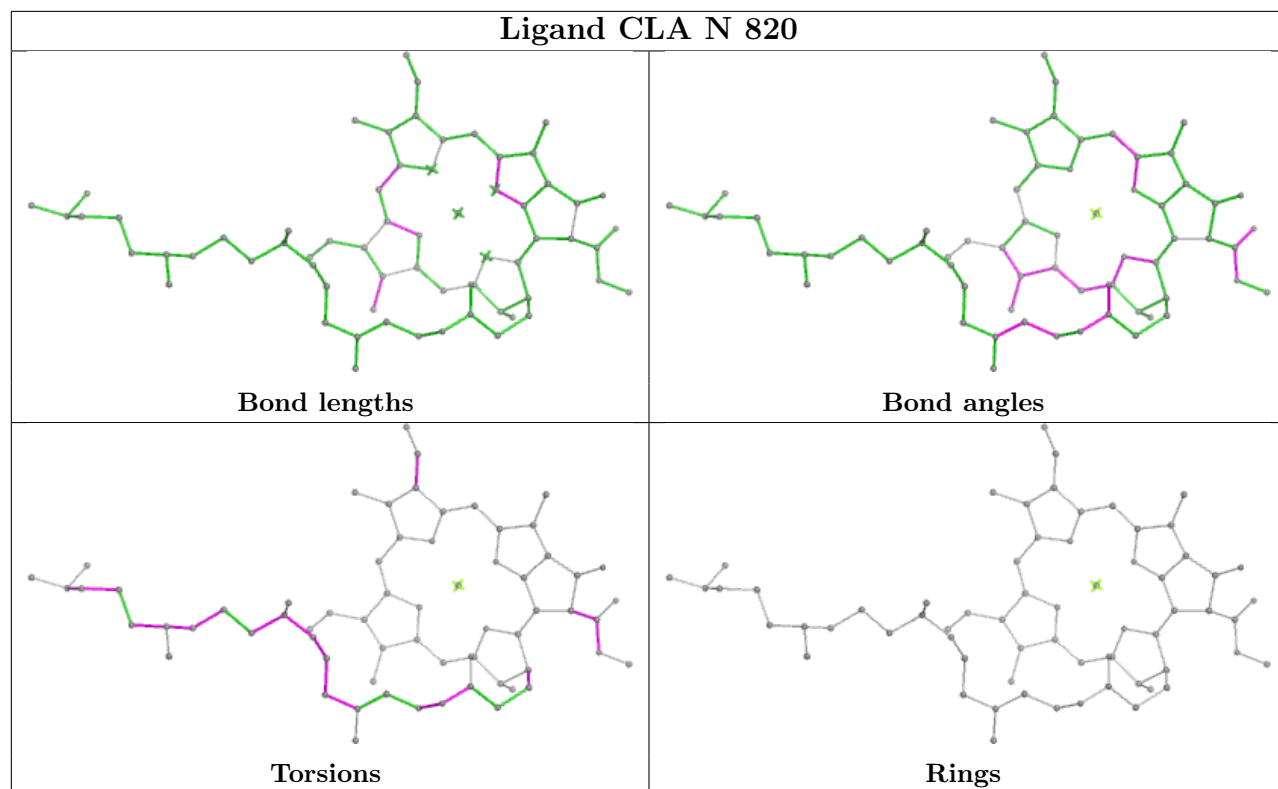
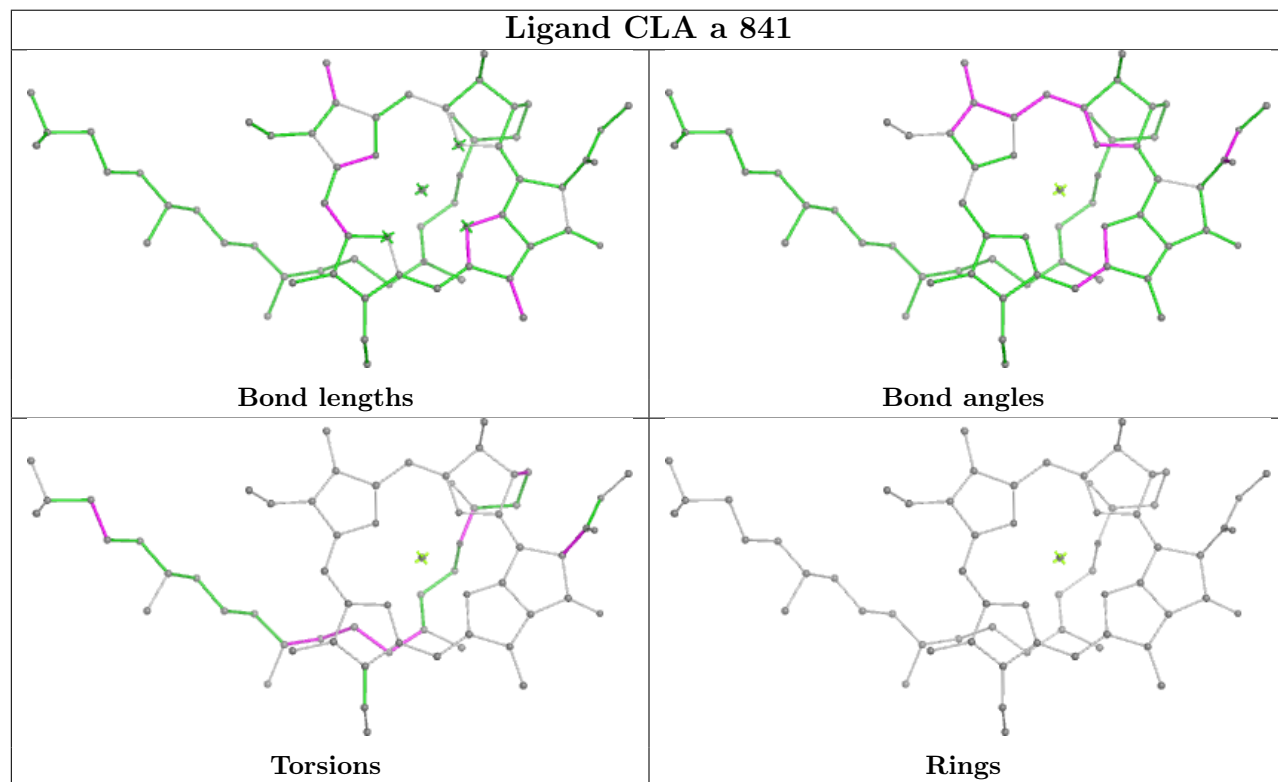


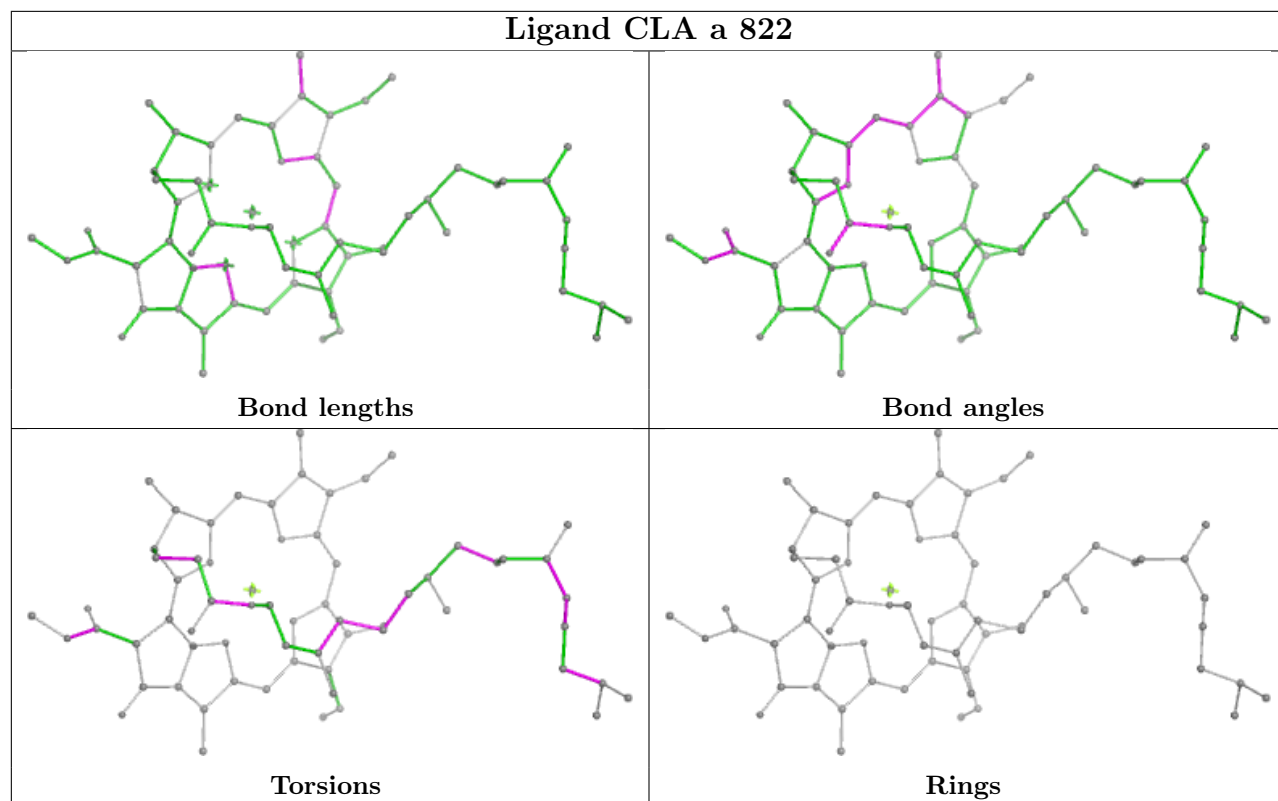
Torsions



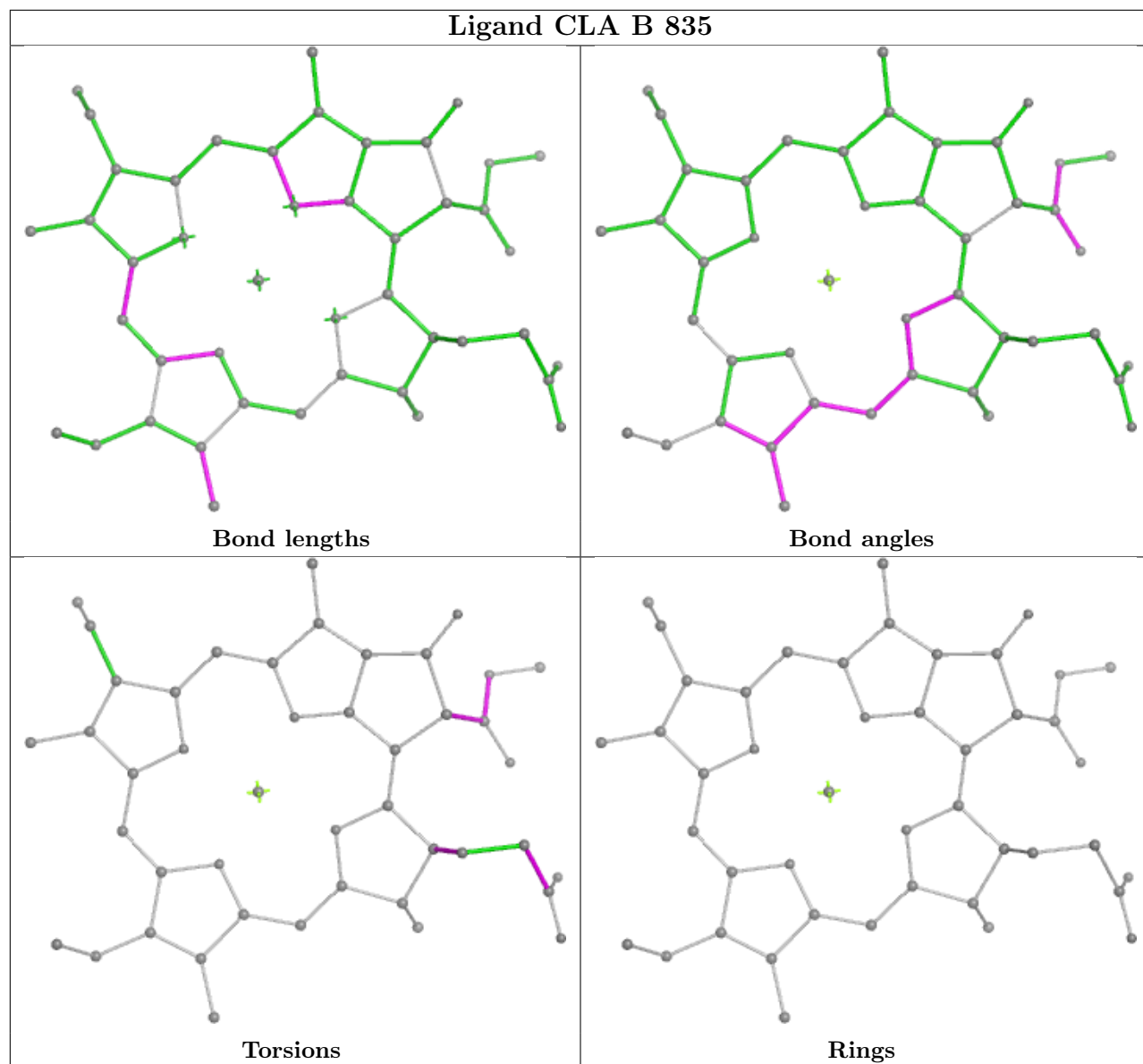
Rings



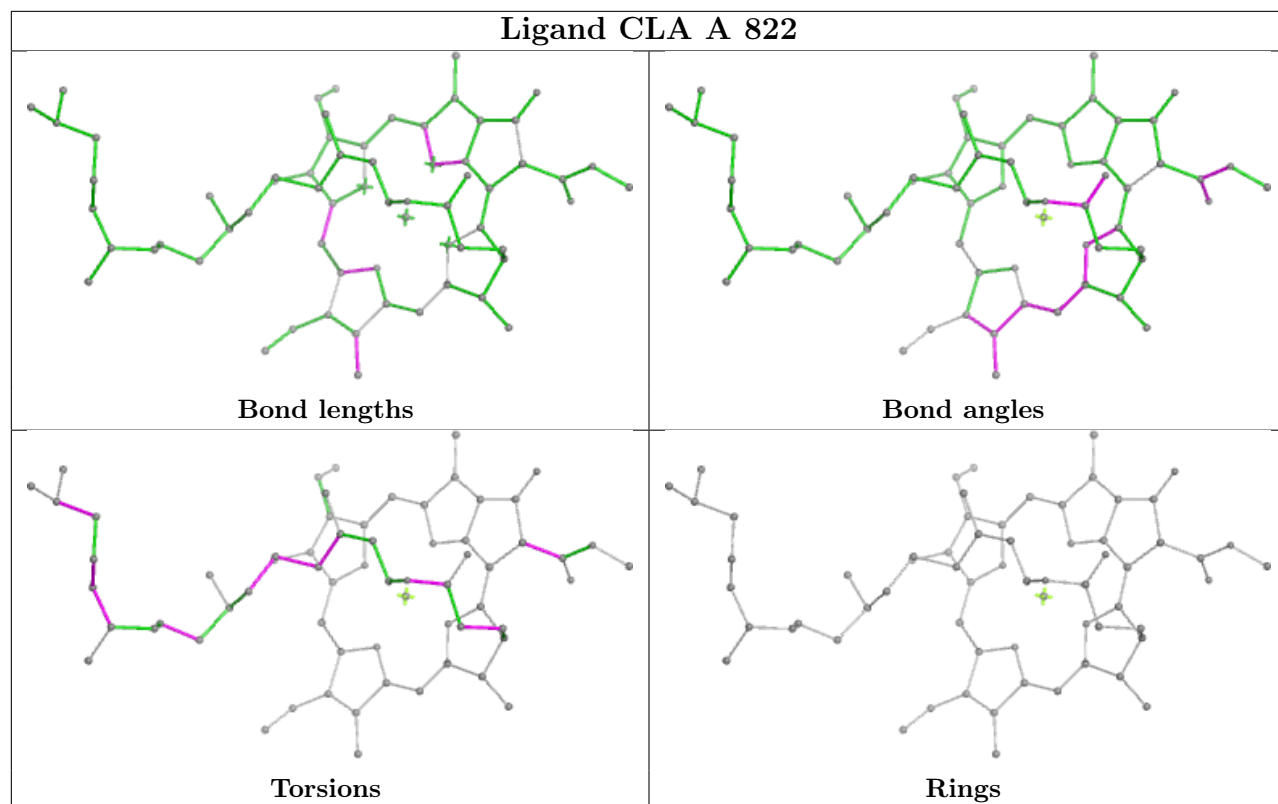
**Ligand CLA N 820****Ligand CLA a 841**



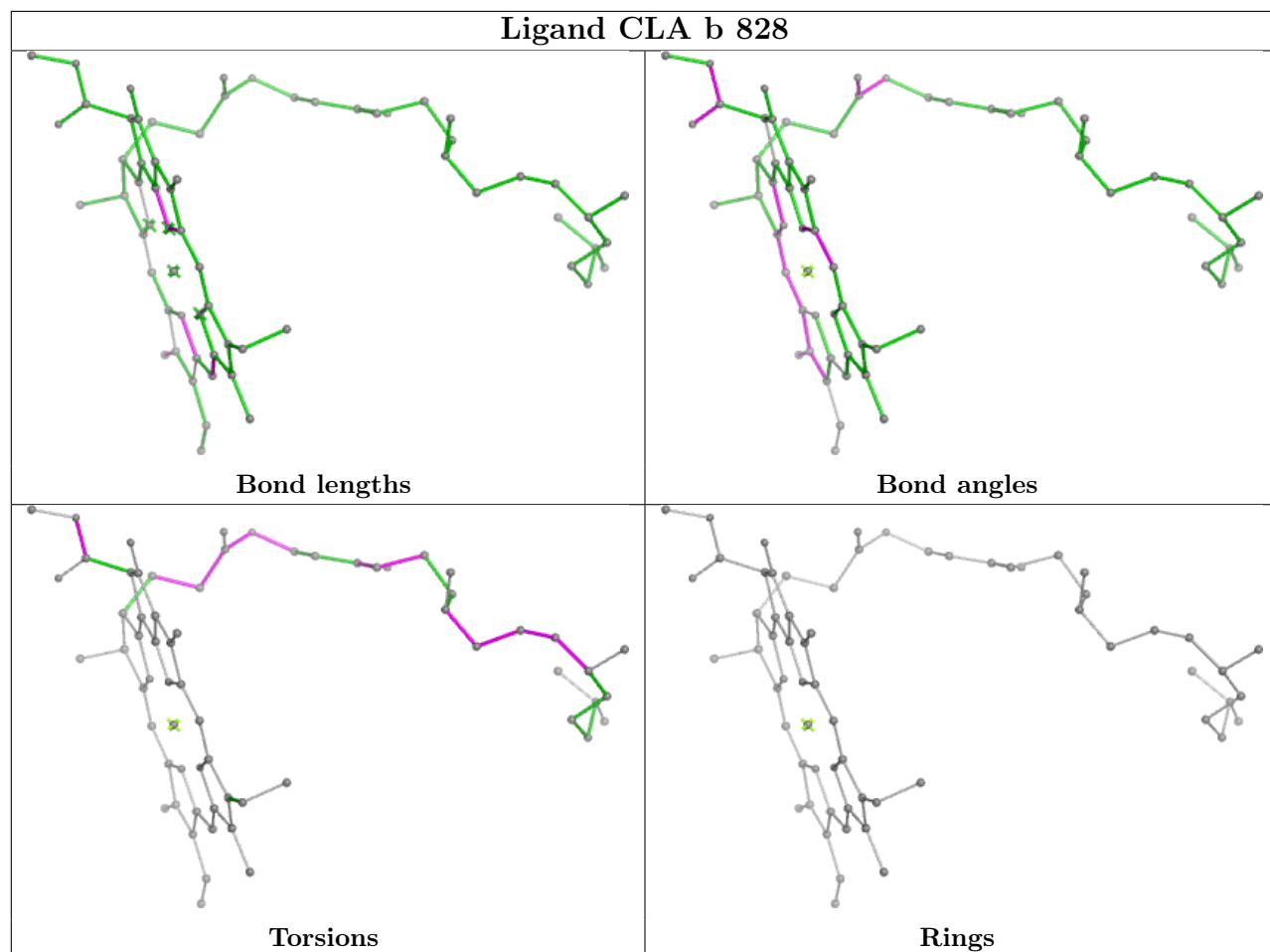
## Ligand CLA B 835



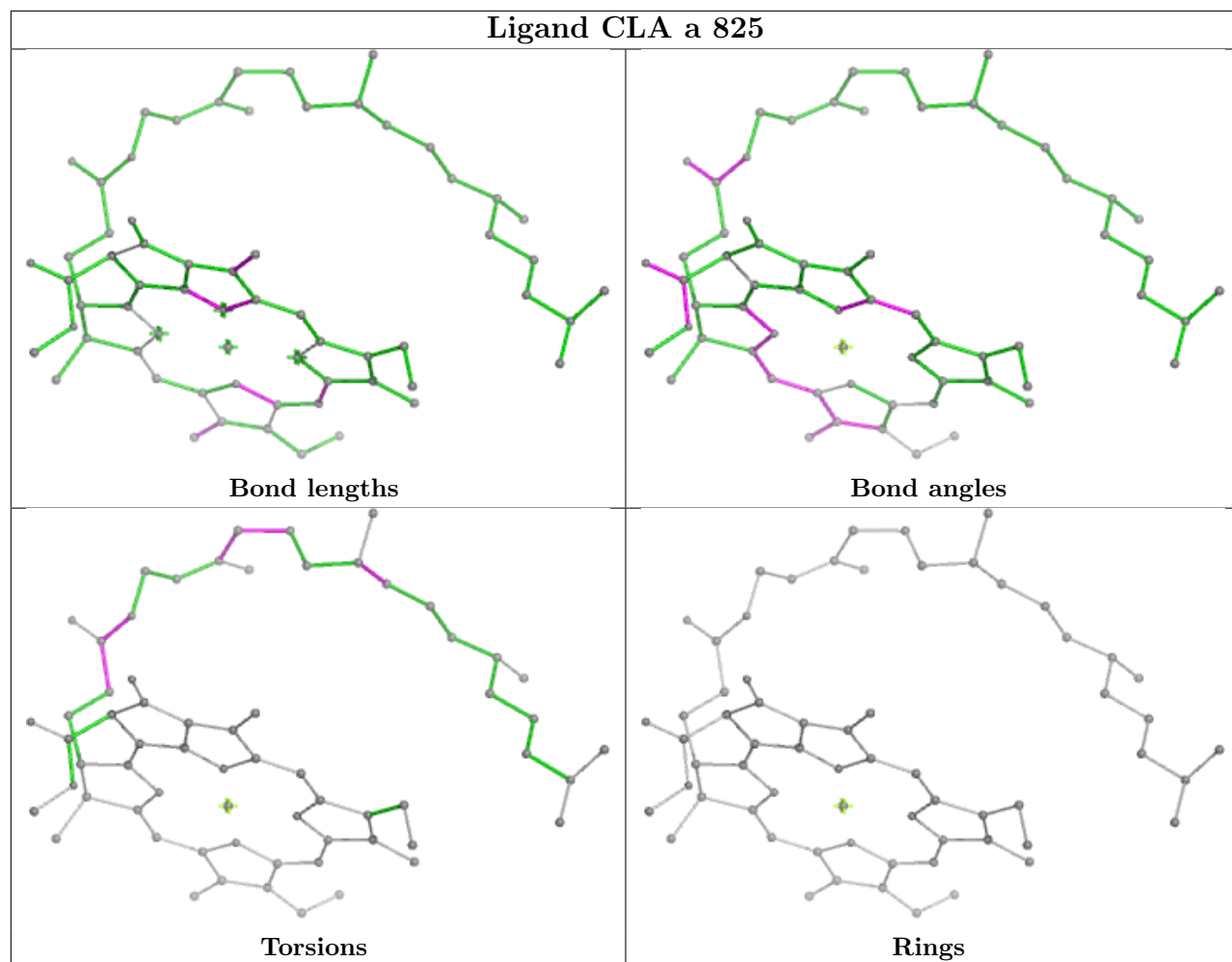
## Ligand CLA A 822



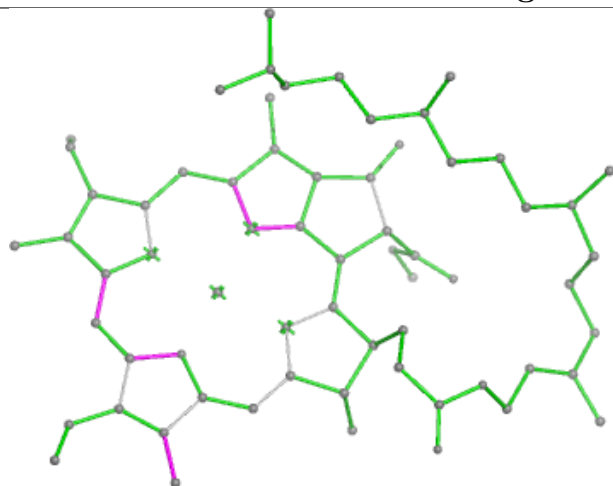
## Ligand CLA b 828



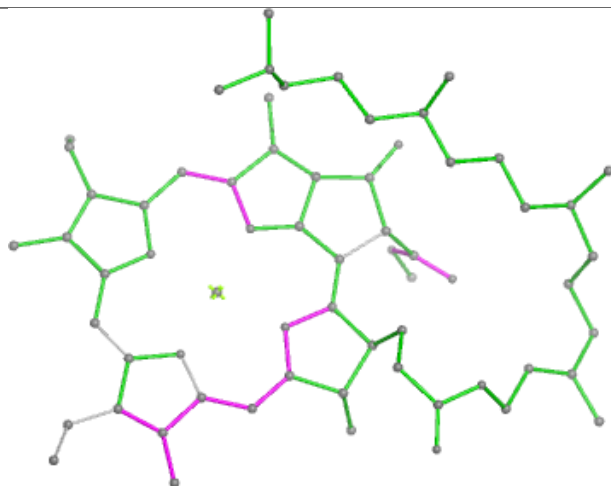
## Ligand CLA a 825



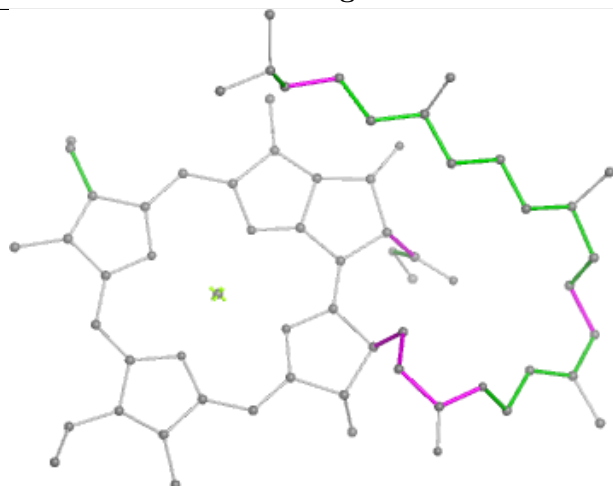
## Ligand CLA b 805



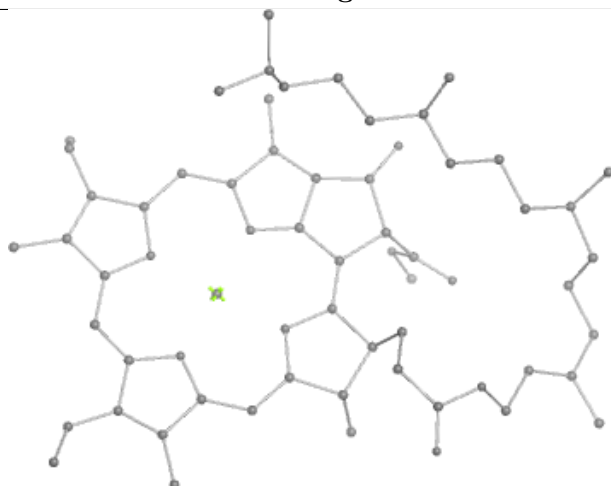
Bond lengths



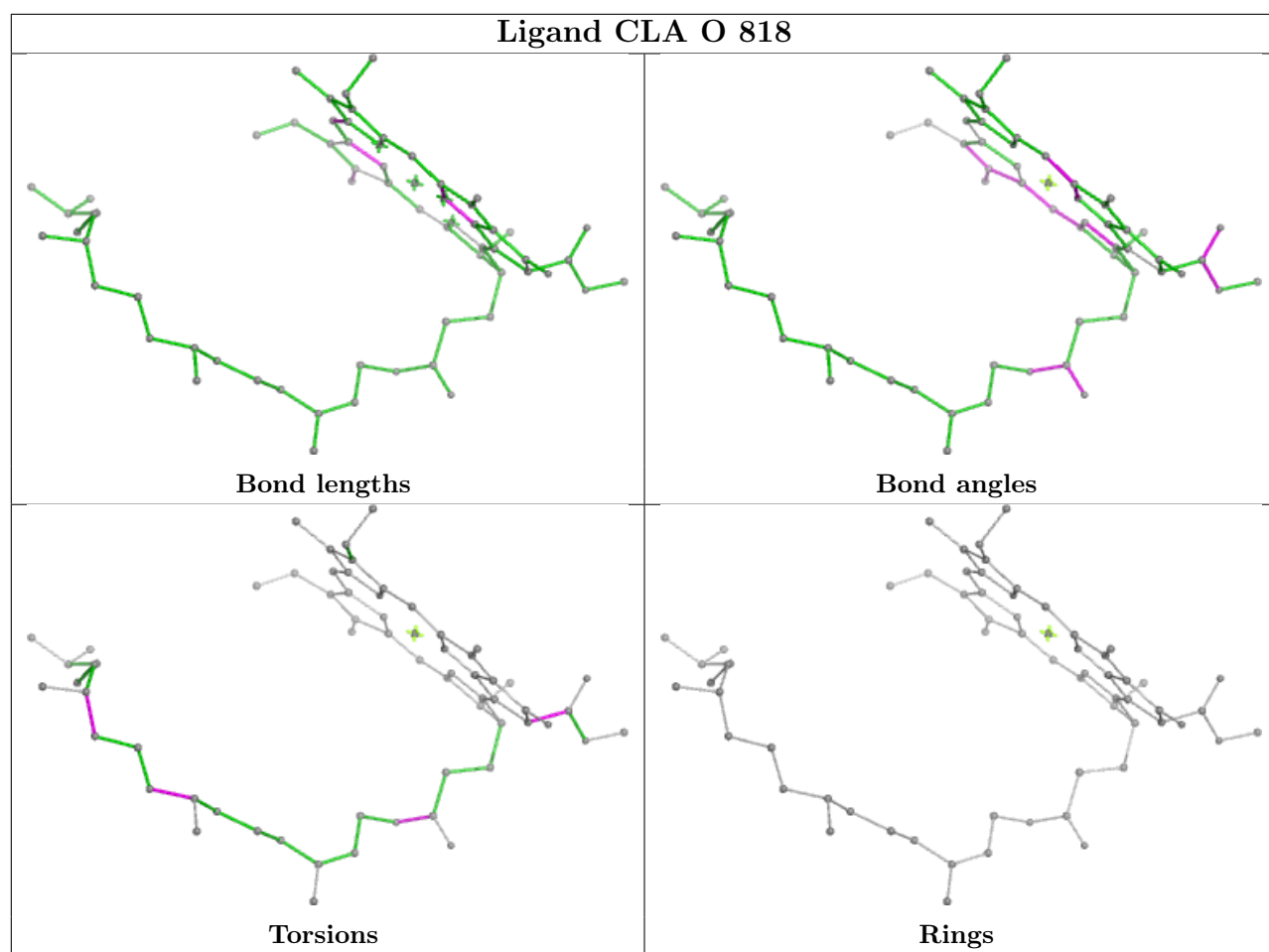
Bond angles

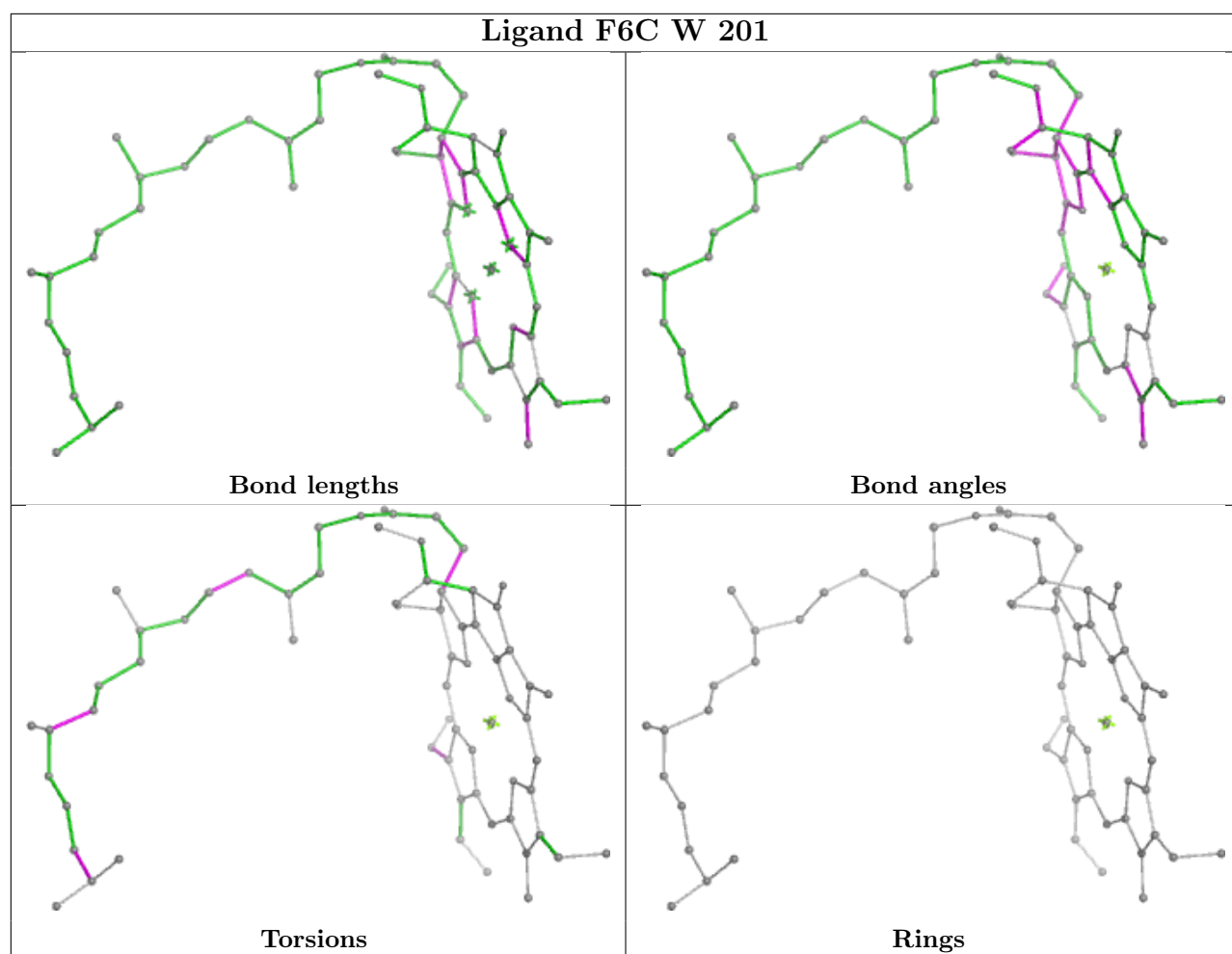


Torsions



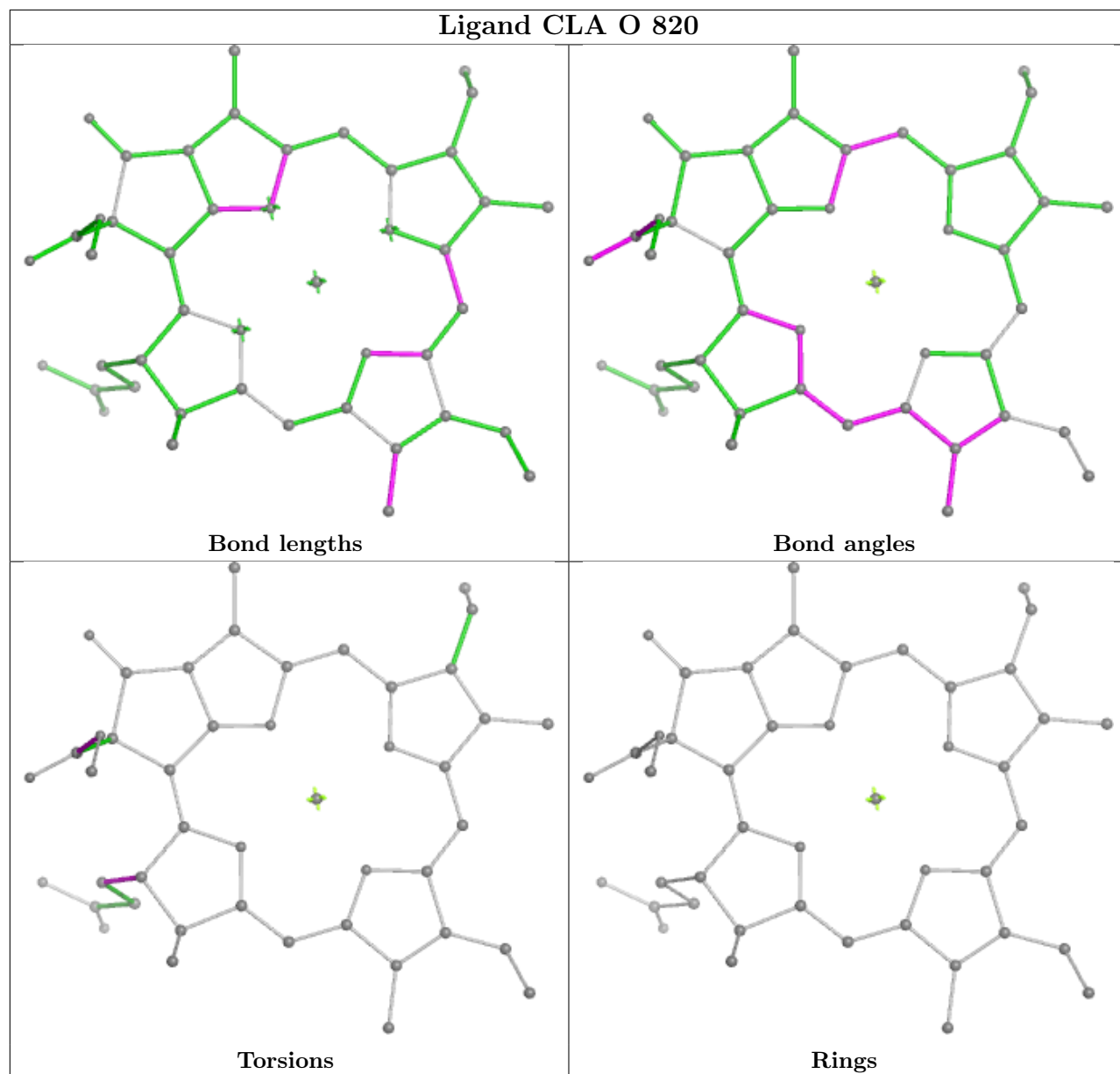
Rings

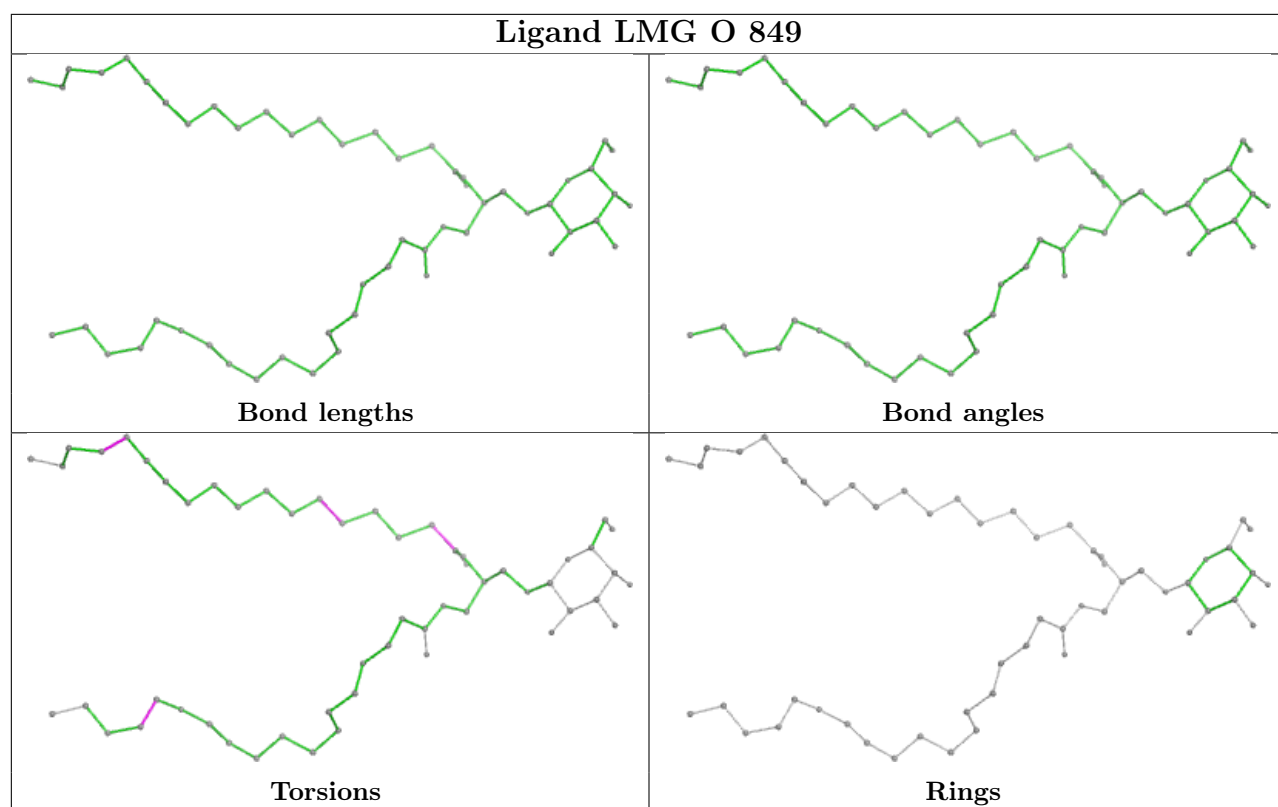




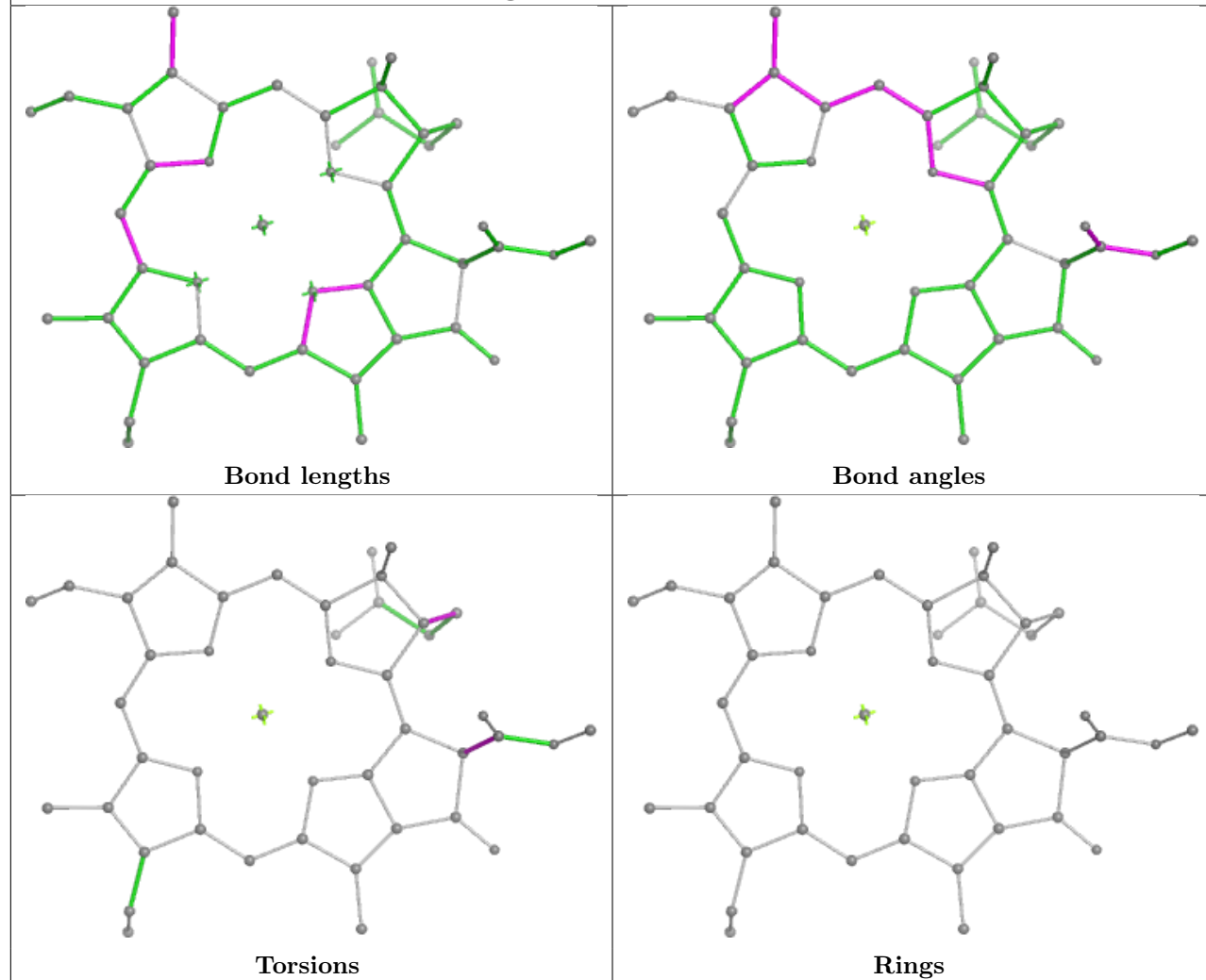


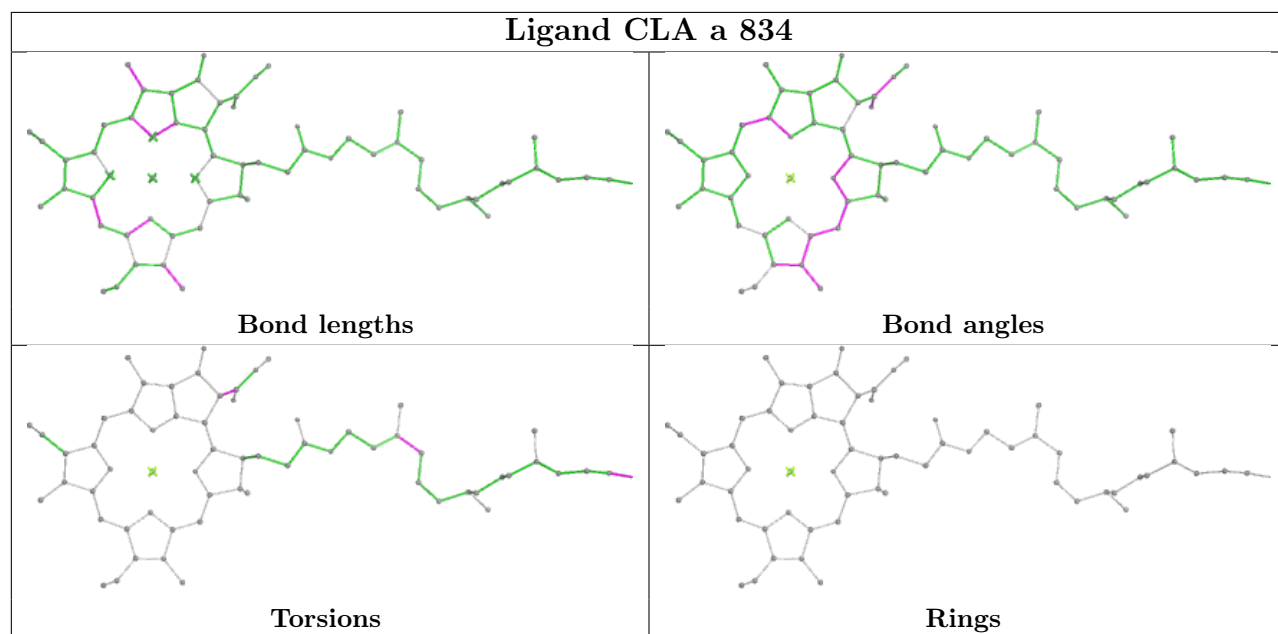
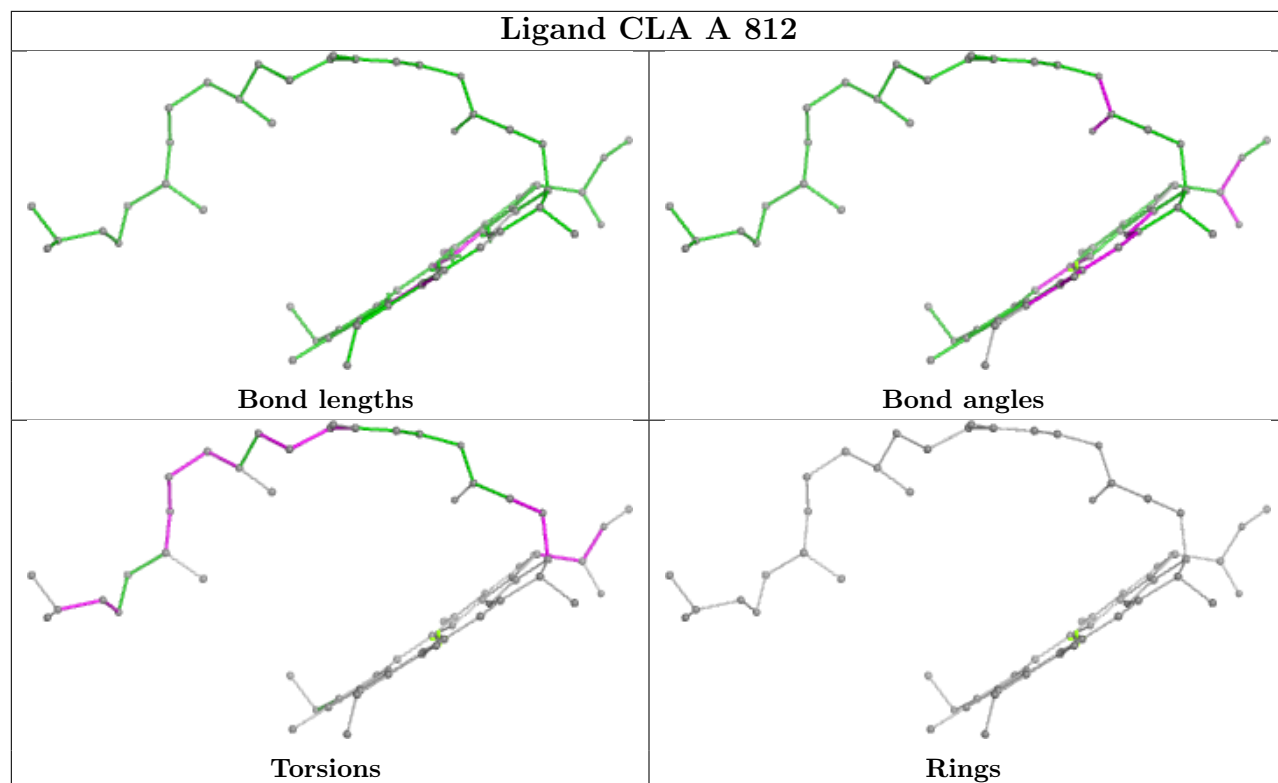
## Ligand CLA O 820

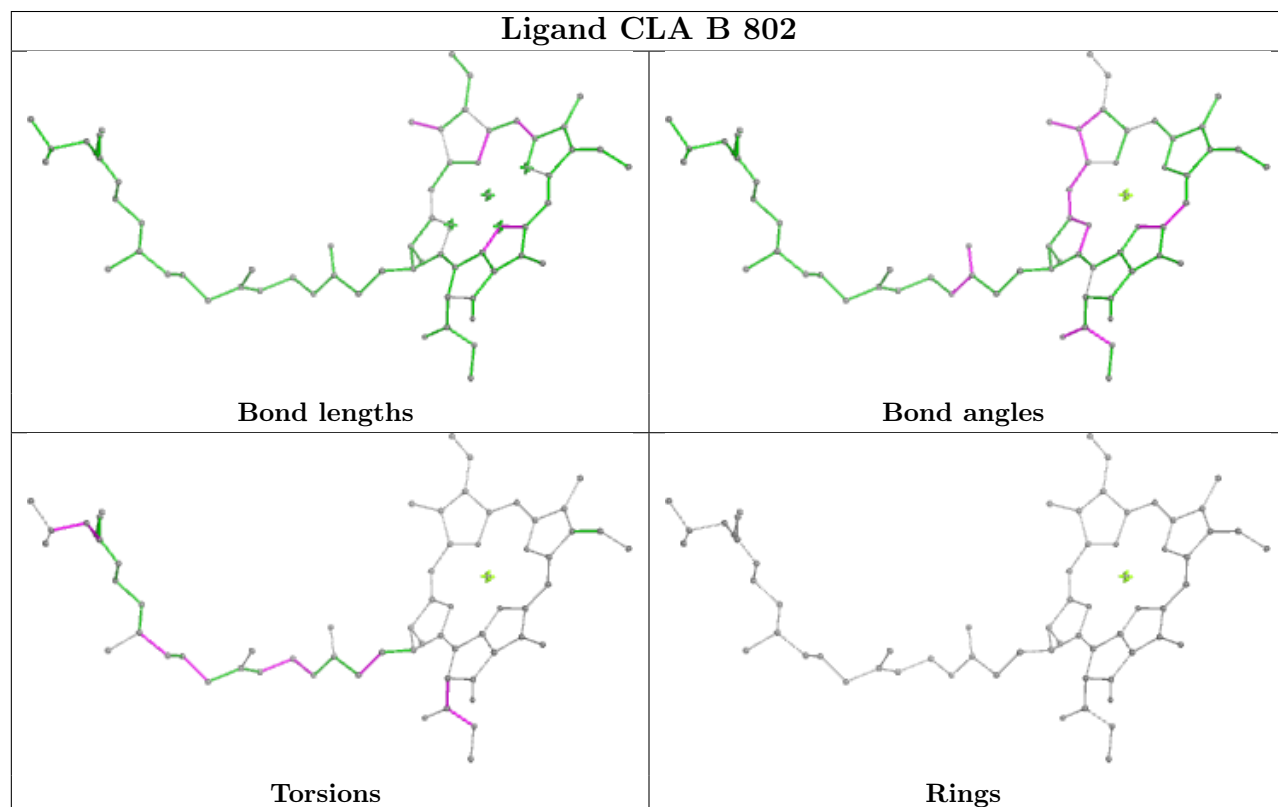
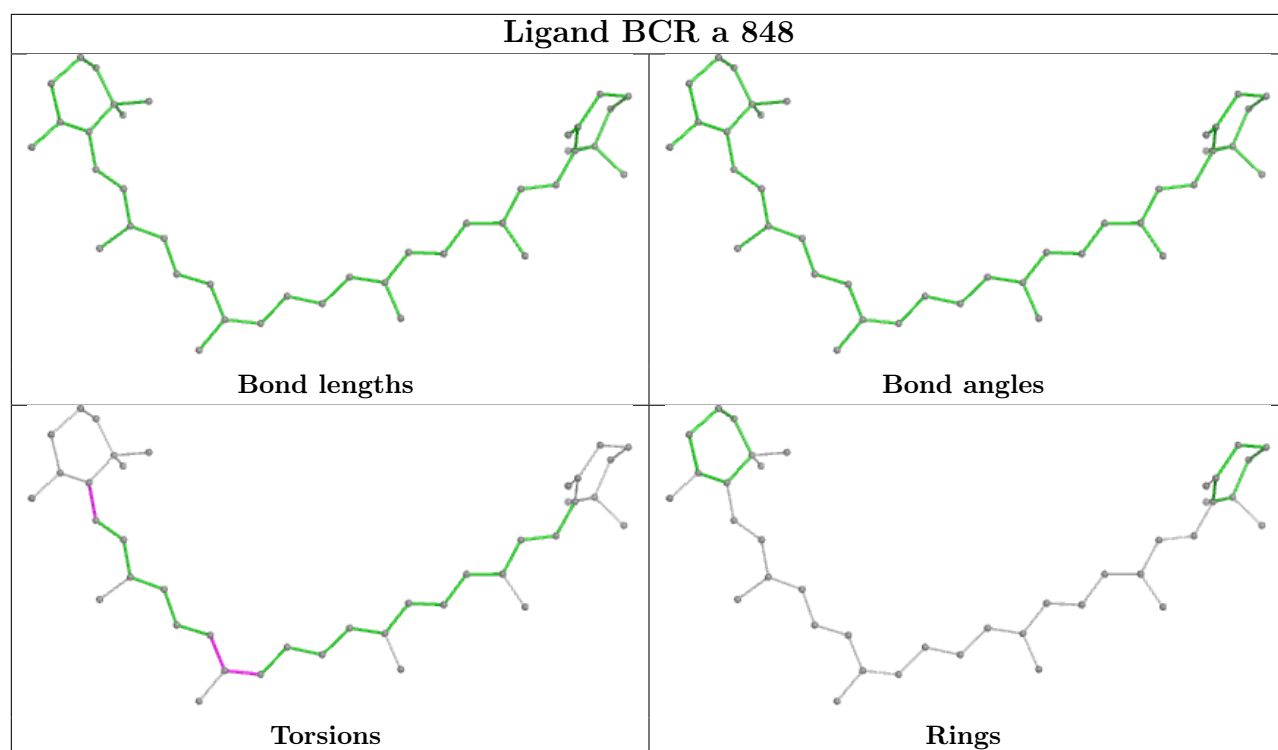




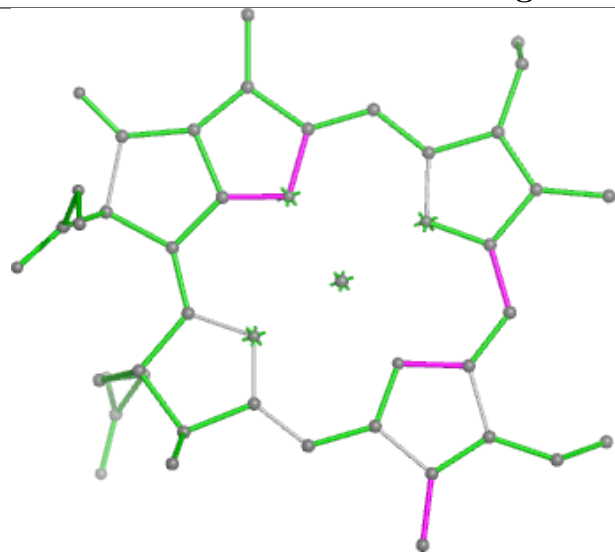
## Ligand CLA B 811



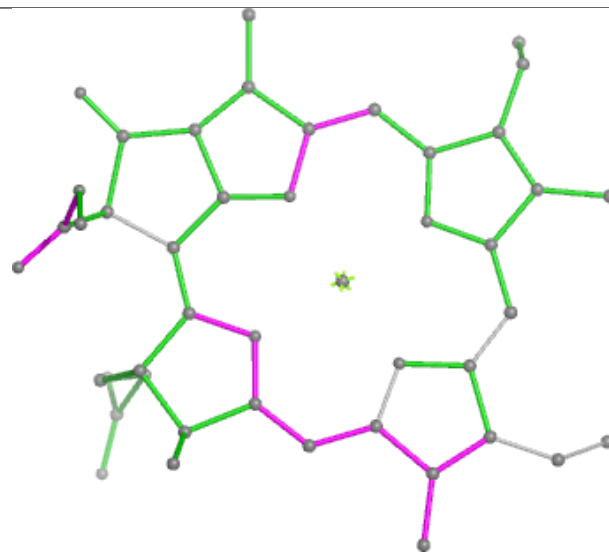




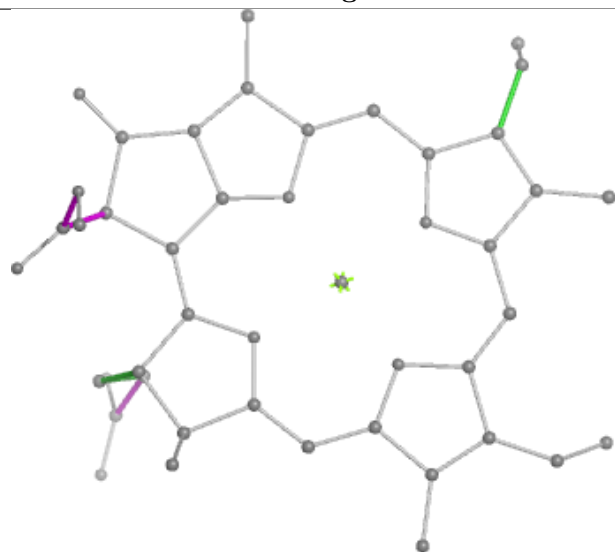
## Ligand CLA A 816



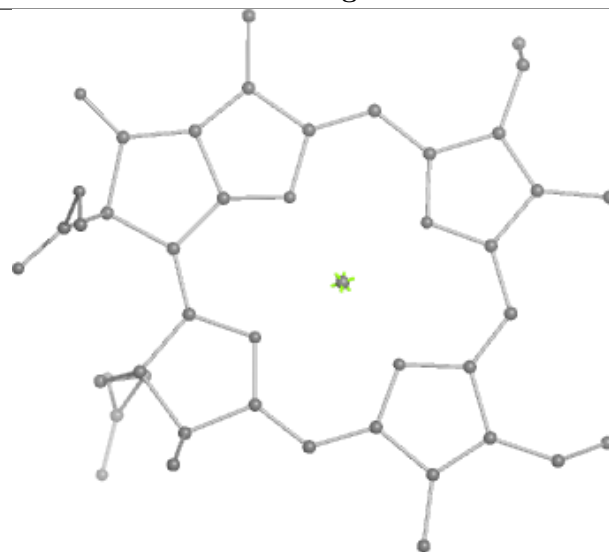
Bond lengths



Bond angles

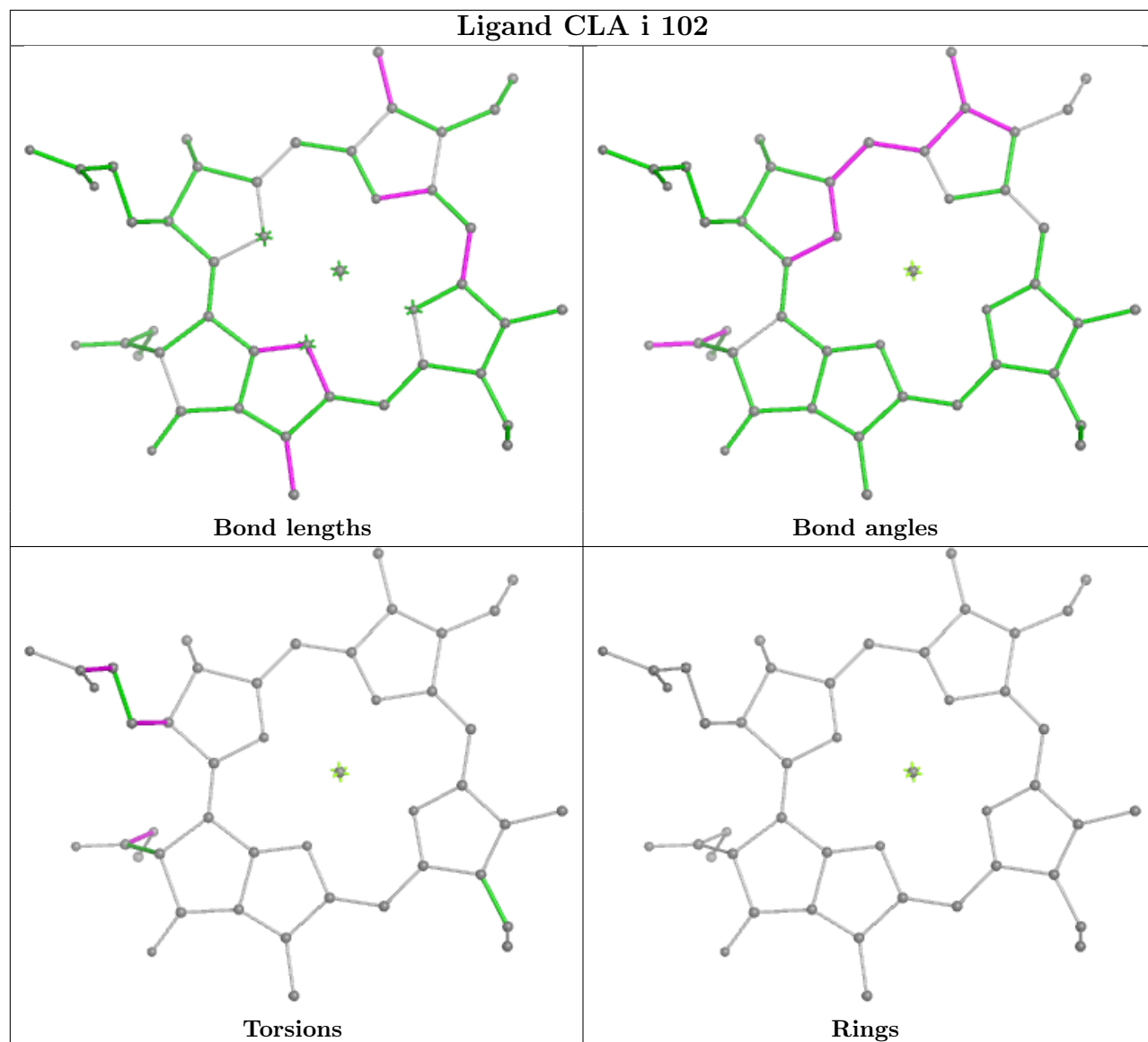


Torsions

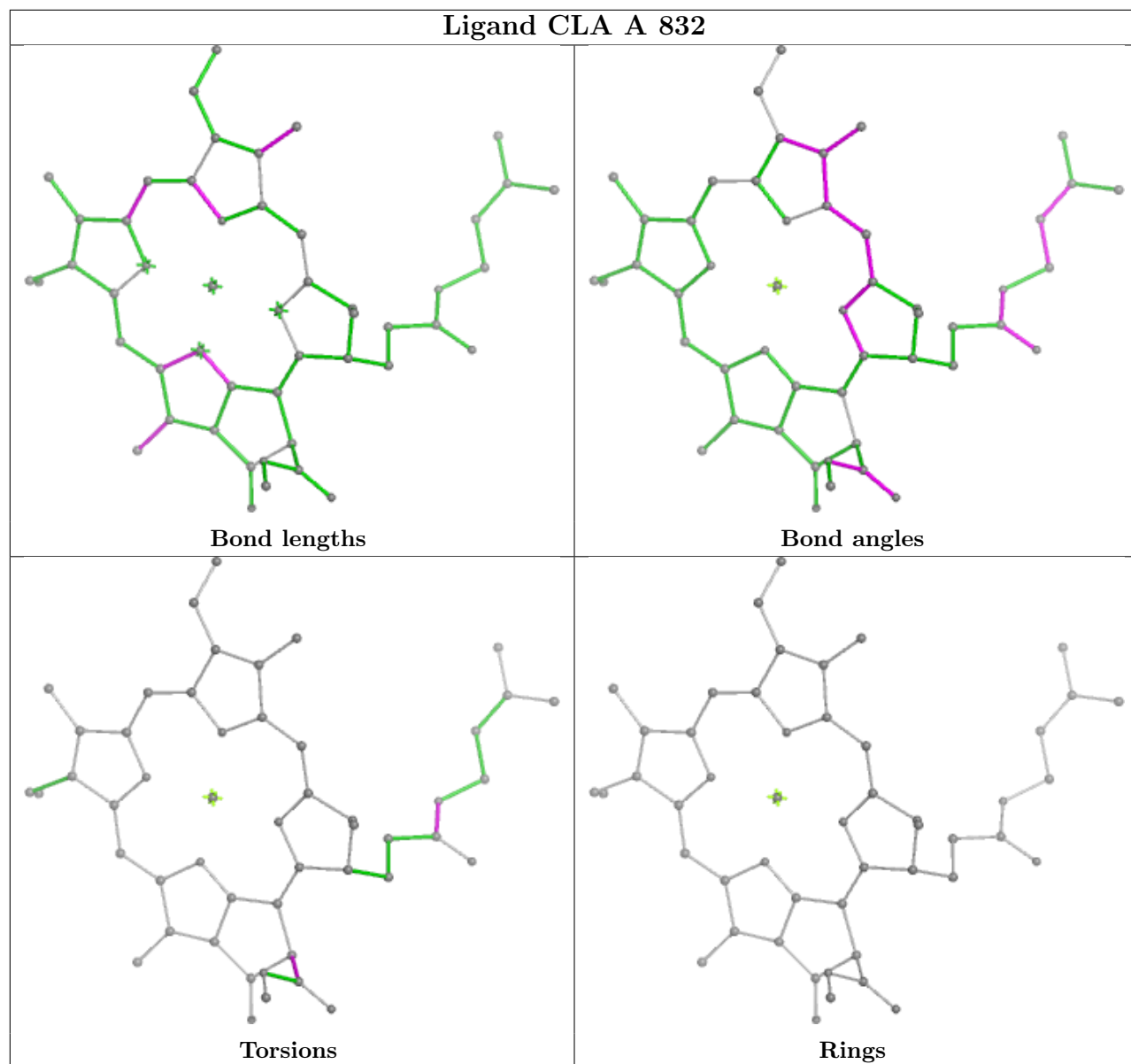


Rings

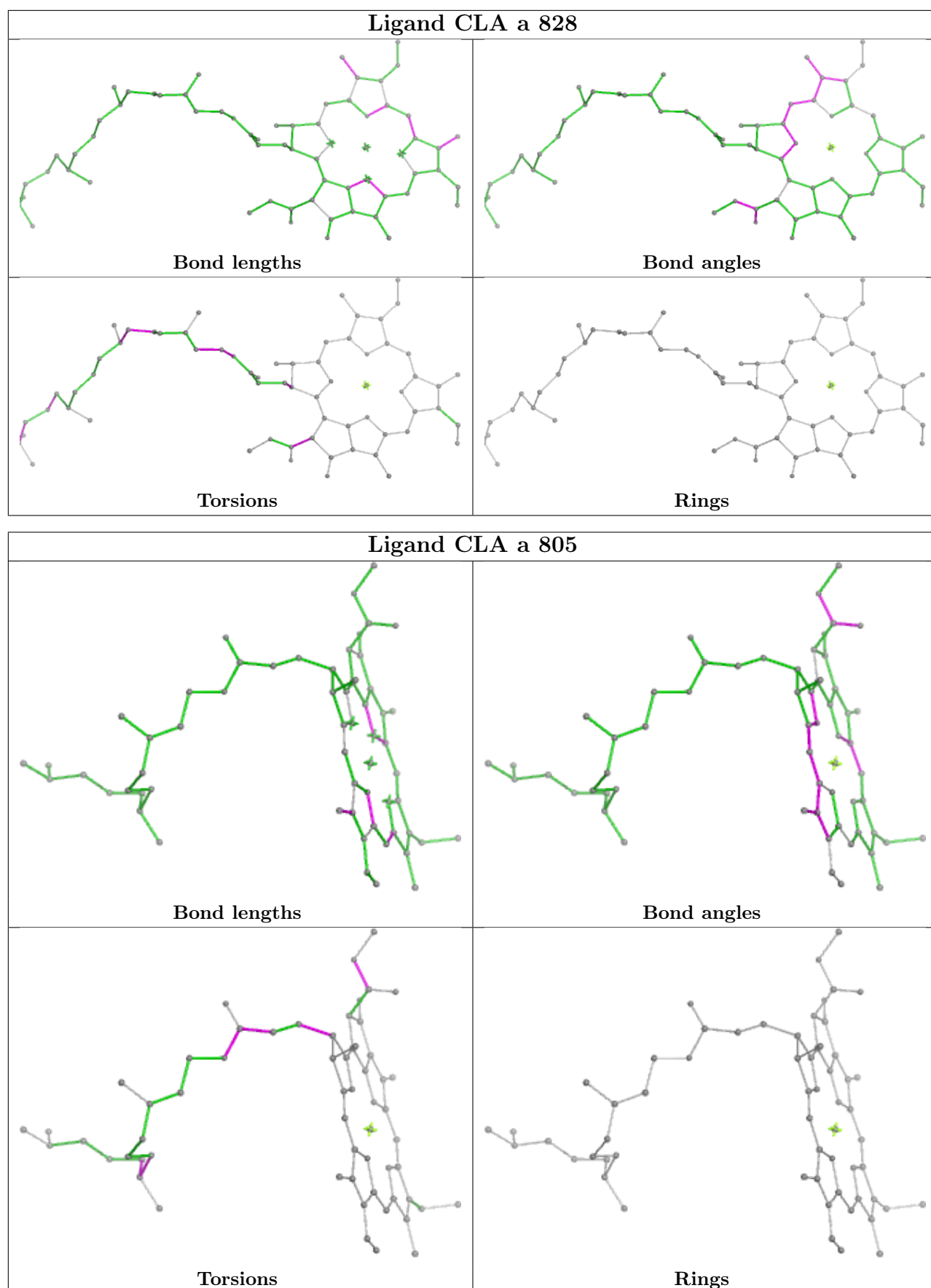
## Ligand CLA i 102



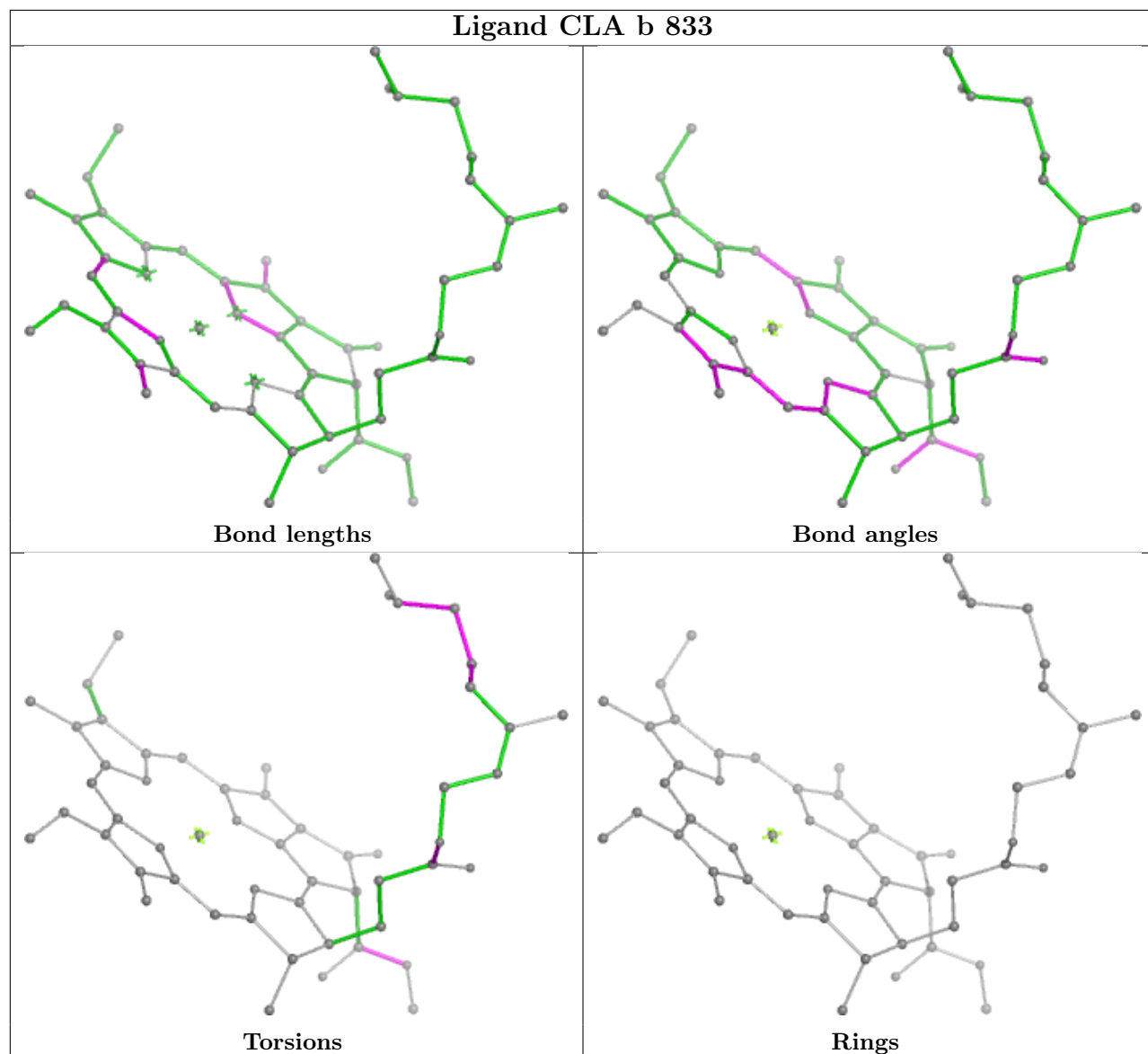
## Ligand CLA A 832



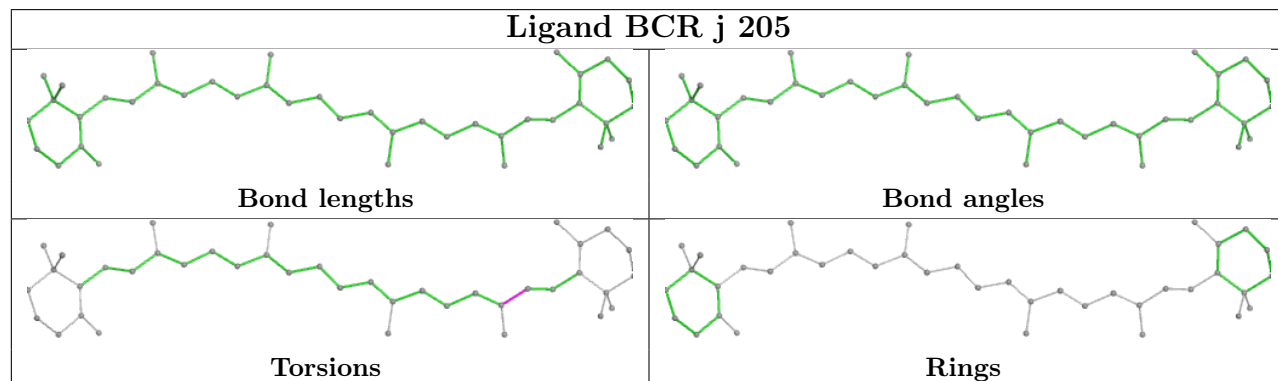




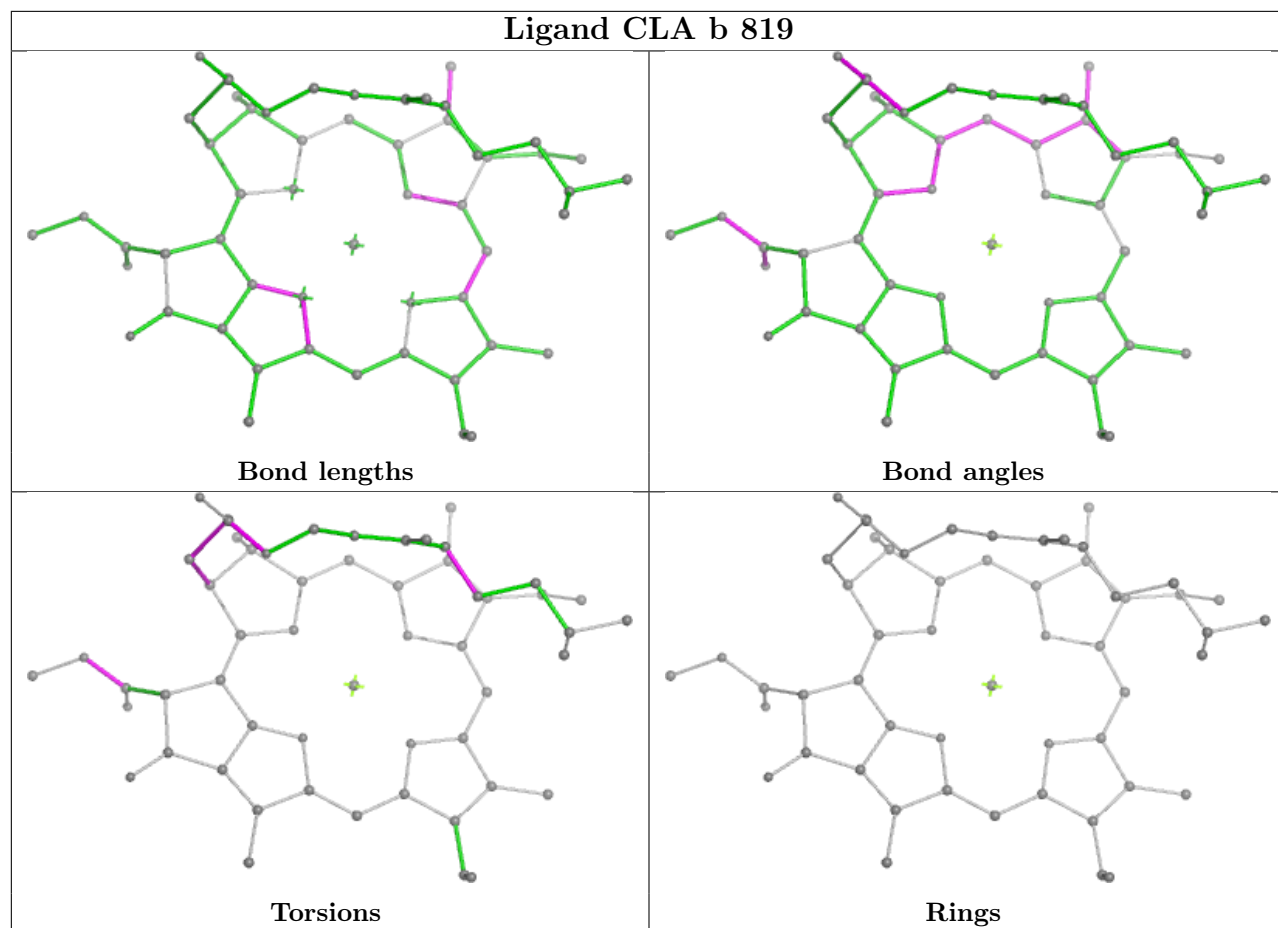
## Ligand CLA b 833



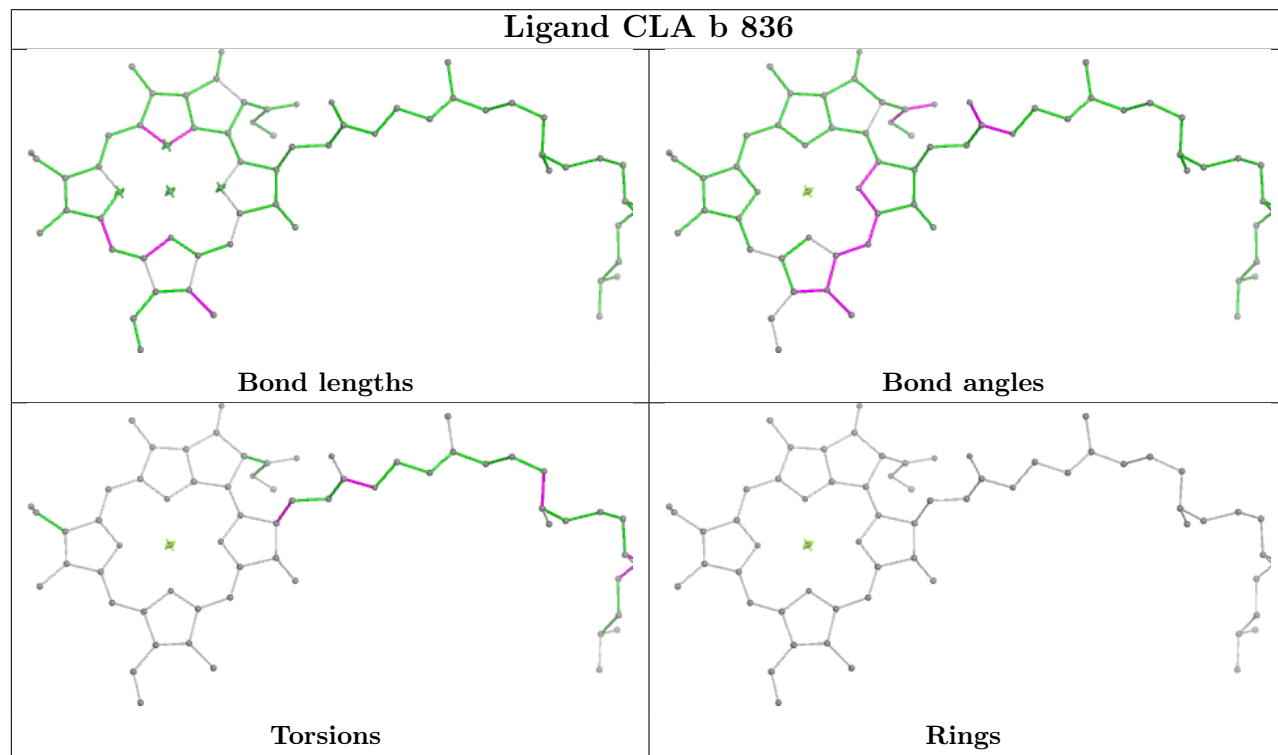
## Ligand BCR j 205

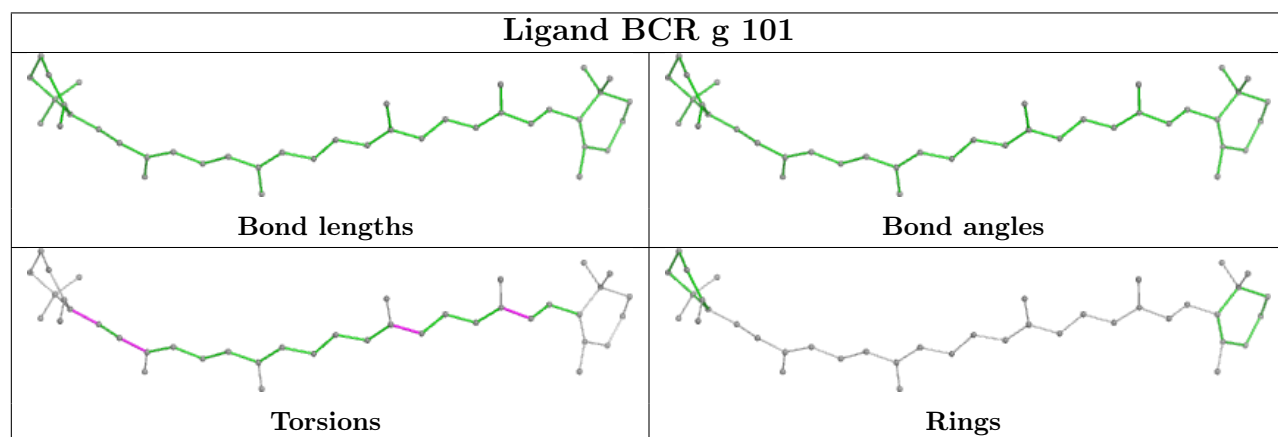
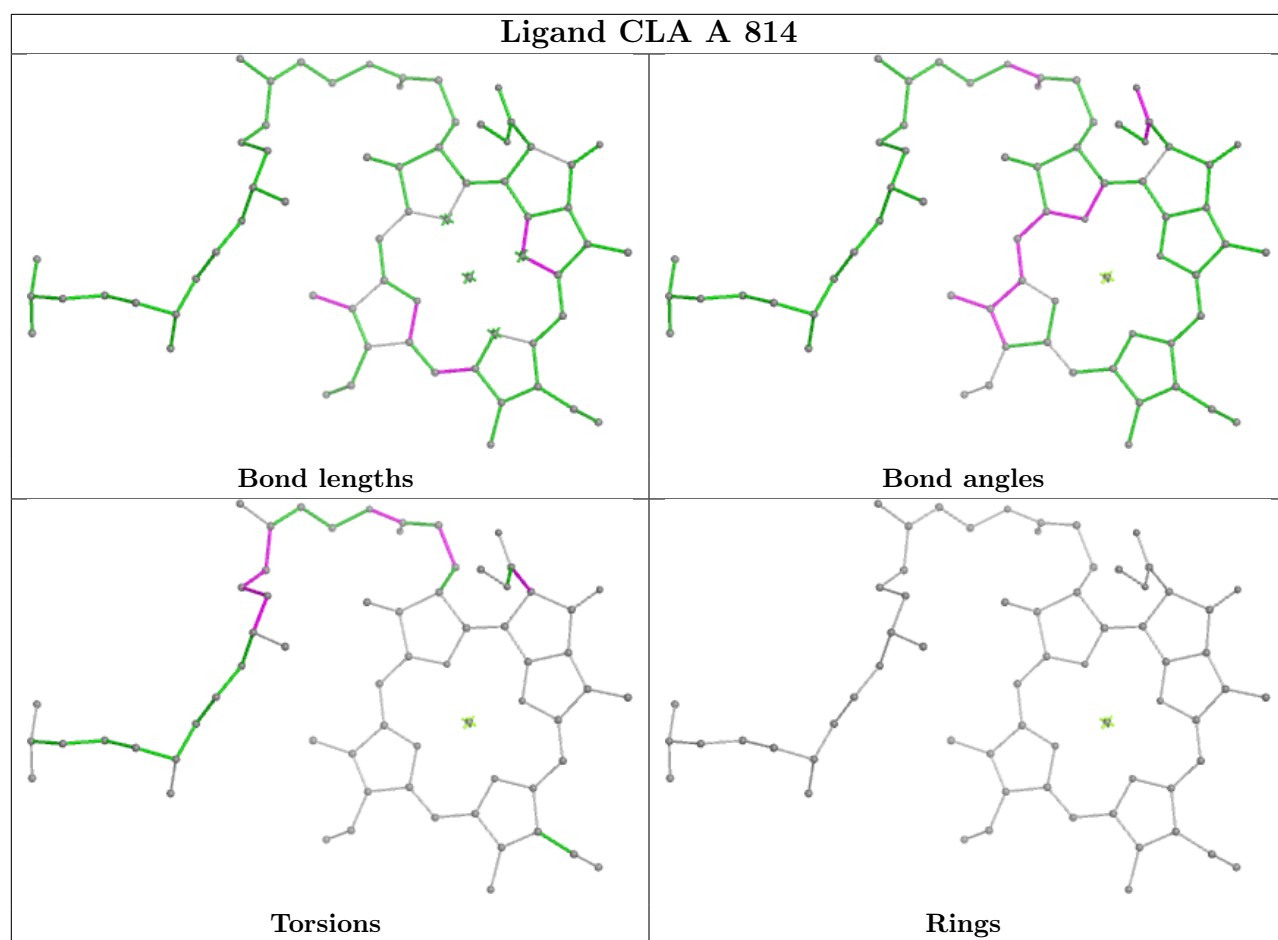


## Ligand CLA b 819

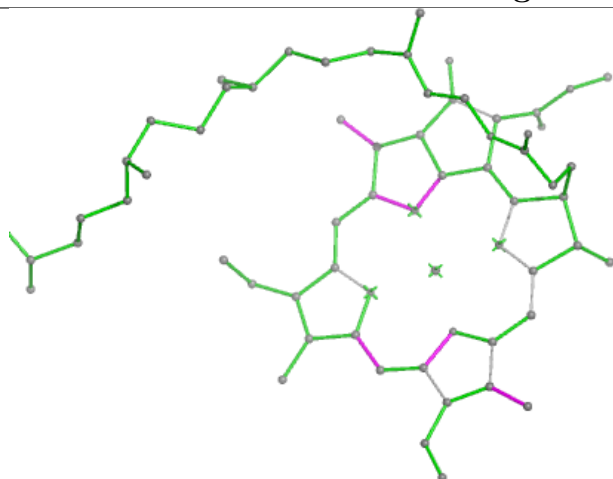


## Ligand CLA b 836

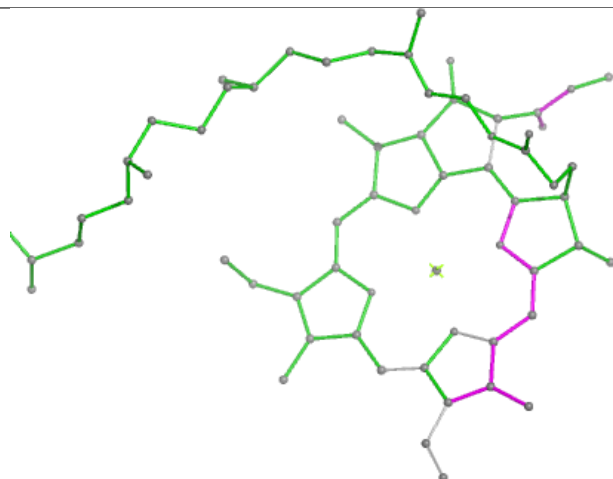




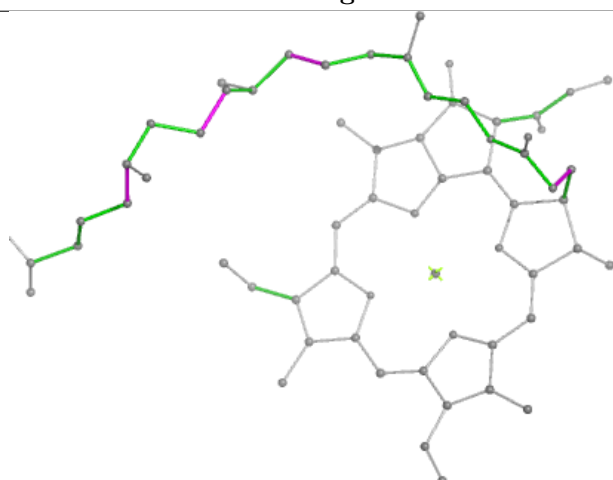
## Ligand CLA N 830



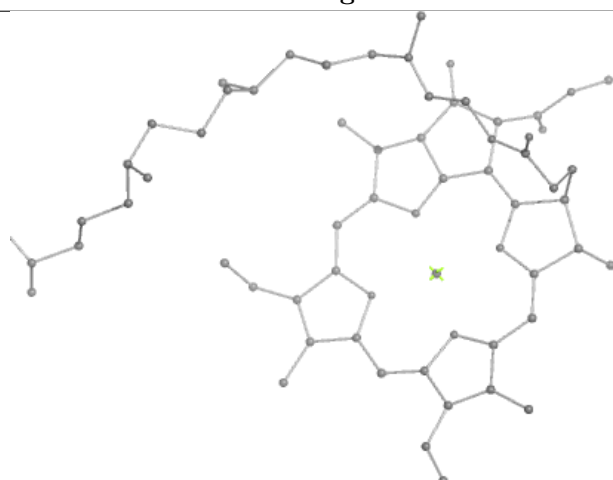
Bond lengths



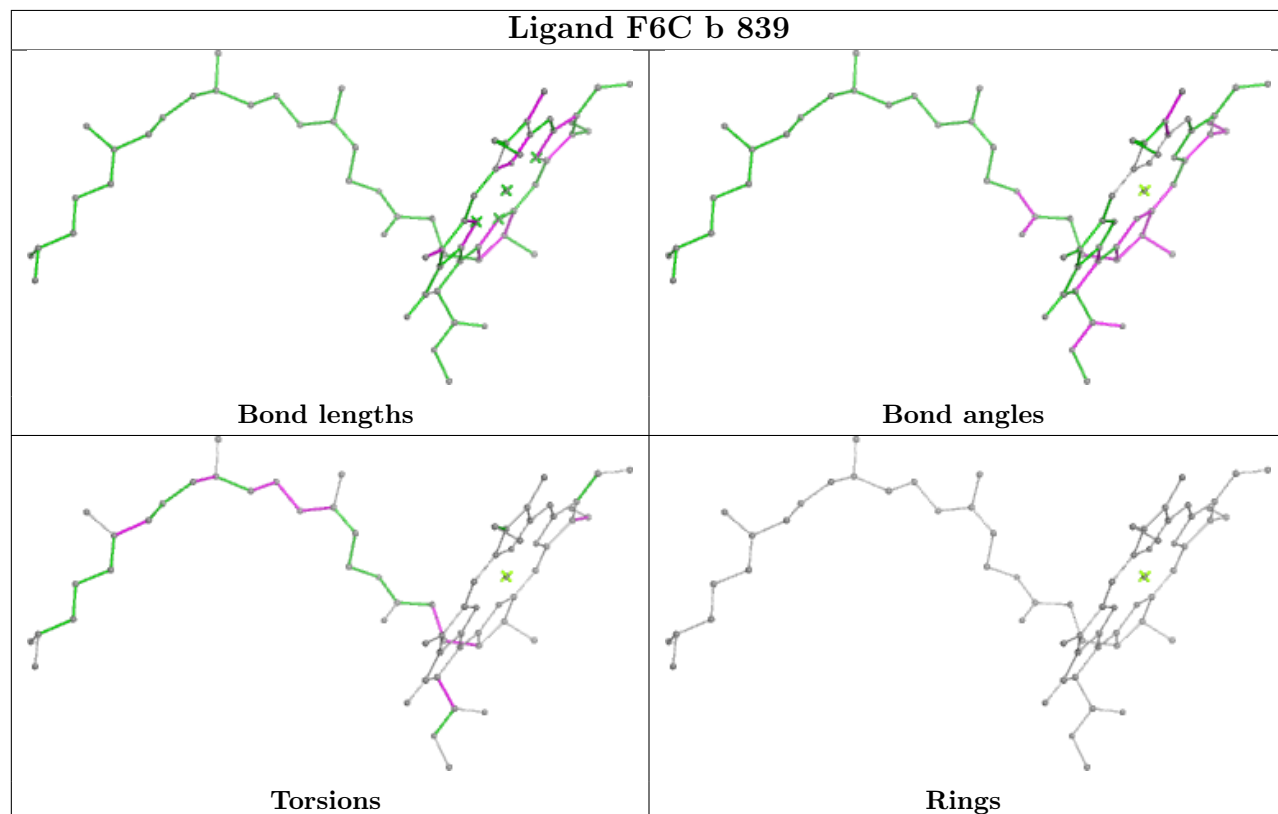
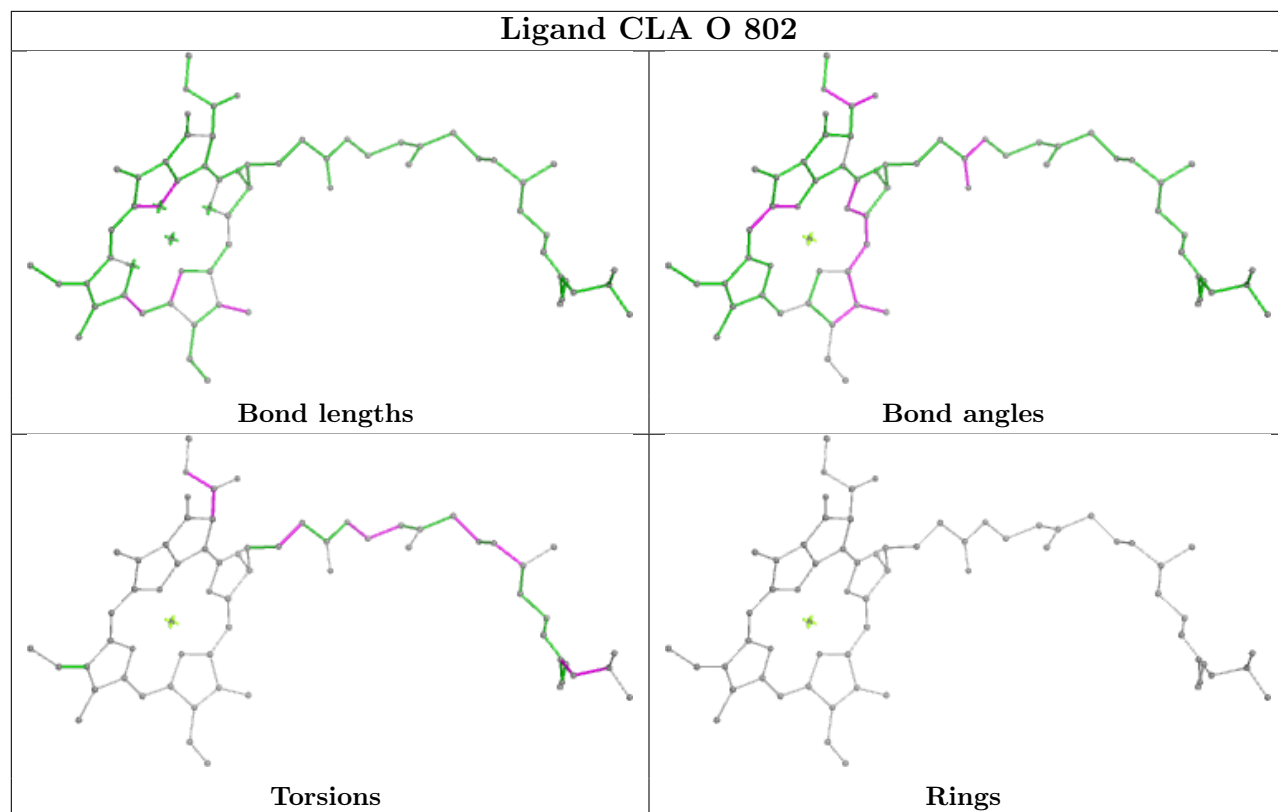
Bond angles

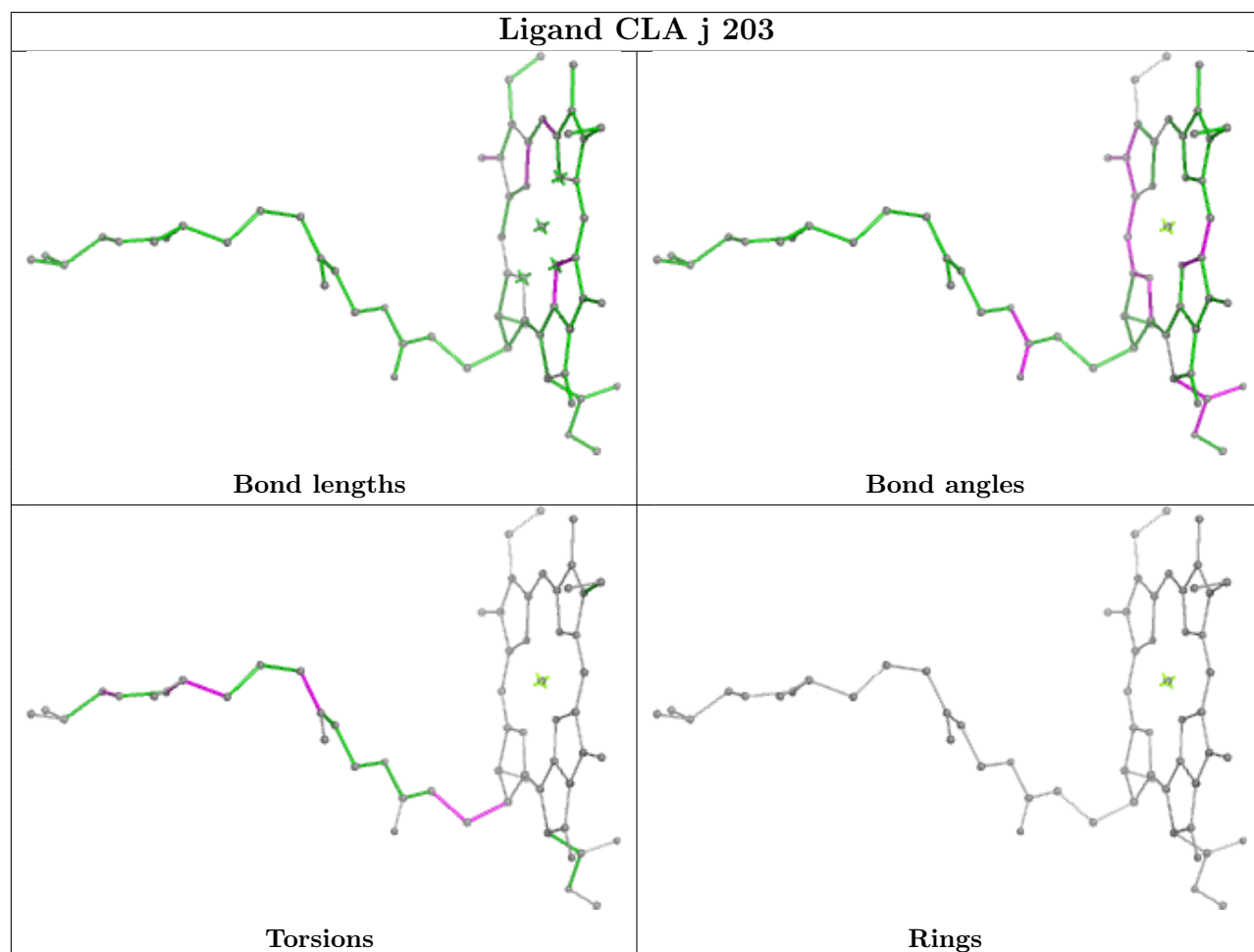
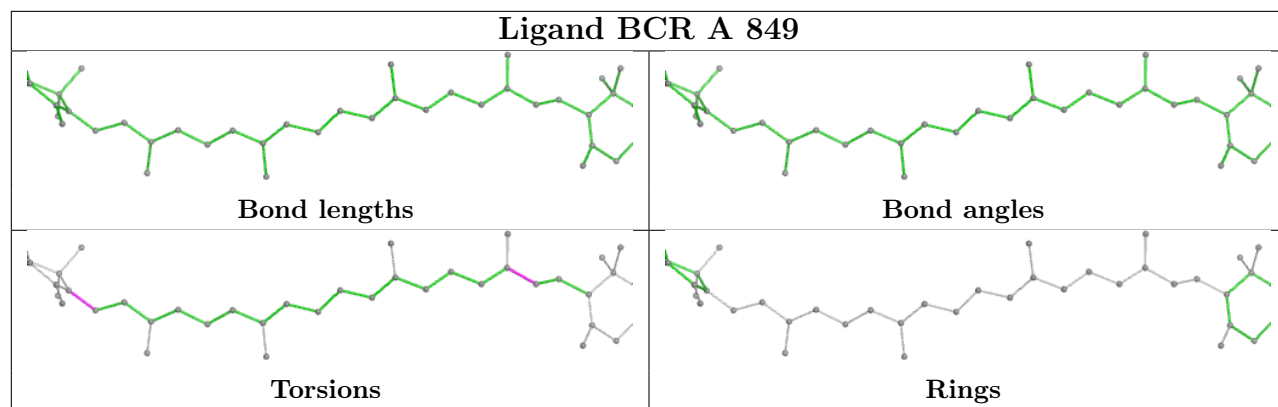


Torsions

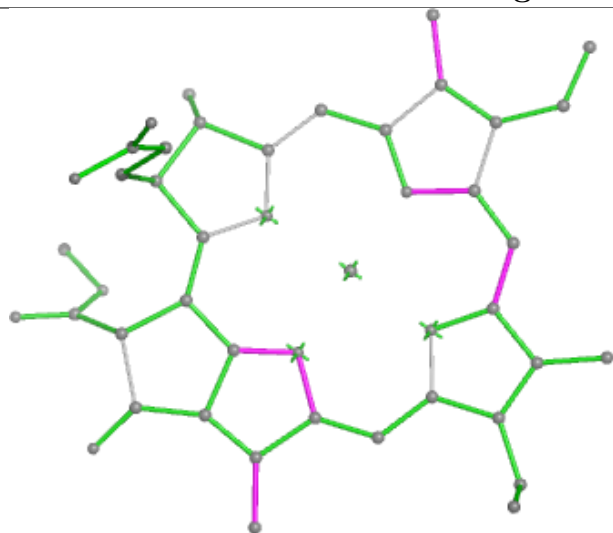


Rings

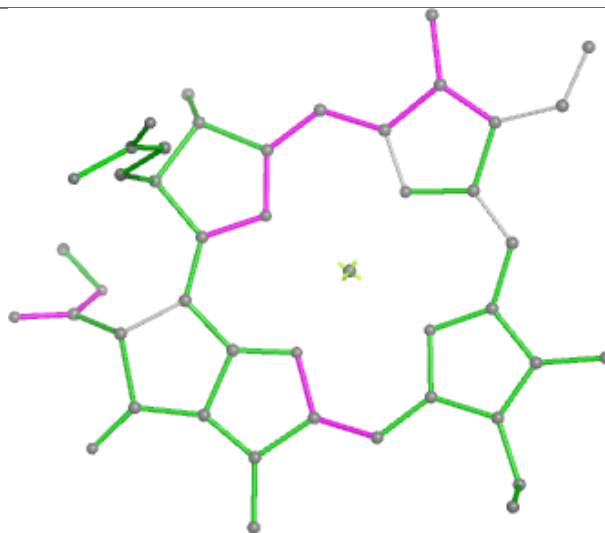




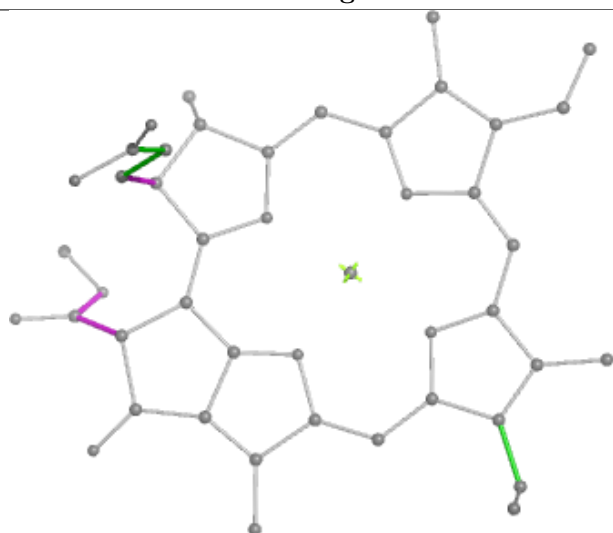
## Ligand CLA O 814



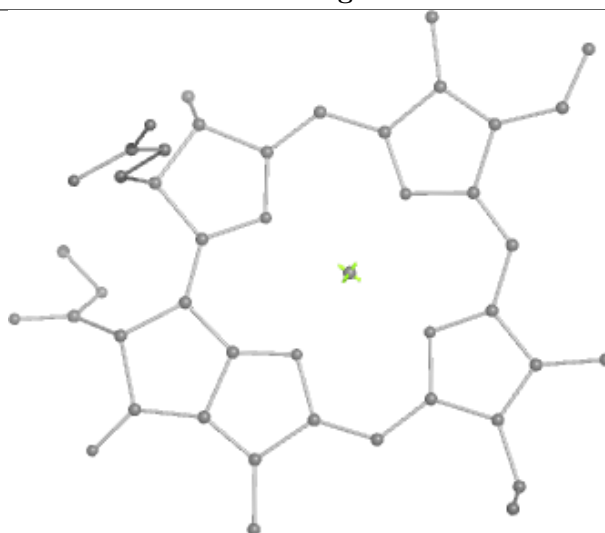
Bond lengths



Bond angles

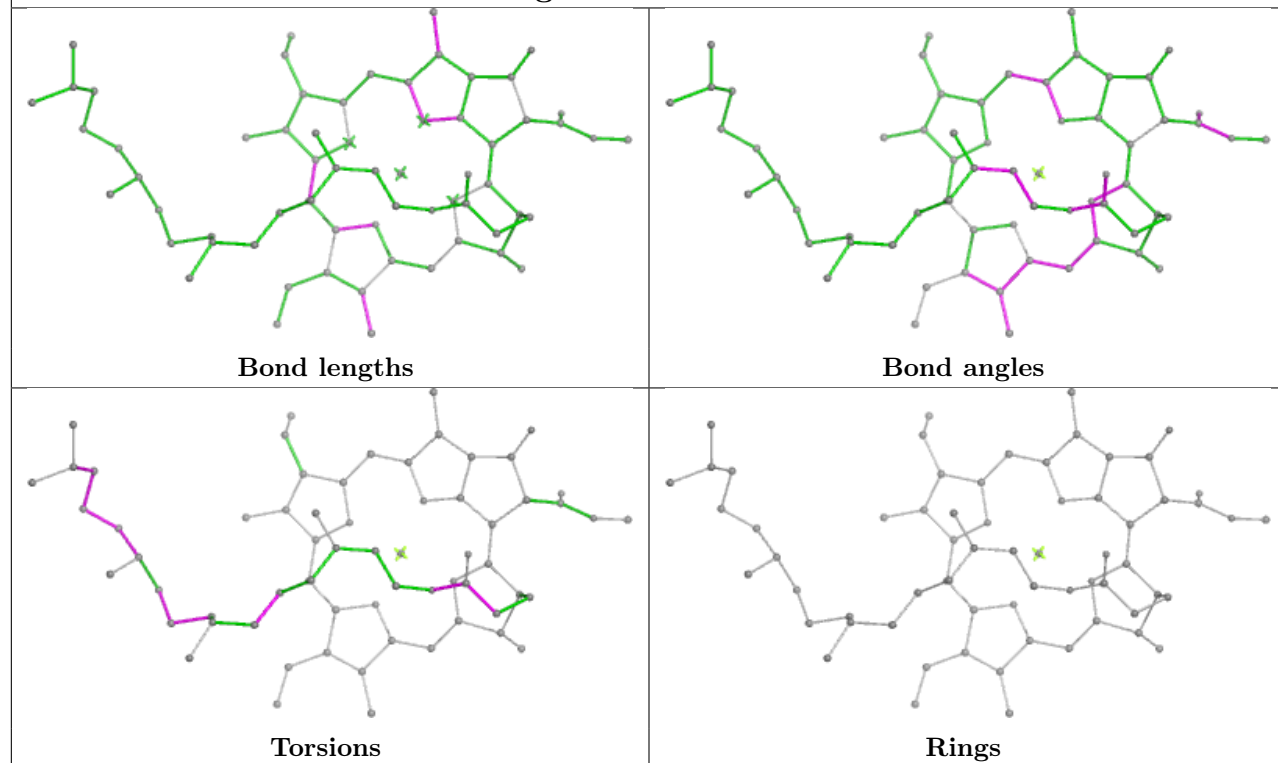
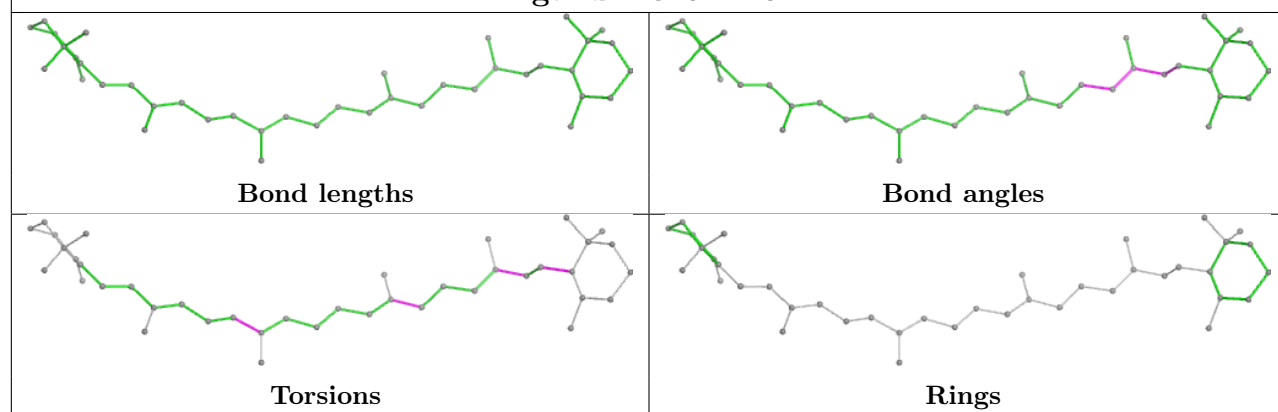


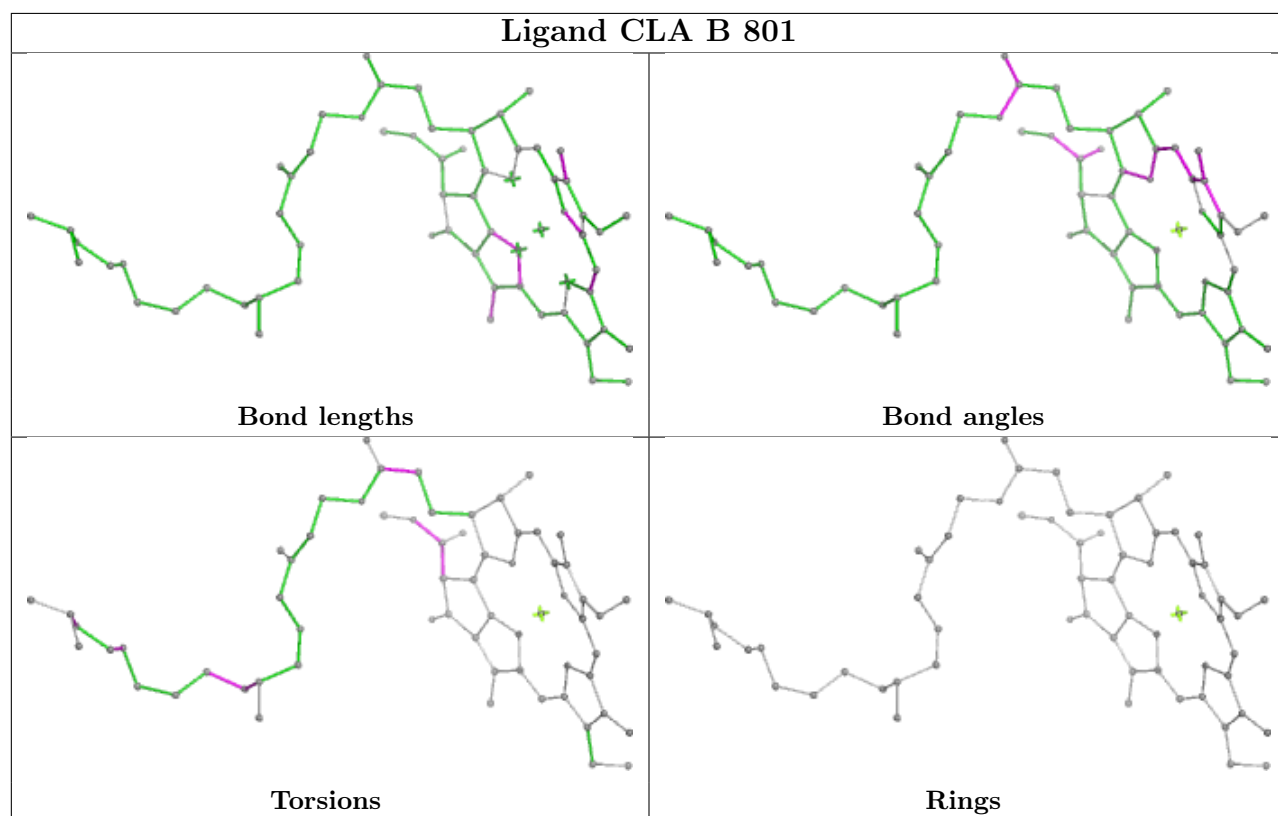
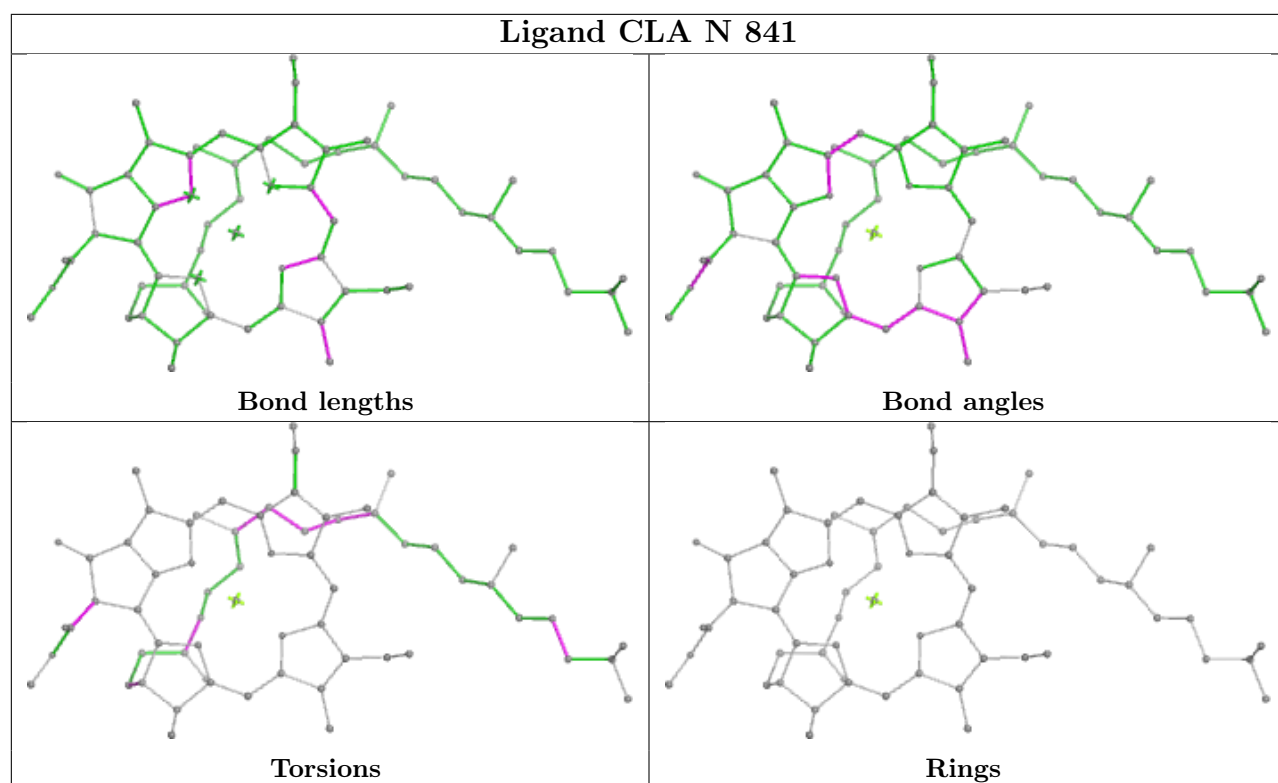
Torsions

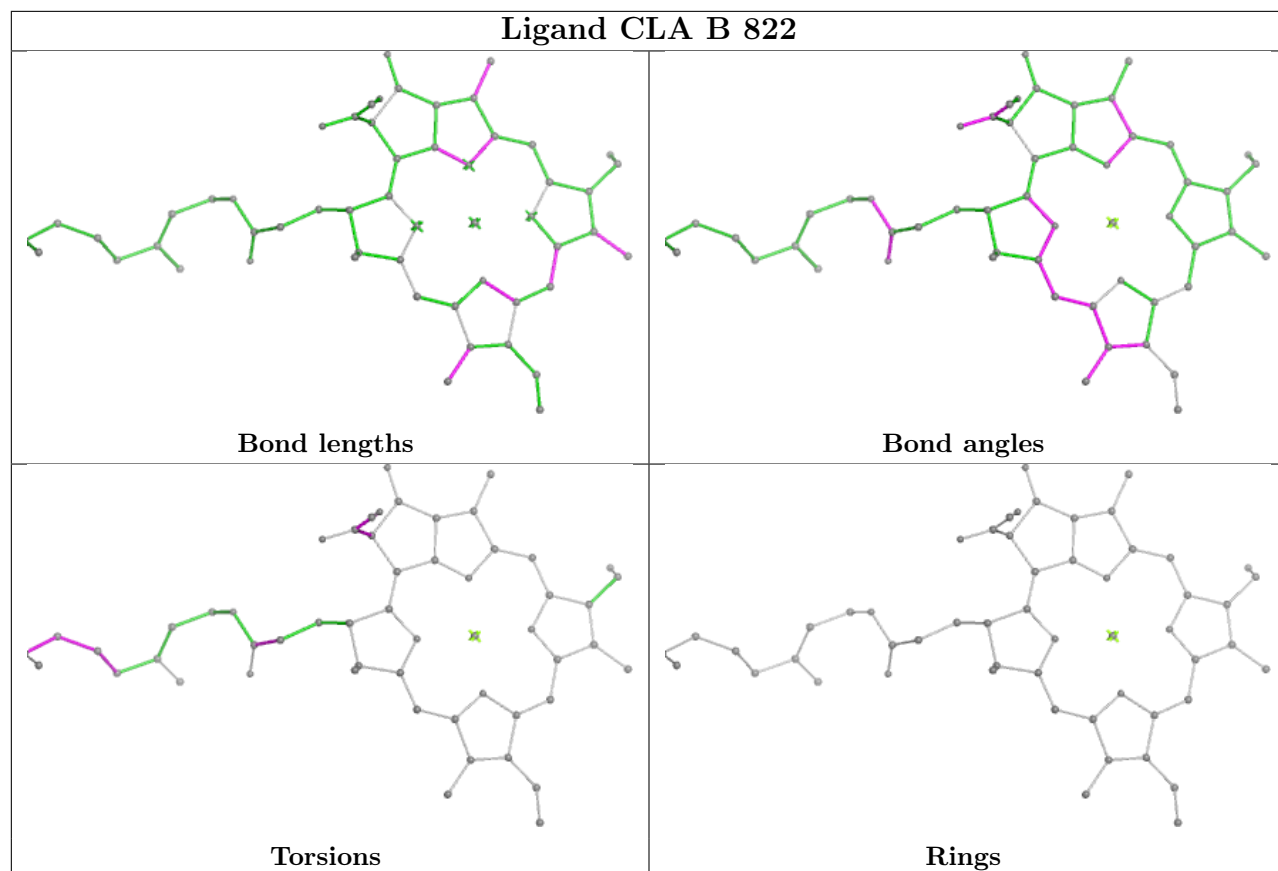
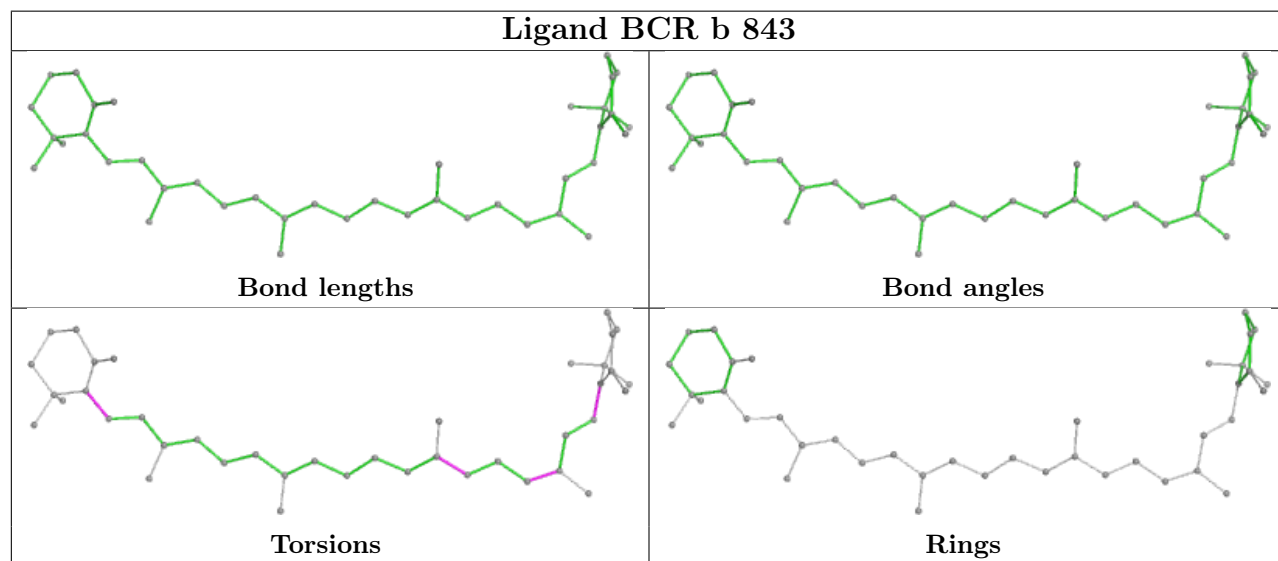


Rings

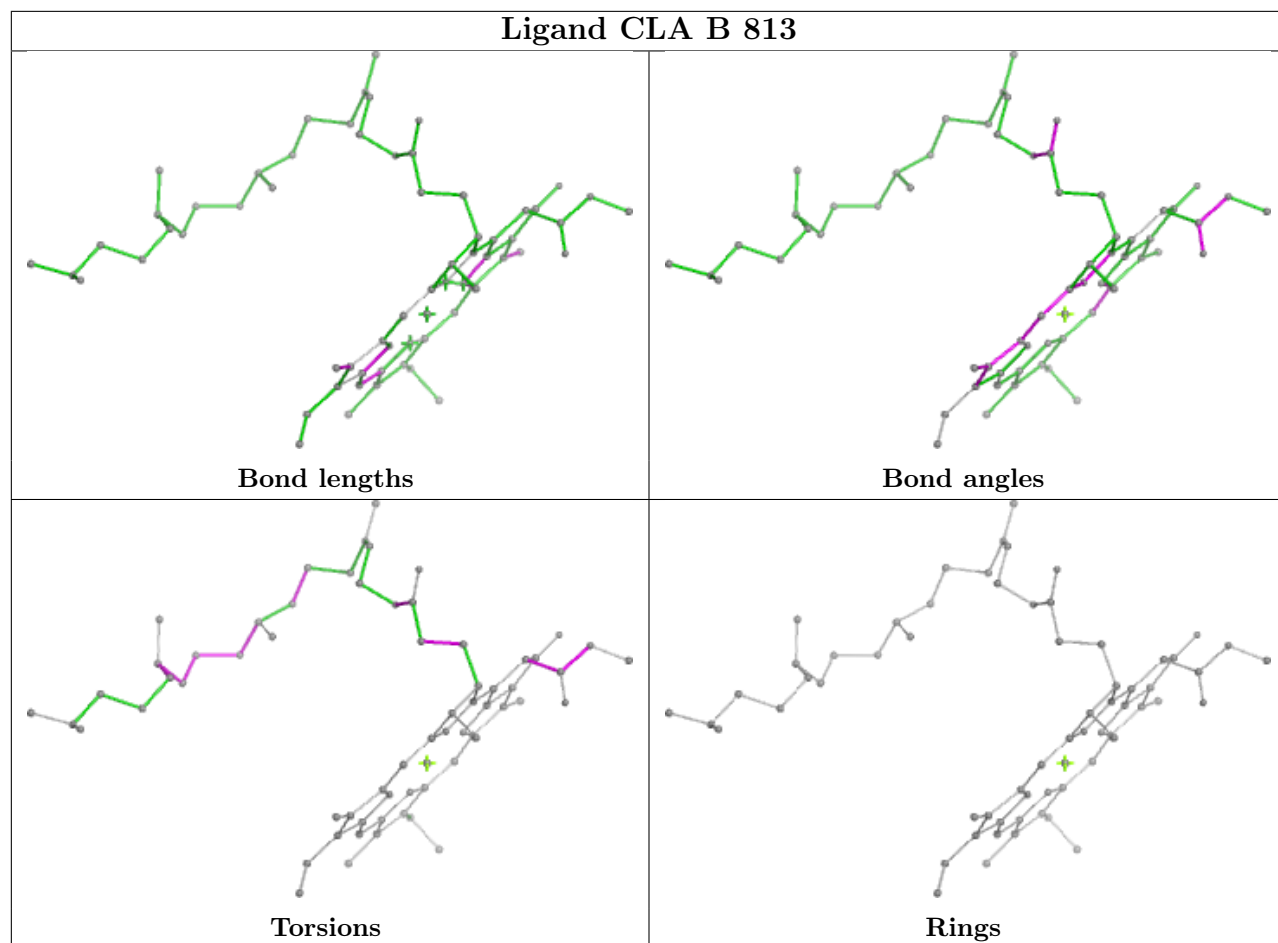


**Ligand CLA b 837****Ligand BCR F 202**

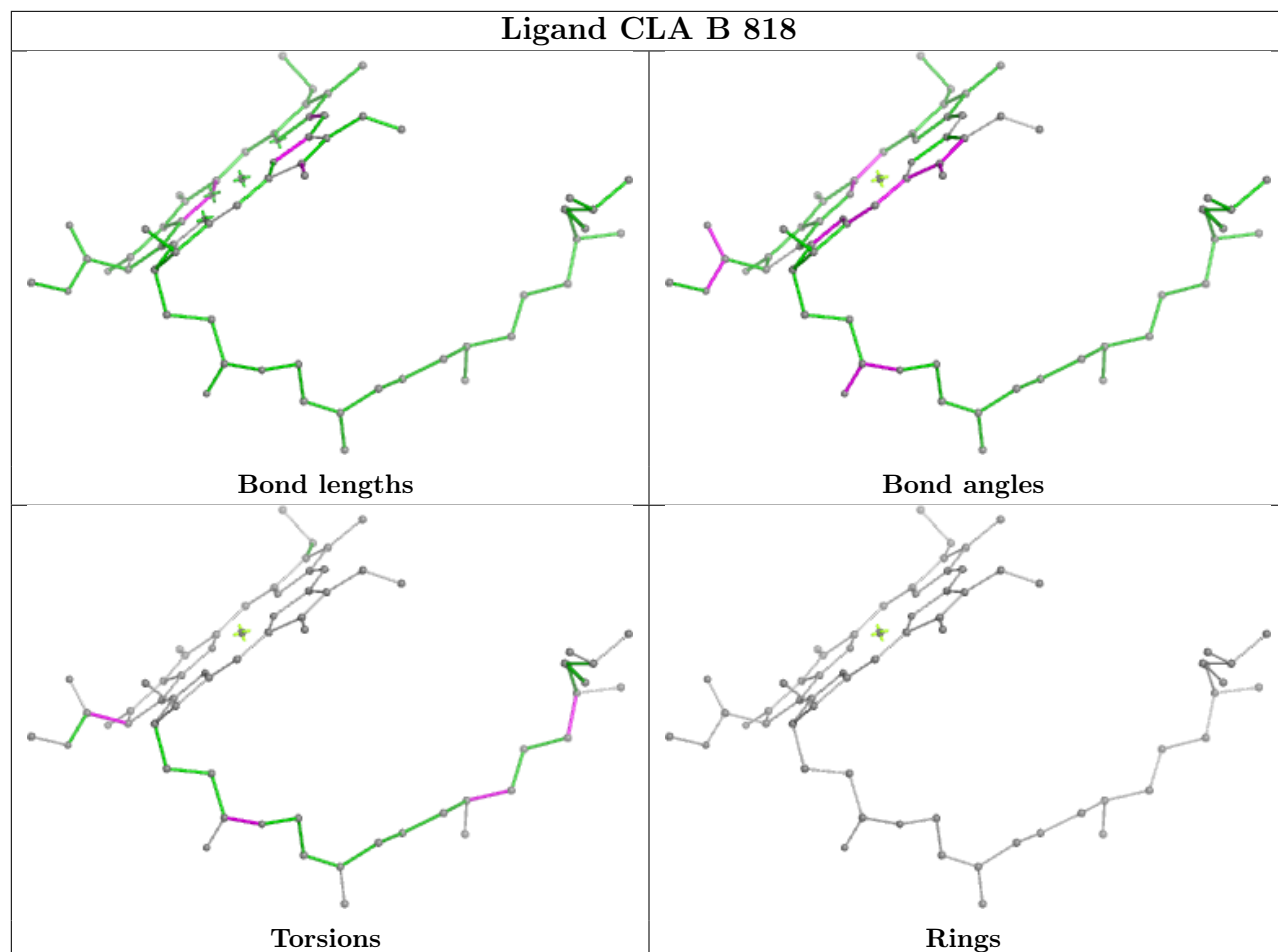


**Ligand CLA B 822****Ligand BCR b 843**

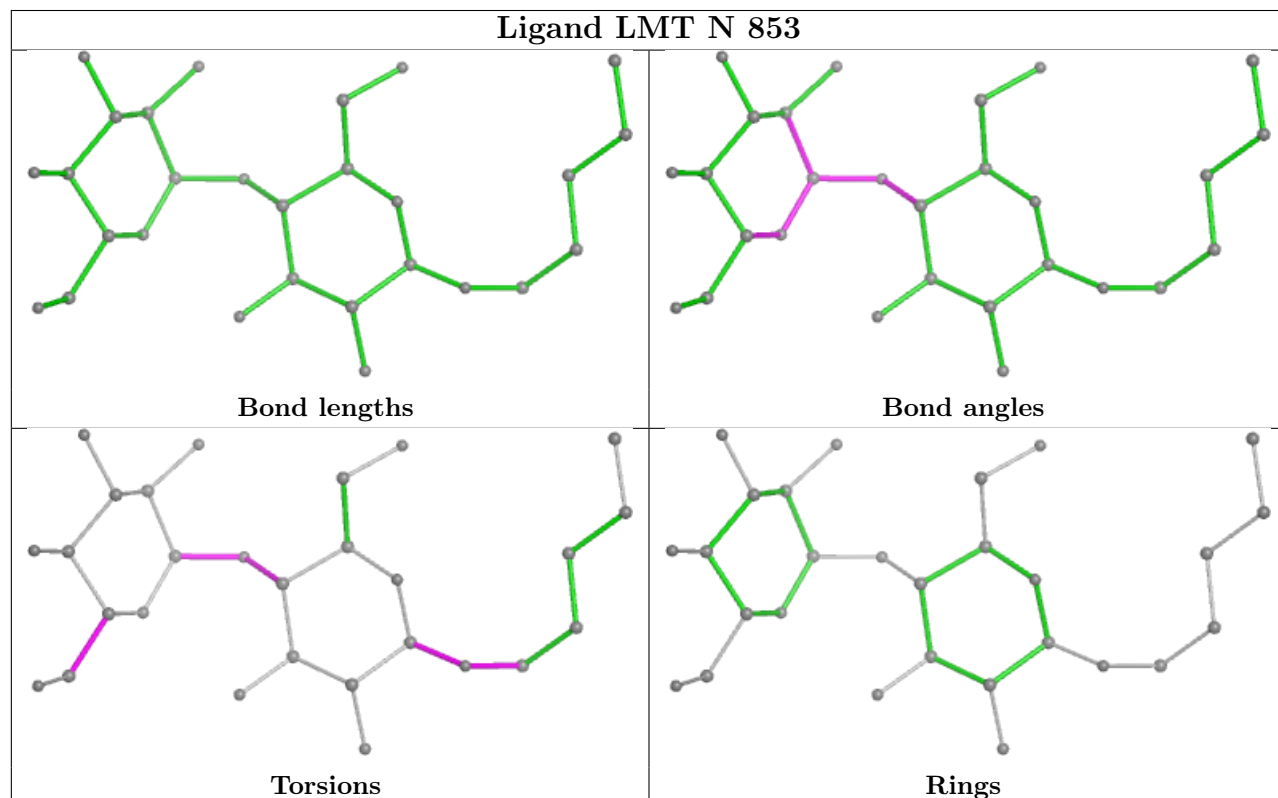
## Ligand CLA B 813

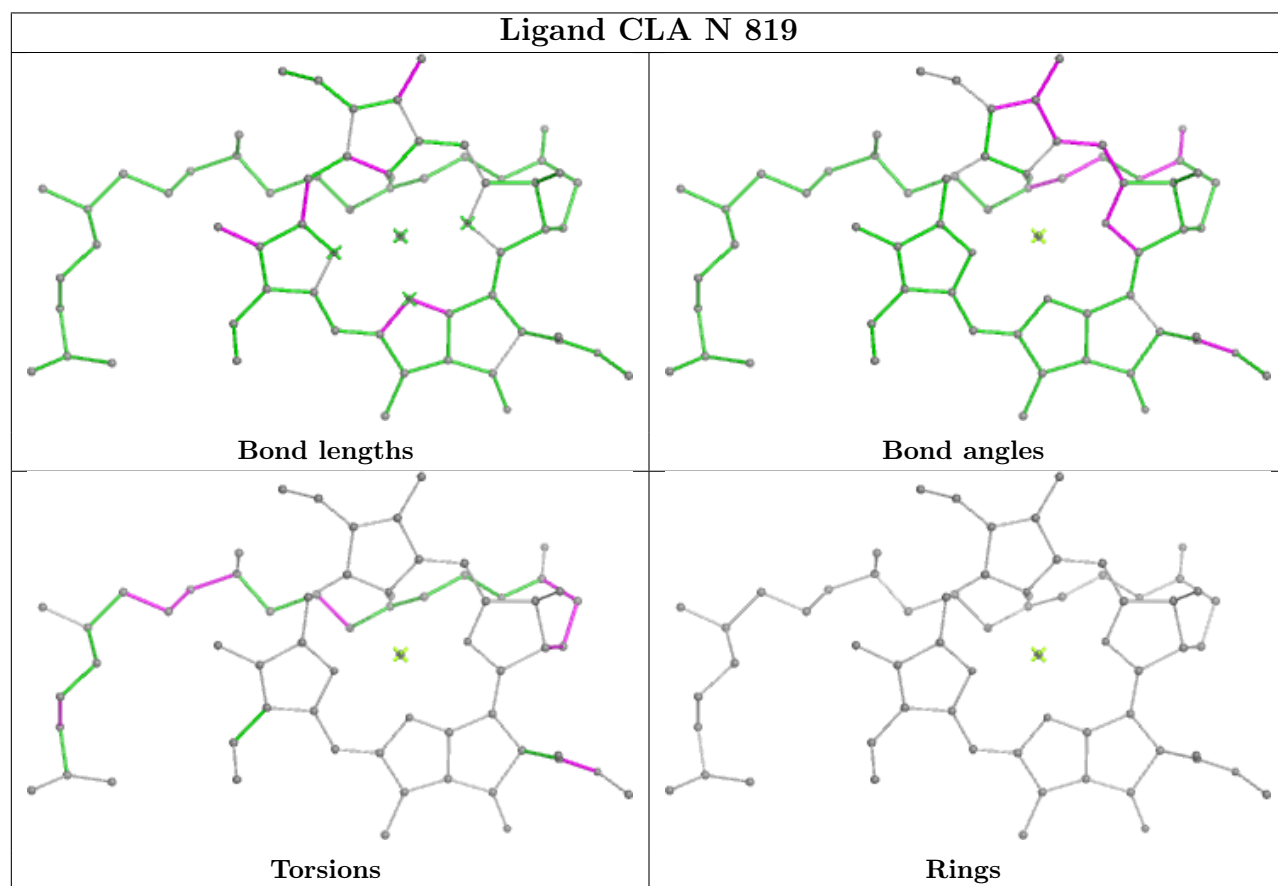
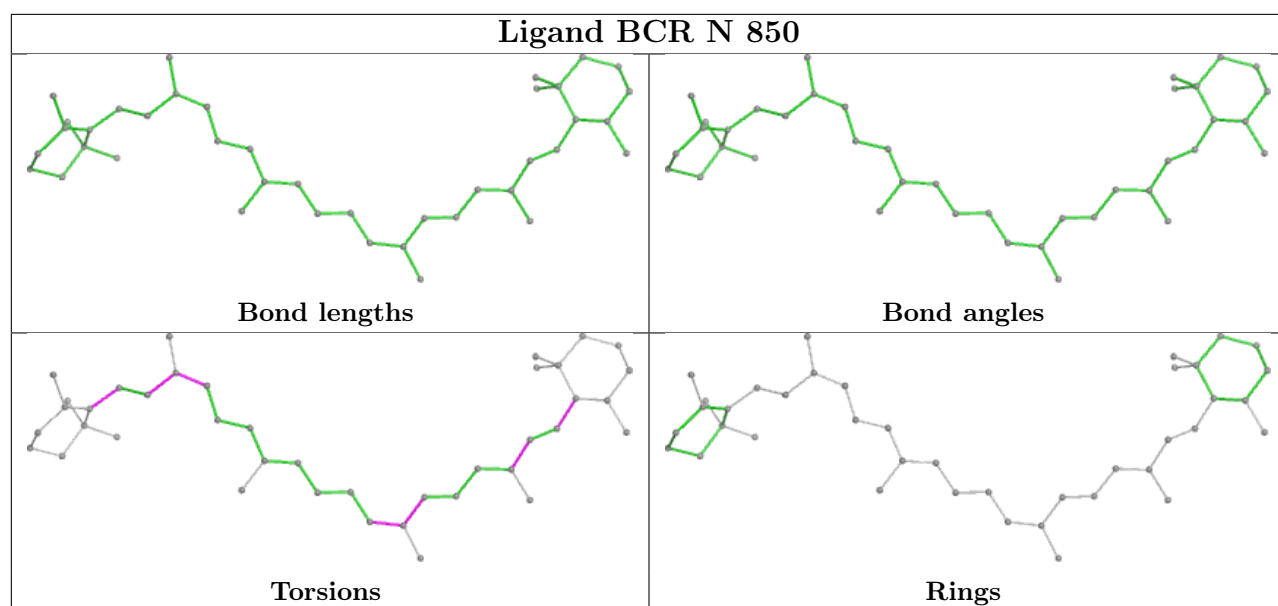


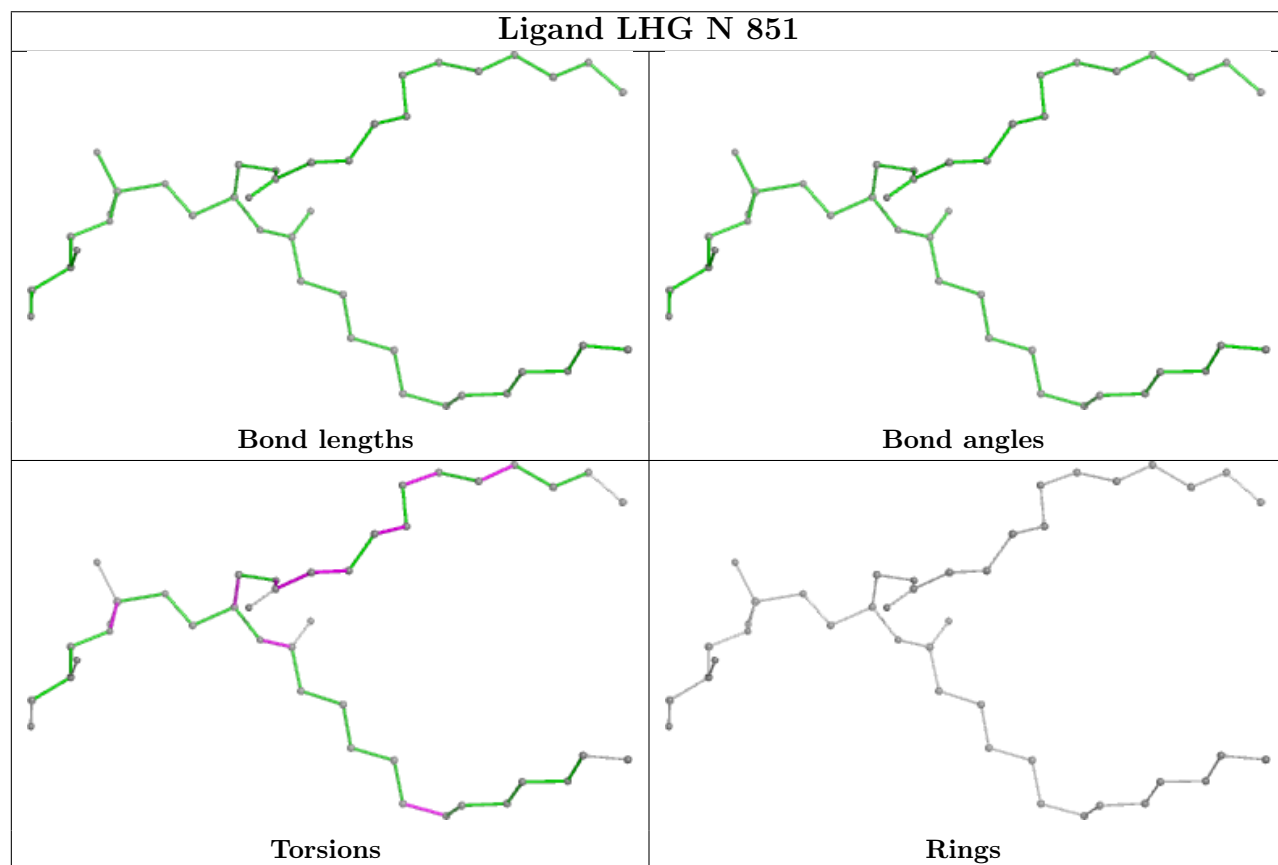
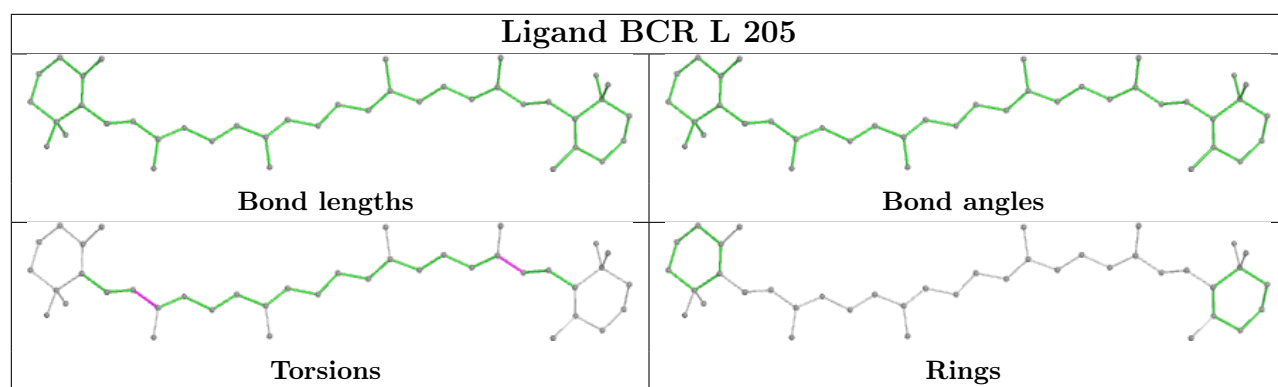
## Ligand CLA B 818

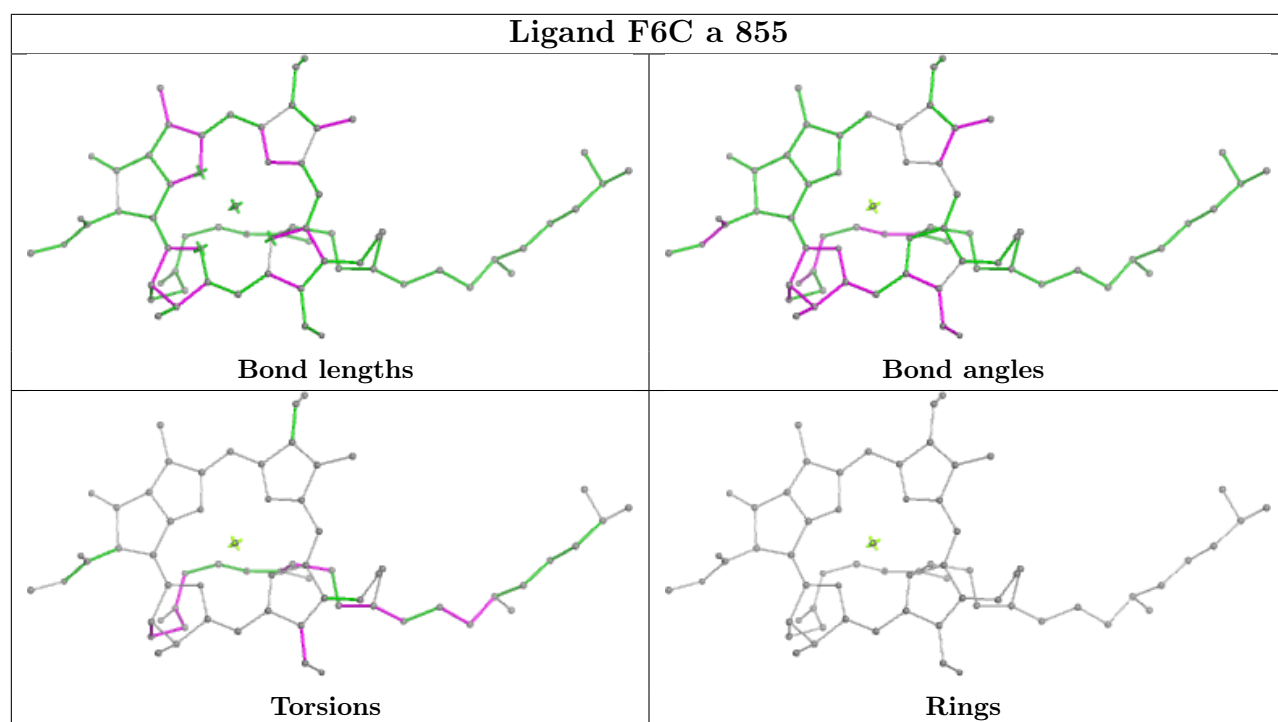


## Ligand LMT N 853



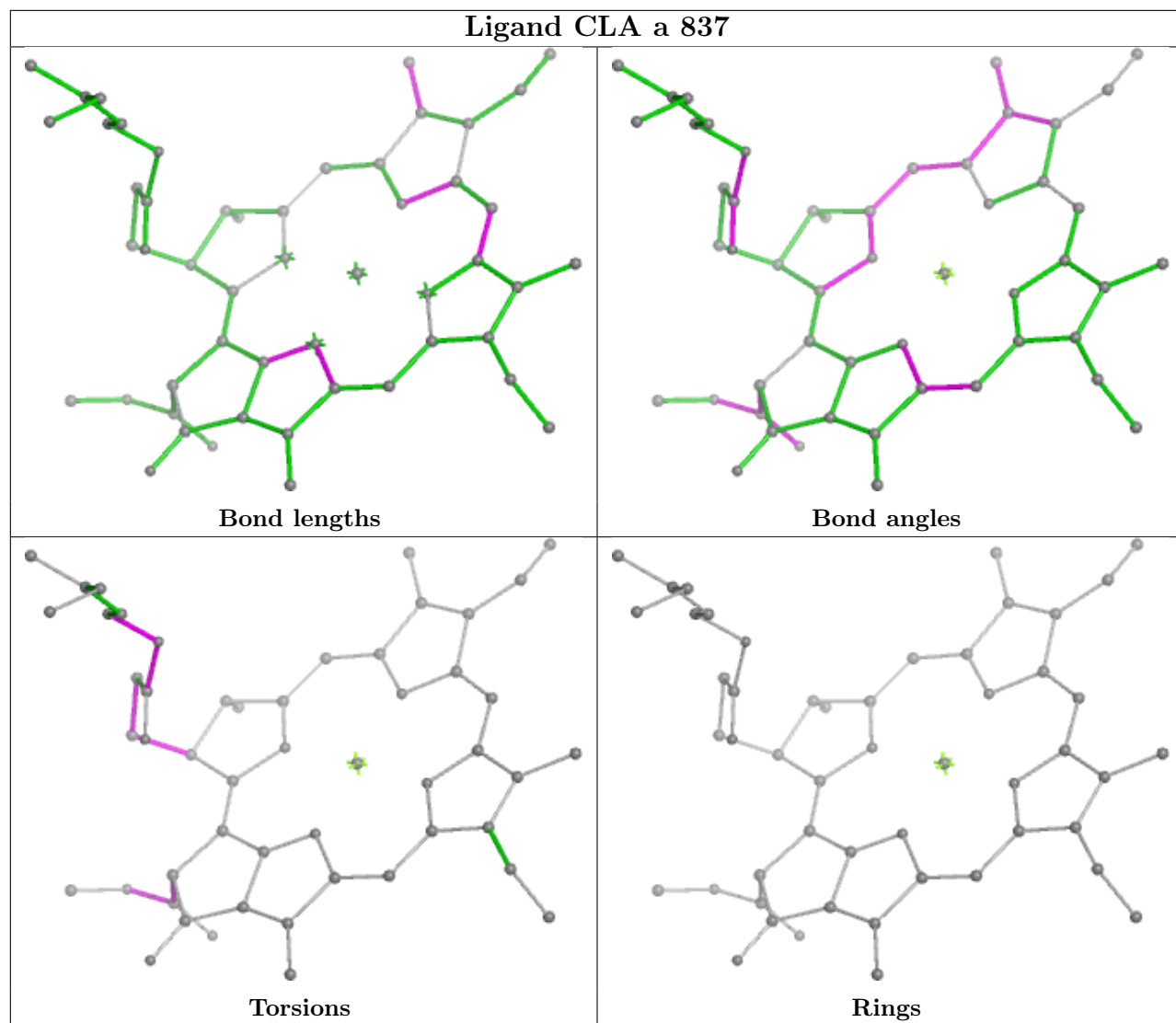


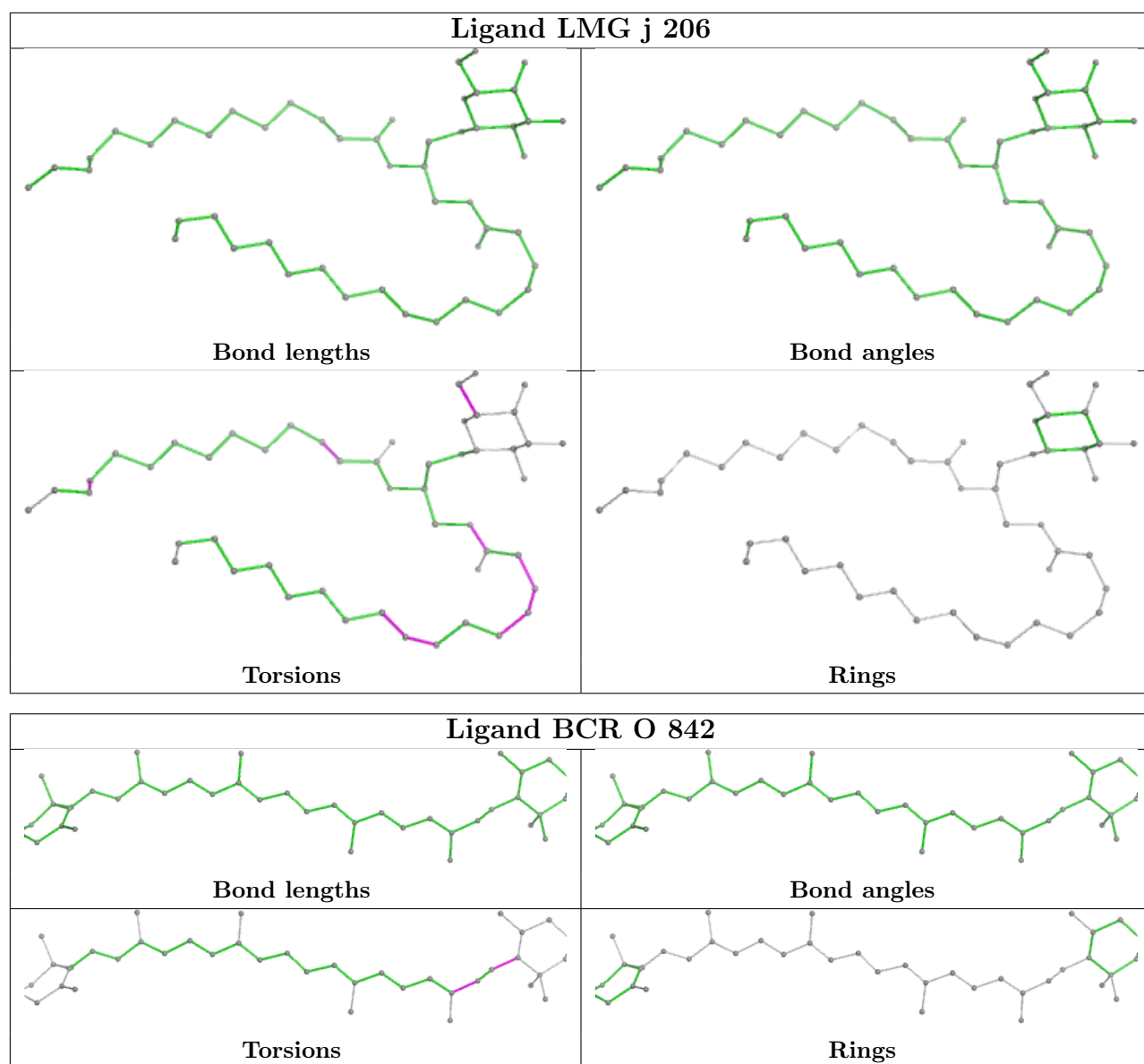


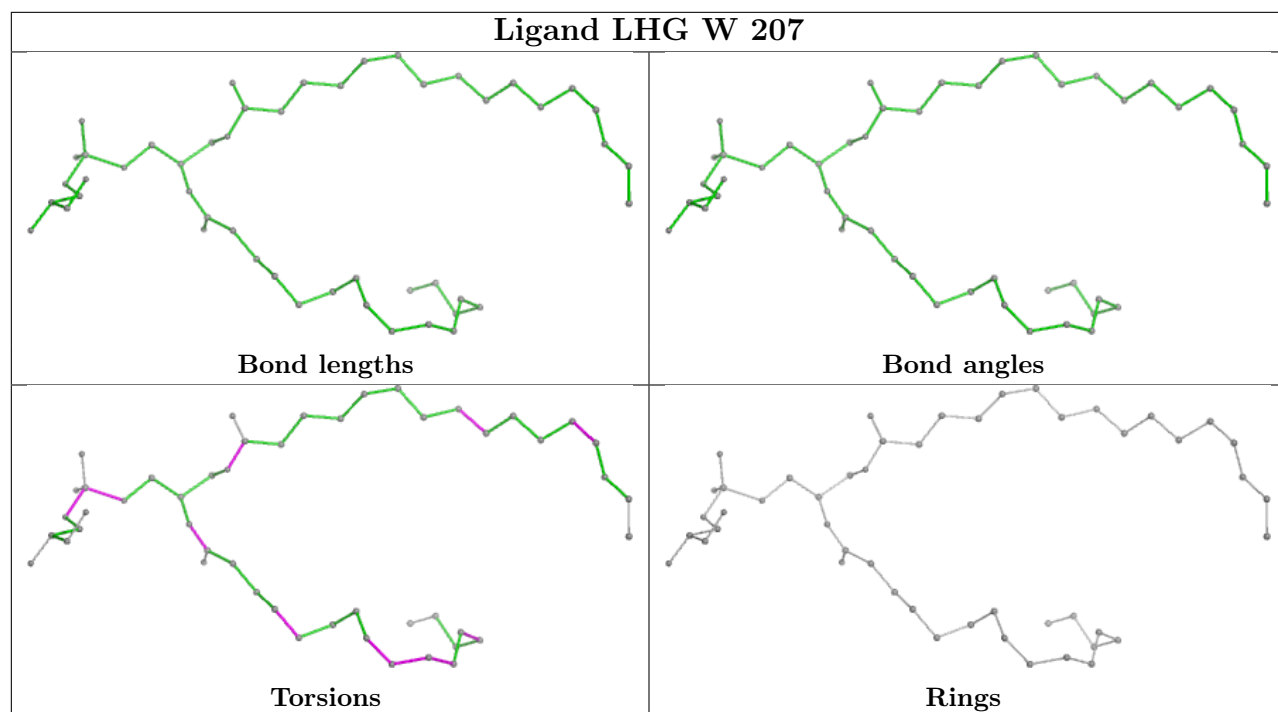
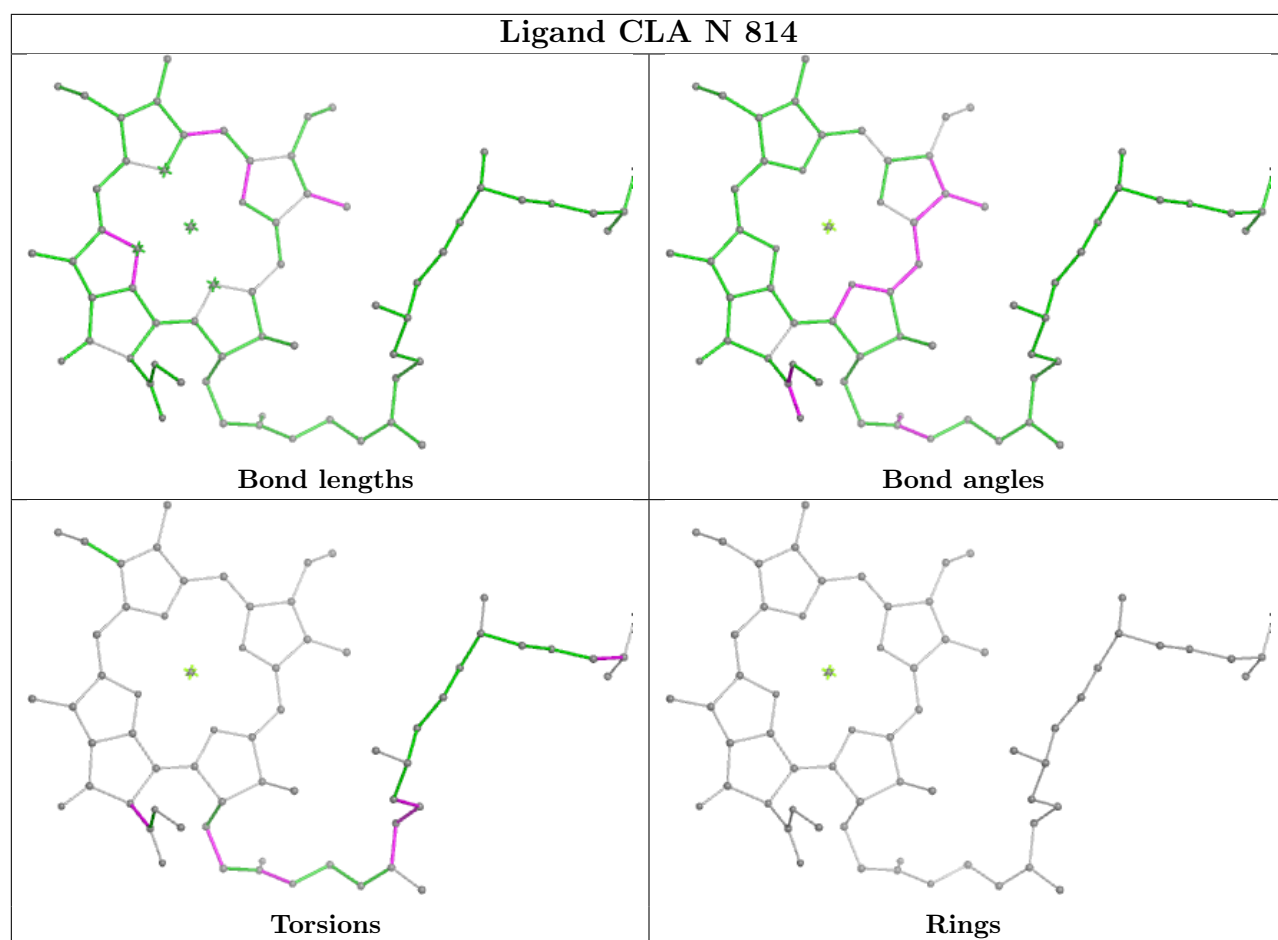




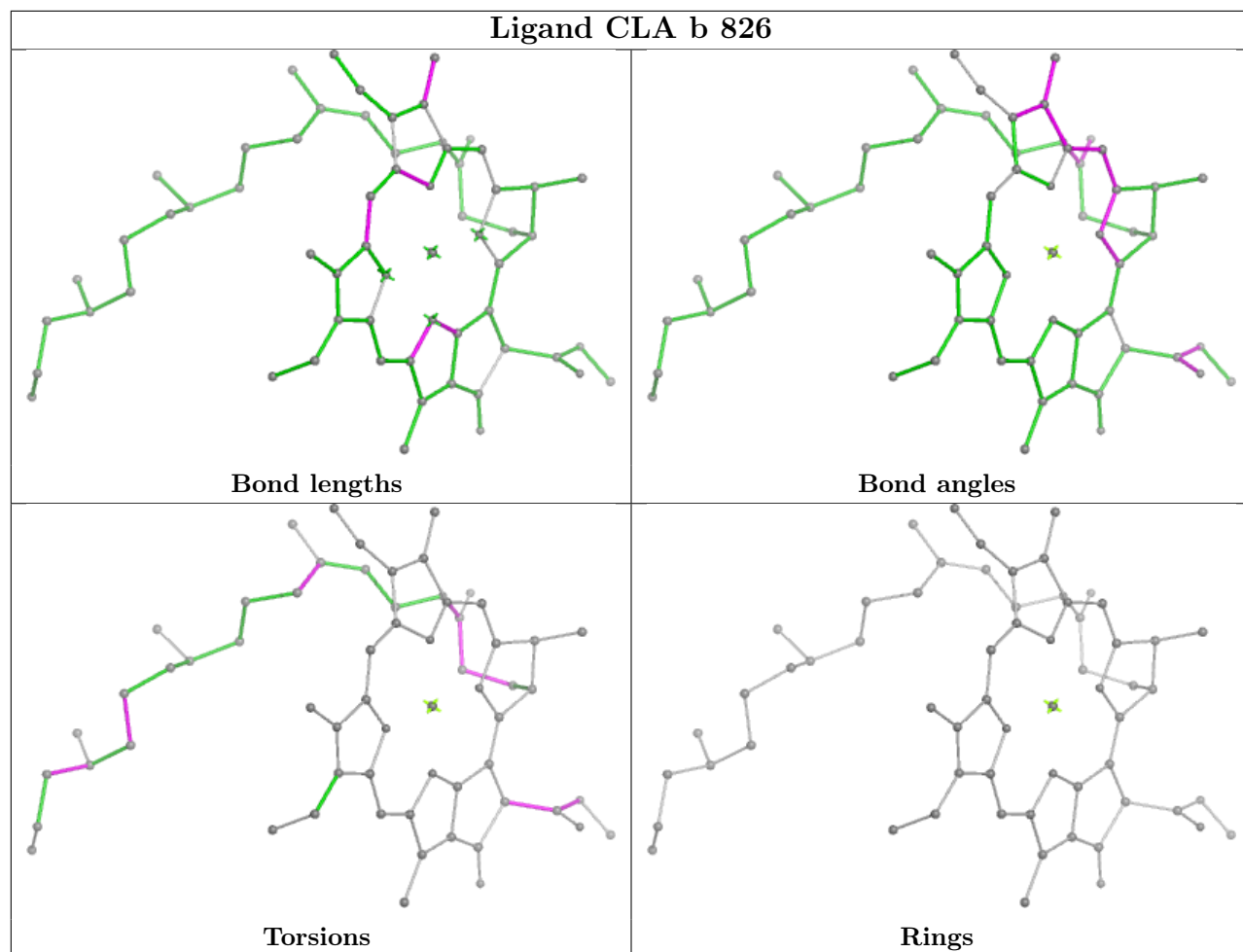
## Ligand CLA a 837

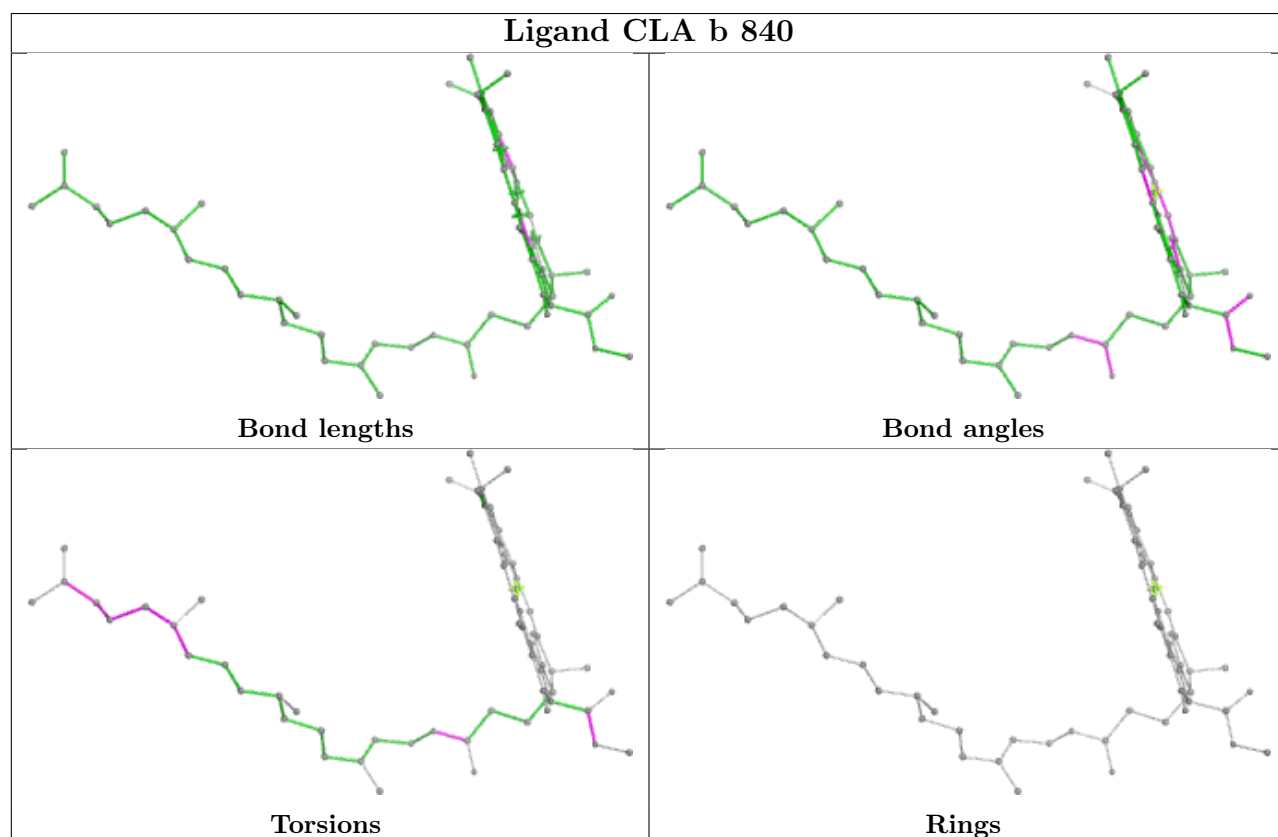
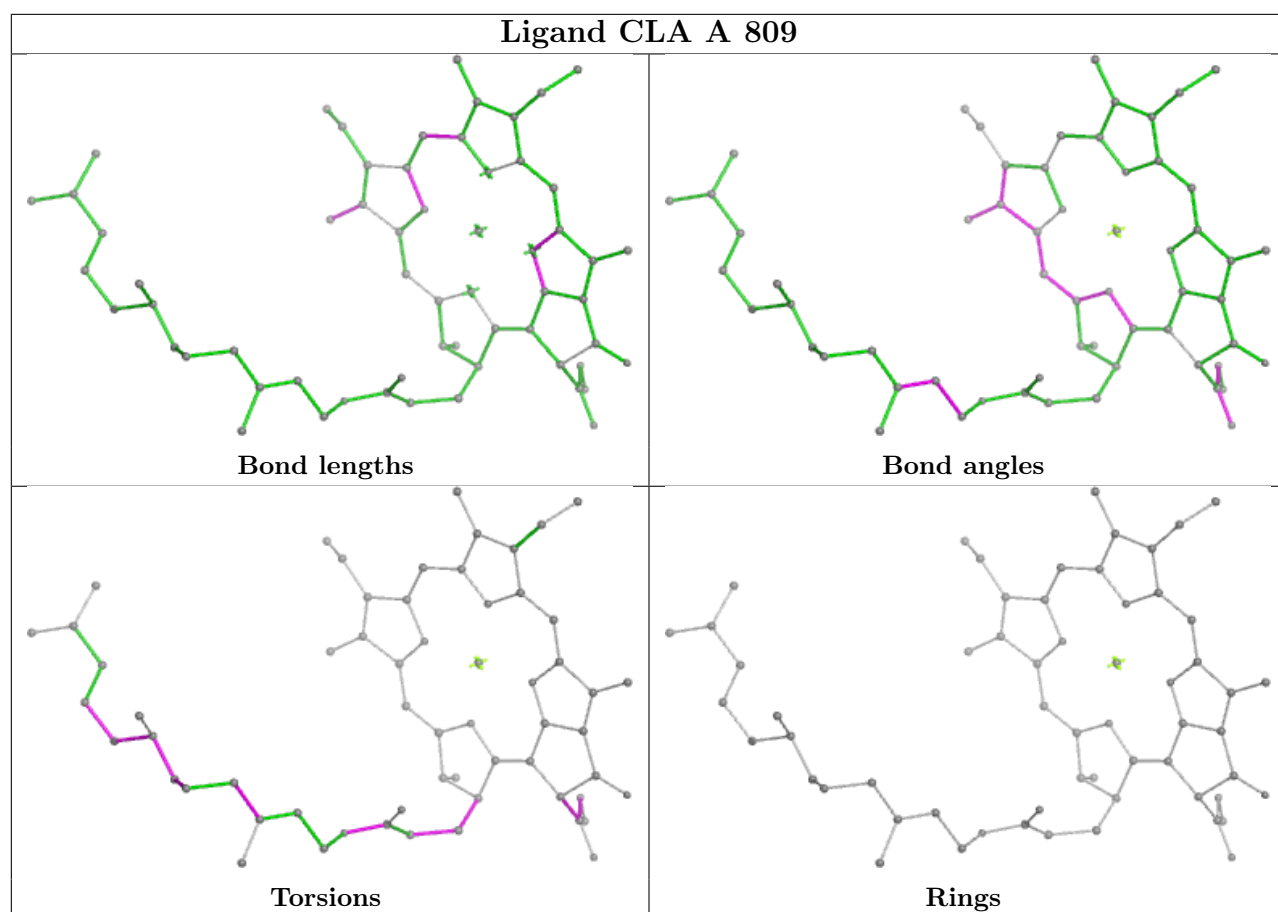


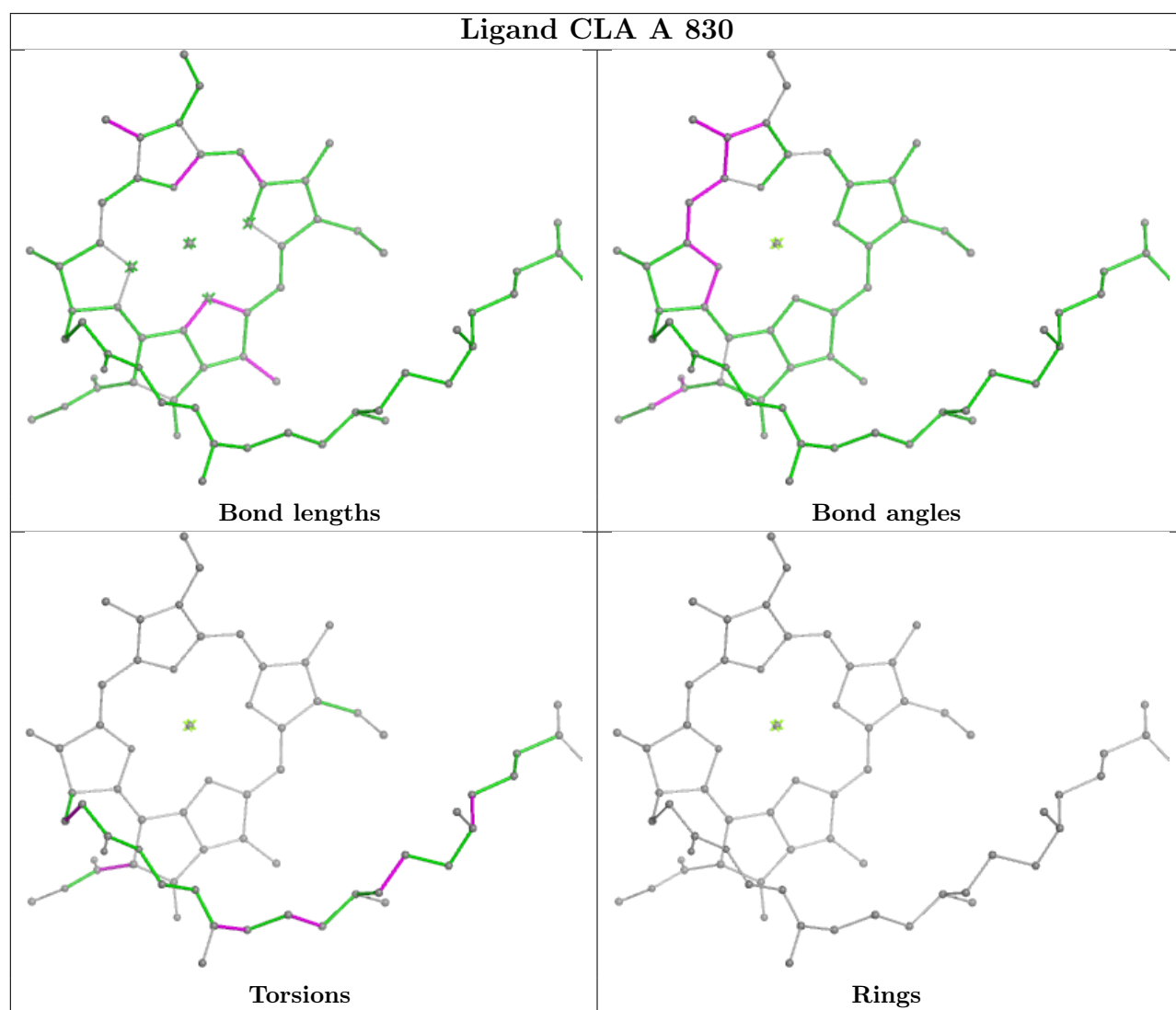
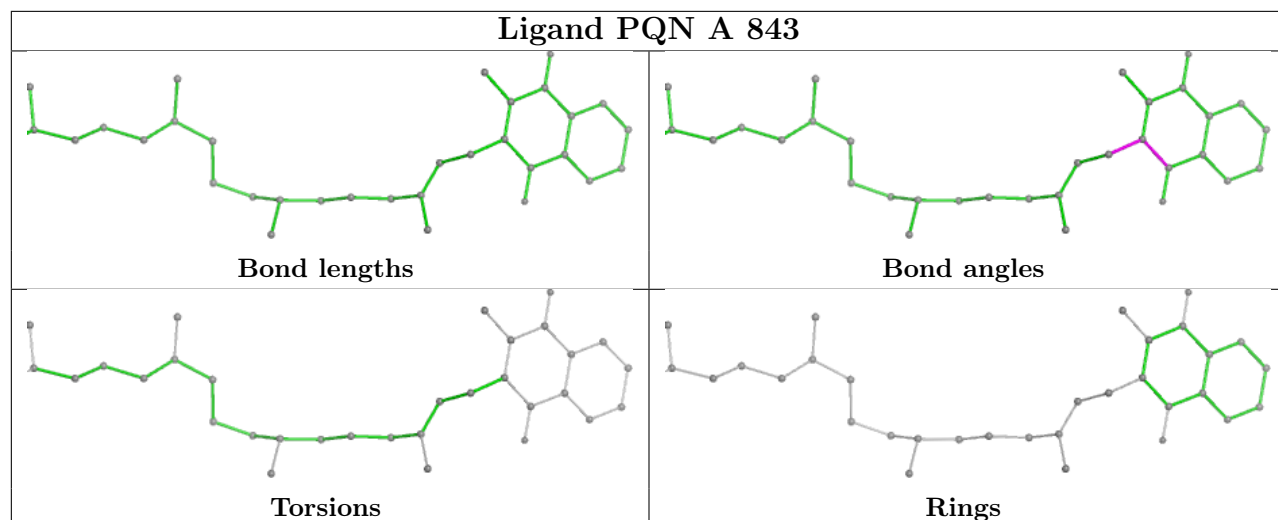


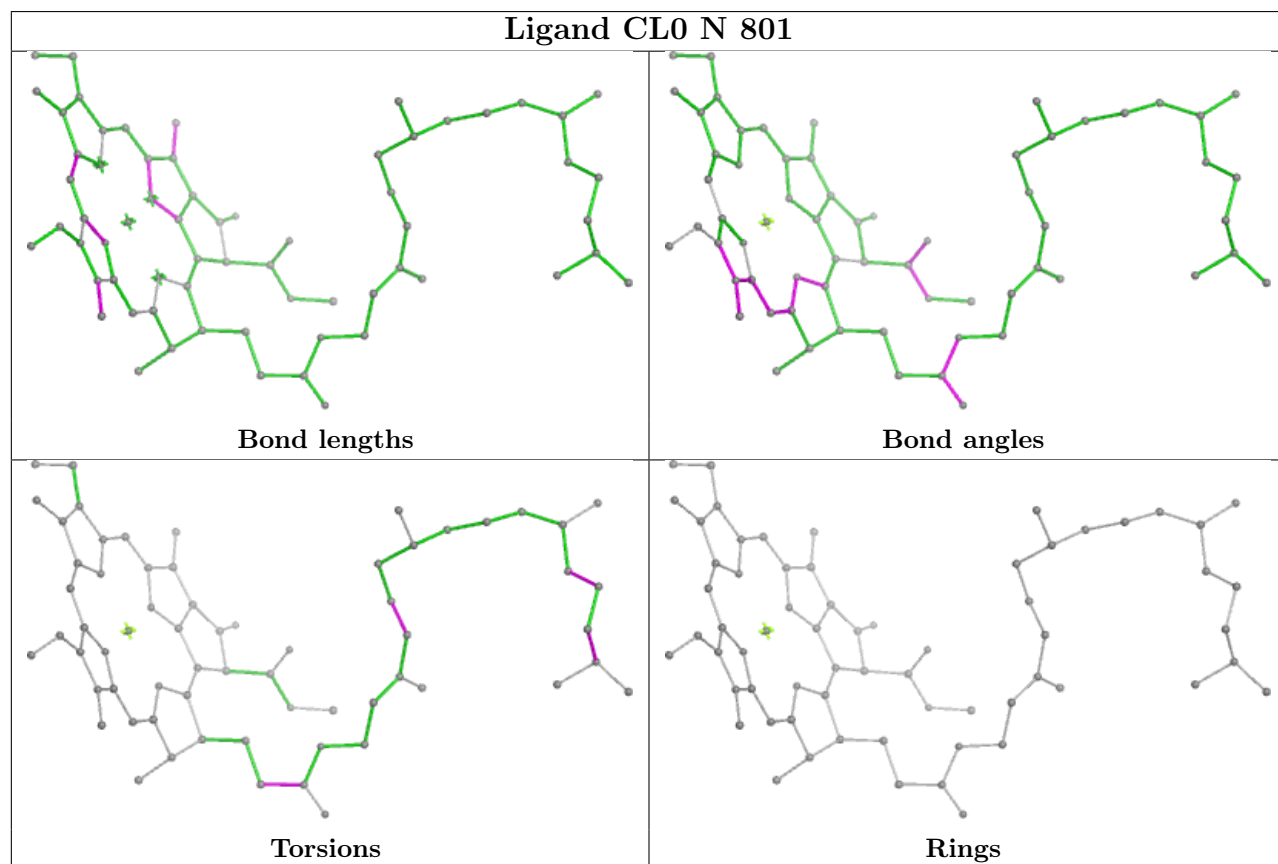
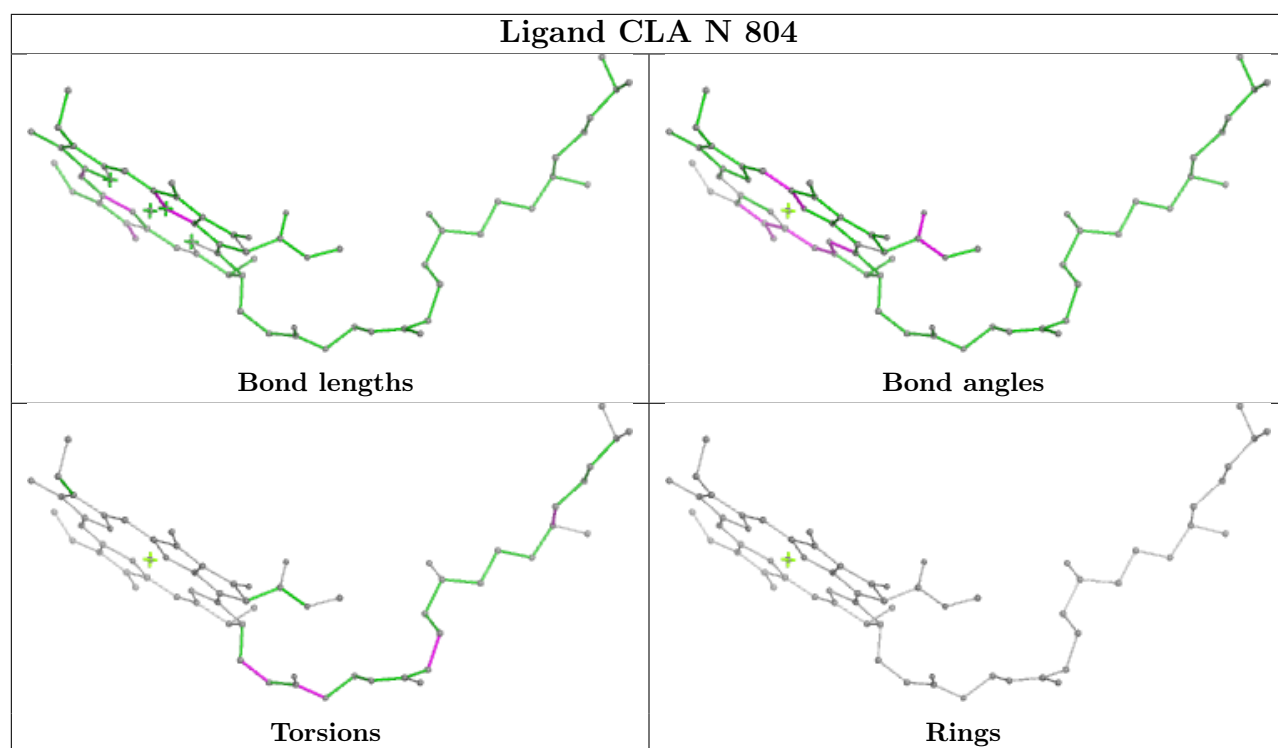


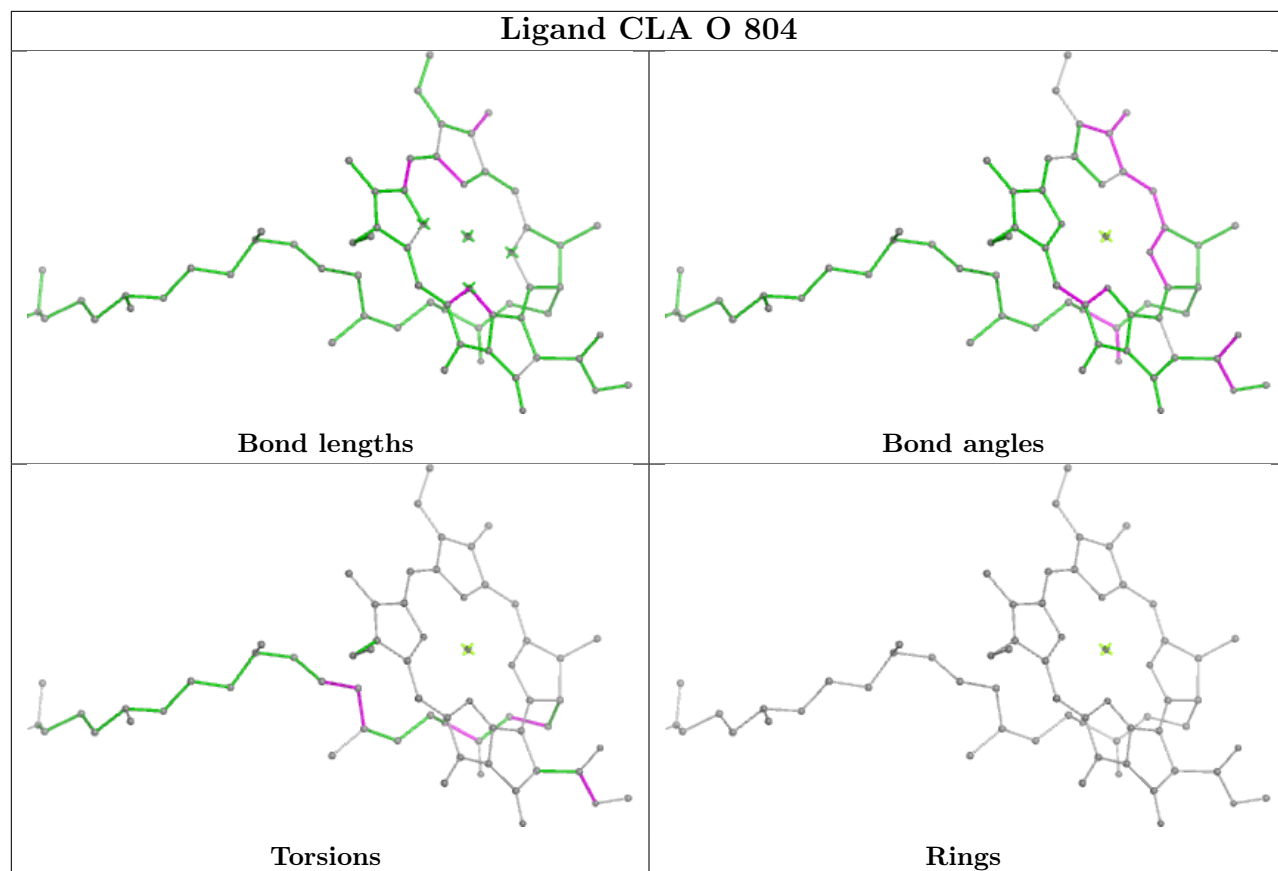
## Ligand CLA b 826





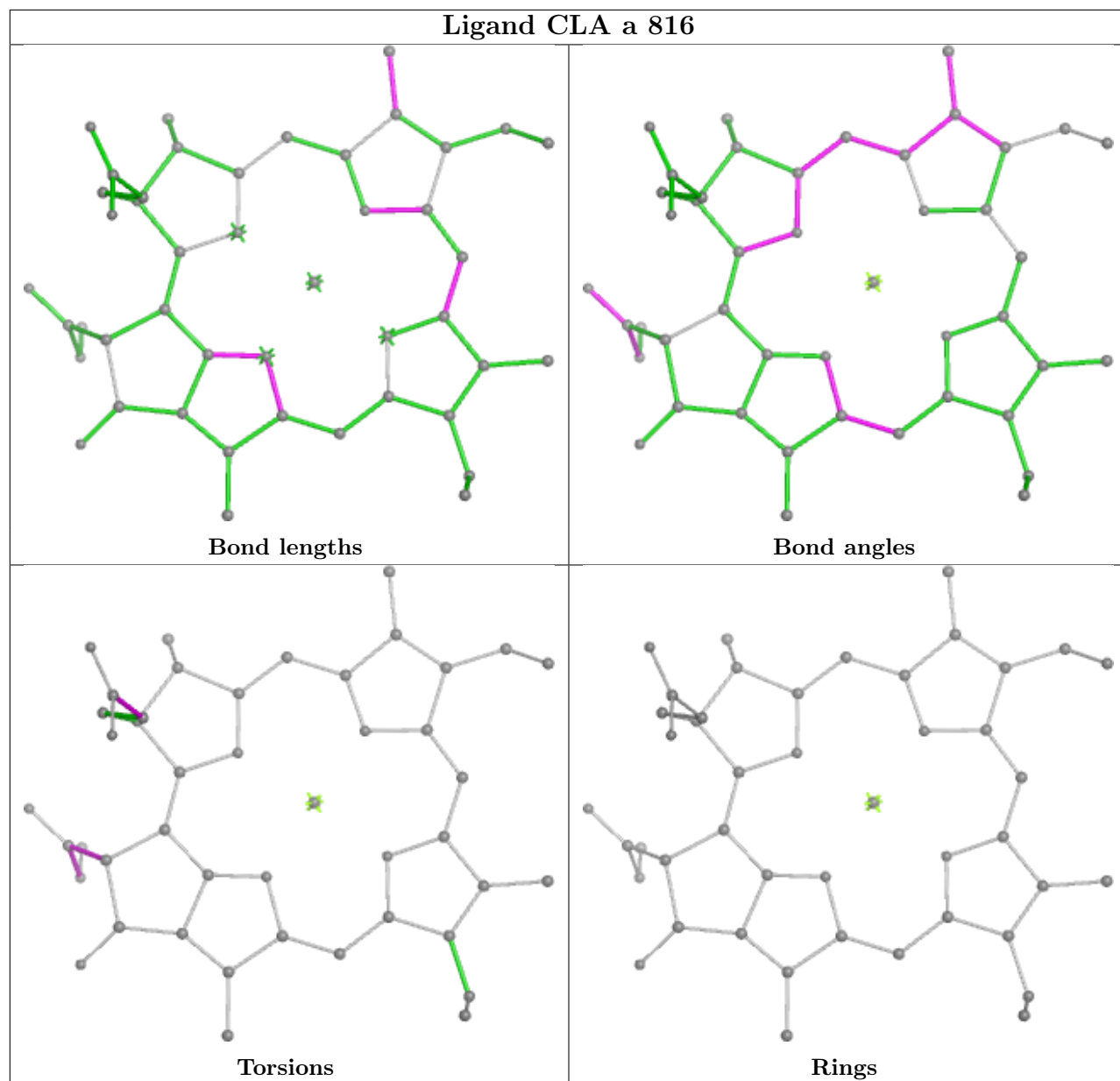




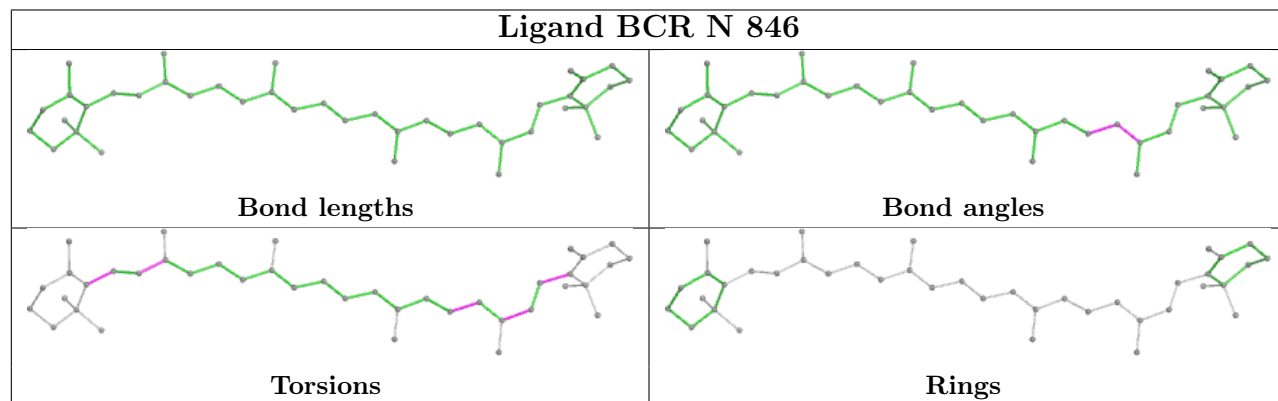


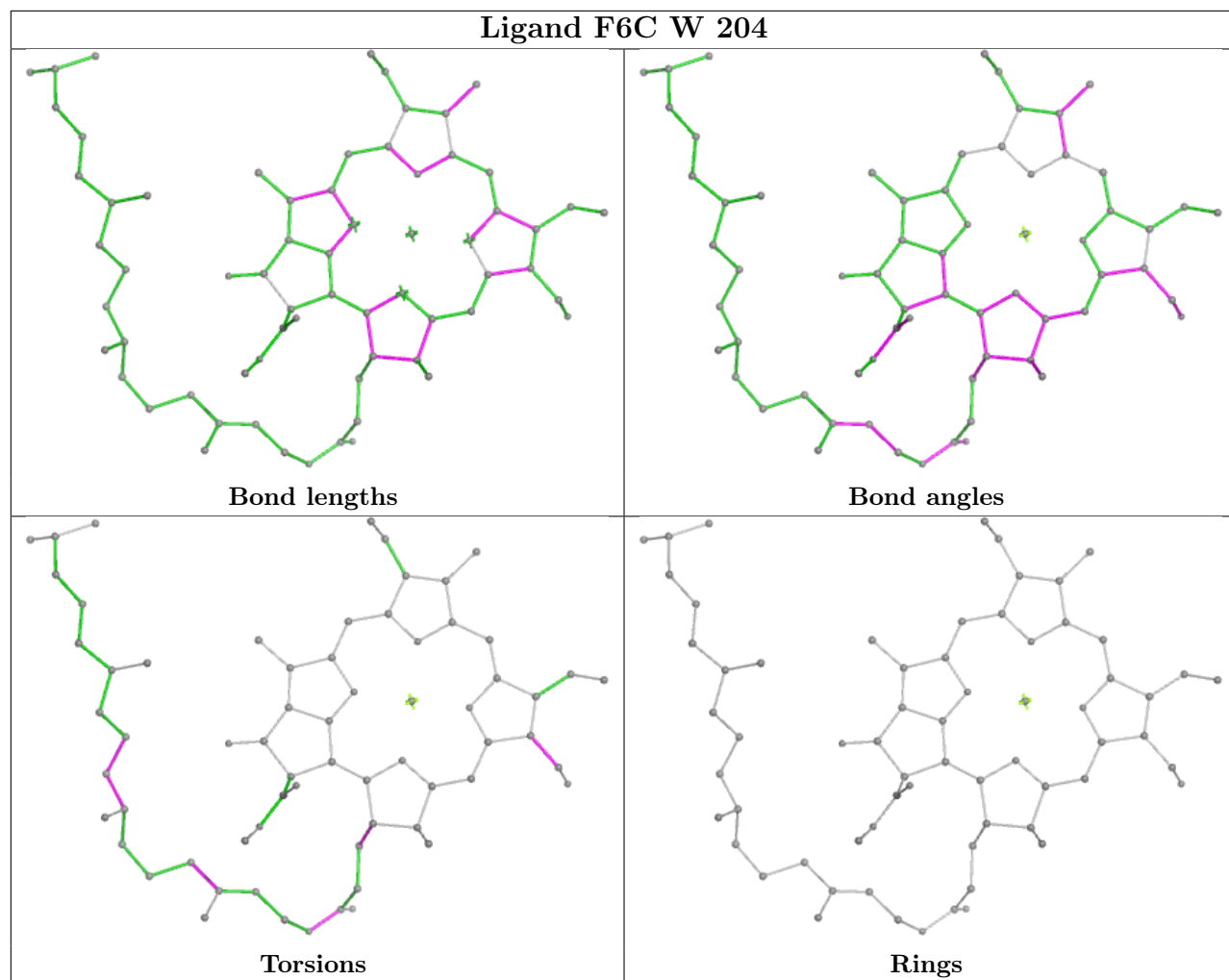


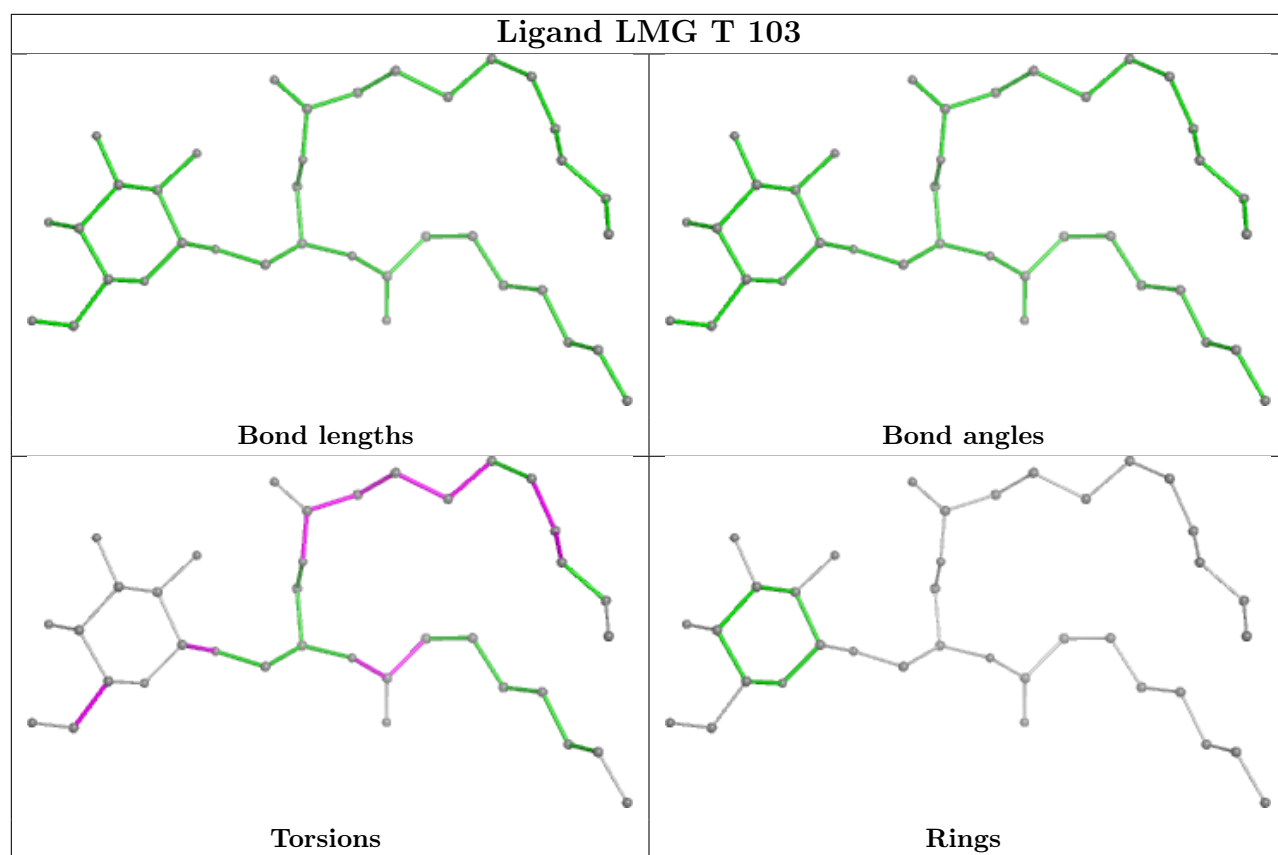
## Ligand CLA a 816



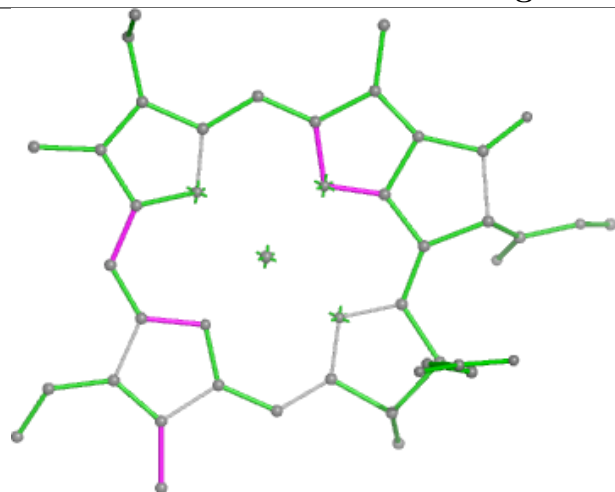
## Ligand BCR N 846



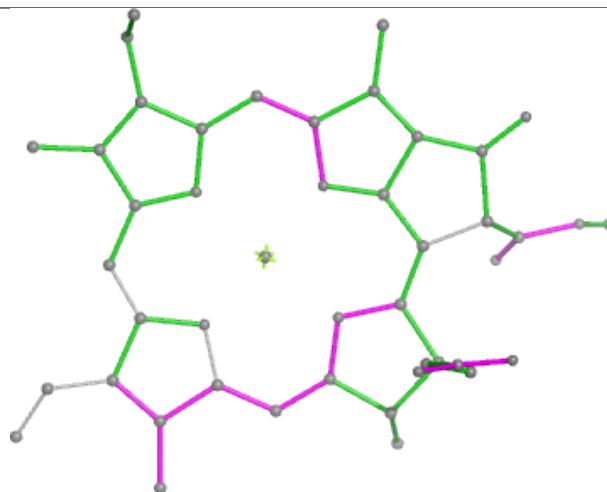




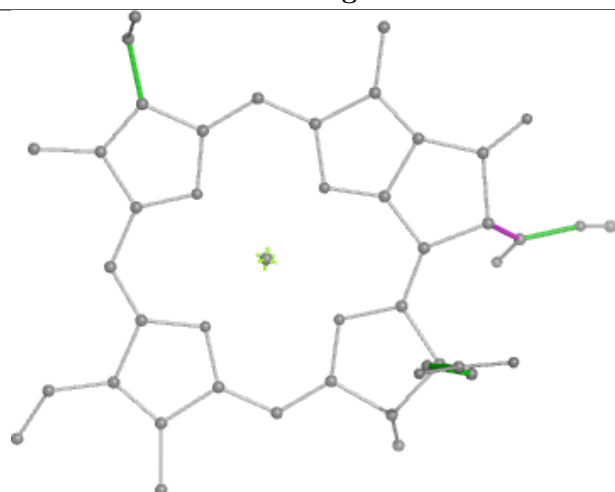
## Ligand CLA N 808



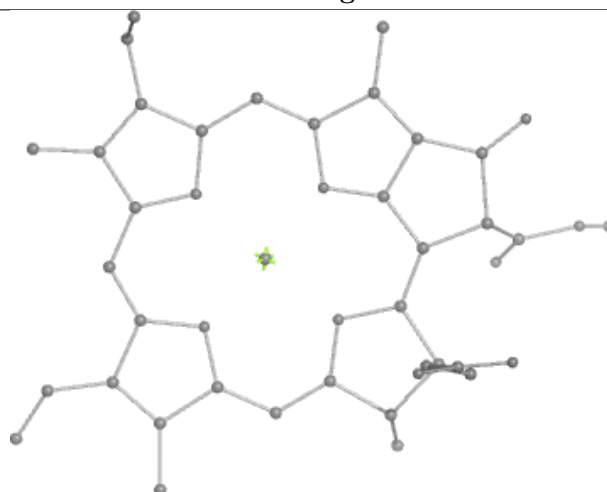
Bond lengths



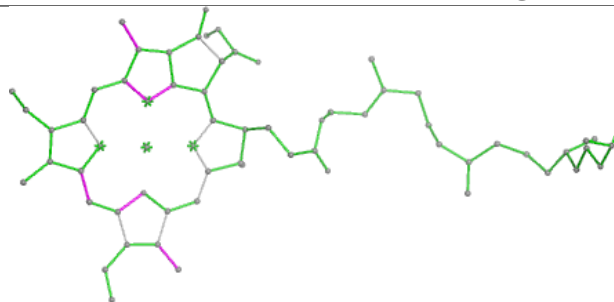
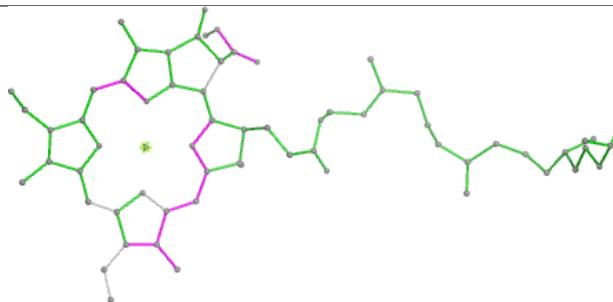
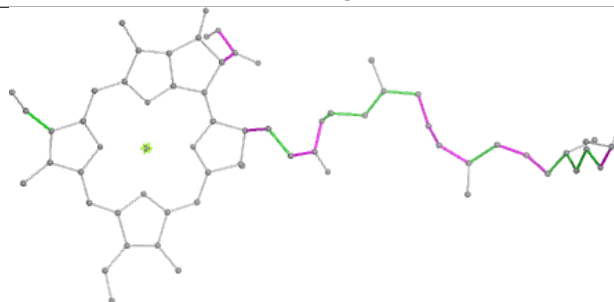
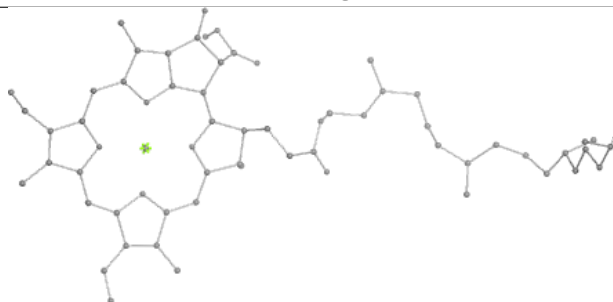
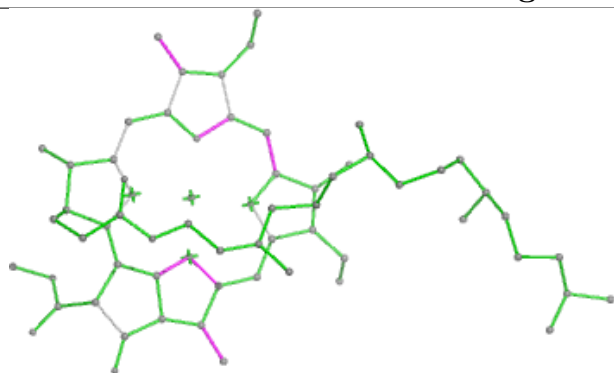
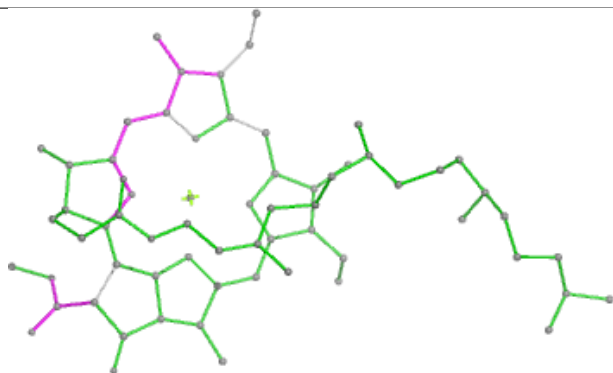
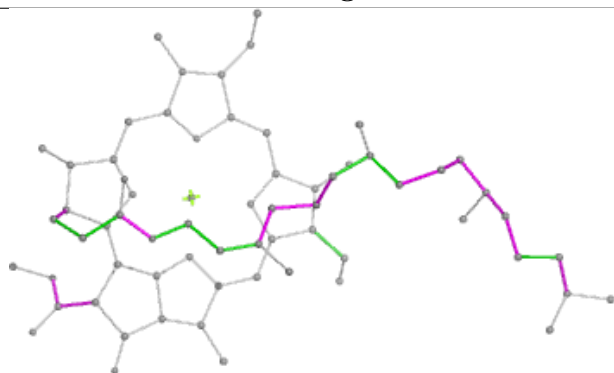
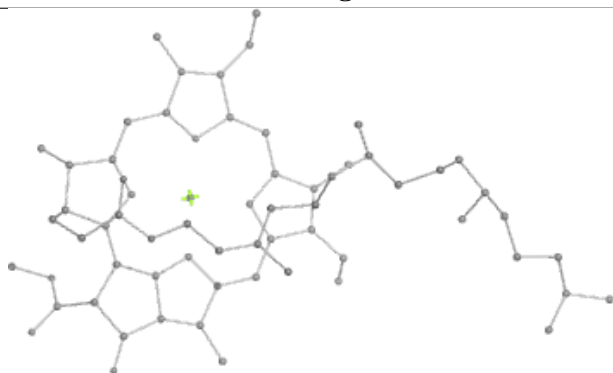
Bond angles



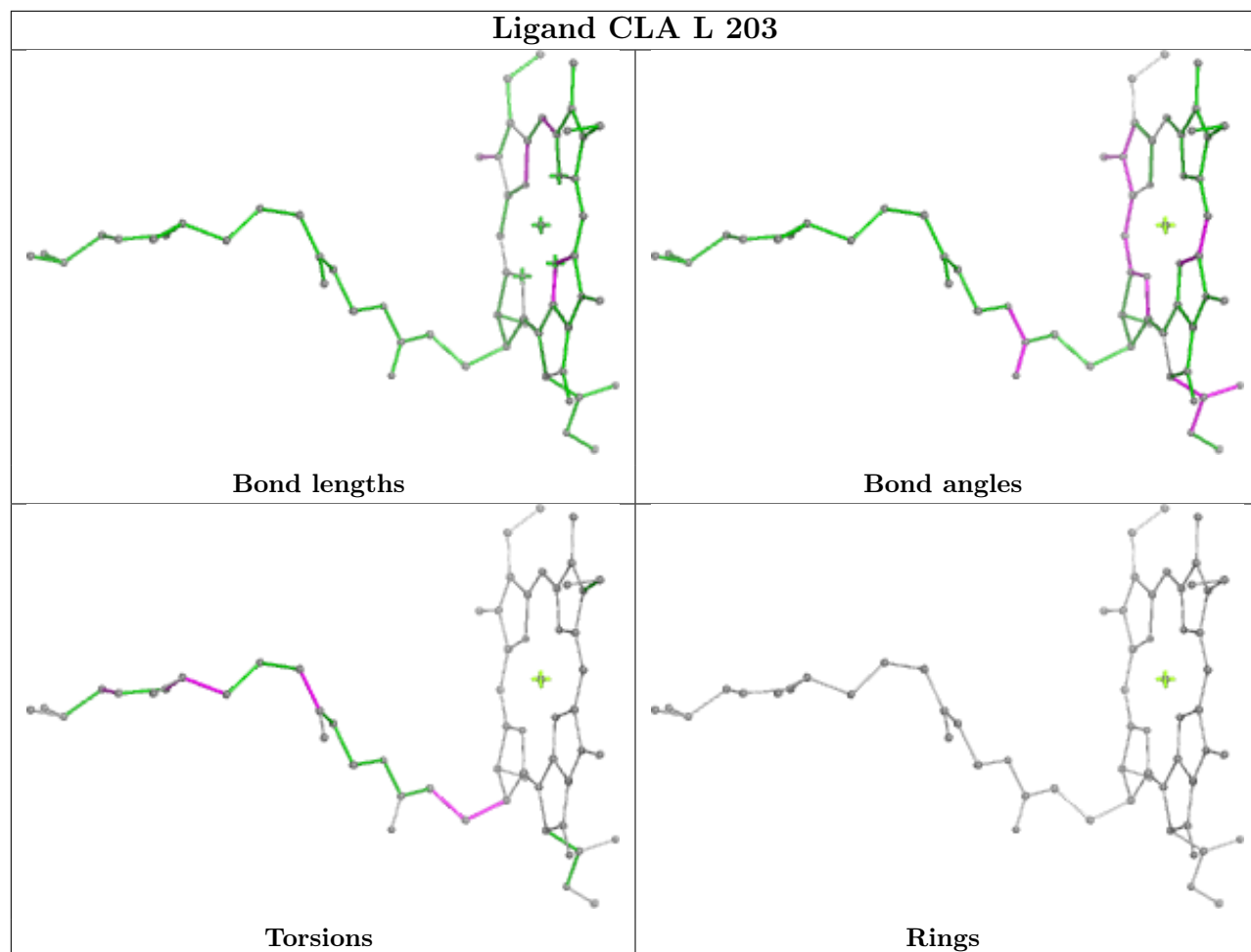
Torsions



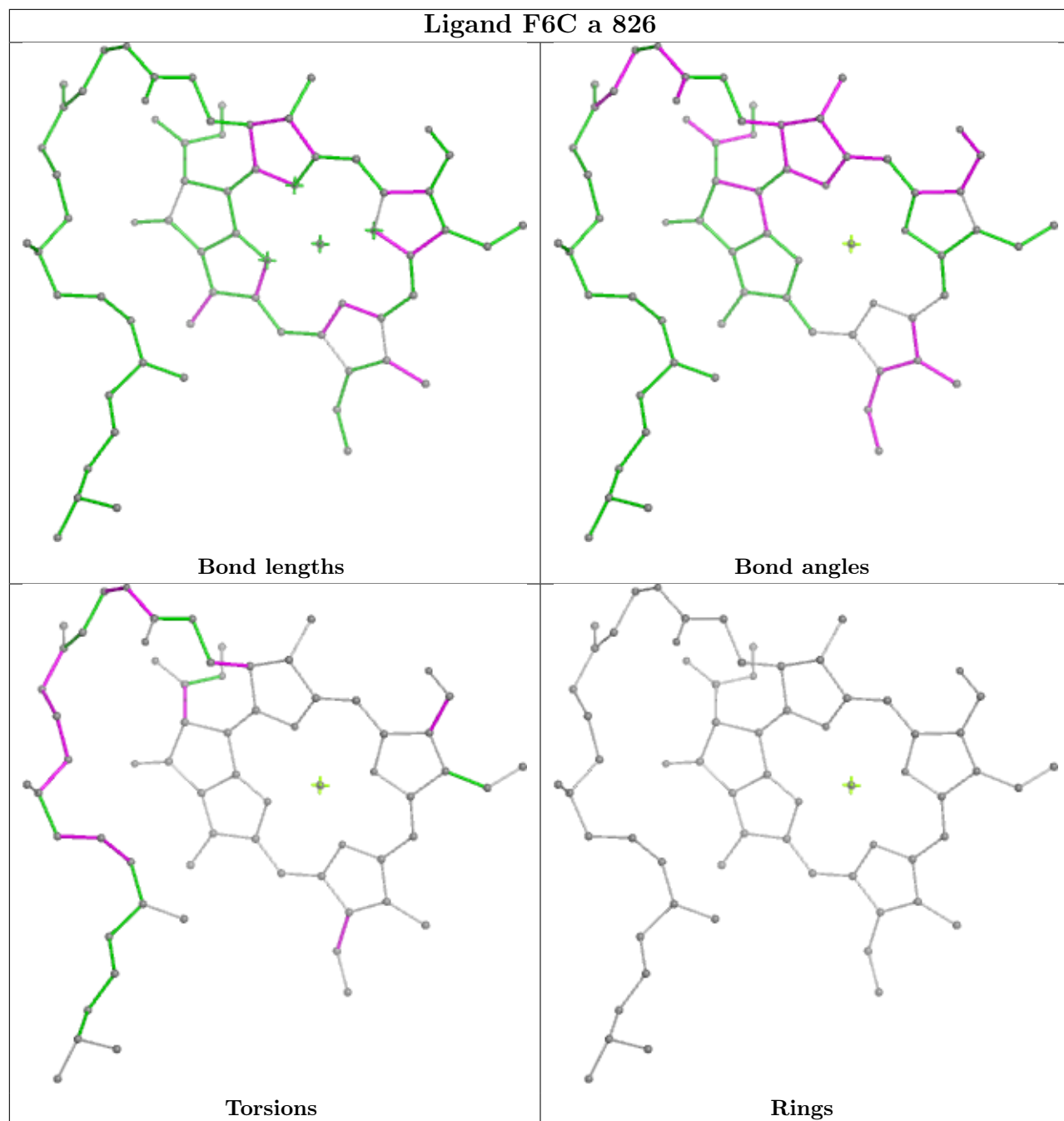
Rings

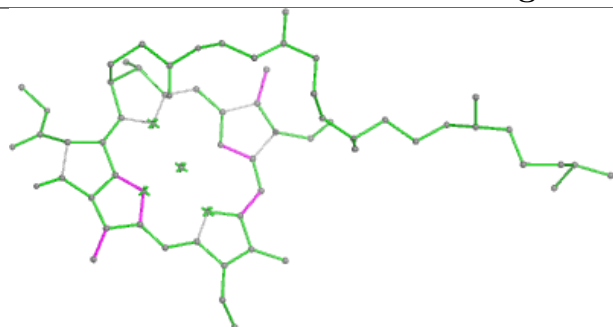
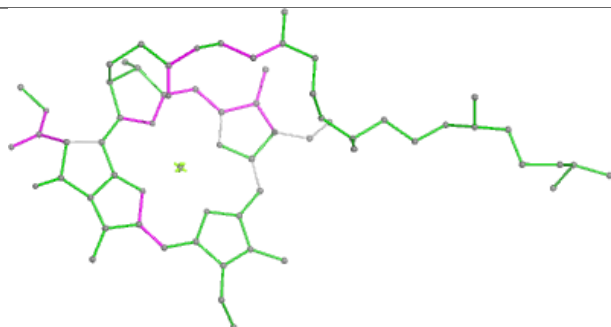
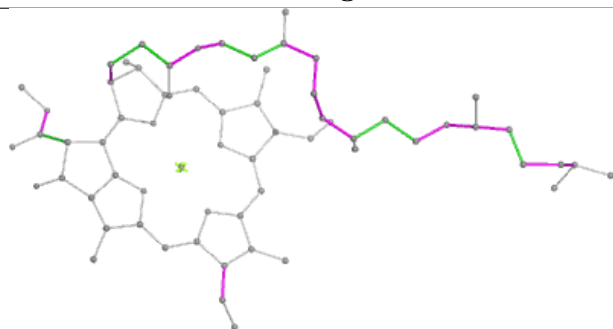
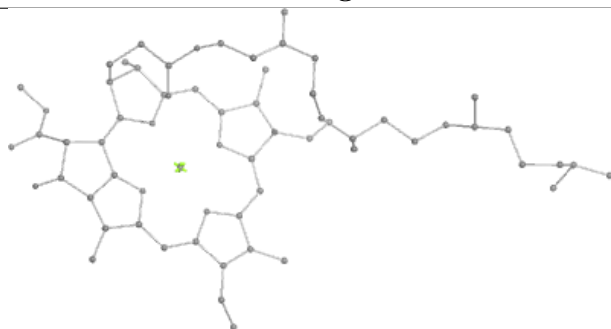
**Ligand CLA N 806****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 818****Bond lengths****Bond angles****Torsions****Rings**

## Ligand CLA L 203



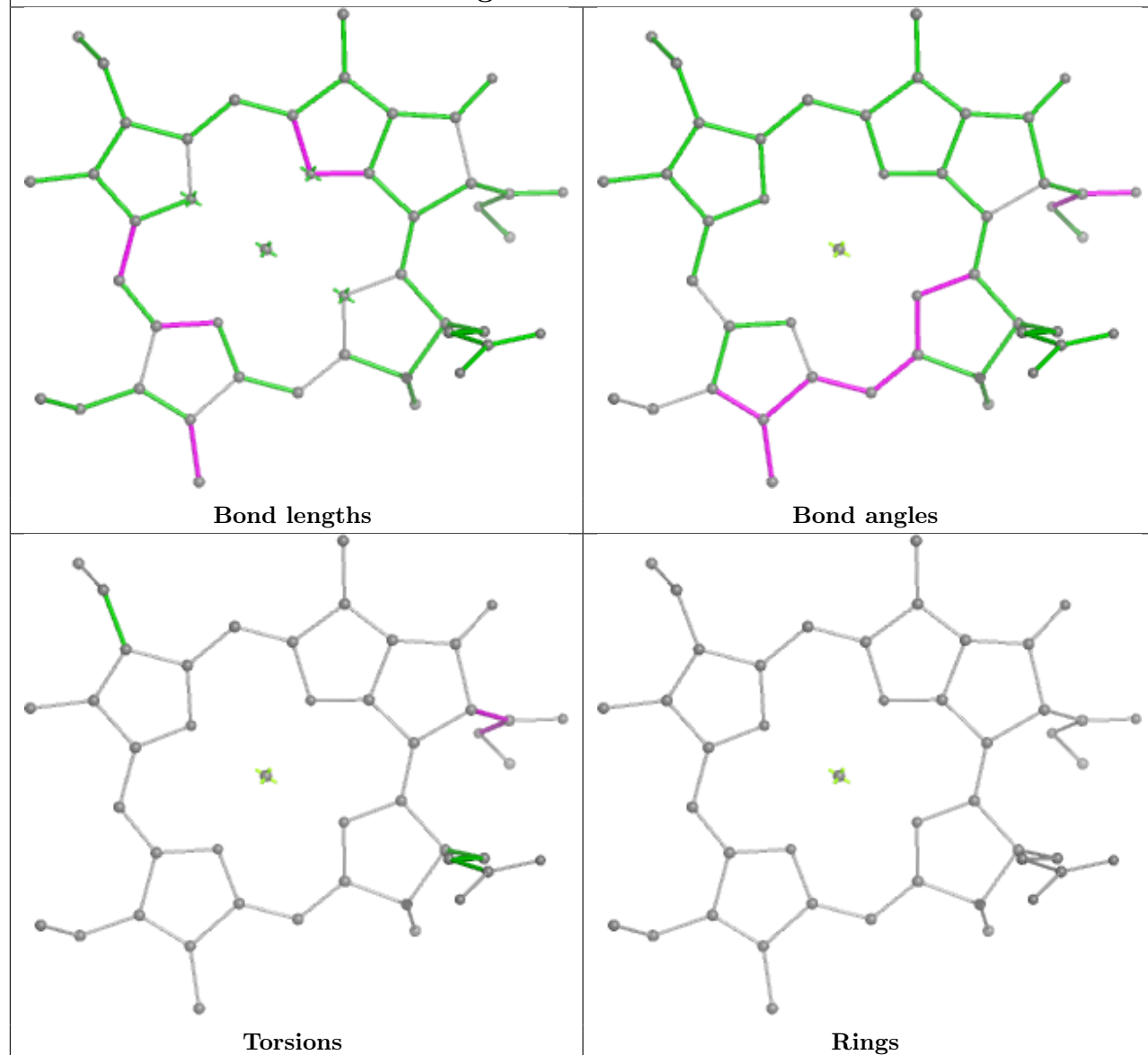
## Ligand F6C a 826



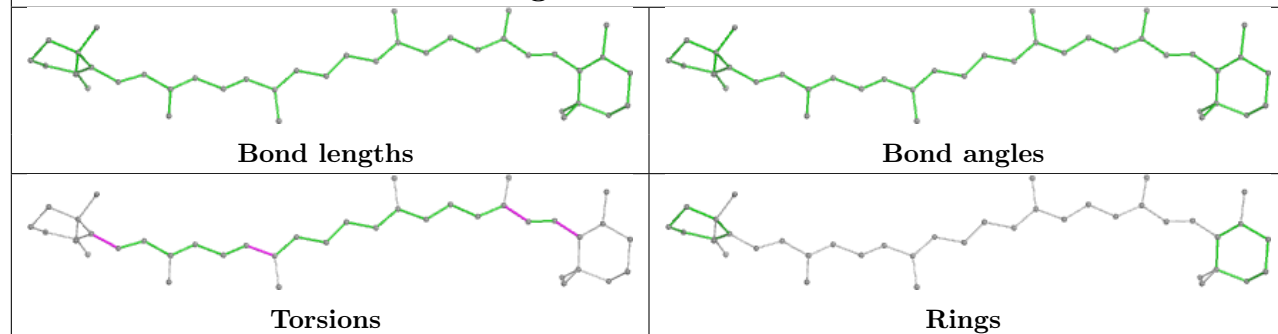
**Ligand CLA a 820****Bond lengths****Bond angles****Torsions****Rings**



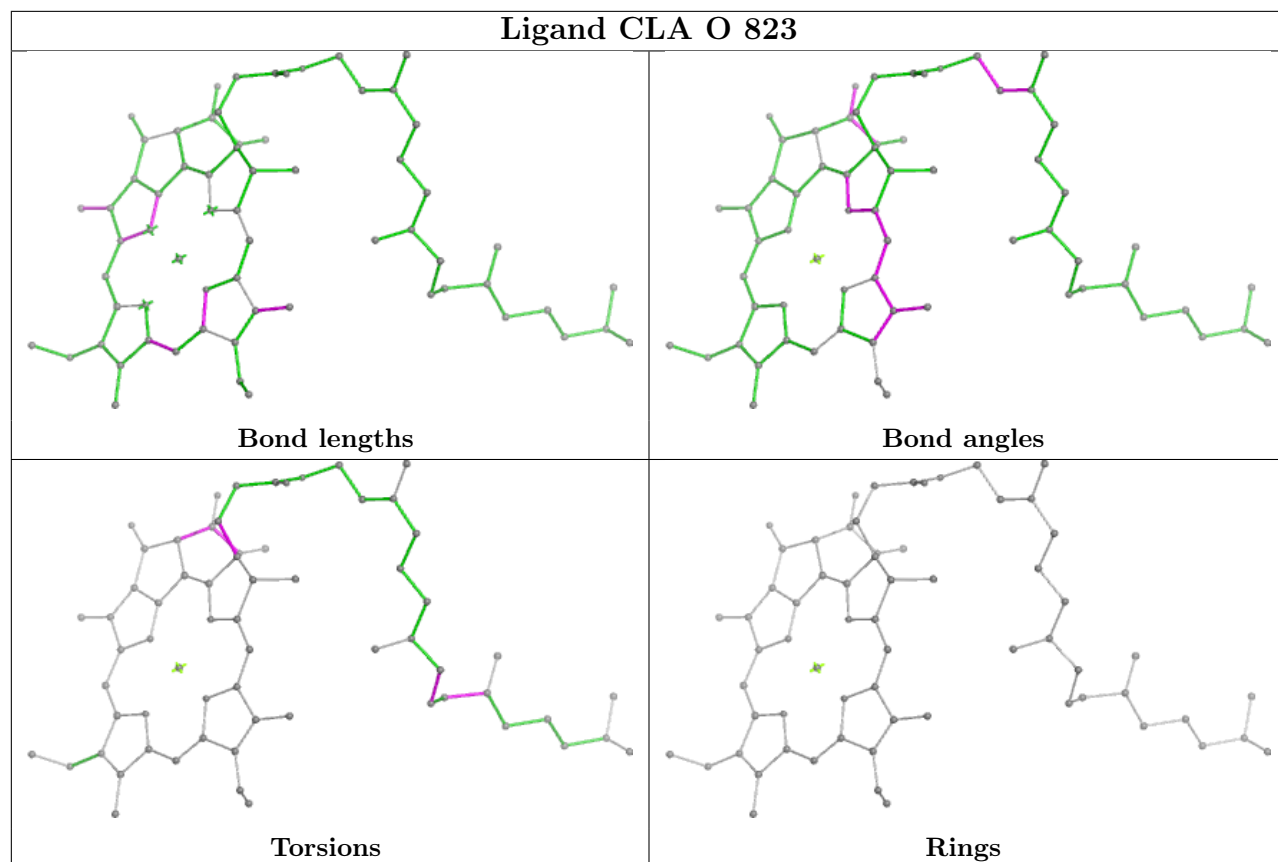
## Ligand CLA N 817



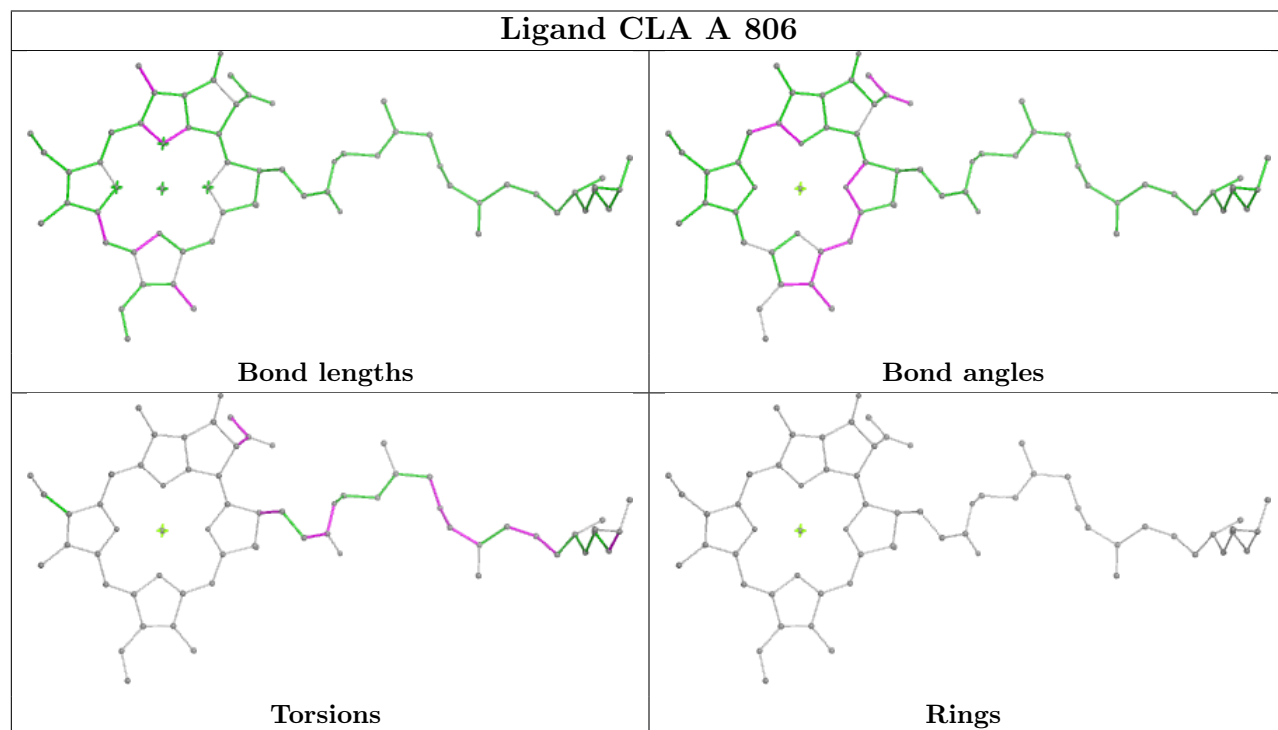
## Ligand BCR U 101

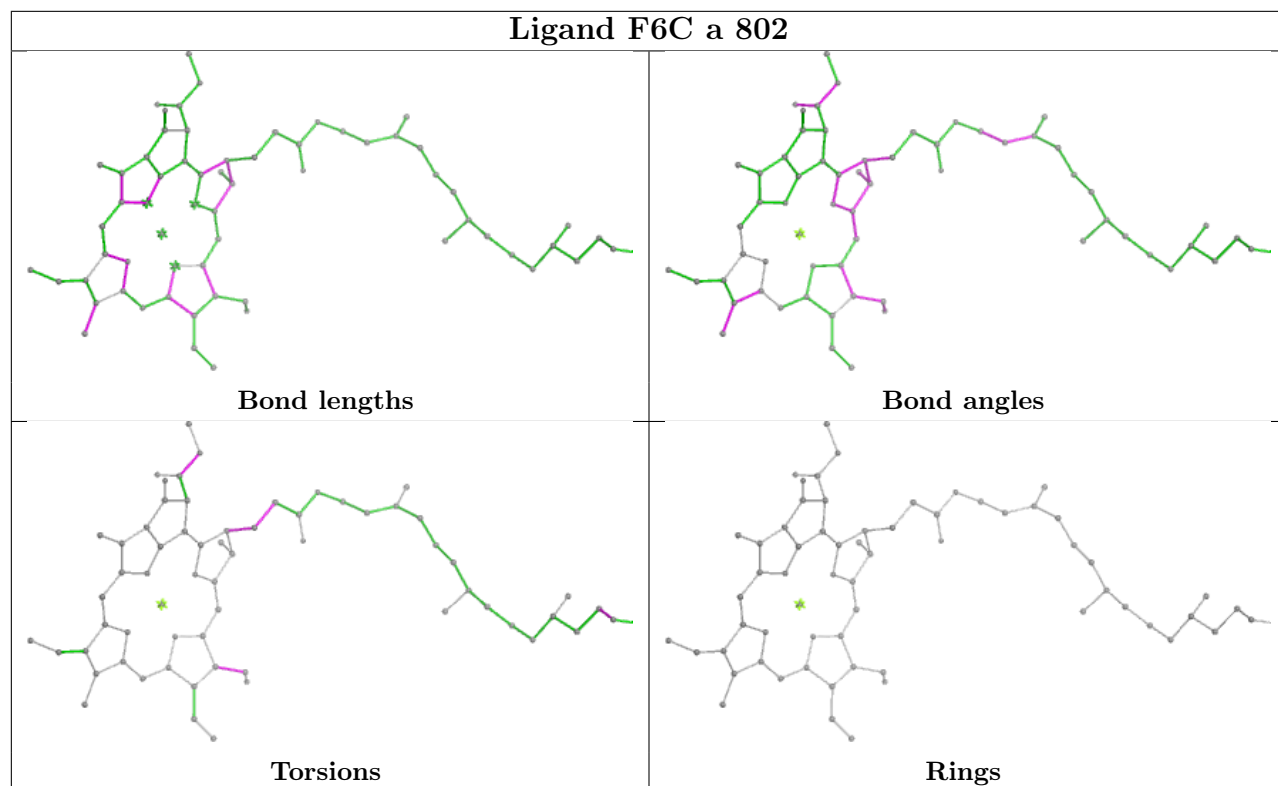
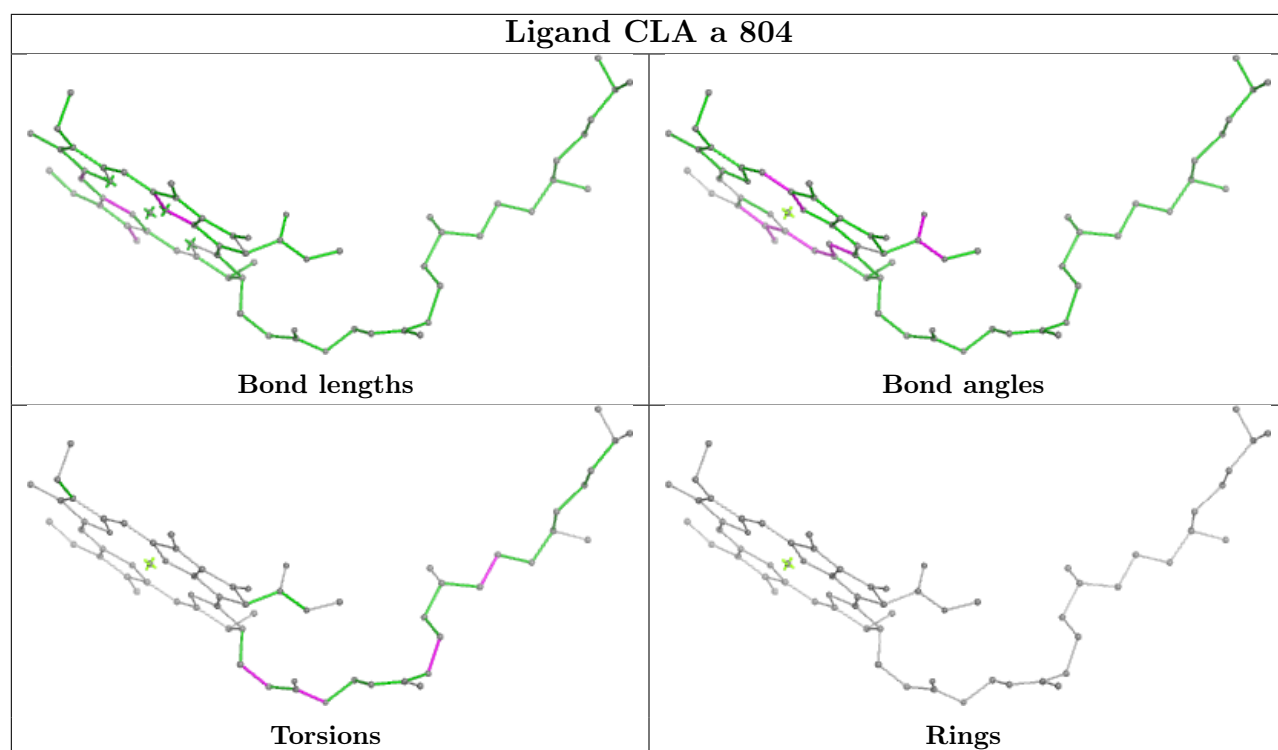


## Ligand CLA O 823

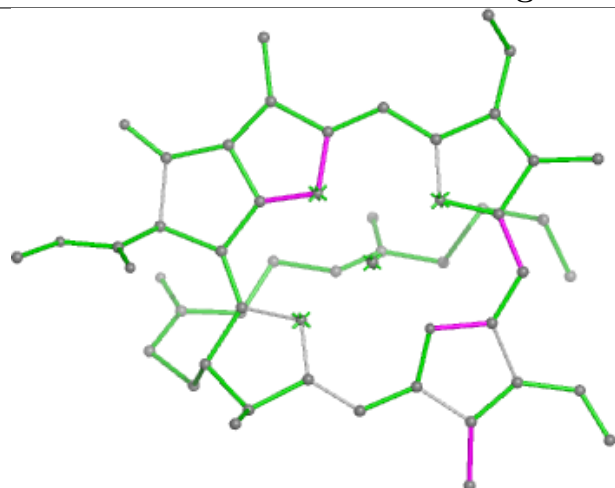


## Ligand CLA A 806

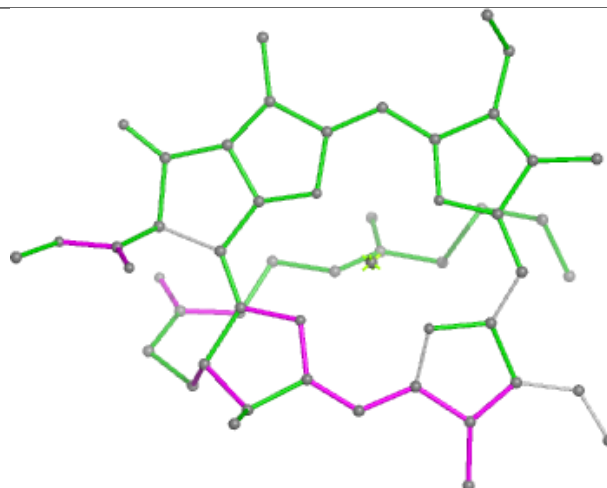




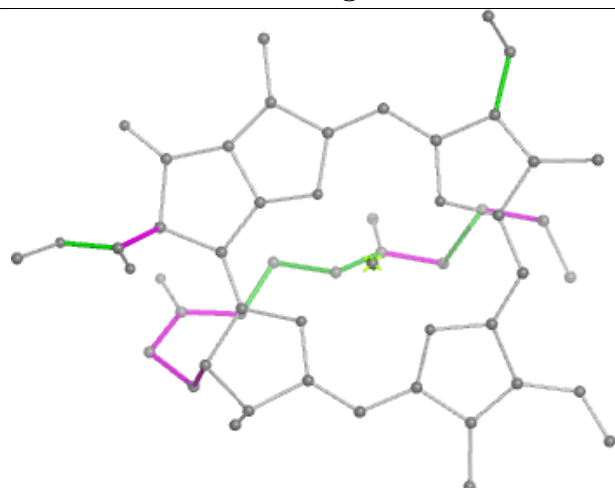
## Ligand CLA B 821



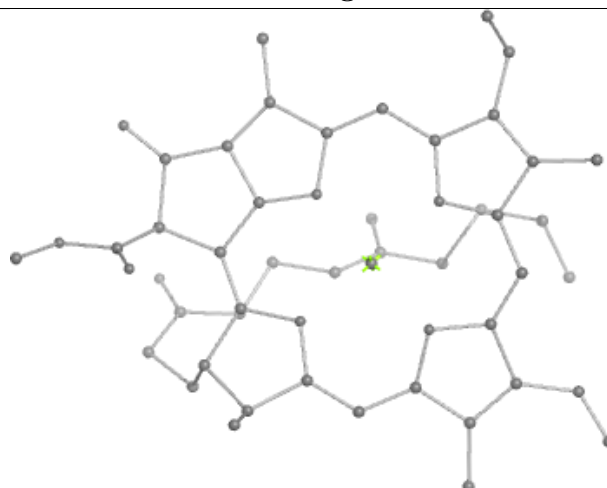
Bond lengths



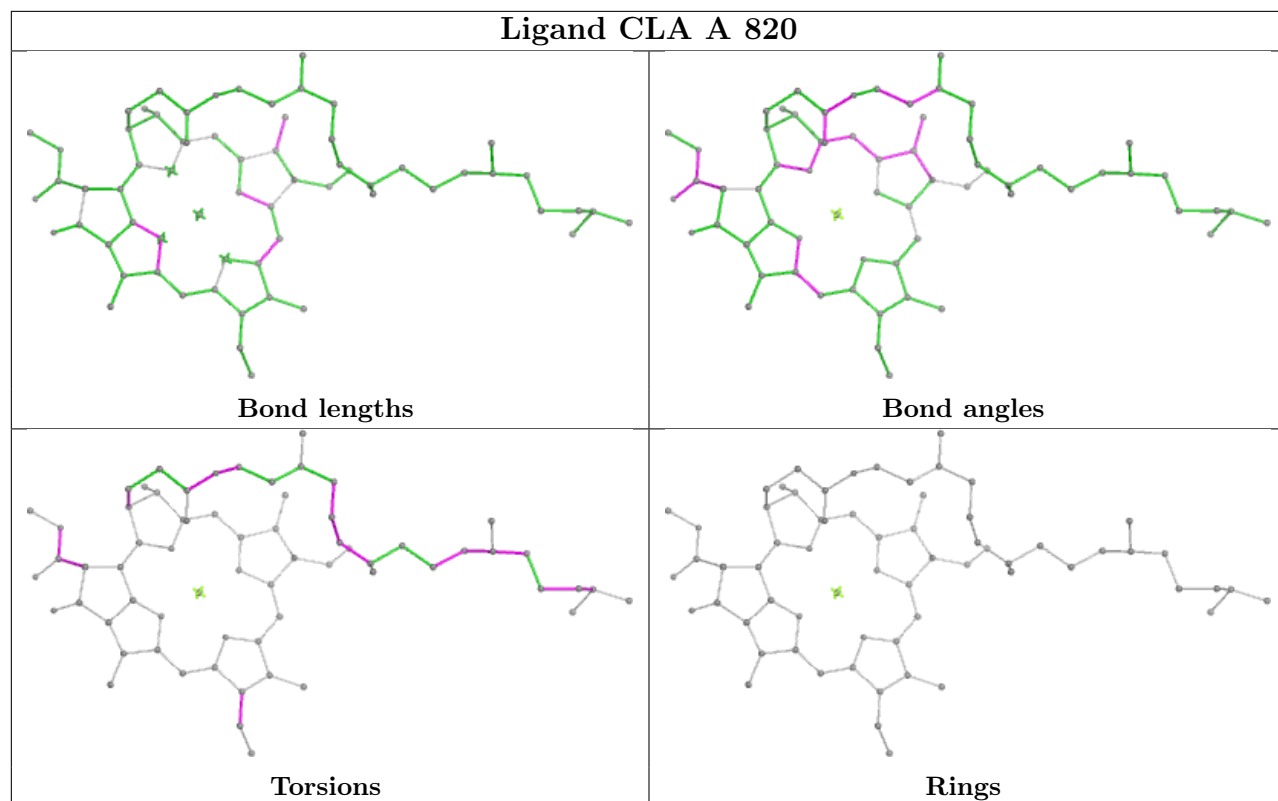
Bond angles



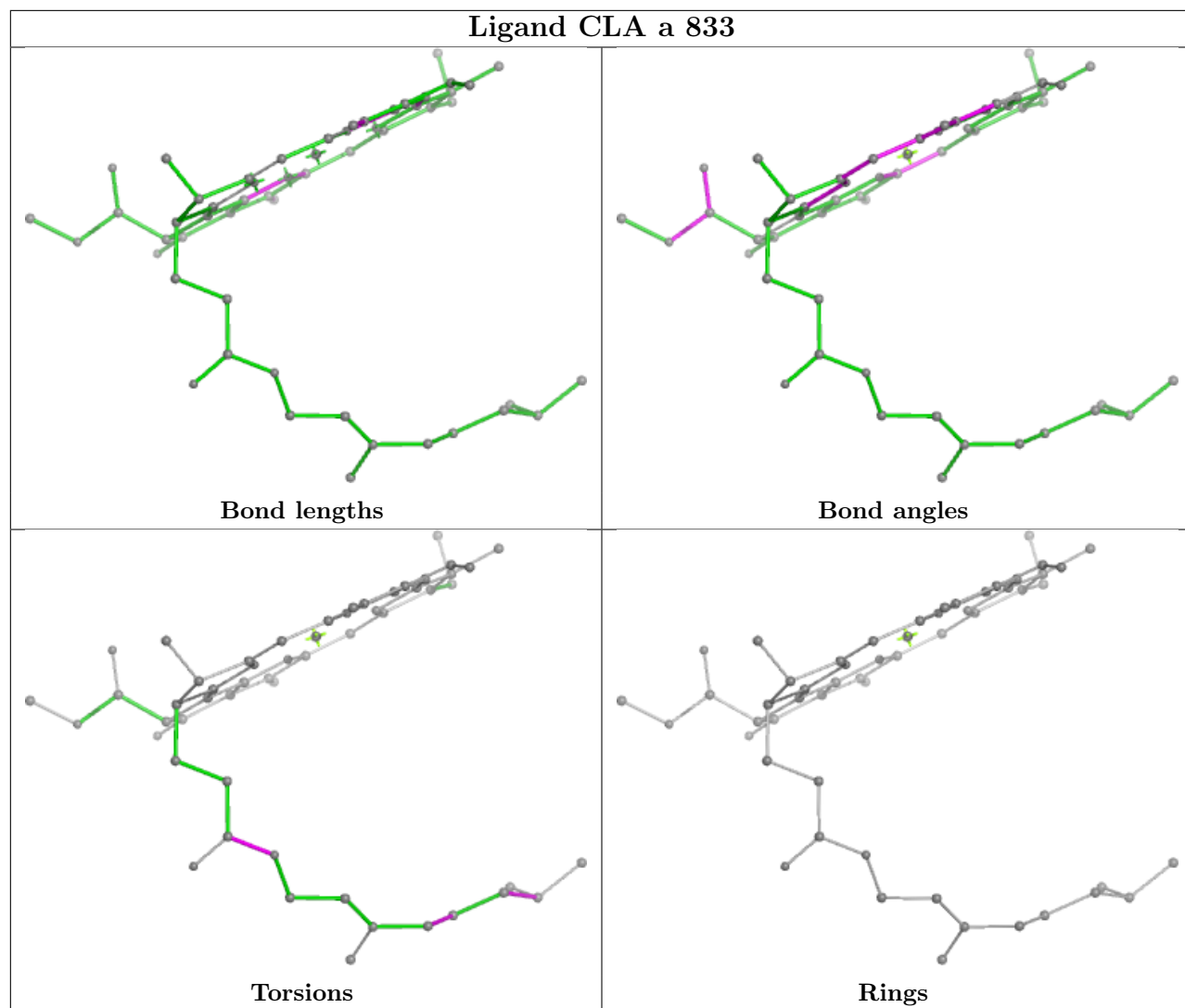
Torsions

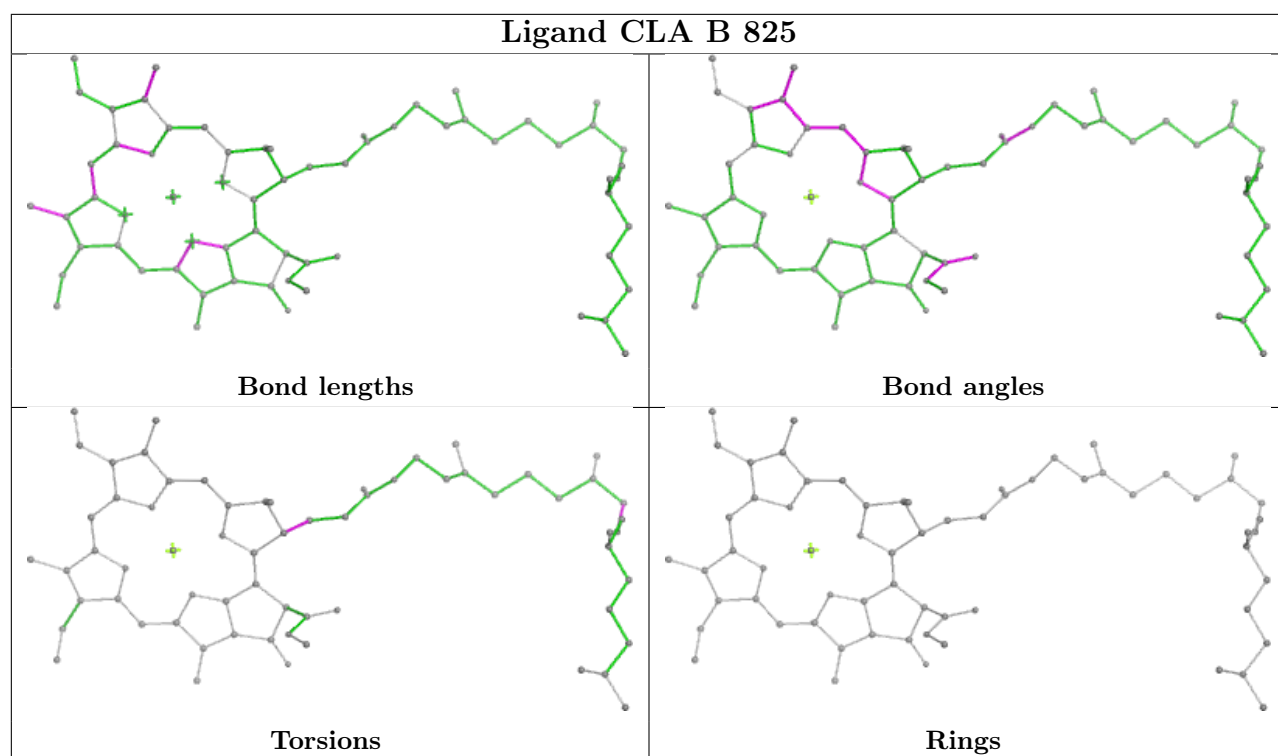


Rings

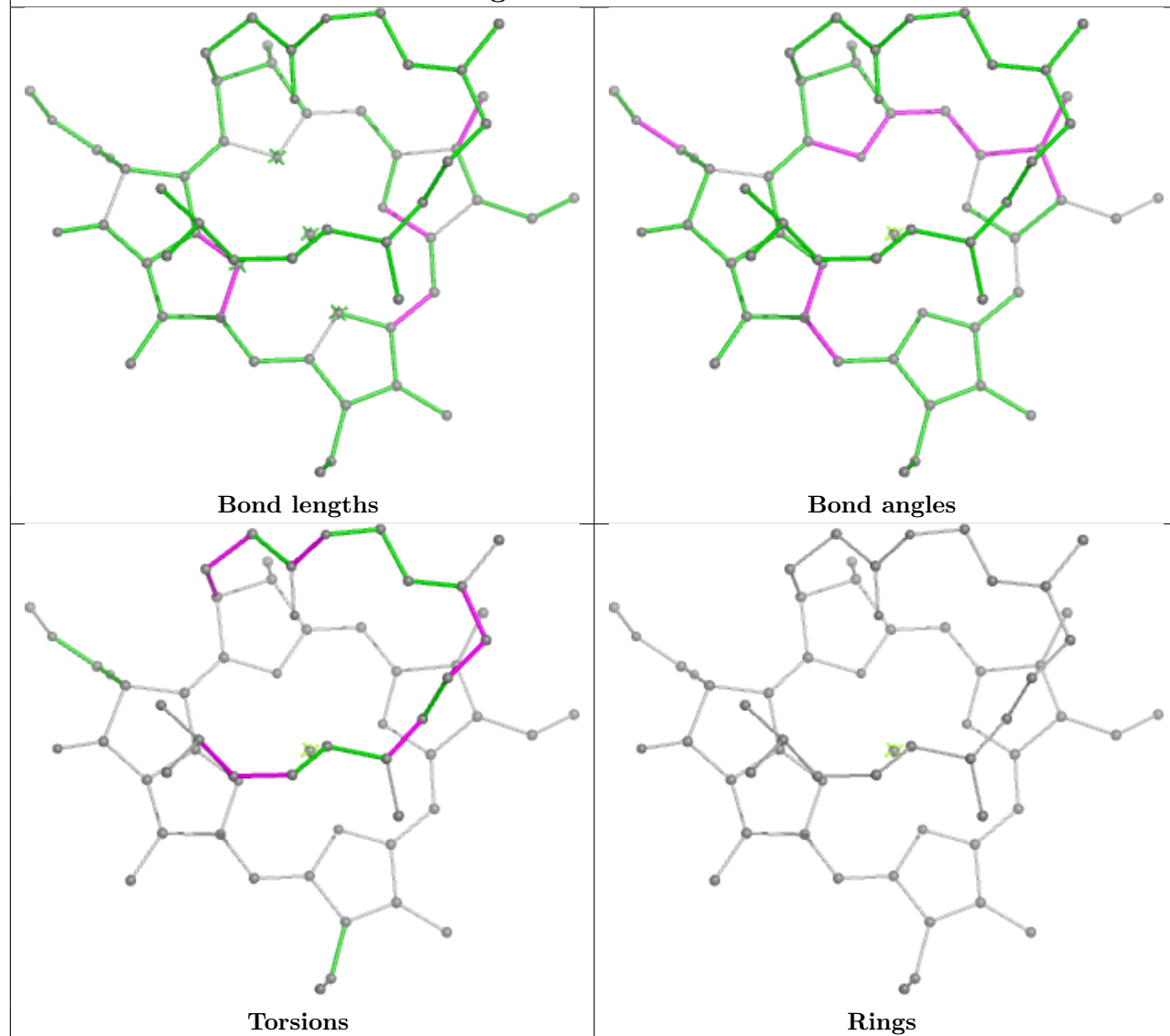


## Ligand CLA a 833



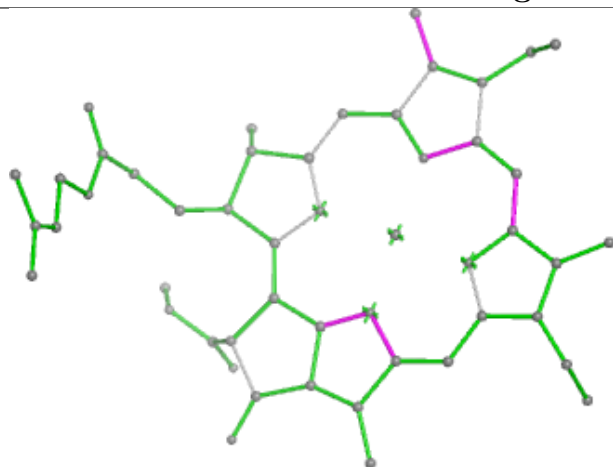


## Ligand CLA b 817

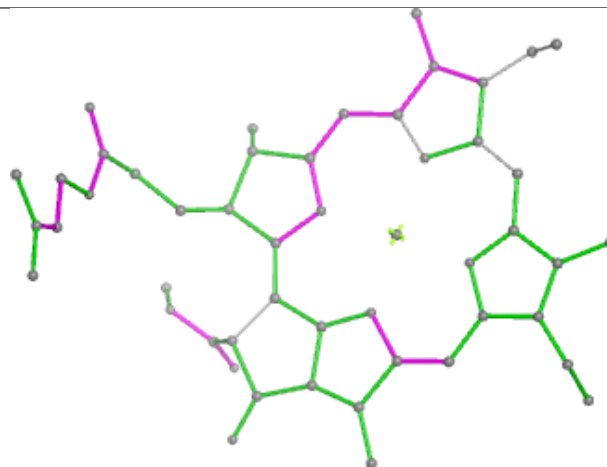




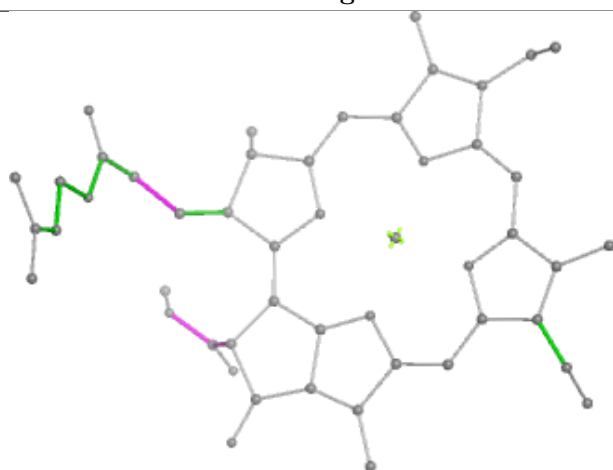
## Ligand CLA V 103



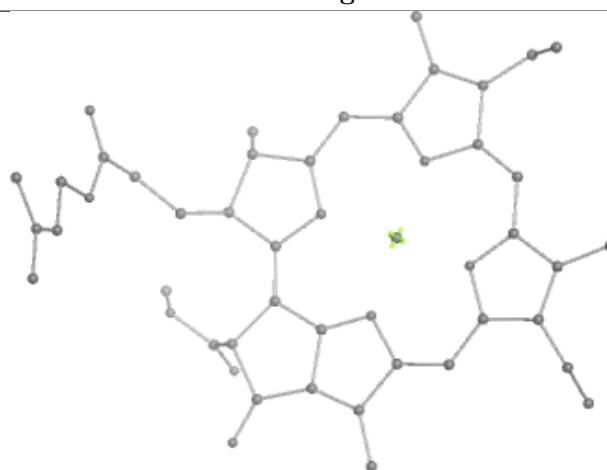
Bond lengths



Bond angles

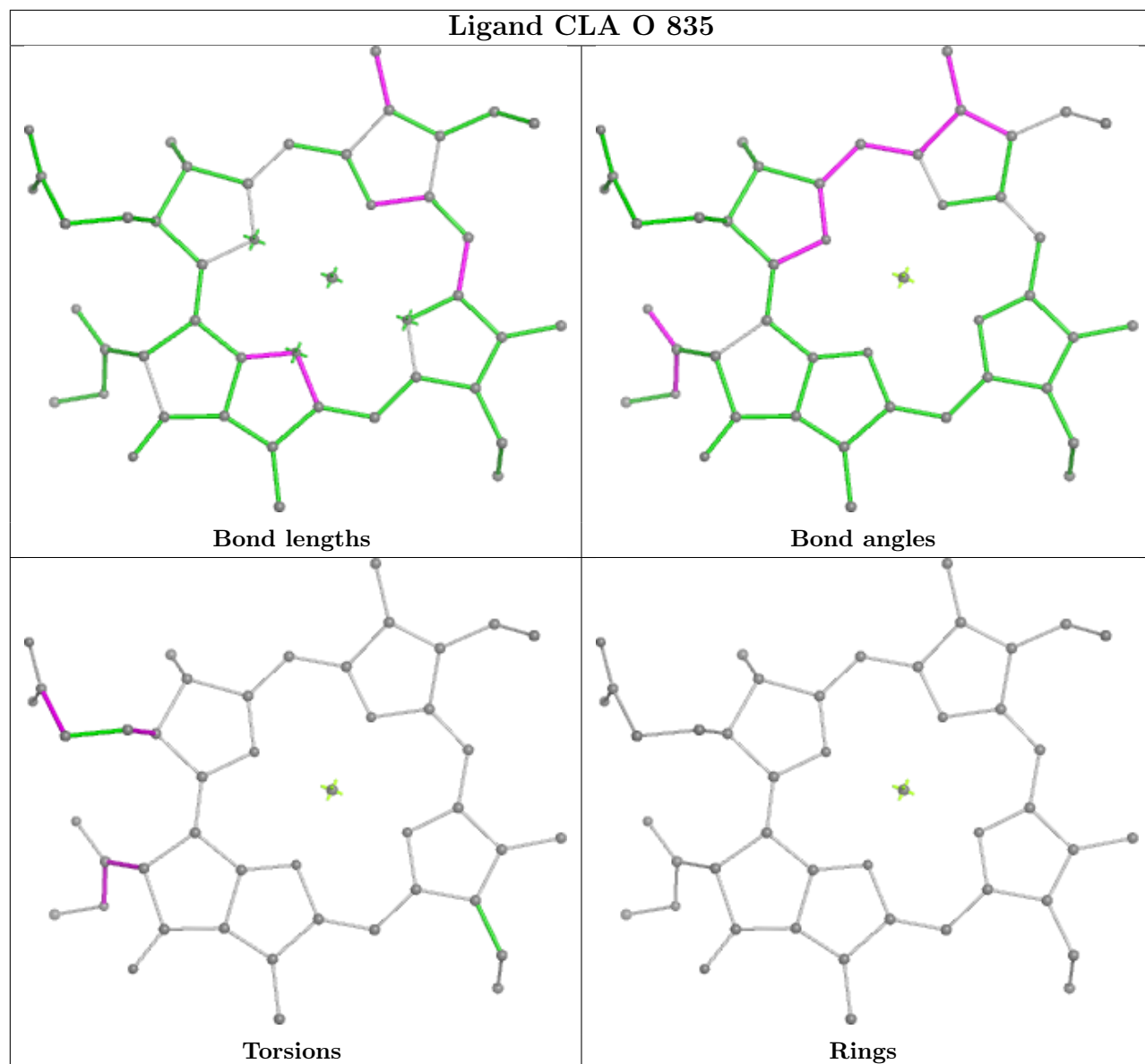


Torsions

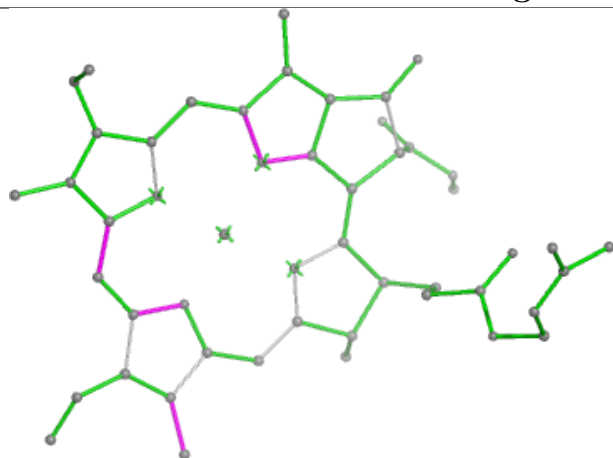


Rings

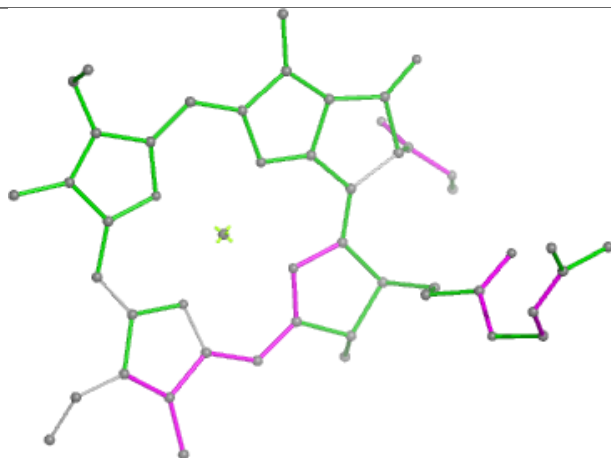
## Ligand CLA O 835



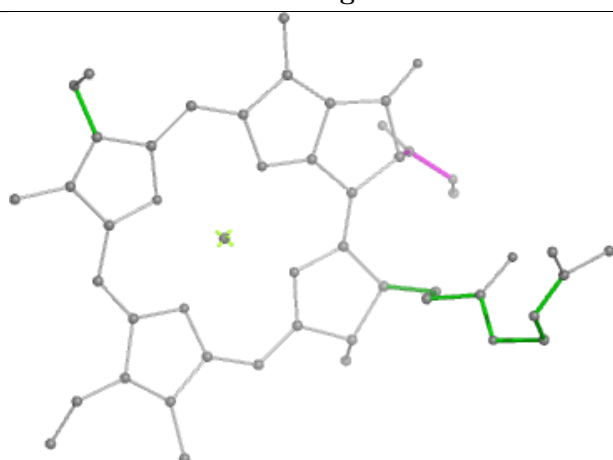
## Ligand CLA N 840



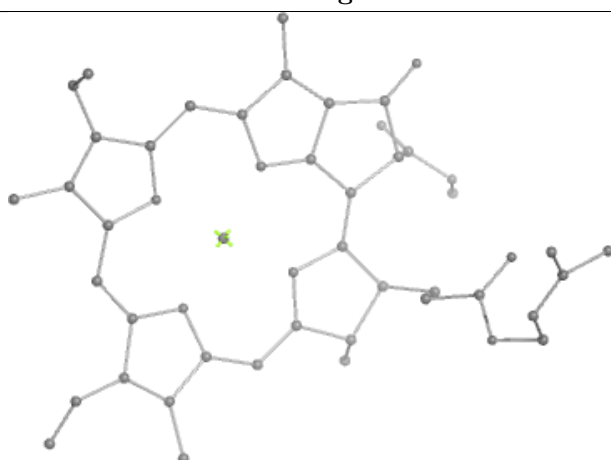
Bond lengths



Bond angles

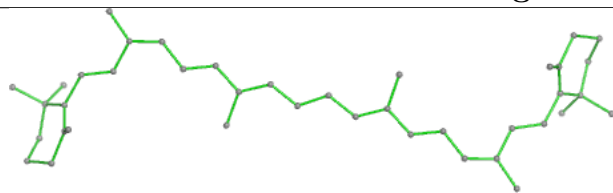


Torsions

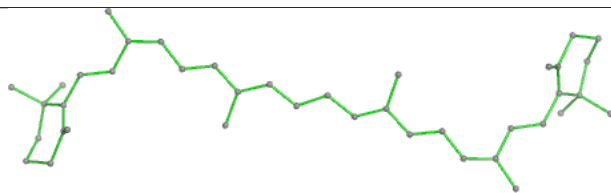


Rings

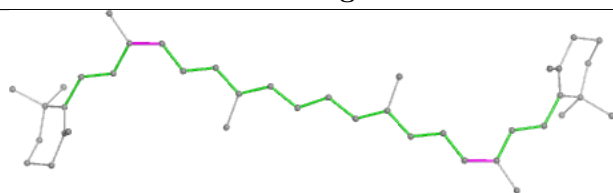
## Ligand BCR B 844



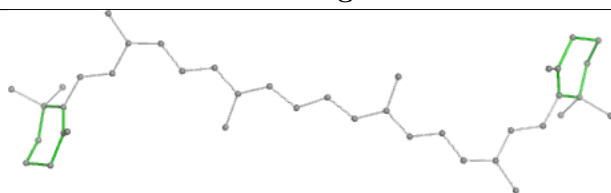
Bond lengths



Bond angles

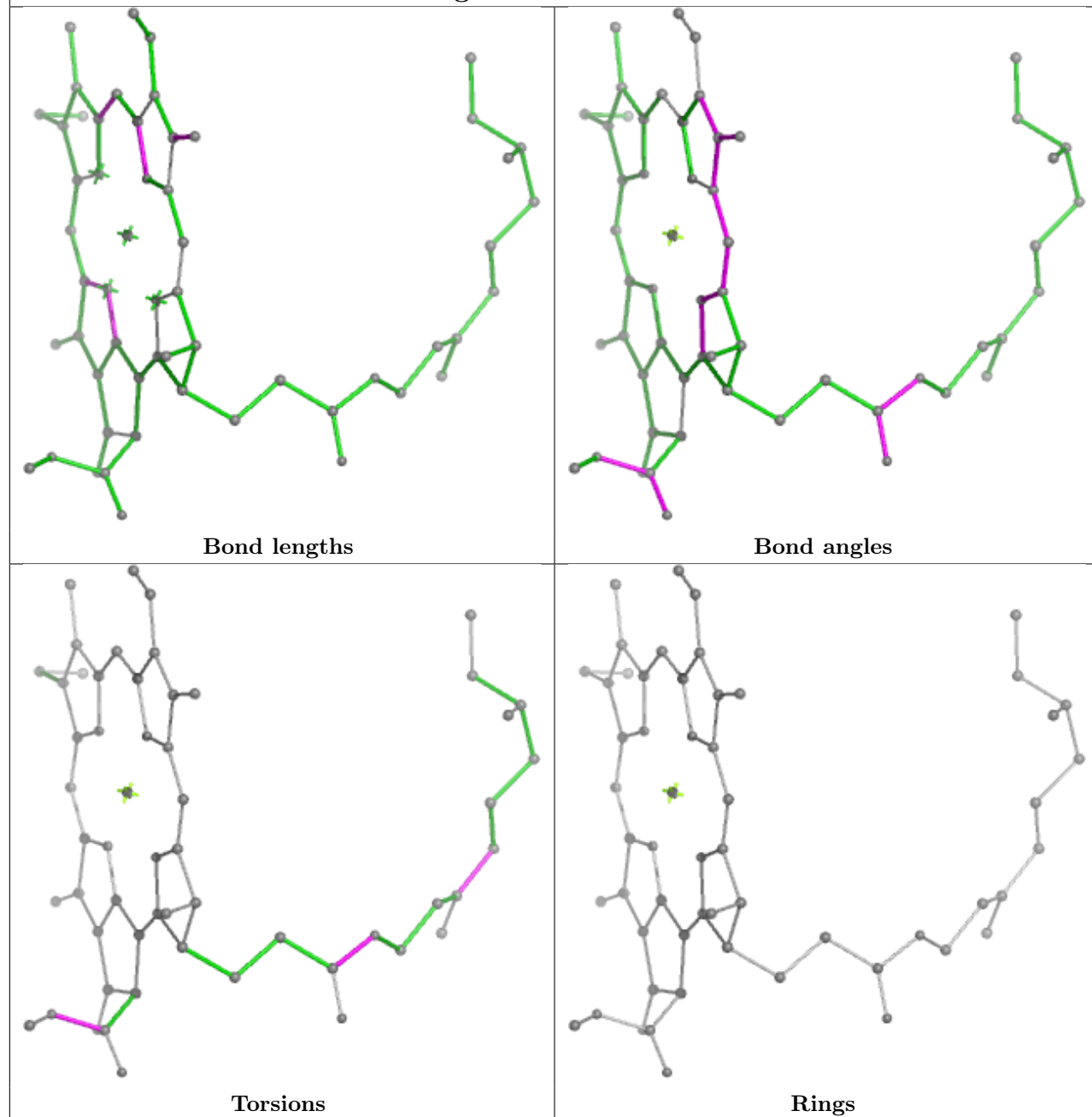


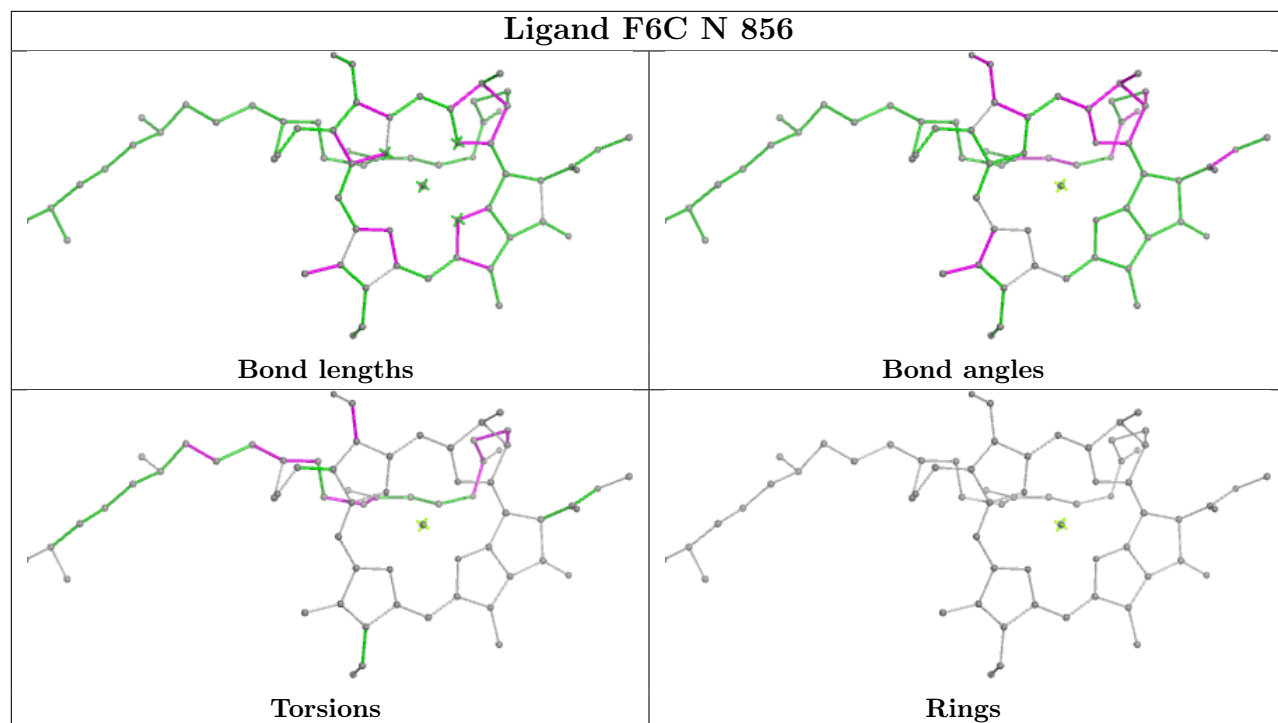
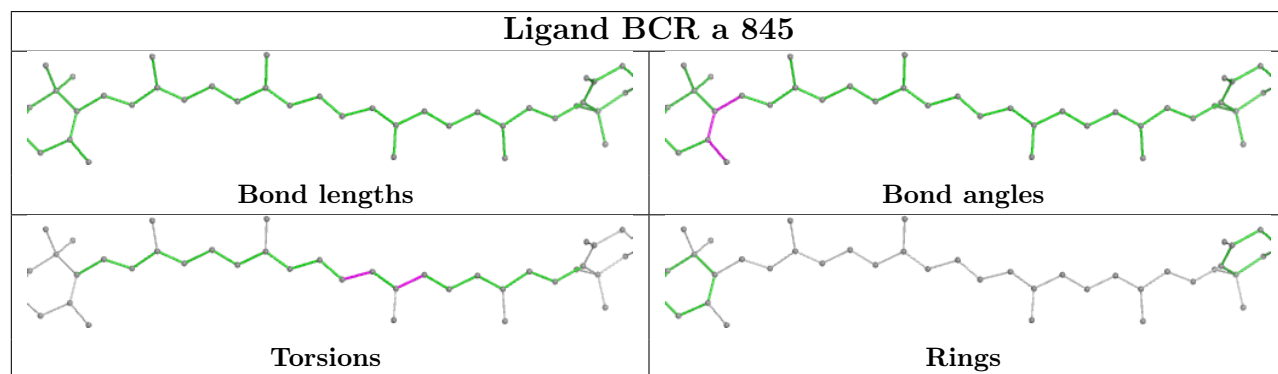
Torsions



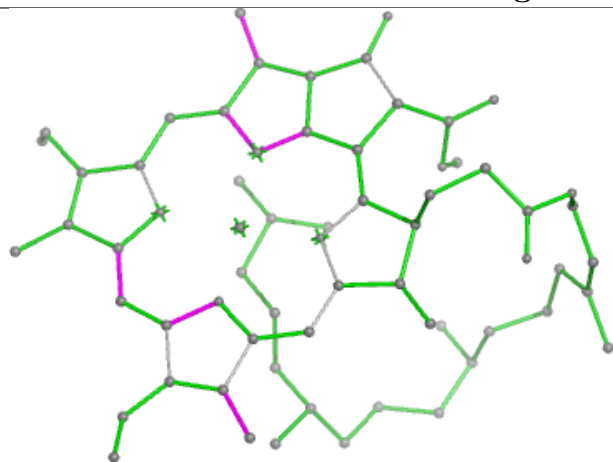
Rings

## Ligand CLA A 823

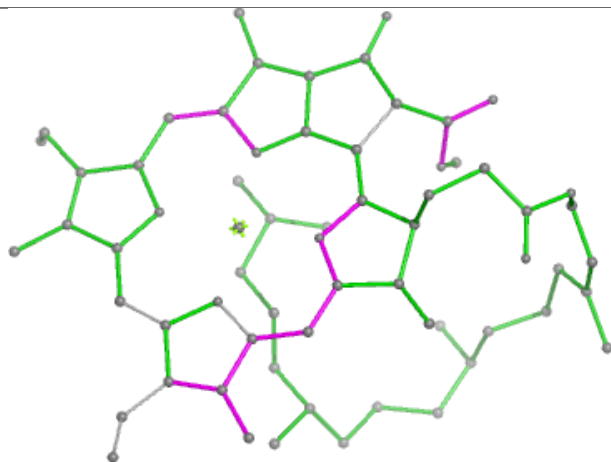


**Ligand F6C N 856****Ligand BCR a 845**

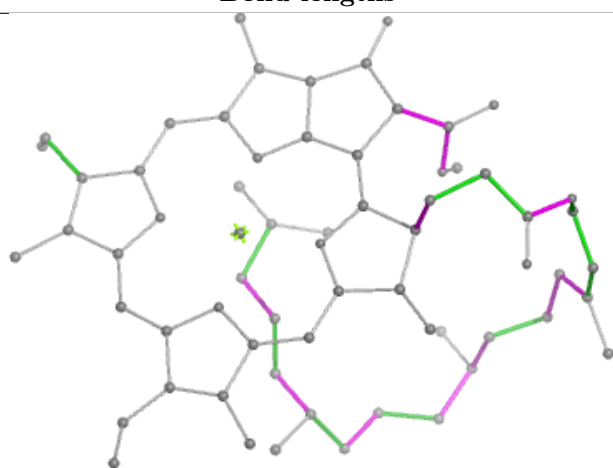
## Ligand CLA O 806



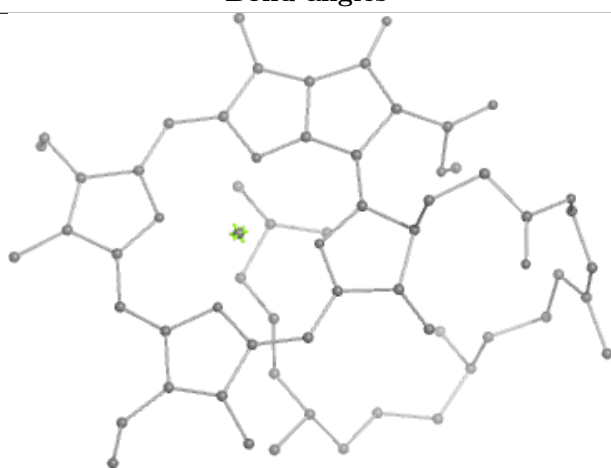
Bond lengths



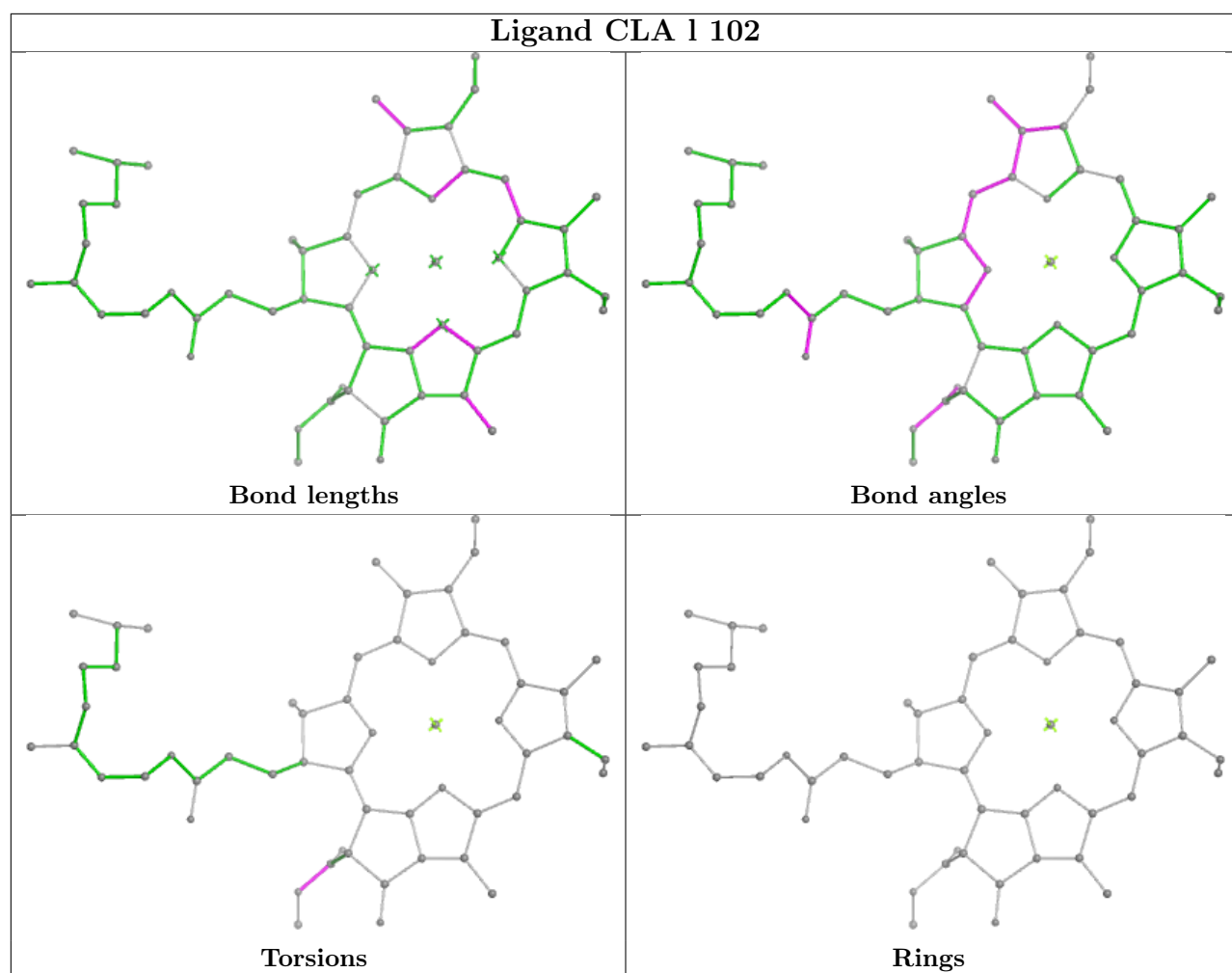
Bond angles



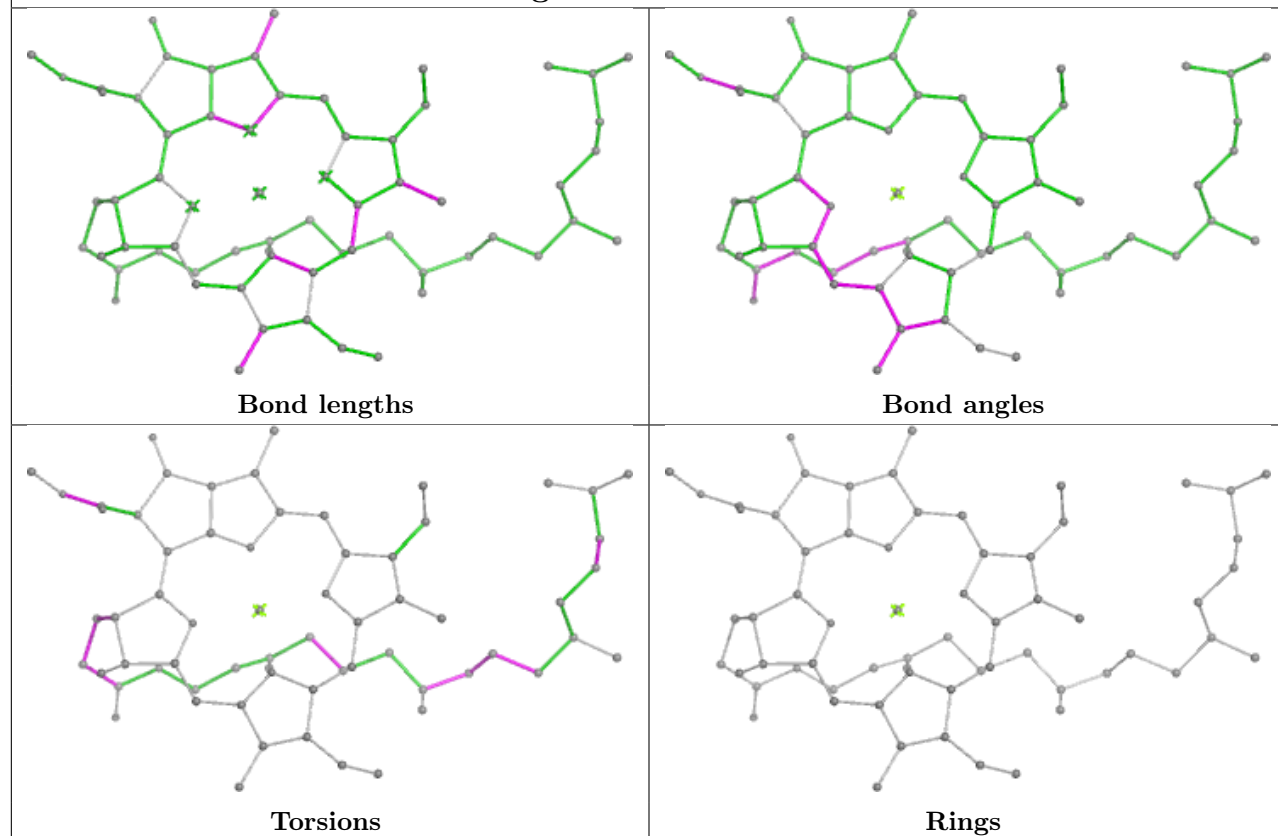
Torsions



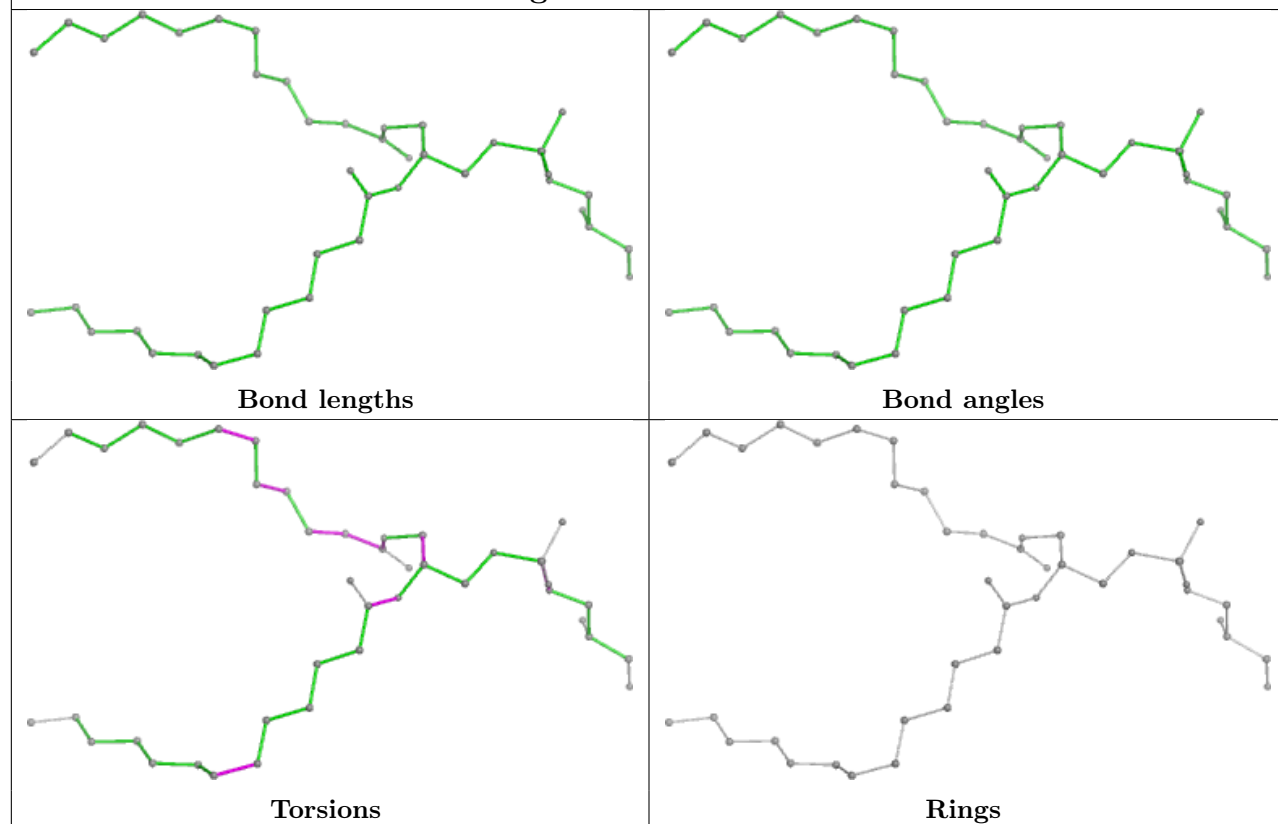
Rings



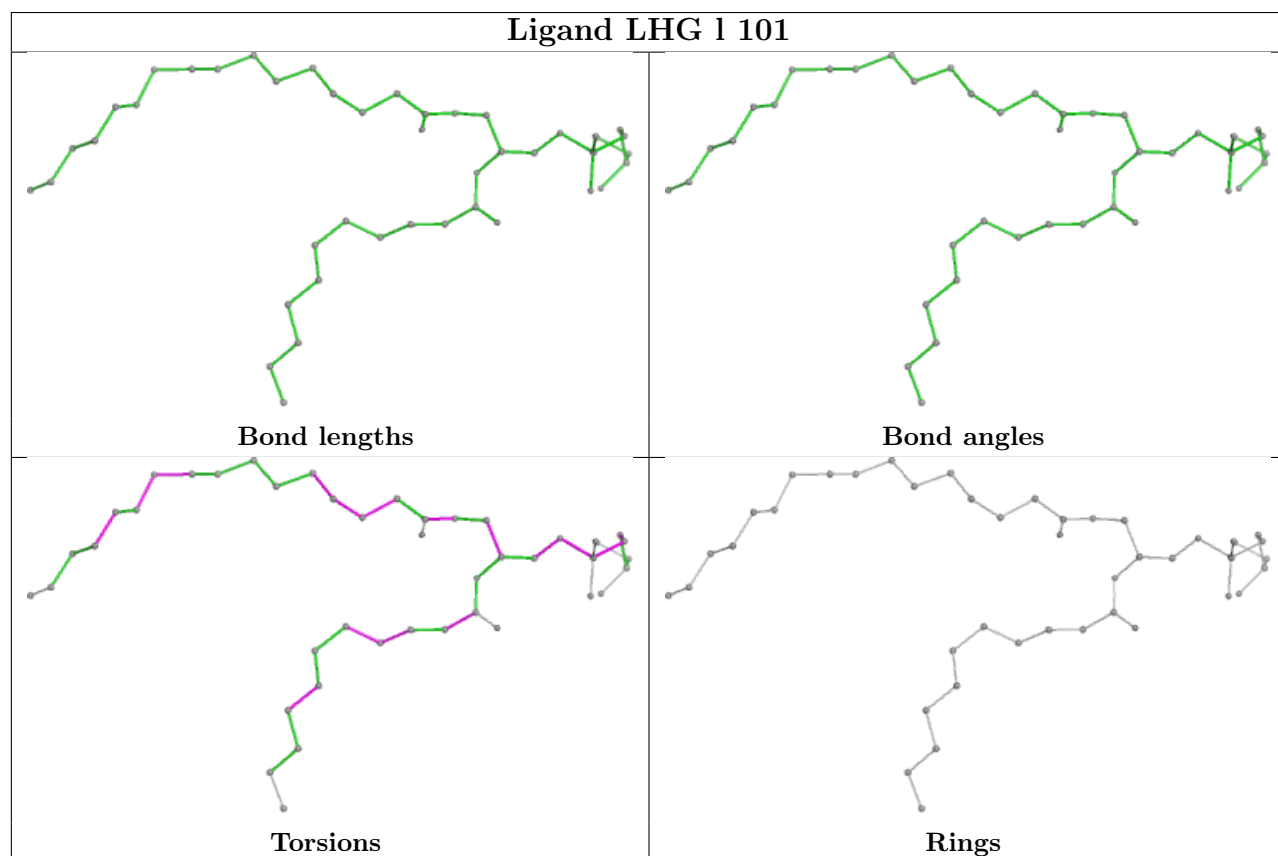
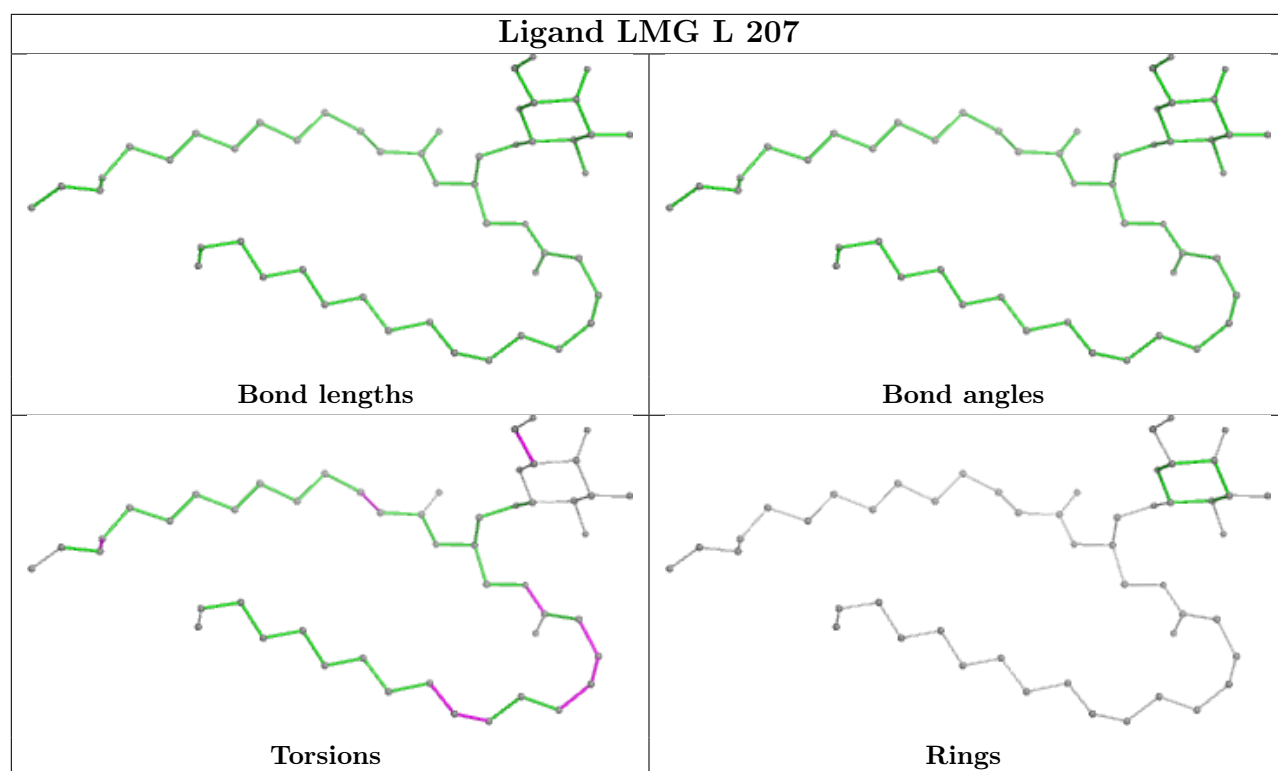
## Ligand CLA A 819



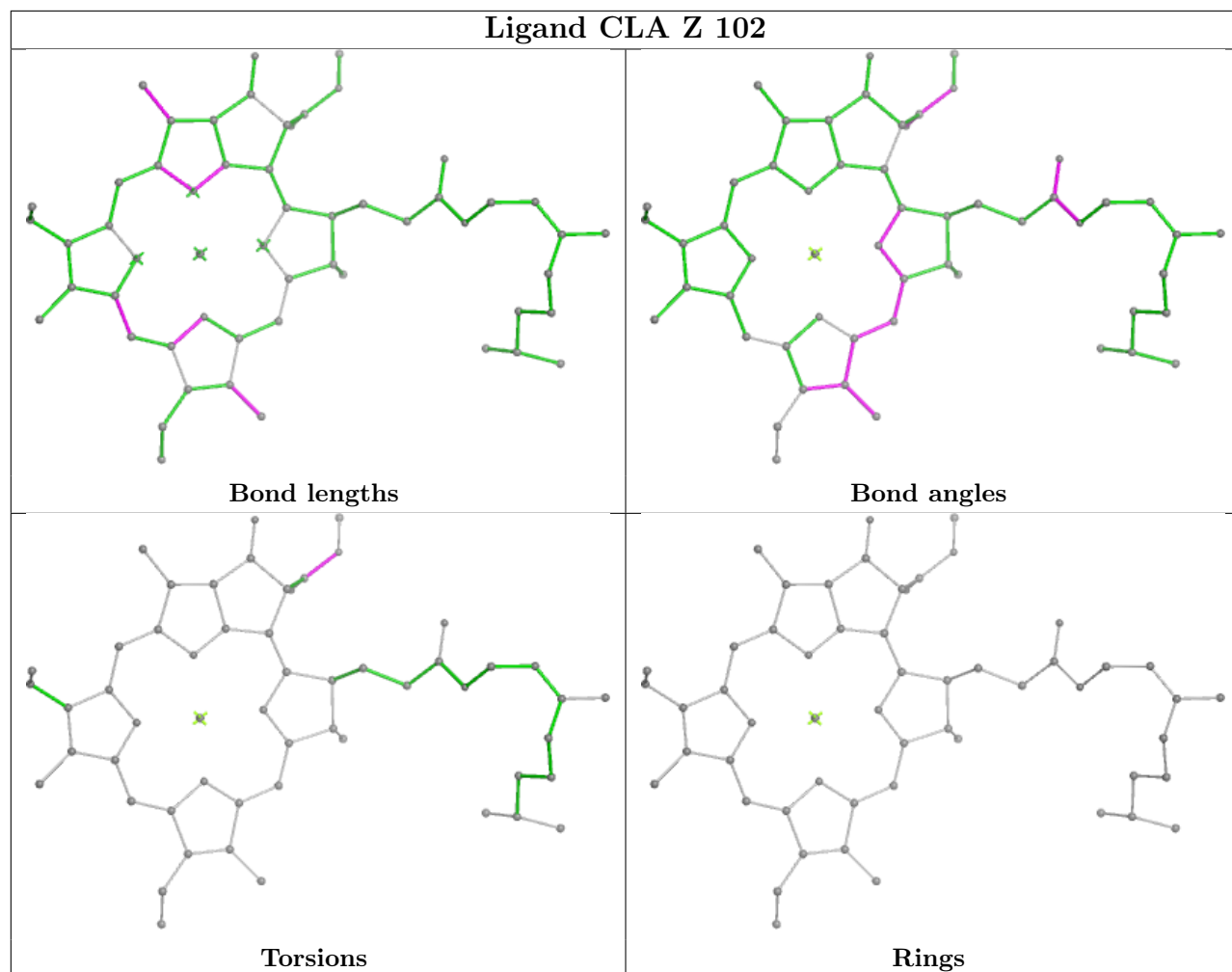
## Ligand LHG A 851



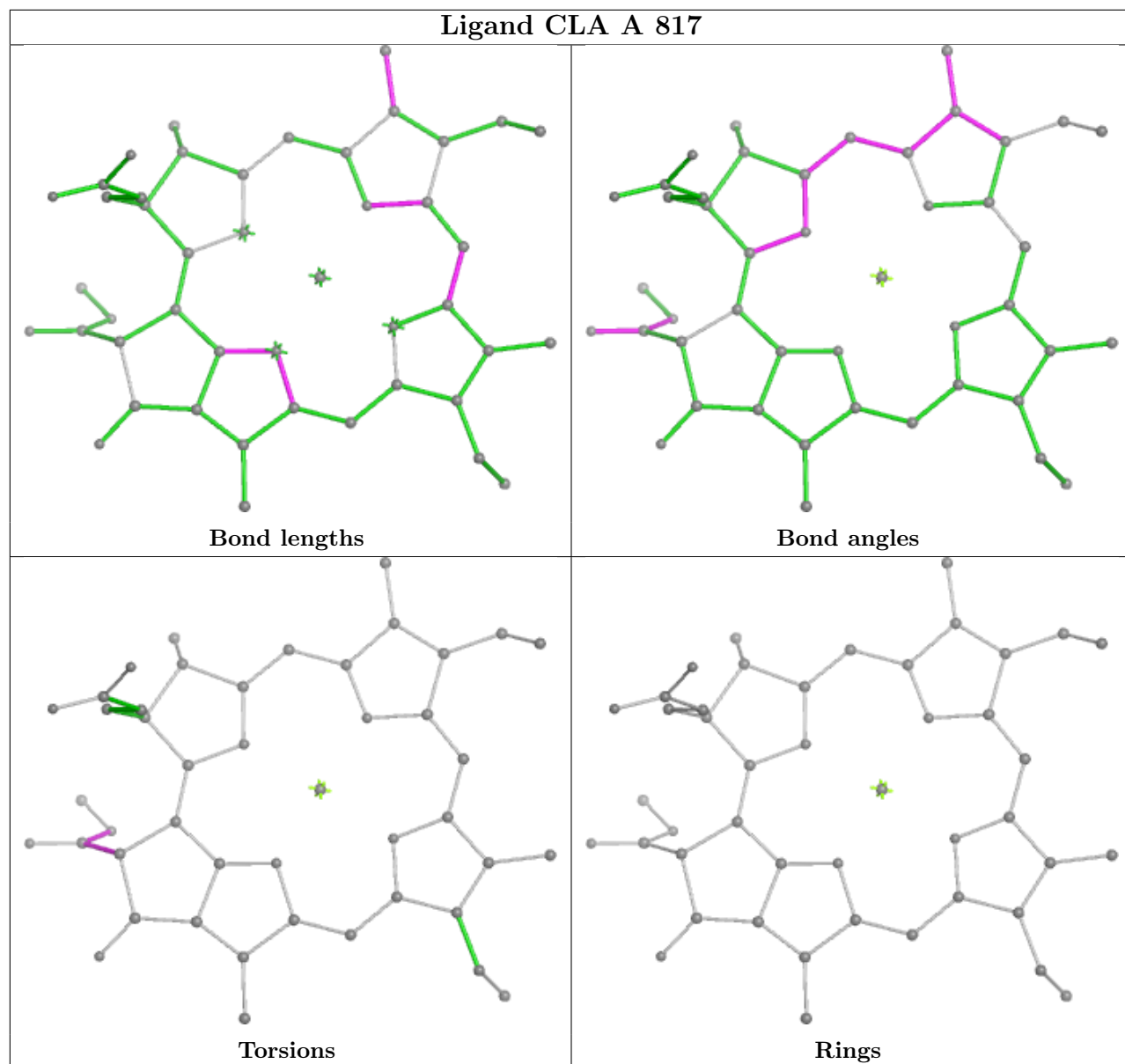


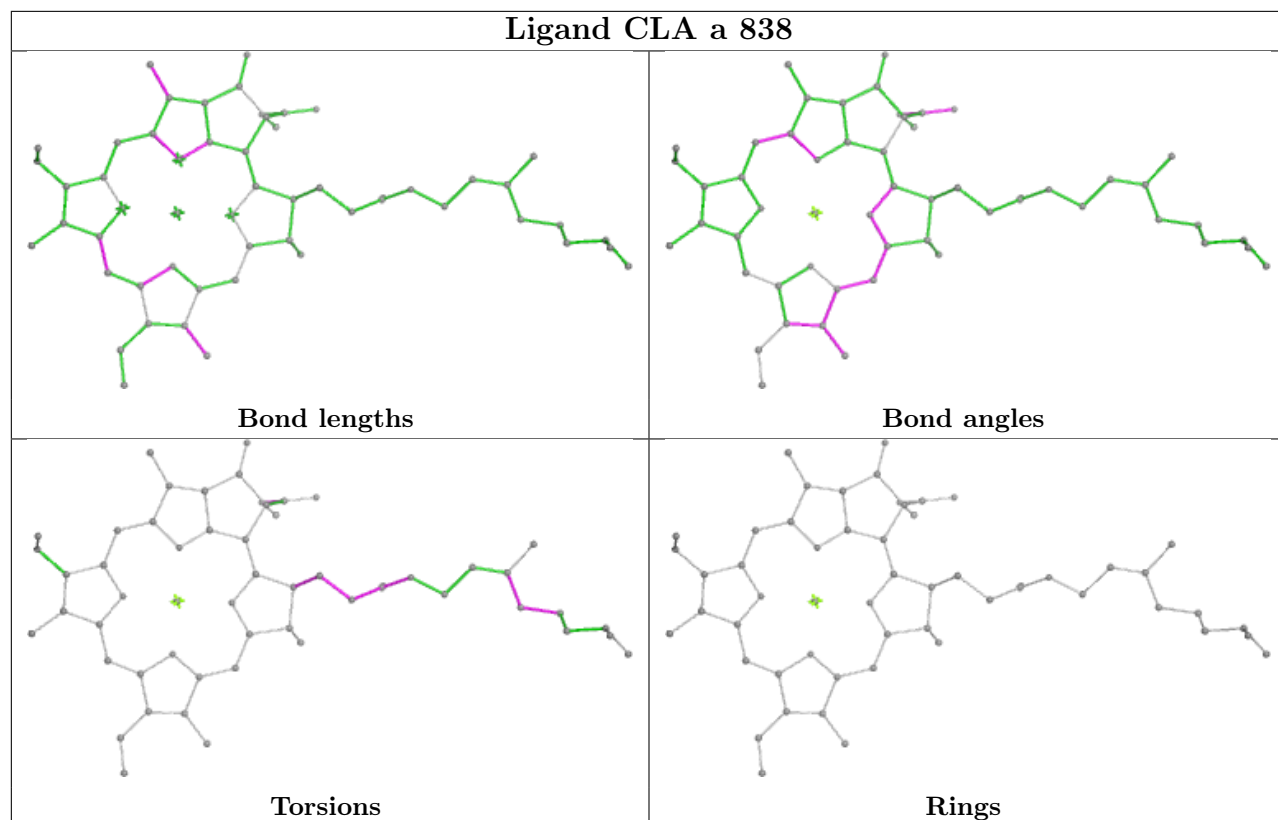
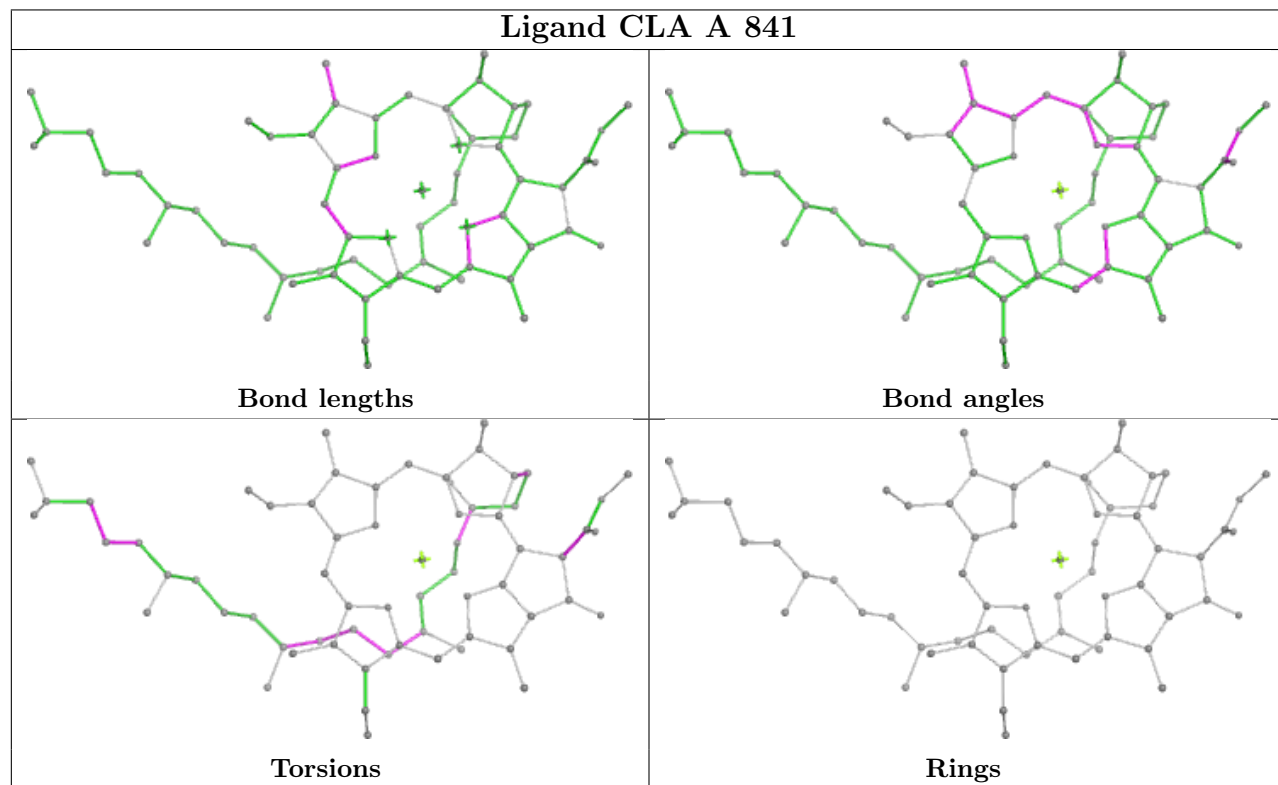


## Ligand CLA Z 102

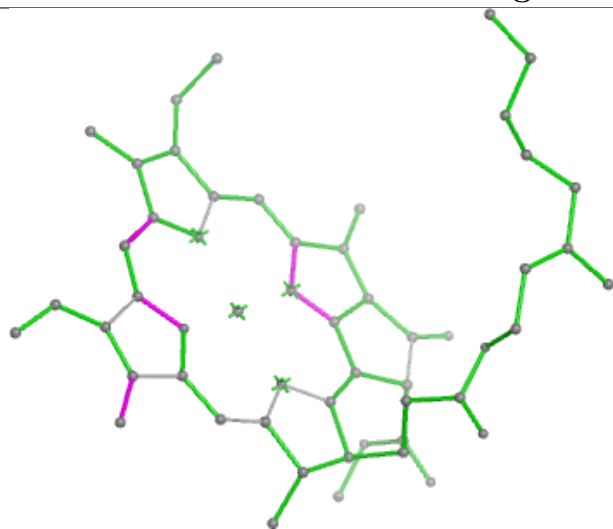


## Ligand CLA A 817

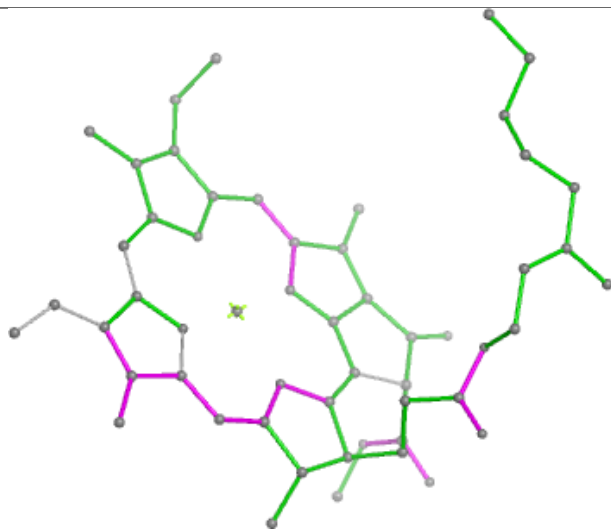


**Ligand CLA a 838****Ligand CLA A 841**

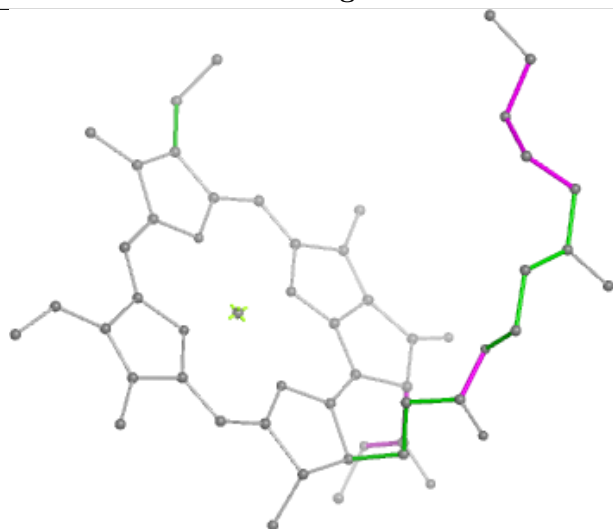
## Ligand CLA N 836



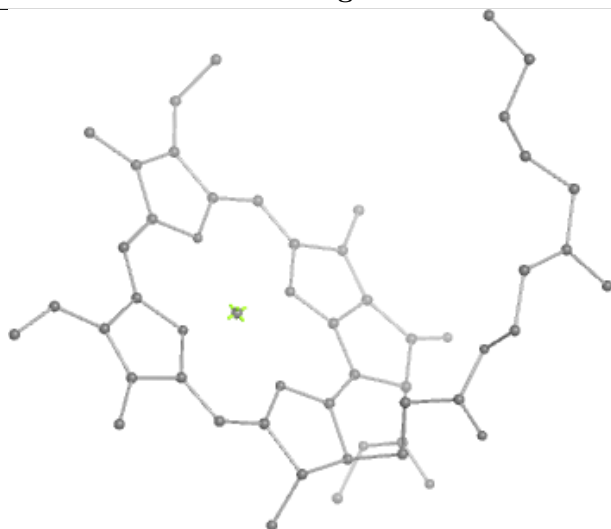
Bond lengths



Bond angles

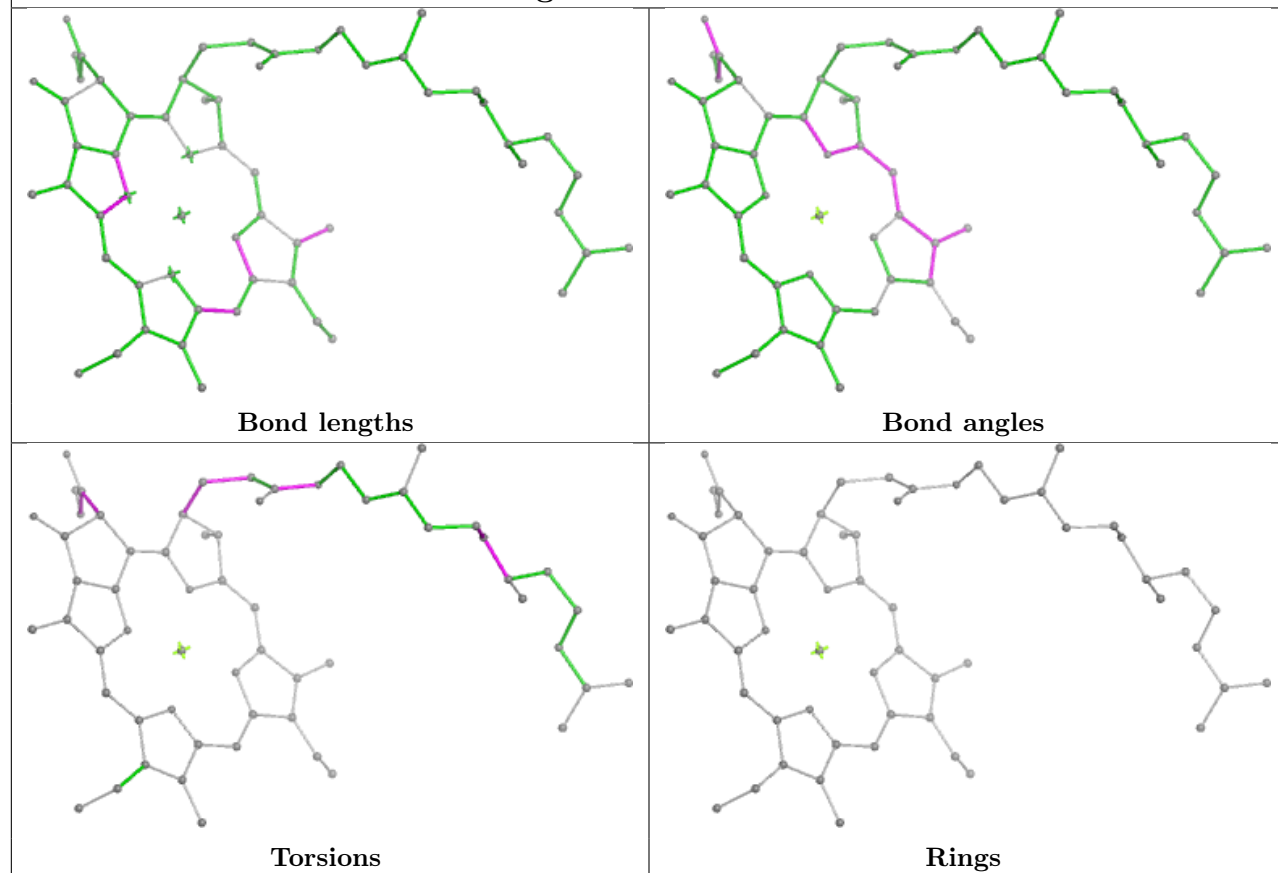


Torsions

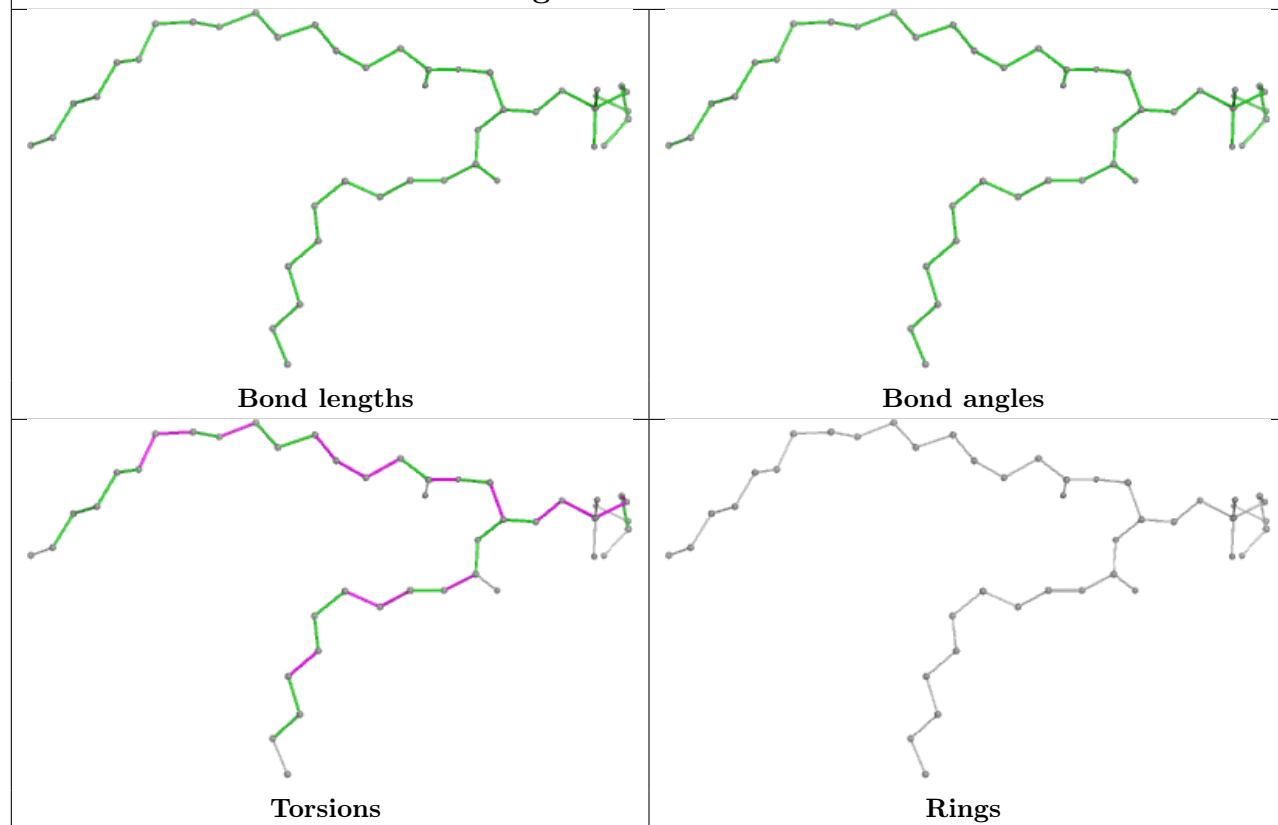


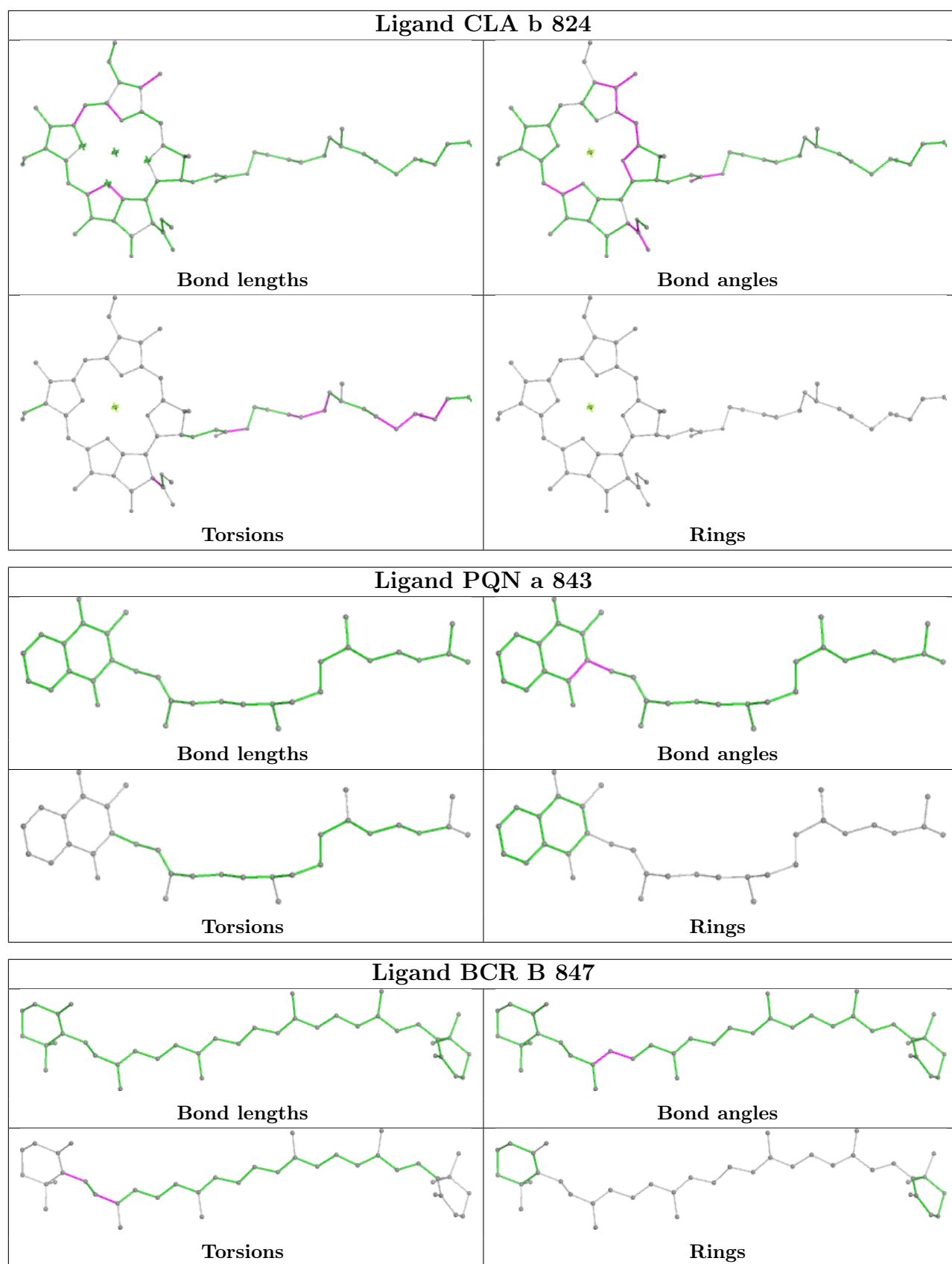
Rings

## Ligand CLA a 809

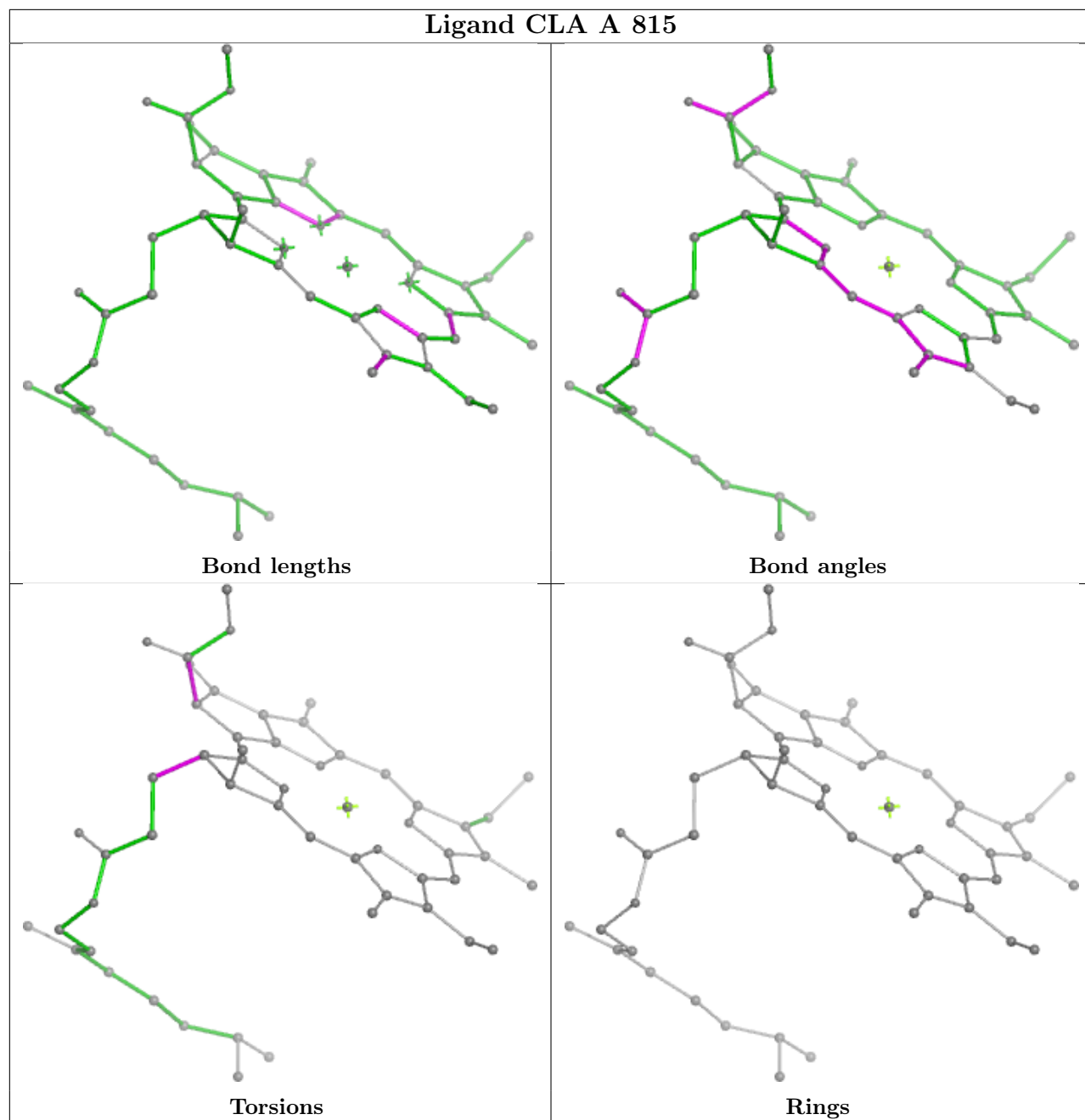


## Ligand LHG Z 101



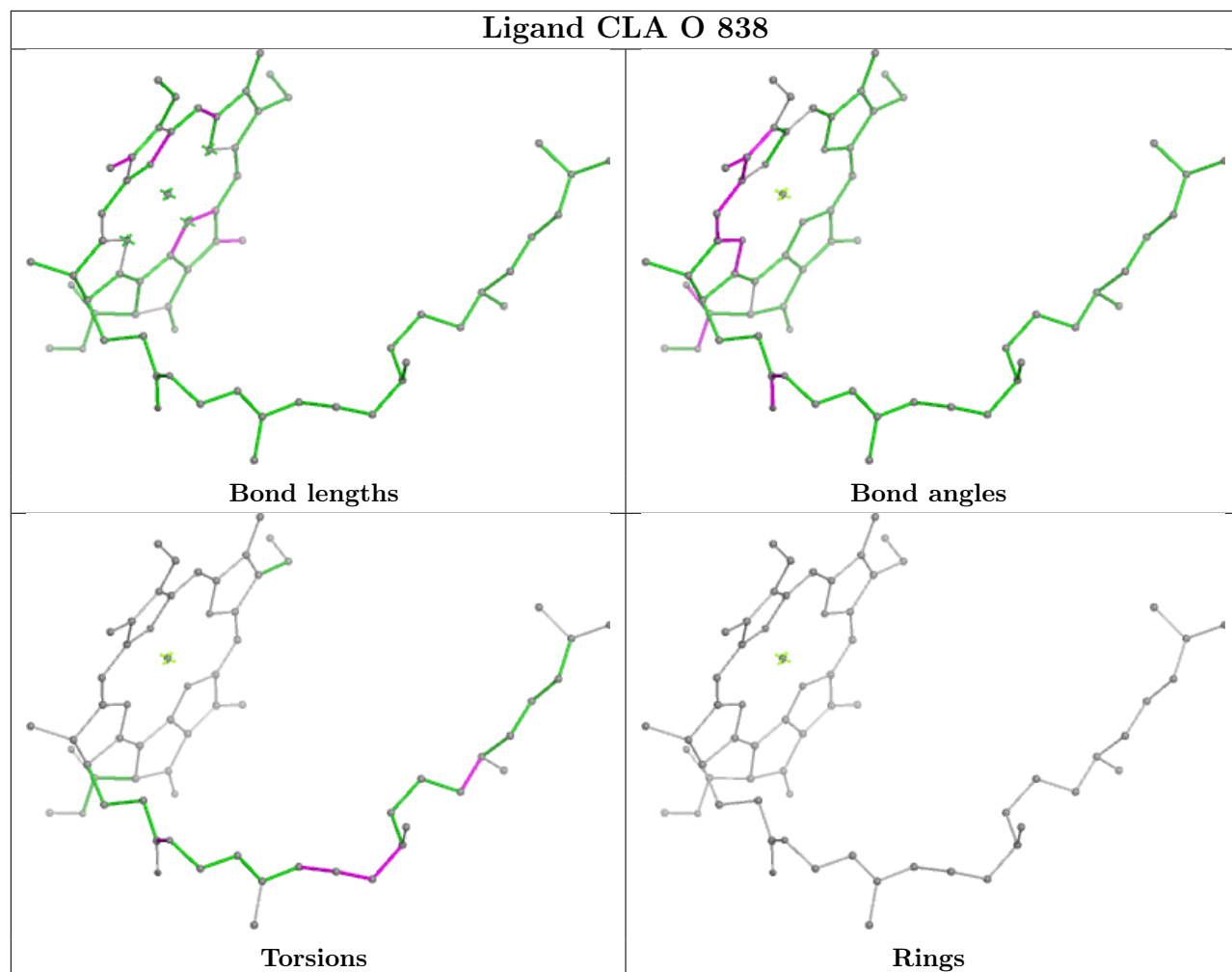


## Ligand CLA A 815

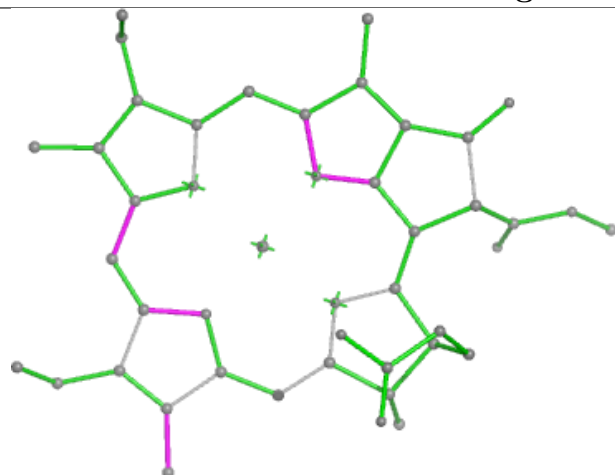




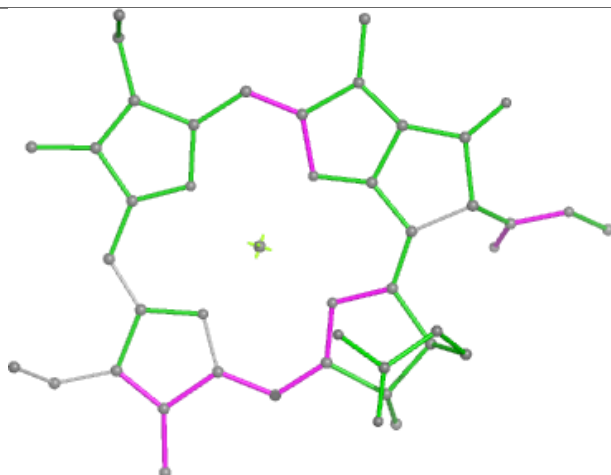
## Ligand CLA O 838



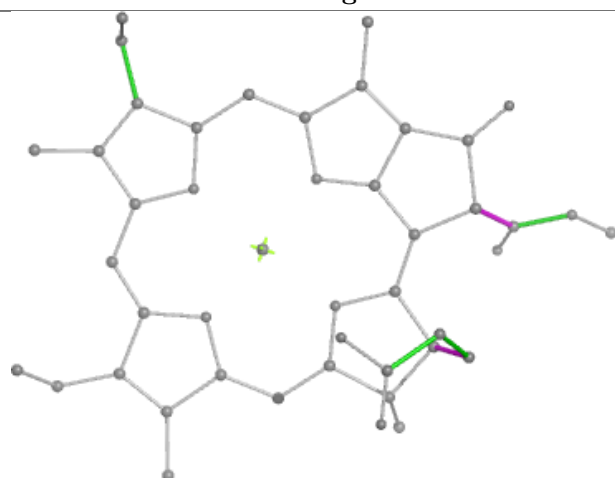
## Ligand CLA O 811



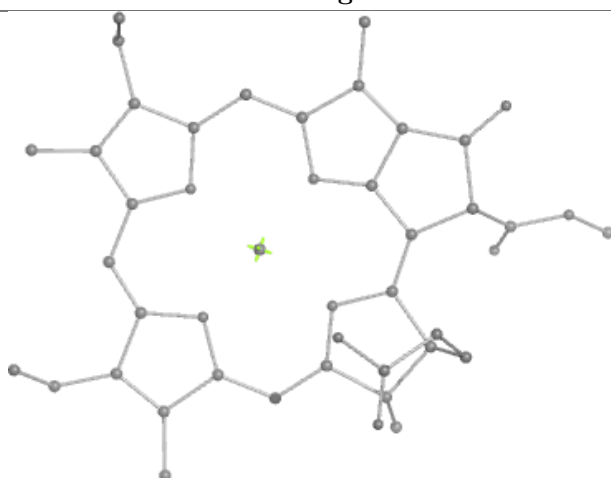
Bond lengths



Bond angles

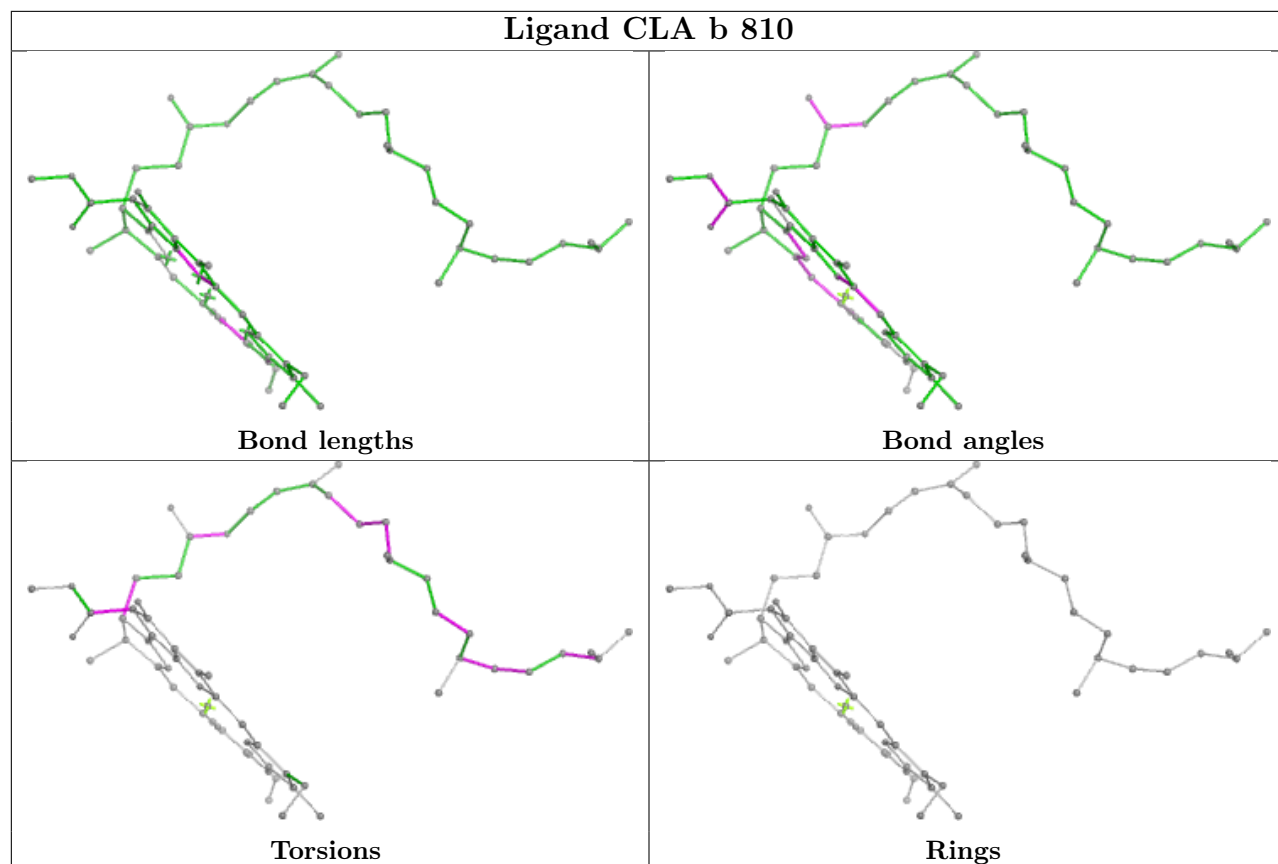


Torsions

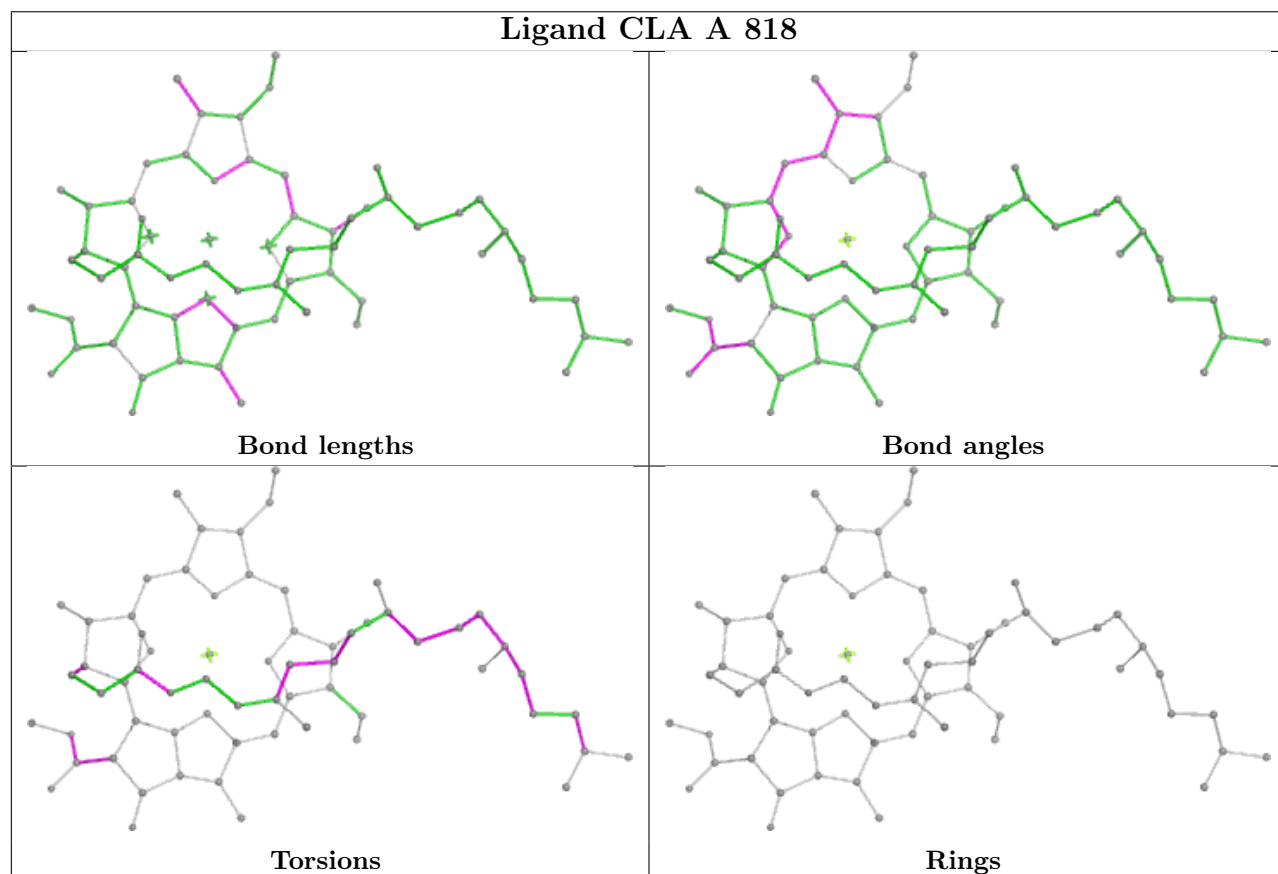


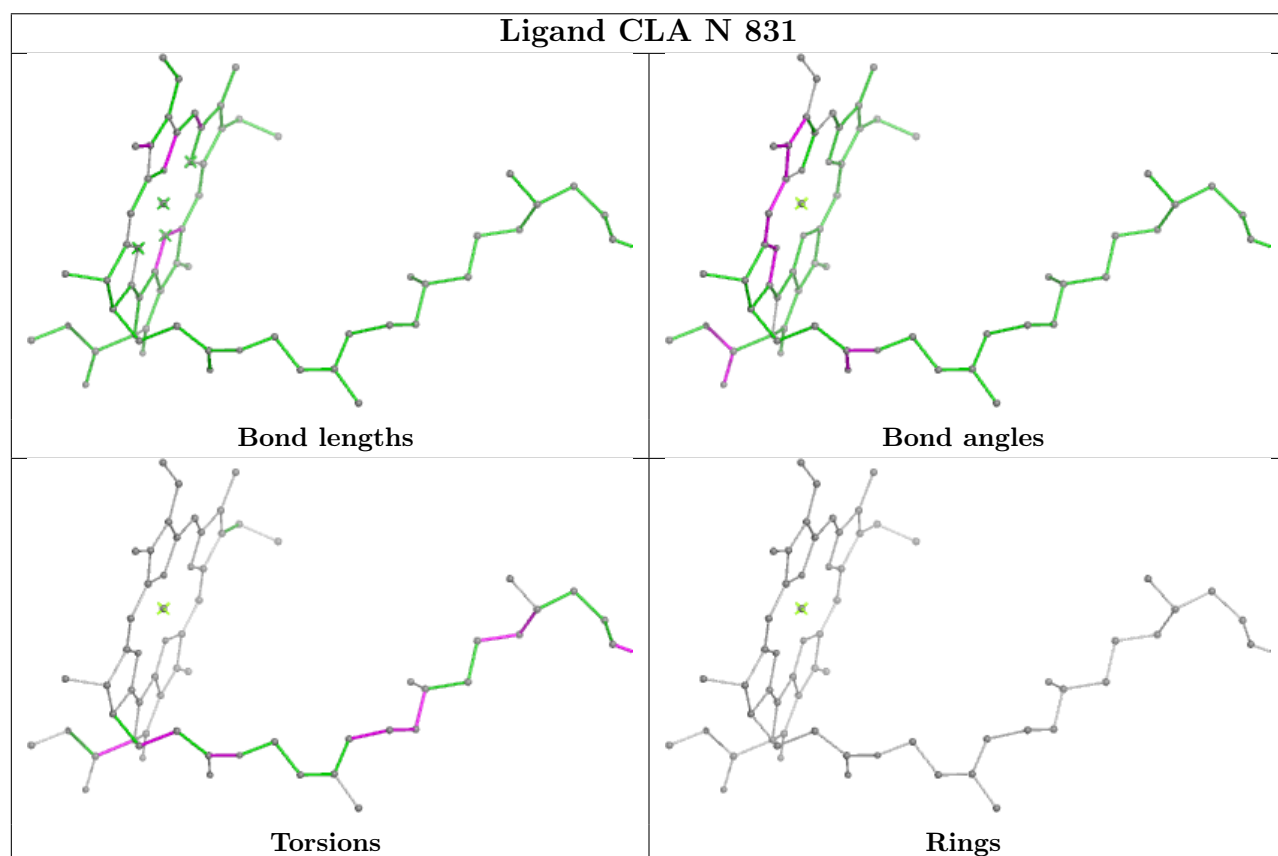
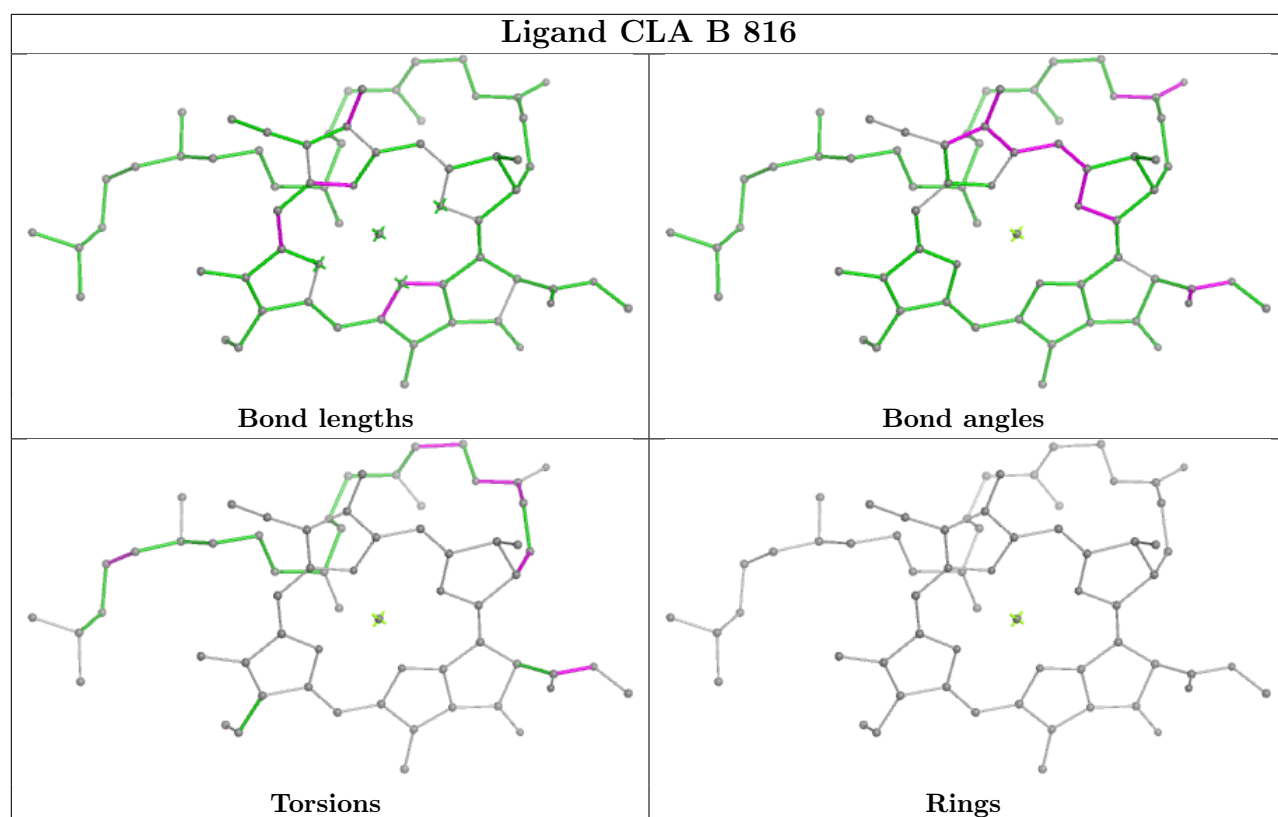
Rings

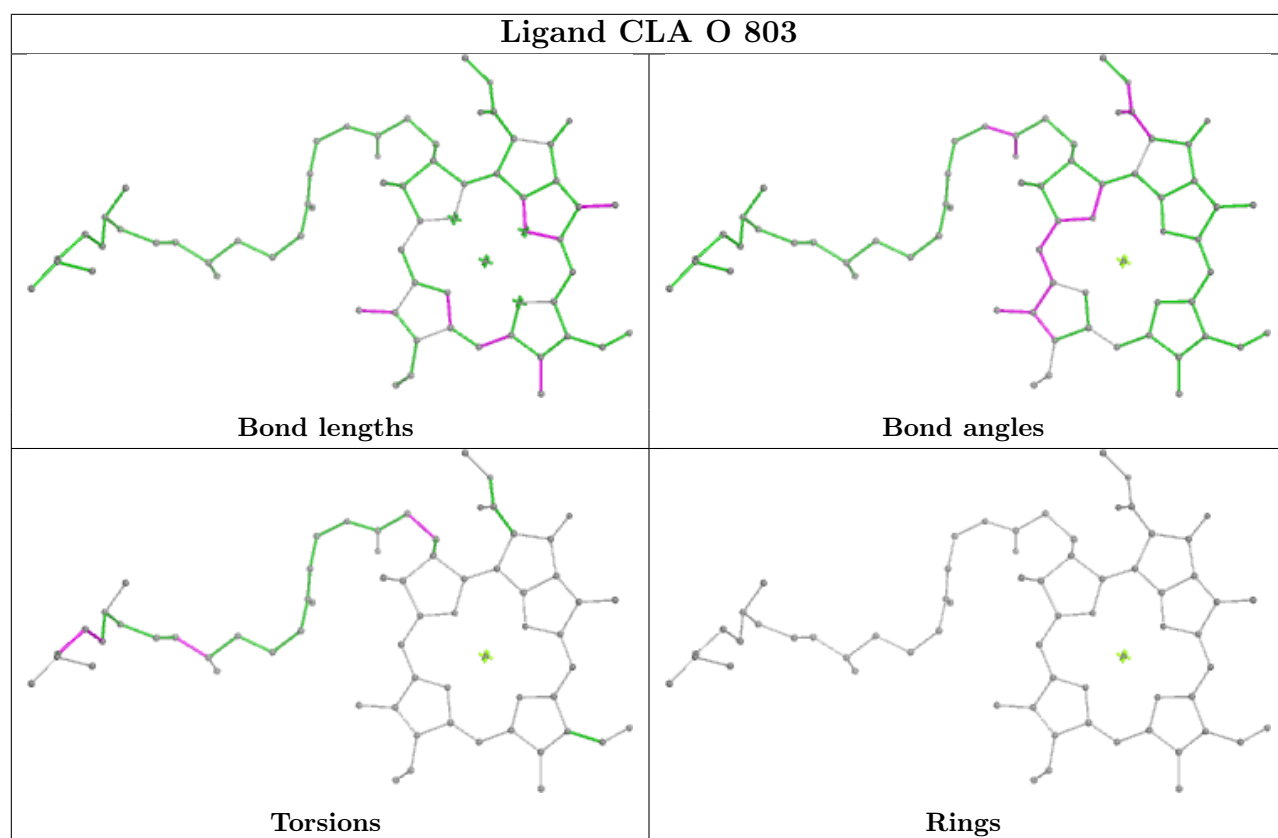
## Ligand CLA b 810



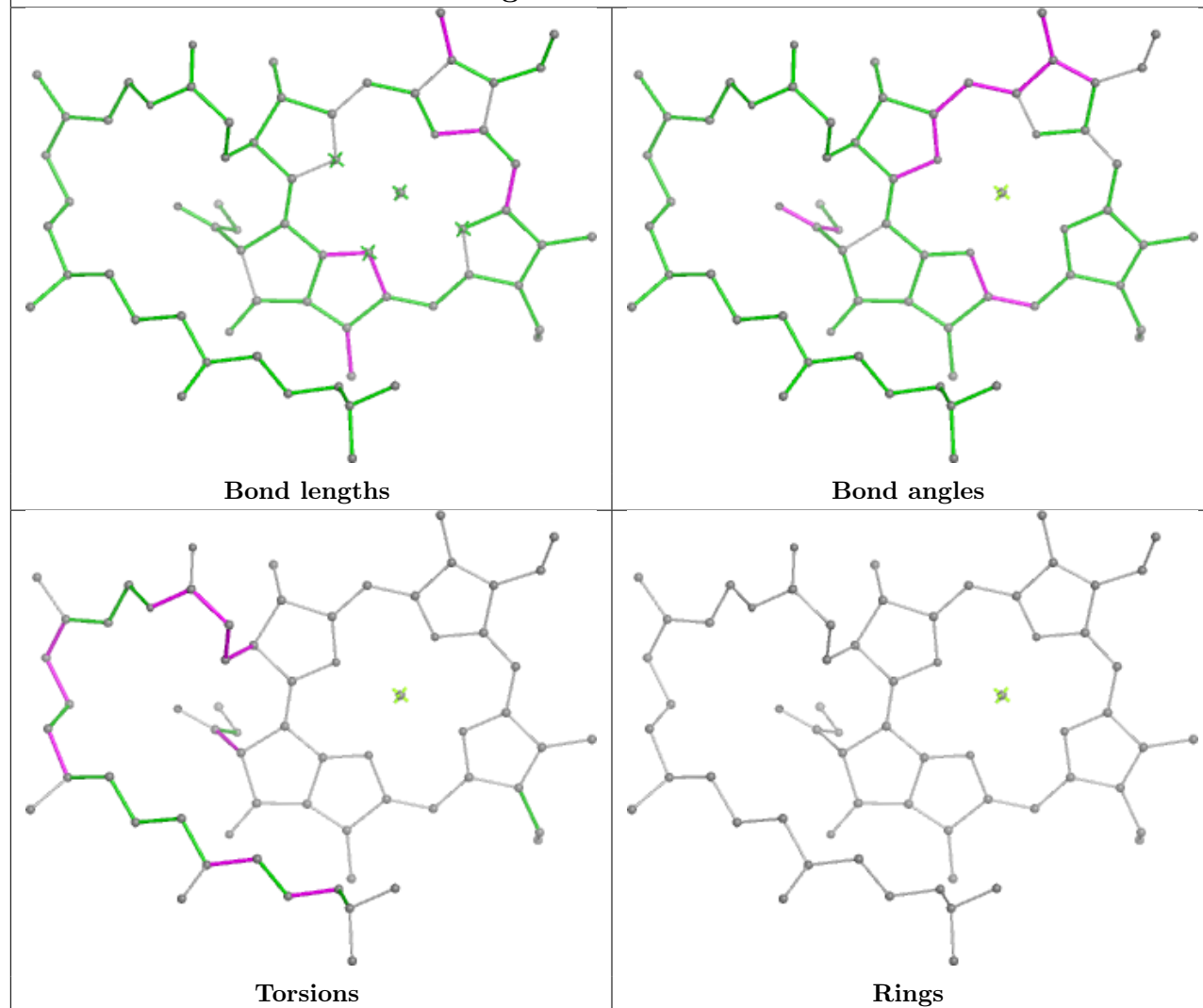
## Ligand CLA A 818



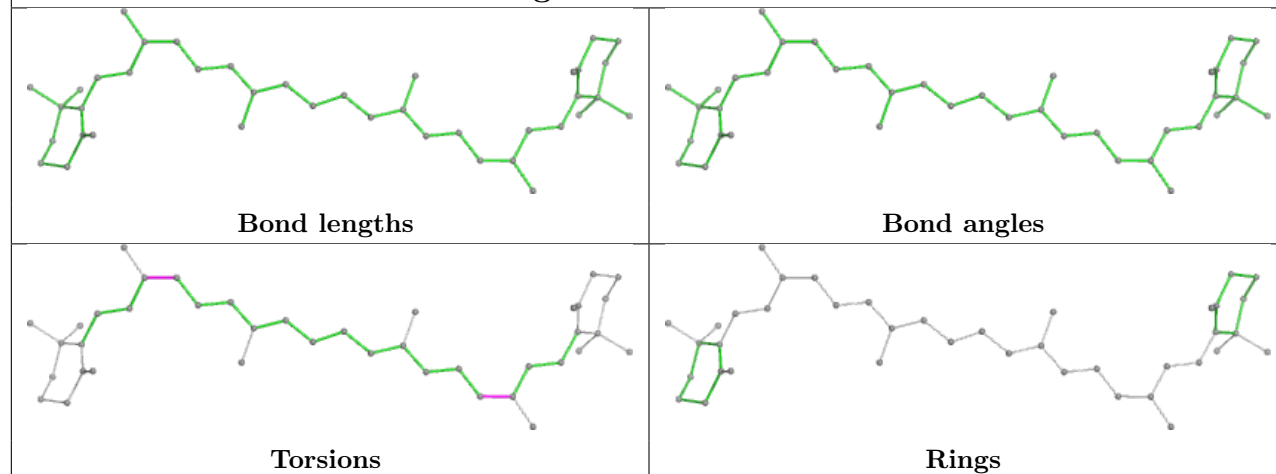




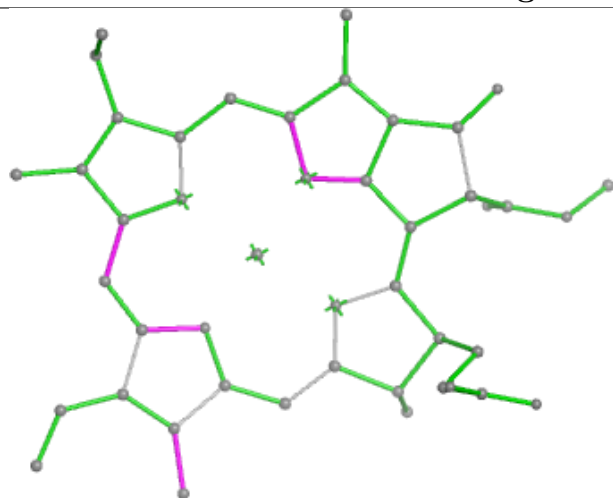
## Ligand CLA B 805



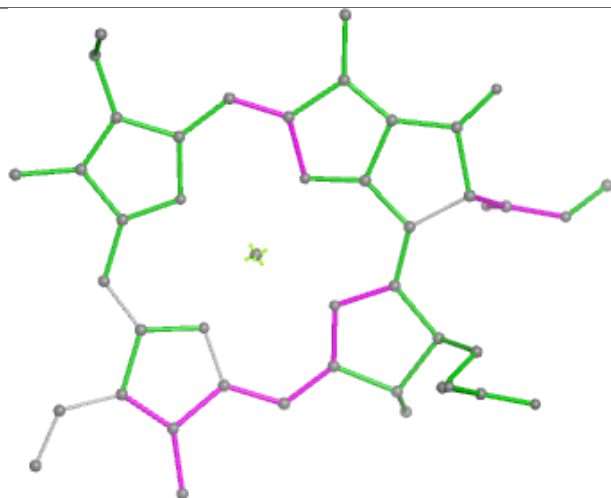
## Ligand BCR b 844



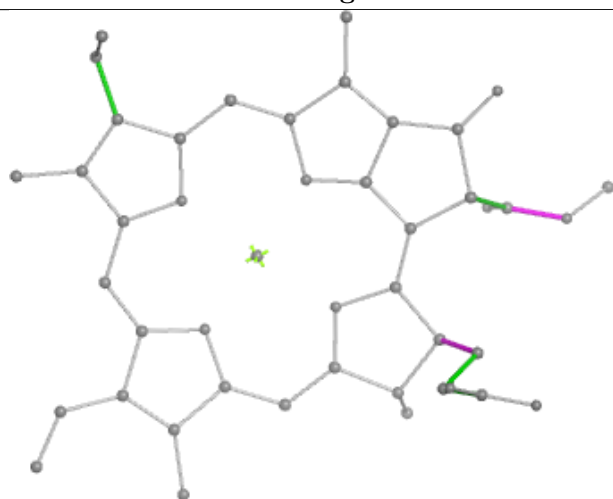
## Ligand CLA b 834



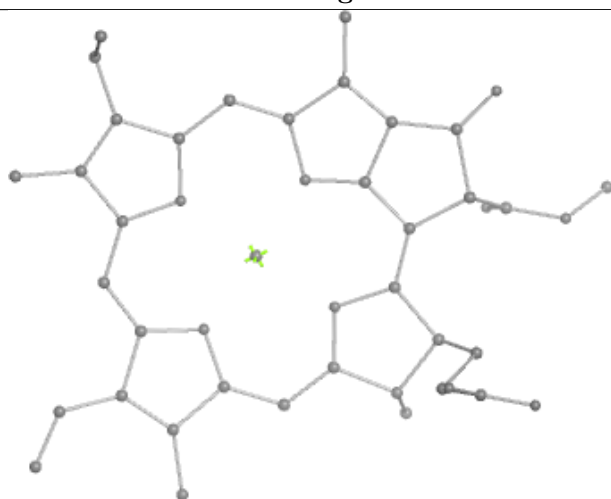
Bond lengths



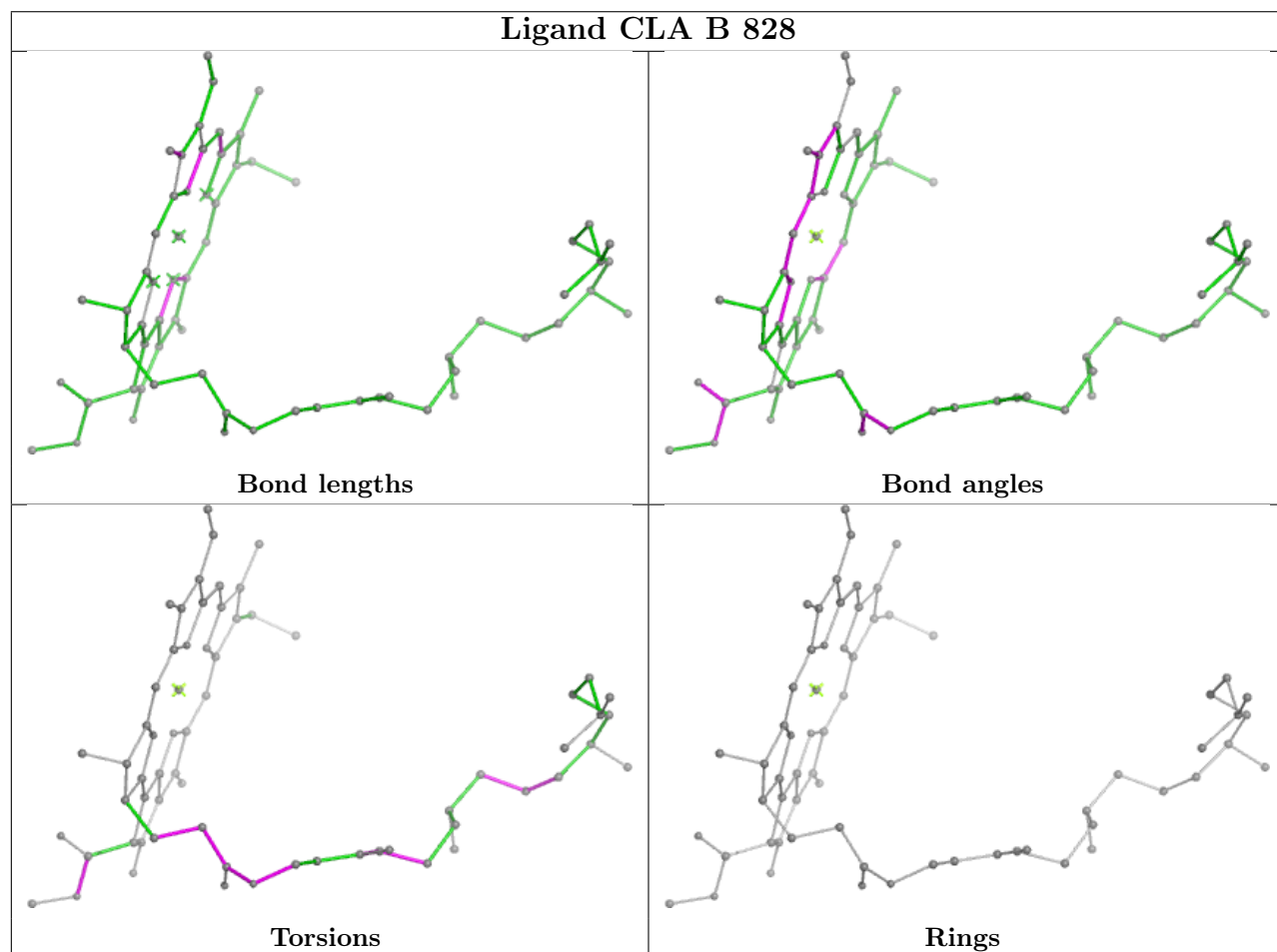
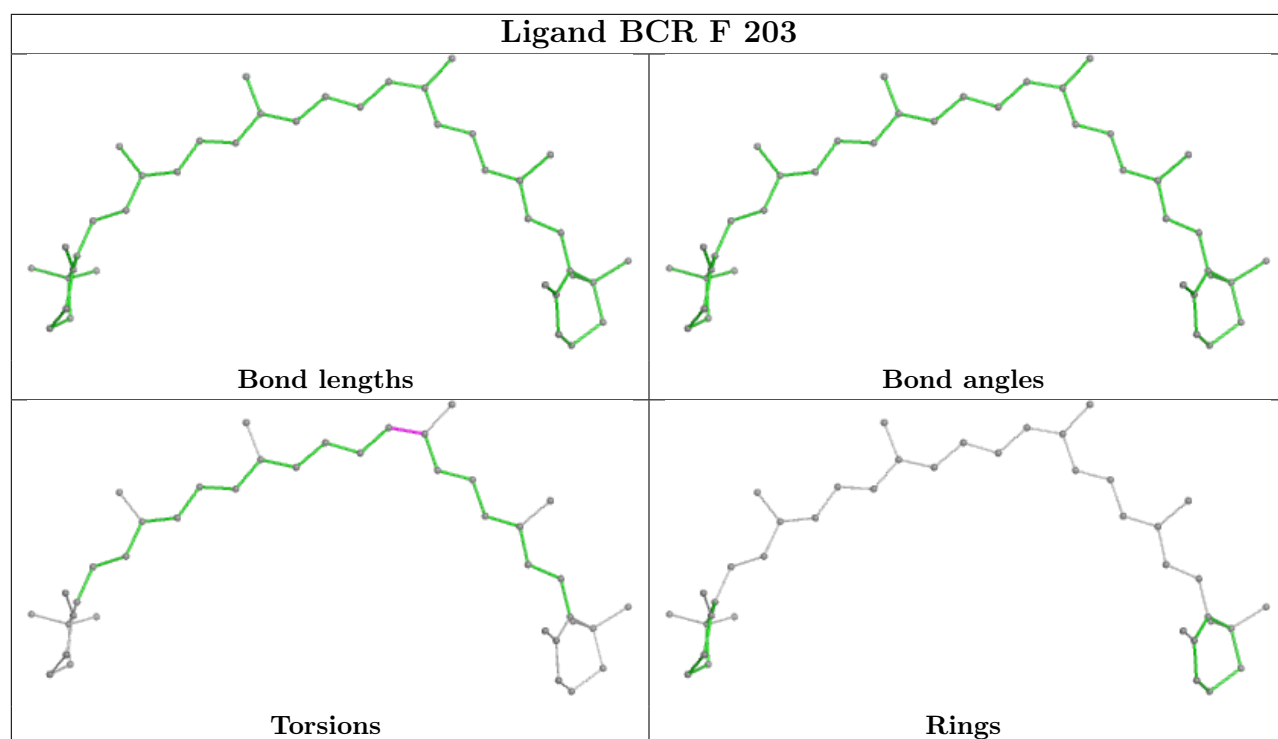
Bond angles



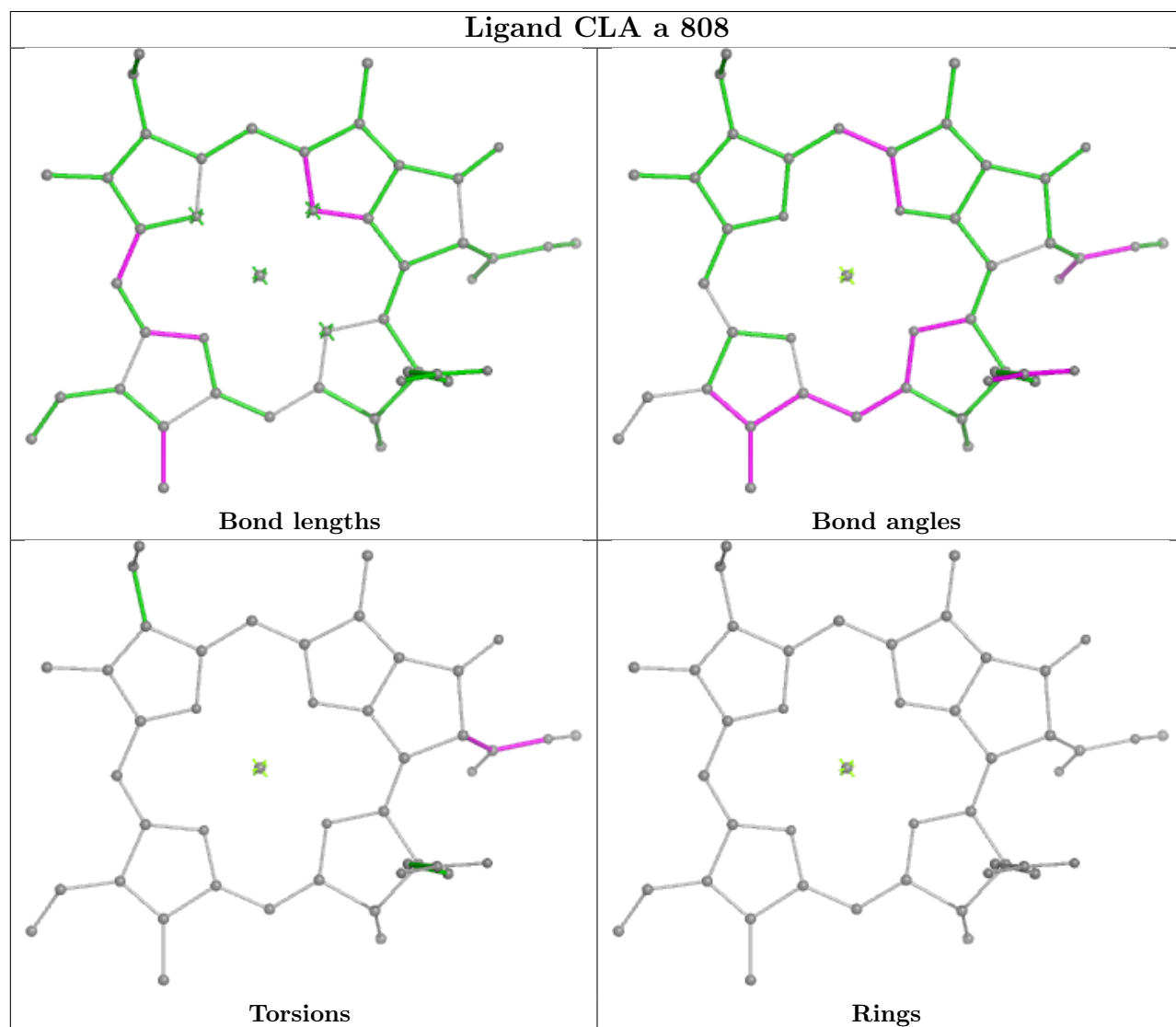
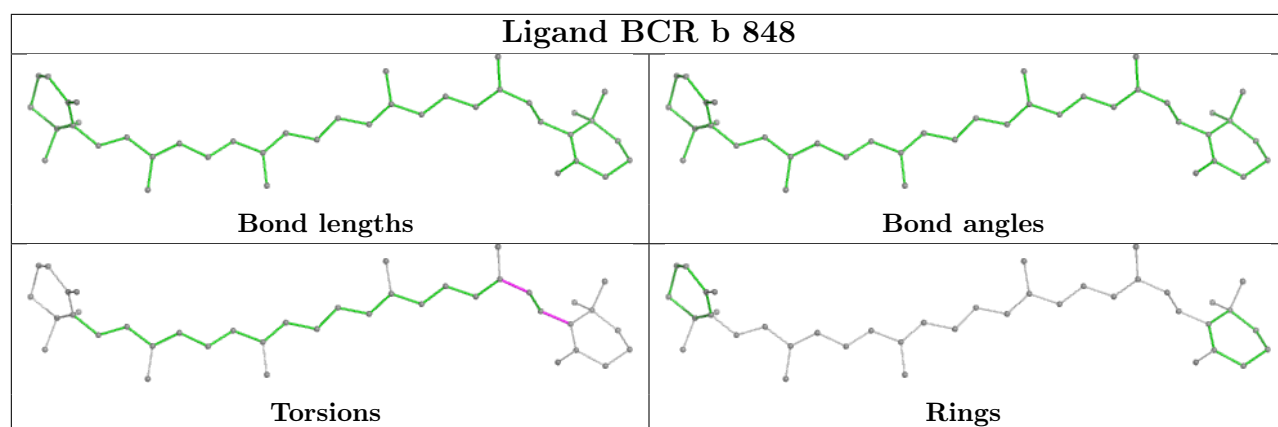
Torsions



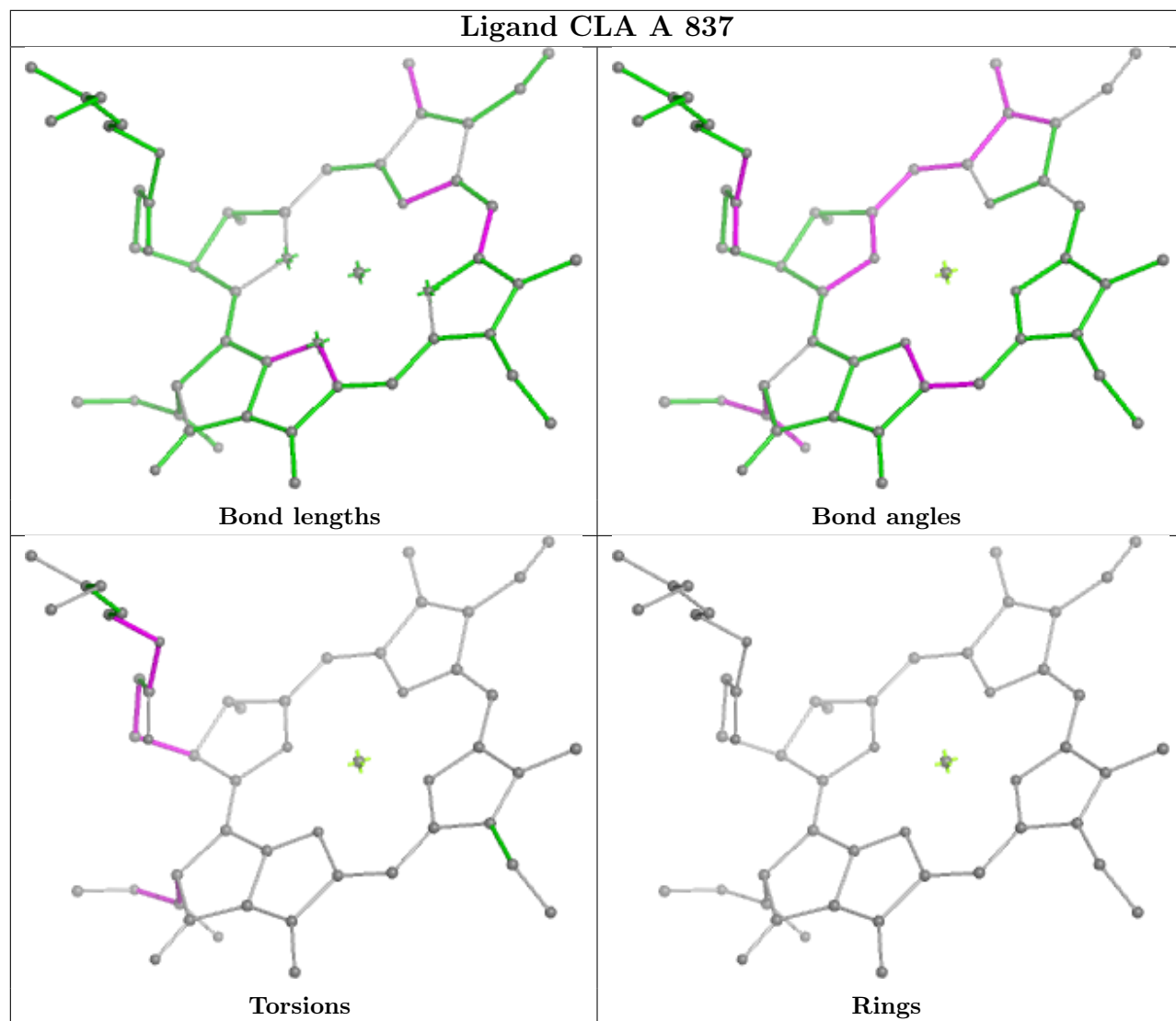
Rings

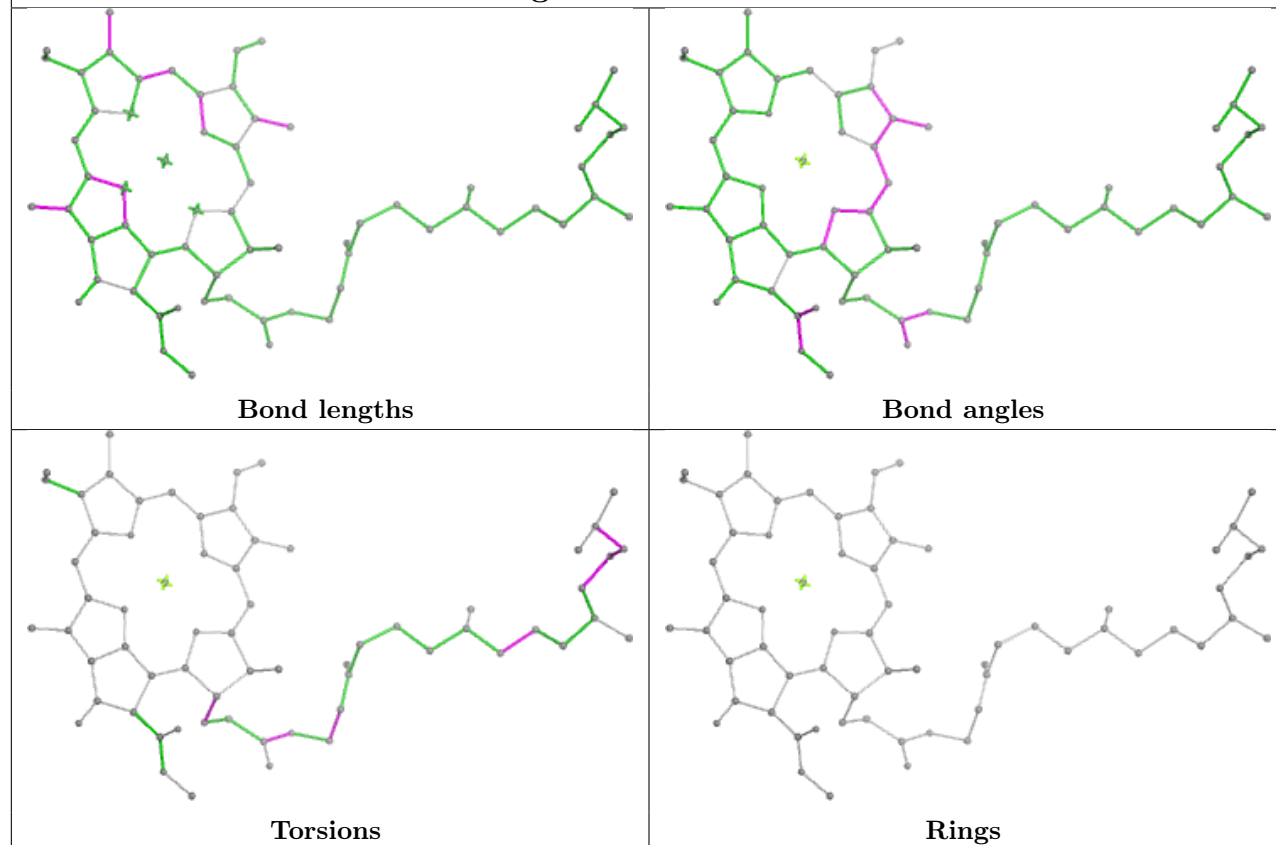
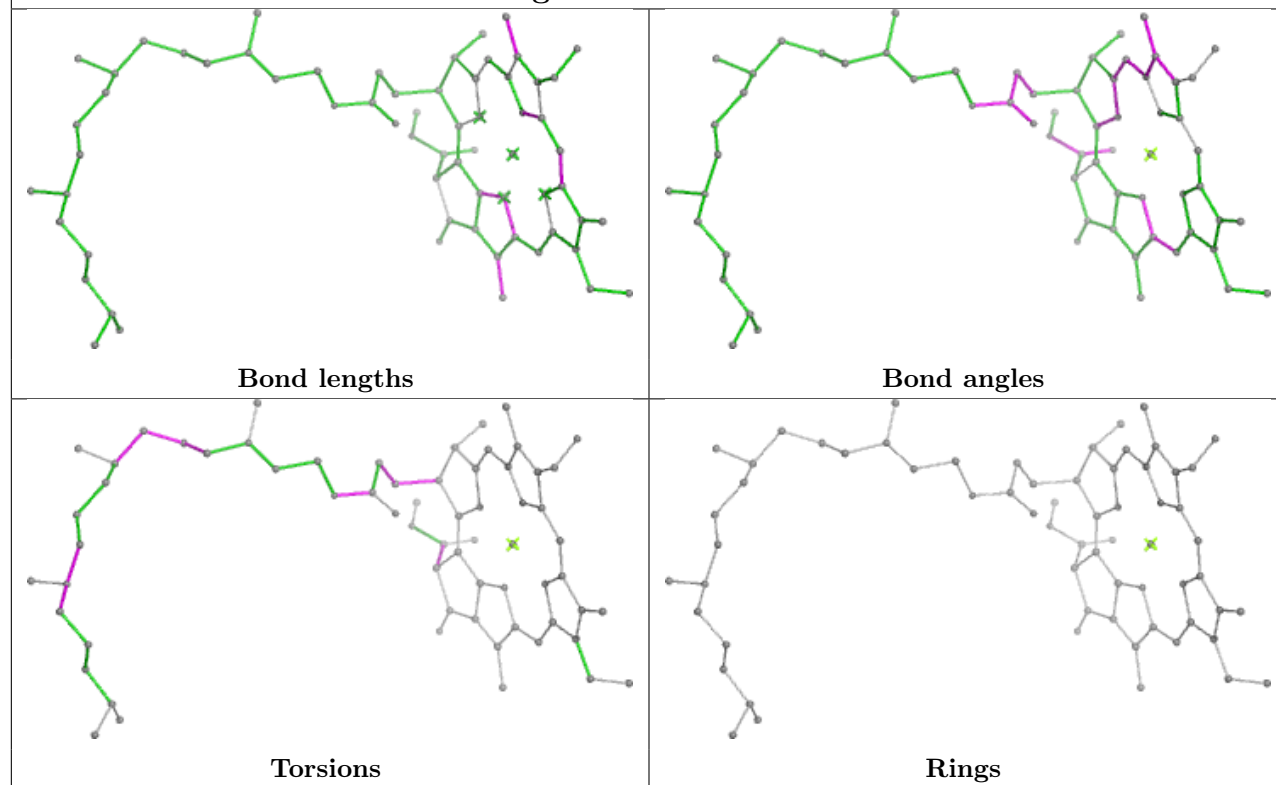


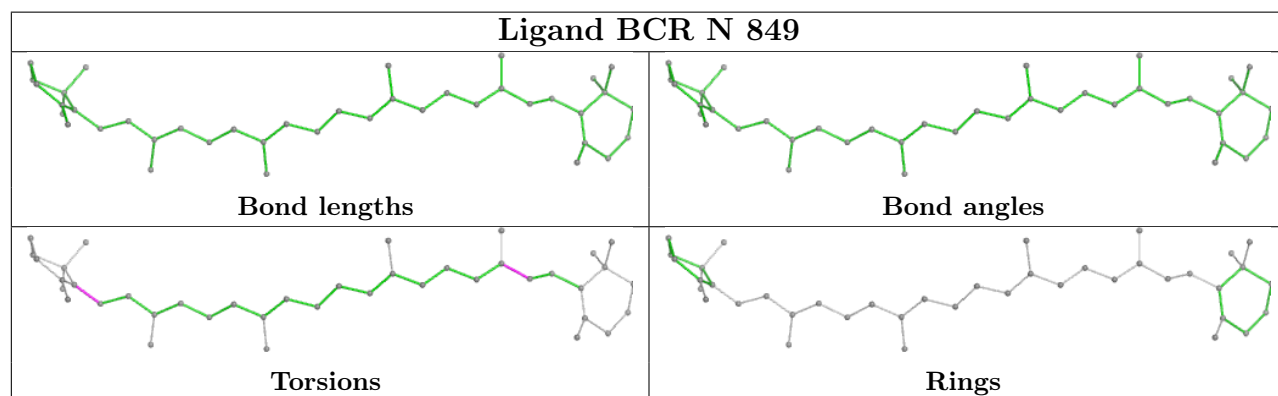
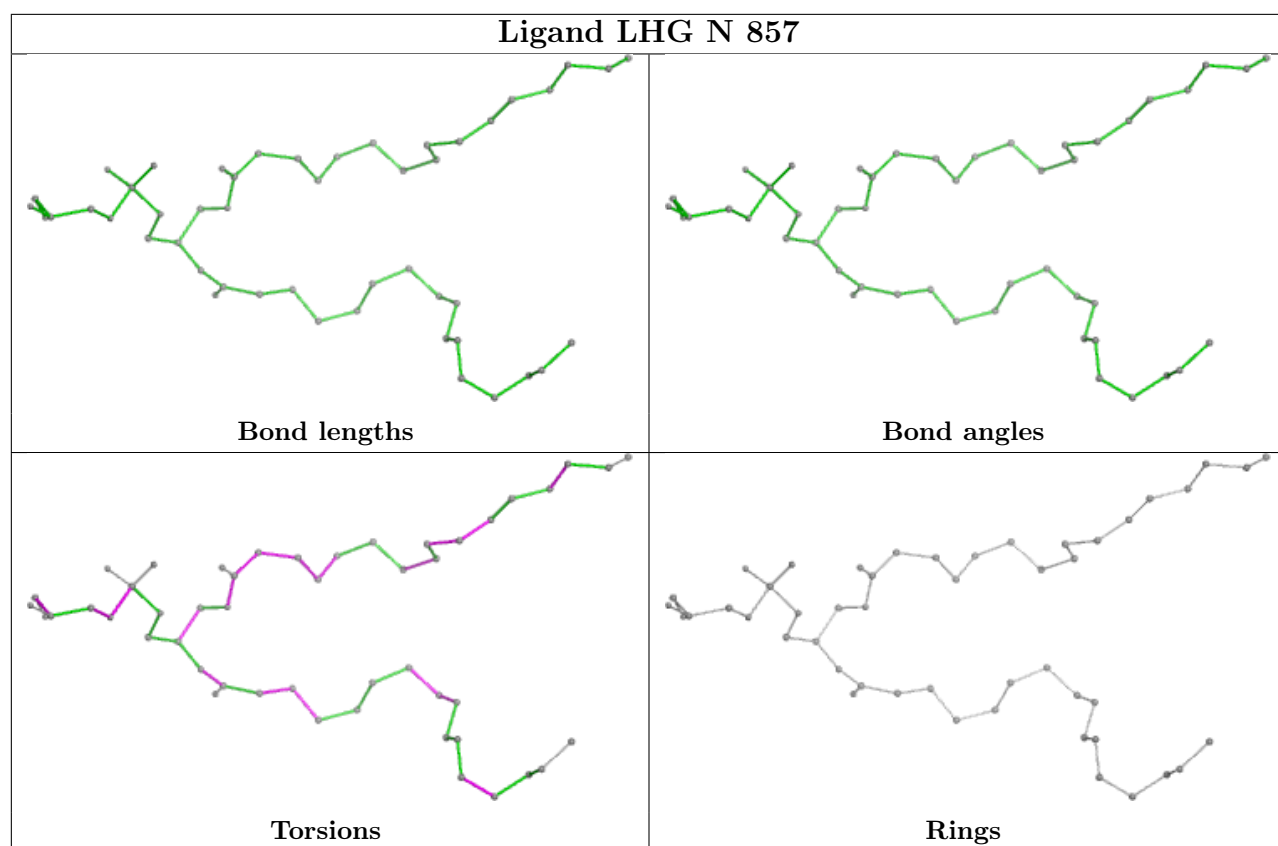




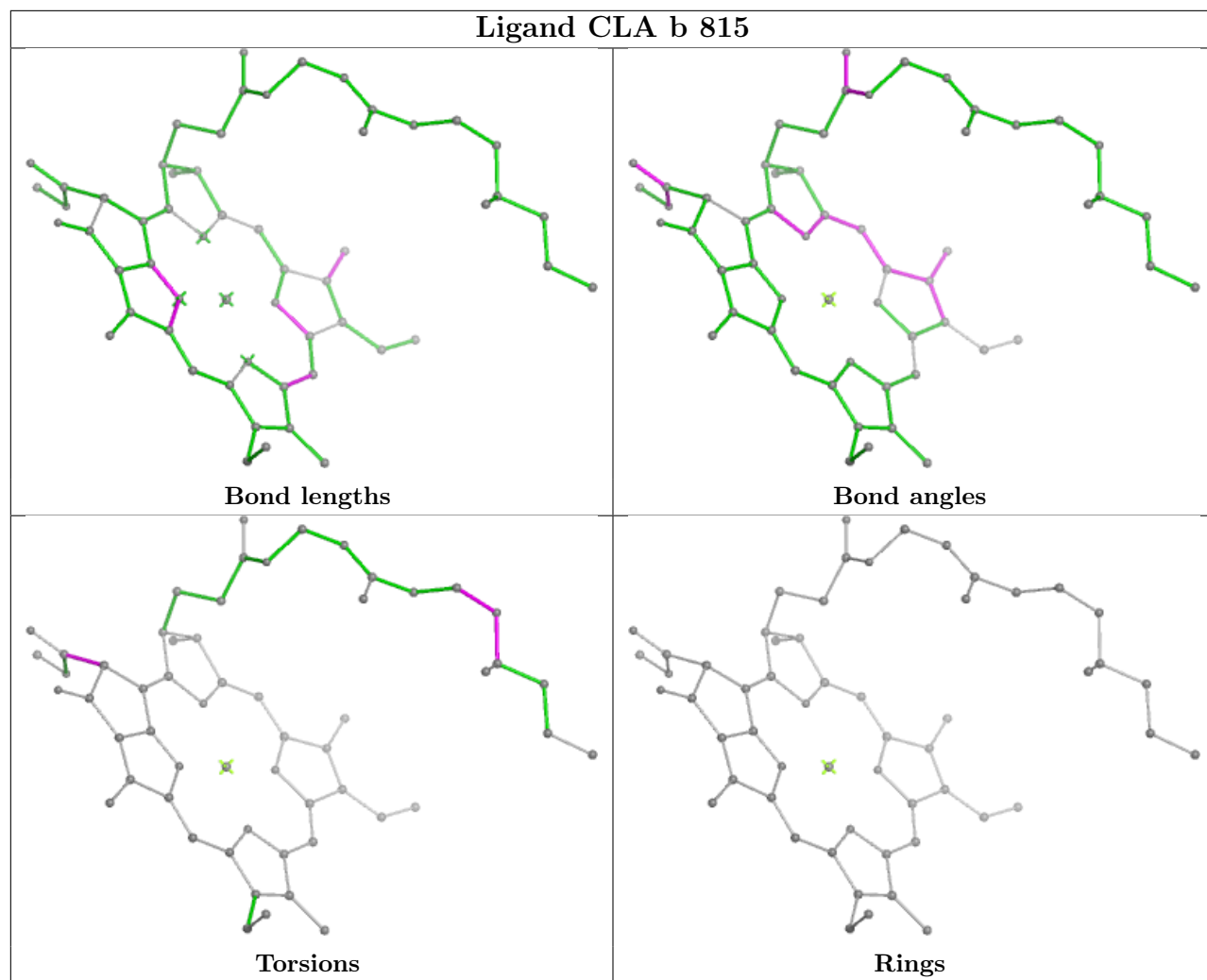
## Ligand CLA A 837

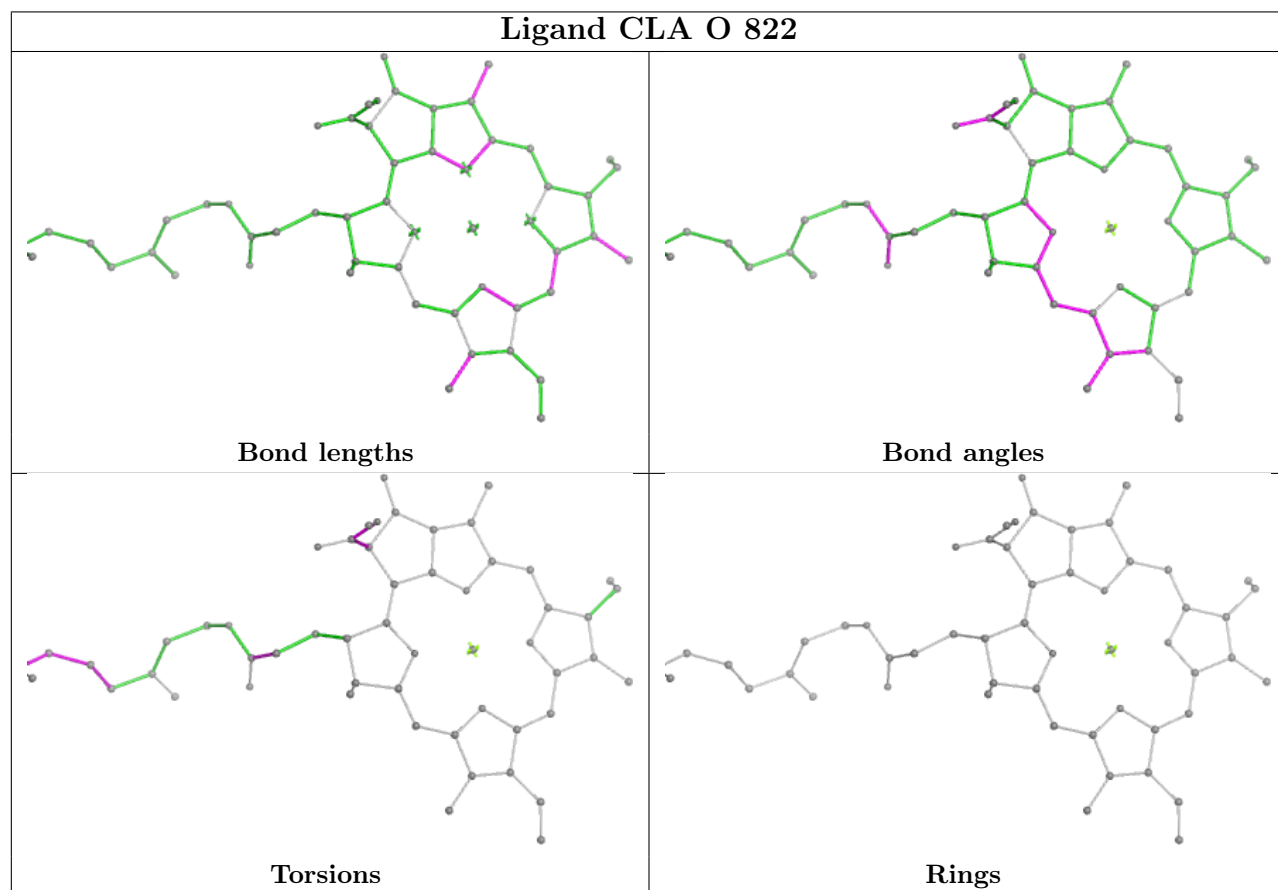
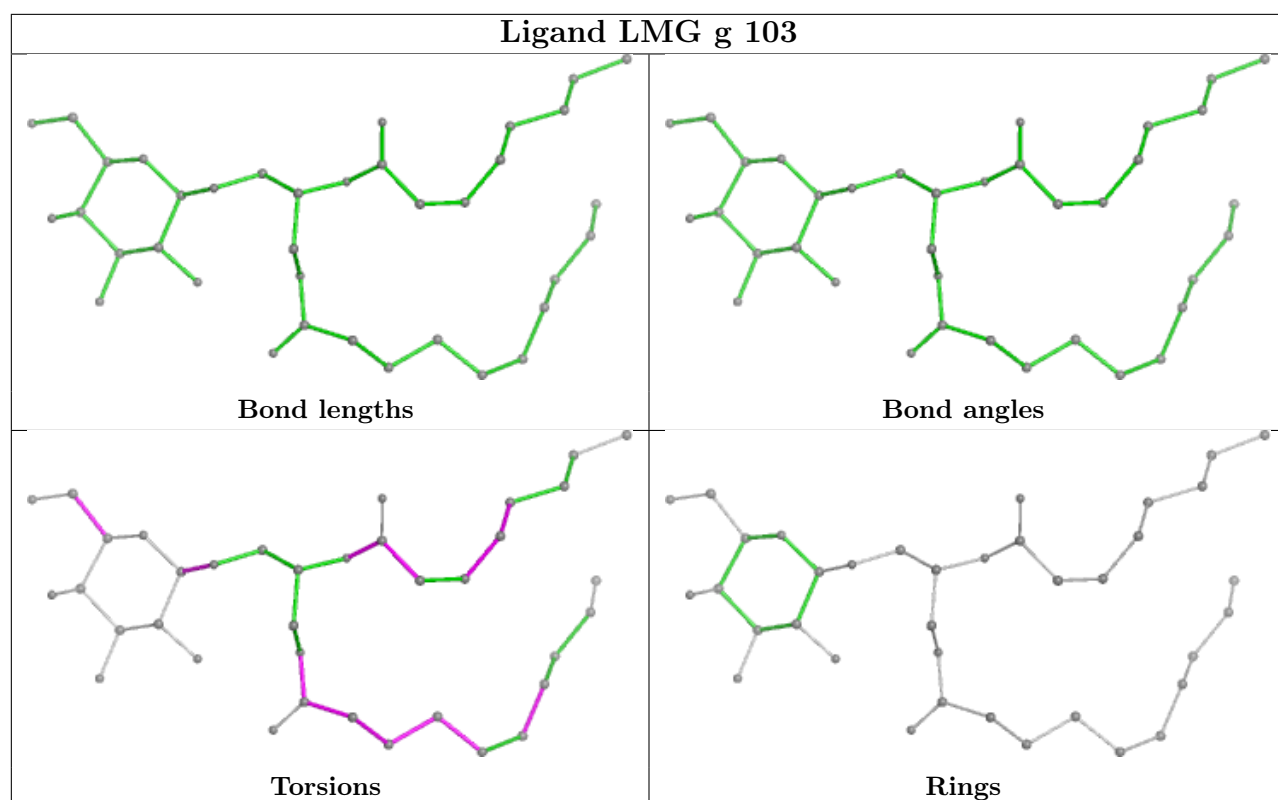


**Ligand CLA N 803****Ligand CLA B 809**

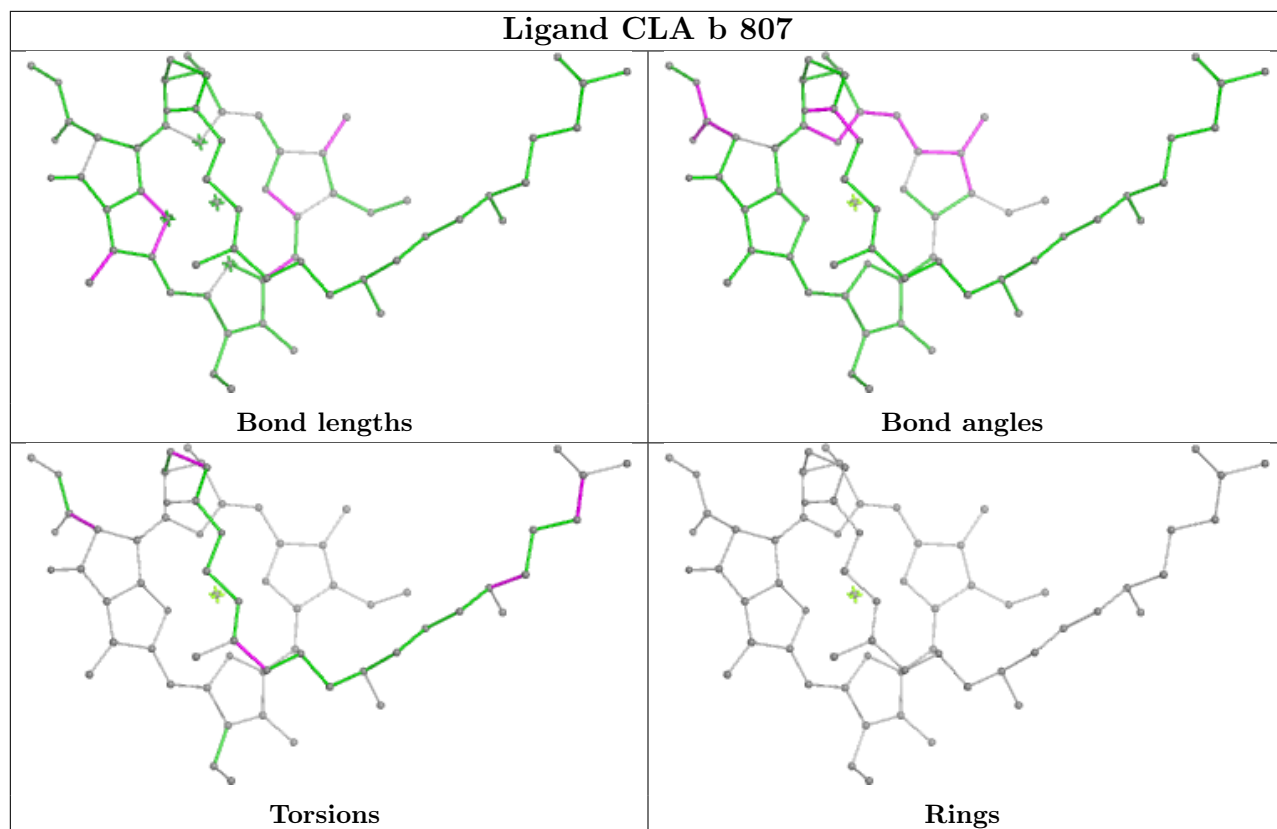


## Ligand CLA b 815

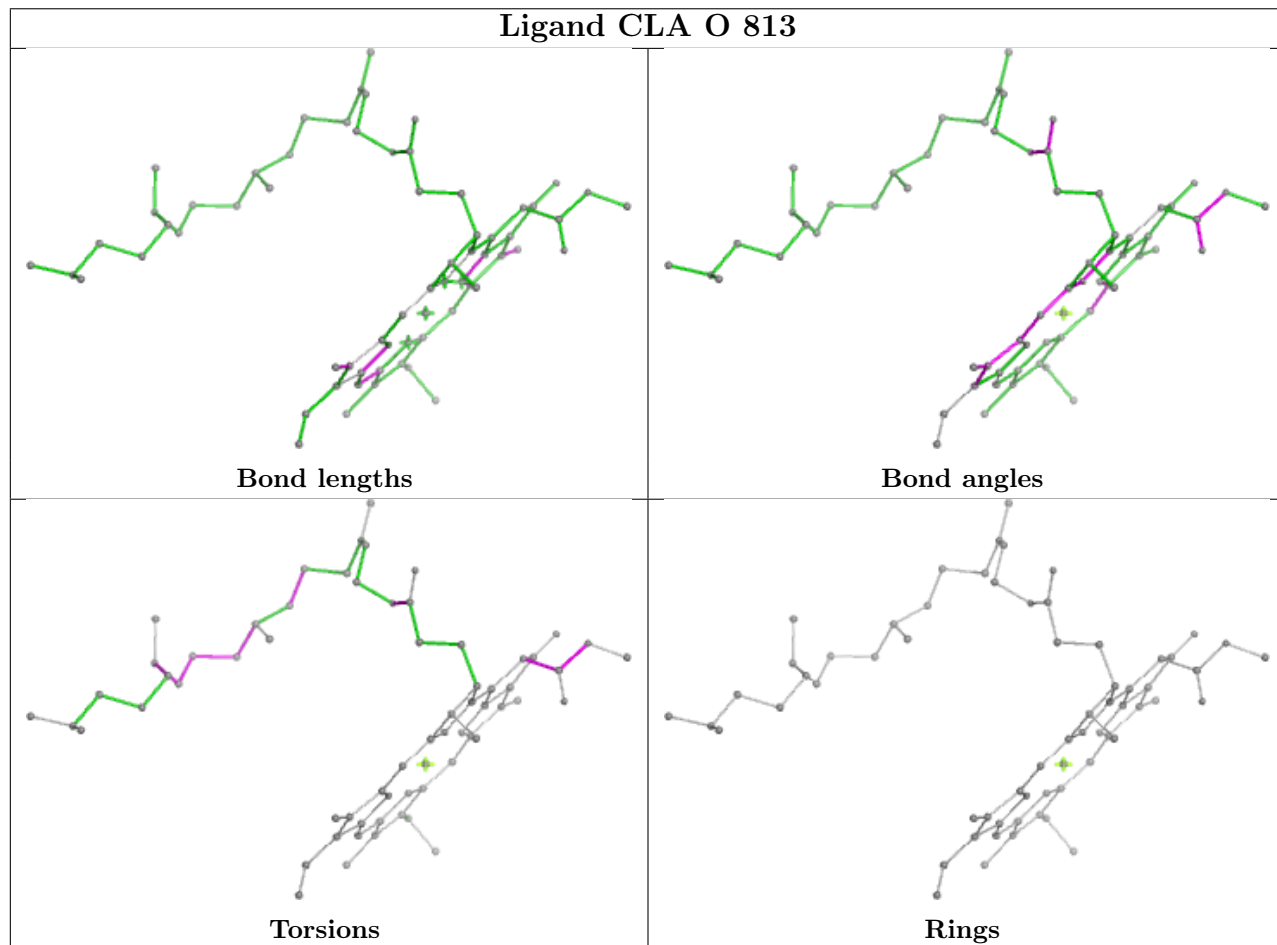




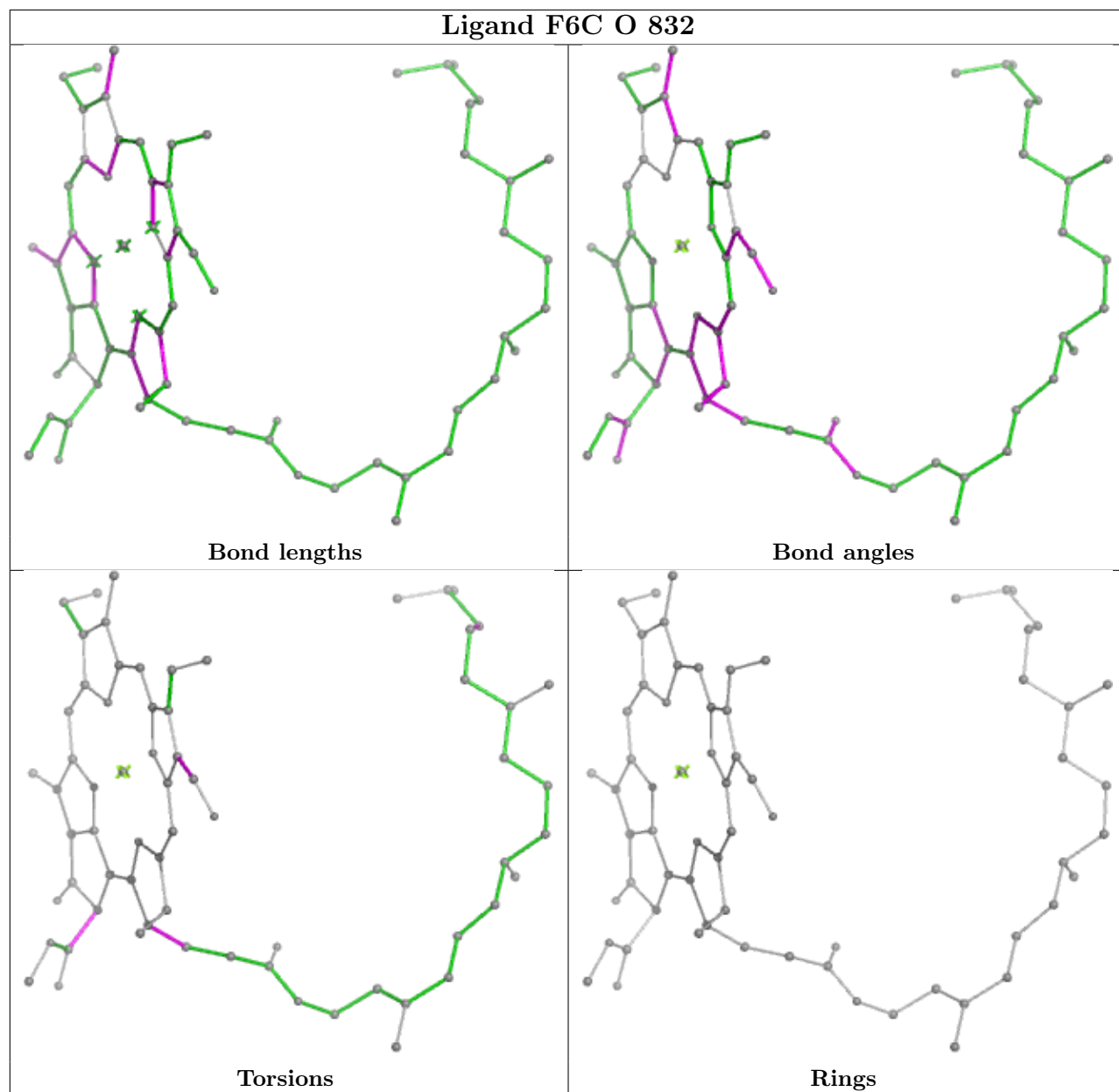
## Ligand CLA b 807



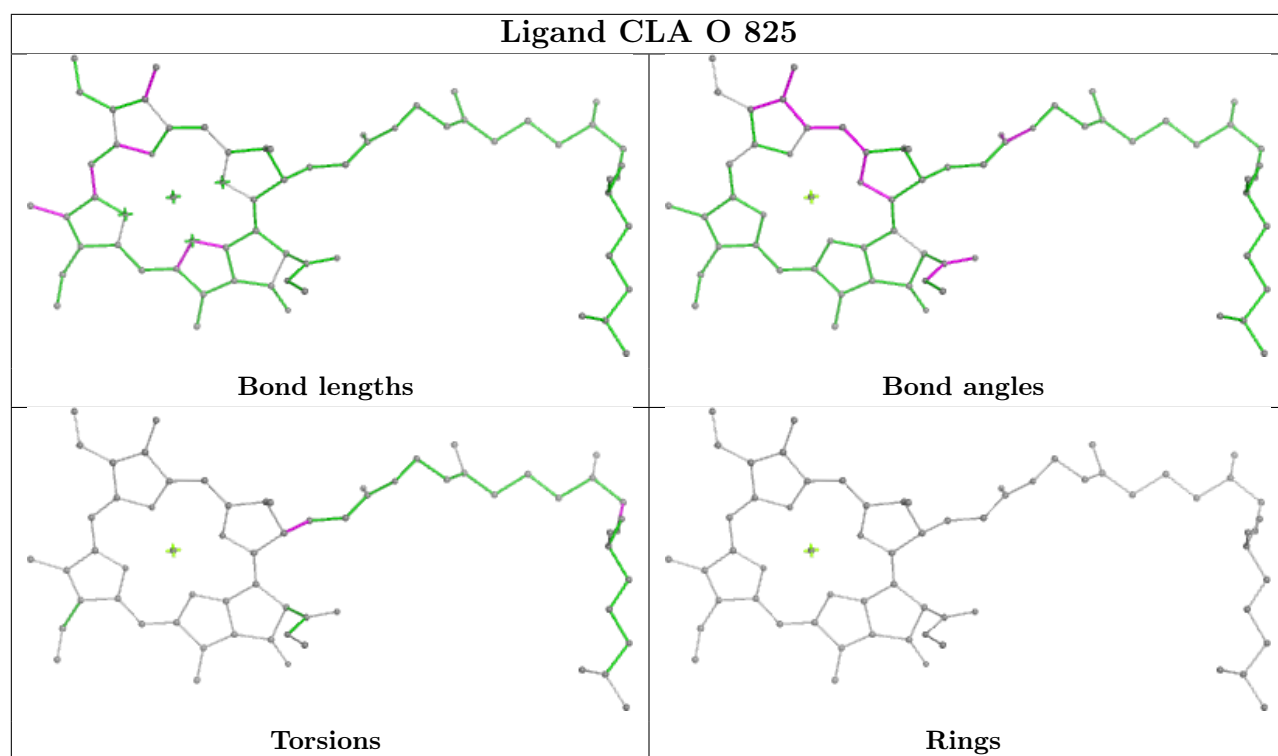
## Ligand CLA O 813



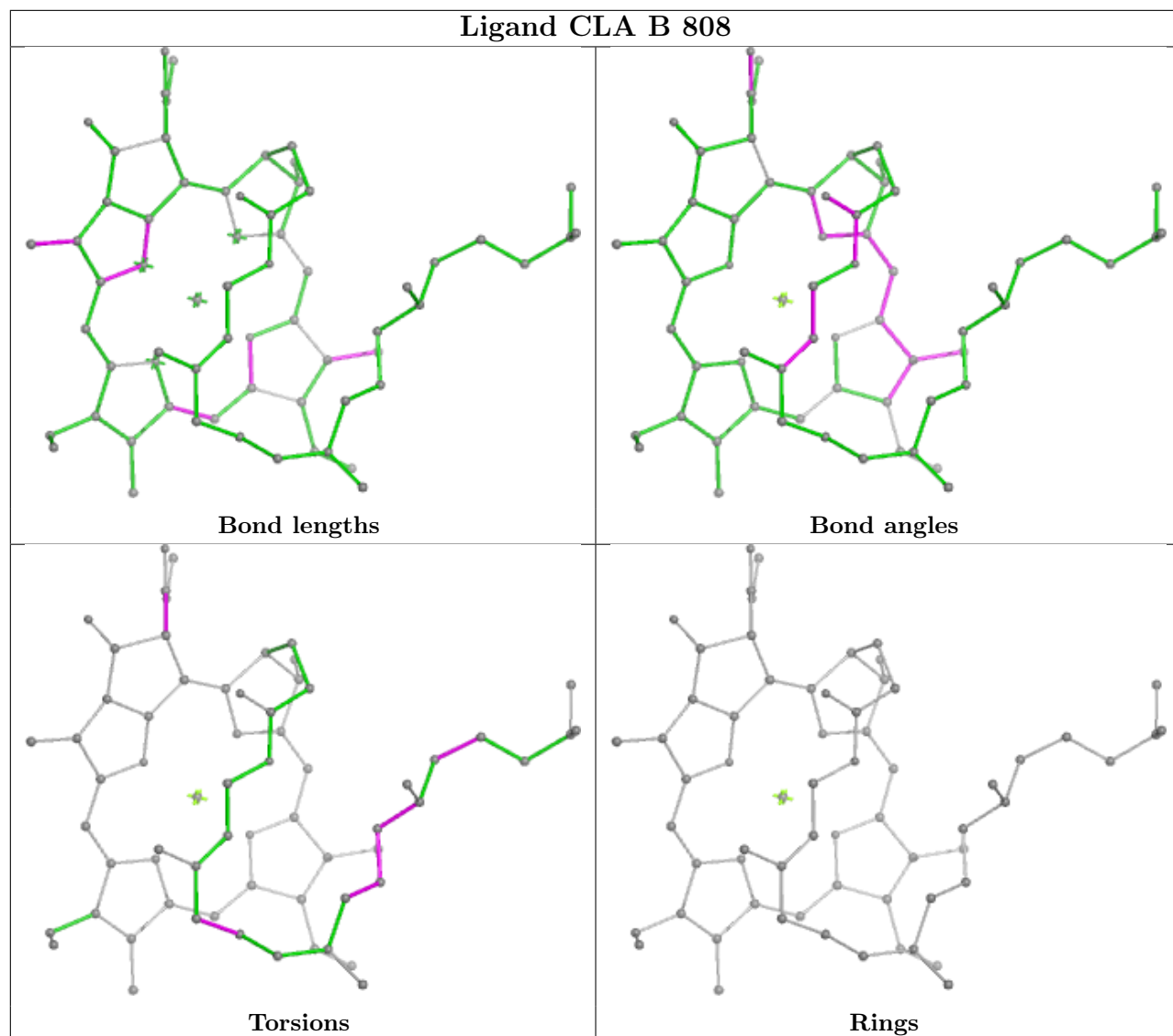
## Ligand F6C O 832



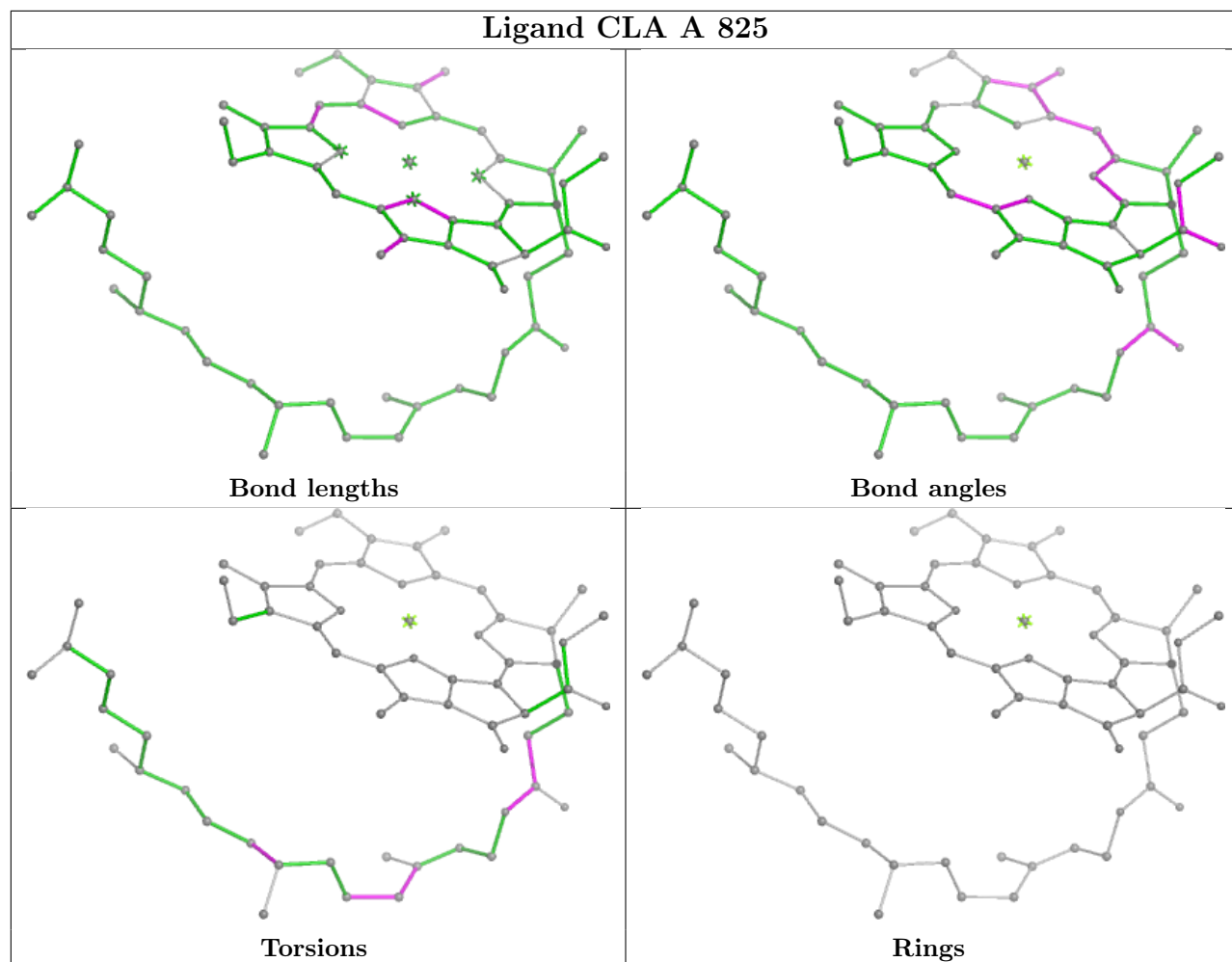


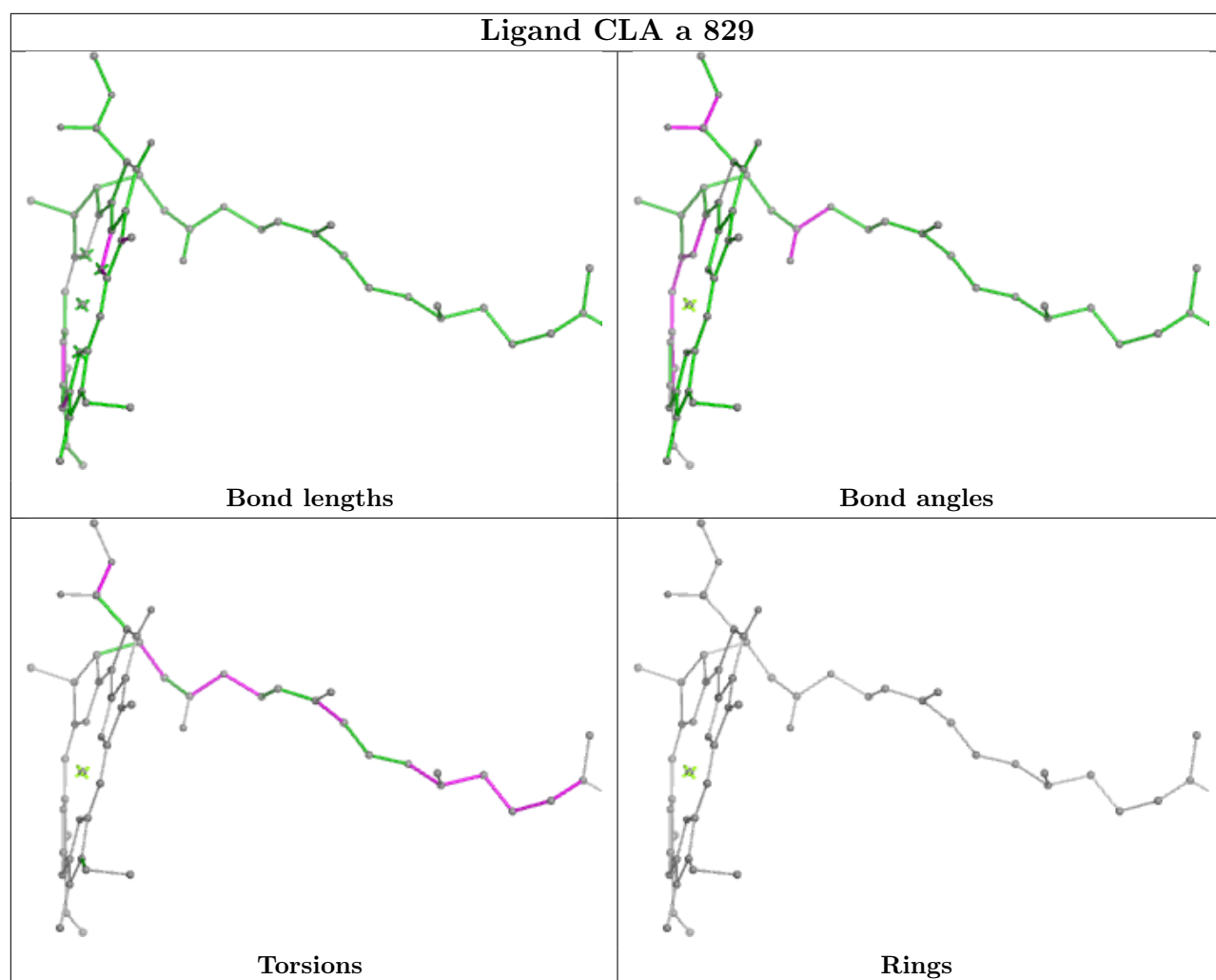


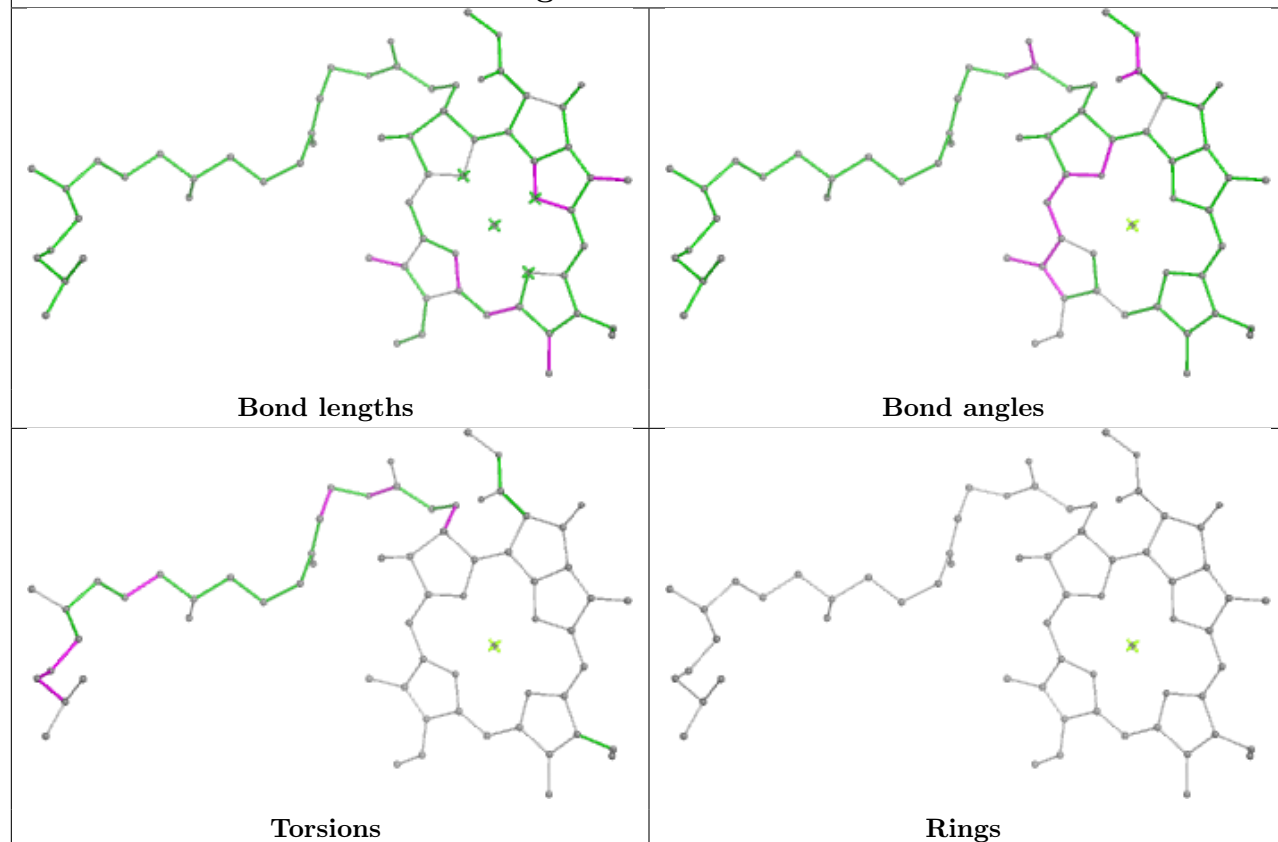
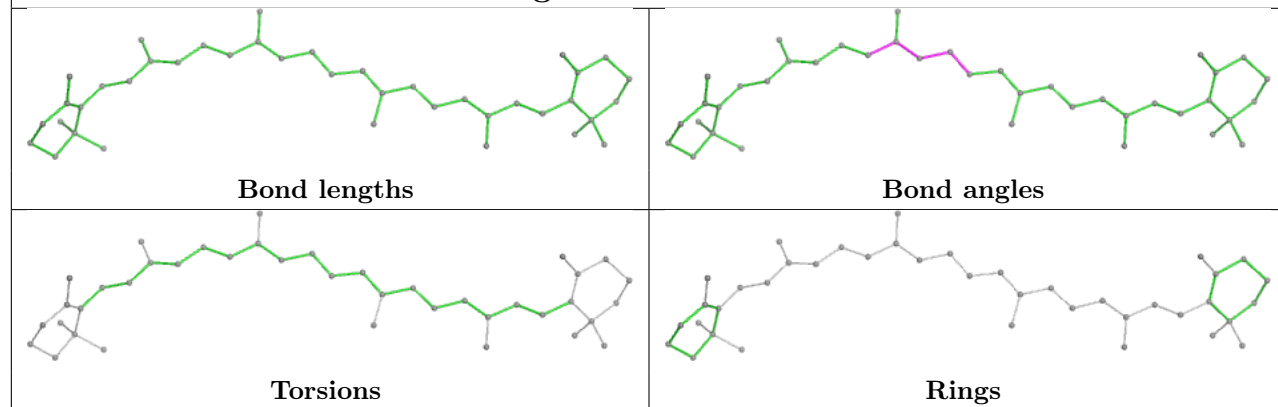
## Ligand CLA B 808



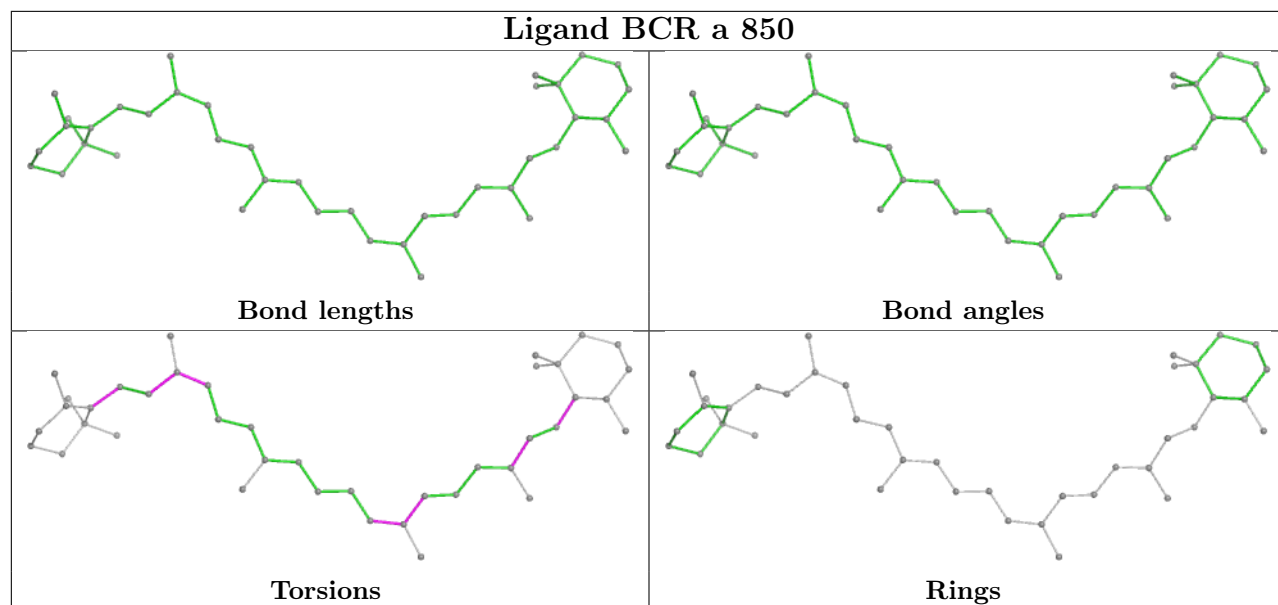
## Ligand CLA A 825



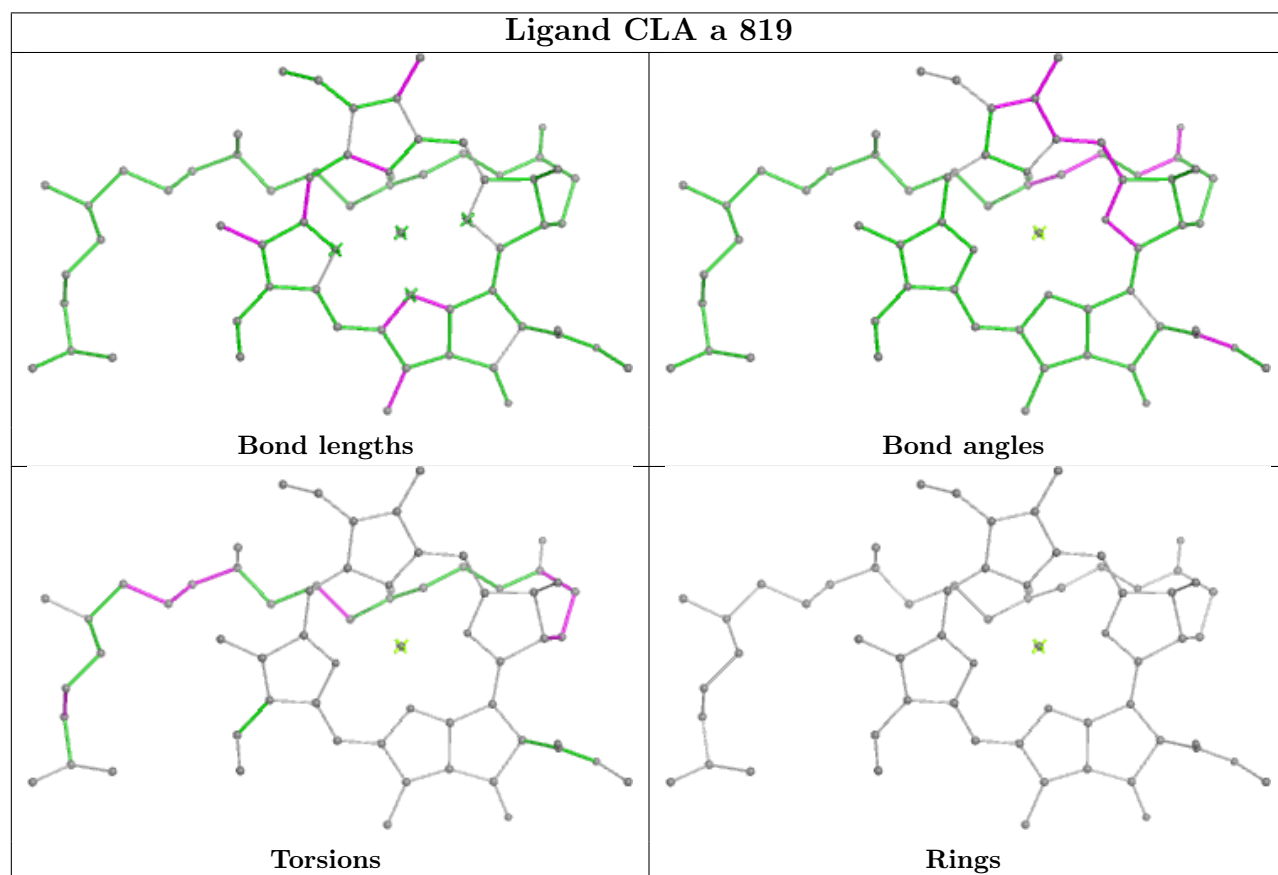


**Ligand CLA a 803****Ligand BCR b 846**

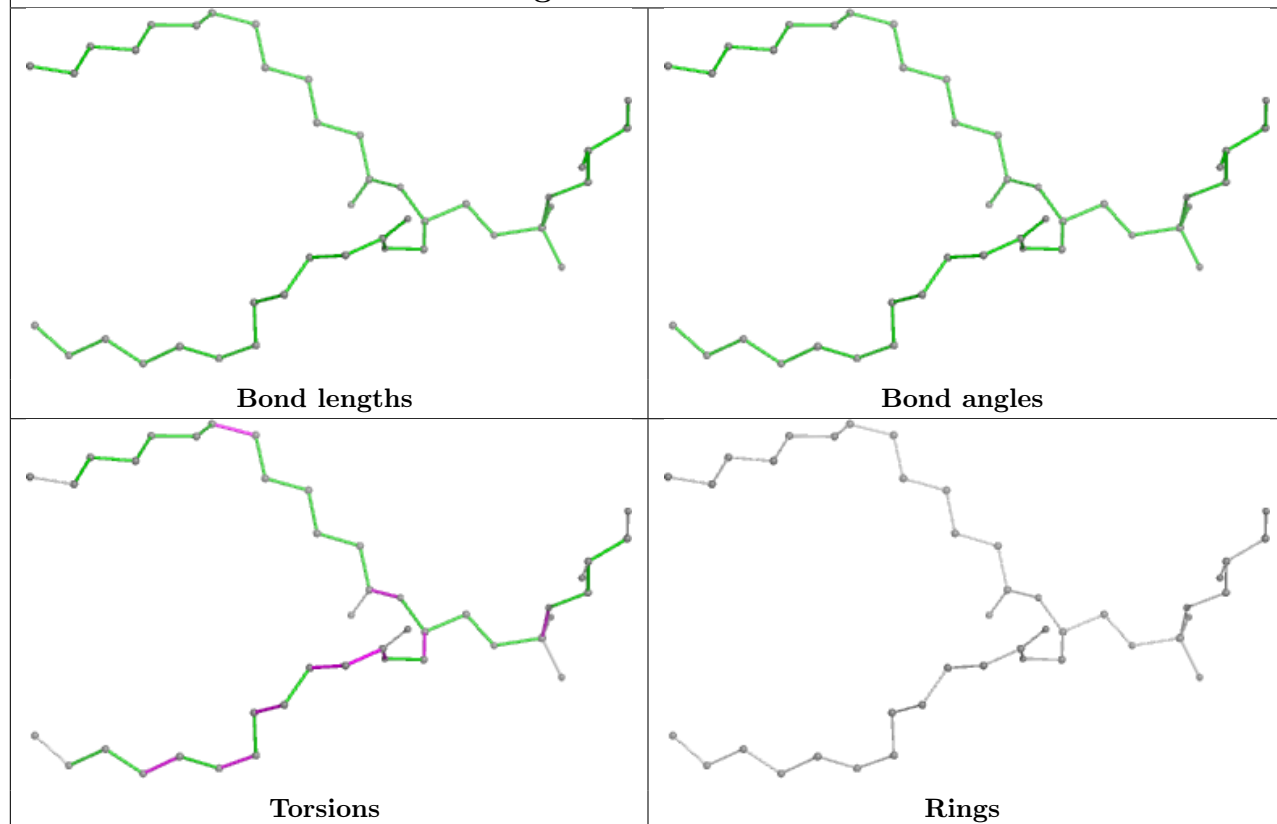
## Ligand BCR a 850



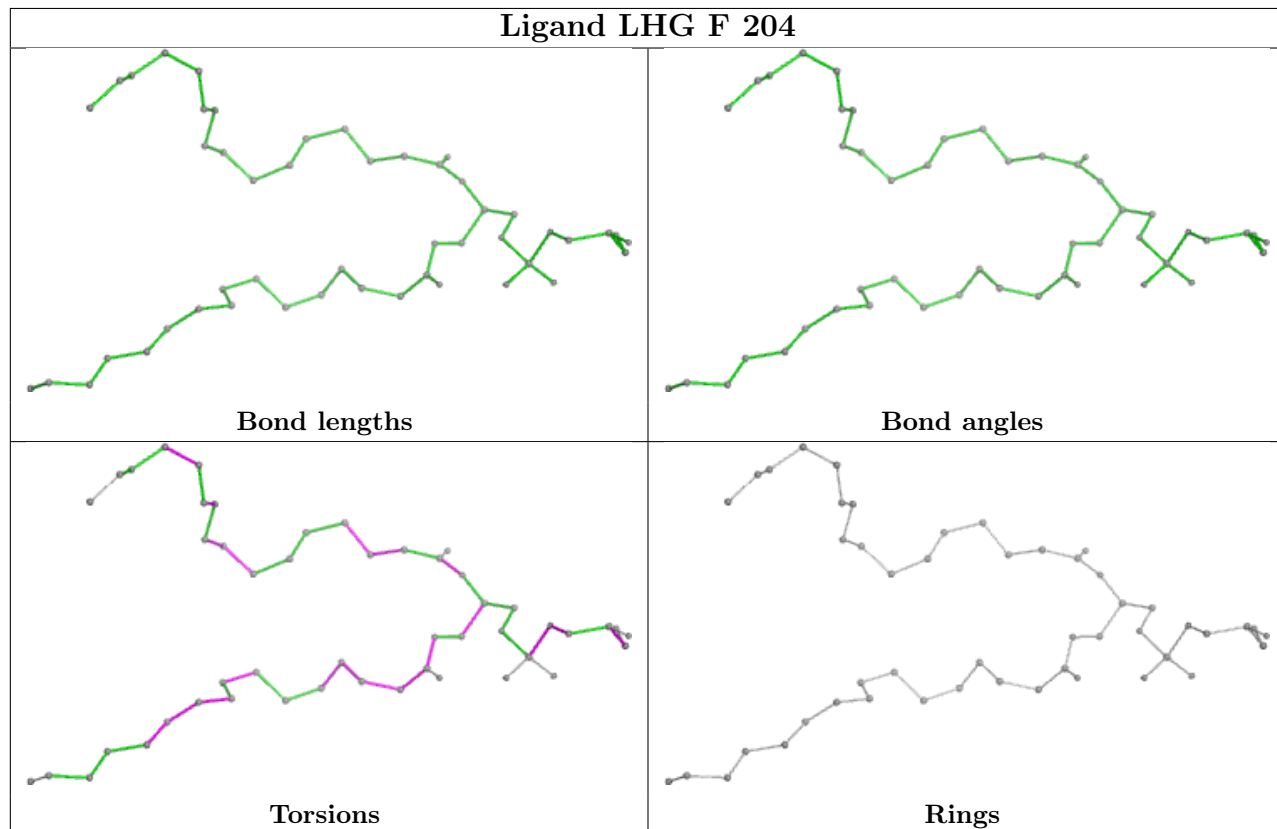
## Ligand CLA a 819

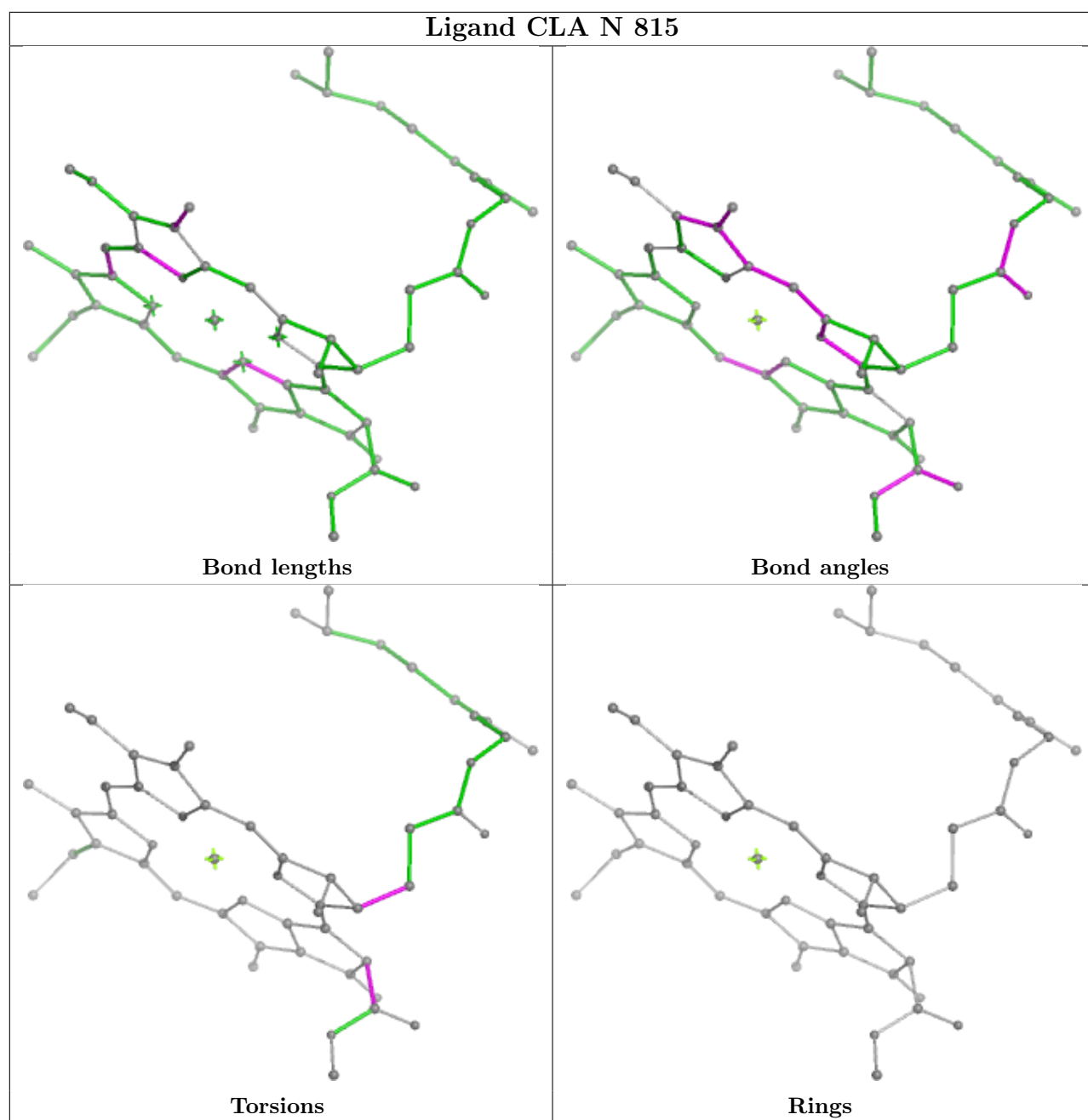


## Ligand LHG a 851

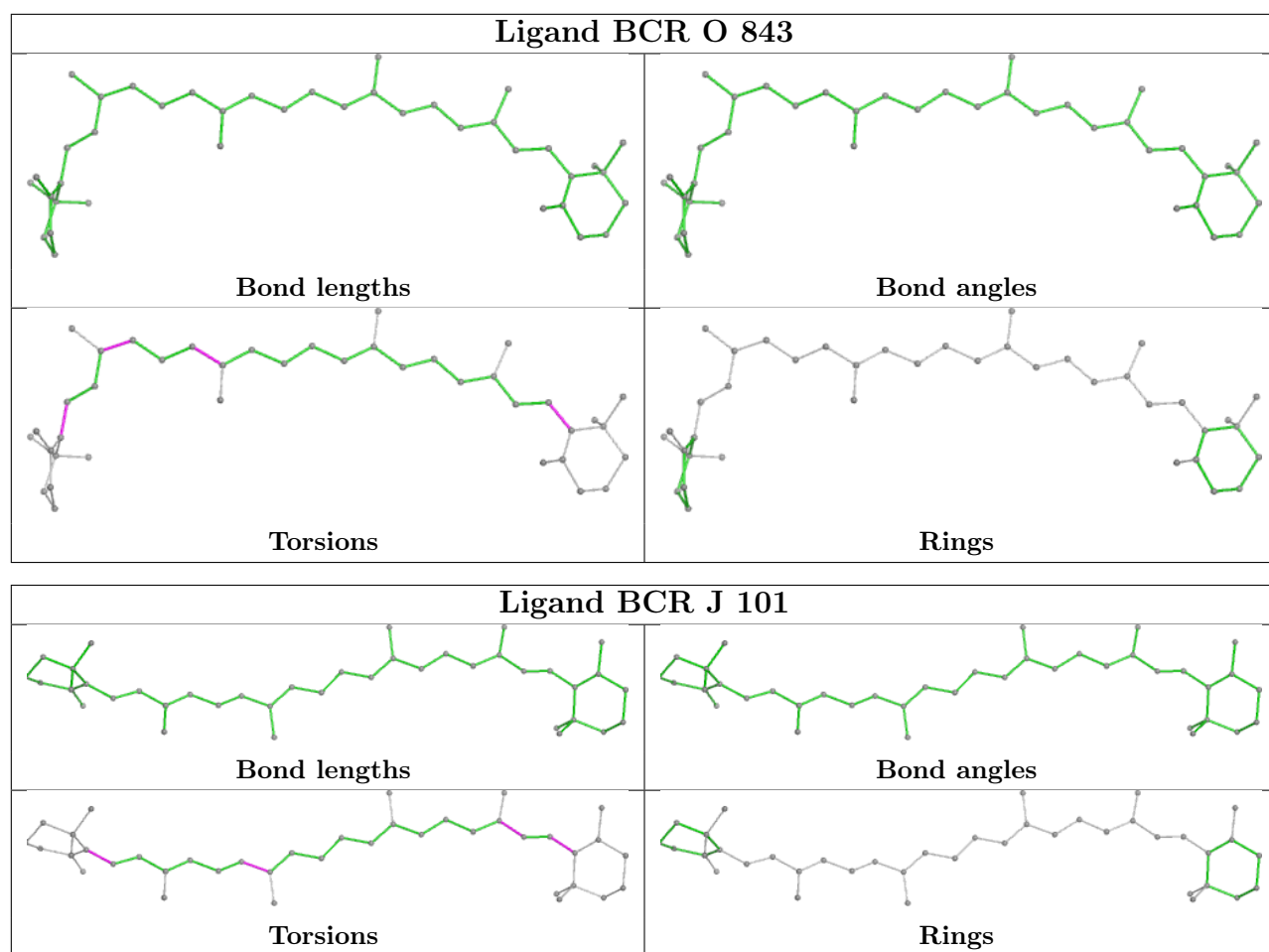


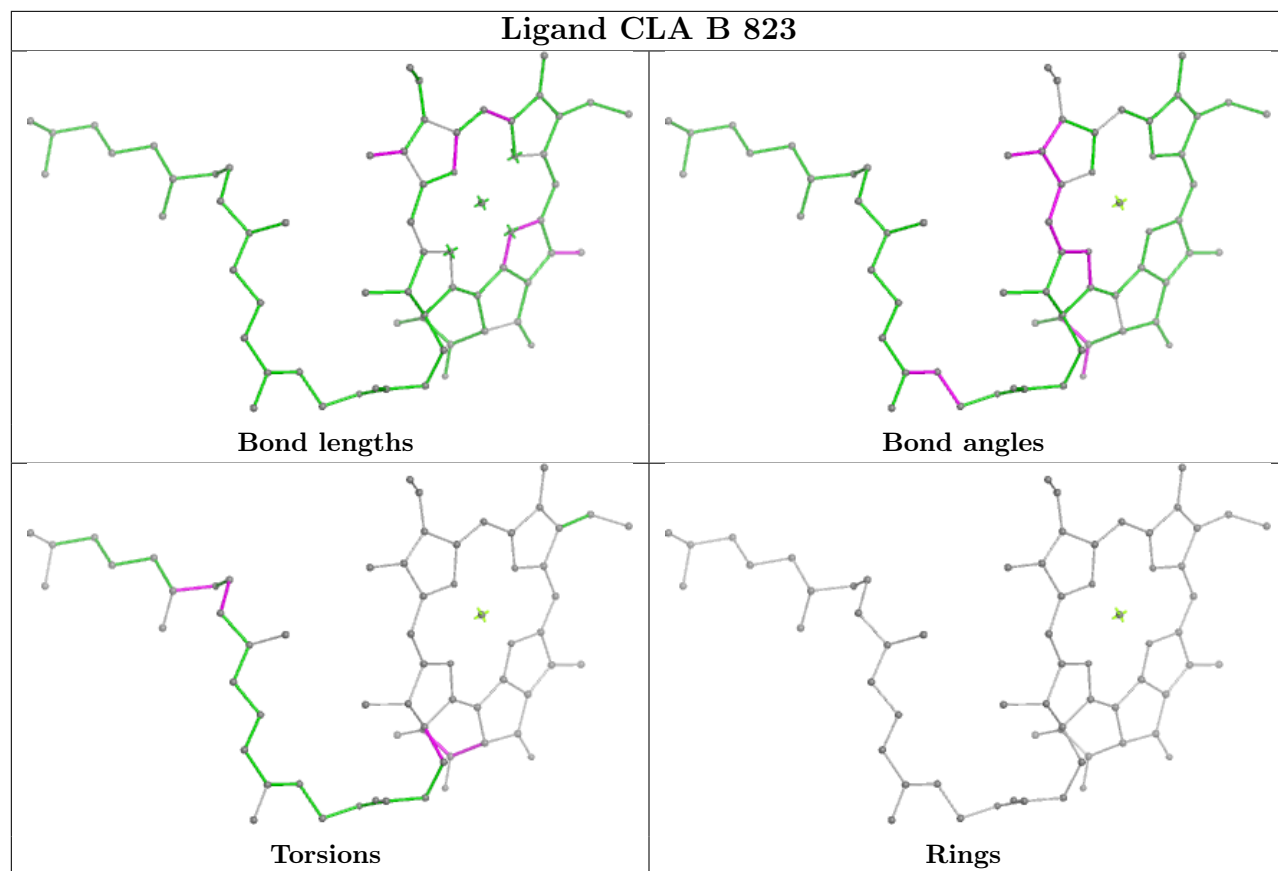
## Ligand LHG F 204



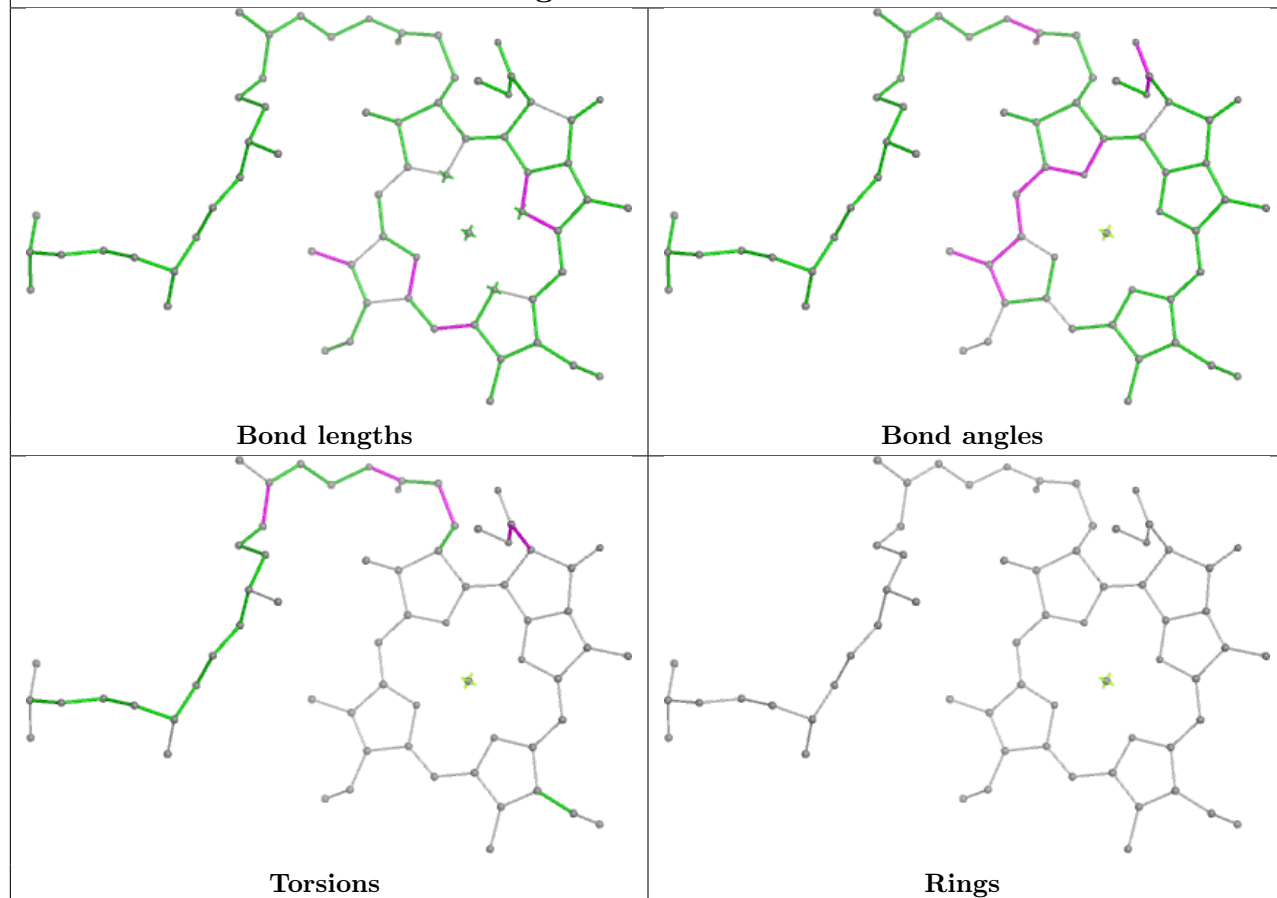




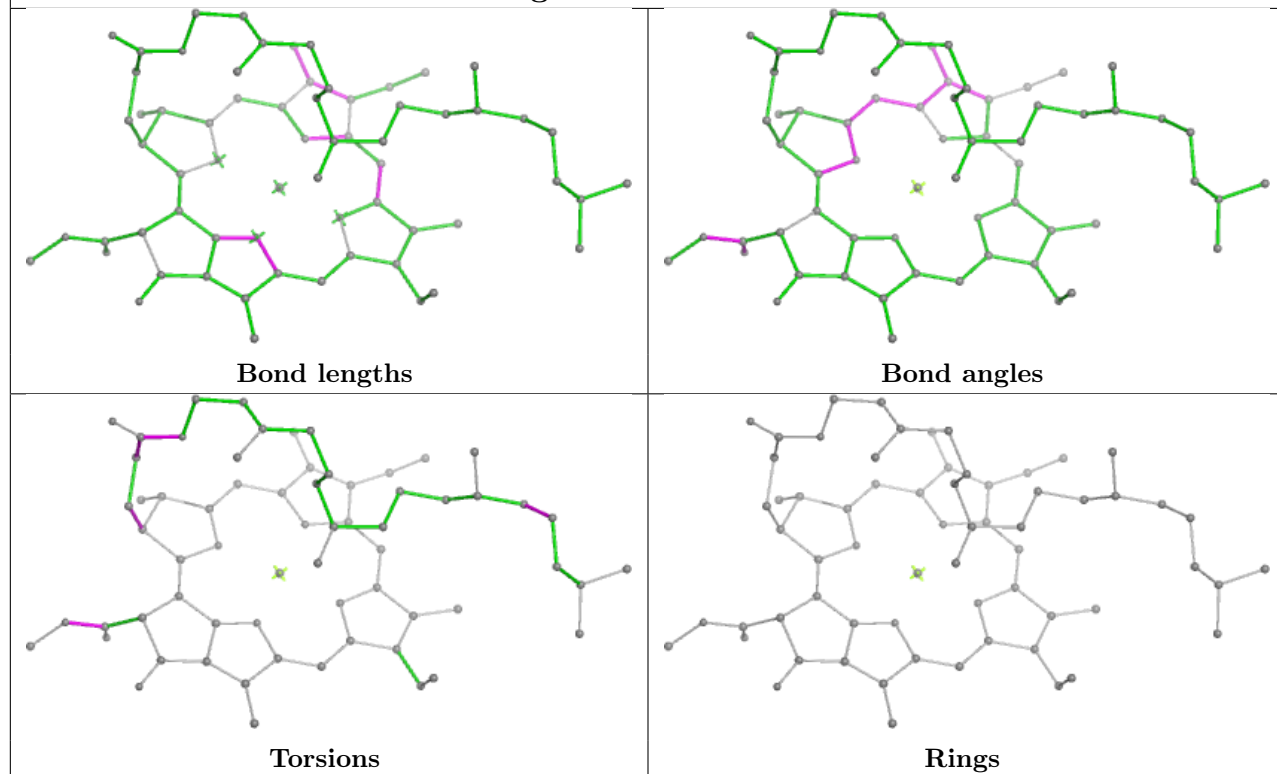




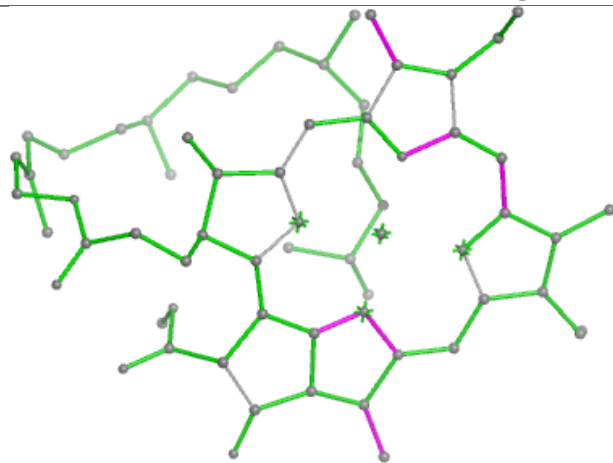
## Ligand CLA a 814



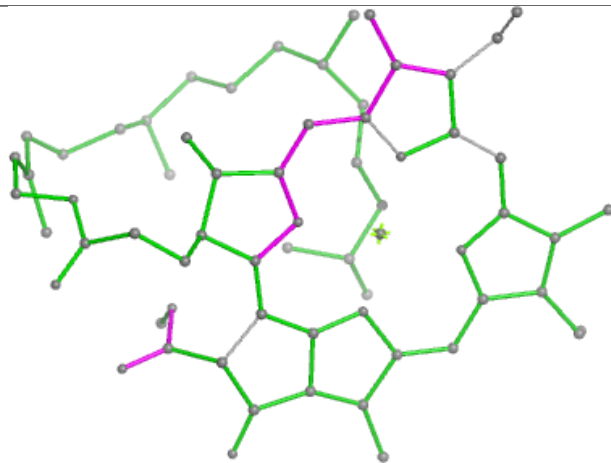
## Ligand CLA O 816



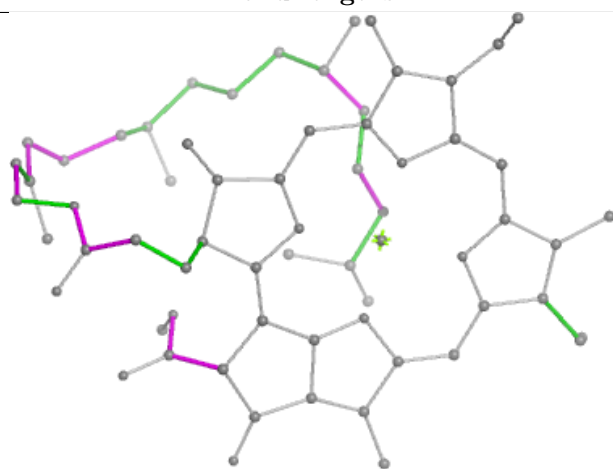
## Ligand CLA A 807



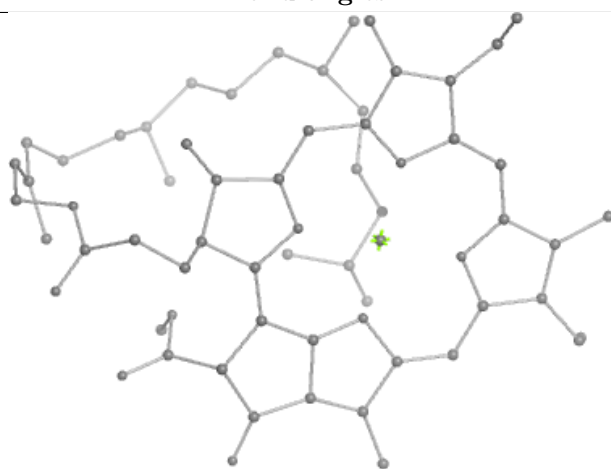
Bond lengths



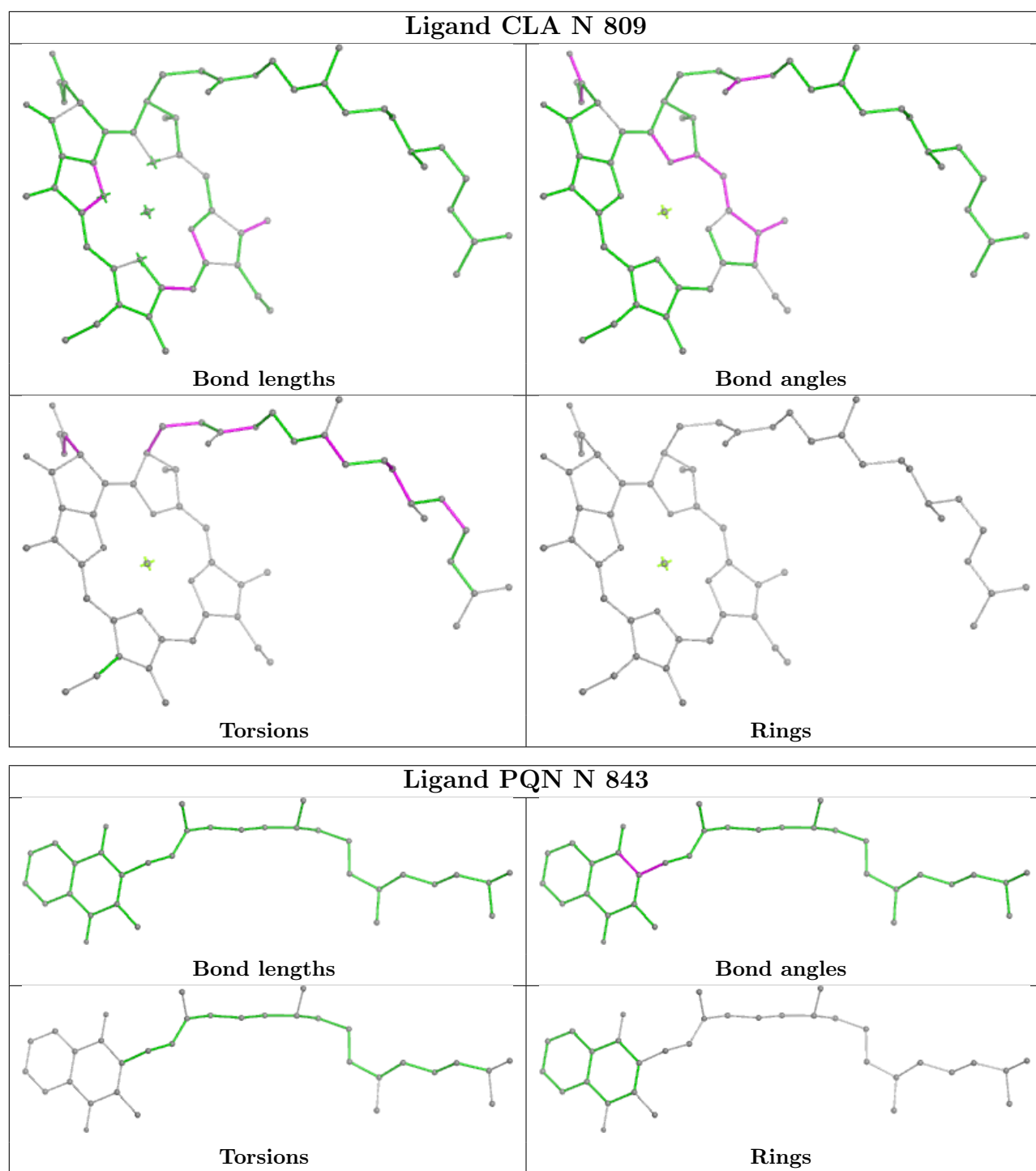
Bond angles

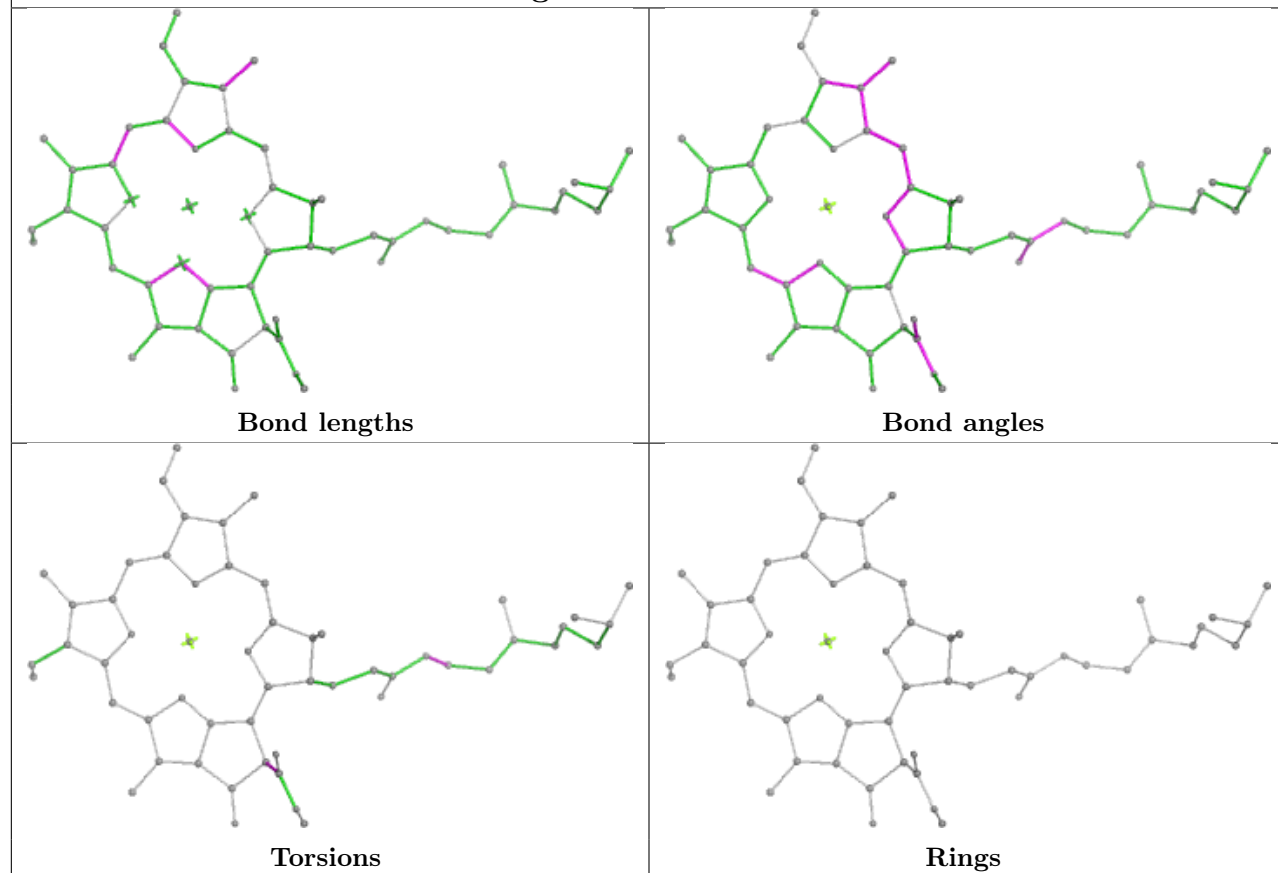
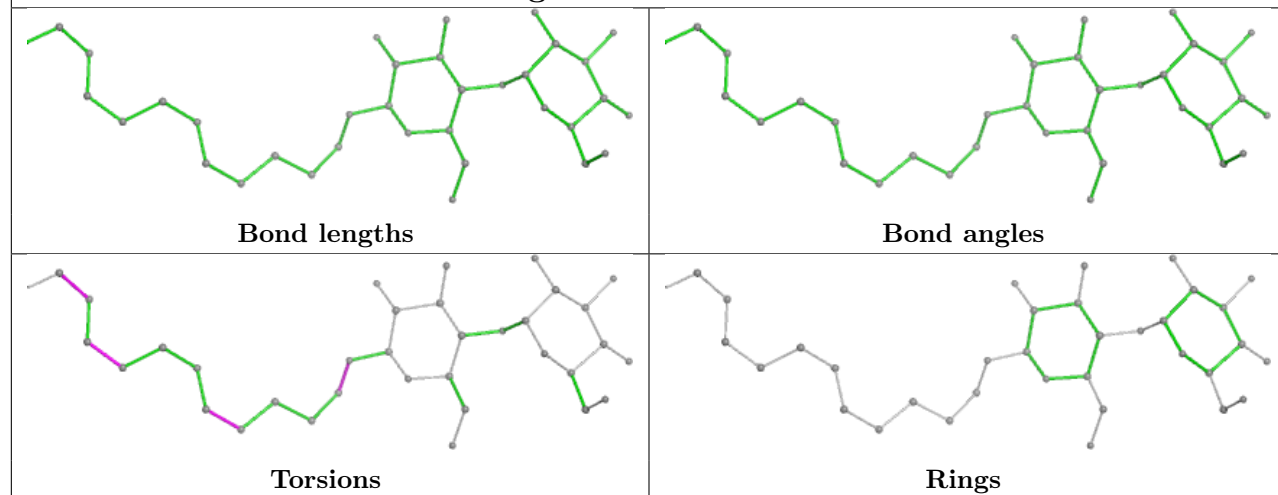


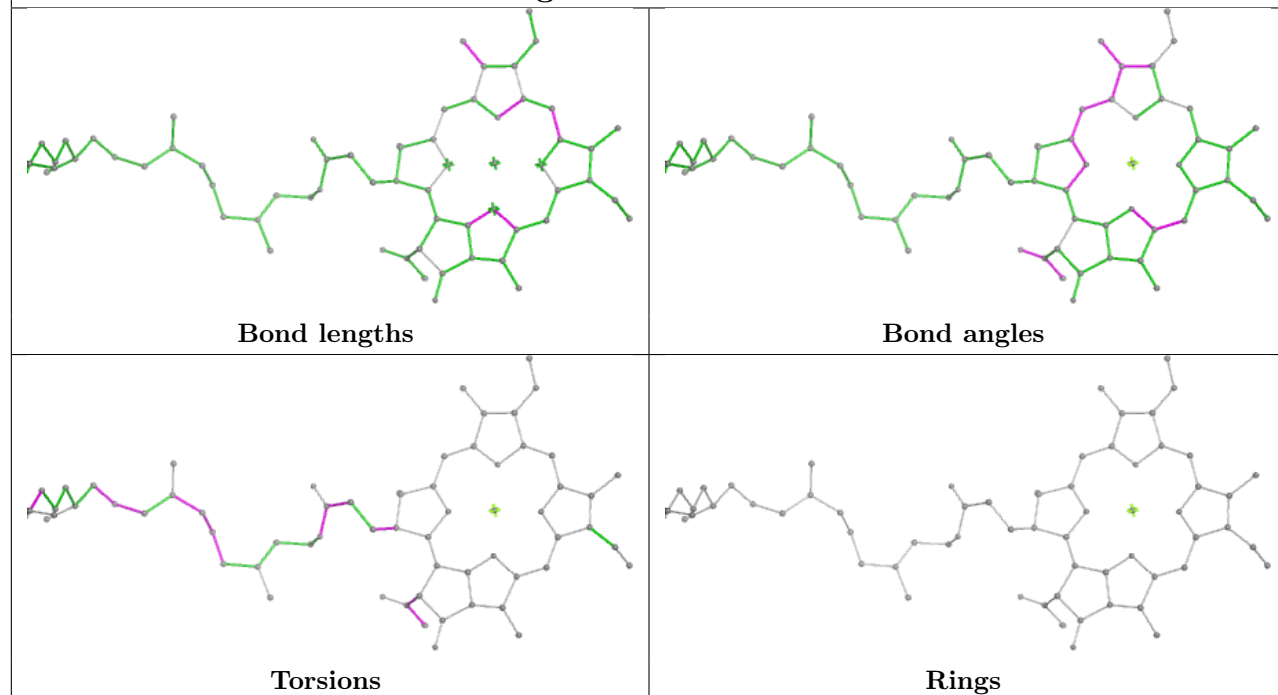
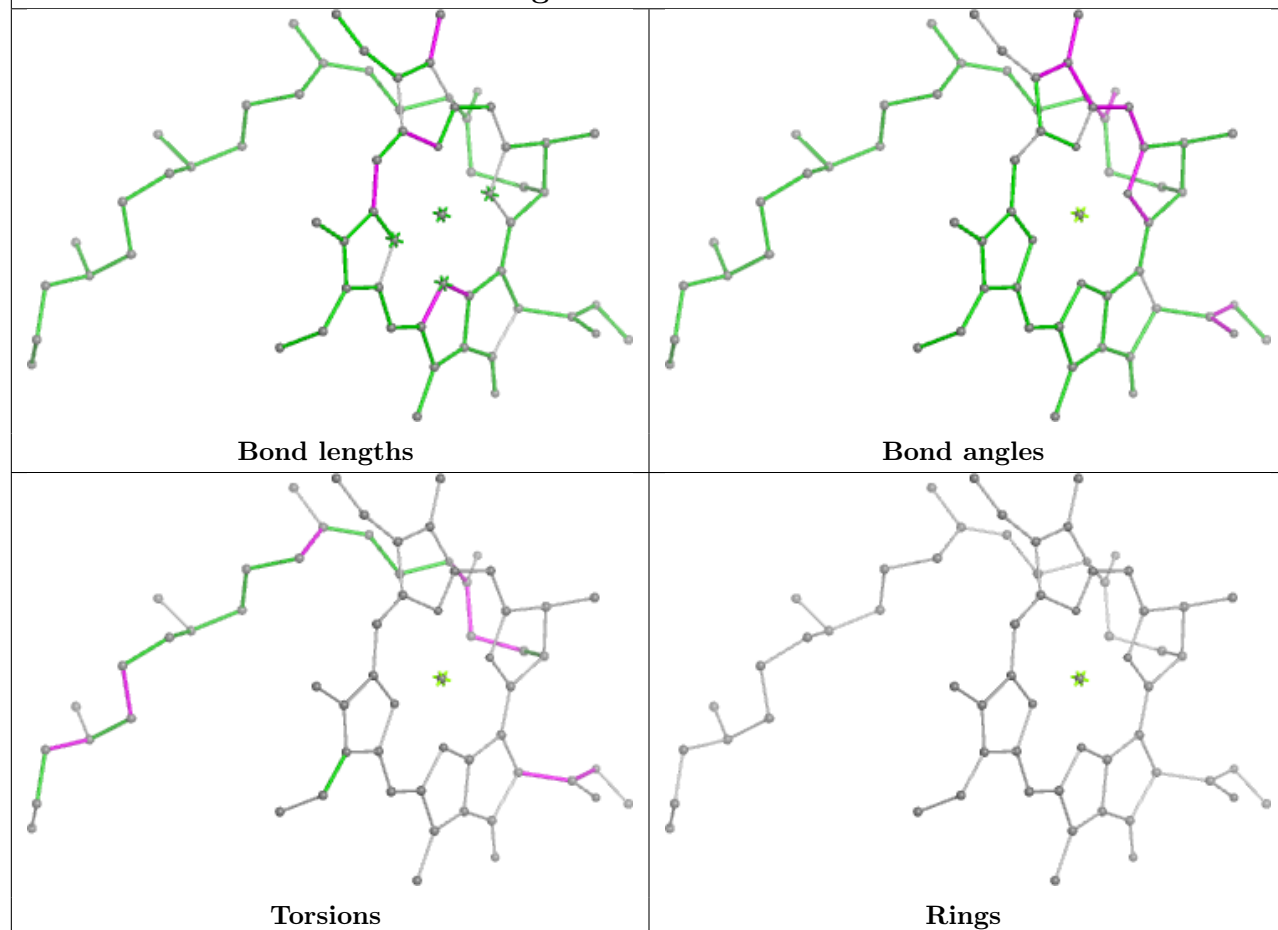
Torsions

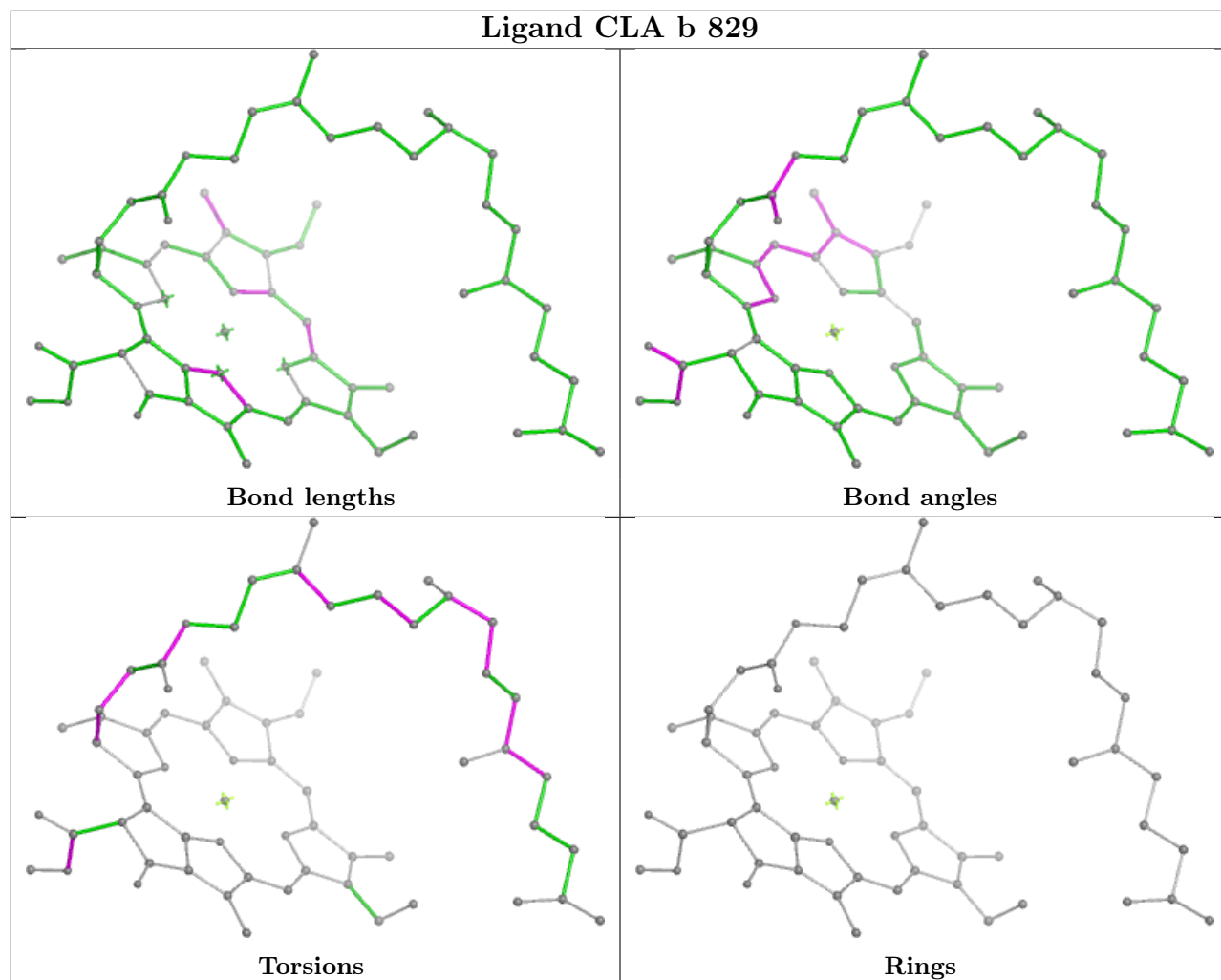
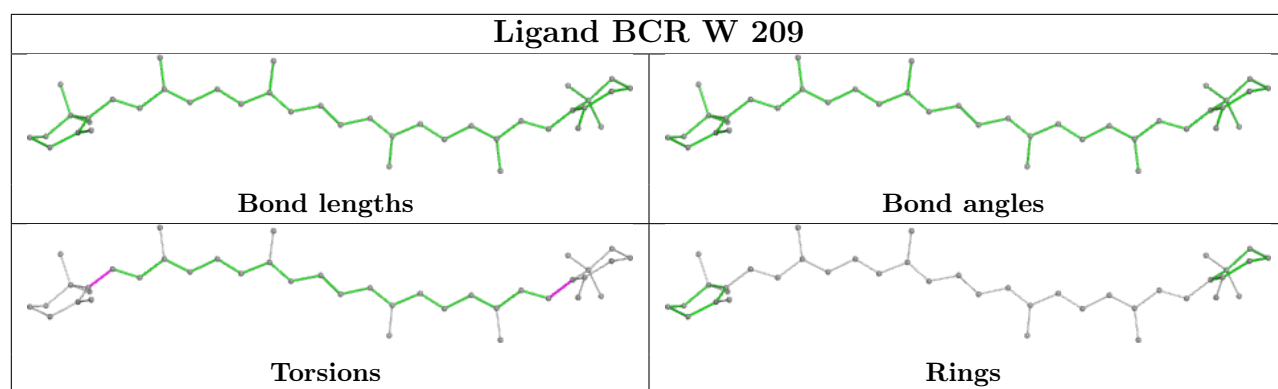


Rings

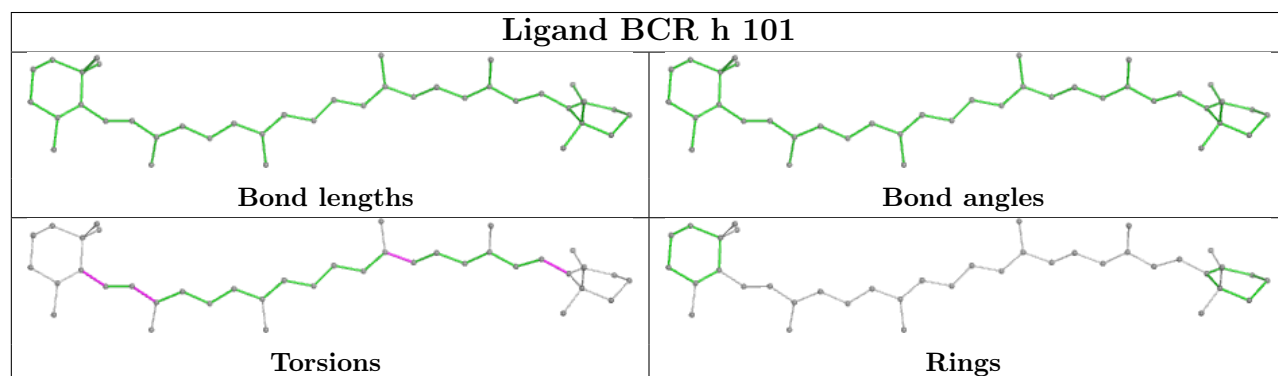
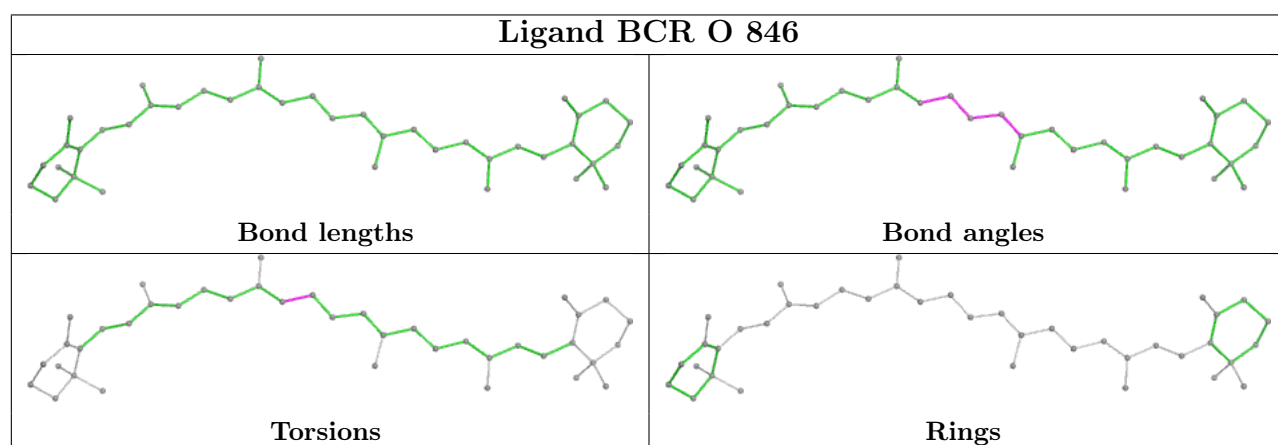
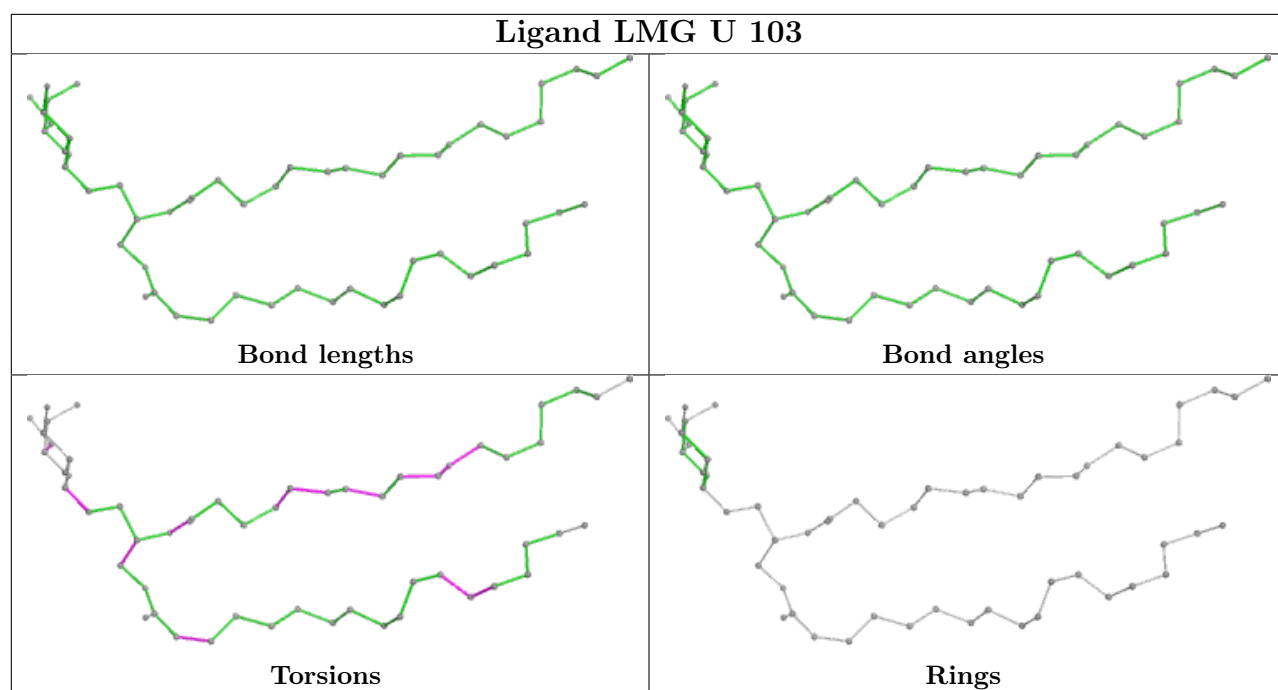


**Ligand CLA A 827****Ligand LMT N 854**

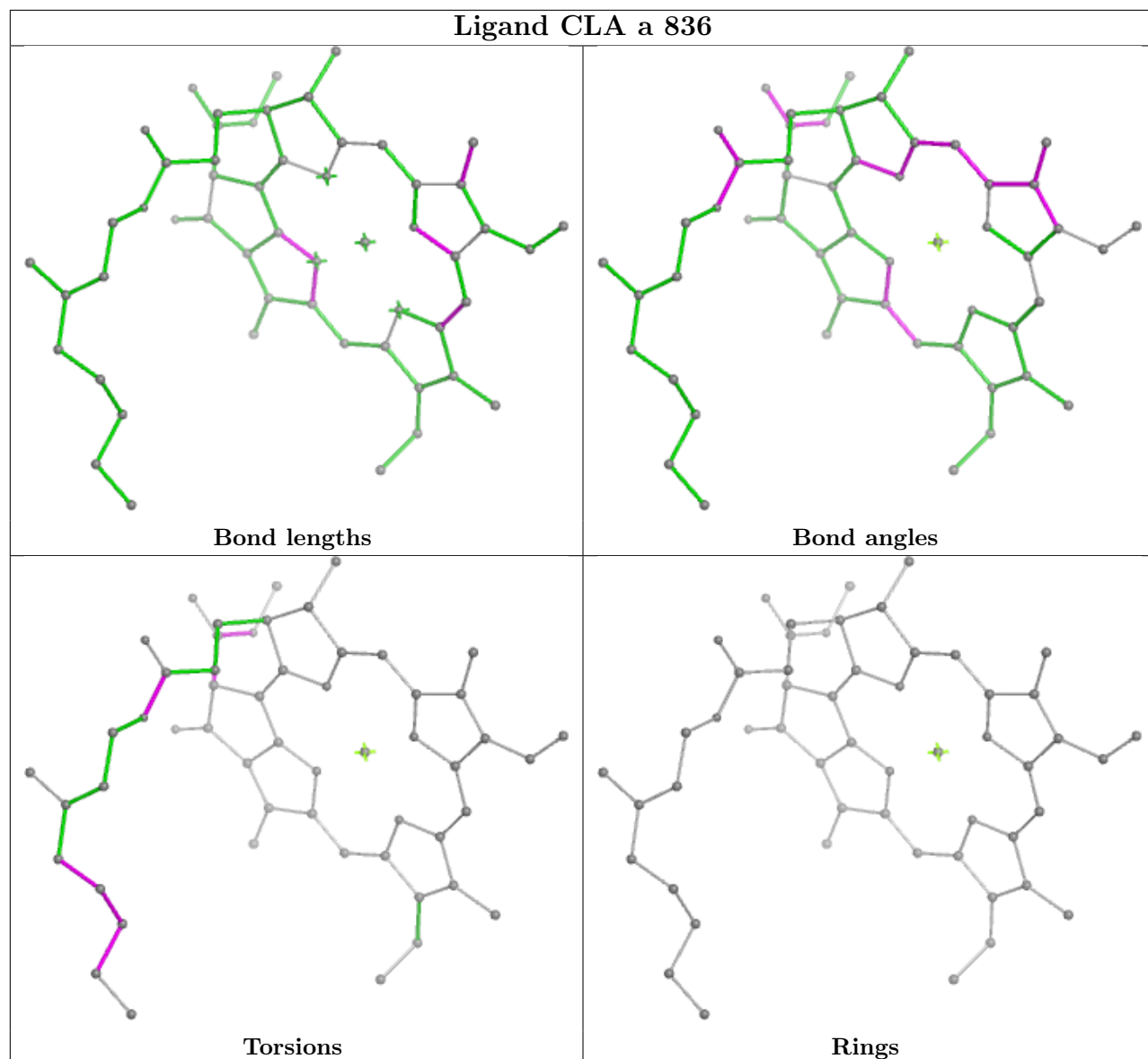
**Ligand CLA a 806****Ligand CLA O 826**



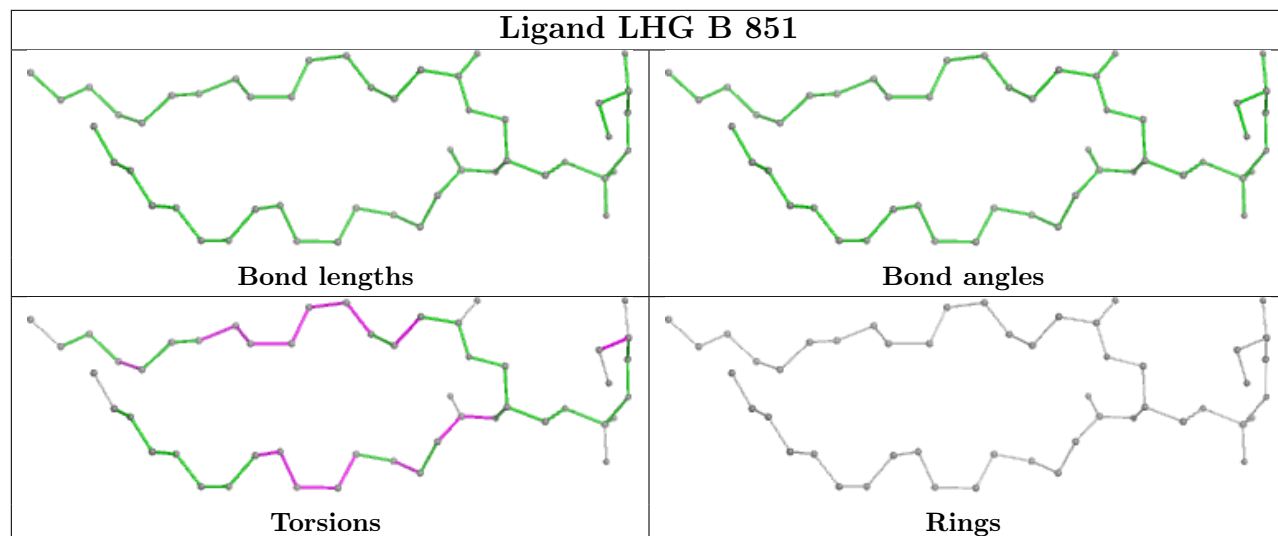


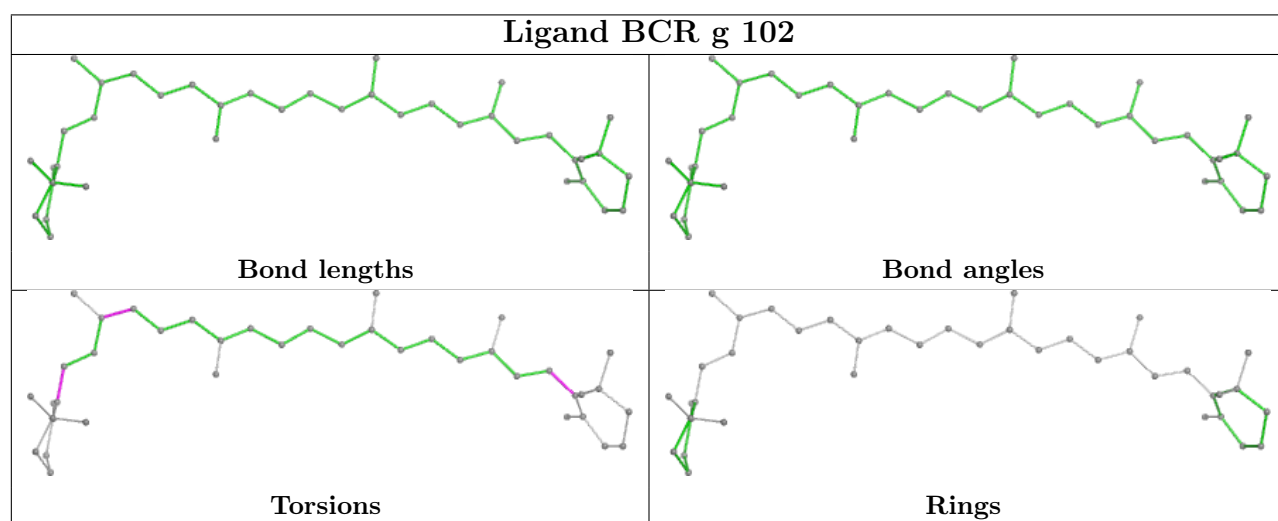
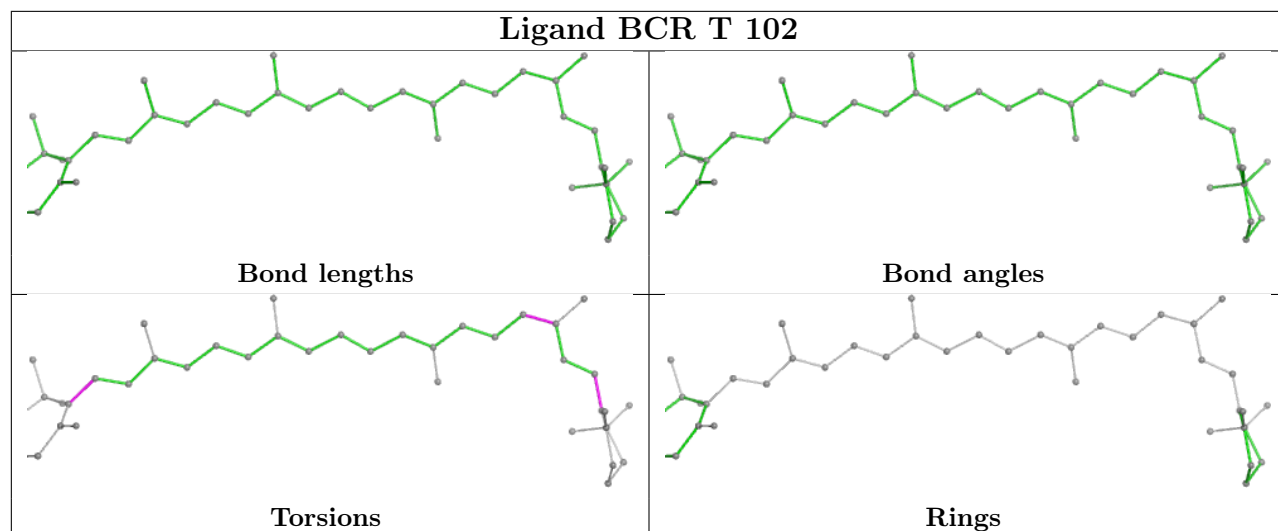


## Ligand CLA a 836

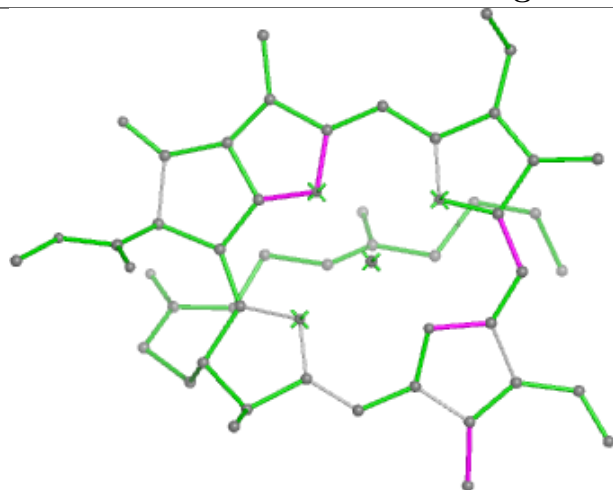


## Ligand LHG B 851

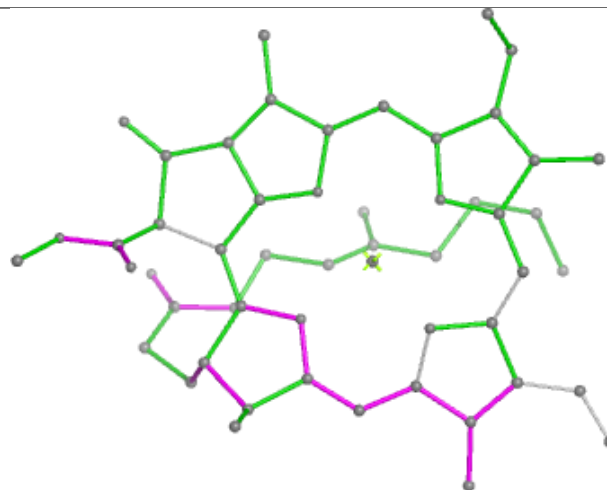




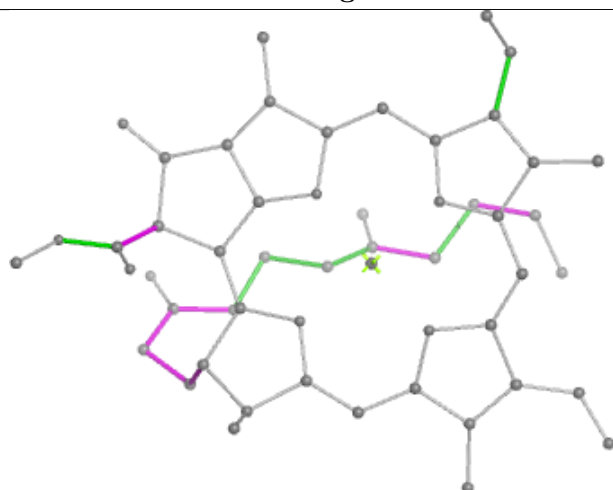
## Ligand CLA O 821



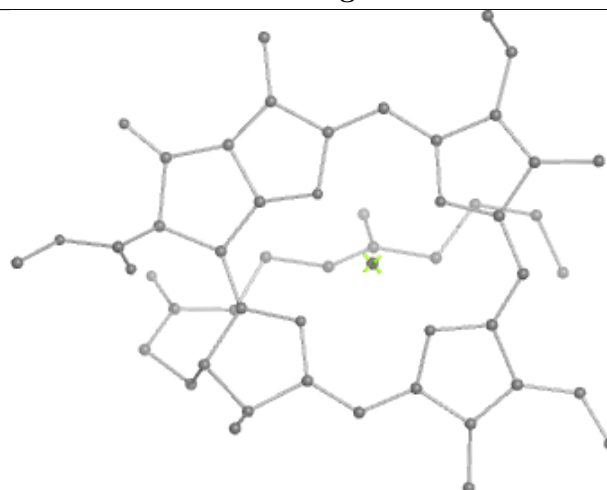
Bond lengths



Bond angles

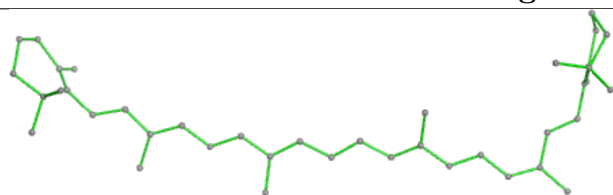


Torsions

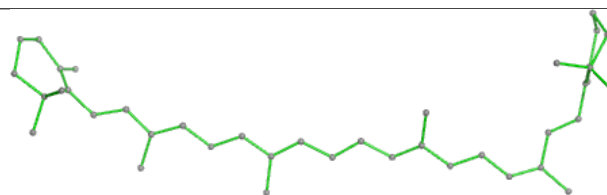


Rings

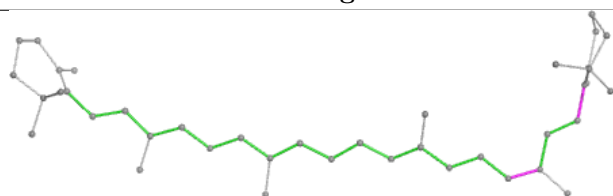
## Ligand BCR I 102



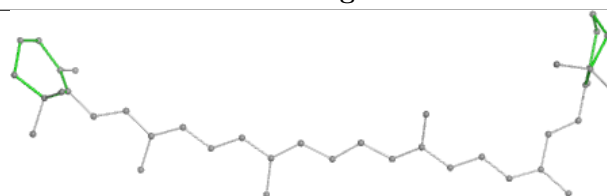
Bond lengths



Bond angles

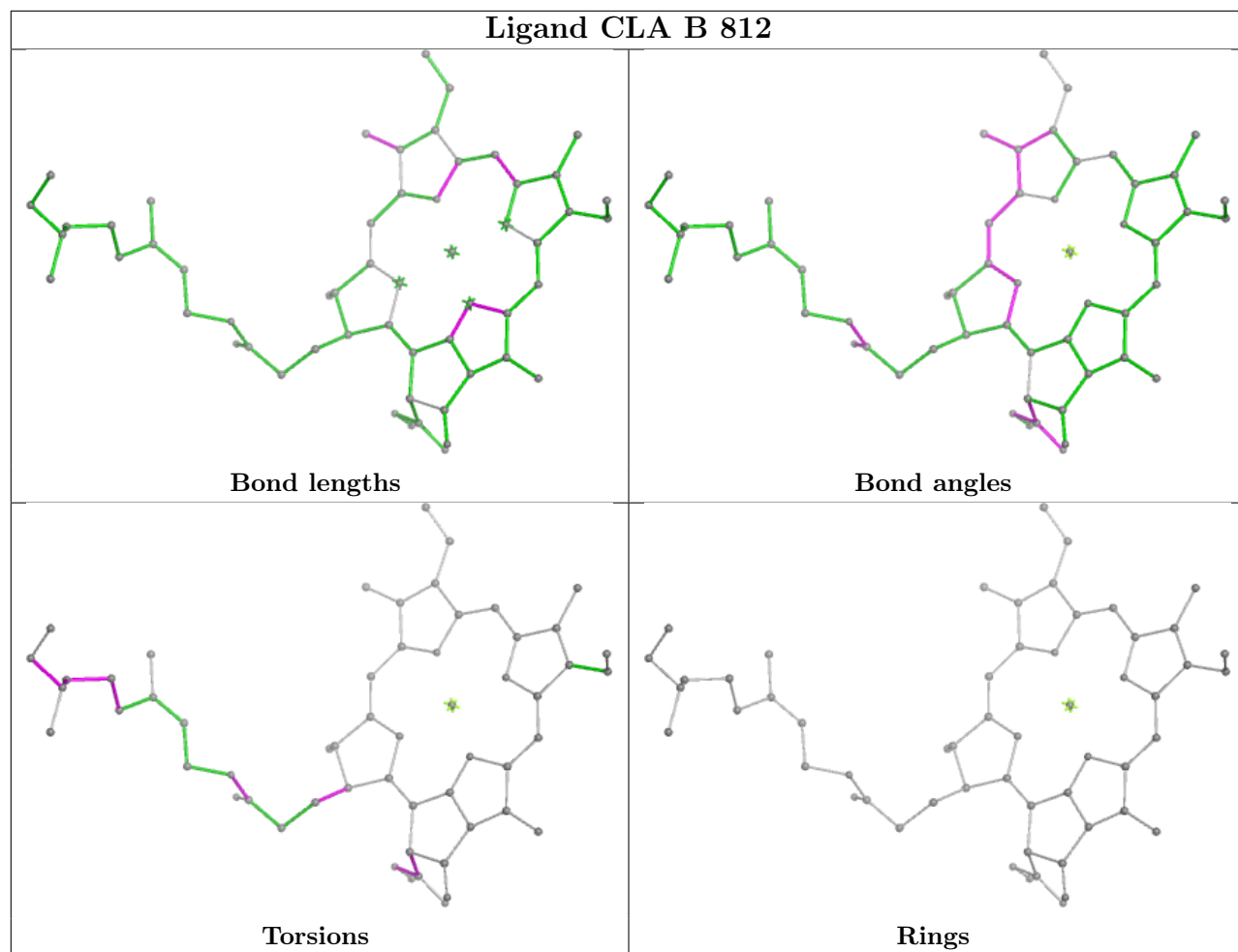


Torsions

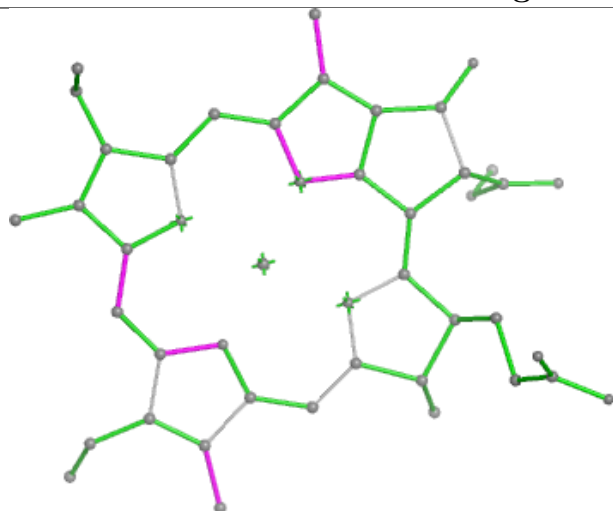


Rings

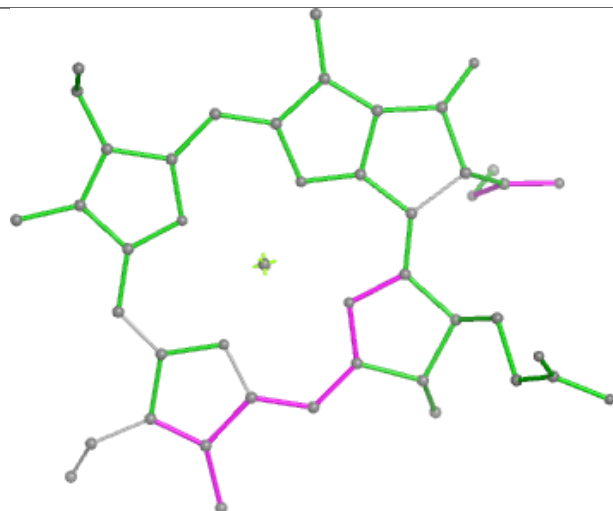
## Ligand CLA B 812



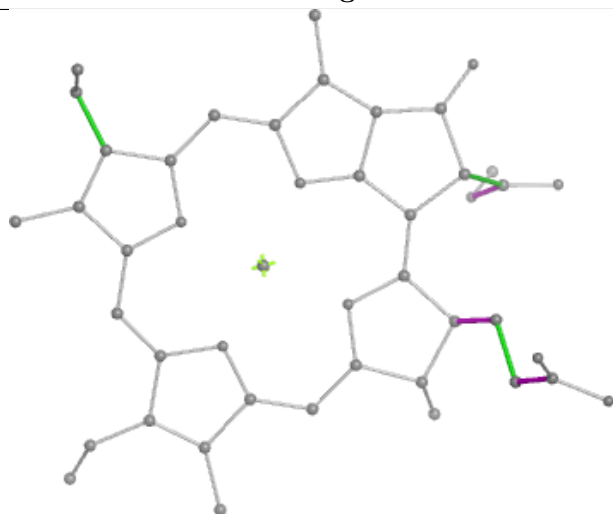
## Ligand CLA K 102



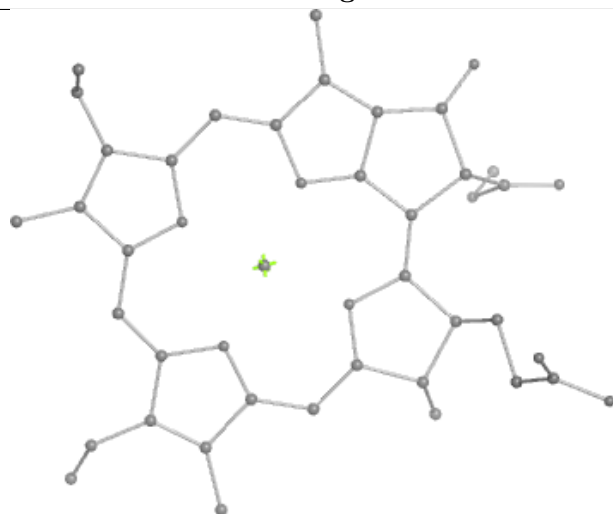
Bond lengths



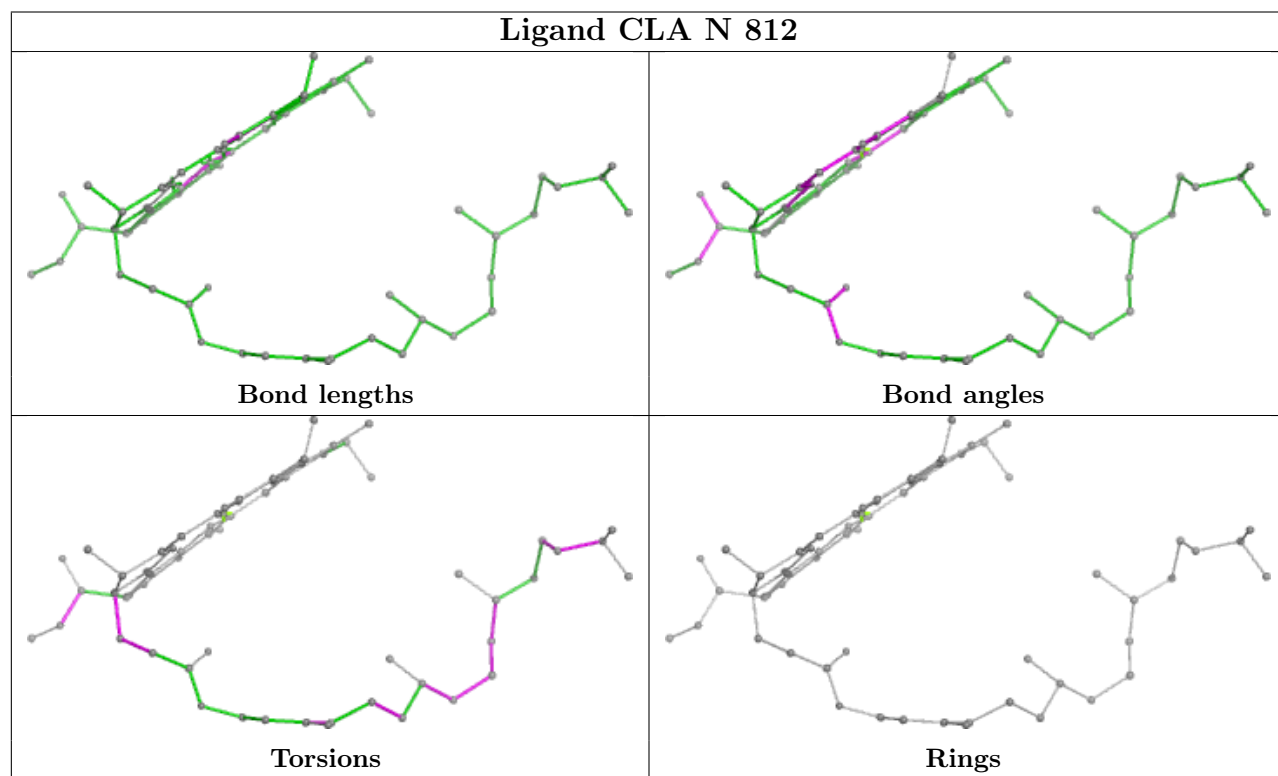
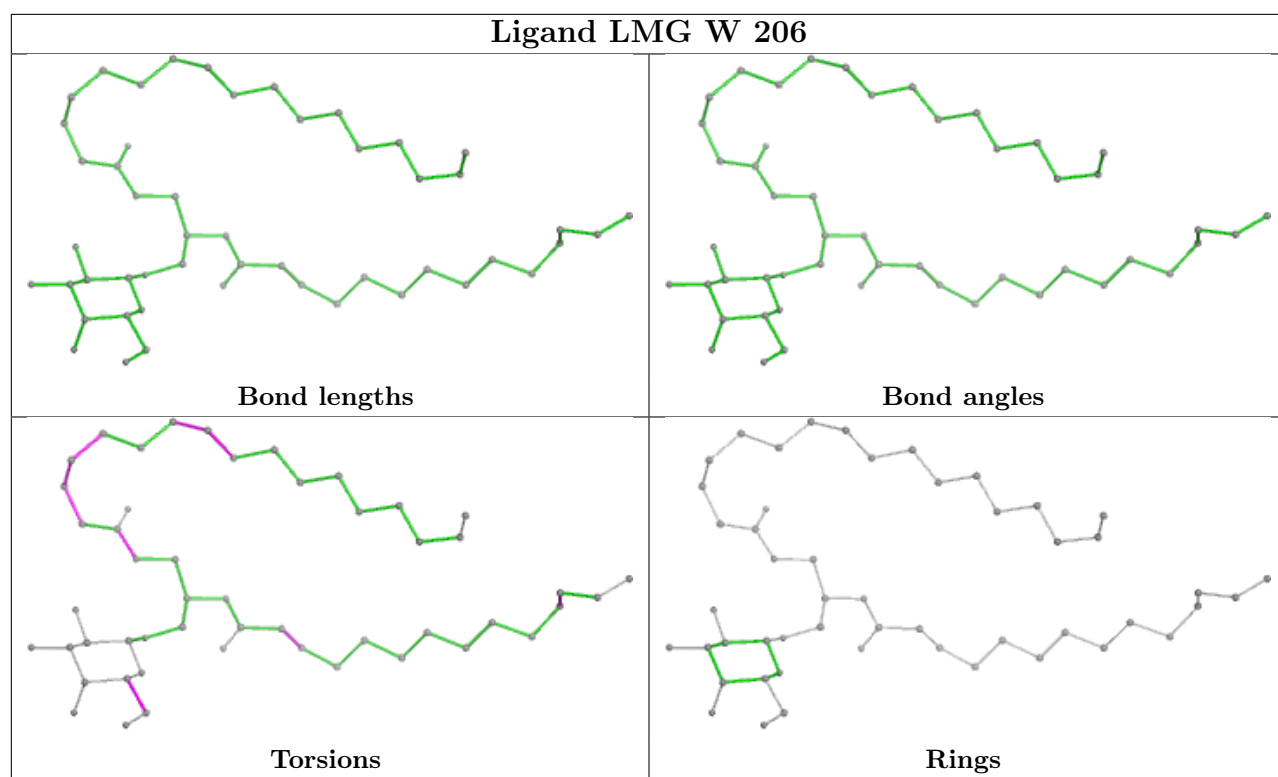
Bond angles



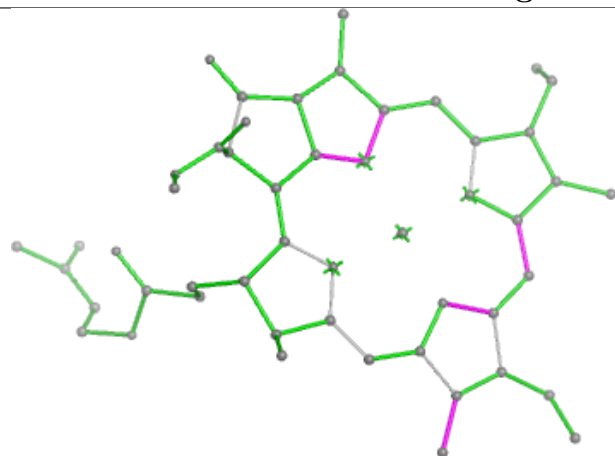
Torsions



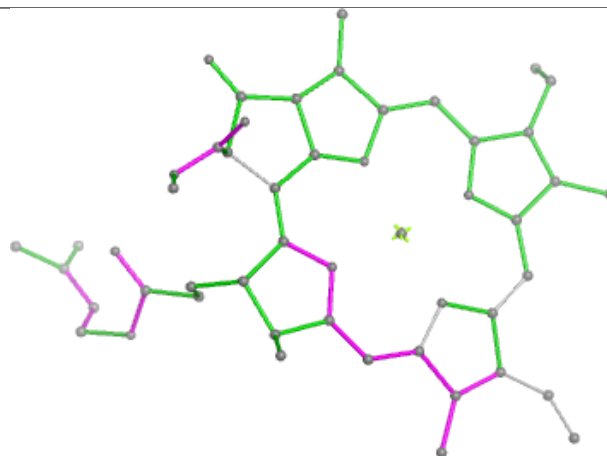
Rings



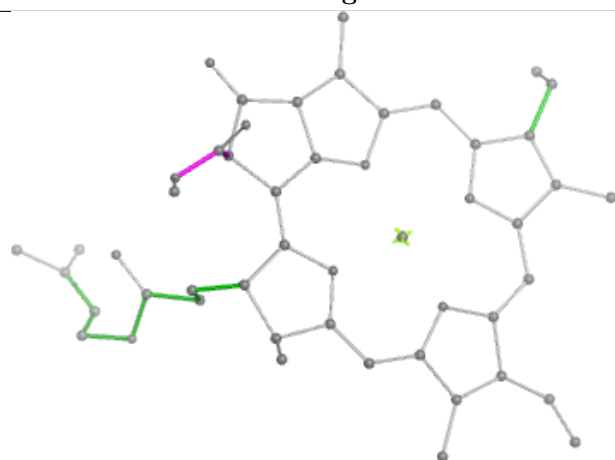
## Ligand CLA A 840



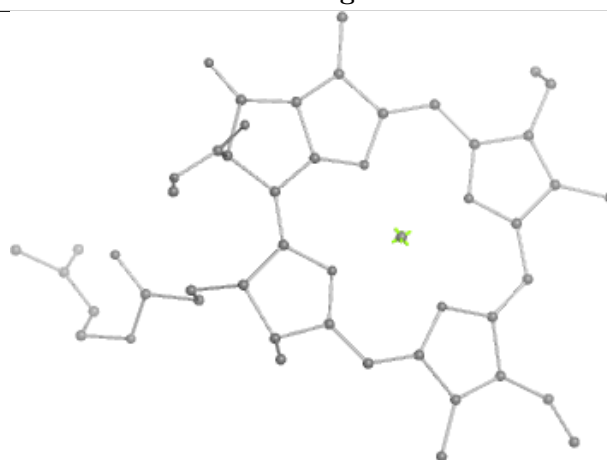
Bond lengths



Bond angles



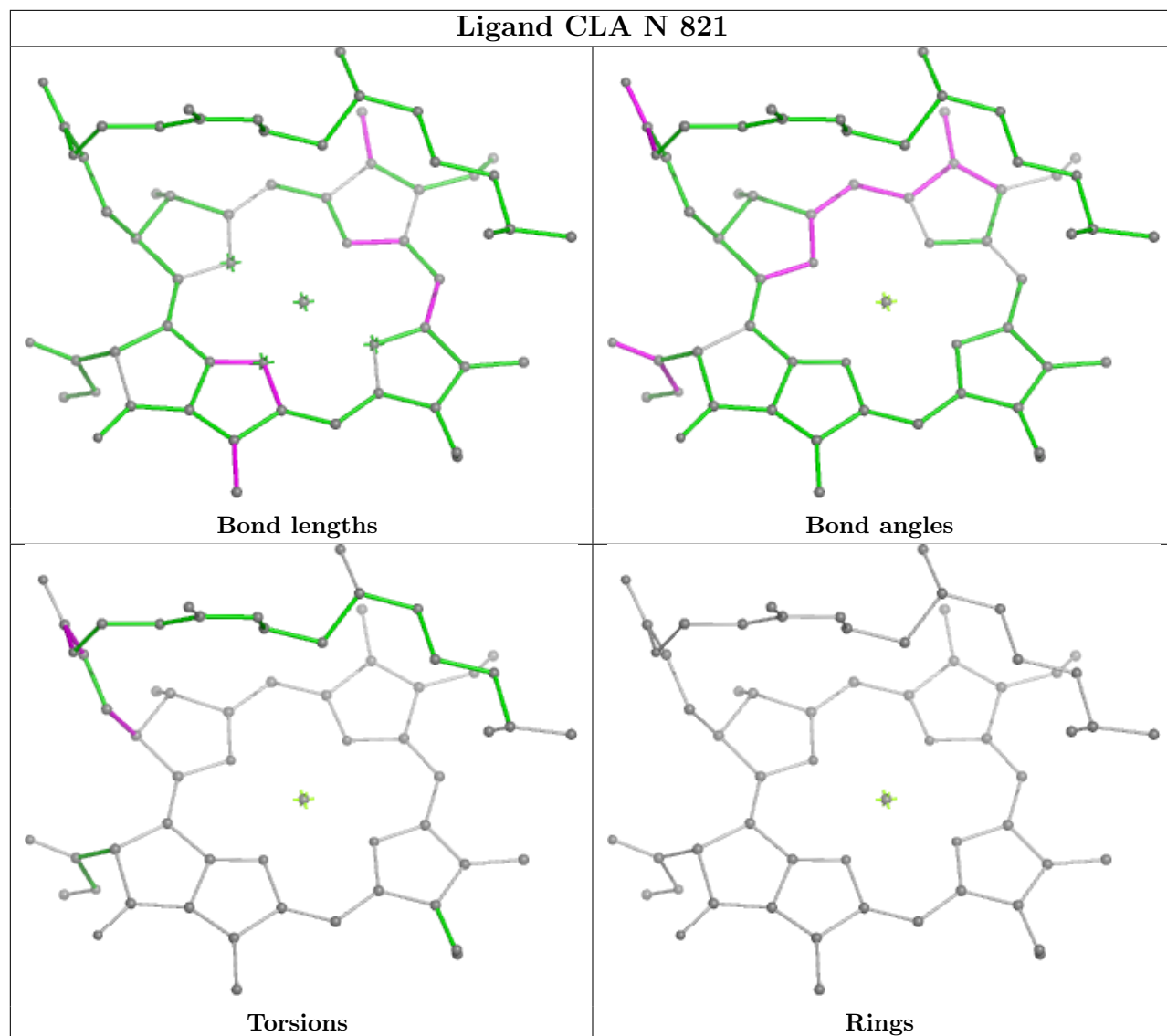
Torsions

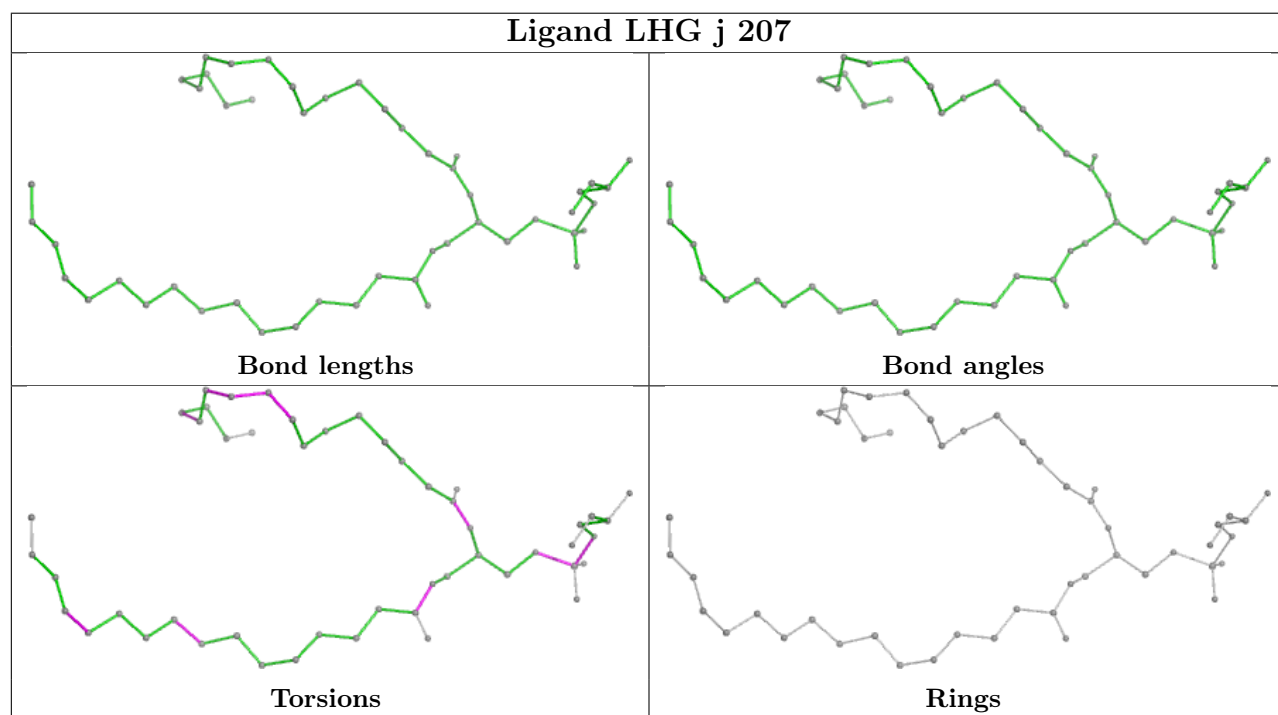
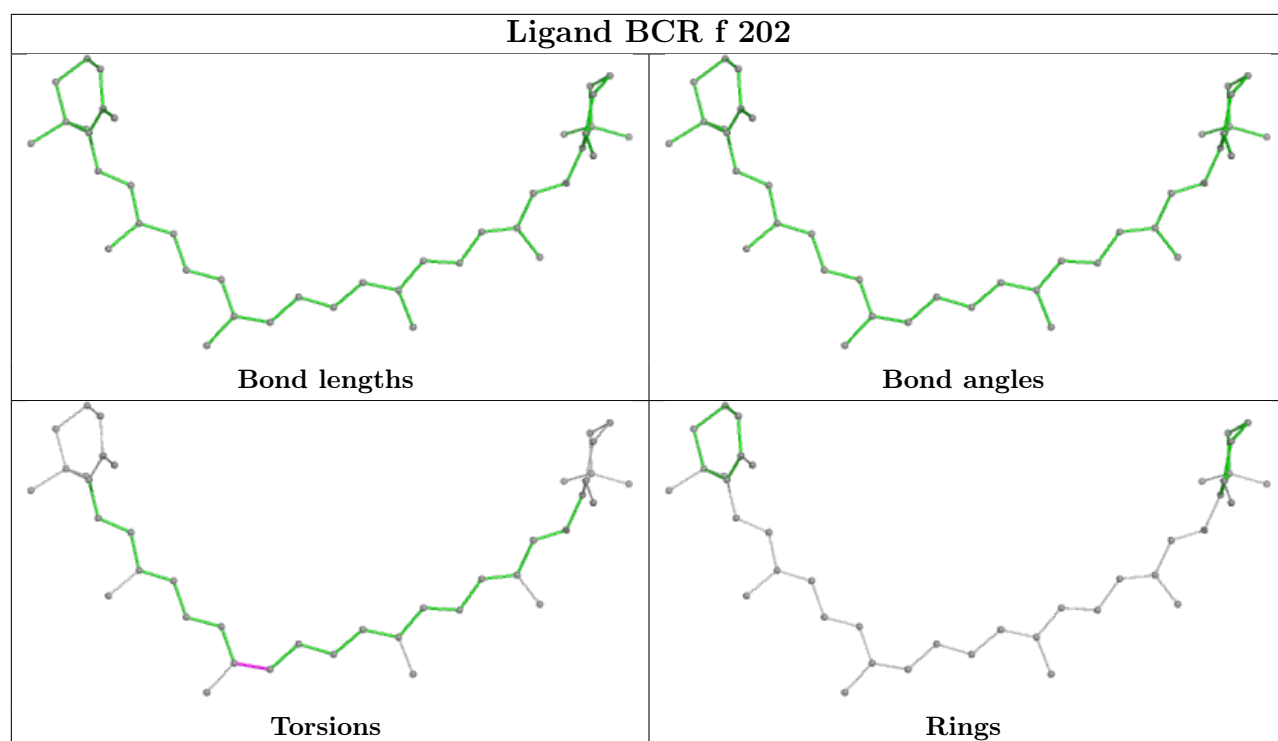


Rings

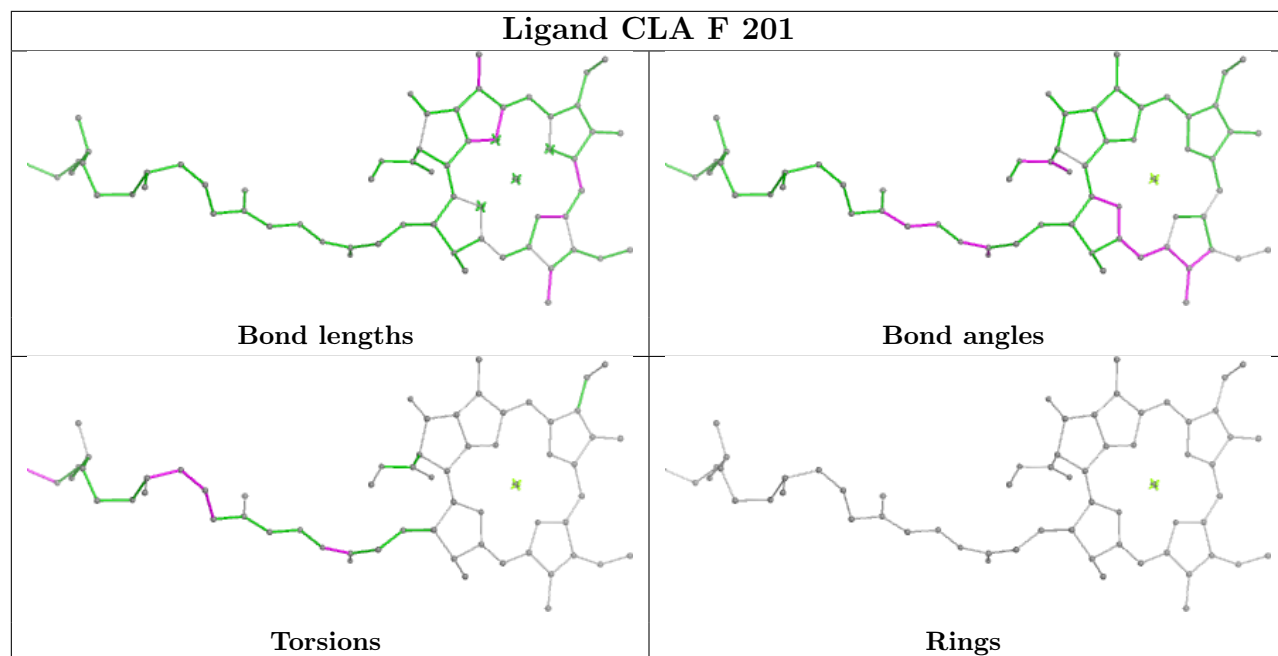


## Ligand CLA N 821

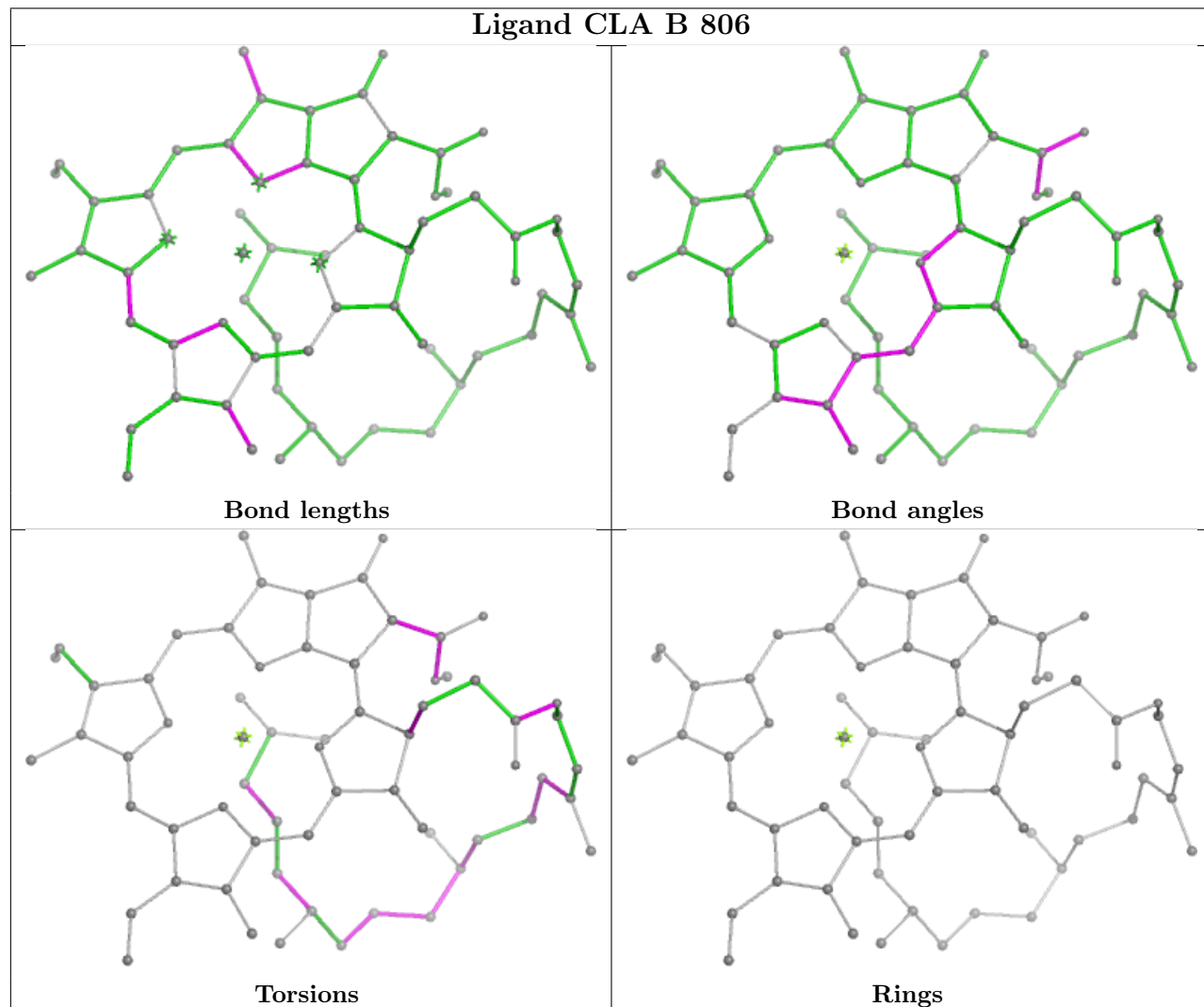


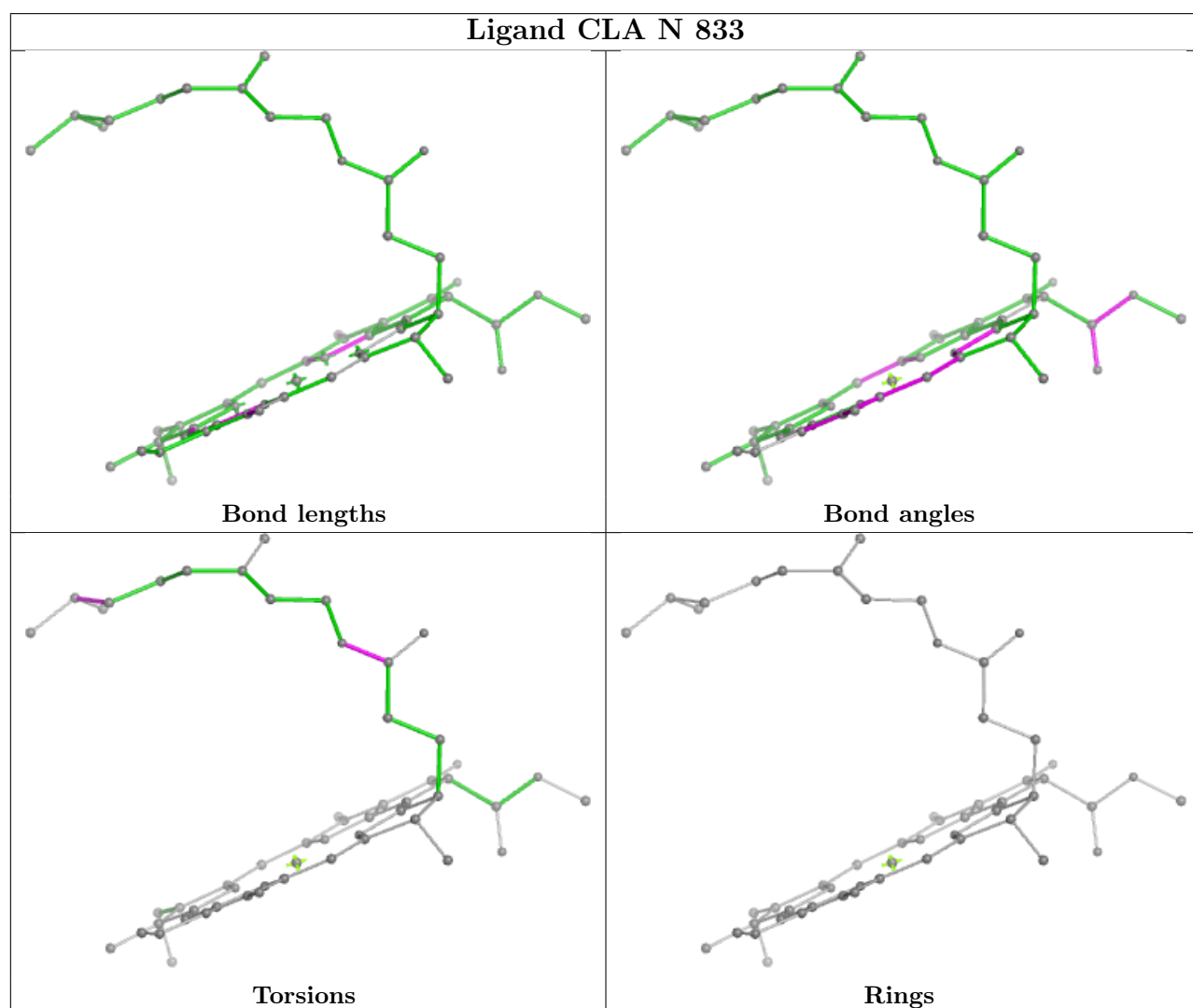
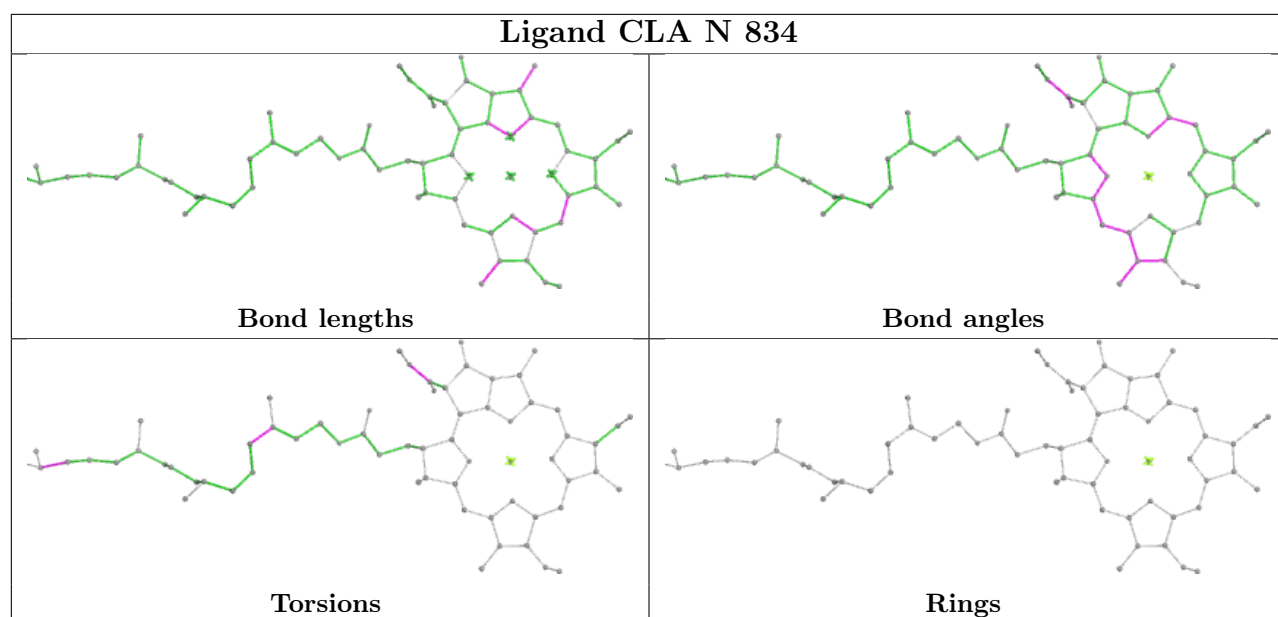


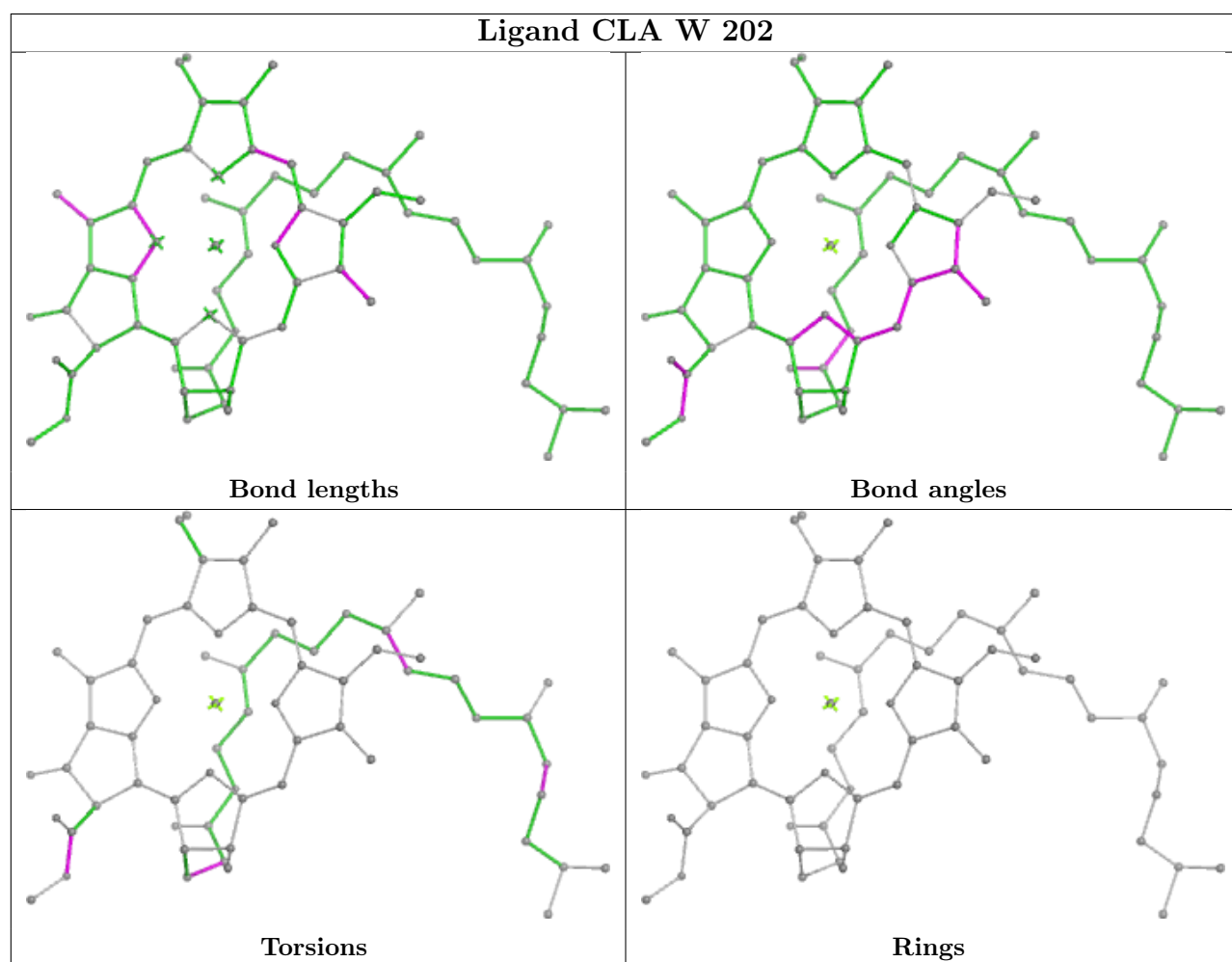
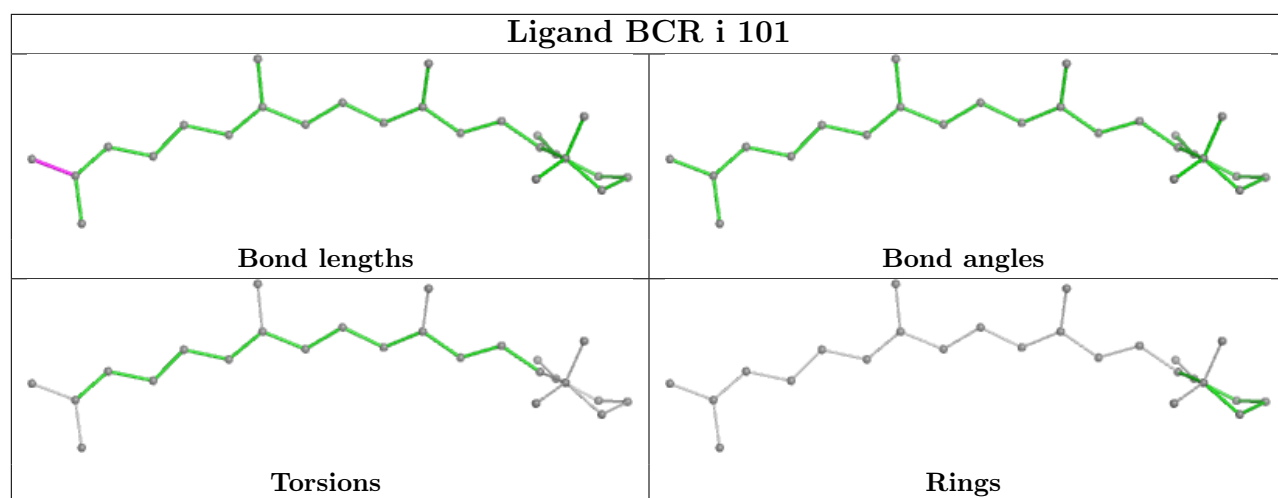
## Ligand CLA F 201



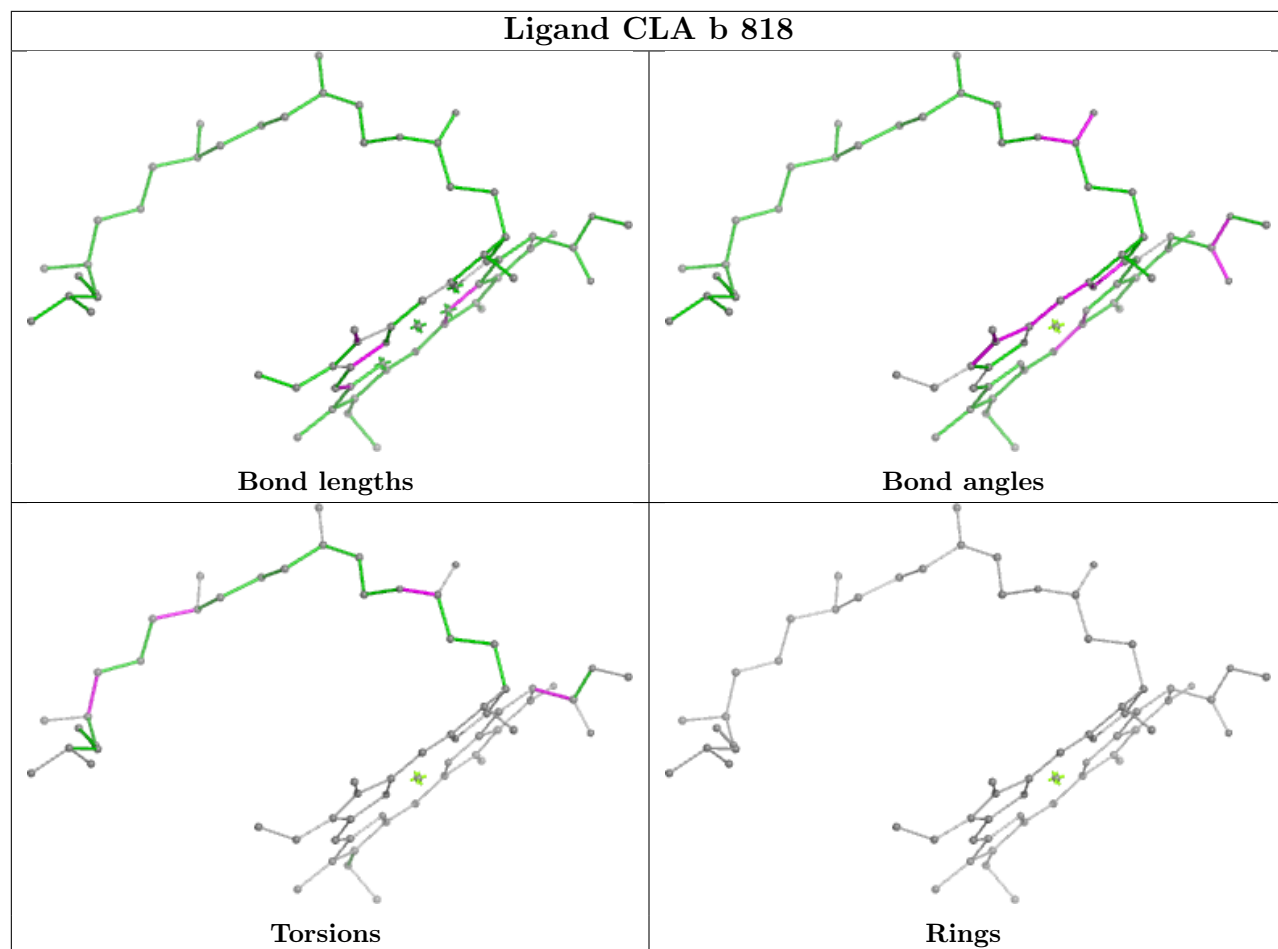
## Ligand CLA B 806



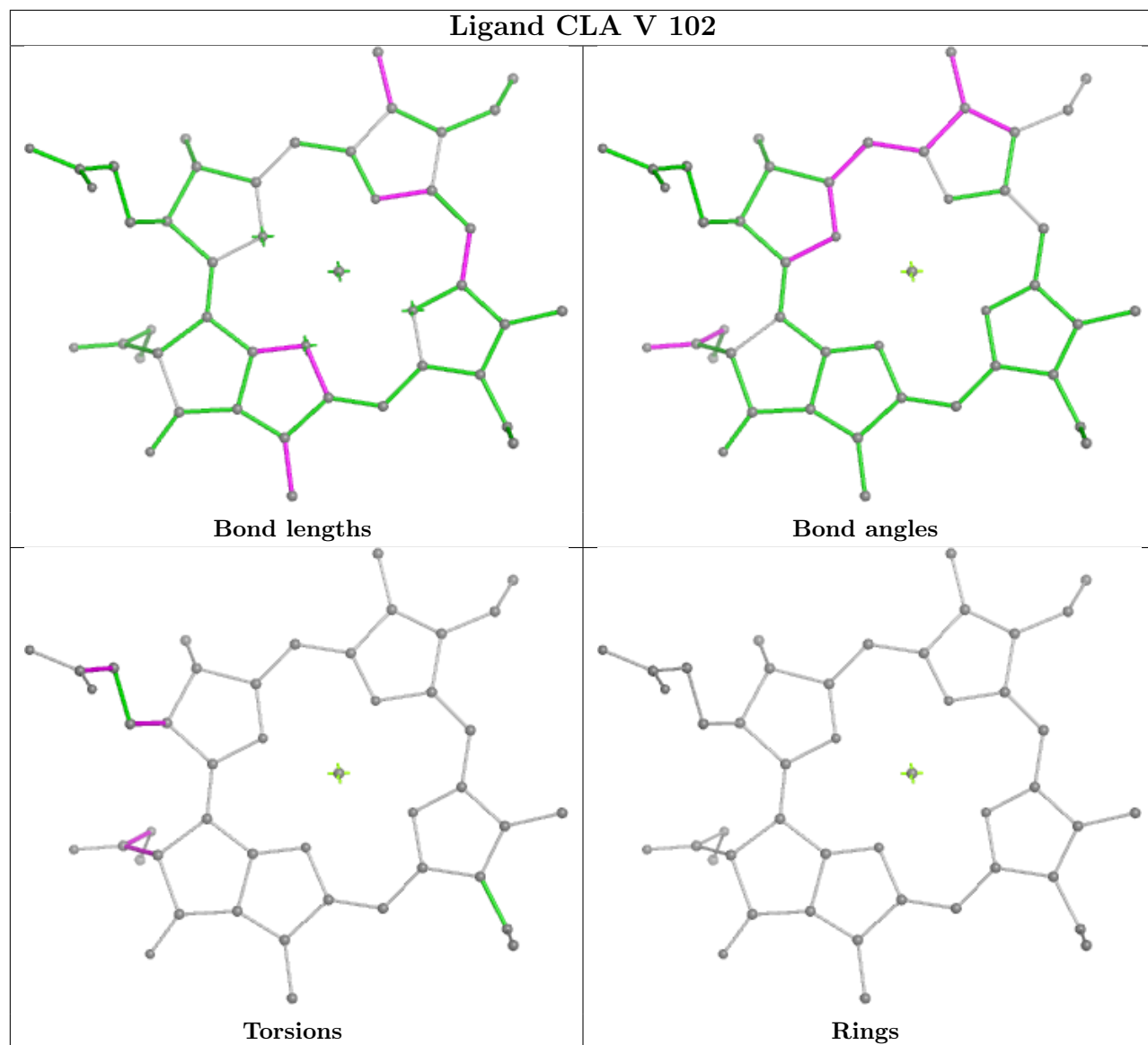




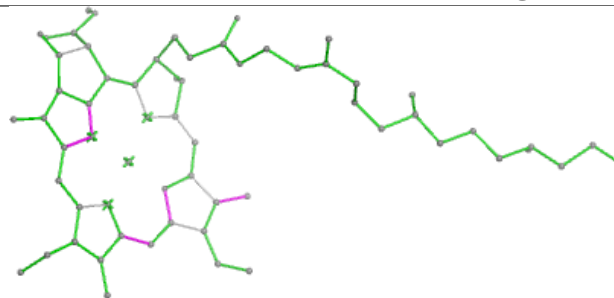
## Ligand CLA b 818



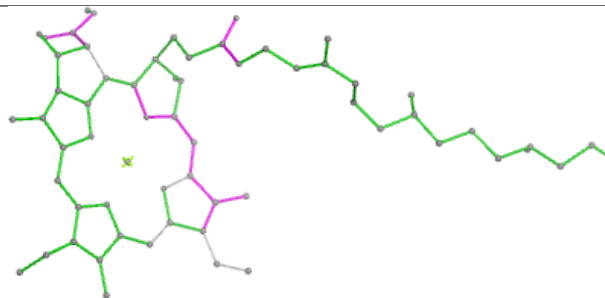
## Ligand CLA V 102



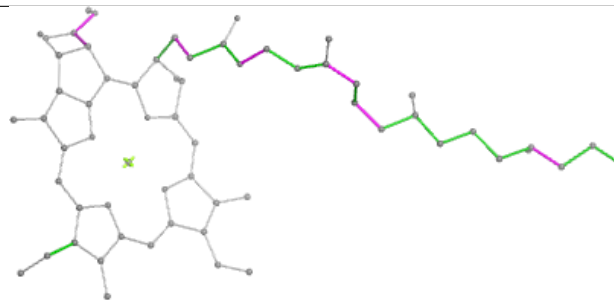
## Ligand CLA A 835



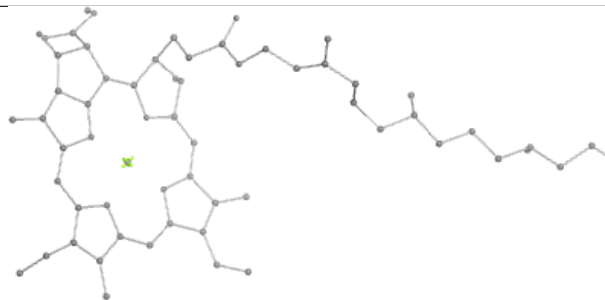
Bond lengths



Bond angles

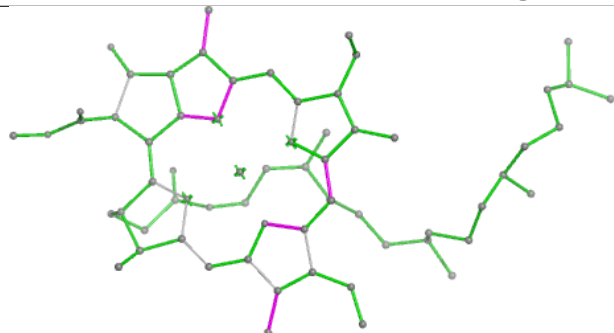


Torsions

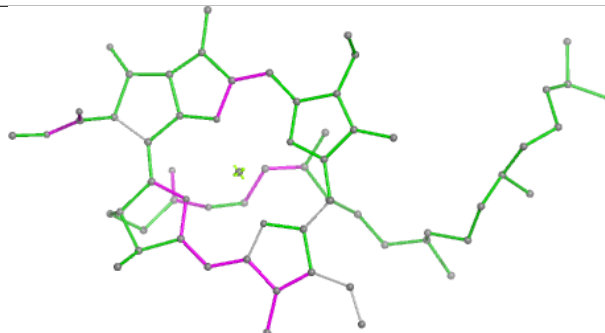


Rings

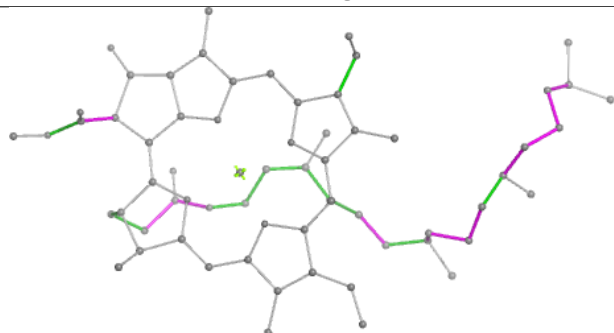
## Ligand CLA B 837



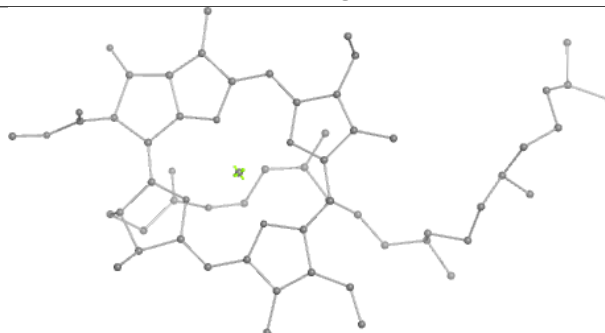
Bond lengths



Bond angles



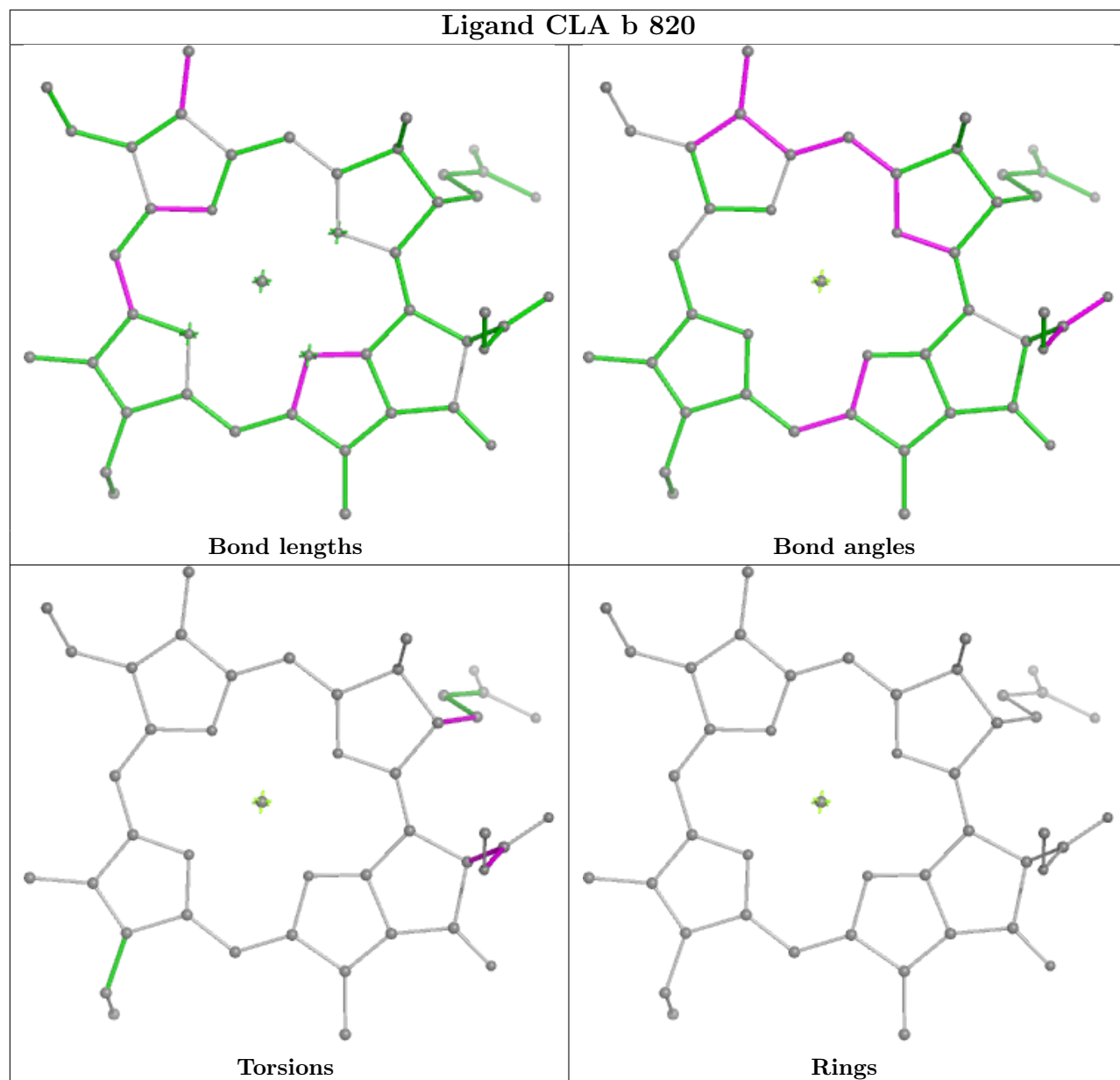
Torsions

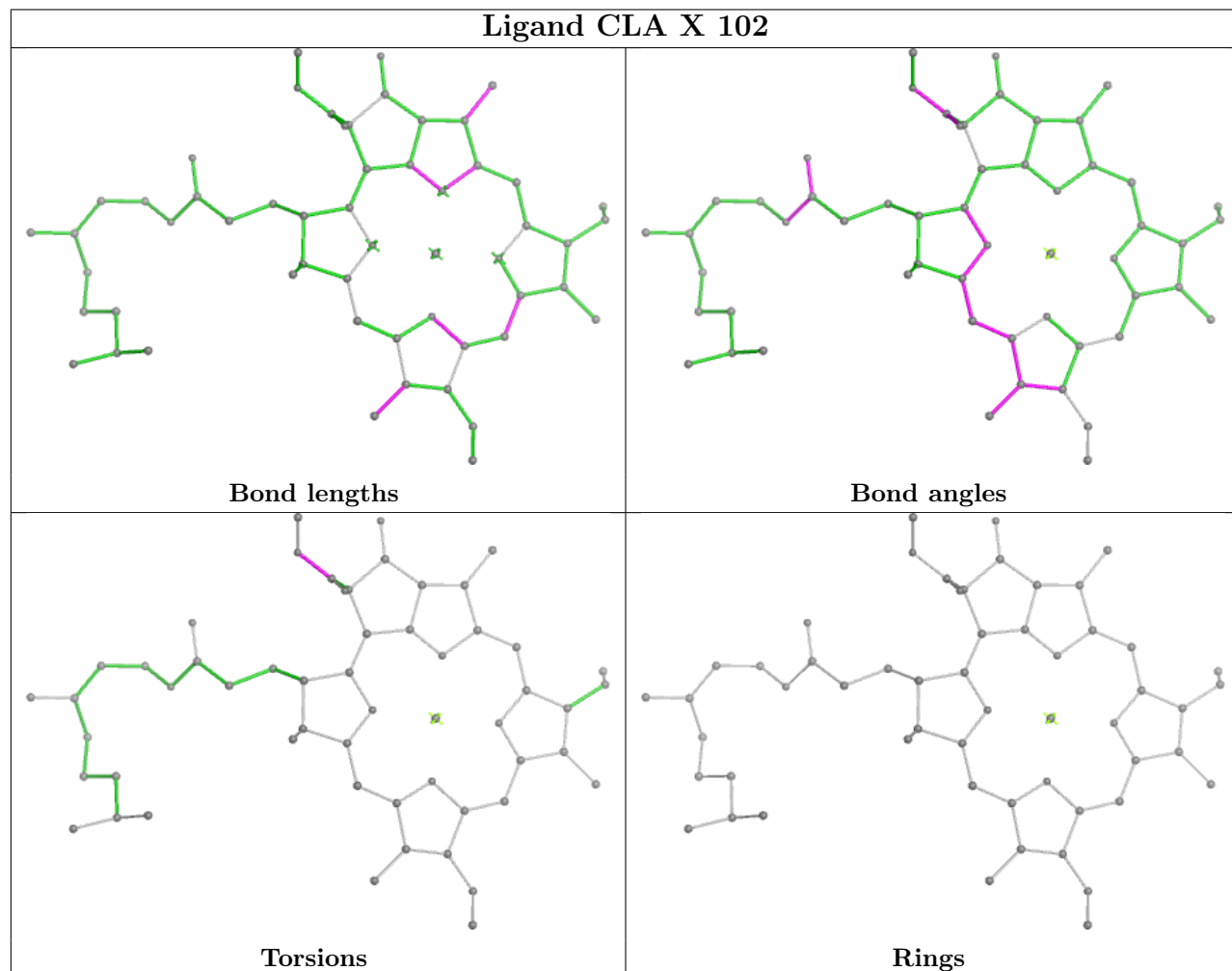
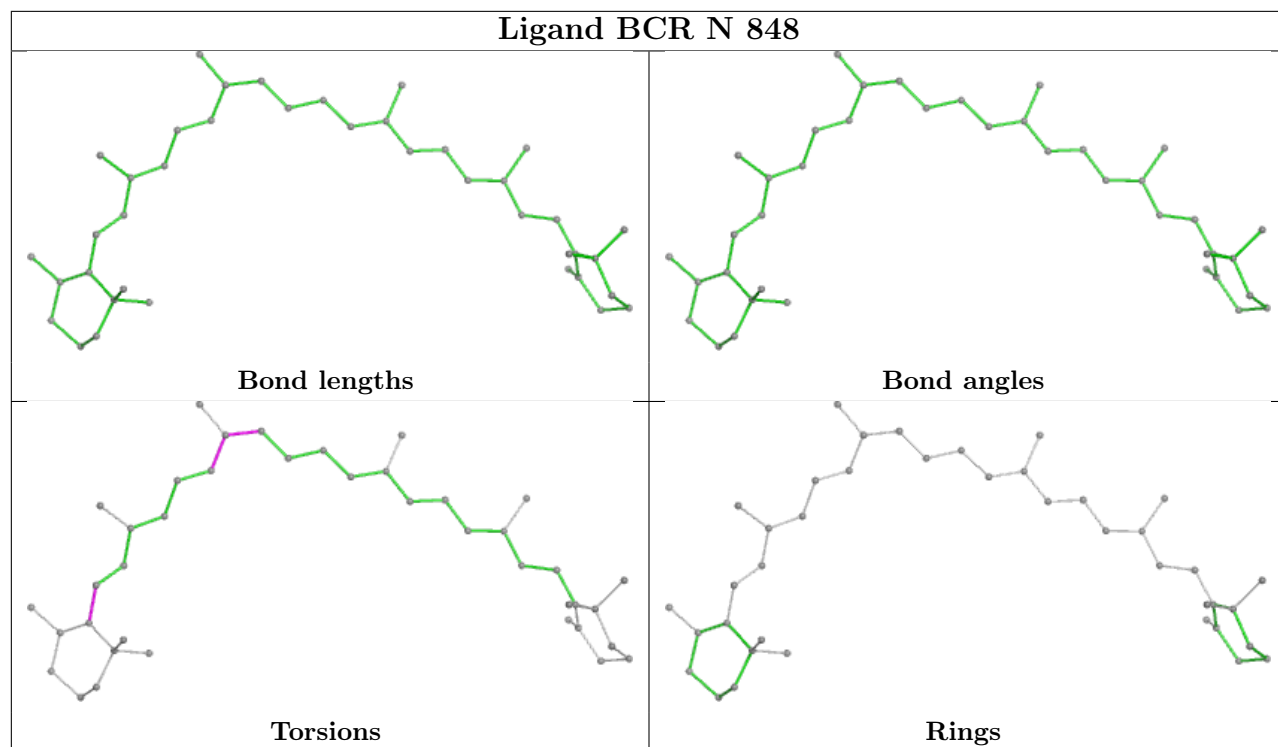


Rings

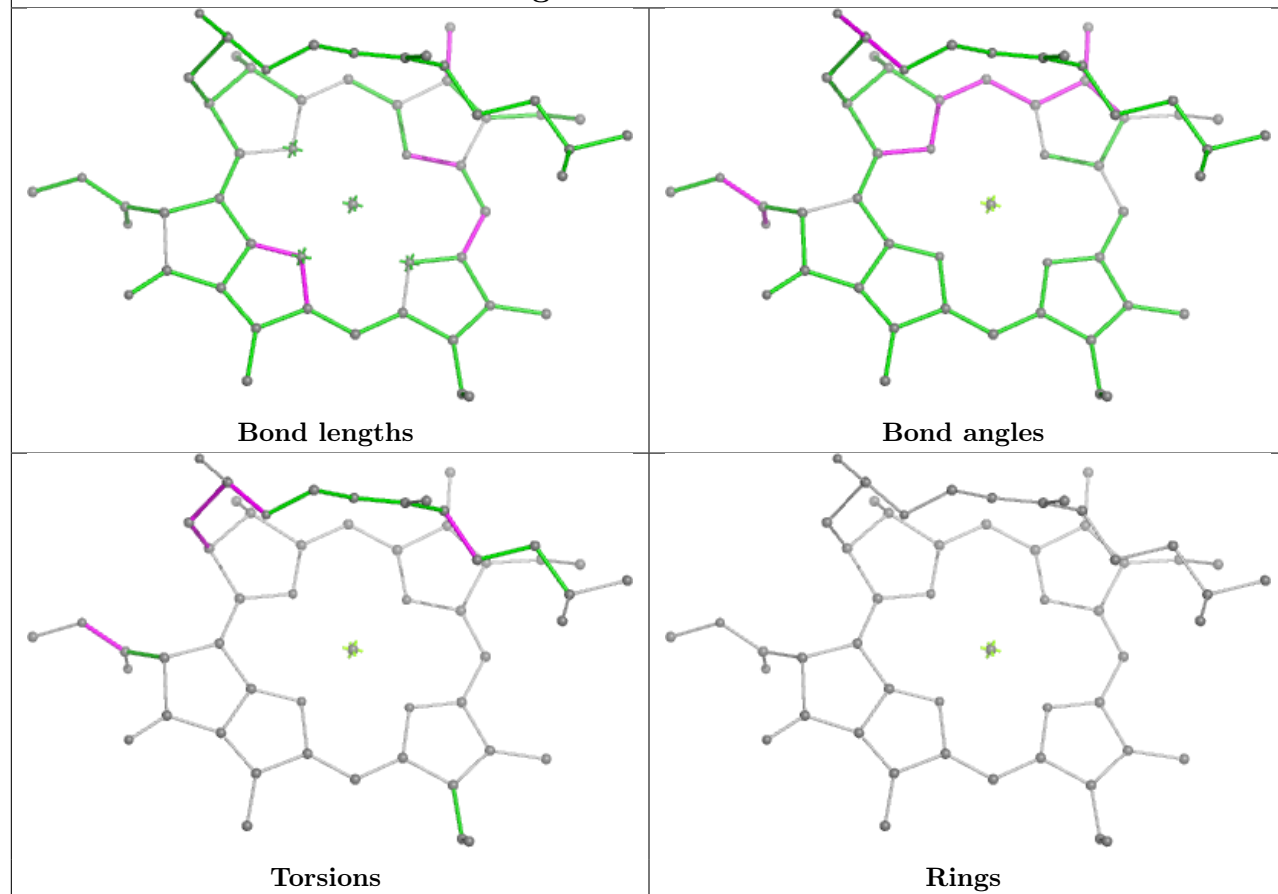


## Ligand CLA b 820

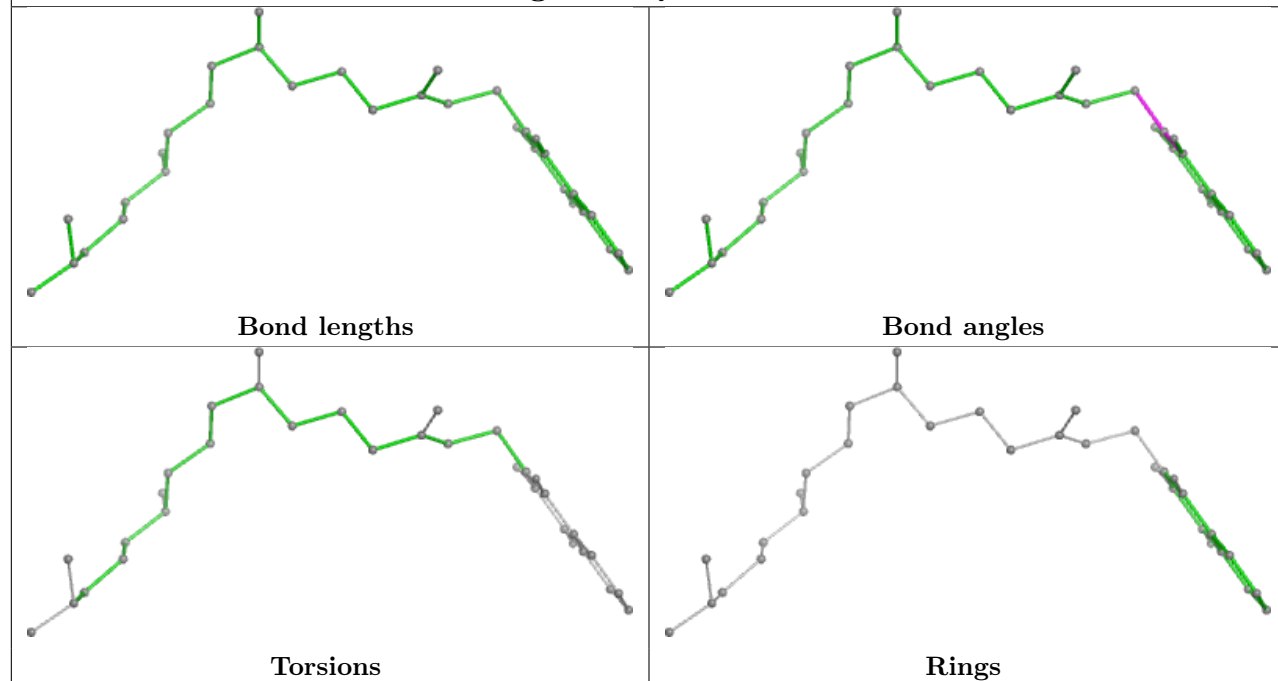


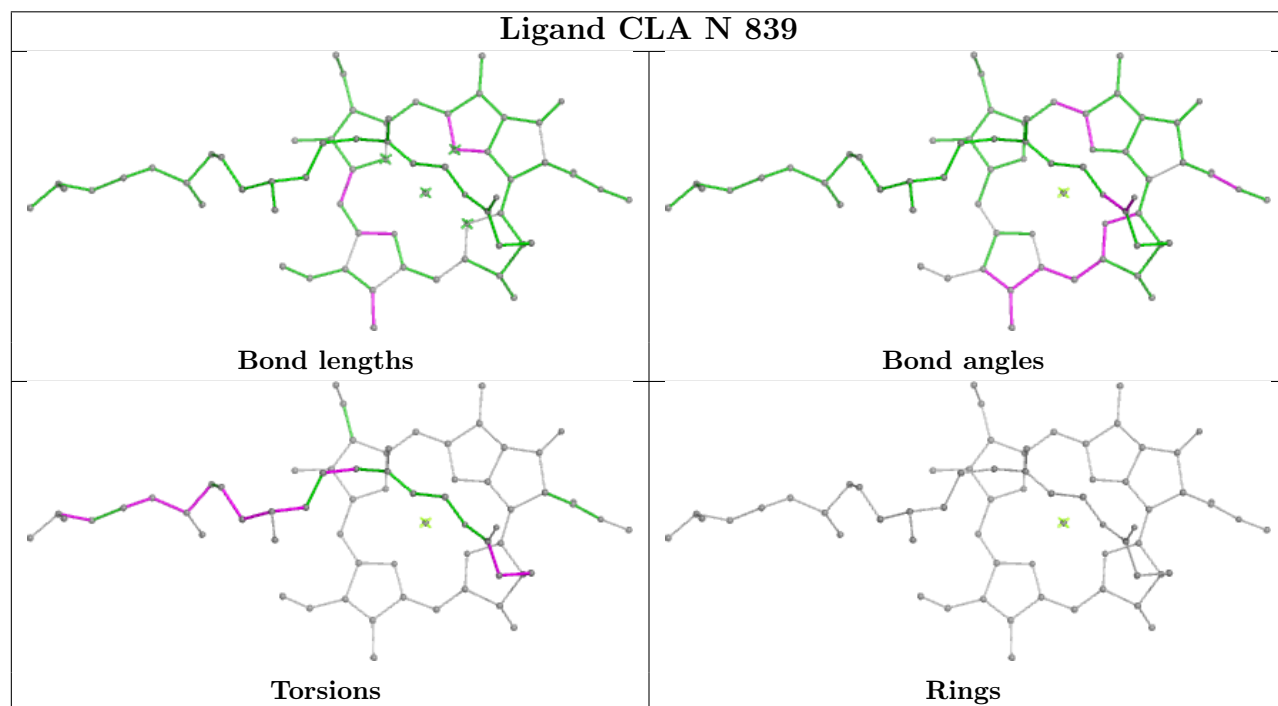
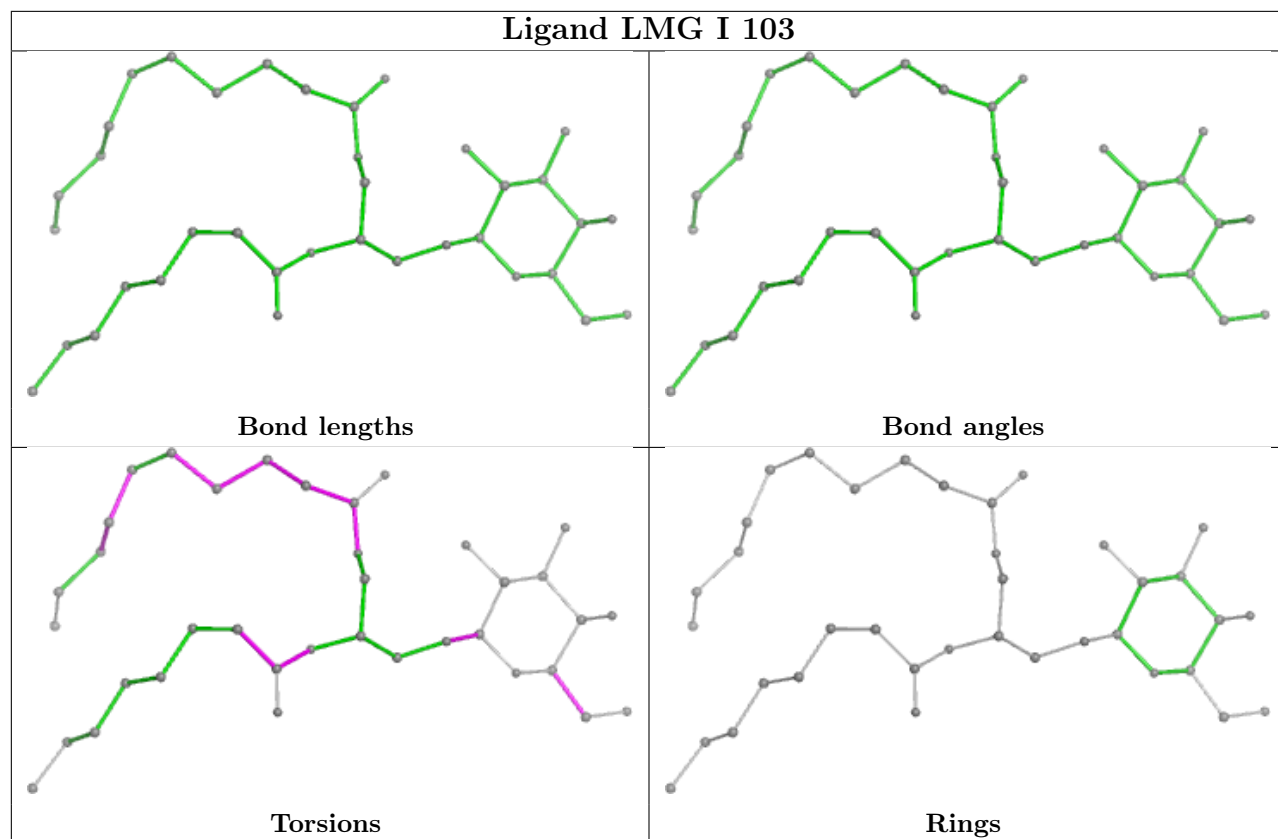


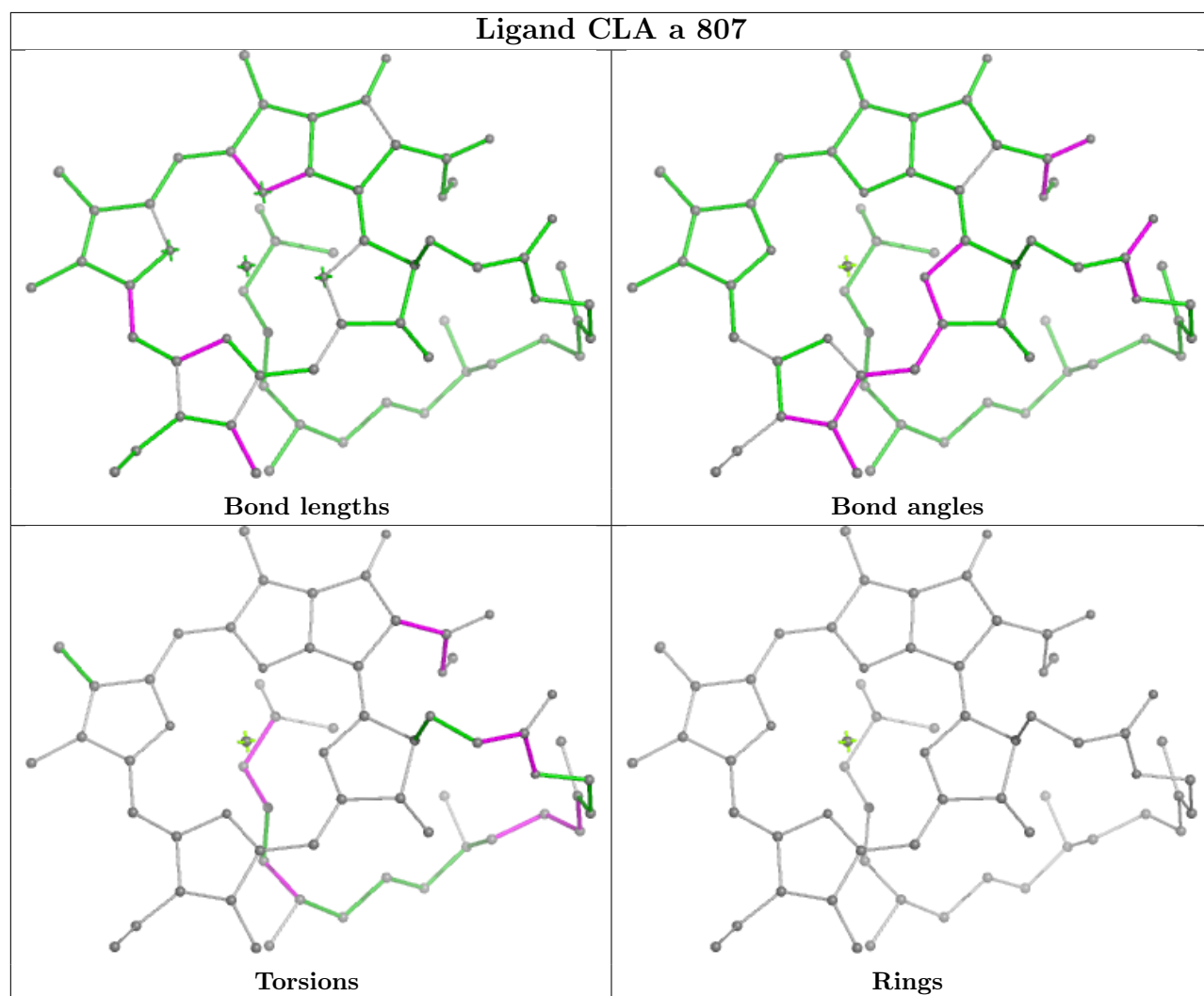
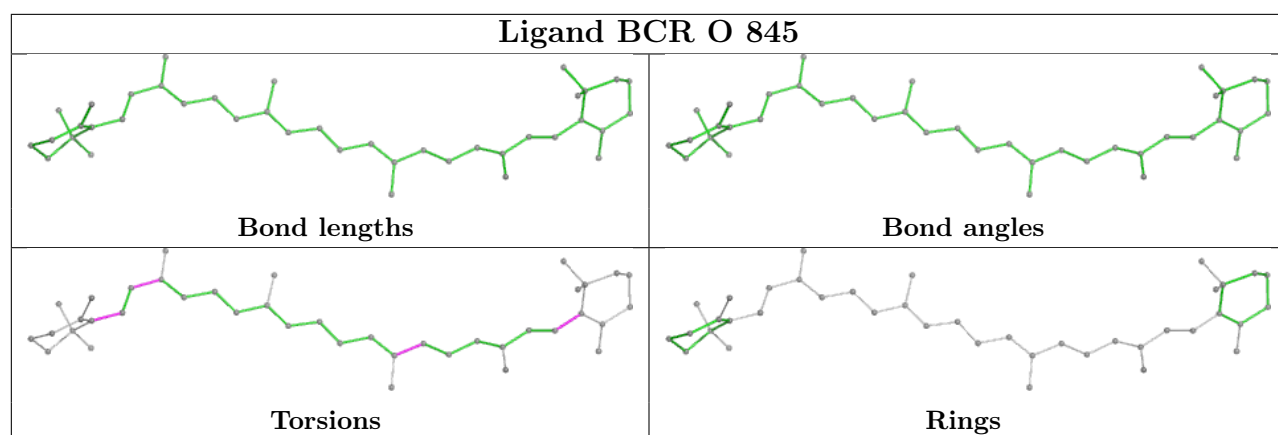
## Ligand CLA B 819

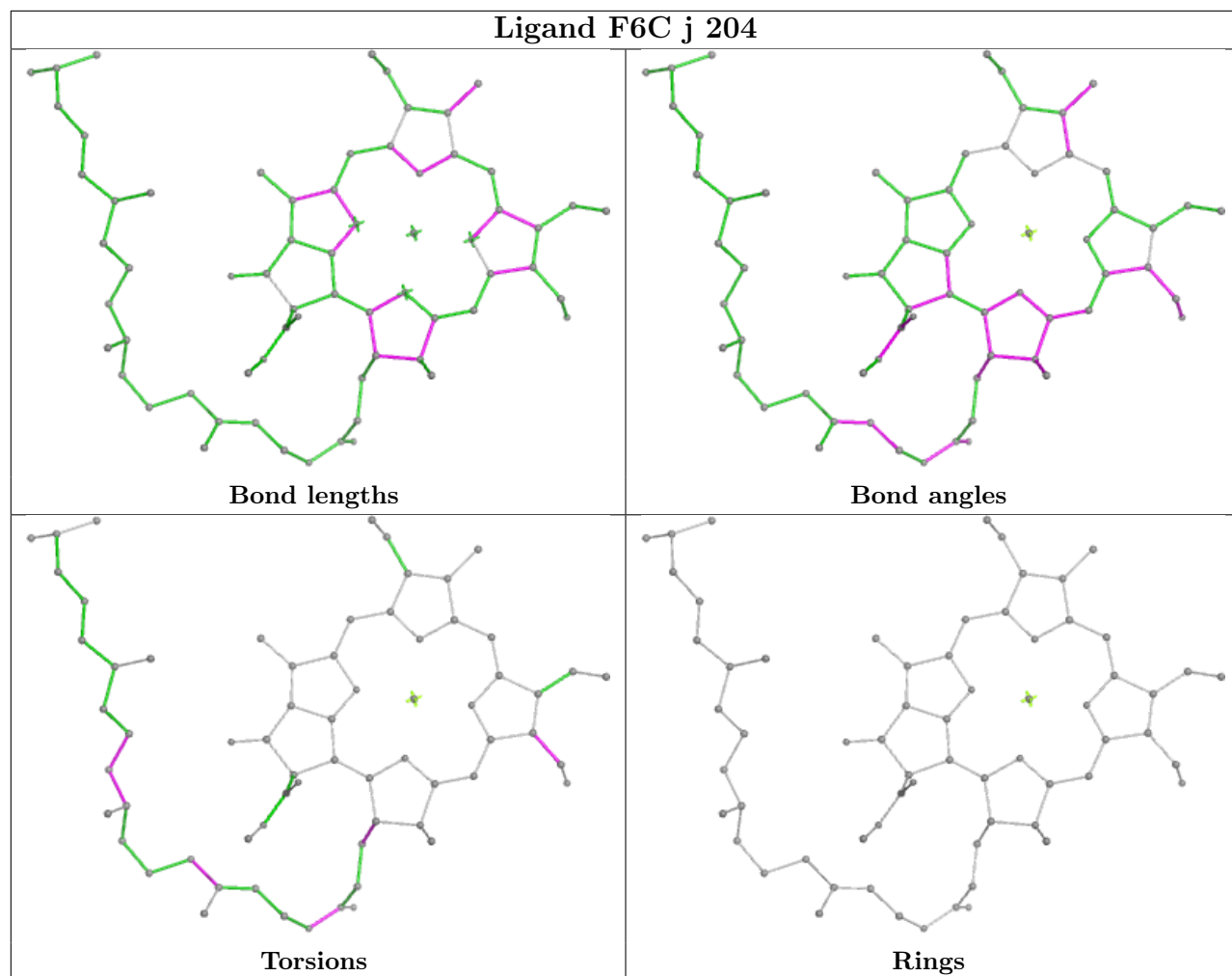


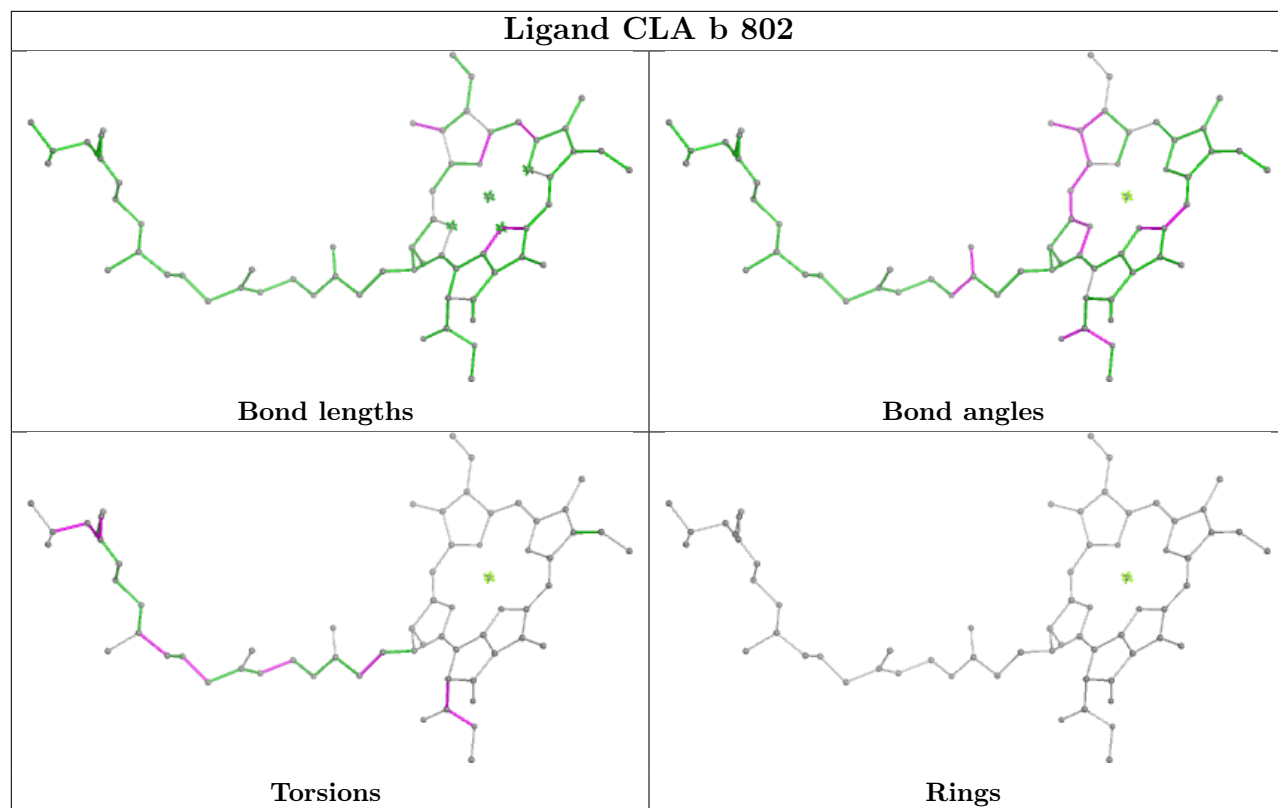
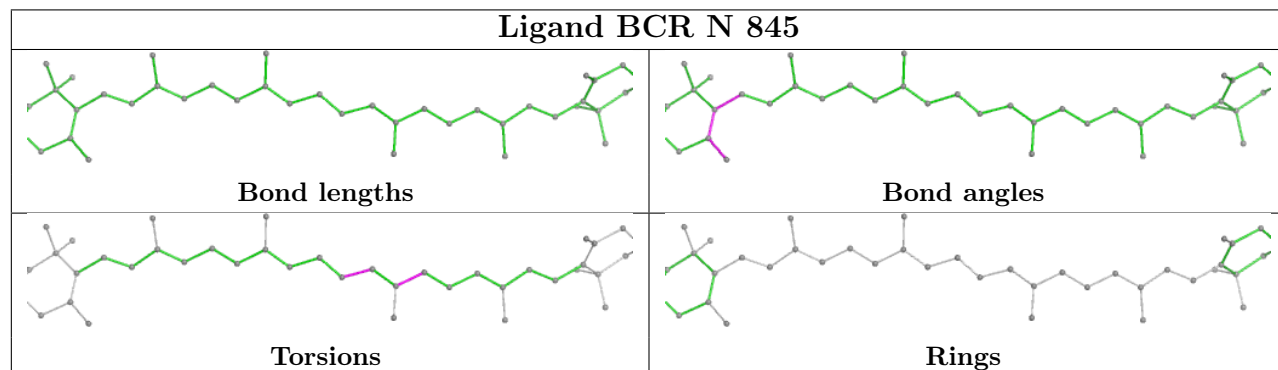
## Ligand PQN O 841



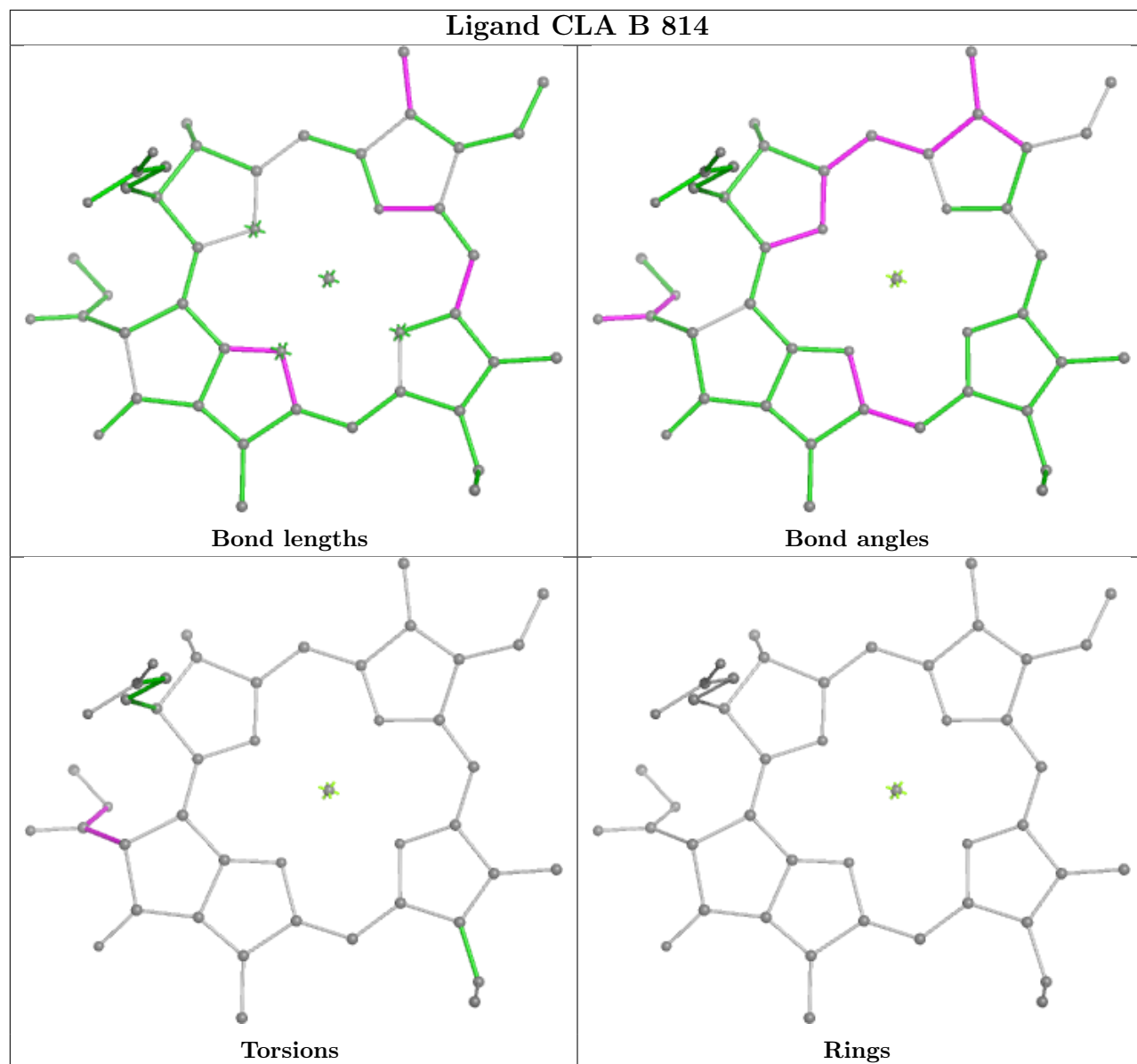




**Ligand F6C j 204**

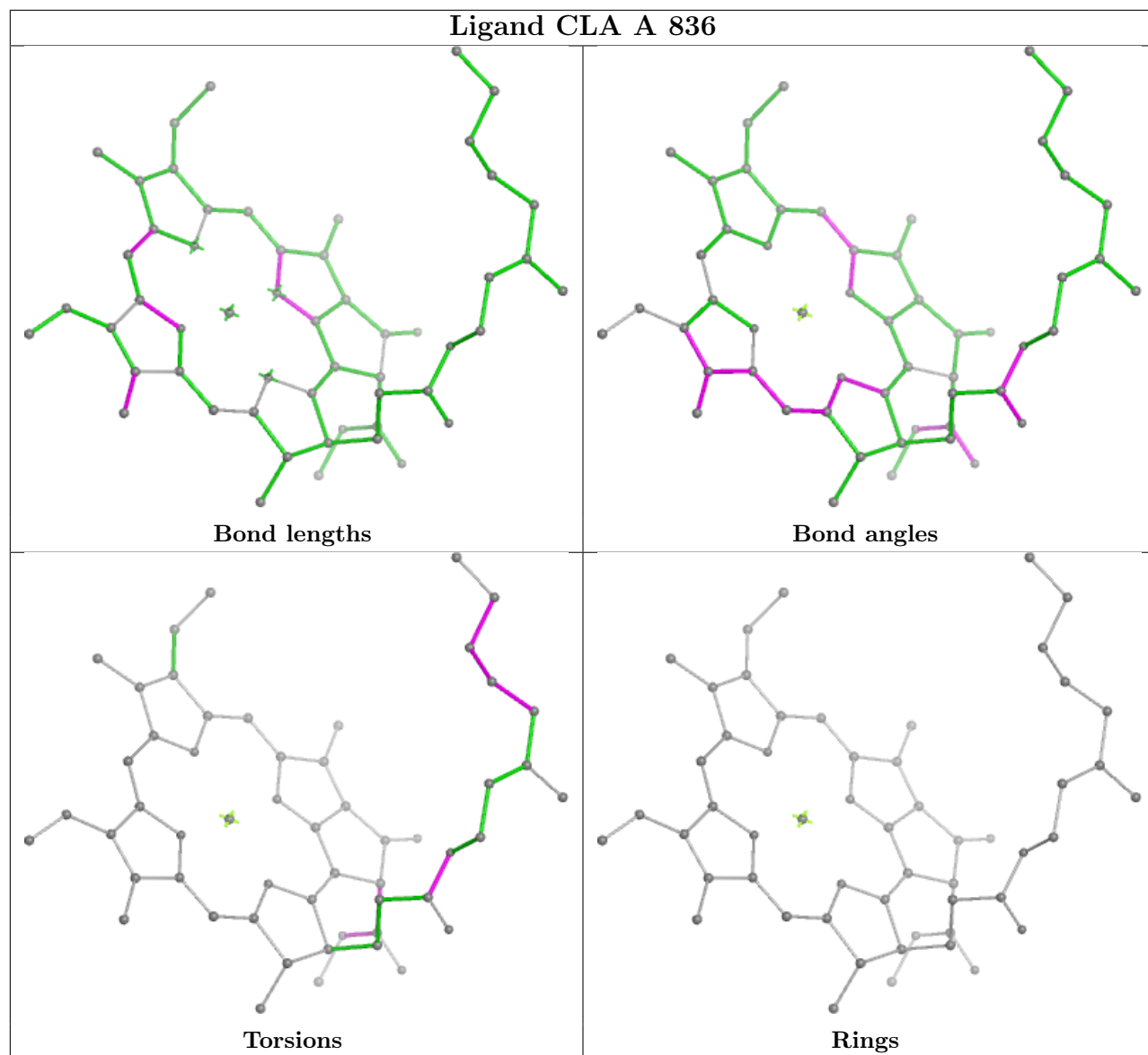
**Ligand CLA b 802****Ligand BCR N 845**

## Ligand CLA B 814

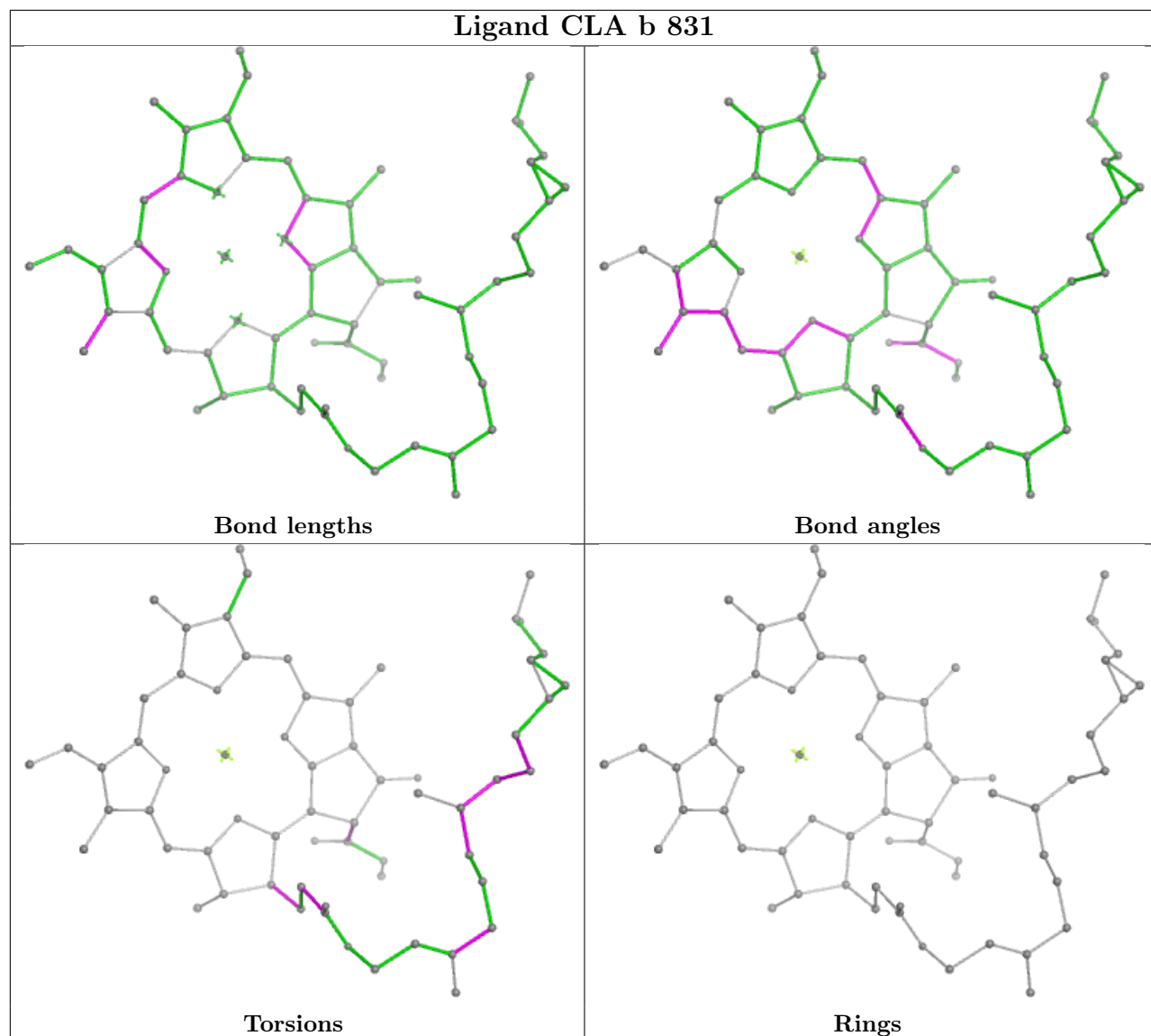




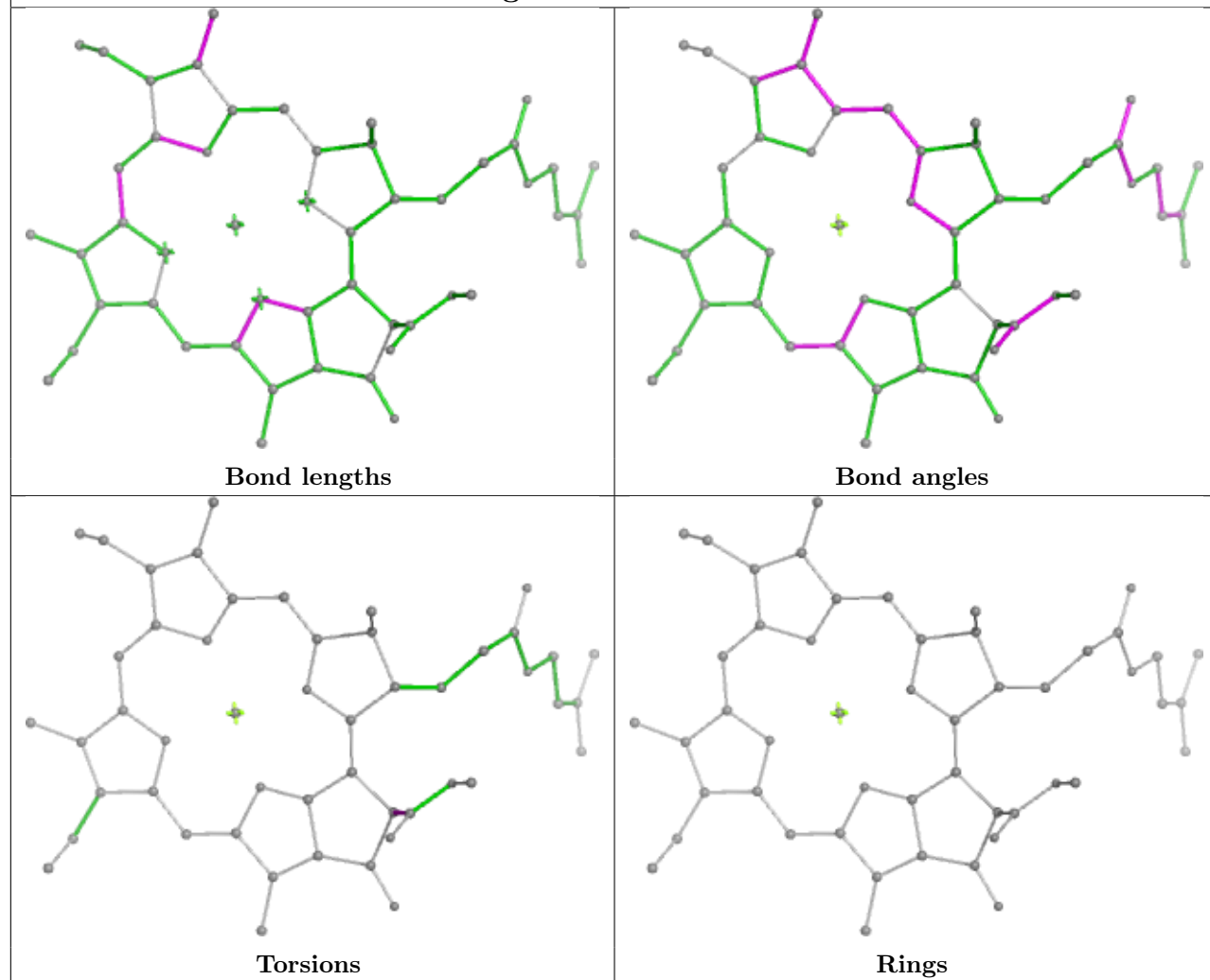
## Ligand CLA A 836

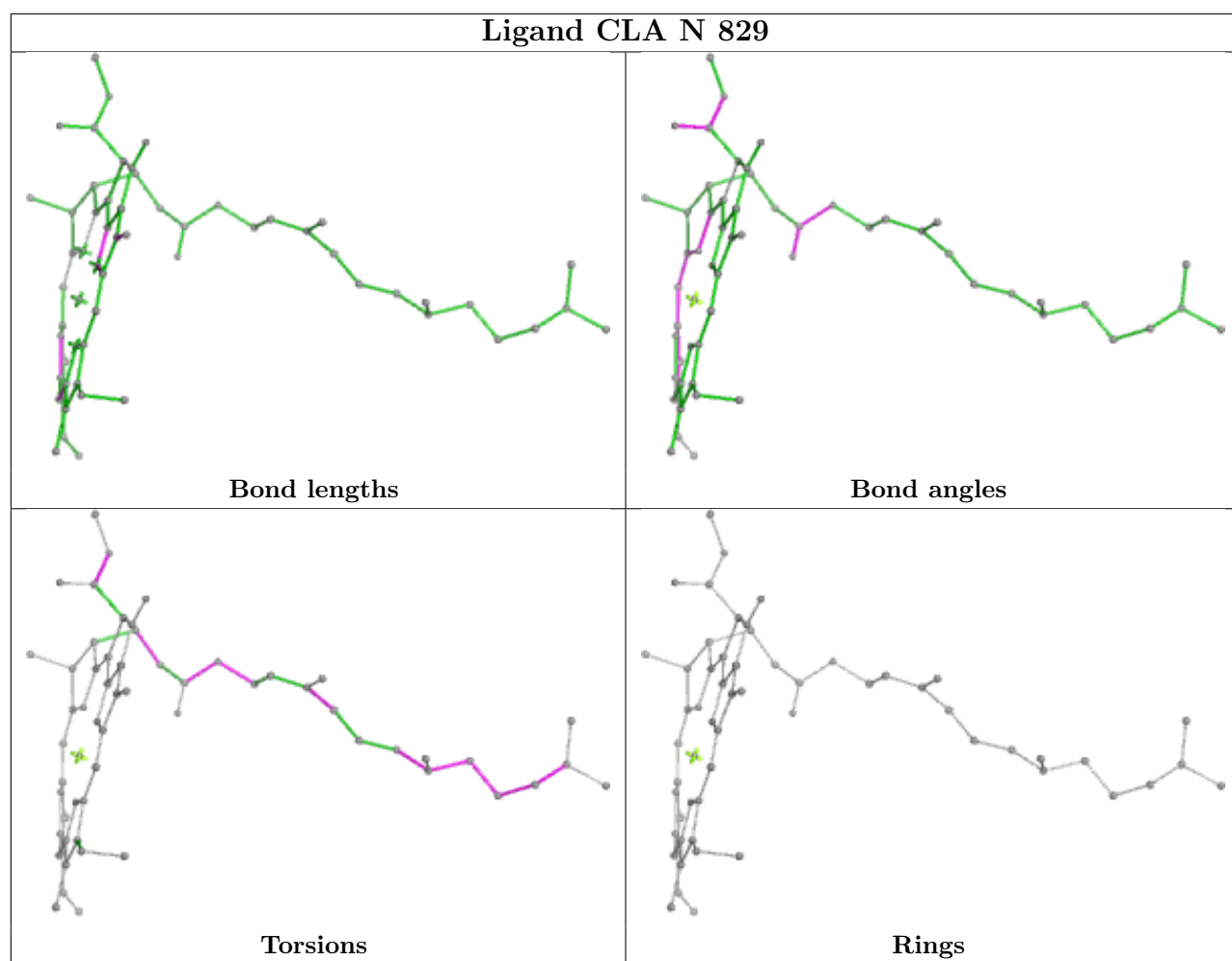


## Ligand CLA b 831

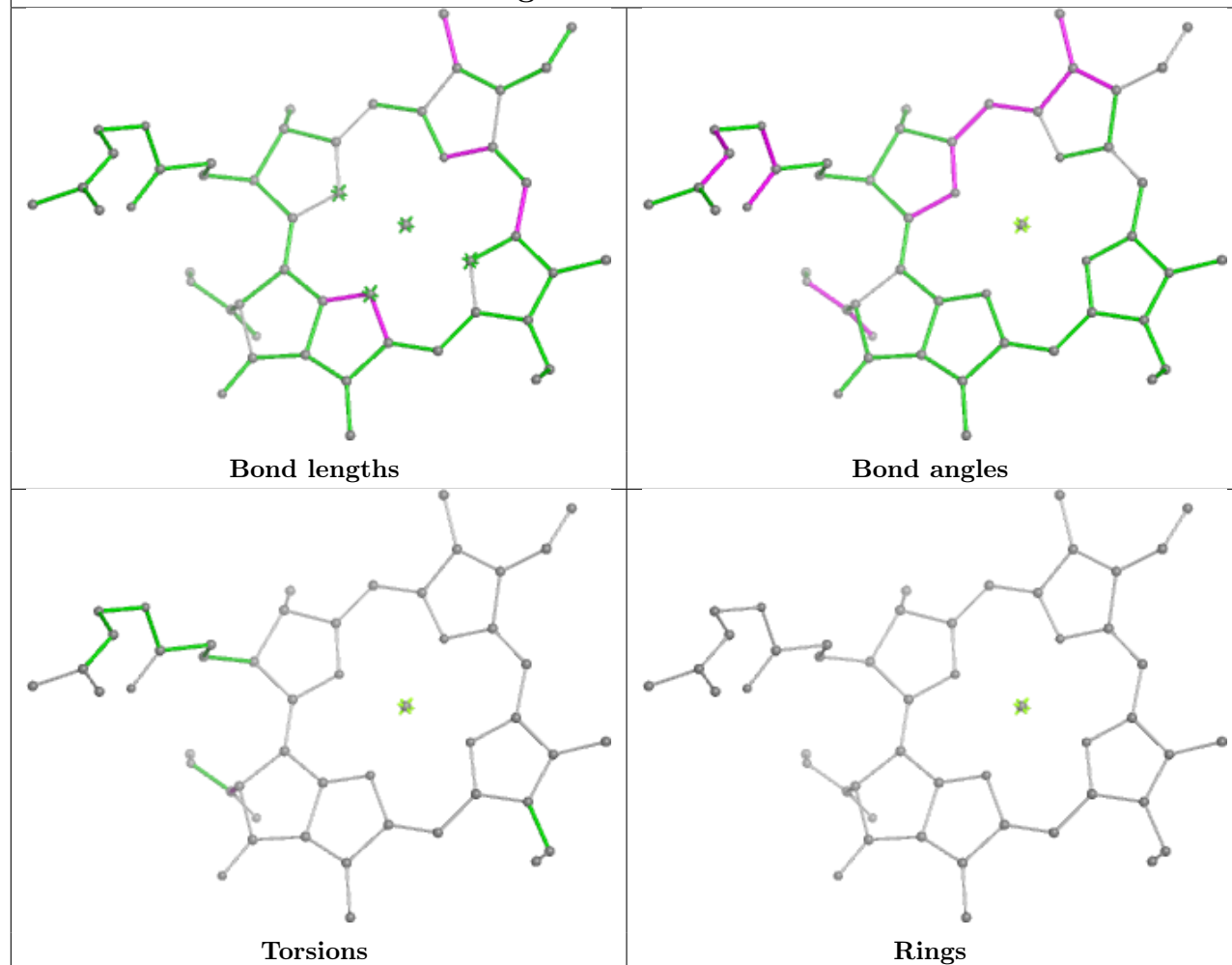


## Ligand CLA K 103

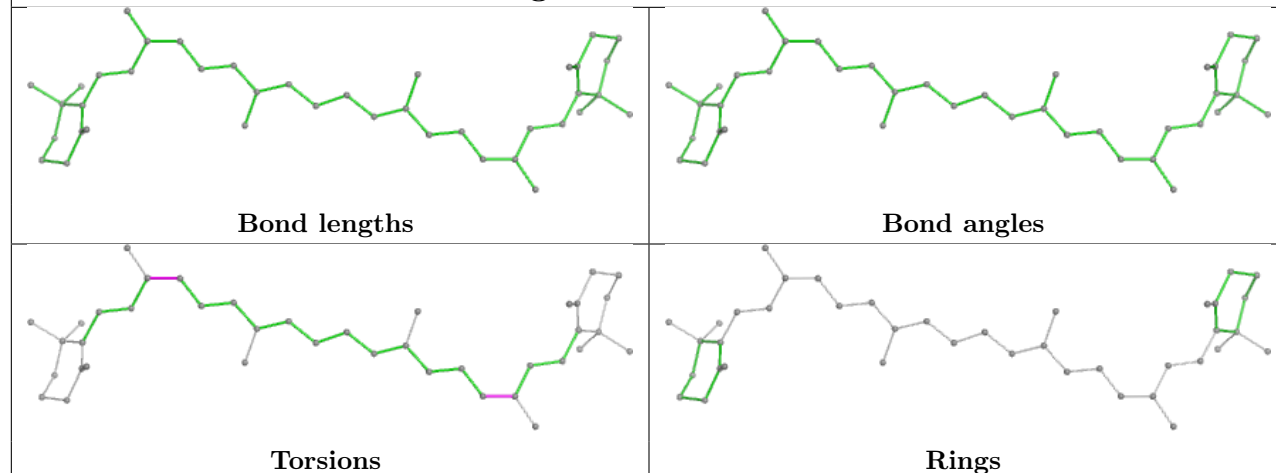


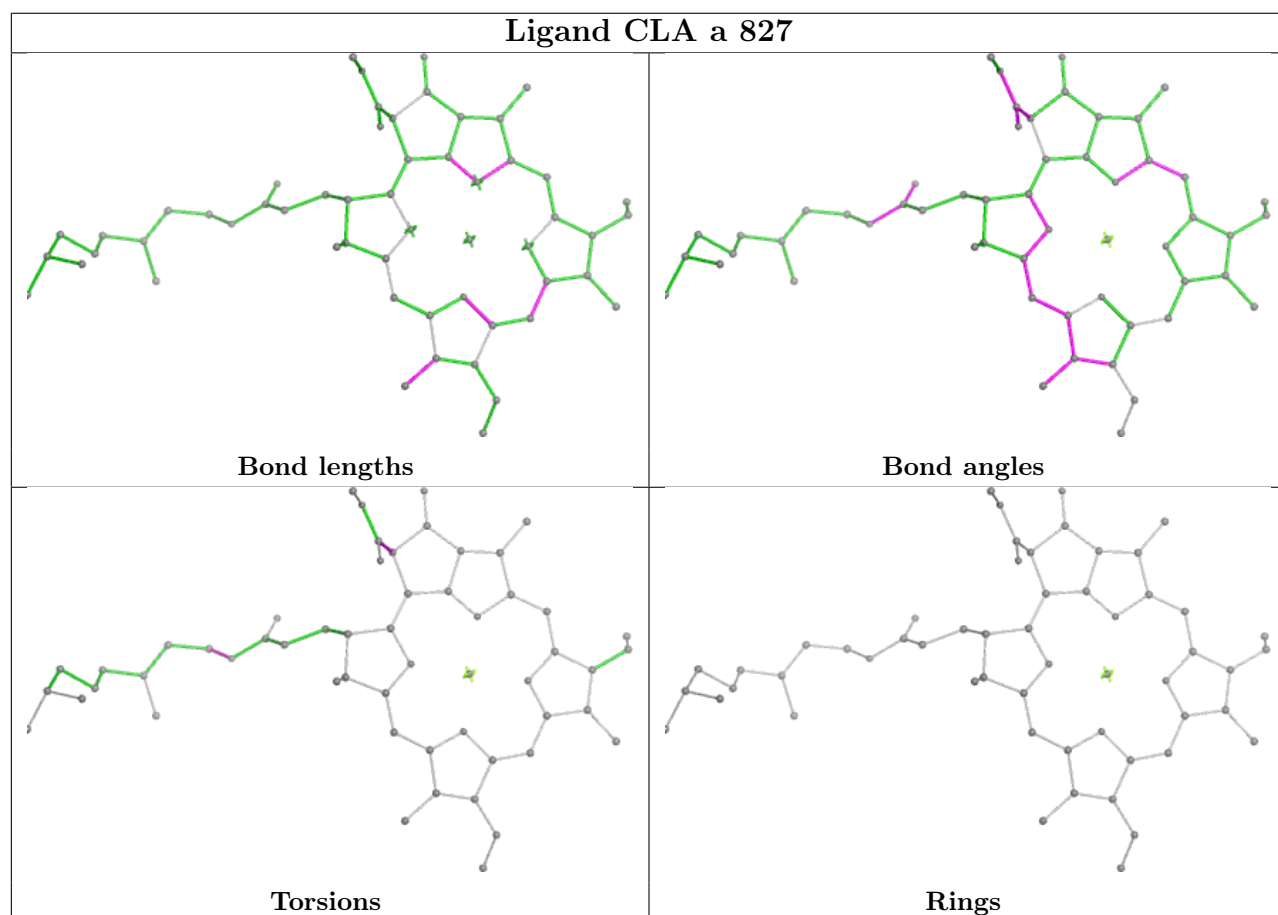
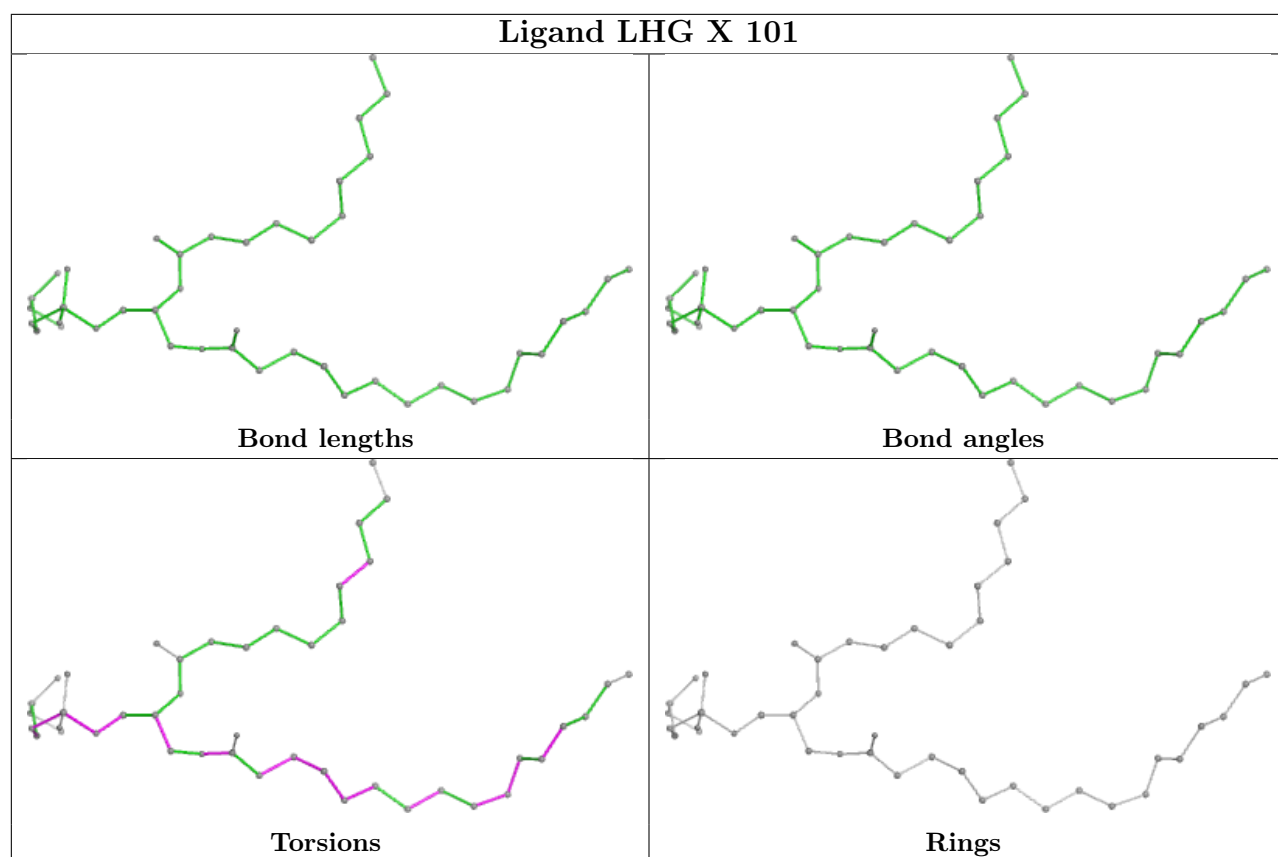


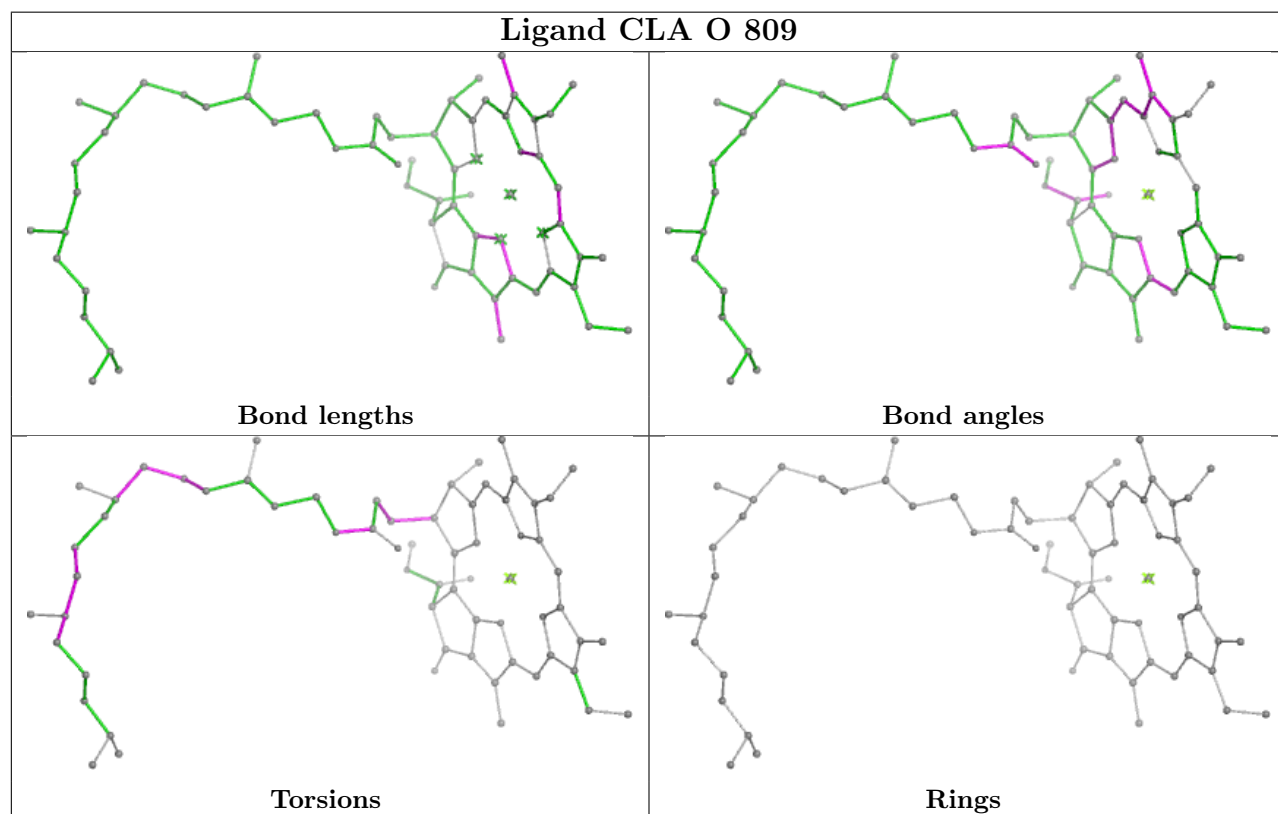
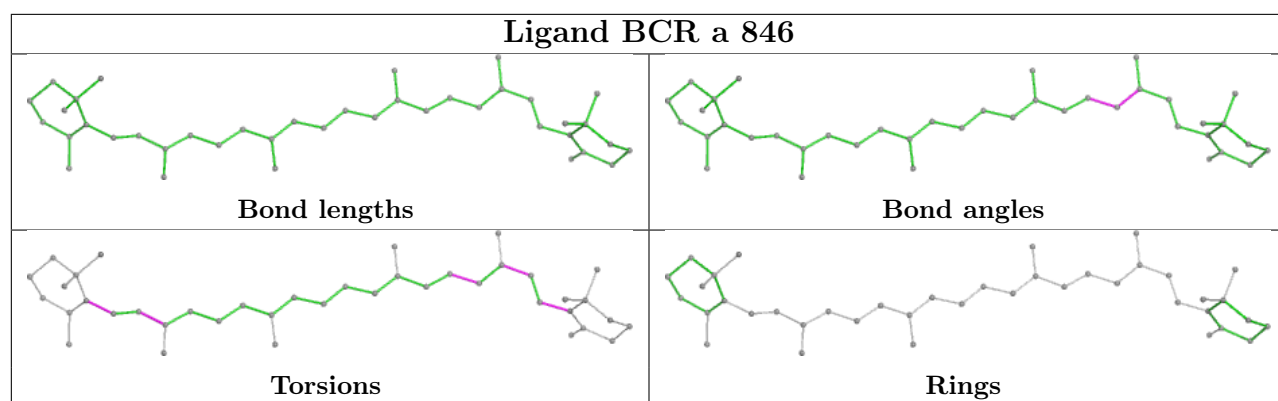
## Ligand CLA a 840

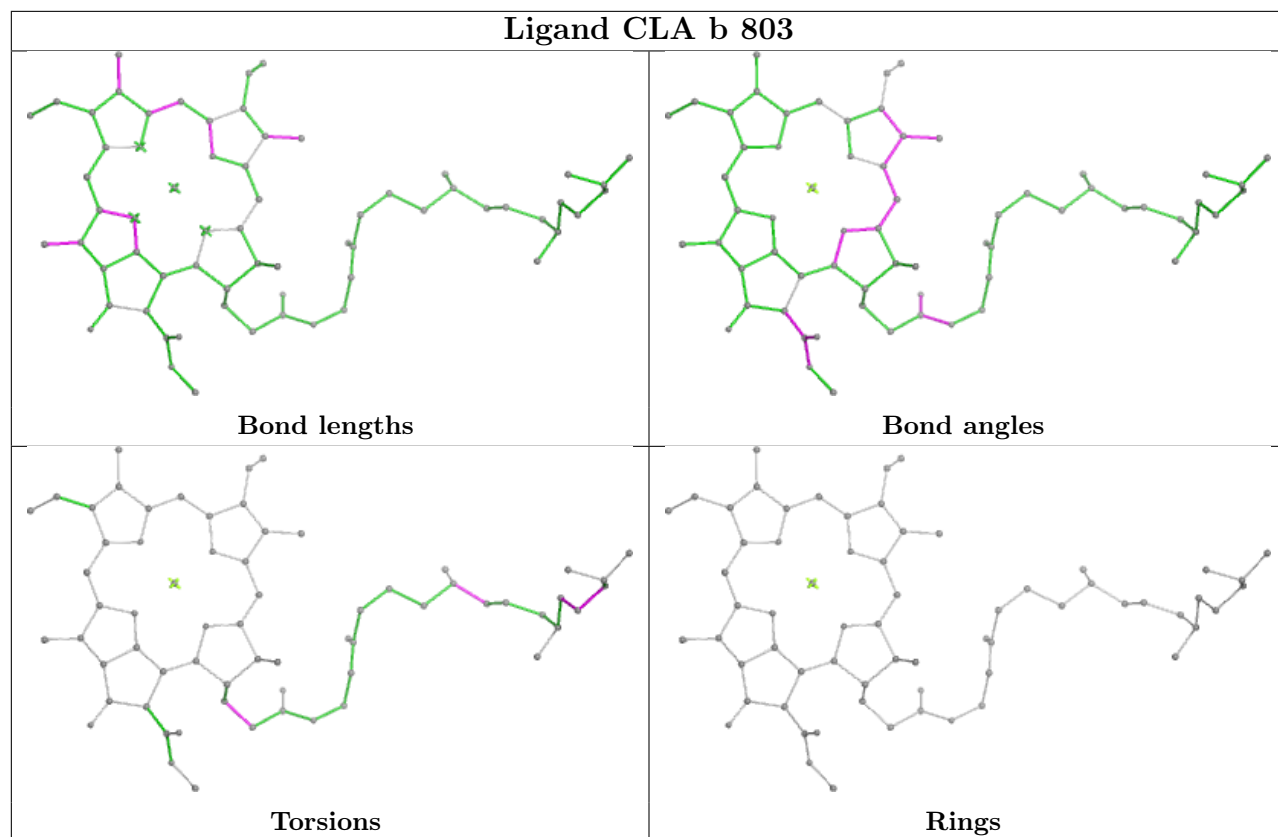
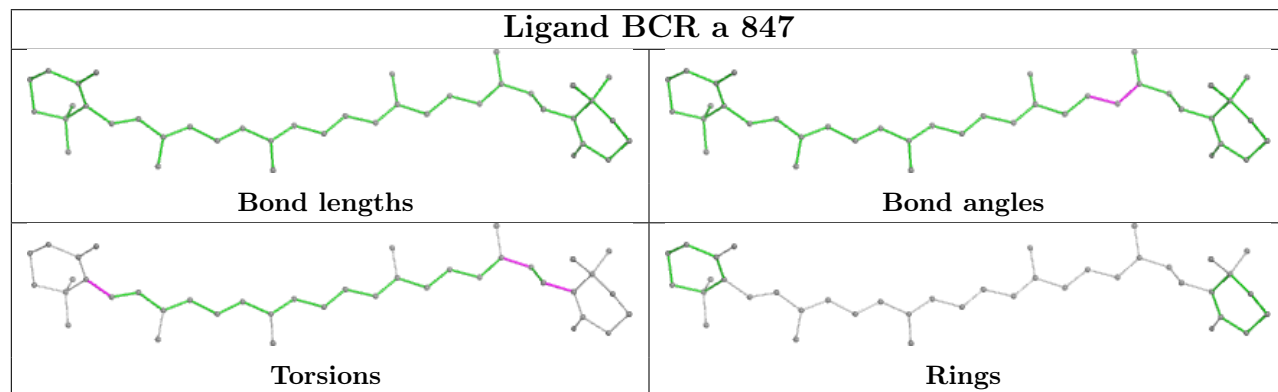


## Ligand BCR O 844

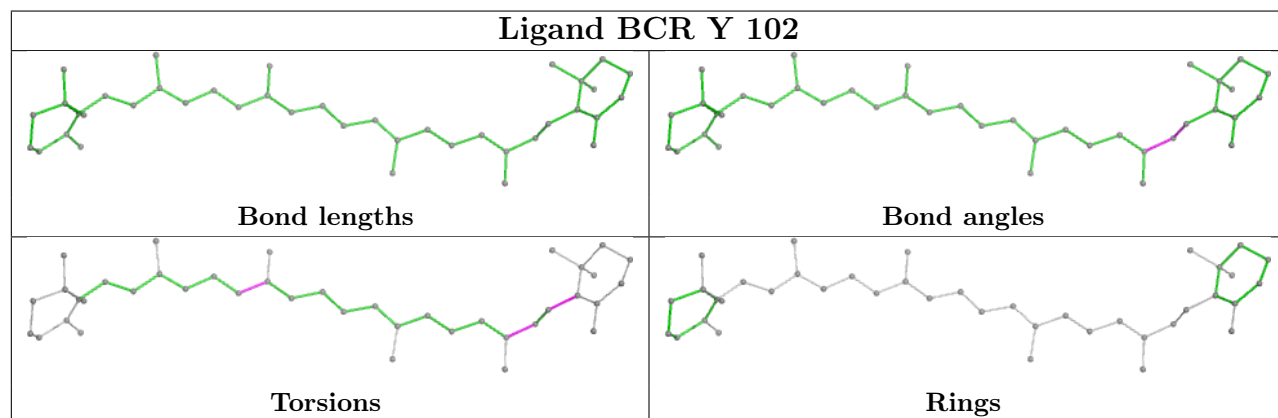
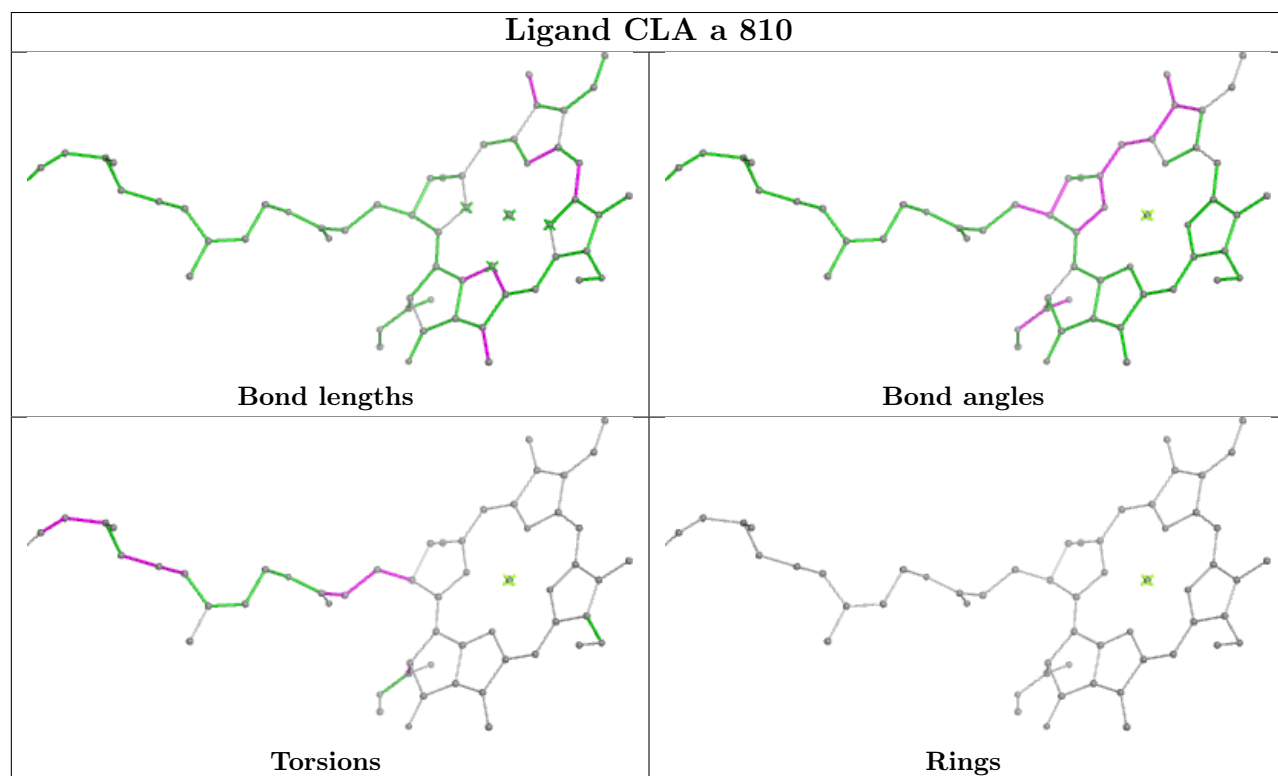
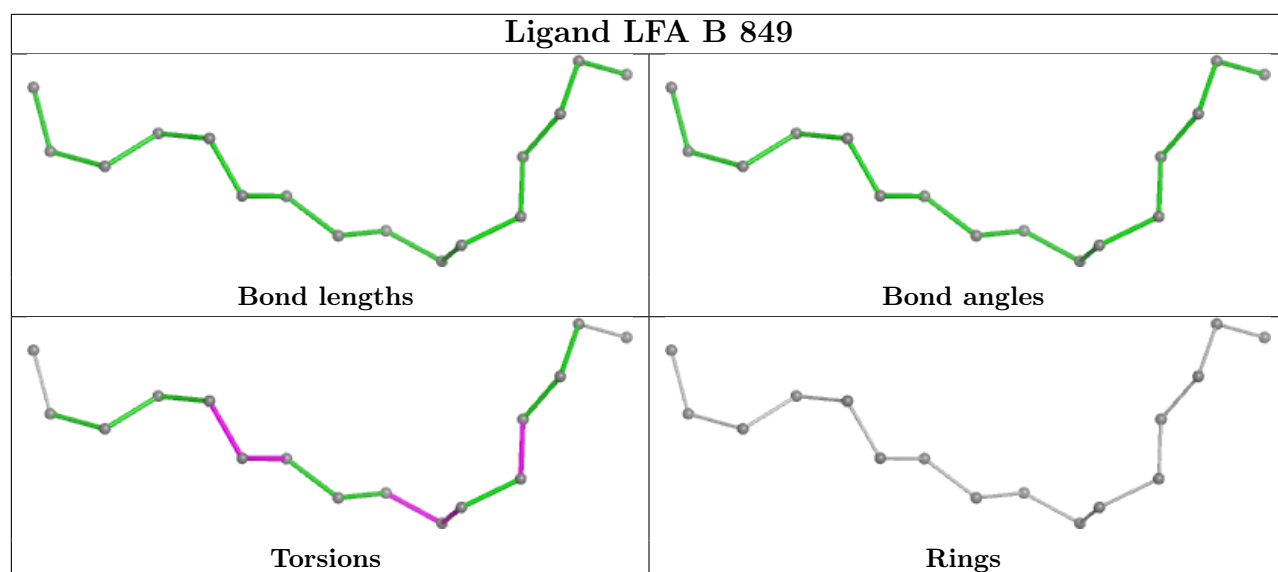


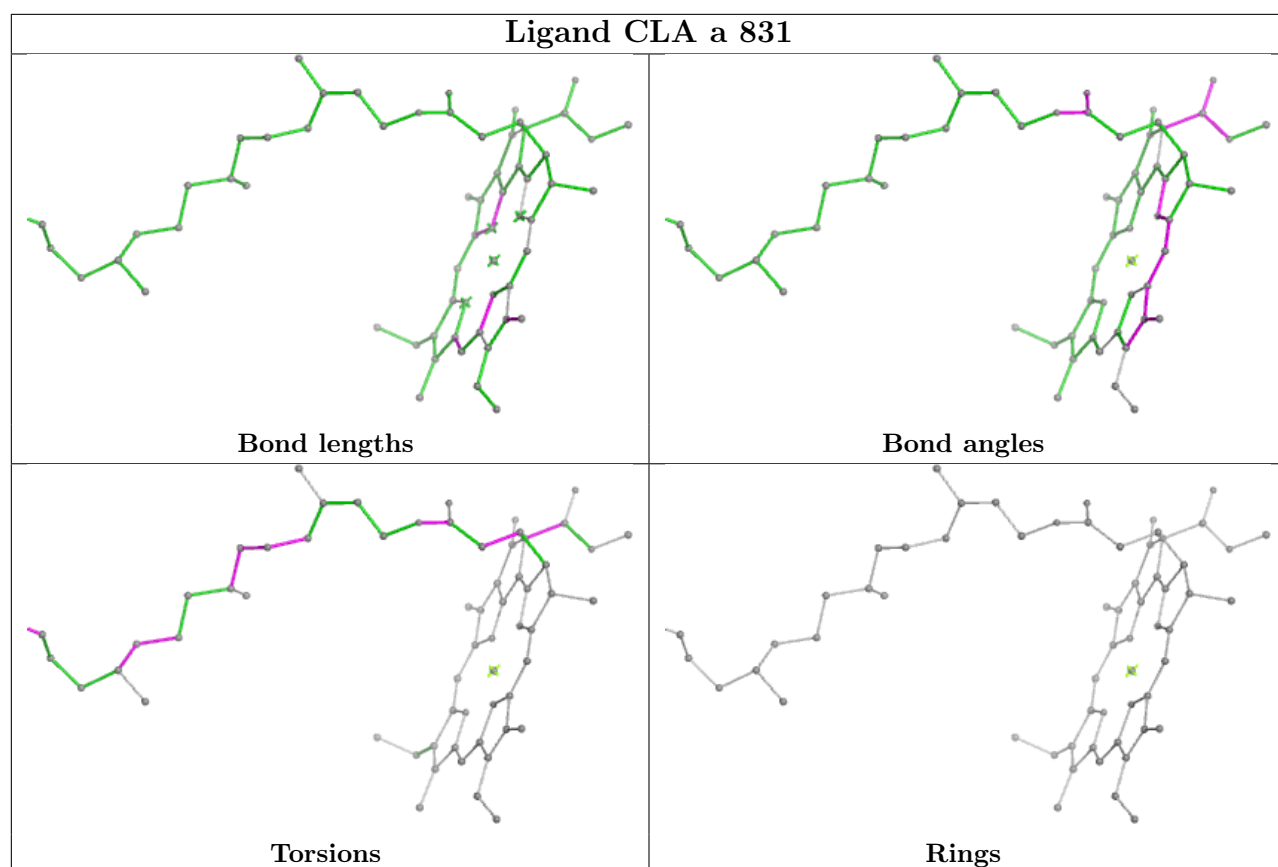




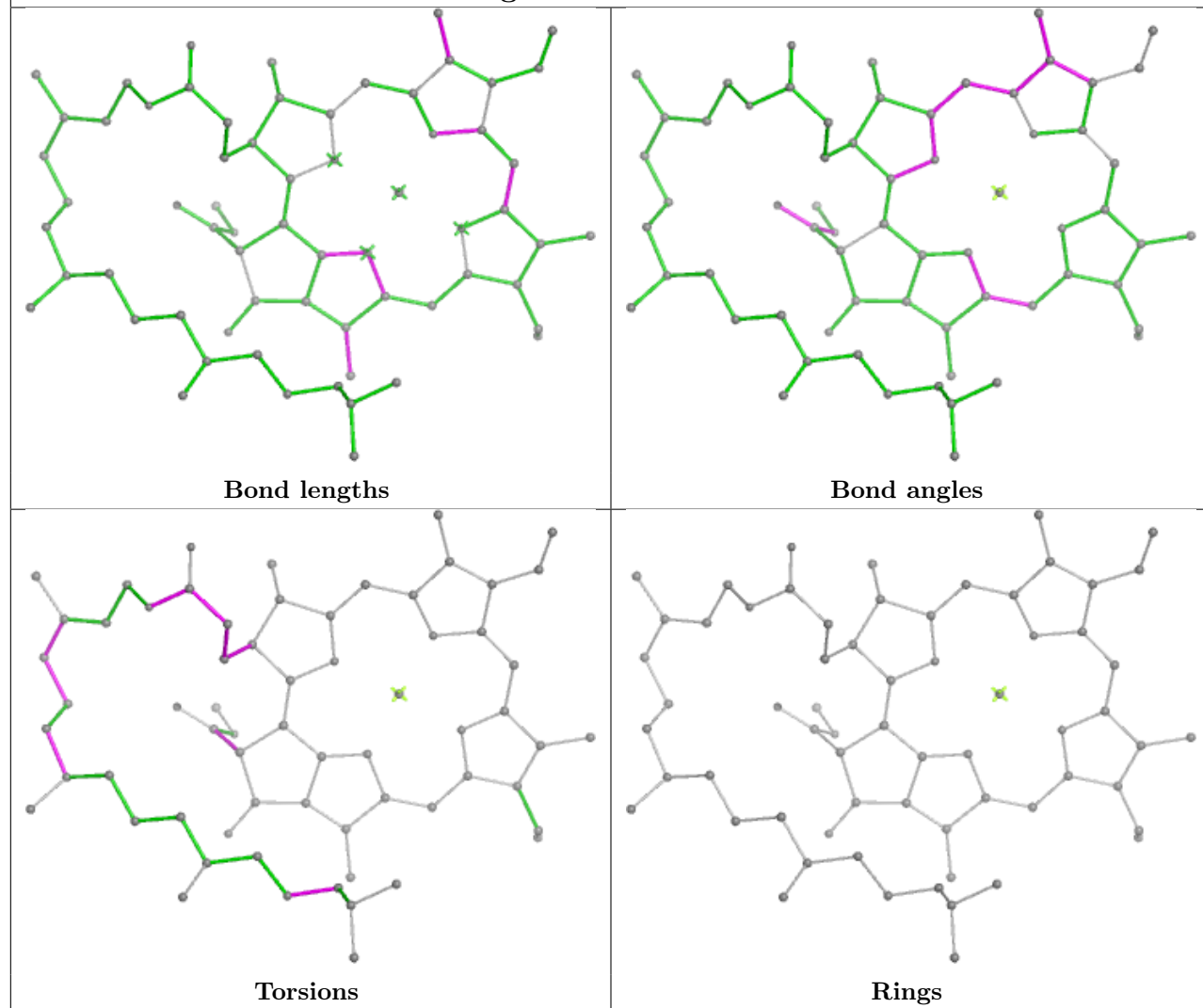
**Ligand CLA b 803****Ligand BCR a 847**

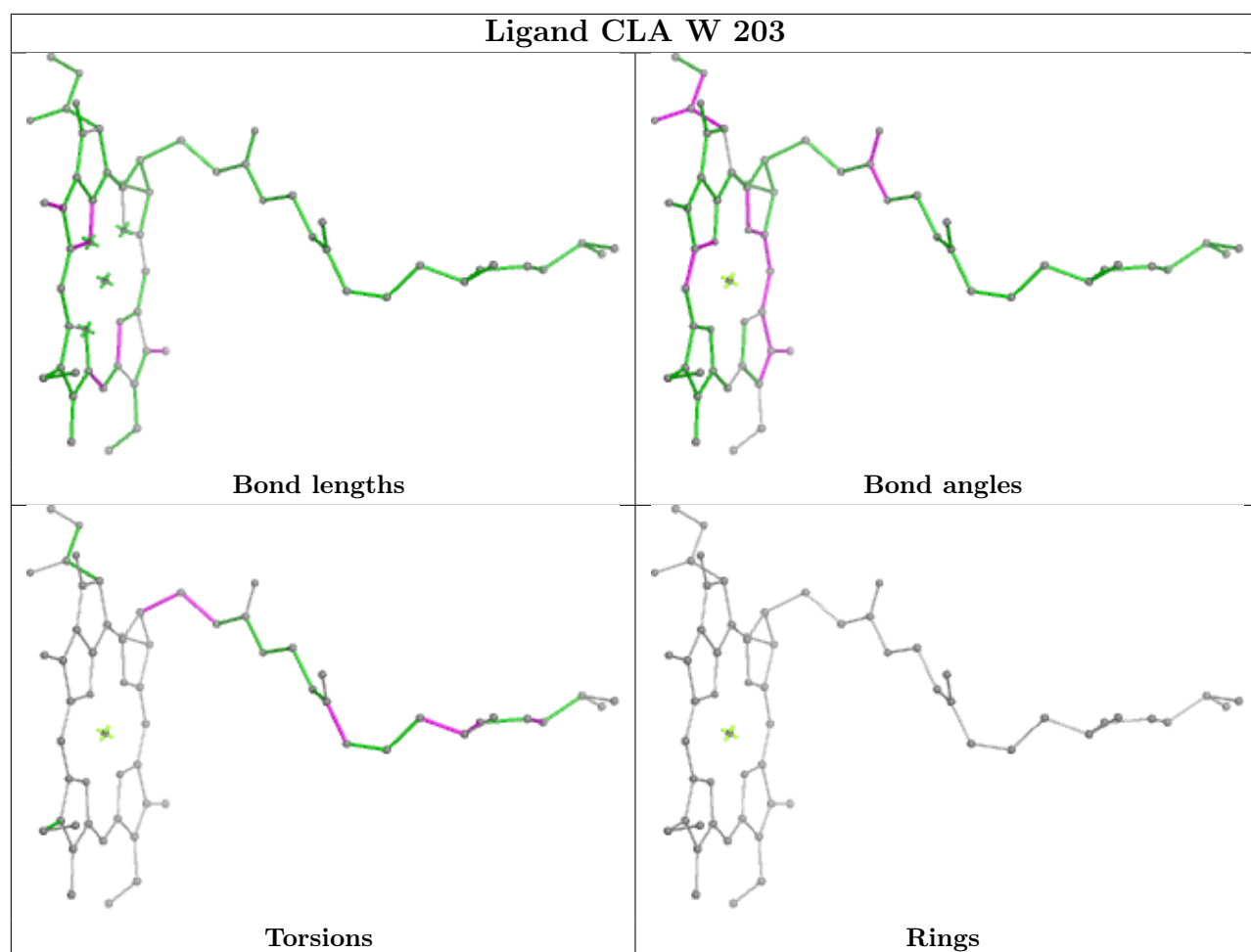


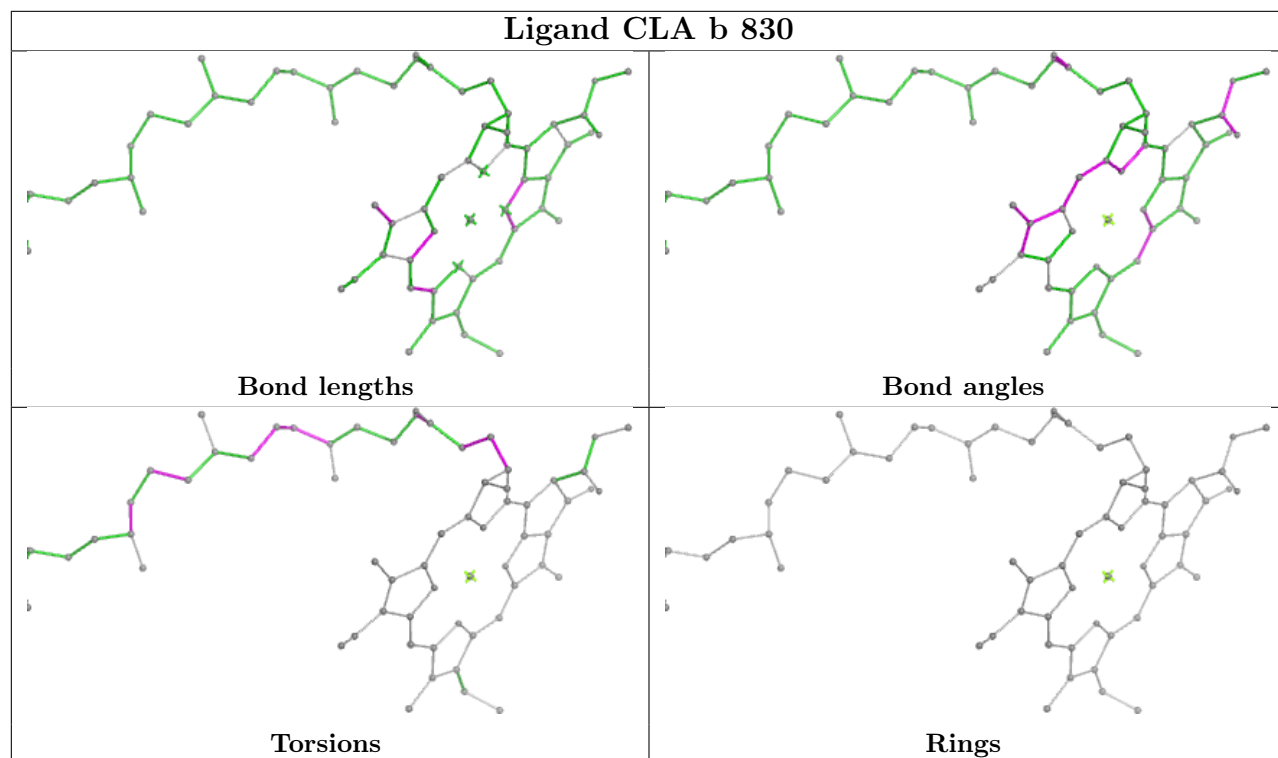
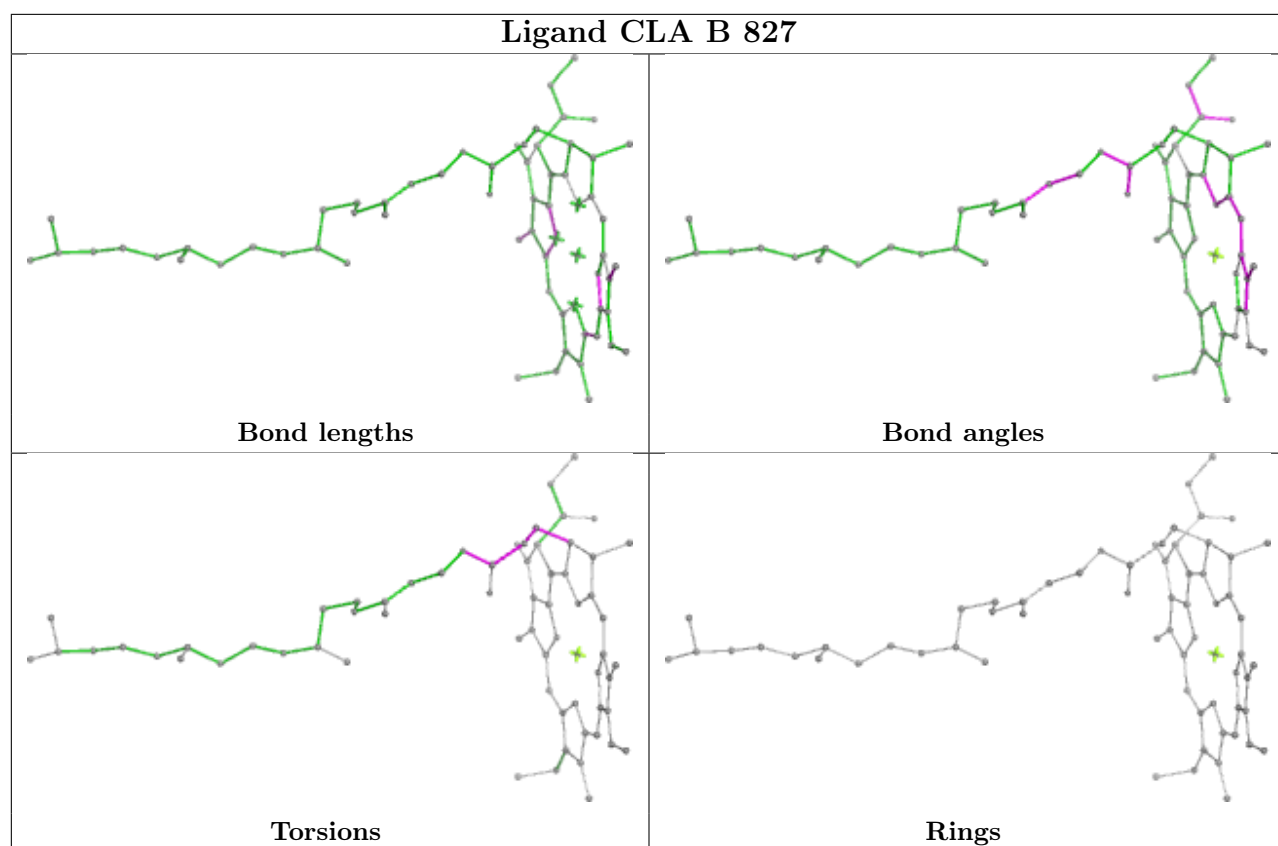


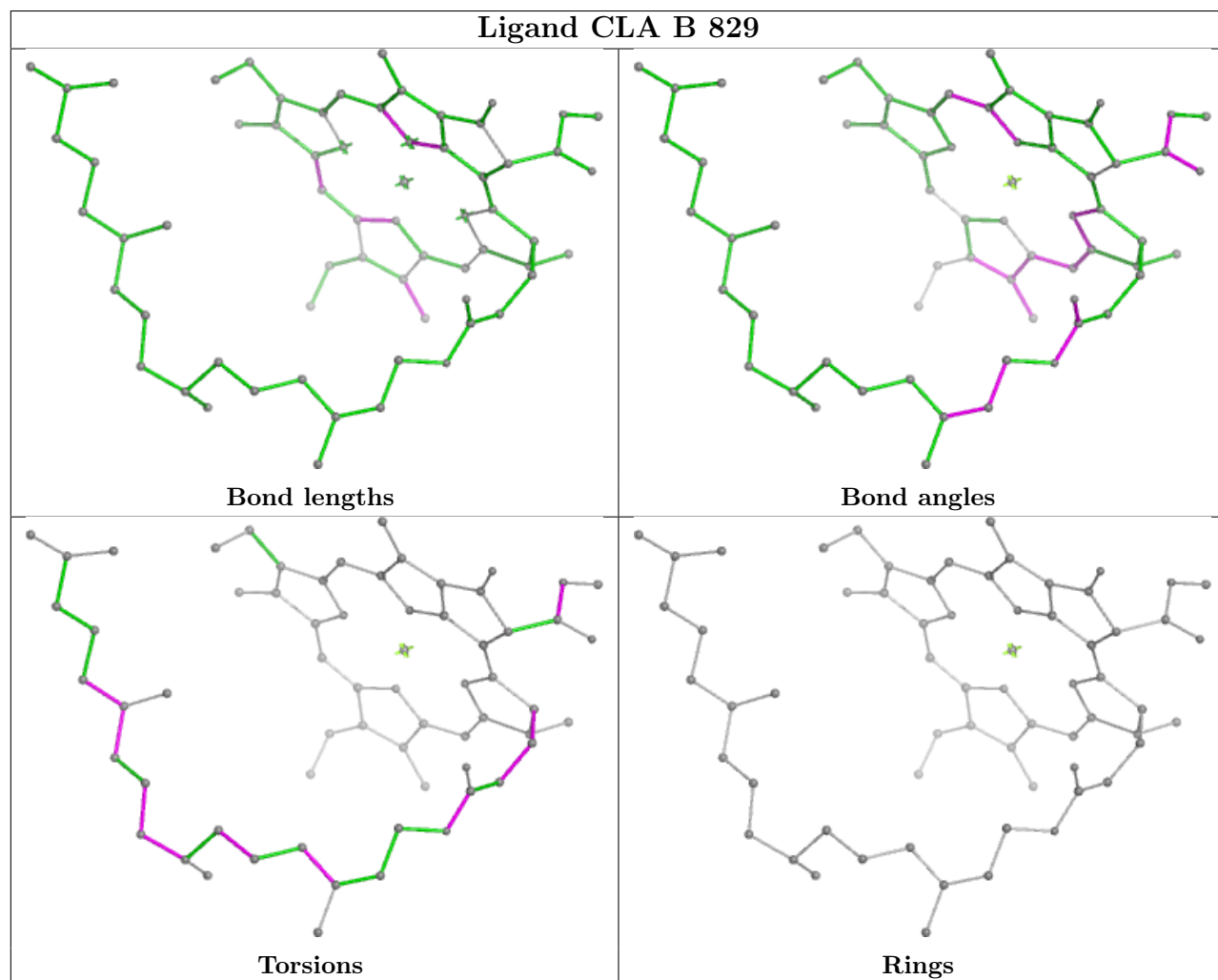
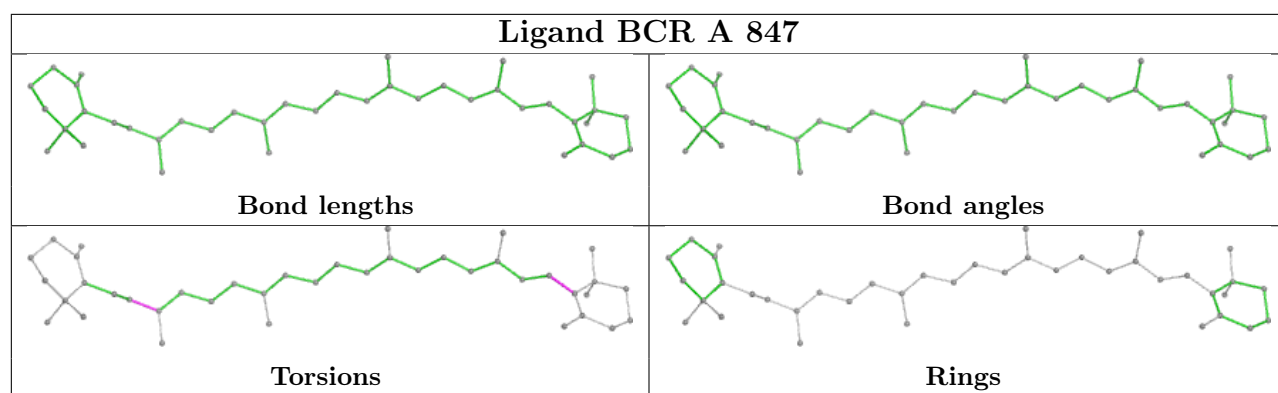


## Ligand CLA O 805

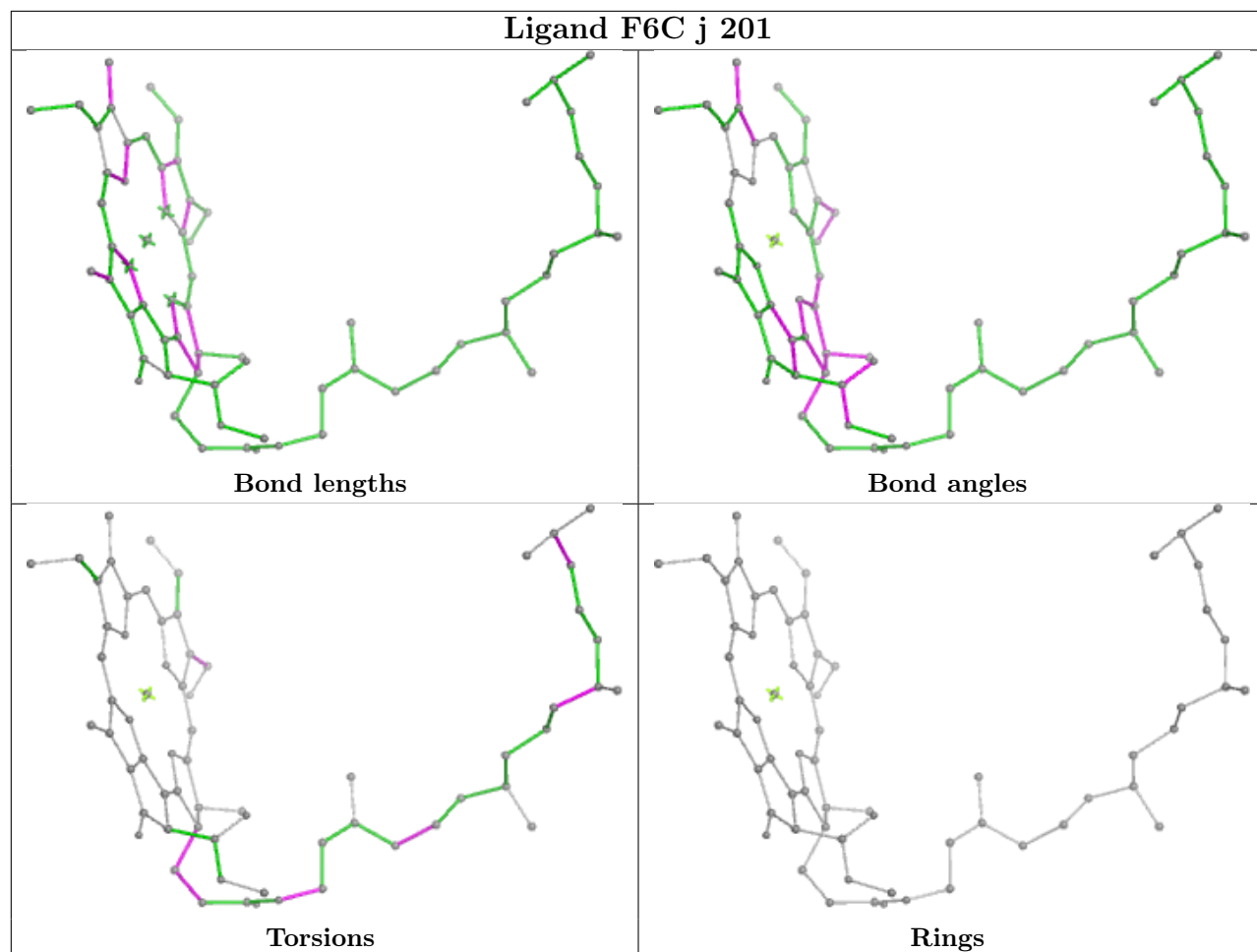




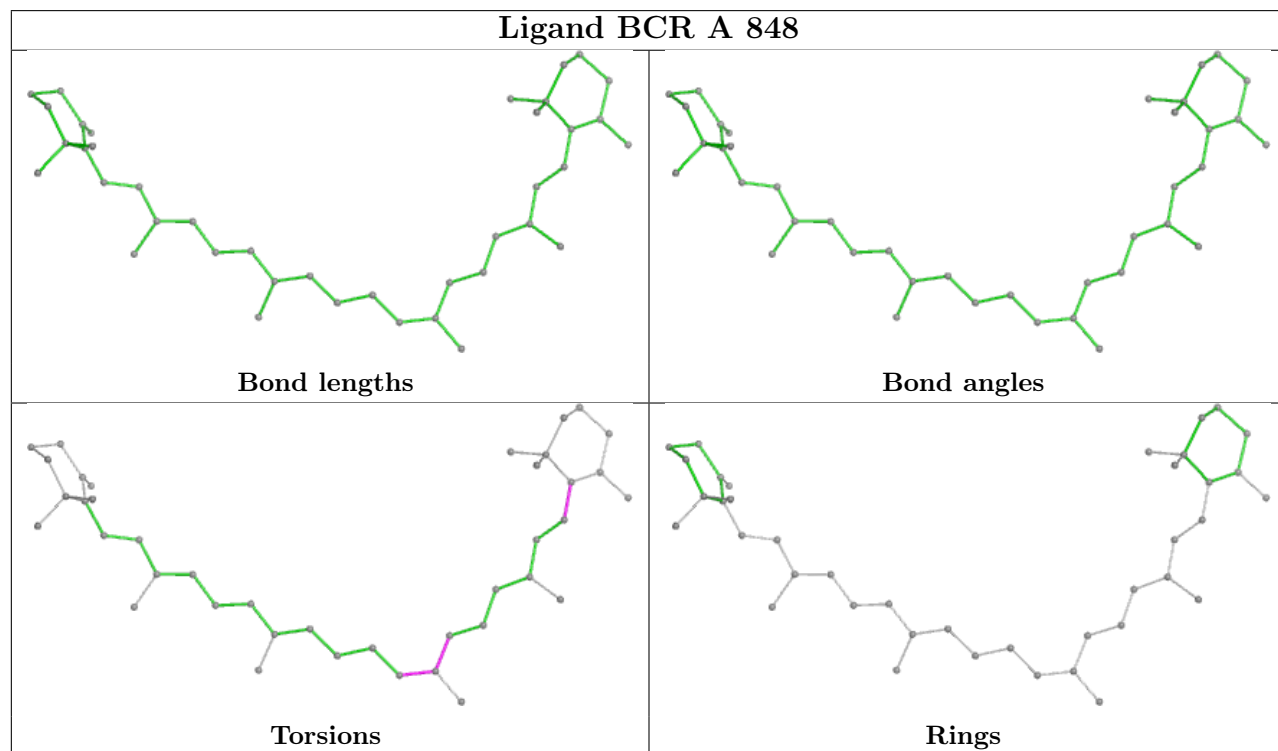


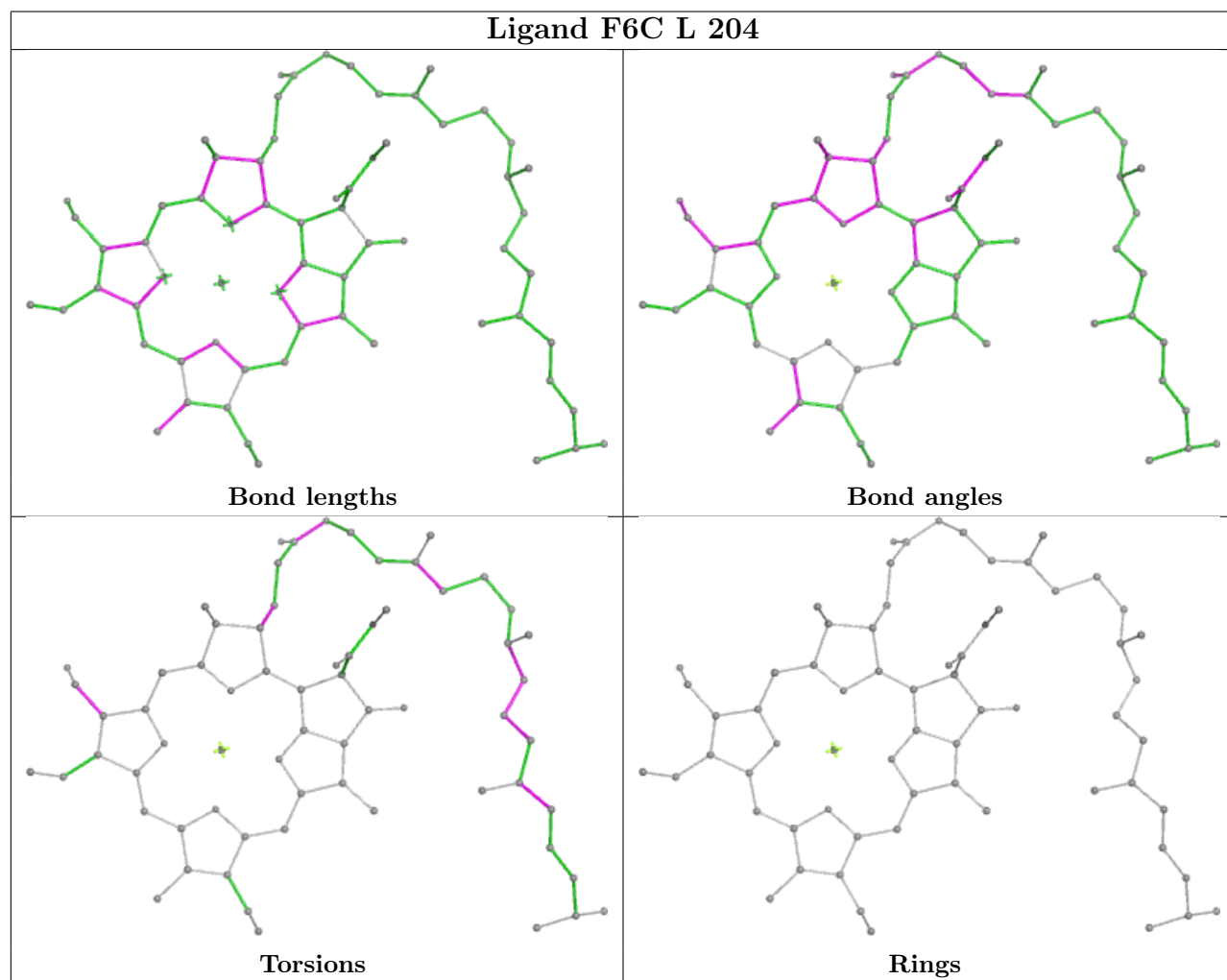
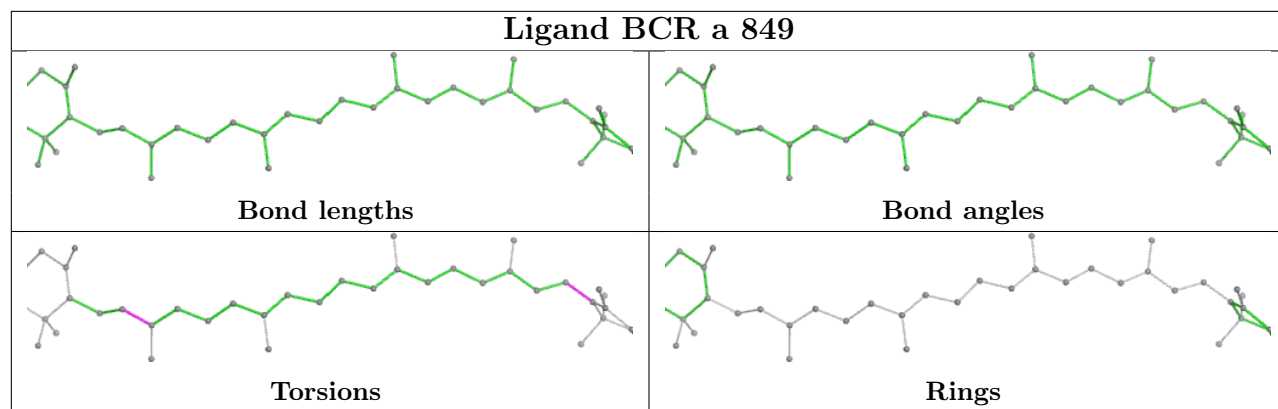


## Ligand F6C j 201



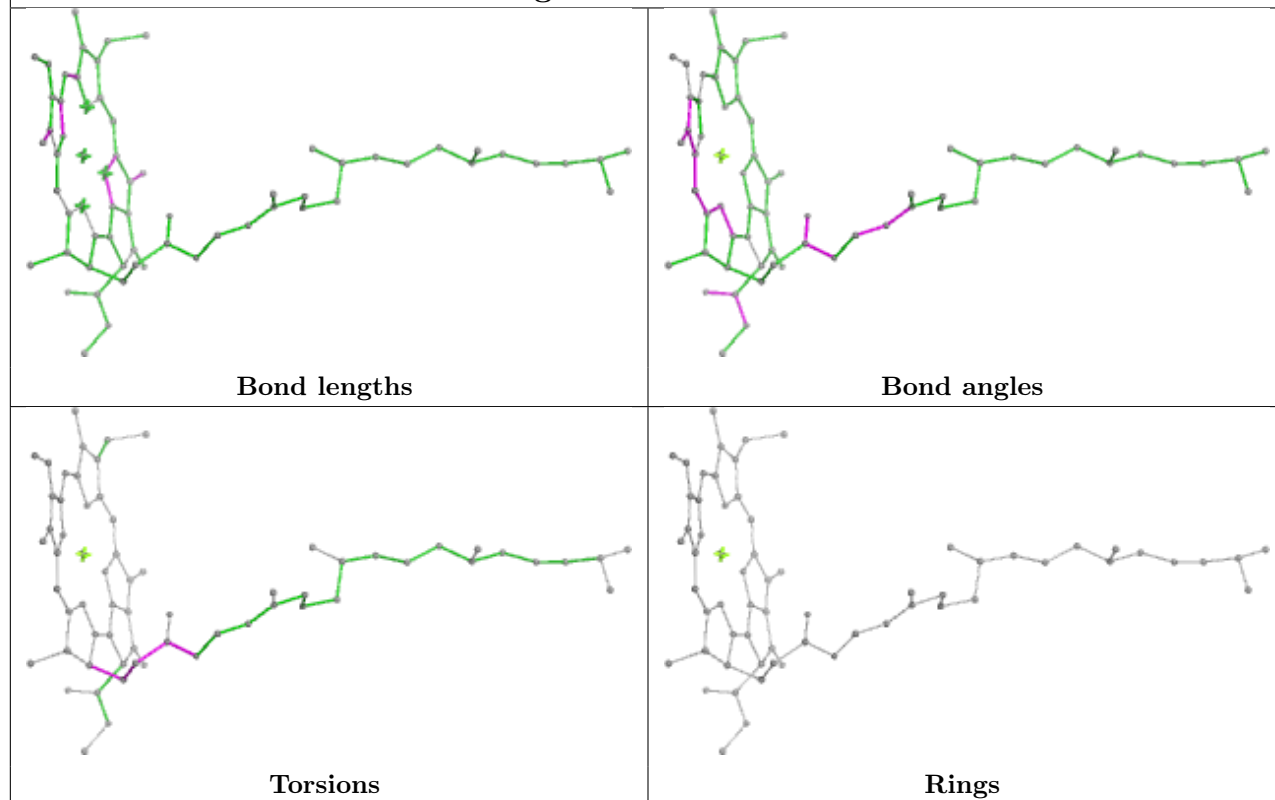
## Ligand BCR A 848



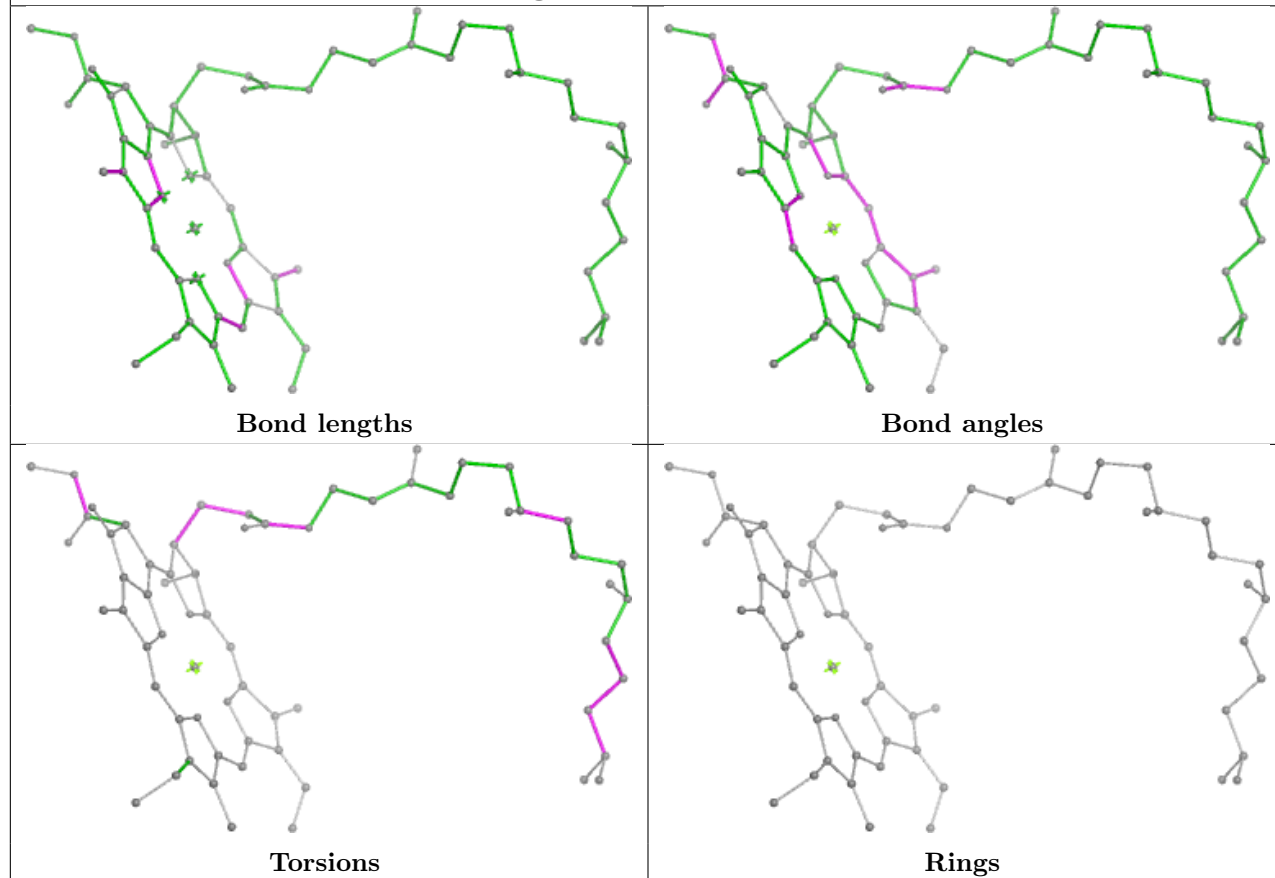


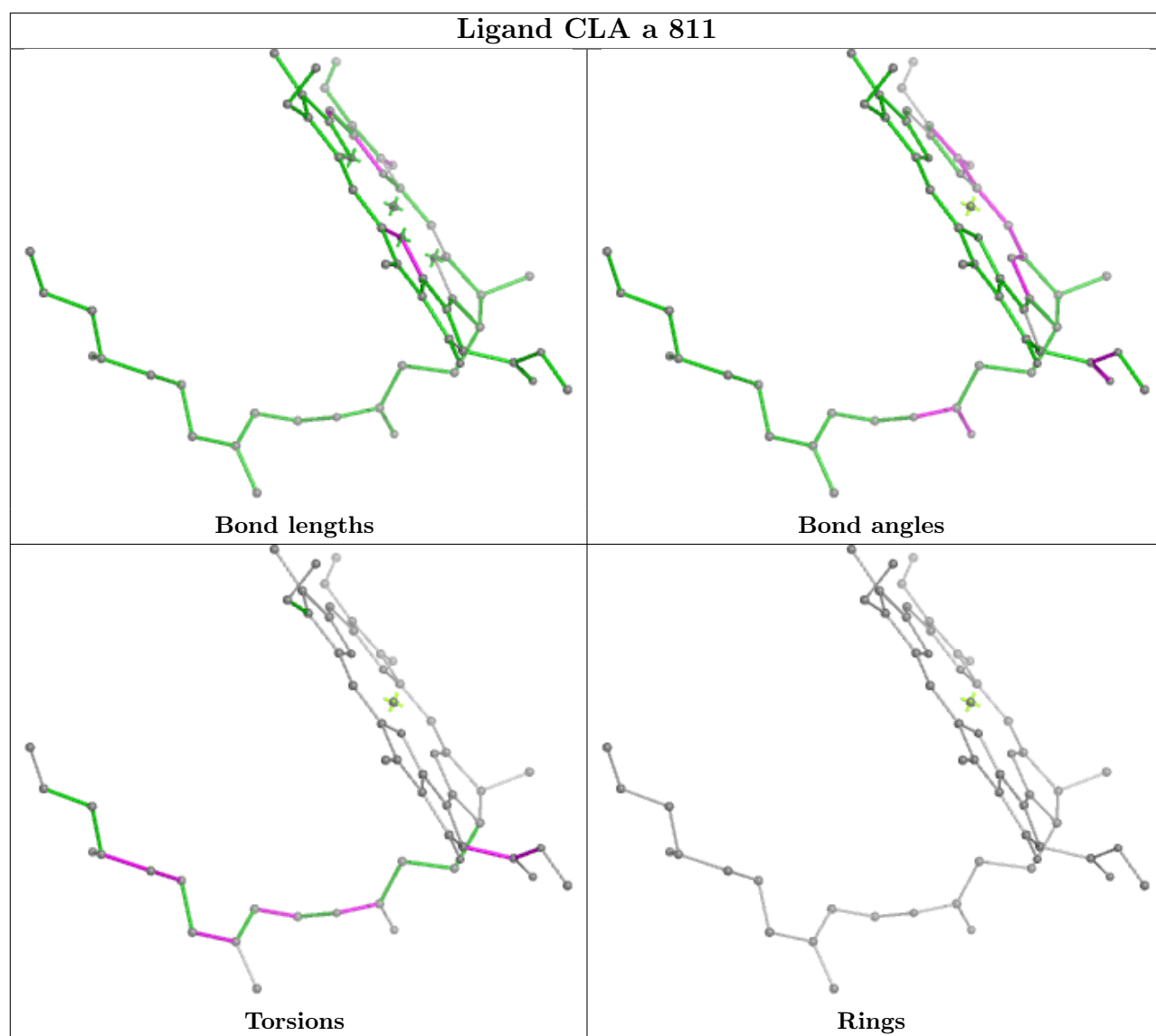


## Ligand CLA b 827

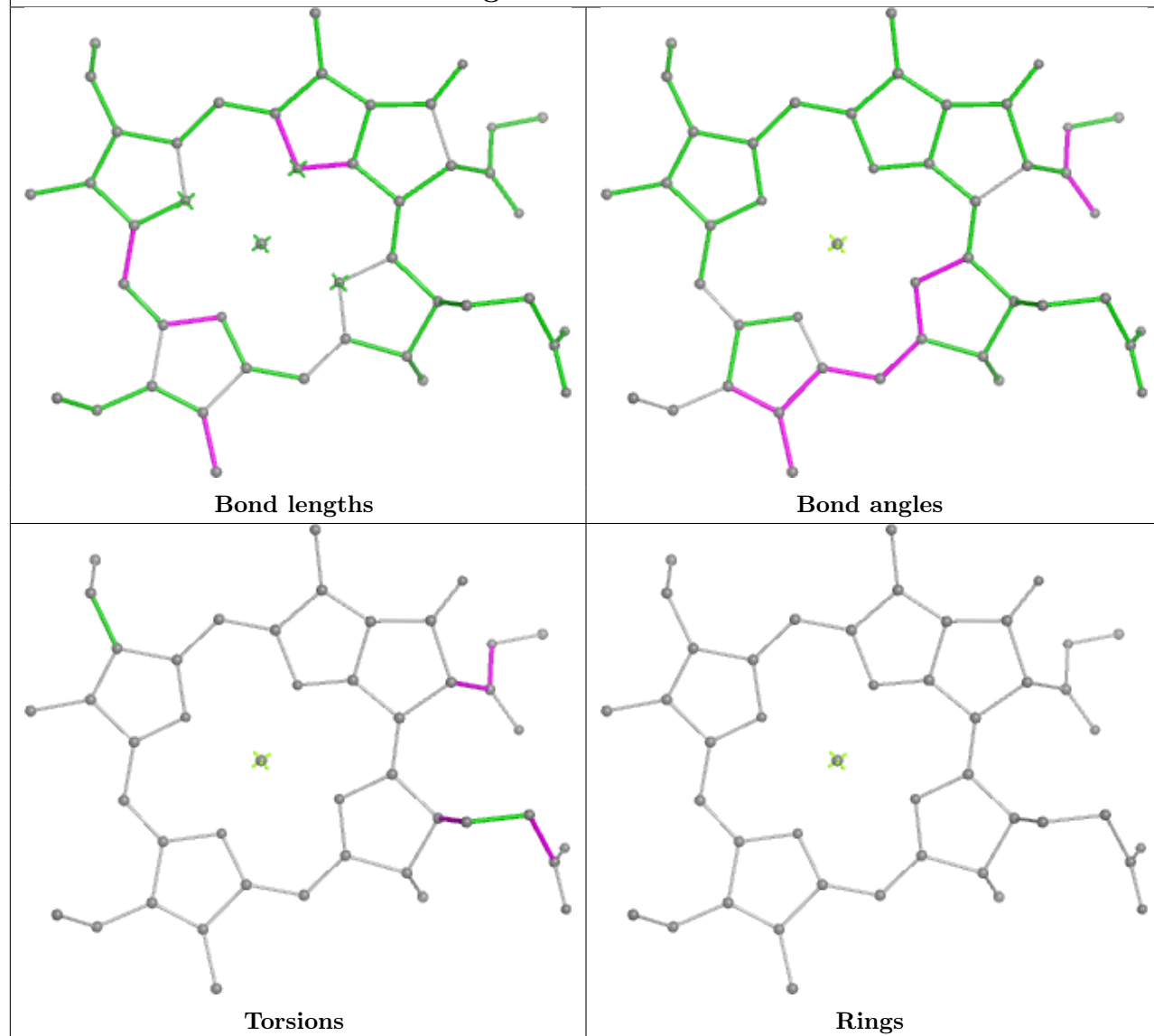


## Ligand CLA N 842

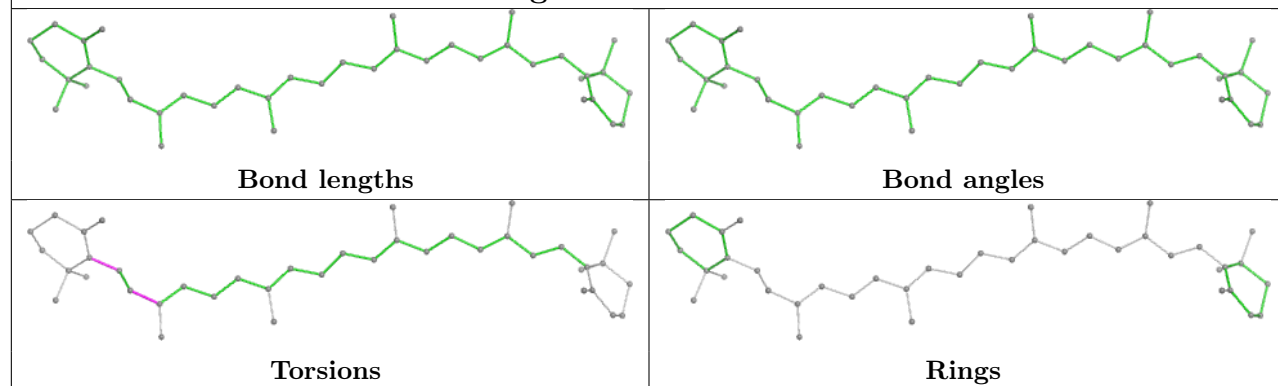


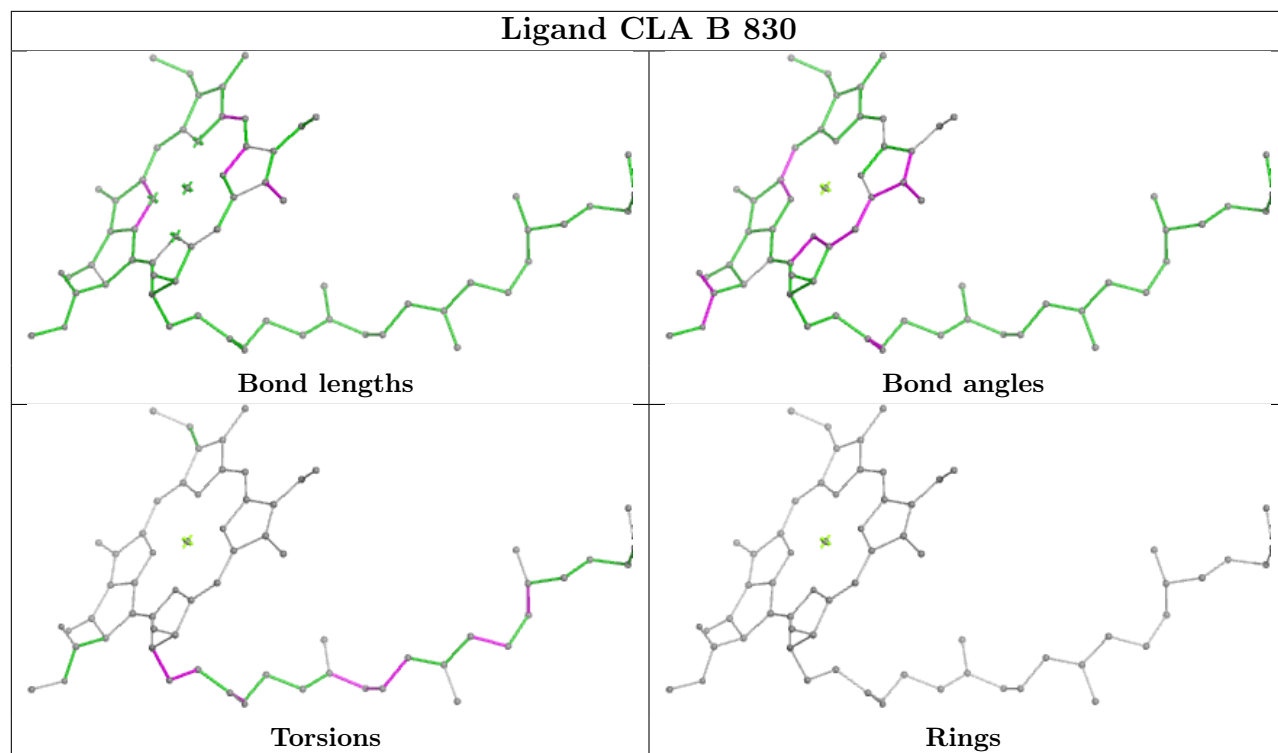


## Ligand CLA b 835

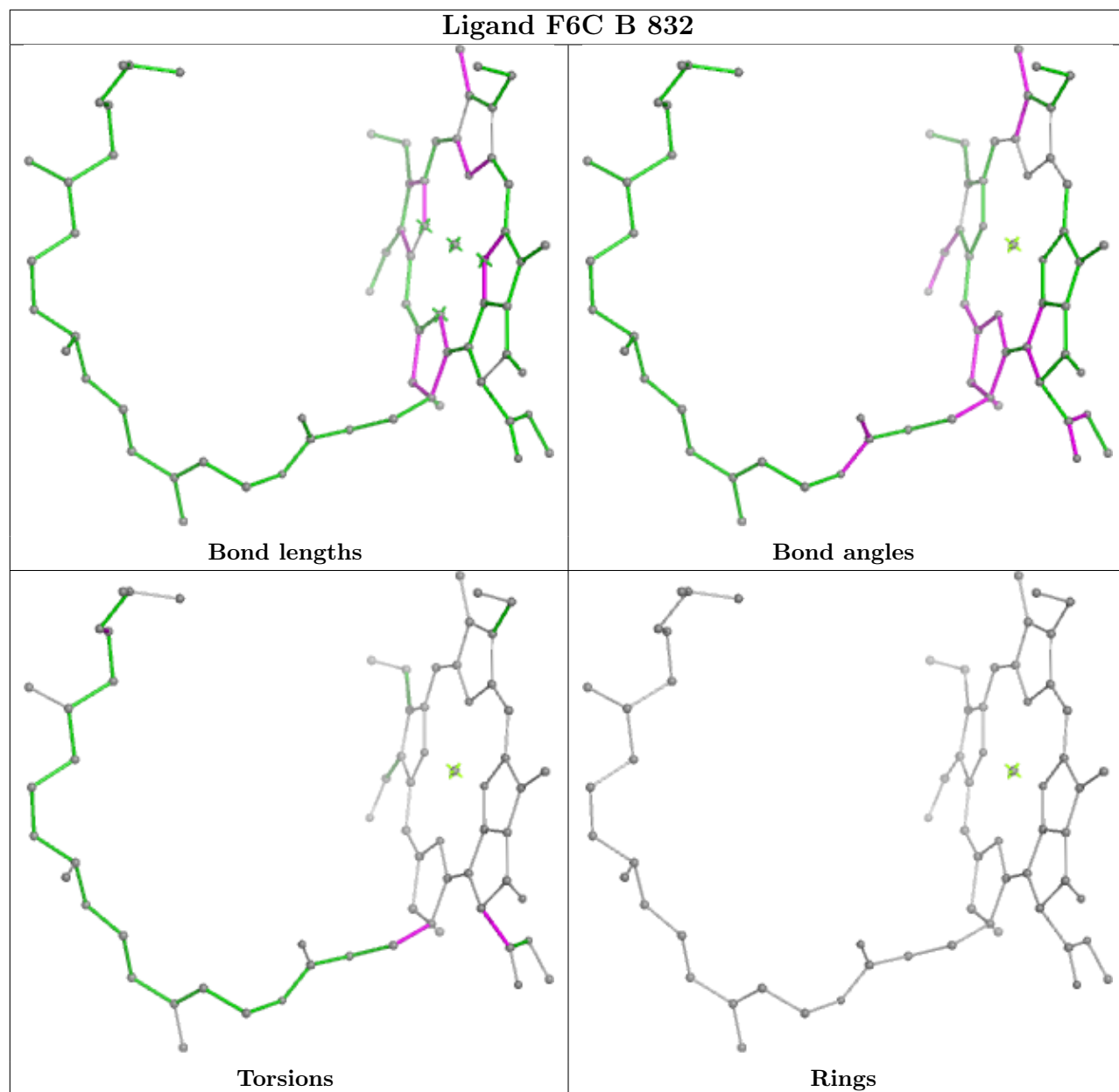


## Ligand BCR O 848

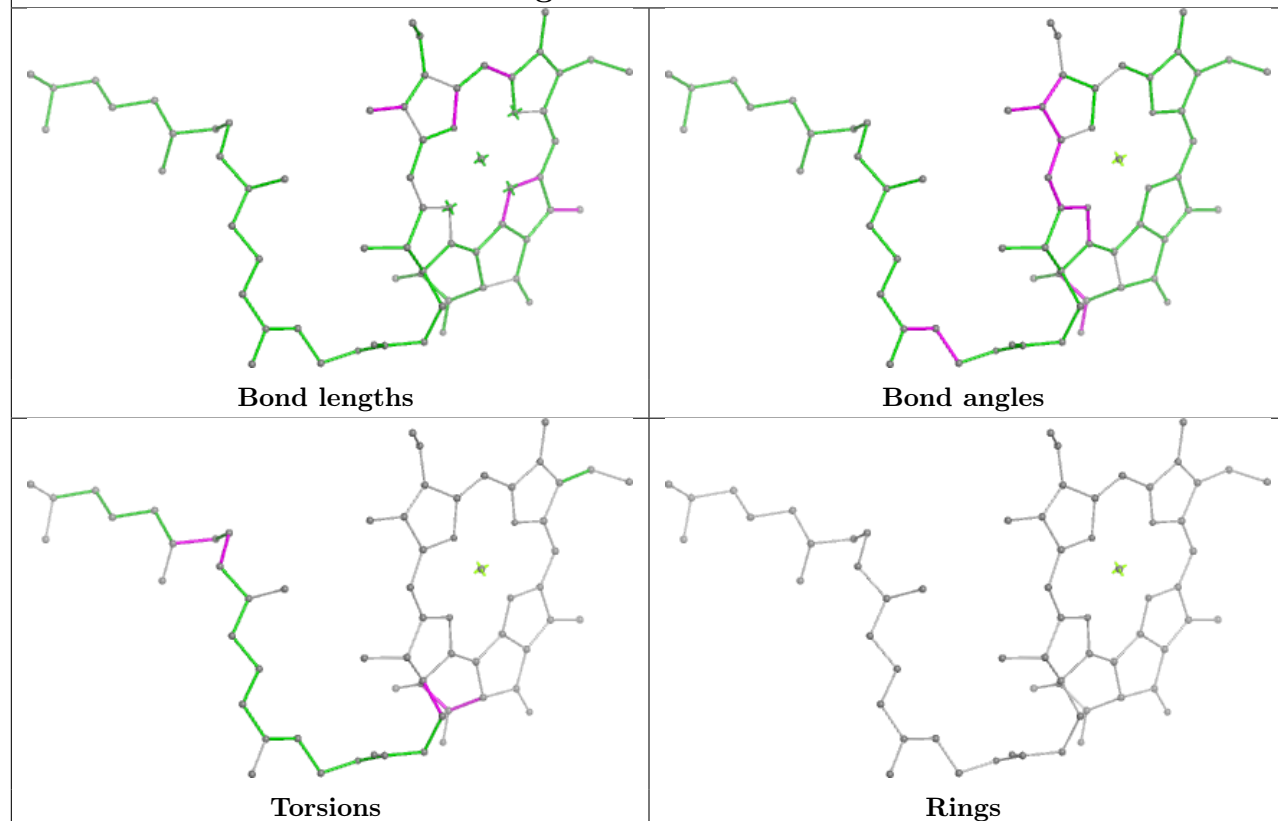




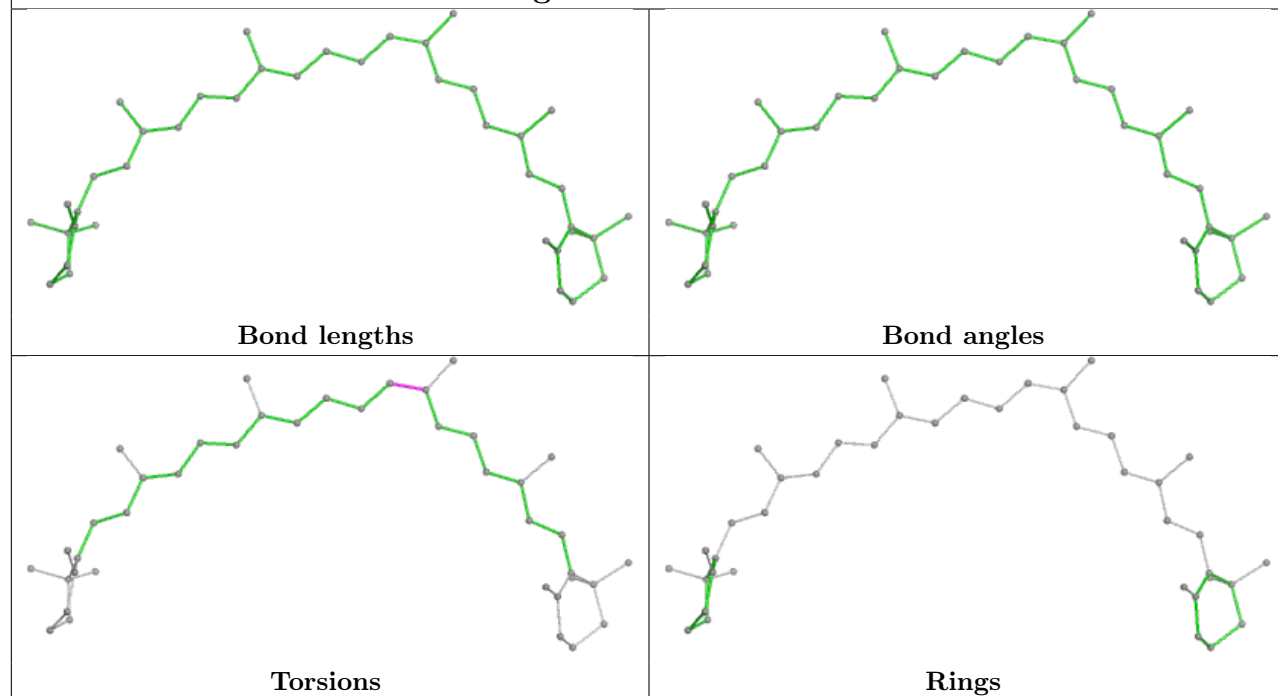
## Ligand F6C B 832

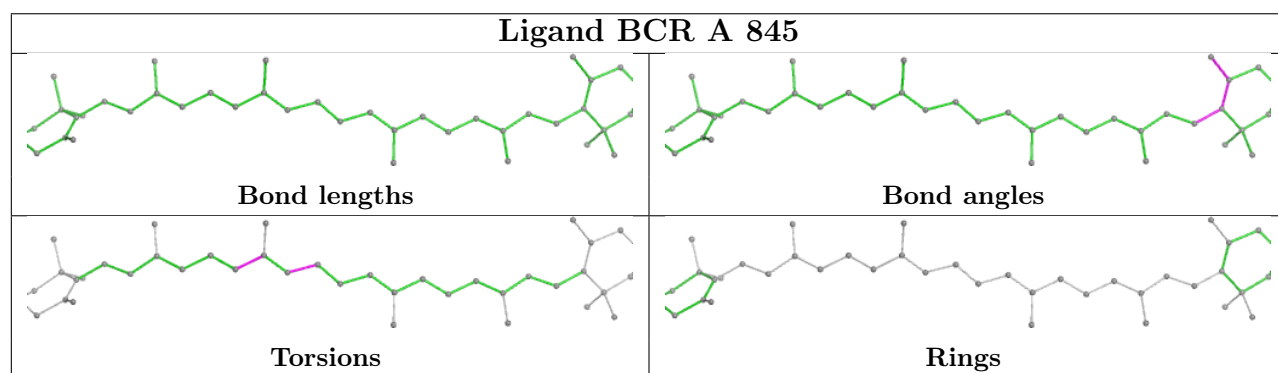
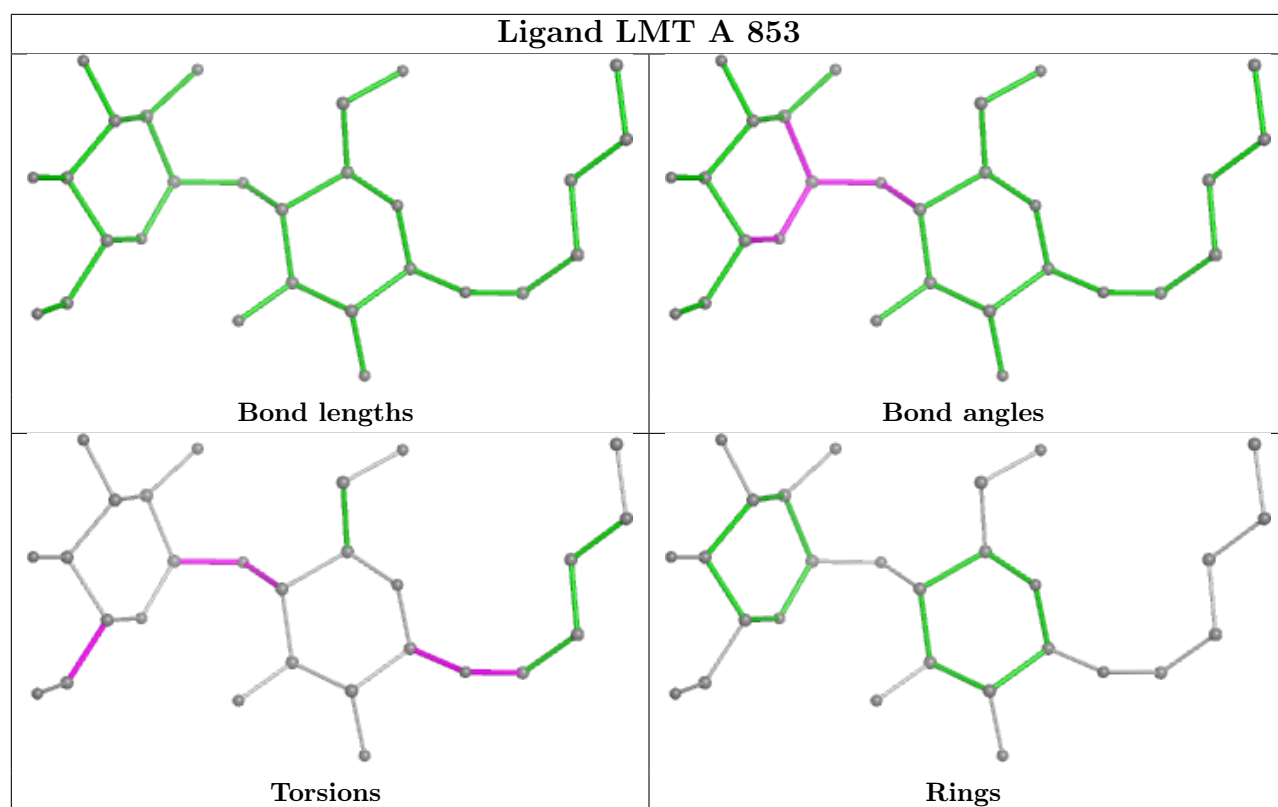


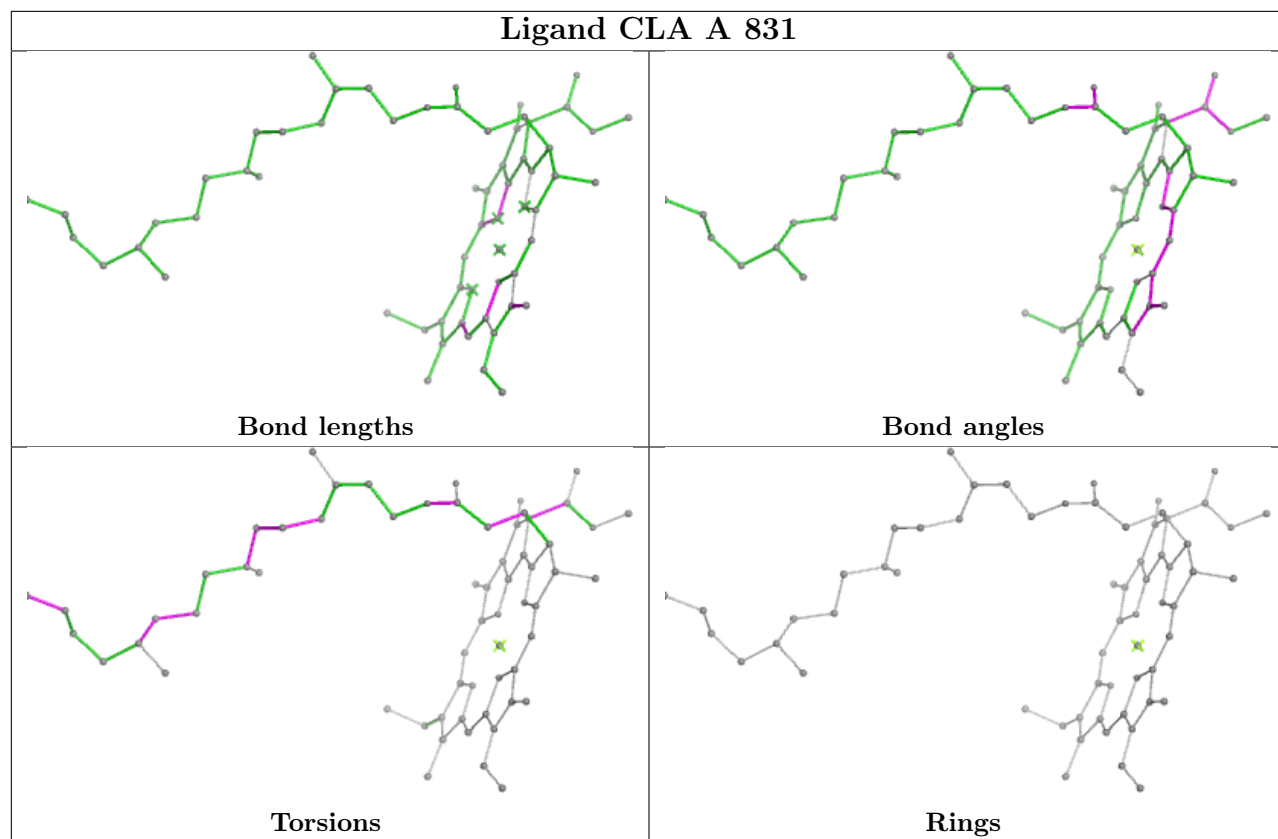
## Ligand CLA b 823



## Ligand BCR S 202

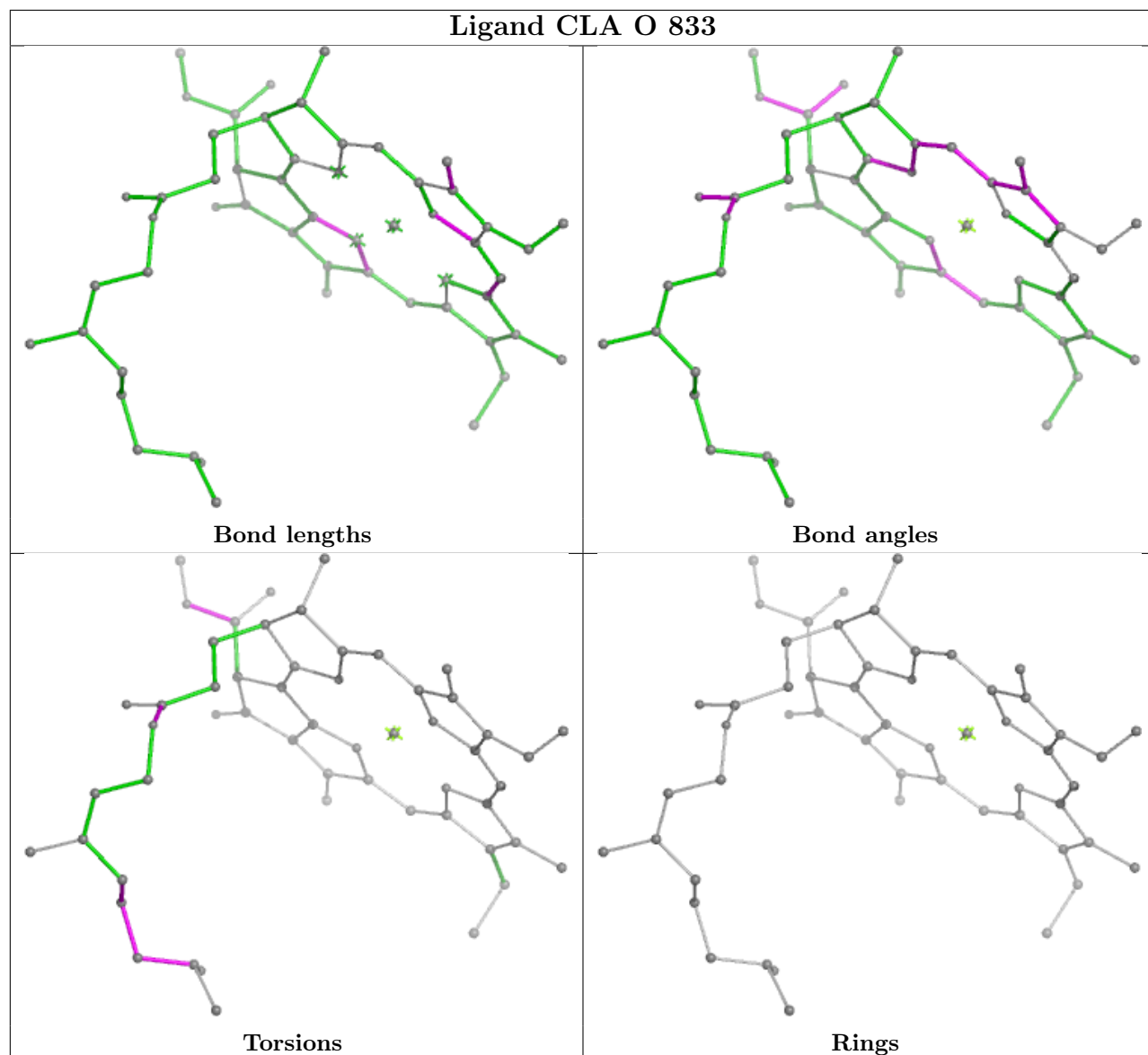




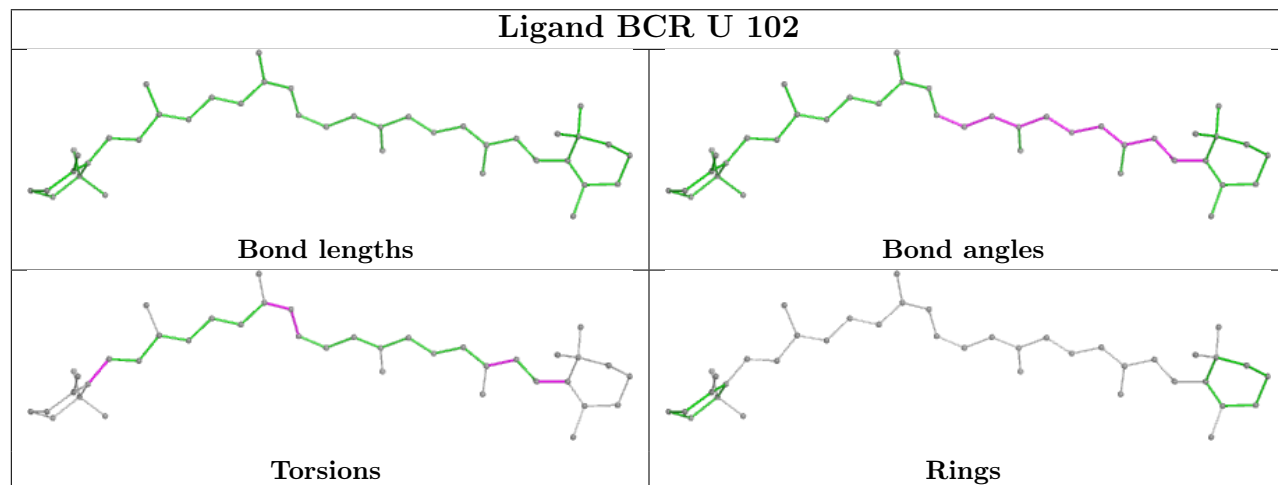


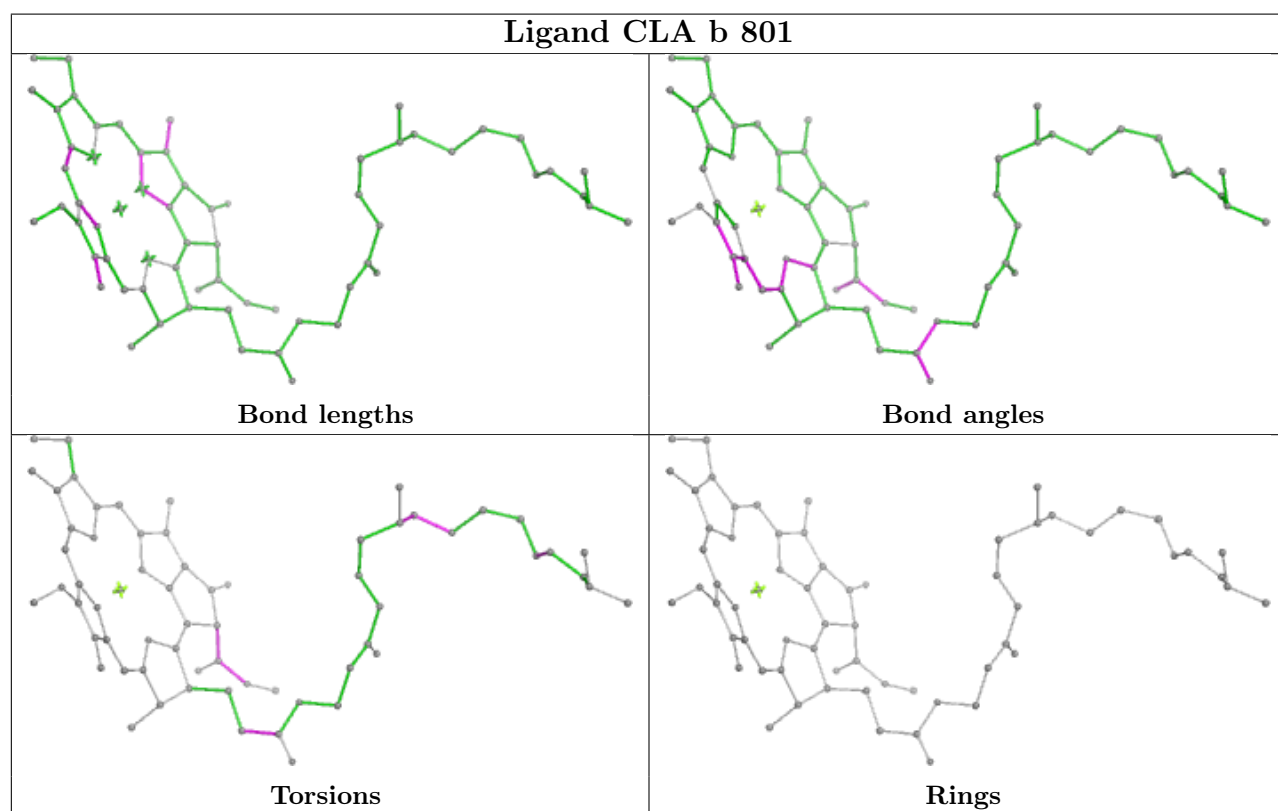
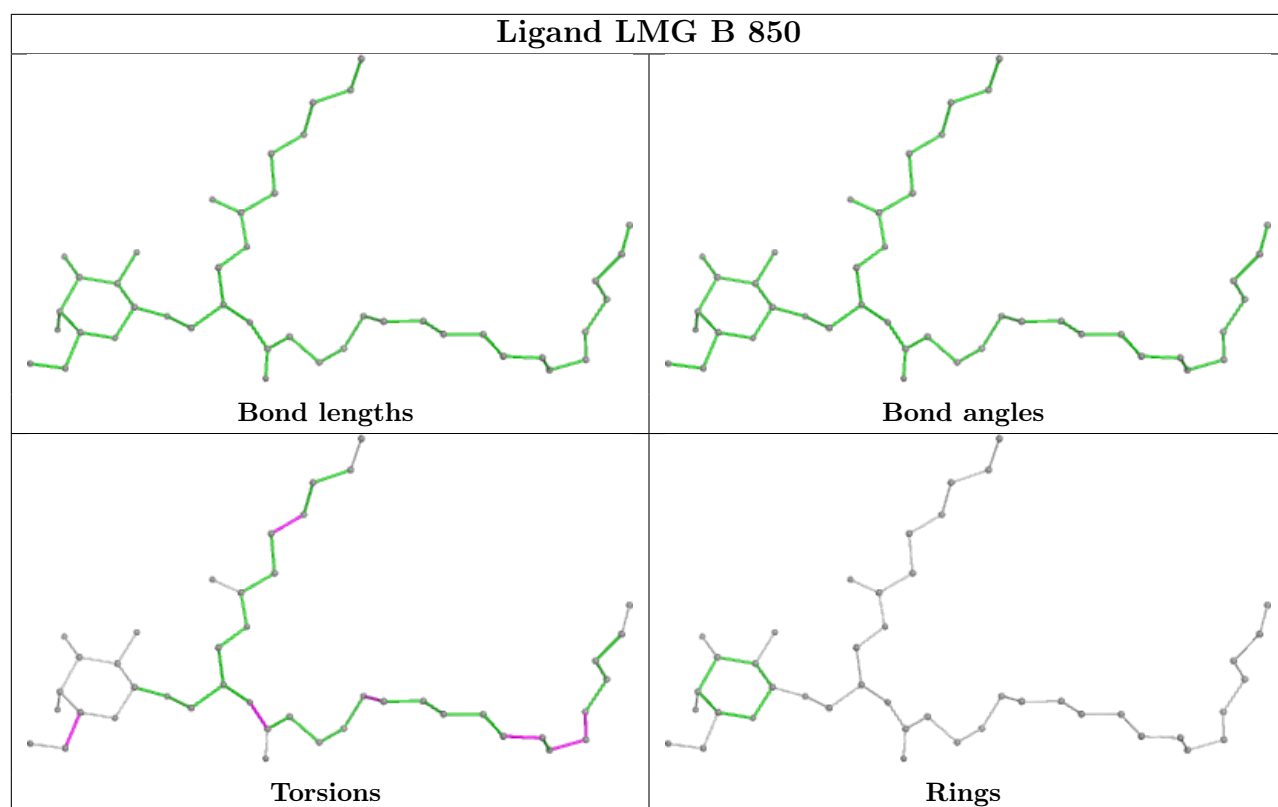


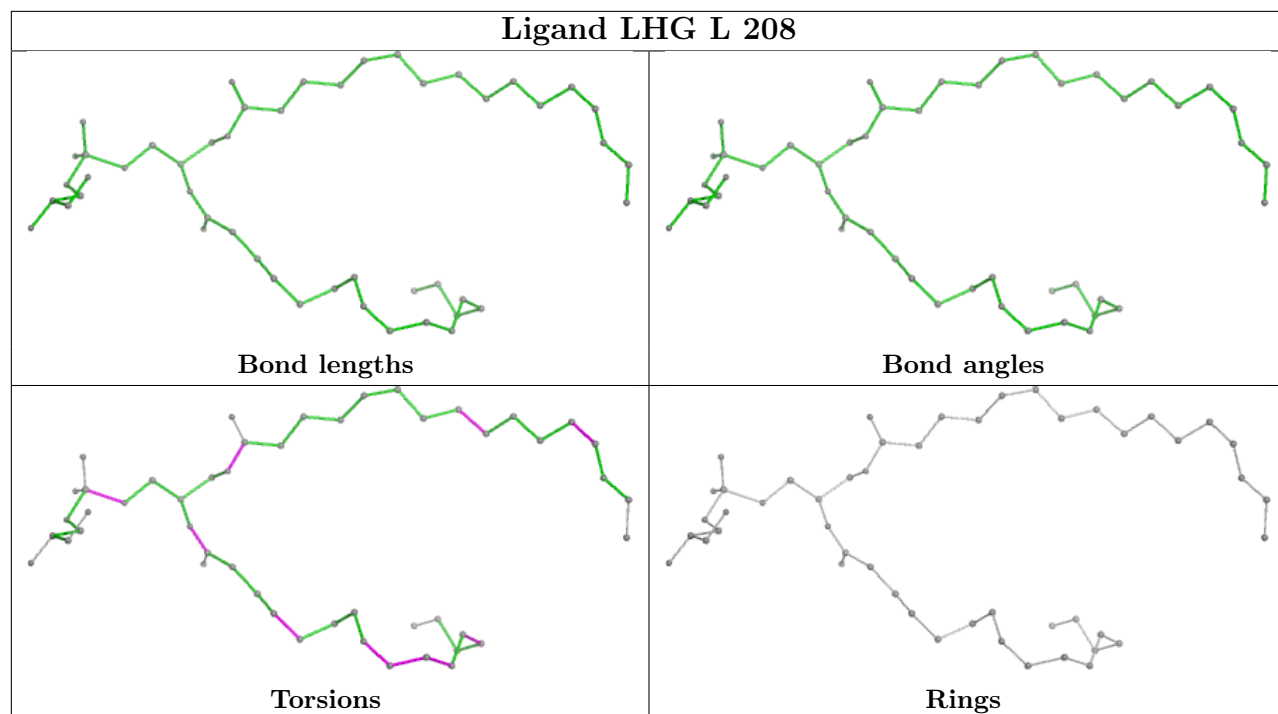
## Ligand CLA O 833



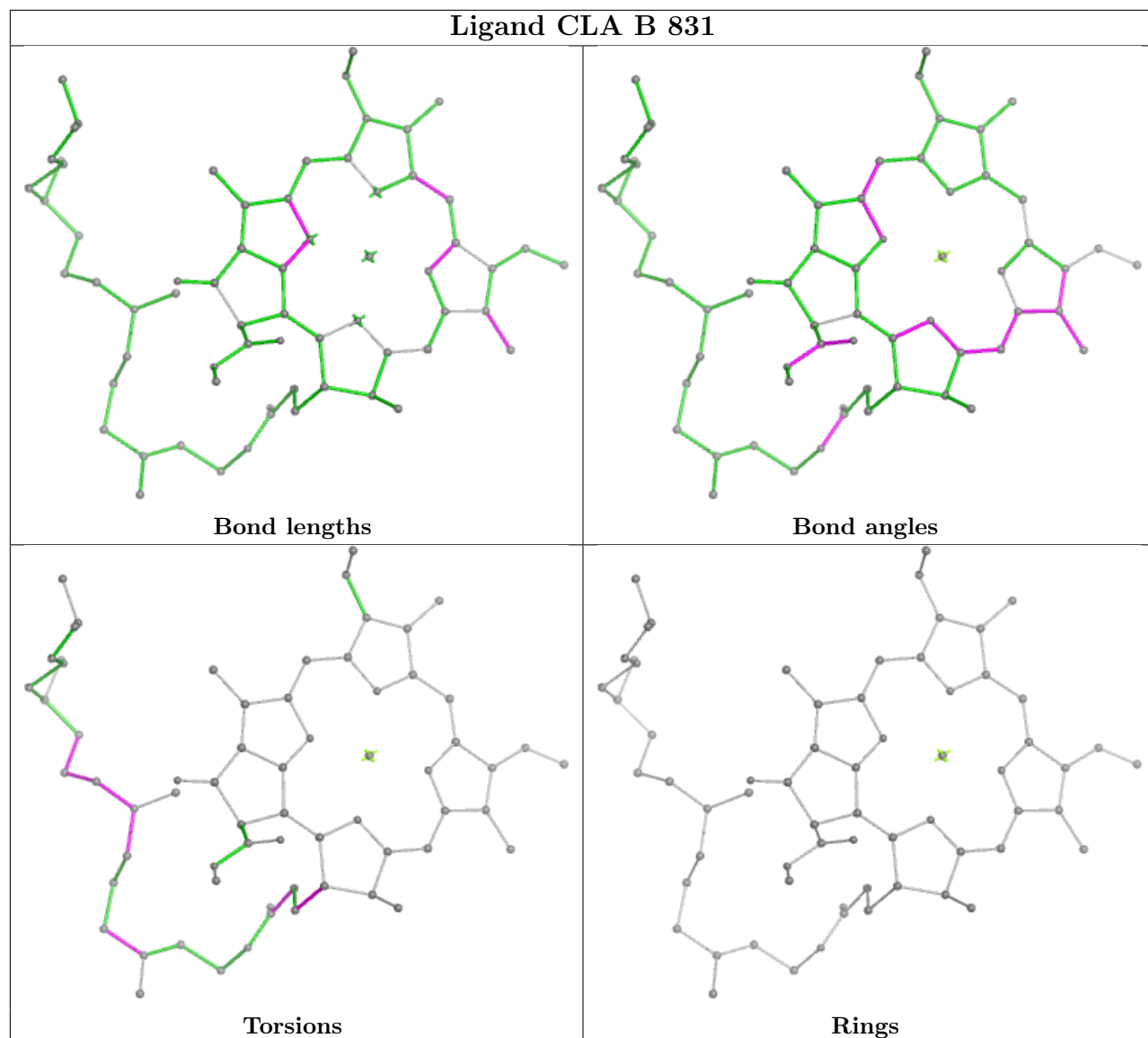
## Ligand BCR U 102

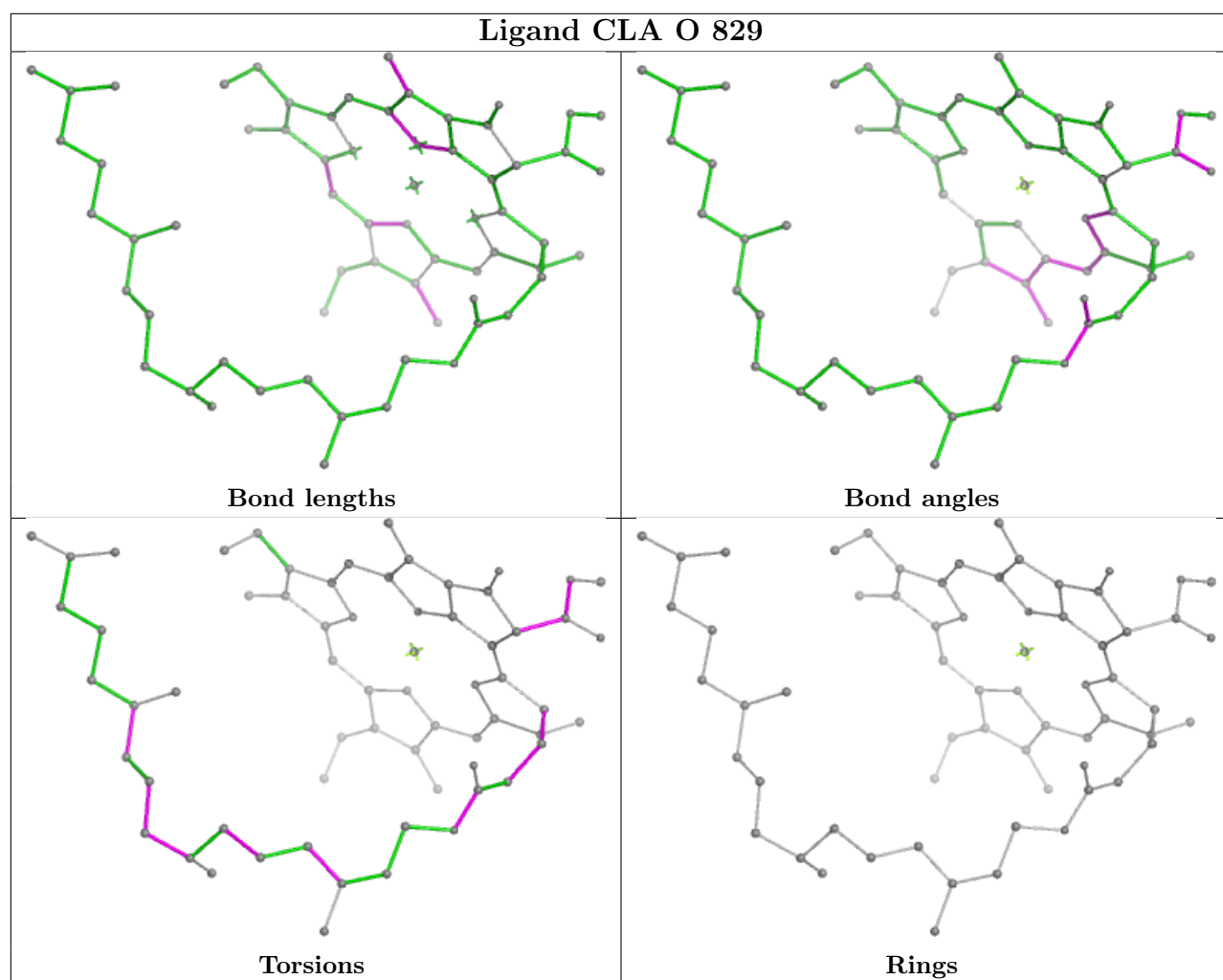


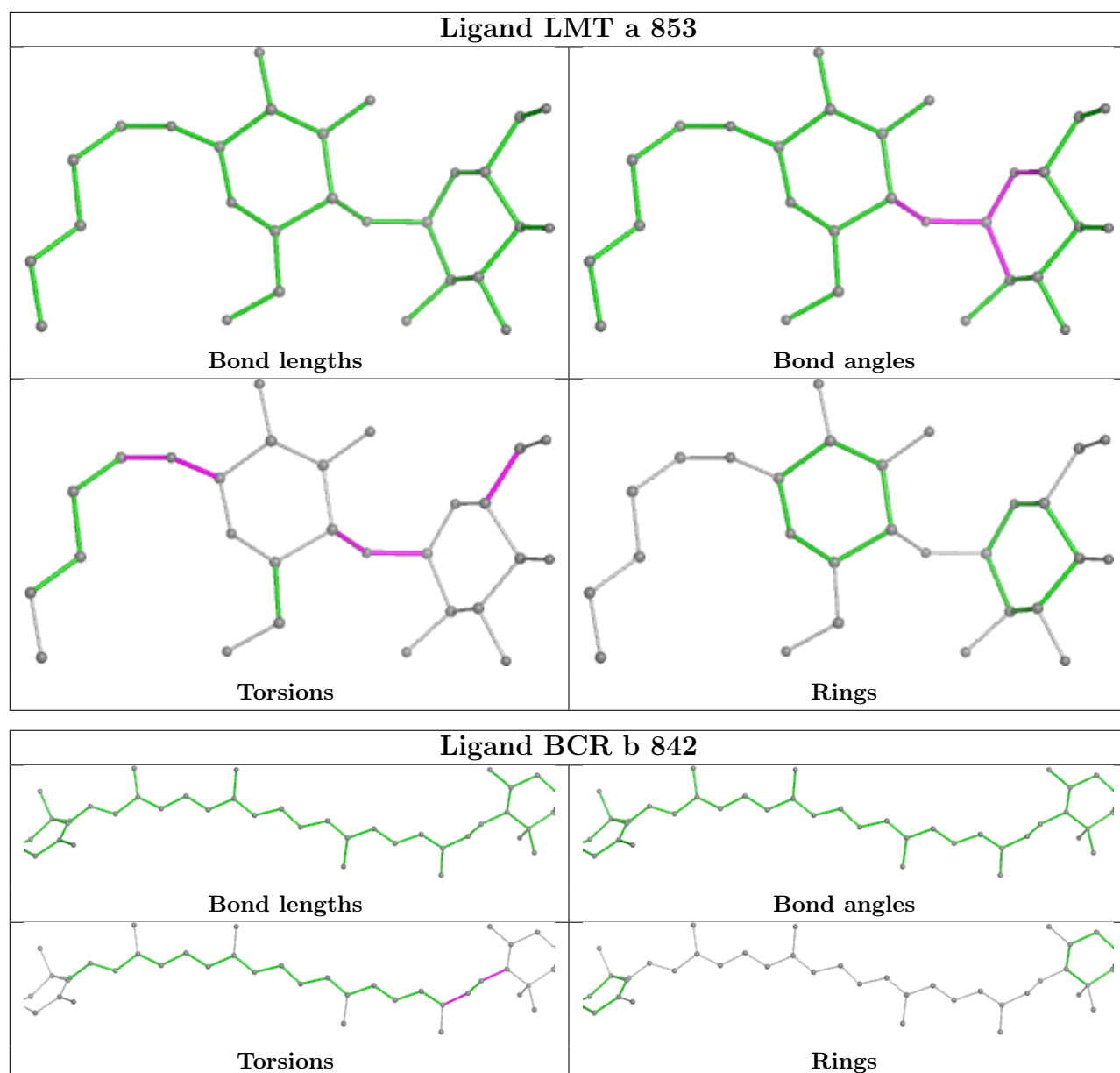


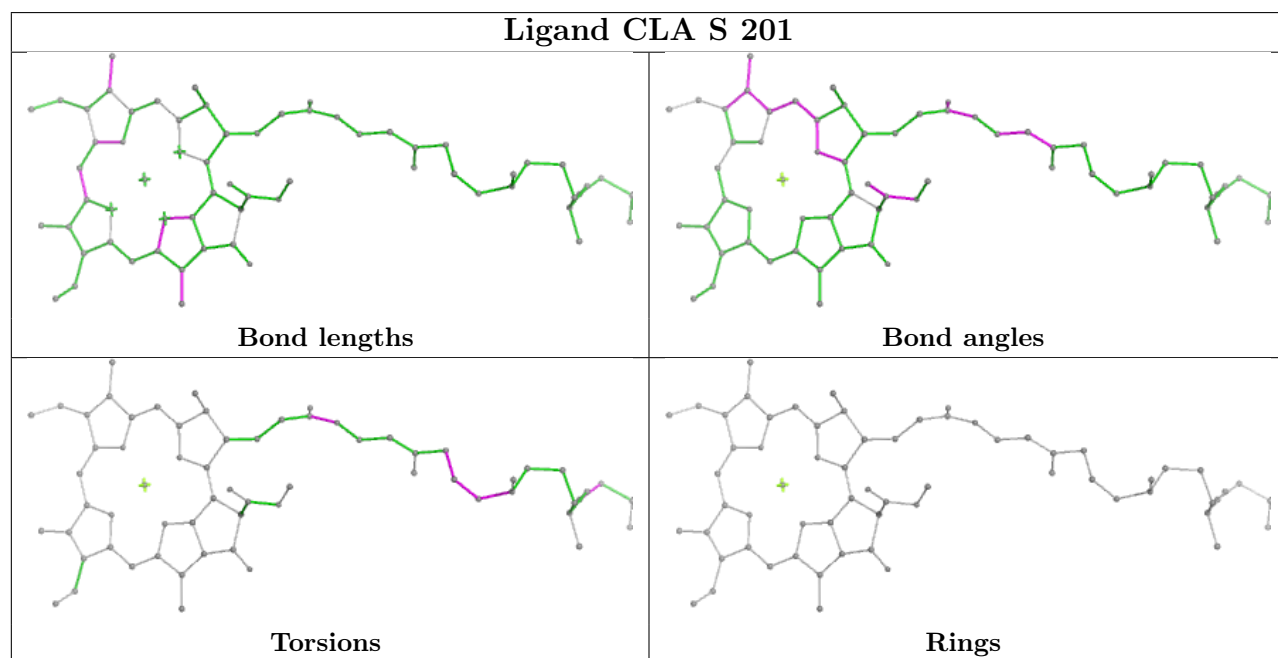
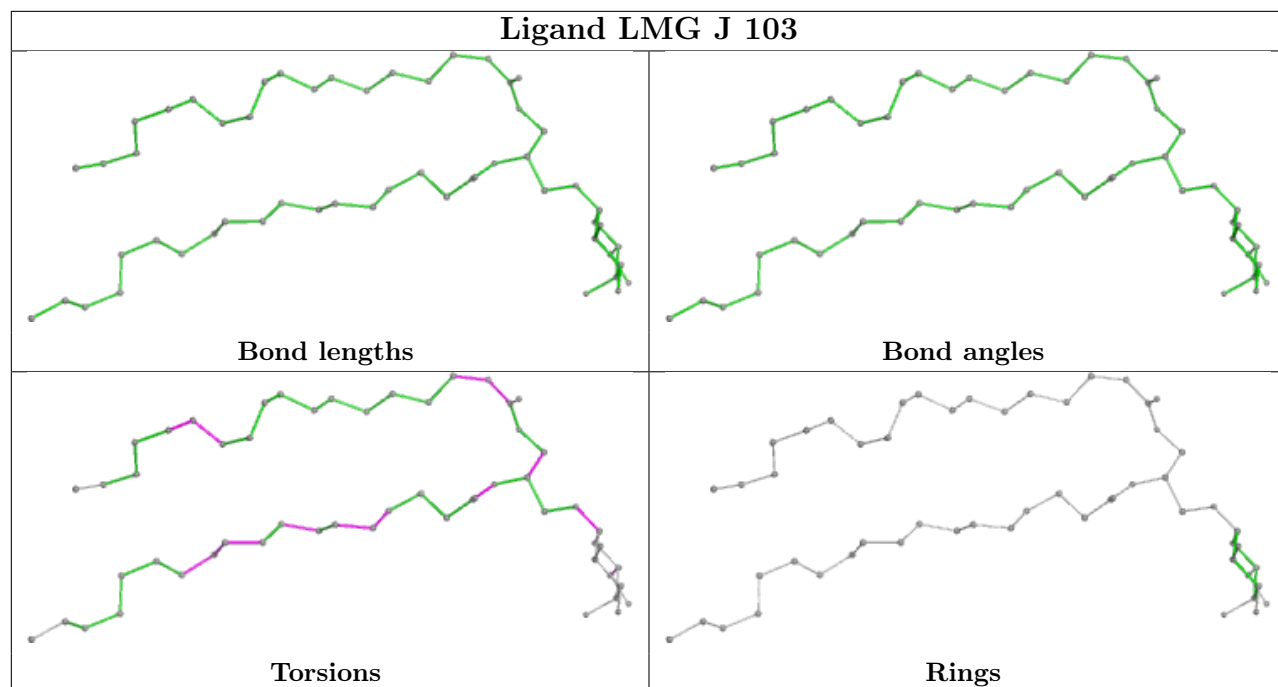


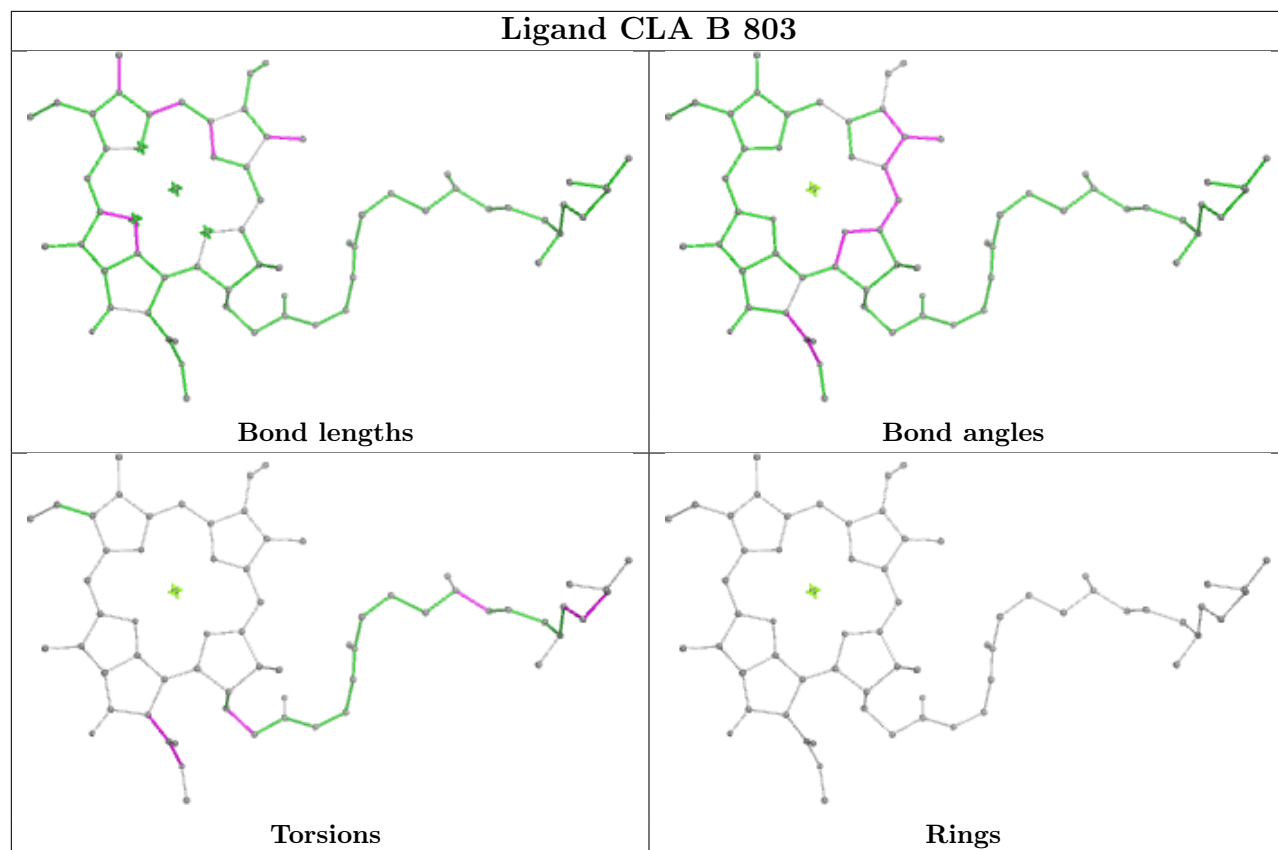
## Ligand CLA B 831





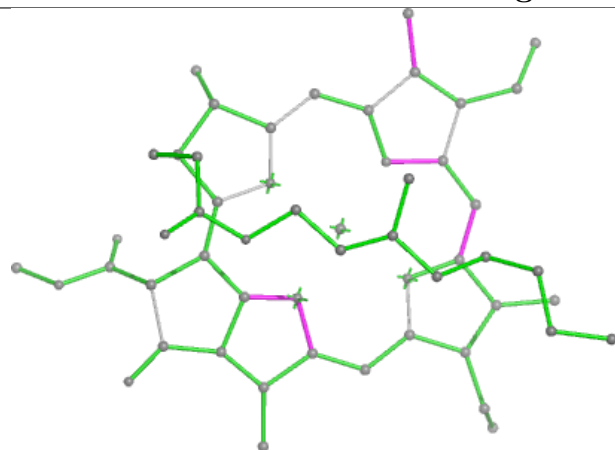




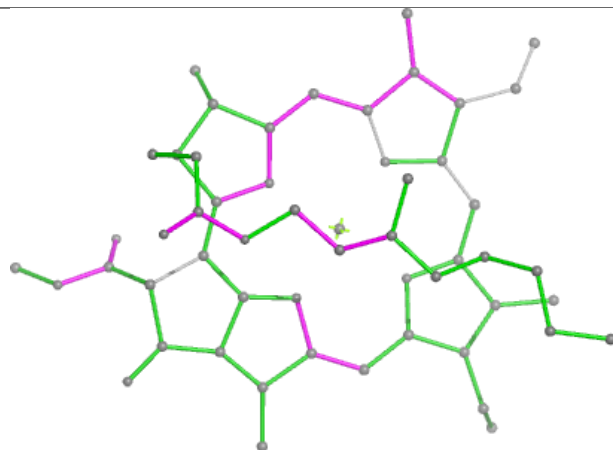




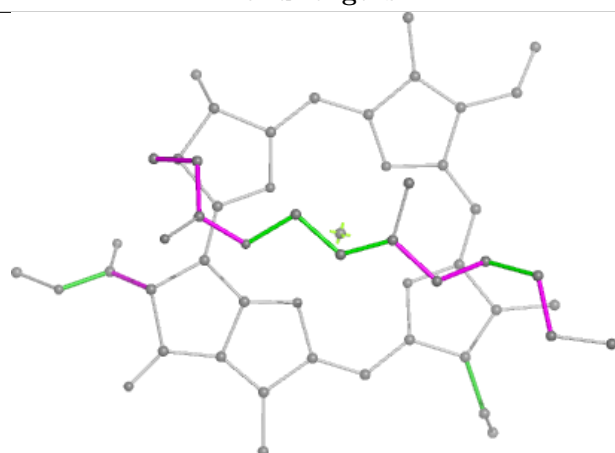
## Ligand CLA N 813



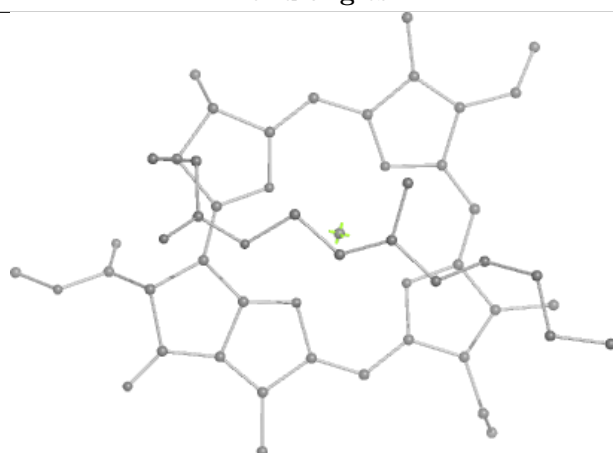
Bond lengths



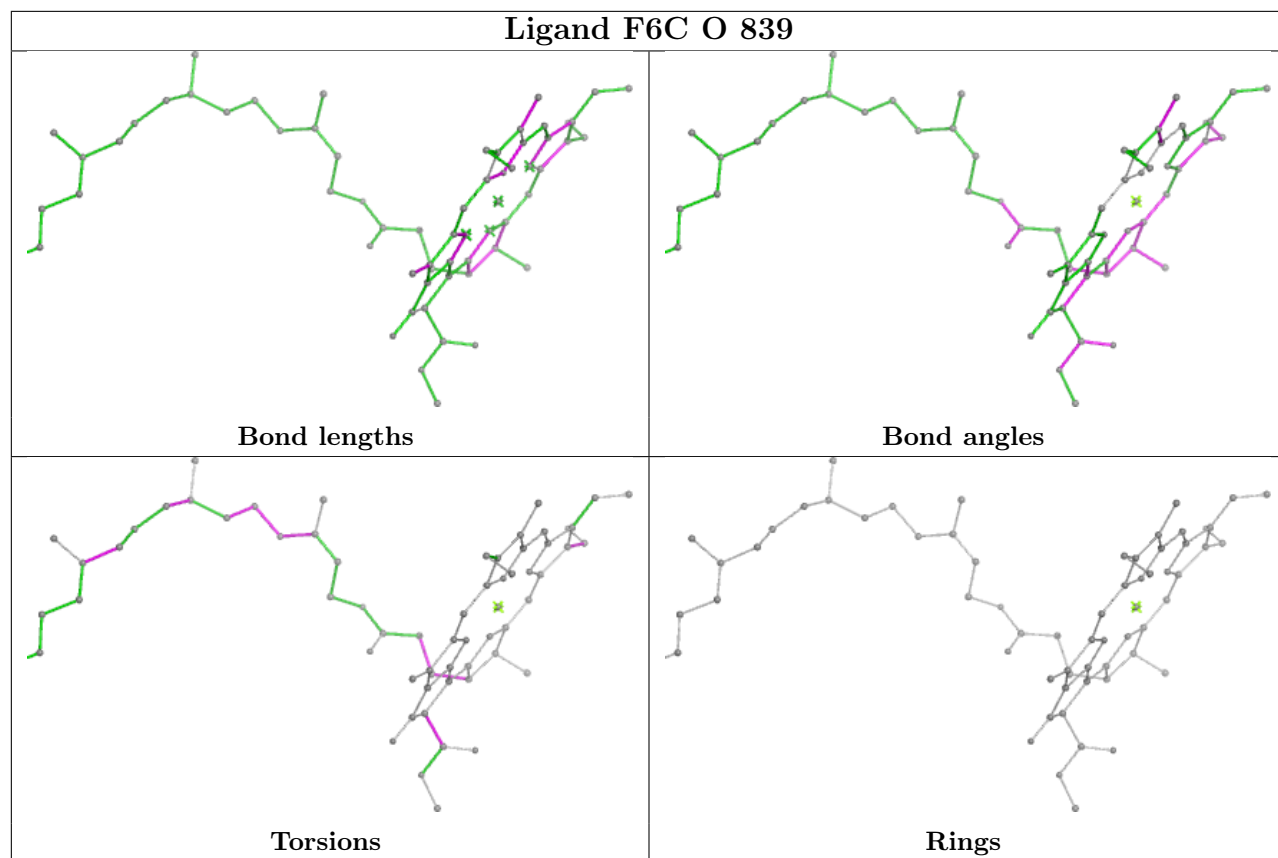
Bond angles



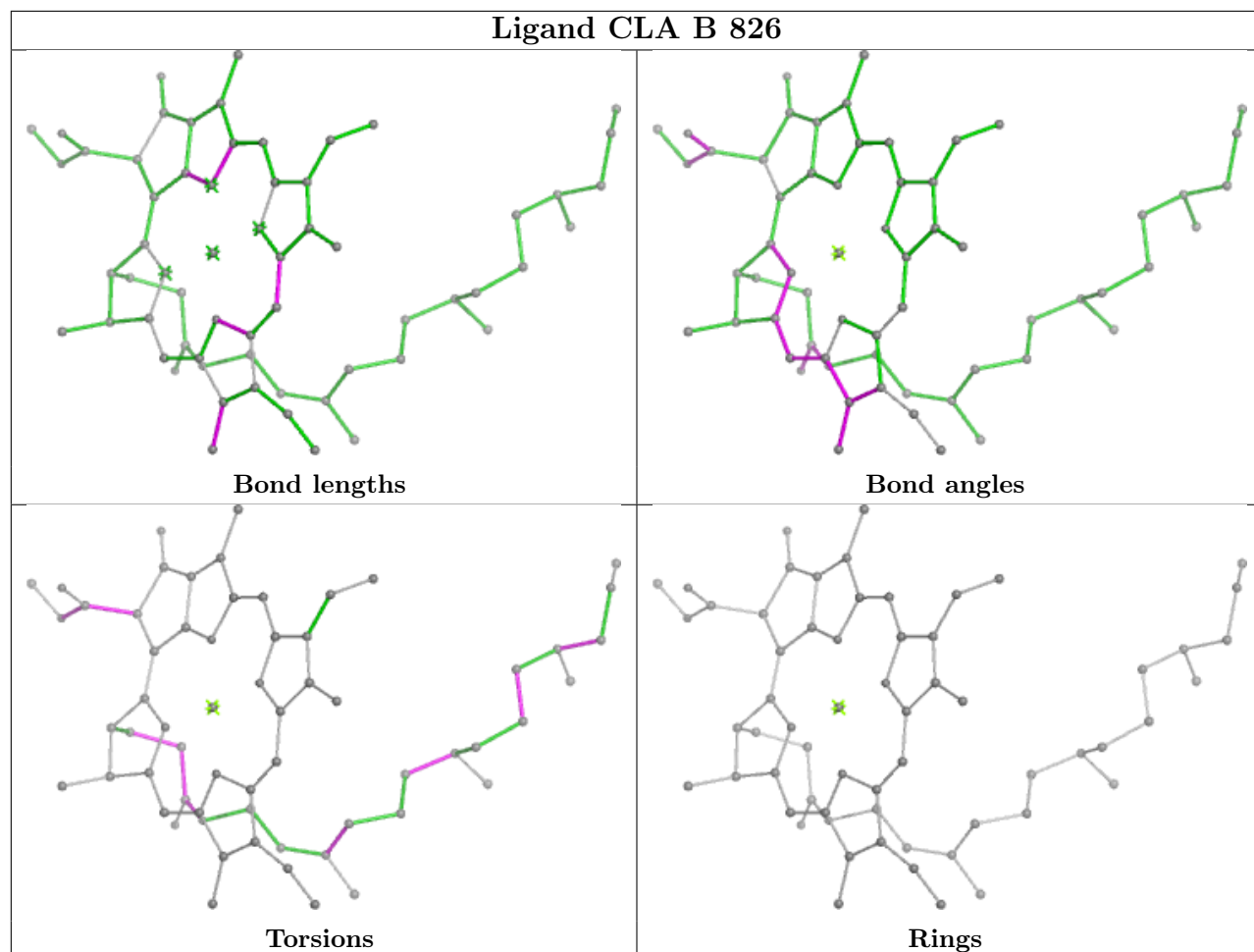
Torsions



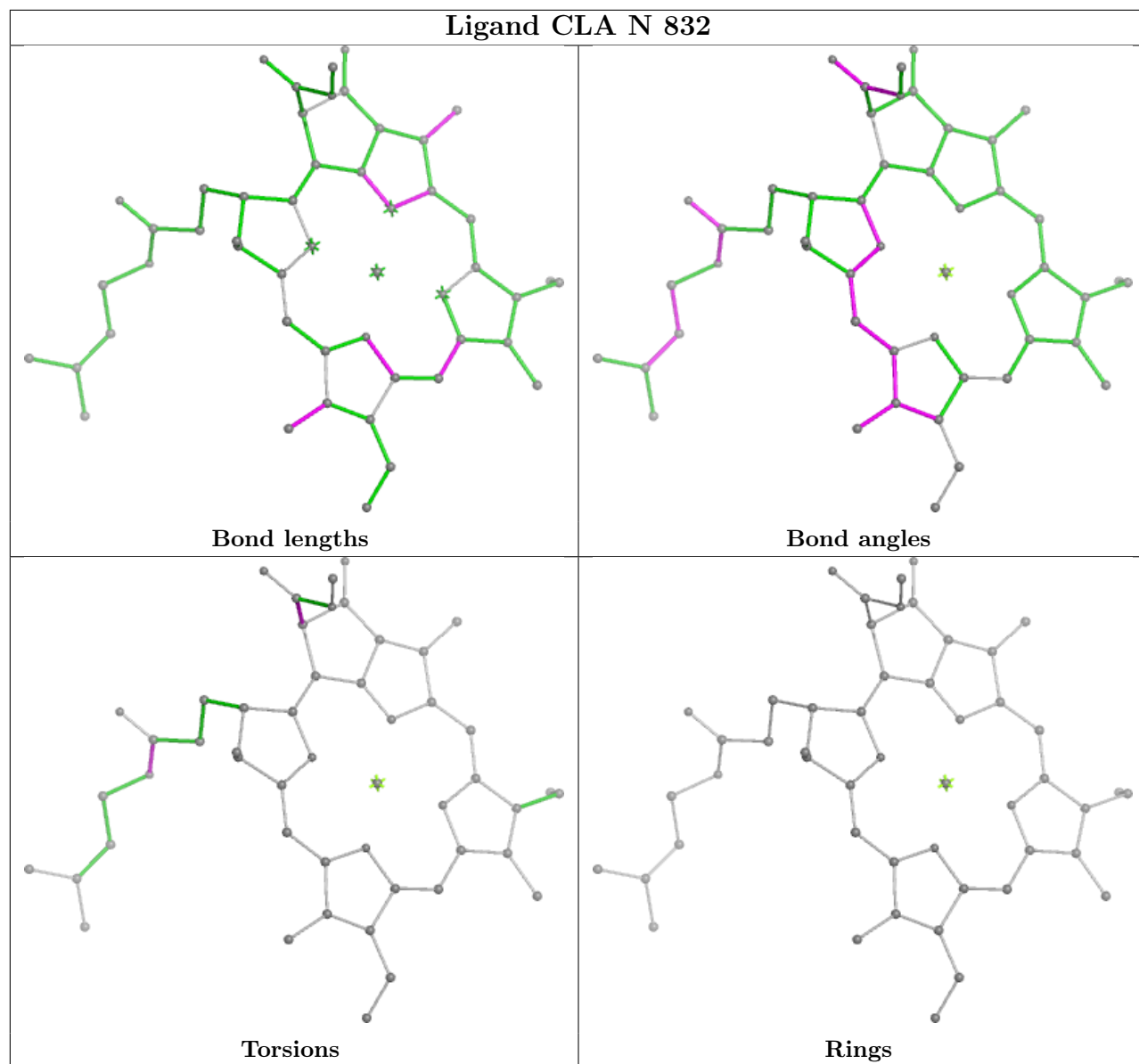
Rings



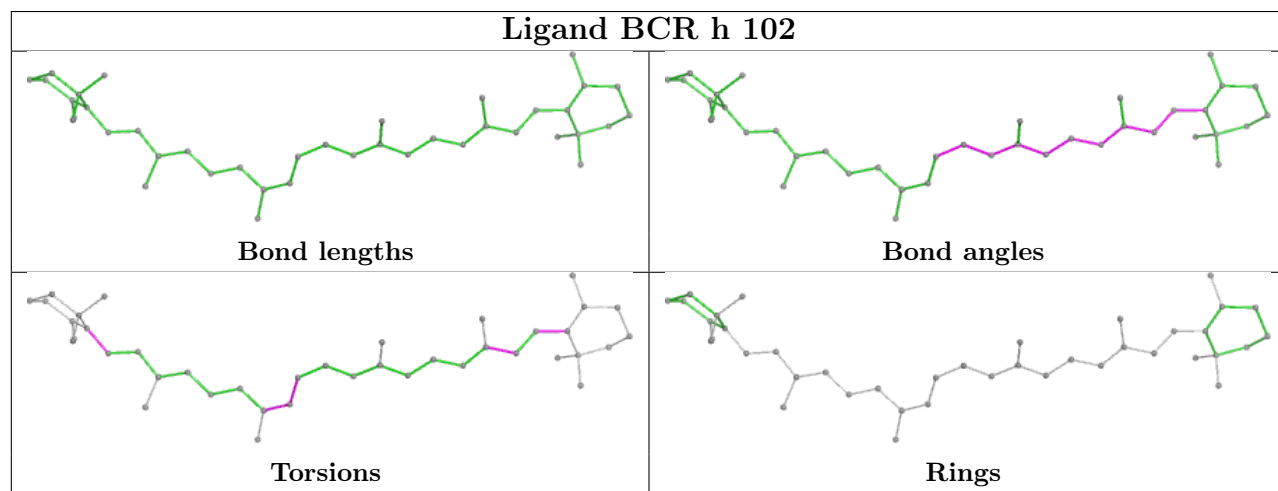
## Ligand CLA B 826



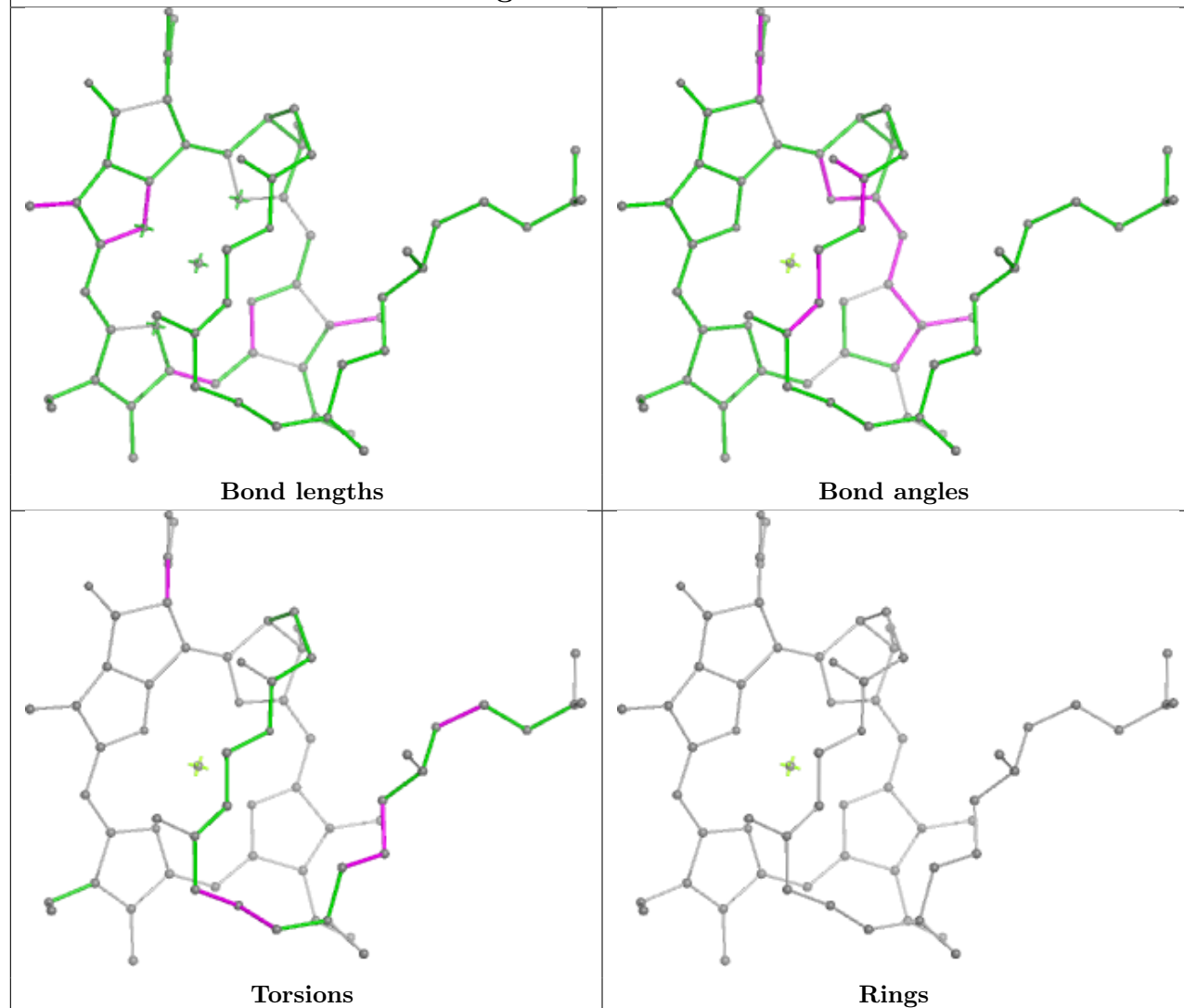
## Ligand CLA N 832



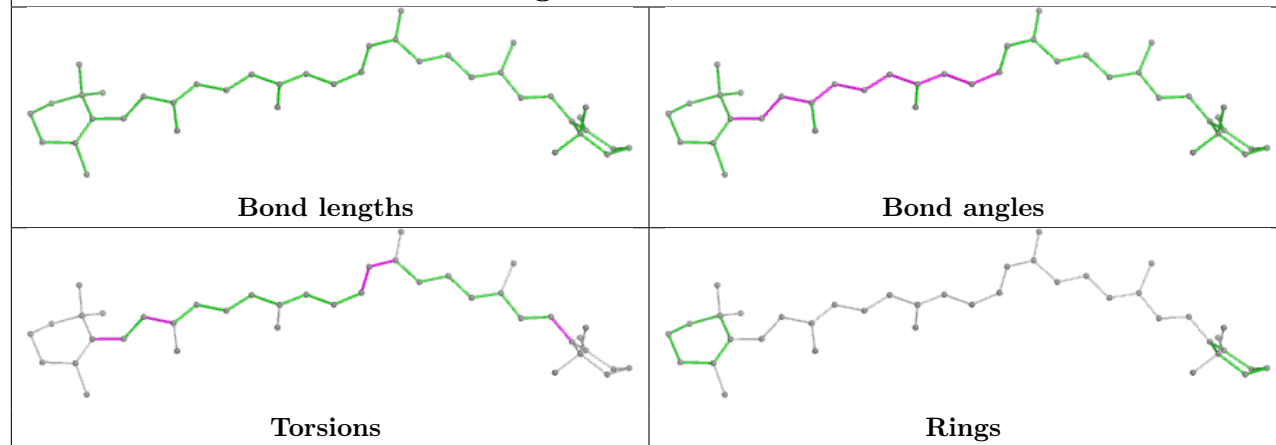
## Ligand BCR h 102



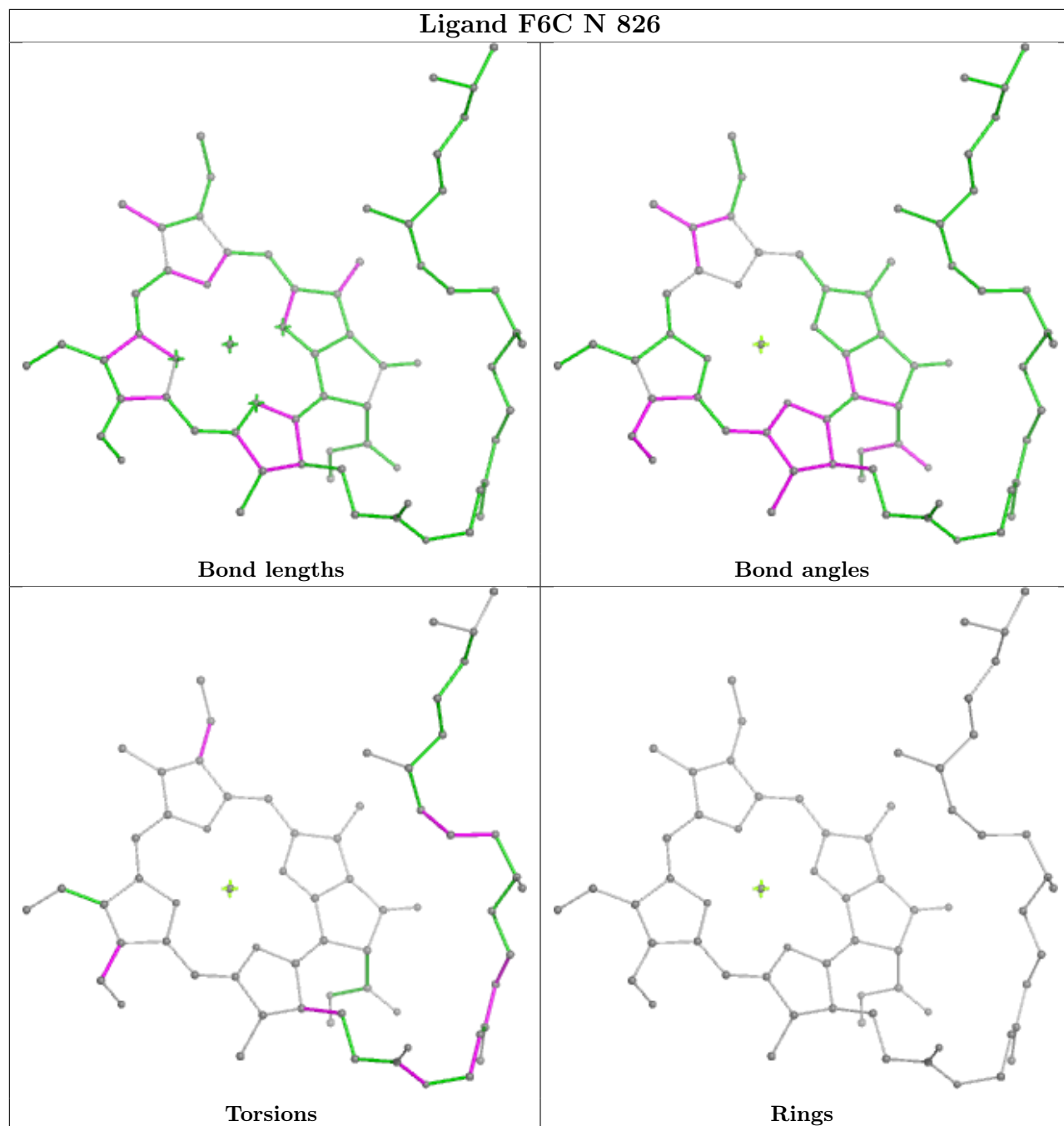
## Ligand CLA b 808

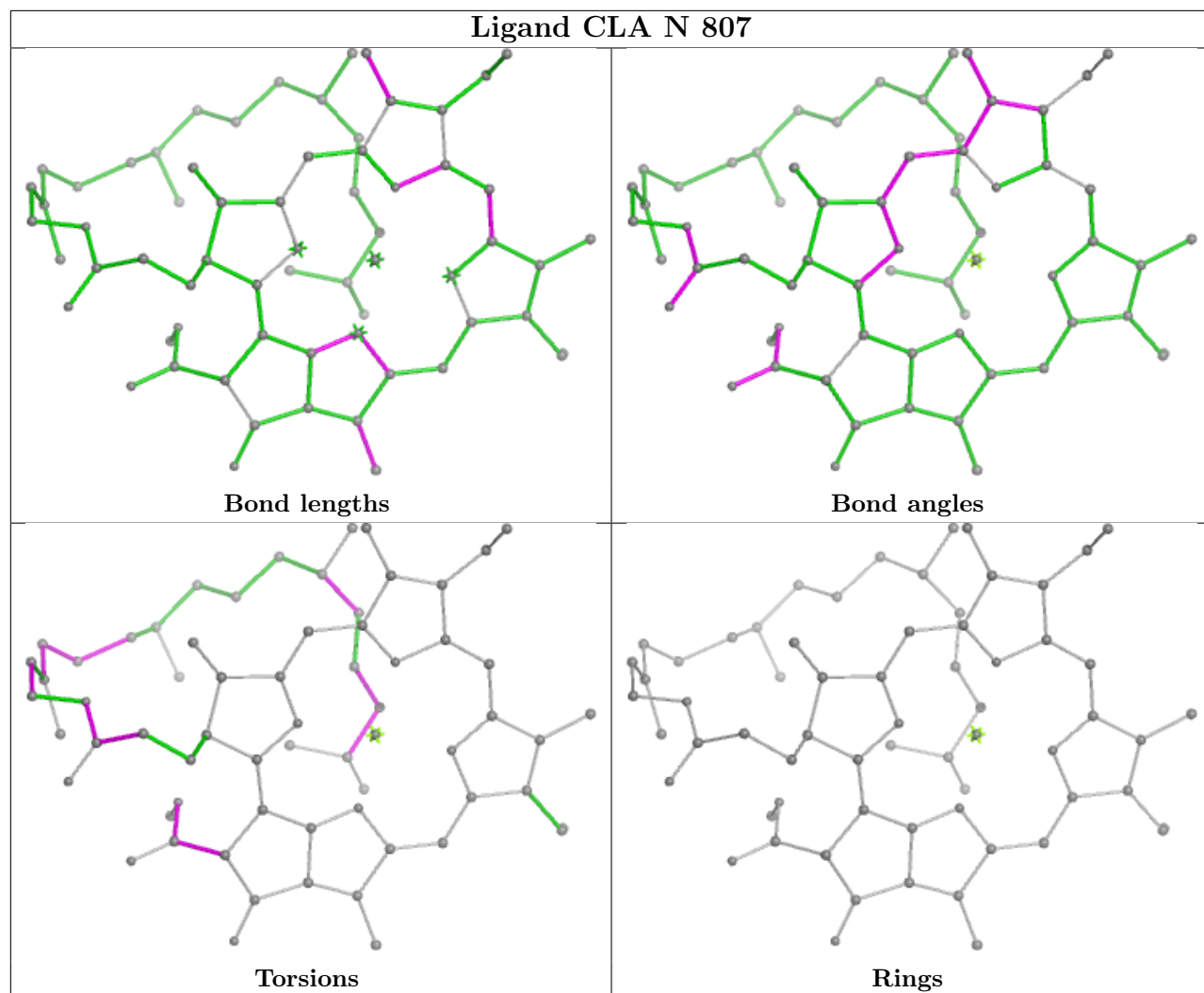


## Ligand BCR J 102

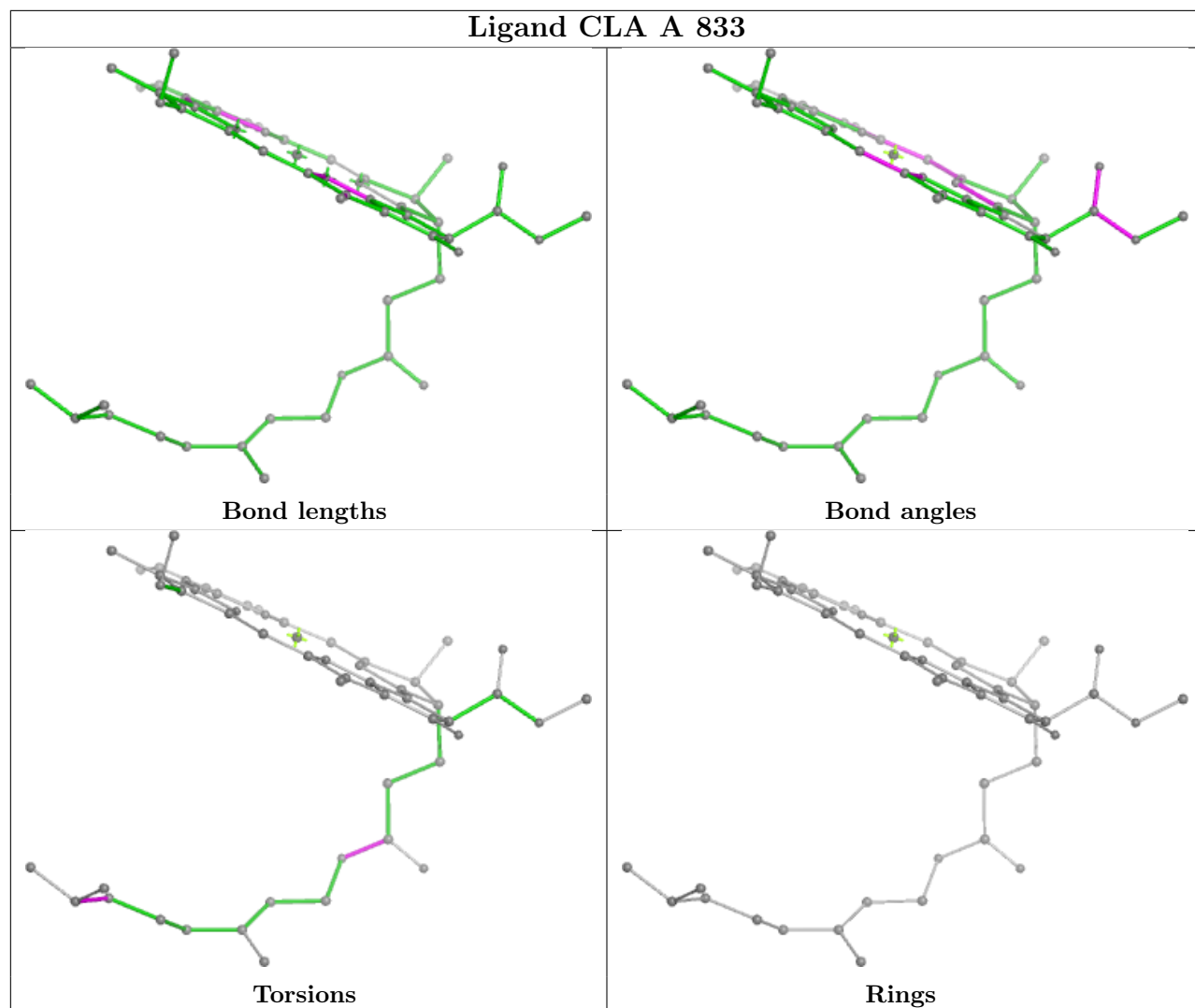


## Ligand F6C N 826

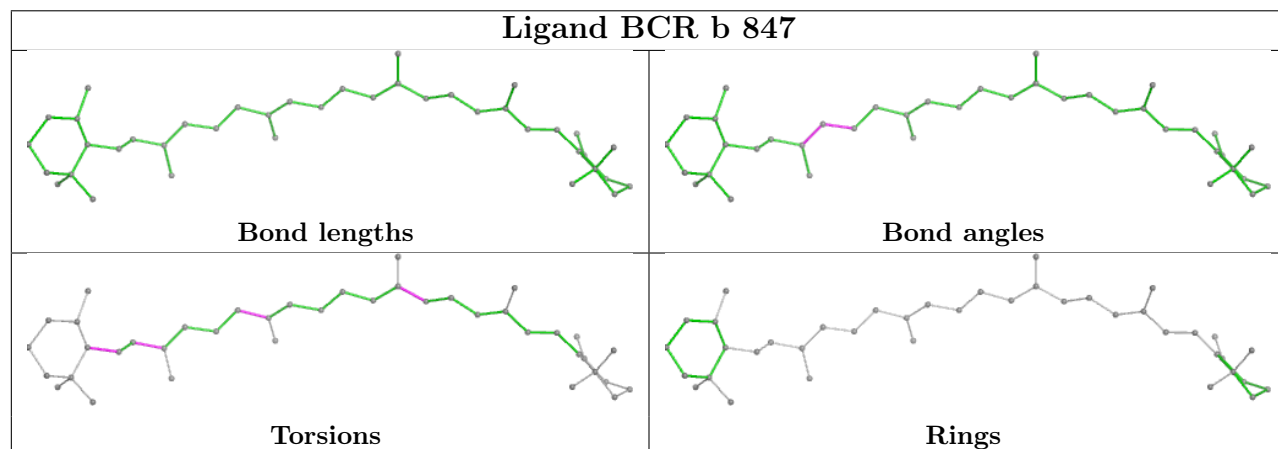




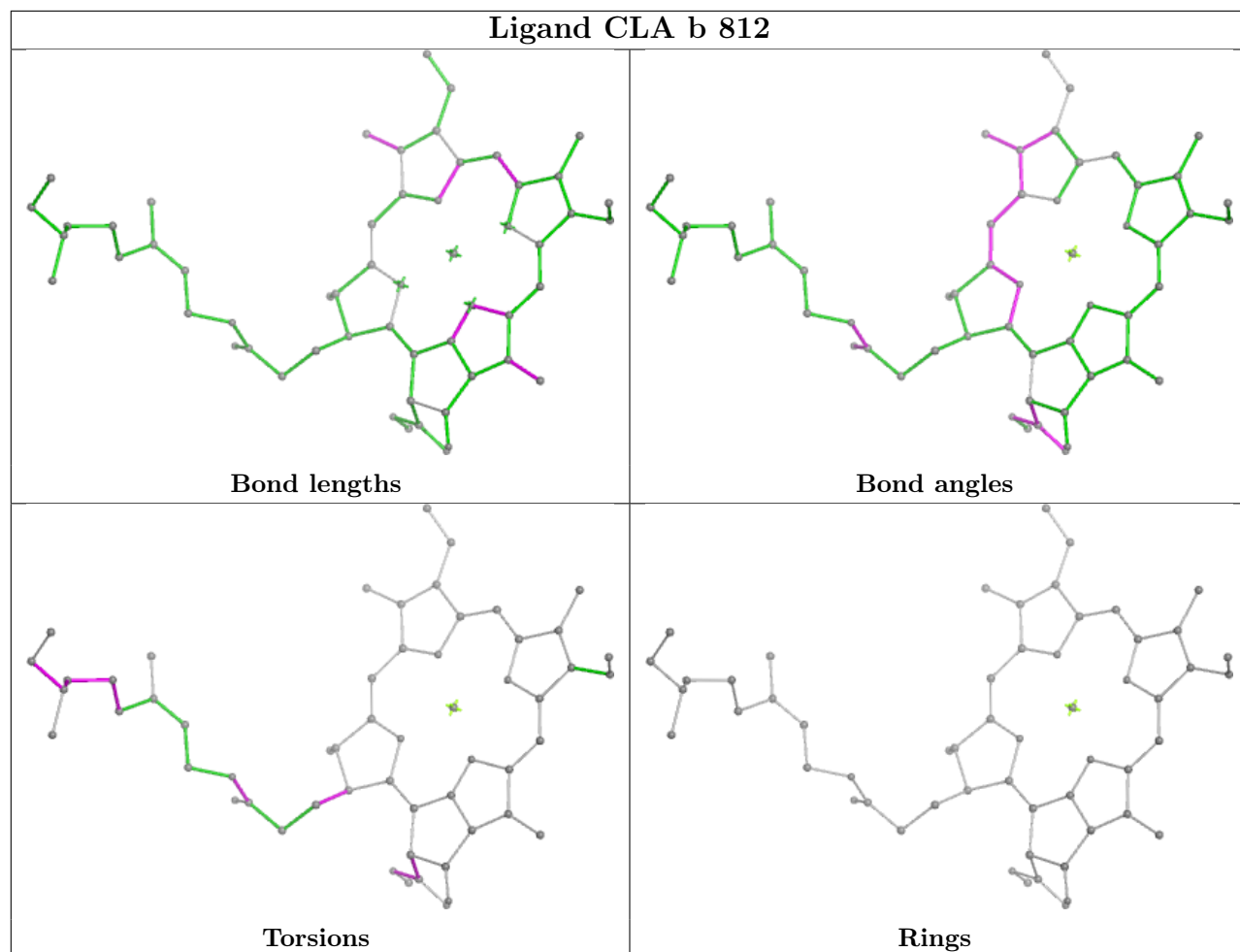
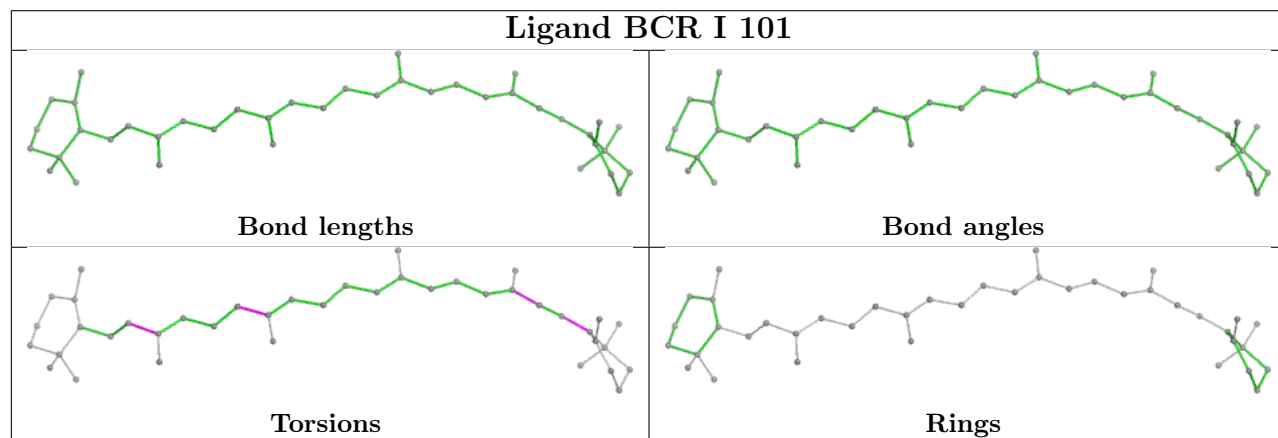
## Ligand CLA A 833



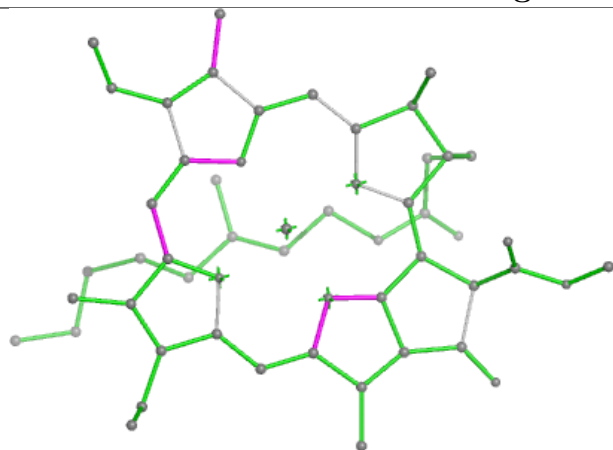
## Ligand BCR b 847



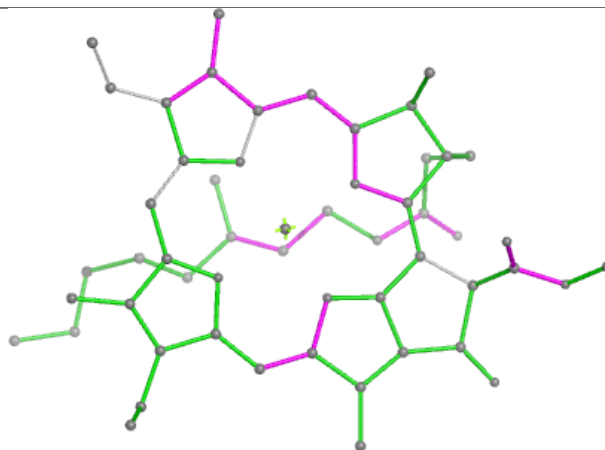


**Ligand CLA b 812****Ligand BCR I 101**

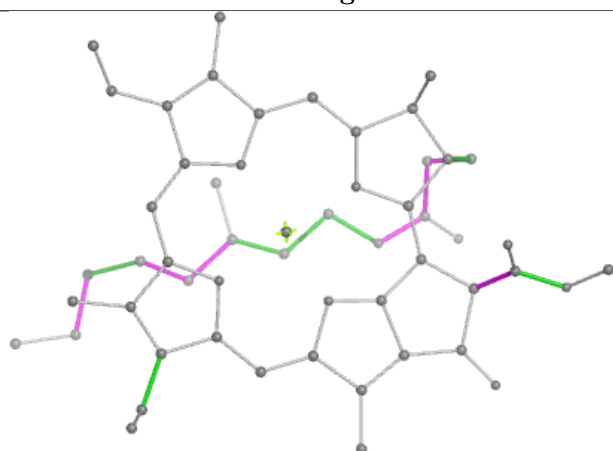
## Ligand CLA A 813



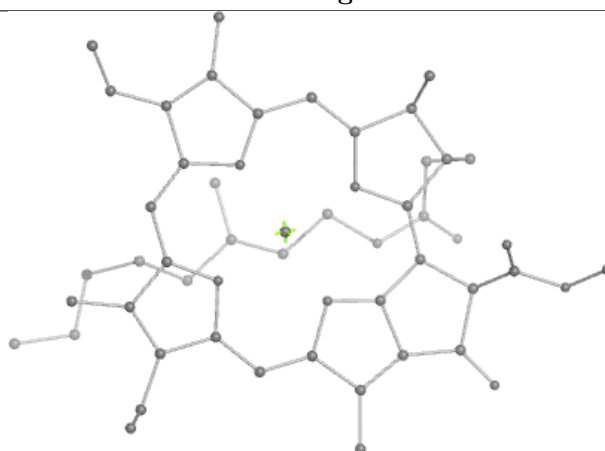
Bond lengths



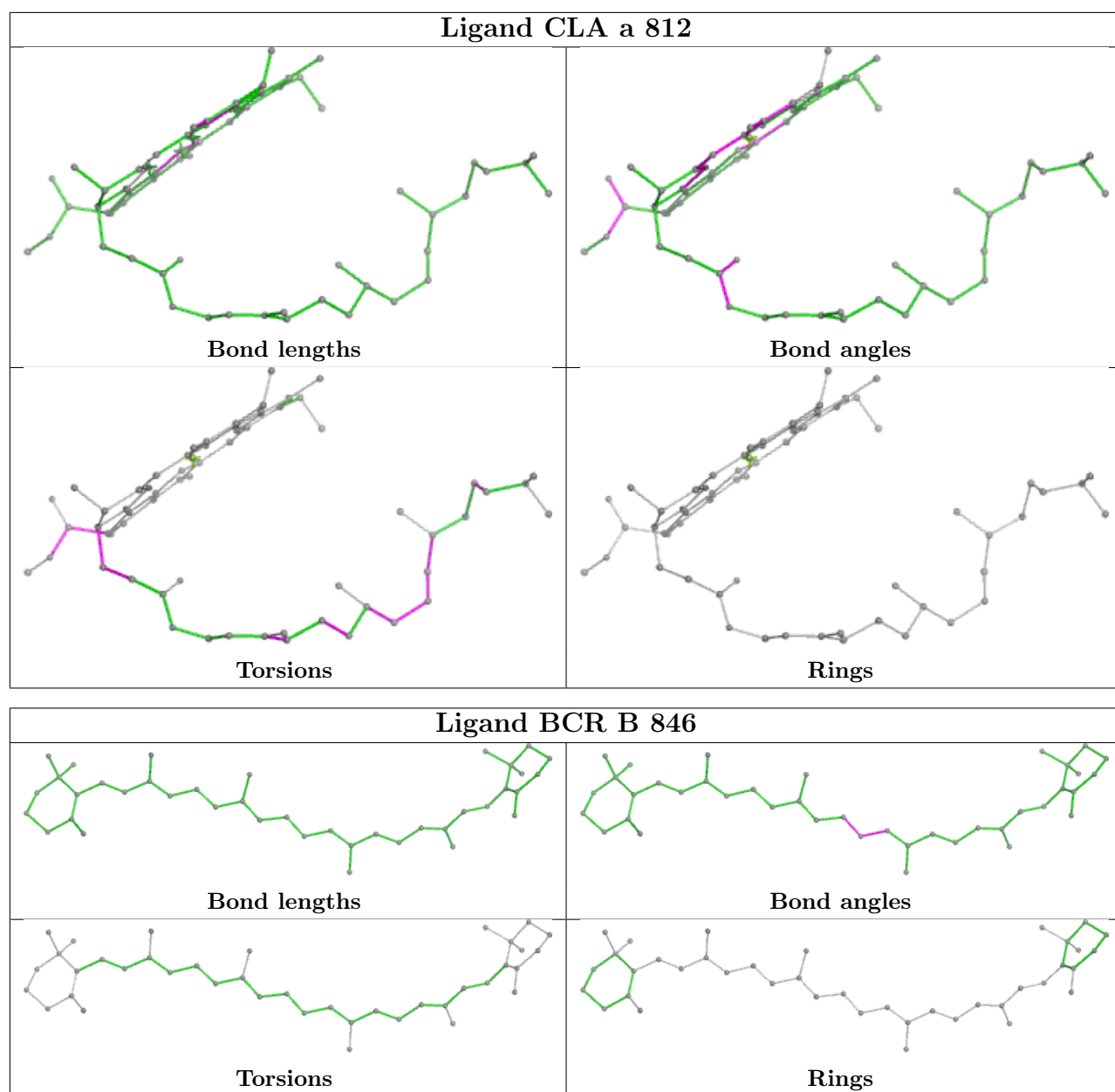
Bond angles



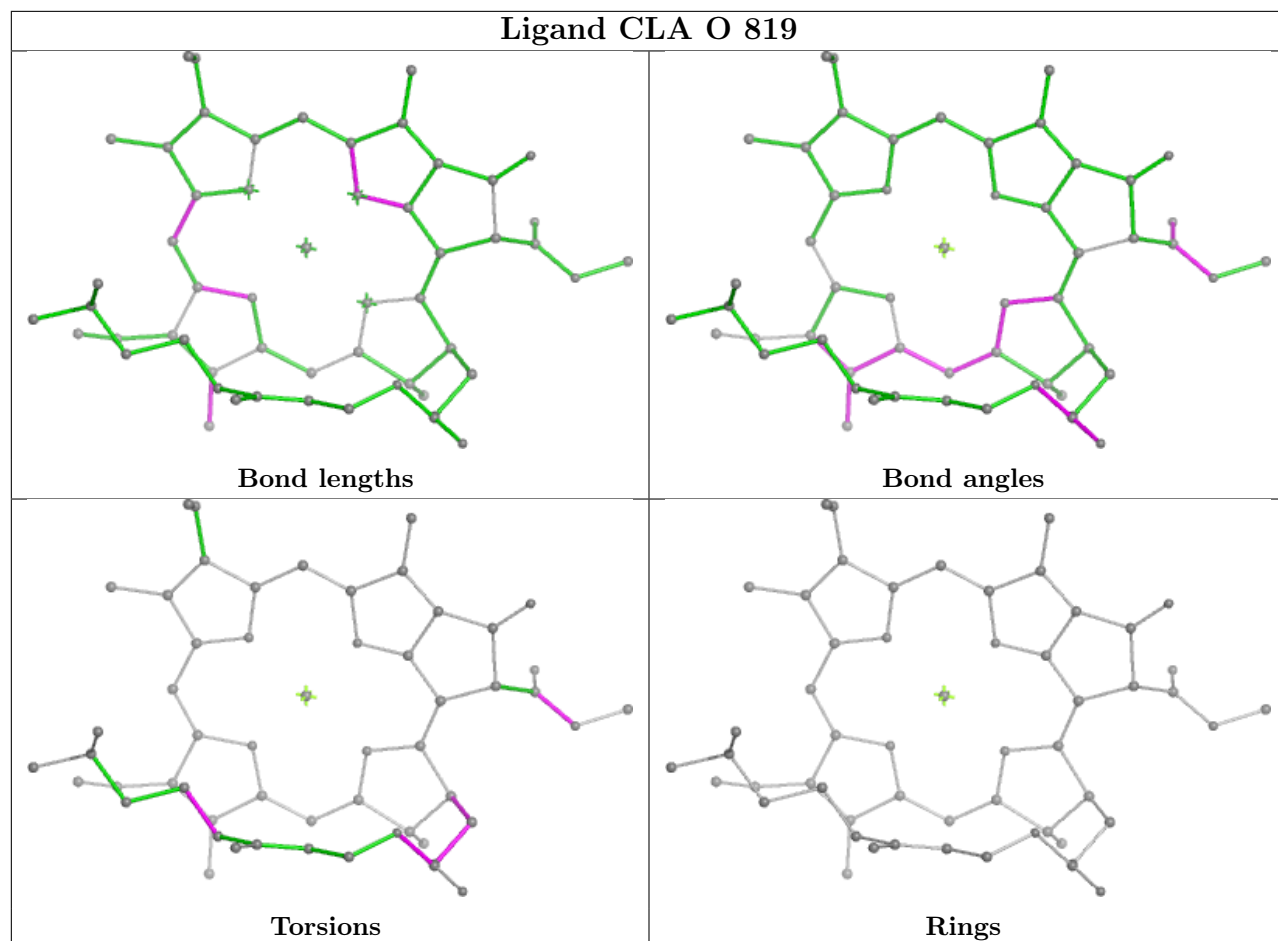
Torsions



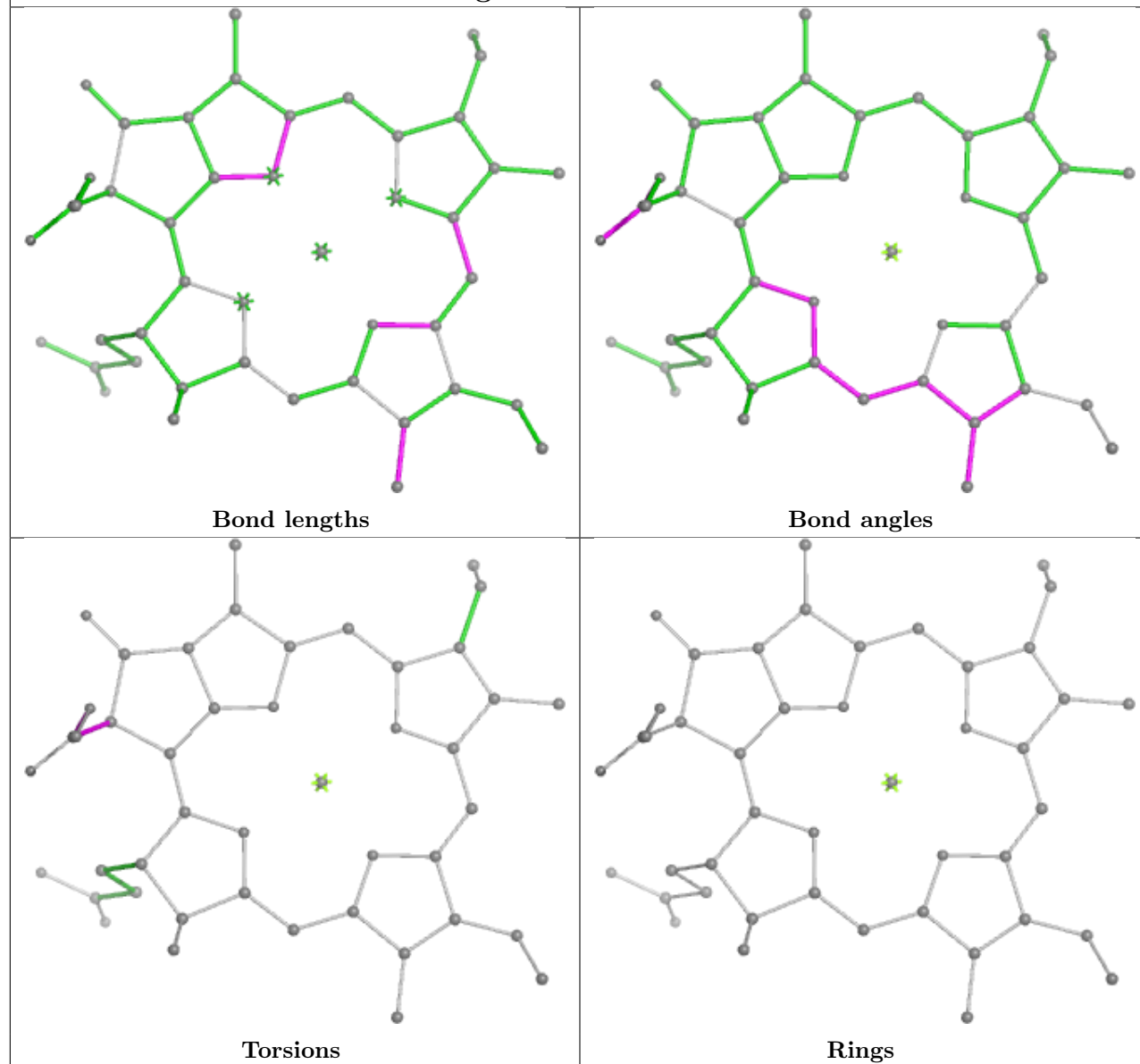
Rings



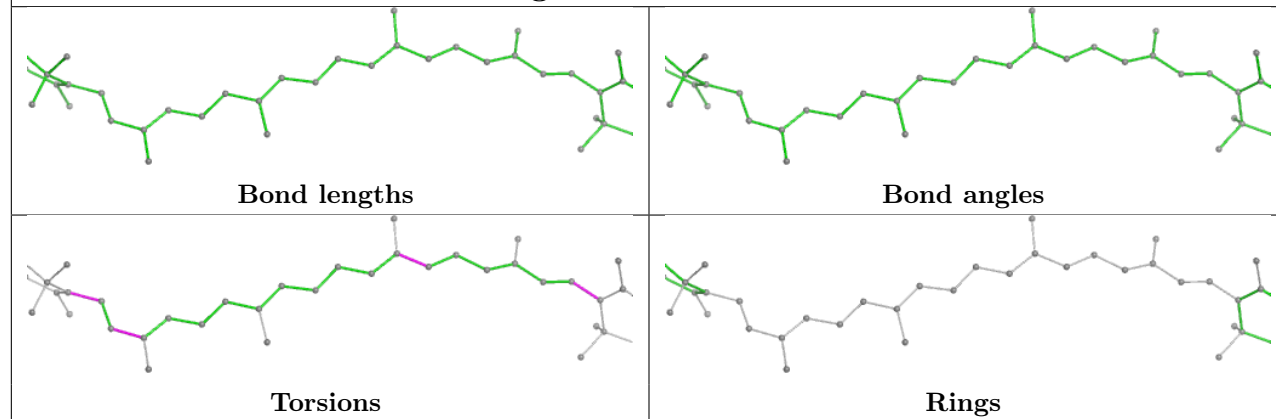
## Ligand CLA O 819



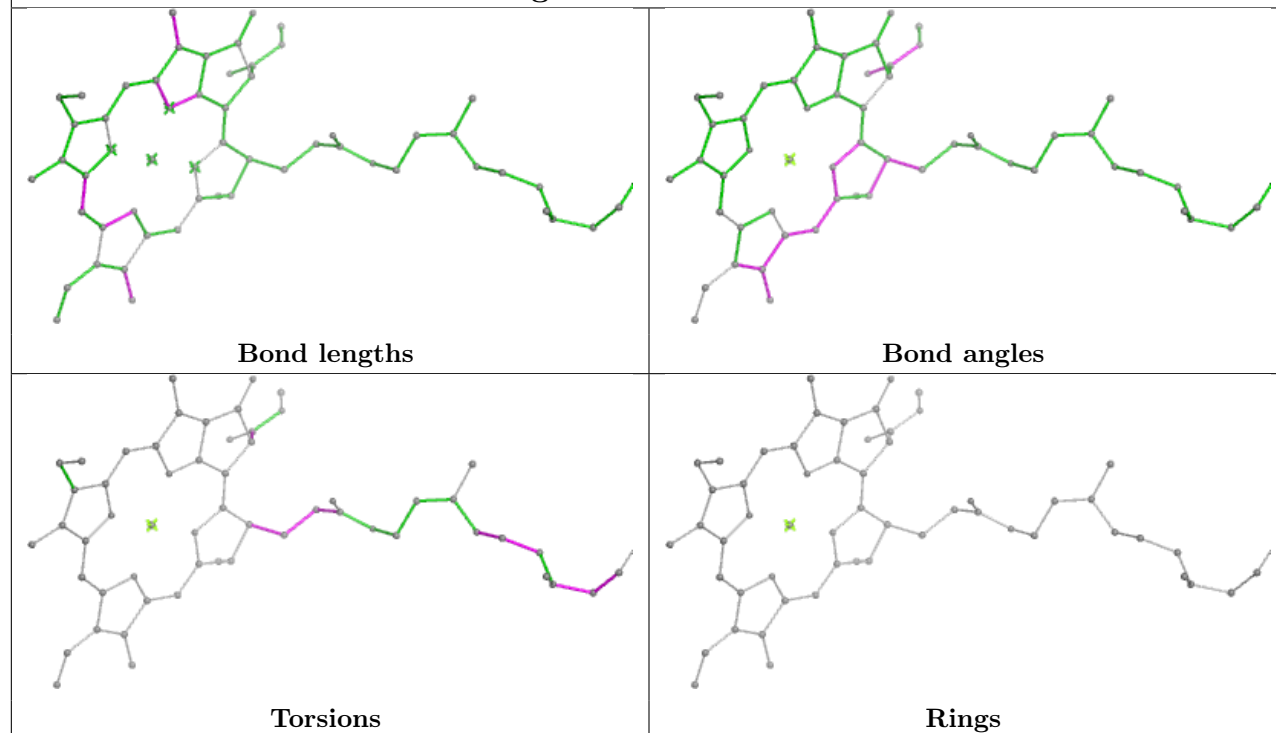
## Ligand CLA B 820



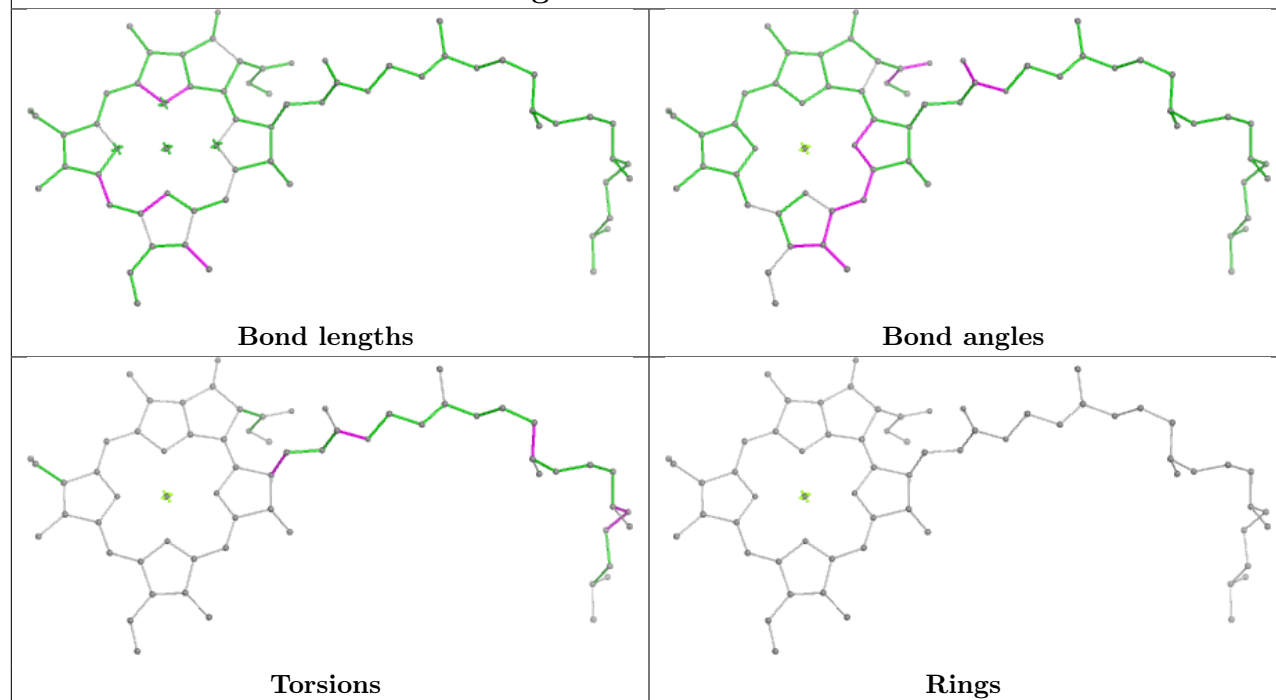
## Ligand BCR B 845

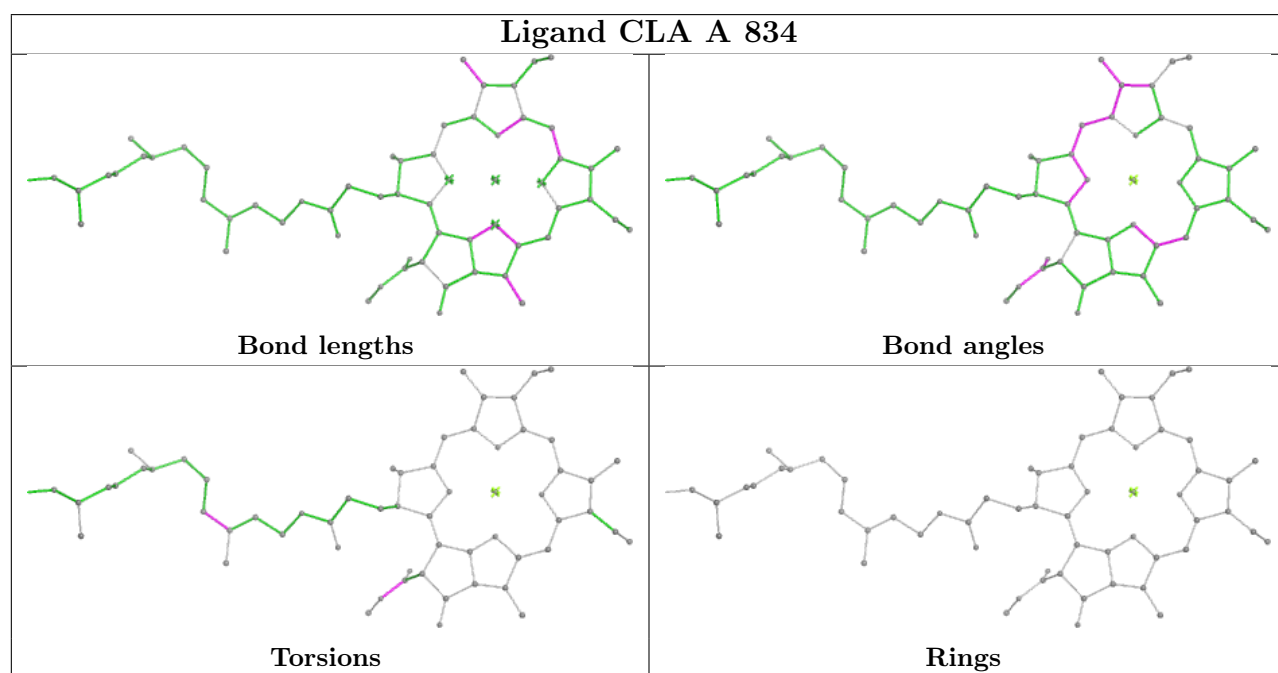
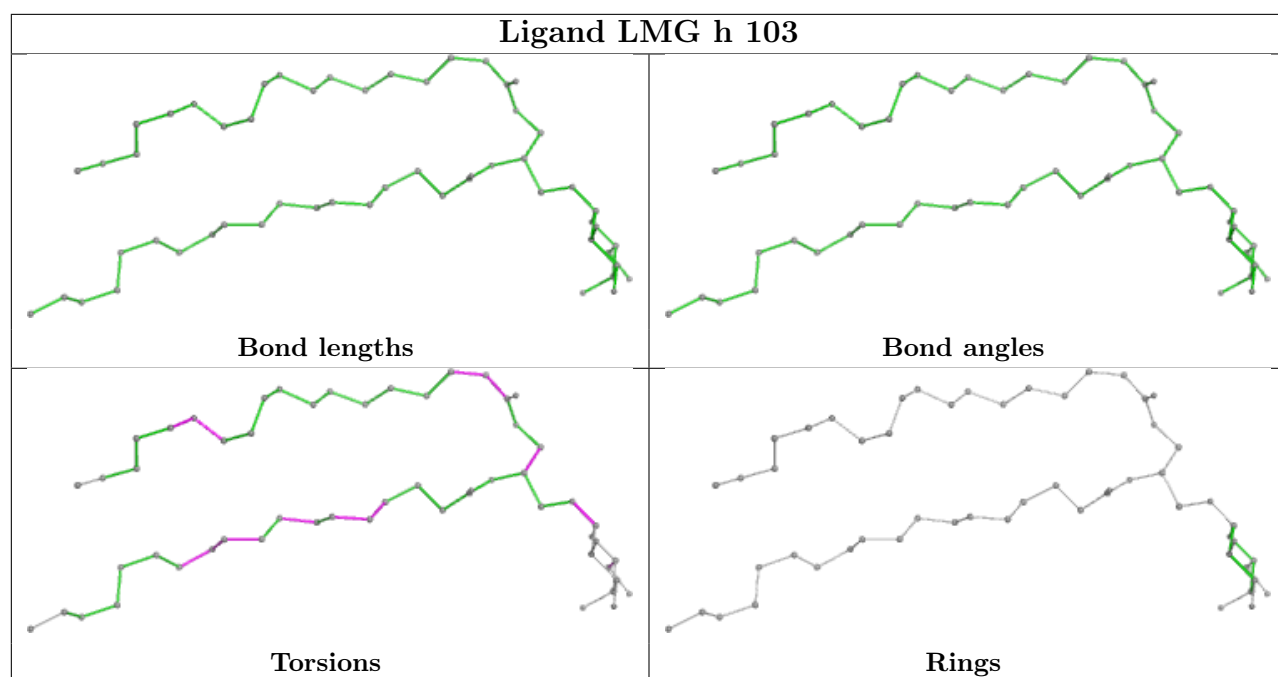


## Ligand CLA N 810

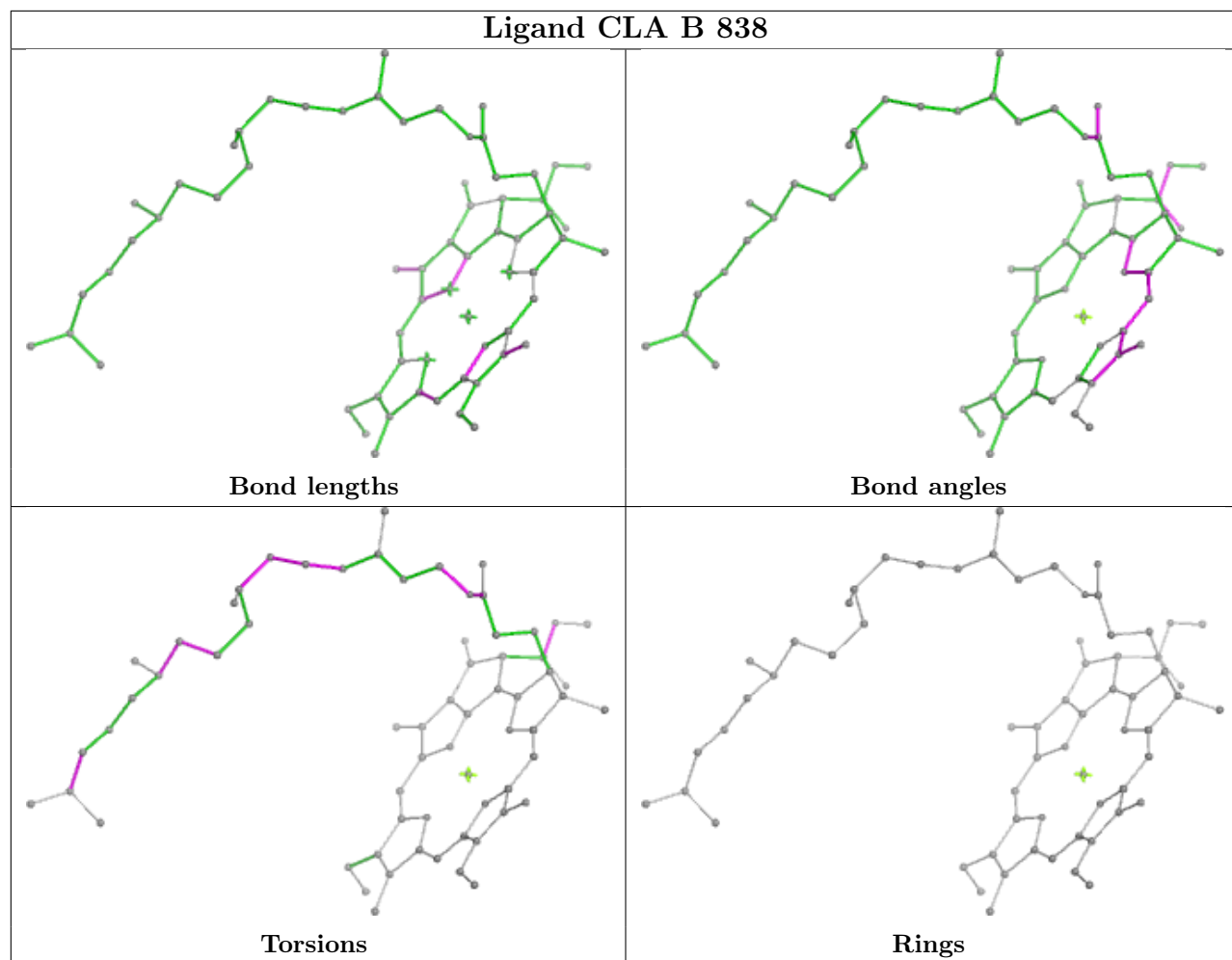


## Ligand CLA O 836

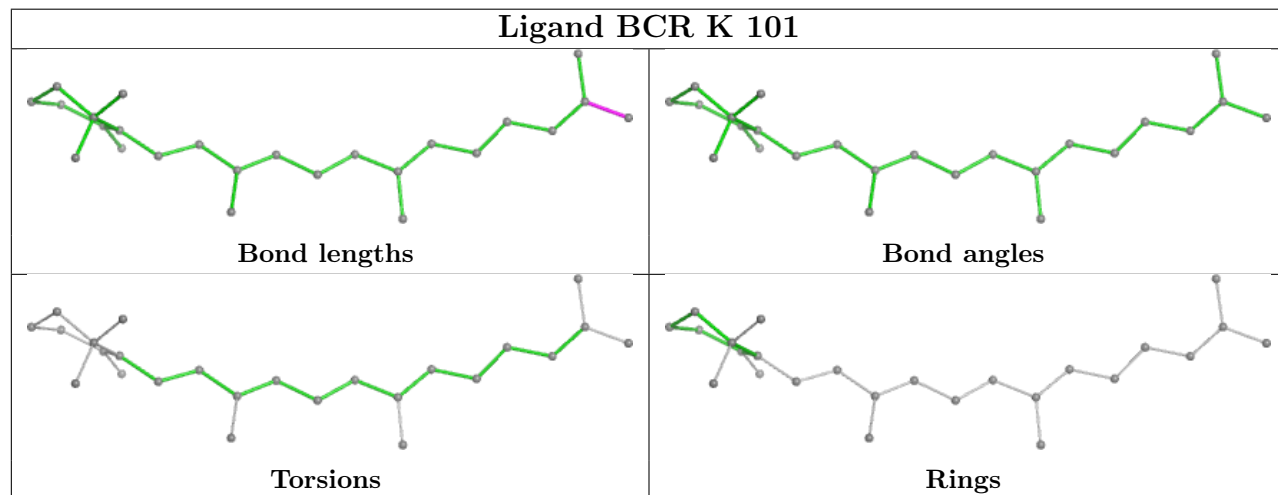




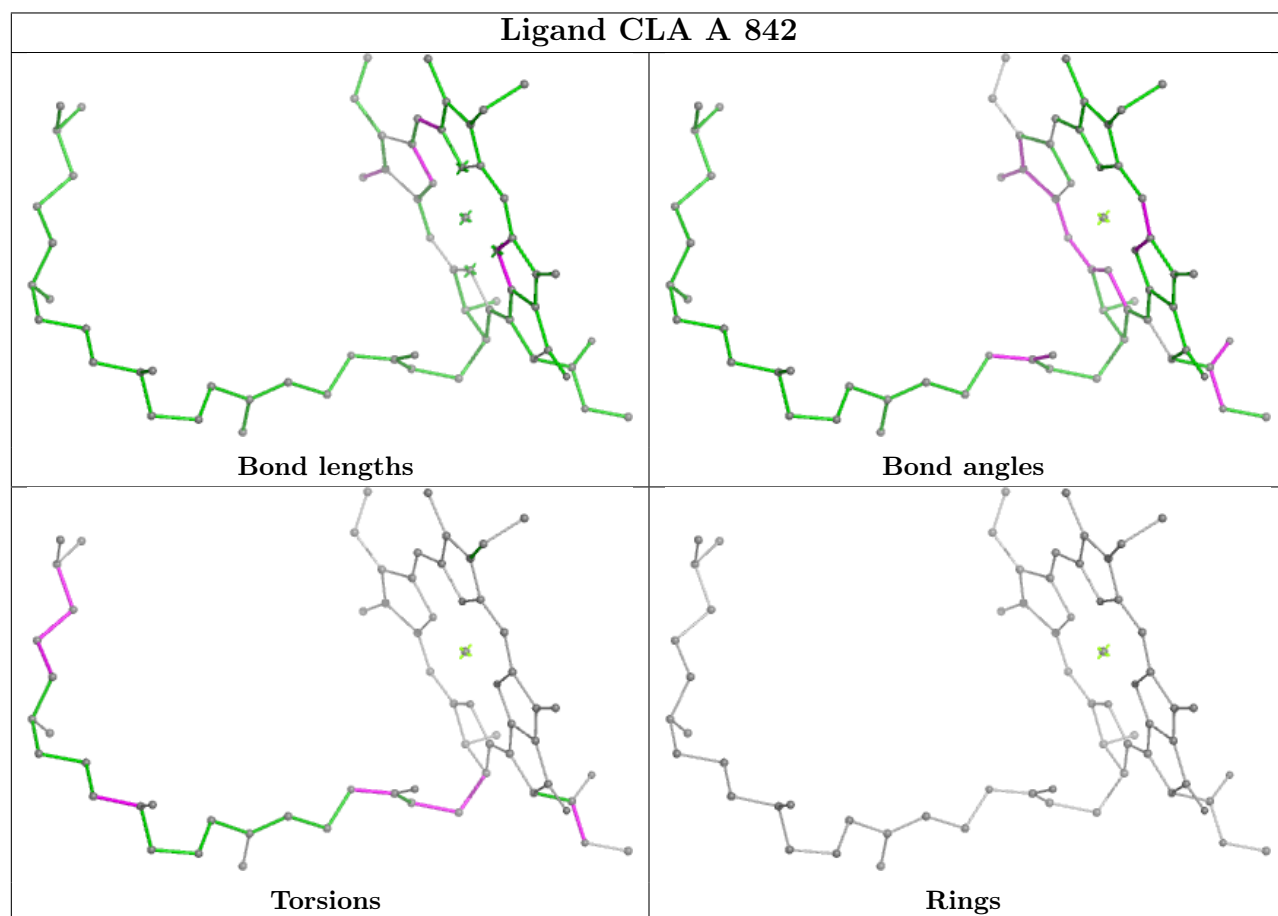
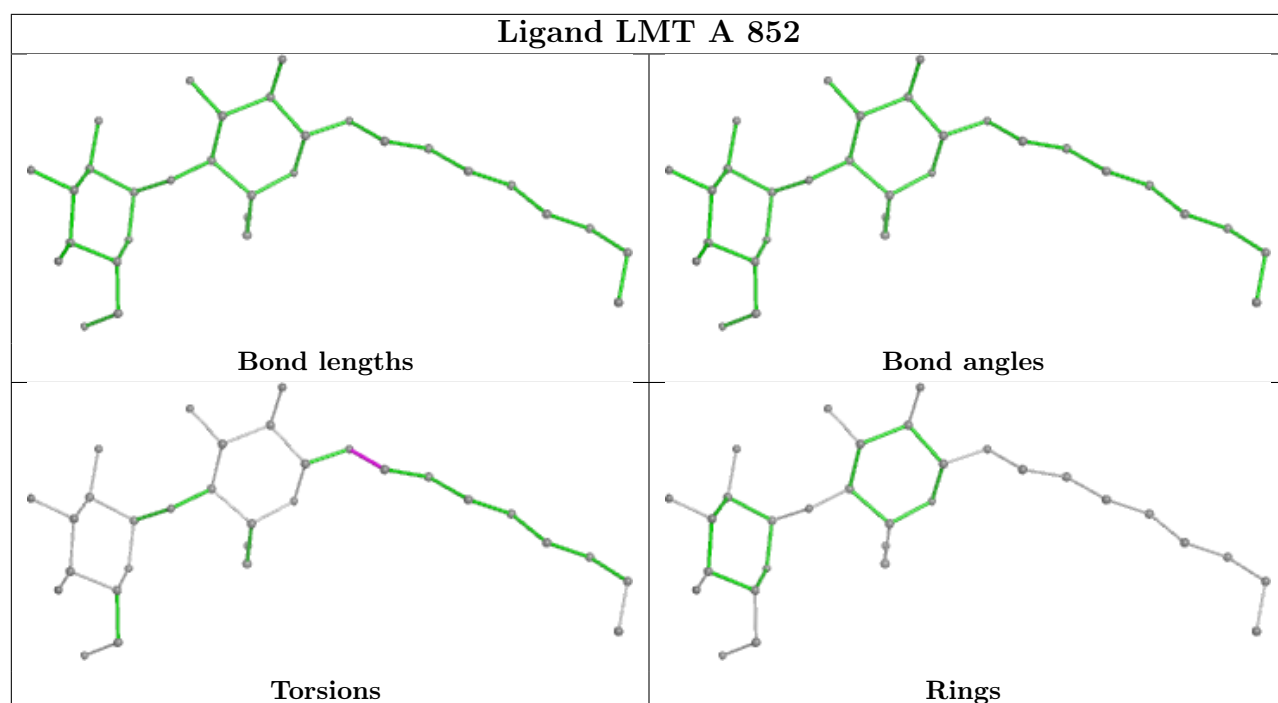
## Ligand CLA B 838

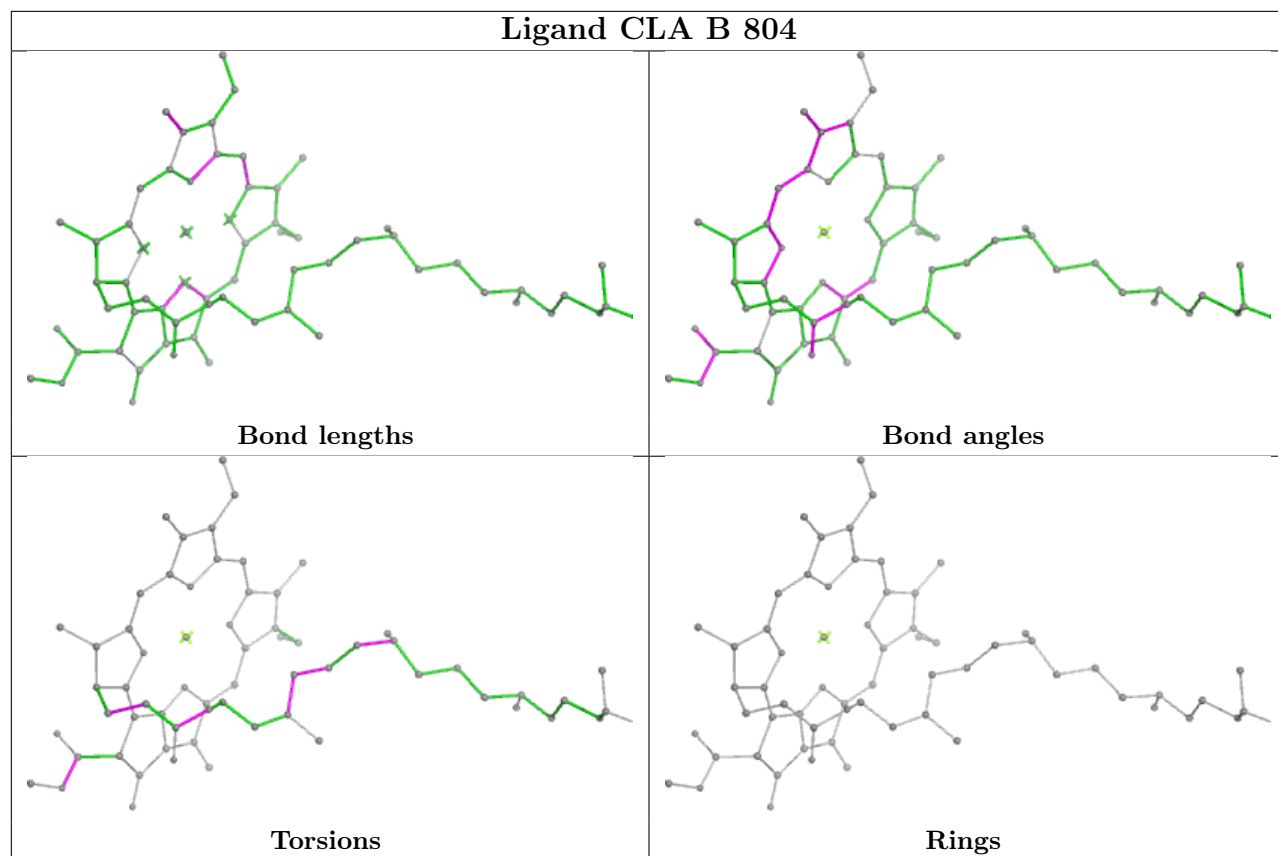


## Ligand BCR K 101

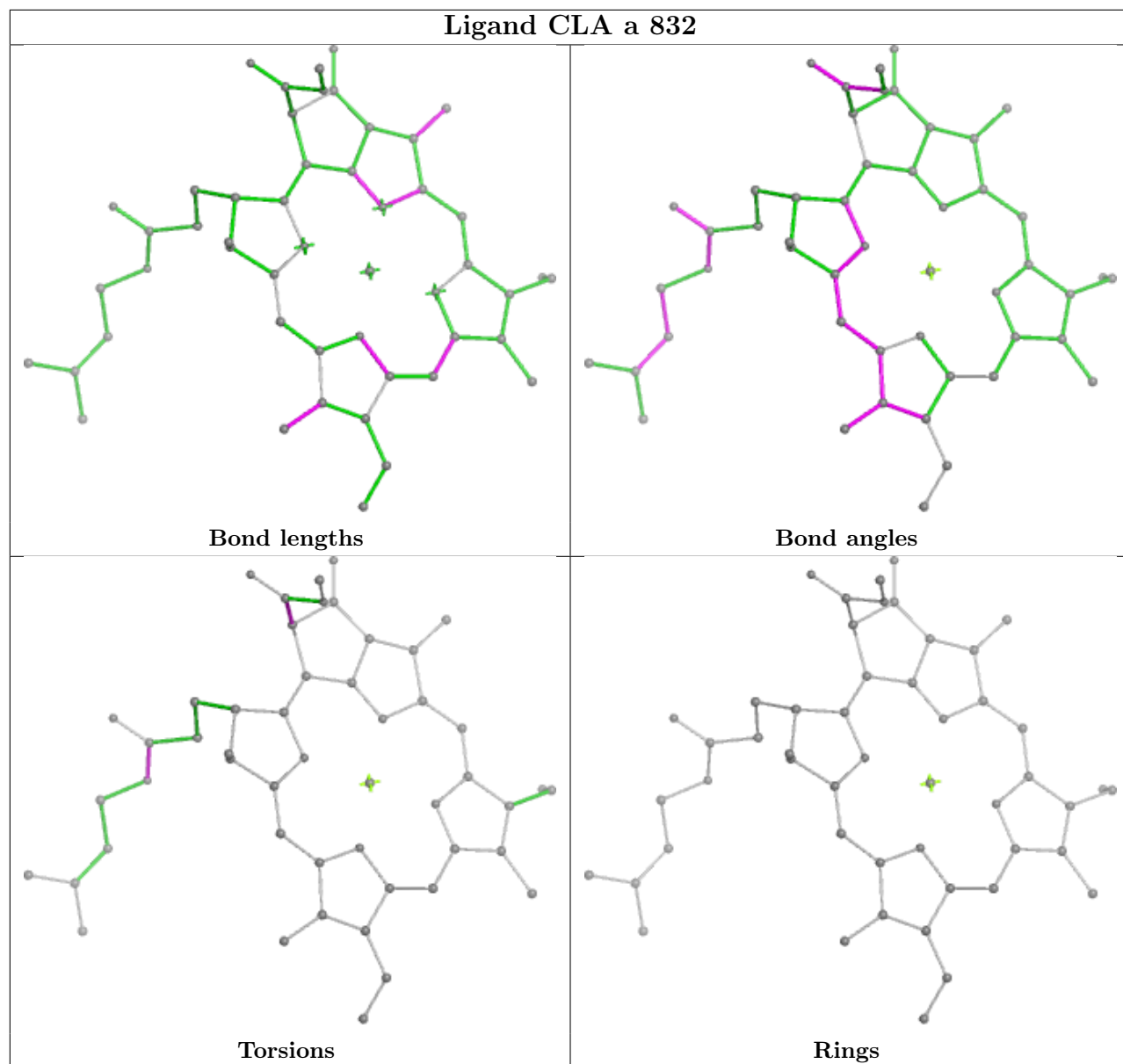


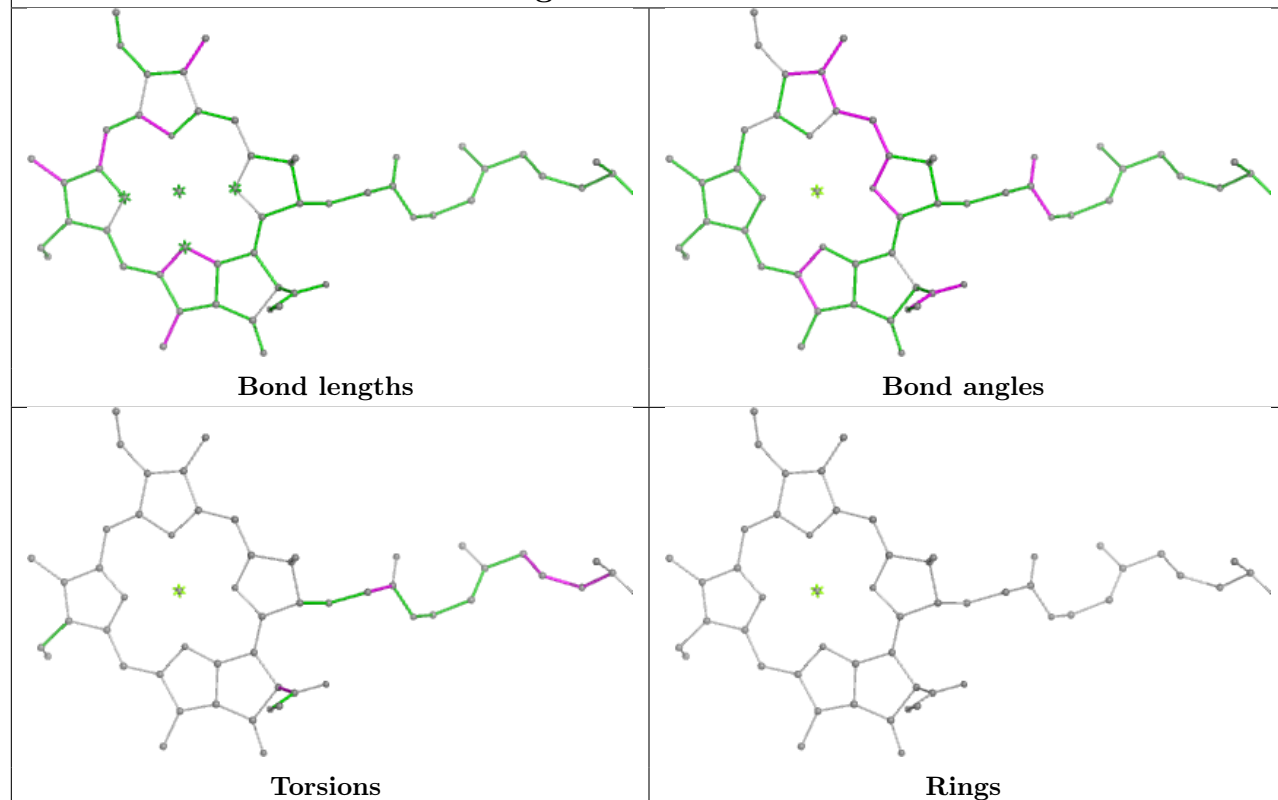
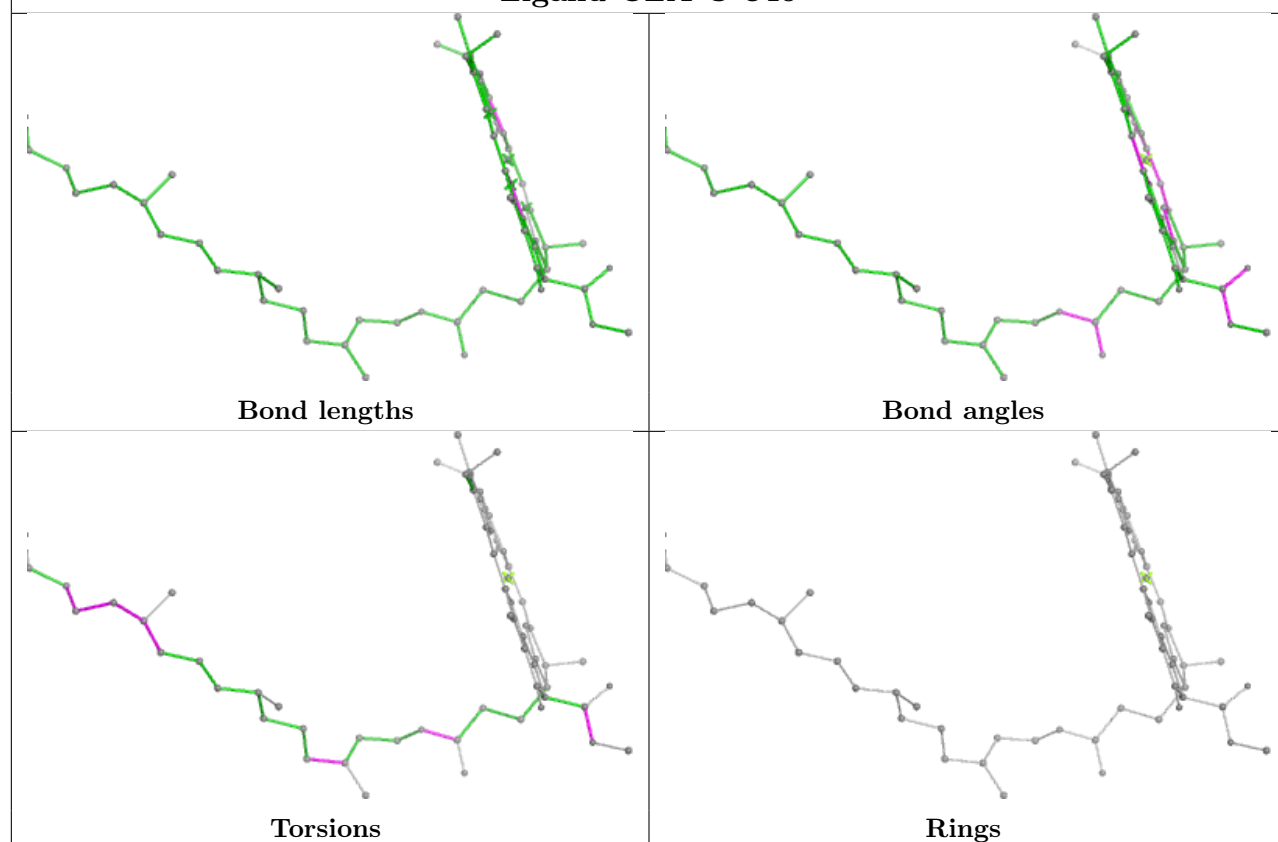




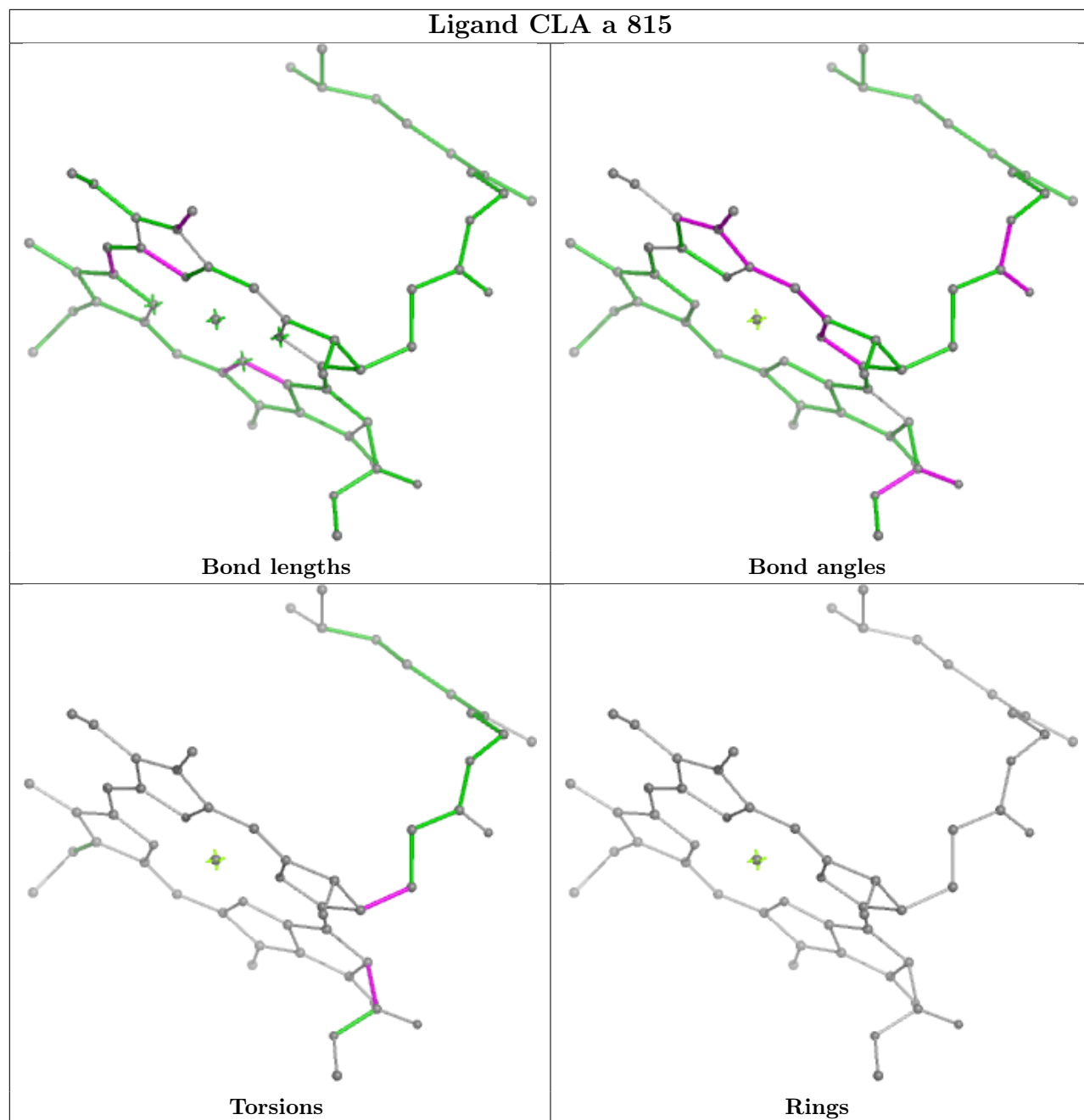


## Ligand CLA a 832

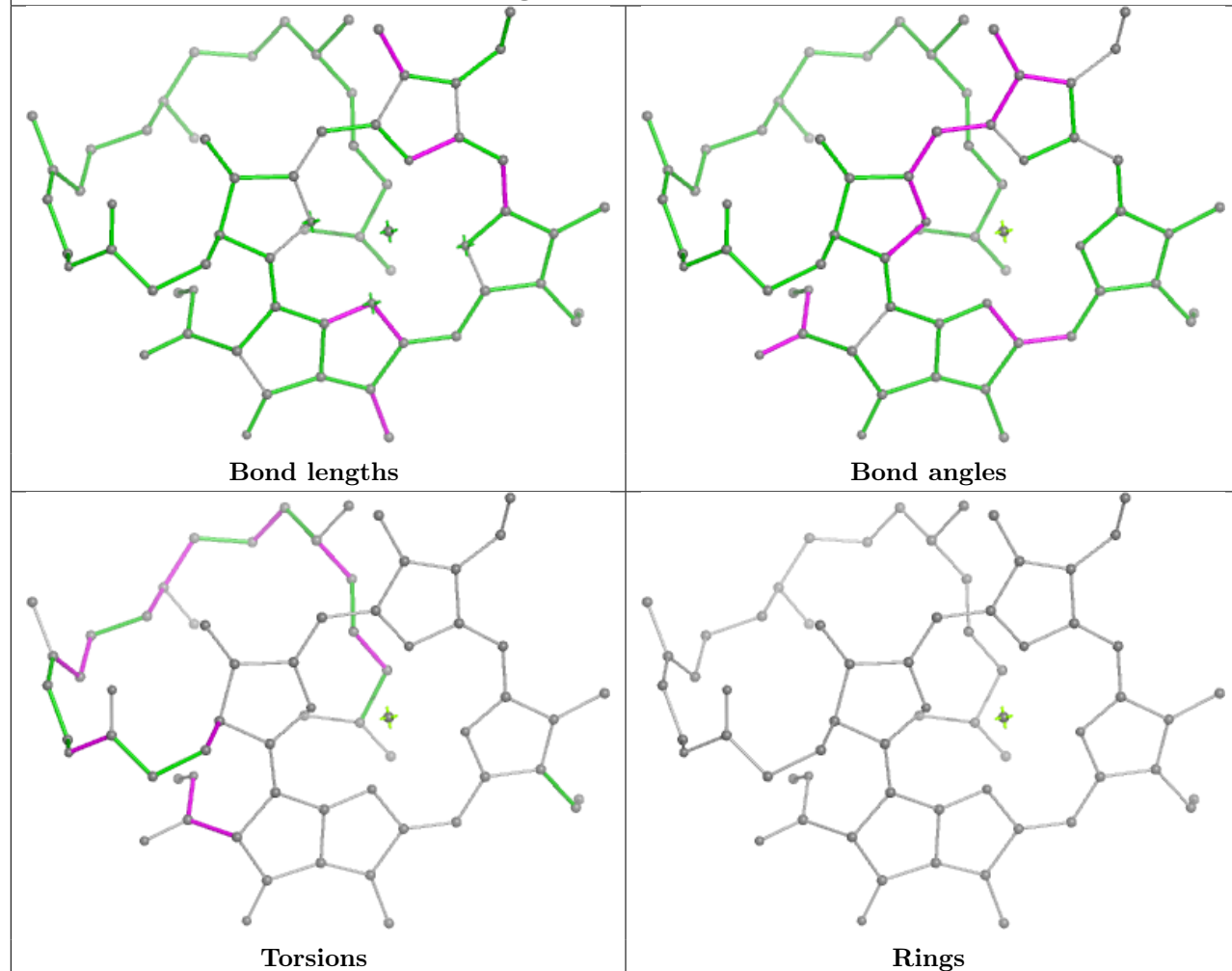


**Ligand CLA b 822****Ligand CLA O 840**

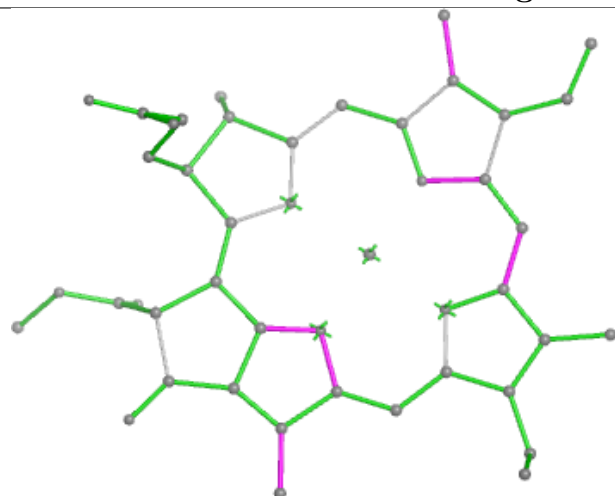
## Ligand CLA a 815



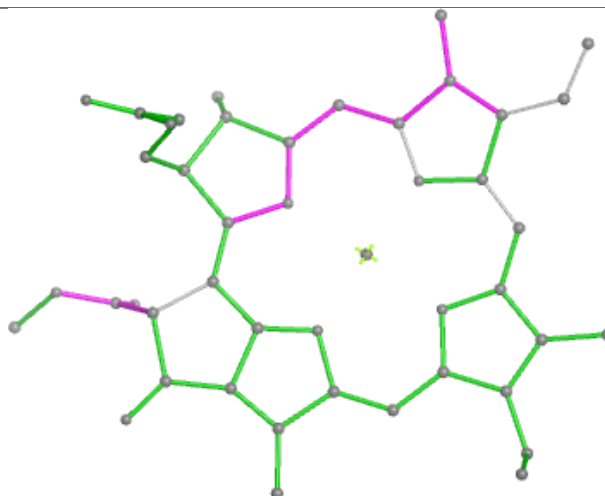
## Ligand CLA b 806



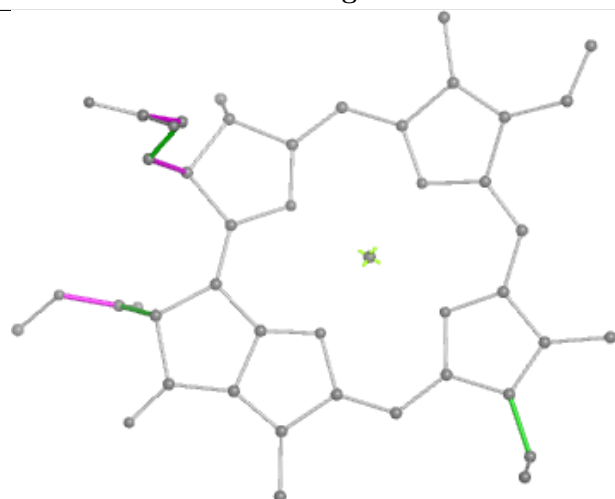
## Ligand CLA O 834



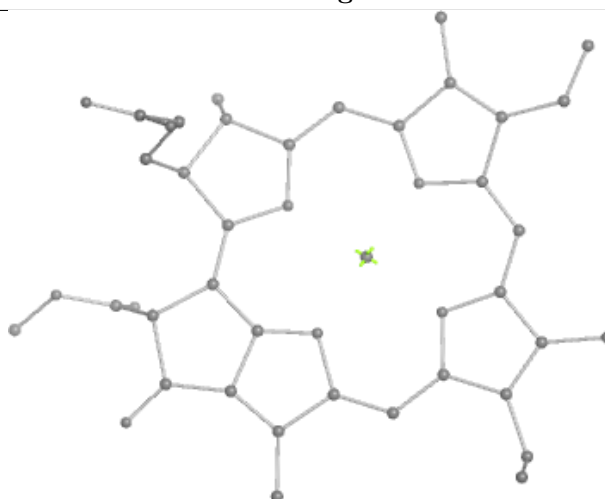
Bond lengths



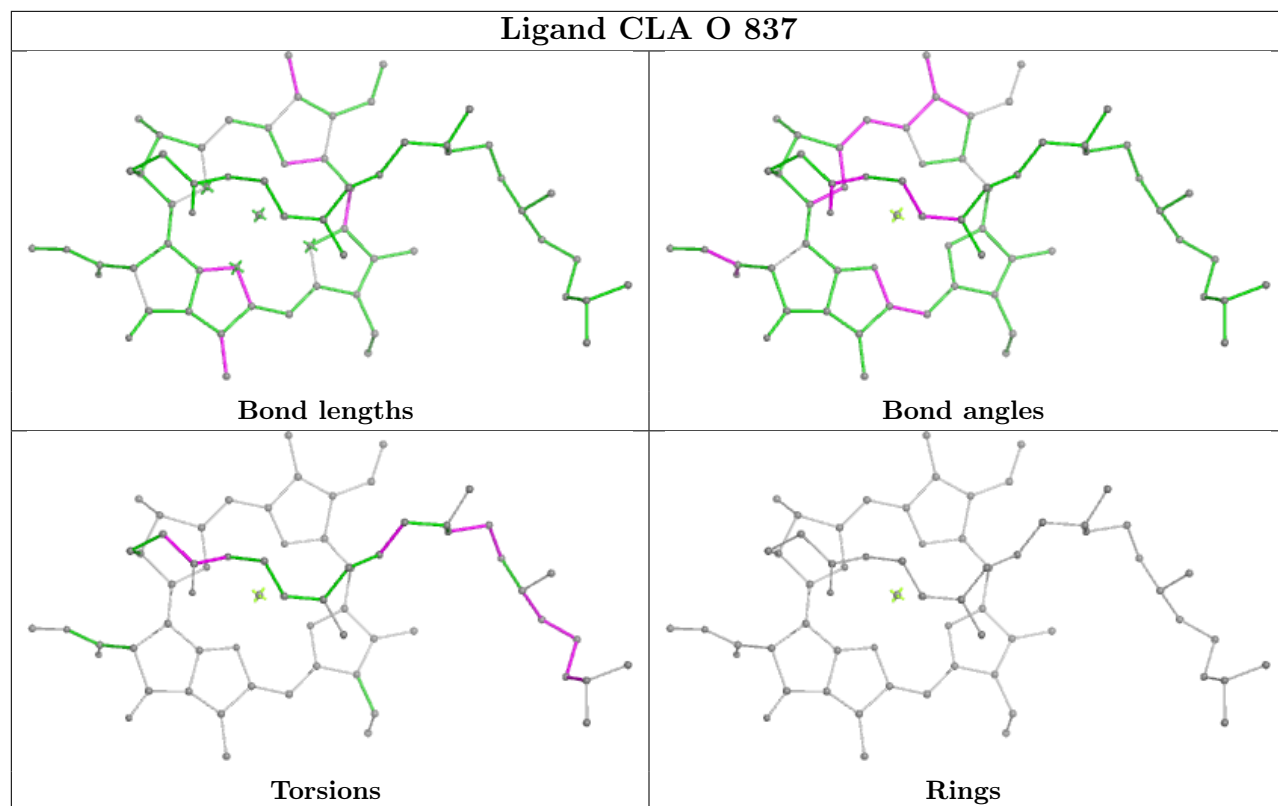
Bond angles



Torsions

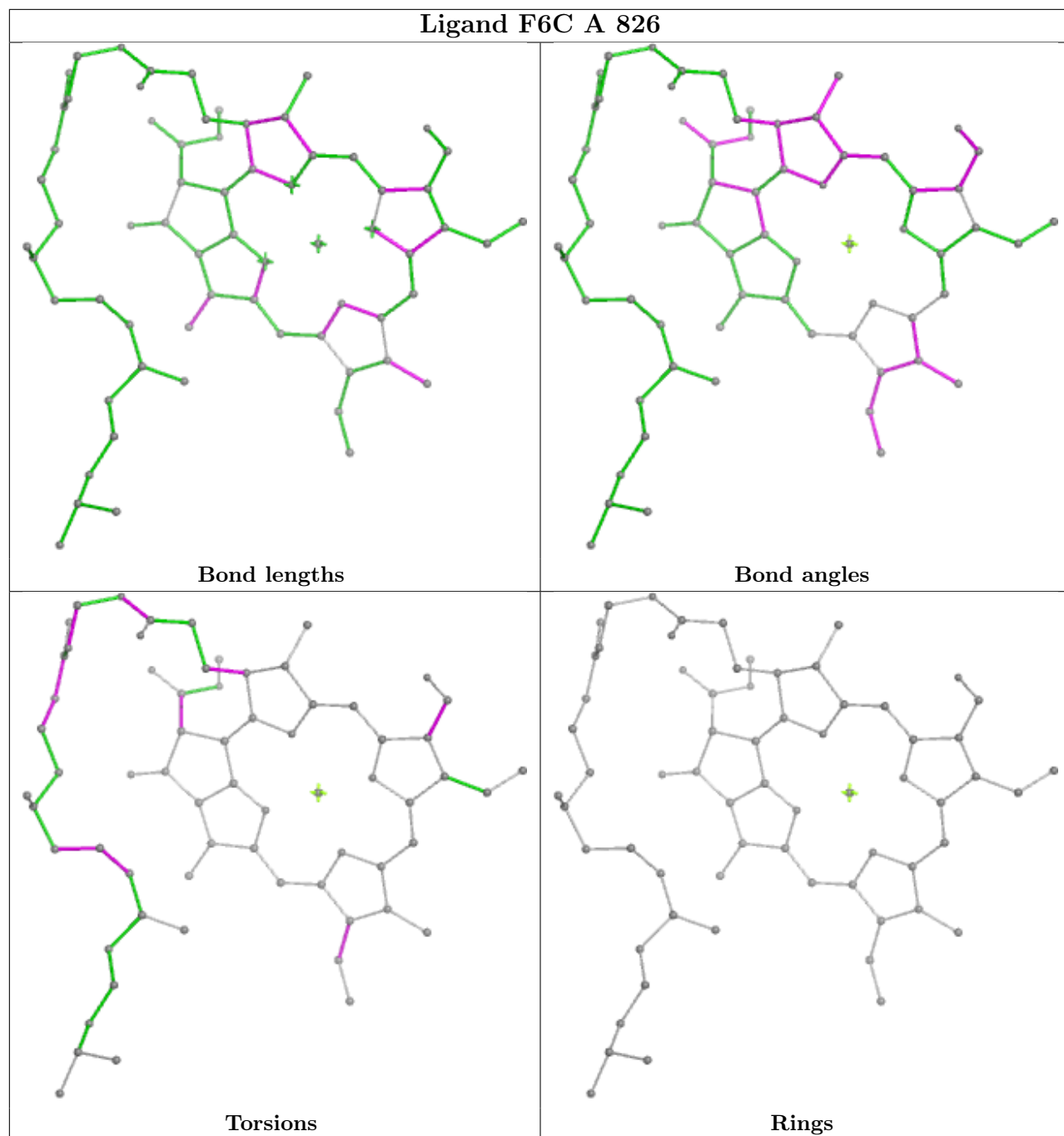


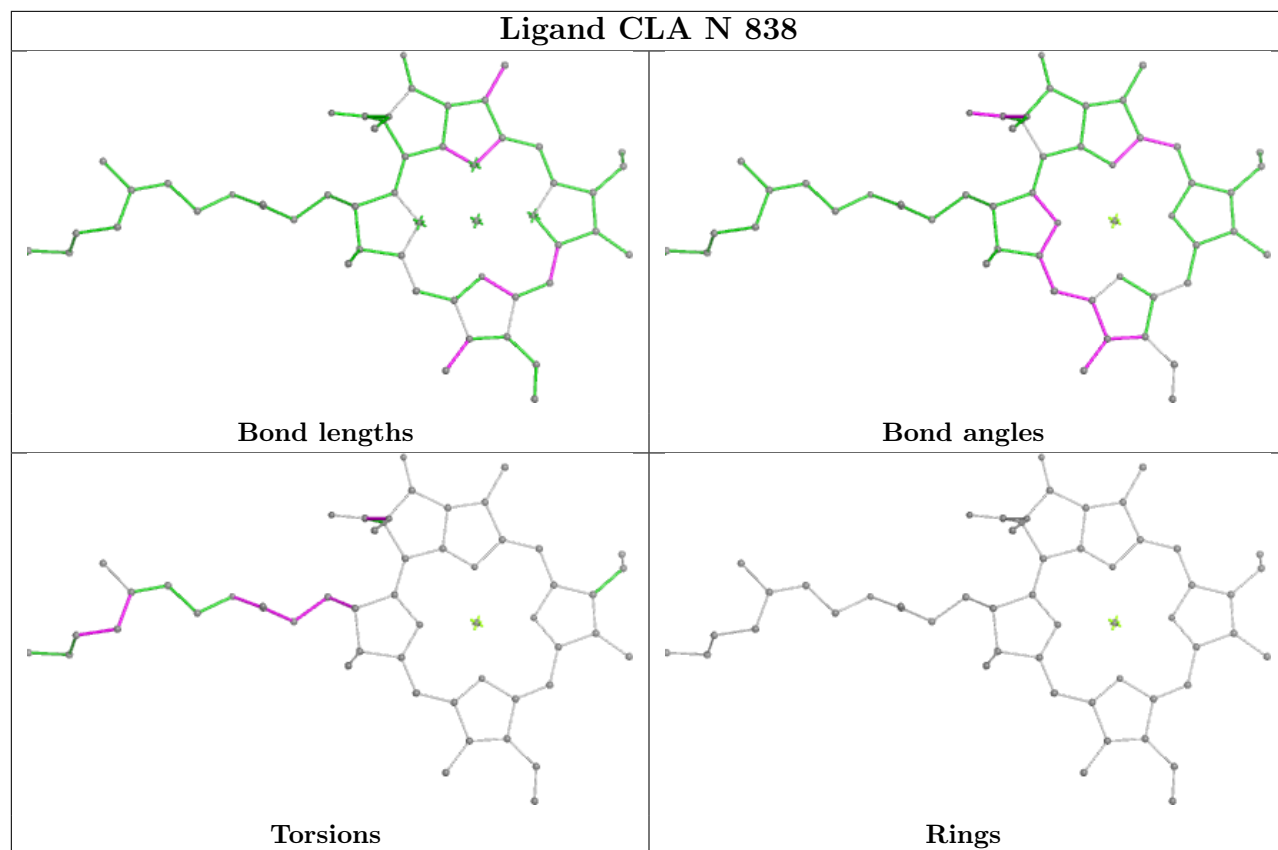
Rings



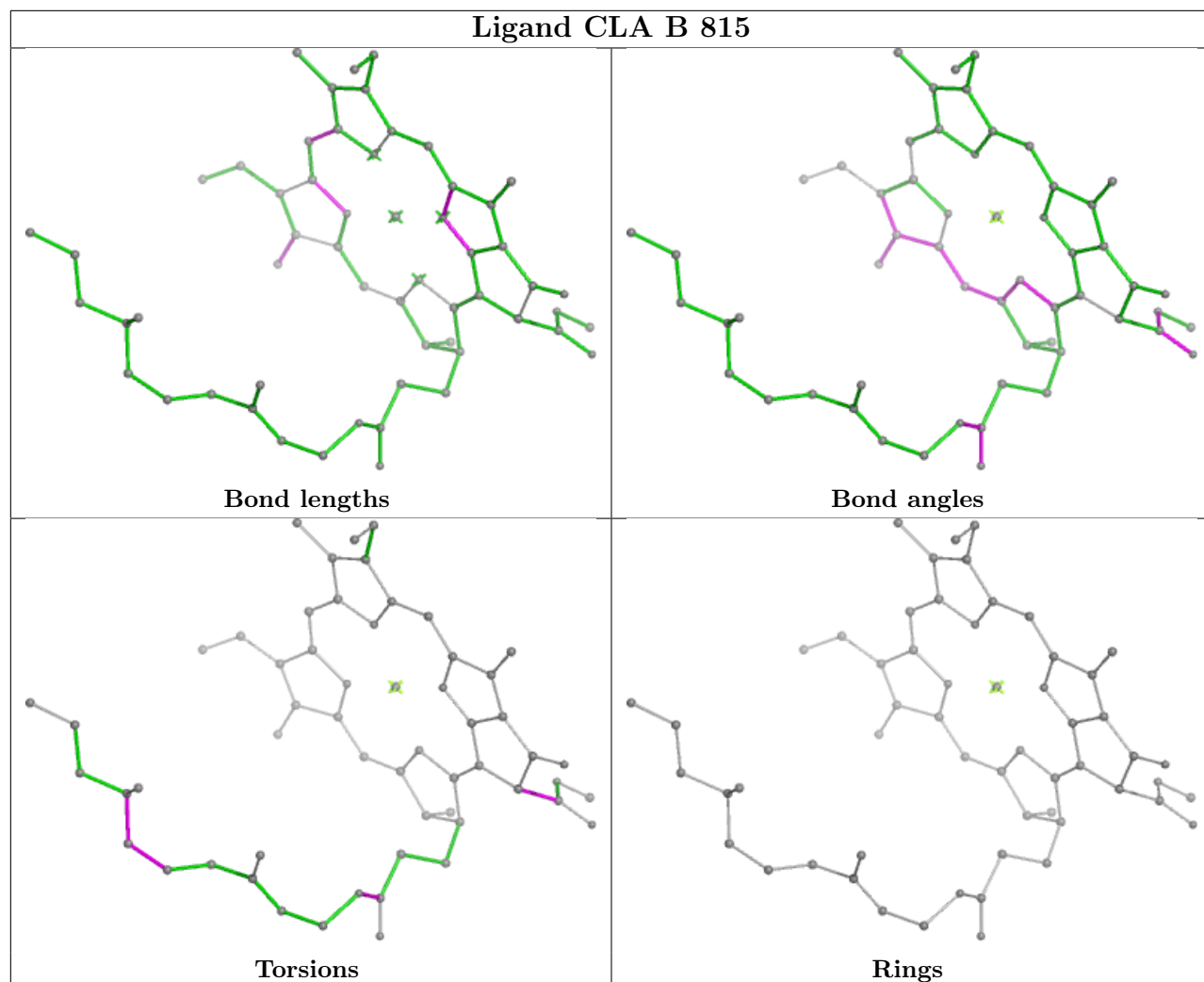


## Ligand F6C A 826

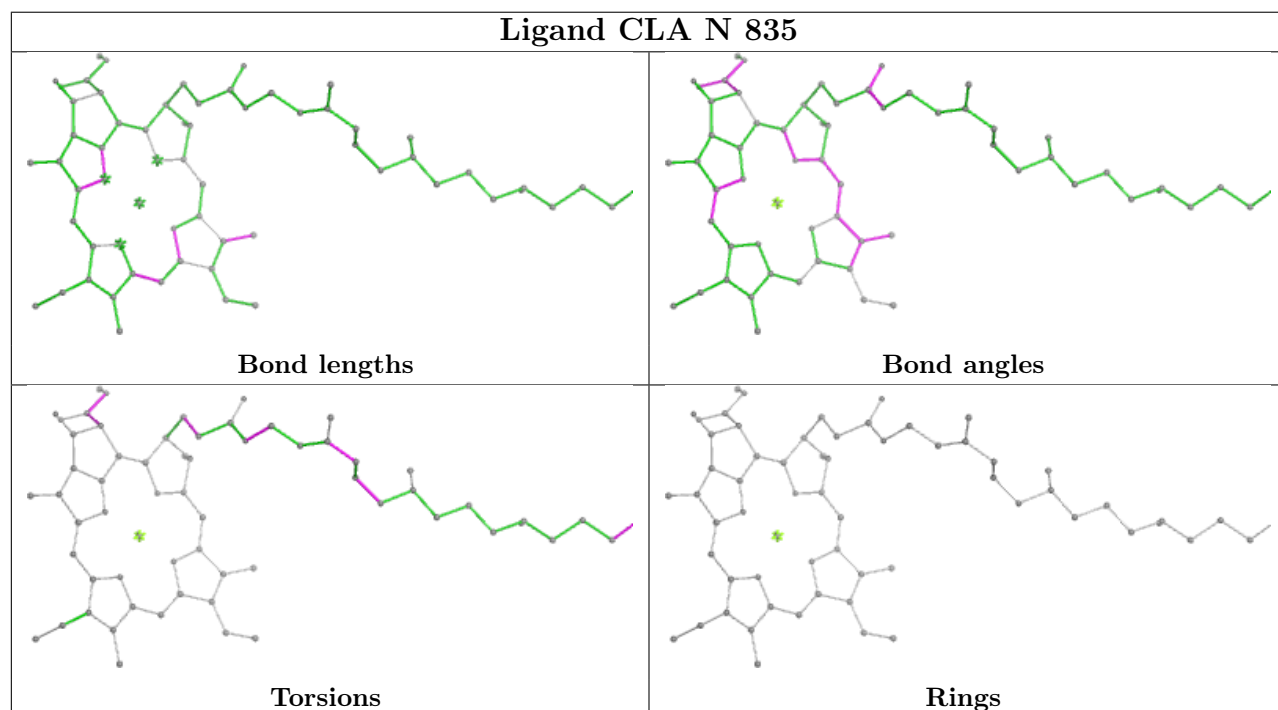


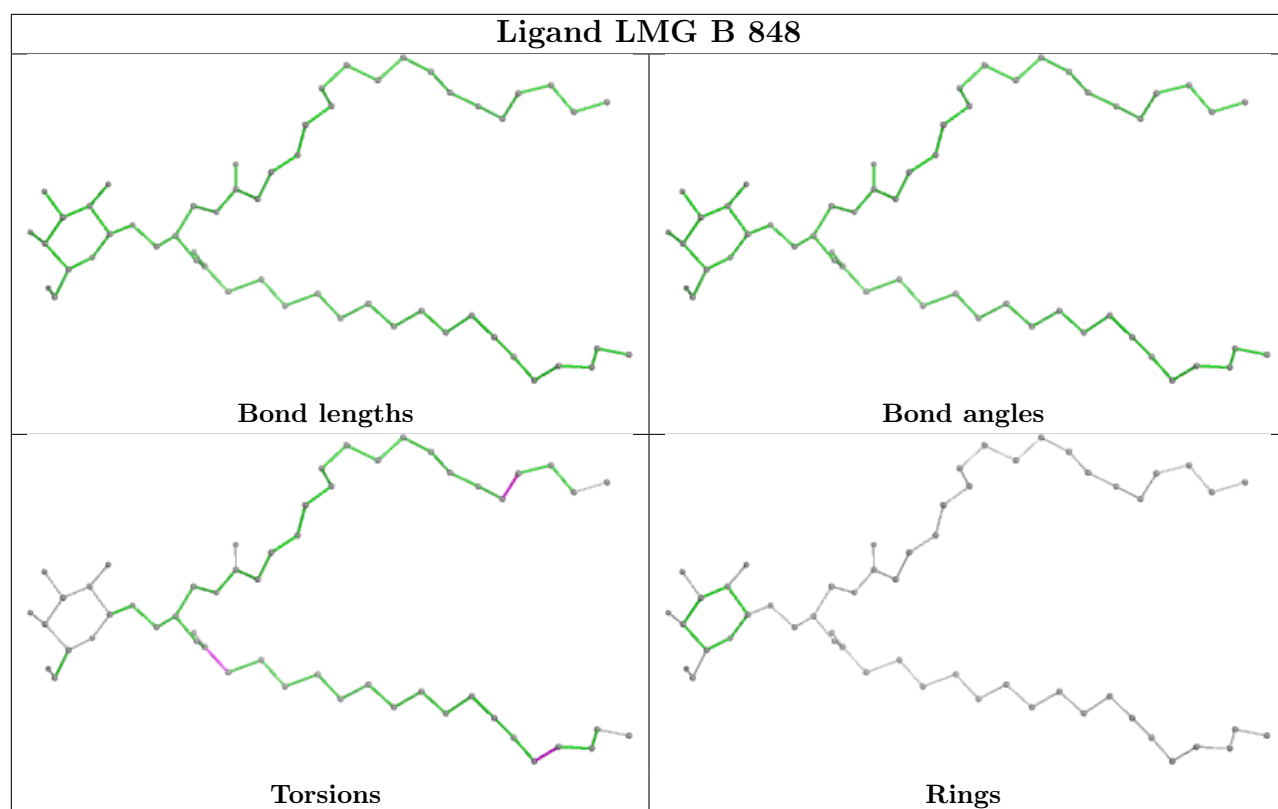


## Ligand CLA B 815

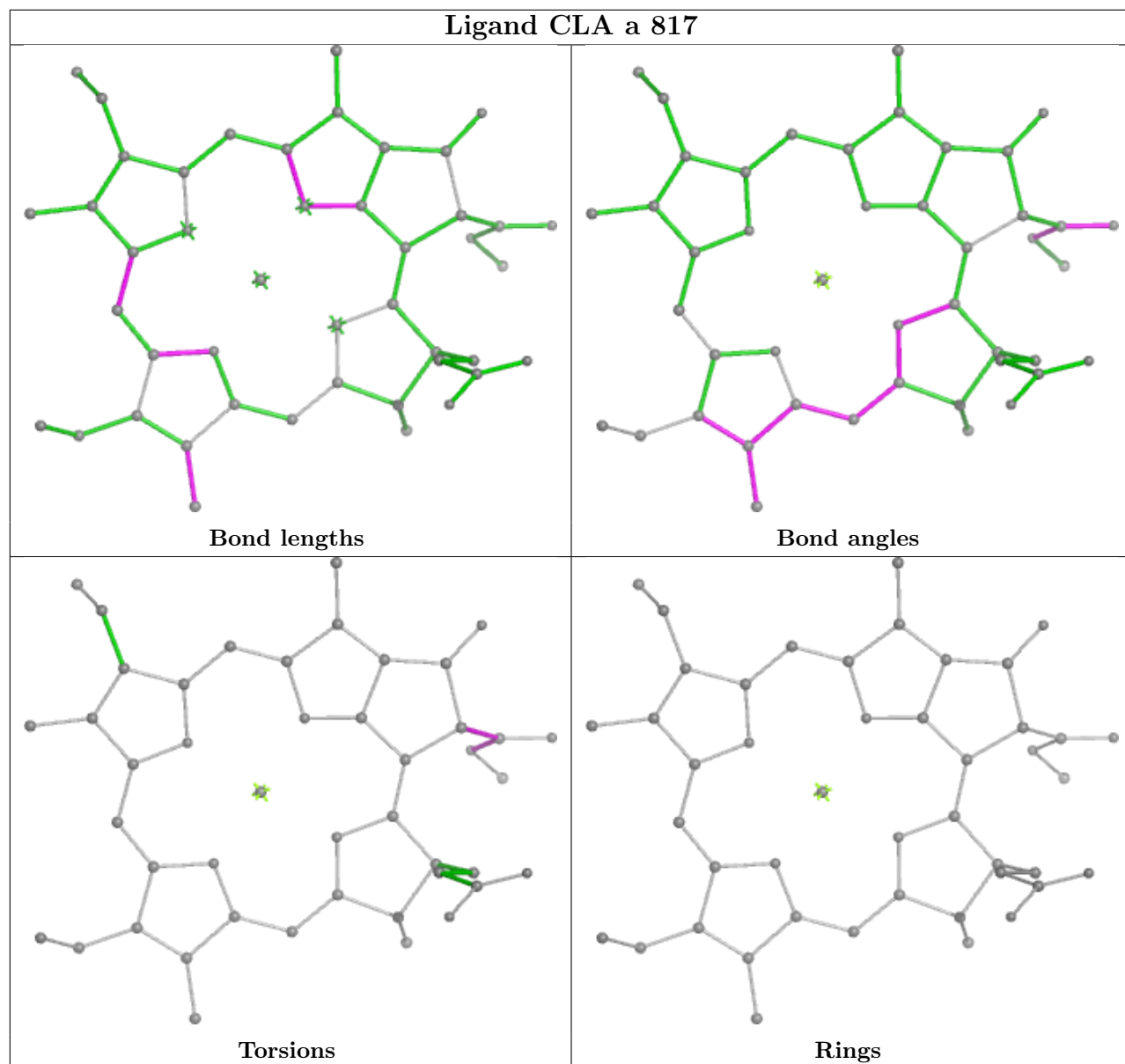


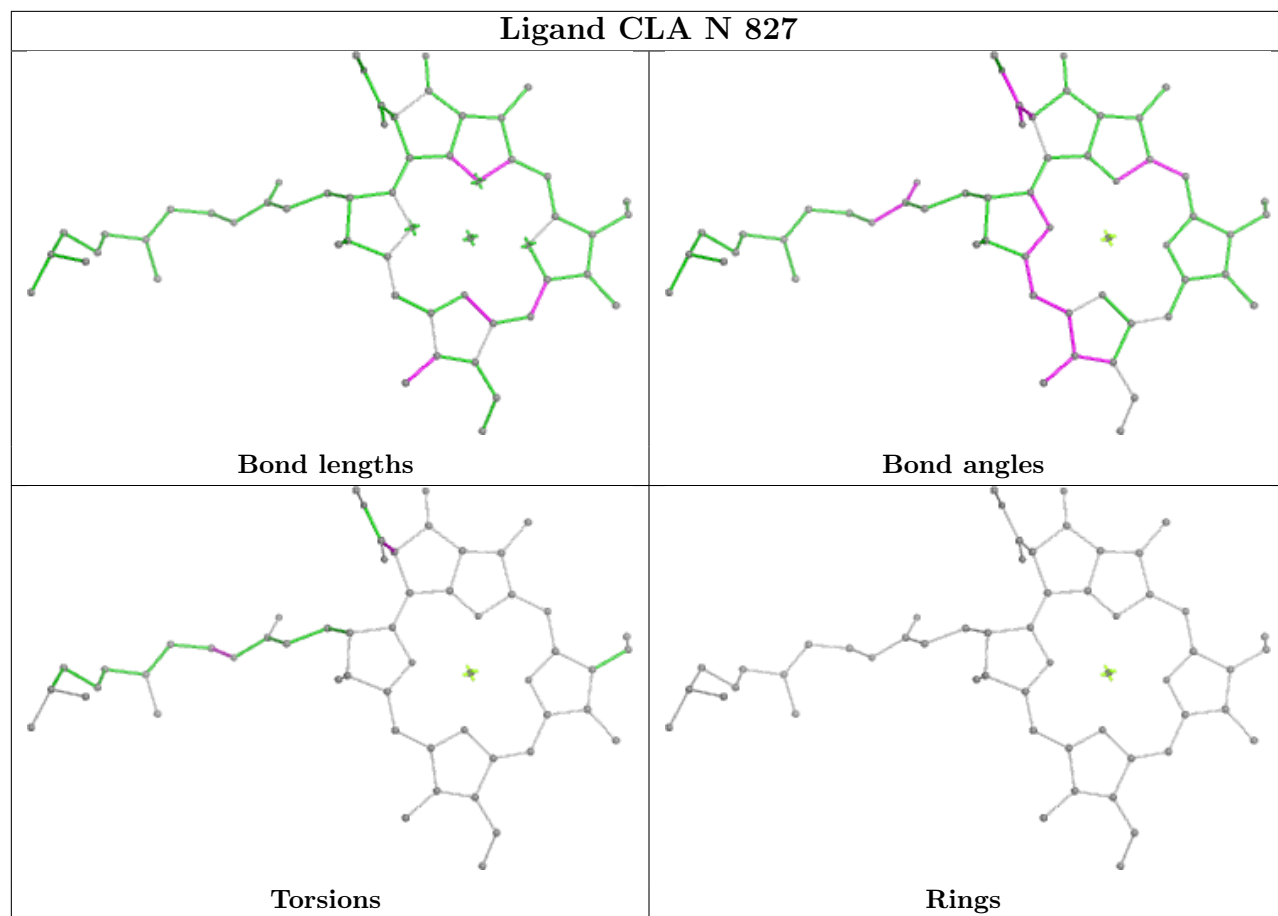
## Ligand CLA N 835



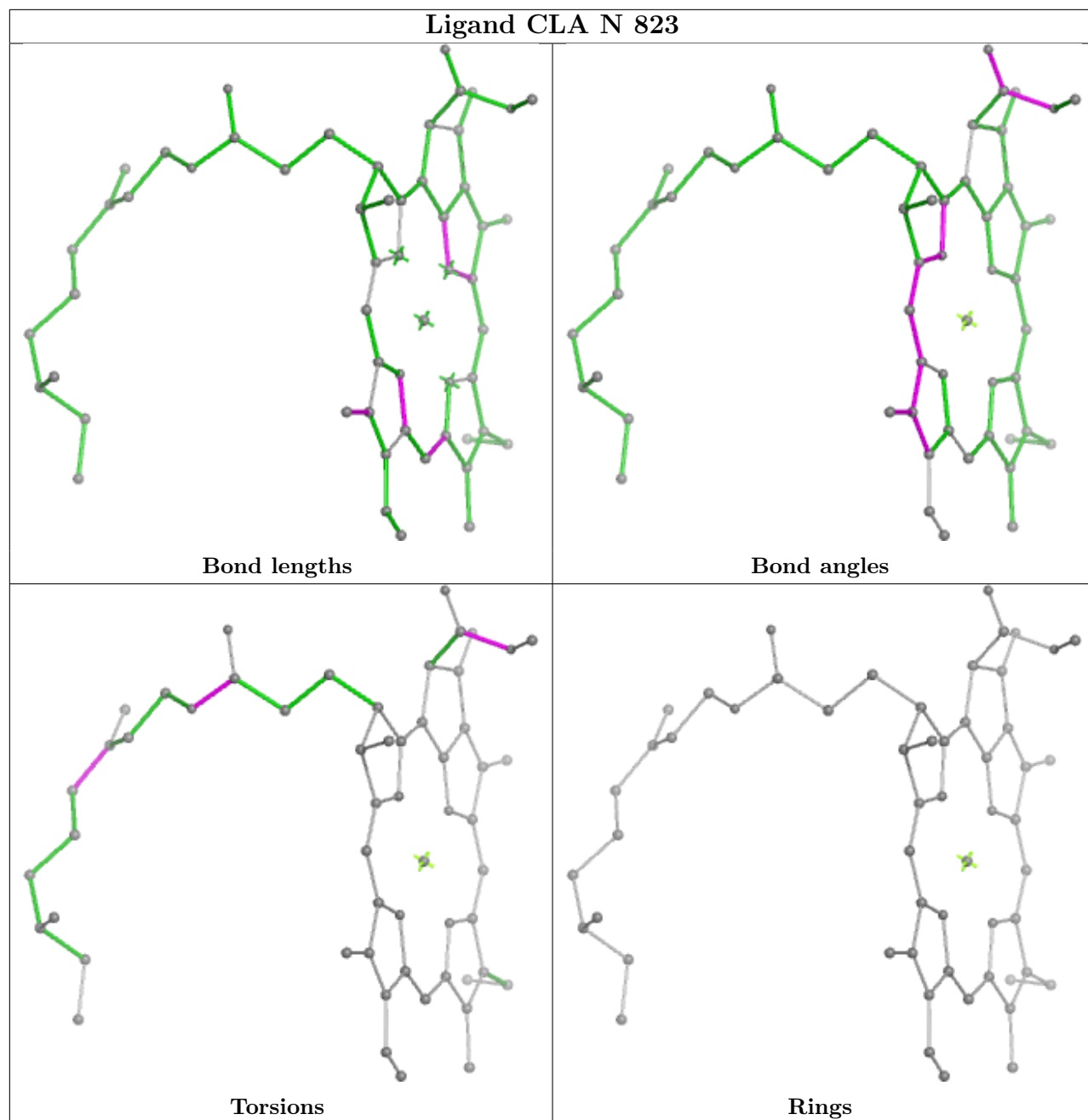


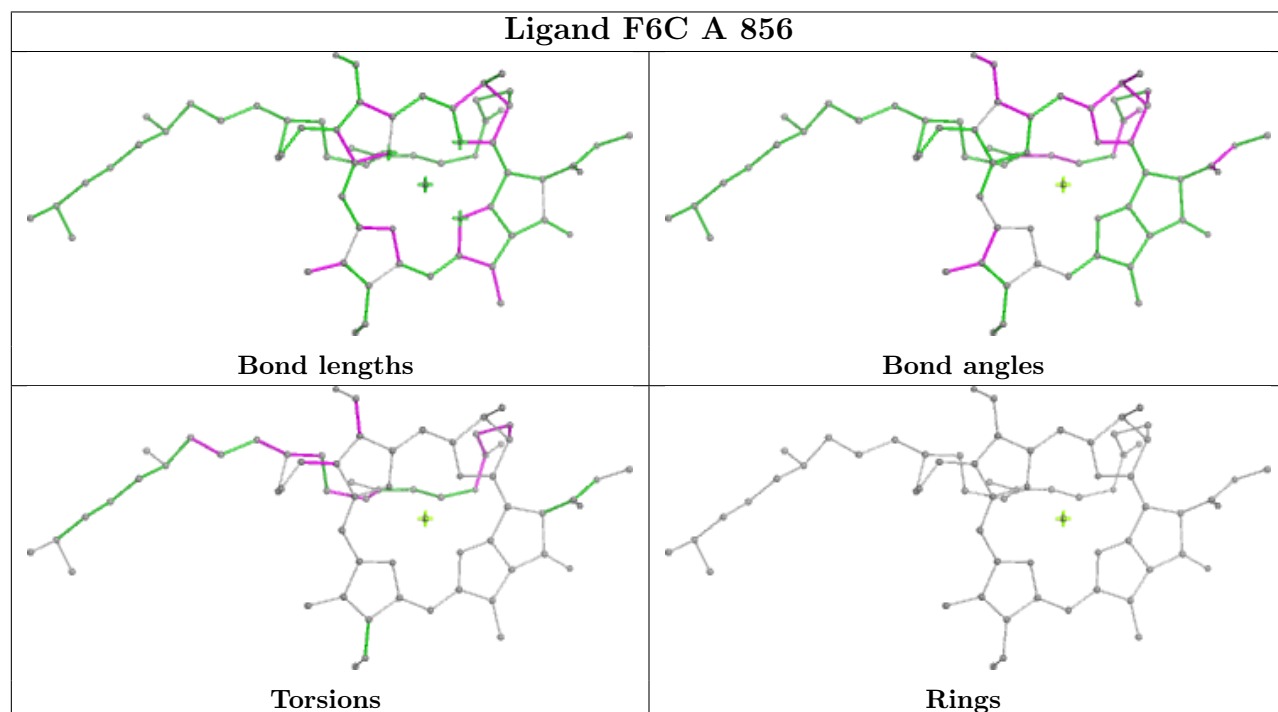
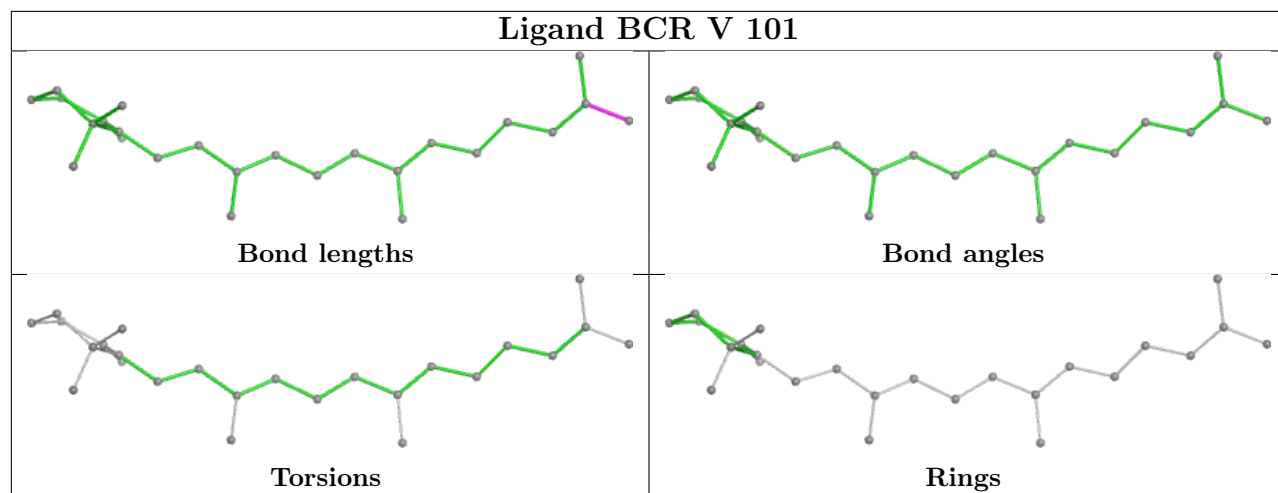
## Ligand CLA a 817





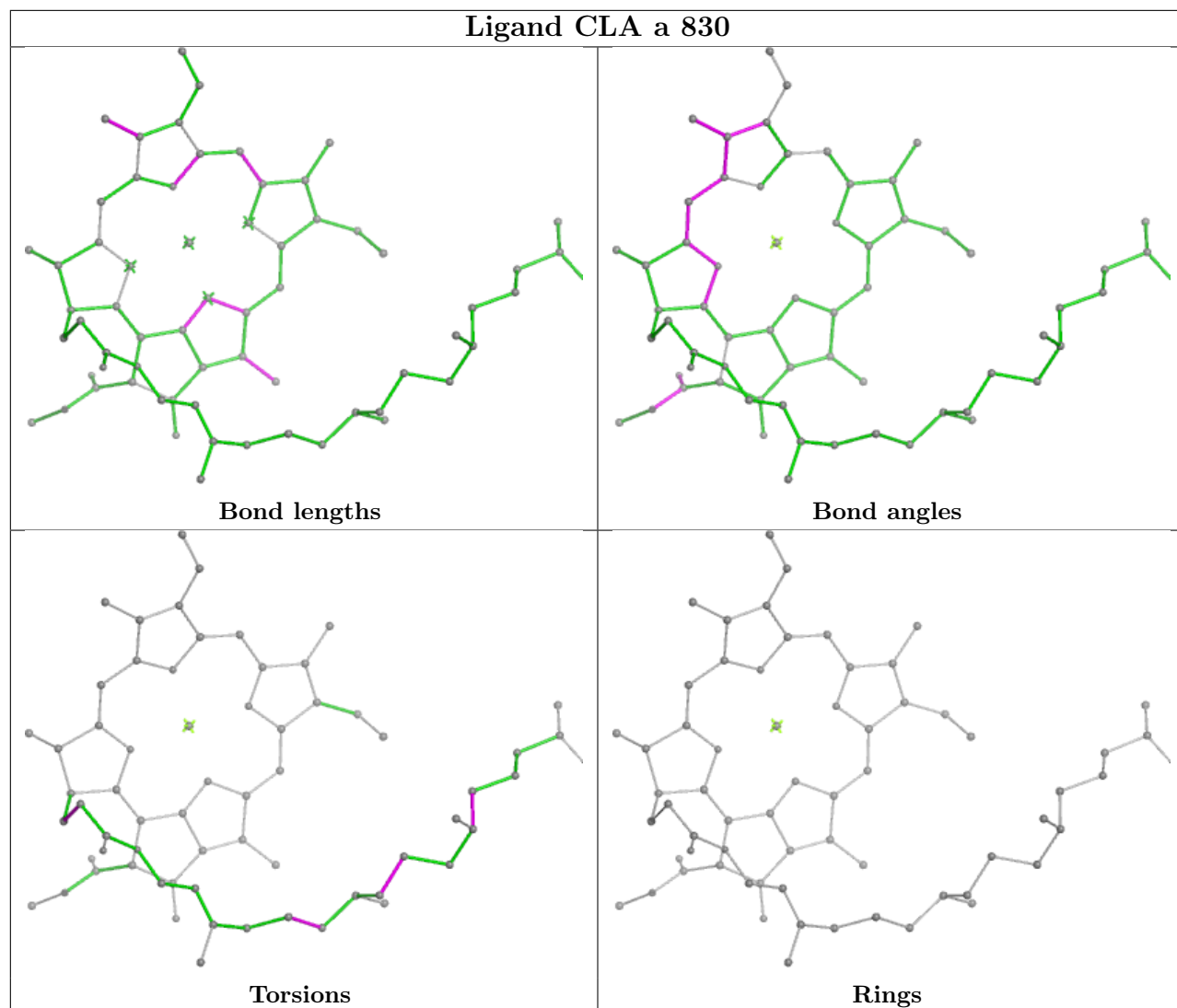
## Ligand CLA N 823



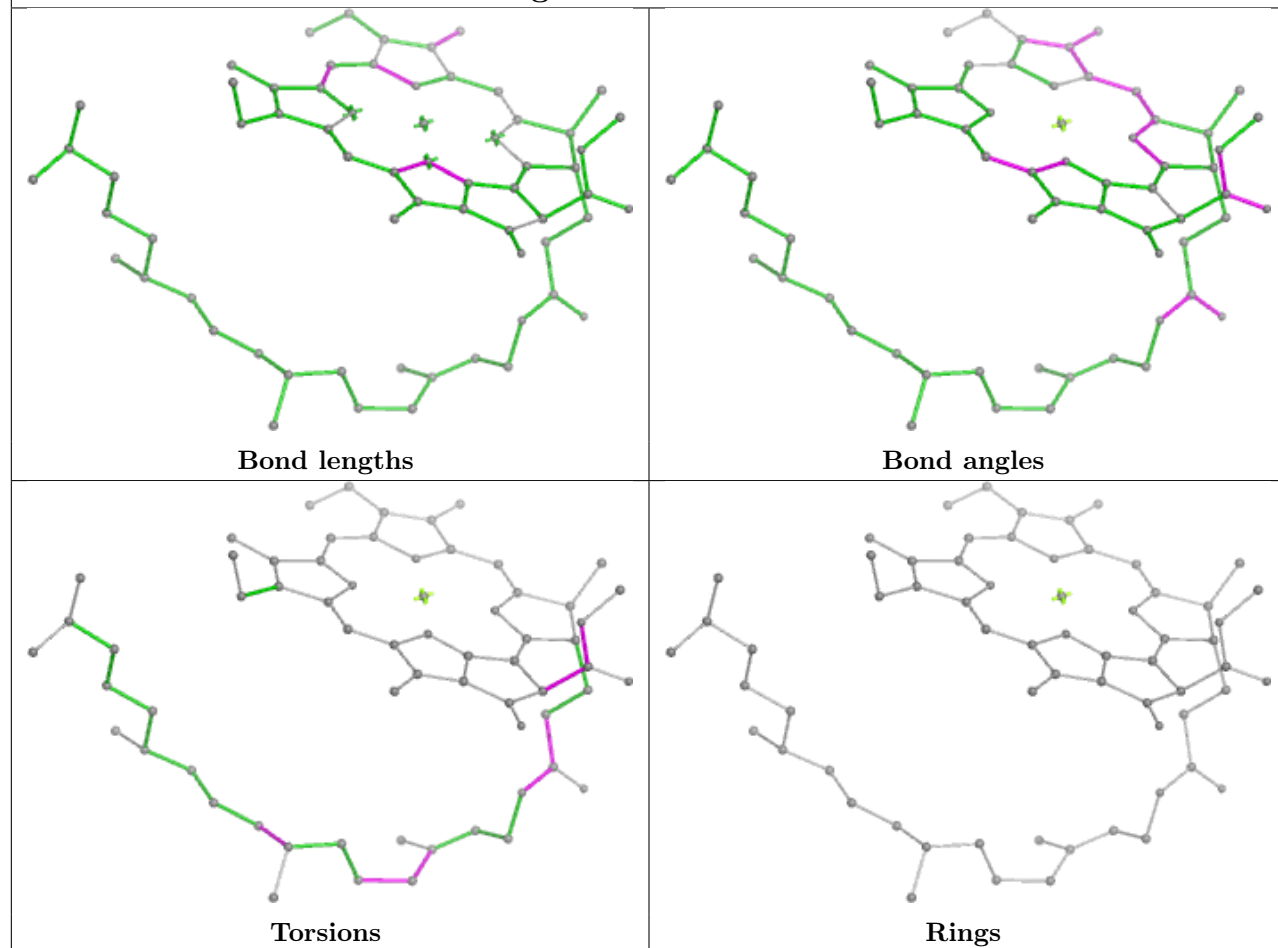




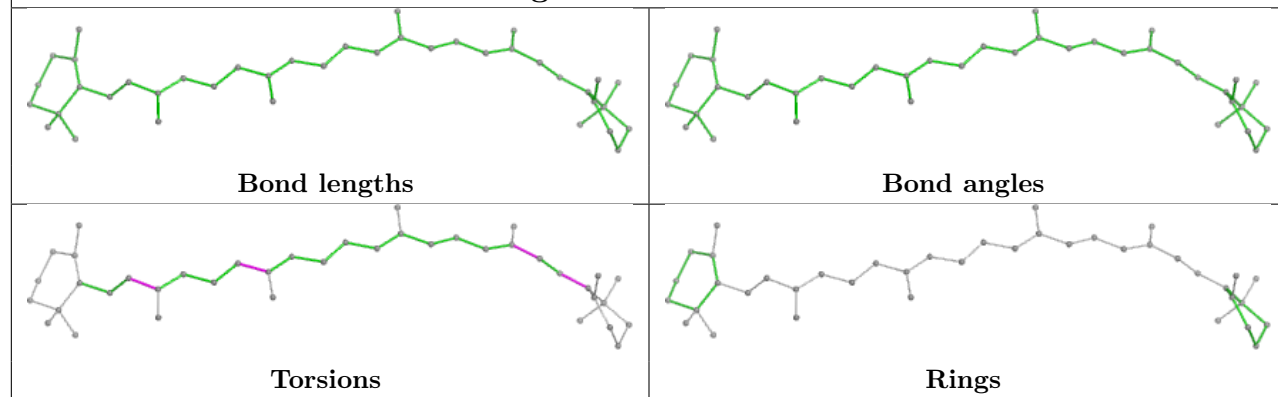
## Ligand CLA a 830



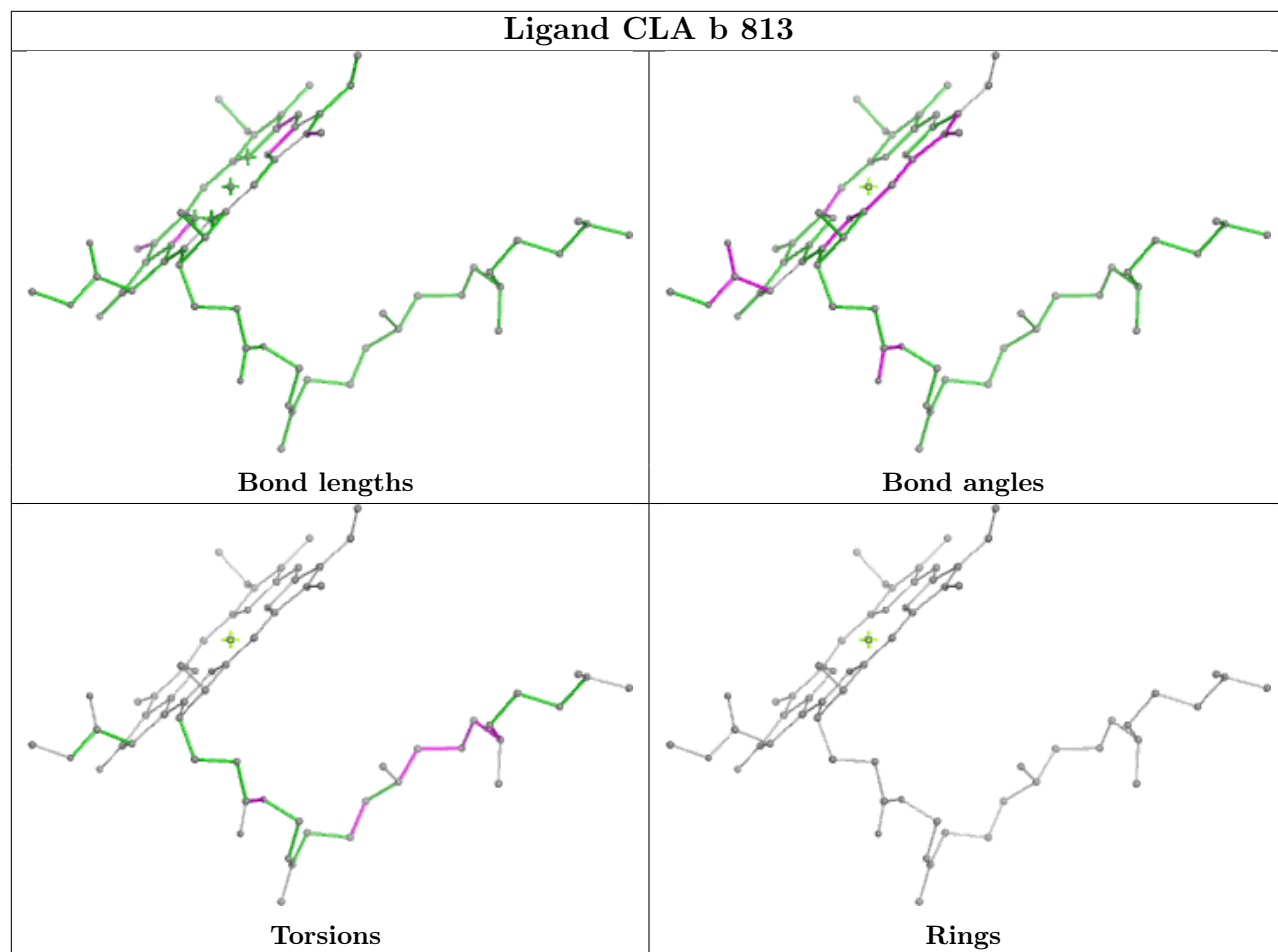
## Ligand CLA N 825



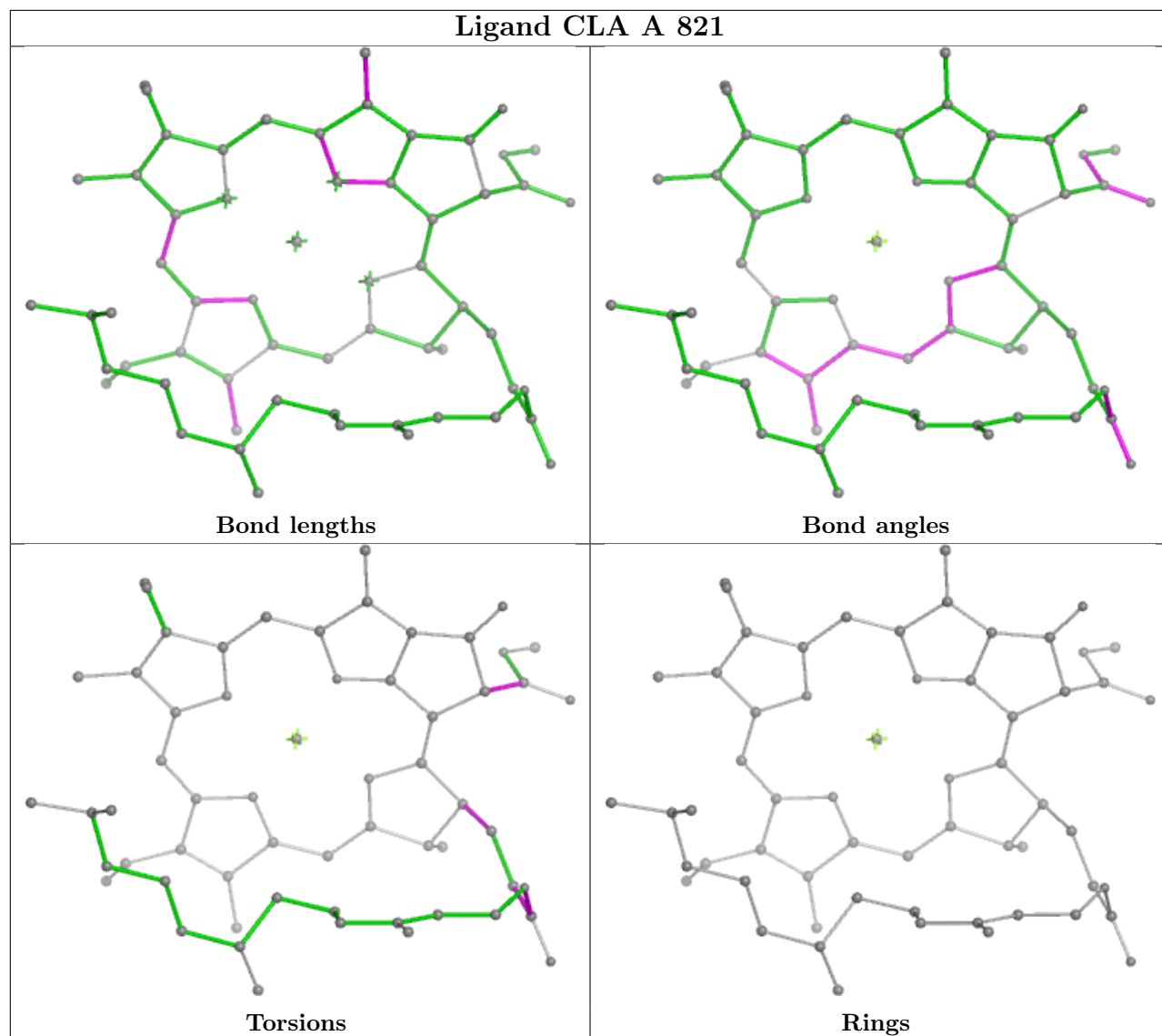
## Ligand BCR T 101



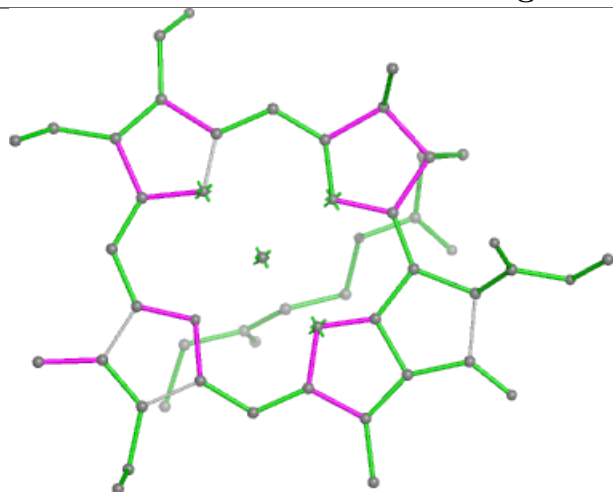
## Ligand CLA b 813



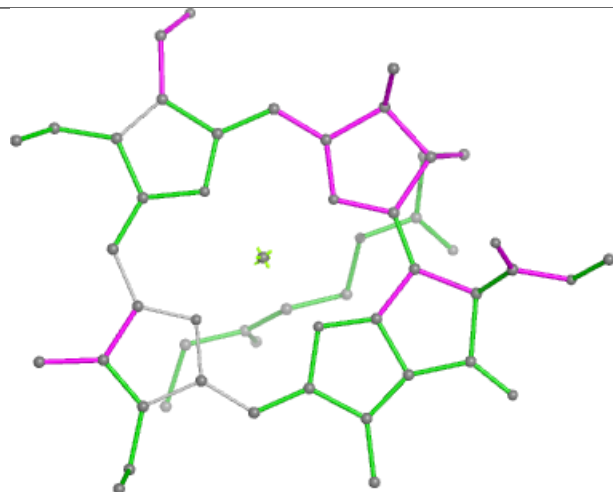
## Ligand CLA A 821



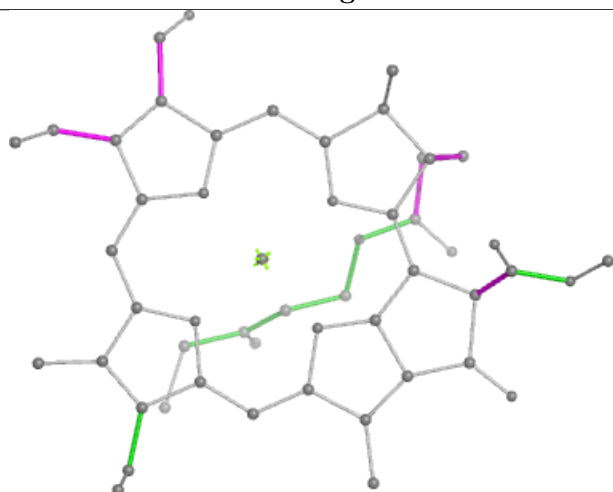
## Ligand F6C N 824



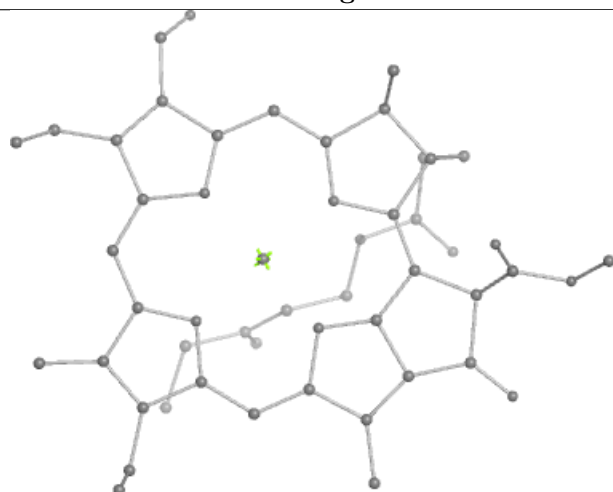
Bond lengths



Bond angles

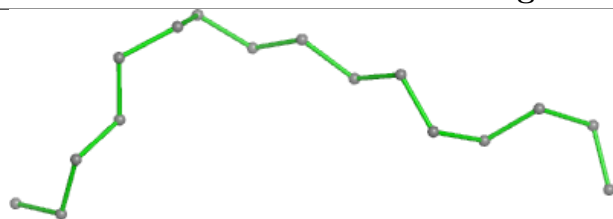


Torsions

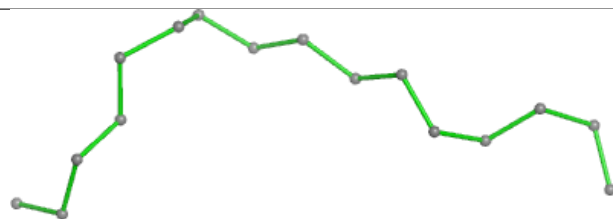


Rings

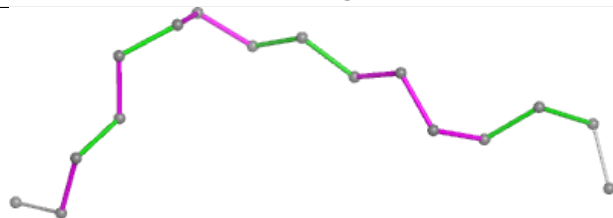
## Ligand LFA O 850



Bond lengths



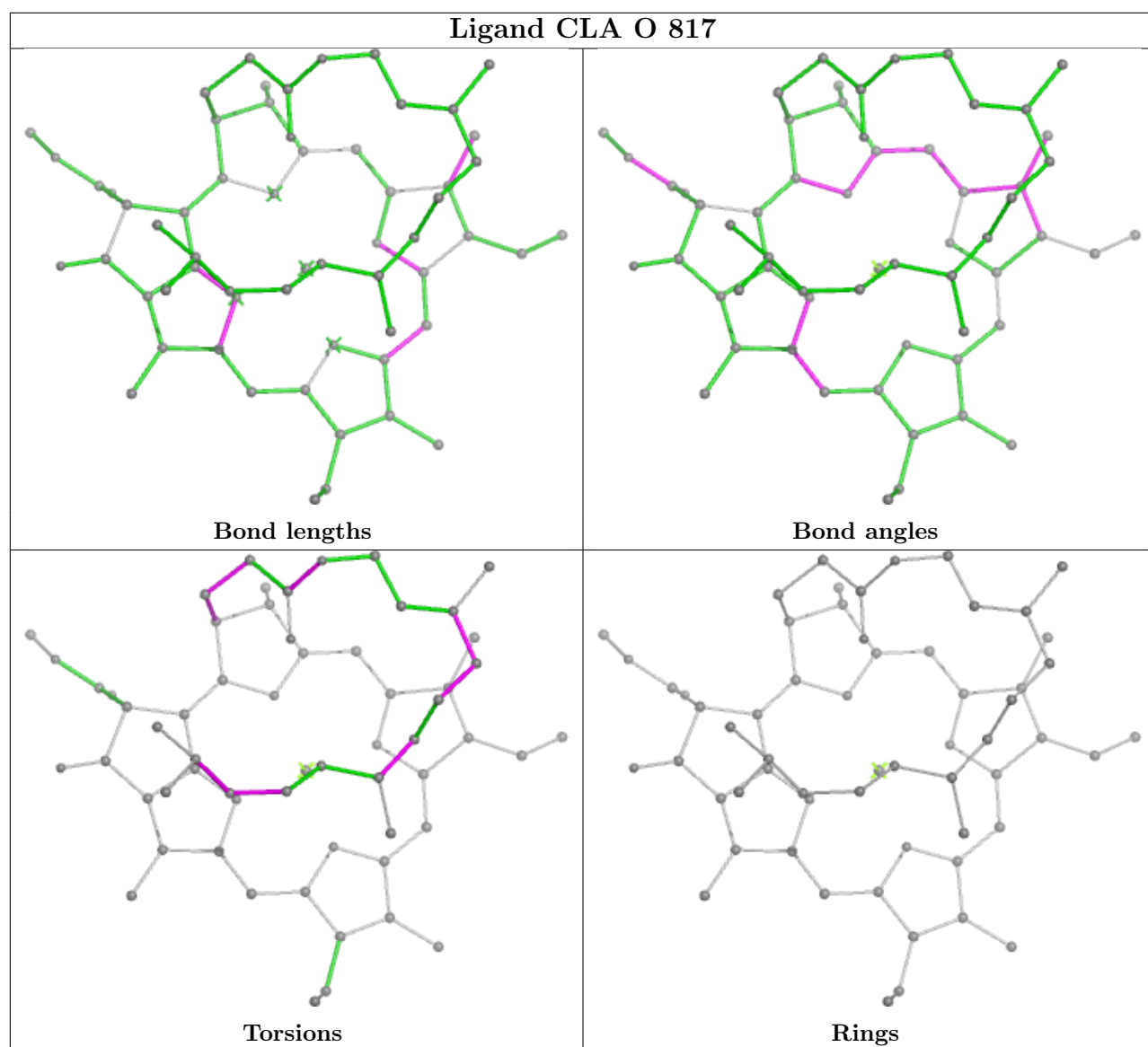
Bond angles

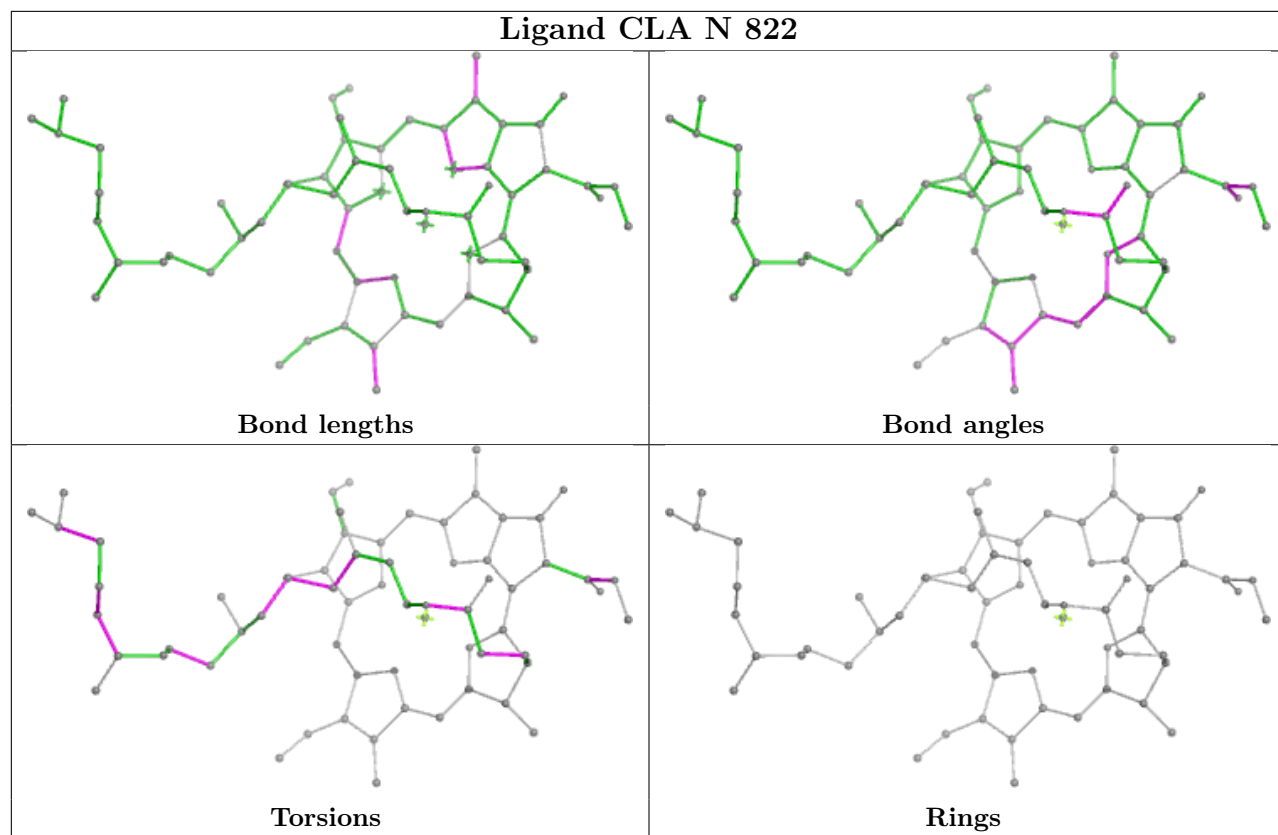


Torsions

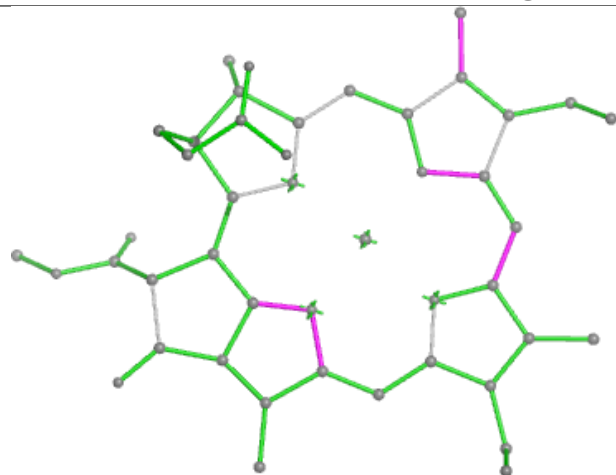


Rings

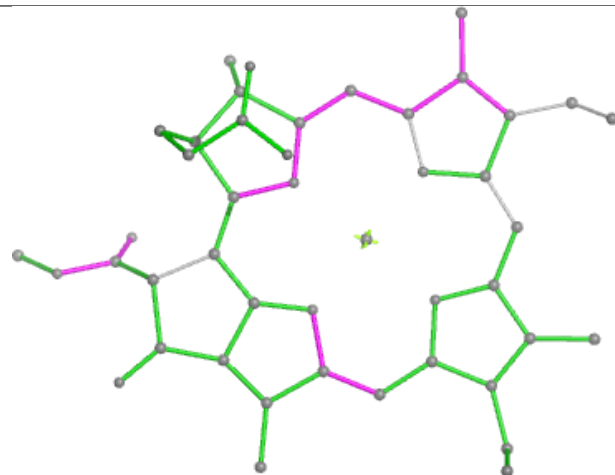




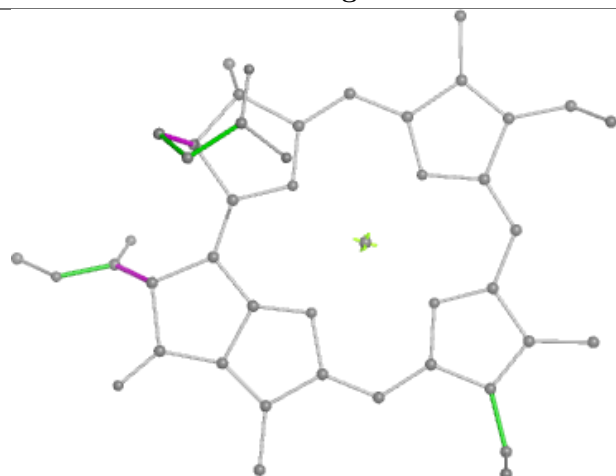
## Ligand CLA b 811



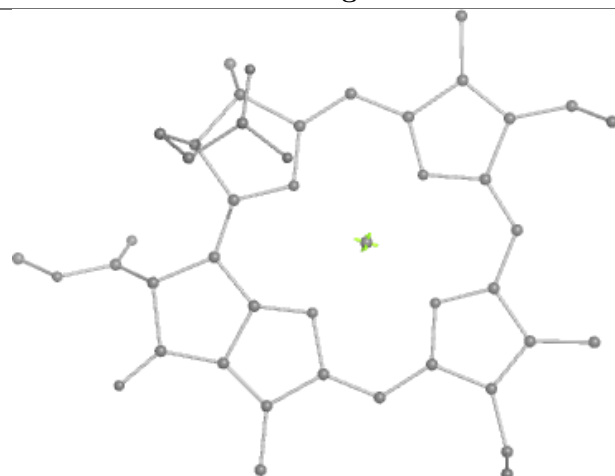
Bond lengths



Bond angles

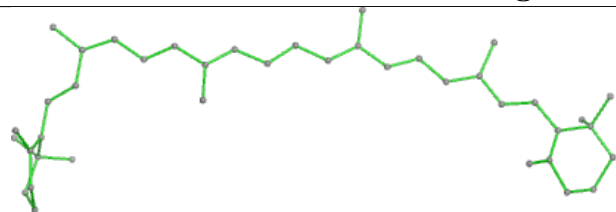


Torsions

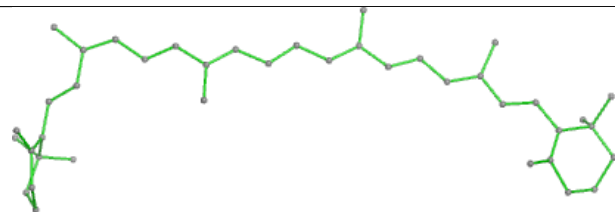


Rings

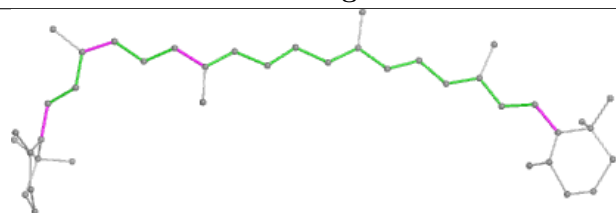
## Ligand BCR B 843



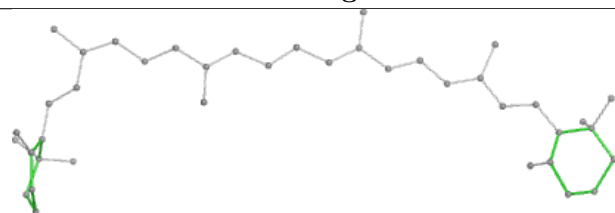
Bond lengths



Bond angles

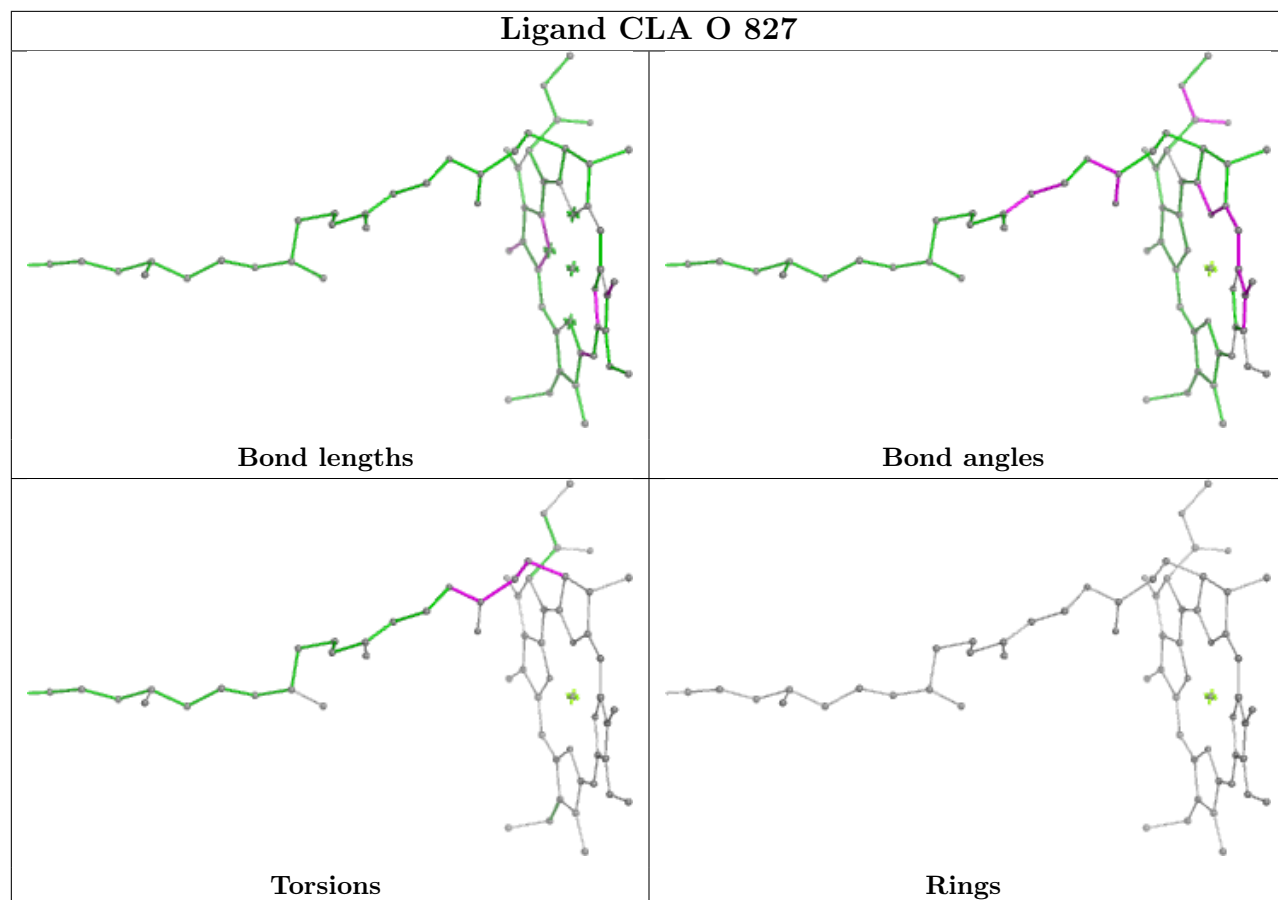
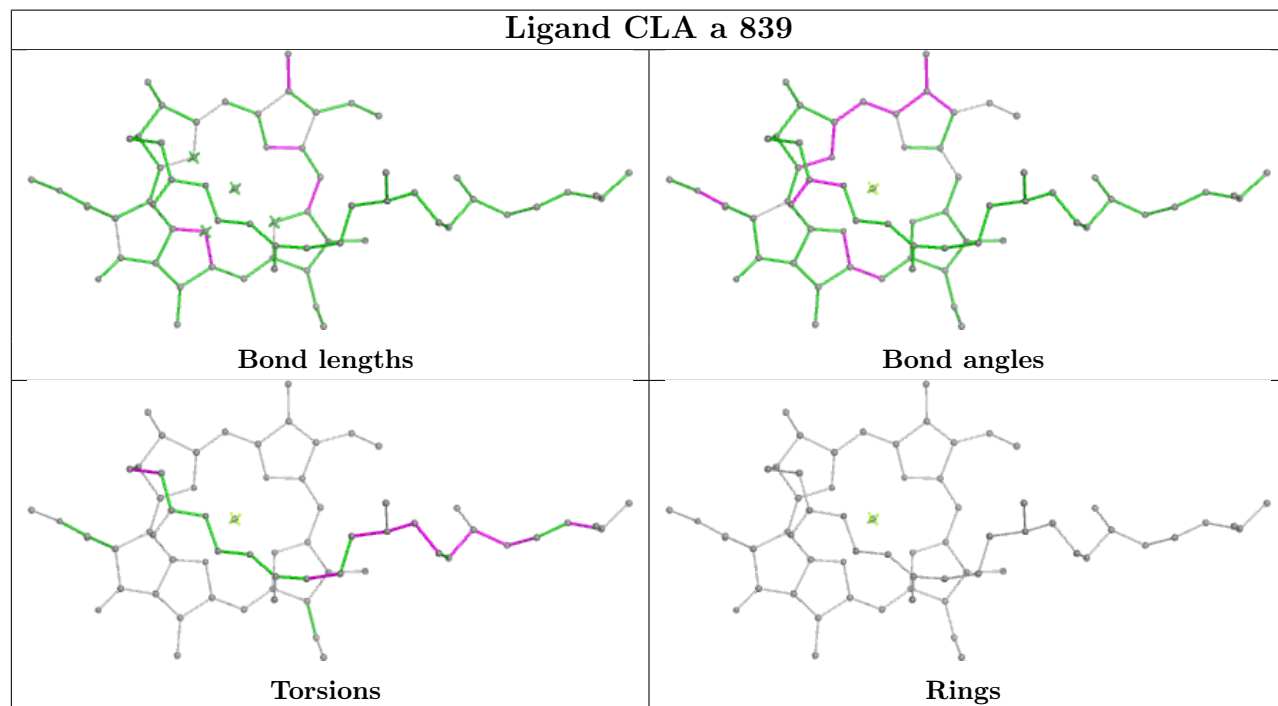


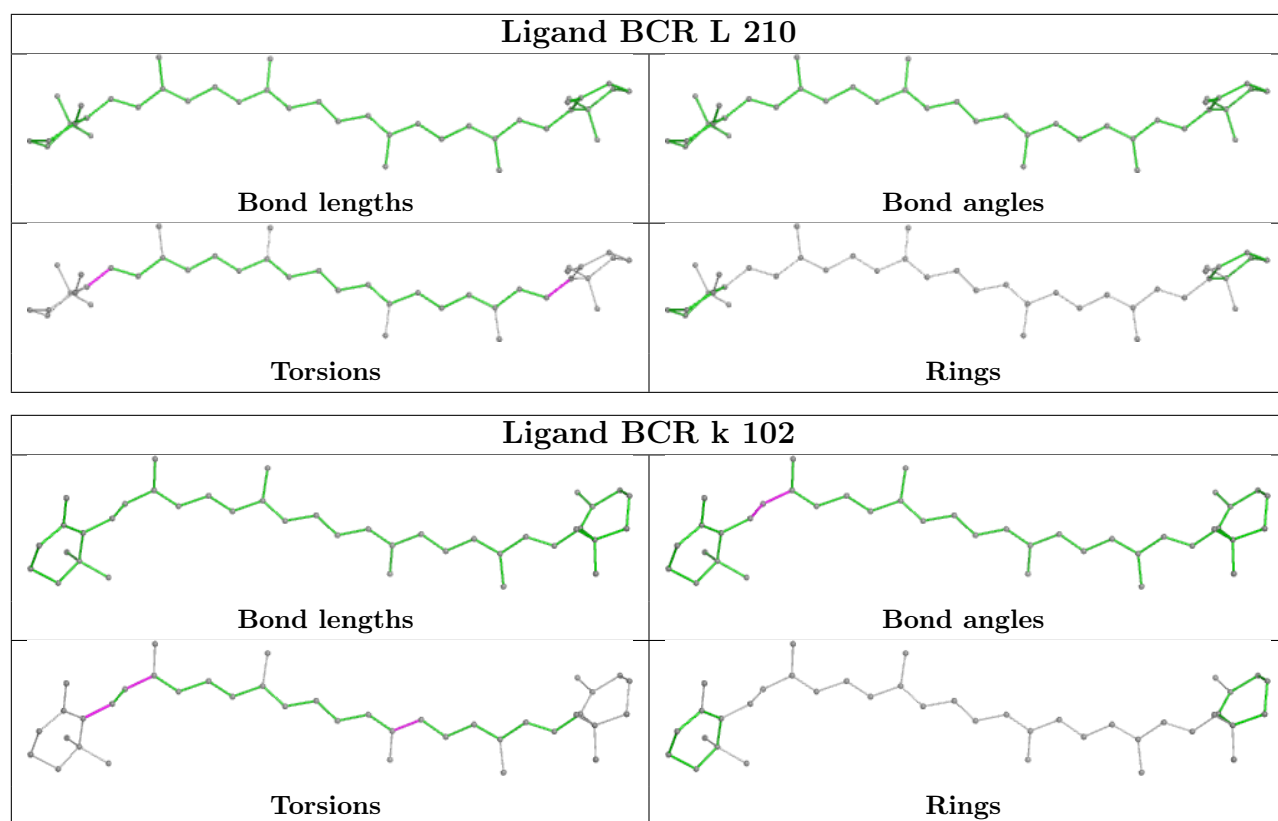
Torsions

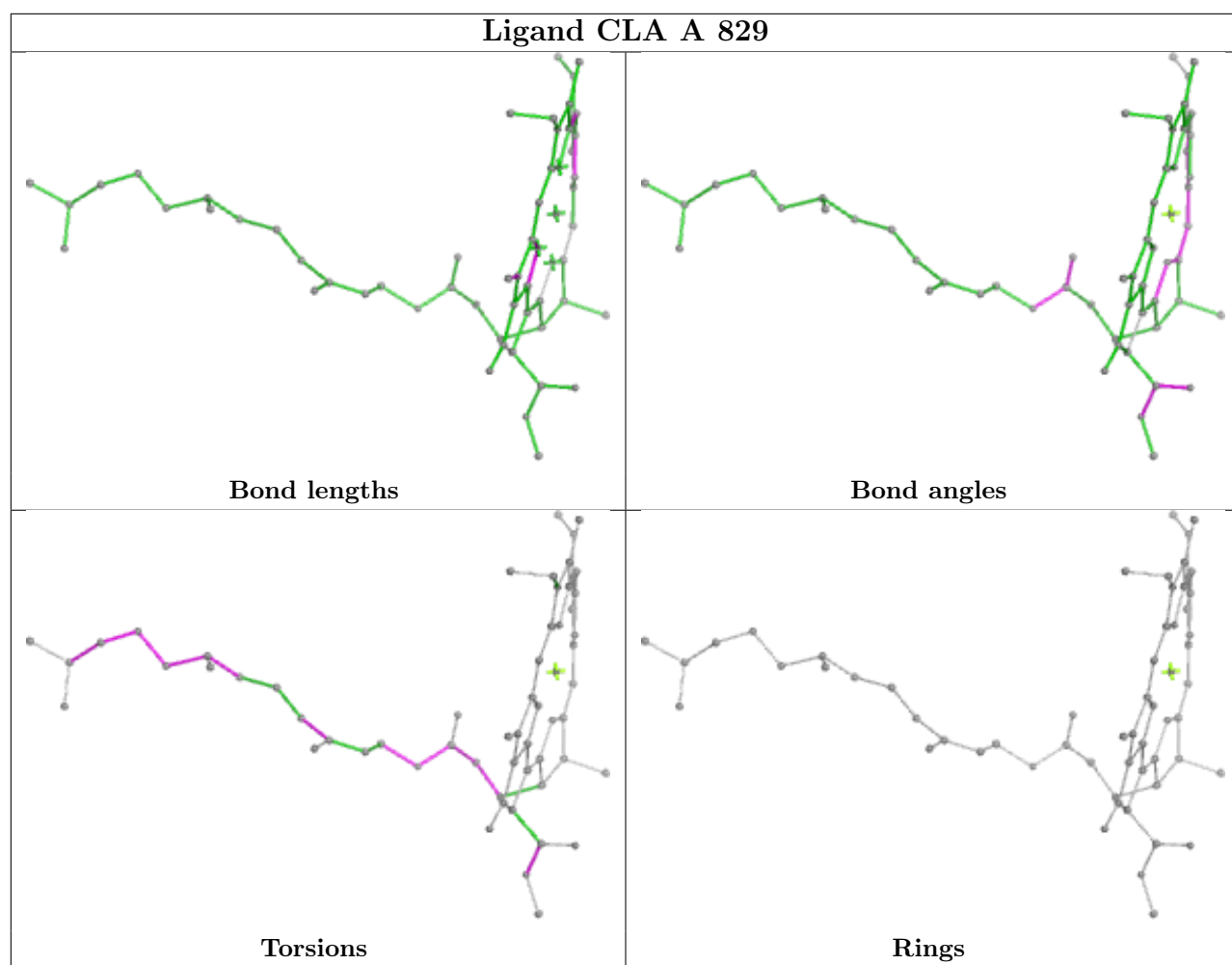


Rings

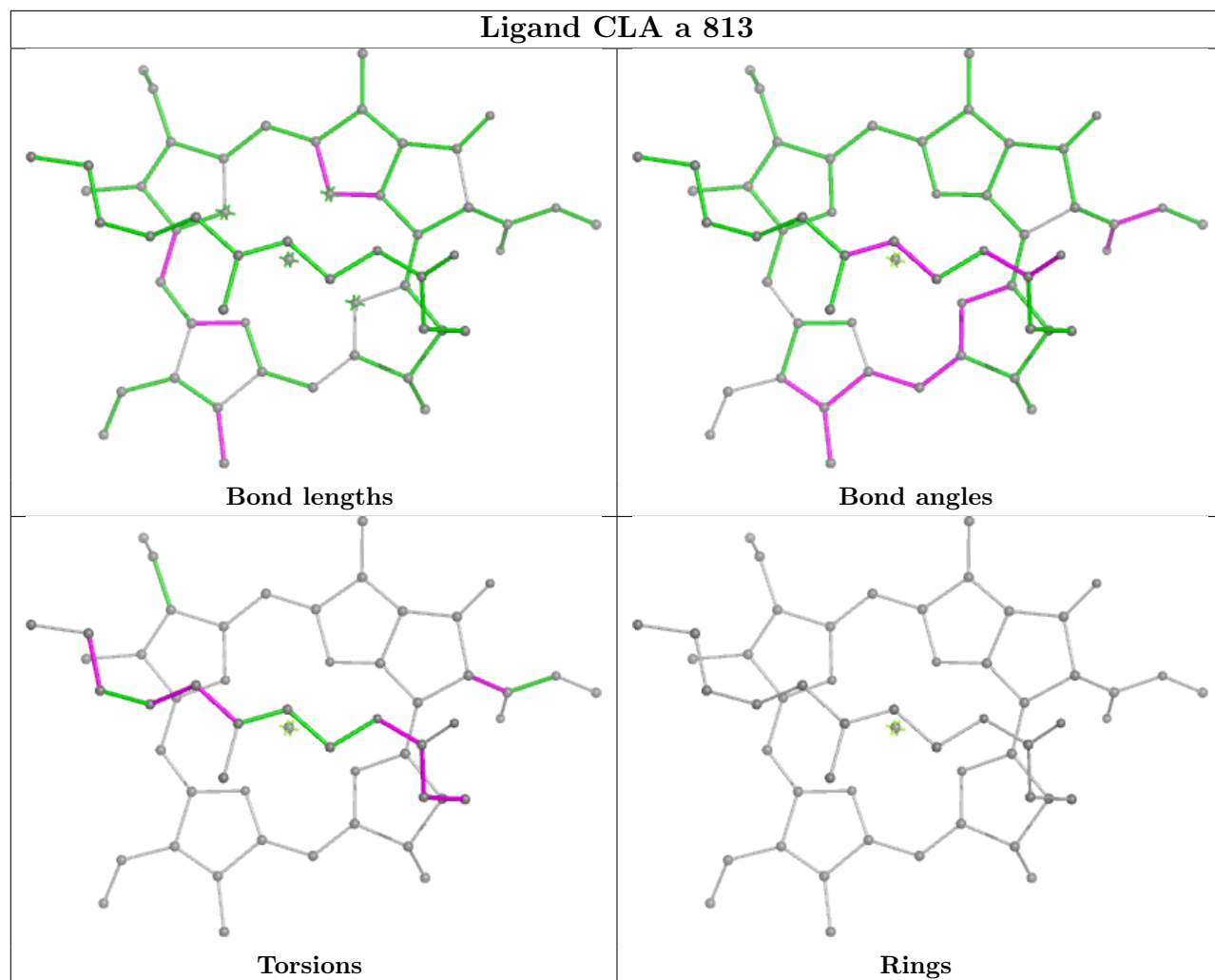


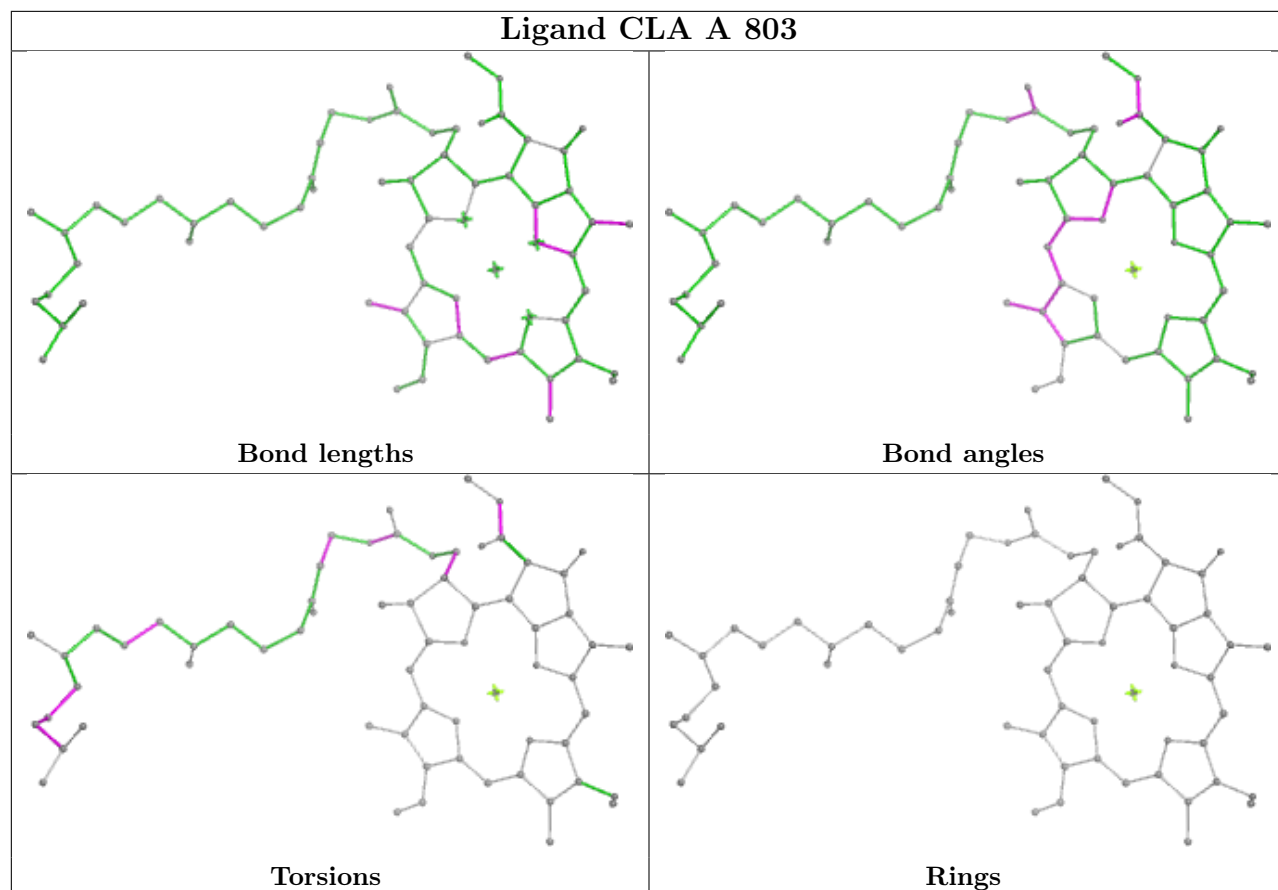
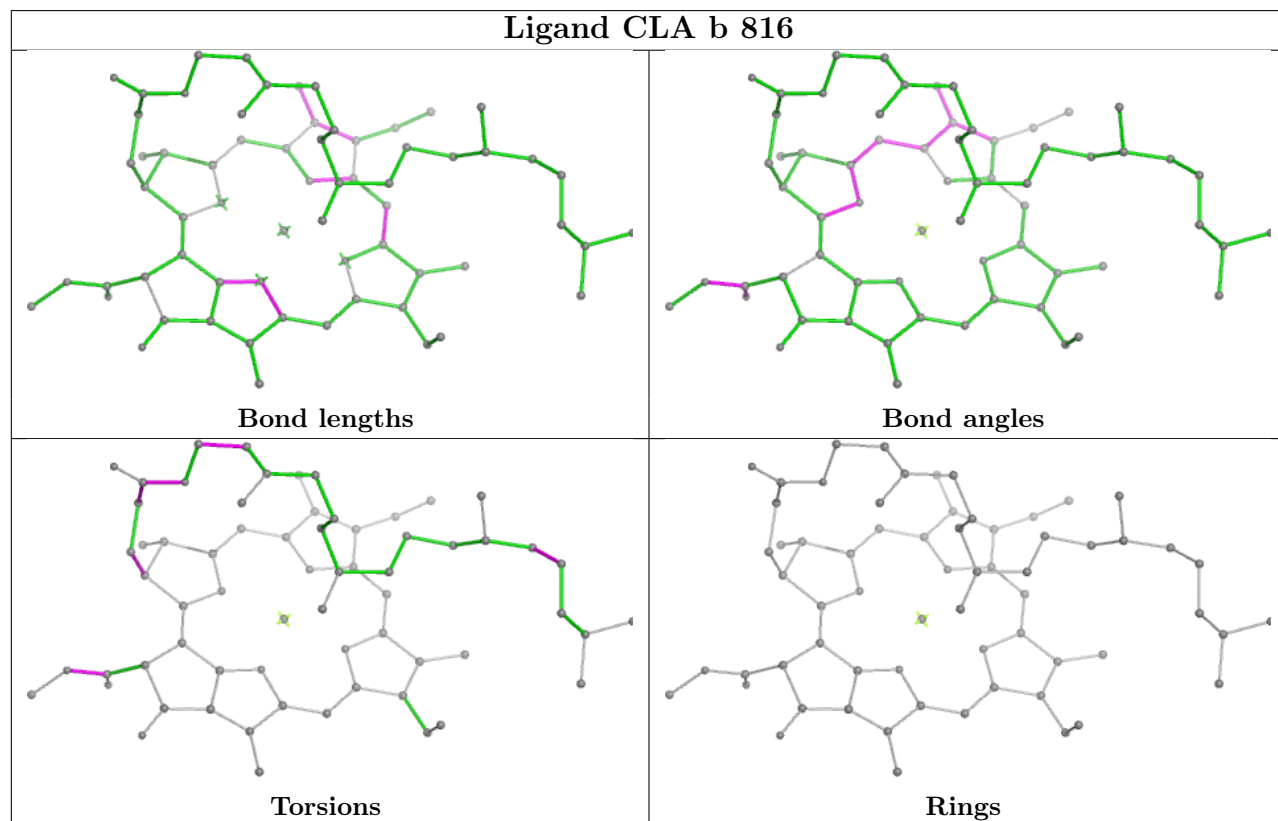
**Ligand CLA O 827****Ligand CLA a 839**

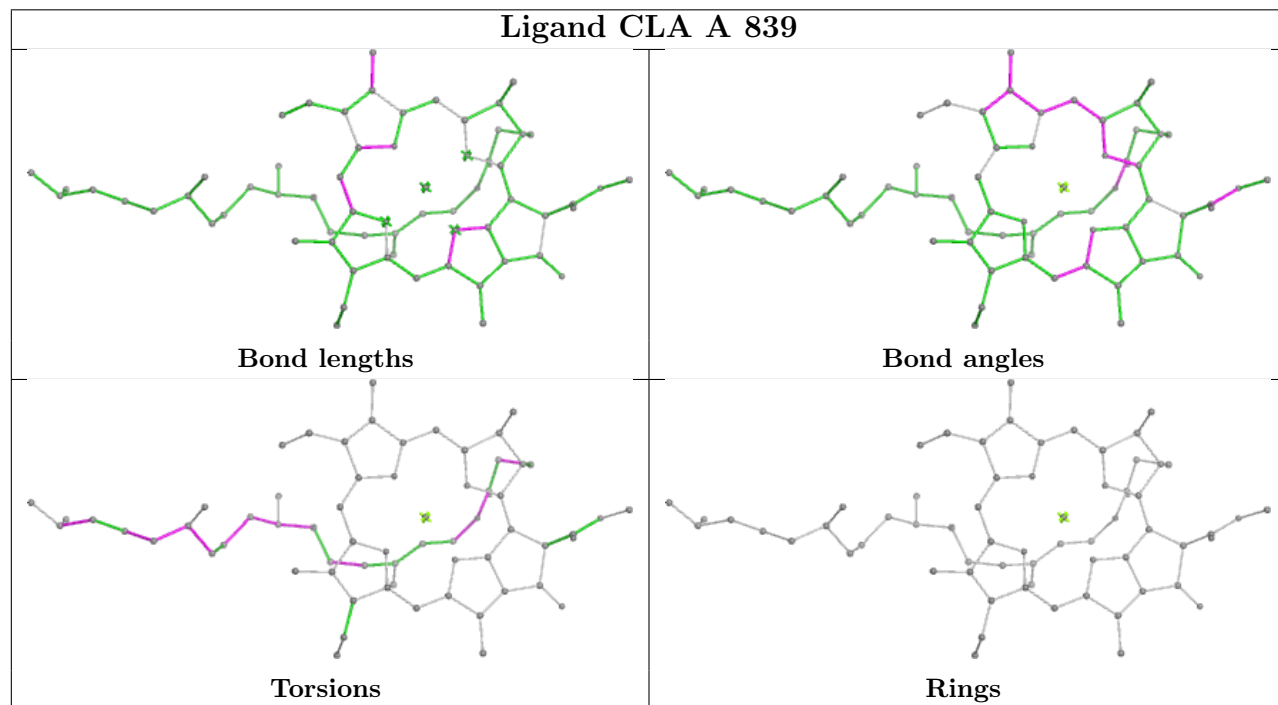
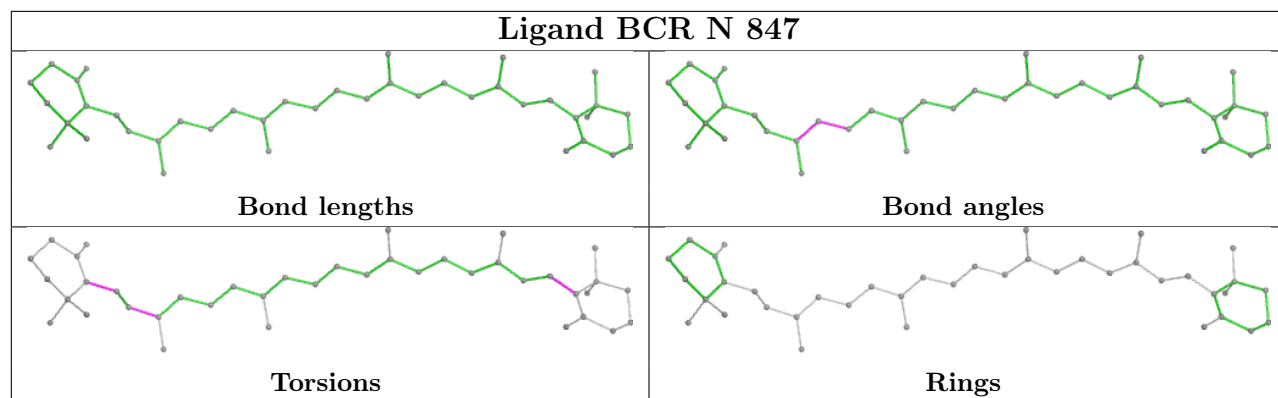


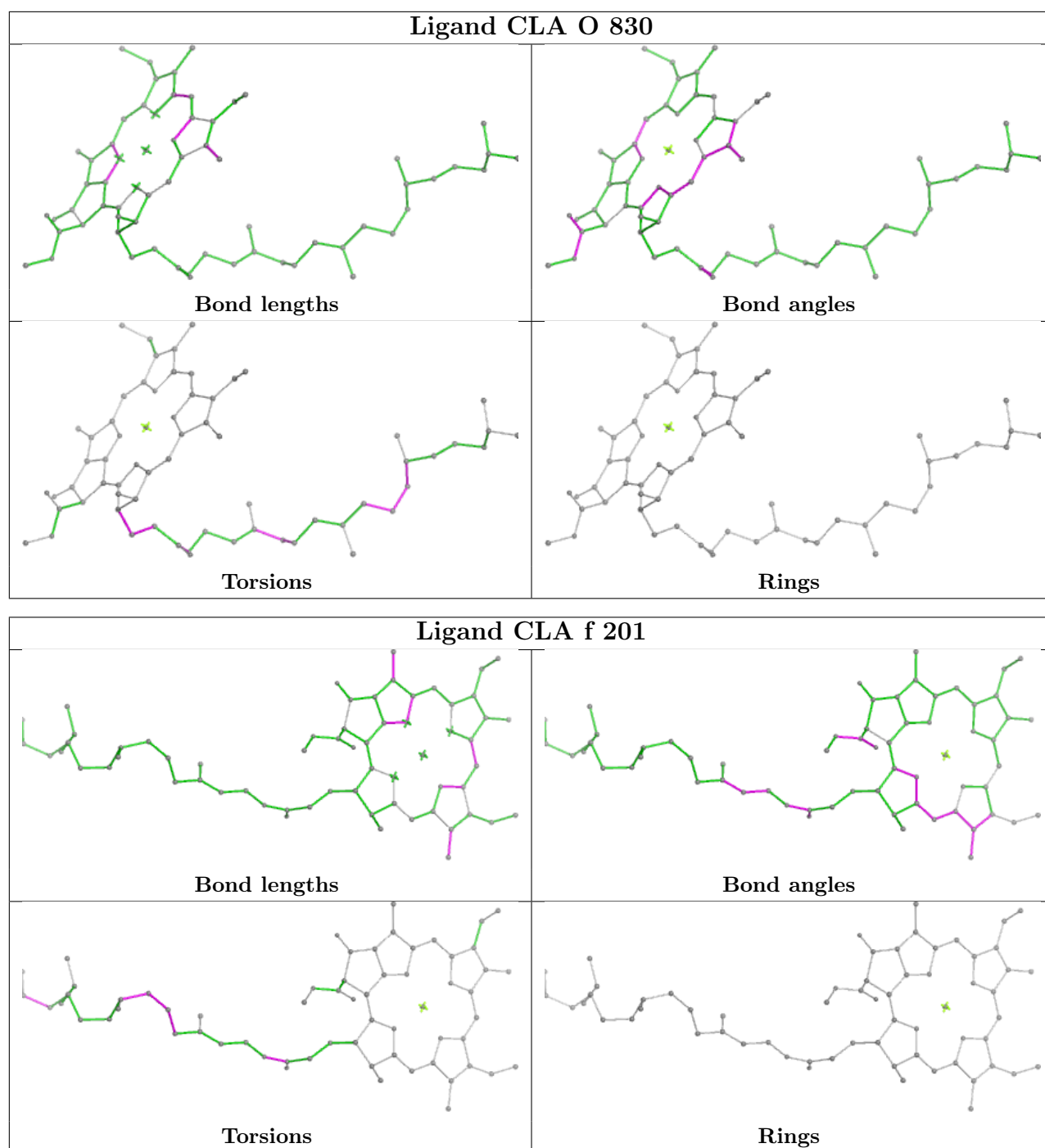


## Ligand CLA a 813



**Ligand CLA A 803****Ligand CLA b 816**





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52762. These allow visual inspection of the internal detail of the map and identification of artifacts.

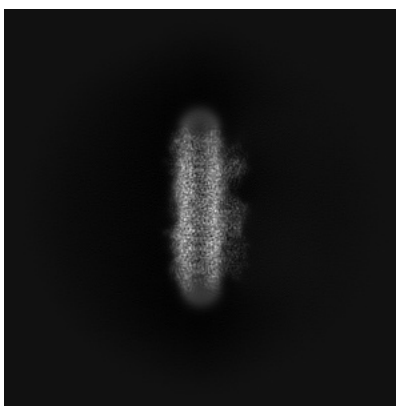
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

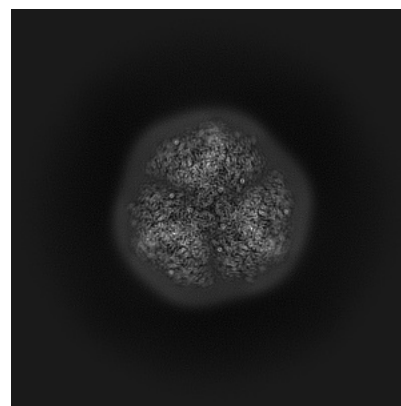
#### 6.1.1 Primary map



X

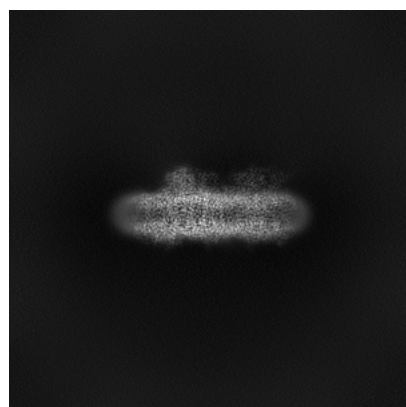


Y

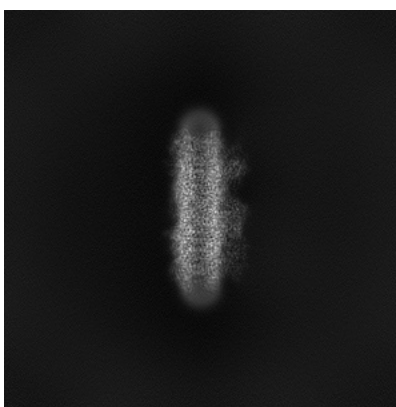


Z

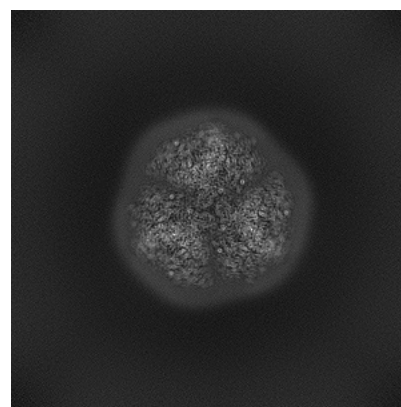
#### 6.1.2 Raw map



X



Y



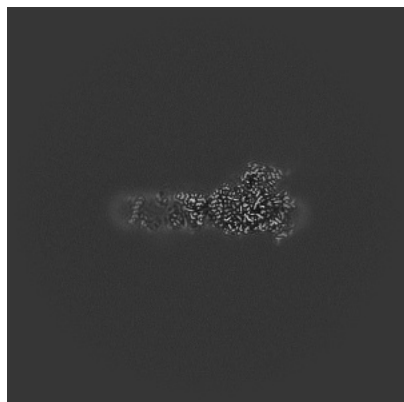
Z

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

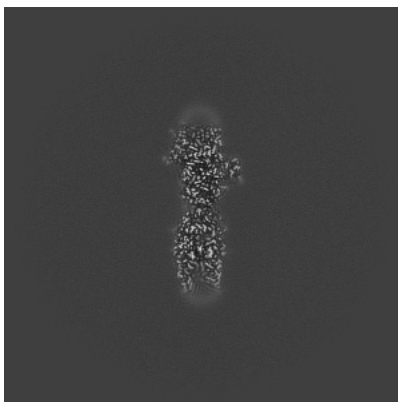


## 6.2 Central slices [i](#)

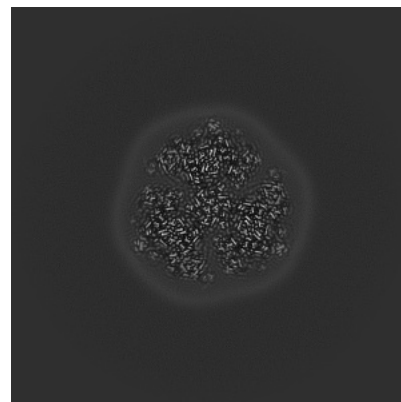
### 6.2.1 Primary map



X Index: 300

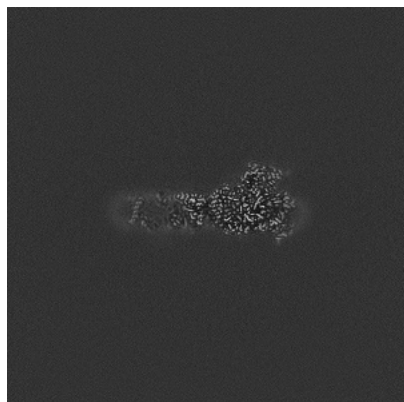


Y Index: 300

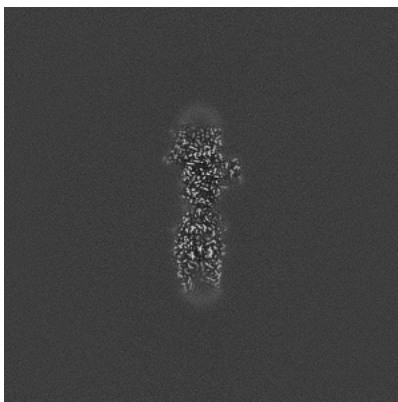


Z Index: 300

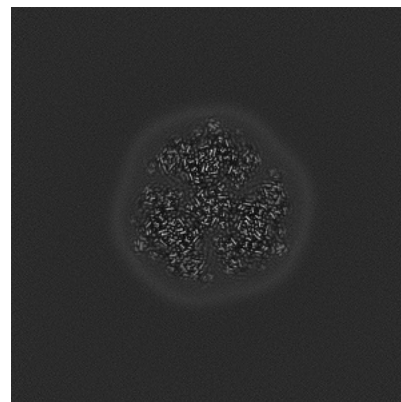
### 6.2.2 Raw map



X Index: 300



Y Index: 300

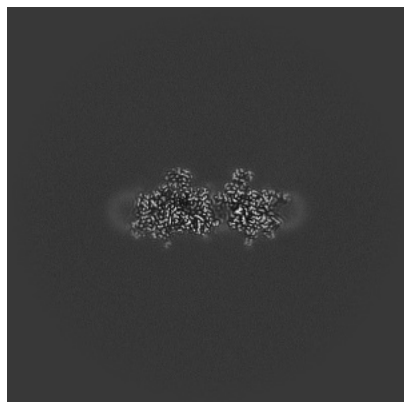


Z Index: 300

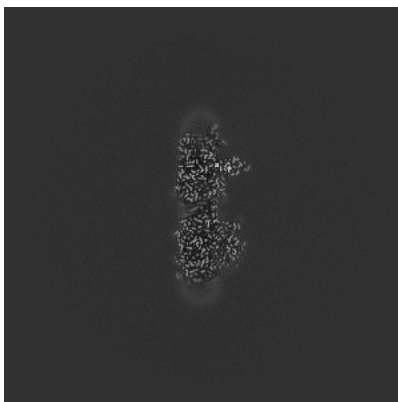
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

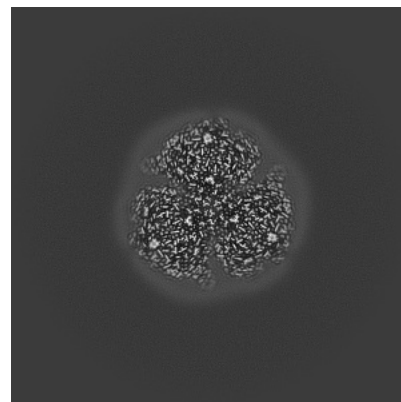
### 6.3.1 Primary map



X Index: 267

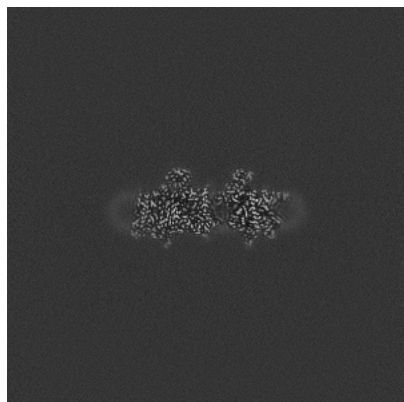


Y Index: 270

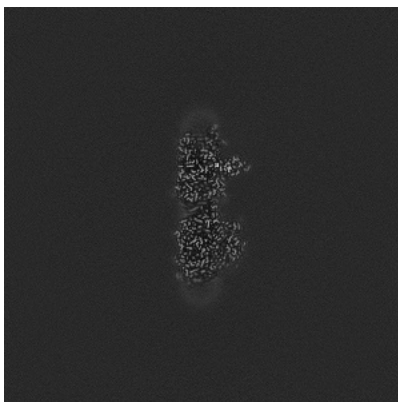


Z Index: 311

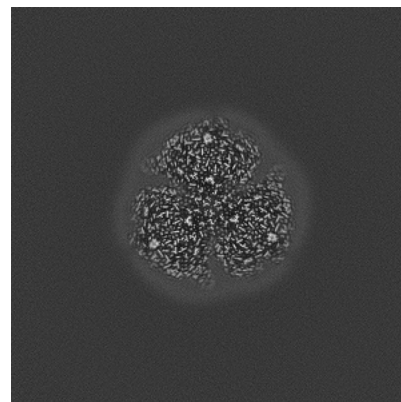
### 6.3.2 Raw map



X Index: 266



Y Index: 270

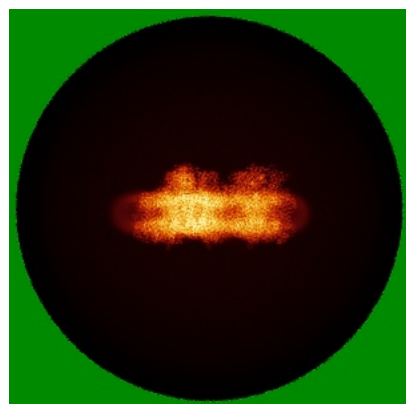


Z Index: 311

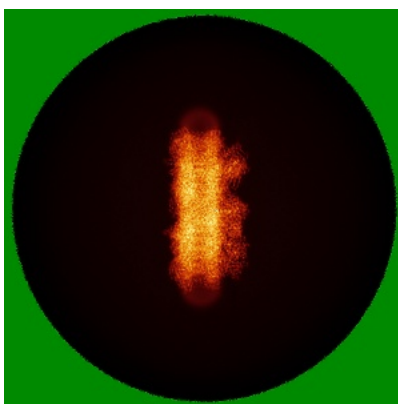
The images above show the largest variance slices of the map in three orthogonal directions.

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

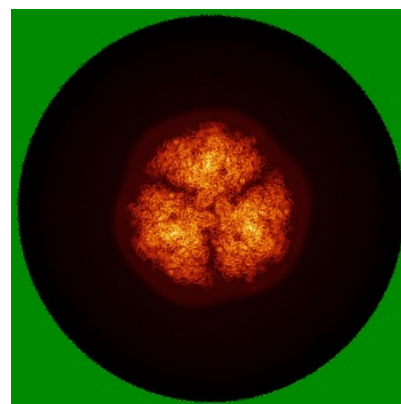
### 6.4.1 Primary map



X

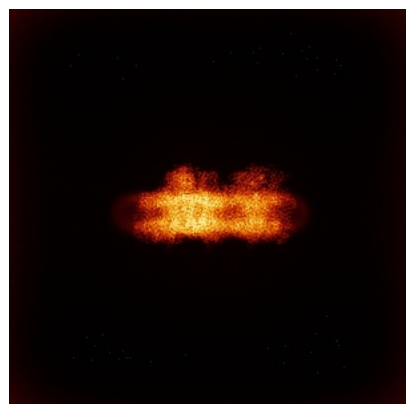


Y

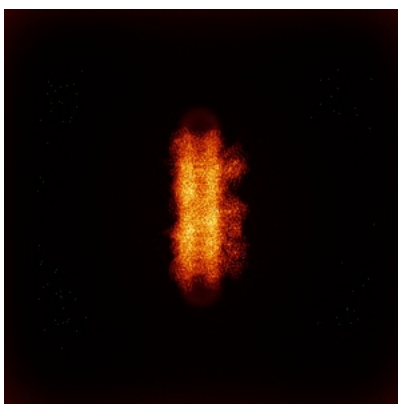


Z

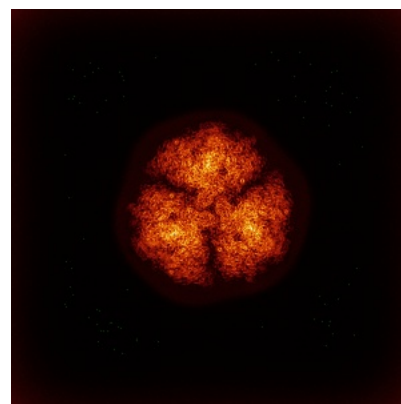
### 6.4.2 Raw map



X



Y

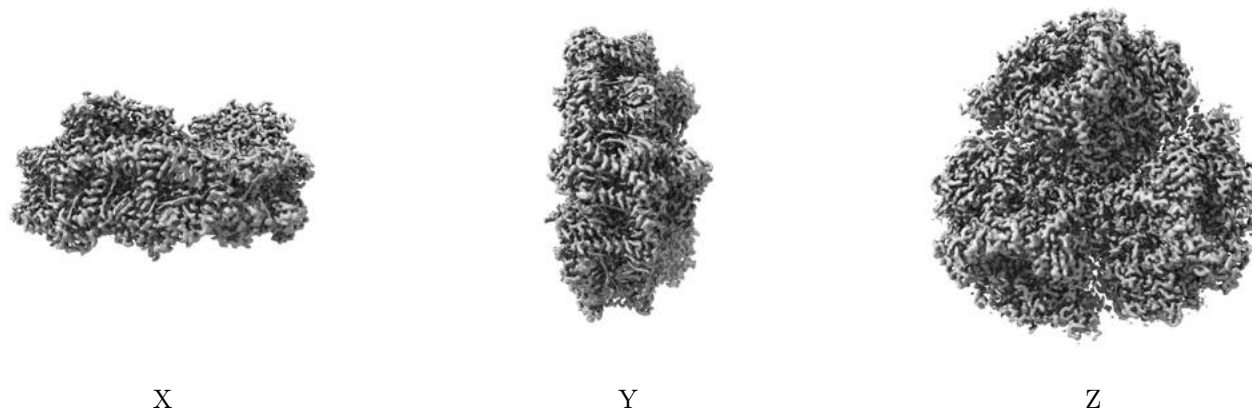


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

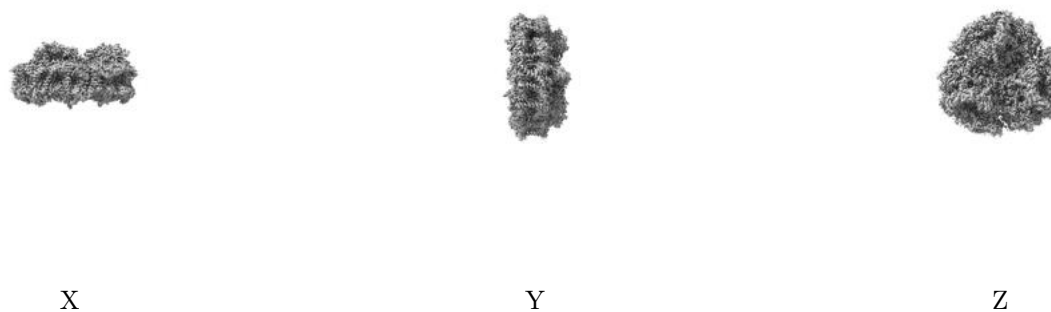
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.13. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

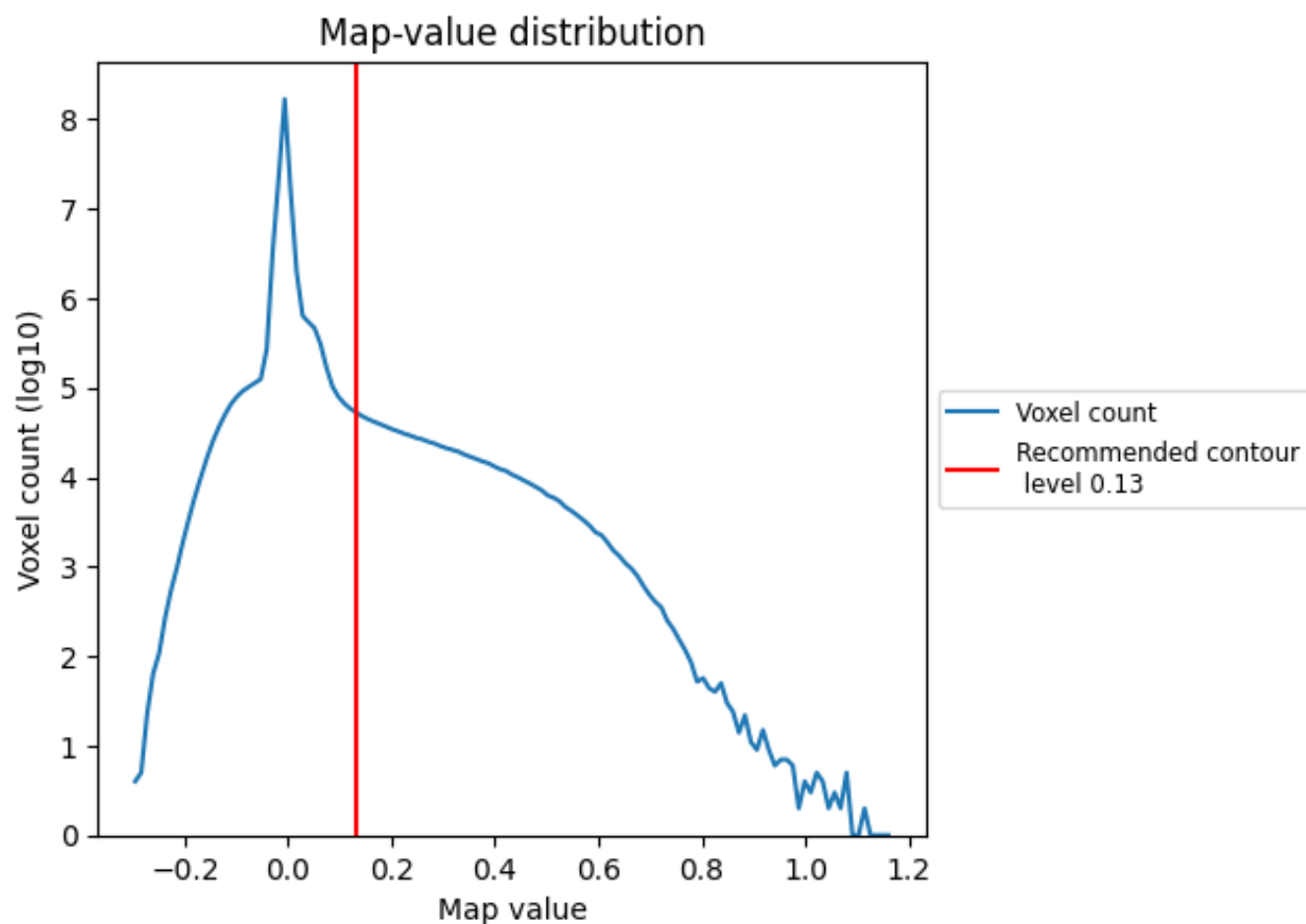
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

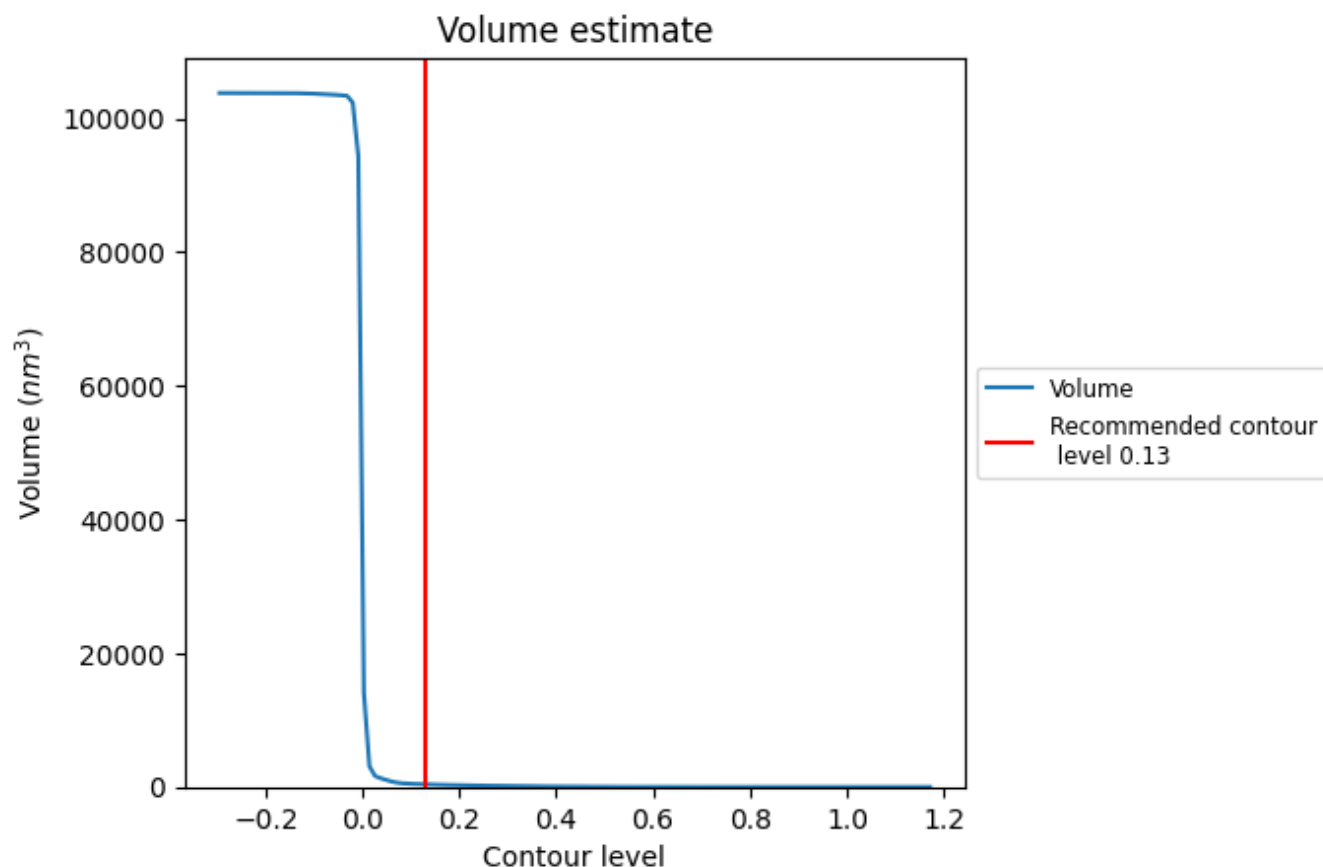
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

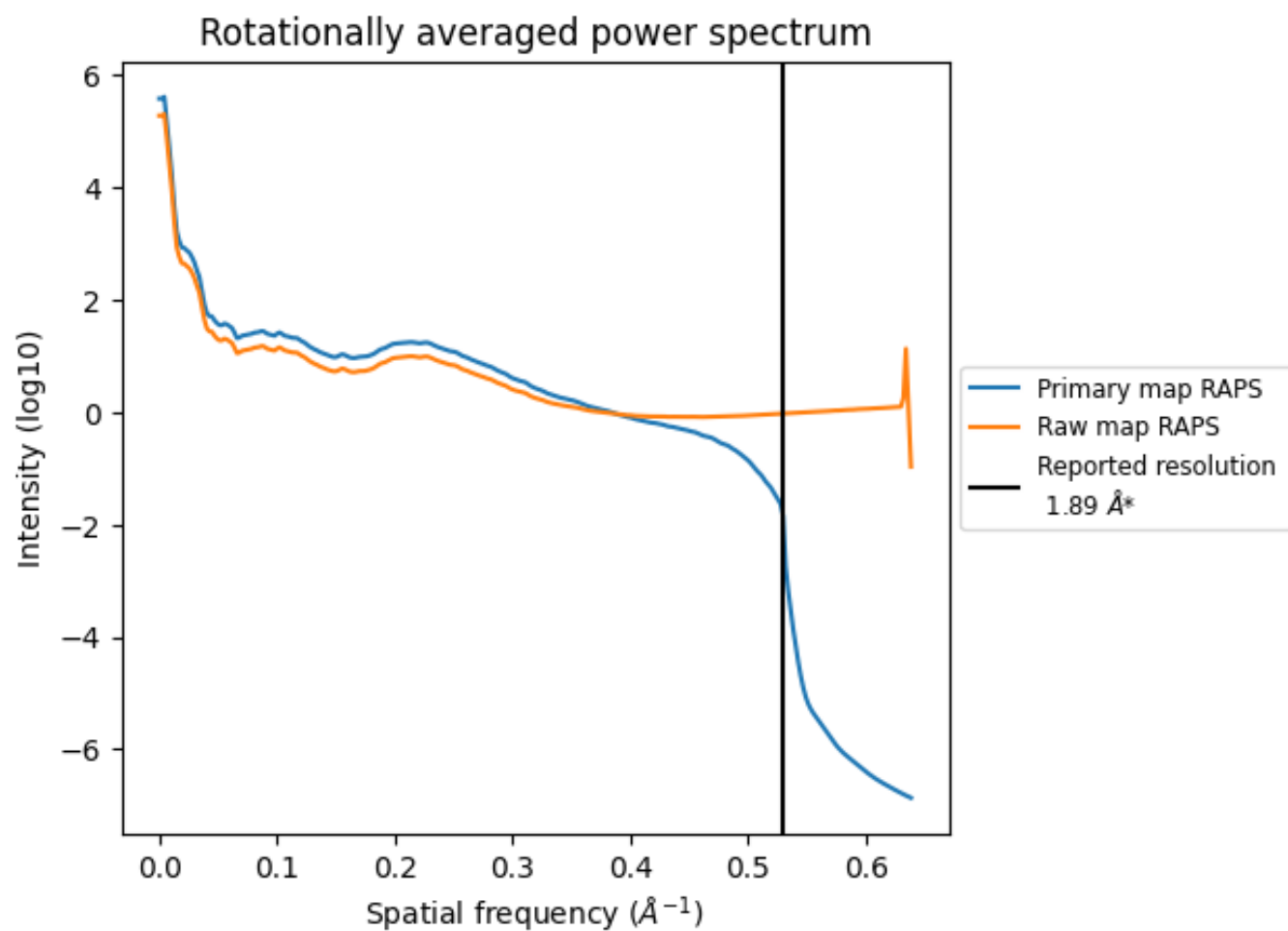
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 389  $\text{nm}^3$ ; this corresponds to an approximate mass of 352 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum [i](#)

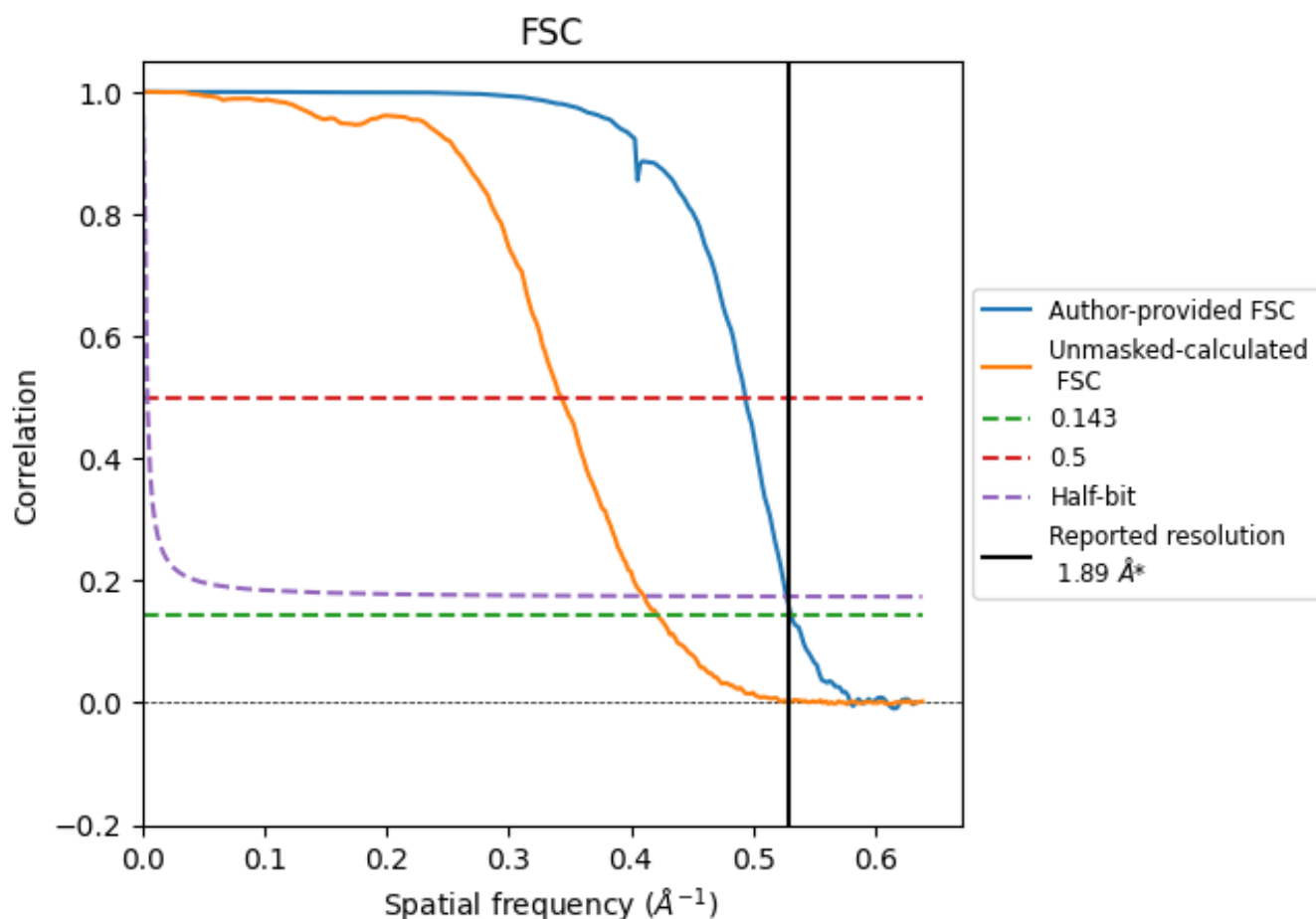


\*Reported resolution corresponds to spatial frequency of 0.529 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.529  $\text{\AA}^{-1}$



## 8.2 Resolution estimates [i](#)

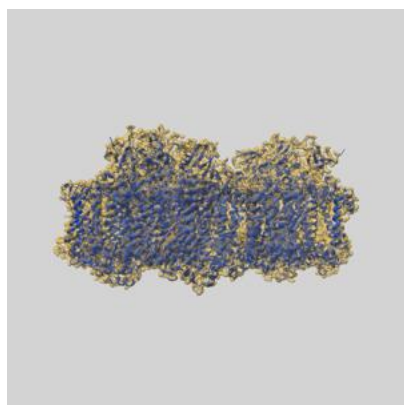
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.89	-	-
Author-provided FSC curve	1.88	2.03	1.90
Unmasked-calculated*	2.37	2.91	2.44

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.37 differs from the reported value 1.89 by more than 10 %

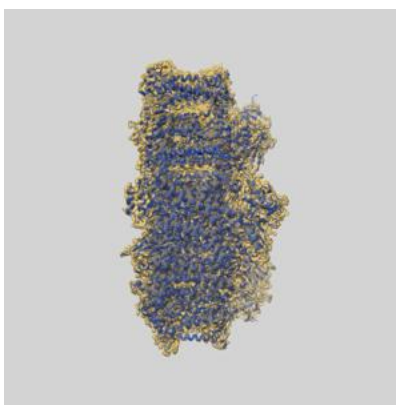
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52762 and PDB model 9I9L. Per-residue inclusion information can be found in section [3](#) on page [41](#).

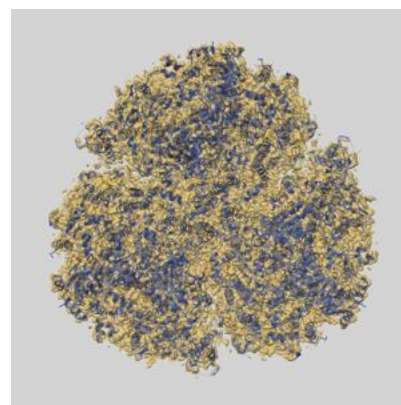
### 9.1 Map-model overlay [i](#)



X



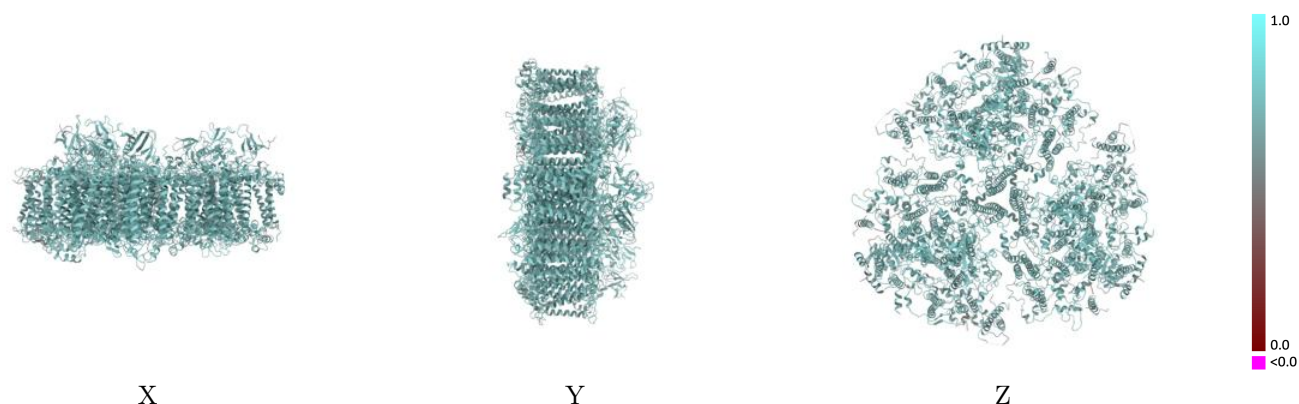
Y



Z

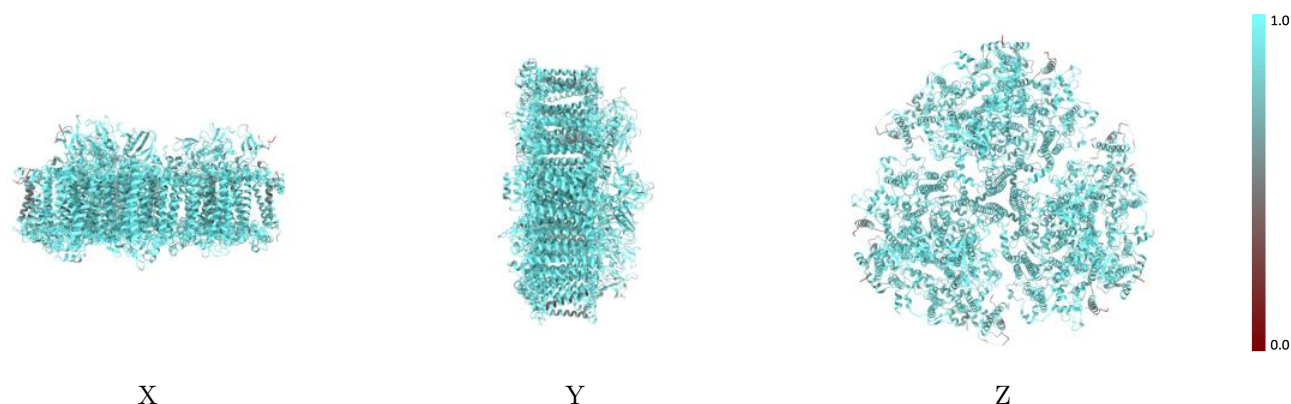
The images above show the 3D surface view of the map at the recommended contour level 0.13 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



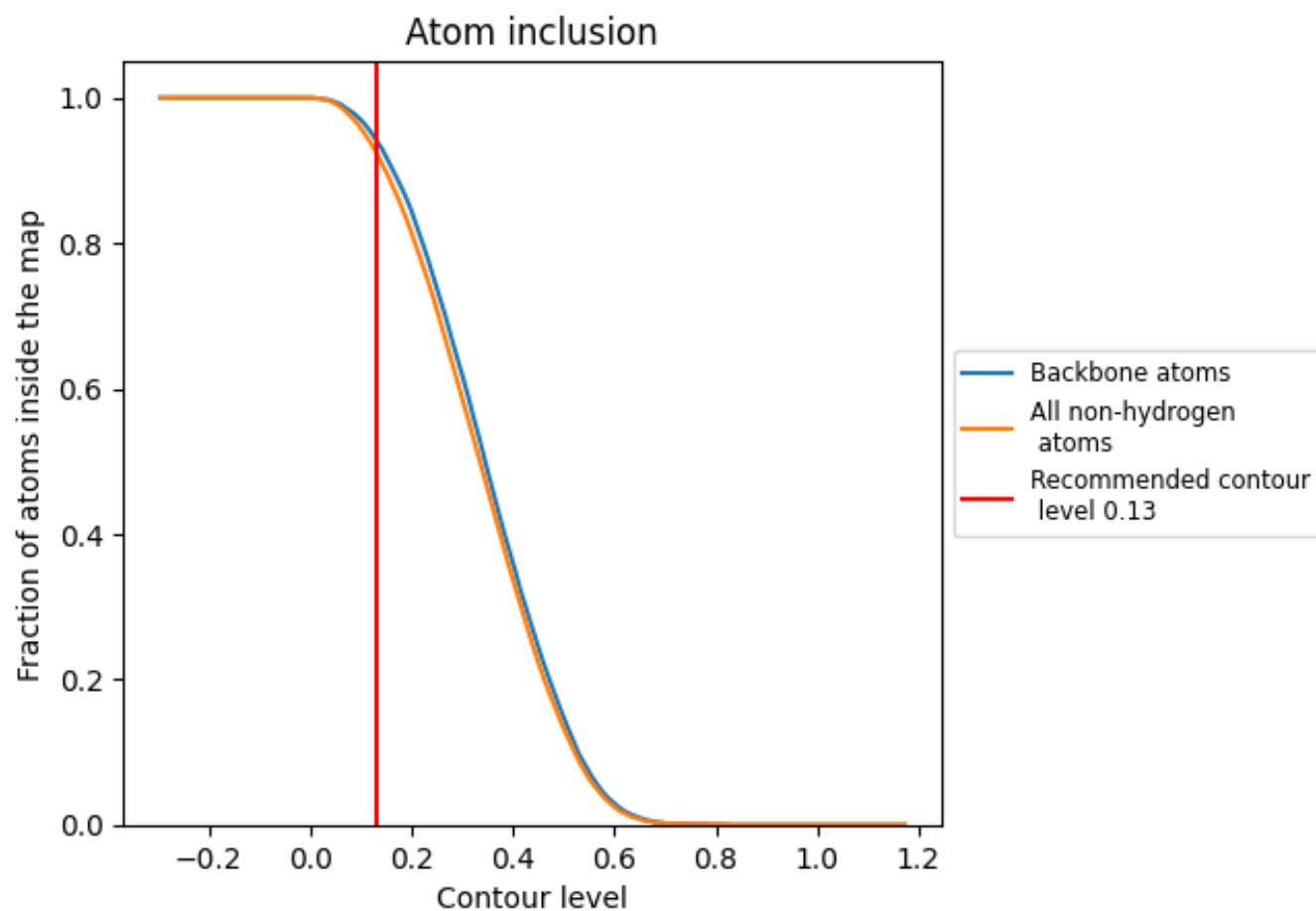
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.13).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.13) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9250	 0.6960
A	 0.9400	 0.6990
B	 0.9400	 0.7000
C	 0.9880	 0.7270
D	 0.9310	 0.6920
E	 0.8470	 0.6580
F	 0.8290	 0.6420
I	 0.9550	 0.7160
J	 0.8330	 0.6500
K	 0.7150	 0.6260
L	 0.9560	 0.7200
M	 0.9390	 0.7080
N	 0.9360	 0.7010
O	 0.9440	 0.7040
P	 0.9920	 0.7290
Q	 0.9340	 0.6980
R	 0.8470	 0.6600
S	 0.8560	 0.6530
T	 0.9500	 0.7190
U	 0.8450	 0.6540
V	 0.7140	 0.6210
W	 0.9550	 0.7210
X	 0.6580	 0.6300
Y	 0.8930	 0.6890
Z	 0.6580	 0.6320
a	 0.9420	 0.7030
b	 0.9440	 0.7030
c	 0.9870	 0.7260
d	 0.9260	 0.6960
e	 0.8520	 0.6570
f	 0.8360	 0.6460
g	 0.9500	 0.7210
h	 0.8430	 0.6530
i	 0.7180	 0.6270
j	 0.9580	 0.7220



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
k	 0.8930	 0.6890
l	 0.6580	 0.6270