



wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 05:21 am GMT

PDB ID : 7QCO
EMDB ID : EMD-13898
Title : The structure of Photosystem I tetramer from *Chroococcidiopsis* TS-821, a thermophilic, unicellular, non-heterocyst-forming cyanobacterium
Authors : Semchonok, D.A.; Mondal, J.; Cooper, J.C.; Schlum, K.; Li, M.; Amin, M.; Sorzano, C.O.S.; Ramirez-Aportela, E.; Kastritis, P.L.; Boekema, E.J.; Guskov, A.; Bruce, B.D.
Deposited on : 2021-11-24
Resolution : 3.70 Å(reported)
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

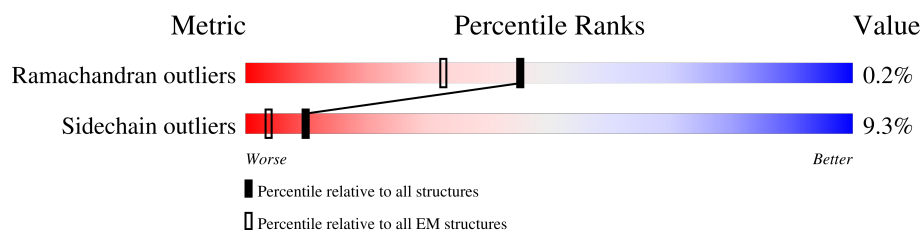
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	752	
1	E	752	
1	a	752	
1	e	752	
2	B	737	
2	G	737	
2	b	737	
2	g	737	

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Mol	Chain	Length	Quality of chain
3	C	82	
3	H	82	
3	c	82	
3	h	82	
4	D	168	
4	N	168	
4	d	168	
4	n	168	
5	V	126	
5	W	126	
5	v	126	
5	w	126	
6	F	164	
6	O	164	
6	f	164	
6	o	164	
7	I	39	
7	P	39	
7	i	39	
7	p	39	
8	J	49	
8	Q	49	
8	j	49	
8	q	49	
9	K	93	

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Mol	Chain	Length	Quality of chain
9	R	93	
9	k	93	
9	r	93	
10	L	172	
10	S	172	
10	l	172	
10	s	172	
11	M	31	
11	T	31	
11	m	31	
11	t	31	

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	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	809	X	-	-	-
13	CLA	A	810	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	812	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	-
13	CLA	A	817	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	821	X	-	-	-
13	CLA	A	822	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	825	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	830	X	-	-	-
13	CLA	A	831	X	-	-	-
13	CLA	A	832	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	834	X	-	-	-
13	CLA	A	835	X	-	-	-
13	CLA	A	836	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	840	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	843	X	-	-	-
13	CLA	A	844	X	-	-	-
13	CLA	A	845	X	-	-	-
13	CLA	A	853	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	802	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	808	X	-	-	-
13	CLA	B	809	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	814	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	817	X	-	-	-
13	CLA	B	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	819	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	821	X	-	-	-
13	CLA	B	822	X	-	-	-
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	826	X	-	-	-
13	CLA	B	827	X	-	-	-
13	CLA	B	828	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	837	X	-	-	-
13	CLA	B	838	X	-	-	-
13	CLA	B	839	X	-	-	-
13	CLA	B	840	X	-	-	-
13	CLA	B	841	X	-	-	-
13	CLA	E	803	X	-	-	-
13	CLA	E	804	X	-	-	-
13	CLA	E	805	X	-	-	-
13	CLA	E	806	X	-	-	-
13	CLA	E	807	X	-	-	-
13	CLA	E	808	X	-	-	-
13	CLA	E	809	X	-	-	-
13	CLA	E	810	X	-	-	-
13	CLA	E	811	X	-	-	-
13	CLA	E	812	X	-	-	-
13	CLA	E	813	X	-	-	-
13	CLA	E	814	X	-	-	-
13	CLA	E	815	X	-	-	-
13	CLA	E	816	X	-	-	-
13	CLA	E	817	X	-	-	-
13	CLA	E	818	X	-	-	-
13	CLA	E	819	X	-	-	-
13	CLA	E	820	X	-	-	-
13	CLA	E	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	E	822	X	-	-	-
13	CLA	E	823	X	-	-	-
13	CLA	E	824	X	-	-	-
13	CLA	E	825	X	-	-	-
13	CLA	E	826	X	-	-	-
13	CLA	E	827	X	-	-	-
13	CLA	E	828	X	-	-	-
13	CLA	E	829	X	-	-	-
13	CLA	E	830	X	-	-	-
13	CLA	E	831	X	-	-	-
13	CLA	E	832	X	-	-	-
13	CLA	E	833	X	-	-	-
13	CLA	E	834	X	-	-	-
13	CLA	E	835	X	-	-	-
13	CLA	E	836	X	-	-	-
13	CLA	E	837	X	-	-	-
13	CLA	E	839	X	-	-	-
13	CLA	E	840	X	-	-	-
13	CLA	E	841	X	-	-	-
13	CLA	E	842	X	-	-	-
13	CLA	E	843	X	-	-	-
13	CLA	E	844	X	-	-	-
13	CLA	E	845	X	-	-	-
13	CLA	E	846	X	-	-	-
13	CLA	F	202	X	-	-	-
13	CLA	G	801	X	-	-	-
13	CLA	G	802	X	-	-	-
13	CLA	G	803	X	-	-	-
13	CLA	G	804	X	-	-	-
13	CLA	G	805	X	-	-	-
13	CLA	G	806	X	-	-	-
13	CLA	G	807	X	-	-	-
13	CLA	G	808	X	-	-	-
13	CLA	G	809	X	-	-	-
13	CLA	G	810	X	-	-	-
13	CLA	G	811	X	-	-	-
13	CLA	G	812	X	-	-	-
13	CLA	G	813	X	-	-	-
13	CLA	G	814	X	-	-	-
13	CLA	G	815	X	-	-	-
13	CLA	G	816	X	-	-	-
13	CLA	G	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	G	818	X	-	-	-
13	CLA	G	819	X	-	-	-
13	CLA	G	820	X	-	-	-
13	CLA	G	821	X	-	-	-
13	CLA	G	822	X	-	-	-
13	CLA	G	823	X	-	-	-
13	CLA	G	824	X	-	-	-
13	CLA	G	825	X	-	-	-
13	CLA	G	826	X	-	-	-
13	CLA	G	827	X	-	-	-
13	CLA	G	828	X	-	-	-
13	CLA	G	829	X	-	-	-
13	CLA	G	830	X	-	-	-
13	CLA	G	831	X	-	-	-
13	CLA	G	832	X	-	-	-
13	CLA	G	833	X	-	-	-
13	CLA	G	834	X	-	-	-
13	CLA	G	835	X	-	-	-
13	CLA	G	836	X	-	-	-
13	CLA	G	837	X	-	-	-
13	CLA	G	838	X	-	-	-
13	CLA	G	839	X	-	-	-
13	CLA	G	840	X	-	-	-
13	CLA	G	841	X	-	-	-
13	CLA	K	101	X	-	-	-
13	CLA	K	102	X	-	-	-
13	CLA	L	202	X	-	-	-
13	CLA	L	203	X	-	-	-
13	CLA	L	204	X	-	-	-
13	CLA	O	203	X	-	-	-
13	CLA	R	102	X	-	-	-
13	CLA	S	203	X	-	-	-
13	CLA	S	204	X	-	-	-
13	CLA	S	206	X	-	-	-
13	CLA	a	804	X	-	-	-
13	CLA	a	805	X	-	-	-
13	CLA	a	806	X	-	-	-
13	CLA	a	807	X	-	-	-
13	CLA	a	808	X	-	-	-
13	CLA	a	809	X	-	-	-
13	CLA	a	810	X	-	-	-
13	CLA	a	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	812	X	-	-	-
13	CLA	a	813	X	-	-	-
13	CLA	a	814	X	-	-	-
13	CLA	a	815	X	-	-	-
13	CLA	a	816	X	-	-	-
13	CLA	a	817	X	-	-	-
13	CLA	a	818	X	-	-	-
13	CLA	a	819	X	-	-	-
13	CLA	a	820	X	-	-	-
13	CLA	a	821	X	-	-	-
13	CLA	a	822	X	-	-	-
13	CLA	a	823	X	-	-	-
13	CLA	a	824	X	-	-	-
13	CLA	a	825	X	-	-	-
13	CLA	a	826	X	-	-	-
13	CLA	a	827	X	-	-	-
13	CLA	a	828	X	-	-	-
13	CLA	a	829	X	-	-	-
13	CLA	a	830	X	-	-	-
13	CLA	a	831	X	-	-	-
13	CLA	a	832	X	-	-	-
13	CLA	a	833	X	-	-	-
13	CLA	a	834	X	-	-	-
13	CLA	a	835	X	-	-	-
13	CLA	a	836	X	-	-	-
13	CLA	a	837	X	-	-	-
13	CLA	a	839	X	-	-	-
13	CLA	a	840	X	-	-	-
13	CLA	a	841	X	-	-	-
13	CLA	a	842	X	-	-	-
13	CLA	a	843	X	-	-	-
13	CLA	a	844	X	-	-	-
13	CLA	a	845	X	-	-	-
13	CLA	a	852	X	-	-	-
13	CLA	b	801	X	-	-	-
13	CLA	b	802	X	-	-	-
13	CLA	b	803	X	-	-	-
13	CLA	b	804	X	-	-	-
13	CLA	b	805	X	-	-	-
13	CLA	b	806	X	-	-	-
13	CLA	b	807	X	-	-	-
13	CLA	b	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	809	X	-	-	-
13	CLA	b	810	X	-	-	-
13	CLA	b	811	X	-	-	-
13	CLA	b	812	X	-	-	-
13	CLA	b	813	X	-	-	-
13	CLA	b	814	X	-	-	-
13	CLA	b	815	X	-	-	-
13	CLA	b	816	X	-	-	-
13	CLA	b	817	X	-	-	-
13	CLA	b	818	X	-	-	-
13	CLA	b	819	X	-	-	-
13	CLA	b	820	X	-	-	-
13	CLA	b	821	X	-	-	-
13	CLA	b	822	X	-	-	-
13	CLA	b	823	X	-	-	-
13	CLA	b	824	X	-	-	-
13	CLA	b	825	X	-	-	-
13	CLA	b	826	X	-	-	-
13	CLA	b	827	X	-	-	-
13	CLA	b	828	X	-	-	-
13	CLA	b	829	X	-	-	-
13	CLA	b	830	X	-	-	-
13	CLA	b	831	X	-	-	-
13	CLA	b	832	X	-	-	-
13	CLA	b	833	X	-	-	-
13	CLA	b	834	X	-	-	-
13	CLA	b	835	X	-	-	-
13	CLA	b	836	X	-	-	-
13	CLA	b	837	X	-	-	-
13	CLA	b	838	X	-	-	-
13	CLA	b	839	X	-	-	-
13	CLA	b	840	X	-	-	-
13	CLA	e	803	X	-	-	-
13	CLA	e	804	X	-	-	-
13	CLA	e	805	X	-	-	-
13	CLA	e	806	X	-	-	-
13	CLA	e	807	X	-	-	-
13	CLA	e	808	X	-	-	-
13	CLA	e	809	X	-	-	-
13	CLA	e	810	X	-	-	-
13	CLA	e	811	X	-	-	-
13	CLA	e	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	813	X	-	-	-
13	CLA	e	814	X	-	-	-
13	CLA	e	815	X	-	-	-
13	CLA	e	816	X	-	-	-
13	CLA	e	817	X	-	-	-
13	CLA	e	818	X	-	-	-
13	CLA	e	819	X	-	-	-
13	CLA	e	820	X	-	-	-
13	CLA	e	821	X	-	-	-
13	CLA	e	822	X	-	-	-
13	CLA	e	823	X	-	-	-
13	CLA	e	824	X	-	-	-
13	CLA	e	825	X	-	-	-
13	CLA	e	826	X	-	-	-
13	CLA	e	827	X	-	-	-
13	CLA	e	828	X	-	-	-
13	CLA	e	829	X	-	-	-
13	CLA	e	830	X	-	-	-
13	CLA	e	831	X	-	-	-
13	CLA	e	832	X	-	-	-
13	CLA	e	833	X	-	-	-
13	CLA	e	834	X	-	-	-
13	CLA	e	835	X	-	-	-
13	CLA	e	837	X	-	-	-
13	CLA	e	838	X	-	-	-
13	CLA	e	839	X	-	-	-
13	CLA	e	840	X	-	-	-
13	CLA	e	841	X	-	-	-
13	CLA	e	842	X	-	-	-
13	CLA	e	843	X	-	-	-
13	CLA	e	844	X	-	-	-
13	CLA	e	852	X	-	-	-
13	CLA	f	203	X	-	-	-
13	CLA	g	801	X	-	-	-
13	CLA	g	802	X	-	-	-
13	CLA	g	803	X	-	-	-
13	CLA	g	805	X	-	-	-
13	CLA	g	806	X	-	-	-
13	CLA	g	807	X	-	-	-
13	CLA	g	808	X	-	-	-
13	CLA	g	809	X	-	-	-
13	CLA	g	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	g	811	X	-	-	-
13	CLA	g	812	X	-	-	-
13	CLA	g	813	X	-	-	-
13	CLA	g	814	X	-	-	-
13	CLA	g	815	X	-	-	-
13	CLA	g	816	X	-	-	-
13	CLA	g	817	X	-	-	-
13	CLA	g	818	X	-	-	-
13	CLA	g	819	X	-	-	-
13	CLA	g	820	X	-	-	-
13	CLA	g	821	X	-	-	-
13	CLA	g	822	X	-	-	-
13	CLA	g	823	X	-	-	-
13	CLA	g	824	X	-	-	-
13	CLA	g	825	X	-	-	-
13	CLA	g	826	X	-	-	-
13	CLA	g	827	X	-	-	-
13	CLA	g	828	X	-	-	-
13	CLA	g	829	X	-	-	-
13	CLA	g	830	X	-	-	-
13	CLA	g	831	X	-	-	-
13	CLA	g	832	X	-	-	-
13	CLA	g	833	X	-	-	-
13	CLA	g	834	X	-	-	-
13	CLA	g	835	X	-	-	-
13	CLA	g	836	X	-	-	-
13	CLA	g	837	X	-	-	-
13	CLA	g	838	X	-	-	-
13	CLA	g	839	X	-	-	-
13	CLA	g	840	X	-	-	-
13	CLA	g	841	X	-	-	-
13	CLA	g	842	X	-	-	-
13	CLA	k	4002	X	-	-	-
13	CLA	l	201	X	-	-	-
13	CLA	l	203	X	-	-	-
13	CLA	l	204	X	-	-	-
13	CLA	l	205	X	-	-	-
13	CLA	o	202	X	-	-	-
13	CLA	r	101	X	-	-	-
13	CLA	r	102	X	-	-	-
13	CLA	s	202	X	-	-	-
13	CLA	s	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	s	205	X	-	-	-

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 90396 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	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	E	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	e	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	a	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	G	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	g	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	b	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	H	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	h	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	c	81	Total	C	N	O	S	0	0
			605	370	105	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	N	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		
4	n	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	d	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	V	61	Total	C	N	O	0	0
			494	315	86	93		
5	W	61	Total	C	N	O	0	0
			494	315	86	93		
5	v	61	Total	C	N	O	0	0
			494	315	86	93		
5	w	61	Total	C	N	O	0	0
			494	315	86	93		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	O	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	o	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	f	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	P	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	p	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	37	Total	C	N	O		0	0
			311	218	44	49			
8	Q	37	Total	C	N	O		0	0
			311	218	44	49			
8	q	37	Total	C	N	O		0	0
			311	218	44	49			
8	j	37	Total	C	N	O		0	0
			311	218	44	49			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	R	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	r	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	k	65	Total	C	N	O	S	0	0
			474	316	80	77	1		

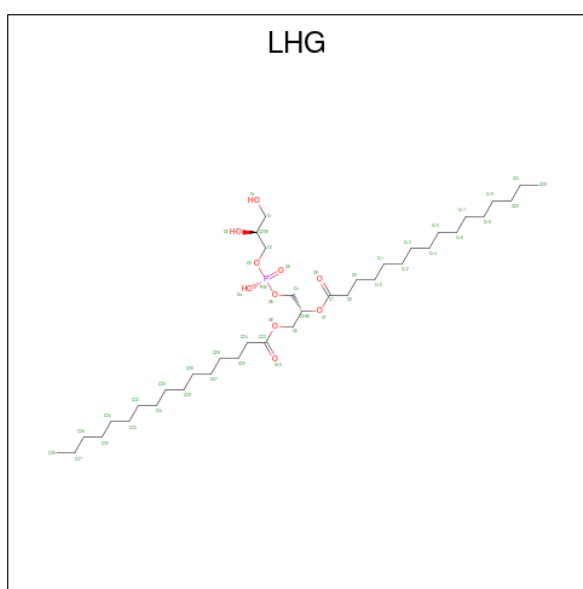
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	S	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	s	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	l	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		

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

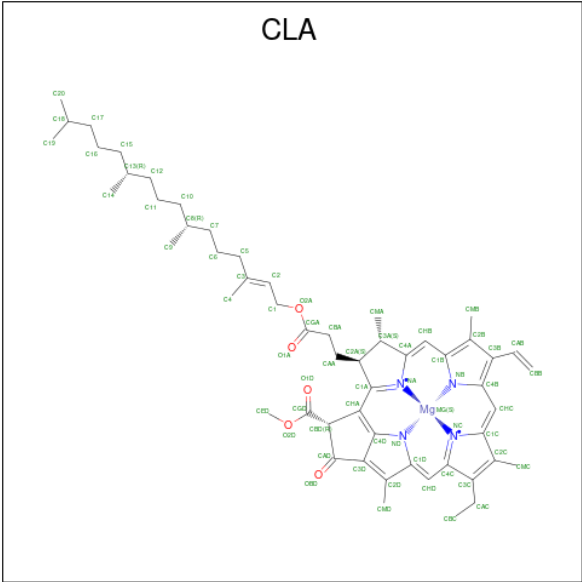
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	T	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	t	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	A	1	Total	C	O	P	0
			38	27	10	1	
12	e	1	Total	C	O	P	0
			49	38	10	1	
12	e	1	Total	C	O	P	0
			38	27	10	1	
12	a	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	L	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	E	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	E	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	G	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	G	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	r	1	Total 41	C 33	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
13	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	s	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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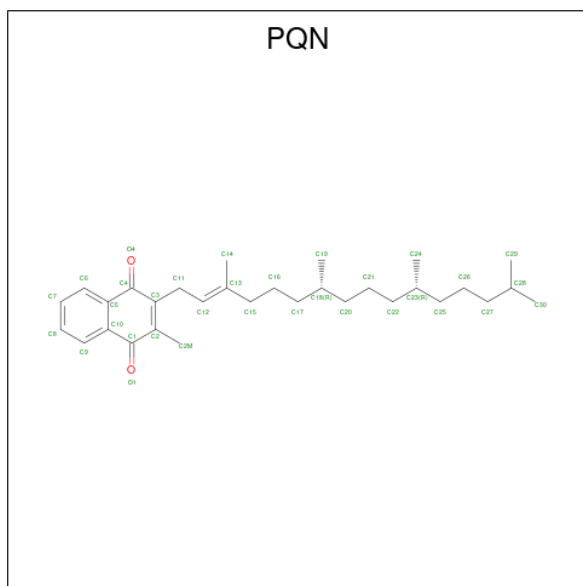
Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	f	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	l	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

- Molecule 14 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



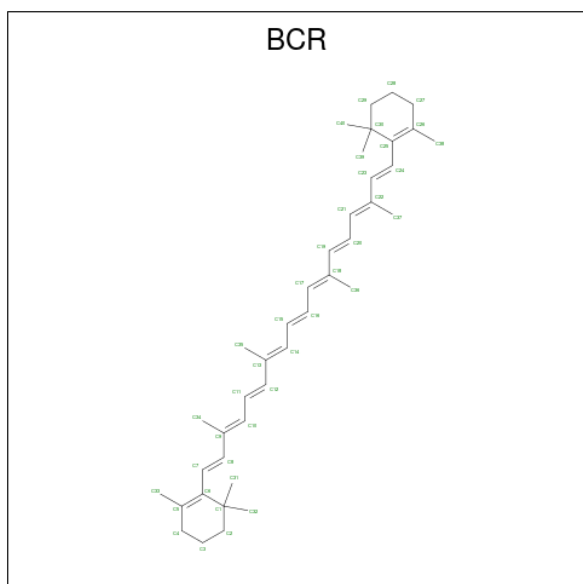
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	

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Mol	Chain	Residues	Atoms			AltConf
14	E	1	Total	C	O	0
			33	31	2	
14	G	1	Total	C	O	0
			33	31	2	
14	e	1	Total	C	O	0
			33	31	2	
14	g	1	Total	C	O	0
			33	31	2	
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	
15	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	F	1	Total C 40 40	0
15	I	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	J	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	L	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	E	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	G	1	Total C 40 40	0
15	O	1	Total C 40 40	0
15	O	1	Total C 40 40	0
15	P	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	T	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	e	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0

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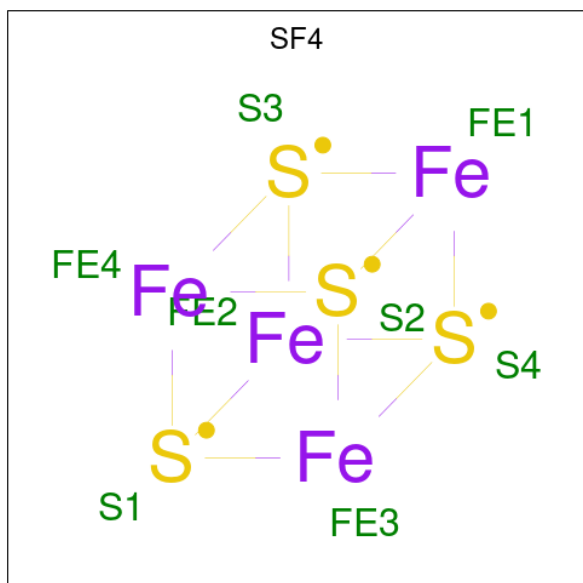
Mol	Chain	Residues	Atoms	AltConf
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	o	1	Total C 40 40	0
15	p	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	m	1	Total C 40 40	0

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



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

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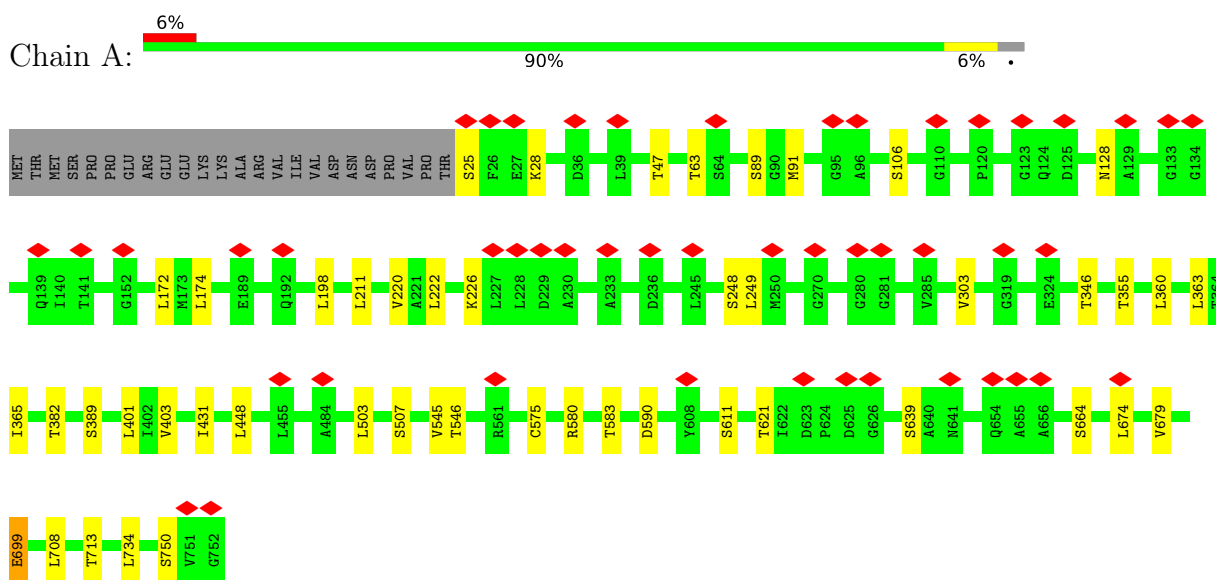
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Mol	Chain	Residues	Atoms			AltConf
16	C	1	Total 8	Fe 4	S 4	0
16	C	1	Total 8	Fe 4	S 4	0
16	E	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	g	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	a	1	Total 8	Fe 4	S 4	0
16	c	1	Total 8	Fe 4	S 4	0
16	c	1	Total 8	Fe 4	S 4	0

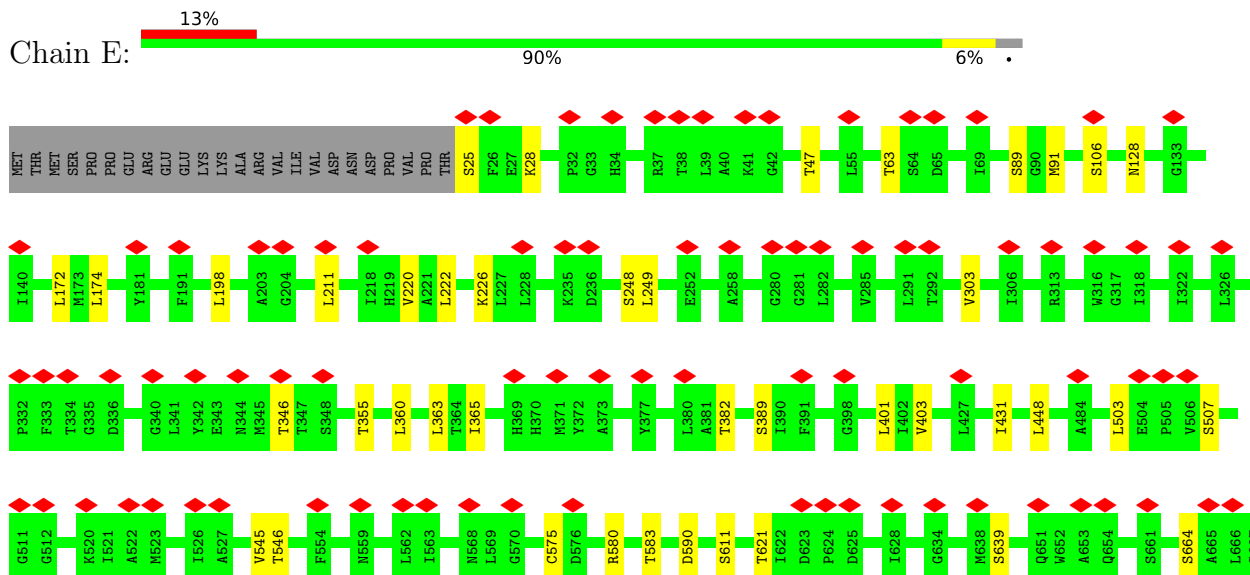
3 Residue-property plots

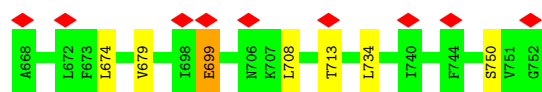
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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



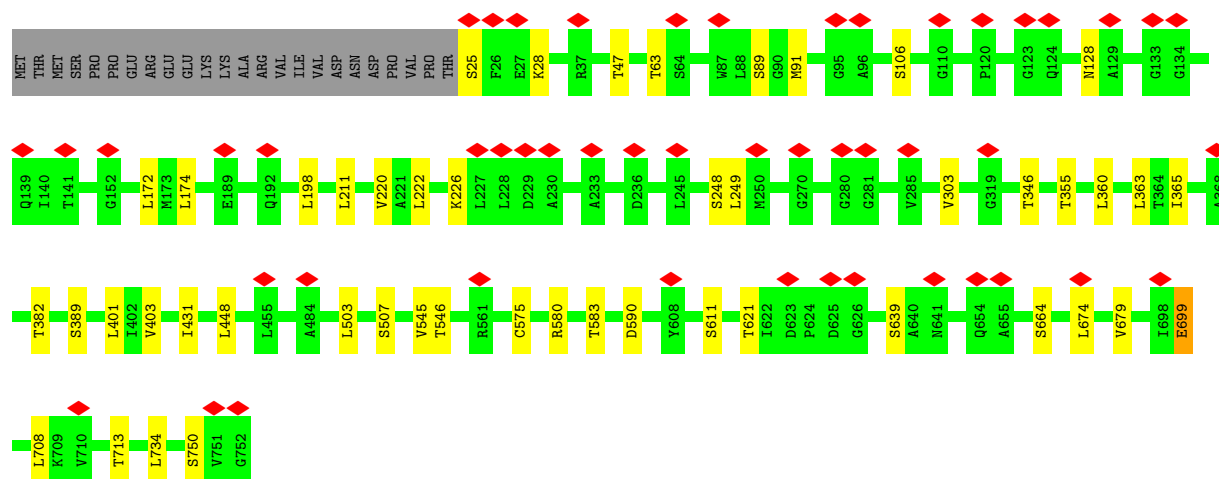
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





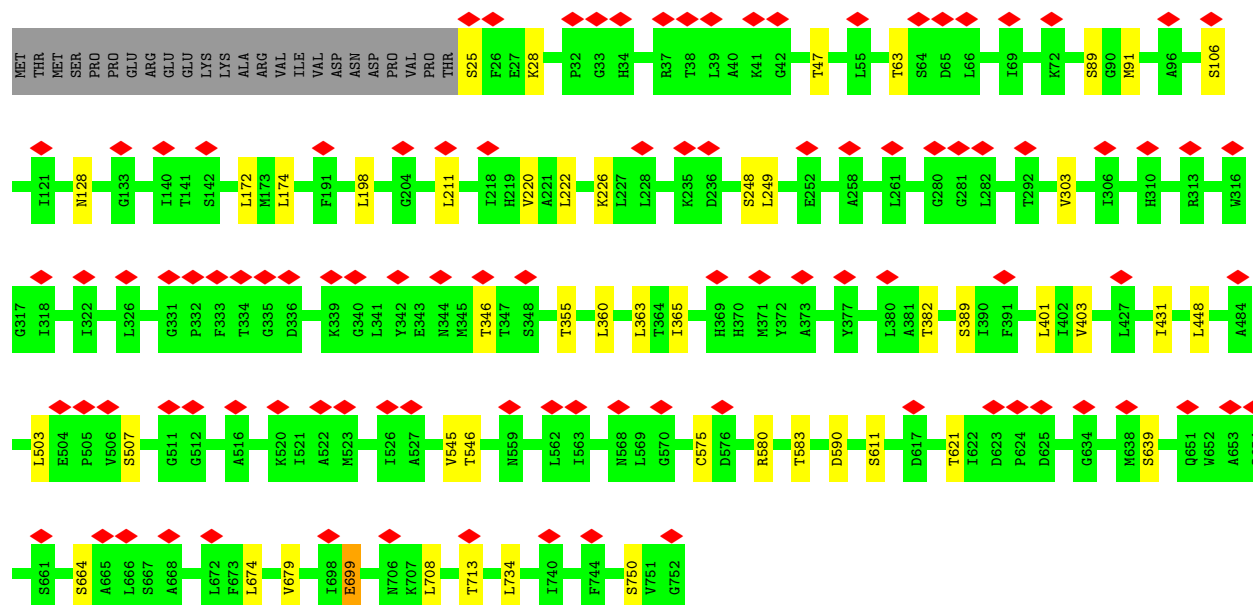
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e: 7% 90% 6%



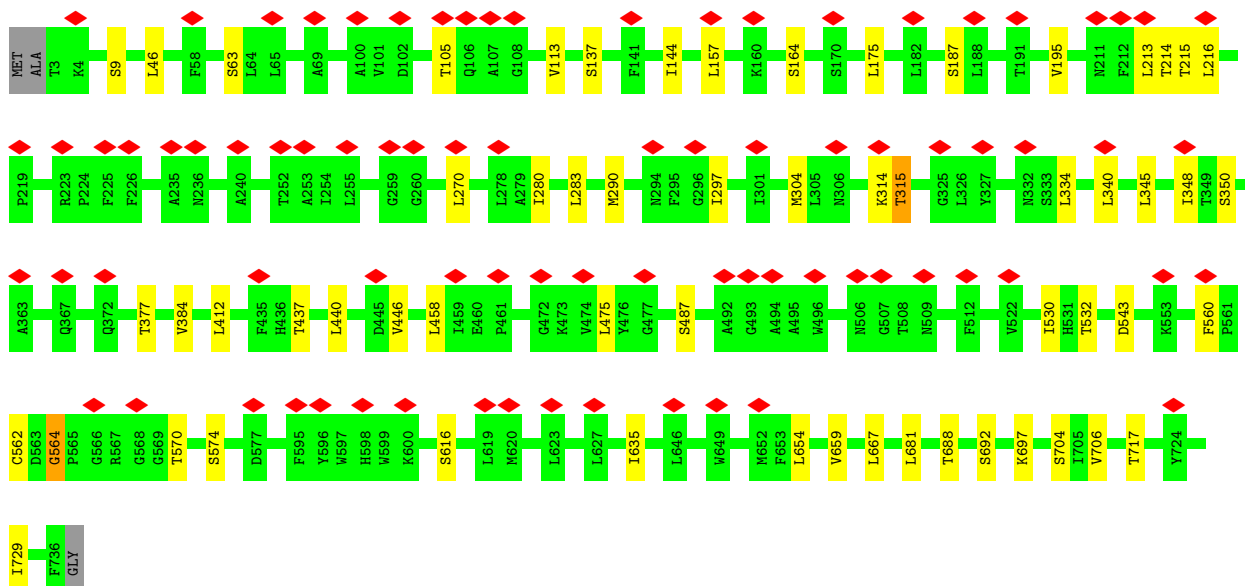
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 13% 90% 6%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

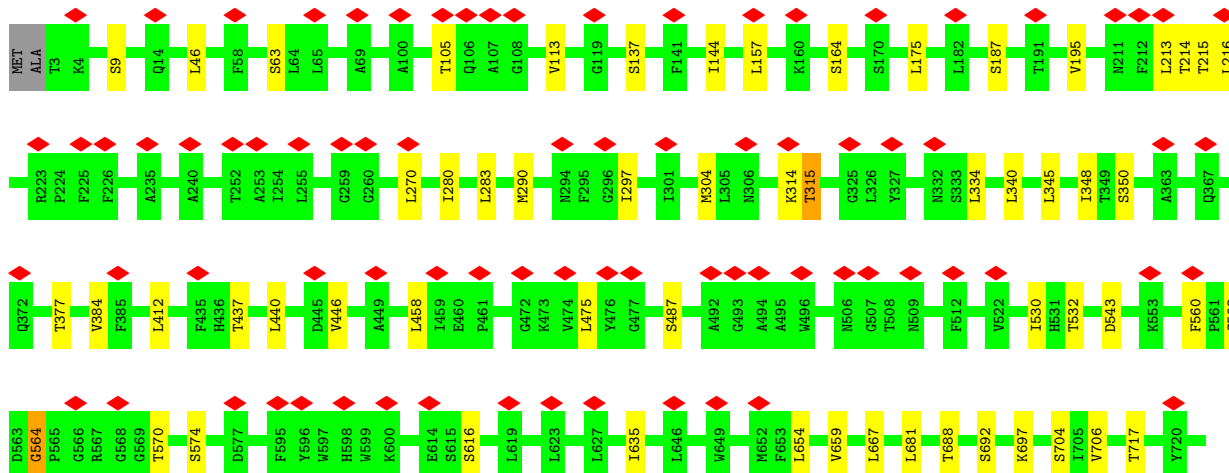
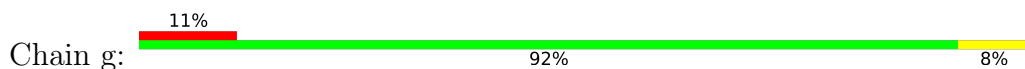
Chain B: 11% 92% 8%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

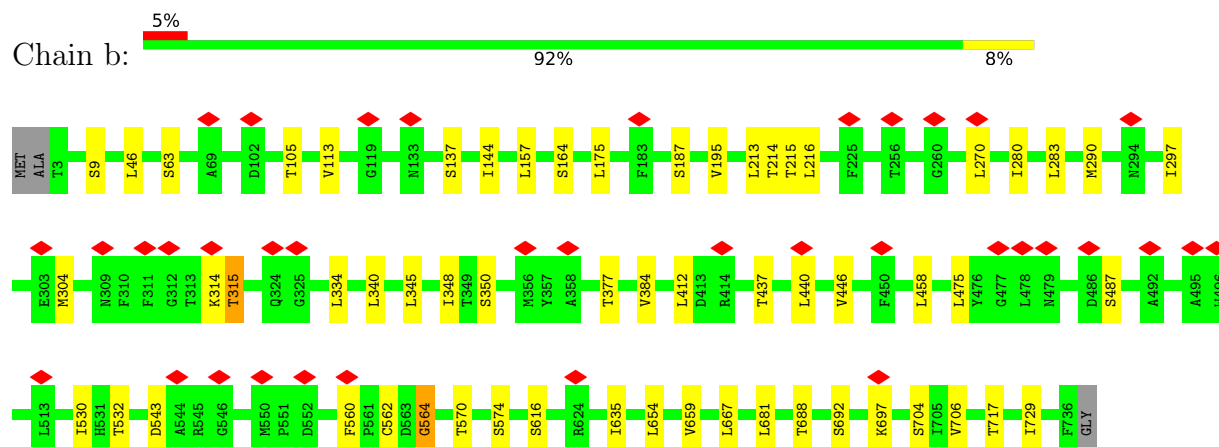


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

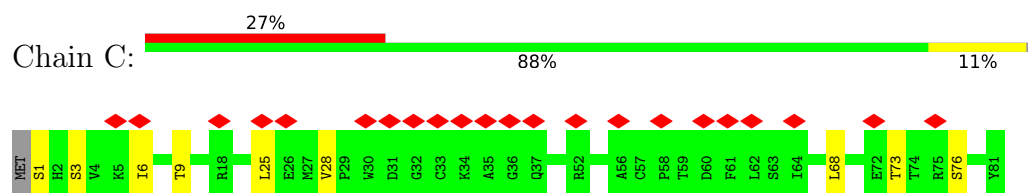




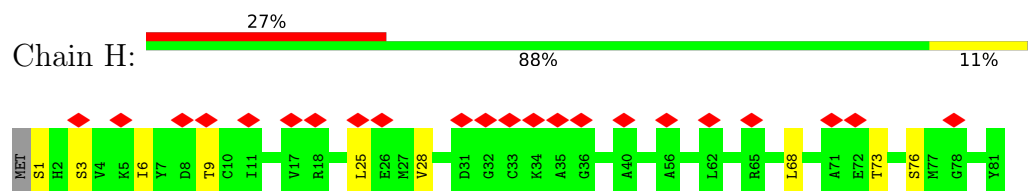
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



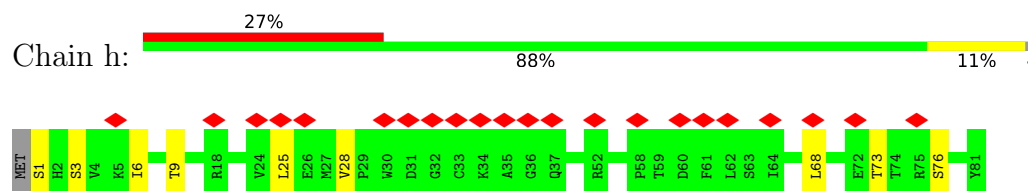
- Molecule 3: Photosystem I iron-sulfur center



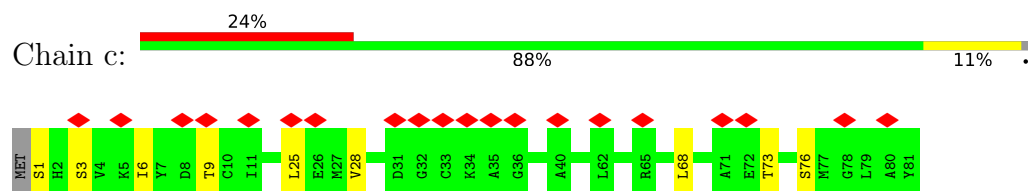
- Molecule 3: Photosystem I iron-sulfur center



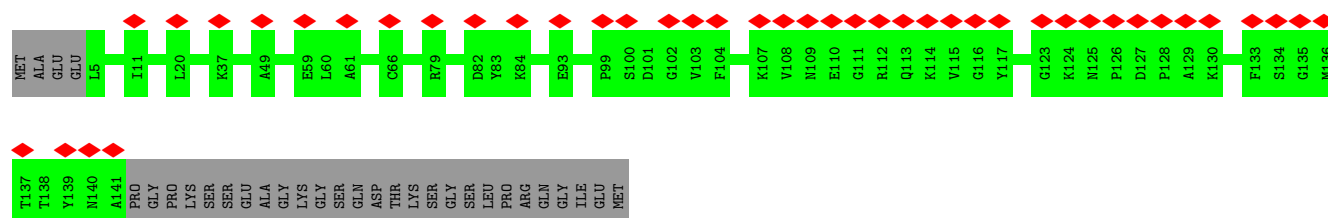
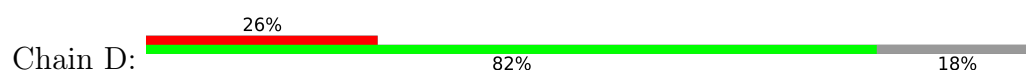
- Molecule 3: Photosystem I iron-sulfur center



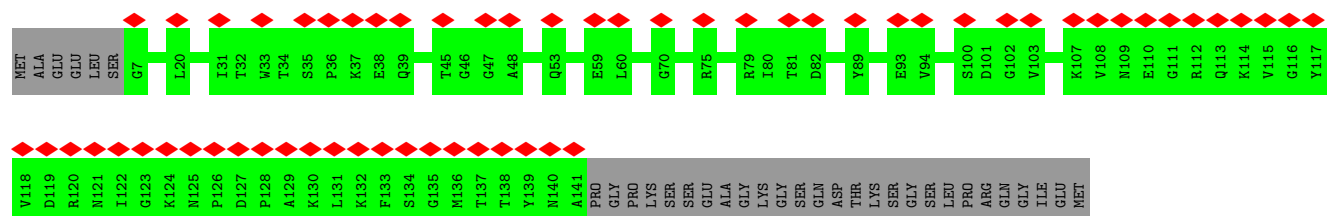
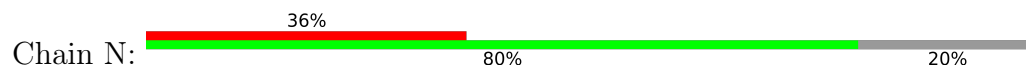
- Molecule 3: Photosystem I iron-sulfur center



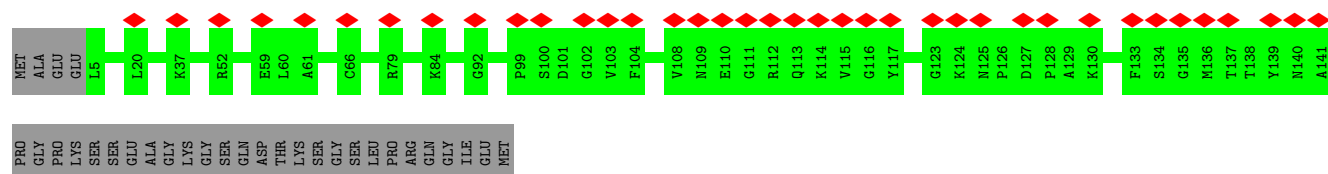
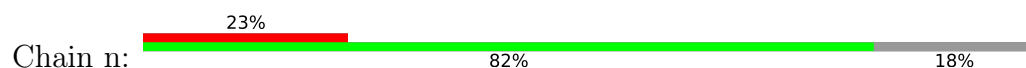
- Molecule 4: Photosystem I reaction center subunit II



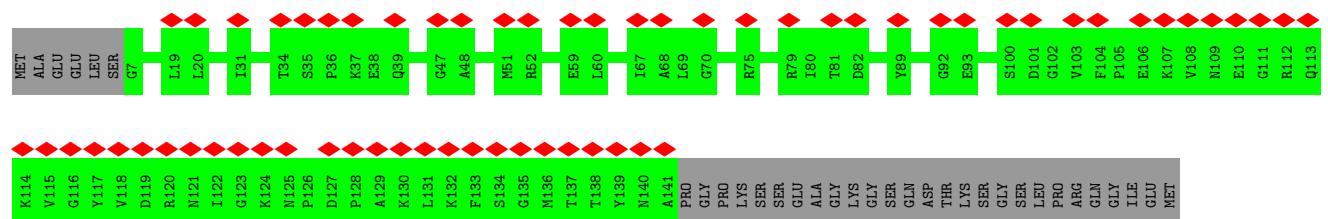
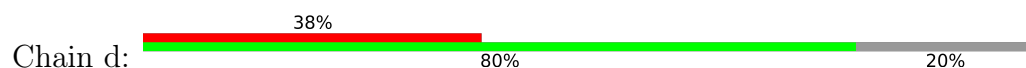
• Molecule 4: Photosystem I reaction center subunit II



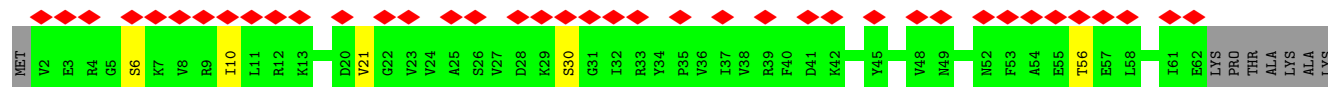
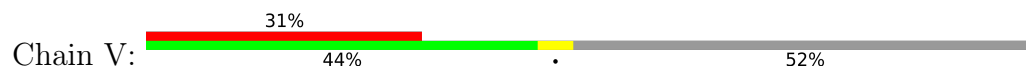
• Molecule 4: Photosystem I reaction center subunit II



• Molecule 4: Photosystem I reaction center subunit II




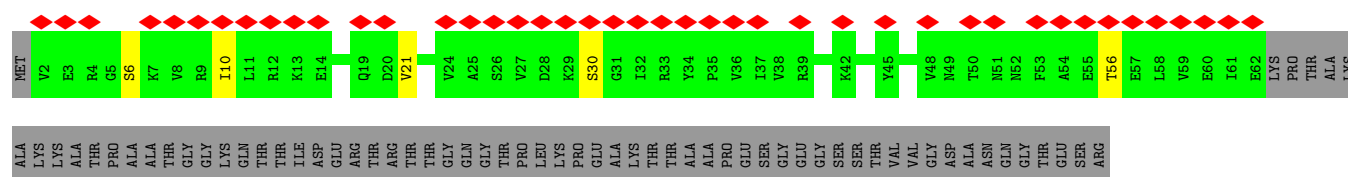
• Molecule 5: Photosystem I reaction center subunit IV




LYS
ALA
THR
PRO
THR
ALA
ALA
THR
GLY
GLY
LYS
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THR
THR
THR
ILE
ASP
GLU
ARG
THR
THR
ARG
THR
THR
GLY
GLN
GLY
THR
THR
PRO
LEU
LYS
PRO
GLU
ALA
LYS
THR
THR
ALA
ALA
ALA
PRO
GLU
SER
GLY
GLY
GLY
SER
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SER
SER
ARG

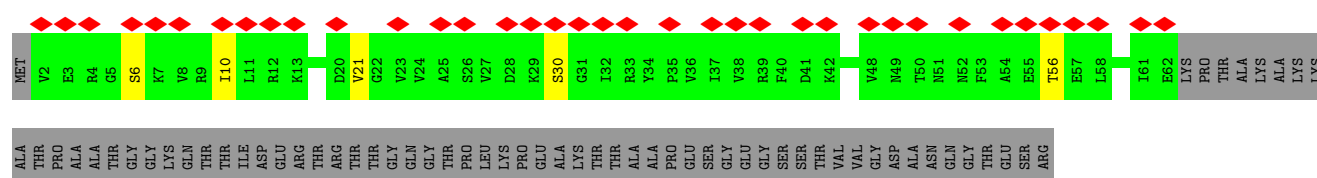
• Molecule 5: Photosystem I reaction center subunit IV

Chain W: 




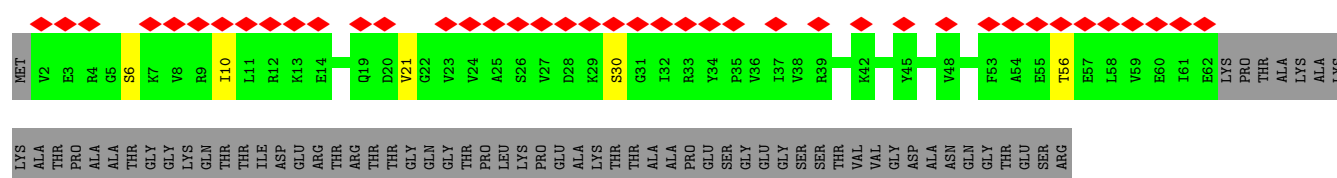
• Molecule 5: Photosystem I reaction center subunit IV

Chain v: 




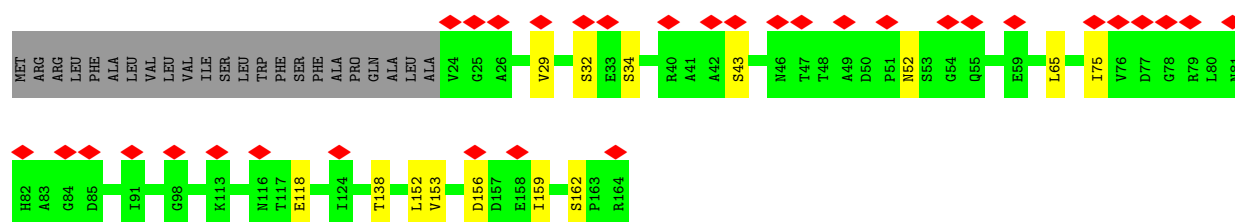
• Molecule 5: Photosystem I reaction center subunit IV

Chain w: 



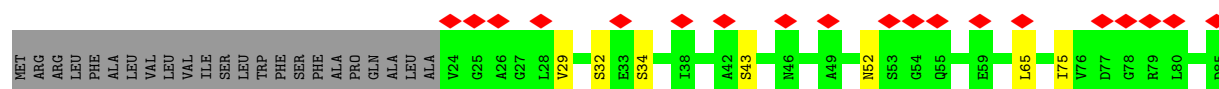
• Molecule 6: Photosystem I reaction center subunit III

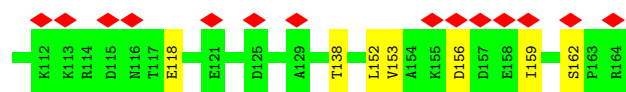
Chain F: 



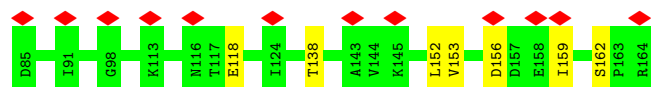
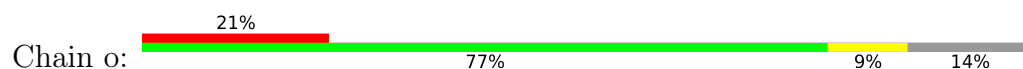
• Molecule 6: Photosystem I reaction center subunit III

Chain O: 

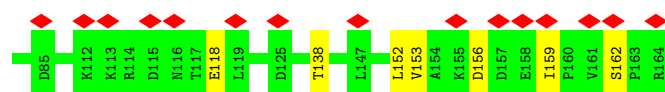
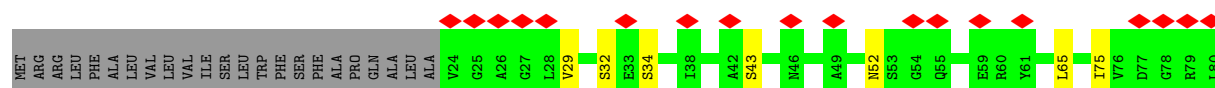
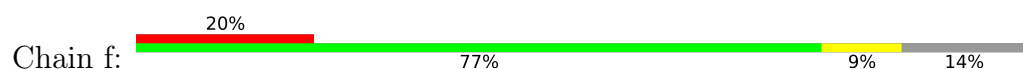




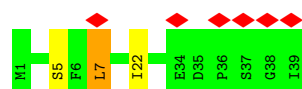
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



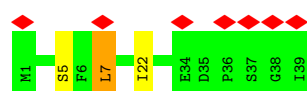
- Molecule 7: Photosystem I reaction center subunit VIII



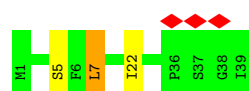
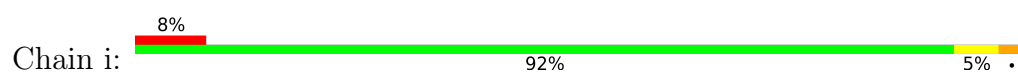
- Molecule 7: Photosystem I reaction center subunit VIII



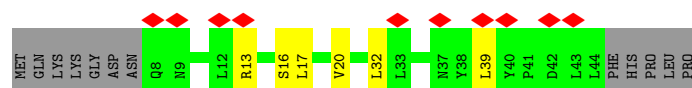
- Molecule 7: Photosystem I reaction center subunit VIII



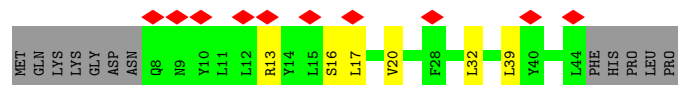
- Molecule 7: Photosystem I reaction center subunit VIII



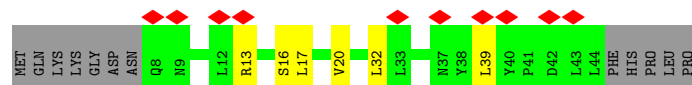
- Molecule 8: Photosystem I reaction center subunit IX



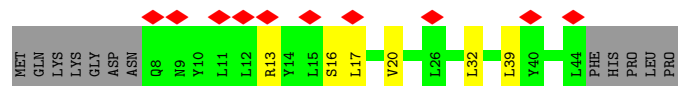
- Molecule 8: Photosystem I reaction center subunit IX



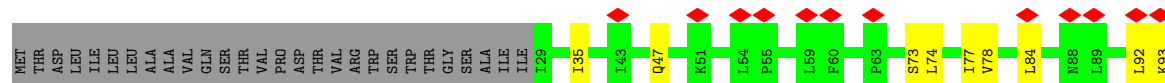
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

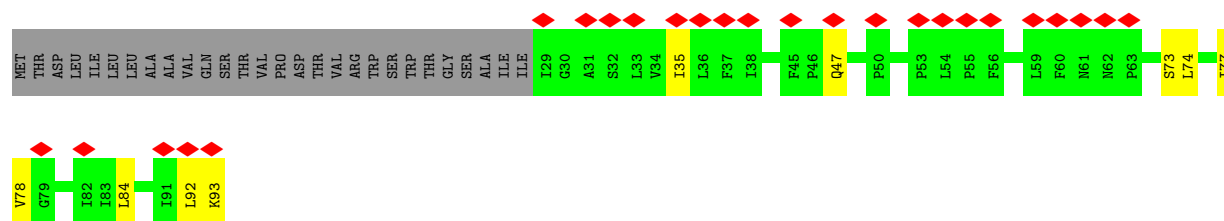


- Molecule 9: Photosystem I reaction center subunit PsaK

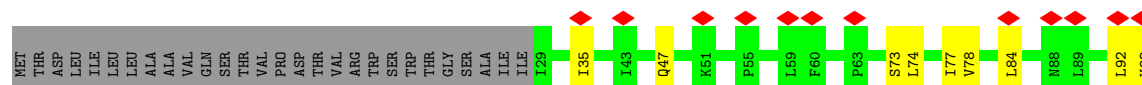


- Molecule 9: Photosystem I reaction center subunit PsaK

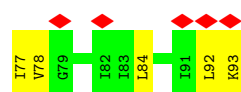
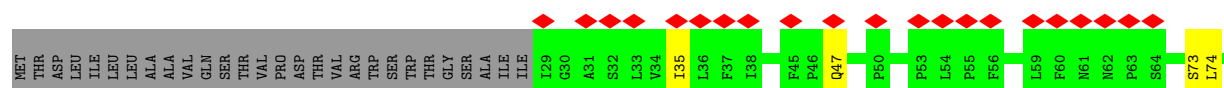




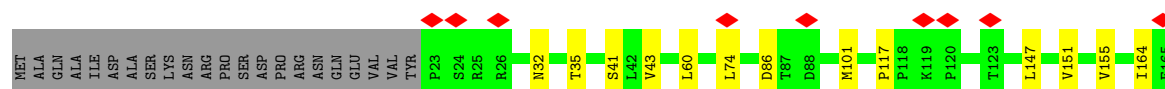
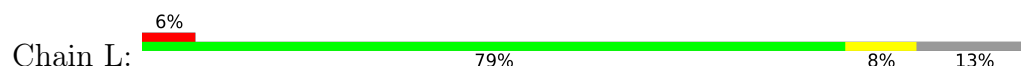
• Molecule 9: Photosystem I reaction center subunit PsaK



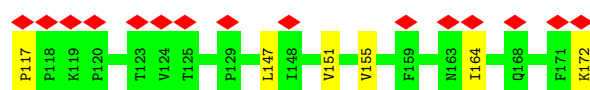
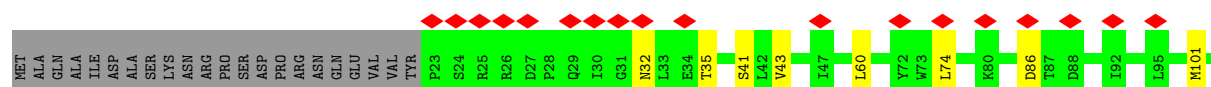
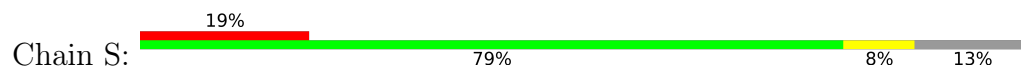
• Molecule 9: Photosystem I reaction center subunit PsaK



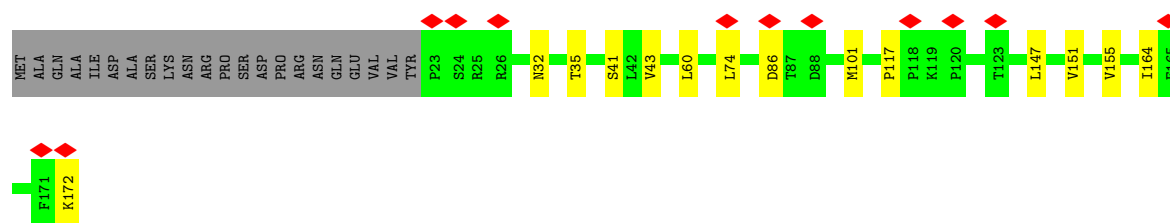
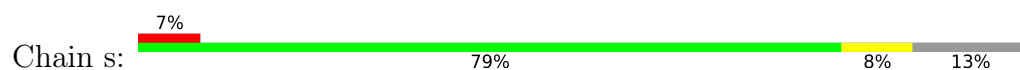
• Molecule 10: Photosystem I reaction center subunit XI



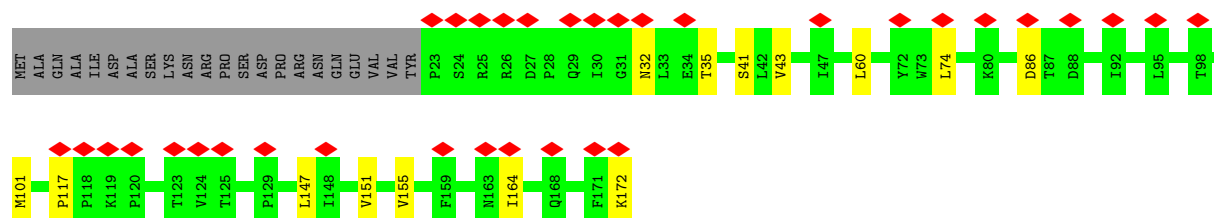
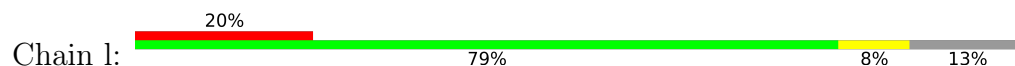
• Molecule 10: Photosystem I reaction center subunit XI



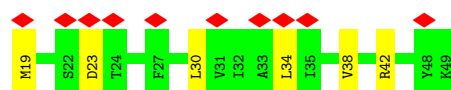
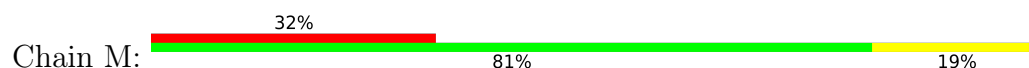
• Molecule 10: Photosystem I reaction center subunit XI



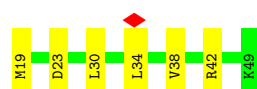
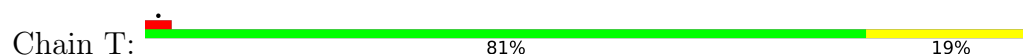
- Molecule 10: Photosystem I reaction center subunit XI



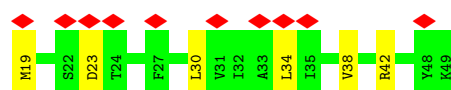
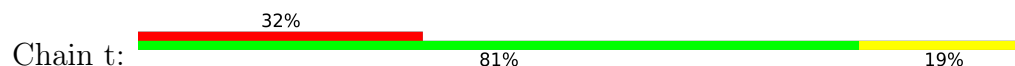
- Molecule 11: Photosystem I reaction center subunit XII



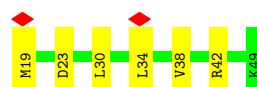
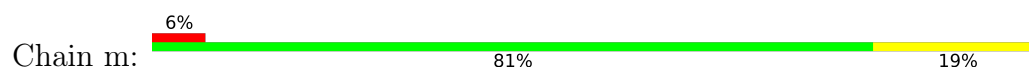
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	66130	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.3	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.053	Depositor
Minimum map value	-0.029	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.0125	Depositor
Map size (Å)	425.47202, 425.47202, 425.47202	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.108, 1.108, 1.108	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/5908	0.49	1/8056 (0.0%)
1	E	0.31	0/5908	0.49	1/8056 (0.0%)
1	a	0.31	0/5908	0.49	1/8056 (0.0%)
1	e	0.31	0/5908	0.49	1/8056 (0.0%)
2	B	0.30	0/6072	0.49	0/8301
2	G	0.30	0/6072	0.49	0/8301
2	b	0.30	0/6072	0.49	0/8301
2	g	0.30	0/6072	0.49	0/8301
3	C	0.28	0/615	0.49	0/833
3	H	0.28	0/615	0.49	0/833
3	c	0.28	0/615	0.49	0/833
3	h	0.28	0/615	0.49	0/833
4	D	0.28	0/1105	0.50	0/1489
4	N	0.27	0/1091	0.50	0/1470
4	d	0.28	0/1091	0.51	0/1470
4	n	0.30	0/1105	0.50	0/1489
5	V	0.30	0/502	0.49	0/678
5	W	0.30	0/502	0.49	0/678
5	v	0.29	0/502	0.49	0/678
5	w	0.30	0/502	0.49	0/678
6	F	0.28	0/1119	0.48	0/1522
6	O	0.28	0/1119	0.48	0/1522
6	f	0.28	0/1119	0.48	0/1522
6	o	0.28	0/1119	0.48	0/1522
7	I	0.29	0/302	0.60	1/411 (0.2%)
7	P	0.29	0/302	0.60	1/411 (0.2%)
7	i	0.29	0/302	0.60	1/411 (0.2%)
7	p	0.29	0/302	0.60	1/411 (0.2%)
8	J	0.29	0/321	0.48	0/441
8	Q	0.29	0/321	0.48	0/441
8	j	0.29	0/321	0.48	0/441
8	q	0.29	0/321	0.48	0/441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	K	0.29	0/484	0.65	1/659 (0.2%)
9	R	0.29	0/484	0.65	1/659 (0.2%)
9	k	0.29	0/484	0.65	1/659 (0.2%)
9	r	0.29	0/484	0.65	1/659 (0.2%)
10	L	0.31	0/1165	0.50	0/1597
10	S	0.31	0/1165	0.50	0/1597
10	l	0.31	0/1165	0.50	0/1597
10	s	0.31	0/1165	0.50	0/1597
11	M	0.33	0/241	0.59	0/326
11	T	0.33	0/241	0.59	0/326
11	m	0.33	0/241	0.59	0/326
11	t	0.34	0/241	0.59	0/326
All	All	0.30	0/71308	0.50	12/97214 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	3
2	G	0	3
2	b	0	3
2	g	0	3
10	L	0	1
10	S	0	1
10	l	0	1
10	s	0	1
All	All	0	16

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	74	LEU	CA-CB-CG	-6.34	100.71	115.30
9	K	74	LEU	CA-CB-CG	-6.34	100.72	115.30
9	k	74	LEU	CA-CB-CG	-6.33	100.74	115.30
9	R	74	LEU	CA-CB-CG	-6.33	100.75	115.30
1	e	699	GLU	CA-CB-CG	6.11	126.85	113.40

There are no chirality outliers.

5 of 16 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	315	THR	Peptide
2	B	560	PHE	Peptide
2	B	564	GLY	Peptide
2	G	315	THR	Peptide
10	L	117	PRO	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	E	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	a	726/752 (96%)	625 (86%)	101 (14%)	0	100	100
1	e	726/752 (96%)	626 (86%)	100 (14%)	0	100	100
2	B	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
2	G	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
2	b	732/737 (99%)	644 (88%)	85 (12%)	3 (0%)	30	62
2	g	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	62
3	C	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	H	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	c	79/82 (96%)	65 (82%)	14 (18%)	0	100	100
3	h	79/82 (96%)	66 (84%)	13 (16%)	0	100	100
4	D	135/168 (80%)	115 (85%)	20 (15%)	0	100	100
4	N	133/168 (79%)	113 (85%)	20 (15%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	133/168 (79%)	114 (86%)	19 (14%)	0	100	100
4	n	135/168 (80%)	117 (87%)	18 (13%)	0	100	100
5	V	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	W	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	v	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
5	w	59/126 (47%)	47 (80%)	12 (20%)	0	100	100
6	F	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	O	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	f	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
6	o	139/164 (85%)	120 (86%)	19 (14%)	0	100	100
7	I	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	P	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	i	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
7	p	37/39 (95%)	30 (81%)	7 (19%)	0	100	100
8	J	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	Q	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	j	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
8	q	35/49 (71%)	30 (86%)	5 (14%)	0	100	100
9	K	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	R	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	k	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
9	r	63/93 (68%)	52 (82%)	11 (18%)	0	100	100
10	L	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	S	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	l	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
10	s	148/172 (86%)	129 (87%)	19 (13%)	0	100	100
11	M	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	T	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	m	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
11	t	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	26
All	All	8724/9652 (90%)	7499 (86%)	1209 (14%)	16 (0%)	45	72

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	314	LYS
2	B	315	THR
2	G	314	LYS
2	G	315	THR
2	g	314	LYS

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	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	E	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	a	578/601 (96%)	530 (92%)	48 (8%)	9	34
1	e	578/601 (96%)	530 (92%)	48 (8%)	9	34
2	B	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	G	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	b	594/595 (100%)	539 (91%)	55 (9%)	7	30
2	g	594/595 (100%)	539 (91%)	55 (9%)	7	30
3	C	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	H	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	c	68/70 (97%)	59 (87%)	9 (13%)	3	18
3	h	68/70 (97%)	59 (87%)	9 (13%)	3	18
4	D	113/137 (82%)	113 (100%)	0	100	100
4	N	111/137 (81%)	111 (100%)	0	100	100
4	d	111/137 (81%)	111 (100%)	0	100	100
4	n	113/137 (82%)	113 (100%)	0	100	100
5	V	54/102 (53%)	49 (91%)	5 (9%)	7	30
5	W	54/102 (53%)	49 (91%)	5 (9%)	7	30
5	v	54/102 (53%)	49 (91%)	5 (9%)	7	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	w	54/102 (53%)	49 (91%)	5 (9%)	7	30
6	F	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	O	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	f	116/135 (86%)	102 (88%)	14 (12%)	4	20
6	o	116/135 (86%)	102 (88%)	14 (12%)	4	20
7	I	33/33 (100%)	30 (91%)	3 (9%)	7	30
7	P	33/33 (100%)	30 (91%)	3 (9%)	7	30
7	i	33/33 (100%)	30 (91%)	3 (9%)	7	30
7	p	33/33 (100%)	30 (91%)	3 (9%)	7	30
8	J	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	Q	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	j	34/45 (76%)	28 (82%)	6 (18%)	1	10
8	q	34/45 (76%)	28 (82%)	6 (18%)	1	10
9	K	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	R	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	k	53/77 (69%)	45 (85%)	8 (15%)	2	15
9	r	53/77 (69%)	45 (85%)	8 (15%)	2	15
10	L	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	S	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	l	121/140 (86%)	108 (89%)	13 (11%)	5	25
10	s	121/140 (86%)	108 (89%)	13 (11%)	5	25
11	M	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	T	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	m	26/26 (100%)	21 (81%)	5 (19%)	1	8
11	t	26/26 (100%)	21 (81%)	5 (19%)	1	8
All	All	7156/7844 (91%)	6492 (91%)	664 (9%)	10	30

5 of 664 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	p	5	SER
2	b	377	THR
9	r	78	VAL

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Mol	Chain	Res	Type
6	o	162	SER
1	a	365	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 176 such sidechains are listed below:

Mol	Chain	Res	Type
2	g	436	HIS
1	a	480	GLN
2	g	531	HIS
8	q	37	ASN
2	b	41	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

462 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	CLA	E	845	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	837	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	E	807	-	50,58,73	1.63	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	B	804	-	50,58,73	1.65	7 (14%)	58,95,113	1.46	8 (13%)
13	CLA	G	832	-	49,57,73	1.68	7 (14%)	55,93,113	1.53	7 (12%)
15	BCR	S	202	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	a	805	-	50,58,73	1.63	8 (16%)	58,95,113	1.45	7 (12%)
14	PQN	G	842	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	G	840	-	50,58,73	1.68	9 (18%)	58,95,113	1.52	8 (13%)
13	CLA	E	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.48	9 (15%)
13	CLA	g	838	-	50,58,73	1.64	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	l	203	10	50,58,73	1.64	6 (12%)	58,95,113	1.54	9 (15%)
13	CLA	e	825	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	9 (15%)
13	CLA	l	204	-	45,53,73	1.75	7 (15%)	52,89,113	1.63	7 (13%)
13	CLA	G	803	-	50,58,73	1.65	7 (14%)	58,95,113	1.46	8 (13%)
13	CLA	g	820	-	50,58,73	1.65	7 (14%)	58,95,113	1.53	6 (10%)
13	CLA	G	841	-	50,58,73	1.66	8 (16%)	58,95,113	1.57	7 (12%)
15	BCR	A	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	G	838	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	a	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.55	8 (13%)
13	CLA	A	819	-	49,57,73	1.71	7 (14%)	55,93,113	1.55	7 (12%)
13	CLA	e	814	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	7 (12%)
15	BCR	Q	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	g	837	-	45,53,73	1.76	6 (13%)	52,89,113	1.70	7 (13%)
13	CLA	g	823	-	45,53,73	1.74	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	g	801	-	50,58,73	1.63	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	B	811	2	50,58,73	1.67	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	g	818	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	E	838	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	G	812	-	45,53,73	1.77	7 (15%)	52,89,113	1.50	7 (13%)
13	CLA	B	816	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	B	828	-	50,58,73	1.66	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	a	822	-	50,58,73	1.67	7 (14%)	58,95,113	1.47	8 (13%)
15	BCR	I	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.18	2 (3%)
13	CLA	e	819	-	50,58,73	1.67	7 (14%)	58,95,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	R	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.43	7 (12%)
13	CLA	B	833	-	50,58,73	1.73	8 (16%)	58,95,113	1.46	9 (15%)
13	CLA	E	823	-	50,58,73	1.65	8 (16%)	58,95,113	1.46	6 (10%)
13	CLA	A	842	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
13	CLA	b	827	-	50,58,73	1.67	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	e	829	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	e	836	-	50,58,73	1.69	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	A	820	-	50,58,73	1.66	7 (14%)	58,95,113	1.58	8 (13%)
13	CLA	e	834	-	50,58,73	1.72	8 (16%)	58,95,113	1.66	9 (15%)
13	CLA	G	836	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
16	SF4	a	846	-	0,12,12	-	-	-	-	-
13	CLA	B	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
13	CLA	G	813	-	45,53,73	1.79	8 (17%)	52,89,113	1.52	7 (13%)
15	BCR	G	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	E	814	-	50,58,73	1.70	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	B	807	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	b	822	2	50,58,73	1.69	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	g	809	-	50,58,73	1.67	9 (18%)	58,95,113	1.50	8 (13%)
13	CLA	b	824	-	50,58,73	1.63	6 (12%)	58,95,113	1.63	8 (13%)
15	BCR	m	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	9 (16%)
13	CLA	E	834	-	50,58,73	1.64	9 (18%)	58,95,113	1.48	7 (12%)
13	CLA	B	813	-	45,53,73	1.79	6 (13%)	52,89,113	1.53	7 (13%)
13	CLA	E	826	-	50,58,73	1.69	7 (14%)	58,95,113	1.53	9 (15%)
13	CLA	g	839	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	e	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.60	8 (13%)
13	CLA	B	801	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	A	815	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	7 (12%)
15	BCR	k	4001	-	41,41,41	1.17	3 (7%)	56,56,56	1.59	10 (17%)
13	CLA	a	836	-	50,58,73	1.71	8 (16%)	58,95,113	1.66	8 (13%)
15	BCR	s	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.16	5 (8%)
13	CLA	a	817	-	50,58,73	1.73	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	e	810	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	9 (15%)
15	BCR	G	845	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	G	824	-	45,53,73	1.78	6 (13%)	52,89,113	1.60	7 (13%)
13	CLA	b	832	-	50,58,73	1.72	8 (16%)	58,95,113	1.46	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	834	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
15	BCR	A	851	-	41,41,41	1.25	2 (4%)	56,56,56	1.26	7 (12%)
15	BCR	b	842	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	G	811	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	7 (12%)
13	CLA	e	840	-	47,55,73	1.72	8 (17%)	54,91,113	1.55	6 (11%)
16	SF4	g	804	-	0,12,12	-	-	-	-	-
15	BCR	b	843	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	E	824	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	e	841	-	50,58,73	1.62	6 (12%)	58,95,113	1.60	9 (15%)
15	BCR	O	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	A	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	A	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
13	CLA	E	827	-	50,58,73	1.69	7 (14%)	58,95,113	1.50	9 (15%)
15	BCR	G	847	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	e	837	1	45,53,73	1.75	6 (13%)	52,89,113	1.66	8 (15%)
13	CLA	B	819	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	7 (12%)
13	CLA	g	812	2	50,58,73	1.68	7 (14%)	58,95,113	1.56	8 (13%)
13	CLA	A	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	G	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
13	CLA	b	802	-	50,58,73	1.64	7 (14%)	58,95,113	1.57	9 (15%)
13	CLA	E	836	-	50,58,73	1.72	8 (16%)	58,95,113	1.66	8 (13%)
12	LHG	e	801	-	48,48,48	0.67	1 (2%)	51,54,54	1.30	7 (13%)
14	PQN	E	848	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	b	808	-	50,58,73	1.71	7 (14%)	58,95,113	1.48	7 (12%)
13	CLA	b	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	g	826	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
13	CLA	E	828	-	50,58,73	1.64	6 (12%)	58,95,113	1.58	9 (15%)
13	CLA	G	820	-	50,58,73	1.67	8 (16%)	58,95,113	1.56	7 (12%)
13	CLA	g	807	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
15	BCR	q	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	L	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.63	7 (13%)
13	CLA	g	806	-	50,58,73	1.64	9 (18%)	58,95,113	1.60	8 (13%)
13	CLA	e	818	-	49,57,73	1.72	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	g	813	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	7 (12%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	827	-	50,58,73	1.70	6 (12%)	58,95,113	1.45	8 (13%)
13	CLA	g	833	-	49,57,73	1.68	7 (14%)	55,93,113	1.53	7 (12%)
13	CLA	b	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	b	825	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	841	-	50,58,73	1.64	9 (18%)	58,95,113	1.53	8 (13%)
15	BCR	E	852	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	A	838	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
15	BCR	g	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	5 (8%)
13	CLA	E	840	-	50,58,73	1.65	6 (12%)	58,95,113	1.62	9 (15%)
13	CLA	E	846	-	42,49,73	1.81	7 (16%)	48,83,113	1.71	7 (14%)
15	BCR	E	801	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	b	818	-	50,58,73	1.66	7 (14%)	58,95,113	1.53	6 (10%)
13	CLA	k	4002	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	9 (17%)
13	CLA	G	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	g	825	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
13	CLA	b	836	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)
13	CLA	e	805	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	a	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	f	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	7 (12%)
15	BCR	e	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	G	818	-	50,58,73	1.69	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	o	202	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	e	846	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
15	BCR	A	850	-	41,41,41	1.20	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	L	202	10	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	E	833	-	50,58,73	1.62	6 (12%)	58,95,113	1.64	7 (12%)
13	CLA	a	844	-	50,58,73	1.66	7 (14%)	58,95,113	1.54	7 (12%)
13	CLA	e	820	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	A	832	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	9 (15%)
13	CLA	F	202	-	45,53,73	1.75	5 (11%)	52,89,113	1.58	6 (11%)
13	CLA	A	843	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	a	852	-	50,58,73	1.65	5 (10%)	58,95,113	1.55	9 (15%)
15	BCR	b	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	B	840	-	50,58,73	1.68	9 (18%)	58,95,113	1.53	8 (13%)
13	CLA	B	841	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SF4	B	803	-	0,12,12	-	-	-		
13	CLA	l	205	-	50,58,73	2.51	11 (22%)	58,95,113	3.07	15 (25%)
15	BCR	e	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.27	9 (16%)
13	CLA	A	853	-	50,58,73	1.65	7 (14%)	58,95,113	1.56	9 (15%)
15	BCR	g	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	e	828	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	a	814	-	45,53,73	1.79	7 (15%)	52,89,113	1.58	7 (13%)
13	CLA	E	822	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
15	BCR	e	850	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	f	203	-	45,53,73	1.75	7 (15%)	52,89,113	1.70	6 (11%)
16	SF4	h	101	-	0,12,12	-	-	-		
13	CLA	b	823	-	45,53,73	1.78	6 (13%)	52,89,113	1.62	7 (13%)
13	CLA	G	830	-	50,58,73	1.64	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	G	827	-	50,58,73	1.70	6 (12%)	58,95,113	1.46	8 (13%)
15	BCR	B	847	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
15	BCR	B	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	a	845	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	b	828	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	a	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	G	831	-	45,53,73	1.77	6 (13%)	52,89,113	1.54	8 (15%)
15	BCR	a	803	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)
13	CLA	e	827	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
13	CLA	a	815	-	50,58,73	1.65	6 (12%)	58,95,113	1.55	7 (12%)
13	CLA	G	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	E	819	-	49,57,73	1.71	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	G	801	-	50,58,73	1.68	8 (16%)	58,95,113	1.57	9 (15%)
14	PQN	a	847	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	a	839	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
13	CLA	A	824	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	g	835	-	50,58,73	1.67	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	G	828	-	50,58,73	1.66	8 (16%)	58,95,113	1.46	8 (13%)
13	CLA	b	826	-	50,58,73	1.71	6 (12%)	58,95,113	1.46	8 (13%)
13	CLA	A	845	12	50,58,73	1.65	6 (12%)	58,95,113	1.63	7 (12%)
13	CLA	g	832	-	45,53,73	1.77	6 (13%)	52,89,113	1.54	8 (15%)
13	CLA	a	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	841	-	50,58,73	1.64	9 (18%)	58,95,113	1.52	8 (13%)
13	CLA	a	838	-	50,58,73	1.69	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	e	806	-	50,58,73	1.63	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	b	807	-	50,58,73	1.66	9 (18%)	58,95,113	1.48	8 (13%)
13	CLA	B	831	-	45,53,73	1.77	6 (13%)	52,89,113	1.53	8 (15%)
13	CLA	a	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.58	9 (15%)
13	CLA	A	829	-	50,58,73	1.70	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	K	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
13	CLA	A	805	-	50,58,73	1.64	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	G	819	-	50,58,73	1.66	7 (14%)	58,95,113	1.53	7 (12%)
13	CLA	B	836	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
13	CLA	a	823	-	50,58,73	1.66	8 (16%)	58,95,113	1.45	6 (10%)
13	CLA	E	809	1	50,58,73	1.68	8 (16%)	58,95,113	1.48	6 (10%)
13	CLA	g	814	-	45,53,73	1.78	6 (13%)	52,89,113	1.52	7 (13%)
13	CLA	G	834	-	50,58,73	1.67	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	a	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
14	PQN	e	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	E	810	-	50,58,73	1.69	6 (12%)	58,95,113	1.50	8 (13%)
13	CLA	B	830	-	50,58,73	1.64	6 (12%)	58,95,113	1.61	8 (13%)
13	CLA	a	809	1	50,58,73	1.68	8 (16%)	58,95,113	1.48	7 (12%)
13	CLA	e	831	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	9 (15%)
13	CLA	a	840	-	50,58,73	1.64	7 (14%)	58,95,113	1.62	9 (15%)
13	CLA	B	838	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	9 (15%)
13	CLA	B	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.55	7 (12%)
13	CLA	g	841	-	50,58,73	1.68	9 (18%)	58,95,113	1.53	8 (13%)
13	CLA	e	821	-	50,58,73	1.68	7 (14%)	58,95,113	1.48	8 (13%)
15	BCR	A	852	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
13	CLA	e	832	-	50,58,73	1.62	6 (12%)	58,95,113	1.63	7 (12%)
15	BCR	j	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	5 (8%)
13	CLA	g	842	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
15	BCR	g	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
15	BCR	e	851	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	b	829	-	50,58,73	1.65	6 (12%)	58,95,113	1.61	8 (13%)
15	BCR	J	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	B	837	-	50,58,73	1.65	6 (12%)	58,95,113	1.58	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	812	-	45,53,73	1.78	7 (15%)	52,89,113	1.53	7 (13%)
15	BCR	T	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	4 (7%)
13	CLA	E	832	-	50,58,73	1.67	7 (14%)	58,95,113	1.48	9 (15%)
13	CLA	g	831	-	50,58,73	1.64	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)
15	BCR	G	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	B	818	-	50,58,73	1.69	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	G	829	-	50,58,73	1.67	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	e	815	-	50,58,73	1.67	6 (12%)	58,95,113	1.55	9 (15%)
13	CLA	e	842	-	50,58,73	1.67	7 (14%)	58,95,113	1.53	8 (13%)
13	CLA	E	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.59	9 (16%)
13	CLA	b	835	-	45,53,73	1.76	6 (13%)	52,89,113	1.69	7 (13%)
13	CLA	g	810	-	50,58,73	1.69	7 (14%)	58,95,113	1.48	7 (12%)
13	CLA	r	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
15	BCR	B	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	g	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.60	6 (11%)
13	CLA	E	842	-	47,55,73	1.73	8 (17%)	54,91,113	1.56	6 (11%)
13	CLA	e	852	-	50,58,73	1.65	7 (14%)	58,95,113	1.56	9 (15%)
13	CLA	G	815	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
13	CLA	E	820	-	50,58,73	1.67	7 (14%)	58,95,113	1.58	9 (15%)
14	PQN	g	843	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	g	803	-	50,58,73	1.67	8 (16%)	58,95,113	1.54	7 (12%)
13	CLA	a	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	E	802	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
13	CLA	G	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.54	7 (13%)
15	BCR	S	201	-	41,41,41	1.19	2 (4%)	56,56,56	1.13	3 (5%)
15	BCR	l	202	-	41,41,41	1.19	2 (4%)	56,56,56	1.16	5 (8%)
12	LHG	e	802	13	37,37,48	0.74	1 (2%)	40,43,54	1.34	5 (12%)
13	CLA	g	830	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	E	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	9 (15%)
15	BCR	a	802	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	b	817	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	G	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	g	821	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
15	BCR	E	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SF4	h	102	3	0,12,12	-	-	-		
13	CLA	A	809	1	50,58,73	1.67	7 (14%)	58,95,113	1.49	6 (10%)
15	BCR	f	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	a	807	-	50,58,73	1.64	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	810	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	A	841	-	47,55,73	1.72	8 (17%)	54,91,113	1.56	6 (11%)
15	BCR	a	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	a	813	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	A	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	A	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	G	802	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	9 (15%)
13	CLA	b	801	-	42,49,73	1.80	8 (19%)	48,83,113	1.54	6 (12%)
13	CLA	G	808	-	50,58,73	1.69	7 (14%)	58,95,113	1.48	7 (12%)
14	PQN	B	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	b	809	-	50,58,73	1.66	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	E	830	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	8 (13%)
13	CLA	b	839	-	50,58,73	1.69	9 (18%)	58,95,113	1.52	8 (13%)
15	BCR	o	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	K	101	-	42,49,73	1.80	7 (16%)	48,83,113	1.57	6 (12%)
12	LHG	A	802	13	37,37,48	0.77	1 (2%)	40,43,54	1.33	5 (12%)
15	BCR	p	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)
15	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
15	BCR	g	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	g	824	2	50,58,73	1.68	8 (16%)	58,95,113	1.57	8 (13%)
13	CLA	B	832	-	49,57,73	1.68	6 (12%)	55,93,113	1.54	7 (12%)
13	CLA	a	833	-	50,58,73	1.63	6 (12%)	58,95,113	1.63	7 (12%)
15	BCR	l	206	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	E	837	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	A	817	-	45,53,73	1.83	7 (15%)	52,89,113	1.55	6 (11%)
13	CLA	B	809	-	50,58,73	1.70	7 (14%)	58,95,113	1.47	7 (12%)
13	CLA	s	203	-	50,58,73	2.51	11 (22%)	58,95,113	3.06	16 (27%)
15	BCR	E	851	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	g	836	-	45,53,73	1.82	7 (15%)	52,89,113	1.55	7 (13%)
13	CLA	e	835	-	50,58,73	1.68	7 (14%)	58,95,113	1.47	8 (13%)
13	CLA	A	816	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	g	834	-	50,58,73	1.73	8 (16%)	58,95,113	1.46	9 (15%)
13	CLA	E	818	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)
15	BCR	b	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	A	826	-	50,58,73	1.68	7 (14%)	58,95,113	1.54	9 (15%)
13	CLA	G	822	-	45,53,73	1.74	5 (11%)	52,89,113	1.67	7 (13%)
15	BCR	g	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	a	819	-	49,57,73	1.71	6 (12%)	55,93,113	1.55	7 (12%)
13	CLA	G	817	-	50,58,73	1.68	6 (12%)	58,95,113	1.47	8 (13%)
13	CLA	A	807	-	50,58,73	1.63	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	834	-	50,58,73	1.66	9 (18%)	58,95,113	1.48	8 (13%)
15	BCR	L	201	-	41,41,41	1.22	2 (4%)	56,56,56	1.13	3 (5%)
13	CLA	a	827	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	9 (15%)
13	CLA	A	813	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	S	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.62	7 (13%)
13	CLA	B	808	-	50,58,73	1.67	9 (18%)	58,95,113	1.49	9 (15%)
13	CLA	B	806	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
13	CLA	g	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.64	9 (15%)
13	CLA	G	826	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	805	-	50,58,73	1.64	7 (14%)	58,95,113	1.45	7 (12%)
13	CLA	G	821	-	47,55,73	1.74	7 (14%)	54,91,113	1.53	7 (12%)
13	CLA	e	809	-	50,58,73	1.68	7 (14%)	58,95,113	1.51	8 (13%)
15	BCR	P	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)
13	CLA	b	810	2	50,58,73	1.67	8 (16%)	58,95,113	1.56	8 (13%)
15	BCR	a	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	5 (8%)
15	BCR	B	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	E	821	-	50,58,73	1.69	8 (16%)	58,95,113	1.50	9 (15%)
13	CLA	g	816	-	50,58,73	1.68	7 (14%)	58,95,113	1.56	7 (12%)
15	BCR	s	204	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	8 (14%)
16	SF4	H	101	-	0,12,12	-	-	-	-	-
13	CLA	G	823	2	50,58,73	1.69	8 (16%)	58,95,113	1.57	8 (13%)
13	CLA	B	824	-	45,53,73	1.77	6 (13%)	52,89,113	1.61	7 (13%)
16	SF4	E	847	-	0,12,12	-	-	-	-	-
13	CLA	a	835	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	G	825	-	50,58,73	1.64	7 (14%)	58,95,113	1.63	8 (13%)
13	CLA	b	814	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	829	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	8 (13%)
13	CLA	g	828	-	50,58,73	1.70	6 (12%)	58,95,113	1.45	8 (13%)
16	SF4	c	101	-	0,12,12	-	-	-	-	-
13	CLA	A	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
13	CLA	s	202	-	45,53,73	1.75	7 (15%)	52,89,113	1.62	7 (13%)
13	CLA	E	844	-	50,58,73	1.66	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.74	11 (19%)
13	CLA	g	822	-	47,55,73	1.73	7 (14%)	54,91,113	1.52	7 (12%)
13	CLA	b	838	-	47,55,73	1.70	7 (14%)	54,91,113	1.61	6 (11%)
13	CLA	g	819	-	50,58,73	1.69	7 (14%)	58,95,113	1.56	8 (13%)
13	CLA	S	204	-	45,53,73	2.64	12 (26%)	52,89,113	3.21	15 (28%)
13	CLA	A	828	-	50,58,73	1.64	7 (14%)	58,95,113	1.59	9 (15%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
15	BCR	J	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	e	824	-	49,57,73	1.67	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	A	835	-	50,58,73	1.71	7 (14%)	58,95,113	1.66	8 (13%)
13	CLA	E	812	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	G	807	-	50,58,73	1.66	8 (16%)	58,95,113	1.49	9 (15%)
13	CLA	E	803	-	50,58,73	1.66	5 (10%)	58,95,113	1.47	7 (12%)
13	CLA	g	829	-	50,58,73	1.66	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	B	815	-	50,58,73	1.68	6 (12%)	58,95,113	1.56	7 (12%)
13	CLA	a	810	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	8 (13%)
13	CLA	O	203	-	45,53,73	1.76	7 (15%)	52,89,113	1.68	6 (11%)
13	CLA	a	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	b	819	-	50,58,73	1.67	8 (16%)	58,95,113	1.55	7 (12%)
13	CLA	R	102	-	45,53,73	1.76	6 (13%)	52,89,113	1.55	8 (15%)
15	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	b	831	-	49,57,73	1.68	6 (12%)	55,93,113	1.54	7 (12%)
13	CLA	a	826	-	50,58,73	1.68	7 (14%)	58,95,113	1.53	9 (15%)
15	BCR	i	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.18	3 (5%)
13	CLA	e	838	-	50,58,73	1.64	7 (14%)	58,95,113	1.60	9 (15%)
13	CLA	e	822	-	50,58,73	1.66	8 (16%)	58,95,113	1.46	6 (10%)
13	CLA	b	811	-	45,53,73	1.77	7 (15%)	52,89,113	1.49	7 (13%)
13	CLA	B	802	-	50,58,73	1.67	8 (16%)	58,95,113	1.53	7 (12%)
13	CLA	e	817	-	45,53,73	1.76	6 (13%)	52,89,113	1.62	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	844	-	50,58,73	1.65	7 (14%)	58,95,113	1.50	8 (13%)
13	CLA	a	834	-	50,58,73	1.65	9 (18%)	58,95,113	1.47	8 (13%)
15	BCR	F	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	E	806	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	9 (15%)
15	BCR	a	853	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	l	201	-	45,53,73	1.78	8 (17%)	52,89,113	1.50	7 (13%)
15	BCR	G	843	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	g	827	-	46,54,73	1.71	7 (15%)	53,90,113	1.63	7 (13%)
13	CLA	E	829	-	50,58,73	1.69	9 (18%)	58,95,113	1.50	6 (10%)
13	CLA	E	817	-	45,53,73	1.83	8 (17%)	52,89,113	1.55	6 (11%)
13	CLA	e	826	-	50,58,73	1.69	7 (14%)	58,95,113	1.51	9 (15%)
13	CLA	A	825	-	49,57,73	1.66	7 (14%)	55,93,113	1.60	9 (16%)
13	CLA	a	832	-	50,58,73	1.67	8 (16%)	58,95,113	1.48	9 (15%)
13	CLA	e	843	-	50,58,73	1.66	7 (14%)	58,95,113	1.51	8 (13%)
13	CLA	b	816	-	50,58,73	1.69	6 (12%)	58,95,113	1.48	8 (13%)
13	CLA	b	804	-	50,58,73	1.65	7 (14%)	58,95,113	1.59	8 (13%)
13	CLA	A	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.51	9 (15%)
13	CLA	b	821	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	7 (13%)
13	CLA	e	811	1	50,58,73	1.67	5 (10%)	58,95,113	1.54	8 (13%)
13	CLA	e	813	-	50,58,73	1.71	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	b	815	-	45,53,73	1.76	7 (15%)	52,89,113	1.61	6 (11%)
13	CLA	A	814	-	50,58,73	1.70	7 (14%)	58,95,113	1.51	7 (12%)
13	CLA	g	817	-	45,53,73	1.76	6 (13%)	52,89,113	1.61	6 (11%)
13	CLA	b	840	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
13	CLA	e	812	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	G	816	-	45,53,73	1.75	6 (13%)	52,89,113	1.61	6 (11%)
15	BCR	b	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	e	839	-	50,58,73	1.65	9 (18%)	58,95,113	1.52	8 (13%)
15	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	a	842	-	47,55,73	1.72	8 (17%)	54,91,113	1.56	6 (11%)
13	CLA	e	823	-	50,58,73	1.66	6 (12%)	58,95,113	1.57	8 (13%)
13	CLA	E	811	-	50,58,73	1.66	7 (14%)	58,95,113	1.52	9 (15%)
14	PQN	b	841	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	A	808	-	50,58,73	1.66	6 (12%)	58,95,113	1.62	8 (13%)
13	CLA	e	807	-	50,58,73	1.67	6 (12%)	58,95,113	1.62	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	843	-	50,58,73	1.63	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	g	815	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	8 (13%)
13	CLA	A	833	-	50,58,73	1.62	6 (12%)	58,95,113	1.63	7 (12%)
13	CLA	e	808	1	50,58,73	1.67	7 (14%)	58,95,113	1.49	6 (10%)
13	CLA	a	829	-	50,58,73	1.69	9 (18%)	58,95,113	1.49	6 (10%)
13	CLA	E	839	1	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
13	CLA	a	824	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	8 (13%)
13	CLA	B	822	-	45,53,73	1.75	7 (15%)	52,89,113	1.68	7 (13%)
13	CLA	G	839	-	47,55,73	1.70	7 (14%)	54,91,113	1.59	6 (11%)
13	CLA	A	804	-	50,58,73	1.62	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	e	833	-	50,58,73	1.65	9 (18%)	58,95,113	1.47	8 (13%)
13	CLA	a	811	-	50,58,73	1.66	6 (12%)	58,95,113	1.53	9 (15%)
13	CLA	b	833	-	50,58,73	1.68	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	B	810	-	50,58,73	1.65	6 (12%)	58,95,113	1.64	9 (15%)
13	CLA	E	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.61	8 (13%)
13	CLA	B	805	-	50,58,73	1.65	8 (16%)	58,95,113	1.60	8 (13%)
13	CLA	a	837	-	50,58,73	1.68	8 (16%)	58,95,113	1.47	8 (13%)
13	CLA	B	812	-	50,58,73	1.67	6 (12%)	58,95,113	1.49	7 (12%)
13	CLA	G	814	-	50,58,73	1.65	6 (12%)	58,95,113	1.56	8 (13%)
12	LHG	a	801	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	7 (13%)
15	BCR	E	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	5 (8%)
13	CLA	E	816	-	50,58,73	1.66	6 (12%)	58,95,113	1.54	9 (15%)
13	CLA	G	833	-	50,58,73	1.73	7 (14%)	58,95,113	1.46	7 (12%)
13	CLA	a	816	-	50,58,73	1.67	7 (14%)	58,95,113	1.54	9 (15%)
14	PQN	A	846	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	a	804	-	50,58,73	1.61	7 (14%)	58,95,113	1.61	8 (13%)
15	BCR	a	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	b	803	-	50,58,73	1.65	6 (12%)	58,95,113	1.45	8 (13%)
13	CLA	g	802	-	50,58,73	1.64	8 (16%)	58,95,113	1.57	7 (12%)
13	CLA	E	815	-	50,58,73	1.66	6 (12%)	58,95,113	1.55	7 (12%)
13	CLA	A	827	-	50,58,73	1.68	6 (12%)	58,95,113	1.50	9 (15%)
13	CLA	E	843	-	50,58,73	1.63	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	g	808	-	50,58,73	1.65	7 (14%)	58,95,113	1.55	9 (15%)
13	CLA	L	204	-	50,58,73	2.51	11 (22%)	58,95,113	3.05	16 (27%)
13	CLA	s	205	-	50,58,73	1.67	6 (12%)	58,95,113	1.50	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	828	-	50,58,73	1.65	7 (14%)	58,95,113	1.60	9 (15%)
15	BCR	B	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	E	835	-	50,58,73	1.65	8 (16%)	58,95,113	1.56	7 (12%)
15	BCR	O	201	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	A	831	-	50,58,73	1.69	7 (14%)	58,95,113	1.57	8 (13%)
15	BCR	S	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	E	813	-	45,53,73	1.77	6 (13%)	52,89,113	1.55	7 (13%)
13	CLA	b	813	-	50,58,73	1.64	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	A	836	-	50,58,73	1.69	8 (16%)	58,95,113	1.48	8 (13%)
15	BCR	q	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	a	808	-	50,58,73	1.65	6 (12%)	58,95,113	1.63	8 (13%)
13	CLA	B	817	-	50,58,73	1.68	6 (12%)	58,95,113	1.46	8 (13%)
13	CLA	B	825	-	50,58,73	1.63	7 (14%)	58,95,113	1.64	9 (15%)
13	CLA	b	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.57	8 (13%)
12	LHG	A	801	-	48,48,48	0.68	1 (2%)	51,54,54	1.31	7 (13%)
13	CLA	B	823	2	50,58,73	1.69	8 (16%)	58,95,113	1.56	8 (13%)
13	CLA	r	101	-	42,49,73	1.81	7 (16%)	48,83,113	1.59	6 (12%)
16	SF4	C	101	-	0,12,12	-	-	-	-	-
15	BCR	e	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	B	826	-	46,54,73	1.71	7 (15%)	53,90,113	1.64	7 (13%)
15	BCR	g	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	A	830	-	50,58,73	1.69	7 (14%)	58,95,113	1.54	8 (13%)
15	BCR	G	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	S	206	-	45,53,73	1.78	7 (15%)	52,89,113	1.49	7 (13%)
15	BCR	B	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	B	814	-	50,58,73	1.64	6 (12%)	58,95,113	1.55	8 (13%)
13	CLA	g	805	-	50,58,73	1.65	7 (14%)	58,95,113	1.45	8 (13%)
13	CLA	b	830	-	45,53,73	1.76	6 (13%)	52,89,113	1.53	8 (15%)
13	CLA	B	834	-	50,58,73	1.68	6 (12%)	58,95,113	1.60	9 (15%)
13	CLA	B	821	-	47,55,73	1.72	7 (14%)	54,91,113	1.52	7 (12%)
16	SF4	H	102	3	0,12,12	-	-	-	-	-
13	CLA	A	840	-	50,58,73	1.65	9 (18%)	58,95,113	1.52	9 (15%)
13	CLA	A	839	-	50,58,73	1.65	7 (14%)	58,95,113	1.61	9 (15%)
13	CLA	A	823	-	50,58,73	1.65	8 (16%)	58,95,113	1.45	6 (10%)
13	CLA	G	804	-	50,58,73	1.65	8 (16%)	58,95,113	1.59	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	816	-	45,53,73	1.82	8 (17%)	52,89,113	1.54	6 (11%)
13	CLA	B	839	-	47,55,73	1.71	7 (14%)	54,91,113	1.60	6 (11%)
13	CLA	e	844	12	50,58,73	1.66	7 (14%)	58,95,113	1.63	9 (15%)
15	BCR	b	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	b	820	-	47,55,73	1.72	7 (14%)	54,91,113	1.52	7 (12%)
13	CLA	G	810	2	50,58,73	1.68	7 (14%)	58,95,113	1.55	8 (13%)

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
13	CLA	E	845	-	1/1/12/20	6/19/97/115	-
13	CLA	G	832	-	1/1/11/20	6/18/96/115	-
13	CLA	E	807	-	1/1/12/20	7/19/97/115	-
13	CLA	B	804	-	1/1/12/20	6/19/97/115	-
13	CLA	A	837	-	-	7/19/97/115	-
15	BCR	S	202	-	-	17/29/63/63	0/2/2/2
13	CLA	a	805	-	1/1/12/20	7/19/97/115	-
14	PQN	G	842	-	-	11/23/43/43	0/2/2/2
13	CLA	G	840	-	1/1/12/20	7/19/97/115	-
13	CLA	E	808	-	1/1/12/20	6/19/97/115	-
13	CLA	e	803	-	1/1/12/20	8/19/97/115	-
13	CLA	g	838	-	1/1/12/20	6/19/97/115	-
13	CLA	l	203	10	1/1/12/20	7/19/97/115	-
13	CLA	e	825	-	1/1/12/20	13/19/97/115	-
13	CLA	l	204	-	1/1/11/20	5/13/91/115	-
13	CLA	G	803	-	1/1/12/20	6/19/97/115	-
13	CLA	g	820	-	1/1/12/20	7/19/97/115	-
13	CLA	G	841	-	1/1/12/20	7/19/97/115	-
15	BCR	A	847	-	-	19/29/63/63	0/2/2/2
13	CLA	G	838	-	1/1/12/20	6/19/97/115	-
13	CLA	a	812	1	1/1/12/20	6/19/97/115	-
13	CLA	A	819	-	1/1/11/20	10/18/96/115	-
13	CLA	e	814	-	1/1/12/20	8/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	Q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	g	837	-	1/1/11/20	8/13/91/115	-
13	CLA	g	823	-	1/1/11/20	6/13/91/115	-
13	CLA	g	801	-	1/1/12/20	7/19/97/115	-
13	CLA	B	811	2	1/1/12/20	6/19/97/115	-
13	CLA	g	818	-	1/1/12/20	8/19/97/115	-
13	CLA	E	838	-	-	7/19/97/115	-
13	CLA	G	812	-	1/1/11/20	4/13/91/115	-
13	CLA	B	816	-	1/1/11/20	6/13/91/115	-
13	CLA	B	828	-	1/1/12/20	6/19/97/115	-
13	CLA	a	822	-	1/1/12/20	9/19/97/115	-
15	BCR	I	101	-	-	10/29/63/63	0/2/2/2
13	CLA	e	819	-	1/1/12/20	2/19/97/115	-
15	BCR	R	101	-	-	16/29/63/63	0/2/2/2
13	CLA	B	833	-	1/1/12/20	4/19/97/115	-
13	CLA	E	823	-	1/1/12/20	10/19/97/115	-
13	CLA	A	842	-	1/1/12/20	6/19/97/115	-
13	CLA	b	827	-	1/1/12/20	6/19/97/115	-
13	CLA	e	829	-	1/1/12/20	8/19/97/115	-
13	CLA	e	836	-	-	7/19/97/115	-
13	CLA	A	820	-	1/1/12/20	2/19/97/115	-
13	CLA	e	834	-	1/1/12/20	6/19/97/115	-
13	CLA	G	836	-	1/1/11/20	8/13/91/115	-
16	SF4	a	846	-	-	-	0/6/5/5
13	CLA	B	835	-	1/1/11/20	7/13/91/115	-
13	CLA	G	813	-	1/1/11/20	5/13/91/115	-
15	BCR	G	846	-	-	22/29/63/63	0/2/2/2
13	CLA	E	814	-	1/1/12/20	3/19/97/115	-
13	CLA	B	807	-	1/1/12/20	10/19/97/115	-
13	CLA	b	822	2	1/1/12/20	7/19/97/115	-
13	CLA	g	809	-	1/1/12/20	4/19/97/115	-
13	CLA	b	824	-	1/1/12/20	6/19/97/115	-
15	BCR	m	101	-	-	11/29/63/63	0/2/2/2
13	CLA	E	834	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	813	-	1/1/11/20	5/13/91/115	-
13	CLA	E	826	-	1/1/12/20	13/19/97/115	-
13	CLA	g	839	-	1/1/12/20	6/19/97/115	-
13	CLA	e	804	-	1/1/12/20	8/19/97/115	-
13	CLA	B	801	-	1/1/12/20	5/19/97/115	-
13	CLA	A	815	-	1/1/12/20	8/19/97/115	-
15	BCR	k	4001	-	-	21/29/63/63	0/2/2/2
13	CLA	a	836	-	1/1/12/20	6/19/97/115	-
15	BCR	s	201	-	-	18/29/63/63	0/2/2/2
13	CLA	a	817	-	1/1/12/20	3/19/97/115	-
13	CLA	e	810	-	1/1/12/20	3/19/97/115	-
15	BCR	G	845	-	-	17/29/63/63	0/2/2/2
13	CLA	G	824	-	1/1/11/20	6/13/91/115	-
13	CLA	b	832	-	1/1/12/20	4/19/97/115	-
13	CLA	b	834	-	1/1/11/20	7/13/91/115	-
15	BCR	A	851	-	-	5/29/63/63	0/2/2/2
15	BCR	b	842	-	-	9/29/63/63	0/2/2/2
13	CLA	G	811	-	1/1/12/20	12/19/97/115	-
13	CLA	e	840	-	1/1/11/20	6/16/94/115	-
16	SF4	g	804	-	-	-	0/6/5/5
15	BCR	b	843	-	-	20/29/63/63	0/2/2/2
13	CLA	E	824	-	1/1/12/20	8/19/97/115	-
13	CLA	e	841	-	1/1/12/20	6/19/97/115	-
15	BCR	O	202	-	-	16/29/63/63	0/2/2/2
13	CLA	A	818	-	1/1/11/20	4/13/91/115	-
13	CLA	A	822	-	1/1/12/20	9/19/97/115	-
13	CLA	E	827	-	1/1/12/20	11/19/97/115	-
15	BCR	G	847	-	-	12/29/63/63	0/2/2/2
13	CLA	e	837	1	1/1/11/20	5/13/91/115	-
13	CLA	B	819	-	1/1/12/20	7/19/97/115	-
13	CLA	g	812	2	1/1/12/20	6/19/97/115	-
13	CLA	A	806	-	1/1/12/20	8/19/97/115	-
13	CLA	G	805	-	1/1/12/20	2/19/97/115	-
13	CLA	b	802	-	1/1/12/20	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	836	-	1/1/12/20	6/19/97/115	-
12	LHG	e	801	-	-	31/53/53/53	-
14	PQN	E	848	-	-	6/23/43/43	0/2/2/2
13	CLA	b	808	-	1/1/12/20	5/19/97/115	-
13	CLA	b	806	-	1/1/12/20	10/19/97/115	-
13	CLA	g	826	-	1/1/12/20	6/19/97/115	-
13	CLA	E	828	-	1/1/12/20	6/19/97/115	-
13	CLA	G	820	-	1/1/12/20	5/19/97/115	-
13	CLA	g	807	-	1/1/12/20	2/19/97/115	-
15	BCR	q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	L	203	-	1/1/11/20	5/13/91/115	-
13	CLA	g	806	-	1/1/12/20	7/19/97/115	-
13	CLA	e	818	-	1/1/11/20	10/18/96/115	-
13	CLA	g	813	-	1/1/12/20	12/19/97/115	-
16	SF4	C	102	3	-	-	0/6/5/5
13	CLA	B	827	-	1/1/12/20	2/19/97/115	-
13	CLA	g	833	-	1/1/11/20	6/18/96/115	-
13	CLA	b	837	-	1/1/12/20	6/19/97/115	-
13	CLA	b	825	-	1/1/11/20	6/15/93/115	-
13	CLA	E	841	-	1/1/12/20	6/19/97/115	-
15	BCR	E	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	838	1	1/1/11/20	7/13/91/115	-
15	BCR	g	847	-	-	22/29/63/63	0/2/2/2
13	CLA	E	840	-	1/1/12/20	6/19/97/115	-
13	CLA	E	846	-	1/1/9/20	3/7/81/115	-
15	BCR	E	801	-	-	12/29/63/63	0/2/2/2
13	CLA	b	818	-	1/1/12/20	7/19/97/115	-
13	CLA	k	4002	-	1/1/11/20	6/13/91/115	-
13	CLA	G	837	-	1/1/12/20	6/19/97/115	-
13	CLA	g	825	-	1/1/11/20	6/13/91/115	-
13	CLA	b	836	-	1/1/12/20	6/19/97/115	-
13	CLA	e	805	-	1/1/12/20	8/19/97/115	-
13	CLA	a	818	-	1/1/11/20	4/13/91/115	-
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	e	847	-	-	13/29/63/63	0/2/2/2
13	CLA	G	818	-	1/1/12/20	10/19/97/115	-
13	CLA	o	202	-	1/1/11/20	5/13/91/115	-
15	BCR	e	846	-	-	19/29/63/63	0/2/2/2
15	BCR	A	850	-	-	21/29/63/63	0/2/2/2
13	CLA	L	202	10	1/1/12/20	6/19/97/115	-
13	CLA	E	833	-	1/1/12/20	6/19/97/115	-
13	CLA	a	844	-	1/1/12/20	7/19/97/115	-
13	CLA	e	820	-	1/1/12/20	7/19/97/115	-
13	CLA	A	832	-	1/1/12/20	4/19/97/115	-
13	CLA	F	202	-	1/1/11/20	5/13/91/115	-
13	CLA	A	843	-	1/1/12/20	7/19/97/115	-
13	CLA	a	852	-	1/1/12/20	8/19/97/115	-
15	BCR	b	846	-	-	12/29/63/63	0/2/2/2
13	CLA	B	840	-	1/1/12/20	7/19/97/115	-
13	CLA	B	841	-	1/1/12/20	7/19/97/115	-
16	SF4	B	803	-	-	-	0/6/5/5
13	CLA	l	205	-	1/1/12/20	8/19/97/115	-
15	BCR	e	849	-	-	20/29/63/63	0/2/2/2
13	CLA	A	853	-	1/1/12/20	10/19/97/115	-
15	BCR	g	846	-	-	17/29/63/63	0/2/2/2
13	CLA	e	828	-	1/1/12/20	9/19/97/115	-
13	CLA	a	814	-	1/1/11/20	3/13/91/115	-
13	CLA	E	822	-	1/1/12/20	9/19/97/115	-
15	BCR	e	850	-	-	6/29/63/63	0/2/2/2
13	CLA	f	203	-	1/1/11/20	7/13/91/115	-
16	SF4	h	101	-	-	-	0/6/5/5
13	CLA	b	823	-	1/1/11/20	6/13/91/115	-
13	CLA	G	830	-	1/1/12/20	6/19/97/115	-
13	CLA	G	827	-	1/1/12/20	2/19/97/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	a	845	-	1/1/12/20	6/19/97/115	-
13	CLA	b	828	-	1/1/12/20	11/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	821	-	1/1/12/20	7/19/97/115	-
13	CLA	G	831	-	1/1/11/20	10/13/91/115	-
15	BCR	a	803	-	-	23/29/63/63	0/2/2/2
13	CLA	e	827	-	1/1/12/20	6/19/97/115	-
13	CLA	a	815	-	1/1/12/20	8/19/97/115	-
13	CLA	G	806	-	1/1/12/20	10/19/97/115	-
13	CLA	E	819	-	1/1/11/20	10/18/96/115	-
13	CLA	G	801	-	1/1/12/20	6/19/97/115	-
14	PQN	a	847	-	-	10/23/43/43	0/2/2/2
13	CLA	a	839	1	1/1/11/20	6/13/91/115	-
13	CLA	A	824	-	1/1/12/20	8/19/97/115	-
13	CLA	g	835	-	1/1/12/20	11/19/97/115	-
13	CLA	G	828	-	1/1/12/20	6/19/97/115	-
13	CLA	b	826	-	1/1/12/20	2/19/97/115	-
13	CLA	a	841	-	1/1/12/20	6/19/97/115	-
13	CLA	A	845	12	1/1/12/20	6/19/97/115	-
13	CLA	g	832	-	1/1/11/20	10/13/91/115	-
13	CLA	a	831	-	1/1/12/20	7/19/97/115	-
13	CLA	a	838	-	-	7/19/97/115	-
13	CLA	e	806	-	1/1/12/20	7/19/97/115	-
13	CLA	b	807	-	1/1/12/20	4/19/97/115	-
13	CLA	B	831	-	1/1/11/20	10/13/91/115	-
13	CLA	a	820	-	1/1/12/20	2/19/97/115	-
13	CLA	A	829	-	1/1/12/20	9/19/97/115	-
13	CLA	K	102	-	1/1/11/20	6/13/91/115	-
13	CLA	A	805	-	1/1/12/20	7/19/97/115	-
13	CLA	G	819	-	1/1/12/20	7/19/97/115	-
13	CLA	B	836	-	1/1/11/20	8/13/91/115	-
13	CLA	a	823	-	1/1/12/20	10/19/97/115	-
13	CLA	E	809	1	1/1/12/20	5/19/97/115	-
13	CLA	g	814	-	1/1/11/20	5/13/91/115	-
13	CLA	G	834	-	1/1/12/20	11/19/97/115	-
13	CLA	a	806	-	1/1/12/20	8/19/97/115	-
14	PQN	e	845	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	810	-	1/1/12/20	8/19/97/115	-
13	CLA	B	830	-	1/1/12/20	6/19/97/115	-
13	CLA	a	809	1	1/1/12/20	5/19/97/115	-
13	CLA	e	831	-	1/1/12/20	4/19/97/115	-
13	CLA	a	840	-	1/1/12/20	7/19/97/115	-
13	CLA	B	838	-	1/1/12/20	6/19/97/115	-
13	CLA	B	820	-	1/1/12/20	5/19/97/115	-
13	CLA	g	841	-	1/1/12/20	7/19/97/115	-
13	CLA	e	821	-	1/1/12/20	9/19/97/115	-
15	BCR	A	852	-	-	15/29/63/63	0/2/2/2
13	CLA	e	832	-	1/1/12/20	6/19/97/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
13	CLA	g	842	-	1/1/12/20	7/19/97/115	-
15	BCR	g	848	-	-	12/29/63/63	0/2/2/2
15	BCR	e	851	-	-	16/29/63/63	0/2/2/2
13	CLA	b	829	-	1/1/12/20	6/19/97/115	-
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
13	CLA	B	837	-	1/1/12/20	6/19/97/115	-
13	CLA	b	812	-	1/1/11/20	5/13/91/115	-
15	BCR	T	101	-	-	11/29/63/63	0/2/2/2
13	CLA	E	832	-	1/1/12/20	4/19/97/115	-
13	CLA	g	831	-	1/1/12/20	6/19/97/115	-
13	CLA	e	830	-	1/1/12/20	8/19/97/115	-
15	BCR	G	844	-	-	20/29/63/63	0/2/2/2
13	CLA	B	818	-	1/1/12/20	10/19/97/115	-
13	CLA	G	829	-	1/1/12/20	11/19/97/115	-
13	CLA	e	815	-	1/1/12/20	5/19/97/115	-
13	CLA	e	842	-	1/1/12/20	7/19/97/115	-
13	CLA	E	825	-	1/1/11/20	9/18/96/115	-
13	CLA	b	835	-	1/1/11/20	8/13/91/115	-
13	CLA	g	810	-	1/1/12/20	5/19/97/115	-
13	CLA	r	102	-	1/1/11/20	6/13/91/115	-
15	BCR	B	845	-	-	17/29/63/63	0/2/2/2
13	CLA	g	840	-	1/1/11/20	8/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	842	-	1/1/11/20	6/16/94/115	-
13	CLA	e	852	-	1/1/12/20	10/19/97/115	-
13	CLA	G	815	-	1/1/12/20	3/19/97/115	-
13	CLA	E	820	-	1/1/12/20	2/19/97/115	-
14	PQN	g	843	-	-	11/23/43/43	0/2/2/2
13	CLA	g	803	-	1/1/12/20	6/19/97/115	-
13	CLA	a	830	-	1/1/12/20	8/19/97/115	-
15	BCR	E	802	-	-	20/29/63/63	0/2/2/2
13	CLA	G	835	-	1/1/11/20	7/13/91/115	-
15	BCR	S	201	-	-	17/29/63/63	0/2/2/2
15	BCR	l	202	-	-	18/29/63/63	0/2/2/2
12	LHG	e	802	13	-	14/42/42/53	-
13	CLA	g	830	-	1/1/12/20	11/19/97/115	-
13	CLA	E	831	-	1/1/12/20	7/19/97/115	-
15	BCR	a	802	-	-	10/29/63/63	0/2/2/2
13	CLA	b	817	-	1/1/12/20	10/19/97/115	-
13	CLA	G	809	-	1/1/12/20	4/19/97/115	-
13	CLA	g	821	-	1/1/12/20	5/19/97/115	-
15	BCR	E	849	-	-	19/29/63/63	0/2/2/2
16	SF4	h	102	3	-	-	0/6/5/5
13	CLA	A	809	1	1/1/12/20	5/19/97/115	-
15	BCR	f	201	-	-	8/29/63/63	0/2/2/2
13	CLA	a	807	-	1/1/12/20	7/19/97/115	-
13	CLA	A	810	-	1/1/12/20	8/19/97/115	-
13	CLA	A	841	-	1/1/11/20	6/16/94/115	-
15	BCR	a	849	-	-	19/29/63/63	0/2/2/2
13	CLA	a	813	-	1/1/11/20	4/13/91/115	-
13	CLA	A	821	-	1/1/12/20	7/19/97/115	-
13	CLA	A	812	1	1/1/12/20	6/19/97/115	-
13	CLA	G	802	-	1/1/12/20	10/19/97/115	-
13	CLA	b	801	-	1/1/9/20	2/7/81/115	-
13	CLA	G	808	-	1/1/12/20	5/19/97/115	-
14	PQN	B	842	-	-	11/23/43/43	0/2/2/2
13	CLA	b	809	-	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	830	-	1/1/12/20	8/19/97/115	-
13	CLA	b	839	-	1/1/12/20	7/19/97/115	-
15	BCR	o	201	-	-	8/29/63/63	0/2/2/2
13	CLA	K	101	-	1/1/9/20	3/7/81/115	-
12	LHG	A	802	13	-	17/42/42/53	-
15	BCR	p	101	-	-	10/29/63/63	0/2/2/2
15	BCR	A	849	-	-	8/29/63/63	0/2/2/2
15	BCR	g	845	-	-	20/29/63/63	0/2/2/2
13	CLA	g	824	2	1/1/12/20	6/19/97/115	-
13	CLA	B	832	-	1/1/11/20	6/18/96/115	-
13	CLA	a	833	-	1/1/12/20	6/19/97/115	-
15	BCR	l	206	-	-	17/29/63/63	0/2/2/2
13	CLA	E	837	-	1/1/12/20	10/19/97/115	-
13	CLA	A	817	-	1/1/11/20	5/13/91/115	-
13	CLA	B	809	-	1/1/12/20	5/19/97/115	-
13	CLA	s	203	-	1/1/12/20	8/19/97/115	-
15	BCR	E	851	-	-	8/29/63/63	0/2/2/2
13	CLA	g	836	-	1/1/11/20	7/13/91/115	-
13	CLA	e	835	-	1/1/12/20	10/19/97/115	-
13	CLA	A	816	-	1/1/12/20	5/19/97/115	-
13	CLA	g	834	-	1/1/12/20	4/19/97/115	-
13	CLA	E	818	-	1/1/11/20	4/13/91/115	-
15	BCR	b	845	-	-	22/29/63/63	0/2/2/2
13	CLA	A	826	-	1/1/12/20	13/19/97/115	-
13	CLA	G	822	-	1/1/11/20	6/13/91/115	-
15	BCR	g	849	-	-	16/29/63/63	0/2/2/2
13	CLA	a	819	-	1/1/11/20	10/18/96/115	-
13	CLA	G	817	-	1/1/12/20	7/19/97/115	-
13	CLA	A	807	-	1/1/12/20	7/19/97/115	-
13	CLA	A	834	-	1/1/12/20	6/19/97/115	-
15	BCR	L	201	-	-	17/29/63/63	0/2/2/2
13	CLA	a	827	-	1/1/12/20	11/19/97/115	-
13	CLA	A	813	-	1/1/11/20	4/13/91/115	-
13	CLA	S	203	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	808	-	1/1/12/20	4/19/97/115	-
13	CLA	B	806	-	1/1/12/20	2/19/97/115	-
13	CLA	g	811	-	1/1/12/20	4/19/97/115	-
13	CLA	G	826	-	1/1/11/20	6/15/93/115	-
13	CLA	E	805	-	1/1/12/20	7/19/97/115	-
13	CLA	G	821	-	1/1/11/20	8/16/94/115	-
13	CLA	e	809	-	1/1/12/20	8/19/97/115	-
15	BCR	P	101	-	-	10/29/63/63	0/2/2/2
13	CLA	b	810	2	1/1/12/20	6/19/97/115	-
15	BCR	a	850	-	-	13/29/63/63	0/2/2/2
15	BCR	B	846	-	-	22/29/63/63	0/2/2/2
13	CLA	E	821	-	1/1/12/20	7/19/97/115	-
13	CLA	g	816	-	1/1/12/20	3/19/97/115	-
15	BCR	s	204	-	-	12/29/63/63	0/2/2/2
16	SF4	H	101	-	-	-	0/6/5/5
13	CLA	G	823	2	1/1/12/20	6/19/97/115	-
13	CLA	B	824	-	1/1/11/20	6/13/91/115	-
16	SF4	E	847	-	-	-	0/6/5/5
13	CLA	a	835	-	1/1/12/20	5/19/97/115	-
13	CLA	G	825	-	1/1/12/20	6/19/97/115	-
13	CLA	b	814	-	1/1/12/20	3/19/97/115	-
13	CLA	B	829	-	1/1/12/20	11/19/97/115	-
13	CLA	g	828	-	1/1/12/20	2/19/97/115	-
16	SF4	c	101	-	-	-	0/6/5/5
13	CLA	A	811	-	1/1/12/20	3/19/97/115	-
13	CLA	s	202	-	1/1/11/20	5/13/91/115	-
13	CLA	E	844	-	1/1/12/20	7/19/97/115	-
15	BCR	a	848	-	-	16/29/63/63	0/2/2/2
13	CLA	g	822	-	1/1/11/20	8/16/94/115	-
13	CLA	b	838	-	1/1/11/20	8/16/94/115	-
13	CLA	g	819	-	1/1/12/20	10/19/97/115	-
13	CLA	S	204	-	1/1/11/20	7/13/91/115	-
13	CLA	A	828	-	1/1/12/20	6/19/97/115	-
16	SF4	c	102	3	-	-	0/6/5/5
15	BCR	J	102	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	824	-	1/1/11/20	9/18/96/115	-
13	CLA	A	835	-	1/1/12/20	6/19/97/115	-
13	CLA	E	812	1	1/1/12/20	6/19/97/115	-
13	CLA	G	807	-	1/1/12/20	4/19/97/115	-
13	CLA	E	803	-	1/1/12/20	5/19/97/115	-
13	CLA	g	829	-	1/1/12/20	6/19/97/115	-
13	CLA	B	815	-	1/1/12/20	3/19/97/115	-
13	CLA	a	810	-	1/1/12/20	8/19/97/115	-
13	CLA	O	203	-	1/1/11/20	7/13/91/115	-
13	CLA	a	825	-	1/1/11/20	9/18/96/115	-
13	CLA	b	819	-	1/1/12/20	5/19/97/115	-
13	CLA	R	102	-	1/1/11/20	6/13/91/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
13	CLA	b	831	-	1/1/11/20	6/18/96/115	-
13	CLA	a	826	-	1/1/12/20	13/19/97/115	-
15	BCR	i	101	-	-	10/29/63/63	0/2/2/2
13	CLA	e	838	-	1/1/12/20	7/19/97/115	-
13	CLA	e	822	-	1/1/12/20	10/19/97/115	-
13	CLA	b	811	-	1/1/11/20	4/13/91/115	-
13	CLA	B	802	-	1/1/12/20	6/19/97/115	-
13	CLA	e	817	-	1/1/11/20	4/13/91/115	-
13	CLA	A	844	-	1/1/12/20	6/19/97/115	-
13	CLA	a	834	-	1/1/12/20	6/19/97/115	-
15	BCR	F	201	-	-	8/29/63/63	0/2/2/2
13	CLA	E	806	-	1/1/12/20	8/19/97/115	-
15	BCR	a	853	-	-	12/29/63/63	0/2/2/2
13	CLA	l	201	-	1/1/11/20	4/13/91/115	-
15	BCR	G	843	-	-	9/29/63/63	0/2/2/2
13	CLA	g	827	-	1/1/11/20	6/15/93/115	-
13	CLA	E	829	-	1/1/12/20	9/19/97/115	-
13	CLA	E	817	-	1/1/11/20	5/13/91/115	-
13	CLA	e	826	-	1/1/12/20	11/19/97/115	-
13	CLA	A	825	-	1/1/11/20	9/18/96/115	-
13	CLA	a	832	-	1/1/12/20	4/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	e	843	-	1/1/12/20	6/19/97/115	-
13	CLA	b	816	-	1/1/12/20	8/19/97/115	-
13	CLA	b	804	-	1/1/12/20	7/19/97/115	-
13	CLA	A	803	-	1/1/12/20	8/19/97/115	-
13	CLA	b	821	-	1/1/11/20	6/13/91/115	-
13	CLA	e	811	1	1/1/12/20	6/19/97/115	-
13	CLA	e	813	-	1/1/12/20	3/19/97/115	-
13	CLA	b	815	-	1/1/11/20	6/13/91/115	-
13	CLA	A	814	-	1/1/12/20	3/19/97/115	-
13	CLA	g	817	-	1/1/11/20	6/13/91/115	-
13	CLA	b	840	-	1/1/12/20	7/19/97/115	-
13	CLA	e	812	-	1/1/11/20	4/13/91/115	-
13	CLA	G	816	-	1/1/11/20	6/13/91/115	-
15	BCR	b	847	-	-	16/29/63/63	0/2/2/2
13	CLA	e	839	-	1/1/12/20	6/19/97/115	-
15	BCR	L	205	-	-	13/29/63/63	0/2/2/2
13	CLA	a	842	-	1/1/11/20	6/16/94/115	-
13	CLA	e	823	-	1/1/12/20	8/19/97/115	-
13	CLA	E	811	-	1/1/12/20	3/19/97/115	-
14	PQN	b	841	-	-	11/23/43/43	0/2/2/2
13	CLA	A	808	-	1/1/12/20	6/19/97/115	-
13	CLA	e	807	-	1/1/12/20	6/19/97/115	-
13	CLA	a	843	-	1/1/12/20	6/19/97/115	-
13	CLA	g	815	-	1/1/12/20	5/19/97/115	-
13	CLA	A	833	-	1/1/12/20	6/19/97/115	-
13	CLA	e	808	1	1/1/12/20	5/19/97/115	-
13	CLA	a	829	-	1/1/12/20	9/19/97/115	-
13	CLA	E	839	1	1/1/11/20	6/13/91/115	-
13	CLA	a	824	-	1/1/12/20	8/19/97/115	-
13	CLA	B	822	-	1/1/11/20	6/13/91/115	-
13	CLA	G	839	-	1/1/11/20	7/16/94/115	-
13	CLA	A	804	-	1/1/12/20	8/19/97/115	-
13	CLA	e	833	-	1/1/12/20	6/19/97/115	-
13	CLA	a	811	-	1/1/12/20	3/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	833	-	1/1/12/20	11/19/97/115	-
13	CLA	B	810	-	1/1/12/20	4/19/97/115	-
13	CLA	E	804	-	1/1/12/20	8/19/97/115	-
13	CLA	B	805	-	1/1/12/20	7/19/97/115	-
13	CLA	a	837	-	1/1/12/20	10/19/97/115	-
13	CLA	B	812	-	1/1/12/20	12/19/97/115	-
13	CLA	G	814	-	1/1/12/20	5/19/97/115	-
12	LHG	a	801	-	-	32/53/53/53	-
15	BCR	E	850	-	-	13/29/63/63	0/2/2/2
13	CLA	E	816	-	1/1/12/20	5/19/97/115	-
13	CLA	G	833	-	1/1/12/20	4/19/97/115	-
13	CLA	a	816	-	1/1/12/20	5/19/97/115	-
14	PQN	A	846	-	-	11/23/43/43	0/2/2/2
13	CLA	a	804	-	1/1/12/20	8/19/97/115	-
15	BCR	a	851	-	-	8/29/63/63	0/2/2/2
13	CLA	b	803	-	1/1/12/20	6/19/97/115	-
13	CLA	g	802	-	1/1/12/20	5/19/97/115	-
13	CLA	E	815	-	1/1/12/20	8/19/97/115	-
13	CLA	A	827	-	1/1/12/20	11/19/97/115	-
13	CLA	E	843	-	1/1/12/20	6/19/97/115	-
13	CLA	g	808	-	1/1/12/20	10/19/97/115	-
13	CLA	L	204	-	1/1/12/20	8/19/97/115	-
13	CLA	s	205	-	1/1/12/20	12/19/97/115	-
13	CLA	a	828	-	1/1/12/20	6/19/97/115	-
15	BCR	B	848	-	-	16/29/63/63	0/2/2/2
13	CLA	E	835	-	1/1/12/20	5/19/97/115	-
15	BCR	O	201	-	-	8/29/63/63	0/2/2/2
13	CLA	A	831	-	1/1/12/20	7/19/97/115	-
15	BCR	S	205	-	-	16/29/63/63	0/2/2/2
13	CLA	E	813	-	1/1/11/20	4/13/91/115	-
13	CLA	b	813	-	1/1/12/20	5/19/97/115	-
13	CLA	A	836	-	1/1/12/20	10/19/97/115	-
15	BCR	q	102	-	-	12/29/63/63	0/2/2/2
13	CLA	a	808	-	1/1/12/20	6/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	817	-	1/1/12/20	8/19/97/115	-
13	CLA	B	825	-	1/1/12/20	6/19/97/115	-
13	CLA	b	805	-	1/1/12/20	2/19/97/115	-
12	LHG	A	801	-	-	32/53/53/53	-
13	CLA	B	823	2	1/1/12/20	6/19/97/115	-
13	CLA	r	101	-	1/1/9/20	4/7/81/115	-
16	SF4	C	101	-	-	-	0/6/5/5
15	BCR	e	848	-	-	8/29/63/63	0/2/2/2
13	CLA	B	826	-	1/1/11/20	6/15/93/115	-
15	BCR	g	844	-	-	9/29/63/63	0/2/2/2
13	CLA	A	830	-	1/1/12/20	8/19/97/115	-
15	BCR	G	848	-	-	16/29/63/63	0/2/2/2
13	CLA	S	206	-	1/1/11/20	4/13/91/115	-
15	BCR	B	844	-	-	20/29/63/63	0/2/2/2
13	CLA	B	814	-	1/1/12/20	5/19/97/115	-
13	CLA	g	805	-	1/1/12/20	6/19/97/115	-
13	CLA	b	830	-	1/1/11/20	10/13/91/115	-
13	CLA	B	834	-	1/1/12/20	11/19/97/115	-
13	CLA	B	821	-	1/1/11/20	8/16/94/115	-
16	SF4	H	102	3	-	-	0/6/5/5
13	CLA	A	840	-	1/1/12/20	6/19/97/115	-
13	CLA	A	839	-	1/1/12/20	6/19/97/115	-
13	CLA	A	823	-	1/1/12/20	10/19/97/115	-
13	CLA	G	804	-	1/1/12/20	7/19/97/115	-
13	CLA	e	816	-	1/1/11/20	5/13/91/115	-
13	CLA	B	839	-	1/1/11/20	7/16/94/115	-
13	CLA	e	844	12	1/1/12/20	8/19/97/115	-
15	BCR	b	844	-	-	17/29/63/63	0/2/2/2
13	CLA	b	820	-	1/1/11/20	8/16/94/115	-
13	CLA	G	810	2	1/1/12/20	6/19/97/115	-

The worst 5 of 2682 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	S	204	CLA	MG-ND	9.46	2.24	2.05
13	l	205	CLA	MG-ND	9.45	2.24	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	L	204	CLA	MG-ND	9.43	2.24	2.05
13	s	203	CLA	MG-ND	9.40	2.24	2.05
13	g	834	CLA	C4B-NB	7.84	1.42	1.35

The worst 5 of 3352 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	l	205	CLA	C4A-NA-C1A	17.39	114.53	106.71
13	s	203	CLA	C4A-NA-C1A	17.36	114.51	106.71
13	S	204	CLA	C4A-NA-C1A	17.31	114.49	106.71
13	L	204	CLA	C4A-NA-C1A	17.27	114.47	106.71
13	E	842	CLA	C4A-NA-C1A	7.38	110.03	106.71

5 of 355 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	803	CLA	ND
13	A	804	CLA	ND
13	A	805	CLA	ND
13	A	806	CLA	ND
13	A	807	CLA	ND

5 of 3682 torsion outliers are listed below:

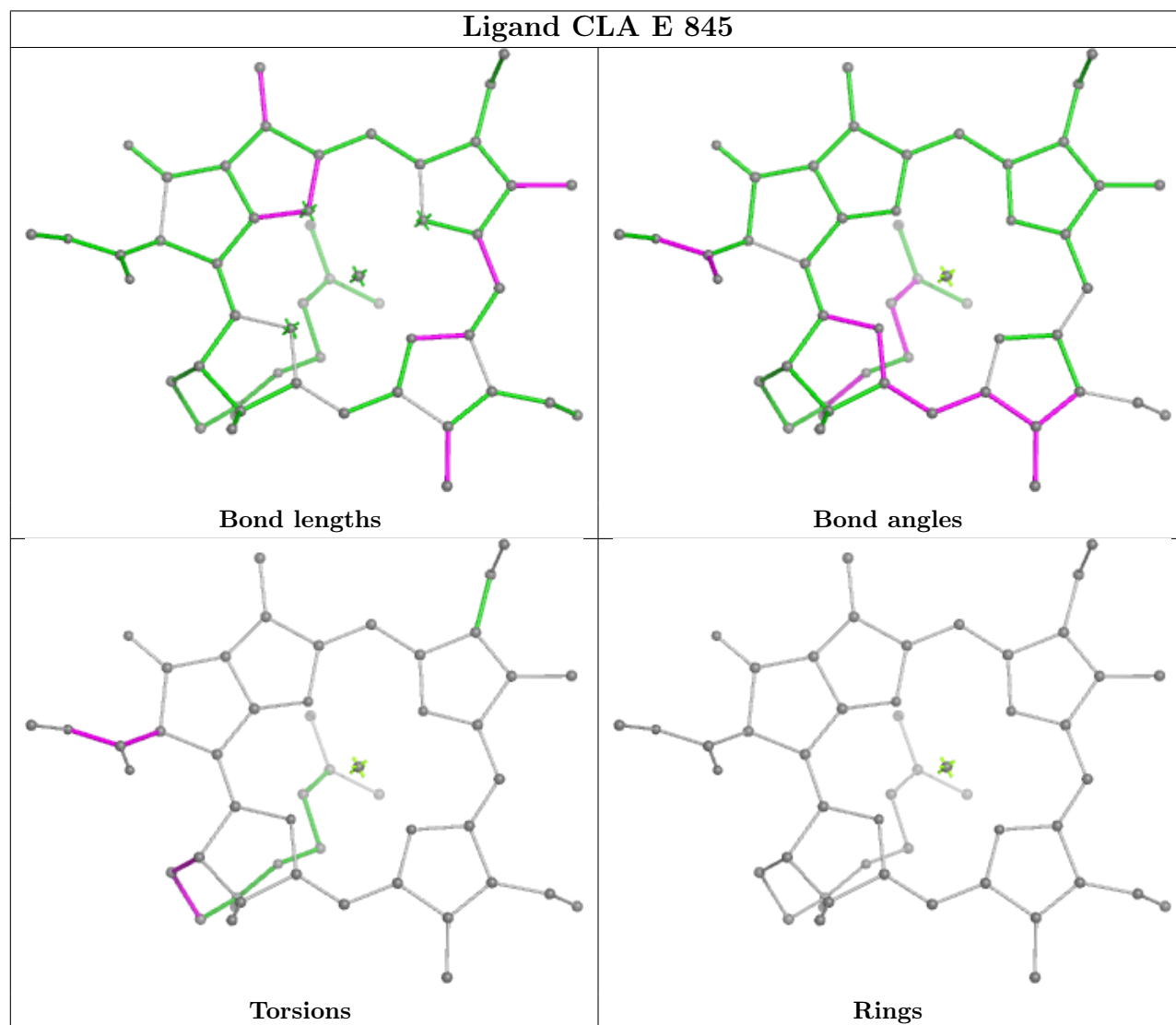
Mol	Chain	Res	Type	Atoms
12	A	801	LHG	O1-C1-C2-C3
12	A	801	LHG	C3-O3-P-O4
12	A	801	LHG	C3-O3-P-O6
12	A	801	LHG	C4-O6-P-O5
12	A	802	LHG	C3-O3-P-O4

There are no ring outliers.

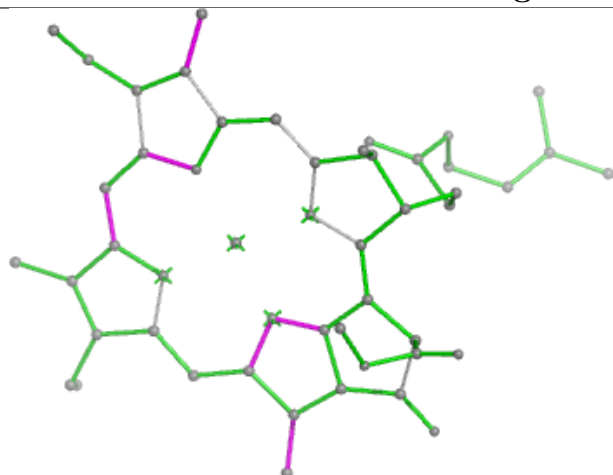
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

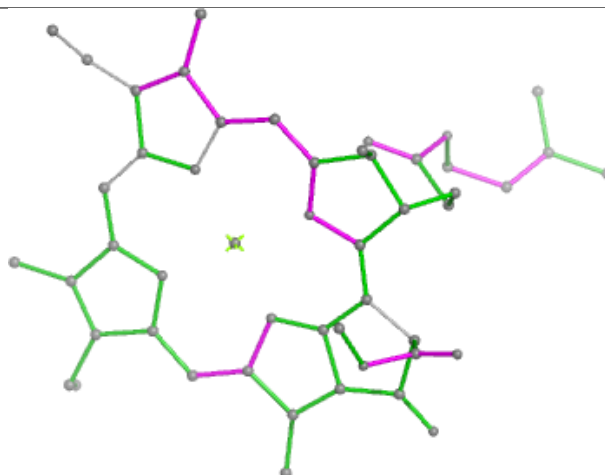
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



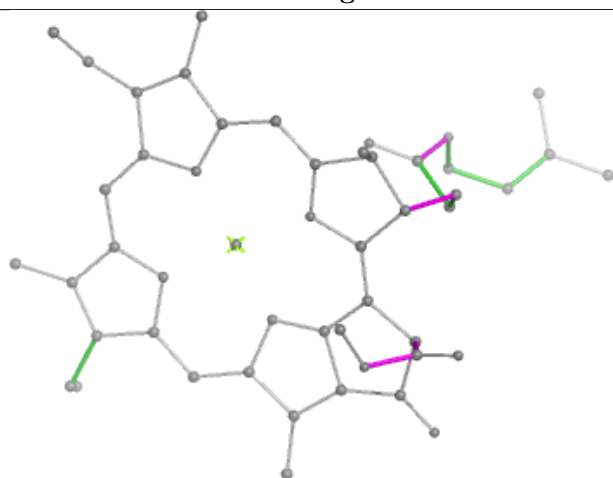
Ligand CLA A 837



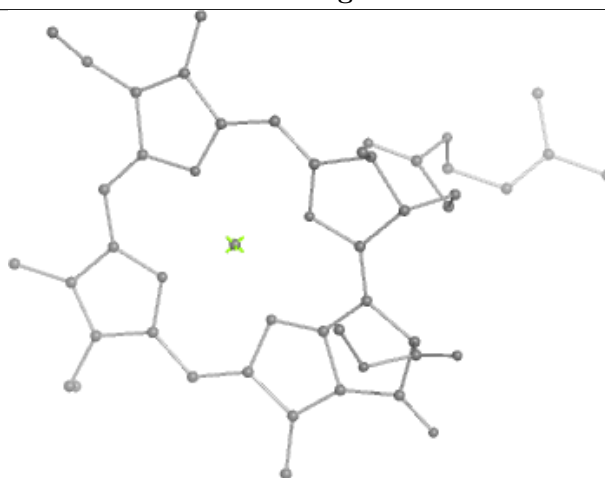
Bond lengths



Bond angles

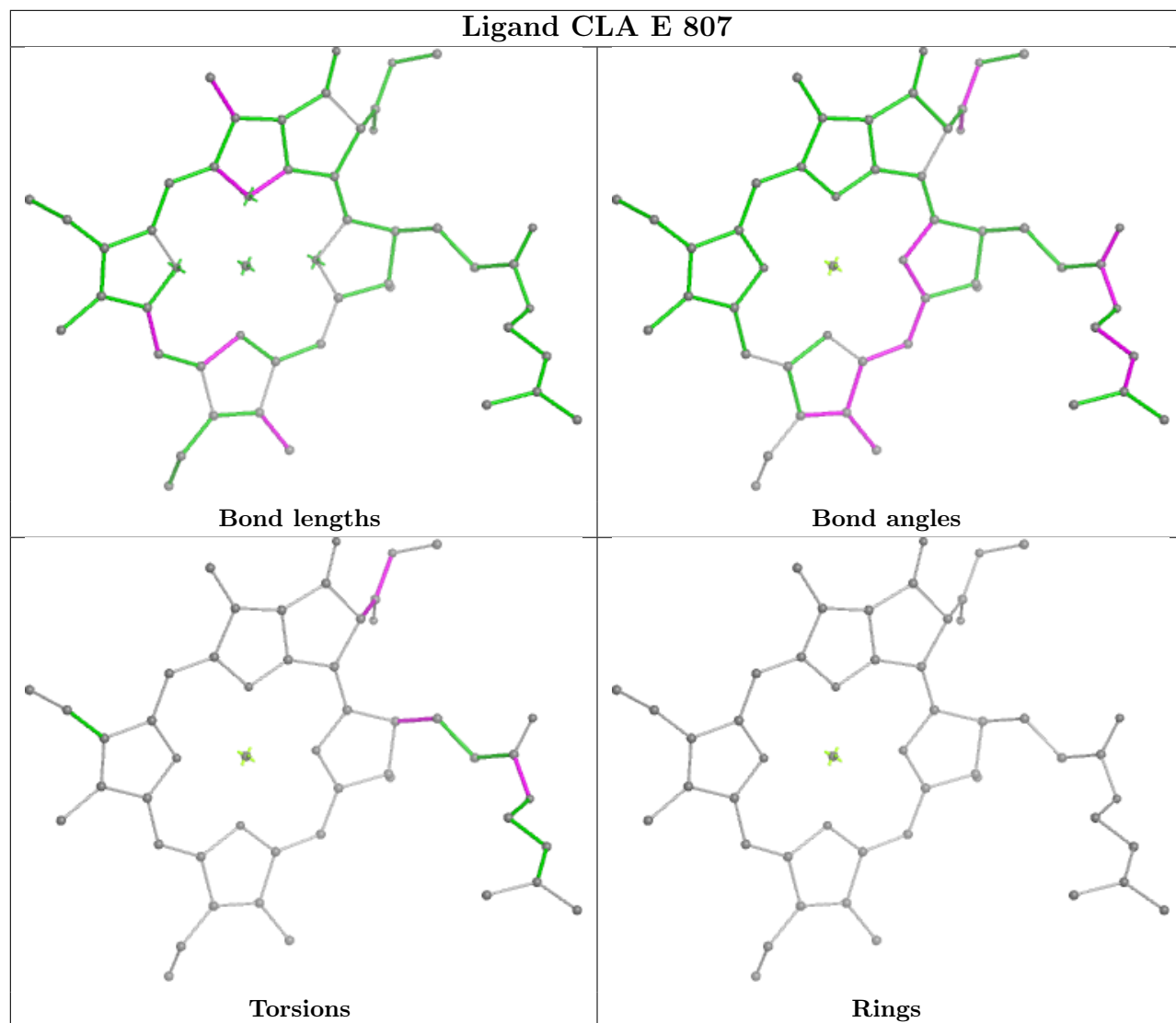


Torsions

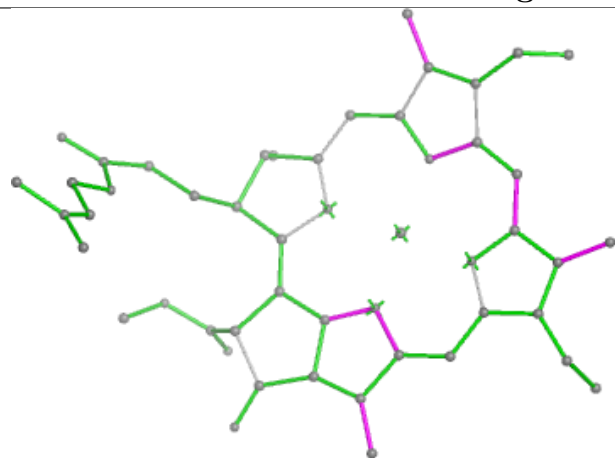


Rings

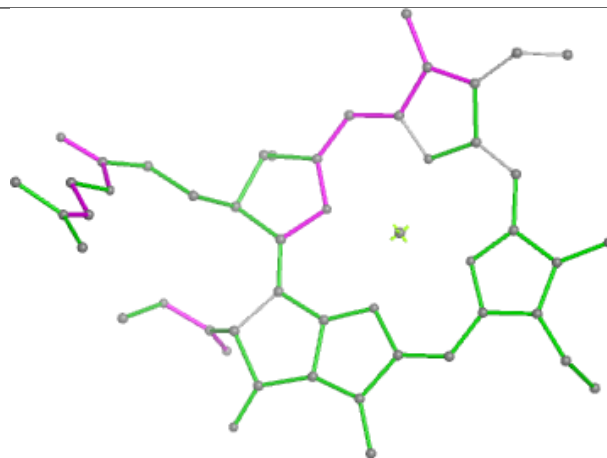
Ligand CLA E 807



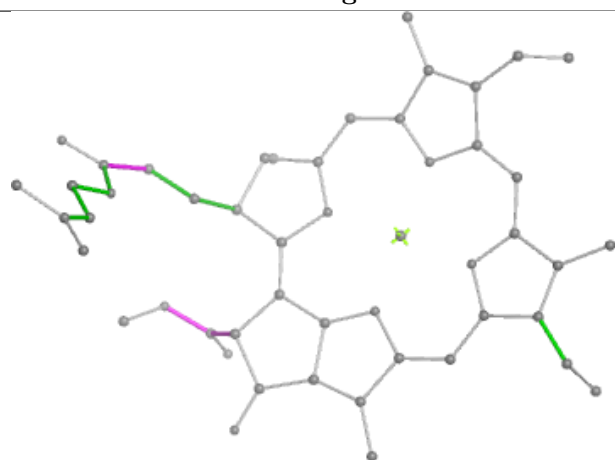
Ligand CLA B 804



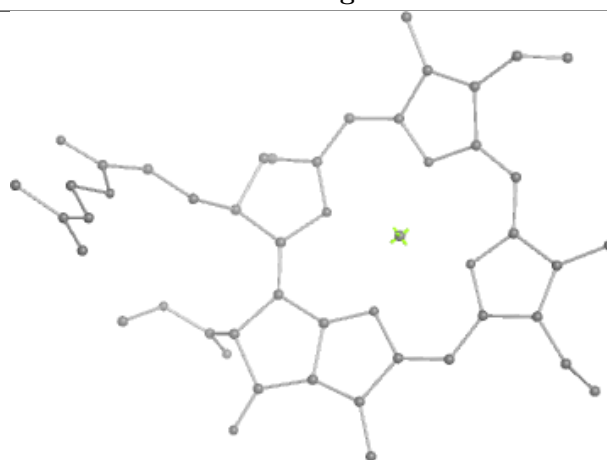
Bond lengths



Bond angles

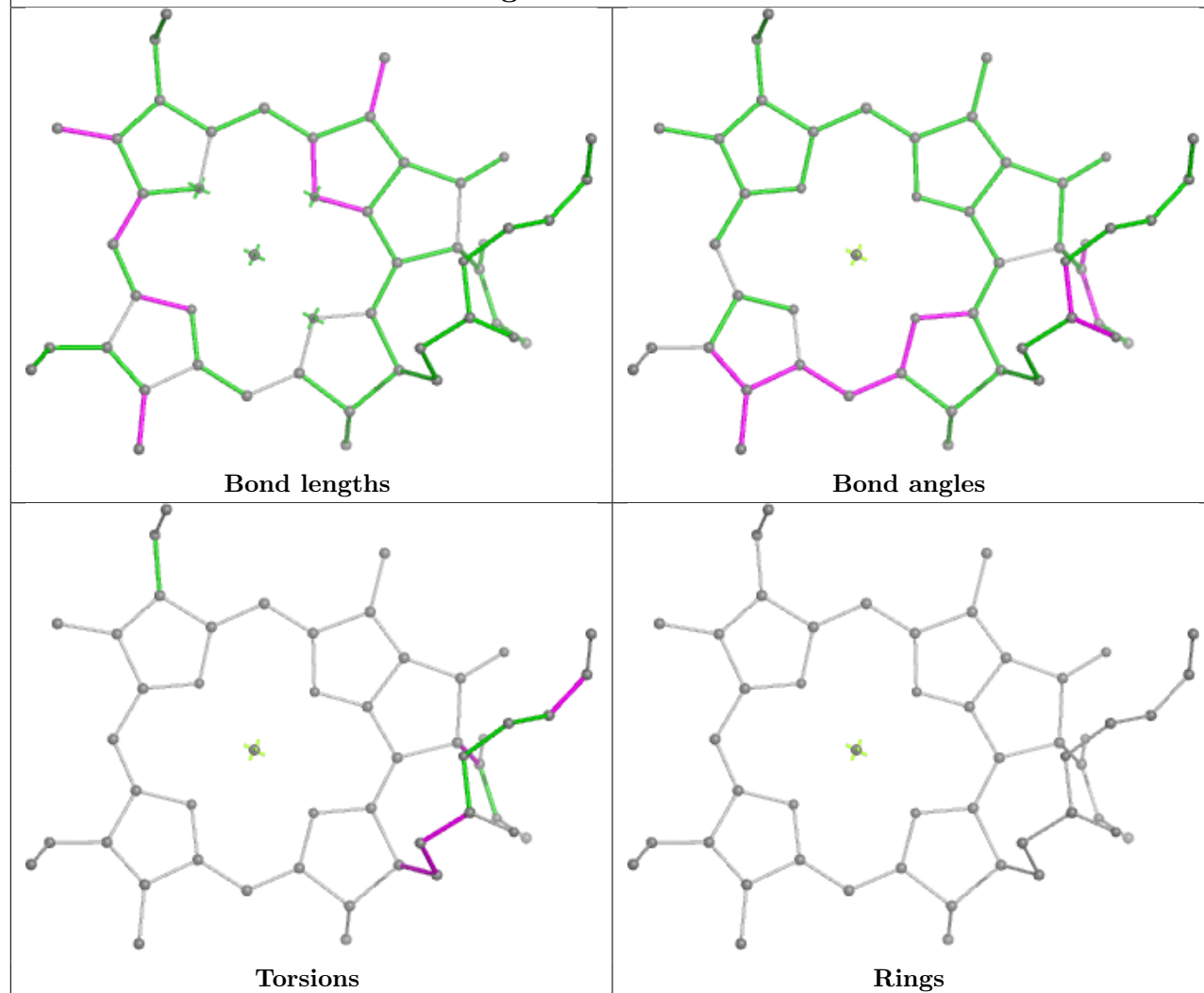


Torsions

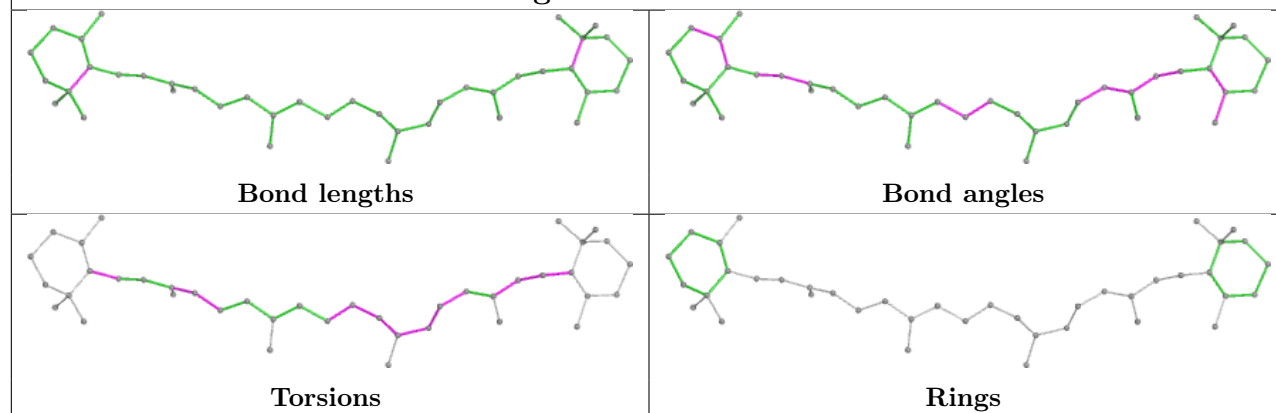


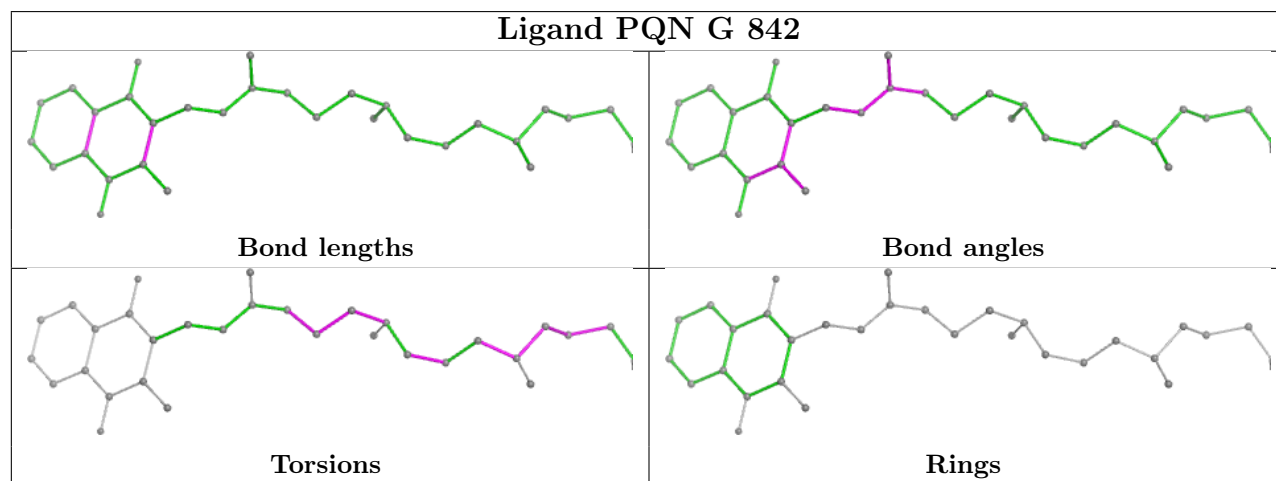
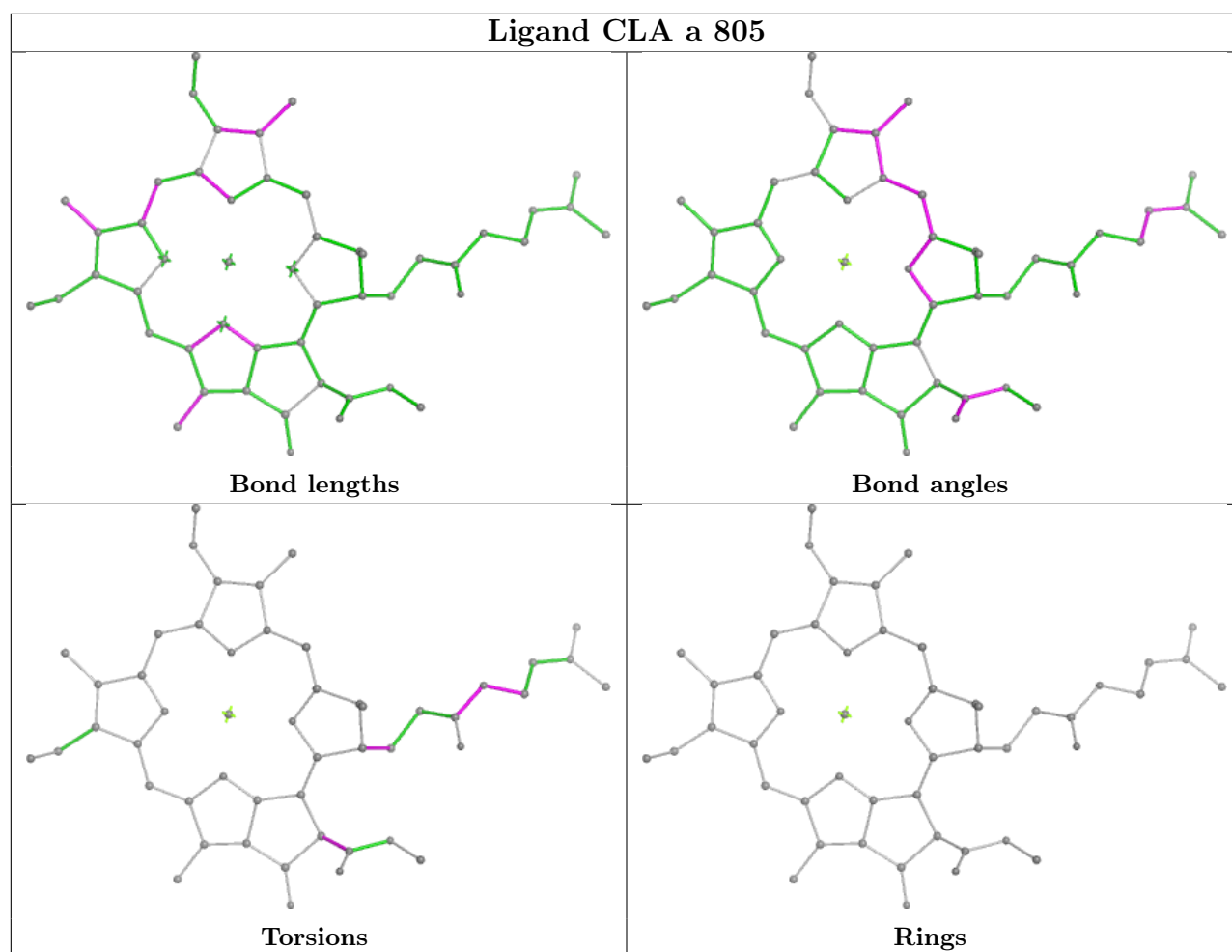
Rings

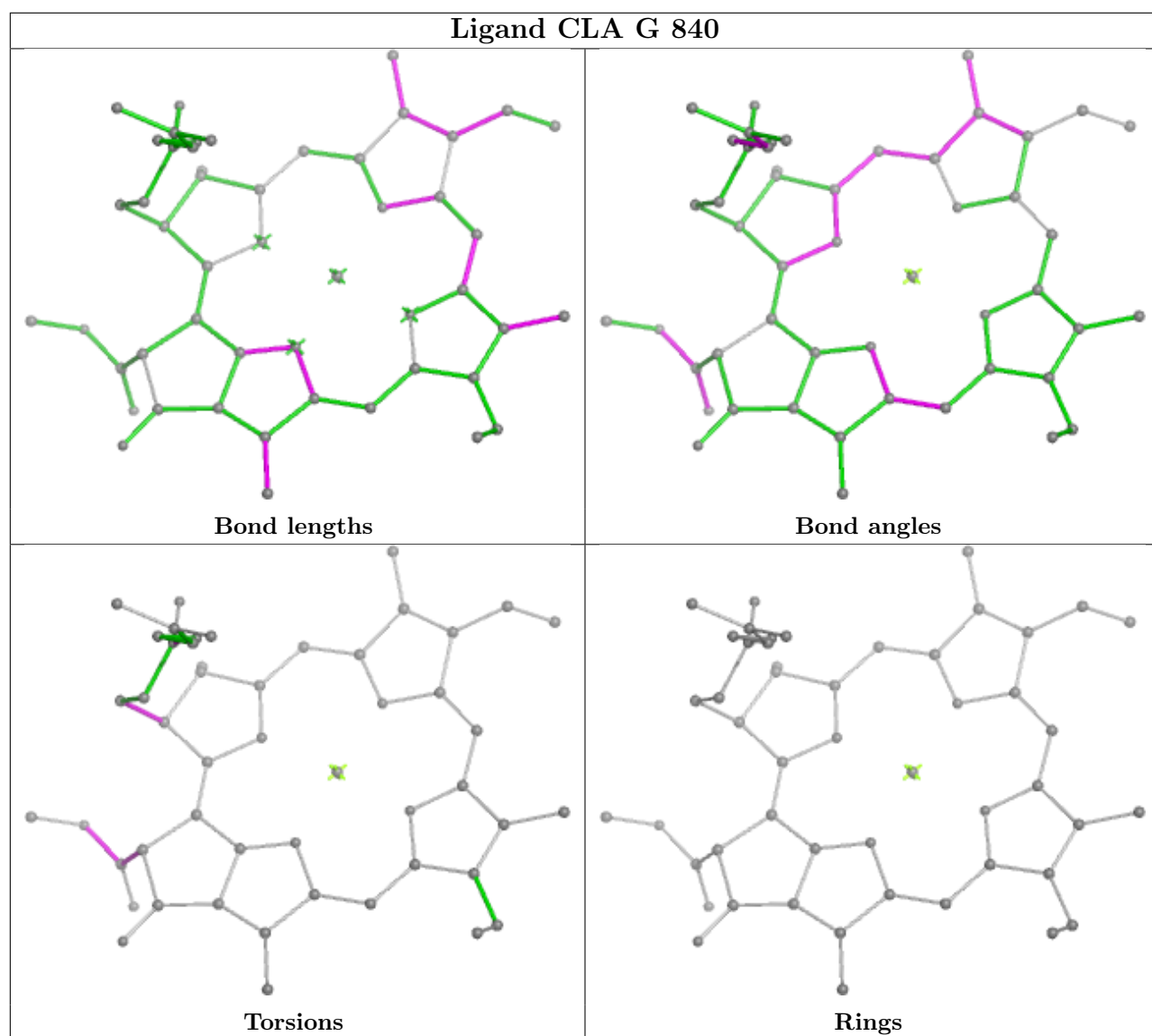
Ligand CLA G 832

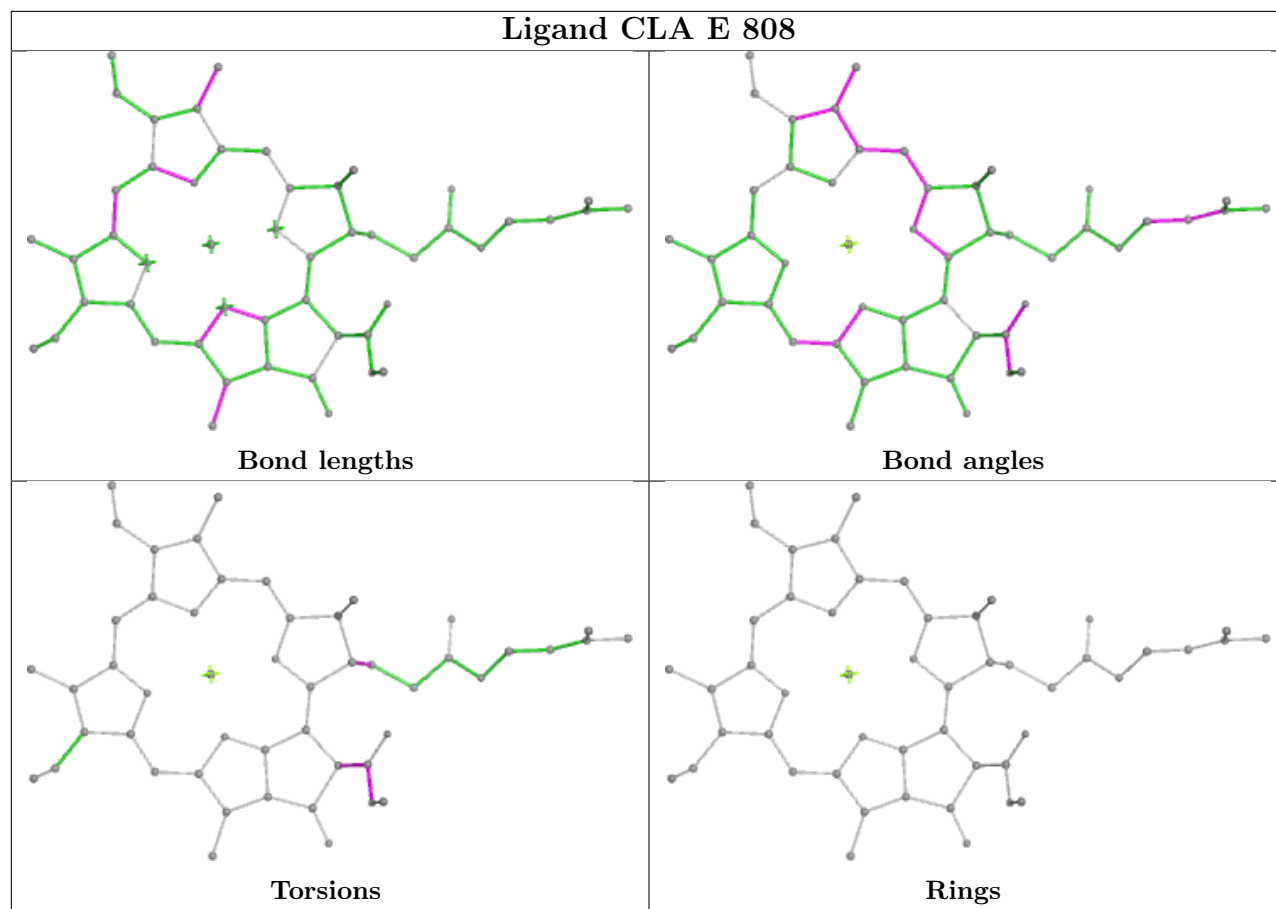


Ligand BCR S 202

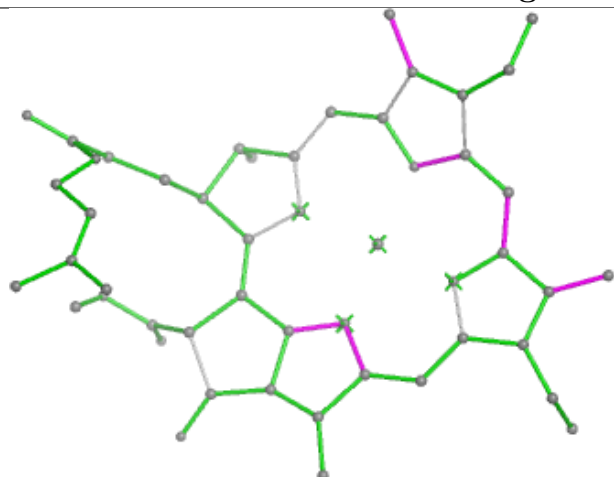




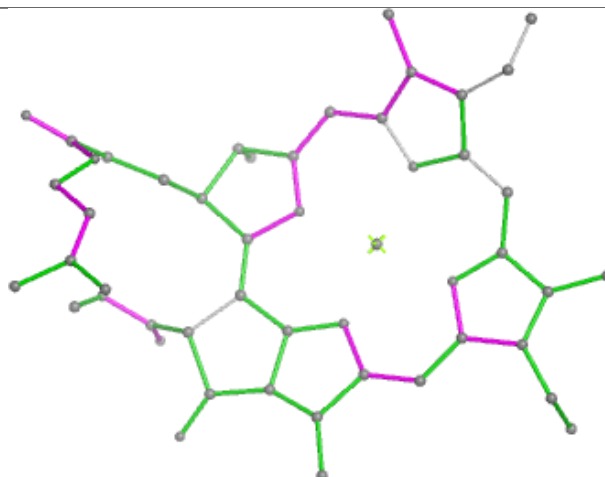




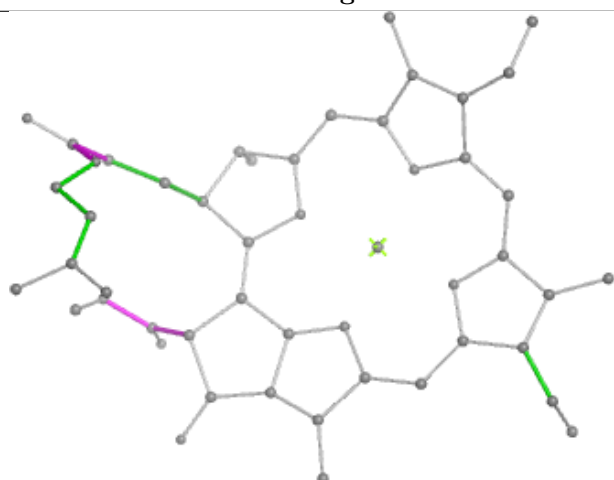
Ligand CLA e 803



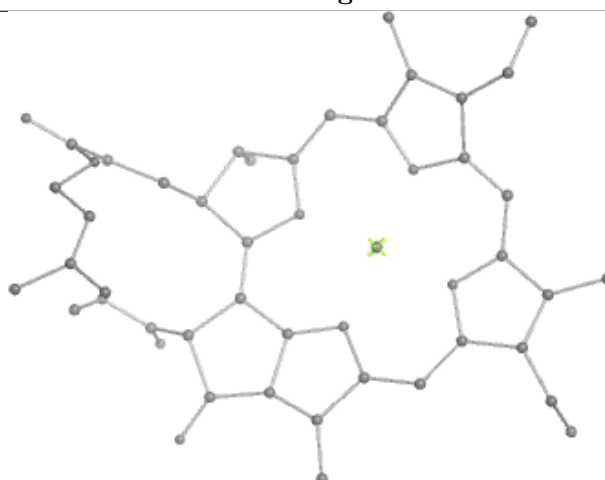
Bond lengths



Bond angles

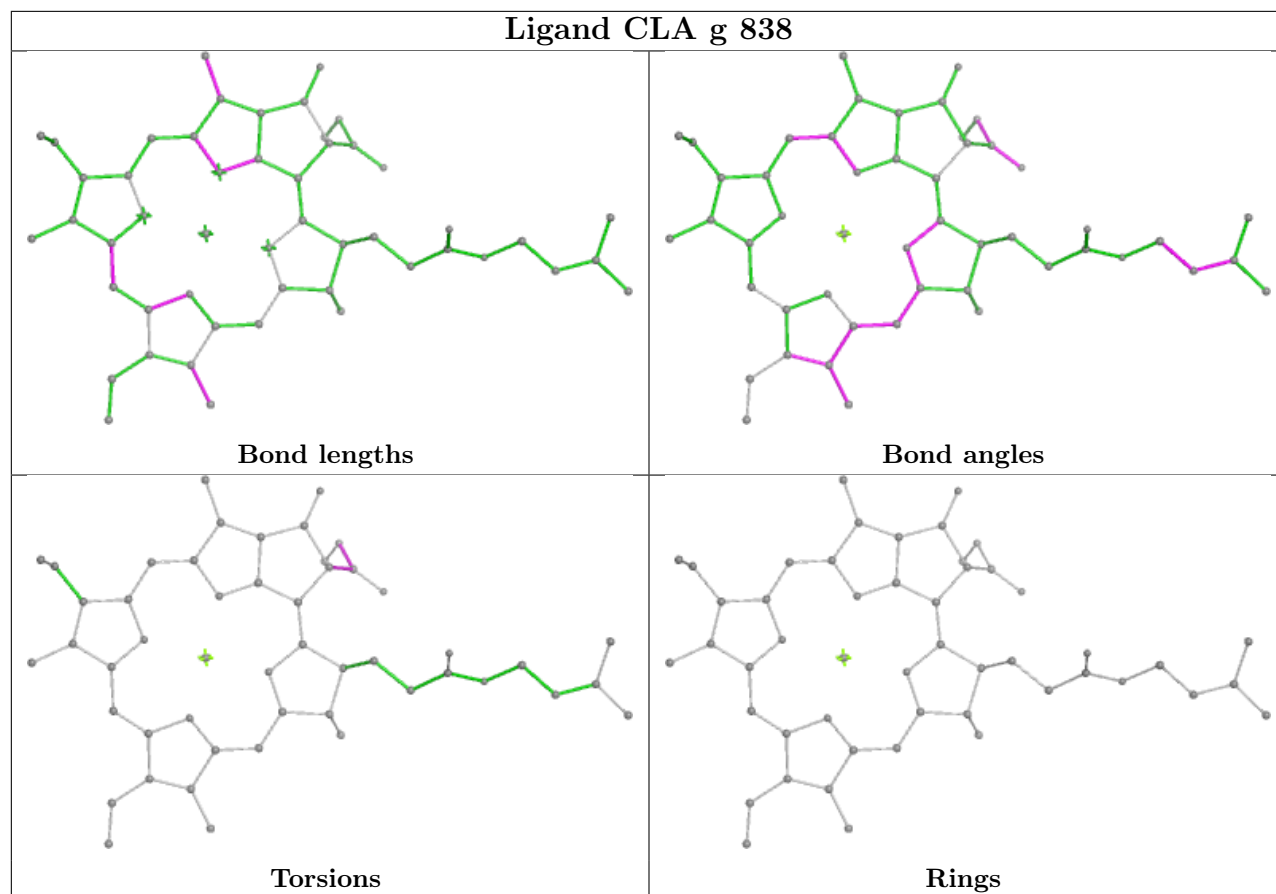


Torsions

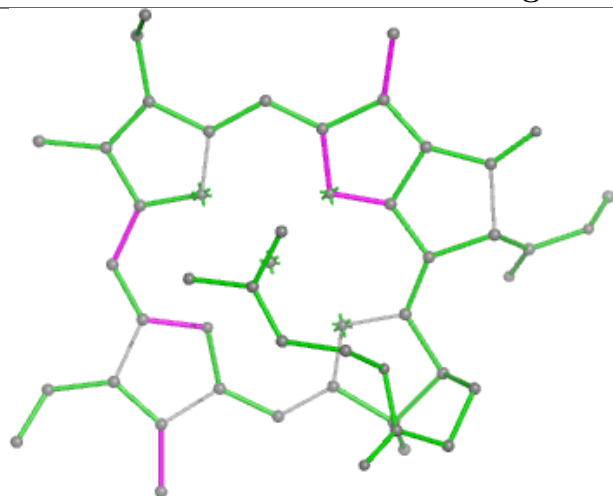


Rings

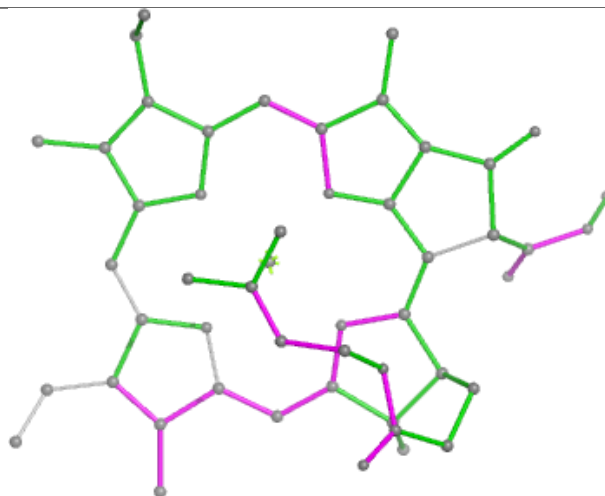
Ligand CLA g 838



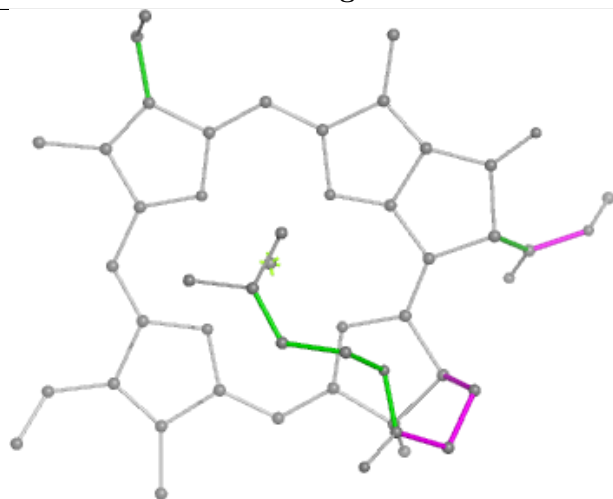
Ligand CLA 1 203



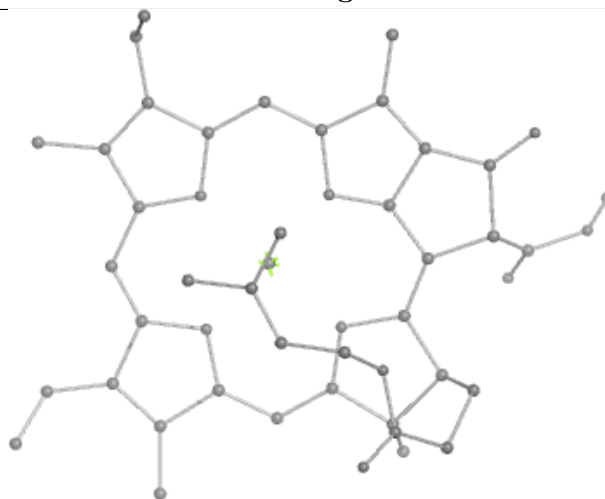
Bond lengths



Bond angles

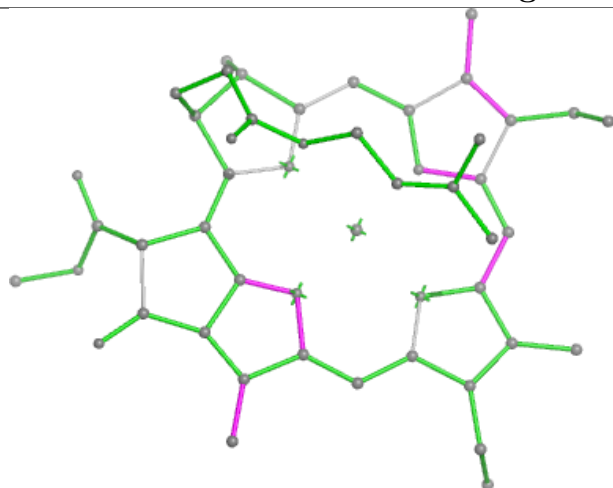


Torsions

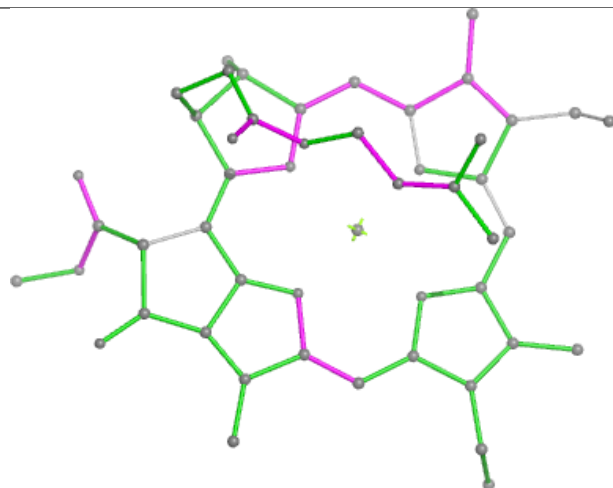


Rings

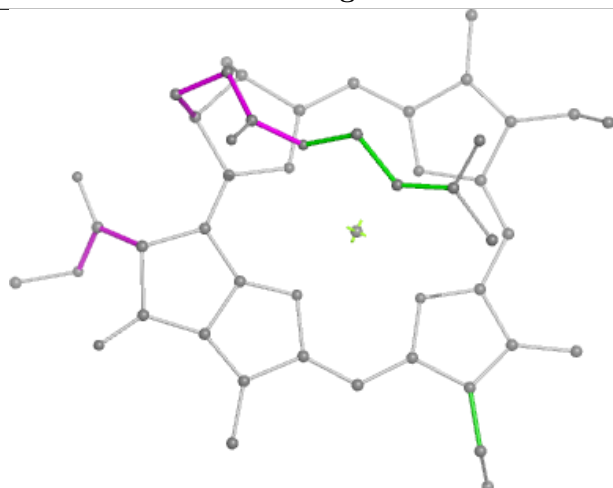
Ligand CLA e 825



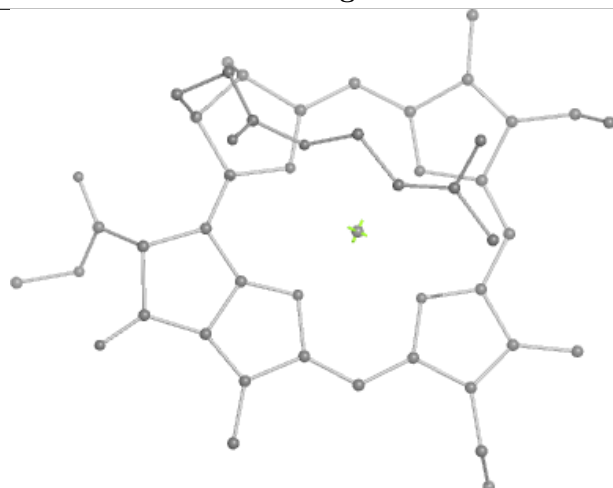
Bond lengths



Bond angles

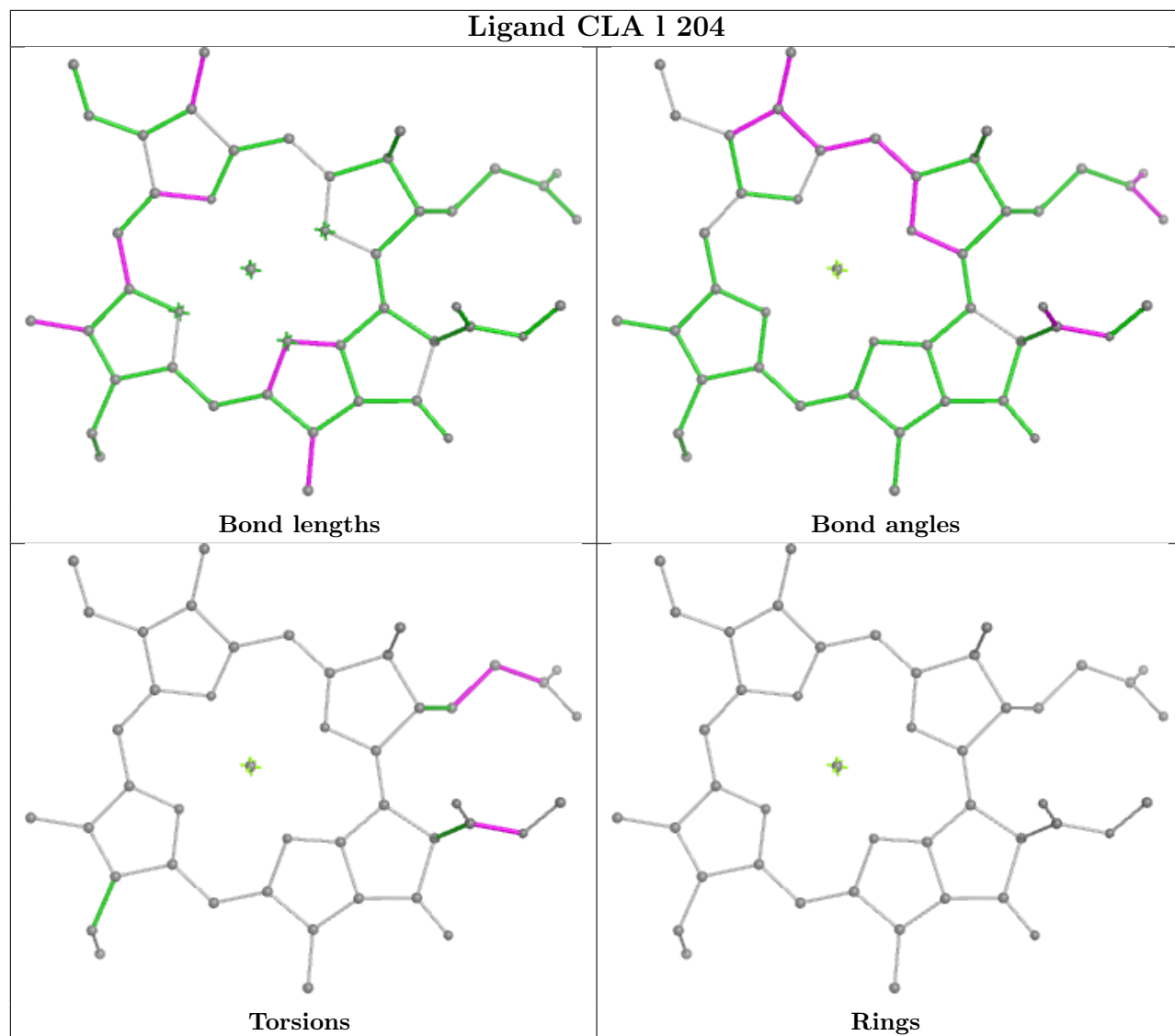


Torsions

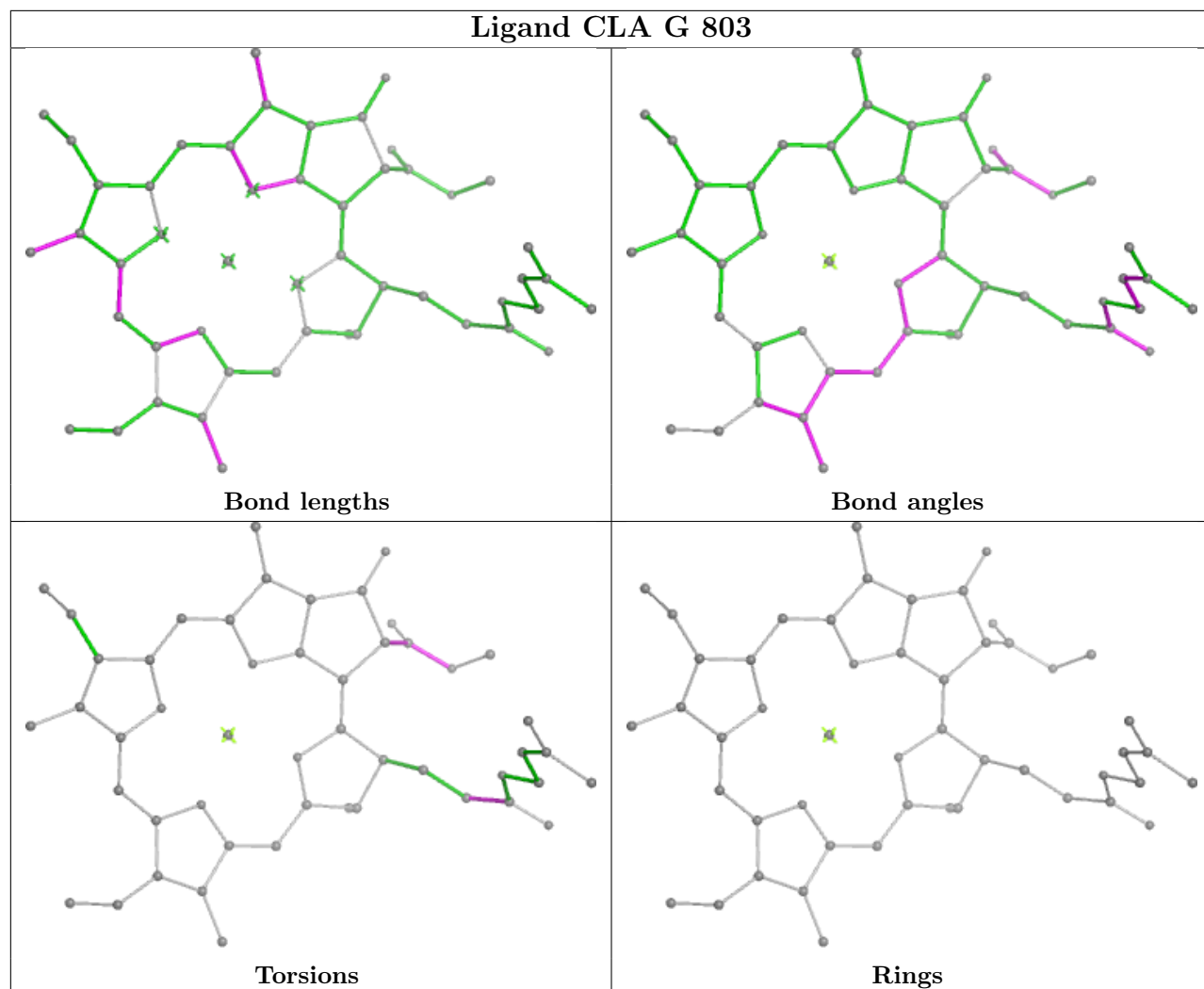


Rings

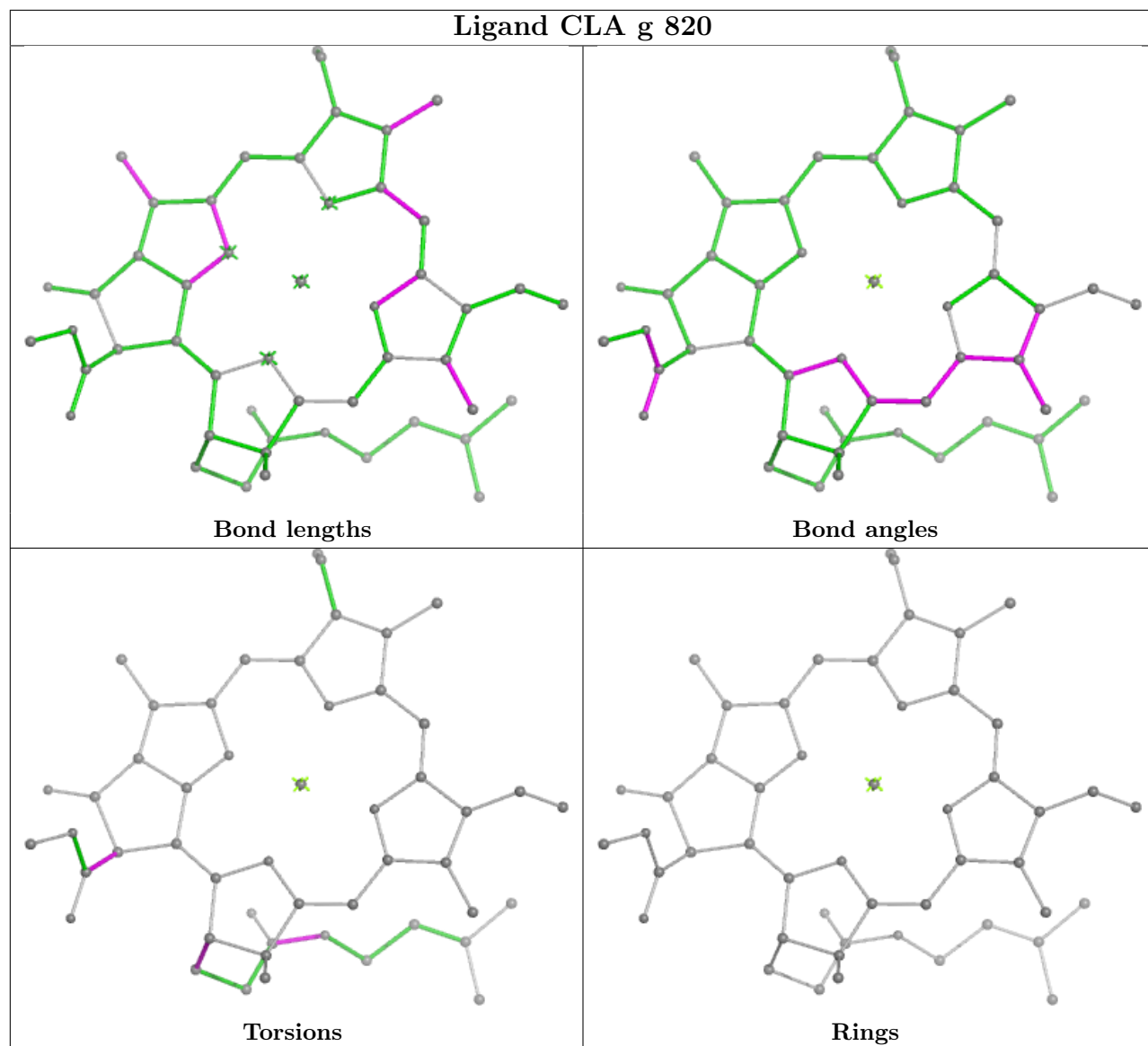
Ligand CLA 1 204

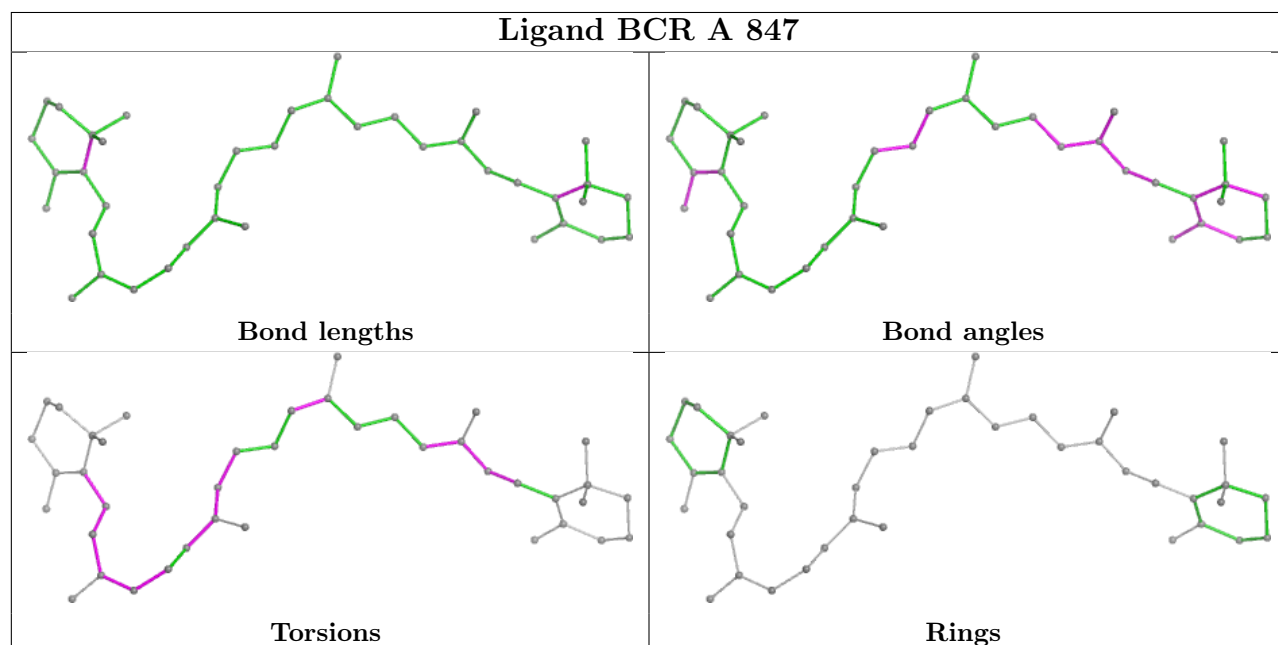
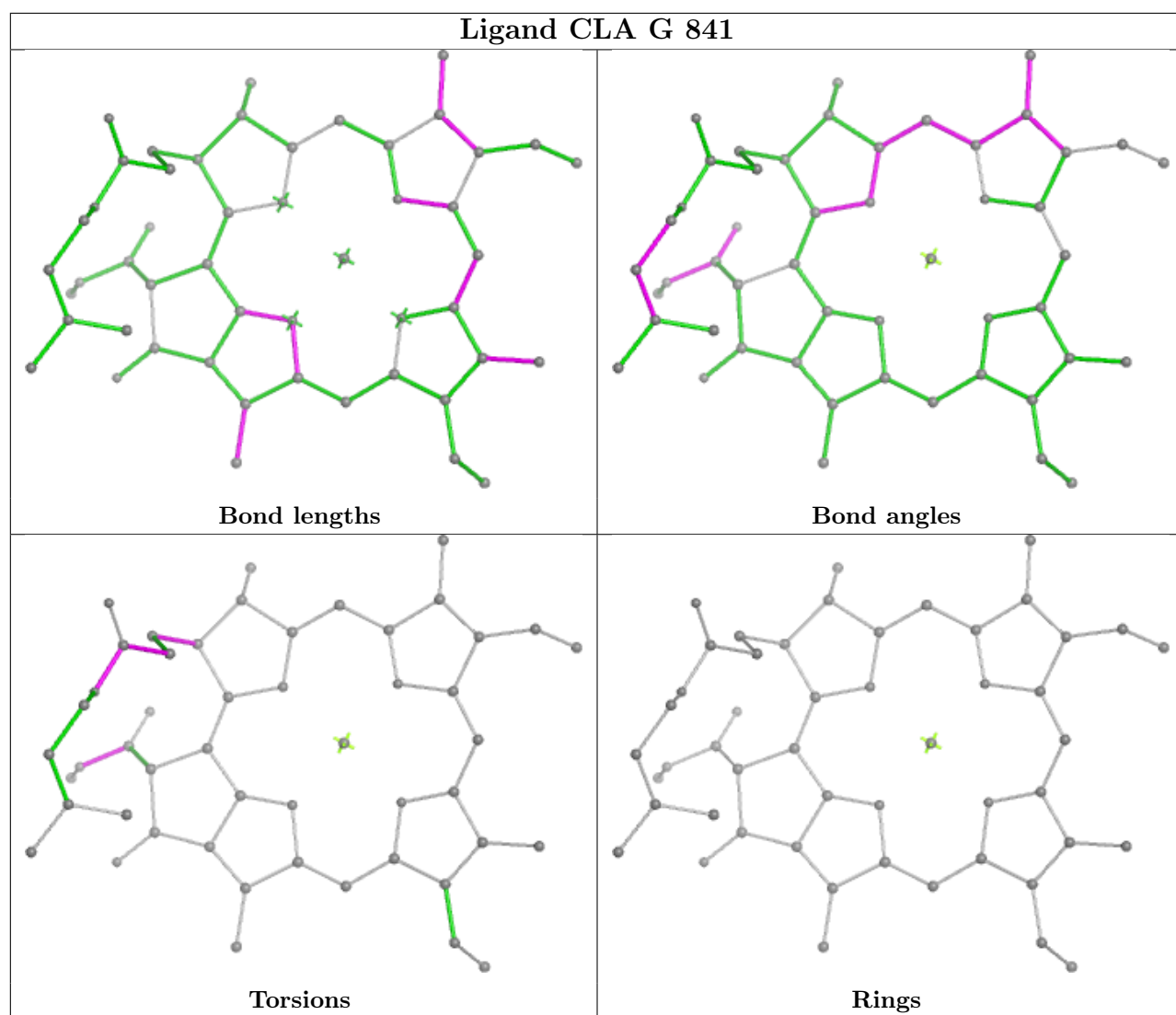


Ligand CLA G 803

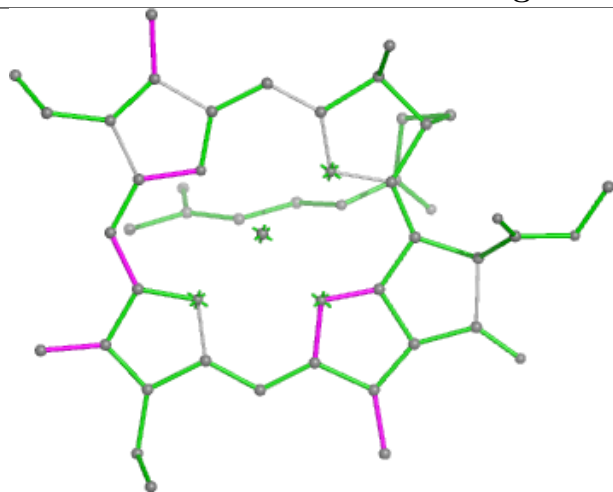


Ligand CLA g 820

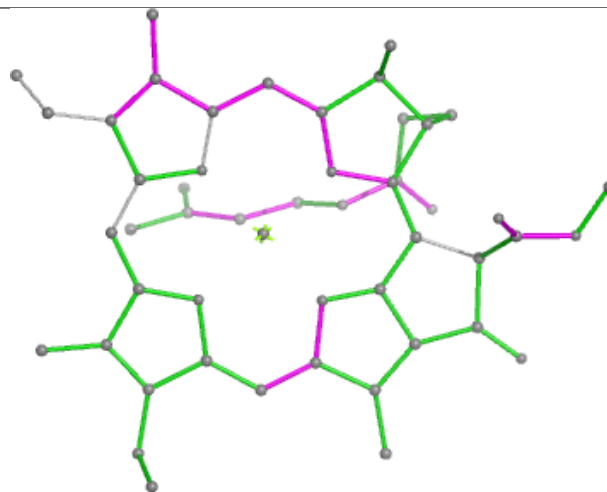




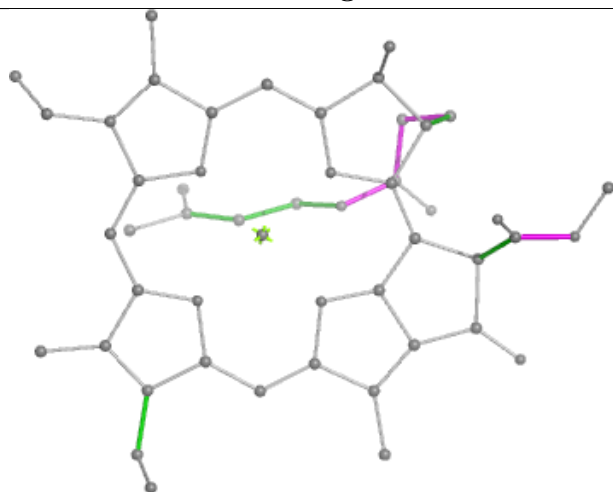
Ligand CLA G 838



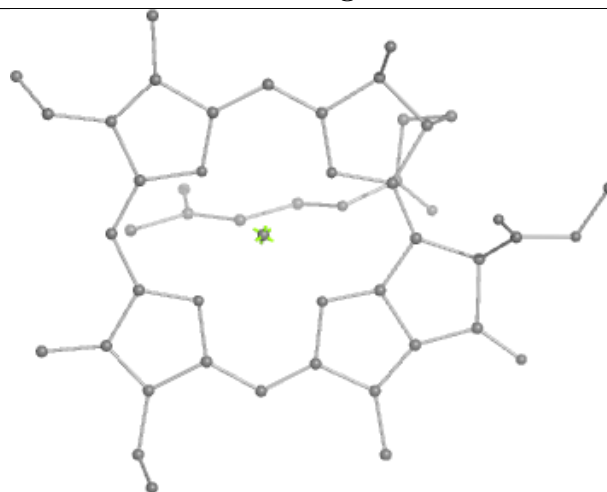
Bond lengths



Bond angles

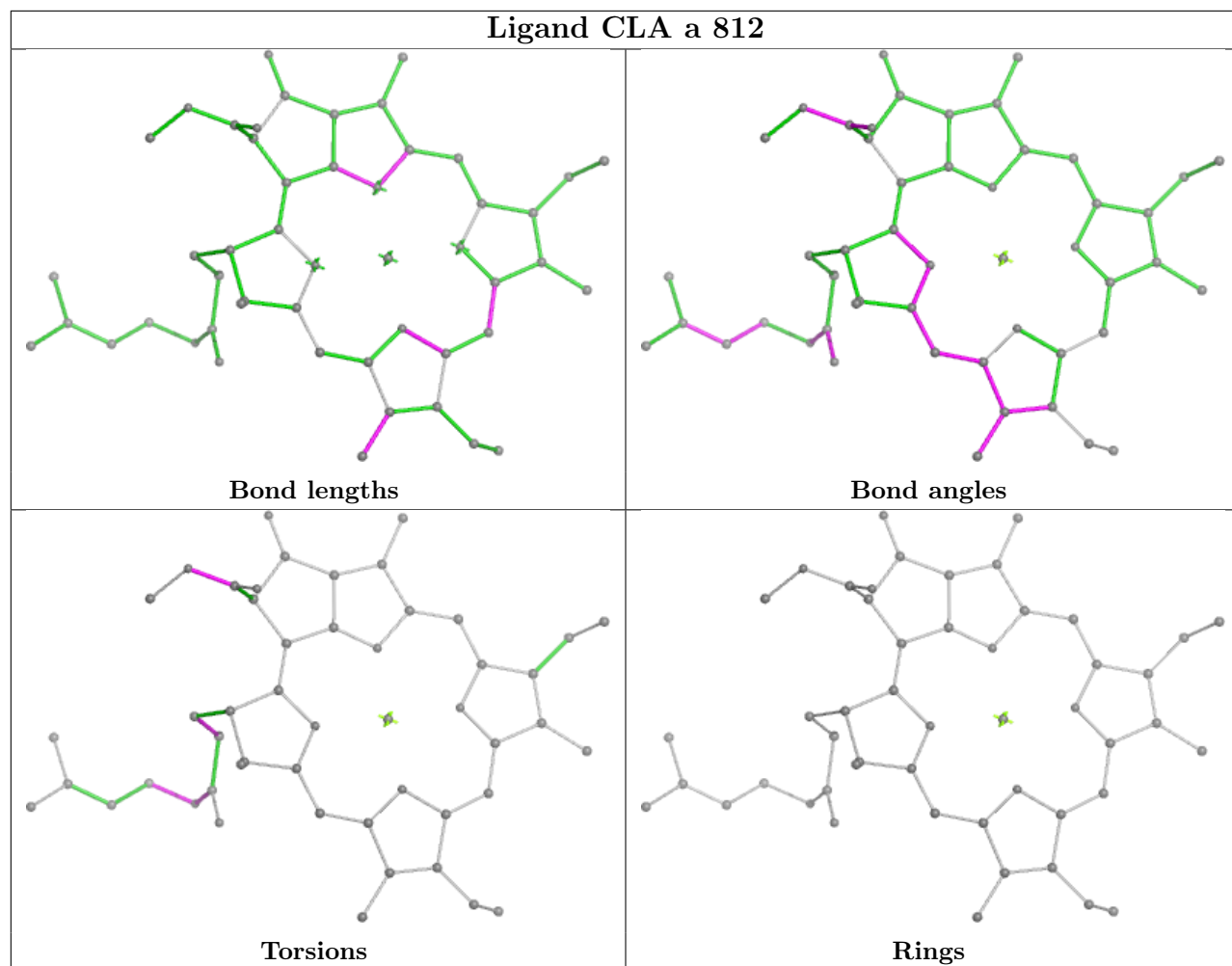


Torsions

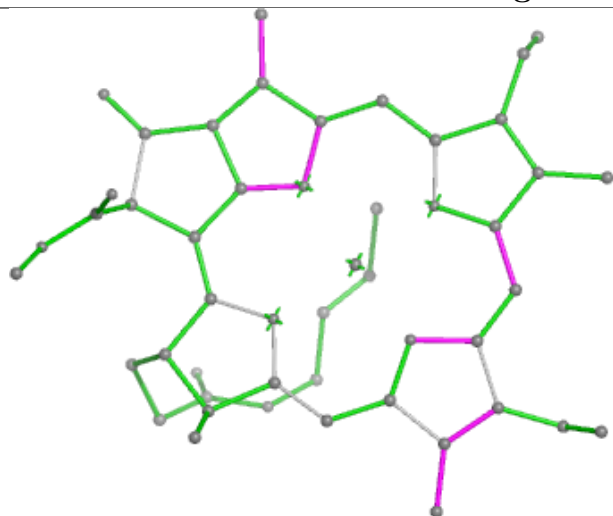


Rings

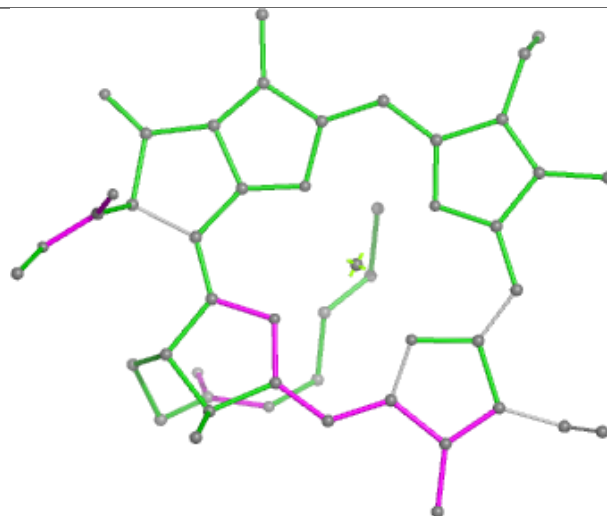
Ligand CLA a 812



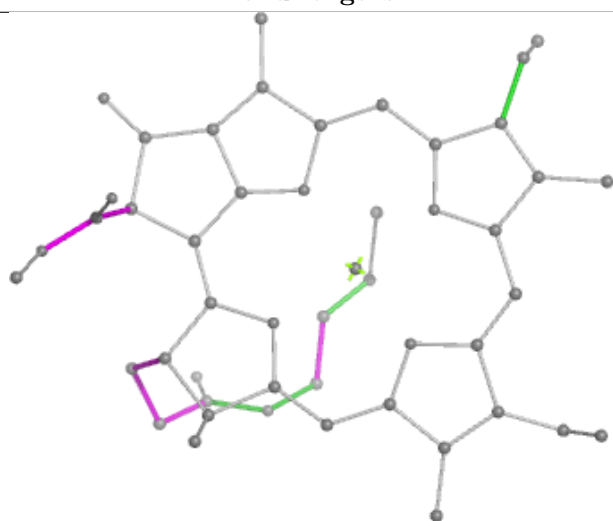
Ligand CLA A 819



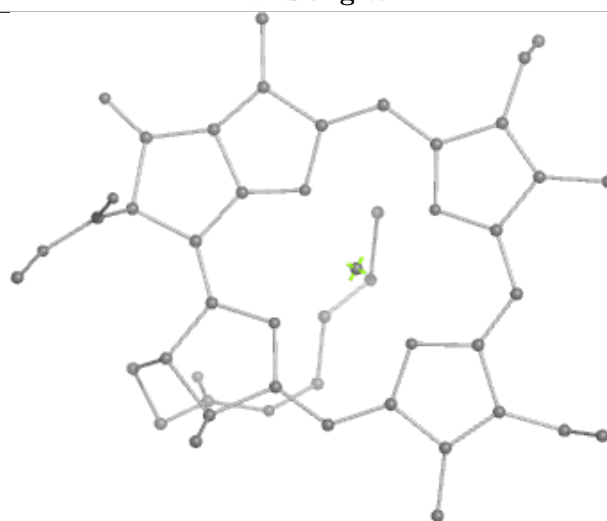
Bond lengths



Bond angles

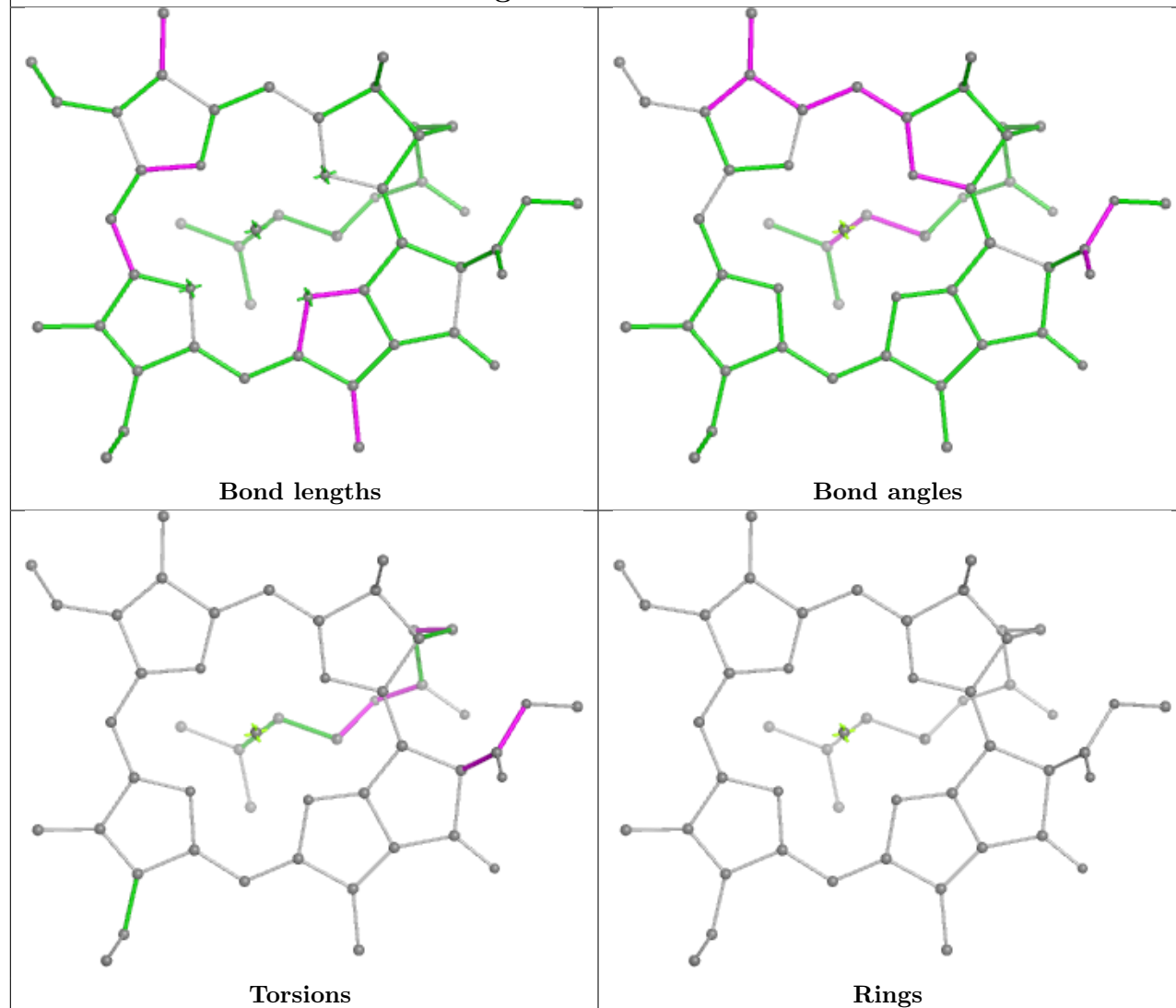


Torsions

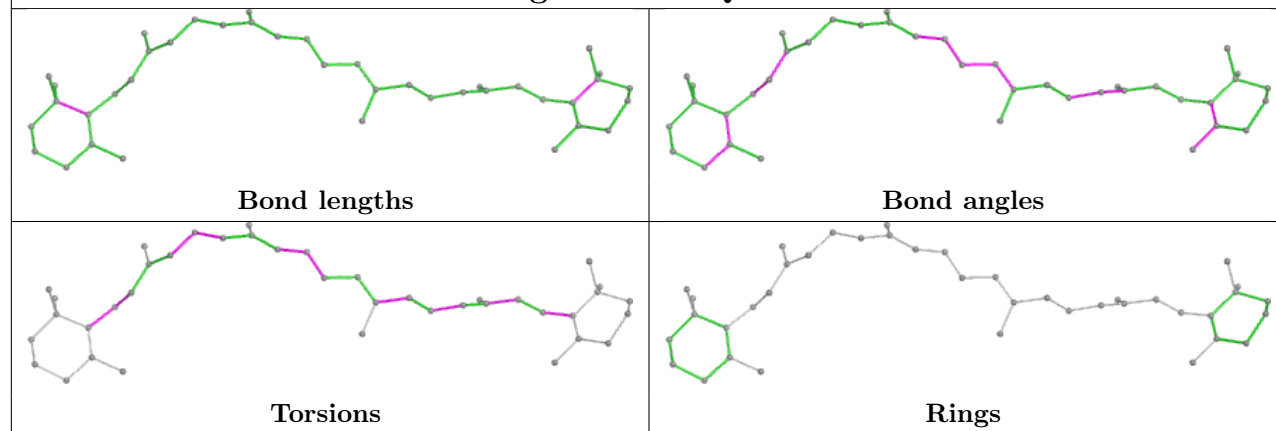


Rings

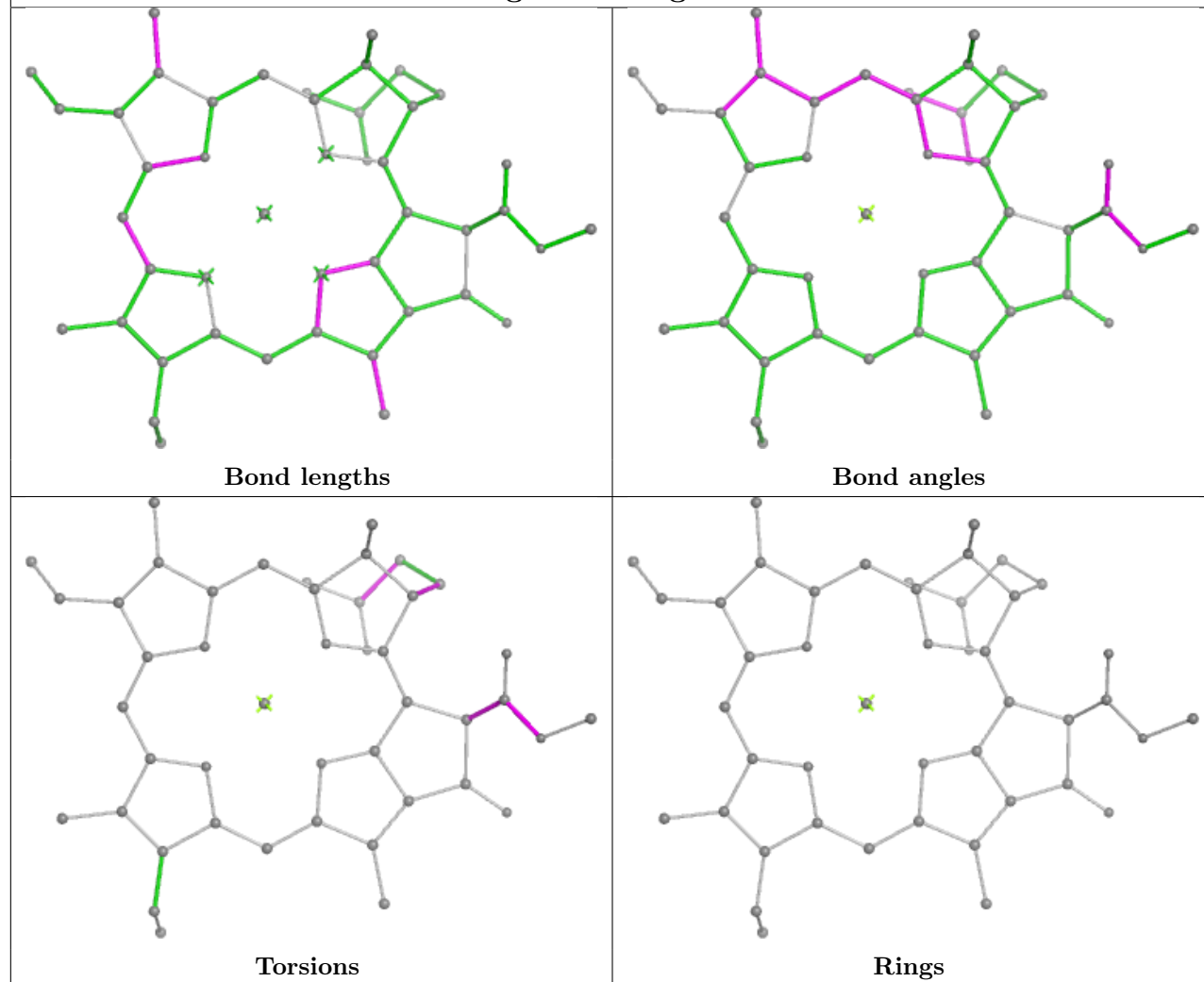
Ligand CLA e 814

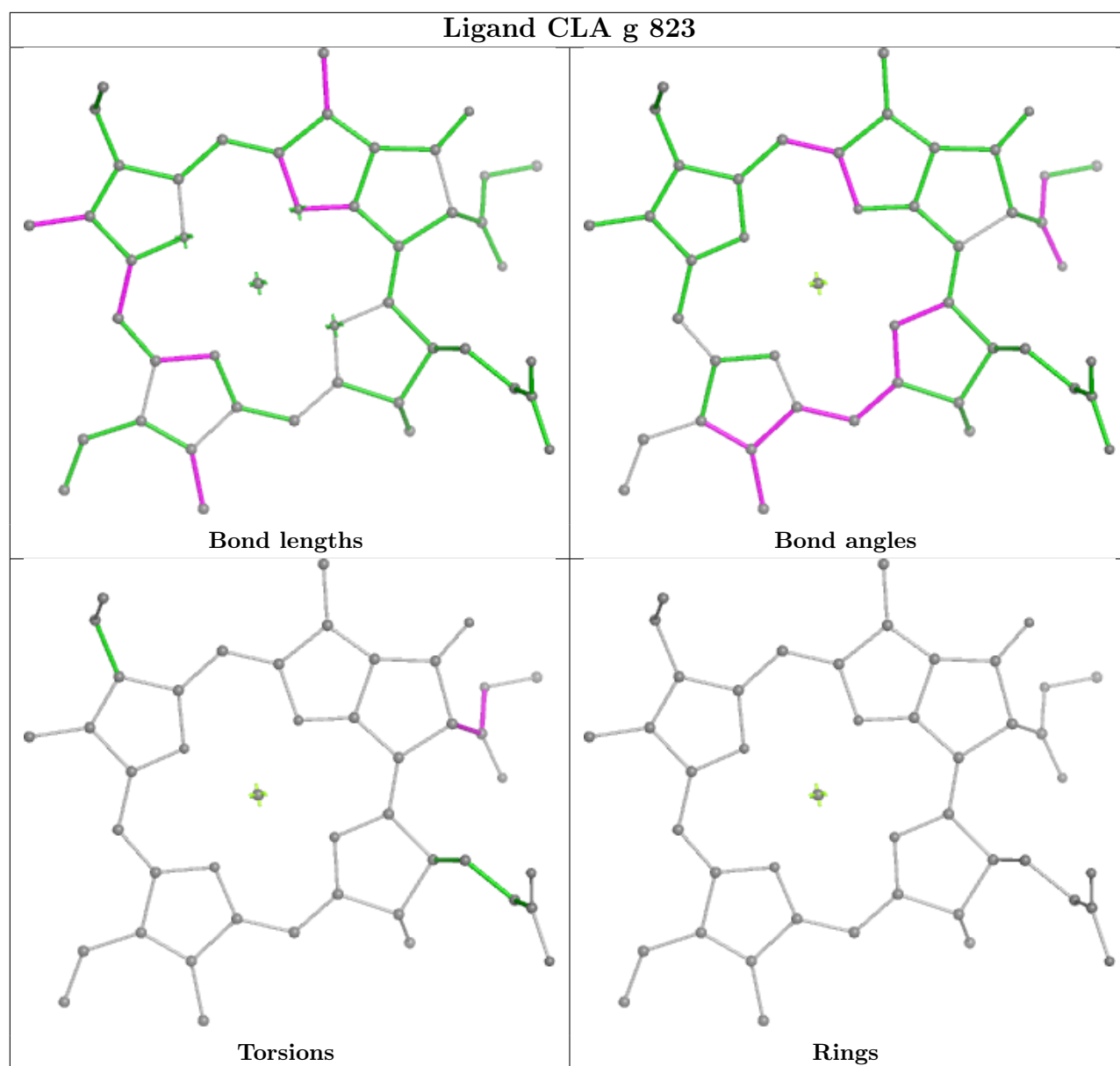


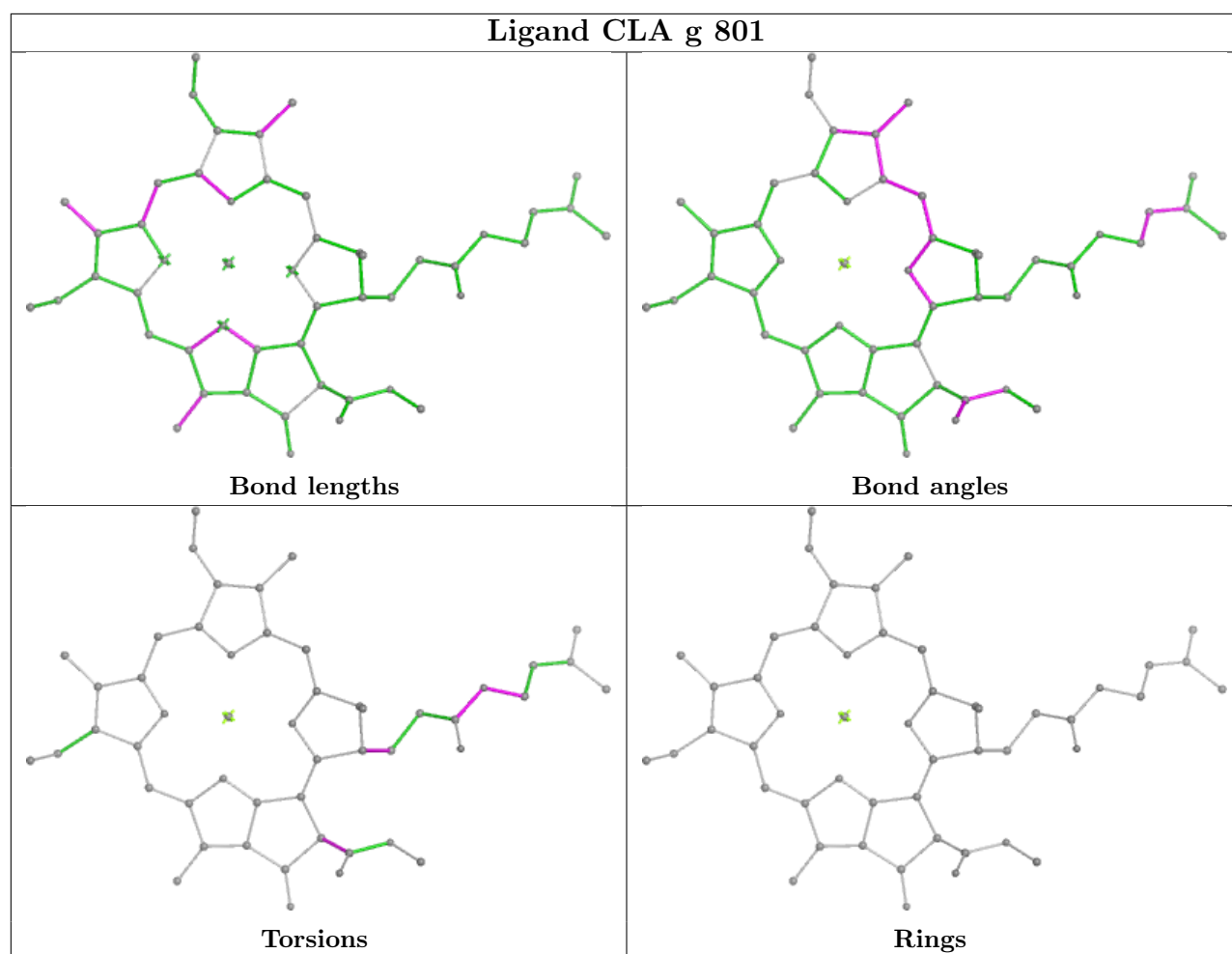
Ligand BCR Q 101



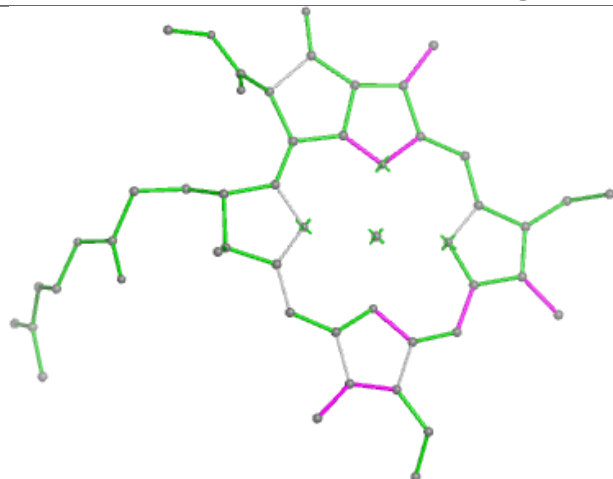
Ligand CLA g 837



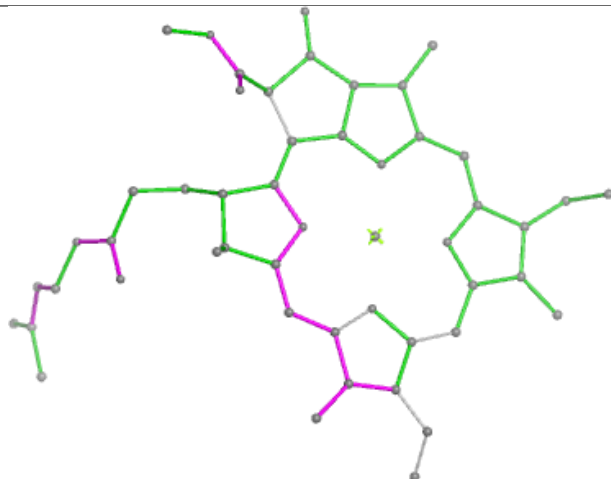




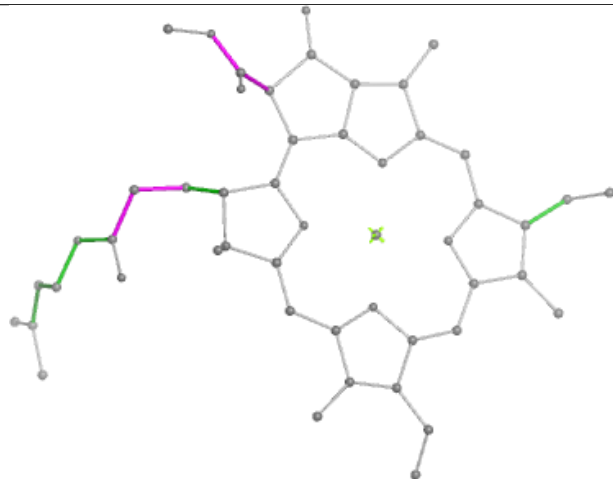
Ligand CLA B 811



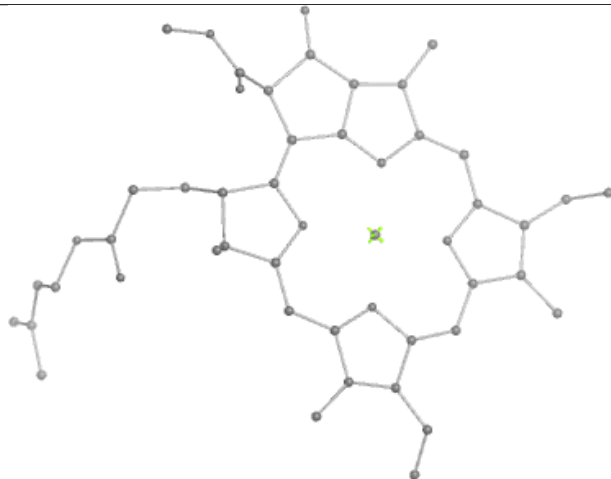
Bond lengths



Bond angles

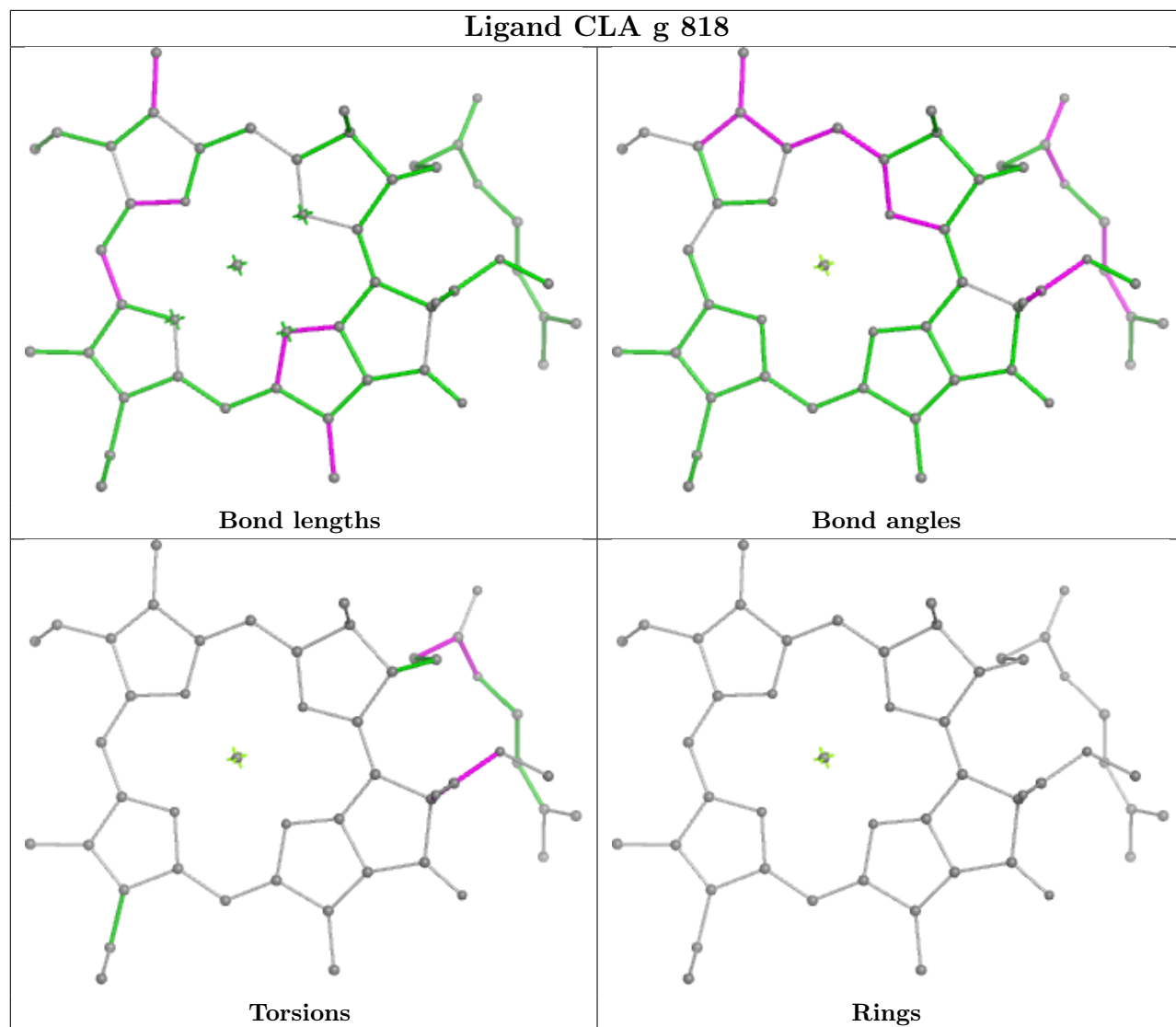


Torsions

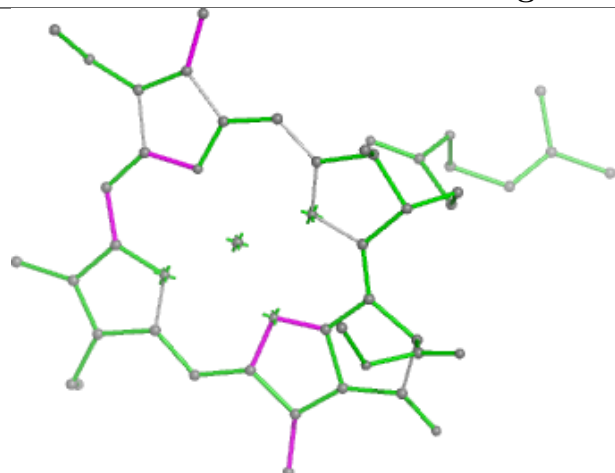


Rings

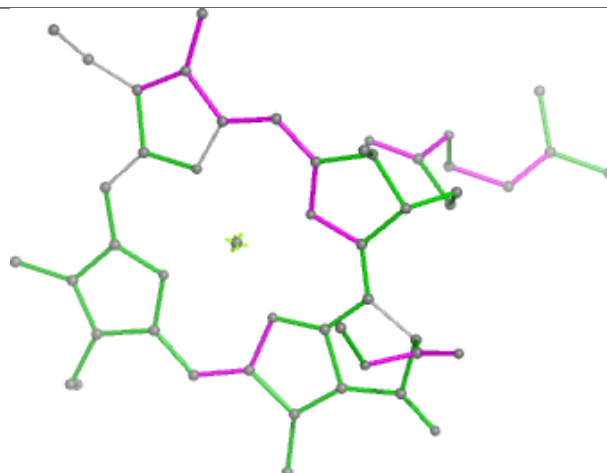
Ligand CLA g 818



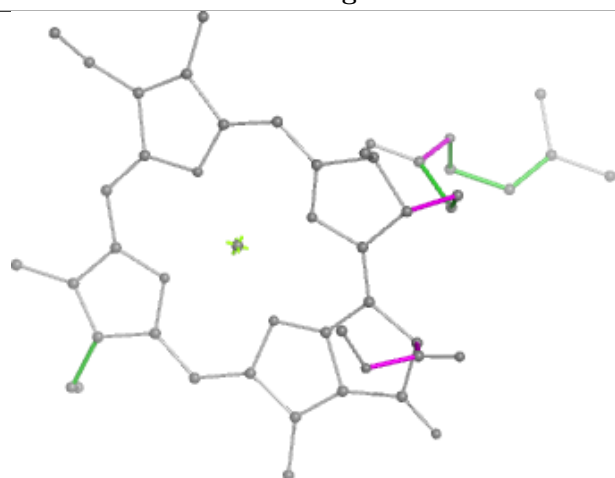
Ligand CLA E 838



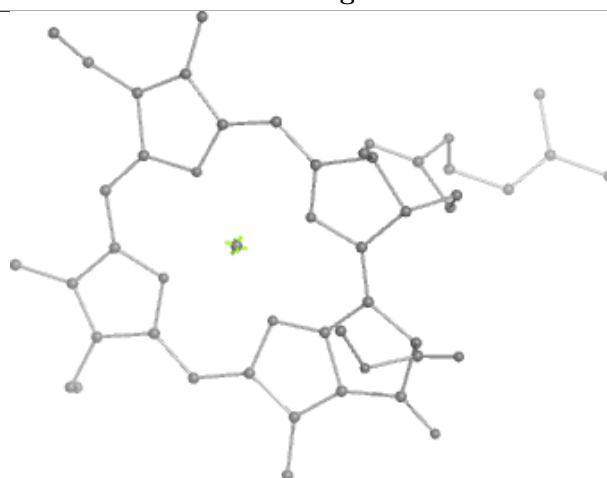
Bond lengths



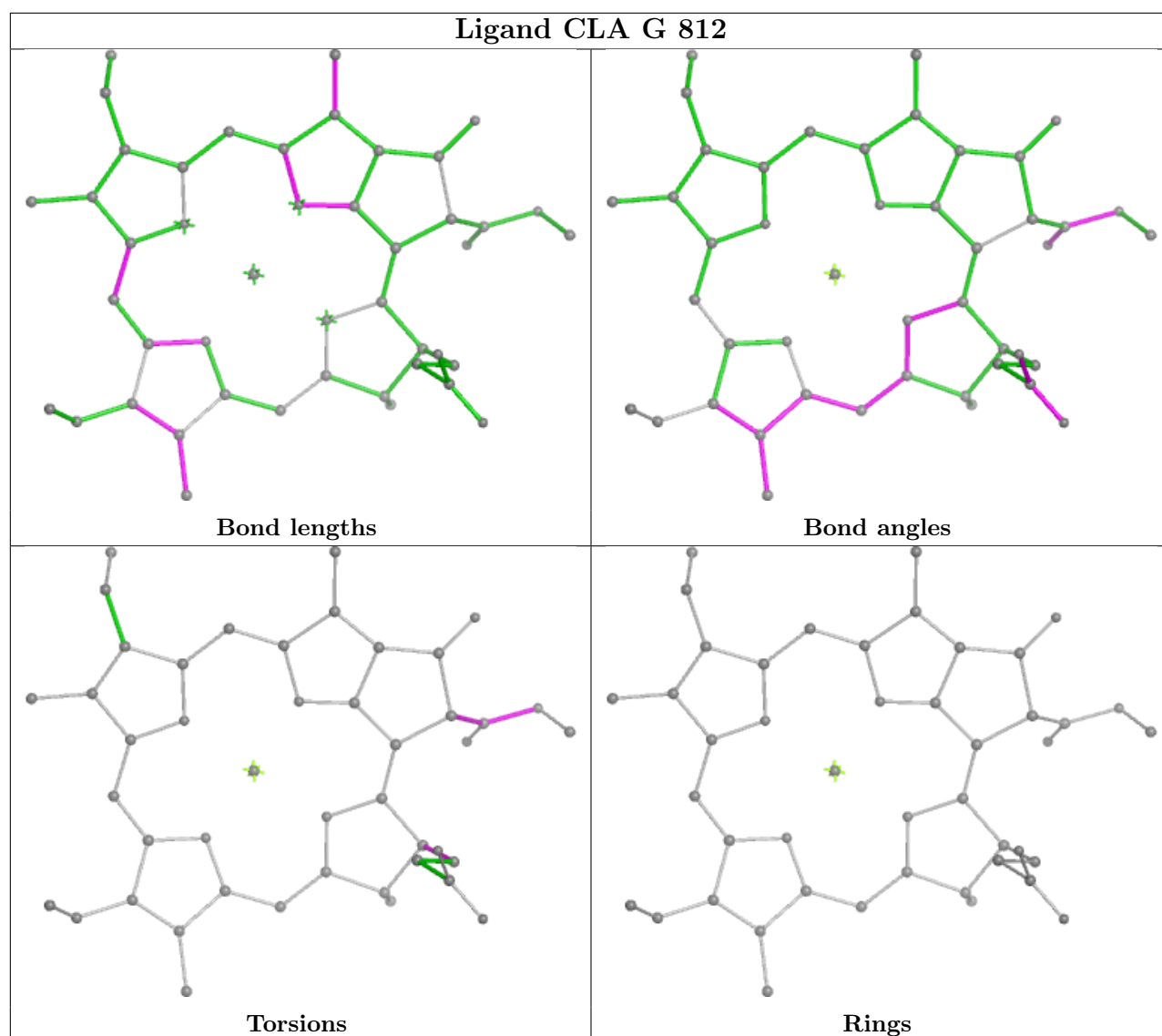
Bond angles



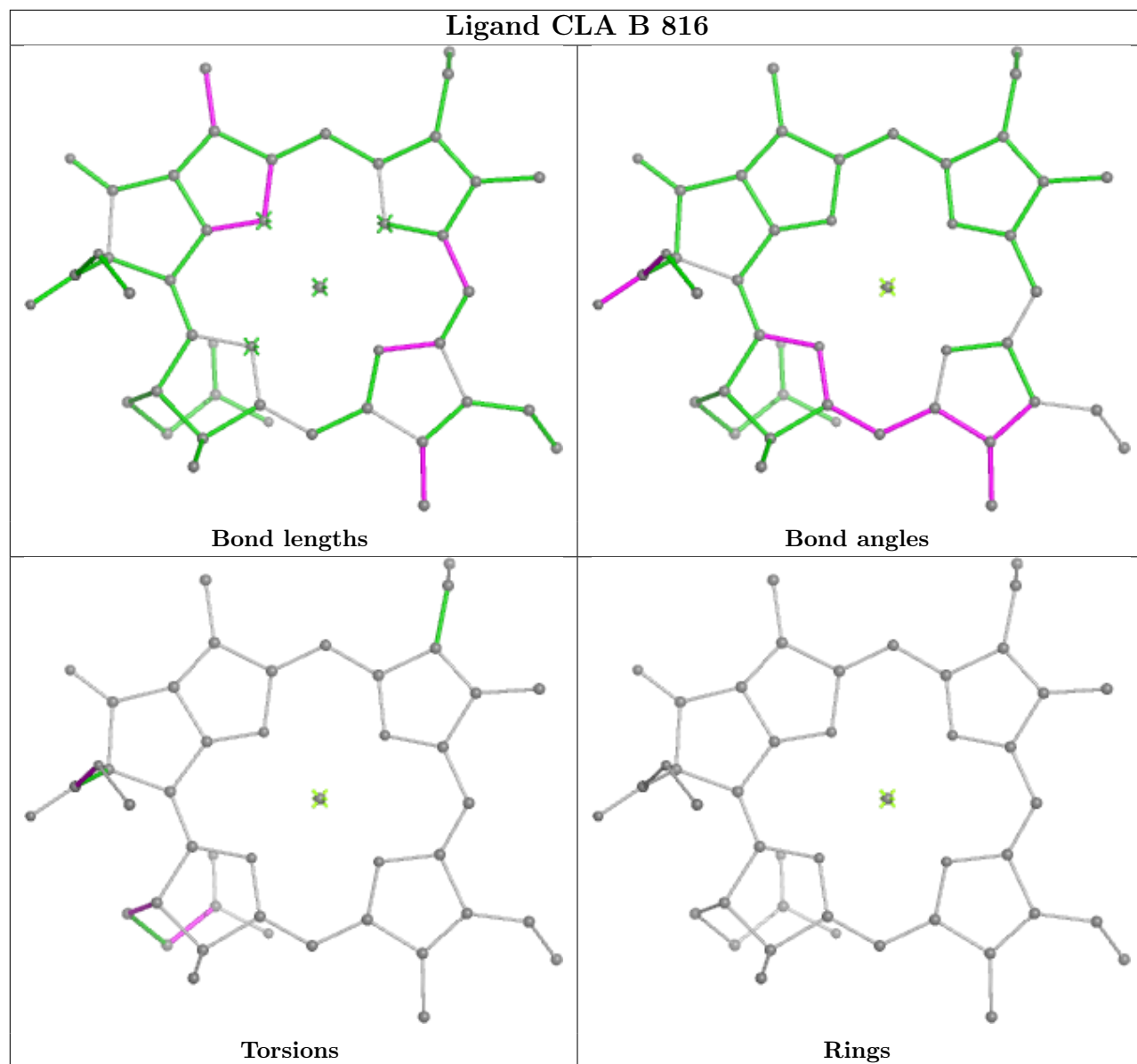
Torsions



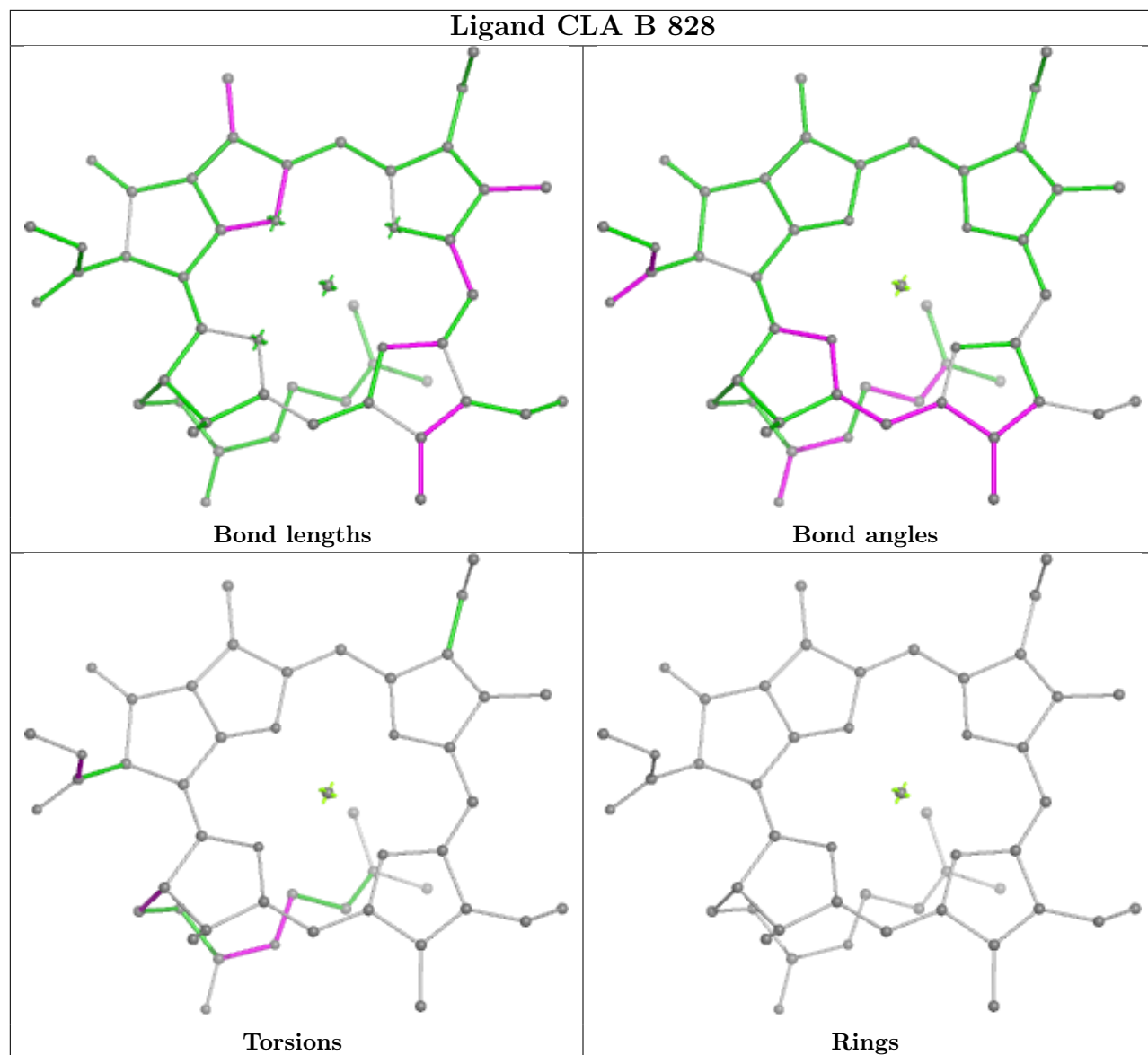
Rings



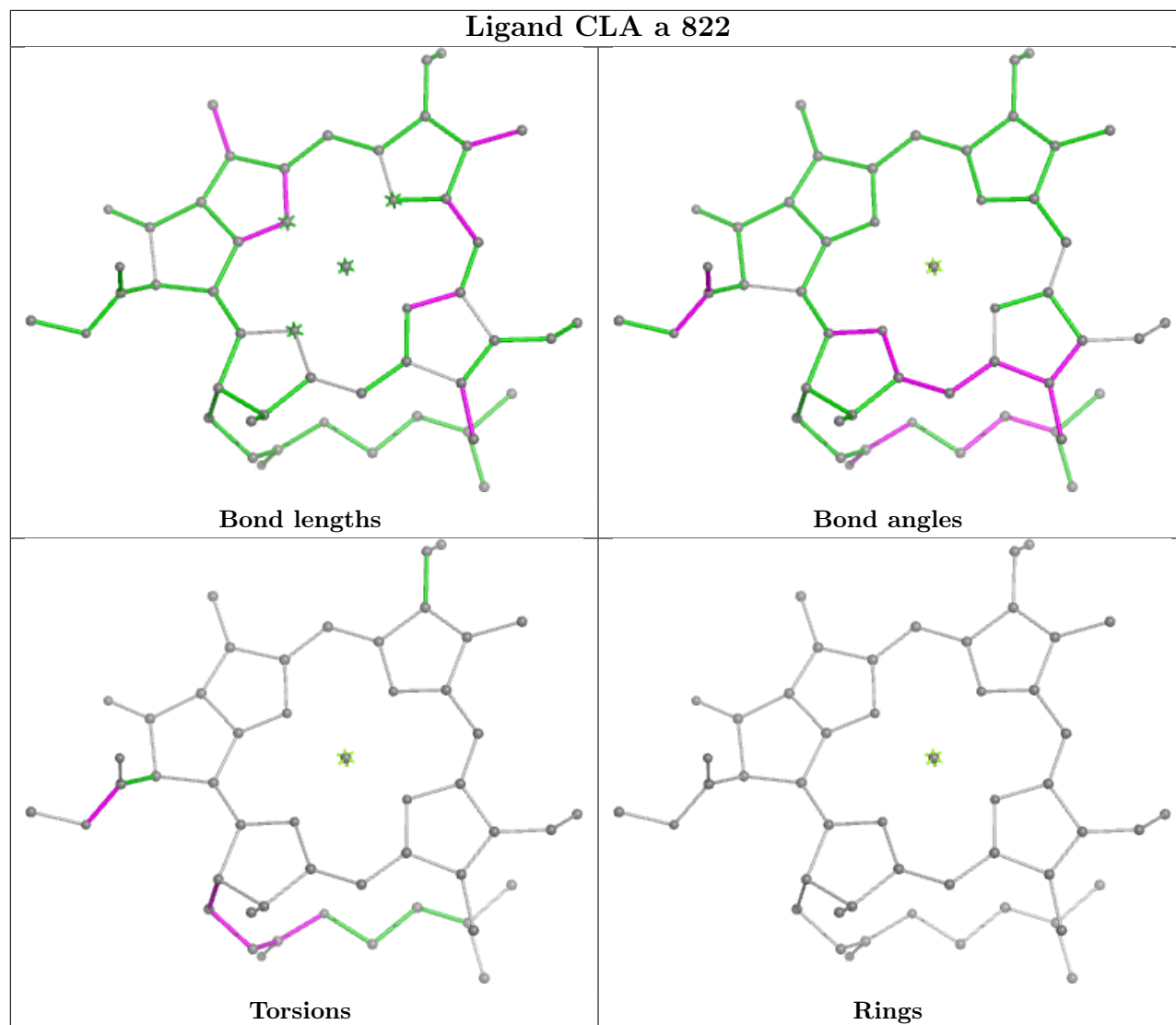
Ligand CLA B 816



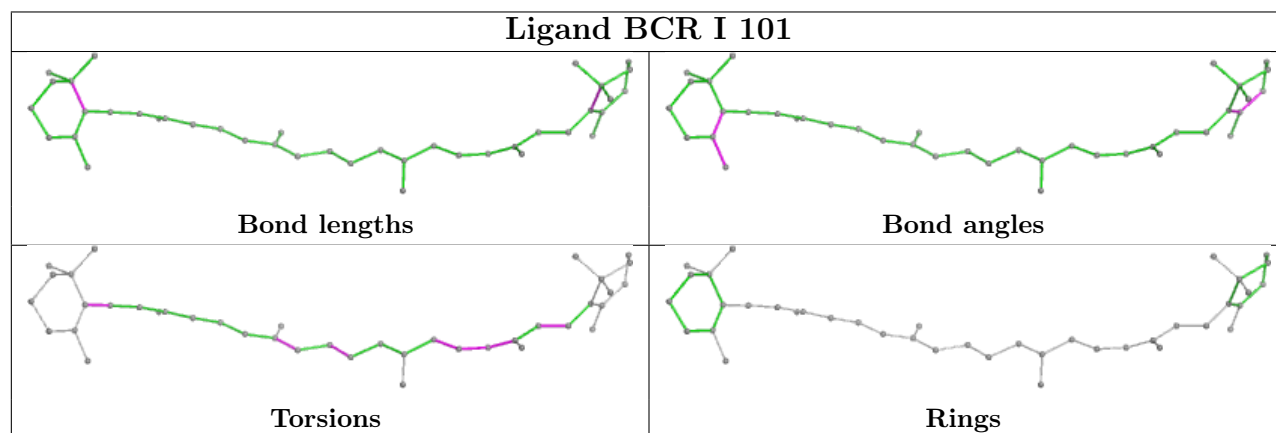
Ligand CLA B 828



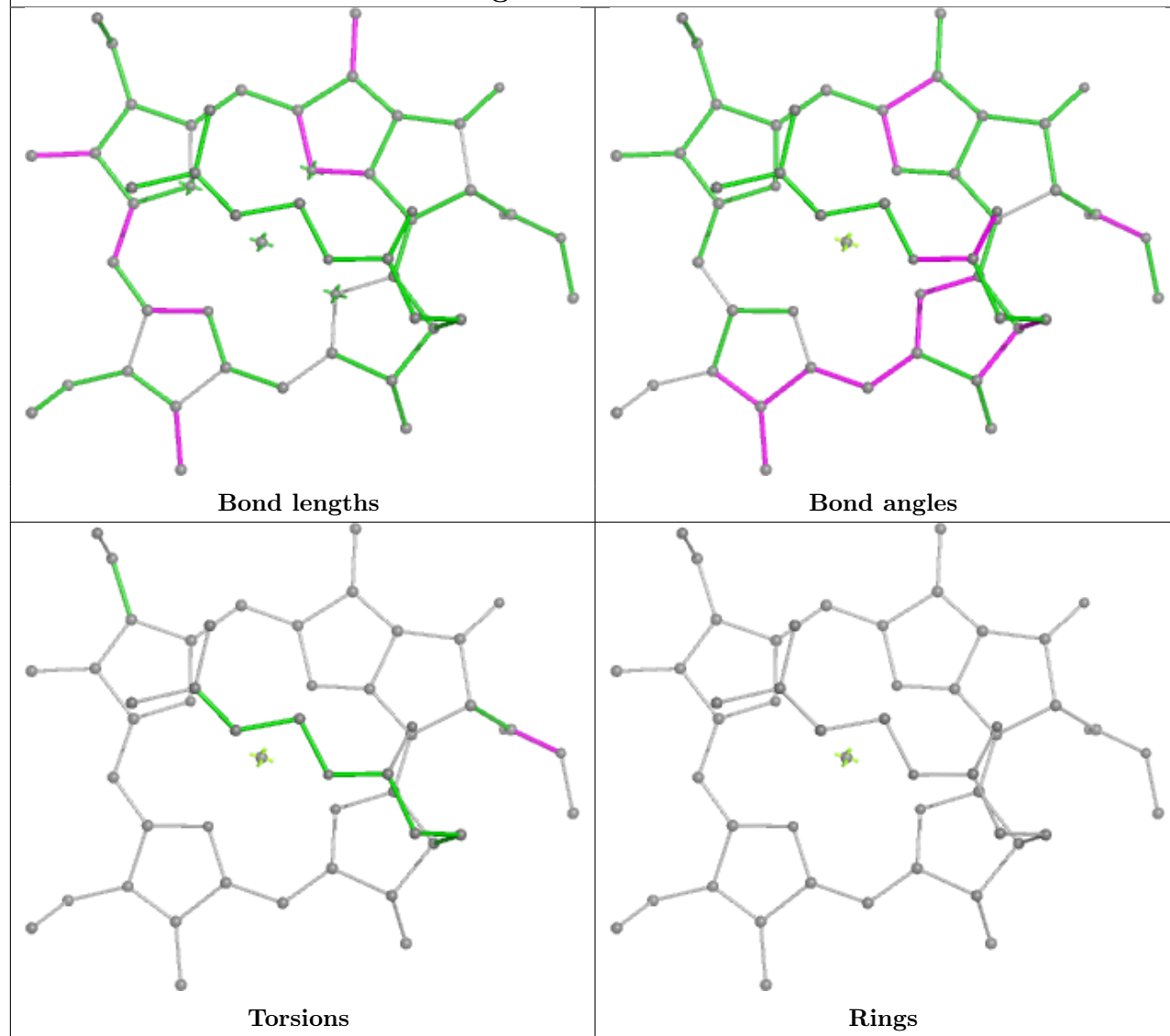
Ligand CLA a 822



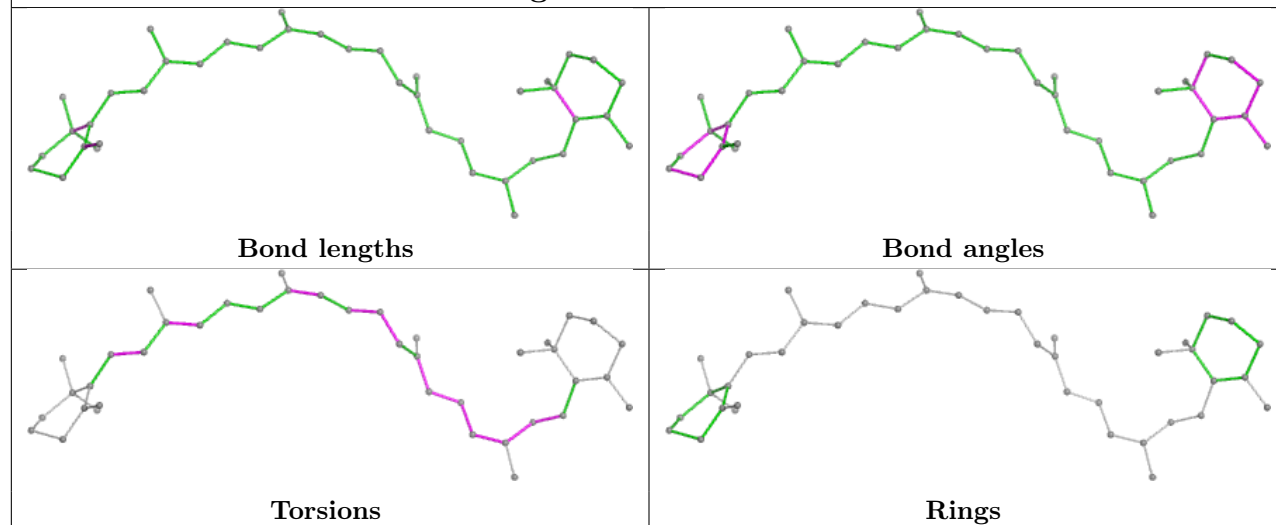
Ligand BCR I 101



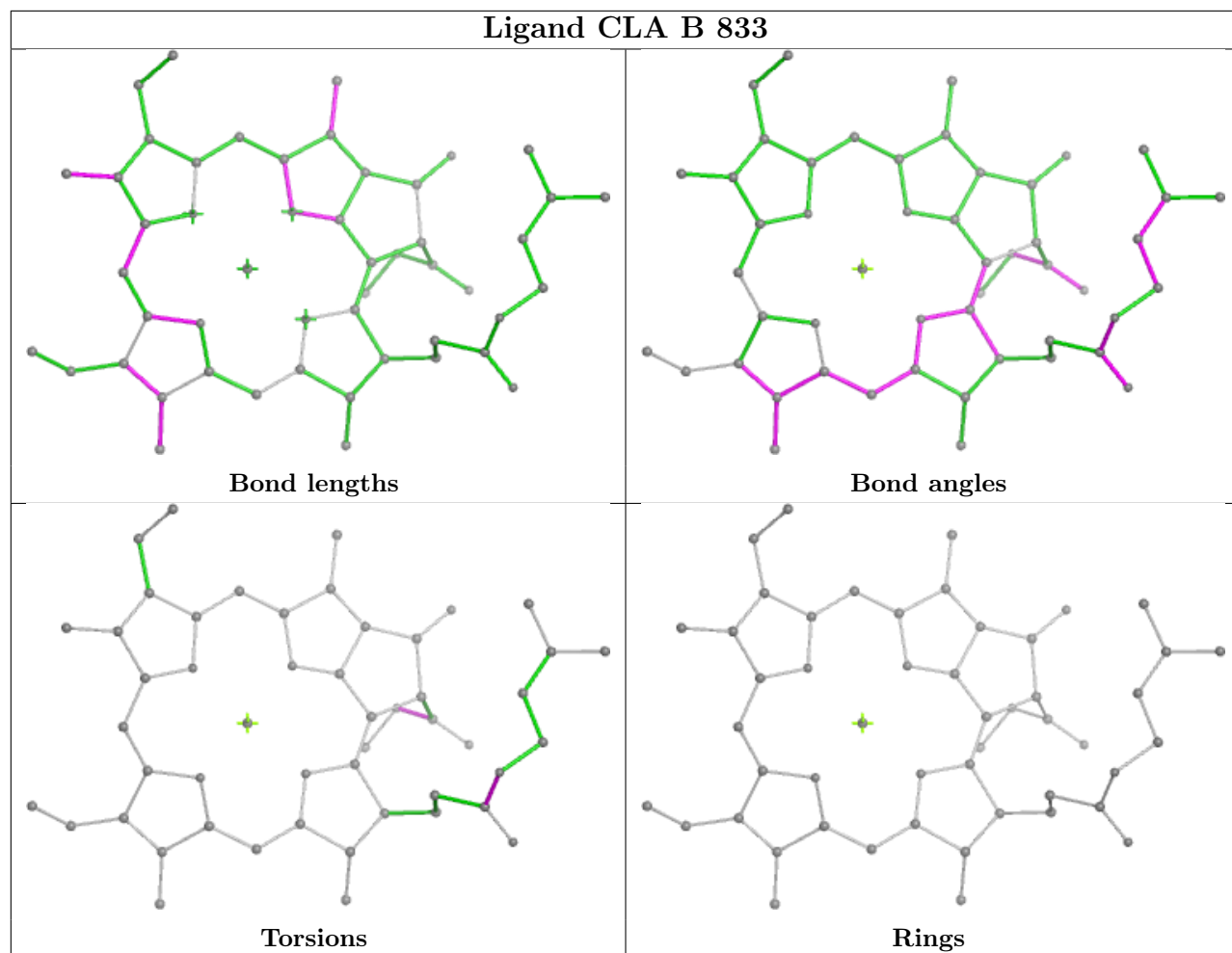
Ligand CLA e 819



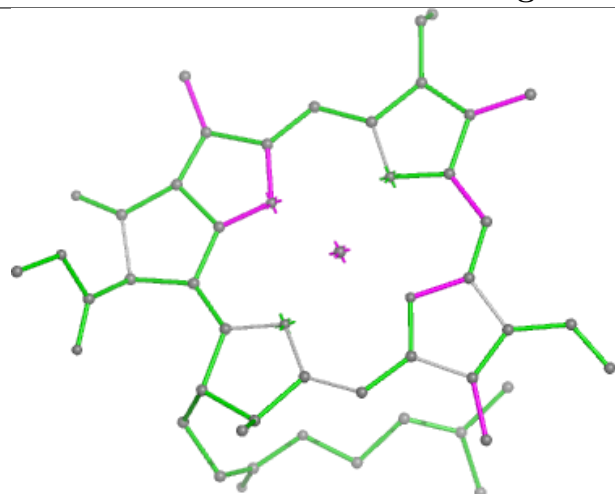
Ligand BCR R 101



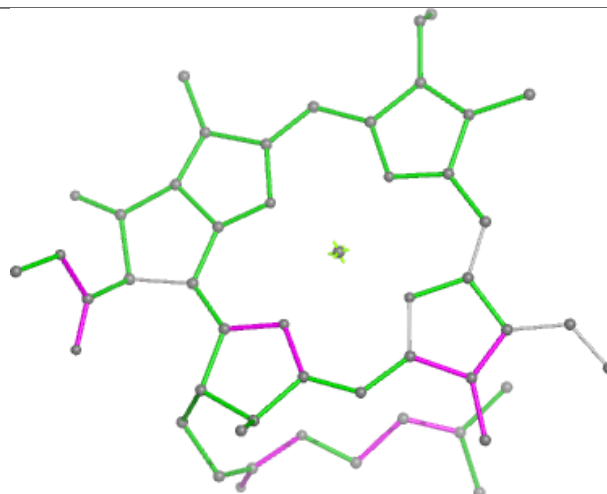
Ligand CLA B 833



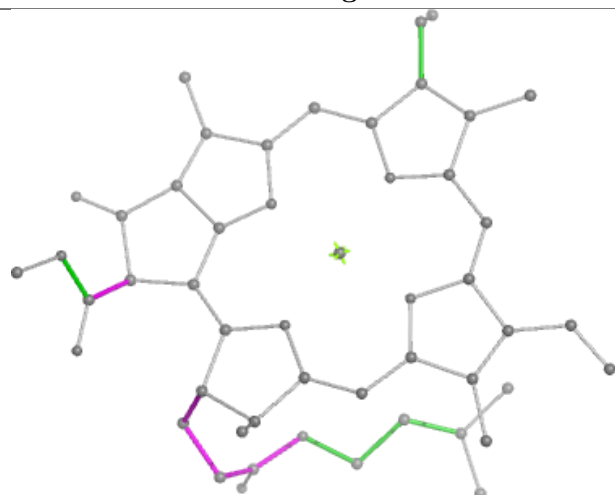
Ligand CLA E 823



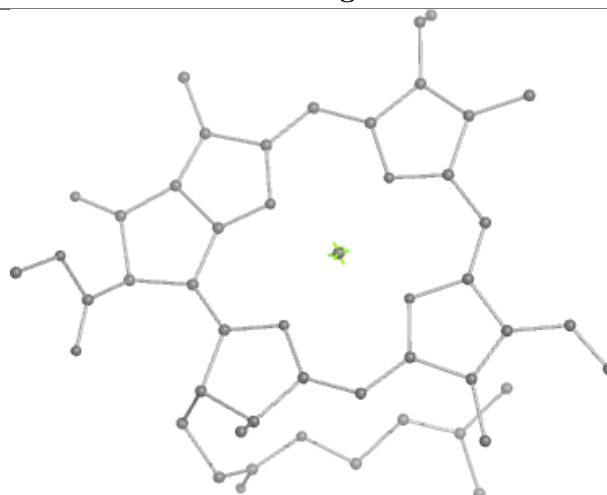
Bond lengths



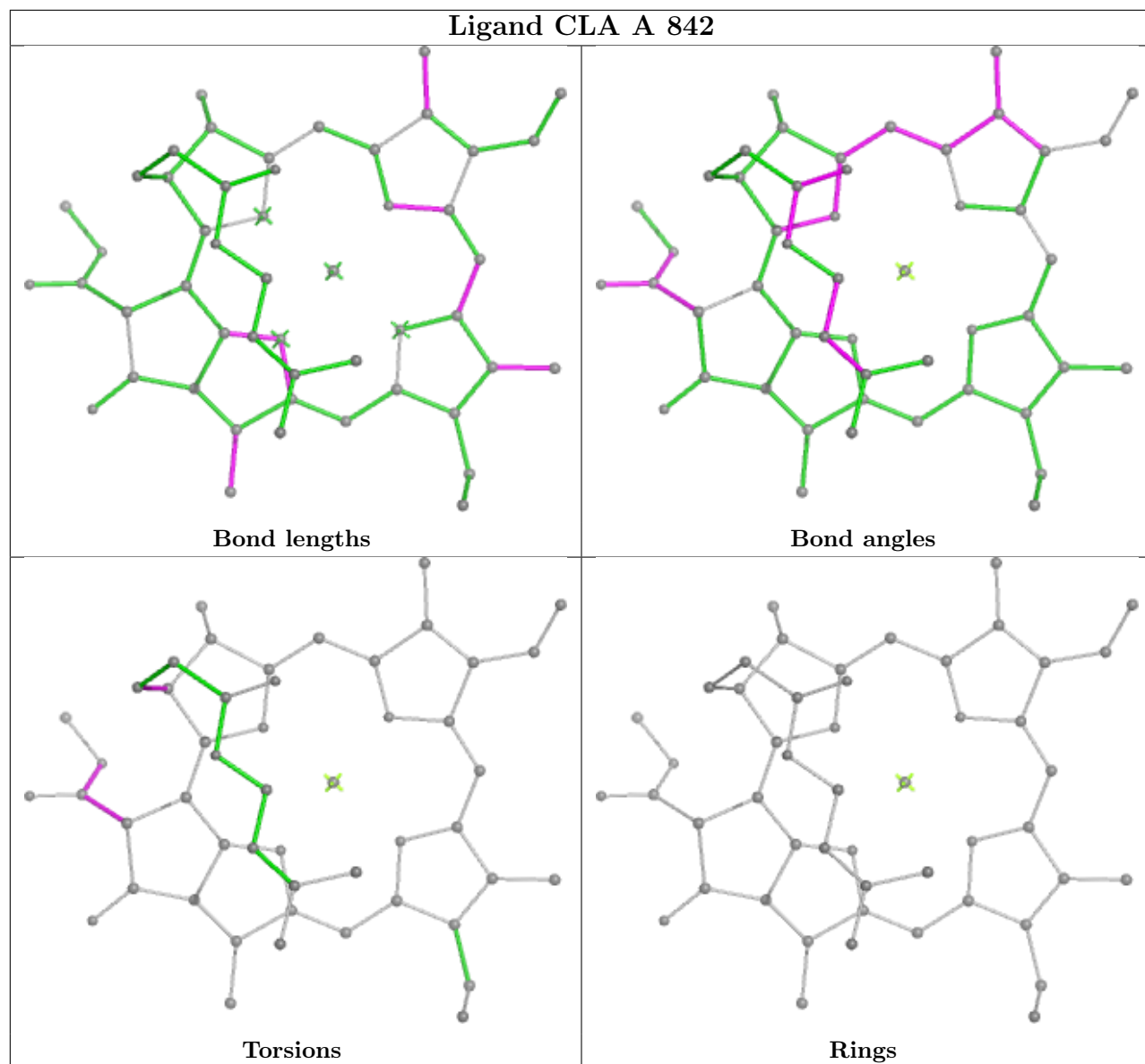
Bond angles



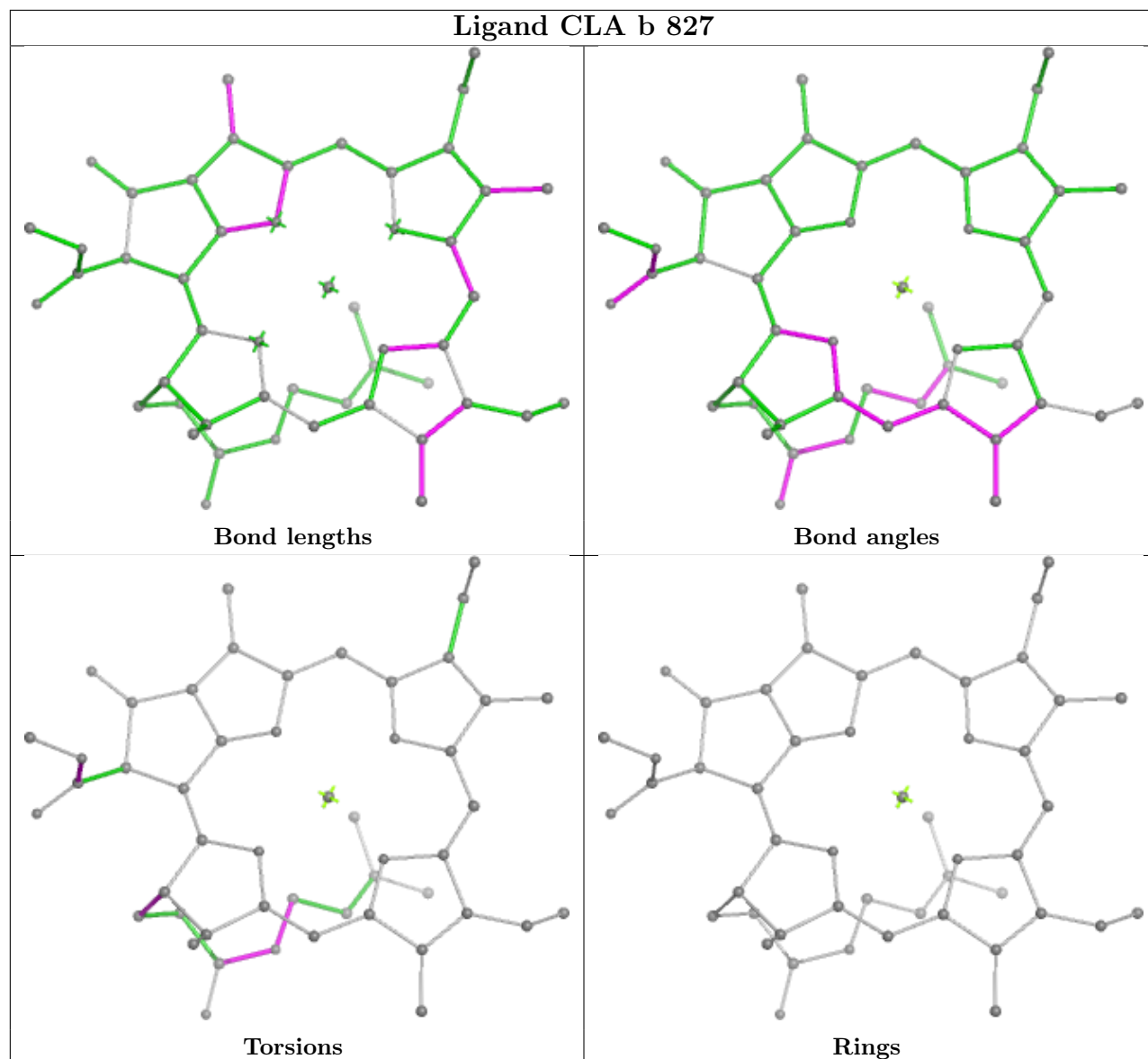
Torsions



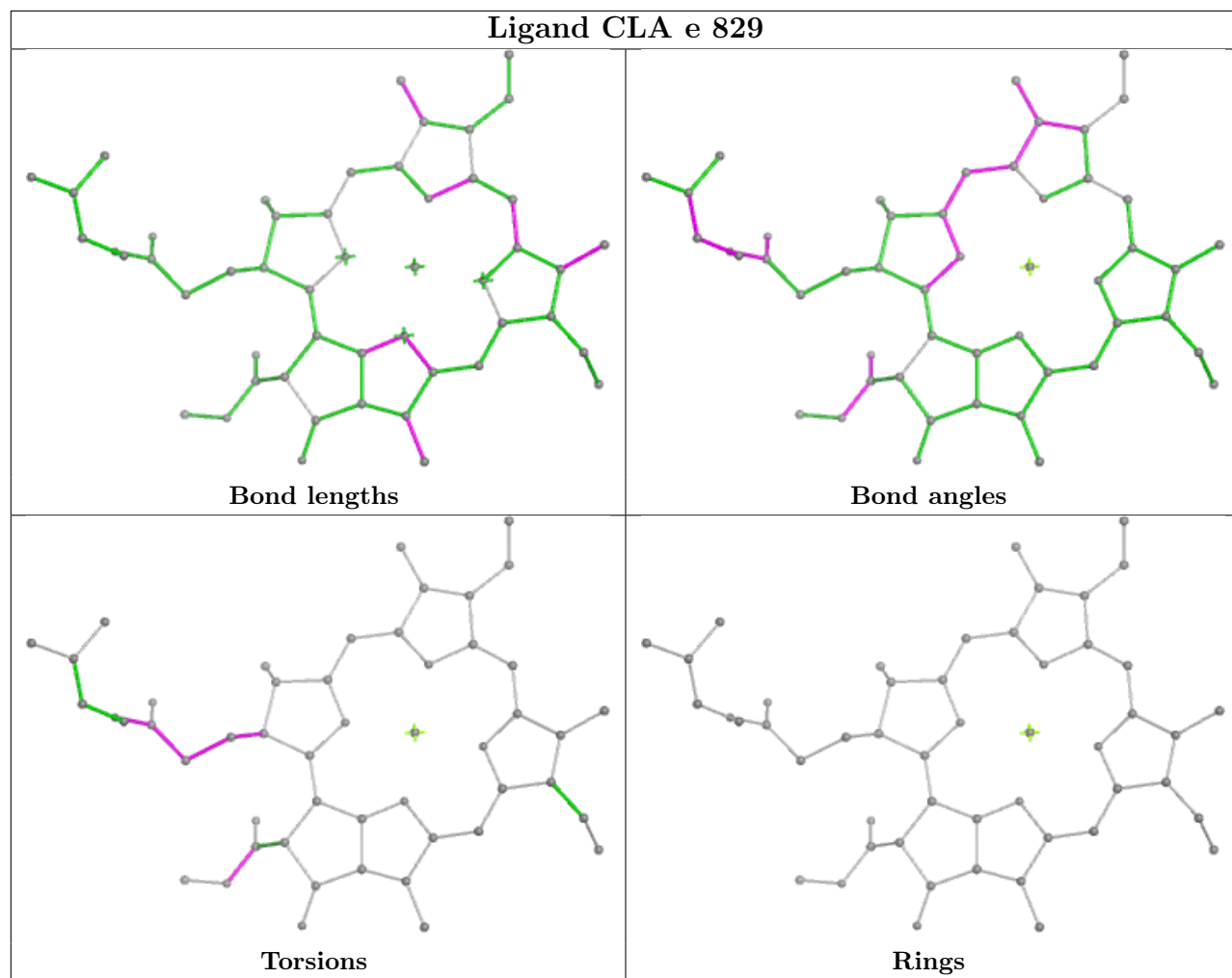
Rings



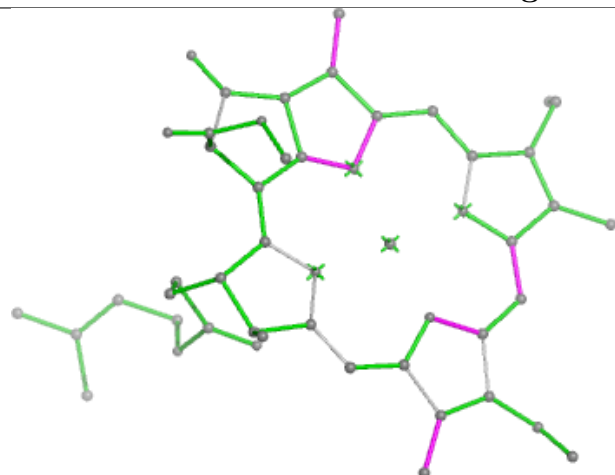
Ligand CLA b 827



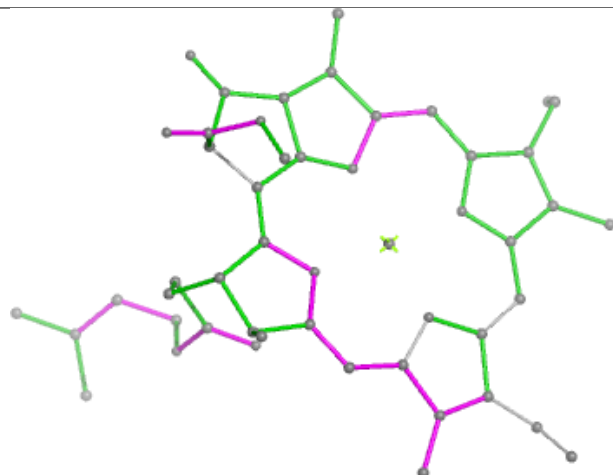
Ligand CLA e 829



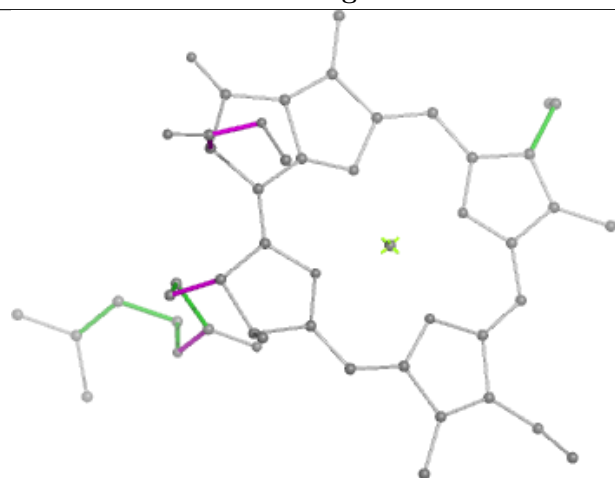
Ligand CLA e 836



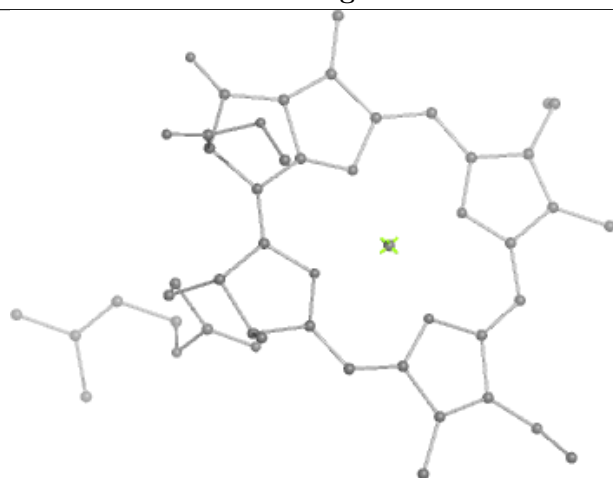
Bond lengths



Bond angles

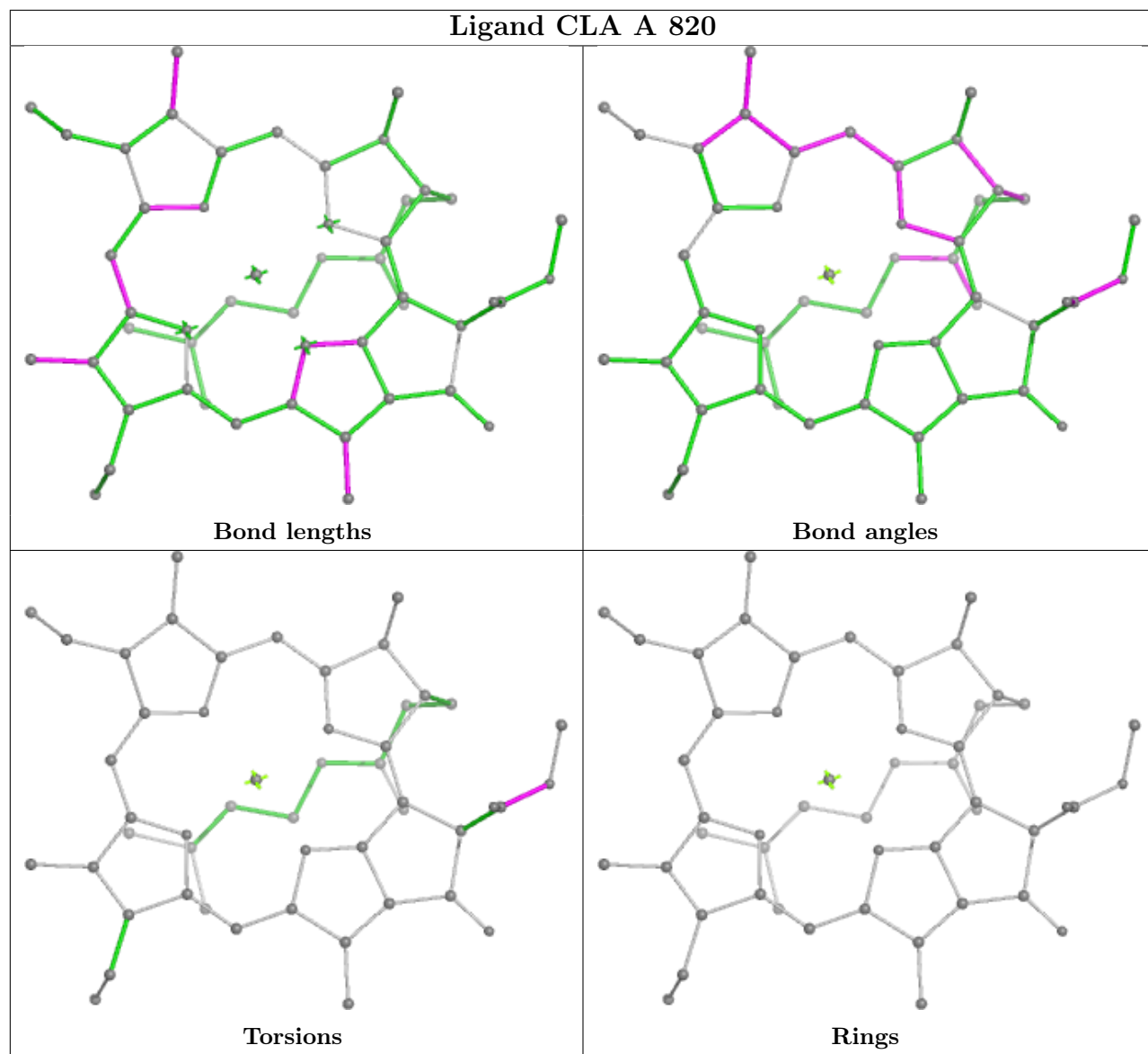


Torsions

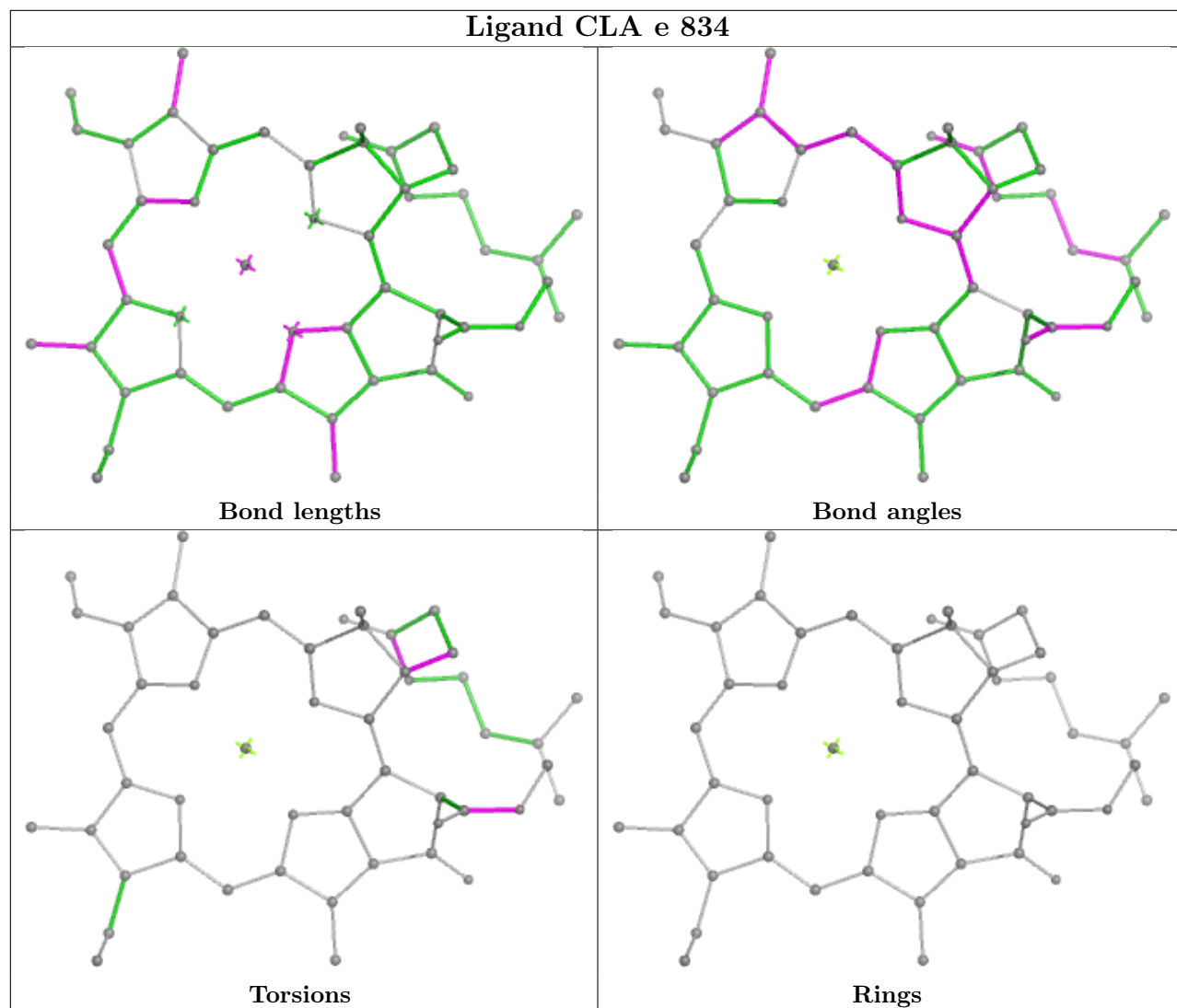


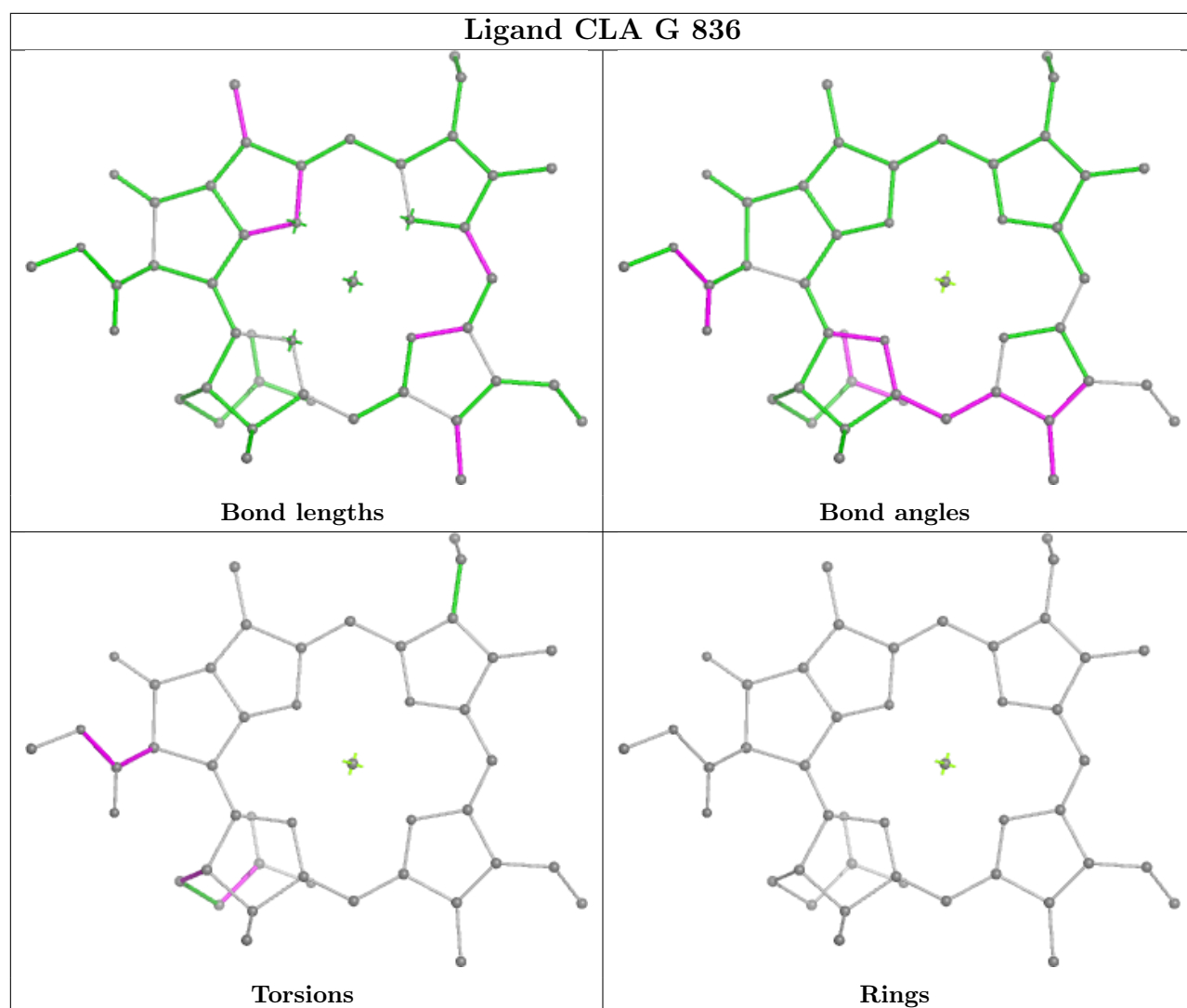
Rings

Ligand CLA A 820

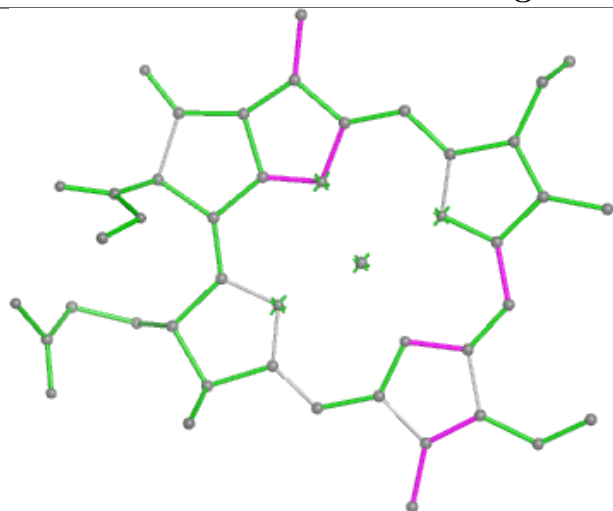


Ligand CLA e 834

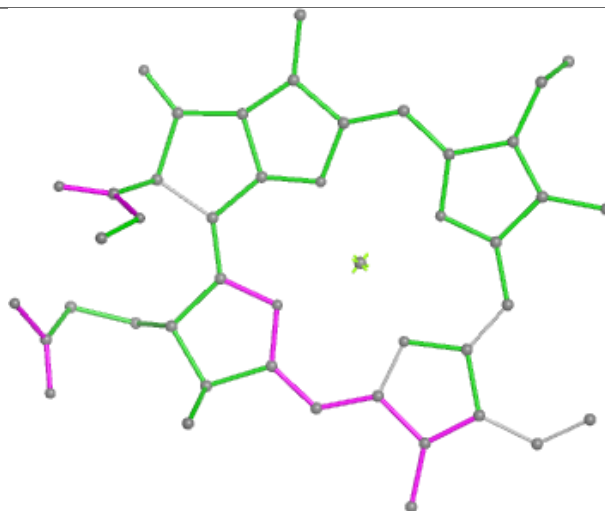




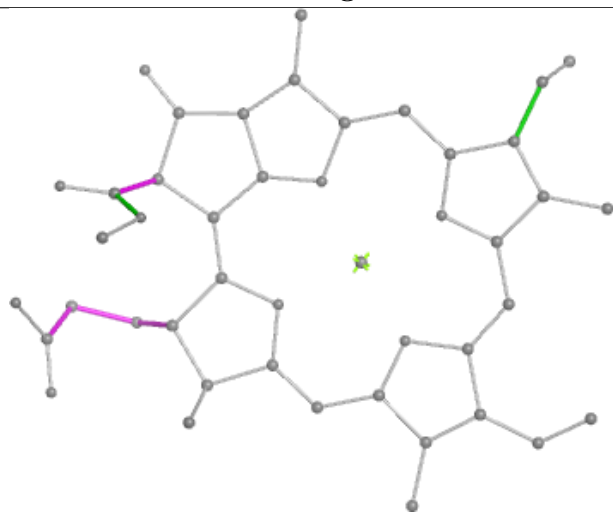
Ligand CLA B 835



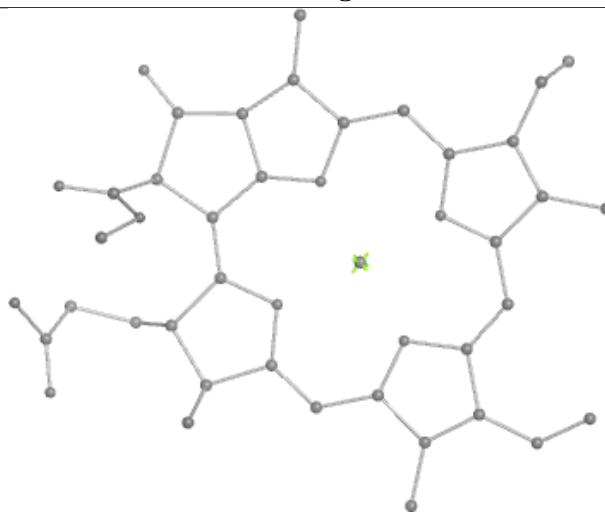
Bond lengths



Bond angles

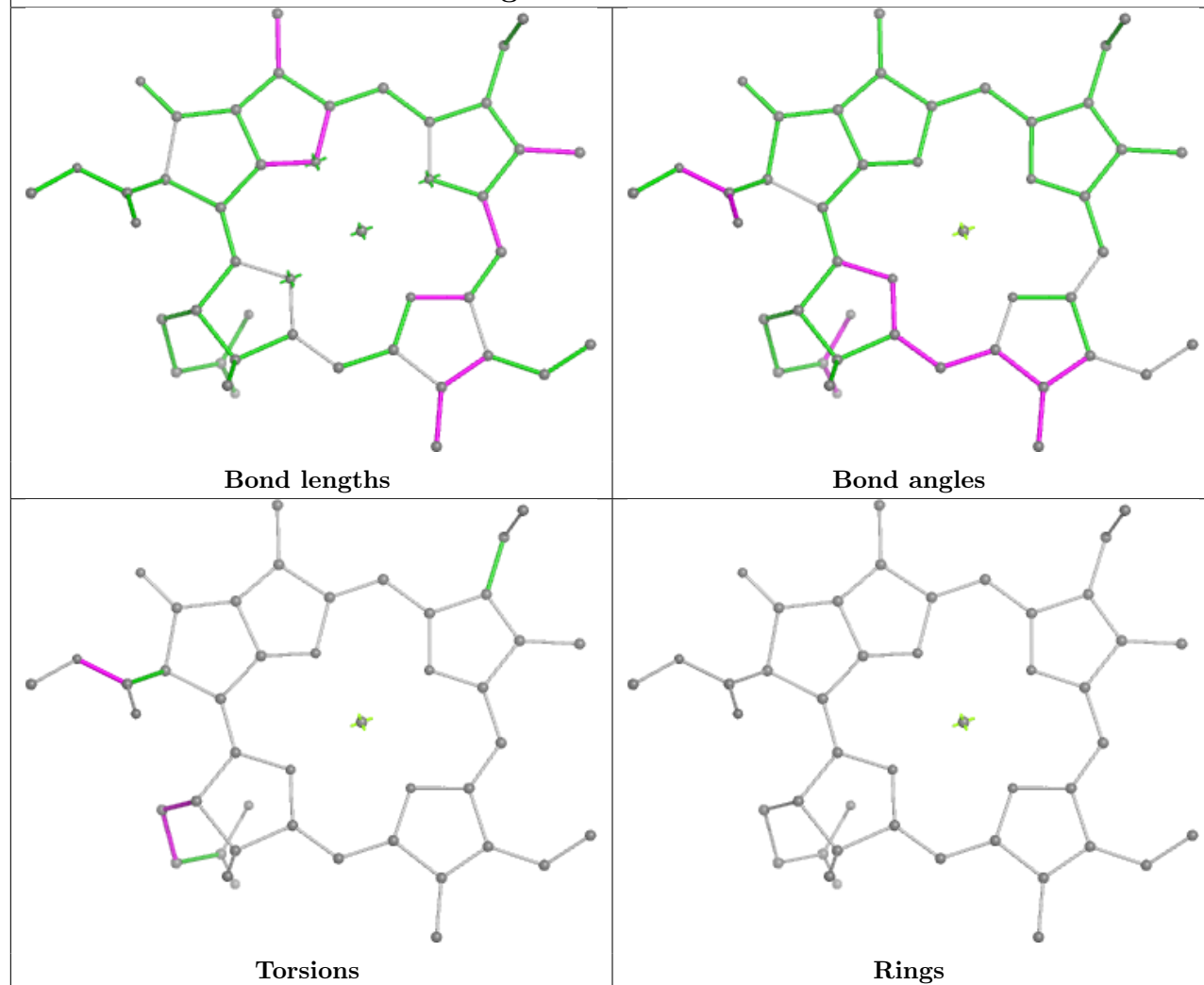


Torsions

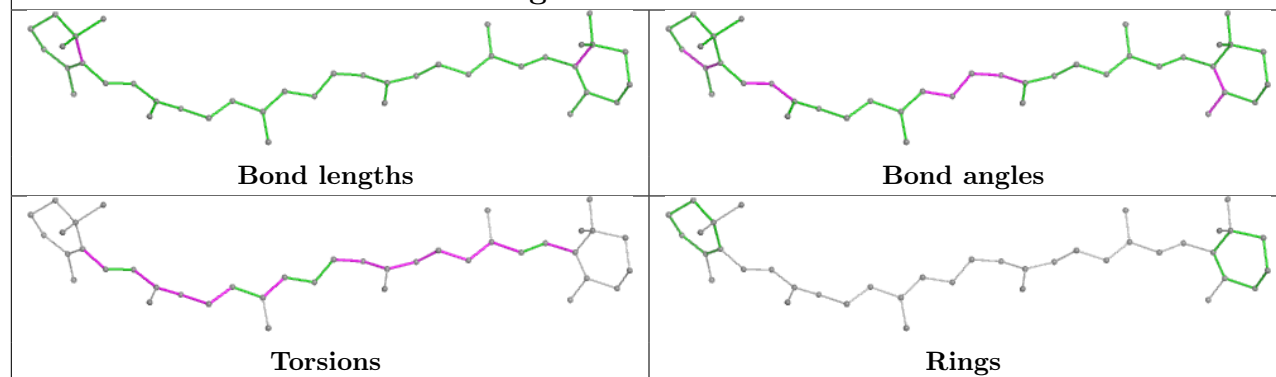


Rings

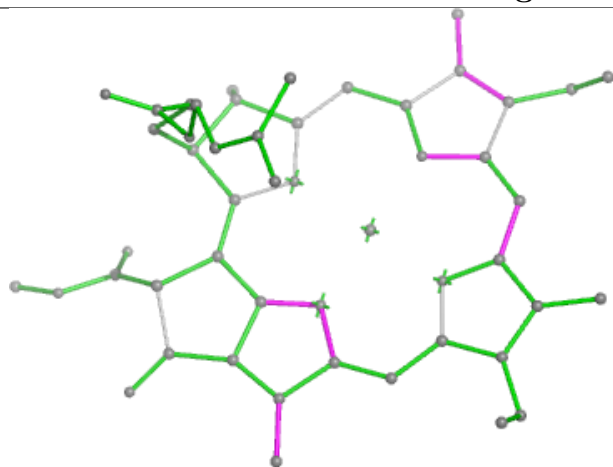
Ligand CLA G 813



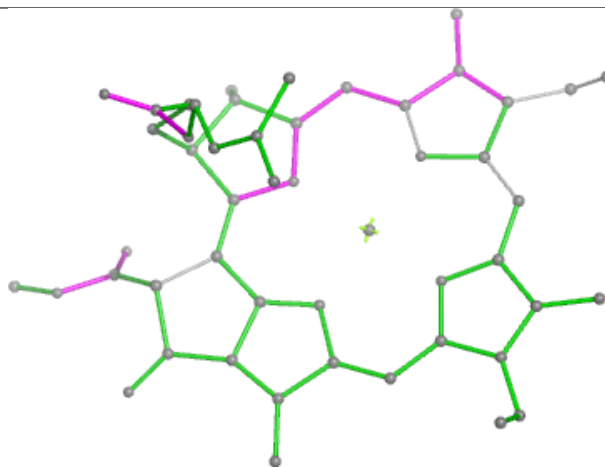
Ligand BCR G 846



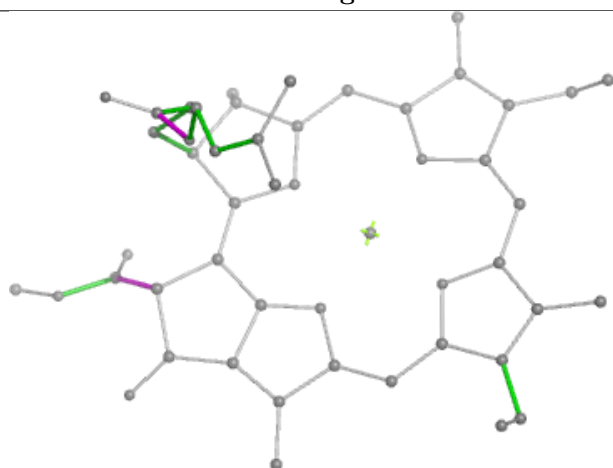
Ligand CLA E 814



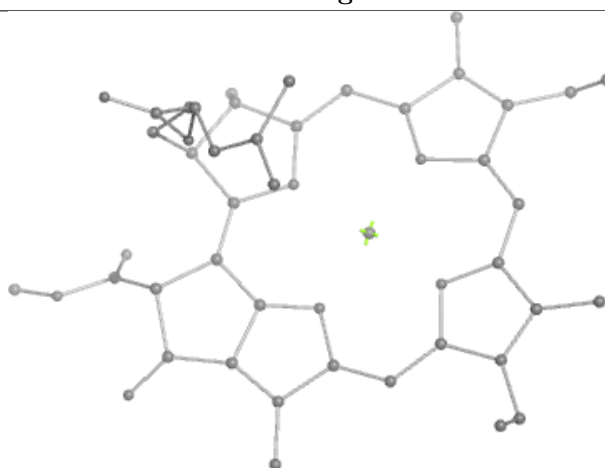
Bond lengths



Bond angles

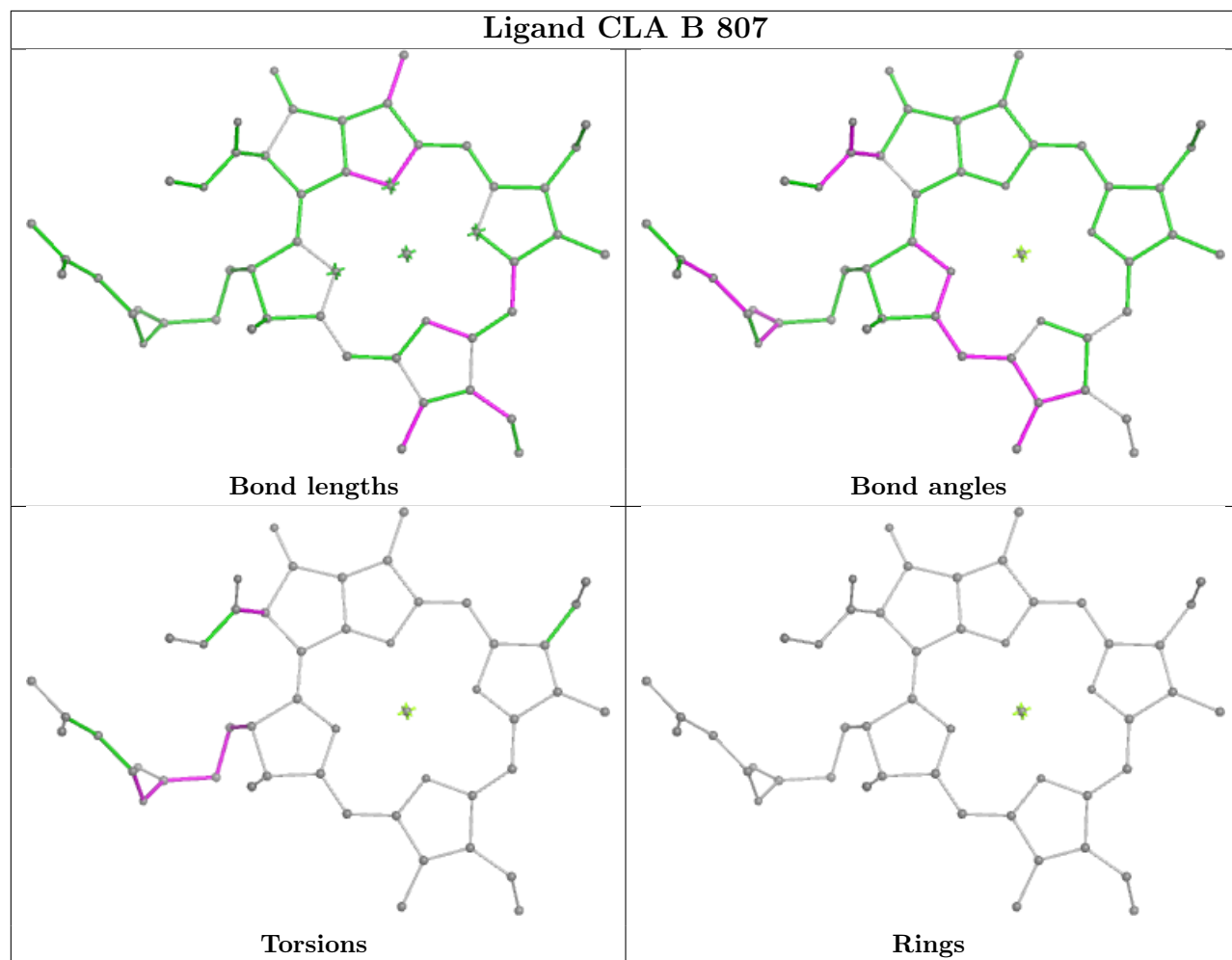


Torsions

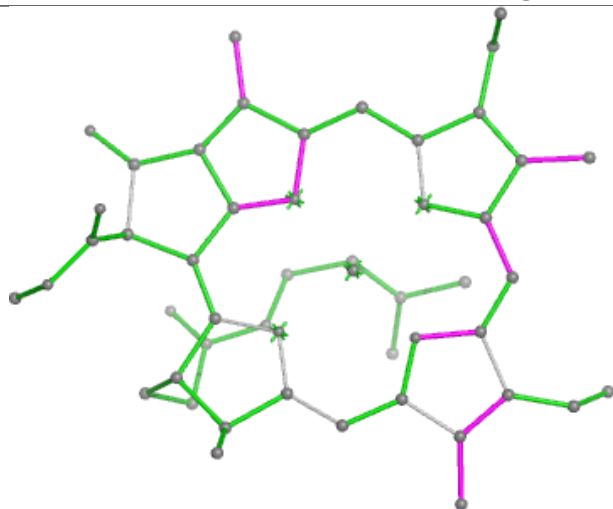


Rings

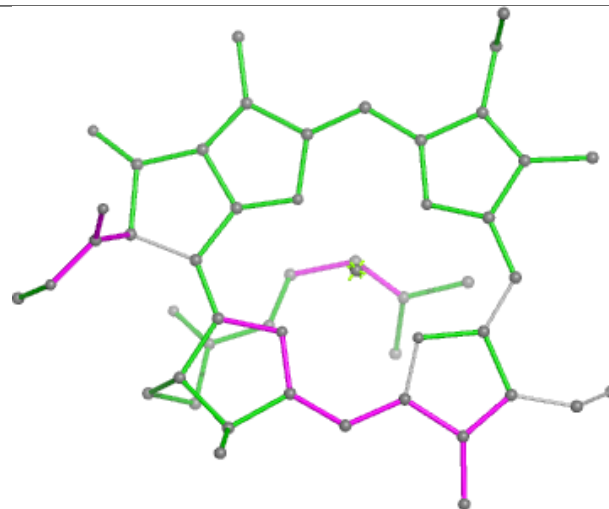
Ligand CLA B 807



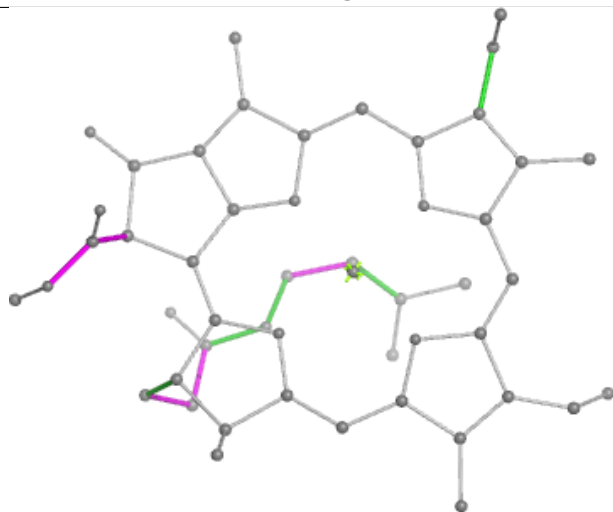
Ligand CLA b 822



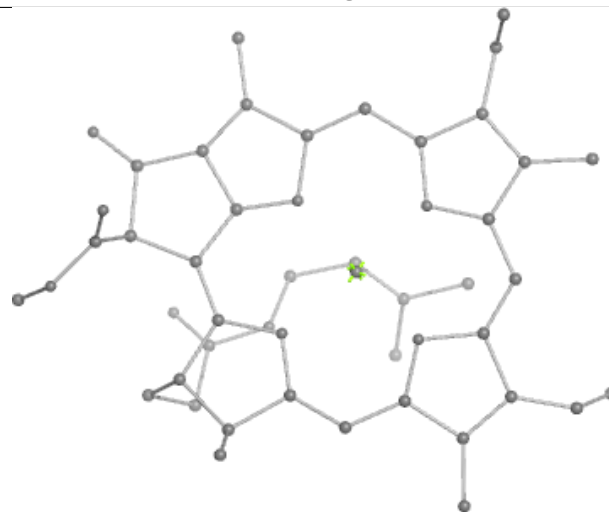
Bond lengths



Bond angles

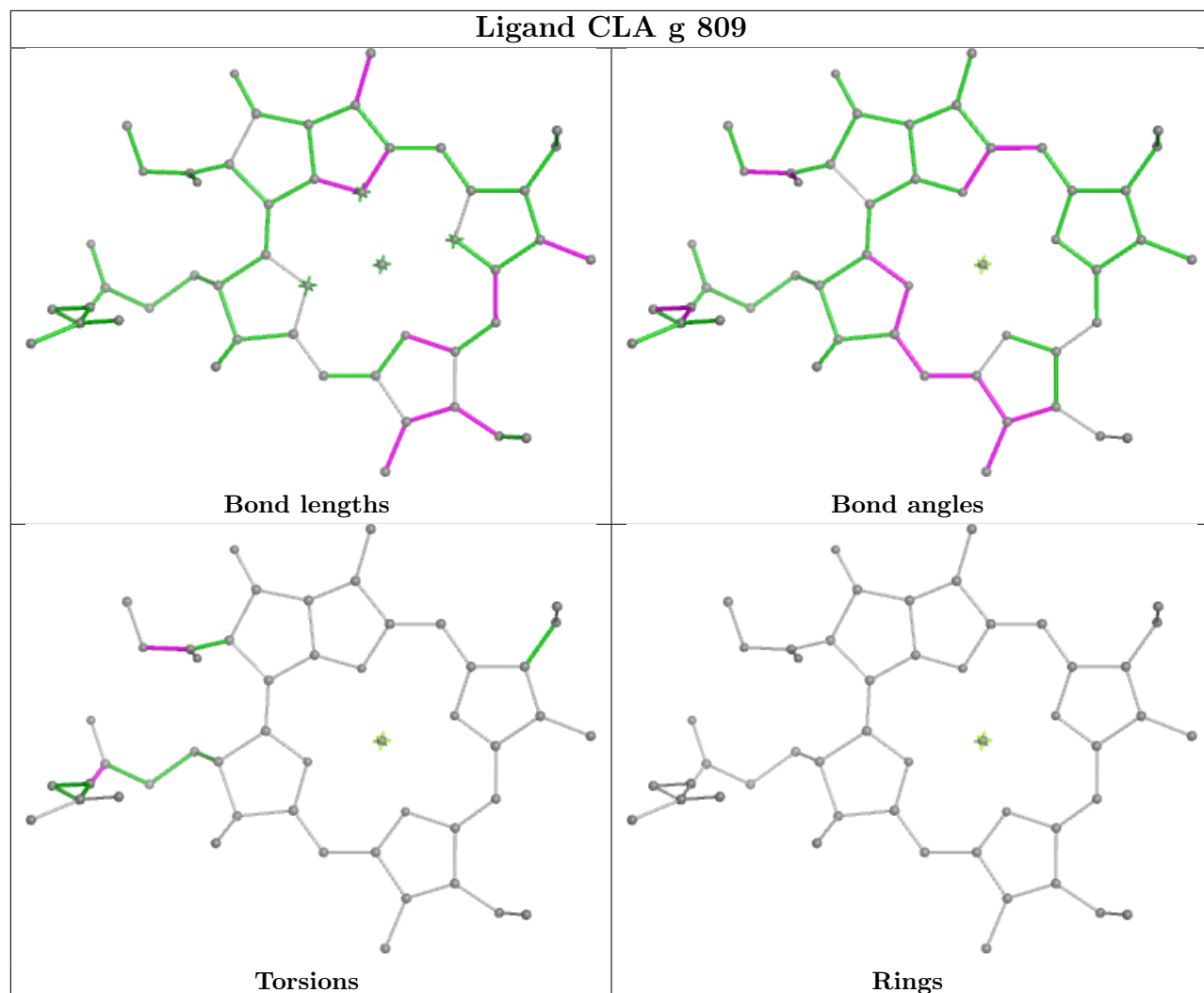


Torsions

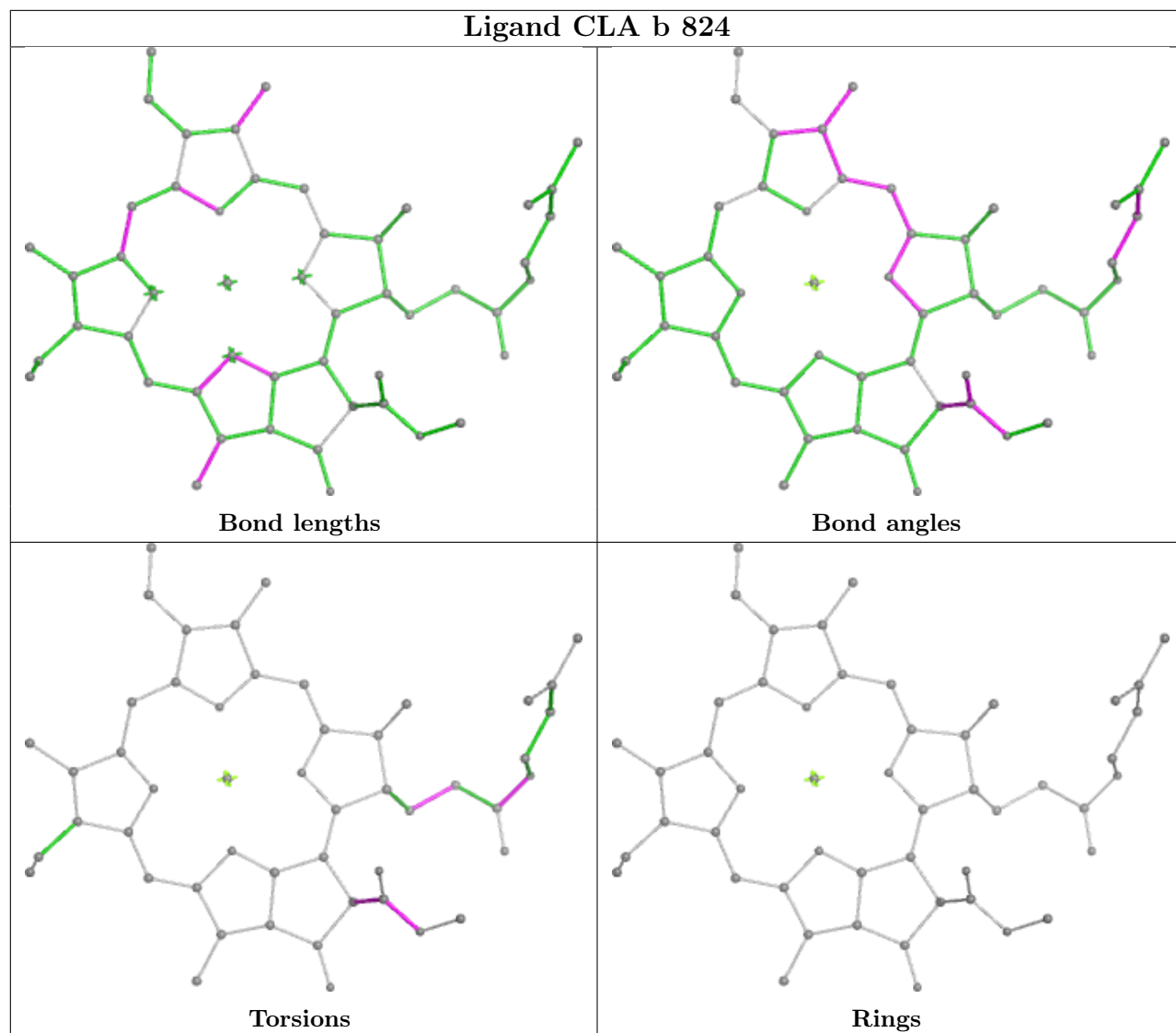


Rings

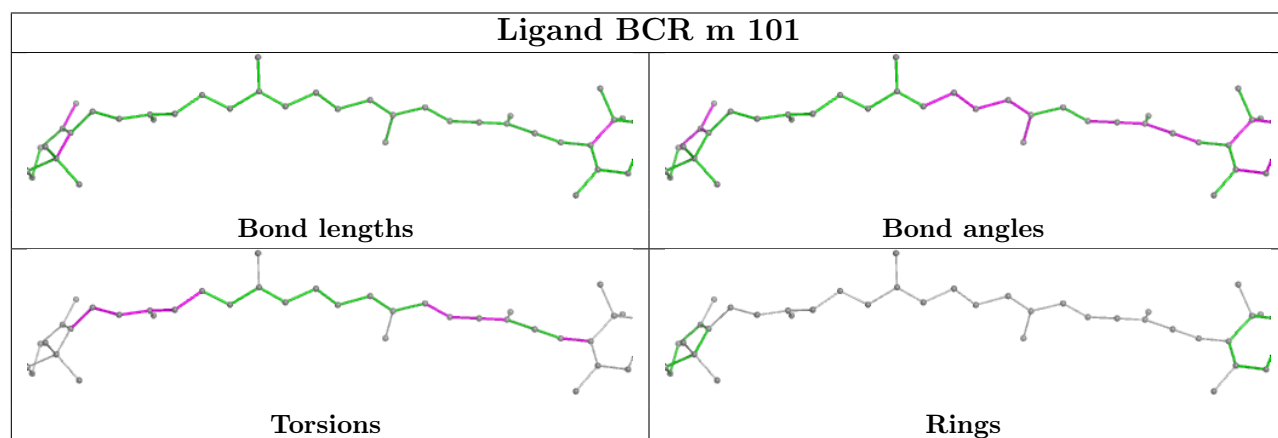
Ligand CLA g 809



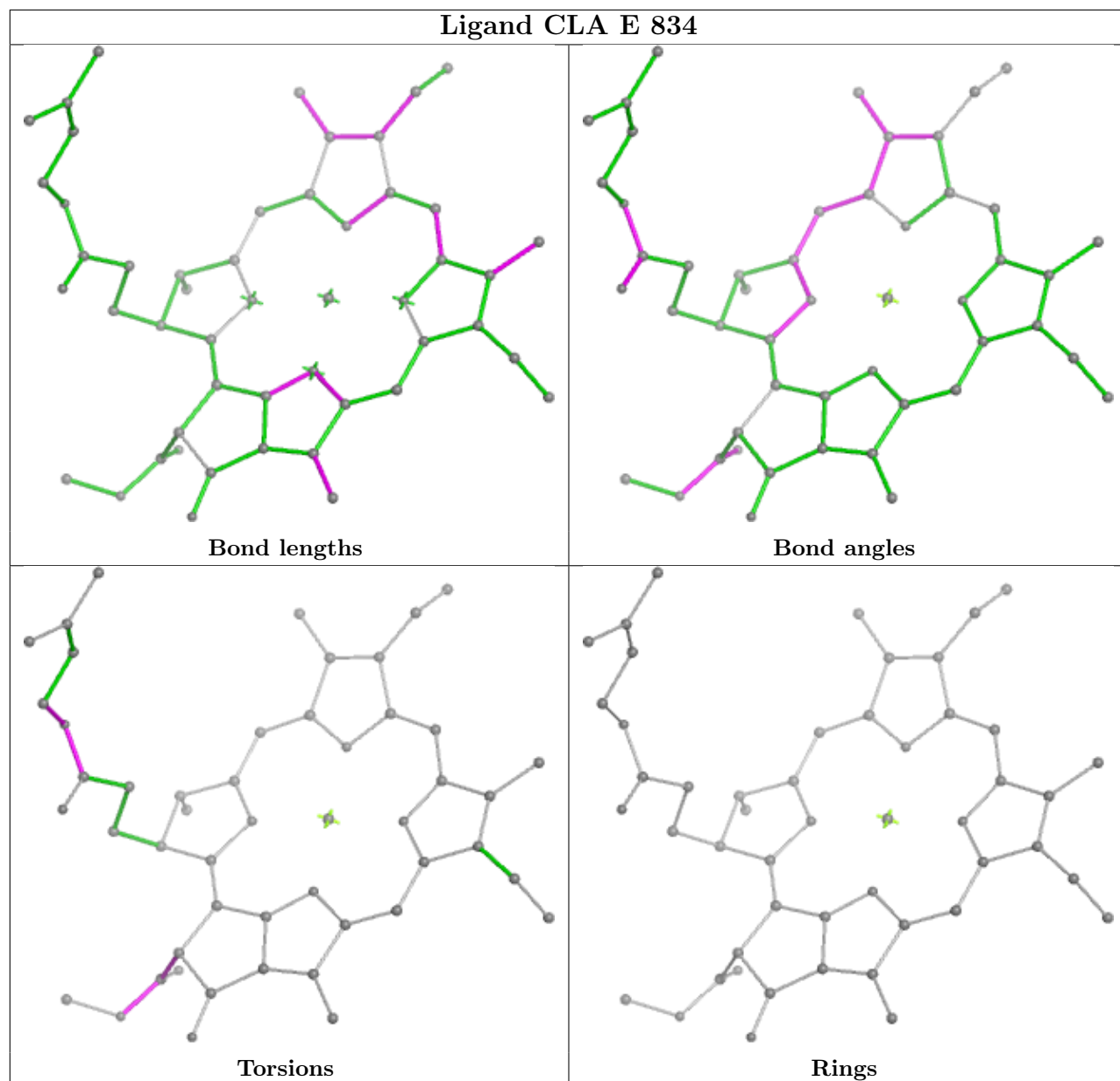
Ligand CLA b 824



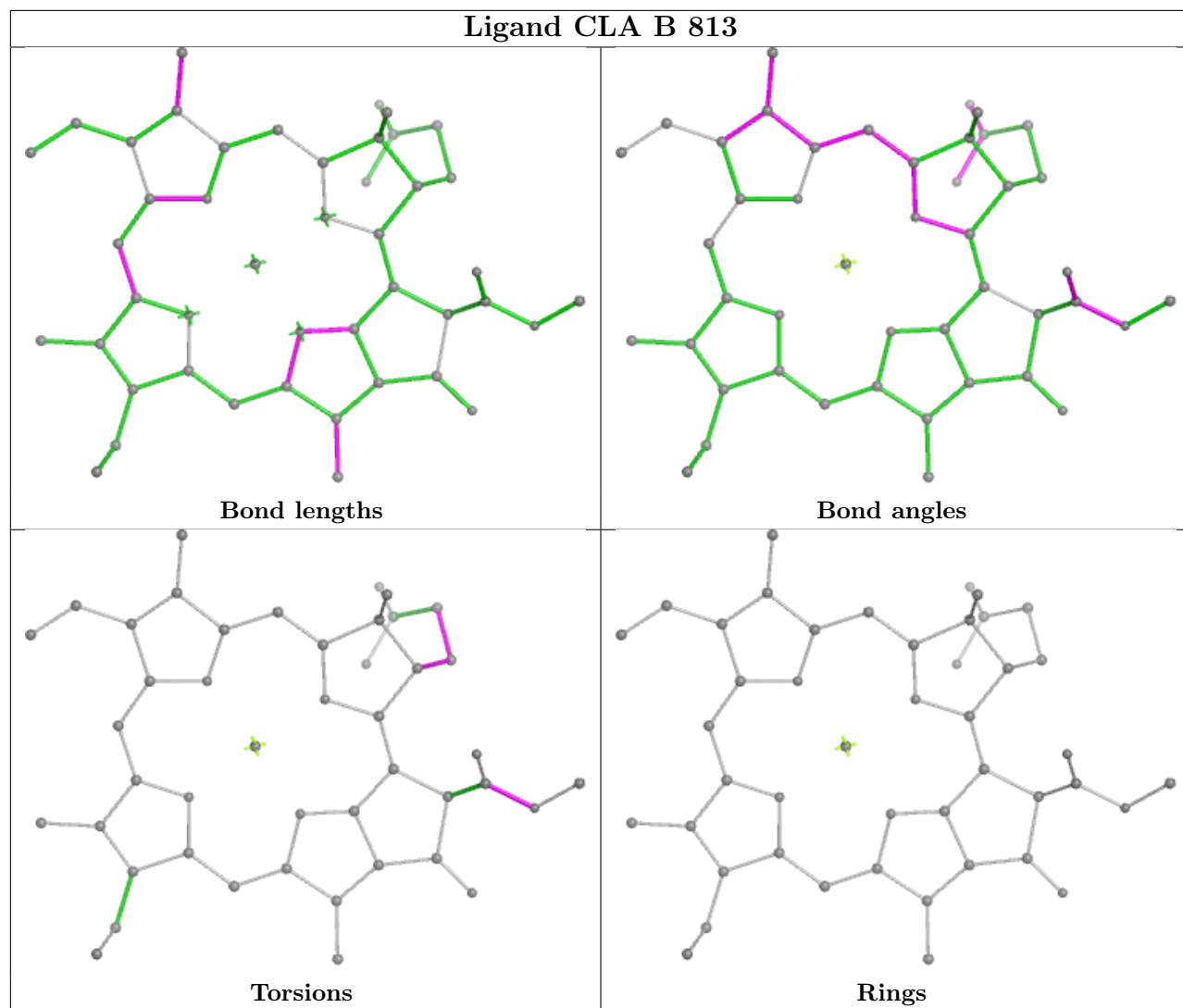
Ligand BCR m 101



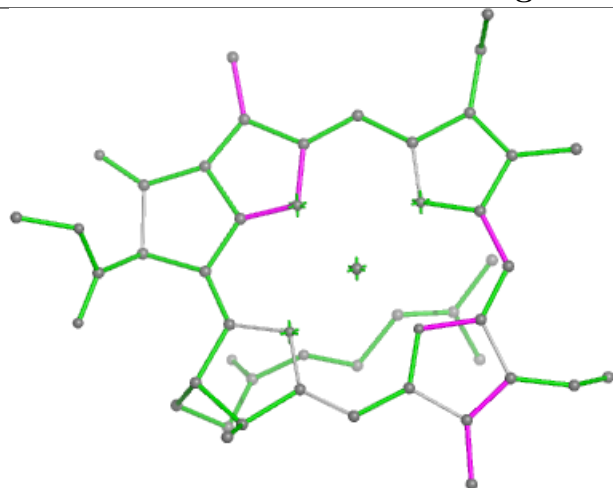
Ligand CLA E 834



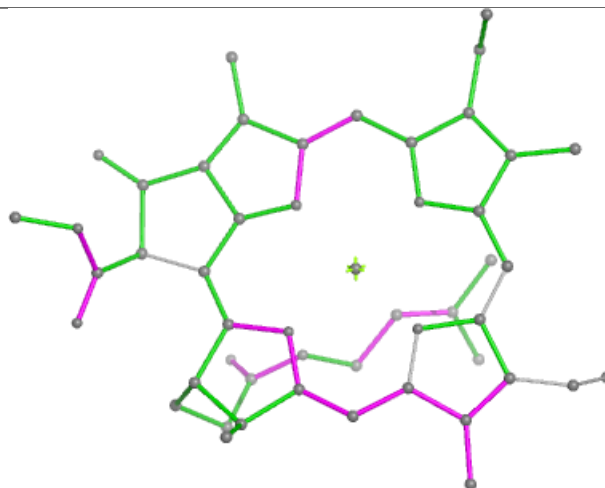
Ligand CLA B 813



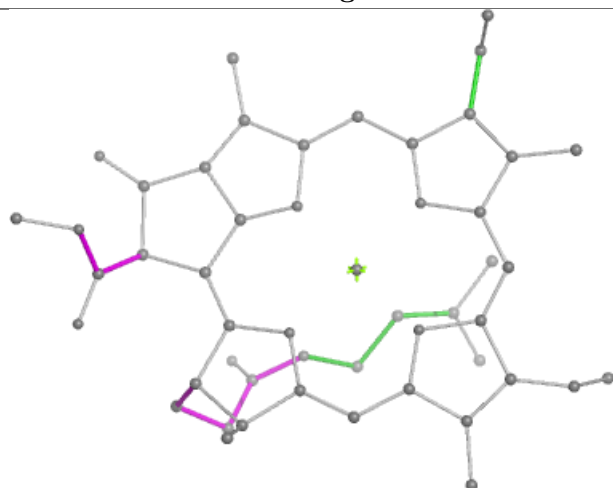
Ligand CLA E 826



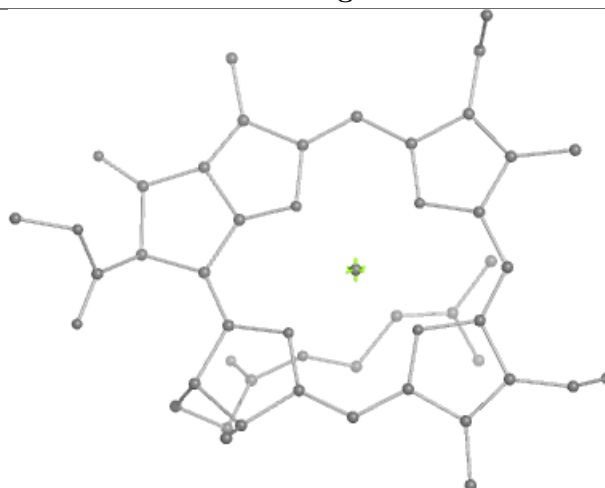
Bond lengths



Bond angles

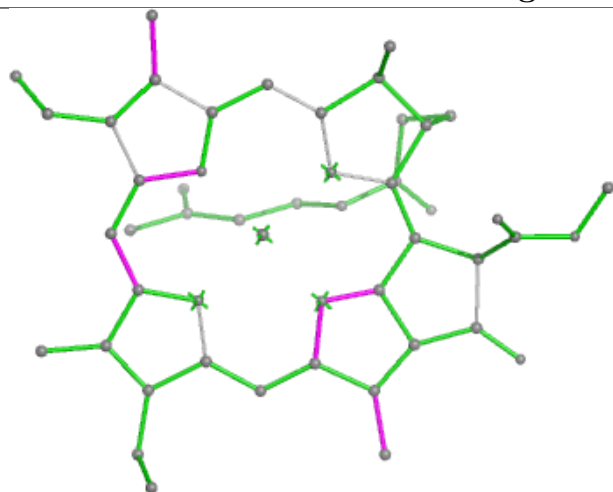


Torsions

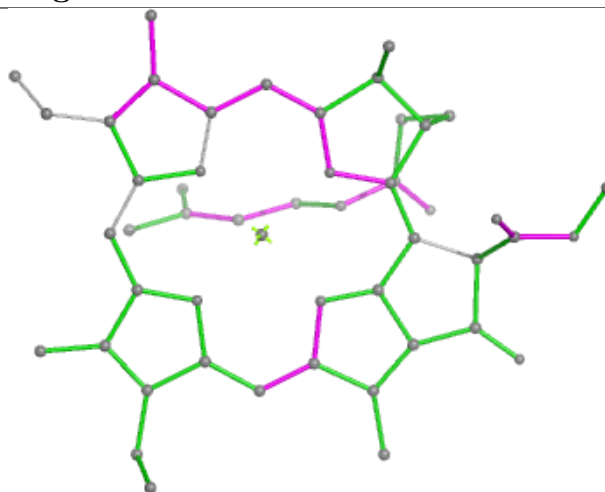


Rings

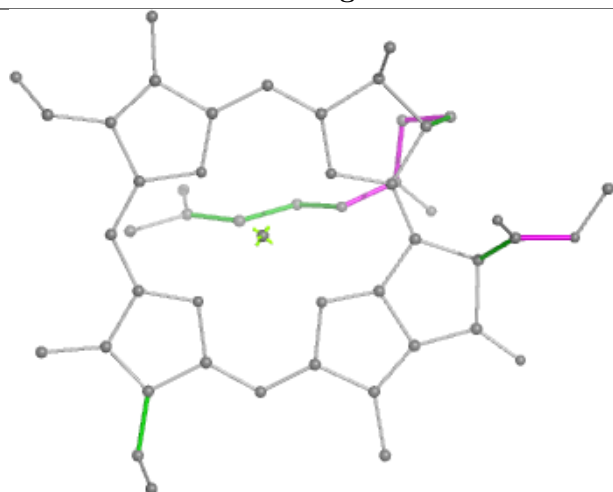
Ligand CLA g 839



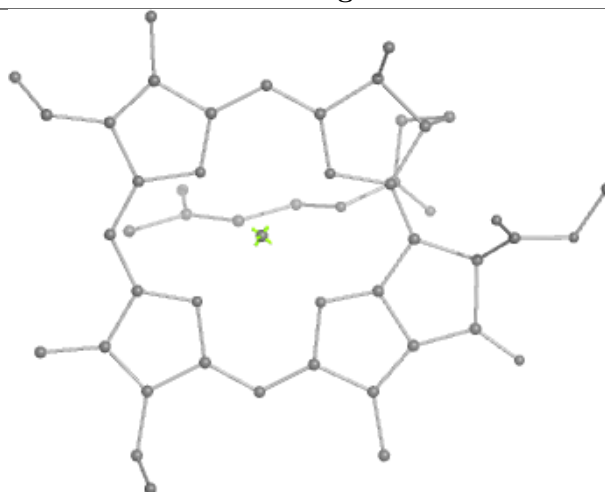
Bond lengths



Bond angles

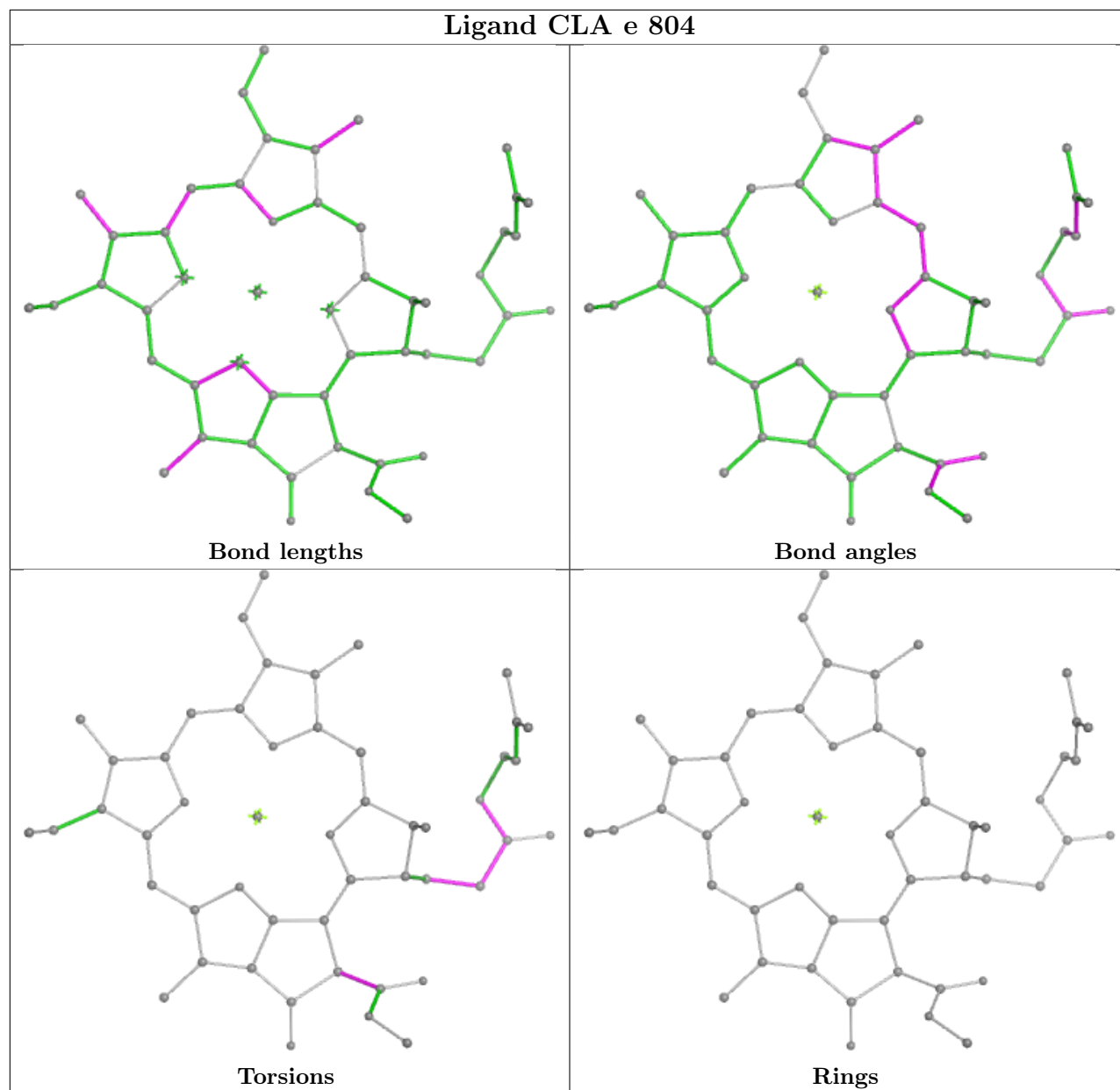


Torsions

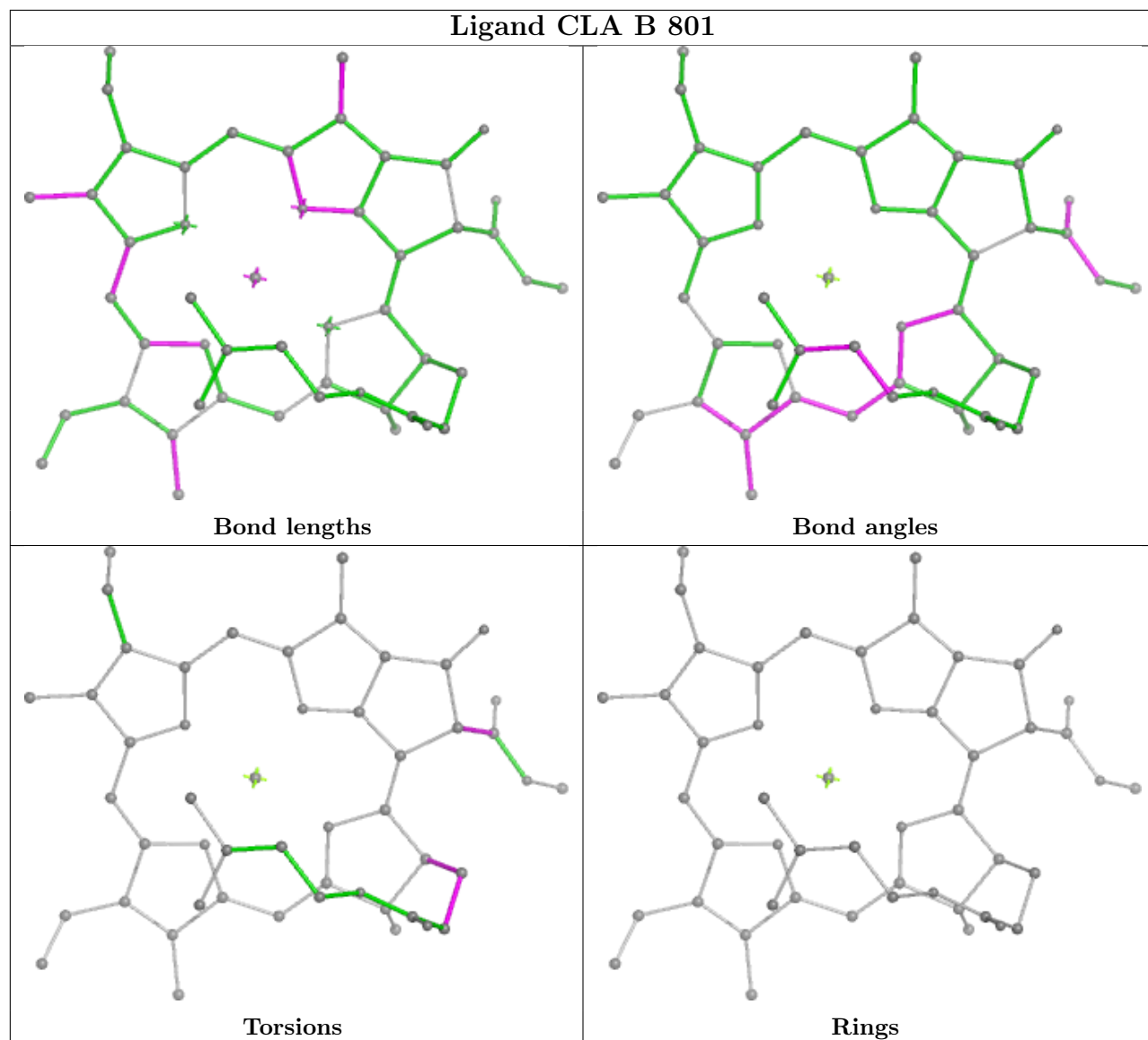


Rings

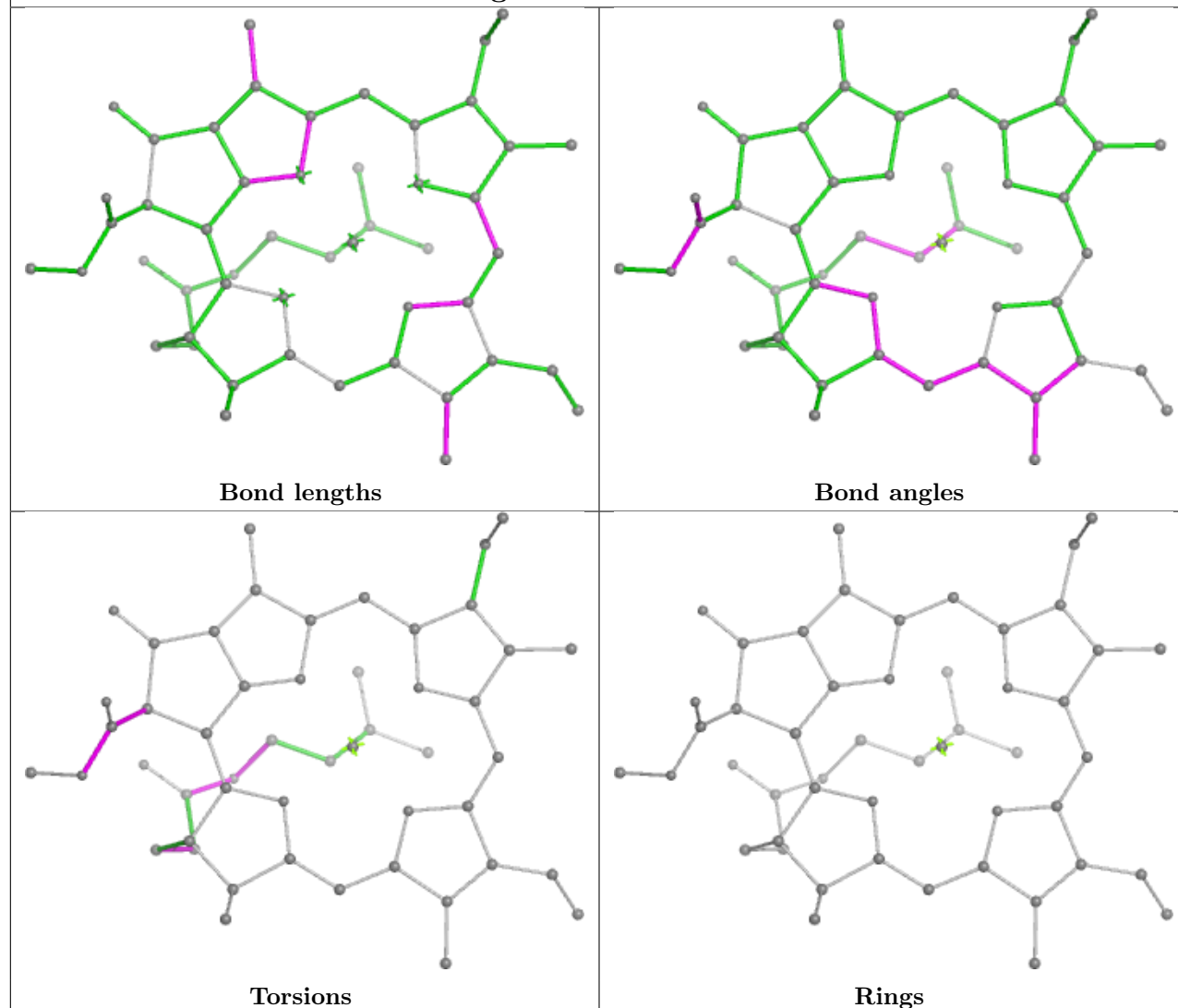
Ligand CLA e 804



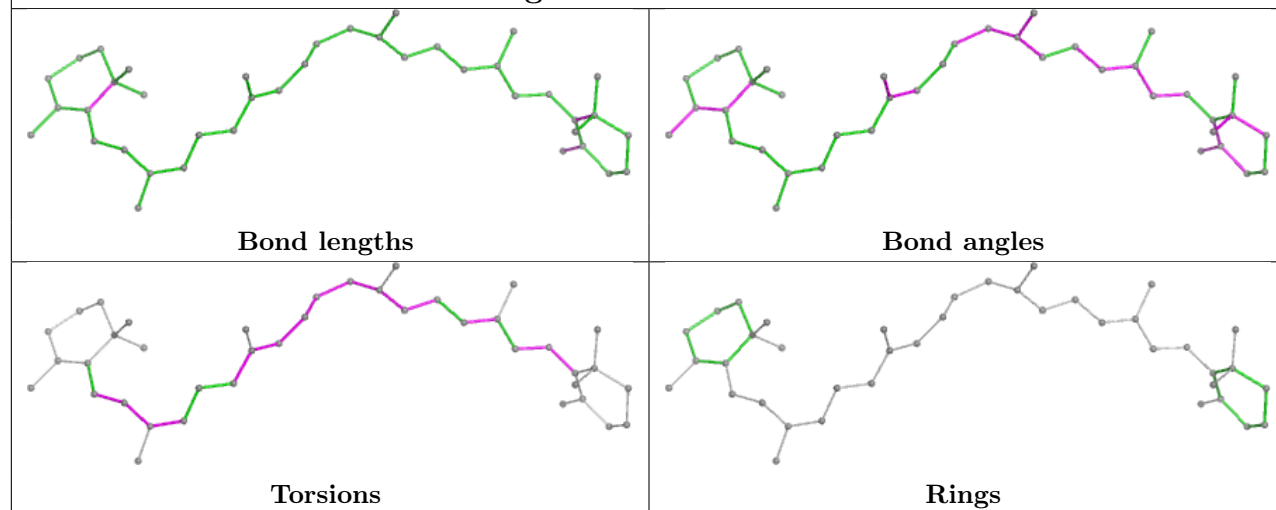
Ligand CLA B 801



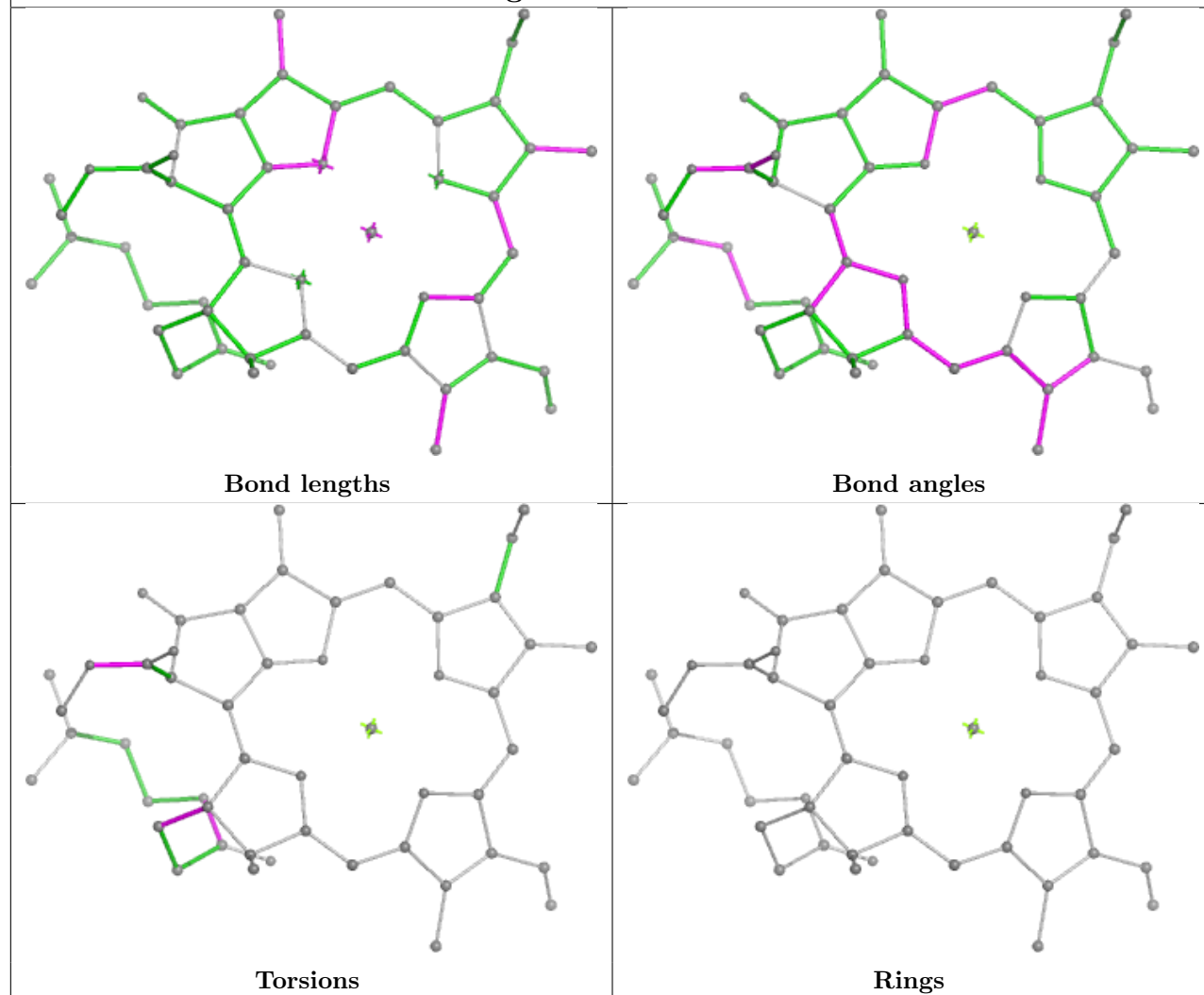
Ligand CLA A 815



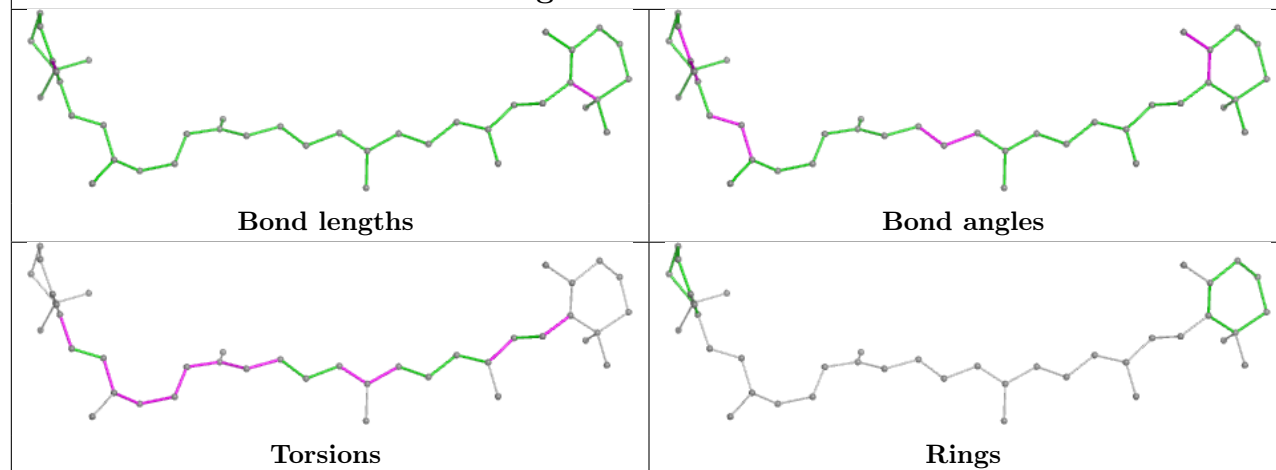
Ligand BCR k 4001



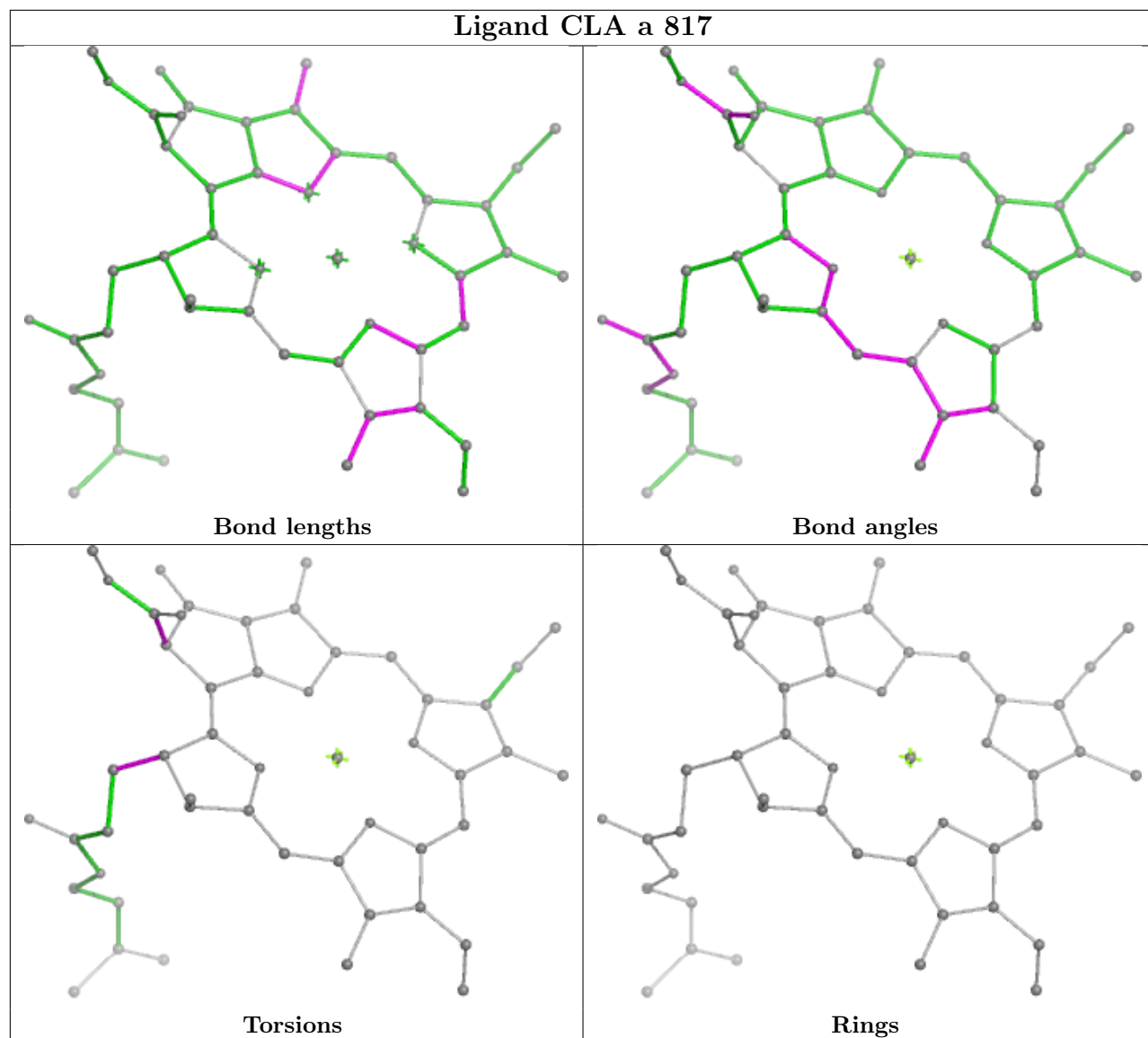
Ligand CLA a 836



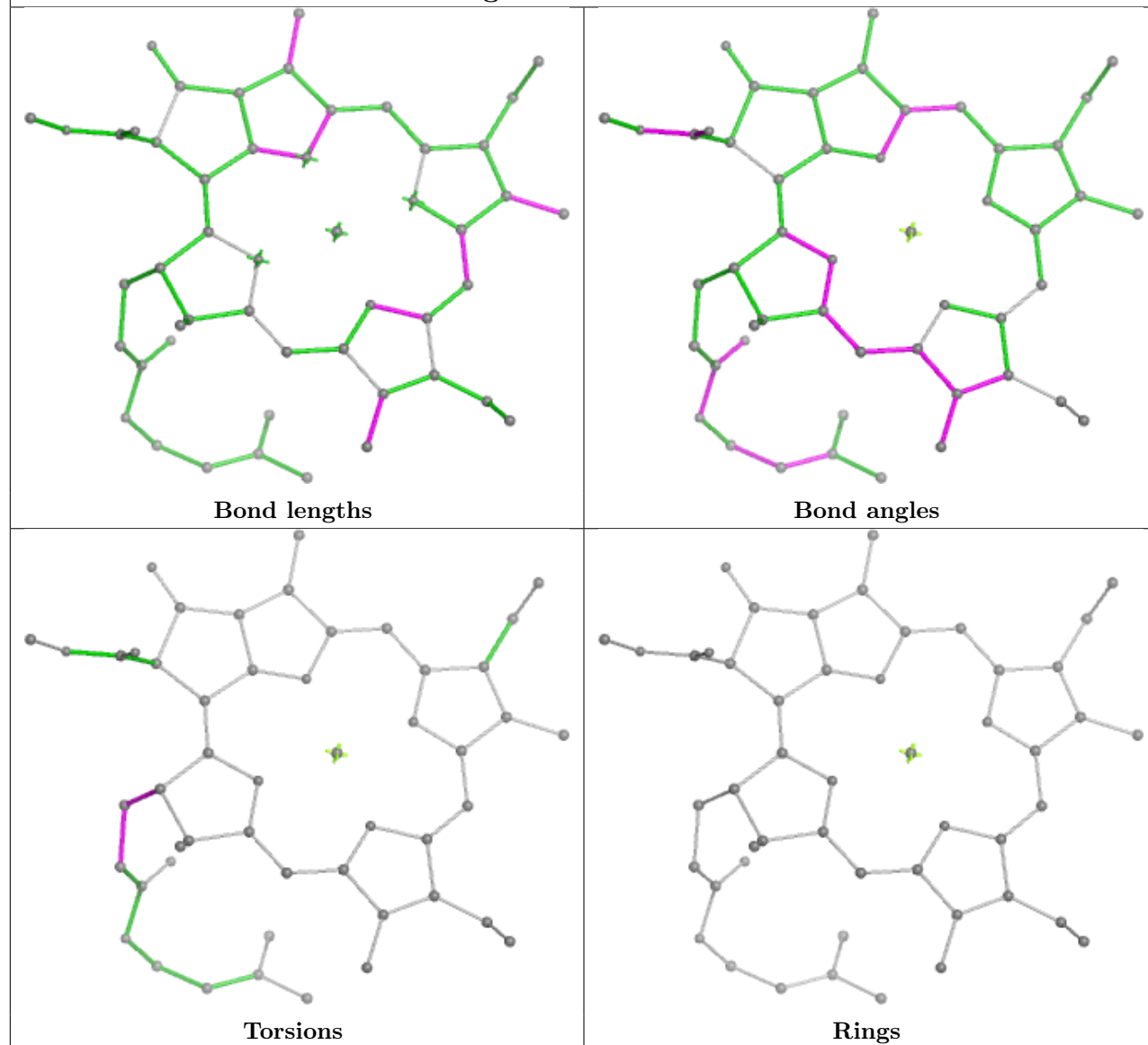
Ligand BCR s 201



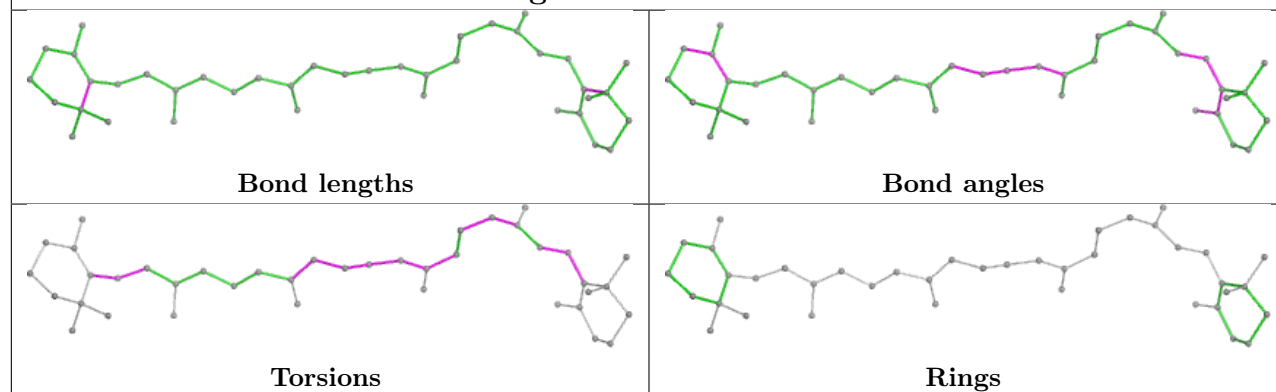
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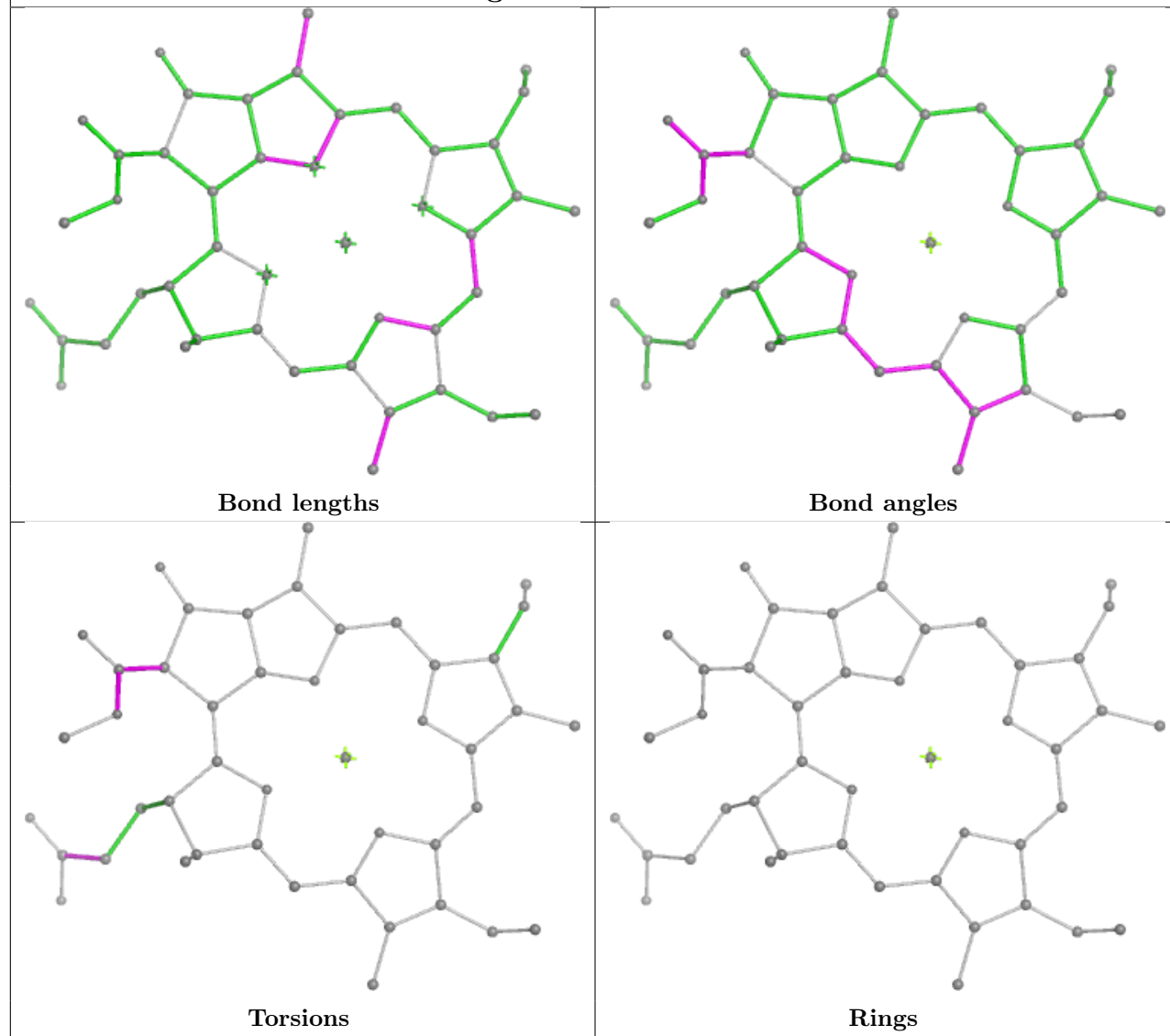
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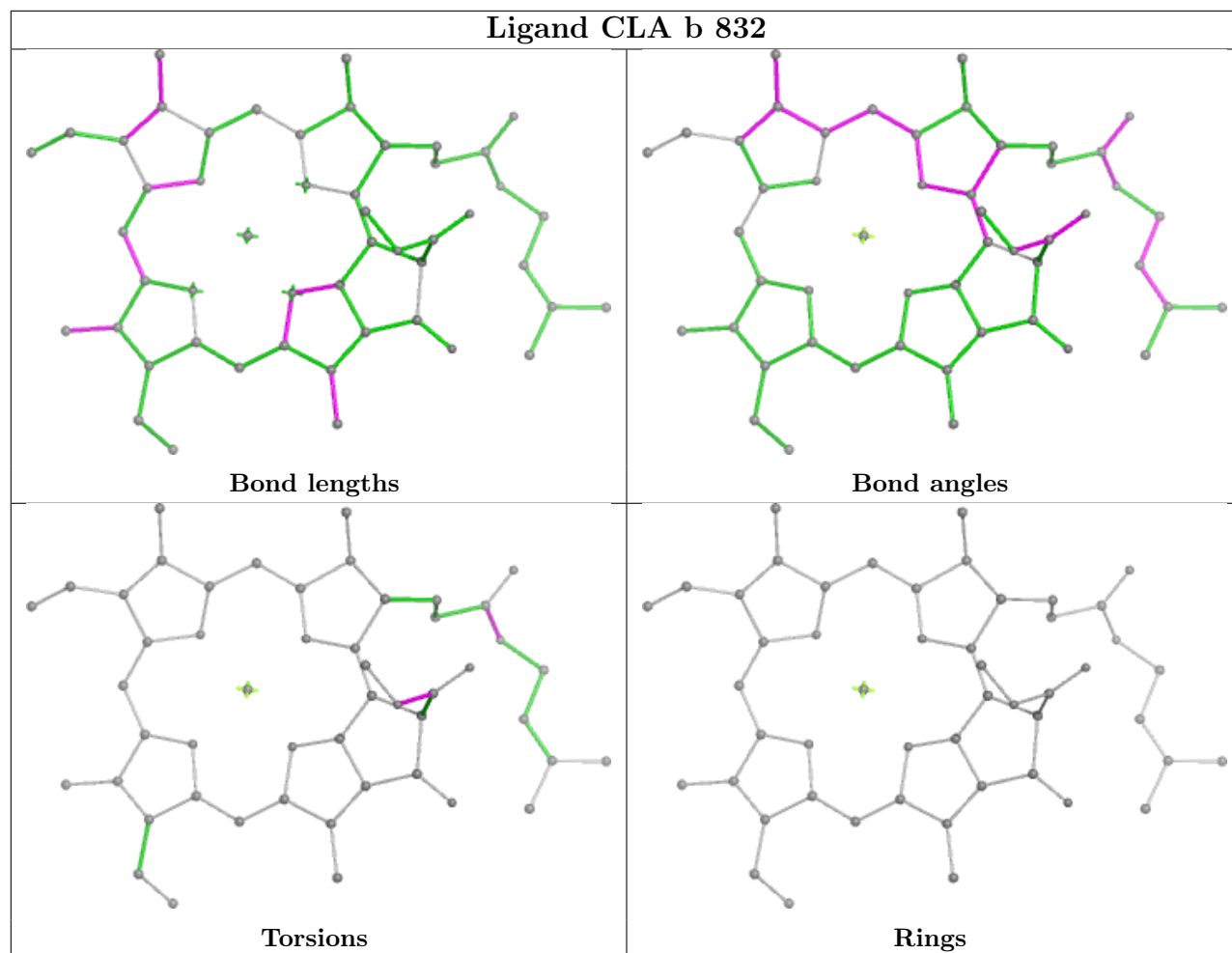
Ligand BCR G 845



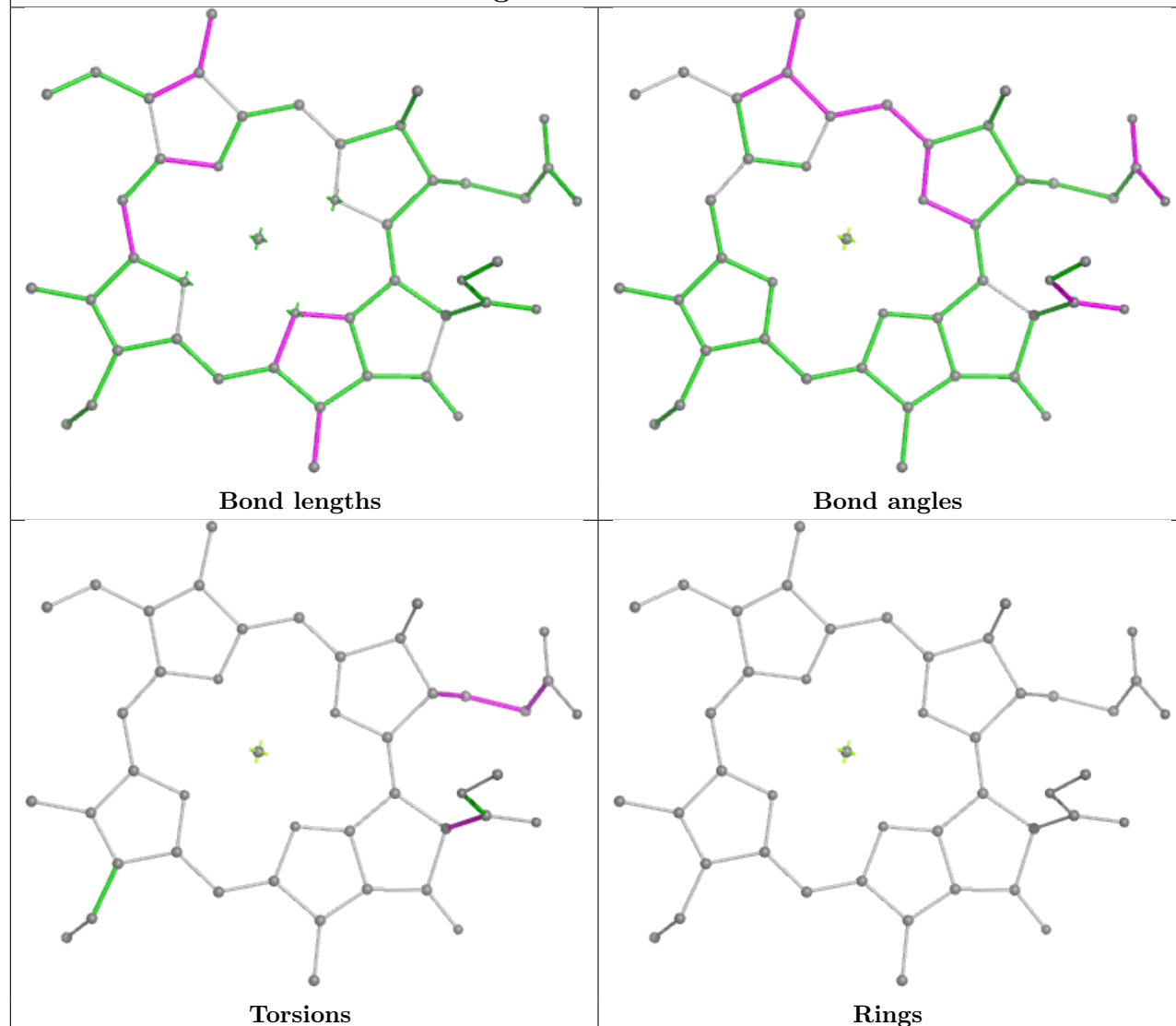
Ligand CLA G 824



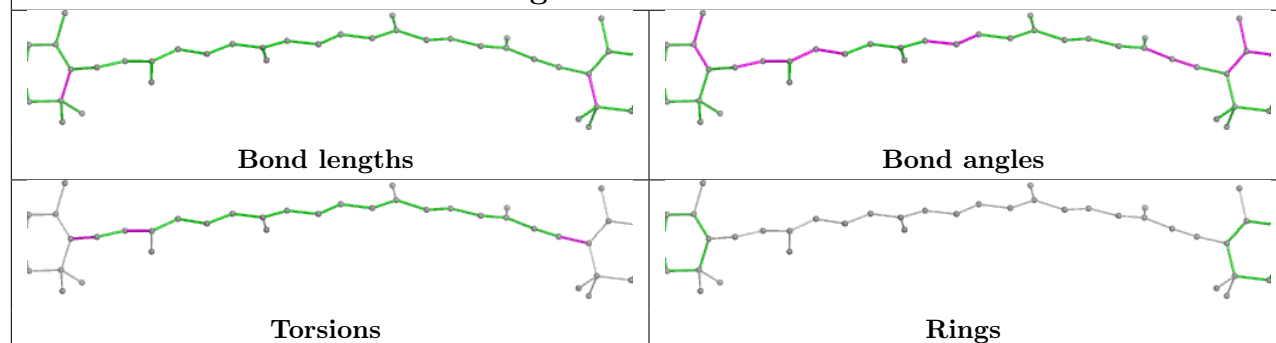
Ligand CLA b 832

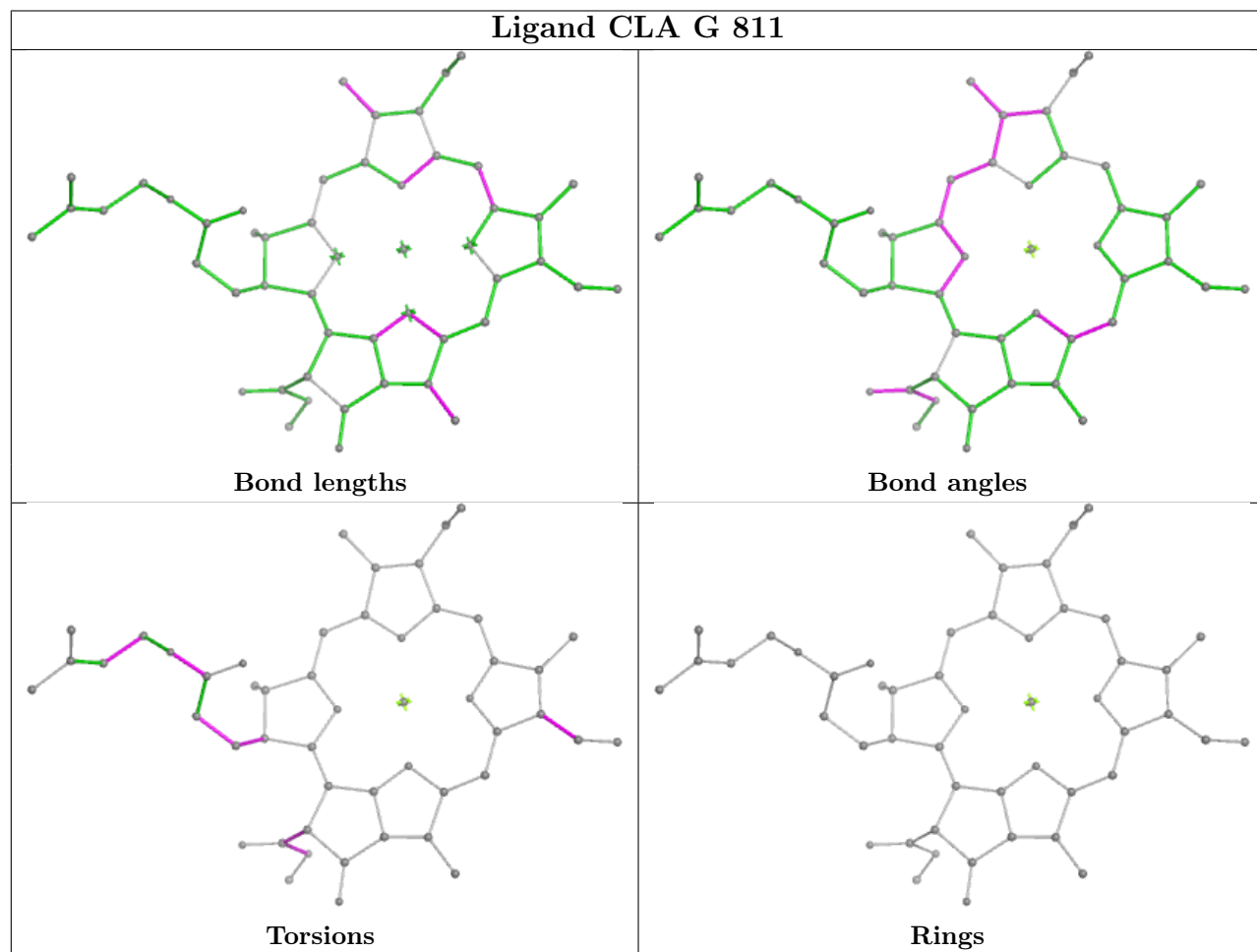
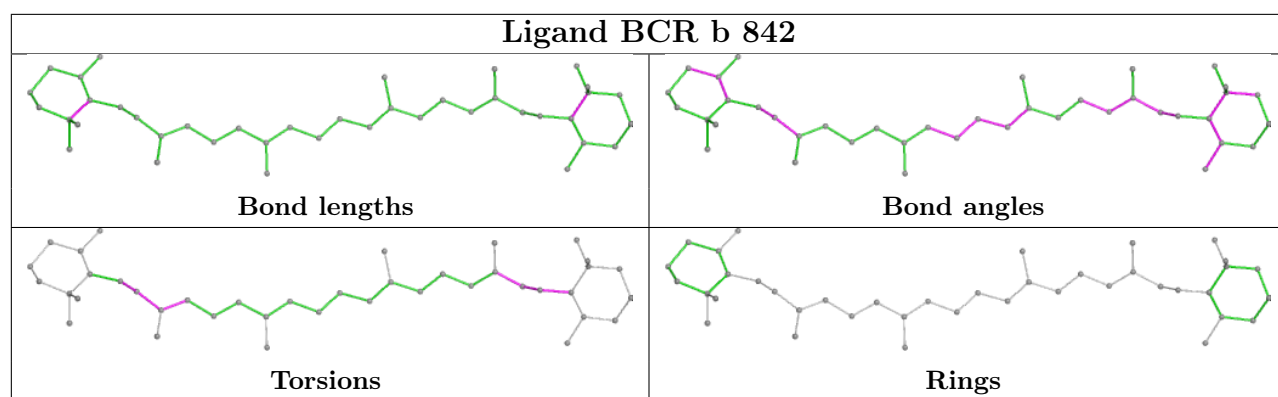


Ligand CLA b 834

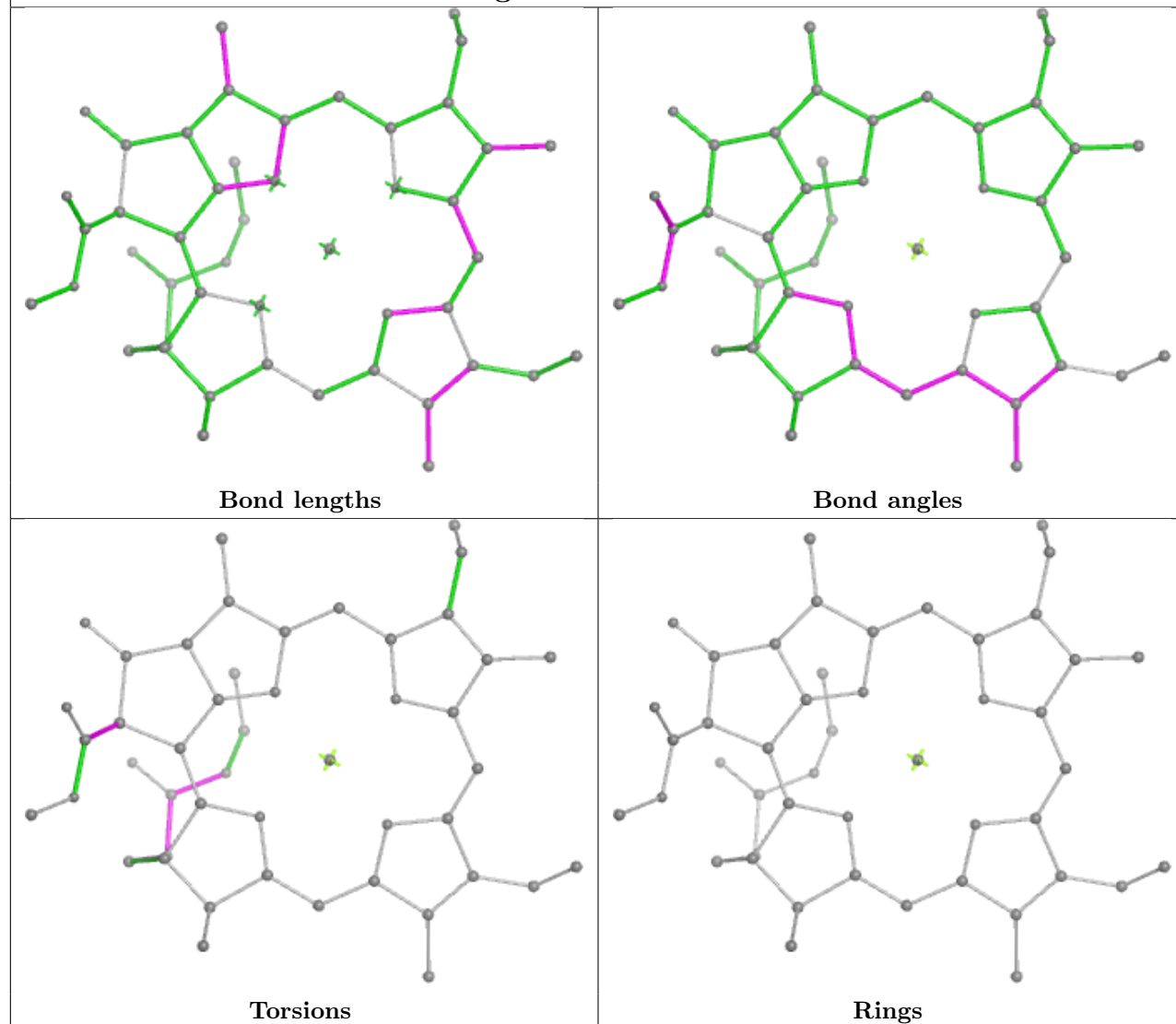


Ligand BCR A 851

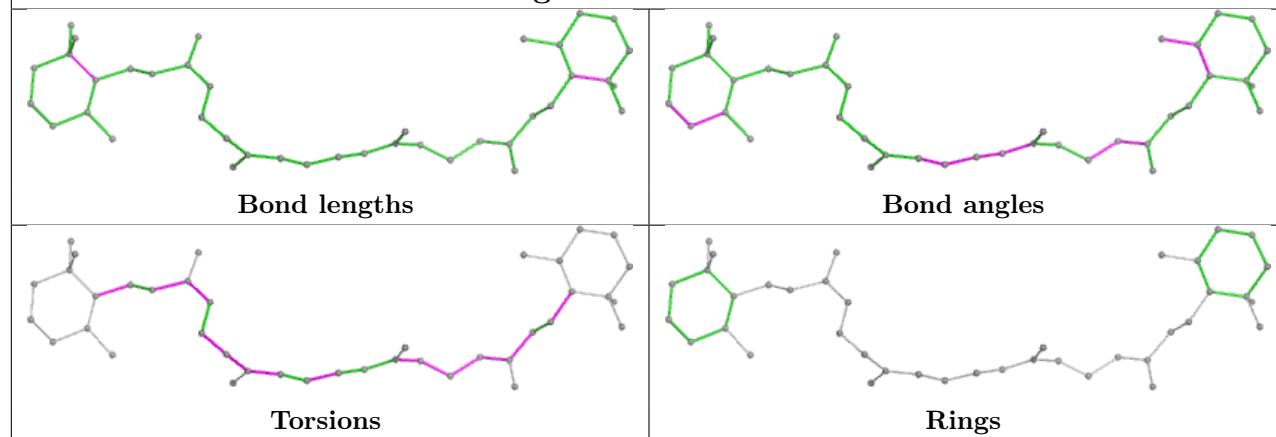




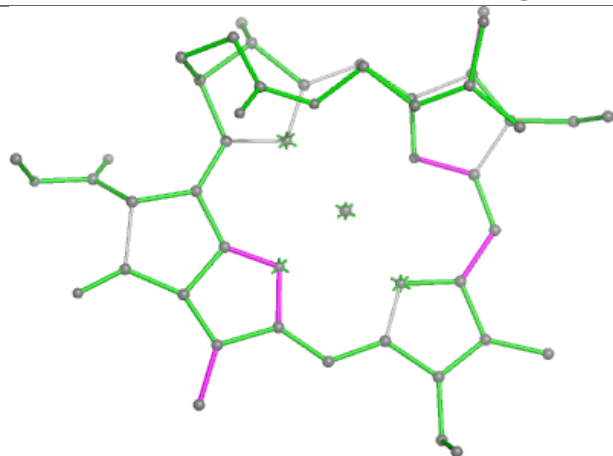
Ligand CLA e 840



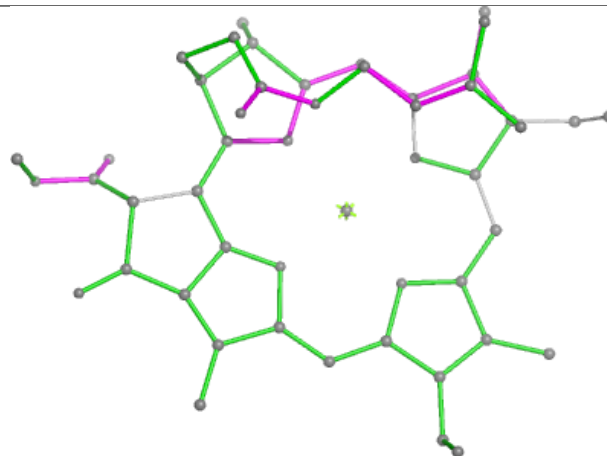
Ligand BCR b 843



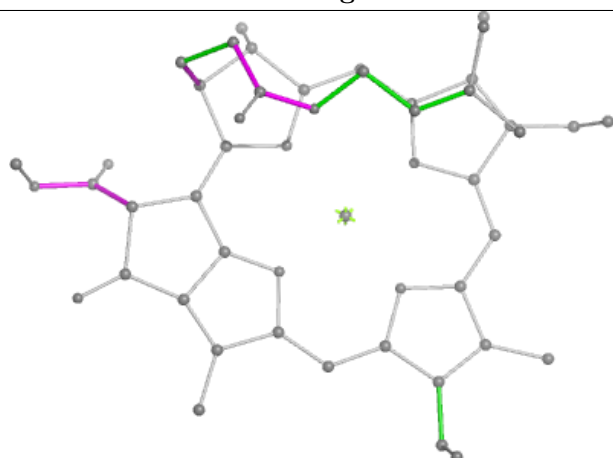
Ligand CLA E 824



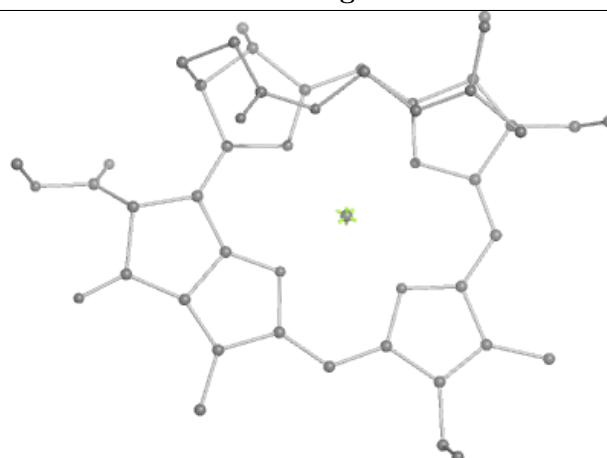
Bond lengths



Bond angles

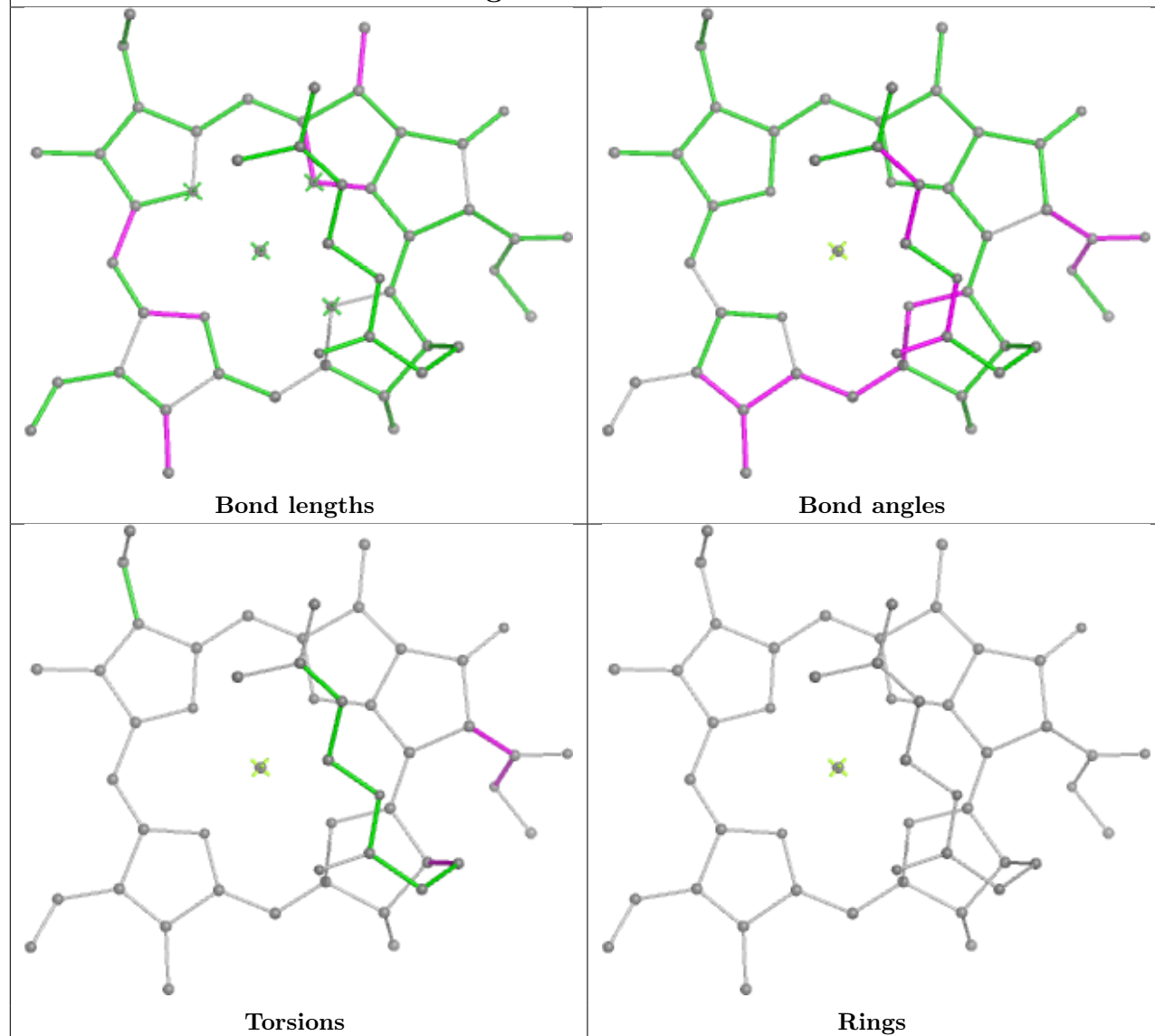


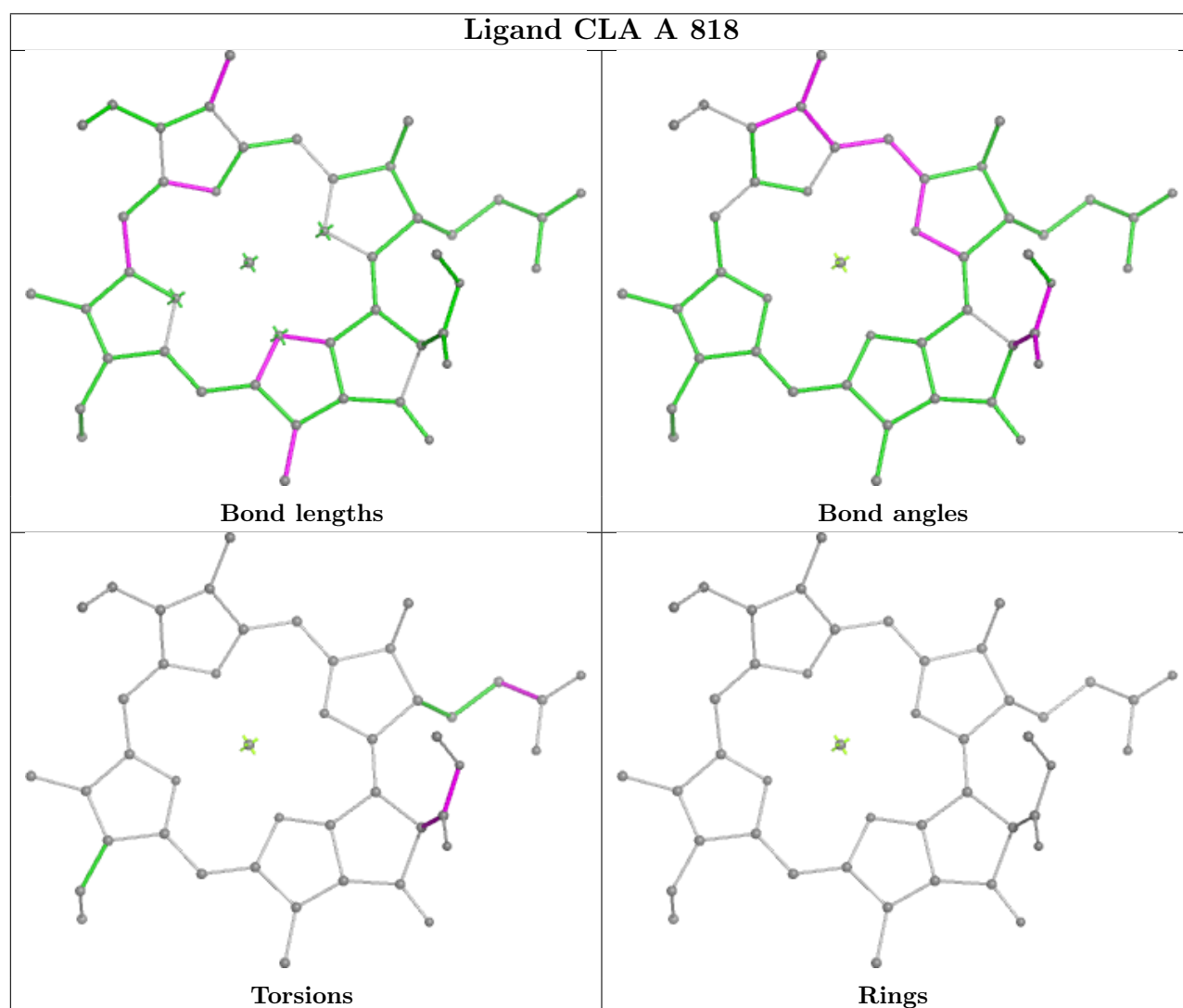
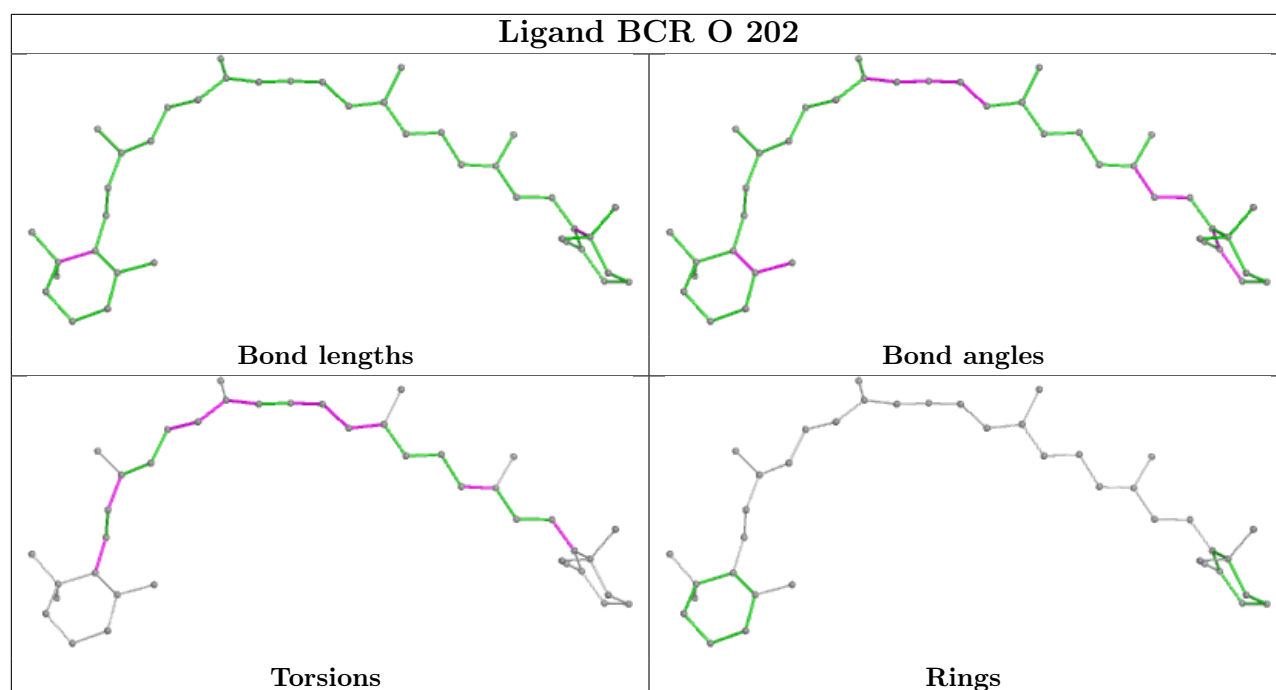
Torsions



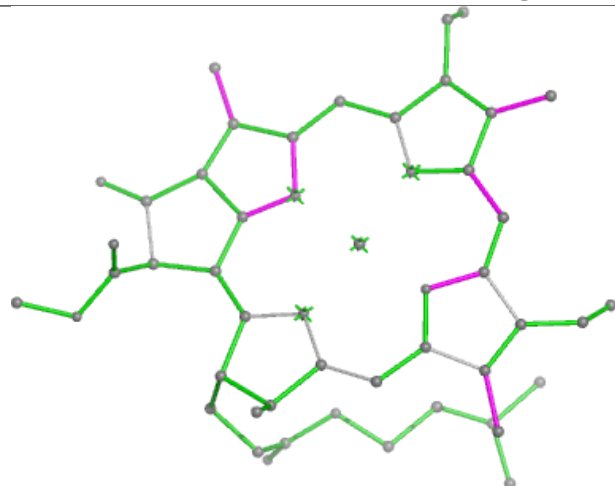
Rings

Ligand CLA e 841

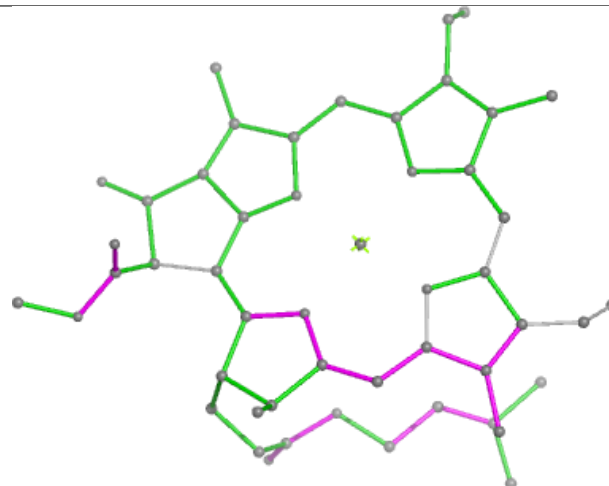




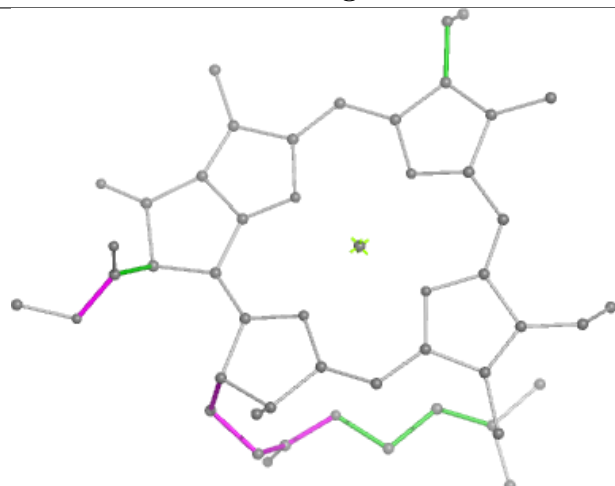
Ligand CLA A 822



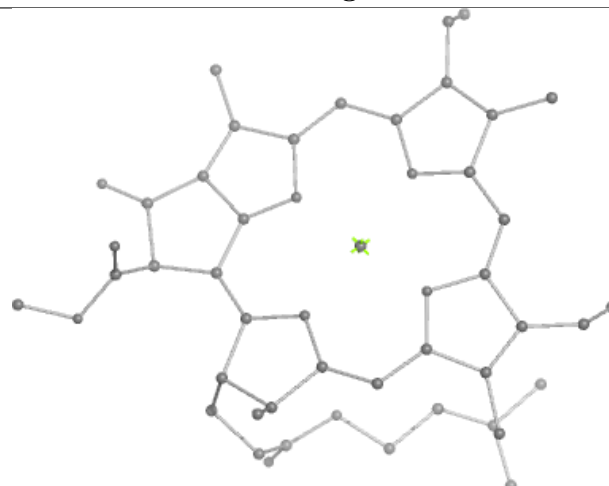
Bond lengths



Bond angles

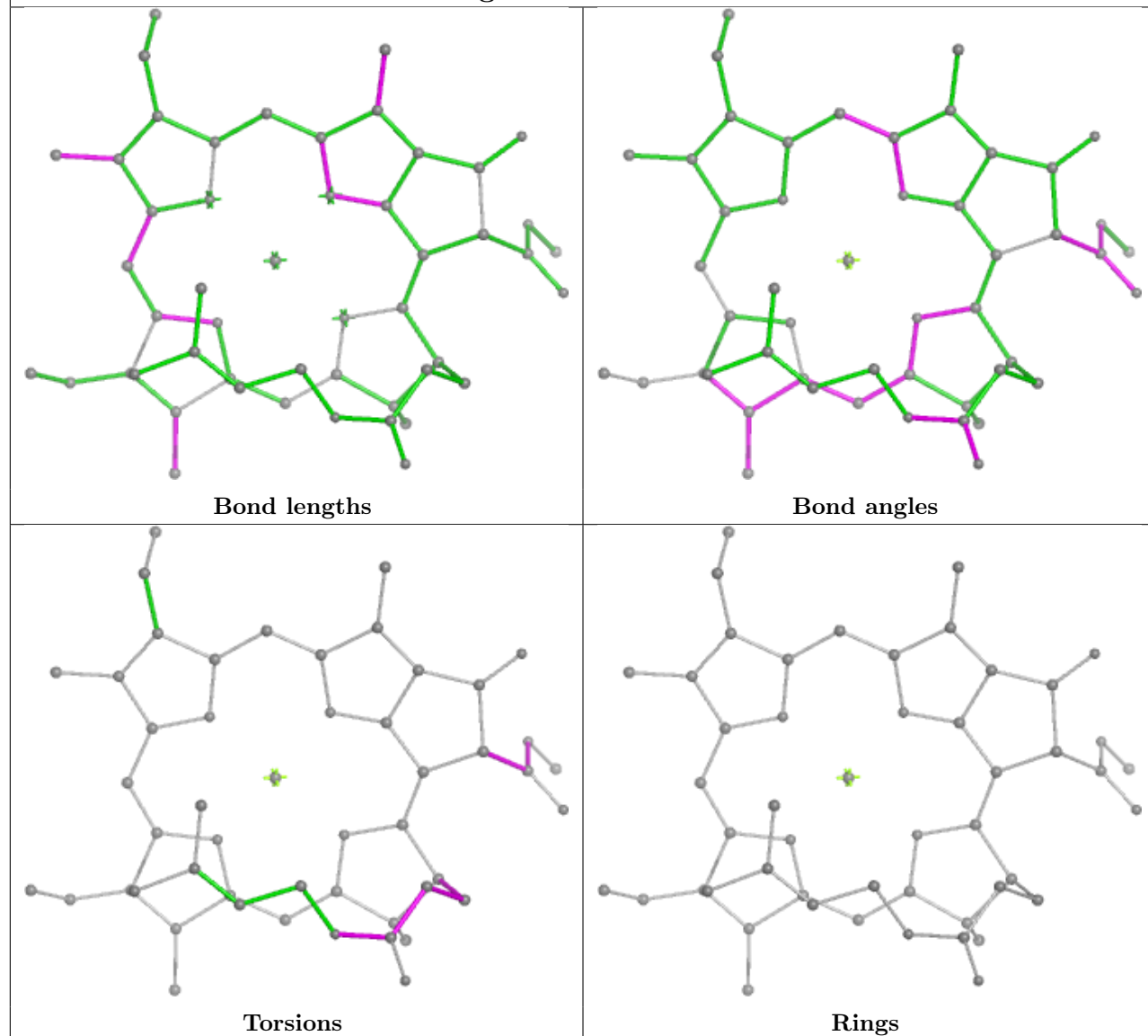


Torsions

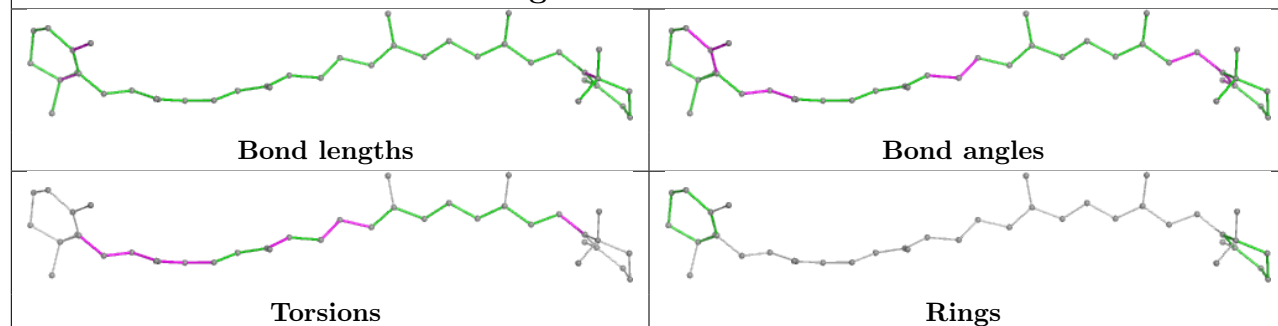


Rings

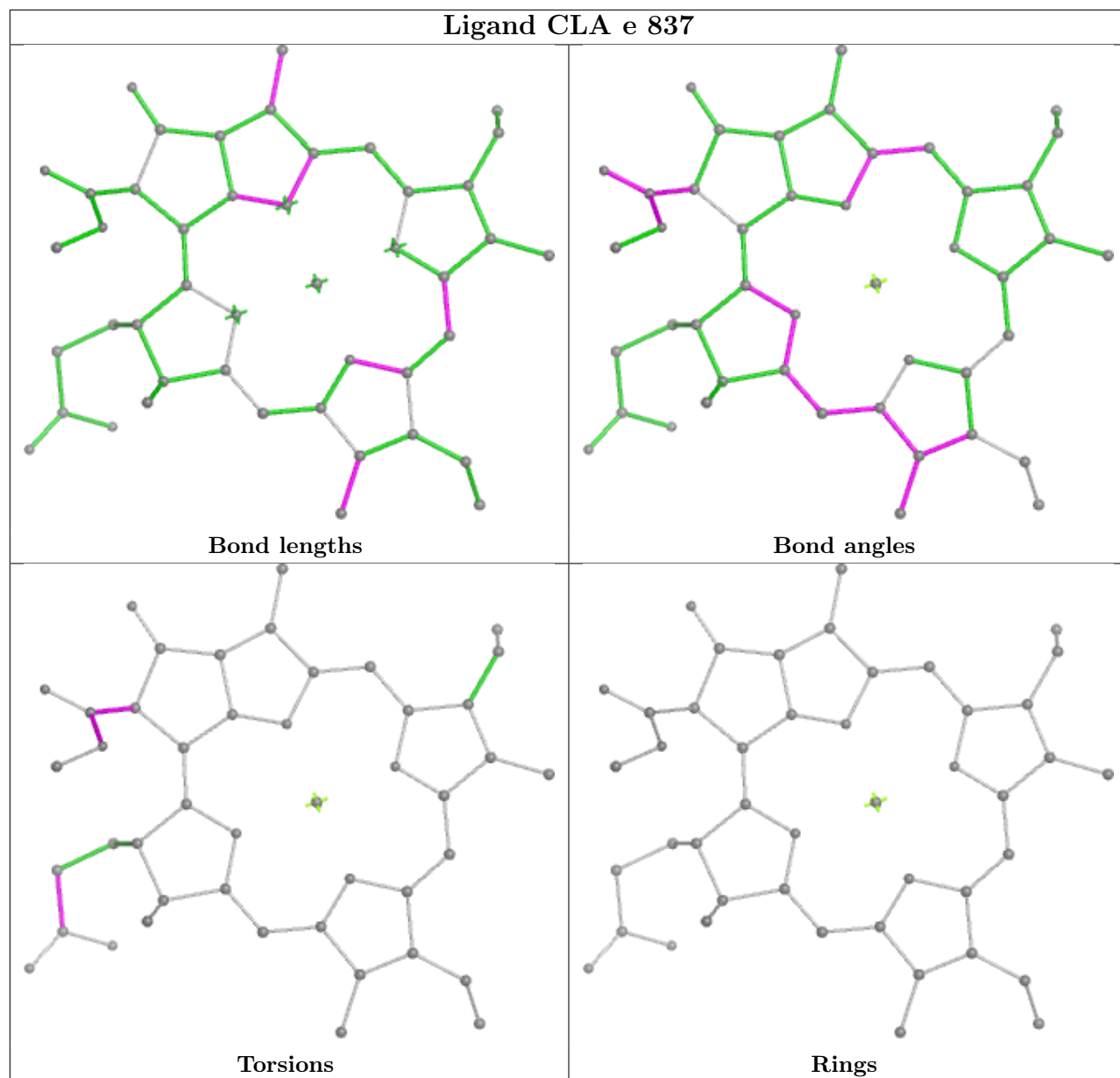
Ligand CLA E 827



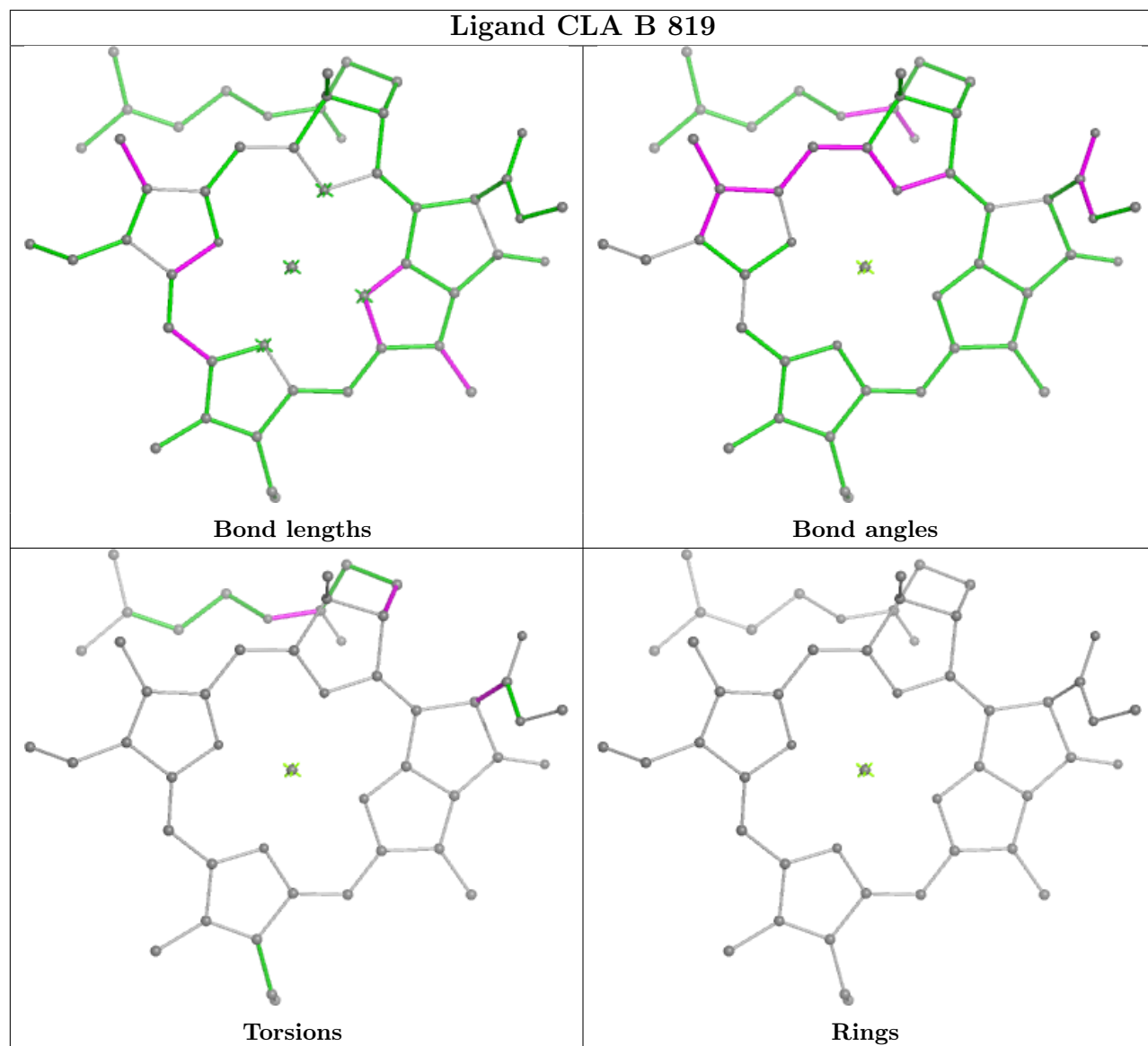
Ligand BCR G 847



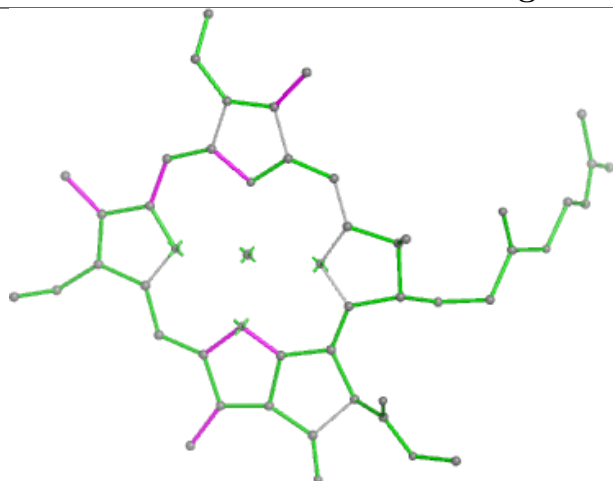
Ligand CLA e 837



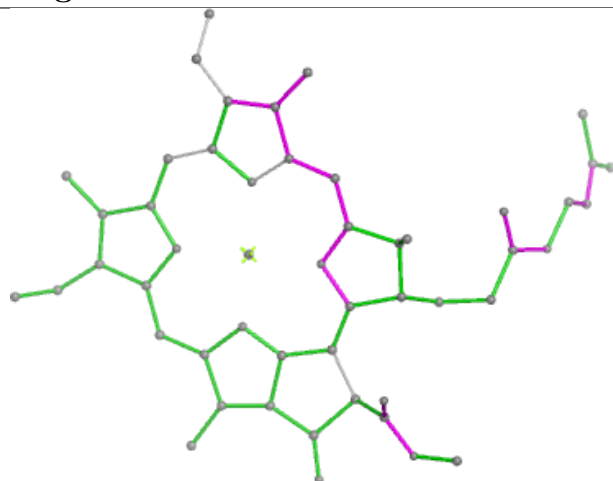
Ligand CLA B 819



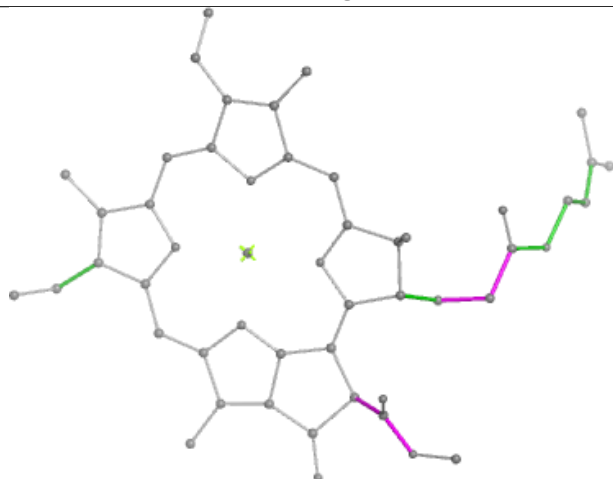
Ligand CLA g 812



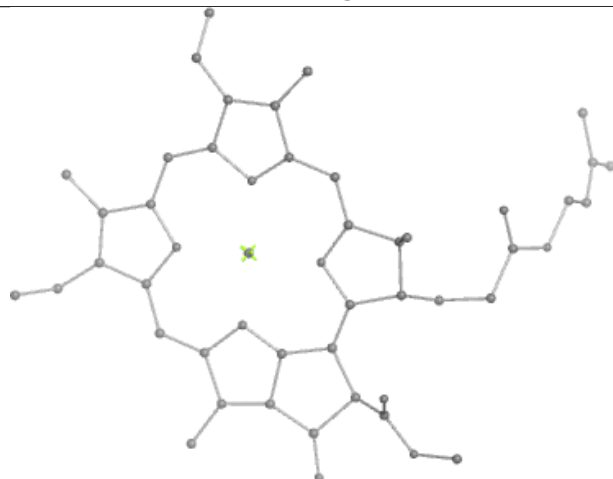
Bond lengths



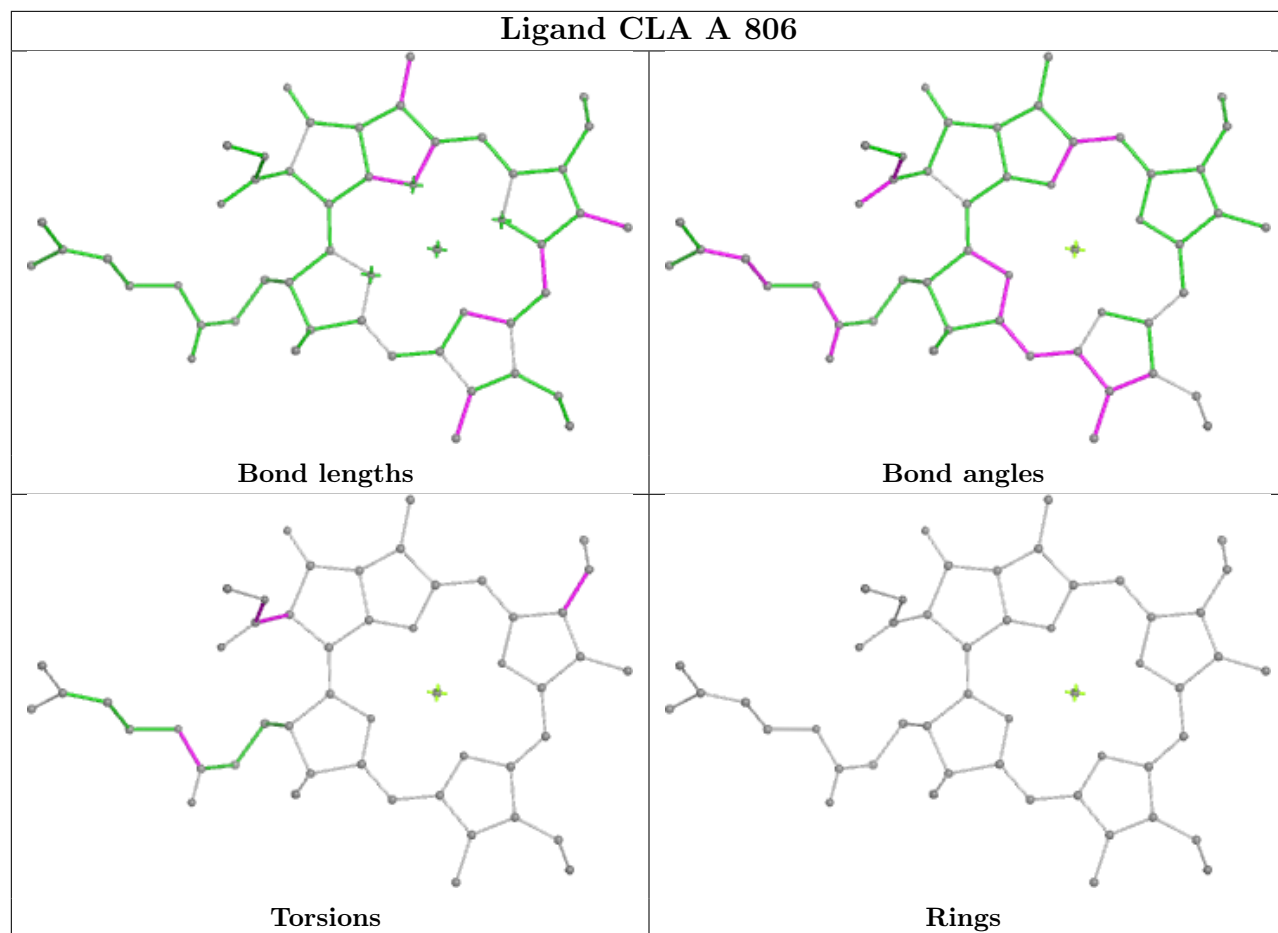
Bond angles

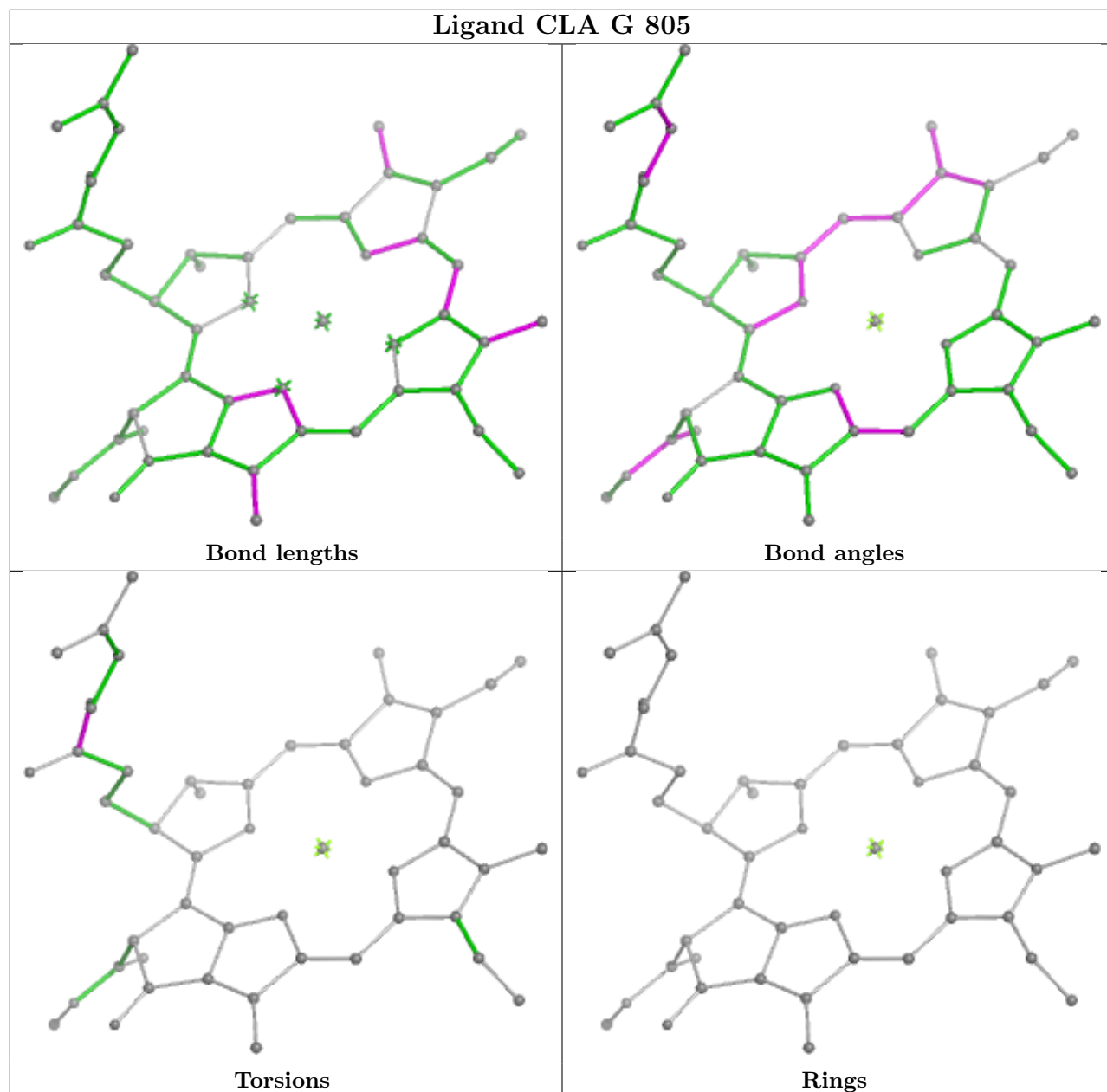


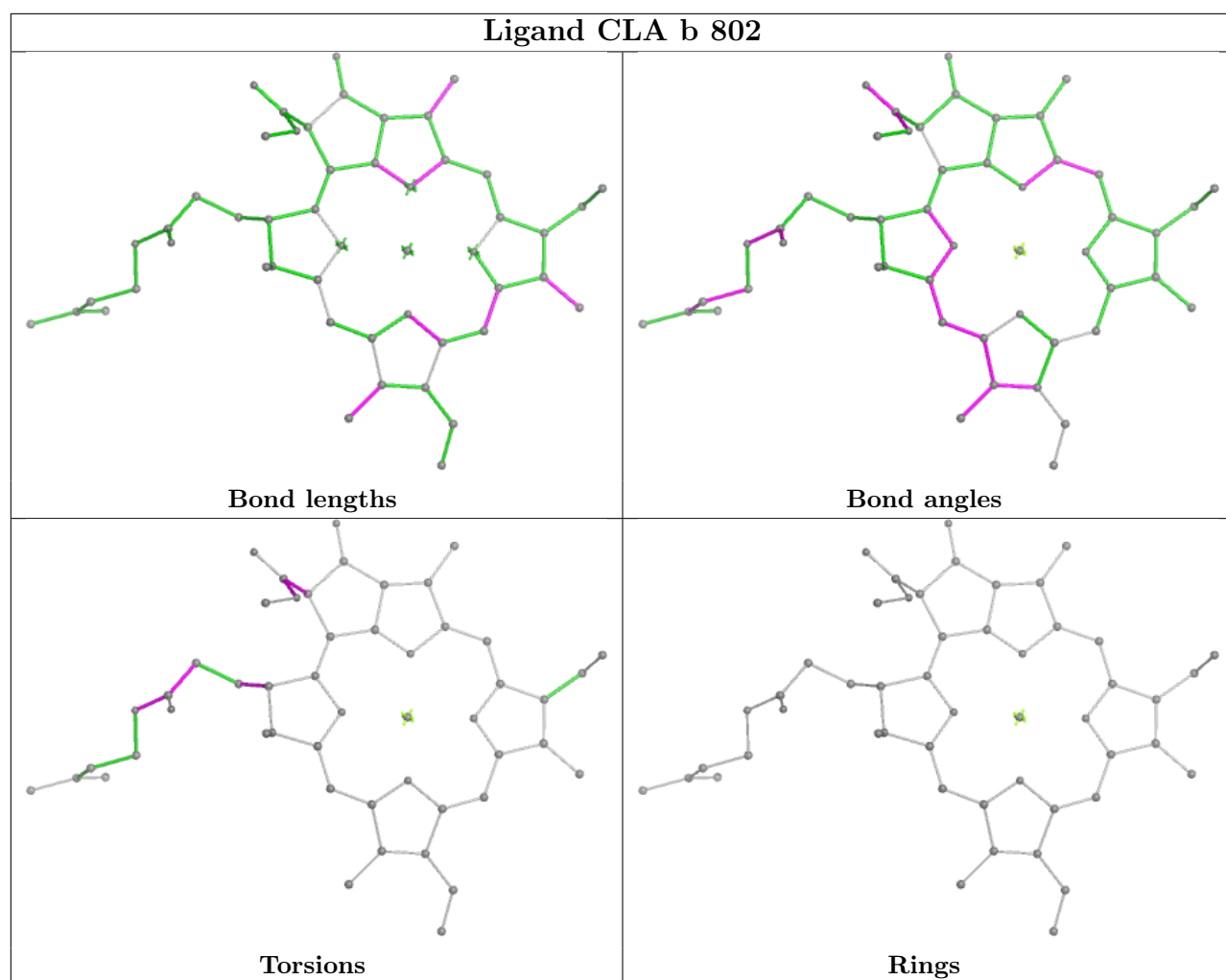
Torsions



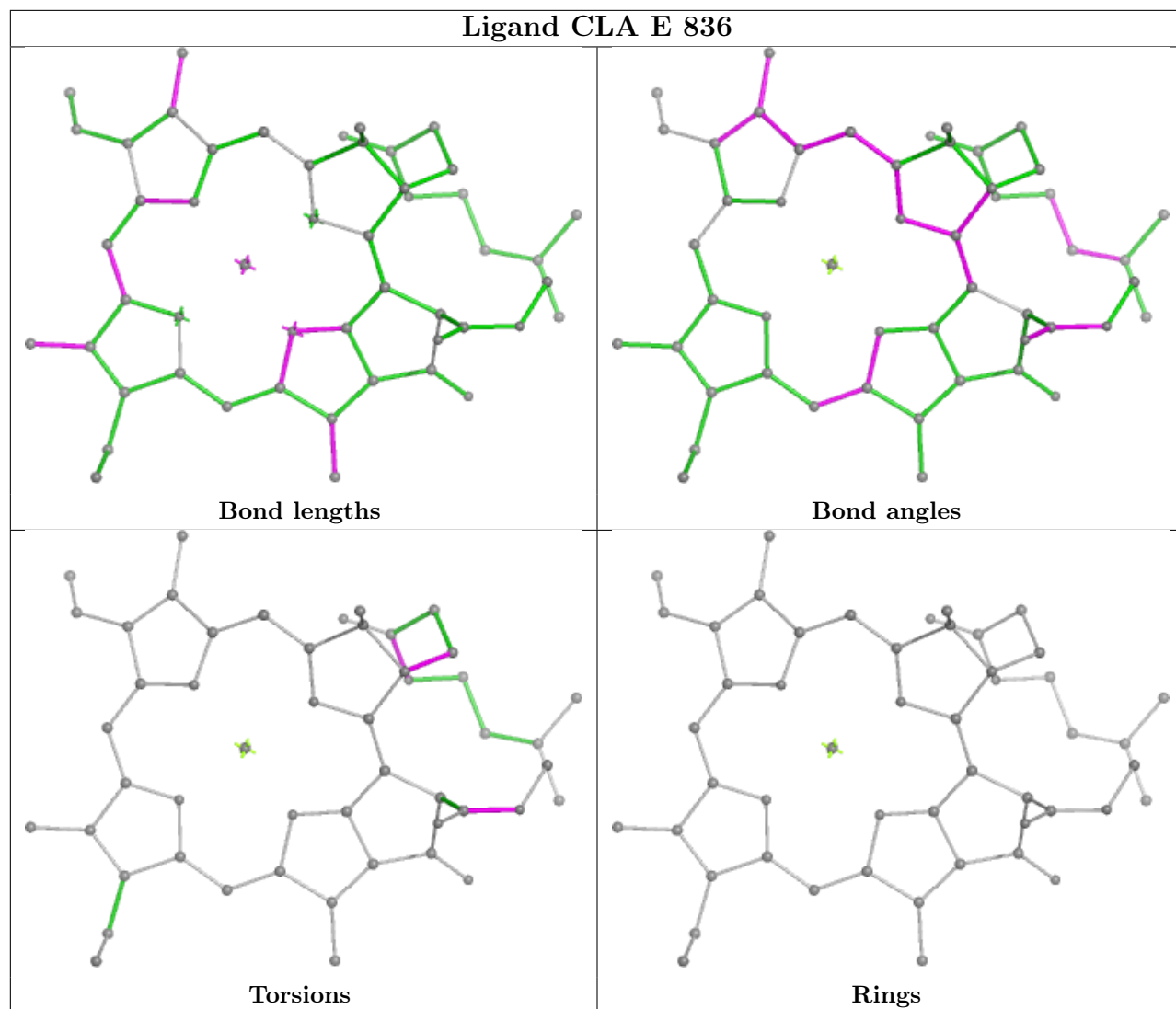
Rings



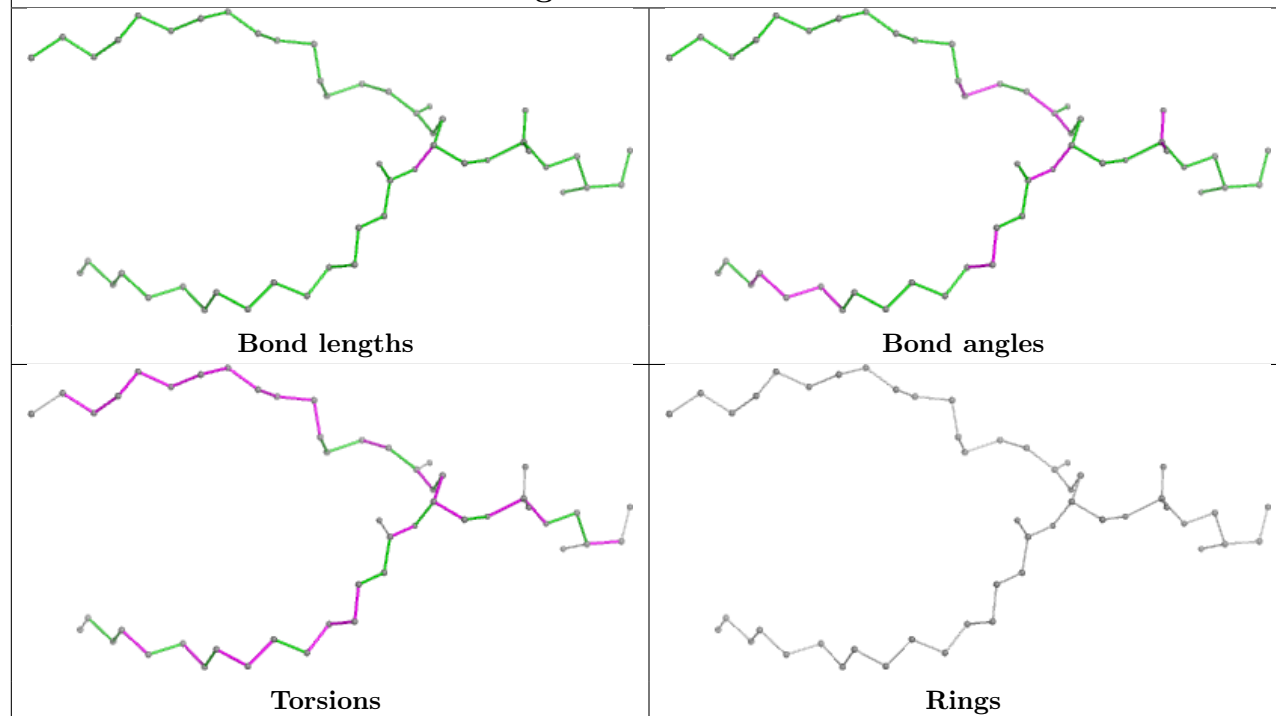




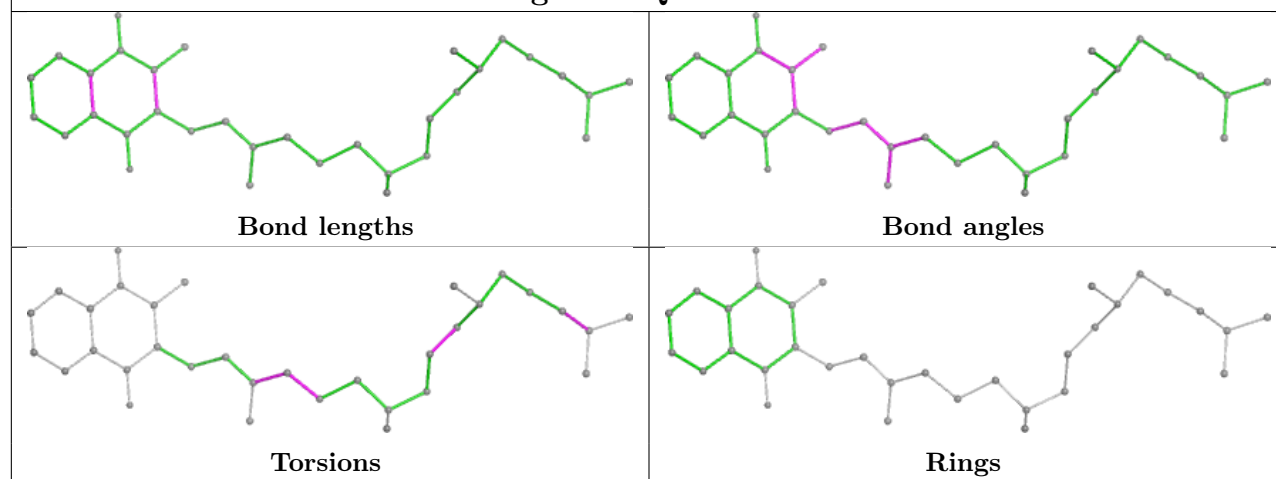
Ligand CLA E 836



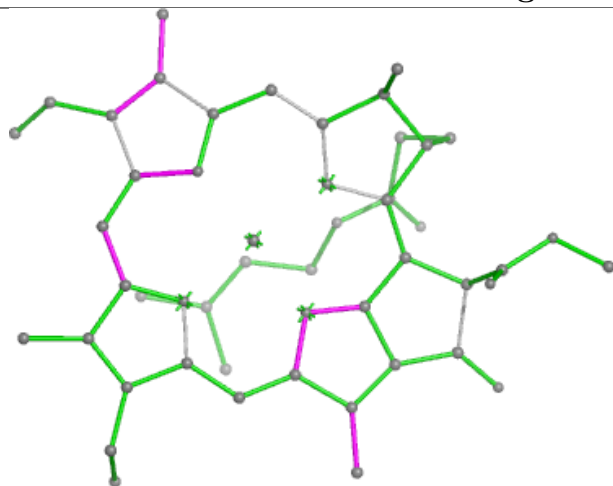
Ligand LHG e 801



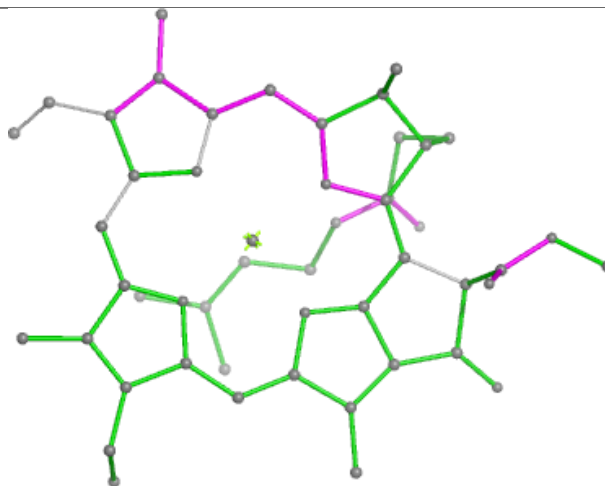
Ligand PQN E 848



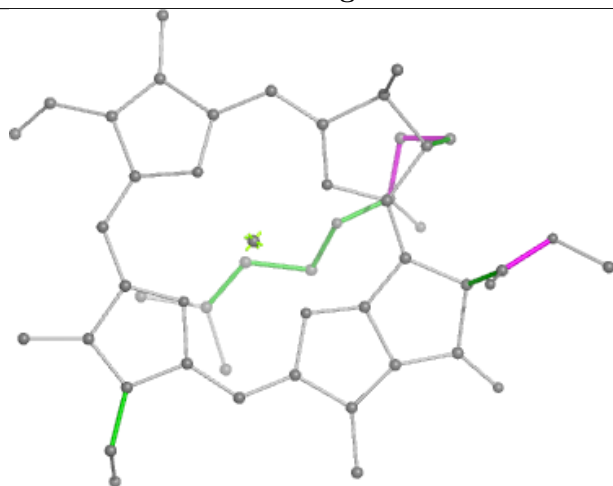
Ligand CLA b 808



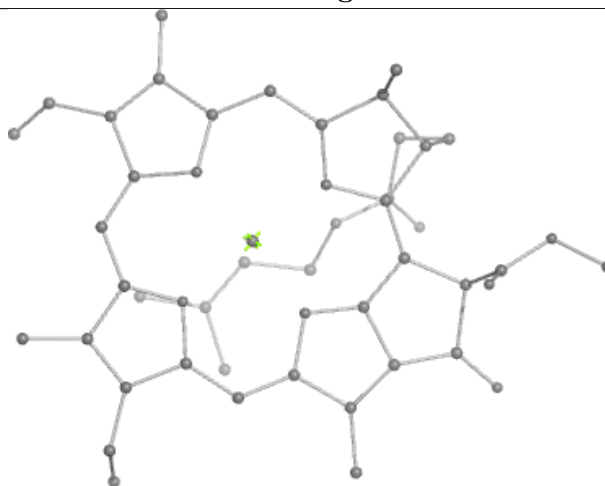
Bond lengths



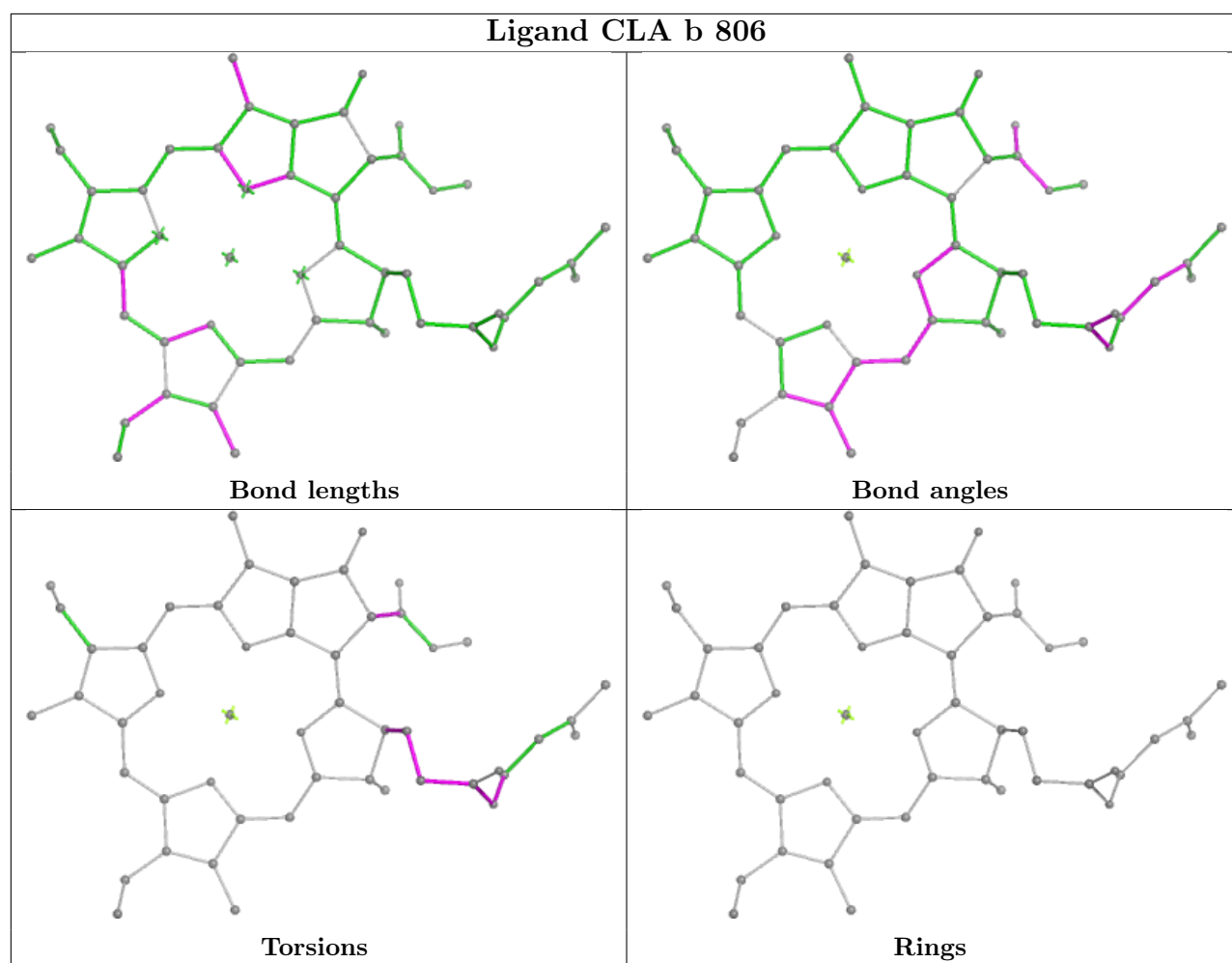
Bond angles



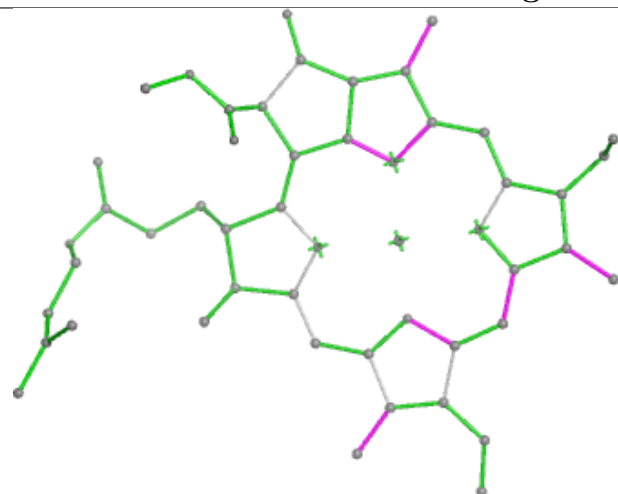
Torsions



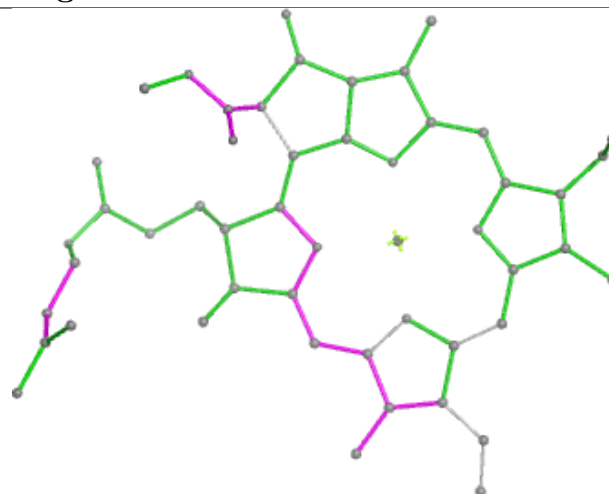
Rings



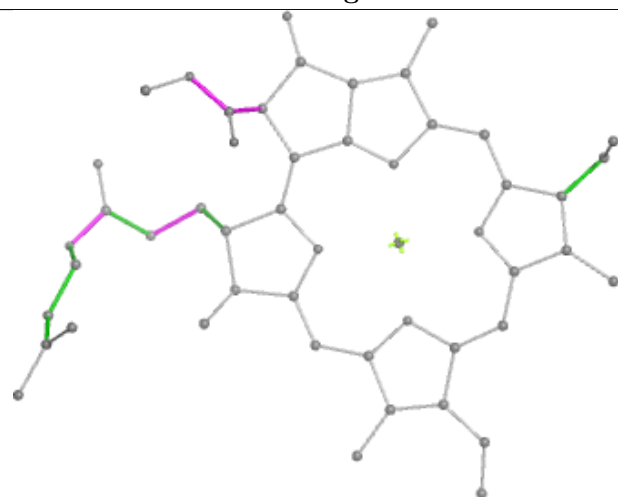
Ligand CLA g 826



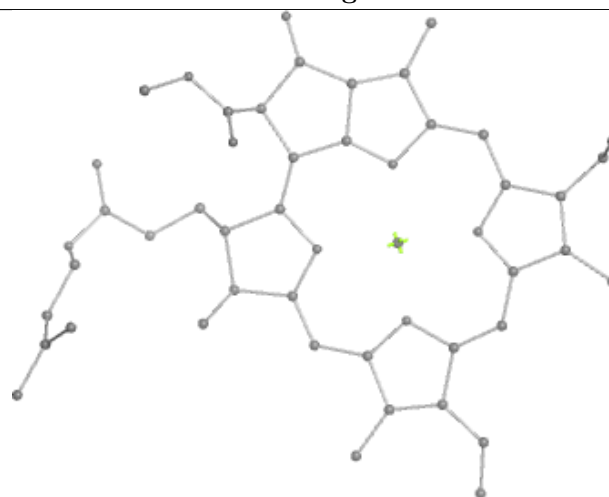
Bond lengths



Bond angles

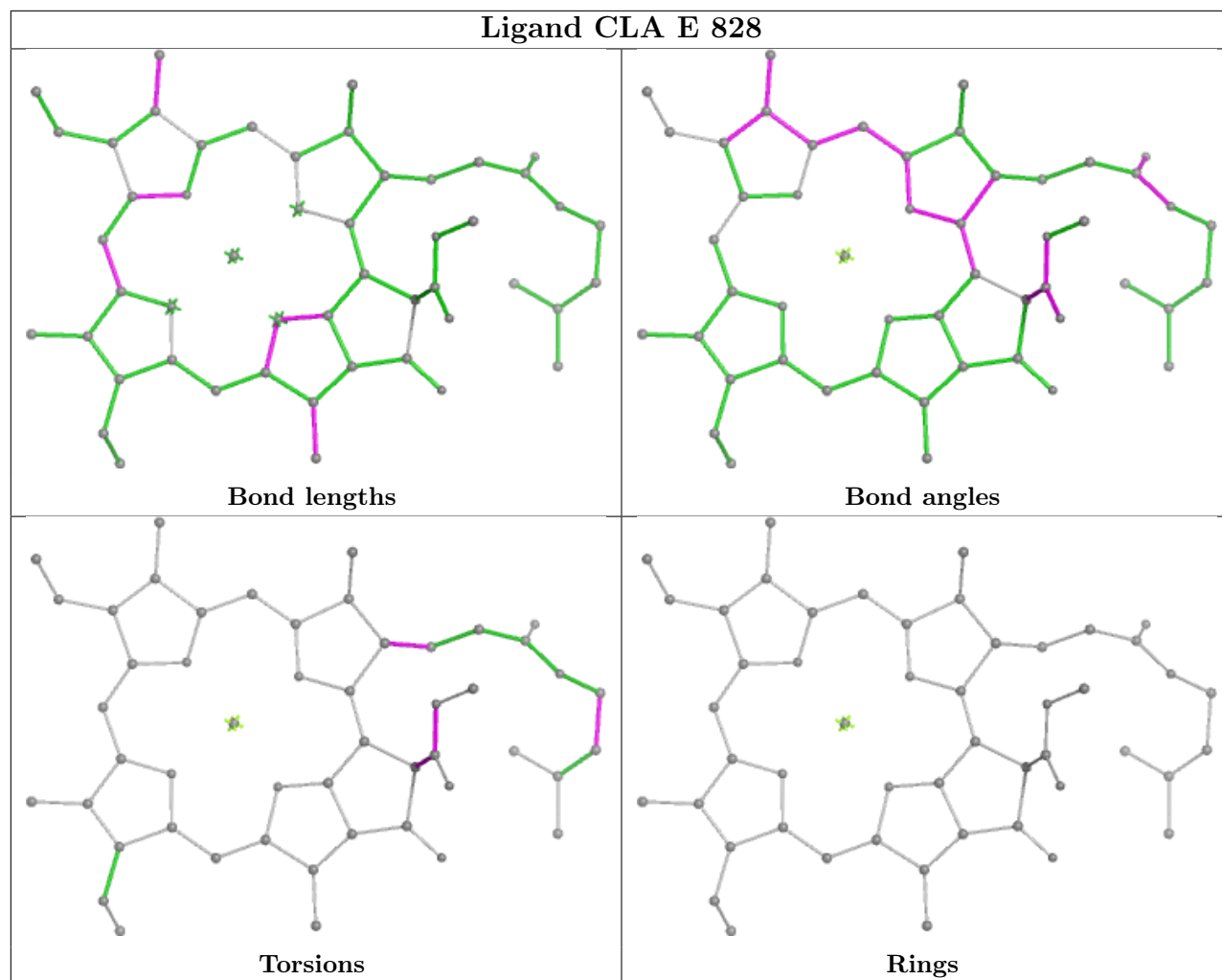


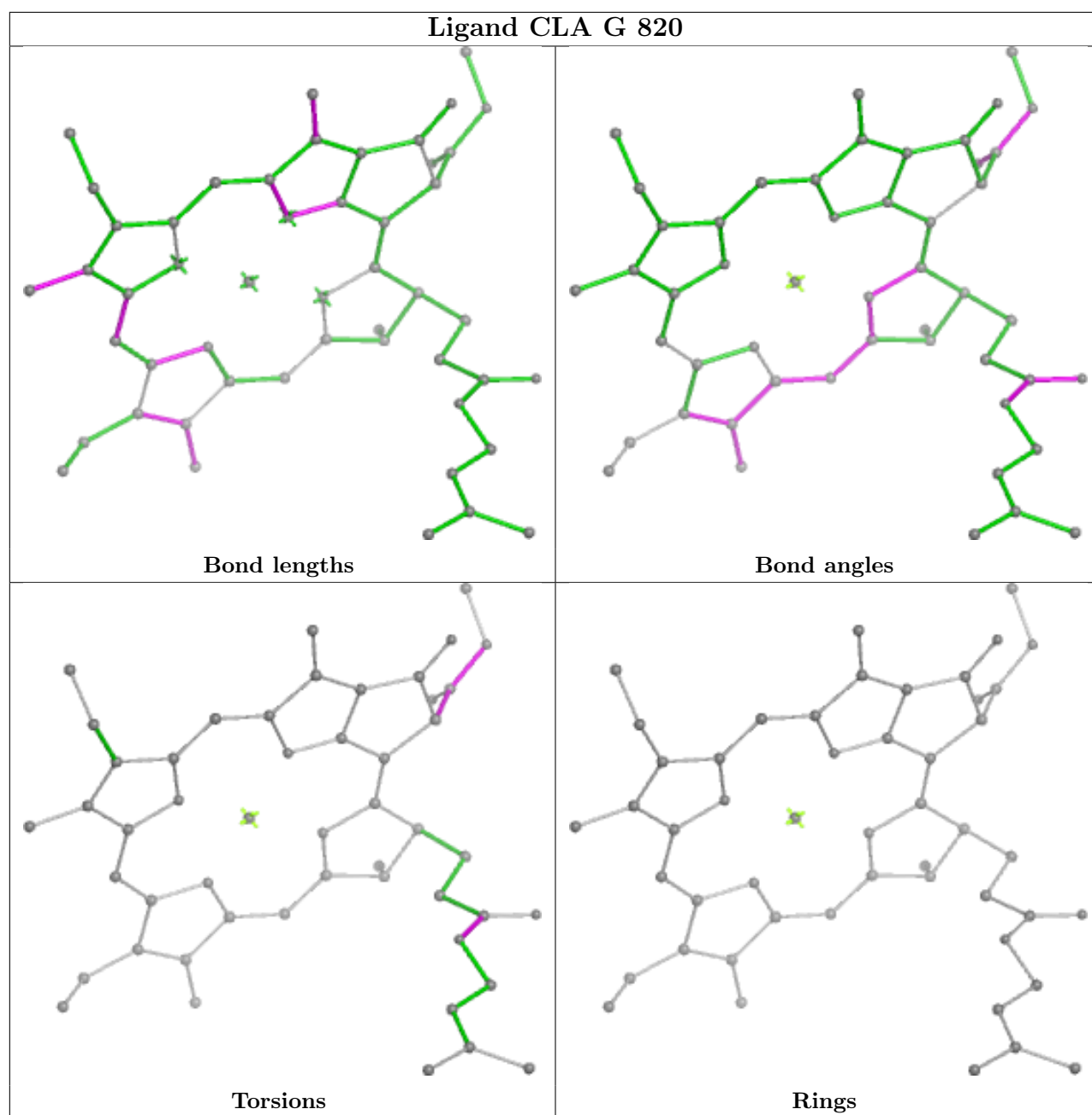
Torsions



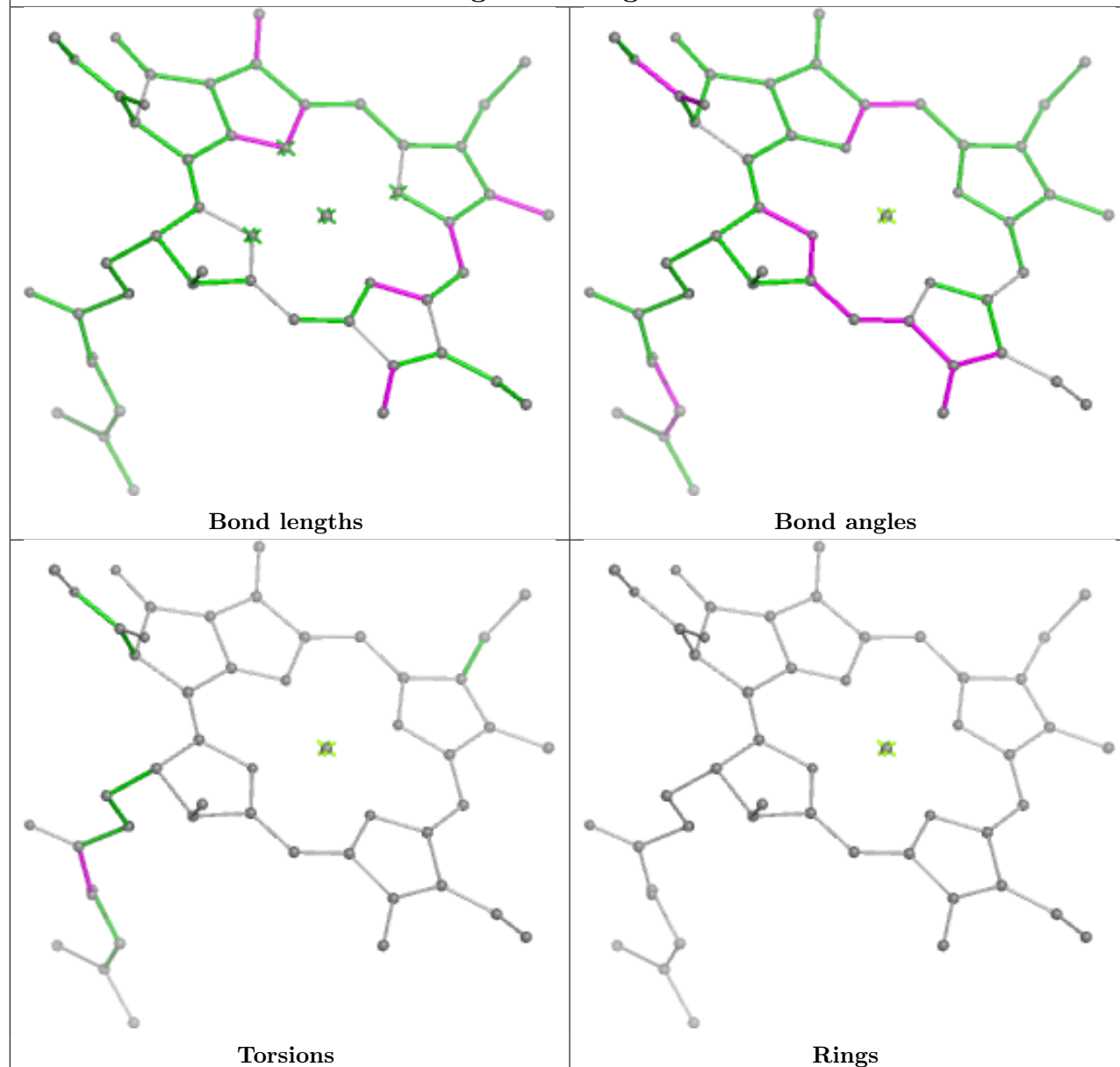
Rings

Ligand CLA E 828

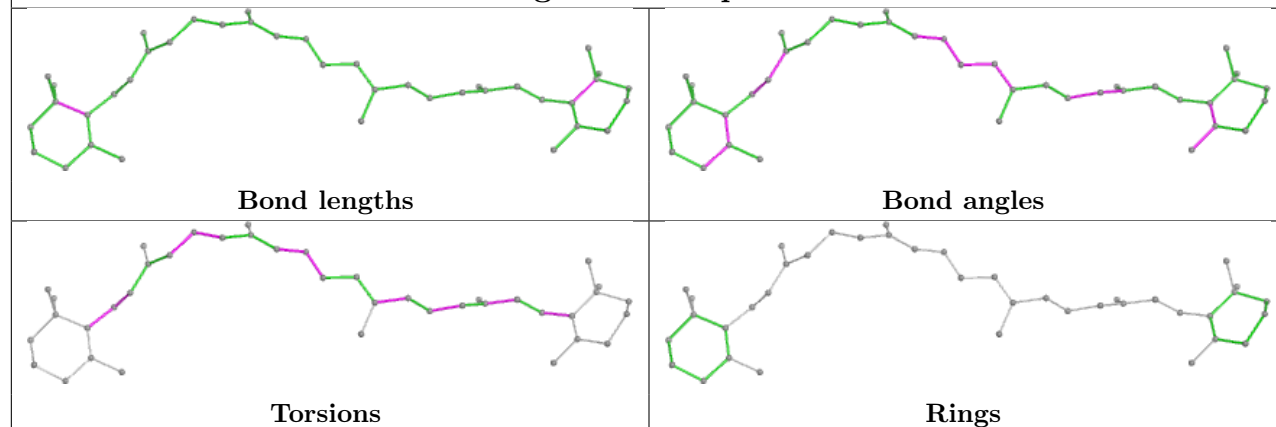




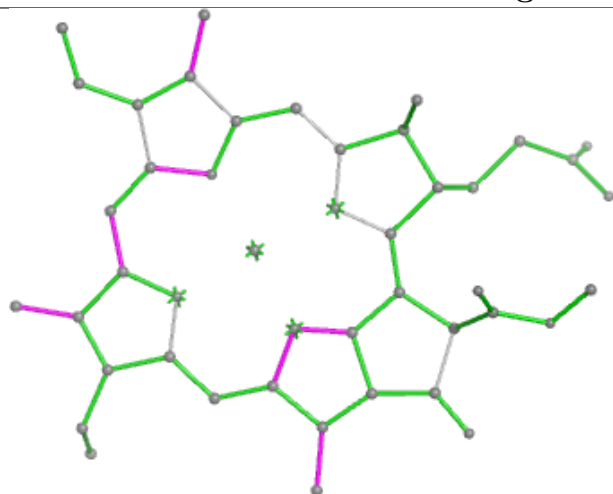
Ligand CLA g 807



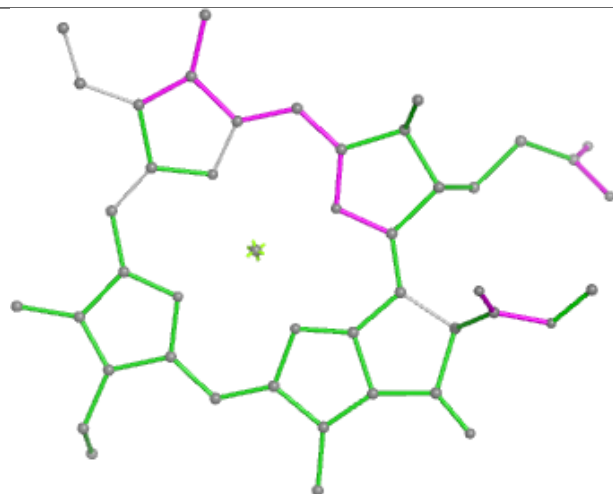
Ligand BCR q 101



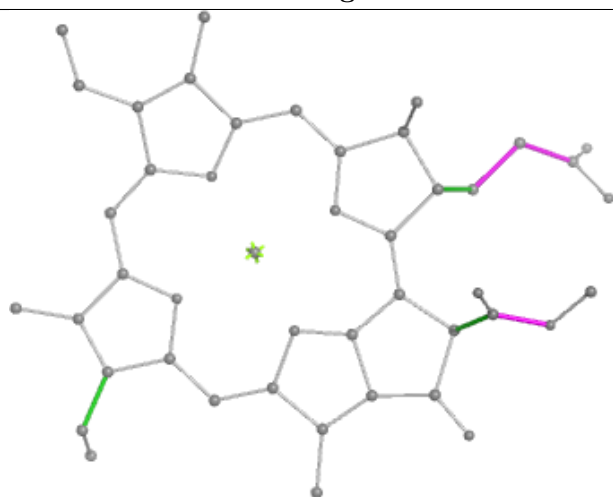
Ligand CLA L 203



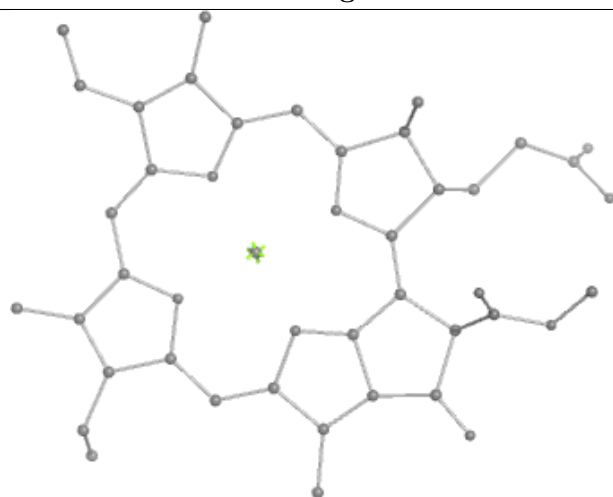
Bond lengths



Bond angles

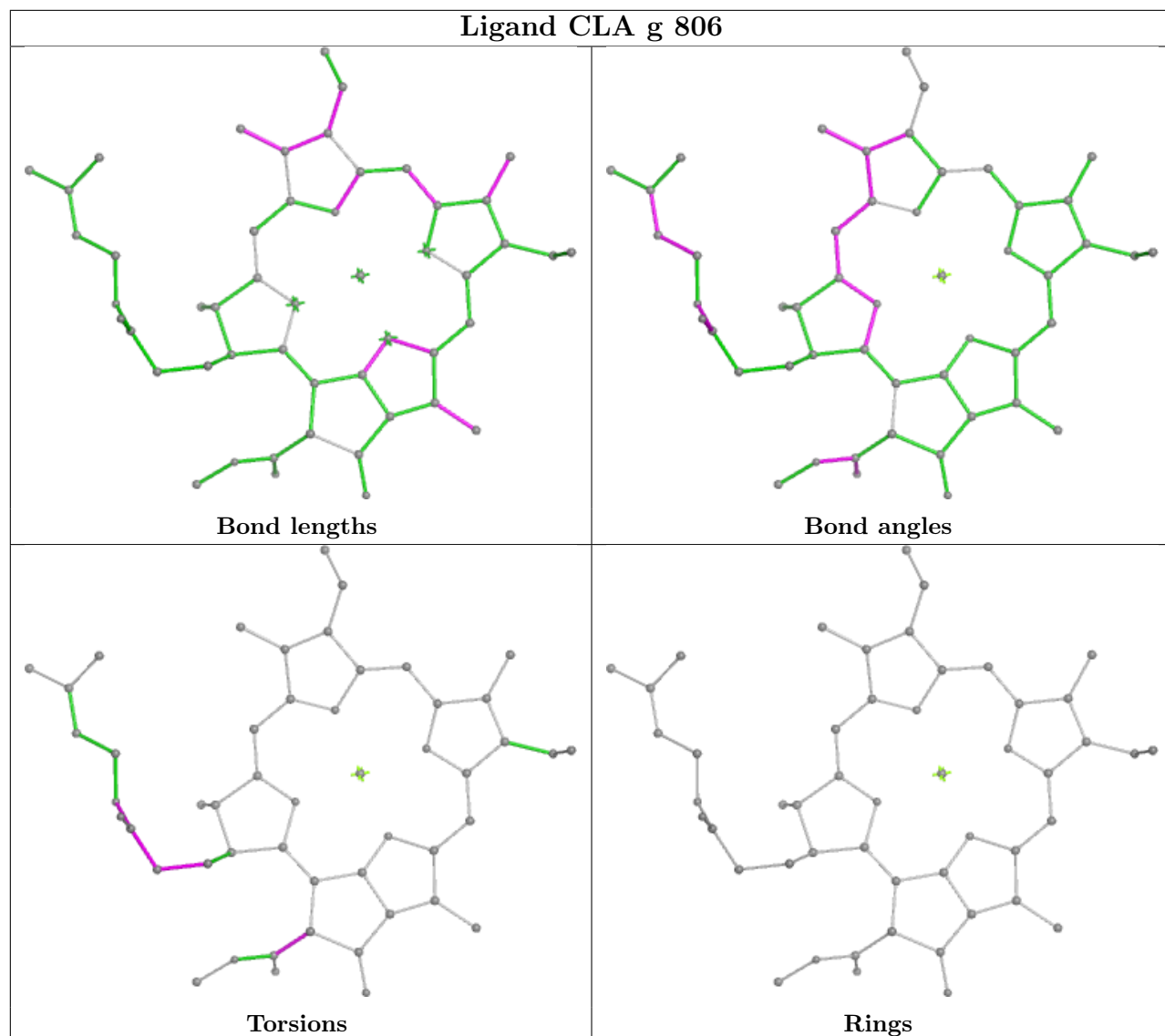


Torsions

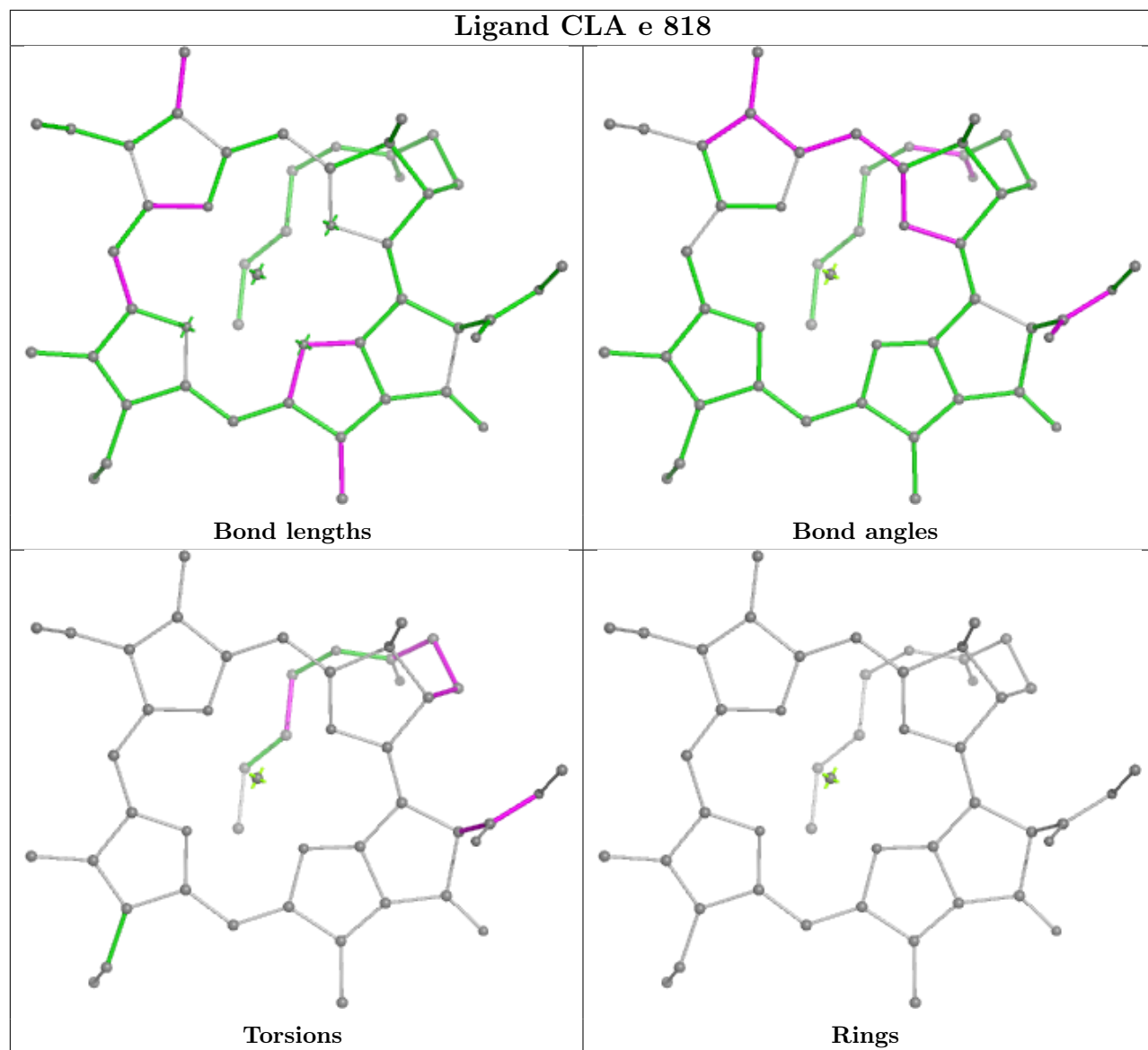


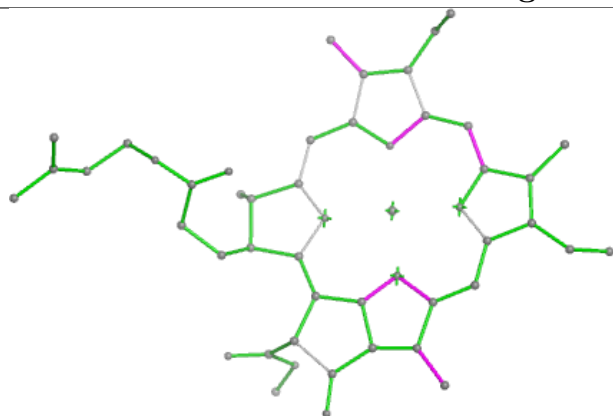
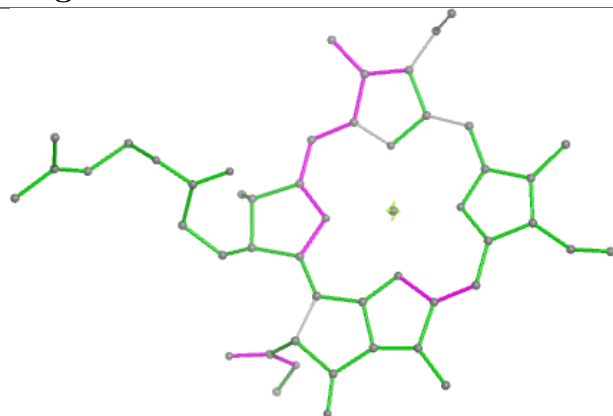
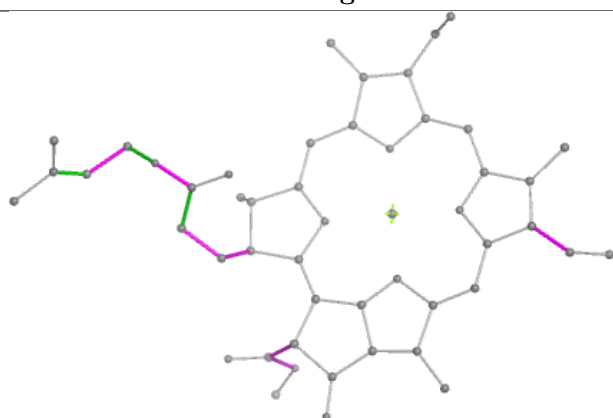
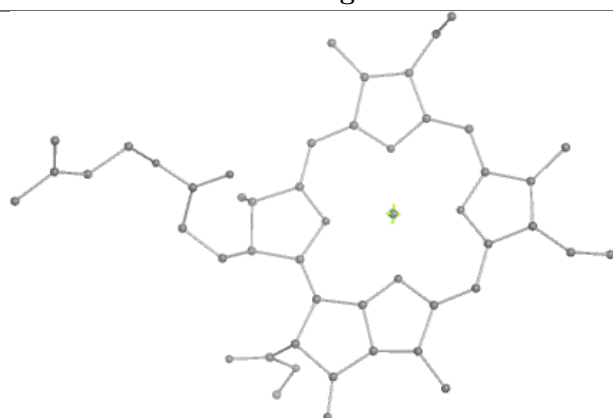
Rings

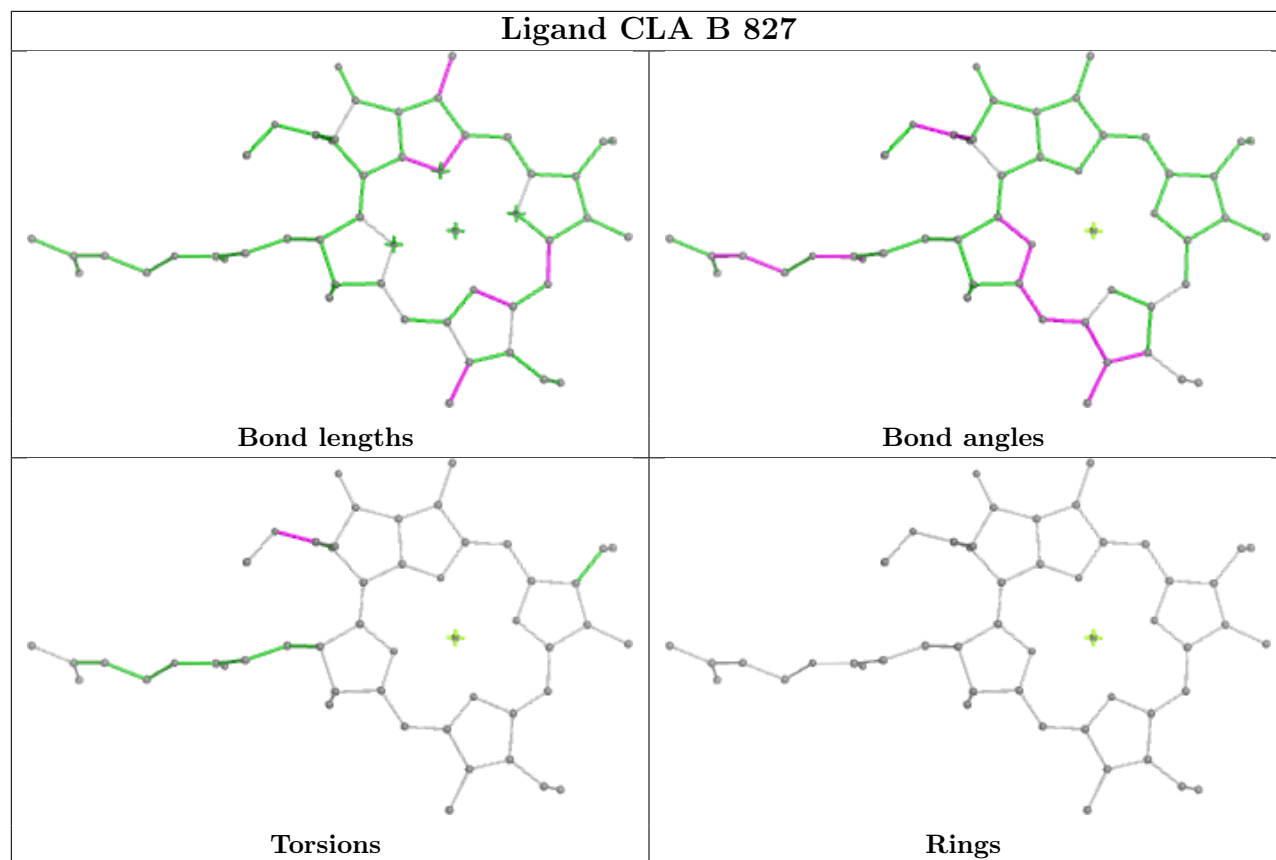
Ligand CLA g 806



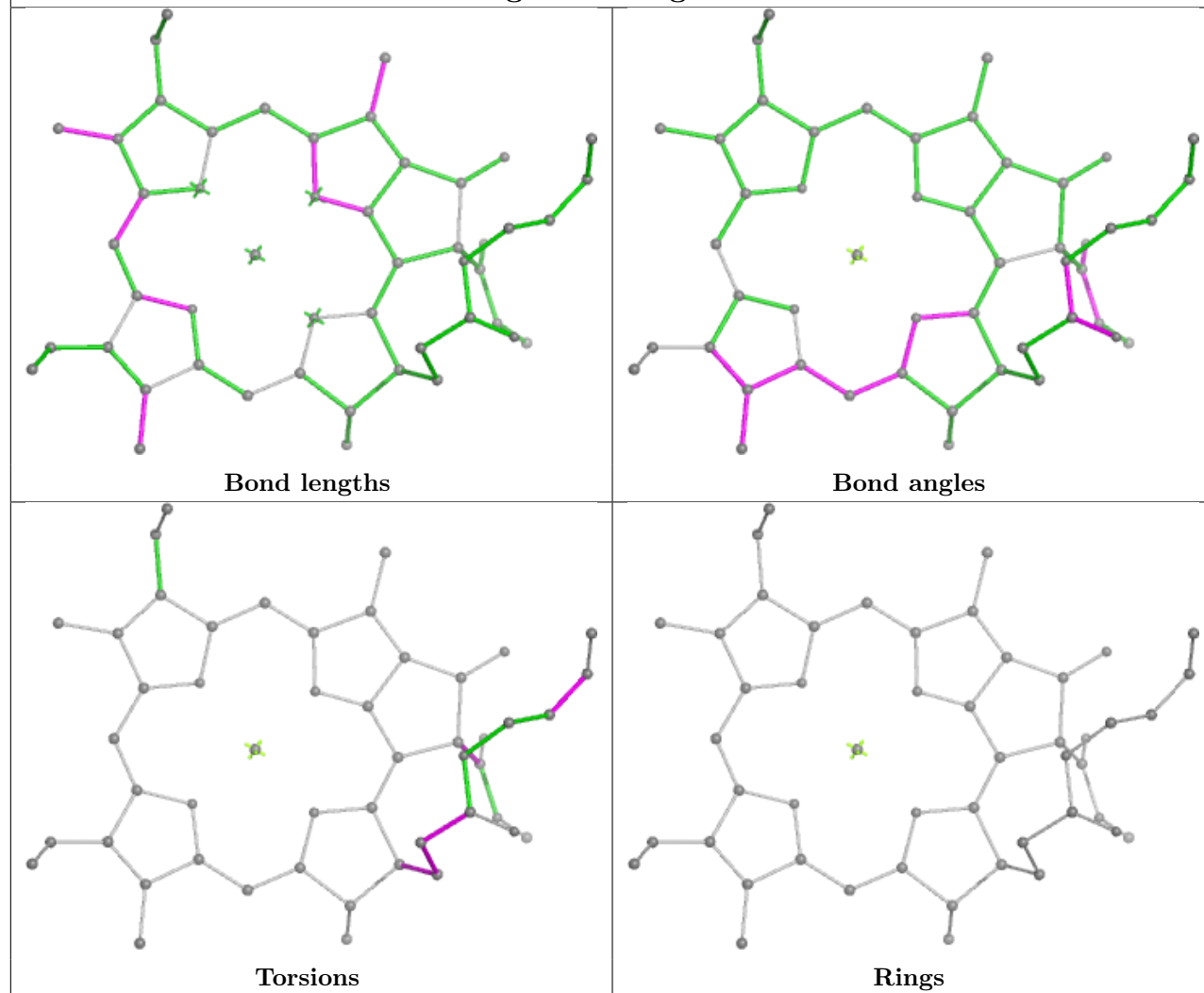
Ligand CLA e 818



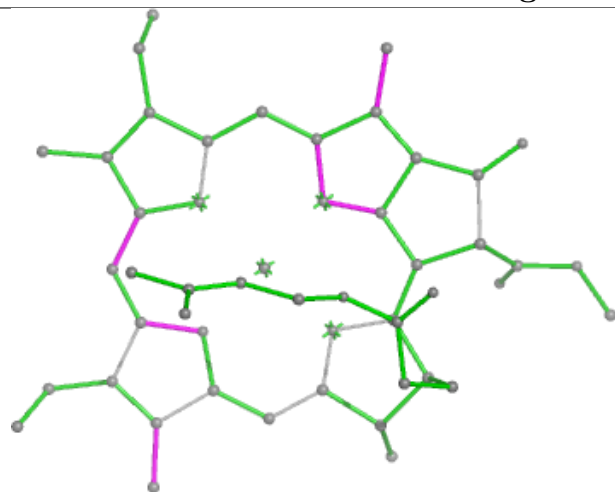
Ligand CLA g 813**Bond lengths****Bond angles****Torsions****Rings**



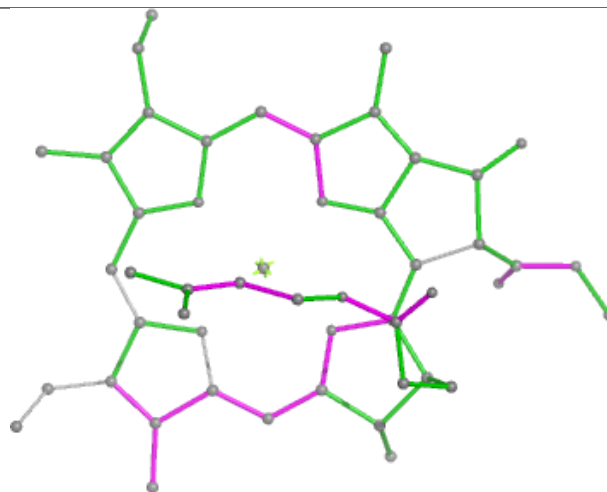
Ligand CLA g 833



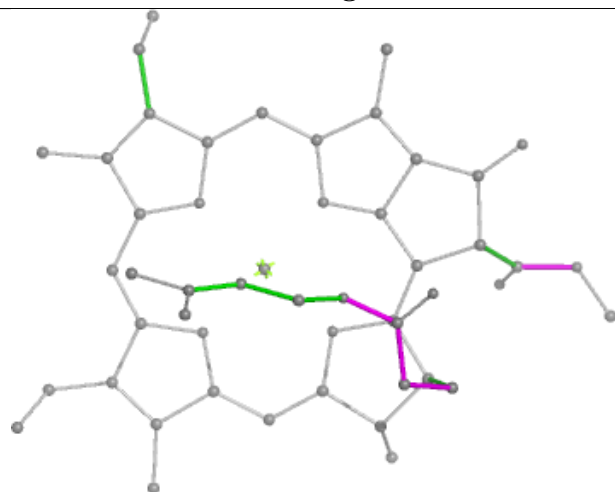
Ligand CLA b 837



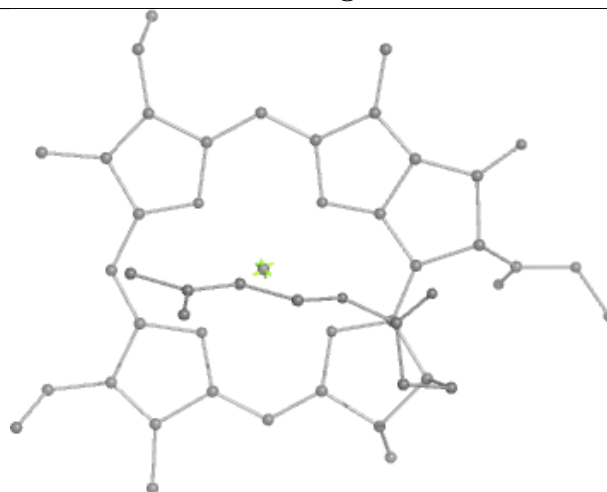
Bond lengths



Bond angles

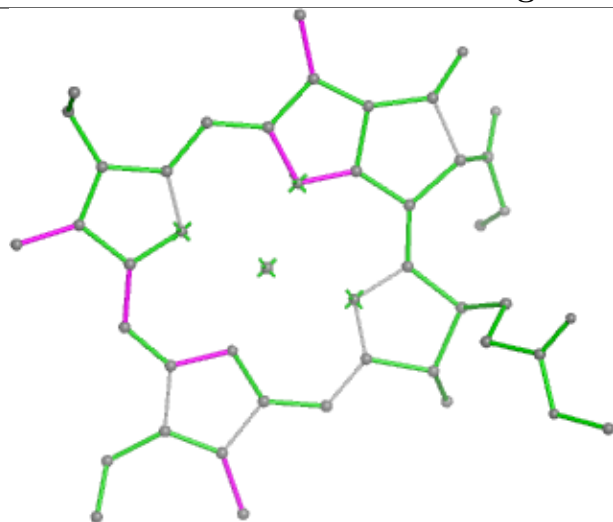


Torsions

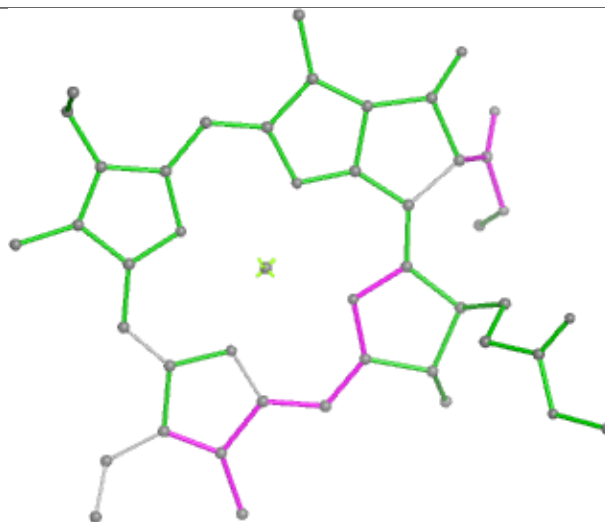


Rings

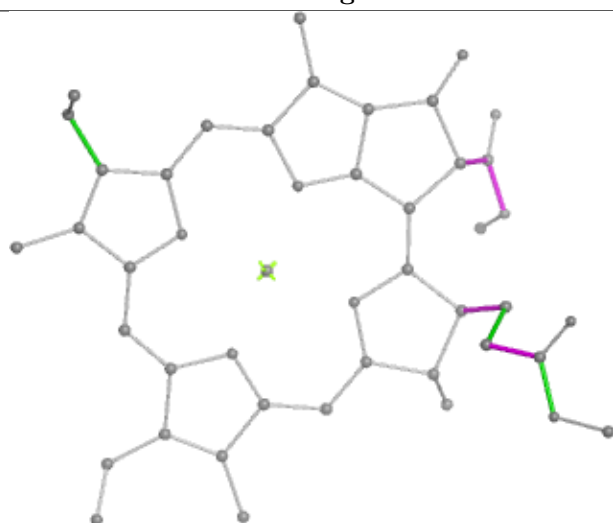
Ligand CLA b 825



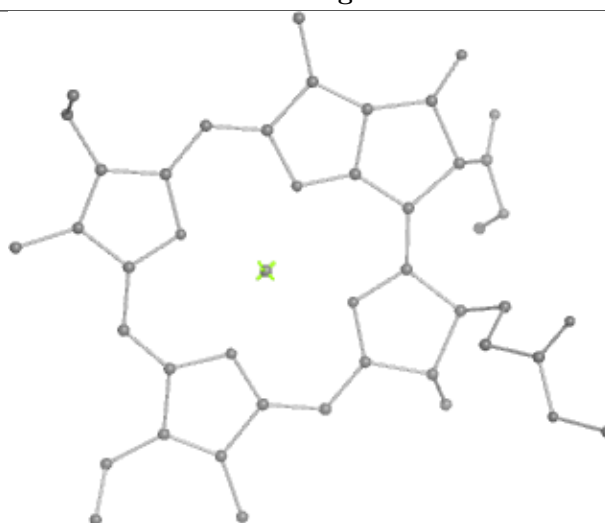
Bond lengths



Bond angles

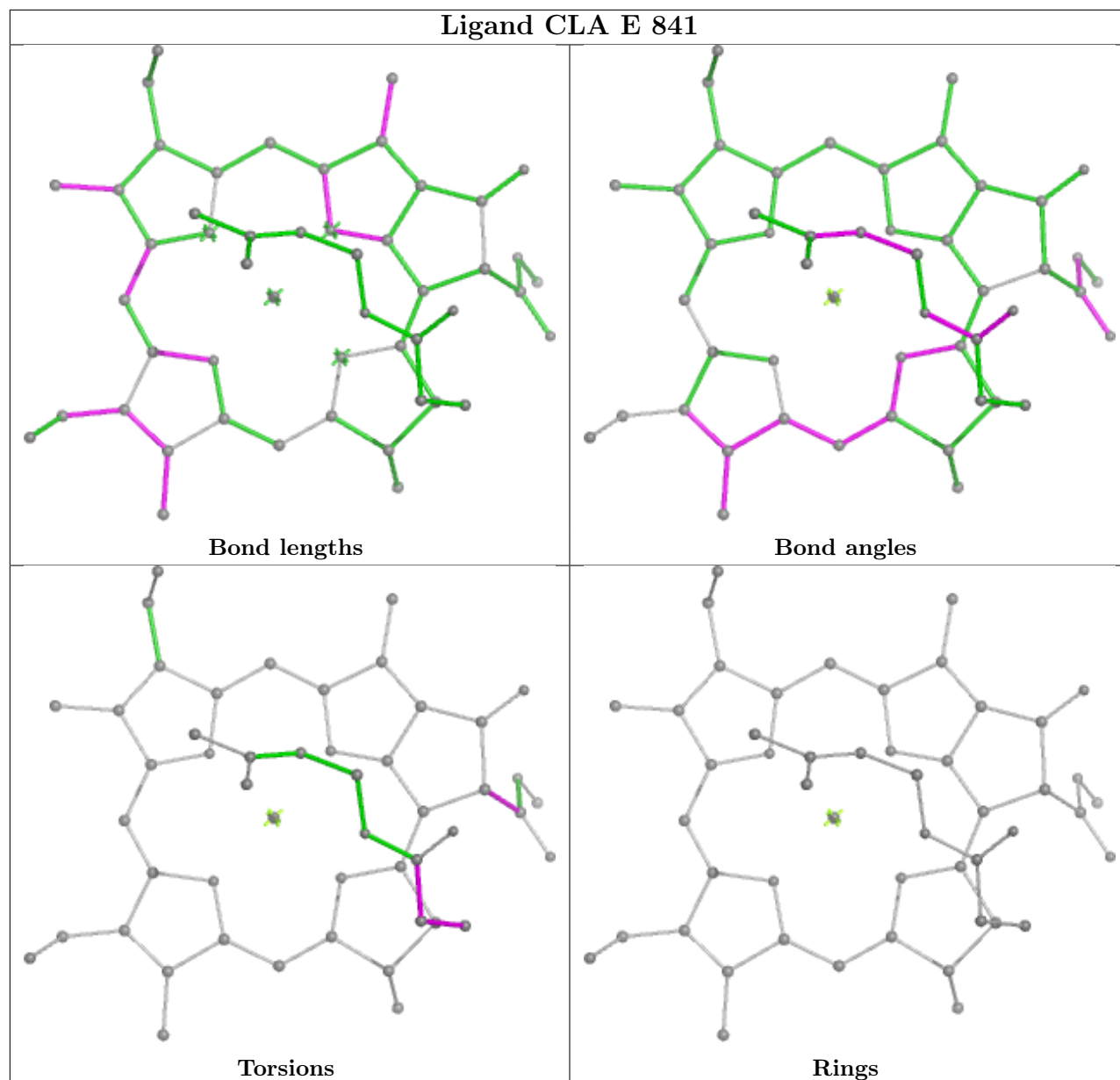


Torsions

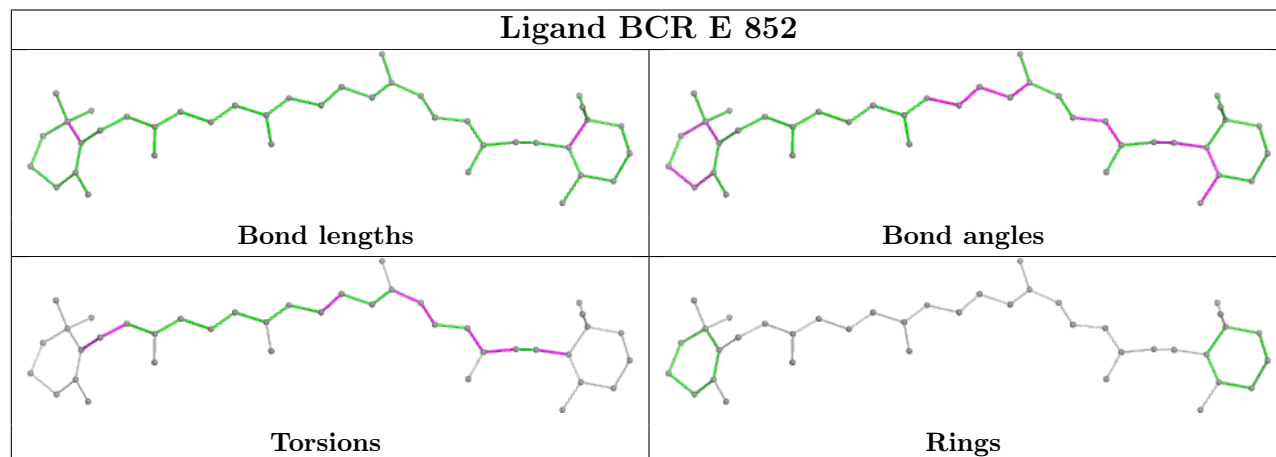


Rings

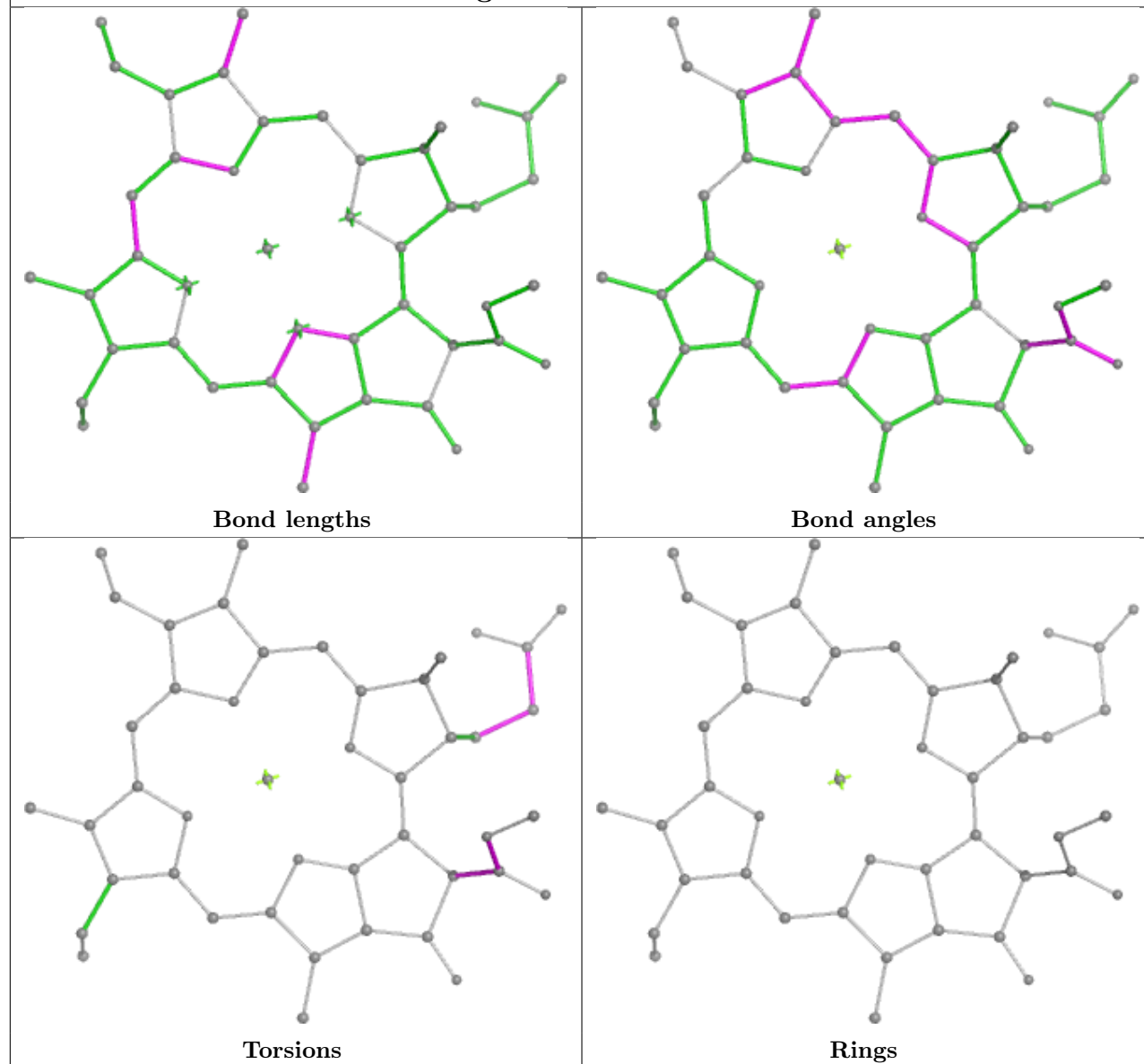
Ligand CLA E 841



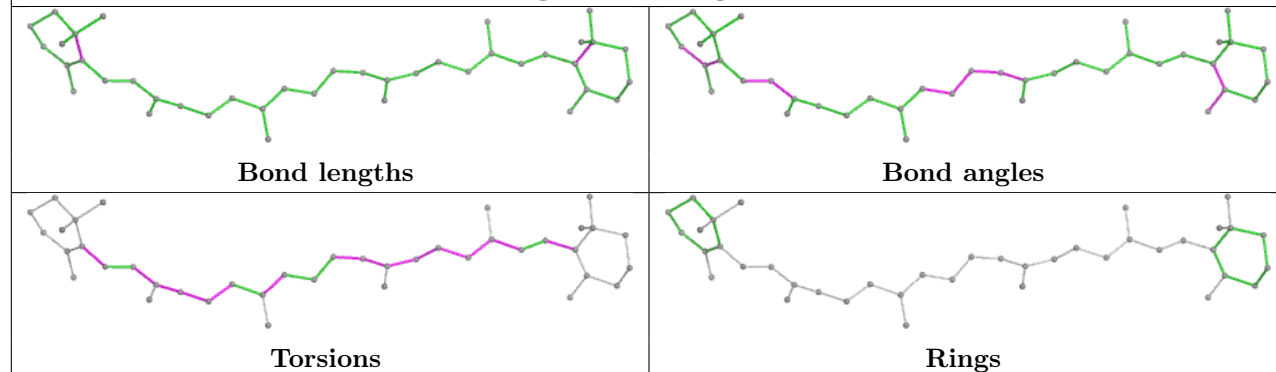
Ligand BCR E 852



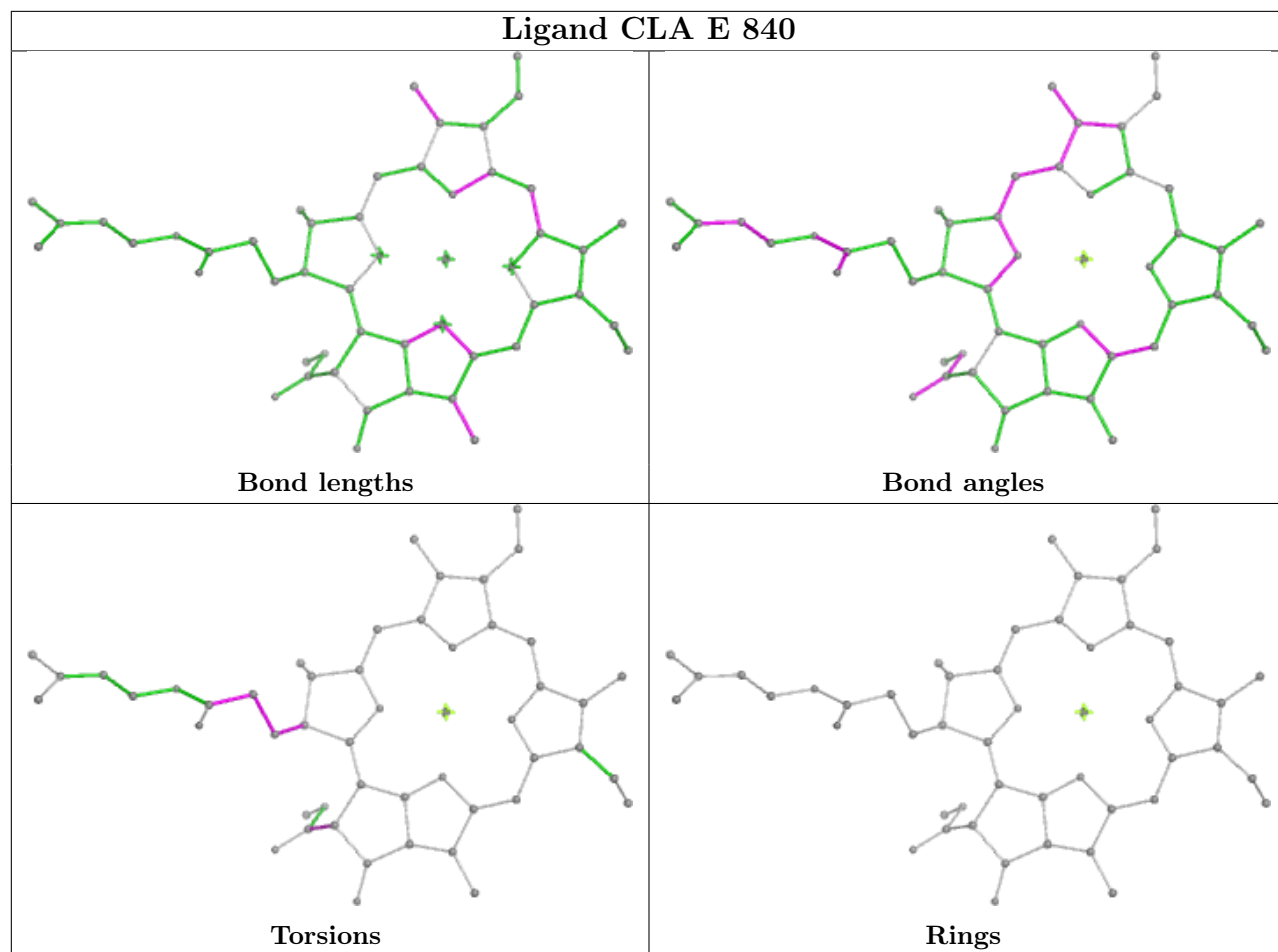
Ligand CLA A 838



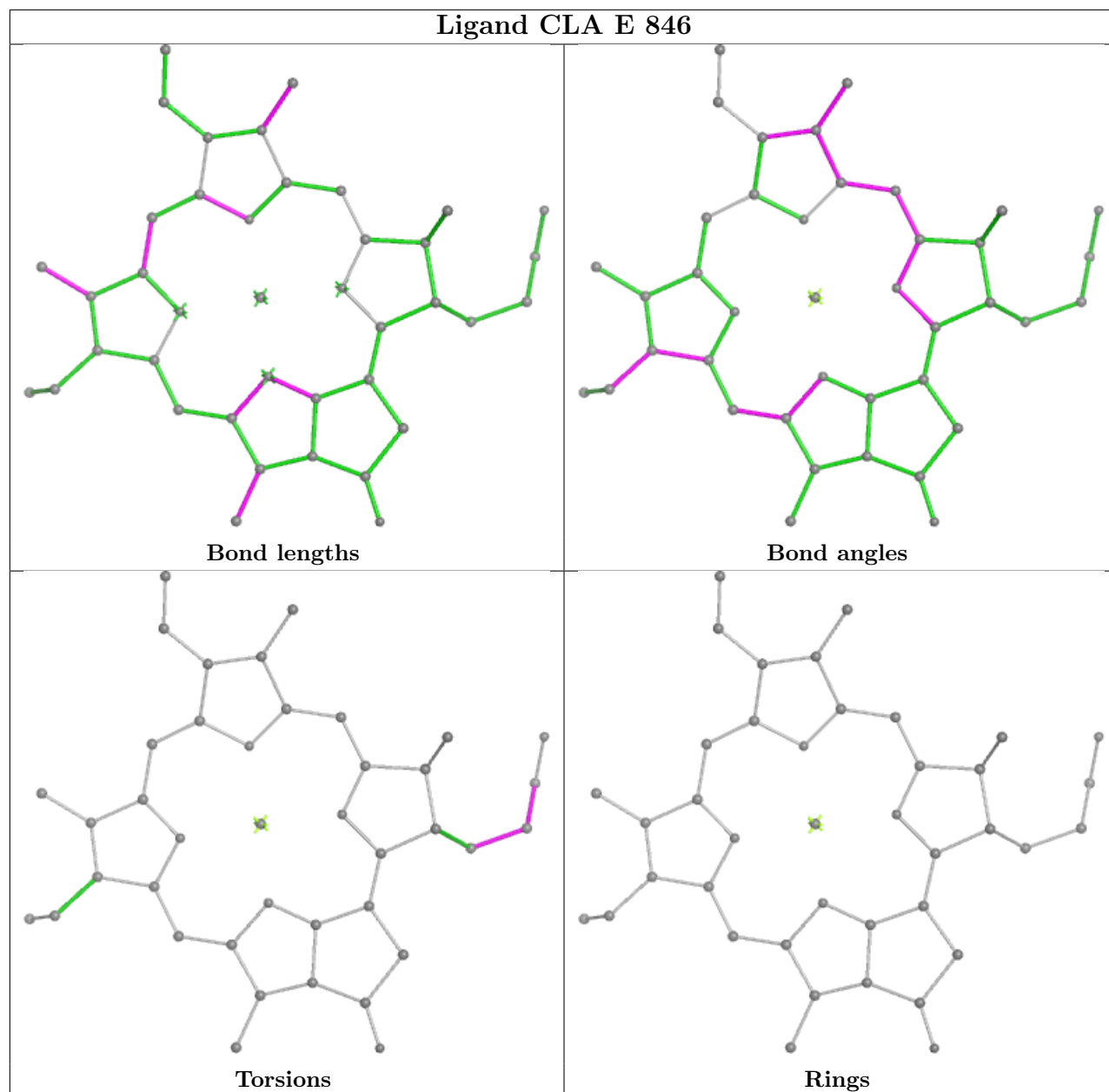
Ligand BCR g 847



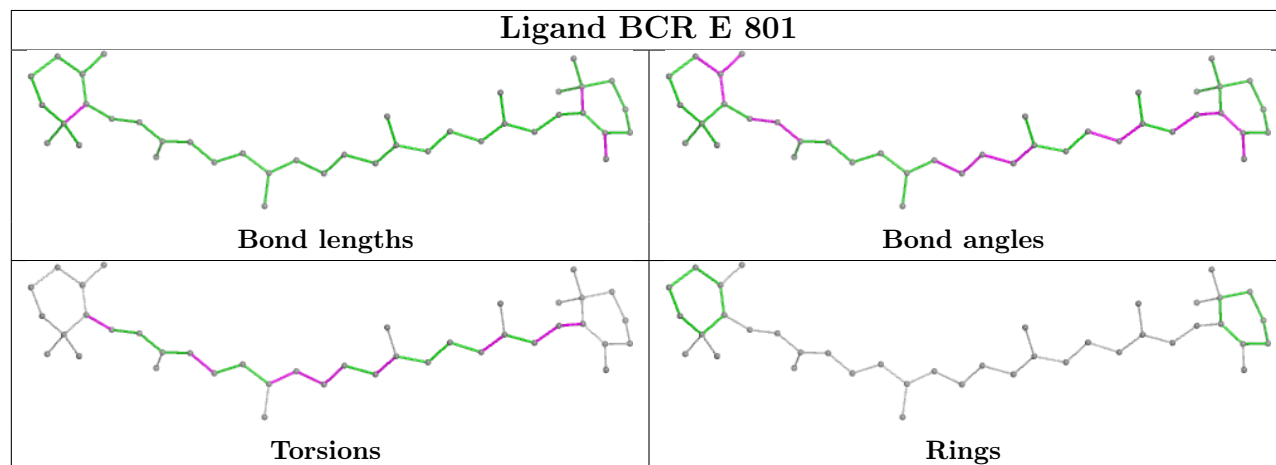
Ligand CLA E 840



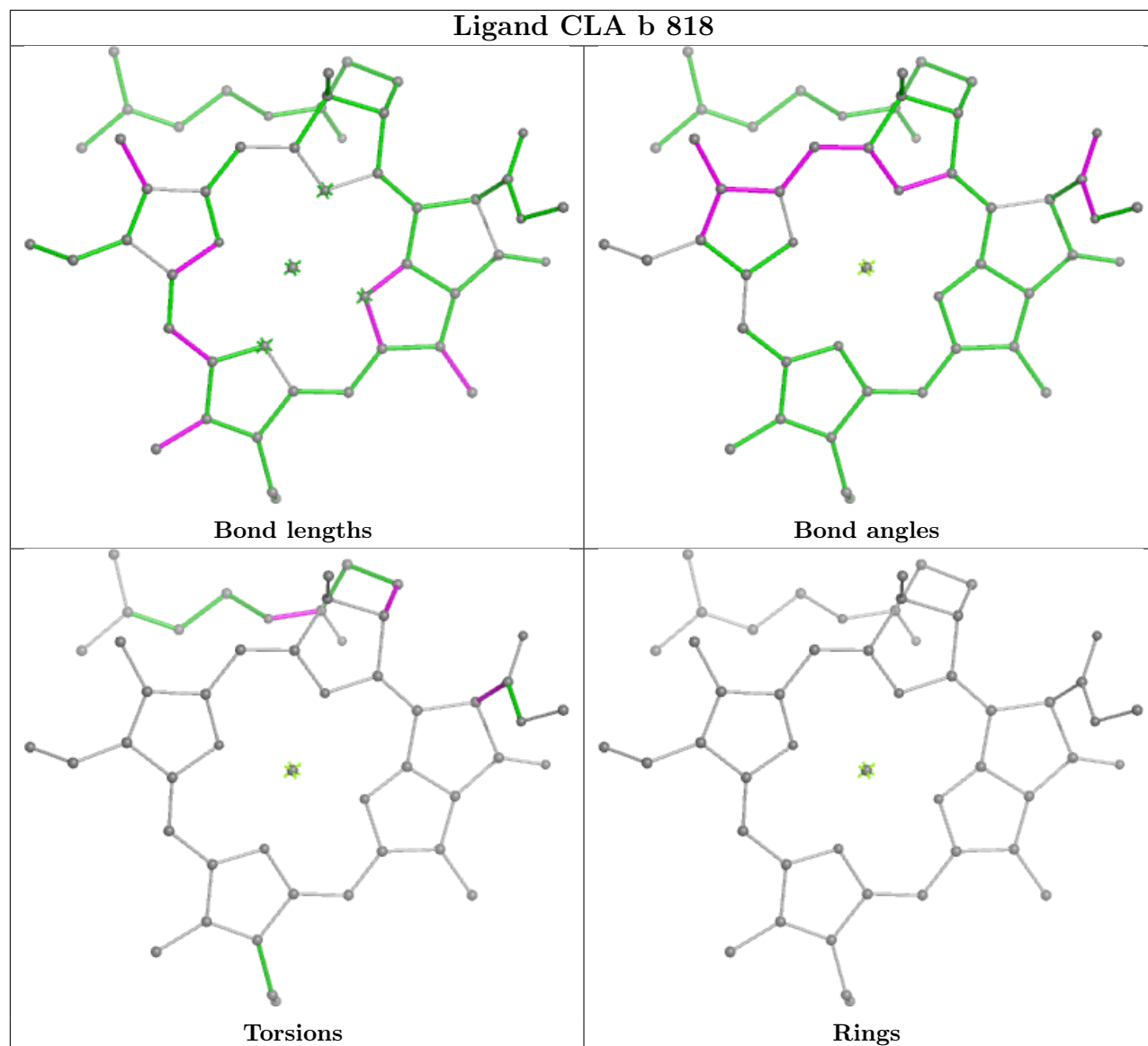
Ligand CLA E 846

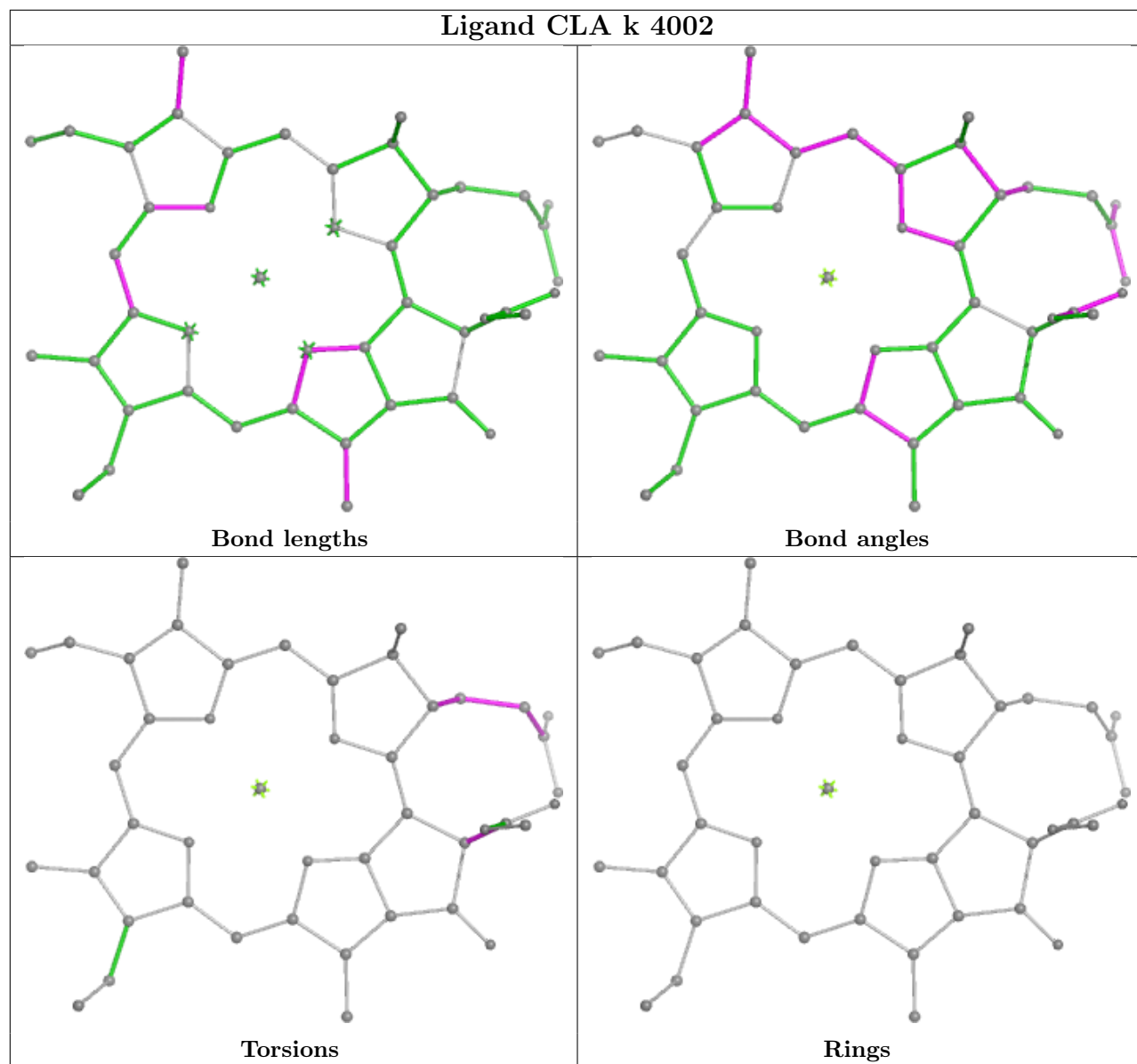


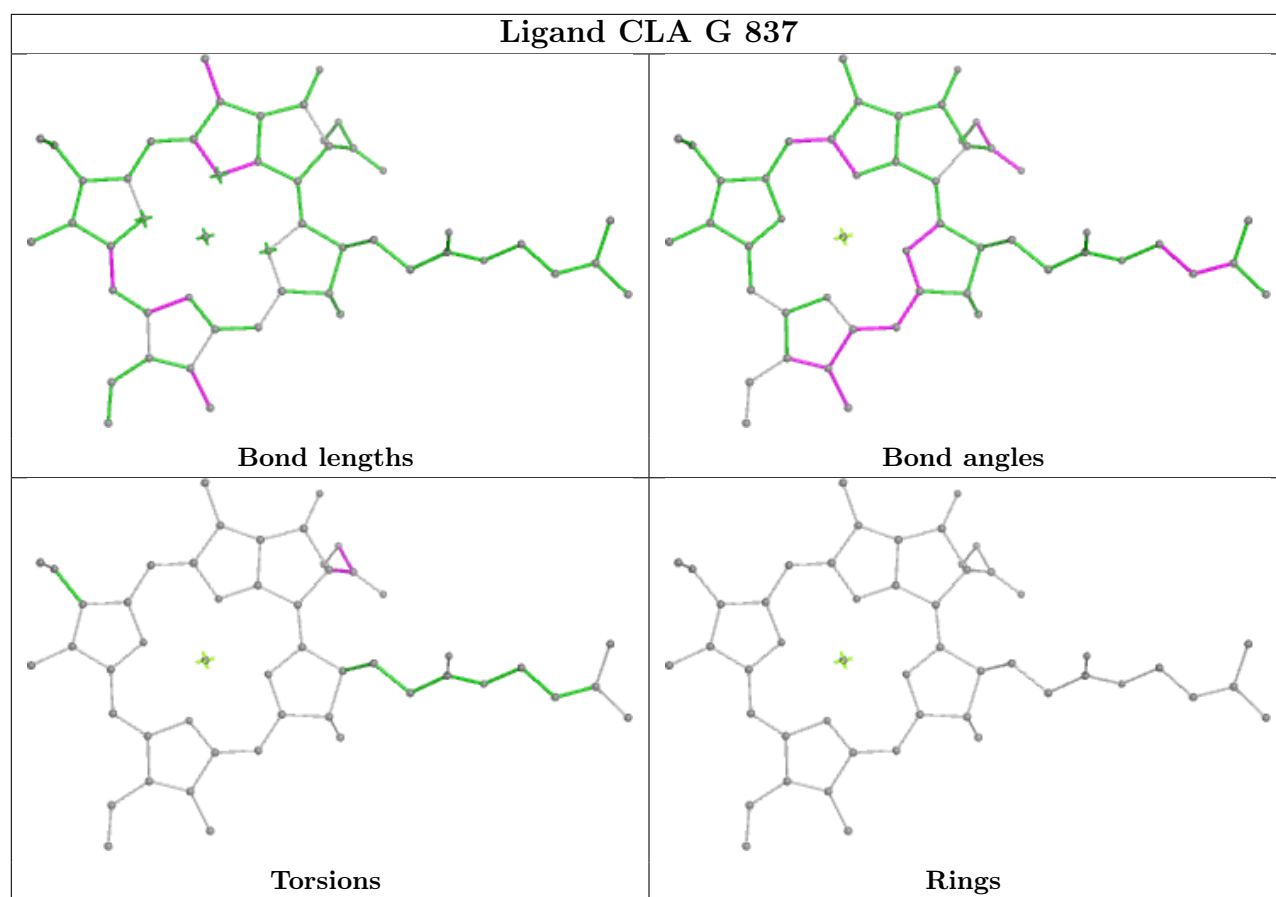
Ligand BCR E 801



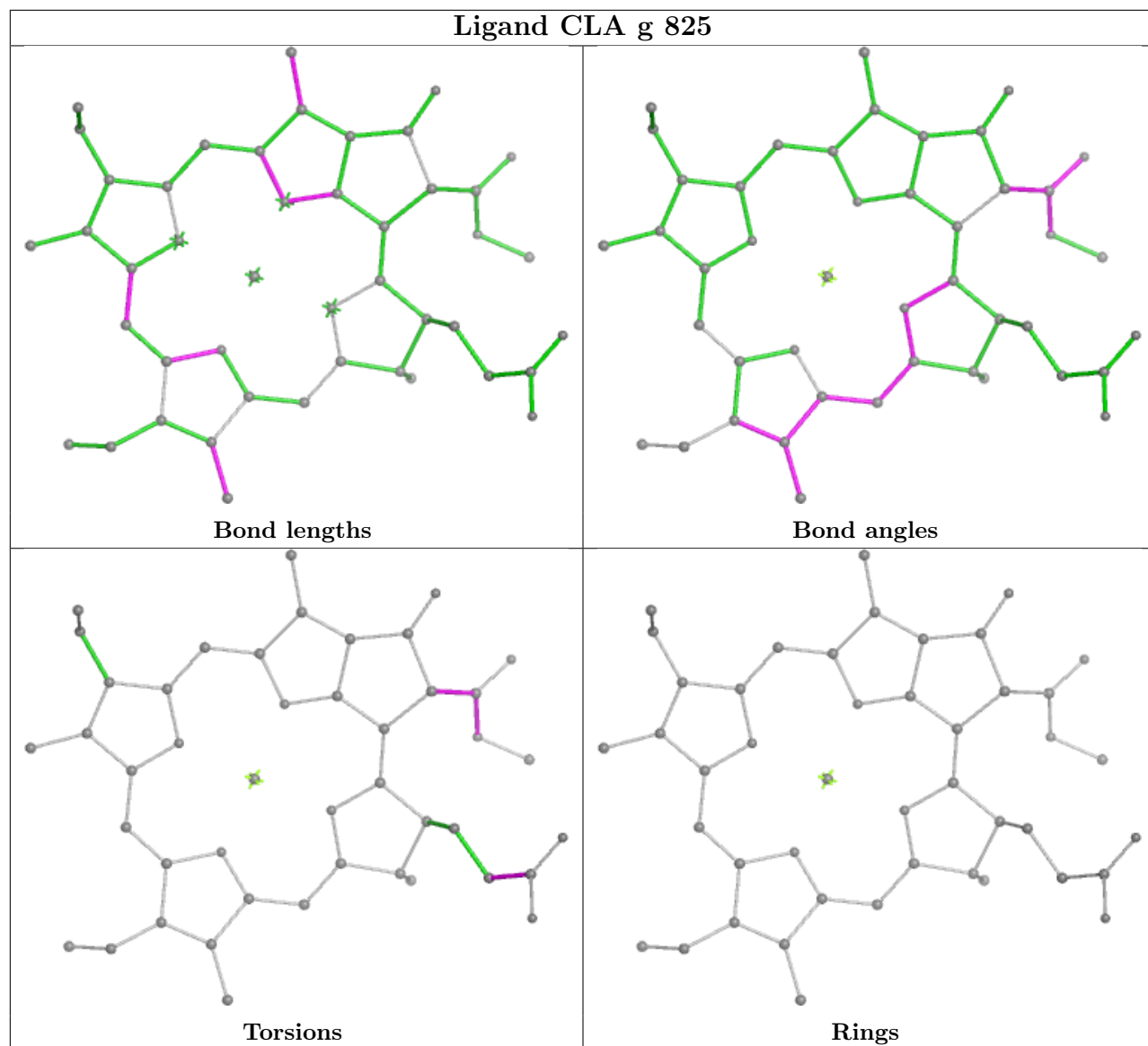
Ligand CLA b 818

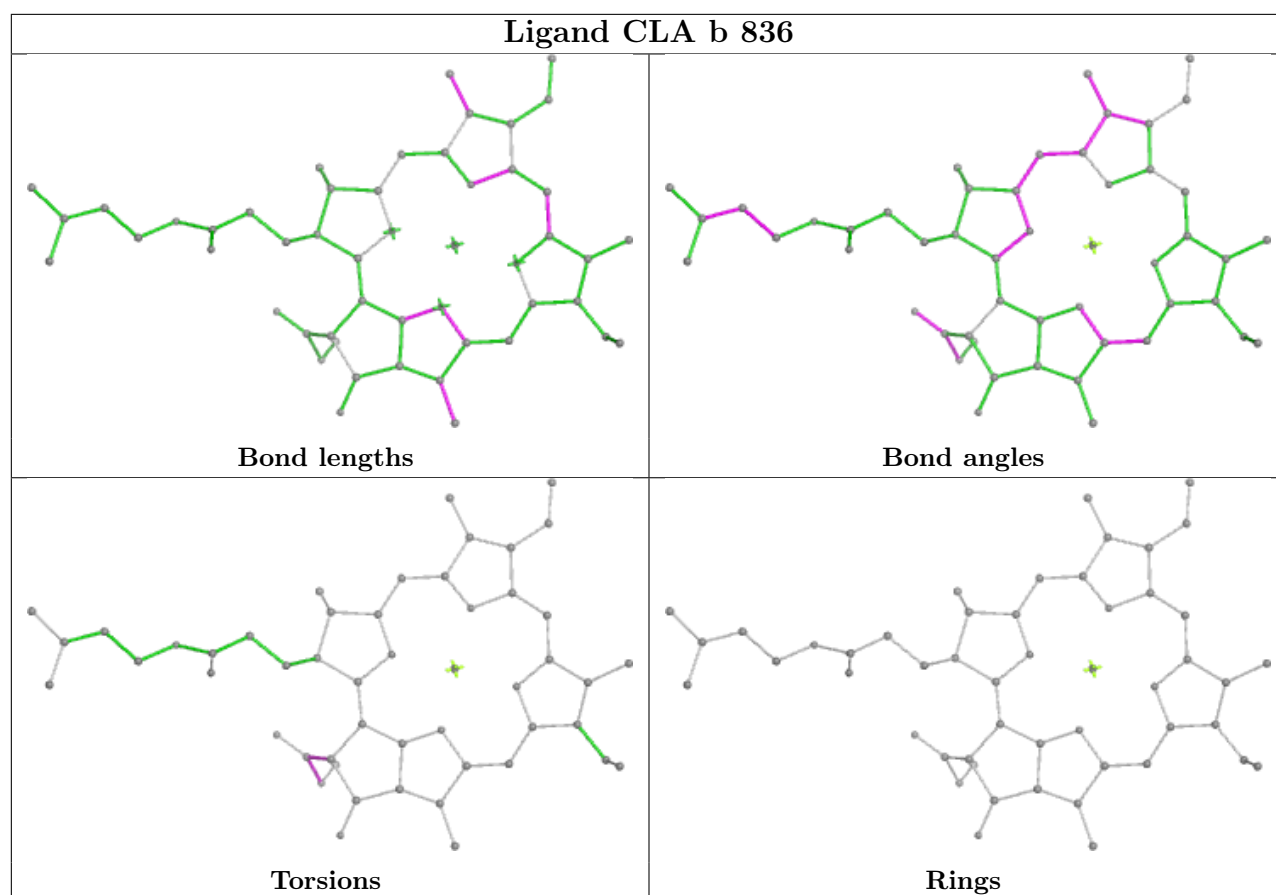




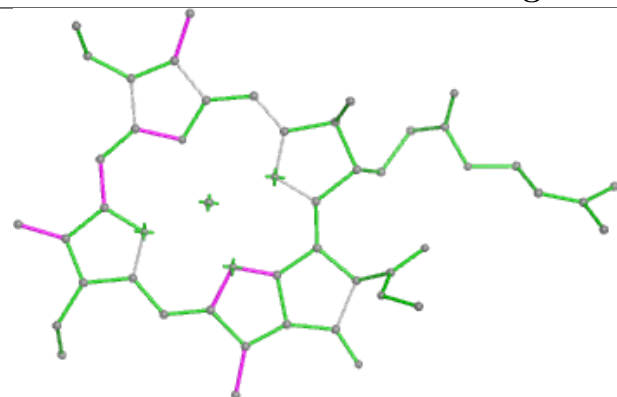


Ligand CLA g 825

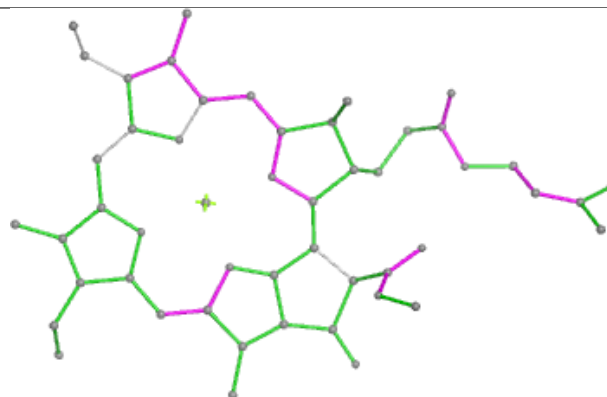




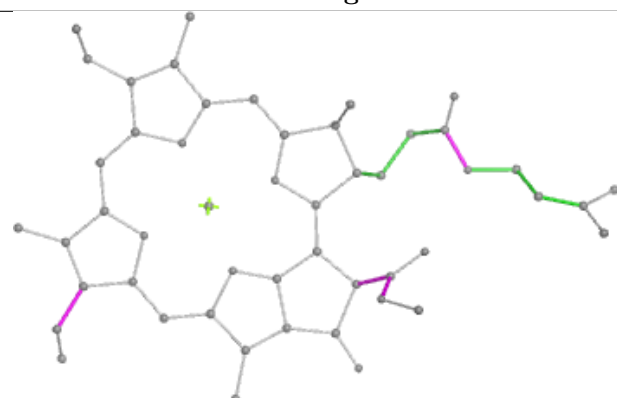
Ligand CLA e 805



Bond lengths



Bond angles

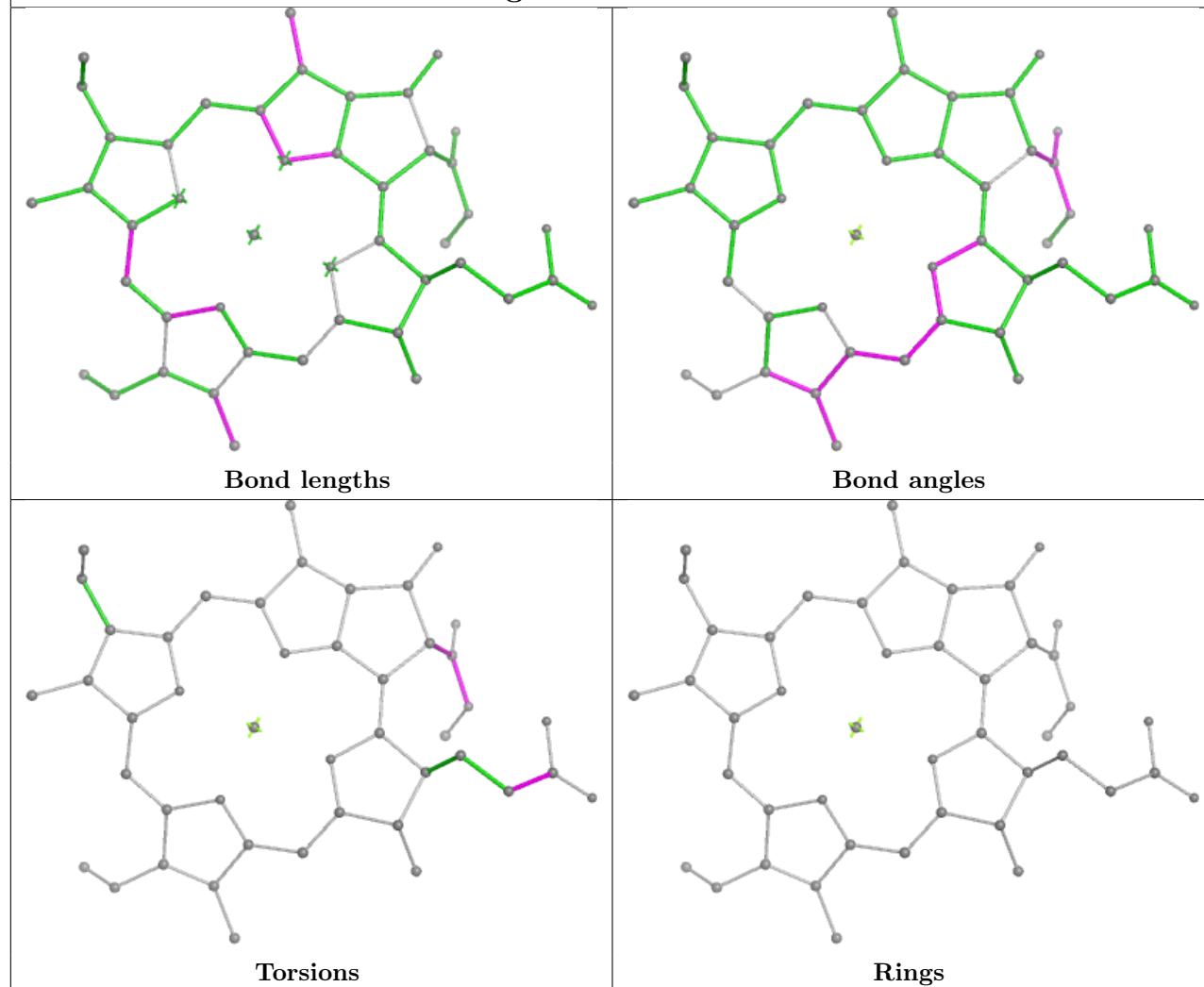


Torsions

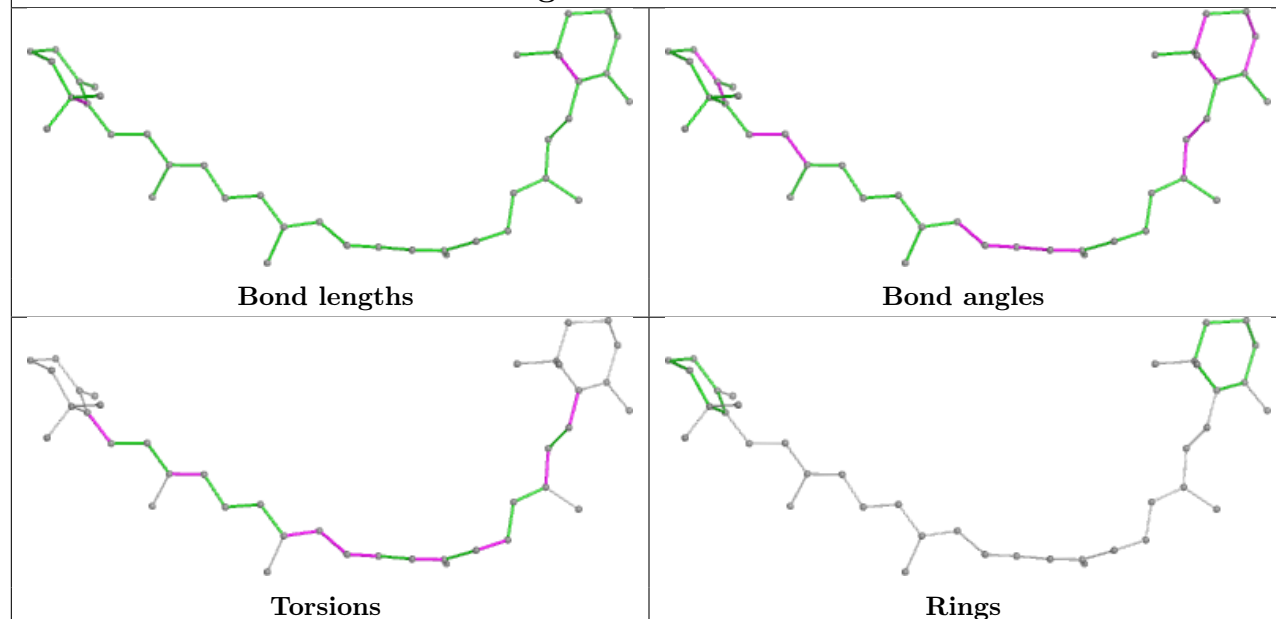


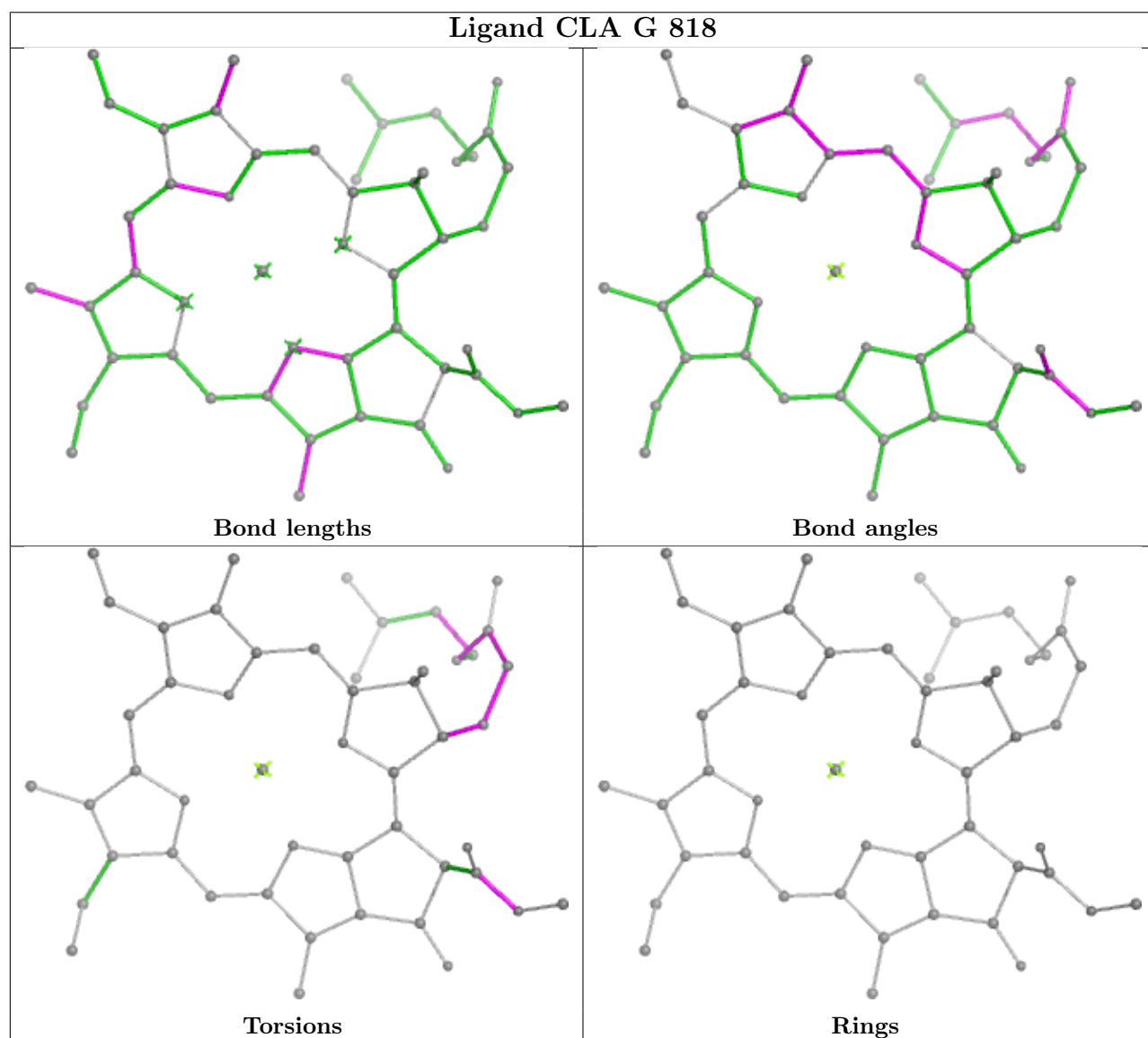
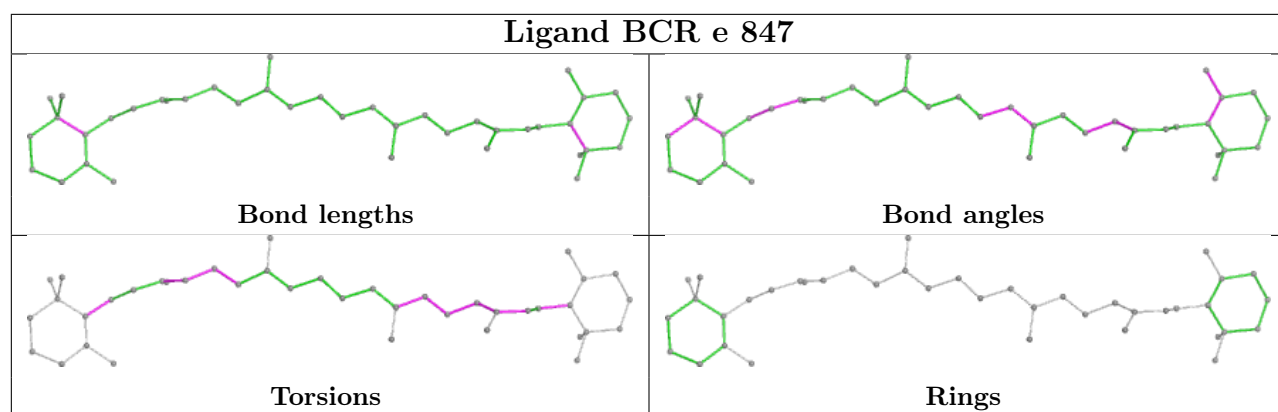
Rings

Ligand CLA a 818

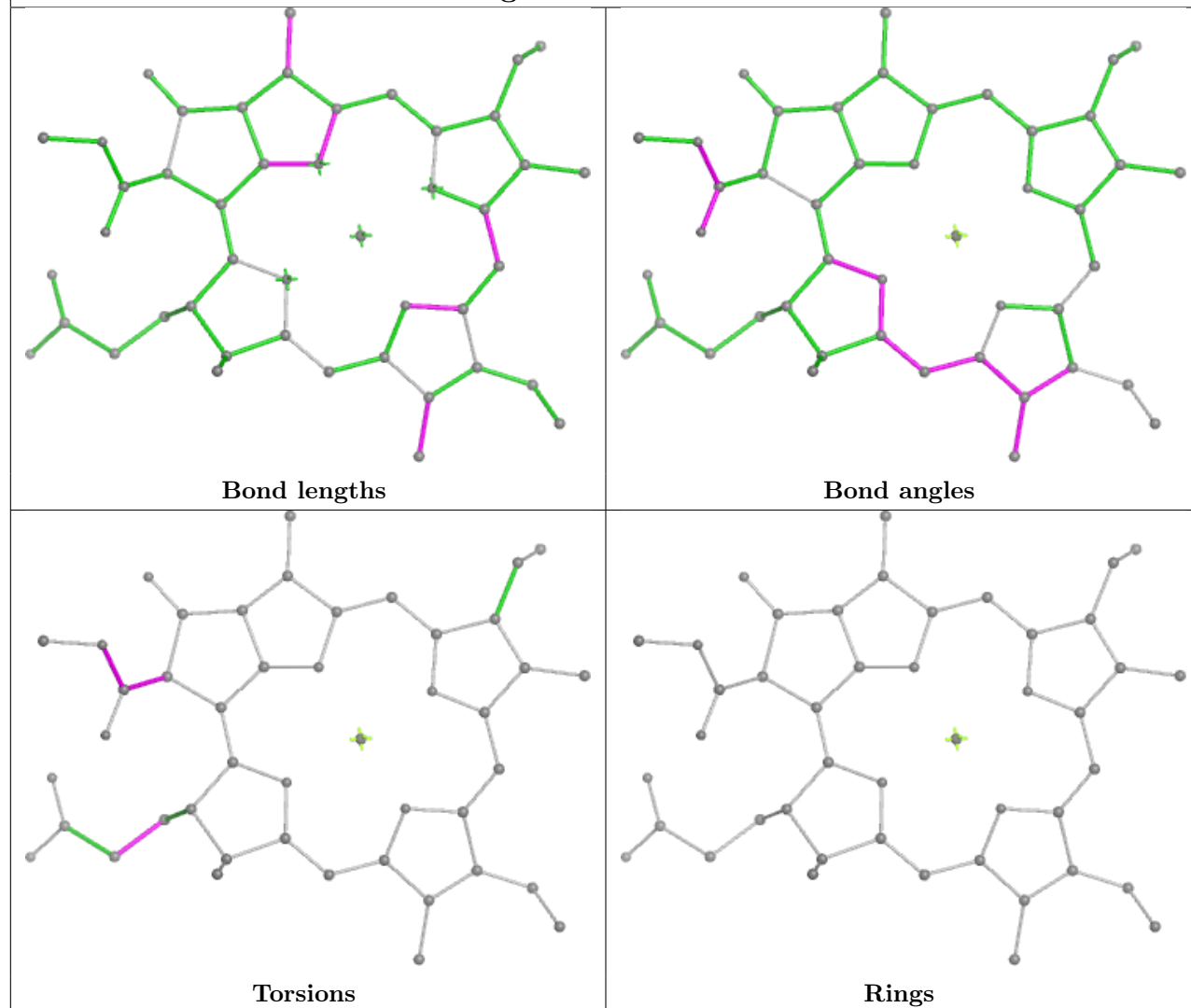


Ligand BCR f 202

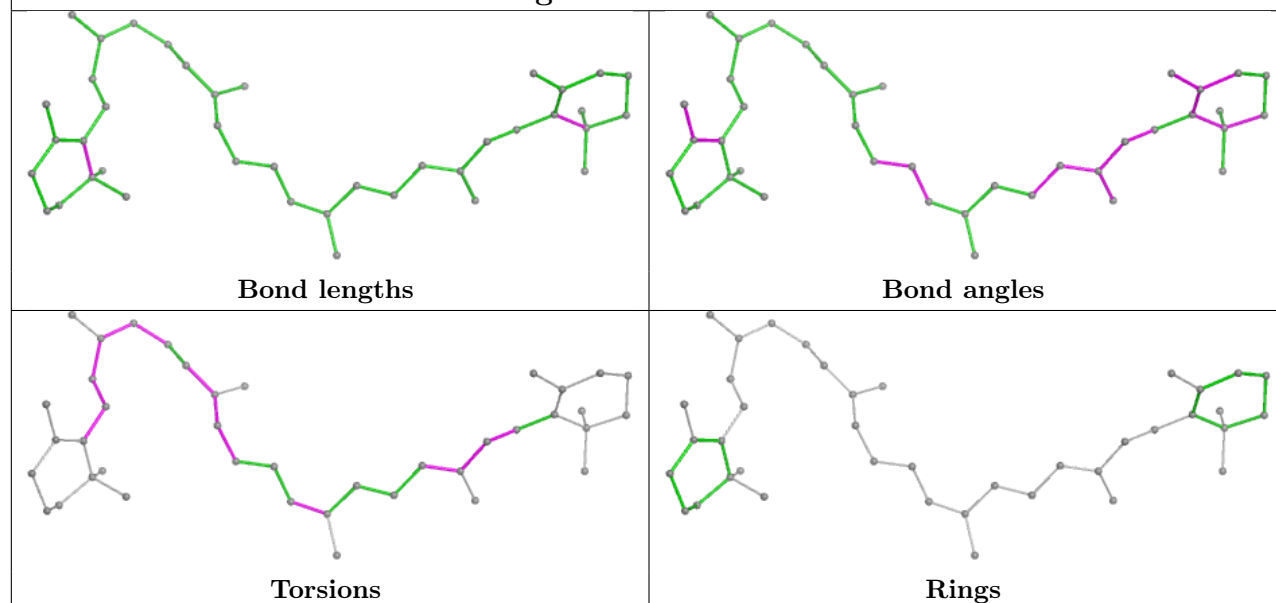


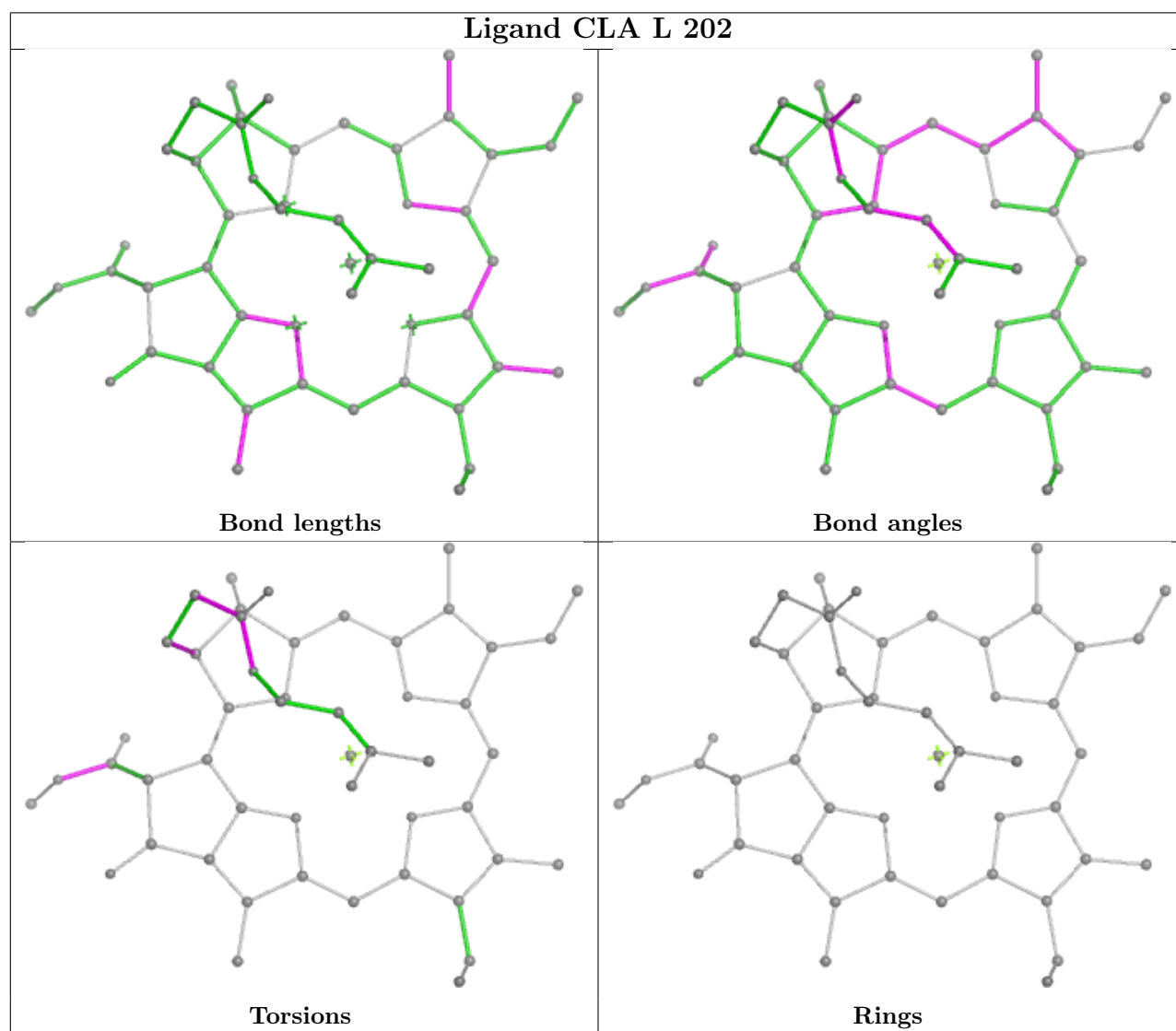
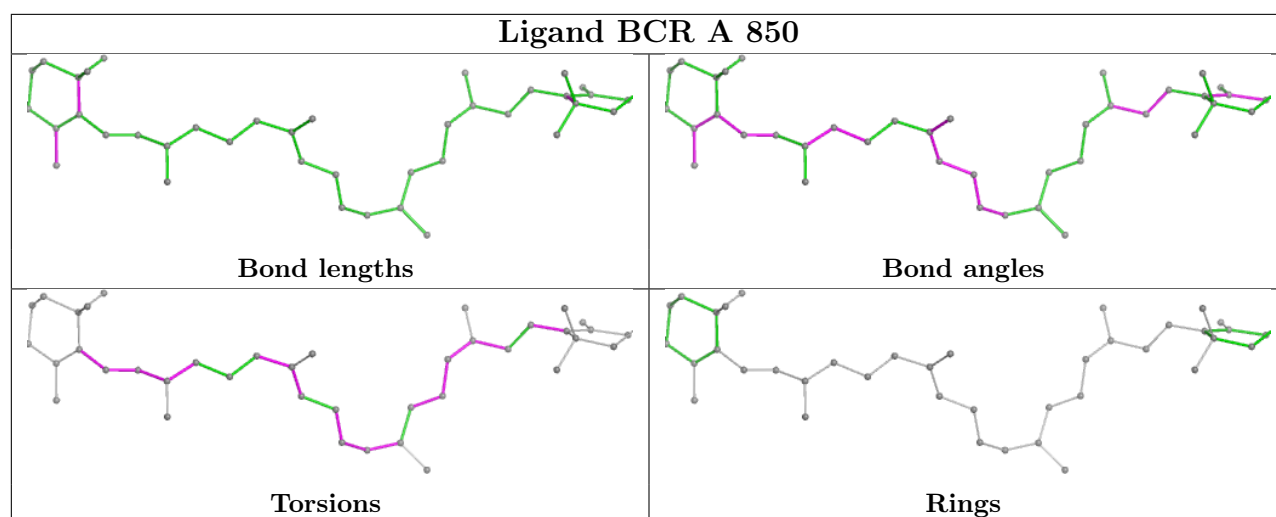


Ligand CLA o 202

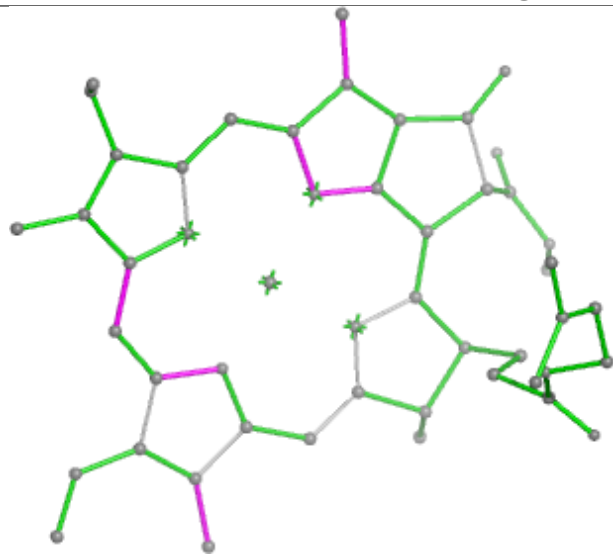


Ligand BCR e 846

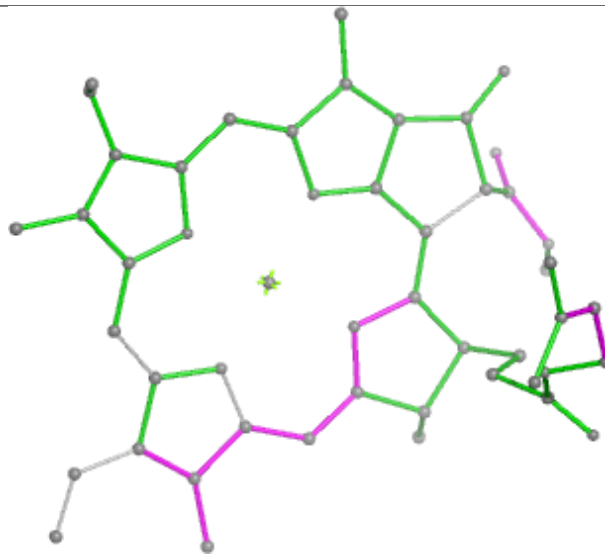




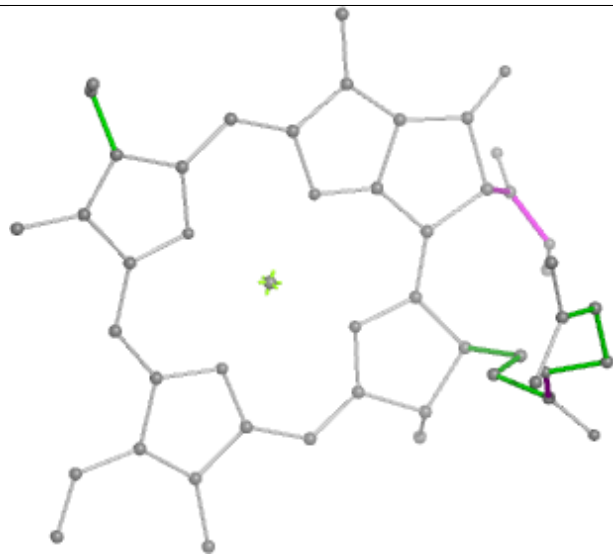
Ligand CLA E 833



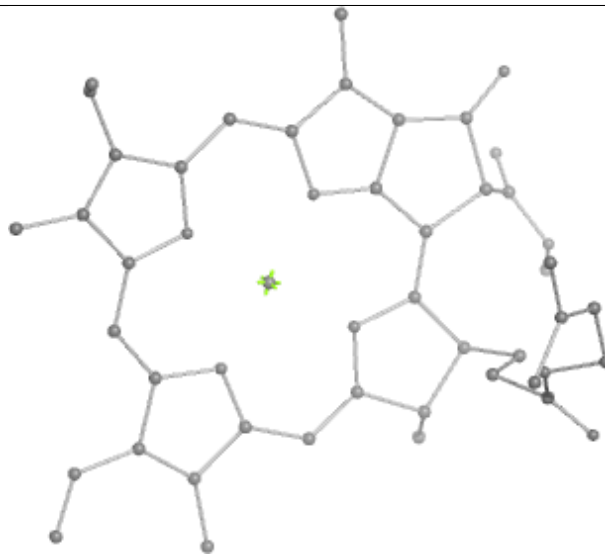
Bond lengths



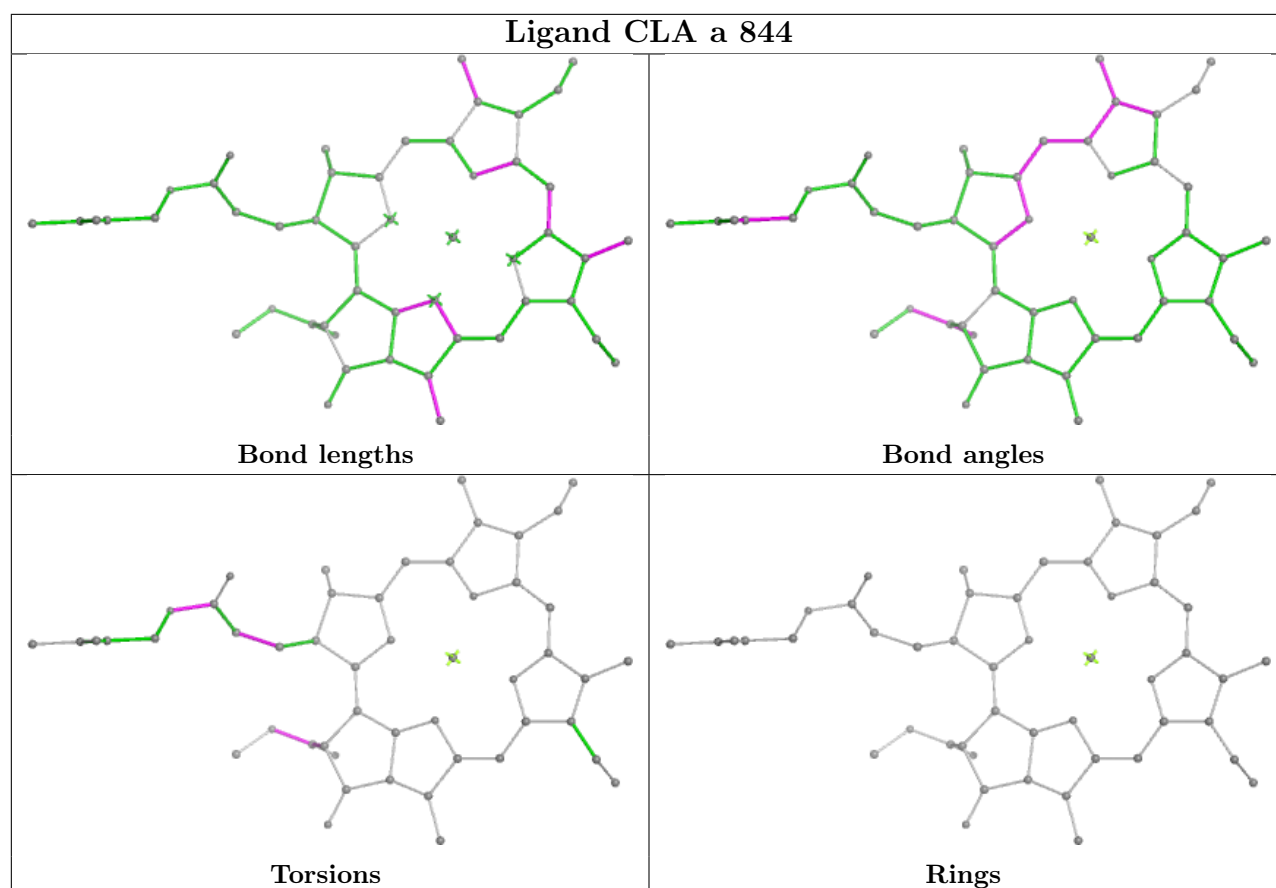
Bond angles



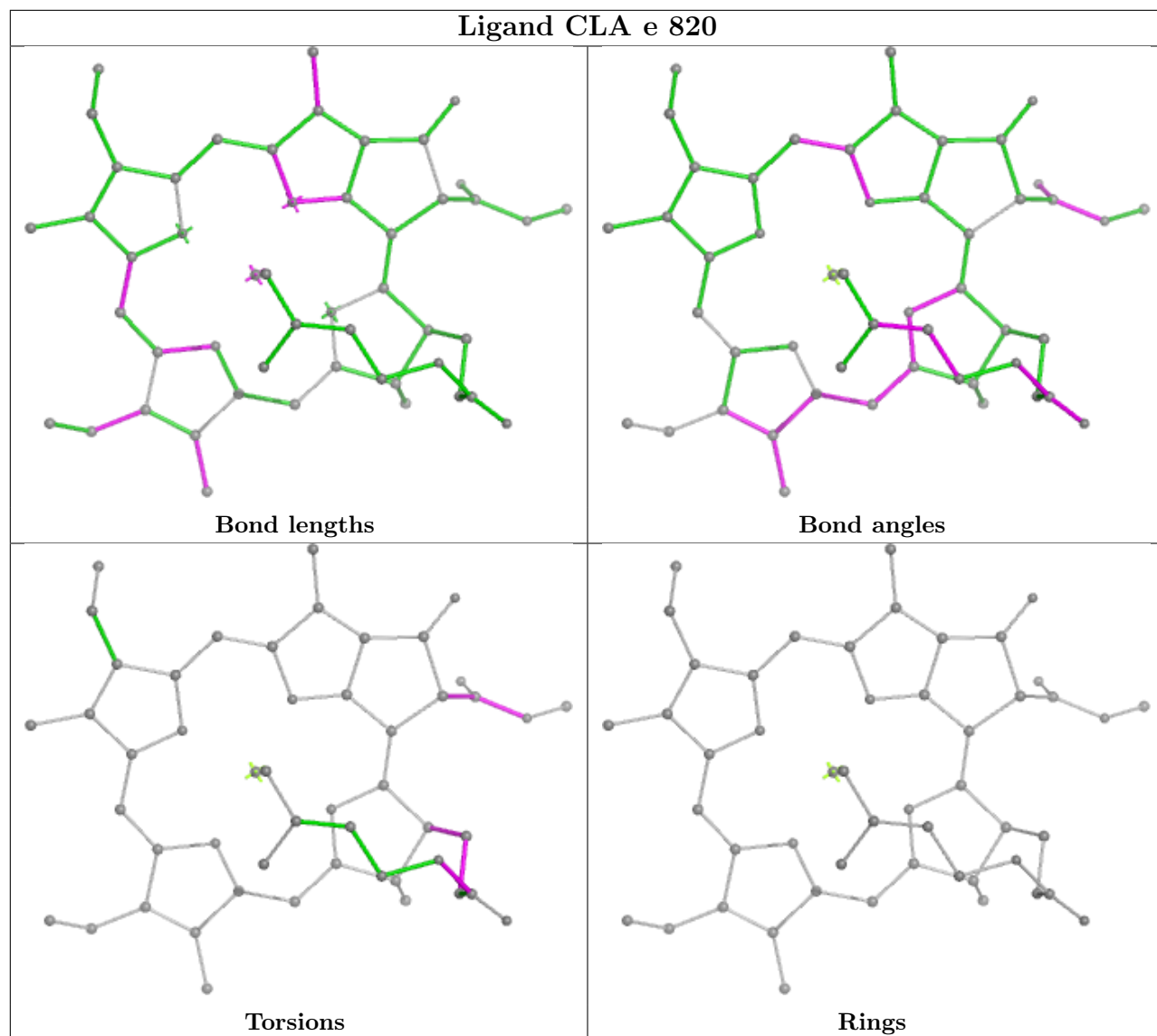
Torsions



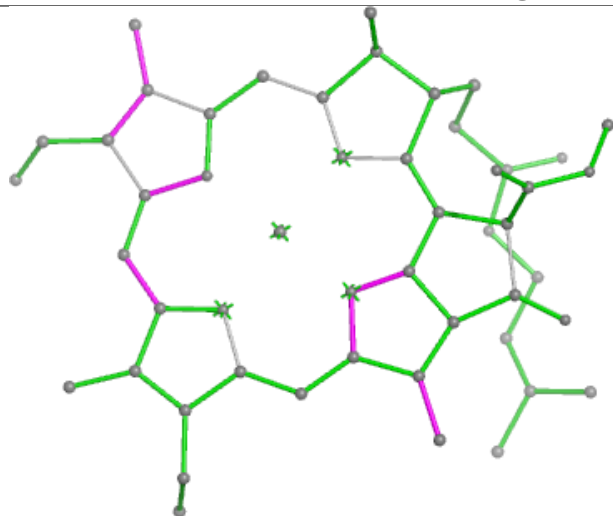
Rings



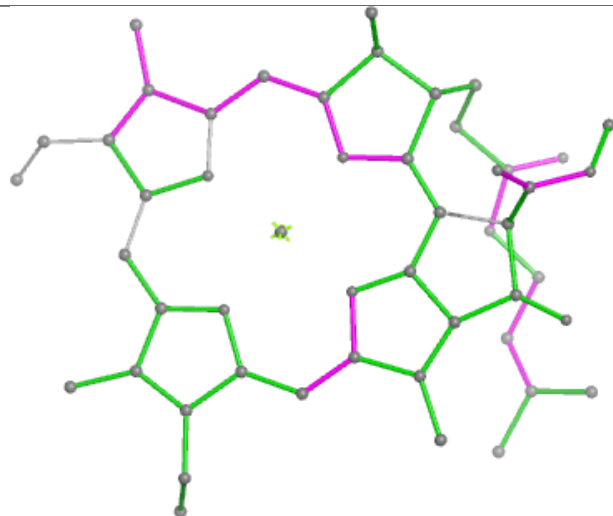
Ligand CLA e 820



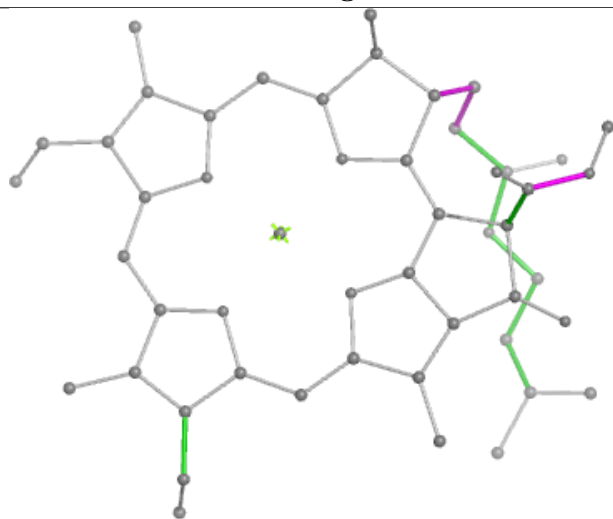
Ligand CLA A 832



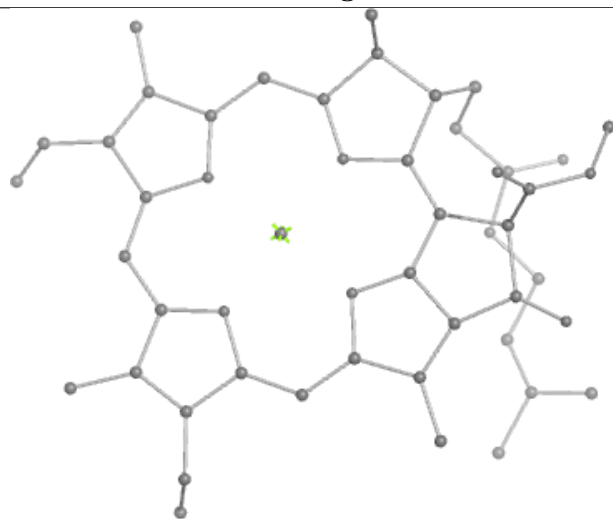
Bond lengths



Bond angles

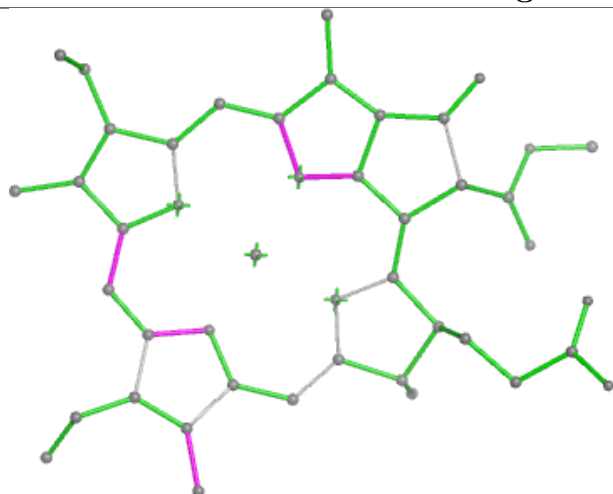


Torsions

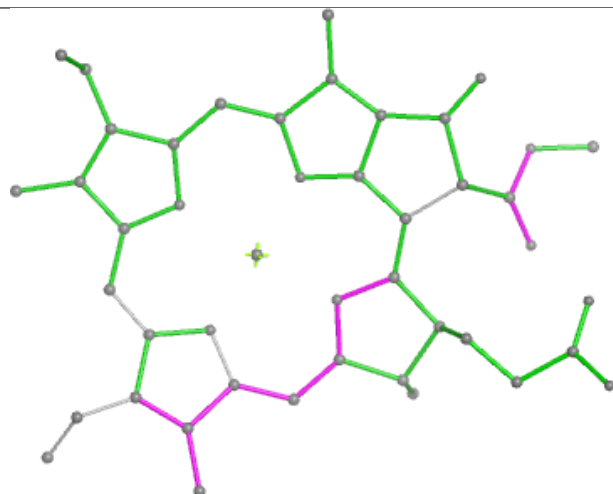


Rings

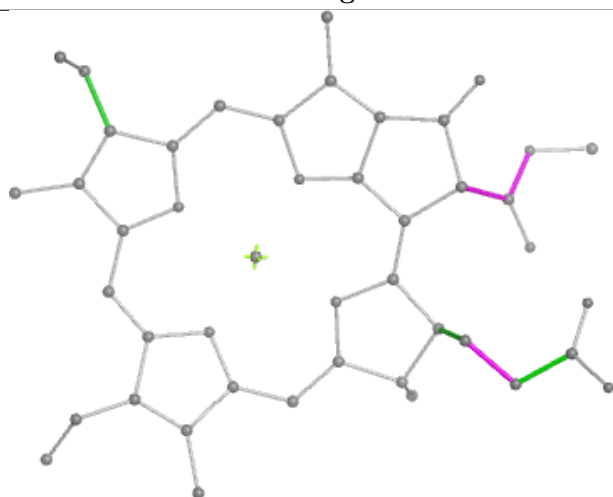
Ligand CLA F 202



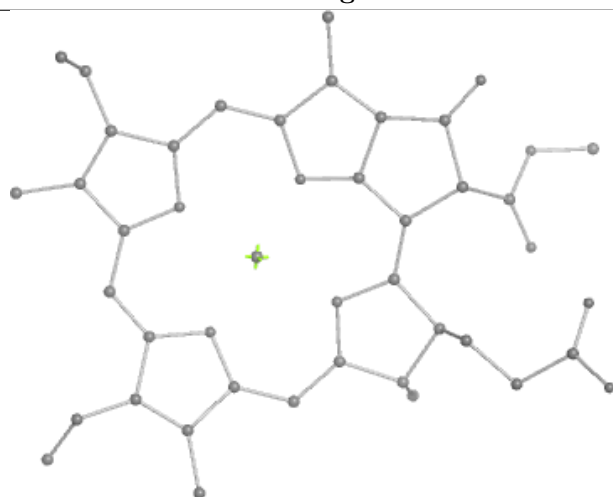
Bond lengths



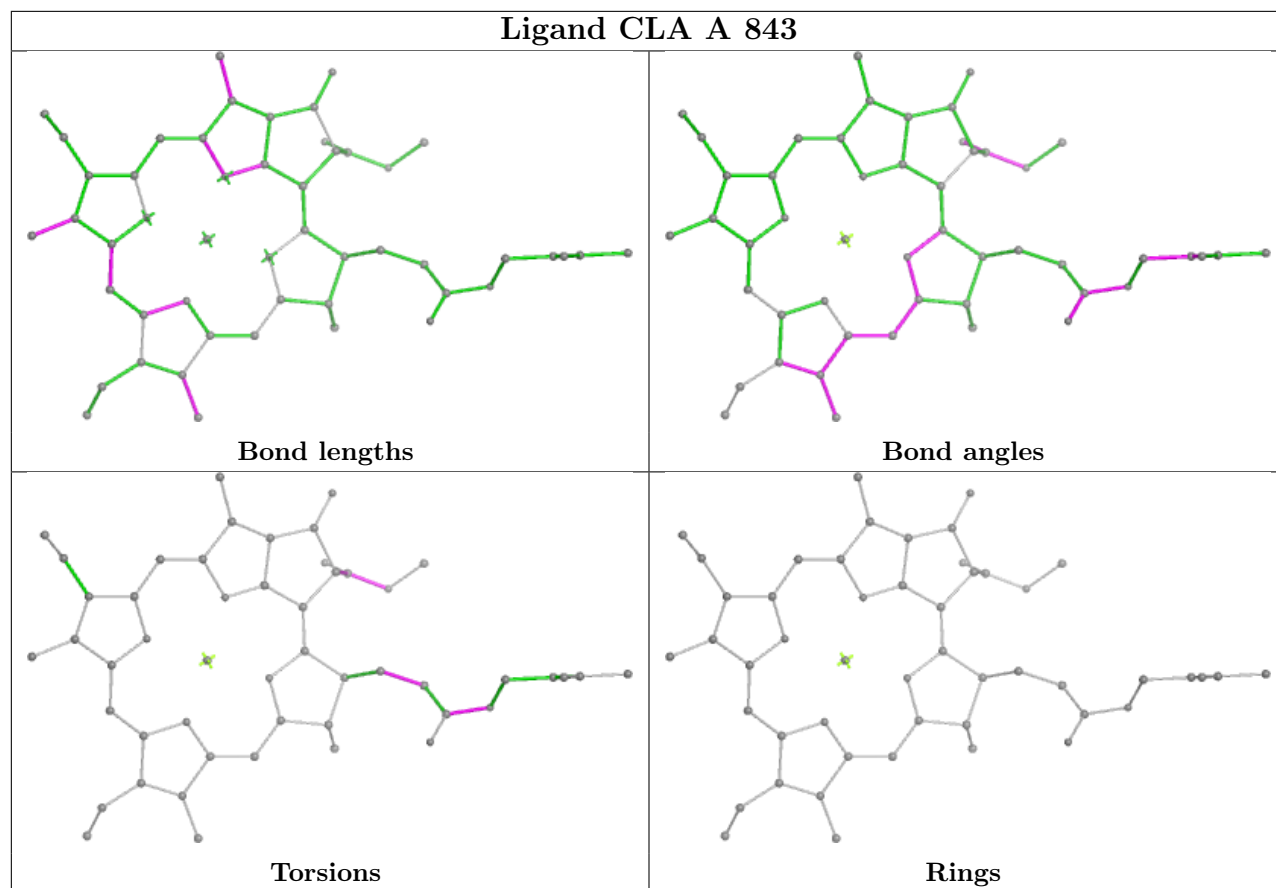
Bond angles



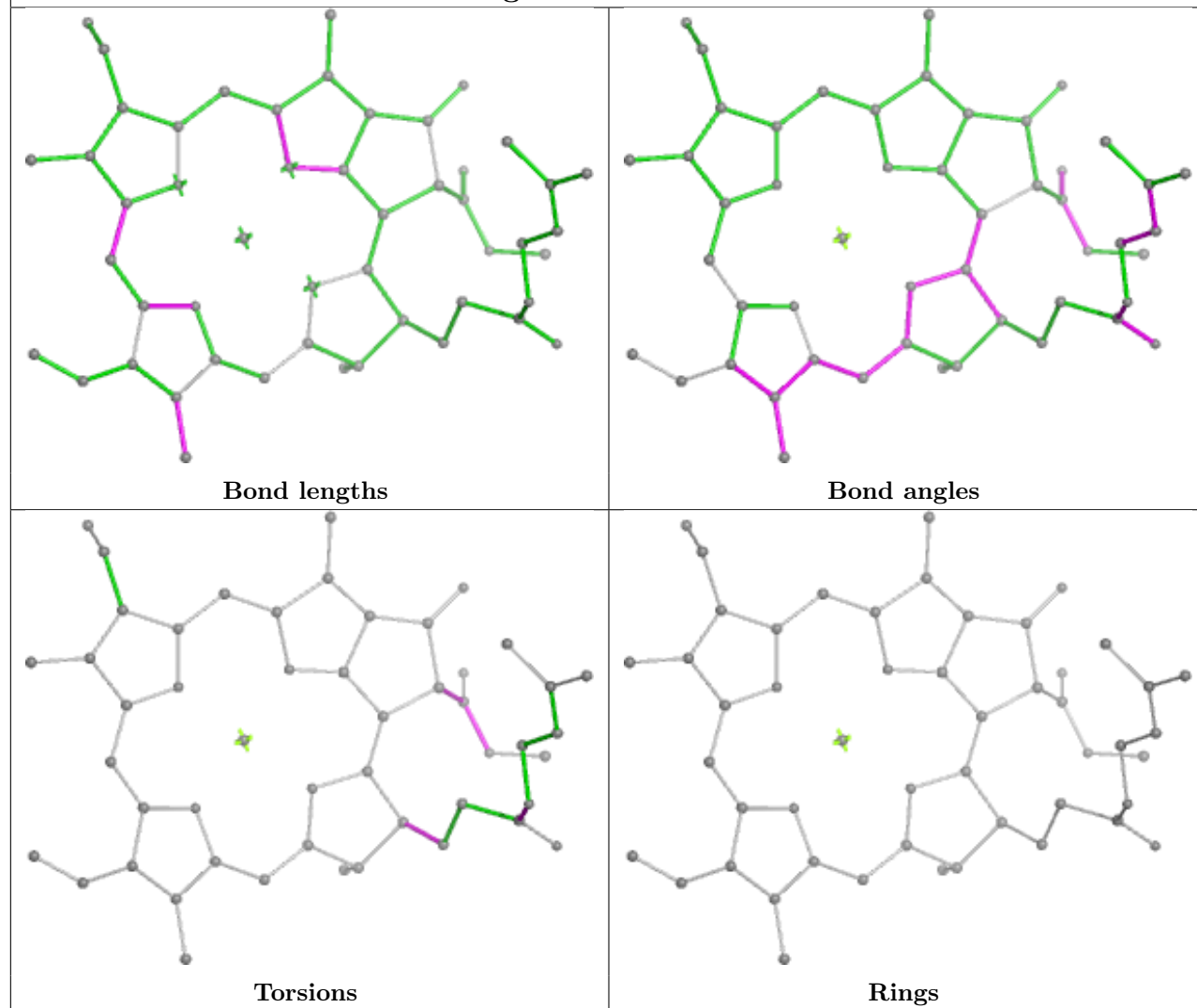
Torsions



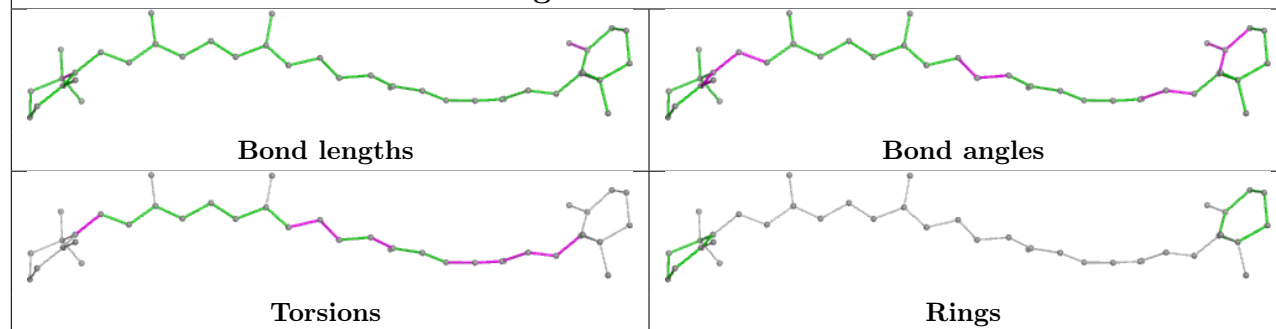
Rings

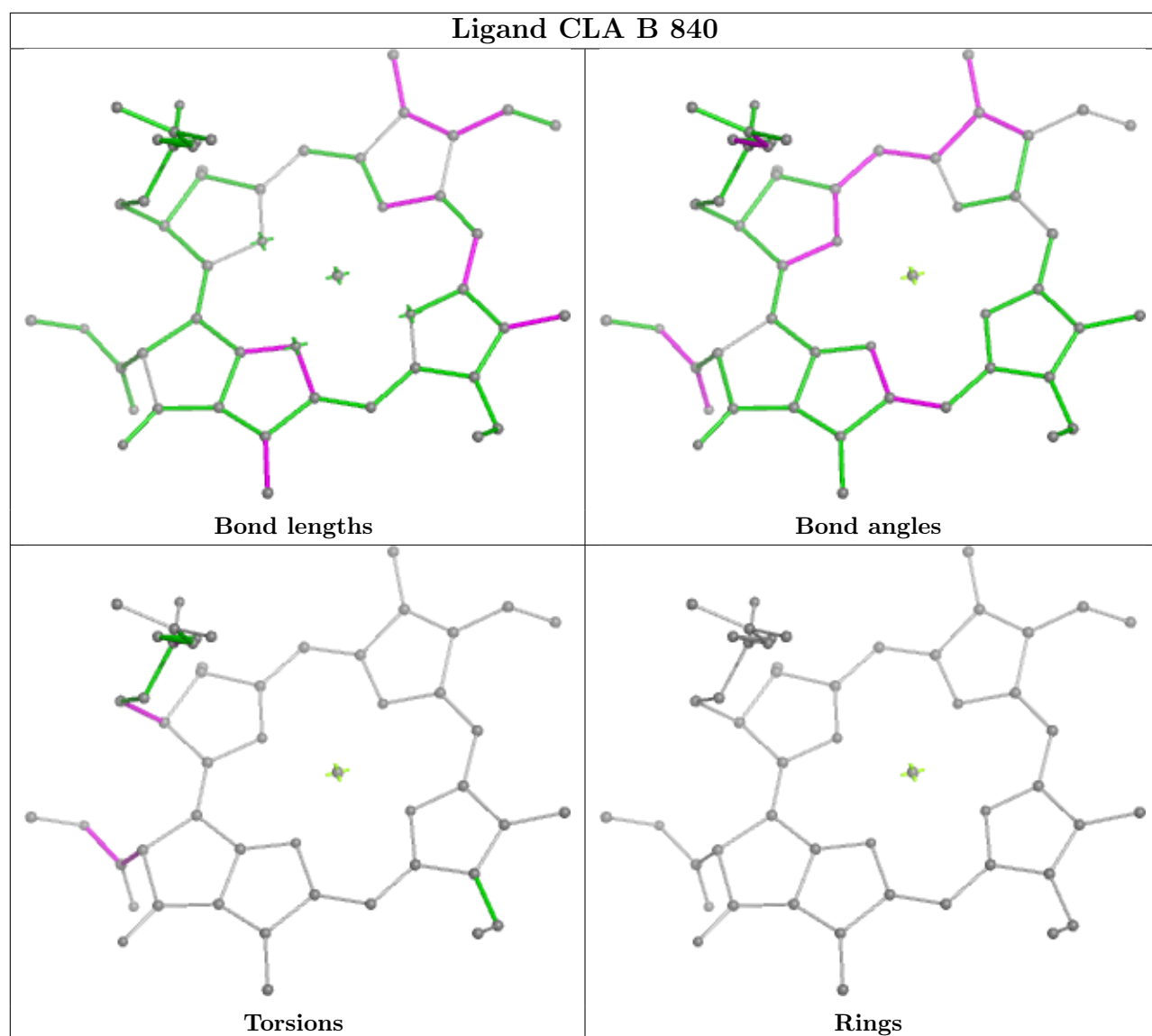


Ligand CLA a 852

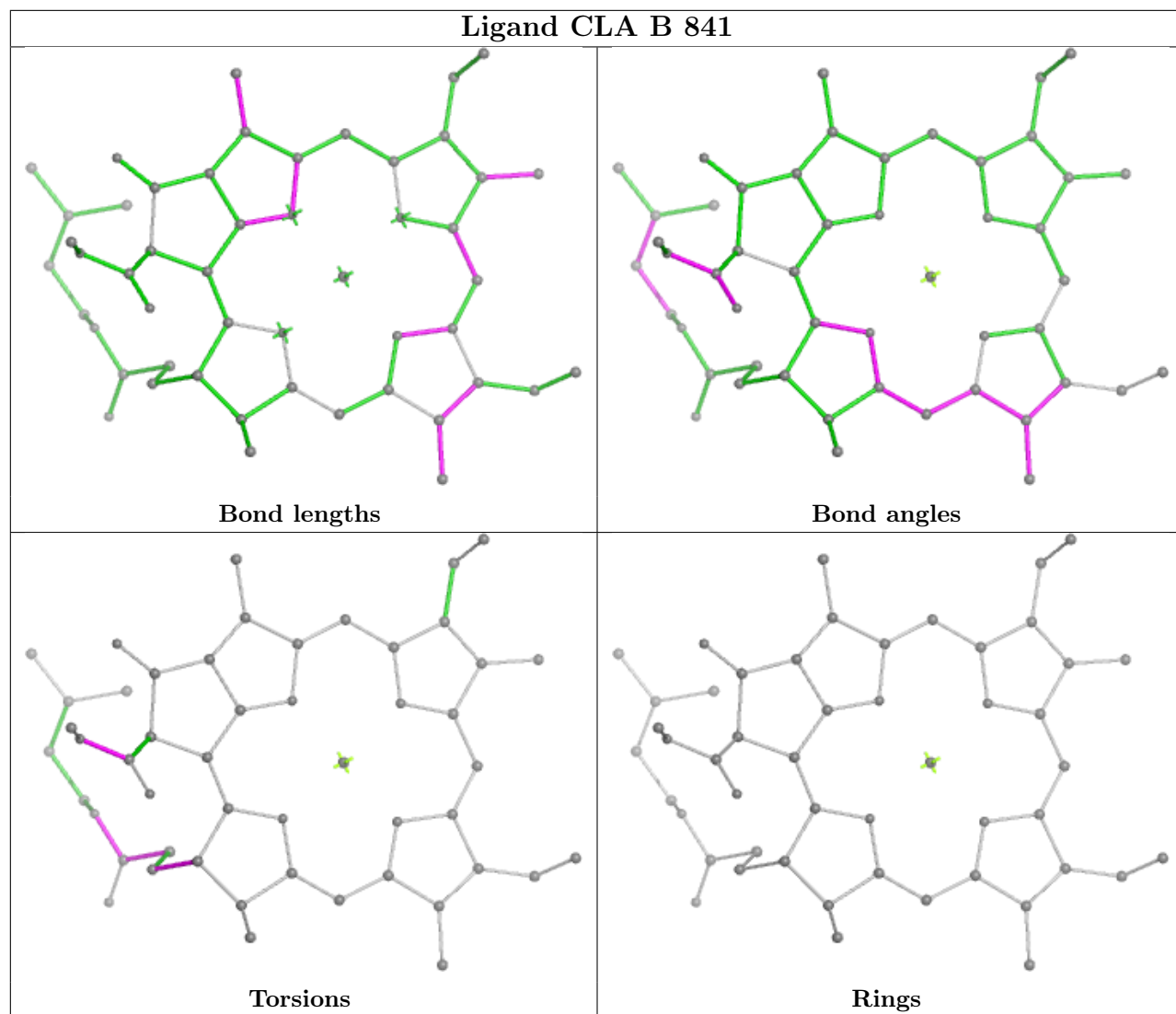


Ligand BCR b 846

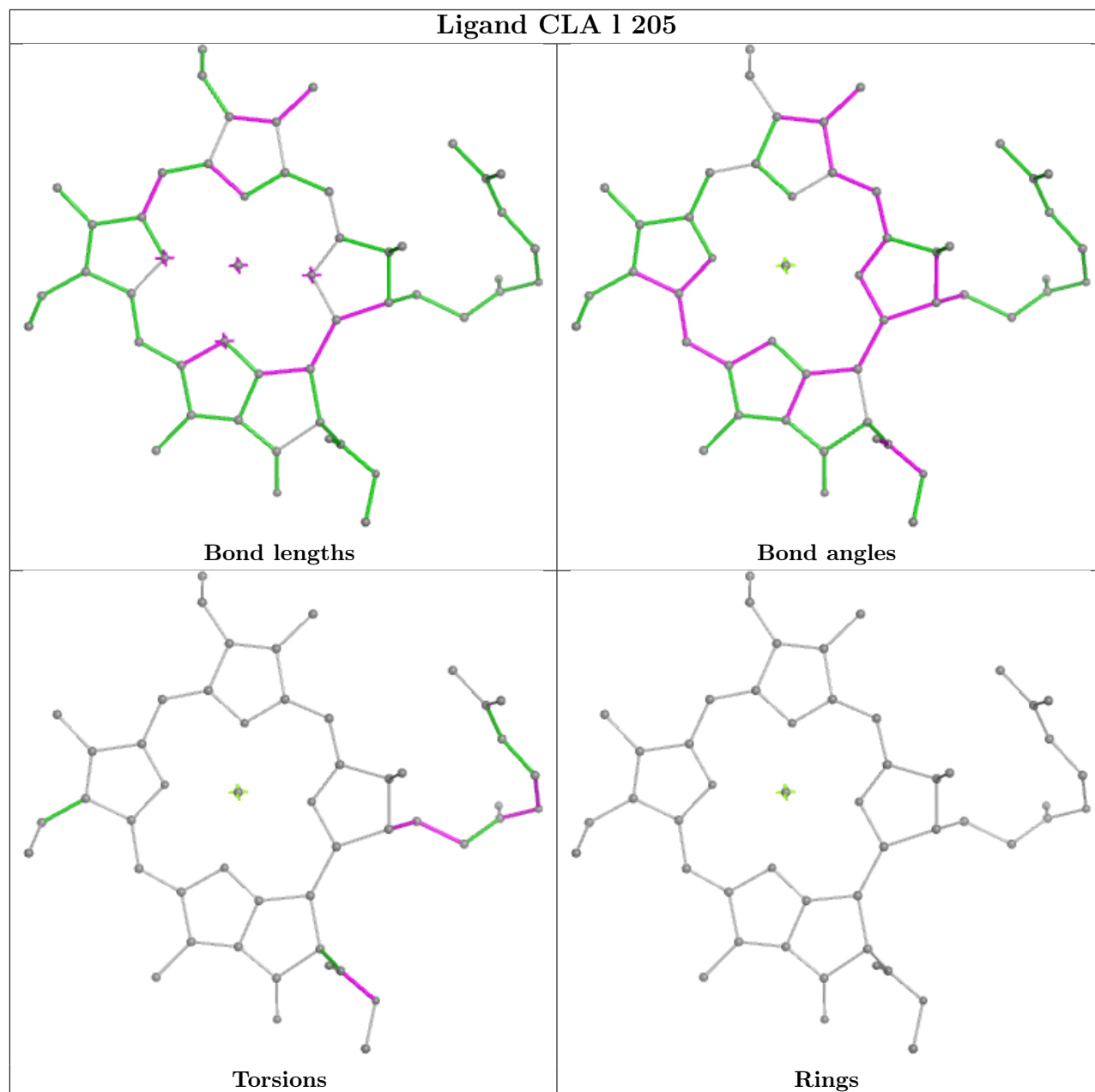




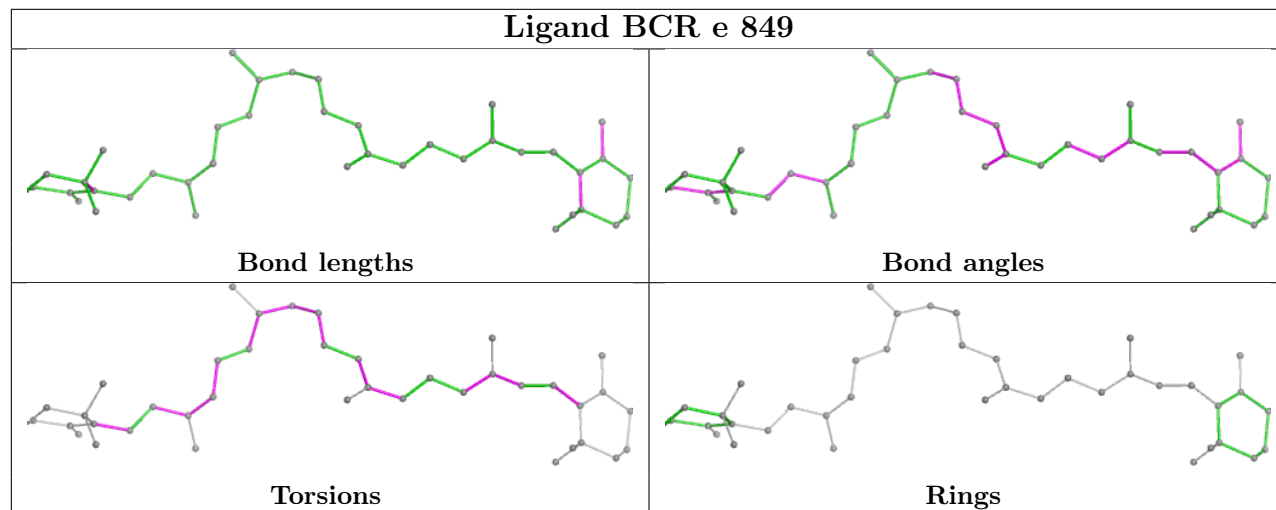
Ligand CLA B 841

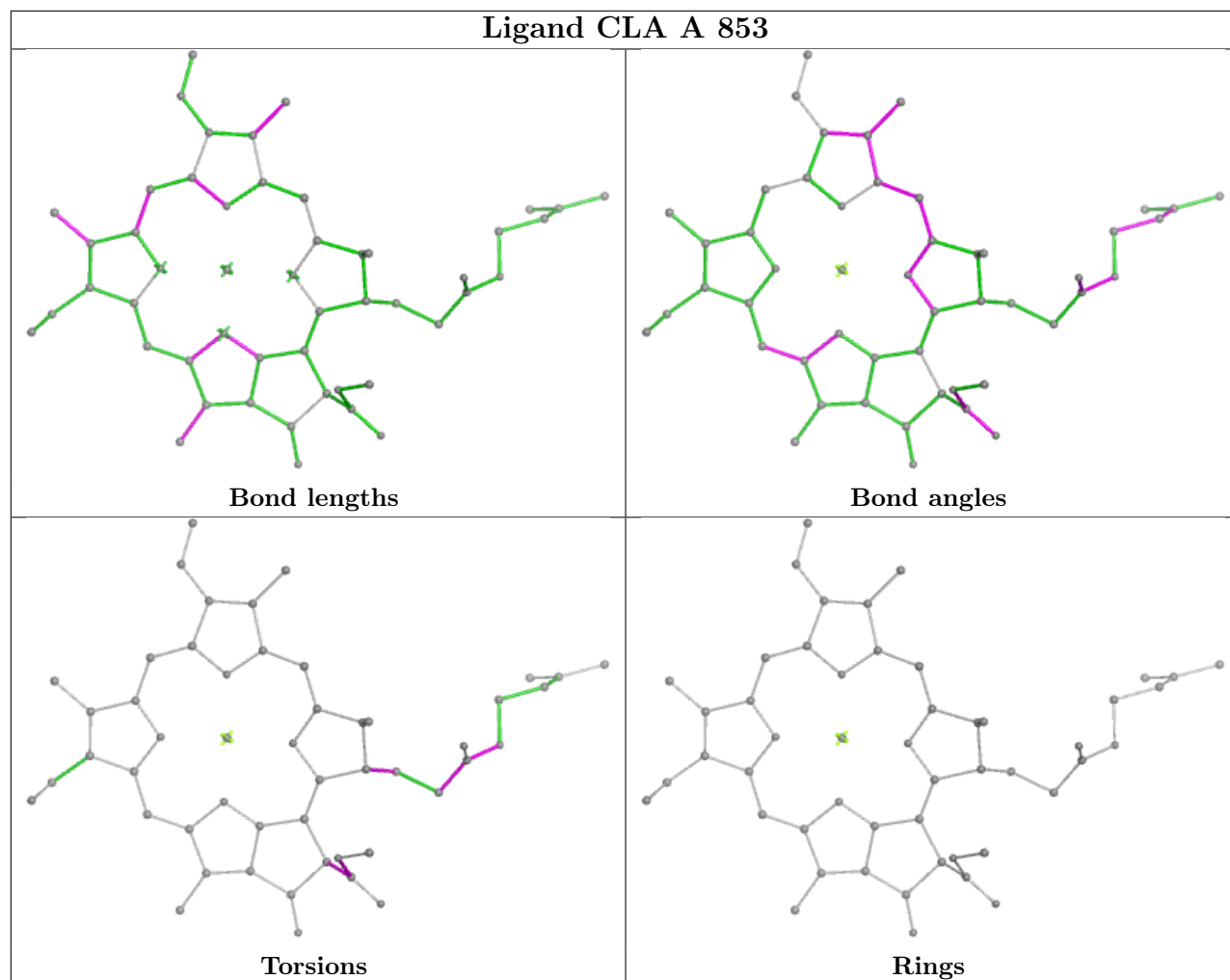
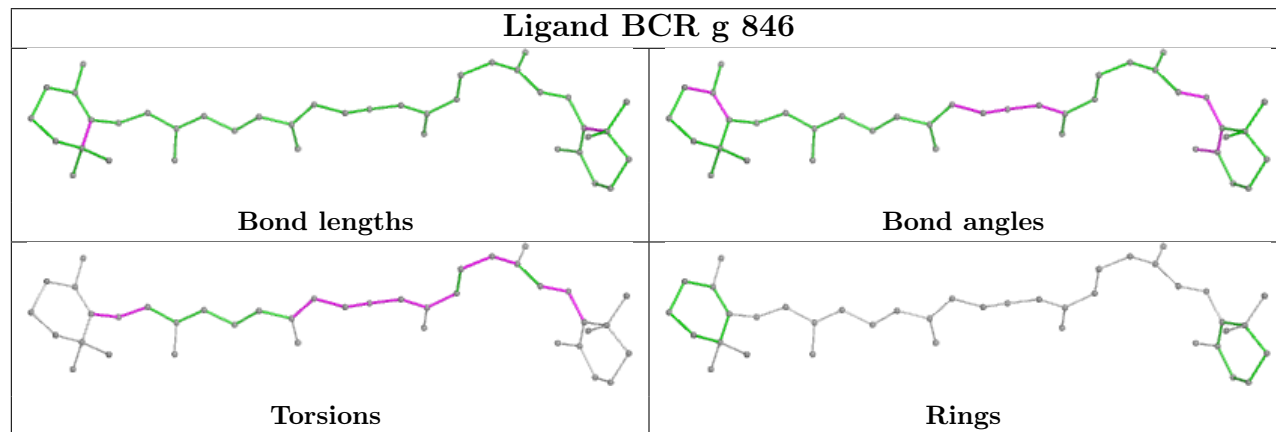


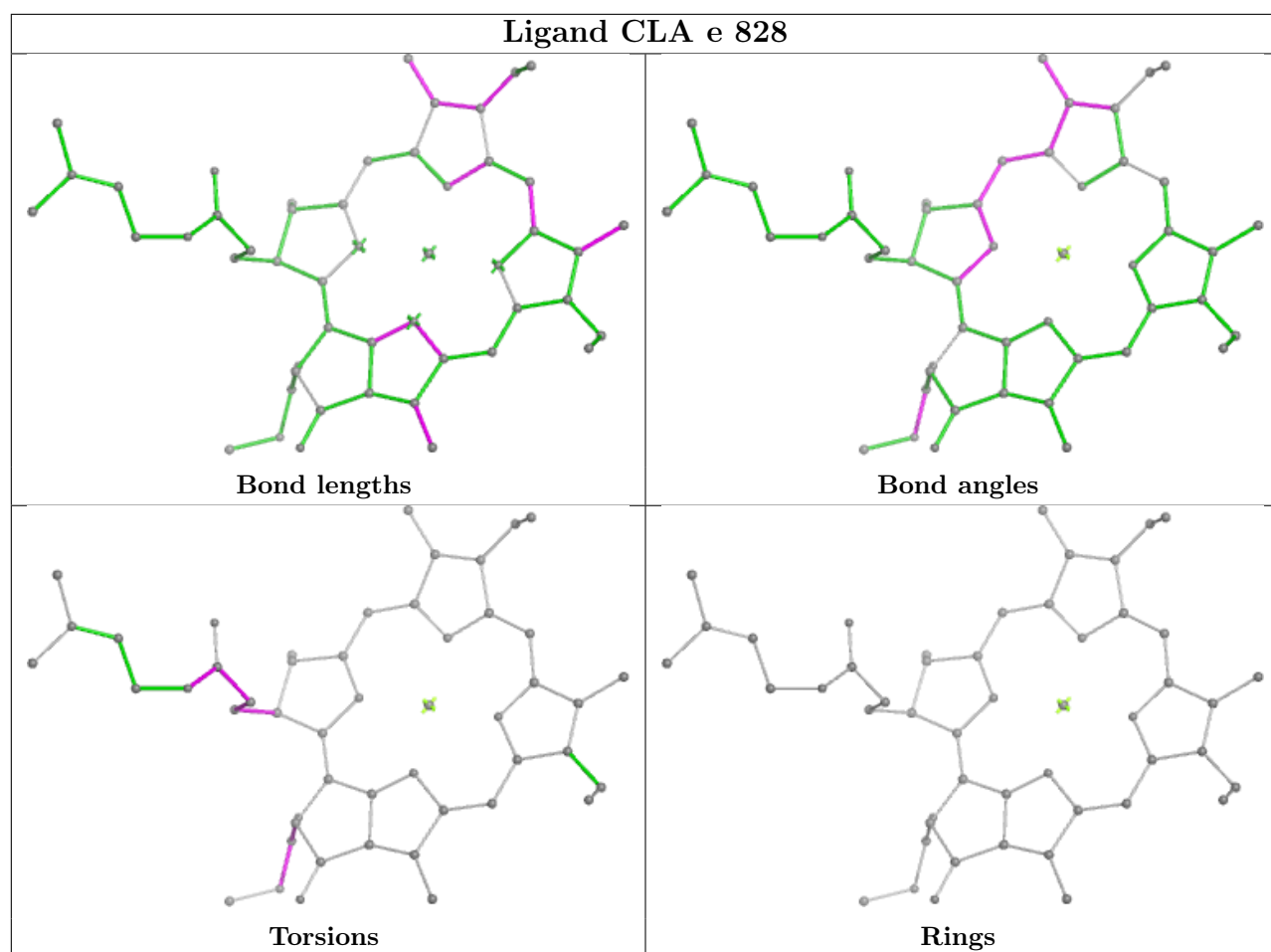
Ligand CLA 1 205



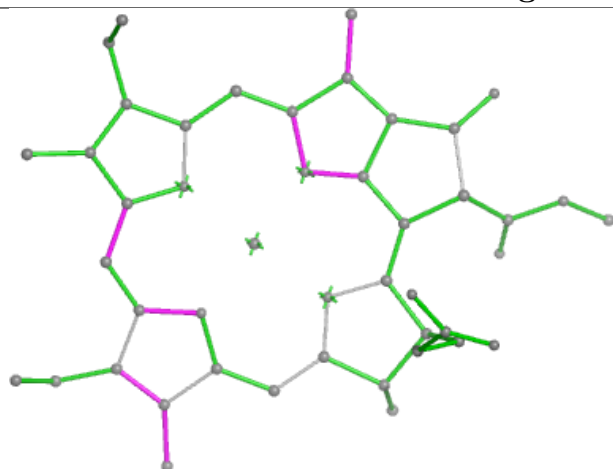
Ligand BCR e 849



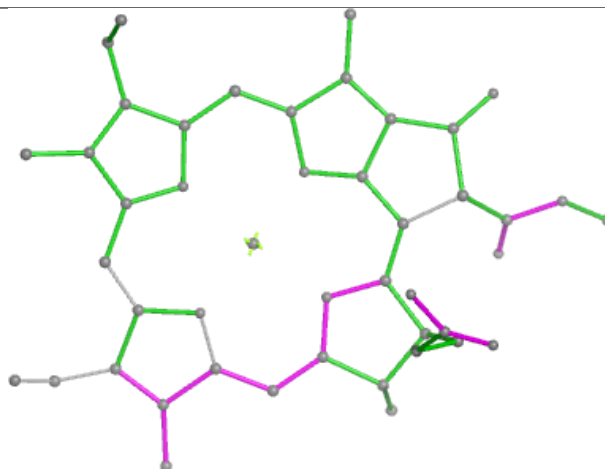
Ligand CLA A 853**Ligand BCR g 846**



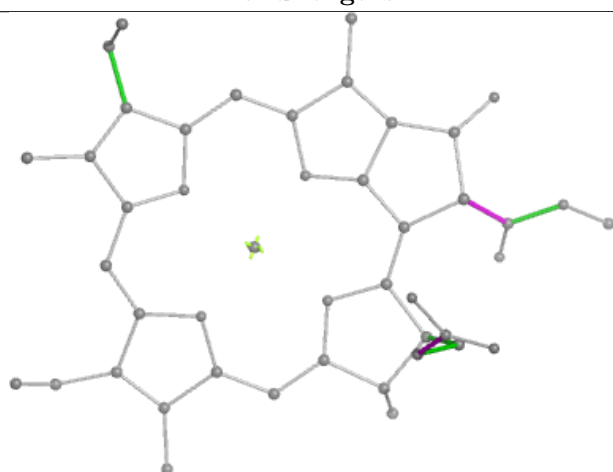
Ligand CLA a 814



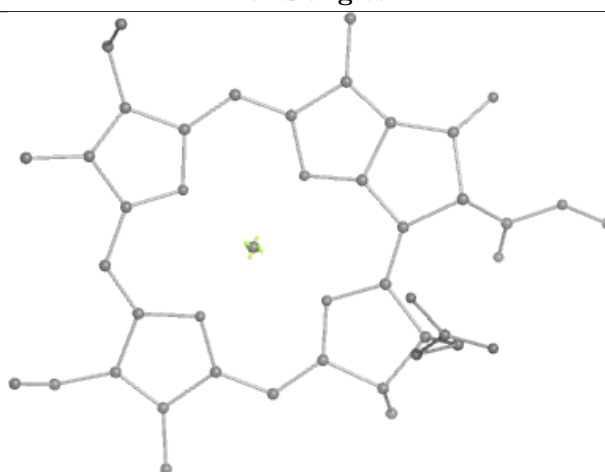
Bond lengths



Bond angles

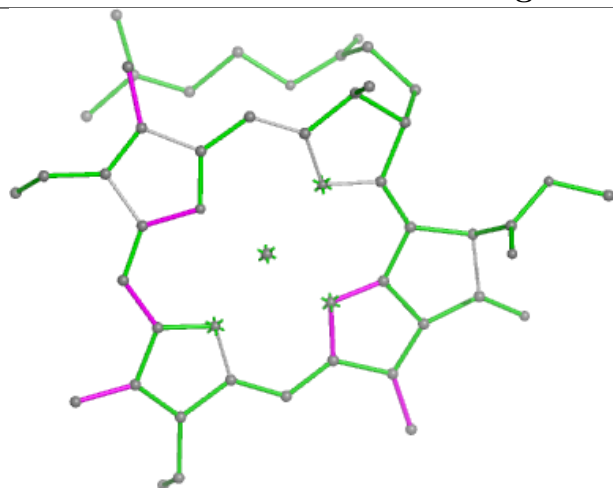


Torsions

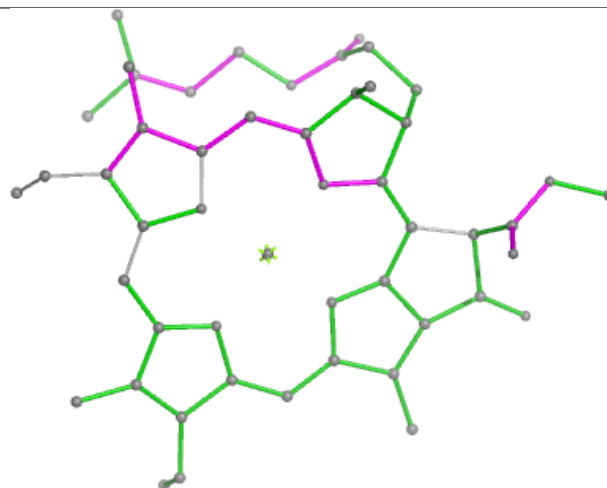


Rings

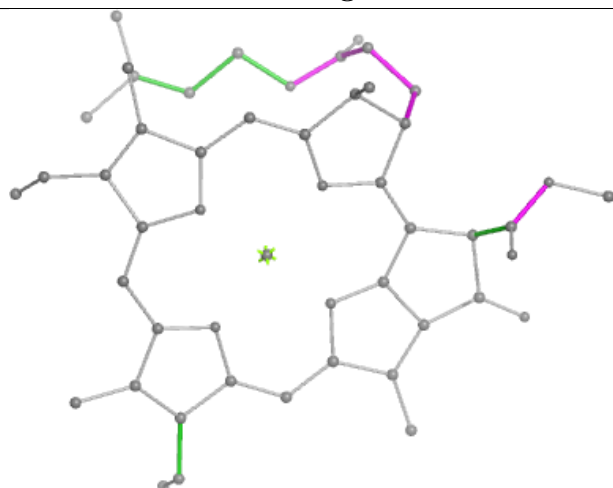
Ligand CLA E 822



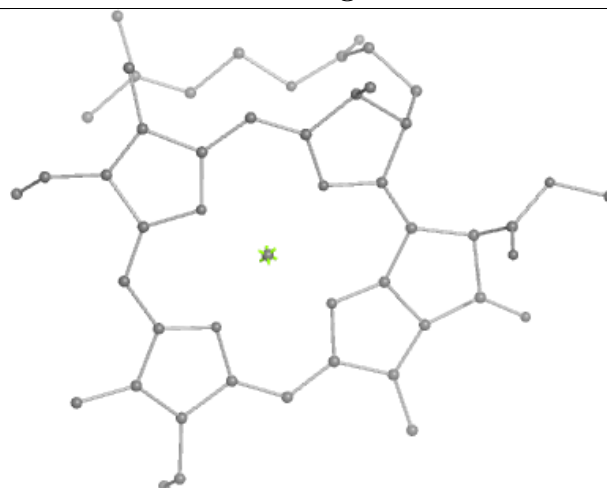
Bond lengths



Bond angles

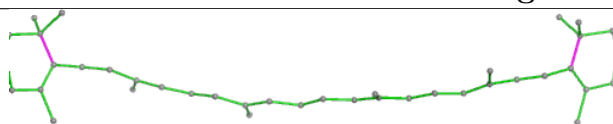


Torsions

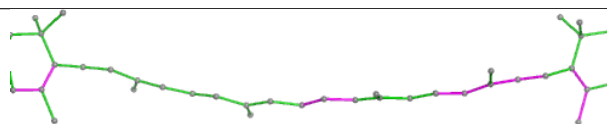


Rings

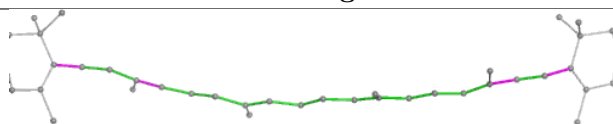
Ligand BCR e 850



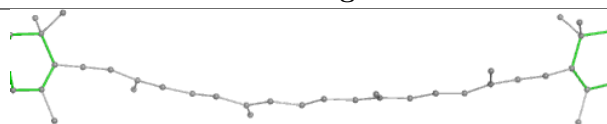
Bond lengths



Bond angles

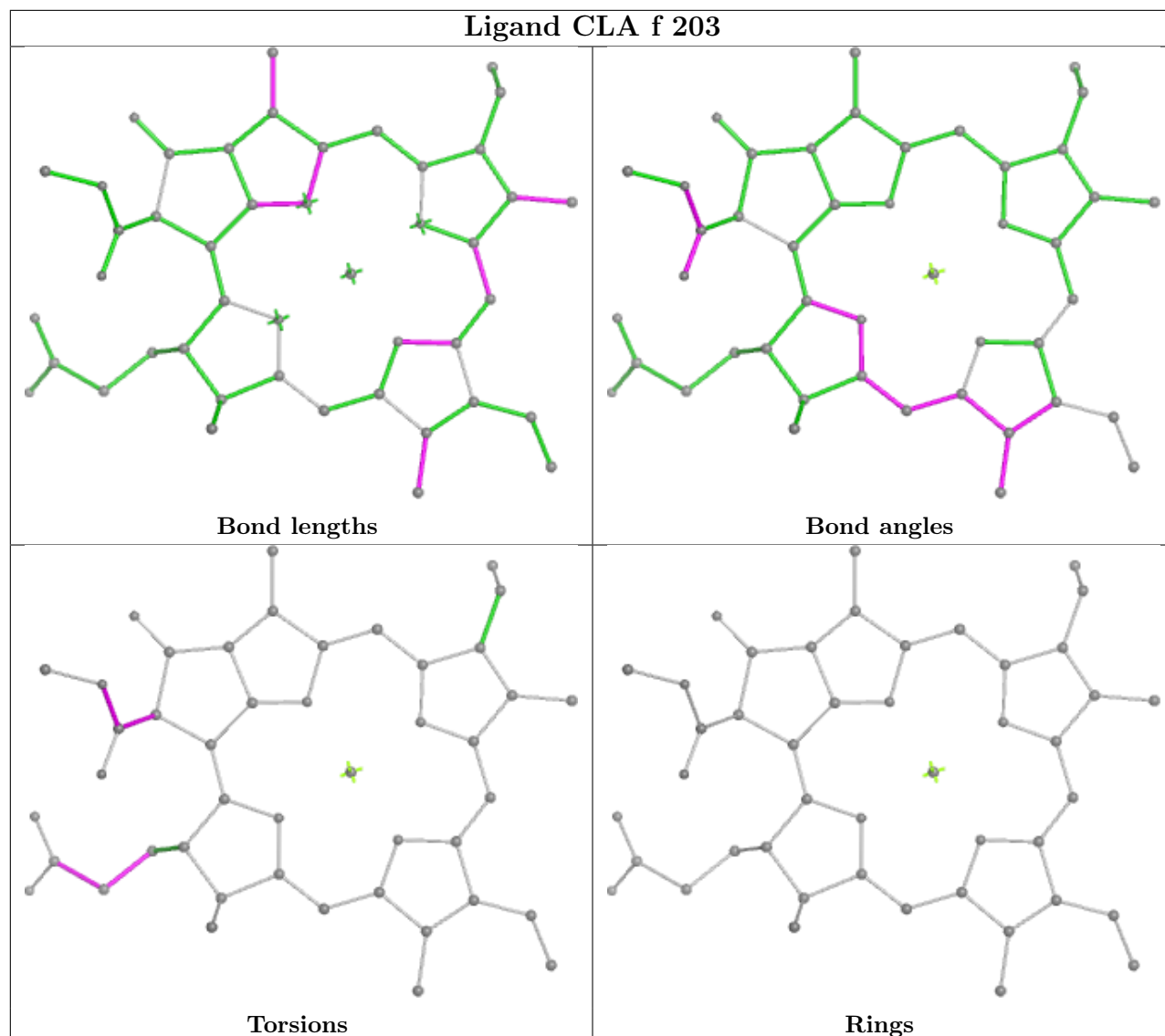


Torsions

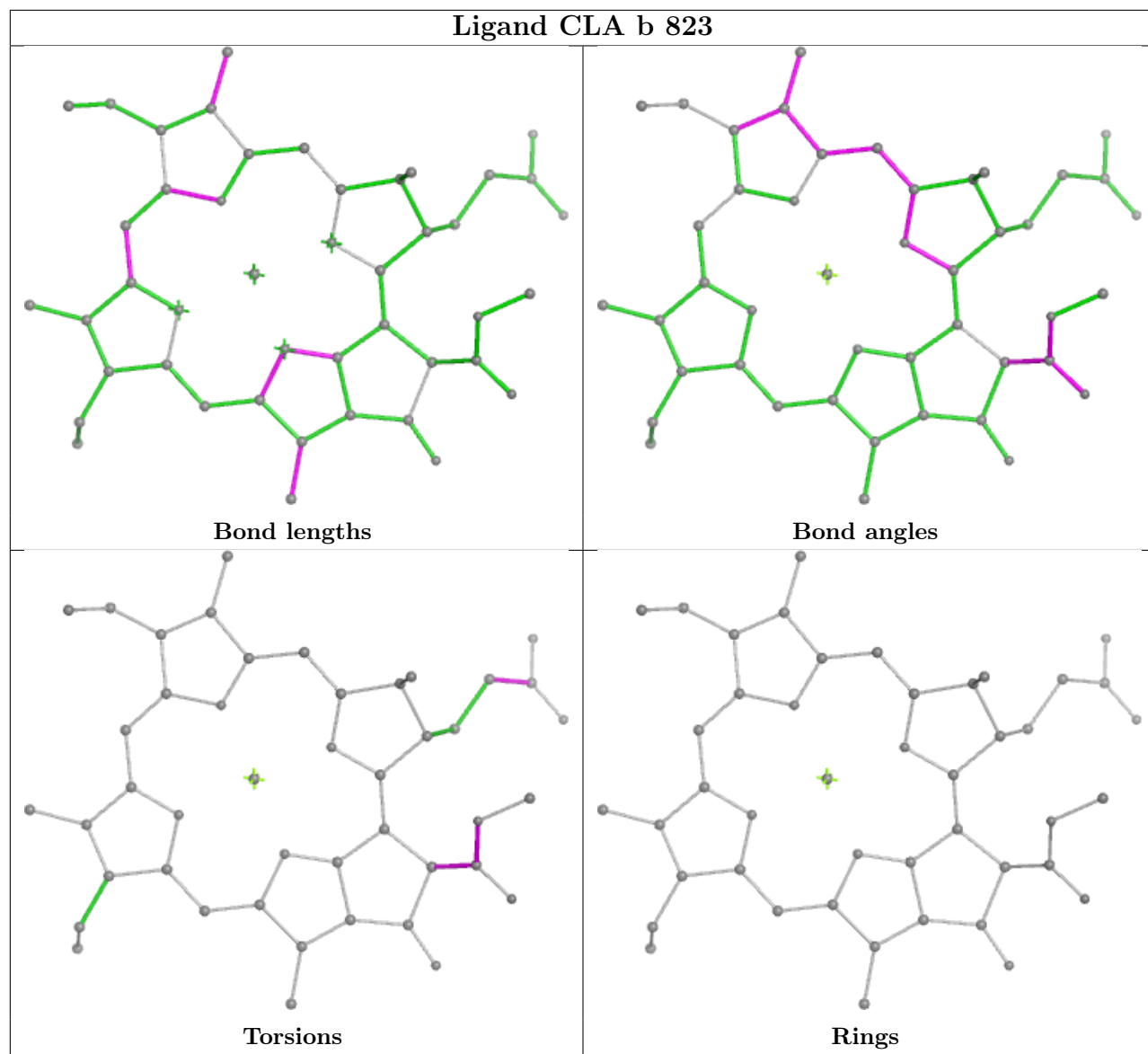


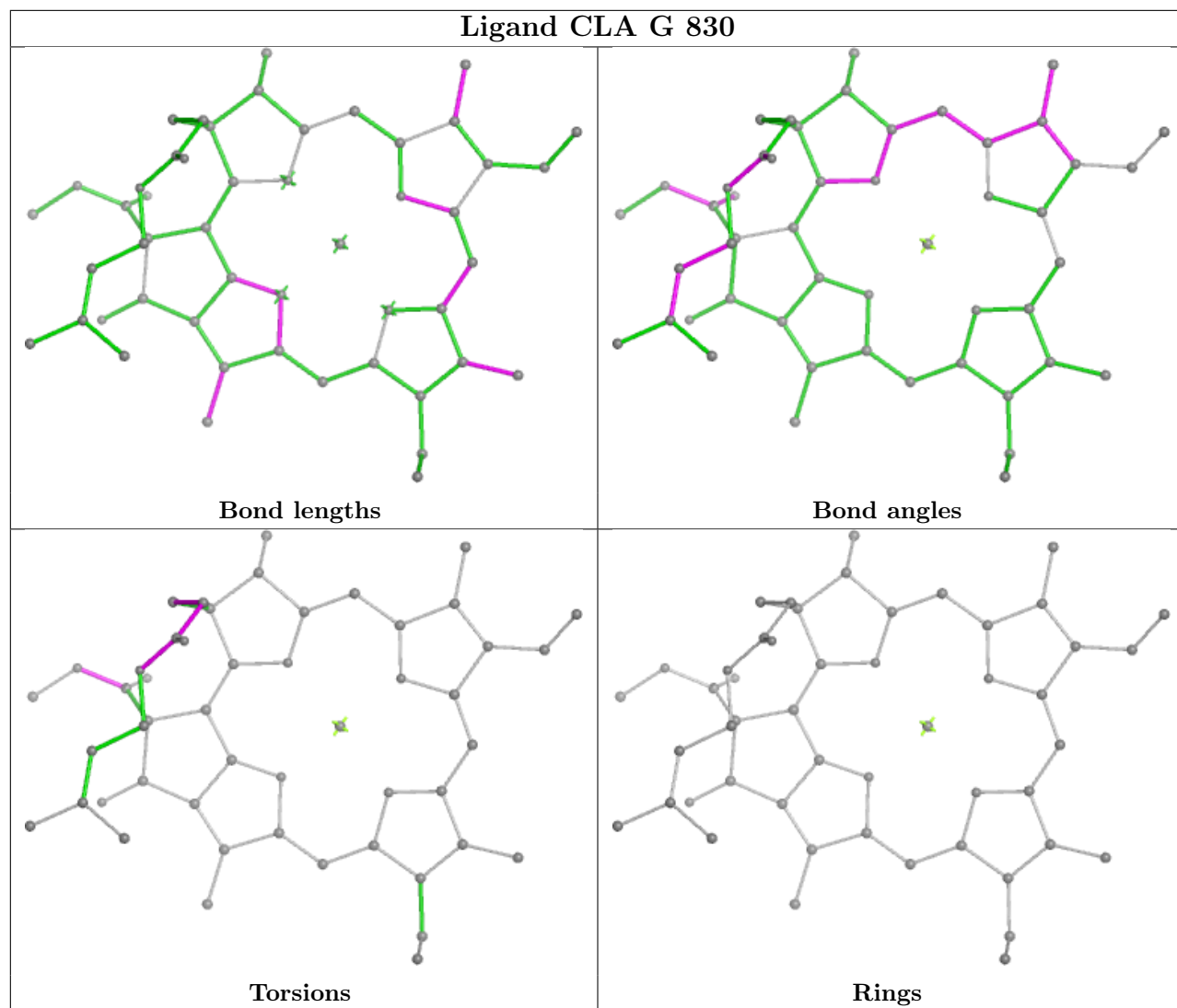
Rings

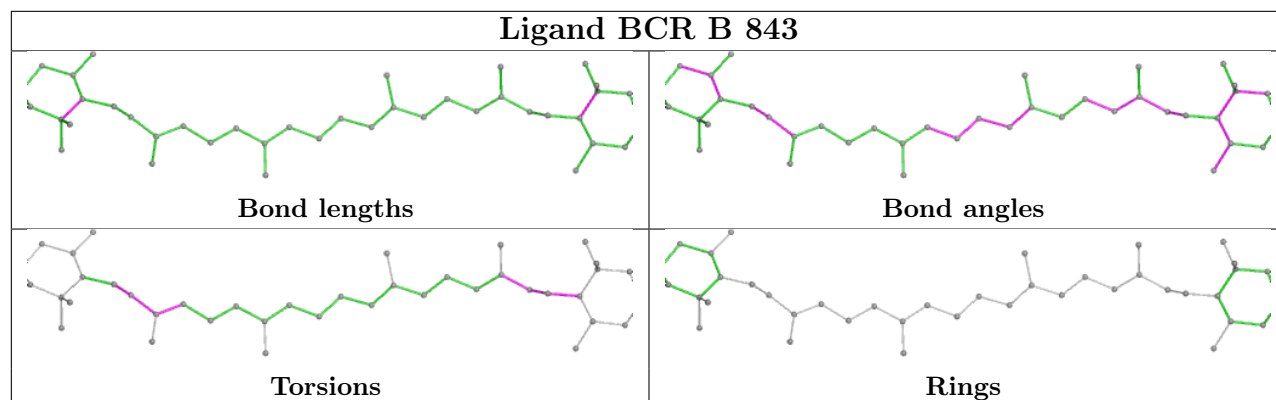
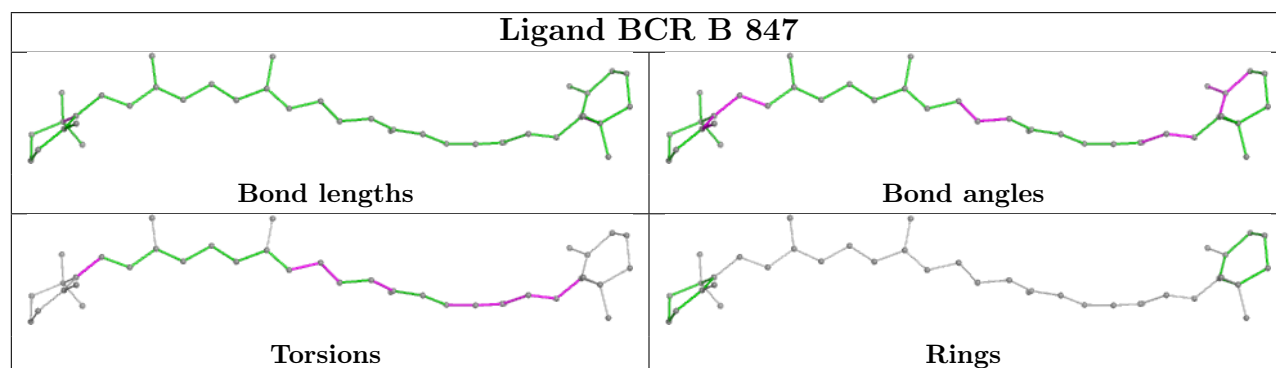
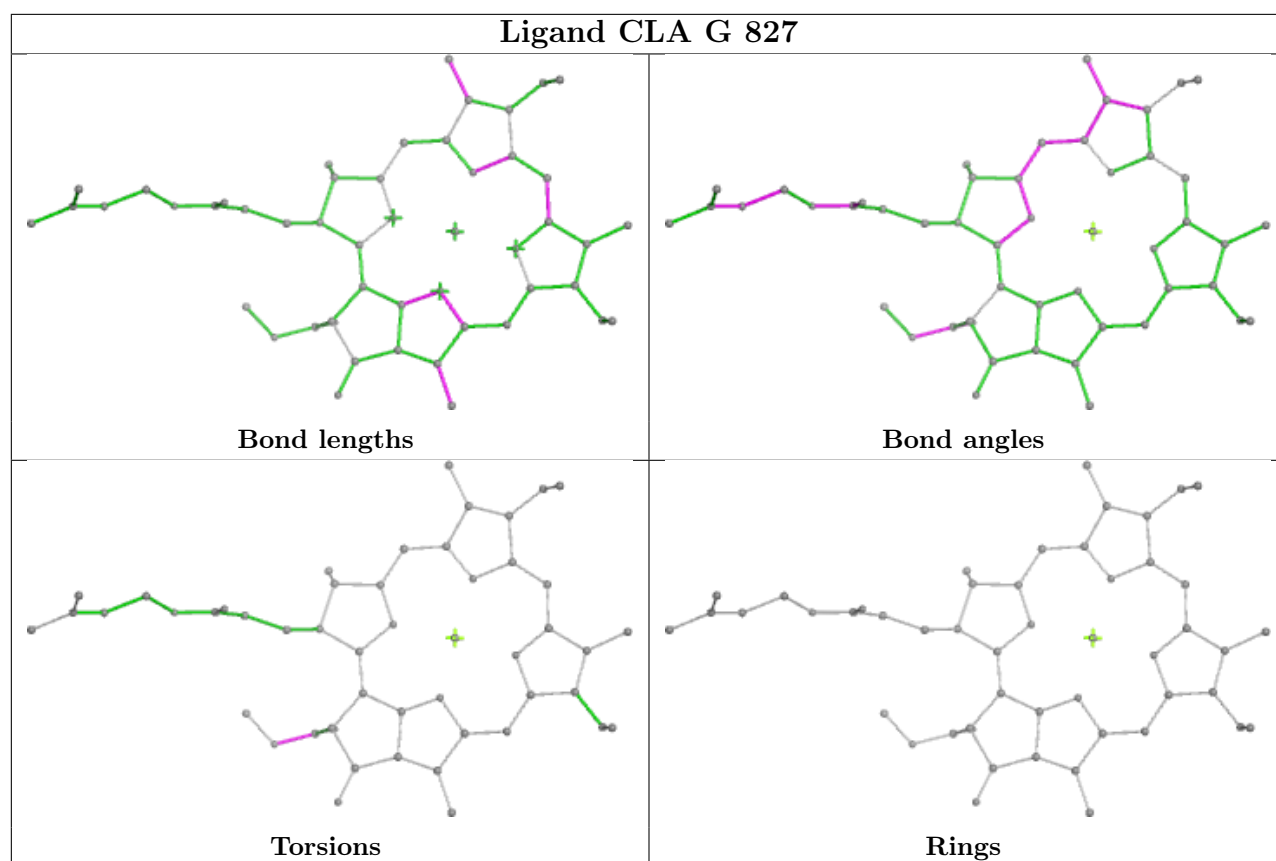
Ligand CLA f 203



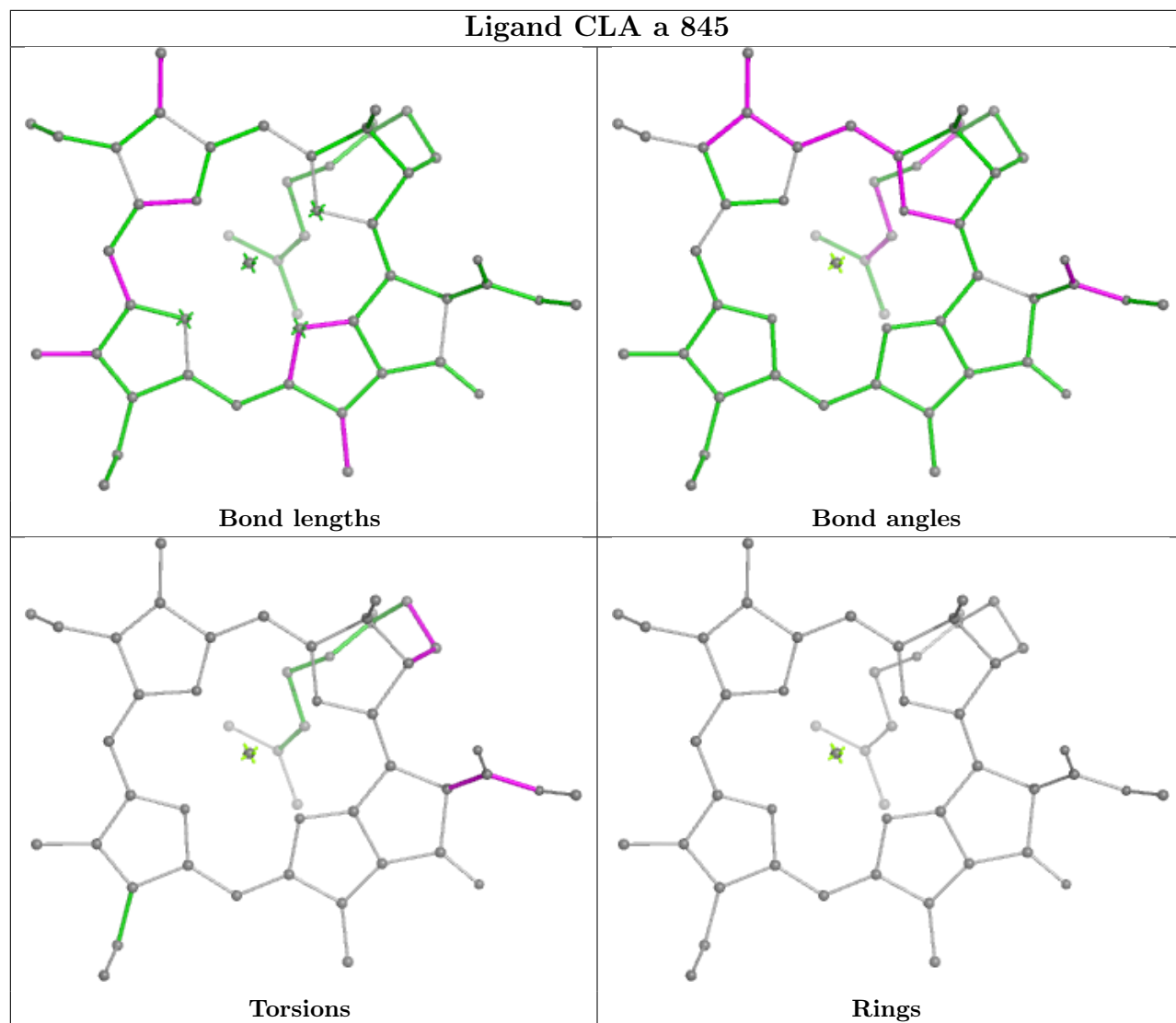
Ligand CLA b 823



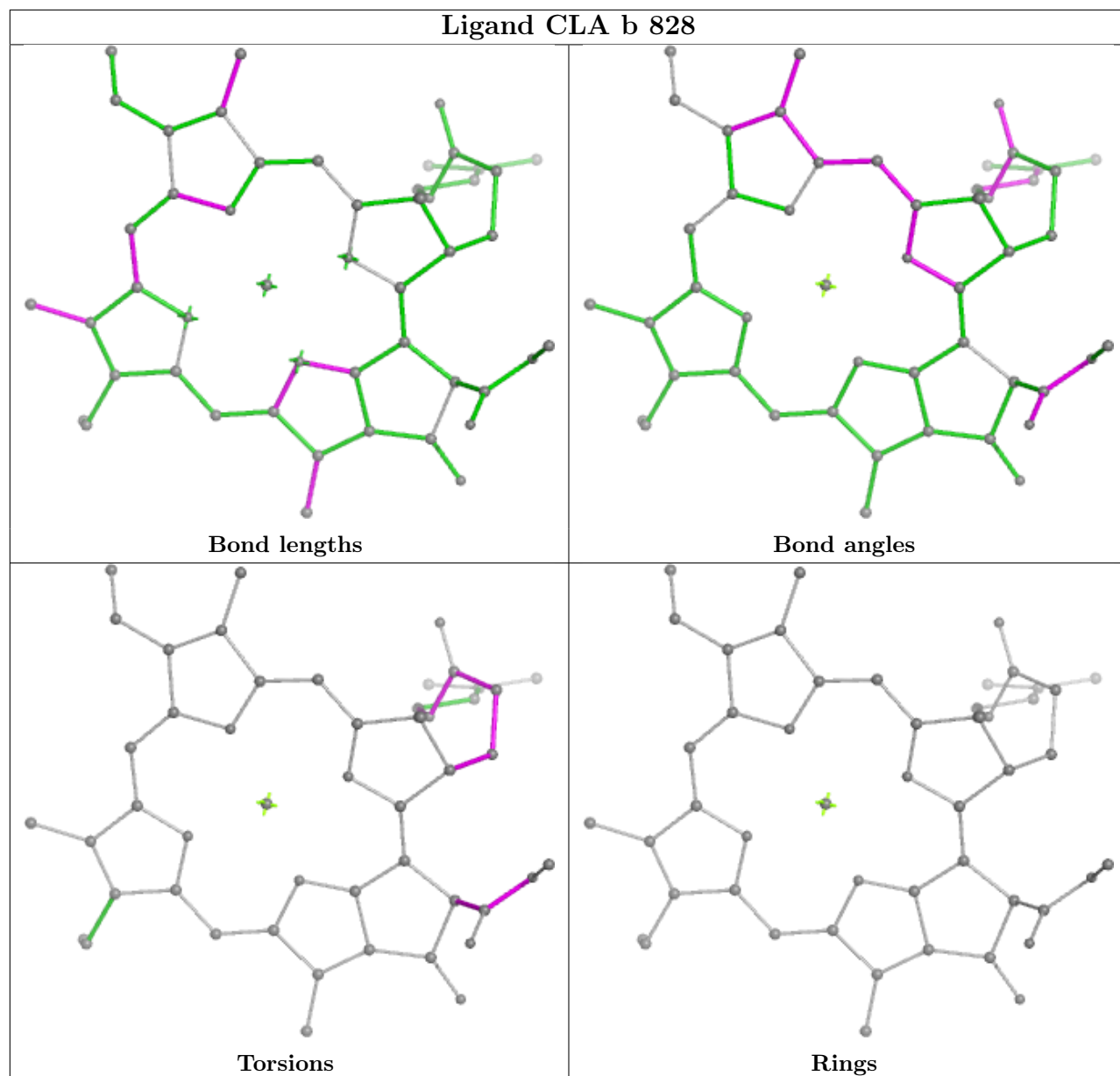




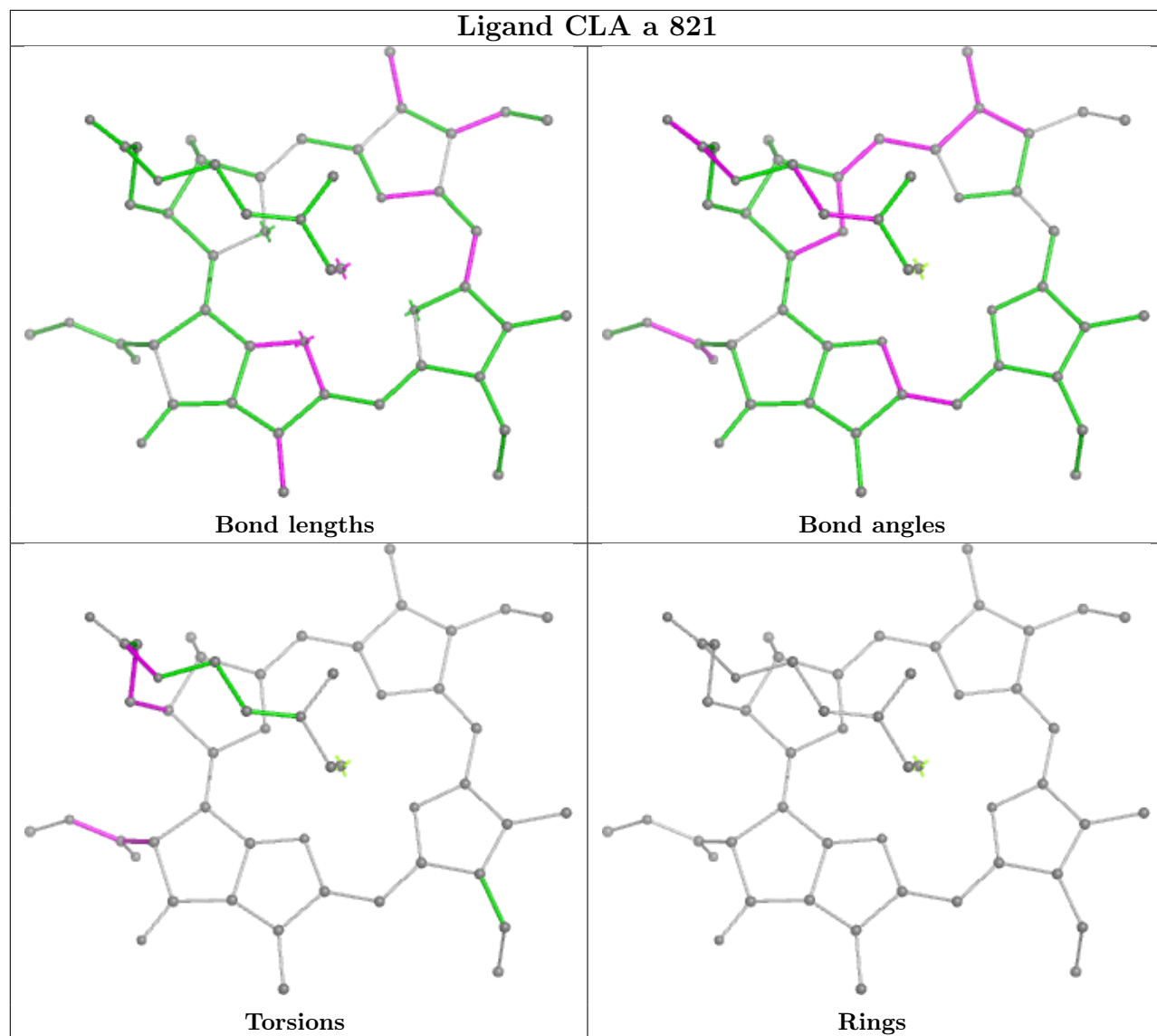
Ligand CLA a 845

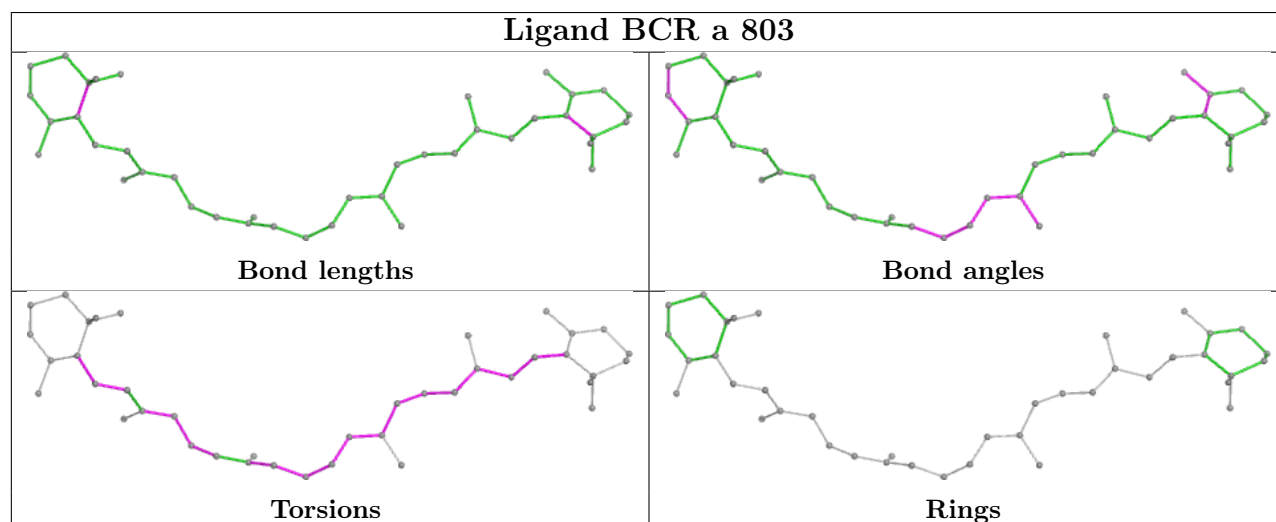
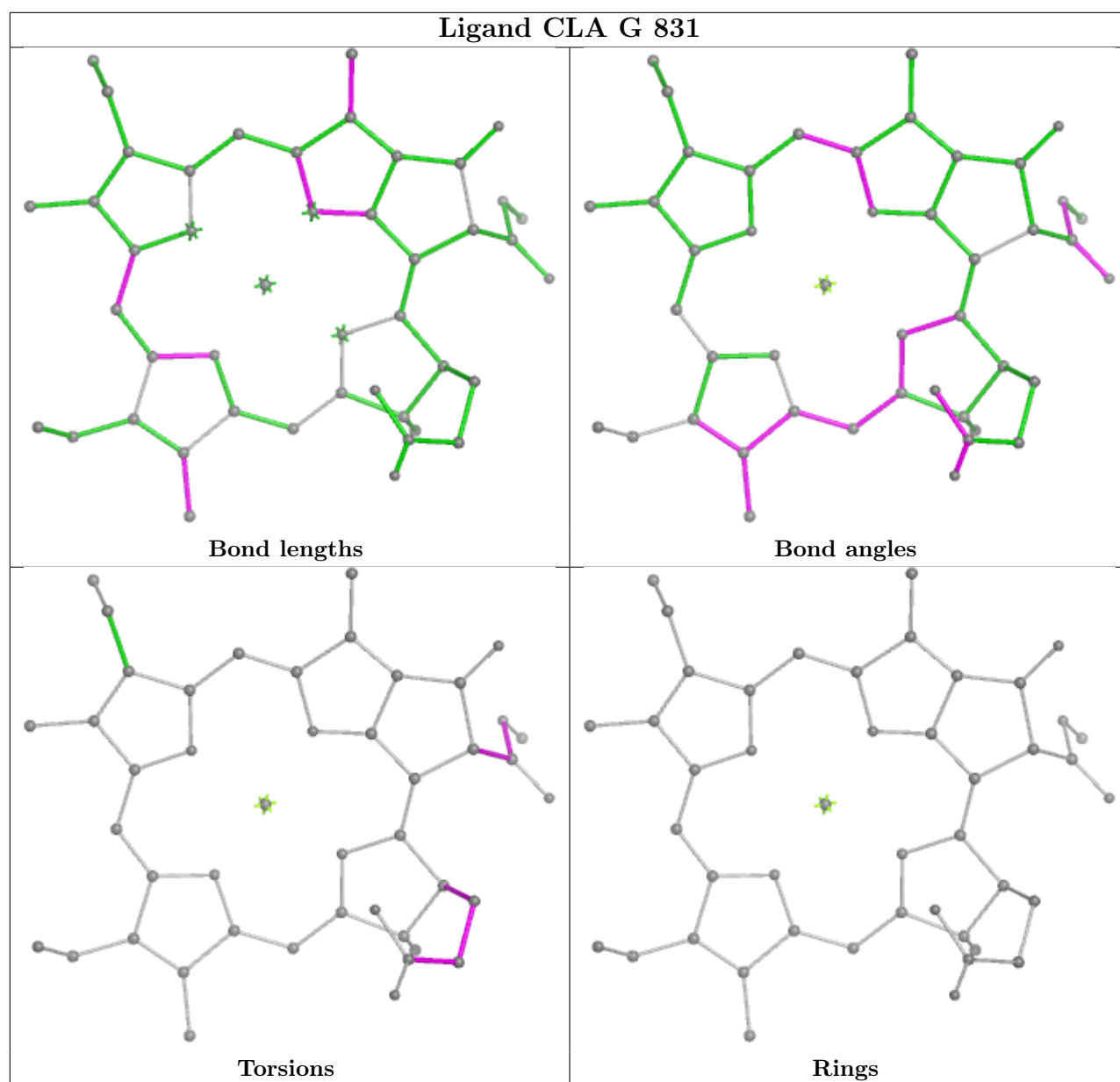


Ligand CLA b 828

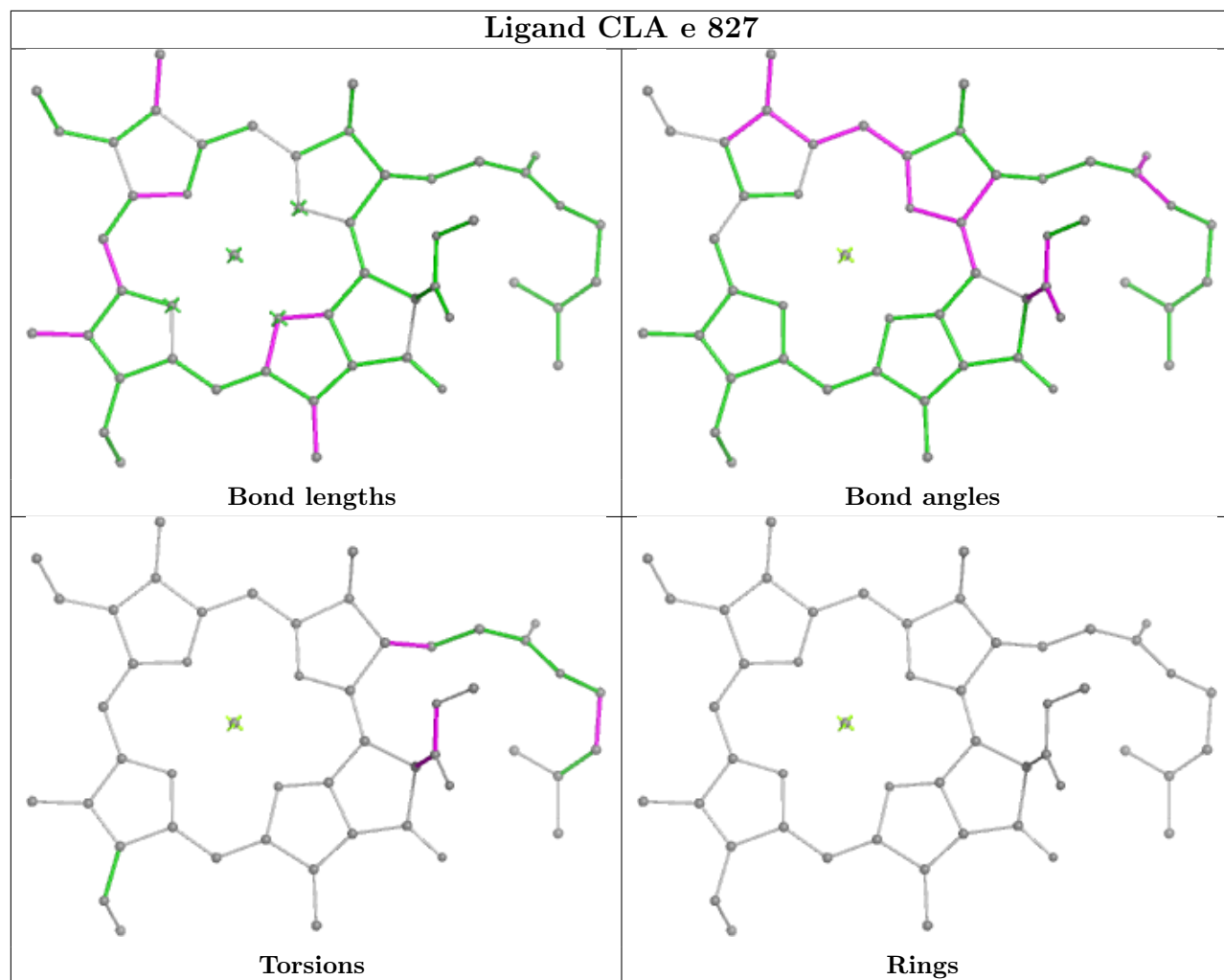


Ligand CLA a 821

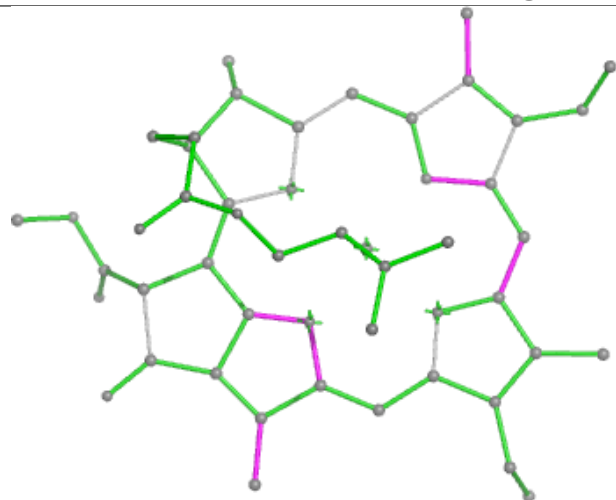




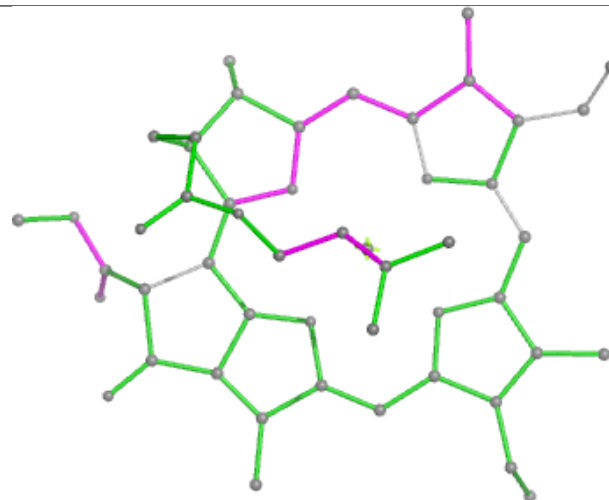
Ligand CLA e 827



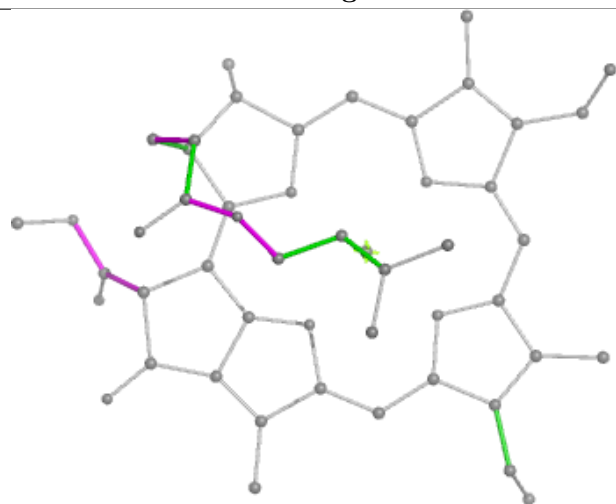
Ligand CLA a 815



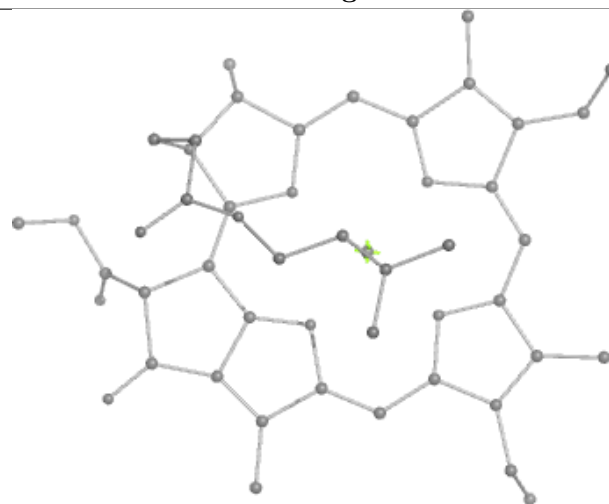
Bond lengths



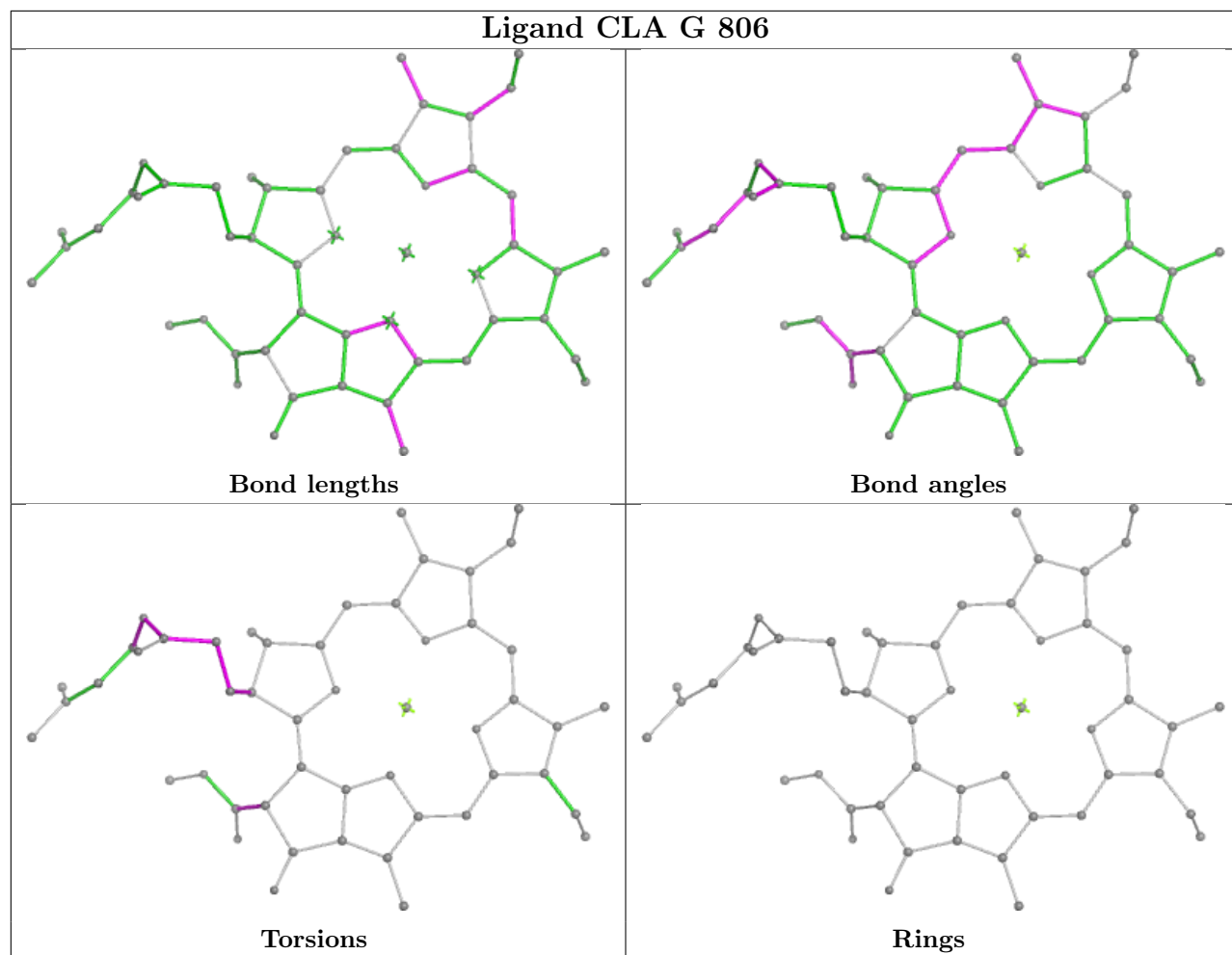
Bond angles



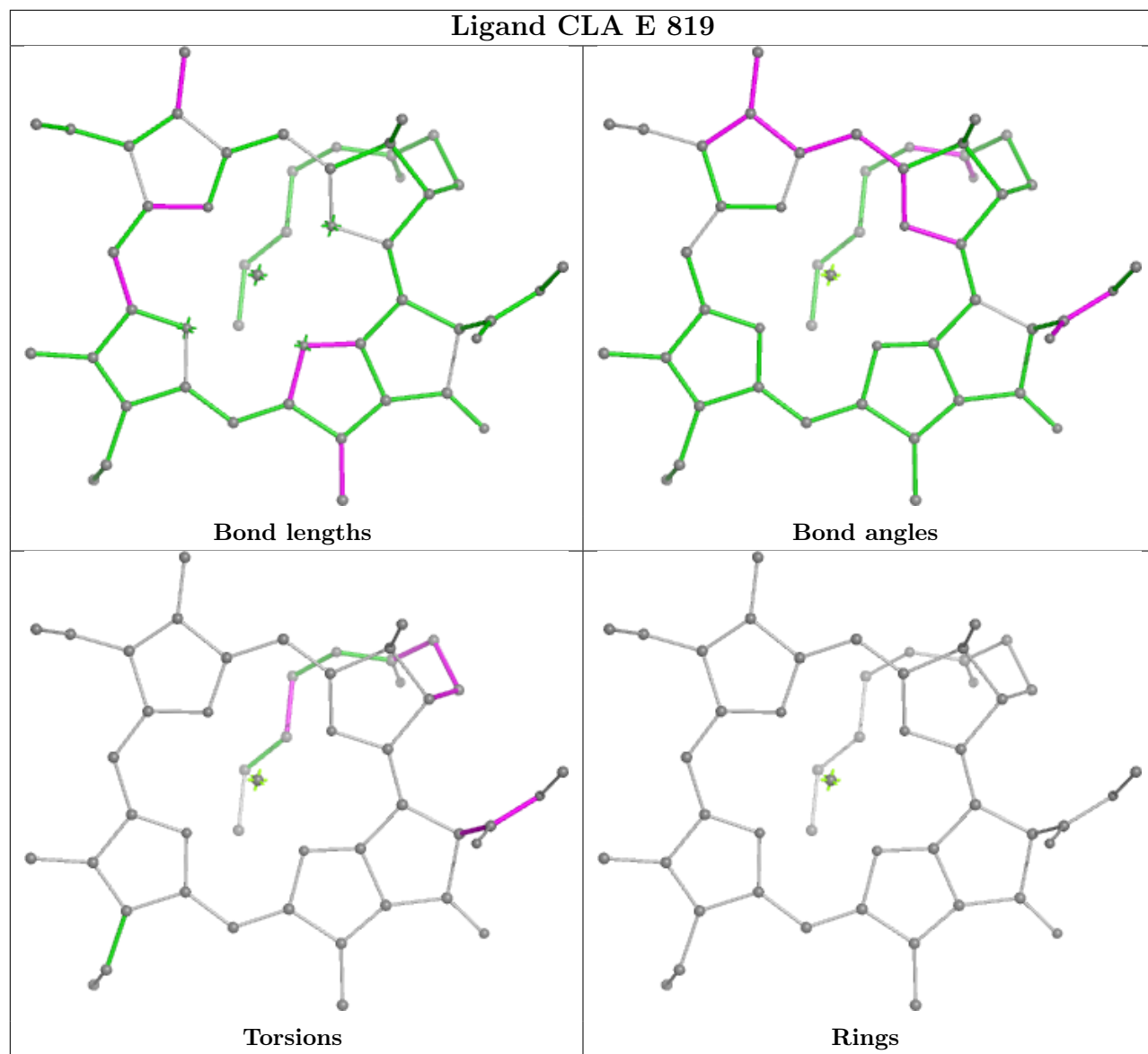
Torsions



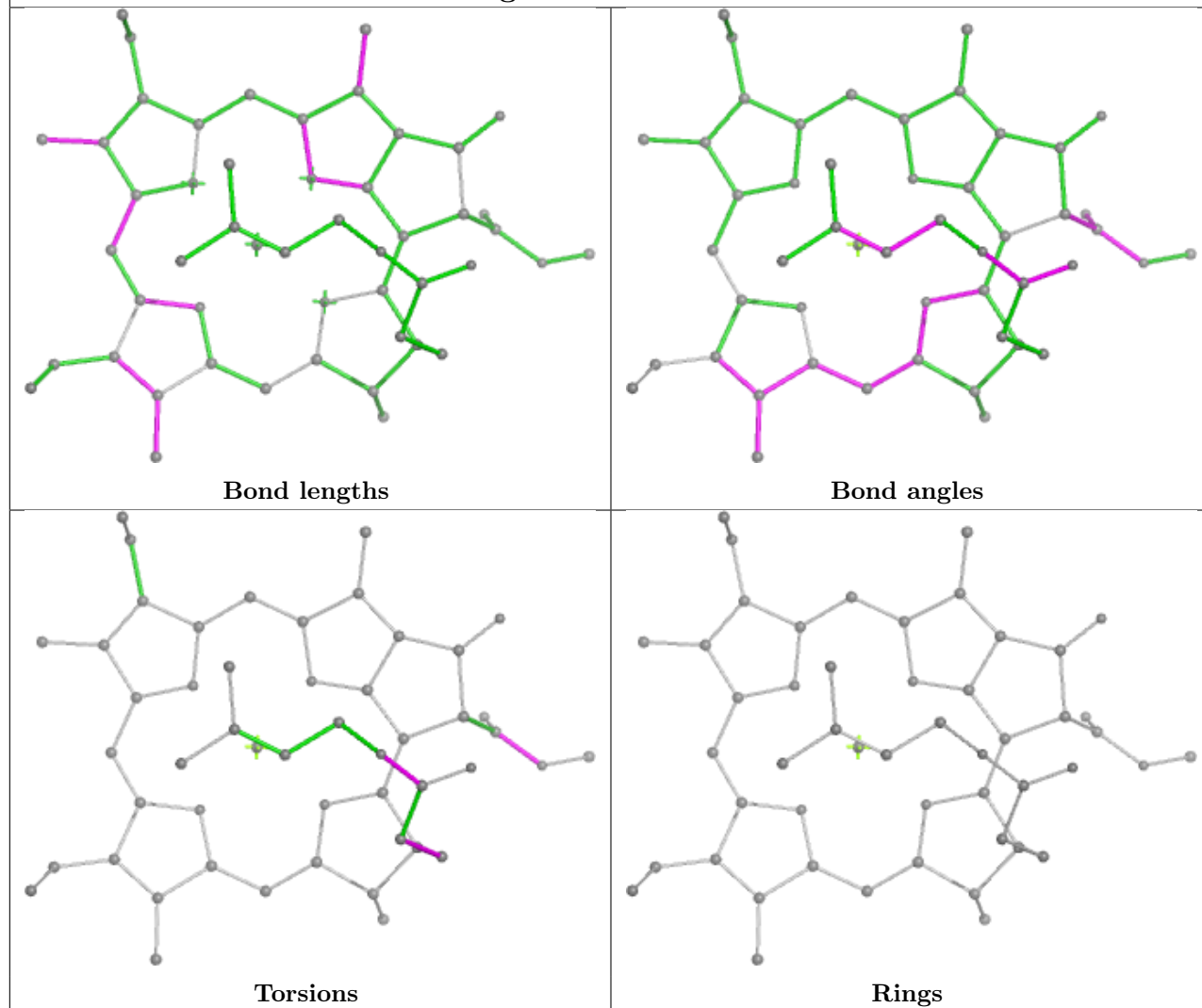
Rings



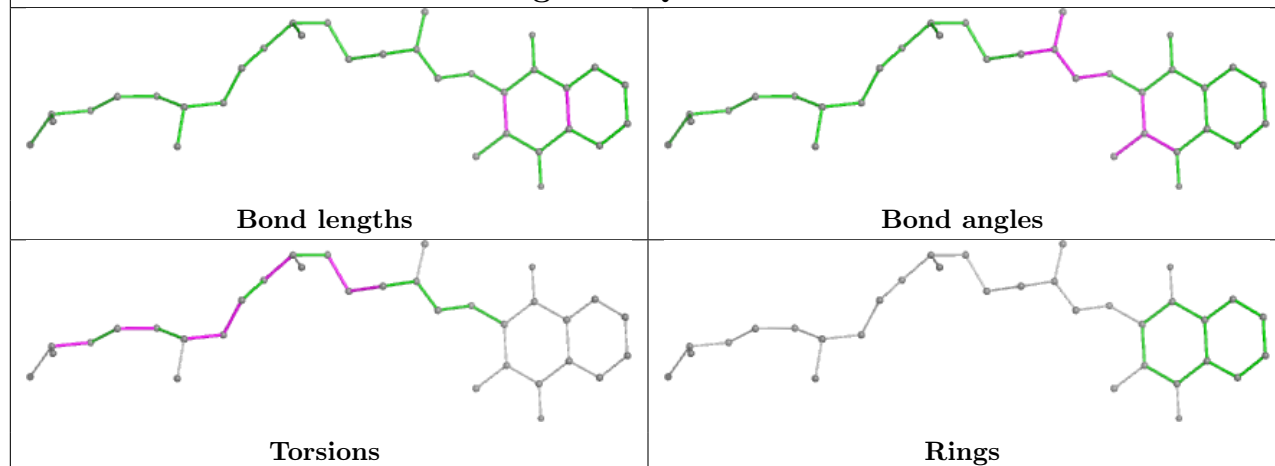
Ligand CLA E 819



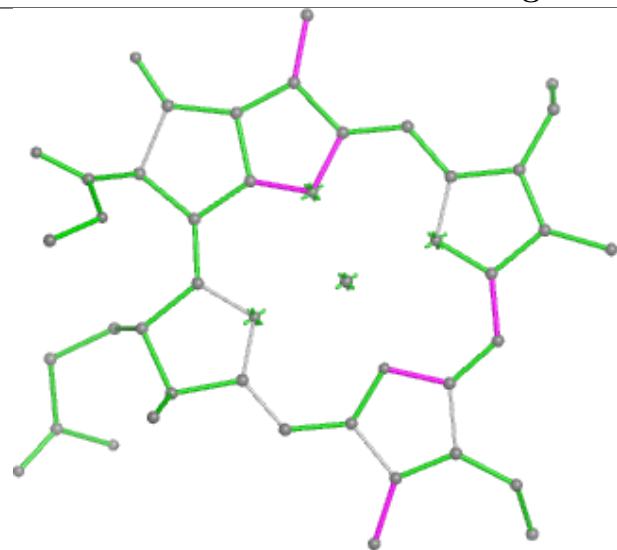
Ligand CLA G 801



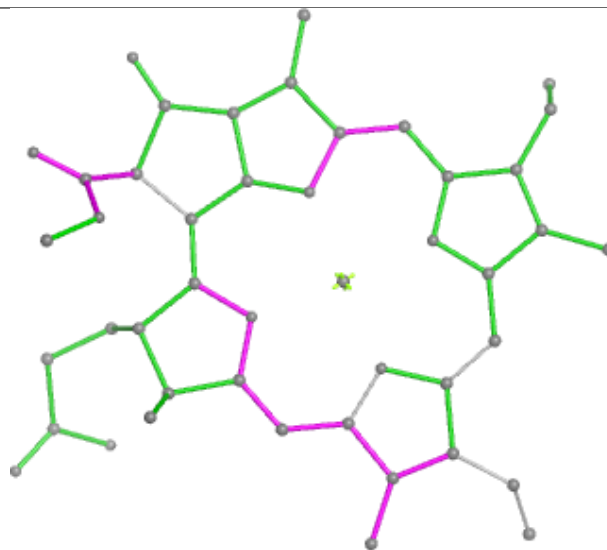
Ligand PQN a 847



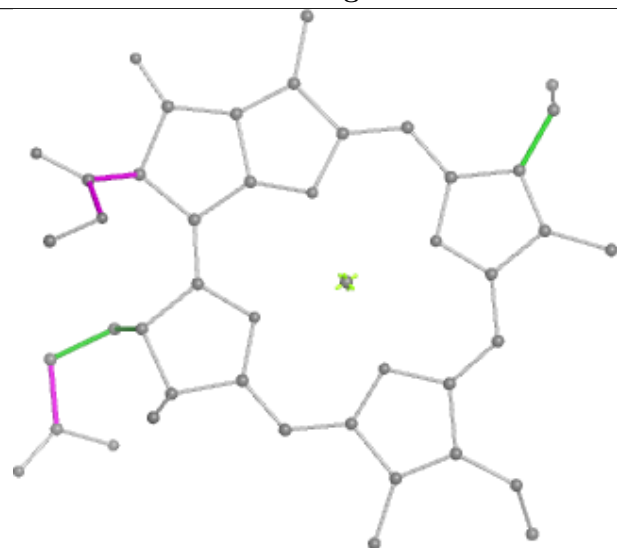
Ligand CLA a 839



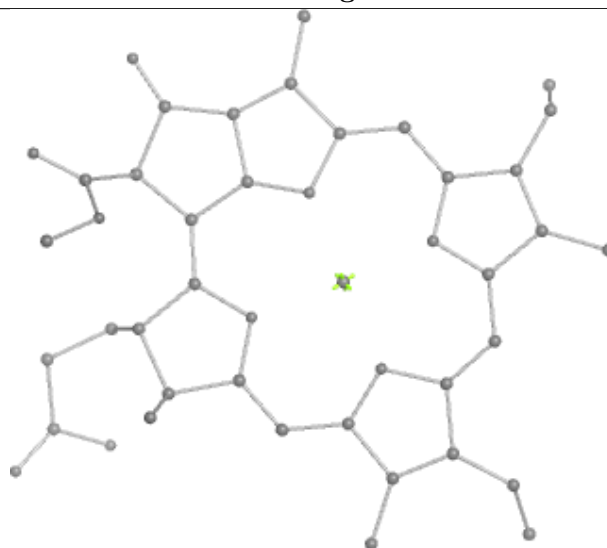
Bond lengths



Bond angles

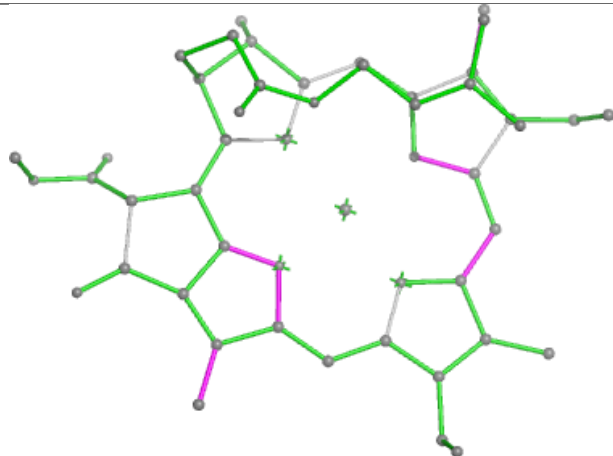


Torsions

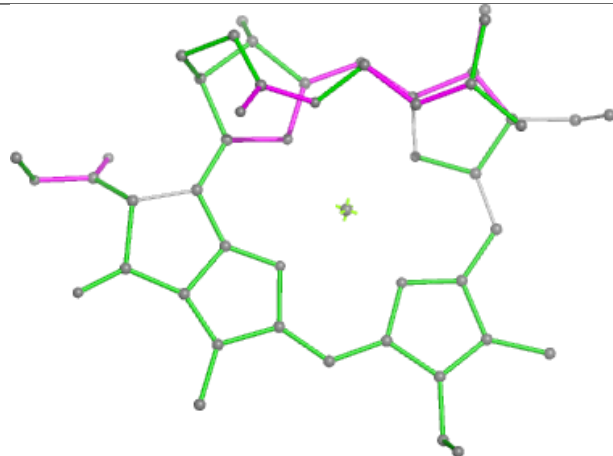


Rings

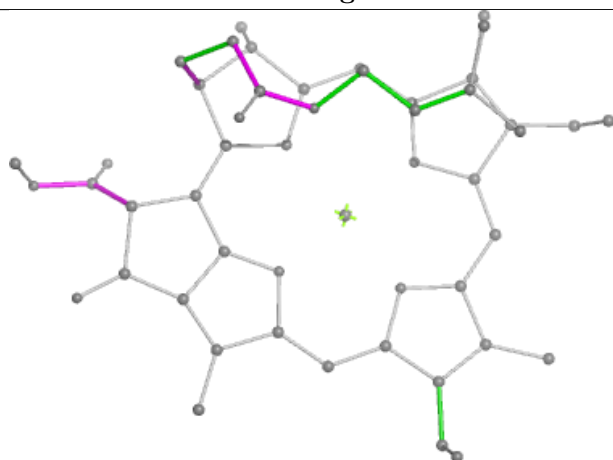
Ligand CLA A 824



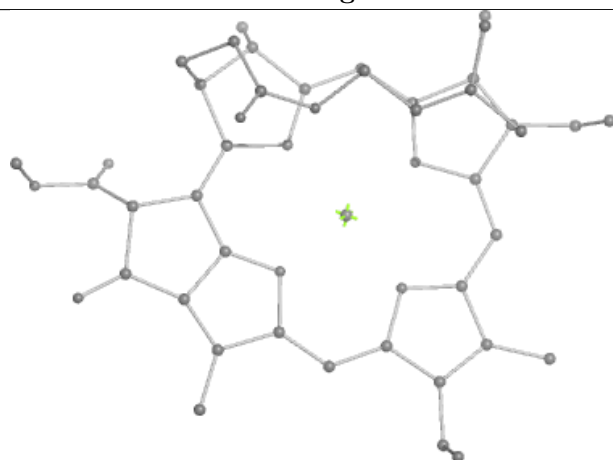
Bond lengths



Bond angles

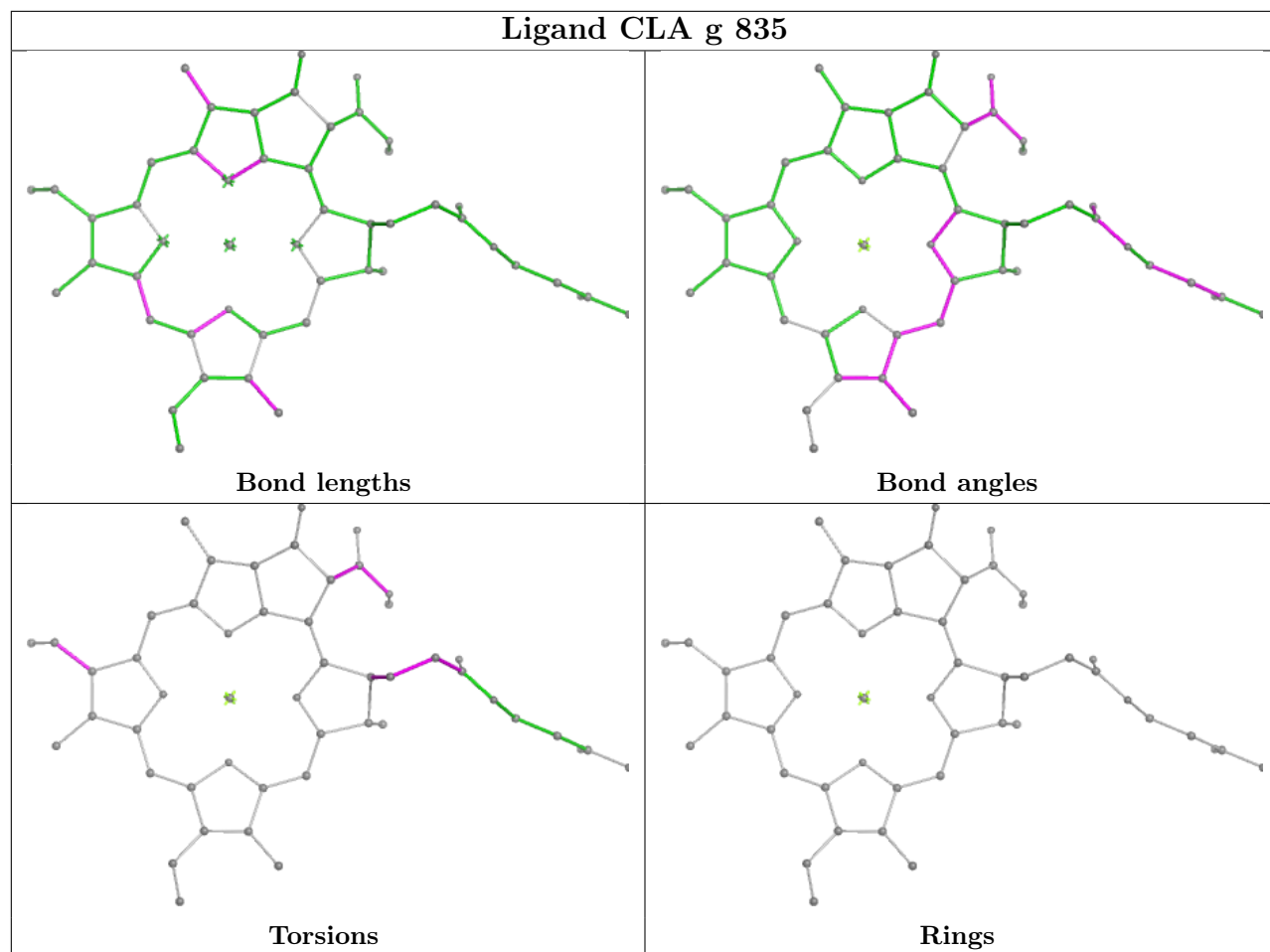


Torsions

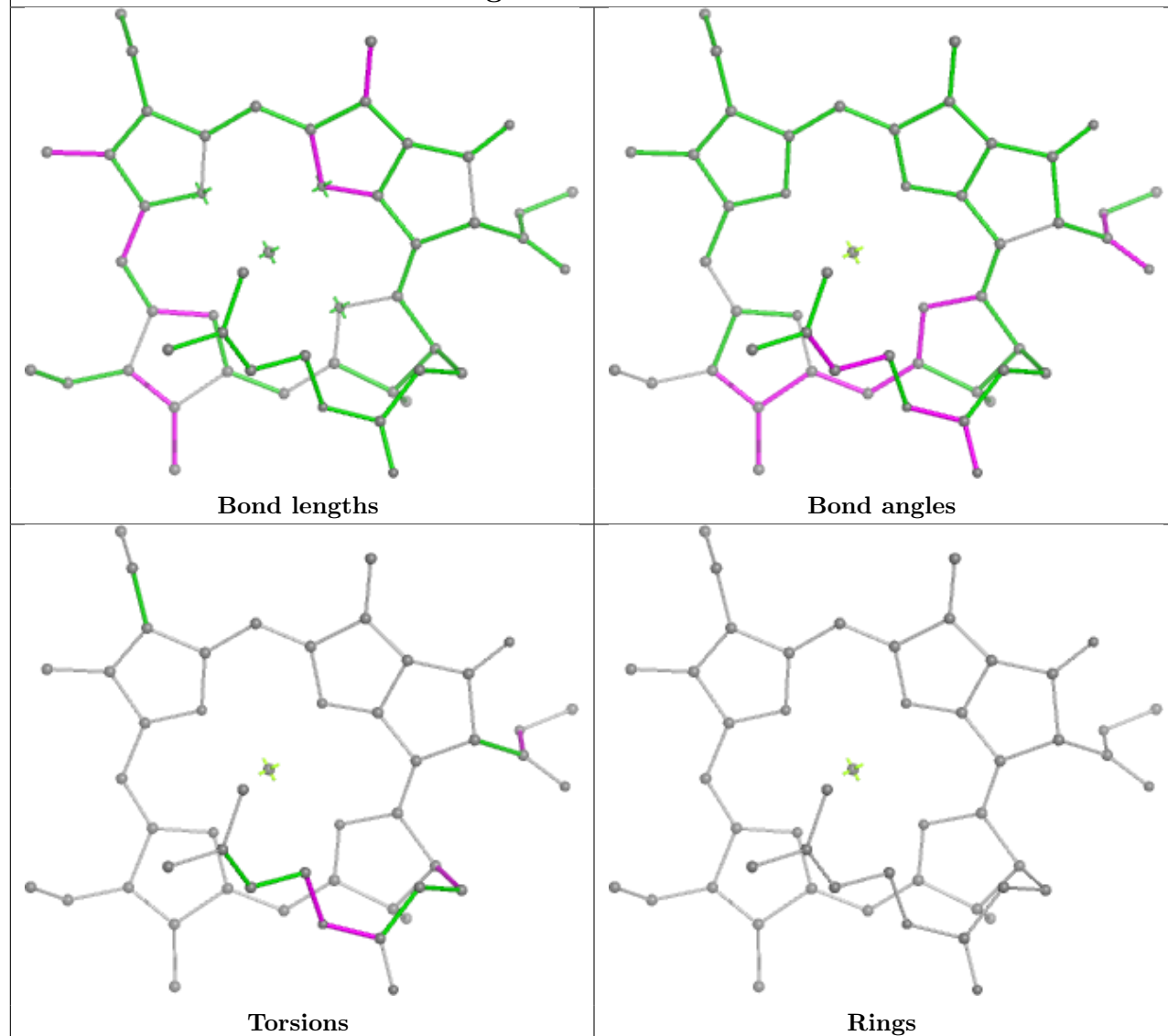


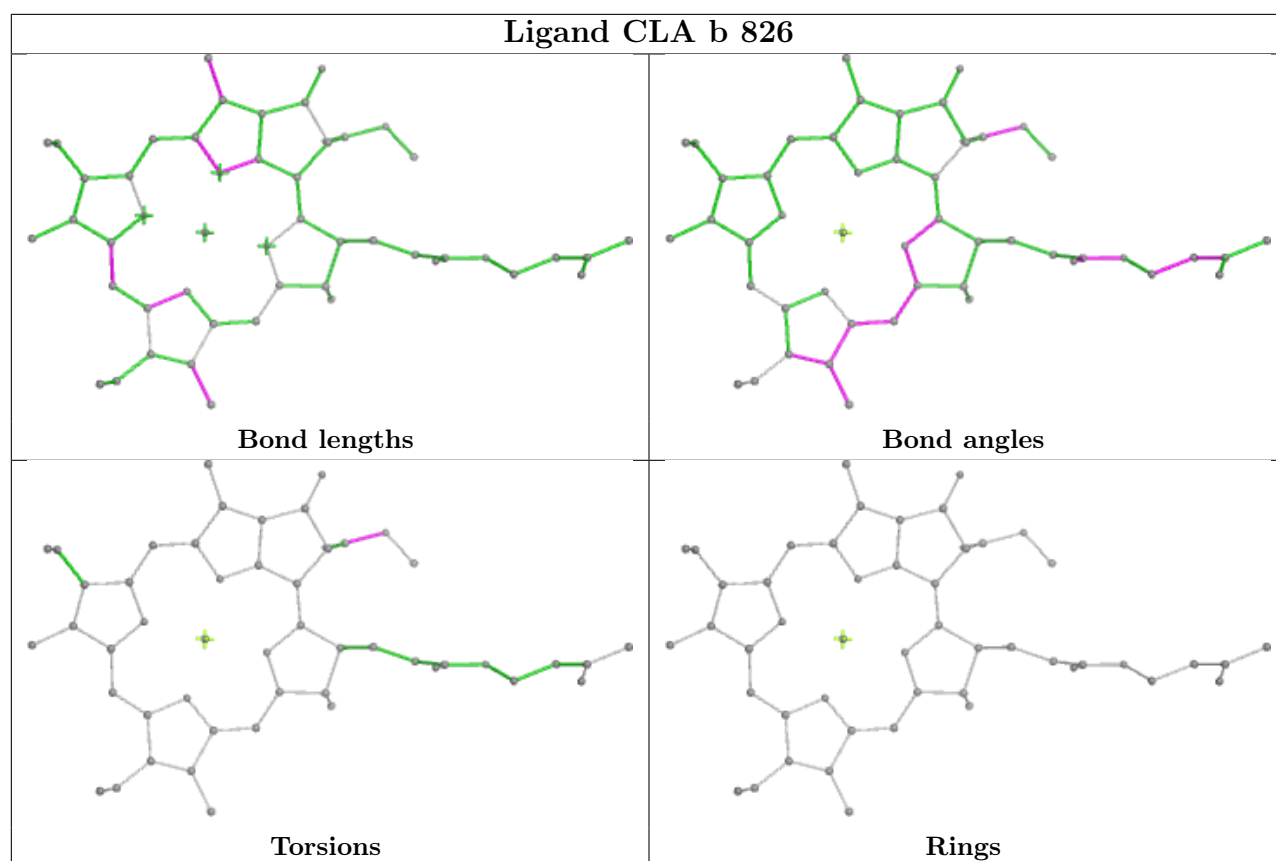
Rings

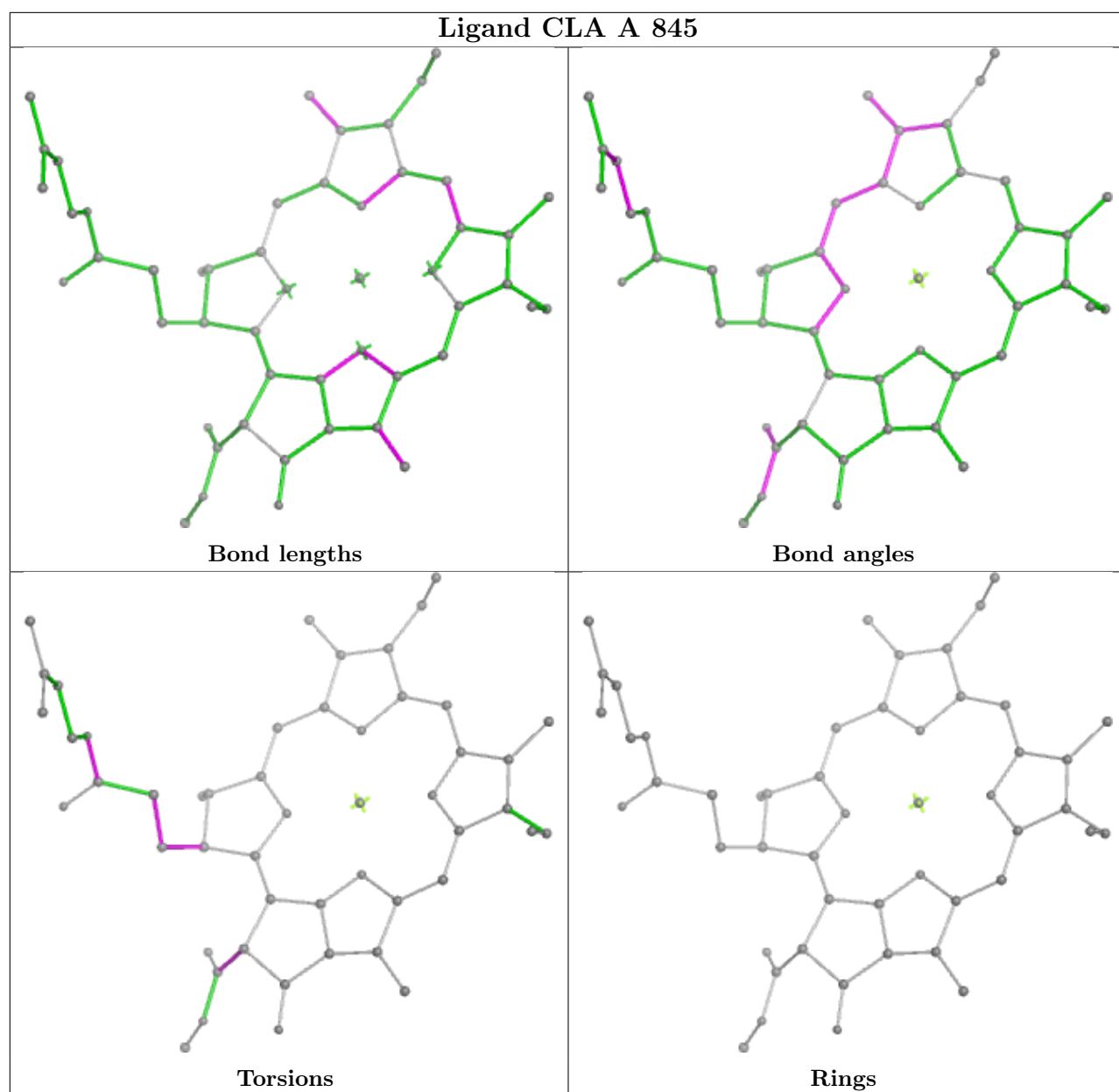
Ligand CLA g 835



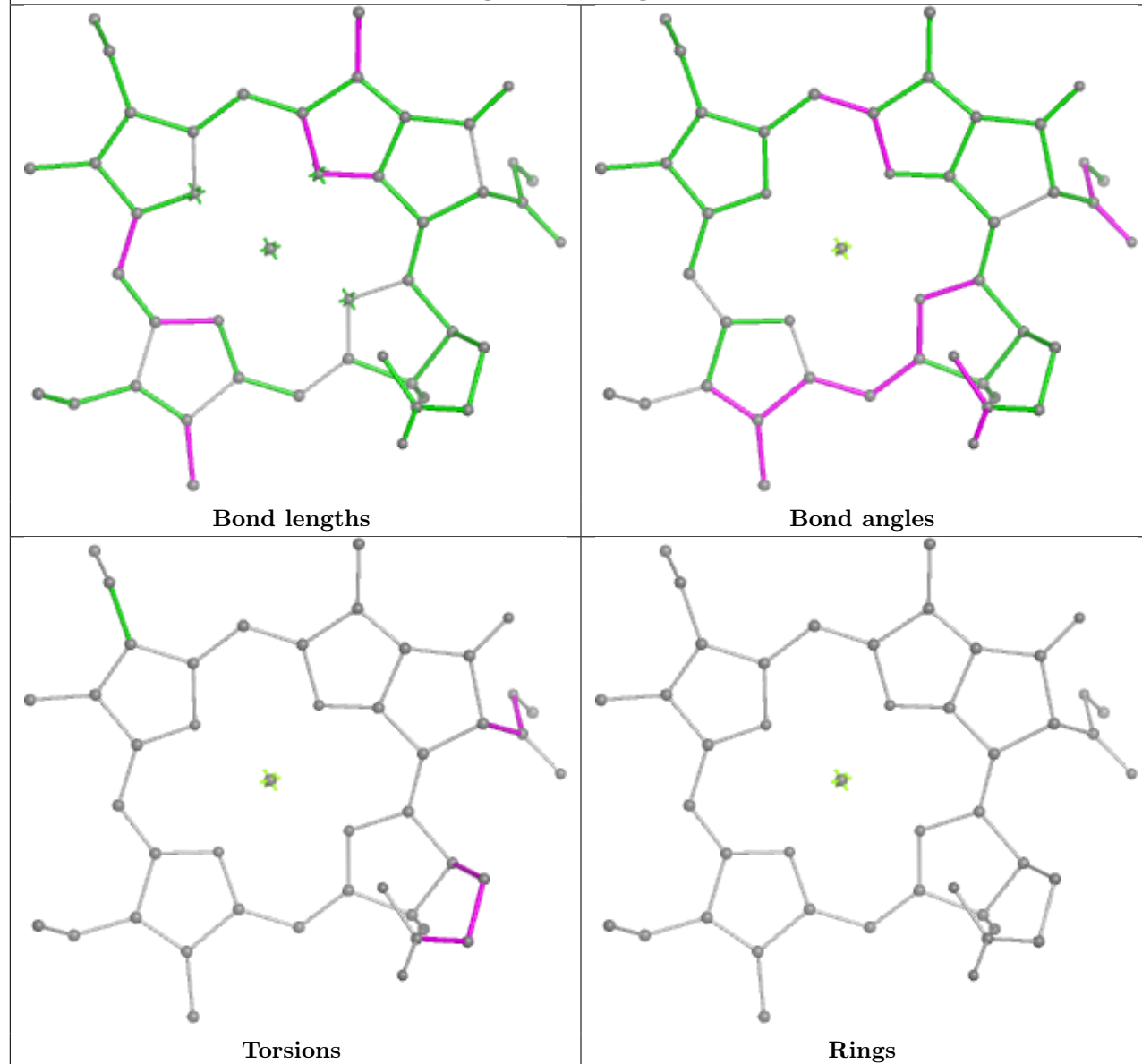
Ligand CLA G 828



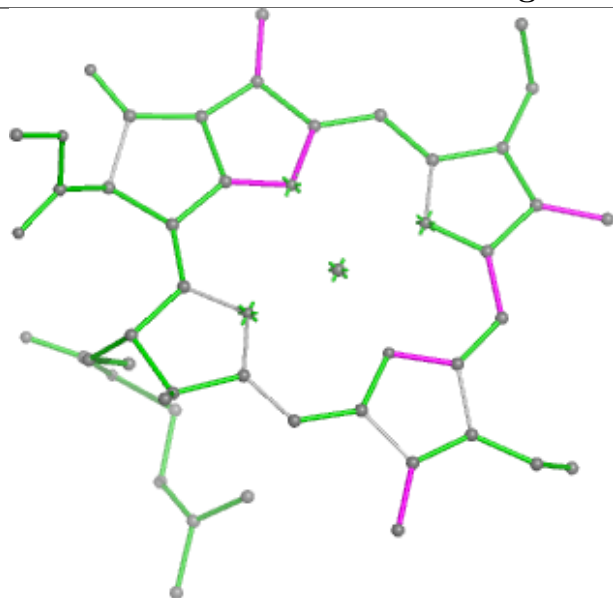




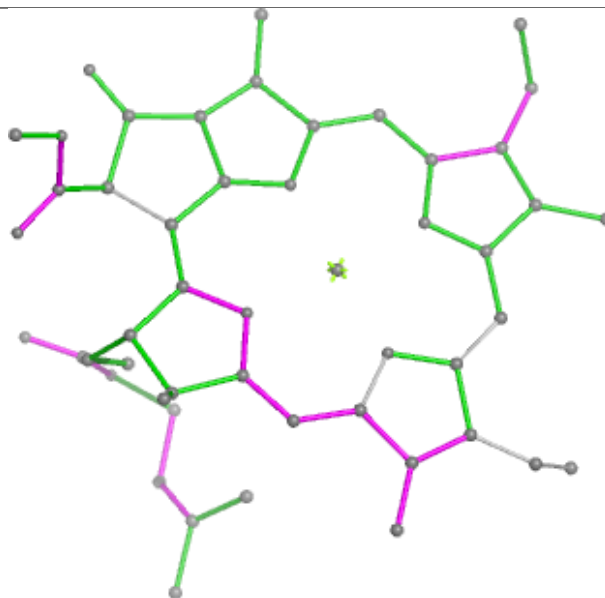
Ligand CLA g 832



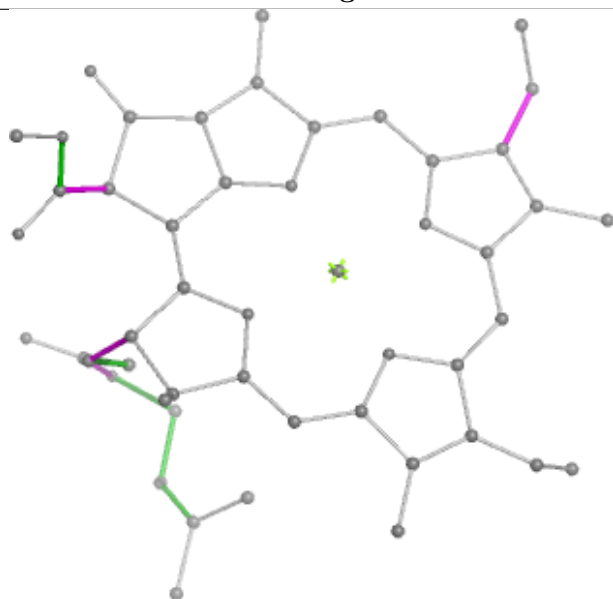
Ligand CLA a 831



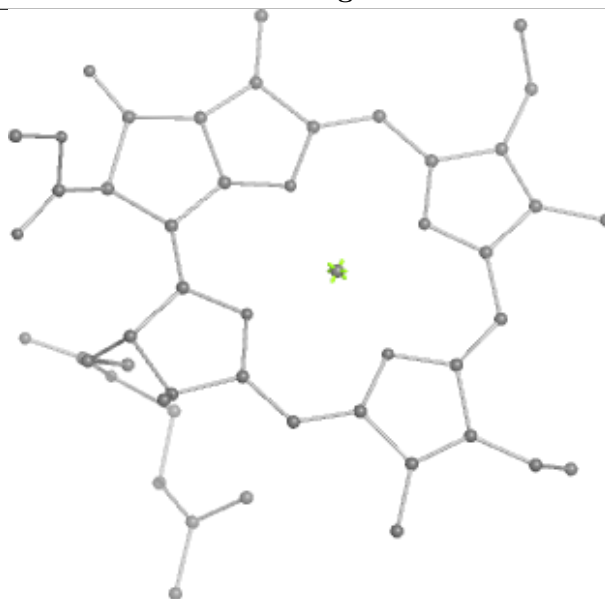
Bond lengths



Bond angles

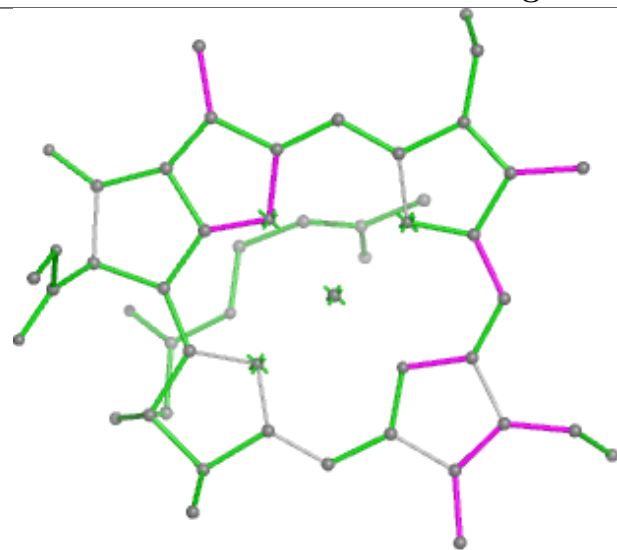


Torsions

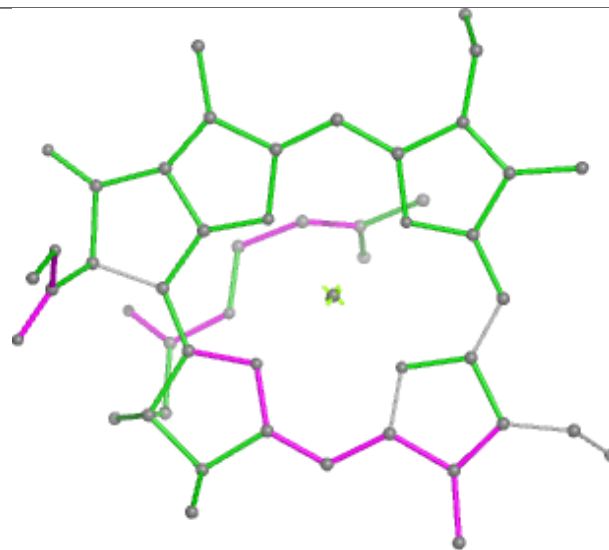


Rings

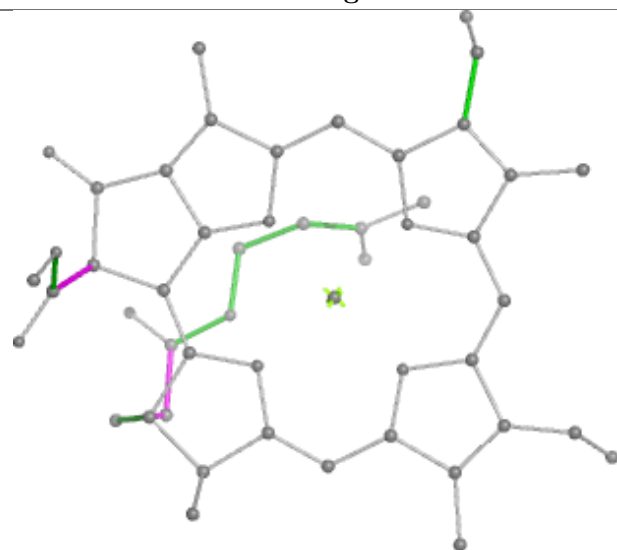
Ligand CLA a 841



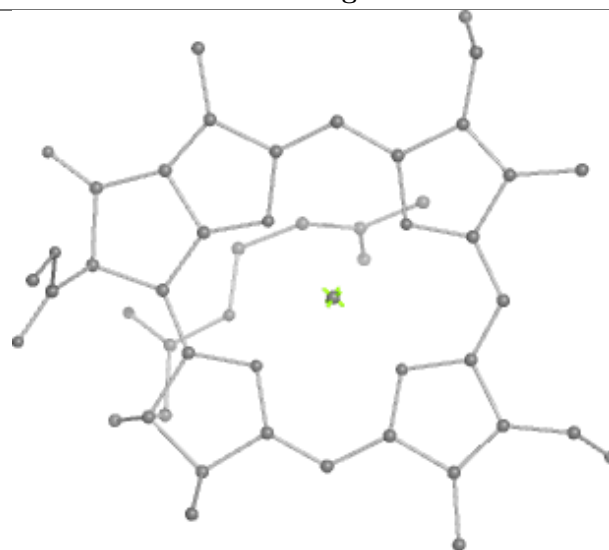
Bond lengths



Bond angles

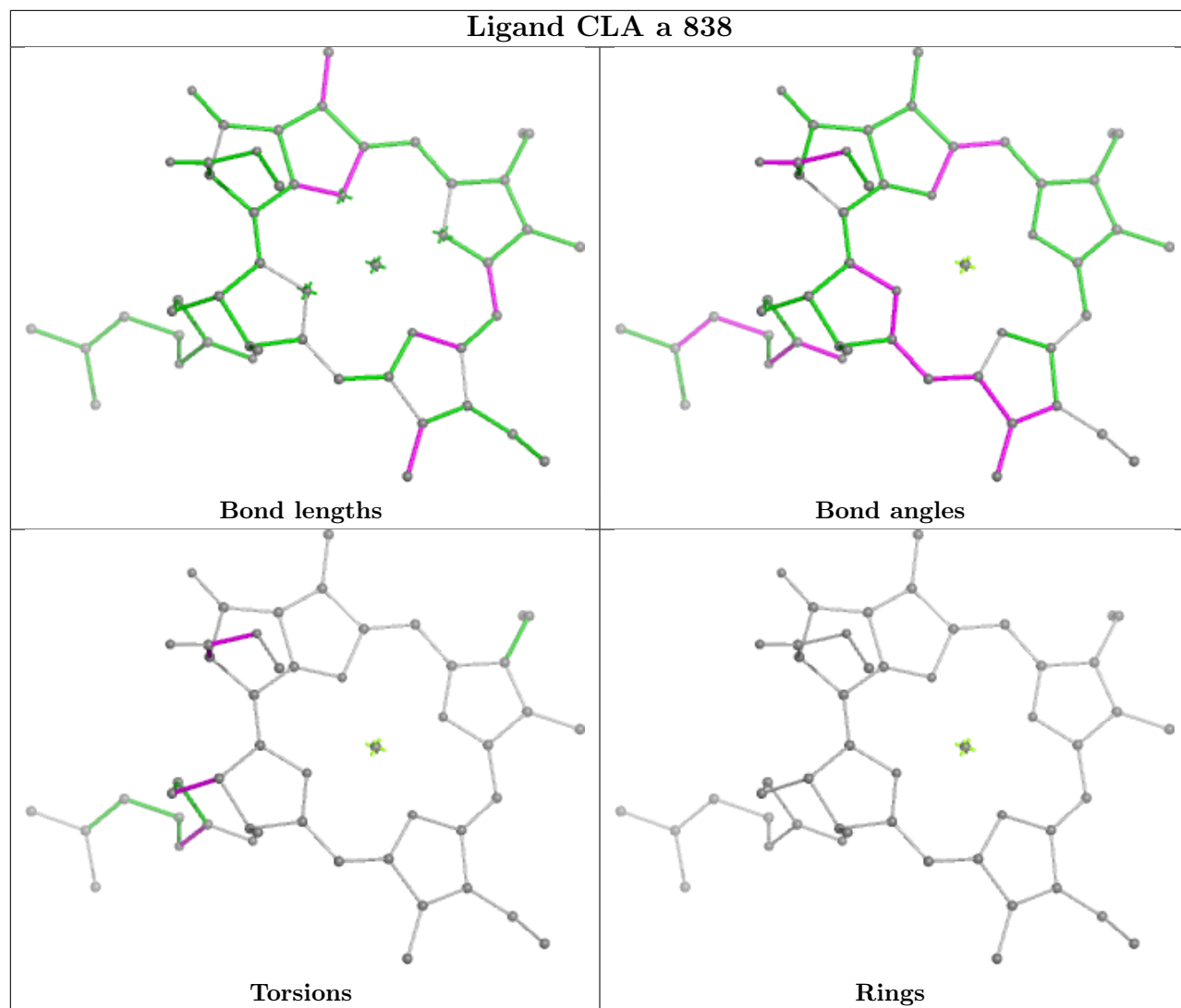


Torsions

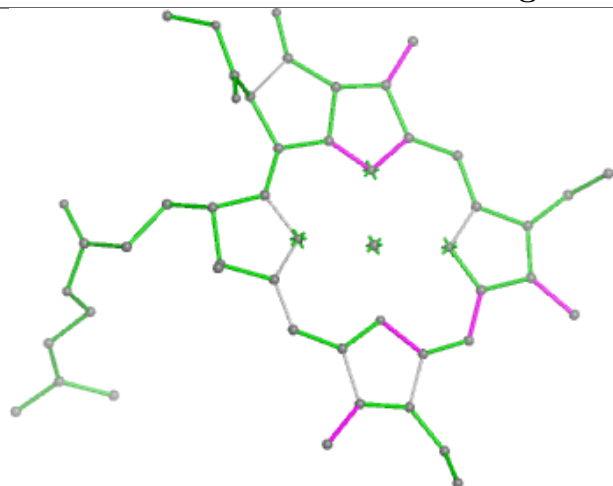


Rings

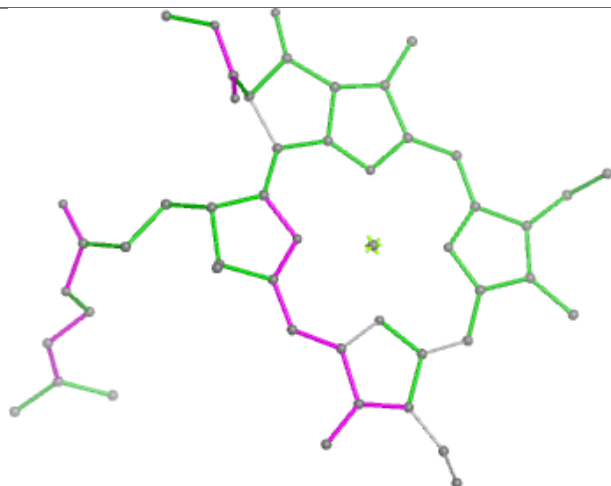
Ligand CLA a 838



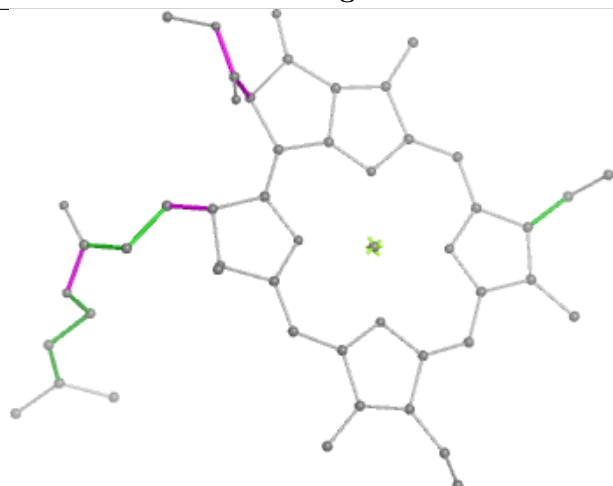
Ligand CLA e 806



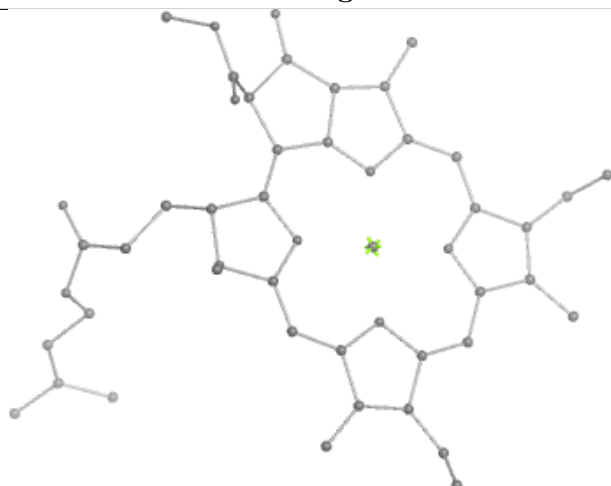
Bond lengths



Bond angles

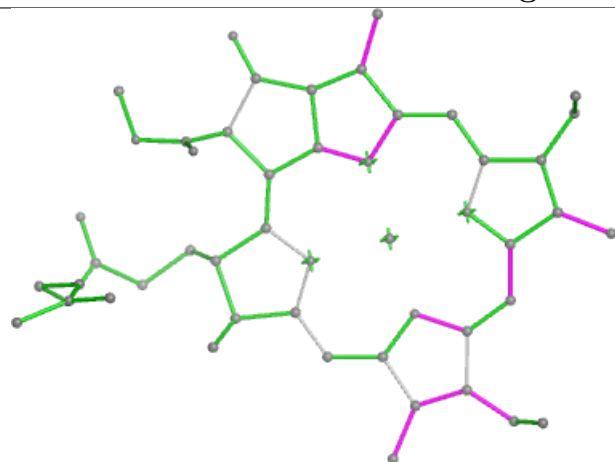


Torsions

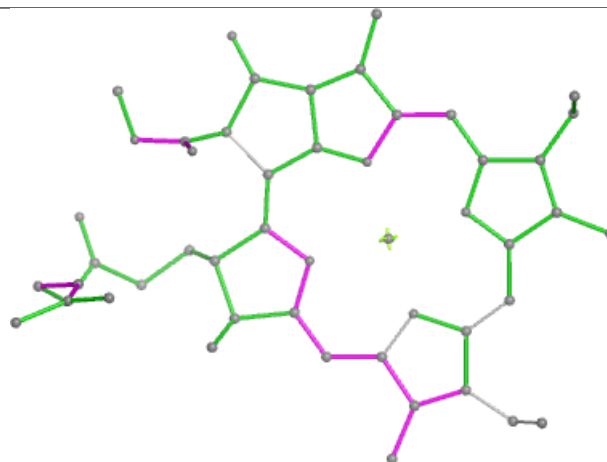


Rings

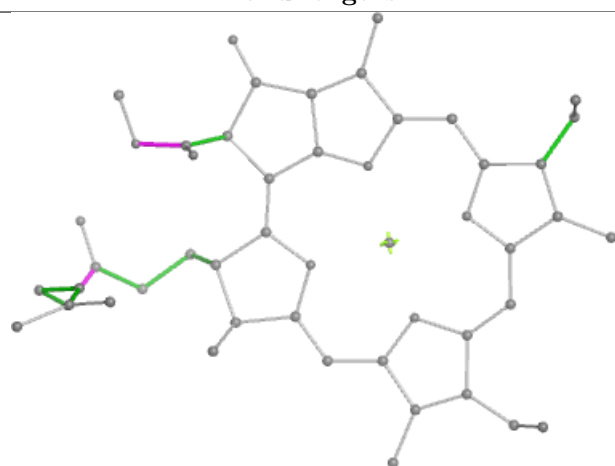
Ligand CLA b 807



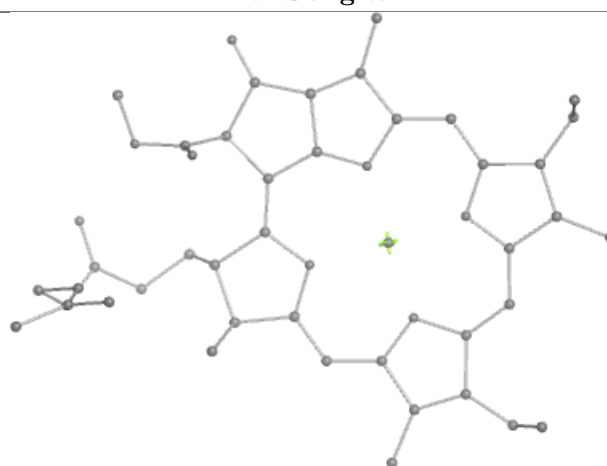
Bond lengths



Bond angles

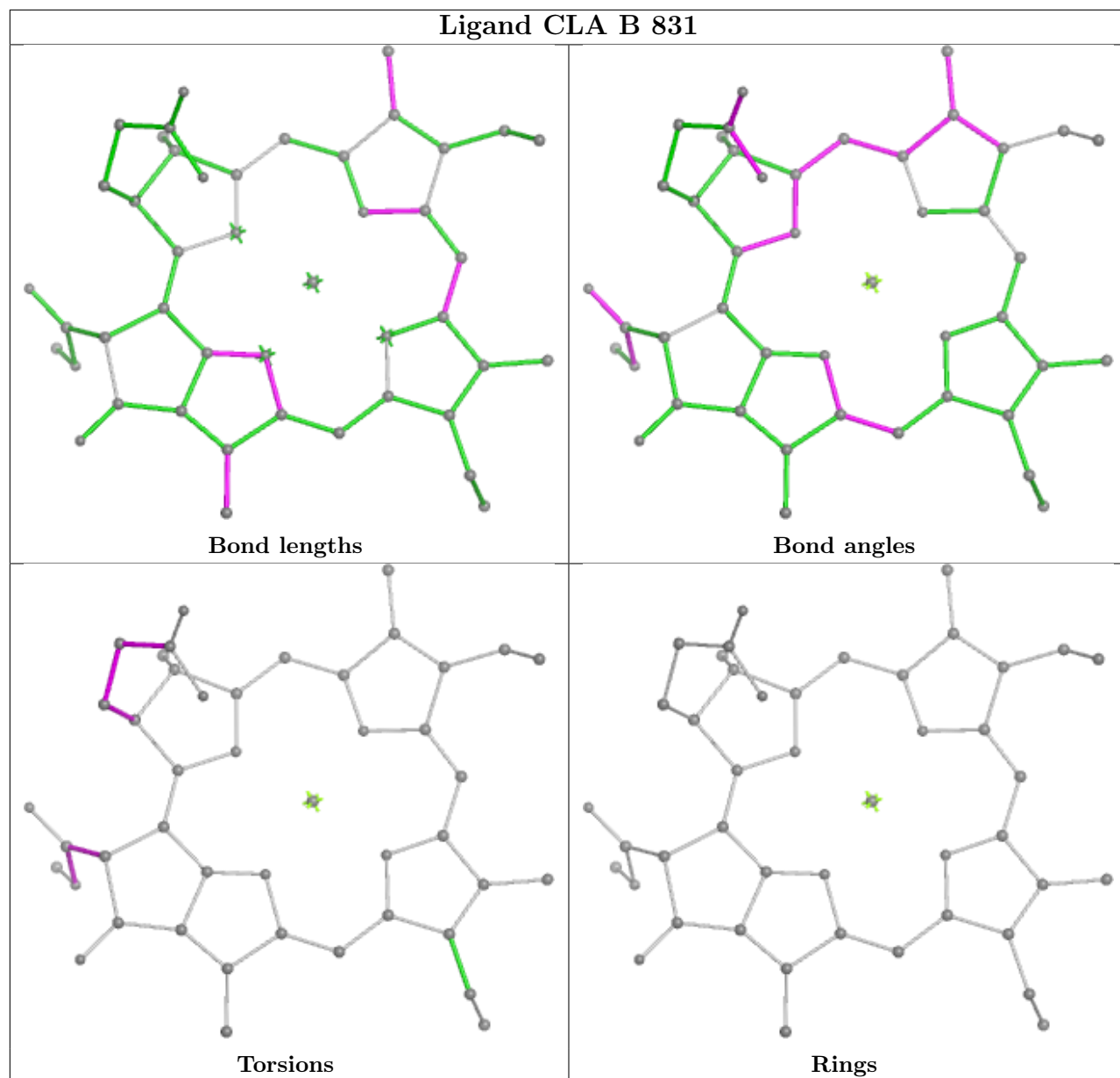


Torsions

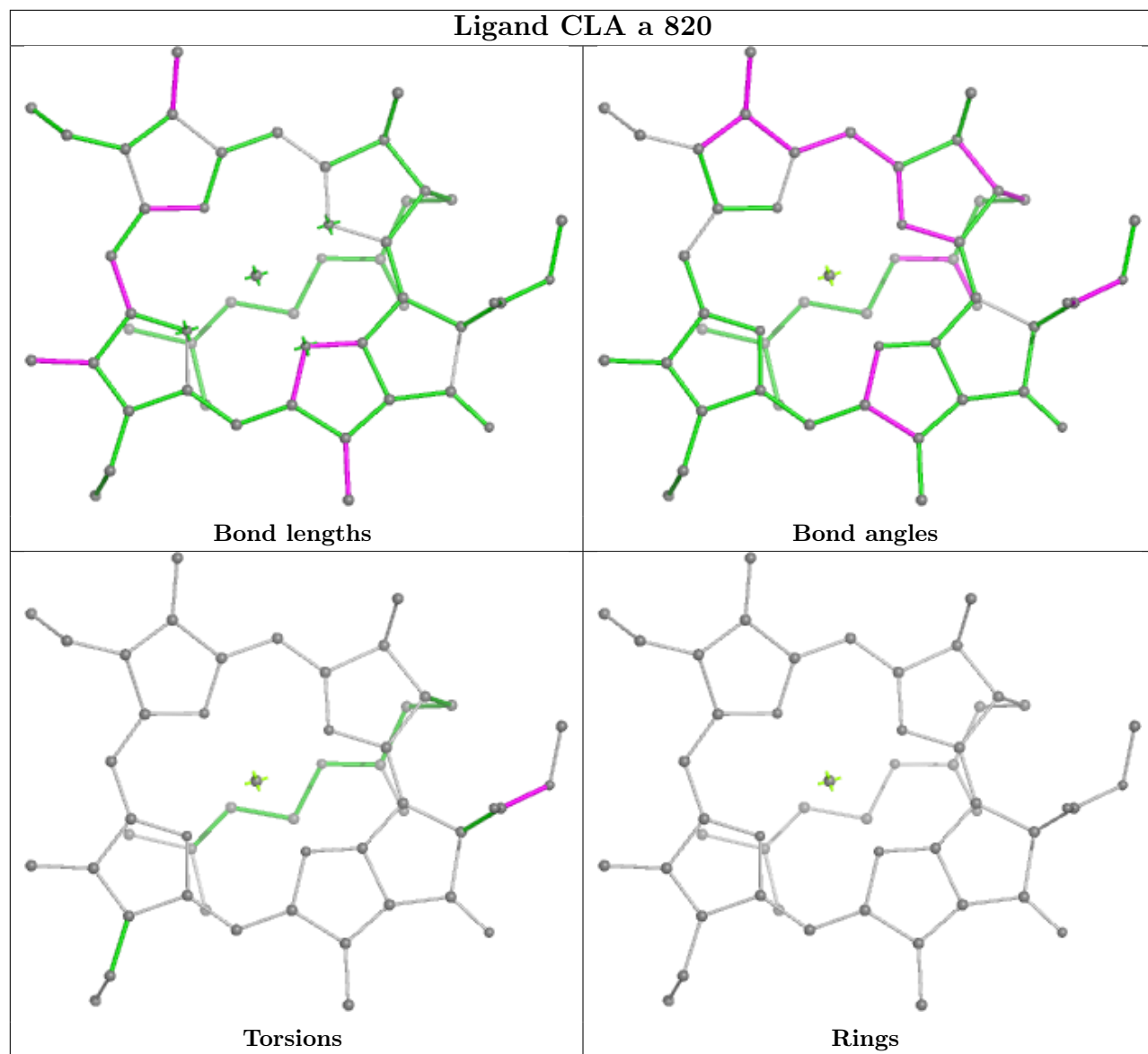


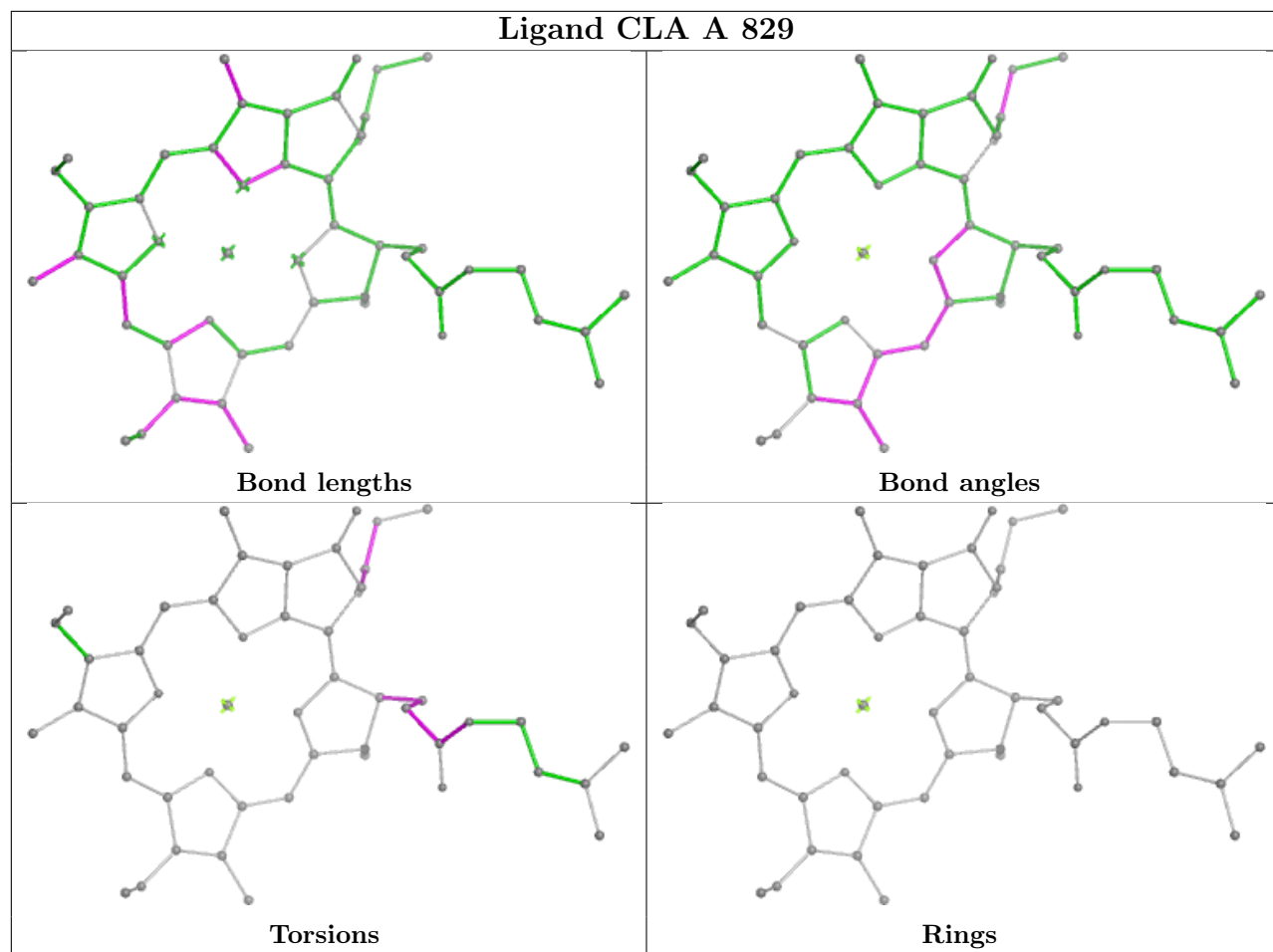
Rings

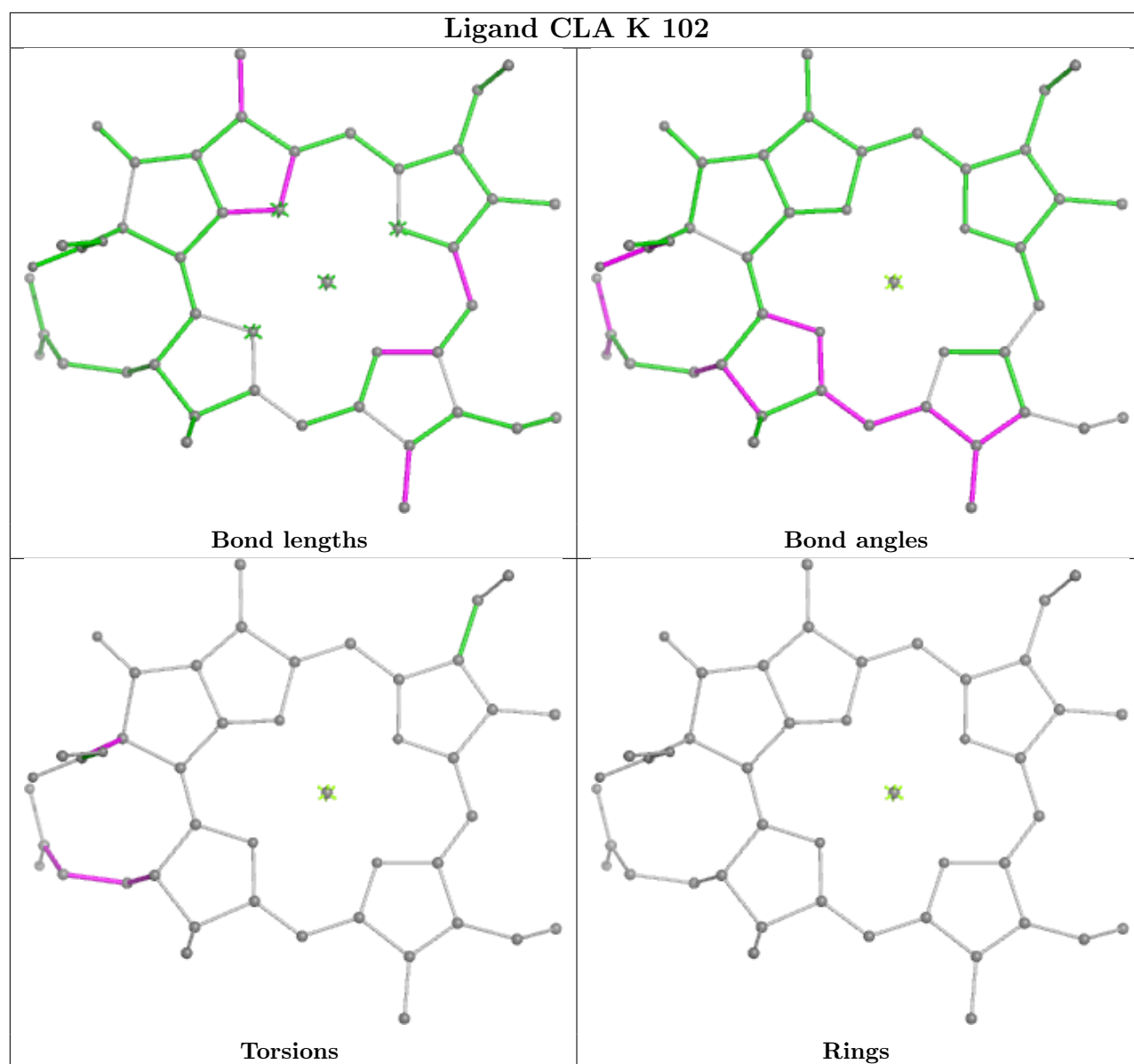
Ligand CLA B 831



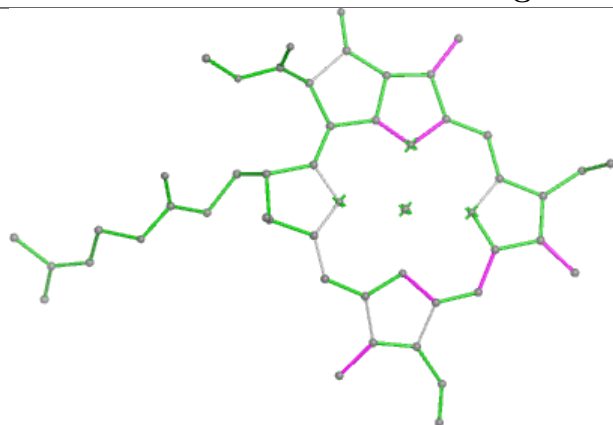
Ligand CLA a 820



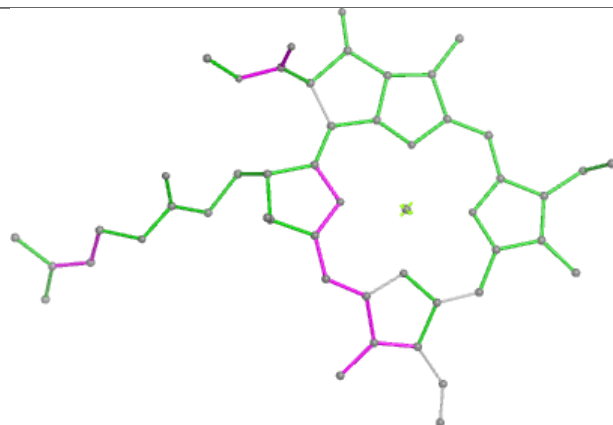




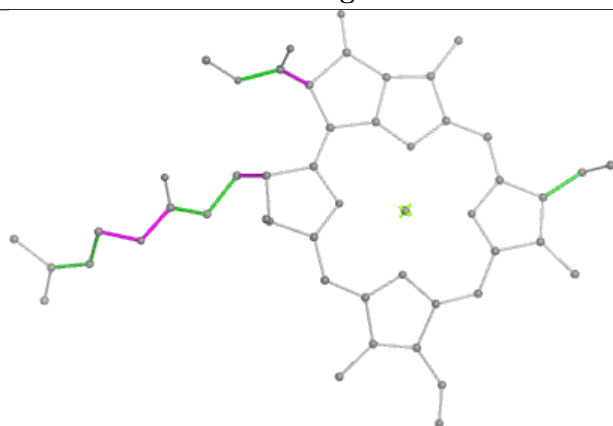
Ligand CLA A 805



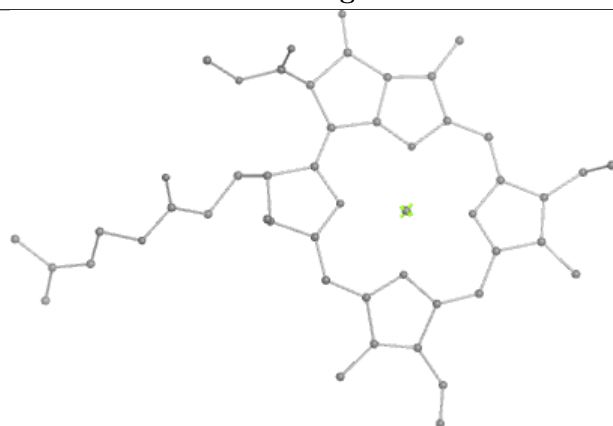
Bond lengths



Bond angles

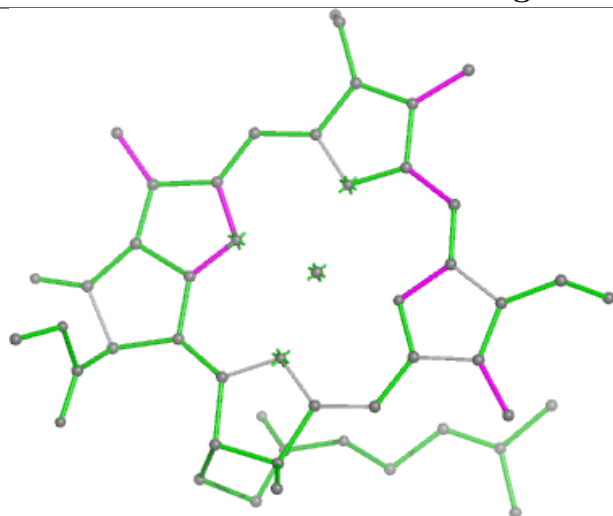


Torsions

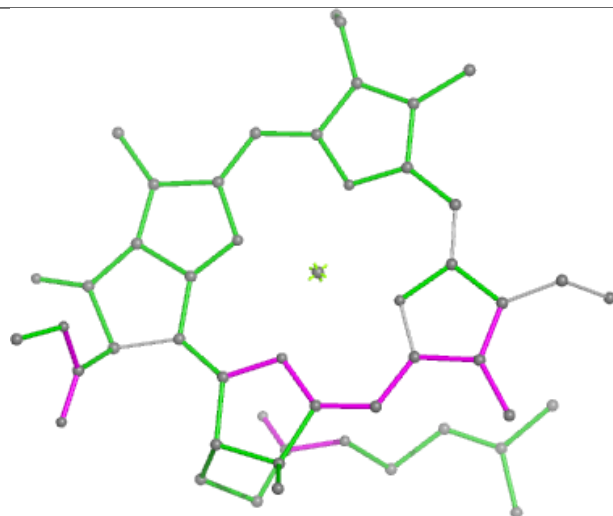


Rings

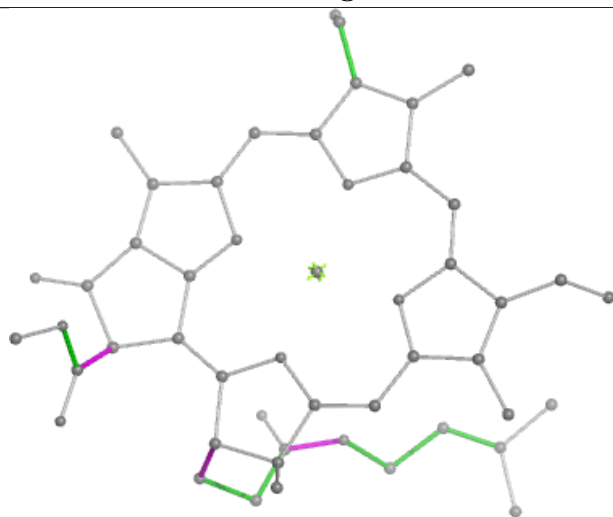
Ligand CLA G 819



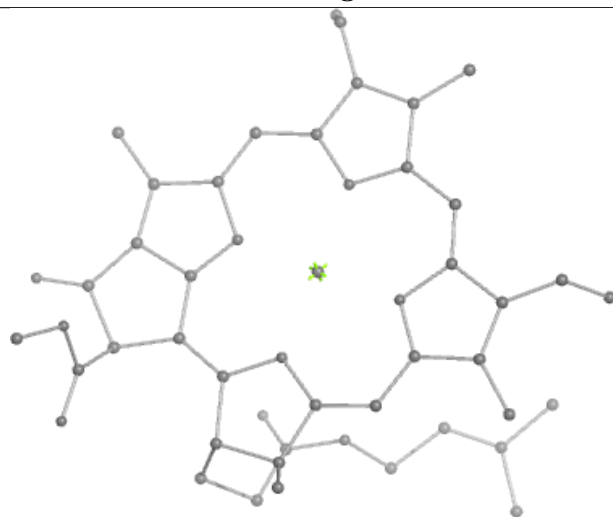
Bond lengths



Bond angles

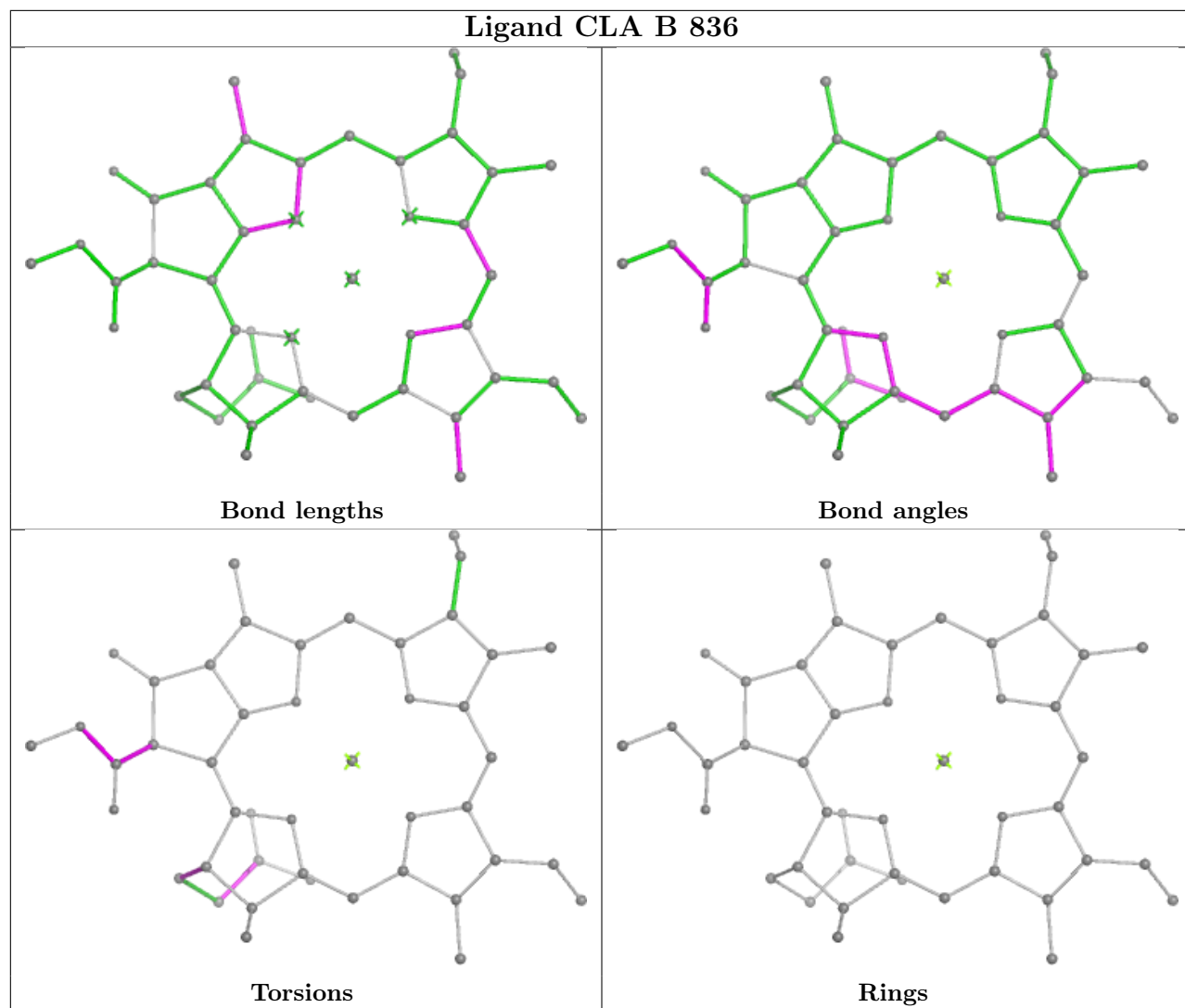


Torsions

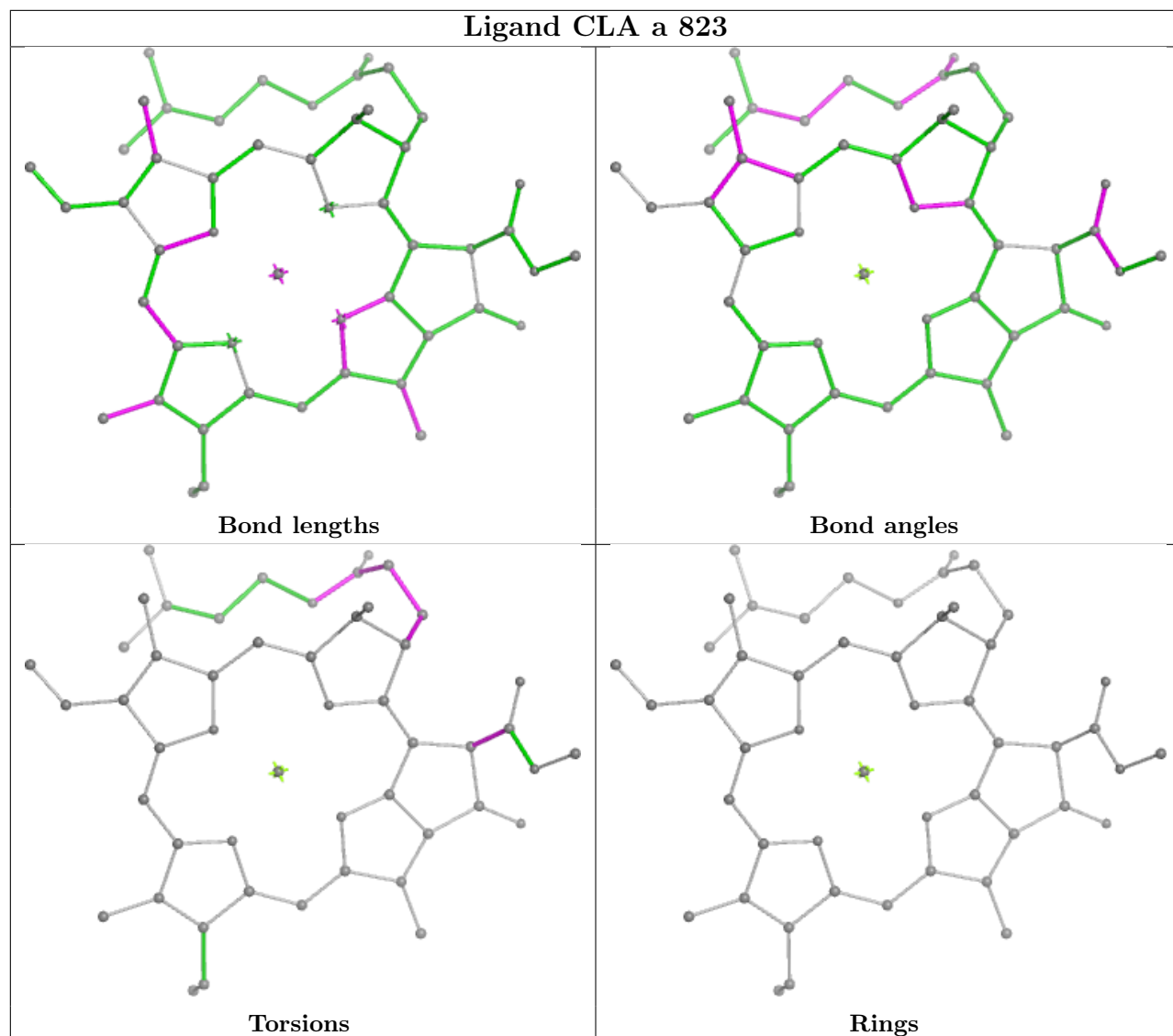


Rings

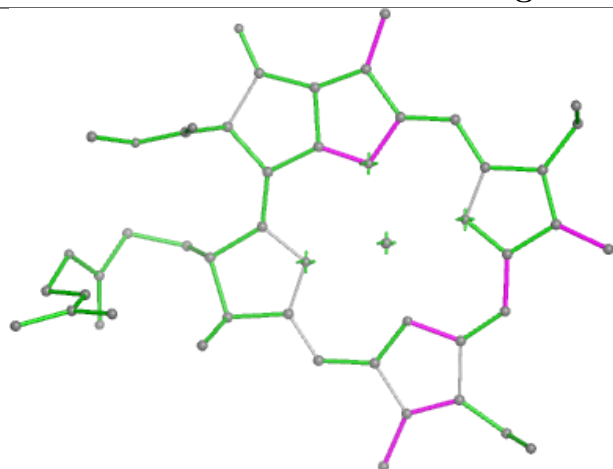
Ligand CLA B 836



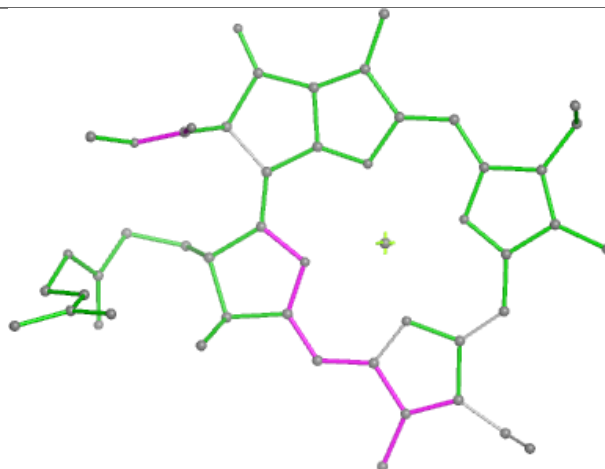
Ligand CLA a 823



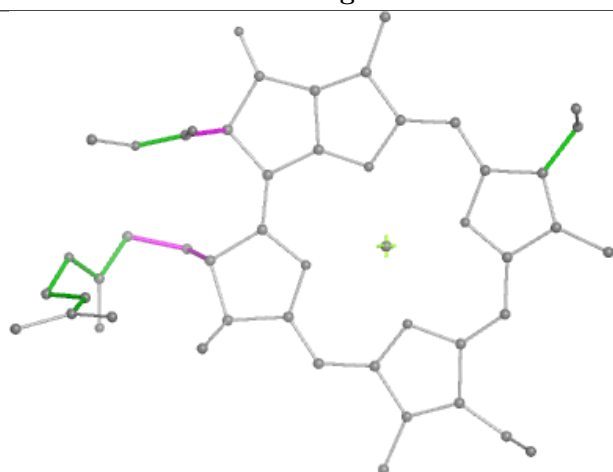
Ligand CLA E 809



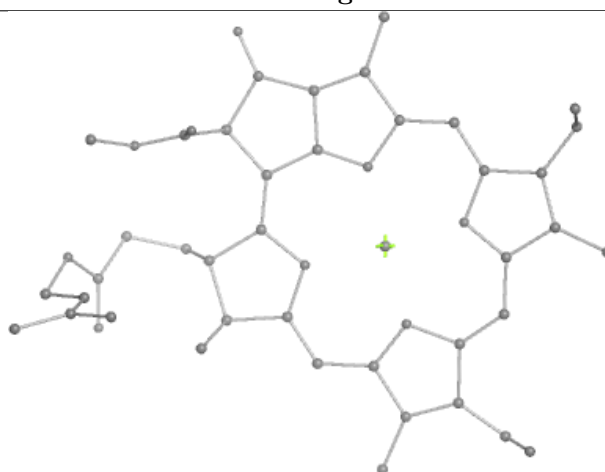
Bond lengths



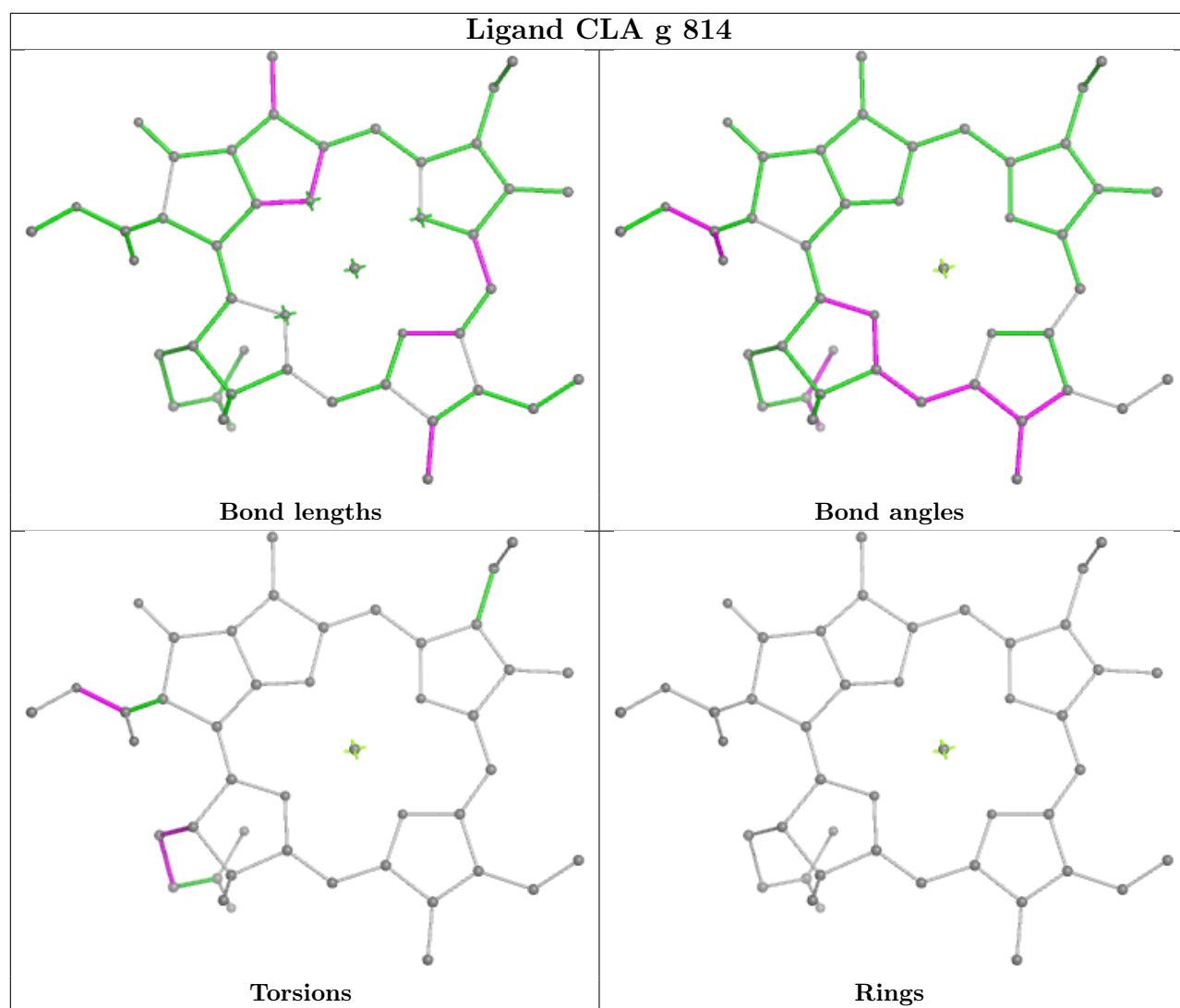
Bond angles

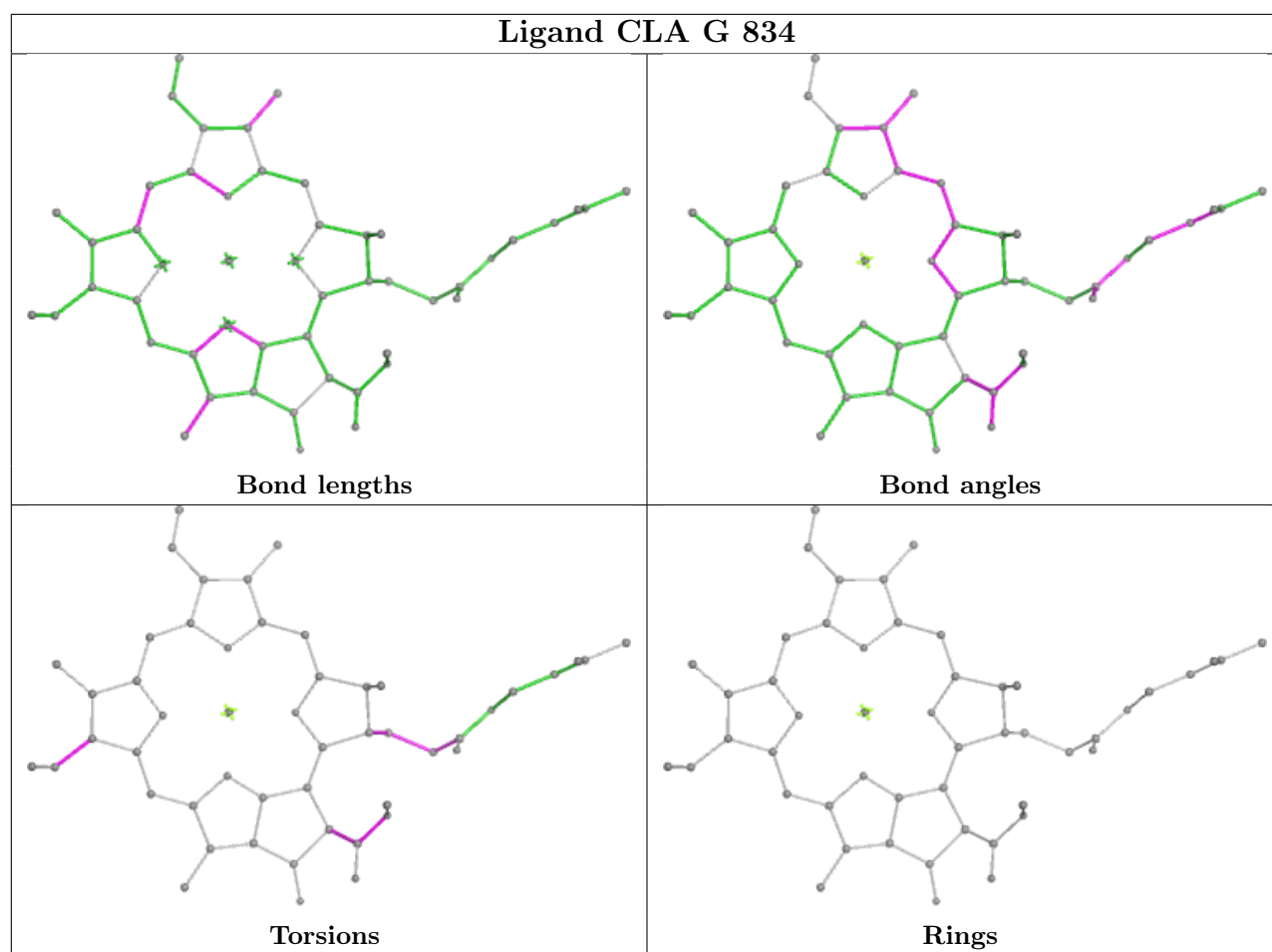


Torsions

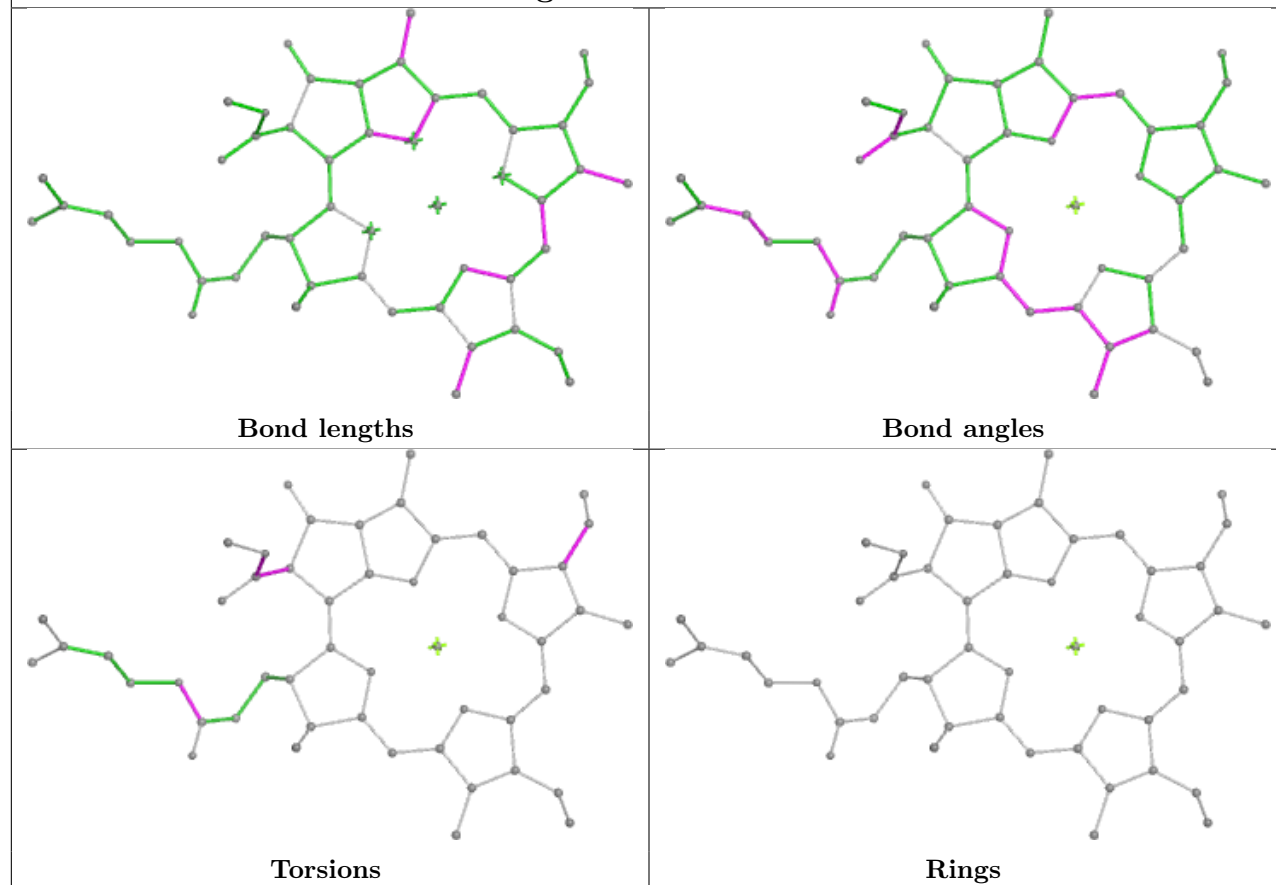


Rings

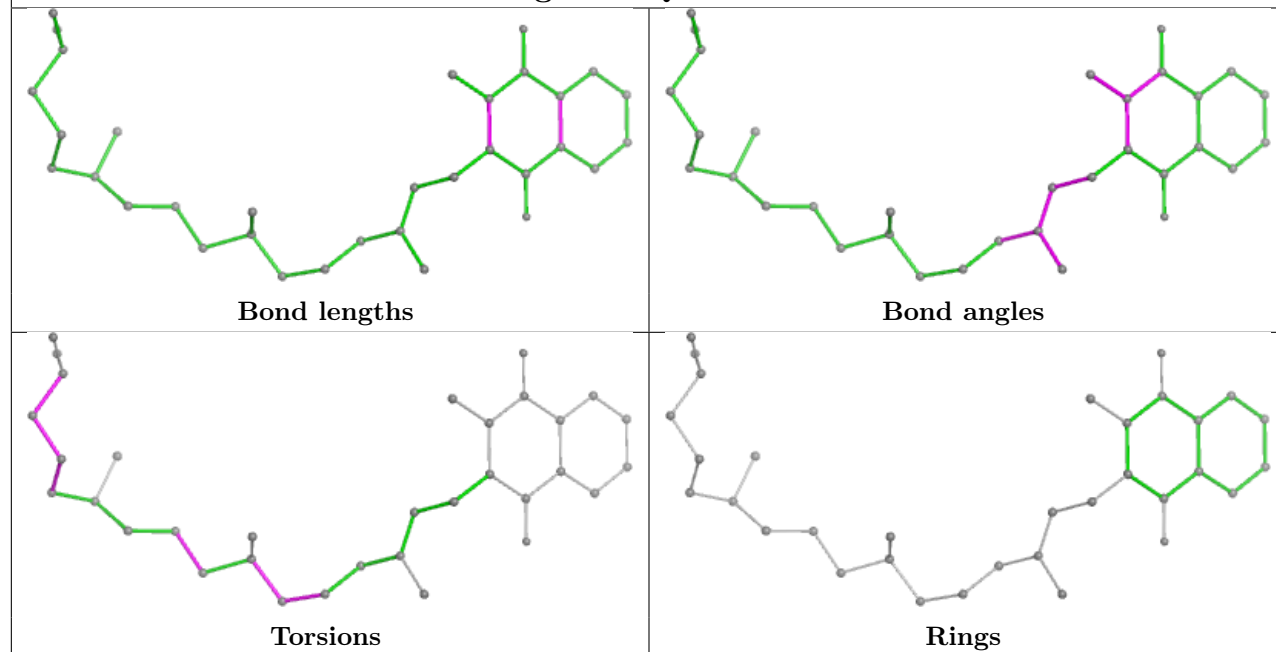




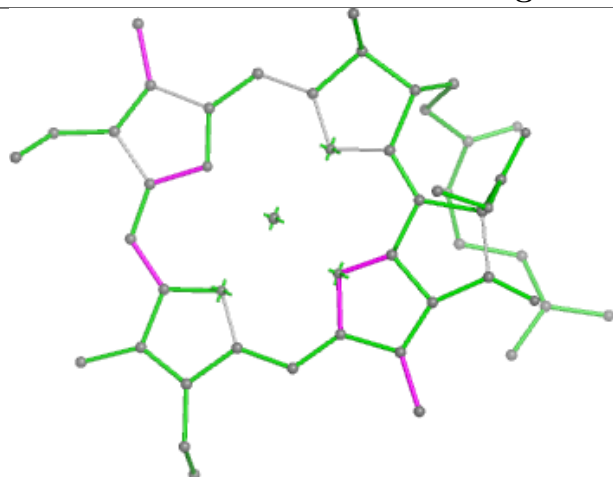
Ligand CLA a 806



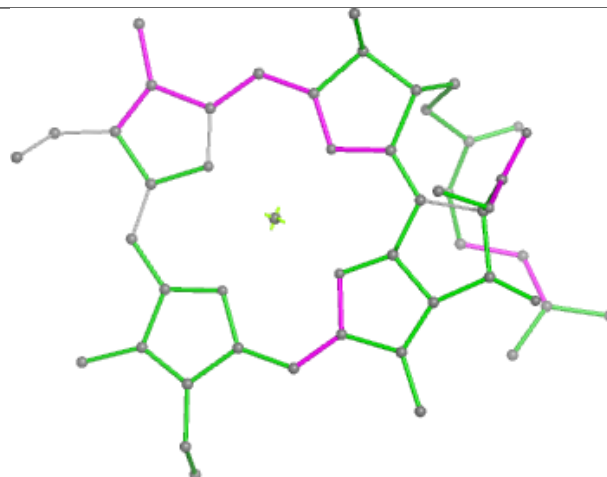
Ligand PQN e 845



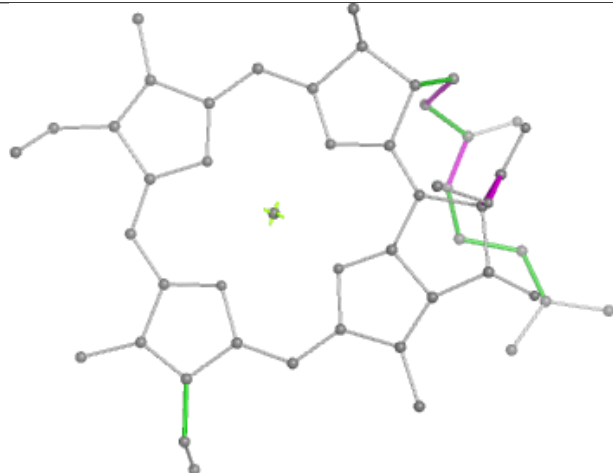
Ligand CLA E 810



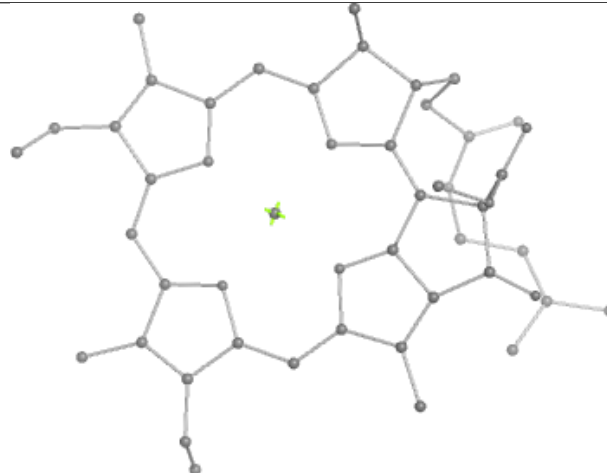
Bond lengths



Bond angles

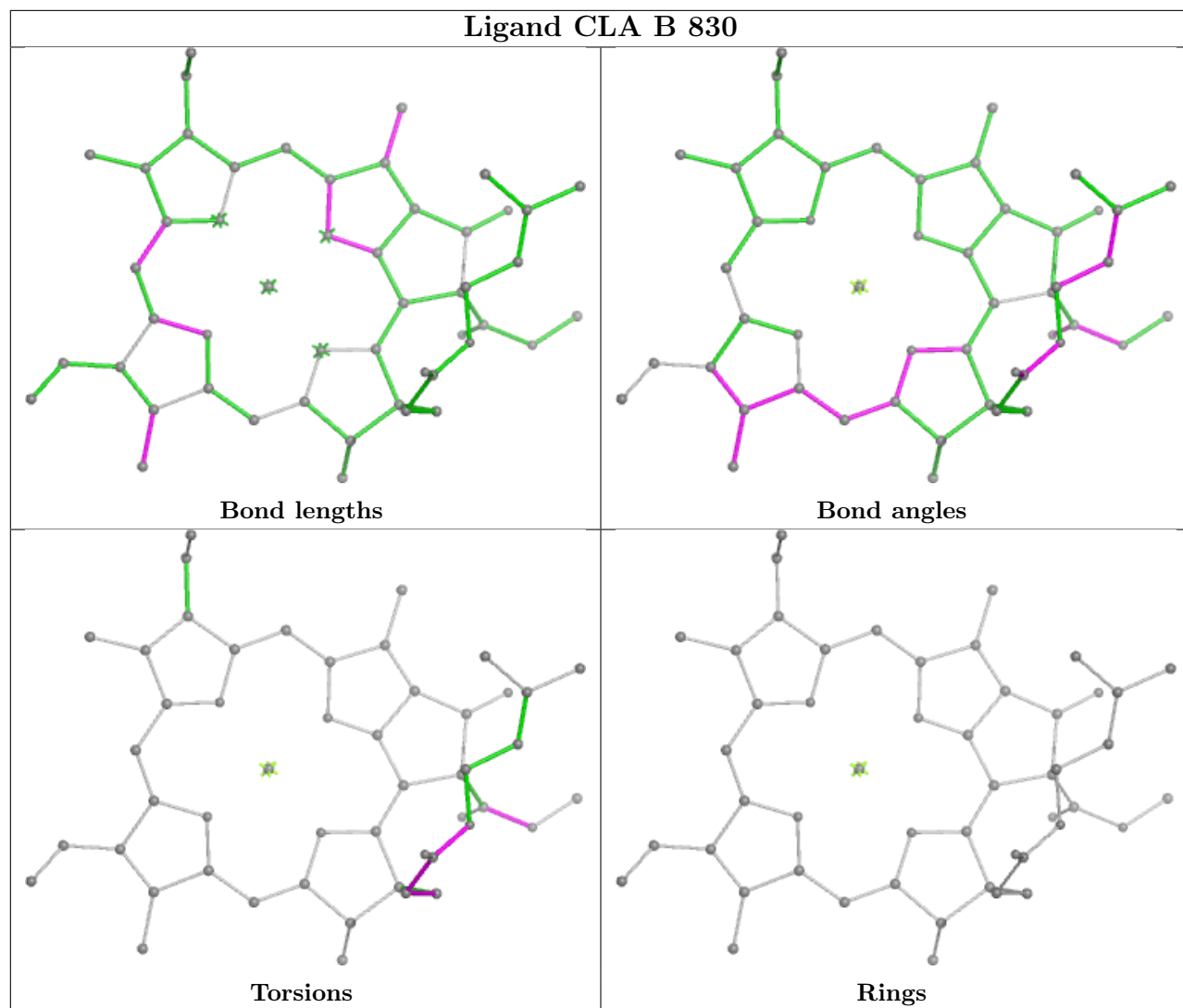


Torsions

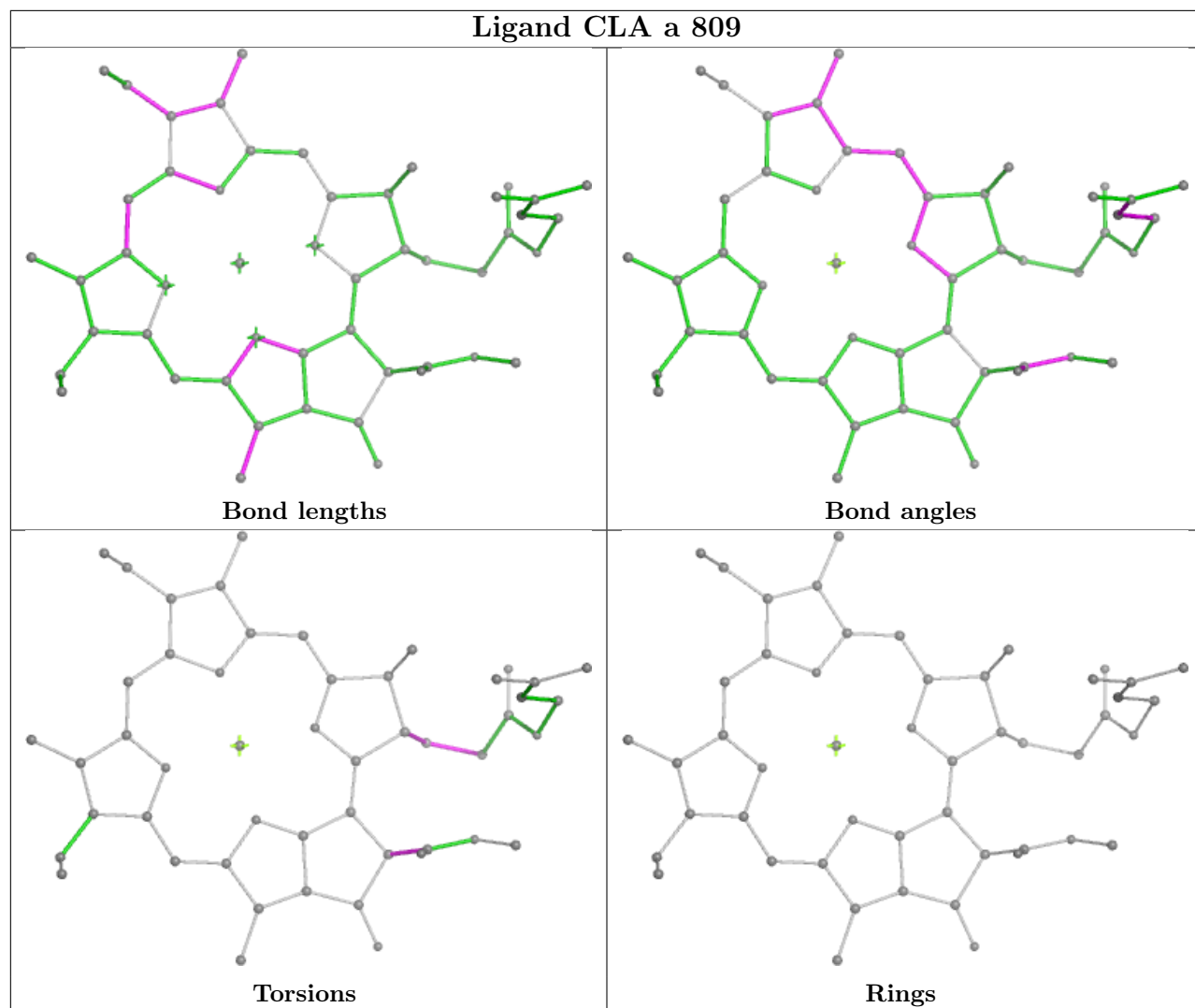


Rings

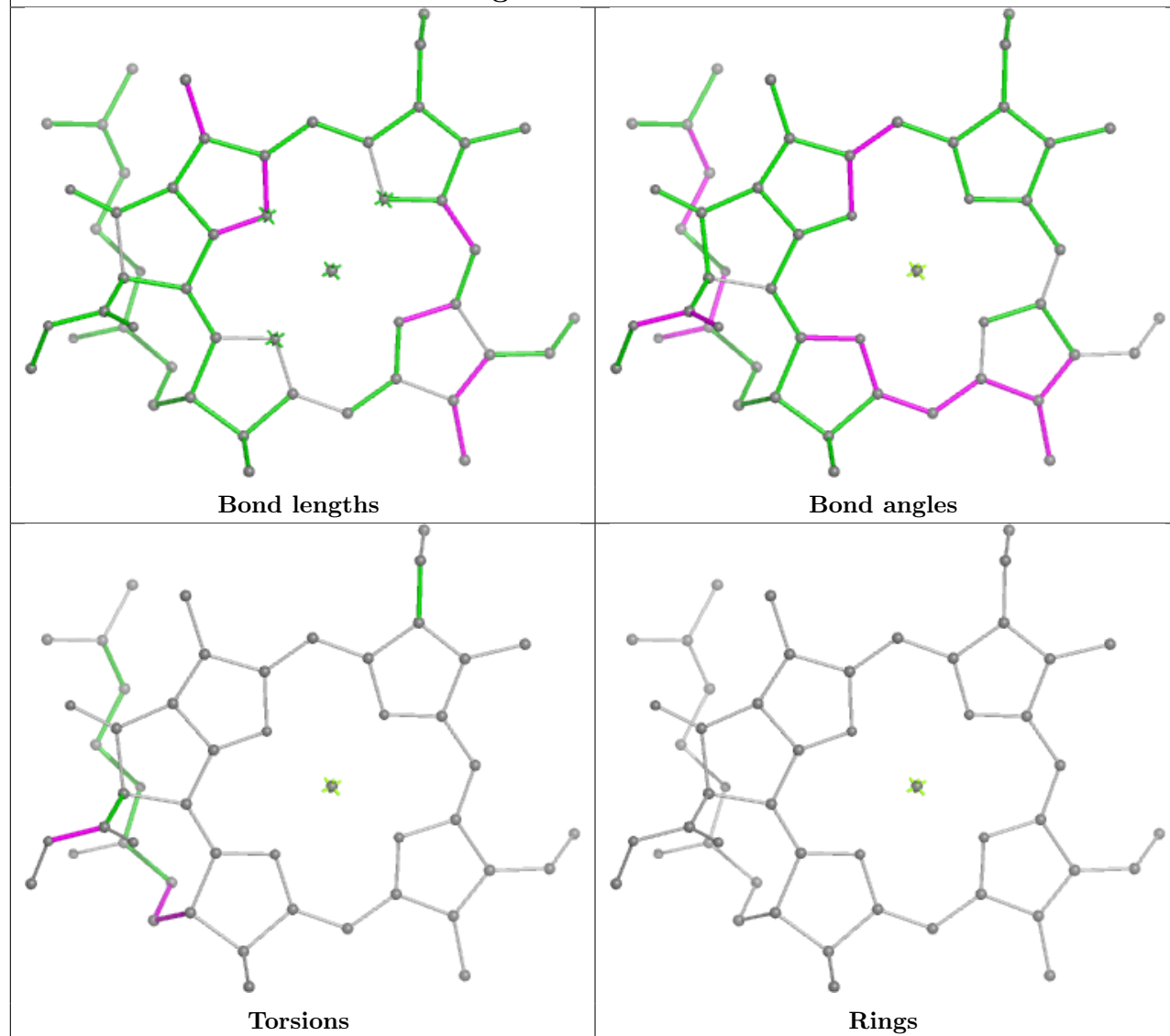
Ligand CLA B 830



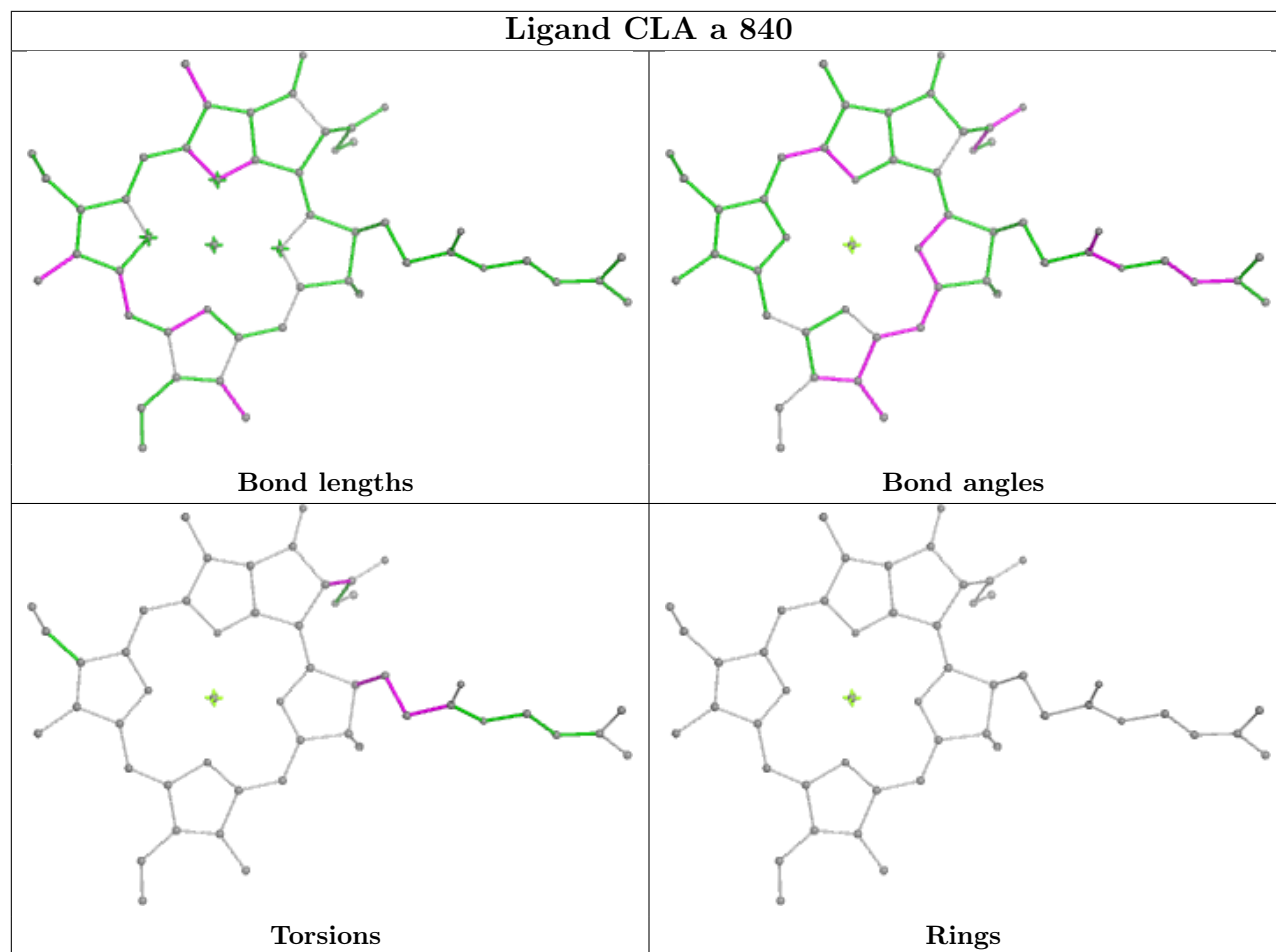
Ligand CLA a 809



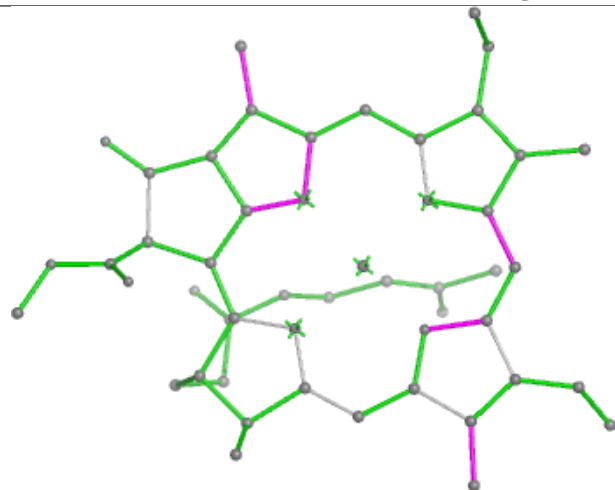
Ligand CLA e 831



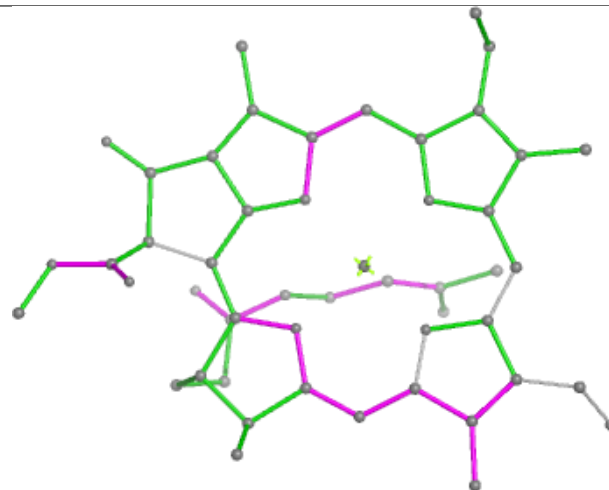
Ligand CLA a 840



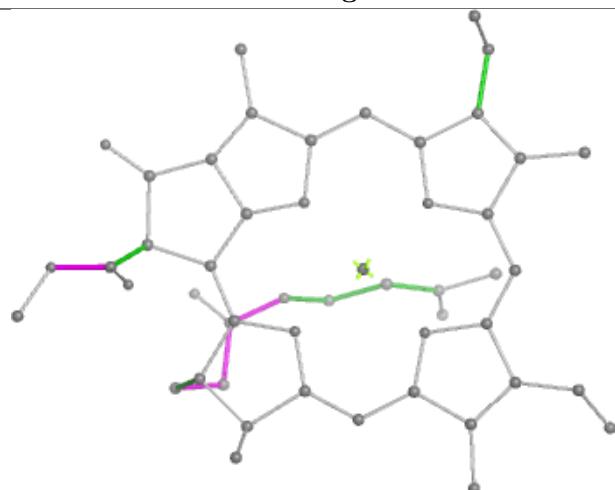
Ligand CLA B 838



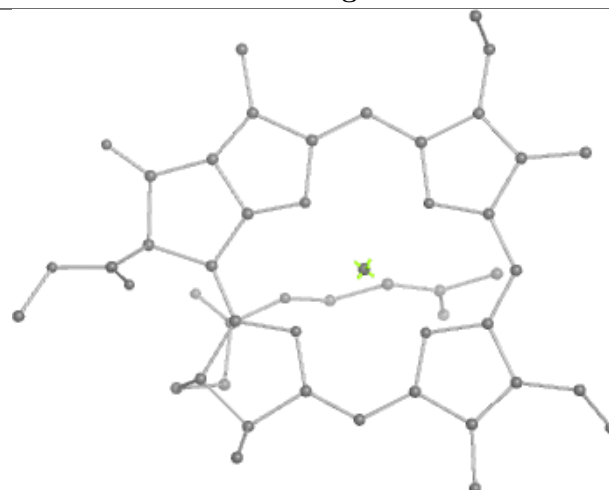
Bond lengths



Bond angles

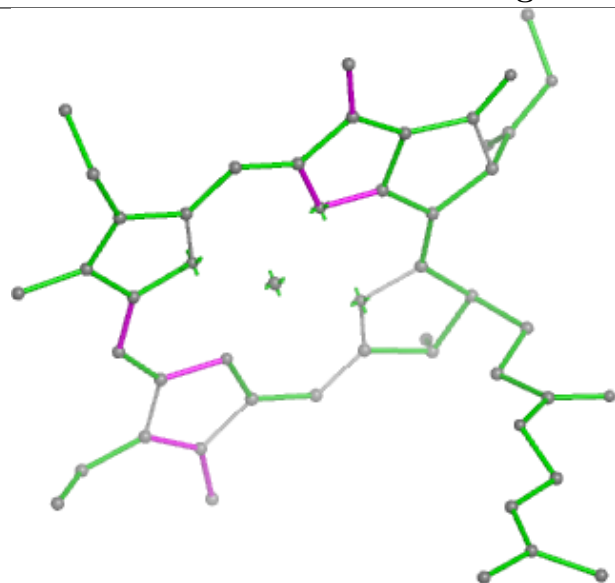


Torsions

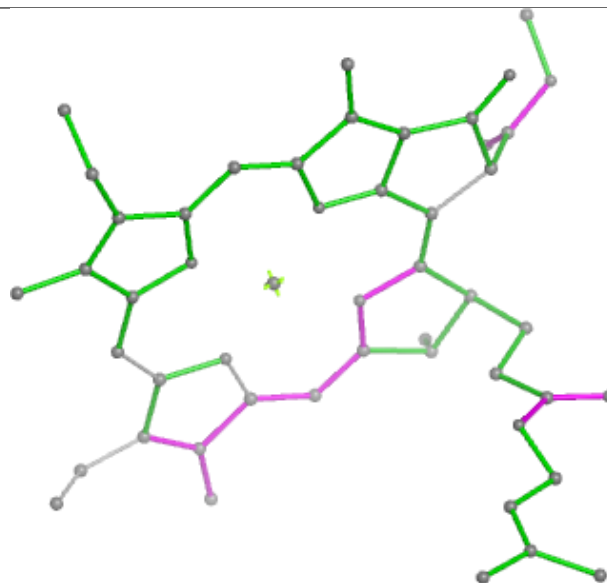


Rings

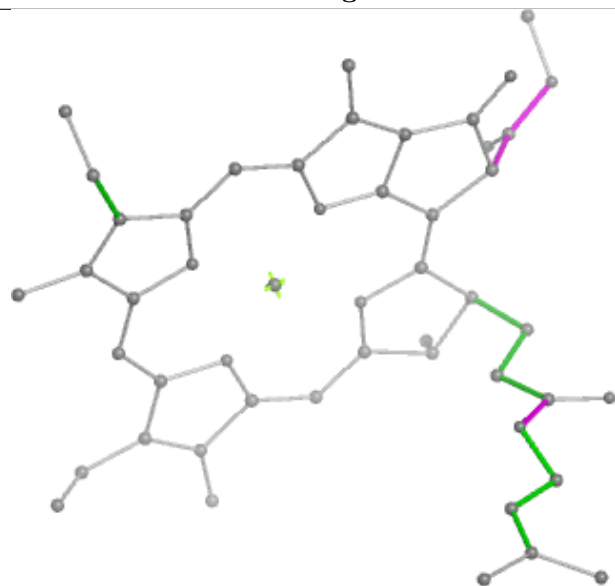
Ligand CLA B 820



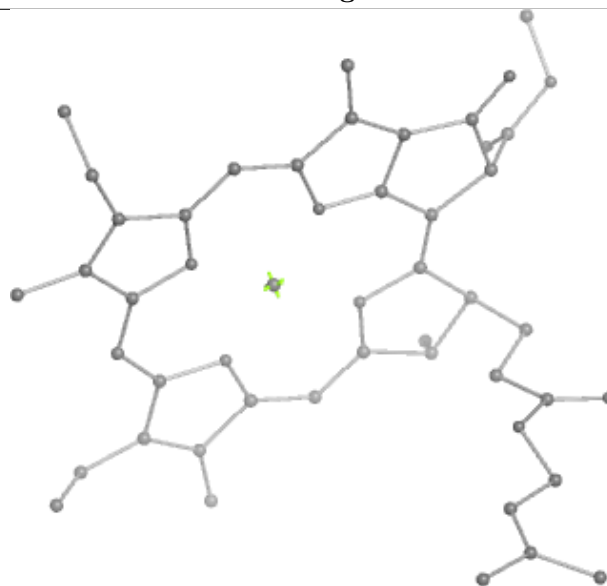
Bond lengths



Bond angles

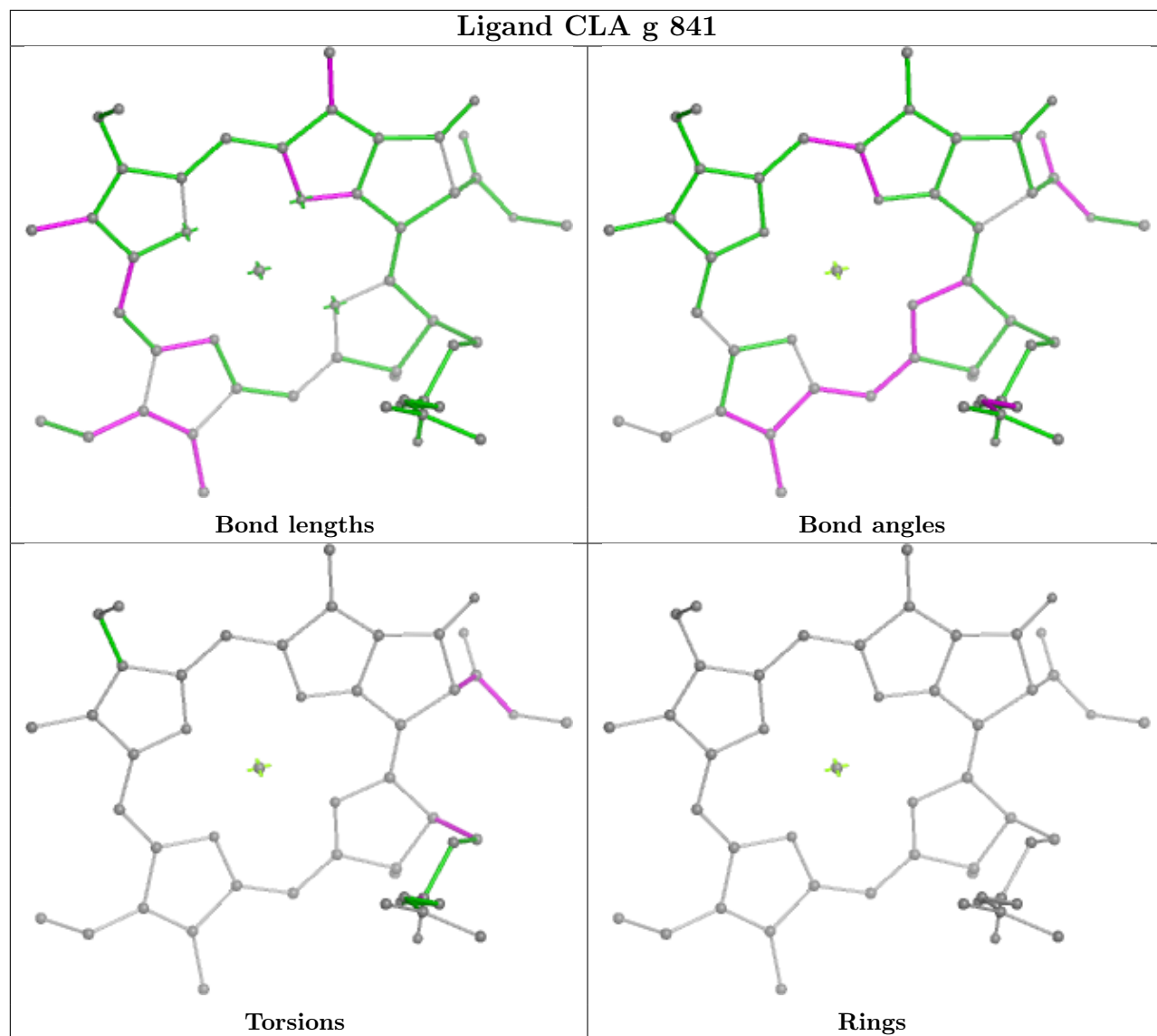


Torsions

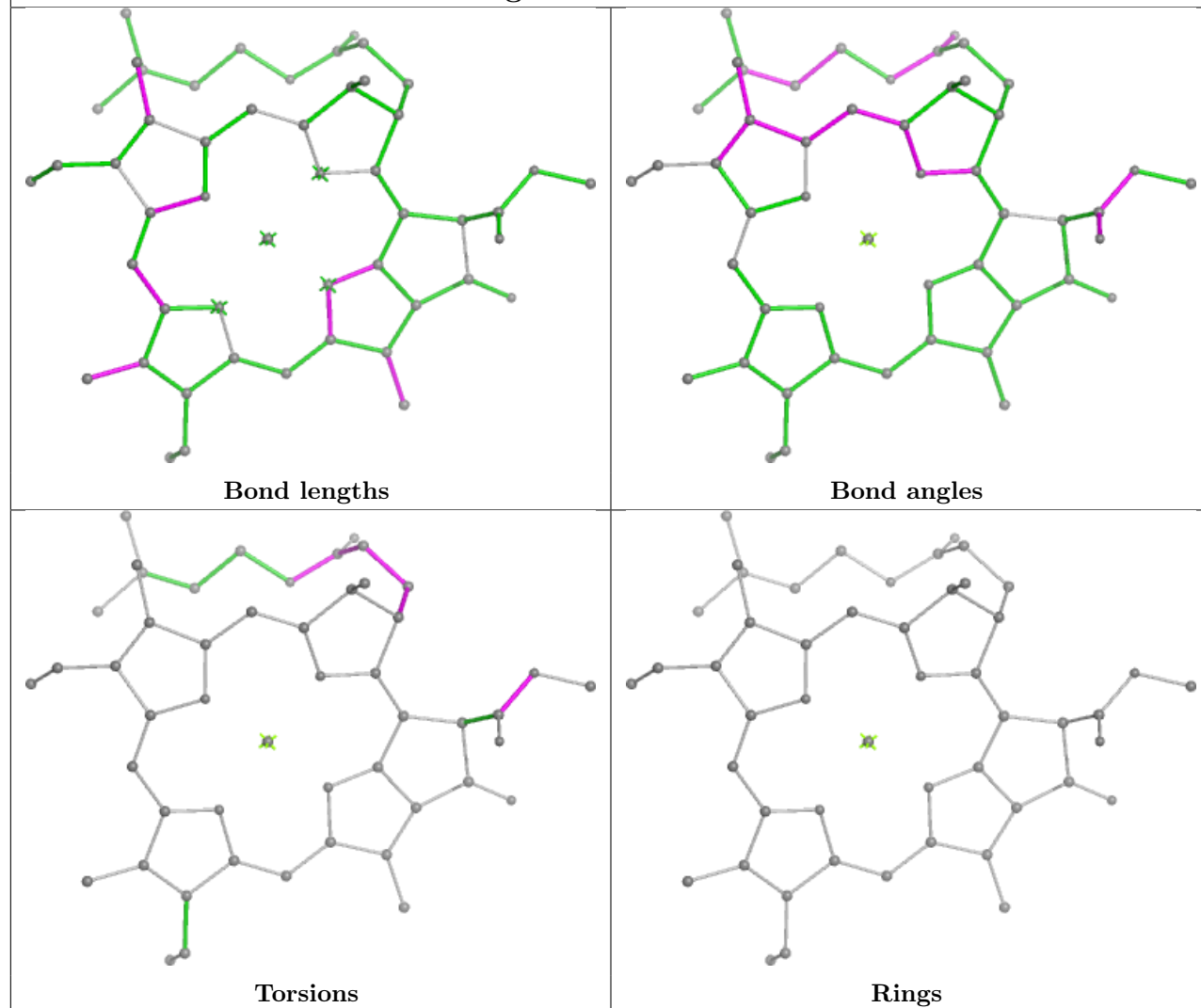


Rings

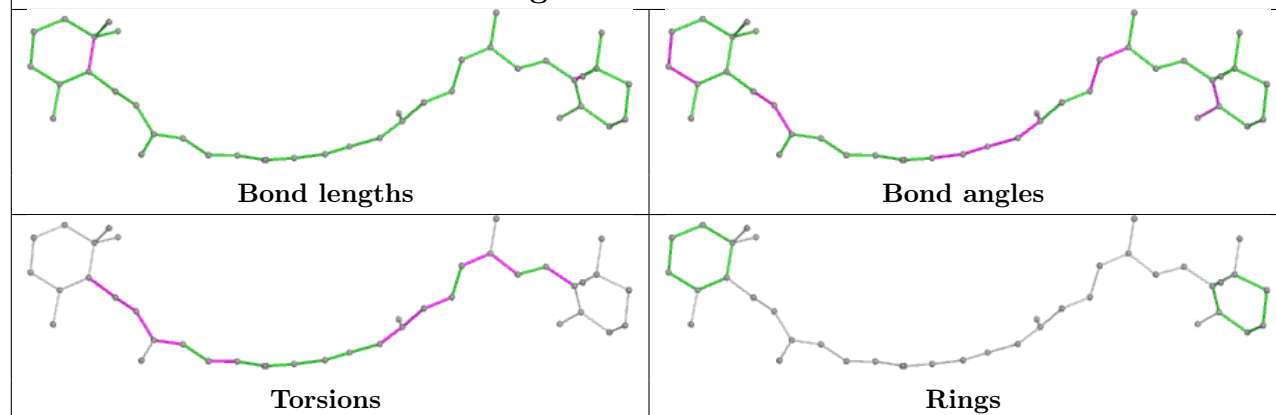
Ligand CLA g 841



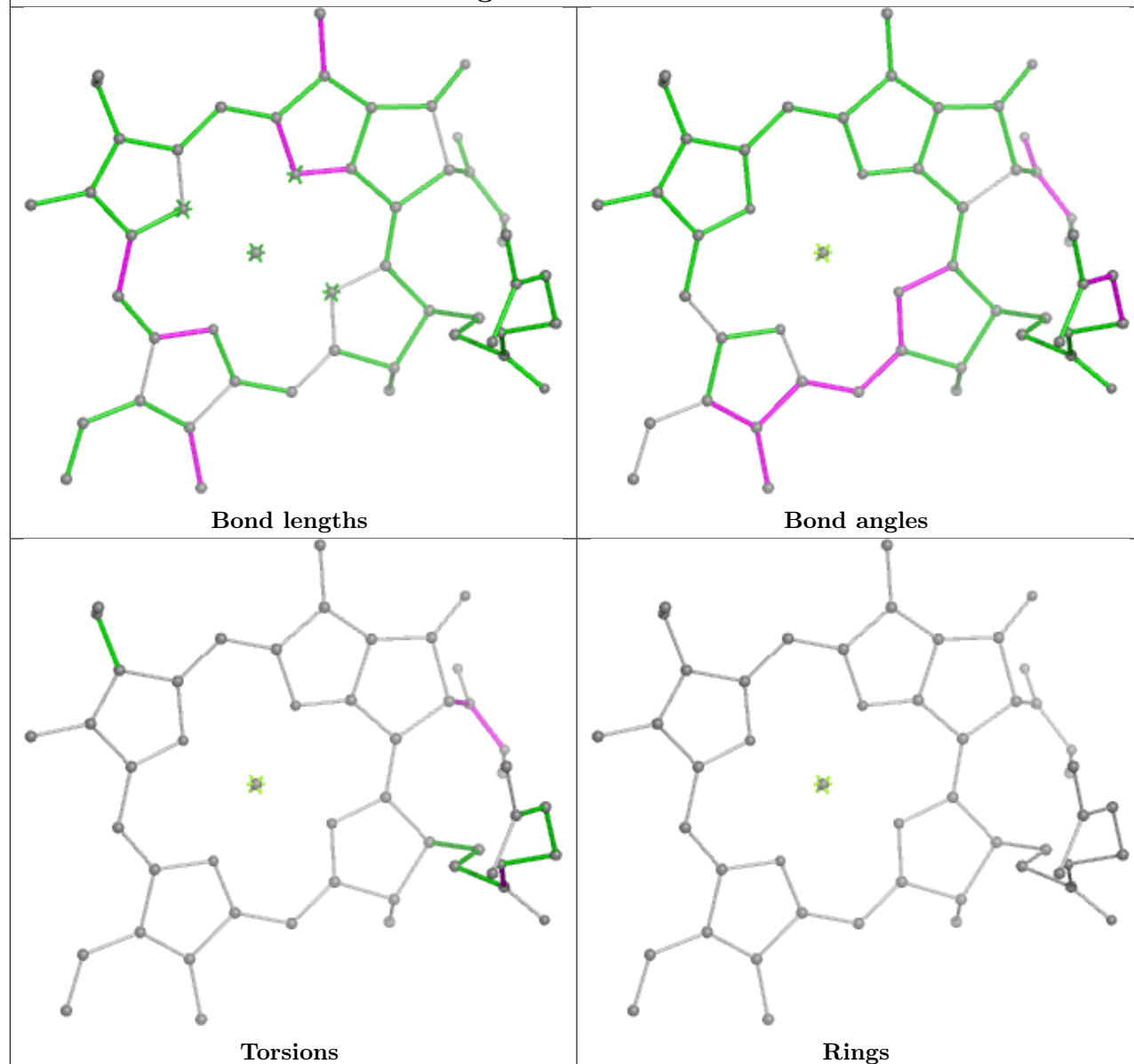
Ligand CLA e 821



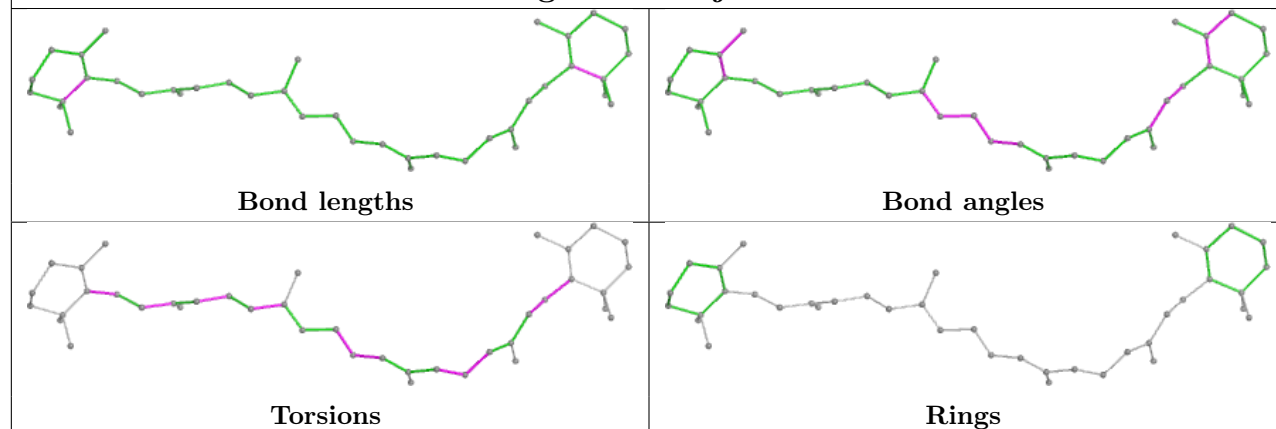
Ligand BCR A 852



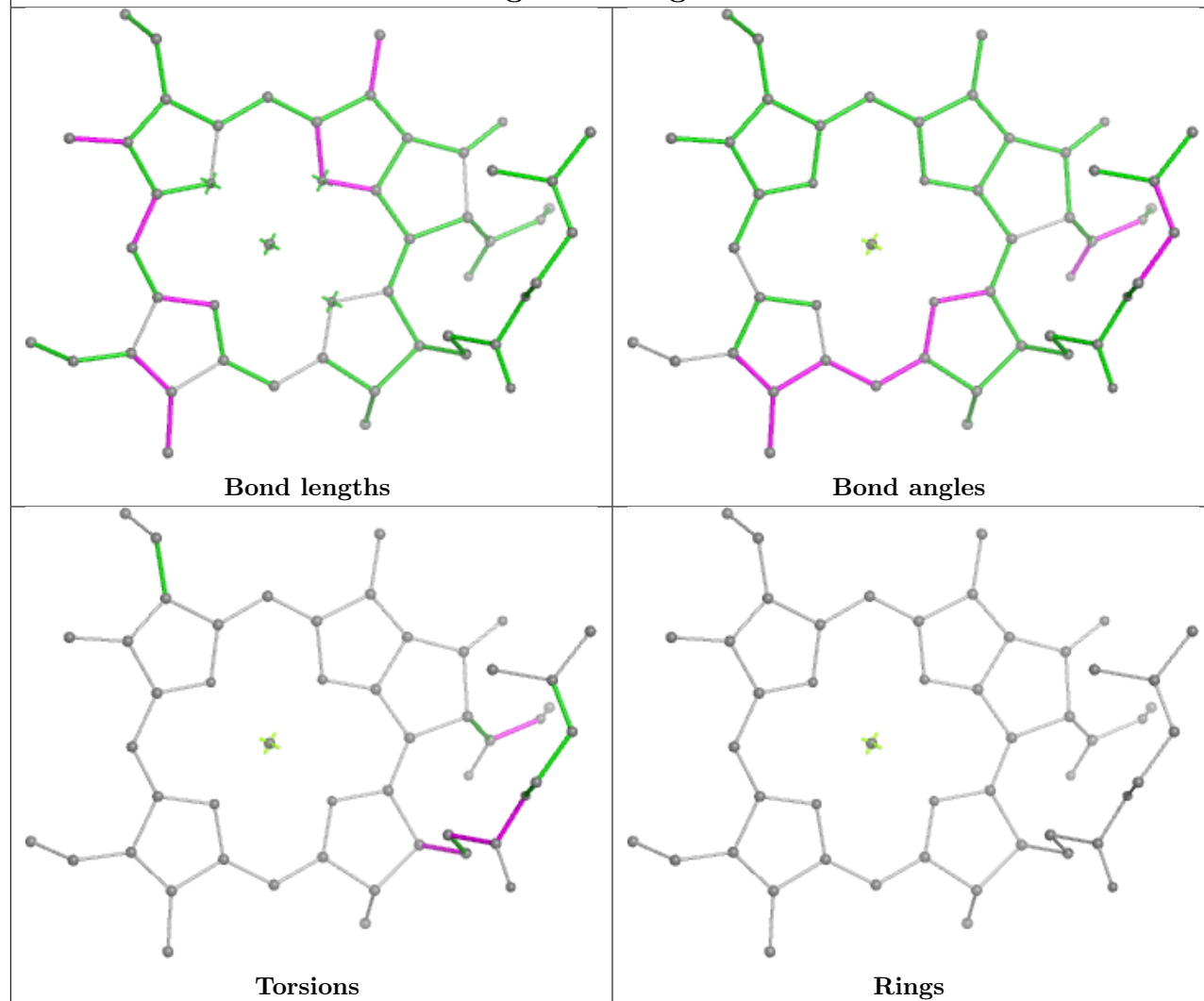
Ligand CLA e 832



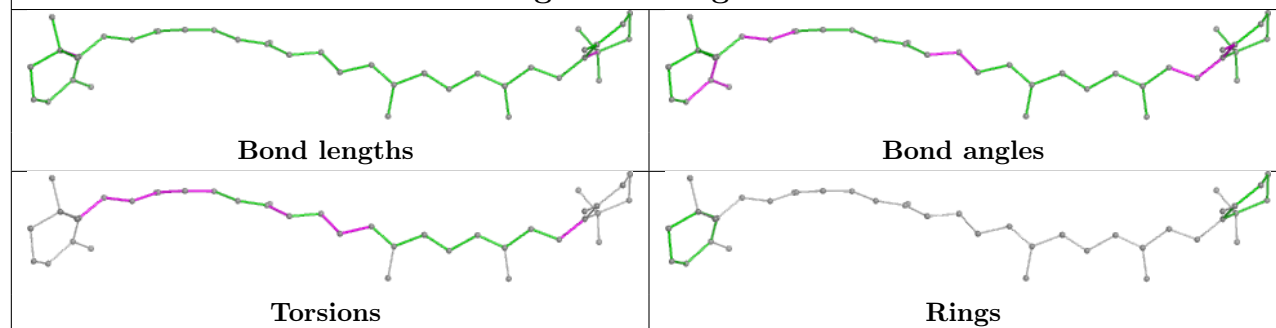
Ligand BCR j 101

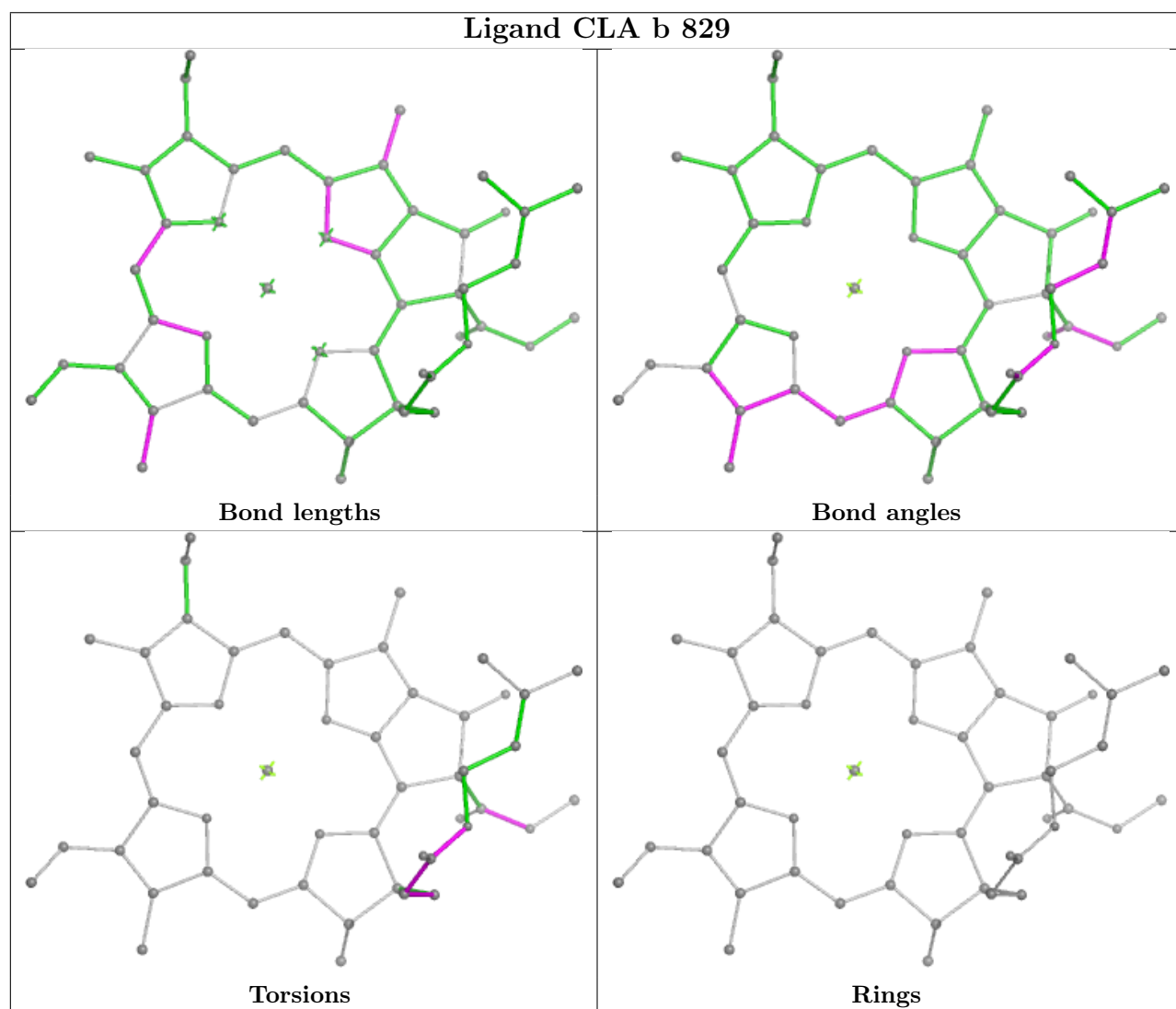
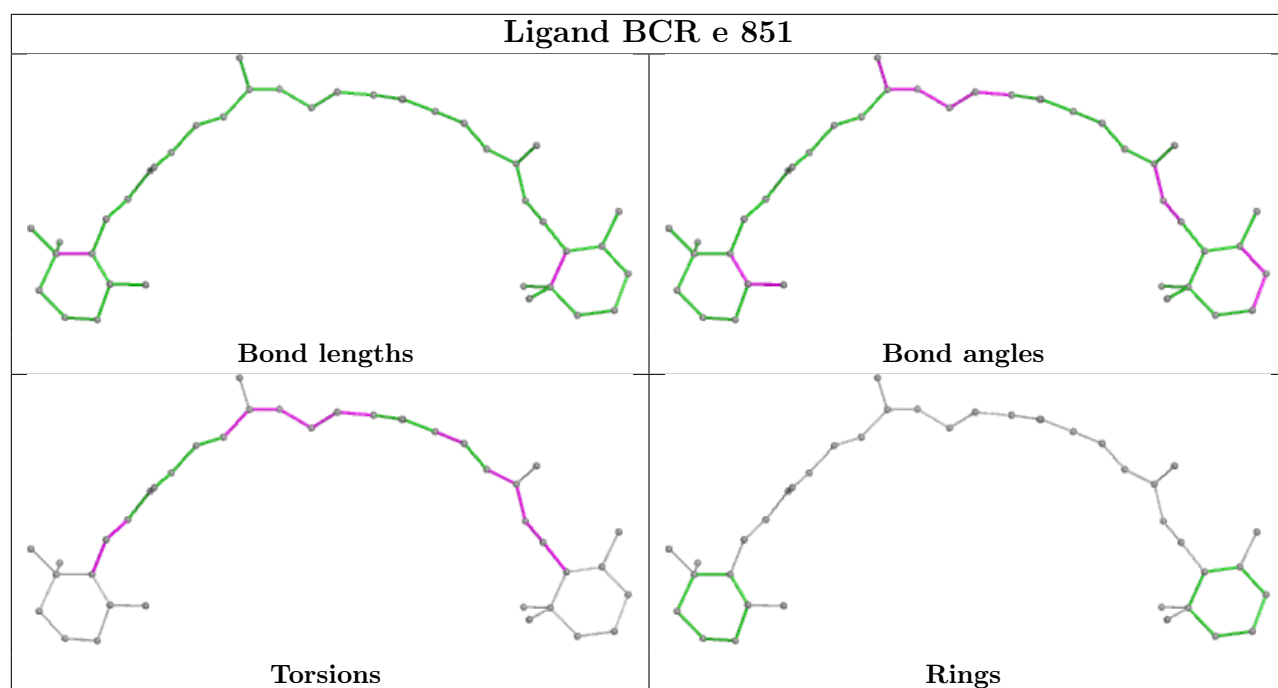


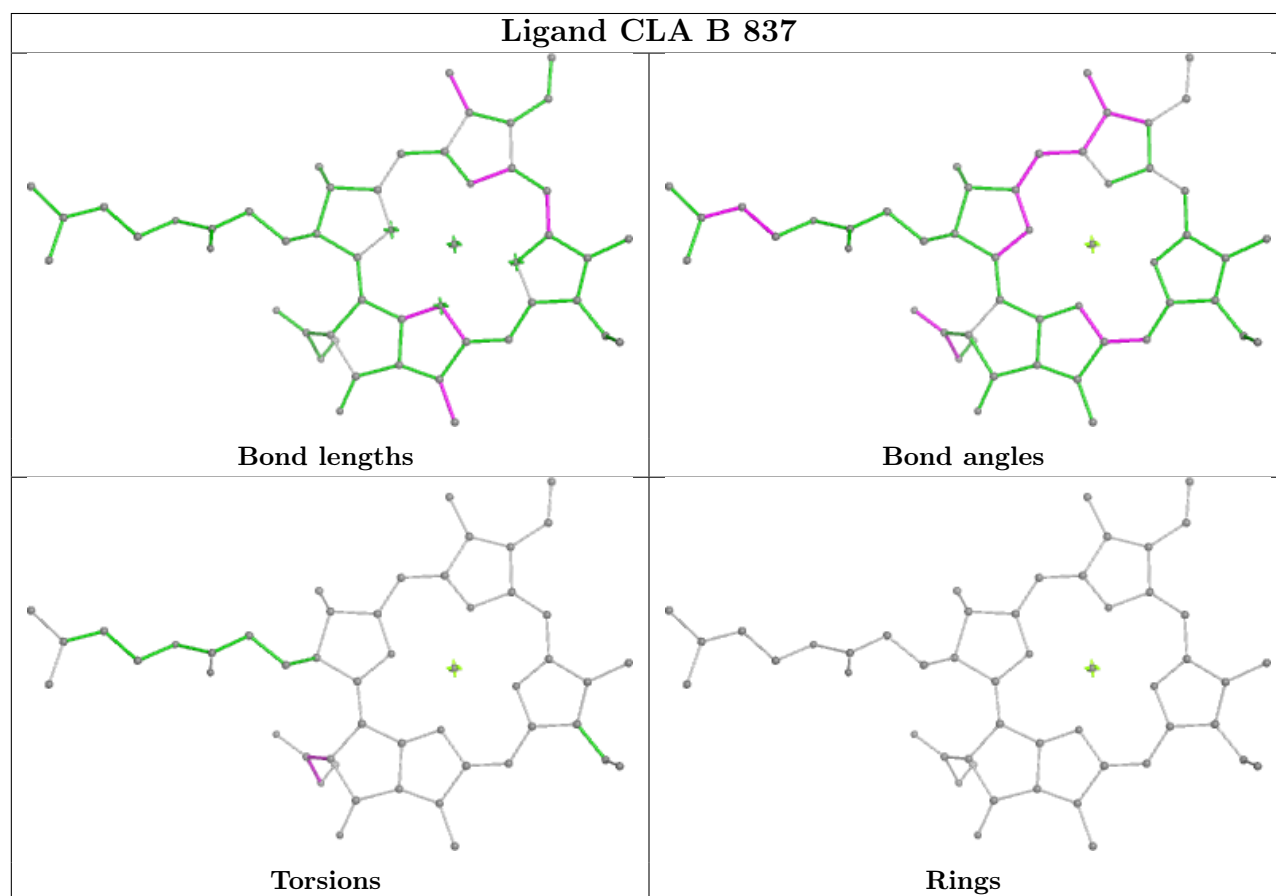
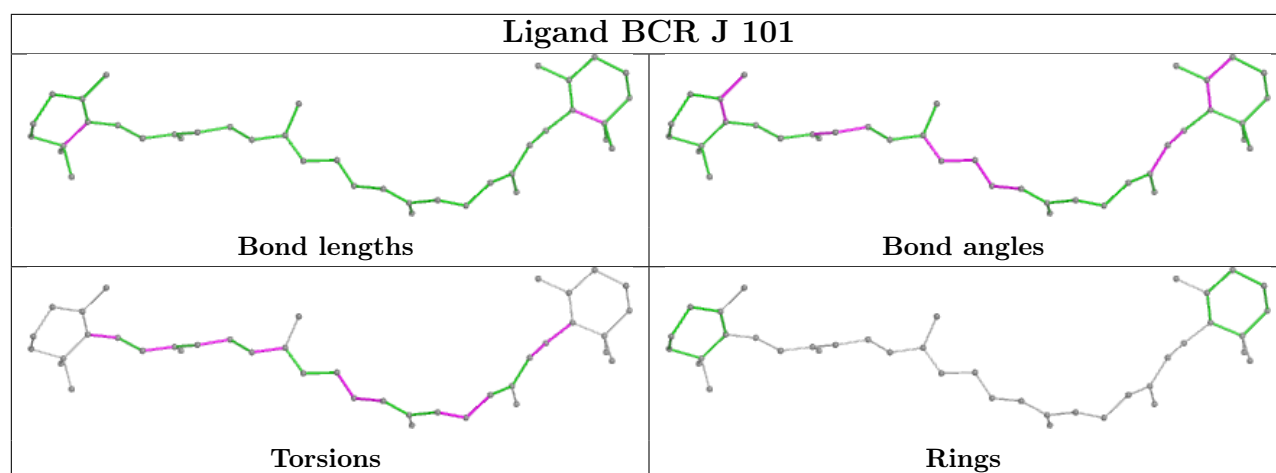
Ligand CLA g 842



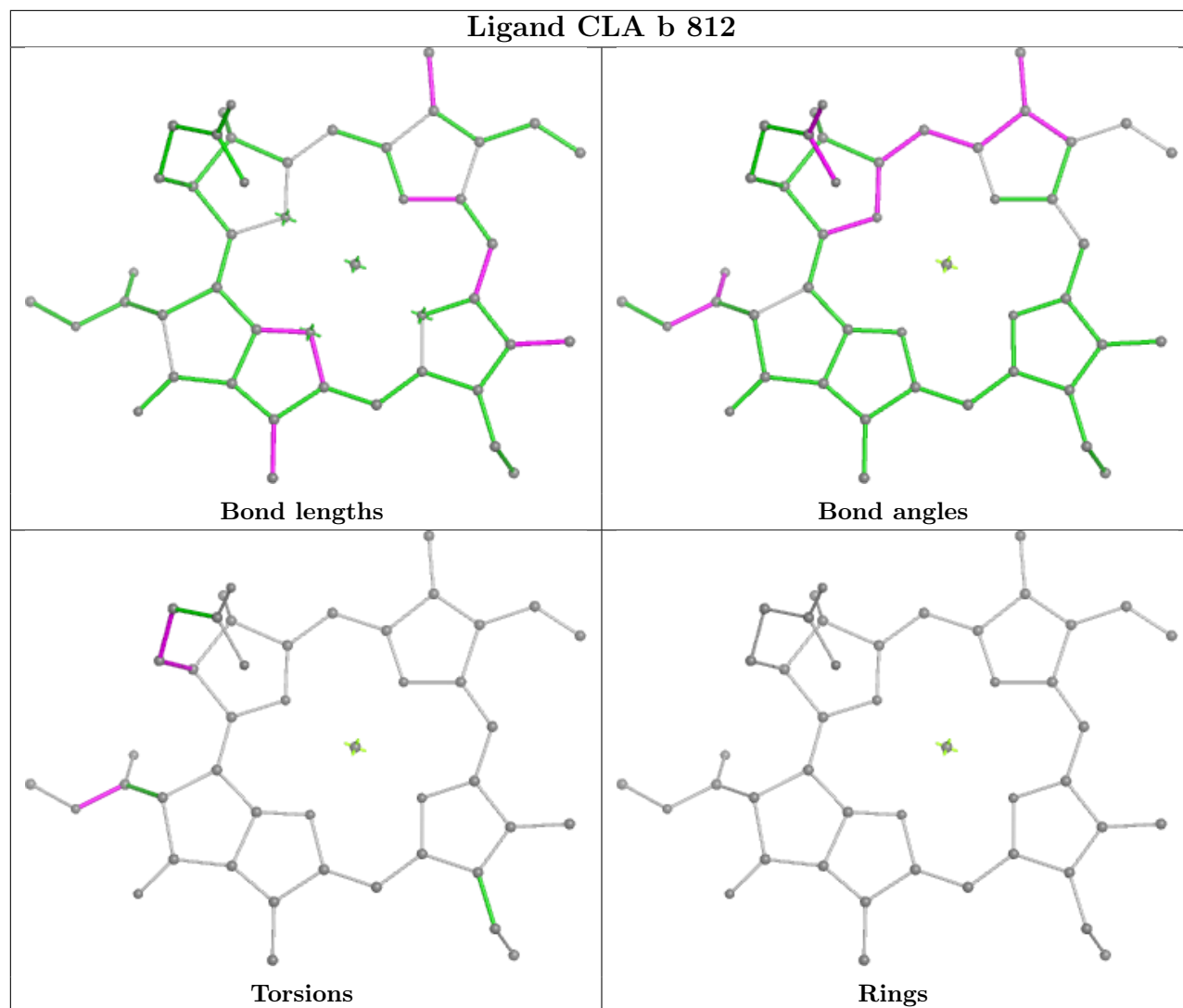
Ligand BCR g 848



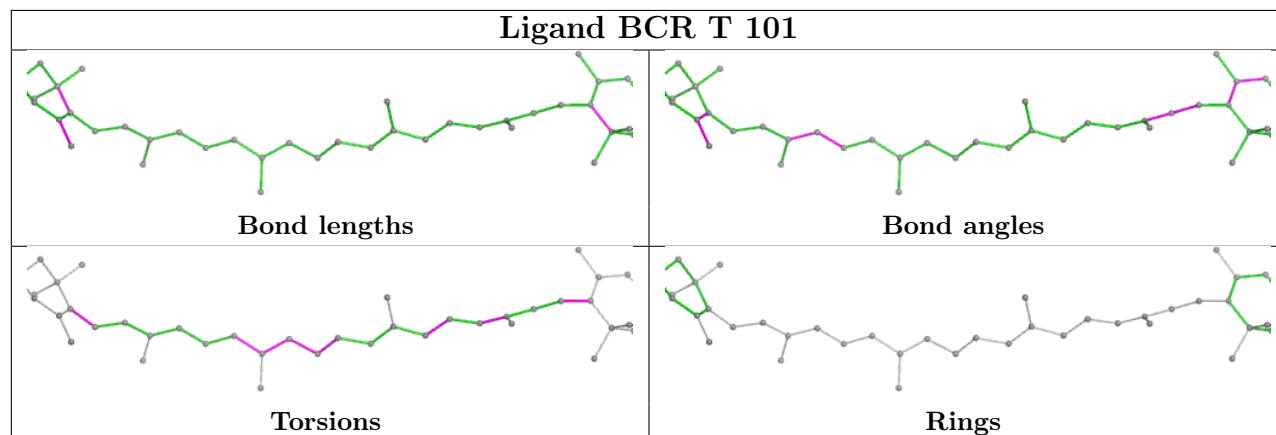




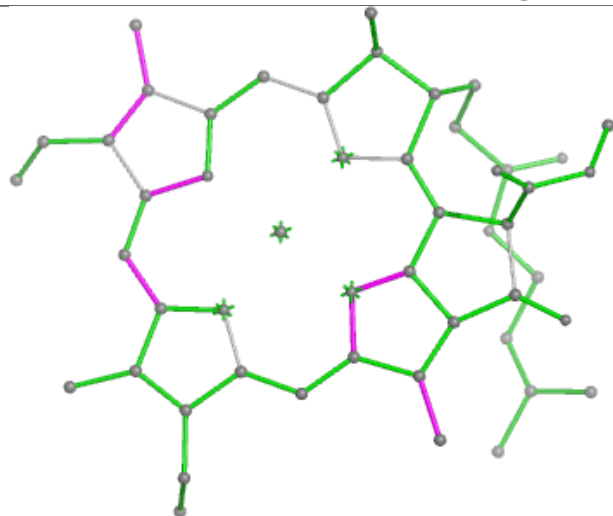
Ligand CLA b 812



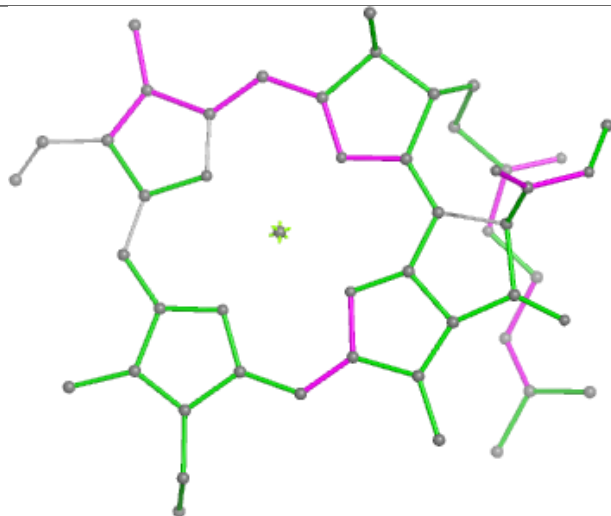
Ligand BCR T 101



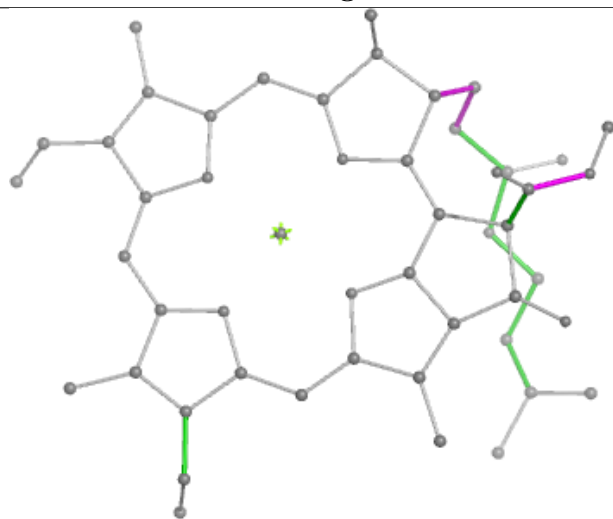
Ligand CLA E 832



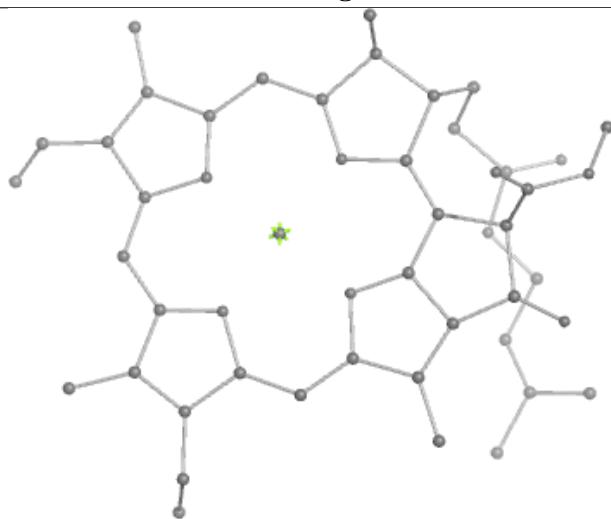
Bond lengths



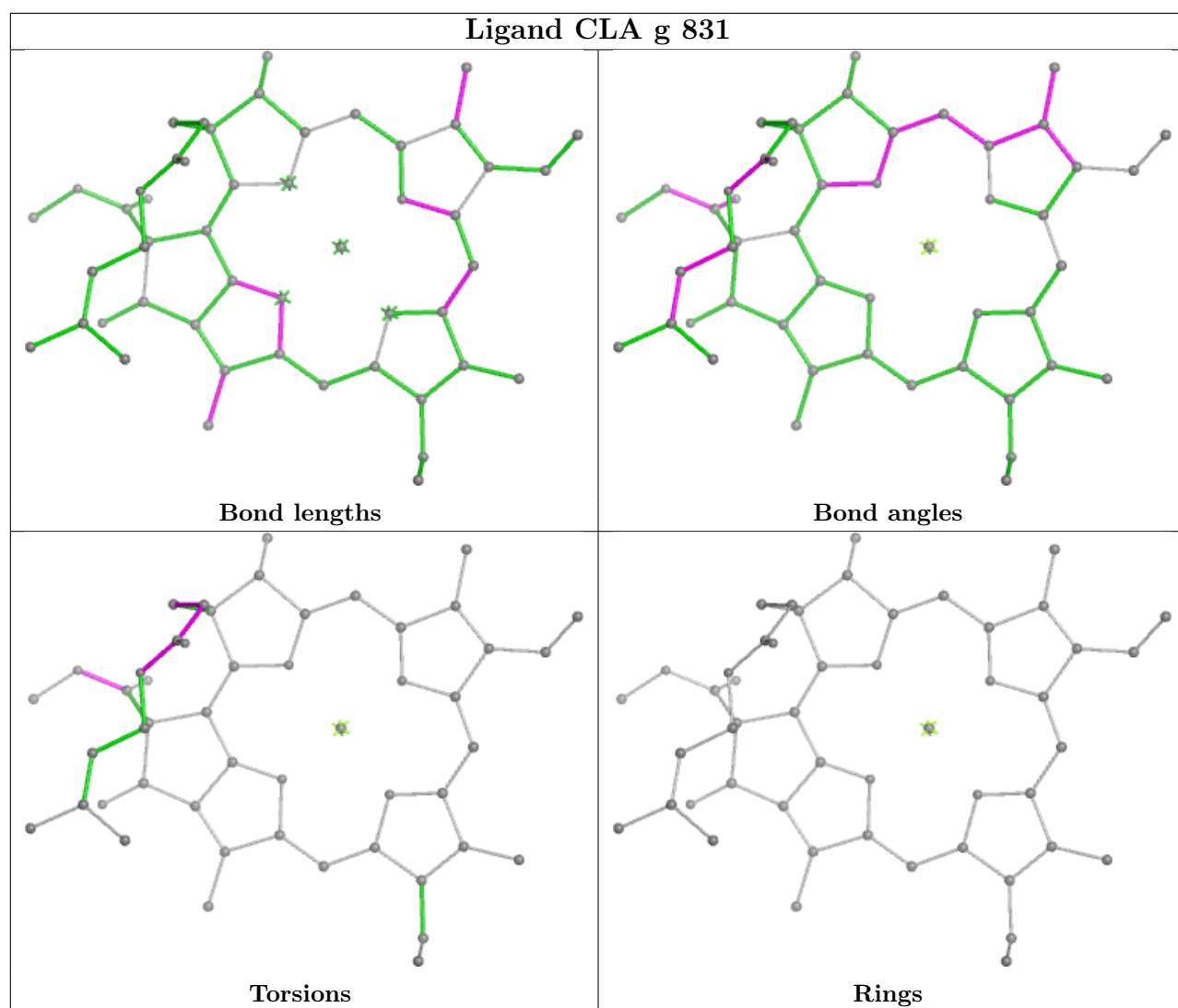
Bond angles



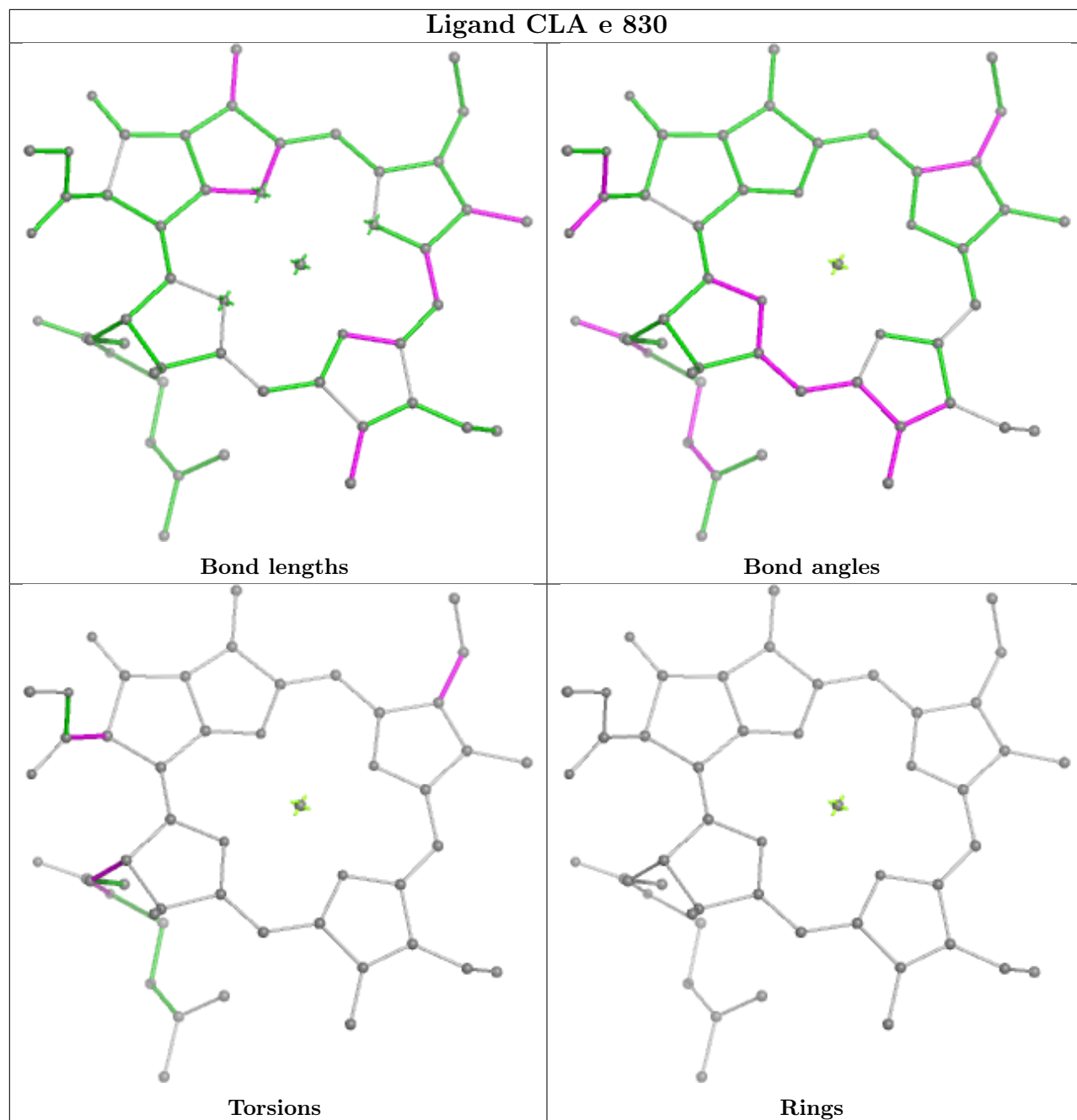
Torsions

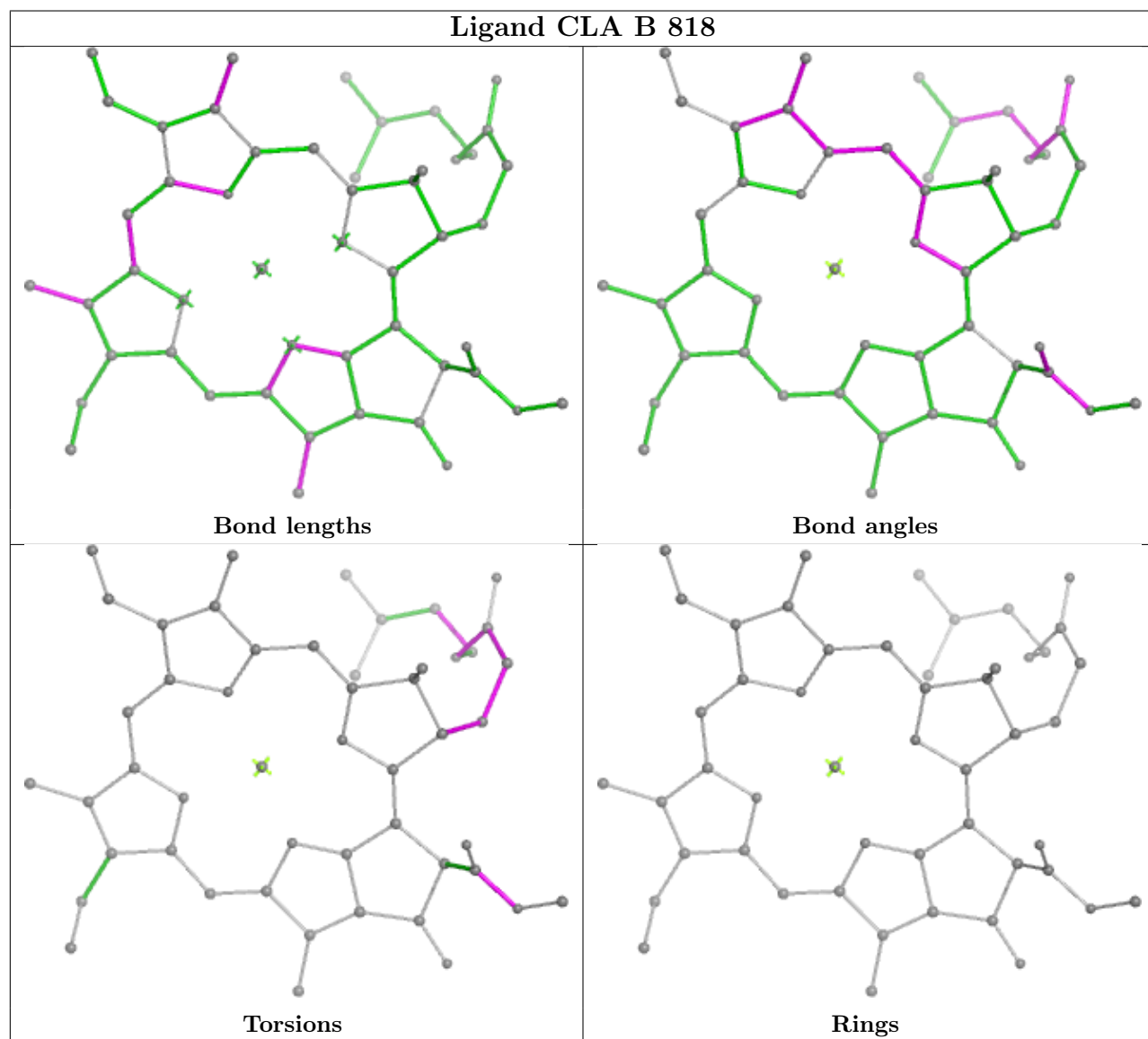
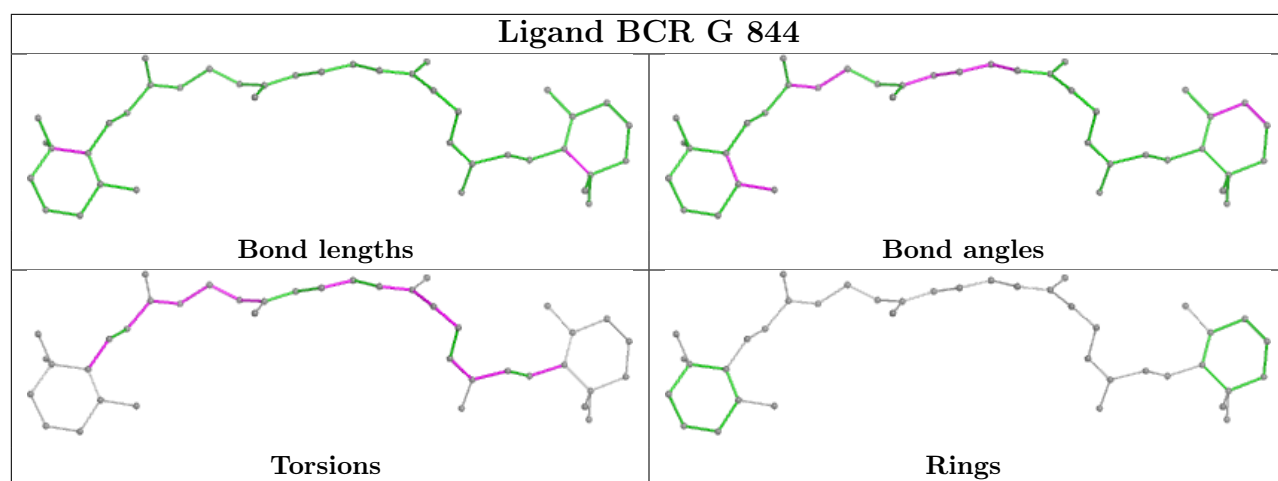


Rings

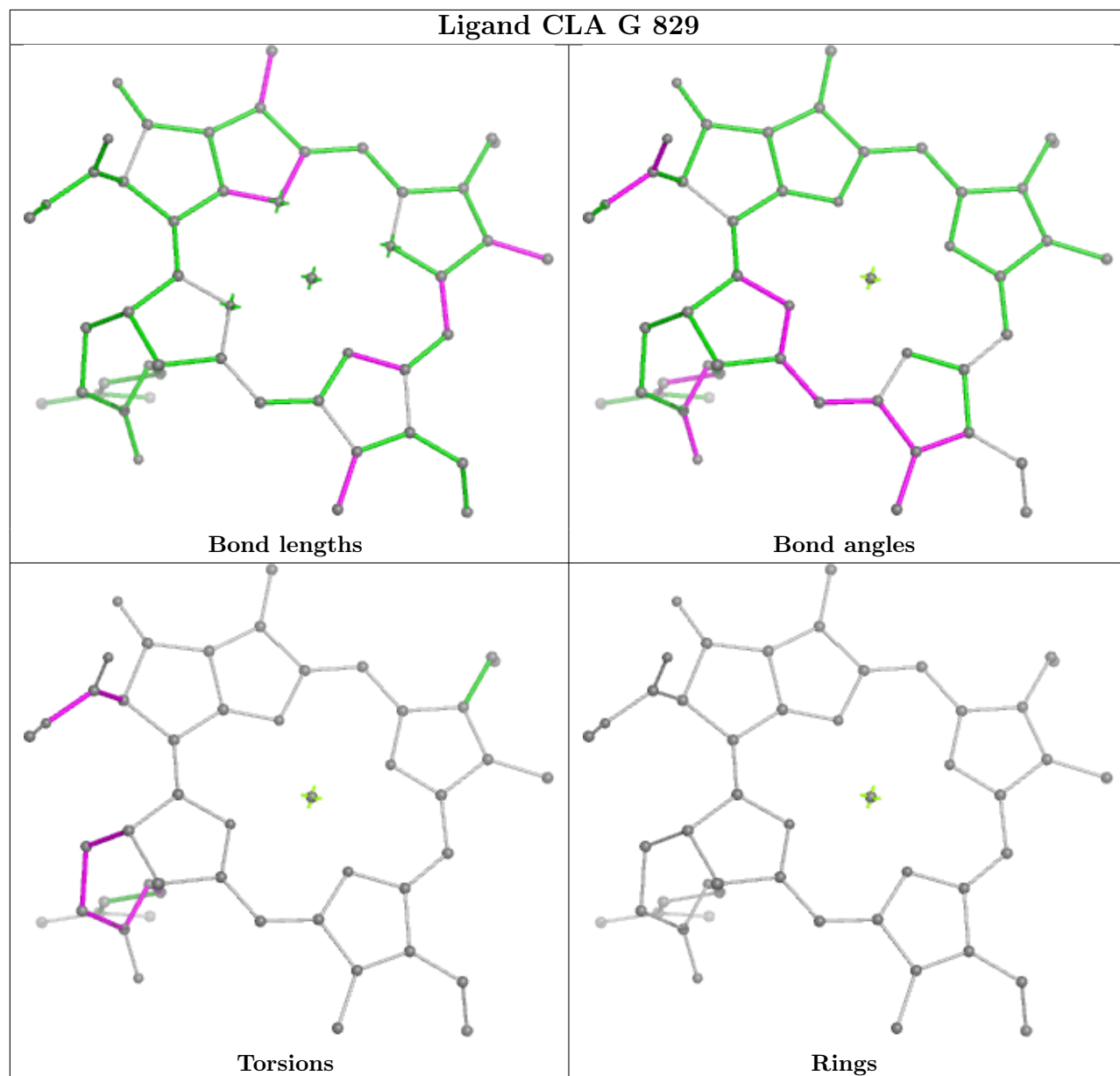


Ligand CLA e 830

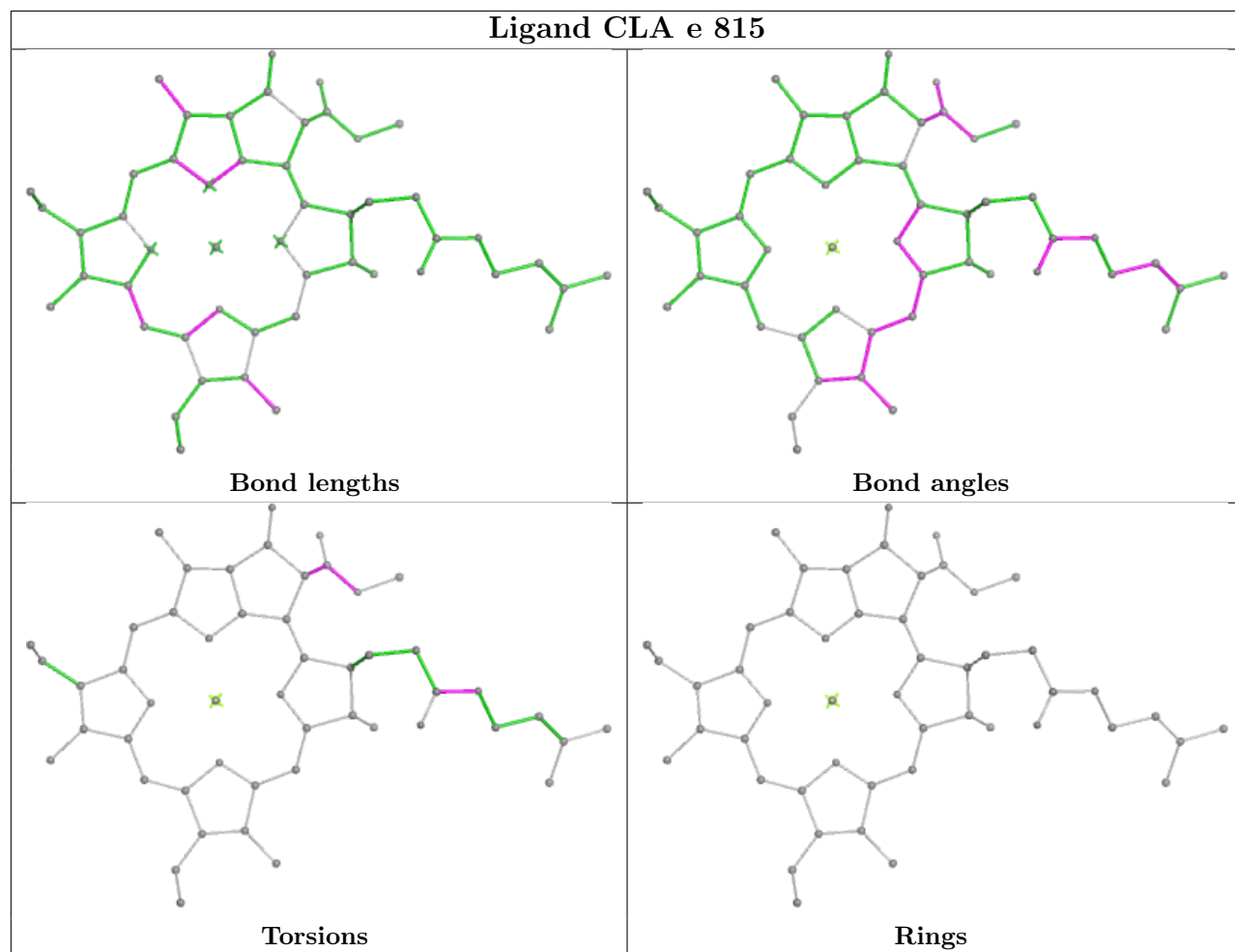


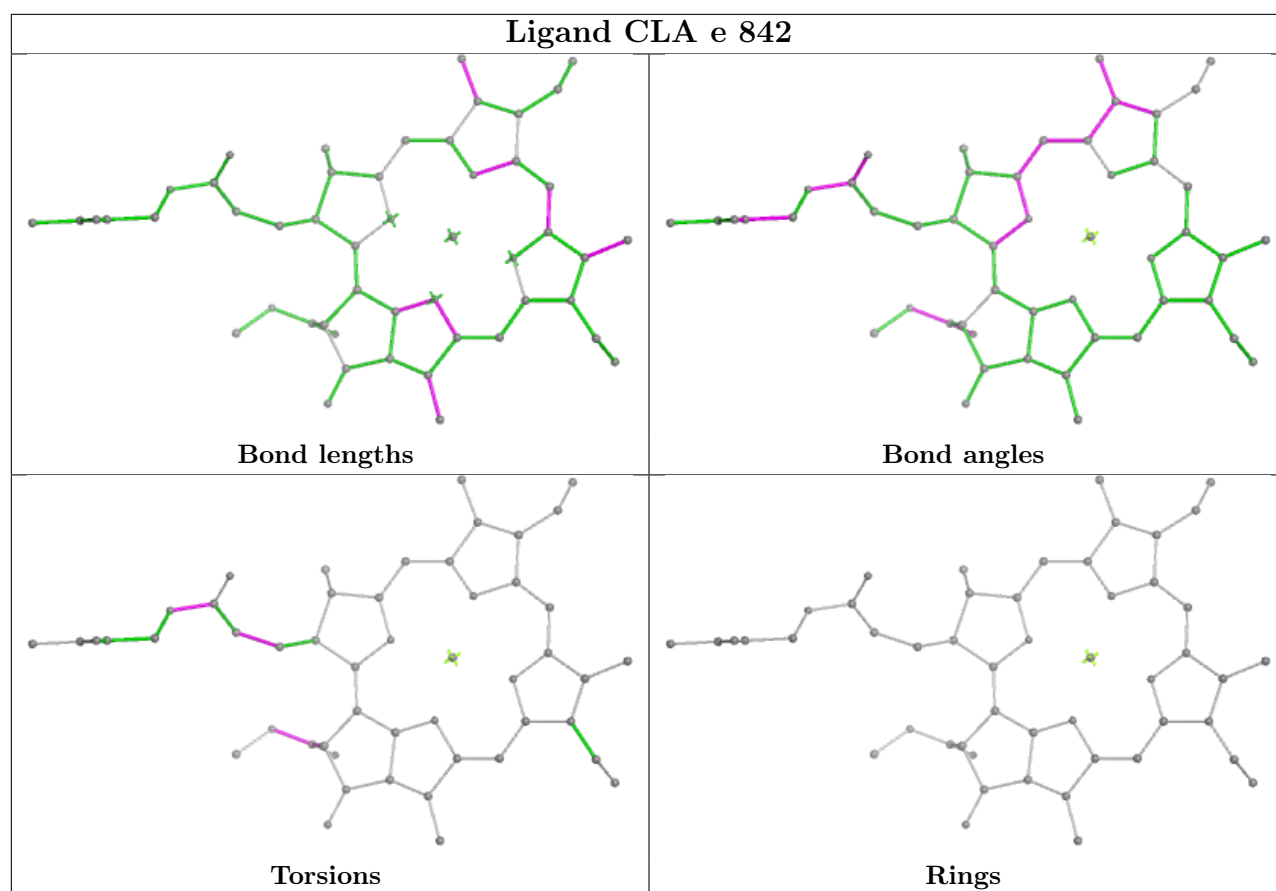


Ligand CLA G 829

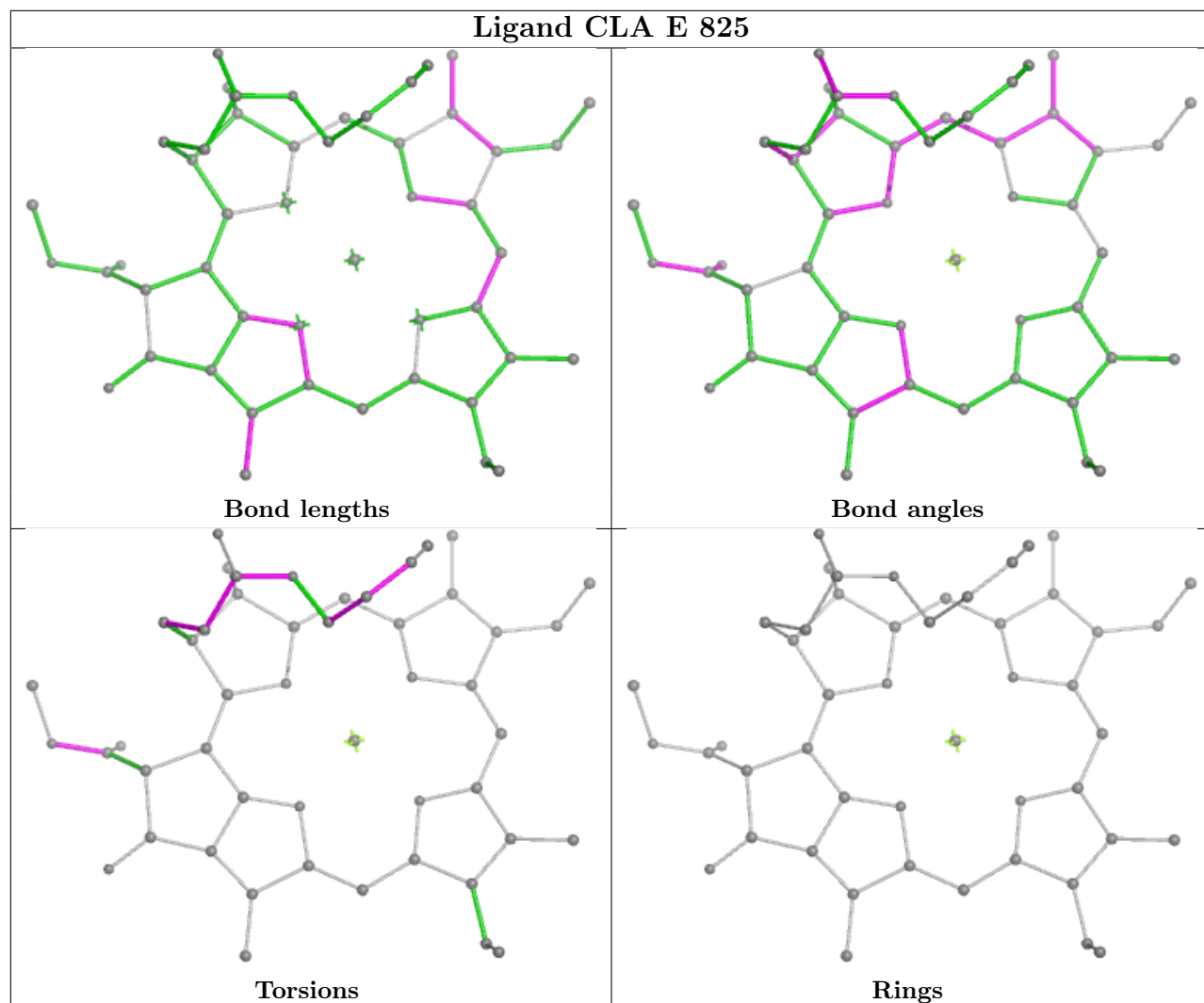


Ligand CLA e 815

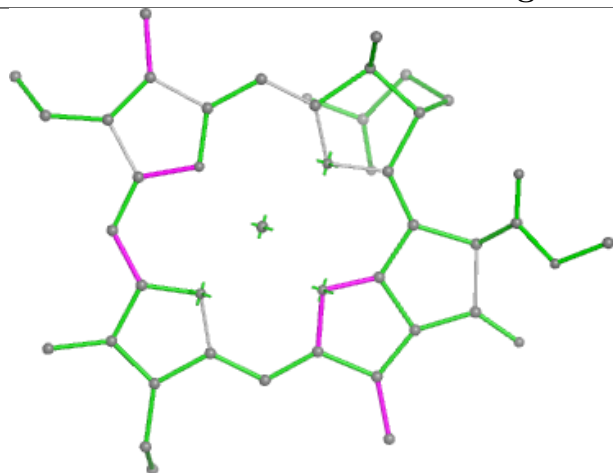




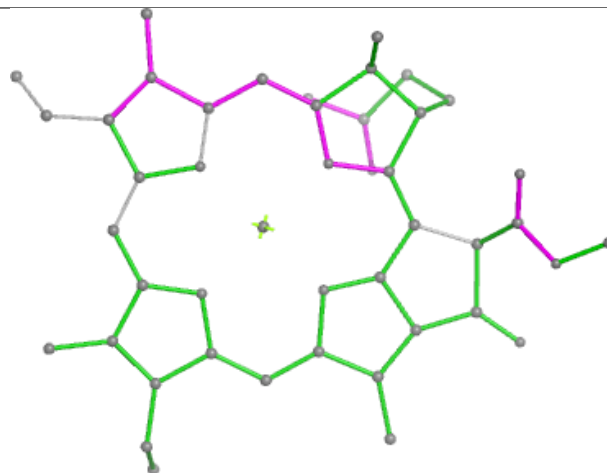
Ligand CLA E 825



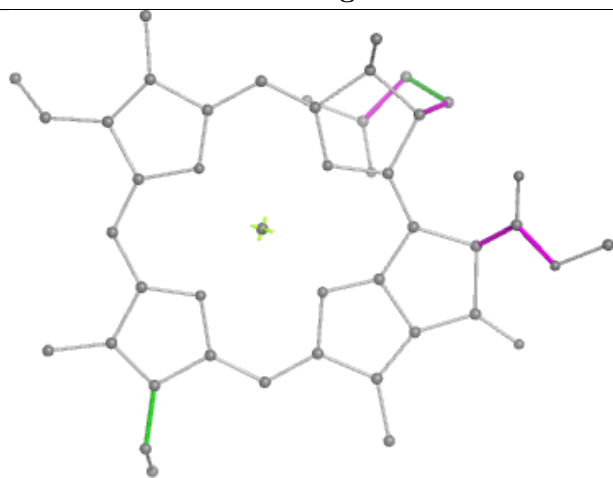
Ligand CLA b 835



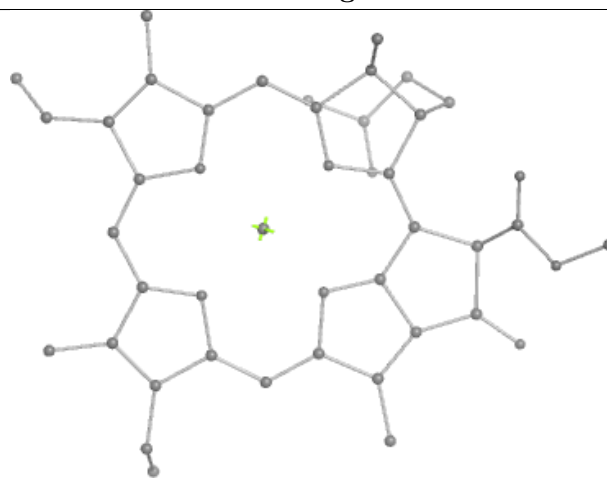
Bond lengths



Bond angles

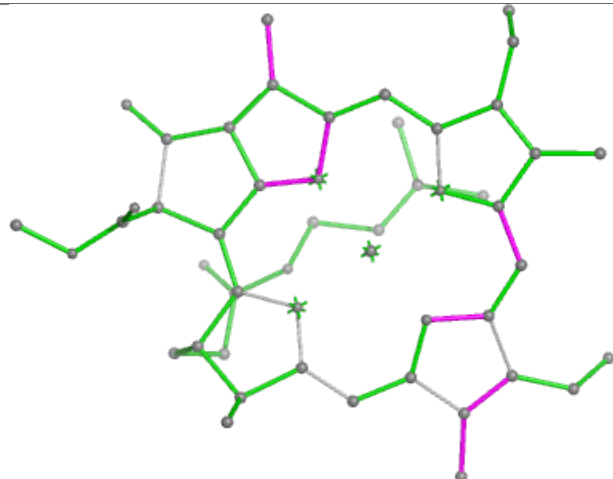


Torsions

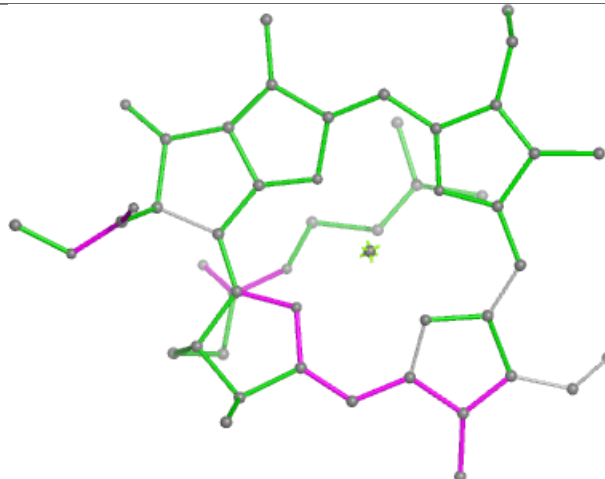


Rings

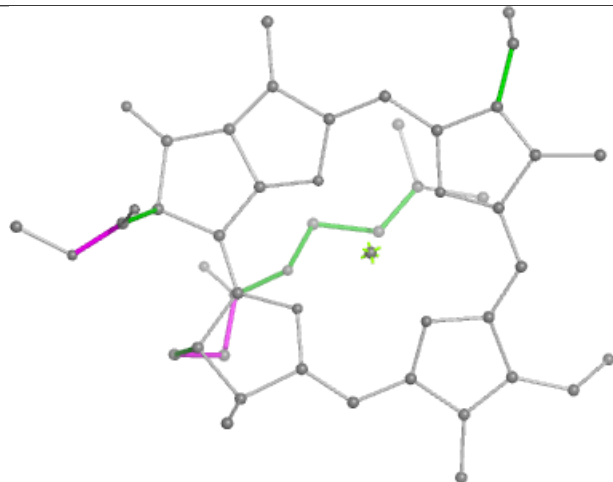
Ligand CLA g 810



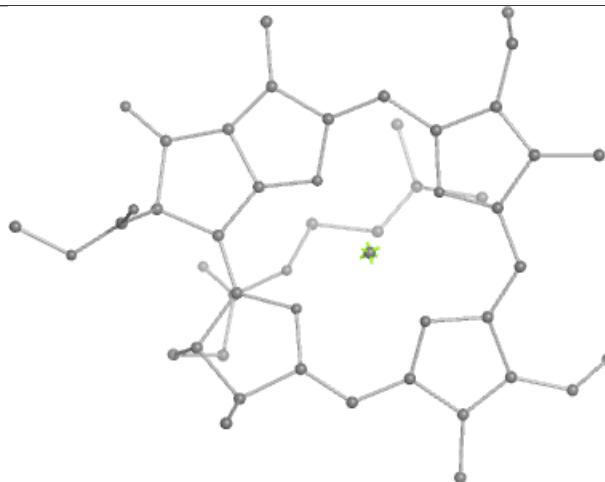
Bond lengths



Bond angles

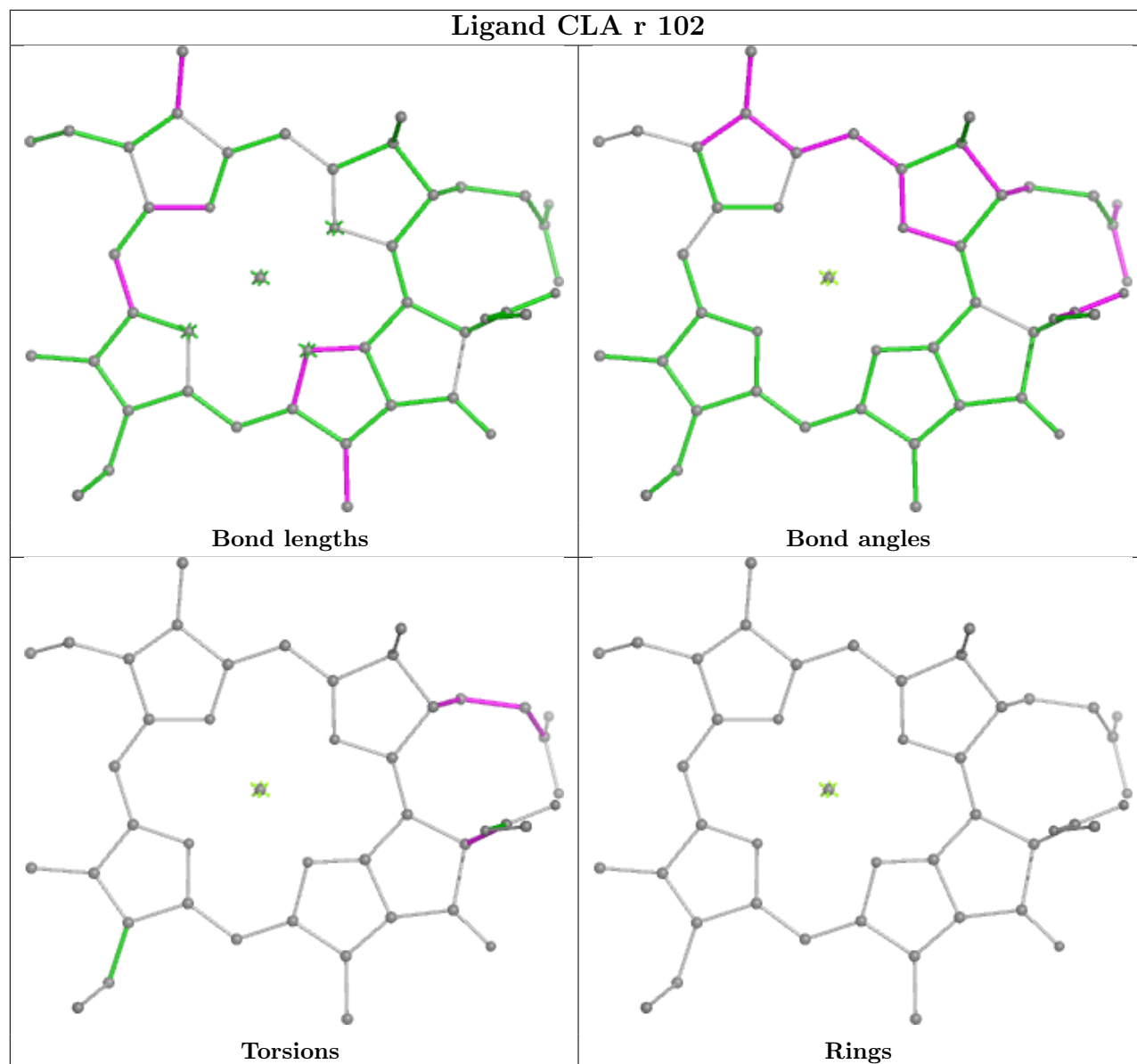


Torsions

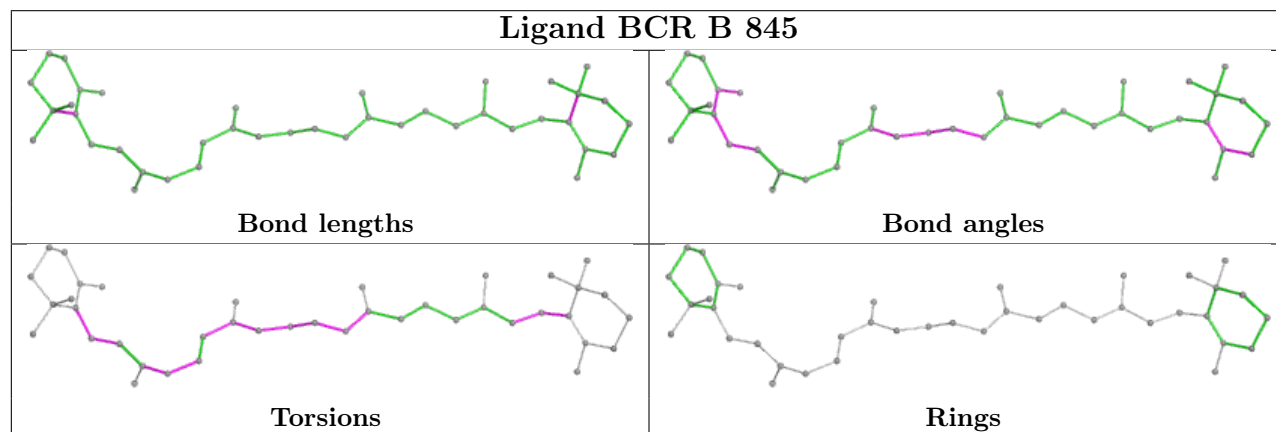


Rings

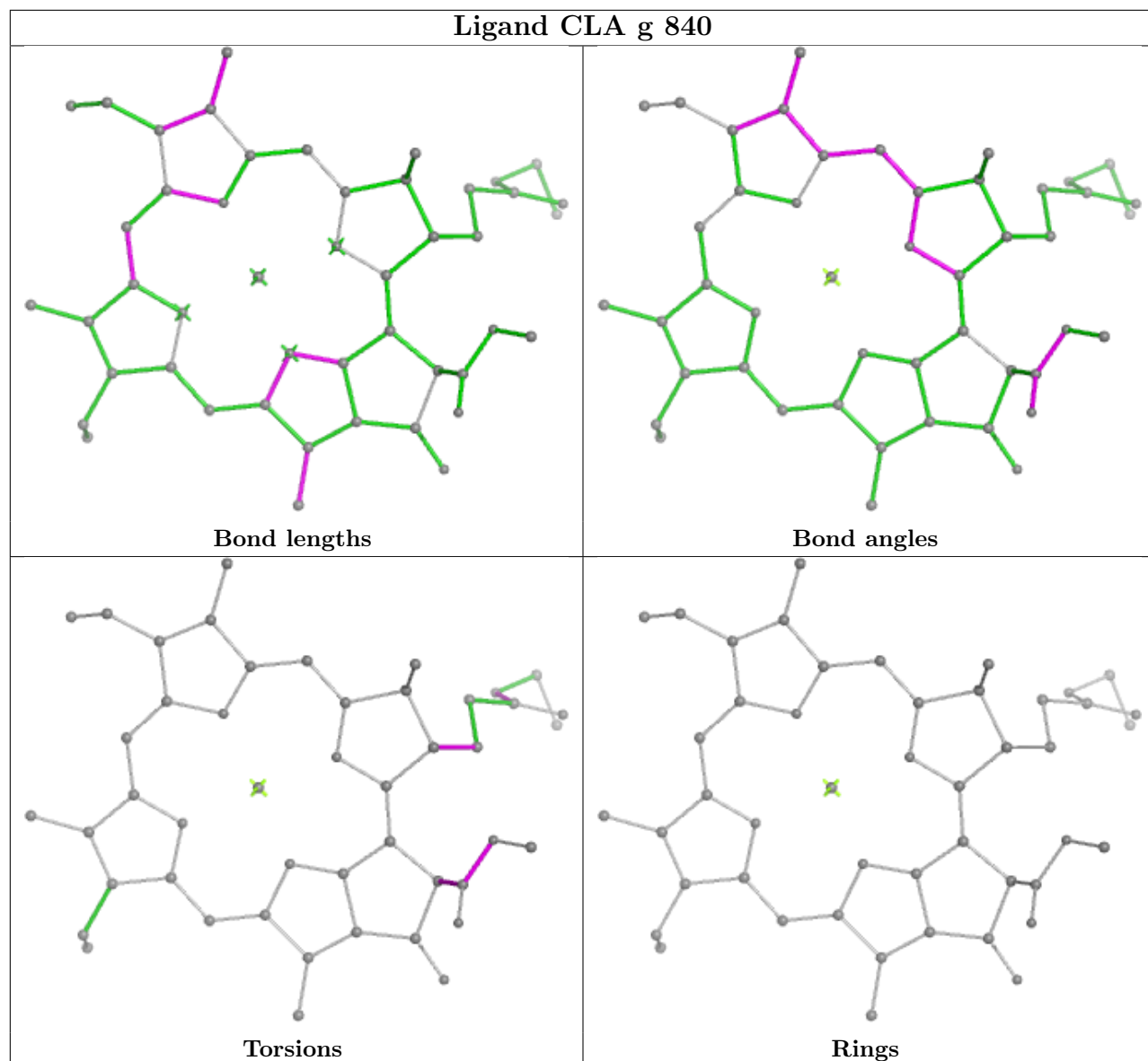
Ligand CLA r 102



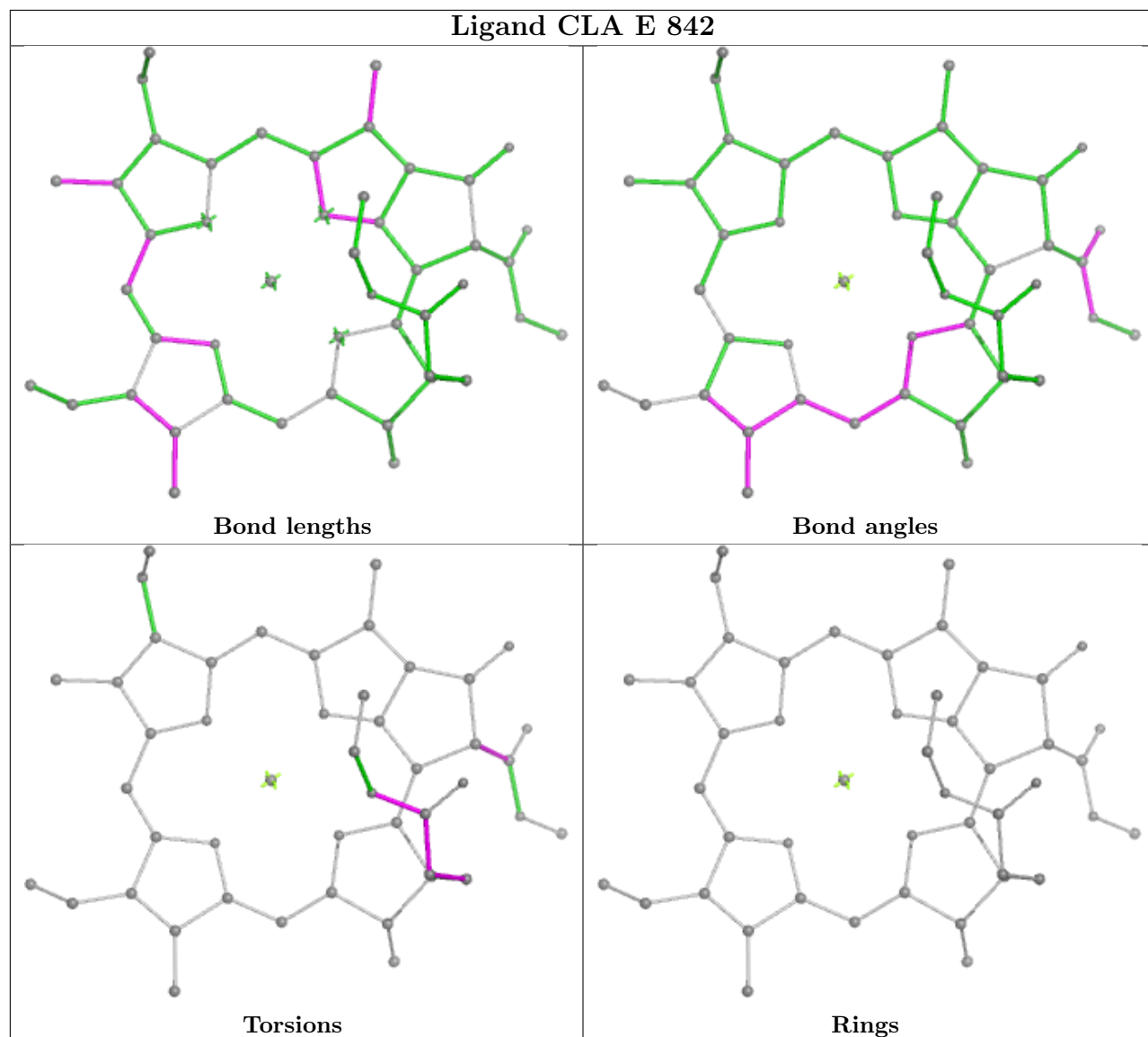
Ligand BCR B 845



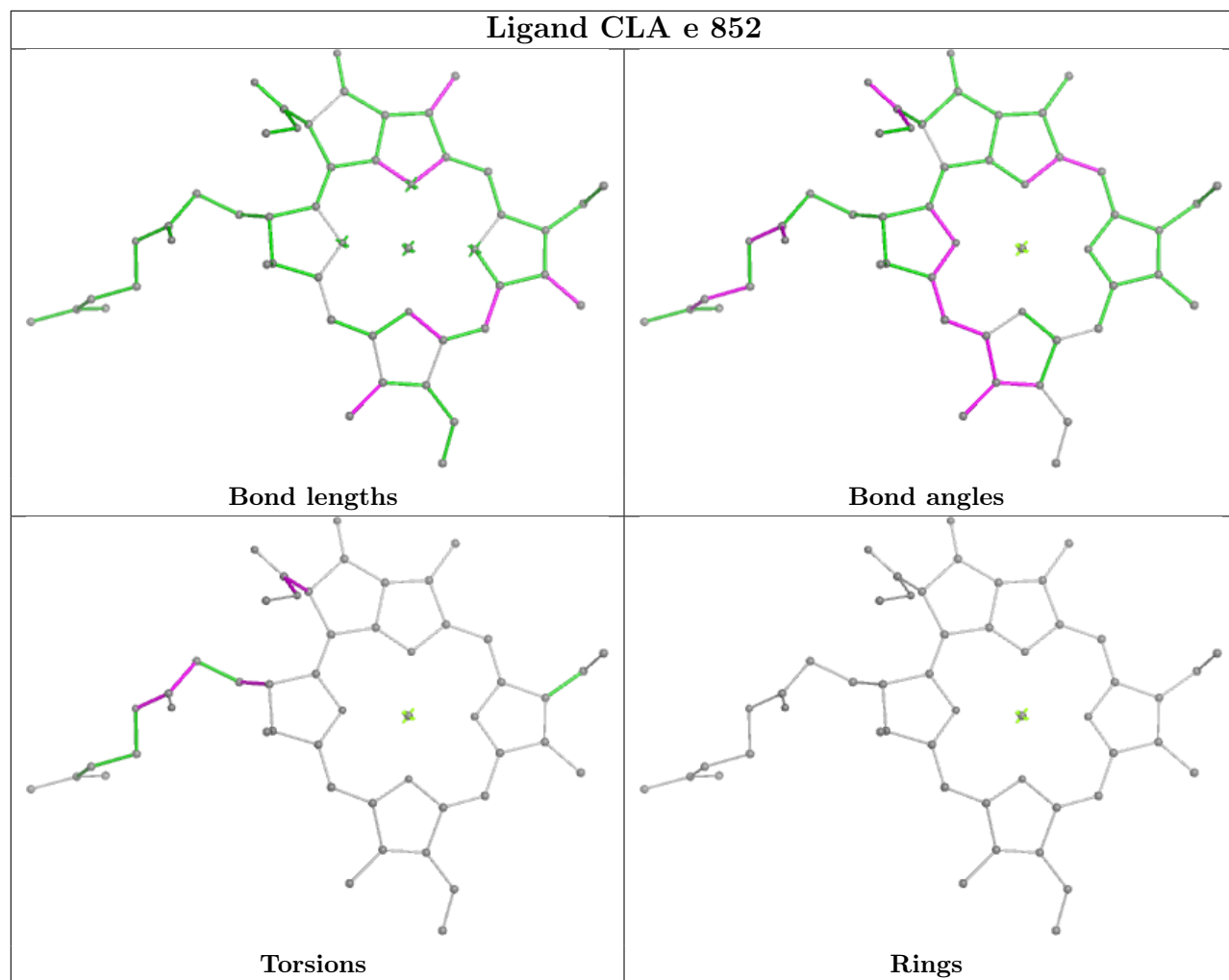
Ligand CLA g 840



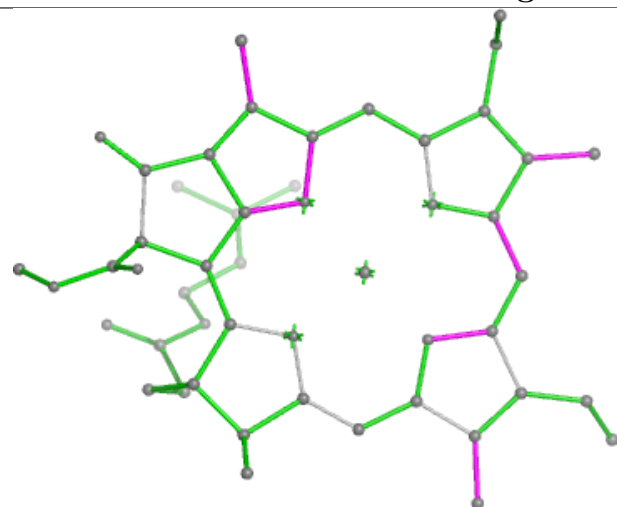
Ligand CLA E 842



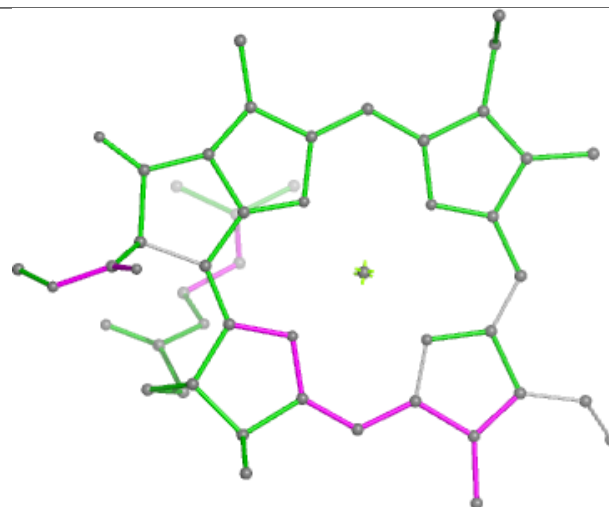
Ligand CLA e 852



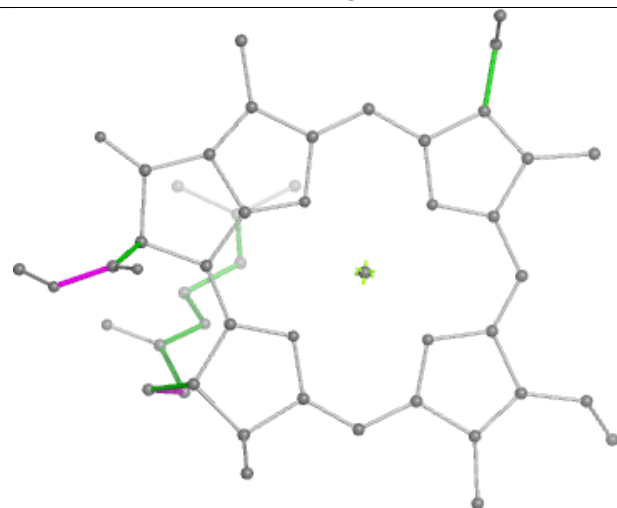
Ligand CLA G 815



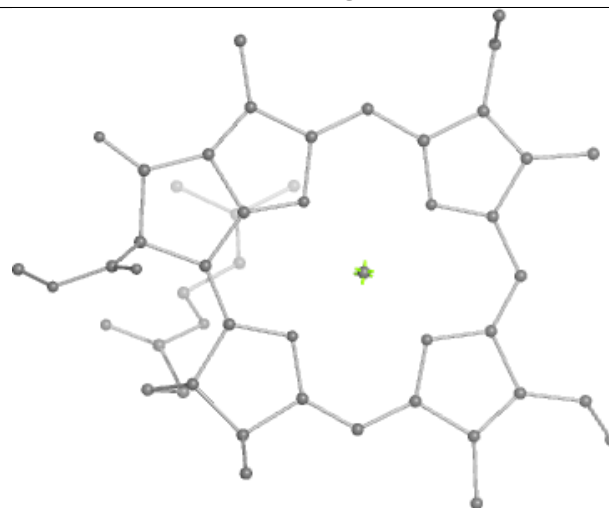
Bond lengths



Bond angles

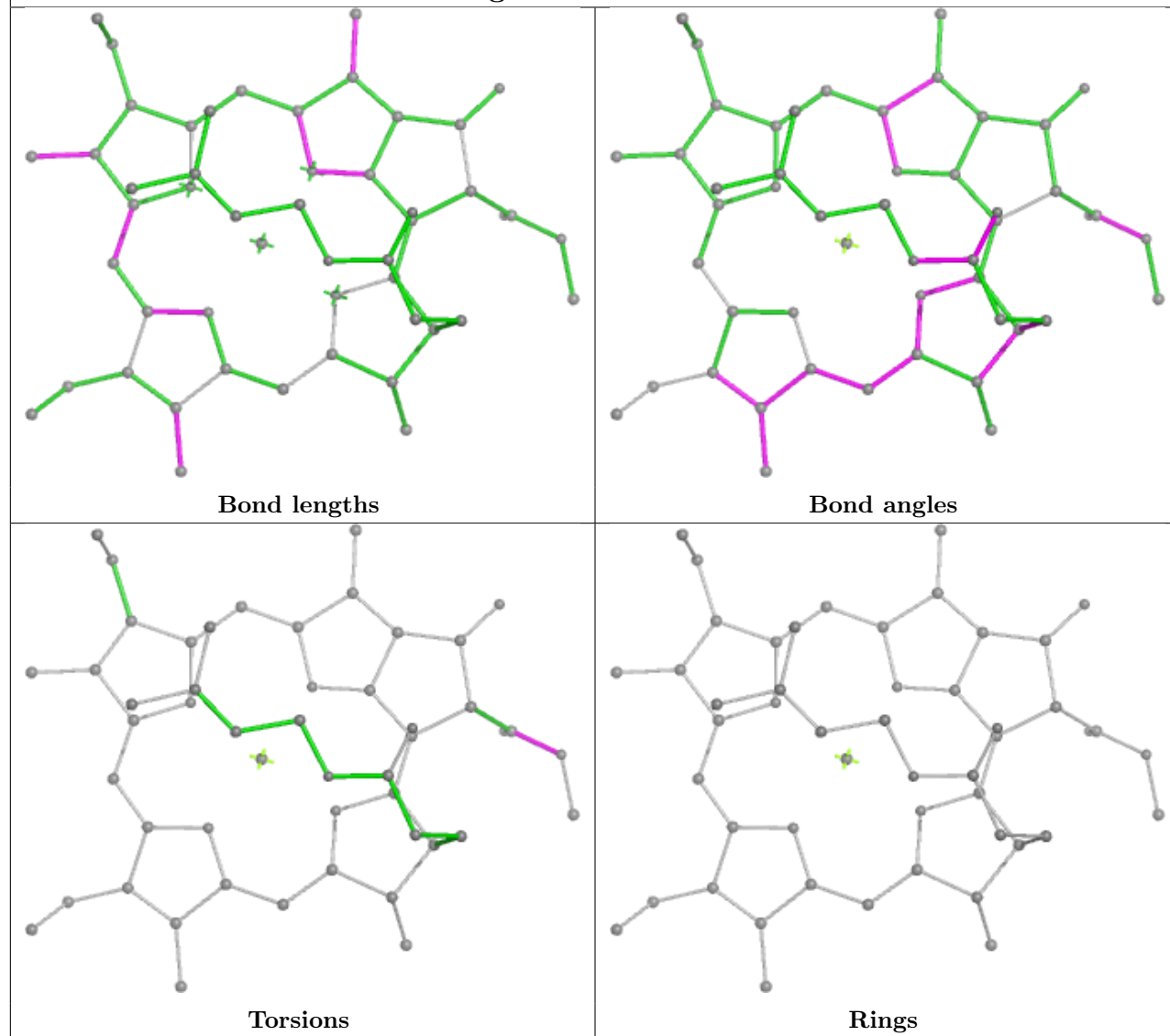


Torsions

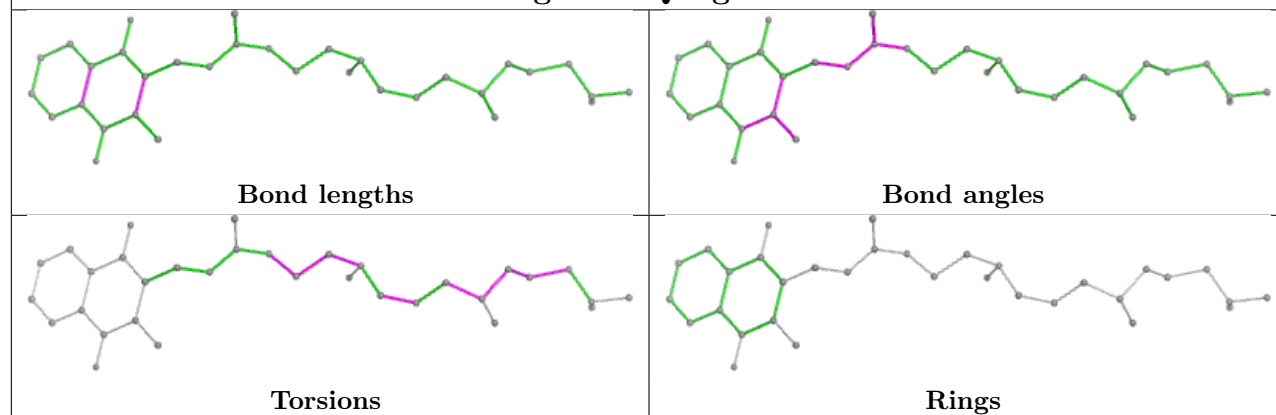


Rings

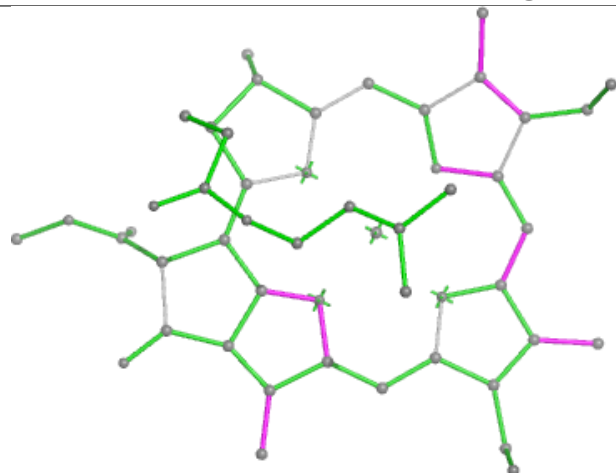
Ligand CLA E 820



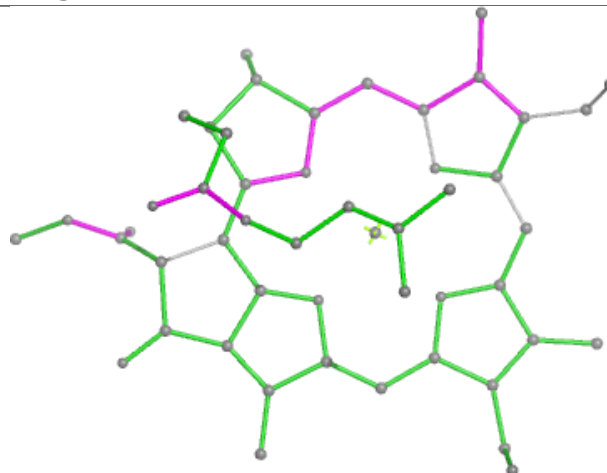
Ligand PQN g 843



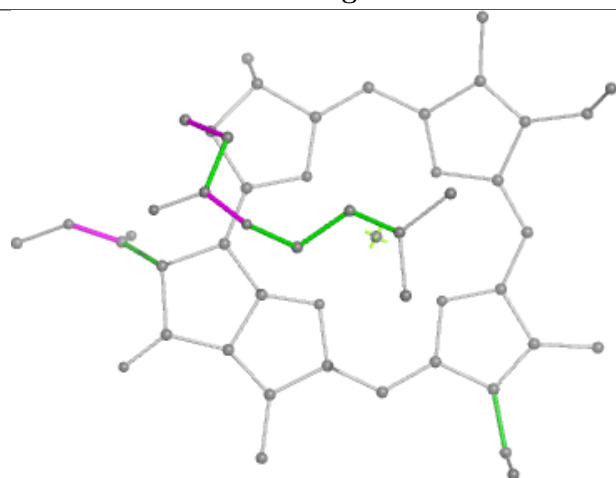
Ligand CLA g 803



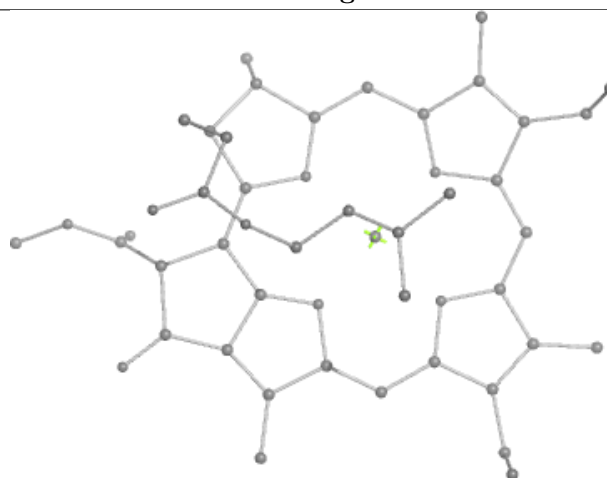
Bond lengths



Bond angles

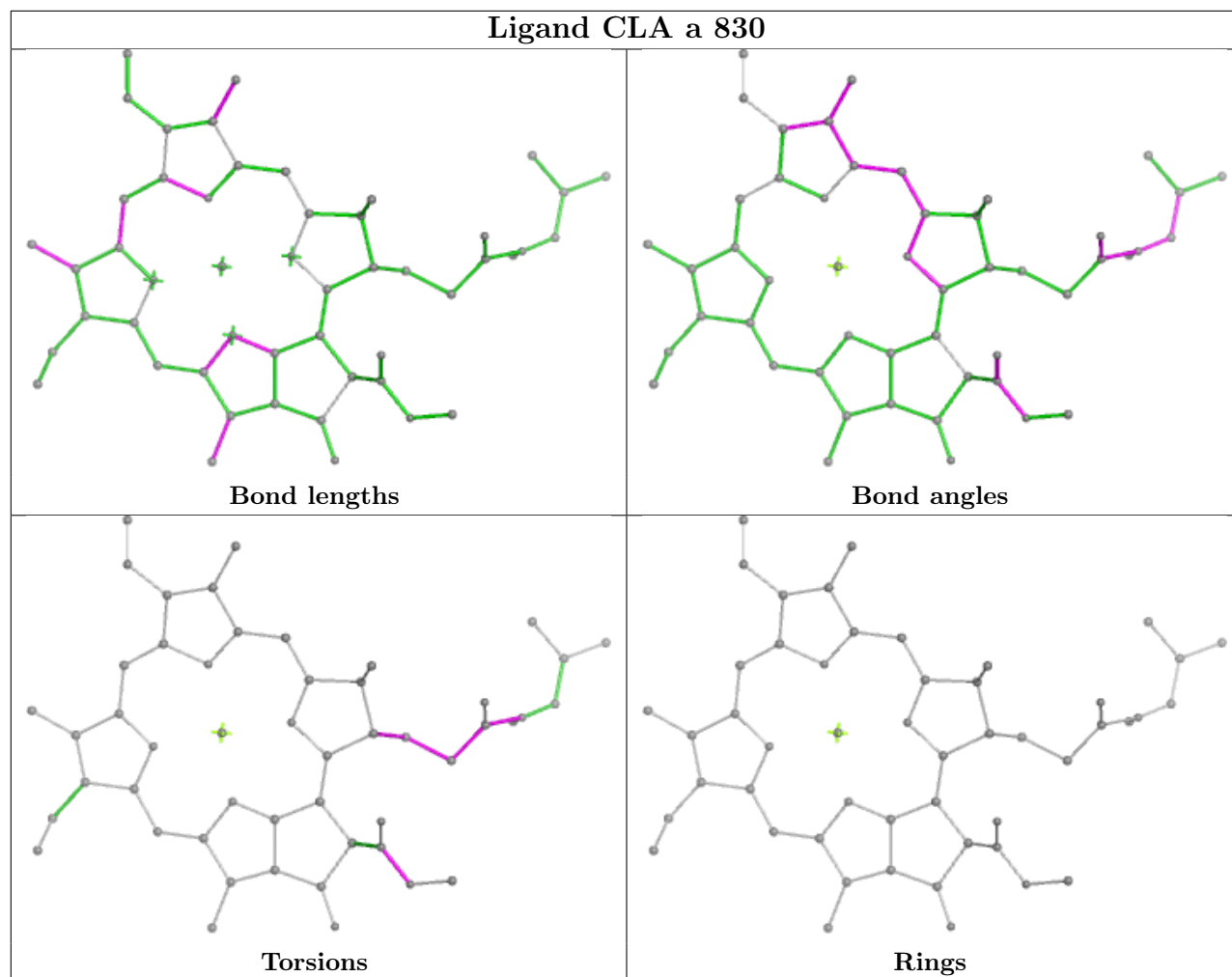


Torsions

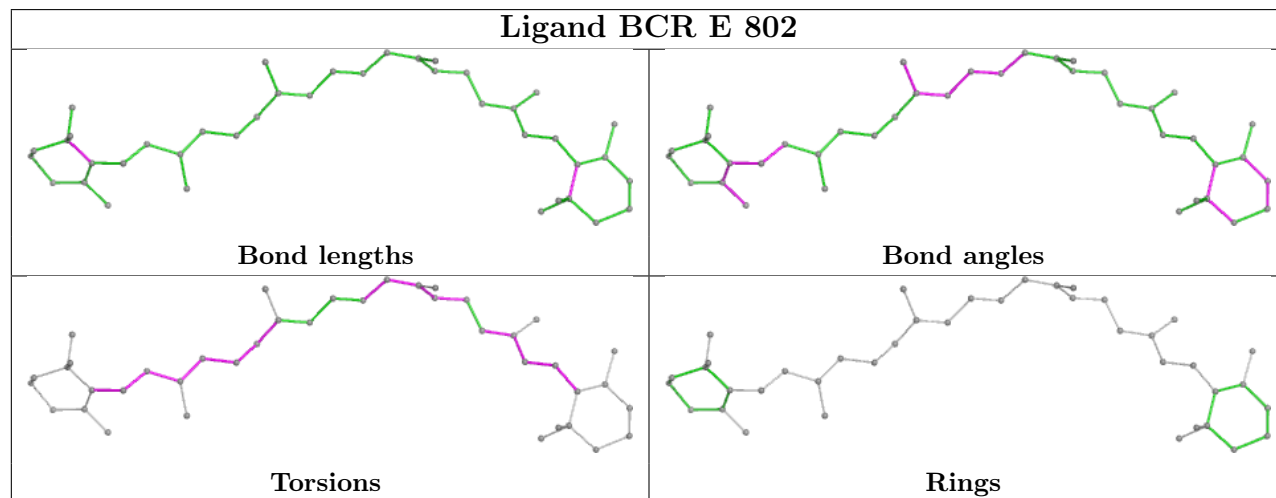


Rings

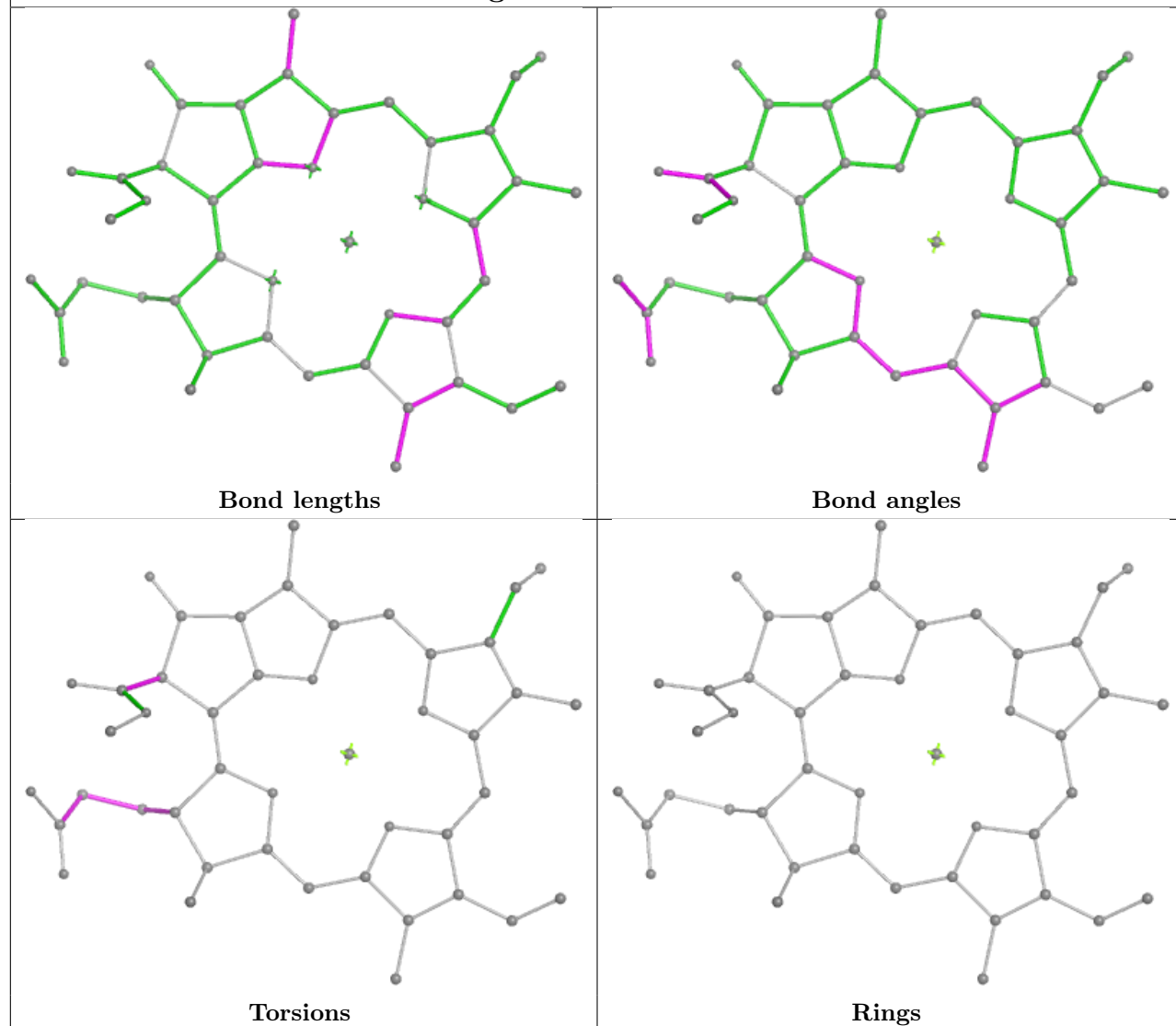
Ligand CLA a 830



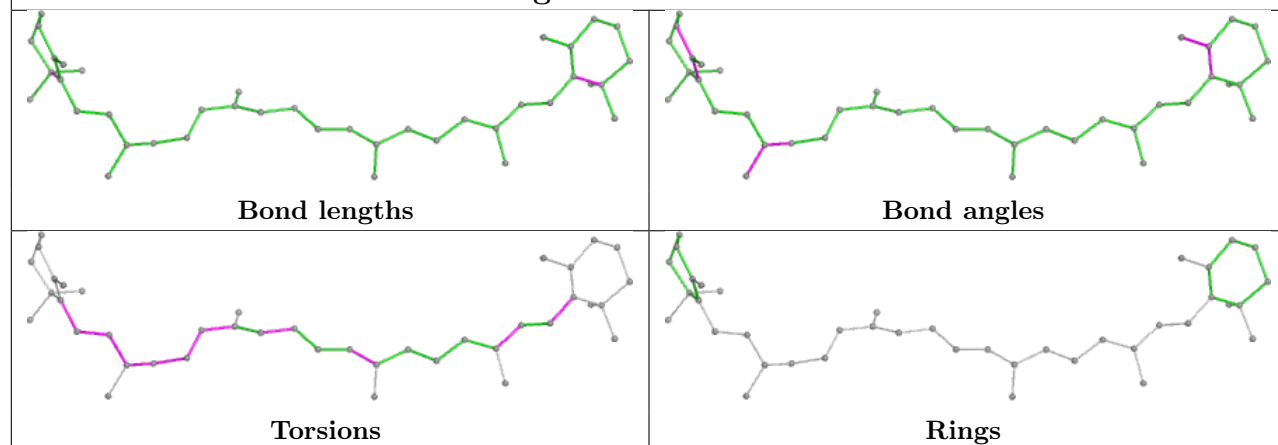
Ligand BCR E 802

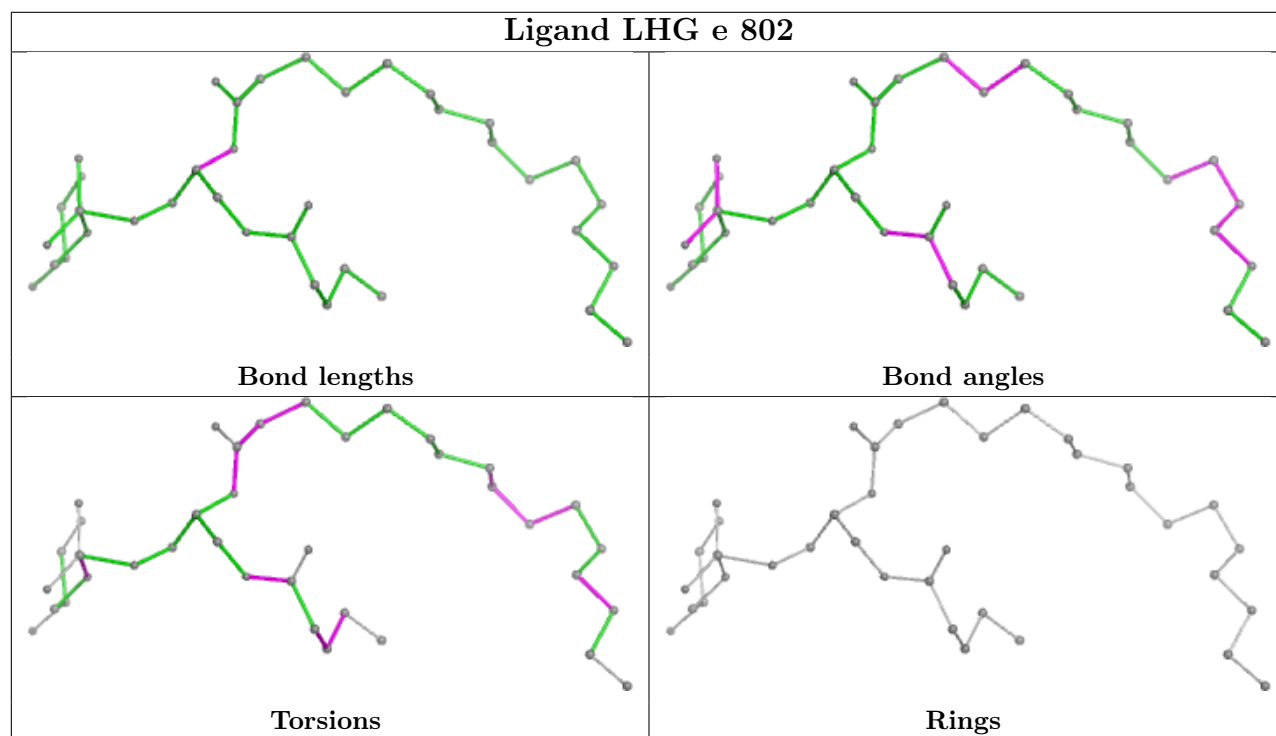
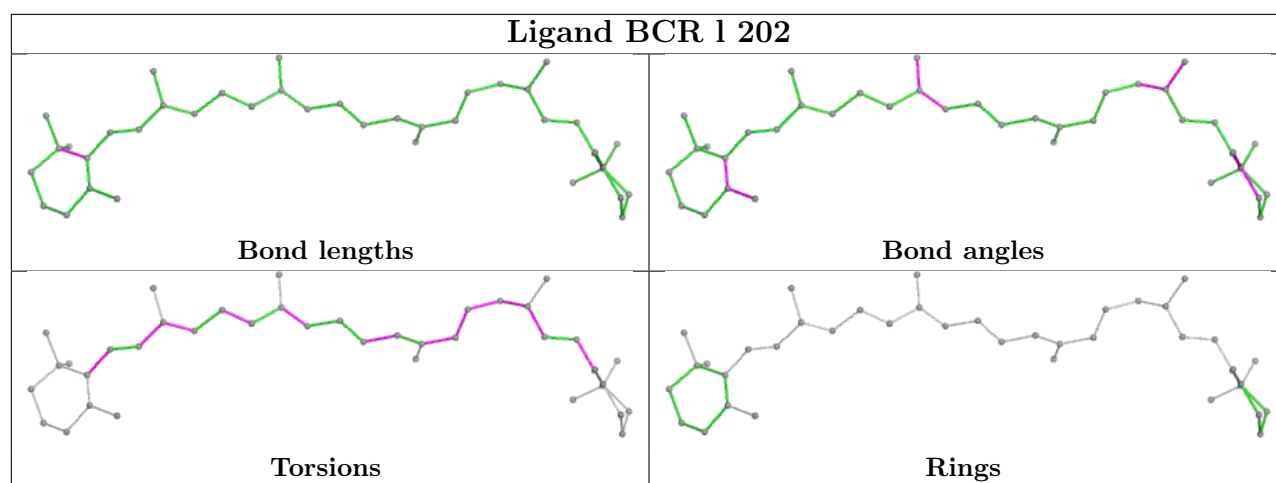


Ligand CLA G 835

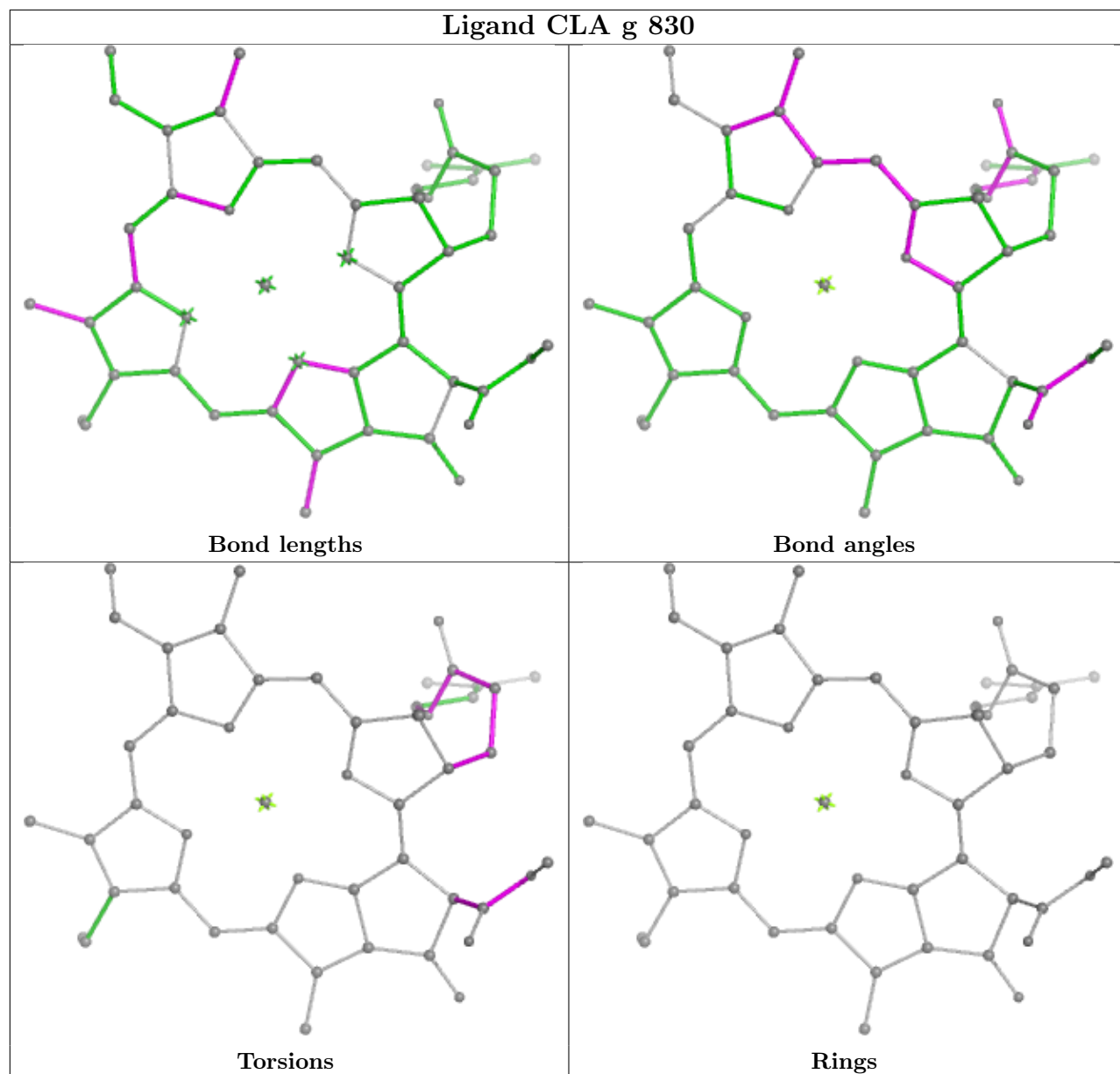


Ligand BCR S 201

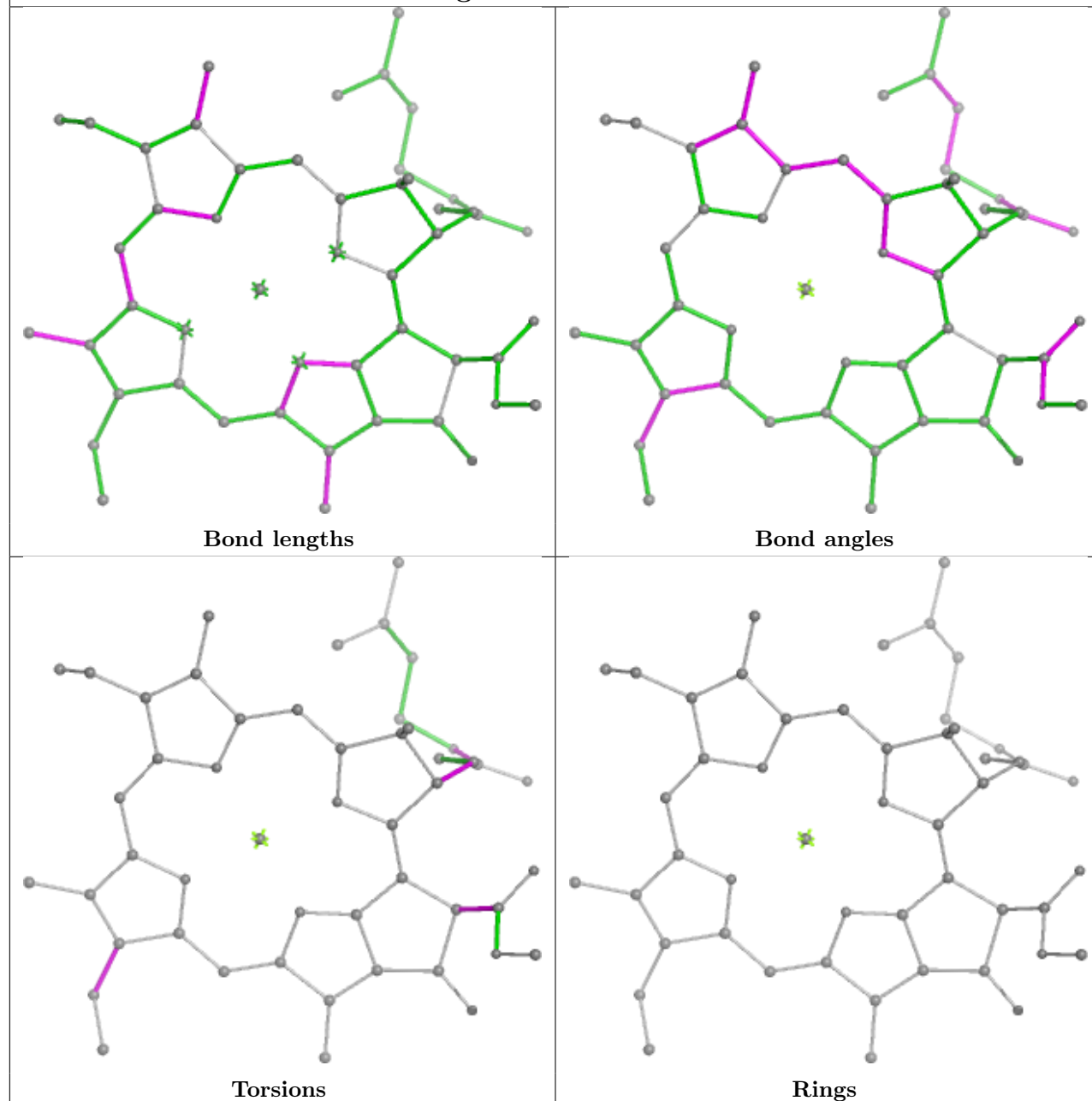




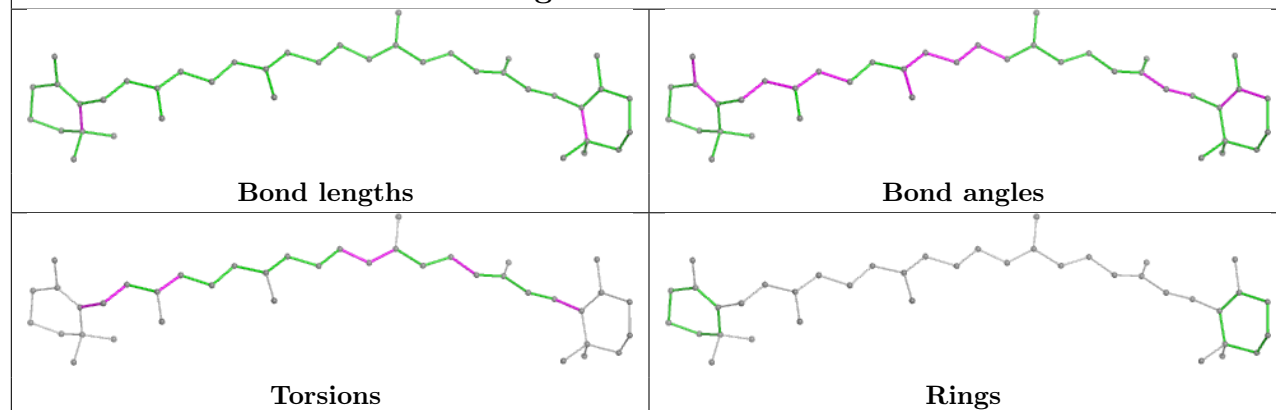
Ligand CLA g 830



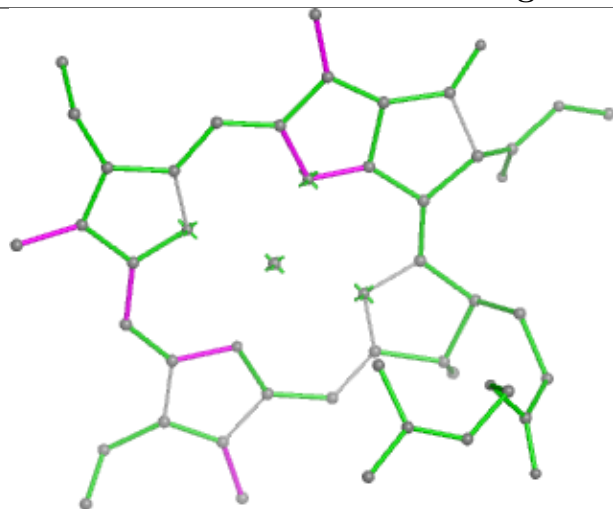
Ligand CLA E 831



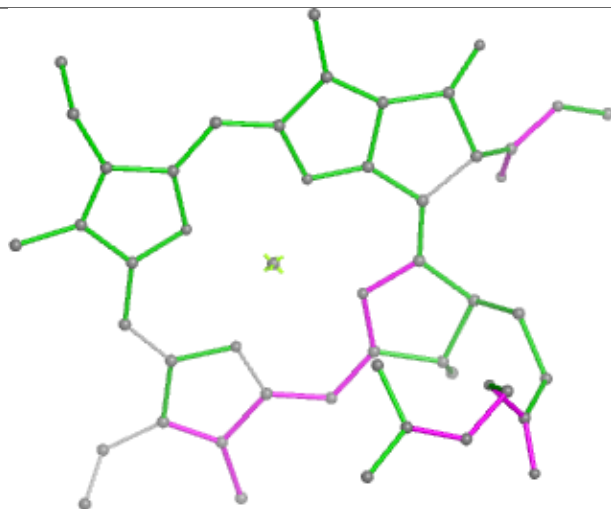
Ligand BCR a 802



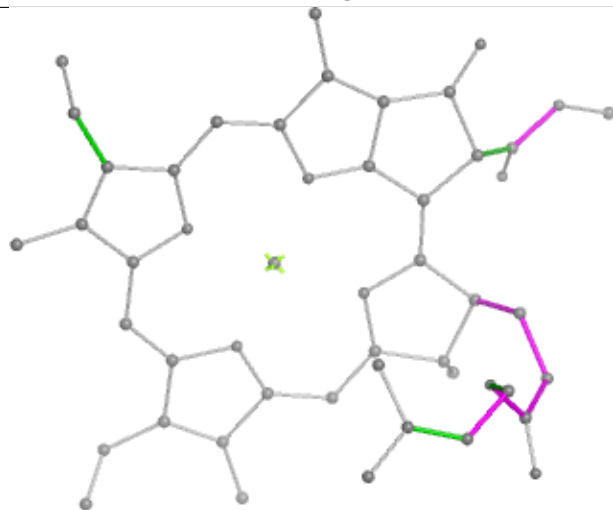
Ligand CLA b 817



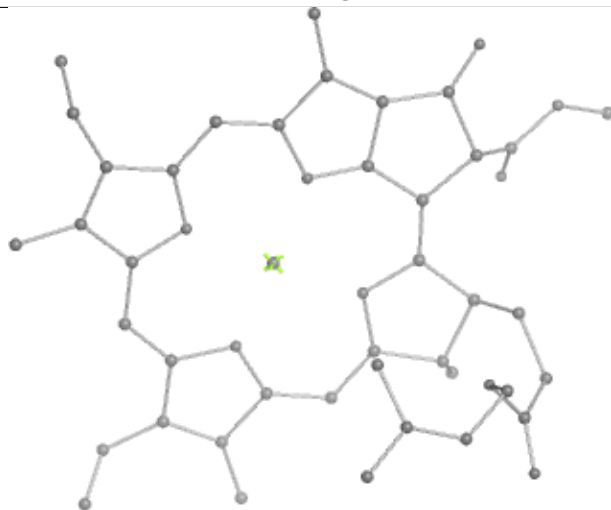
Bond lengths



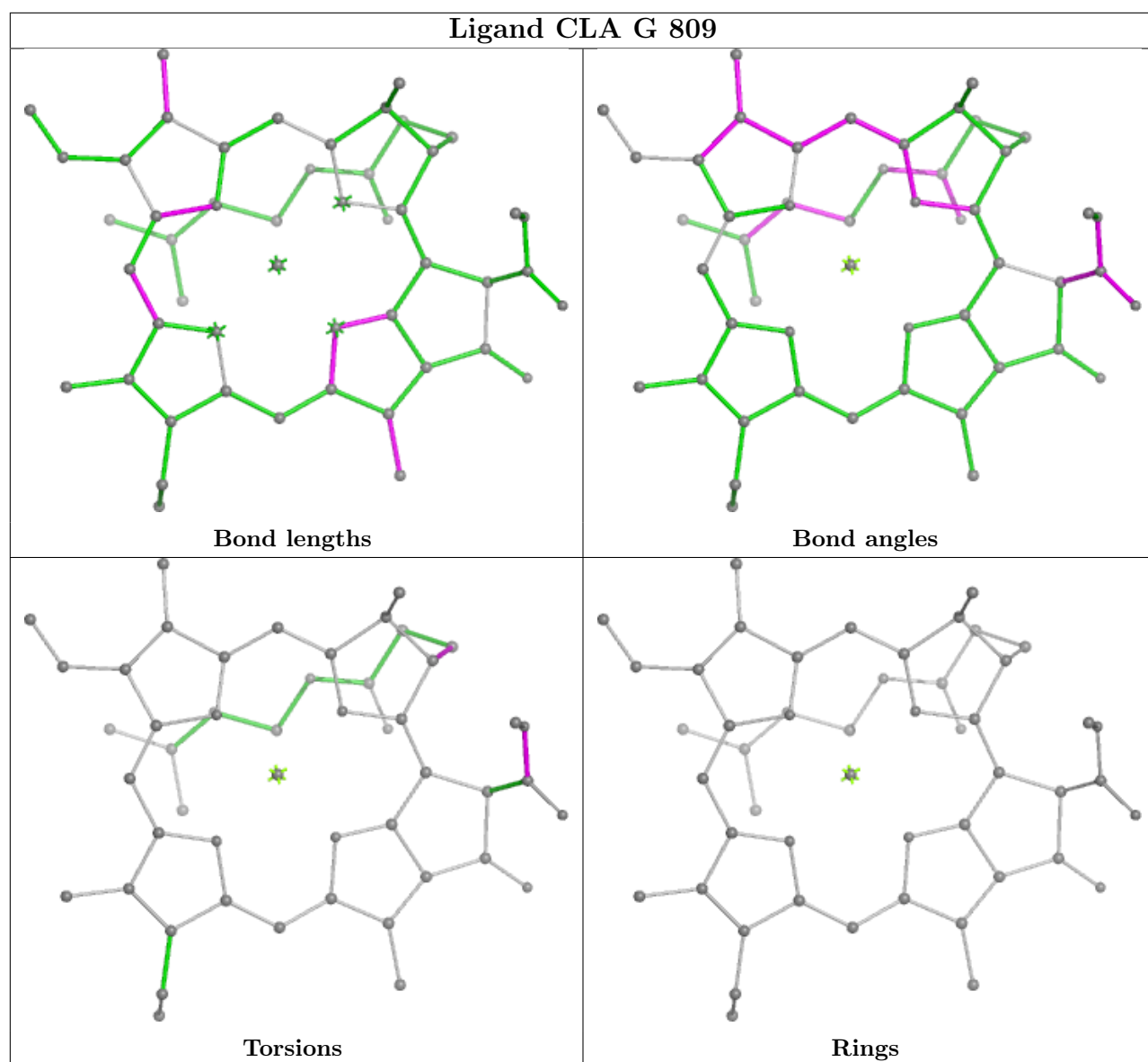
Bond angles



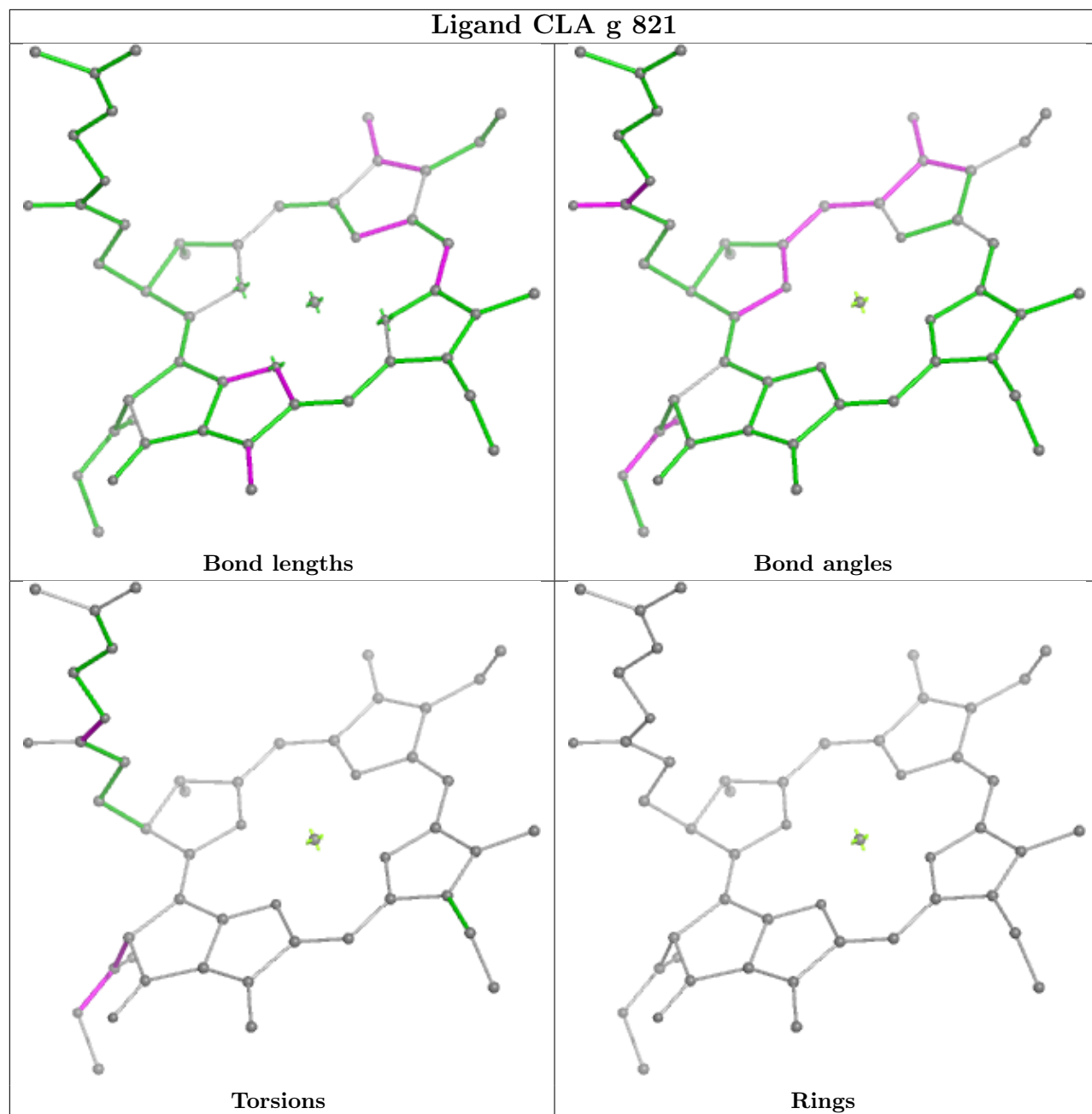
Torsions

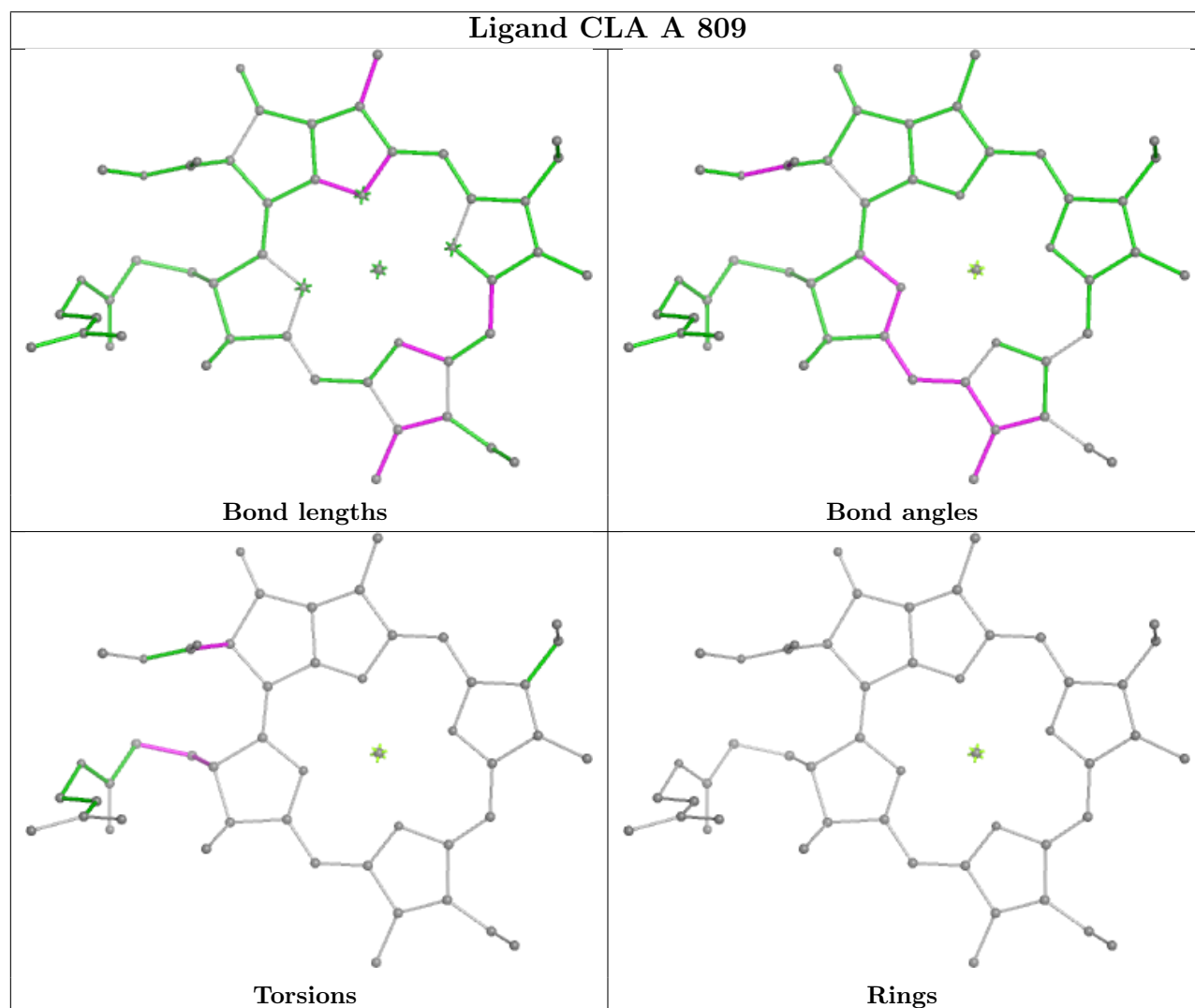
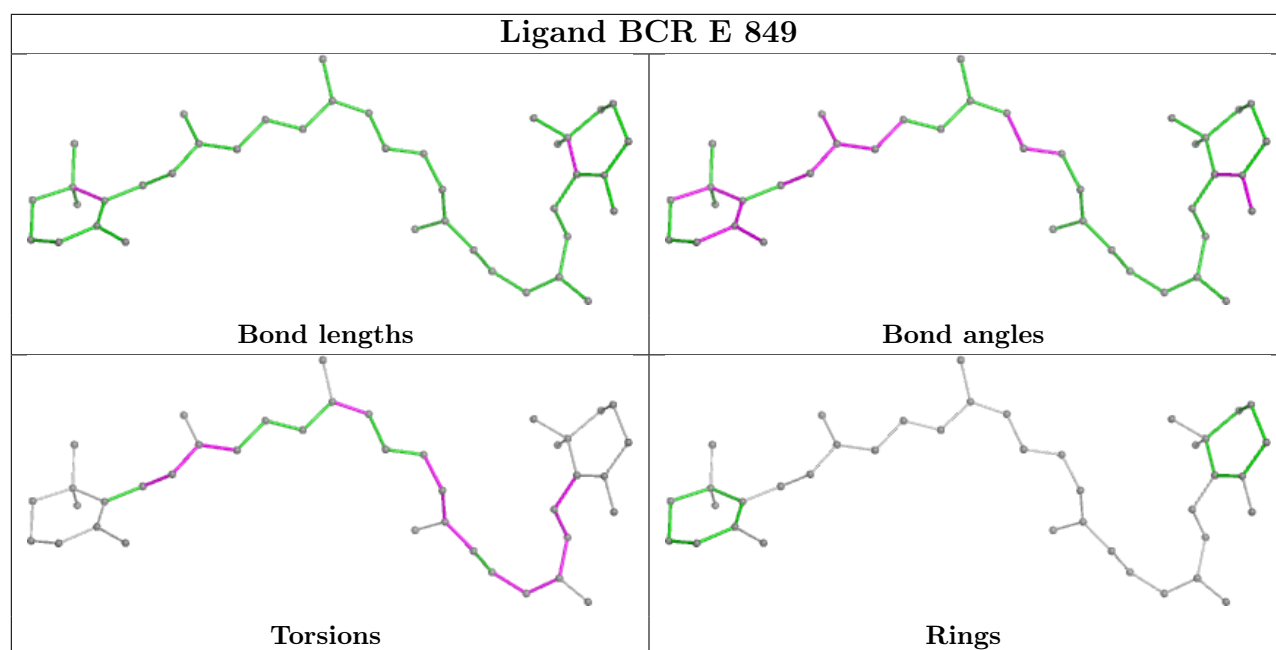


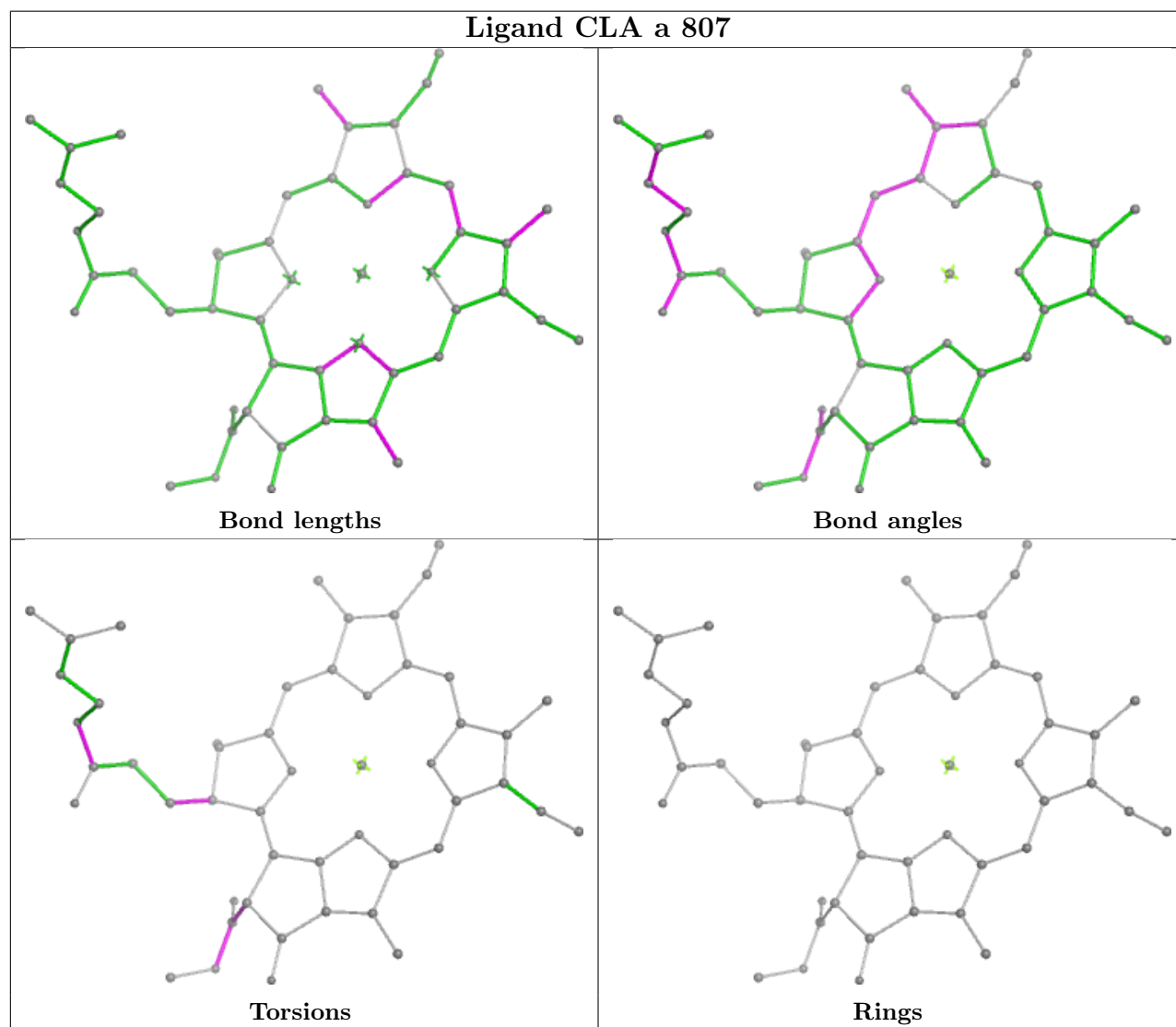
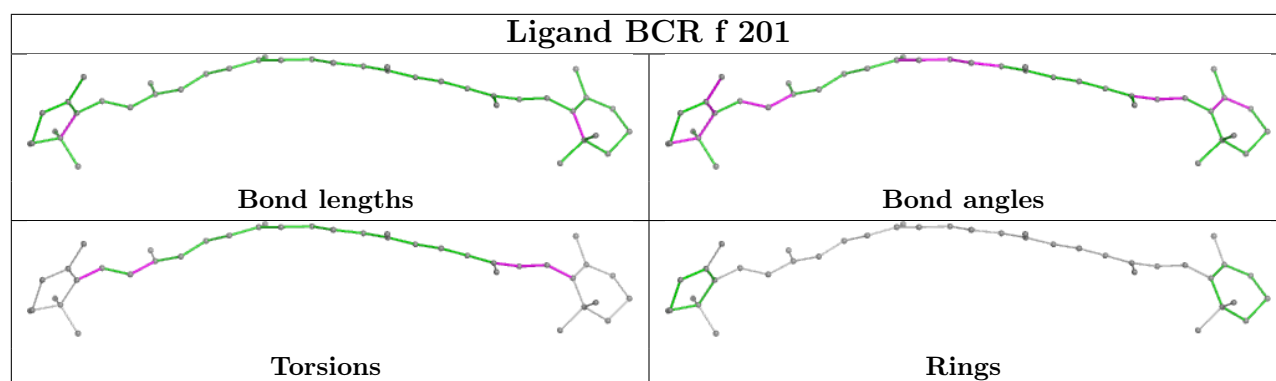
Rings



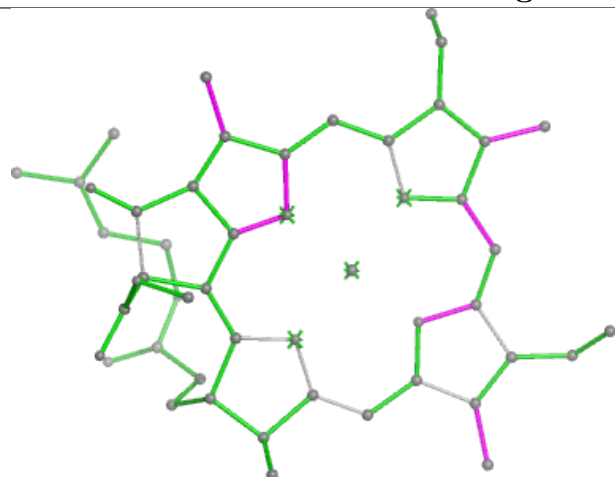
Ligand CLA g 821



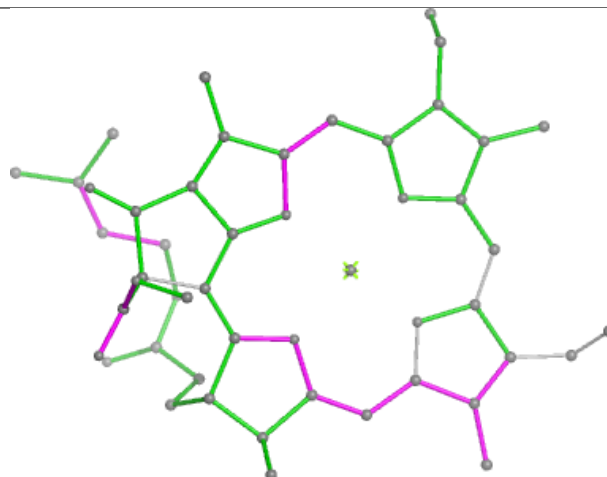




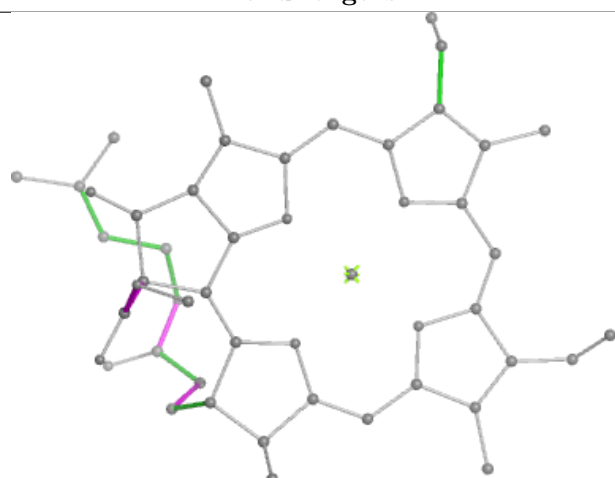
Ligand CLA A 810



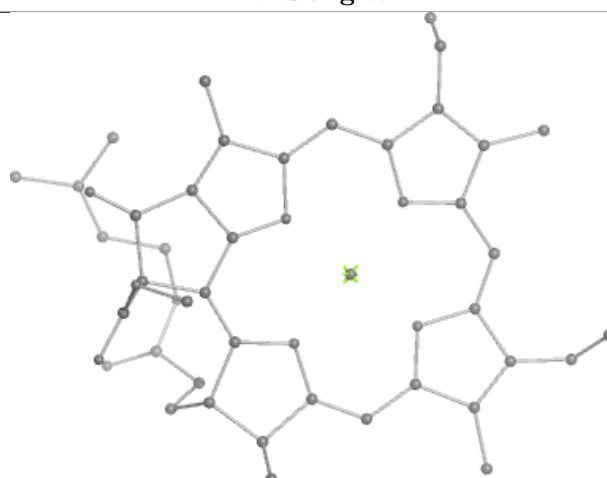
Bond lengths



Bond angles

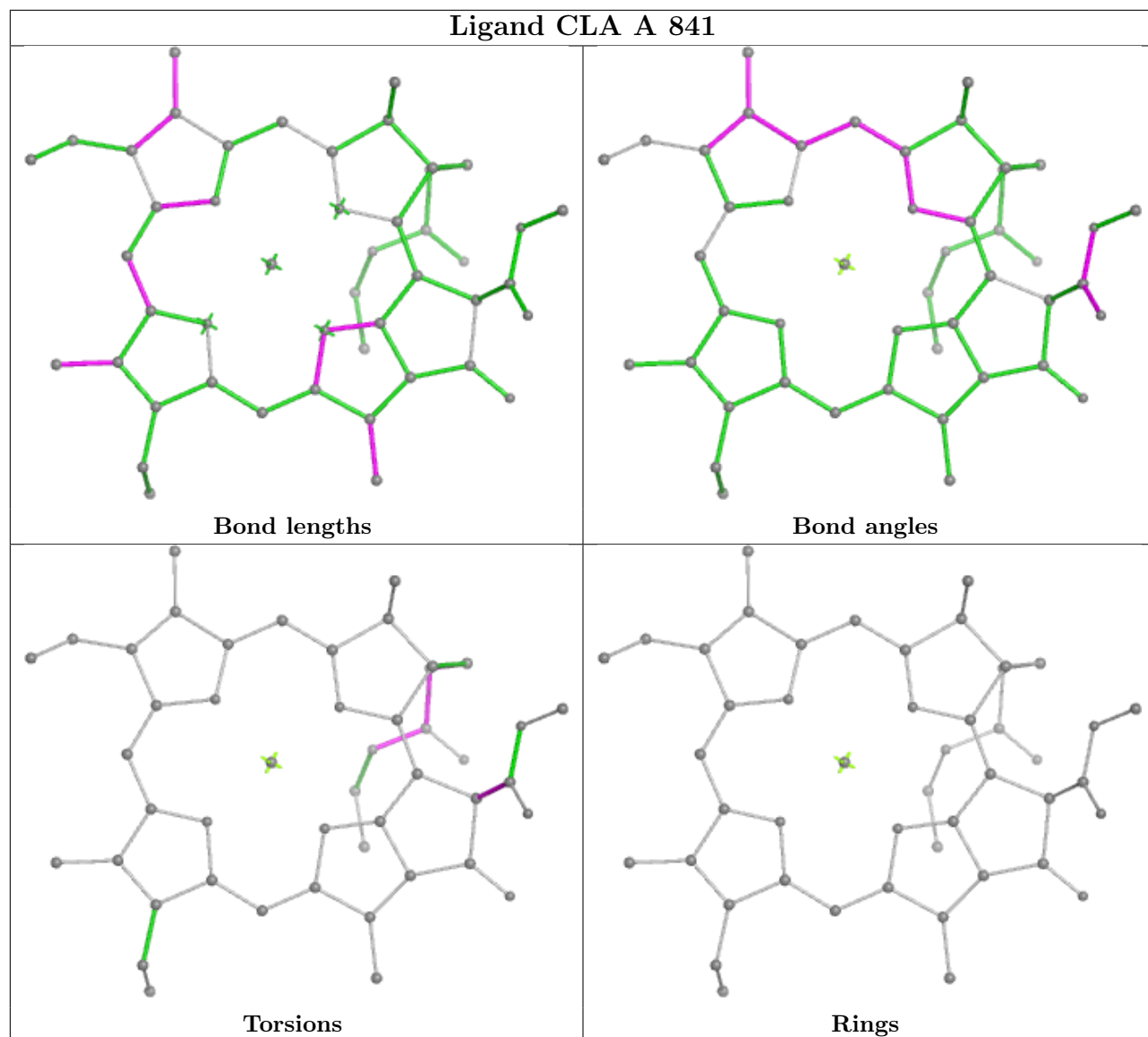


Torsions

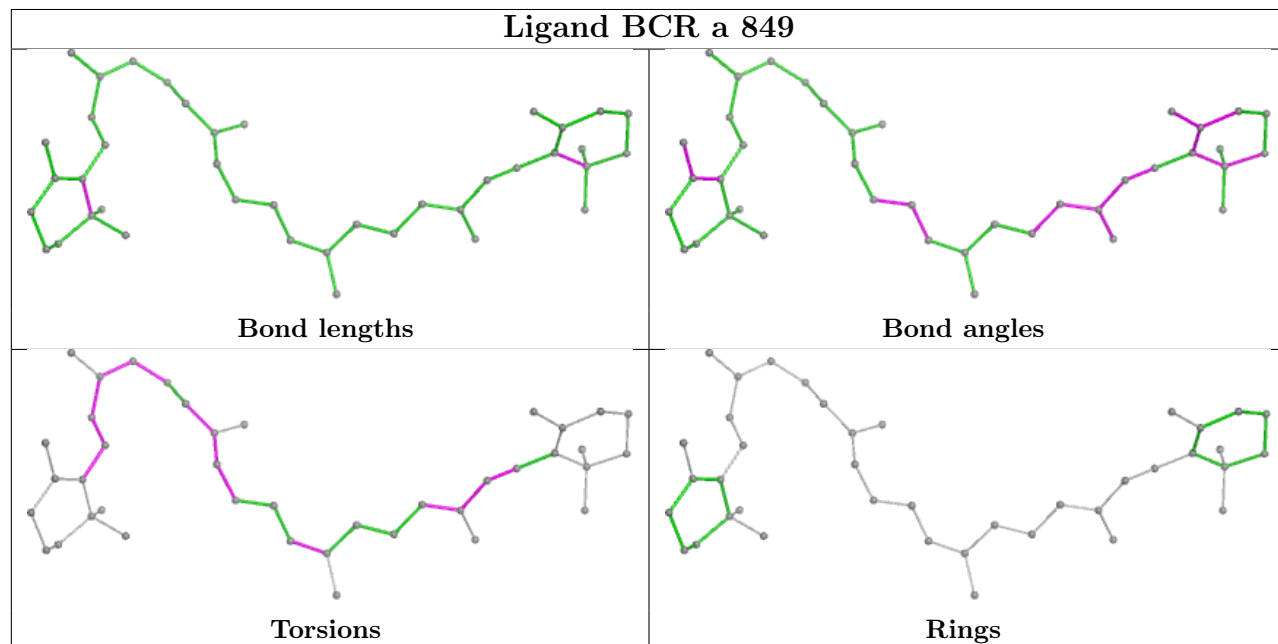


Rings

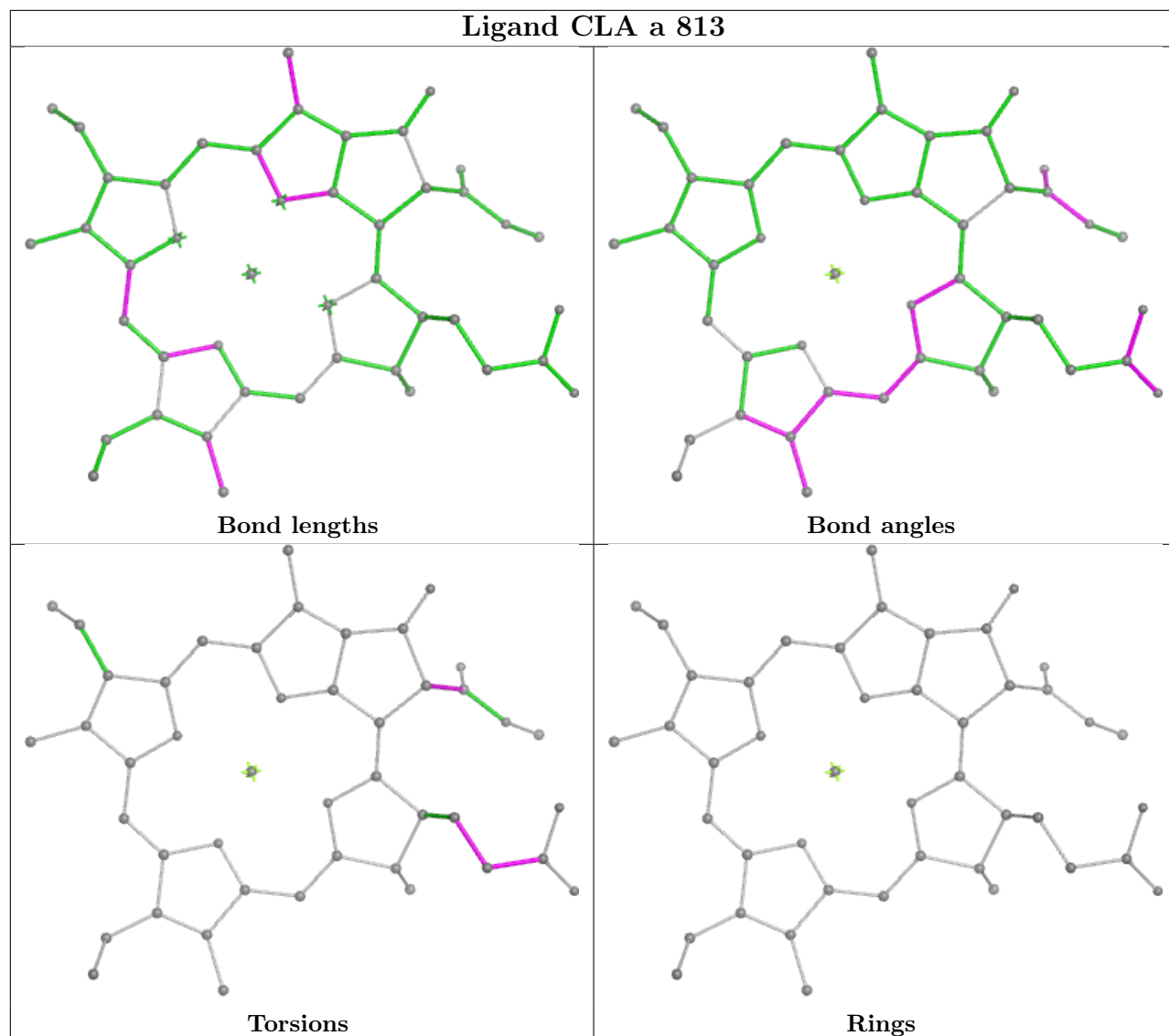
Ligand CLA A 841



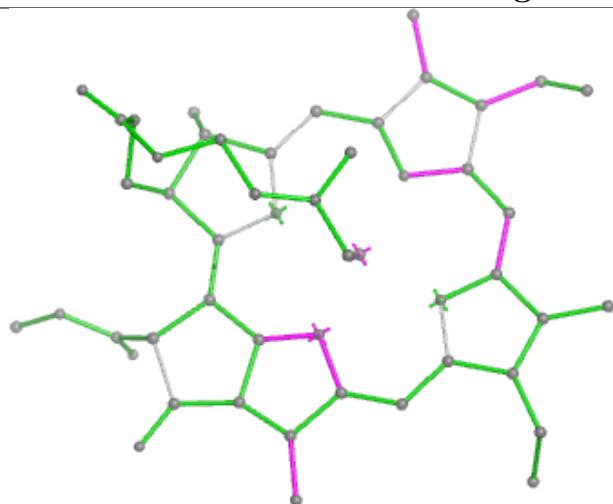
Ligand BCR a 849



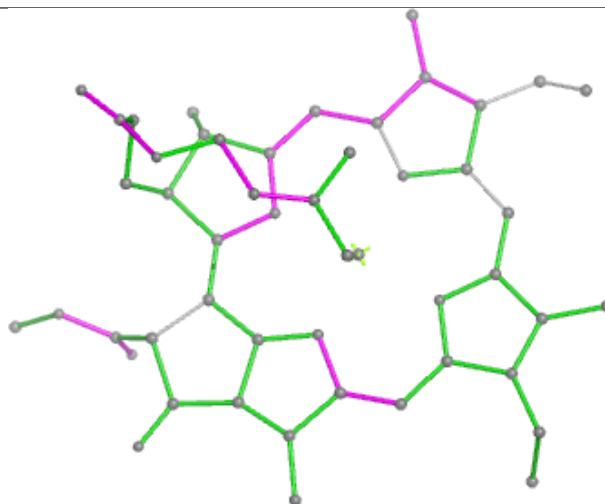
Ligand CLA a 813



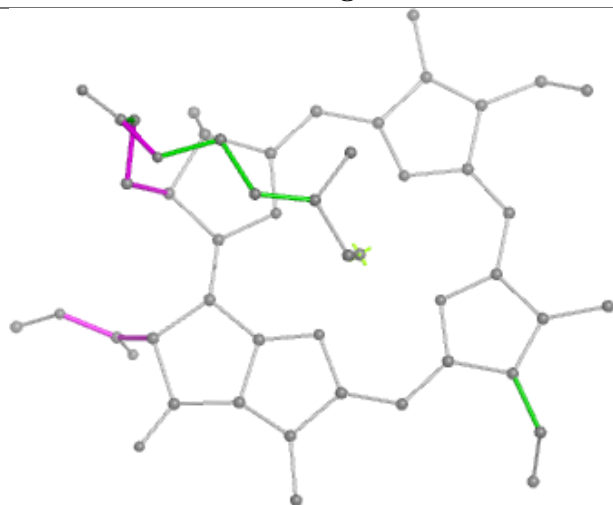
Ligand CLA A 821



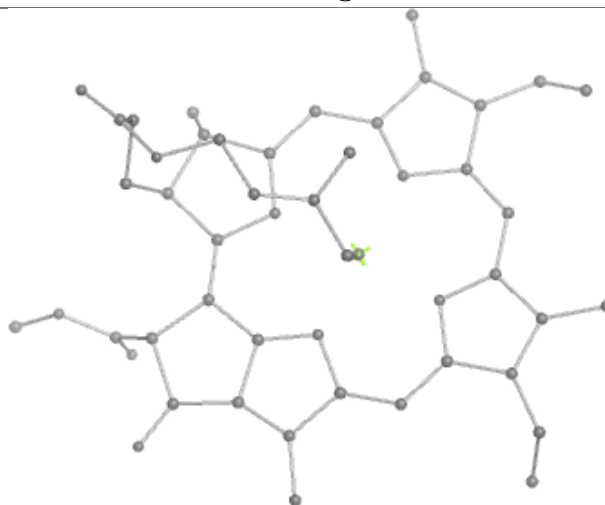
Bond lengths



Bond angles

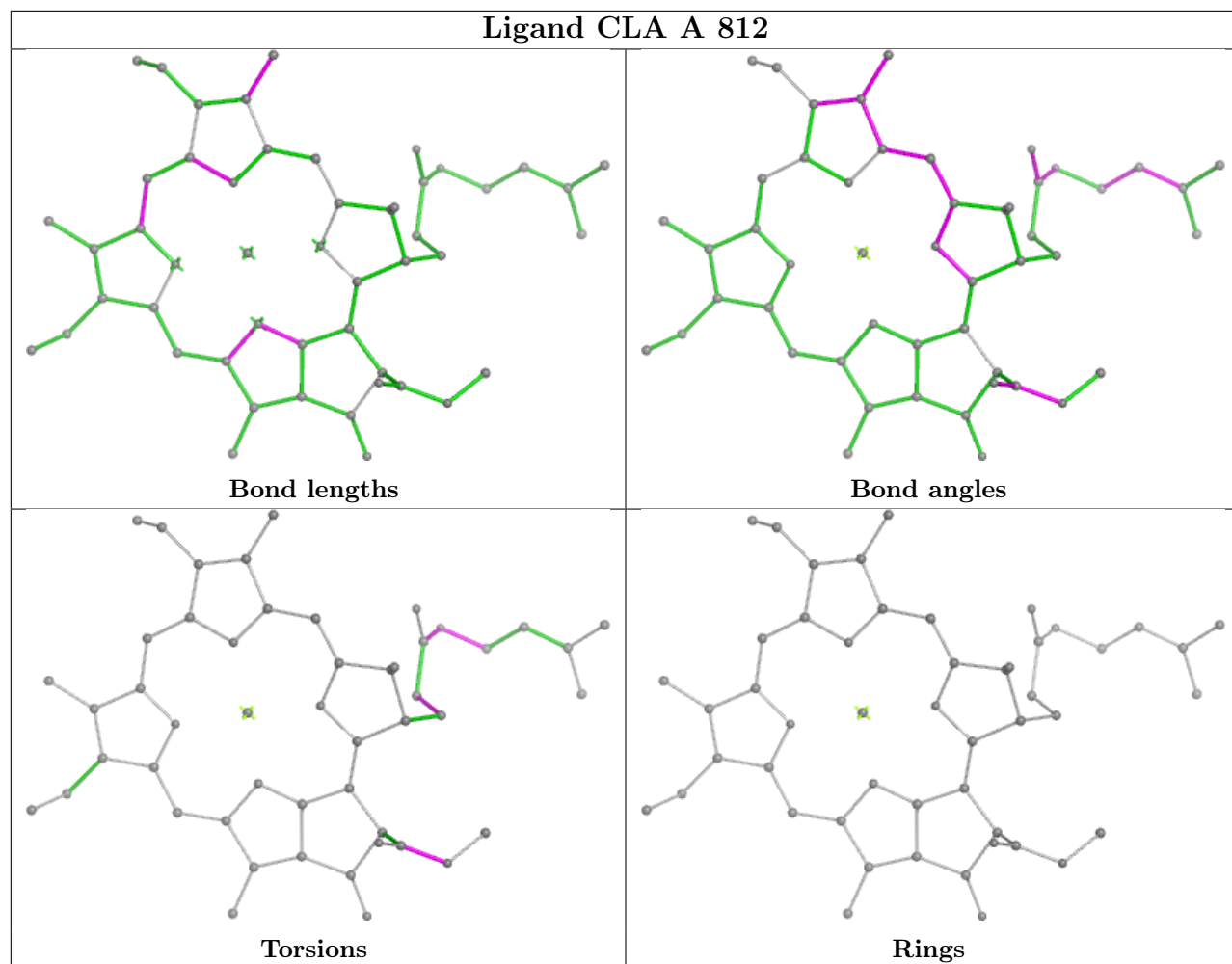


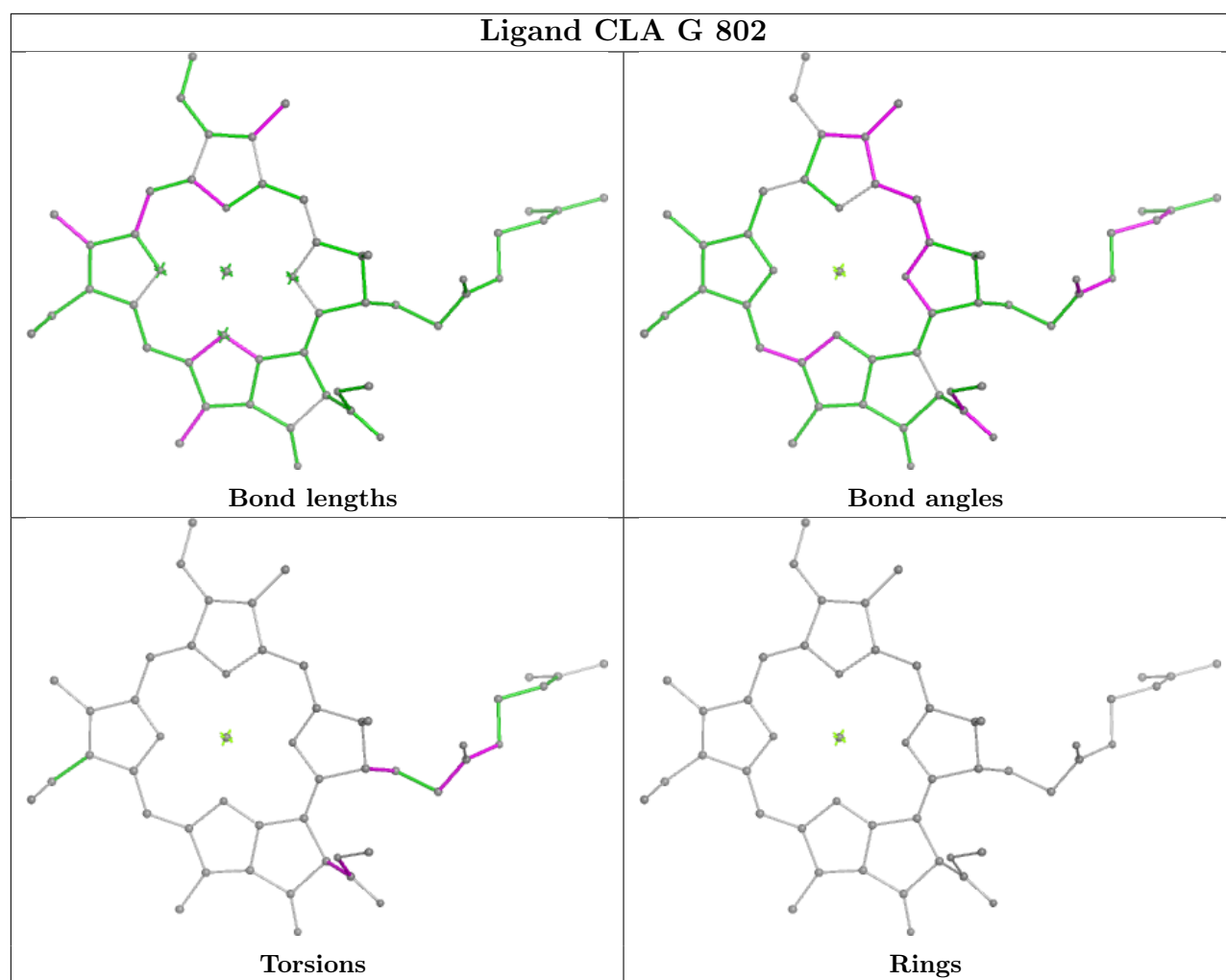
Torsions



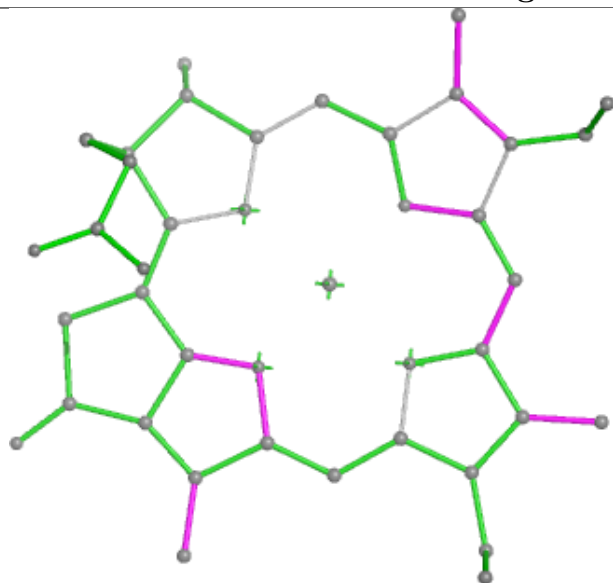
Rings

Ligand CLA A 812

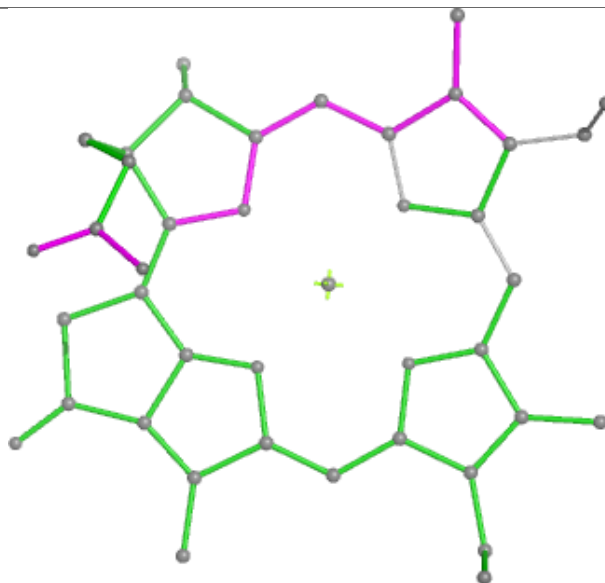




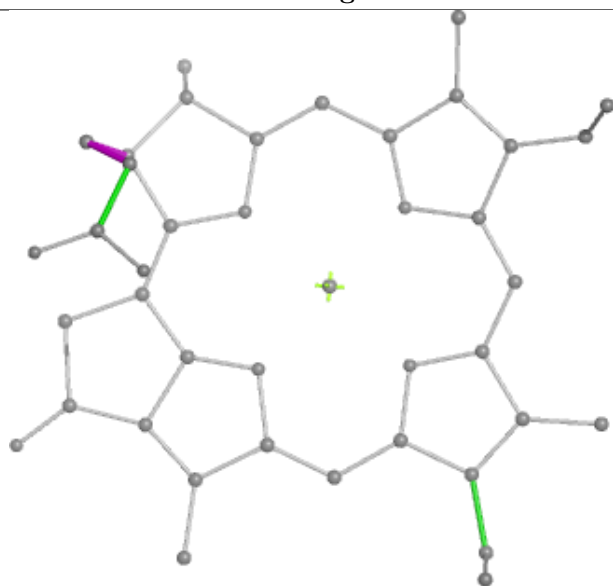
Ligand CLA b 801



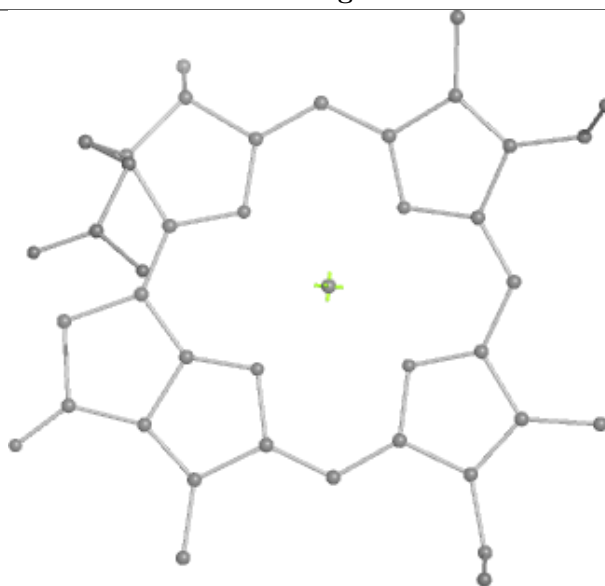
Bond lengths



Bond angles

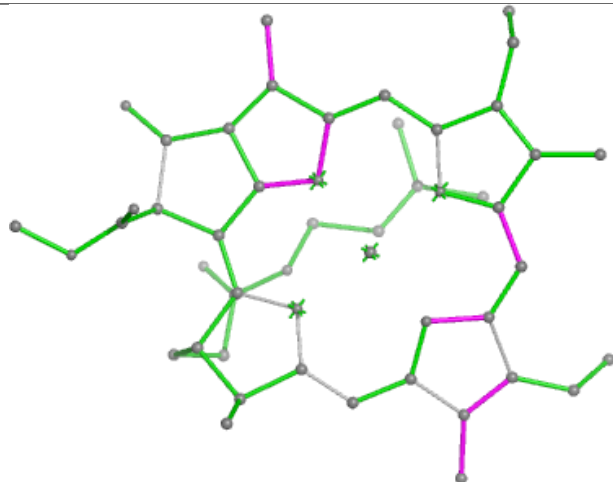


Torsions

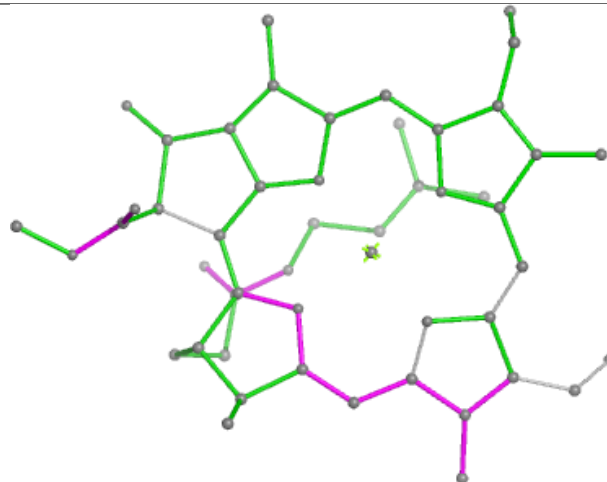


Rings

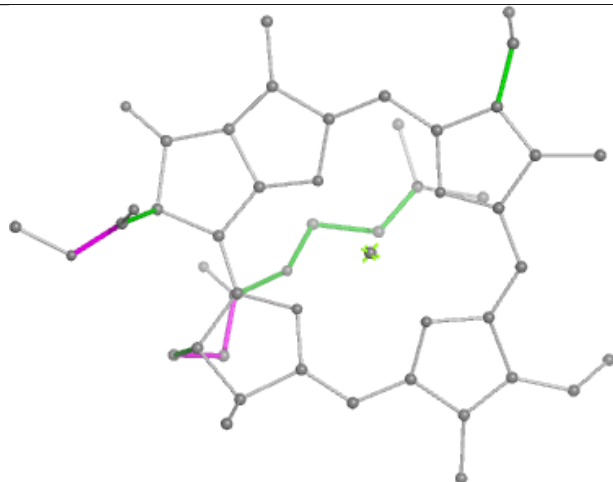
Ligand CLA G 808



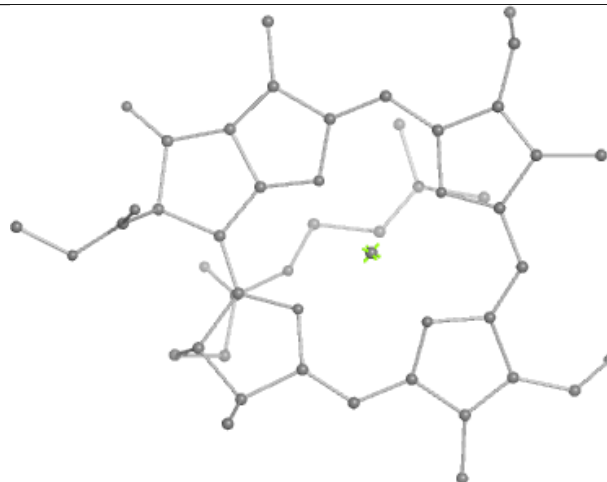
Bond lengths



Bond angles

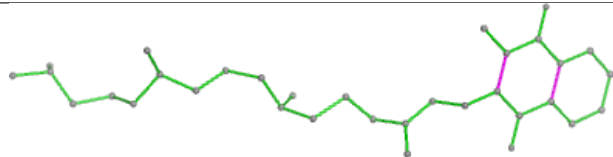


Torsions

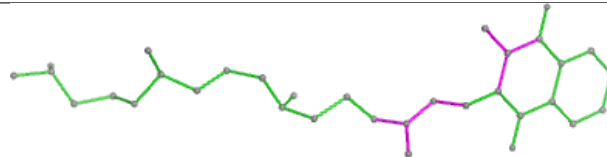


Rings

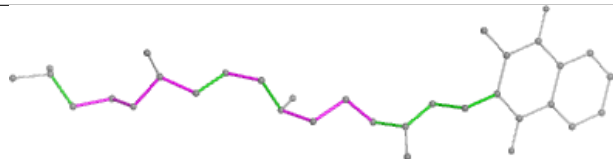
Ligand PQN B 842



Bond lengths



Bond angles

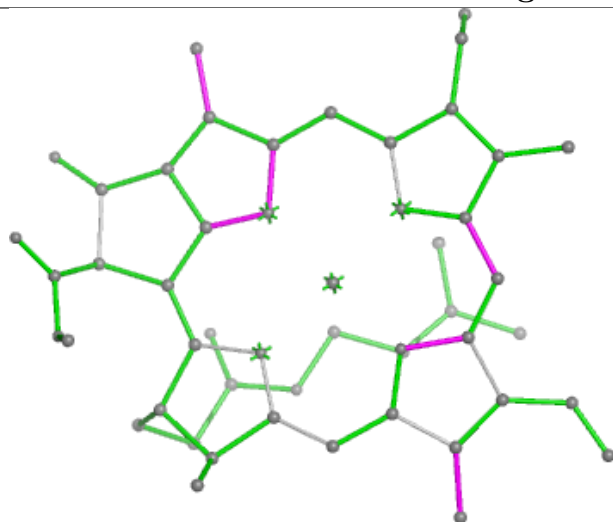


Torsions

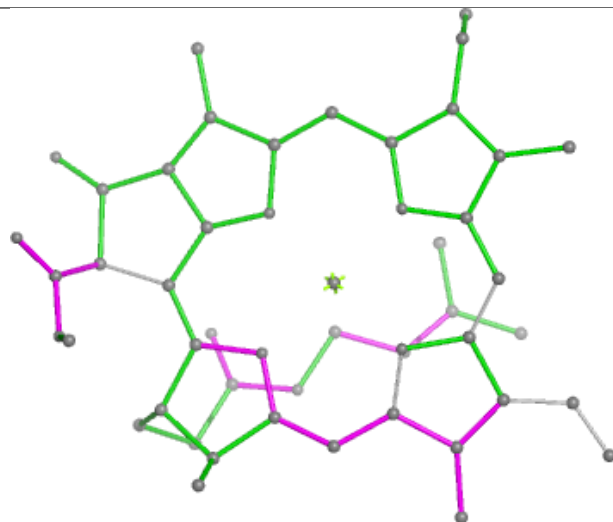


Rings

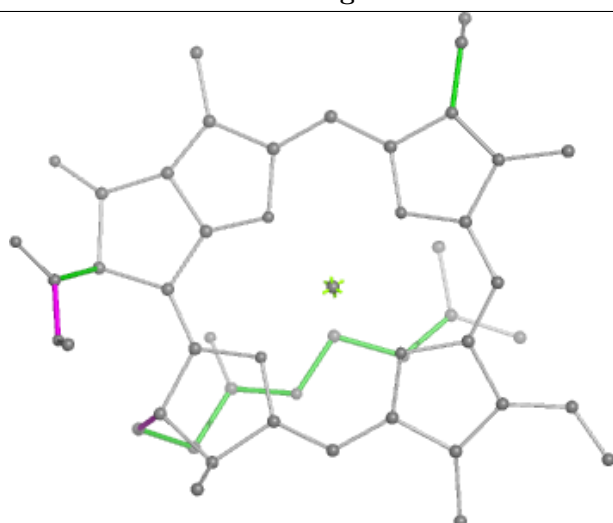
Ligand CLA b 809



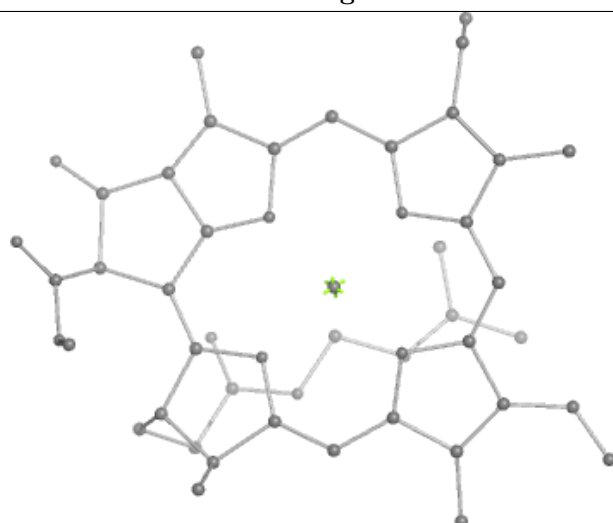
Bond lengths



Bond angles

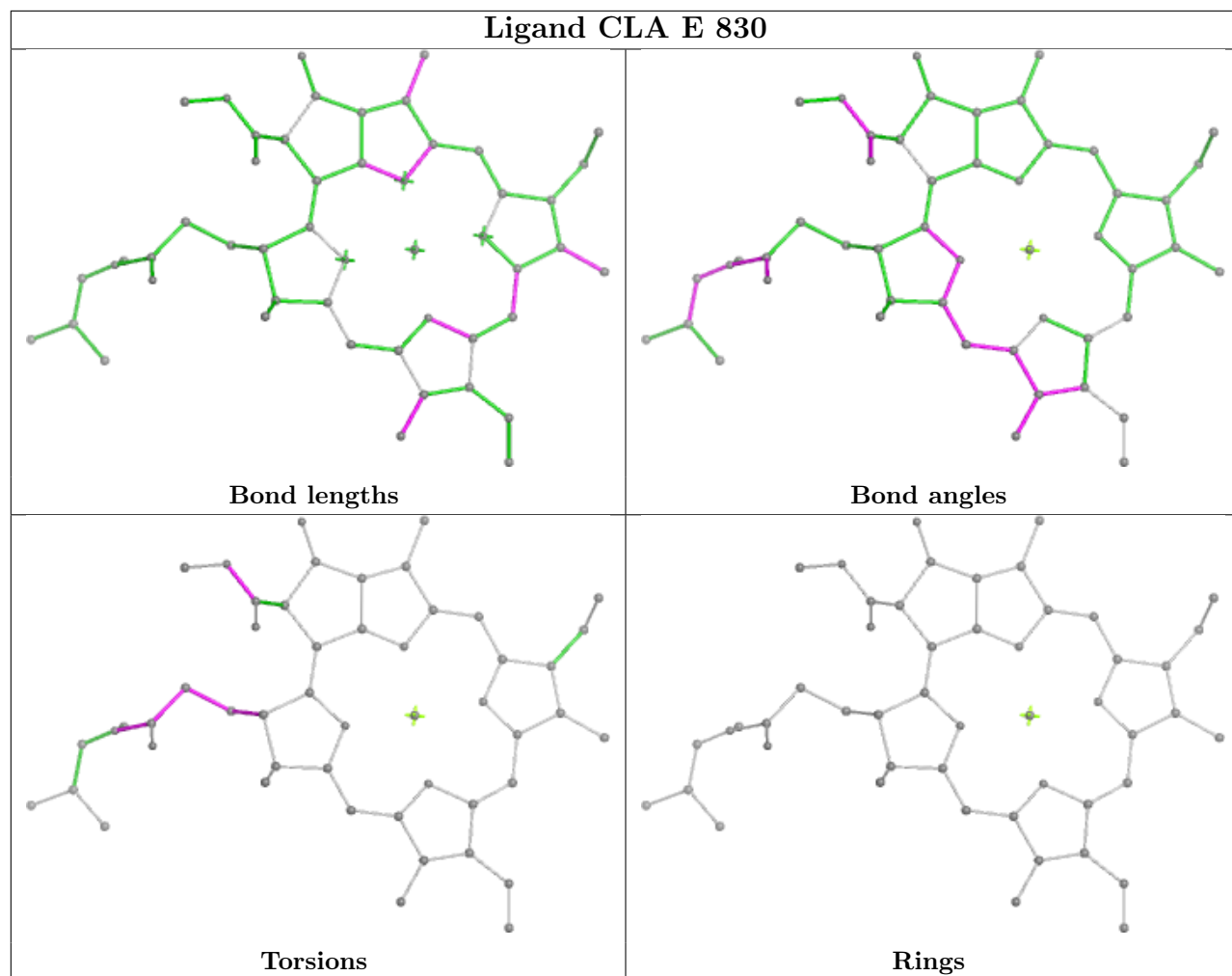


Torsions

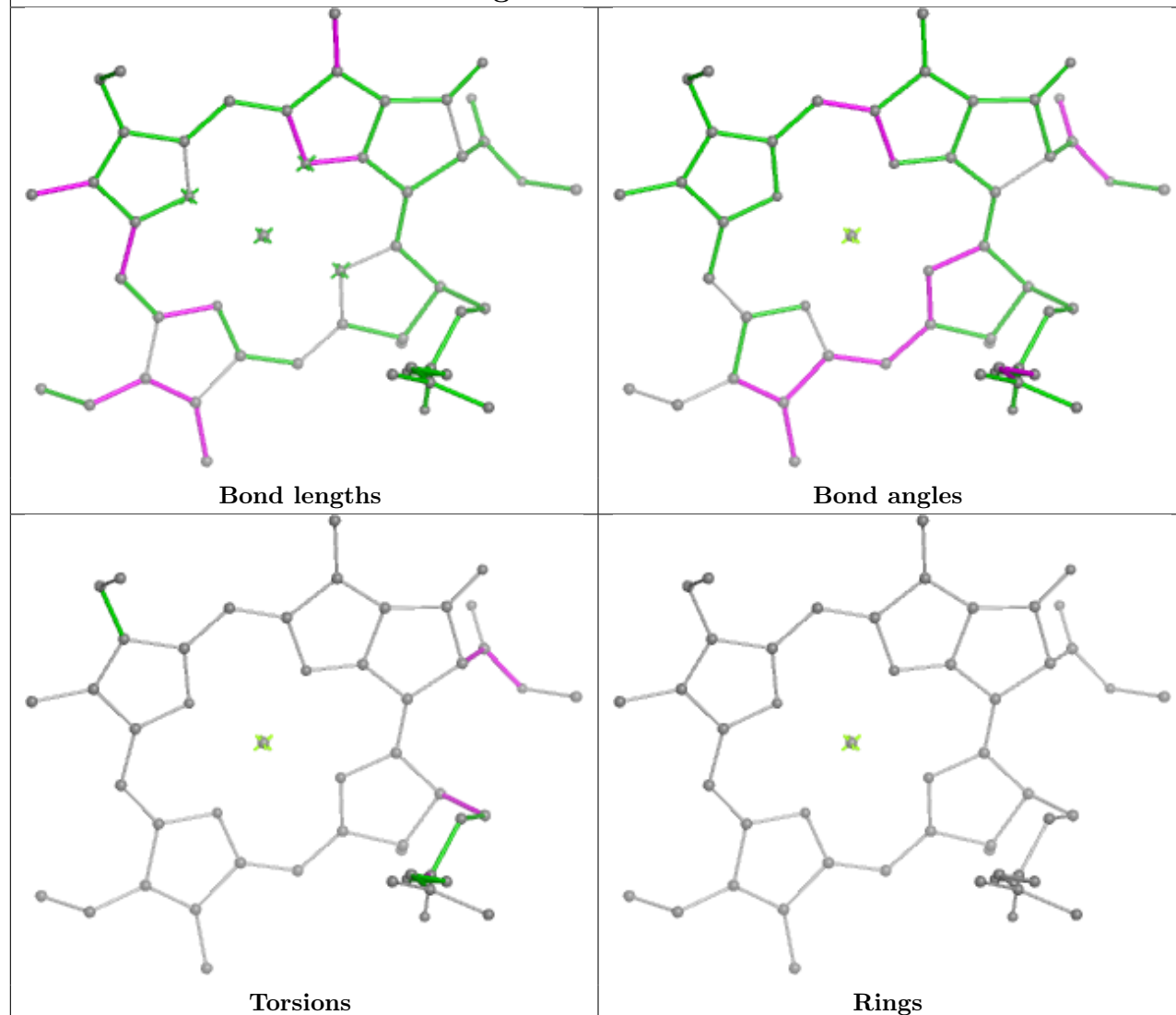


Rings

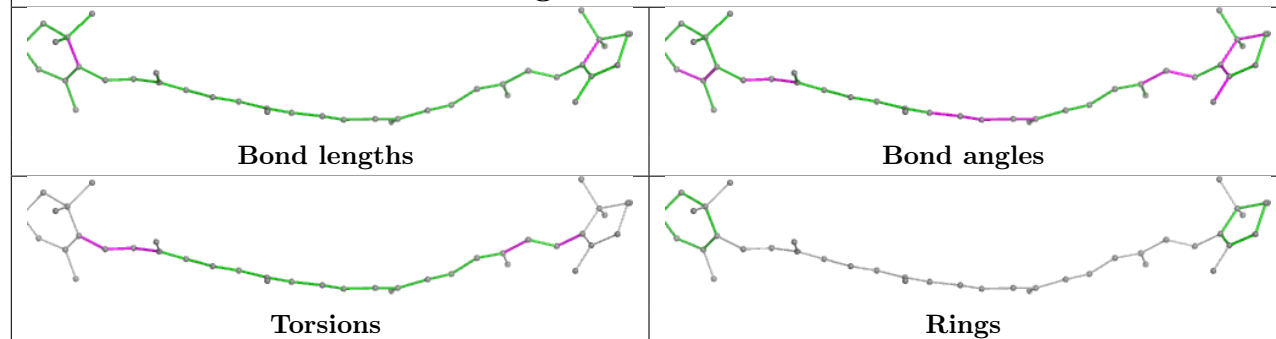
Ligand CLA E 830



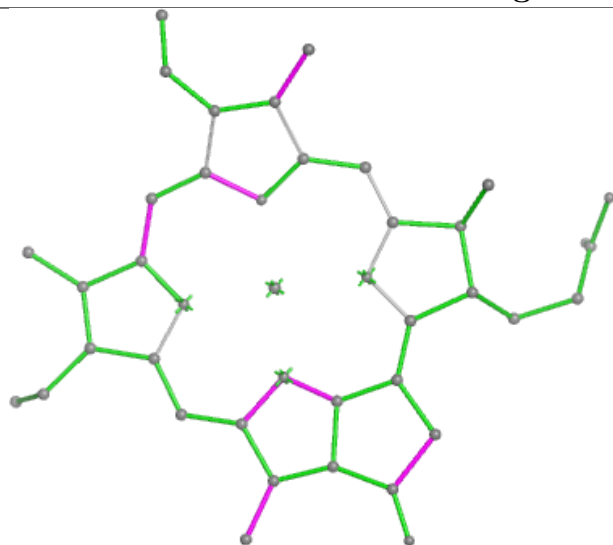
Ligand CLA b 839



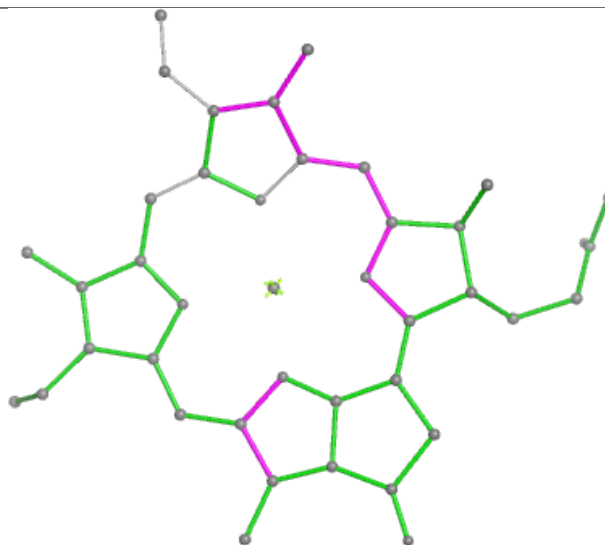
Ligand BCR o 201



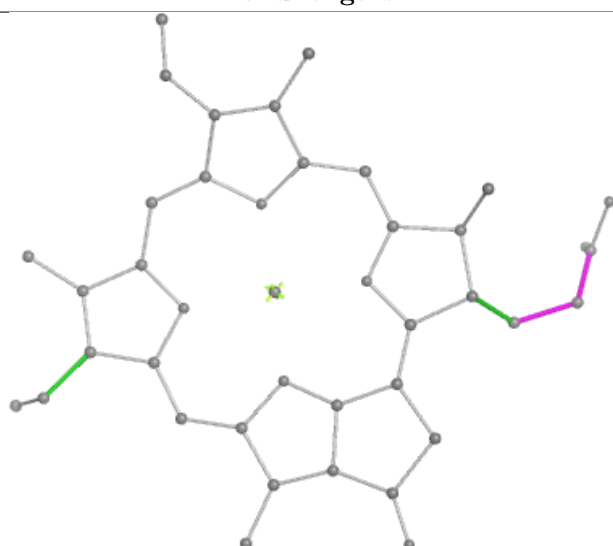
Ligand CLA K 101



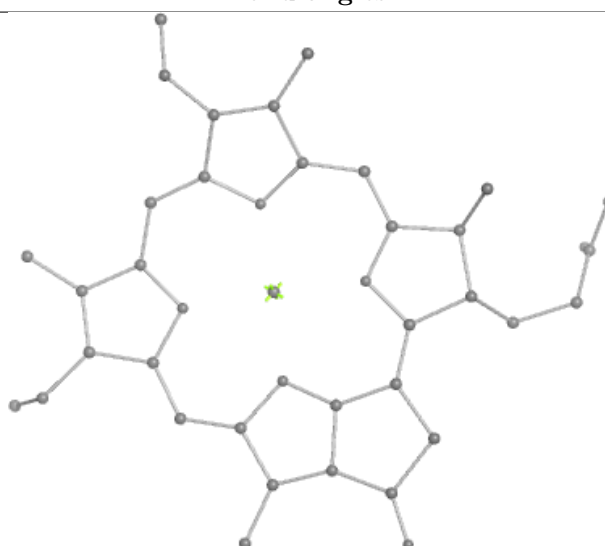
Bond lengths



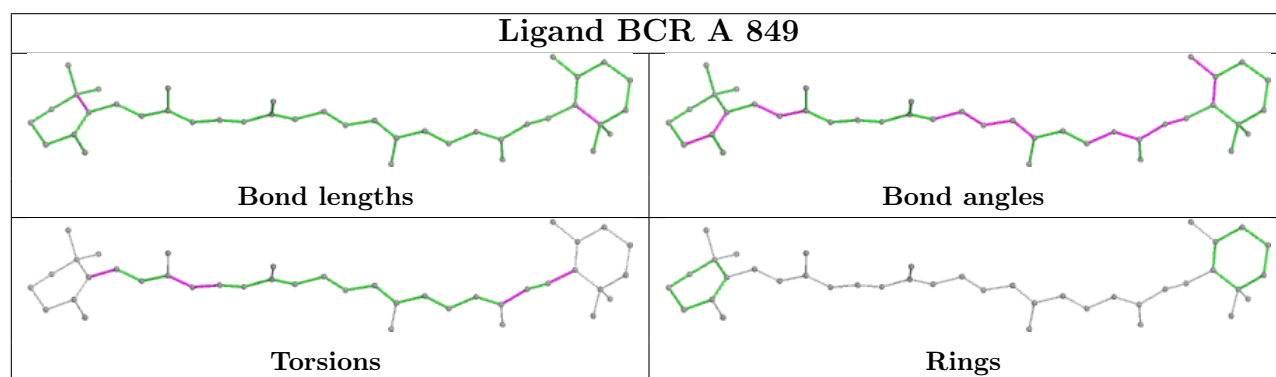
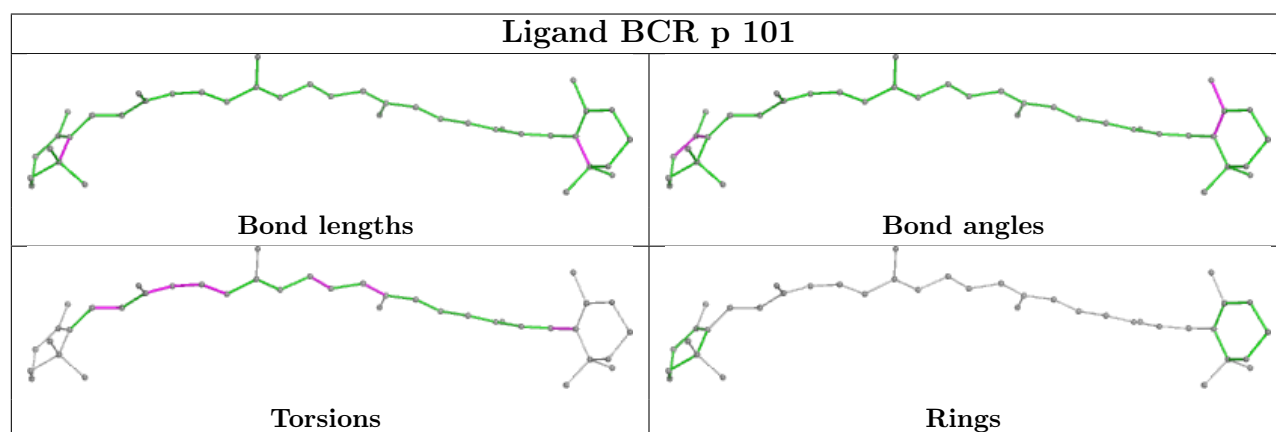
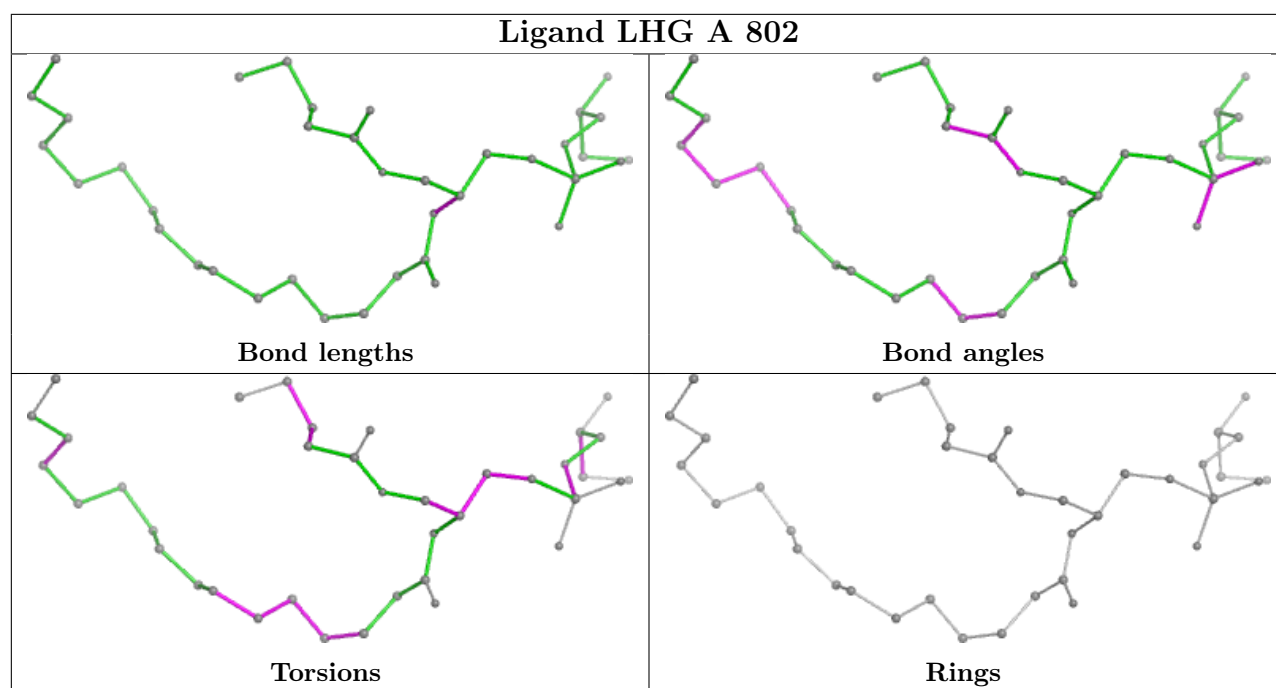
Bond angles

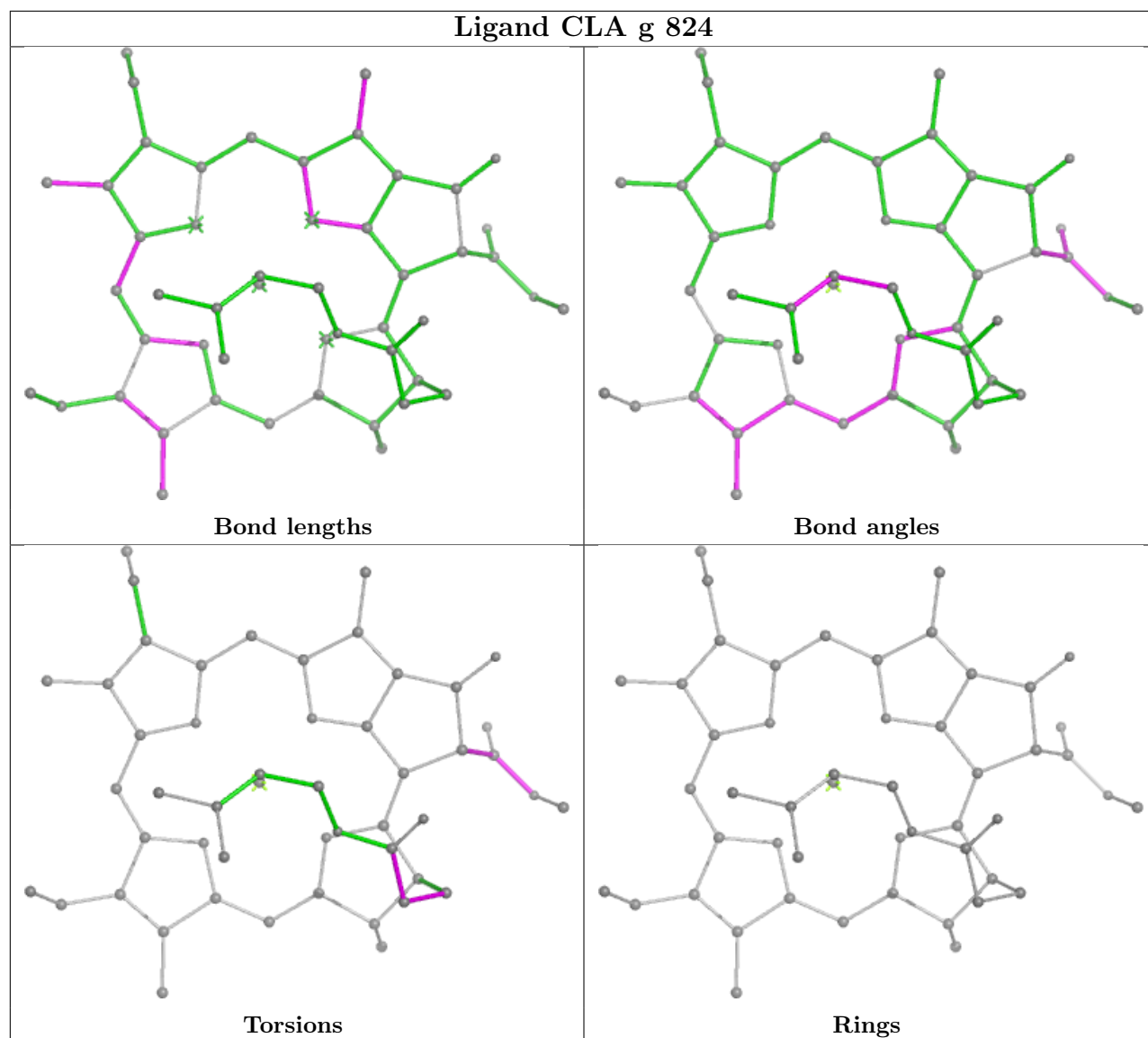
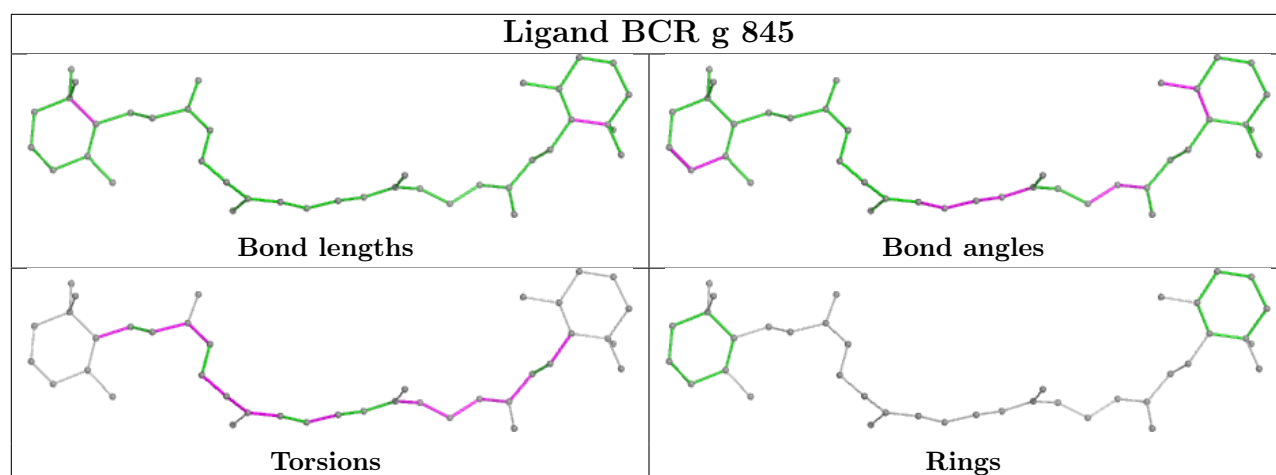


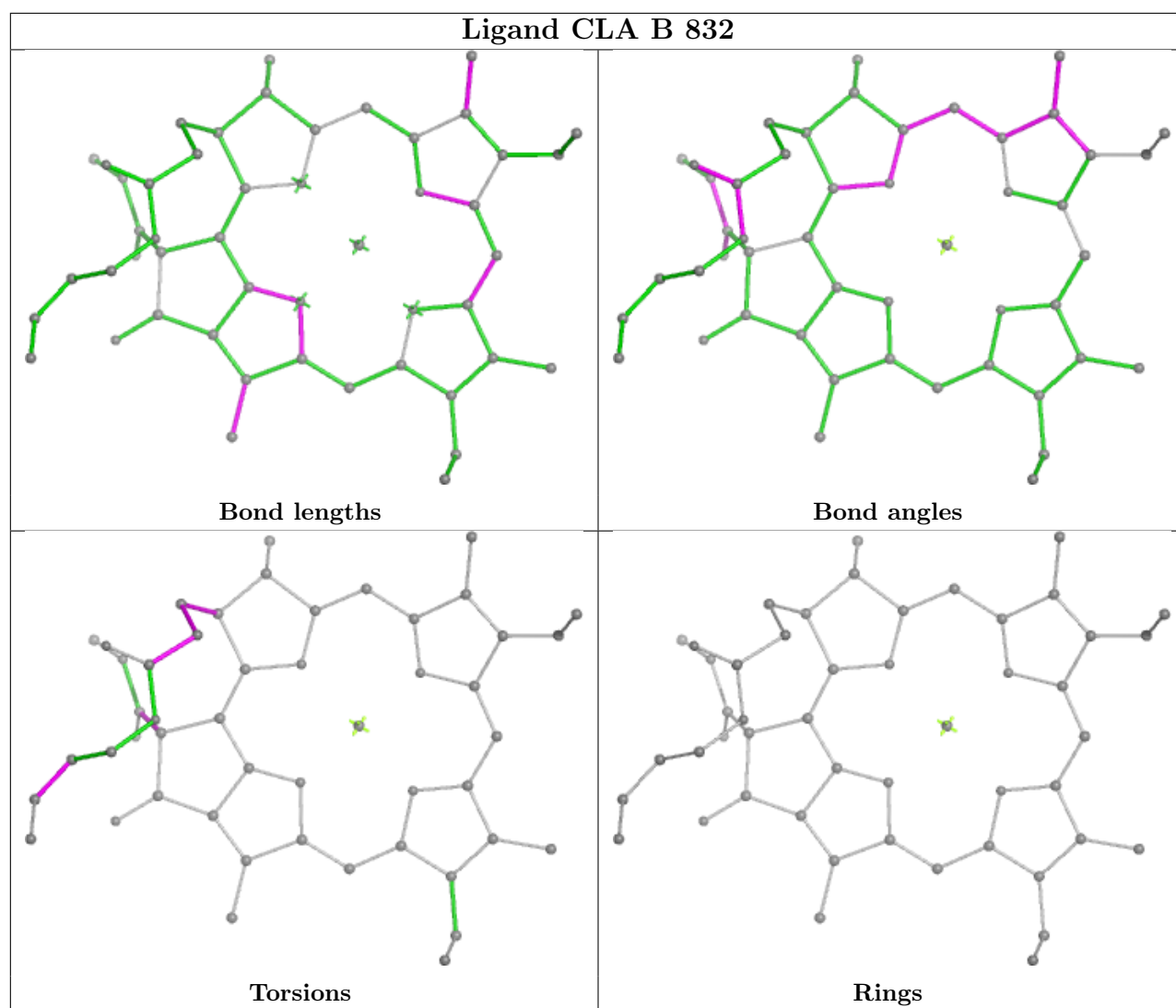
Torsions

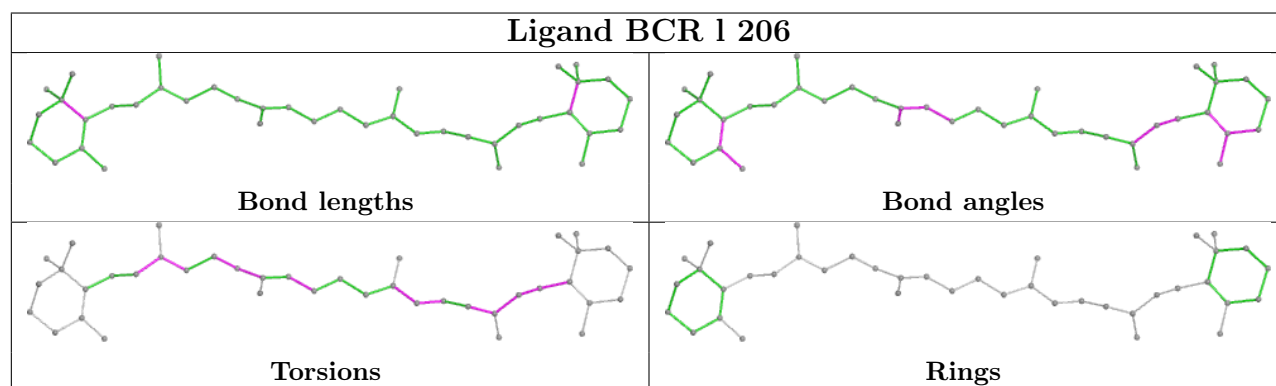
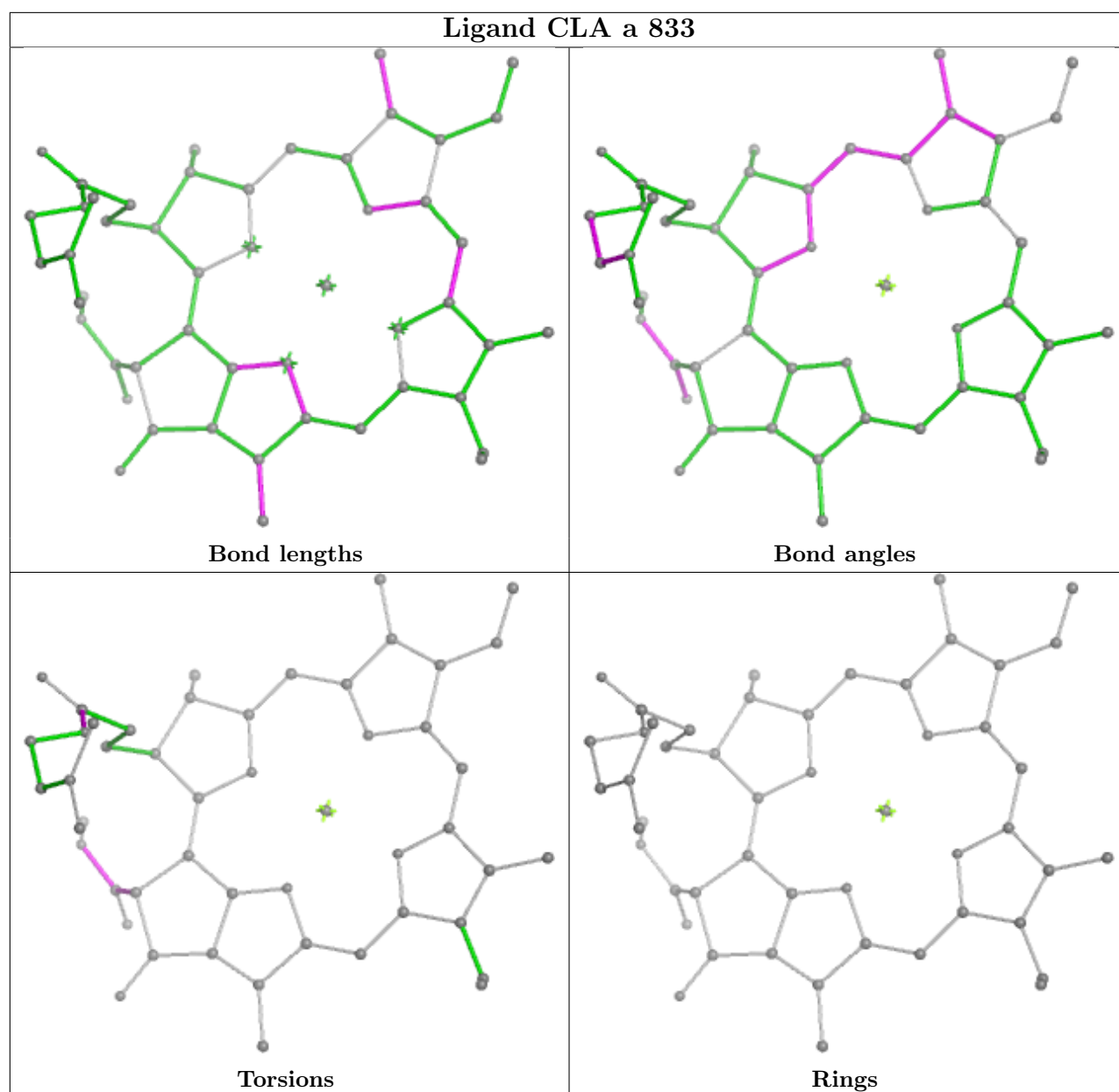


Rings

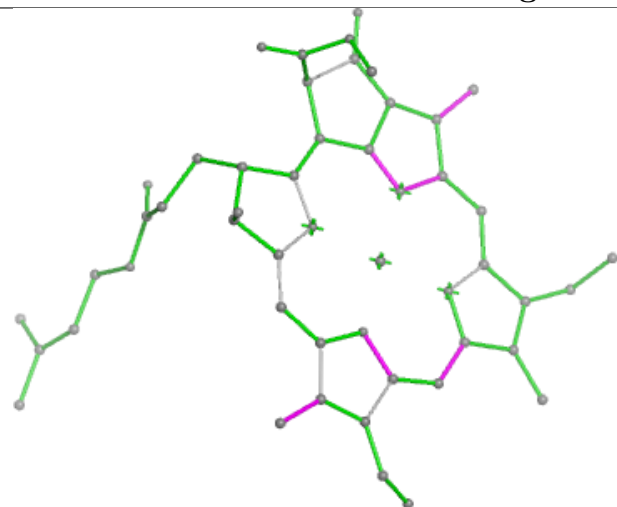




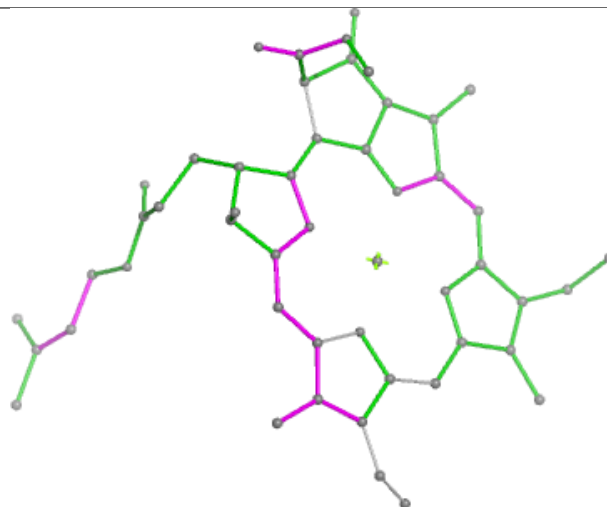




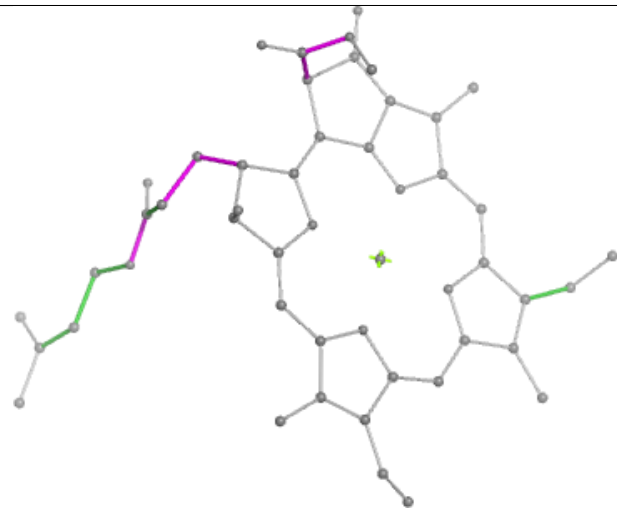
Ligand CLA E 837



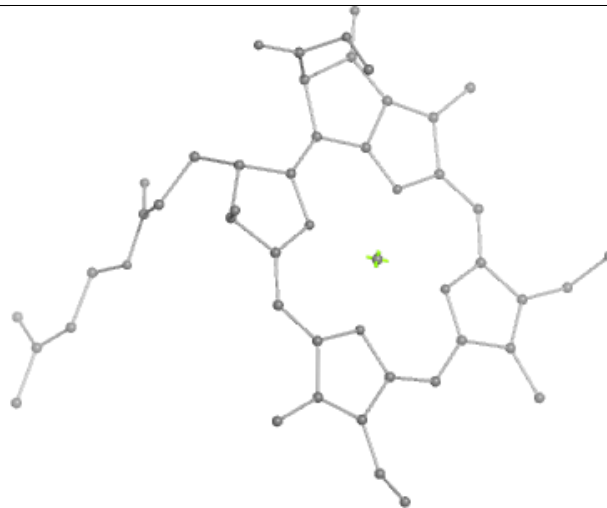
Bond lengths



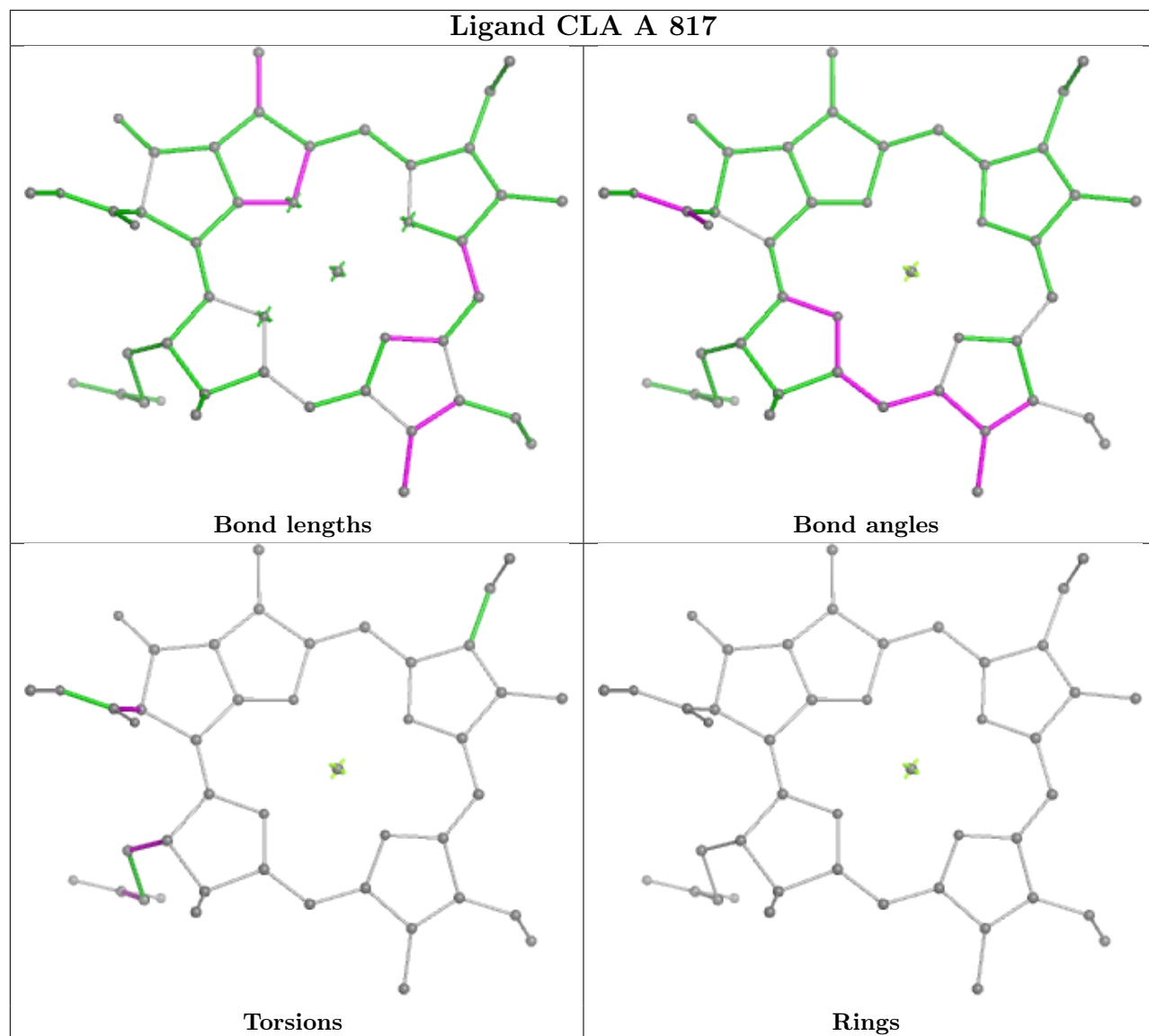
Bond angles



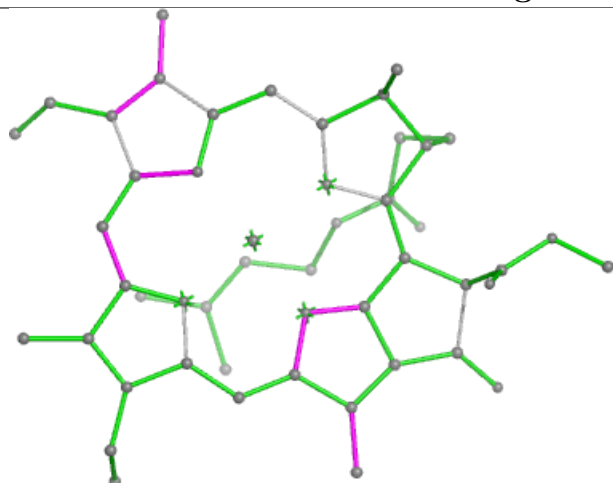
Torsions



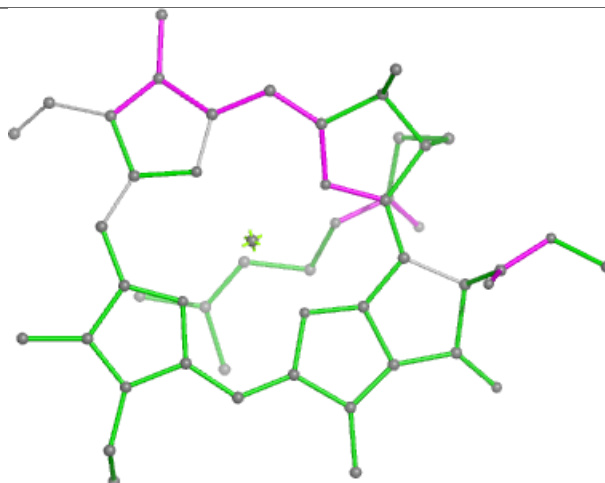
Rings



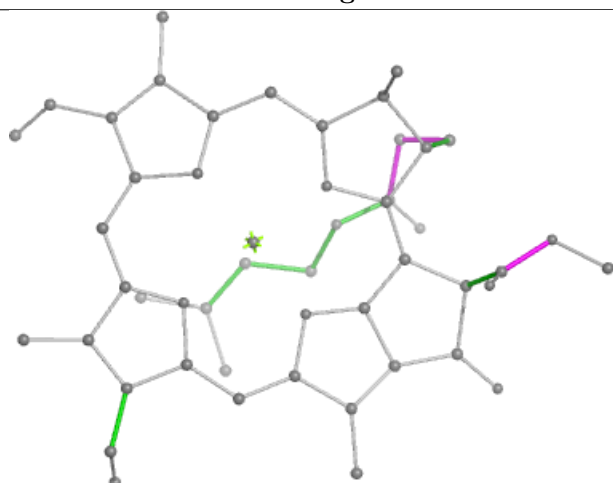
Ligand CLA B 809



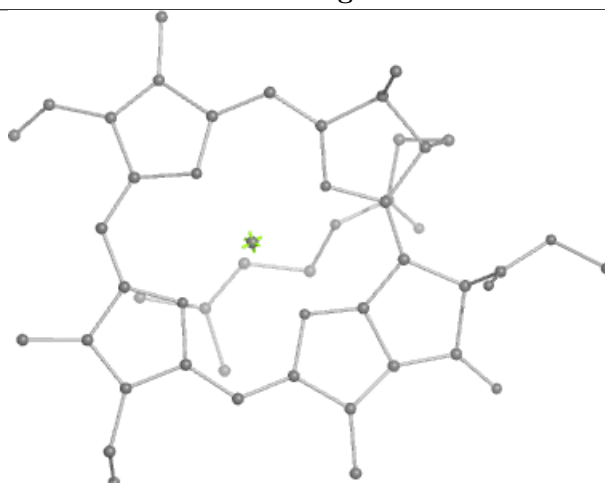
Bond lengths



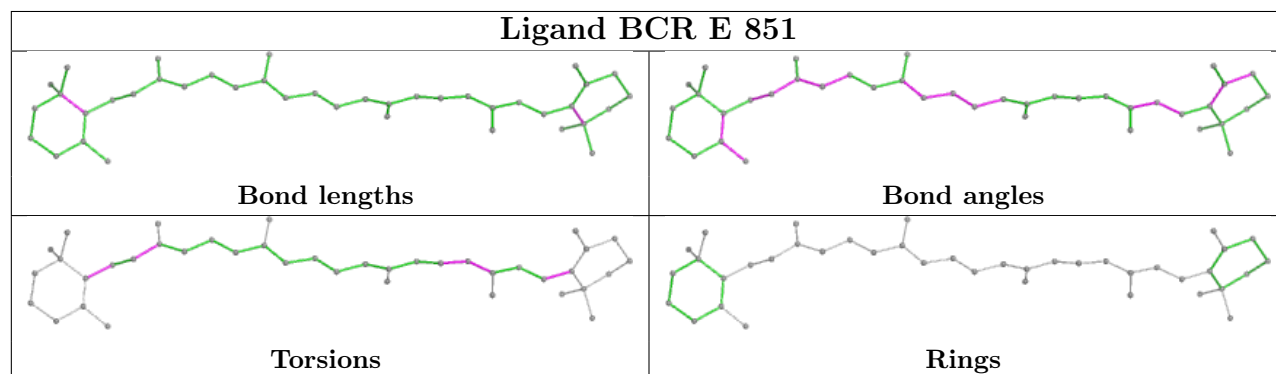
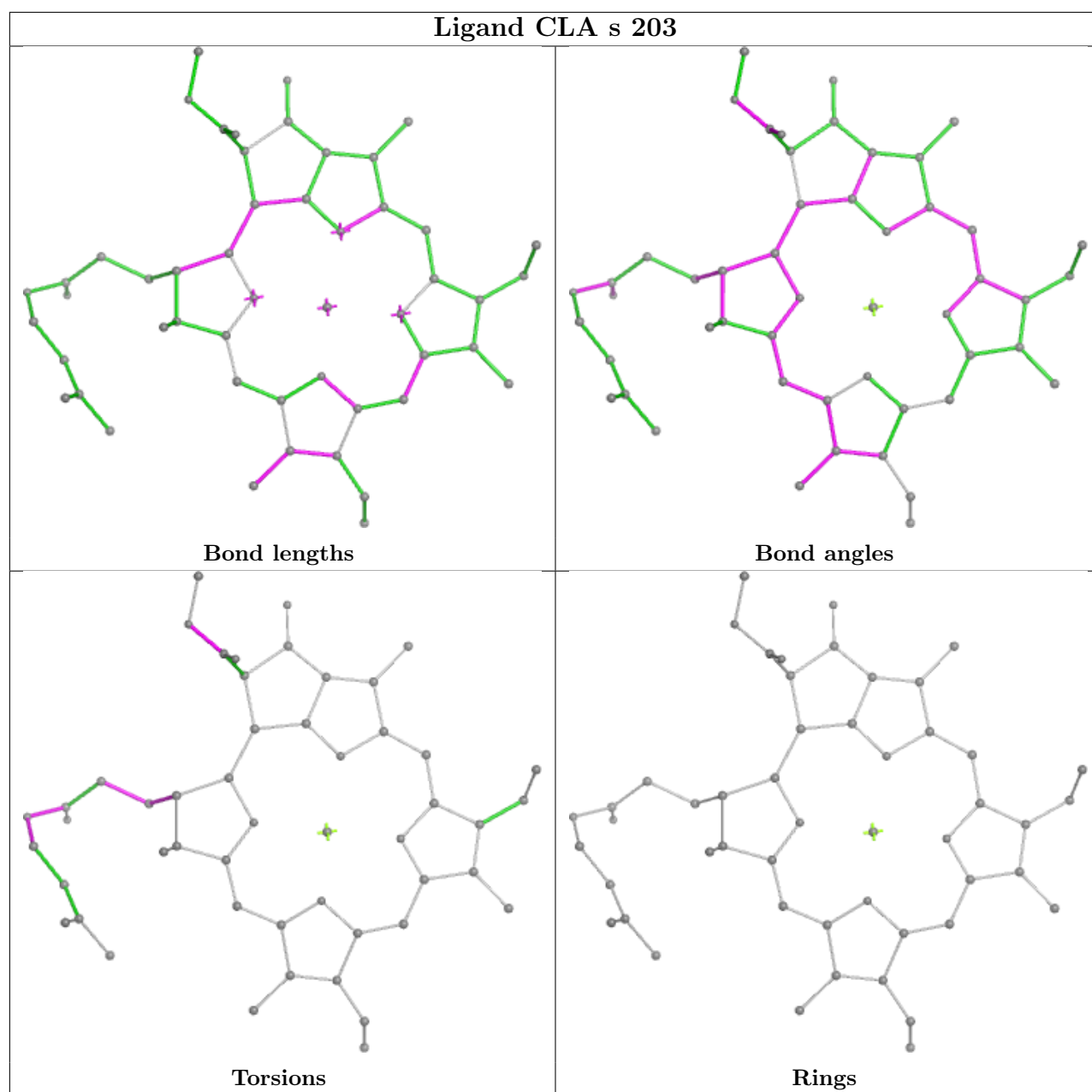
Bond angles



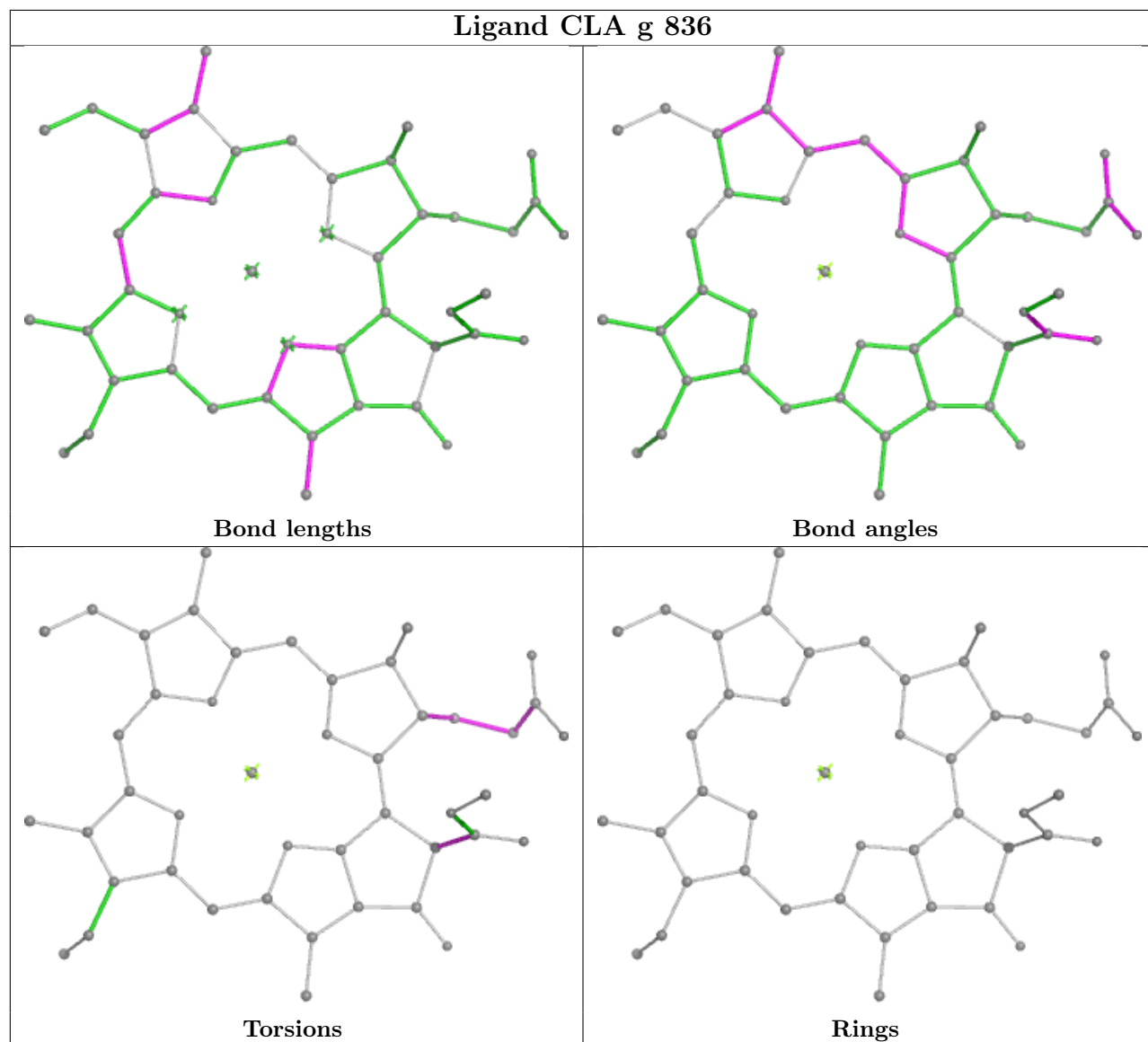
Torsions



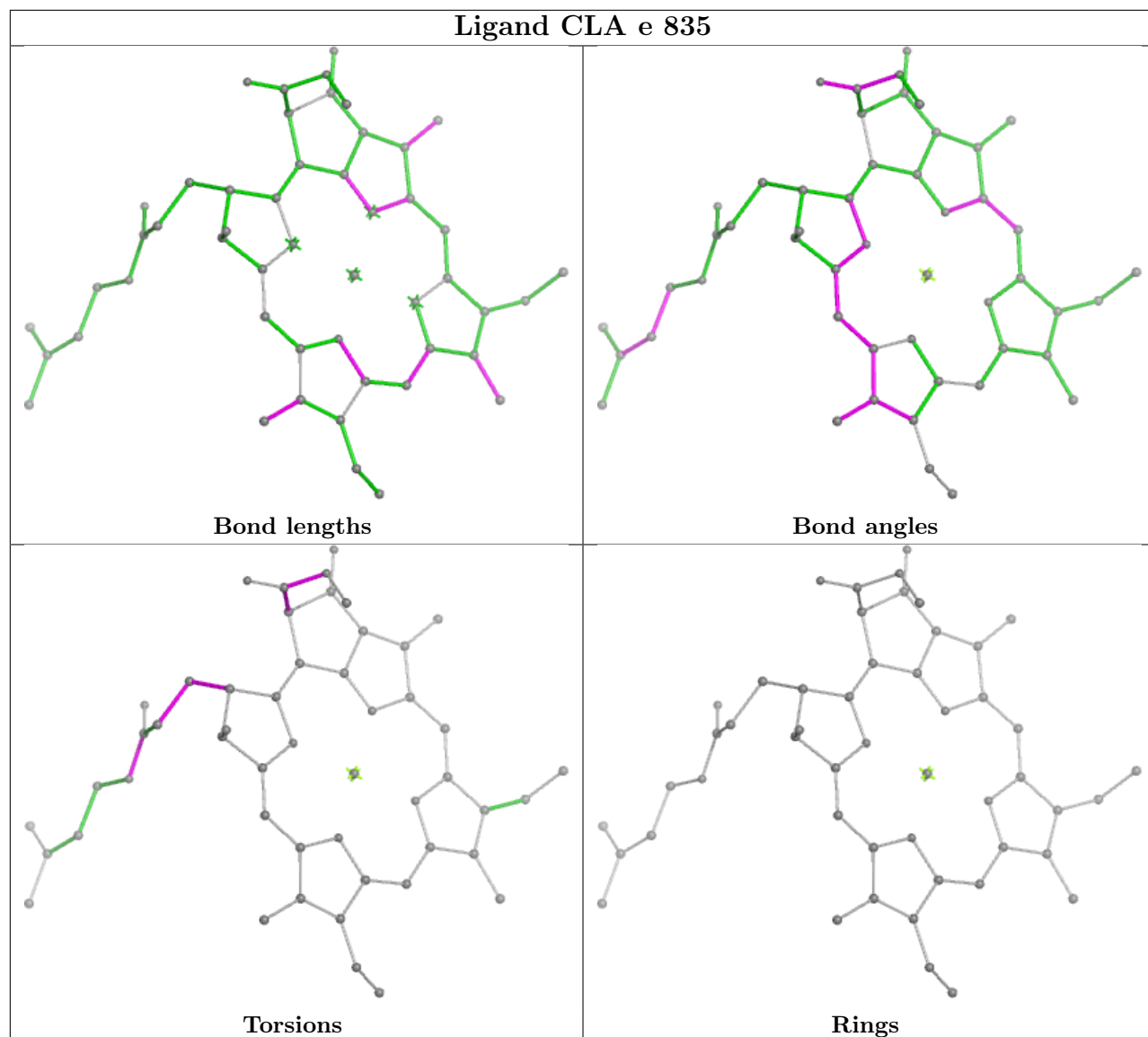
Rings



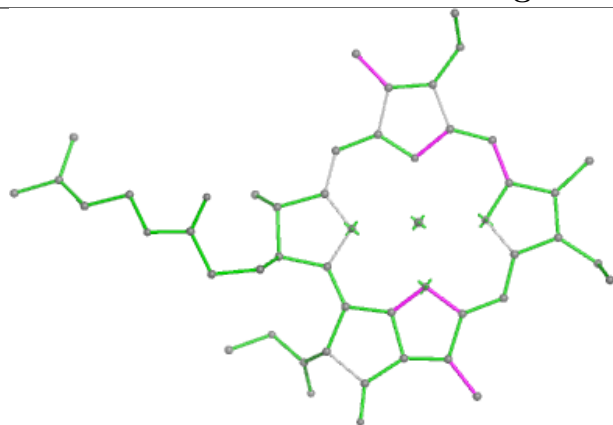
Ligand CLA g 836



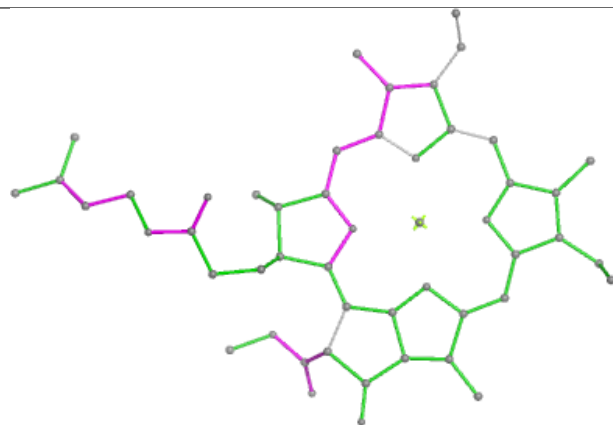
Ligand CLA e 835



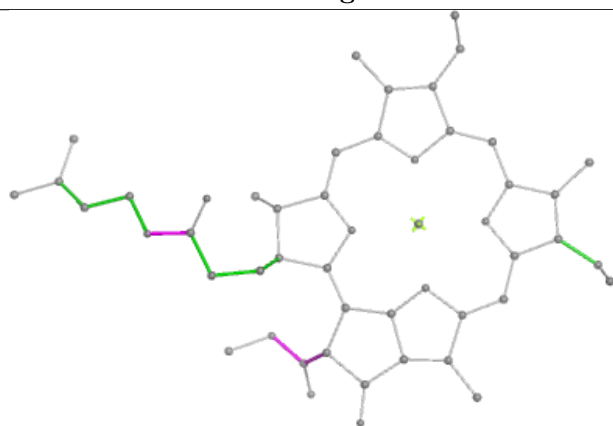
Ligand CLA A 816



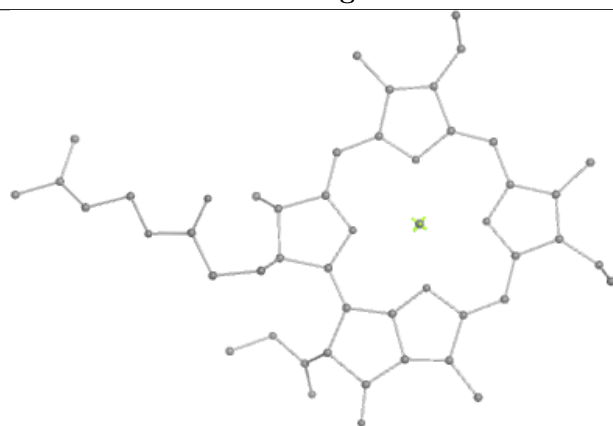
Bond lengths



Bond angles

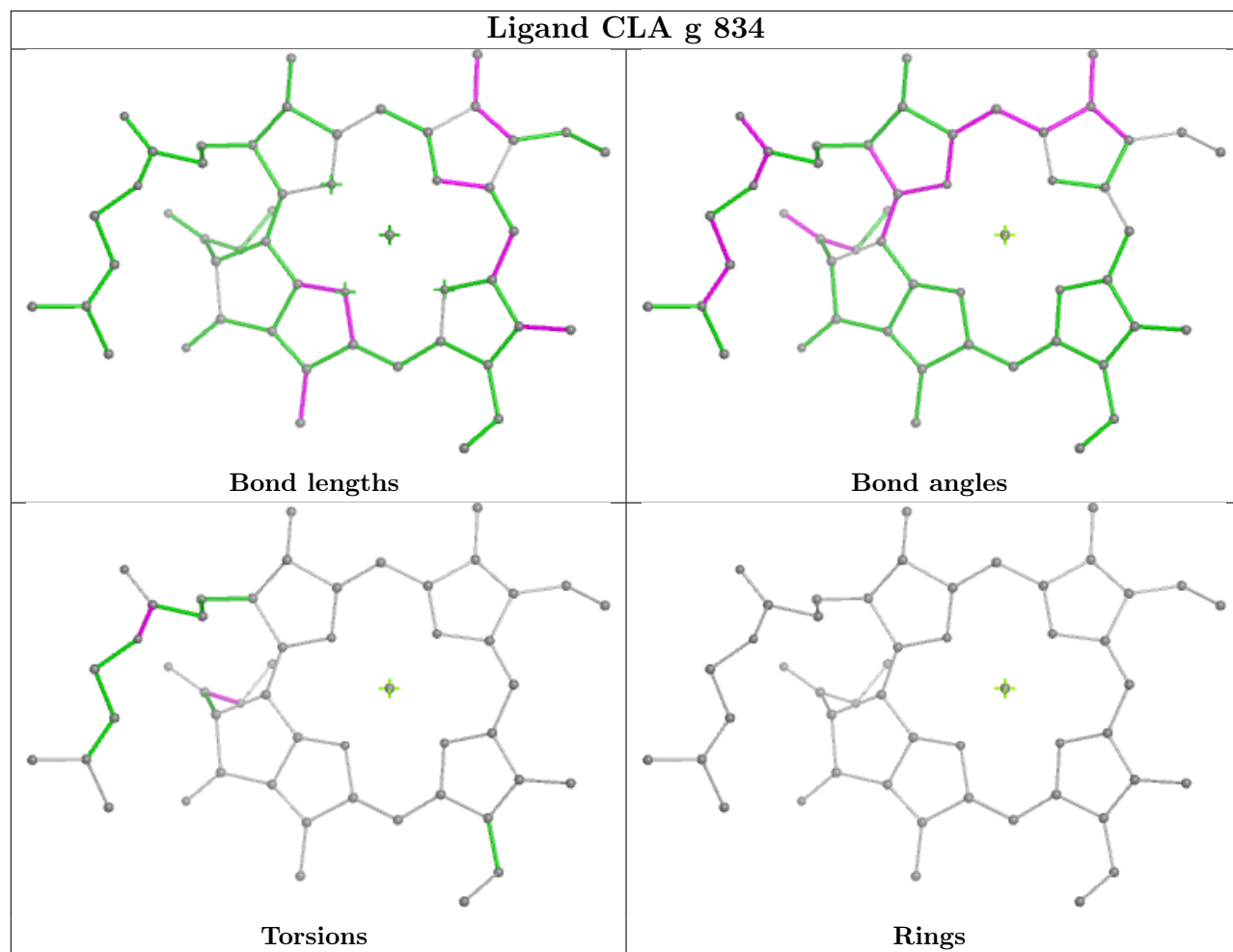


Torsions

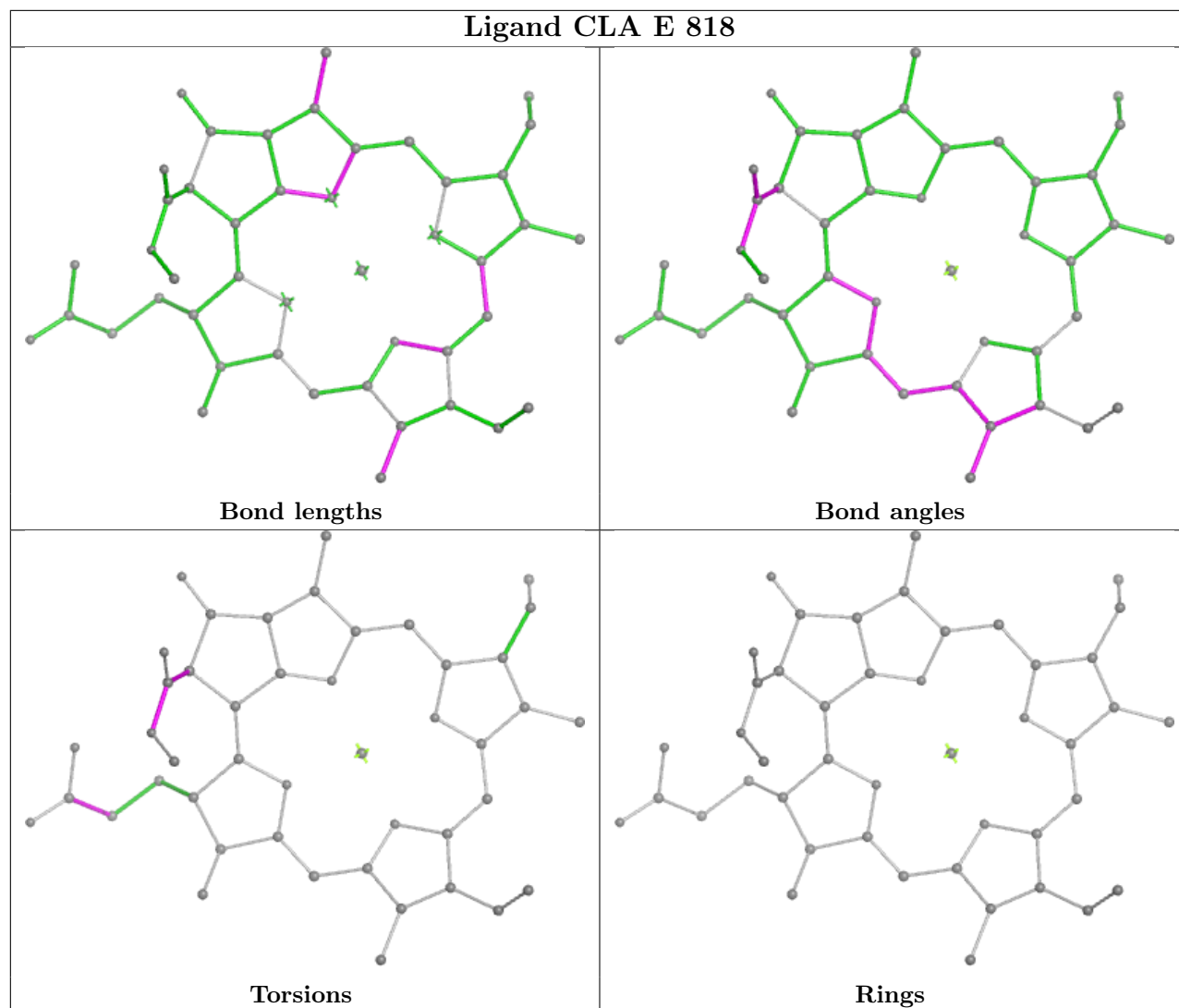


Rings

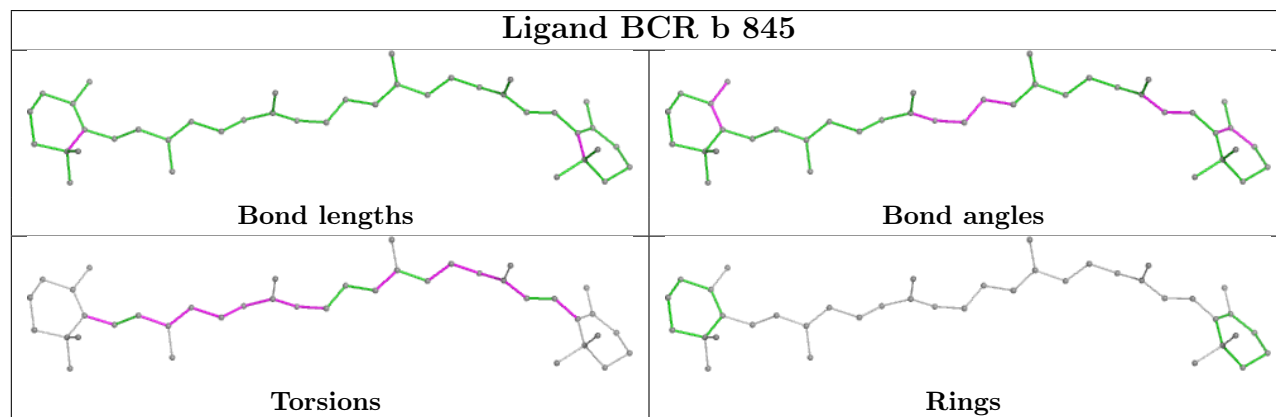
Ligand CLA g 834



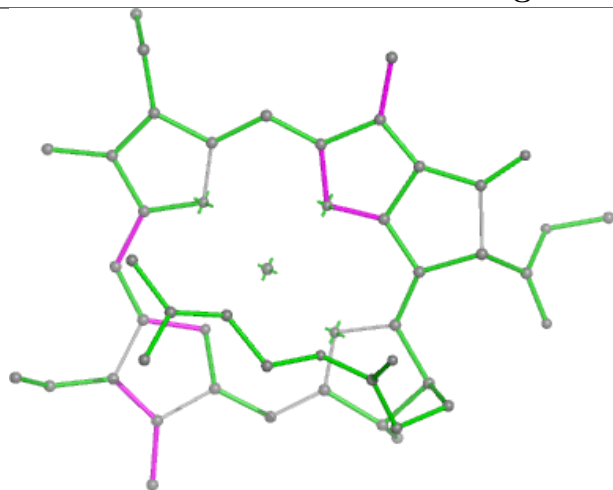
Ligand CLA E 818



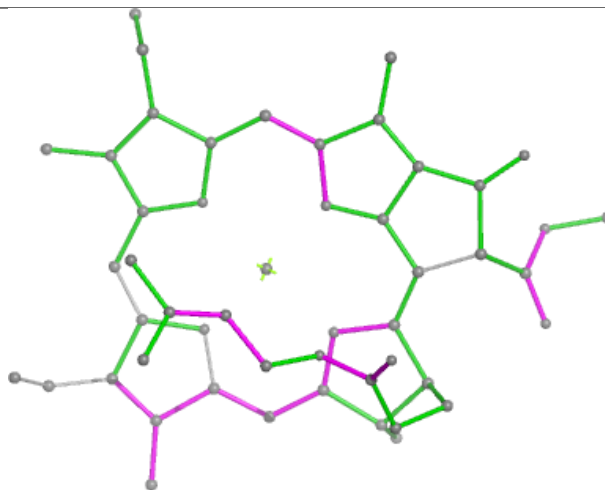
Ligand BCR b 845



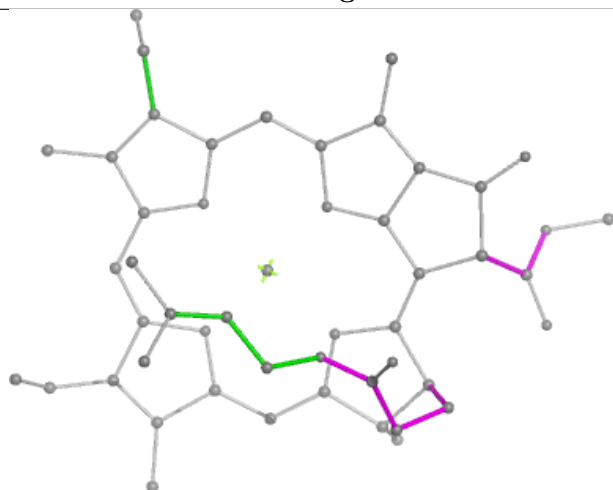
Ligand CLA A 826



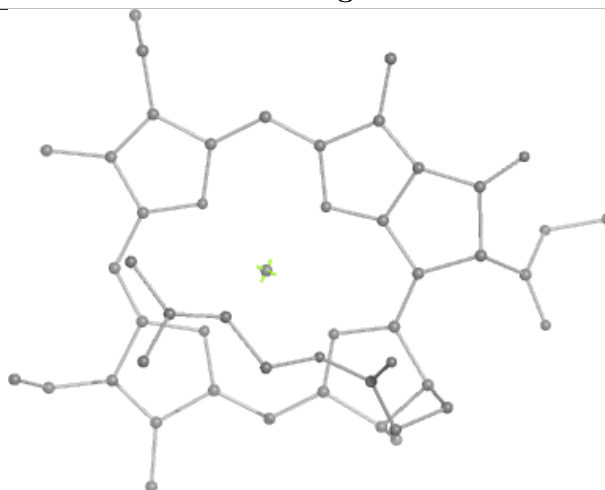
Bond lengths



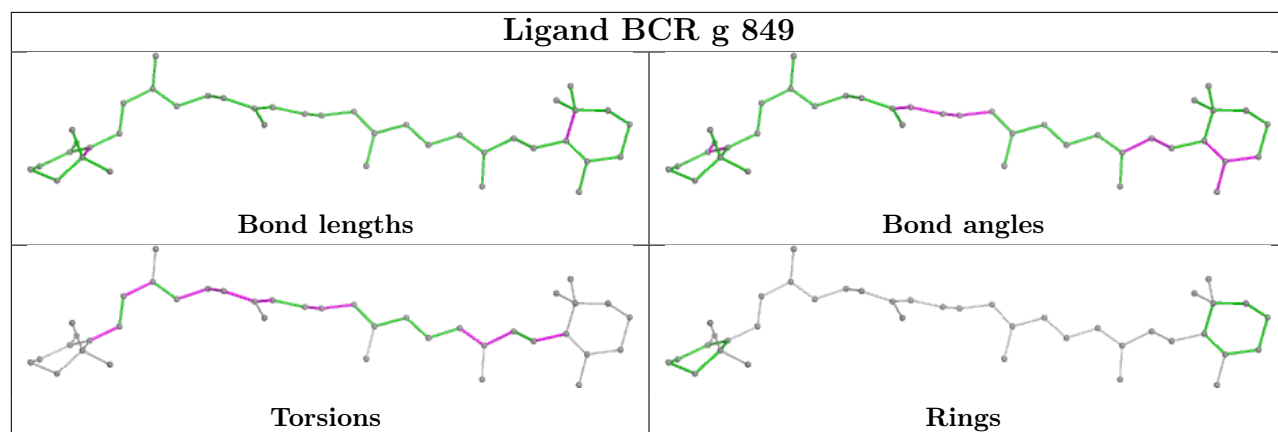
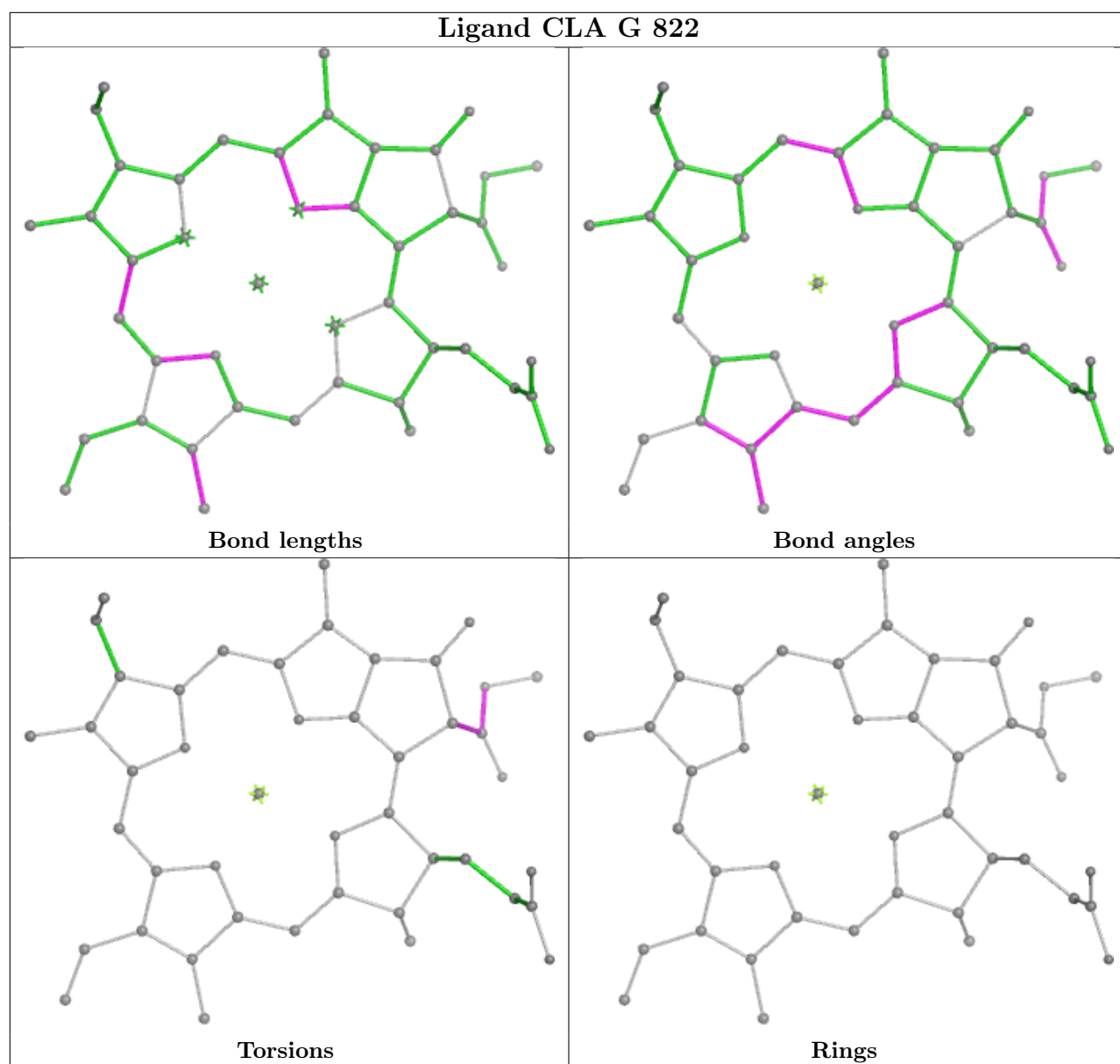
Bond angles



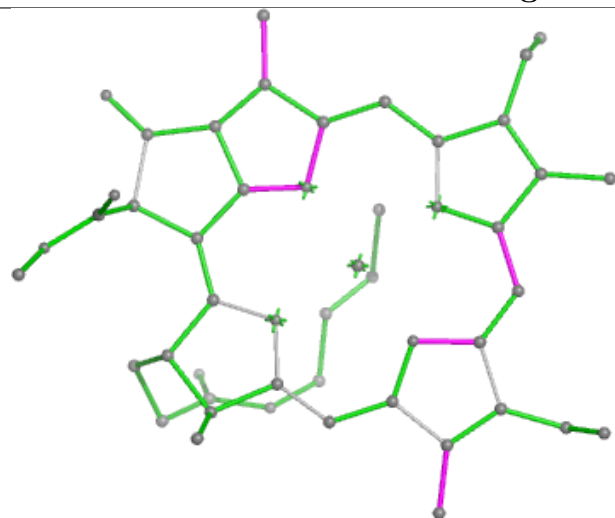
Torsions



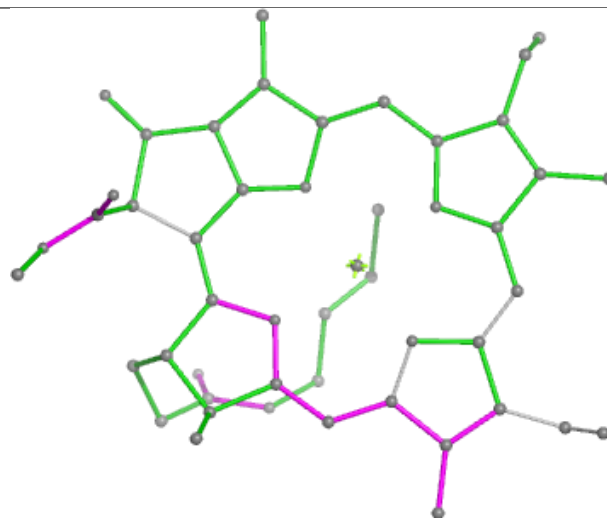
Rings



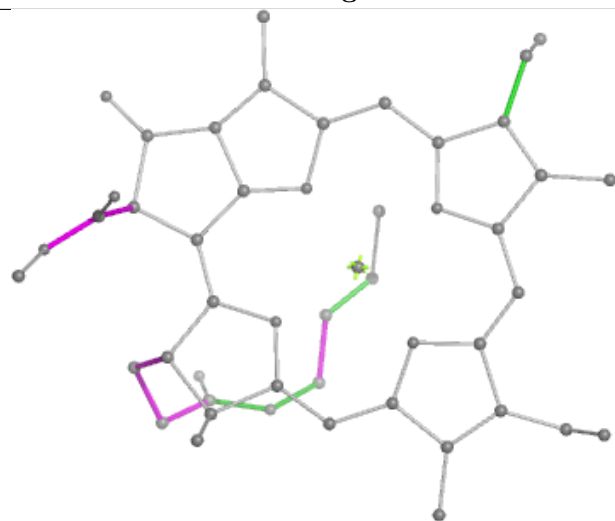
Ligand CLA a 819



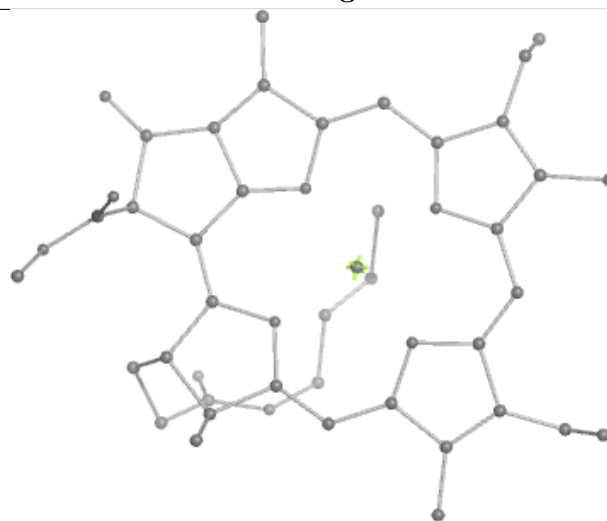
Bond lengths



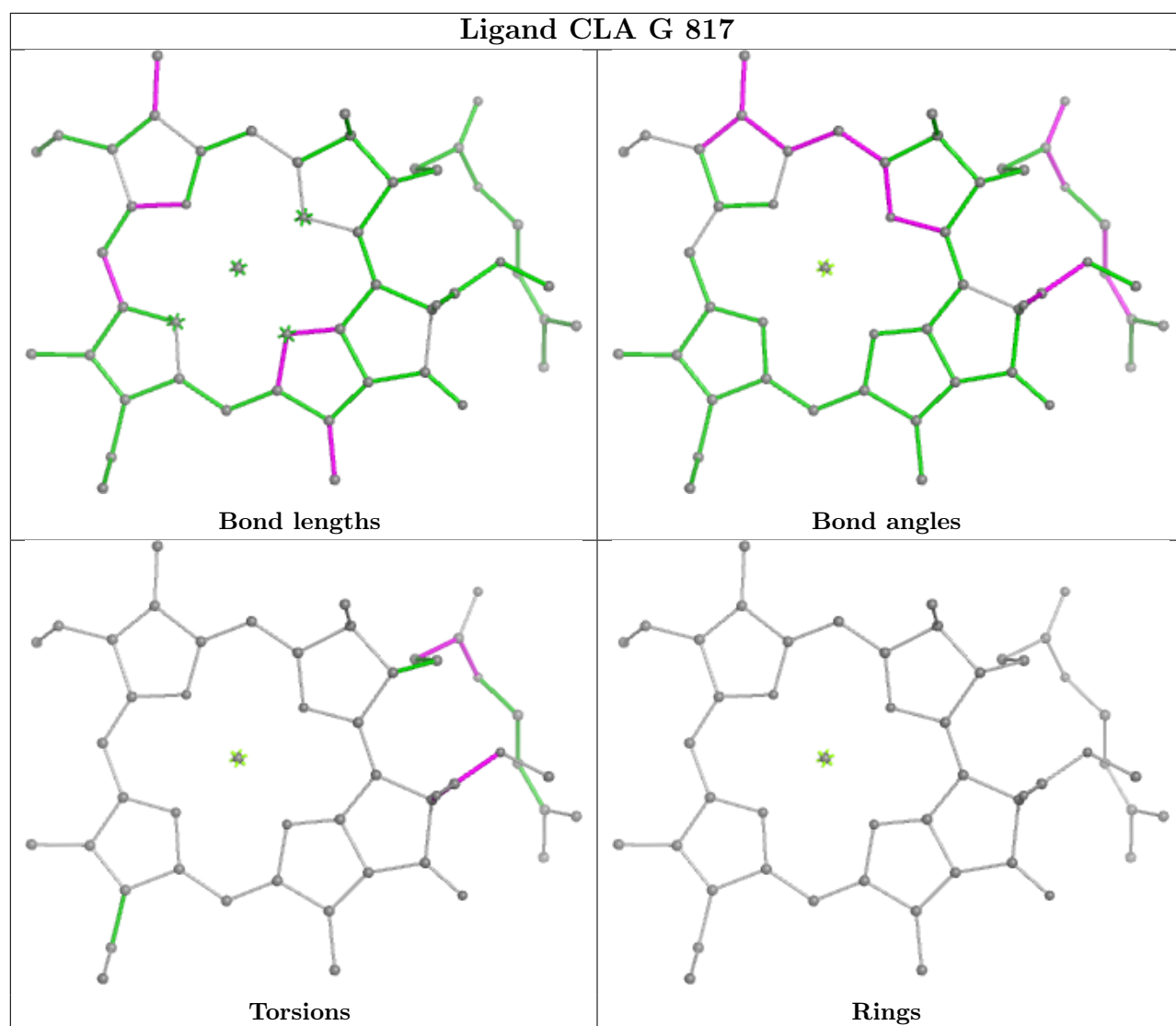
Bond angles



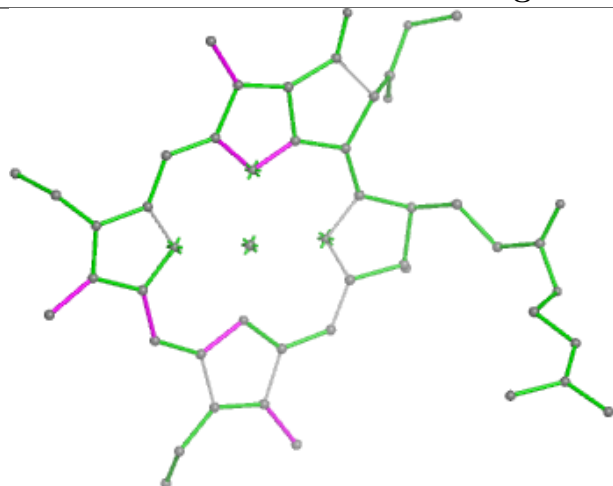
Torsions



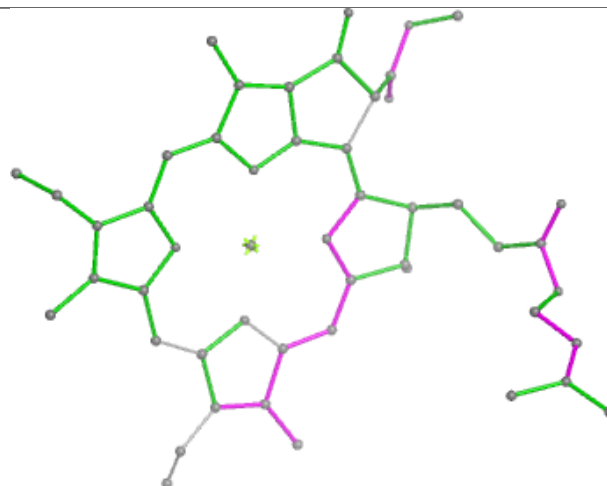
Rings



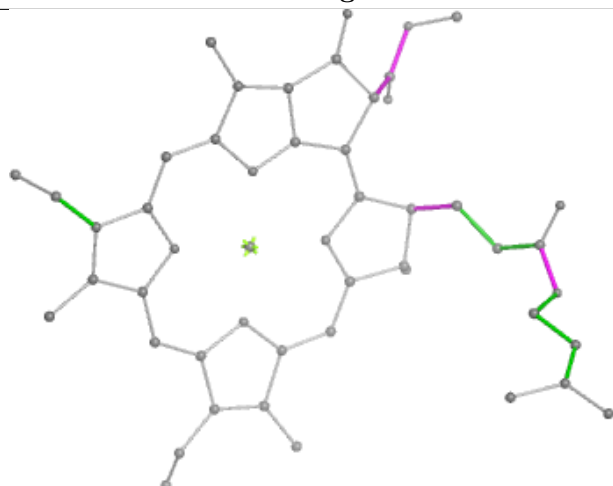
Ligand CLA A 807



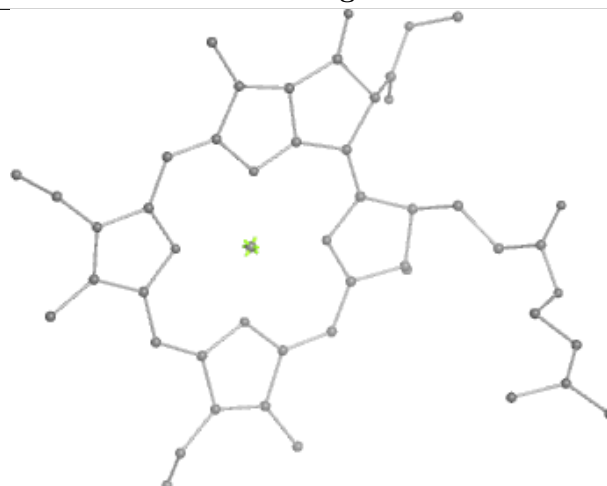
Bond lengths



Bond angles

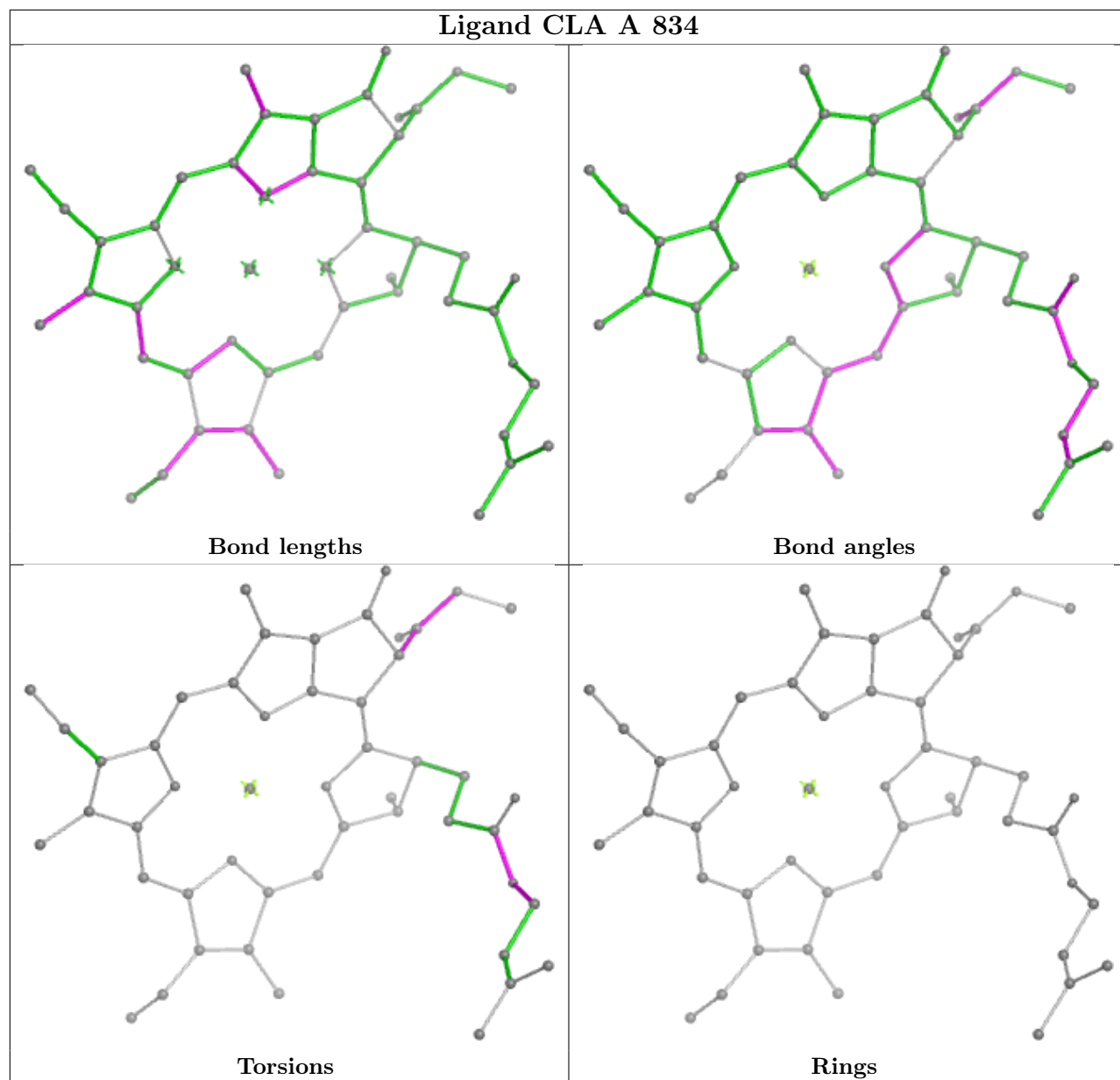


Torsions

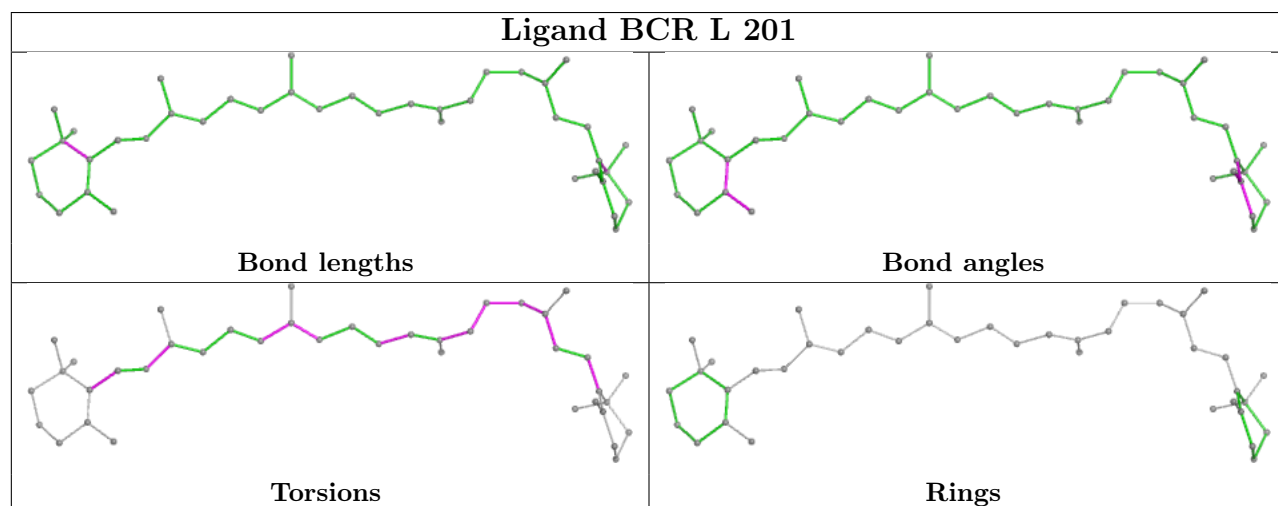


Rings

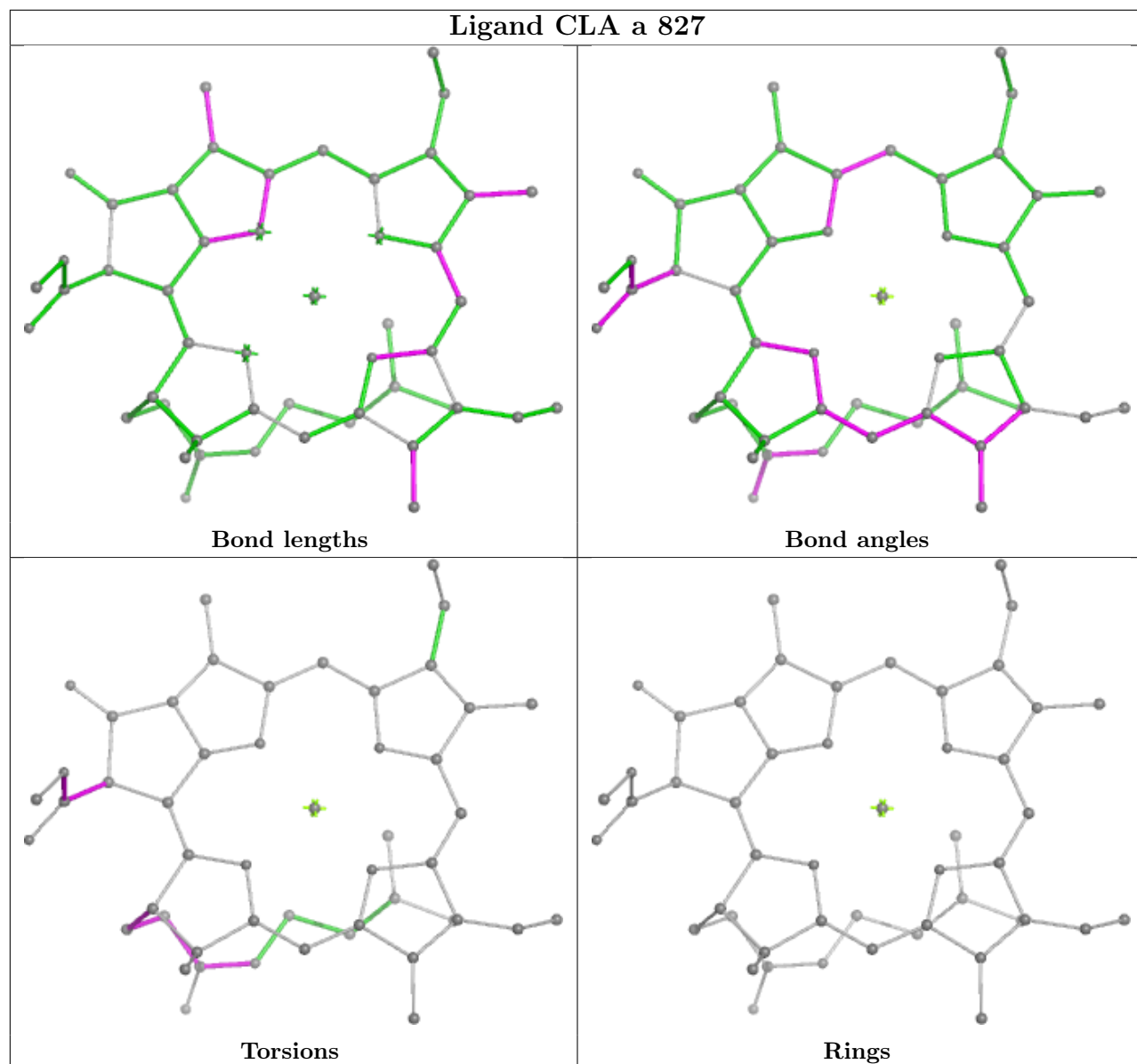
Ligand CLA A 834



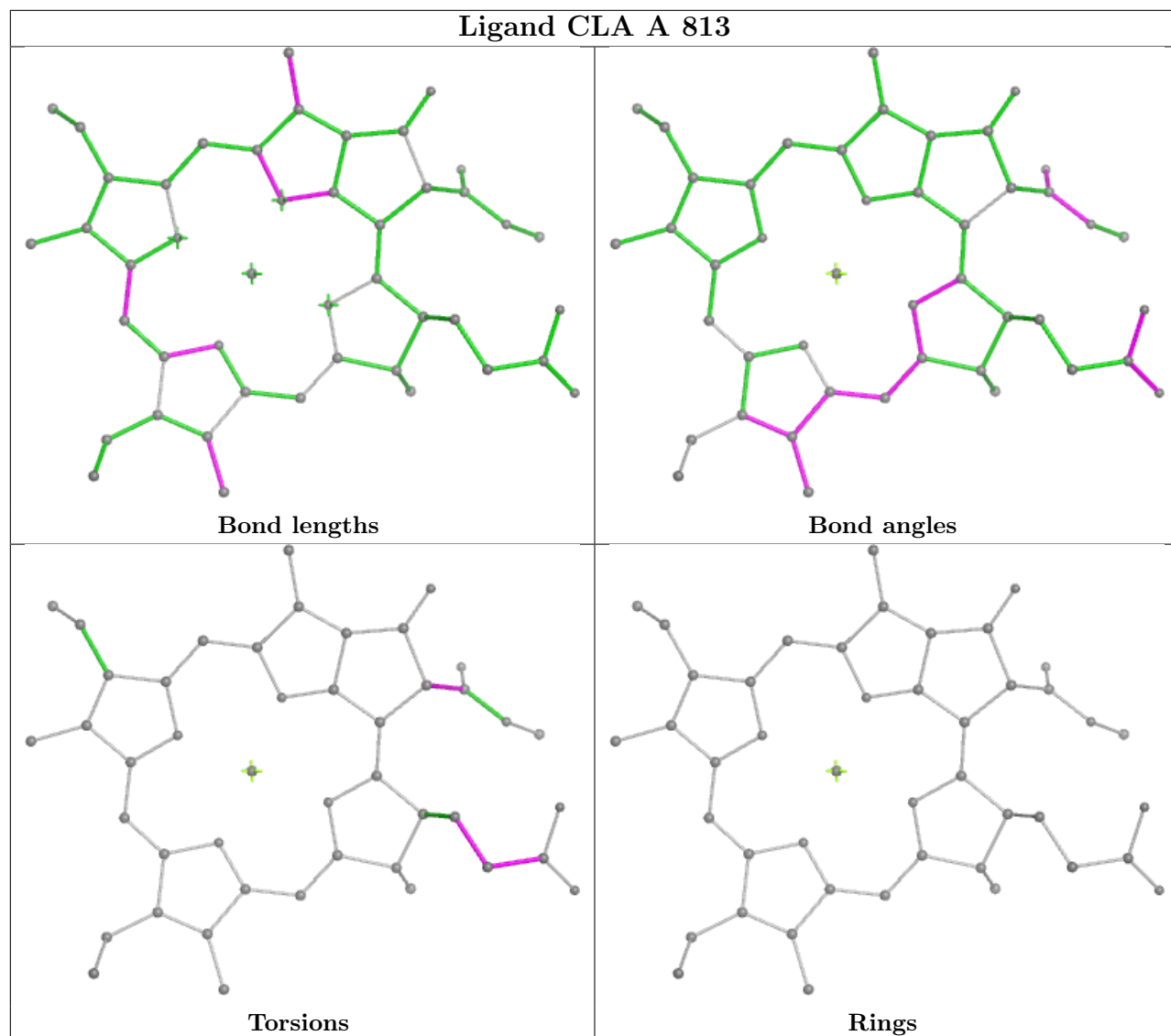
Ligand BCR L 201



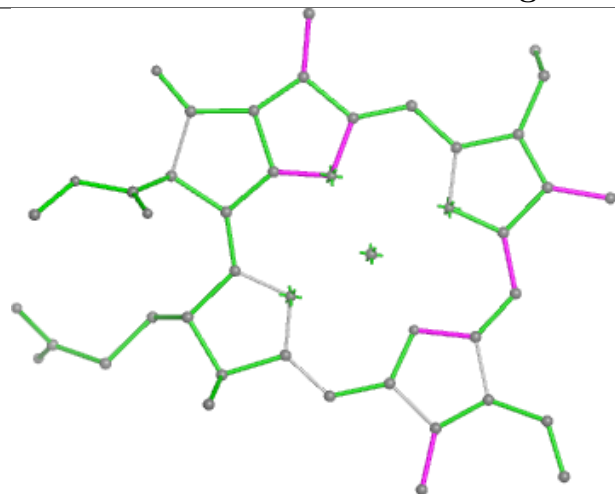
Ligand CLA a 827



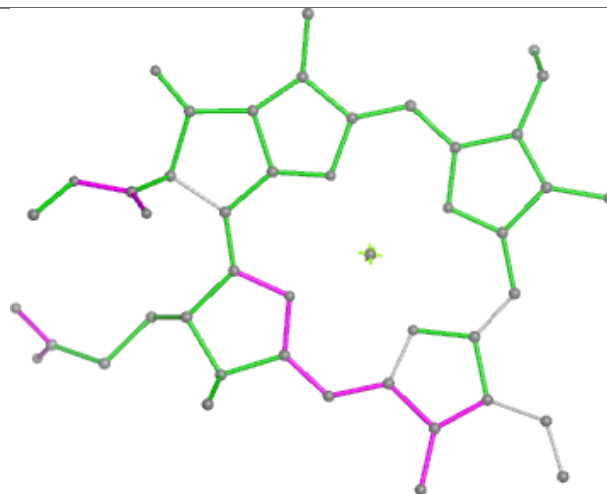
Ligand CLA A 813



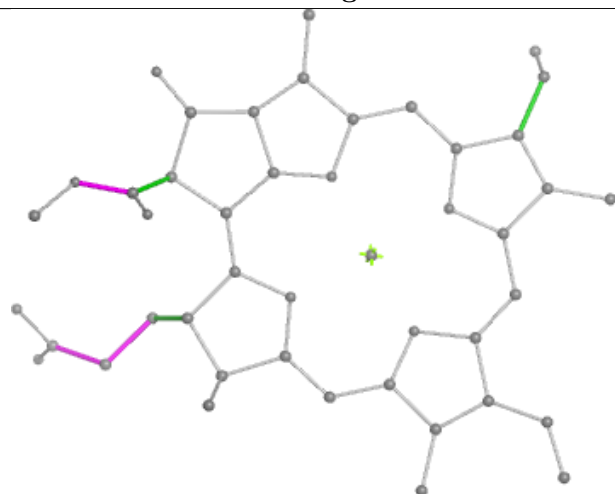
Ligand CLA S 203



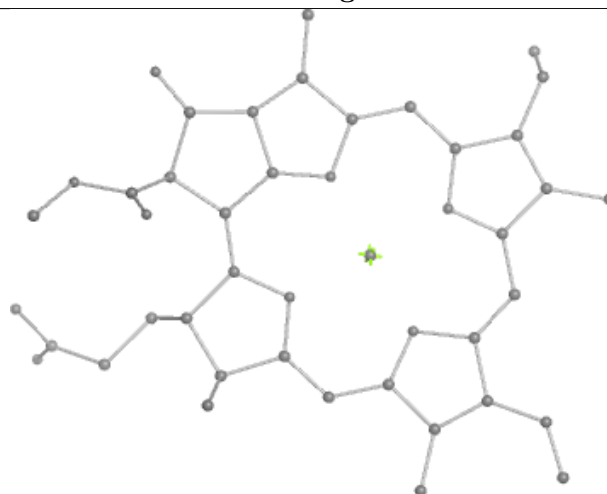
Bond lengths



Bond angles

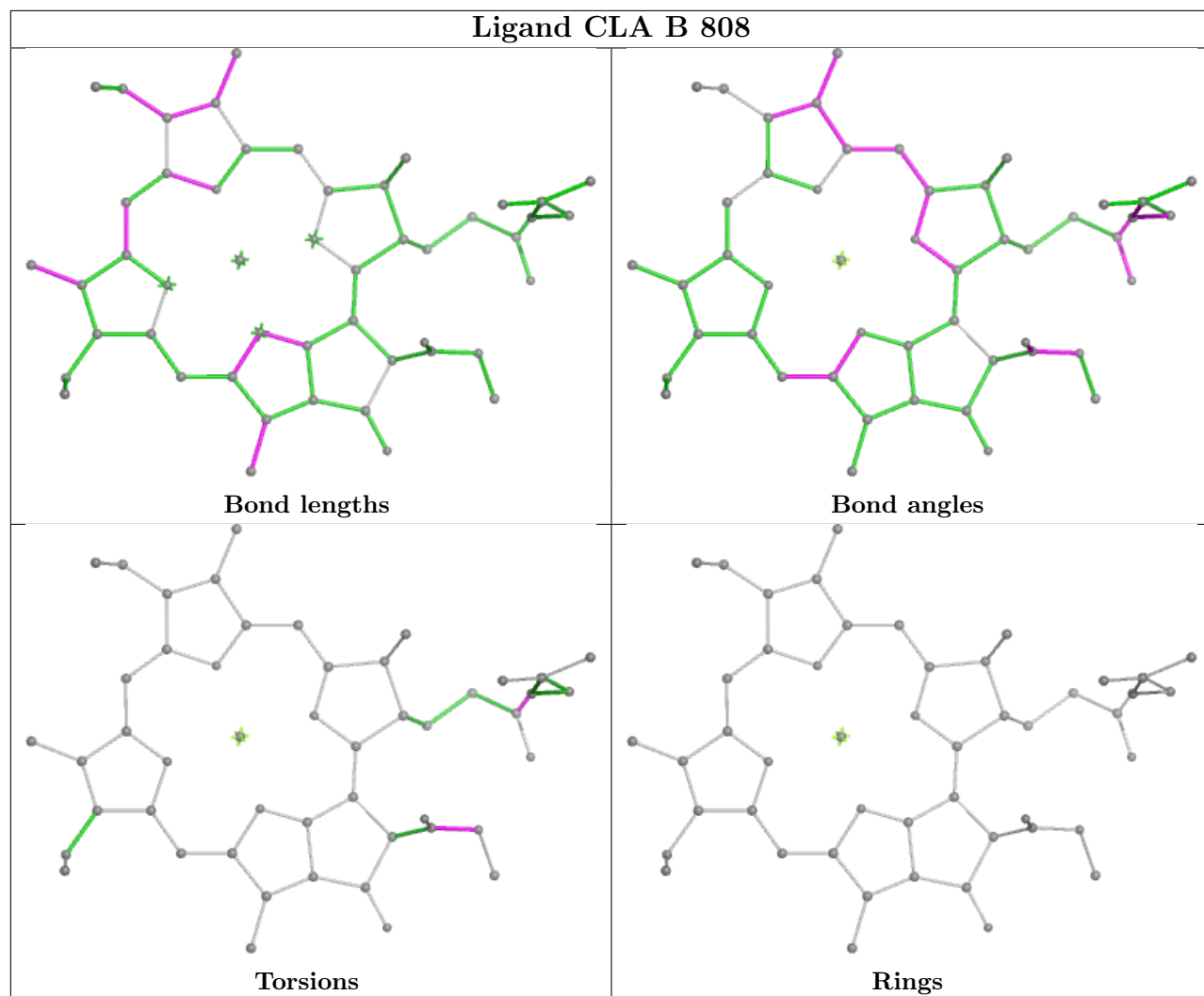


Torsions

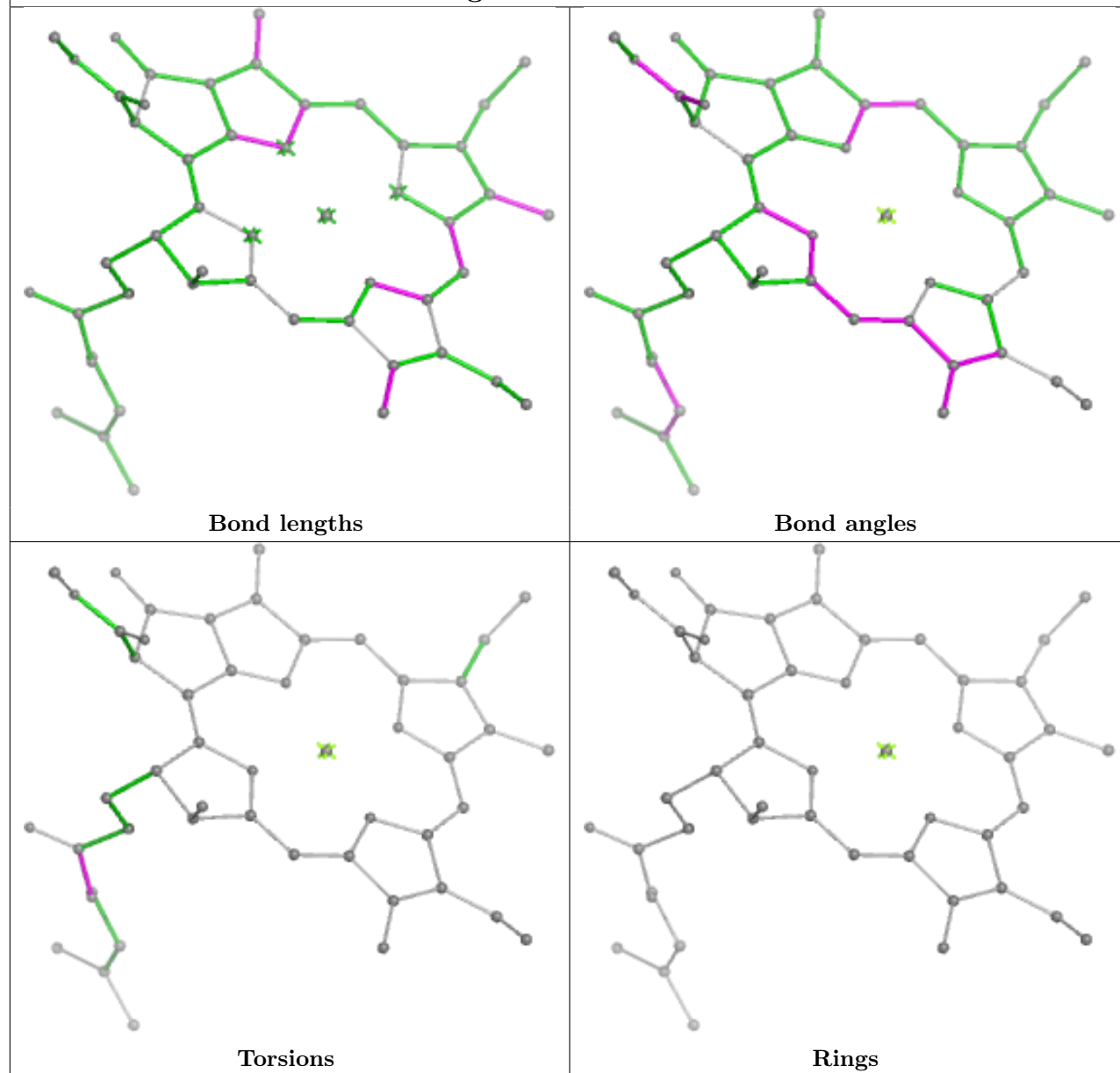


Rings

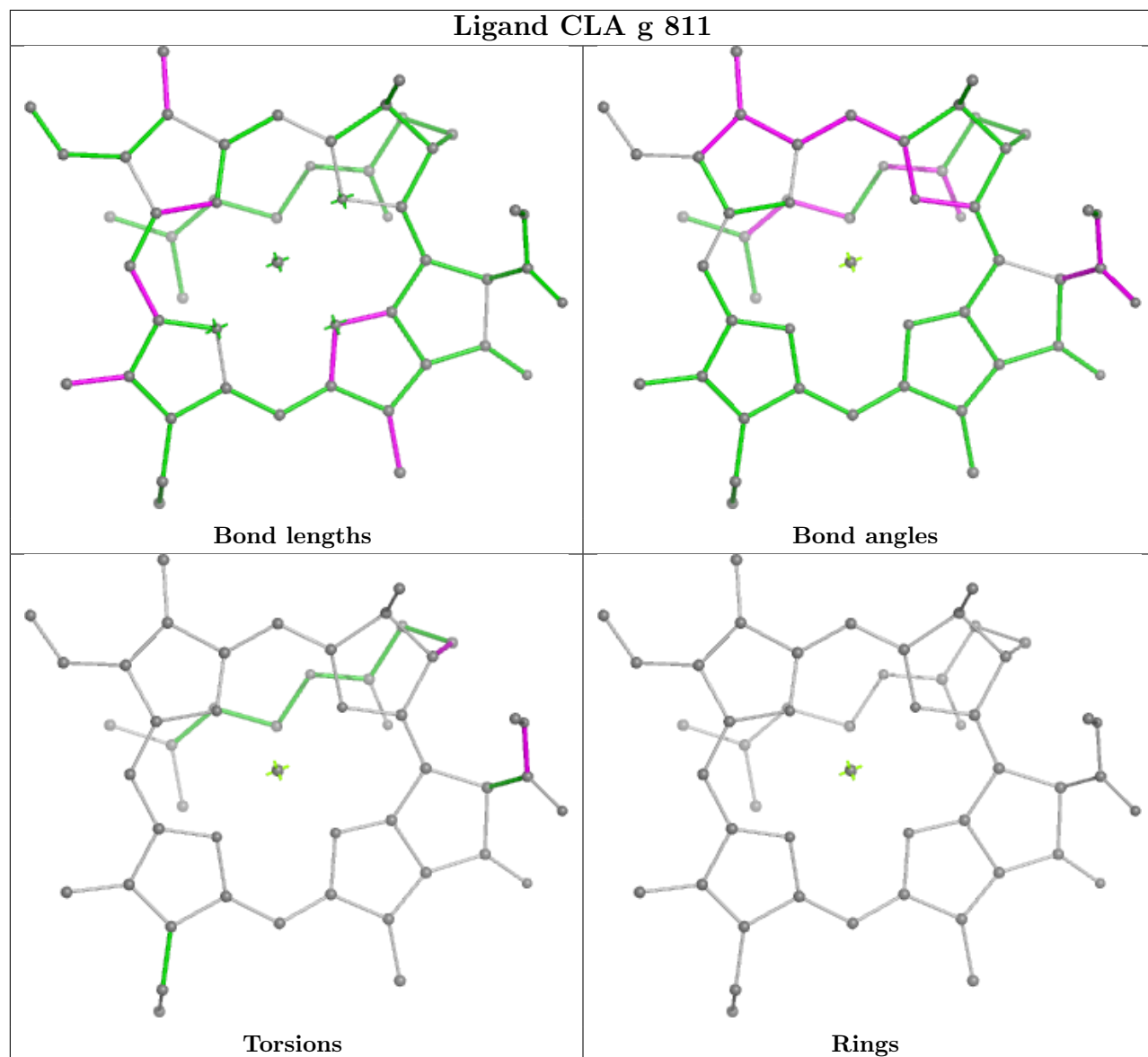
Ligand CLA B 808

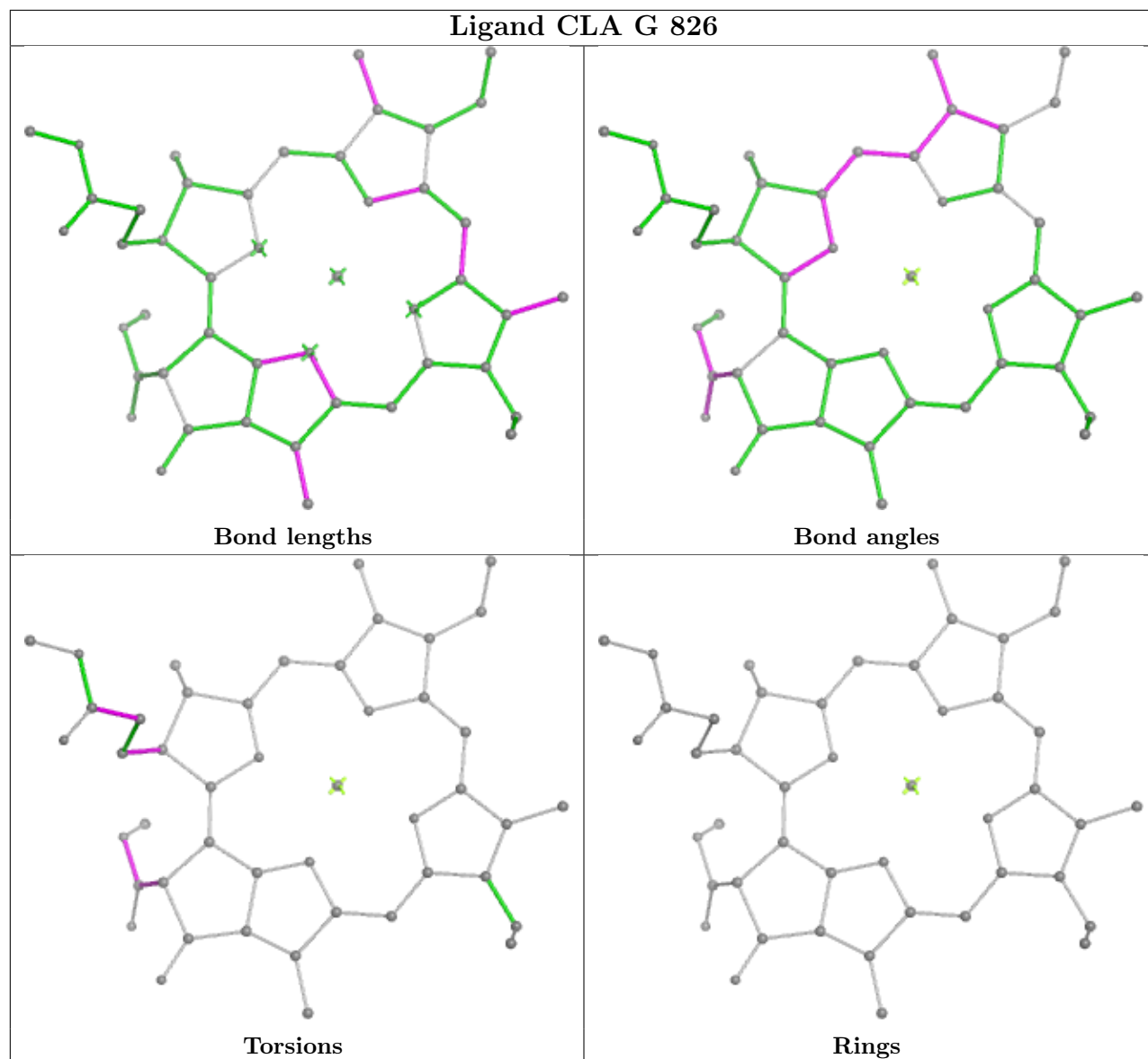


Ligand CLA B 806

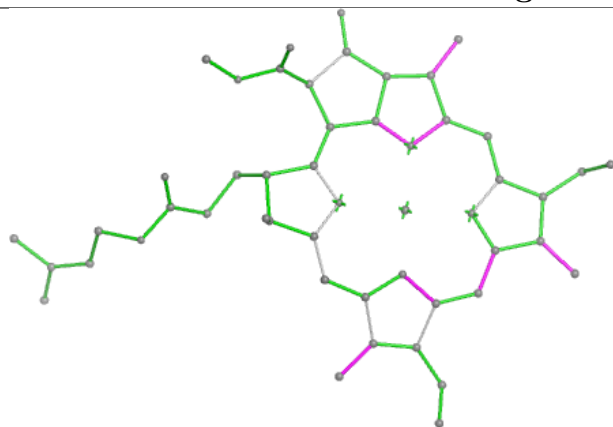


Ligand CLA g 811

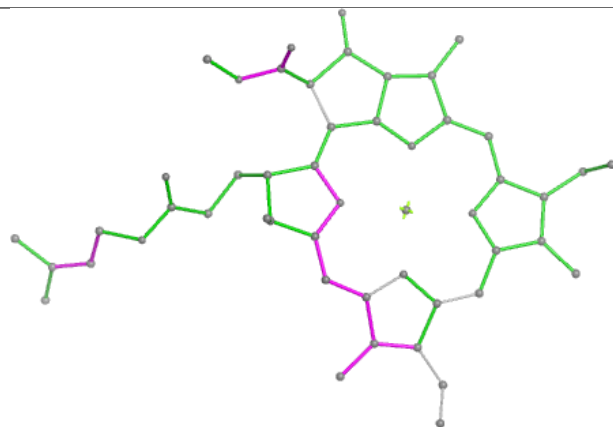




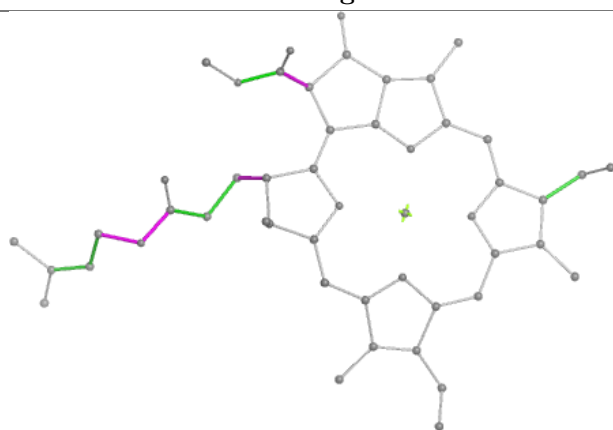
Ligand CLA E 805



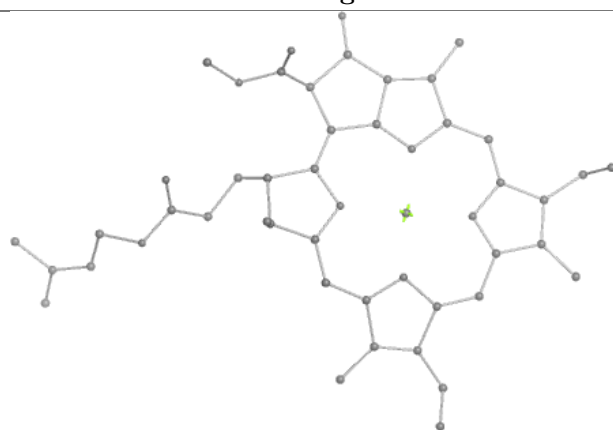
Bond lengths



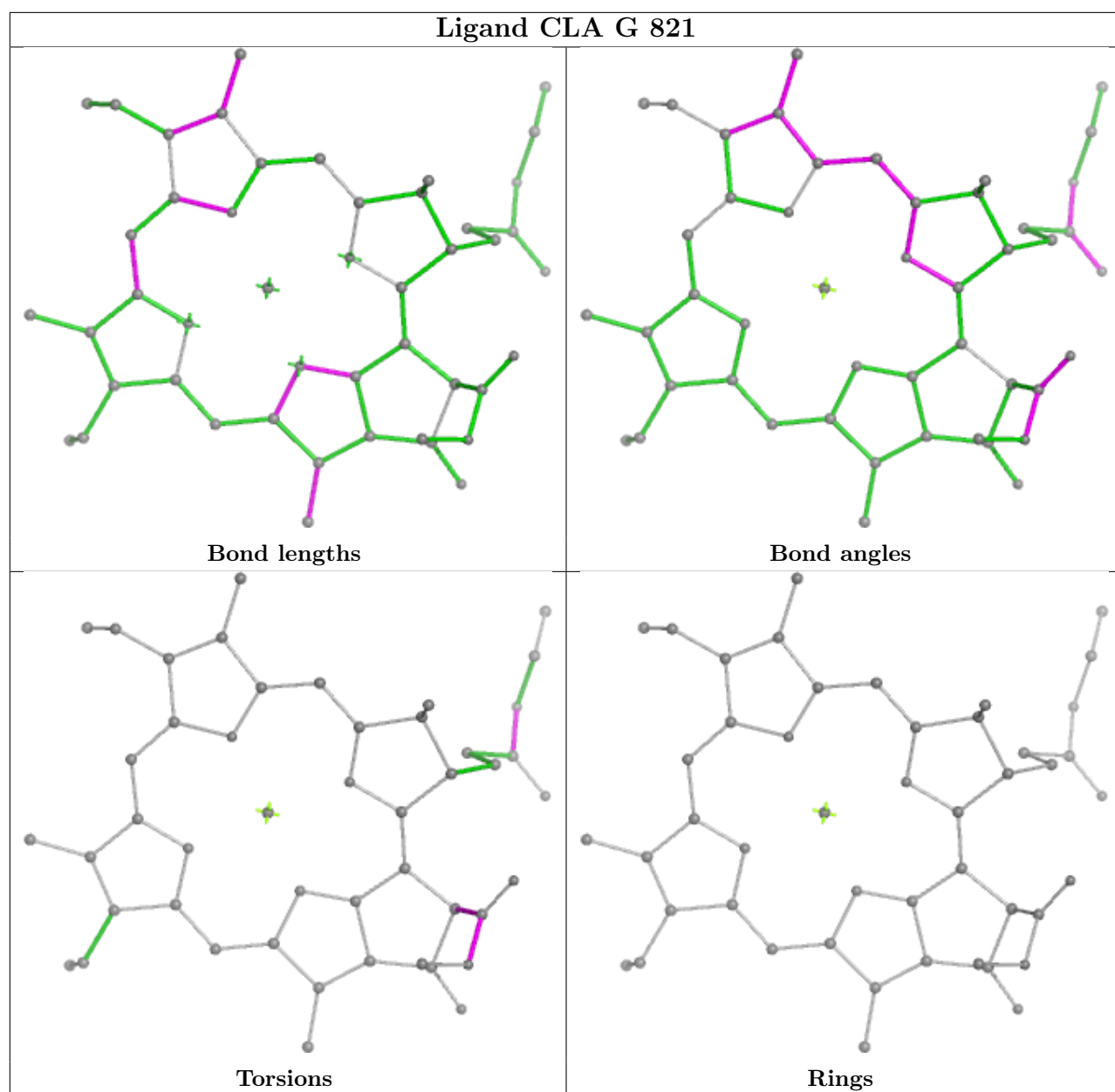
Bond angles



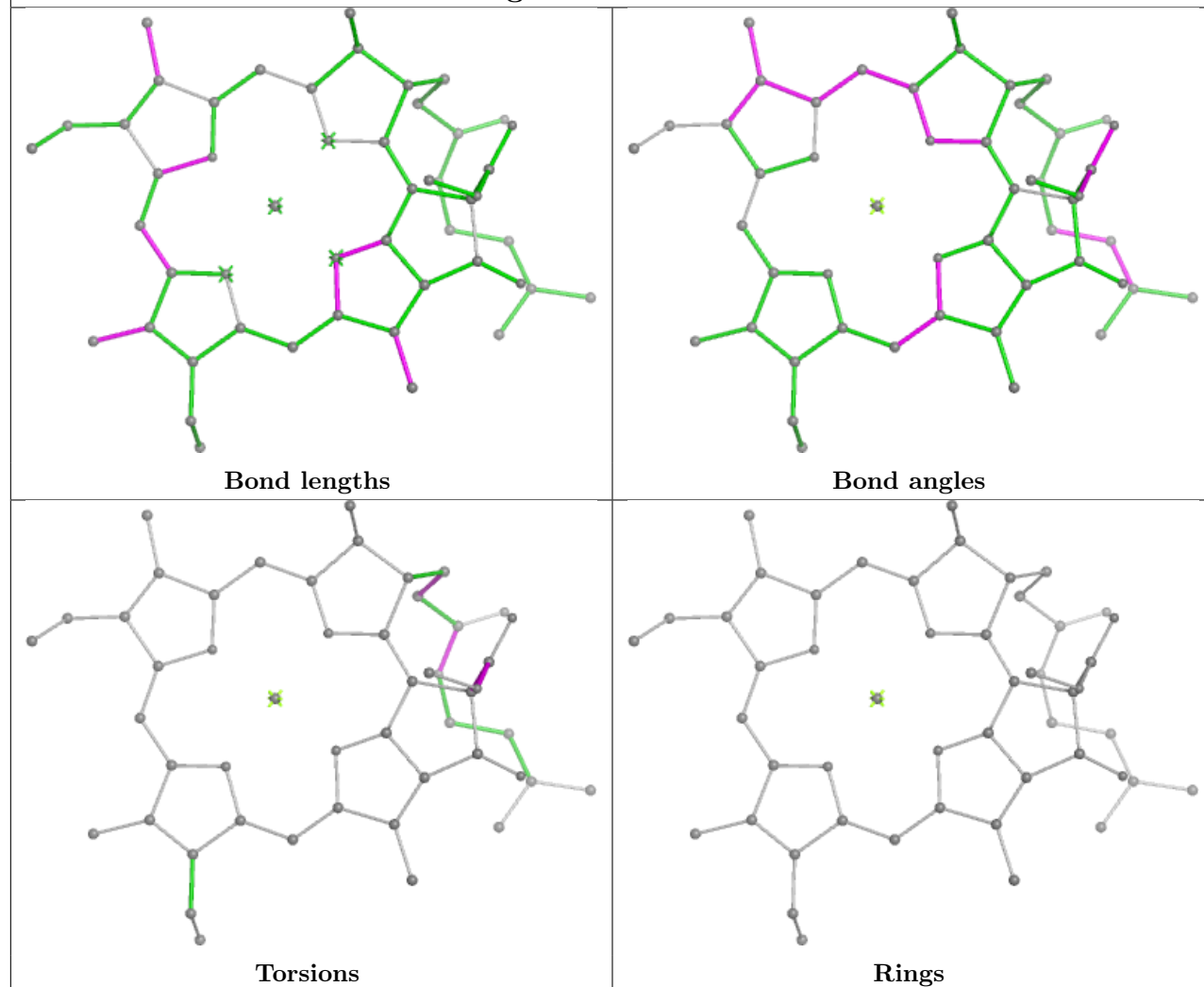
Torsions



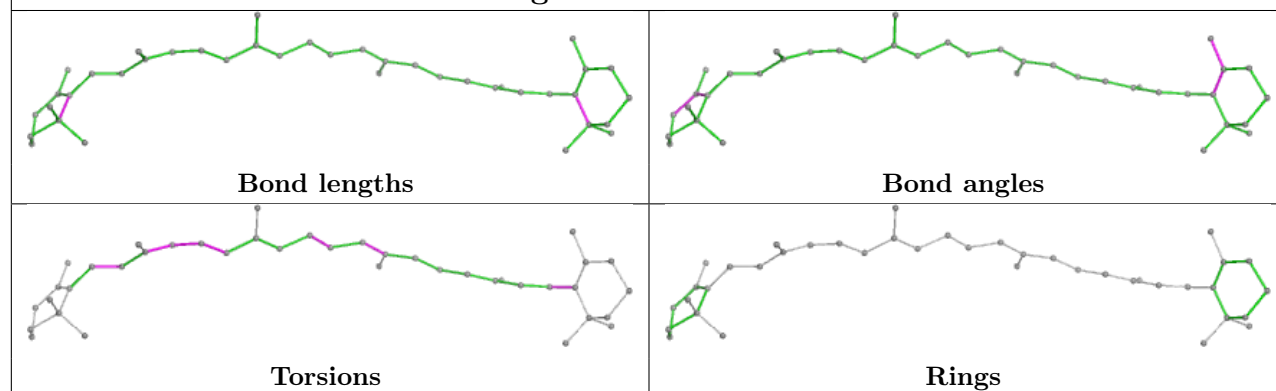
Rings



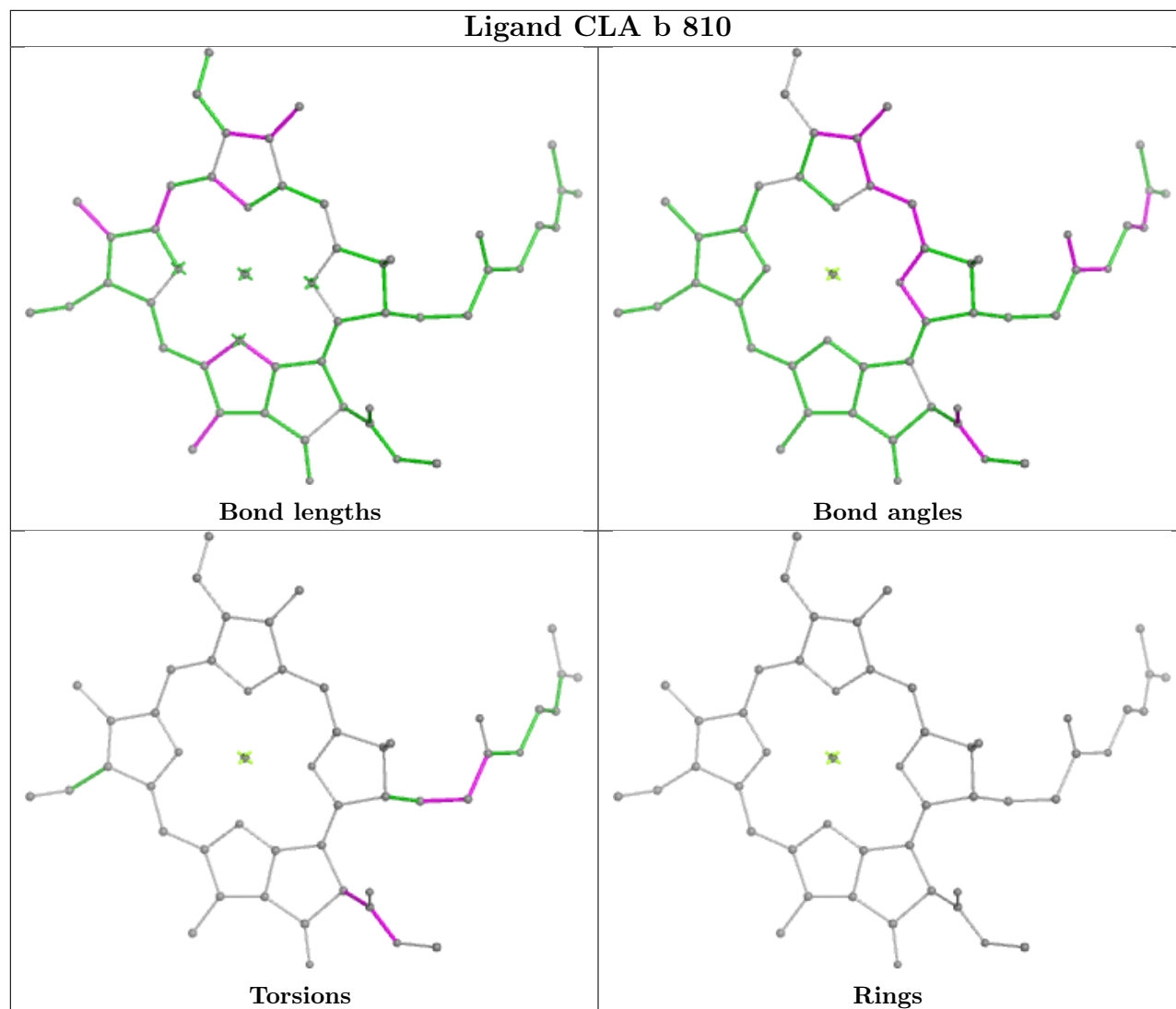
Ligand CLA e 809



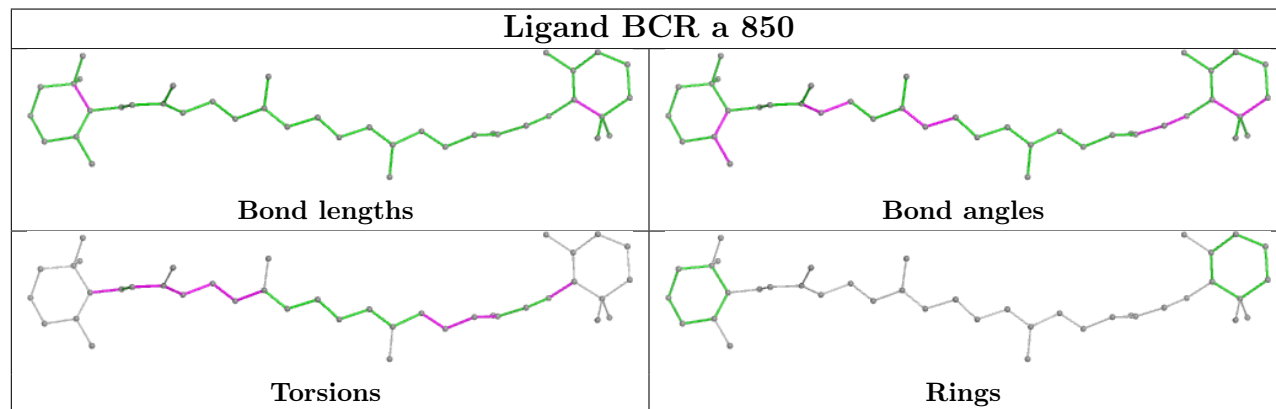
Ligand BCR P 101

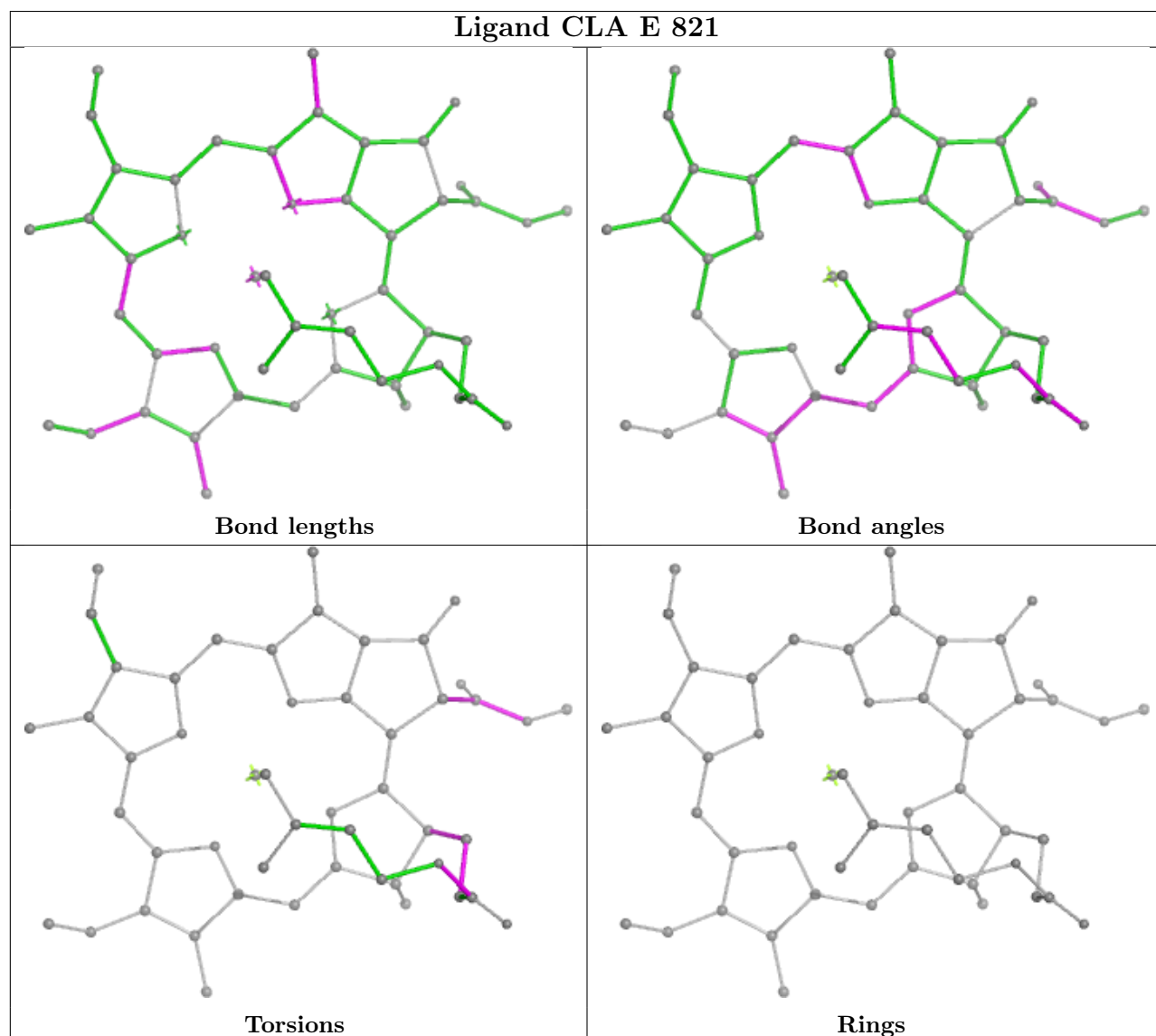
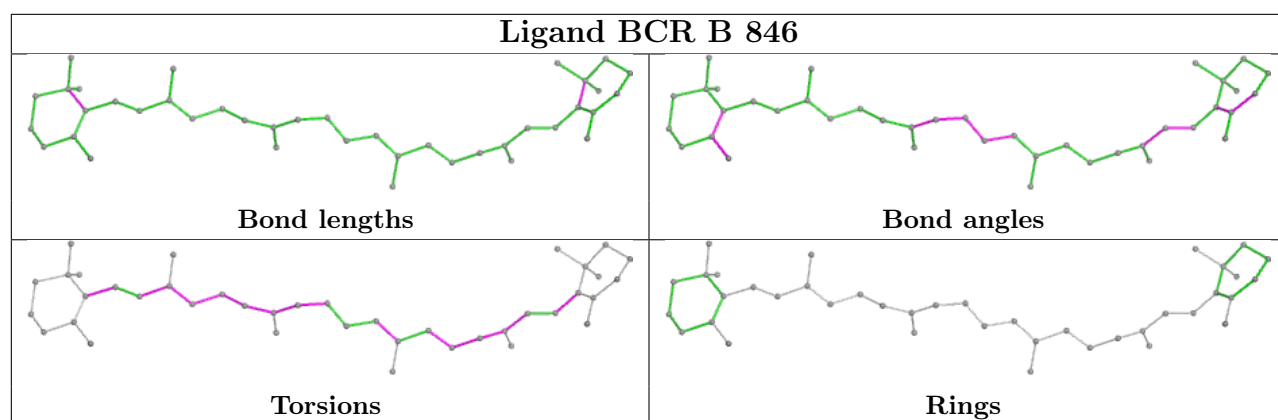


Ligand CLA b 810

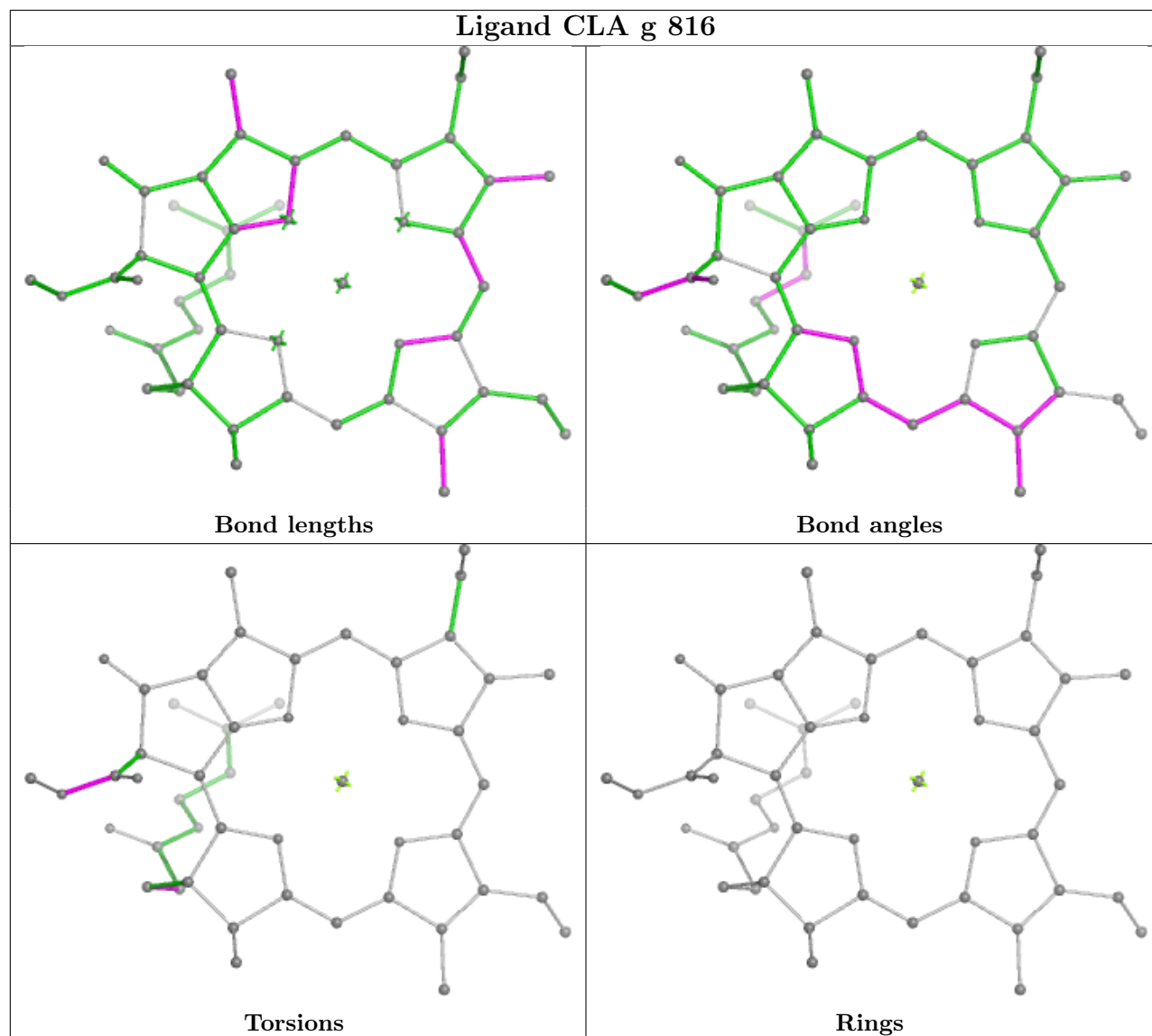


Ligand BCR a 850

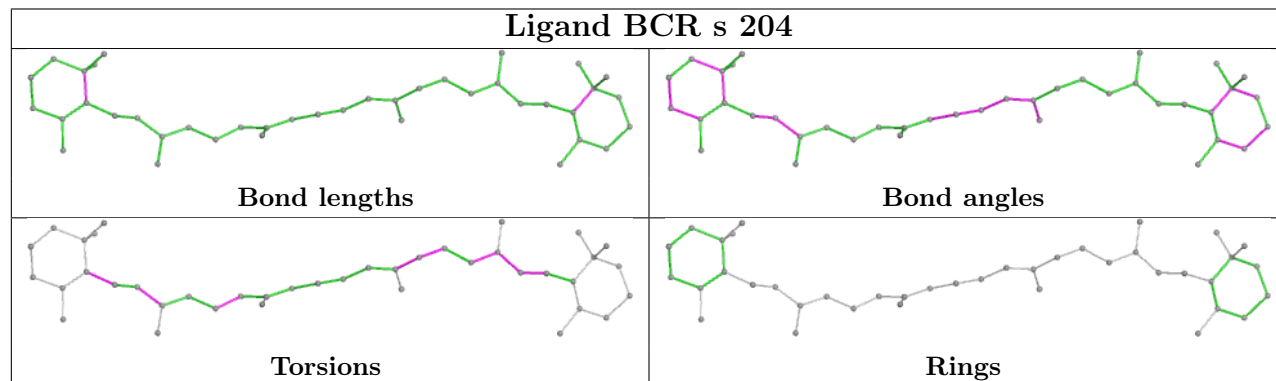




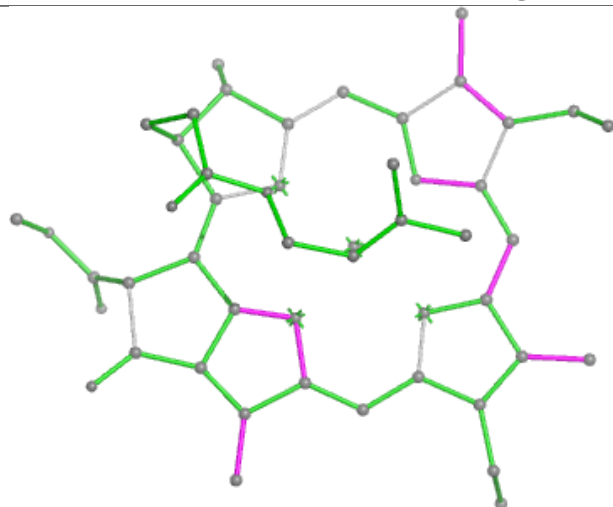
Ligand CLA g 816



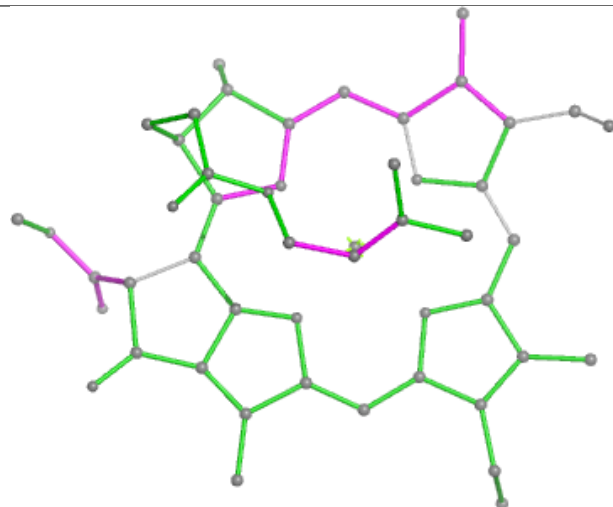
Ligand BCR s 204



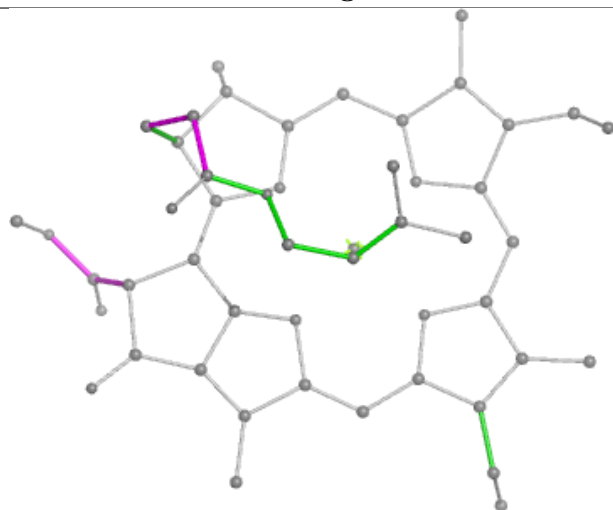
Ligand CLA G 823



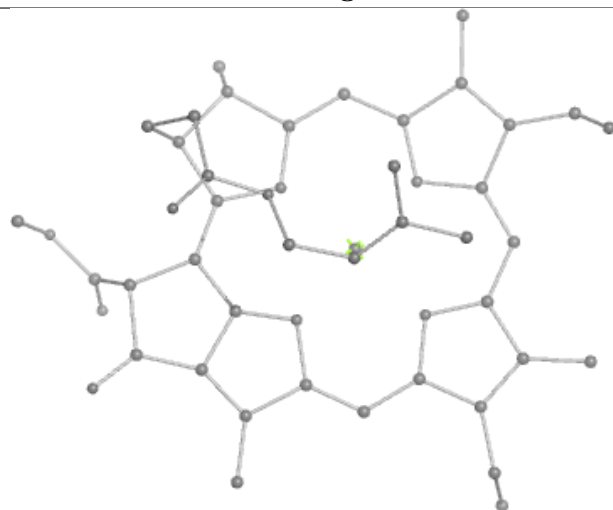
Bond lengths



Bond angles

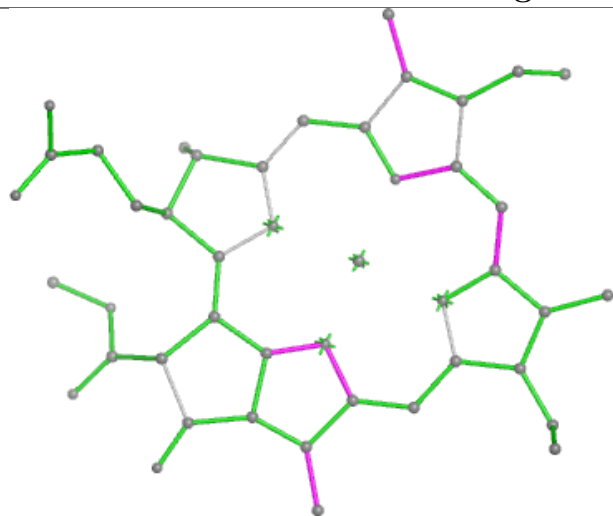


Torsions

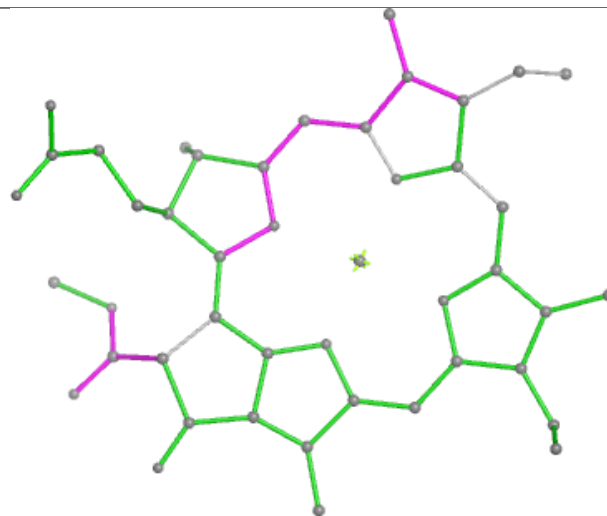


Rings

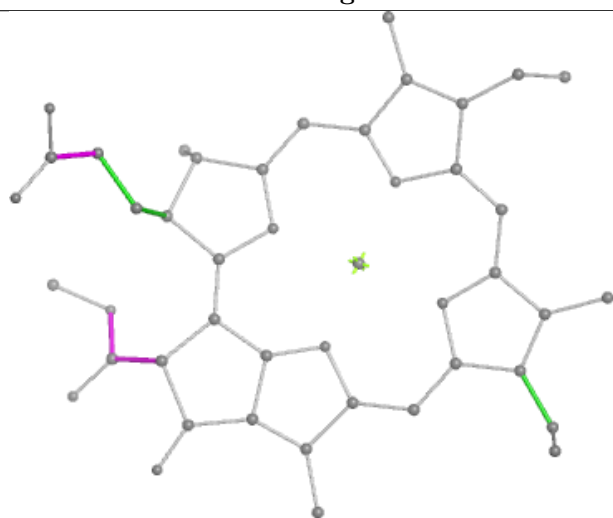
Ligand CLA B 824



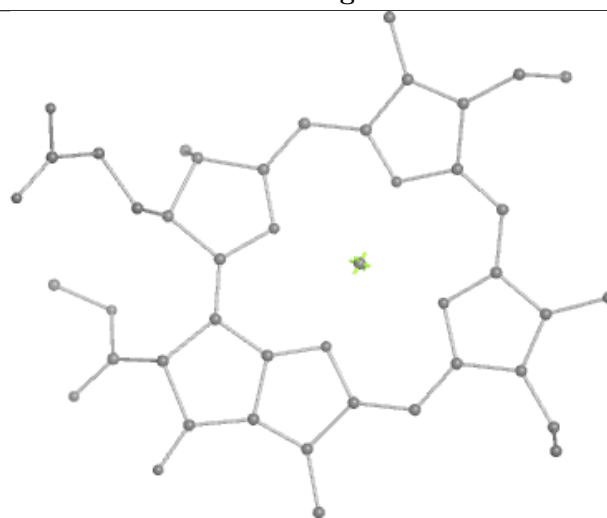
Bond lengths



Bond angles

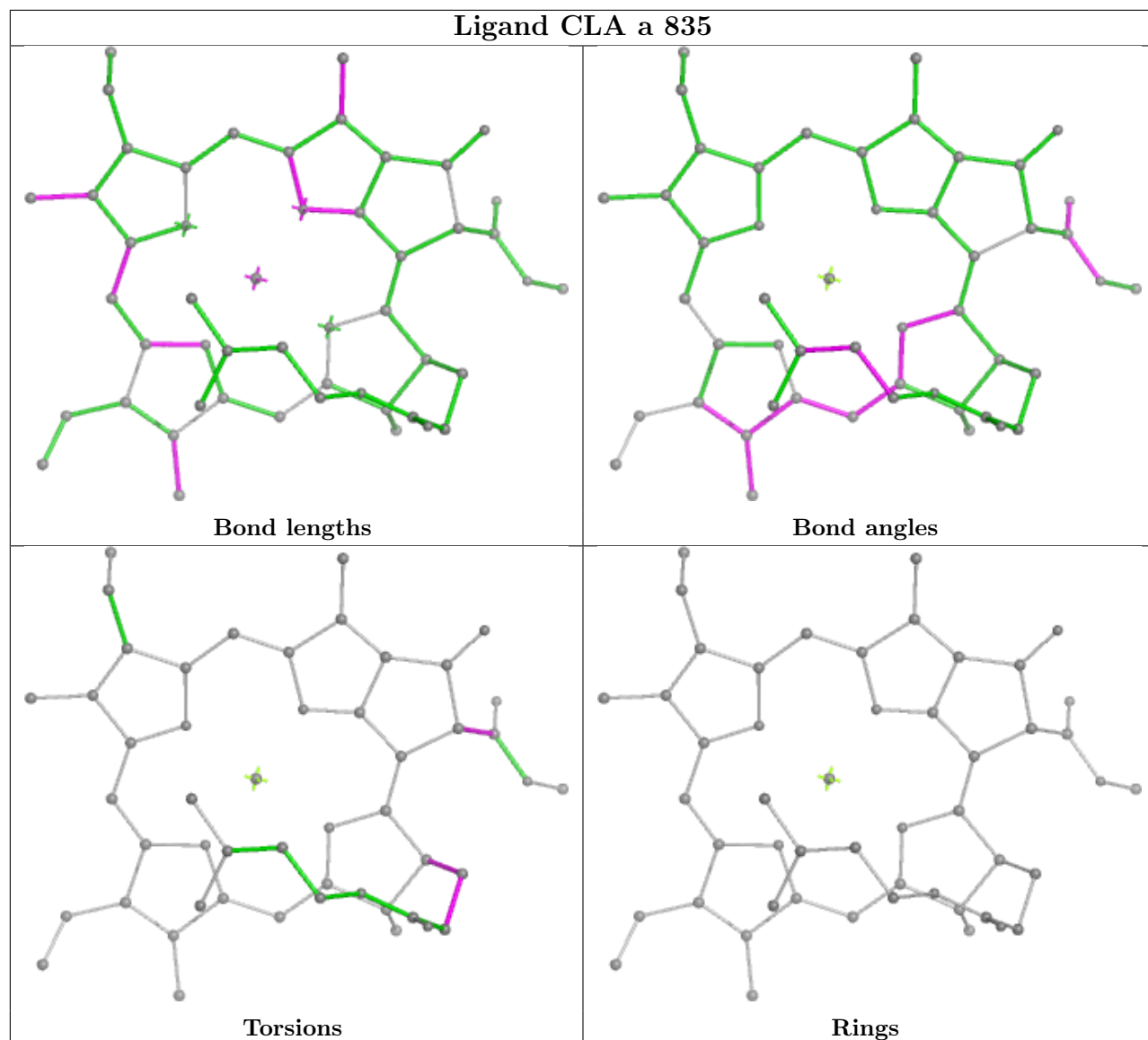


Torsions

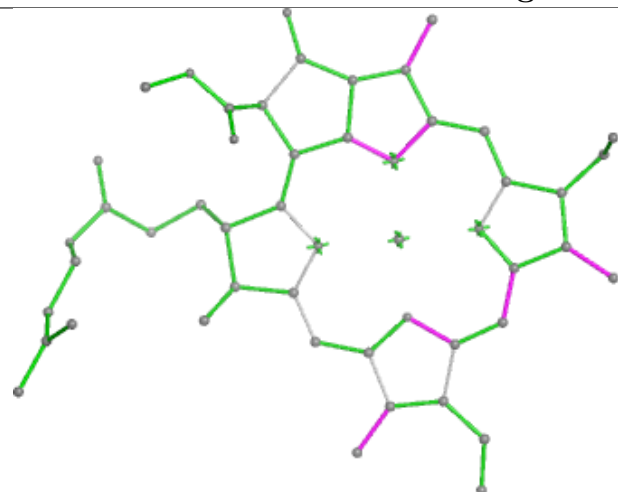


Rings

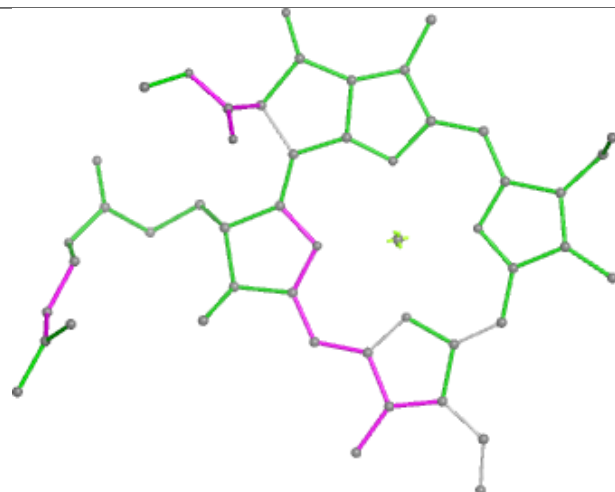
Ligand CLA a 835



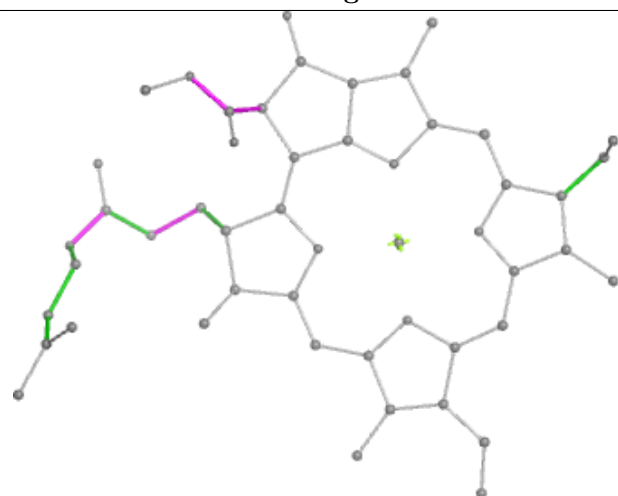
Ligand CLA G 825



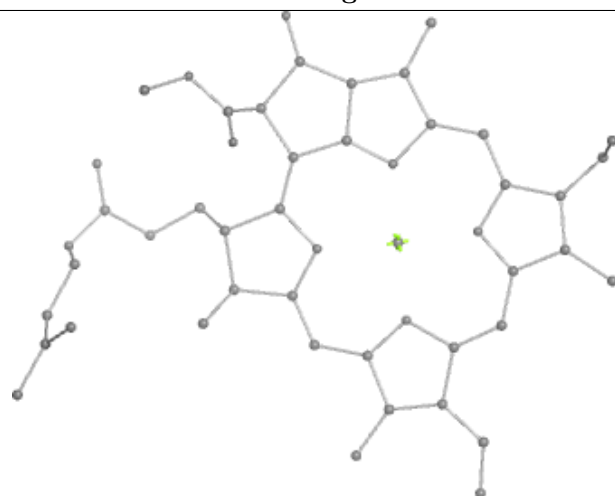
Bond lengths



Bond angles

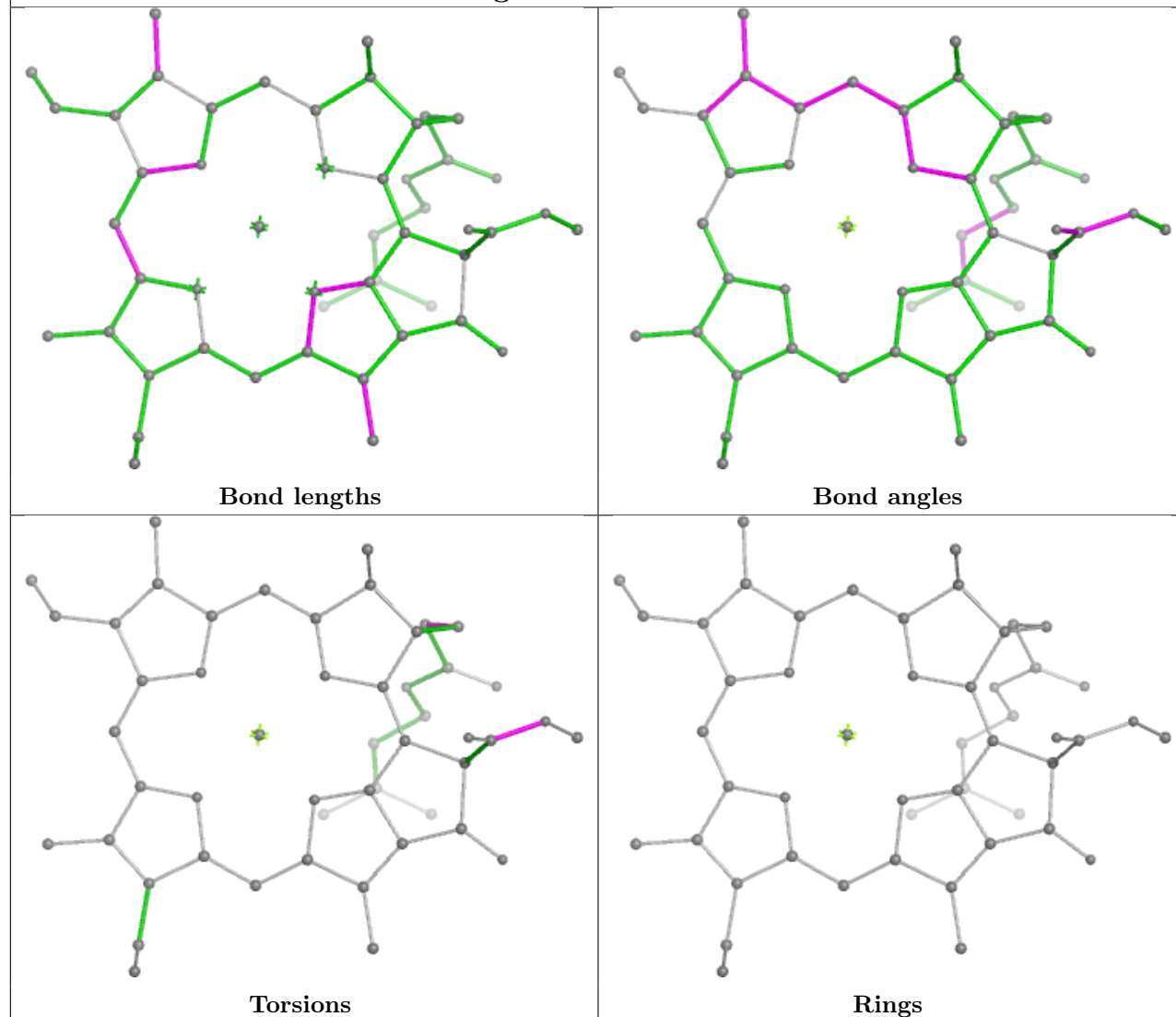


Torsions

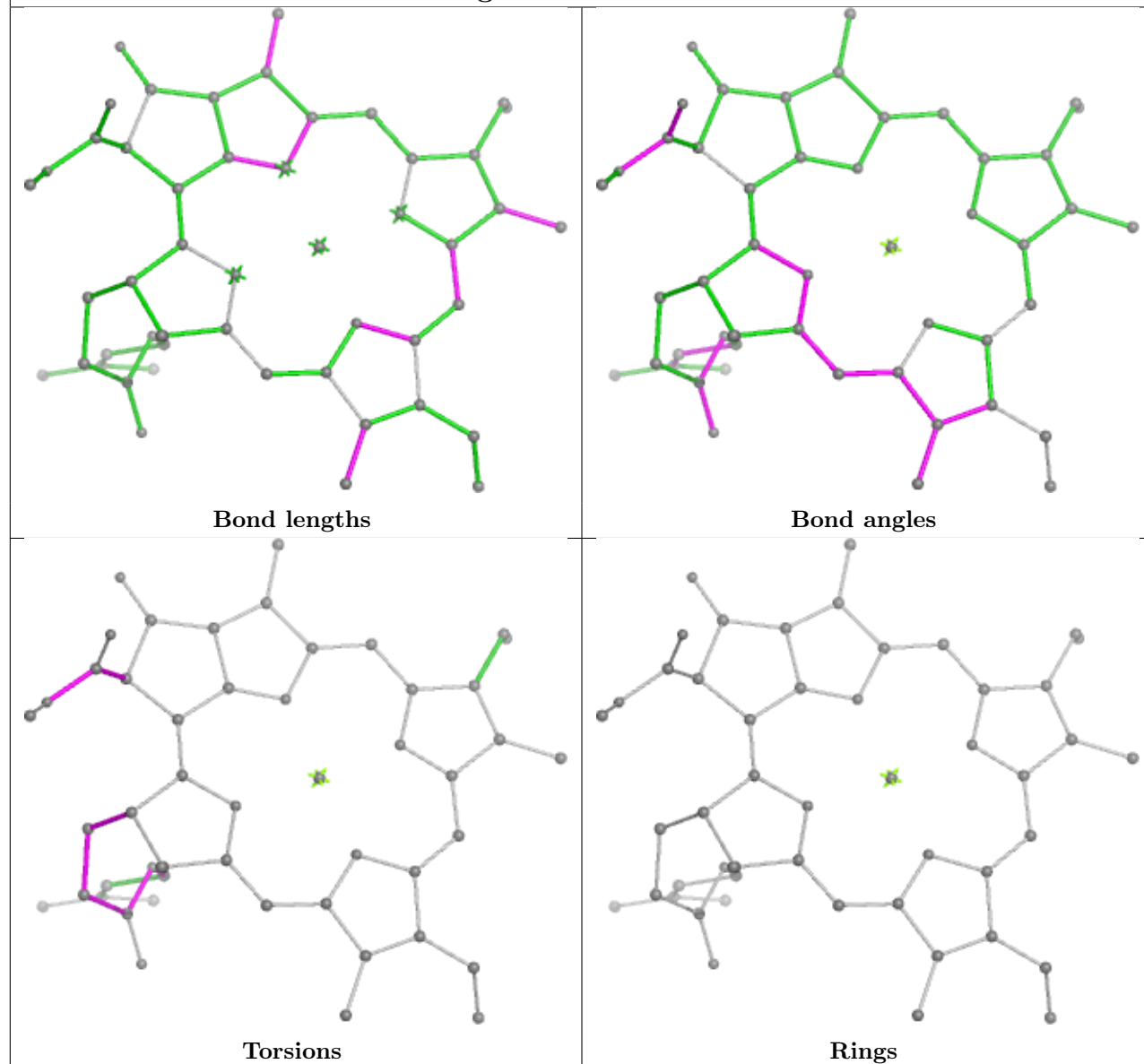


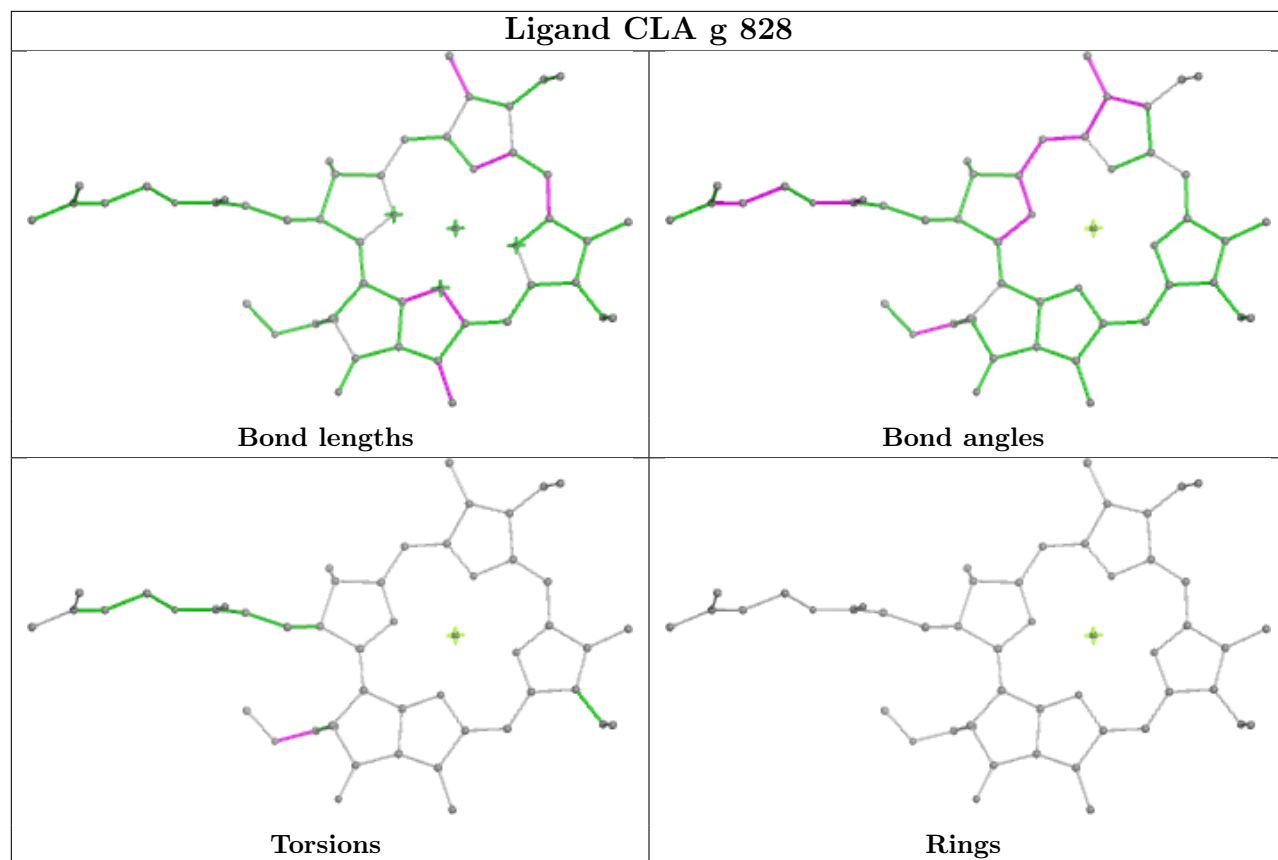
Rings

Ligand CLA b 814

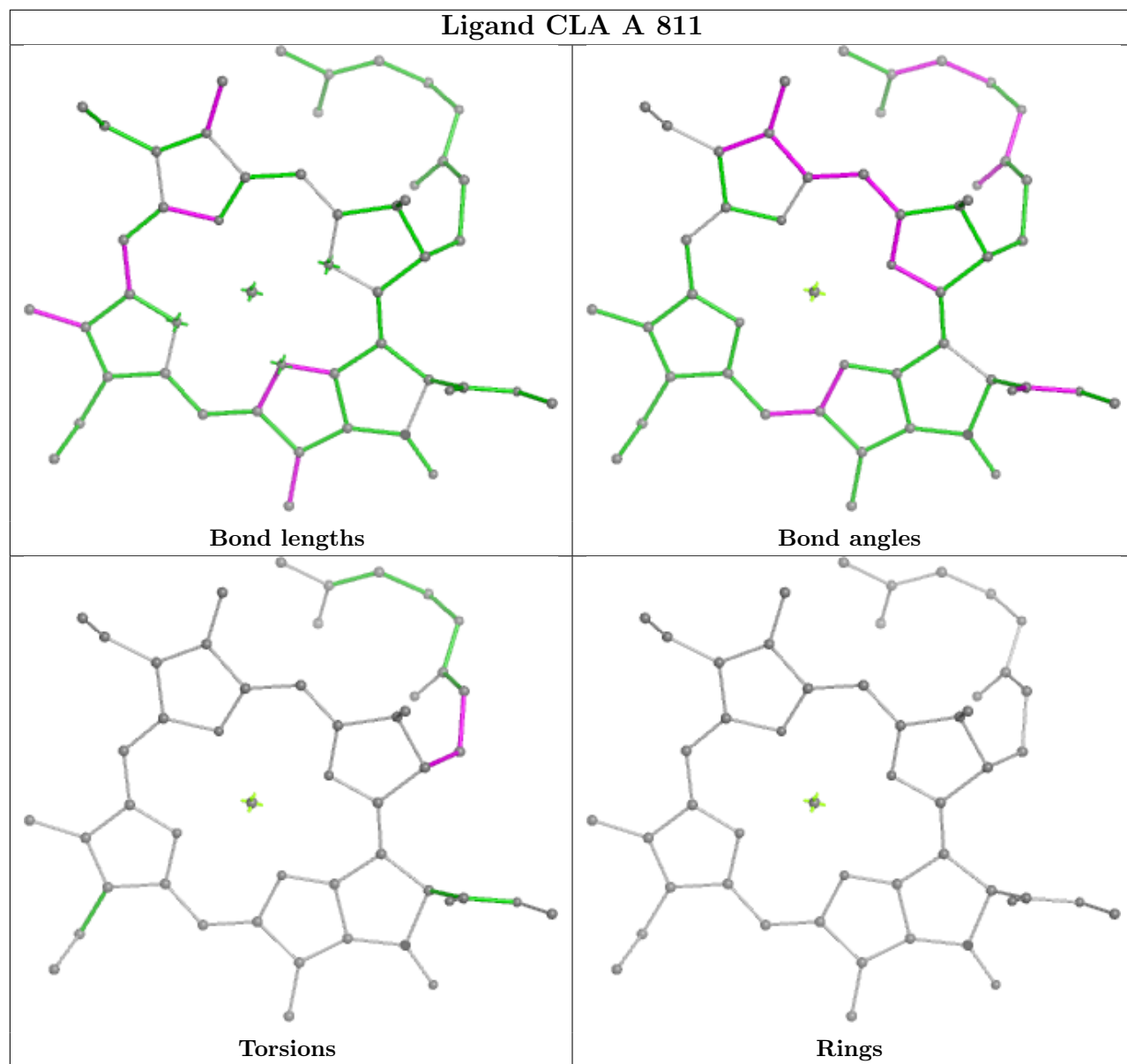


Ligand CLA B 829

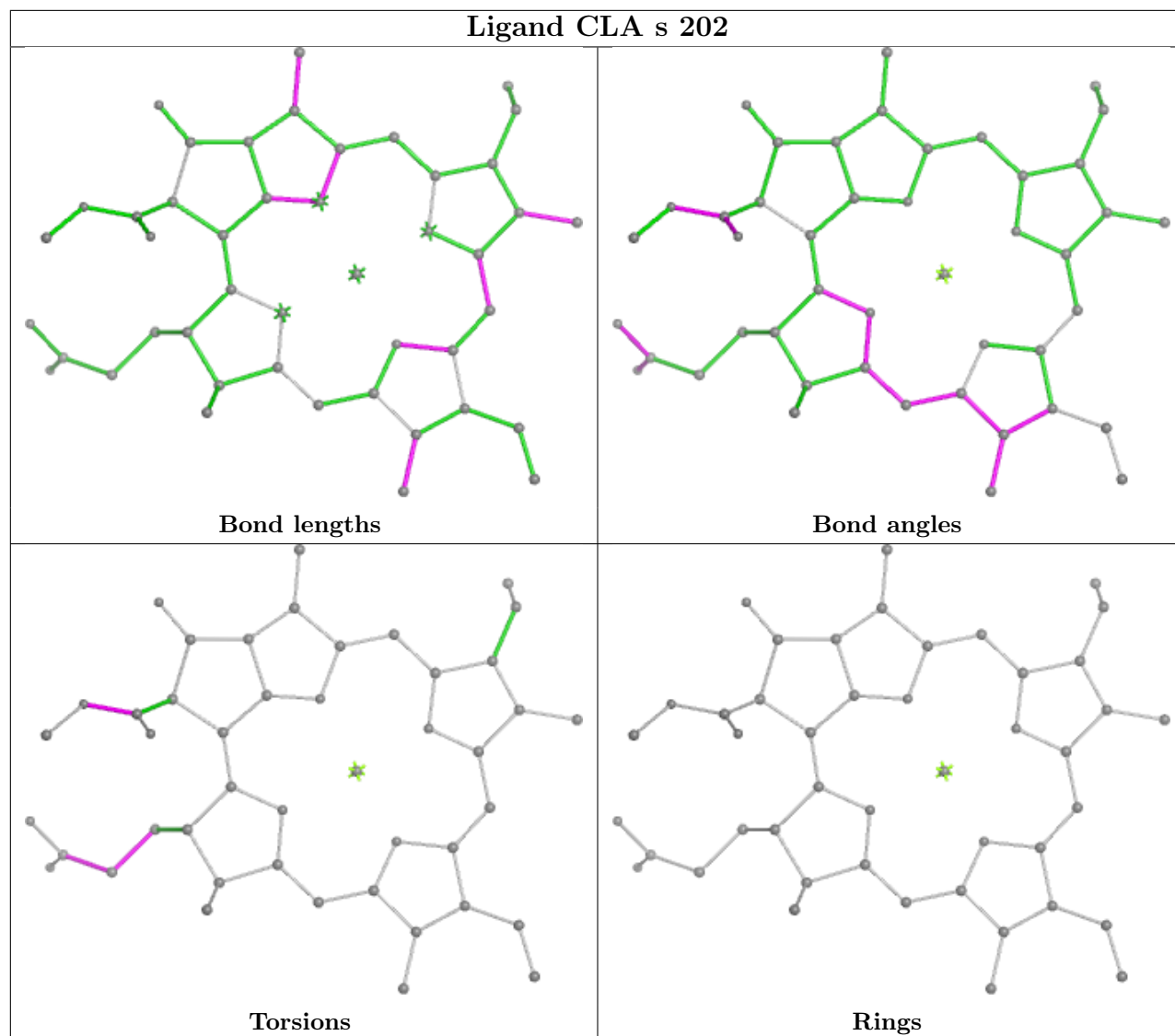




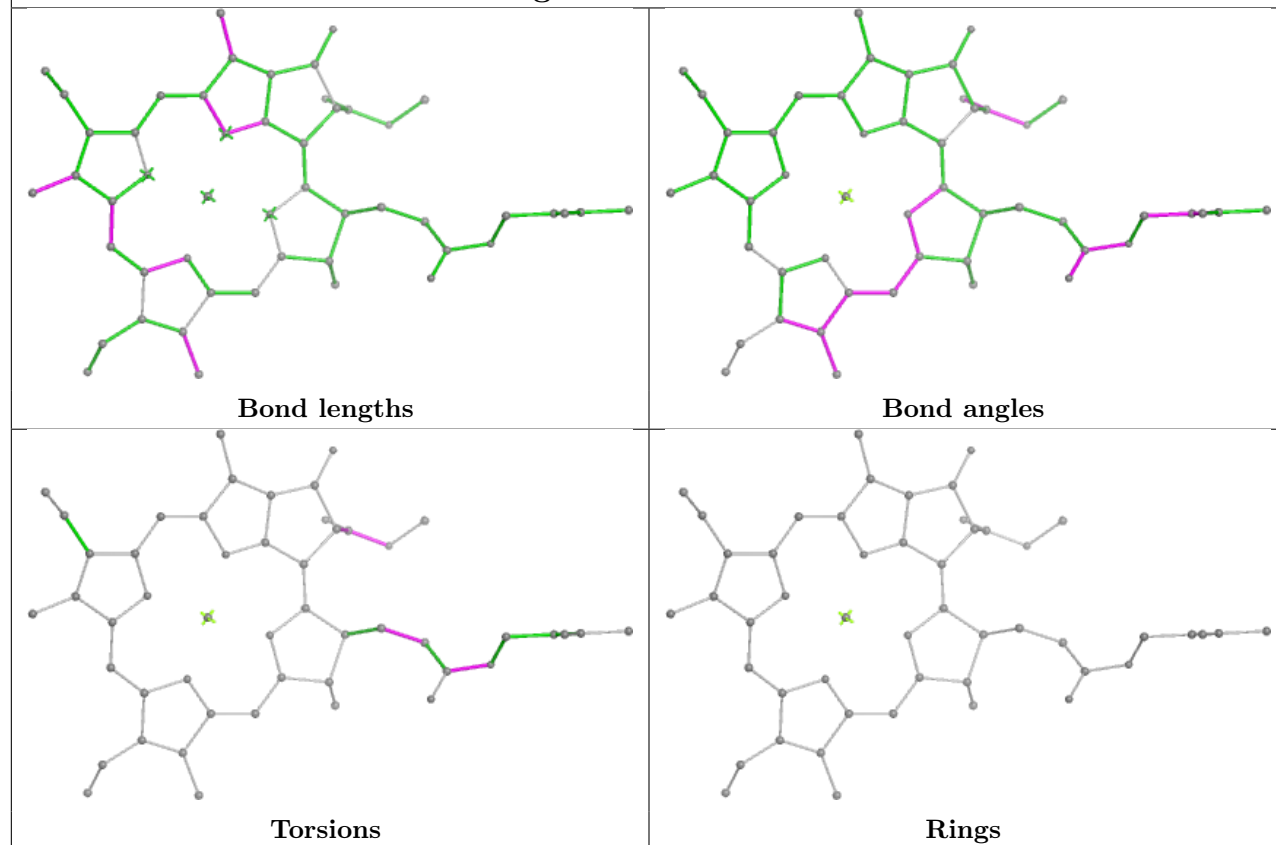
Ligand CLA A 811



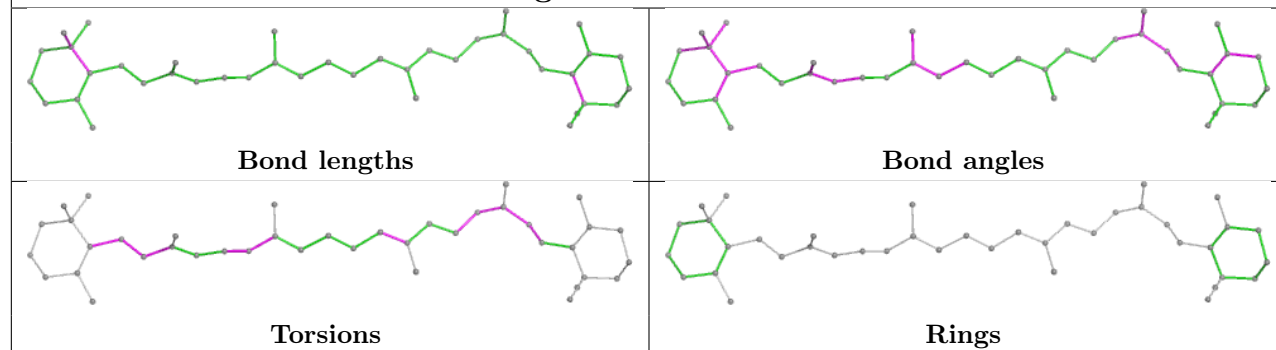
Ligand CLA s 202



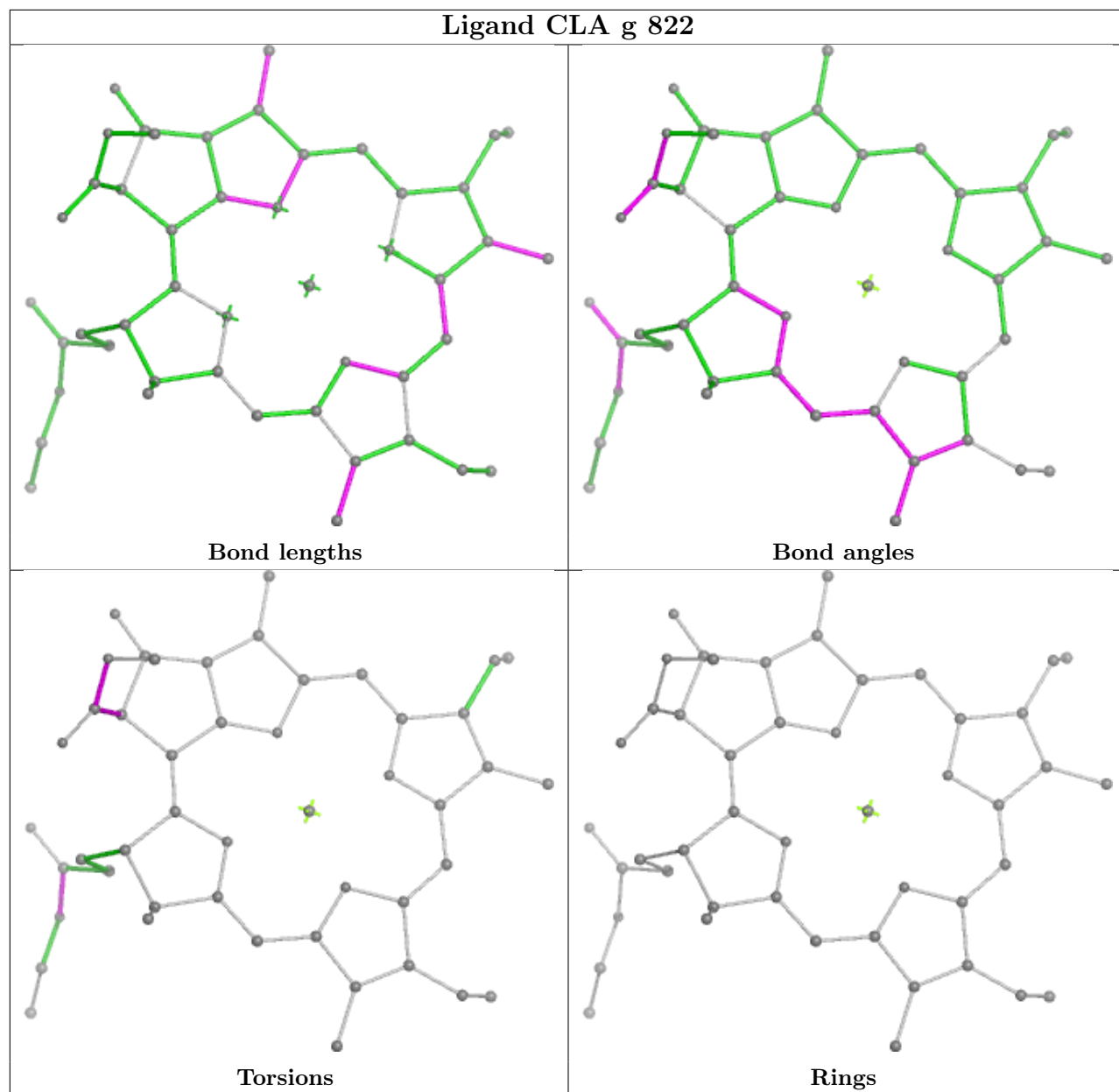
Ligand CLA E 844



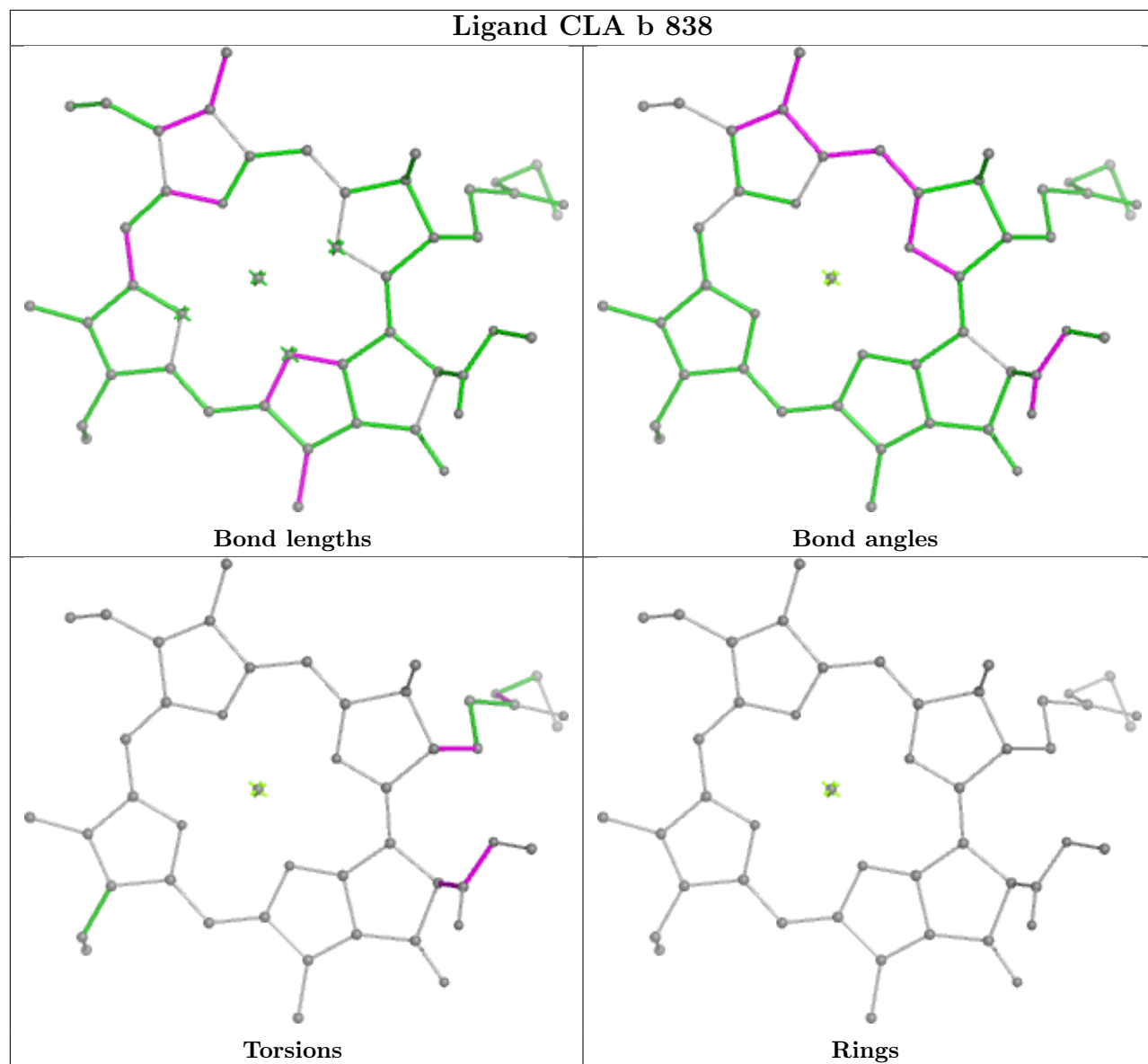
Ligand BCR a 848



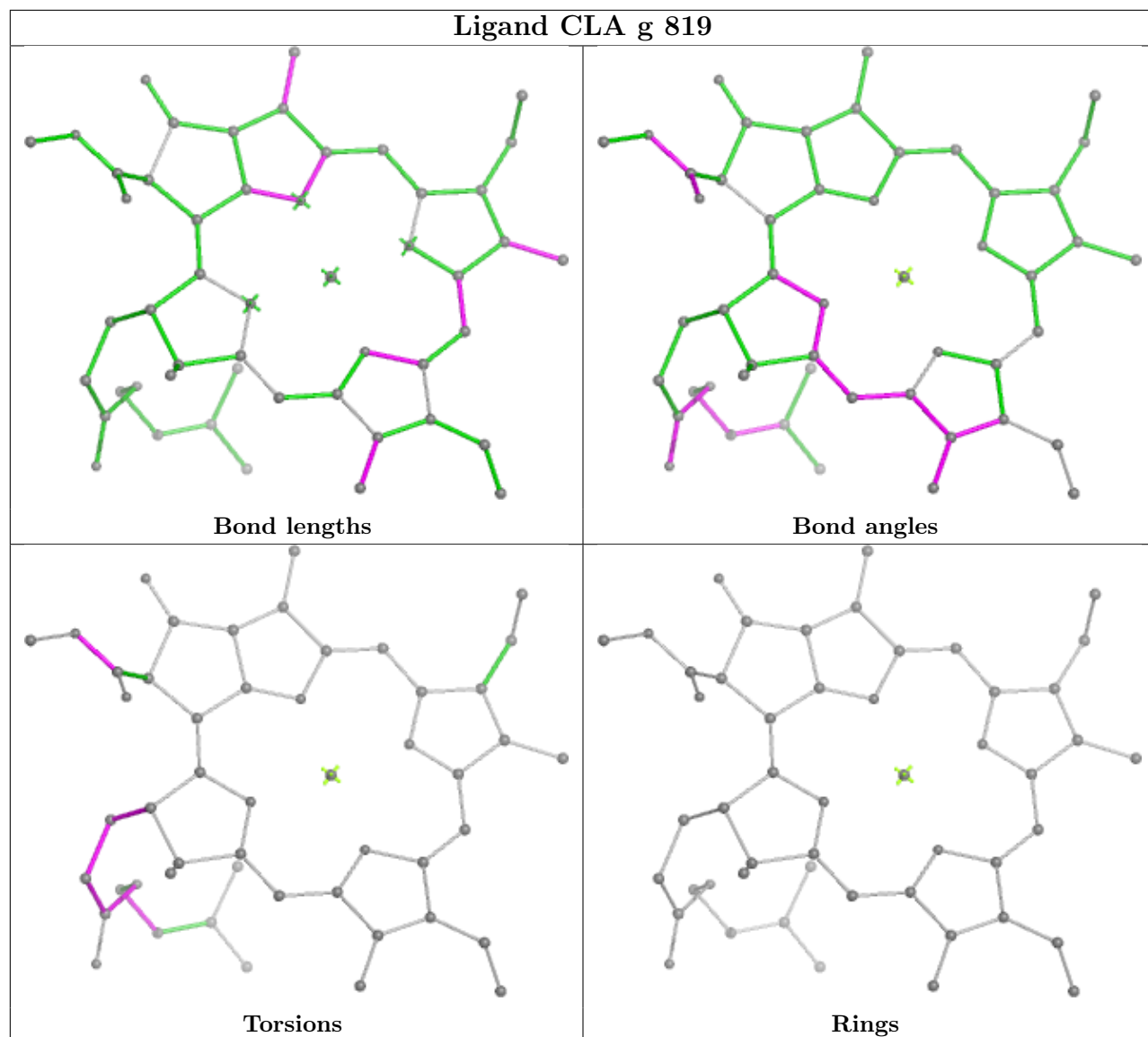
Ligand CLA g 822



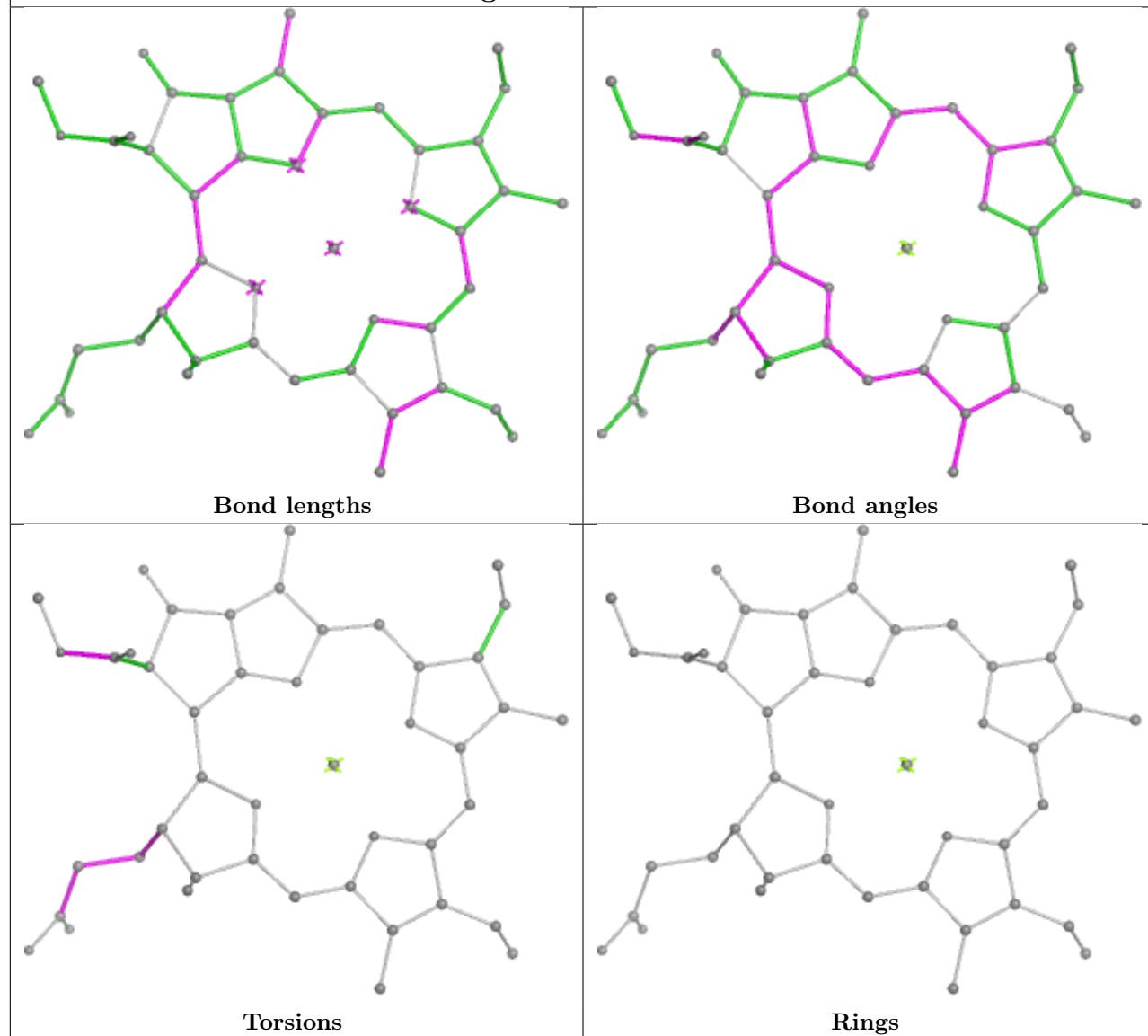
Ligand CLA b 838



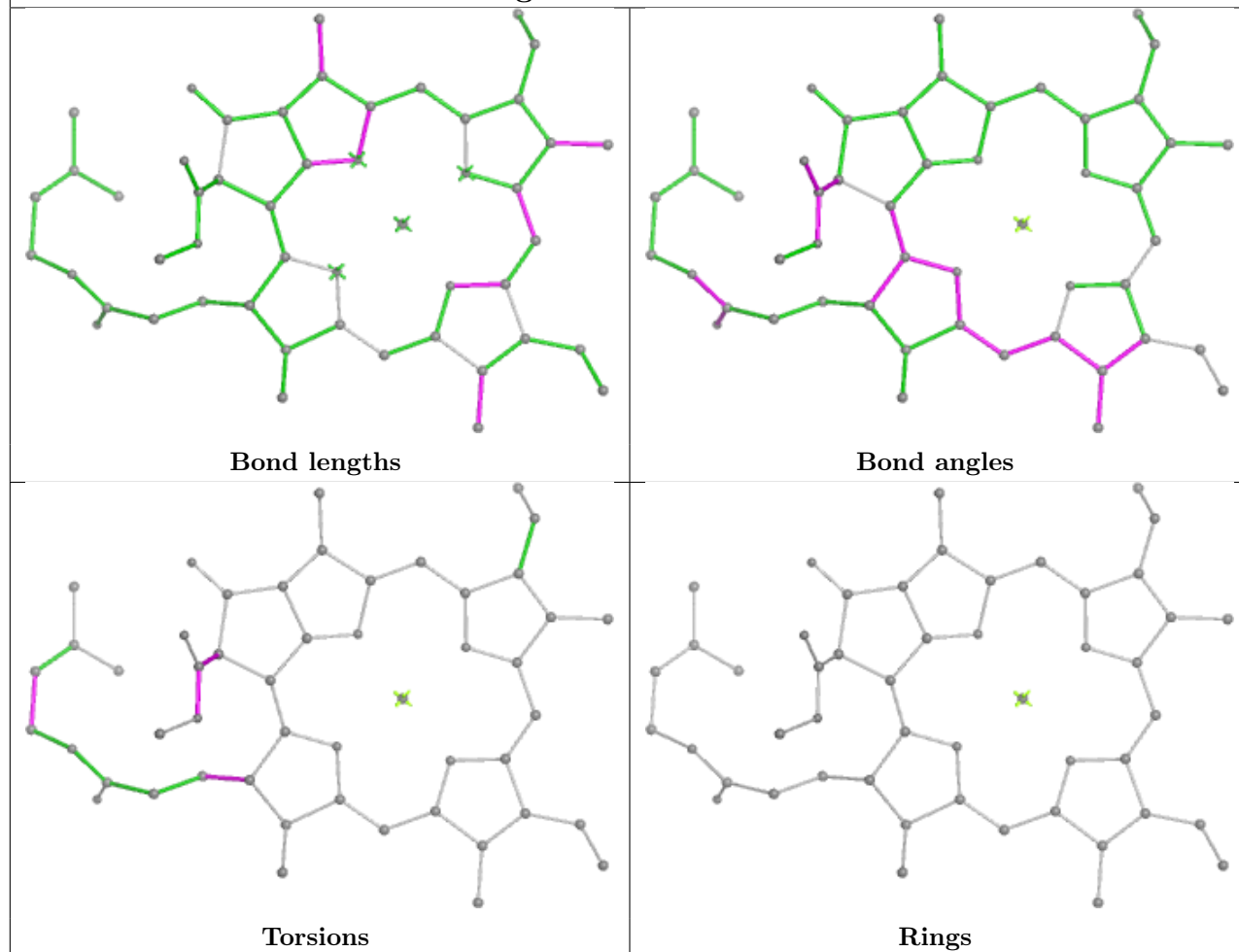
Ligand CLA g 819



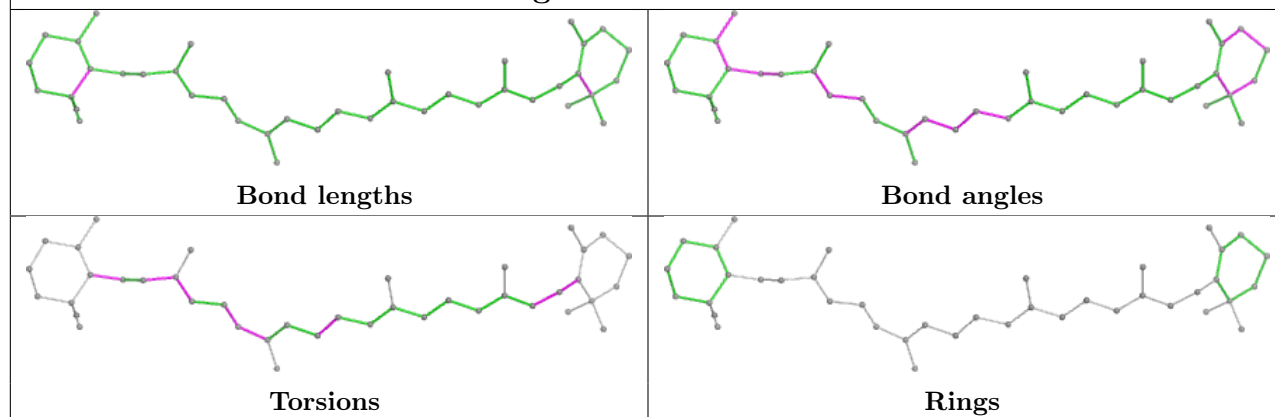
Ligand CLA S 204



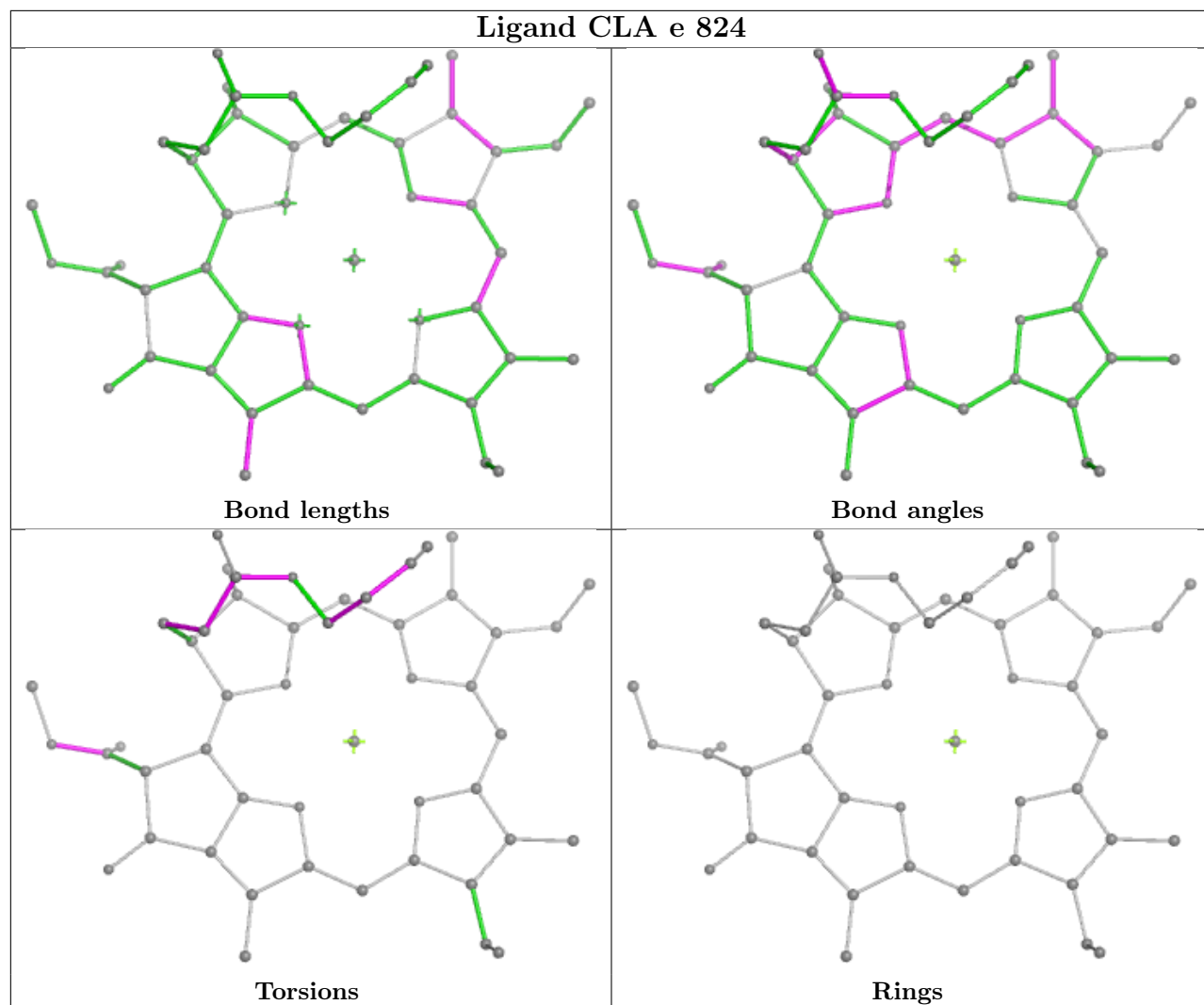
Ligand CLA A 828



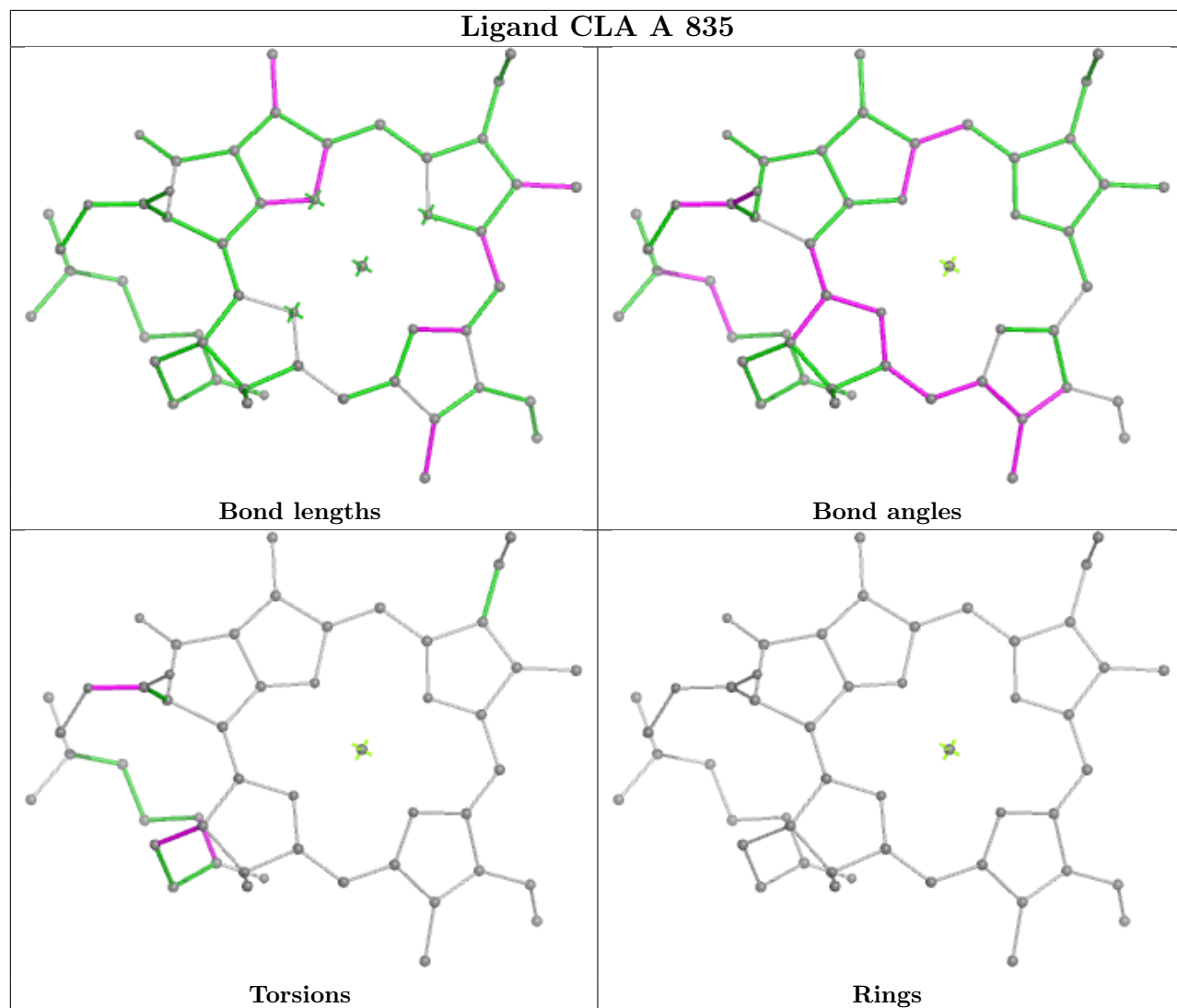
Ligand BCR J 102



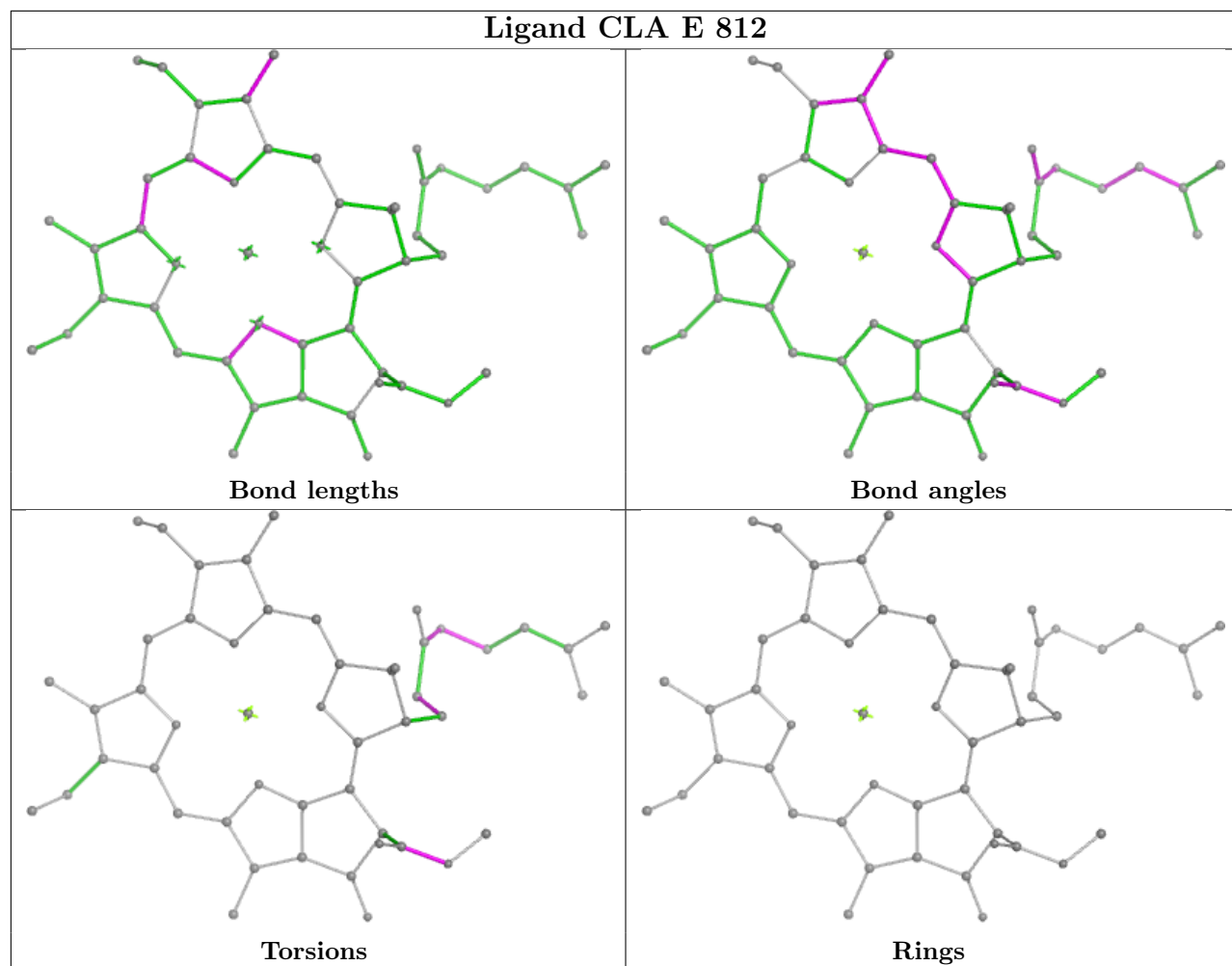
Ligand CLA e 824



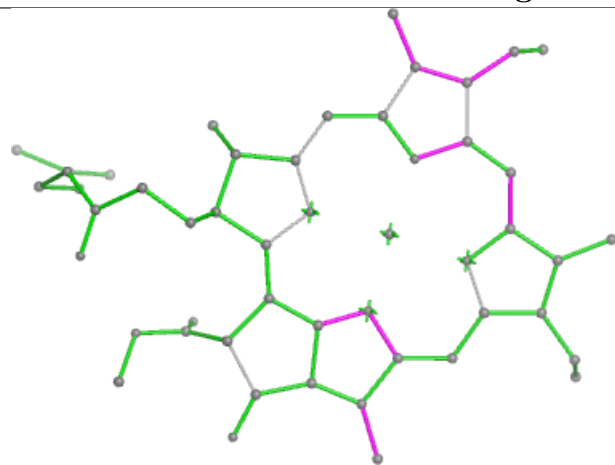
Ligand CLA A 835



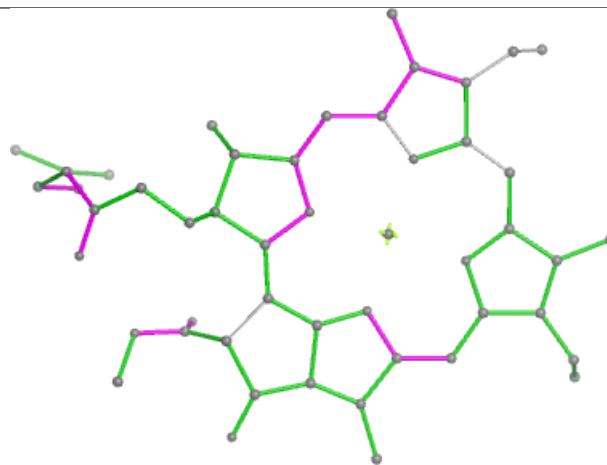
Ligand CLA E 812



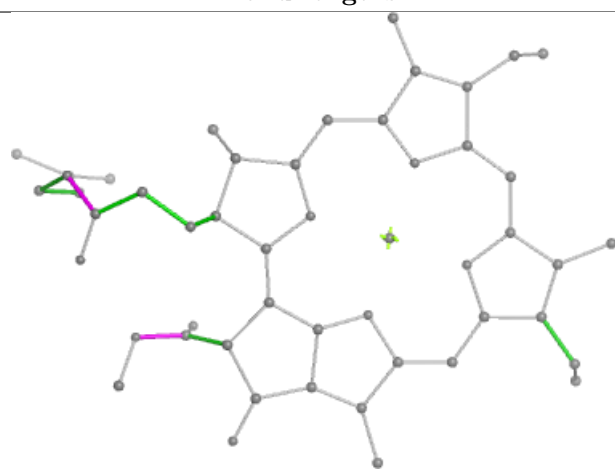
Ligand CLA G 807



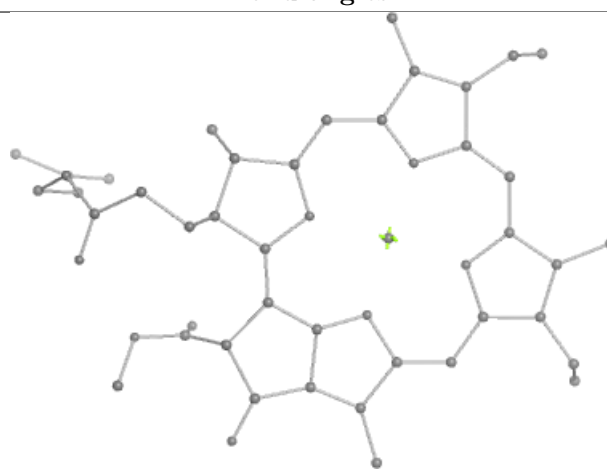
Bond lengths



Bond angles

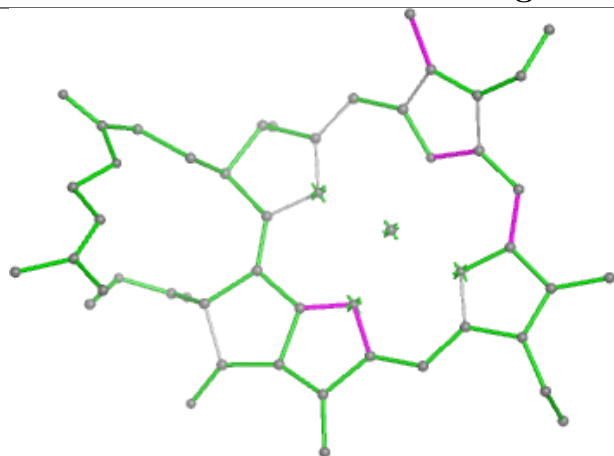


Torsions

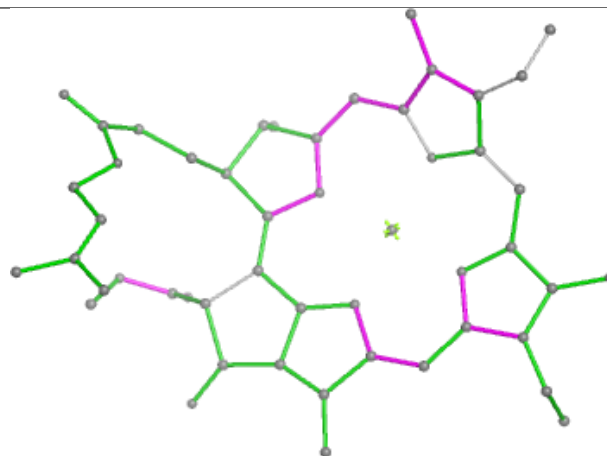


Rings

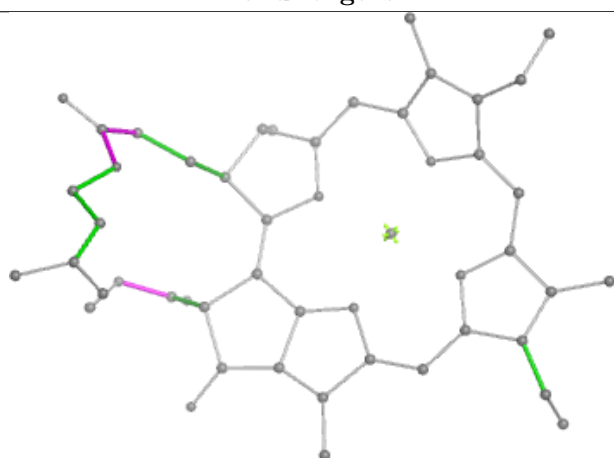
Ligand CLA E 803



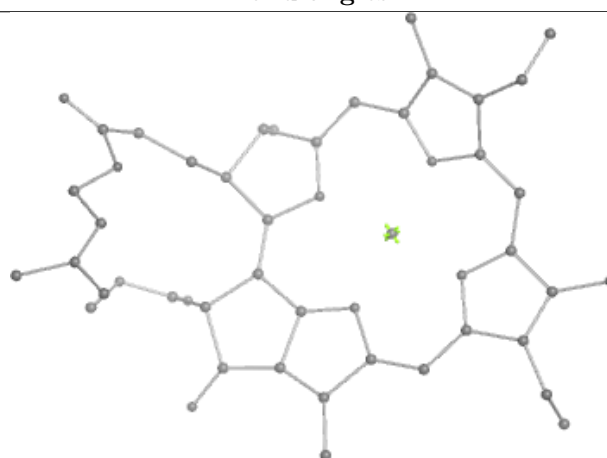
Bond lengths



Bond angles

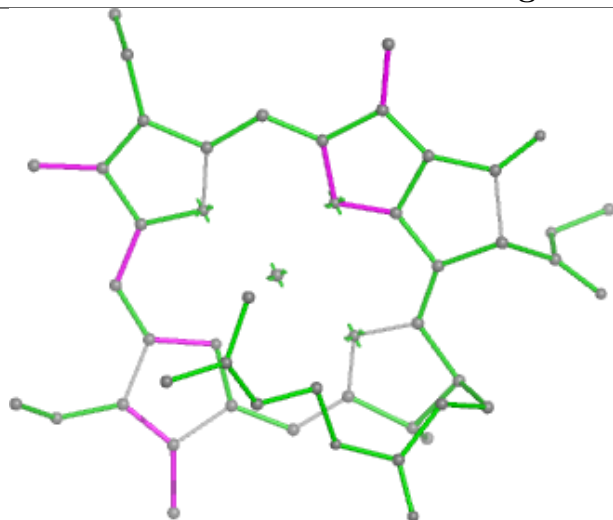


Torsions

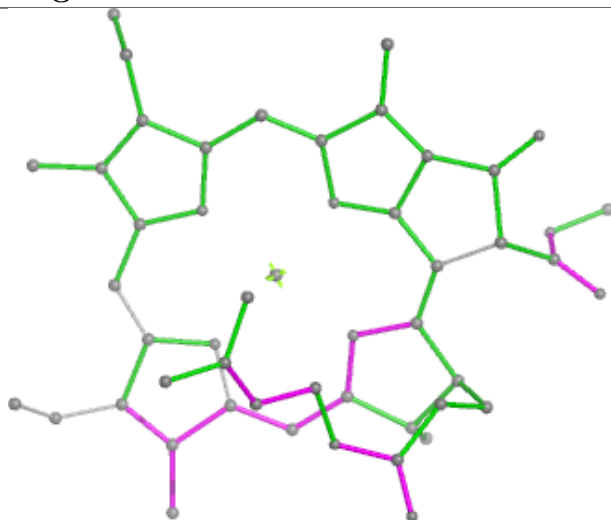


Rings

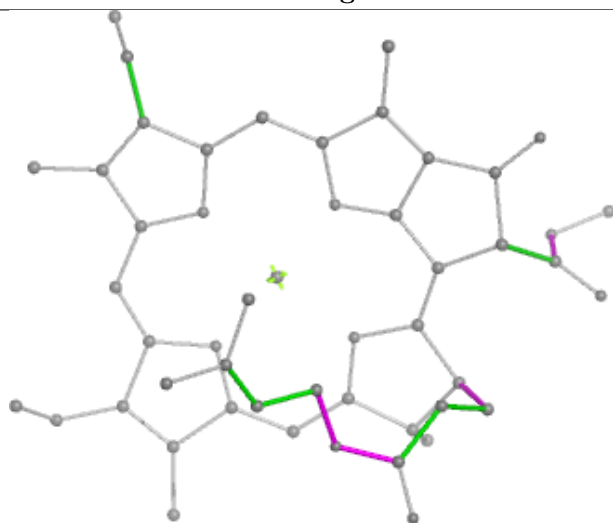
Ligand CLA g 829



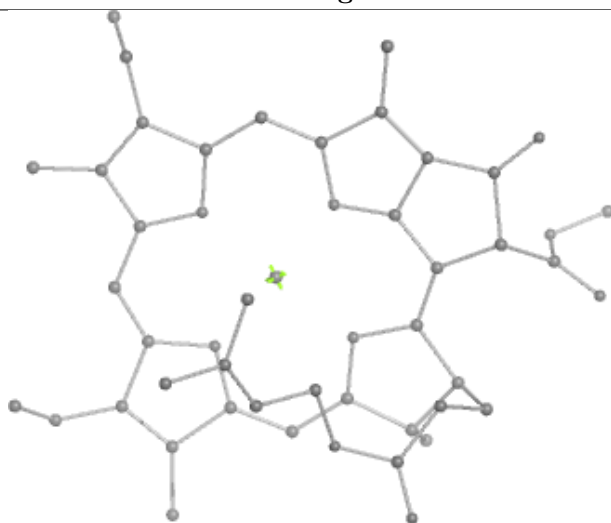
Bond lengths



Bond angles

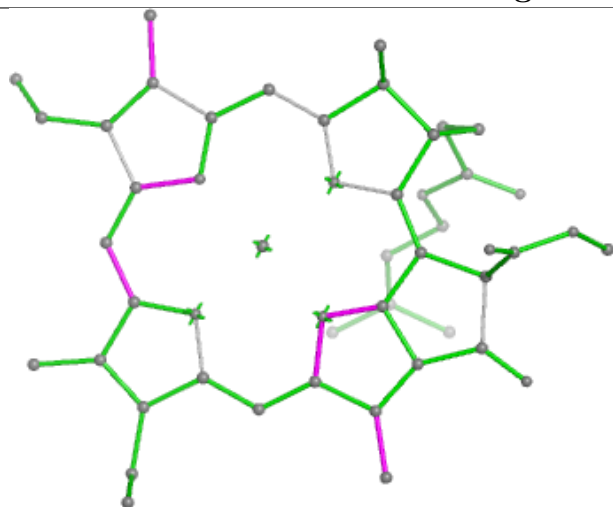


Torsions

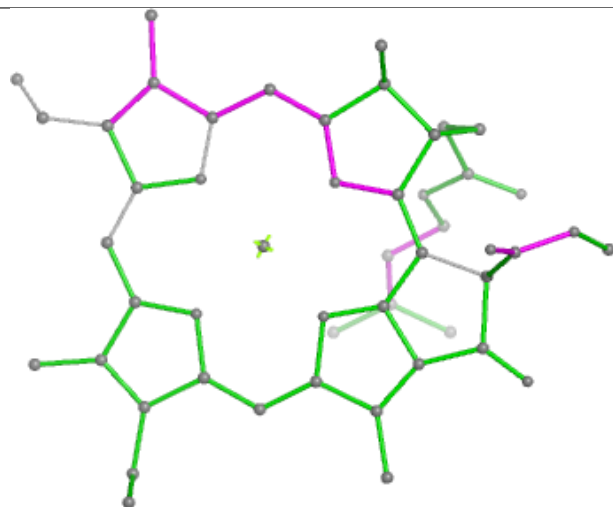


Rings

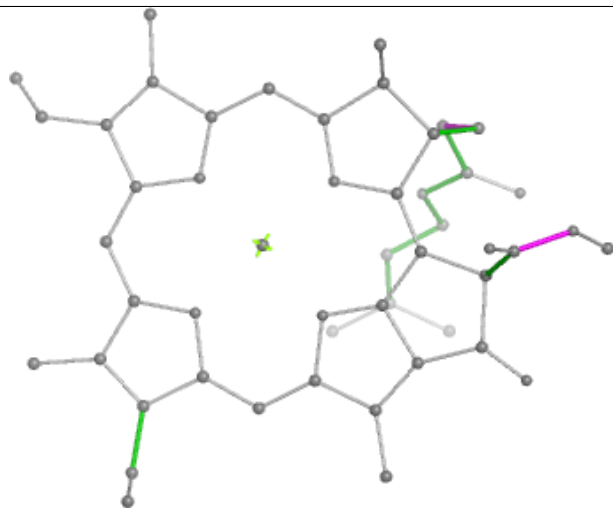
Ligand CLA B 815



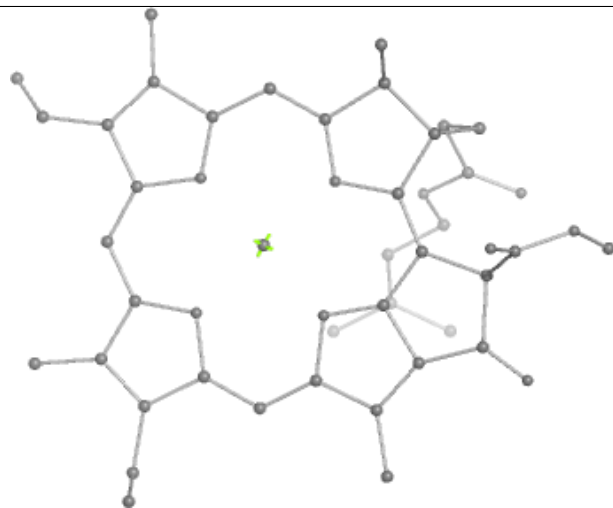
Bond lengths



Bond angles

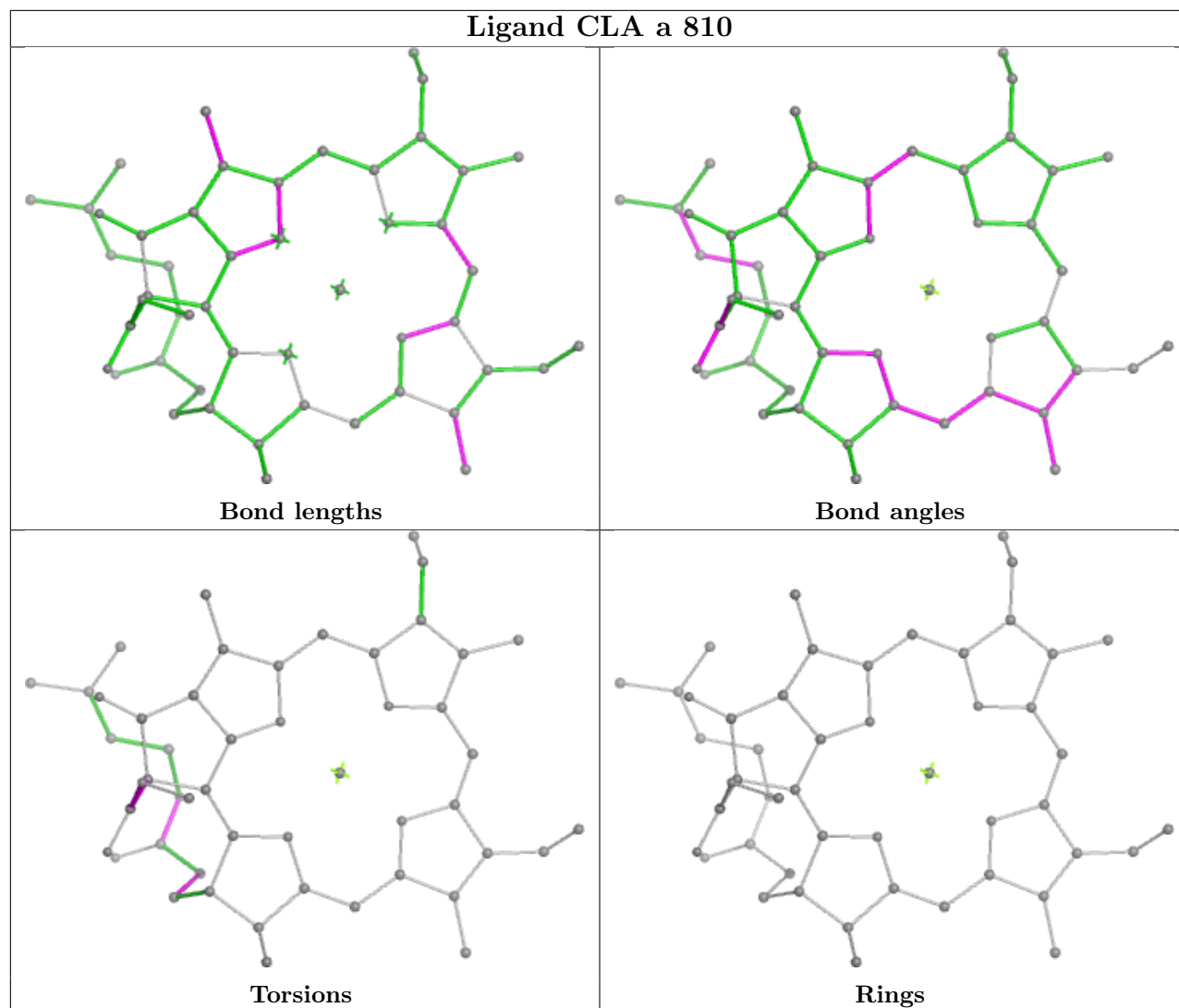


Torsions

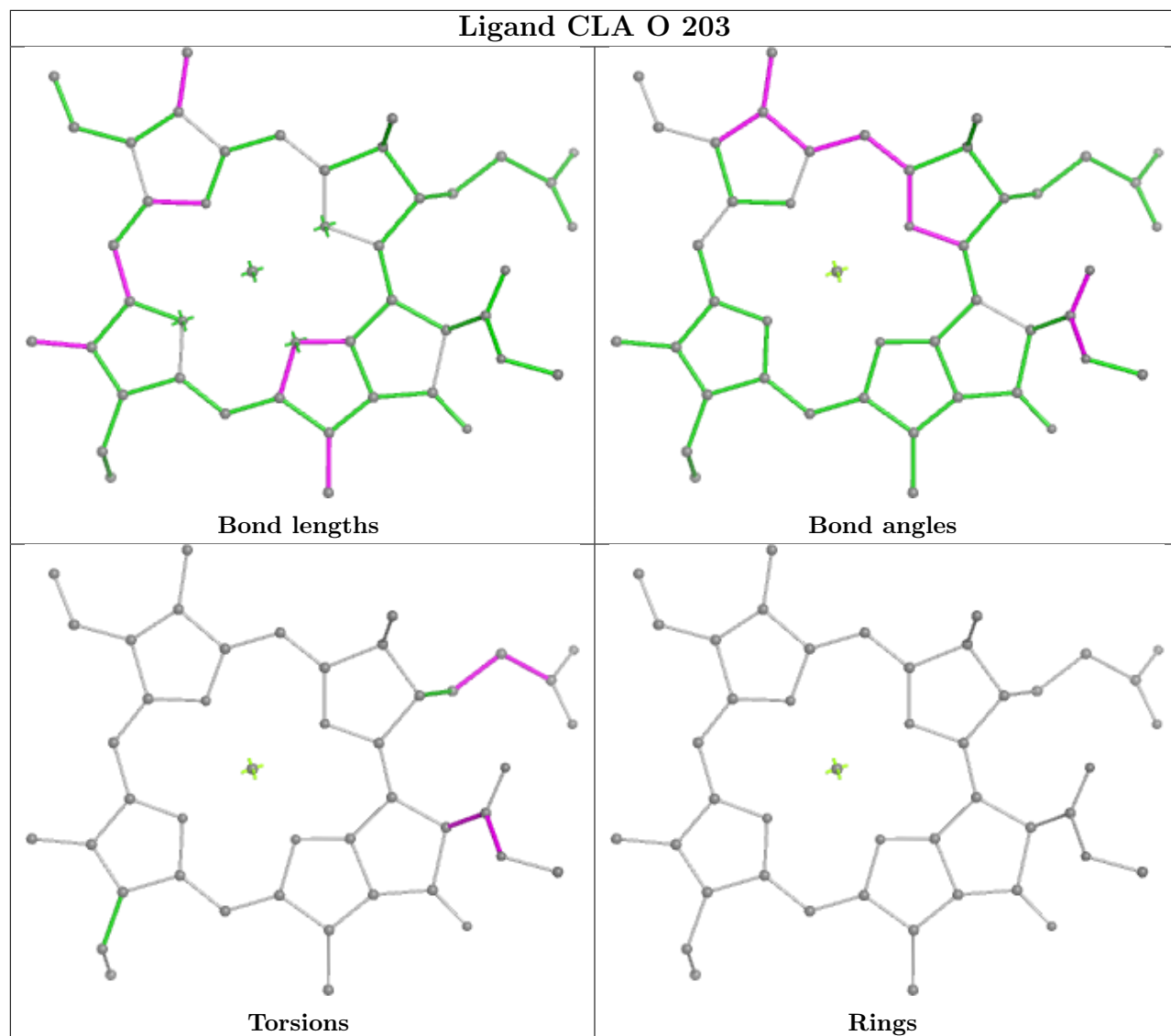


Rings

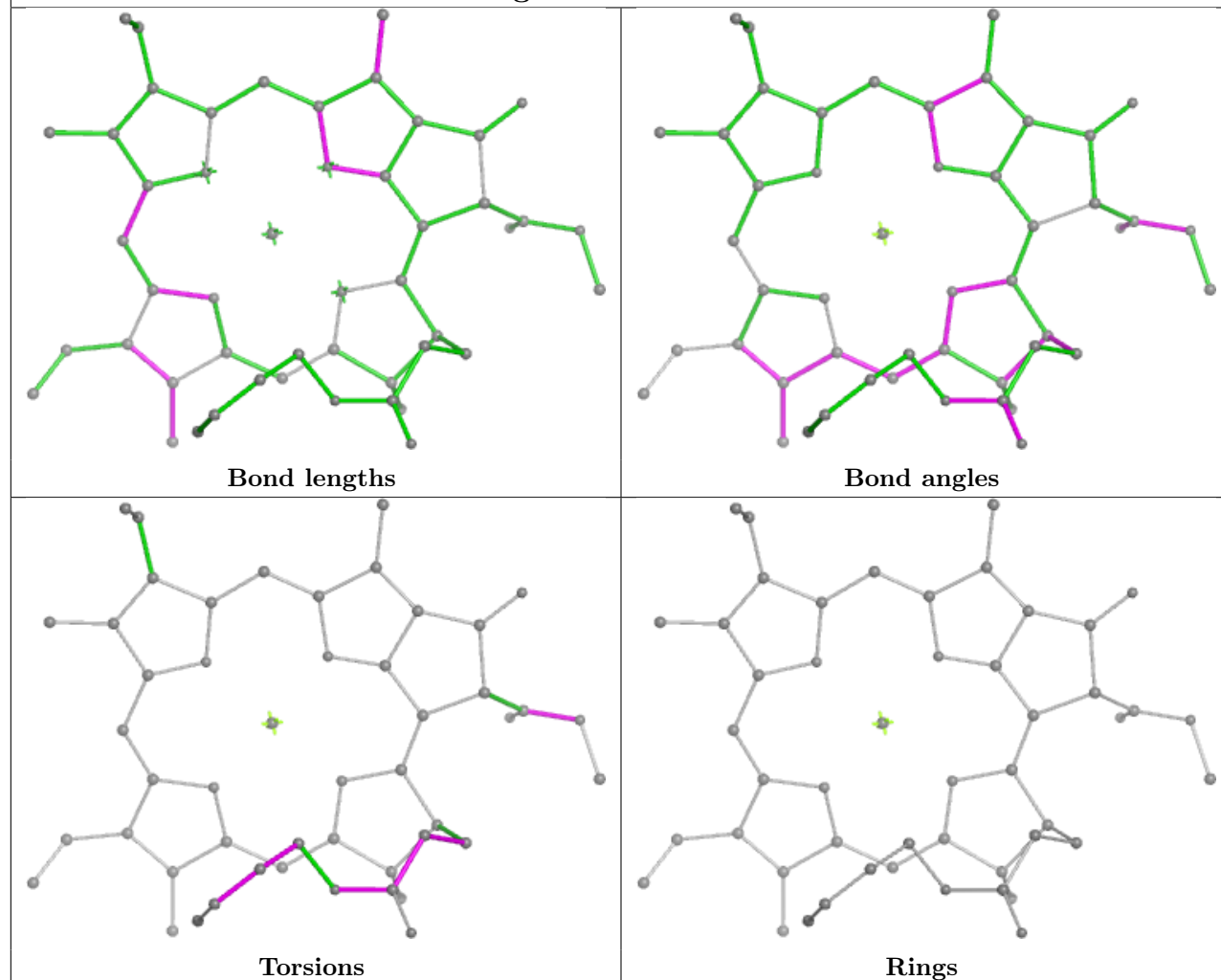
Ligand CLA a 810



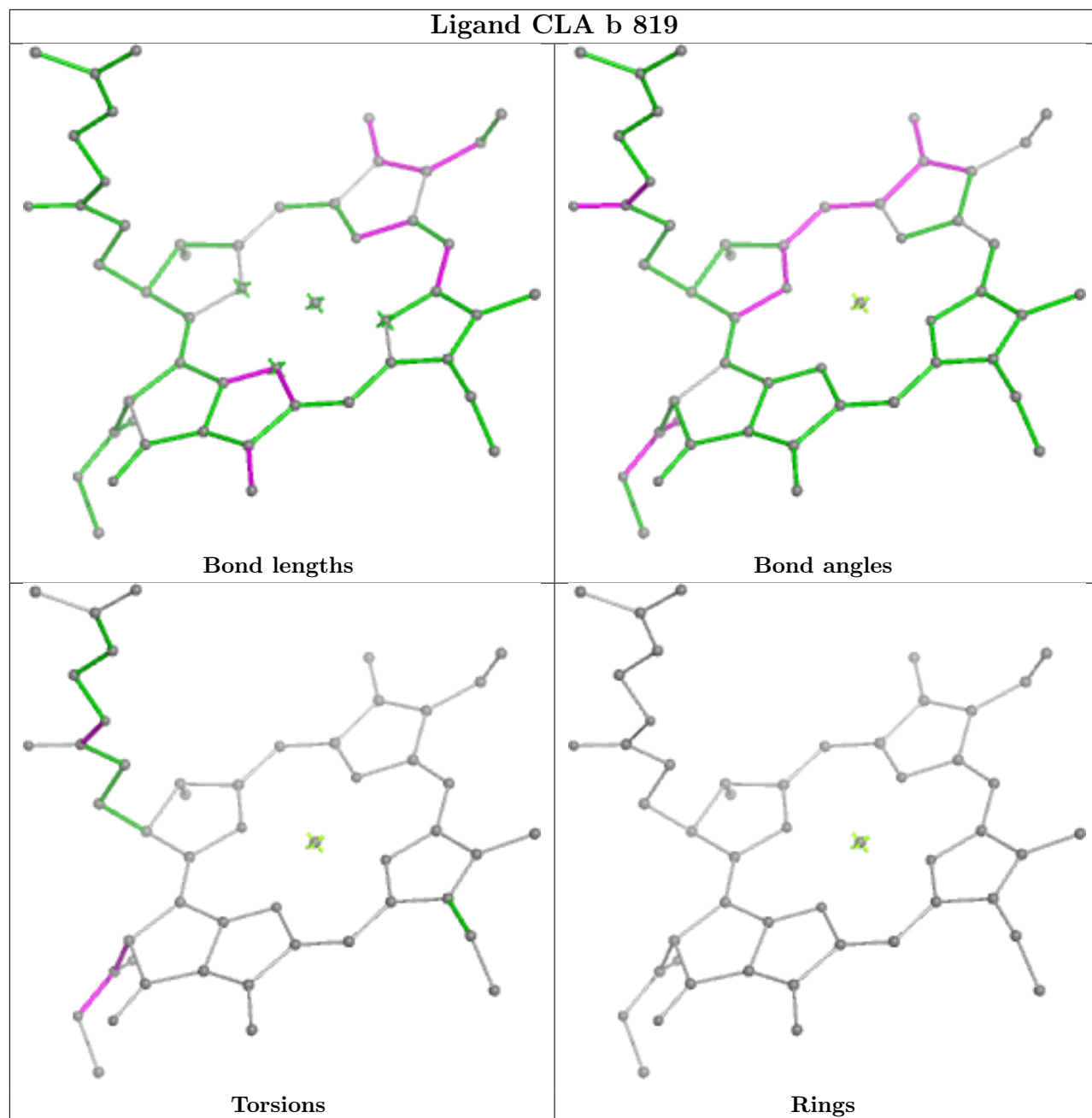
Ligand CLA O 203



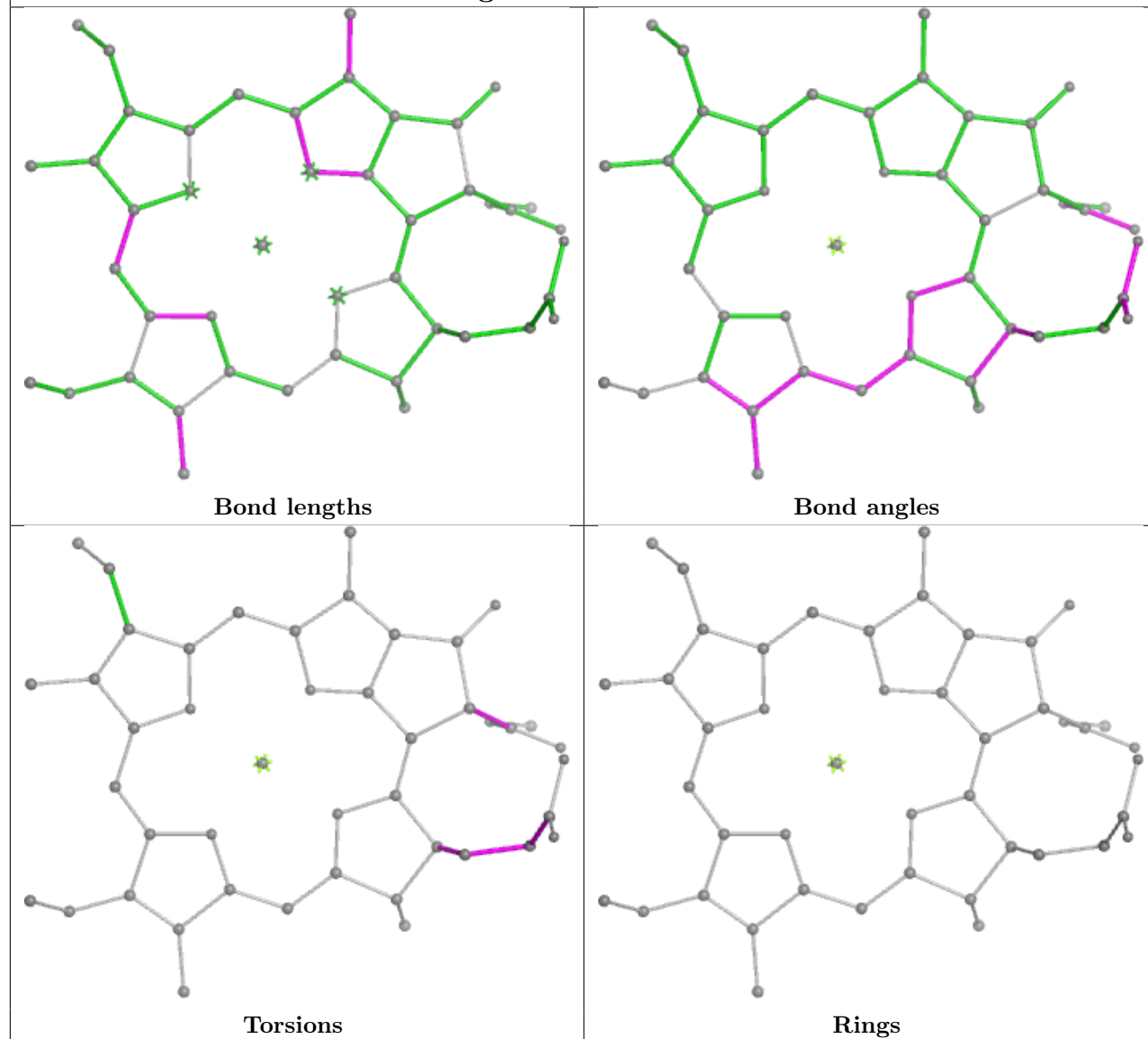
Ligand CLA a 825



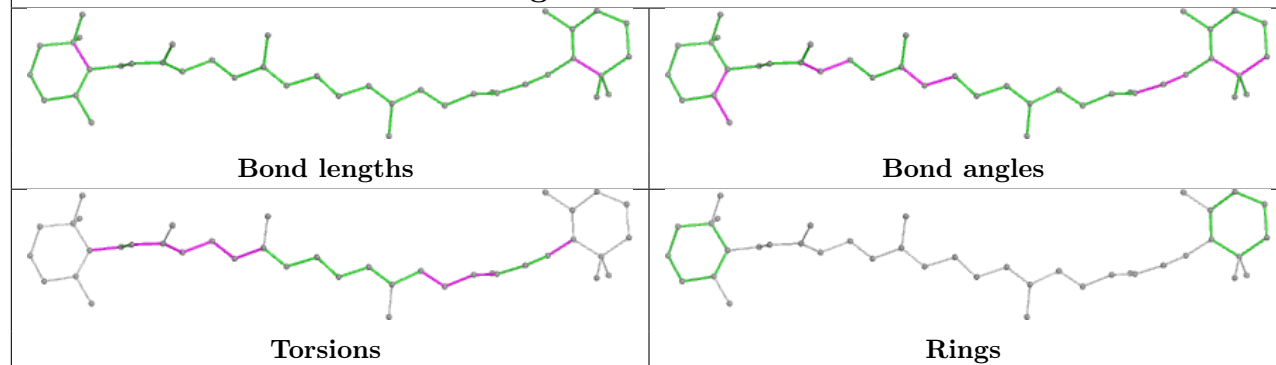
Ligand CLA b 819



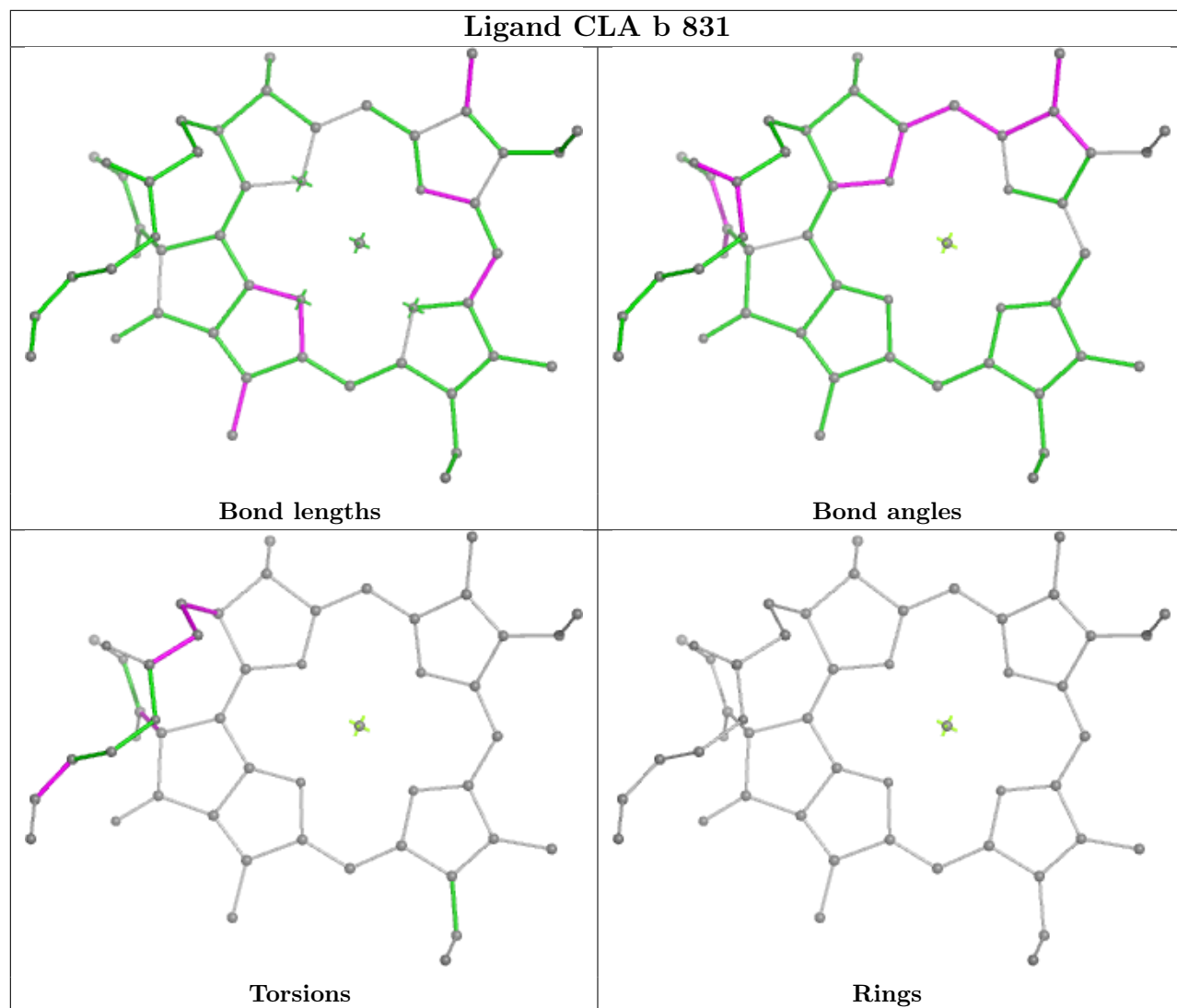
Ligand CLA R 102



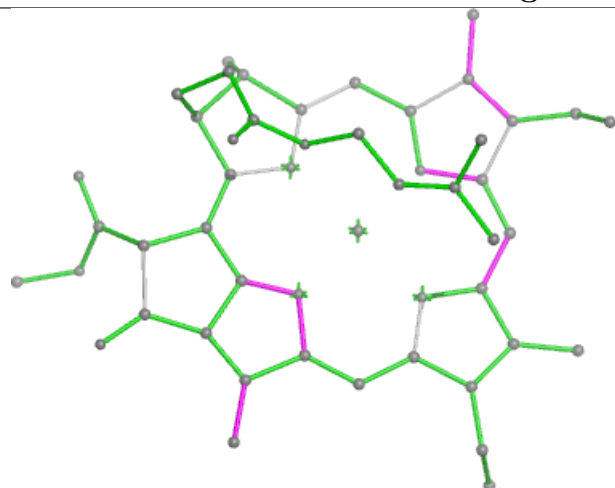
Ligand BCR A 848



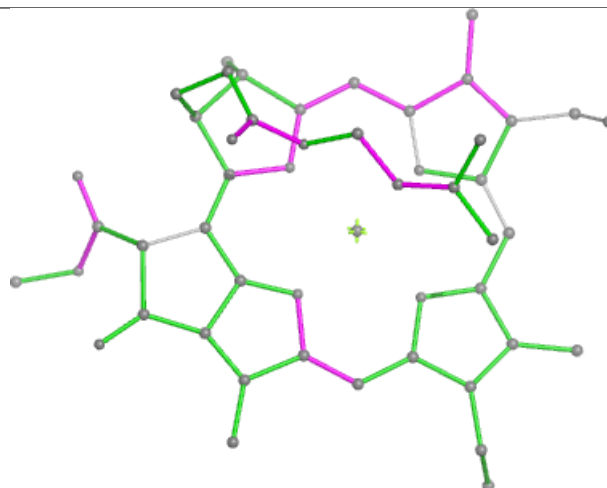
Ligand CLA b 831



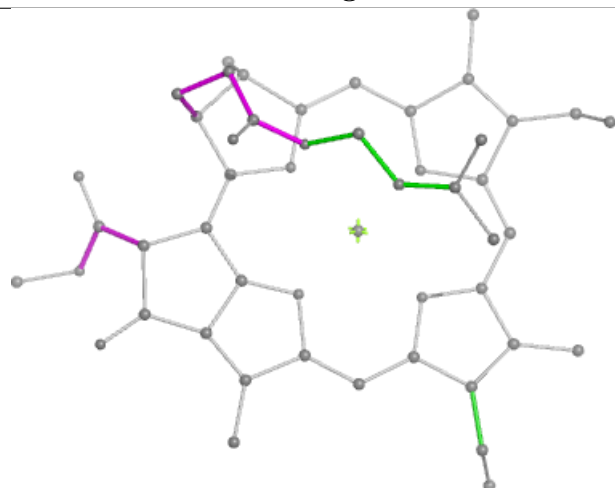
Ligand CLA a 826



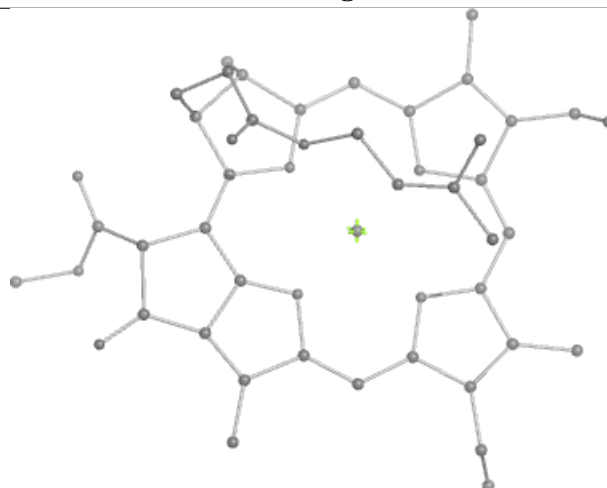
Bond lengths



Bond angles

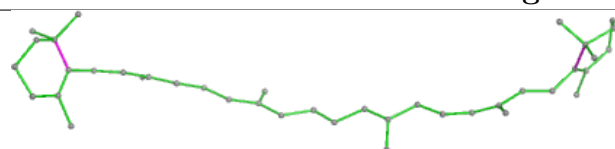


Torsions

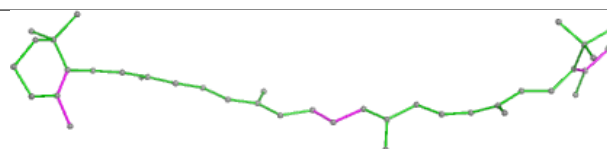


Rings

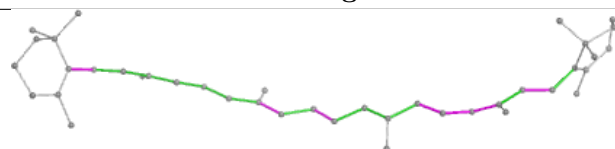
Ligand BCR i 101



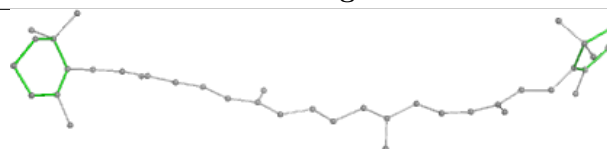
Bond lengths



Bond angles

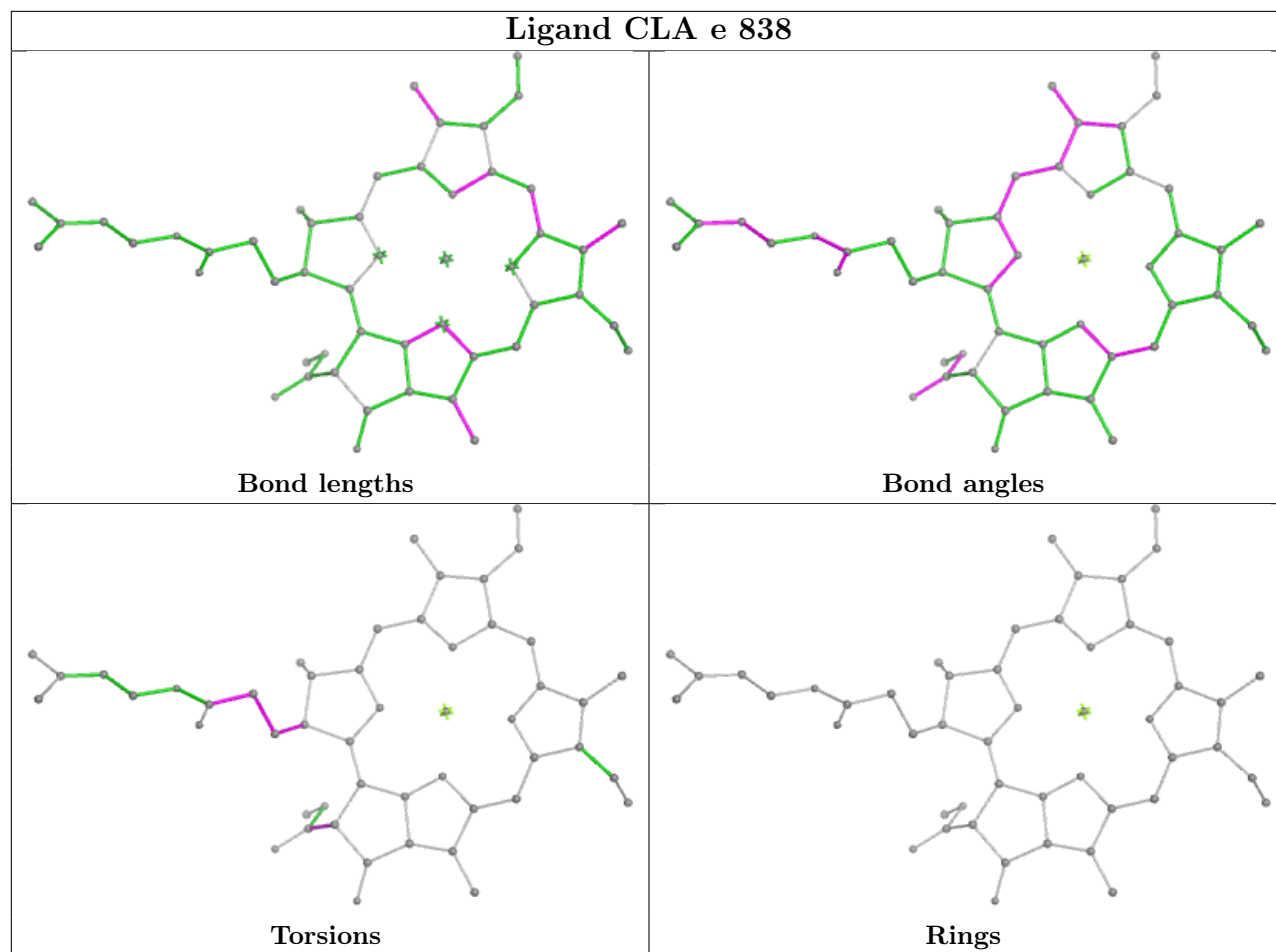


Torsions

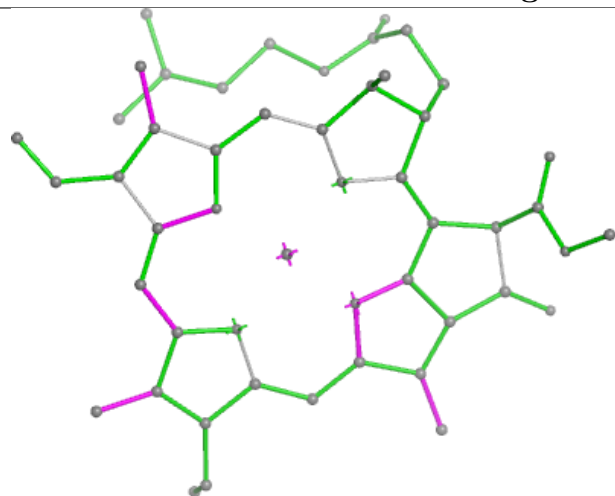


Rings

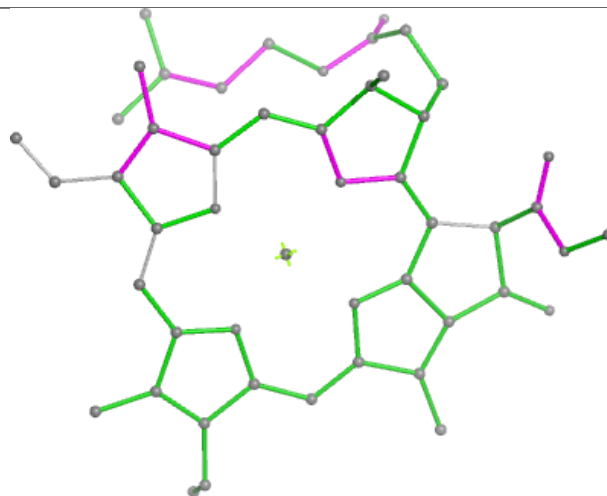
Ligand CLA e 838



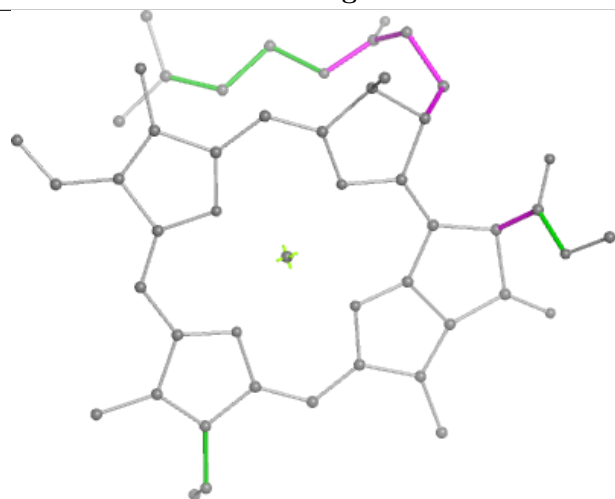
Ligand CLA e 822



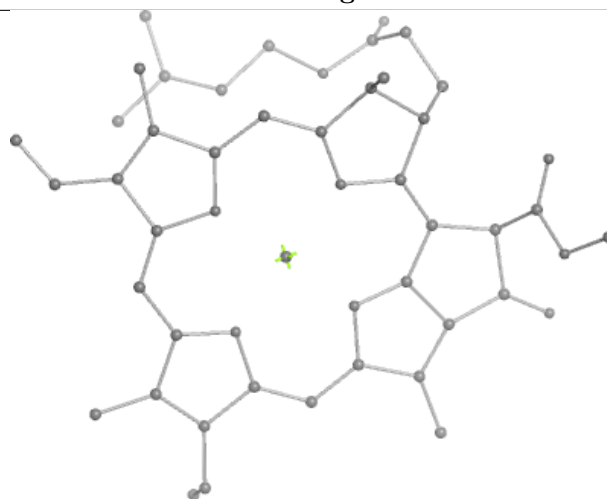
Bond lengths



Bond angles

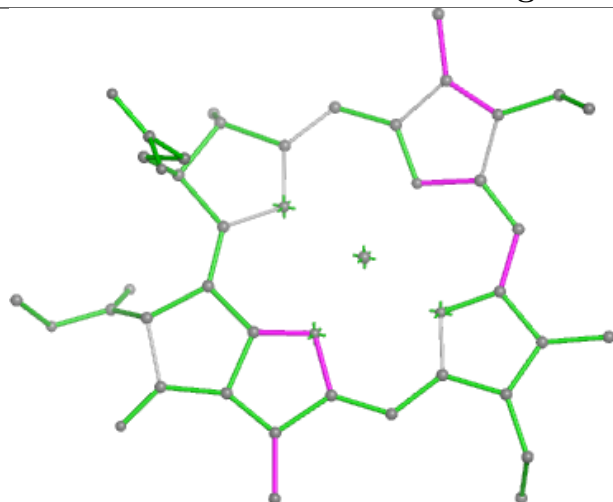


Torsions

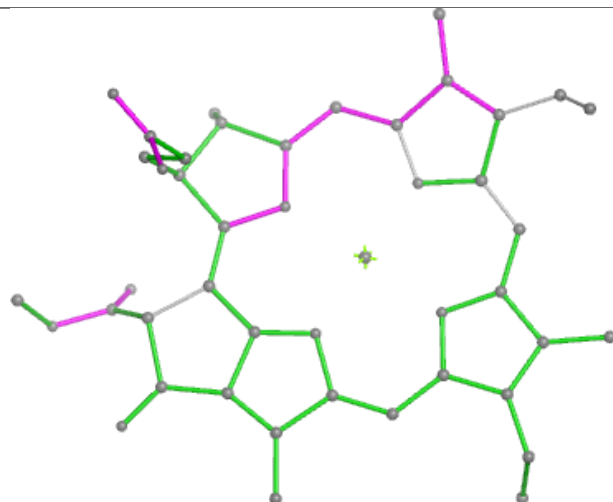


Rings

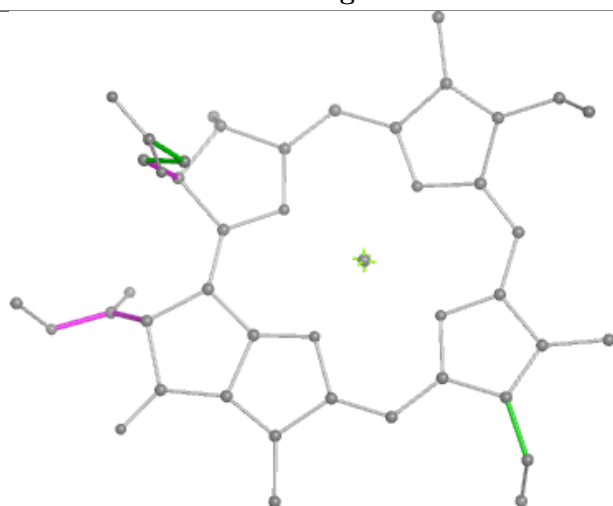
Ligand CLA b 811



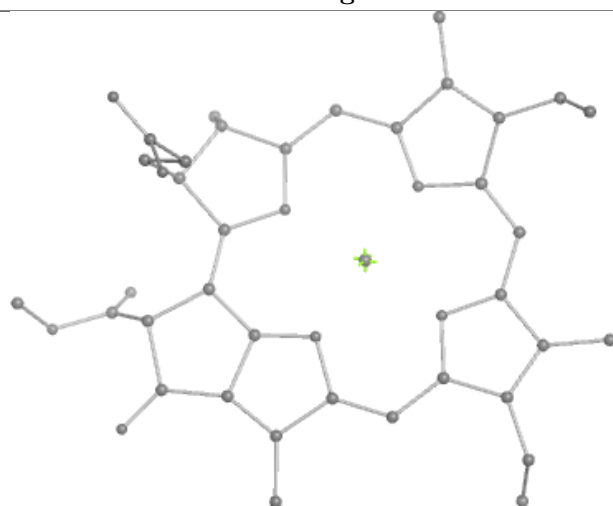
Bond lengths



Bond angles

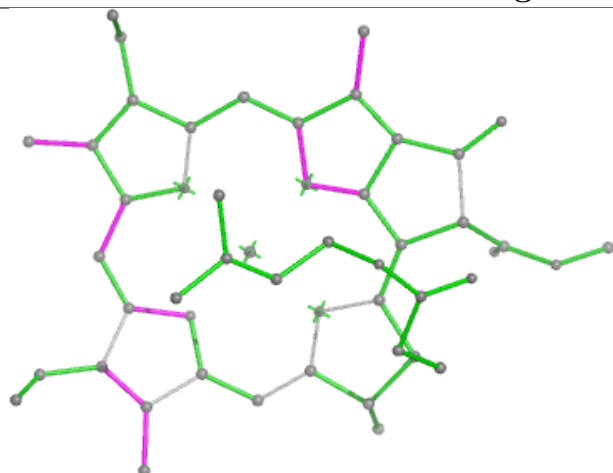


Torsions

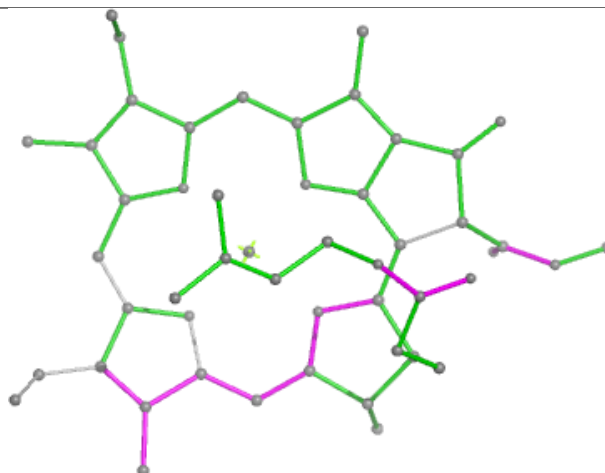


Rings

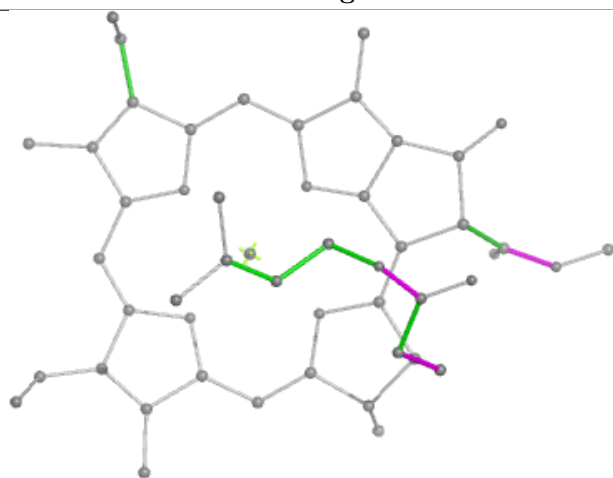
Ligand CLA B 802



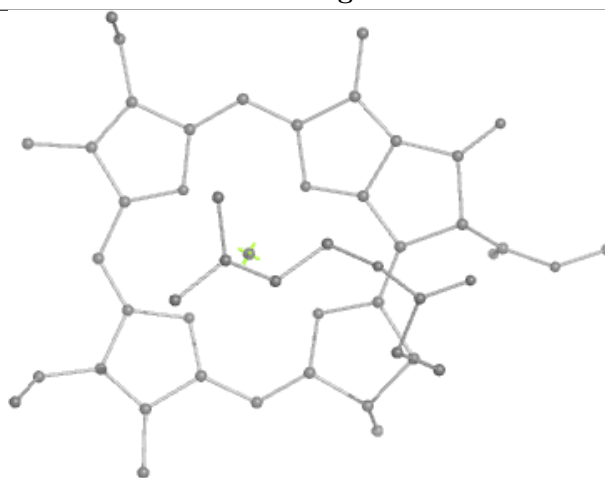
Bond lengths



Bond angles

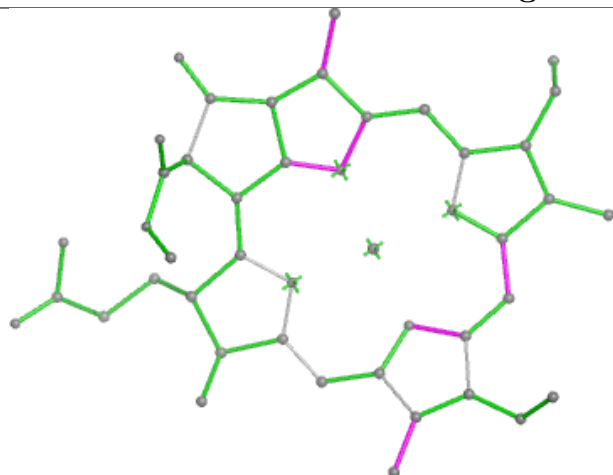


Torsions

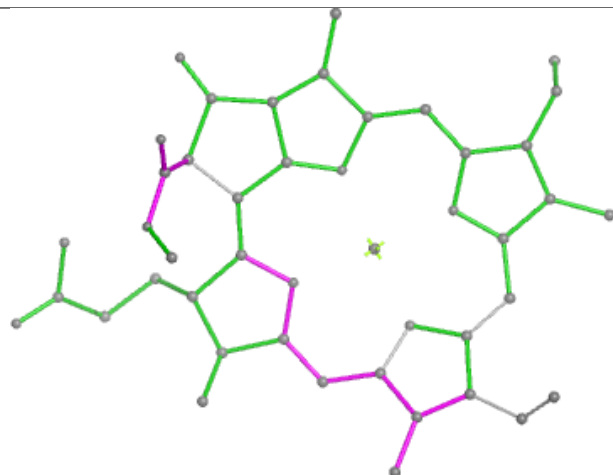


Rings

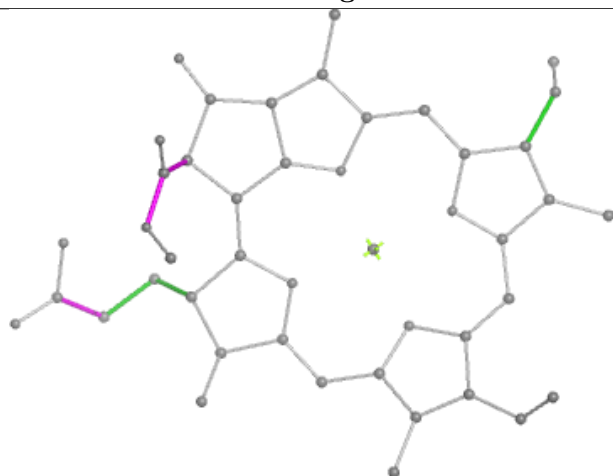
Ligand CLA e 817



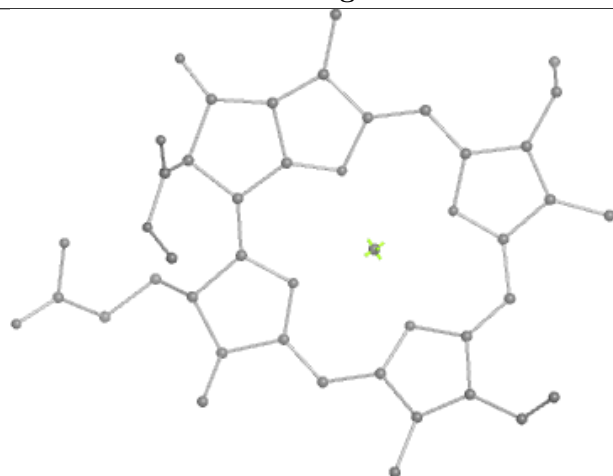
Bond lengths



Bond angles

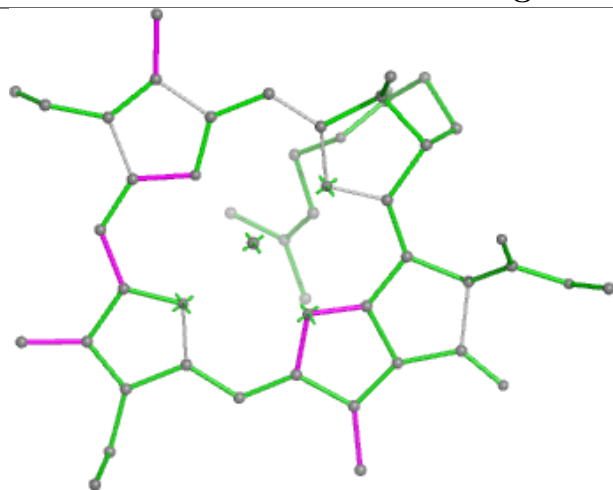


Torsions

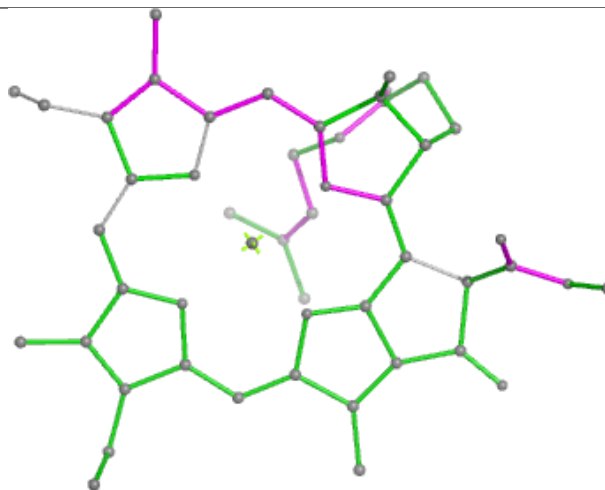


Rings

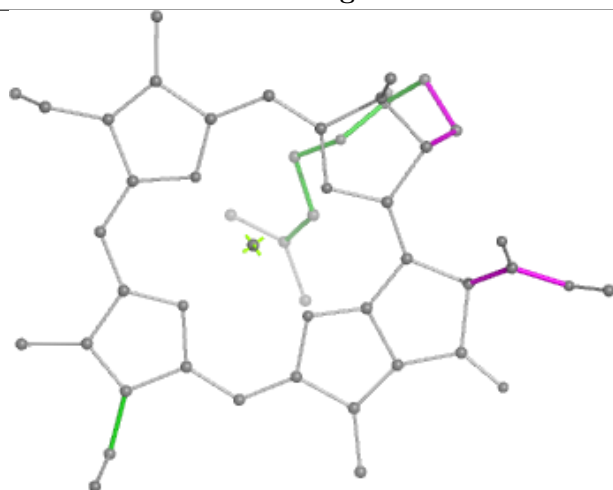
Ligand CLA A 844



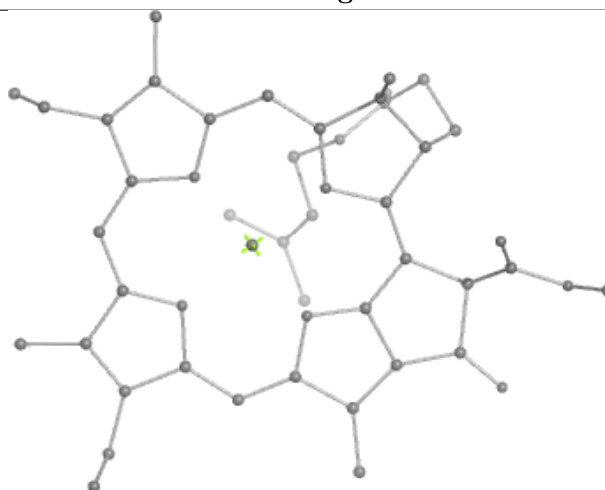
Bond lengths



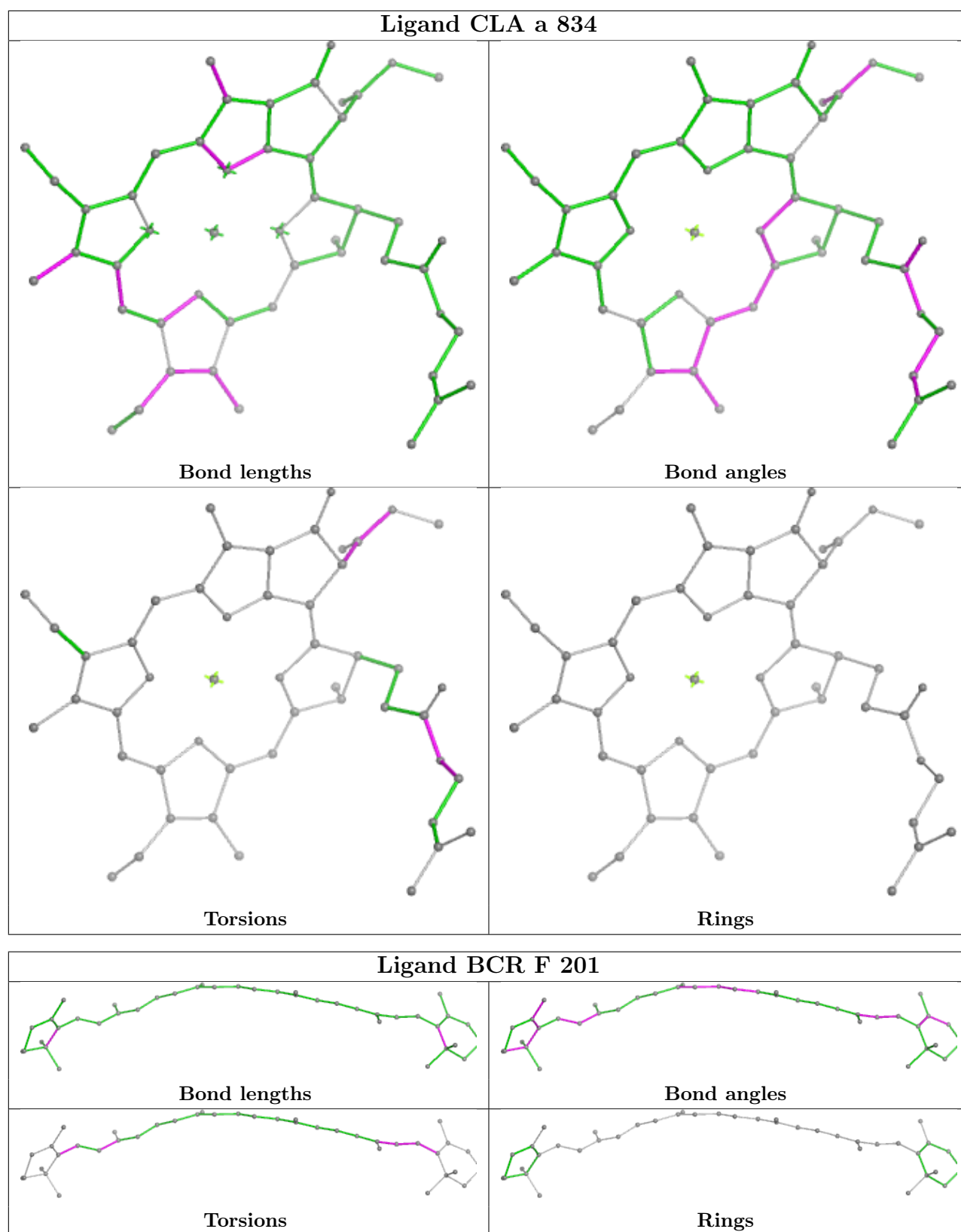
Bond angles



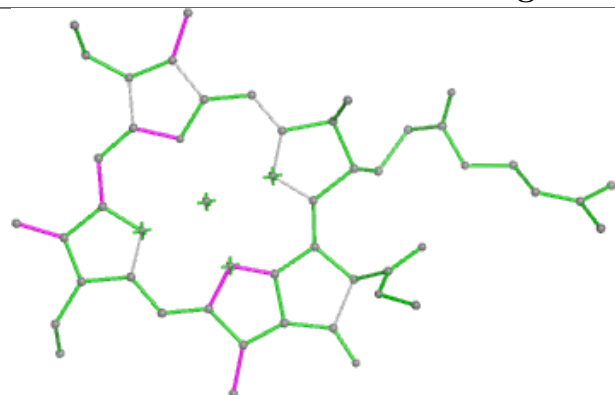
Torsions



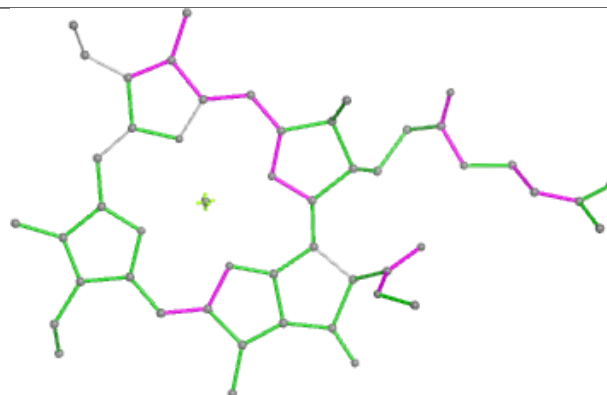
Rings



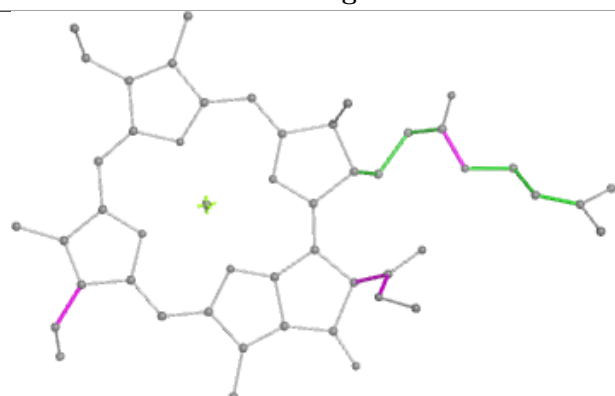
Ligand CLA E 806



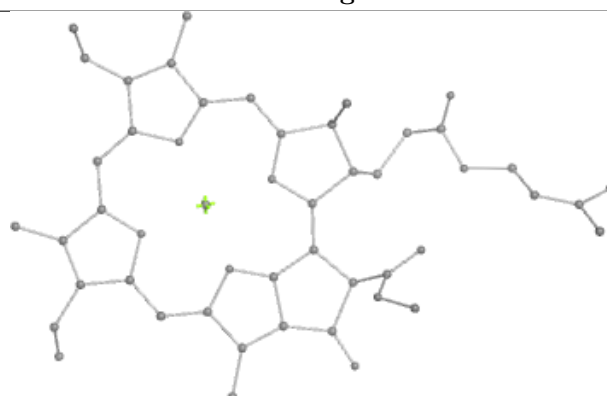
Bond lengths



Bond angles

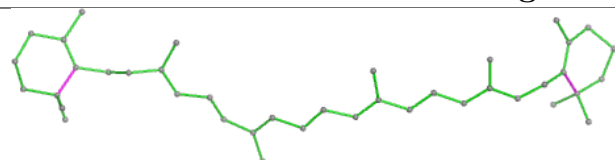


Torsions

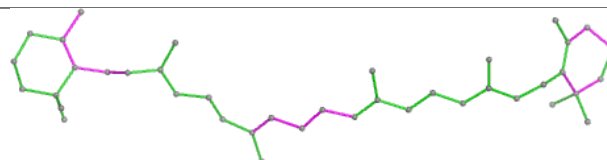


Rings

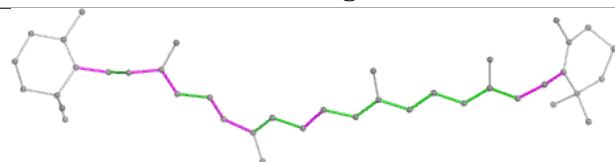
Ligand BCR a 853



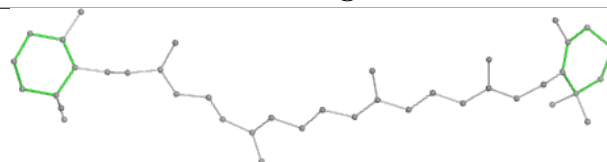
Bond lengths



Bond angles

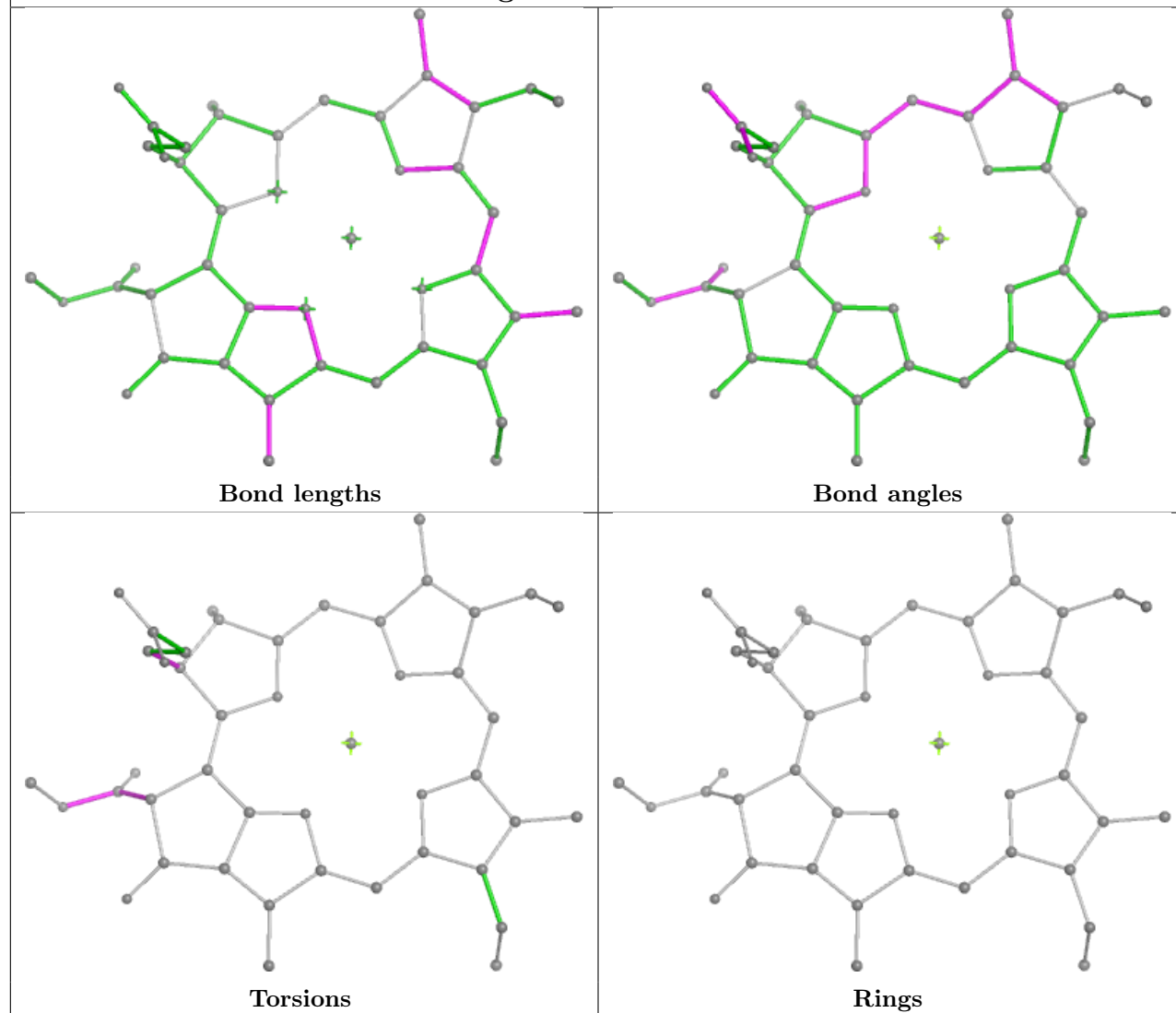


Torsions

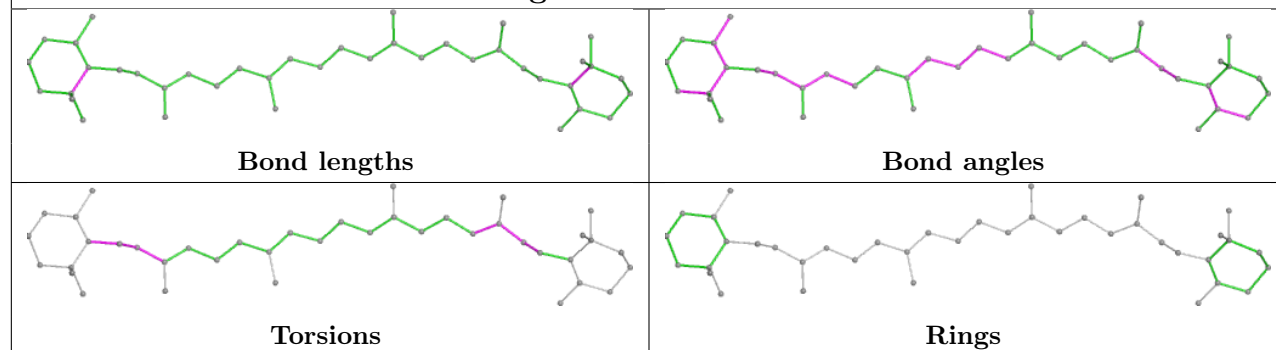


Rings

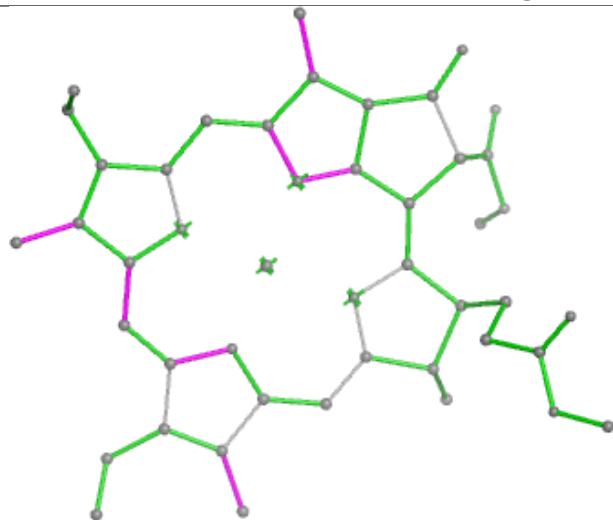
Ligand CLA 1 201



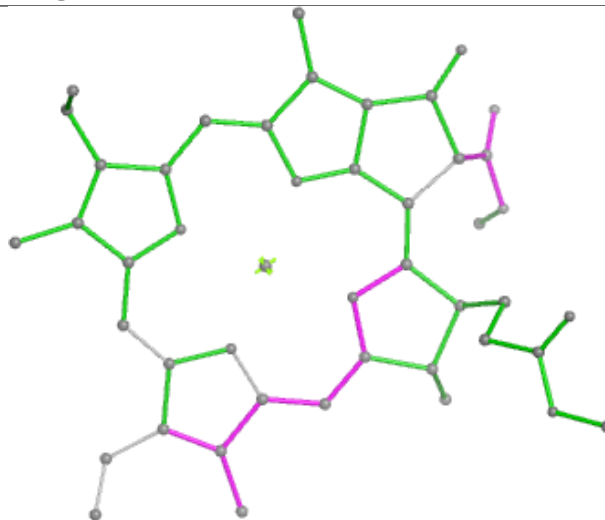
Ligand BCR G 843



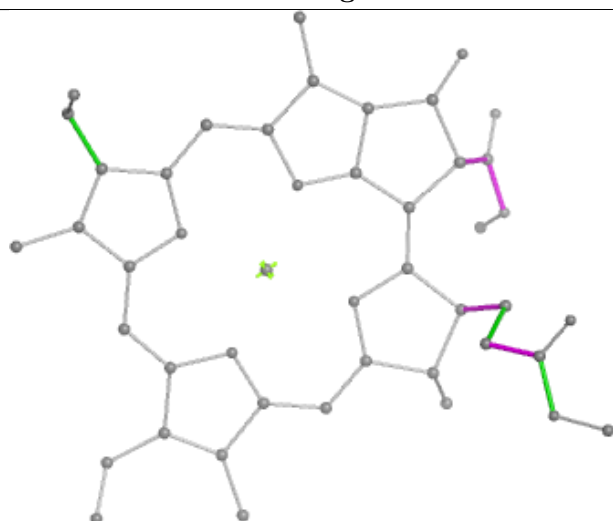
Ligand CLA g 827



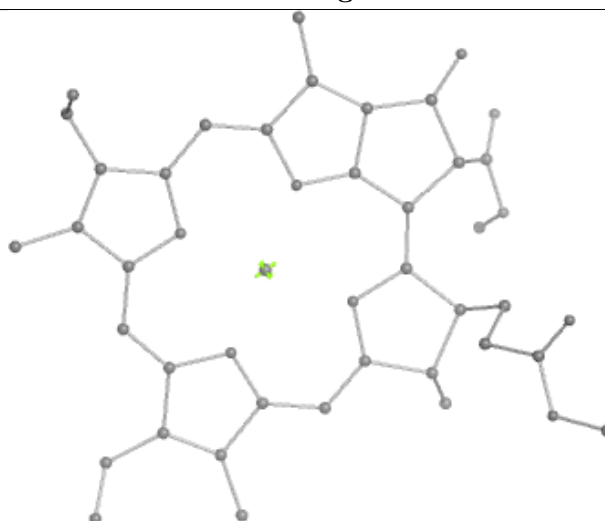
Bond lengths



Bond angles

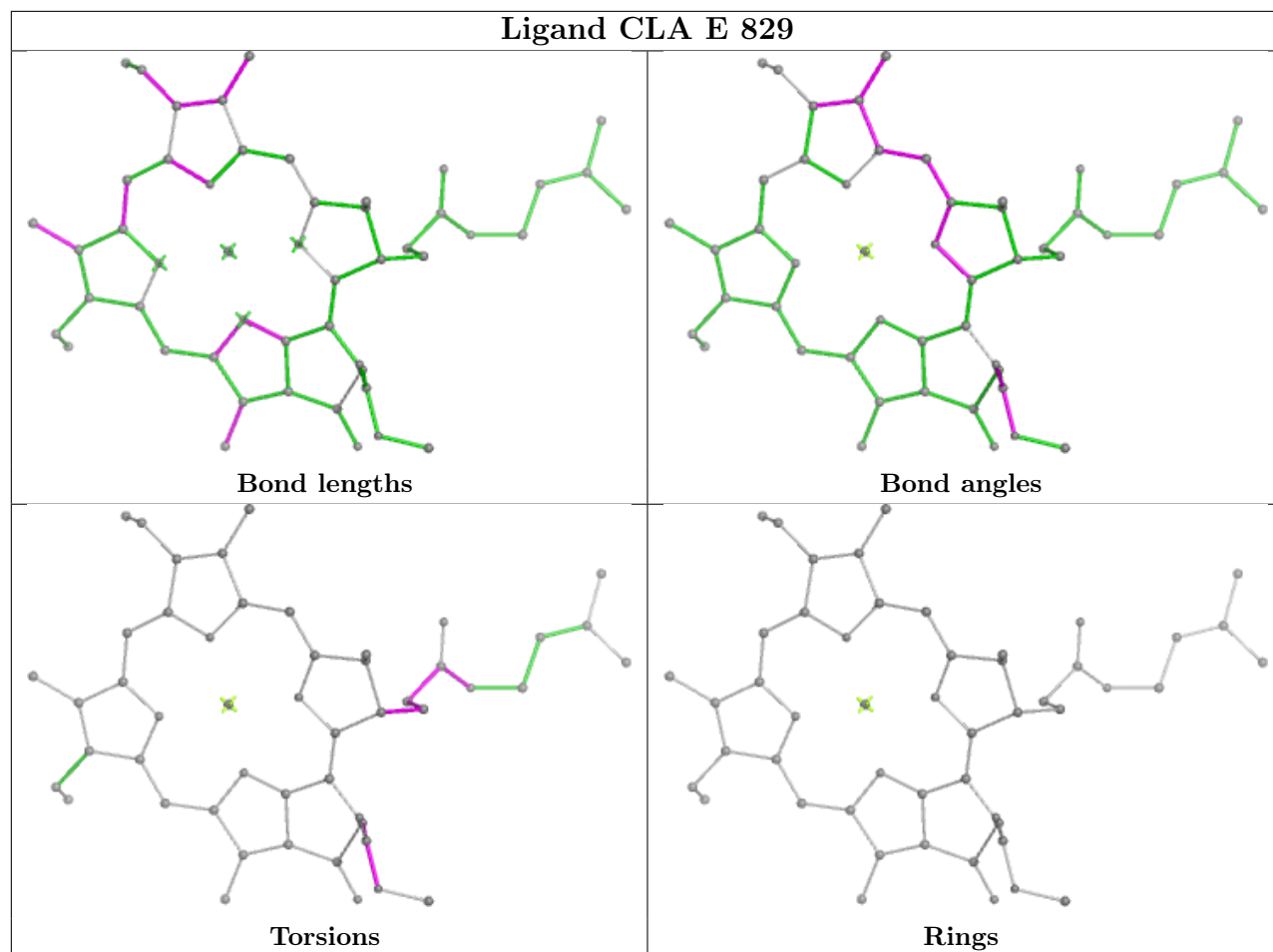


Torsions

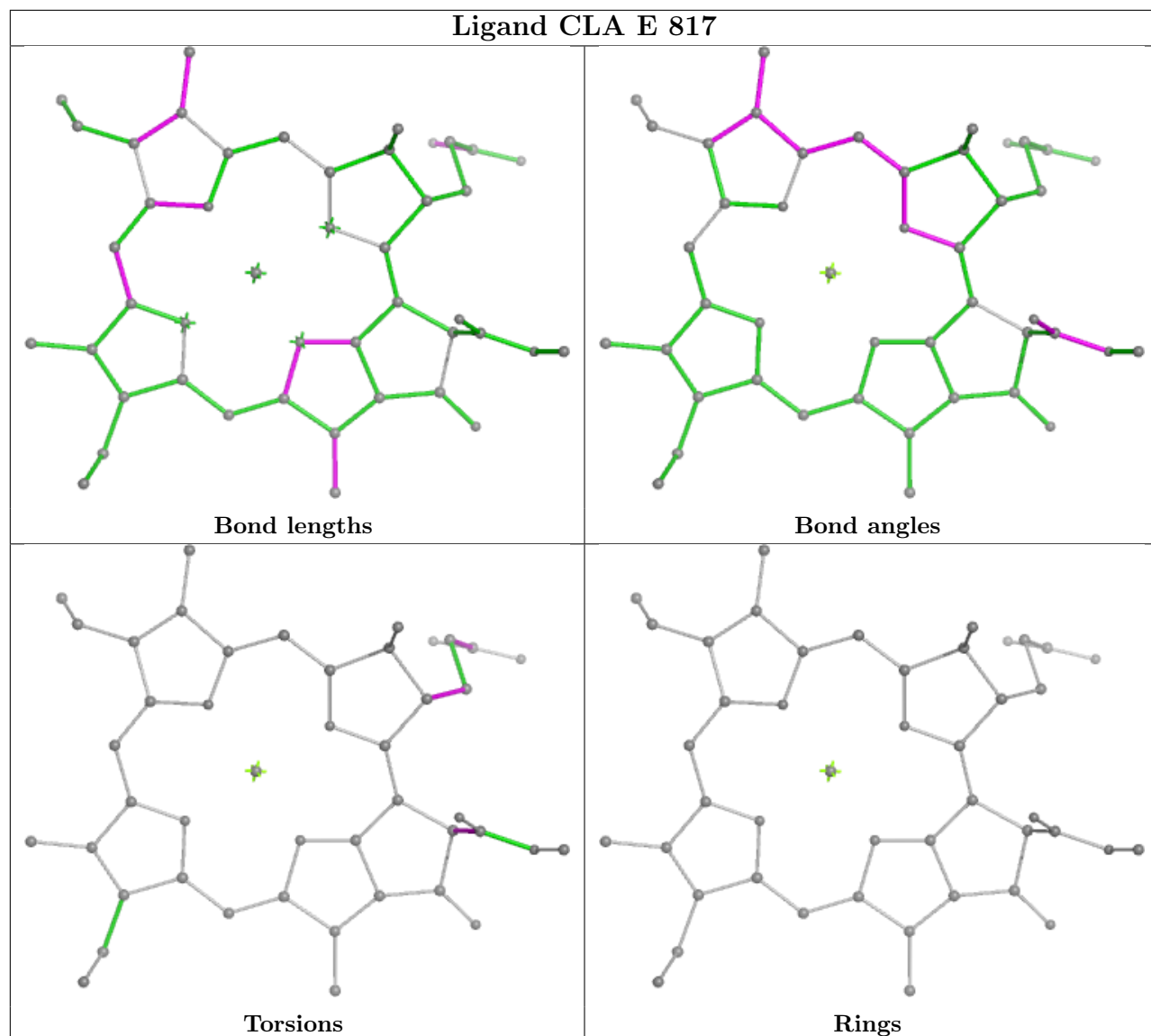


Rings

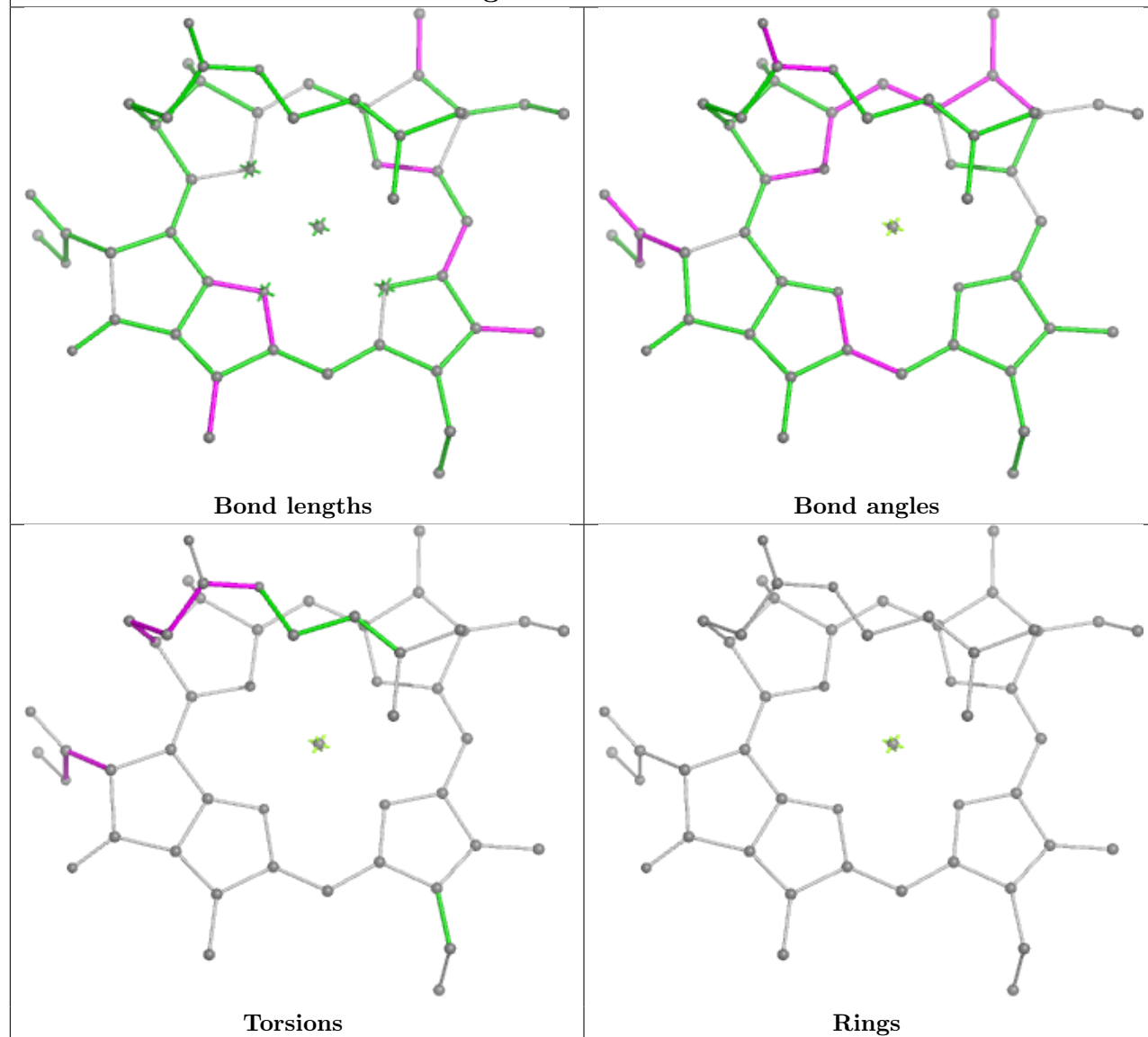
Ligand CLA E 829



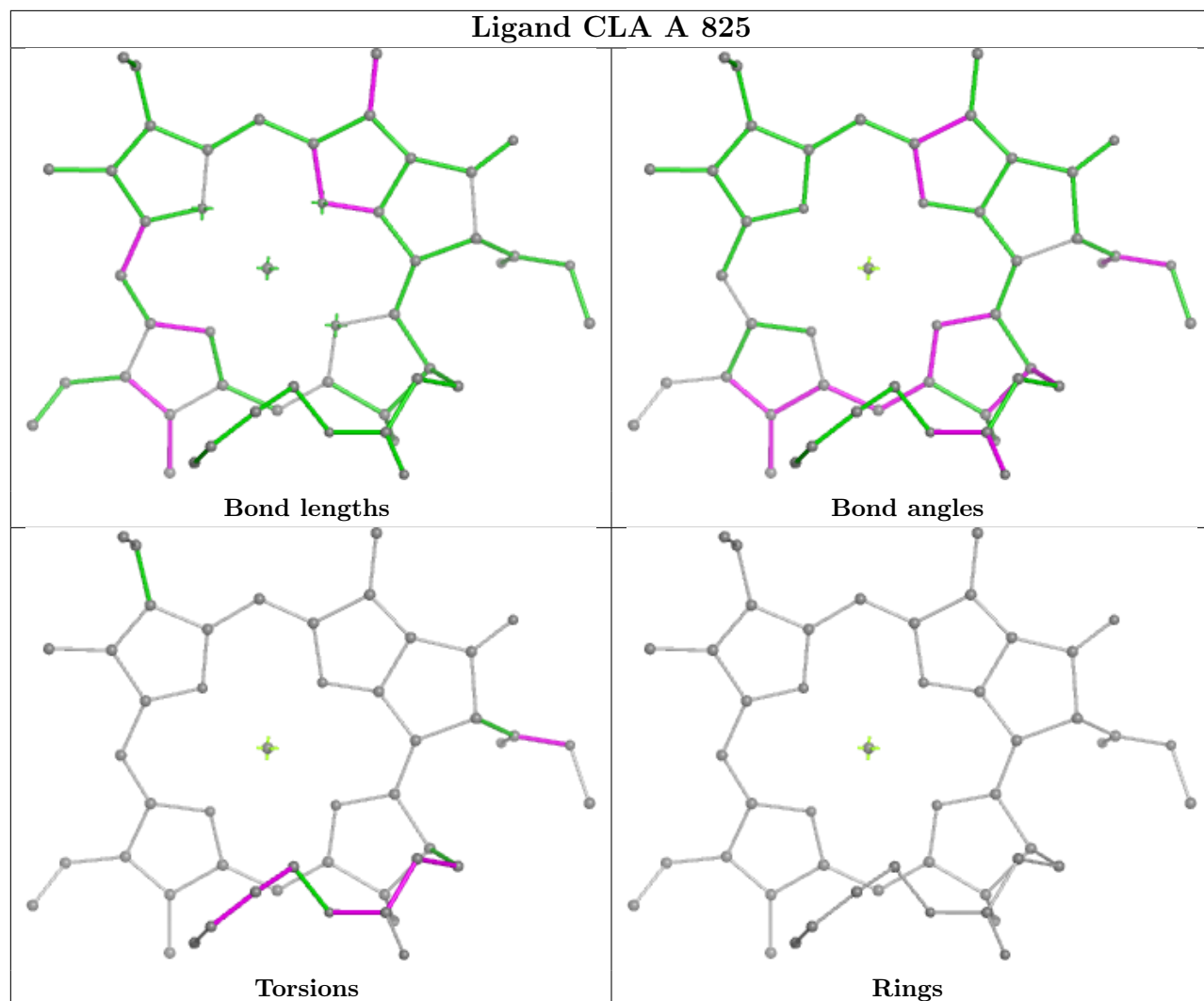
Ligand CLA E 817



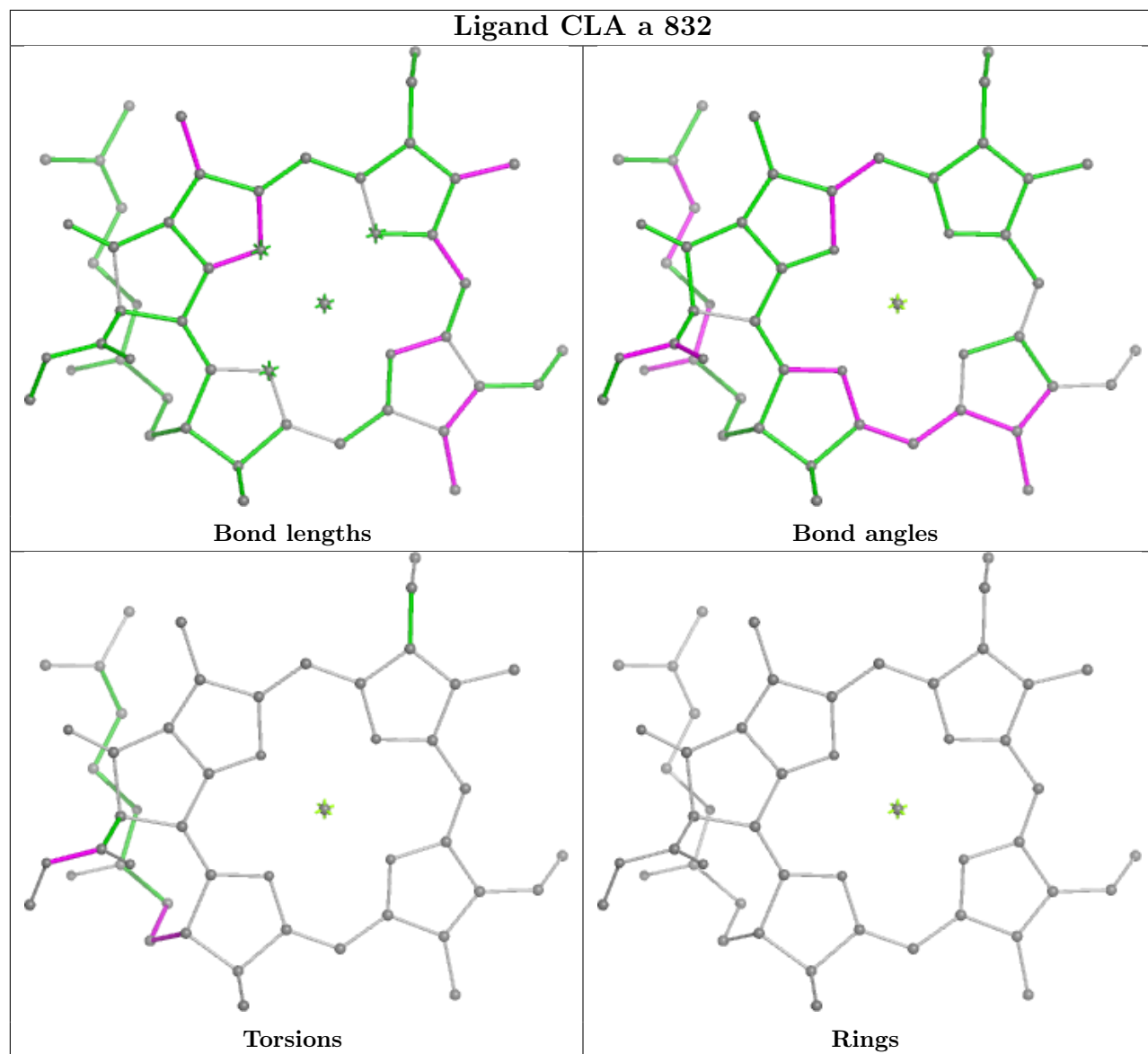
Ligand CLA e 826



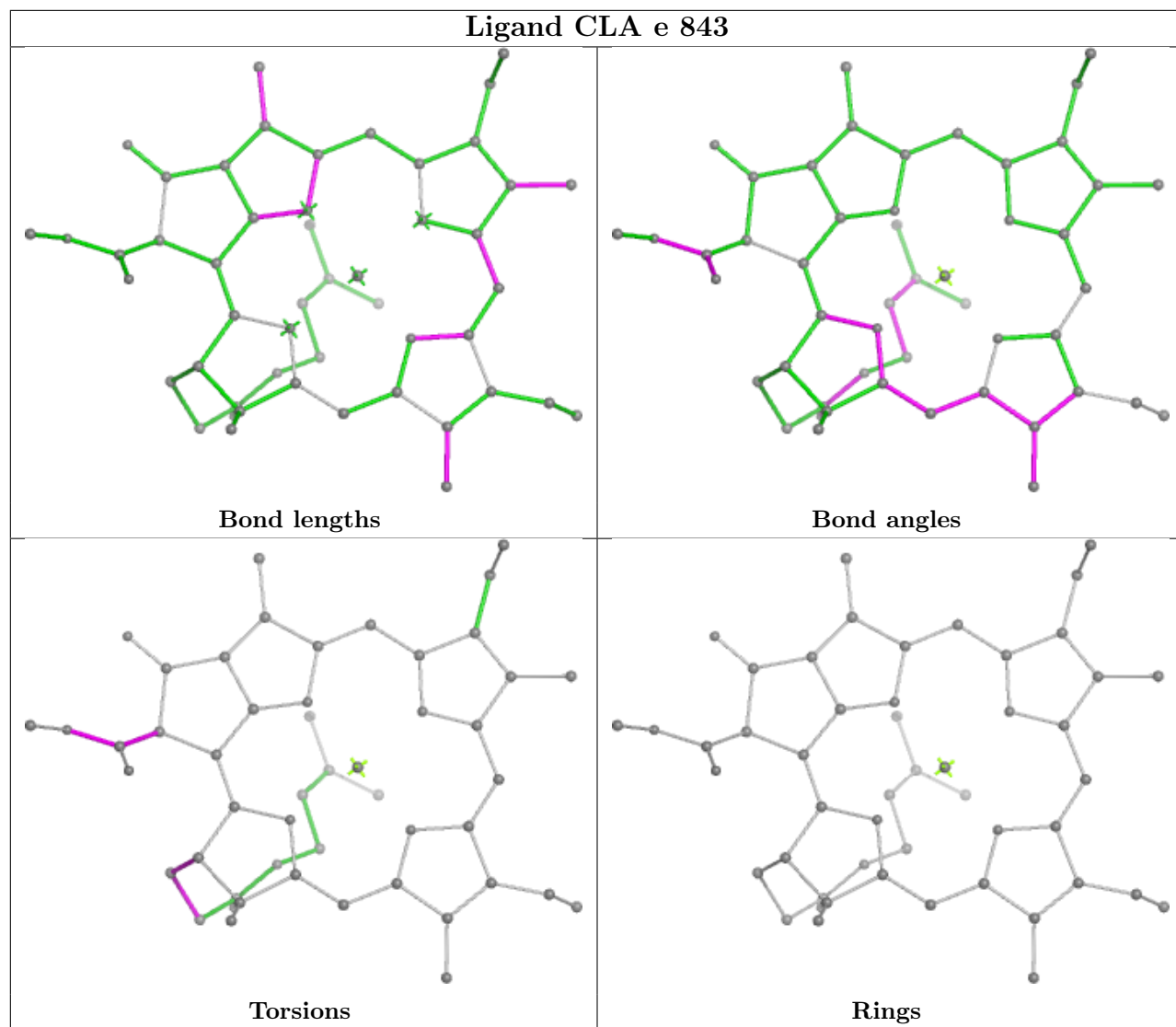
Ligand CLA A 825



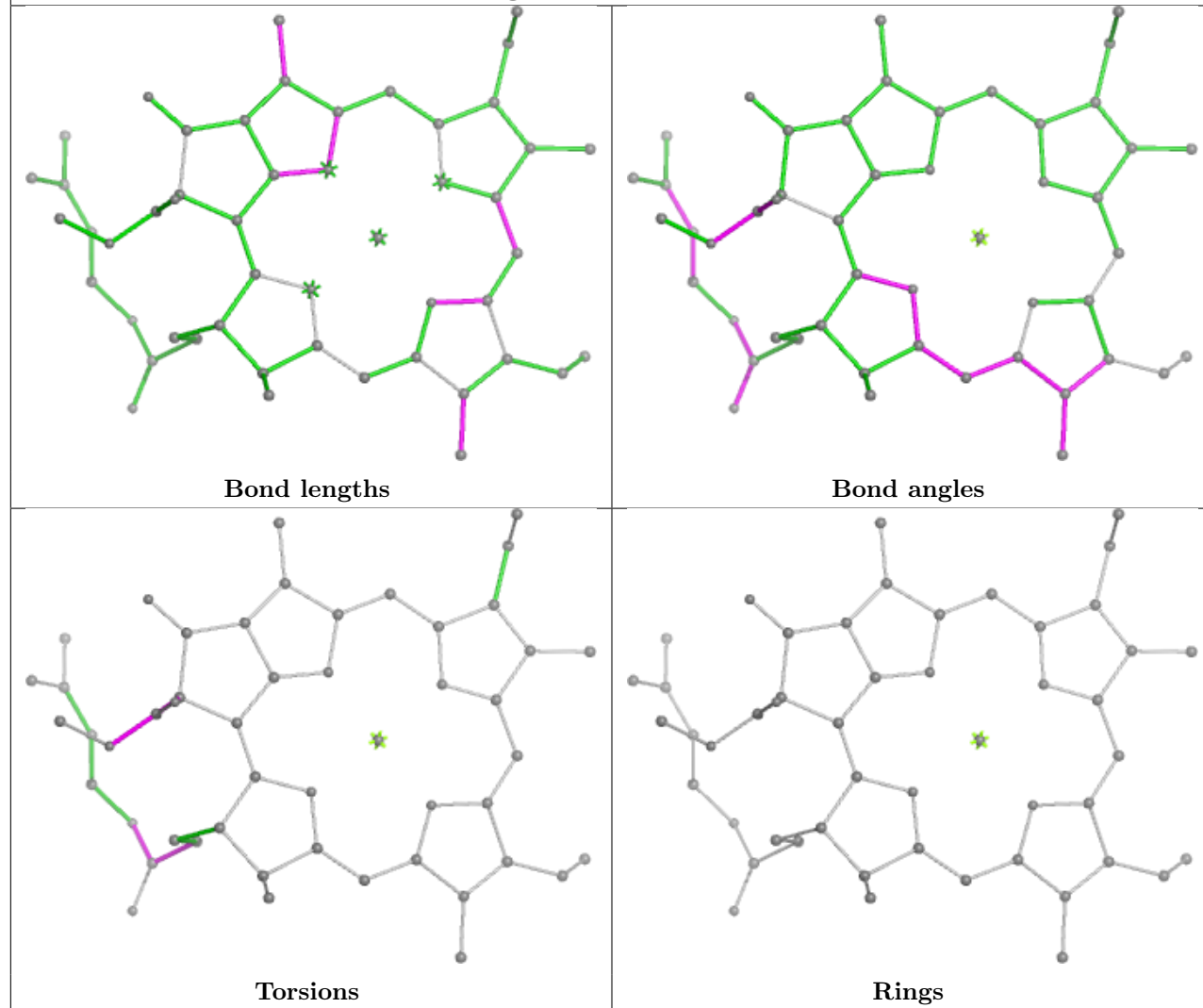
Ligand CLA a 832



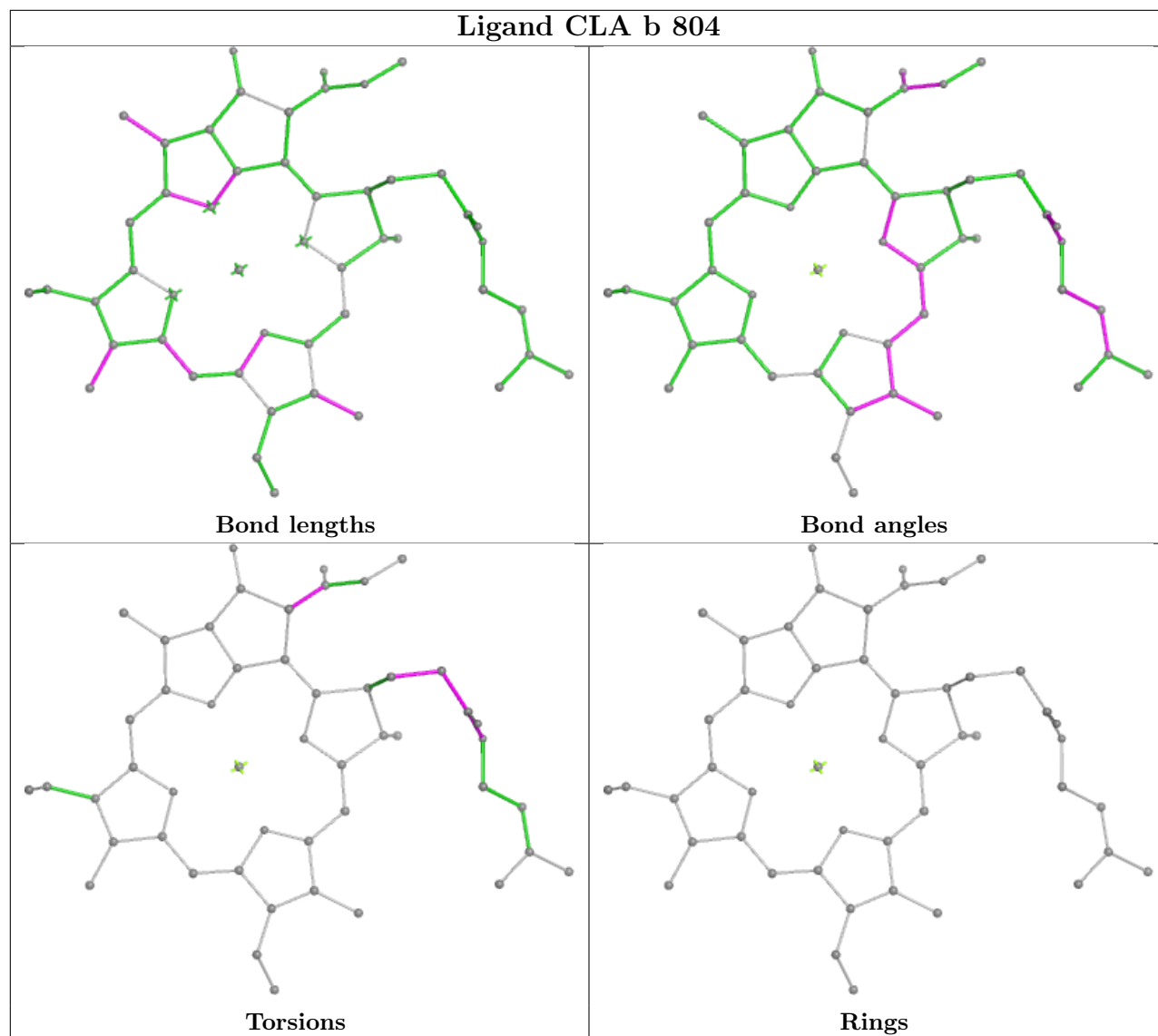
Ligand CLA e 843



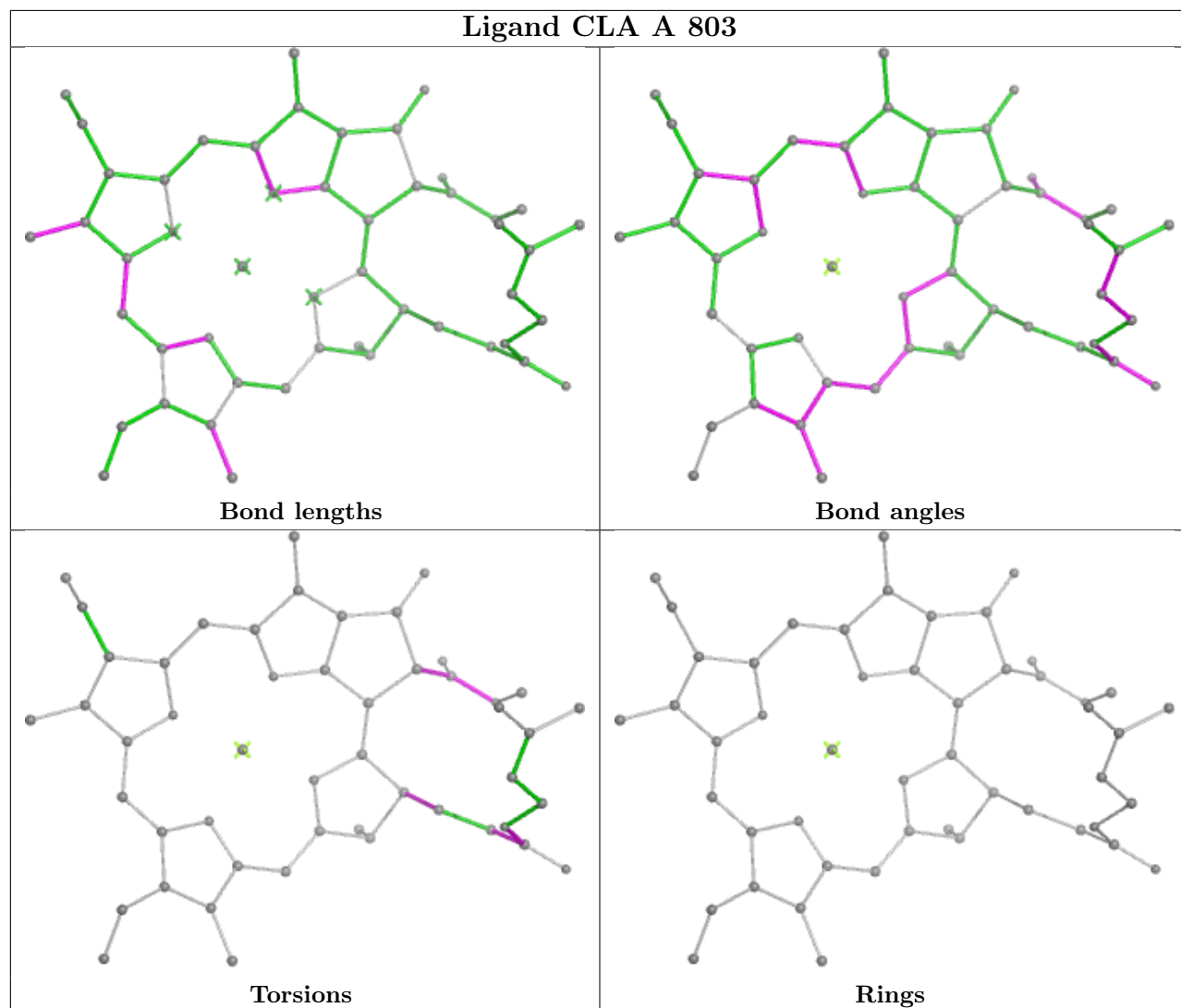
Ligand CLA b 816



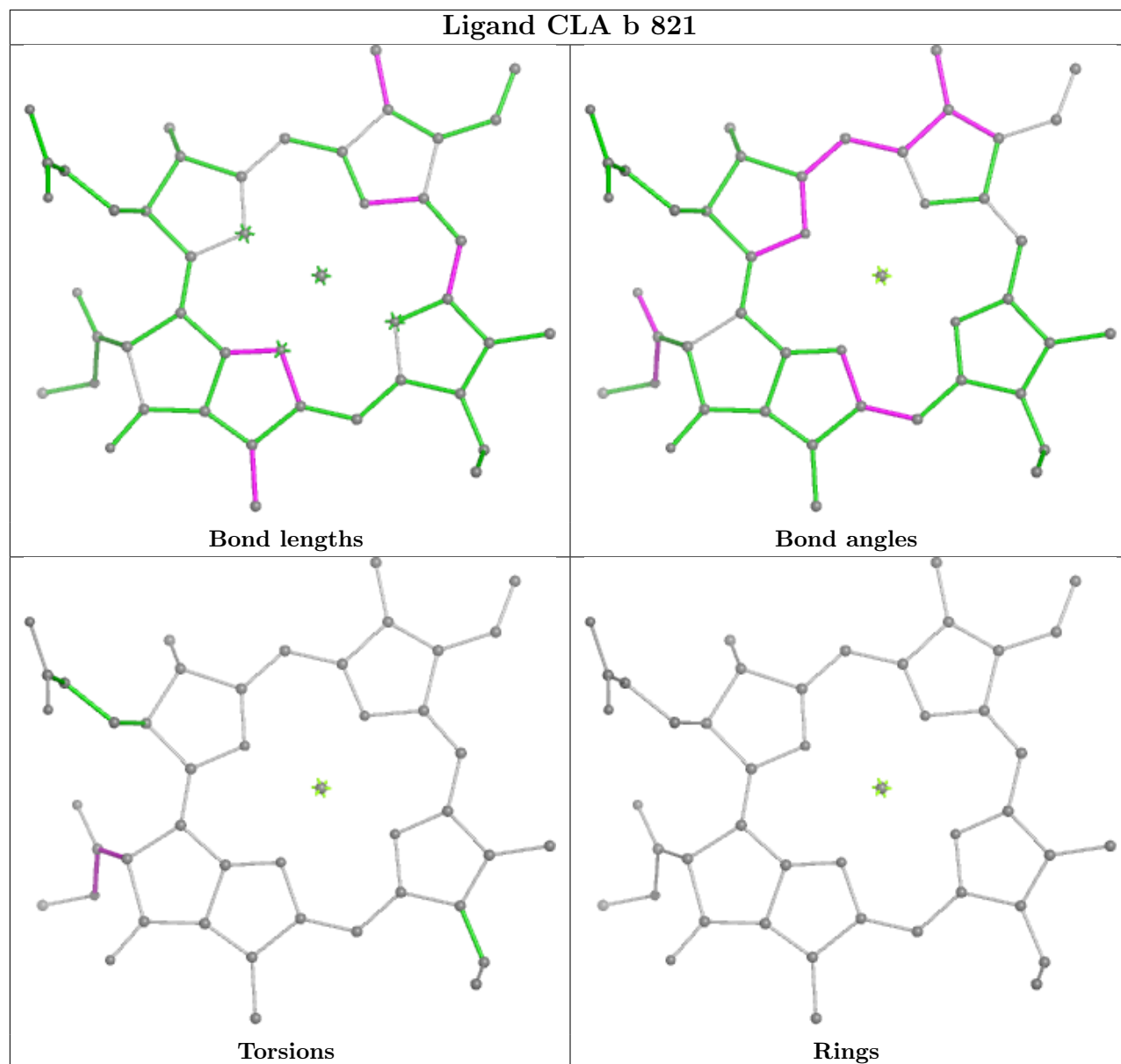
Ligand CLA b 804



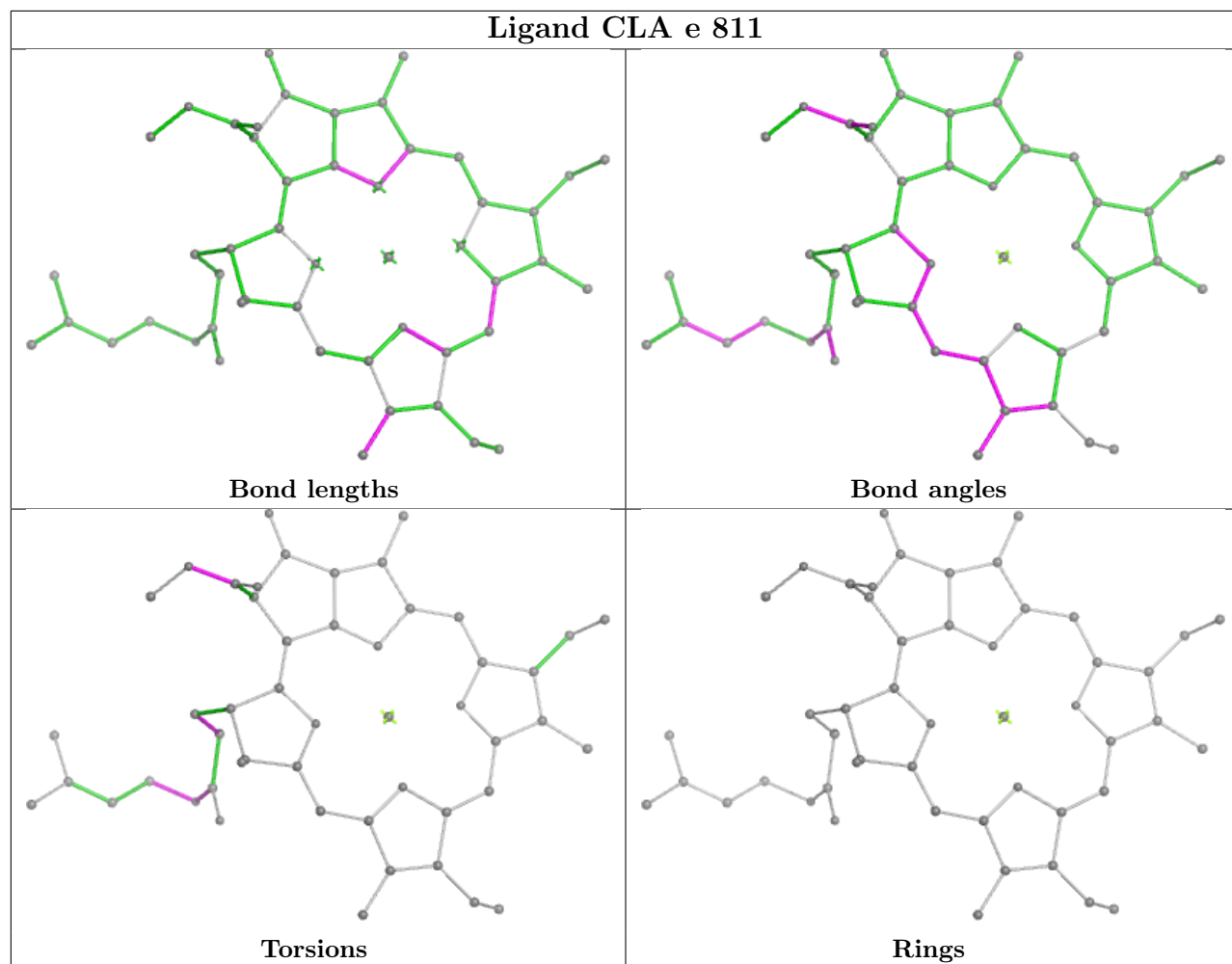
Ligand CLA A 803



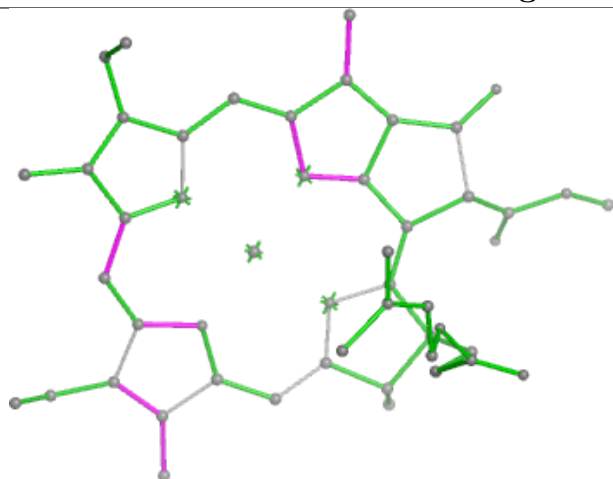
Ligand CLA b 821



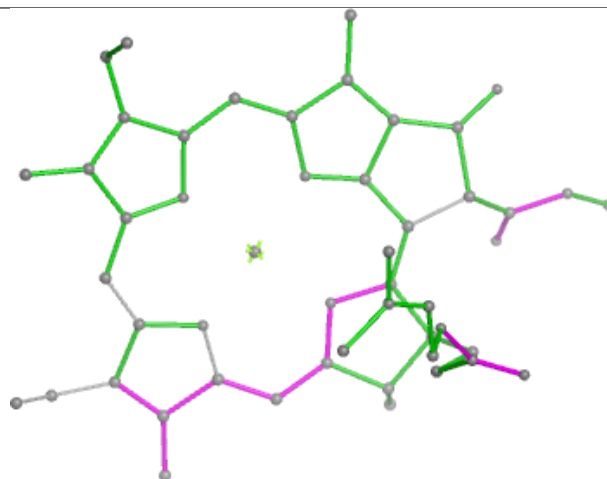
Ligand CLA e 811



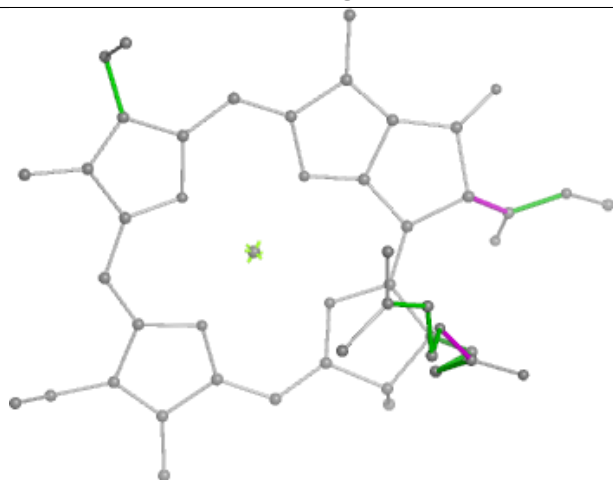
Ligand CLA e 813



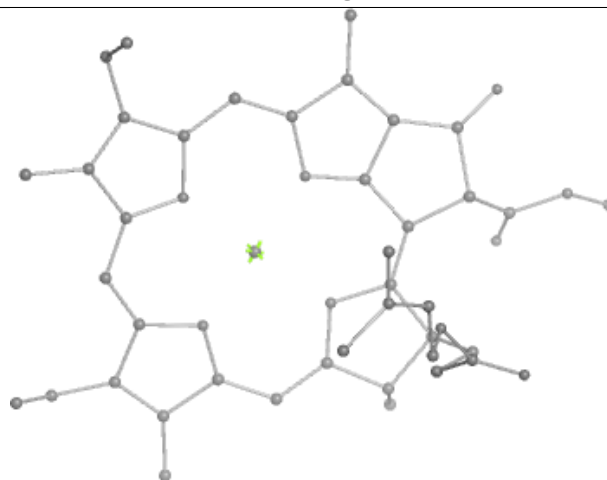
Bond lengths



Bond angles

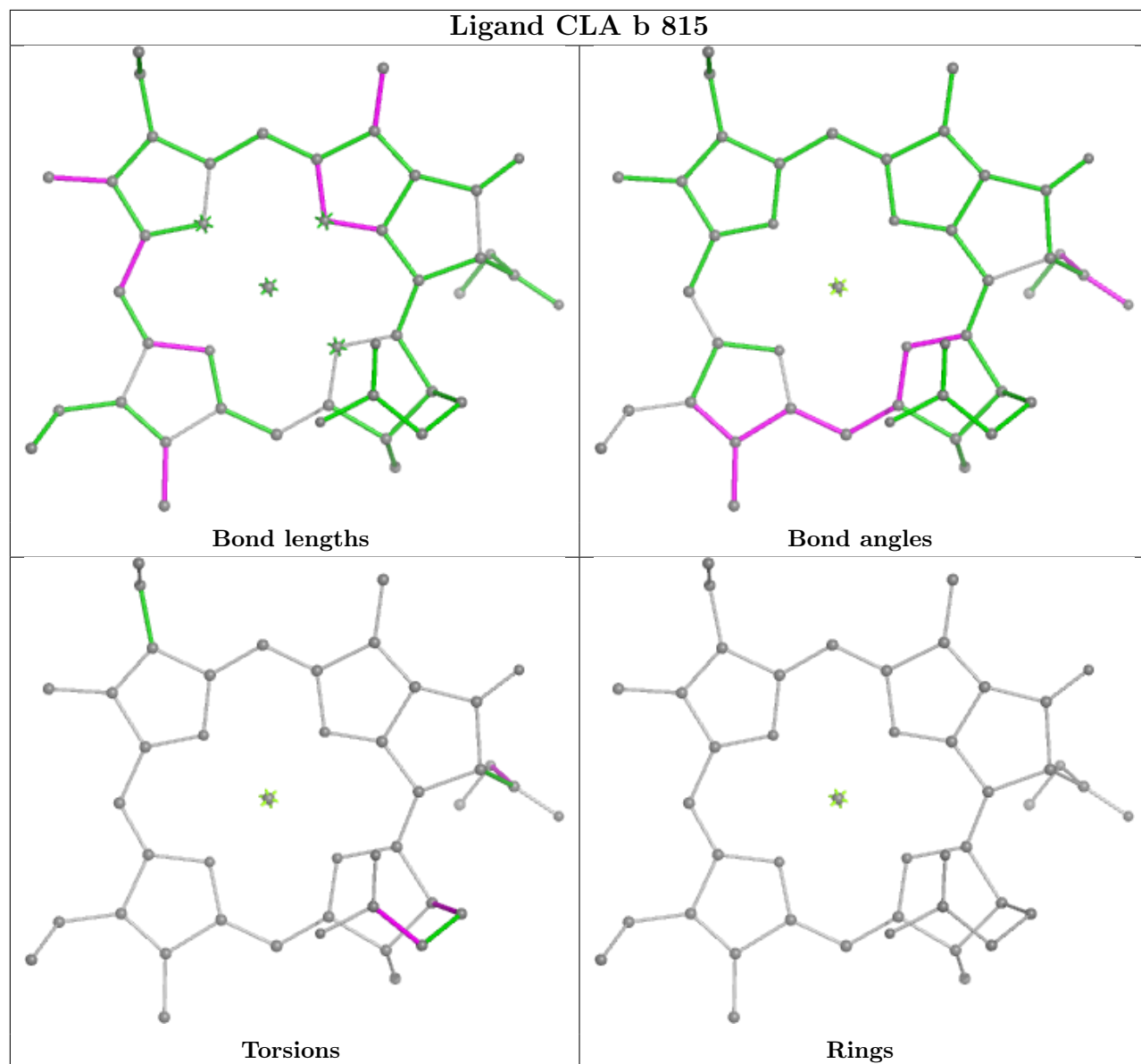


Torsions

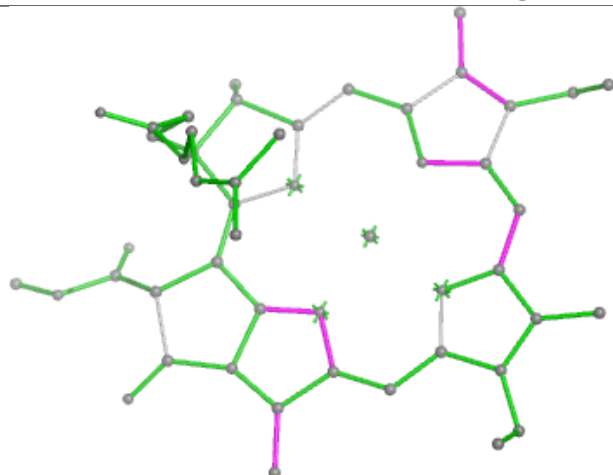


Rings

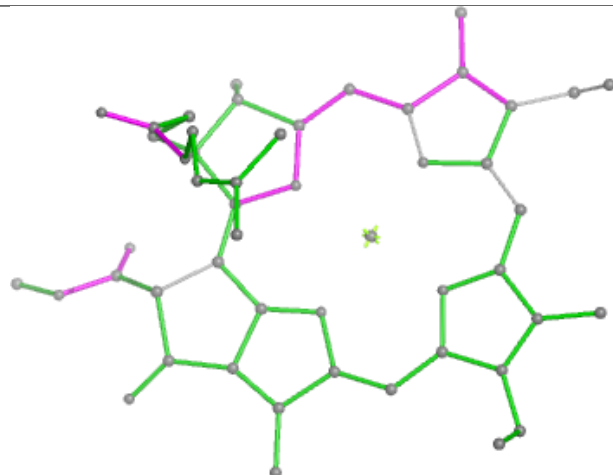
Ligand CLA b 815



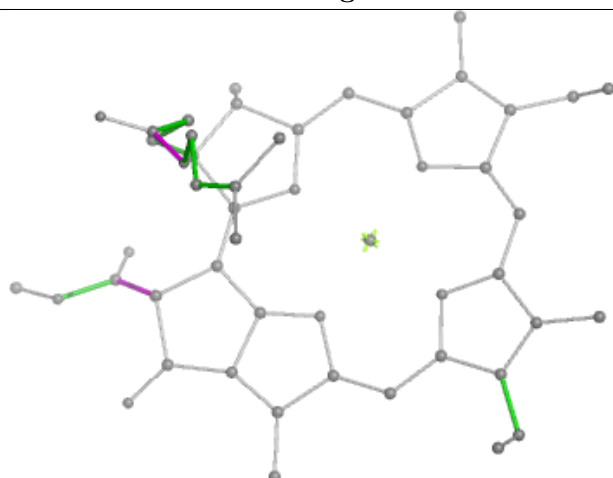
Ligand CLA A 814



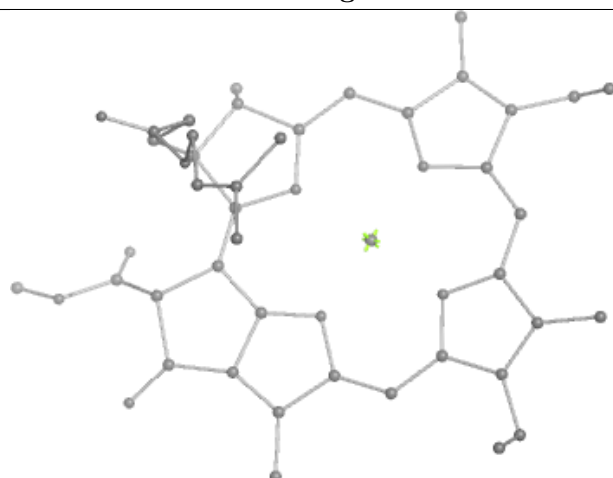
Bond lengths



Bond angles

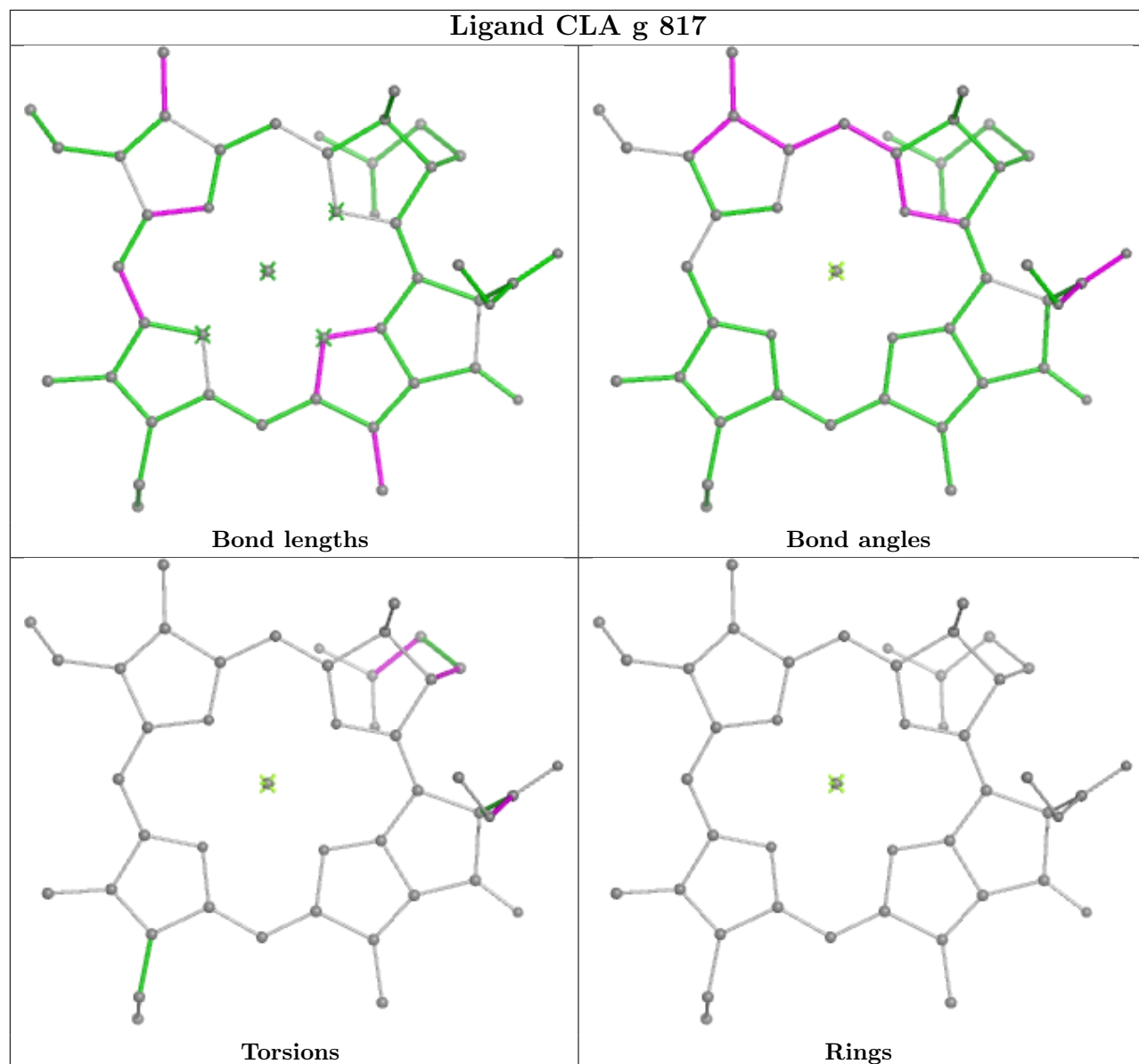


Torsions

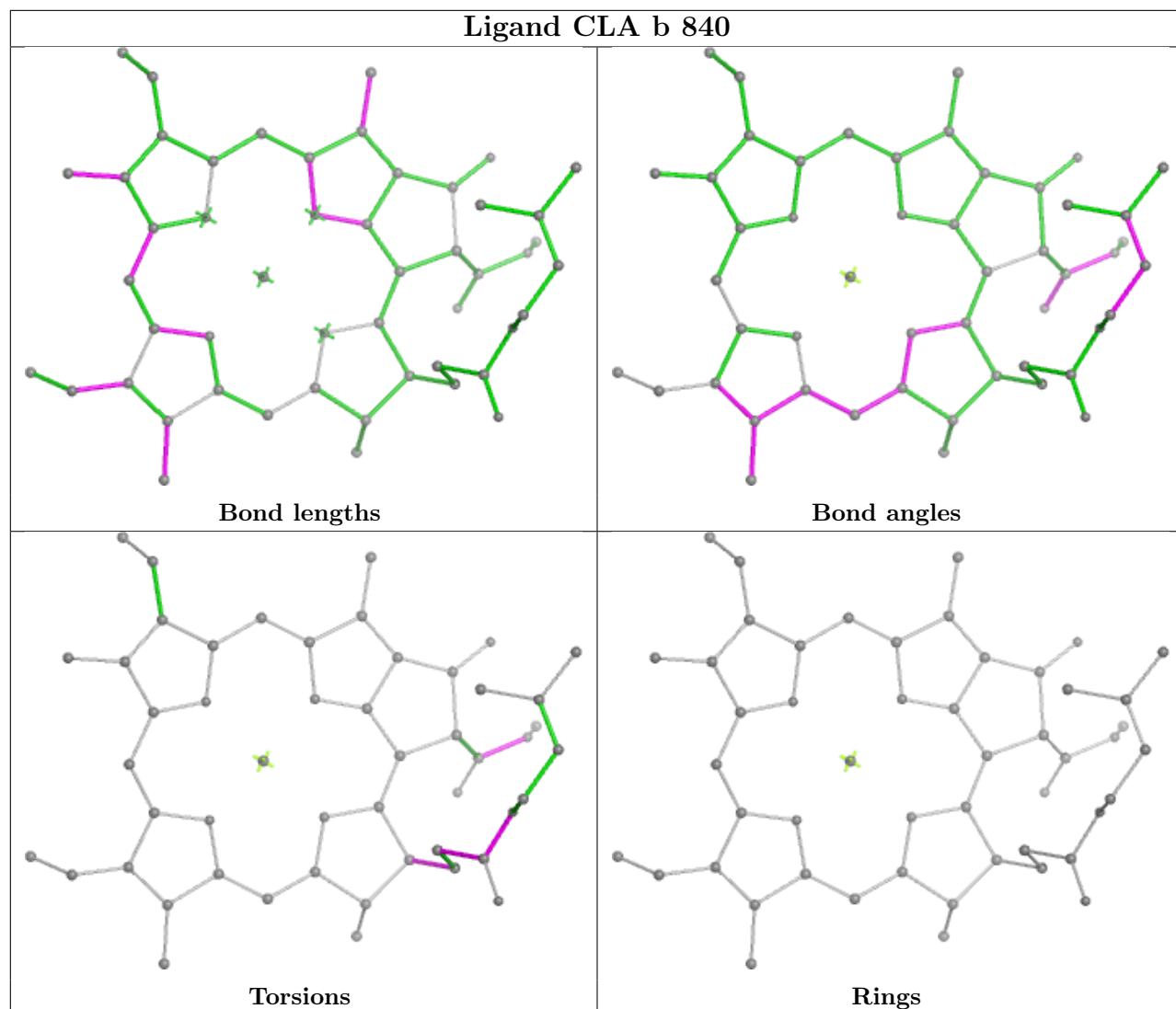


Rings

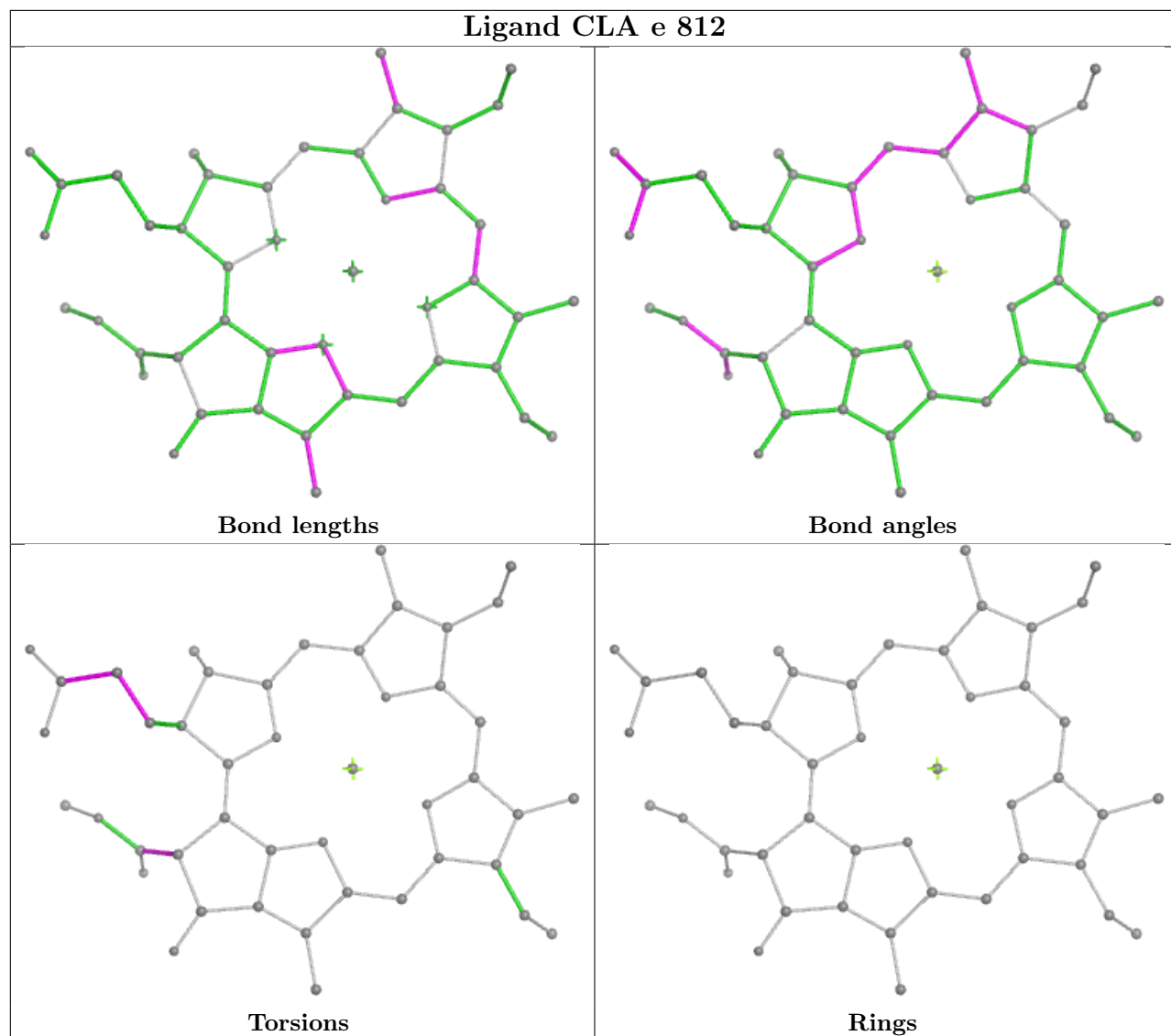
Ligand CLA g 817



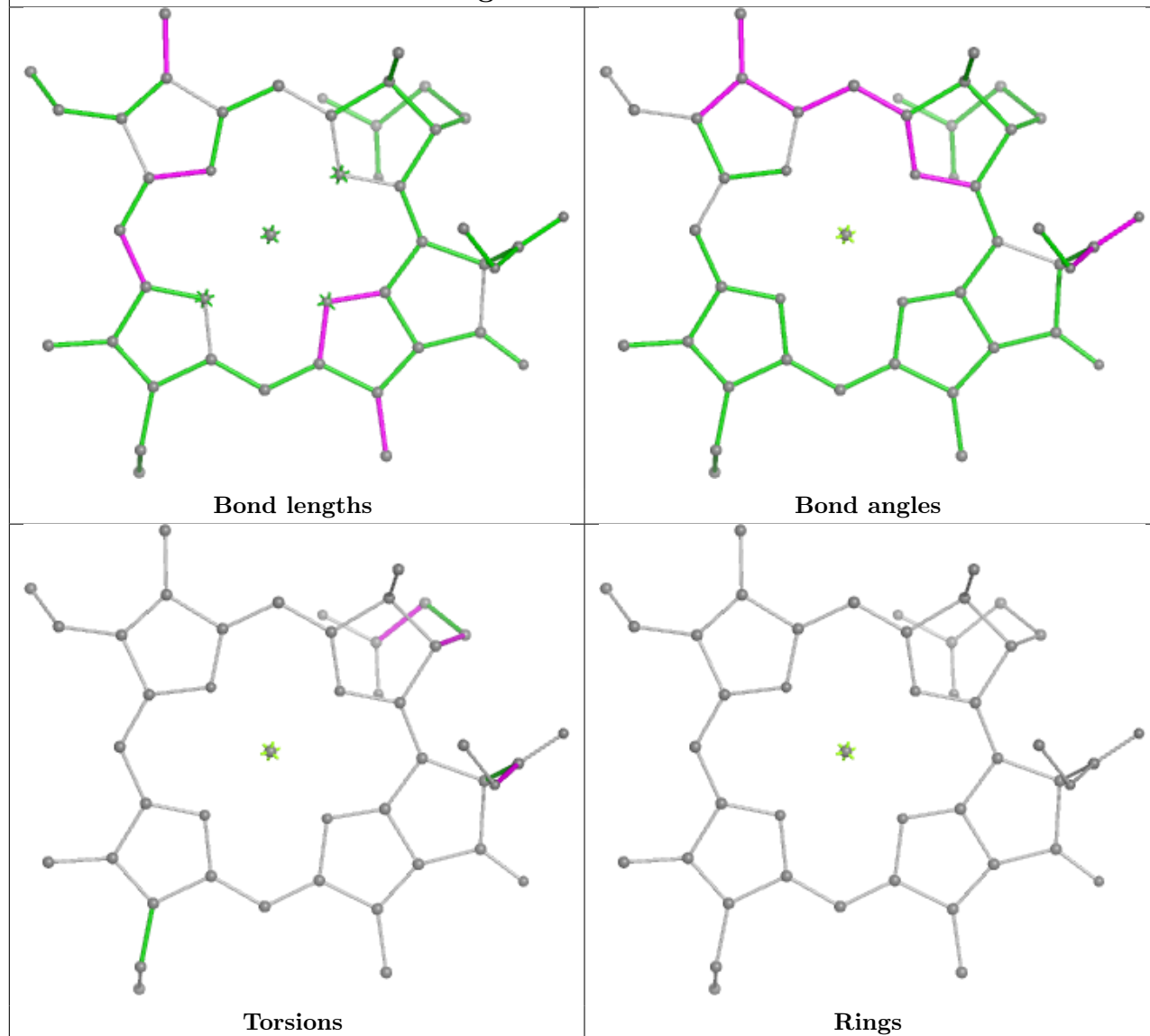
Ligand CLA b 840



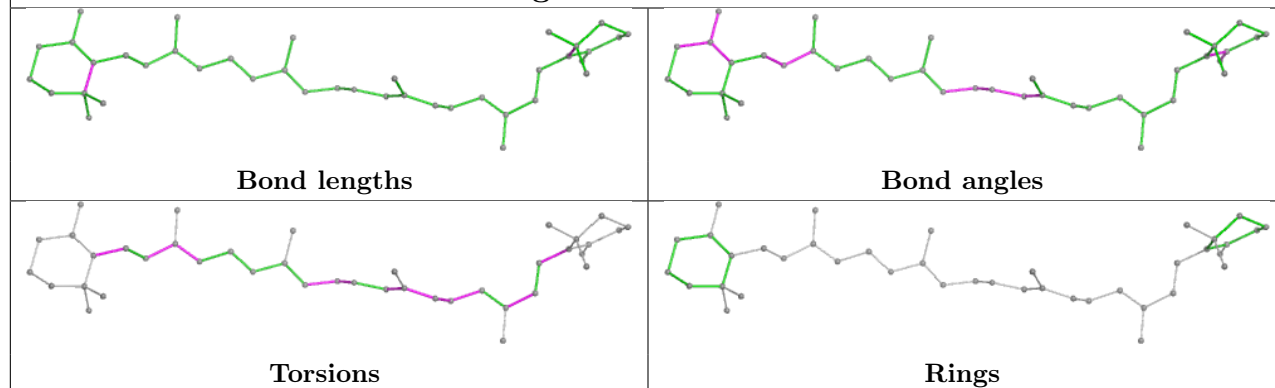
Ligand CLA e 812



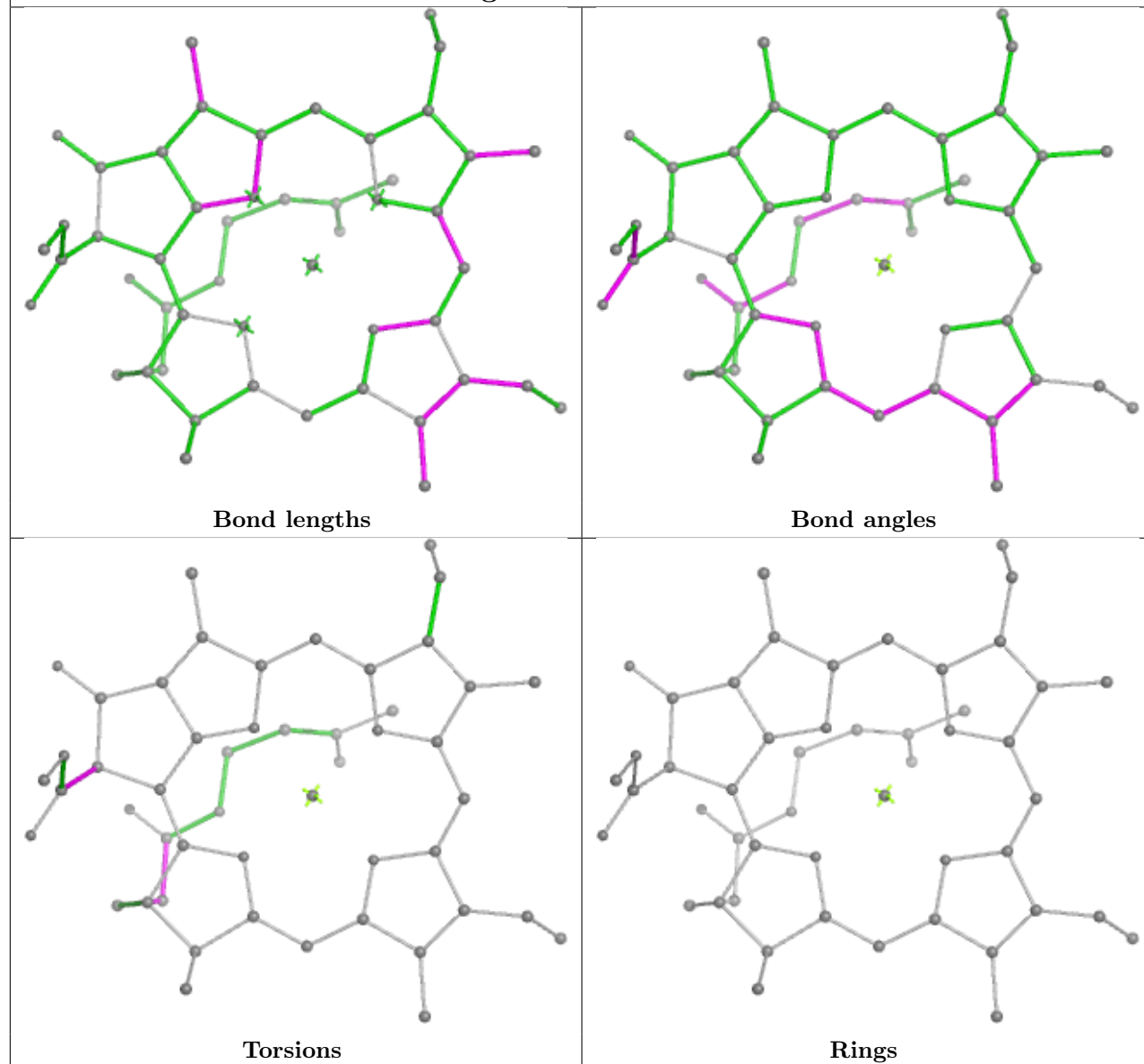
Ligand CLA G 816



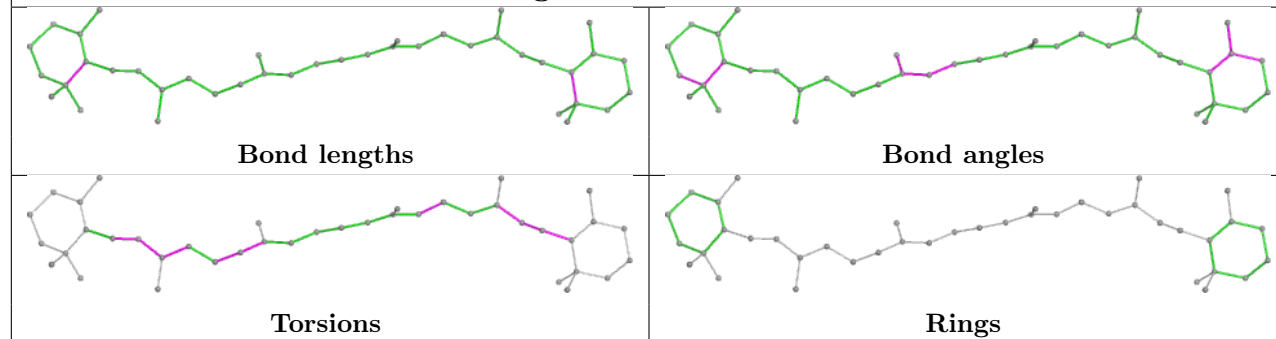
Ligand BCR b 847



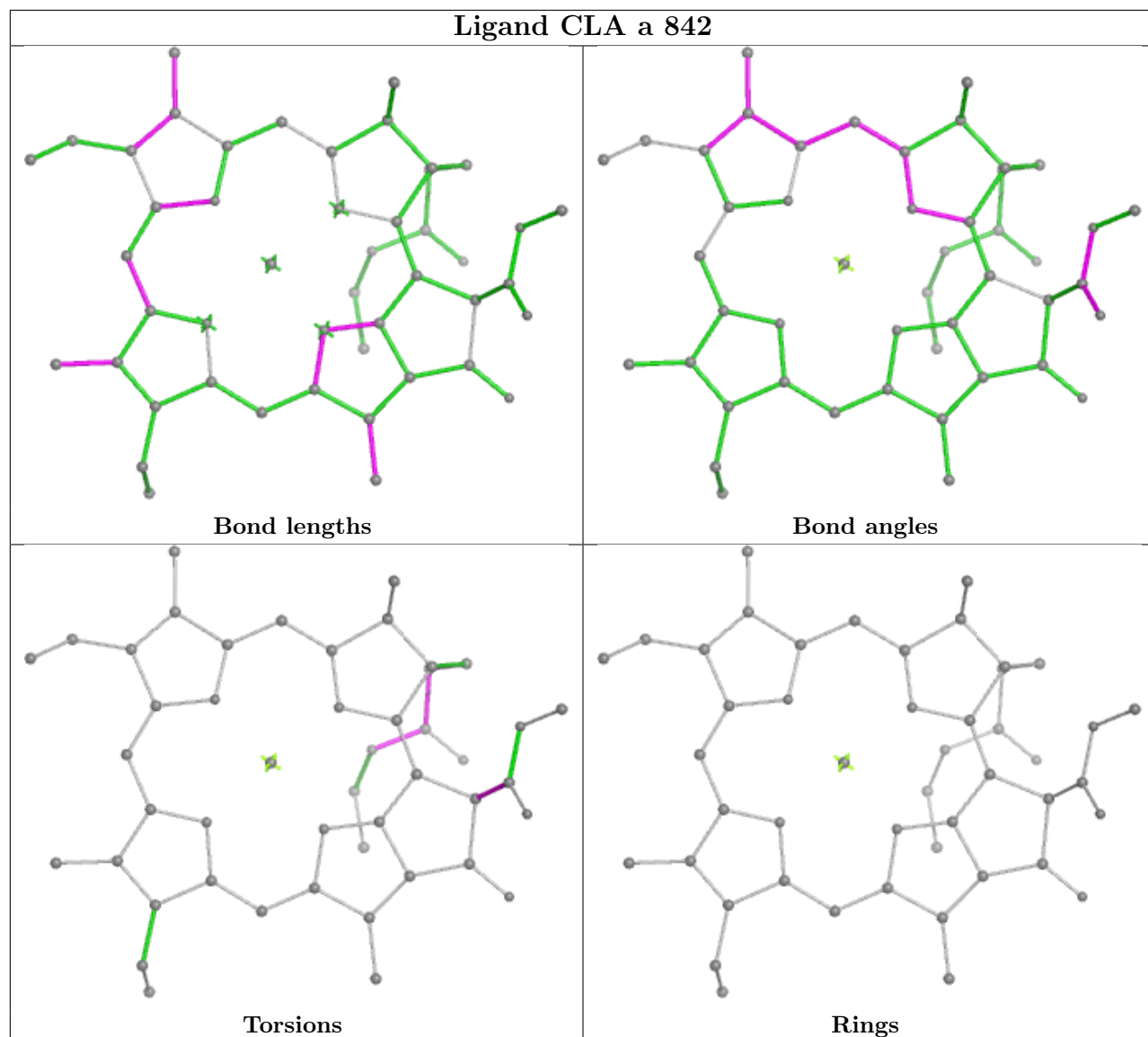
Ligand CLA e 839



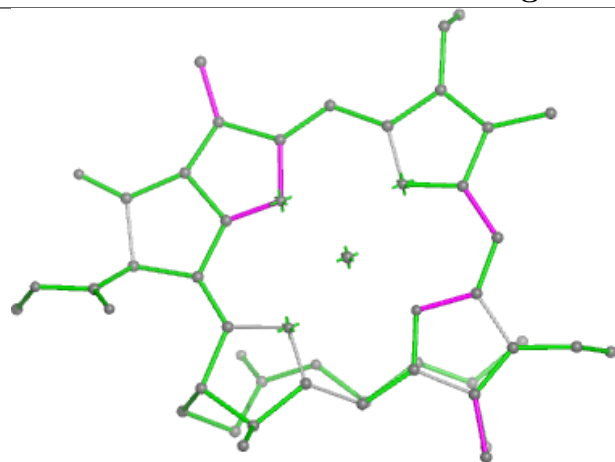
Ligand BCR L 205



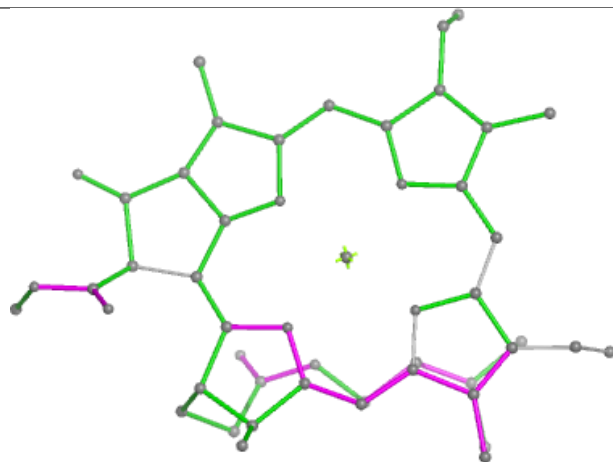
Ligand CLA a 842



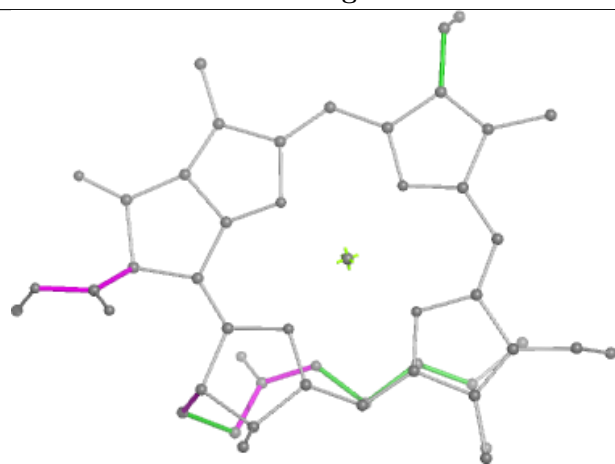
Ligand CLA e 823



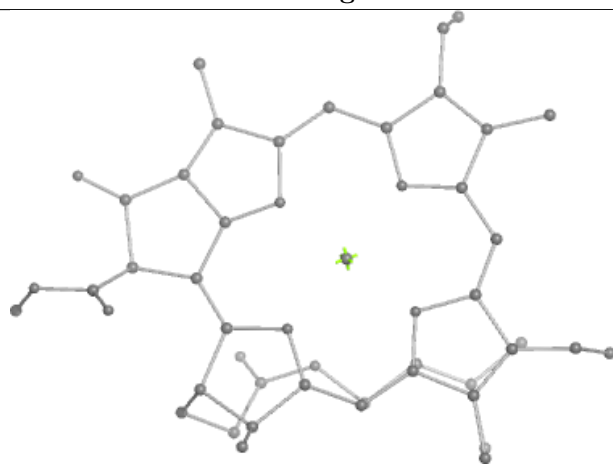
Bond lengths



Bond angles

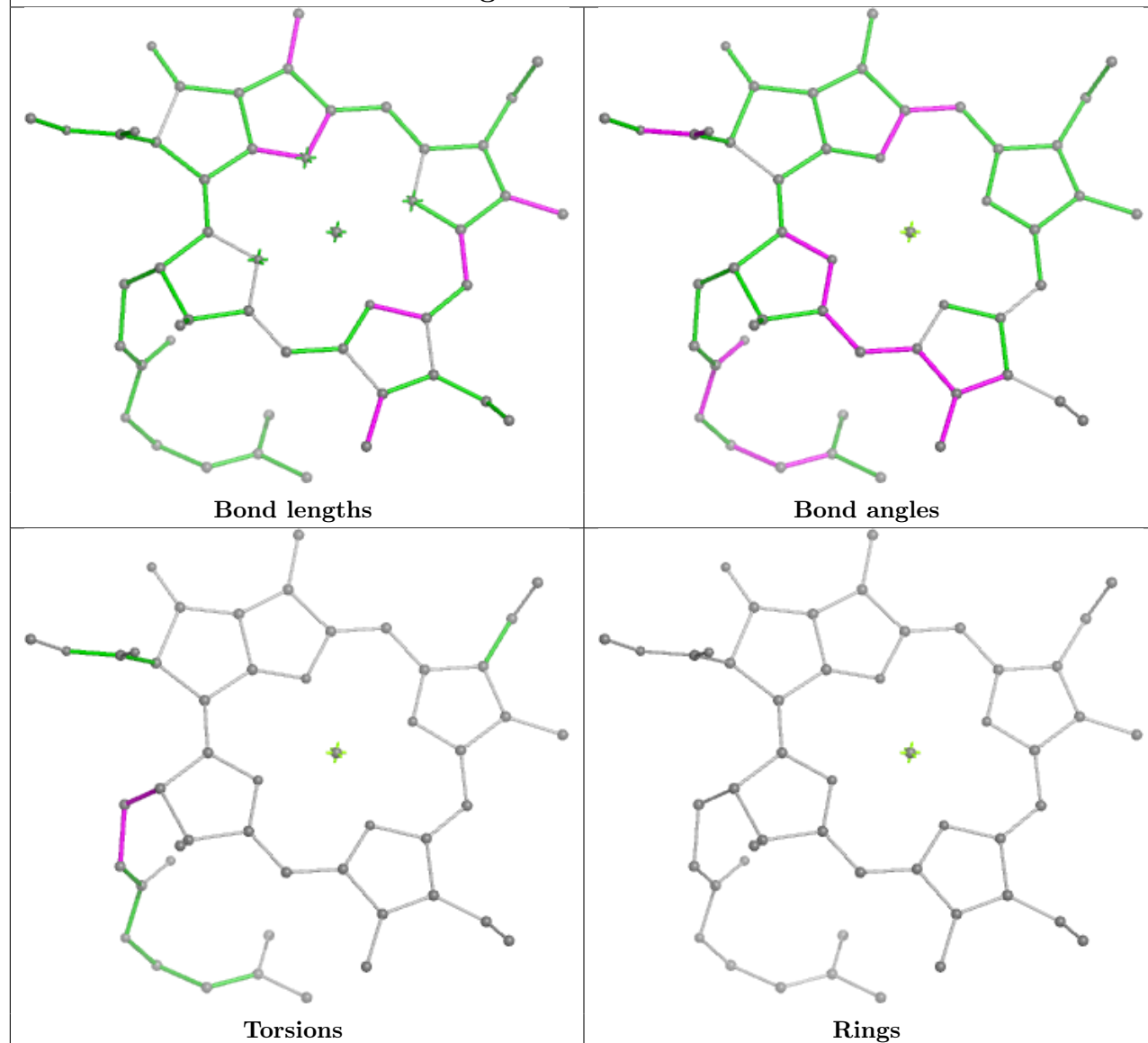


Torsions

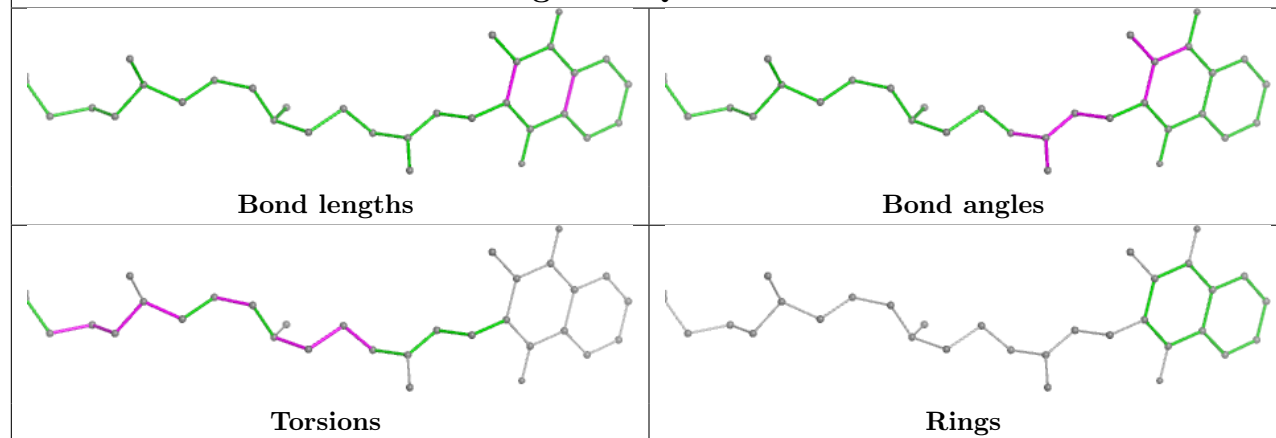


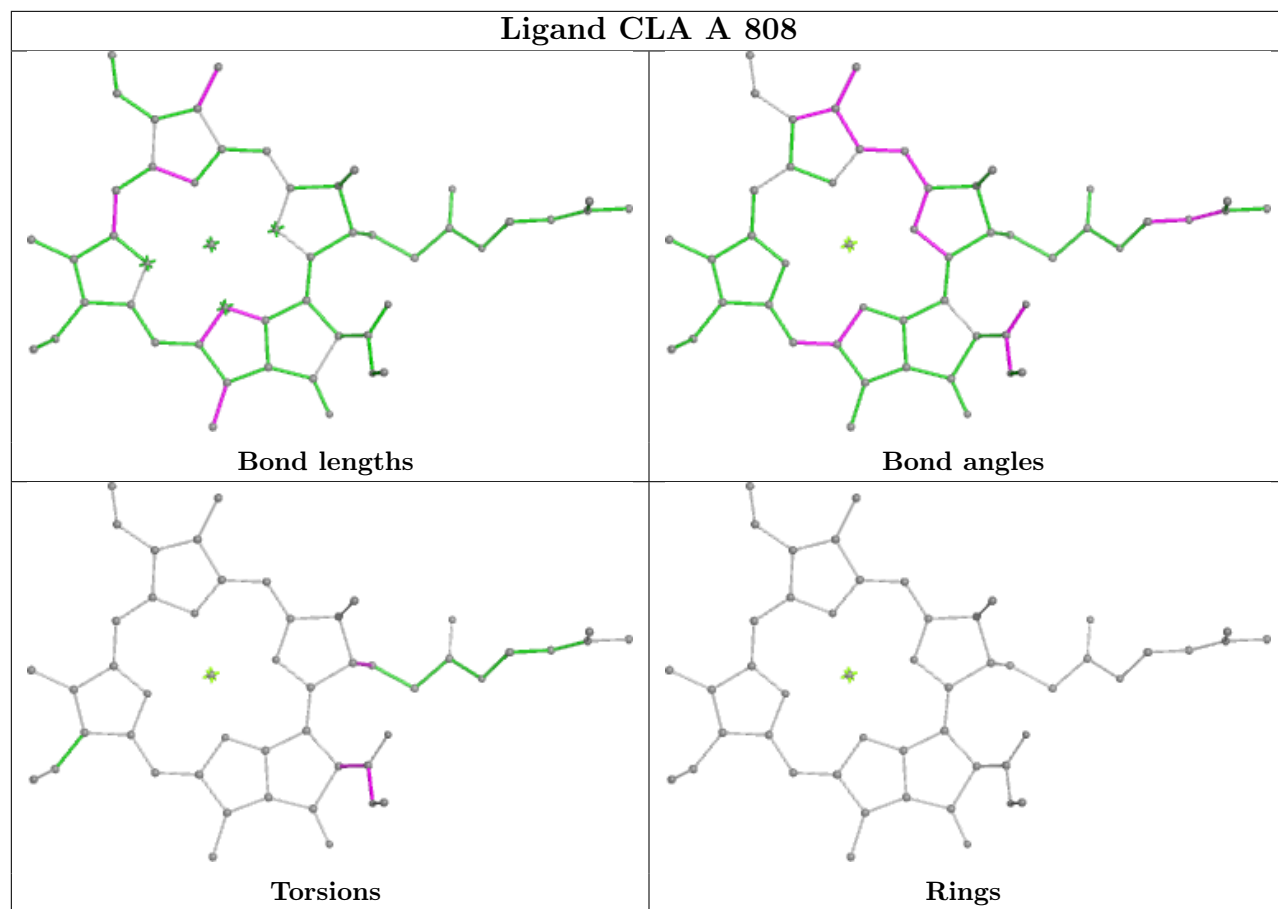
Rings

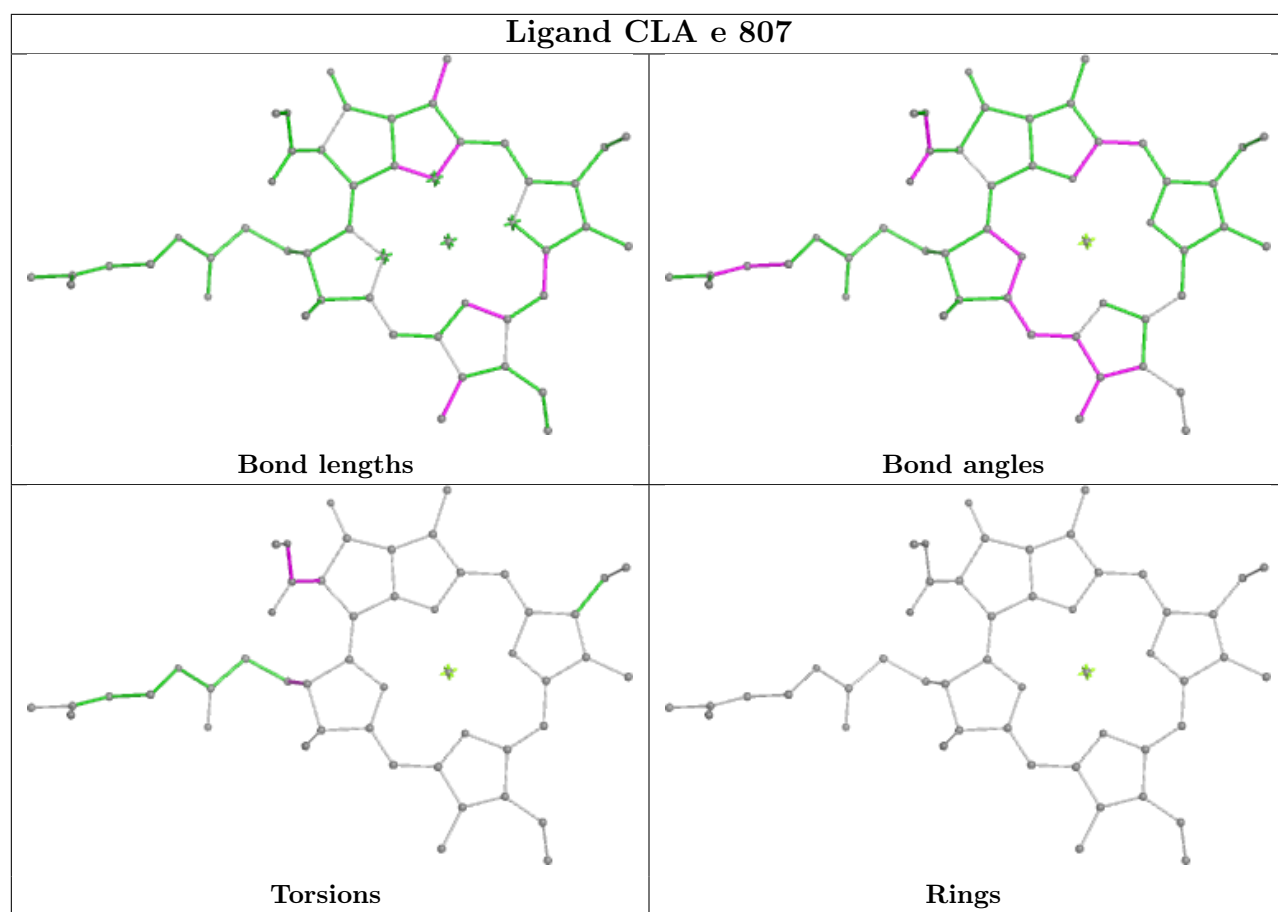
Ligand CLA E 811



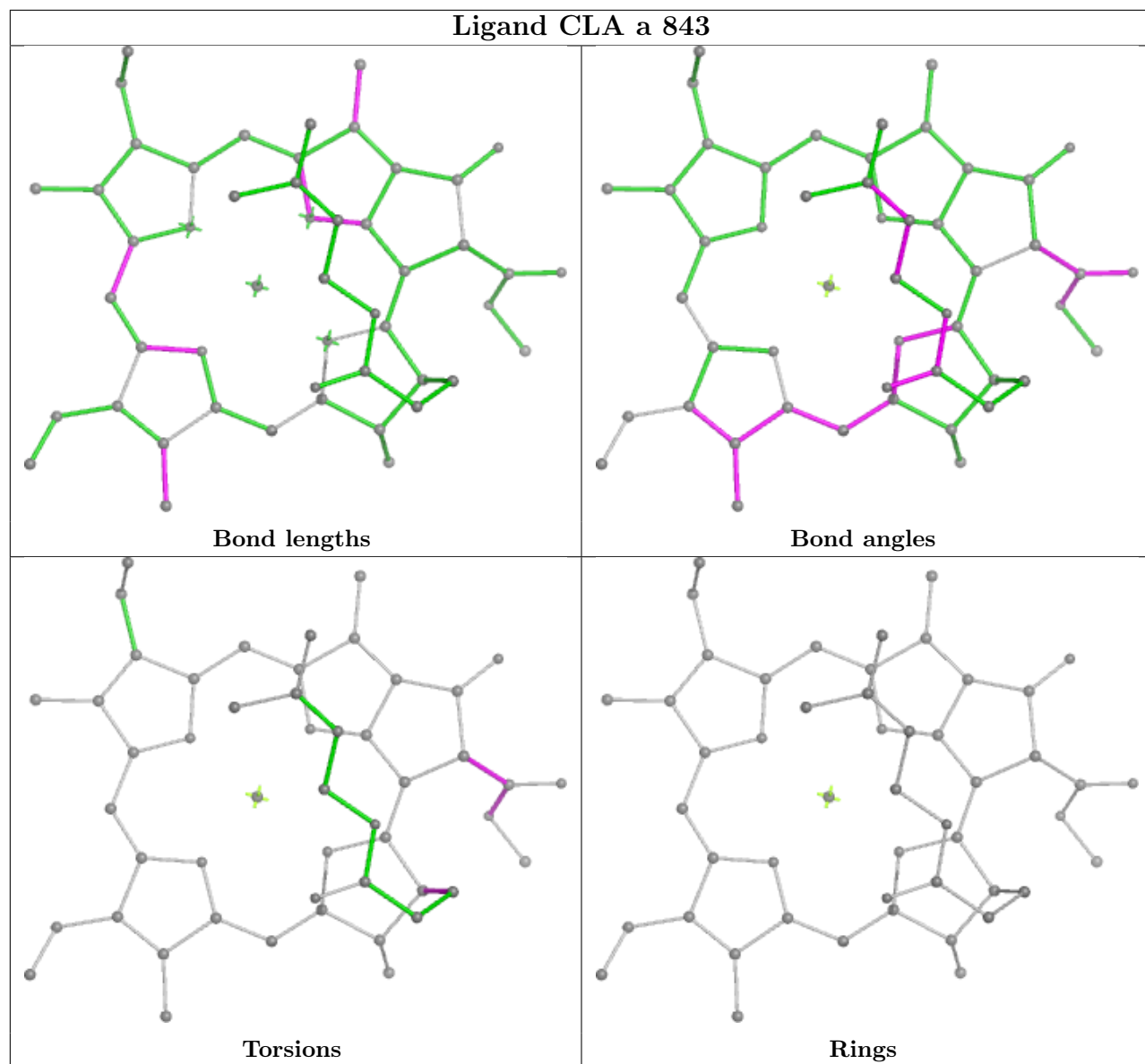
Ligand PQN b 841



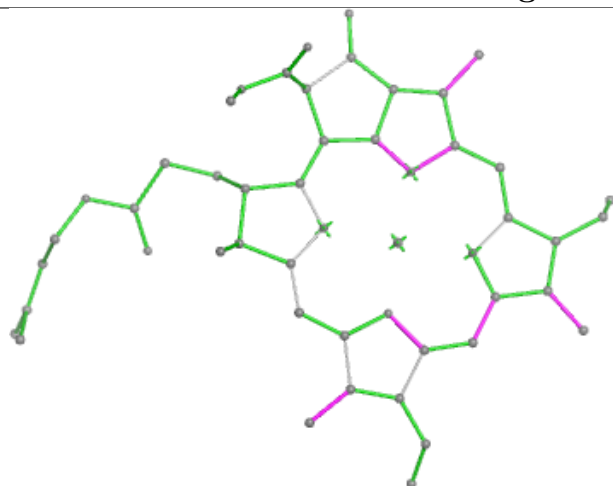




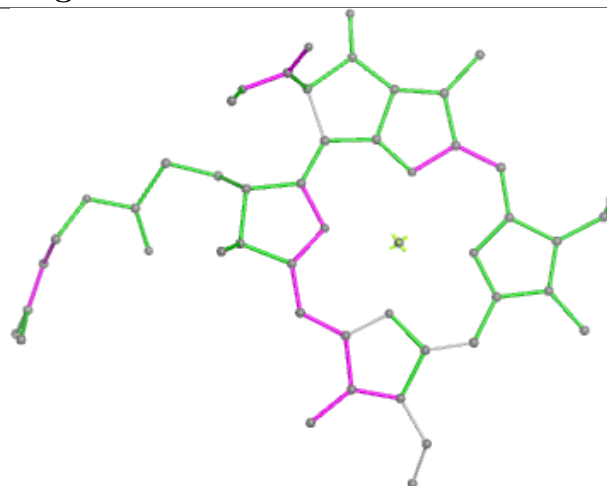
Ligand CLA a 843



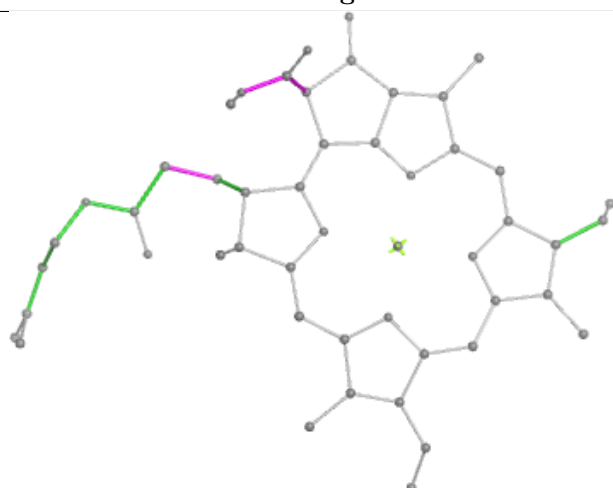
Ligand CLA g 815



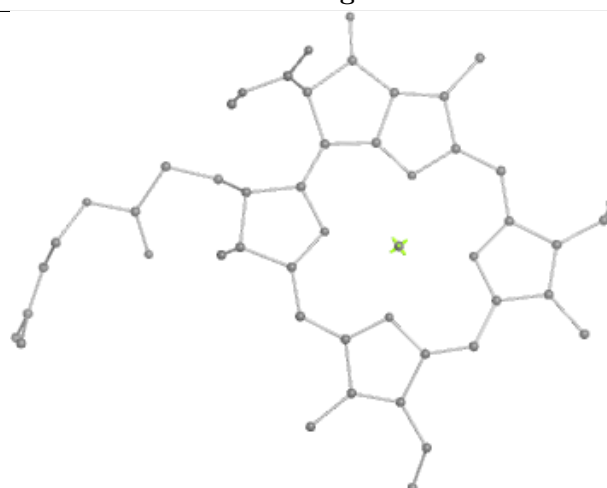
Bond lengths



Bond angles

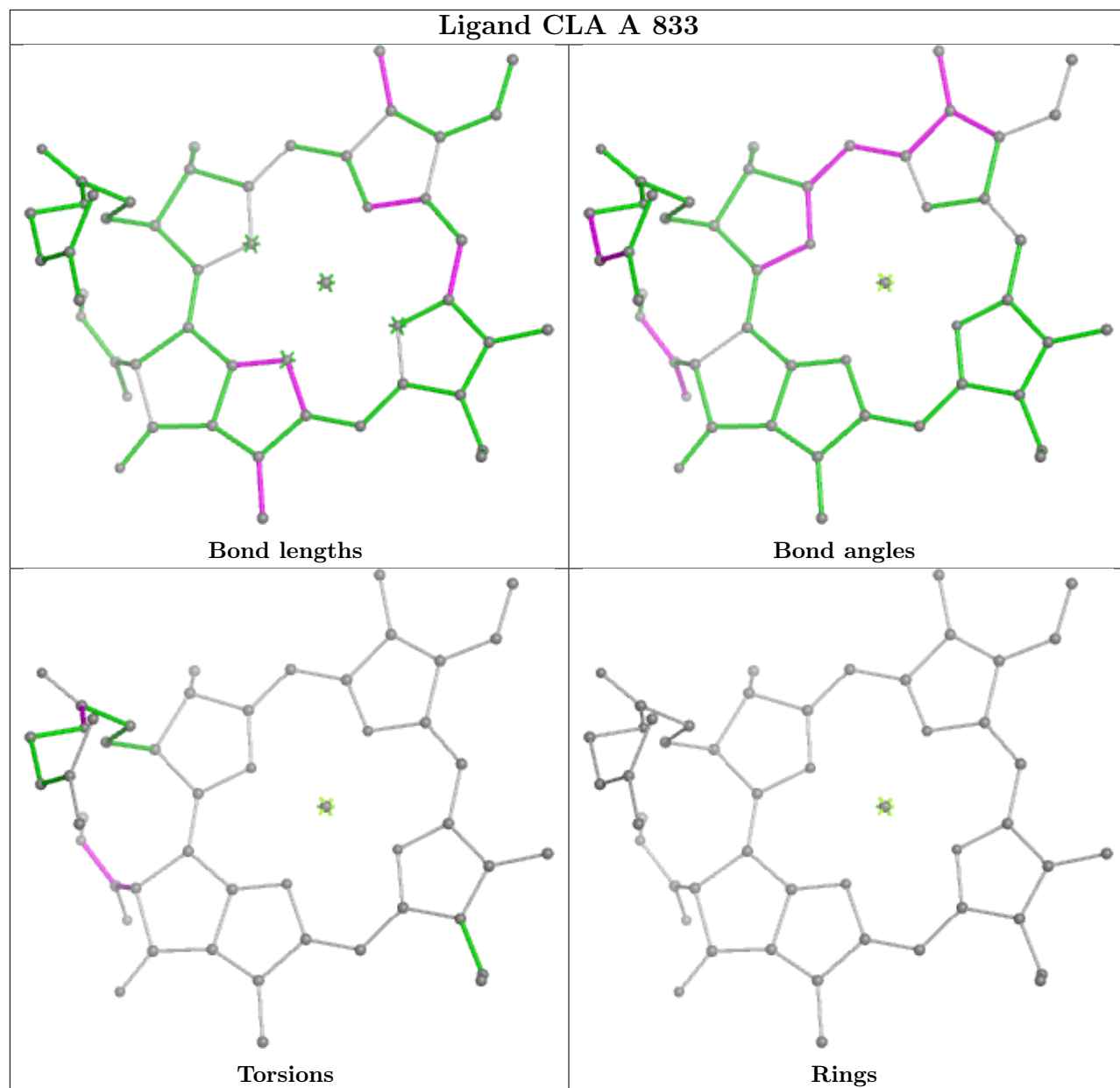


Torsions

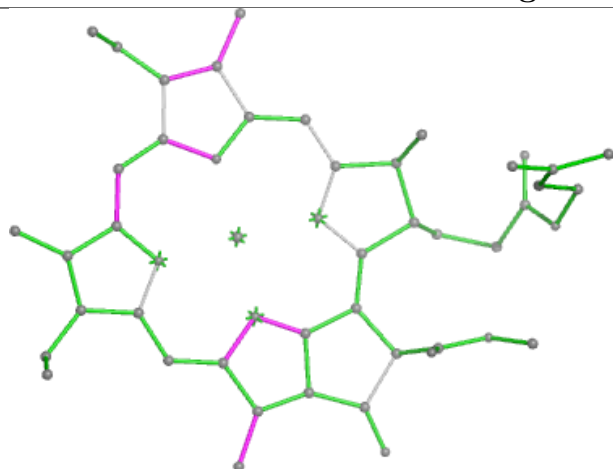


Rings

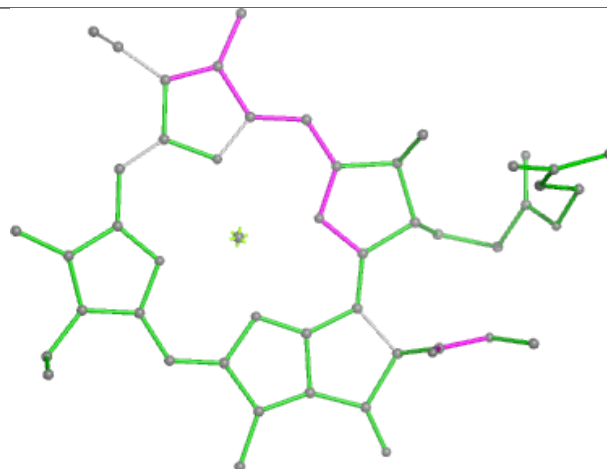
Ligand CLA A 833



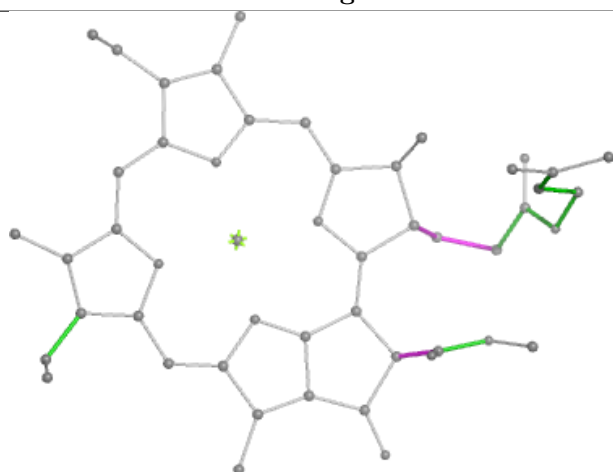
Ligand CLA e 808



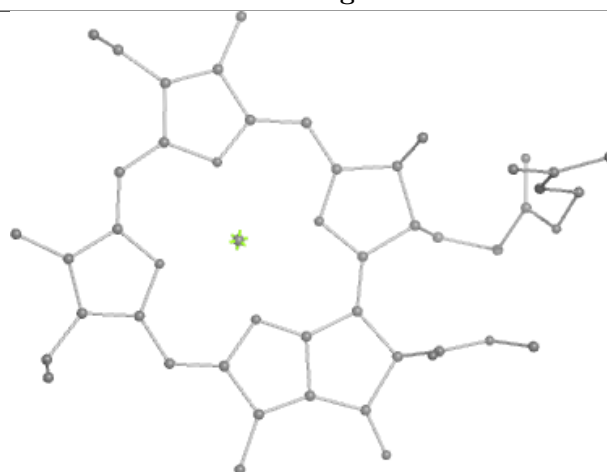
Bond lengths



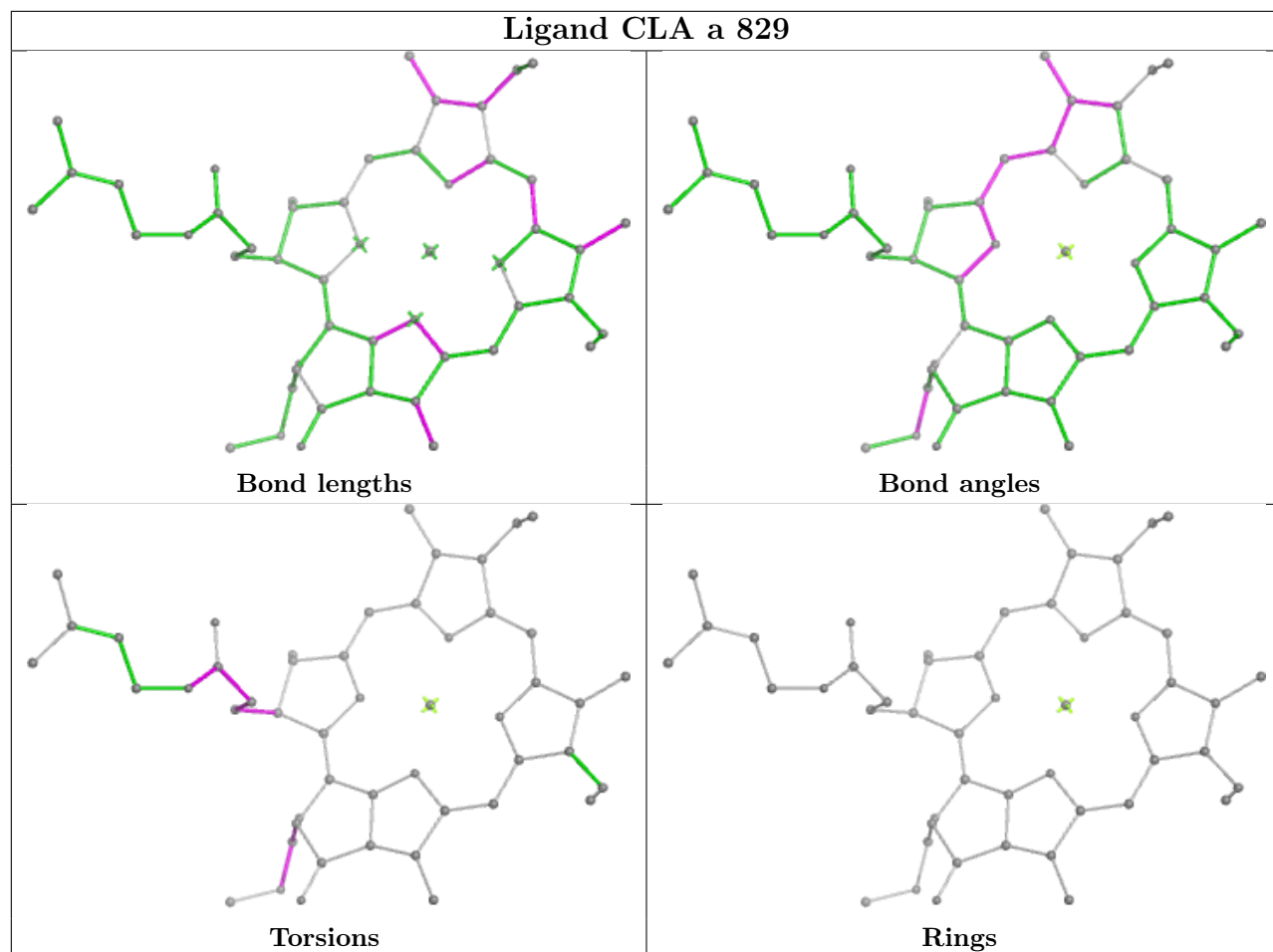
Bond angles



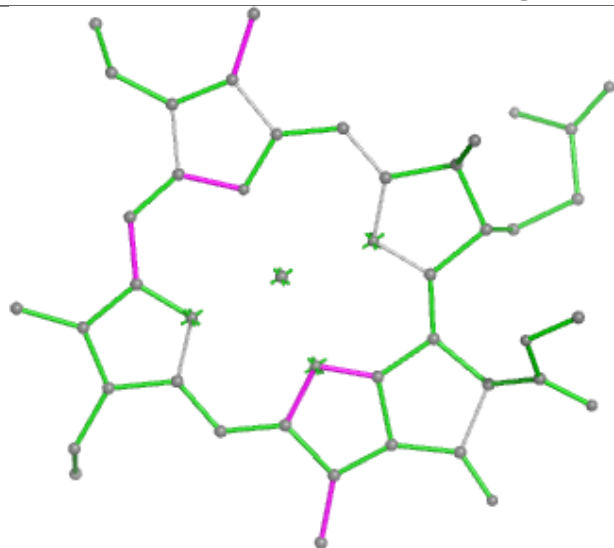
Torsions



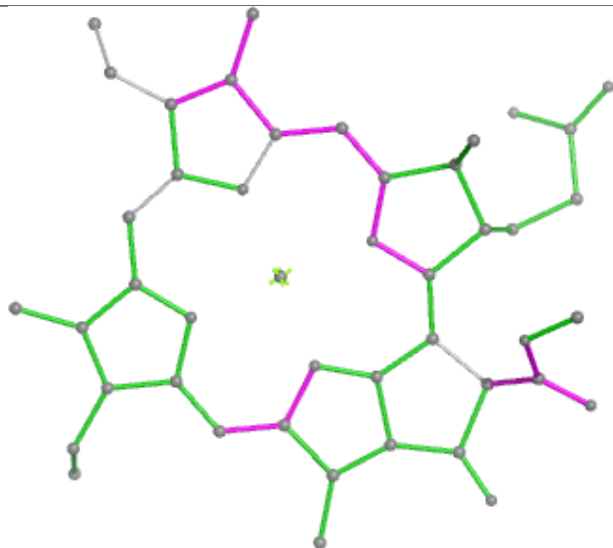
Rings



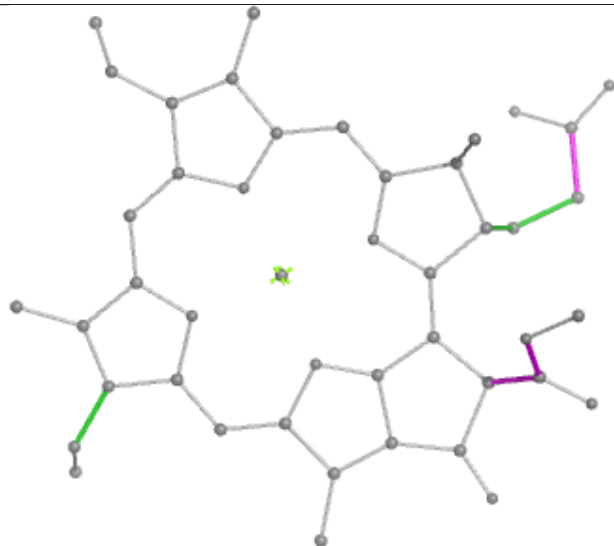
Ligand CLA E 839



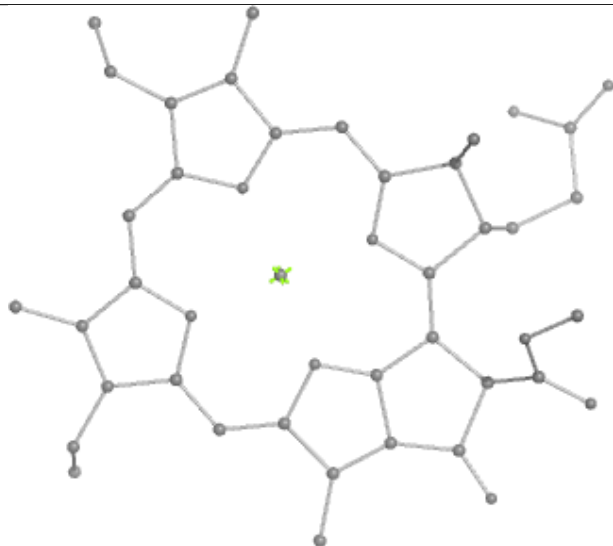
Bond lengths



Bond angles

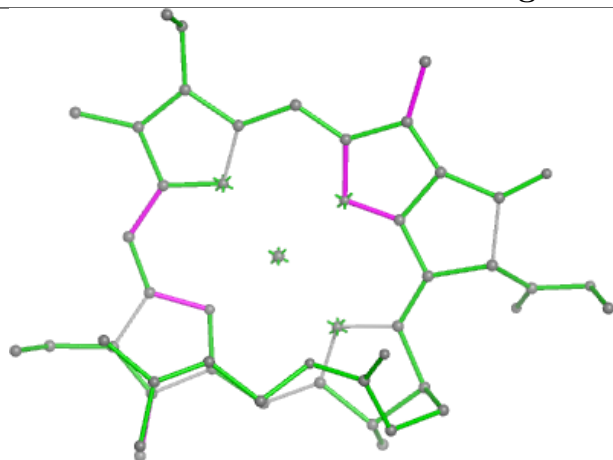


Torsions

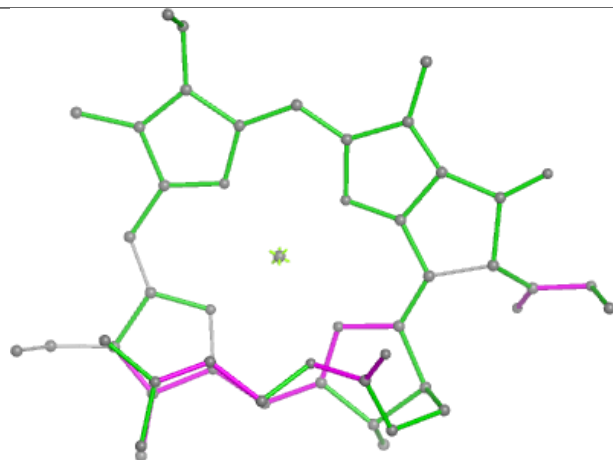


Rings

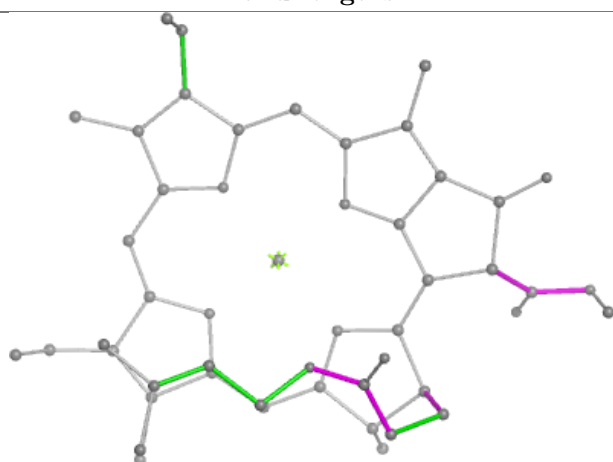
Ligand CLA a 824



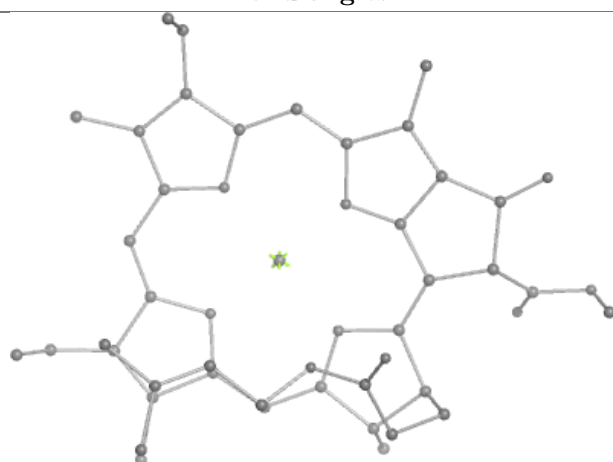
Bond lengths



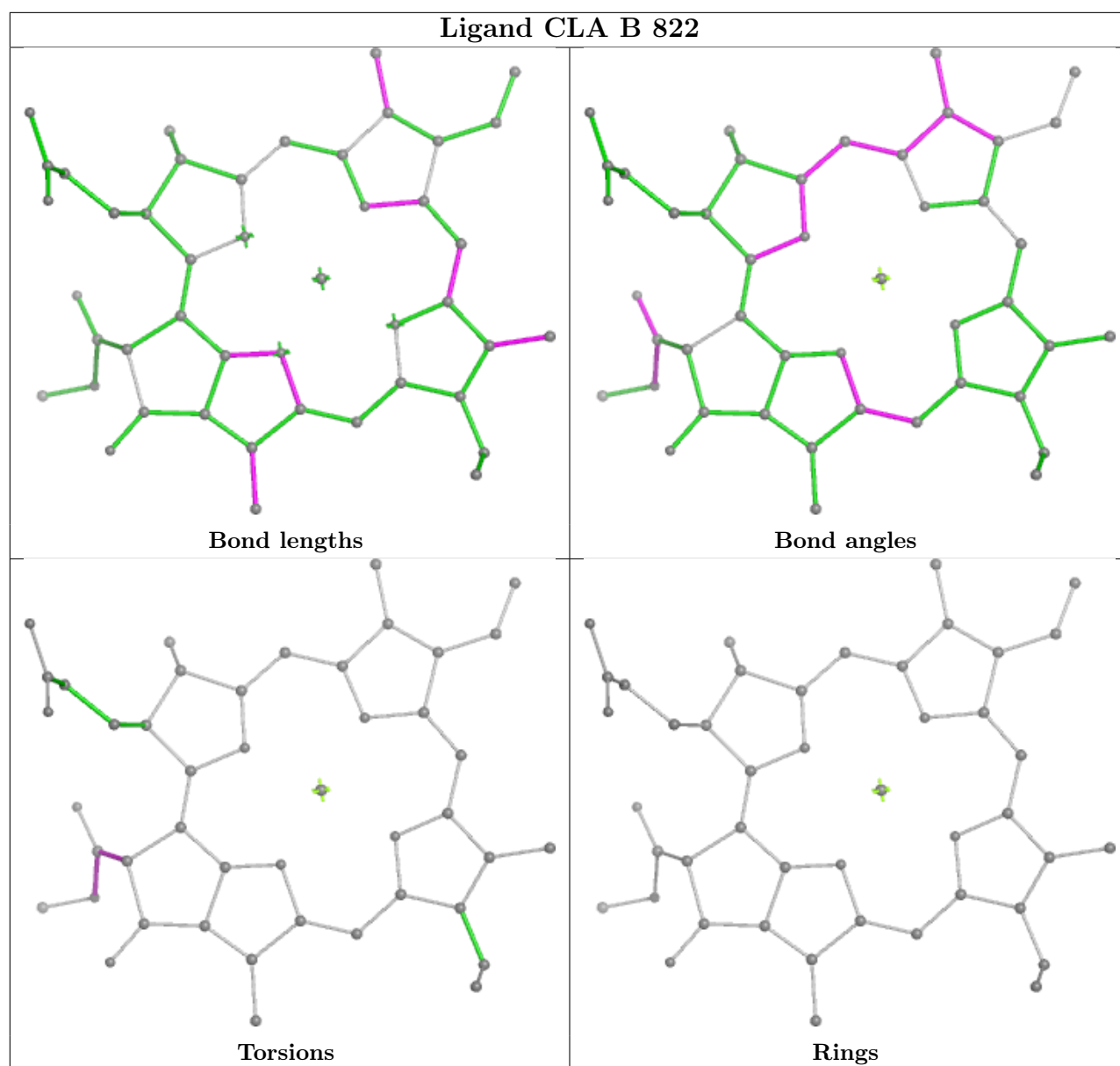
Bond angles

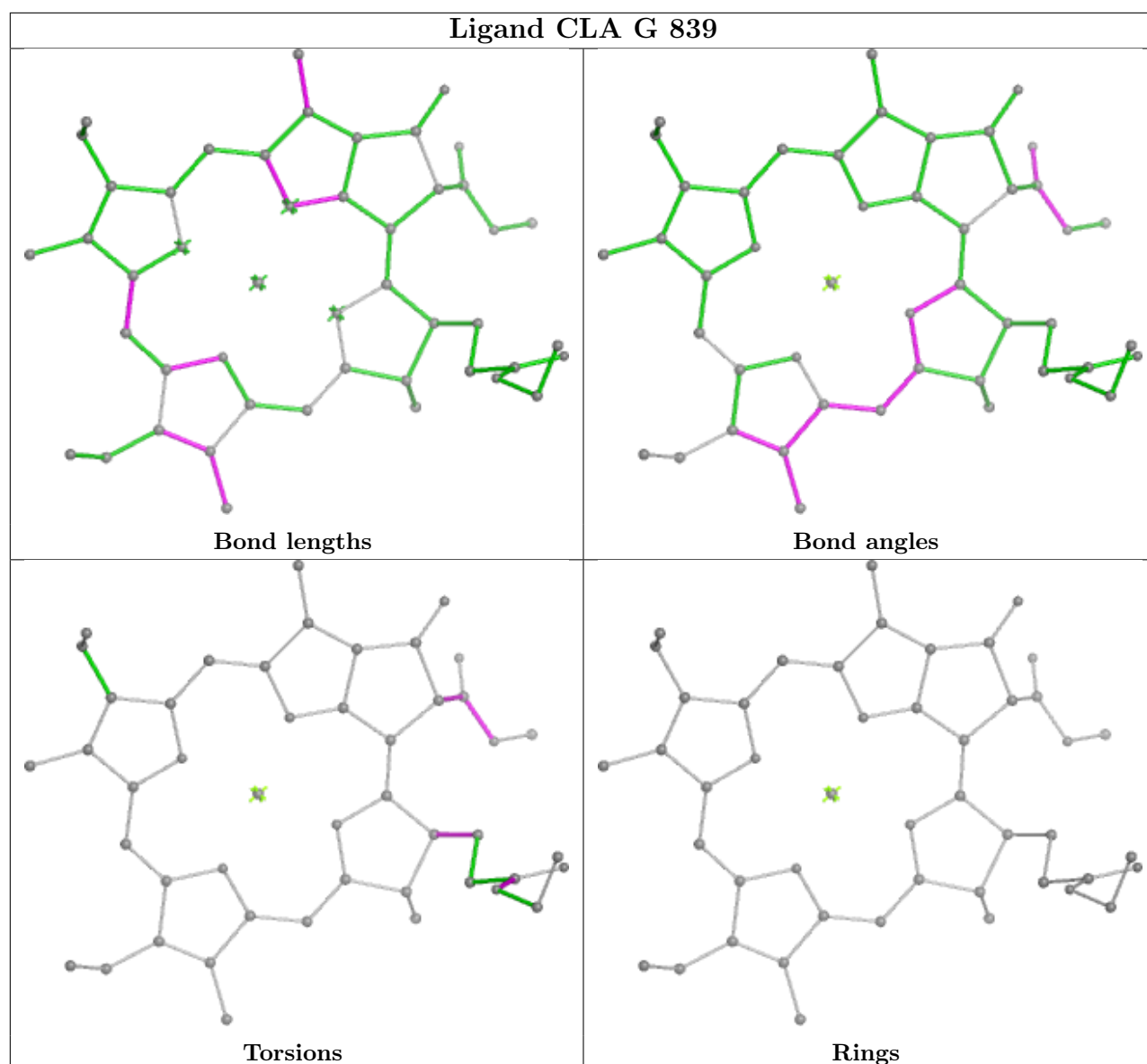


Torsions

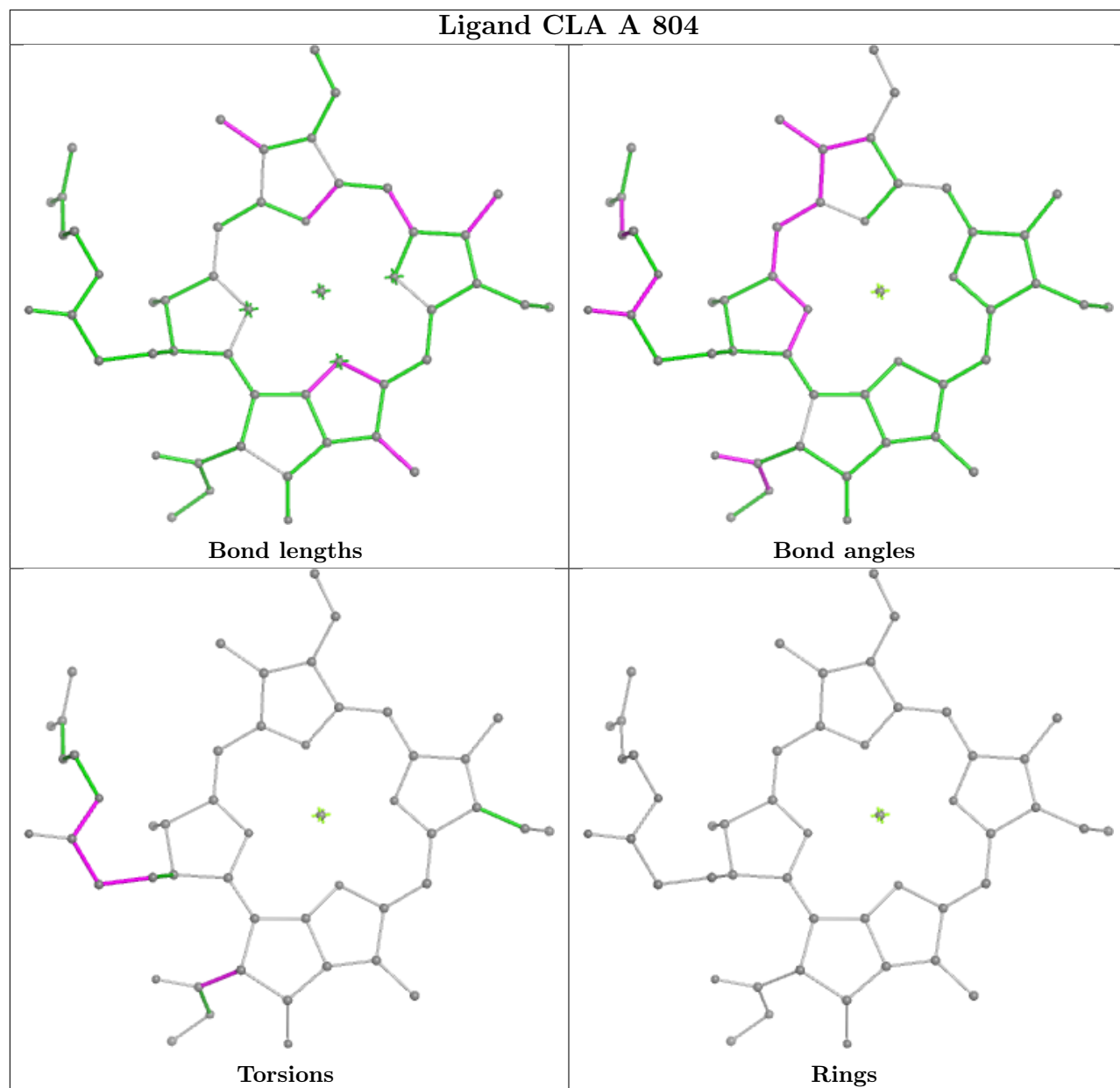


Rings

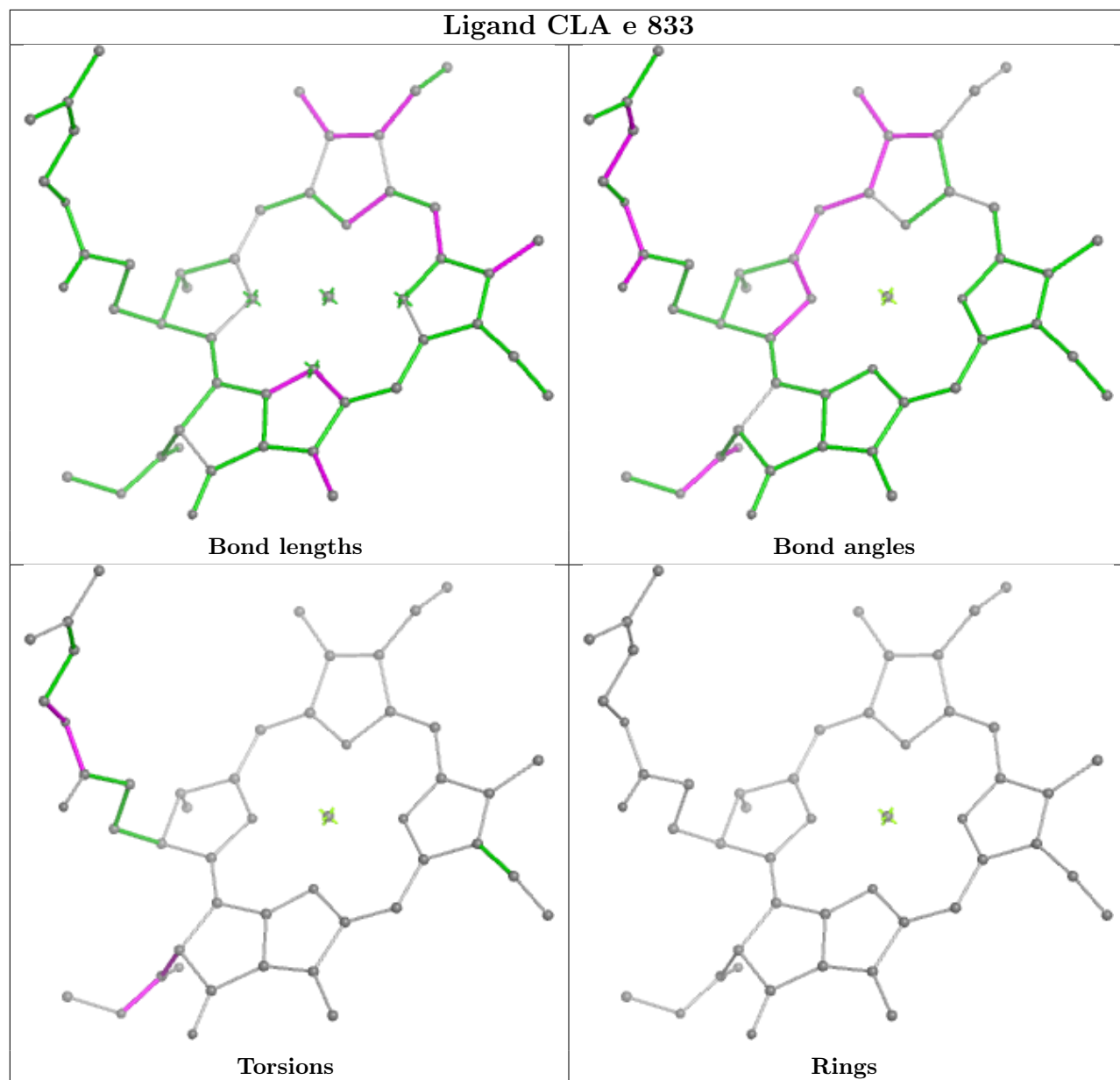




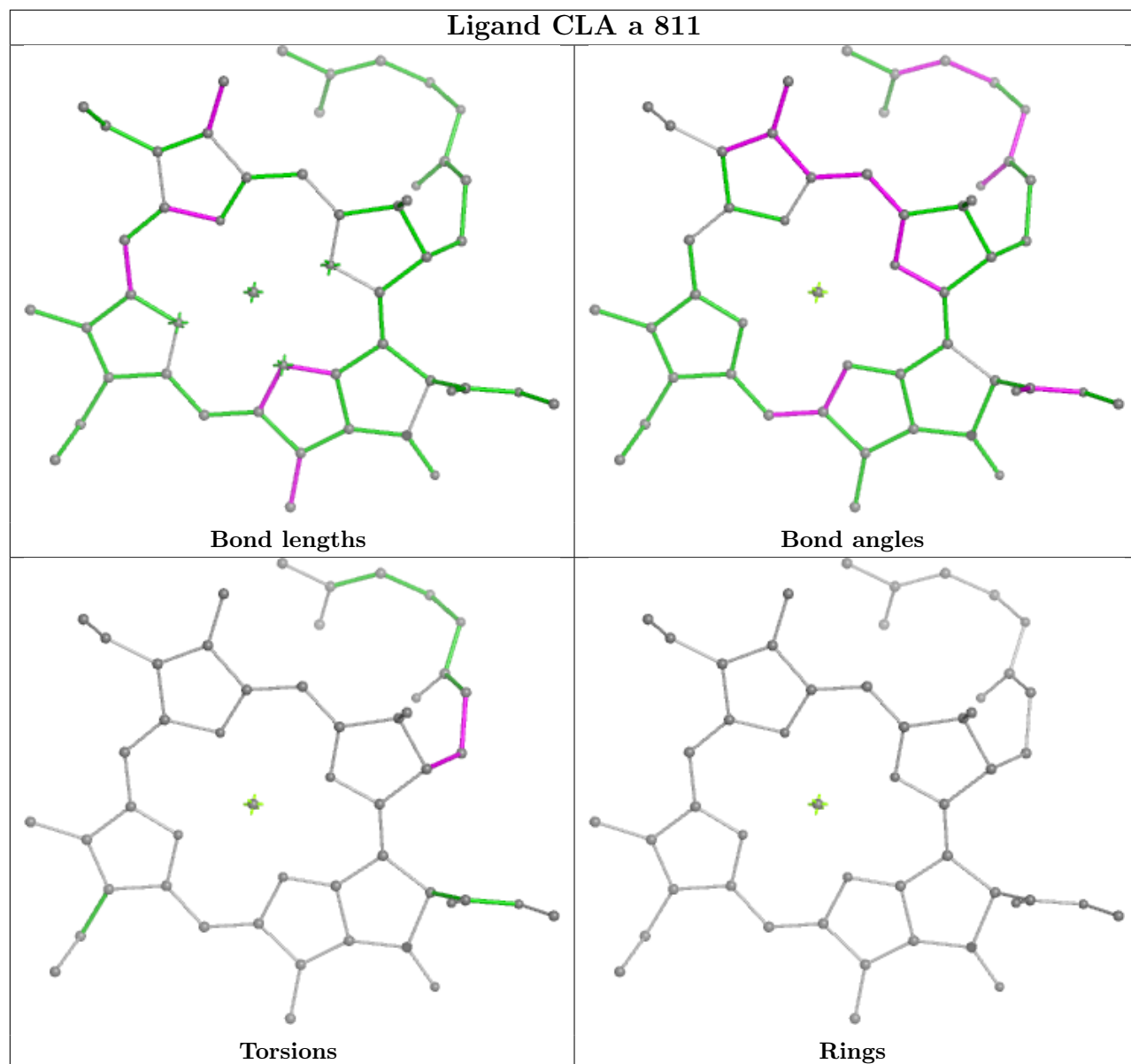
Ligand CLA A 804



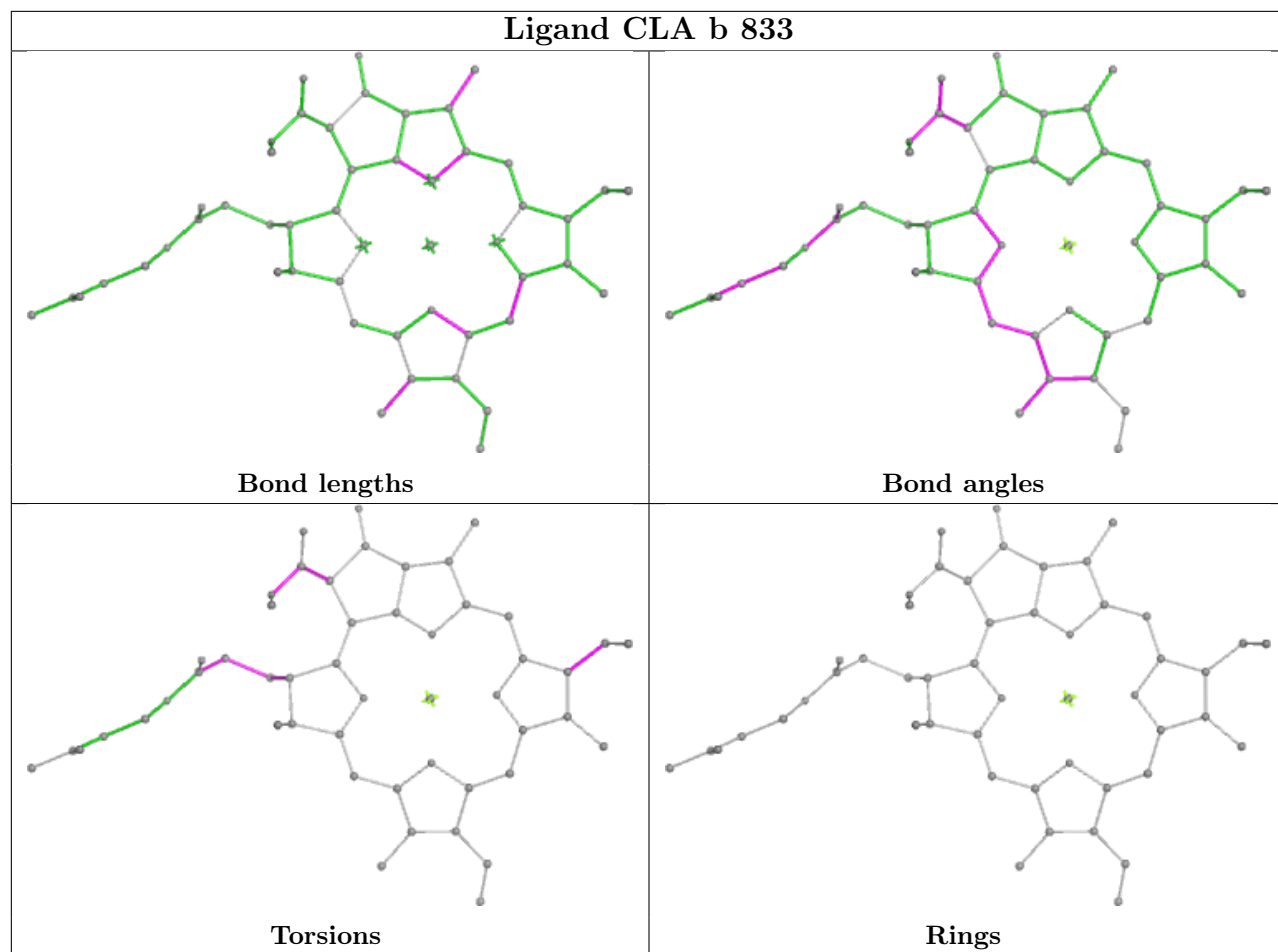
Ligand CLA e 833



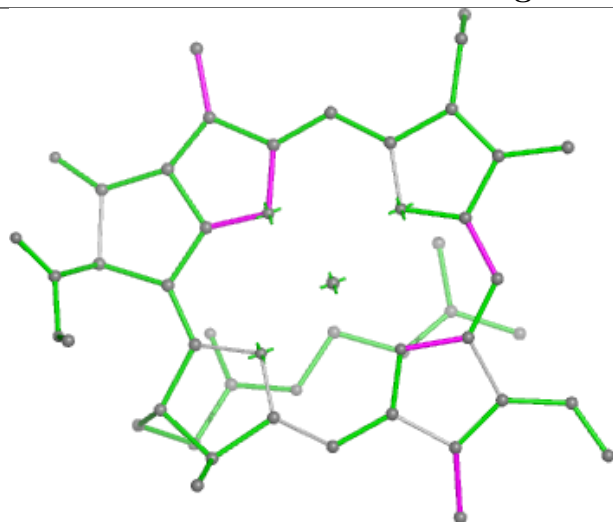
Ligand CLA a 811



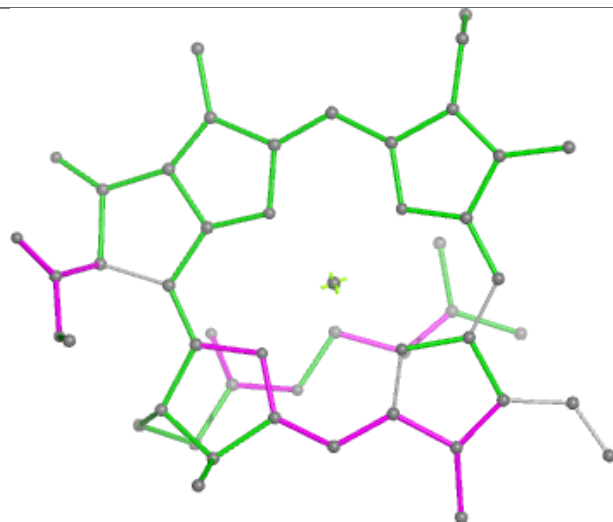
Ligand CLA b 833



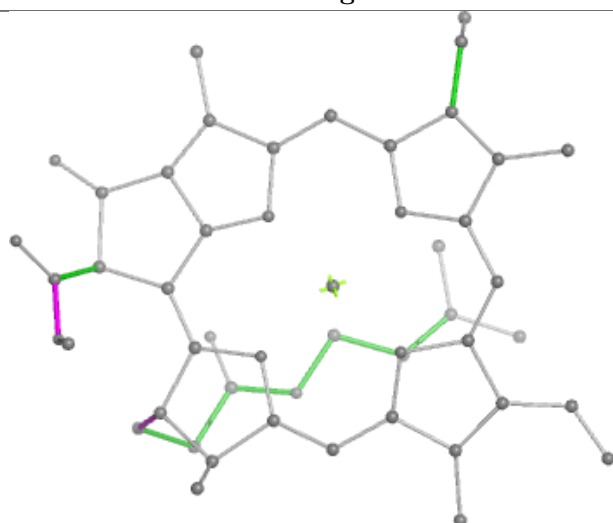
Ligand CLA B 810



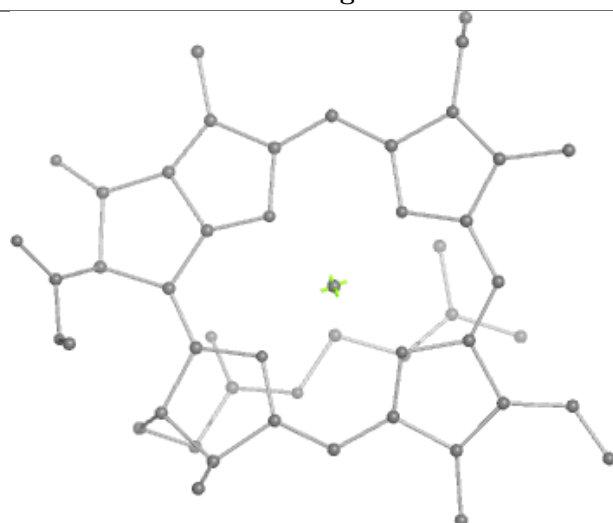
Bond lengths



Bond angles

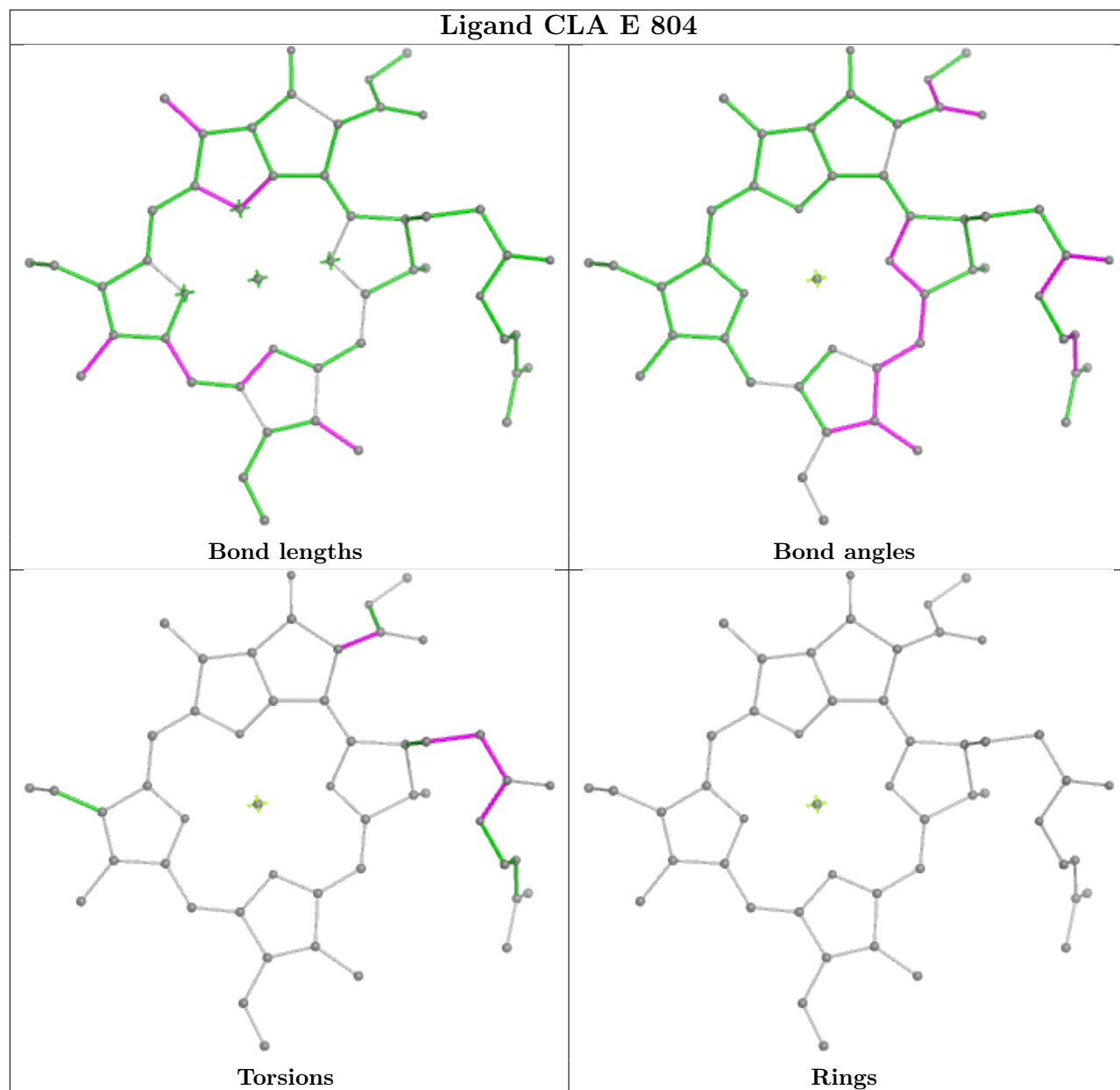


Torsions

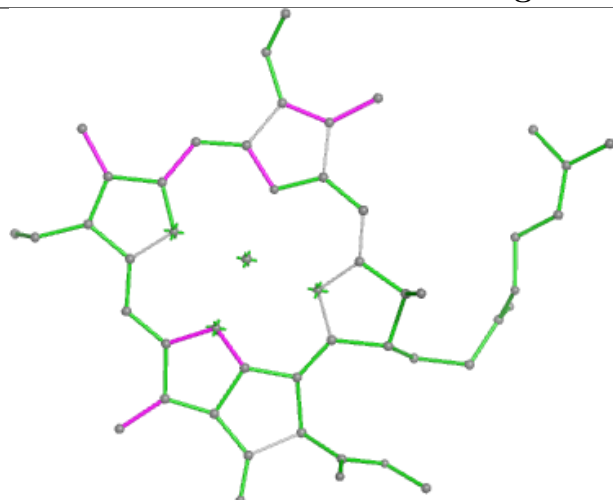


Rings

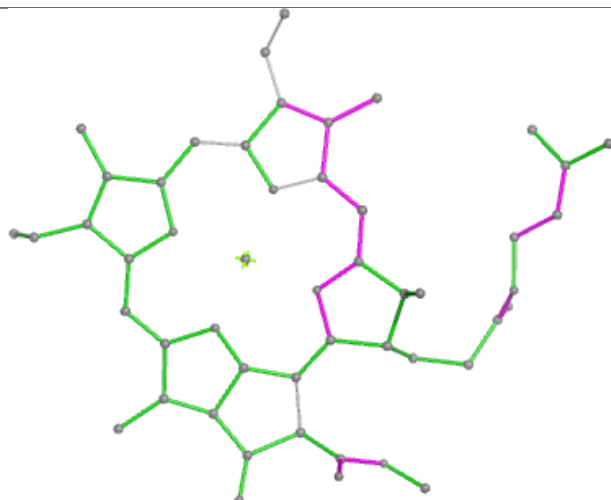
Ligand CLA E 804



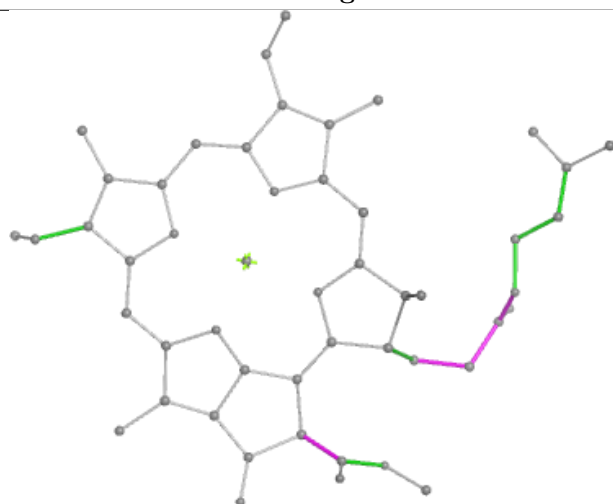
Ligand CLA B 805



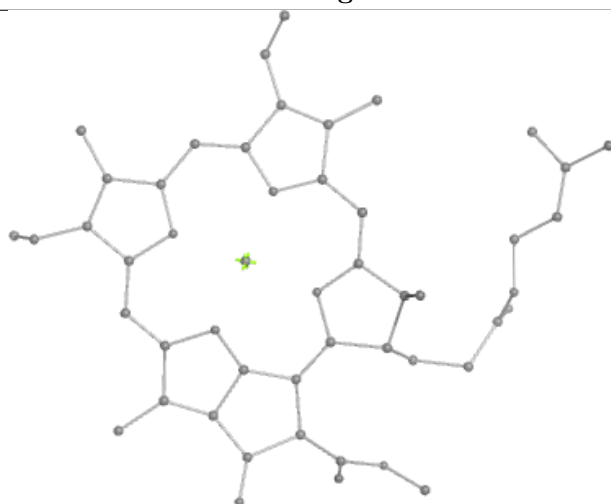
Bond lengths



Bond angles

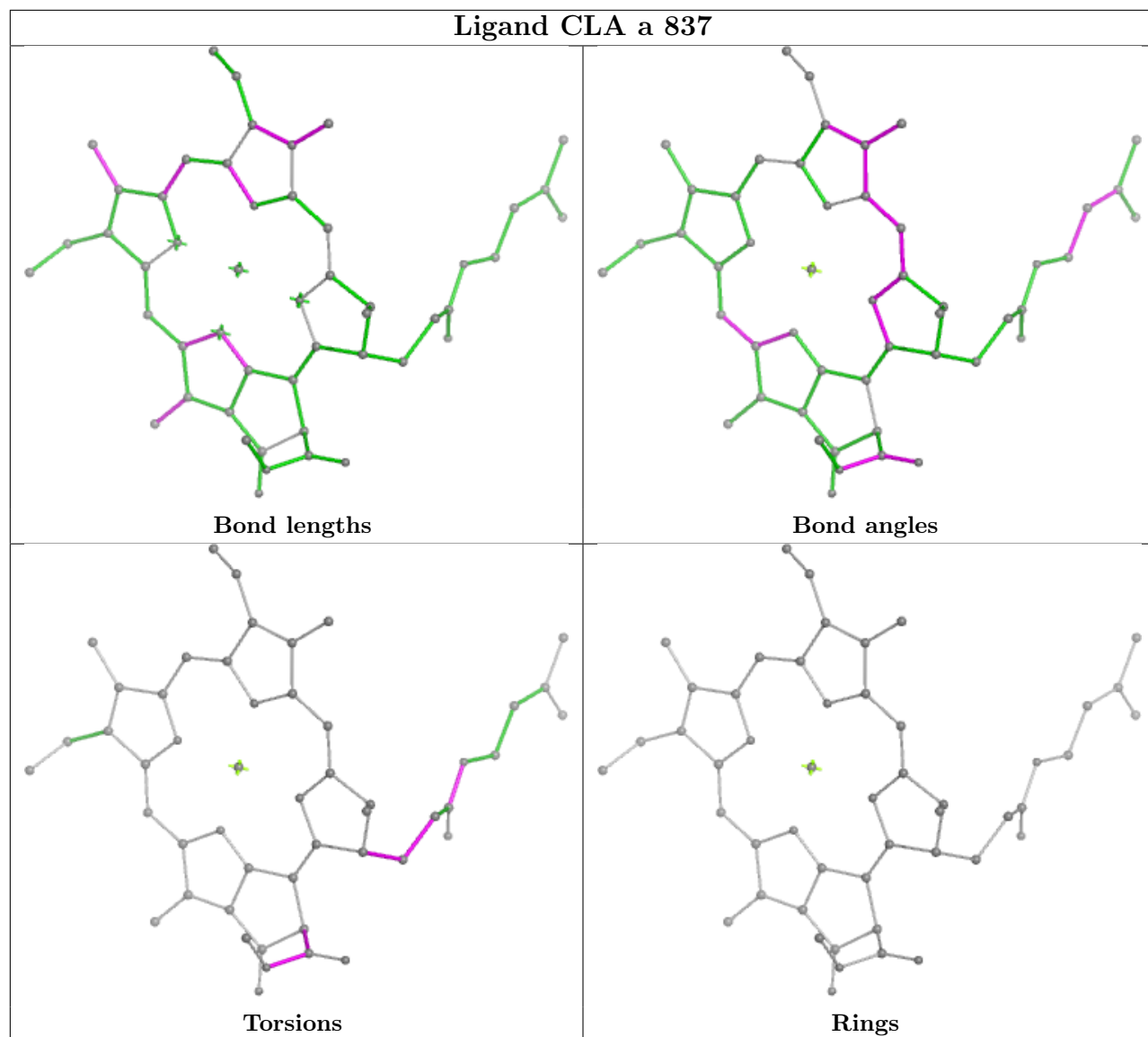


Torsions

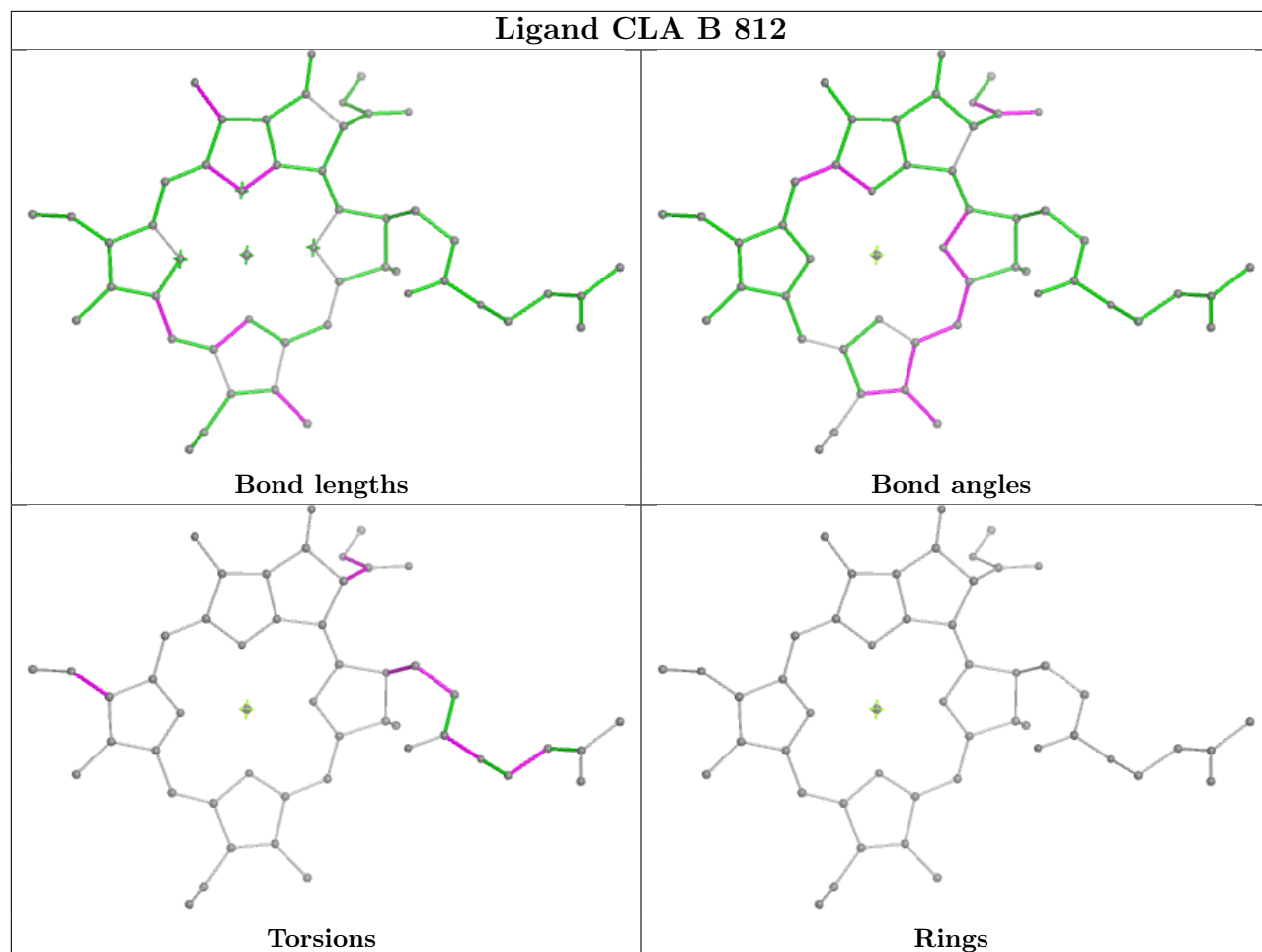


Rings

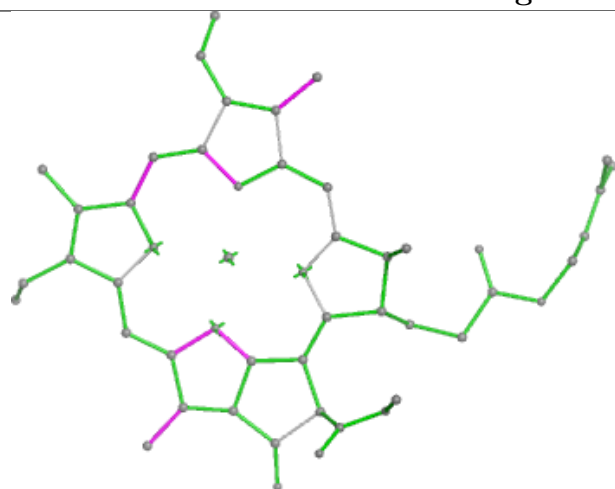
Ligand CLA a 837



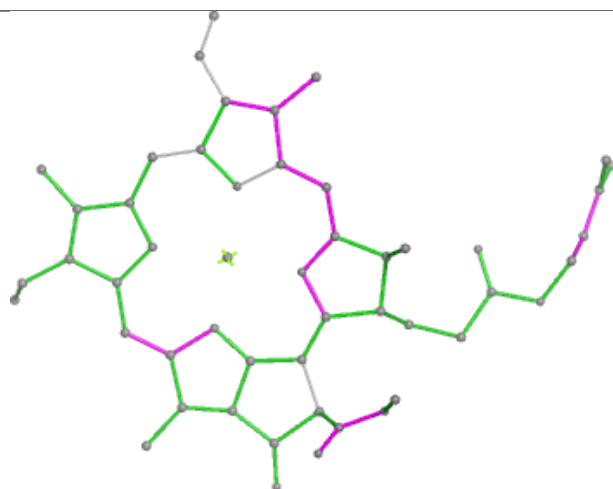
Ligand CLA B 812



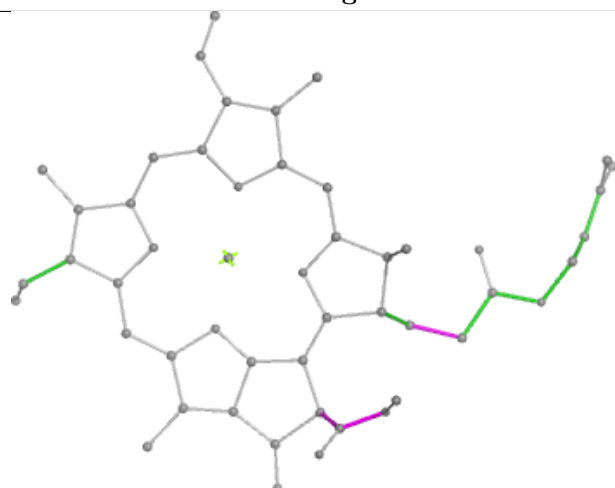
Ligand CLA G 814



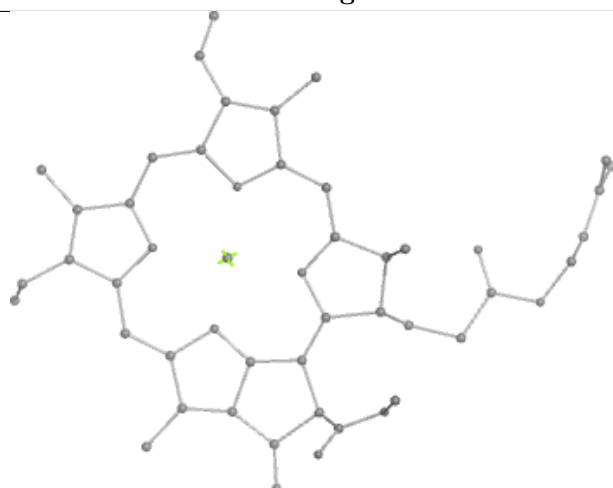
Bond lengths



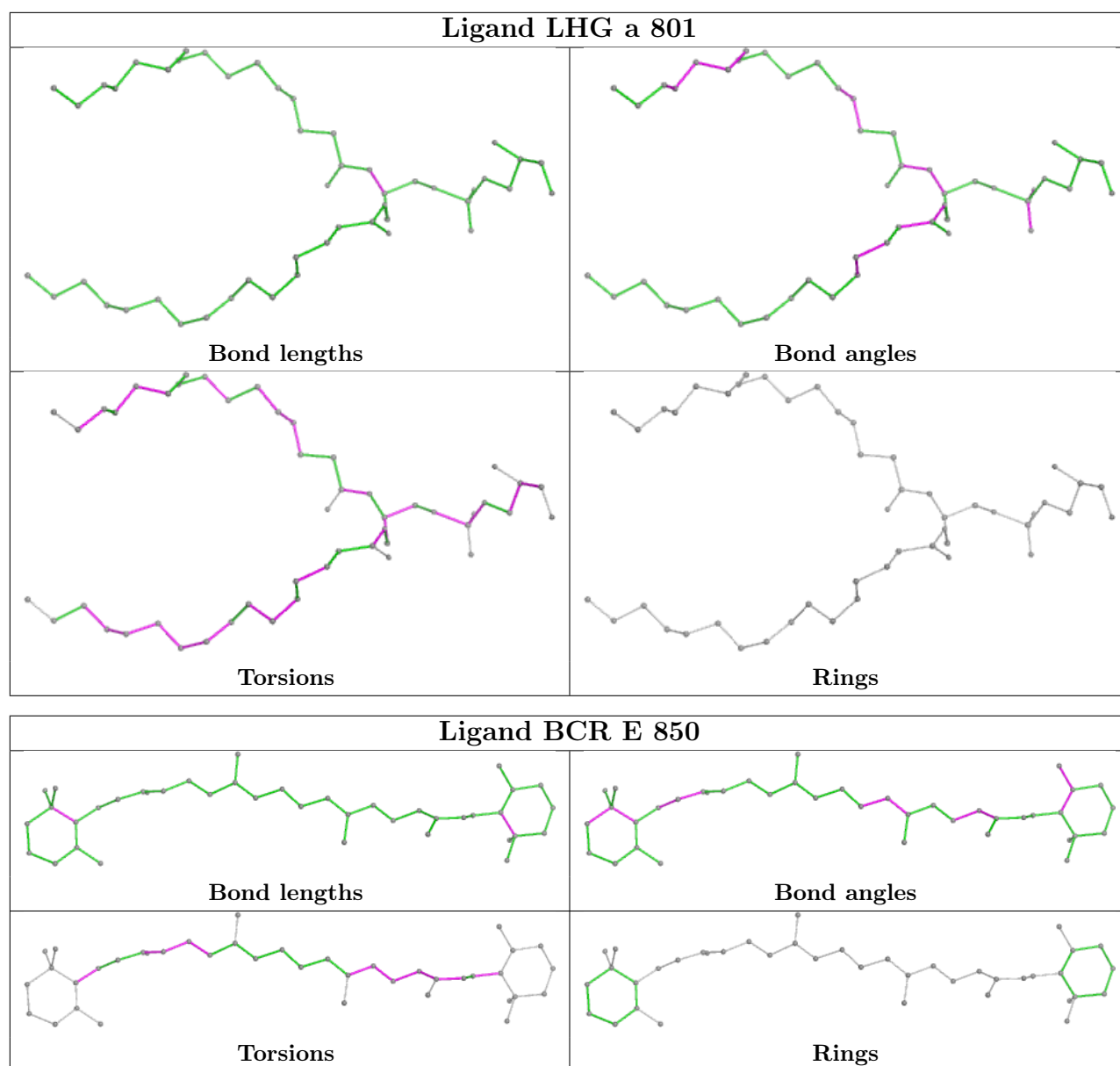
Bond angles



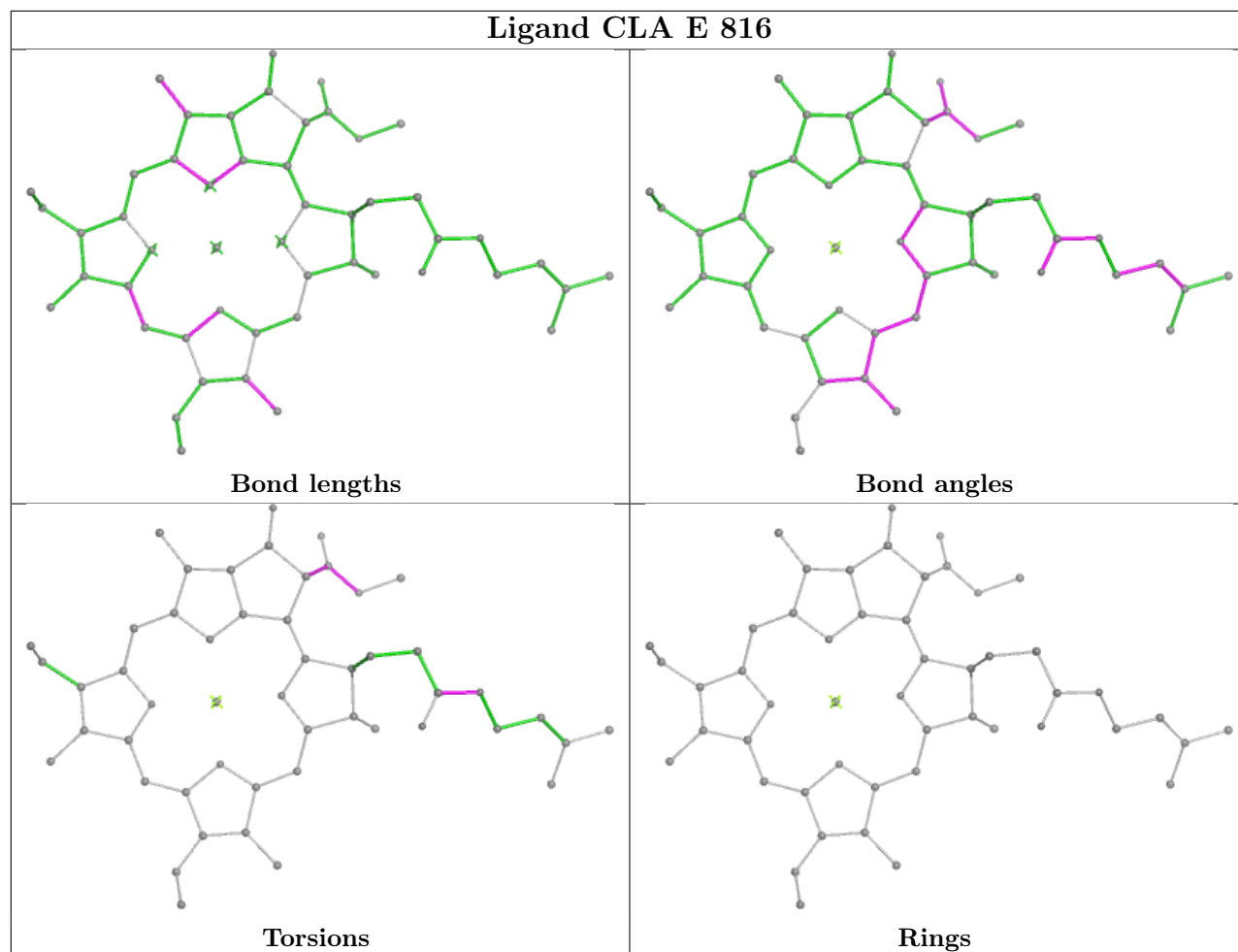
Torsions

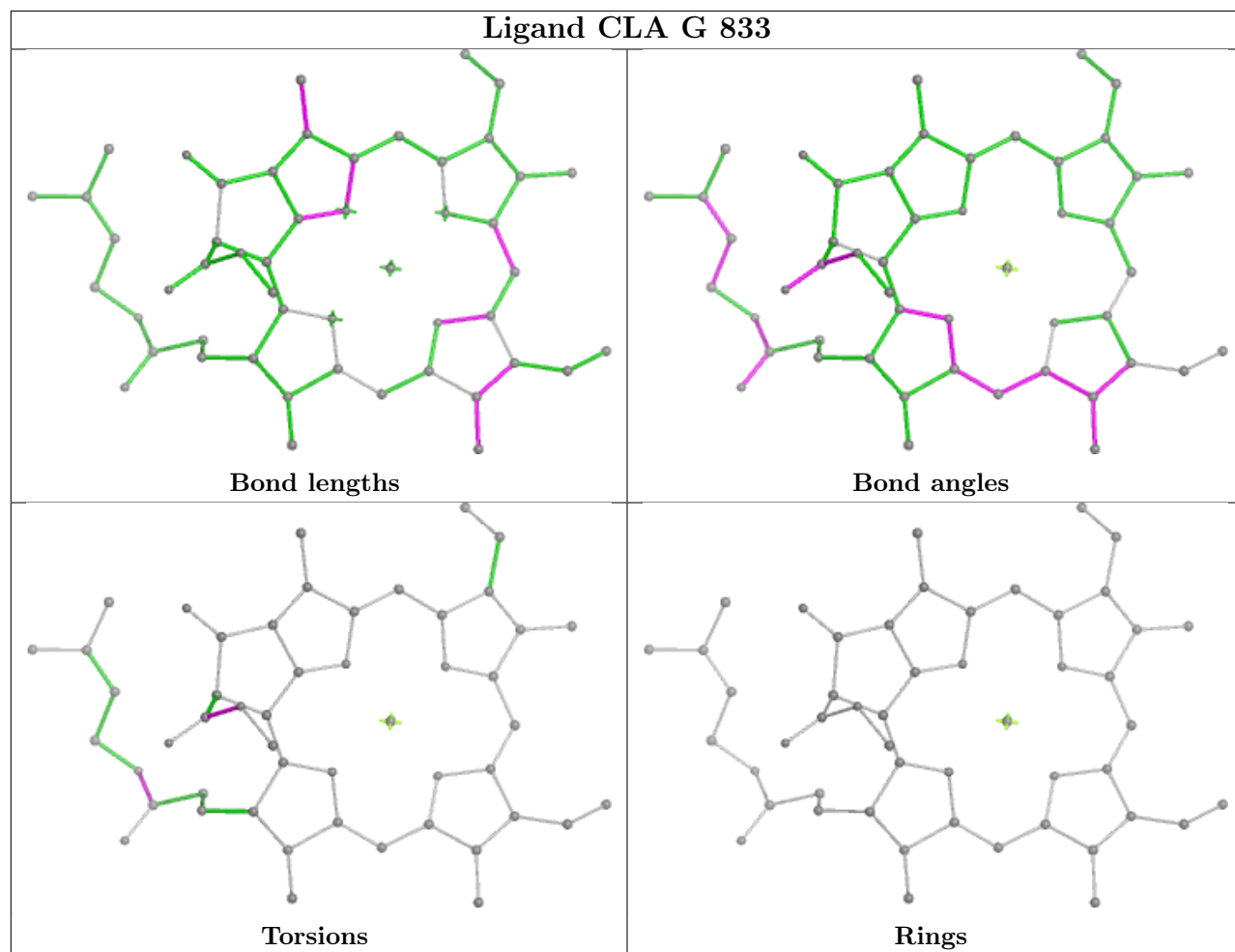


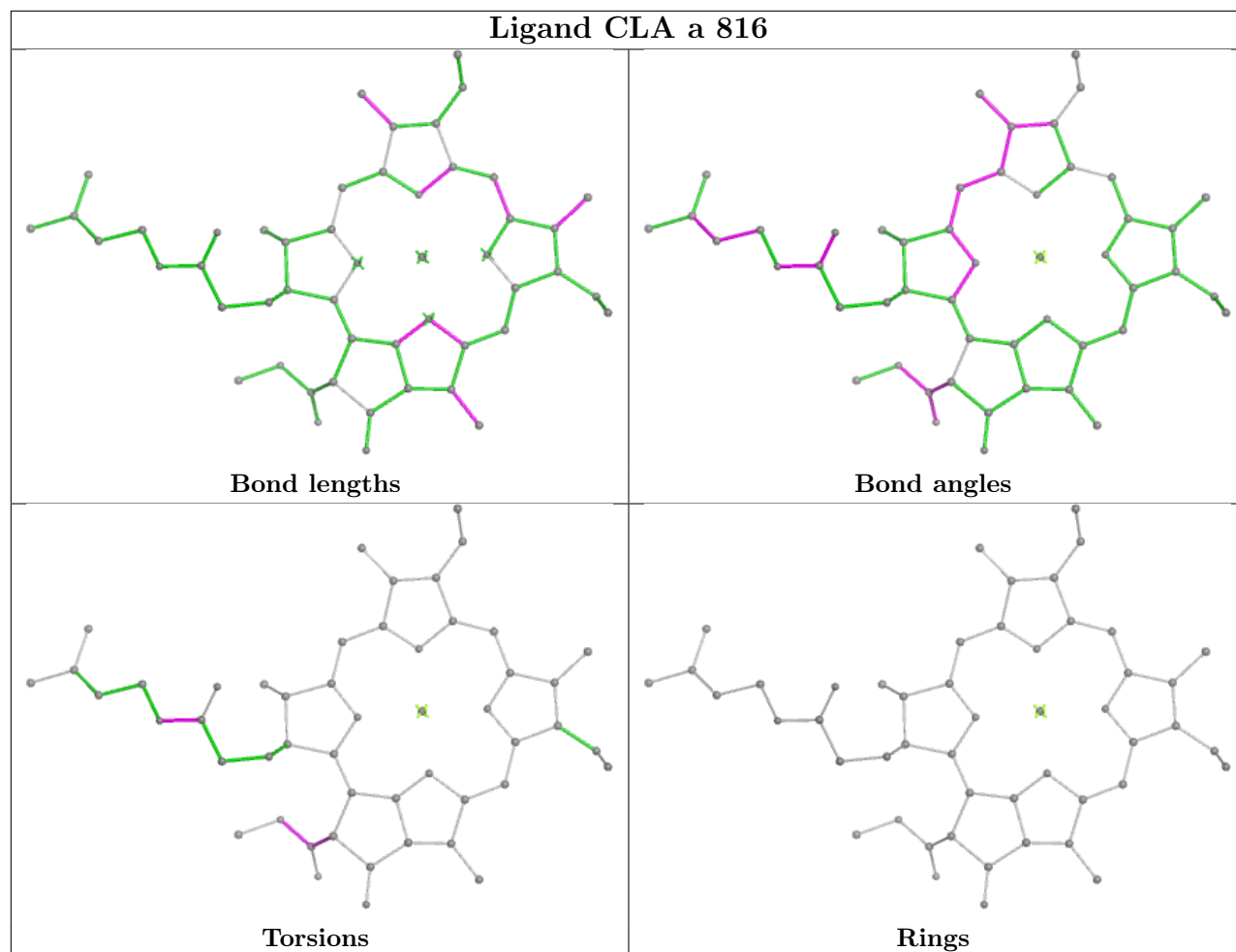
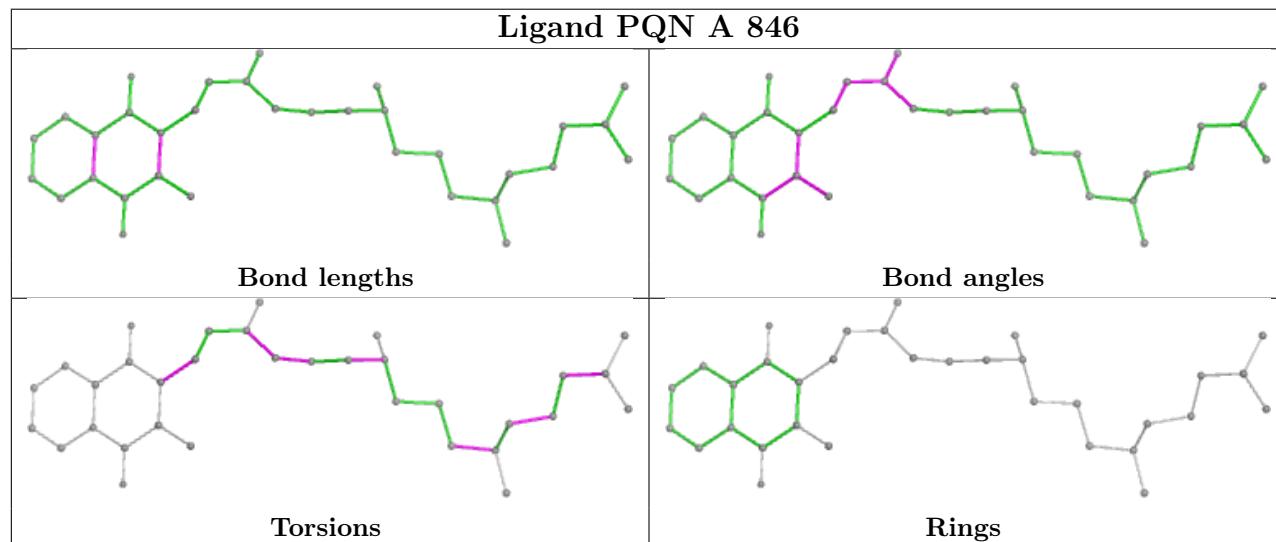
Rings



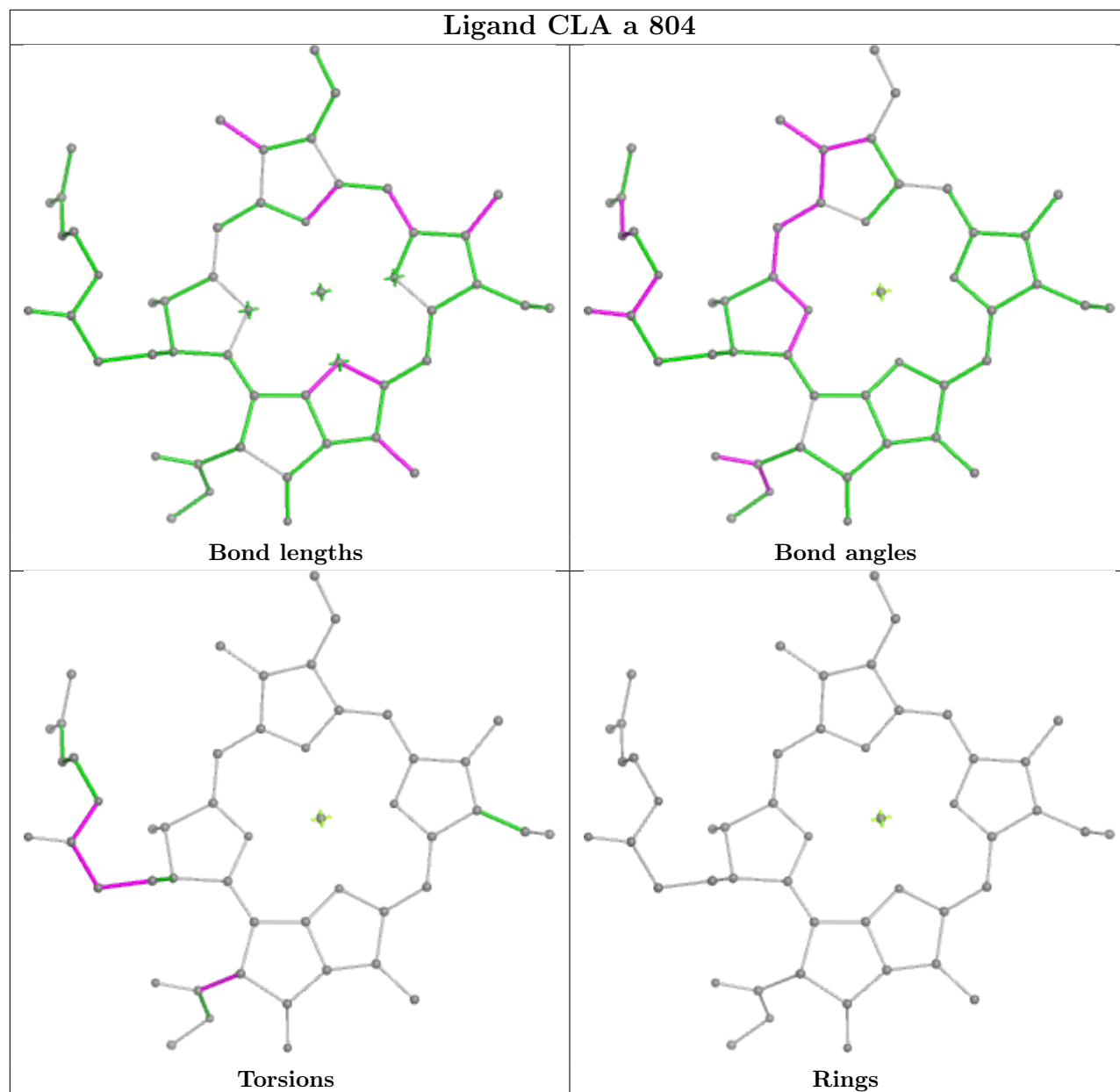
Ligand CLA E 816



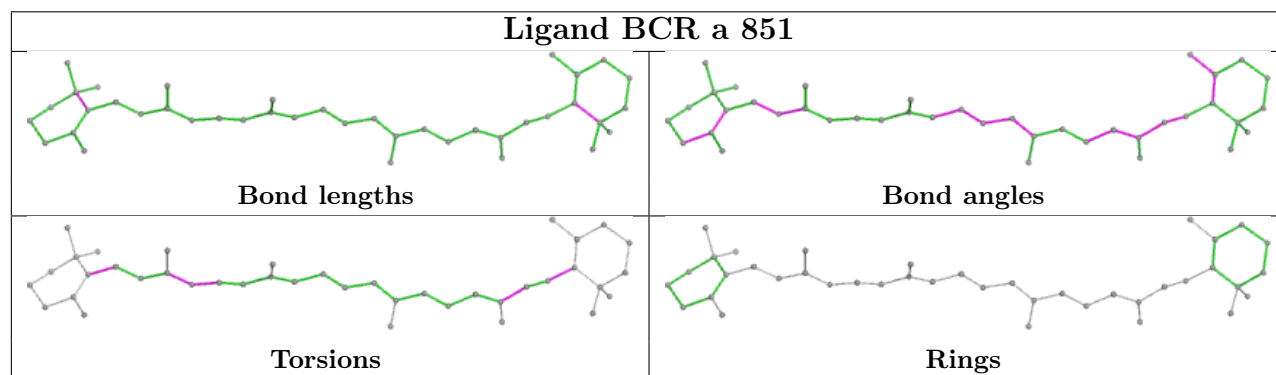


Ligand CLA a 816**Ligand PQN A 846**

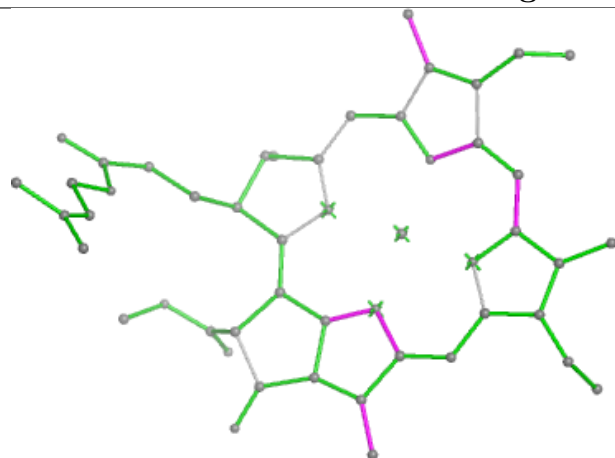
Ligand CLA a 804



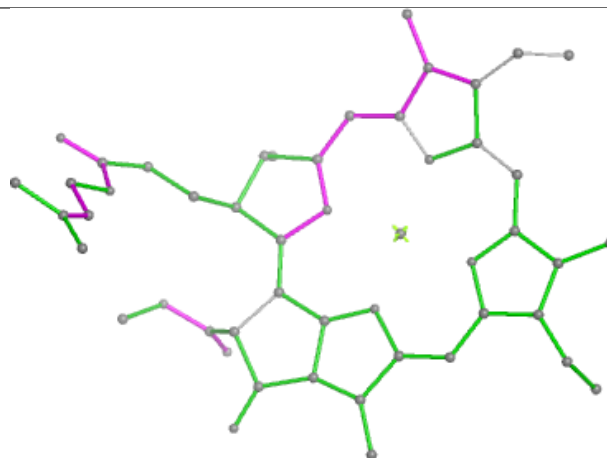
Ligand BCR a 851



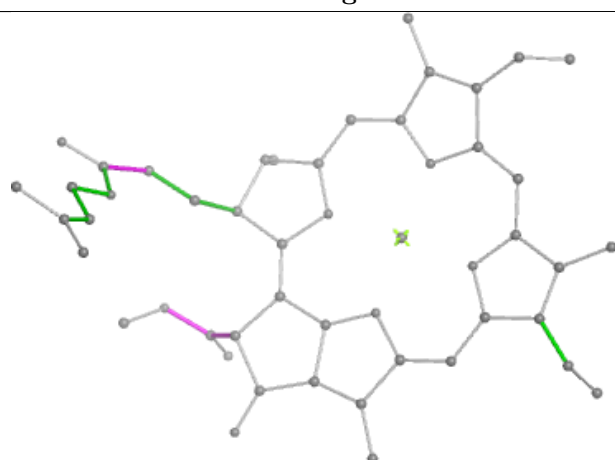
Ligand CLA b 803



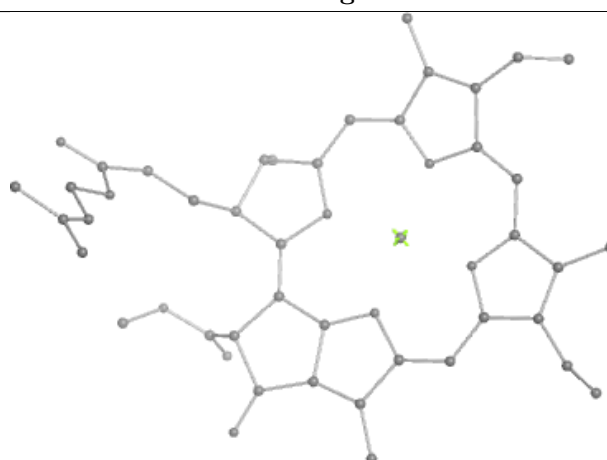
Bond lengths



Bond angles

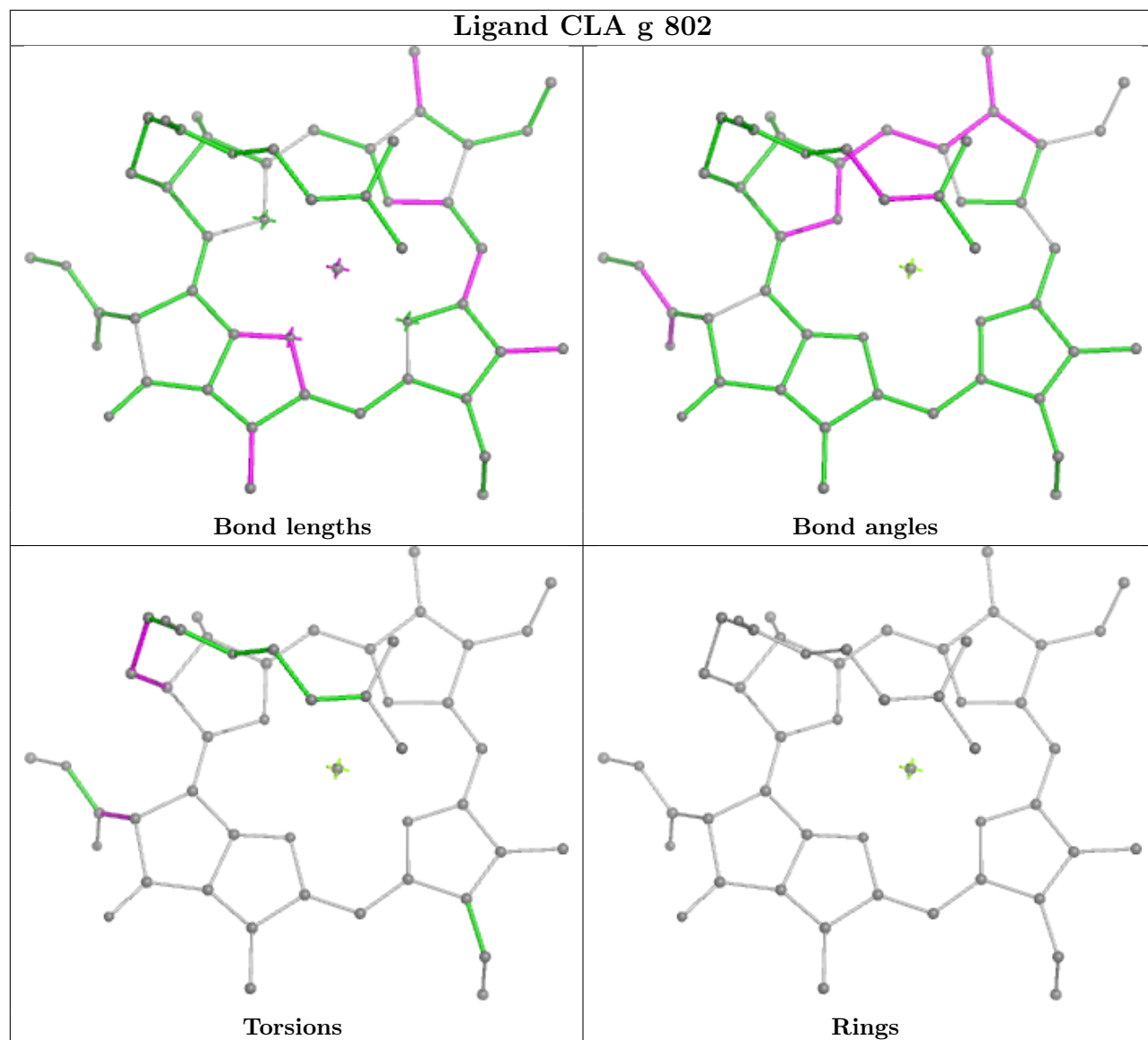


Torsions

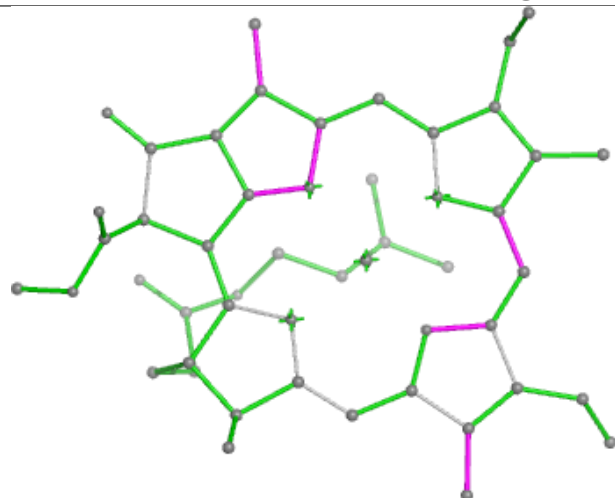


Rings

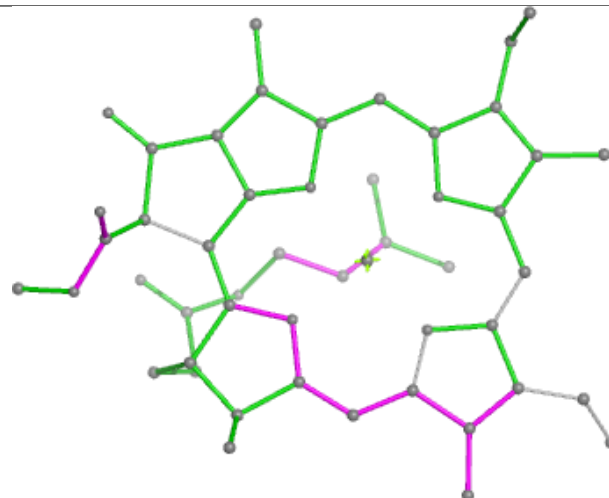
Ligand CLA g 802



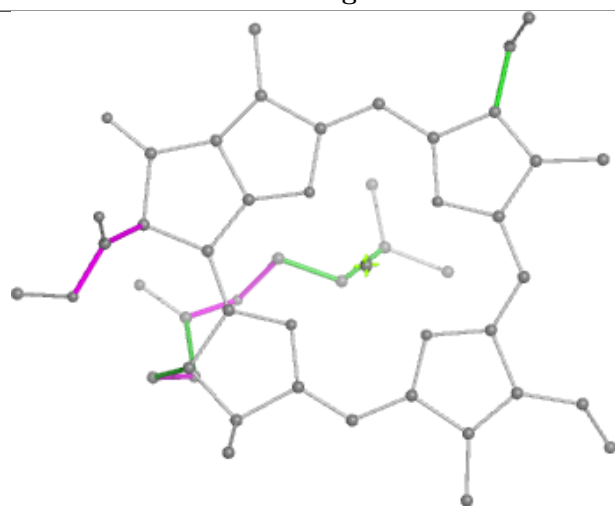
Ligand CLA E 815



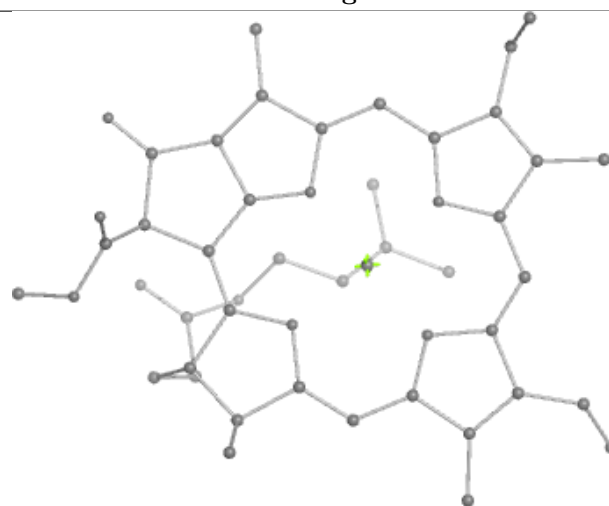
Bond lengths



Bond angles

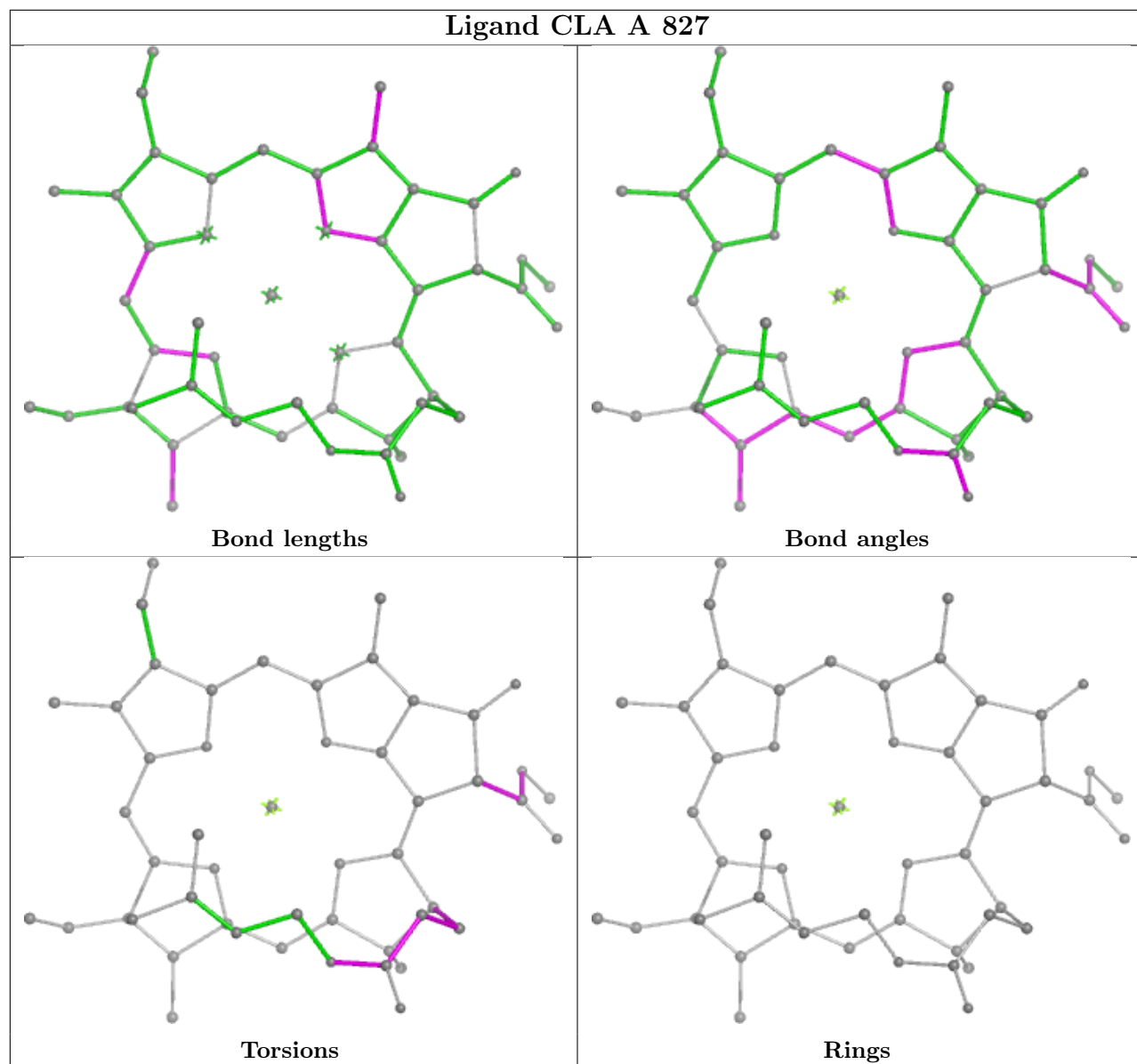


Torsions

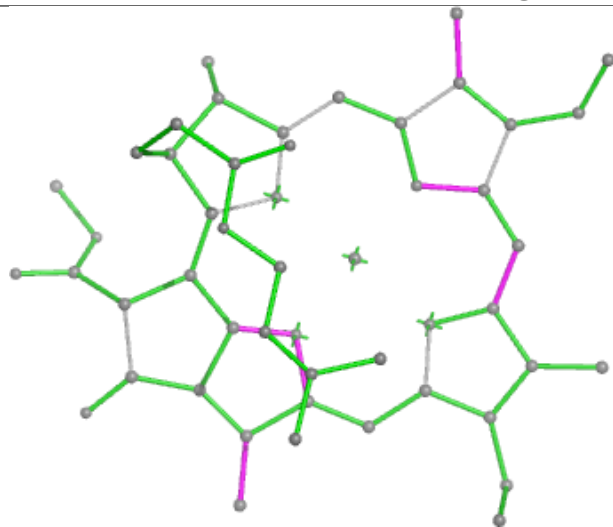


Rings

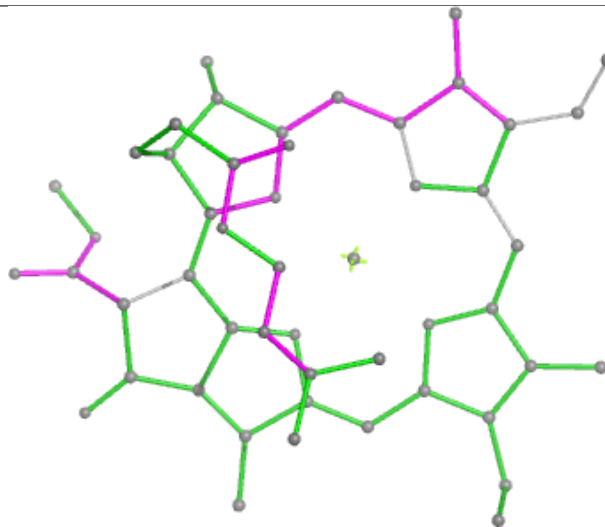
Ligand CLA A 827



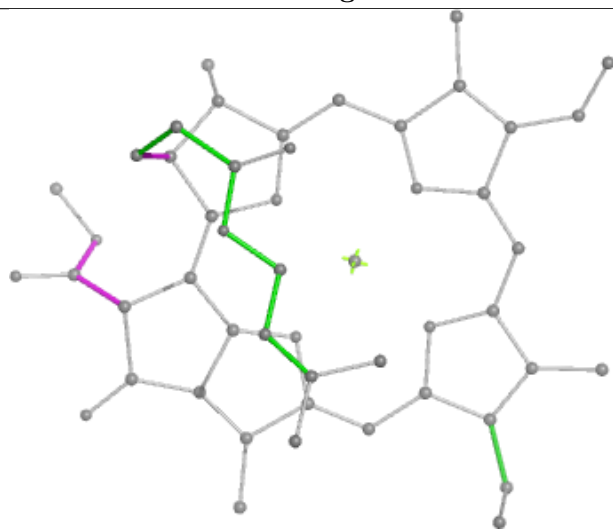
Ligand CLA E 843



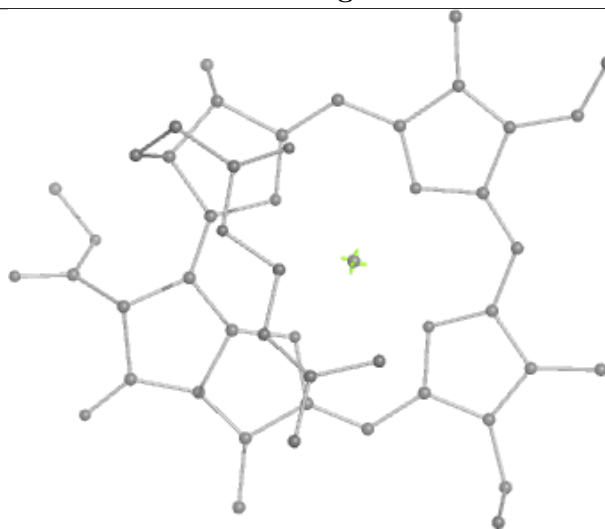
Bond lengths



Bond angles

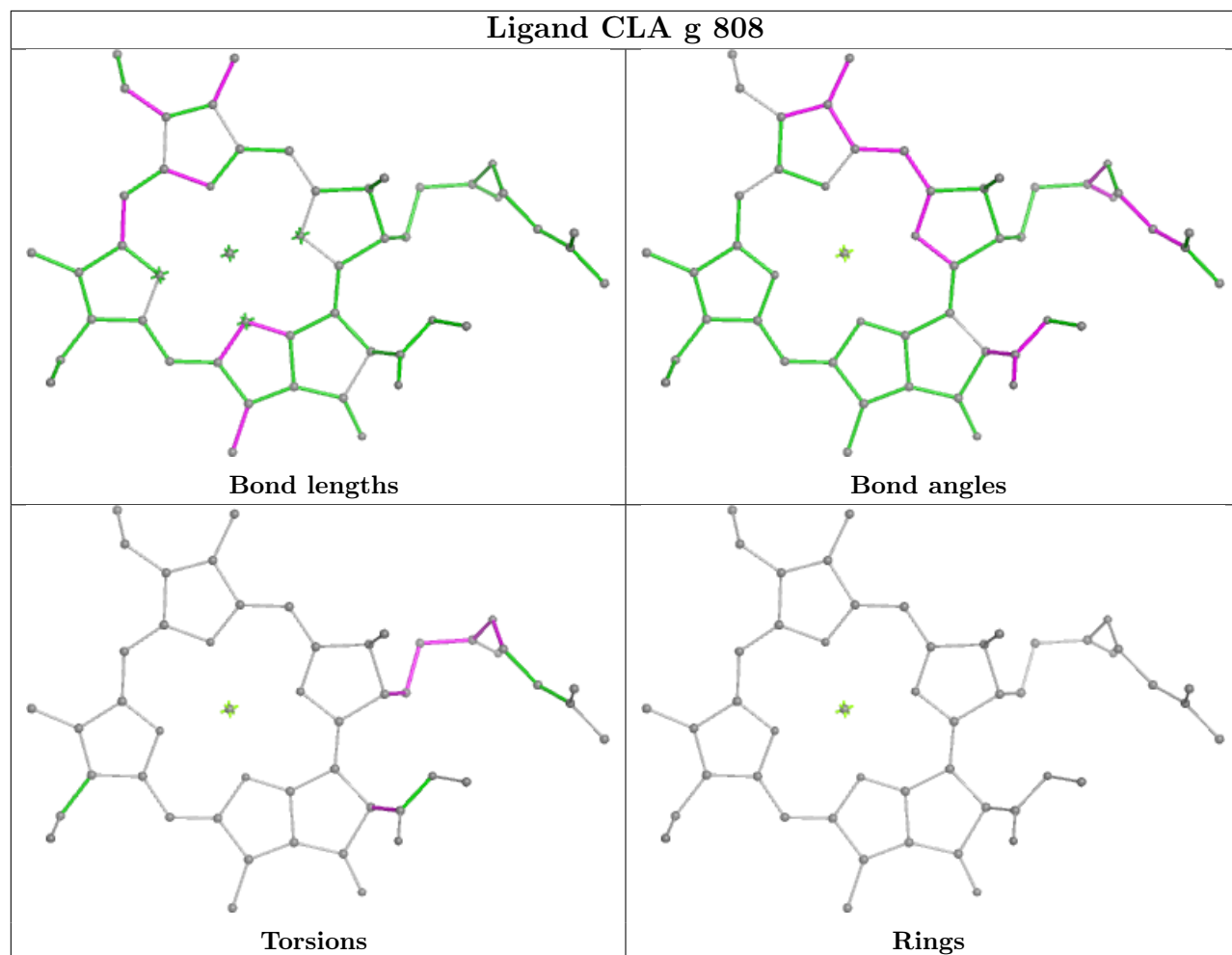


Torsions

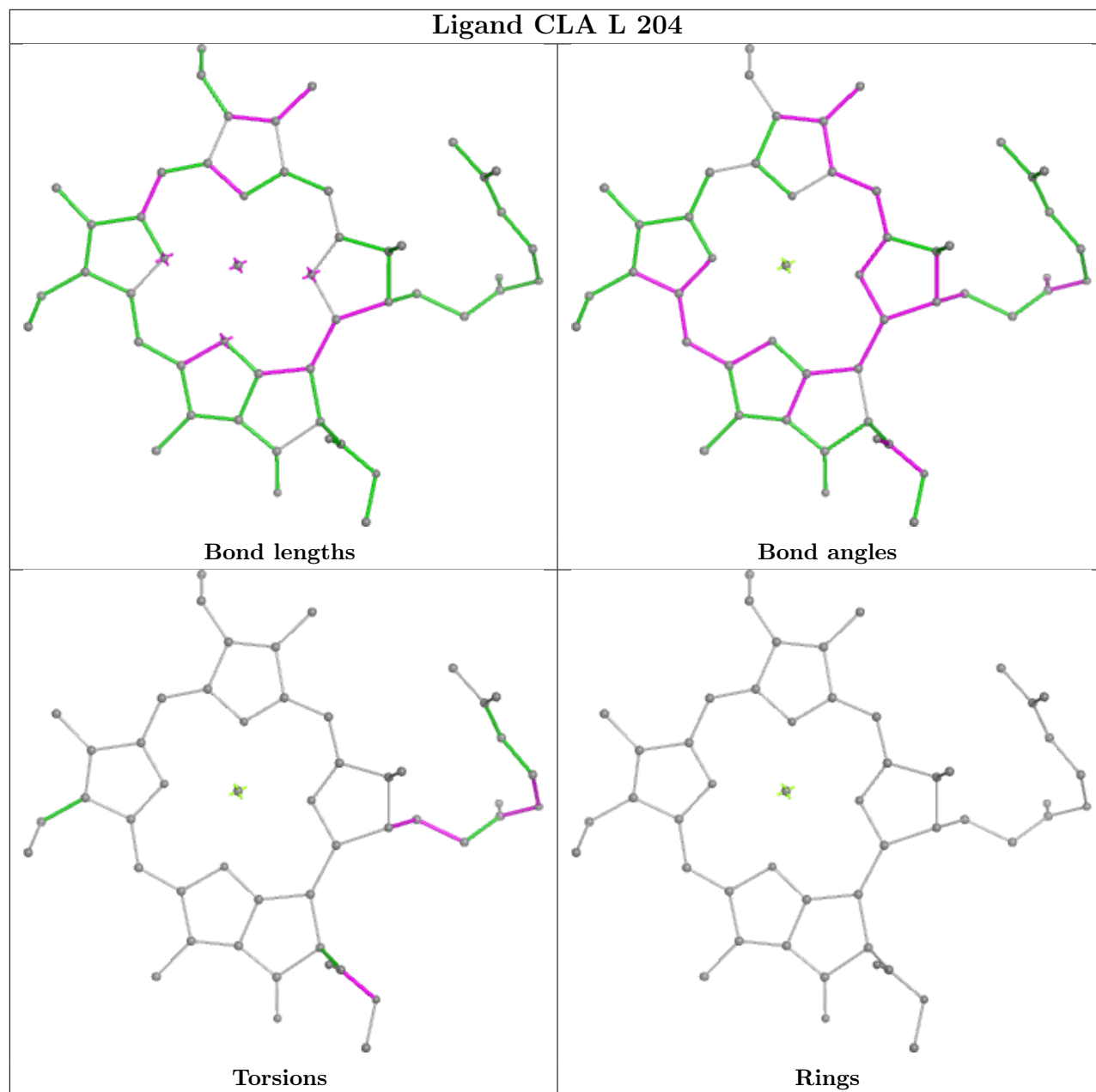


Rings

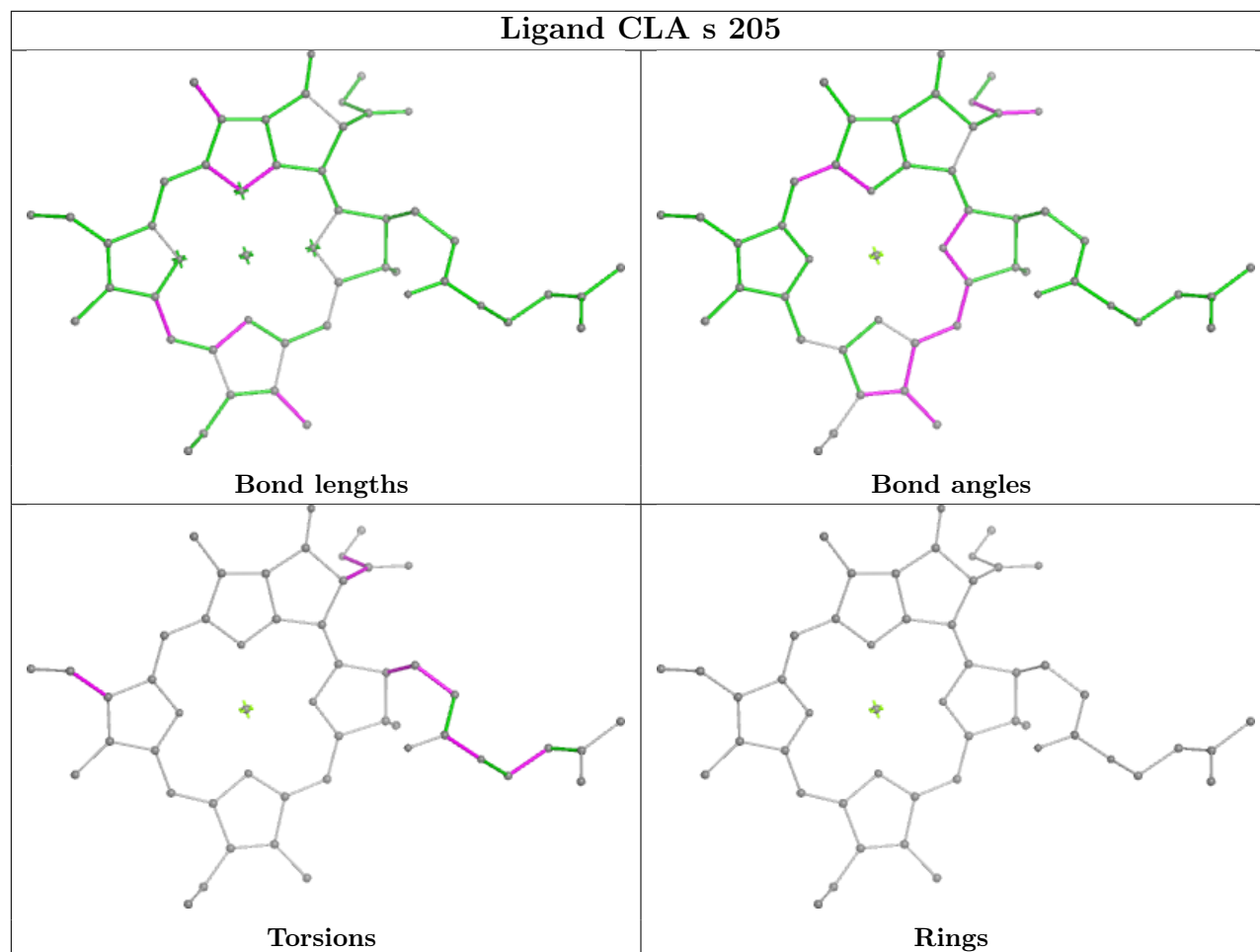
Ligand CLA g 808



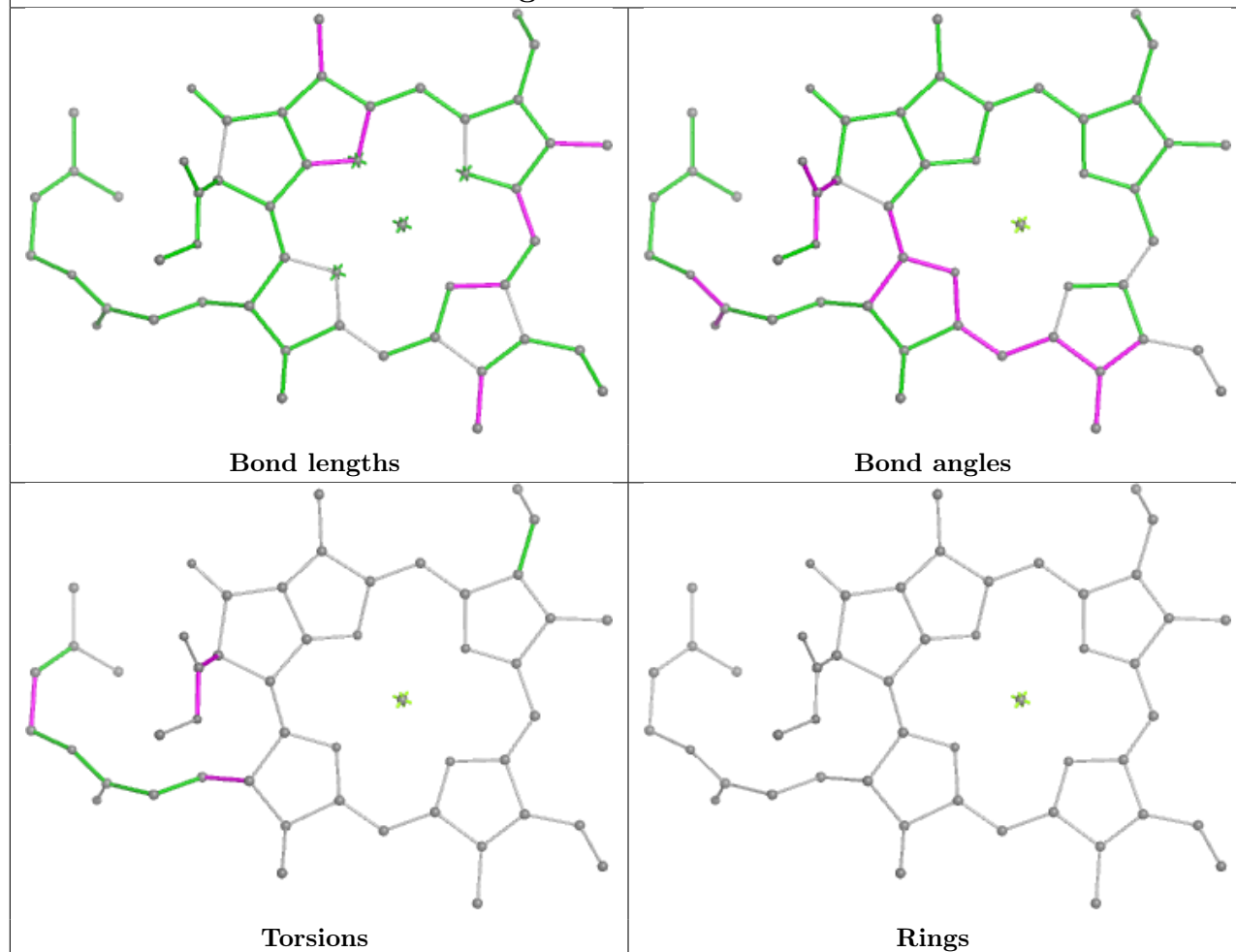
Ligand CLA L 204



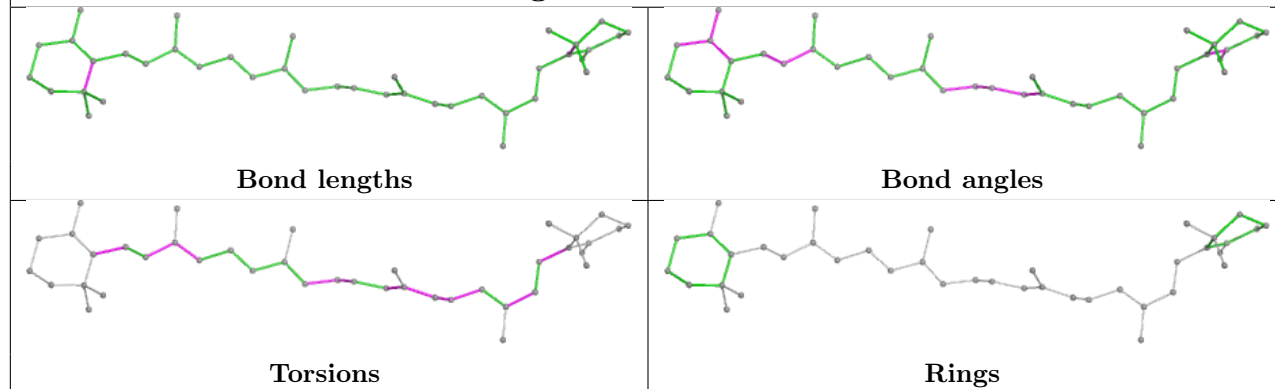
Ligand CLA s 205



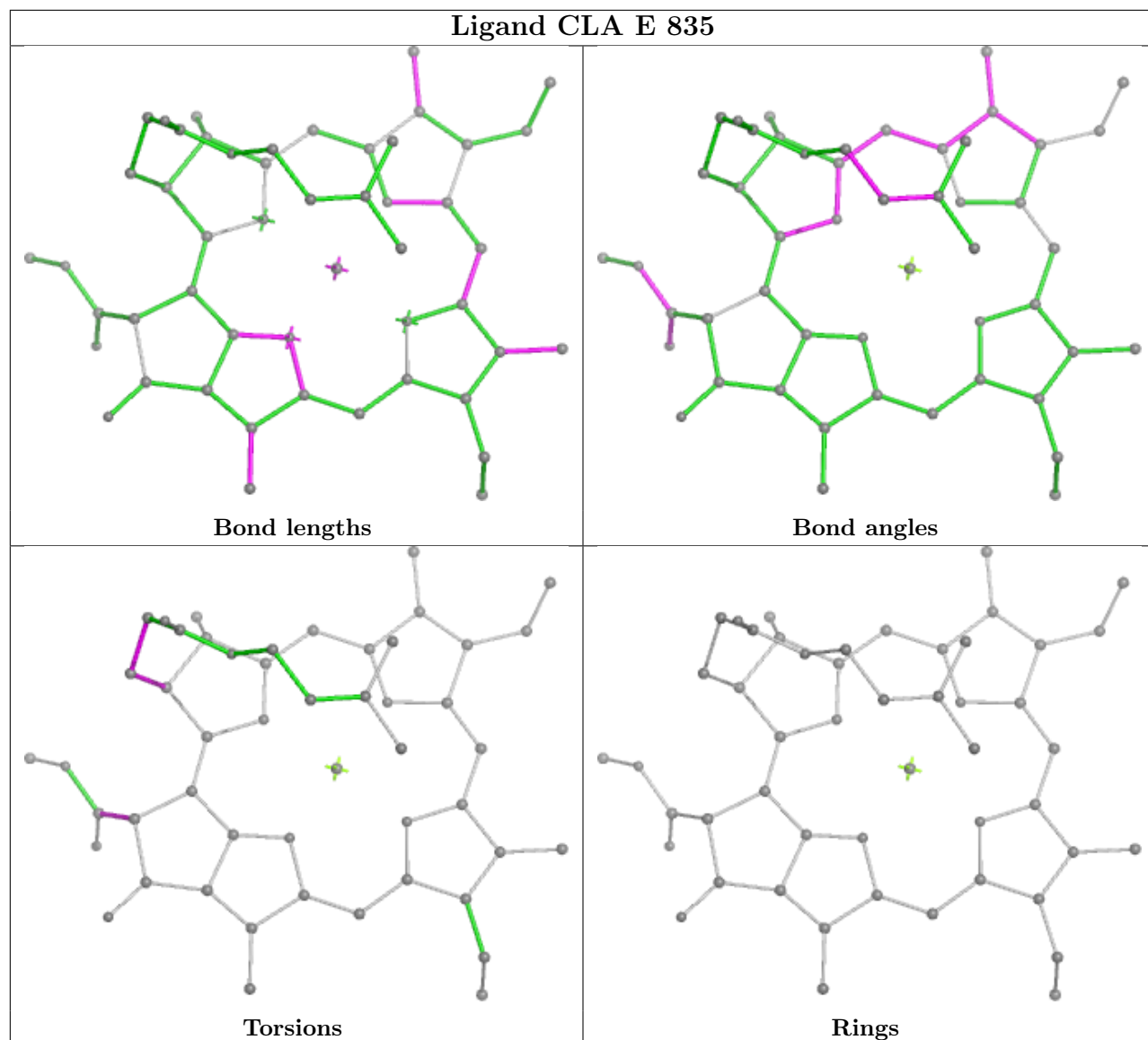
Ligand CLA a 828



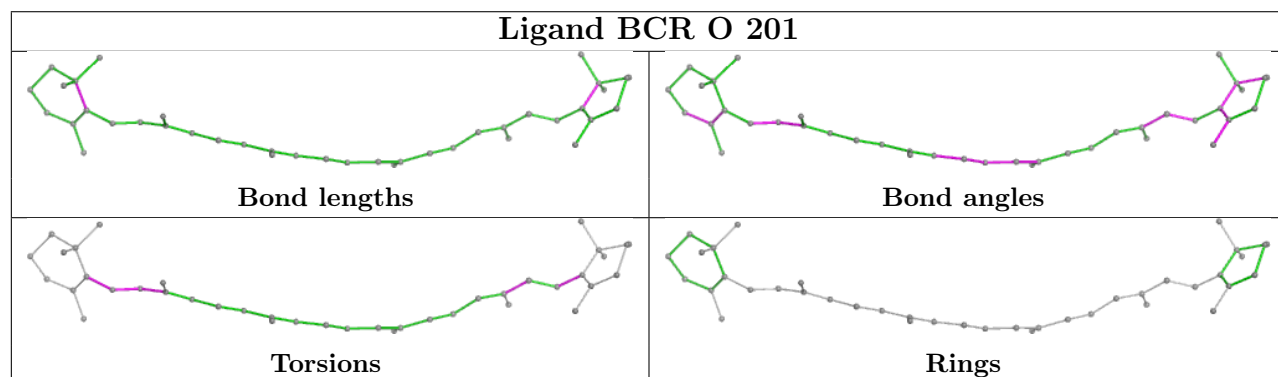
Ligand BCR B 848

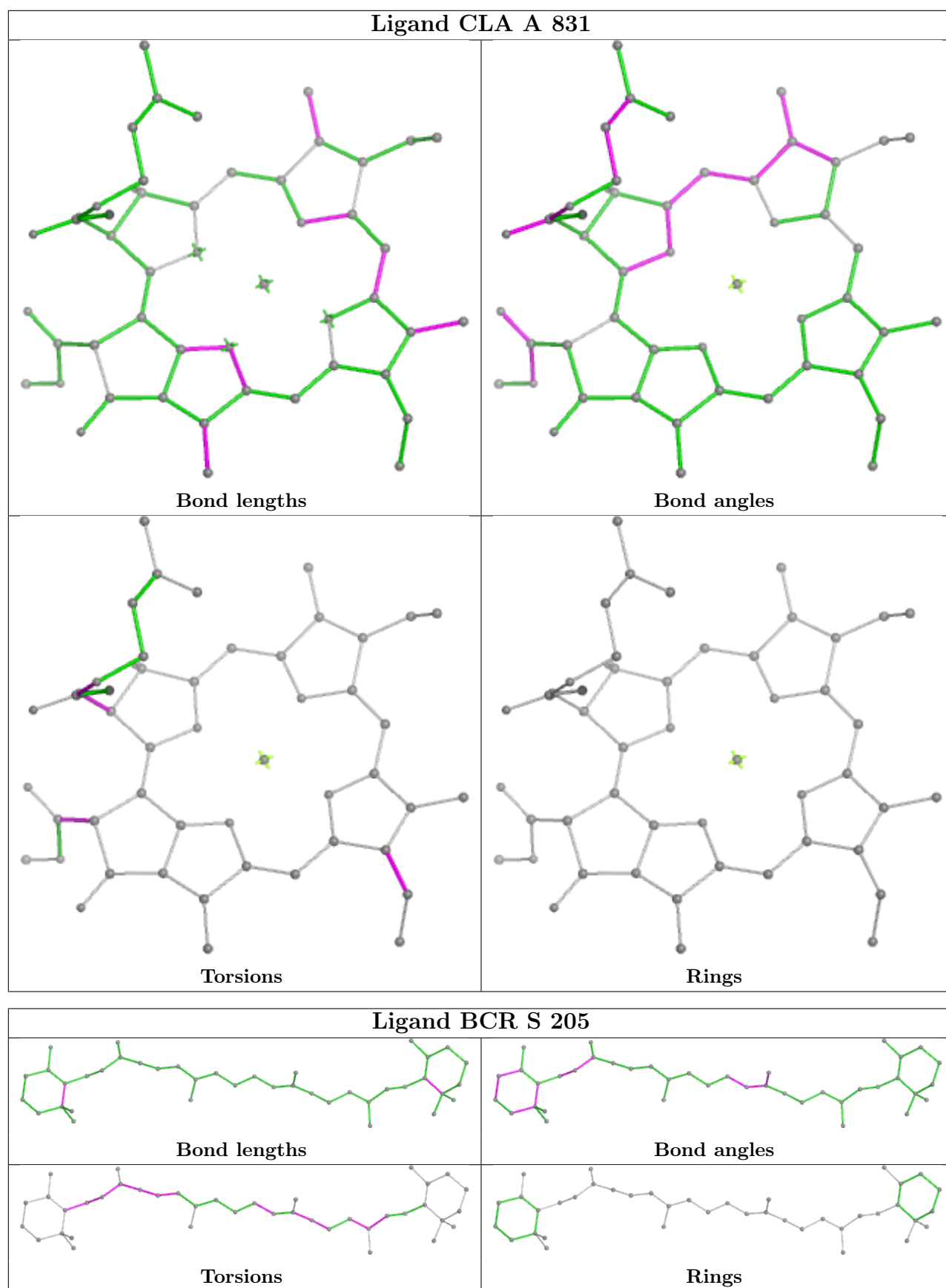


Ligand CLA E 835

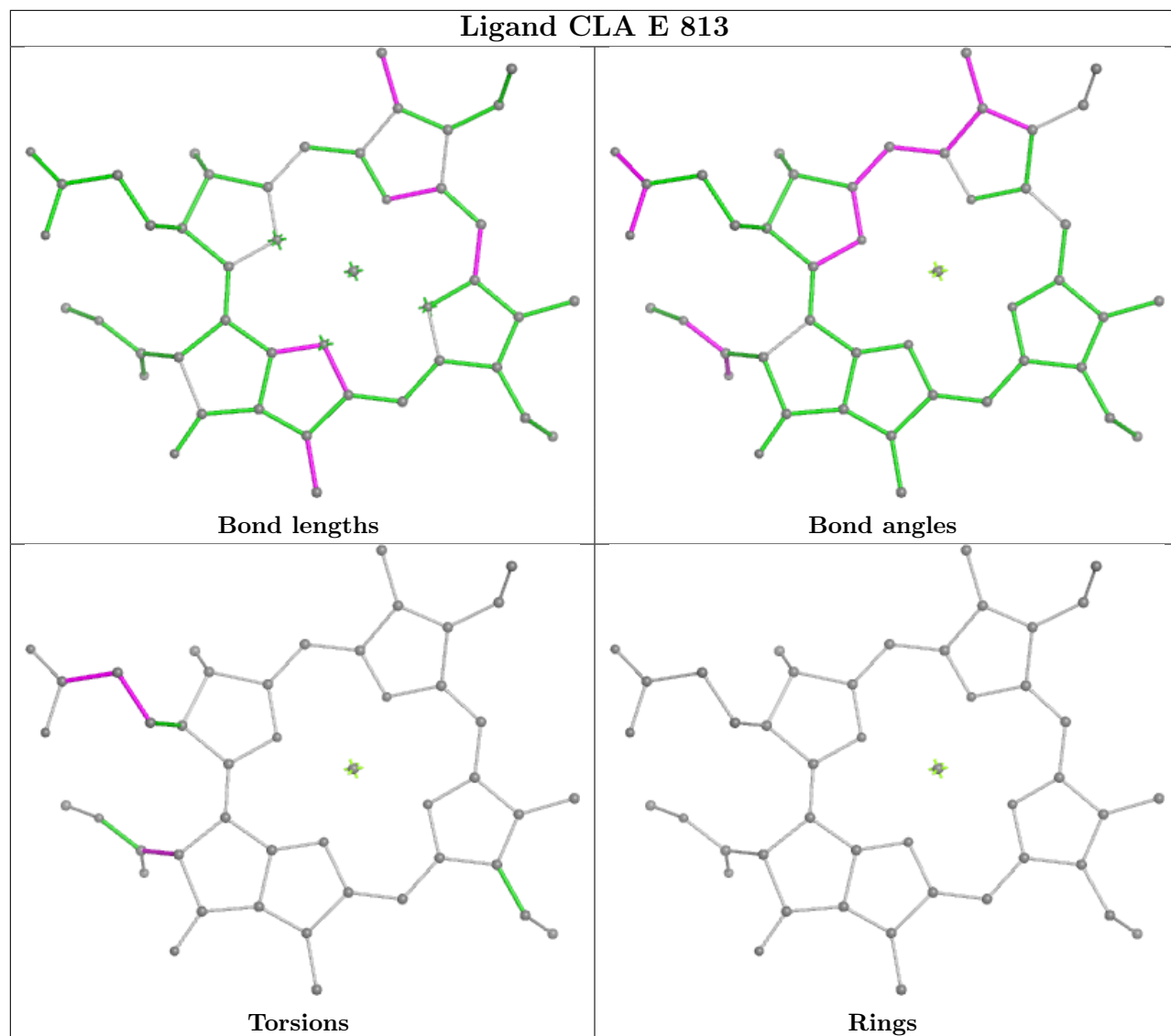


Ligand BCR O 201

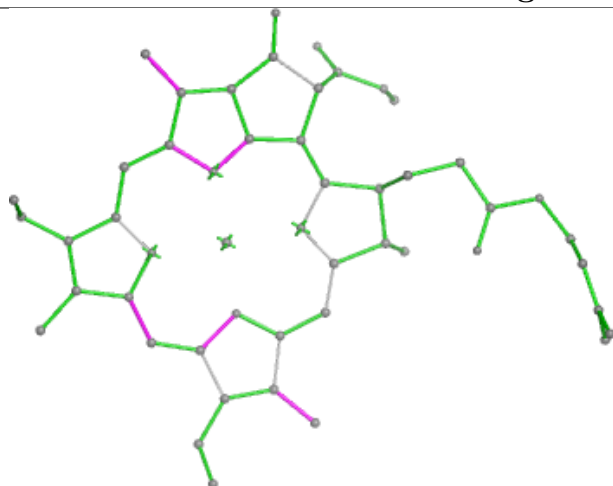




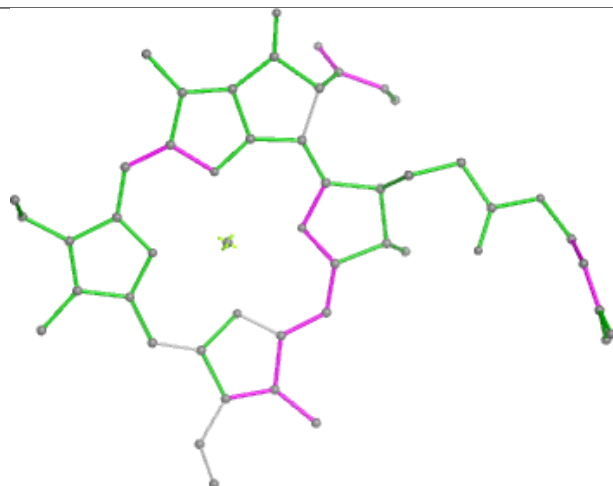
Ligand CLA E 813



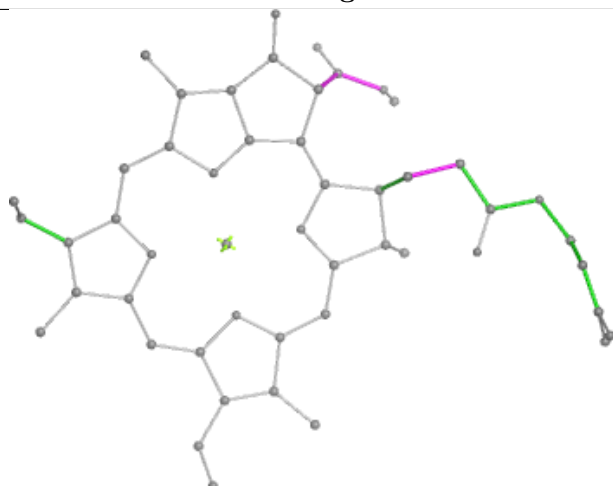
Ligand CLA b 813



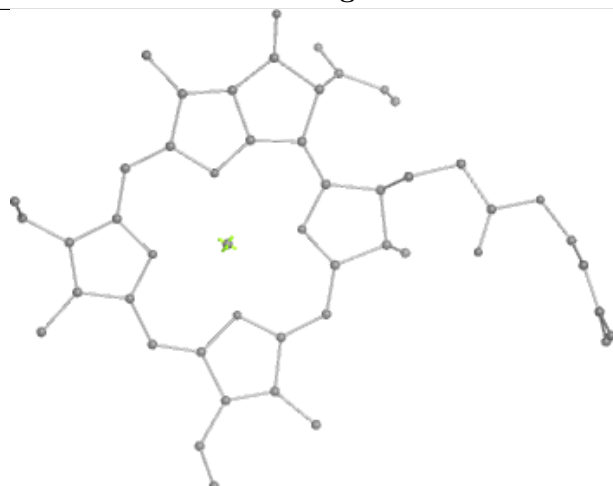
Bond lengths



Bond angles

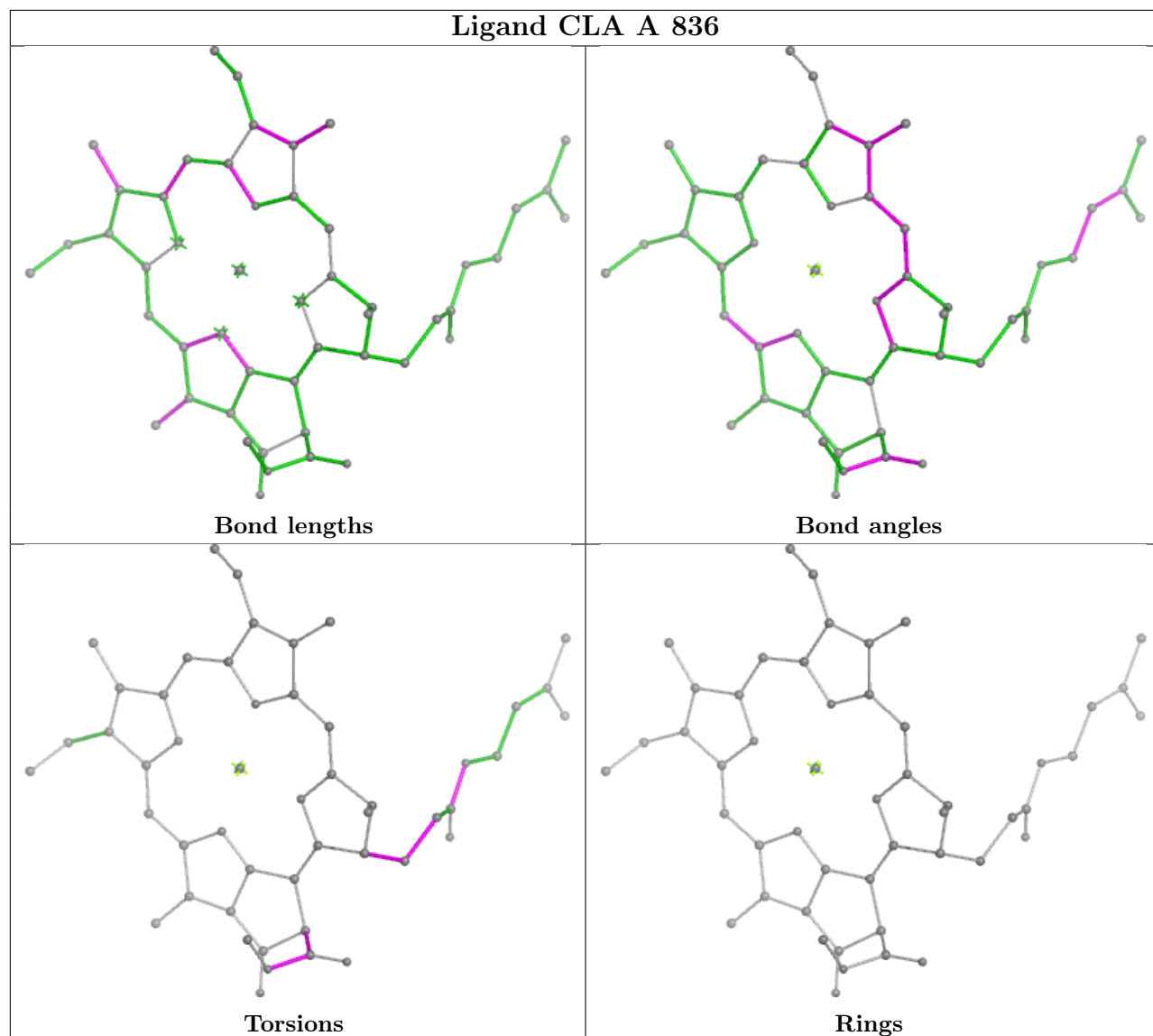


Torsions

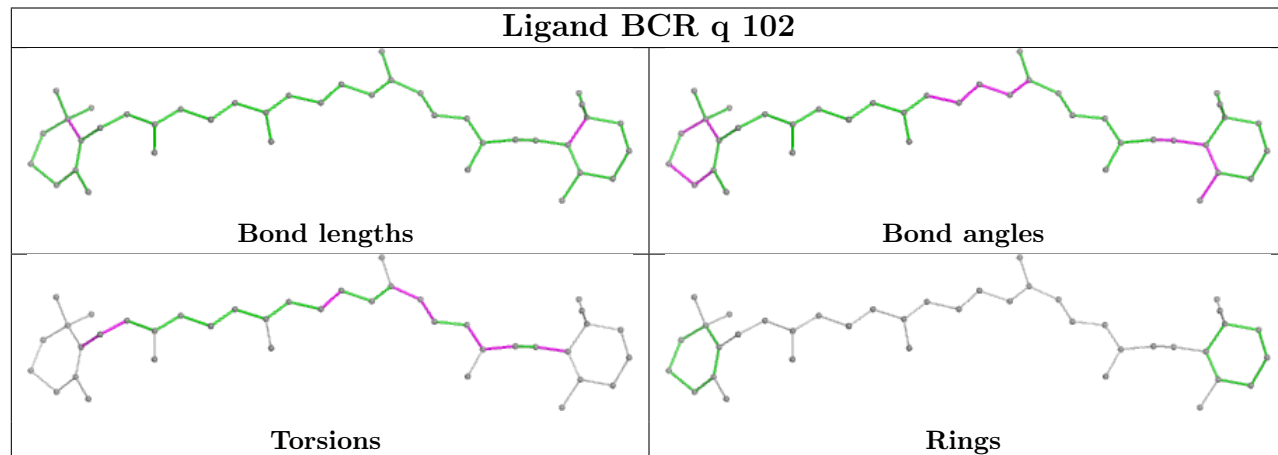


Rings

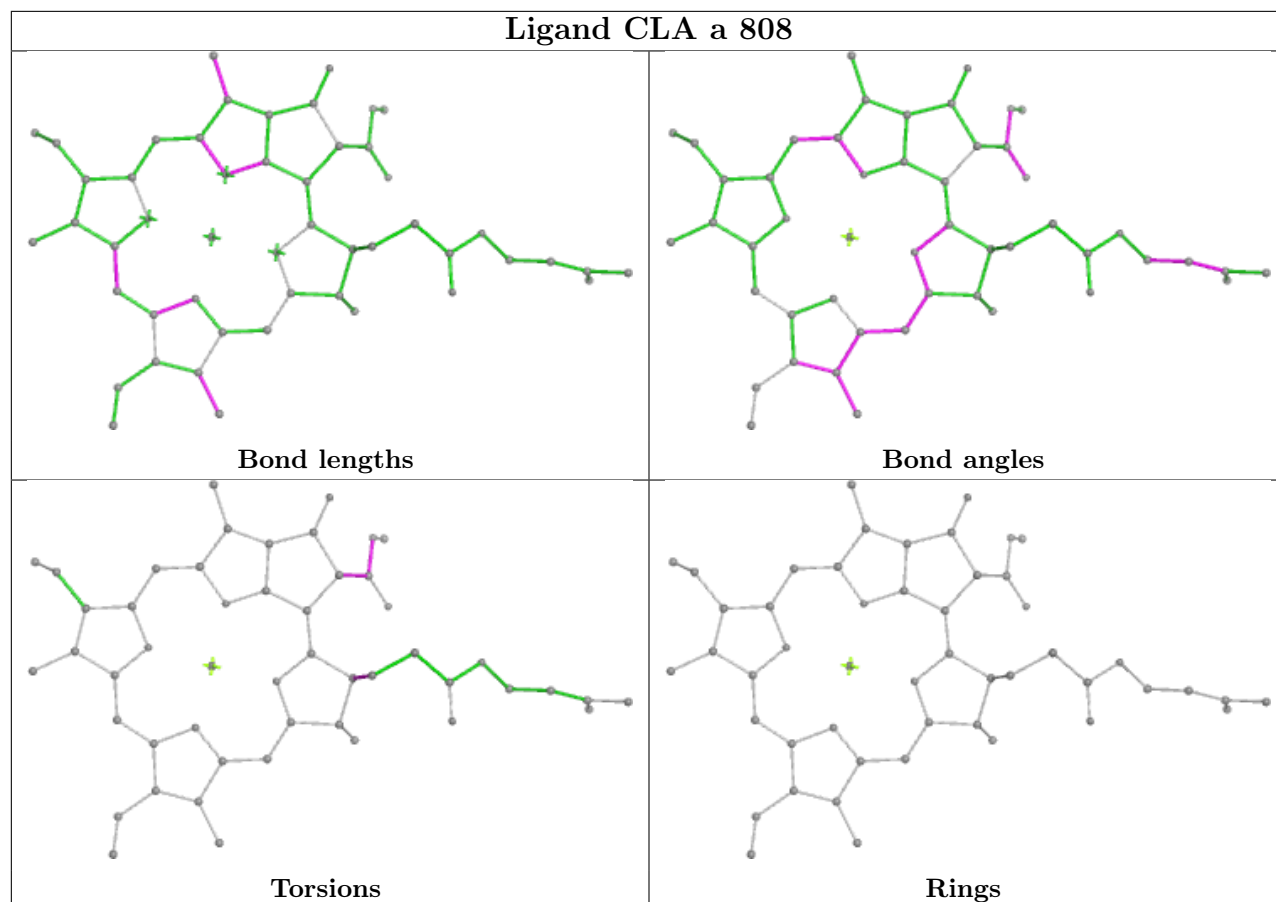
Ligand CLA A 836



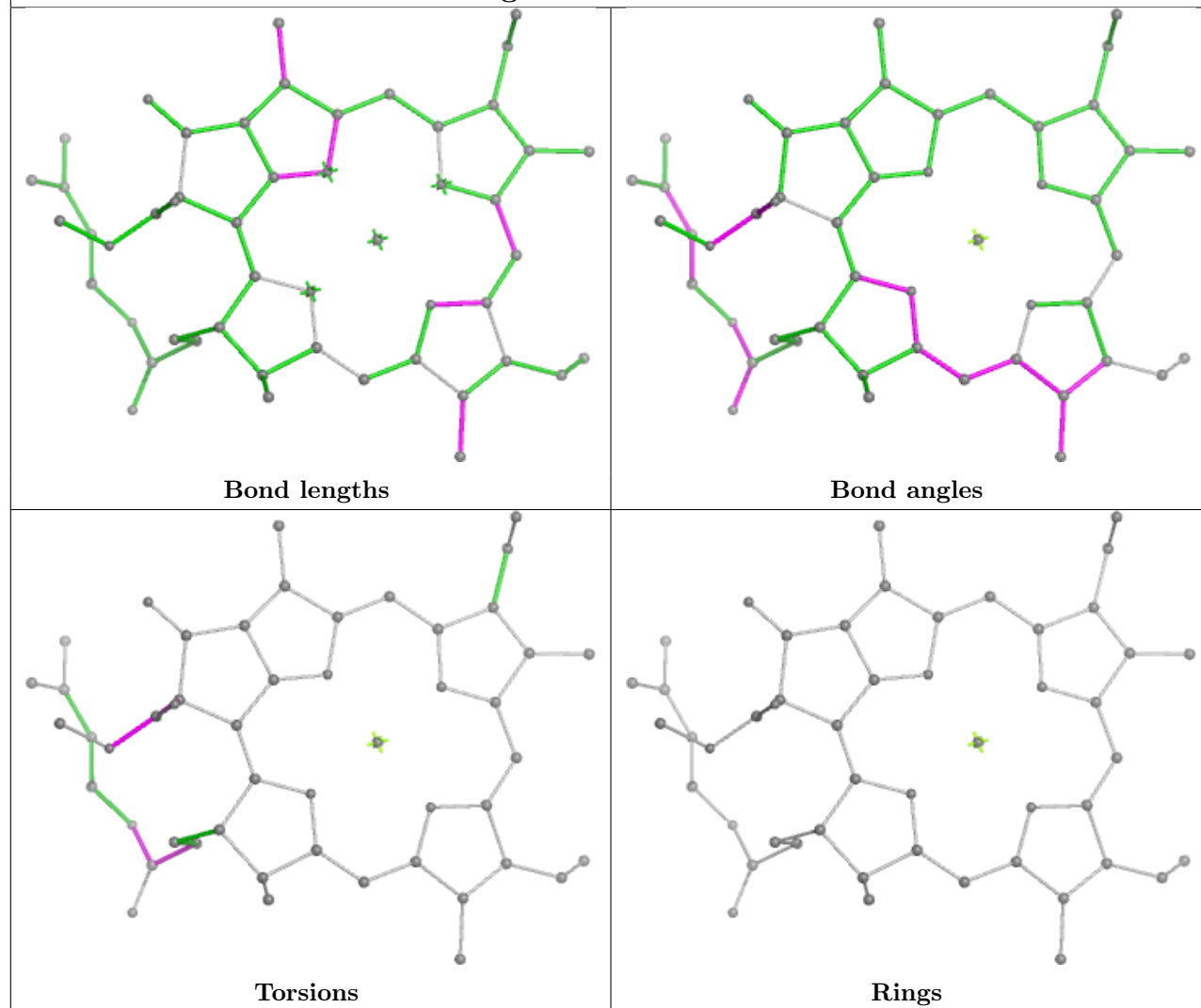
Ligand BCR q 102

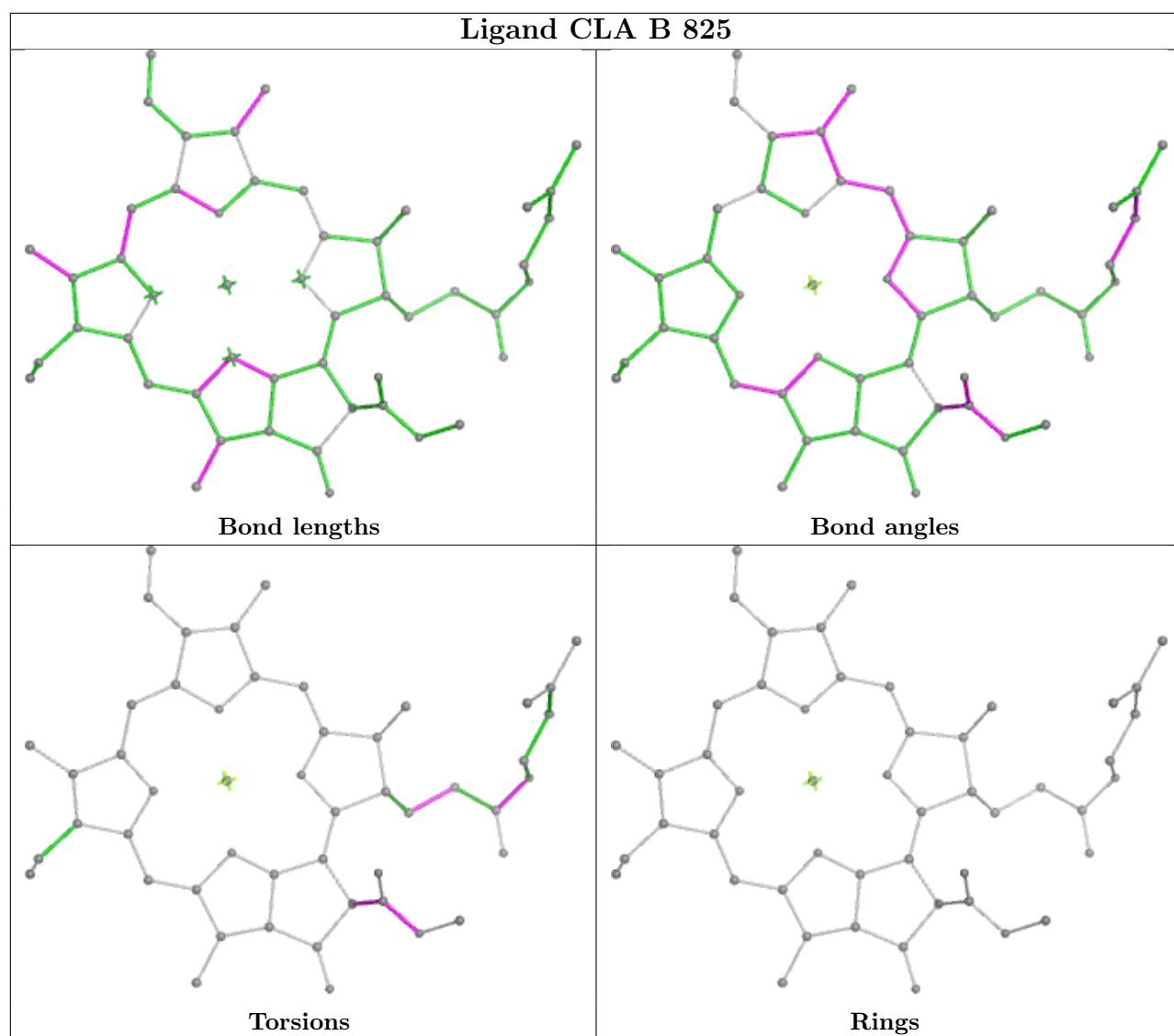


Ligand CLA a 808

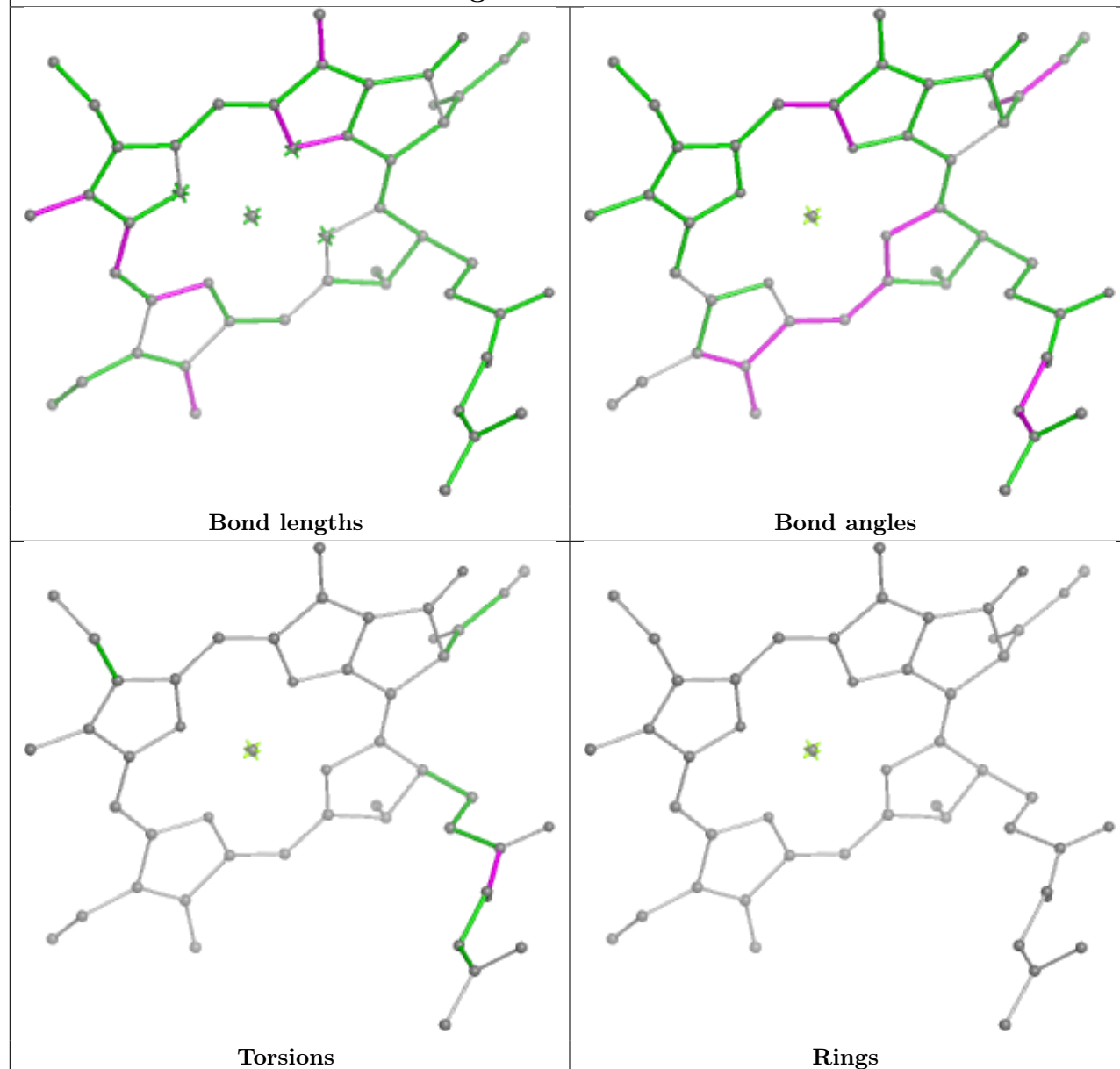


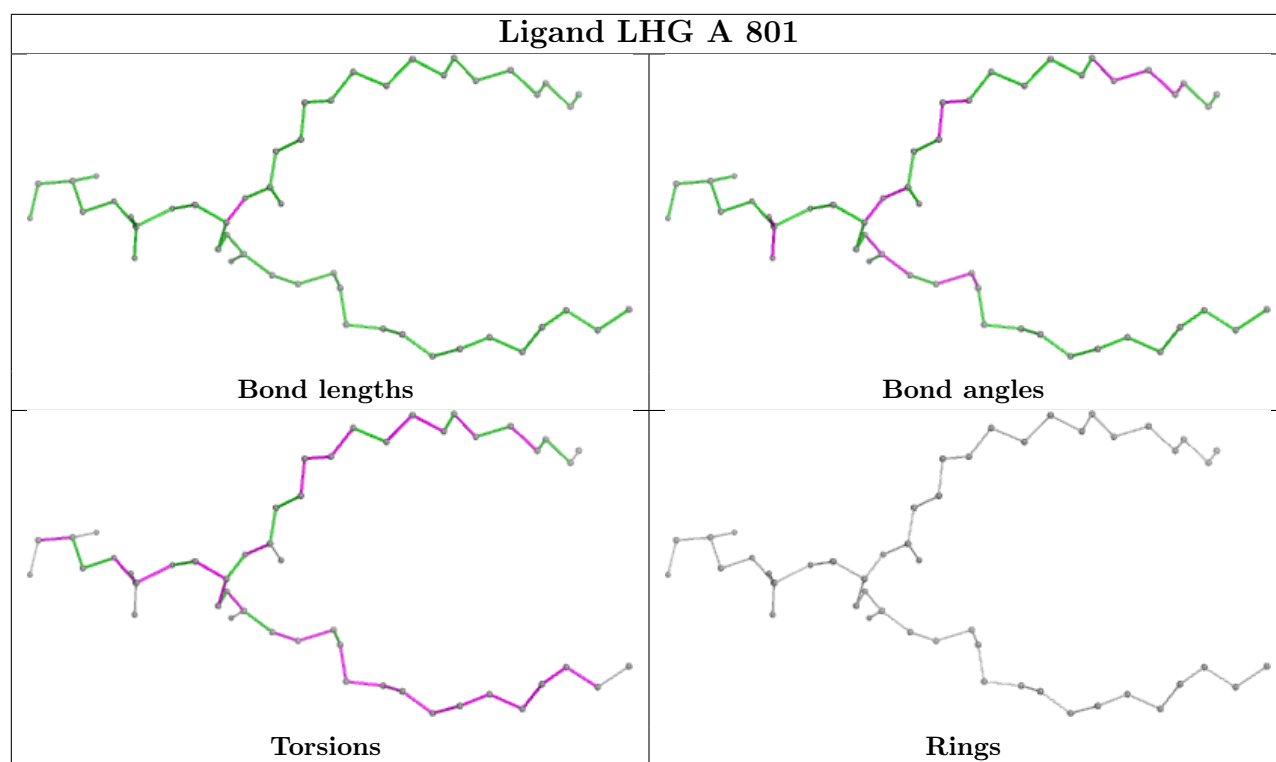
Ligand CLA B 817



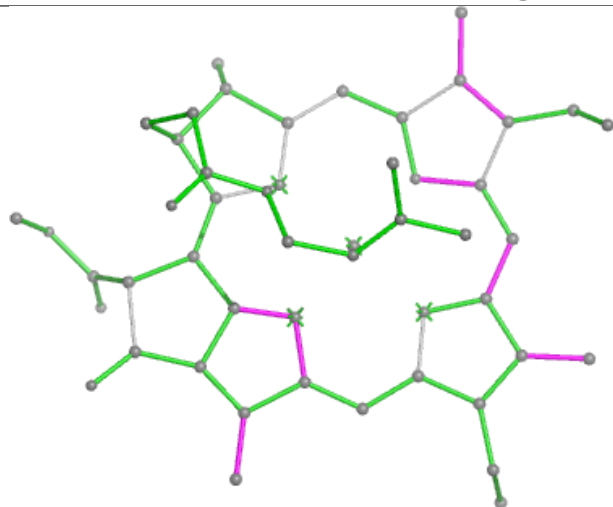


Ligand CLA b 805

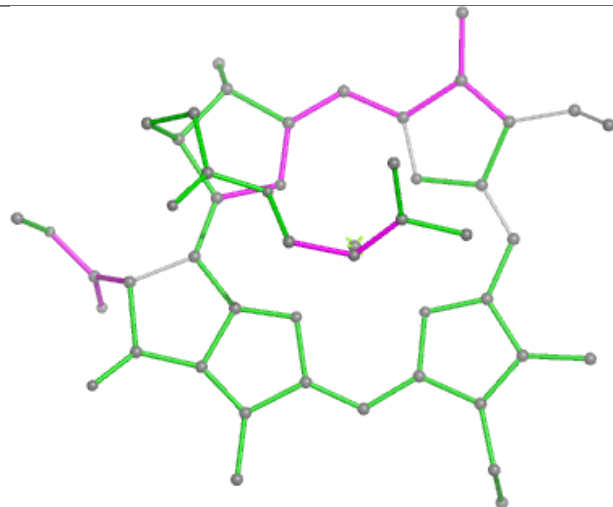




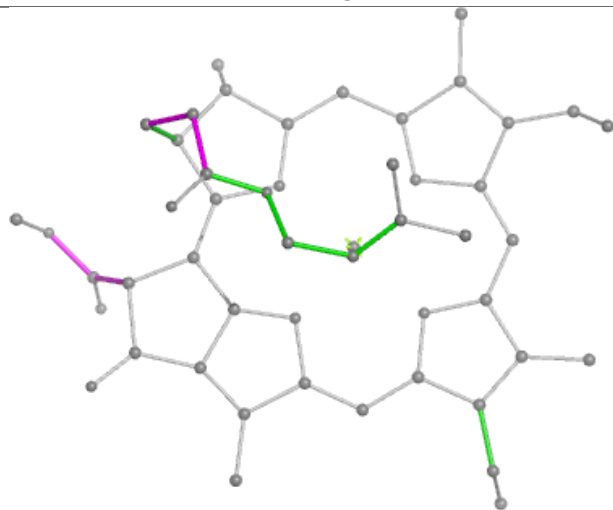
Ligand CLA B 823



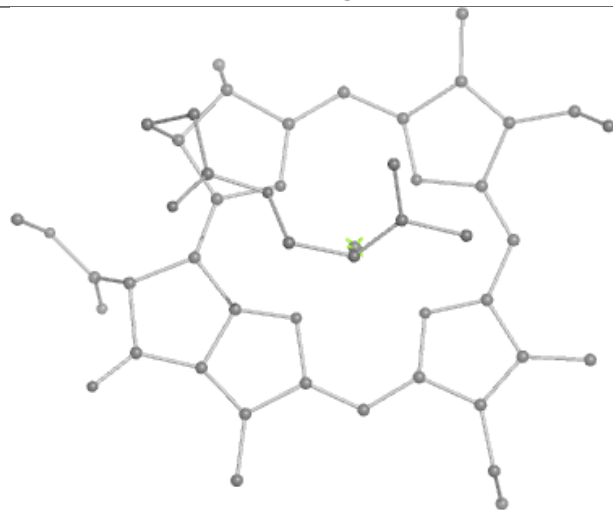
Bond lengths



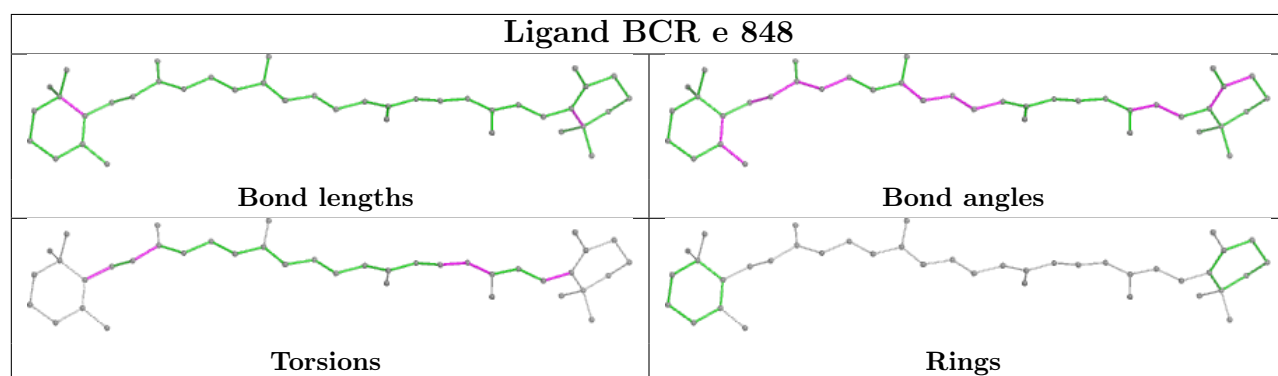
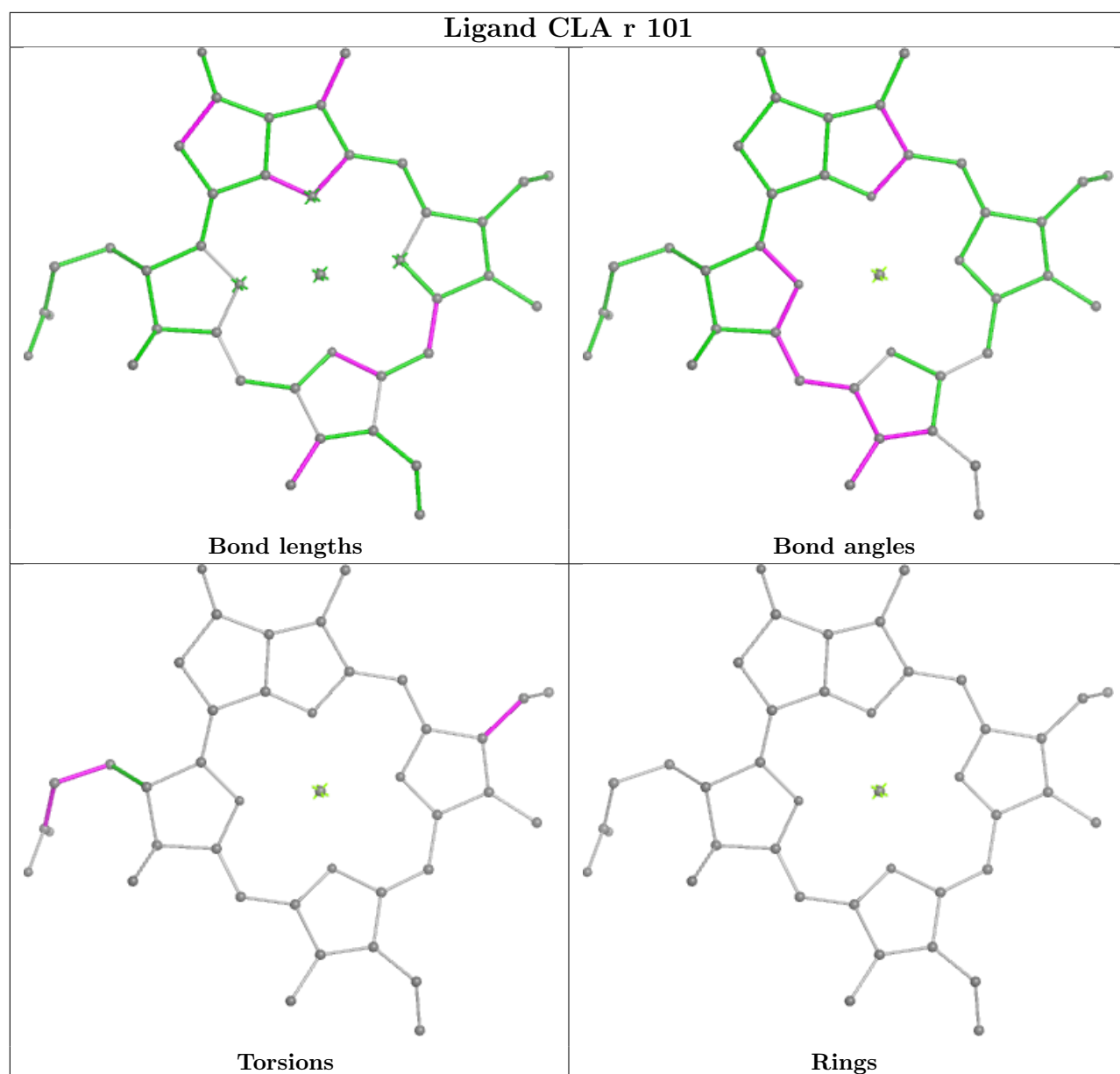
Bond angles



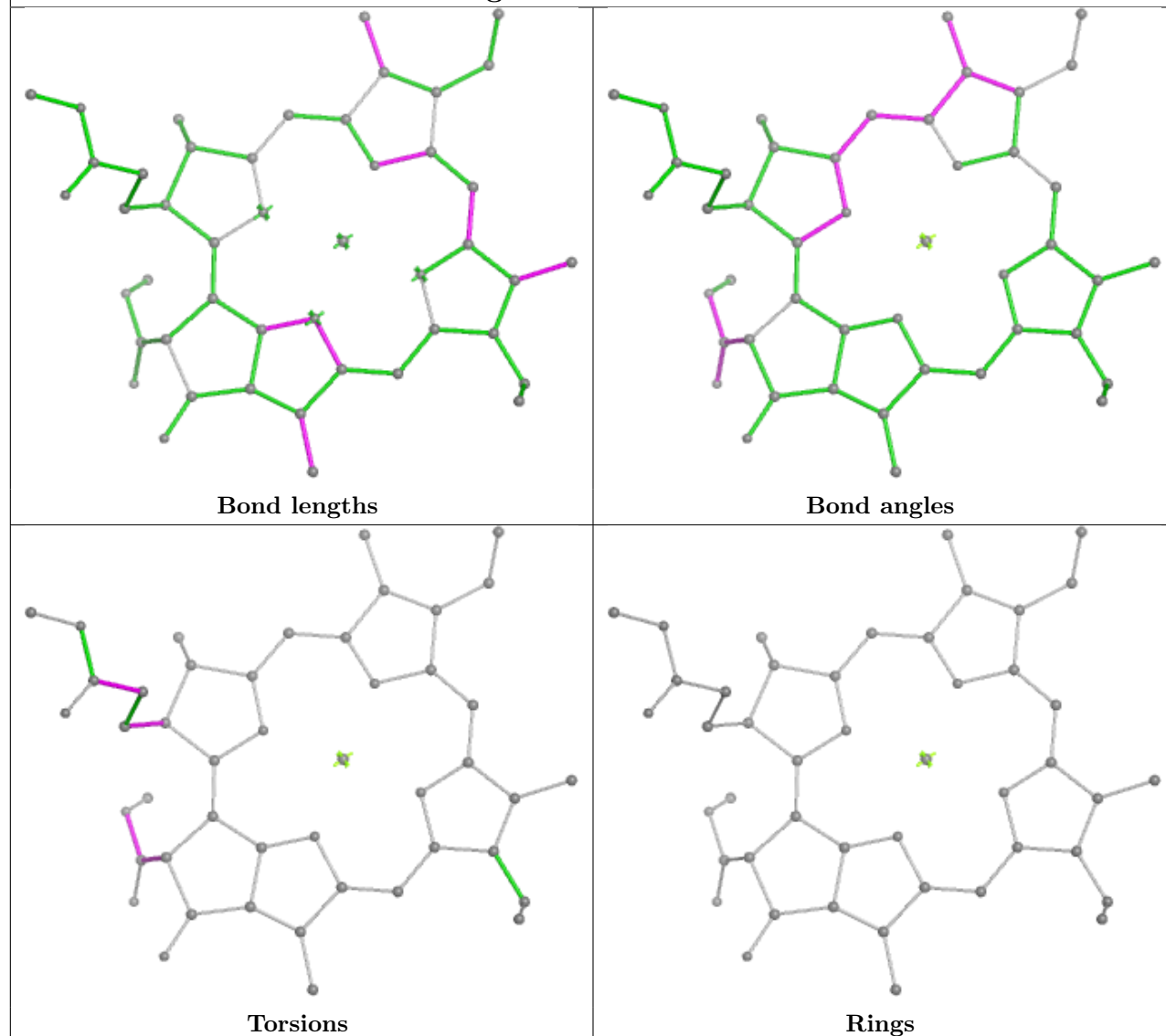
Torsions



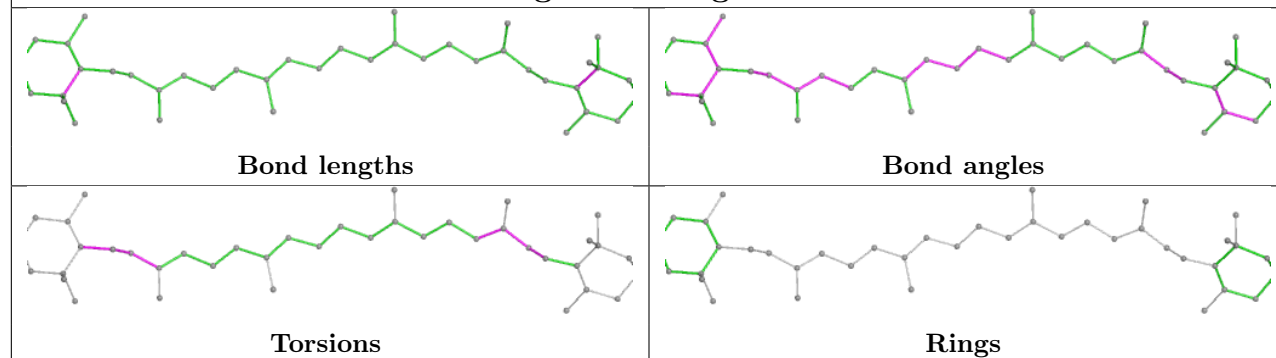
Rings



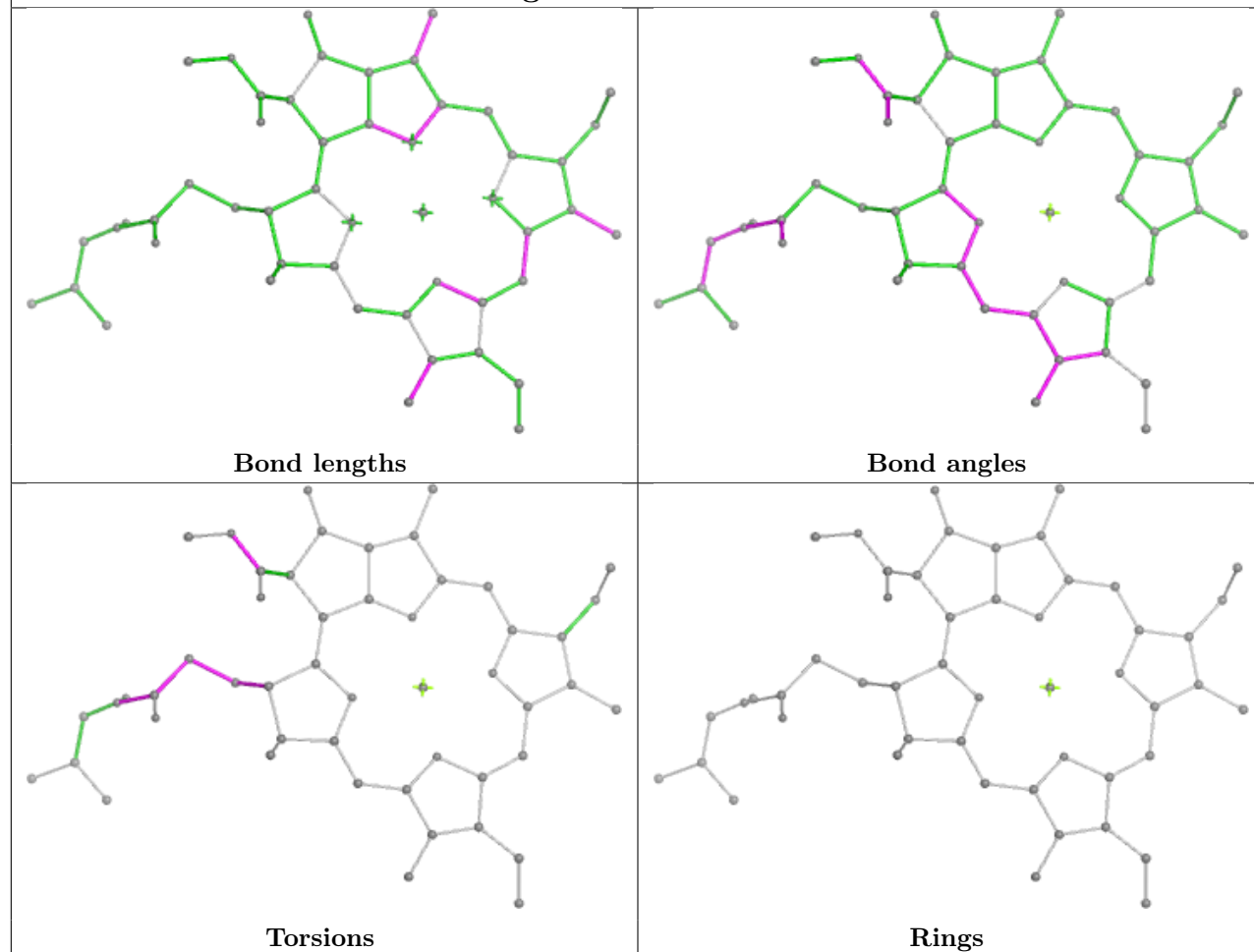
Ligand CLA B 826



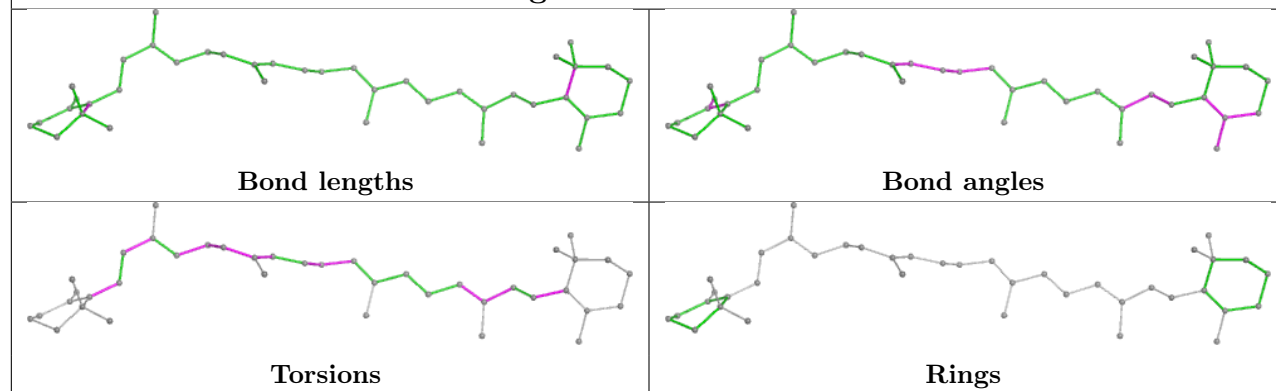
Ligand BCR g 844



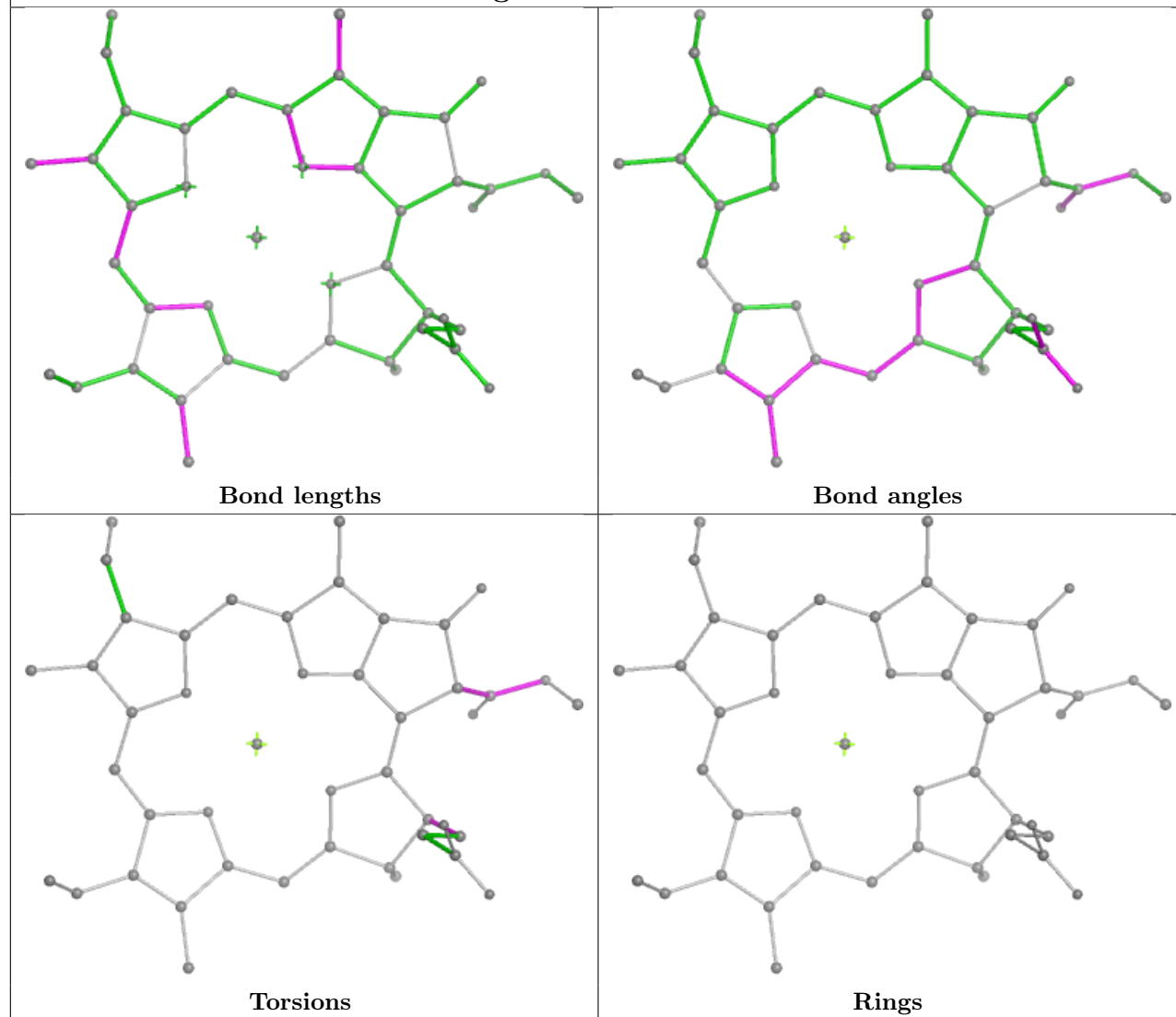
Ligand CLA A 830



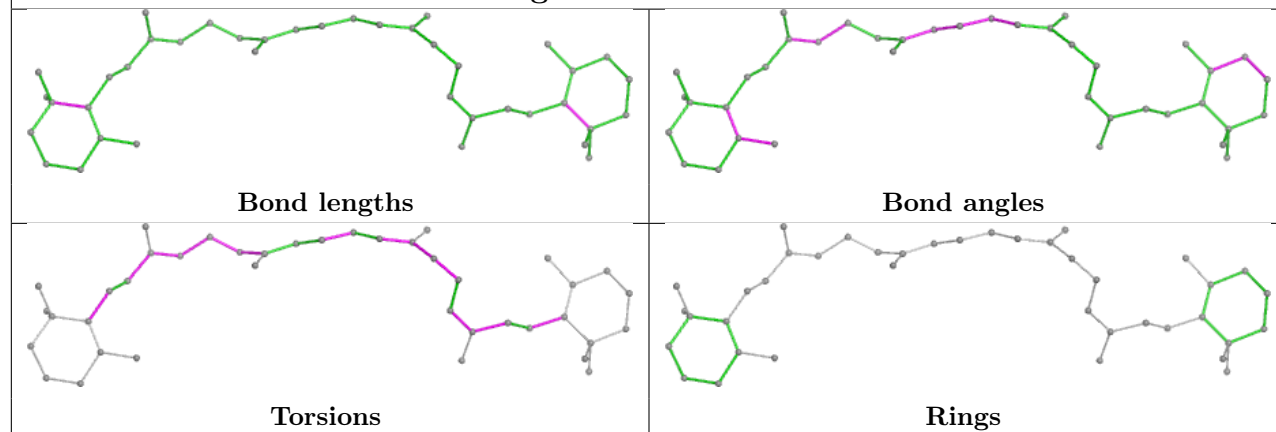
Ligand BCR G 848



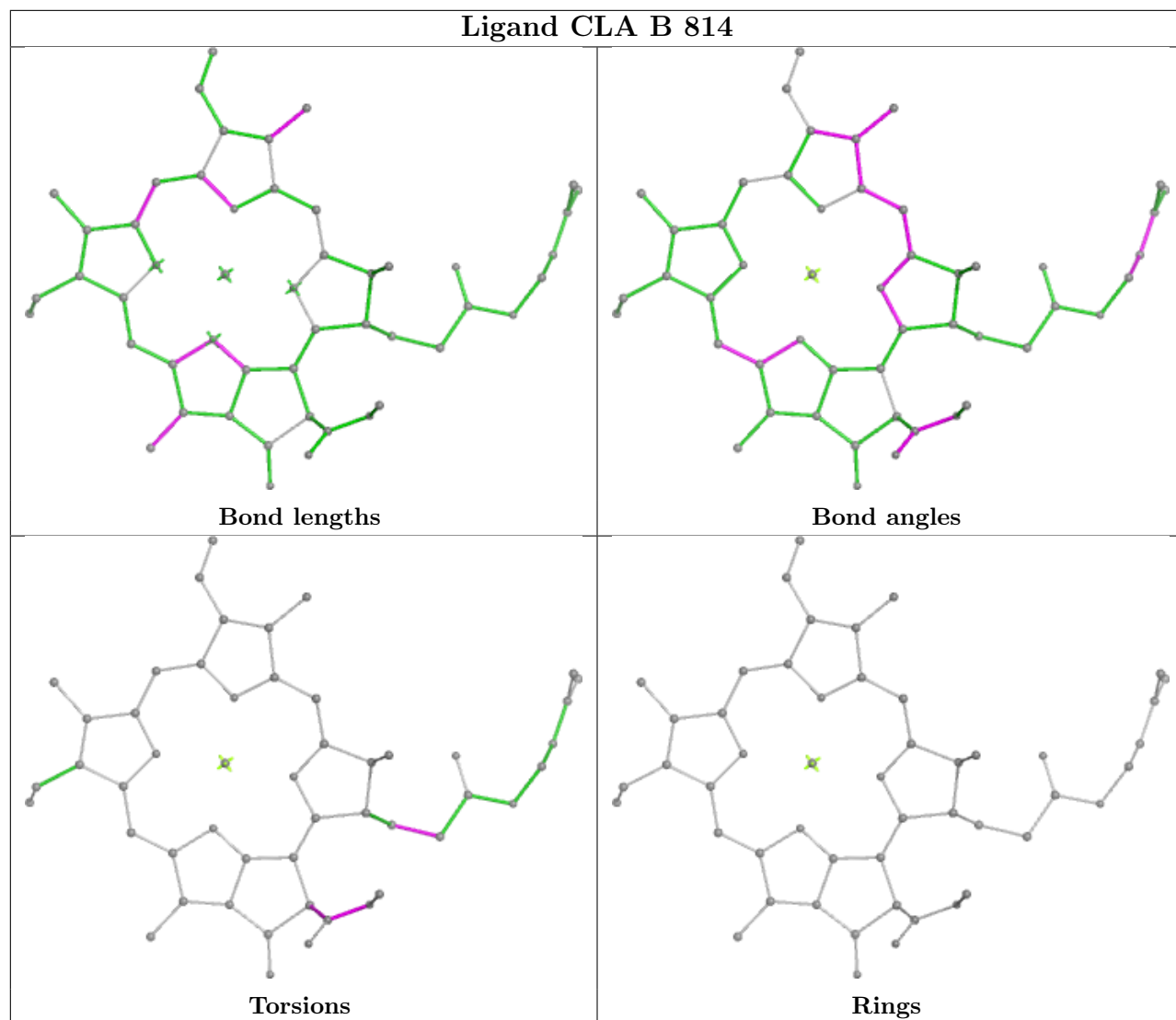
Ligand CLA S 206



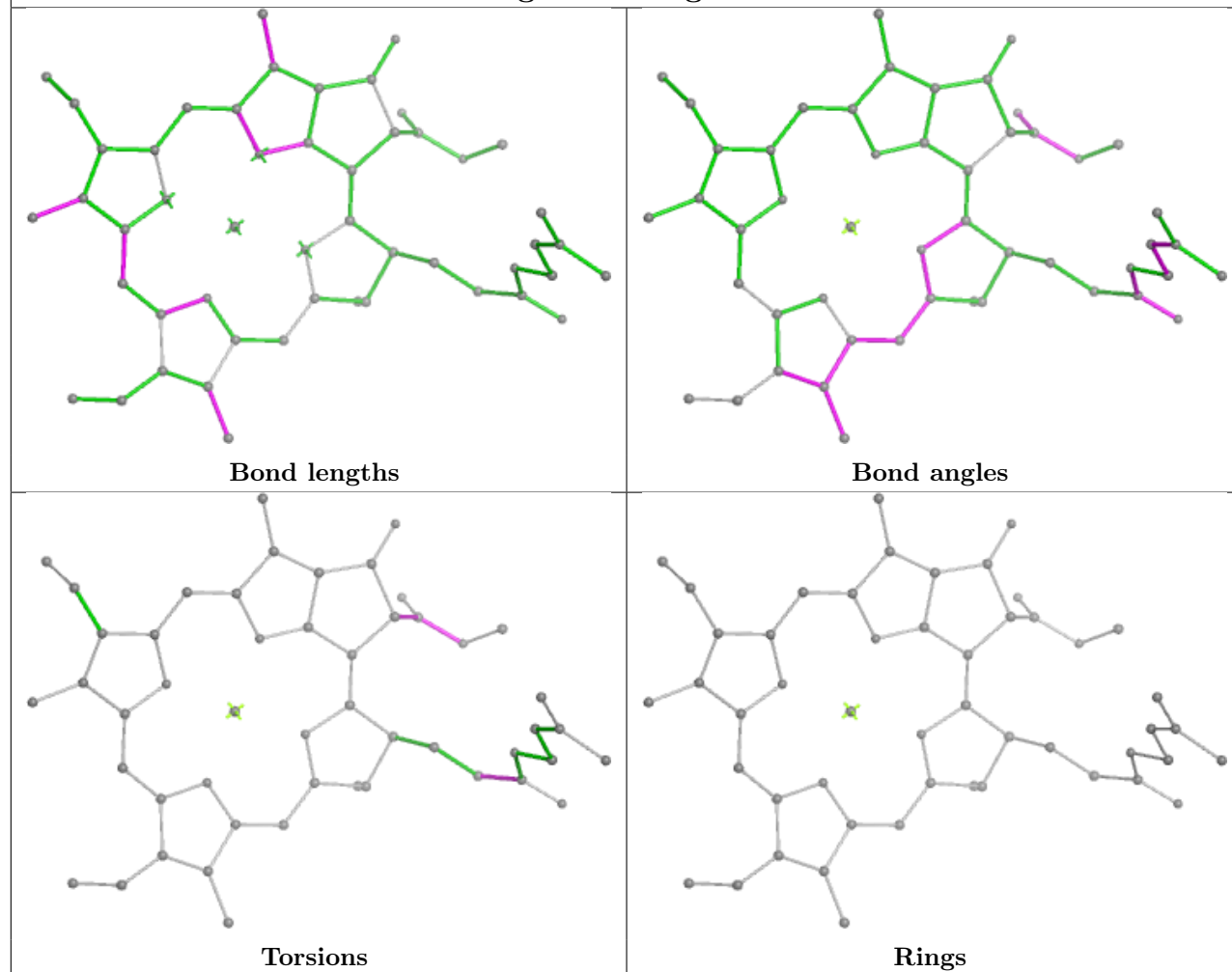
Ligand BCR B 844



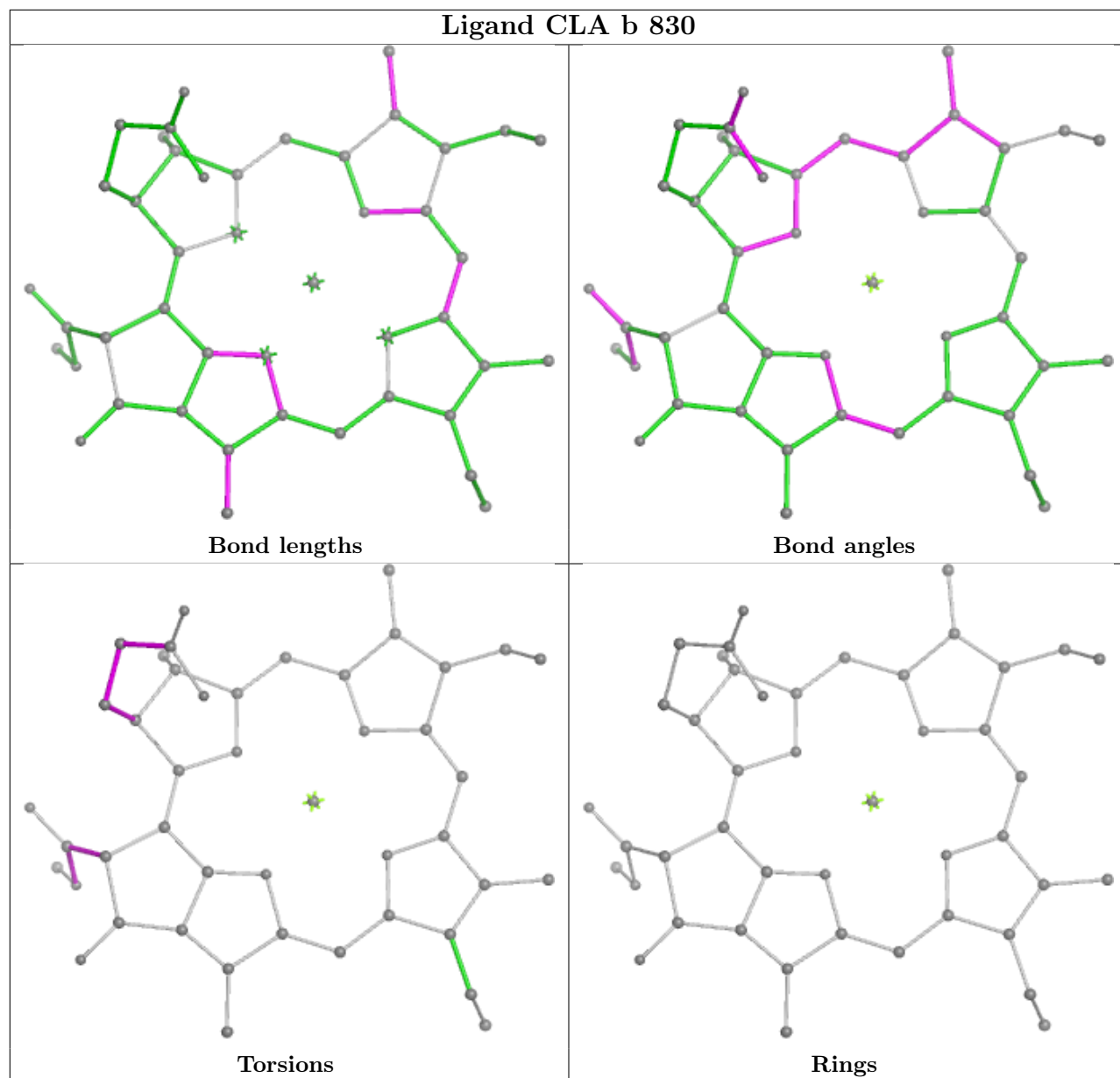
Ligand CLA B 814



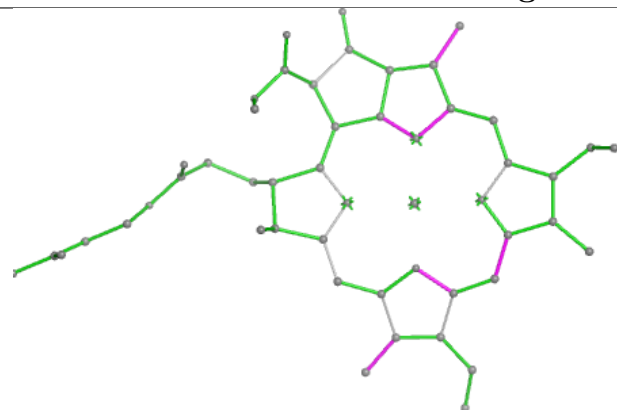
Ligand CLA g 805



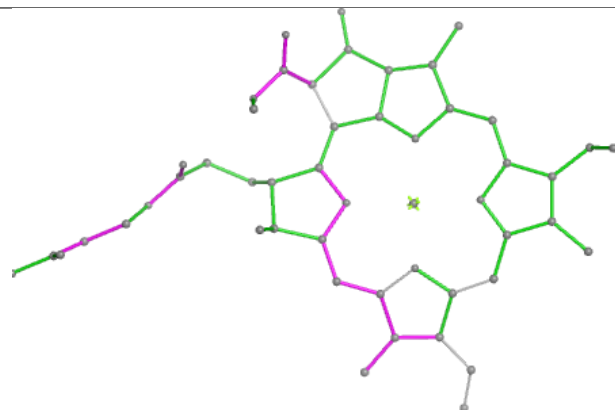
Ligand CLA b 830



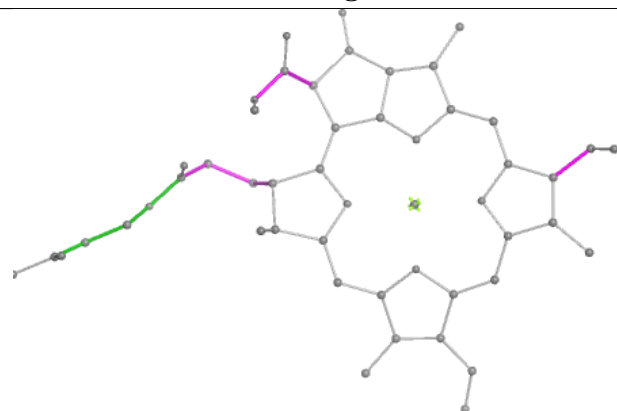
Ligand CLA B 834



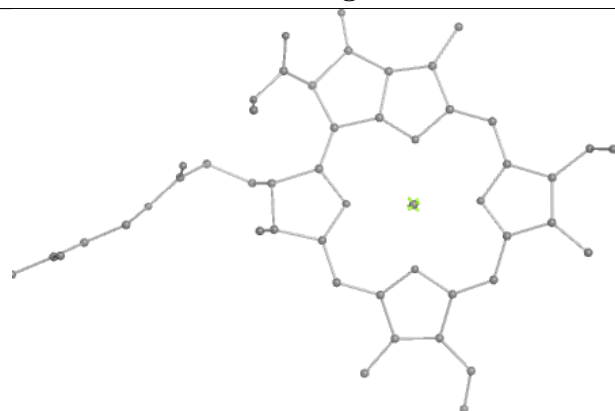
Bond lengths



Bond angles

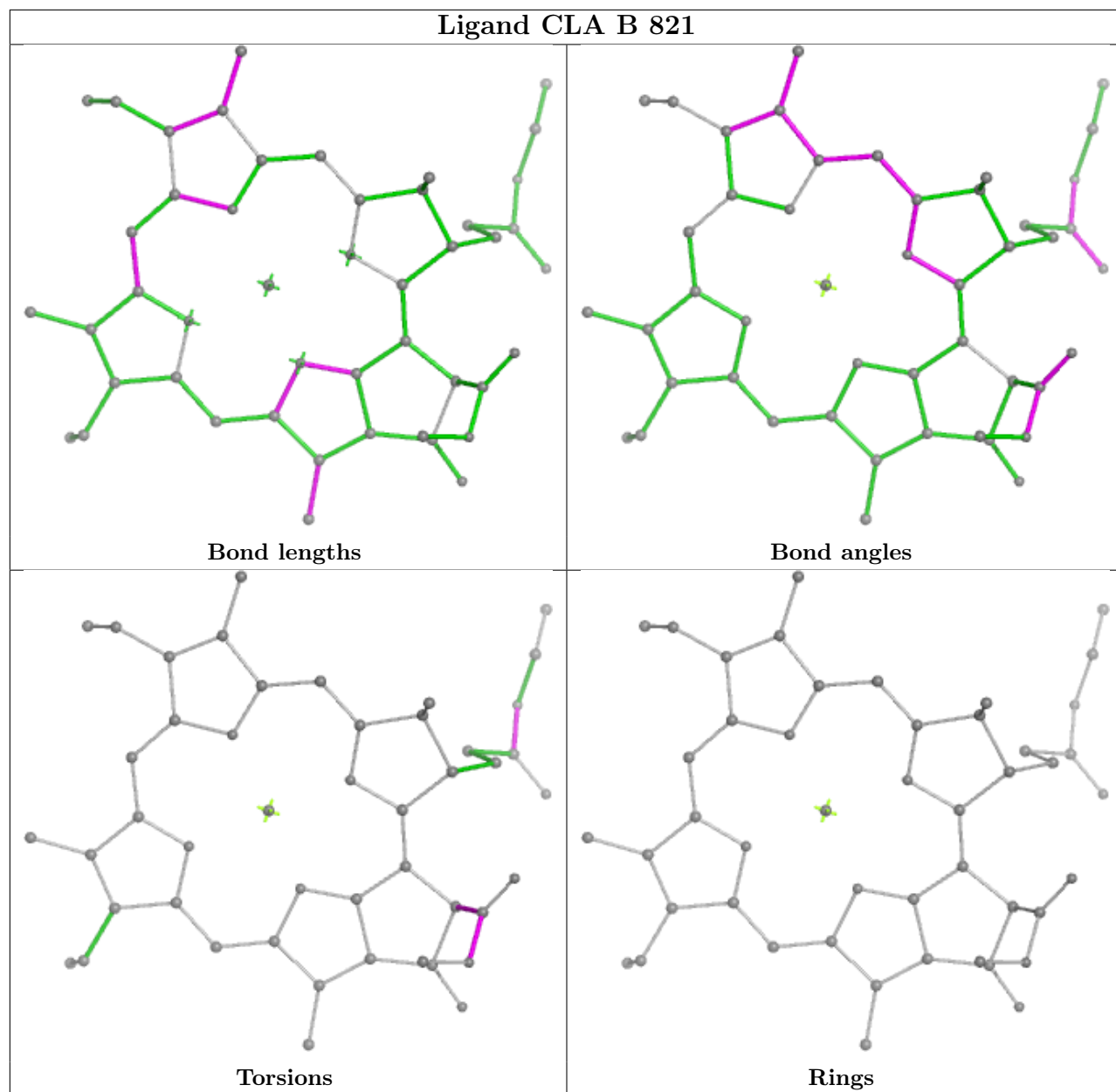


Torsions

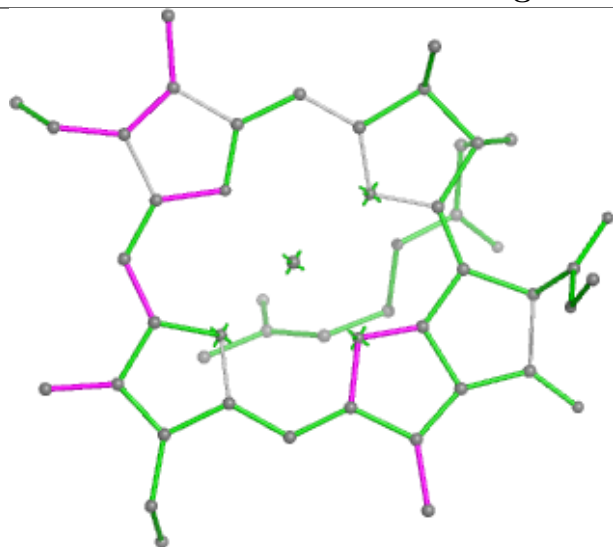


Rings

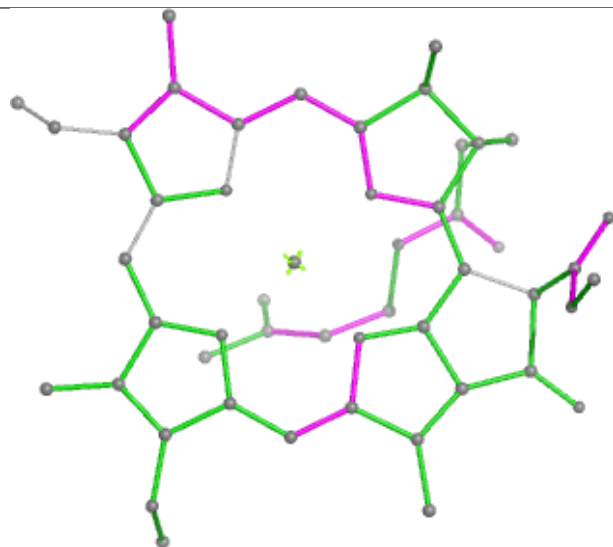
Ligand CLA B 821



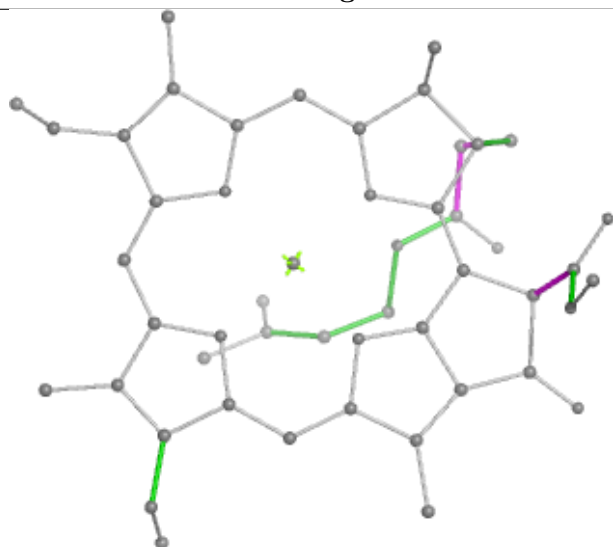
Ligand CLA A 840



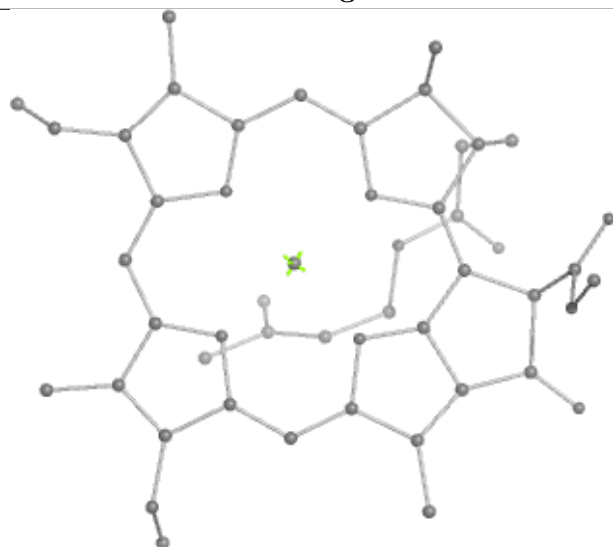
Bond lengths



Bond angles

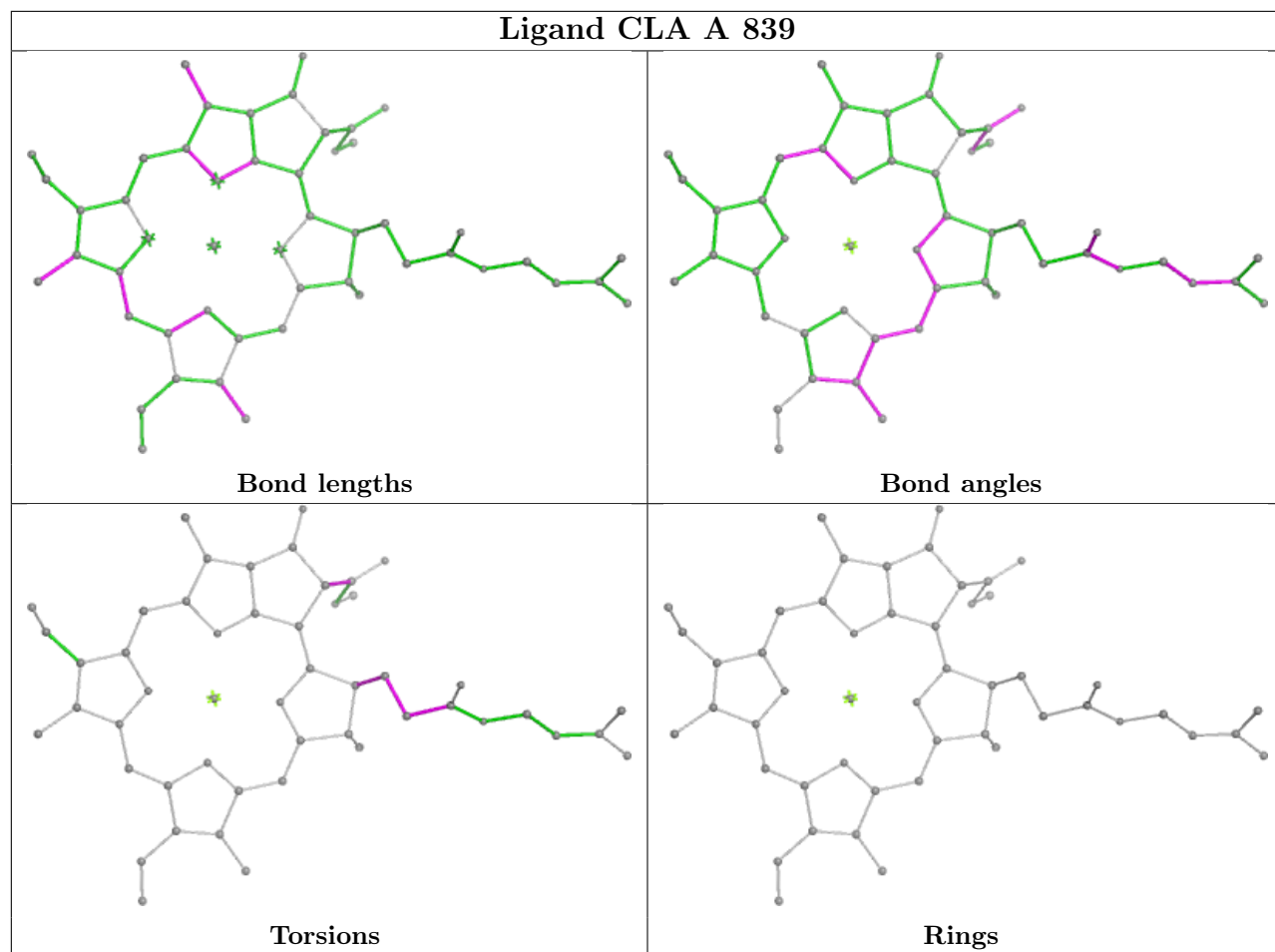


Torsions

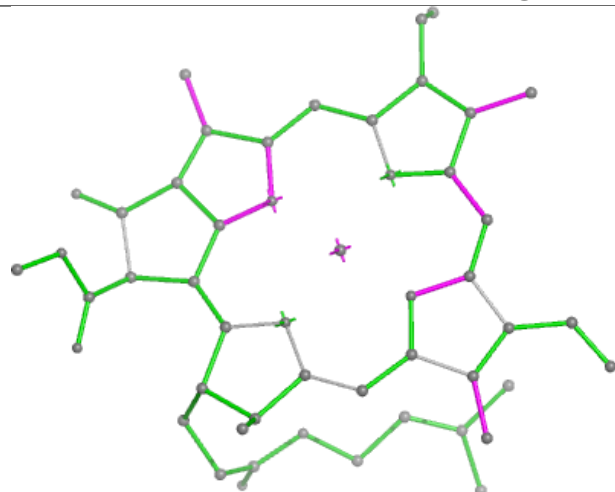


Rings

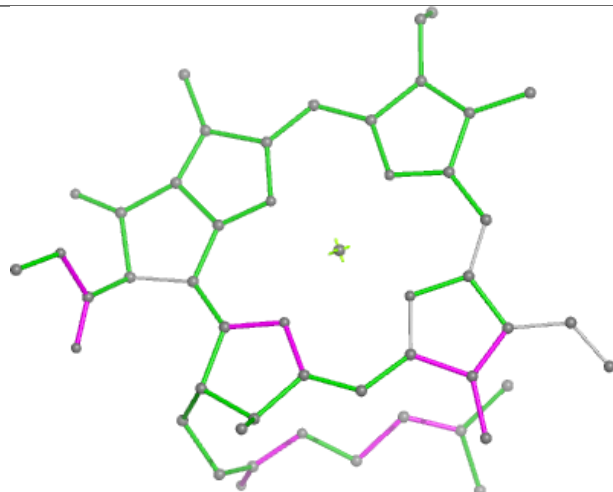
Ligand CLA A 839



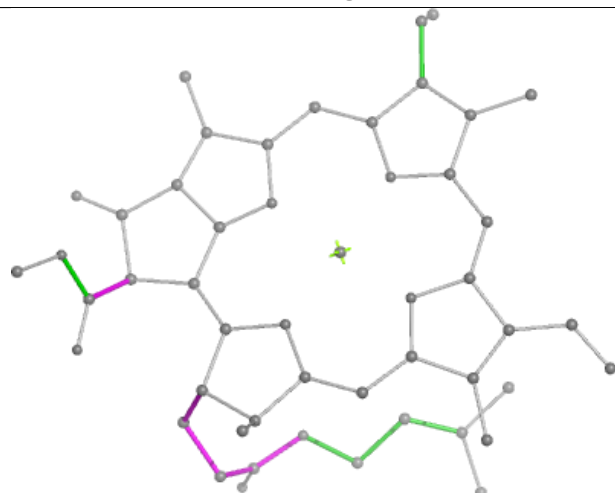
Ligand CLA A 823



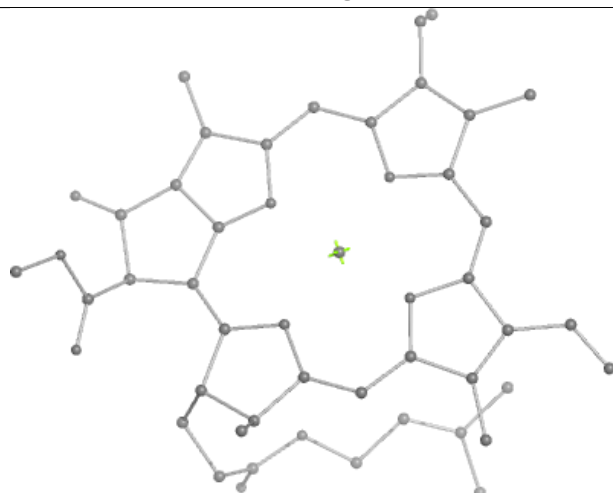
Bond lengths



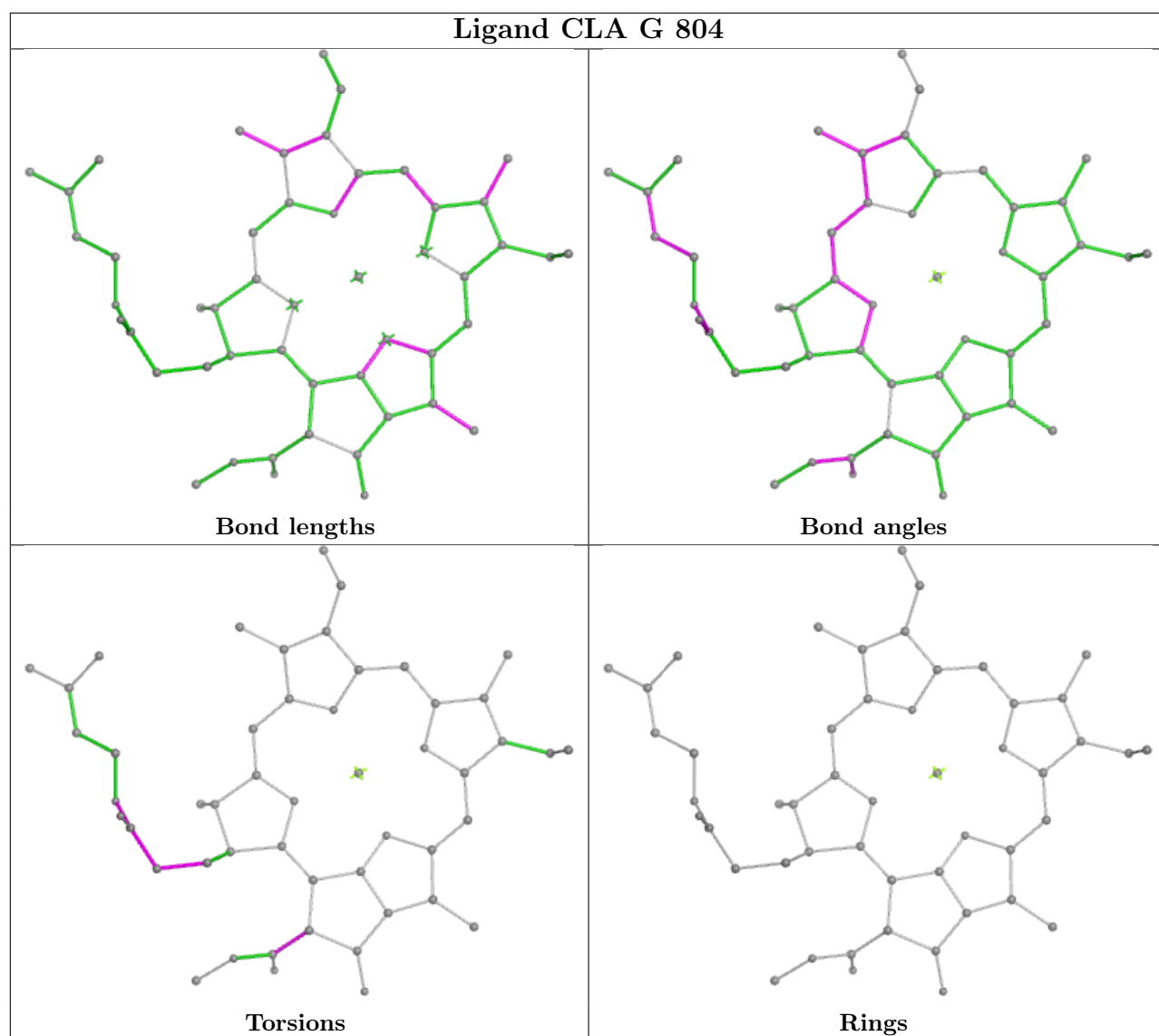
Bond angles



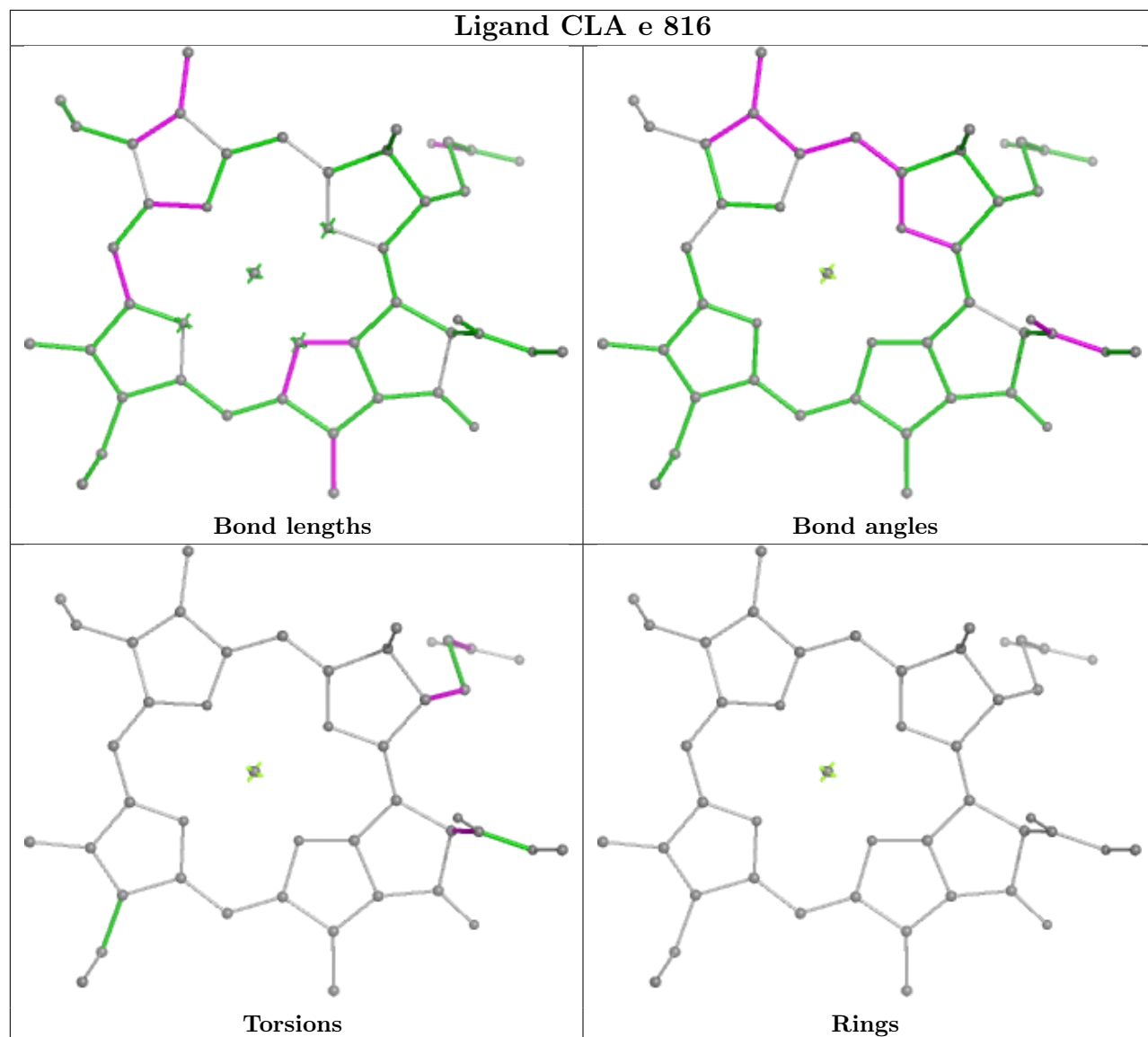
Torsions



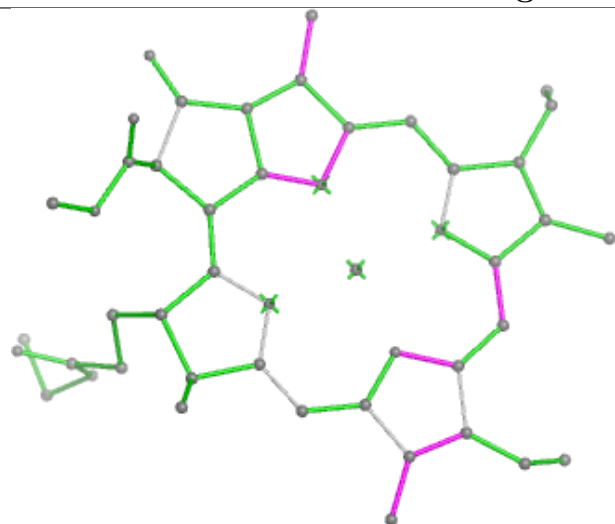
Rings



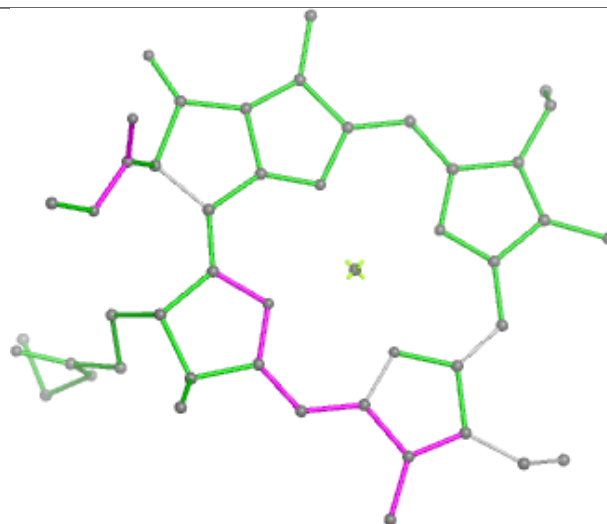
Ligand CLA e 816



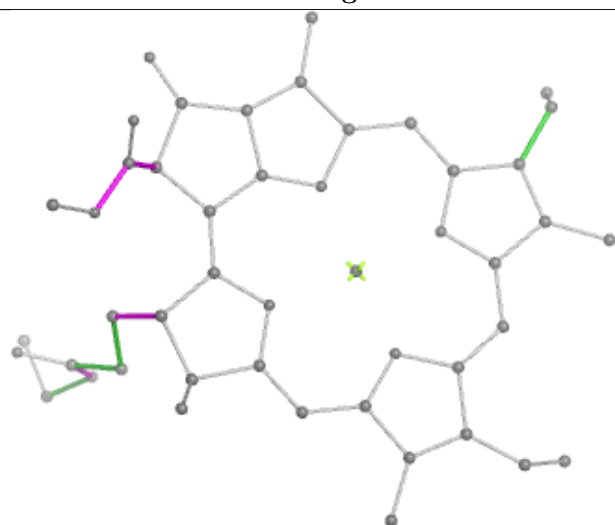
Ligand CLA B 839



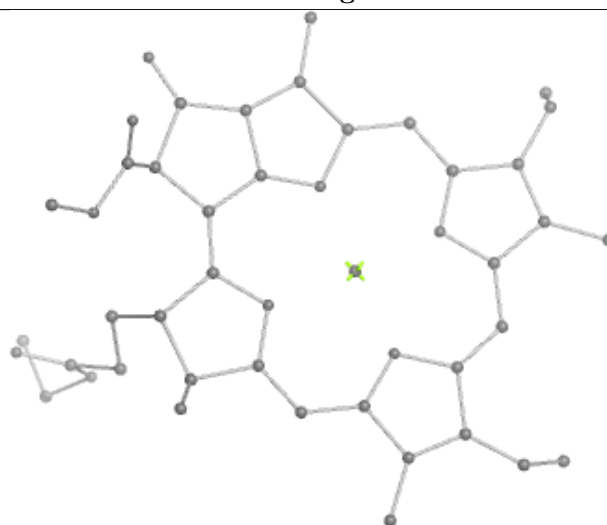
Bond lengths



Bond angles

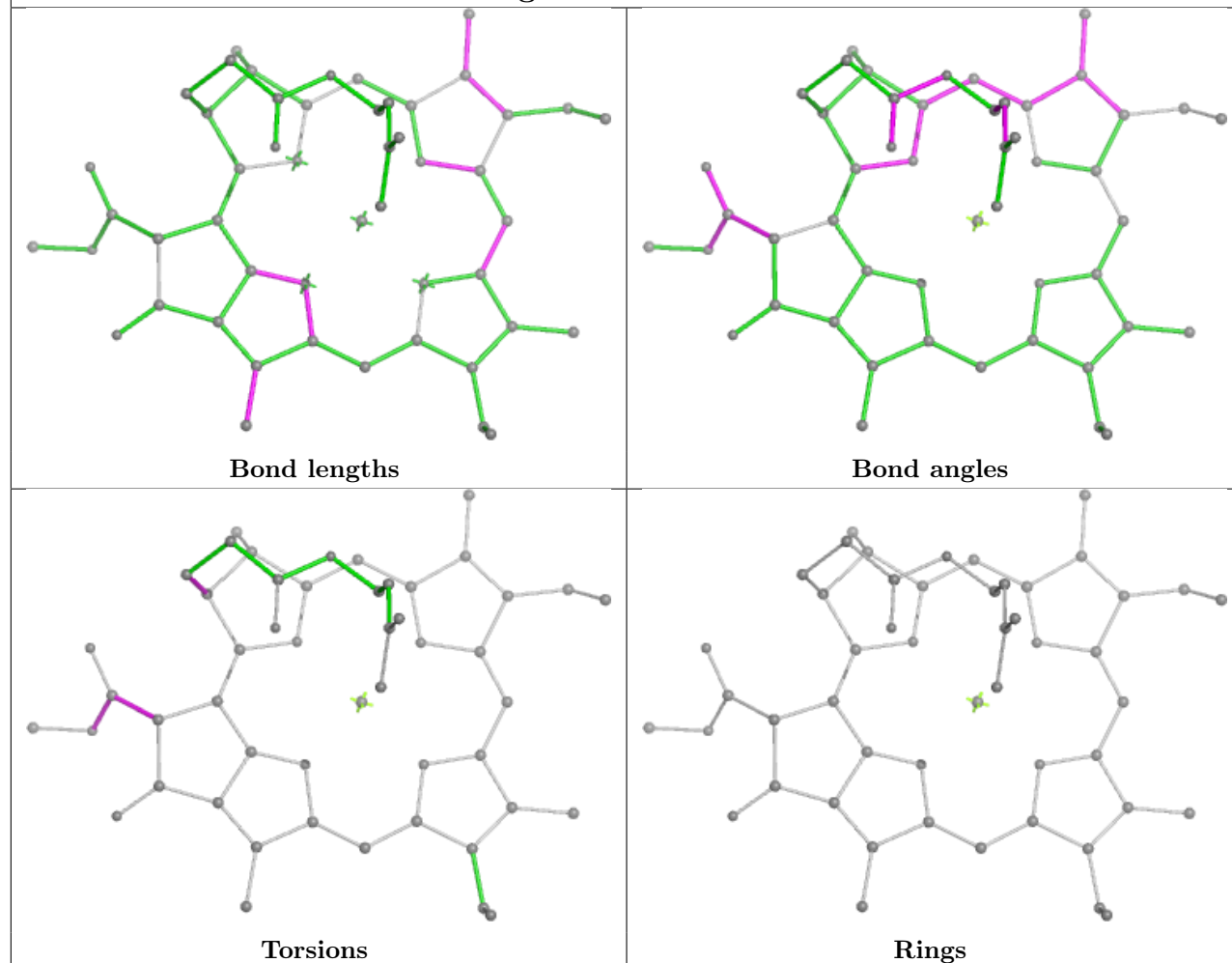


Torsions

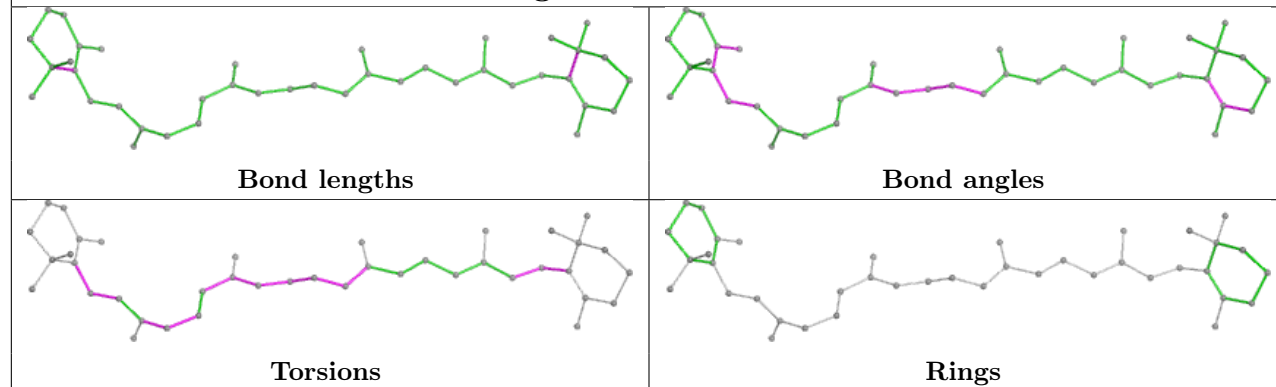


Rings

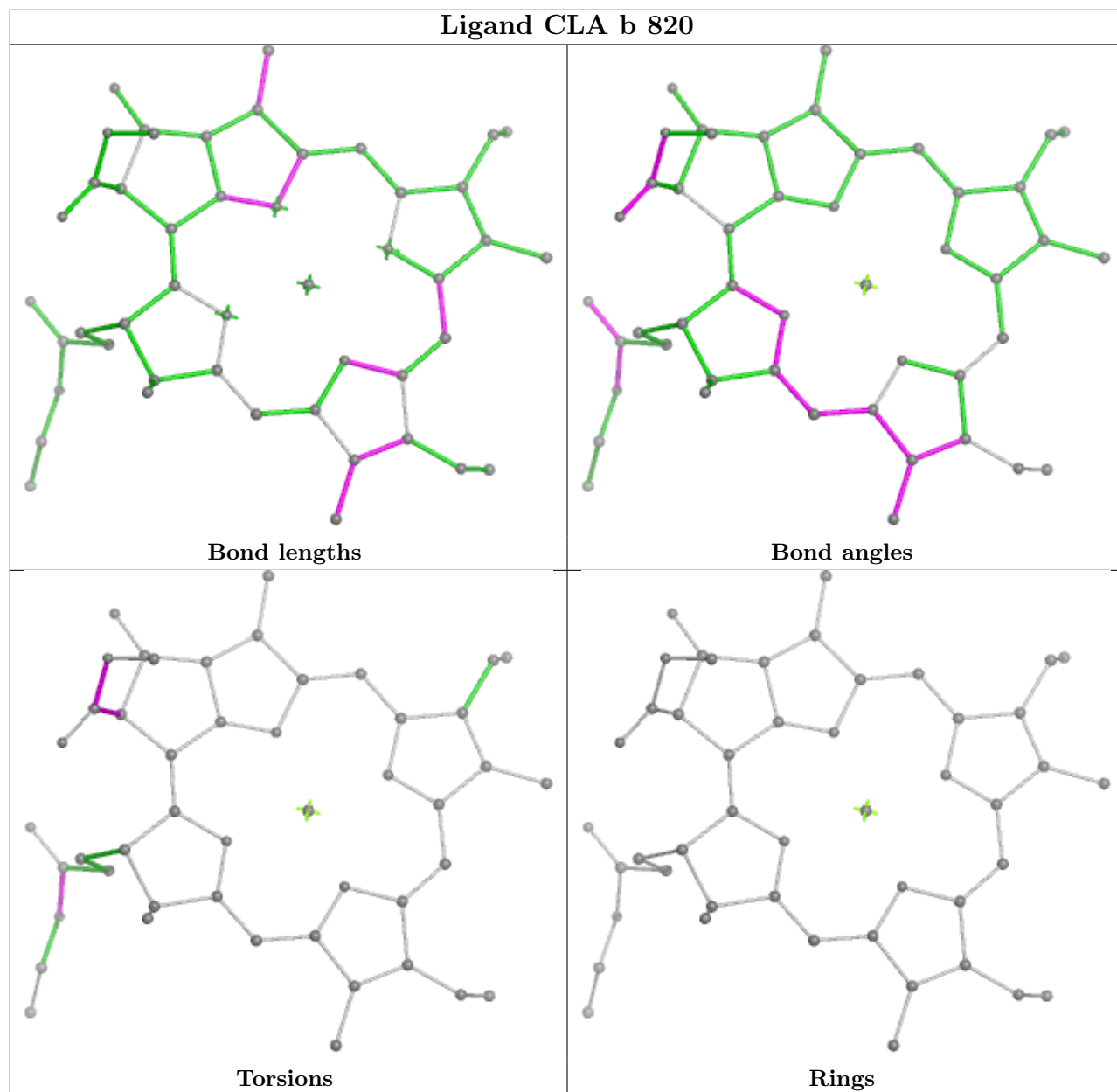
Ligand CLA e 844

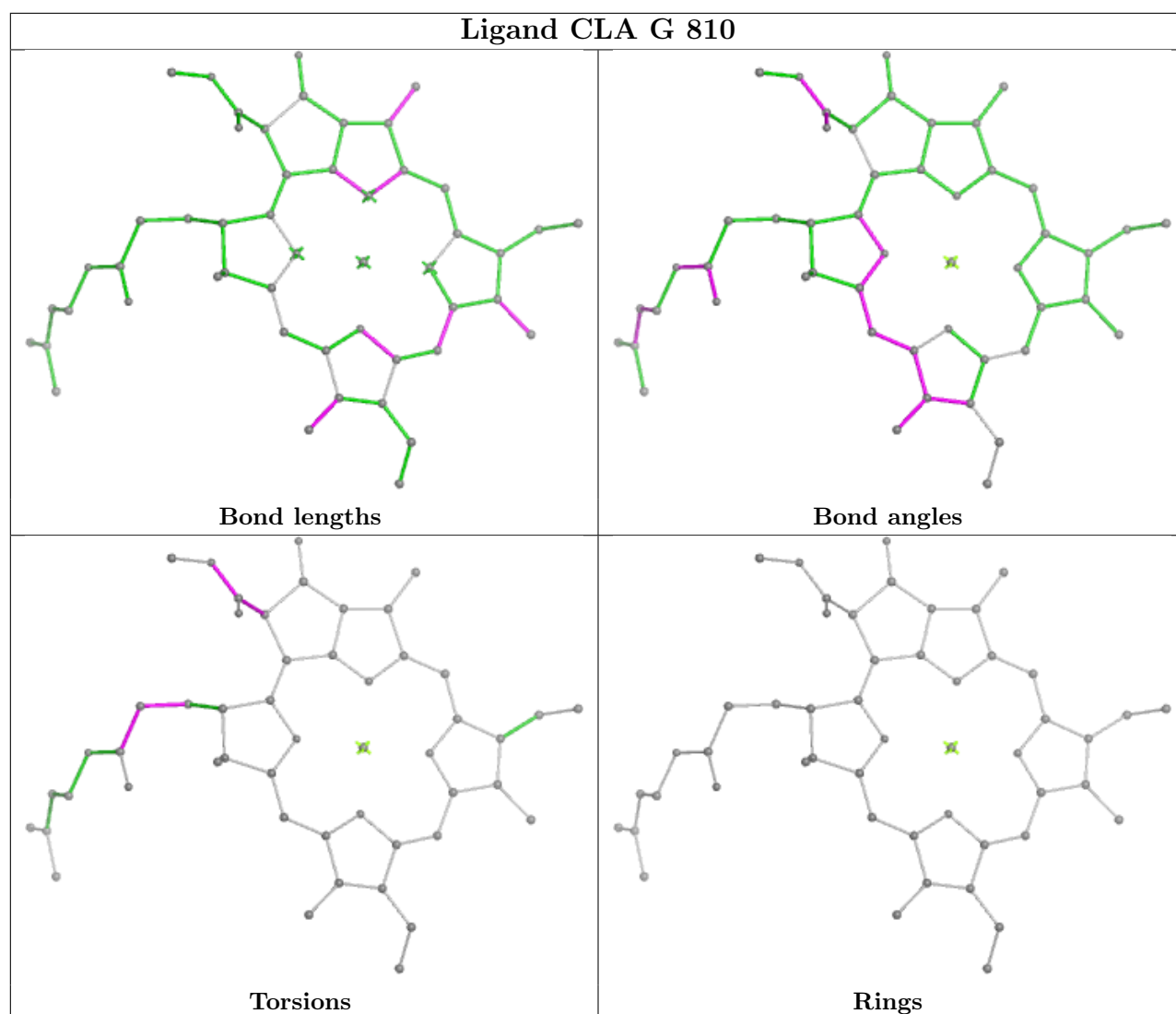


Ligand BCR b 844



Ligand CLA b 820





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.

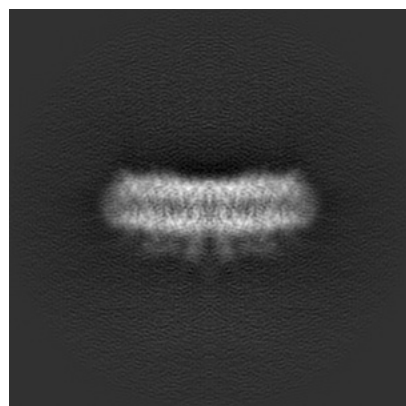
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13898. These allow visual inspection of the internal detail of the map and identification of artifacts.

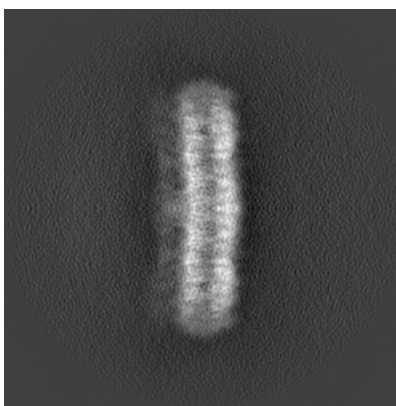
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

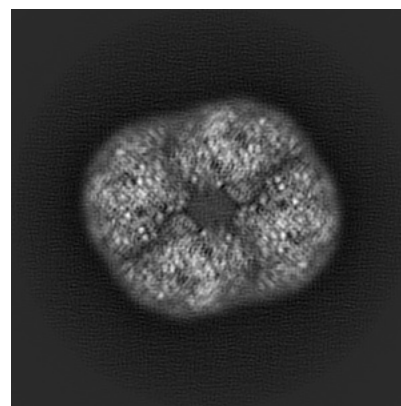
6.1.1 Primary map



X

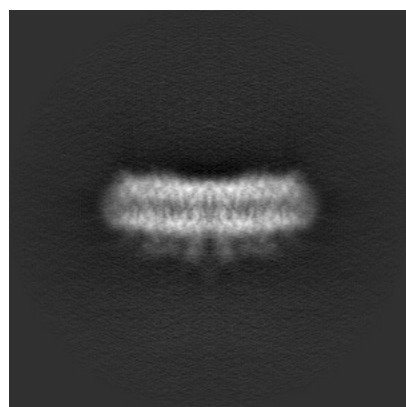


Y

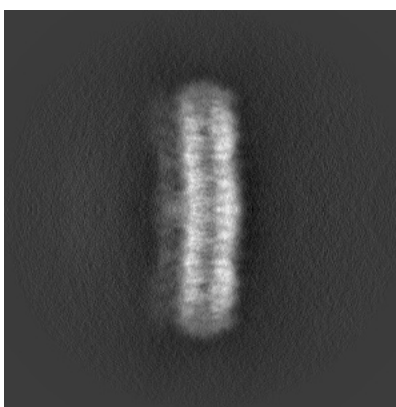


Z

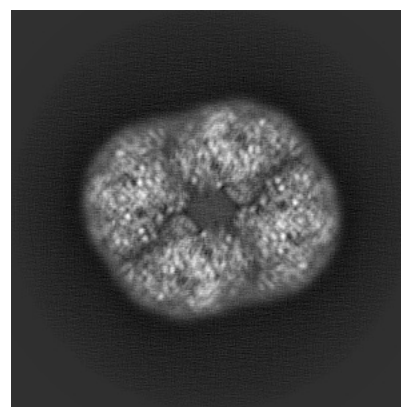
6.1.2 Raw map



X



Y

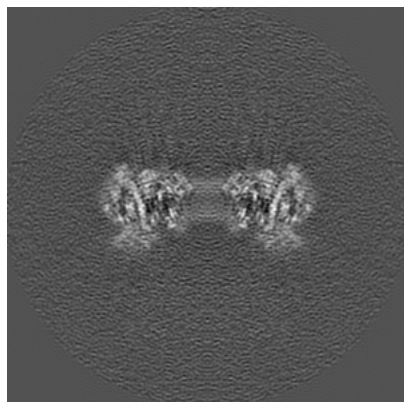


Z

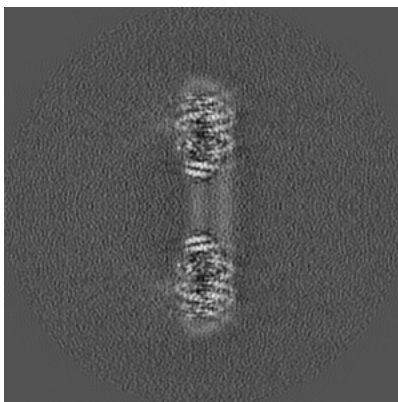
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

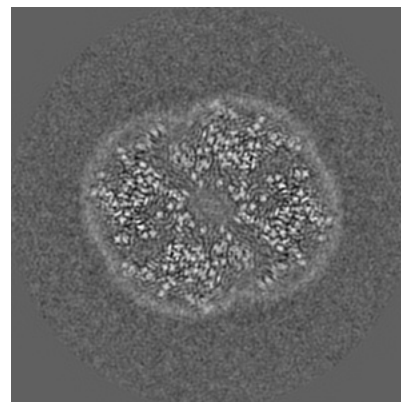
6.2.1 Primary map



X Index: 192

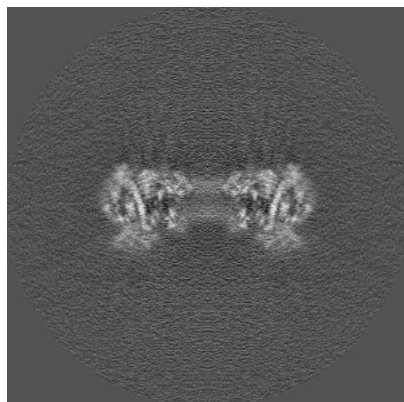


Y Index: 192

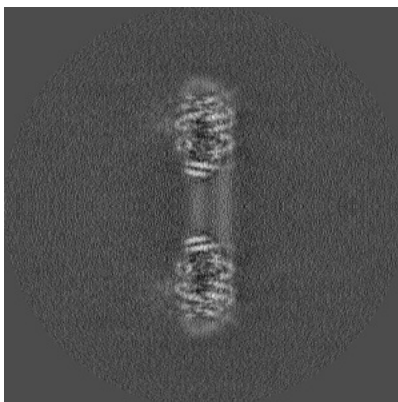


Z Index: 192

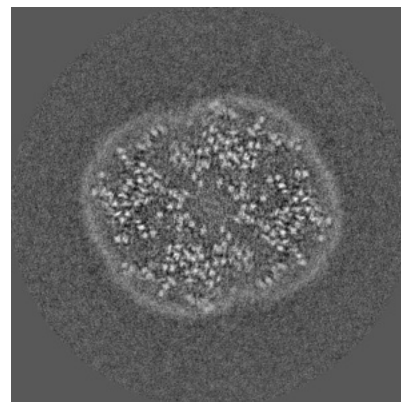
6.2.2 Raw map



X Index: 192



Y Index: 192

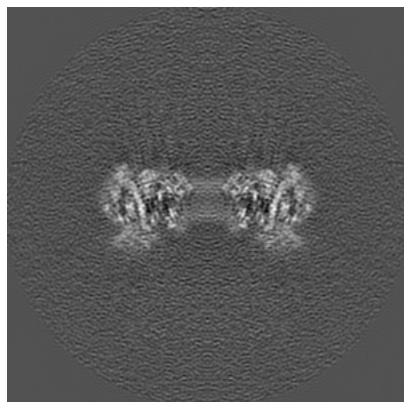


Z Index: 192

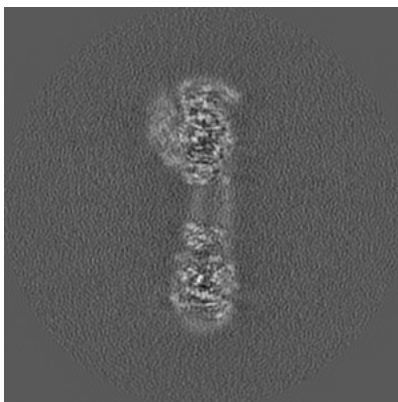
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

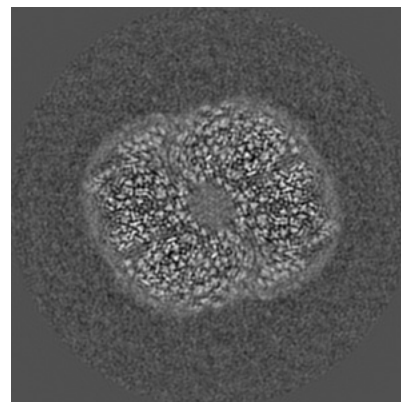
6.3.1 Primary map



X Index: 192

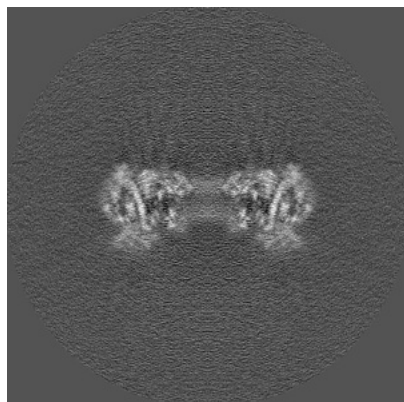


Y Index: 180

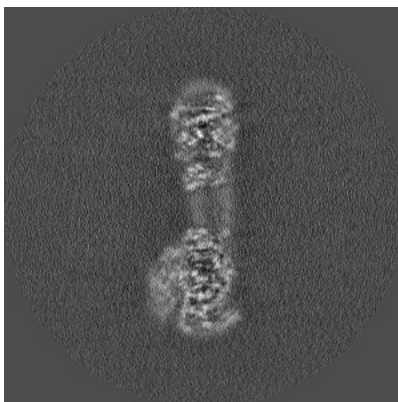


Z Index: 184

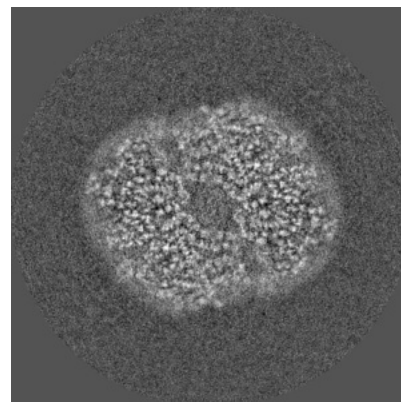
6.3.2 Raw map



X Index: 192



Y Index: 204

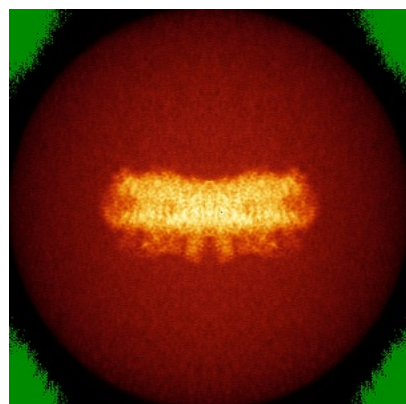


Z Index: 180

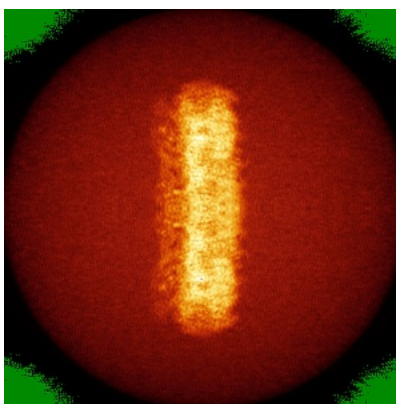
The images above show the largest variance slices of the map in three orthogonal directions.

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

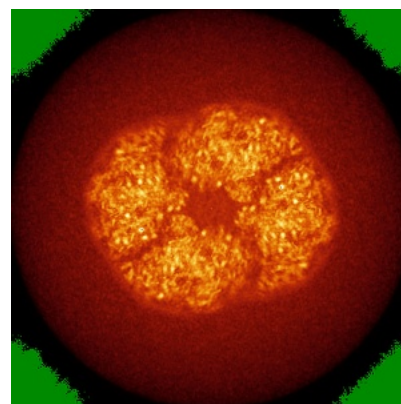
6.4.1 Primary map



X

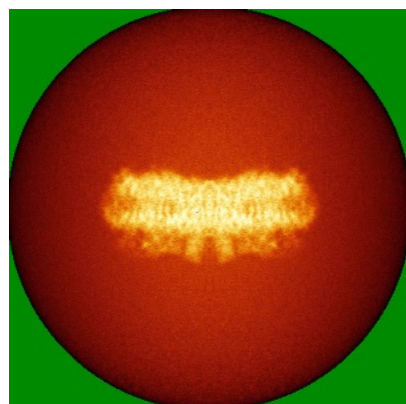


Y

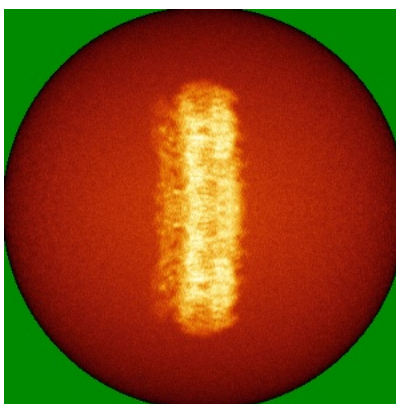


Z

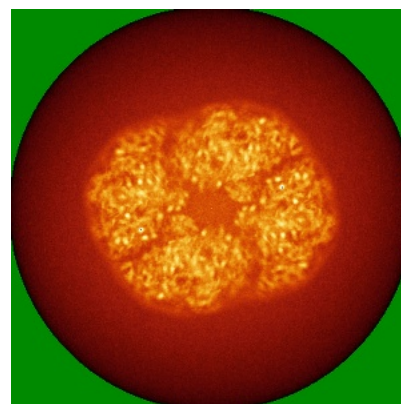
6.4.2 Raw map



X



Y

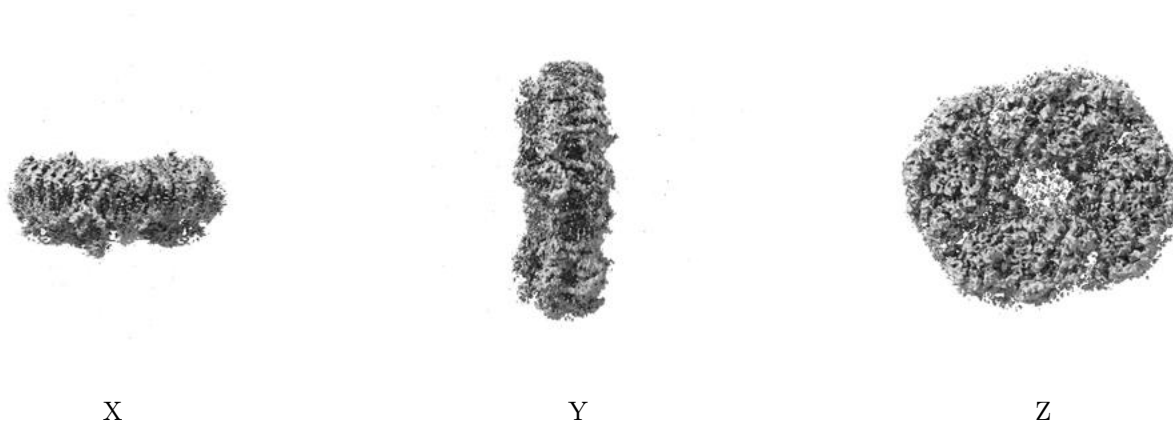


Z

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.

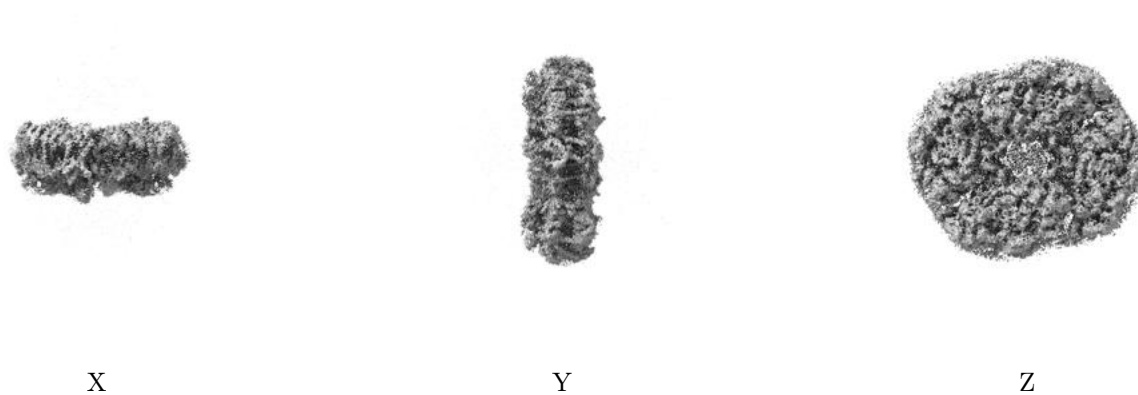
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0125. 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.

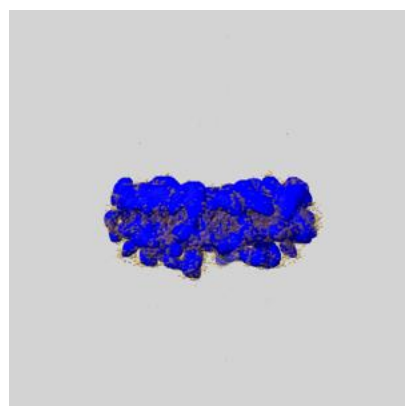
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

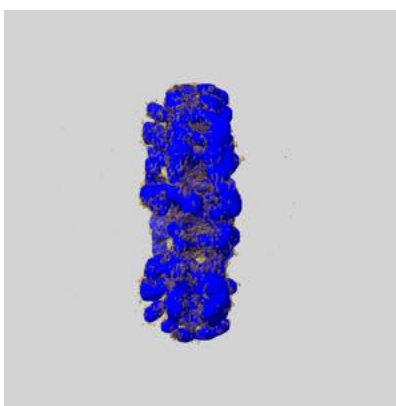
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

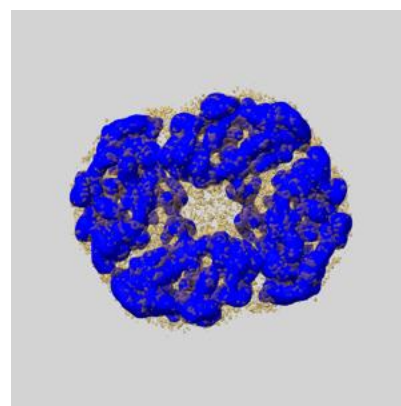
6.6.1 emd_13898_msk_1.map [i](#)



X



Y

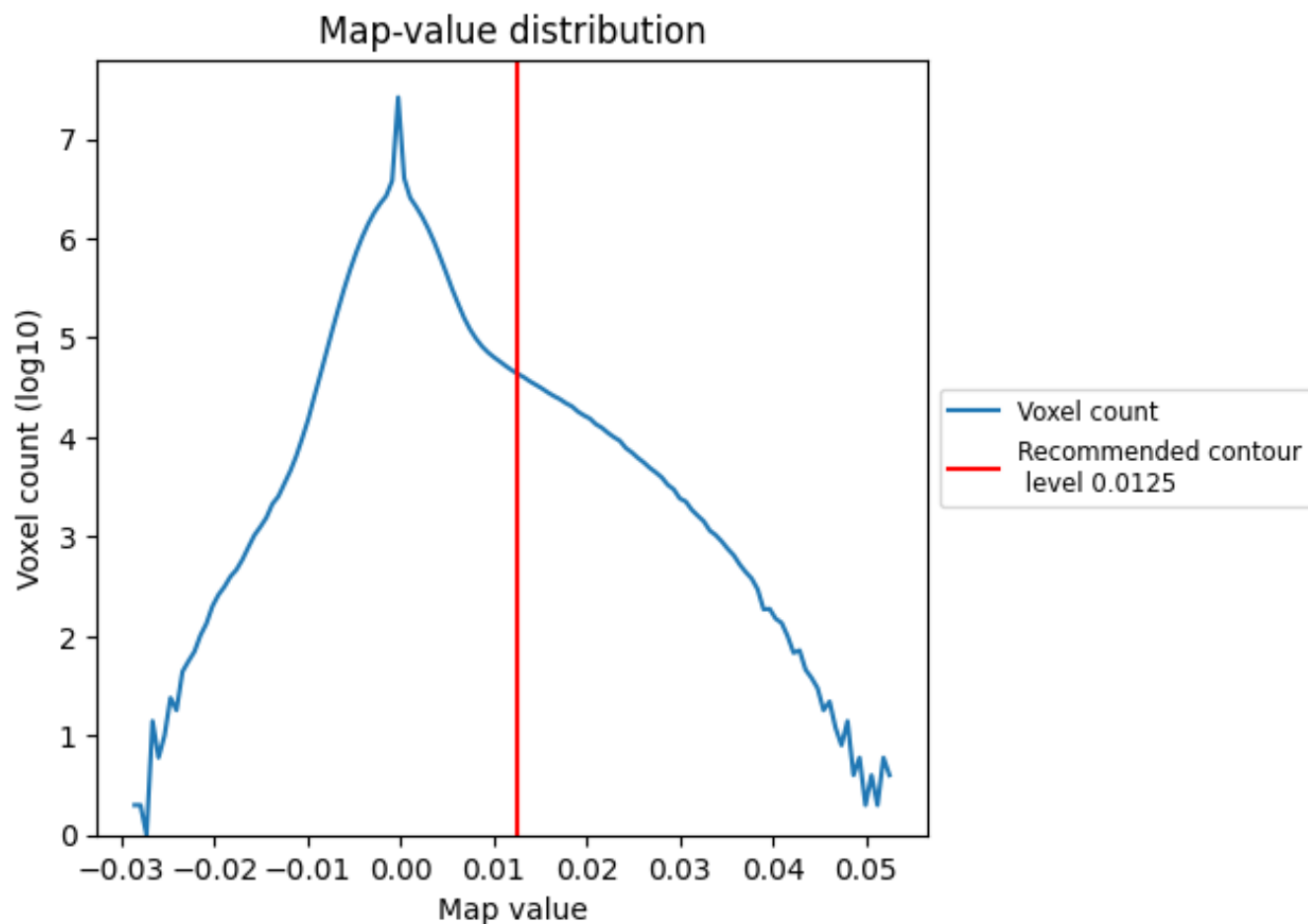


Z

7 Map analysis [i](#)

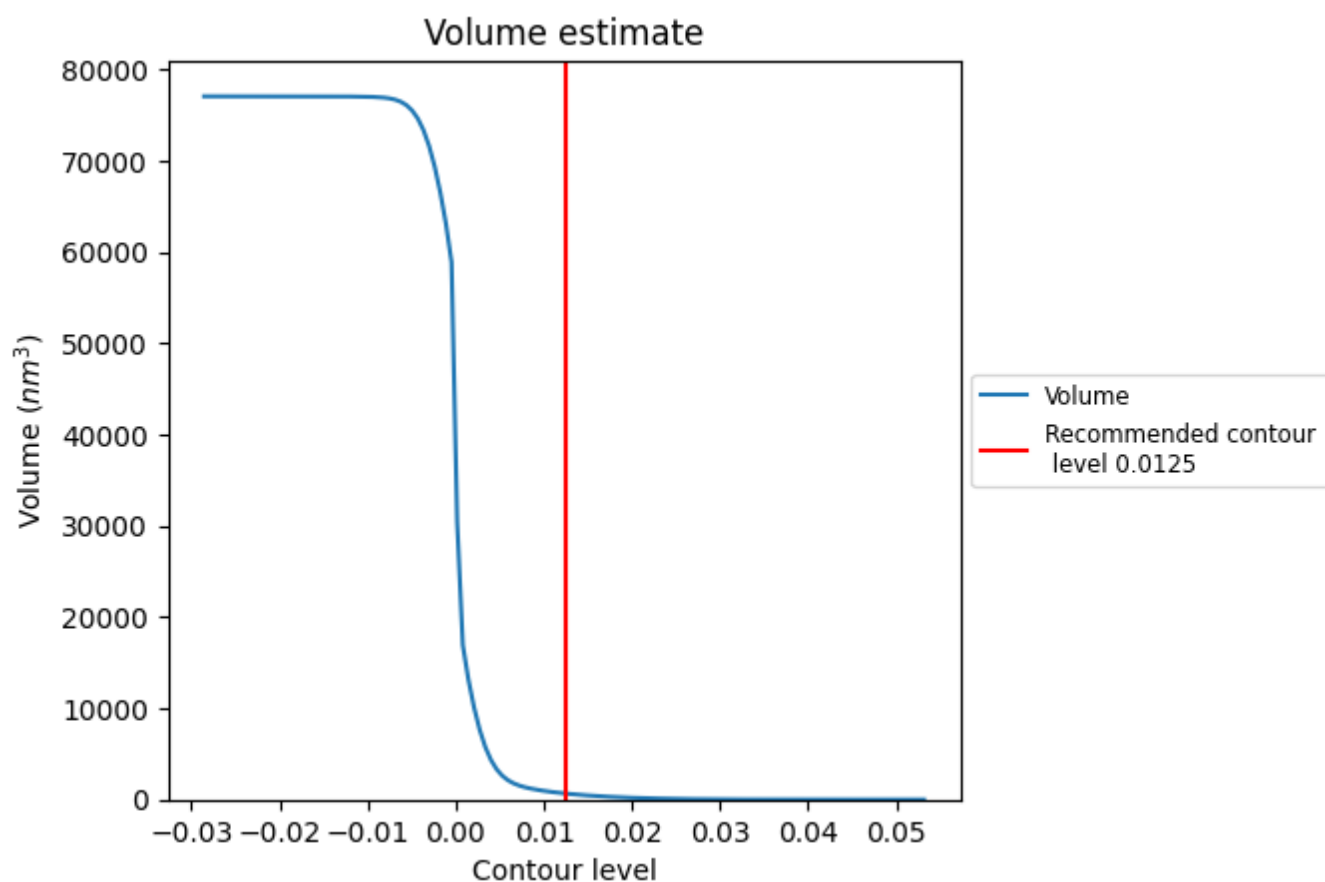
This section contains the results of statistical analysis of the map.

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.

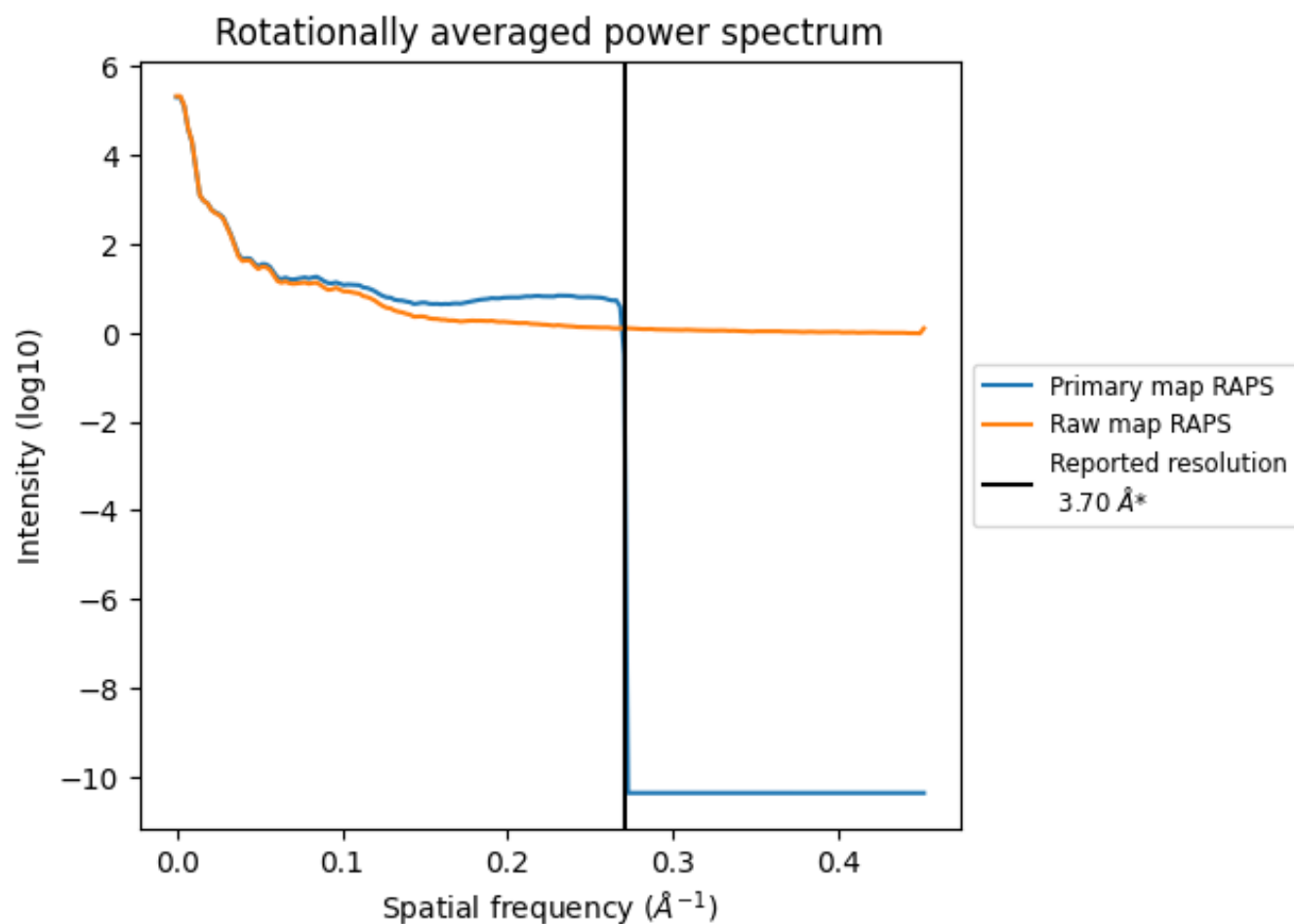
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 658 nm³; this corresponds to an approximate mass of 594 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

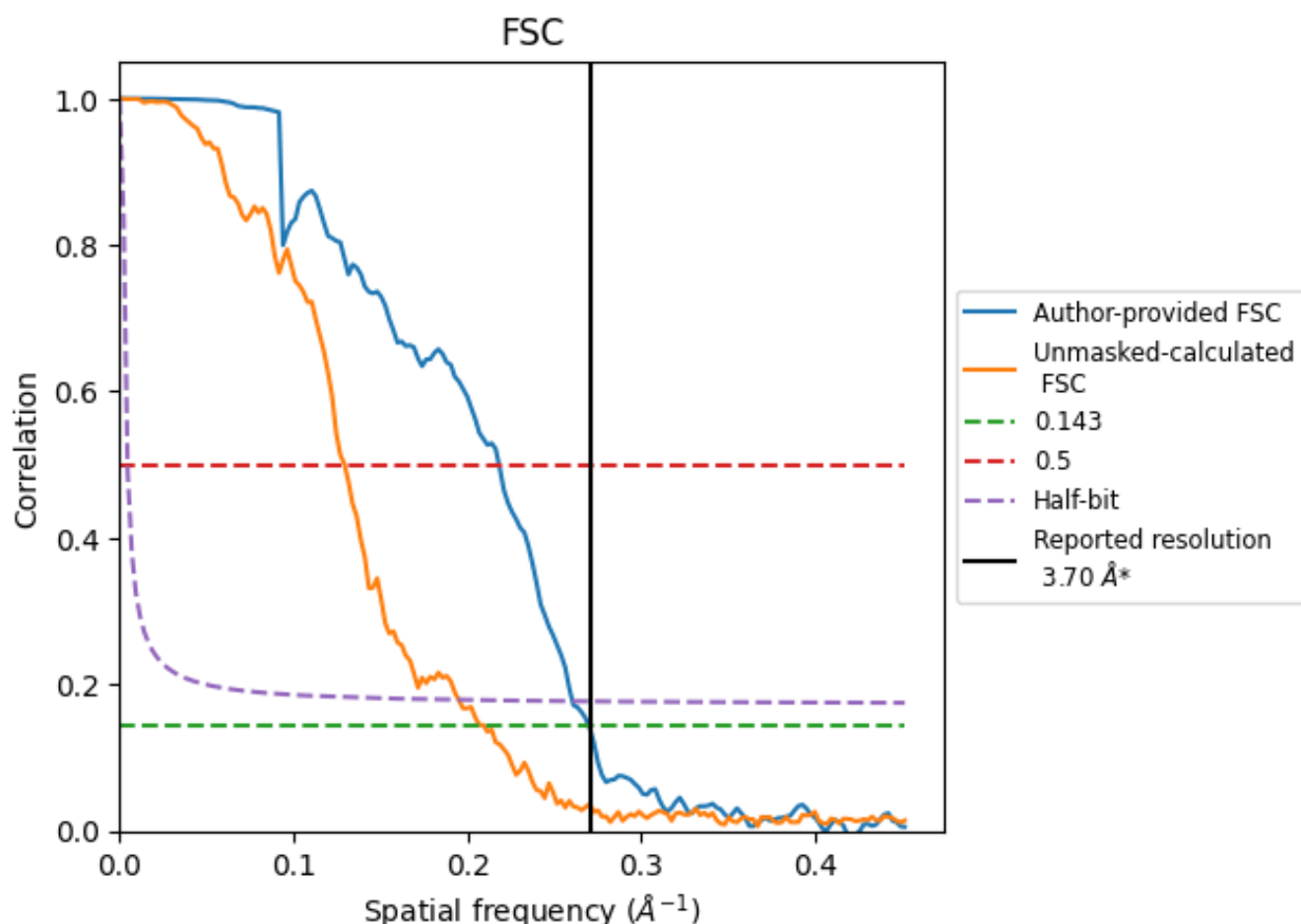


*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8.2 Resolution estimates [i](#)

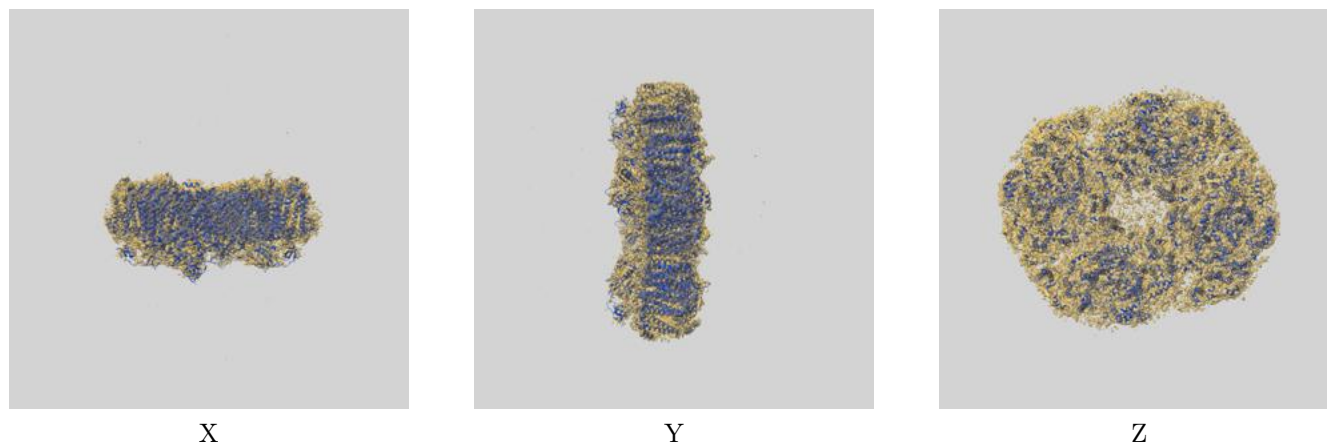
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.59	3.84
Unmasked-calculated*	4.77	7.73	5.13

*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 4.77 differs from the reported value 3.7 by more than 10 %

9 Map-model fit [i](#)

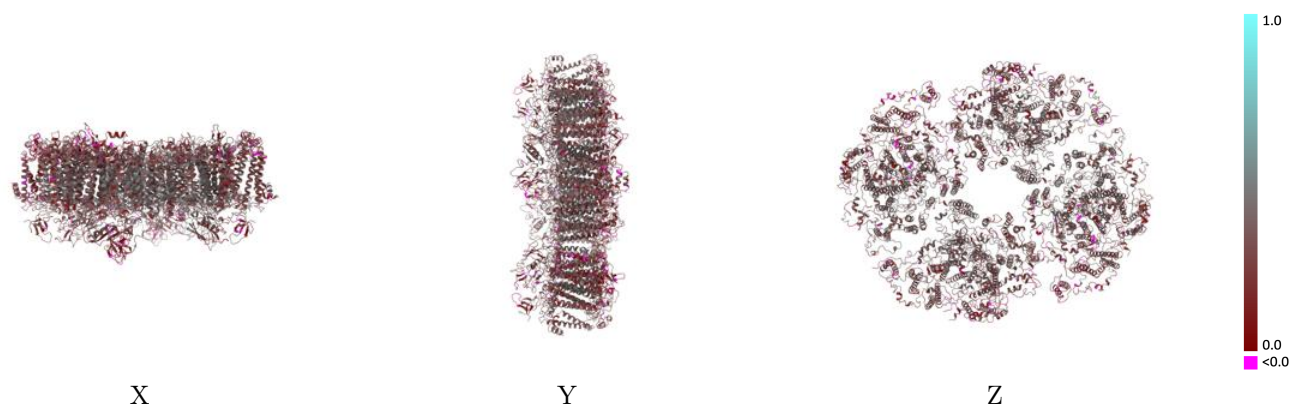
This section contains information regarding the fit between EMDB map EMD-13898 and PDB model 7QCO. Per-residue inclusion information can be found in section [3](#) on page [42](#).

9.1 Map-model overlay [i](#)



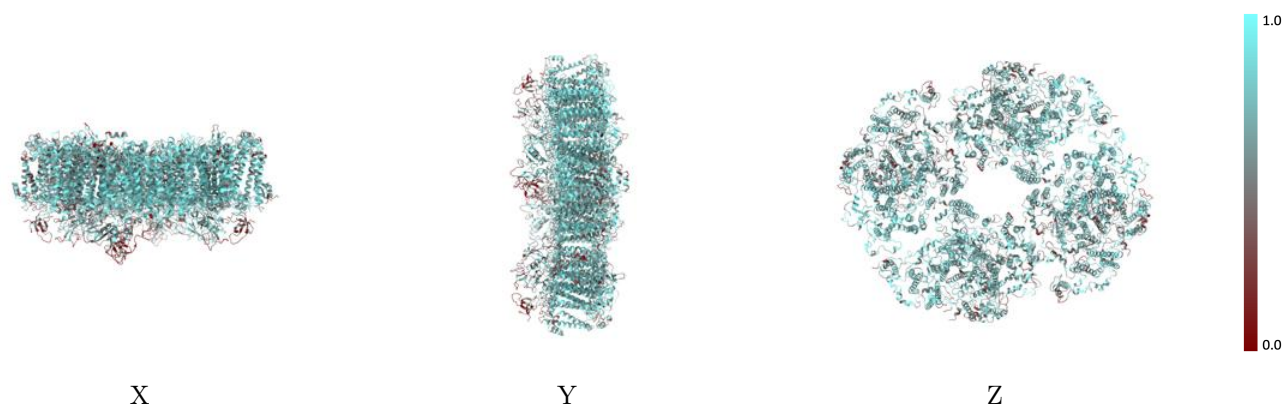
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



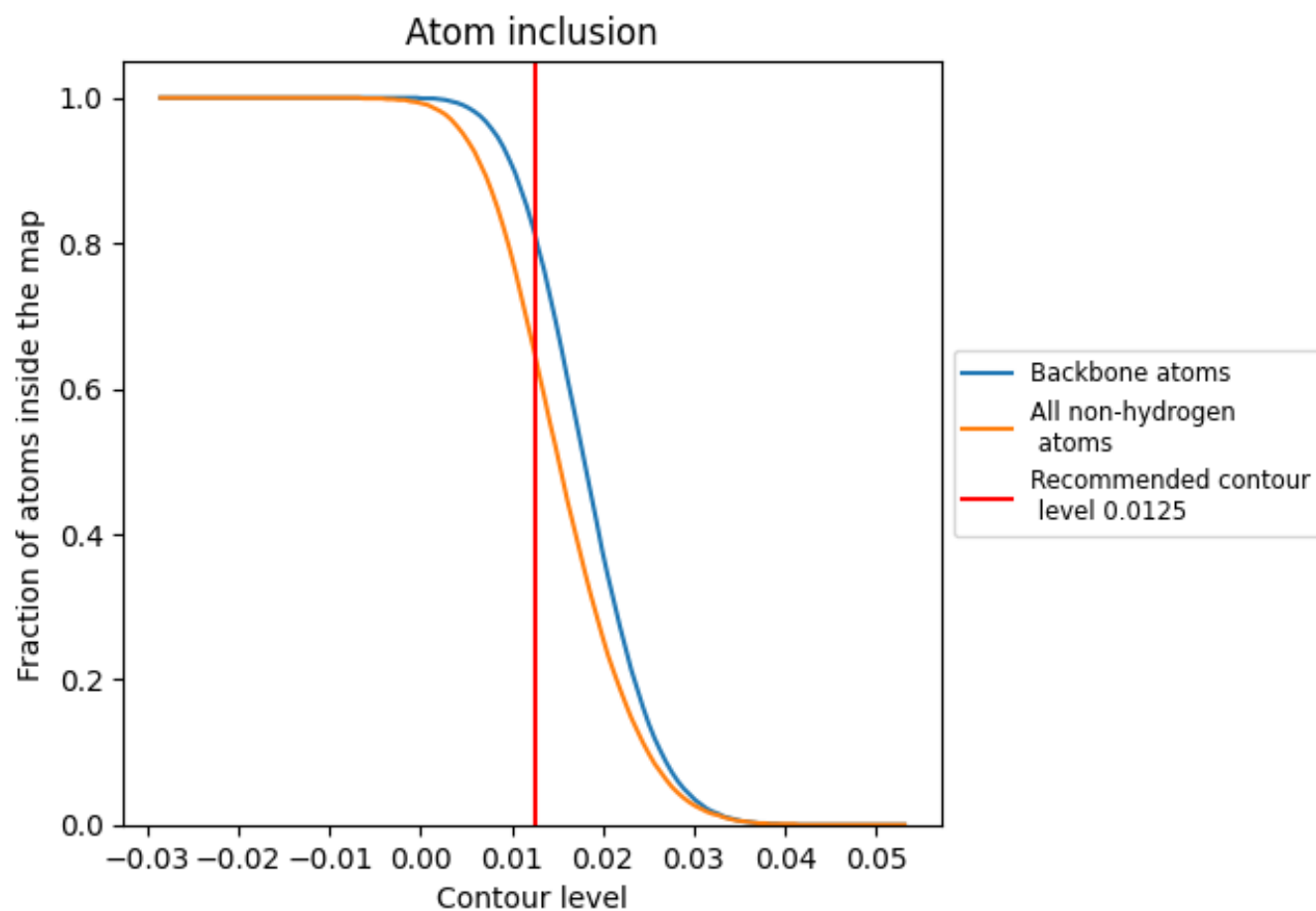
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0125).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 82% of all backbone atoms, 65% 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 (0.0125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6500	 0.3260
A	 0.7060	 0.3530
B	 0.6540	 0.3250
C	 0.6330	 0.2920
D	 0.5610	 0.3410
E	 0.6410	 0.2980
F	 0.6020	 0.2680
G	 0.7410	 0.3840
H	 0.6010	 0.2430
I	 0.5870	 0.3220
J	 0.4660	 0.2660
K	 0.6510	 0.2800
L	 0.7000	 0.3730
M	 0.5400	 0.2970
N	 0.4420	 0.3070
O	 0.5780	 0.3140
P	 0.6930	 0.3780
Q	 0.4970	 0.3000
R	 0.4300	 0.1660
S	 0.5970	 0.3020
T	 0.6760	 0.3850
V	 0.3020	 0.1980
W	 0.2600	 0.1520
a	 0.6340	 0.2930
b	 0.7440	 0.3820
c	 0.6000	 0.2430
d	 0.4280	 0.3040
e	 0.7080	 0.3510
f	 0.5790	 0.3130
g	 0.6580	 0.3250
h	 0.6160	 0.2860
i	 0.6870	 0.3730
j	 0.5170	 0.3010
k	 0.4300	 0.1650
l	 0.5960	 0.3030



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Chain	Atom inclusion	Q-score
m	 0.6650	 0.3820
n	 0.5660	 0.3430
o	 0.6020	 0.2660
p	 0.5720	 0.3100
q	 0.4690	 0.2620
r	 0.6460	 0.2780
s	 0.6880	 0.3610
t	 0.5530	 0.3010
v	 0.3650	 0.2490
w	 0.2600	 0.1690