



wwPDB EM Validation Summary Report ⓘ

Sep 8, 2026 – 04:29 am BST

PDB ID : 7QCO / pdb_00007qco
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.; Kastiris, 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.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

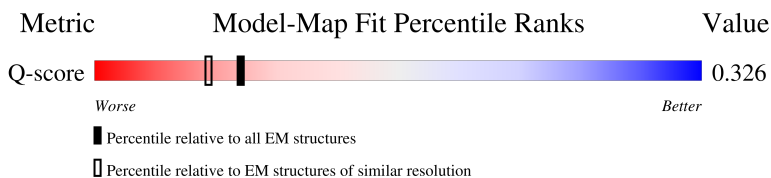
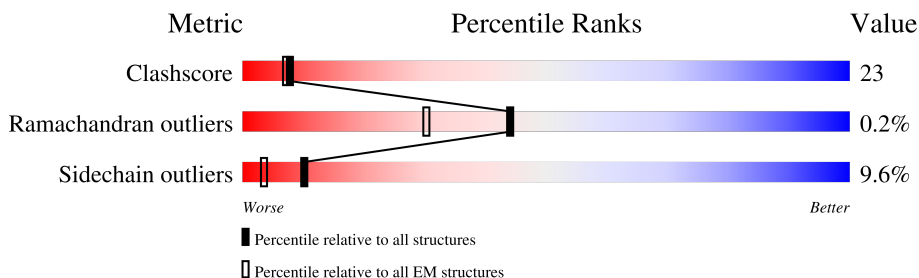
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11569 (3.20 - 4.20)

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	6% 48% 45% • •
1	E	752	13% 49% 44% • •
1	a	752	13% 48% 46% • •

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Validation Pipeline (wwPDB-VP) : 2.50

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

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Mol	Chain	Length	Quality of chain
8	J	49	
8	Q	49	
8	j	49	
8	q	49	
9	K	93	
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	852	-	-	X	-
15	BCR	E	849	-	-	X	-
15	BCR	R	101	-	-	X	-
15	BCR	a	848	-	-	X	-
15	BCR	a	849	-	-	X	-
15	BCR	k	4001	-	-	X	-
16	SF4	C	101	-	-	X	-
16	SF4	C	102	-	-	X	-
16	SF4	H	101	-	-	X	-
16	SF4	H	102	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
16	SF4	c	101	-	-	X	-
16	SF4	c	102	-	-	X	-
16	SF4	h	101	-	-	X	-
16	SF4	h	102	-	-	X	-

2 Entry composition [i](#)

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		

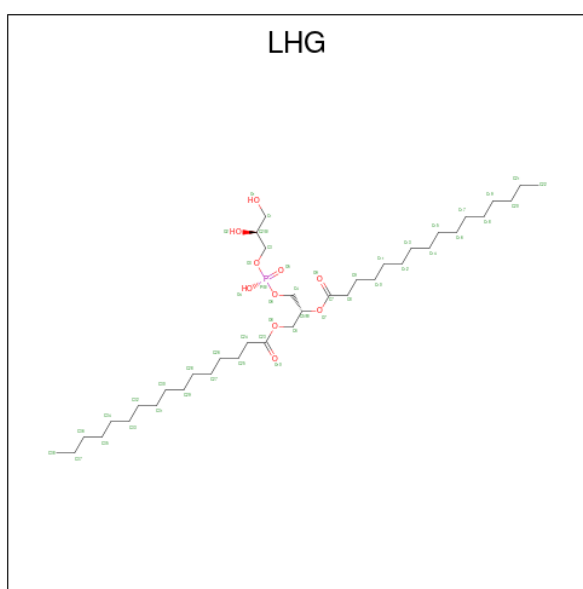
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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 (CCD ID: 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 (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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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 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 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 45	C 35	Mg 1	N 4	O 5	0
13	E	1	Total 49	C 39	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 49	C 39	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
			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 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
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 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 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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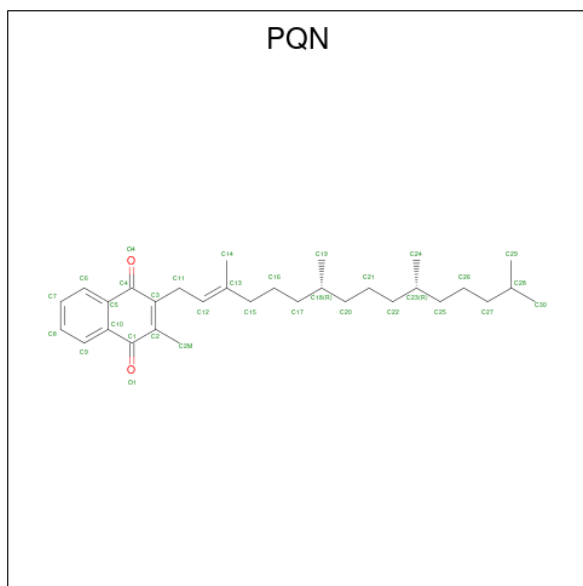
Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 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 (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



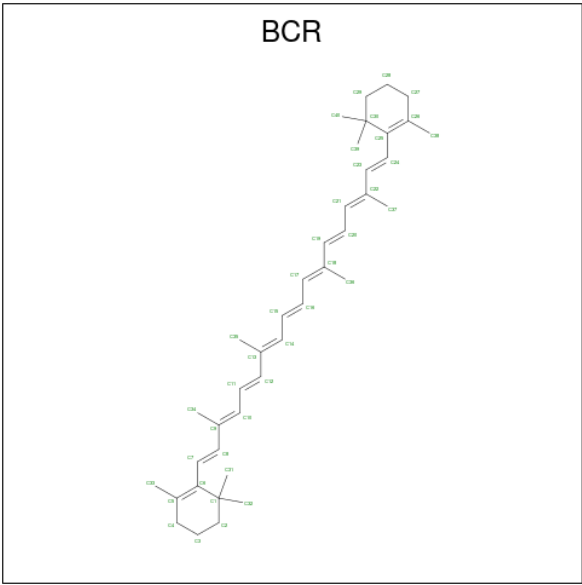
Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	

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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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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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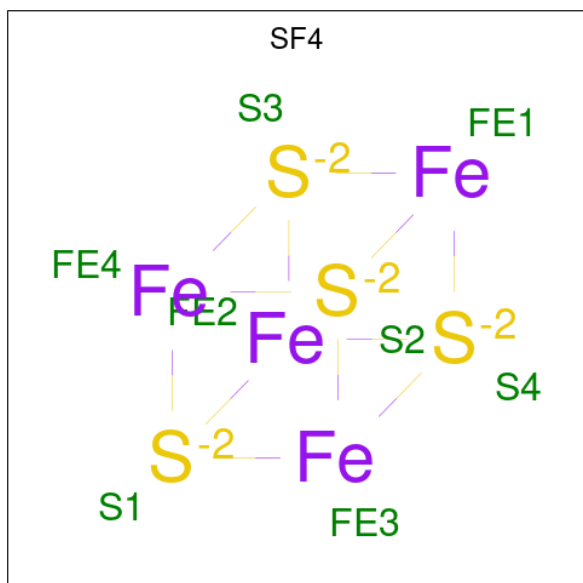
Mol	Chain	Residues	Atoms	AltConf
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	g	1	Total C 40 40	0
15	o	1	Total C 40 40	0
15	p	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	q	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	s	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 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 (CCD ID: SF4) (formula: Fe₄S₄).



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

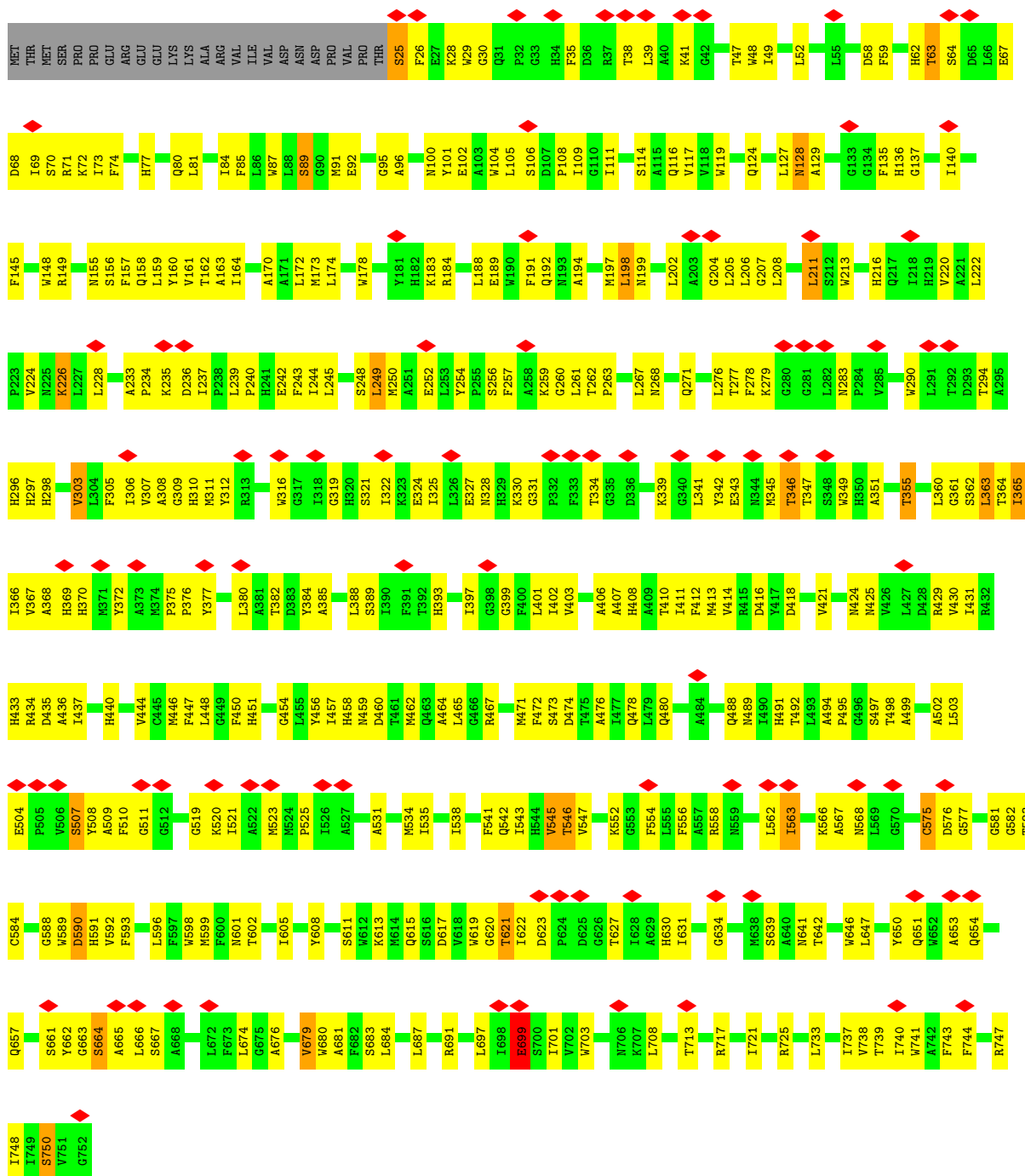
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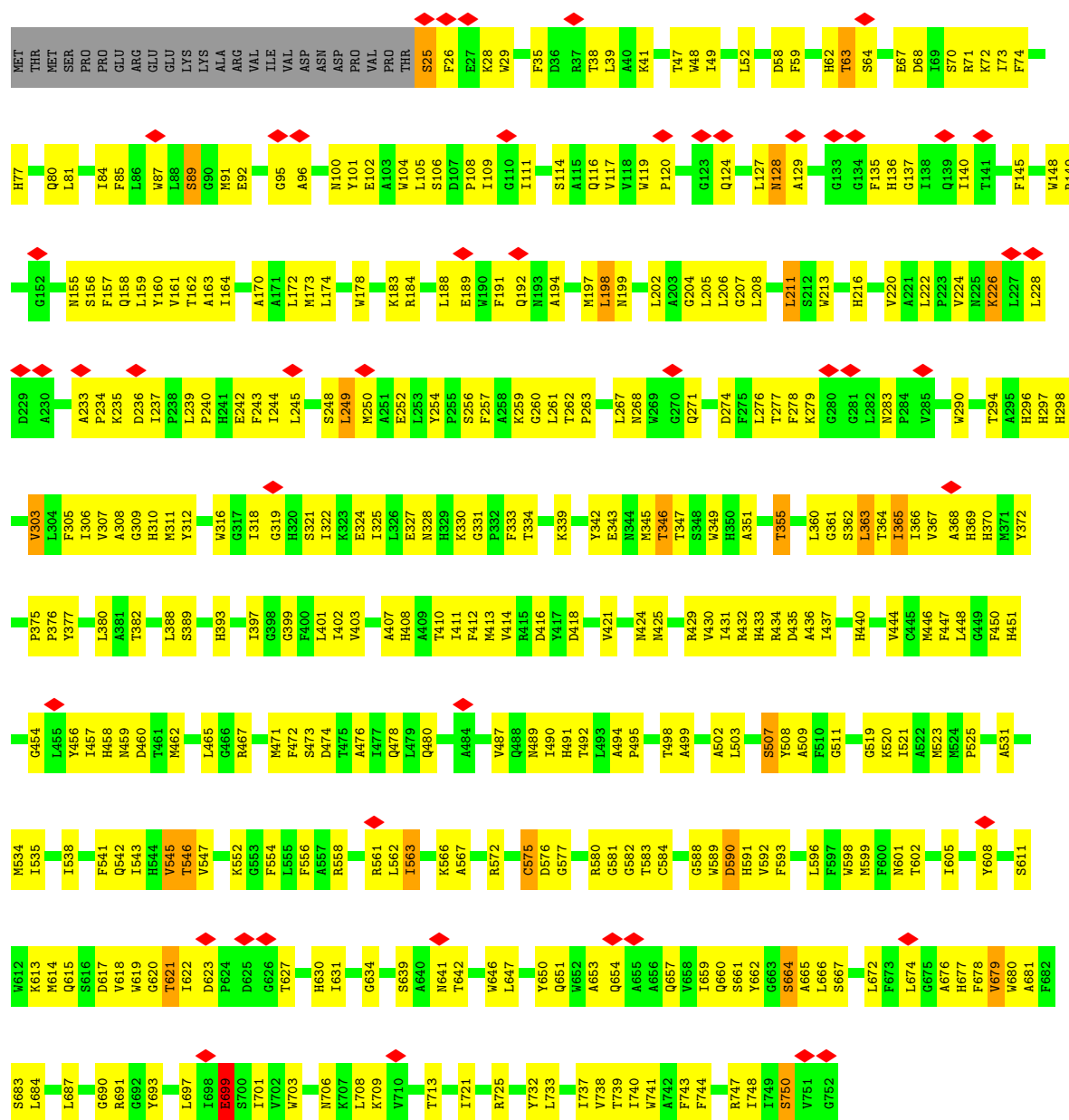
Mol	Chain	Residues	Atoms			AltConf
16	C	1	Total 8	Fe 4	S 4	0
16	C	1	Total 8	Fe 4	S 4	0
16	E	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	H	1	Total 8	Fe 4	S 4	0
16	g	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	h	1	Total 8	Fe 4	S 4	0
16	a	1	Total 8	Fe 4	S 4	0
16	c	1	Total 8	Fe 4	S 4	0
16	c	1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



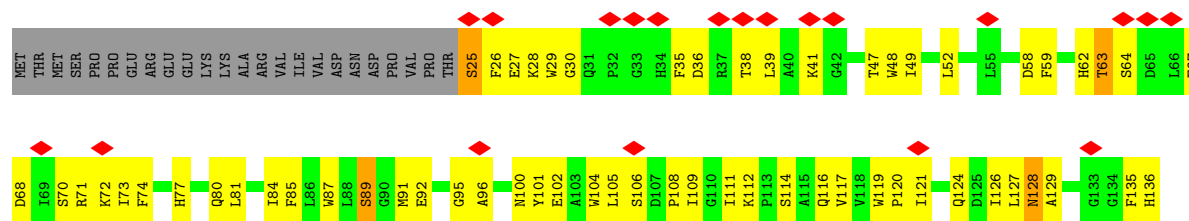
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

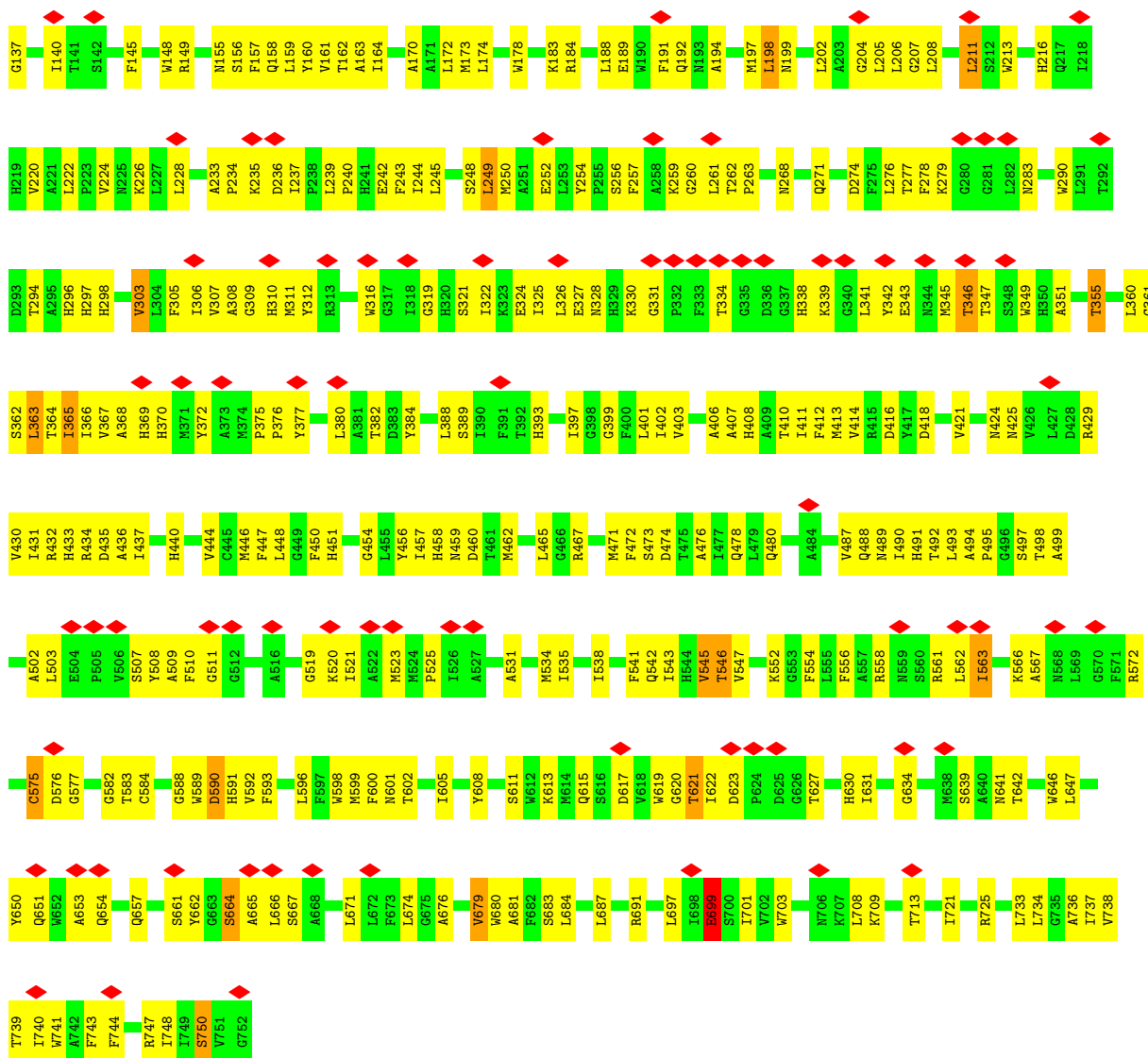


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

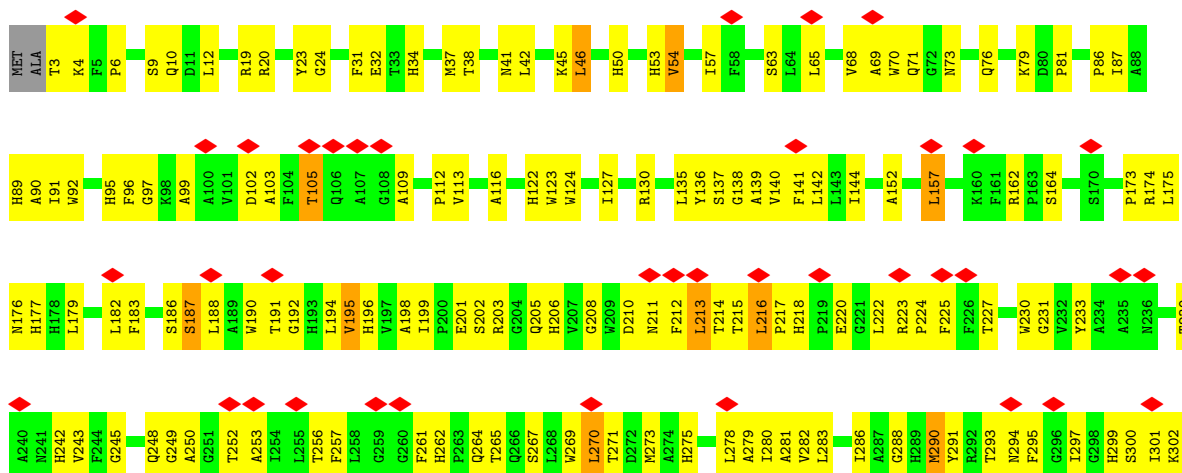


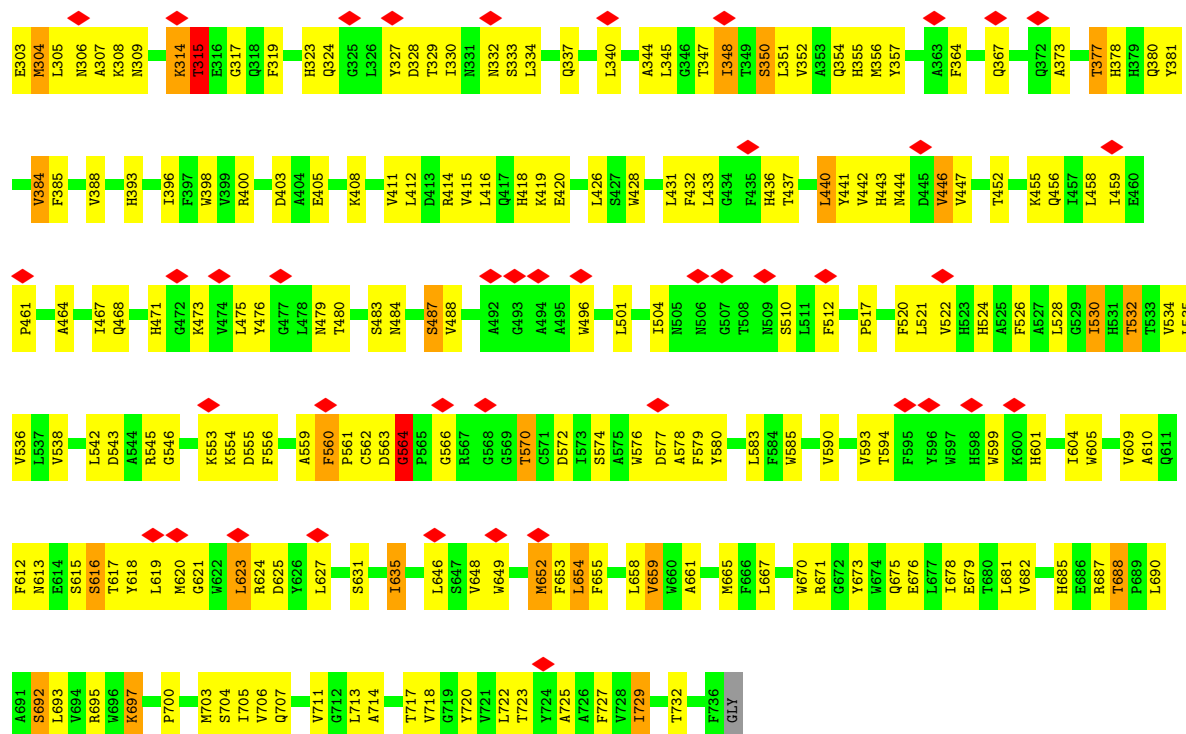
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



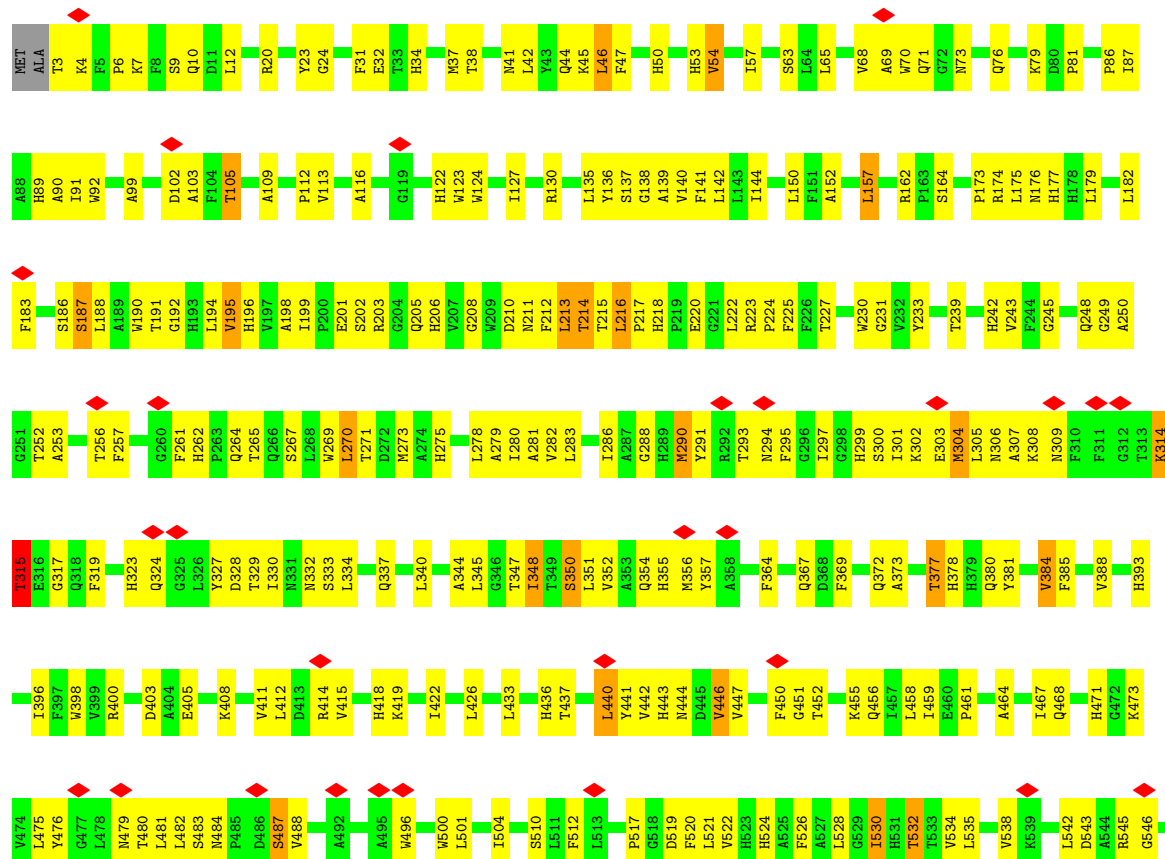


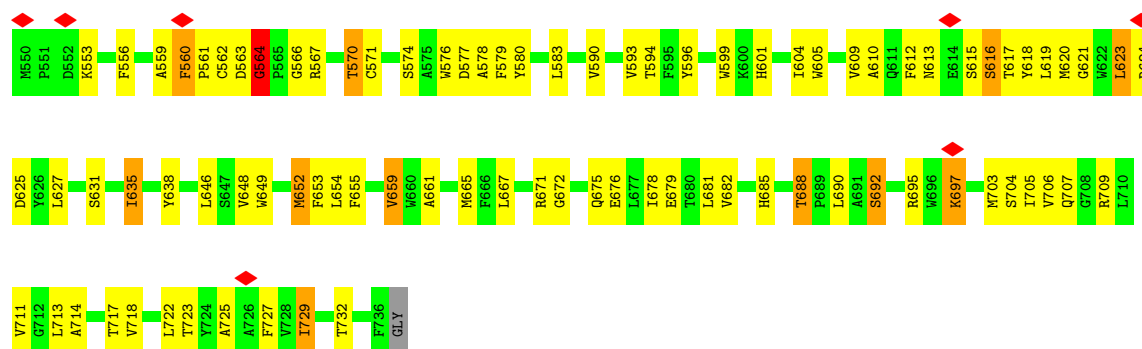
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



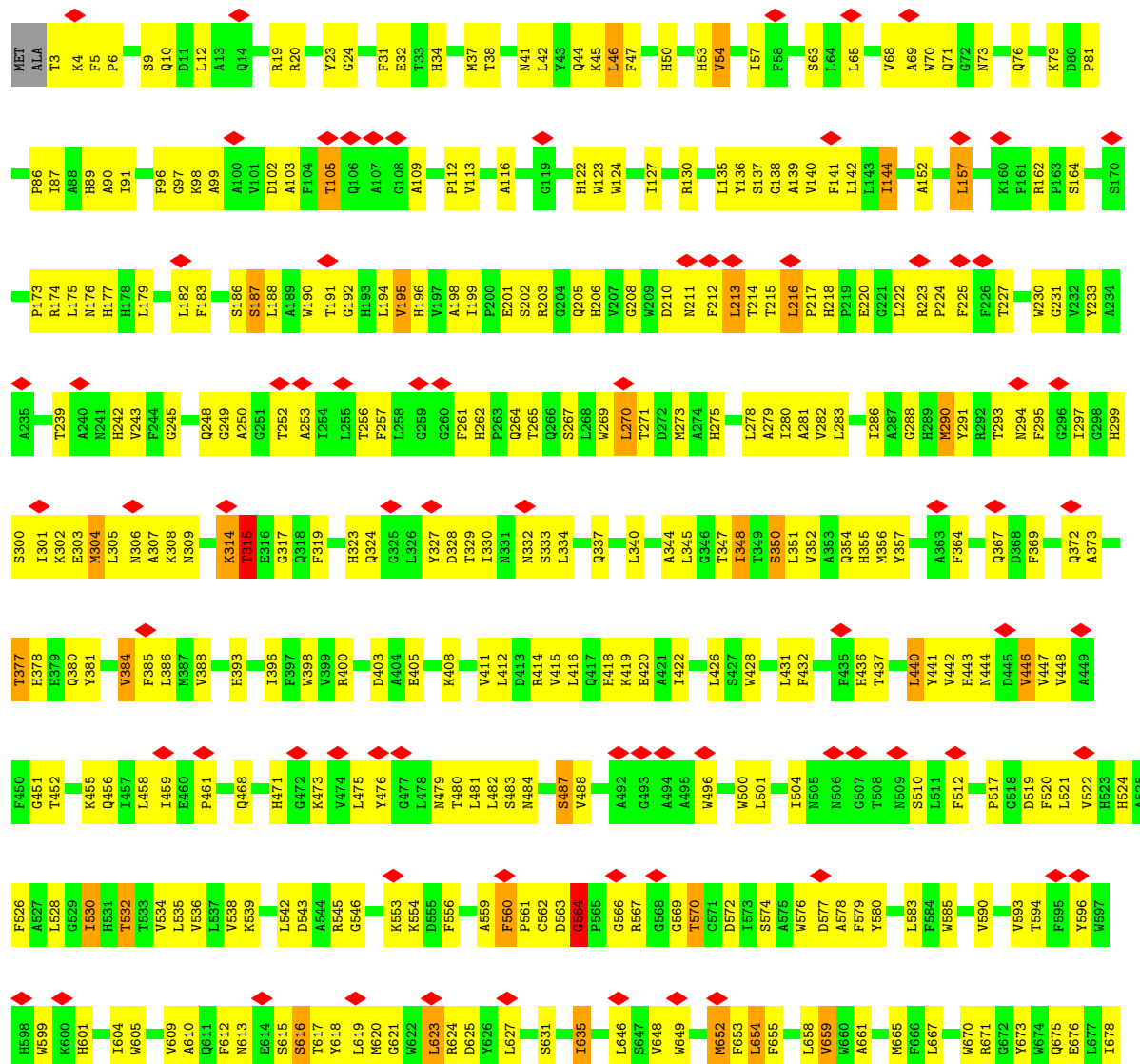


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



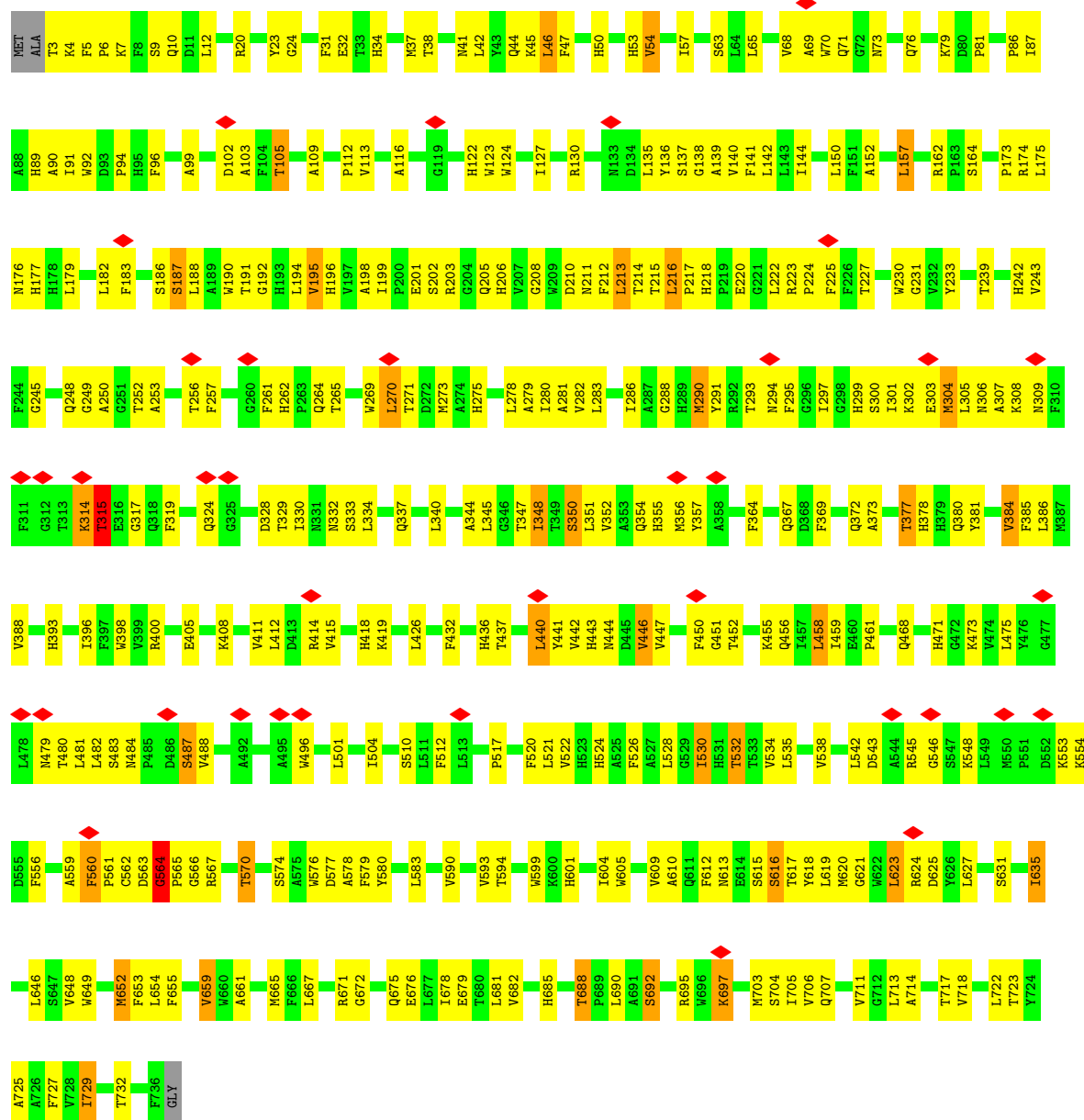


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

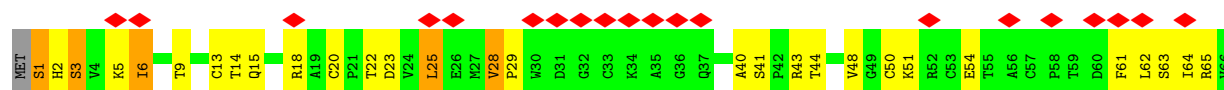


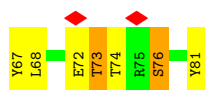


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

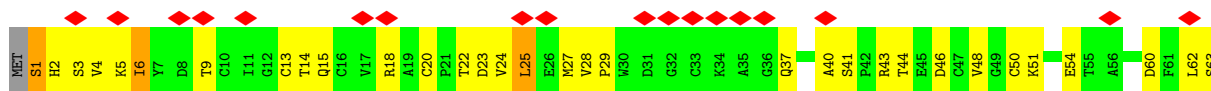


• Molecule 3: Photosystem I iron-sulfur center

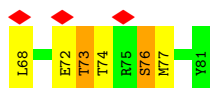
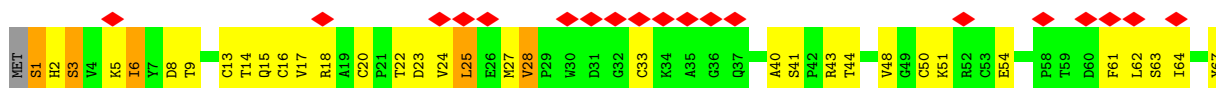




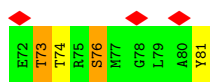
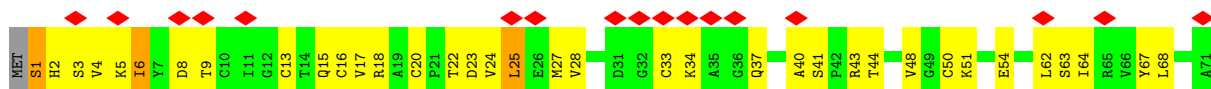
• Molecule 3: Photosystem I iron-sulfur center



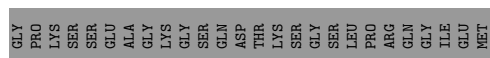
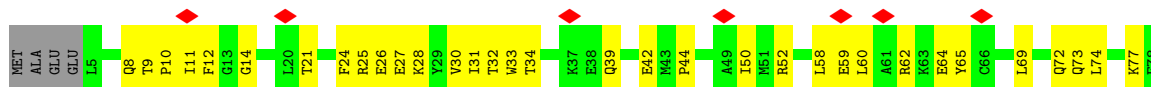
• Molecule 3: Photosystem I iron-sulfur center



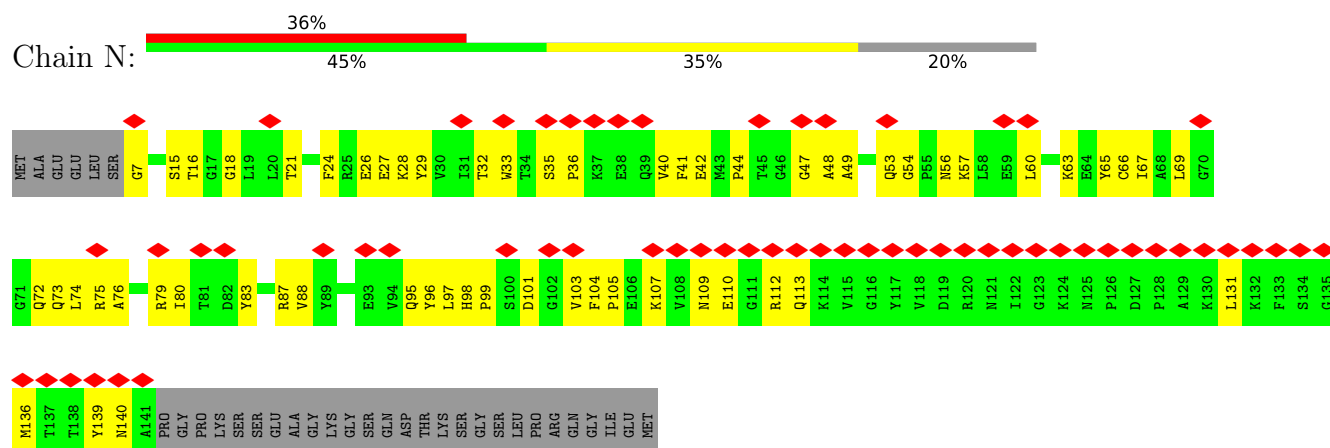
• Molecule 3: Photosystem I iron-sulfur center



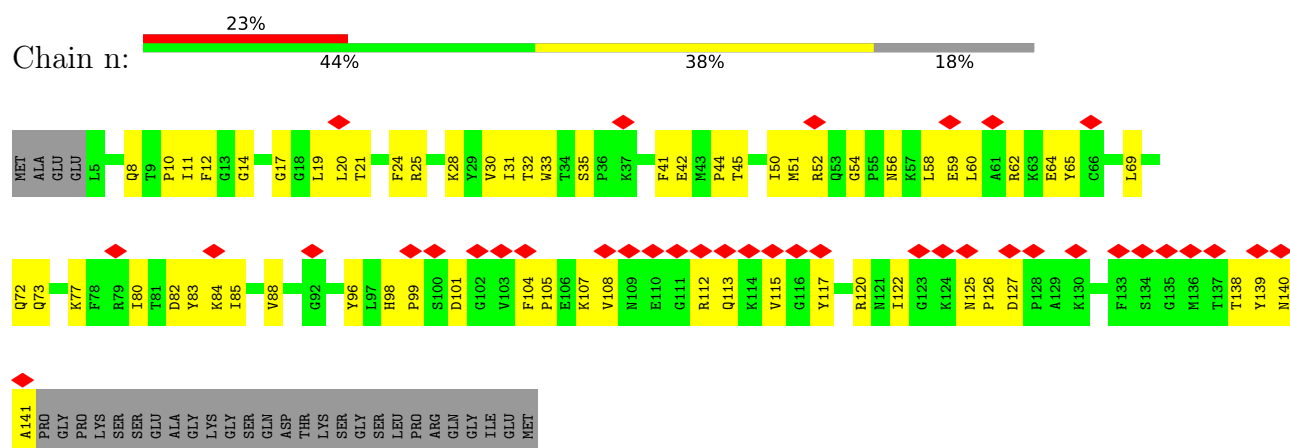
• Molecule 4: Photosystem I reaction center subunit II



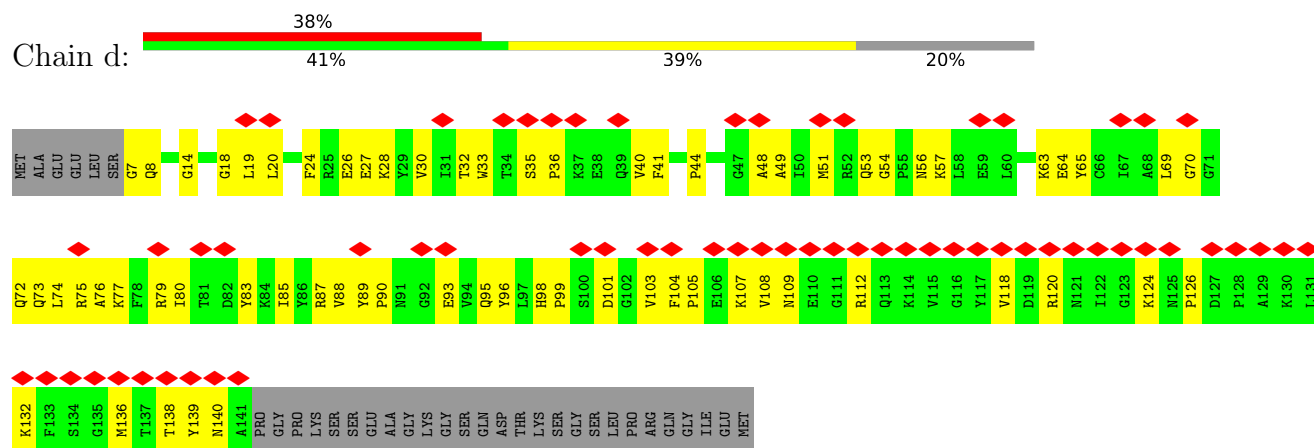
- Molecule 4: Photosystem I reaction center subunit II



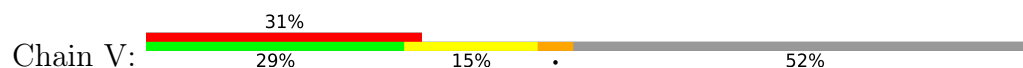
- Molecule 4: Photosystem I reaction center subunit II

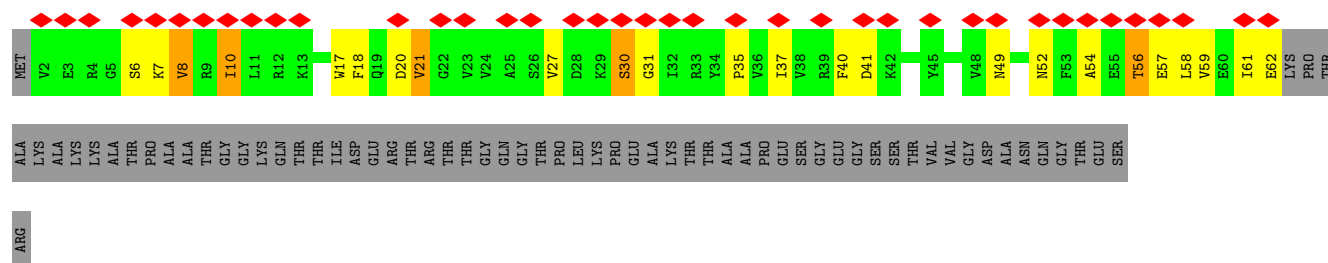


- Molecule 4: Photosystem I reaction center subunit II

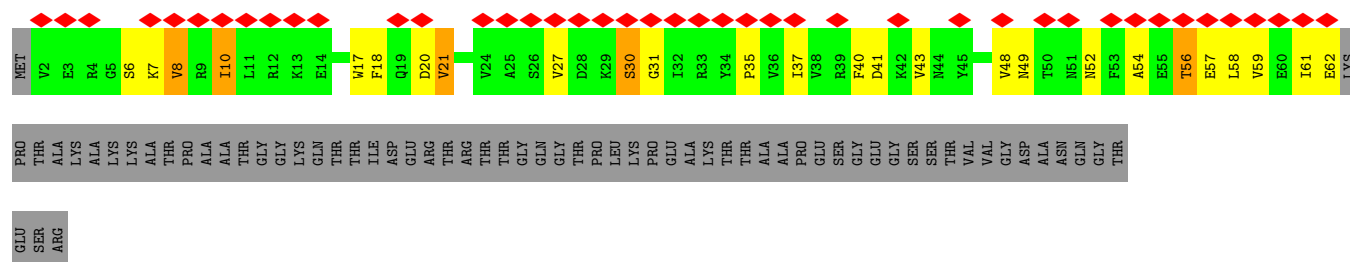
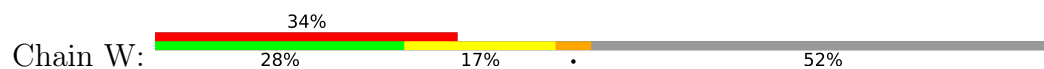


- Molecule 5: Photosystem I reaction center subunit IV

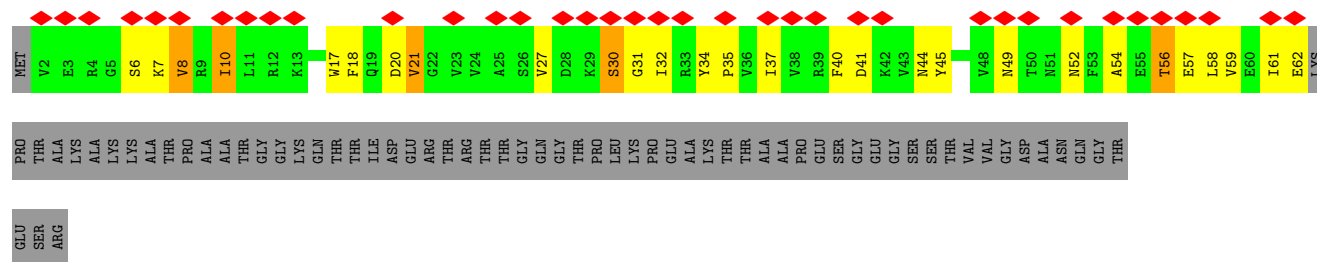




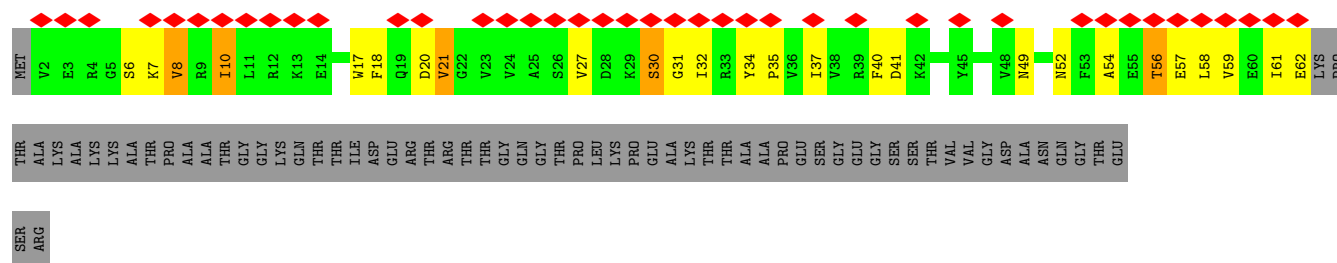
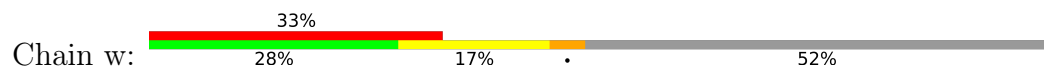
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV

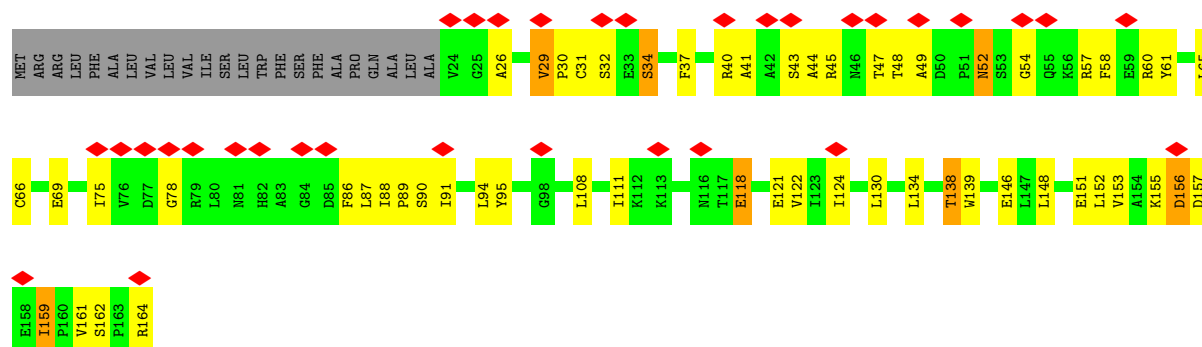


- Molecule 5: Photosystem I reaction center subunit IV

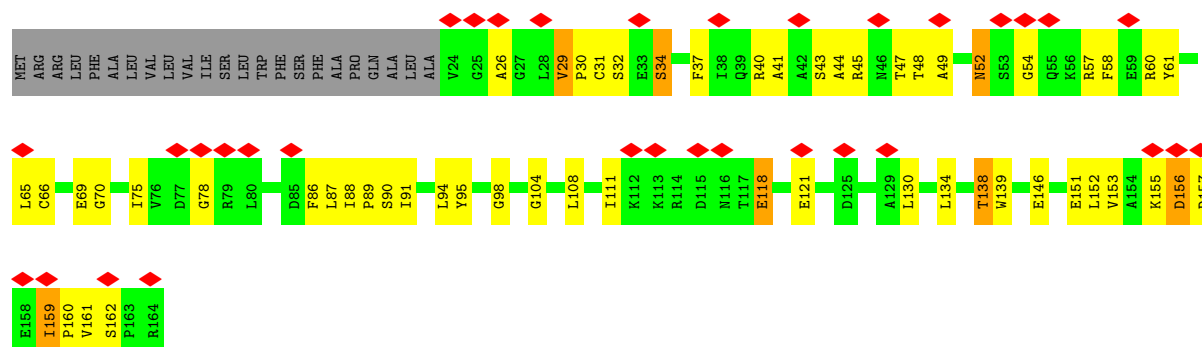


- Molecule 6: Photosystem I reaction center subunit III

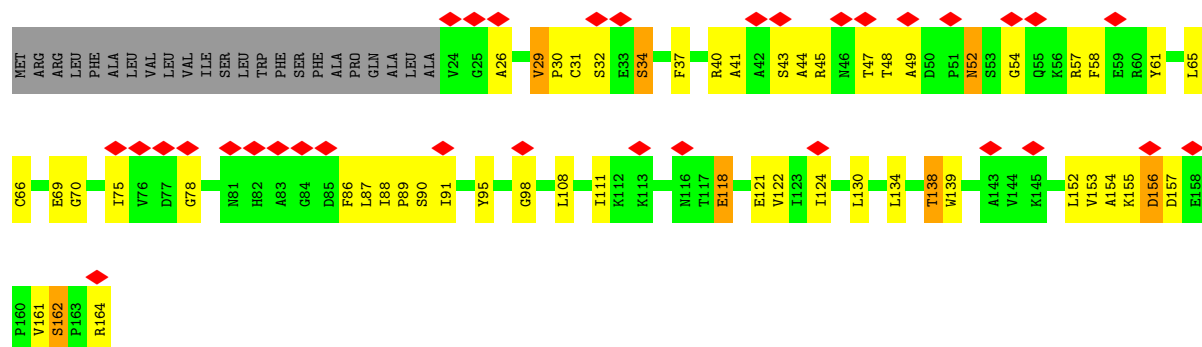




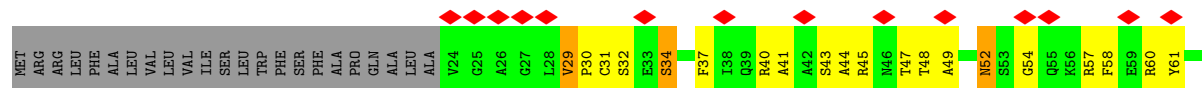
• Molecule 6: Photosystem I reaction center subunit III

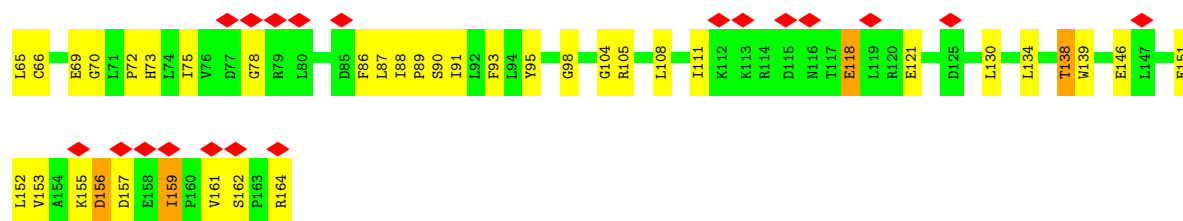


• Molecule 6: Photosystem I reaction center subunit III

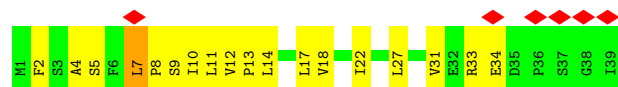


• Molecule 6: Photosystem I reaction center subunit III





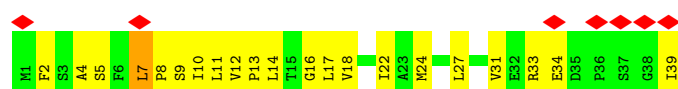
• Molecule 7: Photosystem I reaction center subunit VIII



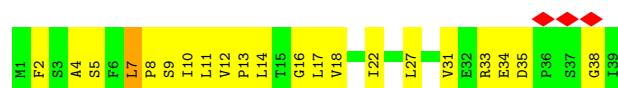
• Molecule 7: Photosystem I reaction center subunit VIII



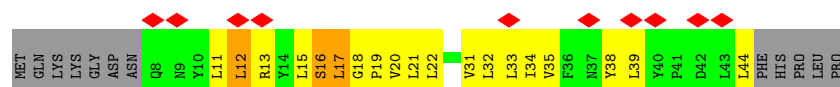
• Molecule 7: Photosystem I reaction center subunit VIII



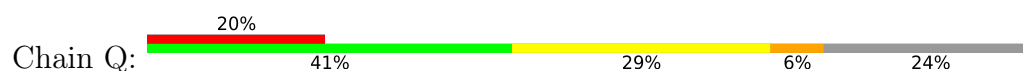
• Molecule 7: Photosystem I reaction center subunit VIII

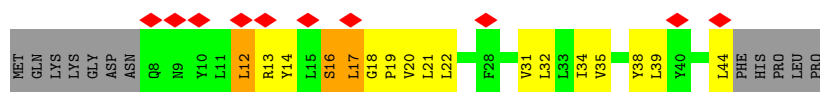


• Molecule 8: Photosystem I reaction center subunit IX

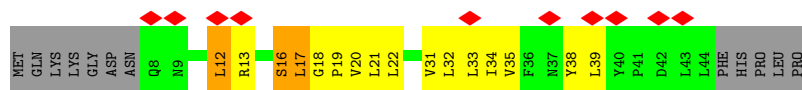
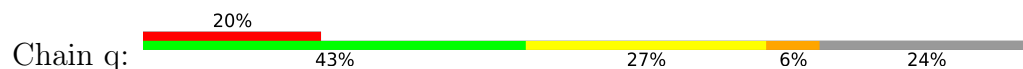


• Molecule 8: Photosystem I reaction center subunit IX

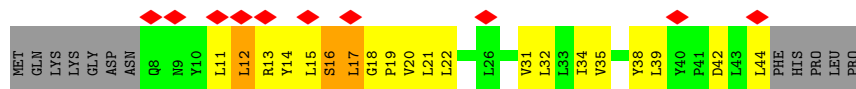




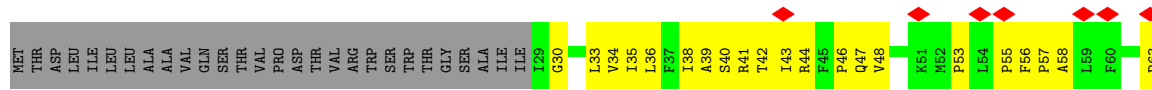
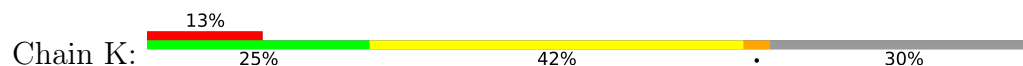
• Molecule 8: Photosystem I reaction center subunit IX



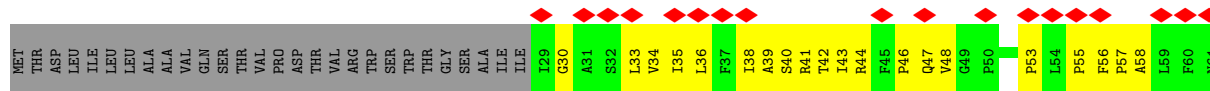
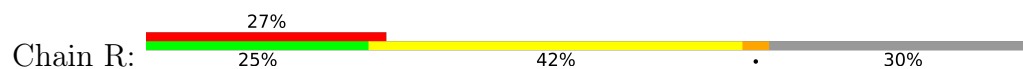
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit Psak

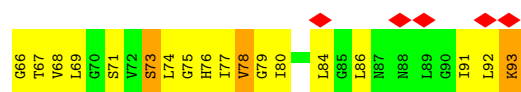


• Molecule 9: Photosystem I reaction center subunit Psak

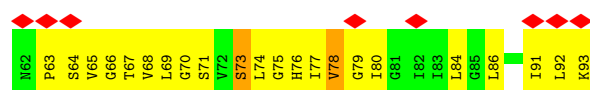
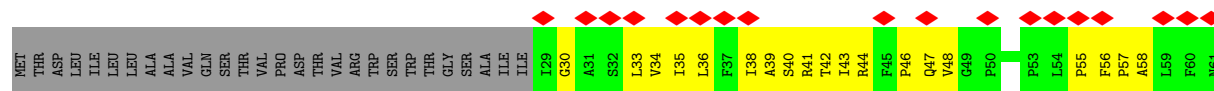


• Molecule 9: Photosystem I reaction center subunit Psak

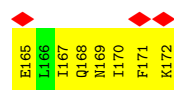
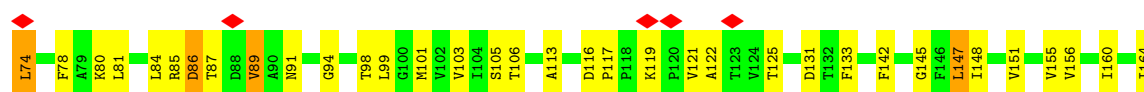




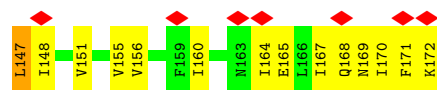
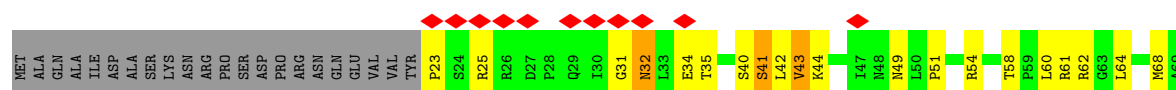
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 10: Photosystem I reaction center subunit XI

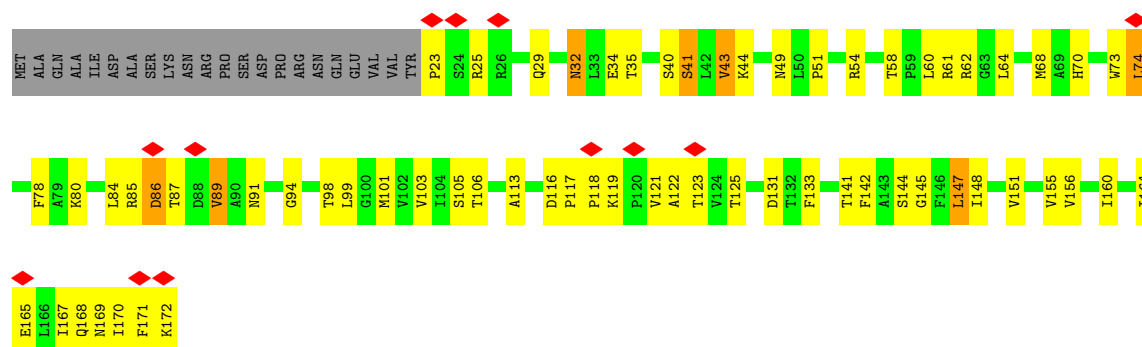


• Molecule 10: Photosystem I reaction center subunit XI

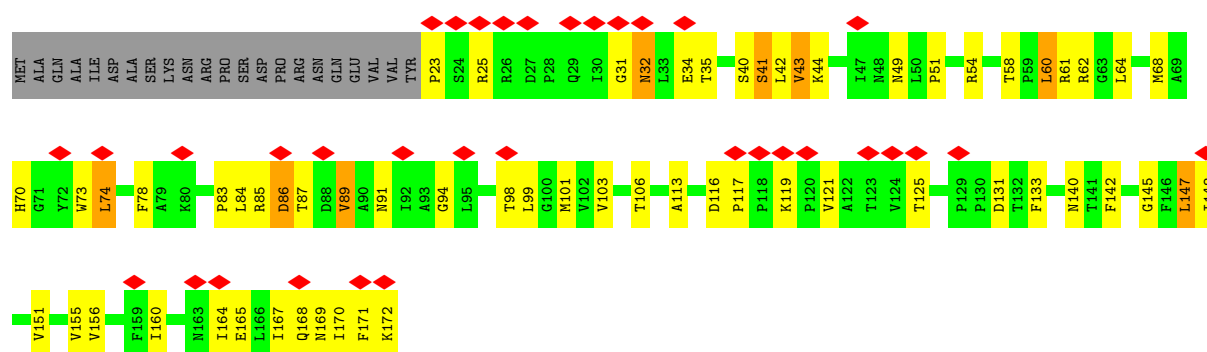


• Molecule 10: Photosystem I reaction center subunit XI





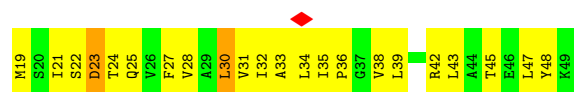
• Molecule 10: Photosystem I reaction center subunit XI



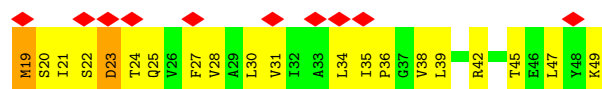
• Molecule 11: Photosystem I reaction center subunit XII



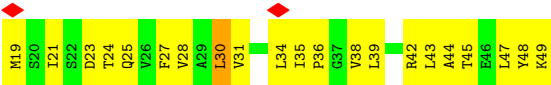
• Molecule 11: Photosystem I reaction center subunit XII



• 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.21	0/5908	0.46	1/8056 (0.0%)
1	E	0.21	0/5908	0.46	1/8056 (0.0%)
1	a	0.21	0/5908	0.46	1/8056 (0.0%)
1	e	0.21	0/5908	0.46	1/8056 (0.0%)
2	B	0.20	0/6072	0.45	0/8301
2	G	0.20	0/6072	0.45	0/8301
2	b	0.20	0/6072	0.45	0/8301
2	g	0.20	0/6072	0.45	0/8301
3	C	0.18	0/615	0.42	0/833
3	H	0.18	0/615	0.42	0/833
3	c	0.18	0/615	0.42	0/833
3	h	0.18	0/615	0.42	0/833
4	D	0.17	0/1105	0.42	0/1489
4	N	0.18	0/1091	0.45	0/1470
4	d	0.18	0/1091	0.46	0/1470
4	n	0.18	0/1105	0.40	0/1489
5	V	0.19	0/502	0.51	0/678
5	W	0.19	0/502	0.51	0/678
5	v	0.19	0/502	0.52	0/678
5	w	0.19	0/502	0.51	0/678
6	F	0.20	0/1119	0.45	0/1522
6	O	0.20	0/1119	0.45	0/1522
6	f	0.20	0/1119	0.45	0/1522
6	o	0.20	0/1119	0.45	0/1522
7	I	0.21	0/302	0.54	0/411
7	P	0.21	0/302	0.54	0/411
7	i	0.21	0/302	0.54	0/411
7	p	0.21	0/302	0.54	0/411
8	J	0.18	0/321	0.44	0/441
8	Q	0.18	0/321	0.43	0/441
8	j	0.18	0/321	0.44	0/441
8	q	0.18	0/321	0.43	0/441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	K	0.21	0/484	0.63	0/659
9	R	0.21	0/484	0.63	0/659
9	k	0.21	0/484	0.63	0/659
9	r	0.21	0/484	0.63	0/659
10	L	0.21	0/1165	0.49	0/1597
10	S	0.21	0/1165	0.49	0/1597
10	l	0.21	0/1165	0.49	0/1597
10	s	0.21	0/1165	0.49	0/1597
11	M	0.24	0/241	0.58	0/326
11	T	0.24	0/241	0.58	0/326
11	m	0.24	0/241	0.58	0/326
11	t	0.24	0/241	0.58	0/326
All	All	0.20	0/71308	0.46	4/97214 (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.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	699	GLU	CA-CB-CG	6.37	126.85	114.10
1	a	699	GLU	CA-CB-CG	6.37	126.83	114.10
1	A	699	GLU	CA-CB-CG	6.36	126.83	114.10
1	E	699	GLU	CA-CB-CG	6.36	126.83	114.10

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5713	0	5565	290	0
1	E	5713	0	5565	285	0
1	a	5713	0	5565	346	0
1	e	5713	0	5565	304	0
2	B	5857	0	5642	293	0
2	G	5857	0	5642	280	0
2	b	5857	0	5642	275	0
2	g	5857	0	5642	309	0
3	C	605	0	590	33	0
3	H	605	0	590	30	0
3	c	605	0	590	38	0
3	h	605	0	590	36	0
4	D	1080	0	1083	58	0
4	N	1066	0	1067	51	0
4	d	1066	0	1067	65	0
4	n	1080	0	1083	58	0
5	V	494	0	493	16	0
5	W	494	0	493	18	0
5	v	494	0	493	22	0
5	w	494	0	493	18	0
6	F	1093	0	1095	38	0
6	O	1093	0	1095	39	0
6	f	1093	0	1095	43	0
6	o	1093	0	1095	39	0
7	I	295	0	314	13	0
7	P	295	0	314	17	0
7	i	295	0	314	21	0
7	p	295	0	314	15	0
8	J	311	0	323	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	Q	311	0	323	12	0
8	j	311	0	323	17	0
8	q	311	0	323	15	0
9	K	474	0	521	29	0
9	R	474	0	521	40	0
9	k	474	0	521	34	0
9	r	474	0	521	29	0
10	L	1134	0	1151	54	0
10	S	1134	0	1151	46	0
10	l	1134	0	1151	44	0
10	s	1134	0	1151	63	0
11	M	238	0	257	10	0
11	T	238	0	257	15	0
11	m	238	0	257	17	0
11	t	238	0	257	11	0
12	A	87	0	123	5	0
12	a	49	0	74	3	0
12	e	87	0	123	5	0
13	A	2175	0	1688	122	0
13	B	1954	0	1504	99	0
13	E	2166	0	1678	121	0
13	F	45	0	33	2	0
13	G	1999	0	1537	105	0
13	K	86	0	62	4	0
13	L	145	0	111	12	0
13	O	45	0	33	1	0
13	R	45	0	33	2	0
13	S	135	0	99	10	0
13	a	2125	0	1649	183	0
13	b	1940	0	1488	106	0
13	e	2125	0	1649	117	0
13	f	45	0	33	0	0
13	g	2004	0	1543	98	0
13	k	45	0	33	2	0
13	l	190	0	144	12	0
13	o	45	0	33	2	0
13	r	86	0	62	3	0
13	s	145	0	111	24	0
14	A	33	0	46	10	0
14	B	33	0	46	2	0
14	E	33	0	46	4	0
14	G	33	0	46	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	a	33	0	46	2	0
14	b	33	0	46	1	0
14	e	33	0	46	1	0
14	g	33	0	46	2	0
15	A	240	0	336	31	0
15	B	240	0	336	10	0
15	E	240	0	336	47	0
15	F	40	0	56	6	0
15	G	240	0	336	16	0
15	I	40	0	56	0	0
15	J	80	0	112	2	0
15	L	80	0	112	6	0
15	O	80	0	112	9	0
15	P	40	0	56	0	0
15	Q	40	0	56	0	0
15	R	40	0	56	37	0
15	S	120	0	168	10	0
15	T	40	0	56	3	0
15	a	280	0	392	86	0
15	b	240	0	336	15	0
15	e	240	0	336	32	0
15	f	80	0	112	8	0
15	g	240	0	336	13	0
15	i	40	0	56	3	0
15	j	40	0	56	4	0
15	k	40	0	56	33	0
15	l	80	0	112	6	0
15	m	40	0	56	6	0
15	o	40	0	56	3	0
15	p	40	0	56	1	0
15	q	80	0	112	1	0
15	s	80	0	112	6	0
16	B	8	0	0	1	0
16	C	16	0	0	4	0
16	E	8	0	0	1	0
16	H	16	0	0	4	0
16	a	8	0	0	1	0
16	c	16	0	0	4	0
16	g	8	0	0	1	0
16	h	16	0	0	4	0
All	All	90396	0	86683	4001	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 23.

The worst 5 of 4001 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:680:TRP:CE3	13:a:852:CLA:HHB	1.40	1.54
1:a:680:TRP:CZ3	13:a:852:CLA:HHB	1.50	1.41
1:a:680:TRP:CZ3	13:a:852:CLA:HMB1	1.55	1.41
1:a:680:TRP:CE2	13:a:852:CLA:H3A	1.65	1.31
10:L:80:LYS:HD3	13:L:204:CLA:C5	1.61	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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	60
2	G	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	60
2	b	732/737 (99%)	644 (88%)	85 (12%)	3 (0%)	30	60
2	g	732/737 (99%)	642 (88%)	87 (12%)	3 (0%)	30	60
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	N	133/168 (79%)	113 (85%)	20 (15%)	0	100	100
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	25
11	T	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	25
11	m	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	25
11	t	29/31 (94%)	19 (66%)	9 (31%)	1 (3%)	3	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	8724/9652 (90%)	7499 (86%)	1209 (14%)	16 (0%)	44 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%)	531 (92%)	47 (8%)	11 36
1	E	578/601 (96%)	531 (92%)	47 (8%)	11 36
1	a	578/601 (96%)	531 (92%)	47 (8%)	11 36
1	e	578/601 (96%)	531 (92%)	47 (8%)	11 36
2	B	594/595 (100%)	535 (90%)	59 (10%)	7 30
2	G	594/595 (100%)	535 (90%)	59 (10%)	7 30
2	b	594/595 (100%)	535 (90%)	59 (10%)	7 30
2	g	594/595 (100%)	535 (90%)	59 (10%)	7 30
3	C	68/70 (97%)	59 (87%)	9 (13%)	4 20
3	H	68/70 (97%)	59 (87%)	9 (13%)	4 20
3	c	68/70 (97%)	59 (87%)	9 (13%)	4 20
3	h	68/70 (97%)	59 (87%)	9 (13%)	4 20
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	V	54/102 (53%)	47 (87%)	7 (13%)	4	20
5	W	54/102 (53%)	47 (87%)	7 (13%)	4	20
5	v	54/102 (53%)	47 (87%)	7 (13%)	4	20
5	w	54/102 (53%)	47 (87%)	7 (13%)	4	20
6	F	116/135 (86%)	103 (89%)	13 (11%)	6	25
6	O	116/135 (86%)	103 (89%)	13 (11%)	6	25
6	f	116/135 (86%)	103 (89%)	13 (11%)	6	25
6	o	116/135 (86%)	103 (89%)	13 (11%)	6	25
7	I	33/33 (100%)	30 (91%)	3 (9%)	9	33
7	P	33/33 (100%)	30 (91%)	3 (9%)	9	33
7	i	33/33 (100%)	30 (91%)	3 (9%)	9	33
7	p	33/33 (100%)	30 (91%)	3 (9%)	9	33
8	J	34/45 (76%)	27 (79%)	7 (21%)	1	8
8	Q	34/45 (76%)	27 (79%)	7 (21%)	1	8
8	j	34/45 (76%)	27 (79%)	7 (21%)	1	8
8	q	34/45 (76%)	27 (79%)	7 (21%)	1	8
9	K	53/77 (69%)	44 (83%)	9 (17%)	2	13
9	R	53/77 (69%)	44 (83%)	9 (17%)	2	13
9	k	53/77 (69%)	44 (83%)	9 (17%)	2	13
9	r	53/77 (69%)	44 (83%)	9 (17%)	2	13
10	L	121/140 (86%)	108 (89%)	13 (11%)	6	27
10	S	121/140 (86%)	108 (89%)	13 (11%)	6	27
10	l	121/140 (86%)	108 (89%)	13 (11%)	6	27
10	s	121/140 (86%)	108 (89%)	13 (11%)	6	27
11	M	26/26 (100%)	21 (81%)	5 (19%)	1	9
11	T	26/26 (100%)	21 (81%)	5 (19%)	1	9
11	m	26/26 (100%)	21 (81%)	5 (19%)	1	9
11	t	26/26 (100%)	21 (81%)	5 (19%)	1	9
All	All	7156/7844 (91%)	6468 (90%)	688 (10%)	10	31

5 of 688 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	v	30	SER
2	b	164	SER
6	o	156	ASP
5	v	21	VAL
1	a	89	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 201 such sidechains are listed below:

Mol	Chain	Res	Type
1	e	641	ASN
4	n	140	ASN
10	l	48	ASN
2	g	10	GLN
2	g	378	HIS

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	g	807	2	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	B	816	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	5 (8%)
16	SF4	H	101	-	0,12,12	-	-	-	-	-
13	CLA	e	829	-	54,58,73	1.42	10 (18%)	65,95,113	1.41	7 (10%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
13	CLA	e	815	1	54,58,73	1.41	8 (14%)	65,95,113	1.43	7 (10%)
13	CLA	b	814	-	54,58,73	1.42	9 (16%)	65,95,113	1.45	6 (9%)
15	BCR	q	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	G	841	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	B	835	-	49,53,73	1.51	9 (18%)	59,89,113	1.43	6 (10%)
13	CLA	a	819	1	53,57,73	1.42	9 (16%)	62,93,113	1.42	7 (11%)
13	CLA	S	206	-	49,53,73	1.48	10 (20%)	59,89,113	1.35	5 (8%)
13	CLA	b	821	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	8 (13%)
13	CLA	b	815	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	5 (8%)
13	CLA	A	803	-	54,58,73	1.41	8 (14%)	65,95,113	1.32	7 (10%)
13	CLA	G	830	2	54,58,73	1.38	9 (16%)	65,95,113	1.47	8 (12%)
13	CLA	l	203	10	54,58,73	1.40	8 (14%)	65,95,113	1.40	10 (15%)
13	CLA	g	830	-	54,58,73	1.40	10 (18%)	65,95,113	1.39	6 (9%)
14	PQN	a	847	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	b	806	2	54,58,73	1.40	9 (16%)	65,95,113	1.43	6 (9%)
13	CLA	a	811	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
13	CLA	e	837	1	49,53,73	1.47	9 (18%)	59,89,113	1.52	6 (10%)
15	BCR	f	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	7 (12%)
13	CLA	B	839	-	51,55,73	1.44	9 (17%)	61,91,113	1.48	5 (8%)
13	CLA	g	838	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
13	CLA	E	817	-	49,53,73	1.50	10 (20%)	59,89,113	1.41	4 (6%)
13	CLA	b	828	-	54,58,73	1.40	10 (18%)	65,95,113	1.38	6 (9%)
15	BCR	e	847	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	e	826	1	54,58,73	1.41	10 (18%)	65,95,113	1.40	8 (12%)
13	CLA	a	840	-	54,58,73	1.39	10 (18%)	65,95,113	1.47	9 (13%)
13	CLA	e	822	-	54,58,73	1.43	10 (18%)	65,95,113	1.32	6 (9%)
15	BCR	I	101	-	41,41,41	1.17	2 (4%)	56,56,56	1.18	2 (3%)
13	CLA	E	840	-	54,58,73	1.40	9 (16%)	65,95,113	1.47	9 (13%)
13	CLA	a	826	1	54,58,73	1.41	9 (16%)	65,95,113	1.41	8 (12%)
15	BCR	L	201	-	41,41,41	1.22	2 (4%)	56,56,56	1.13	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	g	821	-	54,58,73	1.41	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	G	819	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	5 (7%)
13	CLA	E	837	-	54,58,73	1.41	9 (16%)	65,95,113	1.36	7 (10%)
13	CLA	b	818	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	4 (6%)
15	BCR	i	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.18	3 (5%)
15	BCR	J	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	7 (12%)
16	SF4	B	803	-	0,12,12	-	-	-	-	-
13	CLA	b	839	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	6 (9%)
13	CLA	r	101	-	46,49,73	1.51	9 (19%)	55,83,113	1.42	5 (9%)
13	CLA	G	823	2	54,58,73	1.41	10 (18%)	65,95,113	1.45	6 (9%)
15	BCR	O	201	-	41,41,41	1.18	2 (4%)	56,56,56	1.23	7 (12%)
15	BCR	F	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	e	819	-	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	B	809	2	54,58,73	1.41	8 (14%)	65,95,113	1.32	5 (7%)
14	PQN	A	846	-	34,34,34	1.63	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	A	840	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	8 (12%)
13	CLA	b	805	2	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	b	832	2	54,58,73	1.43	9 (16%)	65,95,113	1.30	6 (9%)
13	CLA	e	803	-	54,58,73	1.41	8 (14%)	65,95,113	1.31	7 (10%)
13	CLA	a	843	1	54,58,73	1.39	8 (14%)	65,95,113	1.45	9 (13%)
13	CLA	G	831	2	49,53,73	1.49	9 (18%)	59,89,113	1.42	6 (10%)
13	CLA	s	203	-	54,58,73	2.26	11 (20%)	65,95,113	2.88	15 (23%)
13	CLA	g	831	2	54,58,73	1.38	8 (14%)	65,95,113	1.48	8 (12%)
13	CLA	g	813	2	54,58,73	1.41	9 (16%)	65,95,113	1.39	5 (7%)
15	BCR	o	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	b	804	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	A	820	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	6 (9%)
13	CLA	g	803	-	54,58,73	1.40	9 (16%)	65,95,113	1.43	5 (7%)
13	CLA	G	802	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	8 (12%)
13	CLA	E	813	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	G	821	2	51,55,73	1.45	9 (17%)	61,91,113	1.40	5 (8%)
13	CLA	E	827	1	54,58,73	1.41	10 (18%)	65,95,113	1.39	8 (12%)
15	BCR	a	803	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	5 (8%)
13	CLA	E	809	1	54,58,73	1.42	9 (16%)	65,95,113	1.38	4 (6%)
13	CLA	g	839	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PQN	G	842	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	g	808	2	54,58,73	1.39	9 (16%)	65,95,113	1.43	7 (10%)
15	BCR	E	801	-	41,41,41	1.17	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	B	829	-	54,58,73	1.40	10 (18%)	65,95,113	1.39	6 (9%)
13	CLA	a	820	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	7 (10%)
13	CLA	B	837	-	54,58,73	1.40	8 (14%)	65,95,113	1.43	7 (10%)
16	SF4	E	847	-	0,12,12	-	-	-	-	-
13	CLA	A	828	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
15	BCR	B	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	6 (10%)
13	CLA	G	811	2	54,58,73	1.42	9 (16%)	65,95,113	1.39	5 (7%)
13	CLA	a	829	-	54,58,73	1.41	9 (16%)	65,95,113	1.38	5 (7%)
13	CLA	e	841	1	54,58,73	1.39	9 (16%)	65,95,113	1.45	10 (15%)
15	BCR	a	853	-	41,41,41	1.16	2 (4%)	56,56,56	1.29	6 (10%)
13	CLA	E	835	-	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	E	841	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	7 (10%)
13	CLA	e	807	-	54,58,73	1.41	9 (16%)	65,95,113	1.48	7 (10%)
13	CLA	A	813	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	B	834	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	6 (9%)
14	PQN	e	845	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	A	809	1	54,58,73	1.42	8 (14%)	65,95,113	1.39	4 (6%)
13	CLA	l	205	-	54,58,73	2.26	10 (18%)	65,95,113	2.89	14 (21%)
13	CLA	B	841	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	a	827	1	54,58,73	1.40	10 (18%)	65,95,113	1.40	8 (12%)
13	CLA	G	840	-	54,58,73	1.40	10 (18%)	65,95,113	1.41	7 (10%)
13	CLA	e	842	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	7 (10%)
15	BCR	B	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	b	807	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	8 (12%)
13	CLA	A	819	1	53,57,73	1.43	9 (16%)	62,93,113	1.42	7 (11%)
12	LHG	A	802	13	37,37,48	0.77	1 (2%)	40,43,54	1.33	5 (12%)
13	CLA	G	820	-	54,58,73	1.41	10 (18%)	65,95,113	1.46	6 (9%)
15	BCR	S	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	E	844	-	54,58,73	1.41	10 (18%)	65,95,113	1.42	7 (10%)
13	CLA	G	814	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
13	CLA	f	203	-	49,53,73	1.47	10 (20%)	59,89,113	1.53	7 (11%)
15	BCR	P	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	G	845	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	g	835	-	54,58,73	1.41	8 (14%)	65,95,113	1.40	6 (9%)
15	BCR	B	847	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
16	SF4	c	101	-	0,12,12	-	-	-		
16	SF4	g	804	-	0,12,12	-	-	-		
13	CLA	G	829	-	54,58,73	1.41	10 (18%)	65,95,113	1.39	6 (9%)
13	CLA	a	813	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	A	827	1	54,58,73	1.41	9 (16%)	65,95,113	1.40	8 (12%)
13	CLA	B	826	-	50,54,73	1.45	10 (20%)	60,90,113	1.49	6 (10%)
13	CLA	l	201	-	49,53,73	1.48	10 (20%)	59,89,113	1.36	5 (8%)
13	CLA	A	844	1	54,58,73	1.40	10 (18%)	65,95,113	1.41	7 (10%)
12	LHG	e	801	-	48,48,48	0.67	1 (2%)	51,54,54	1.30	7 (13%)
15	BCR	b	842	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	A	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.41	7 (11%)
15	BCR	b	845	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	s	202	10	49,53,73	1.47	10 (20%)	59,89,113	1.46	7 (11%)
14	PQN	g	843	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
15	BCR	S	202	-	41,41,41	1.15	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	e	813	-	54,58,73	1.41	8 (14%)	65,95,113	1.39	5 (7%)
15	BCR	m	101	-	41,41,41	1.12	3 (7%)	56,56,56	1.33	9 (16%)
13	CLA	a	805	-	54,58,73	1.39	10 (18%)	65,95,113	1.30	5 (7%)
15	BCR	e	846	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	a	835	-	54,58,73	1.40	11 (20%)	65,95,113	1.44	7 (10%)
13	CLA	B	819	-	54,58,73	1.41	9 (16%)	65,95,113	1.42	5 (7%)
13	CLA	e	839	-	54,58,73	1.41	9 (16%)	65,95,113	1.44	7 (10%)
13	CLA	A	830	-	54,58,73	1.42	10 (18%)	65,95,113	1.42	7 (10%)
13	CLA	b	824	-	54,58,73	1.39	9 (16%)	65,95,113	1.48	9 (13%)
15	BCR	A	850	-	41,41,41	1.20	3 (7%)	56,56,56	1.26	8 (14%)
13	CLA	G	804	-	54,58,73	1.41	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	g	806	-	54,58,73	1.40	9 (16%)	65,95,113	1.46	6 (9%)
13	CLA	G	813	2	49,53,73	1.50	10 (20%)	59,89,113	1.40	6 (10%)
13	CLA	e	824	1	53,57,73	1.41	8 (15%)	62,93,113	1.46	8 (12%)
13	CLA	G	815	-	54,58,73	1.42	10 (18%)	65,95,113	1.45	6 (9%)
13	CLA	A	838	1	49,53,73	1.47	9 (18%)	59,89,113	1.52	6 (10%)
13	CLA	e	823	-	54,58,73	1.39	9 (16%)	65,95,113	1.44	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	804	-	54,58,73	1.38	10 (18%)	65,95,113	1.44	9 (13%)
13	CLA	B	821	2	51,55,73	1.44	9 (17%)	61,91,113	1.39	5 (8%)
13	CLA	A	805	-	54,58,73	1.40	10 (18%)	65,95,113	1.30	5 (7%)
13	CLA	b	819	-	54,58,73	1.41	9 (16%)	65,95,113	1.45	6 (9%)
13	CLA	G	806	2	54,58,73	1.40	9 (16%)	65,95,113	1.43	7 (10%)
13	CLA	a	810	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	7 (10%)
13	CLA	b	829	2	54,58,73	1.39	8 (14%)	65,95,113	1.46	6 (9%)
13	CLA	G	808	2	54,58,73	1.41	8 (14%)	65,95,113	1.33	6 (9%)
13	CLA	a	839	1	49,53,73	1.46	9 (18%)	59,89,113	1.52	6 (10%)
13	CLA	b	810	2	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
13	CLA	E	843	1	54,58,73	1.39	9 (16%)	65,95,113	1.45	10 (15%)
13	CLA	g	811	-	54,58,73	1.39	10 (18%)	65,95,113	1.47	8 (12%)
13	CLA	a	817	-	54,58,73	1.42	8 (14%)	65,95,113	1.39	6 (9%)
13	CLA	E	821	1	54,58,73	1.45	11 (20%)	65,95,113	1.41	8 (12%)
15	BCR	B	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
13	CLA	E	811	-	54,58,73	1.40	10 (18%)	65,95,113	1.41	7 (10%)
15	BCR	a	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	5 (8%)
13	CLA	A	829	-	54,58,73	1.40	9 (16%)	65,95,113	1.37	5 (7%)
13	CLA	b	808	2	54,58,73	1.42	8 (14%)	65,95,113	1.33	6 (9%)
13	CLA	a	822	-	54,58,73	1.40	9 (16%)	65,95,113	1.34	6 (9%)
13	CLA	a	814	-	49,53,73	1.47	9 (18%)	59,89,113	1.44	5 (8%)
15	BCR	g	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	b	834	-	49,53,73	1.51	8 (16%)	59,89,113	1.43	6 (10%)
13	CLA	A	810	-	54,58,73	1.41	10 (18%)	65,95,113	1.40	7 (10%)
13	CLA	g	814	2	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
14	PQN	b	841	-	34,34,34	1.64	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	g	829	2	54,58,73	1.40	10 (18%)	65,95,113	1.36	6 (9%)
13	CLA	e	814	1	54,58,73	1.40	9 (16%)	65,95,113	1.42	6 (9%)
13	CLA	b	802	-	54,58,73	1.40	10 (18%)	65,95,113	1.39	8 (12%)
13	CLA	E	814	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	5 (7%)
13	CLA	g	810	2	54,58,73	1.41	8 (14%)	65,95,113	1.33	6 (9%)
13	CLA	A	834	1	54,58,73	1.39	10 (18%)	65,95,113	1.35	7 (10%)
13	CLA	G	825	-	54,58,73	1.40	10 (18%)	65,95,113	1.48	9 (13%)
15	BCR	A	851	-	41,41,41	1.25	2 (4%)	56,56,56	1.26	7 (12%)
13	CLA	g	825	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	831	-	54,58,73	1.42	10 (18%)	65,95,113	1.46	8 (12%)
16	SF4	C	102	3	0,12,12	-	-	-		
13	CLA	a	834	1	54,58,73	1.40	9 (16%)	65,95,113	1.35	7 (10%)
13	CLA	G	805	2	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	G	835	-	49,53,73	1.51	9 (18%)	59,89,113	1.43	6 (10%)
13	CLA	G	826	-	50,54,73	1.45	10 (20%)	60,90,113	1.48	6 (10%)
13	CLA	e	838	-	54,58,73	1.39	10 (18%)	65,95,113	1.45	9 (13%)
13	CLA	A	821	1	54,58,73	1.45	10 (18%)	65,95,113	1.41	8 (12%)
13	CLA	b	837	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	8 (12%)
13	CLA	g	817	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
13	CLA	L	203	10	49,53,73	1.48	10 (20%)	59,89,113	1.47	7 (11%)
13	CLA	A	843	-	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
13	CLA	b	831	-	53,57,73	1.40	8 (15%)	62,93,113	1.41	6 (9%)
15	BCR	e	849	-	41,41,41	1.19	3 (7%)	56,56,56	1.27	9 (16%)
15	BCR	e	850	-	41,41,41	1.22	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	a	807	-	54,58,73	1.40	9 (16%)	65,95,113	1.43	7 (10%)
13	CLA	E	839	1	49,53,73	1.47	9 (18%)	59,89,113	1.52	6 (10%)
13	CLA	E	820	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	7 (10%)
15	BCR	E	852	-	41,41,41	1.15	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	A	831	-	54,58,73	1.42	10 (18%)	65,95,113	1.45	7 (10%)
13	CLA	G	812	-	49,53,73	1.47	9 (18%)	59,89,113	1.36	5 (8%)
13	CLA	a	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.41	7 (11%)
13	CLA	G	834	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	7 (10%)
13	CLA	a	821	1	54,58,73	1.44	11 (20%)	65,95,113	1.41	8 (12%)
13	CLA	G	810	2	54,58,73	1.41	10 (18%)	65,95,113	1.42	7 (10%)
13	CLA	e	810	-	54,58,73	1.40	9 (16%)	65,95,113	1.41	7 (10%)
13	CLA	E	815	1	54,58,73	1.40	9 (16%)	65,95,113	1.42	6 (9%)
13	CLA	E	823	-	54,58,73	1.42	10 (18%)	65,95,113	1.31	6 (9%)
13	CLA	B	801	-	54,58,73	1.39	11 (20%)	65,95,113	1.45	7 (10%)
13	CLA	B	814	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
13	CLA	e	821	-	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
13	CLA	A	817	-	49,53,73	1.50	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	B	823	2	54,58,73	1.41	10 (18%)	65,95,113	1.45	6 (9%)
13	CLA	b	812	2	49,53,73	1.49	10 (20%)	59,89,113	1.41	6 (10%)
15	BCR	e	851	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	841	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	7 (10%)
13	CLA	A	839	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	9 (13%)
13	CLA	a	824	-	54,58,73	1.39	9 (16%)	65,95,113	1.44	7 (10%)
15	BCR	s	201	-	41,41,41	1.24	3 (7%)	56,56,56	1.16	5 (8%)
13	CLA	b	809	-	54,58,73	1.39	9 (16%)	65,95,113	1.47	7 (10%)
13	CLA	b	836	-	54,58,73	1.40	8 (14%)	65,95,113	1.42	8 (12%)
13	CLA	A	814	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	5 (7%)
13	CLA	G	817	-	54,58,73	1.42	9 (16%)	65,95,113	1.36	7 (10%)
13	CLA	G	828	2	54,58,73	1.40	10 (18%)	65,95,113	1.36	6 (9%)
13	CLA	G	807	-	54,58,73	1.41	8 (14%)	65,95,113	1.40	9 (13%)
13	CLA	B	815	-	54,58,73	1.42	9 (16%)	65,95,113	1.45	6 (9%)
13	CLA	e	828	-	54,58,73	1.41	9 (16%)	65,95,113	1.37	5 (7%)
15	BCR	E	802	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
13	CLA	E	831	-	54,58,73	1.42	10 (18%)	65,95,113	1.46	8 (12%)
13	CLA	B	813	2	49,53,73	1.49	9 (18%)	59,89,113	1.41	6 (10%)
13	CLA	a	842	-	51,55,73	1.44	9 (17%)	61,91,113	1.44	5 (8%)
13	CLA	b	833	-	54,58,73	1.42	8 (14%)	65,95,113	1.40	6 (9%)
13	CLA	E	816	1	54,58,73	1.41	9 (16%)	65,95,113	1.43	7 (10%)
13	CLA	G	818	2	54,58,73	1.42	10 (18%)	65,95,113	1.43	7 (10%)
13	CLA	a	809	1	54,58,73	1.41	8 (14%)	65,95,113	1.38	5 (7%)
13	CLA	E	804	-	54,58,73	1.38	10 (18%)	65,95,113	1.44	9 (13%)
13	CLA	b	816	-	54,58,73	1.42	9 (16%)	65,95,113	1.37	7 (10%)
13	CLA	e	830	-	54,58,73	1.42	10 (18%)	65,95,113	1.46	8 (12%)
13	CLA	b	838	-	51,55,73	1.44	8 (15%)	61,91,113	1.48	5 (8%)
13	CLA	E	807	-	54,58,73	1.40	8 (14%)	65,95,113	1.44	7 (10%)
13	CLA	A	853	-	54,58,73	1.40	9 (16%)	65,95,113	1.39	8 (12%)
13	CLA	g	812	2	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
13	CLA	A	824	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	7 (10%)
13	CLA	b	827	2	54,58,73	1.40	10 (18%)	65,95,113	1.36	6 (9%)
13	CLA	g	809	-	54,58,73	1.41	9 (16%)	65,95,113	1.41	7 (10%)
13	CLA	g	836	-	49,53,73	1.52	9 (18%)	59,89,113	1.44	6 (10%)
13	CLA	A	835	-	54,58,73	1.43	8 (14%)	65,95,113	1.49	5 (7%)
13	CLA	A	833	-	54,58,73	1.39	8 (14%)	65,95,113	1.47	8 (12%)
13	CLA	e	811	1	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
13	CLA	e	805	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	811	-	49,53,73	1.48	9 (18%)	59,89,113	1.35	5 (8%)
13	CLA	E	806	-	54,58,73	1.41	10 (18%)	65,95,113	1.40	8 (12%)
13	CLA	E	805	-	54,58,73	1.39	10 (18%)	65,95,113	1.30	5 (7%)
13	CLA	g	833	-	53,57,73	1.40	10 (18%)	62,93,113	1.40	7 (11%)
15	BCR	T	101	-	41,41,41	1.19	3 (7%)	56,56,56	1.26	4 (7%)
13	CLA	A	832	1	54,58,73	1.41	9 (16%)	65,95,113	1.37	7 (10%)
15	BCR	B	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	e	808	1	54,58,73	1.41	8 (14%)	65,95,113	1.39	4 (6%)
13	CLA	e	817	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	7 (11%)
13	CLA	A	823	-	54,58,73	1.42	11 (20%)	65,95,113	1.31	6 (9%)
13	CLA	E	808	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	7 (10%)
13	CLA	a	833	-	54,58,73	1.39	8 (14%)	65,95,113	1.47	8 (12%)
13	CLA	S	204	-	49,53,73	2.37	11 (22%)	59,89,113	3.01	14 (23%)
13	CLA	e	840	-	51,55,73	1.44	9 (17%)	61,91,113	1.44	5 (8%)
13	CLA	a	804	-	54,58,73	1.38	10 (18%)	65,95,113	1.44	9 (13%)
13	CLA	g	816	-	54,58,73	1.42	10 (18%)	65,95,113	1.44	6 (9%)
13	CLA	G	827	-	54,58,73	1.42	9 (16%)	65,95,113	1.37	7 (10%)
14	PQN	E	848	-	34,34,34	1.63	2 (5%)	42,45,45	1.19	4 (9%)
13	CLA	g	832	2	49,53,73	1.48	9 (18%)	59,89,113	1.43	6 (10%)
13	CLA	e	832	-	54,58,73	1.39	9 (16%)	65,95,113	1.46	8 (12%)
13	CLA	e	818	1	53,57,73	1.43	9 (16%)	62,93,113	1.42	7 (11%)
13	CLA	G	822	-	49,53,73	1.47	7 (14%)	59,89,113	1.50	8 (13%)
15	BCR	E	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	5 (8%)
13	CLA	B	840	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	6 (9%)
13	CLA	A	812	1	54,58,73	1.40	8 (14%)	65,95,113	1.41	6 (9%)
13	CLA	B	805	-	54,58,73	1.41	9 (16%)	65,95,113	1.47	6 (9%)
15	BCR	R	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.43	7 (12%)
13	CLA	a	838	1	54,58,73	1.41	8 (14%)	65,95,113	1.42	7 (10%)
13	CLA	a	815	1	54,58,73	1.40	9 (16%)	65,95,113	1.42	6 (9%)
13	CLA	e	820	1	54,58,73	1.45	11 (20%)	65,95,113	1.41	8 (12%)
13	CLA	g	815	-	54,58,73	1.40	10 (18%)	65,95,113	1.42	7 (10%)
13	CLA	g	818	-	54,58,73	1.42	9 (16%)	65,95,113	1.36	7 (10%)
15	BCR	J	101	-	41,41,41	1.11	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	E	812	1	54,58,73	1.41	8 (14%)	65,95,113	1.42	6 (9%)
13	CLA	E	829	-	54,58,73	1.40	10 (18%)	65,95,113	1.38	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	g	801	-	54,58,73	1.40	10 (18%)	65,95,113	1.30	5 (7%)
15	BCR	G	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.22	6 (10%)
15	BCR	b	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	803	-	54,58,73	1.40	8 (14%)	65,95,113	1.32	6 (9%)
13	CLA	G	824	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	6 (10%)
13	CLA	E	810	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	7 (10%)
15	BCR	E	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	A	804	-	54,58,73	1.39	10 (18%)	65,95,113	1.44	9 (13%)
13	CLA	F	202	-	49,53,73	1.47	8 (16%)	59,89,113	1.43	4 (6%)
13	CLA	E	825	1	53,57,73	1.41	8 (15%)	62,93,113	1.45	7 (11%)
15	BCR	B	845	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
15	BCR	L	205	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
13	CLA	G	833	2	54,58,73	1.43	8 (14%)	65,95,113	1.30	4 (6%)
13	CLA	A	807	-	54,58,73	1.40	9 (16%)	65,95,113	1.43	7 (10%)
13	CLA	E	826	1	54,58,73	1.41	9 (16%)	65,95,113	1.41	8 (12%)
15	BCR	E	851	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	a	845	1	54,58,73	1.40	10 (18%)	65,95,113	1.42	8 (12%)
13	CLA	e	816	-	49,53,73	1.49	10 (20%)	59,89,113	1.40	4 (6%)
13	CLA	B	810	-	54,58,73	1.38	8 (14%)	65,95,113	1.47	7 (10%)
13	CLA	E	828	-	54,58,73	1.40	9 (16%)	65,95,113	1.44	8 (12%)
13	CLA	G	838	-	54,58,73	1.40	10 (18%)	65,95,113	1.44	8 (12%)
13	CLA	a	837	-	54,58,73	1.41	10 (18%)	65,95,113	1.36	7 (10%)
13	CLA	E	834	1	54,58,73	1.39	10 (18%)	65,95,113	1.36	7 (10%)
13	CLA	G	839	-	51,55,73	1.44	9 (17%)	61,91,113	1.47	5 (8%)
13	CLA	e	806	-	54,58,73	1.39	9 (16%)	65,95,113	1.43	7 (10%)
15	BCR	g	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	5 (8%)
13	CLA	g	827	-	50,54,73	1.45	10 (20%)	60,90,113	1.48	6 (10%)
15	BCR	A	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	a	836	-	54,58,73	1.43	10 (18%)	65,95,113	1.48	5 (7%)
13	CLA	E	819	1	53,57,73	1.43	9 (16%)	62,93,113	1.42	7 (11%)
13	CLA	e	812	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
13	CLA	B	808	-	54,58,73	1.41	9 (16%)	65,95,113	1.39	8 (12%)
13	CLA	a	825	1	53,57,73	1.40	8 (15%)	62,93,113	1.46	8 (12%)
13	CLA	B	828	2	54,58,73	1.40	10 (18%)	65,95,113	1.36	6 (9%)
13	CLA	s	205	2	54,58,73	1.42	9 (16%)	65,95,113	1.40	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	816	1	54,58,73	1.41	9 (16%)	65,95,113	1.43	7 (10%)
13	CLA	a	832	1	54,58,73	1.41	10 (18%)	65,95,113	1.37	7 (10%)
13	CLA	g	805	-	54,58,73	1.40	9 (16%)	65,95,113	1.33	6 (9%)
13	CLA	b	822	2	54,58,73	1.41	10 (18%)	65,95,113	1.44	6 (9%)
13	CLA	b	801	-	46,49,73	1.49	9 (19%)	55,83,113	1.40	5 (9%)
13	CLA	B	825	-	54,58,73	1.39	10 (18%)	65,95,113	1.48	9 (13%)
13	CLA	G	837	-	54,58,73	1.40	8 (14%)	65,95,113	1.43	7 (10%)
13	CLA	G	836	-	49,53,73	1.47	8 (16%)	59,89,113	1.54	6 (10%)
13	CLA	a	812	1	54,58,73	1.40	8 (14%)	65,95,113	1.42	7 (10%)
15	BCR	p	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.17	2 (3%)
13	CLA	A	825	1	53,57,73	1.40	8 (15%)	62,93,113	1.46	8 (12%)
13	CLA	A	816	1	54,58,73	1.40	8 (14%)	65,95,113	1.43	7 (10%)
13	CLA	B	811	2	54,58,73	1.41	10 (18%)	65,95,113	1.43	7 (10%)
13	CLA	G	803	-	54,58,73	1.40	9 (16%)	65,95,113	1.33	6 (9%)
13	CLA	A	826	1	54,58,73	1.41	9 (16%)	65,95,113	1.42	8 (12%)
13	CLA	E	830	-	54,58,73	1.42	10 (18%)	65,95,113	1.42	7 (10%)
16	SF4	h	102	3	0,12,12	-	-	-	-	-
13	CLA	E	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	7 (11%)
13	CLA	e	836	1	54,58,73	1.41	9 (16%)	65,95,113	1.43	7 (10%)
15	BCR	S	201	-	41,41,41	1.19	2 (4%)	56,56,56	1.13	3 (5%)
13	CLA	G	816	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	5 (8%)
15	BCR	a	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
13	CLA	G	832	-	53,57,73	1.41	10 (18%)	62,93,113	1.41	7 (11%)
13	CLA	B	802	-	54,58,73	1.39	10 (18%)	65,95,113	1.42	6 (9%)
13	CLA	E	824	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	7 (10%)
13	CLA	B	804	-	54,58,73	1.40	9 (16%)	65,95,113	1.33	6 (9%)
15	BCR	l	206	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	E	846	-	46,49,73	1.51	9 (19%)	55,83,113	1.51	6 (10%)
13	CLA	e	844	12	54,58,73	1.40	8 (14%)	65,95,113	1.52	8 (12%)
15	BCR	g	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	830	2	54,58,73	1.39	8 (14%)	65,95,113	1.47	6 (9%)
13	CLA	b	840	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	6 (9%)
13	CLA	B	822	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
13	CLA	o	202	-	49,53,73	1.47	8 (16%)	59,89,113	1.46	4 (6%)
13	CLA	e	825	1	54,58,73	1.41	9 (16%)	65,95,113	1.42	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	852	-	54,58,73	1.40	9 (16%)	65,95,113	1.38	8 (12%)
13	CLA	g	828	-	54,58,73	1.42	9 (16%)	65,95,113	1.36	7 (10%)
13	CLA	E	832	1	54,58,73	1.41	9 (16%)	65,95,113	1.37	7 (10%)
13	CLA	R	102	-	49,53,73	1.48	7 (14%)	59,89,113	1.43	7 (11%)
15	BCR	q	101	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	B	812	2	54,58,73	1.41	9 (16%)	65,95,113	1.39	5 (7%)
13	CLA	e	835	-	54,58,73	1.41	10 (18%)	65,95,113	1.35	7 (10%)
13	CLA	b	820	2	51,55,73	1.44	9 (17%)	61,91,113	1.40	5 (8%)
15	BCR	b	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
16	SF4	a	846	-	0,12,12	-	-	-	-	-
13	CLA	B	824	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	6 (10%)
13	CLA	b	813	-	54,58,73	1.40	9 (16%)	65,95,113	1.42	7 (10%)
13	CLA	B	817	-	54,58,73	1.41	9 (16%)	65,95,113	1.35	7 (10%)
13	CLA	K	102	-	49,53,73	1.48	7 (14%)	59,89,113	1.42	7 (11%)
13	CLA	O	203	-	49,53,73	1.48	10 (20%)	59,89,113	1.51	7 (11%)
15	BCR	b	843	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	B	827	-	54,58,73	1.42	9 (16%)	65,95,113	1.36	7 (10%)
13	CLA	B	833	2	54,58,73	1.43	10 (18%)	65,95,113	1.30	6 (9%)
13	CLA	b	823	-	49,53,73	1.47	9 (18%)	59,89,113	1.51	5 (8%)
13	CLA	g	834	2	54,58,73	1.43	10 (18%)	65,95,113	1.30	6 (9%)
13	CLA	a	808	-	54,58,73	1.41	9 (16%)	65,95,113	1.49	7 (10%)
13	CLA	g	840	-	51,55,73	1.45	9 (17%)	61,91,113	1.48	5 (8%)
13	CLA	A	842	1	54,58,73	1.40	10 (18%)	65,95,113	1.44	9 (13%)
13	CLA	a	823	-	54,58,73	1.42	10 (18%)	65,95,113	1.31	6 (9%)
15	BCR	l	202	-	41,41,41	1.19	2 (4%)	56,56,56	1.16	5 (8%)
13	CLA	e	843	1	54,58,73	1.40	10 (18%)	65,95,113	1.41	7 (10%)
12	LHG	a	801	-	48,48,48	0.64	1 (2%)	51,54,54	1.30	7 (13%)
13	CLA	B	818	2	54,58,73	1.41	10 (18%)	65,95,113	1.42	7 (10%)
15	BCR	k	4001	-	41,41,41	1.17	3 (7%)	56,56,56	1.59	10 (17%)
15	BCR	e	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	B	832	-	53,57,73	1.41	9 (16%)	62,93,113	1.41	7 (11%)
13	CLA	A	845	12	54,58,73	1.40	8 (14%)	65,95,113	1.52	6 (9%)
13	CLA	L	202	10	54,58,73	1.41	9 (16%)	65,95,113	1.42	10 (15%)
13	CLA	g	820	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	4 (6%)
13	CLA	e	834	-	54,58,73	1.44	10 (18%)	65,95,113	1.48	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	f	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	7 (12%)
13	CLA	A	822	-	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
12	LHG	e	802	13	37,37,48	0.74	1 (2%)	40,43,54	1.34	5 (12%)
13	CLA	A	837	1	54,58,73	1.41	9 (16%)	65,95,113	1.42	7 (10%)
13	CLA	K	101	-	46,49,73	1.50	9 (19%)	55,83,113	1.40	5 (9%)
15	BCR	g	844	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	b	817	2	54,58,73	1.41	10 (18%)	65,95,113	1.42	7 (10%)
15	BCR	s	204	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	8 (14%)
15	BCR	O	202	-	41,41,41	1.12	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	E	833	-	54,58,73	1.40	8 (14%)	65,95,113	1.48	8 (12%)
13	CLA	g	837	-	49,53,73	1.47	8 (16%)	59,89,113	1.54	6 (10%)
13	CLA	g	823	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	8 (13%)
15	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.74	11 (19%)
13	CLA	r	102	-	49,53,73	1.48	8 (16%)	59,89,113	1.43	7 (11%)
12	LHG	A	801	-	48,48,48	0.68	1 (2%)	51,54,54	1.31	7 (13%)
13	CLA	g	826	-	54,58,73	1.40	10 (18%)	65,95,113	1.47	9 (13%)
13	CLA	E	838	1	54,58,73	1.41	8 (14%)	65,95,113	1.42	7 (10%)
14	PQN	B	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.18	4 (9%)
13	CLA	S	203	10	49,53,73	1.48	10 (20%)	59,89,113	1.47	7 (11%)
13	CLA	e	831	1	54,58,73	1.41	9 (16%)	65,95,113	1.37	7 (10%)
16	SF4	H	102	3	0,12,12	-	-	-	-	-
13	CLA	B	806	2	54,58,73	1.40	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	B	836	-	49,53,73	1.47	8 (16%)	59,89,113	1.53	6 (10%)
13	CLA	g	824	2	54,58,73	1.40	10 (18%)	65,95,113	1.45	6 (9%)
13	CLA	B	807	2	54,58,73	1.40	9 (16%)	65,95,113	1.43	7 (10%)
15	BCR	G	847	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	B	831	2	49,53,73	1.48	9 (18%)	59,89,113	1.41	6 (10%)
15	BCR	G	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	5 (8%)
16	SF4	h	101	-	0,12,12	-	-	-	-	-
15	BCR	A	848	-	41,41,41	1.13	2 (4%)	56,56,56	1.26	5 (8%)
15	BCR	G	844	-	41,41,41	1.15	2 (4%)	56,56,56	1.23	5 (8%)
13	CLA	g	842	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	6 (9%)
15	BCR	a	802	-	41,41,41	1.11	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	l	204	10	49,53,73	1.47	10 (20%)	59,89,113	1.47	7 (11%)
13	CLA	b	830	2	49,53,73	1.48	9 (18%)	59,89,113	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	E	842	-	51,55,73	1.44	9 (17%)	61,91,113	1.44	4 (6%)
13	CLA	E	845	1	54,58,73	1.40	10 (18%)	65,95,113	1.41	8 (12%)
16	SF4	C	101	-	0,12,12	-	-	-	-	-
13	CLA	G	809	-	54,58,73	1.39	8 (14%)	65,95,113	1.48	8 (12%)
13	CLA	A	811	-	54,58,73	1.40	10 (18%)	65,95,113	1.41	7 (10%)
13	CLA	e	809	-	54,58,73	1.41	10 (18%)	65,95,113	1.40	7 (10%)
13	CLA	E	836	-	54,58,73	1.43	9 (16%)	65,95,113	1.48	5 (7%)
15	BCR	A	852	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	7 (12%)
13	CLA	g	822	2	51,55,73	1.45	10 (19%)	61,91,113	1.40	5 (8%)
13	CLA	E	822	-	54,58,73	1.41	9 (16%)	65,95,113	1.34	6 (9%)
13	CLA	a	844	-	54,58,73	1.41	10 (18%)	65,95,113	1.42	6 (9%)
15	BCR	b	846	-	41,41,41	1.21	3 (7%)	56,56,56	1.17	6 (10%)
13	CLA	B	820	-	54,58,73	1.41	9 (16%)	65,95,113	1.45	6 (9%)
13	CLA	e	827	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	A	841	-	51,55,73	1.43	9 (17%)	61,91,113	1.44	5 (8%)
13	CLA	A	806	-	54,58,73	1.41	9 (16%)	65,95,113	1.41	8 (12%)
15	BCR	j	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	5 (8%)
13	CLA	a	852	-	54,58,73	1.39	7 (12%)	65,95,113	1.39	7 (10%)
15	BCR	g	848	-	41,41,41	1.21	2 (4%)	56,56,56	1.17	6 (10%)
13	CLA	B	838	-	54,58,73	1.40	9 (16%)	65,95,113	1.45	8 (12%)
13	CLA	E	803	-	54,58,73	1.40	7 (12%)	65,95,113	1.30	5 (7%)
13	CLA	a	806	-	54,58,73	1.41	10 (18%)	65,95,113	1.41	8 (12%)
13	CLA	A	808	-	54,58,73	1.41	9 (16%)	65,95,113	1.48	7 (10%)
13	CLA	g	841	-	54,58,73	1.41	10 (18%)	65,95,113	1.42	7 (10%)
13	CLA	g	819	2	54,58,73	1.41	10 (18%)	65,95,113	1.44	7 (10%)
13	CLA	b	825	-	50,54,73	1.45	10 (20%)	60,90,113	1.48	6 (10%)
13	CLA	b	835	-	49,53,73	1.47	9 (18%)	59,89,113	1.53	6 (10%)
13	CLA	k	4002	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	8 (13%)
15	BCR	G	843	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
13	CLA	g	802	-	54,58,73	1.40	11 (20%)	65,95,113	1.45	7 (10%)
13	CLA	a	828	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
13	CLA	e	833	1	54,58,73	1.40	10 (18%)	65,95,113	1.35	7 (10%)
13	CLA	b	826	-	54,58,73	1.42	9 (16%)	65,95,113	1.36	7 (10%)
13	CLA	L	204	-	54,58,73	2.25	11 (20%)	65,95,113	2.87	15 (23%)
13	CLA	A	836	-	54,58,73	1.42	10 (18%)	65,95,113	1.37	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	A	847	-	41,41,41	1.14	2 (4%)	56,56,56	1.38	8 (14%)
15	BCR	a	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	a	830	-	54,58,73	1.42	10 (18%)	65,95,113	1.41	7 (10%)
13	CLA	A	815	1	54,58,73	1.41	9 (16%)	65,95,113	1.42	6 (9%)
15	BCR	Q	101	-	41,41,41	1.12	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	G	801	-	54,58,73	1.40	10 (18%)	65,95,113	1.45	8 (12%)
15	BCR	g	846	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)

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	g	807	2	-	2/21/97/115	-
13	CLA	B	816	-	-	6/15/91/115	-
16	SF4	H	101	-	-	-	0/6/5/5
13	CLA	e	829	-	-	8/21/97/115	-
16	SF4	c	102	3	-	-	0/6/5/5
13	CLA	e	815	1	-	5/21/97/115	-
13	CLA	b	814	-	-	3/21/97/115	-
15	BCR	q	102	-	-	12/29/63/63	0/2/2/2
13	CLA	G	841	-	-	9/21/97/115	-
13	CLA	B	835	-	-	7/15/91/115	-
13	CLA	a	819	1	-	12/20/96/115	-
13	CLA	S	206	-	-	6/15/91/115	-
13	CLA	b	821	-	-	6/15/91/115	-
13	CLA	b	815	-	-	6/15/91/115	-
13	CLA	A	803	-	-	8/21/97/115	-
13	CLA	G	830	2	-	6/21/97/115	-
13	CLA	l	203	10	-	7/21/97/115	-
13	CLA	g	830	-	-	11/21/97/115	-
14	PQN	a	847	-	-	10/23/43/43	0/2/2/2
13	CLA	b	806	2	-	12/21/97/115	-
13	CLA	a	811	-	-	5/21/97/115	-
13	CLA	e	837	1	-	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2
13	CLA	B	839	-	-	9/18/94/115	-
13	CLA	g	838	-	-	6/21/97/115	-
13	CLA	E	817	-	-	7/15/91/115	-
13	CLA	b	828	-	-	11/21/97/115	-
15	BCR	e	847	-	-	13/29/63/63	0/2/2/2
13	CLA	e	826	1	-	13/21/97/115	-
13	CLA	a	840	-	-	7/21/97/115	-
13	CLA	e	822	-	-	10/21/97/115	-
15	BCR	I	101	-	-	10/29/63/63	0/2/2/2
13	CLA	E	840	-	-	6/21/97/115	-
13	CLA	a	826	1	-	15/21/97/115	-
15	BCR	L	201	-	-	17/29/63/63	0/2/2/2
13	CLA	g	821	-	-	7/21/97/115	-
13	CLA	G	819	-	-	9/21/97/115	-
13	CLA	E	837	-	-	10/21/97/115	-
13	CLA	b	818	-	-	9/21/97/115	-
15	BCR	i	101	-	-	10/29/63/63	0/2/2/2
15	BCR	J	102	-	-	12/29/63/63	0/2/2/2
16	SF4	B	803	-	-	-	0/6/5/5
13	CLA	b	839	-	-	9/21/97/115	-
13	CLA	r	101	-	-	4/9/81/115	-
13	CLA	G	823	2	-	8/21/97/115	-
15	BCR	O	201	-	-	8/29/63/63	0/2/2/2
15	BCR	F	201	-	-	8/29/63/63	0/2/2/2
13	CLA	e	819	-	-	4/21/97/115	-
13	CLA	B	809	2	-	7/21/97/115	-
14	PQN	A	846	-	-	11/23/43/43	0/2/2/2
13	CLA	A	840	-	-	8/21/97/115	-
13	CLA	b	805	2	-	2/21/97/115	-
13	CLA	b	832	2	-	4/21/97/115	-
13	CLA	e	803	-	-	8/21/97/115	-
13	CLA	a	843	1	-	6/21/97/115	-
13	CLA	G	831	2	-	12/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	s	203	-	-	10/21/97/115	-
13	CLA	g	831	2	-	6/21/97/115	-
13	CLA	g	813	2	-	14/21/97/115	-
15	BCR	o	201	-	-	8/29/63/63	0/2/2/2
13	CLA	b	804	-	-	7/21/97/115	-
13	CLA	A	820	-	-	4/21/97/115	-
13	CLA	g	803	-	-	8/21/97/115	-
13	CLA	G	802	-	-	10/21/97/115	-
13	CLA	E	813	-	-	6/15/91/115	-
13	CLA	G	821	2	-	10/18/94/115	-
13	CLA	E	827	1	-	13/21/97/115	-
15	BCR	a	803	-	-	23/29/63/63	0/2/2/2
13	CLA	E	809	1	-	7/21/97/115	-
13	CLA	g	839	-	-	8/21/97/115	-
14	PQN	G	842	-	-	11/23/43/43	0/2/2/2
13	CLA	g	808	2	-	12/21/97/115	-
15	BCR	E	801	-	-	12/29/63/63	0/2/2/2
13	CLA	B	829	-	-	11/21/97/115	-
13	CLA	a	820	-	-	4/21/97/115	-
13	CLA	B	837	-	-	6/21/97/115	-
16	SF4	E	847	-	-	-	0/6/5/5
13	CLA	A	828	-	-	6/21/97/115	-
15	BCR	B	848	-	-	16/29/63/63	0/2/2/2
13	CLA	G	811	2	-	14/21/97/115	-
13	CLA	a	829	-	-	11/21/97/115	-
13	CLA	e	841	1	-	6/21/97/115	-
15	BCR	a	853	-	-	12/29/63/63	0/2/2/2
13	CLA	E	835	-	-	5/21/97/115	-
13	CLA	E	841	-	-	8/21/97/115	-
13	CLA	e	807	-	-	6/21/97/115	-
13	CLA	A	813	-	-	6/15/91/115	-
13	CLA	B	834	-	-	11/21/97/115	-
14	PQN	e	845	-	-	7/23/43/43	0/2/2/2
13	CLA	A	809	1	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	l	205	-	-	10/21/97/115	-
13	CLA	B	841	-	-	9/21/97/115	-
13	CLA	a	827	1	-	13/21/97/115	-
13	CLA	G	840	-	-	9/21/97/115	-
13	CLA	e	842	-	-	7/21/97/115	-
15	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	b	807	-	-	6/21/97/115	-
13	CLA	A	819	1	-	12/20/96/115	-
12	LHG	A	802	13	-	17/42/42/53	-
13	CLA	G	820	-	-	7/21/97/115	-
15	BCR	S	205	-	-	16/29/63/63	0/2/2/2
13	CLA	E	844	-	-	7/21/97/115	-
13	CLA	G	814	-	-	5/21/97/115	-
13	CLA	f	203	-	-	7/15/91/115	-
15	BCR	P	101	-	-	10/29/63/63	0/2/2/2
15	BCR	G	845	-	-	17/29/63/63	0/2/2/2
13	CLA	g	835	-	-	11/21/97/115	-
15	BCR	B	847	-	-	12/29/63/63	0/2/2/2
16	SF4	c	101	-	-	-	0/6/5/5
16	SF4	g	804	-	-	-	0/6/5/5
13	CLA	G	829	-	-	11/21/97/115	-
13	CLA	a	813	-	-	6/15/91/115	-
13	CLA	A	827	1	-	13/21/97/115	-
13	CLA	B	826	-	-	6/17/93/115	-
13	CLA	l	201	-	-	6/15/91/115	-
13	CLA	A	844	1	-	8/21/97/115	-
12	LHG	e	801	-	-	31/53/53/53	-
15	BCR	b	842	-	-	9/29/63/63	0/2/2/2
13	CLA	A	818	-	-	6/15/91/115	-
15	BCR	b	845	-	-	22/29/63/63	0/2/2/2
13	CLA	s	202	10	-	5/15/91/115	-
14	PQN	g	843	-	-	11/23/43/43	0/2/2/2
15	BCR	S	202	-	-	17/29/63/63	0/2/2/2
13	CLA	e	813	-	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	m	101	-	-	11/29/63/63	0/2/2/2
13	CLA	a	805	-	-	7/21/97/115	-
15	BCR	e	846	-	-	19/29/63/63	0/2/2/2
13	CLA	a	835	-	-	5/21/97/115	-
13	CLA	B	819	-	-	9/21/97/115	-
13	CLA	e	839	-	-	8/21/97/115	-
13	CLA	A	830	-	-	8/21/97/115	-
13	CLA	b	824	-	-	6/21/97/115	-
15	BCR	A	850	-	-	21/29/63/63	0/2/2/2
13	CLA	G	804	-	-	7/21/97/115	-
13	CLA	g	806	-	-	7/21/97/115	-
13	CLA	G	813	2	-	5/15/91/115	-
13	CLA	e	824	1	-	11/20/96/115	-
13	CLA	G	815	-	-	3/21/97/115	-
13	CLA	A	838	1	-	7/15/91/115	-
13	CLA	e	823	-	-	10/21/97/115	-
13	CLA	e	804	-	-	8/21/97/115	-
13	CLA	B	821	2	-	10/18/94/115	-
13	CLA	A	805	-	-	7/21/97/115	-
13	CLA	b	819	-	-	7/21/97/115	-
13	CLA	G	806	2	-	12/21/97/115	-
13	CLA	a	810	-	-	10/21/97/115	-
13	CLA	b	829	2	-	6/21/97/115	-
13	CLA	G	808	2	-	7/21/97/115	-
13	CLA	a	839	1	-	6/15/91/115	-
13	CLA	b	810	2	-	6/21/97/115	-
13	CLA	E	843	1	-	6/21/97/115	-
13	CLA	g	811	-	-	4/21/97/115	-
13	CLA	a	817	-	-	5/21/97/115	-
13	CLA	E	821	1	-	7/21/97/115	-
15	BCR	B	846	-	-	22/29/63/63	0/2/2/2
13	CLA	E	811	-	-	5/21/97/115	-
15	BCR	a	850	-	-	13/29/63/63	0/2/2/2
13	CLA	A	829	-	-	11/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	808	2	-	7/21/97/115	-
13	CLA	a	822	-	-	11/21/97/115	-
13	CLA	a	814	-	-	5/15/91/115	-
15	BCR	g	845	-	-	20/29/63/63	0/2/2/2
13	CLA	b	834	-	-	7/15/91/115	-
13	CLA	A	810	-	-	10/21/97/115	-
13	CLA	g	814	2	-	5/15/91/115	-
14	PQN	b	841	-	-	11/23/43/43	0/2/2/2
13	CLA	g	829	2	-	8/21/97/115	-
13	CLA	e	814	1	-	8/21/97/115	-
13	CLA	b	802	-	-	10/21/97/115	-
13	CLA	E	814	-	-	5/21/97/115	-
13	CLA	g	810	2	-	7/21/97/115	-
13	CLA	A	834	1	-	8/21/97/115	-
13	CLA	G	825	-	-	6/21/97/115	-
15	BCR	A	851	-	-	5/29/63/63	0/2/2/2
13	CLA	g	825	-	-	8/15/91/115	-
13	CLA	a	831	-	-	9/21/97/115	-
16	SF4	C	102	3	-	-	0/6/5/5
13	CLA	a	834	1	-	8/21/97/115	-
13	CLA	G	805	2	-	2/21/97/115	-
13	CLA	G	835	-	-	7/15/91/115	-
13	CLA	G	826	-	-	6/17/93/115	-
13	CLA	e	838	-	-	7/21/97/115	-
13	CLA	A	821	1	-	7/21/97/115	-
13	CLA	b	837	-	-	8/21/97/115	-
13	CLA	g	817	-	-	6/15/91/115	-
13	CLA	L	203	10	-	5/15/91/115	-
13	CLA	A	843	-	-	7/21/97/115	-
13	CLA	b	831	-	-	8/20/96/115	-
15	BCR	e	849	-	-	20/29/63/63	0/2/2/2
15	BCR	e	850	-	-	6/29/63/63	0/2/2/2
13	CLA	a	807	-	-	8/21/97/115	-
13	CLA	E	839	1	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	820	-	-	4/21/97/115	-
15	BCR	E	852	-	-	12/29/63/63	0/2/2/2
13	CLA	A	831	-	-	9/21/97/115	-
13	CLA	G	812	-	-	6/15/91/115	-
13	CLA	a	818	-	-	6/15/91/115	-
13	CLA	G	834	-	-	11/21/97/115	-
13	CLA	a	821	1	-	7/21/97/115	-
13	CLA	G	810	2	-	6/21/97/115	-
13	CLA	e	810	-	-	5/21/97/115	-
13	CLA	E	815	1	-	8/21/97/115	-
13	CLA	E	823	-	-	10/21/97/115	-
13	CLA	B	801	-	-	5/21/97/115	-
13	CLA	B	814	-	-	5/21/97/115	-
13	CLA	e	821	-	-	11/21/97/115	-
13	CLA	A	817	-	-	7/15/91/115	-
13	CLA	B	823	2	-	8/21/97/115	-
13	CLA	b	812	2	-	5/15/91/115	-
15	BCR	e	851	-	-	16/29/63/63	0/2/2/2
13	CLA	a	841	-	-	8/21/97/115	-
13	CLA	A	839	-	-	6/21/97/115	-
13	CLA	a	824	-	-	10/21/97/115	-
15	BCR	s	201	-	-	18/29/63/63	0/2/2/2
13	CLA	b	809	-	-	4/21/97/115	-
13	CLA	b	836	-	-	6/21/97/115	-
13	CLA	A	814	-	-	5/21/97/115	-
13	CLA	G	817	-	-	9/21/97/115	-
13	CLA	G	828	2	-	8/21/97/115	-
13	CLA	G	807	-	-	6/21/97/115	-
13	CLA	B	815	-	-	3/21/97/115	-
13	CLA	e	828	-	-	11/21/97/115	-
15	BCR	E	802	-	-	20/29/63/63	0/2/2/2
13	CLA	E	831	-	-	9/21/97/115	-
13	CLA	B	813	2	-	5/15/91/115	-
13	CLA	a	842	-	-	7/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	833	-	-	11/21/97/115	-
13	CLA	E	816	1	-	5/21/97/115	-
13	CLA	G	818	2	-	12/21/97/115	-
13	CLA	a	809	1	-	7/21/97/115	-
13	CLA	E	804	-	-	8/21/97/115	-
13	CLA	b	816	-	-	10/21/97/115	-
13	CLA	e	830	-	-	10/21/97/115	-
13	CLA	b	838	-	-	10/18/94/115	-
13	CLA	E	807	-	-	8/21/97/115	-
13	CLA	A	853	-	-	10/21/97/115	-
13	CLA	g	812	2	-	6/21/97/115	-
13	CLA	A	824	-	-	10/21/97/115	-
13	CLA	b	827	2	-	8/21/97/115	-
13	CLA	g	809	-	-	6/21/97/115	-
13	CLA	g	836	-	-	7/15/91/115	-
13	CLA	A	835	-	-	6/21/97/115	-
13	CLA	A	833	-	-	6/21/97/115	-
13	CLA	e	811	1	-	8/21/97/115	-
13	CLA	e	805	-	-	10/21/97/115	-
13	CLA	b	811	-	-	6/15/91/115	-
13	CLA	E	806	-	-	10/21/97/115	-
13	CLA	E	805	-	-	7/21/97/115	-
13	CLA	g	833	-	-	8/20/96/115	-
15	BCR	T	101	-	-	11/29/63/63	0/2/2/2
13	CLA	A	832	1	-	6/21/97/115	-
15	BCR	B	844	-	-	20/29/63/63	0/2/2/2
13	CLA	e	808	1	-	7/21/97/115	-
13	CLA	e	817	-	-	6/15/91/115	-
13	CLA	A	823	-	-	10/21/97/115	-
13	CLA	E	808	-	-	6/21/97/115	-
13	CLA	a	833	-	-	6/21/97/115	-
13	CLA	S	204	-	-	9/15/91/115	-
13	CLA	e	840	-	-	7/18/94/115	-
13	CLA	a	804	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	g	816	-	-	3/21/97/115	-
13	CLA	G	827	-	-	4/21/97/115	-
14	PQN	E	848	-	-	6/23/43/43	0/2/2/2
13	CLA	g	832	2	-	12/15/91/115	-
13	CLA	e	832	-	-	6/21/97/115	-
13	CLA	e	818	1	-	12/20/96/115	-
13	CLA	G	822	-	-	6/15/91/115	-
15	BCR	E	850	-	-	13/29/63/63	0/2/2/2
13	CLA	B	840	-	-	9/21/97/115	-
13	CLA	A	812	1	-	8/21/97/115	-
13	CLA	B	805	-	-	7/21/97/115	-
15	BCR	R	101	-	-	16/29/63/63	0/2/2/2
13	CLA	a	838	1	-	9/21/97/115	-
13	CLA	a	815	1	-	8/21/97/115	-
13	CLA	e	820	1	-	7/21/97/115	-
13	CLA	g	815	-	-	5/21/97/115	-
13	CLA	g	818	-	-	10/21/97/115	-
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
13	CLA	E	812	1	-	8/21/97/115	-
13	CLA	E	829	-	-	11/21/97/115	-
13	CLA	g	801	-	-	7/21/97/115	-
15	BCR	G	848	-	-	16/29/63/63	0/2/2/2
15	BCR	b	847	-	-	16/29/63/63	0/2/2/2
13	CLA	b	803	-	-	8/21/97/115	-
13	CLA	G	824	-	-	8/15/91/115	-
13	CLA	E	810	-	-	10/21/97/115	-
15	BCR	E	849	-	-	19/29/63/63	0/2/2/2
13	CLA	A	804	-	-	8/21/97/115	-
13	CLA	F	202	-	-	7/15/91/115	-
13	CLA	E	825	1	-	11/20/96/115	-
15	BCR	B	845	-	-	17/29/63/63	0/2/2/2
15	BCR	L	205	-	-	13/29/63/63	0/2/2/2
13	CLA	G	833	2	-	4/21/97/115	-
13	CLA	A	807	-	-	8/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	E	826	1	-	15/21/97/115	-
15	BCR	E	851	-	-	8/29/63/63	0/2/2/2
13	CLA	a	845	1	-	8/21/97/115	-
13	CLA	e	816	-	-	7/15/91/115	-
13	CLA	B	810	-	-	4/21/97/115	-
13	CLA	E	828	-	-	6/21/97/115	-
13	CLA	G	838	-	-	8/21/97/115	-
13	CLA	a	837	-	-	10/21/97/115	-
13	CLA	E	834	1	-	8/21/97/115	-
13	CLA	G	839	-	-	9/18/94/115	-
13	CLA	e	806	-	-	8/21/97/115	-
15	BCR	g	847	-	-	22/29/63/63	0/2/2/2
13	CLA	g	827	-	-	6/17/93/115	-
15	BCR	A	849	-	-	8/29/63/63	0/2/2/2
13	CLA	a	836	-	-	6/21/97/115	-
13	CLA	E	819	1	-	12/20/96/115	-
13	CLA	e	812	-	-	6/15/91/115	-
13	CLA	B	808	-	-	6/21/97/115	-
13	CLA	a	825	1	-	11/20/96/115	-
13	CLA	B	828	2	-	8/21/97/115	-
13	CLA	s	205	2	-	14/21/97/115	-
13	CLA	a	816	1	-	5/21/97/115	-
13	CLA	a	832	1	-	6/21/97/115	-
13	CLA	g	805	-	-	8/21/97/115	-
13	CLA	b	822	2	-	9/21/97/115	-
13	CLA	b	801	-	-	4/9/81/115	-
13	CLA	B	825	-	-	6/21/97/115	-
13	CLA	G	837	-	-	6/21/97/115	-
13	CLA	G	836	-	-	8/15/91/115	-
13	CLA	a	812	1	-	8/21/97/115	-
15	BCR	p	101	-	-	10/29/63/63	0/2/2/2
13	CLA	A	825	1	-	11/20/96/115	-
13	CLA	A	816	1	-	5/21/97/115	-
13	CLA	B	811	2	-	6/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	G	803	-	-	8/21/97/115	-
13	CLA	A	826	1	-	15/21/97/115	-
13	CLA	E	830	-	-	8/21/97/115	-
16	SF4	h	102	3	-	-	0/6/5/5
13	CLA	E	818	-	-	6/15/91/115	-
13	CLA	e	836	1	-	9/21/97/115	-
15	BCR	S	201	-	-	17/29/63/63	0/2/2/2
13	CLA	G	816	-	-	6/15/91/115	-
15	BCR	a	849	-	-	19/29/63/63	0/2/2/2
13	CLA	G	832	-	-	8/20/96/115	-
13	CLA	B	802	-	-	8/21/97/115	-
13	CLA	E	824	-	-	10/21/97/115	-
13	CLA	B	804	-	-	8/21/97/115	-
15	BCR	l	206	-	-	17/29/63/63	0/2/2/2
13	CLA	E	846	-	-	3/9/81/115	-
13	CLA	e	844	12	-	10/21/97/115	-
15	BCR	g	849	-	-	16/29/63/63	0/2/2/2
13	CLA	B	830	2	-	6/21/97/115	-
13	CLA	b	840	-	-	9/21/97/115	-
13	CLA	B	822	-	-	6/15/91/115	-
13	CLA	o	202	-	-	7/15/91/115	-
13	CLA	e	825	1	-	15/21/97/115	-
13	CLA	e	852	-	-	10/21/97/115	-
13	CLA	g	828	-	-	4/21/97/115	-
13	CLA	E	832	1	-	6/21/97/115	-
13	CLA	R	102	-	-	8/15/91/115	-
15	BCR	q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	B	812	2	-	14/21/97/115	-
13	CLA	e	835	-	-	10/21/97/115	-
13	CLA	b	820	2	-	10/18/94/115	-
15	BCR	b	844	-	-	17/29/63/63	0/2/2/2
16	SF4	a	846	-	-	-	0/6/5/5
13	CLA	B	824	-	-	8/15/91/115	-
13	CLA	b	813	-	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	817	-	-	10/21/97/115	-
13	CLA	K	102	-	-	8/15/91/115	-
13	CLA	O	203	-	-	7/15/91/115	-
15	BCR	b	843	-	-	20/29/63/63	0/2/2/2
13	CLA	B	827	-	-	4/21/97/115	-
13	CLA	B	833	2	-	4/21/97/115	-
13	CLA	b	823	-	-	8/15/91/115	-
13	CLA	g	834	2	-	4/21/97/115	-
13	CLA	a	808	-	-	6/21/97/115	-
13	CLA	g	840	-	-	10/18/94/115	-
13	CLA	A	842	1	-	6/21/97/115	-
13	CLA	a	823	-	-	10/21/97/115	-
15	BCR	l	202	-	-	18/29/63/63	0/2/2/2
13	CLA	e	843	1	-	8/21/97/115	-
12	LHG	a	801	-	-	32/53/53/53	-
13	CLA	B	818	2	-	12/21/97/115	-
15	BCR	k	4001	-	-	21/29/63/63	0/2/2/2
15	BCR	e	848	-	-	8/29/63/63	0/2/2/2
13	CLA	B	832	-	-	8/20/96/115	-
13	CLA	A	845	12	-	8/21/97/115	-
13	CLA	L	202	10	-	6/21/97/115	-
13	CLA	g	820	-	-	9/21/97/115	-
13	CLA	e	834	-	-	6/21/97/115	-
15	BCR	f	201	-	-	8/29/63/63	0/2/2/2
13	CLA	A	822	-	-	11/21/97/115	-
12	LHG	e	802	13	-	14/42/42/53	-
13	CLA	A	837	1	-	9/21/97/115	-
13	CLA	K	101	-	-	3/9/81/115	-
15	BCR	g	844	-	-	9/29/63/63	0/2/2/2
13	CLA	b	817	2	-	12/21/97/115	-
15	BCR	s	204	-	-	12/29/63/63	0/2/2/2
15	BCR	O	202	-	-	16/29/63/63	0/2/2/2
13	CLA	E	833	-	-	6/21/97/115	-
13	CLA	g	837	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	g	823	-	-	6/15/91/115	-
15	BCR	a	848	-	-	16/29/63/63	0/2/2/2
13	CLA	r	102	-	-	8/15/91/115	-
12	LHG	A	801	-	-	32/53/53/53	-
13	CLA	g	826	-	-	6/21/97/115	-
13	CLA	E	838	1	-	9/21/97/115	-
14	PQN	B	842	-	-	11/23/43/43	0/2/2/2
13	CLA	S	203	10	-	5/15/91/115	-
13	CLA	e	831	1	-	6/21/97/115	-
16	SF4	H	102	3	-	-	0/6/5/5
13	CLA	B	806	2	-	2/21/97/115	-
13	CLA	B	836	-	-	8/15/91/115	-
13	CLA	g	824	2	-	8/21/97/115	-
13	CLA	B	807	2	-	12/21/97/115	-
15	BCR	G	847	-	-	12/29/63/63	0/2/2/2
13	CLA	B	831	2	-	12/15/91/115	-
15	BCR	G	846	-	-	22/29/63/63	0/2/2/2
16	SF4	h	101	-	-	-	0/6/5/5
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
15	BCR	G	844	-	-	20/29/63/63	0/2/2/2
13	CLA	g	842	-	-	9/21/97/115	-
15	BCR	a	802	-	-	10/29/63/63	0/2/2/2
13	CLA	l	204	10	-	5/15/91/115	-
13	CLA	b	830	2	-	12/15/91/115	-
13	CLA	E	842	-	-	7/18/94/115	-
13	CLA	E	845	1	-	8/21/97/115	-
16	SF4	C	101	-	-	-	0/6/5/5
13	CLA	G	809	-	-	4/21/97/115	-
13	CLA	A	811	-	-	5/21/97/115	-
13	CLA	e	809	-	-	10/21/97/115	-
13	CLA	E	836	-	-	6/21/97/115	-
15	BCR	A	852	-	-	15/29/63/63	0/2/2/2
13	CLA	g	822	2	-	10/18/94/115	-
13	CLA	E	822	-	-	11/21/97/115	-
13	CLA	a	844	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	b	846	-	-	12/29/63/63	0/2/2/2
13	CLA	B	820	-	-	7/21/97/115	-
13	CLA	e	827	-	-	6/21/97/115	-
13	CLA	A	841	-	-	6/18/94/115	-
13	CLA	A	806	-	-	10/21/97/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
13	CLA	a	852	-	-	8/21/97/115	-
15	BCR	g	848	-	-	12/29/63/63	0/2/2/2
13	CLA	B	838	-	-	8/21/97/115	-
13	CLA	E	803	-	-	7/21/97/115	-
13	CLA	a	806	-	-	10/21/97/115	-
13	CLA	A	808	-	-	6/21/97/115	-
13	CLA	g	841	-	-	9/21/97/115	-
13	CLA	g	819	2	-	12/21/97/115	-
13	CLA	b	825	-	-	6/17/93/115	-
13	CLA	b	835	-	-	8/15/91/115	-
13	CLA	k	4002	-	-	8/15/91/115	-
15	BCR	G	843	-	-	9/29/63/63	0/2/2/2
13	CLA	g	802	-	-	5/21/97/115	-
13	CLA	a	828	-	-	6/21/97/115	-
13	CLA	e	833	1	-	8/21/97/115	-
13	CLA	b	826	-	-	4/21/97/115	-
13	CLA	L	204	-	-	10/21/97/115	-
13	CLA	A	836	-	-	10/21/97/115	-
15	BCR	A	847	-	-	19/29/63/63	0/2/2/2
15	BCR	a	851	-	-	8/29/63/63	0/2/2/2
13	CLA	a	830	-	-	8/21/97/115	-
13	CLA	A	815	1	-	8/21/97/115	-
15	BCR	Q	101	-	-	13/29/63/63	0/2/2/2
13	CLA	G	801	-	-	8/21/97/115	-
15	BCR	g	846	-	-	17/29/63/63	0/2/2/2

The worst 5 of 3495 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
13	L	204	CLA	MG-ND	9.43	2.24	2.05
13	s	203	CLA	MG-ND	9.40	2.24	2.05
14	G	842	PQN	C3-C2	7.73	1.49	1.35

The worst 5 of 2944 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

There are no chirality outliers.

5 of 4075 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.

410 monomers are involved in 1257 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	816	CLA	1	0
16	H	101	SF4	2	0
16	c	102	SF4	2	0
13	e	815	CLA	5	0
13	b	814	CLA	1	0
15	q	102	BCR	1	0
13	B	835	CLA	2	0
13	a	819	CLA	3	0
13	S	206	CLA	2	0
13	b	821	CLA	1	0
13	b	815	CLA	1	0
13	A	803	CLA	7	0
13	G	830	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	l	203	CLA	2	0
13	g	830	CLA	4	0
14	a	847	PQN	2	0
13	b	806	CLA	2	0
13	a	811	CLA	1	0
13	e	837	CLA	2	0
15	f	202	BCR	4	0
13	B	839	CLA	3	0
13	E	817	CLA	3	0
13	b	828	CLA	3	0
15	e	847	BCR	6	0
13	e	826	CLA	1	0
13	a	840	CLA	5	0
13	e	822	CLA	3	0
13	E	840	CLA	5	0
13	a	826	CLA	2	0
15	L	201	BCR	4	0
13	G	819	CLA	3	0
13	E	837	CLA	5	0
13	b	818	CLA	4	0
15	i	101	BCR	3	0
15	J	102	BCR	1	0
16	B	803	SF4	1	0
13	b	839	CLA	5	0
13	r	101	CLA	2	0
13	G	823	CLA	3	0
15	O	201	BCR	2	0
15	F	201	BCR	6	0
13	e	819	CLA	4	0
13	B	809	CLA	1	0
14	A	846	PQN	10	0
13	A	840	CLA	3	0
13	b	805	CLA	1	0
13	b	832	CLA	3	0
13	e	803	CLA	7	0
13	a	843	CLA	2	0
13	G	831	CLA	2	0
13	s	203	CLA	16	0
13	g	831	CLA	1	0
13	g	813	CLA	1	0
15	o	201	BCR	3	0
13	b	804	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	820	CLA	5	0
13	g	803	CLA	3	0
13	G	802	CLA	1	0
13	E	813	CLA	1	0
15	a	803	BCR	1	0
13	E	809	CLA	3	0
14	G	842	PQN	1	0
13	g	808	CLA	2	0
15	E	801	BCR	2	0
13	B	829	CLA	4	0
13	a	820	CLA	5	0
16	E	847	SF4	1	0
13	A	828	CLA	1	0
15	B	848	BCR	4	0
13	G	811	CLA	3	0
13	a	829	CLA	1	0
13	e	841	CLA	2	0
15	a	853	BCR	6	0
13	E	835	CLA	1	0
13	E	841	CLA	3	0
13	e	807	CLA	3	0
13	A	813	CLA	1	0
13	B	834	CLA	7	0
14	e	845	PQN	1	0
13	A	809	CLA	3	0
13	l	205	CLA	3	0
13	G	840	CLA	6	0
13	b	807	CLA	1	0
12	A	802	LHG	3	0
15	S	205	BCR	2	0
13	G	814	CLA	5	0
15	G	845	BCR	1	0
13	g	835	CLA	7	0
15	B	847	BCR	1	0
16	c	101	SF4	2	0
16	g	804	SF4	1	0
13	G	829	CLA	4	0
13	a	813	CLA	1	0
13	A	827	CLA	2	0
13	B	826	CLA	6	0
13	l	201	CLA	2	0
13	A	844	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	e	801	LHG	2	0
15	b	842	BCR	2	0
13	A	818	CLA	1	0
15	b	845	BCR	2	0
13	s	202	CLA	8	0
14	g	843	PQN	2	0
15	S	202	BCR	1	0
13	e	813	CLA	3	0
15	m	101	BCR	6	0
13	a	805	CLA	3	0
15	e	846	BCR	14	0
13	B	819	CLA	4	0
13	e	839	CLA	3	0
13	b	824	CLA	2	0
15	A	850	BCR	3	0
13	G	804	CLA	6	0
13	g	806	CLA	5	0
13	G	813	CLA	2	0
13	e	824	CLA	10	0
13	G	815	CLA	1	0
13	A	838	CLA	3	0
13	e	823	CLA	1	0
13	e	804	CLA	6	0
13	A	805	CLA	4	0
13	G	806	CLA	1	0
13	a	810	CLA	2	0
13	b	829	CLA	1	0
13	G	808	CLA	1	0
13	a	839	CLA	2	0
13	b	810	CLA	2	0
13	E	843	CLA	3	0
13	g	811	CLA	2	0
13	a	817	CLA	14	0
13	E	821	CLA	7	0
15	B	846	BCR	1	0
13	E	811	CLA	2	0
15	a	850	BCR	19	0
13	b	808	CLA	3	0
13	a	822	CLA	4	0
13	a	814	CLA	1	0
15	g	845	BCR	5	0
13	b	834	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	A	810	CLA	2	0
13	g	814	CLA	2	0
14	b	841	PQN	1	0
13	g	829	CLA	4	0
13	e	814	CLA	1	0
13	b	802	CLA	6	0
13	E	814	CLA	3	0
13	A	834	CLA	2	0
13	G	825	CLA	2	0
15	A	851	BCR	3	0
13	g	825	CLA	8	0
13	a	831	CLA	1	0
16	C	102	SF4	2	0
13	a	834	CLA	2	0
13	G	805	CLA	2	0
13	G	835	CLA	2	0
13	G	826	CLA	6	0
13	e	838	CLA	5	0
13	A	821	CLA	6	0
13	g	817	CLA	2	0
13	L	203	CLA	3	0
13	b	831	CLA	2	0
15	e	849	BCR	3	0
15	e	850	BCR	3	0
13	a	807	CLA	2	0
13	E	839	CLA	2	0
13	E	820	CLA	6	0
15	E	852	BCR	2	0
13	A	831	CLA	1	0
13	G	812	CLA	1	0
13	a	818	CLA	6	0
13	G	834	CLA	7	0
13	a	821	CLA	7	0
13	G	810	CLA	2	0
13	e	810	CLA	2	0
13	E	815	CLA	1	0
13	E	823	CLA	7	0
13	B	801	CLA	1	0
13	B	814	CLA	6	0
13	e	821	CLA	4	0
13	A	817	CLA	3	0
13	B	823	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	812	CLA	2	0
15	e	851	BCR	2	0
13	a	841	CLA	3	0
13	A	839	CLA	5	0
13	a	824	CLA	1	0
15	s	201	BCR	2	0
13	b	809	CLA	3	0
13	A	814	CLA	3	0
13	G	817	CLA	5	0
13	G	828	CLA	4	0
13	G	807	CLA	1	0
13	B	815	CLA	1	0
13	e	828	CLA	1	0
15	E	802	BCR	2	0
13	E	831	CLA	1	0
13	B	813	CLA	3	0
13	a	842	CLA	3	0
13	b	833	CLA	8	0
13	E	816	CLA	5	0
13	G	818	CLA	4	0
13	a	809	CLA	2	0
13	E	804	CLA	4	0
13	b	816	CLA	5	0
13	e	830	CLA	1	0
13	b	838	CLA	3	0
13	E	807	CLA	3	0
13	A	853	CLA	1	0
13	g	812	CLA	2	0
13	b	827	CLA	4	0
13	g	809	CLA	1	0
13	g	836	CLA	2	0
13	A	835	CLA	5	0
13	A	833	CLA	2	0
13	e	811	CLA	2	0
13	e	805	CLA	3	0
13	b	811	CLA	1	0
13	E	806	CLA	2	0
13	E	805	CLA	3	0
15	T	101	BCR	3	0
13	A	832	CLA	6	0
15	B	844	BCR	4	0
13	e	808	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	e	817	CLA	1	0
13	A	823	CLA	2	0
13	E	808	CLA	3	0
13	a	833	CLA	2	0
13	S	204	CLA	2	0
13	e	840	CLA	4	0
13	a	804	CLA	4	0
13	G	827	CLA	2	0
14	E	848	PQN	4	0
13	g	832	CLA	1	0
13	e	832	CLA	2	0
13	G	822	CLA	1	0
15	E	850	BCR	5	0
13	B	840	CLA	6	0
13	A	812	CLA	3	0
13	B	805	CLA	5	0
15	R	101	BCR	37	0
13	a	838	CLA	2	0
13	a	815	CLA	1	0
13	e	820	CLA	7	0
13	g	815	CLA	5	0
13	g	818	CLA	5	0
15	J	101	BCR	1	0
13	E	812	CLA	2	0
13	g	801	CLA	5	0
15	G	848	BCR	5	0
15	b	847	BCR	4	0
13	b	803	CLA	2	0
13	G	824	CLA	8	0
13	E	810	CLA	2	0
15	E	849	BCR	30	0
13	A	804	CLA	5	0
13	F	202	CLA	2	0
13	E	825	CLA	10	0
15	L	205	BCR	2	0
13	G	833	CLA	2	0
13	A	807	CLA	4	0
13	E	826	CLA	2	0
15	E	851	BCR	8	0
13	a	845	CLA	2	0
13	e	816	CLA	4	0
13	B	810	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	828	CLA	1	0
13	a	837	CLA	5	0
13	E	834	CLA	2	0
13	G	839	CLA	4	0
13	e	806	CLA	4	0
15	g	847	BCR	1	0
13	g	827	CLA	7	0
15	A	849	BCR	7	0
13	a	836	CLA	9	0
13	E	819	CLA	1	0
13	e	812	CLA	1	0
13	B	808	CLA	1	0
13	a	825	CLA	11	0
13	B	828	CLA	4	0
13	s	205	CLA	7	0
13	a	816	CLA	5	0
13	a	832	CLA	6	0
13	g	805	CLA	5	0
13	b	822	CLA	3	0
13	b	801	CLA	3	0
13	B	825	CLA	2	0
13	G	836	CLA	2	0
13	a	812	CLA	4	0
15	p	101	BCR	1	0
13	A	825	CLA	10	0
13	A	816	CLA	5	0
13	B	811	CLA	2	0
13	G	803	CLA	2	0
13	A	826	CLA	5	0
16	h	102	SF4	2	0
13	E	818	CLA	1	0
13	e	836	CLA	3	0
15	S	201	BCR	7	0
13	G	816	CLA	2	0
15	a	849	BCR	26	0
13	G	832	CLA	4	0
13	B	802	CLA	5	0
13	E	824	CLA	1	0
13	B	804	CLA	5	0
15	l	206	BCR	1	0
13	E	846	CLA	2	0
13	e	844	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	g	849	BCR	4	0
13	B	830	CLA	1	0
13	B	822	CLA	1	0
13	o	202	CLA	2	0
13	e	825	CLA	5	0
13	e	852	CLA	2	0
13	g	828	CLA	2	0
13	E	832	CLA	5	0
13	R	102	CLA	2	0
13	B	812	CLA	2	0
13	e	835	CLA	4	0
16	a	846	SF4	1	0
13	B	824	CLA	8	0
13	b	813	CLA	5	0
13	B	817	CLA	4	0
13	K	102	CLA	2	0
13	O	203	CLA	1	0
15	b	843	BCR	5	0
13	B	827	CLA	2	0
13	B	833	CLA	2	0
13	b	823	CLA	8	0
13	g	834	CLA	2	0
13	a	808	CLA	3	0
13	g	840	CLA	4	0
13	A	842	CLA	4	0
13	a	823	CLA	8	0
15	l	202	BCR	5	0
12	a	801	LHG	3	0
13	B	818	CLA	4	0
15	k	4001	BCR	33	0
15	e	848	BCR	7	0
13	A	845	CLA	5	0
13	L	202	CLA	2	0
13	g	820	CLA	4	0
13	e	834	CLA	5	0
15	f	201	BCR	4	0
13	A	822	CLA	4	0
12	e	802	LHG	3	0
13	A	837	CLA	3	0
13	K	101	CLA	2	0
15	g	844	BCR	1	0
13	b	817	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	s	204	BCR	4	0
15	O	202	BCR	7	0
13	E	833	CLA	4	0
13	g	837	CLA	2	0
13	g	823	CLA	1	0
15	a	848	BCR	41	0
13	r	102	CLA	1	0
12	A	801	LHG	2	0
13	g	826	CLA	2	0
13	E	838	CLA	2	0
14	B	842	PQN	2	0
13	S	203	CLA	7	0
13	e	831	CLA	5	0
16	H	102	SF4	2	0
13	B	836	CLA	2	0
13	g	824	CLA	3	0
13	B	807	CLA	2	0
15	G	847	BCR	1	0
13	B	831	CLA	2	0
15	G	846	BCR	3	0
16	h	101	SF4	2	0
15	A	848	BCR	5	0
15	G	844	BCR	5	0
15	a	802	BCR	2	0
13	l	204	CLA	7	0
13	b	830	CLA	2	0
13	E	842	CLA	3	0
13	E	845	CLA	3	0
16	C	101	SF4	2	0
13	G	809	CLA	3	0
13	A	811	CLA	1	0
13	e	809	CLA	2	0
13	E	836	CLA	9	0
15	A	852	BCR	4	0
13	E	822	CLA	4	0
15	b	846	BCR	2	0
13	e	827	CLA	1	0
13	A	841	CLA	3	0
13	A	806	CLA	3	0
15	j	101	BCR	4	0
13	a	852	CLA	53	0
15	g	848	BCR	2	0

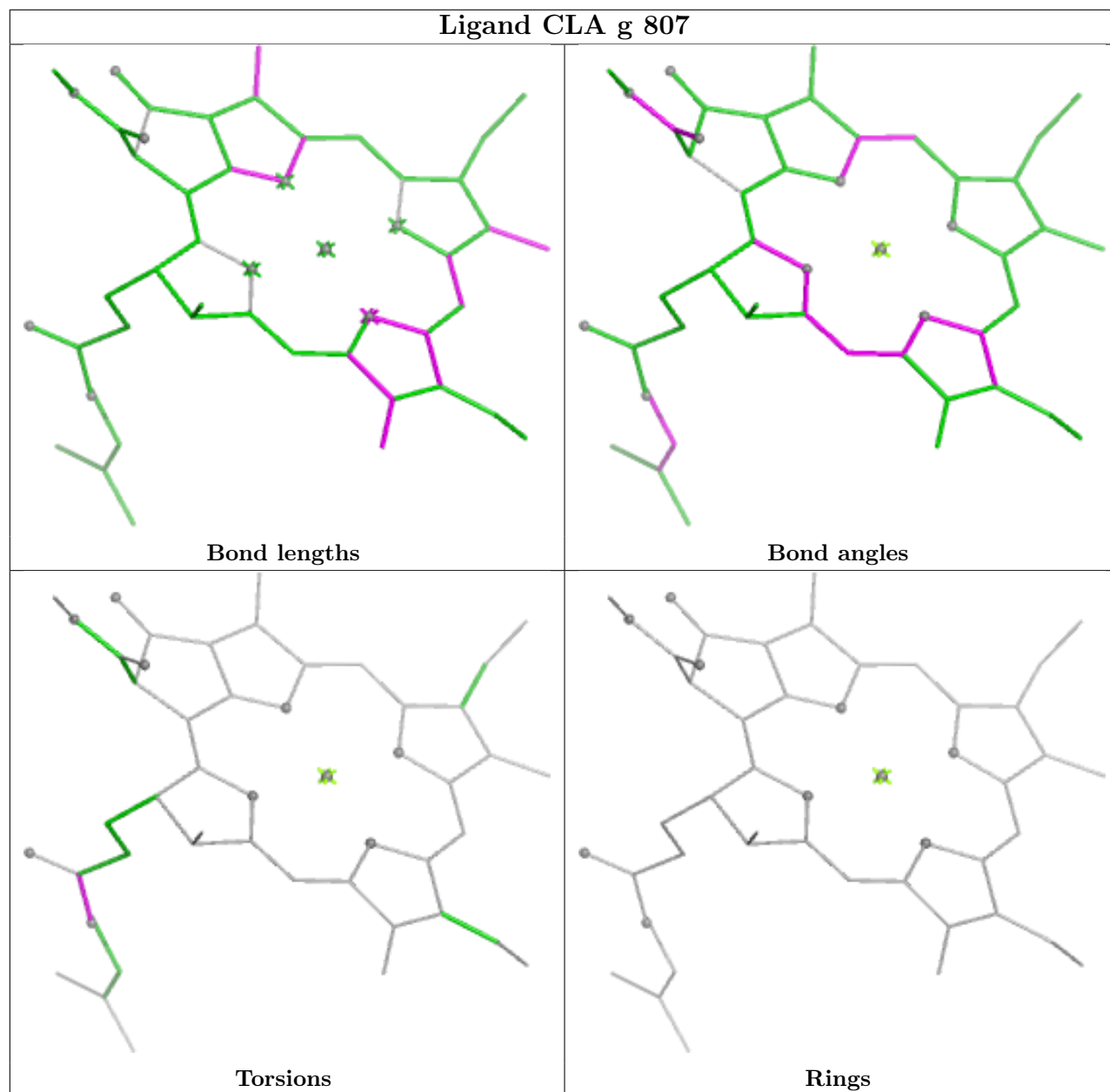
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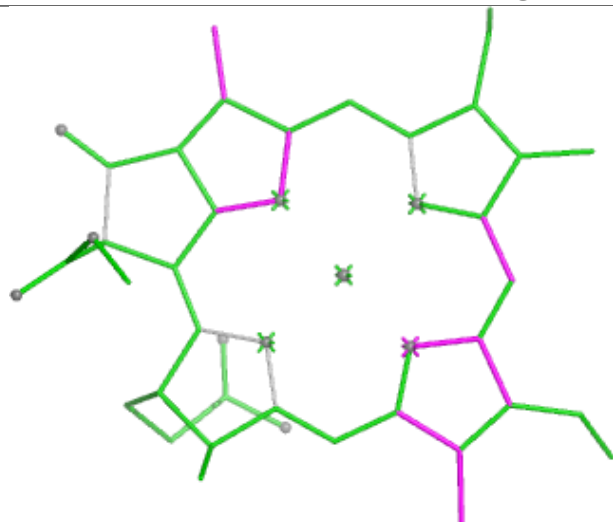
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	E	803	CLA	3	0
13	a	806	CLA	2	0
13	A	808	CLA	3	0
13	g	841	CLA	5	0
13	g	819	CLA	3	0
13	b	825	CLA	7	0
13	b	835	CLA	2	0
13	k	4002	CLA	2	0
15	G	843	BCR	1	0
13	g	802	CLA	1	0
13	a	828	CLA	1	0
13	e	833	CLA	4	0
13	b	826	CLA	2	0
13	L	204	CLA	8	0
13	A	836	CLA	6	0
15	A	847	BCR	12	0
15	a	851	BCR	8	0
13	A	815	CLA	1	0
13	G	801	CLA	5	0

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

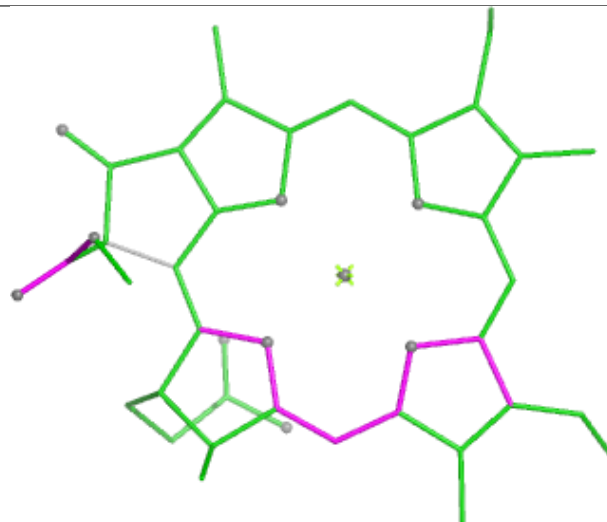
Ligand CLA g 807



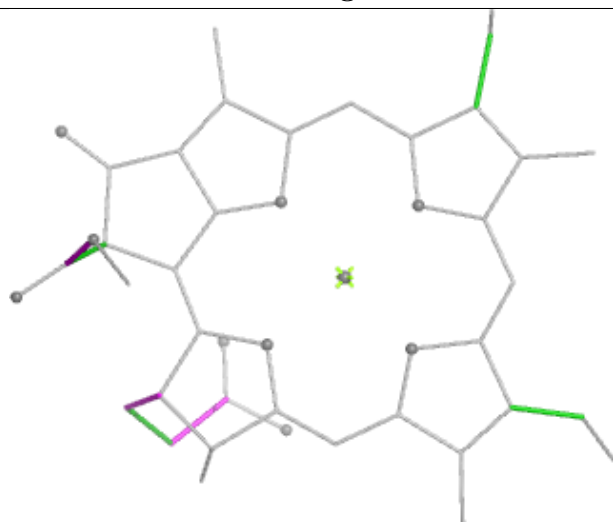
Ligand CLA B 816



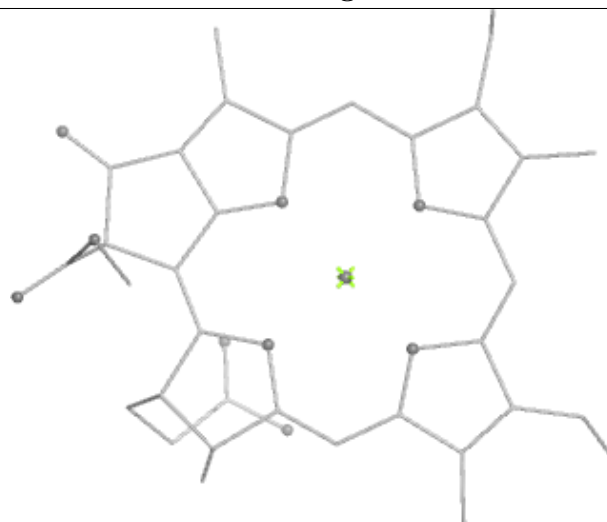
Bond lengths



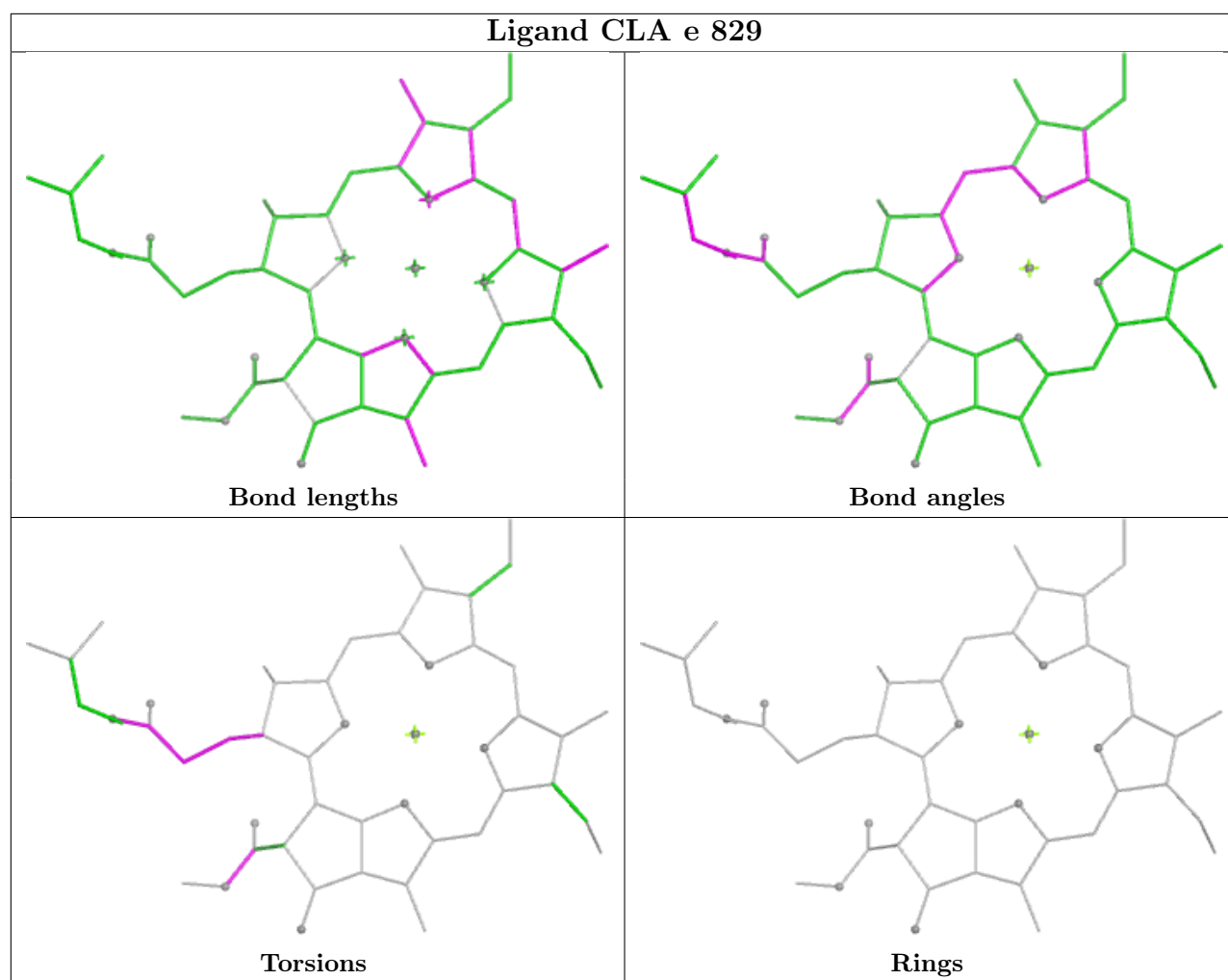
Bond angles



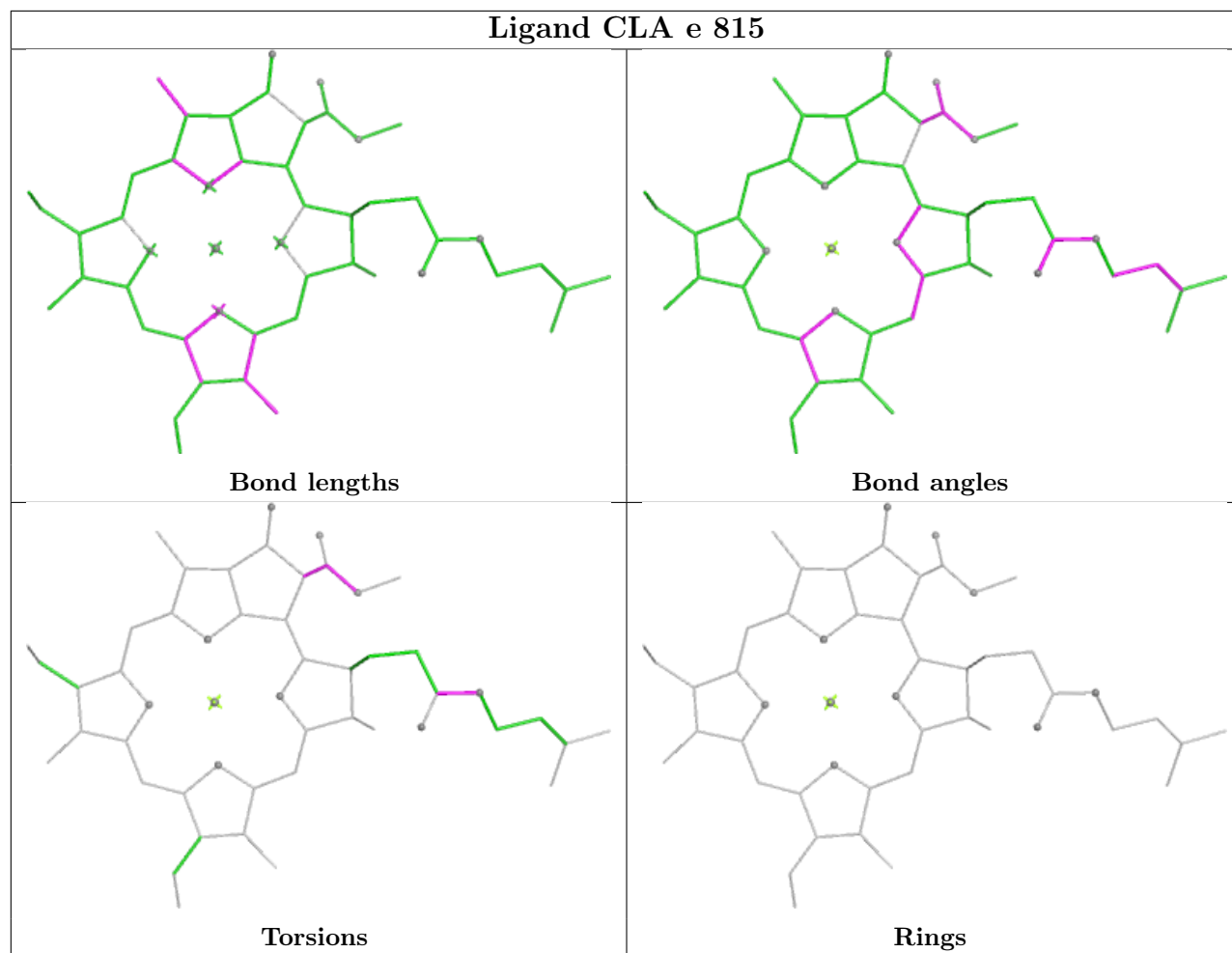
Torsions



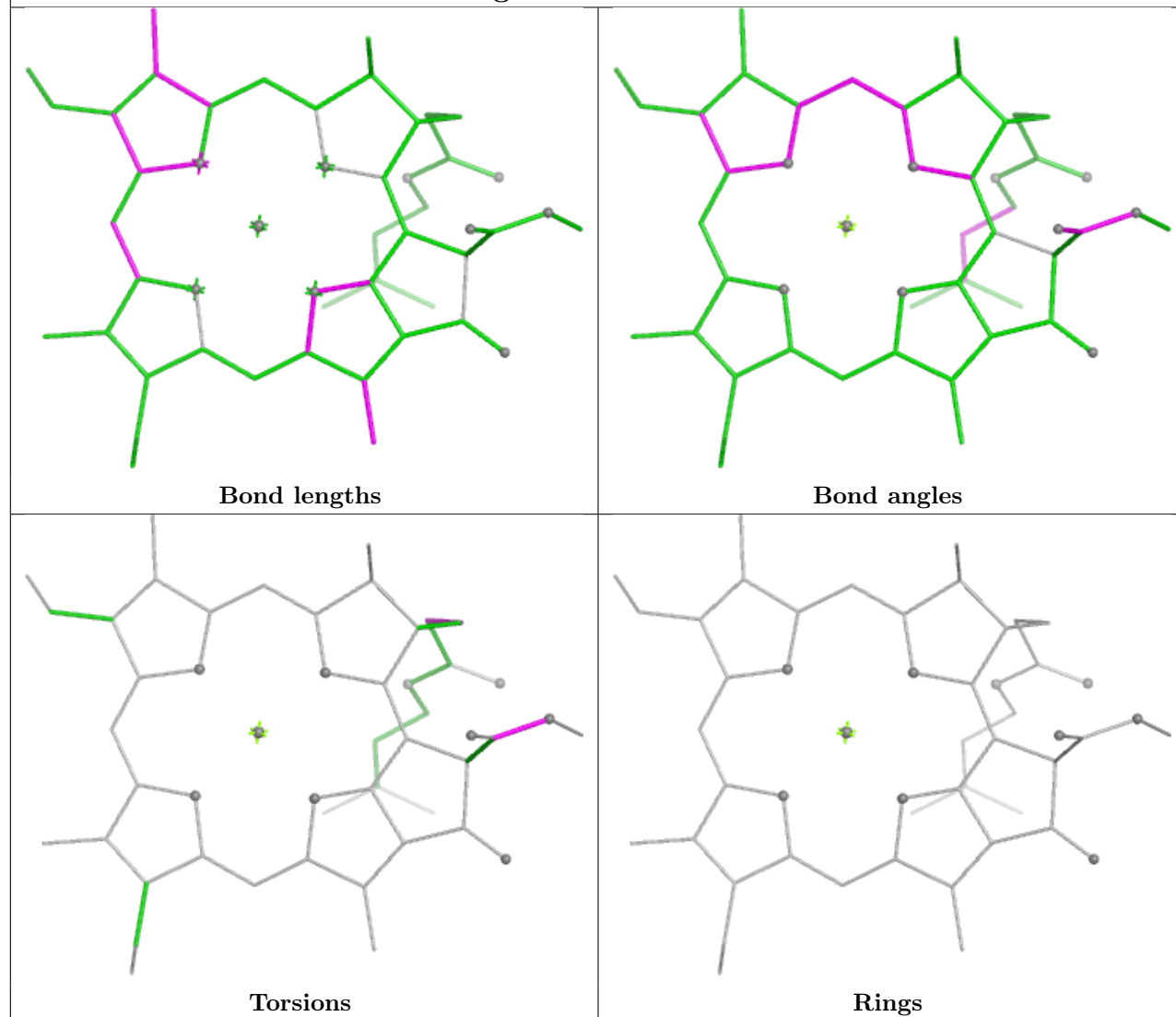
Rings



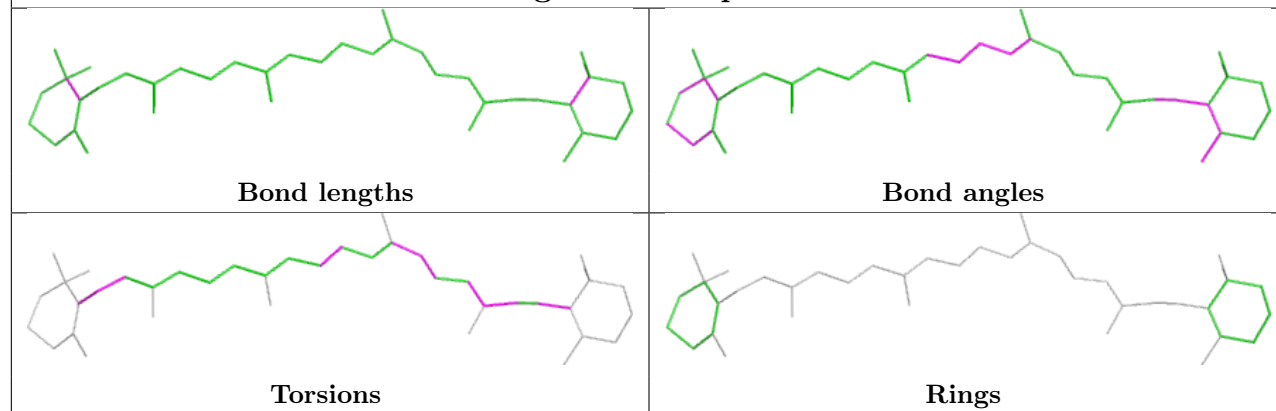
Ligand CLA e 815



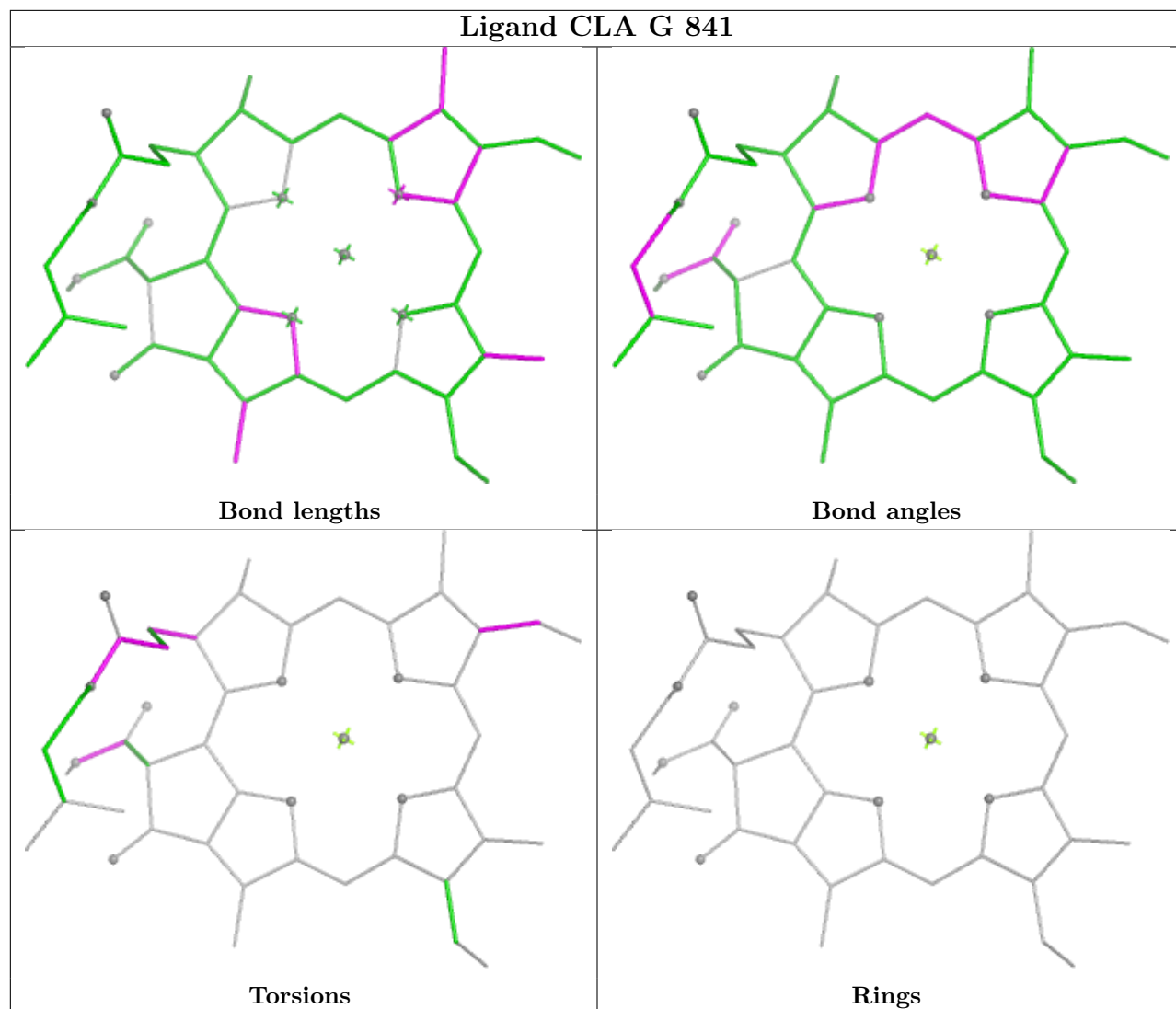
Ligand CLA b 814



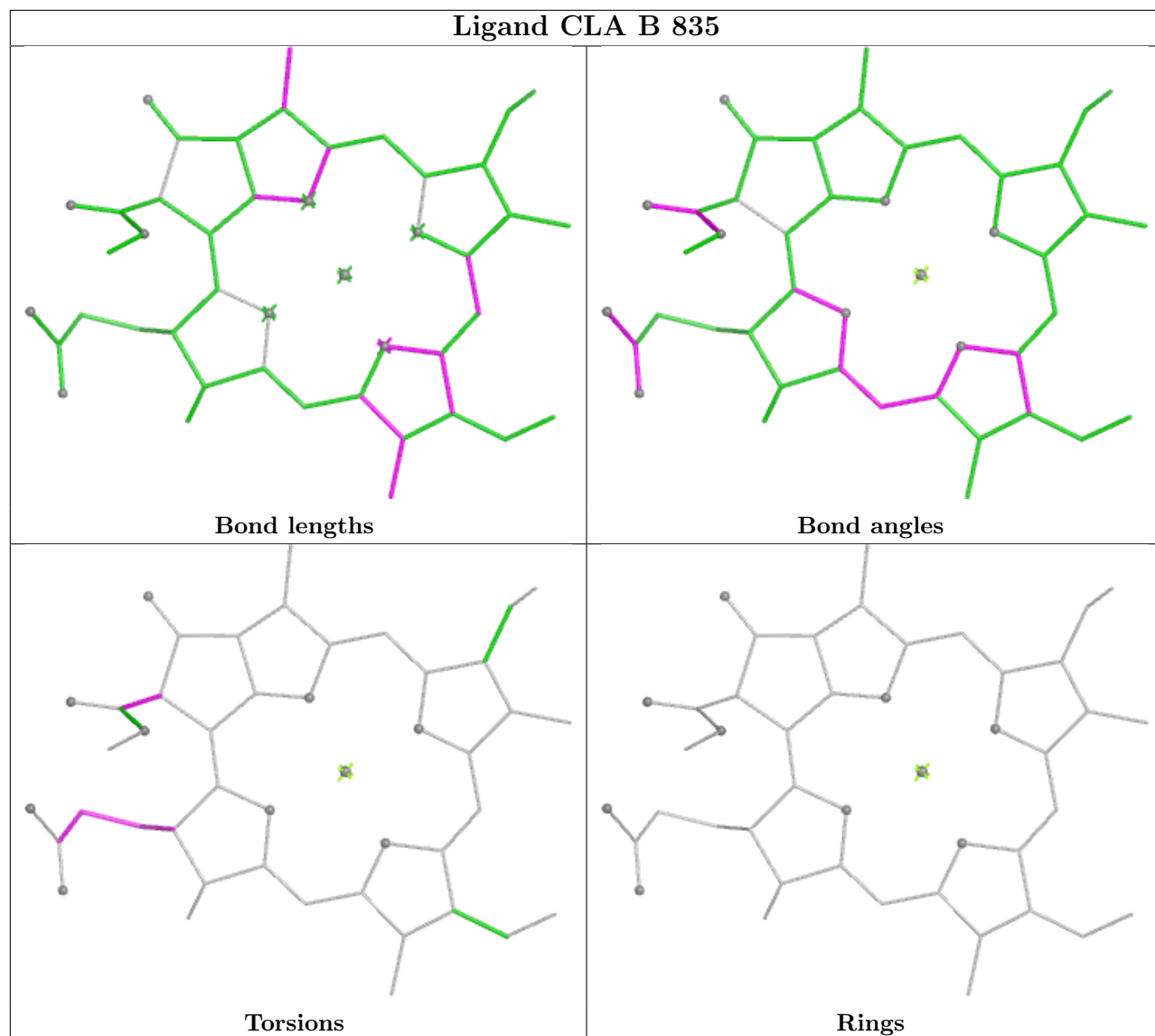
Ligand BCR q 102



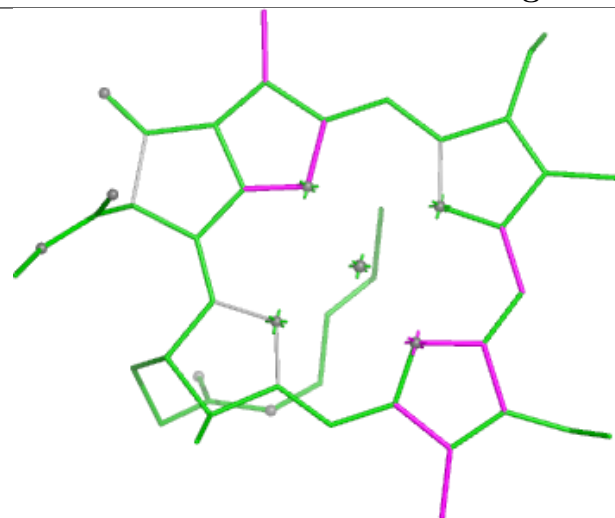
Ligand CLA G 841



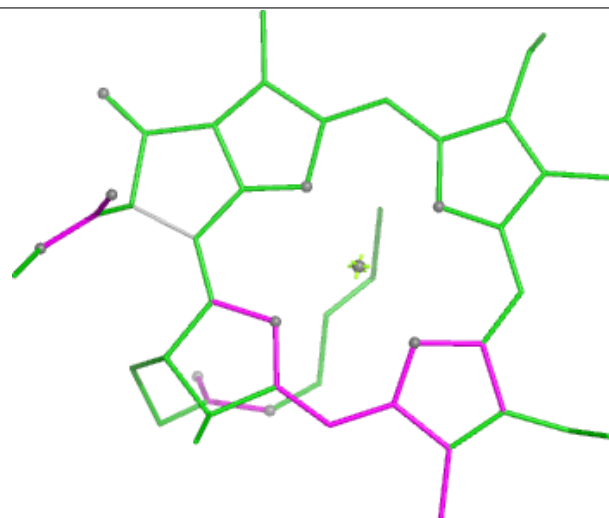
Ligand CLA B 835



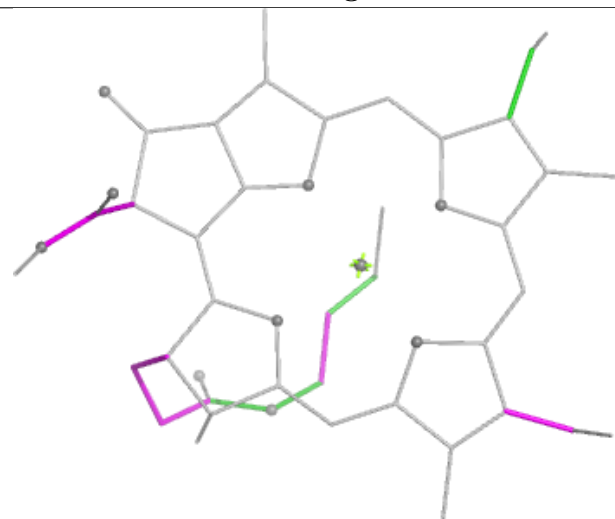
Ligand CLA a 819



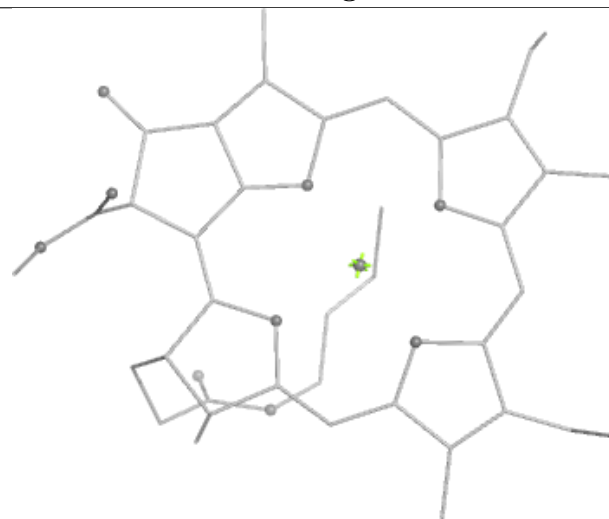
Bond lengths



Bond angles

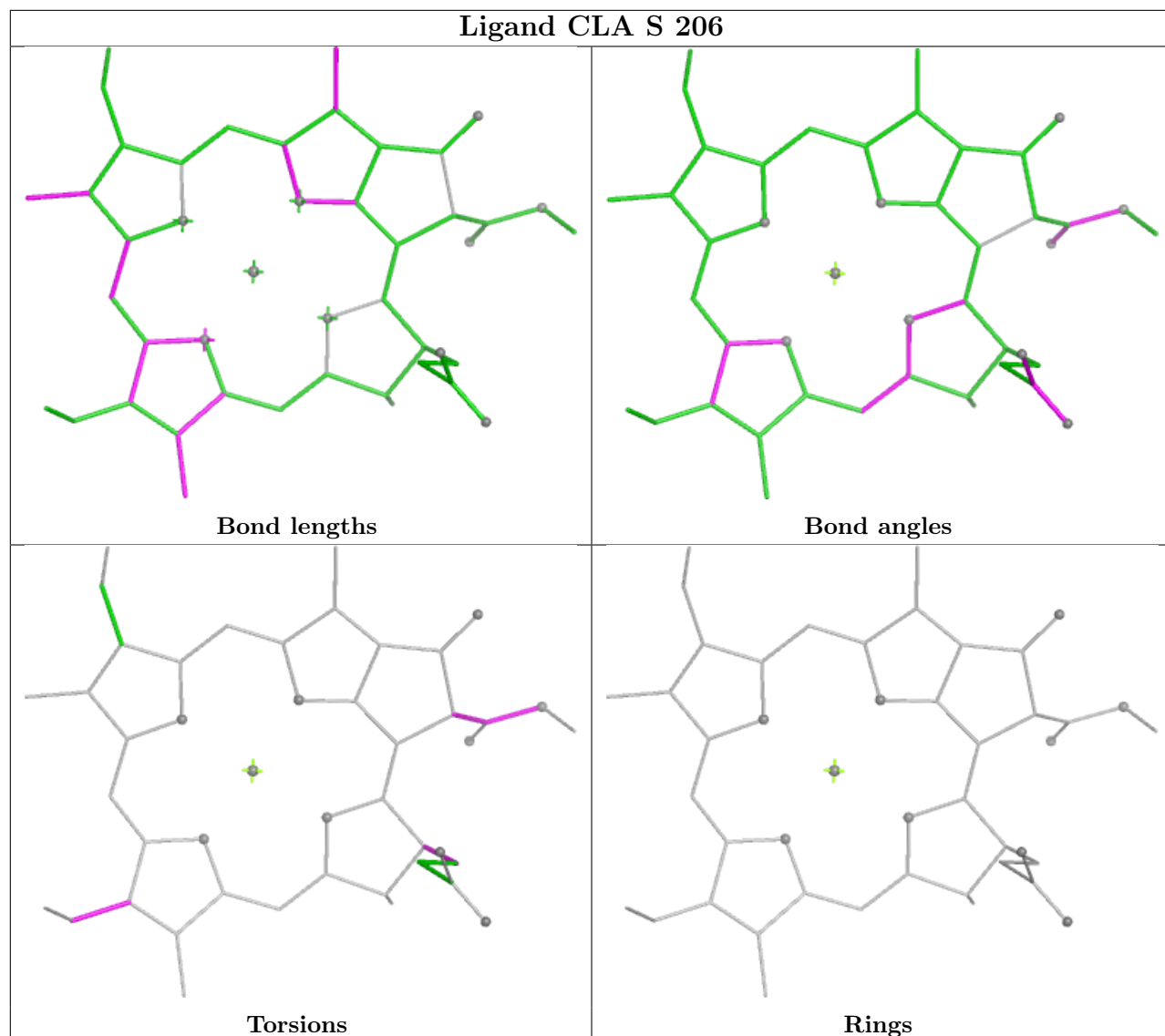


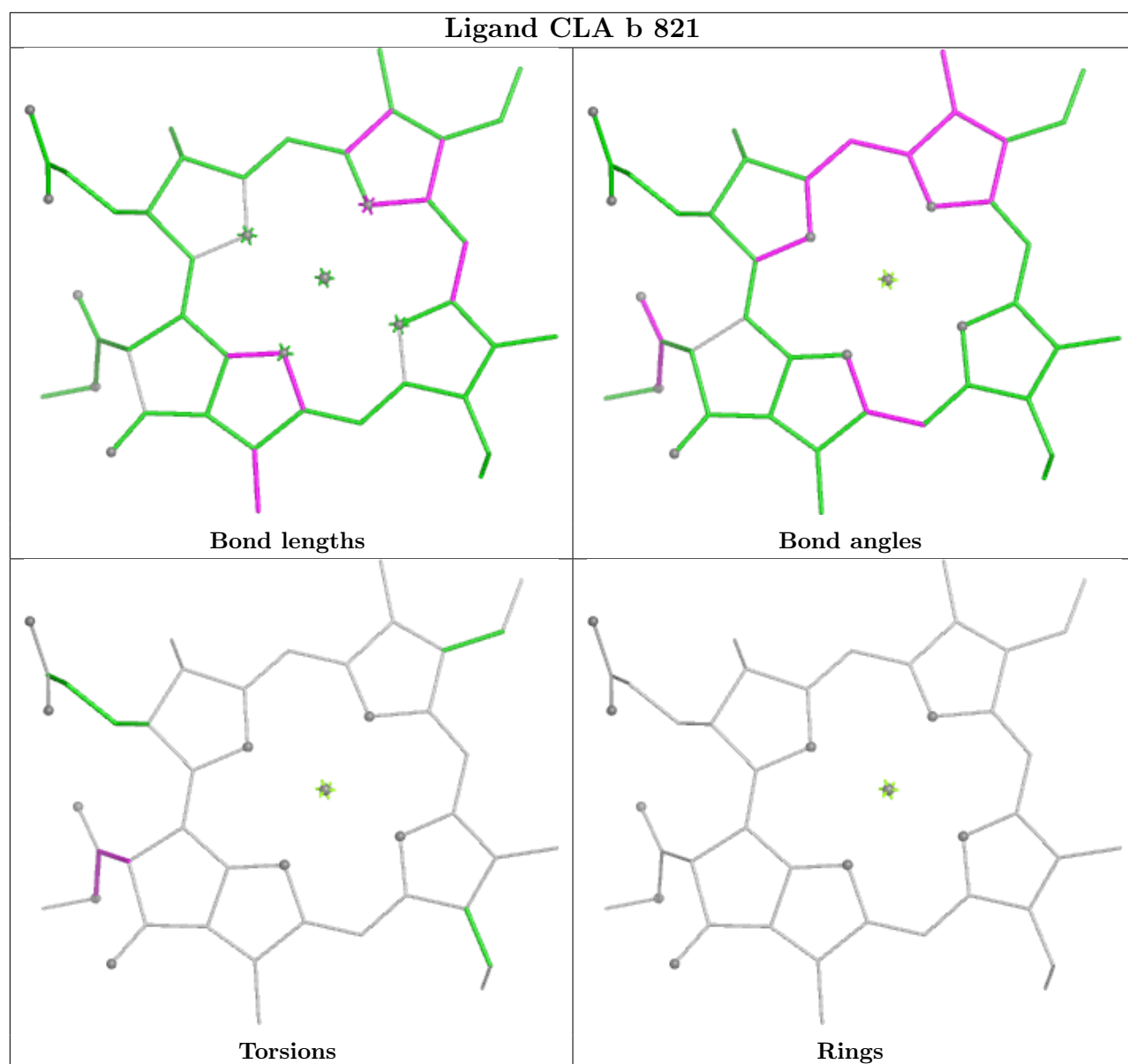
Torsions



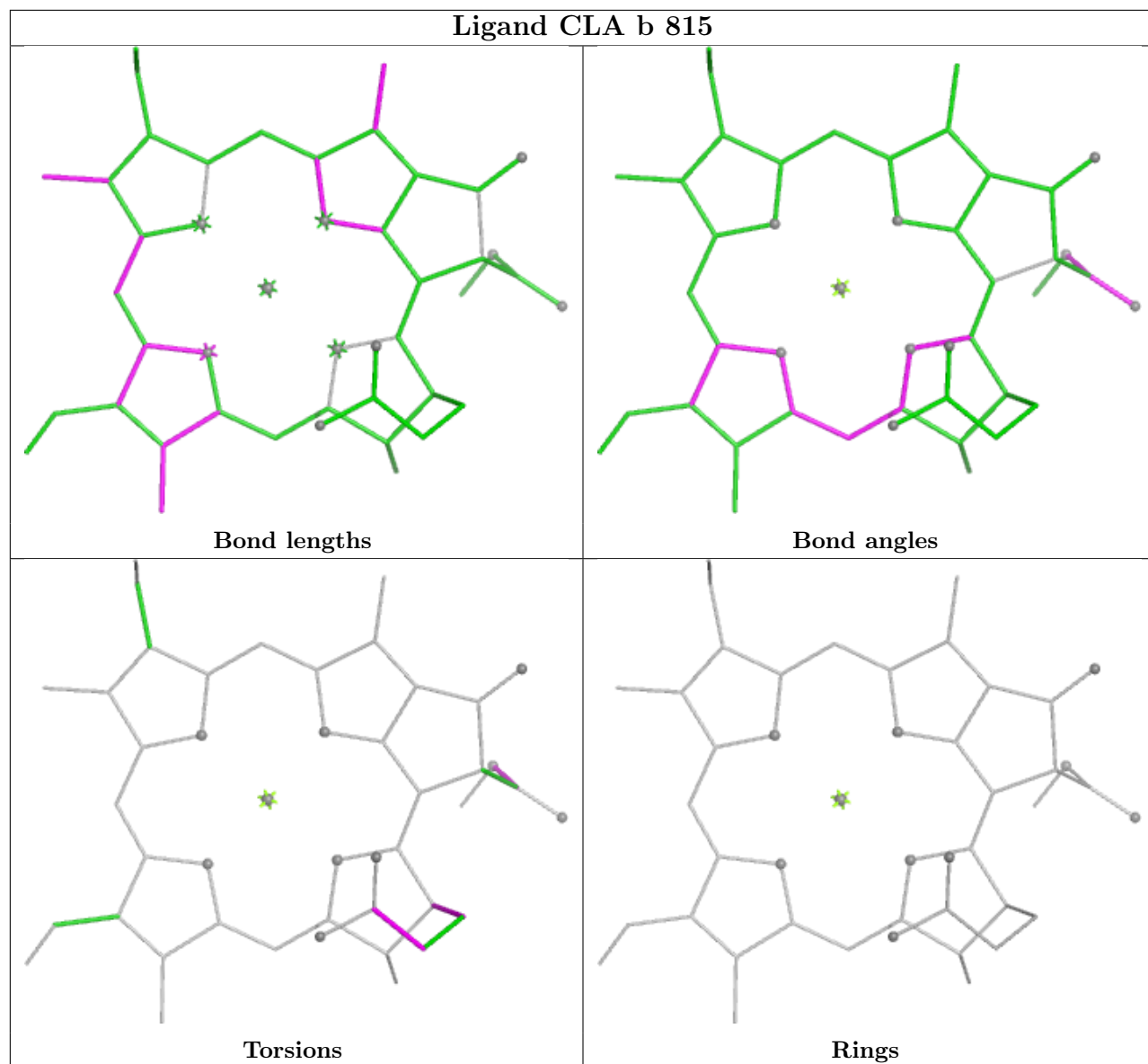
Rings

Ligand CLA S 206

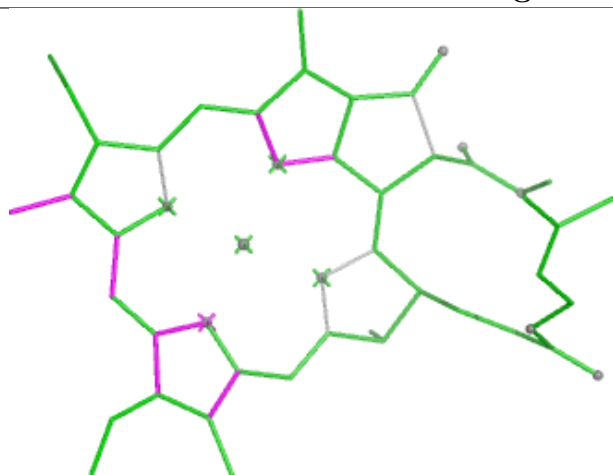




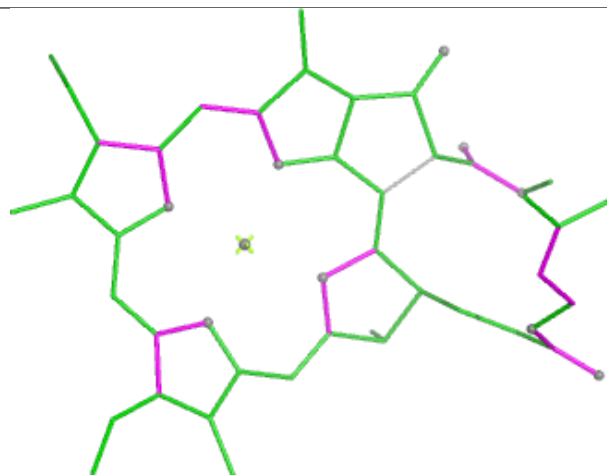
Ligand CLA b 815



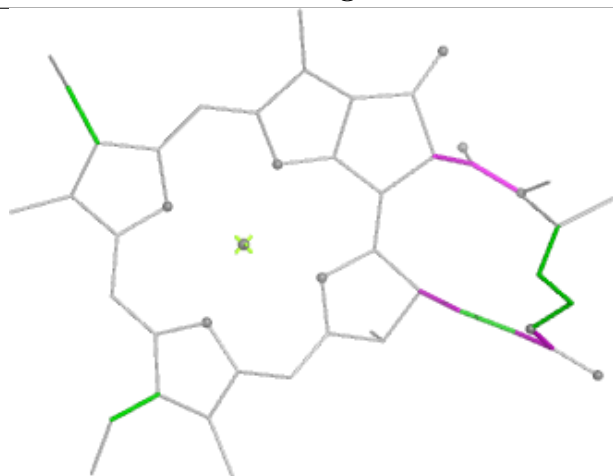
Ligand CLA A 803



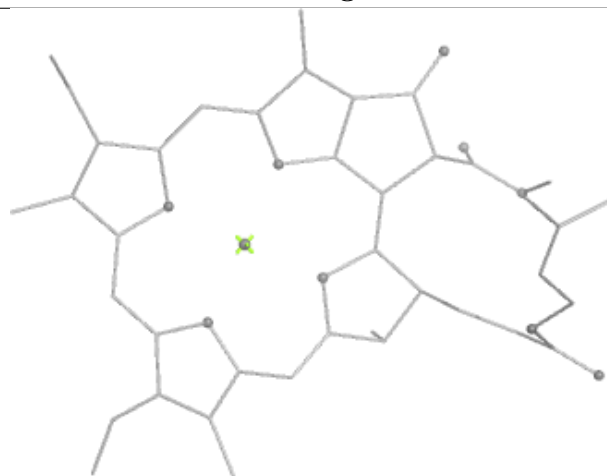
Bond lengths



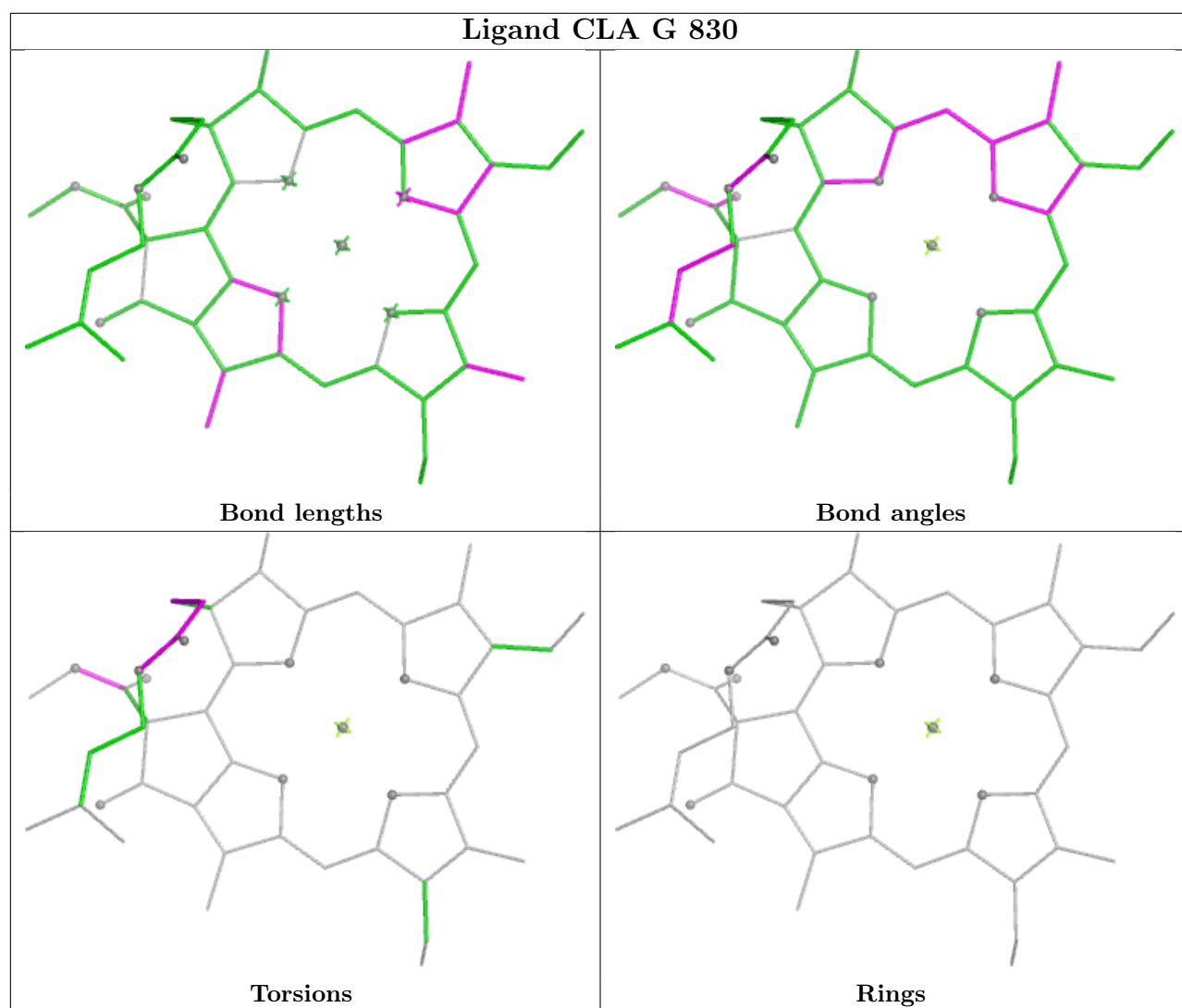
Bond angles



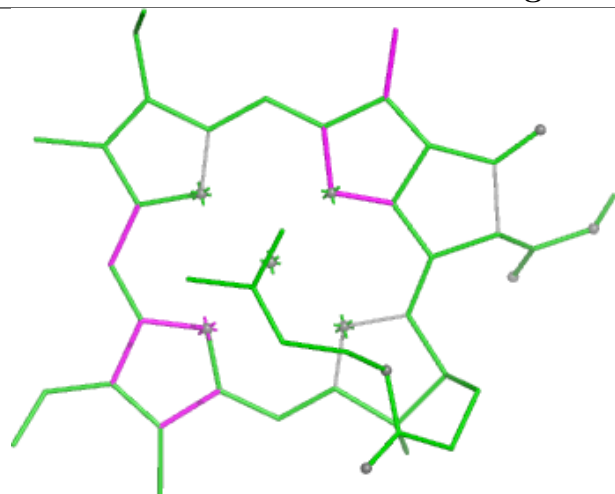
Torsions



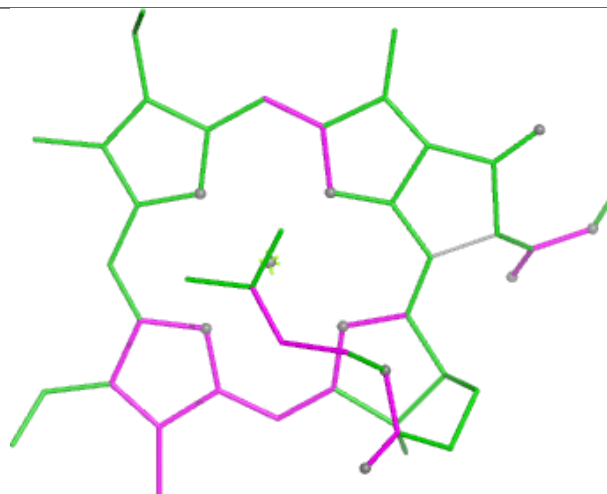
Rings



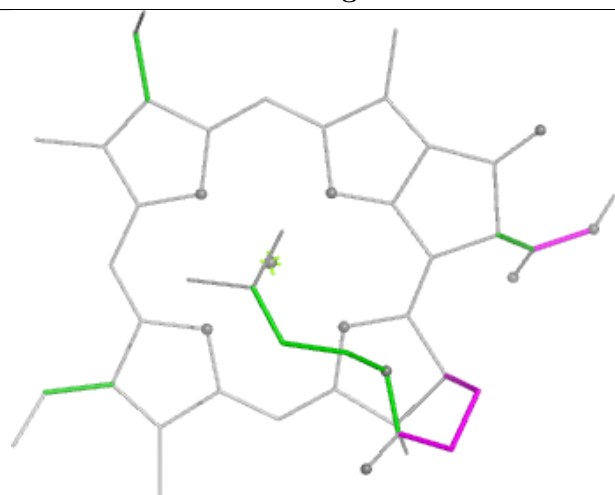
Ligand CLA 1 203



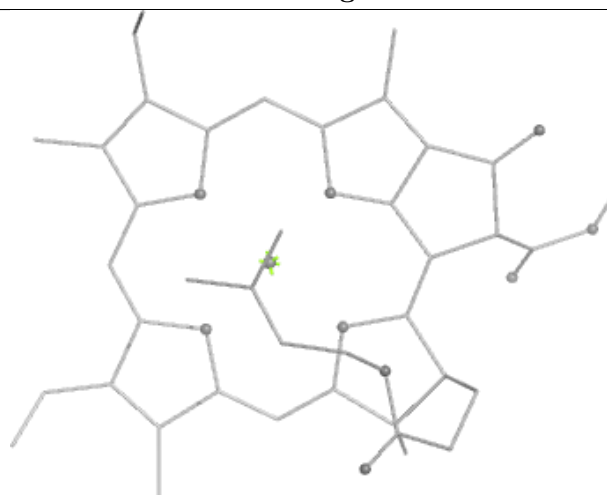
Bond lengths



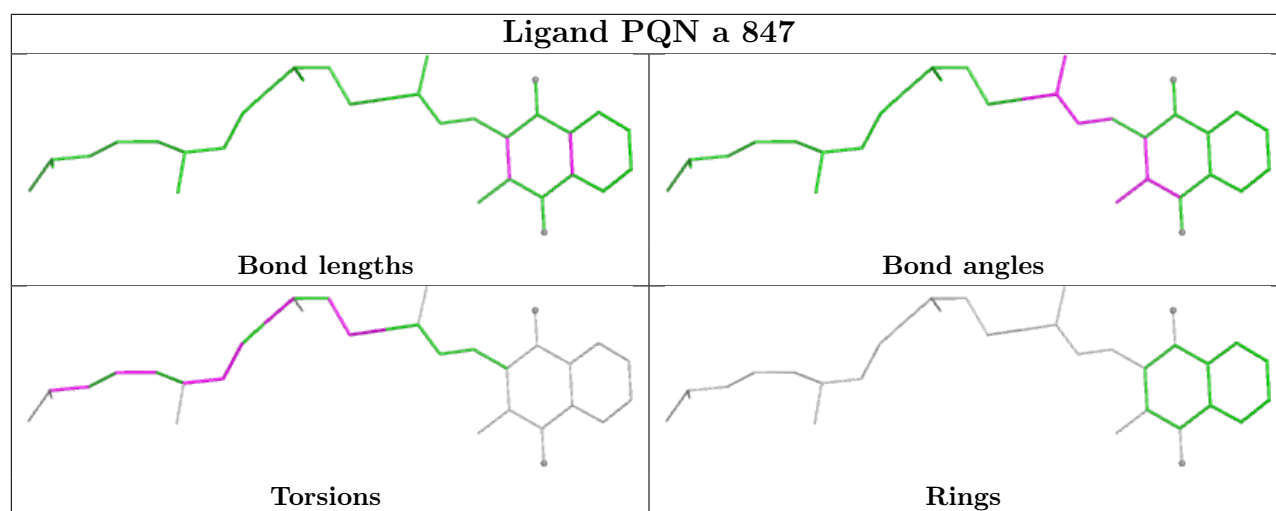
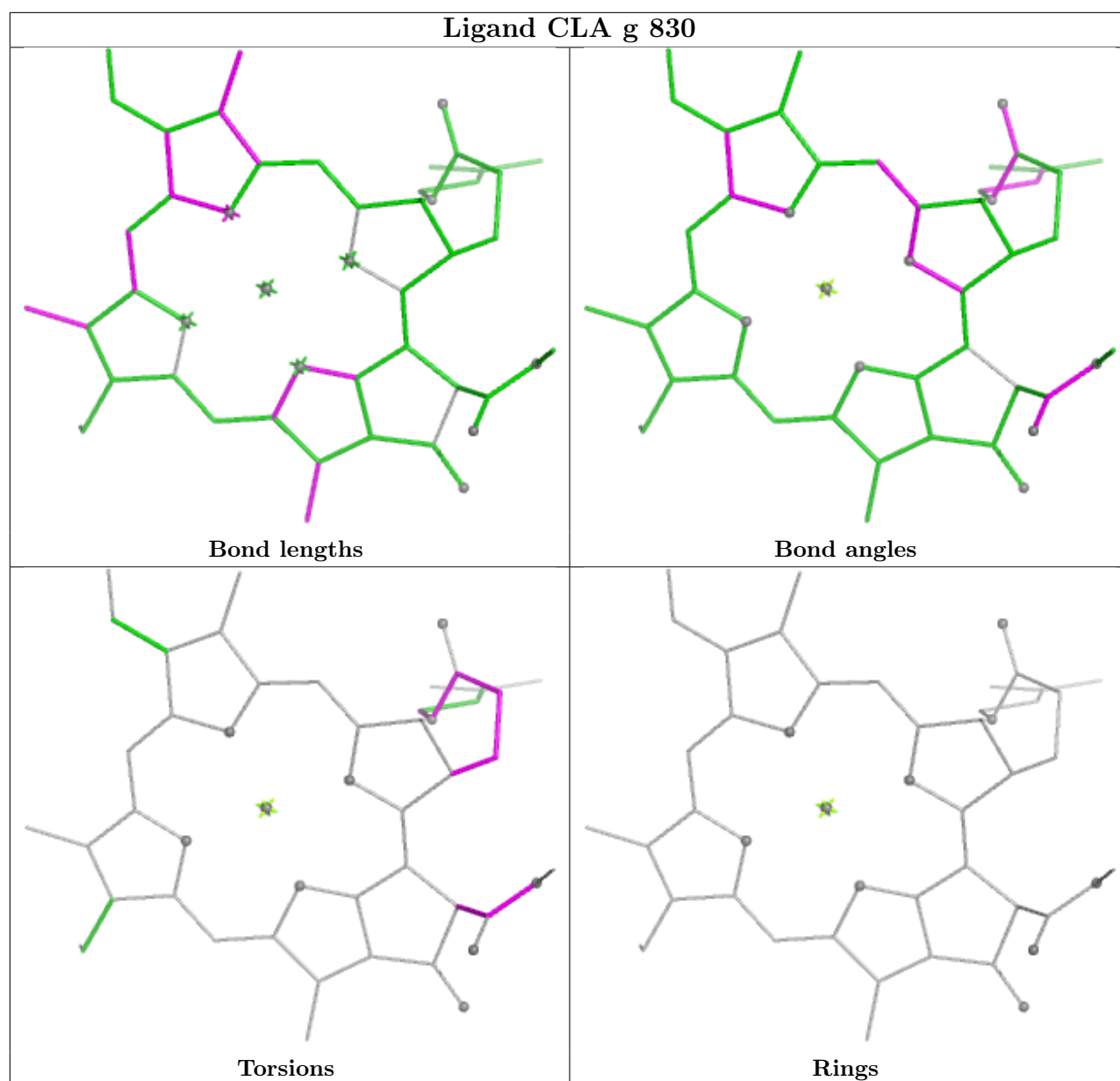
Bond angles



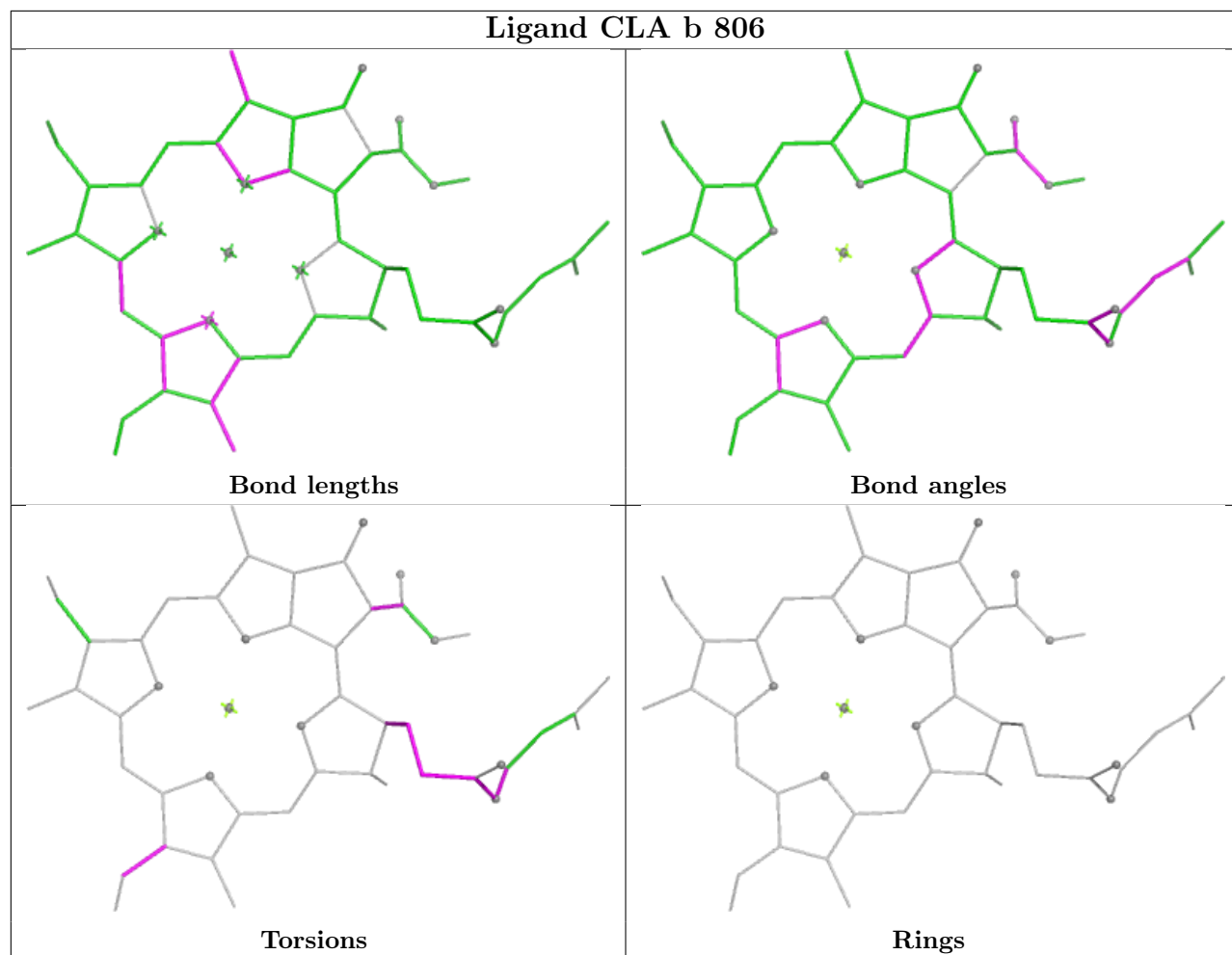
Torsions



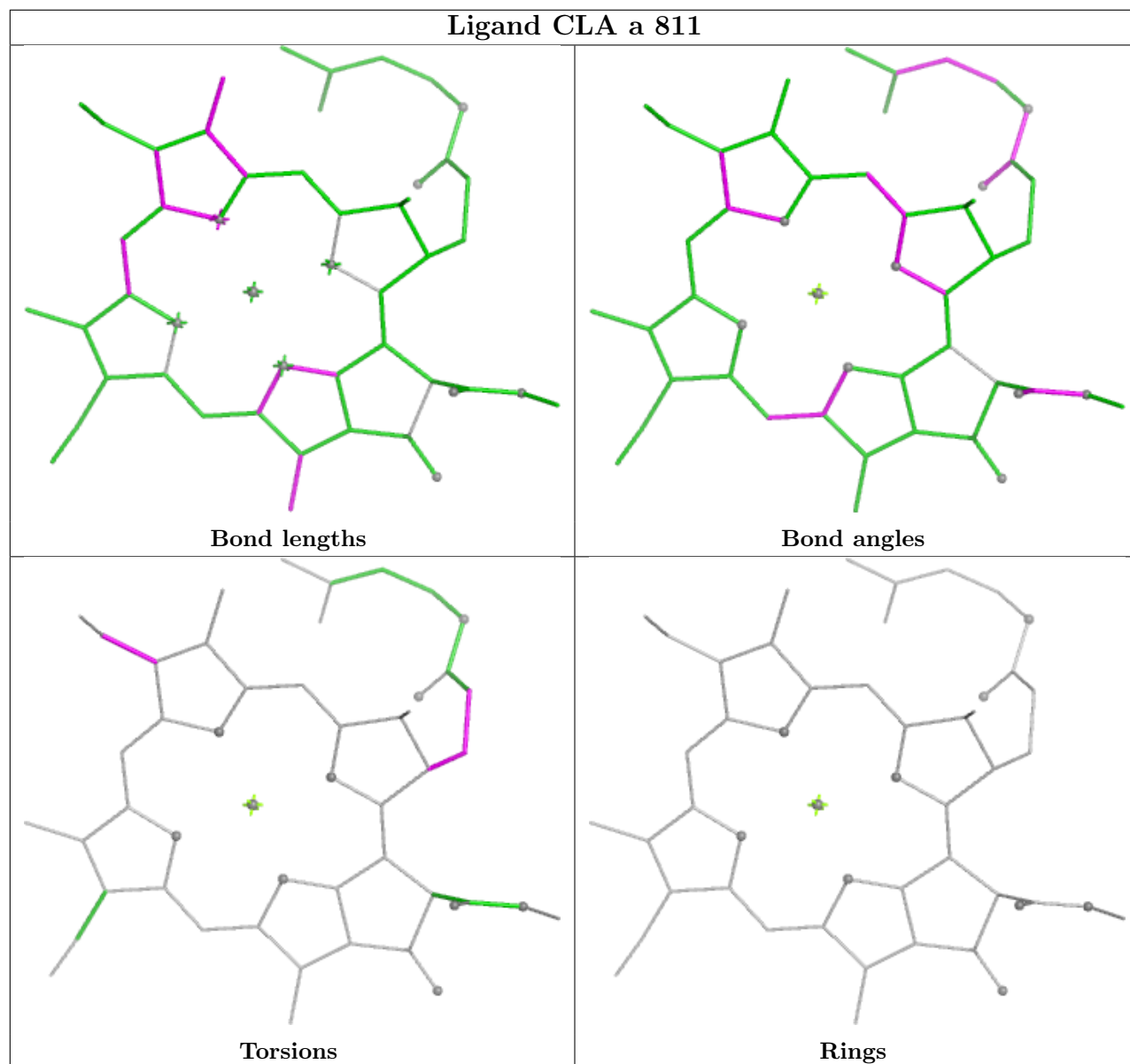
Rings



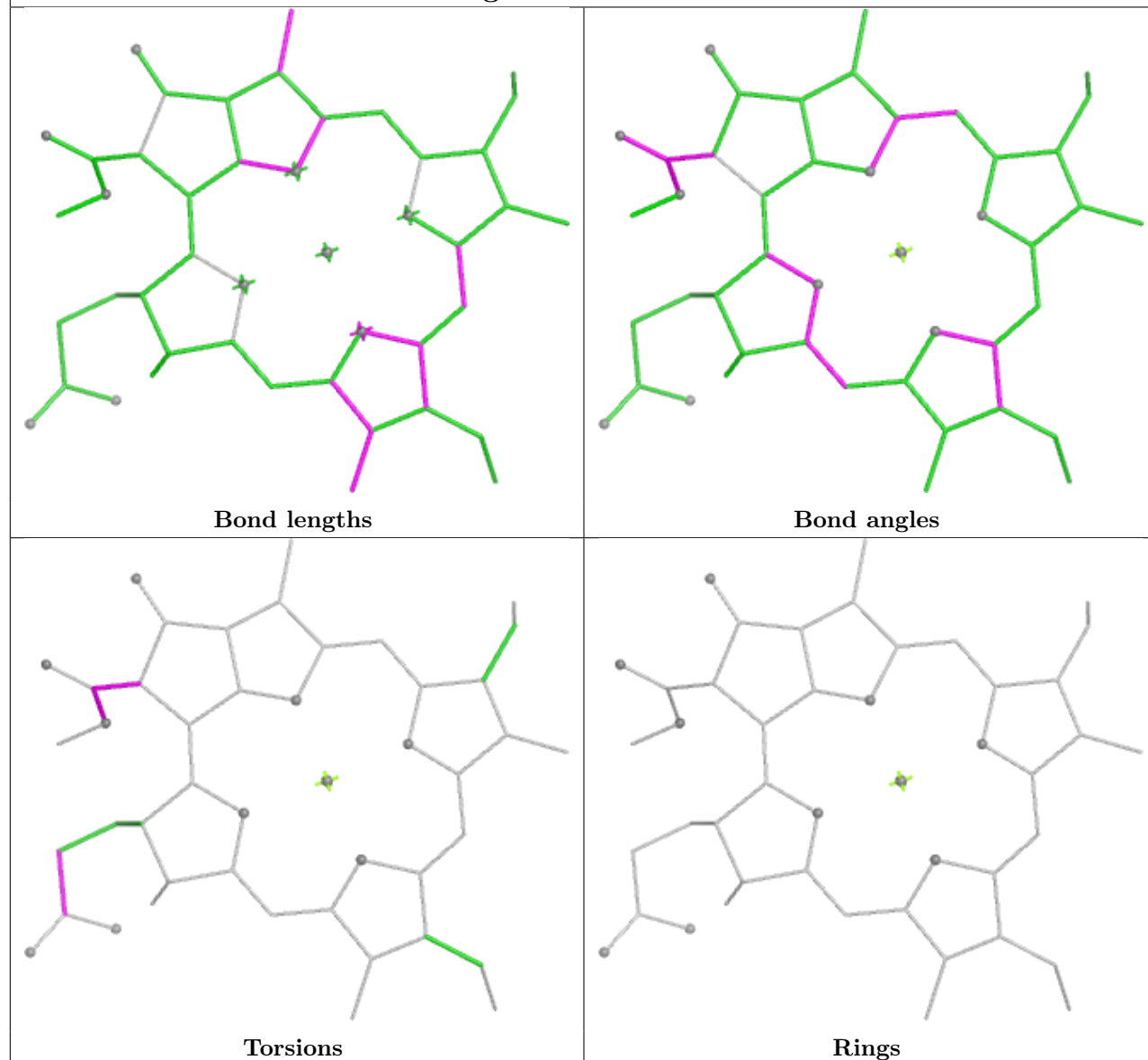
Ligand CLA b 806

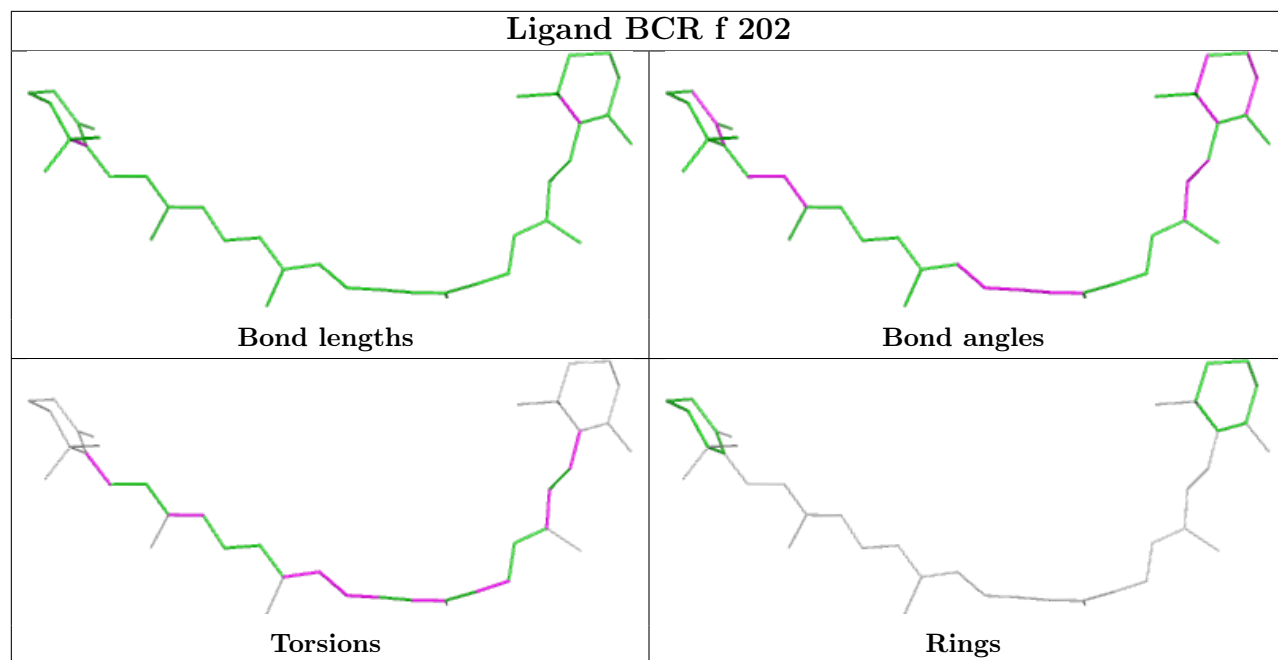


Ligand CLA a 811

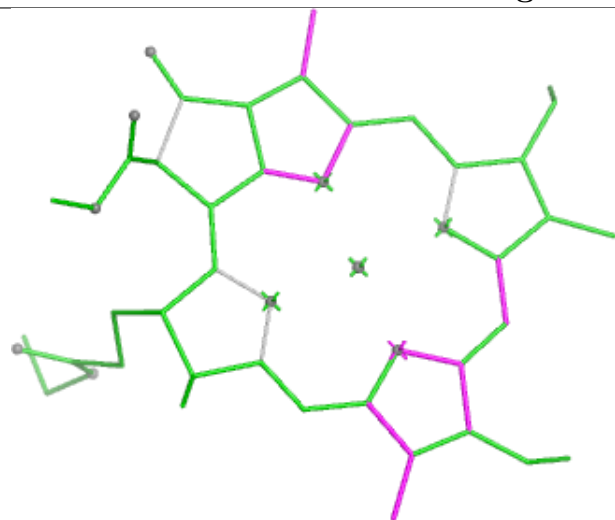


Ligand CLA e 837

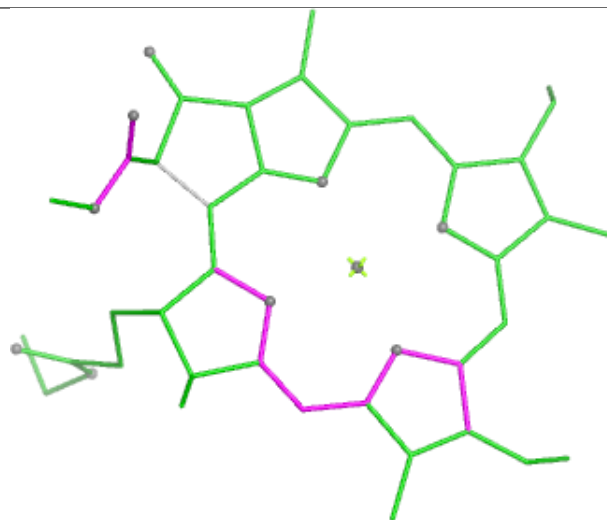




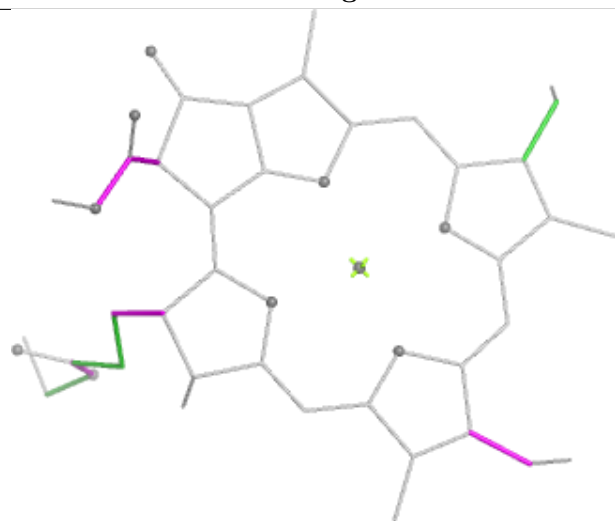
Ligand CLA B 839



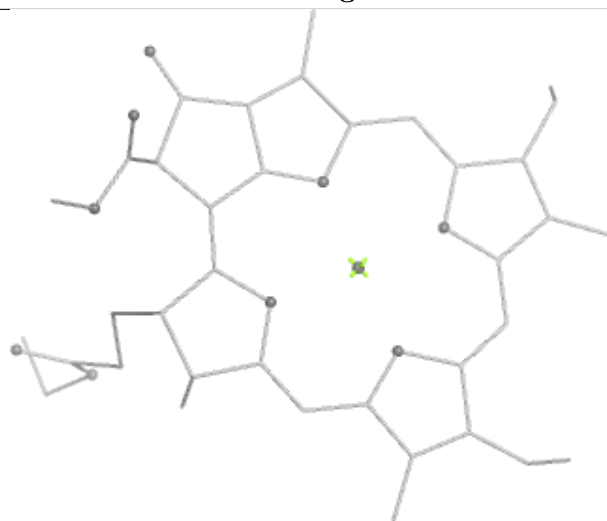
Bond lengths



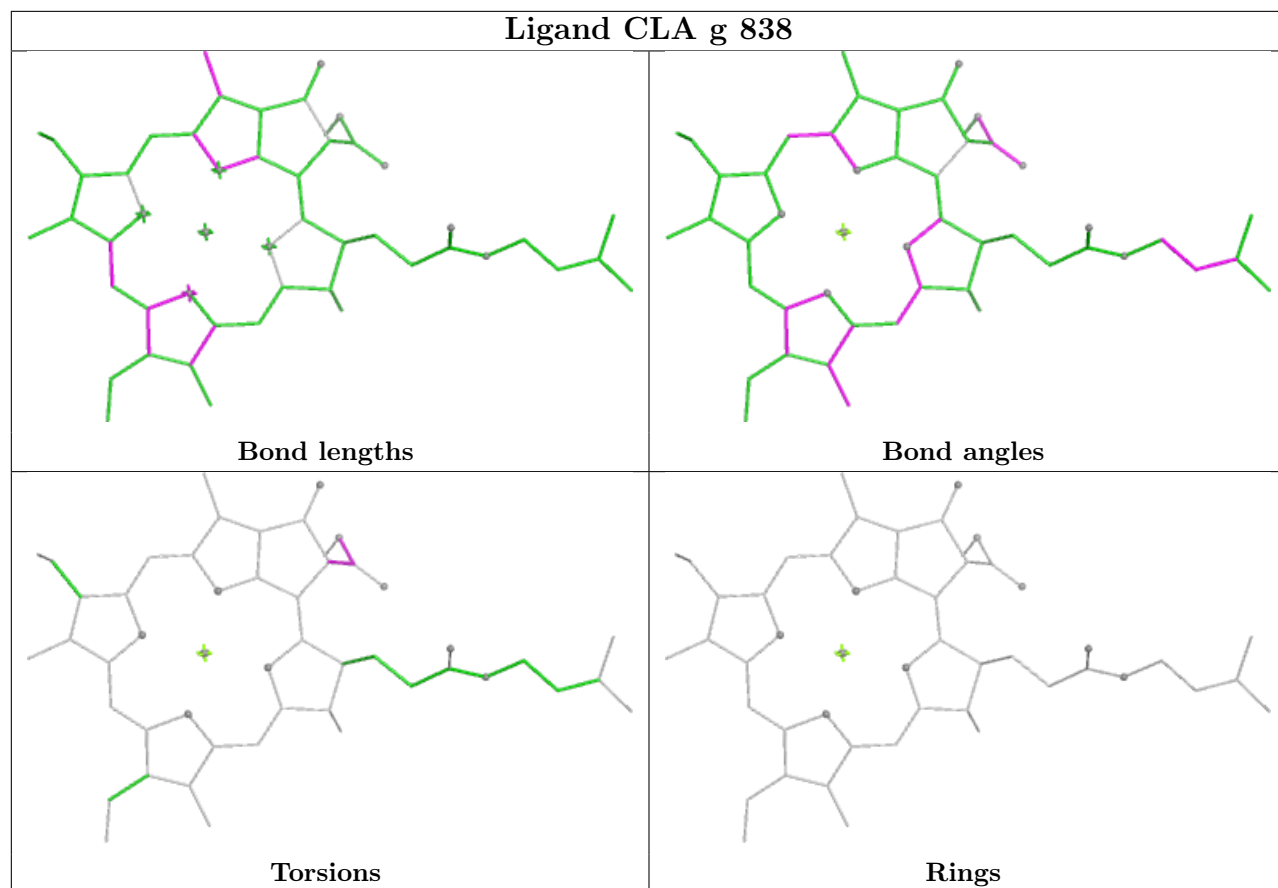
Bond angles



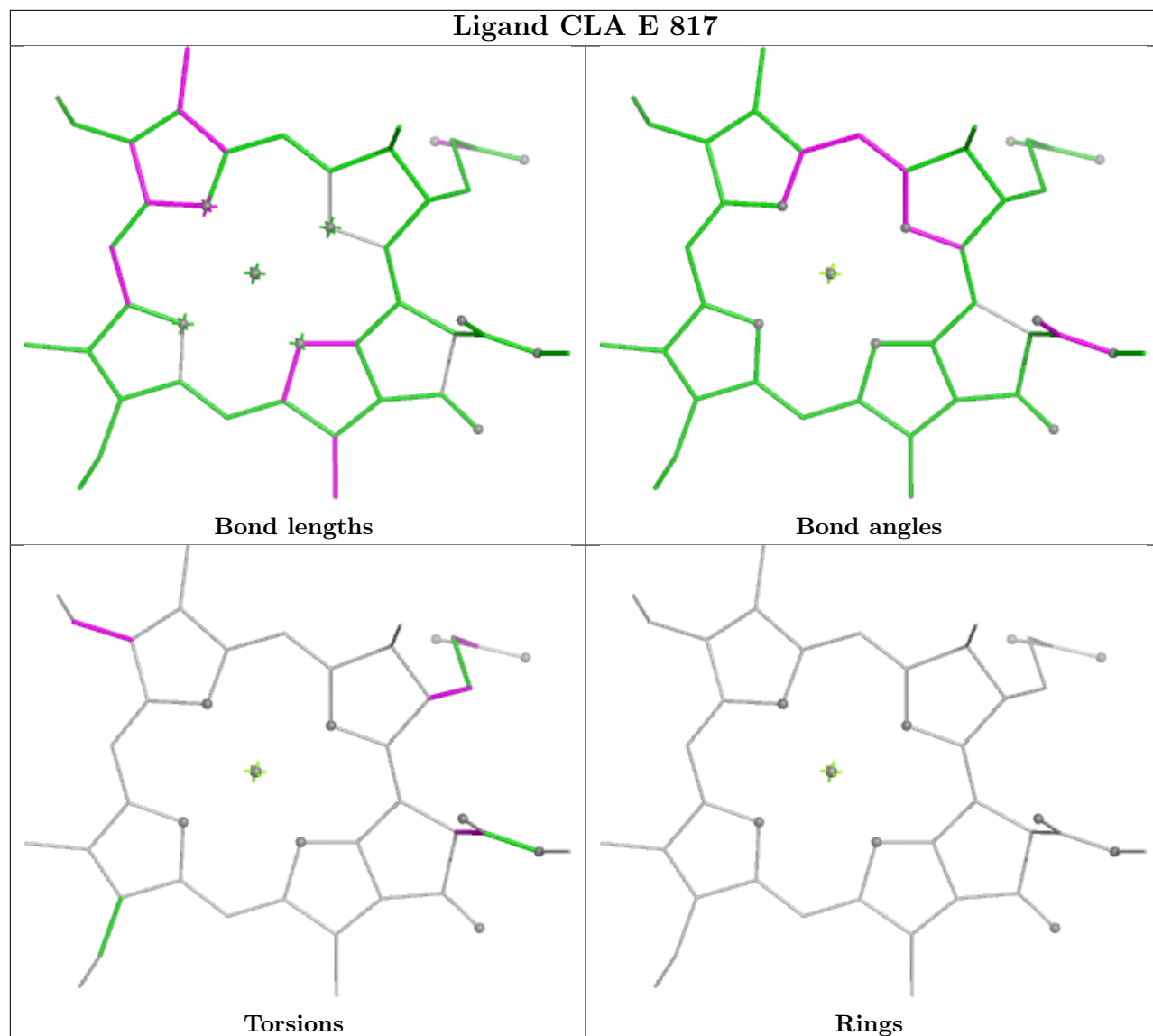
Torsions

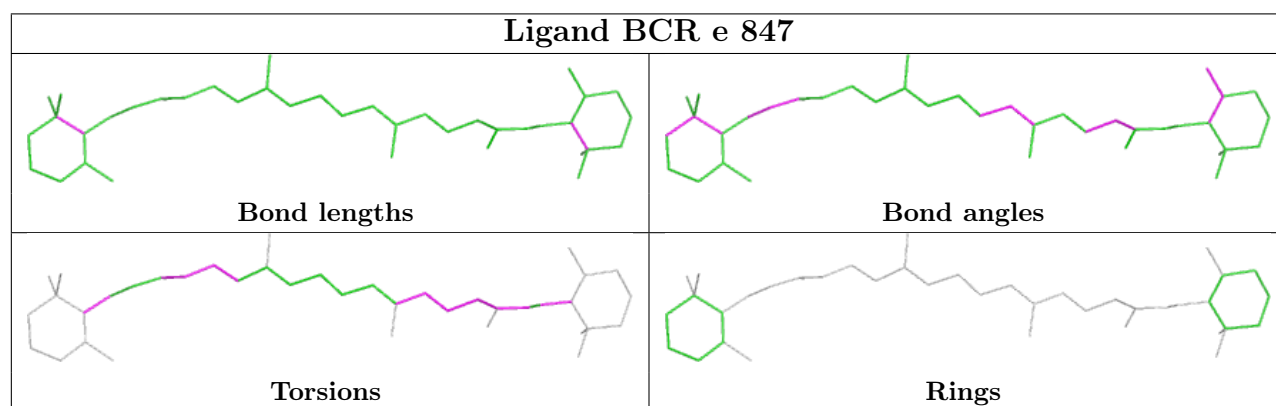
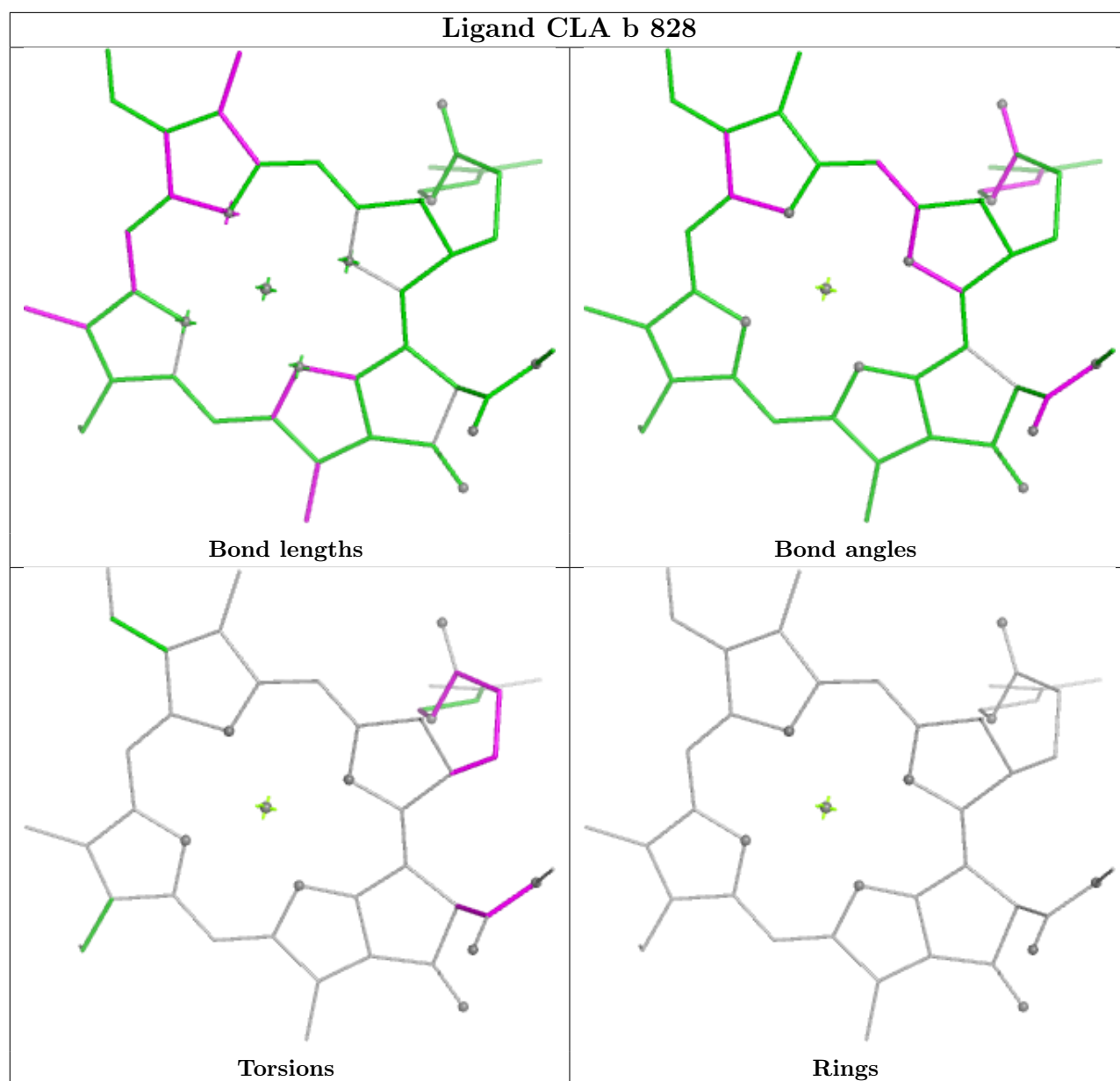


Rings

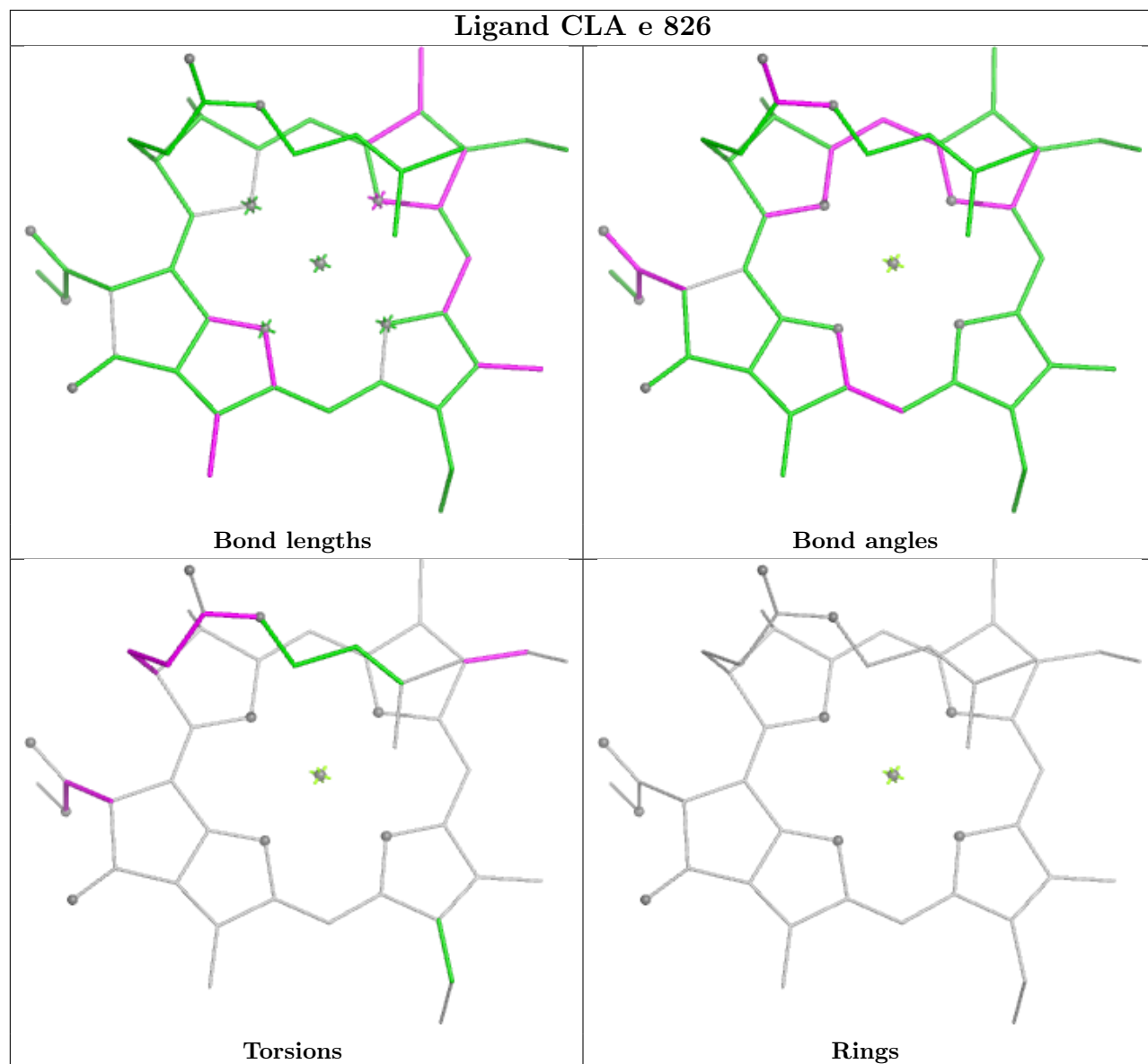


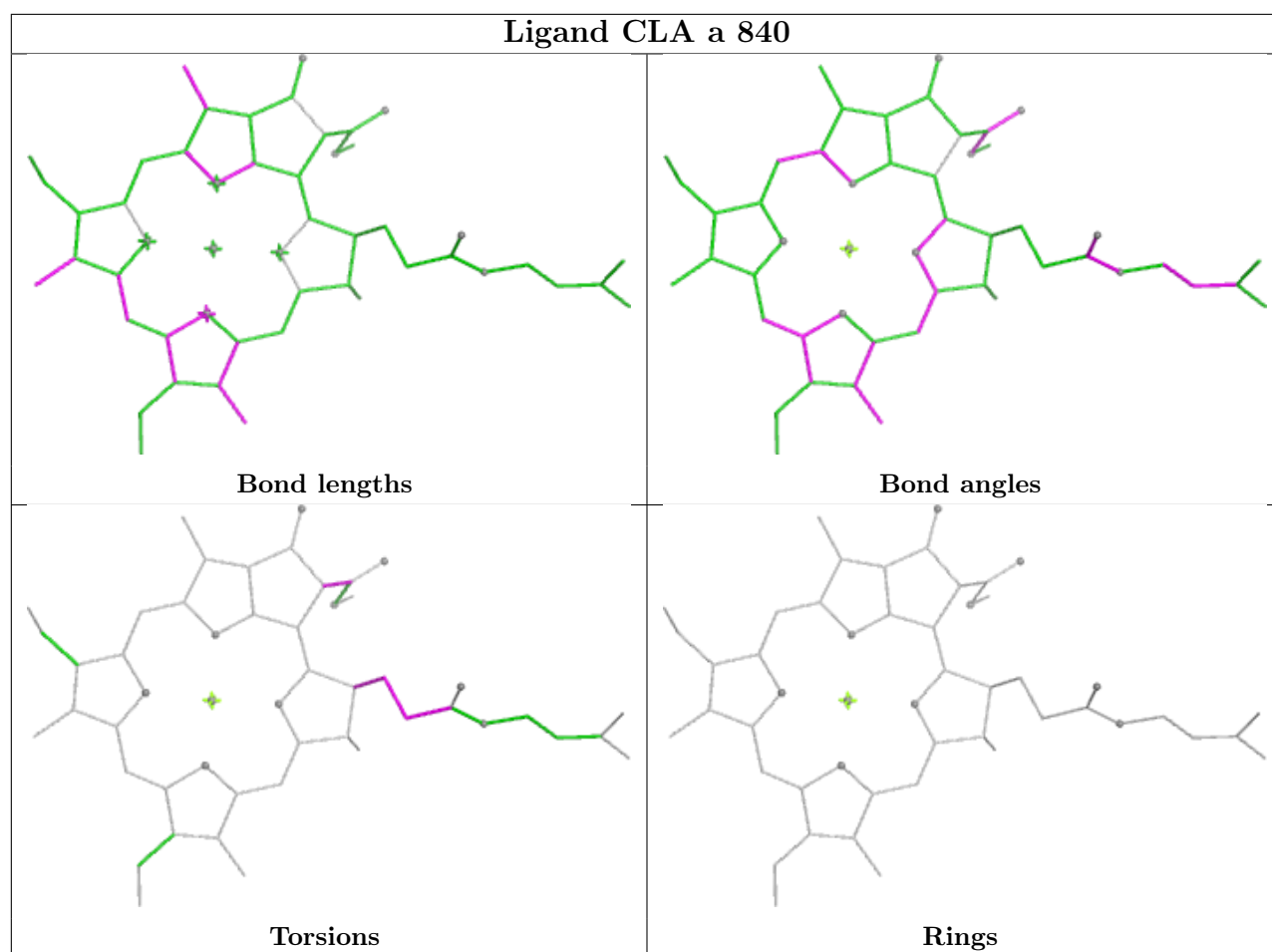
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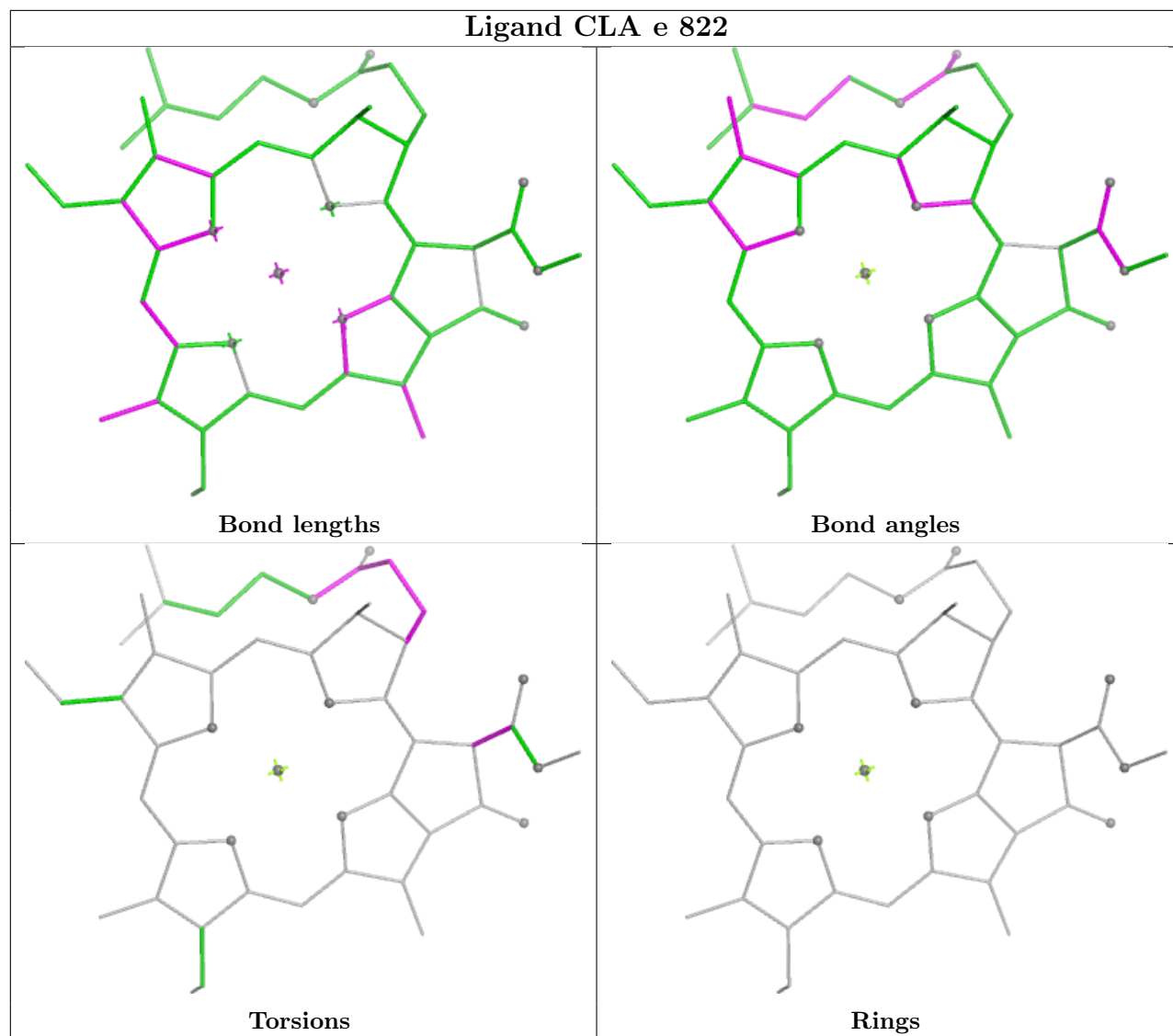


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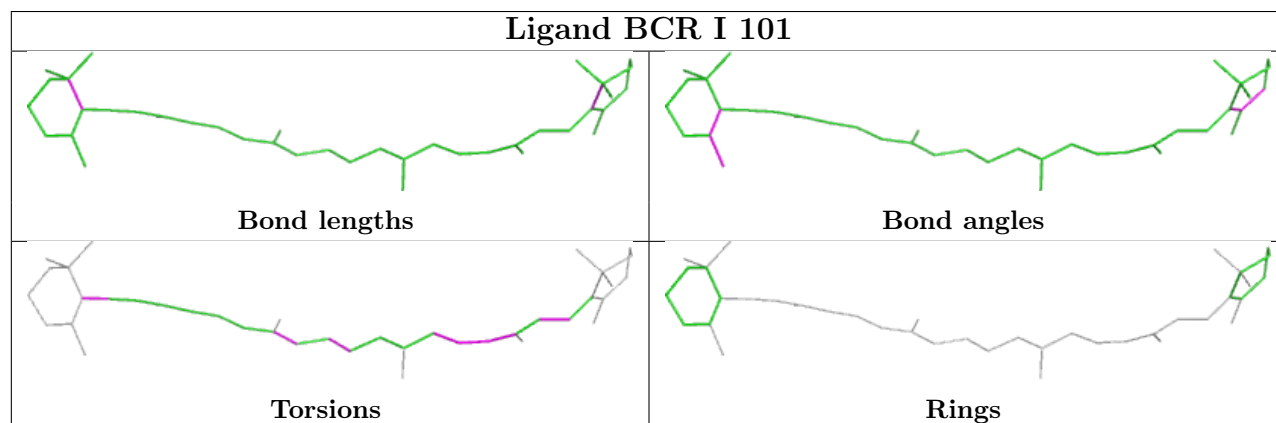


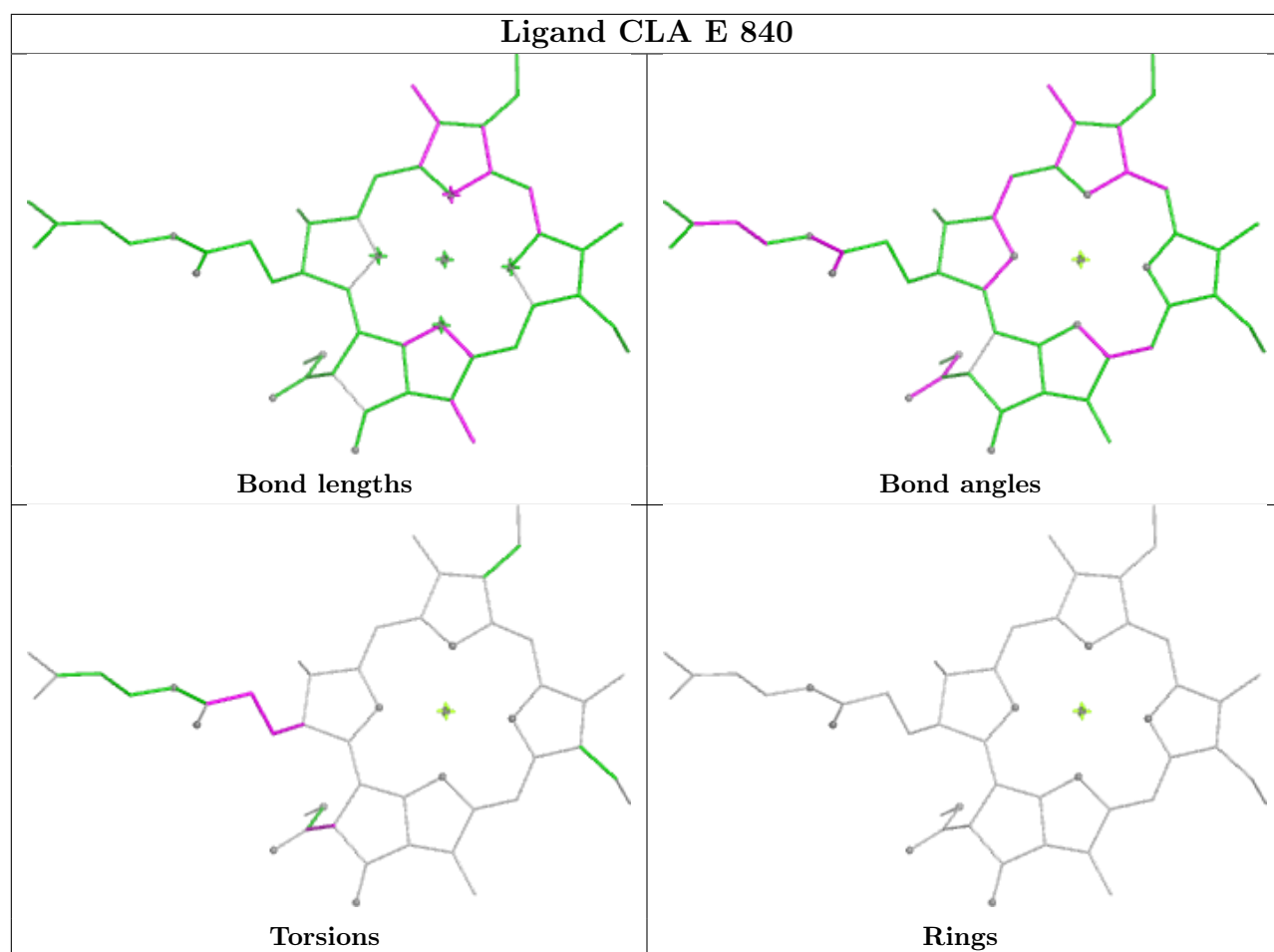


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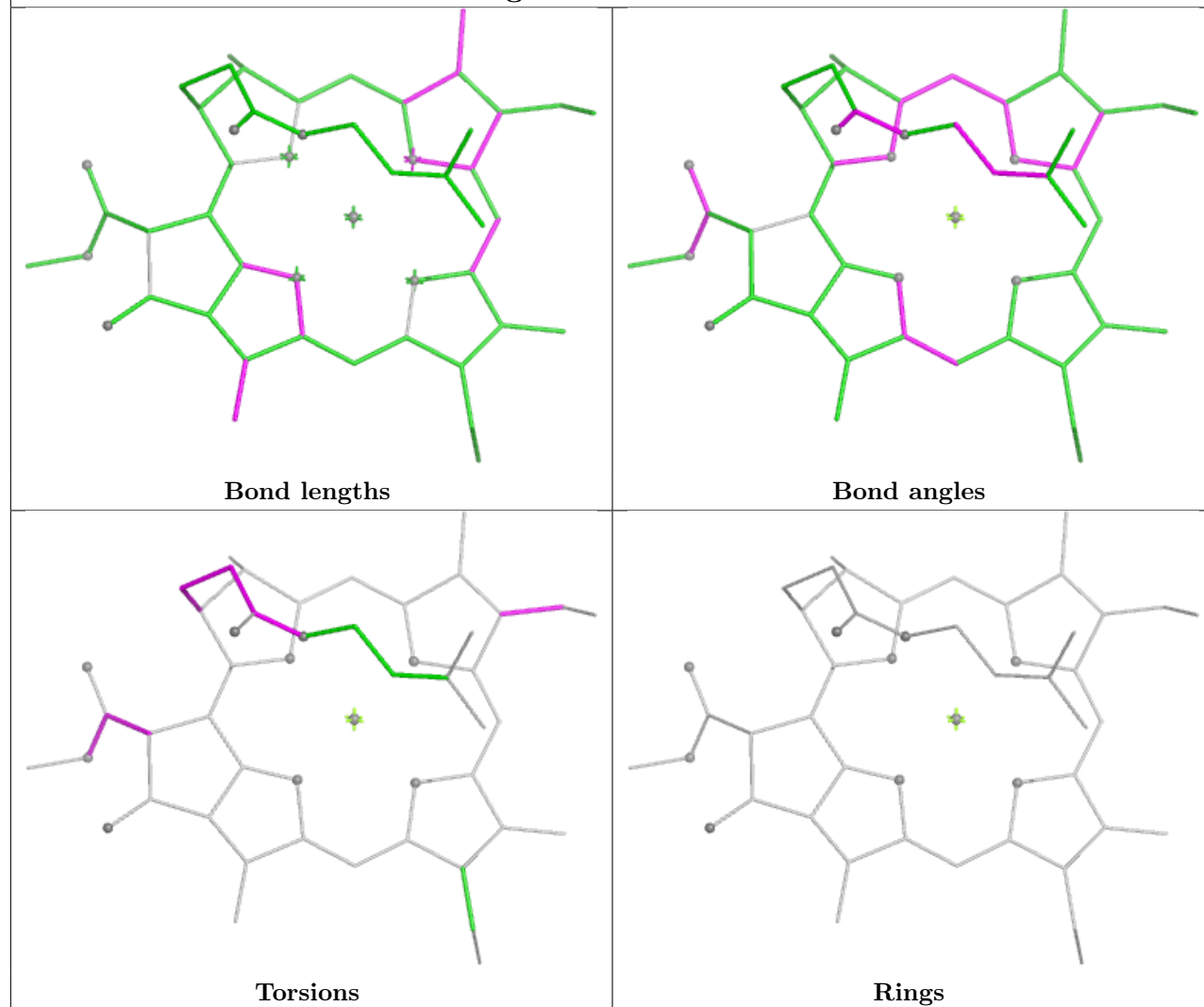


Ligand BCR I 101

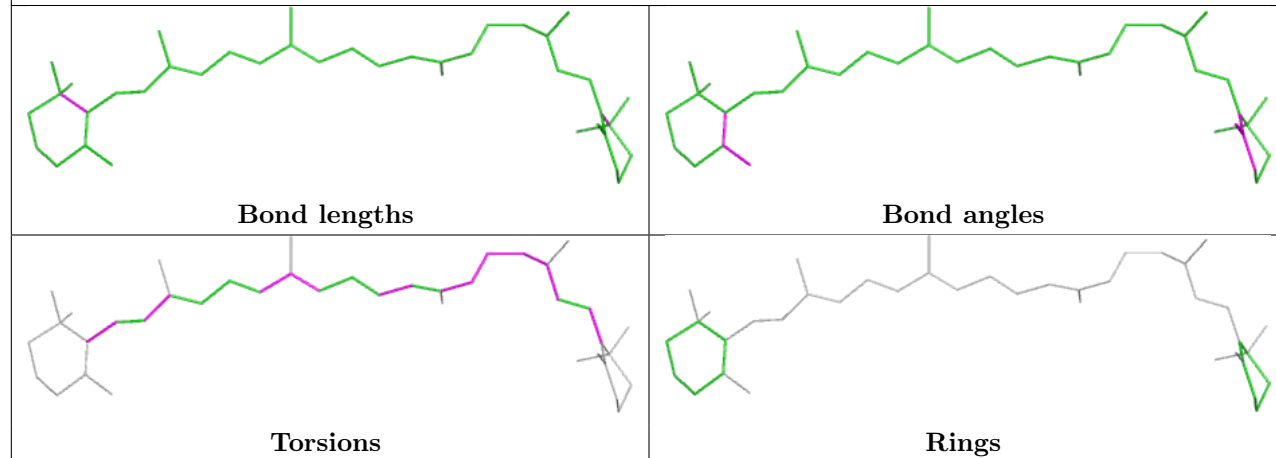




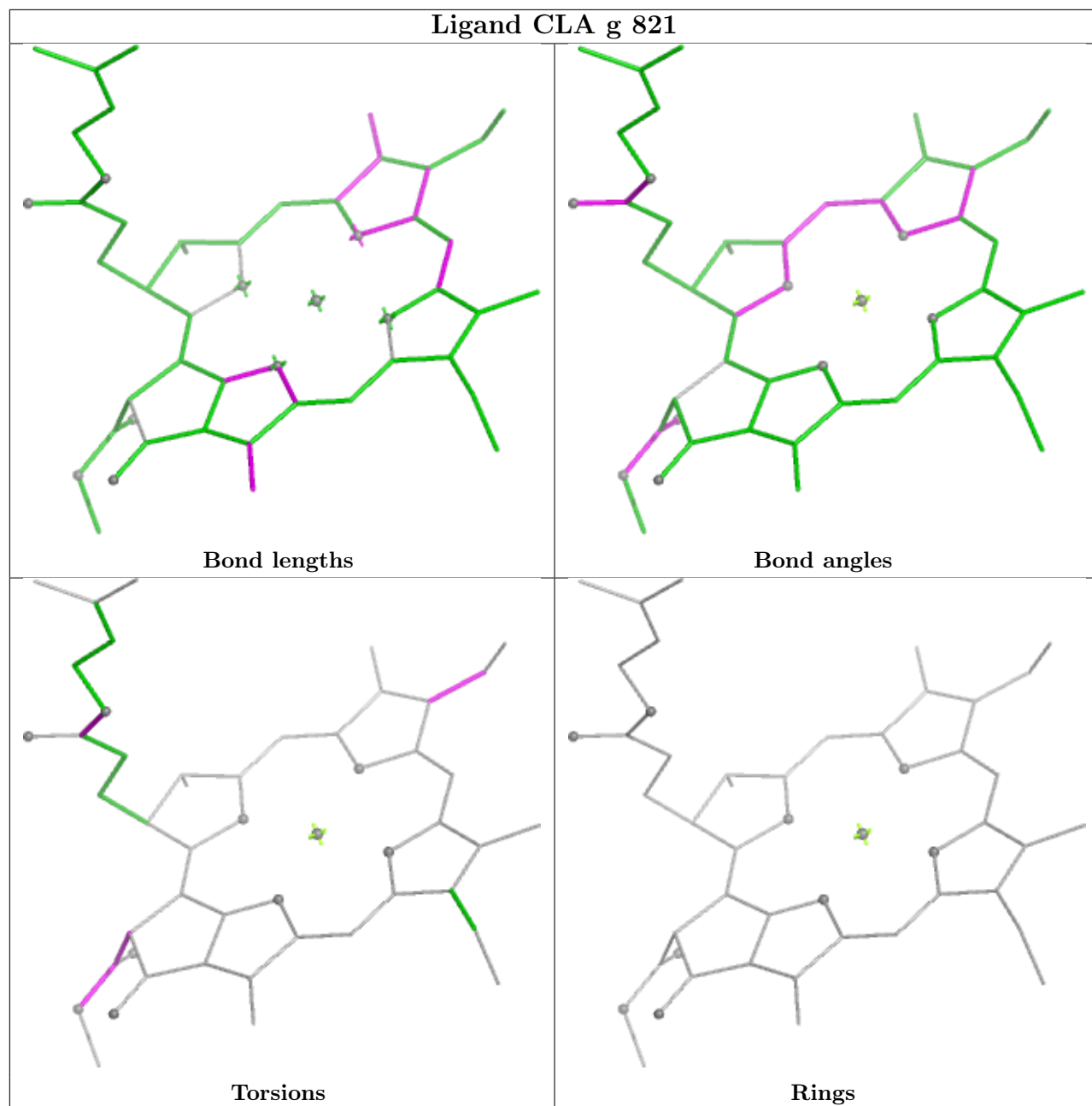
Ligand CLA a 826

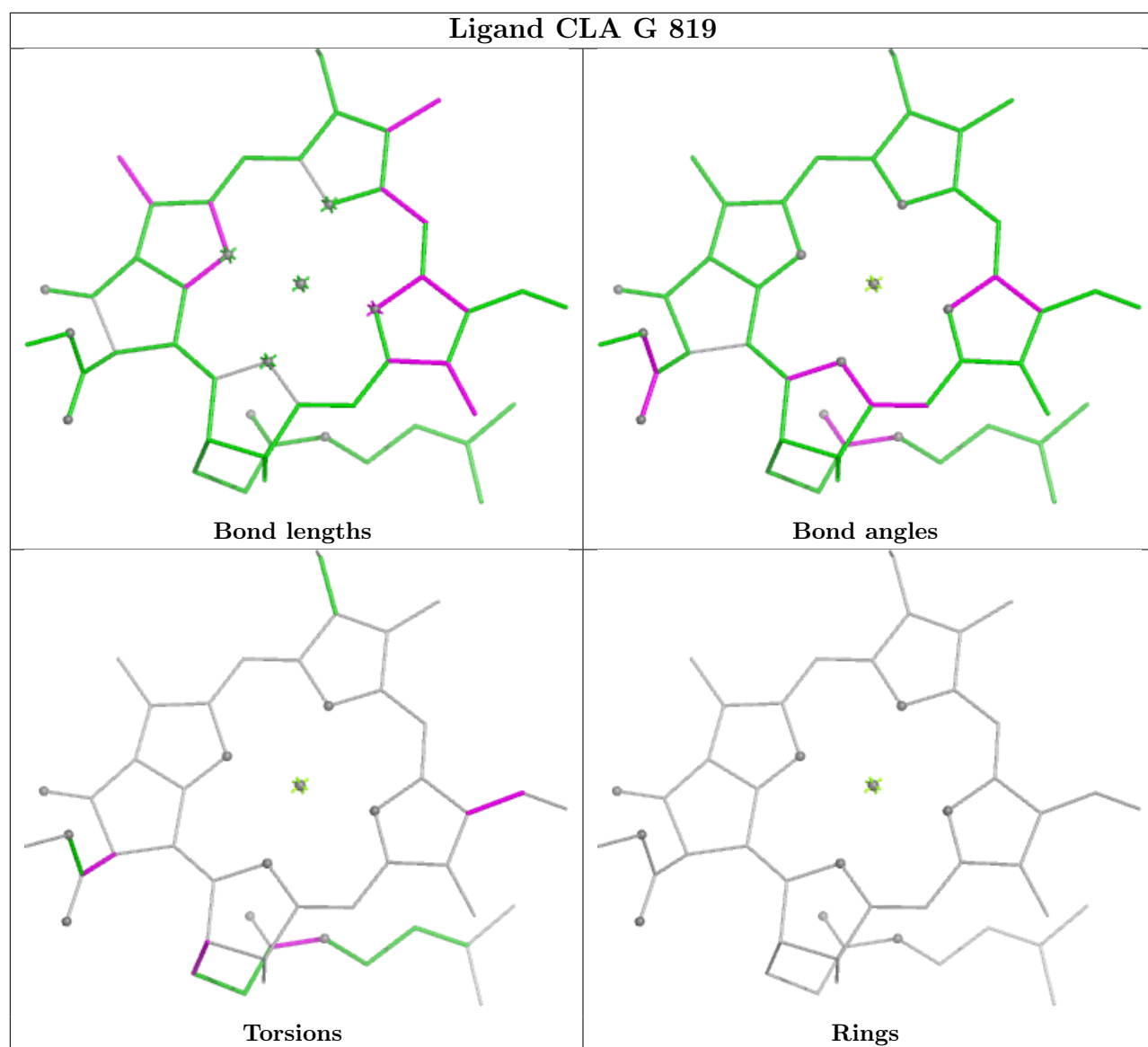


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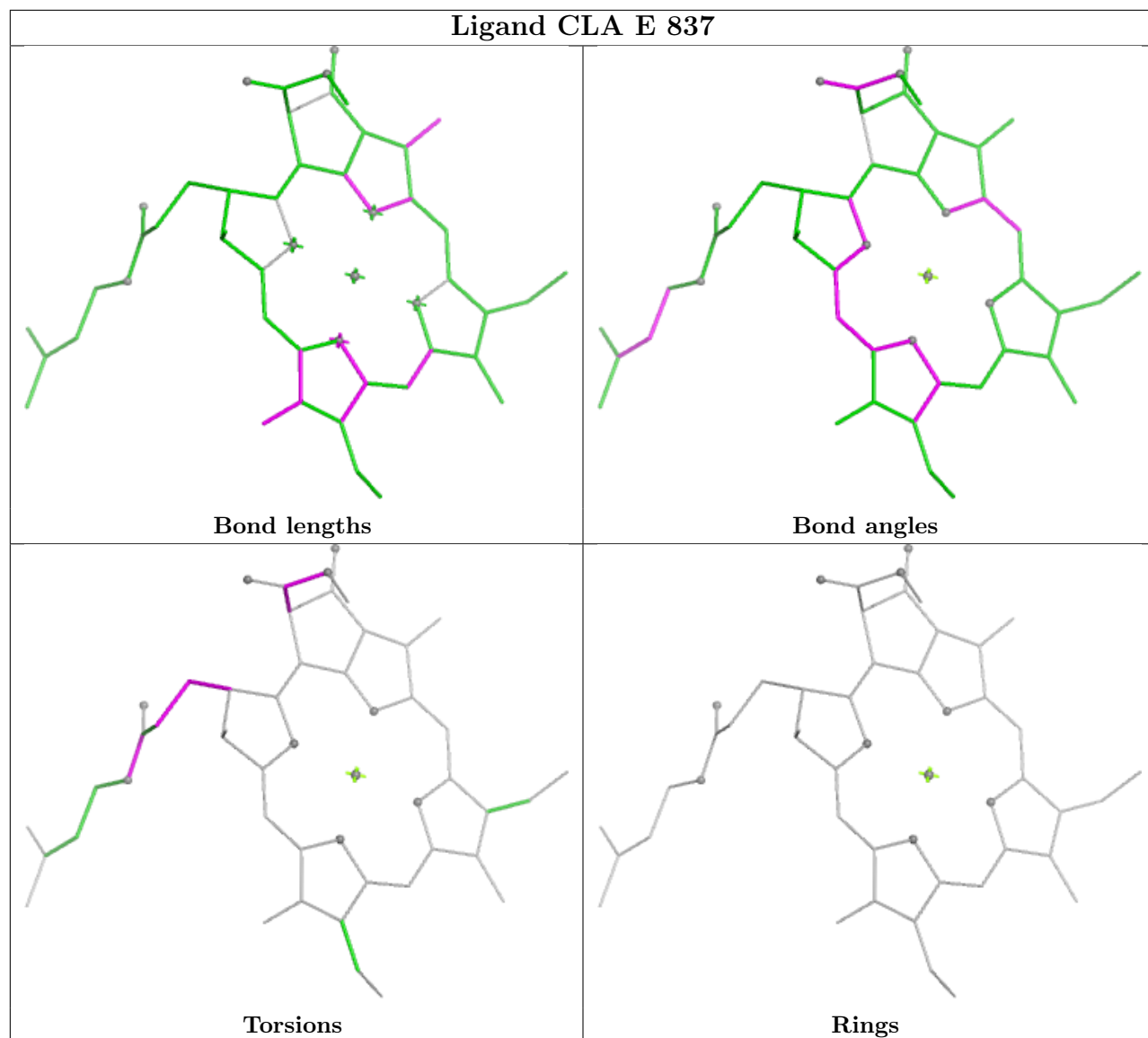


Ligand CLA g 821

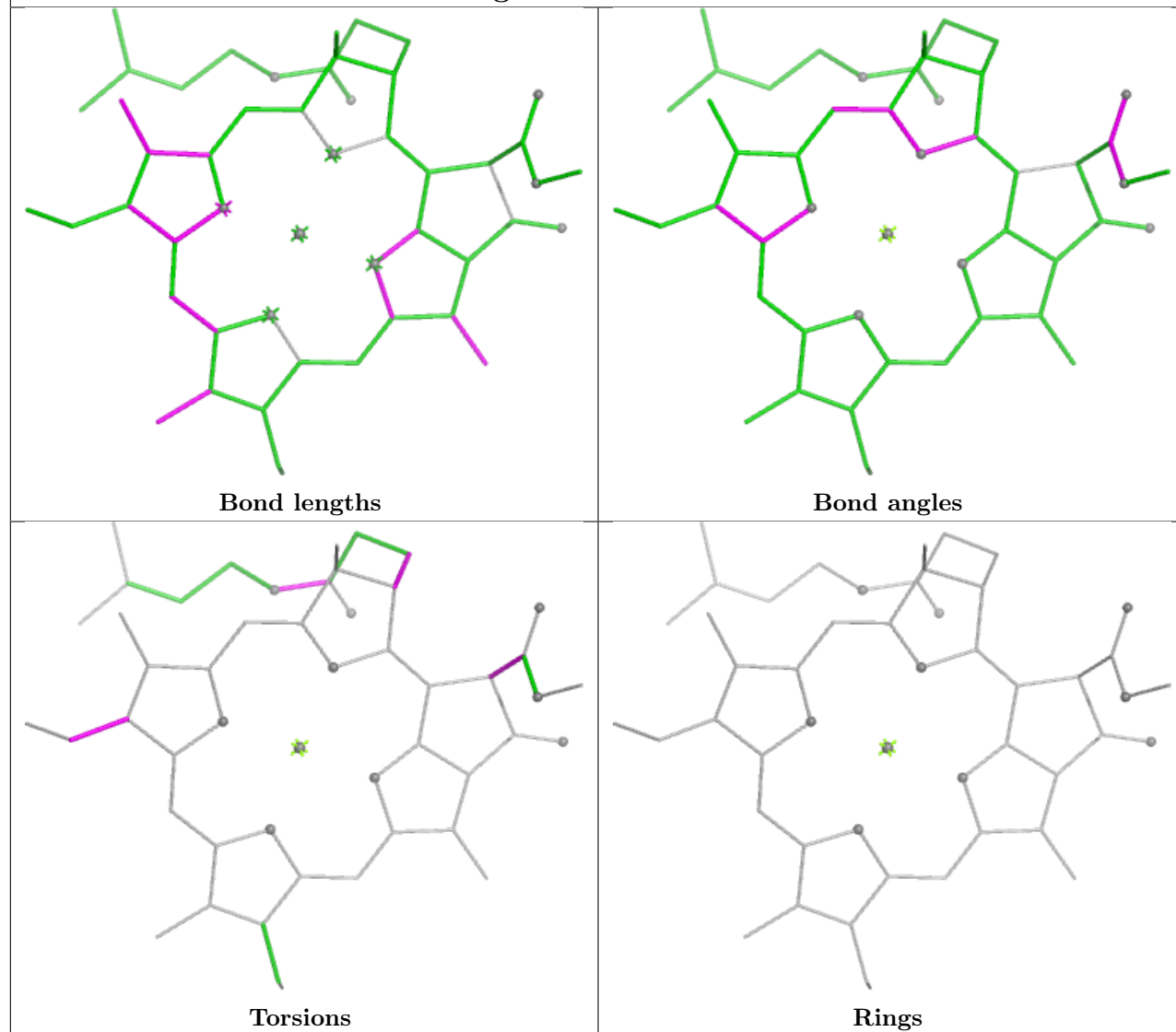




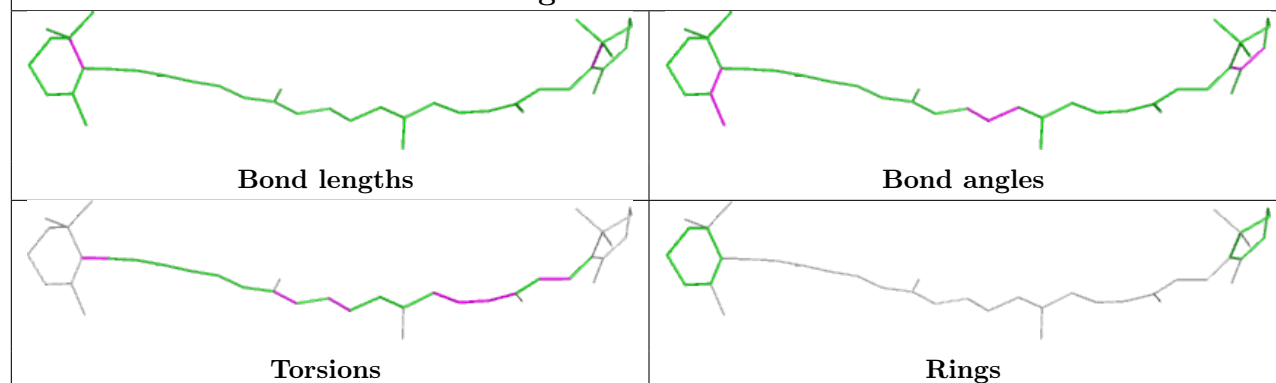
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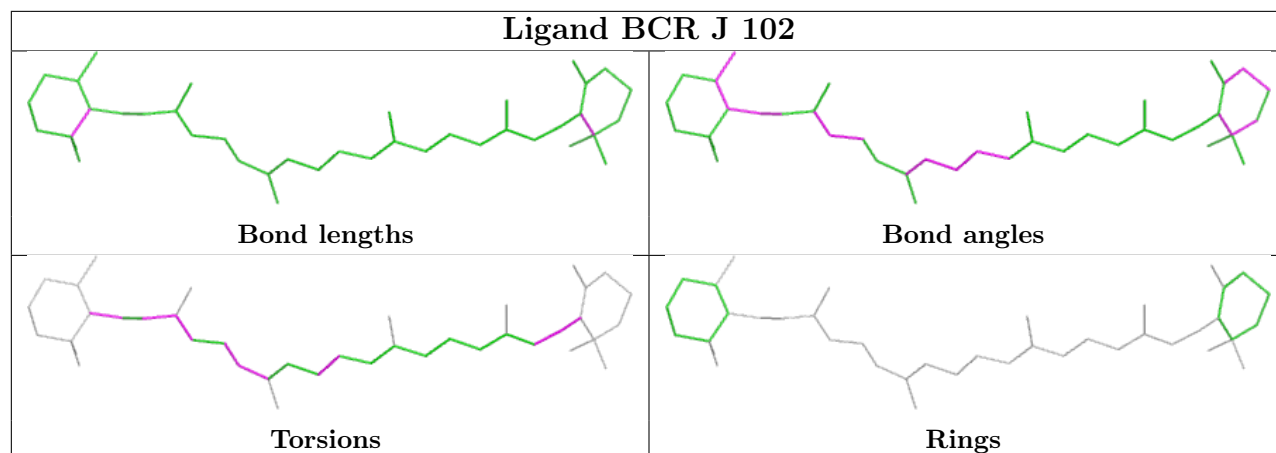
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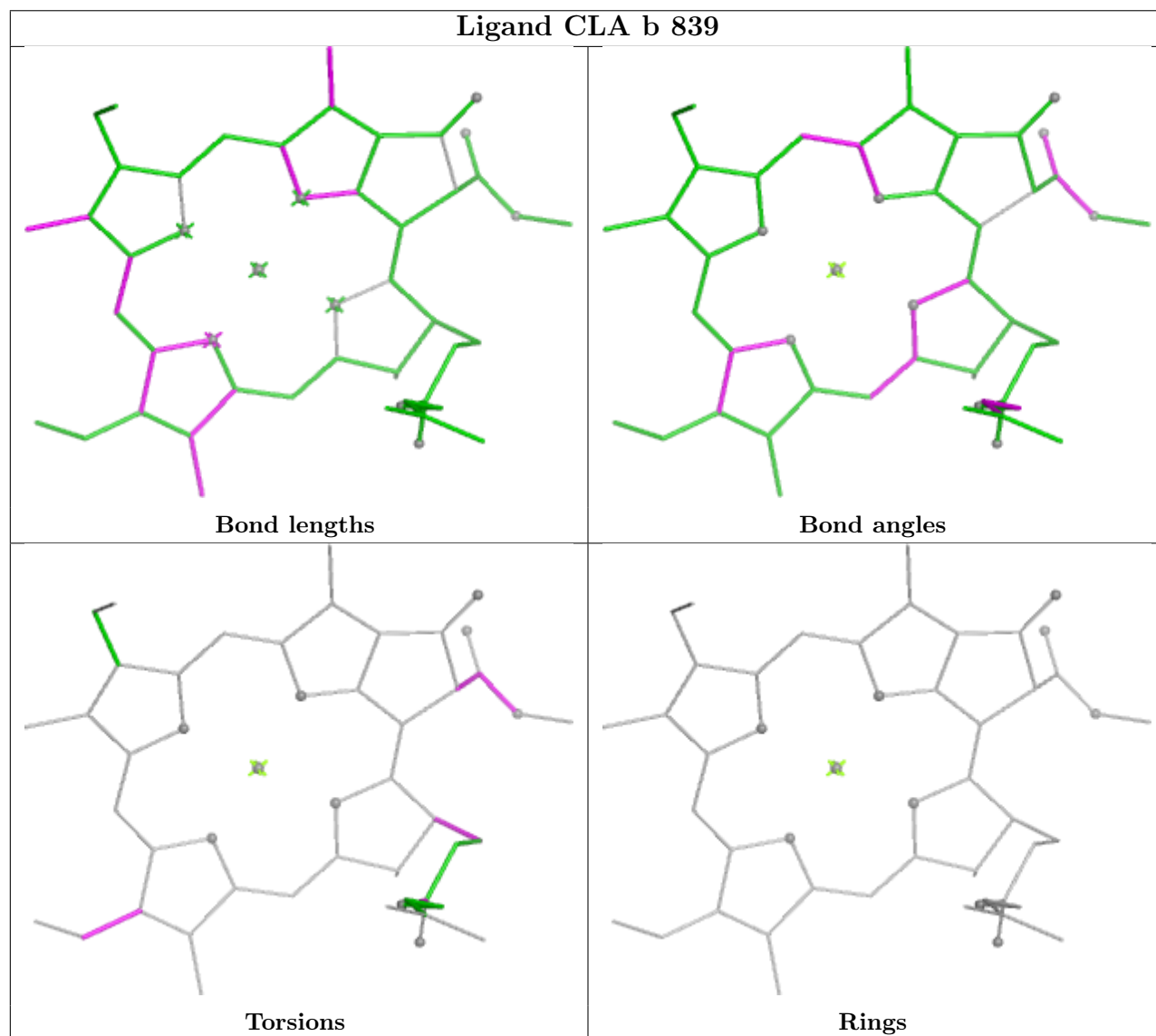
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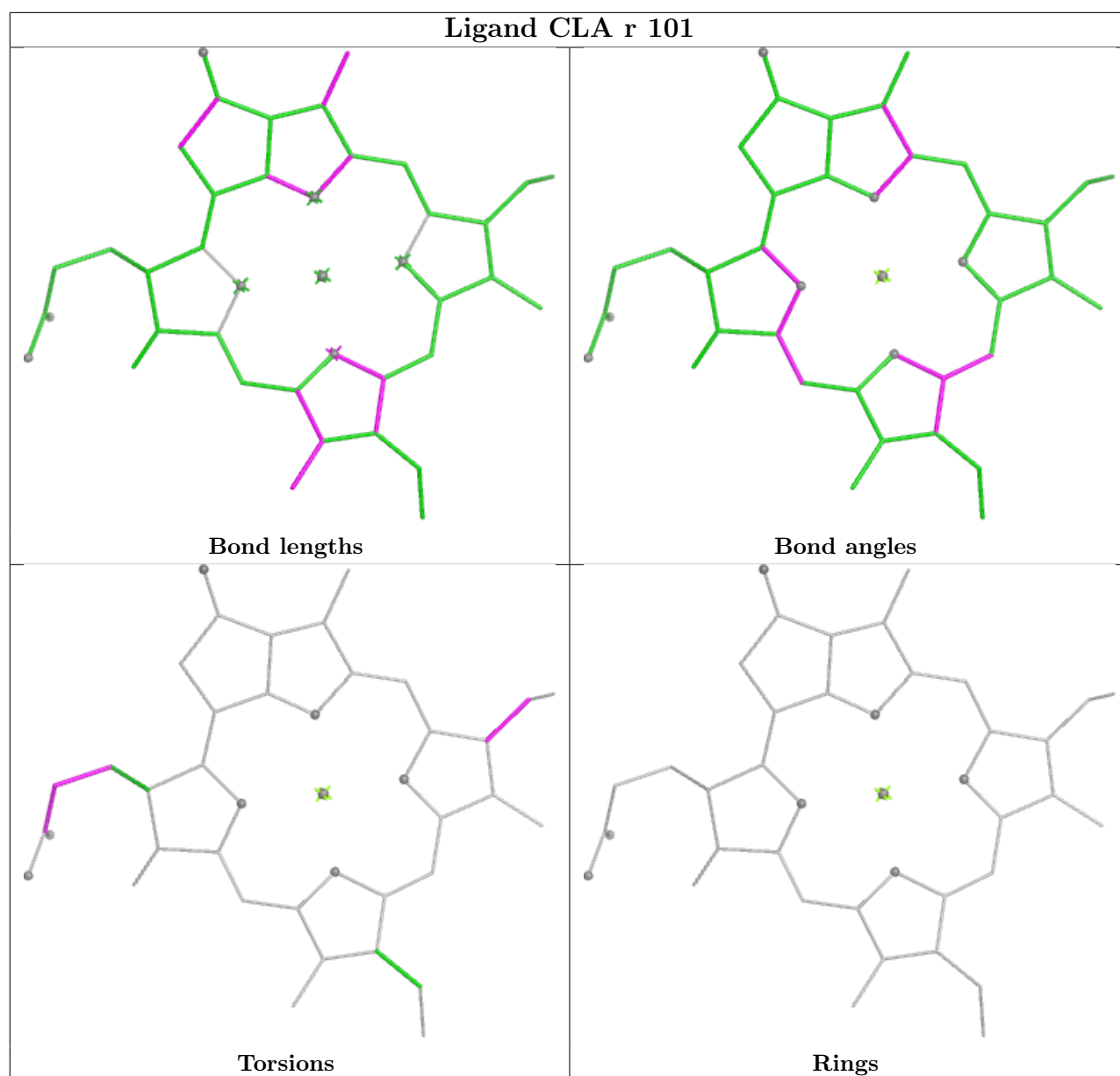


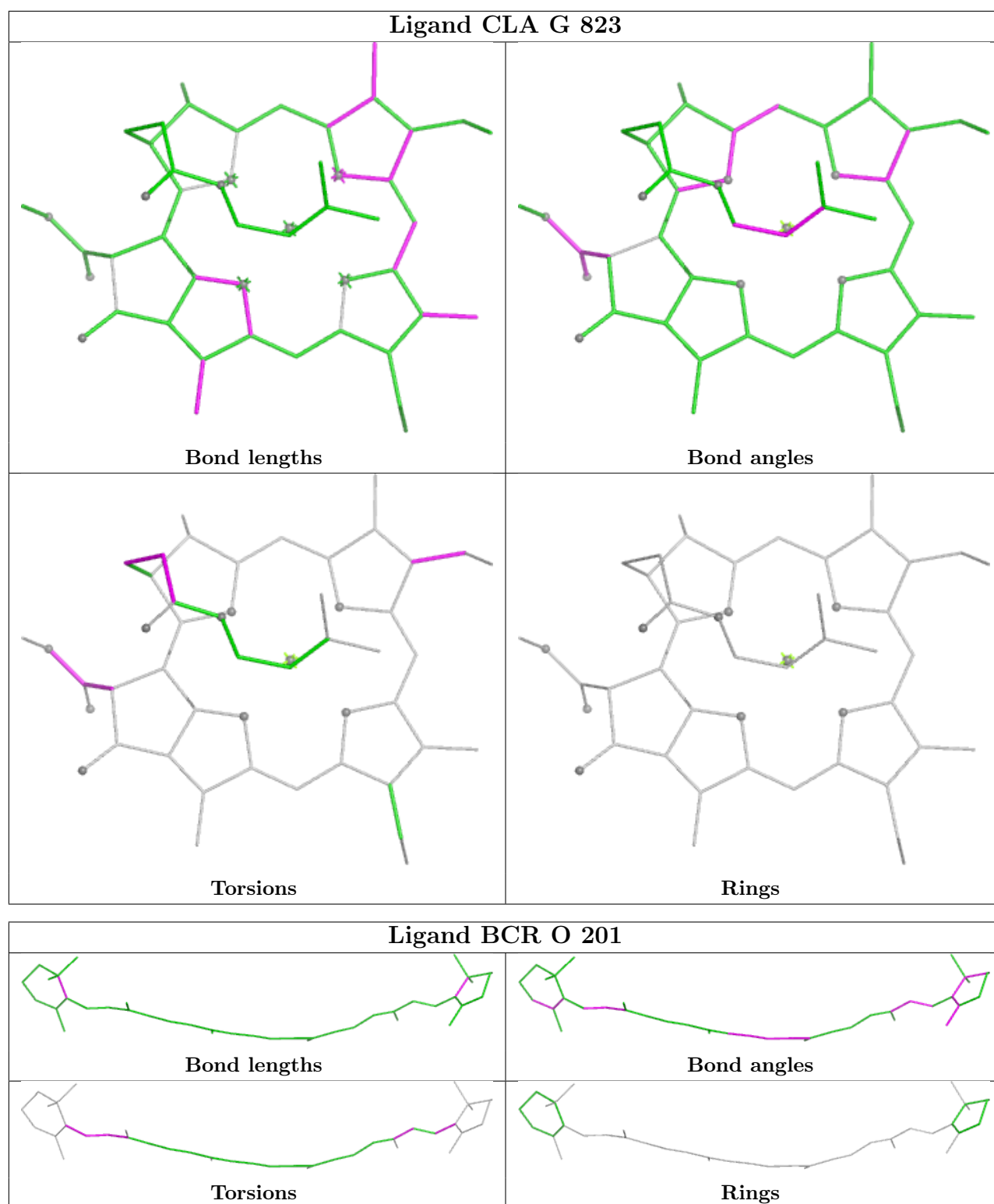
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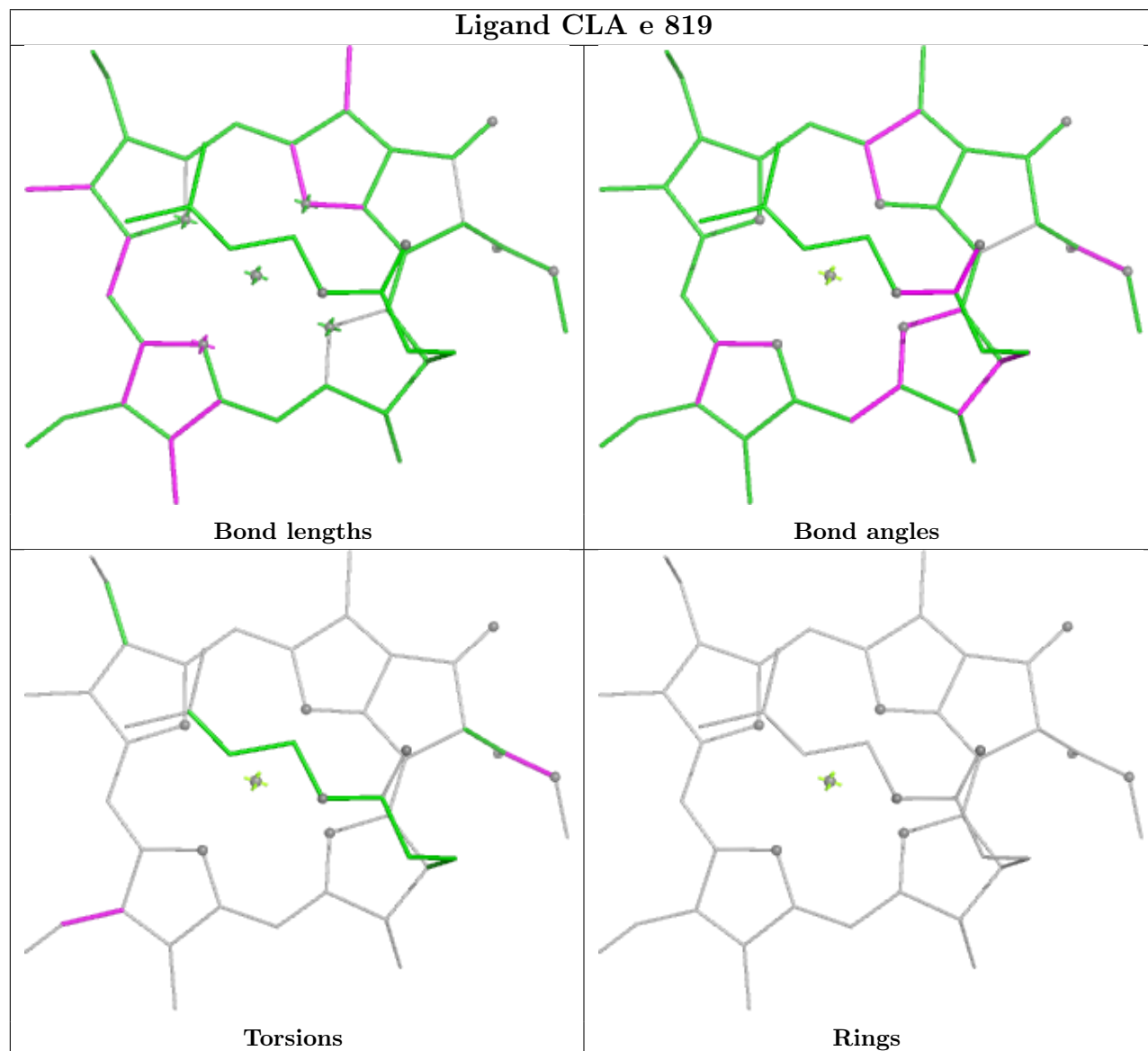
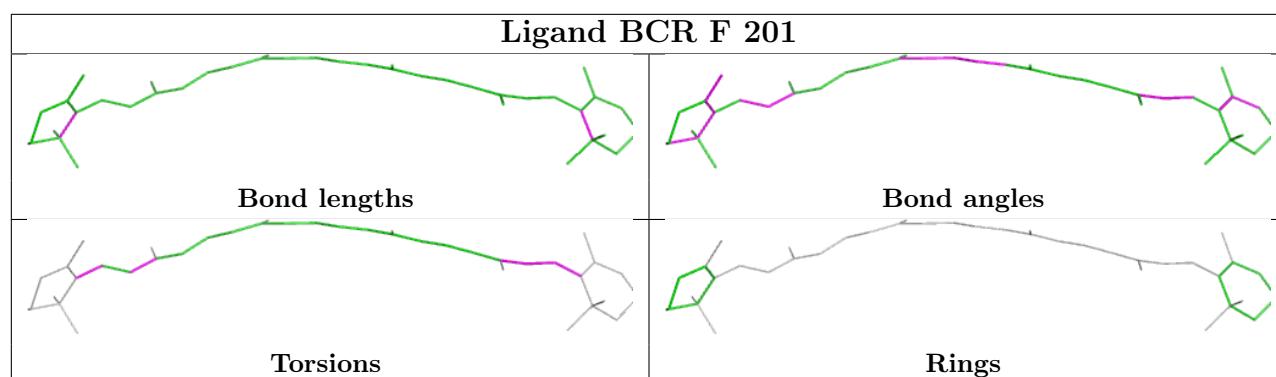


Ligand CLA b 839

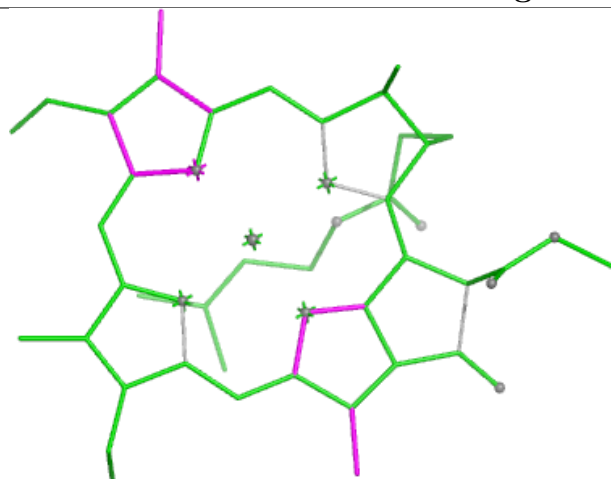




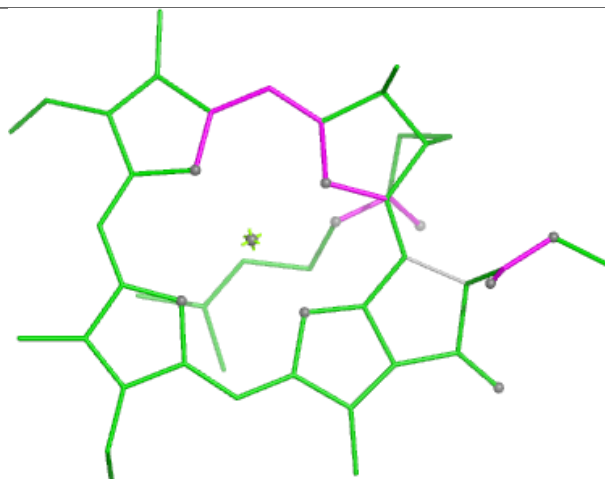




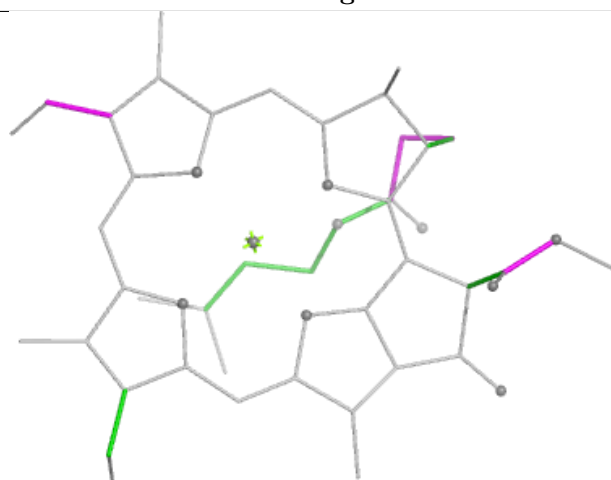
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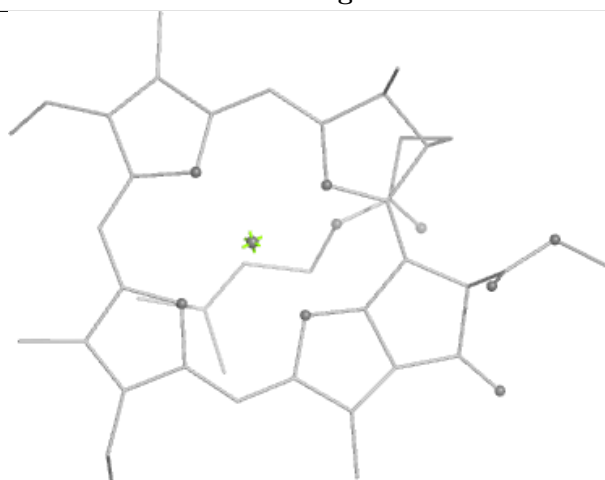
Bond lengths



Bond angles

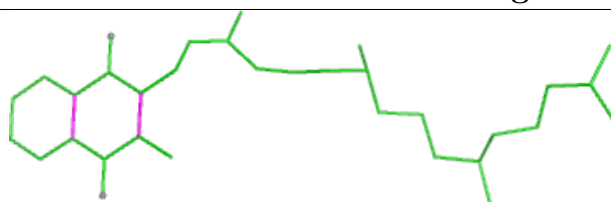


Torsions

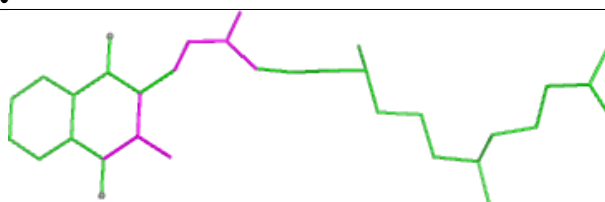


Rings

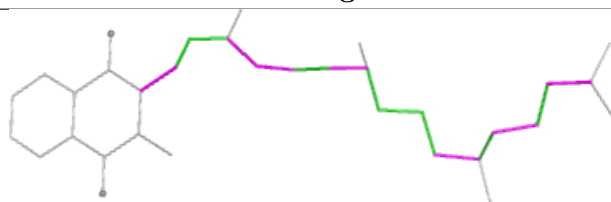
Ligand PQN A 846



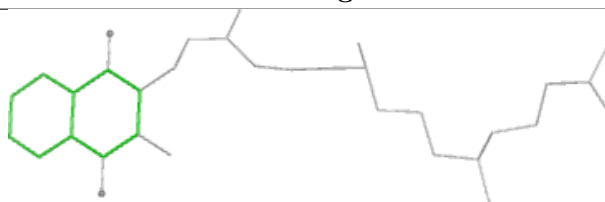
Bond lengths



Bond angles

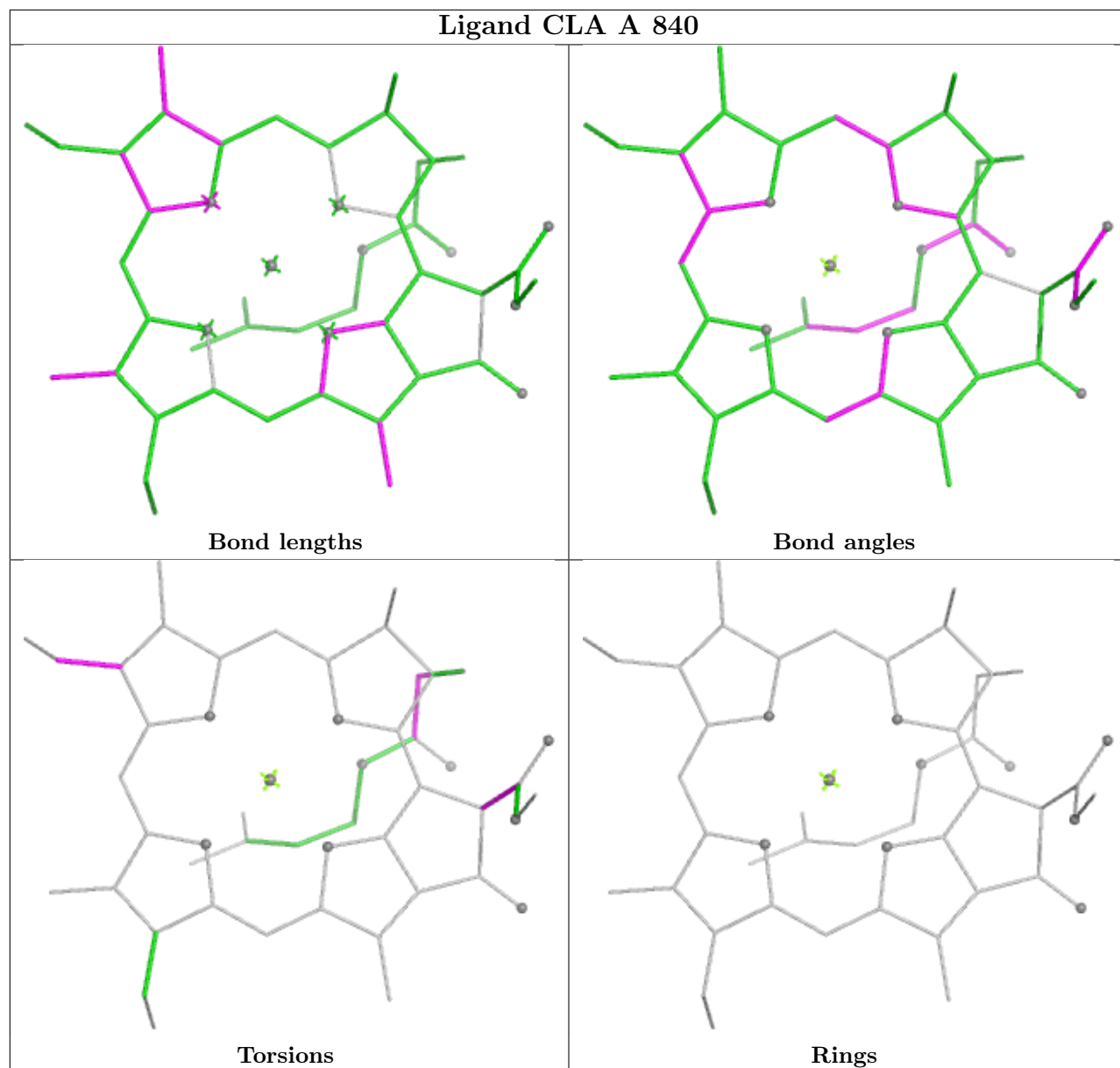


Torsions

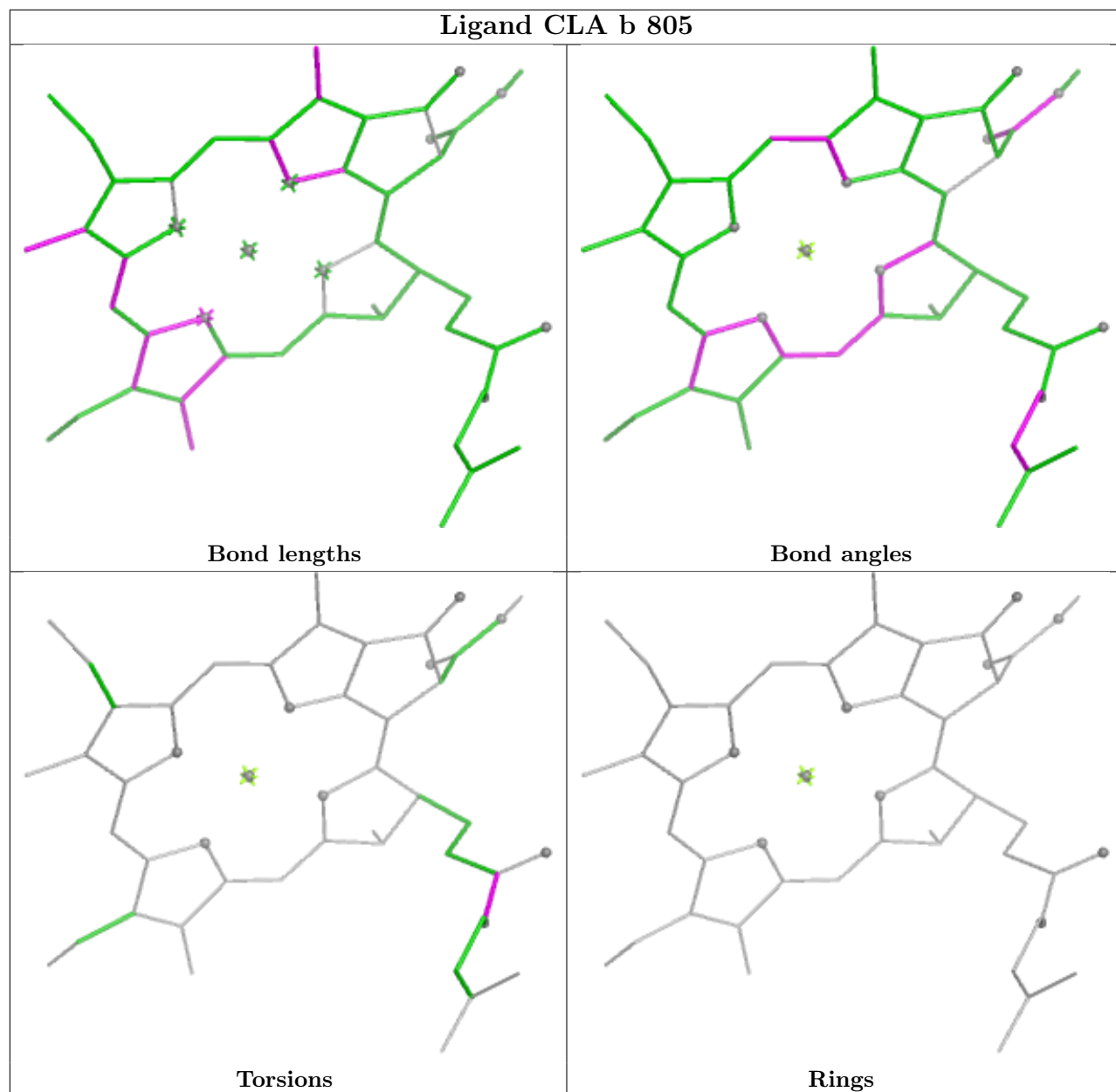


Rings

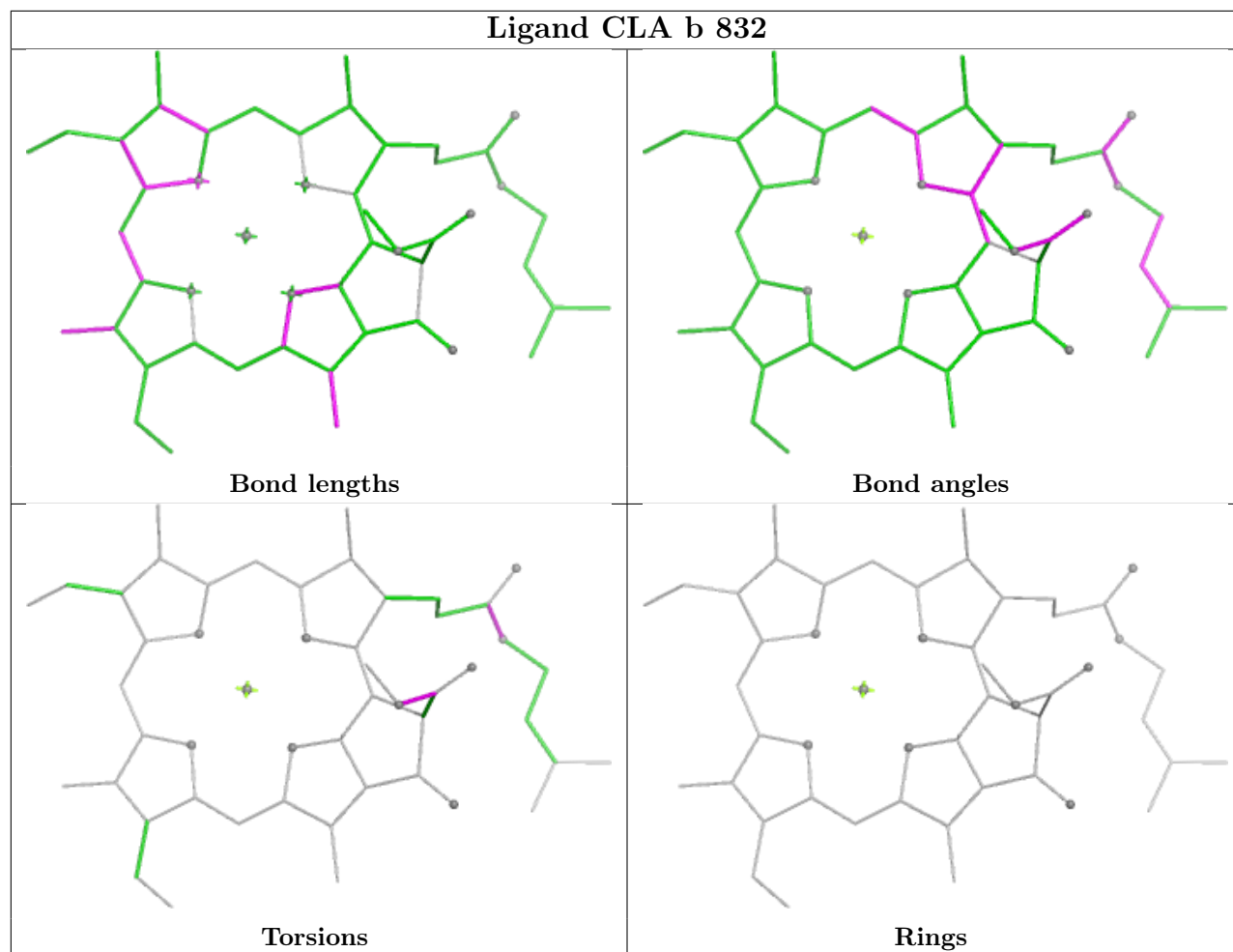
Ligand CLA A 840



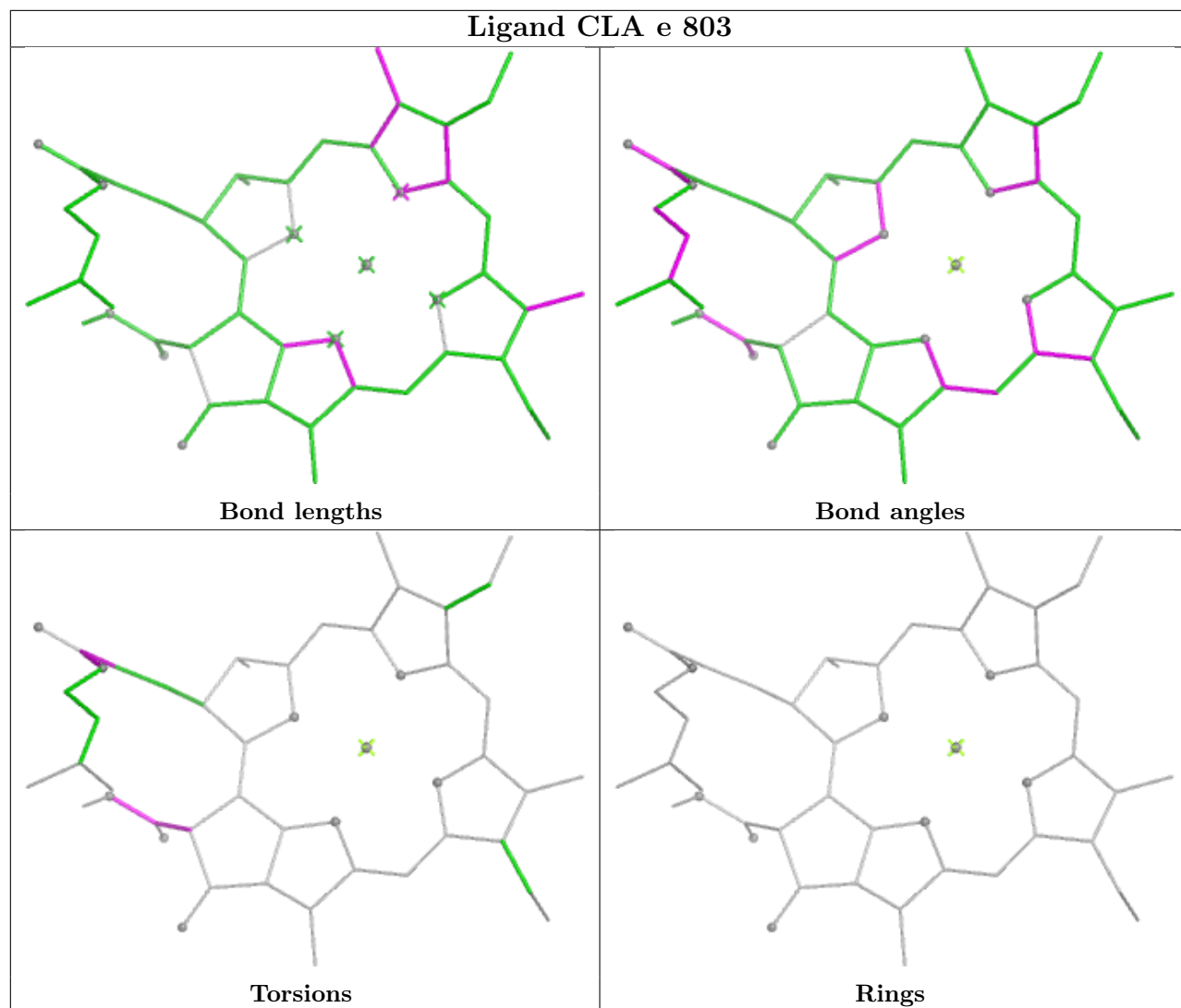
Ligand CLA b 805



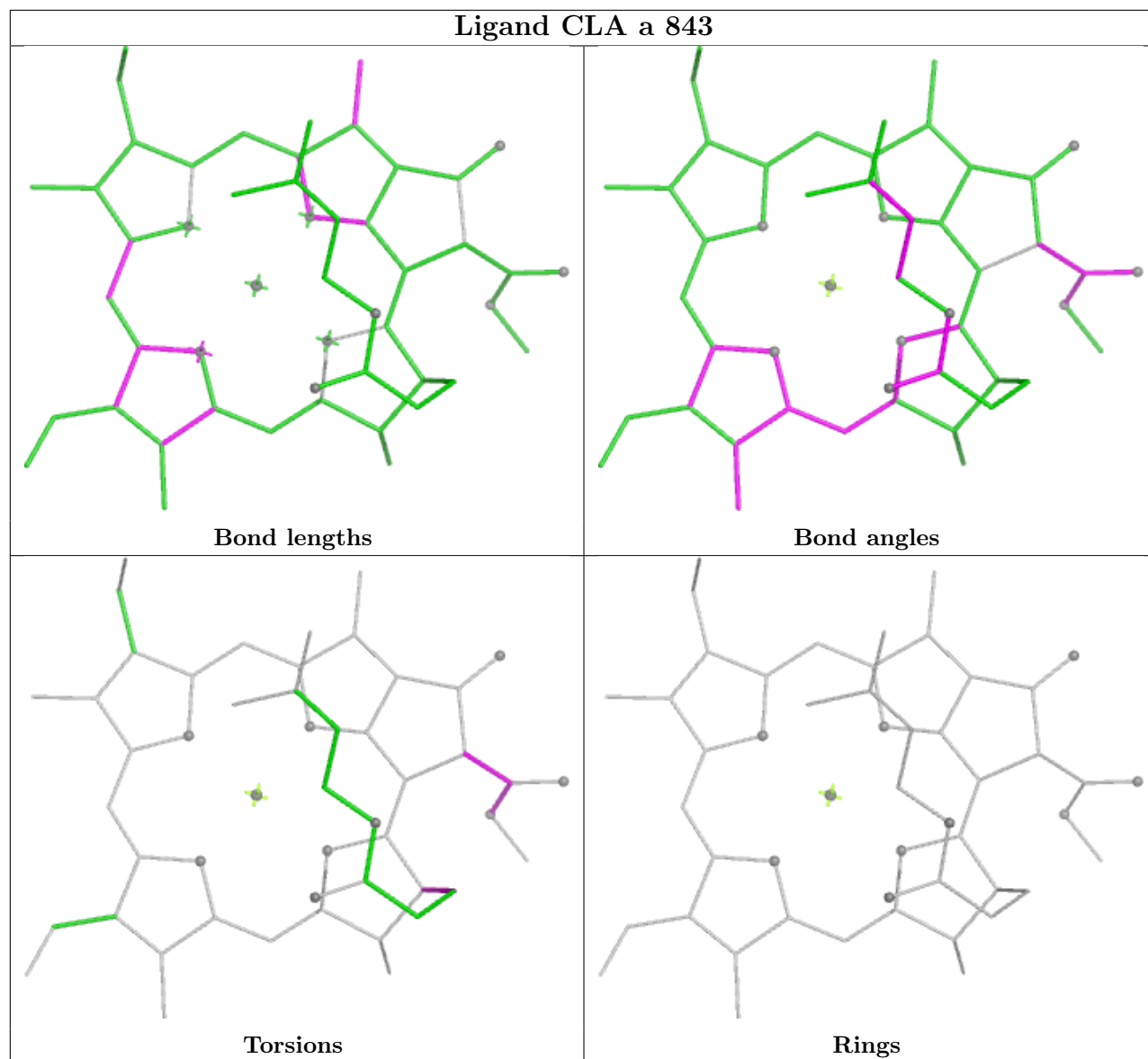
Ligand CLA b 832



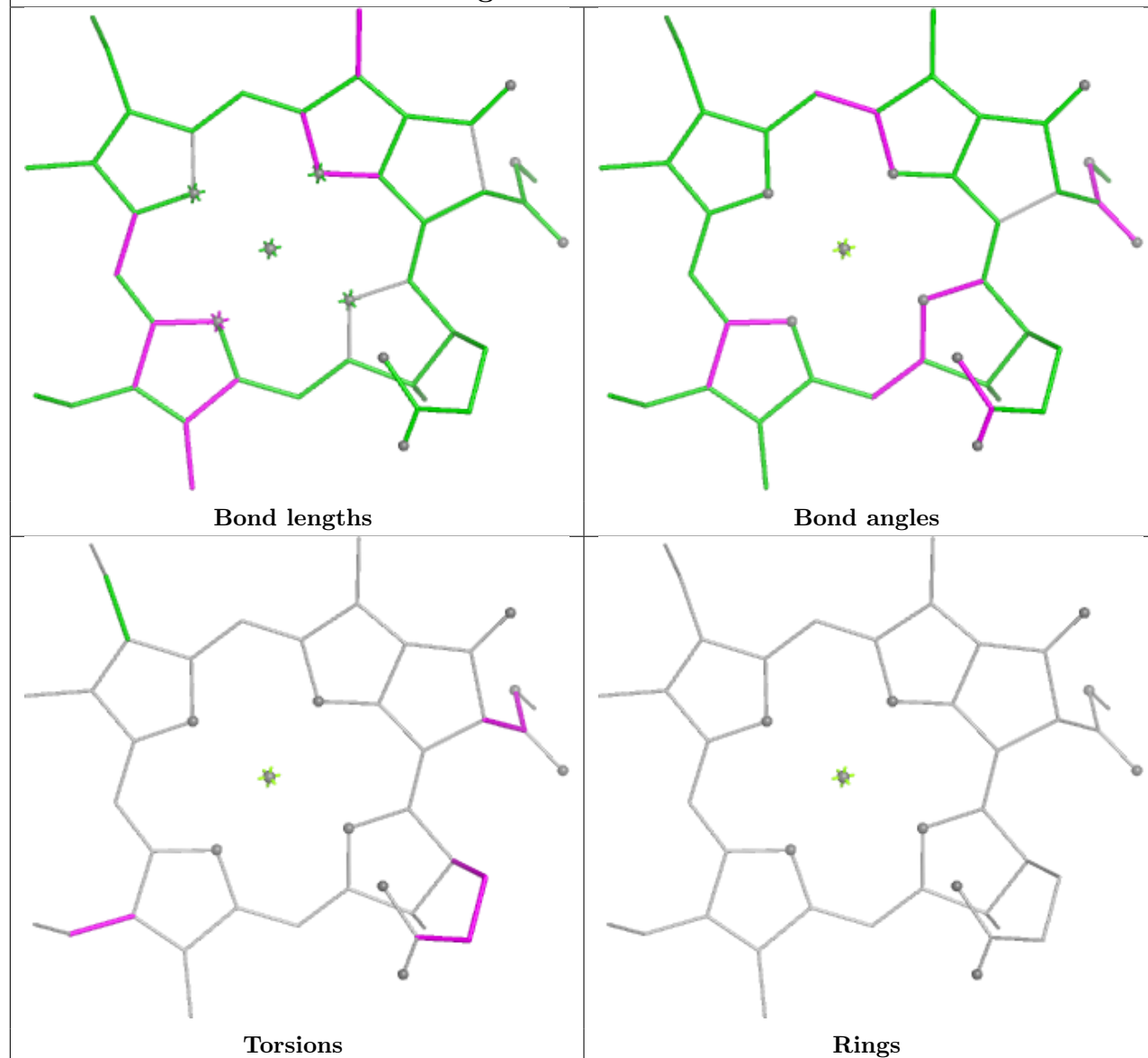
Ligand CLA e 803



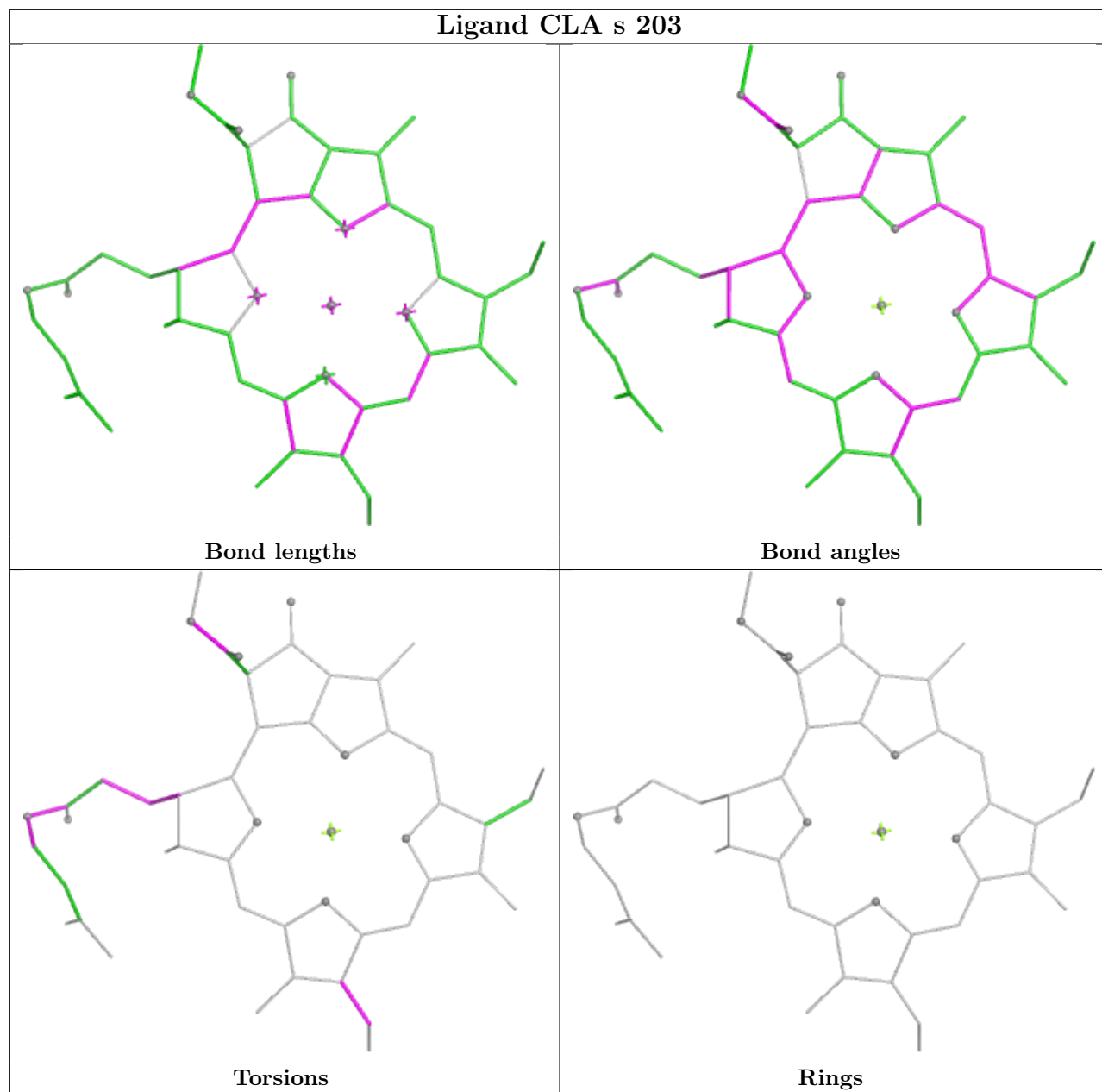
Ligand CLA a 843



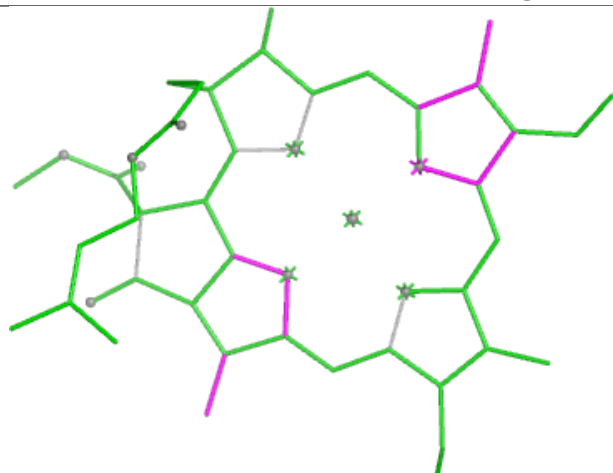
Ligand CLA G 831



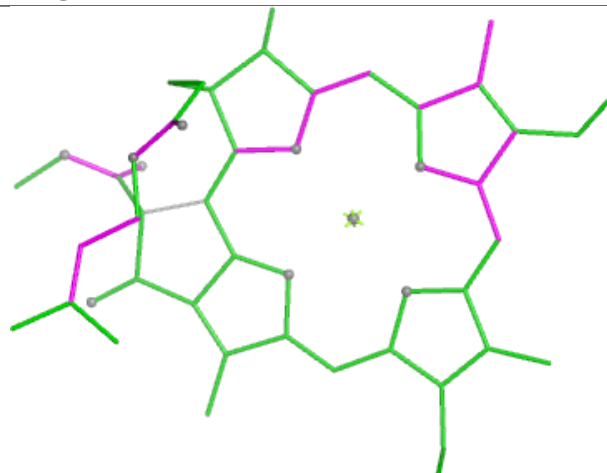
Ligand CLA s 203



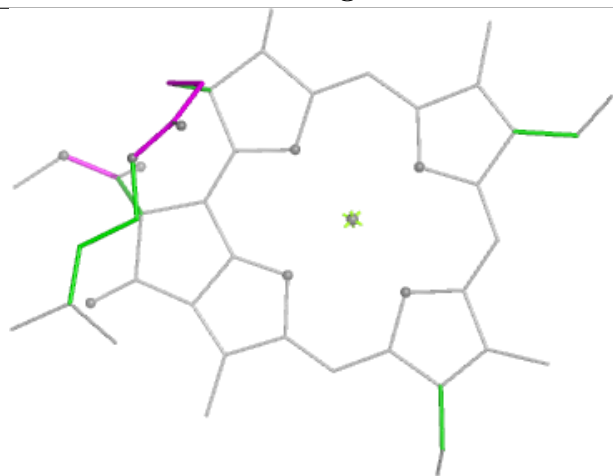
Ligand CLA g 831



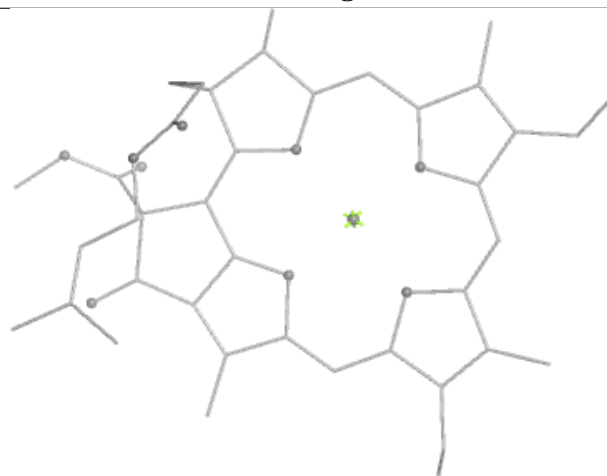
Bond lengths



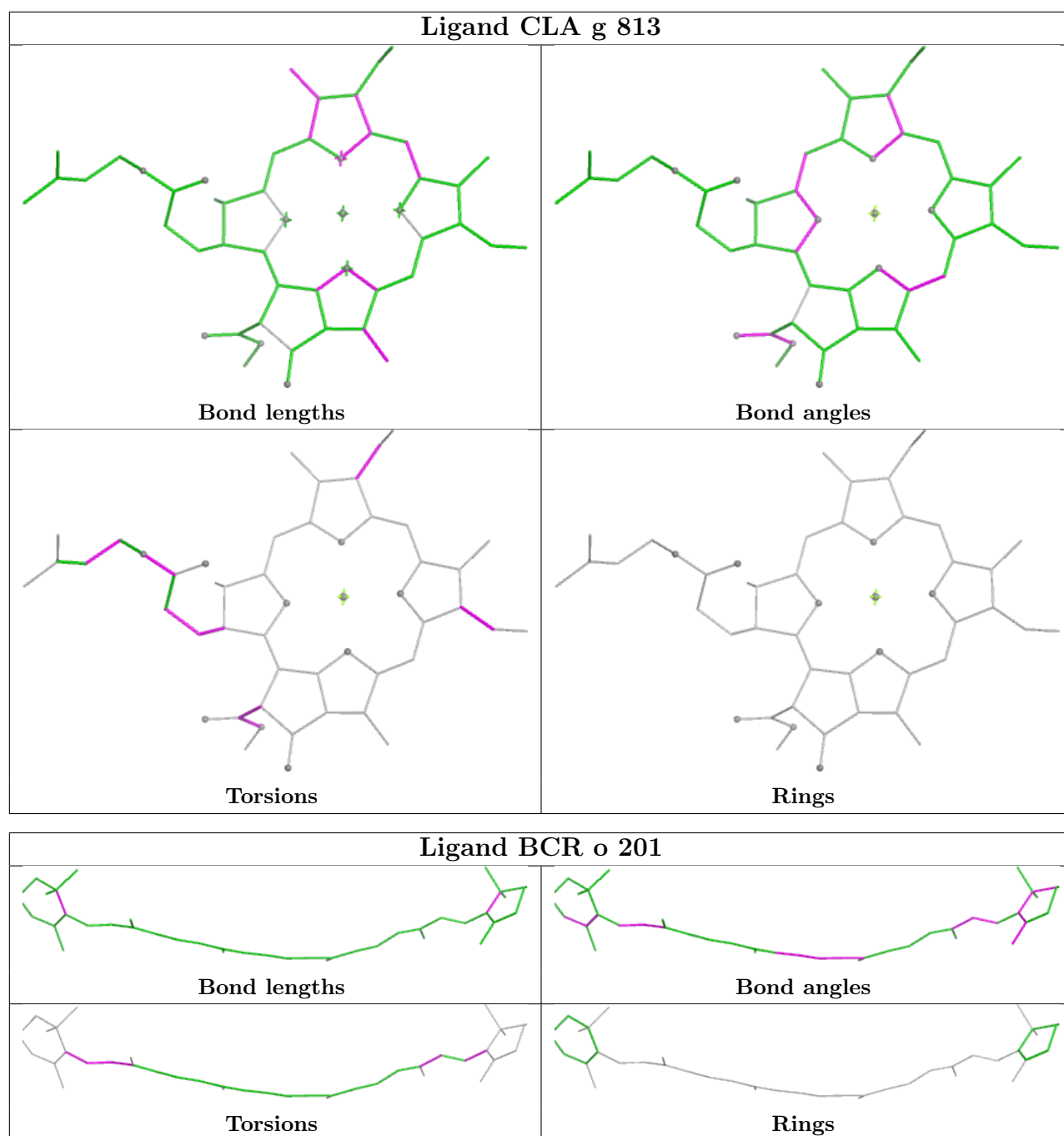
Bond angles



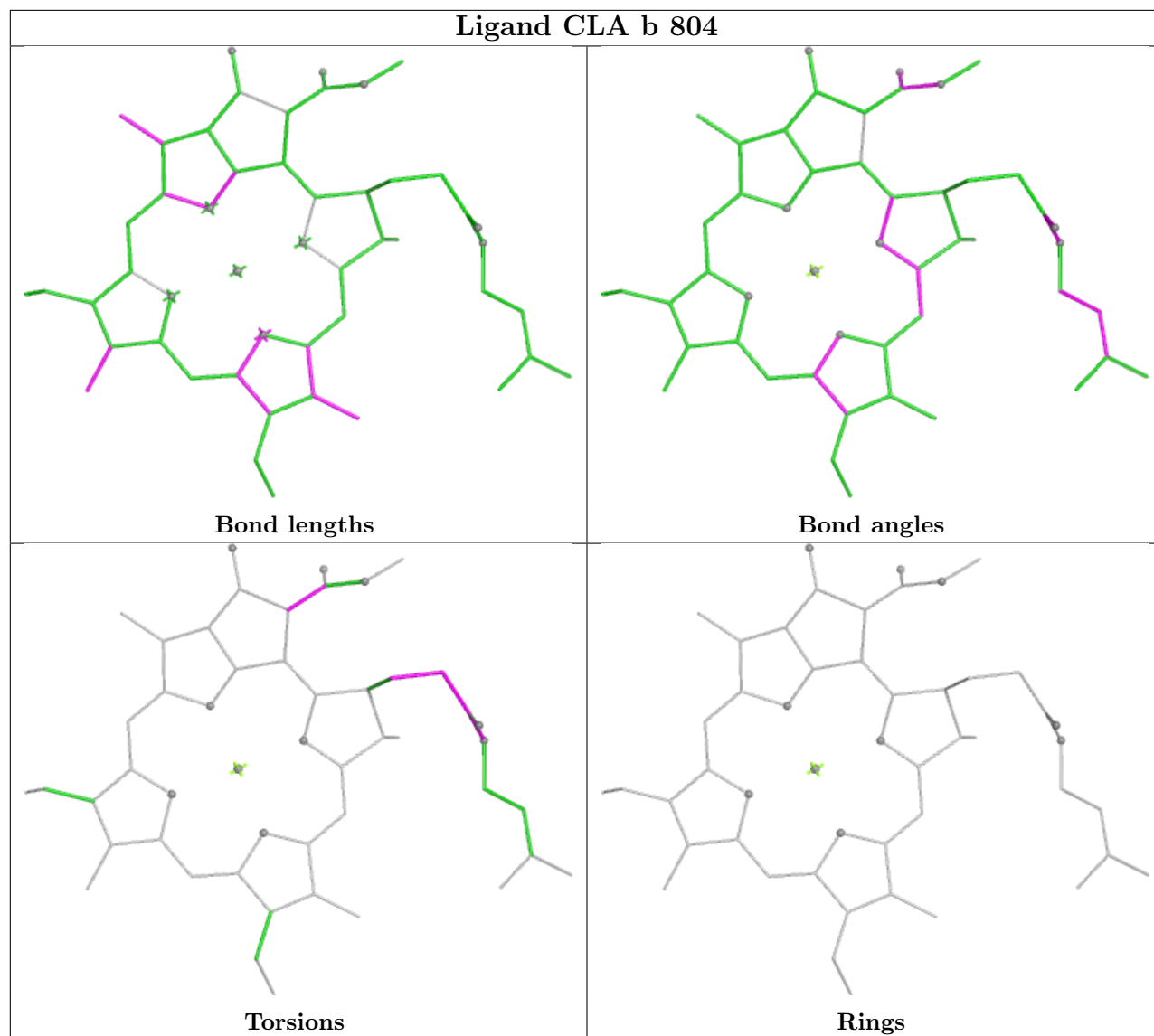
Torsions



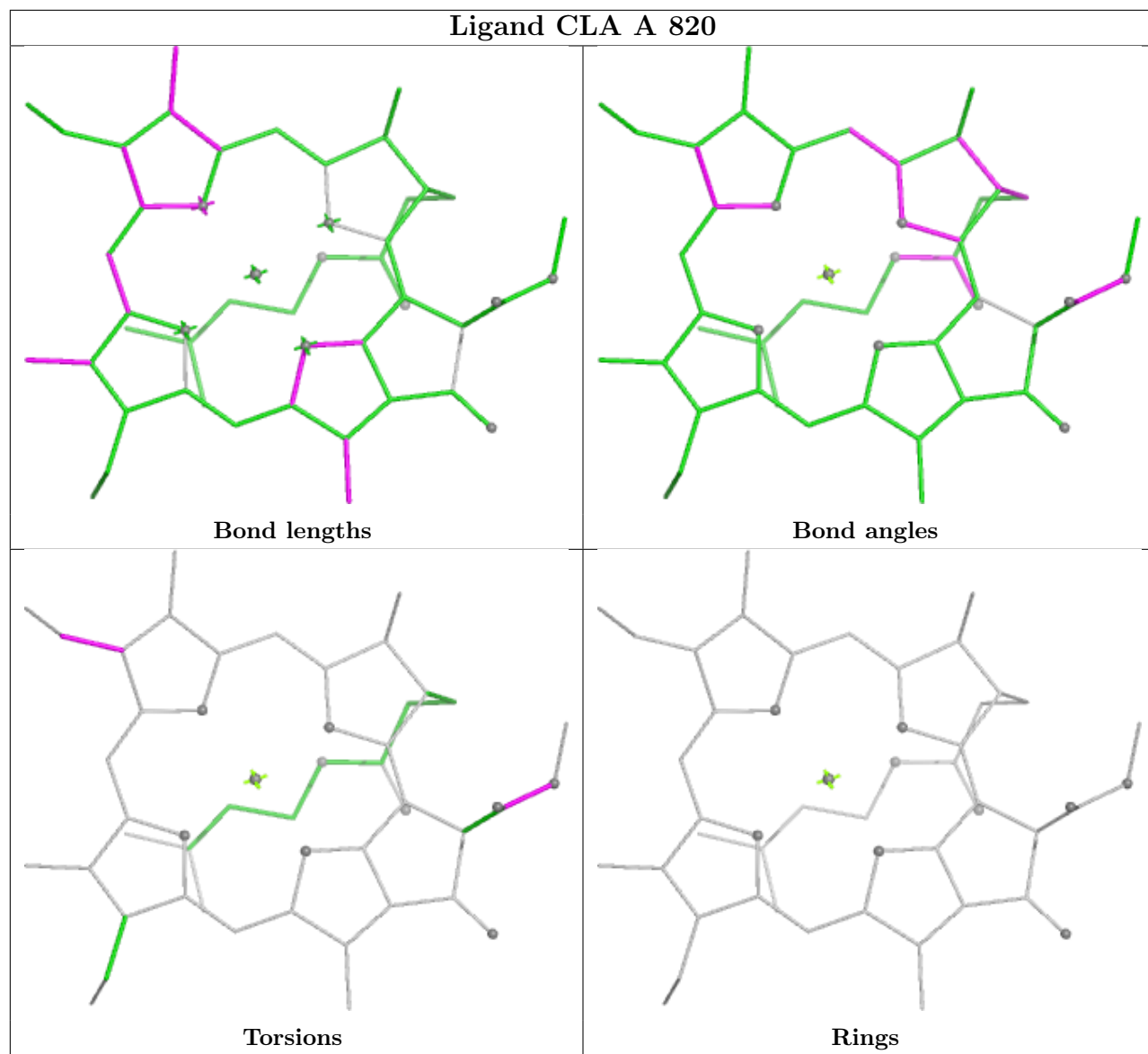
Rings

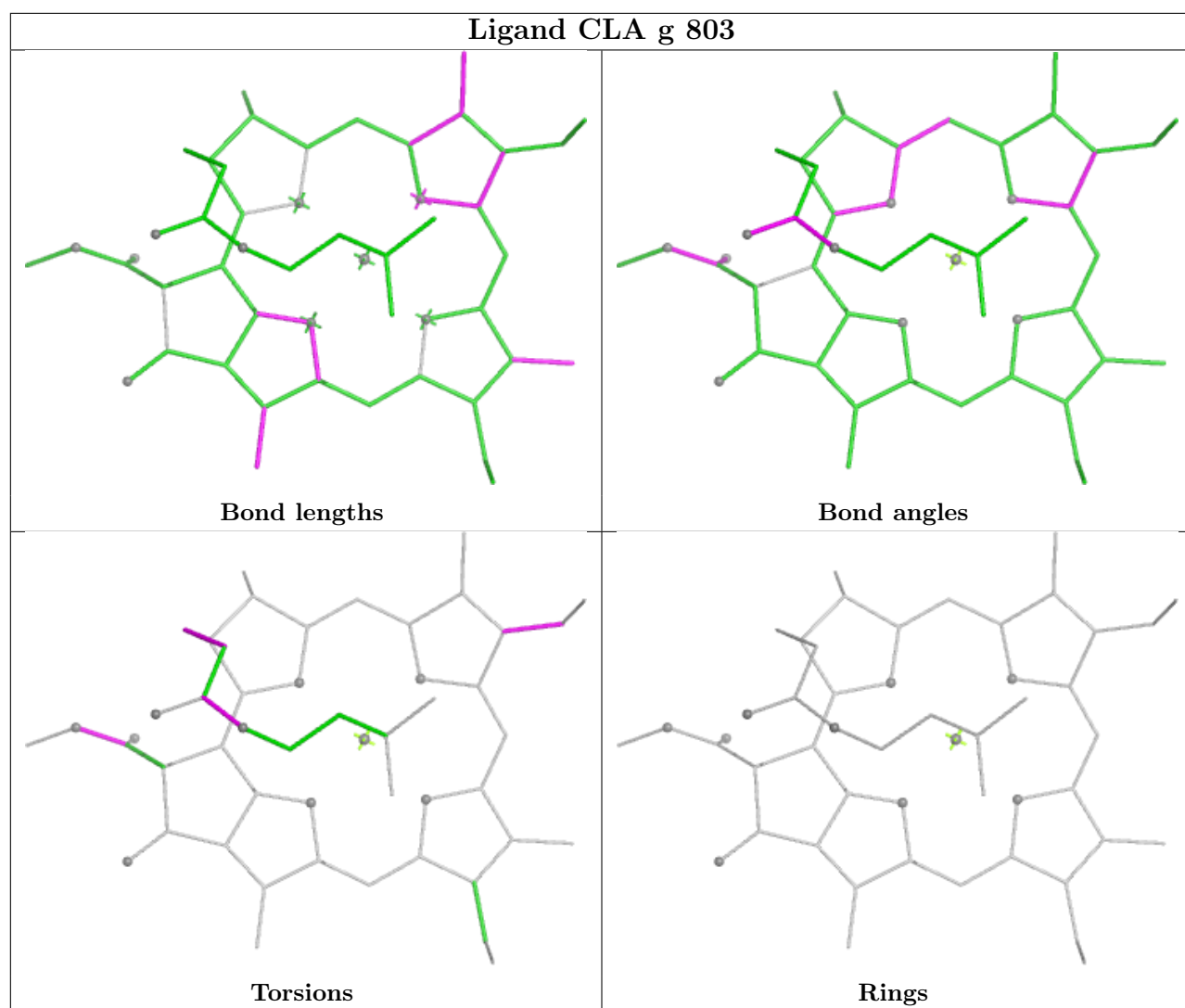


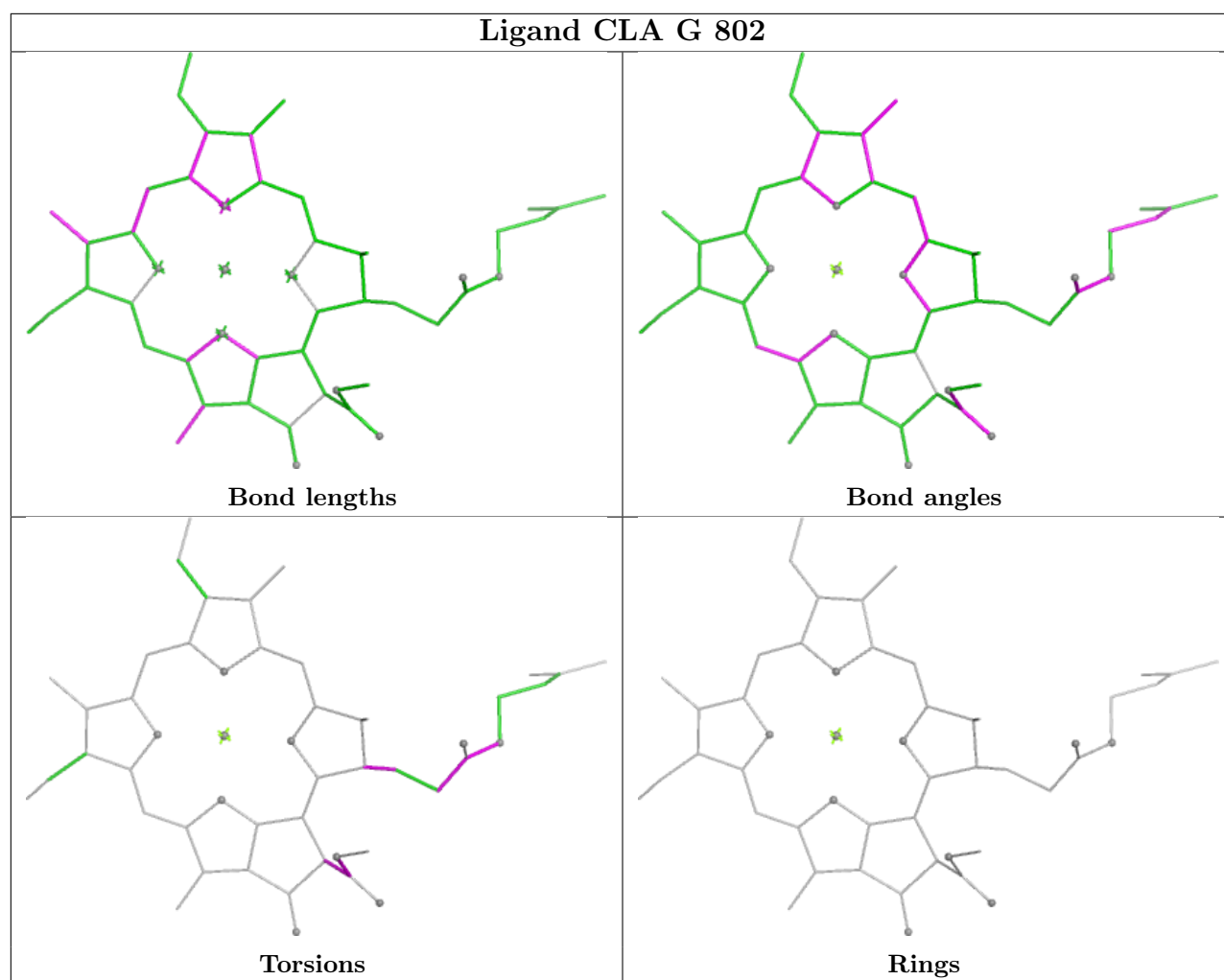
Ligand CLA b 804



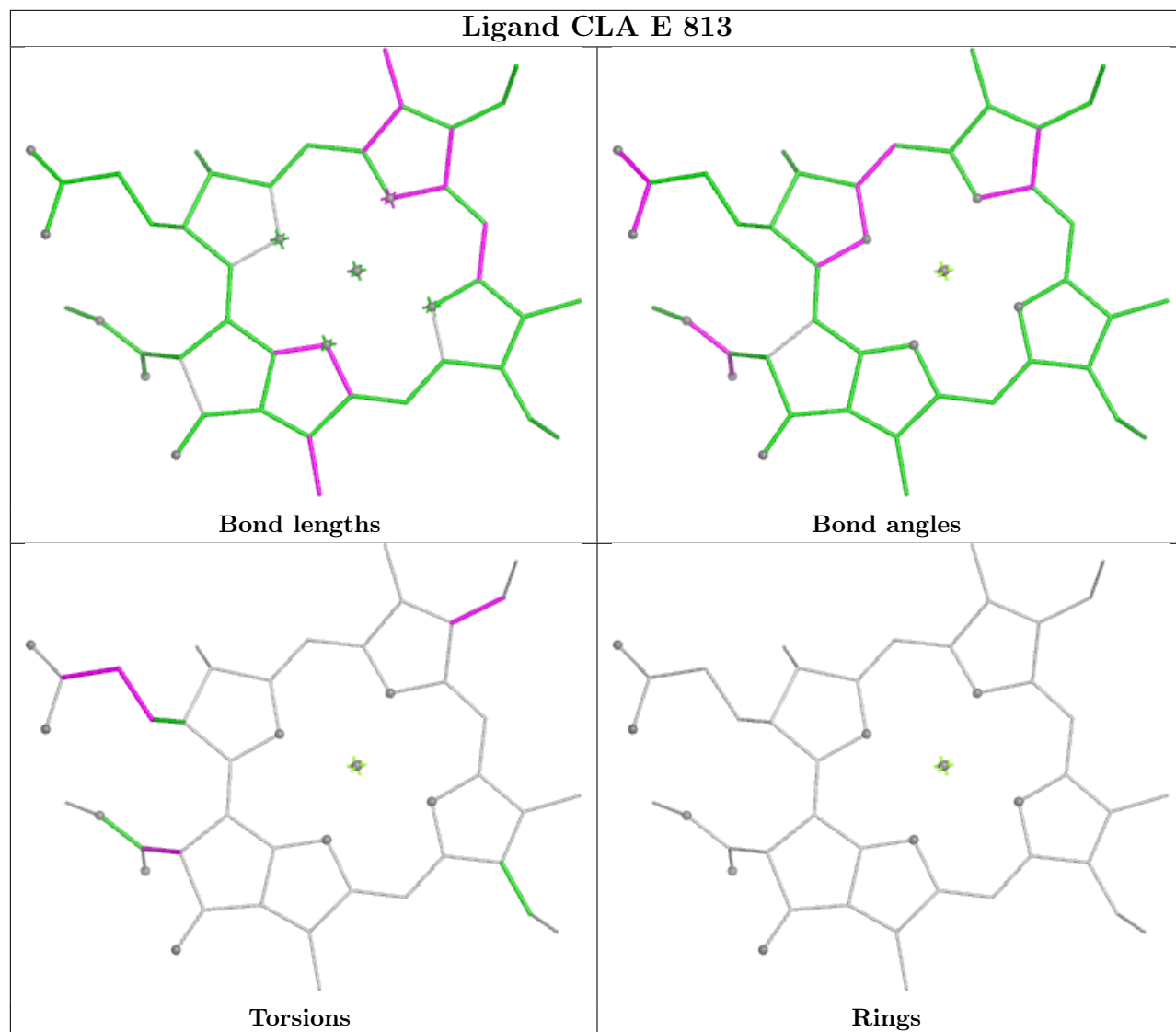
Ligand CLA A 820

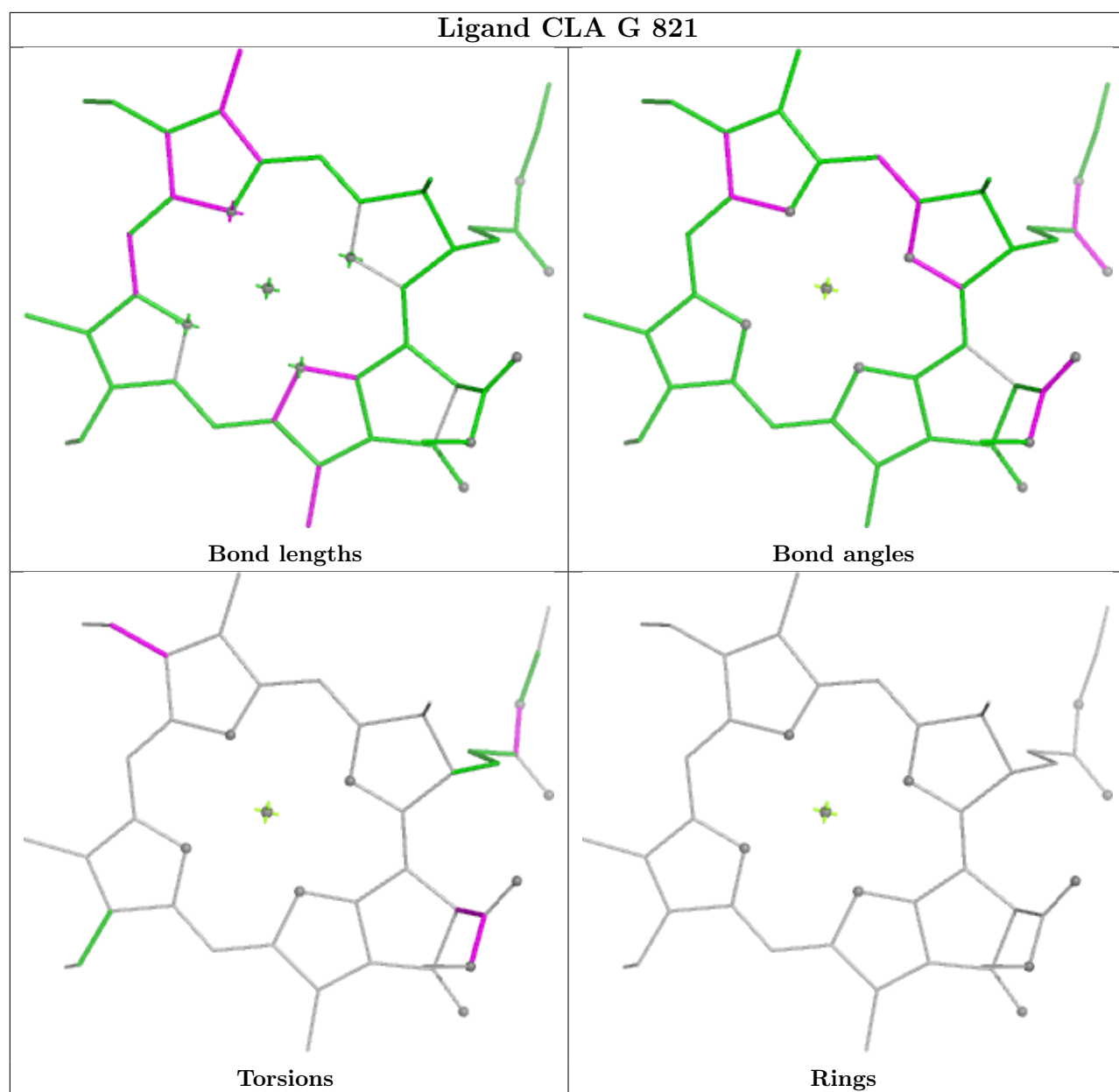




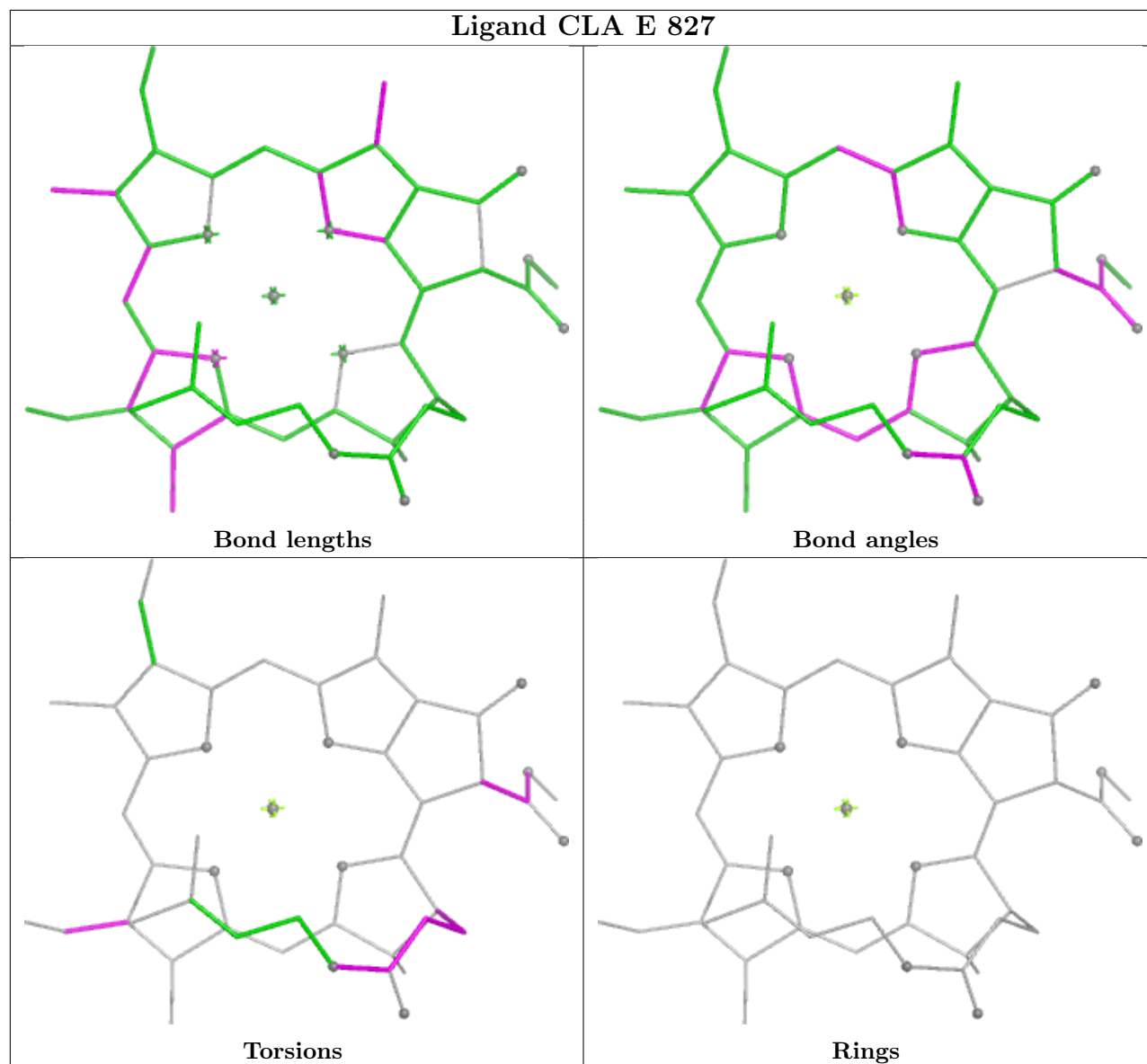


Ligand CLA E 813

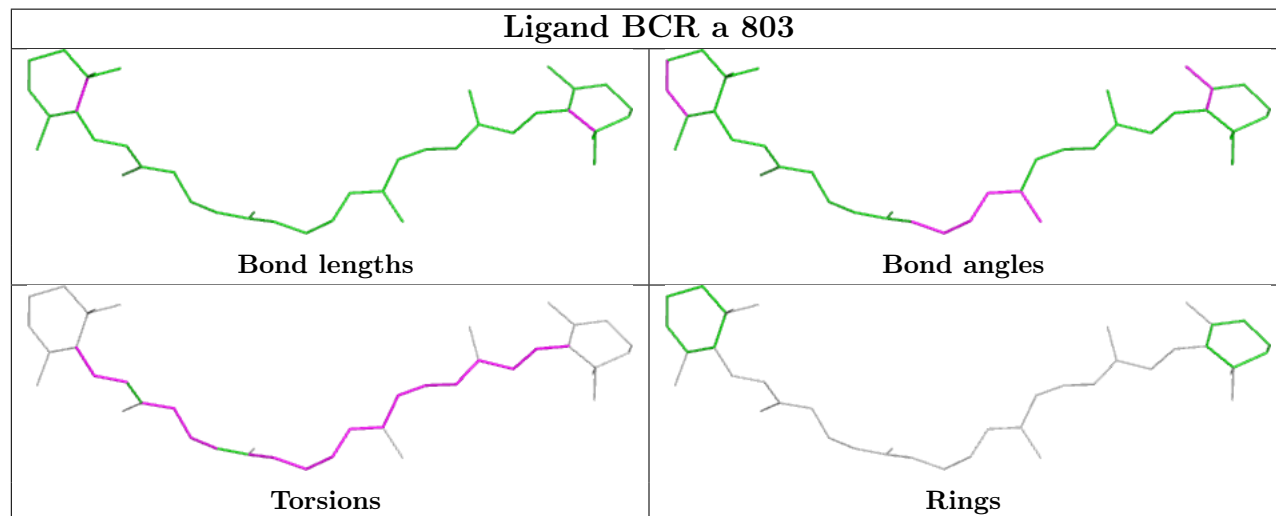




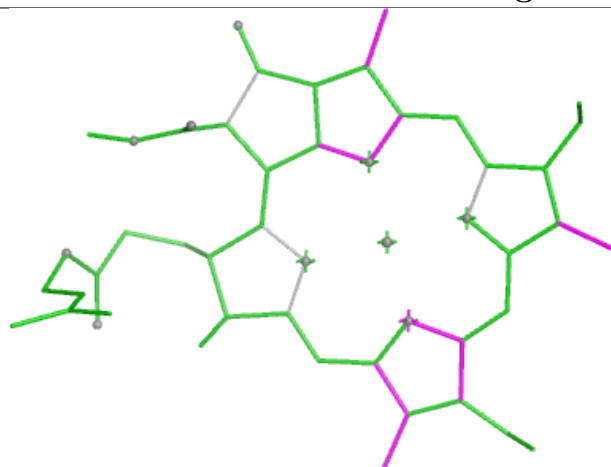
Ligand CLA E 827



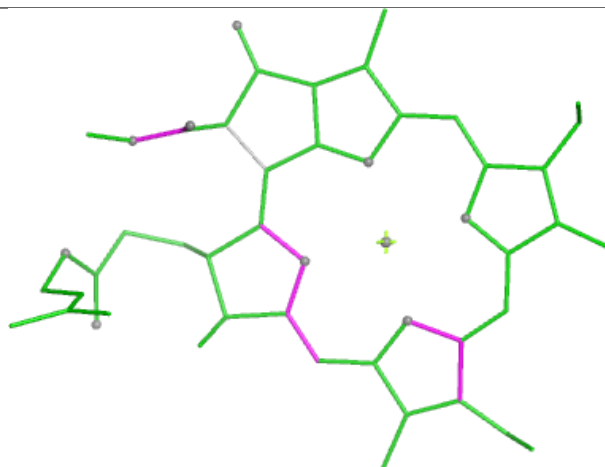
Ligand BCR a 803



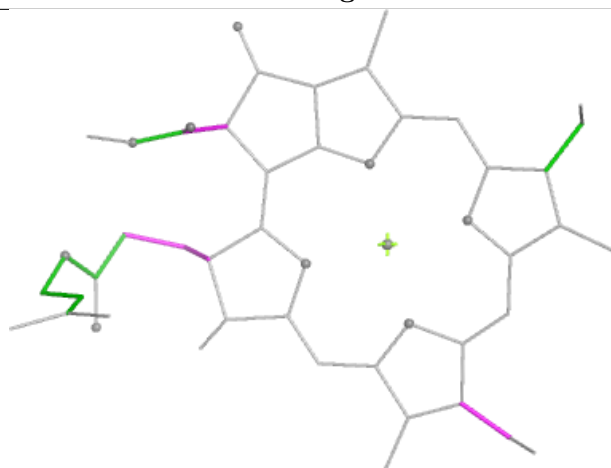
Ligand CLA E 809



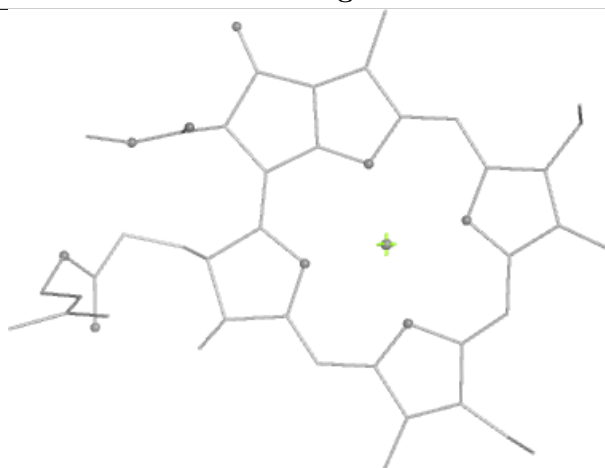
Bond lengths



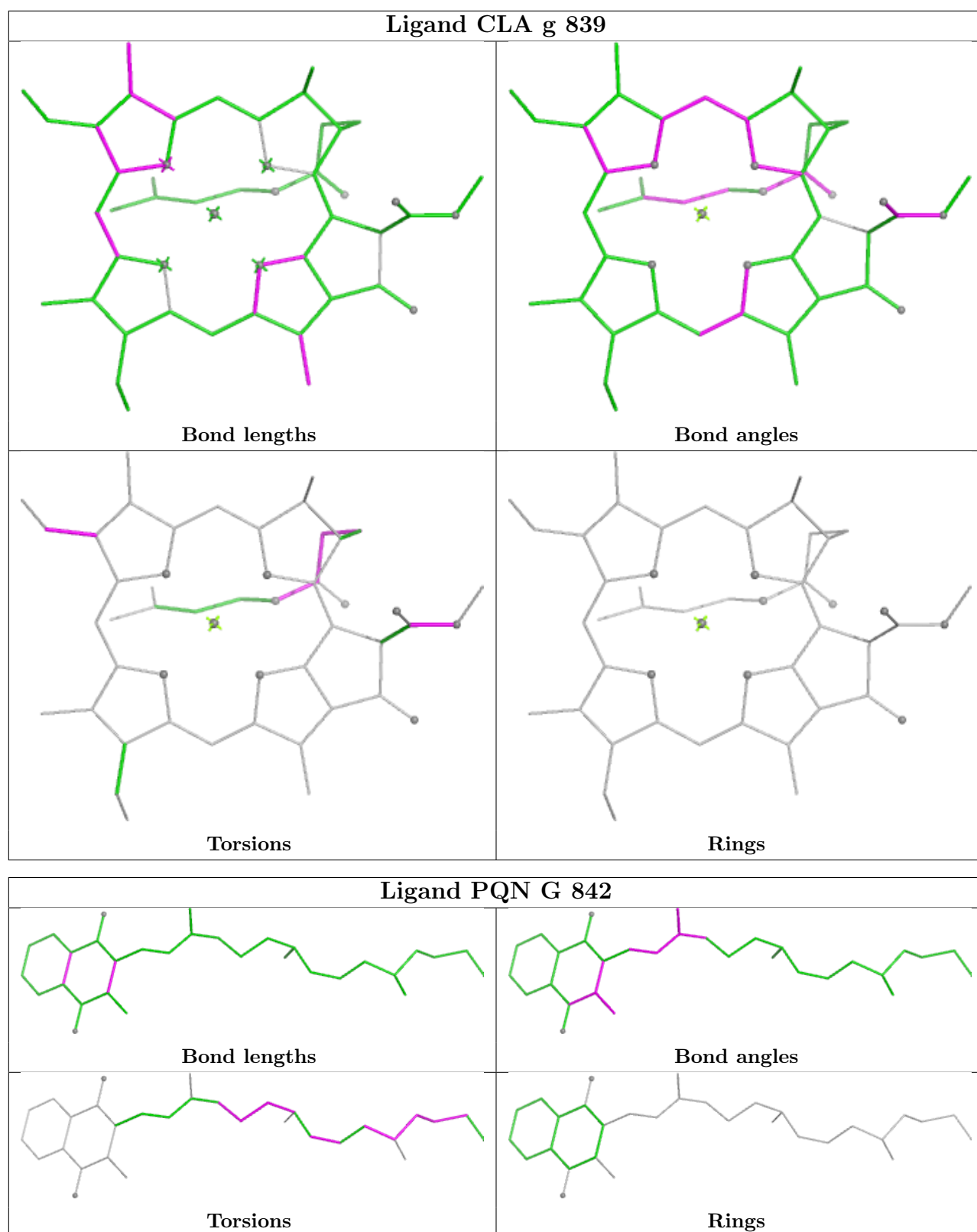
Bond angles



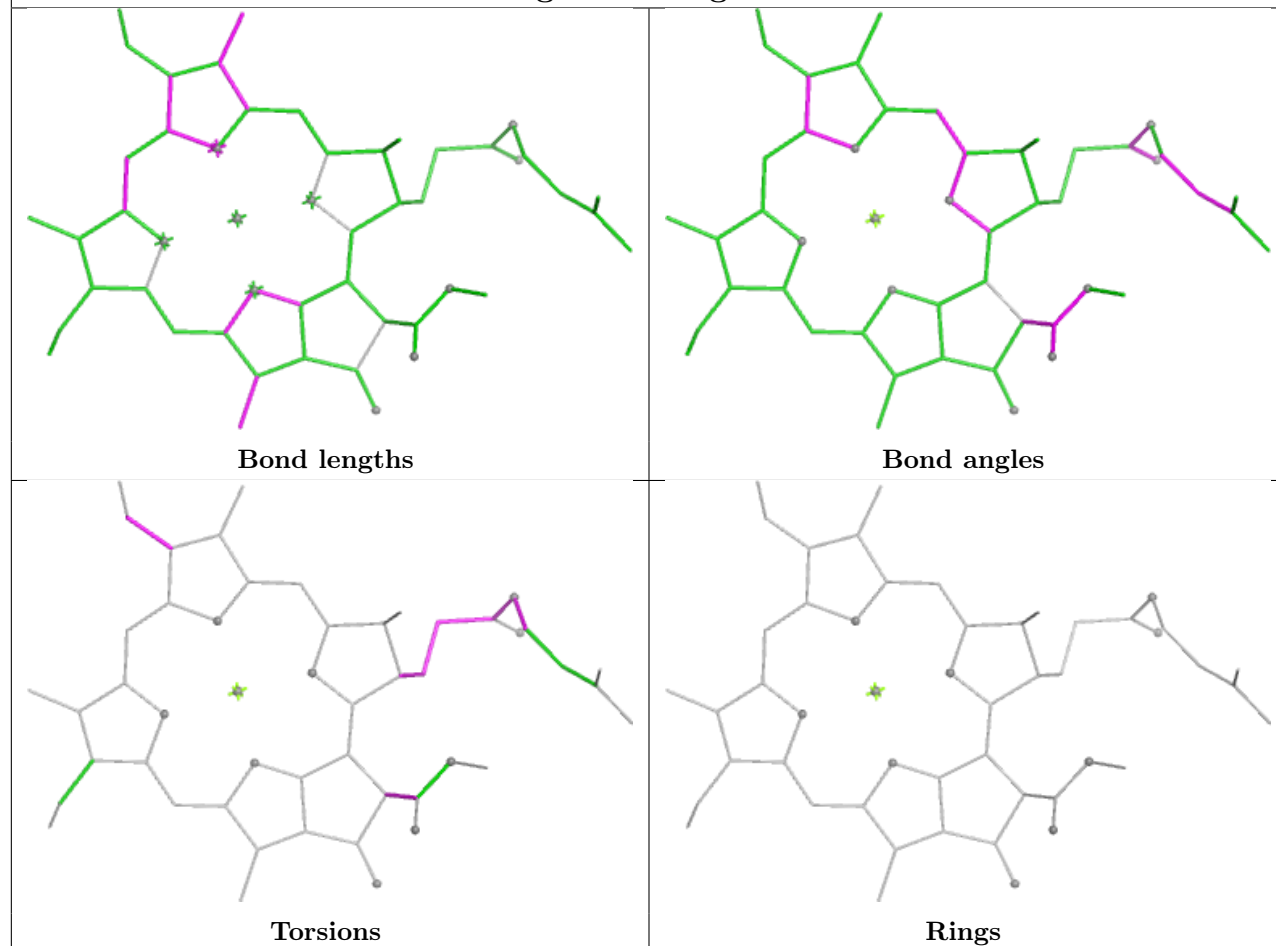
Torsions



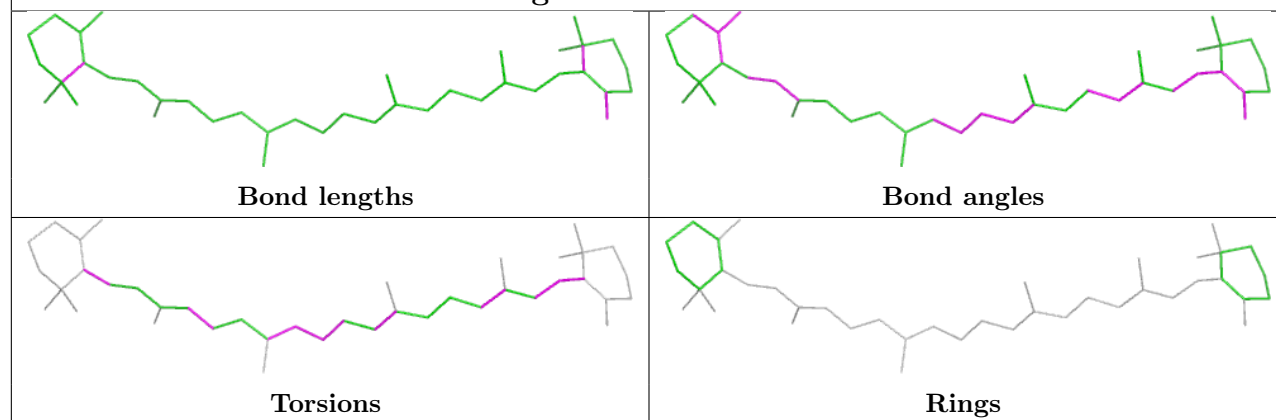
Rings



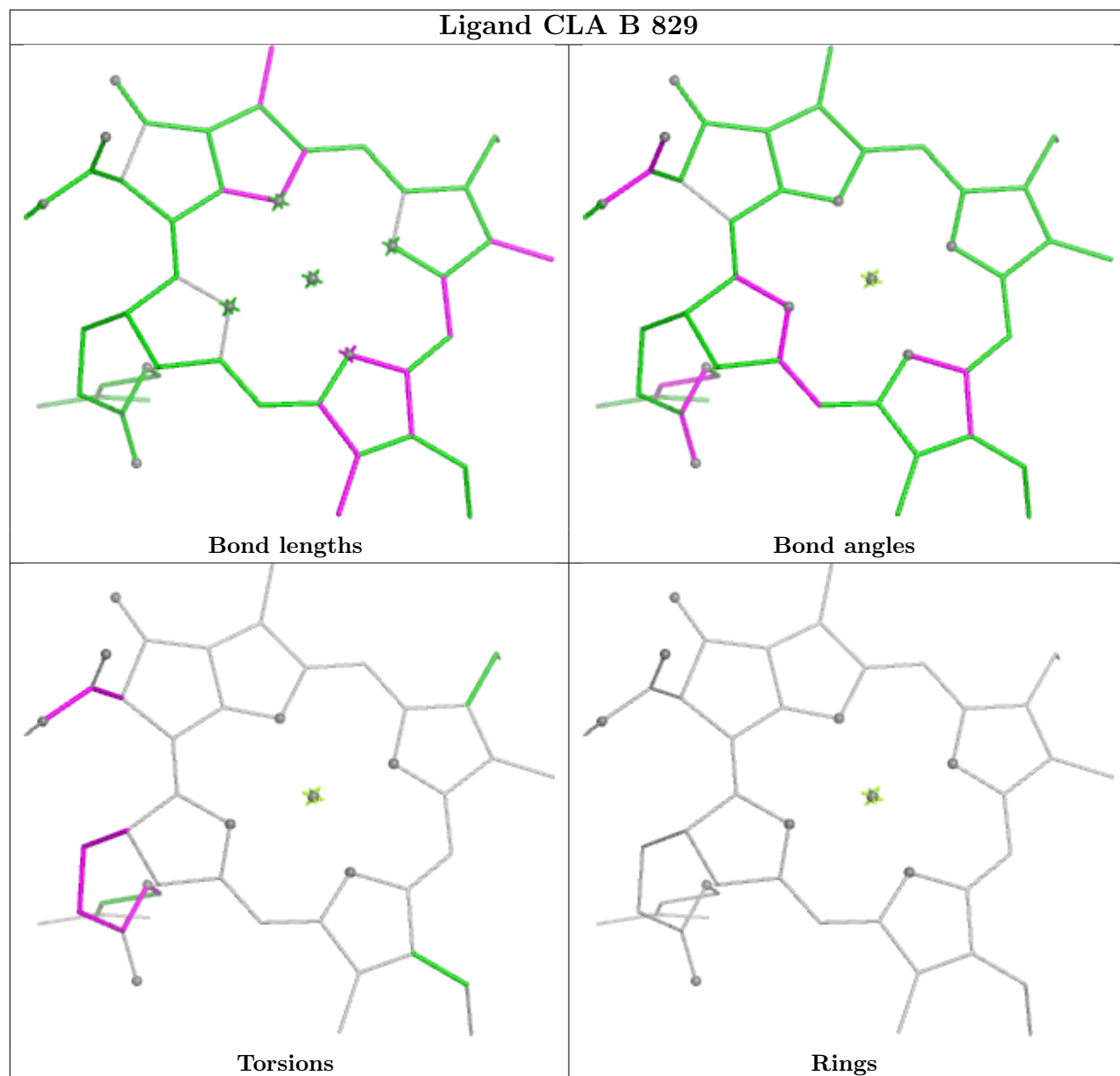
Ligand CLA g 808



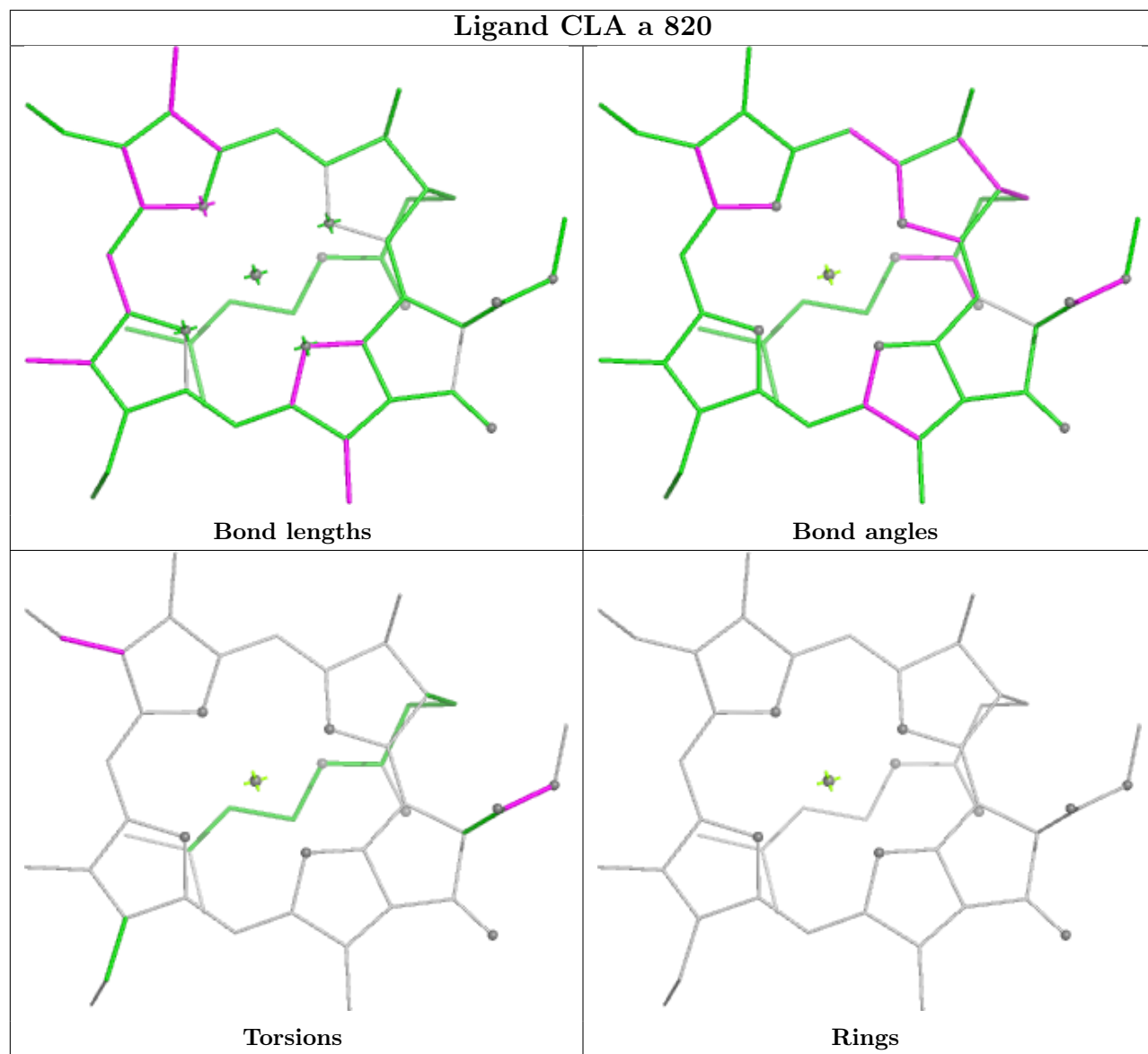
Ligand BCR E 801

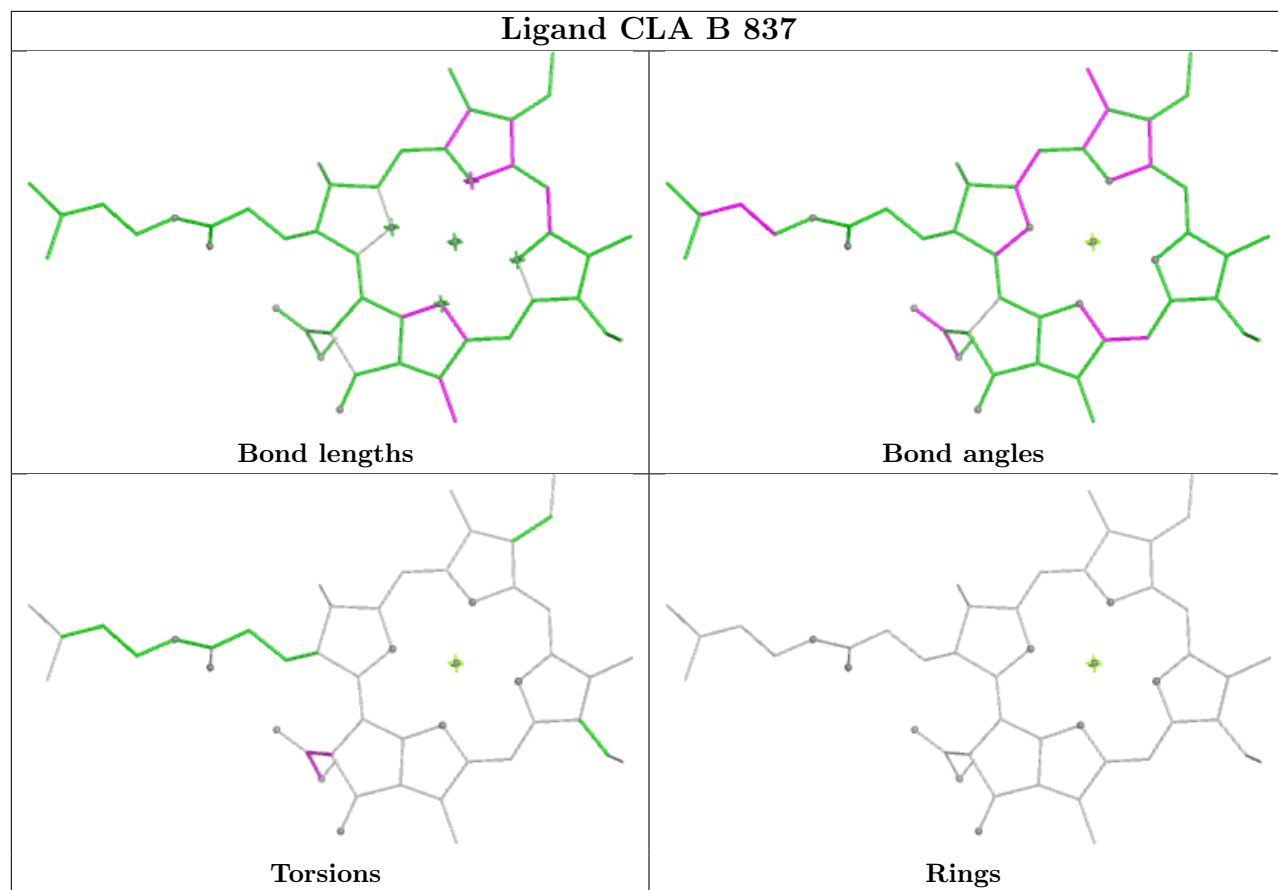


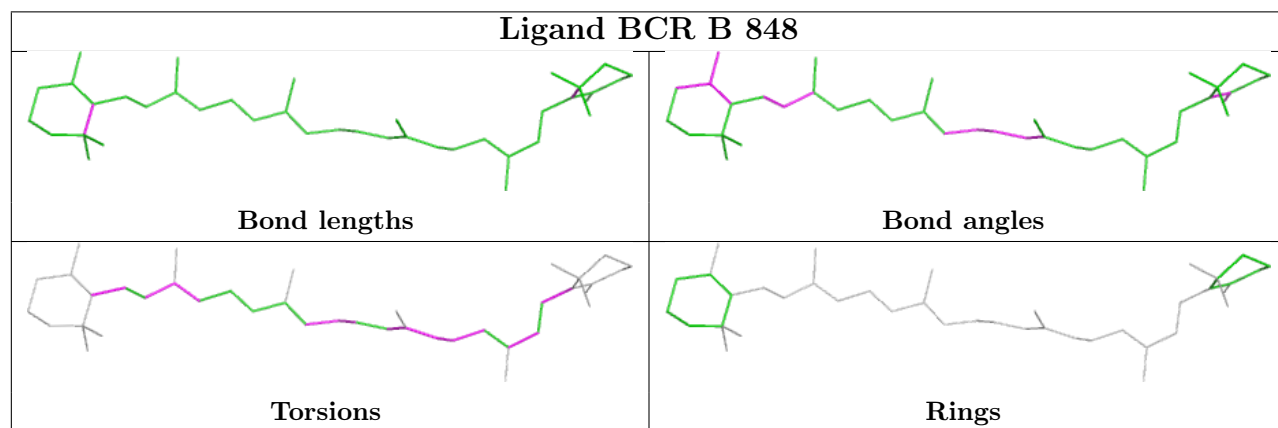
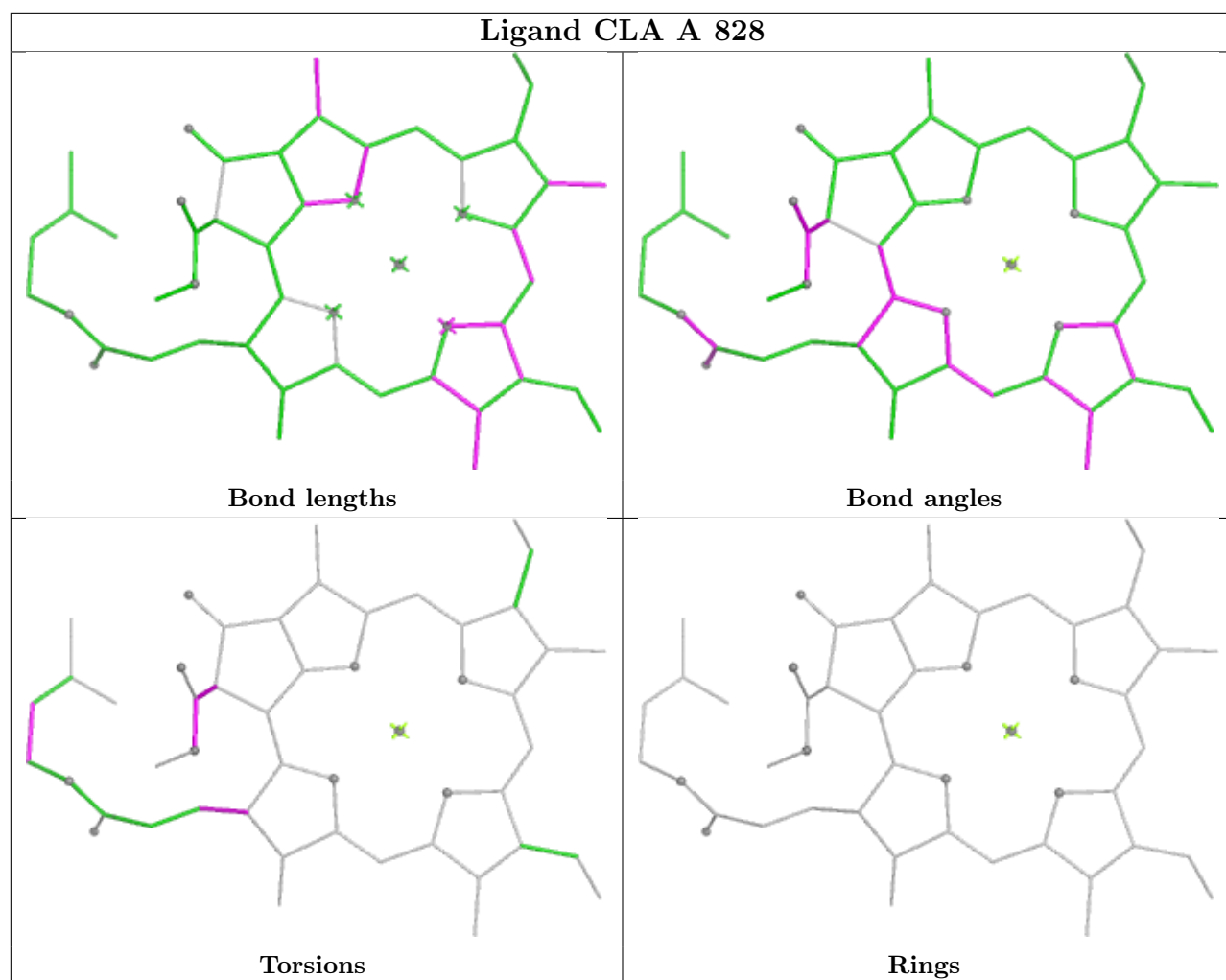
Ligand CLA B 829

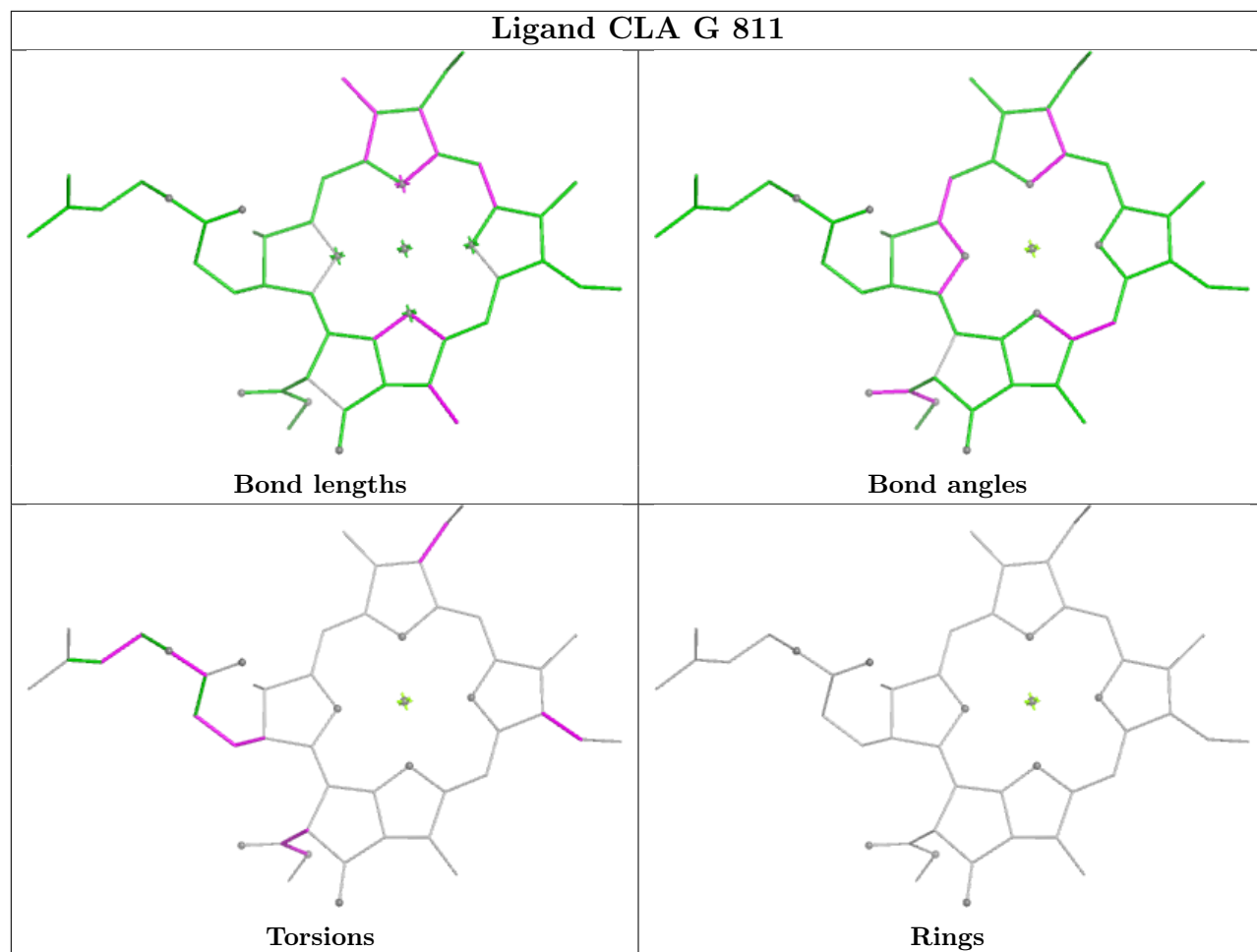


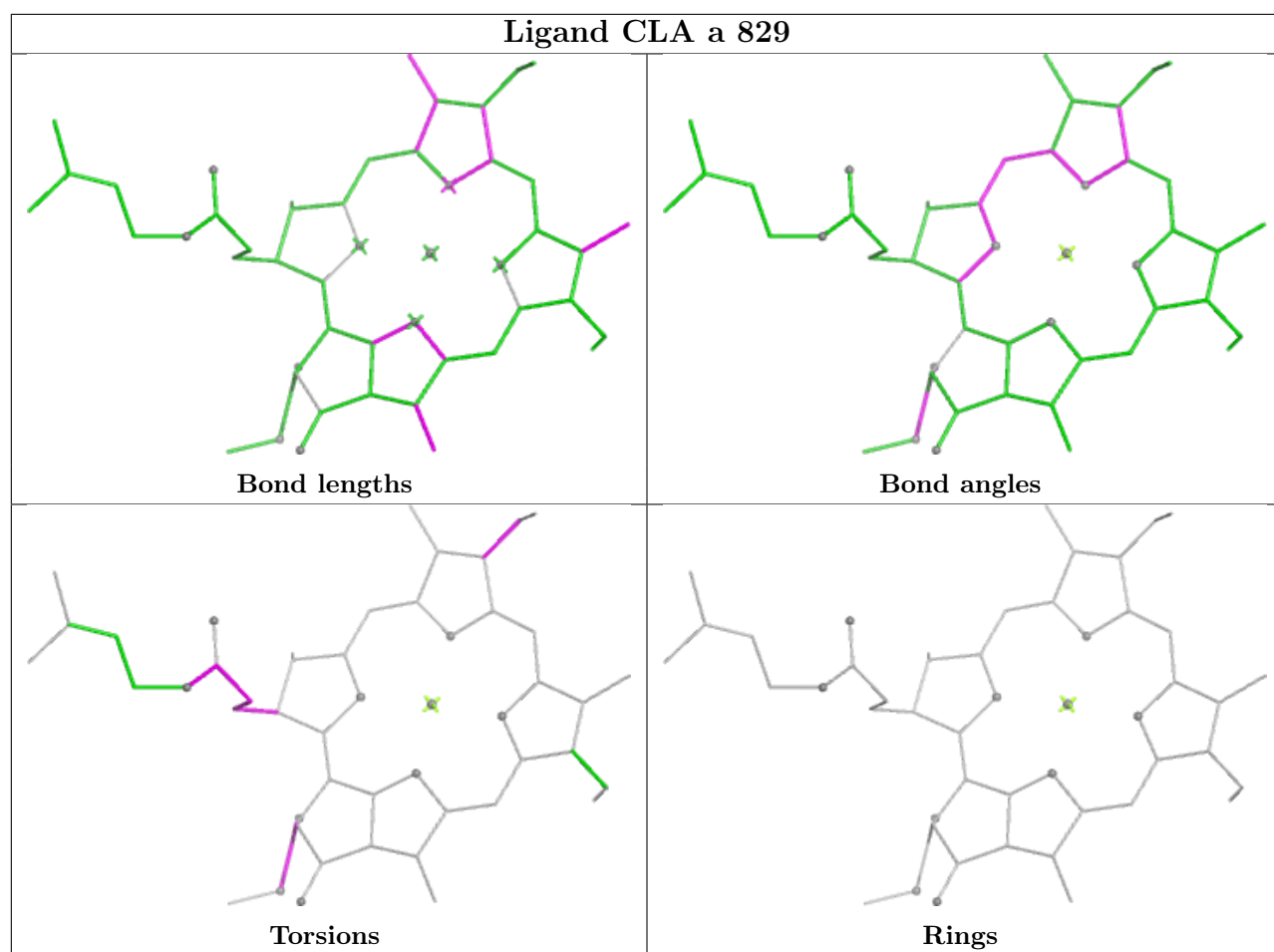
Ligand CLA a 820



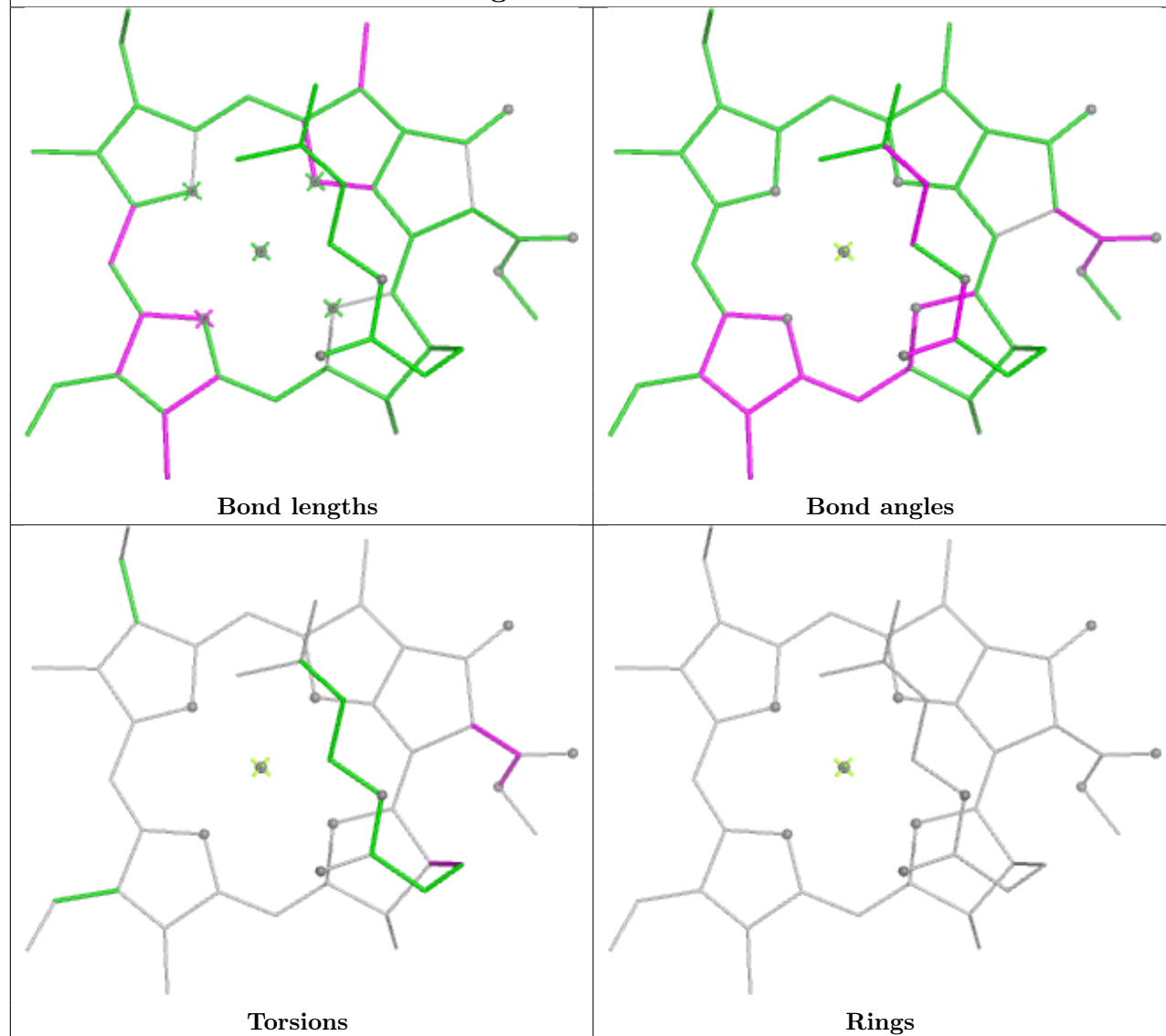




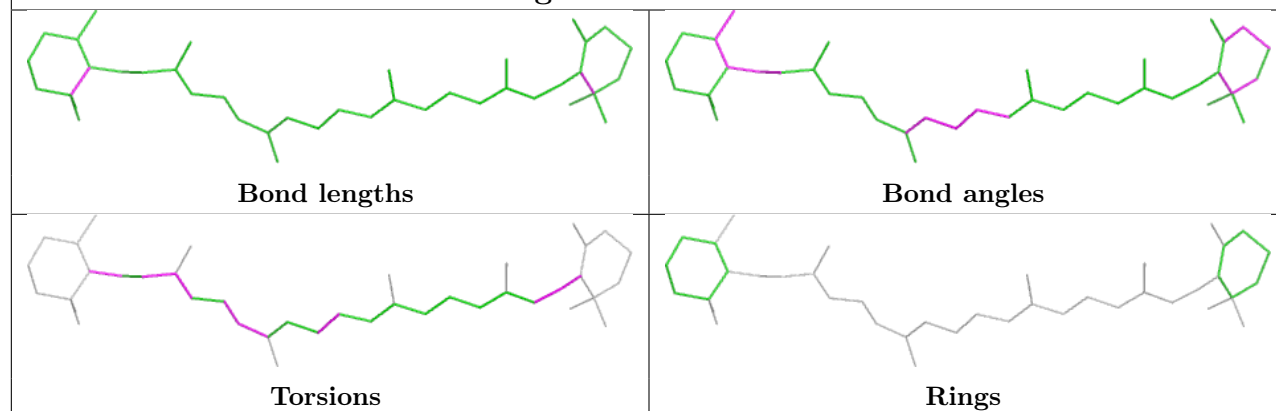




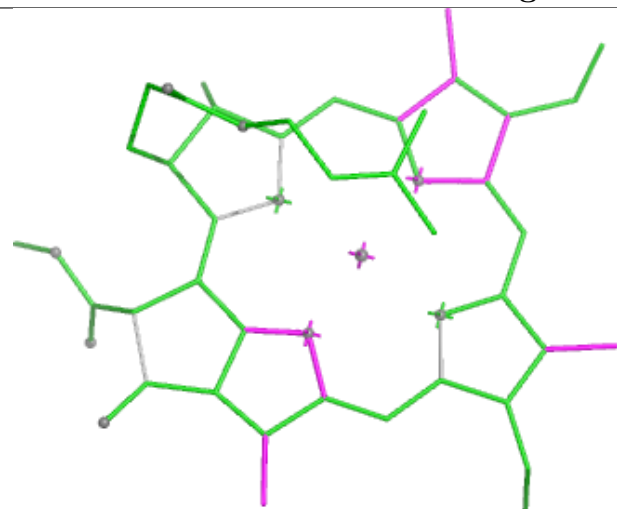
Ligand CLA e 841



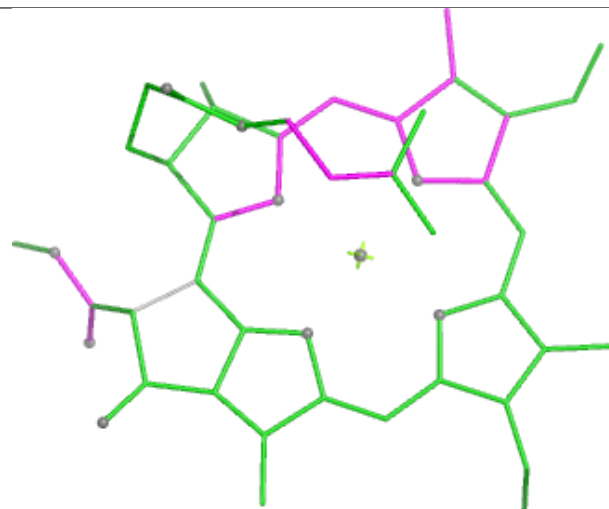
Ligand BCR a 853



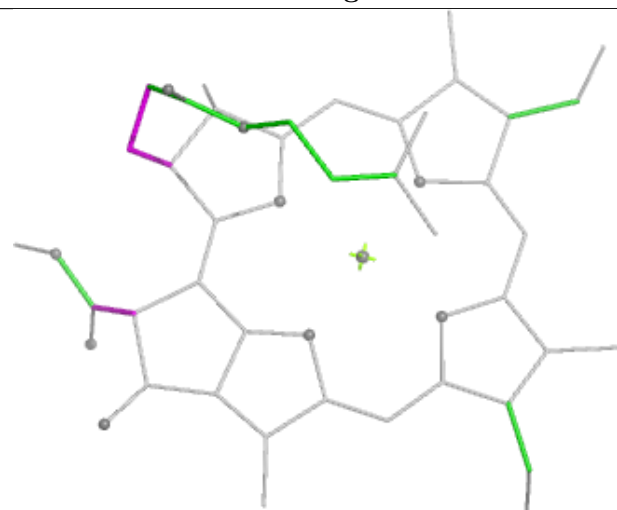
Ligand CLA E 835



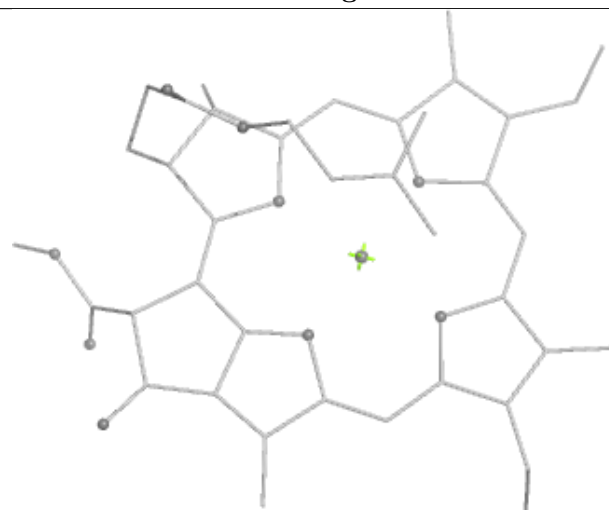
Bond lengths



Bond angles

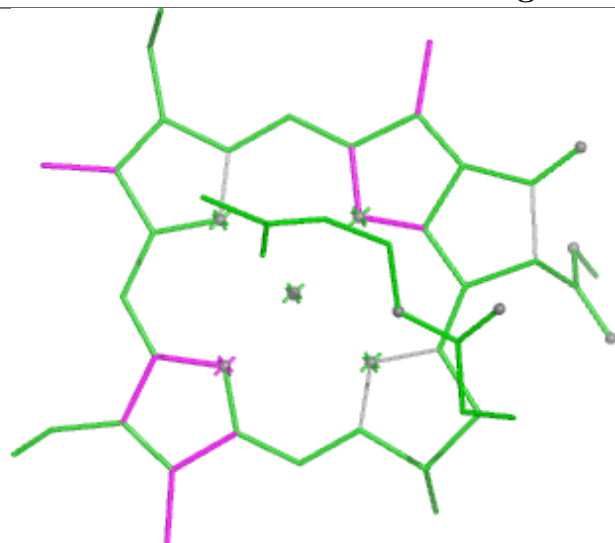


Torsions

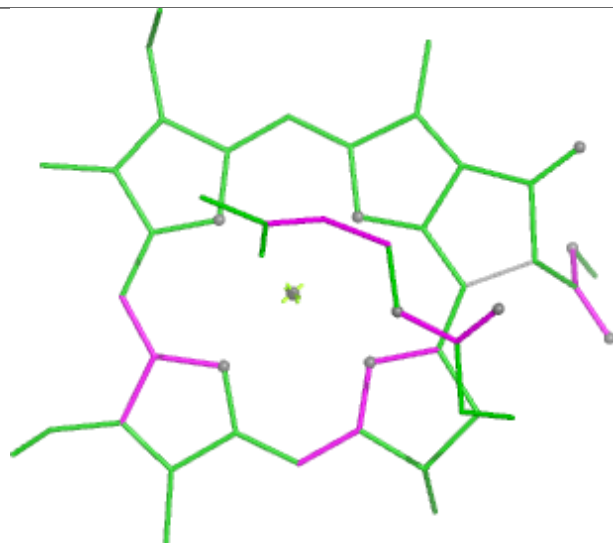


Rings

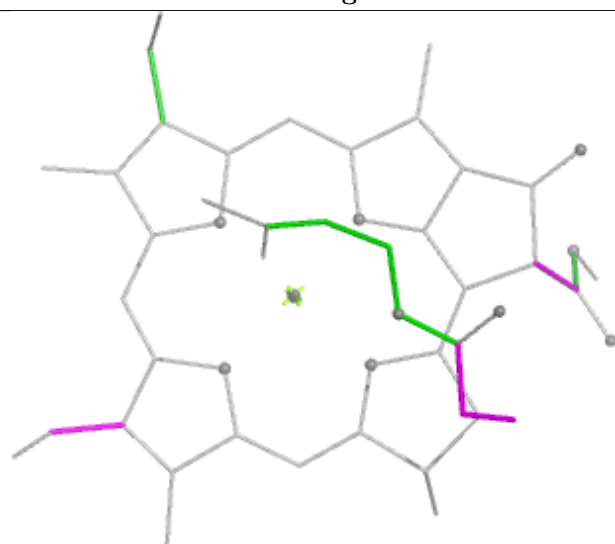
Ligand CLA E 841



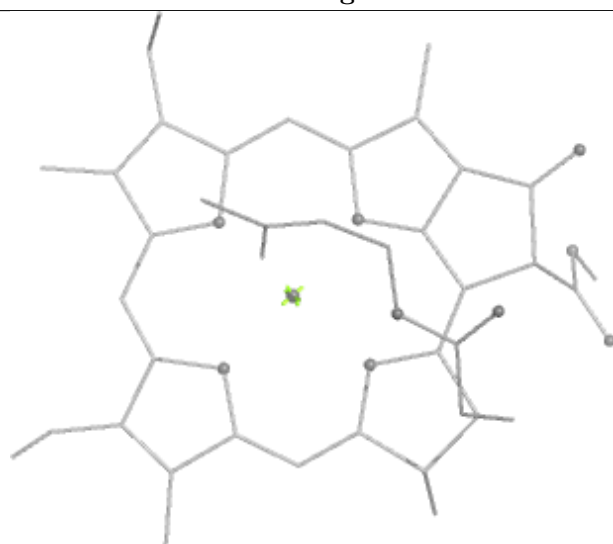
Bond lengths



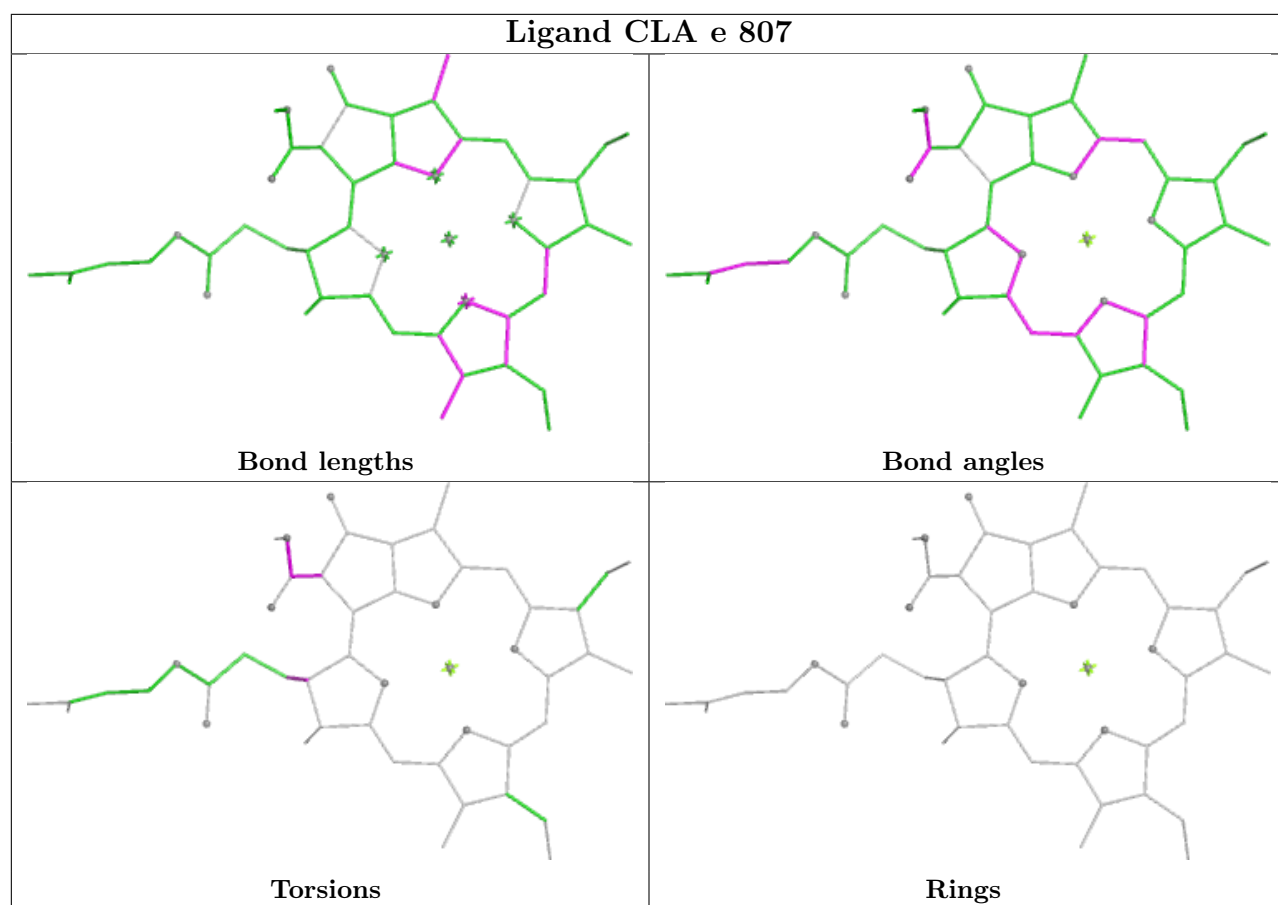
Bond angles



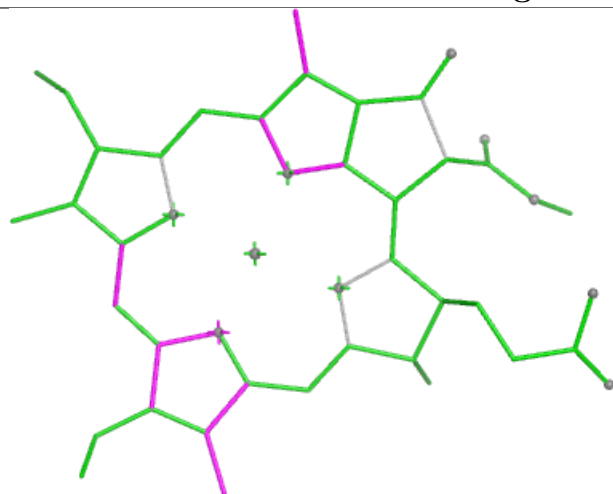
Torsions



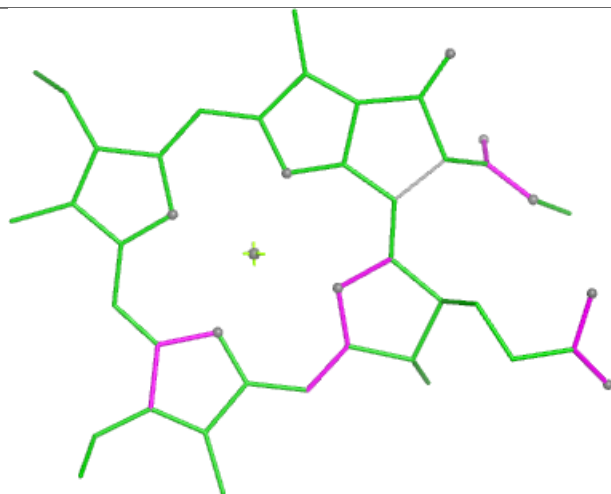
Rings



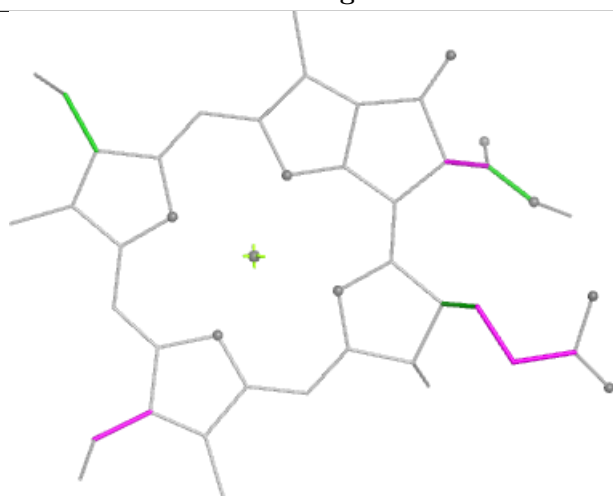
Ligand CLA A 813



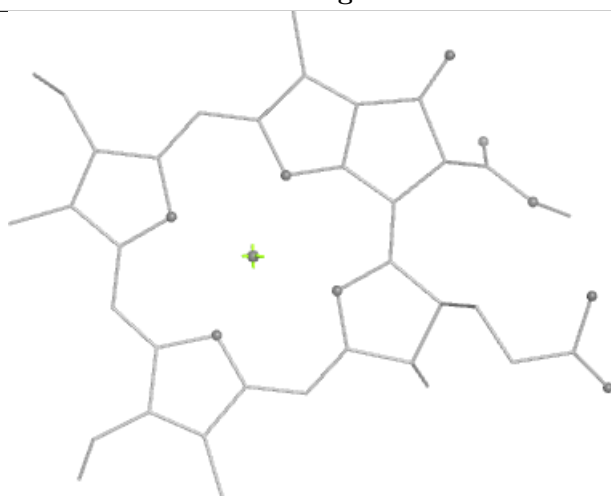
Bond lengths



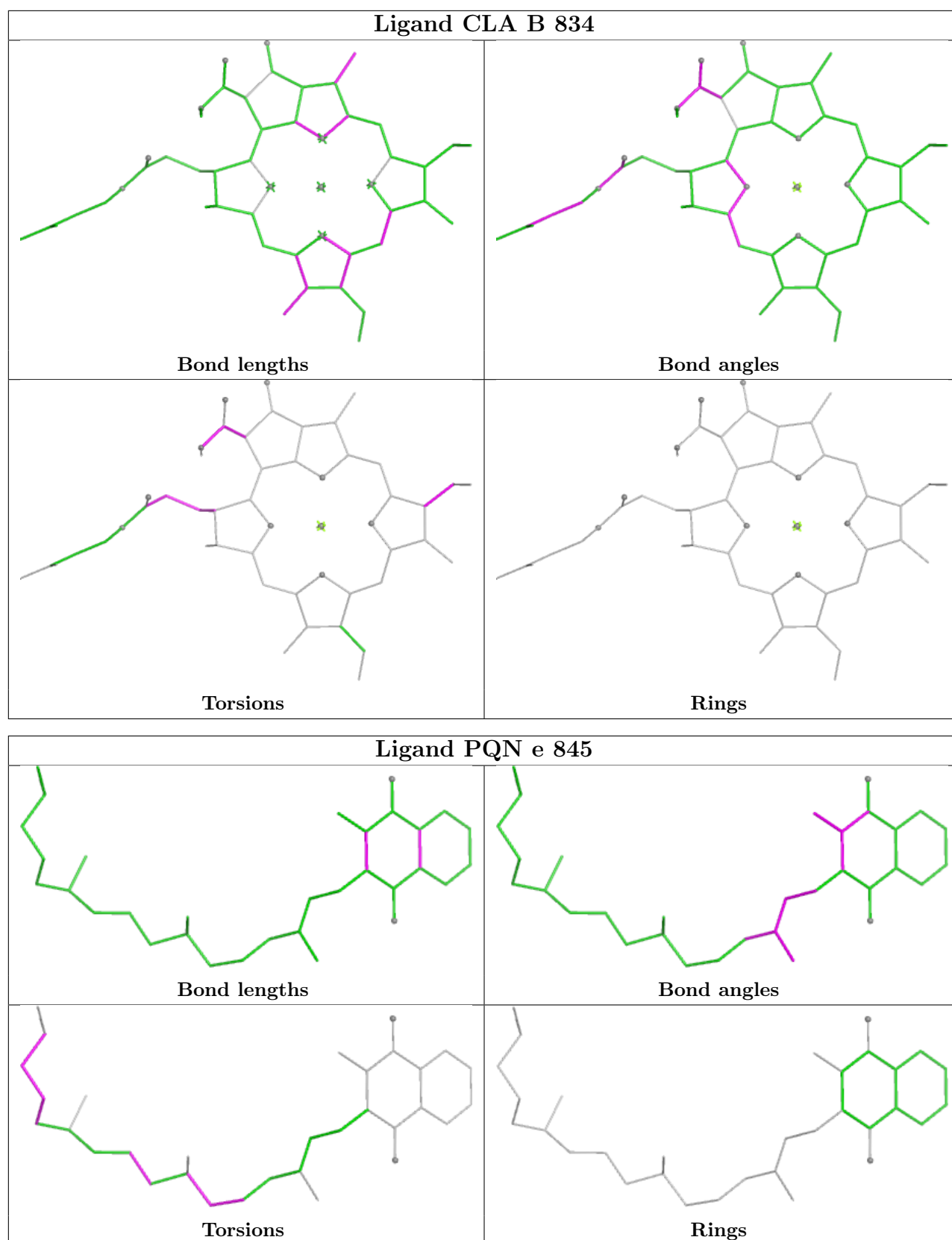
Bond angles



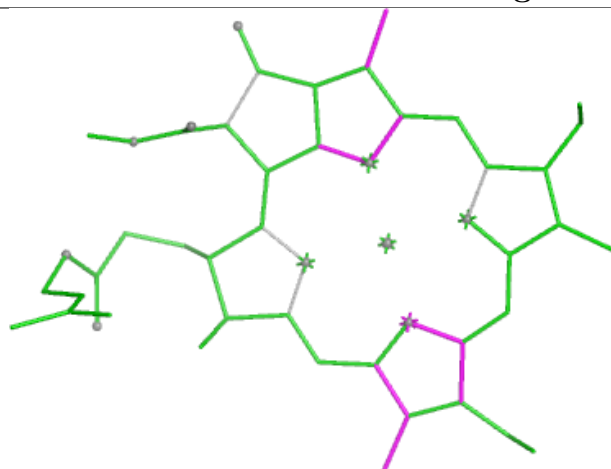
Torsions



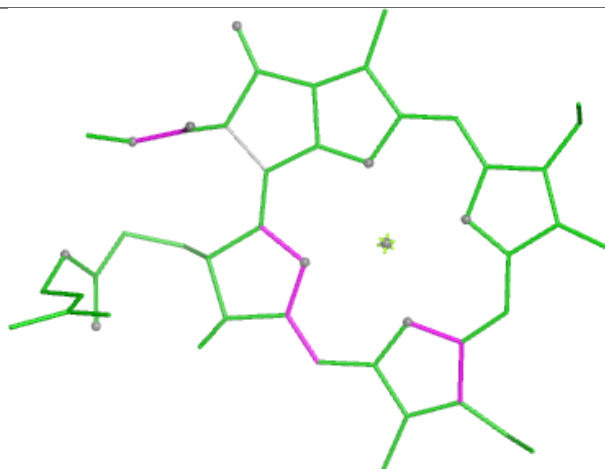
Rings



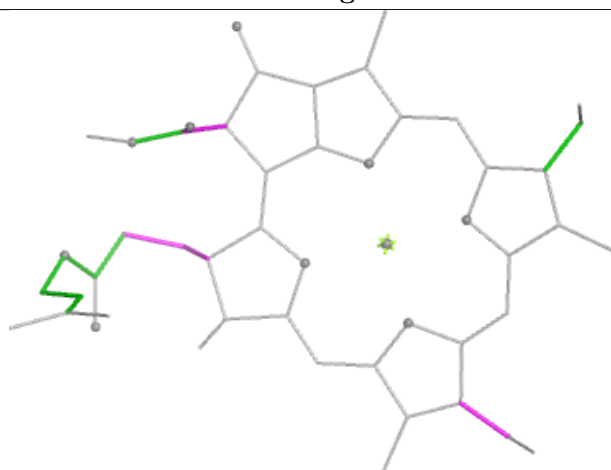
Ligand CLA A 809



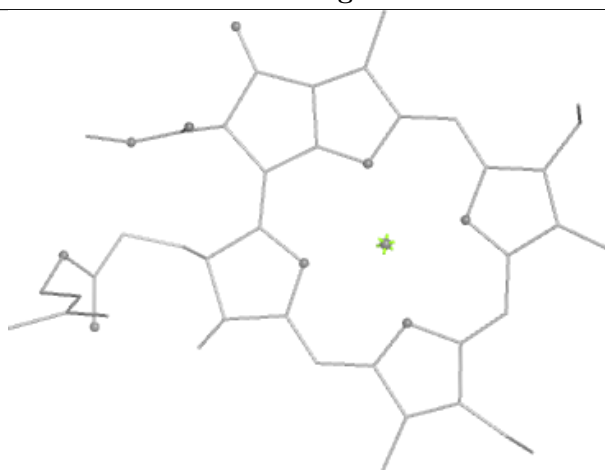
Bond lengths



Bond angles

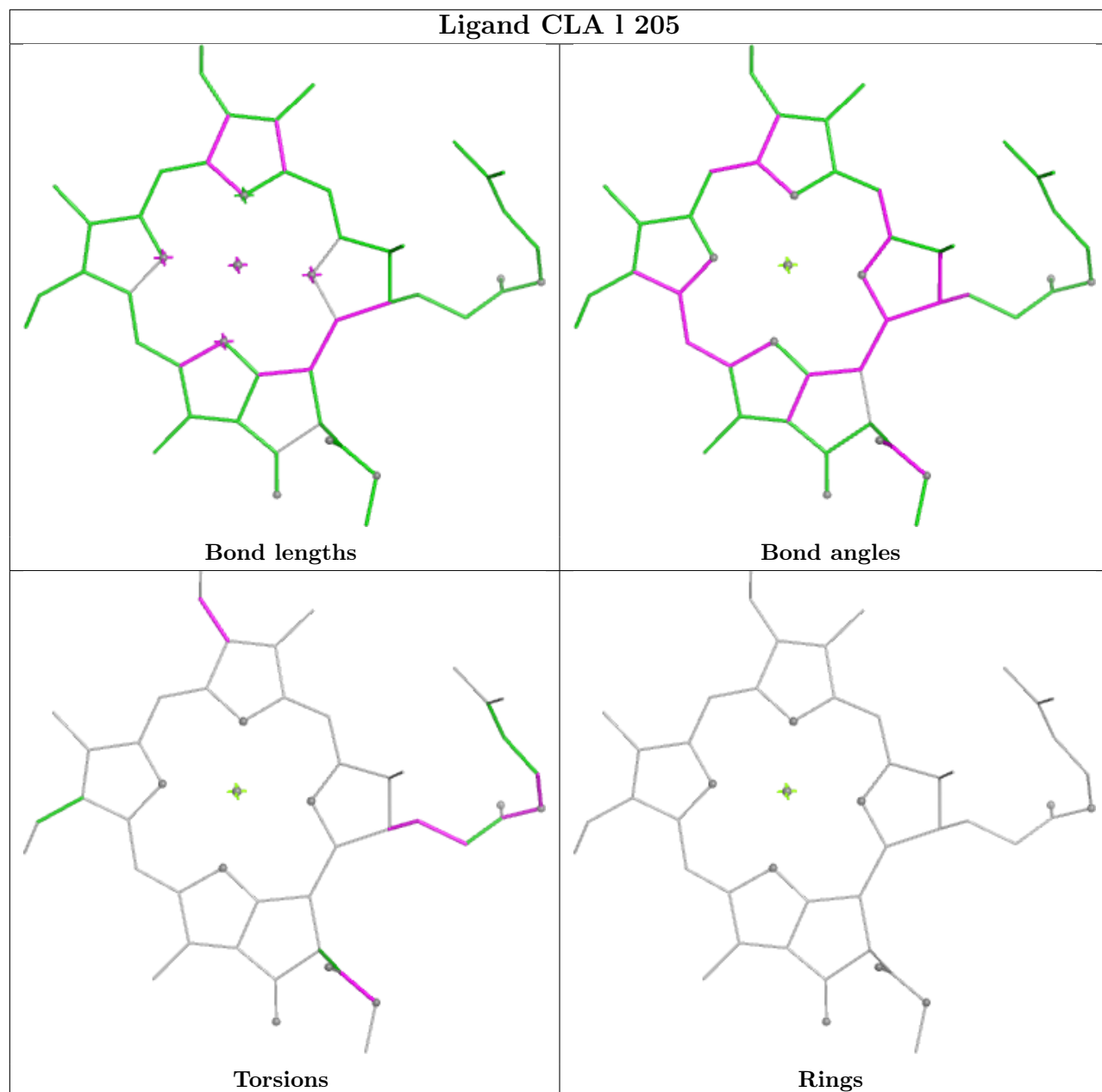


Torsions

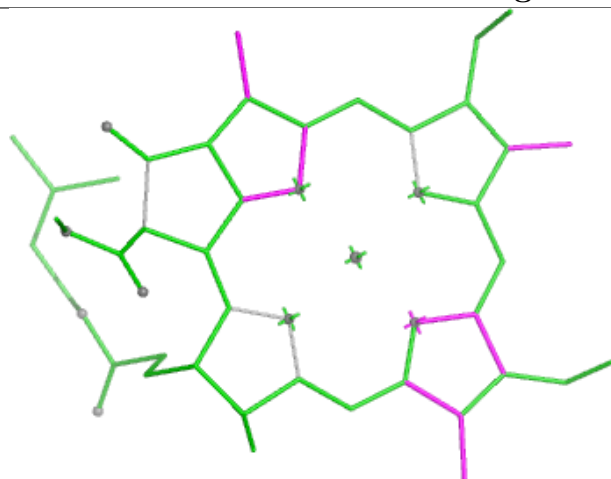


Rings

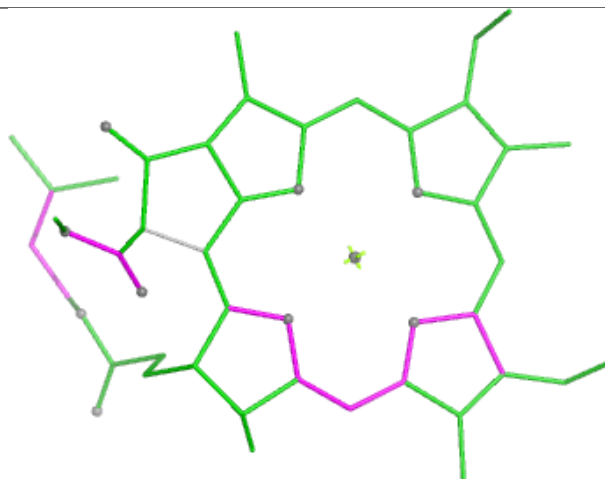
Ligand CLA 1 205



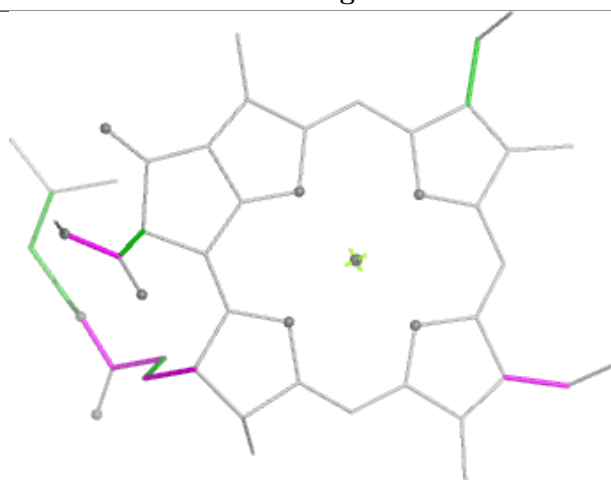
Ligand CLA B 841



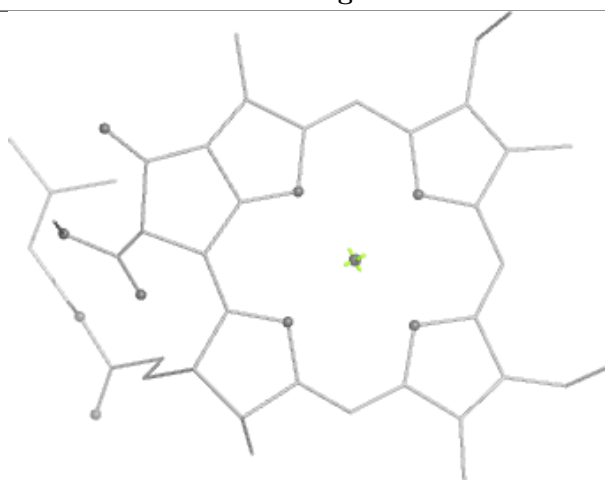
Bond lengths



Bond angles

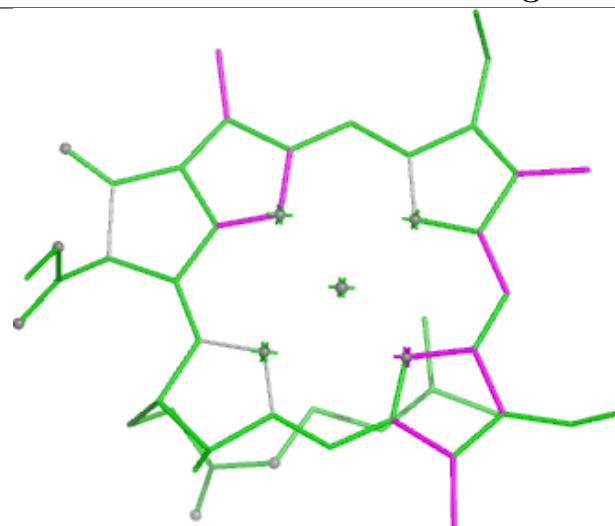


Torsions

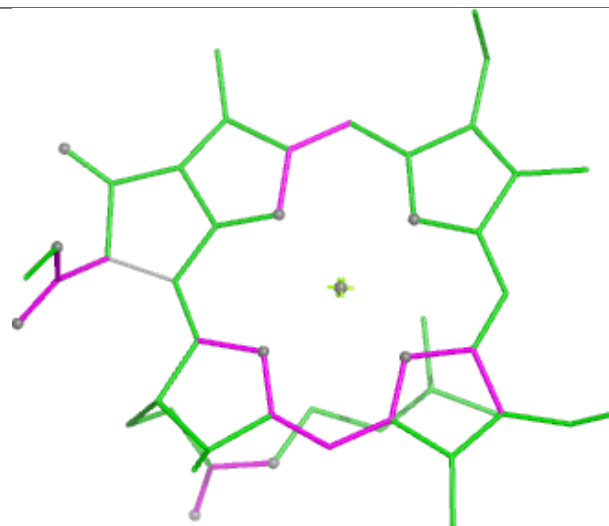


Rings

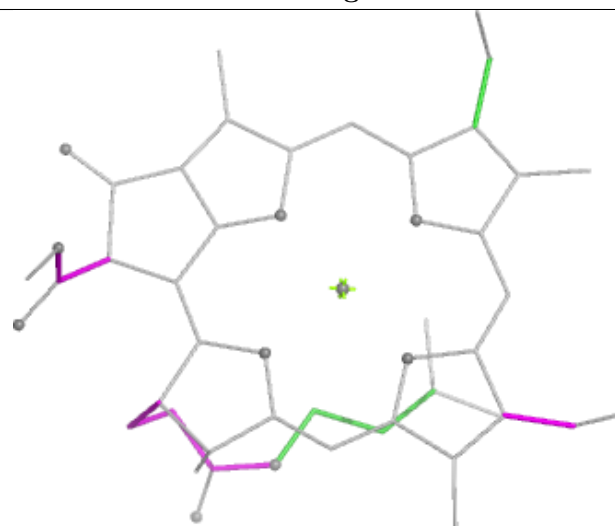
Ligand CLA a 827



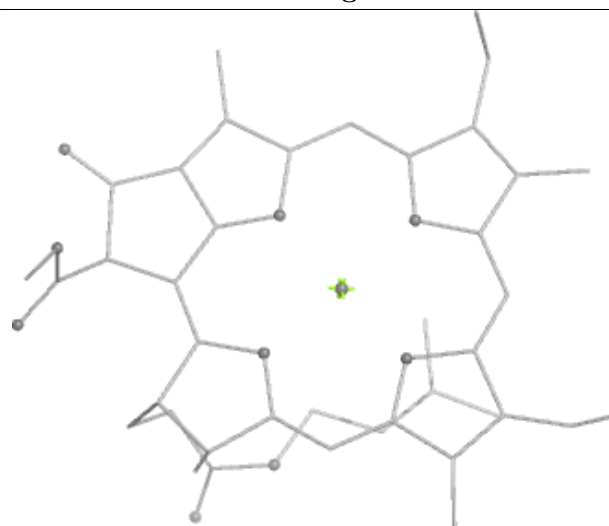
Bond lengths



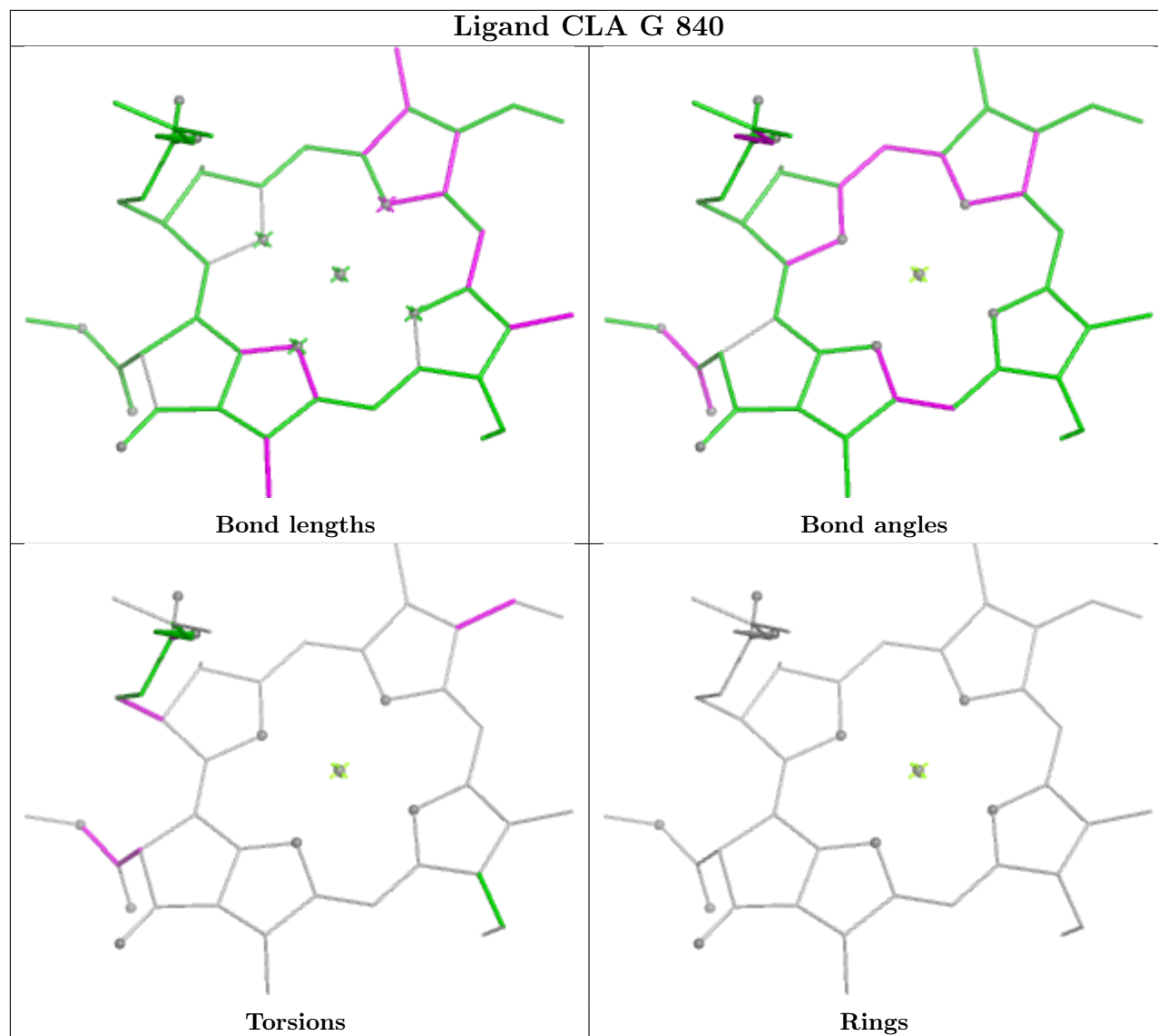
Bond angles

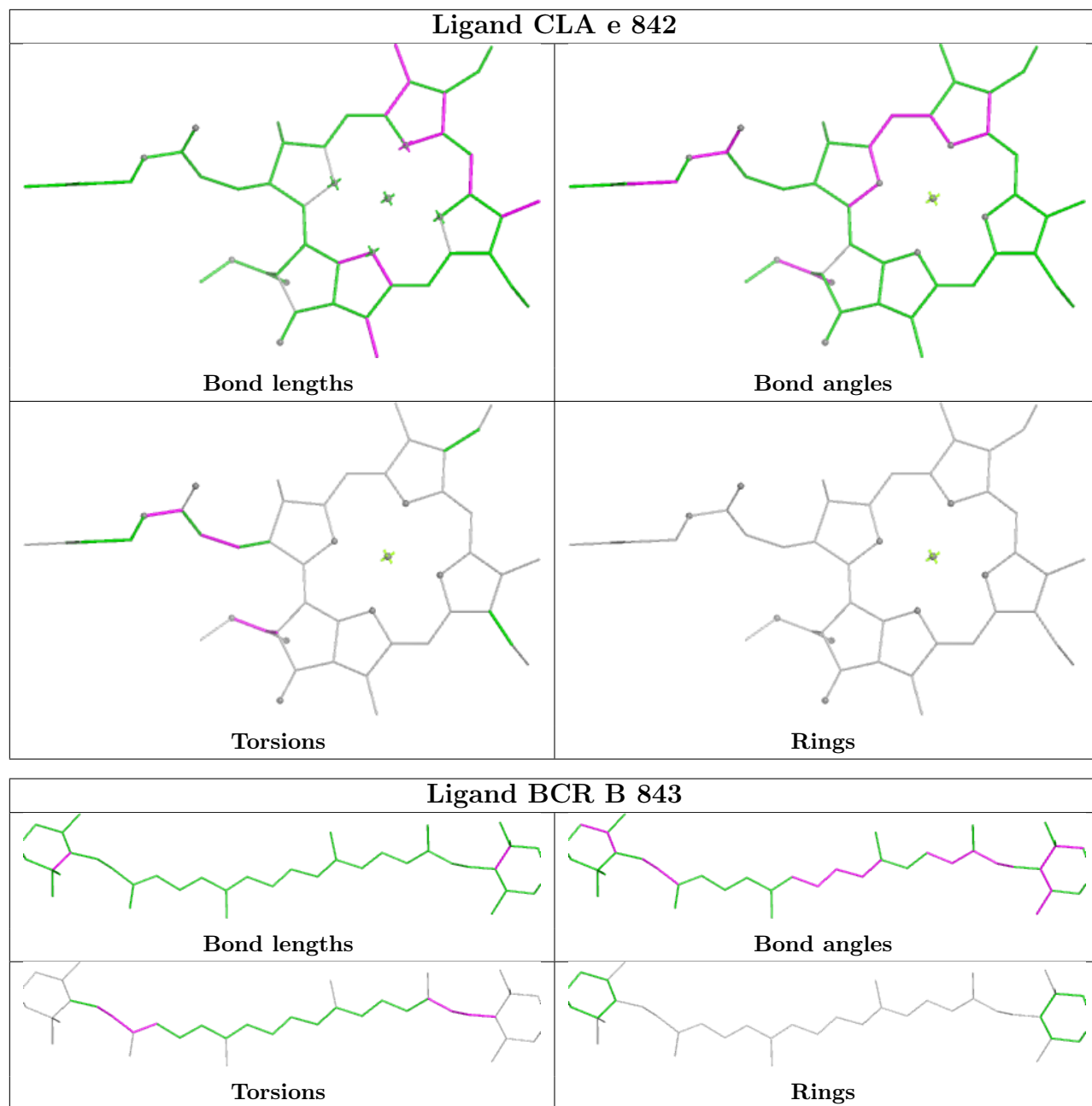


Torsions

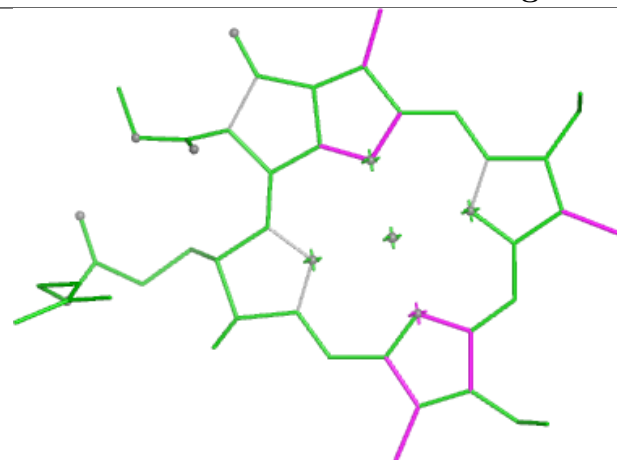


Rings

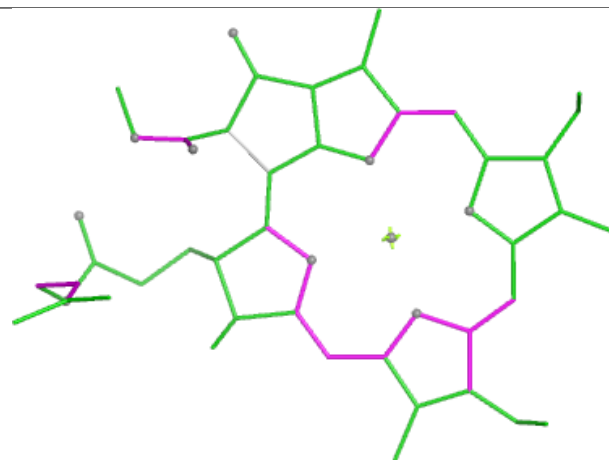




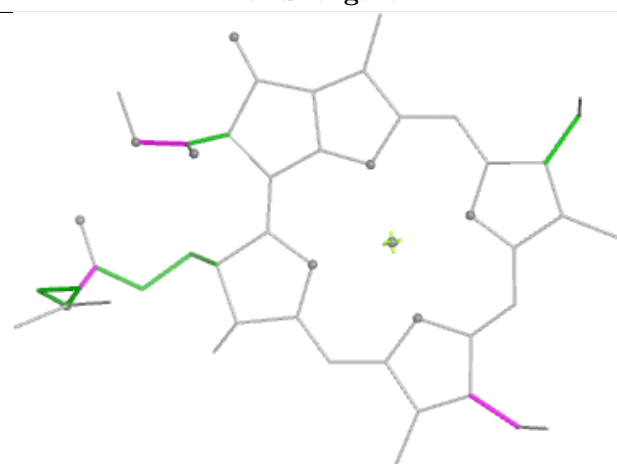
Ligand CLA b 807



Bond lengths



Bond angles

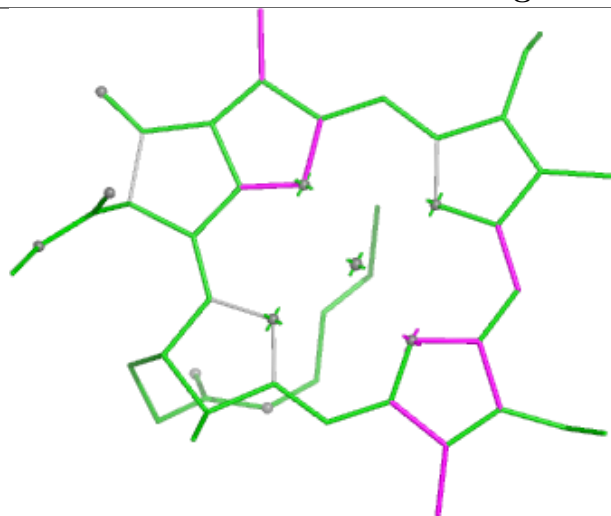


Torsions

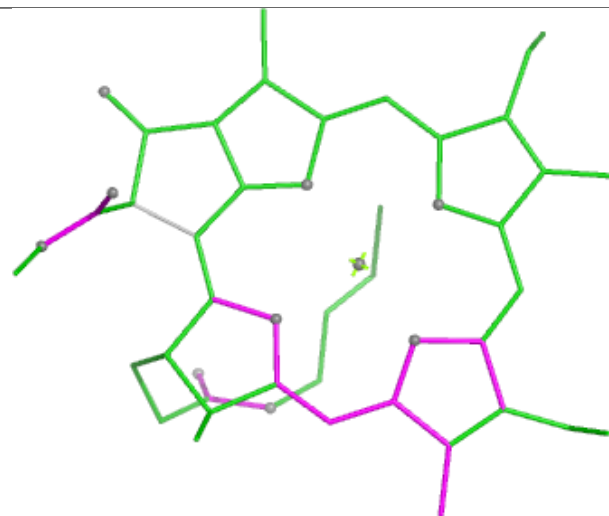


Rings

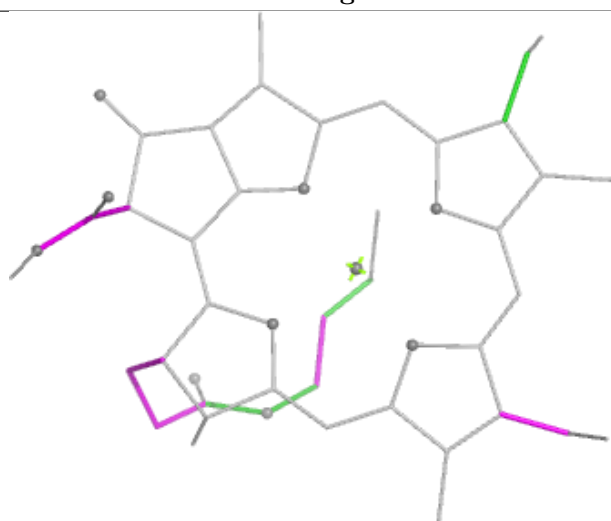
Ligand CLA A 819



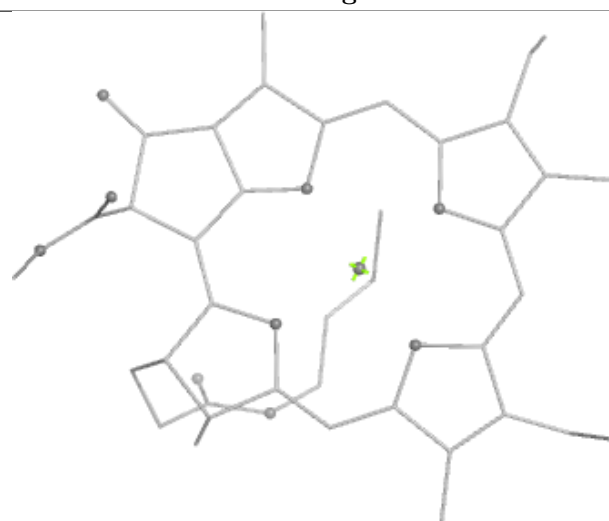
Bond lengths



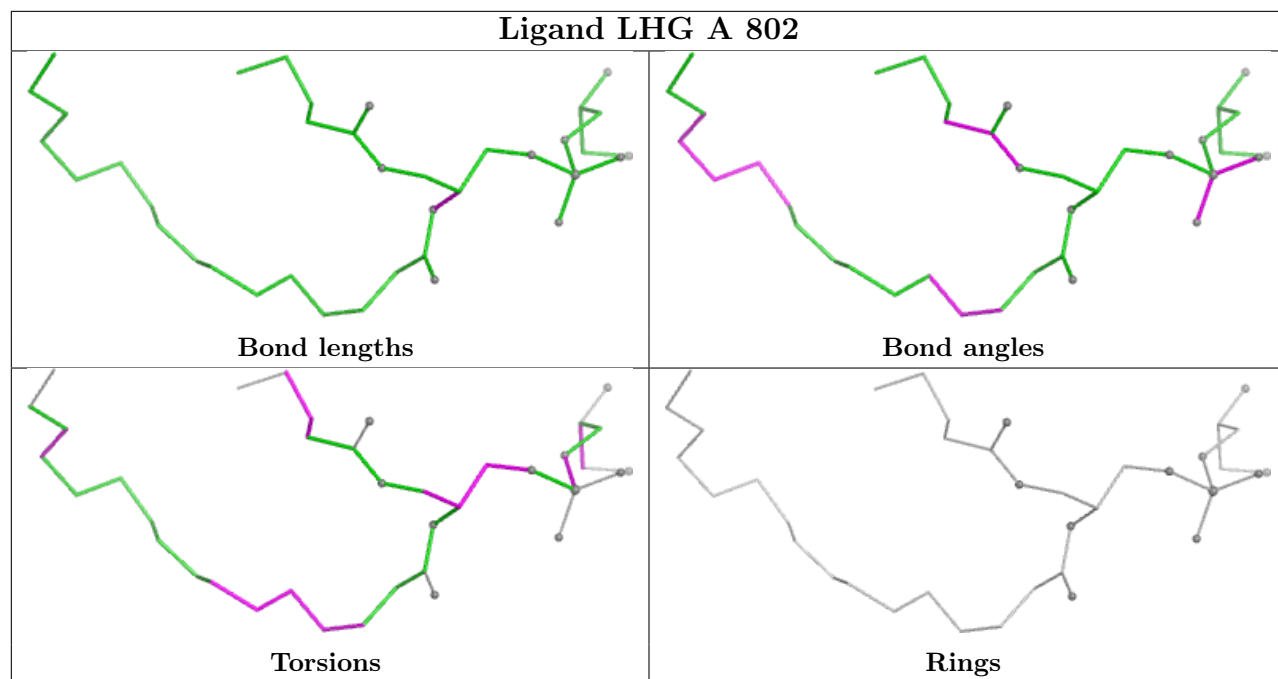
Bond angles

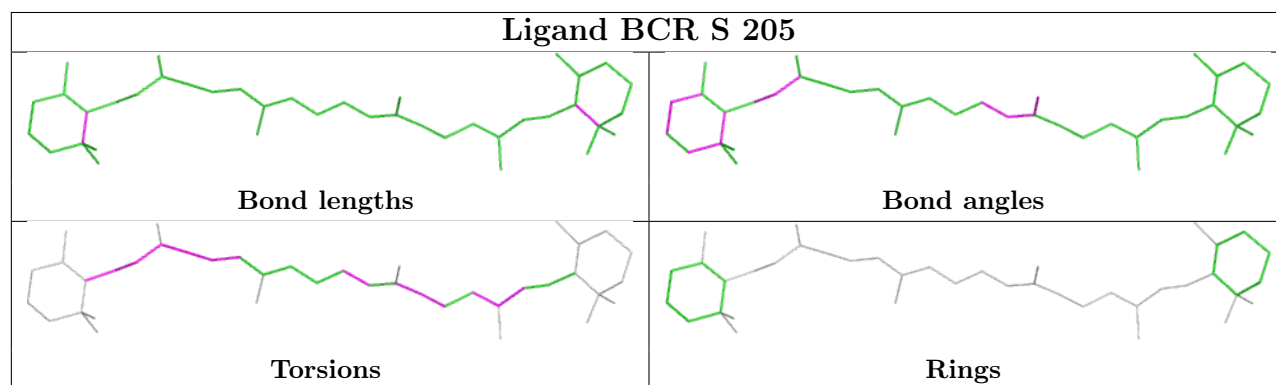
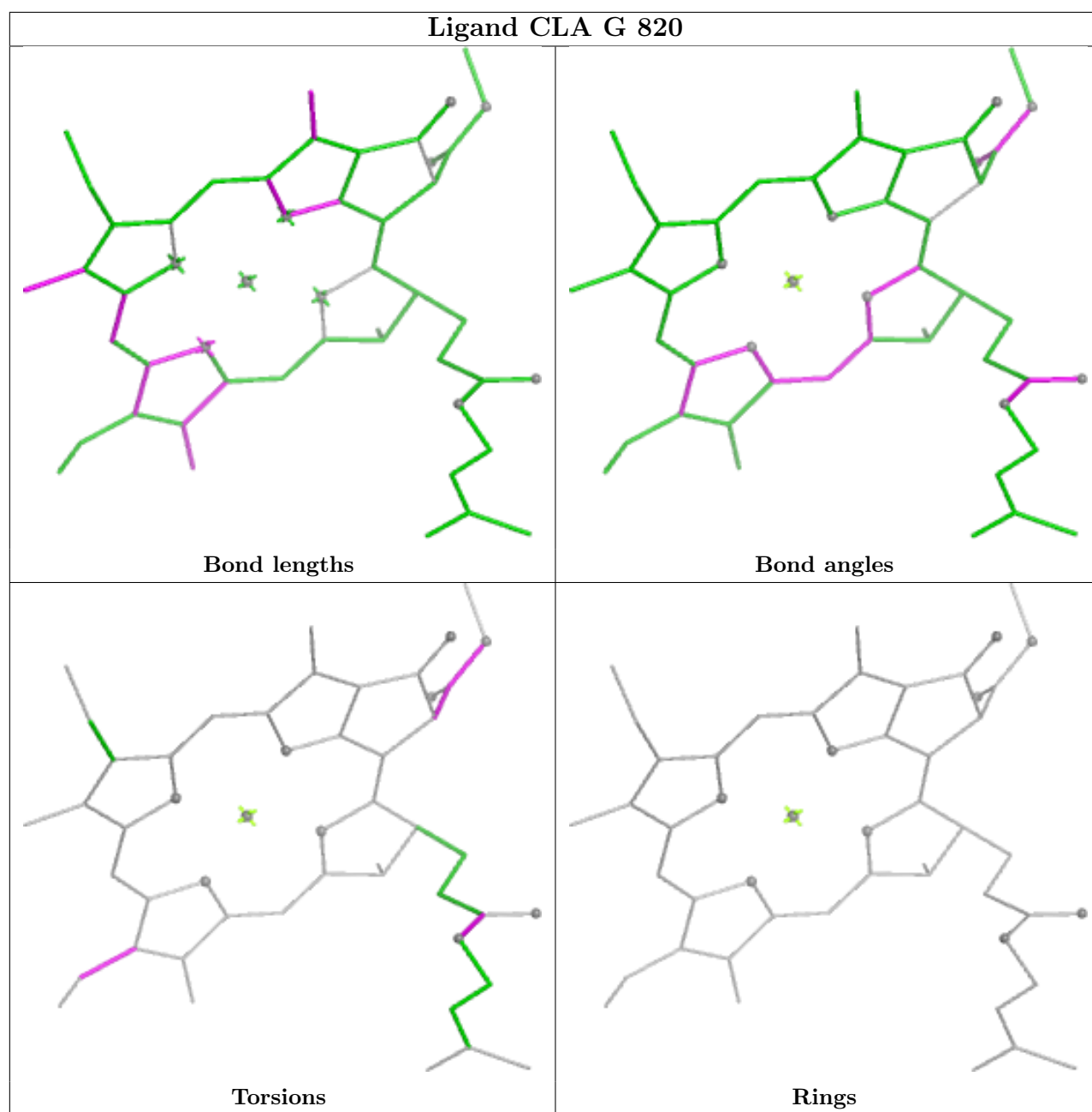


Torsions

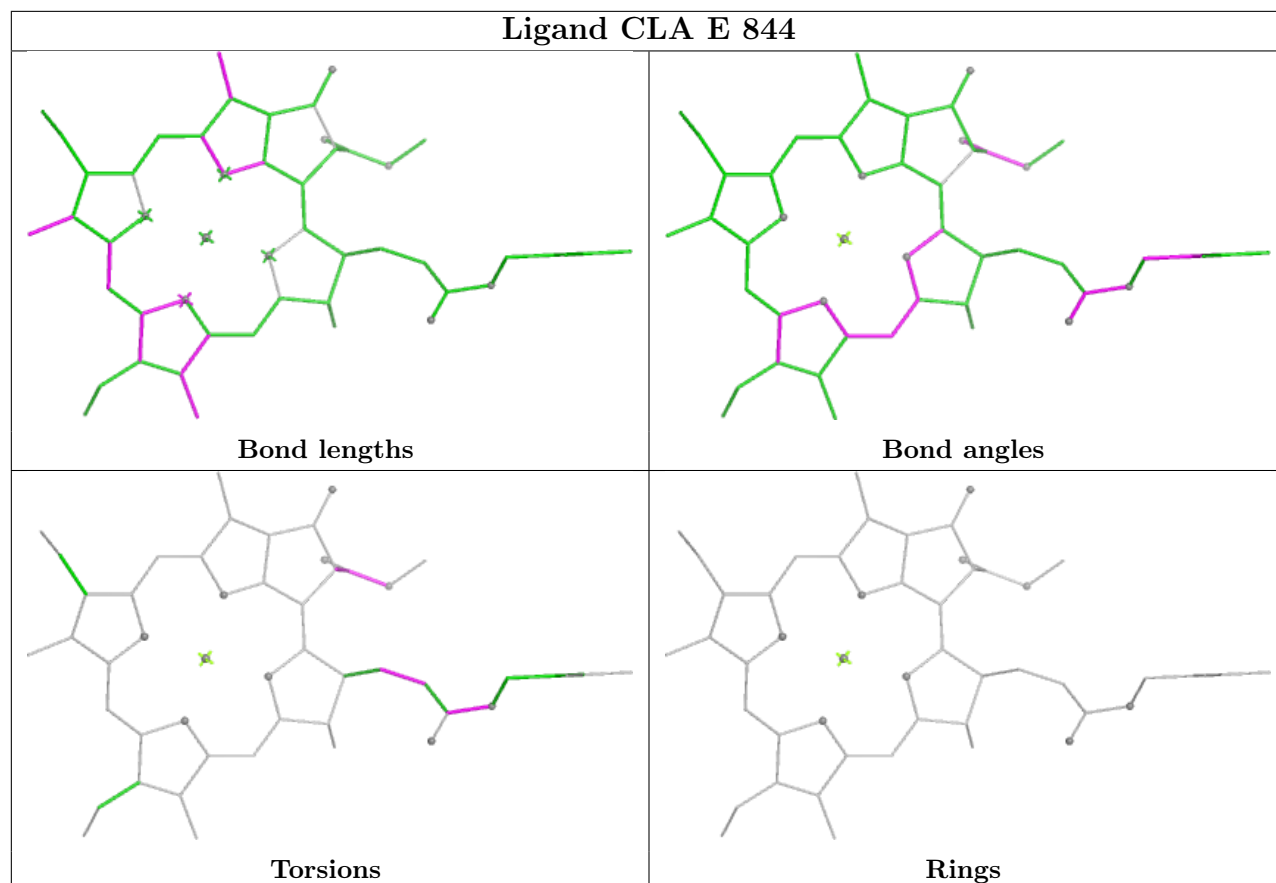


Rings

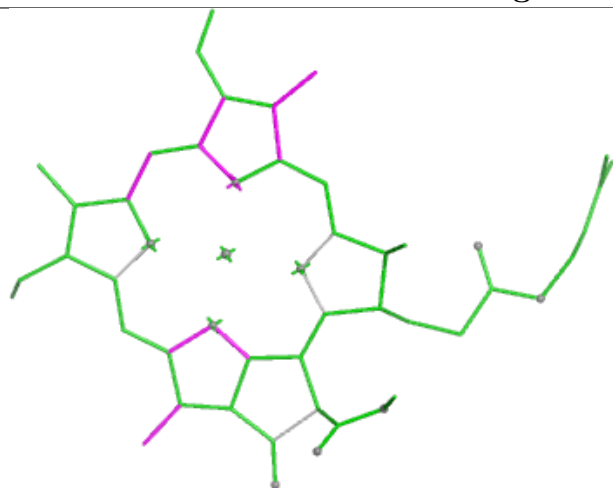




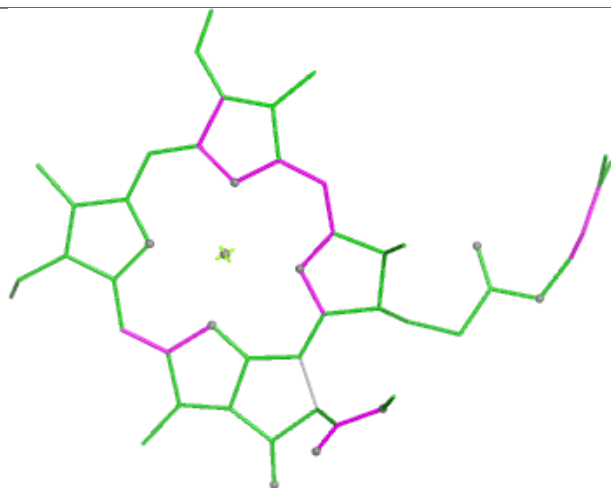
Ligand CLA E 844



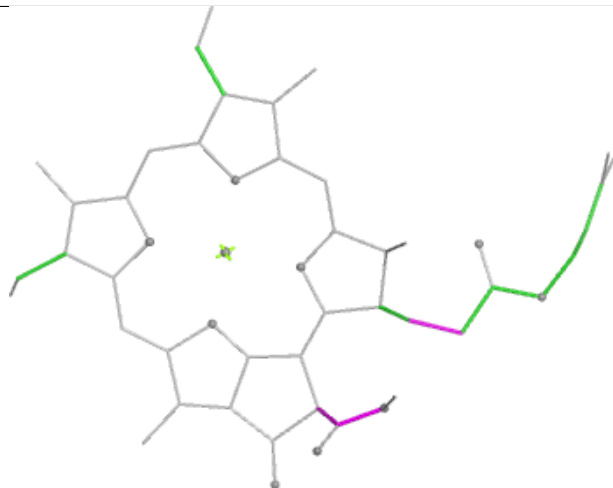
Ligand CLA G 814



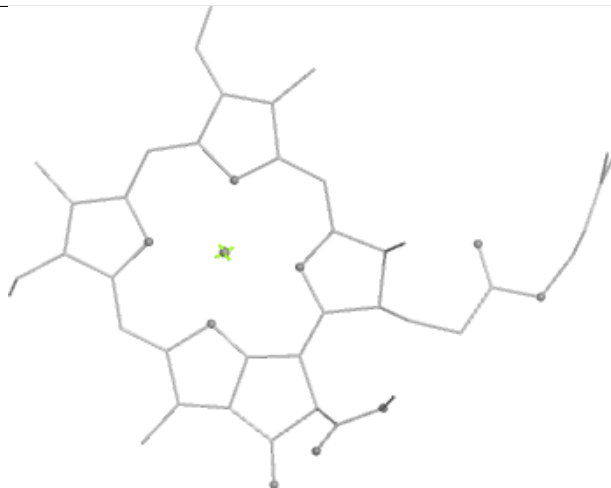
Bond lengths



Bond angles

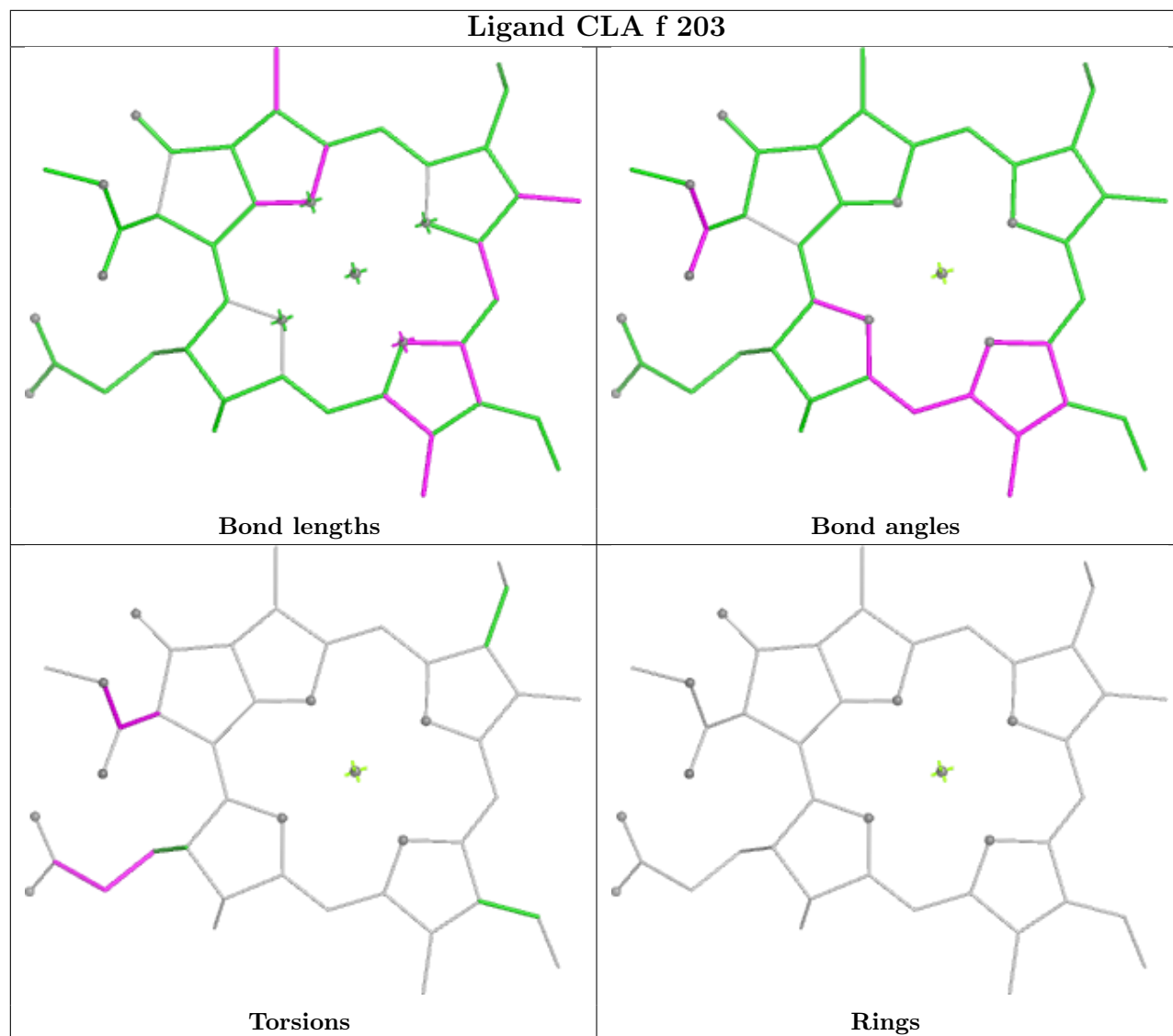


Torsions

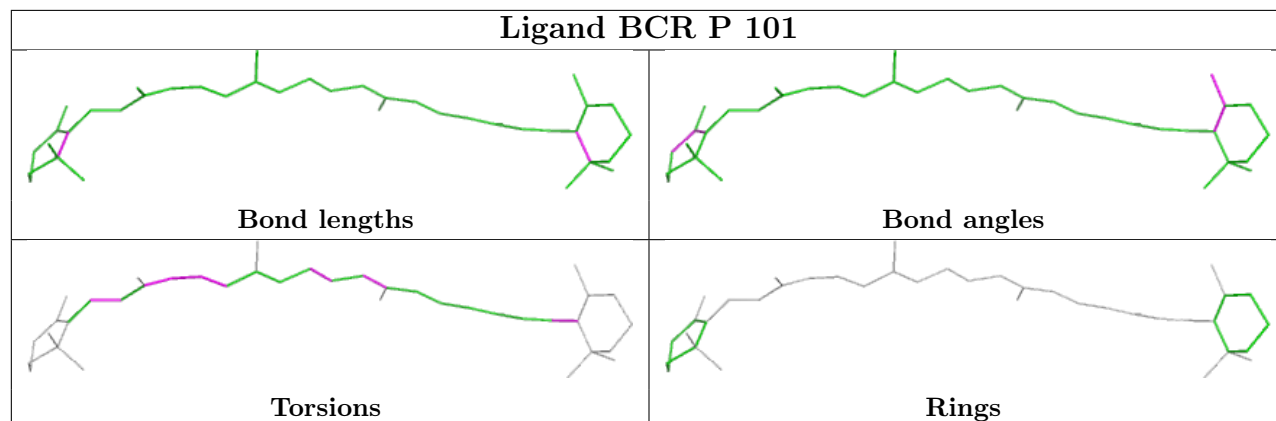


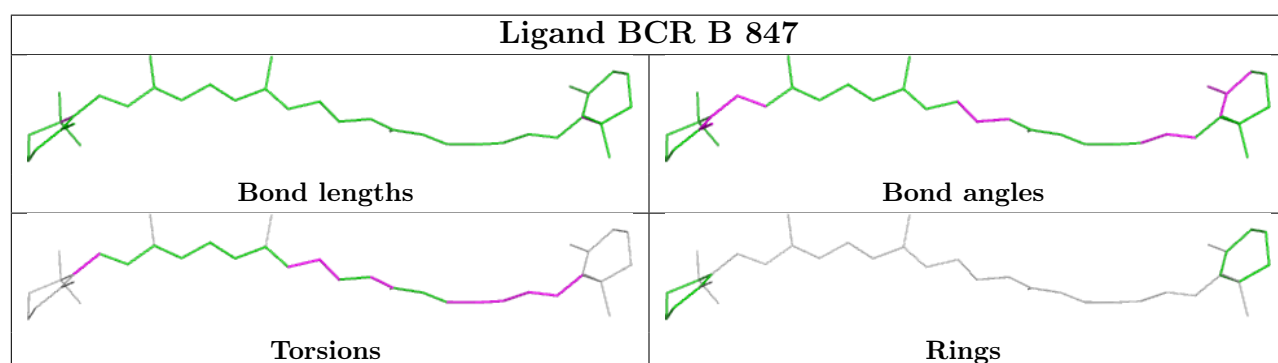
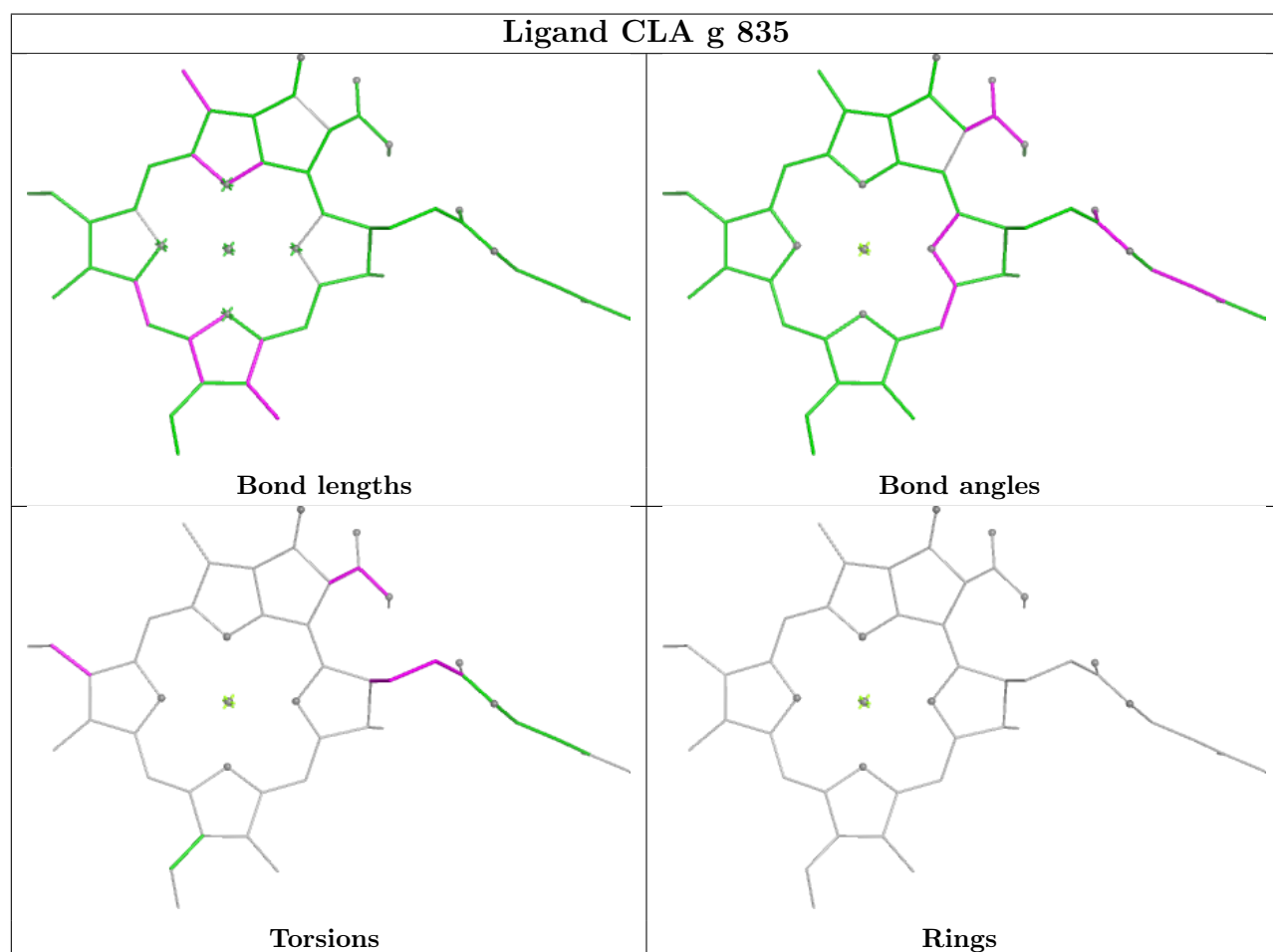
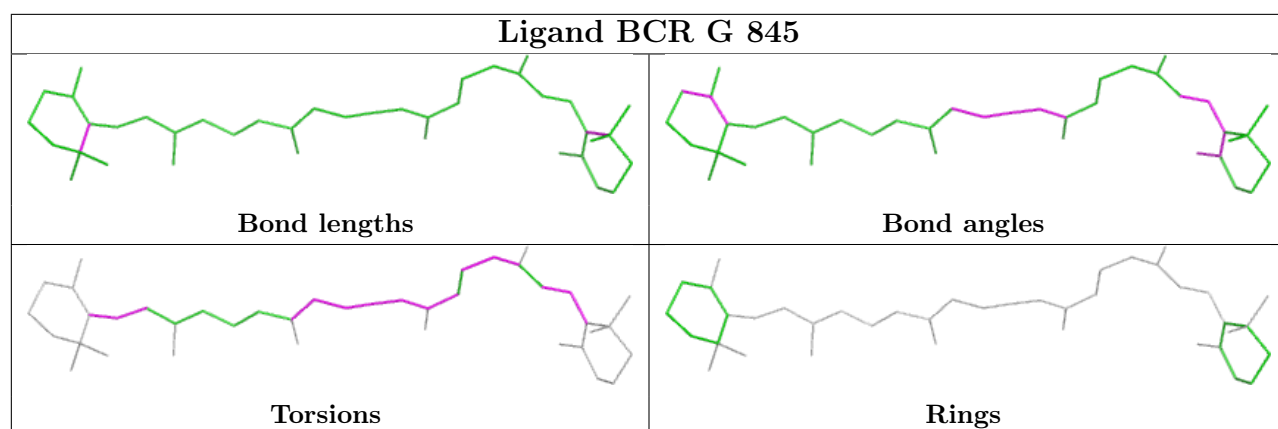
Rings

Ligand CLA f 203

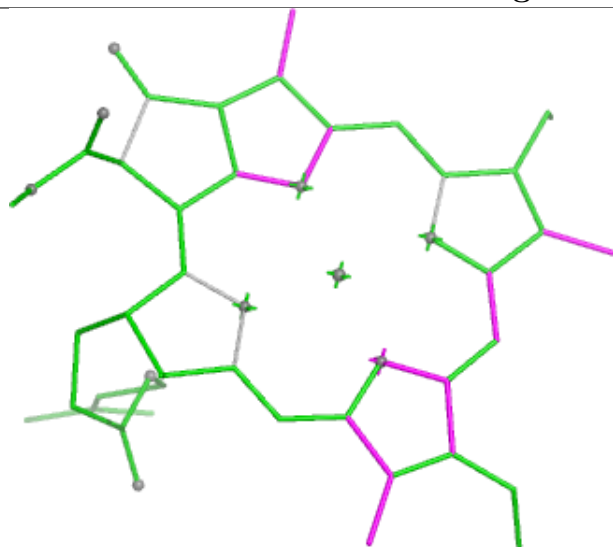


Ligand BCR P 101

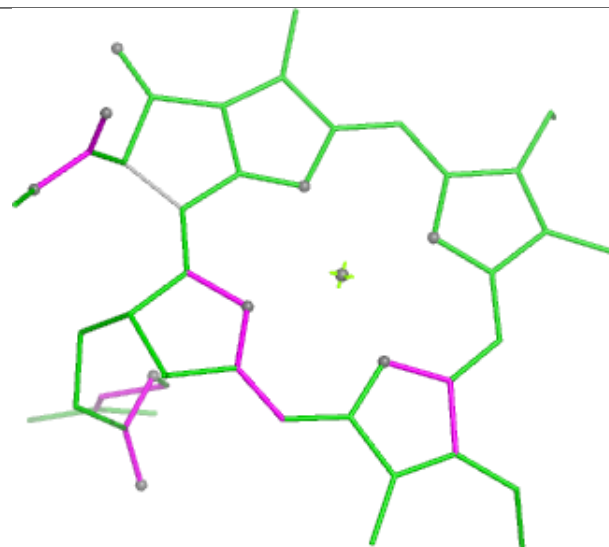




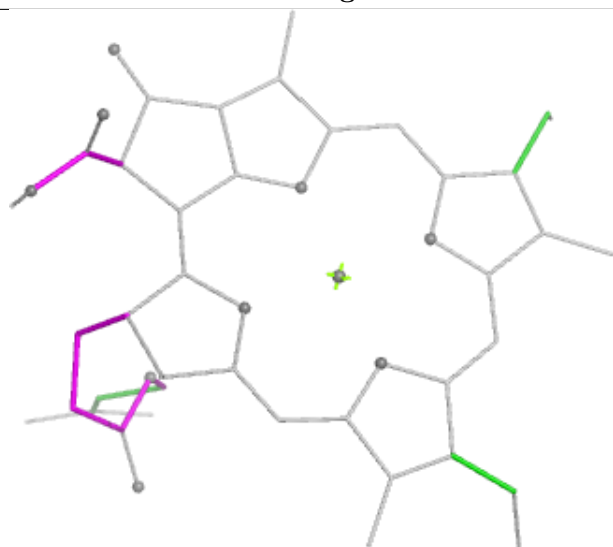
Ligand CLA G 829



Bond lengths



Bond angles

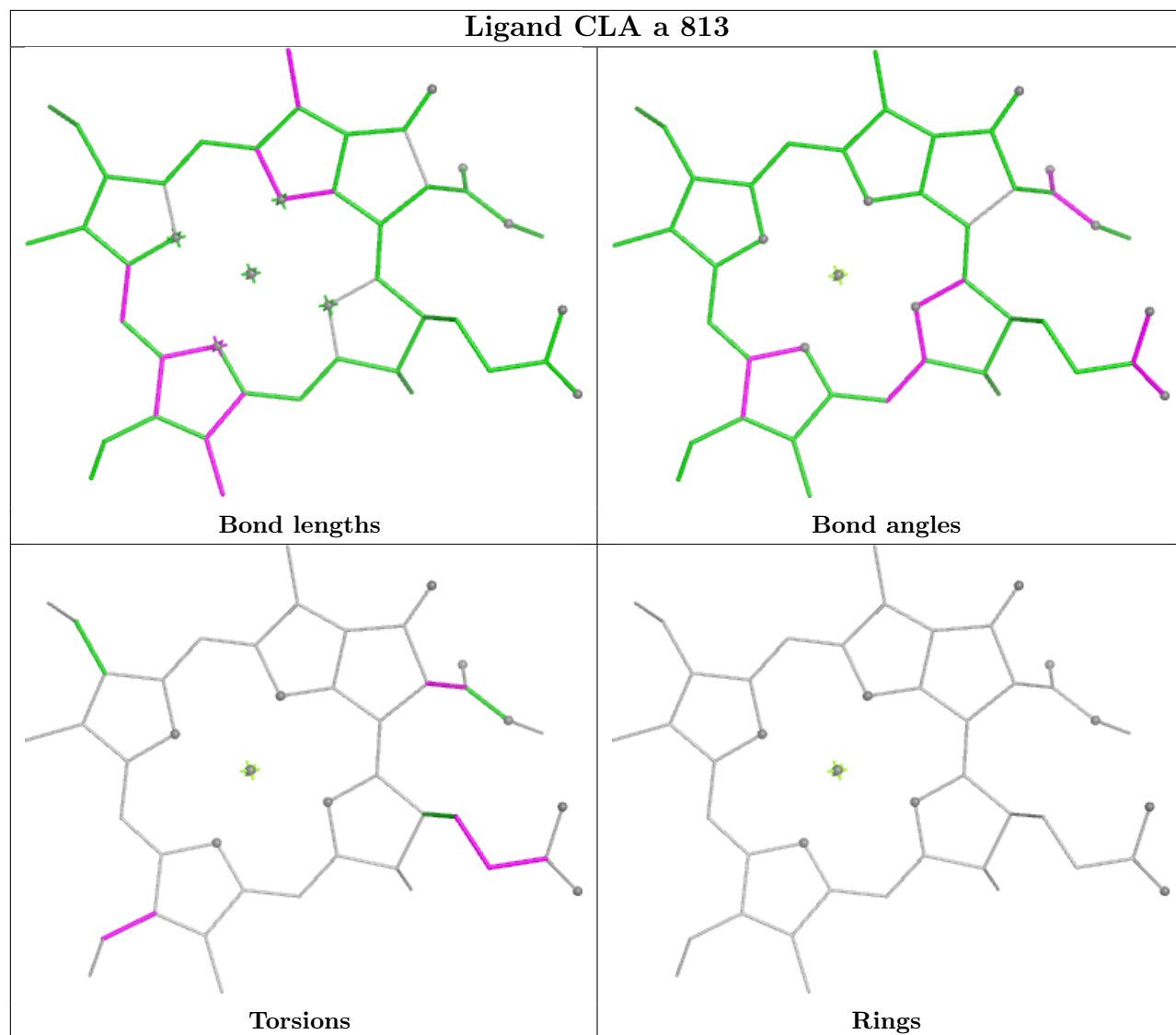


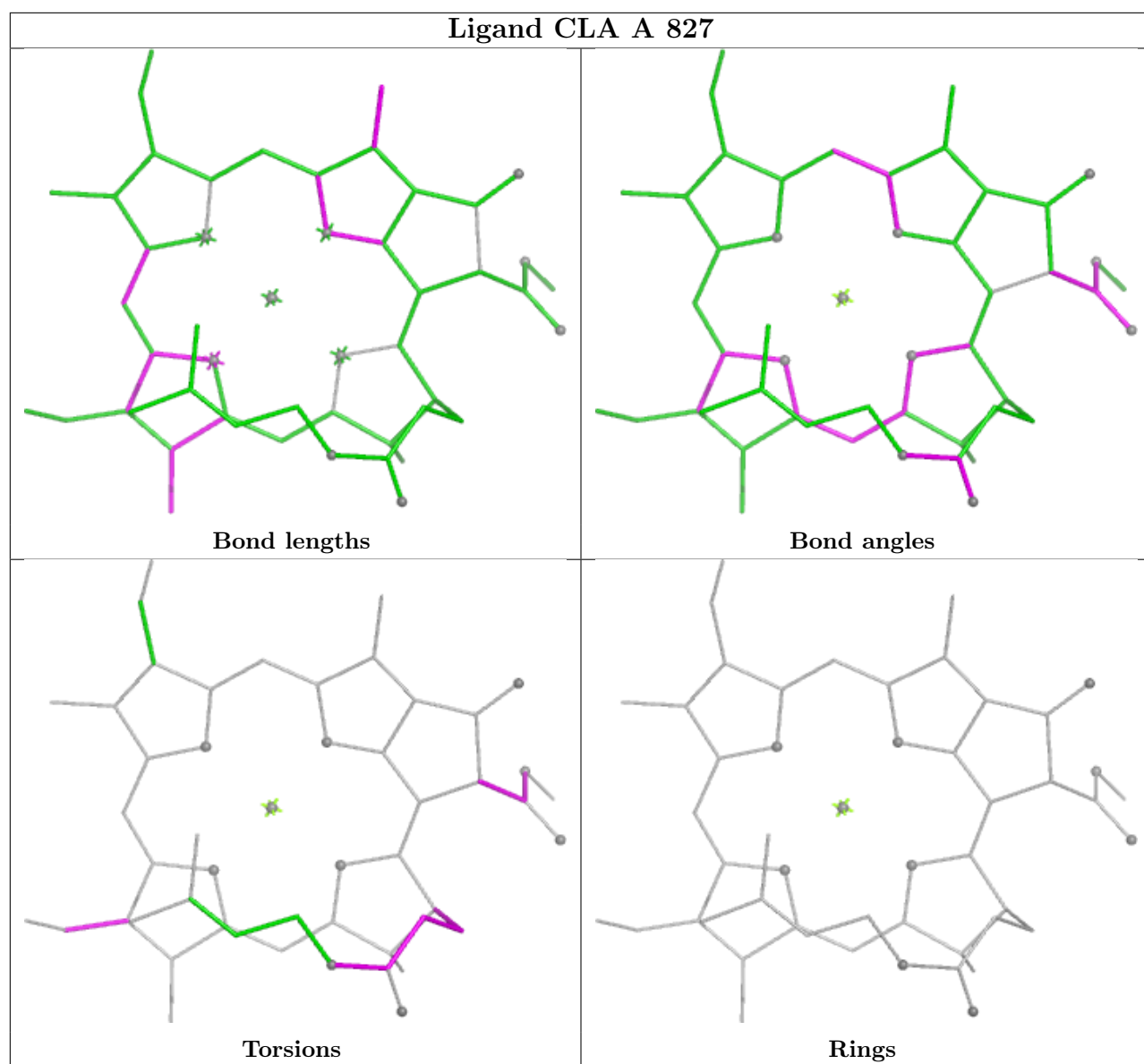
Torsions



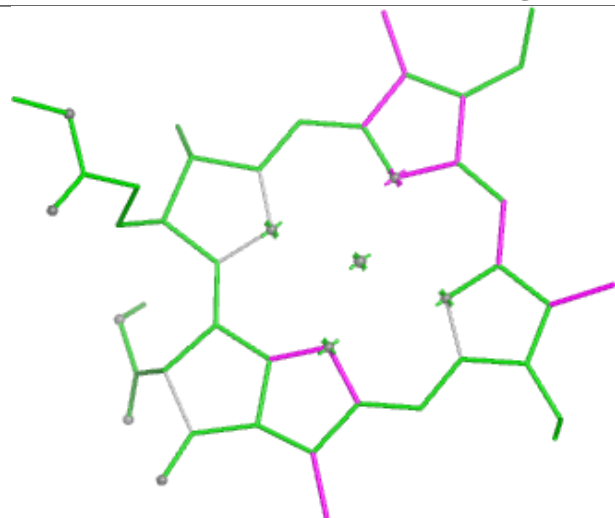
Rings

Ligand CLA a 813

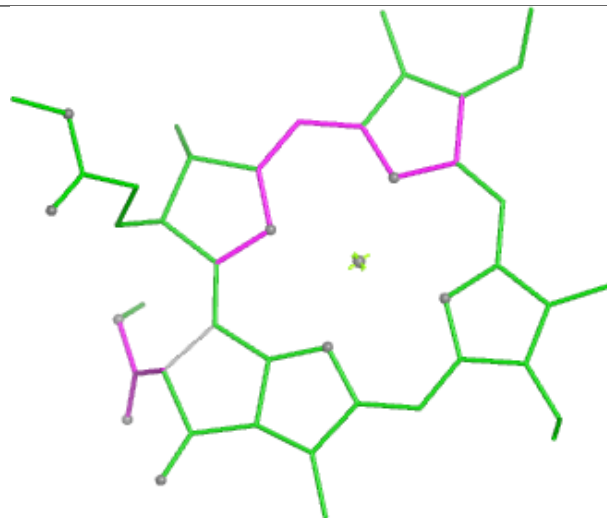




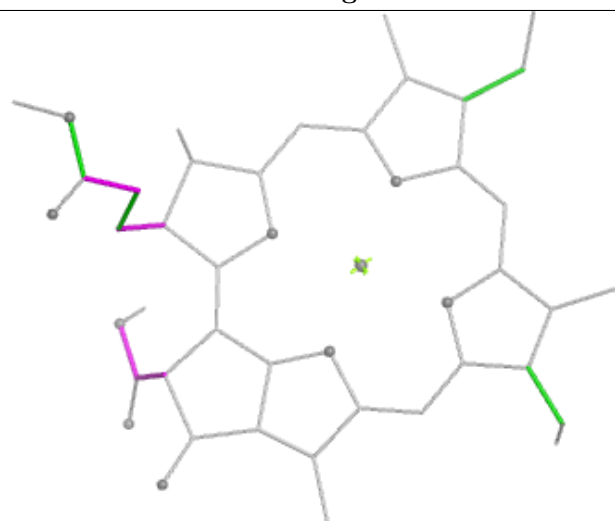
Ligand CLA B 826



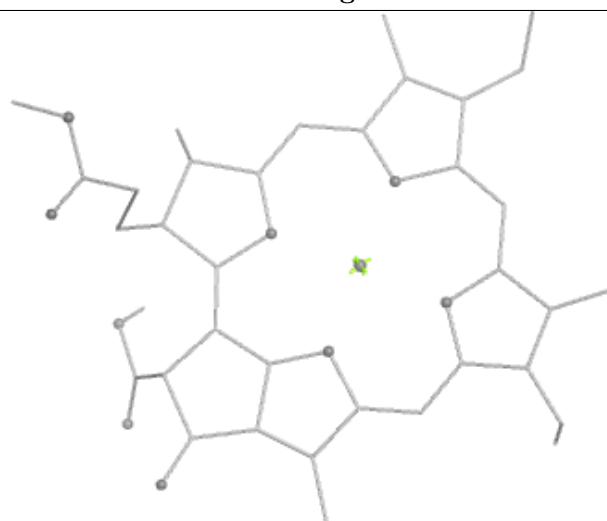
Bond lengths



Bond angles

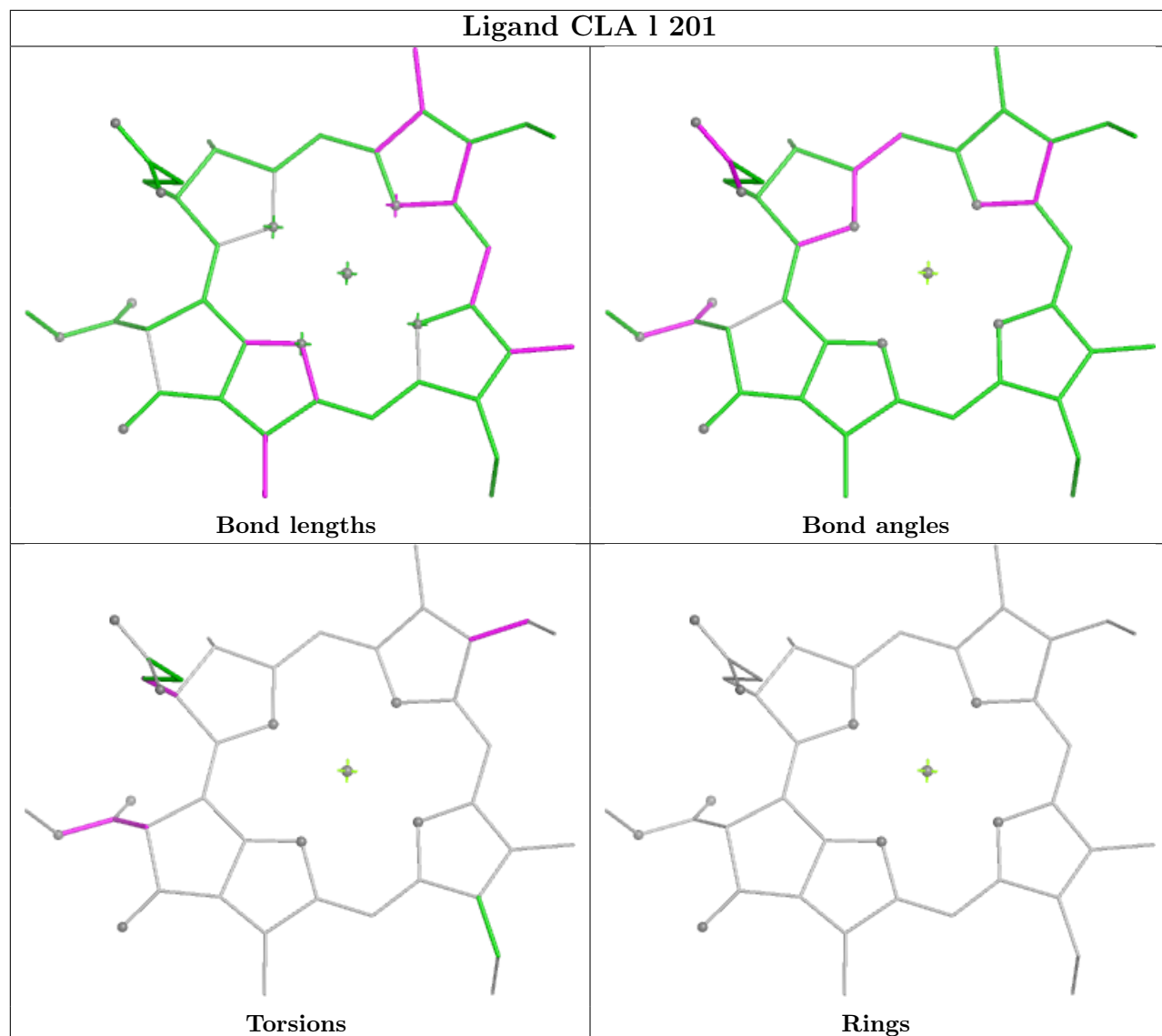


Torsions

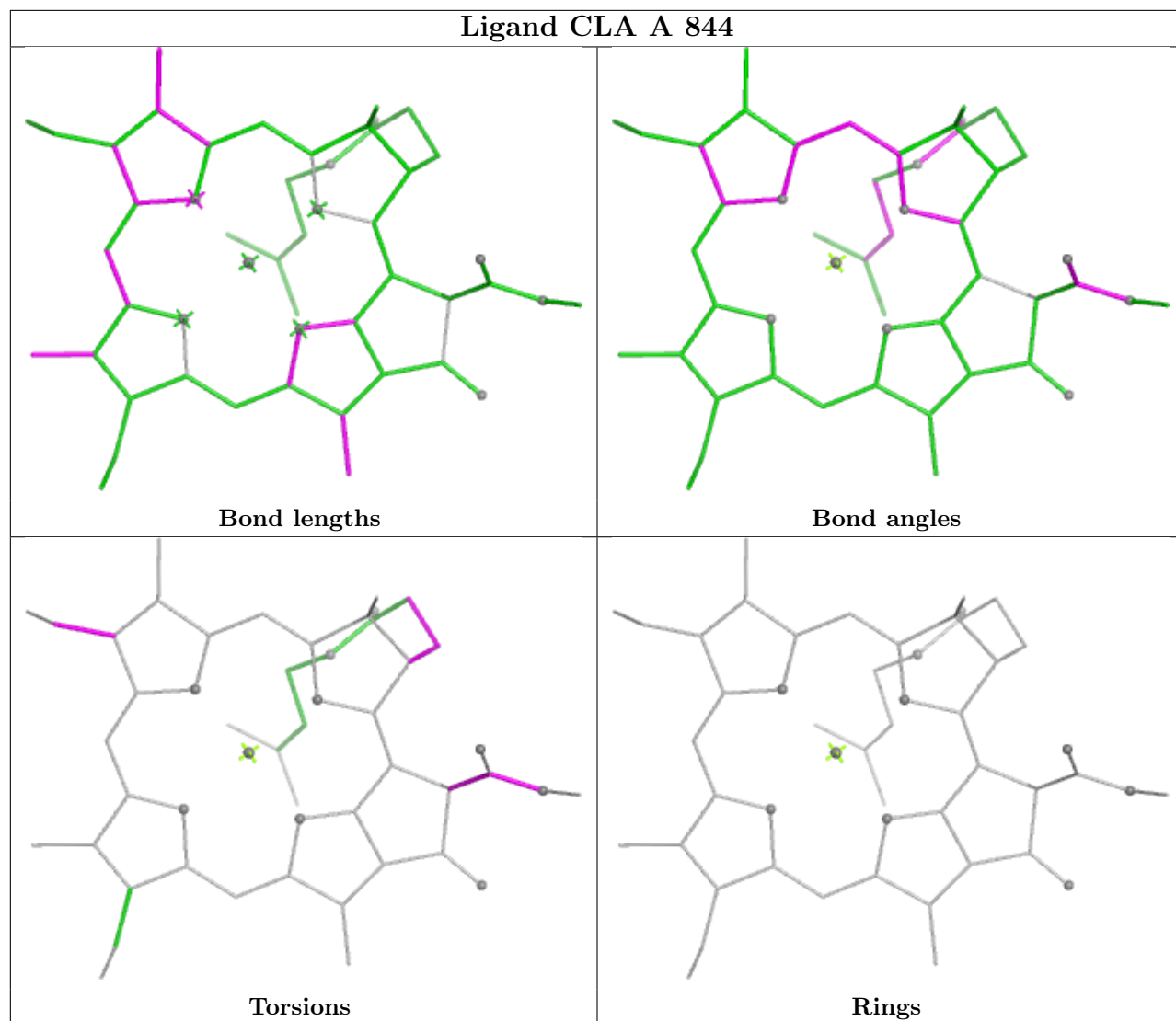


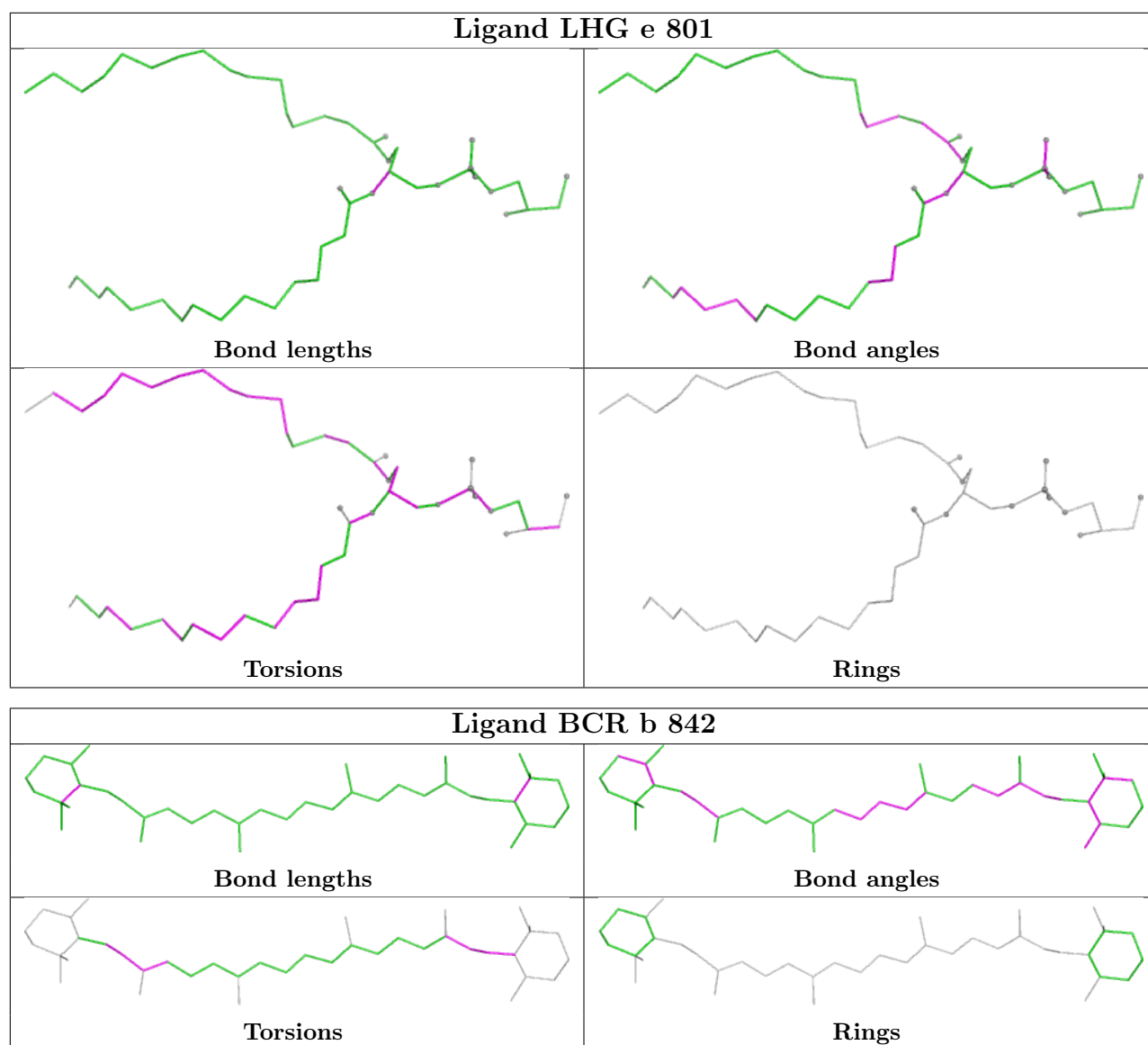
Rings

Ligand CLA 1 201

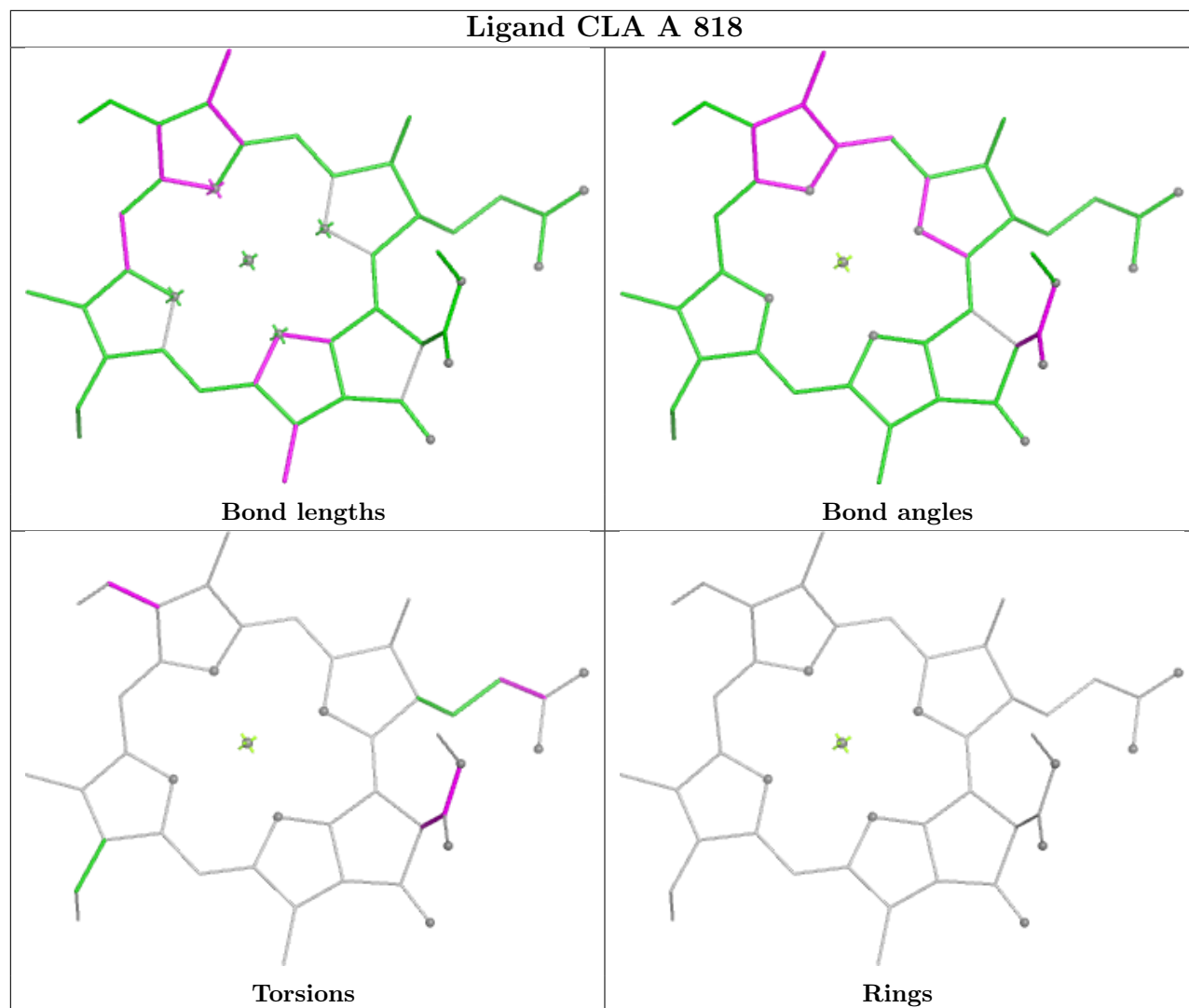


Ligand CLA A 844

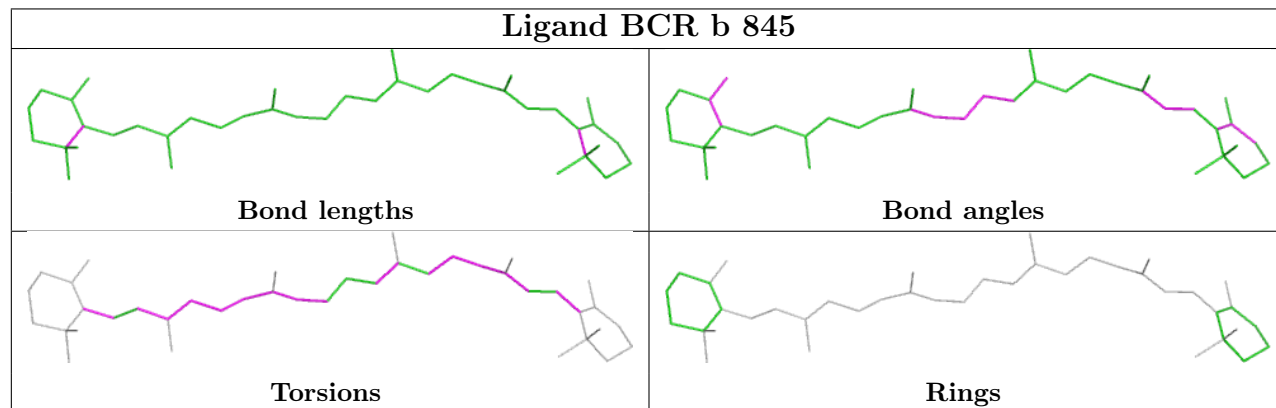




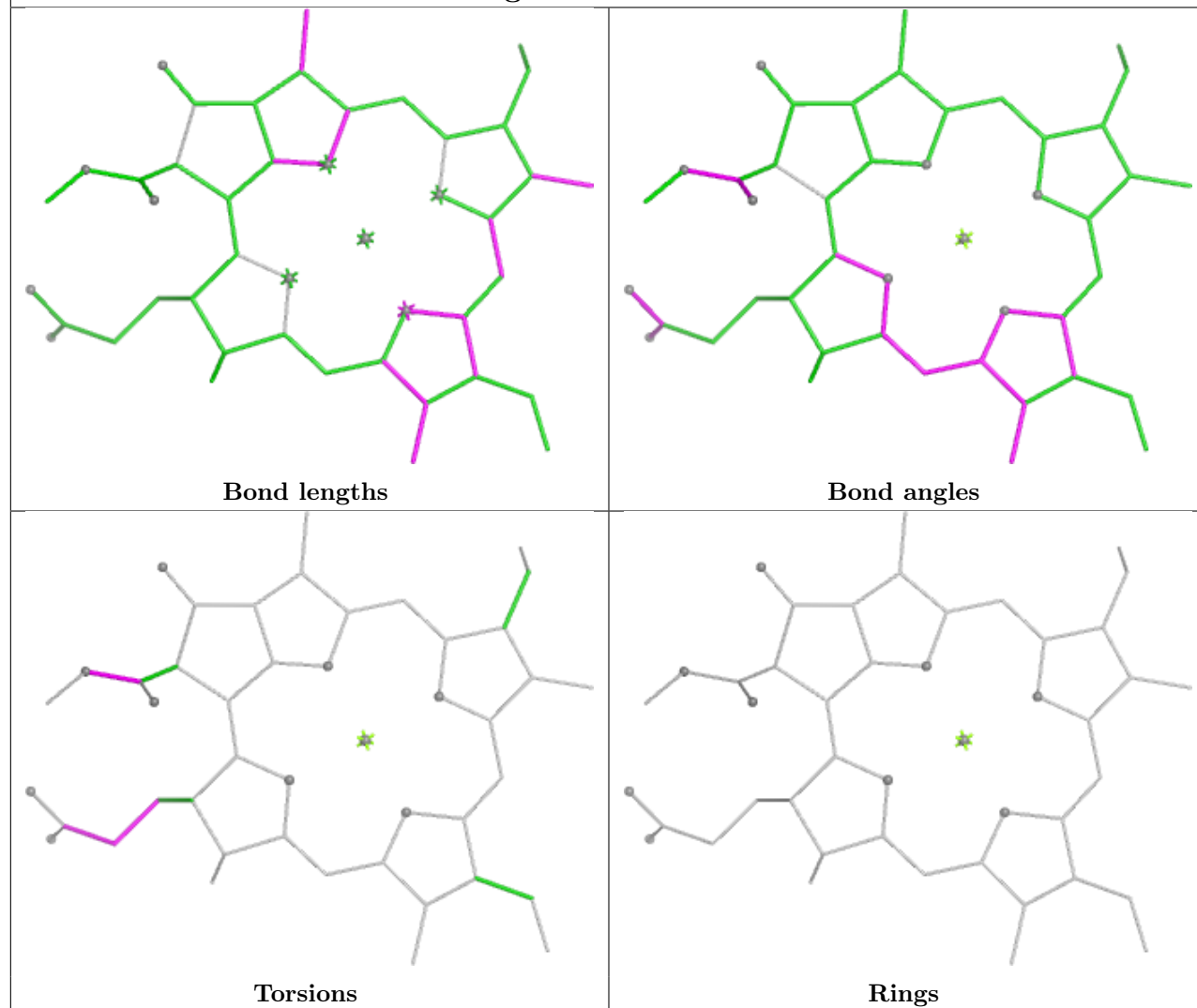
Ligand CLA A 818



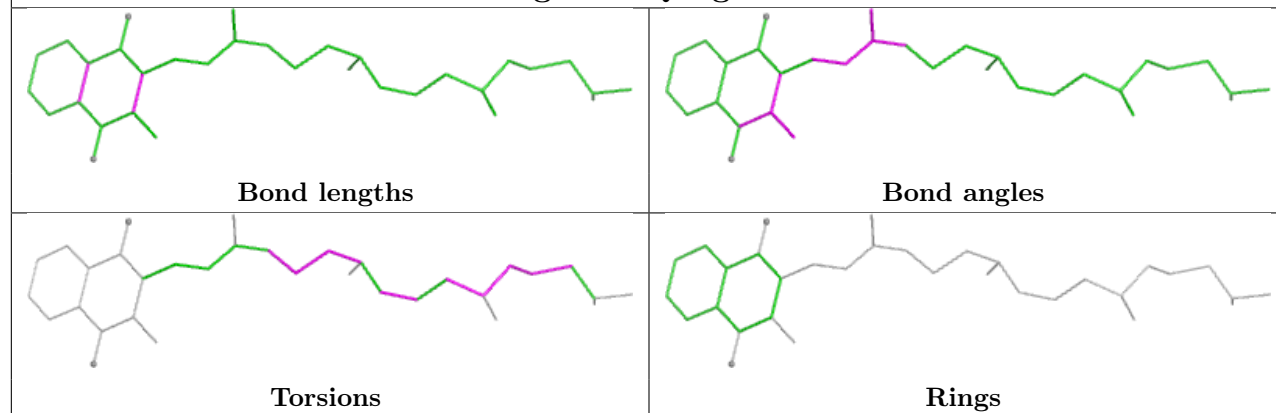
Ligand BCR b 845

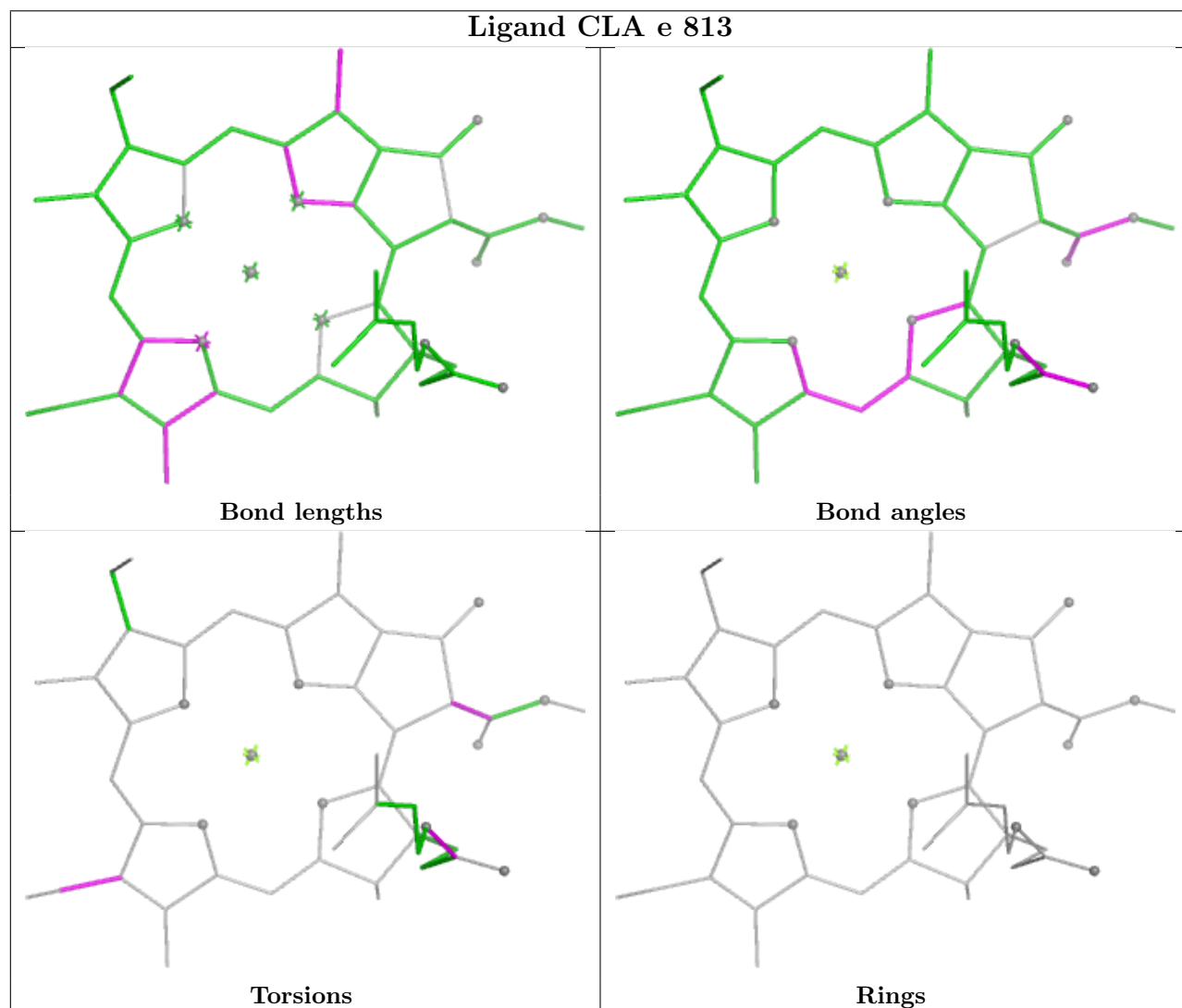
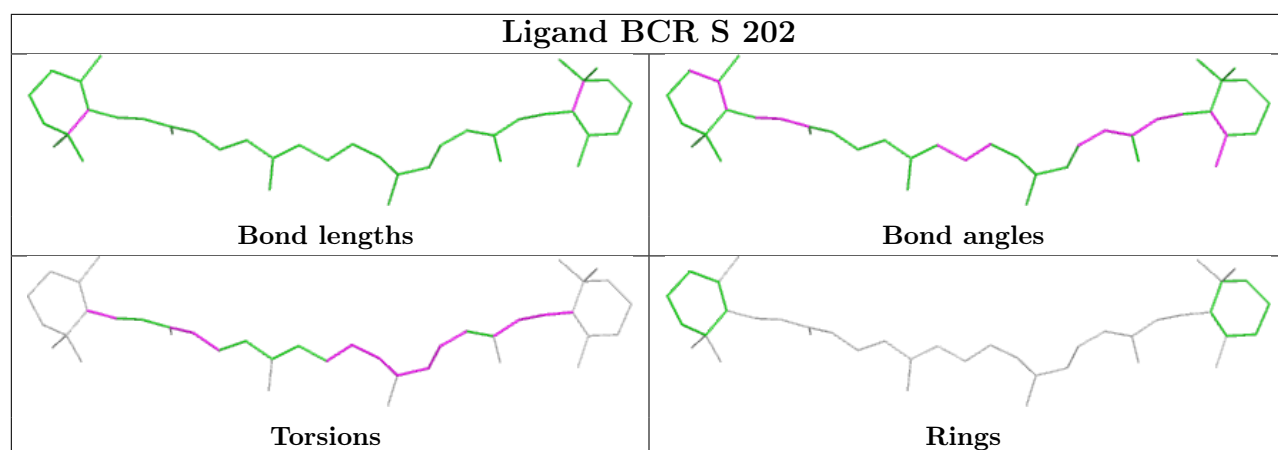


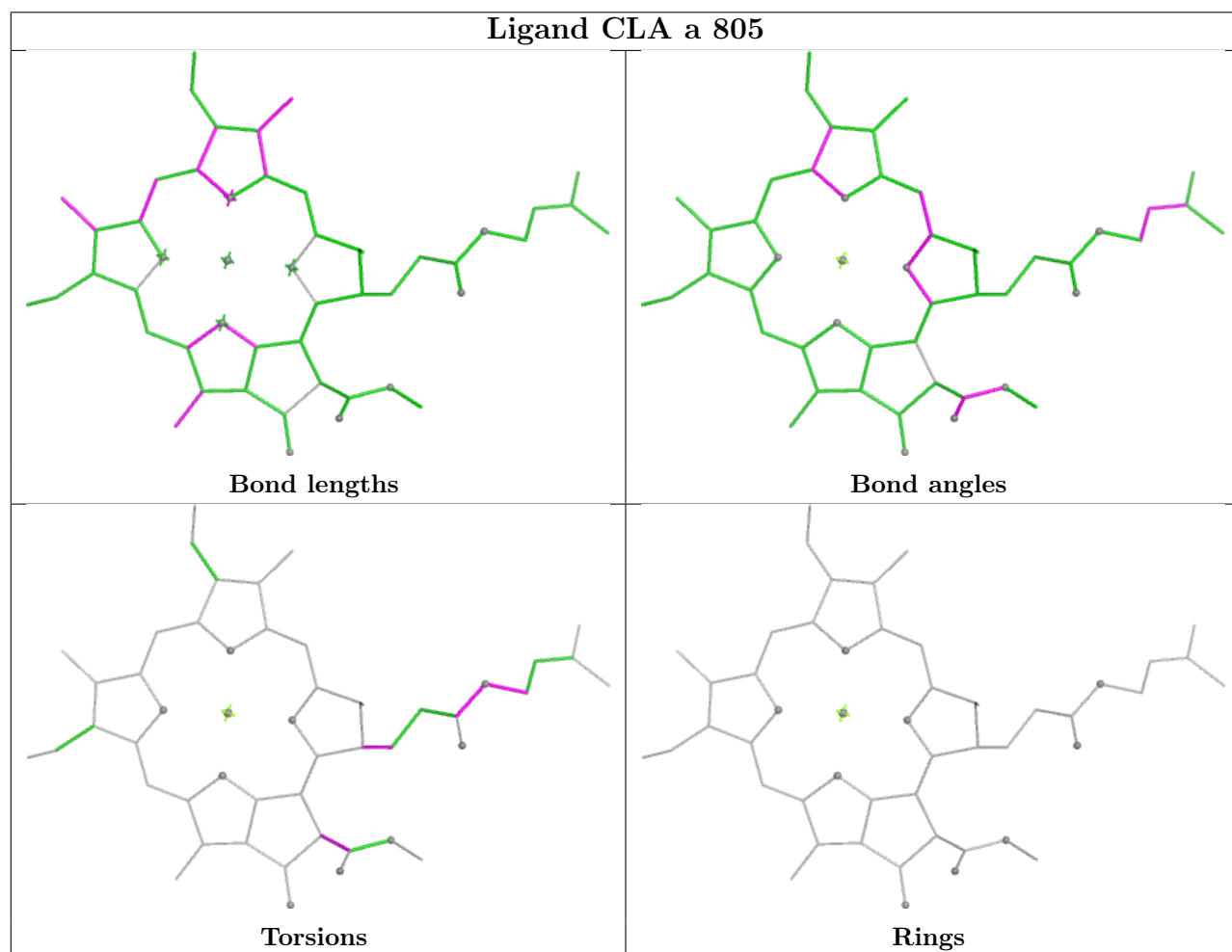
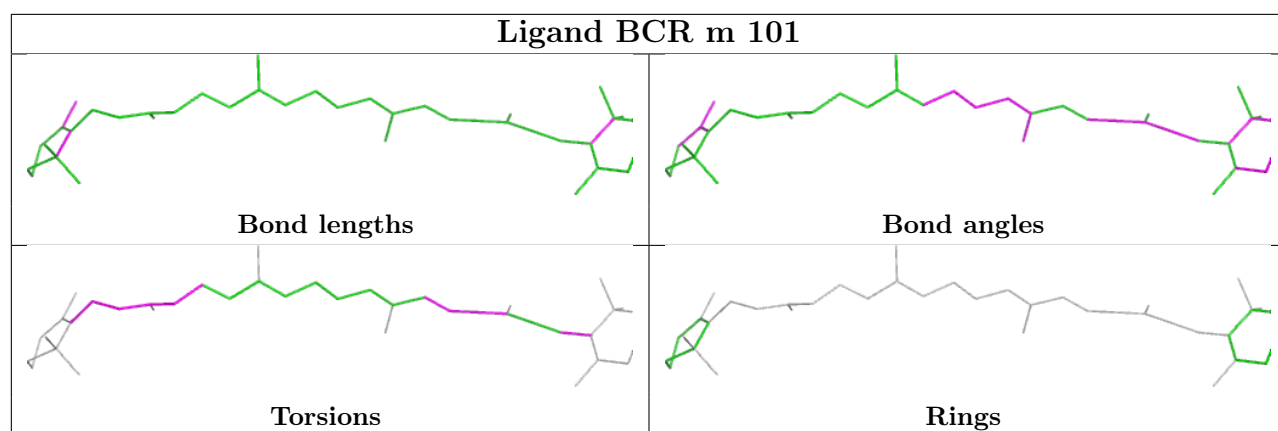
Ligand CLA s 202

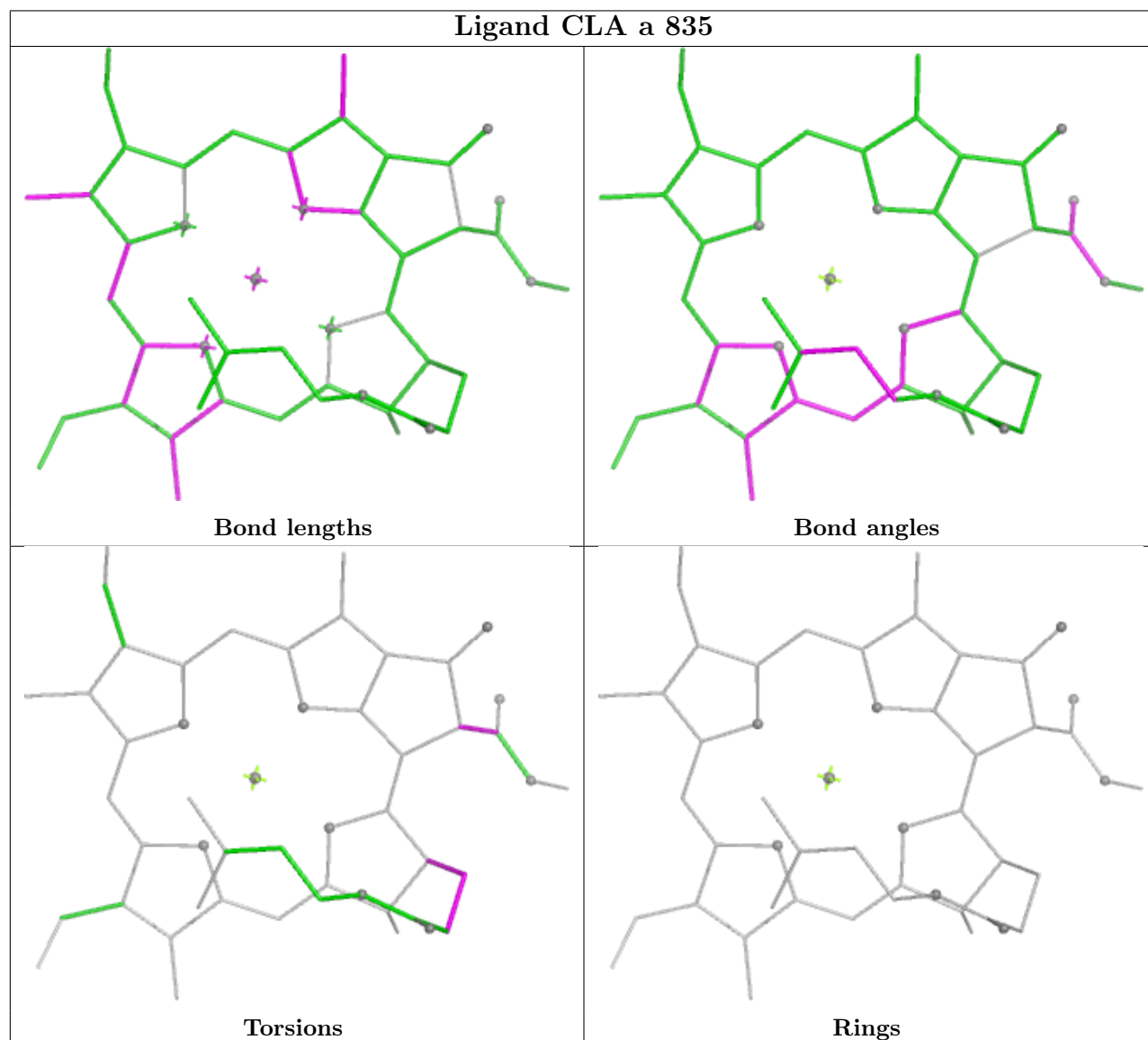
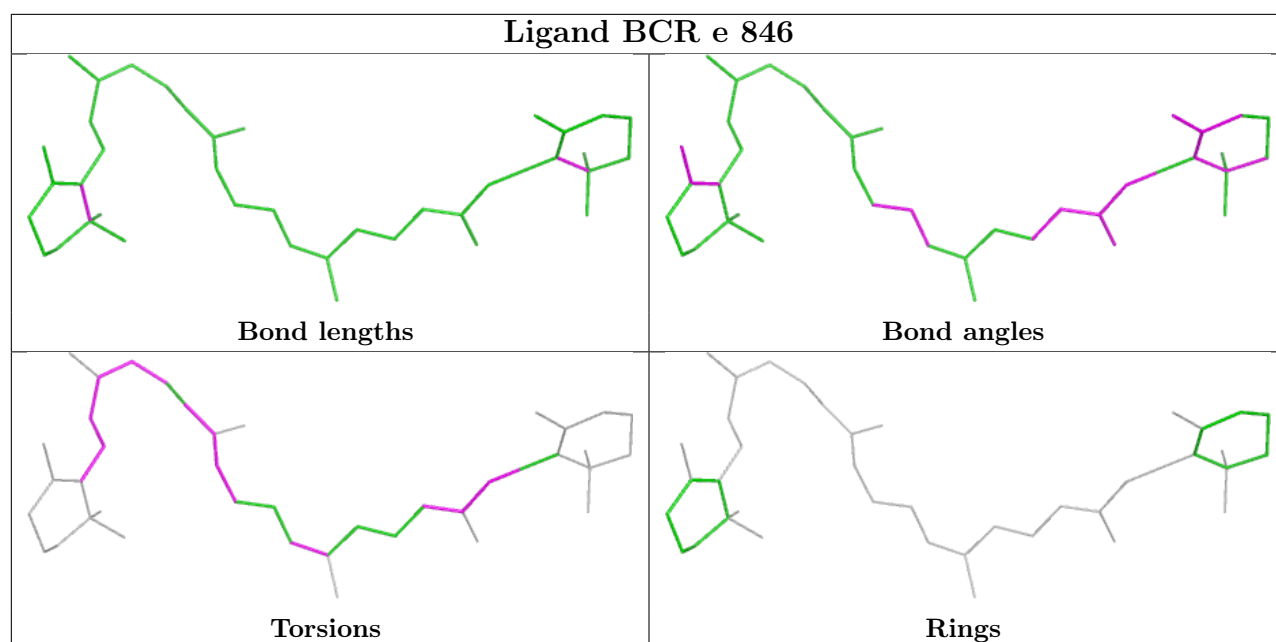


Ligand PQN g 843

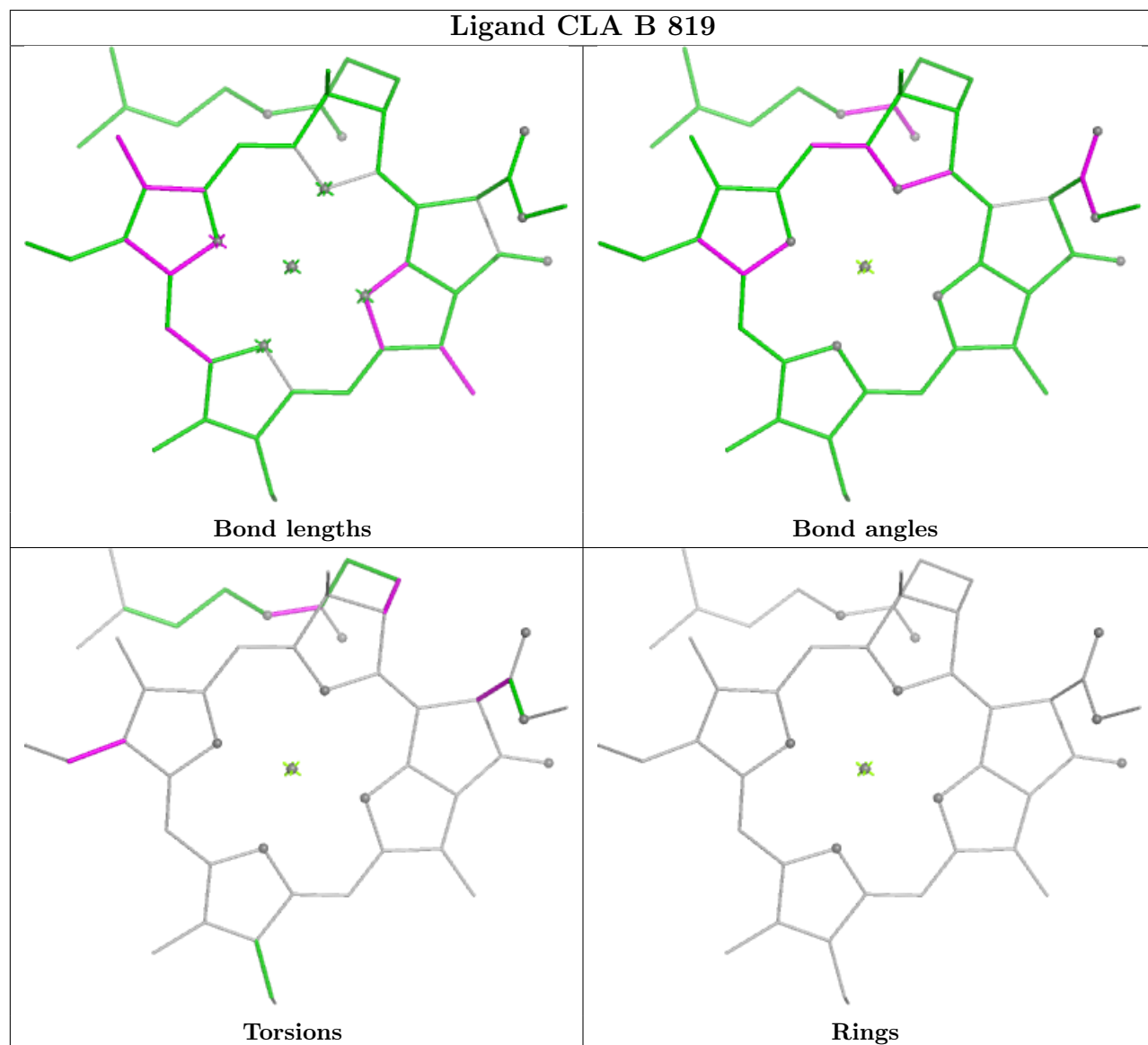




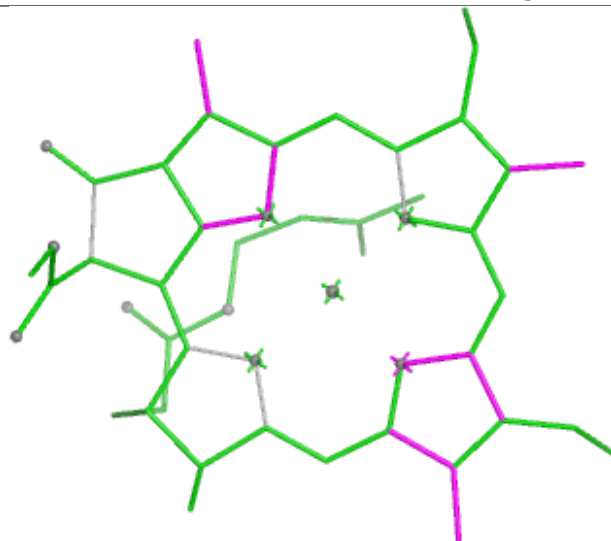




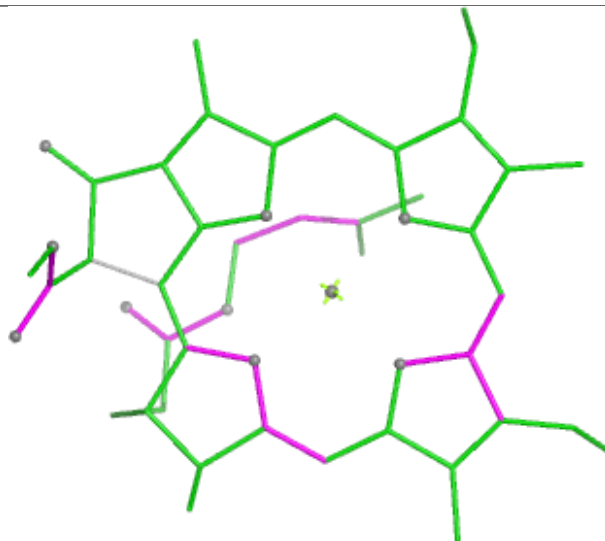
Ligand CLA B 819



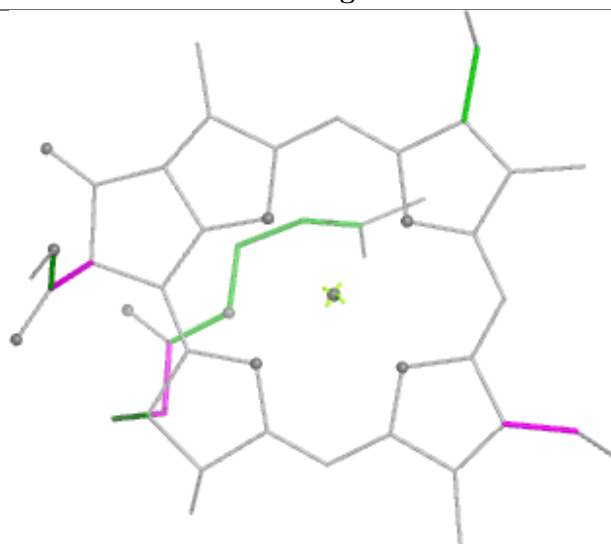
Ligand CLA e 839



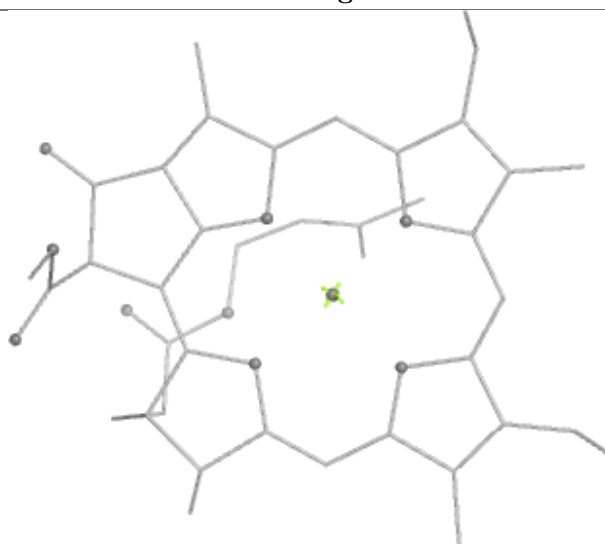
Bond lengths



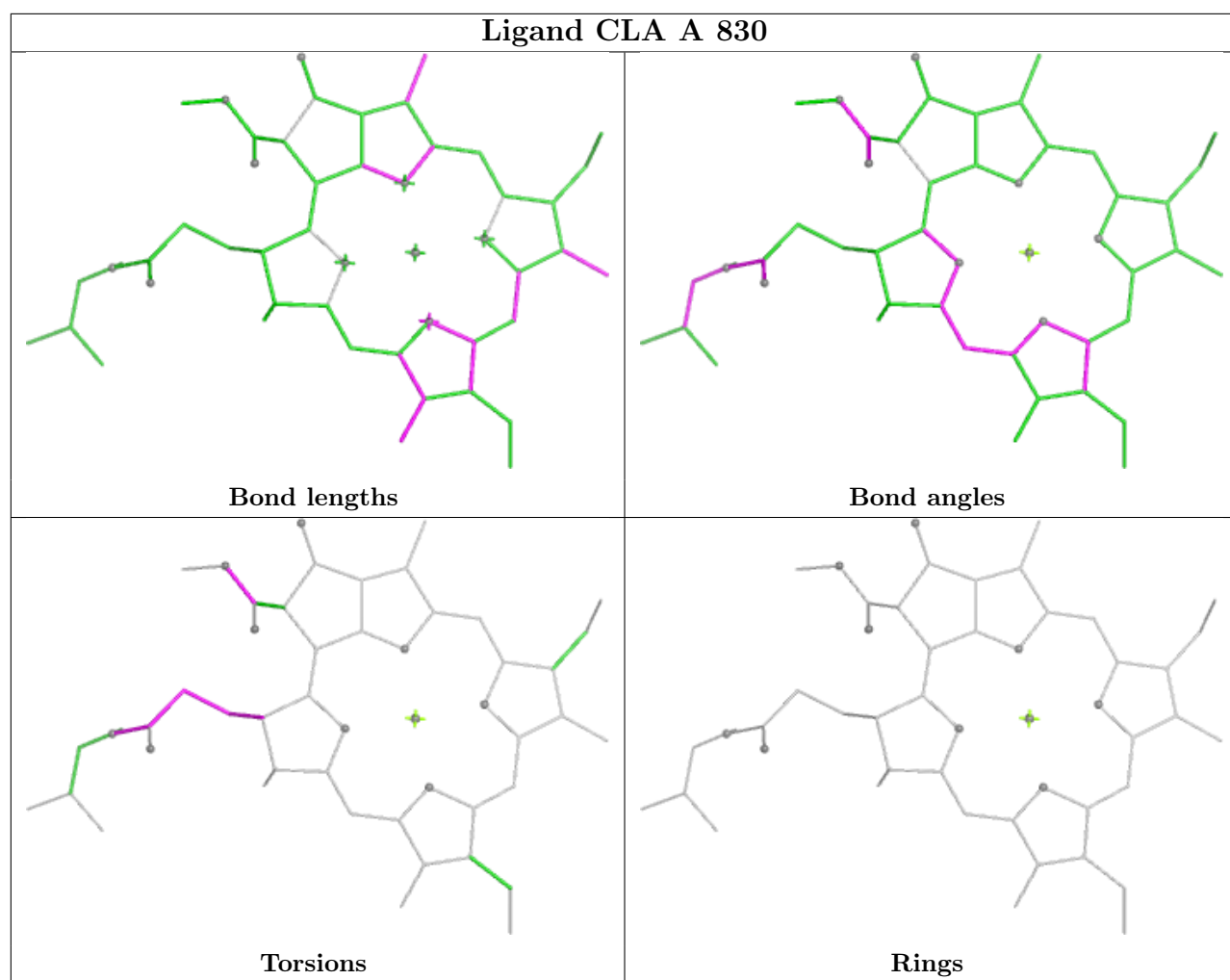
Bond angles



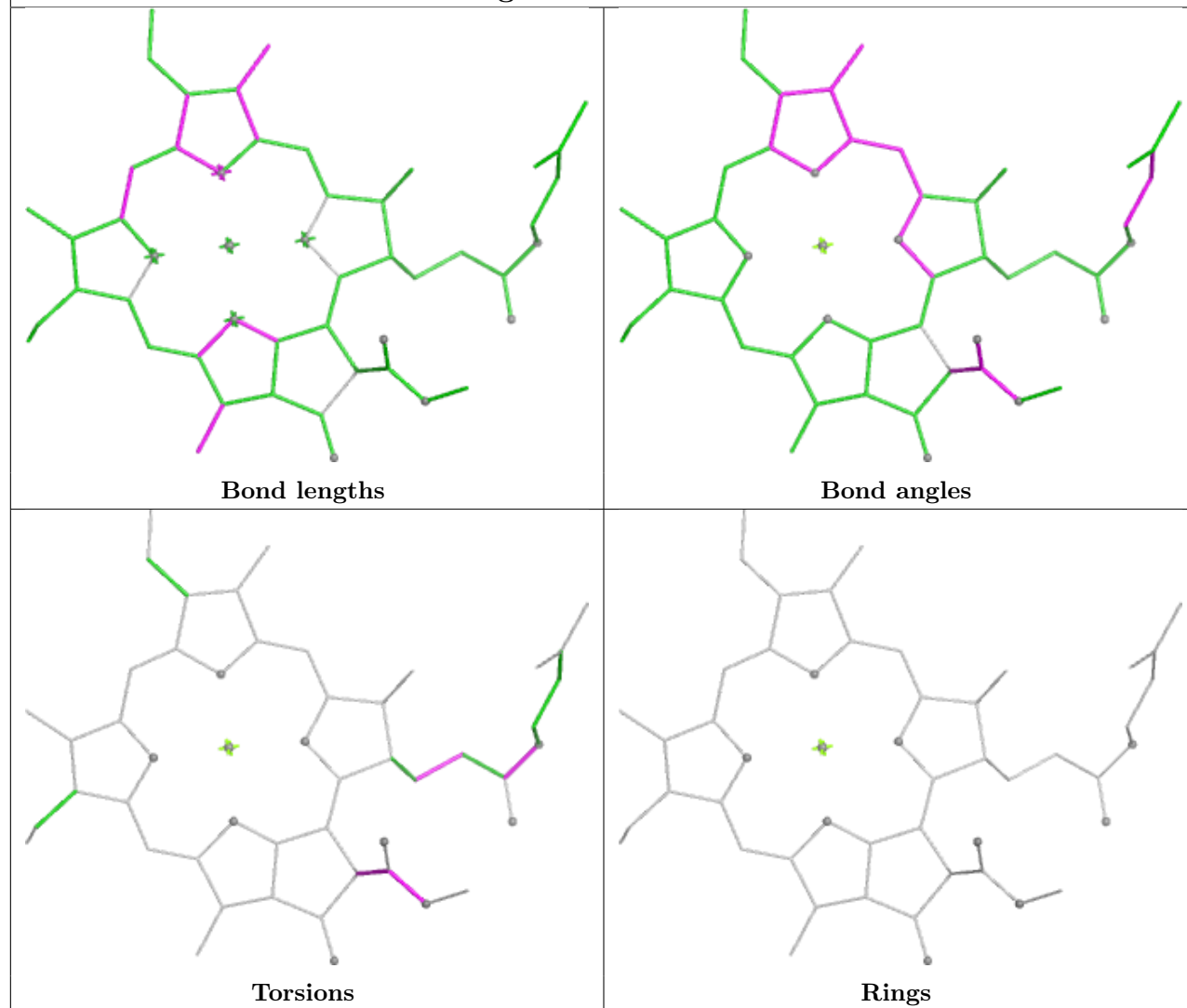
Torsions



Rings

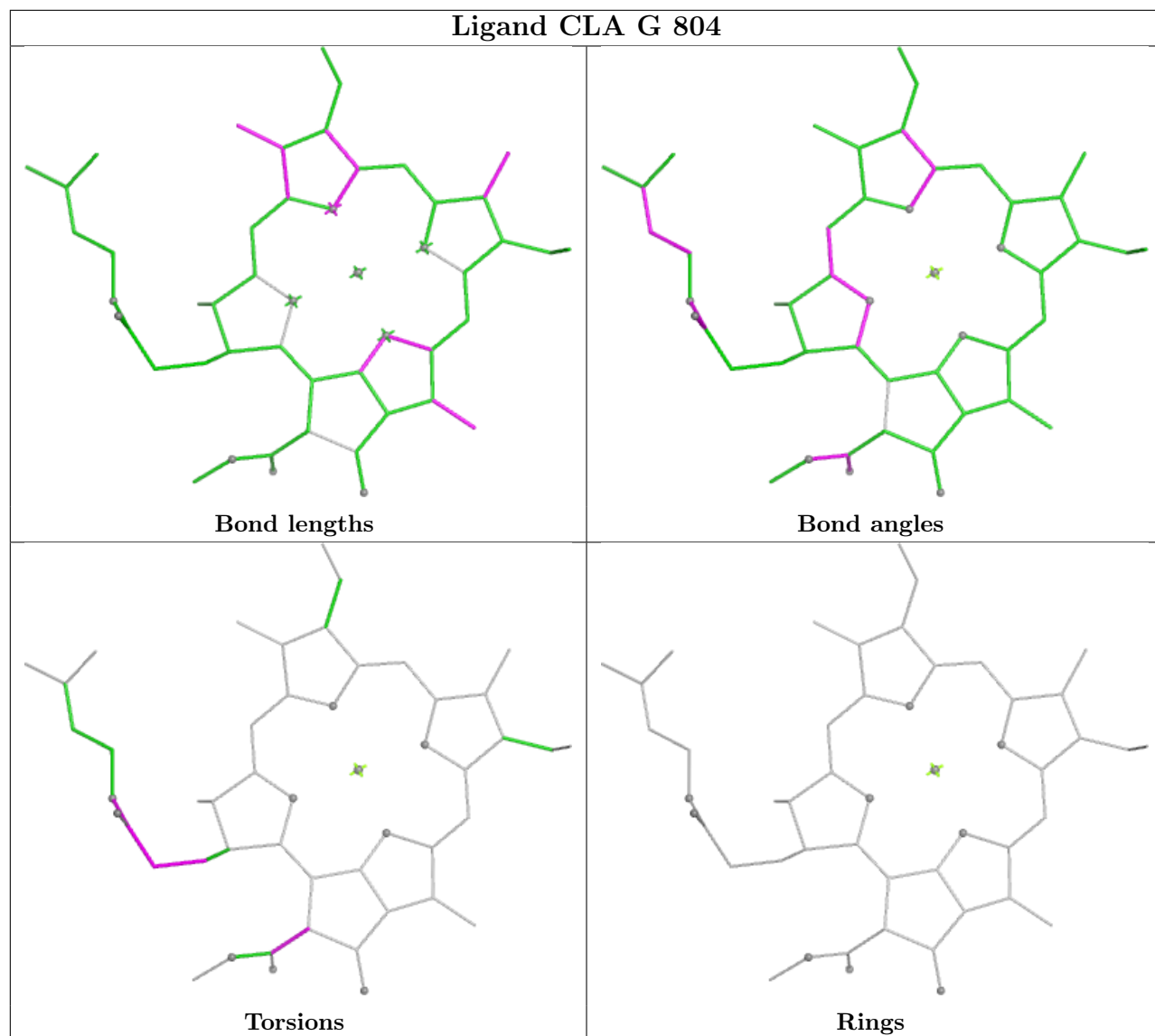


Ligand CLA b 824

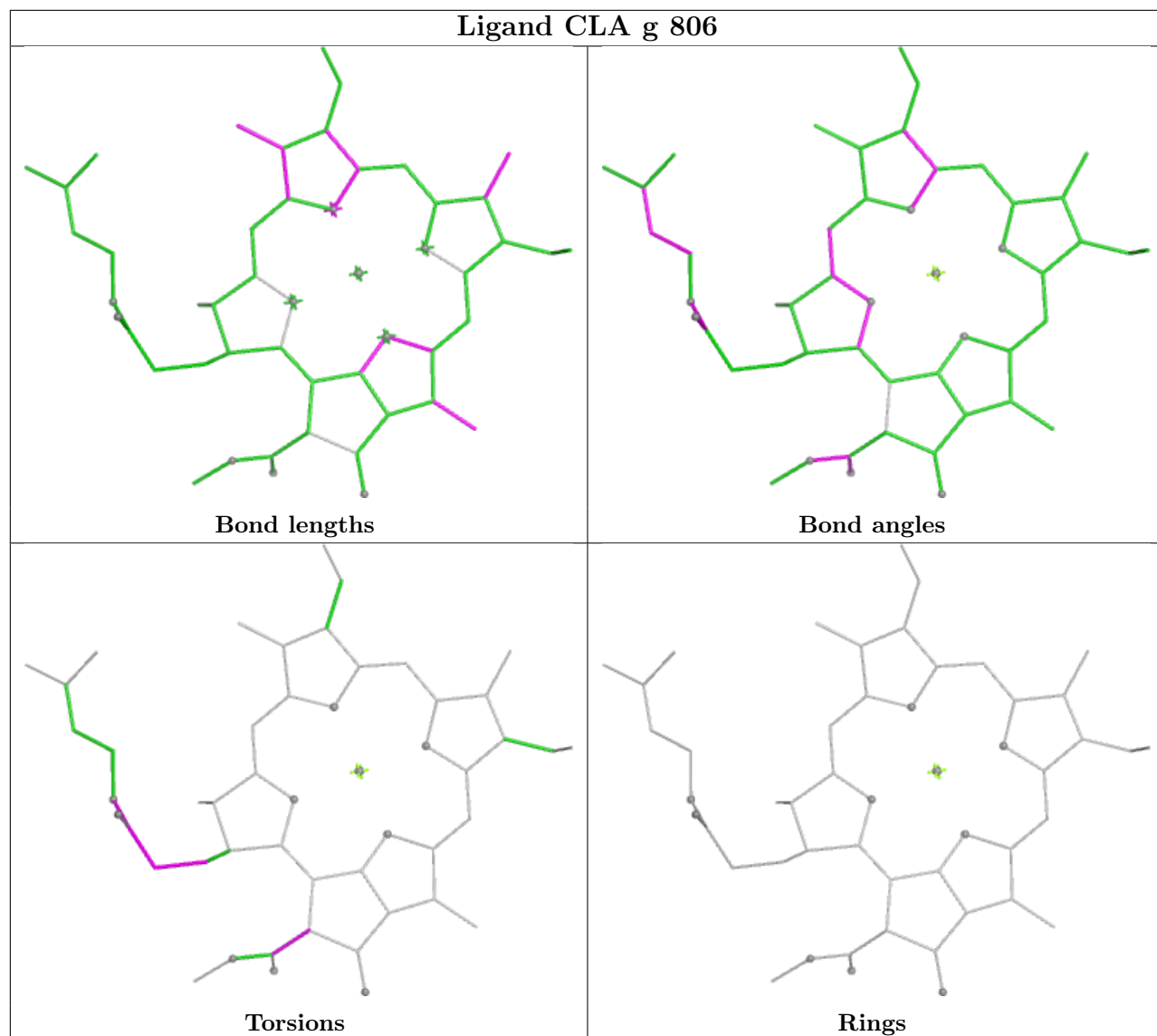


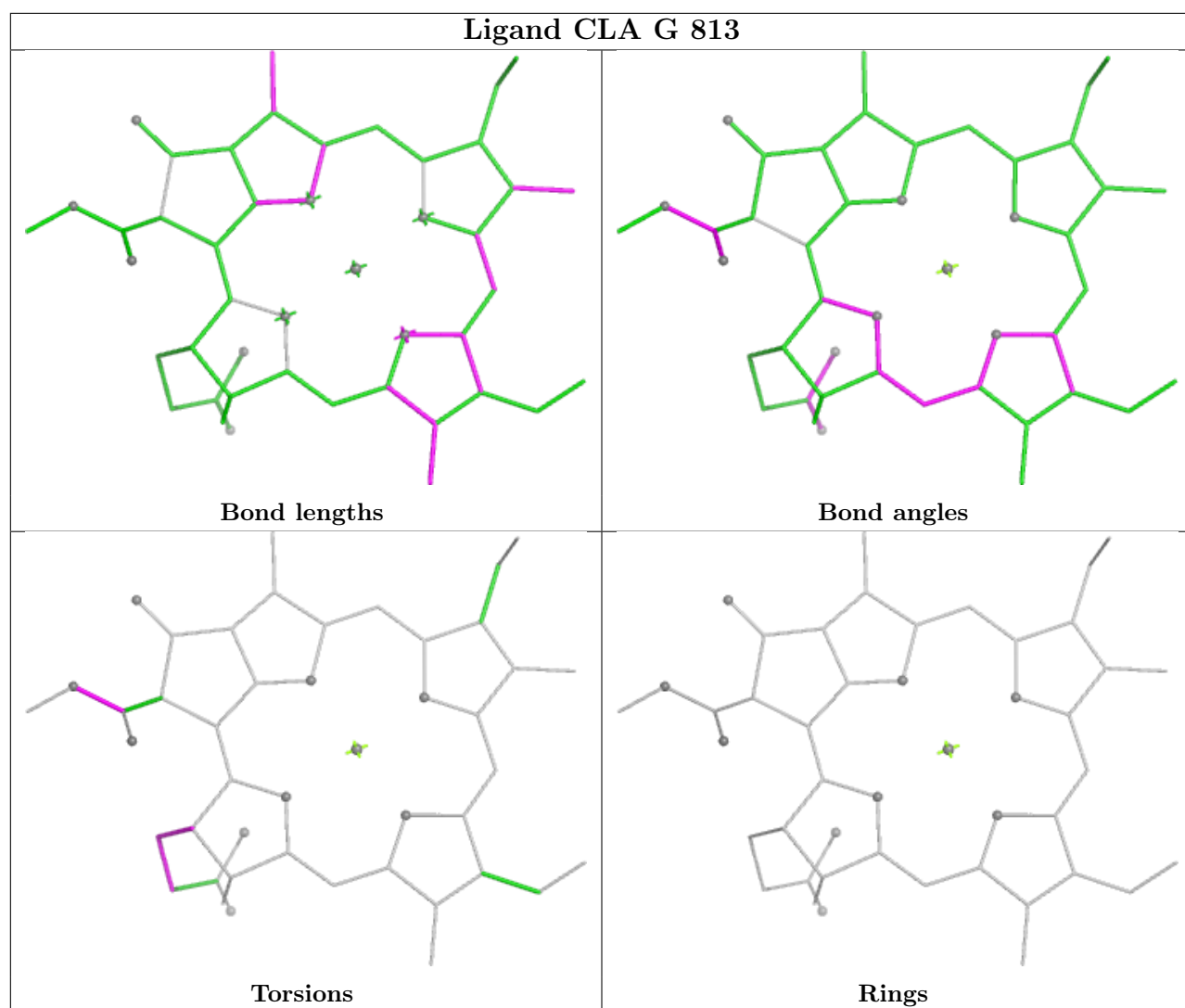
Ligand BCR A 850

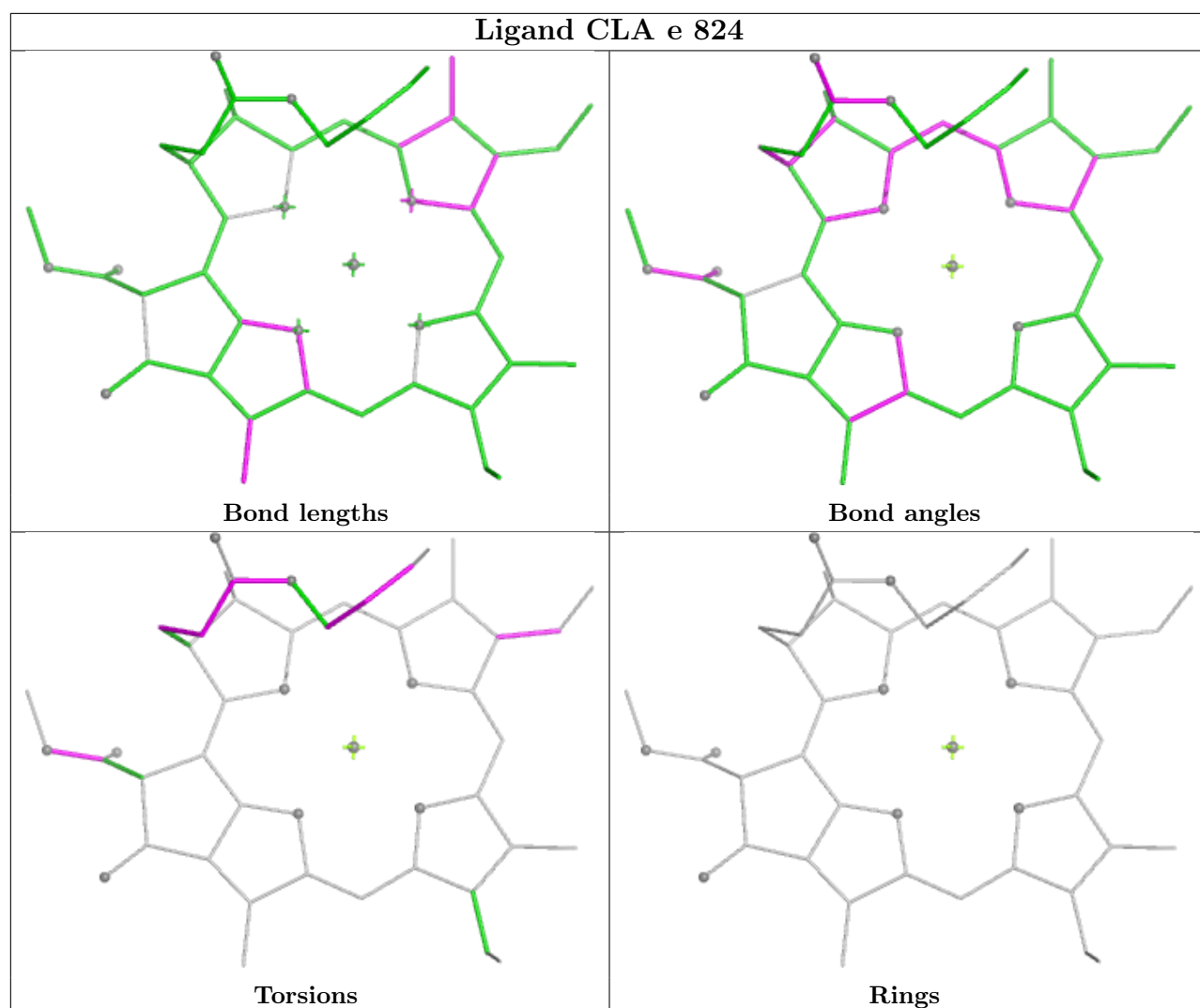




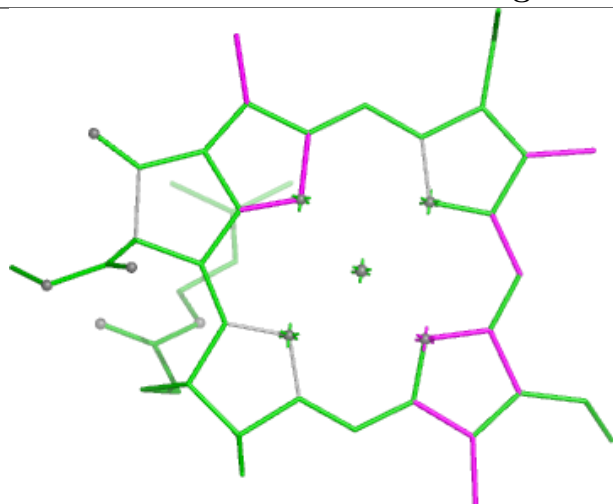
Ligand CLA g 806



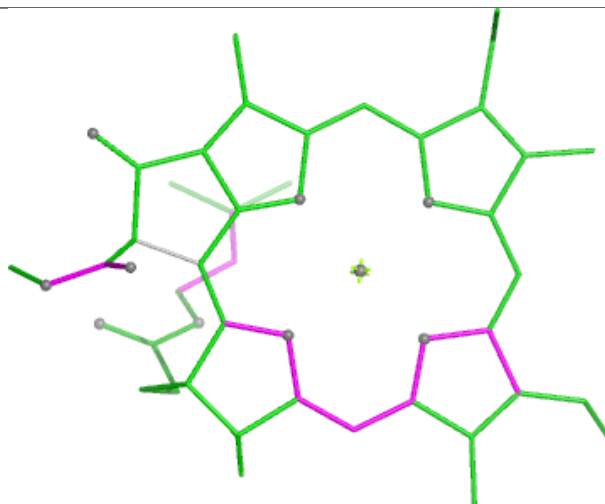




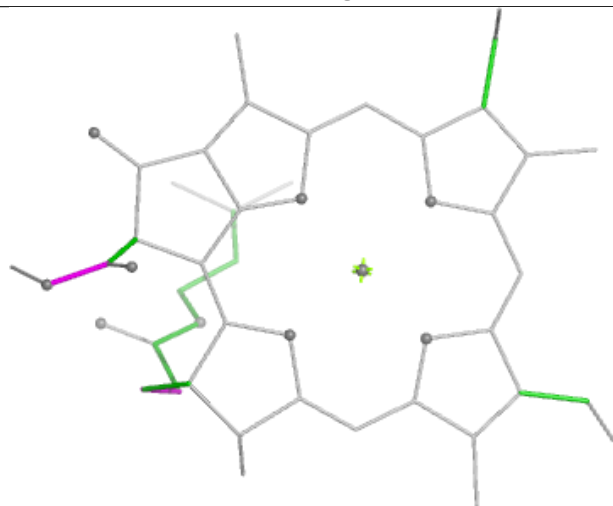
Ligand CLA G 815



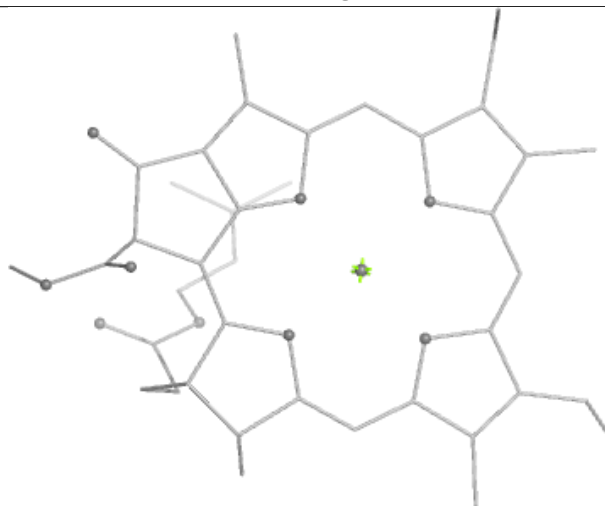
Bond lengths



Bond angles

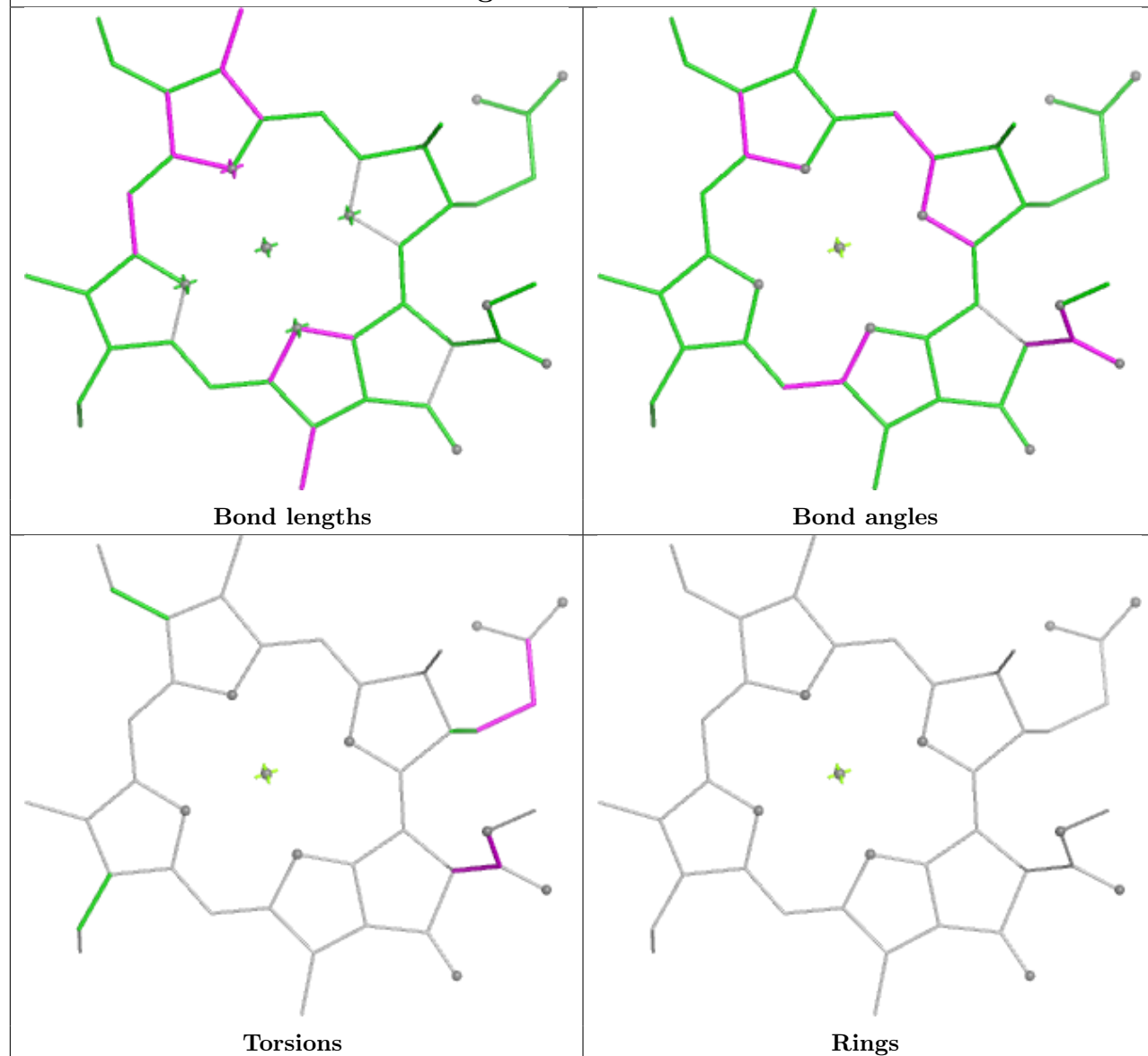


Torsions

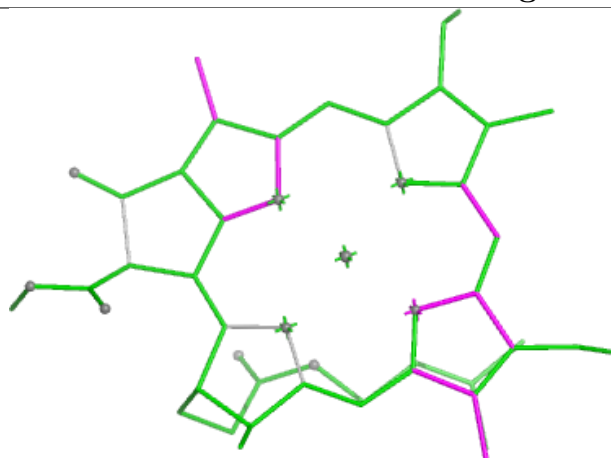


Rings

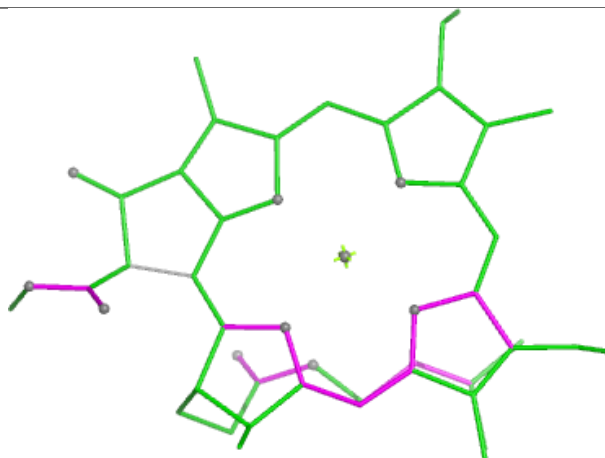
Ligand CLA A 838



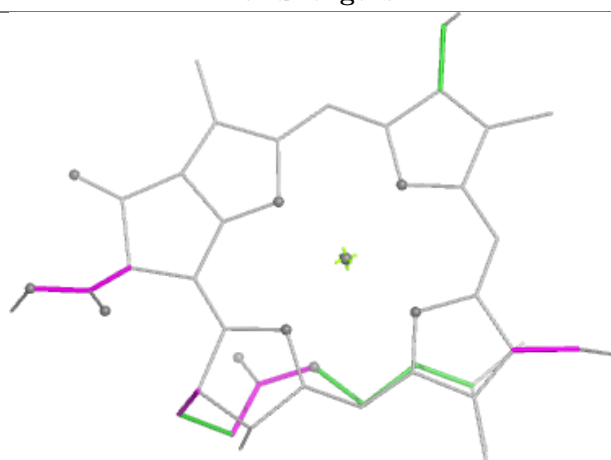
Ligand CLA e 823



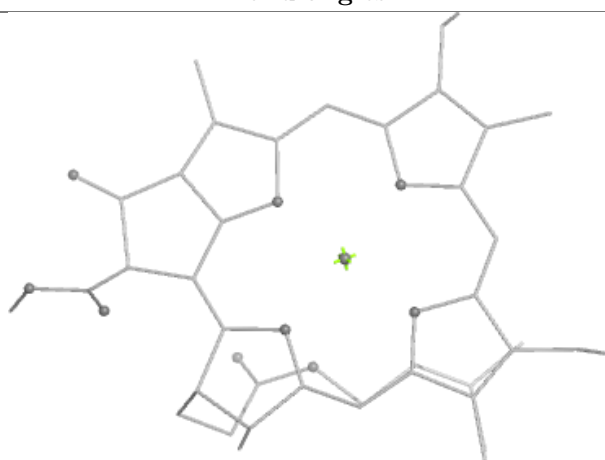
Bond lengths



Bond angles

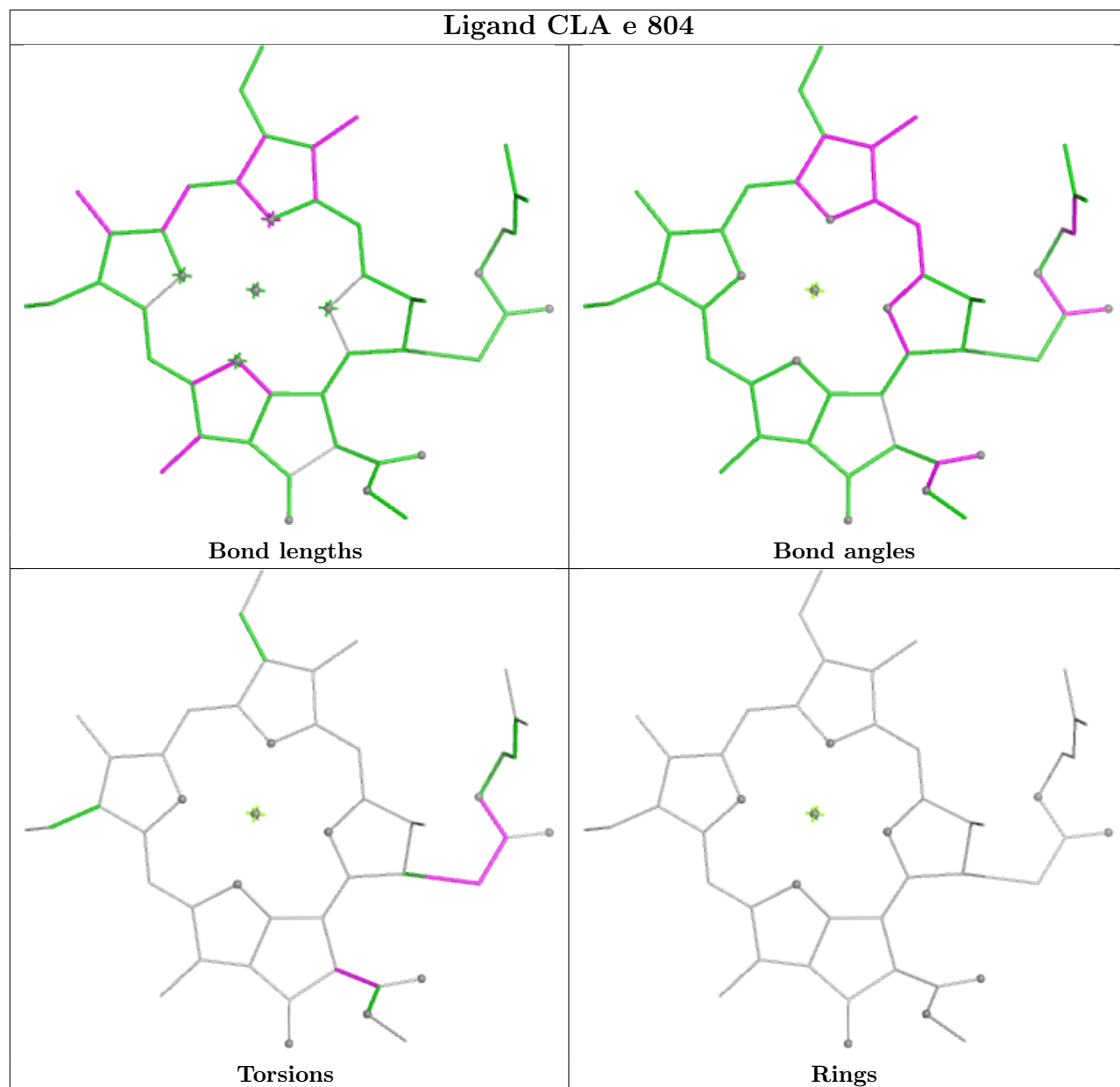


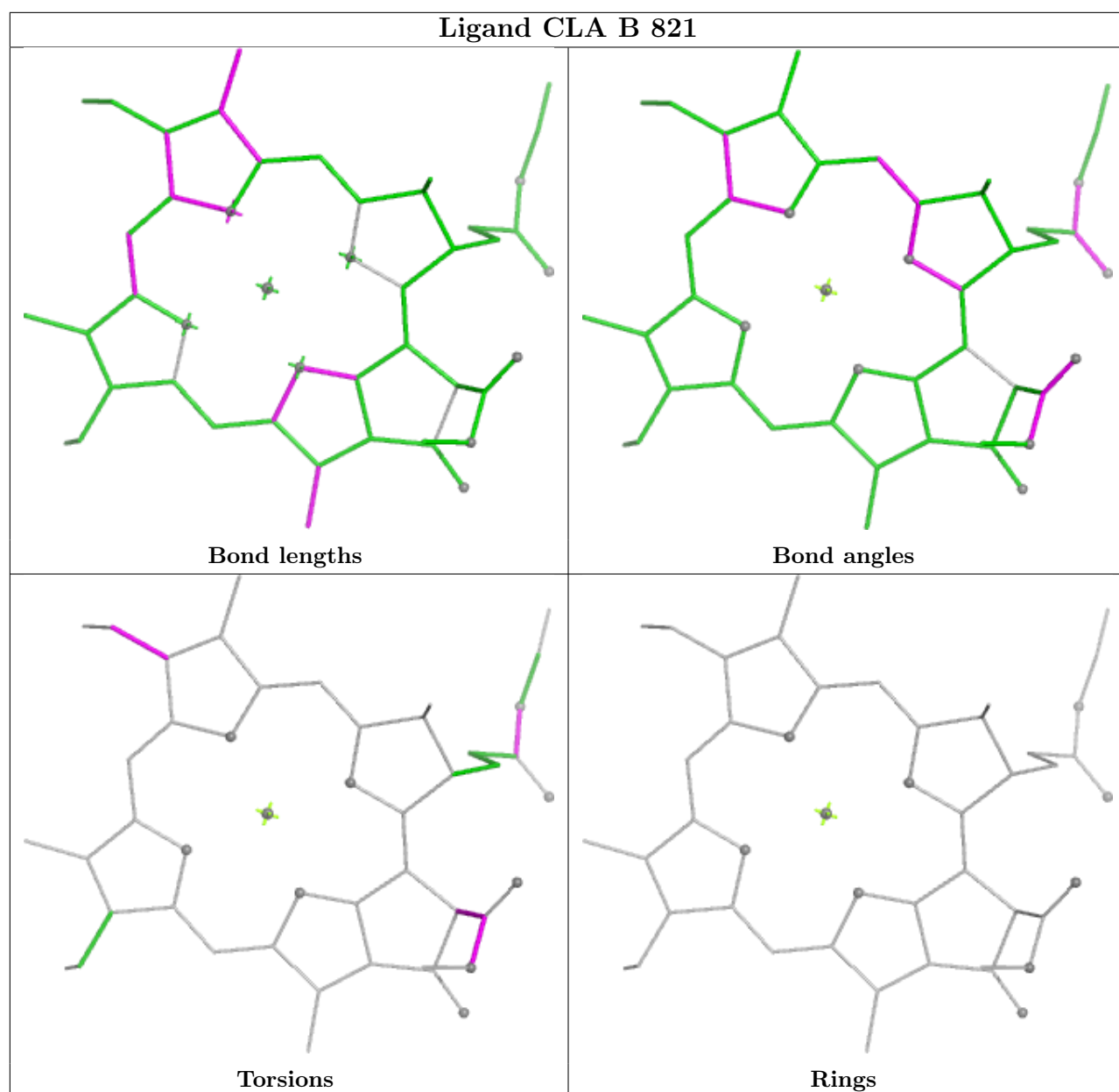
Torsions

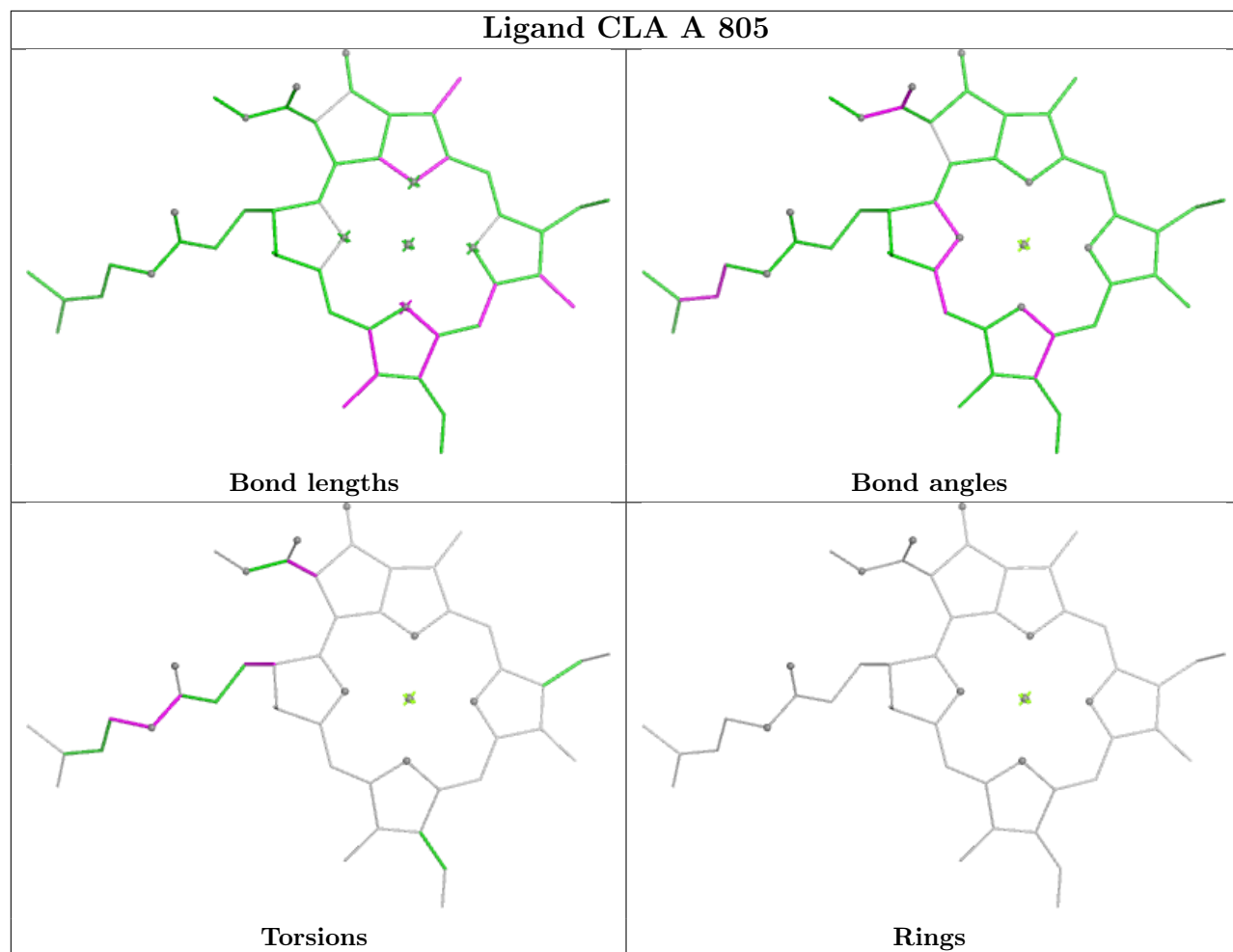


Rings

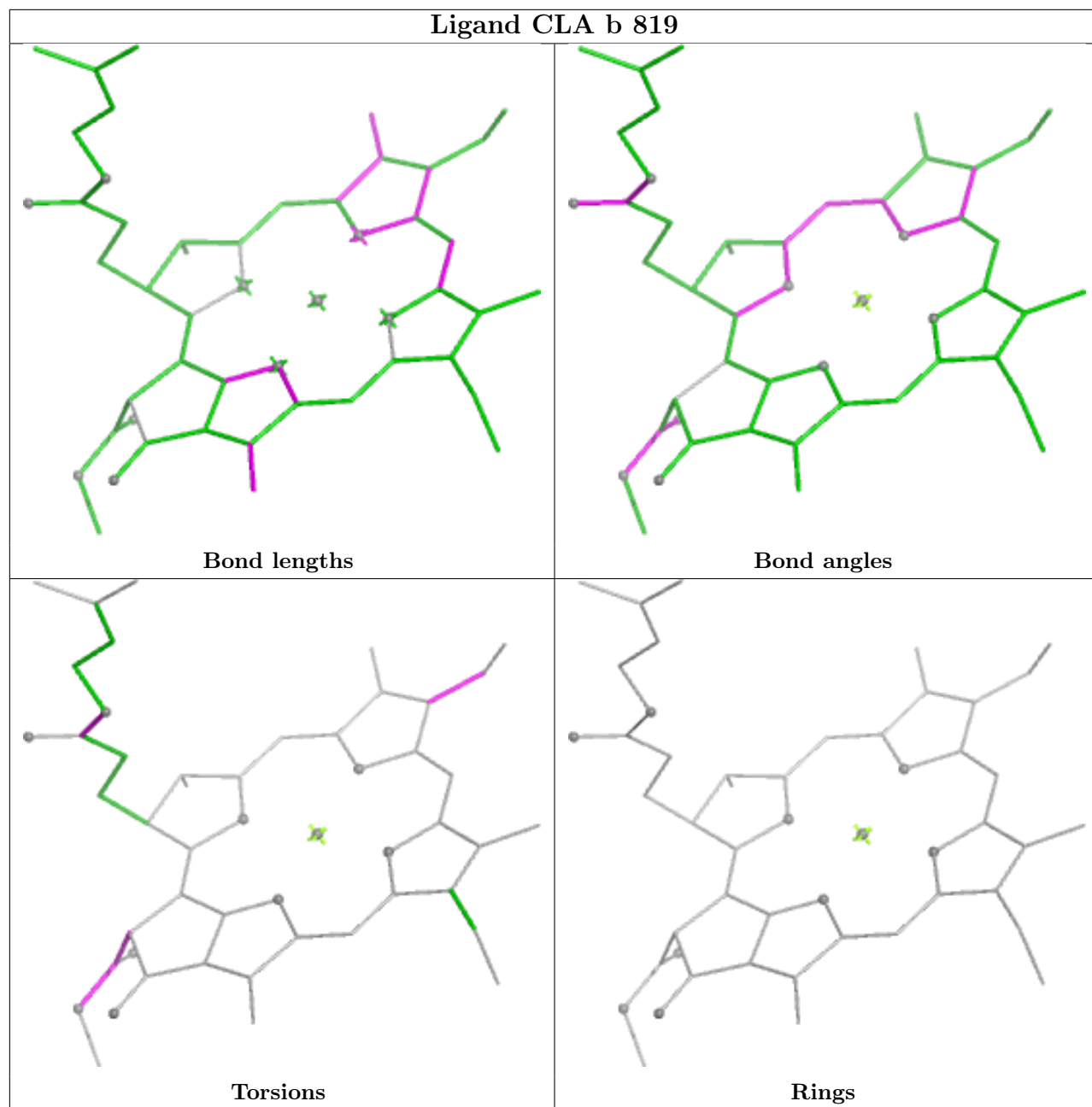
Ligand CLA e 804

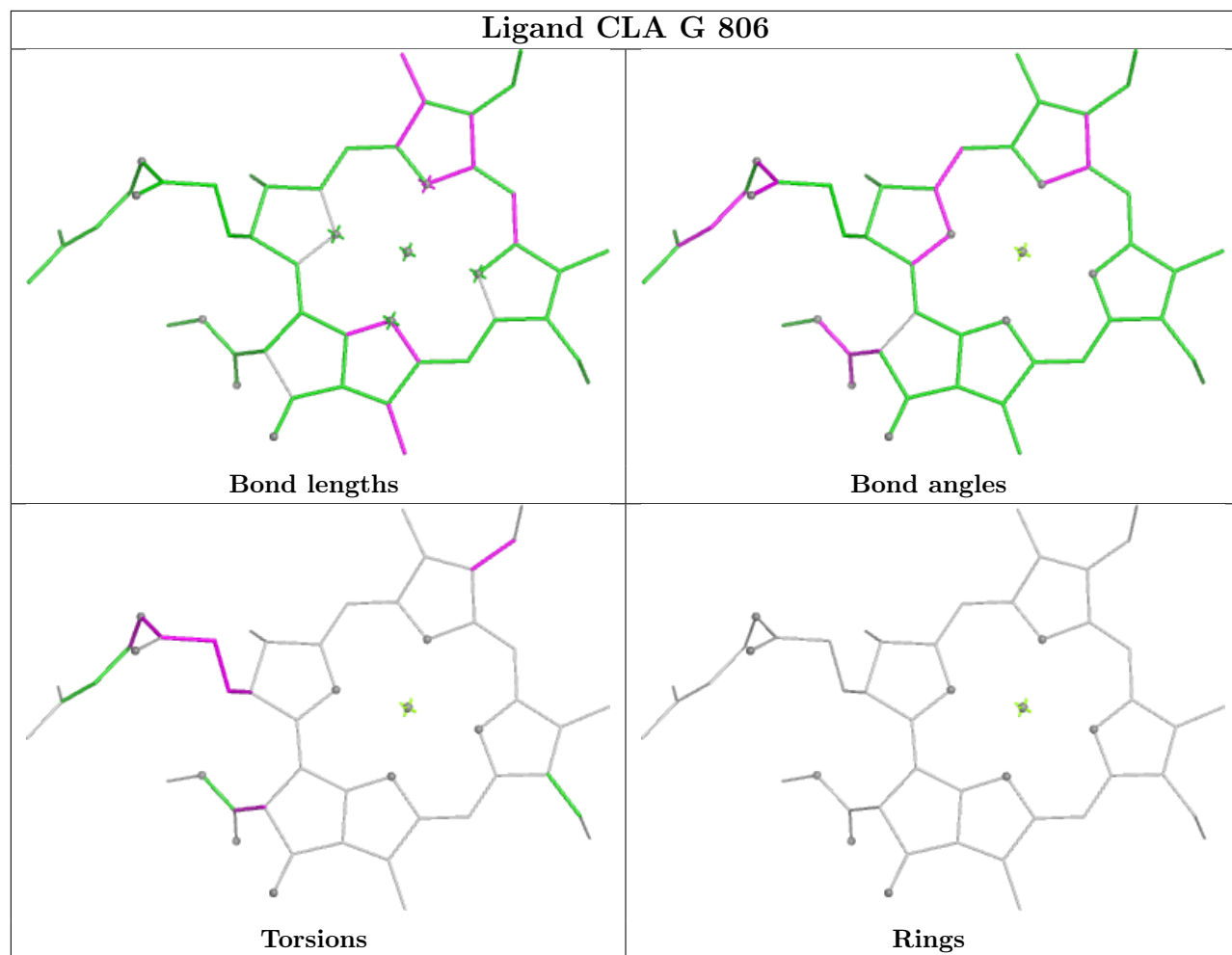




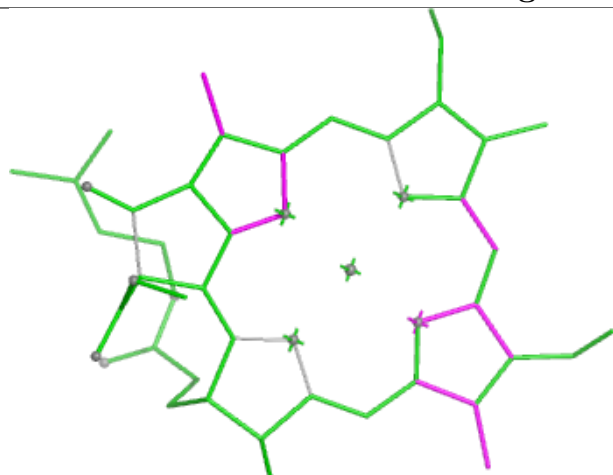


Ligand CLA b 819

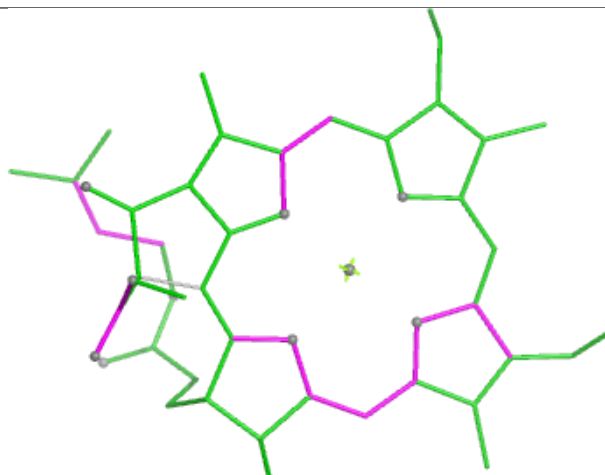




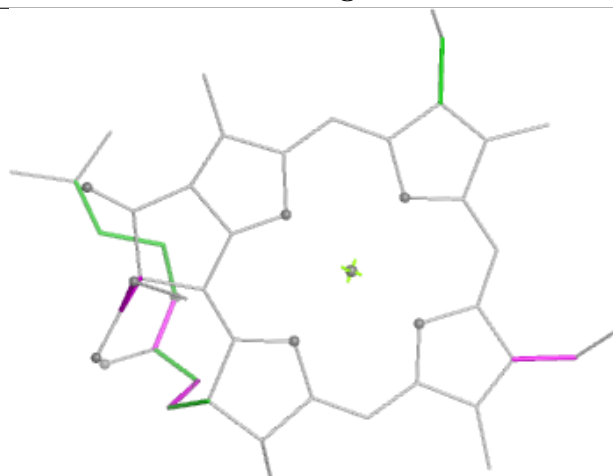
Ligand CLA a 810



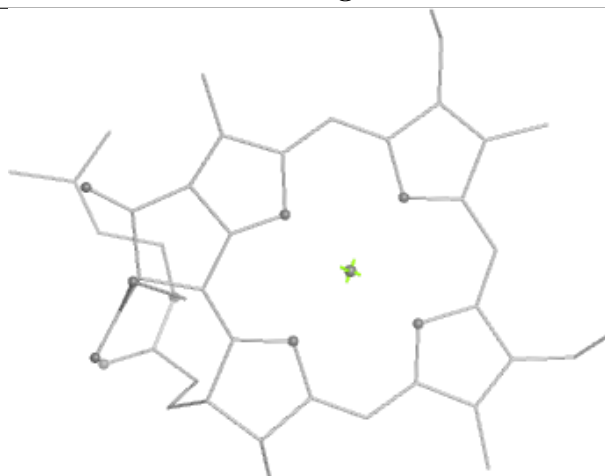
Bond lengths



Bond angles

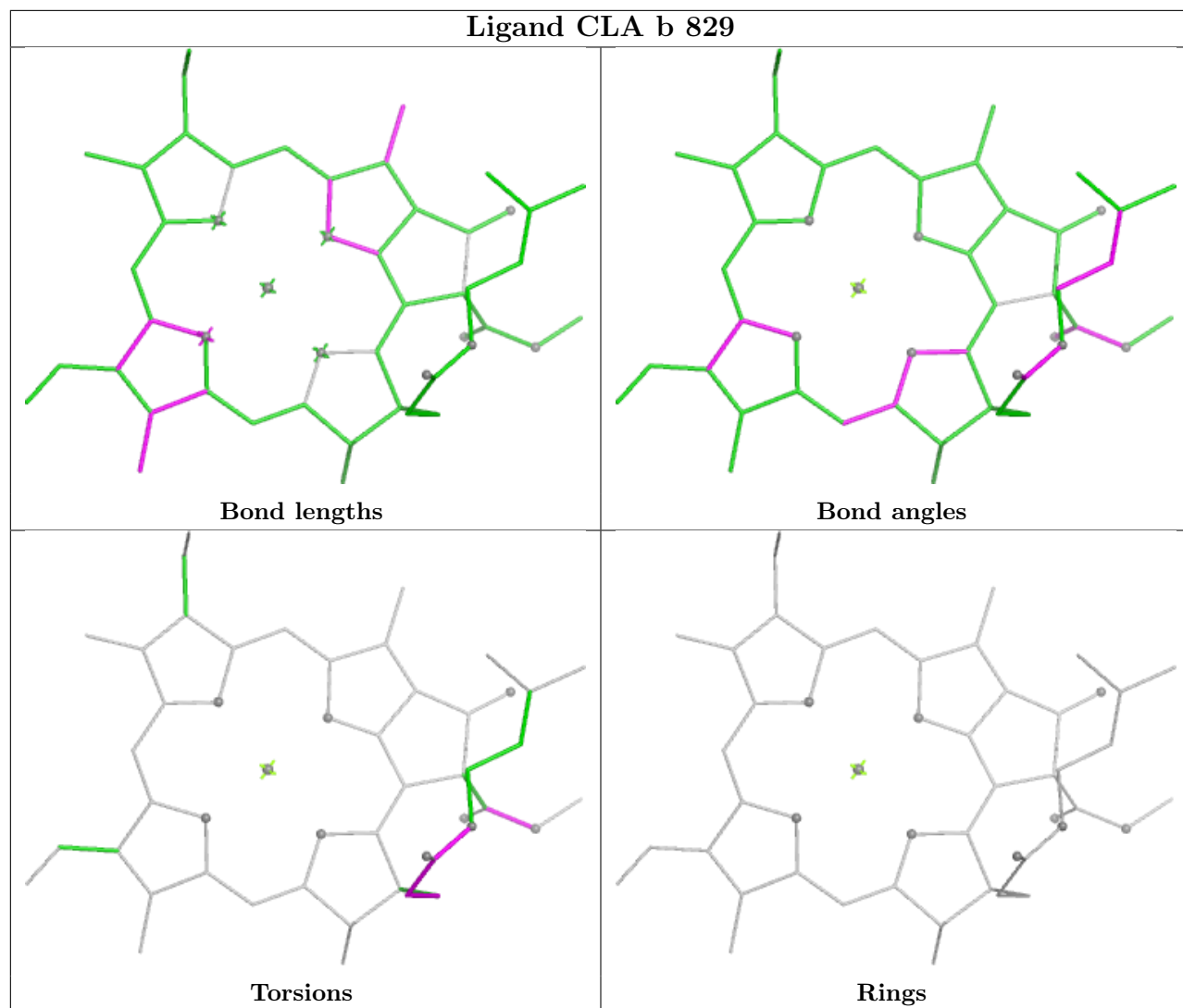


Torsions

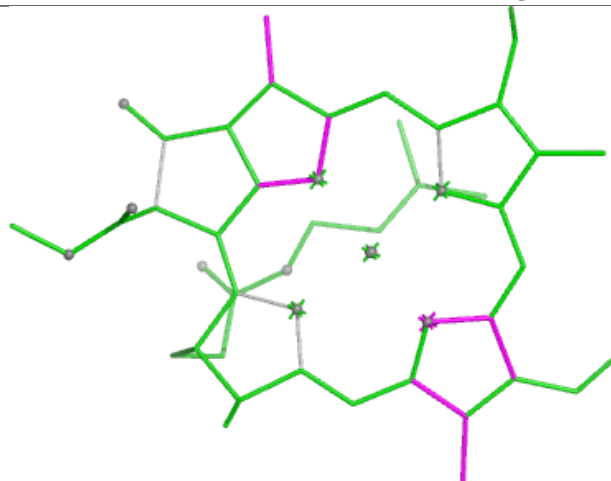


Rings

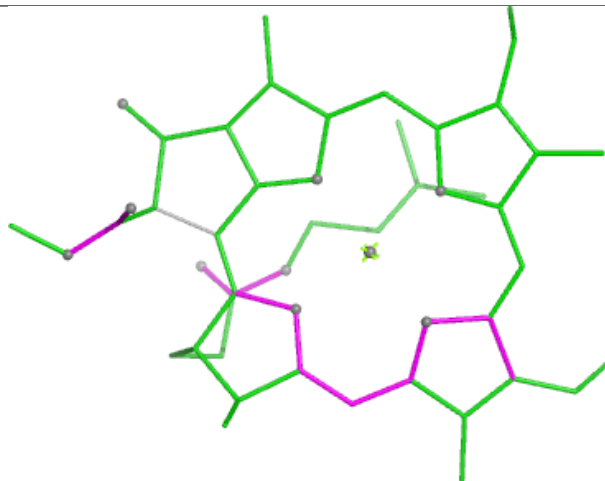
Ligand CLA b 829



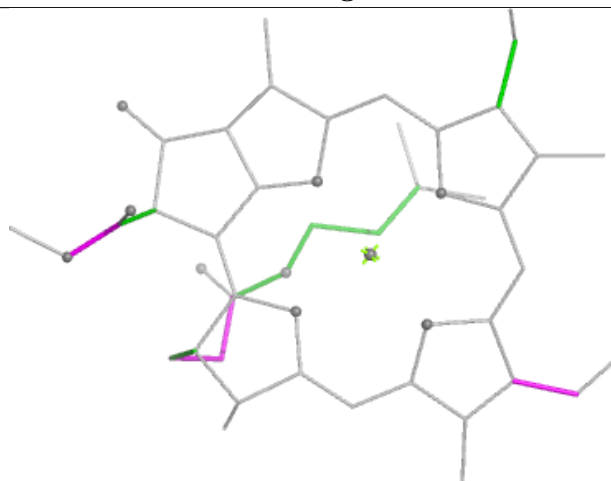
Ligand CLA G 808



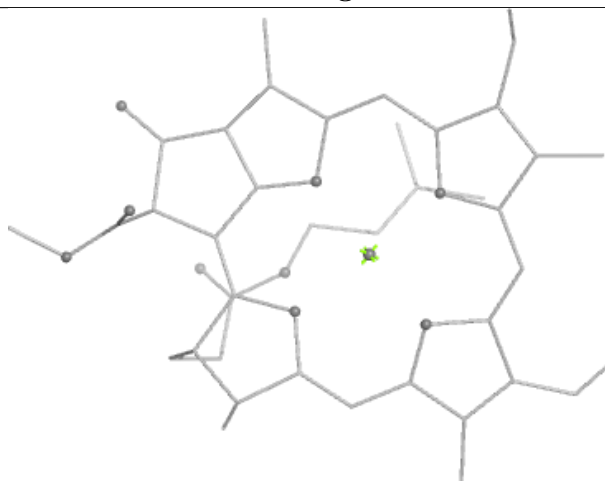
Bond lengths



Bond angles

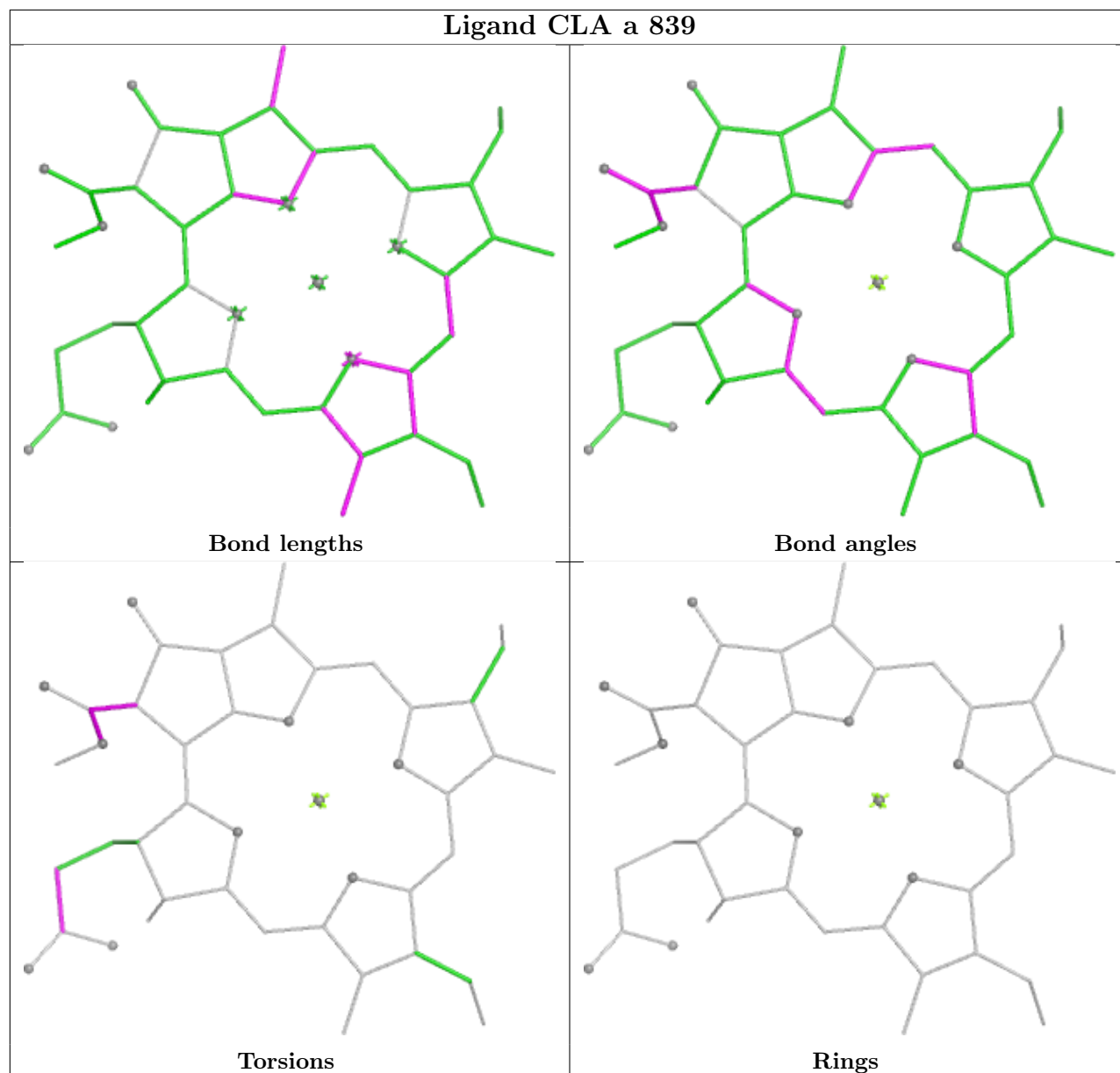


Torsions

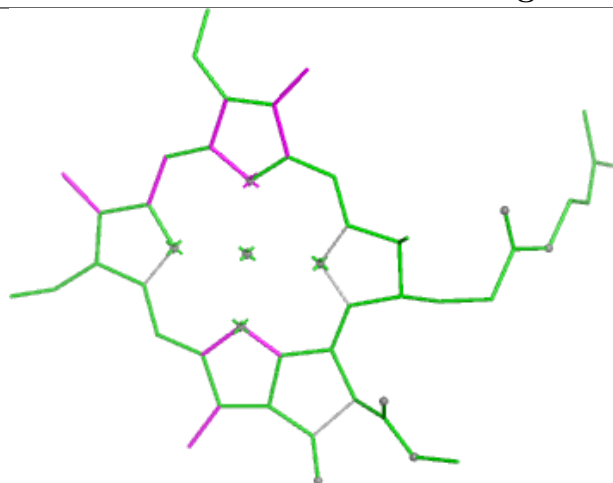


Rings

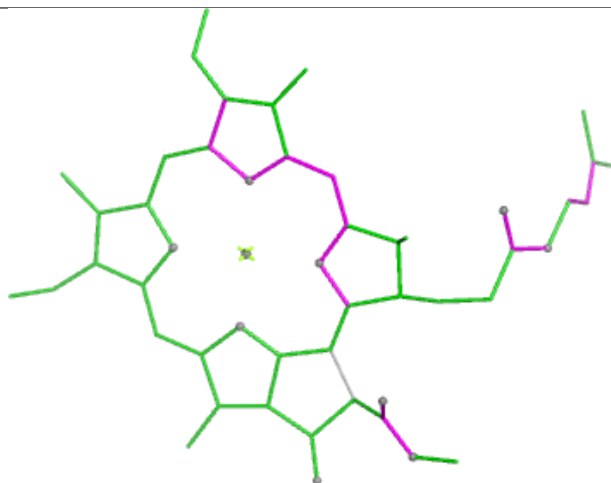
Ligand CLA a 839



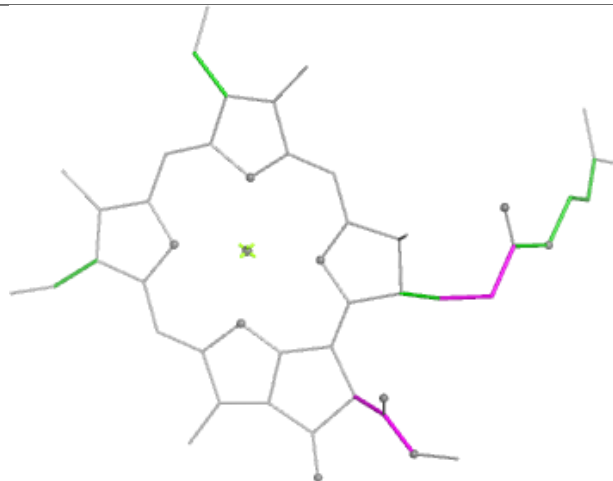
Ligand CLA b 810



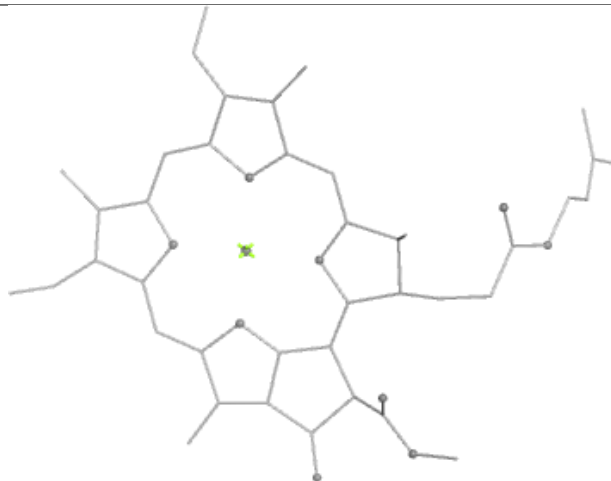
Bond lengths



Bond angles

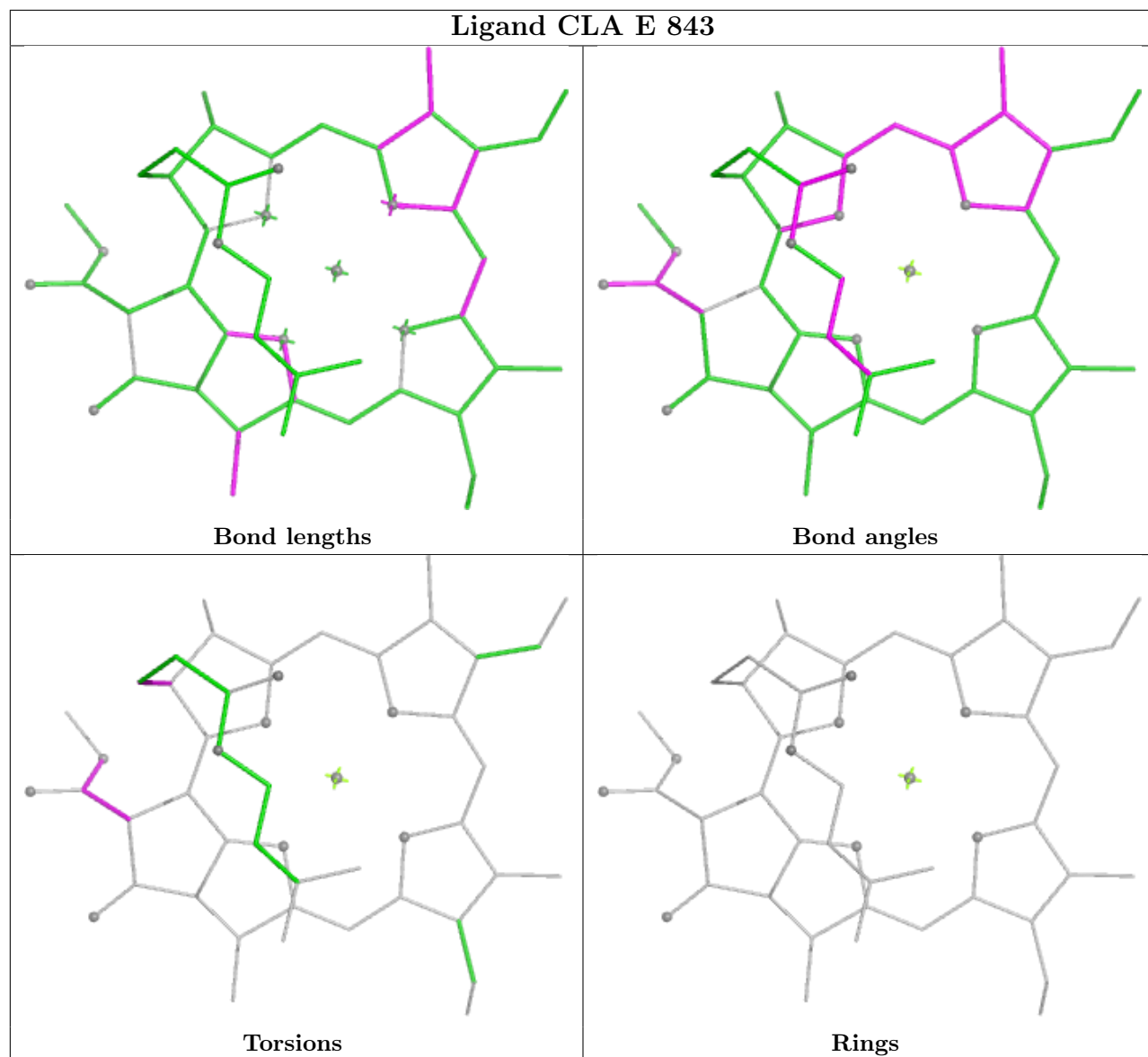


Torsions

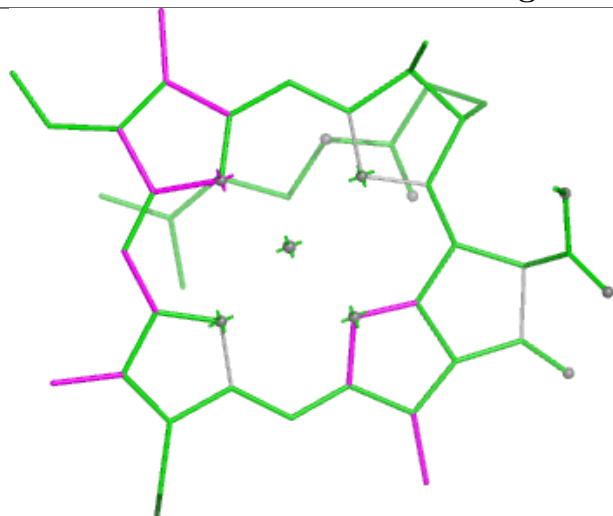


Rings

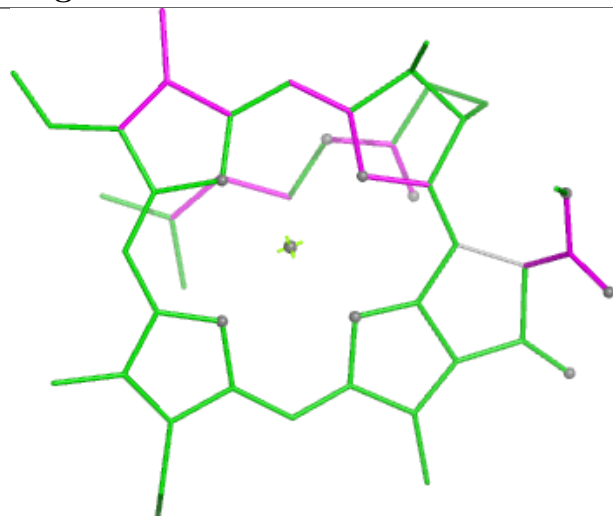
Ligand CLA E 843



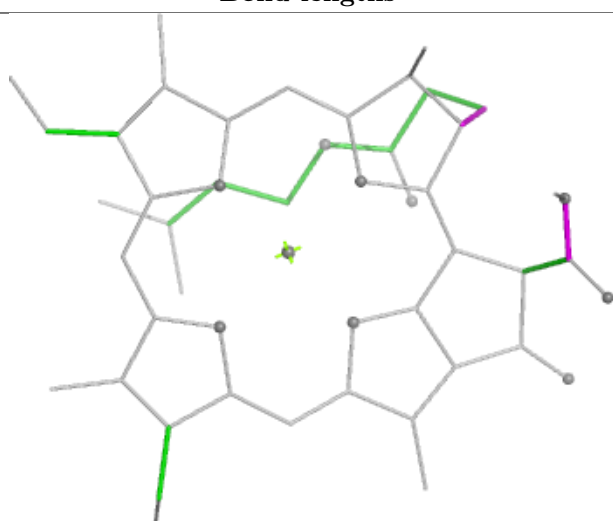
Ligand CLA g 811



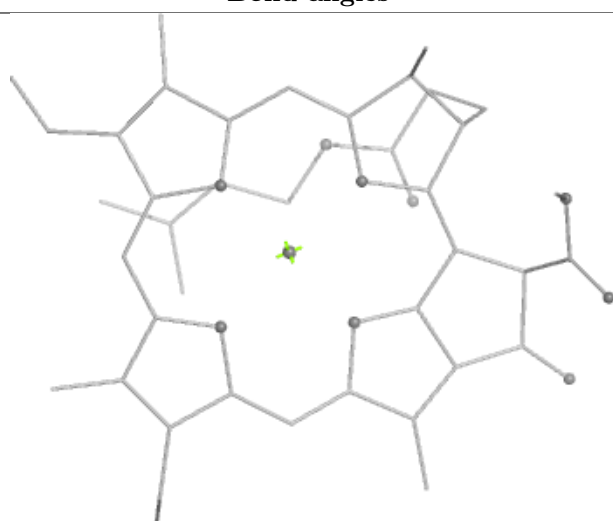
Bond lengths



Bond angles

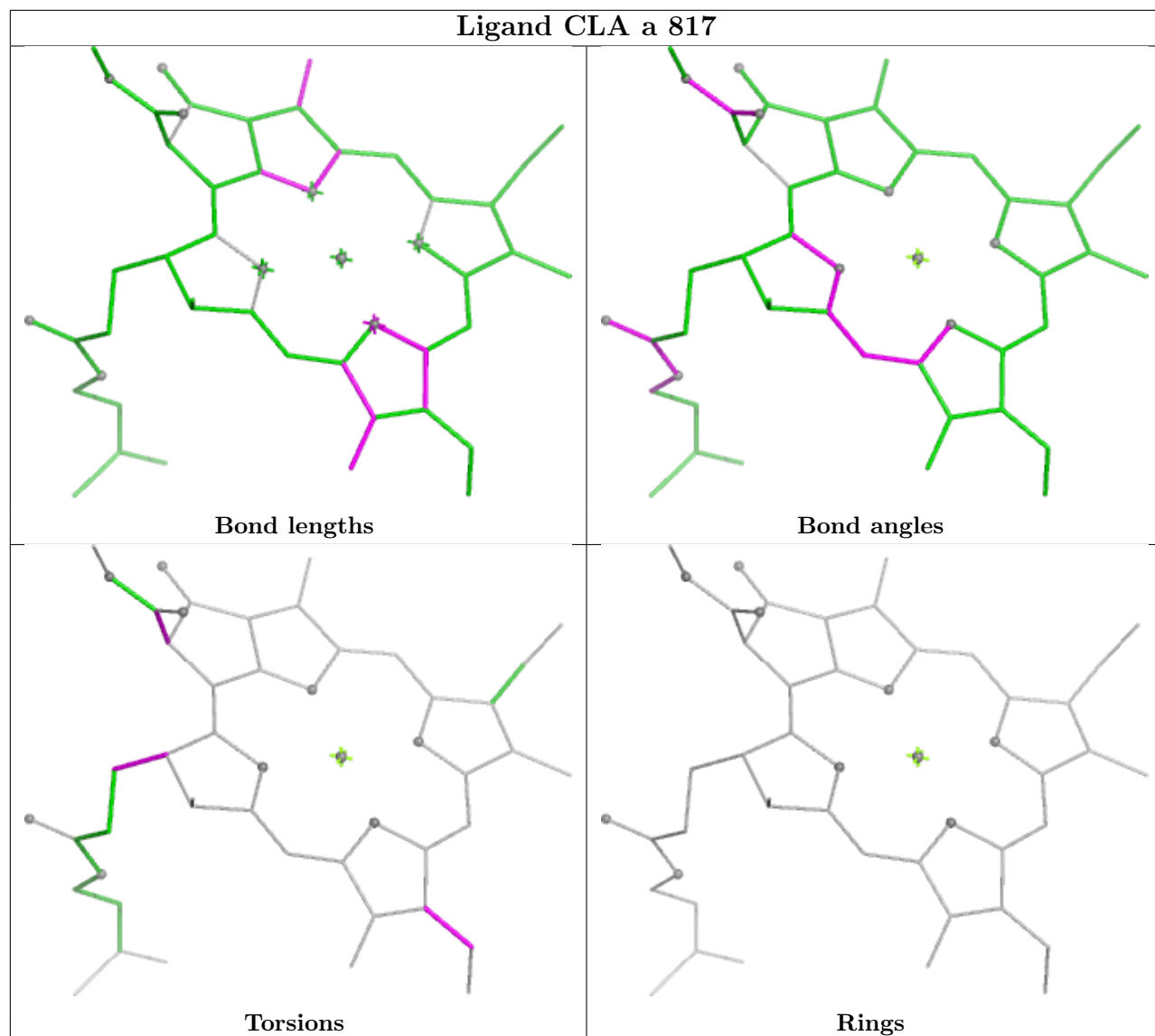


Torsions

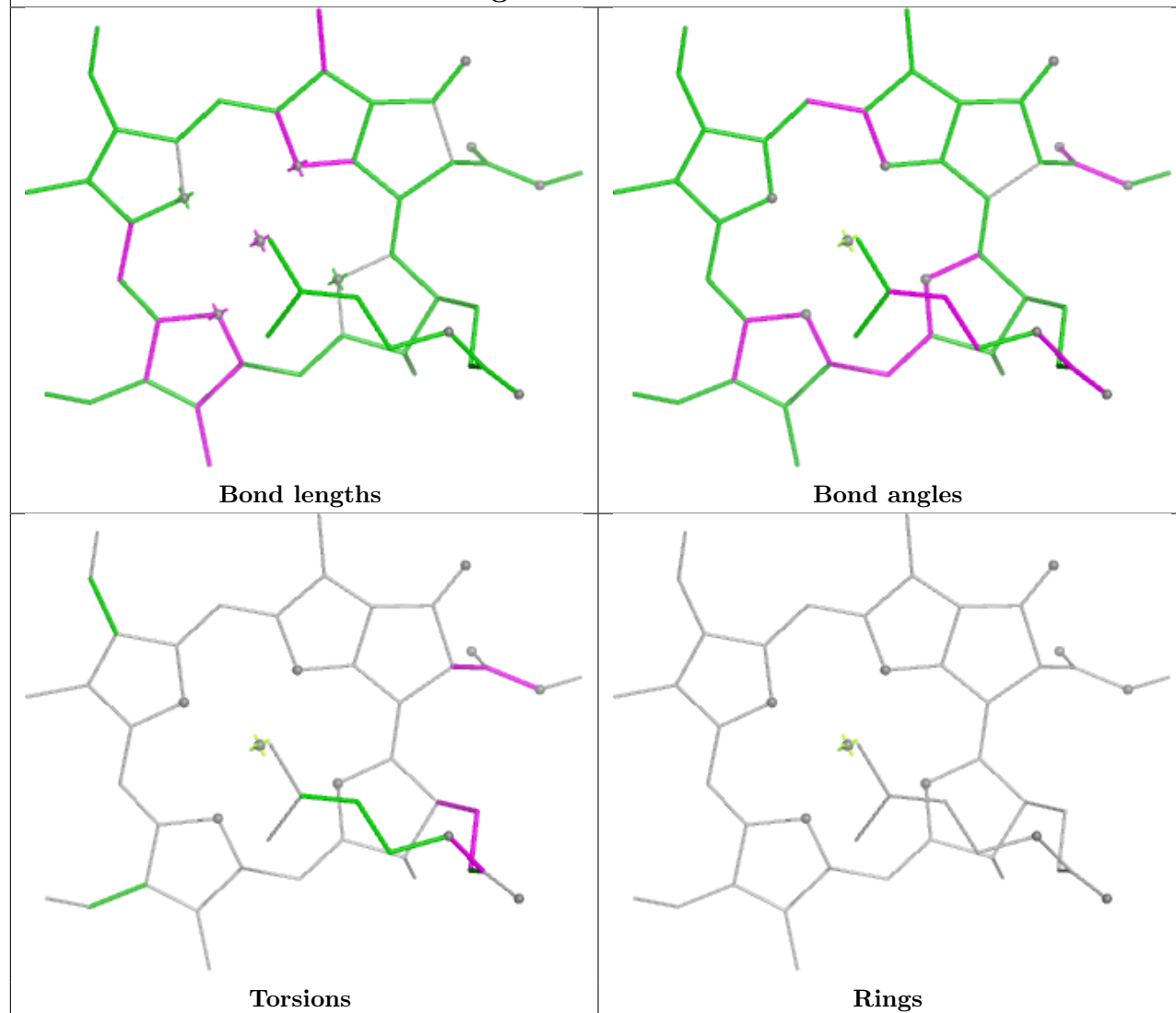


Rings

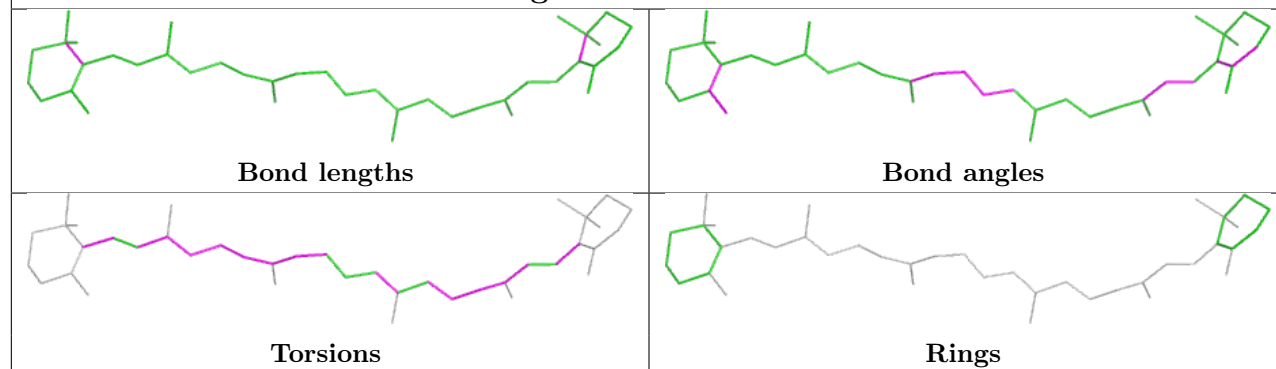
Ligand CLA a 817



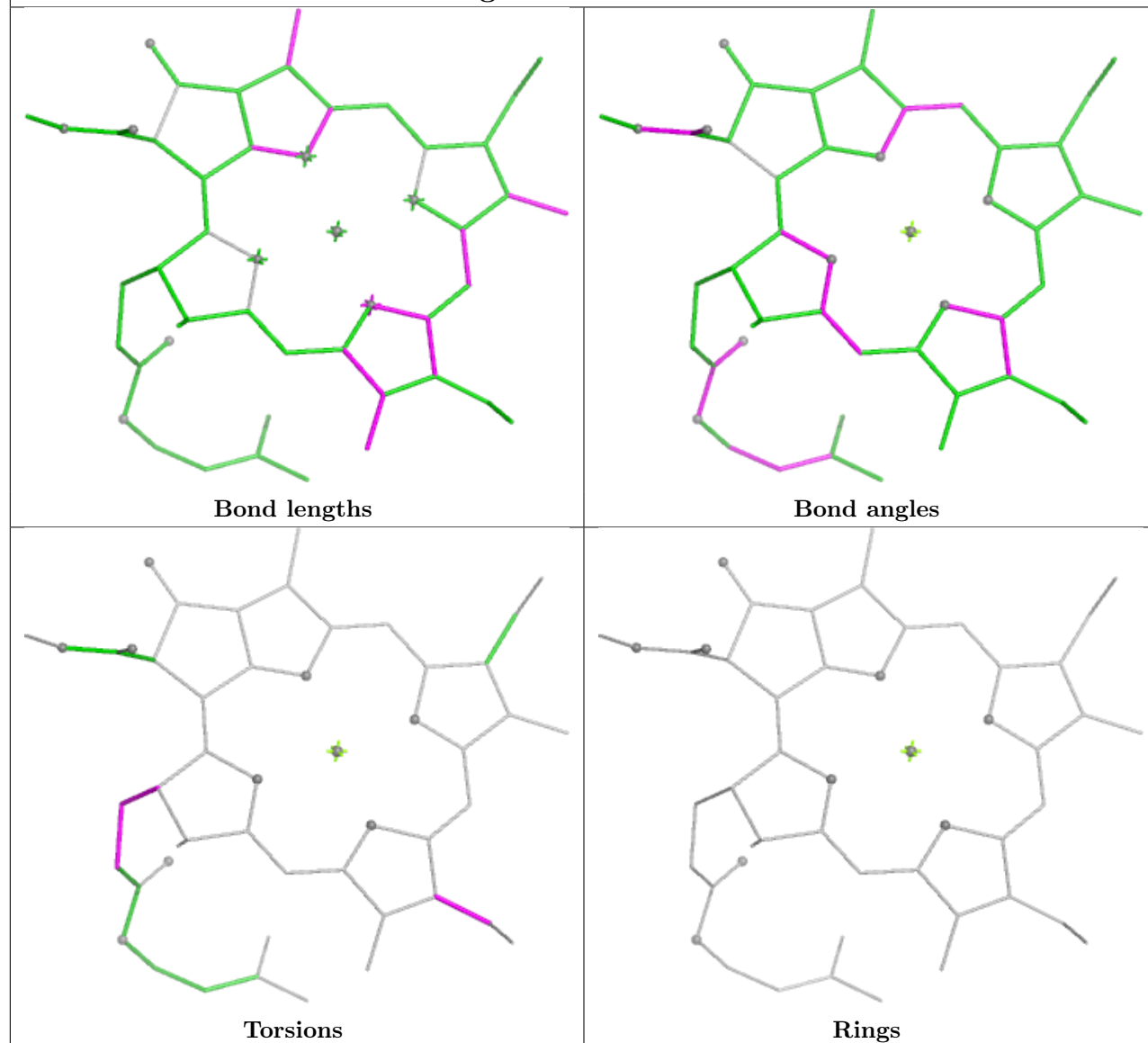
Ligand CLA E 821



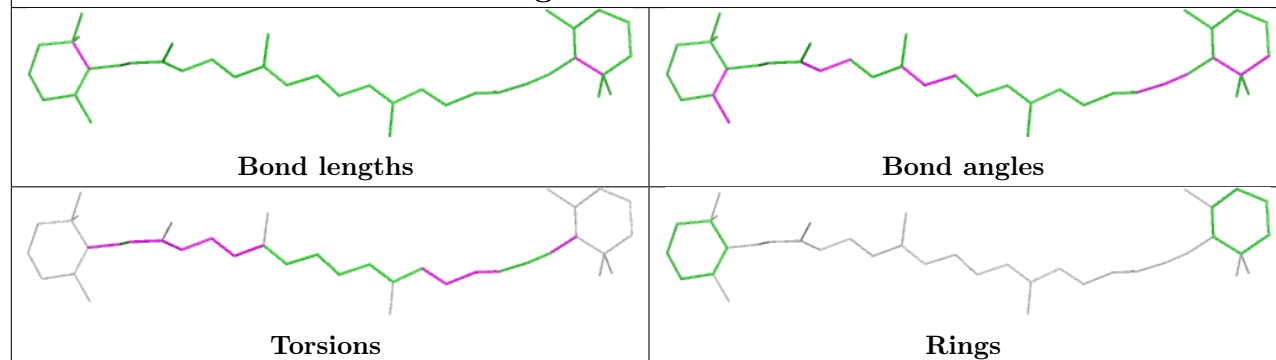
Ligand BCR B 846

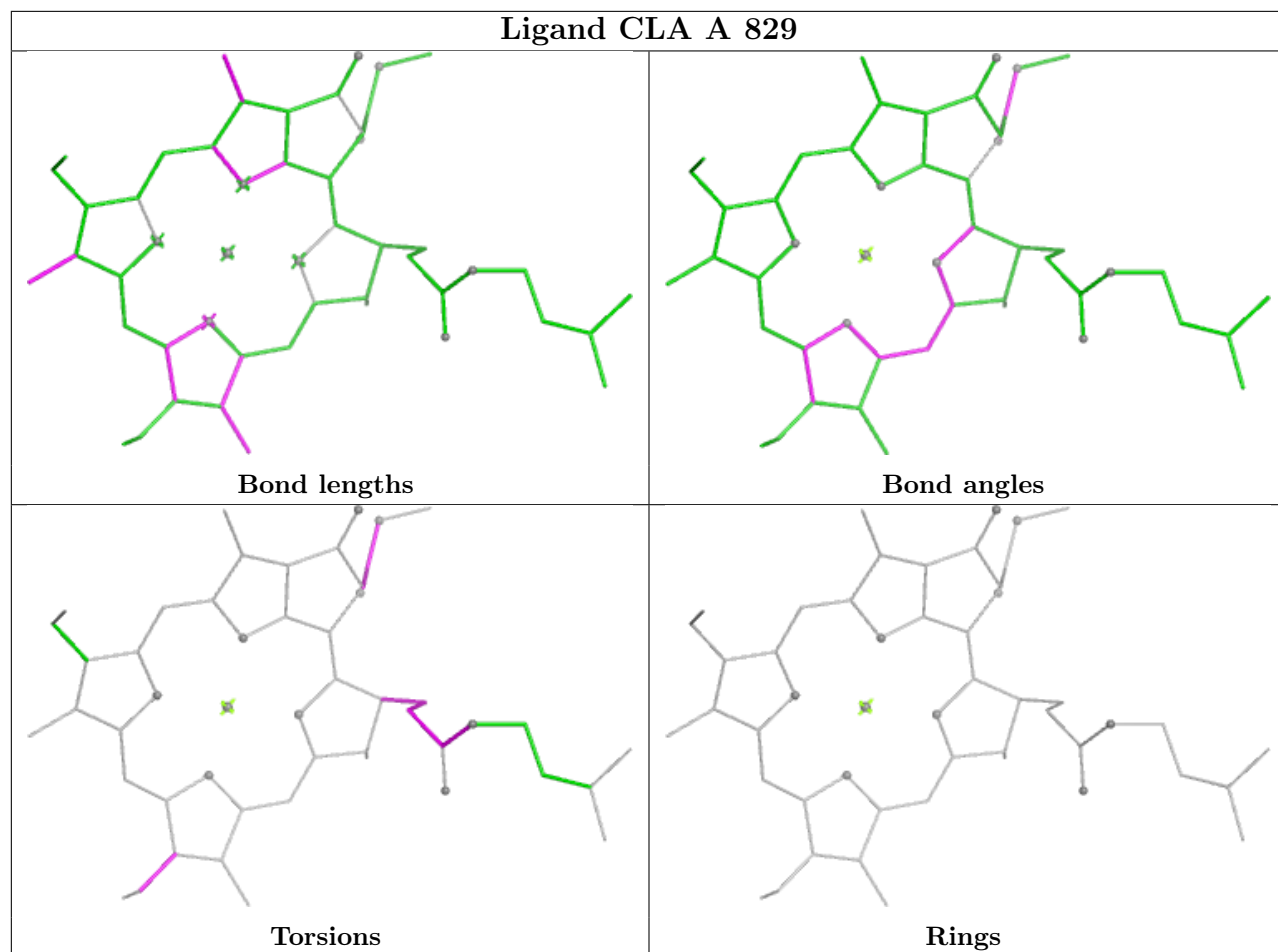


Ligand CLA E 811

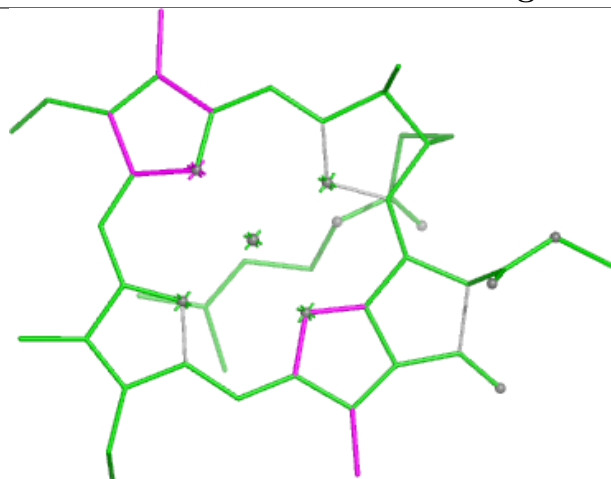


Ligand BCR a 850

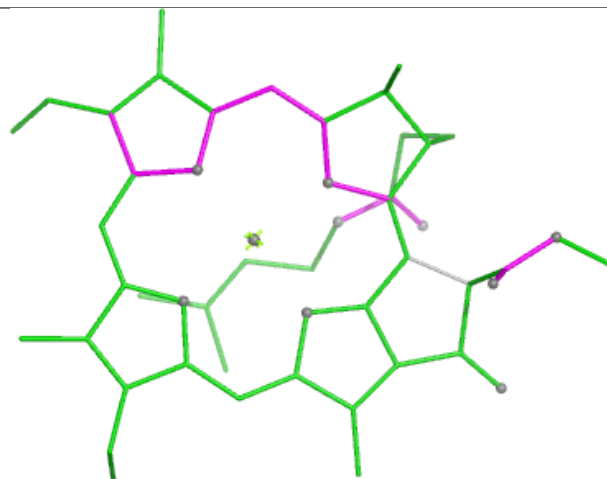




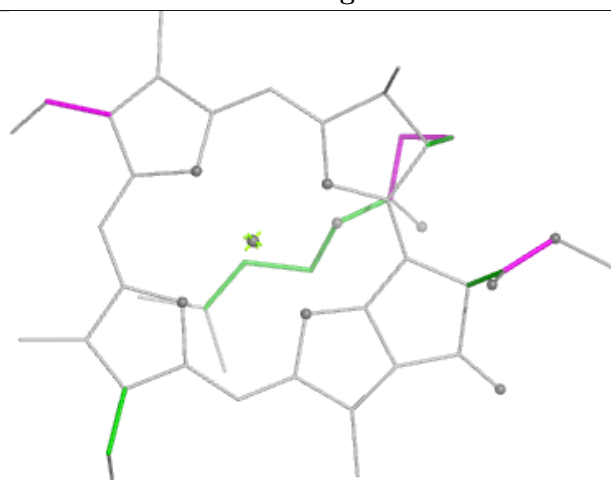
Ligand CLA b 808



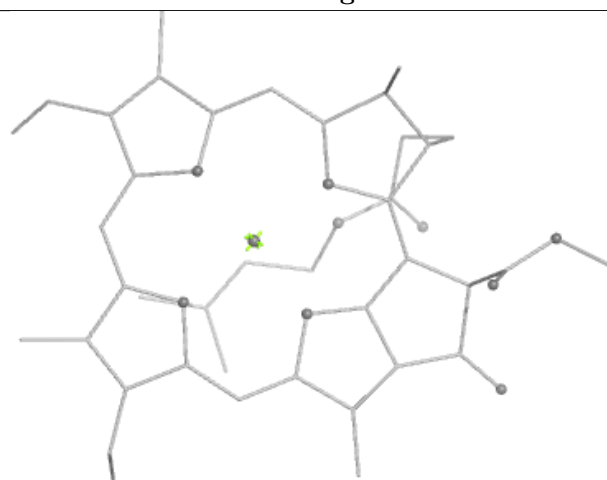
Bond lengths



Bond angles

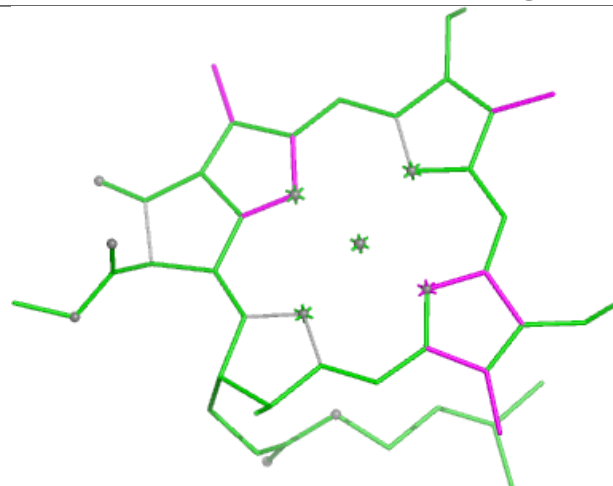


Torsions

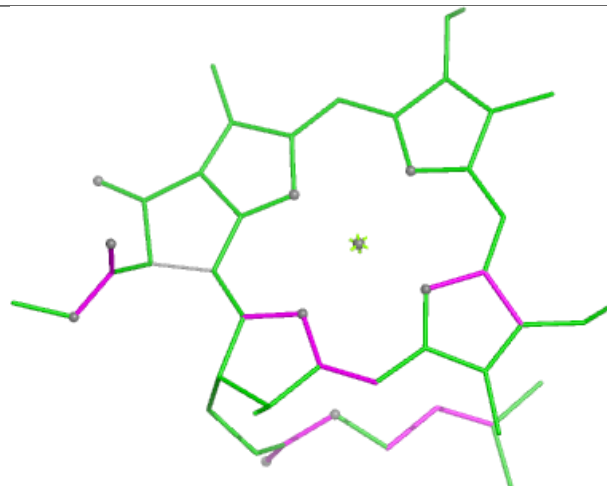


Rings

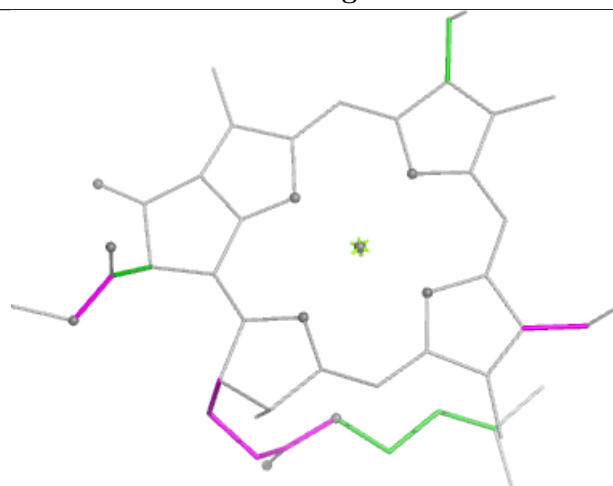
Ligand CLA a 822



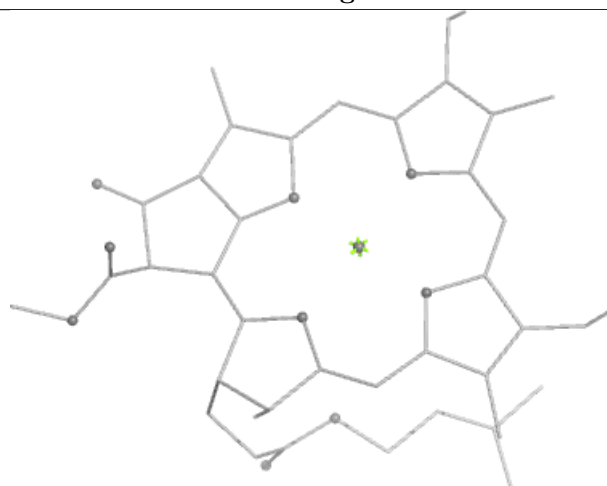
Bond lengths



Bond angles

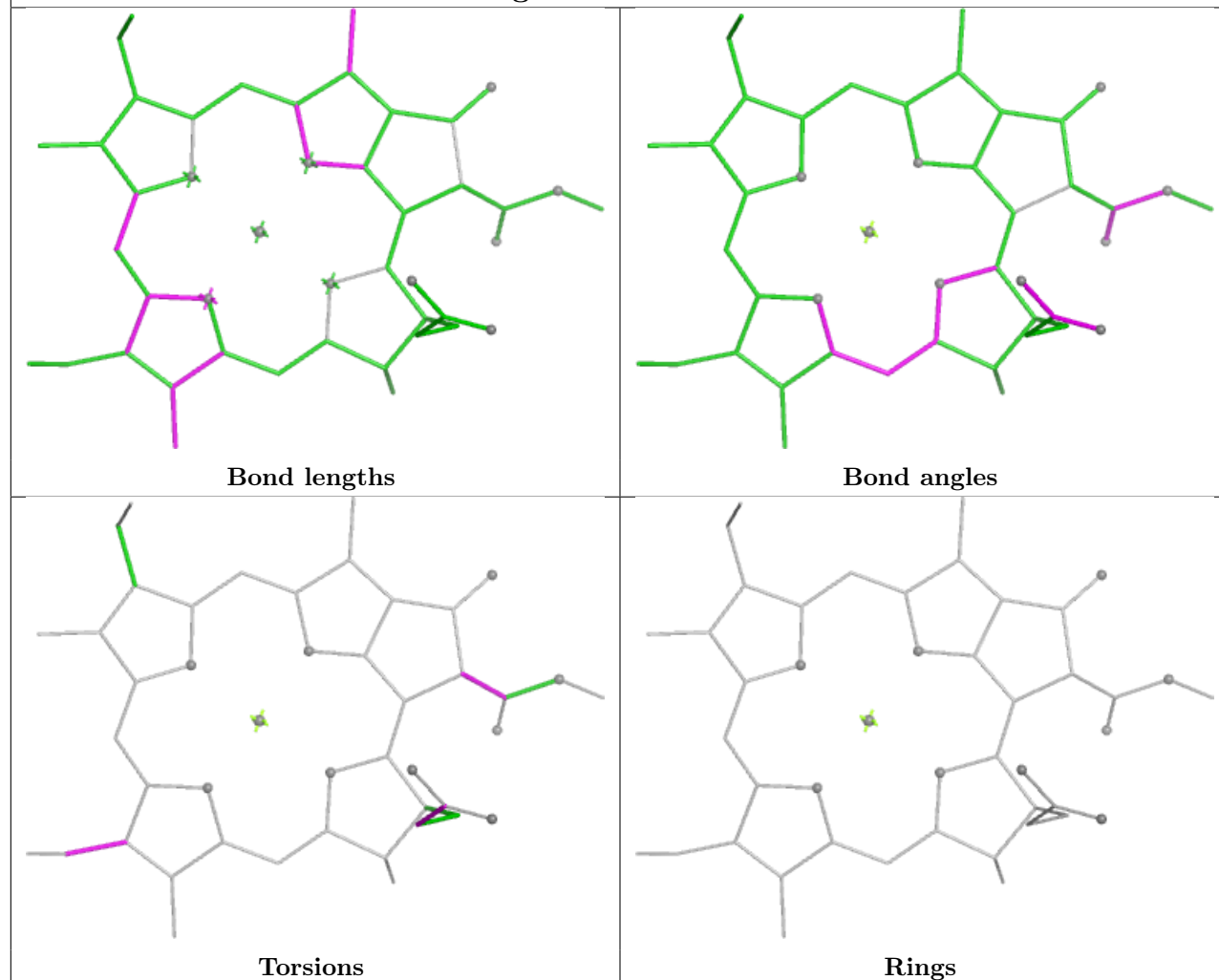


Torsions

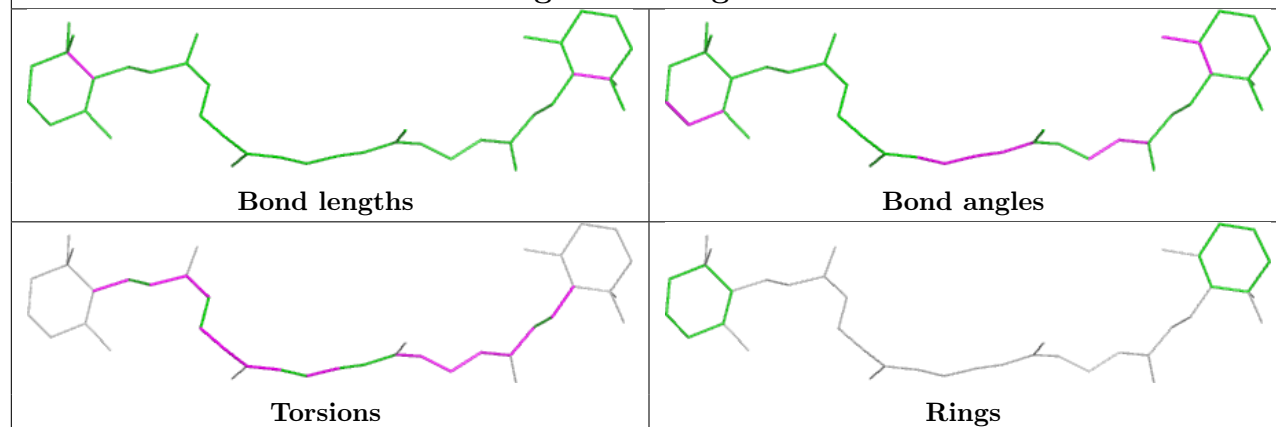


Rings

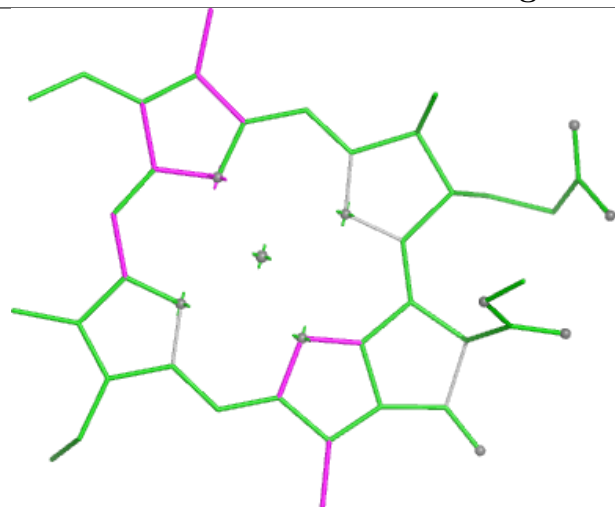
Ligand CLA a 814



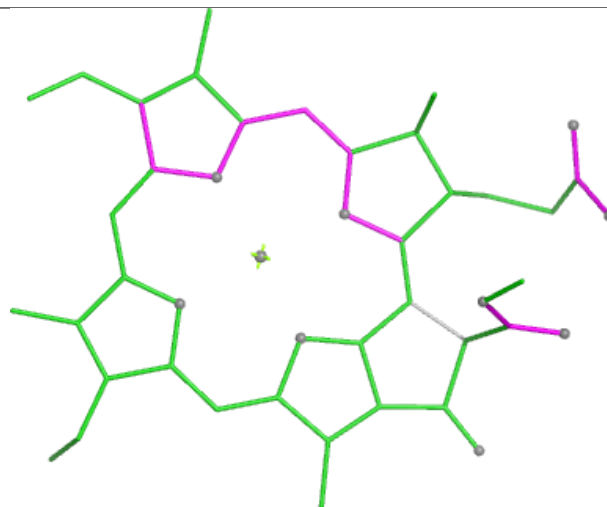
Ligand BCR g 845



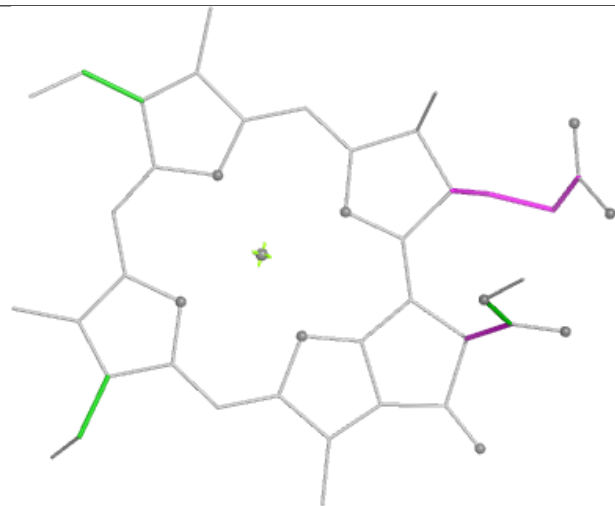
Ligand CLA b 834



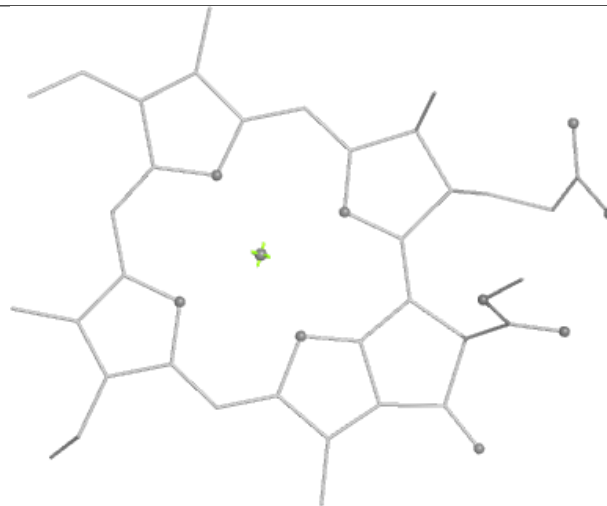
Bond lengths



Bond angles

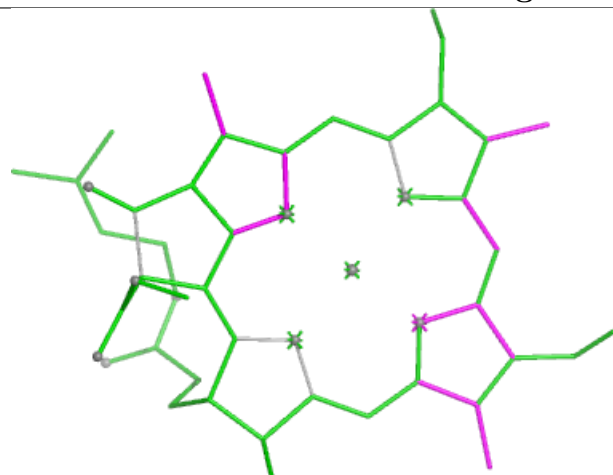


Torsions

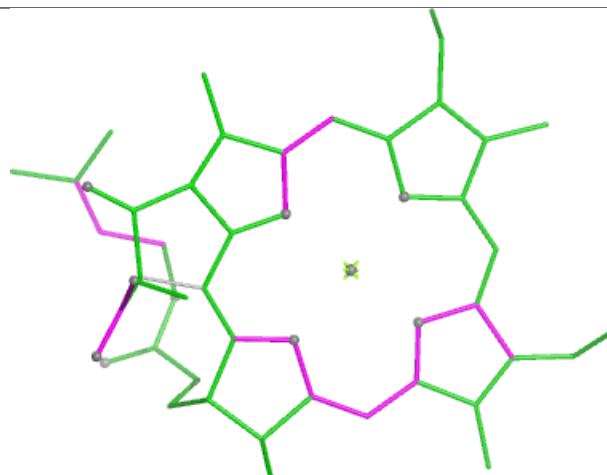


Rings

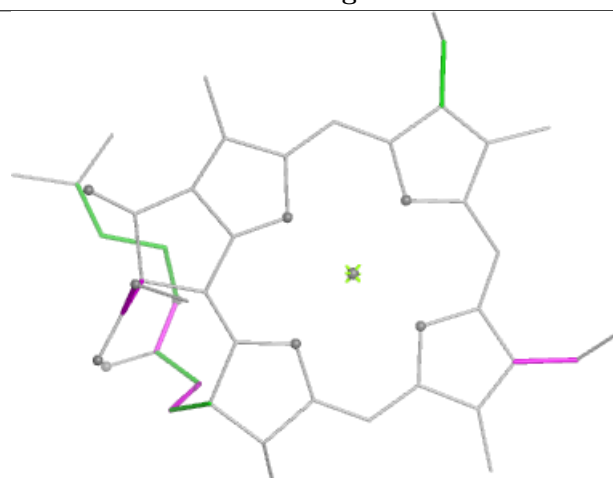
Ligand CLA A 810



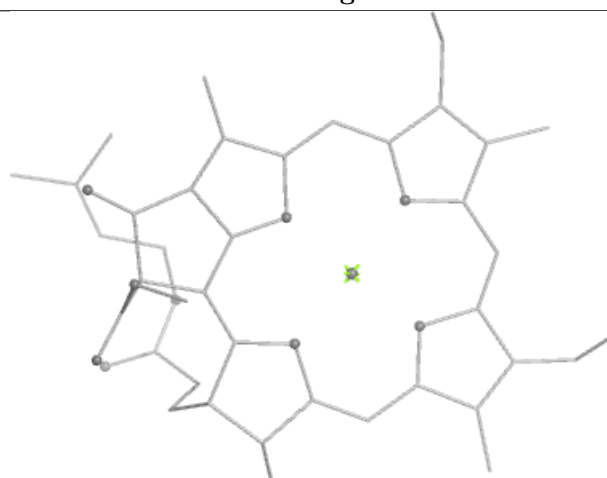
Bond lengths



Bond angles

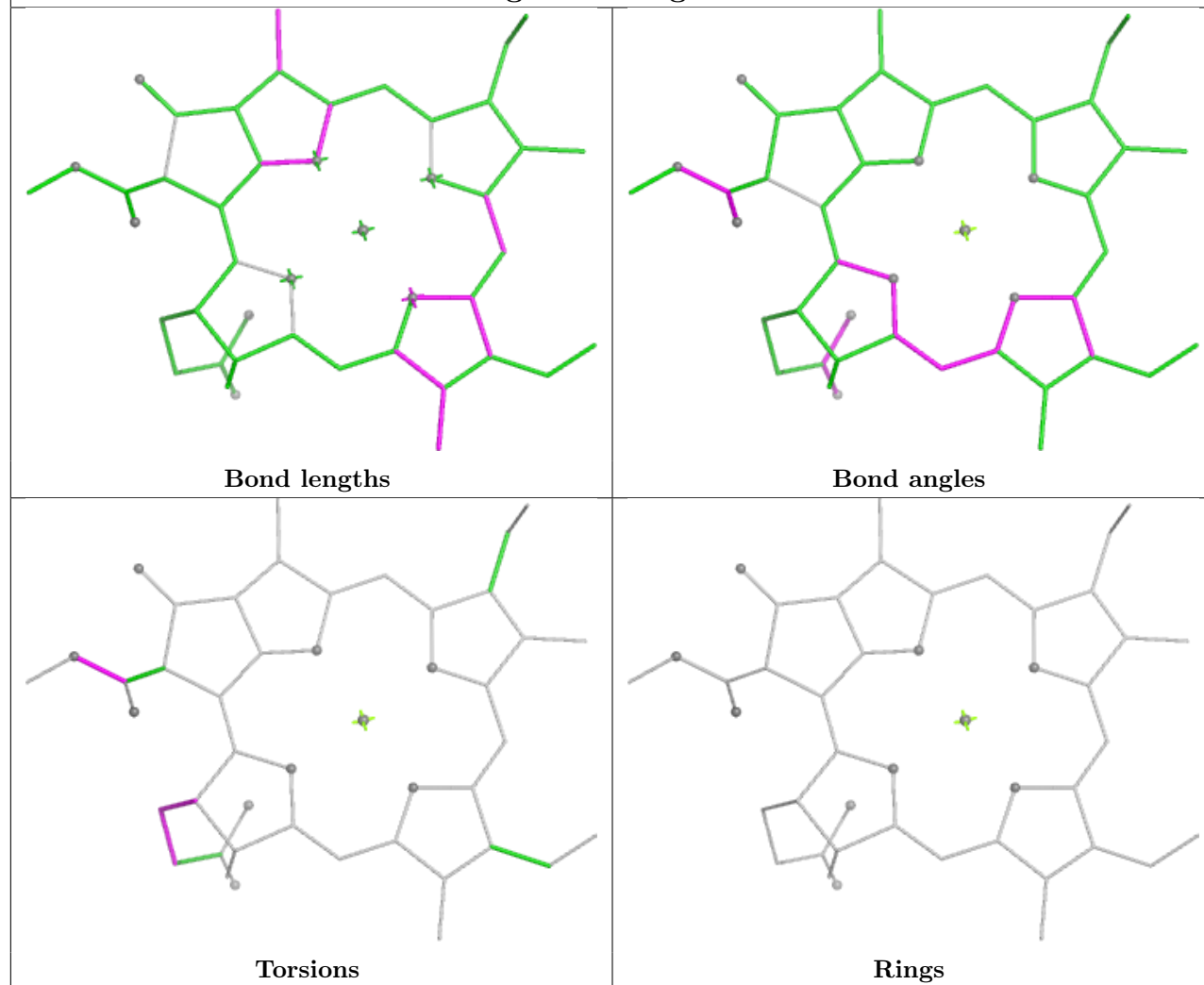


Torsions

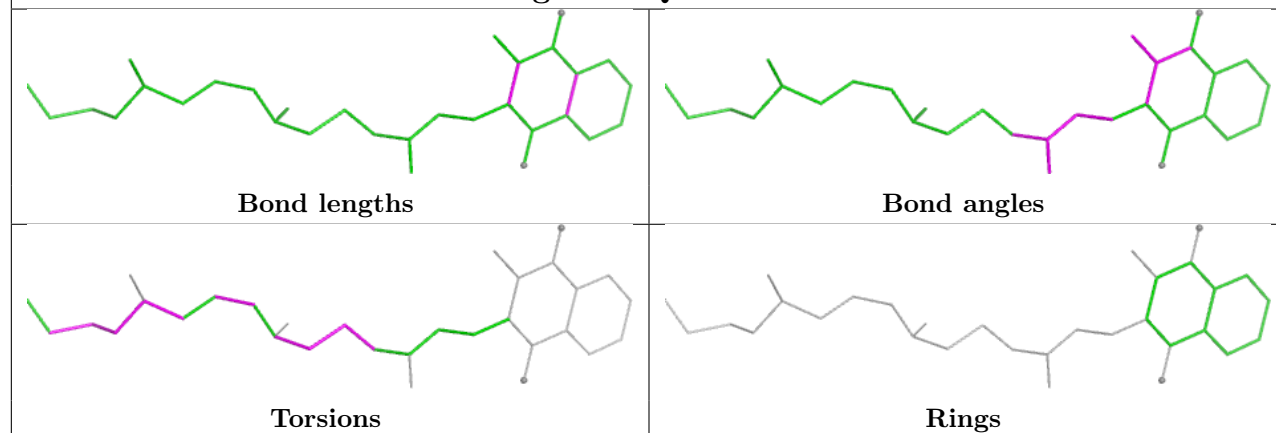


Rings

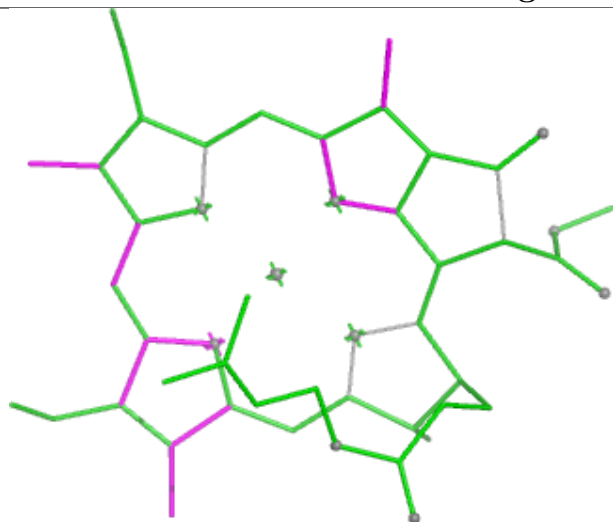
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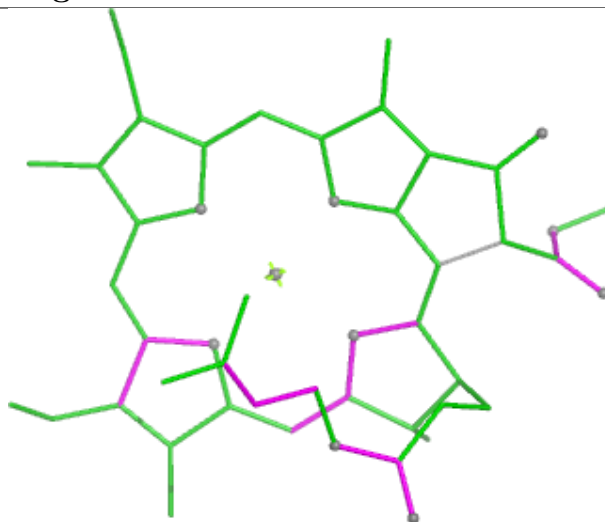
Ligand PQN b 841



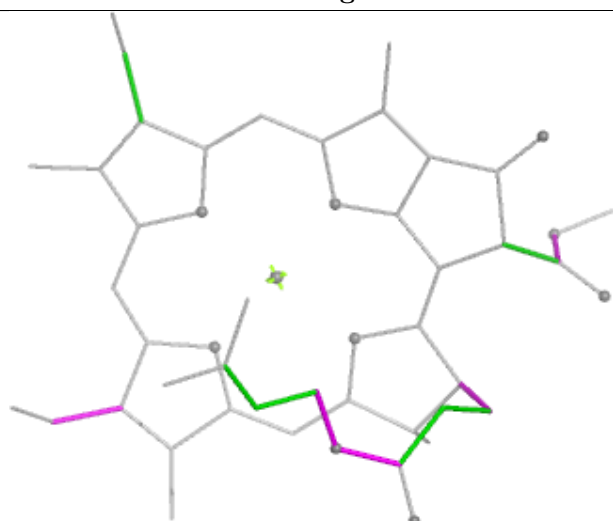
Ligand CLA g 829



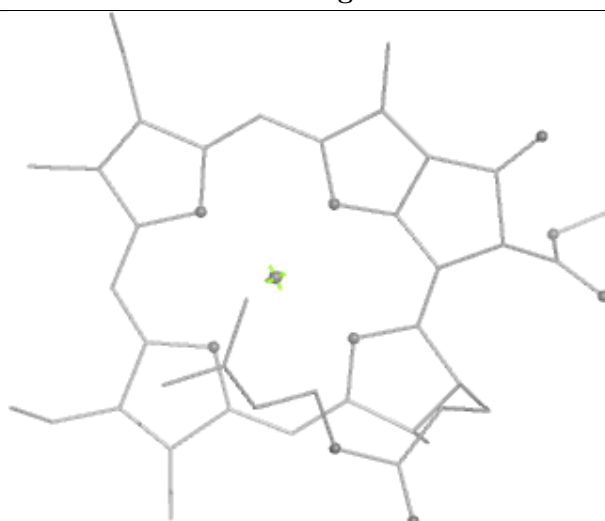
Bond lengths



Bond angles

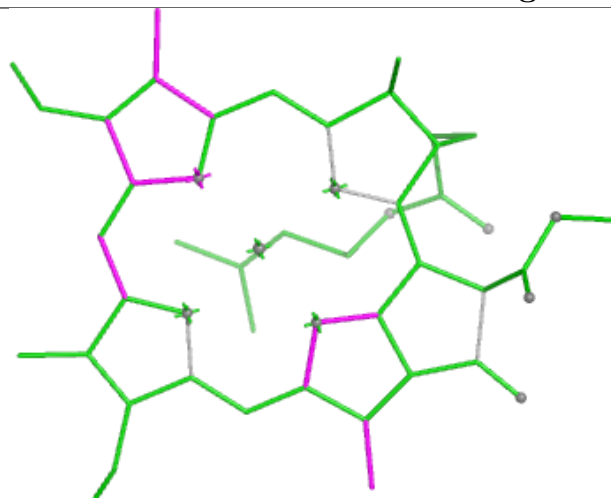


Torsions

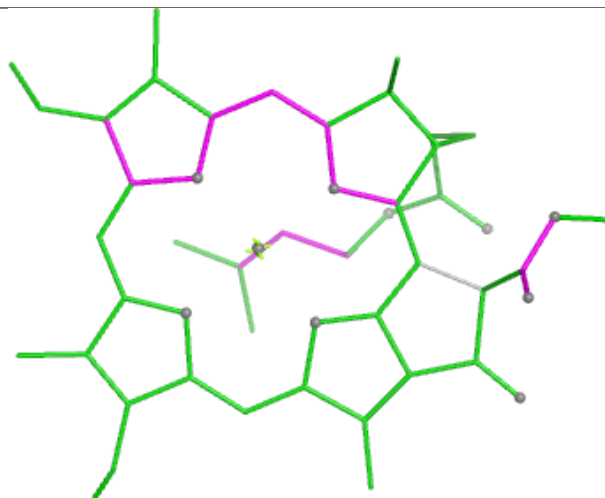


Rings

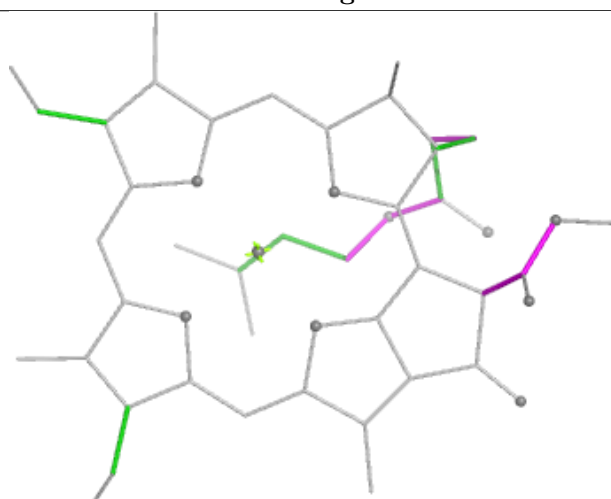
Ligand CLA e 814



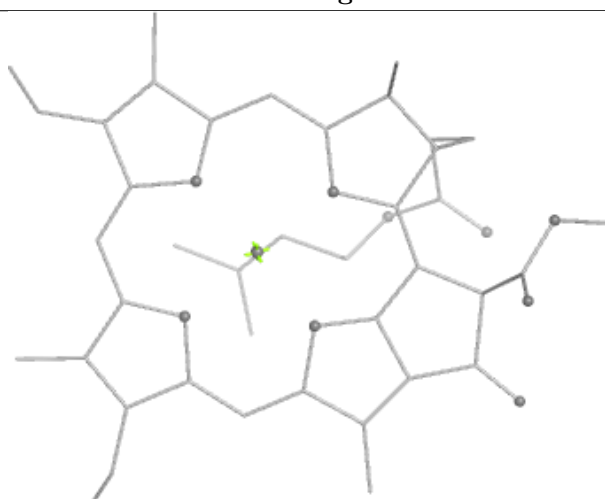
Bond lengths



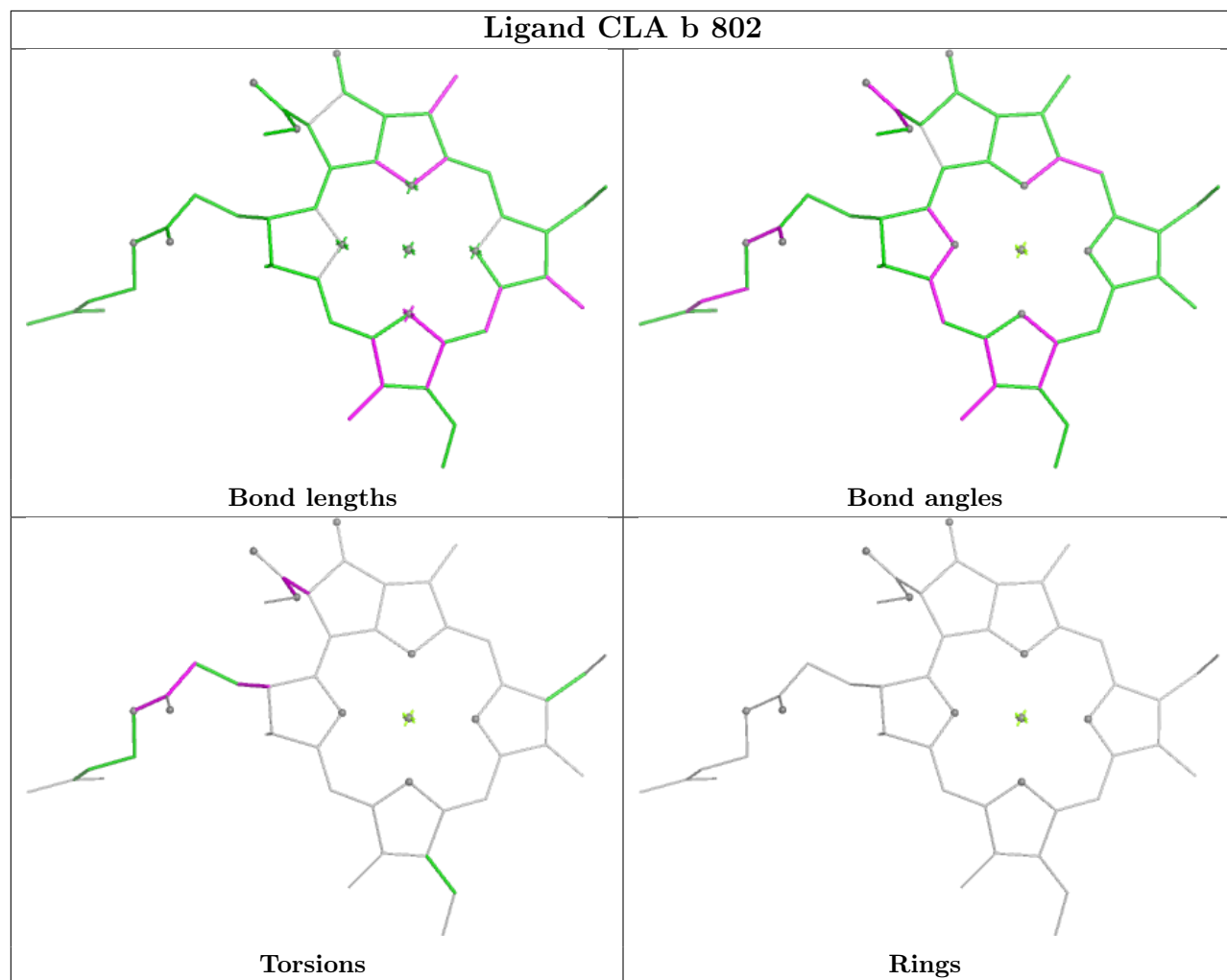
Bond angles



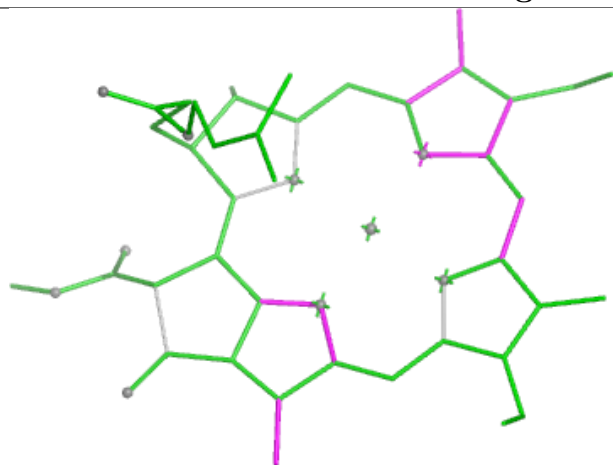
Torsions



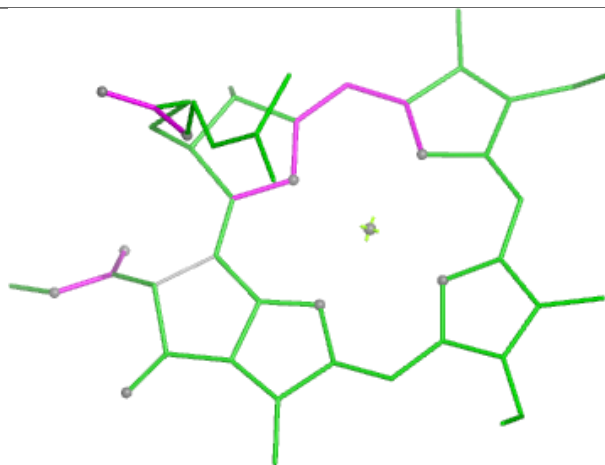
Rings



Ligand CLA E 814



Bond lengths



Bond angles

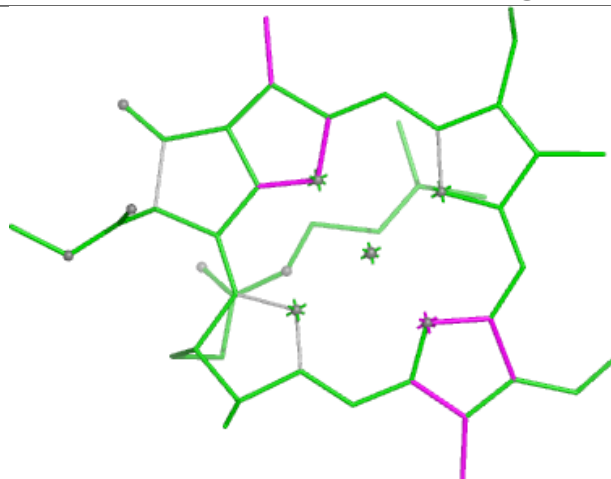


Torsions

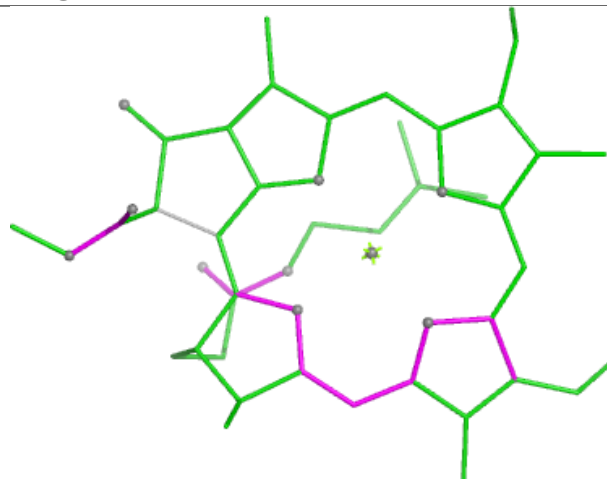


Rings

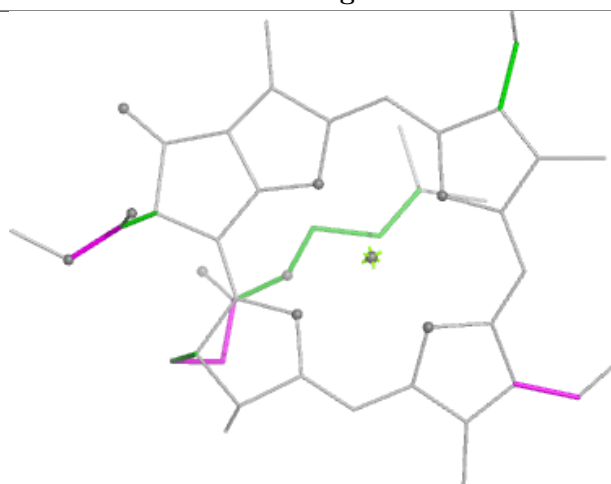
Ligand CLA g 810



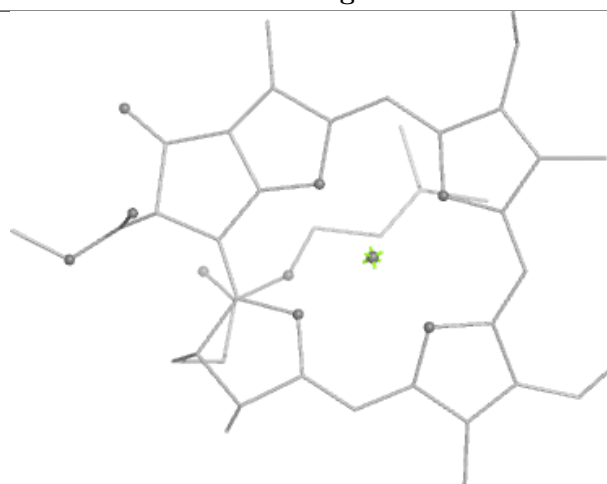
Bond lengths



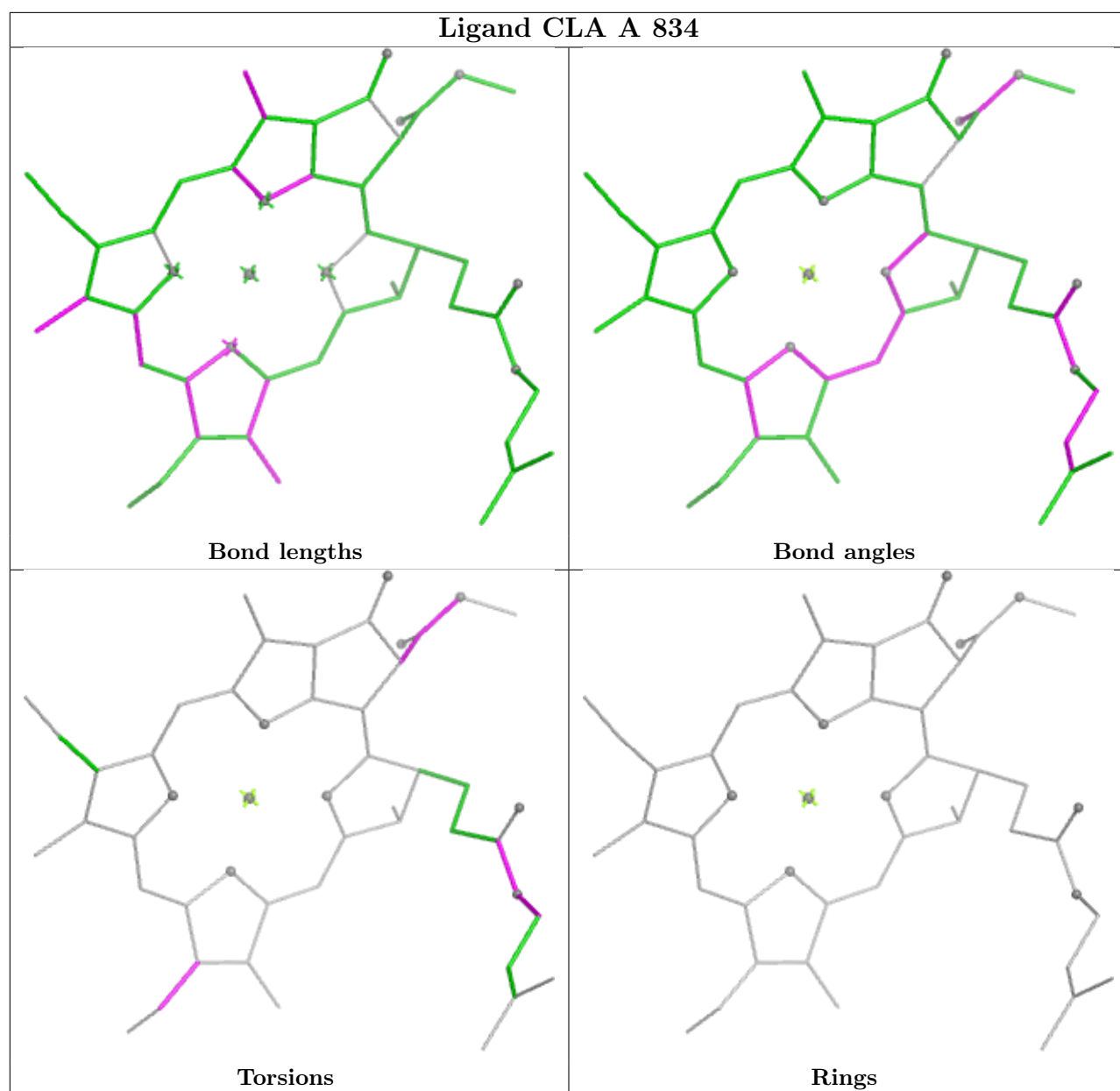
Bond angles



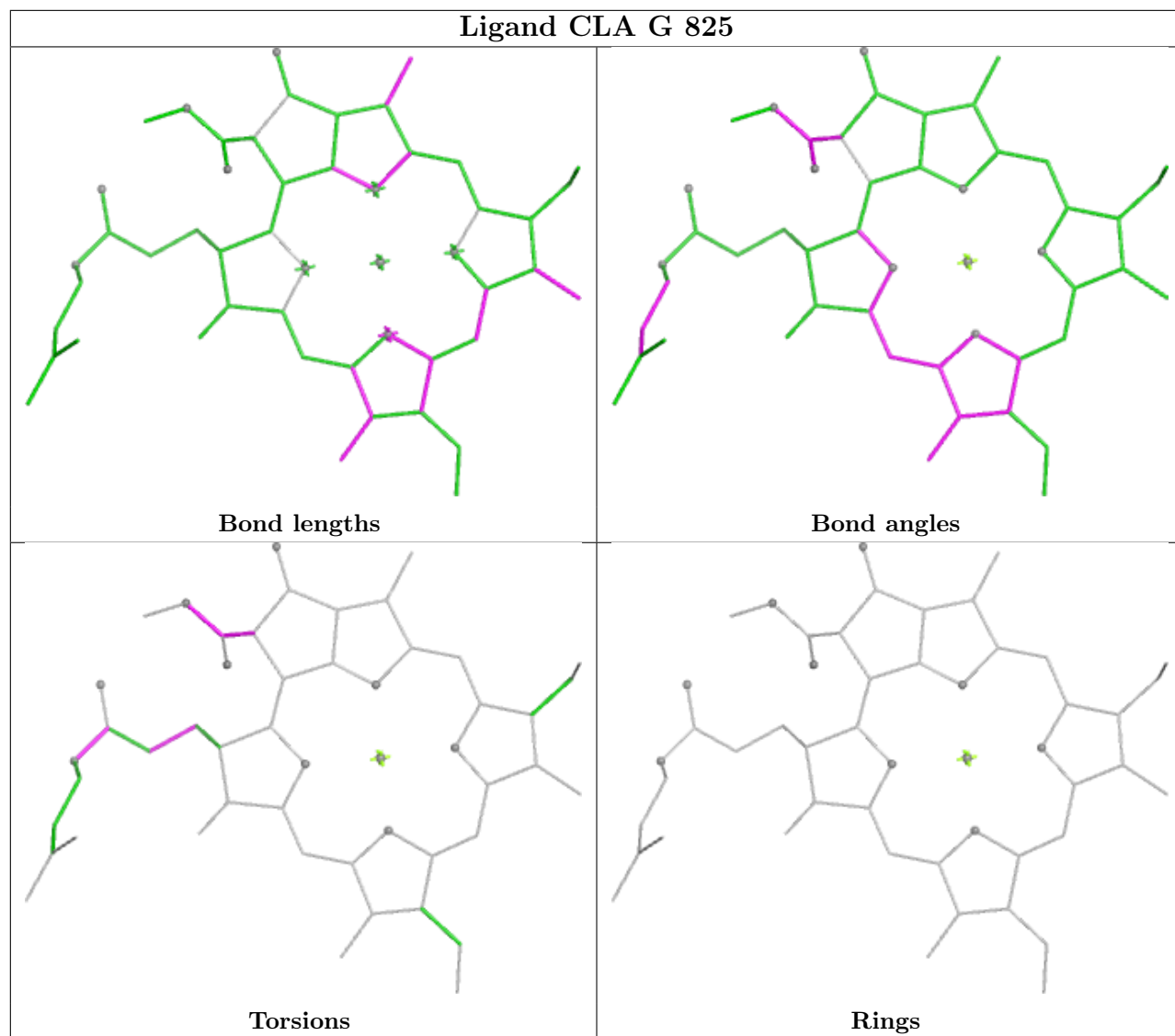
Torsions



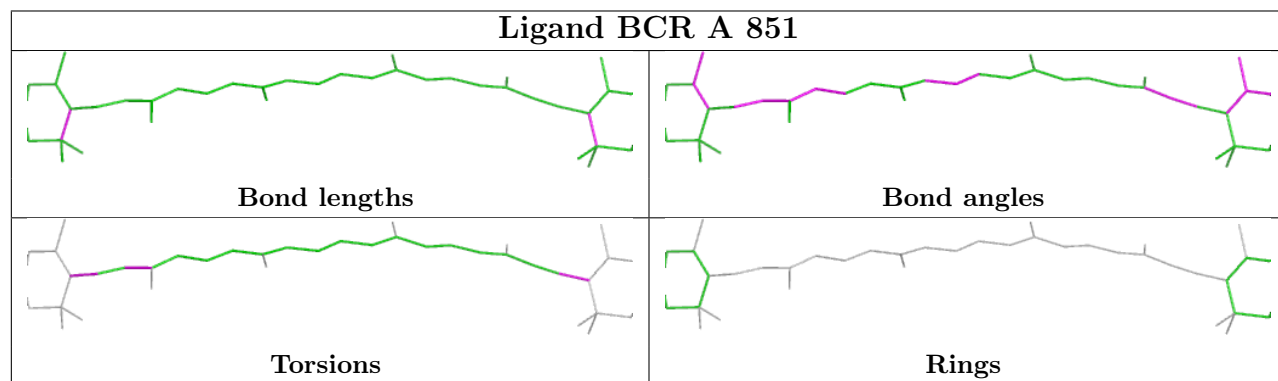
Rings



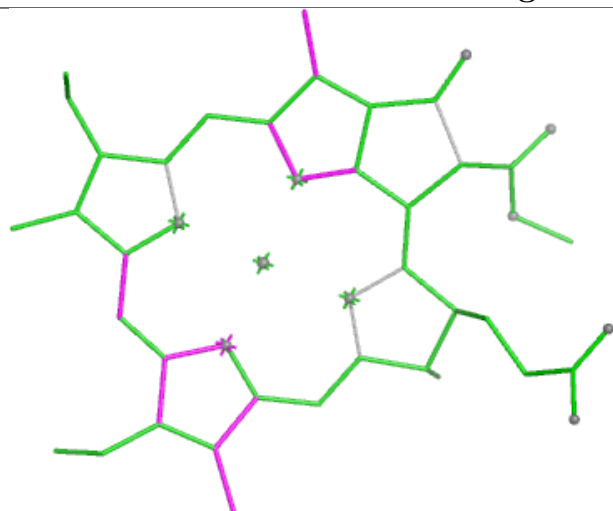
Ligand CLA G 825



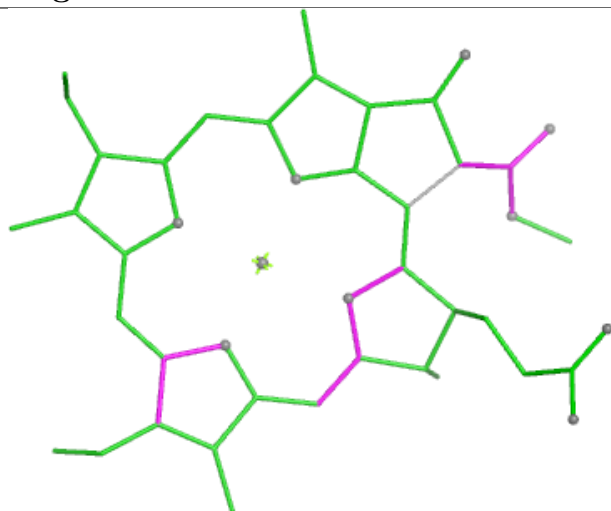
Ligand BCR A 851



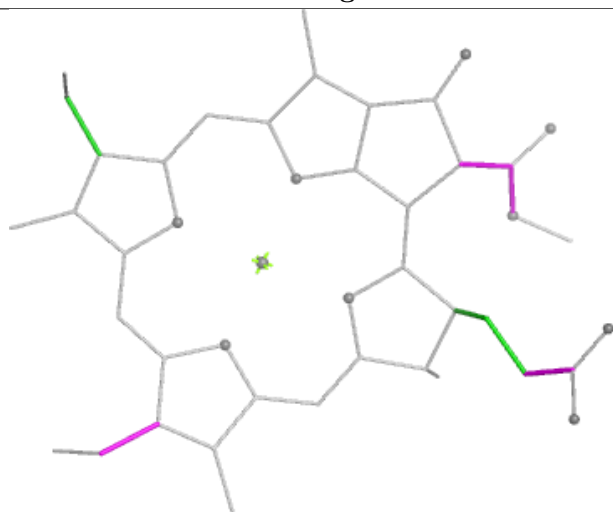
Ligand CLA g 825



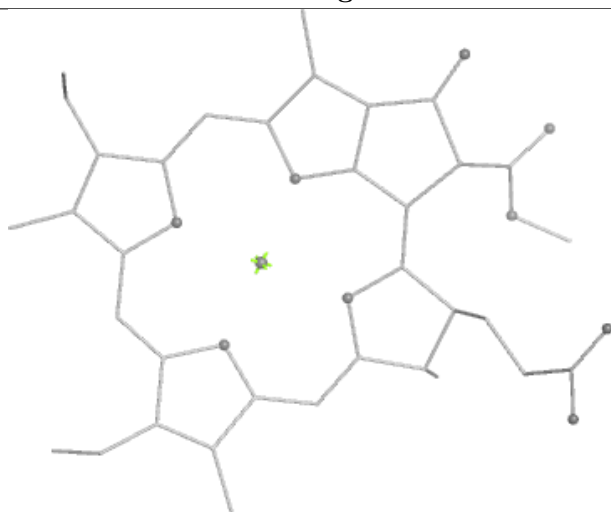
Bond lengths



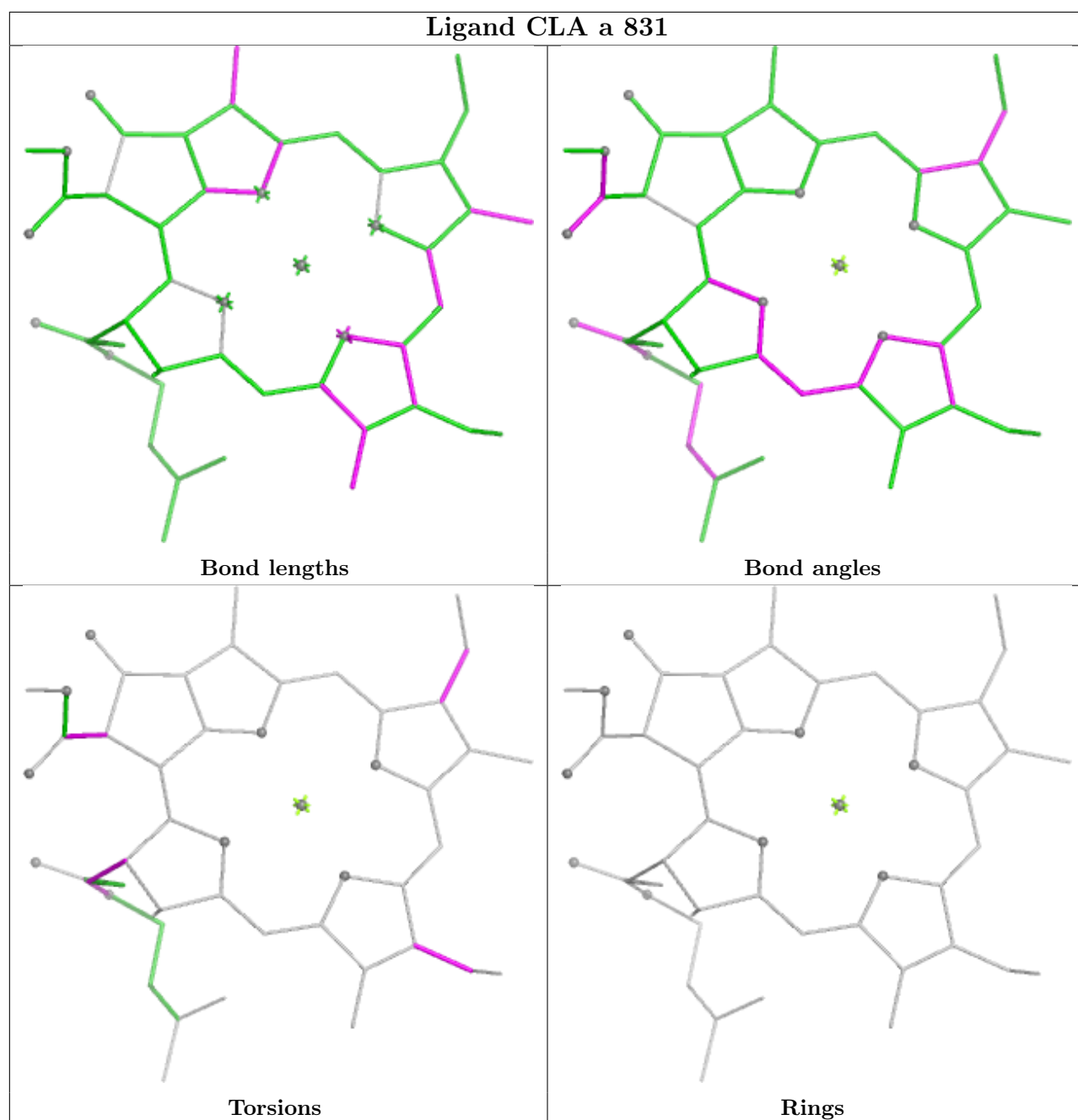
Bond angles

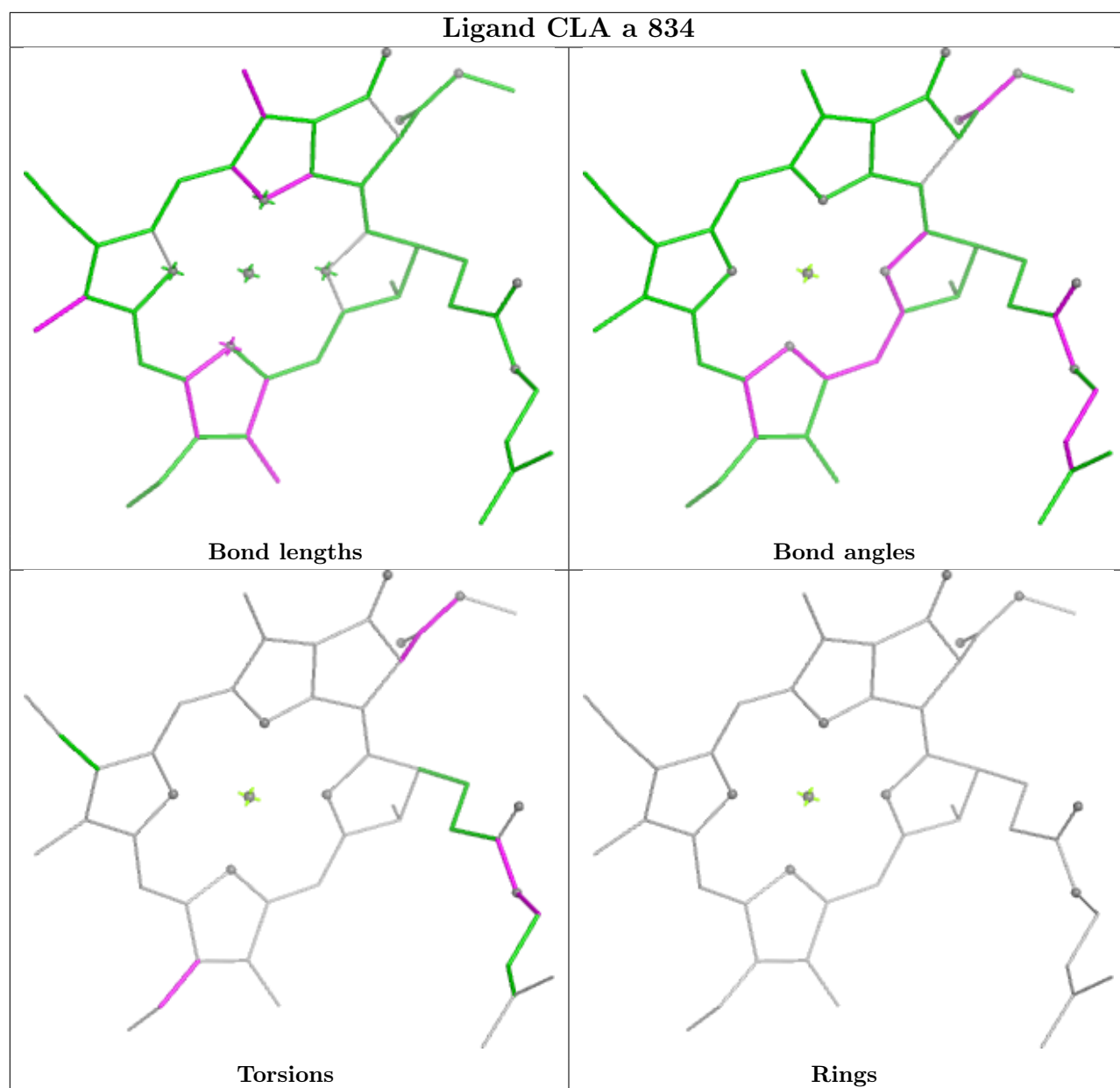


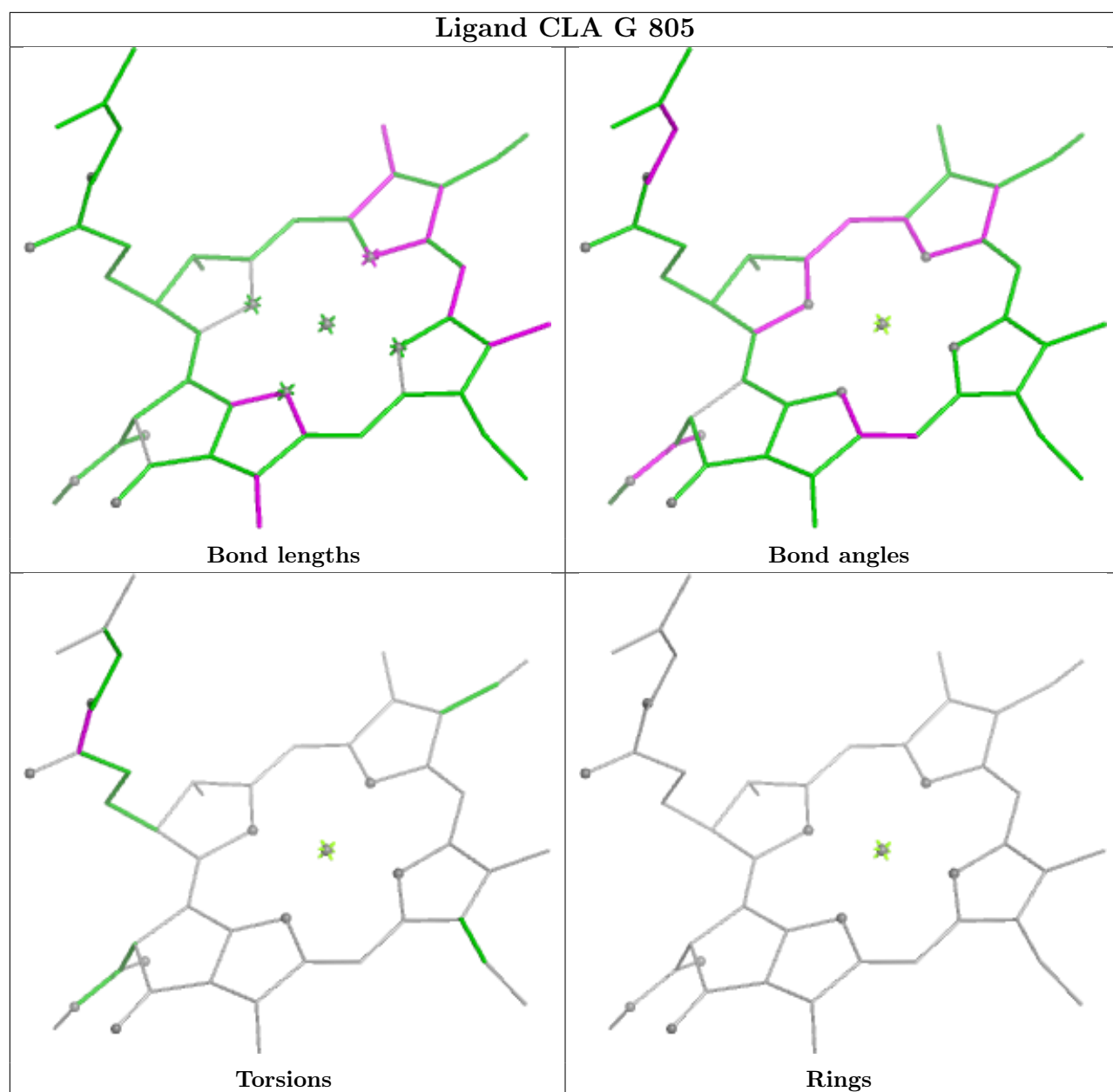
Torsions



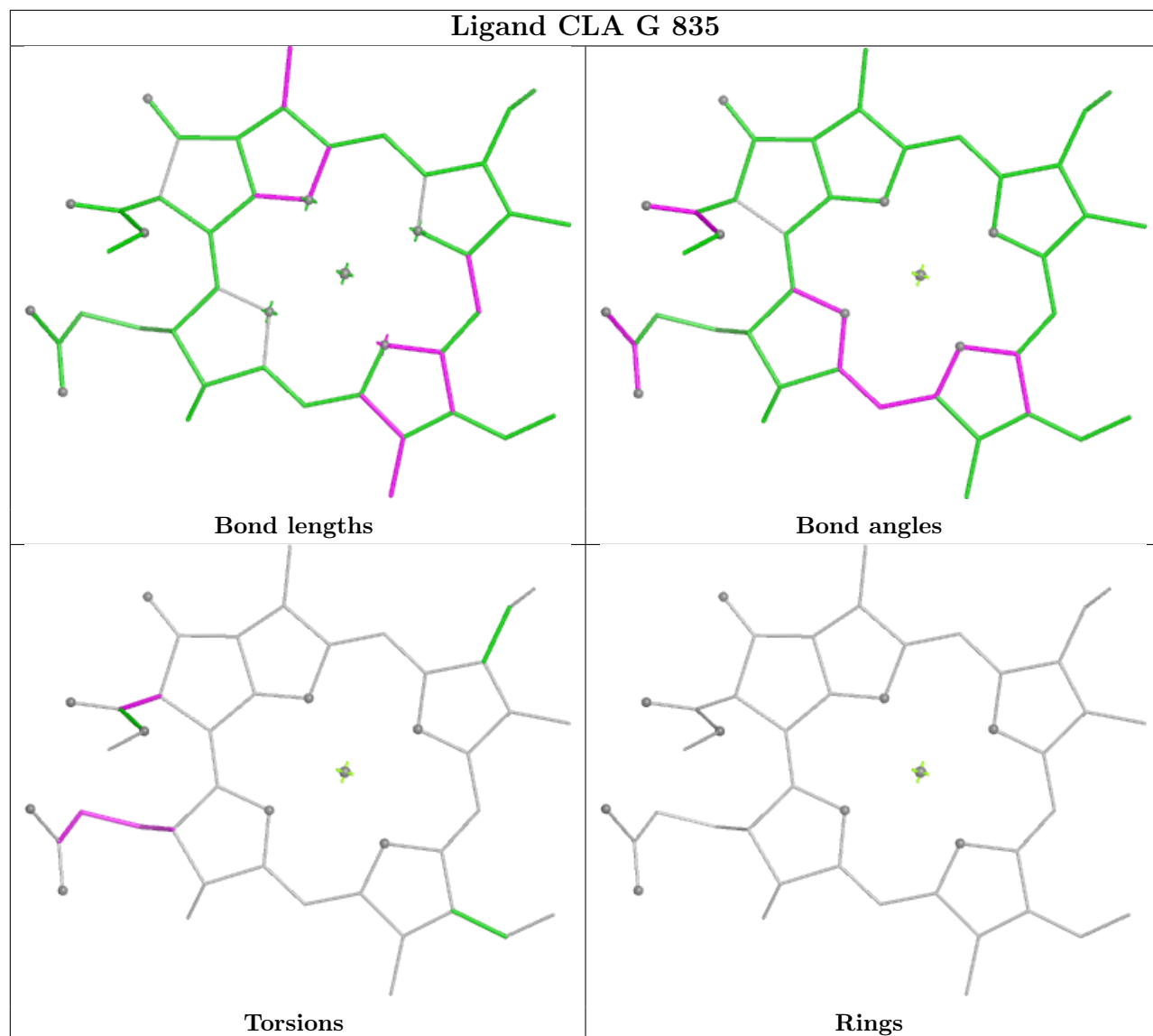
Rings

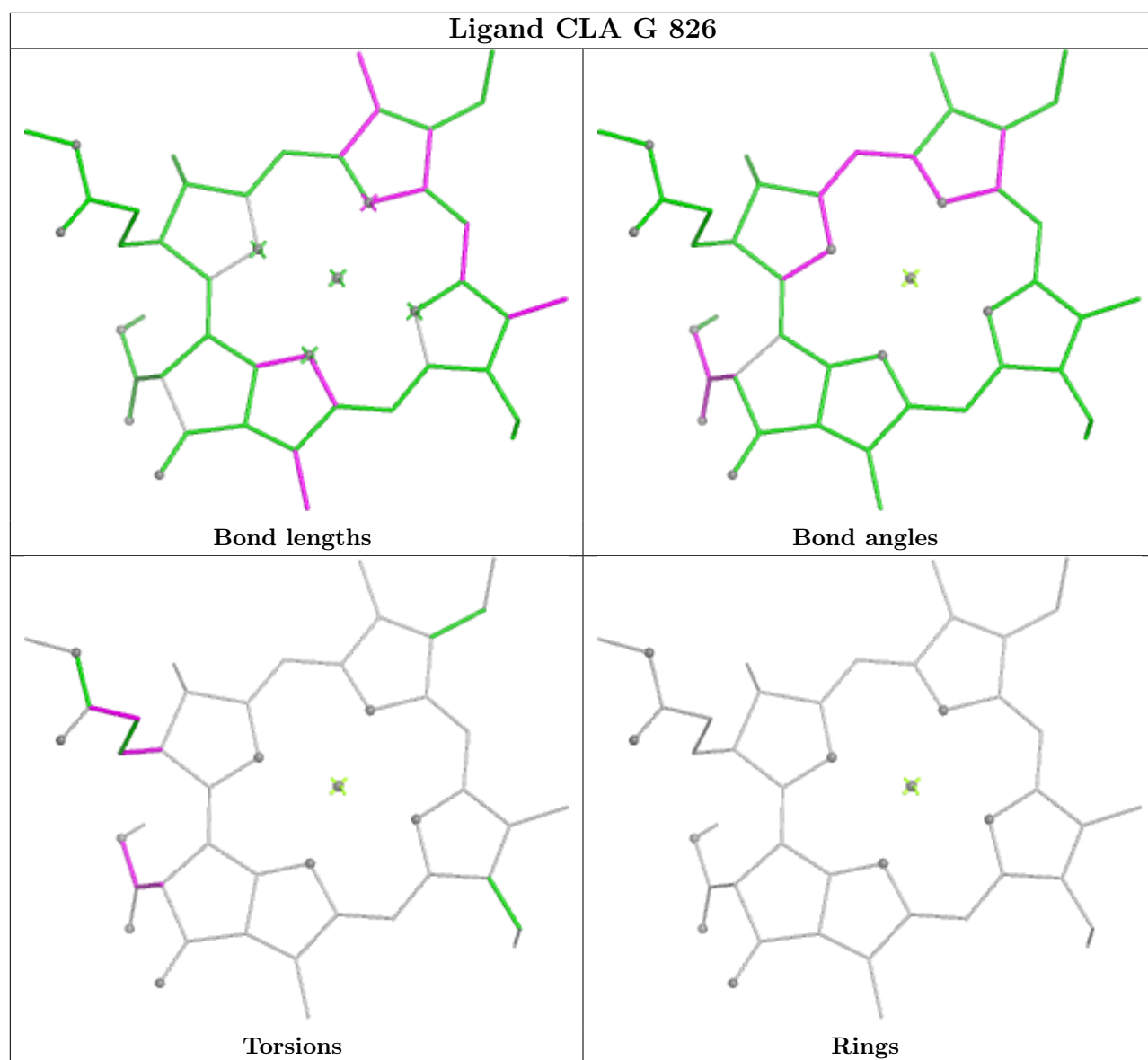


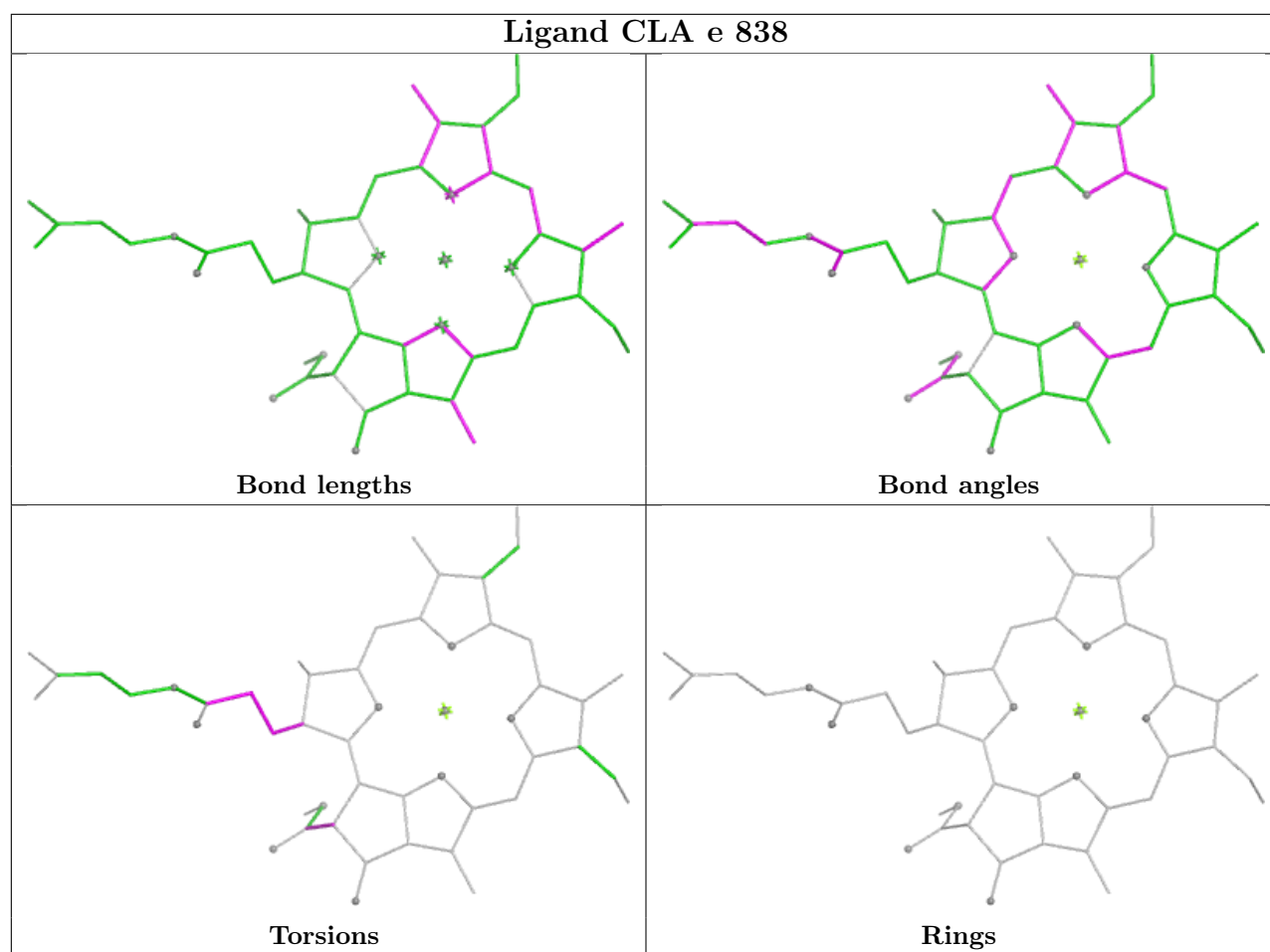




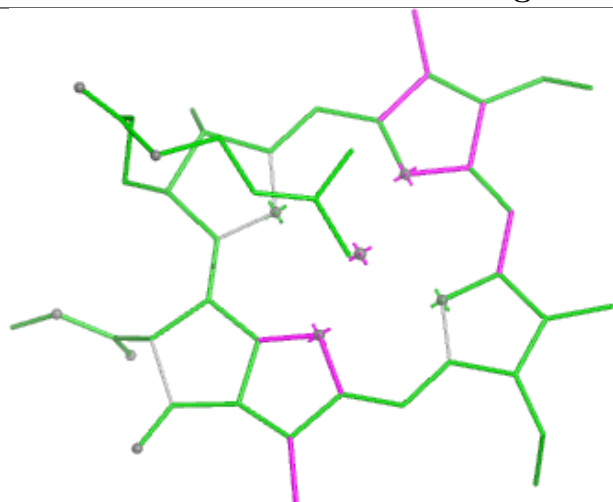
Ligand CLA G 835



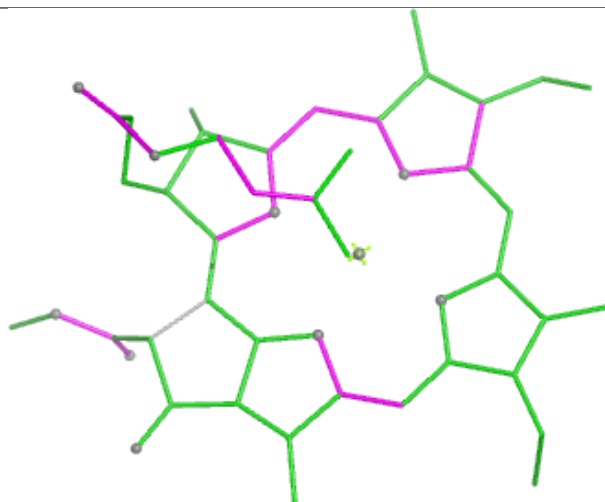




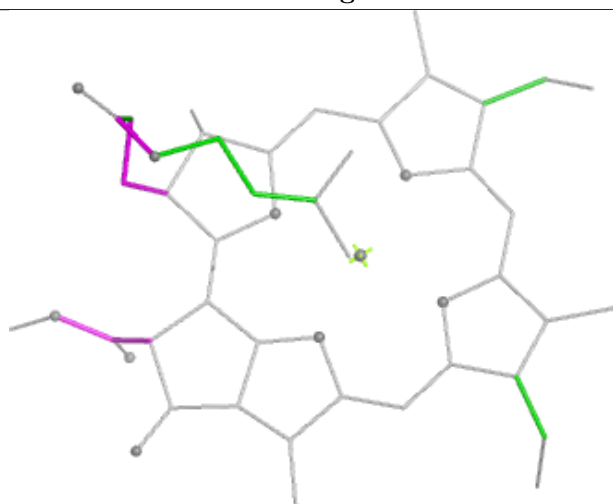
Ligand CLA A 821



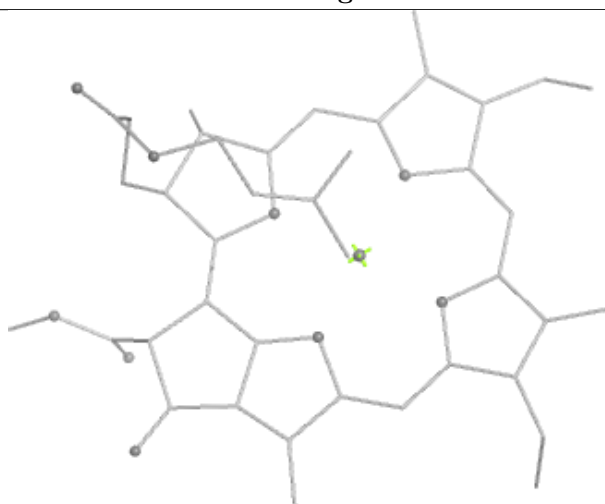
Bond lengths



Bond angles

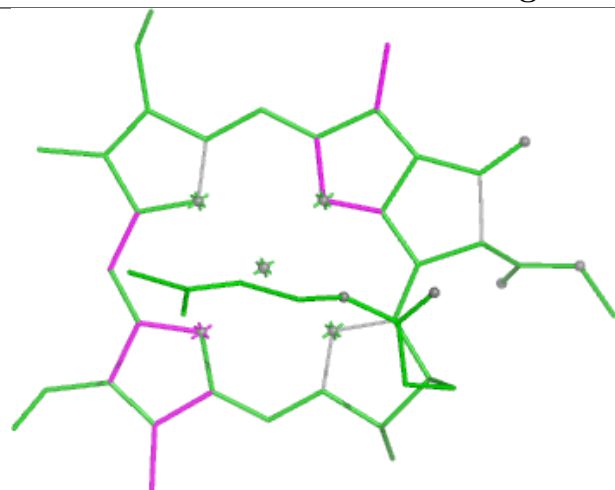


Torsions

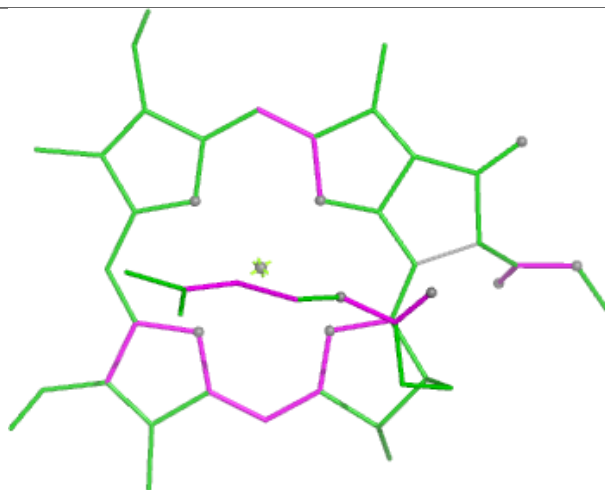


Rings

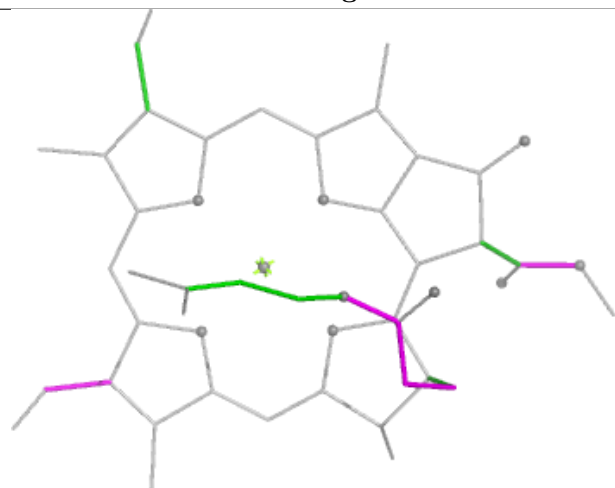
Ligand CLA b 837



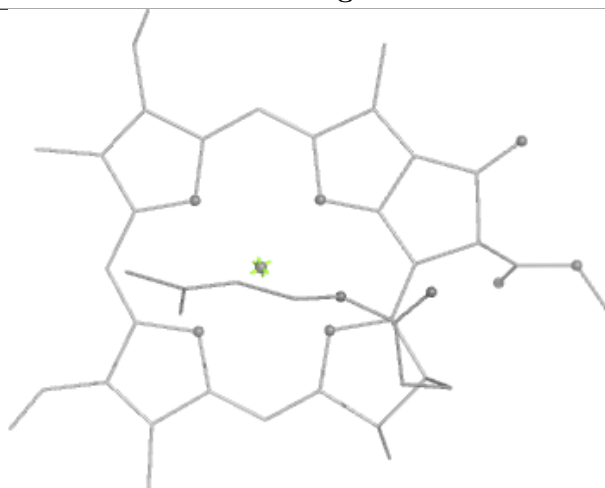
Bond lengths



Bond angles

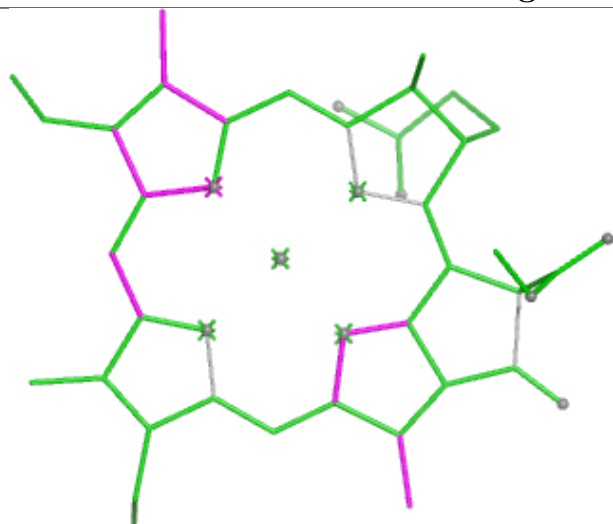


Torsions

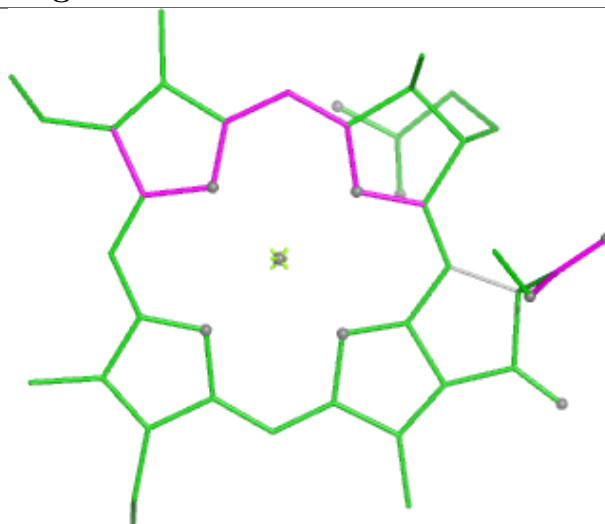


Rings

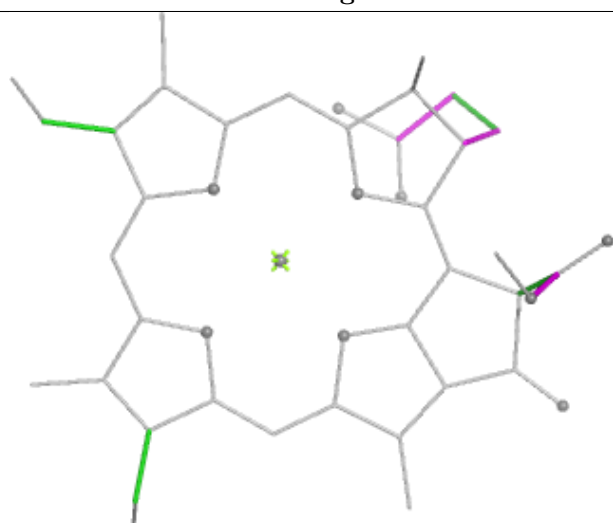
Ligand CLA g 817



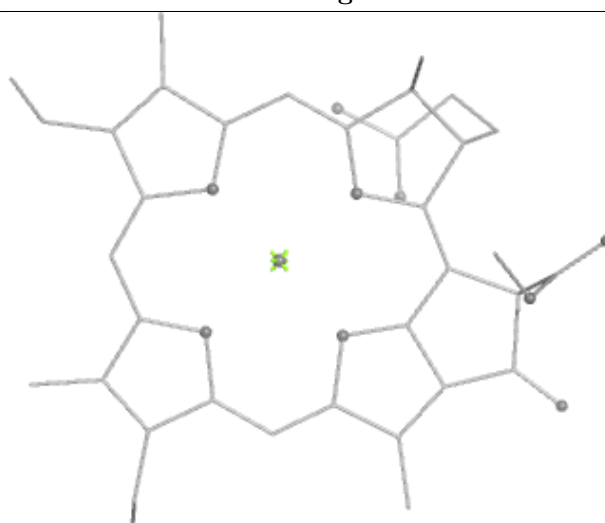
Bond lengths



Bond angles

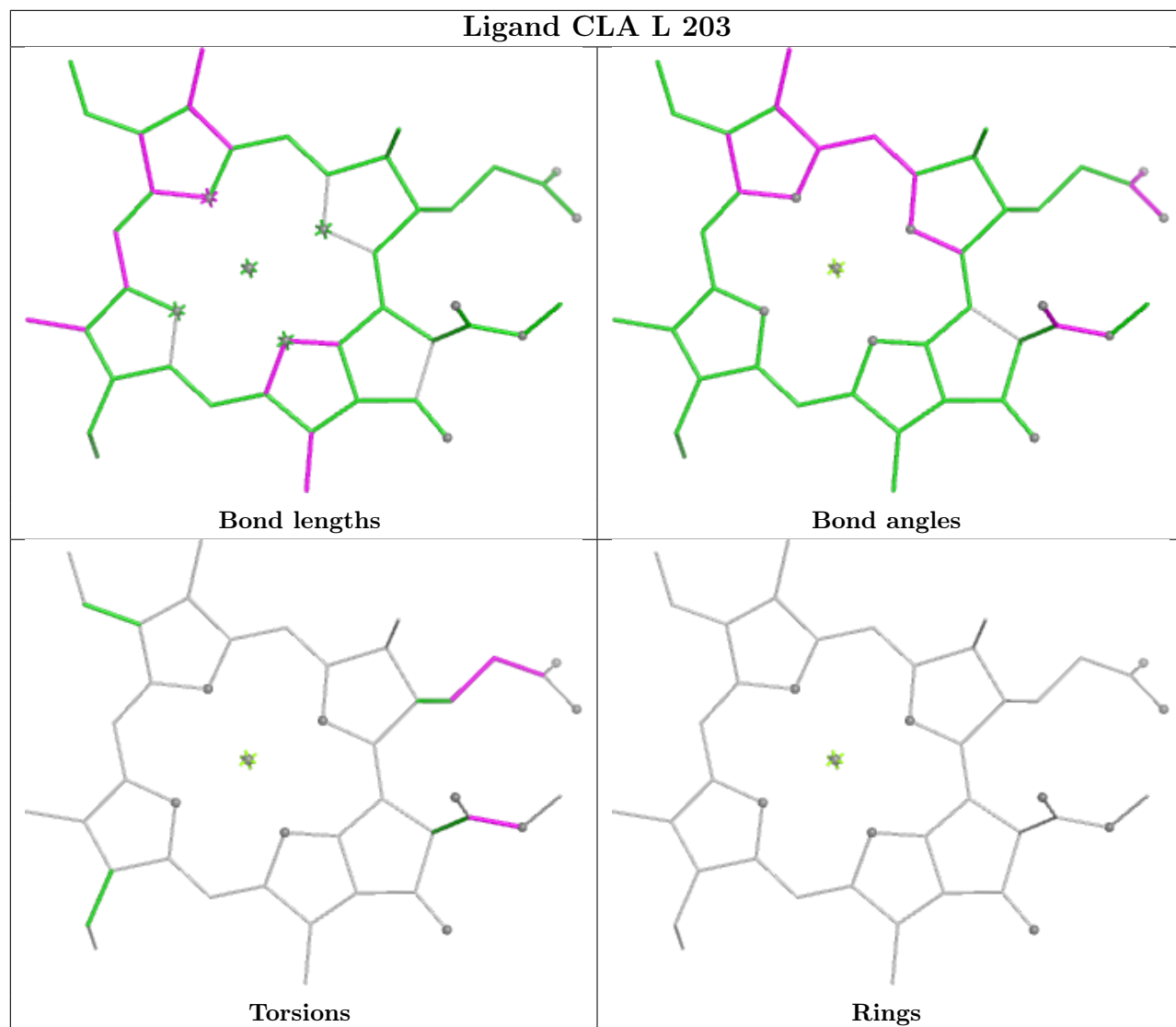


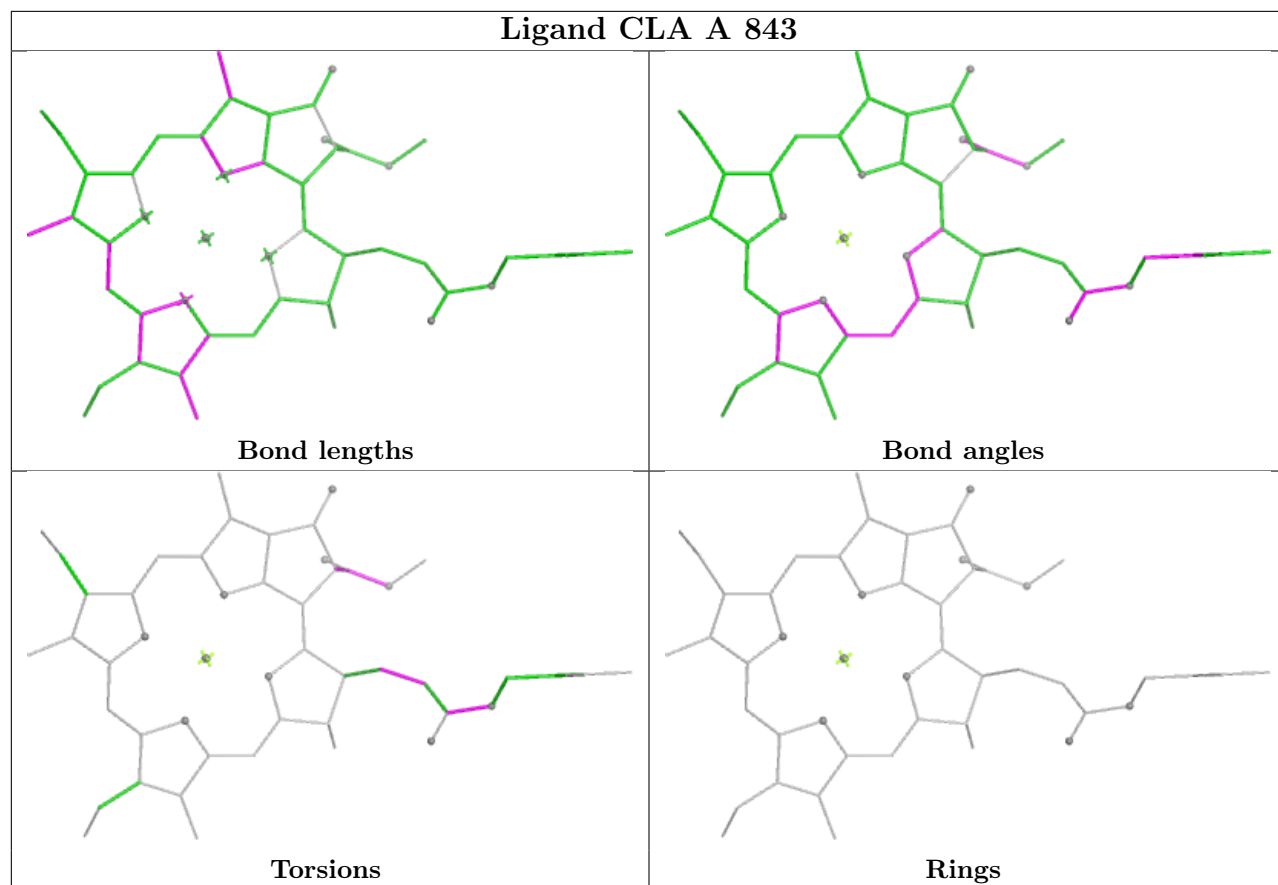
Torsions



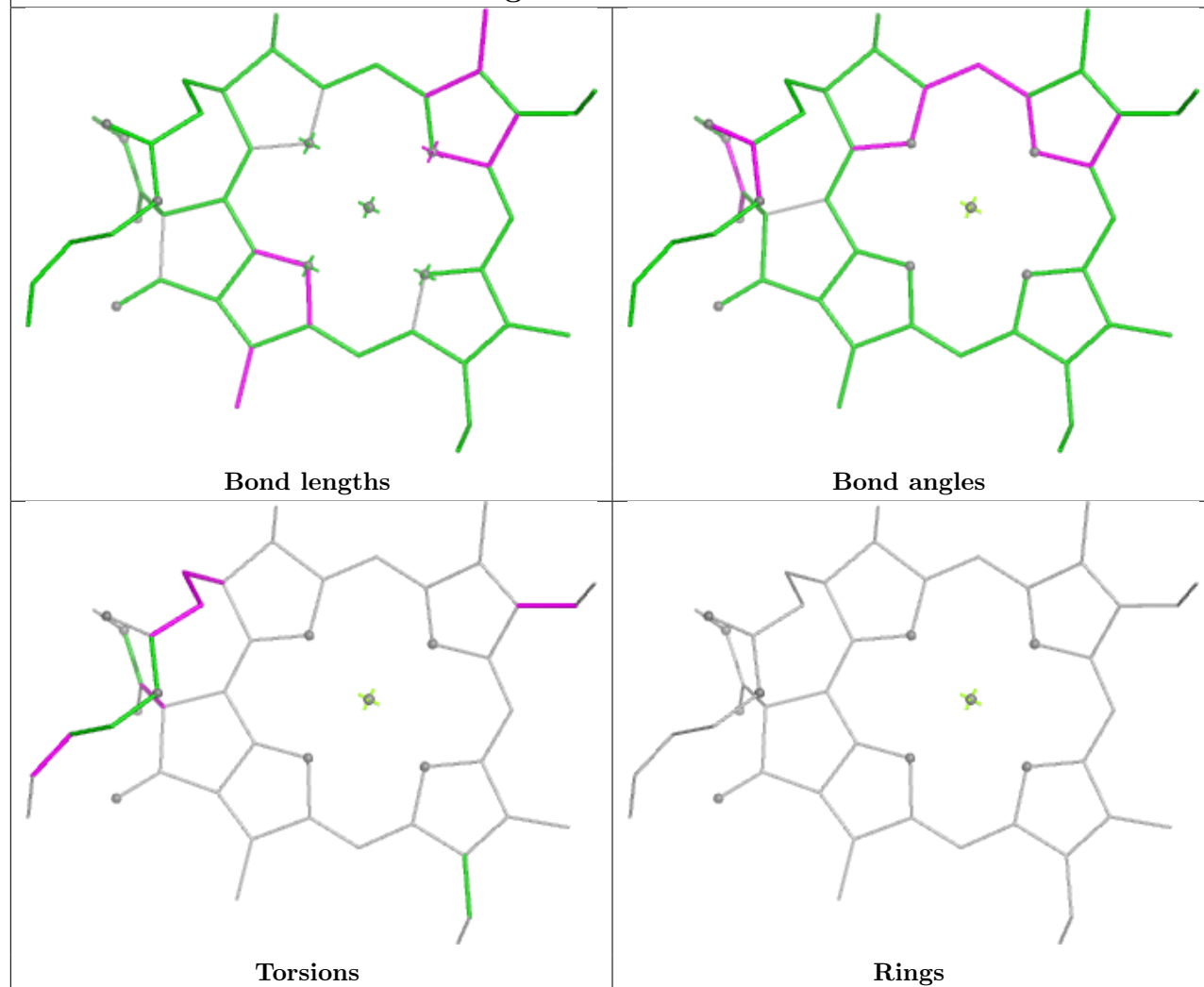
Rings

Ligand CLA L 203

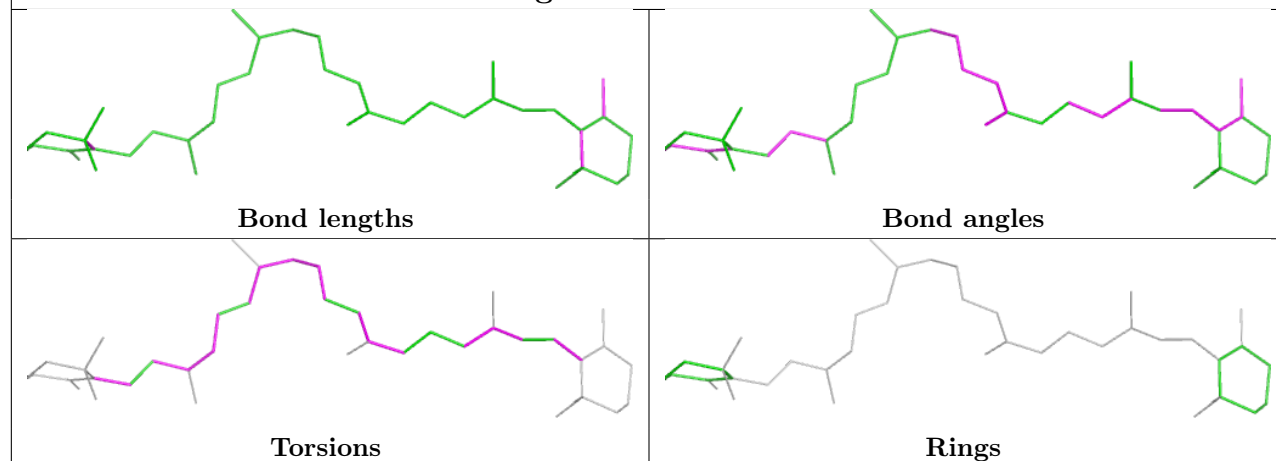


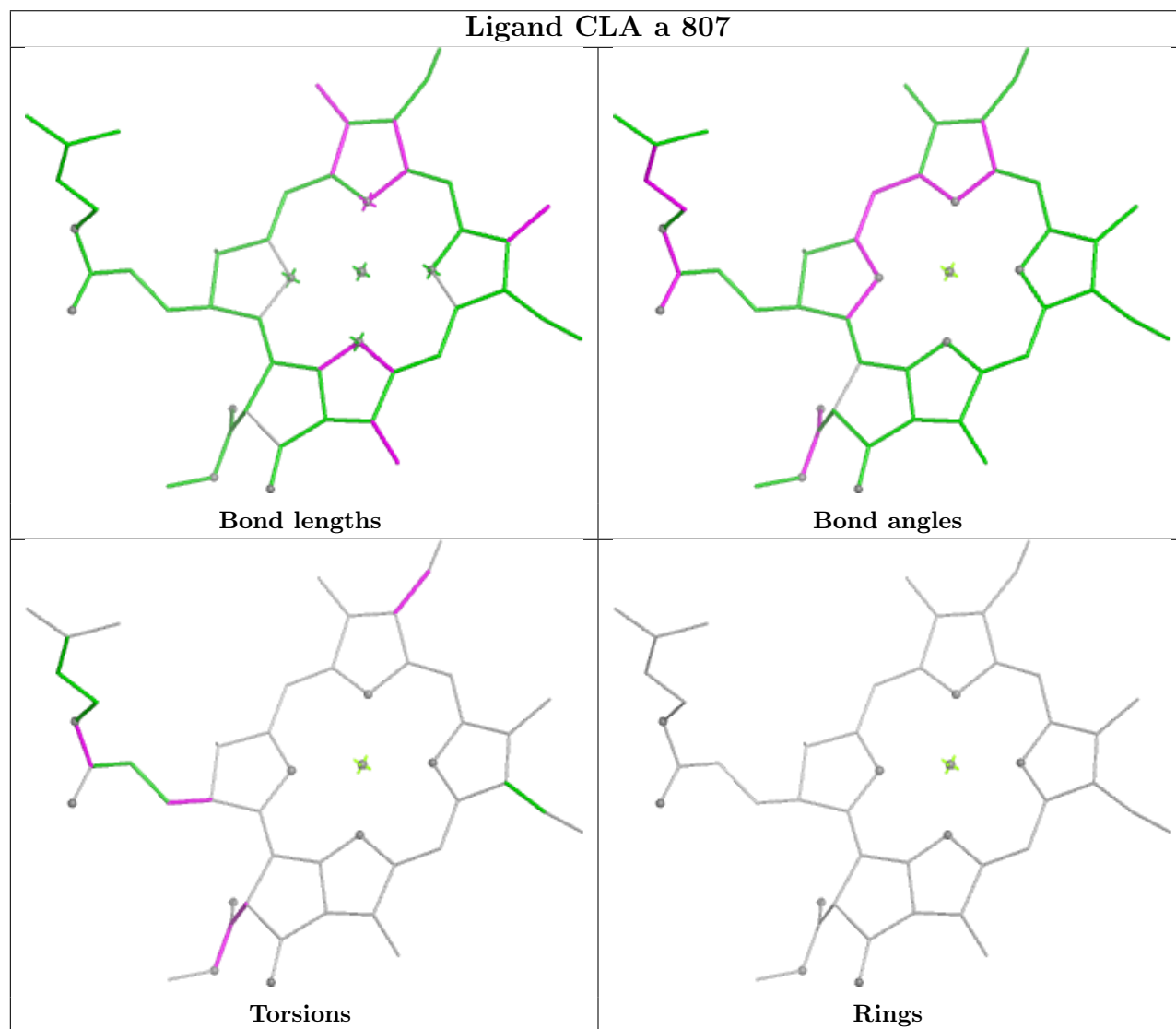
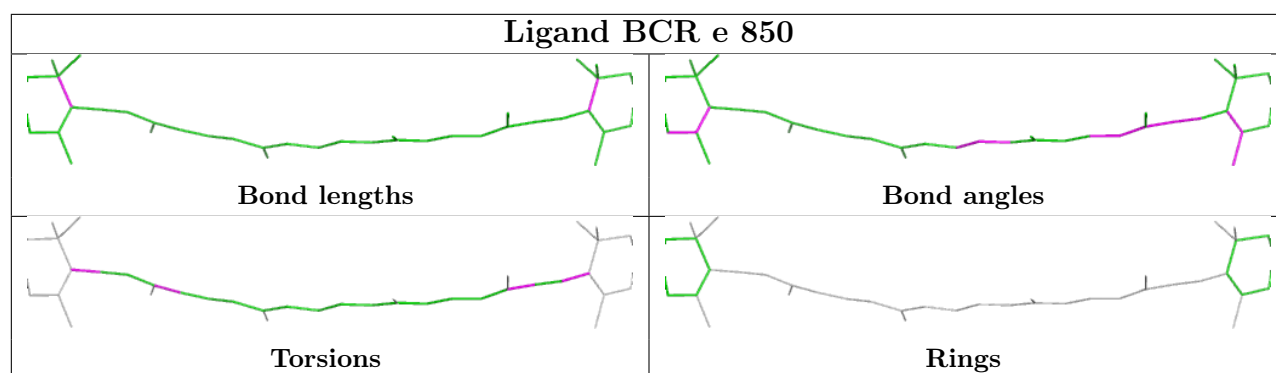


Ligand CLA b 831

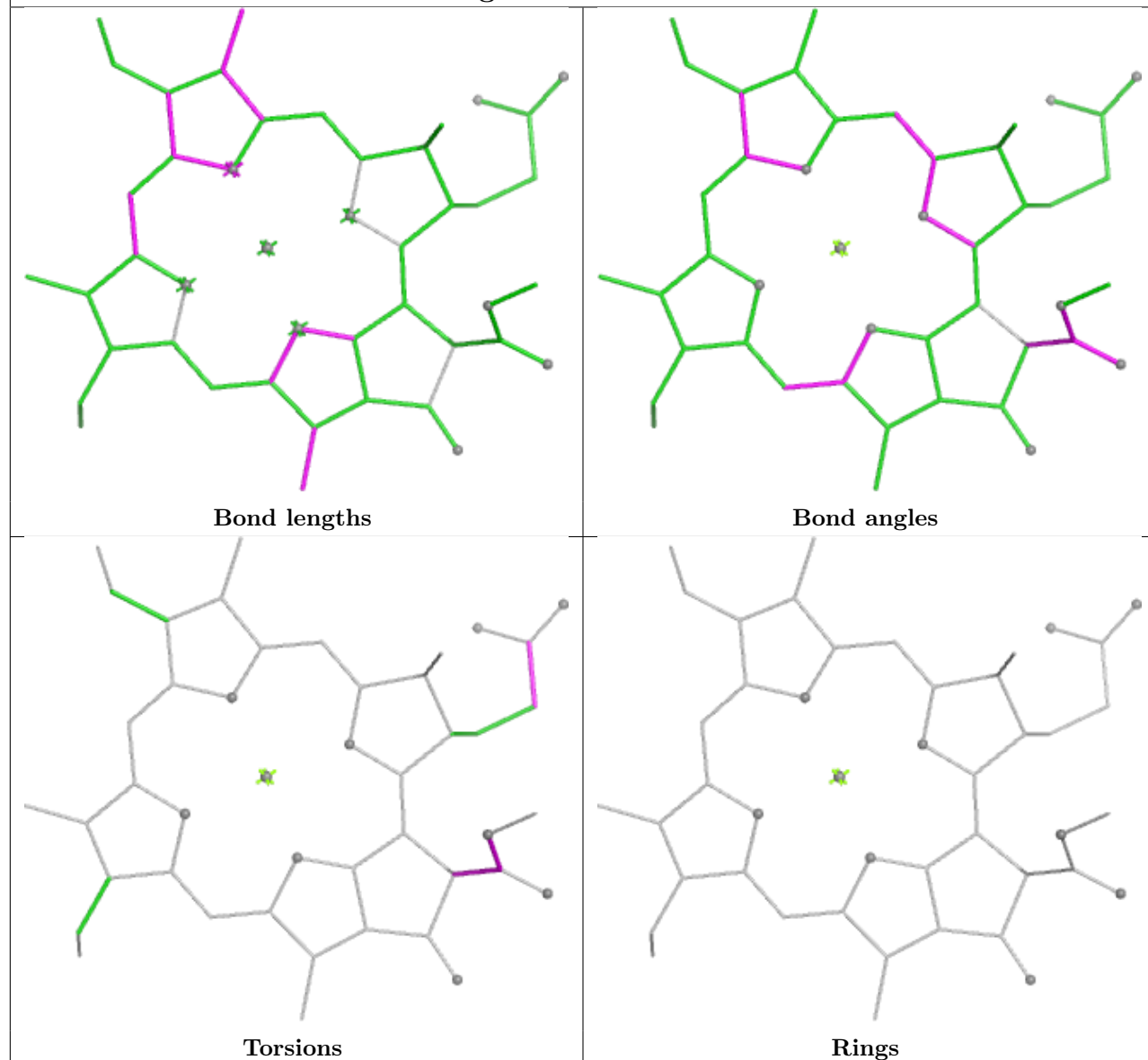


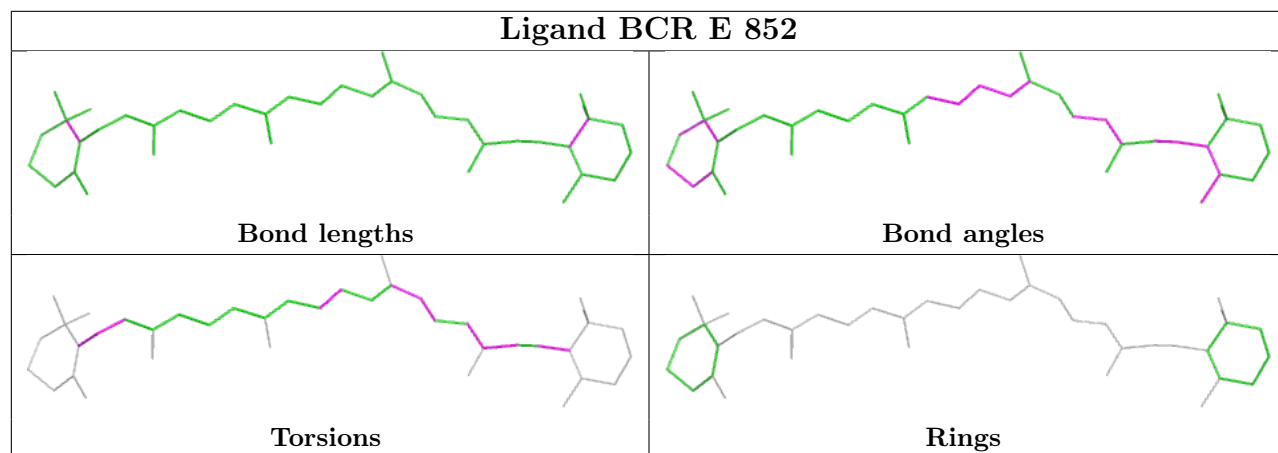
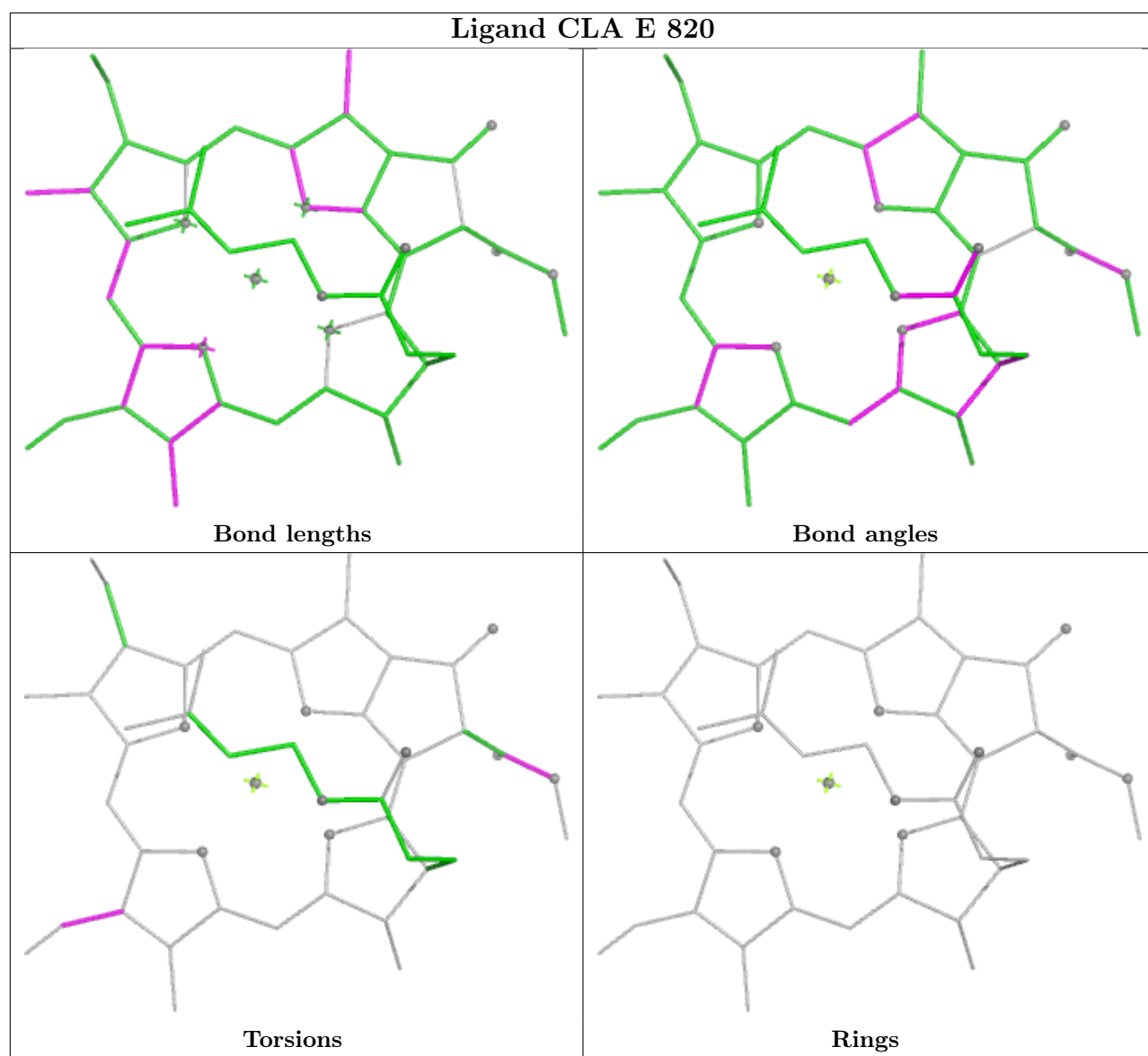
Ligand BCR e 849



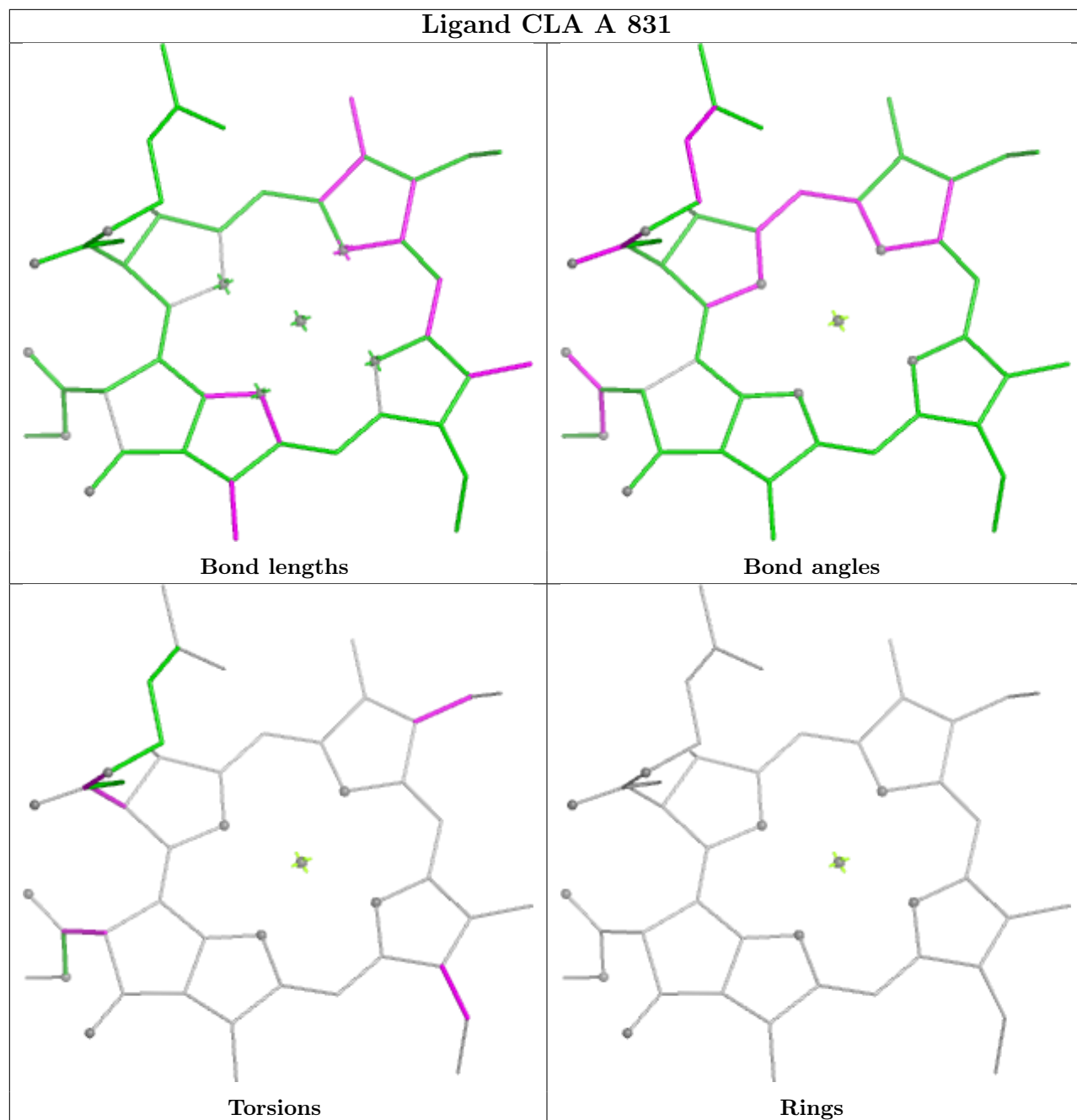


Ligand CLA E 839

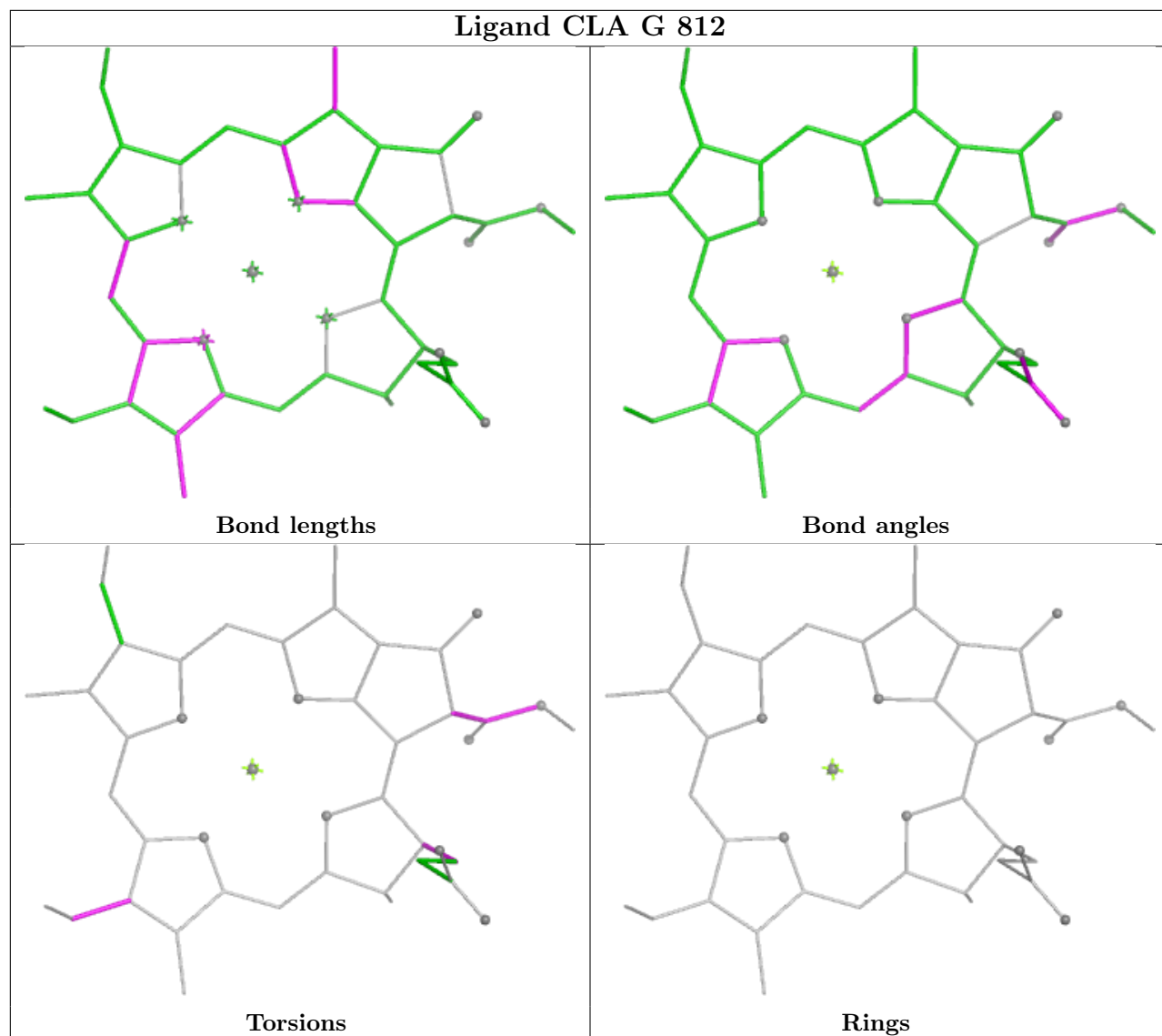




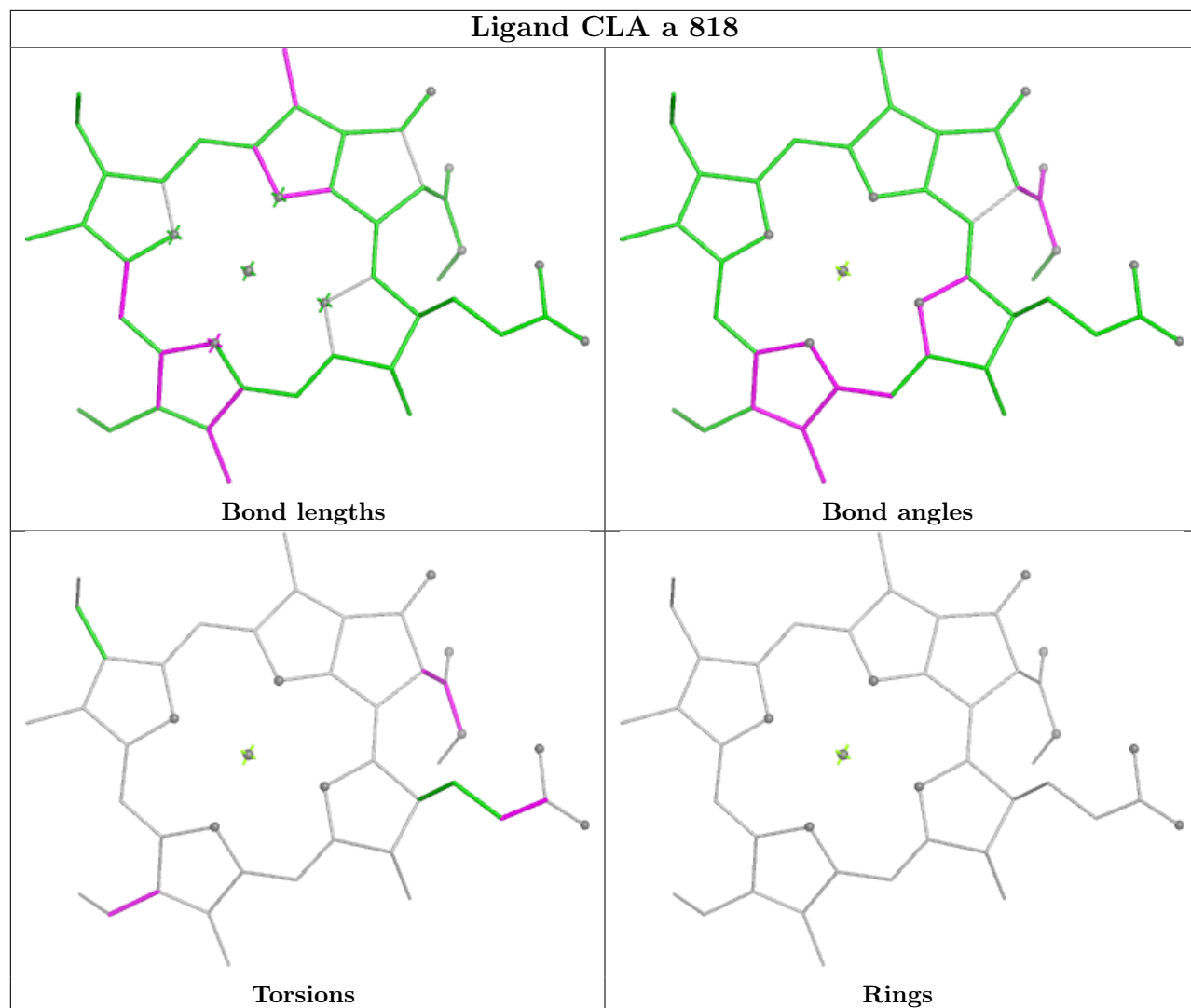
Ligand CLA A 831

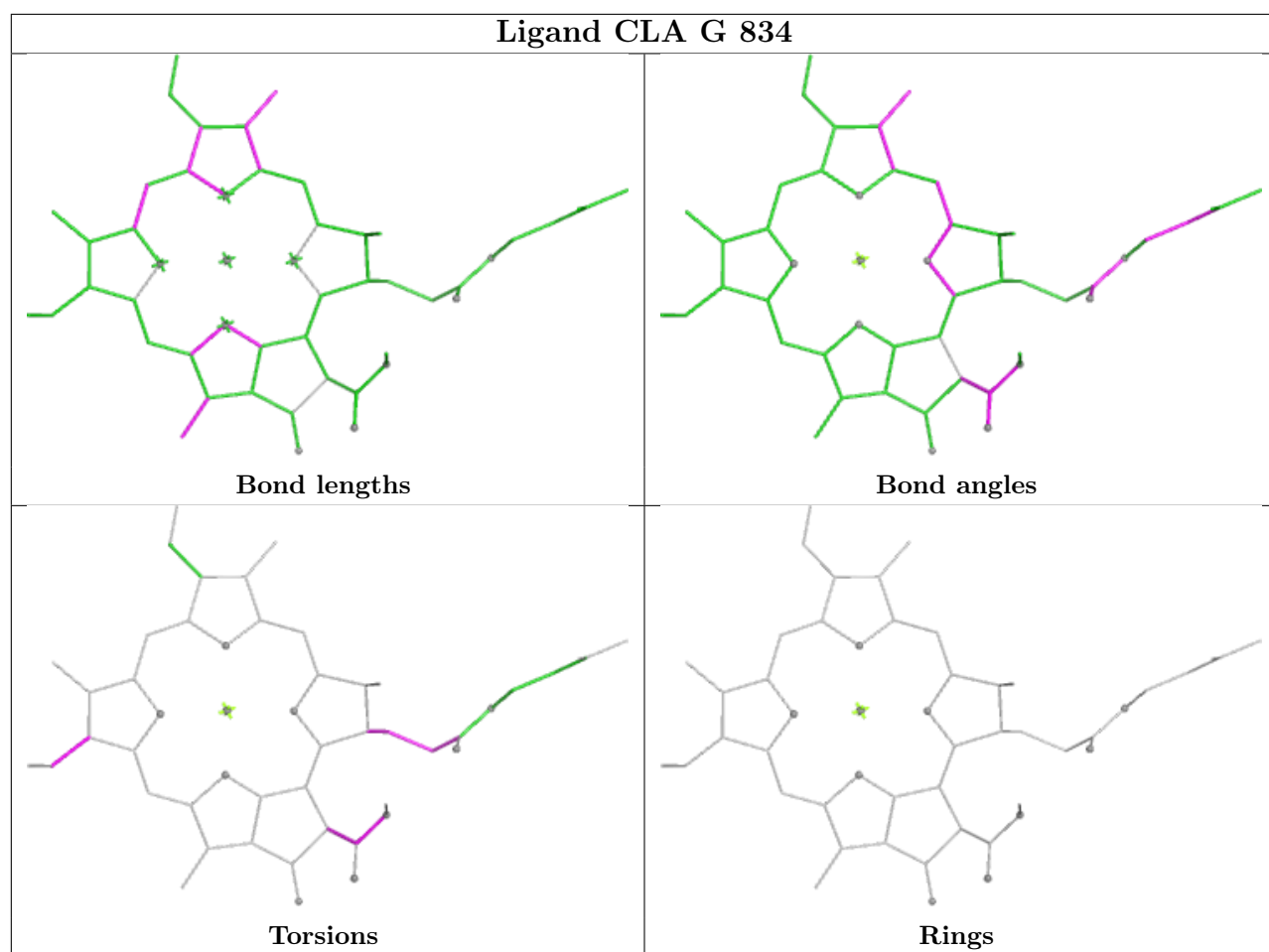


Ligand CLA G 812

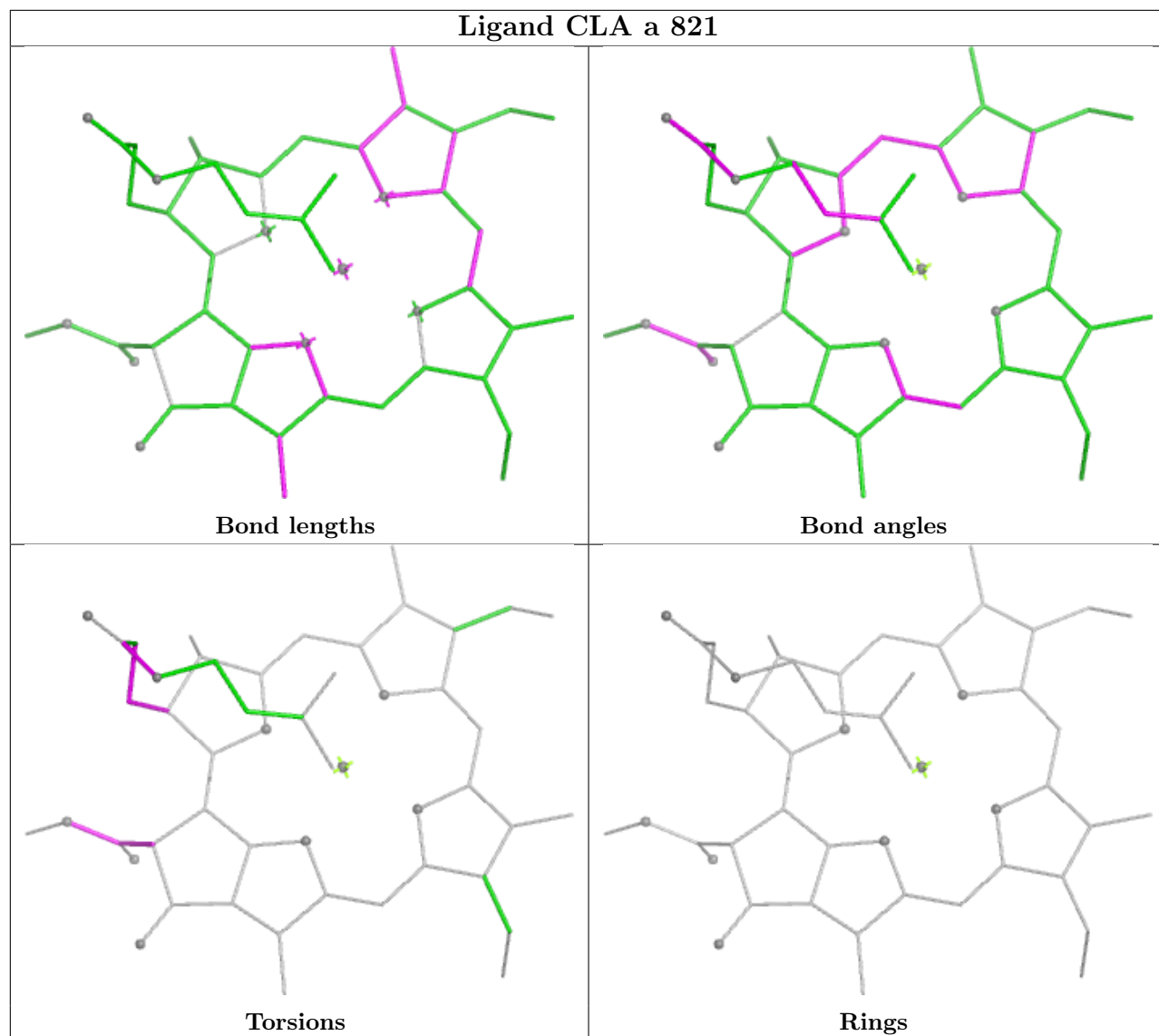


Ligand CLA a 818

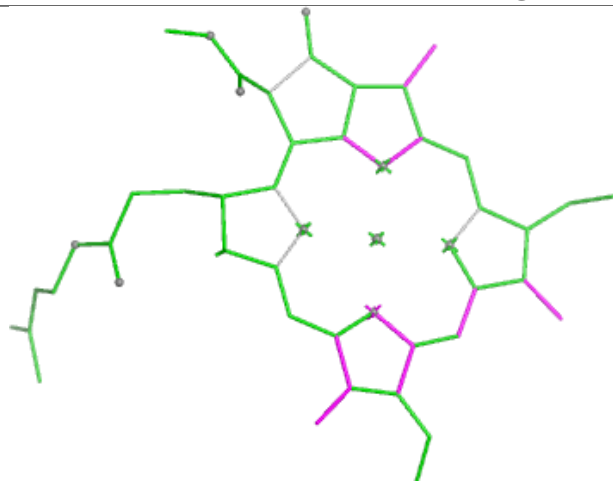




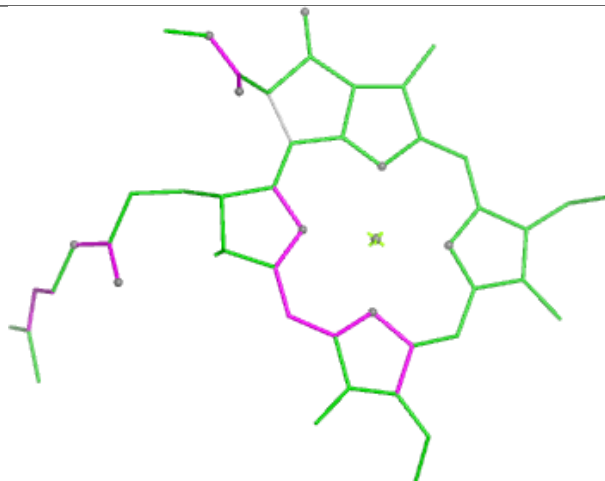
Ligand CLA a 821



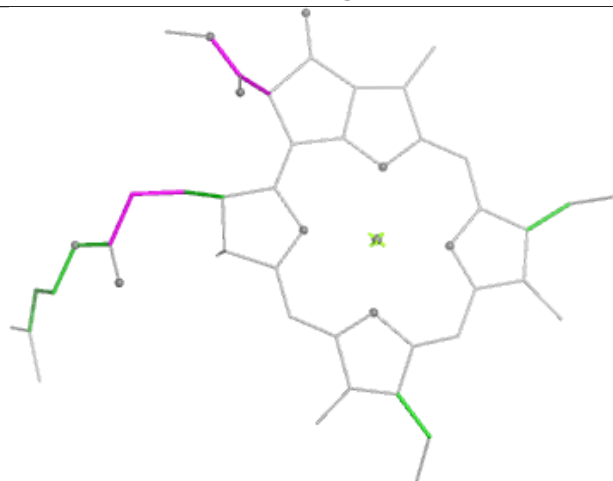
Ligand CLA G 810



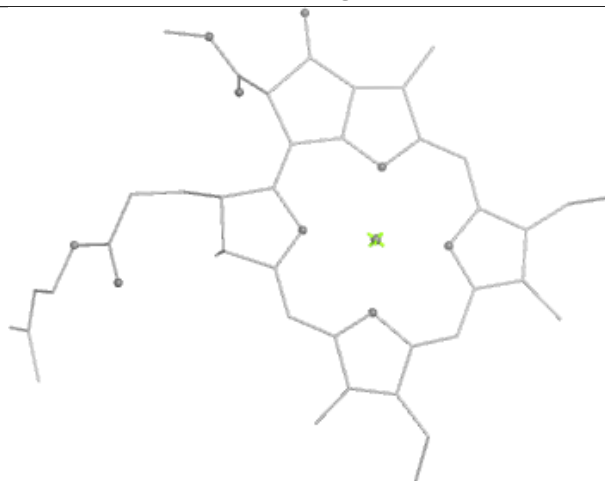
Bond lengths



Bond angles

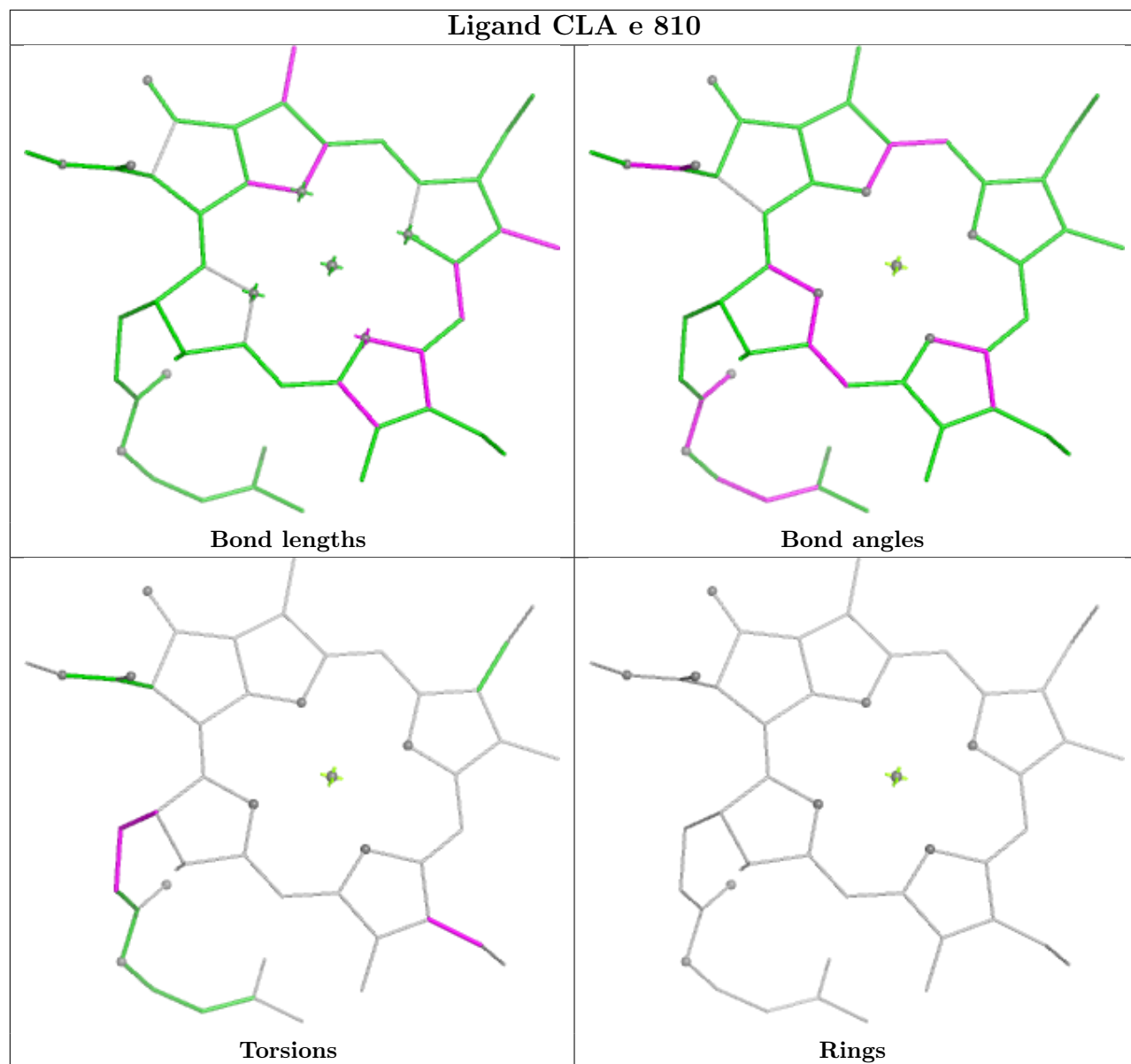


Torsions

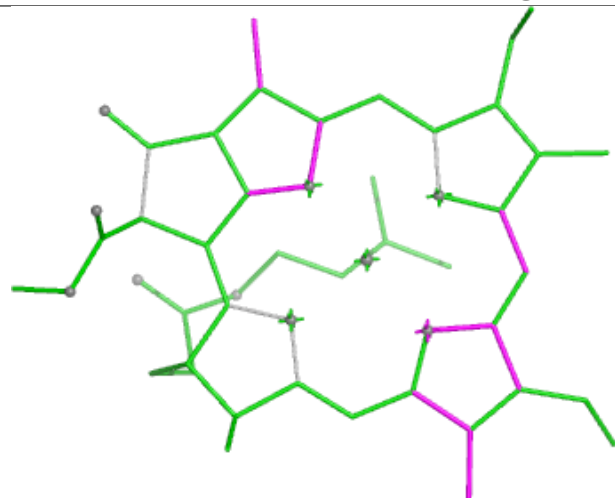


Rings

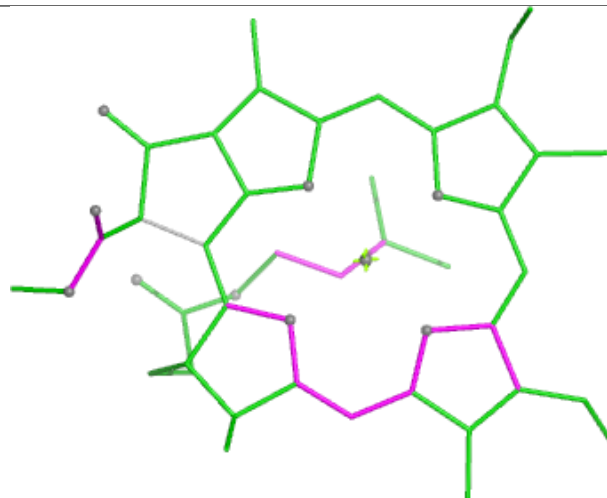
Ligand CLA e 810



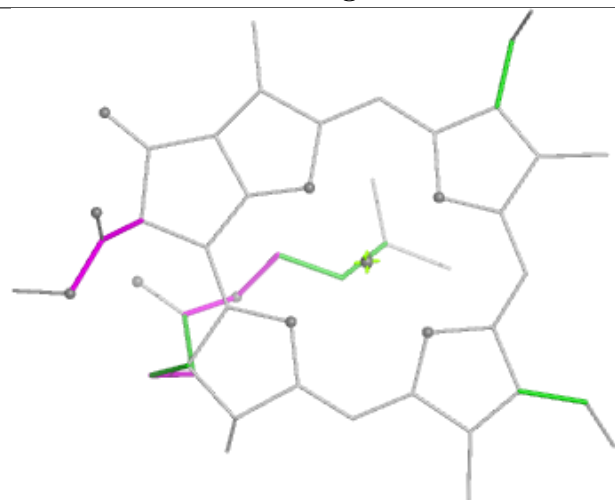
Ligand CLA E 815



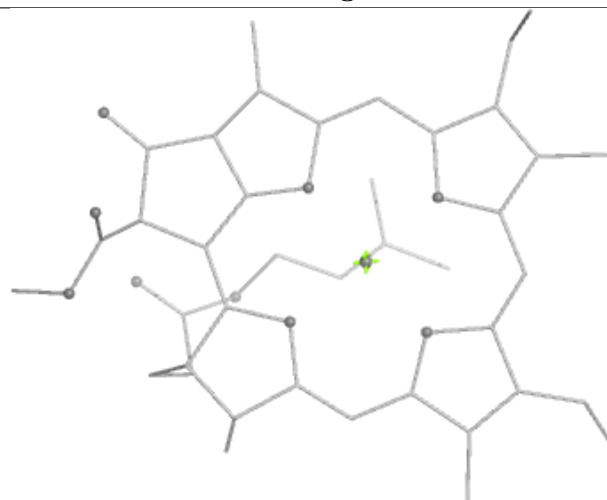
Bond lengths



Bond angles

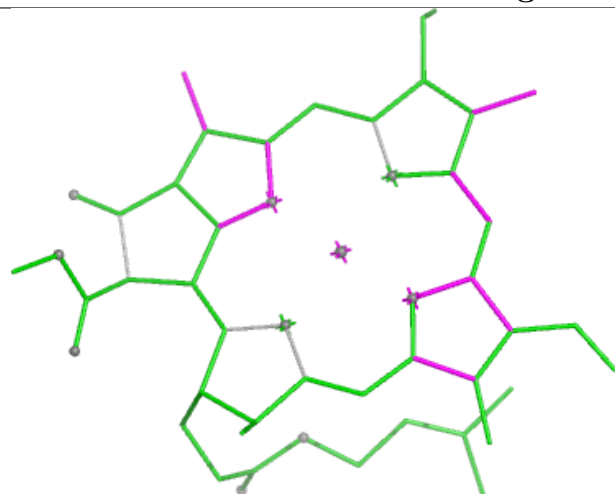


Torsions

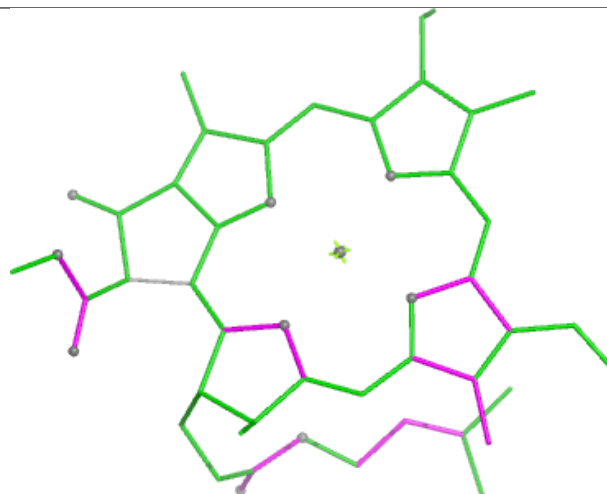


Rings

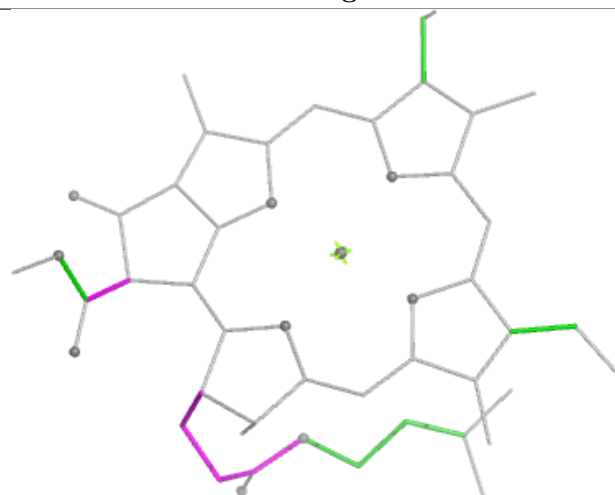
Ligand CLA E 823



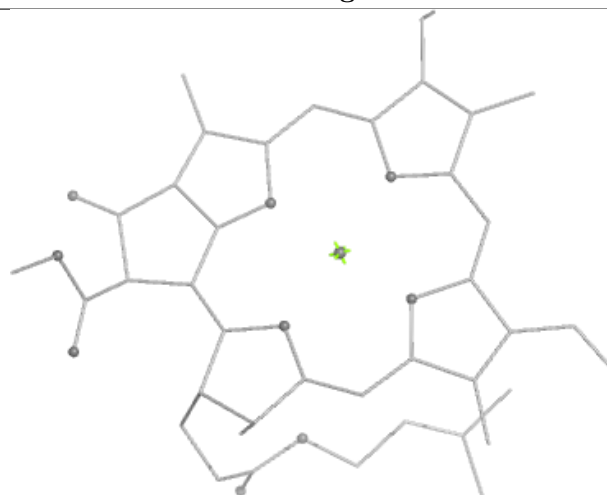
Bond lengths



Bond angles

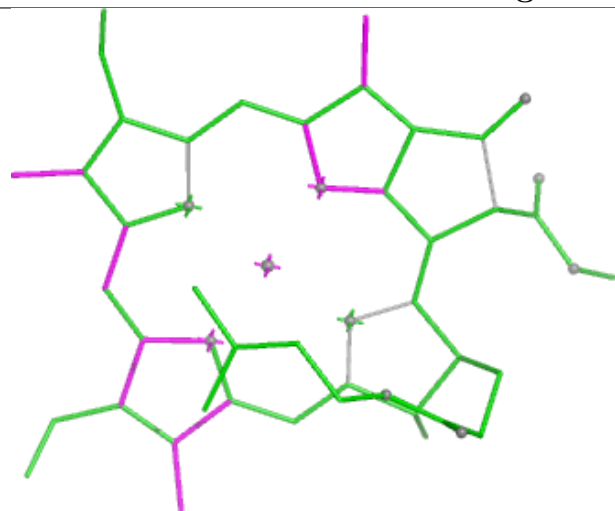


Torsions

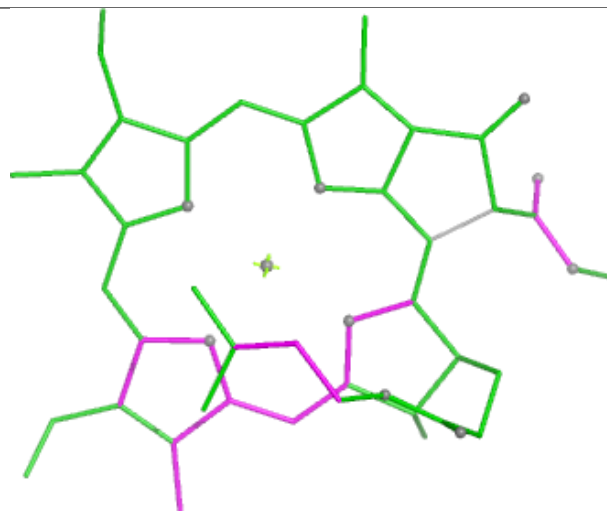


Rings

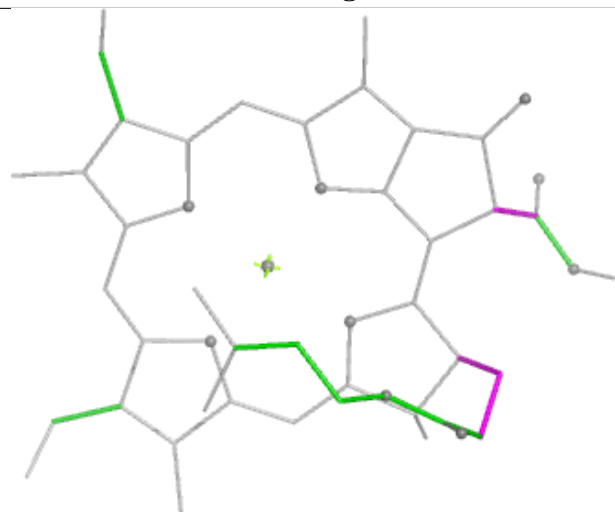
Ligand CLA B 801



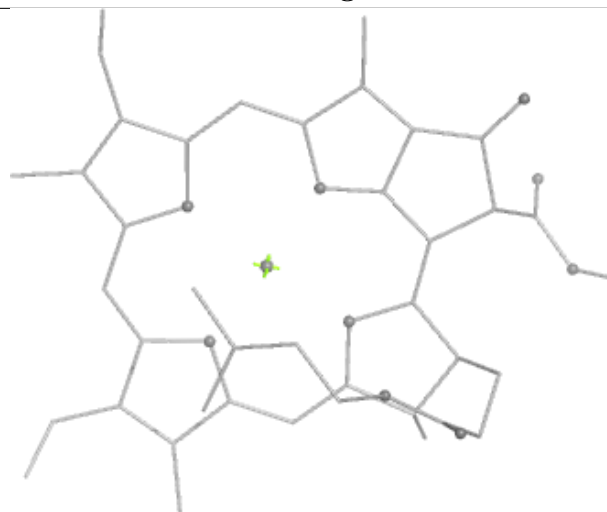
Bond lengths



Bond angles

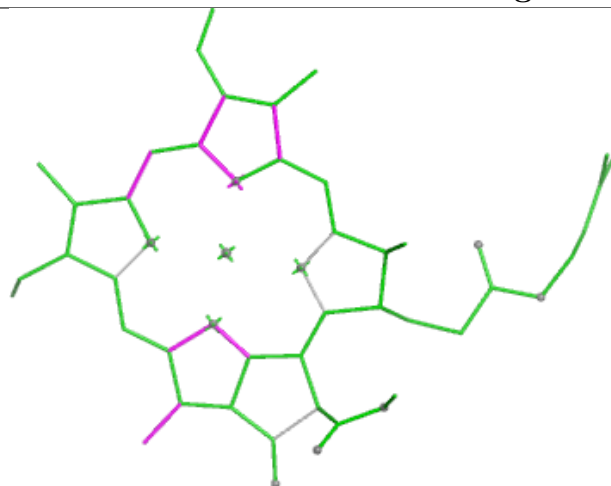


Torsions

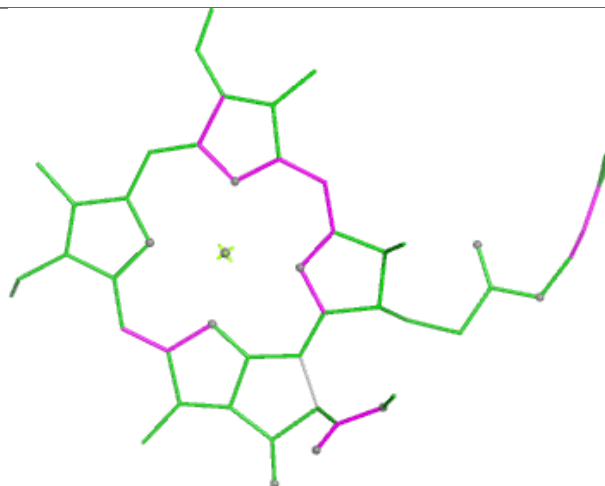


Rings

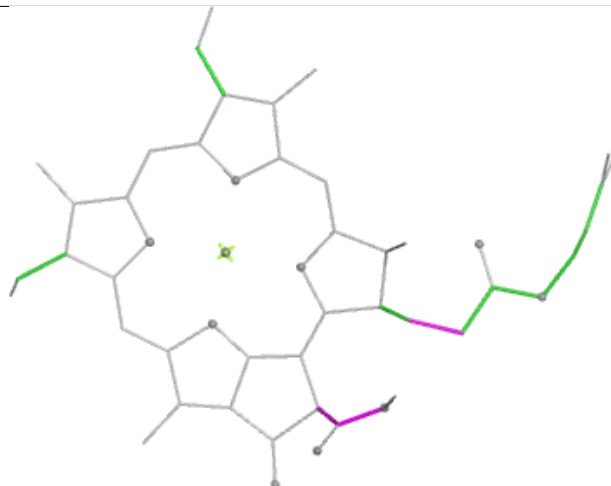
Ligand CLA B 814



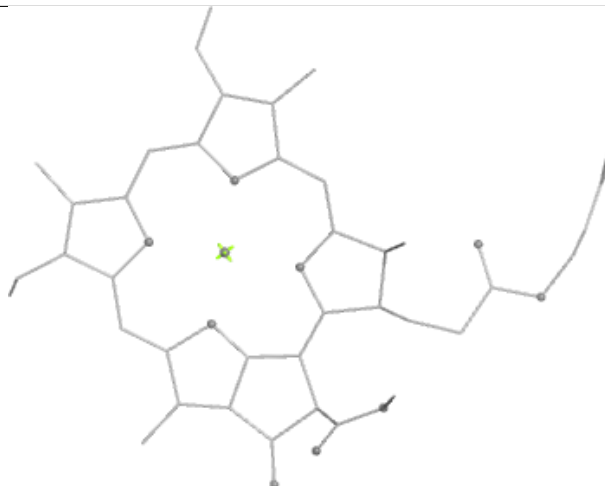
Bond lengths



Bond angles

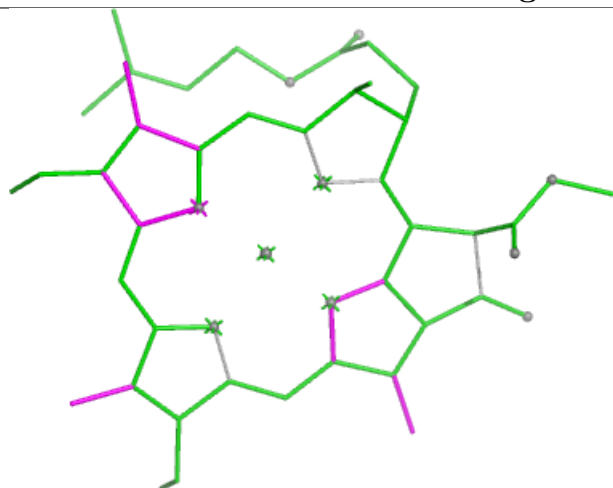


Torsions

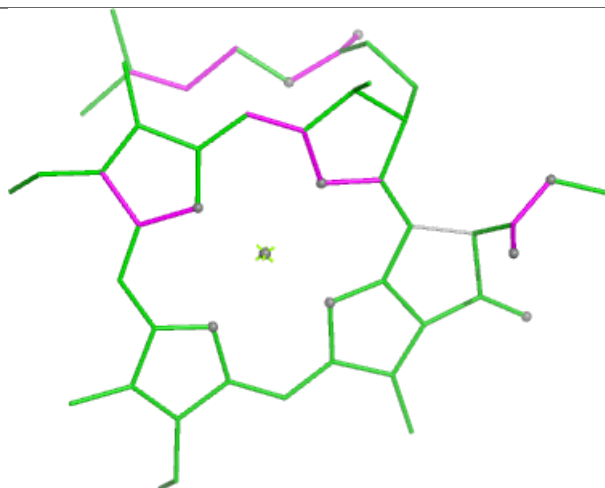


Rings

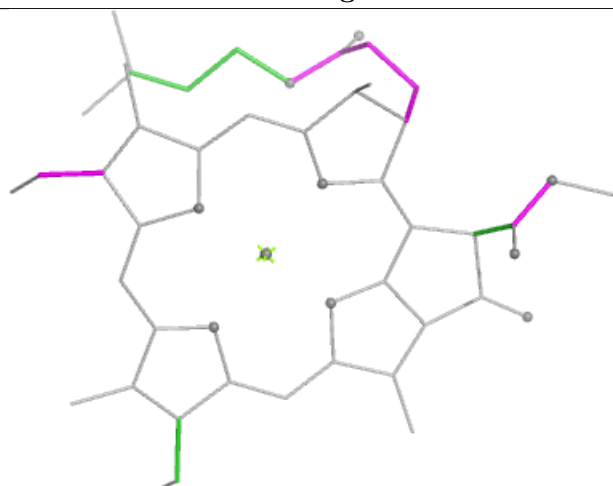
Ligand CLA e 821



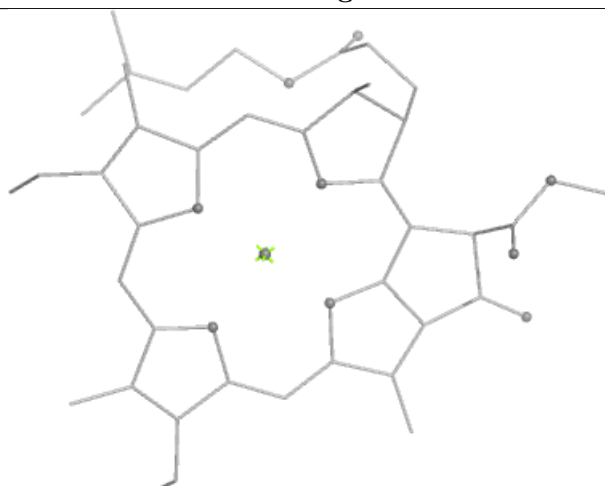
Bond lengths



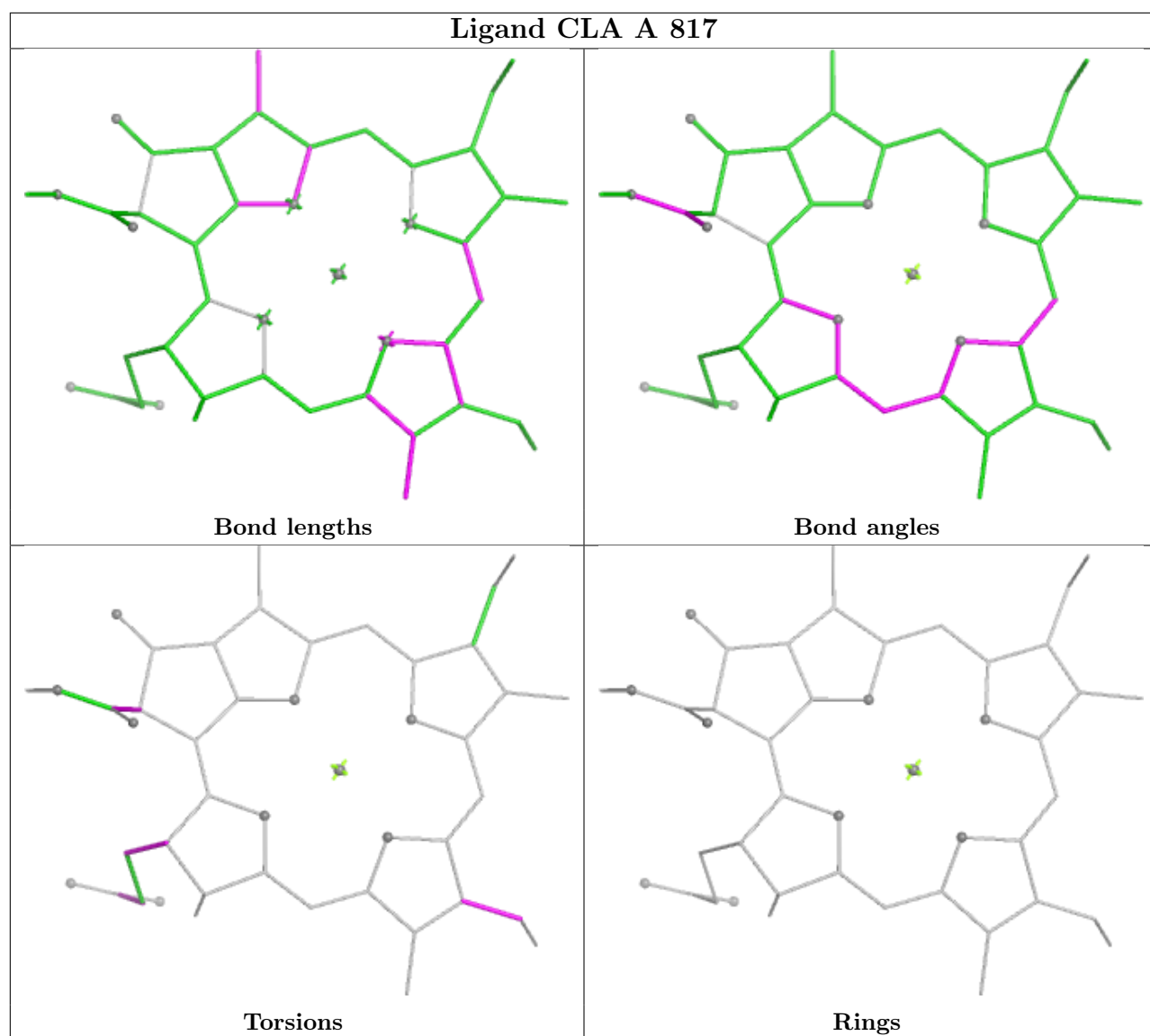
Bond angles



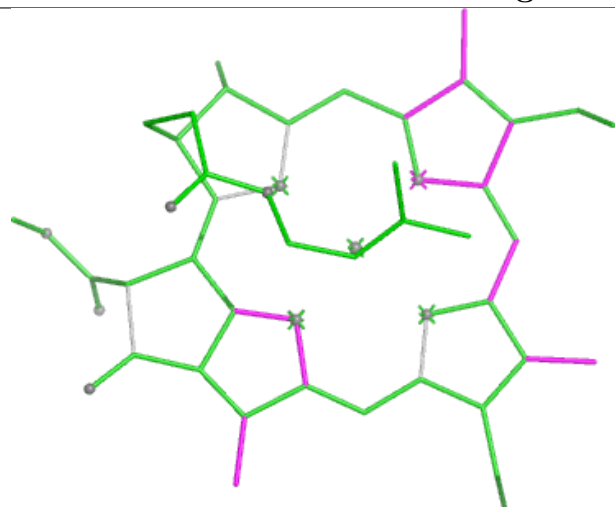
Torsions



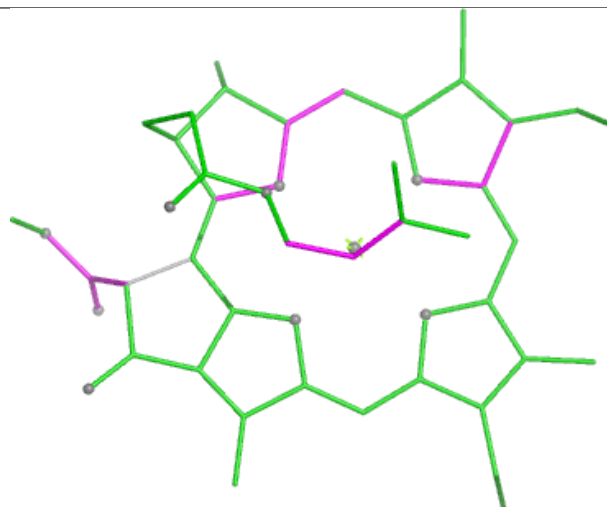
Rings



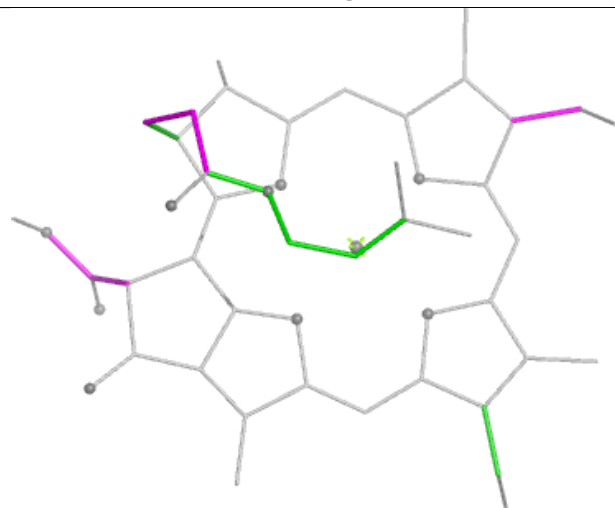
Ligand CLA B 823



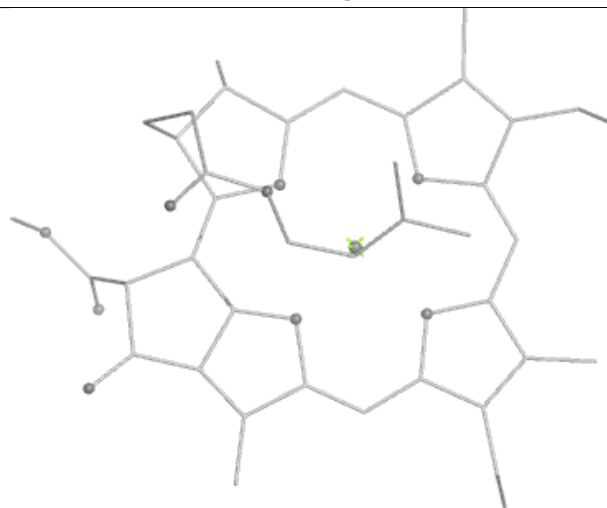
Bond lengths



Bond angles

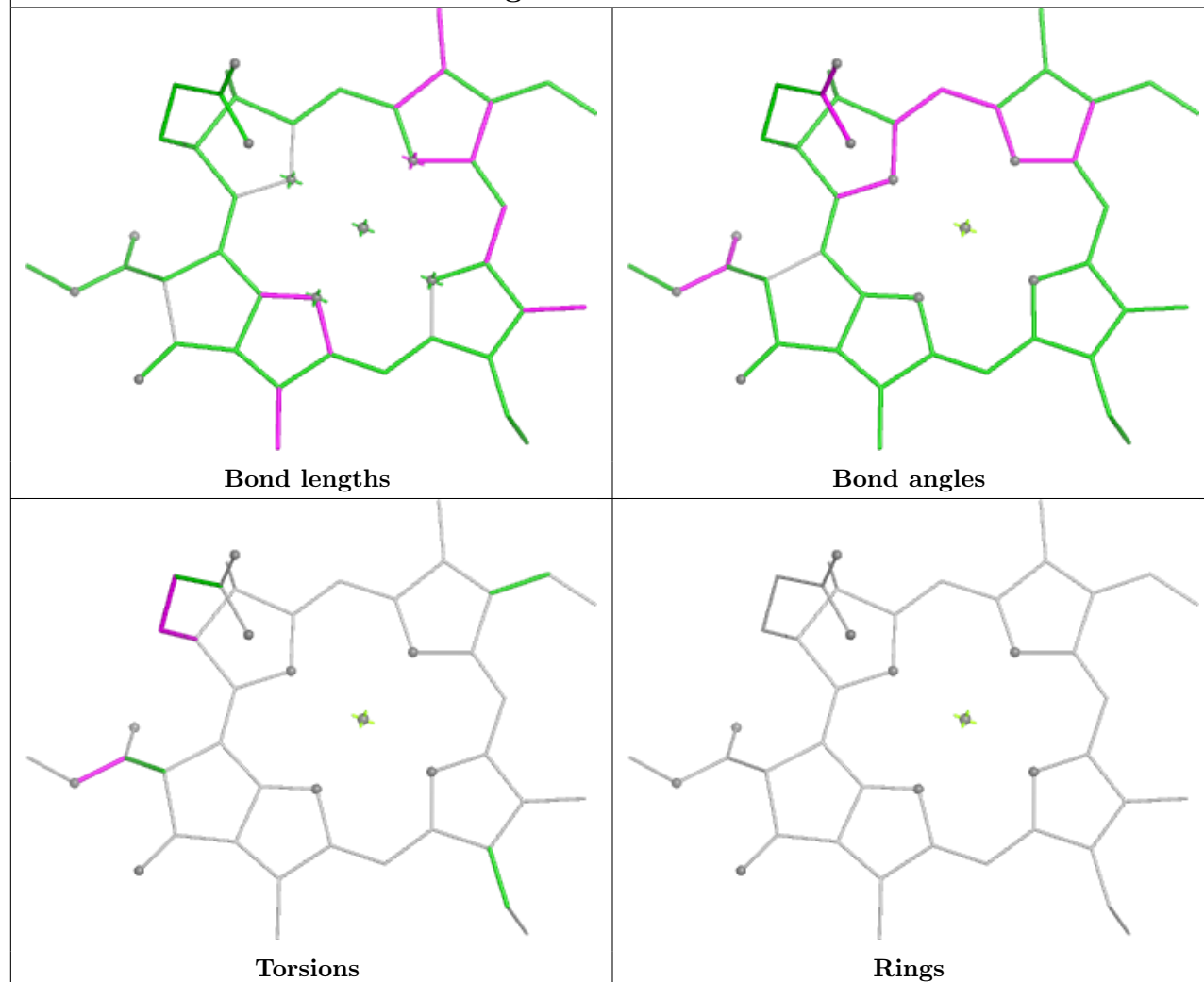


Torsions

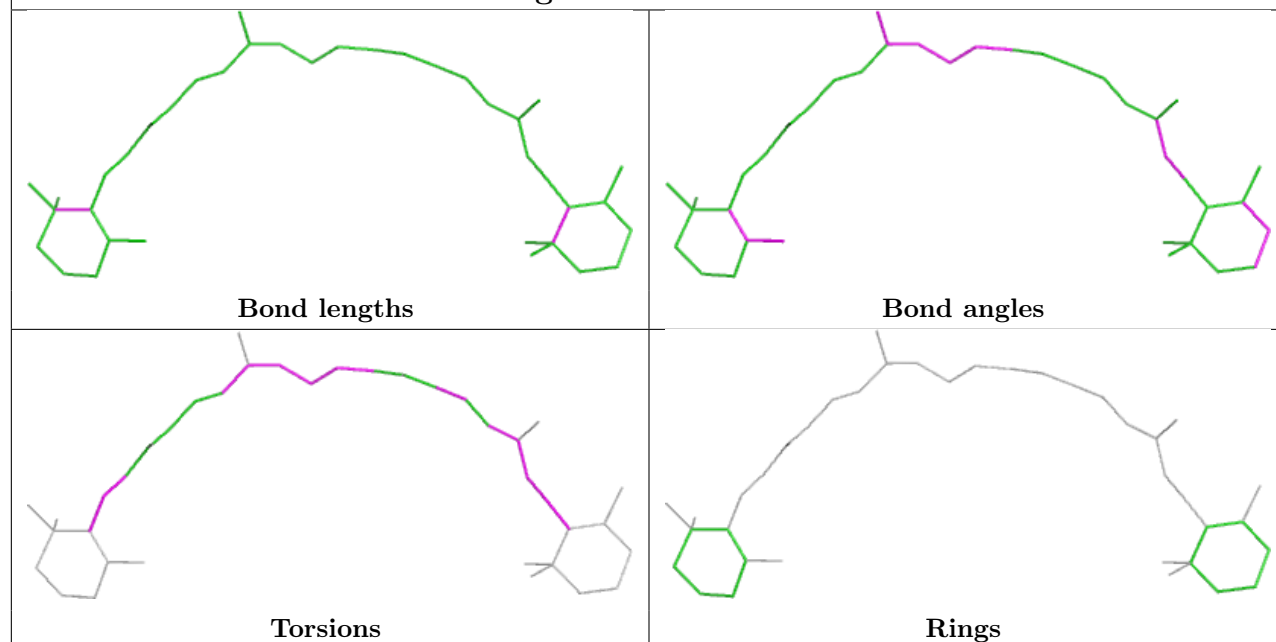


Rings

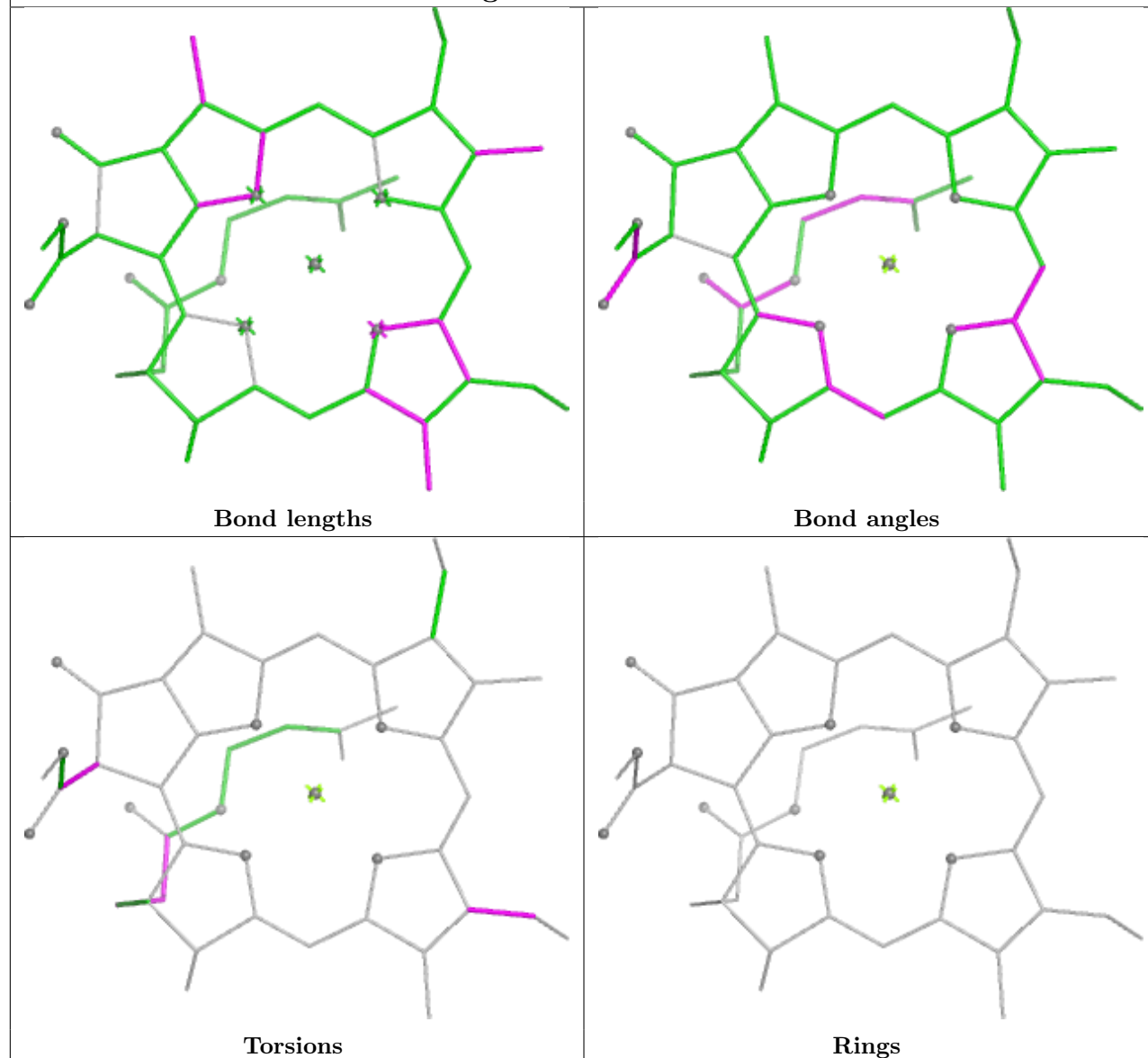
Ligand CLA b 812

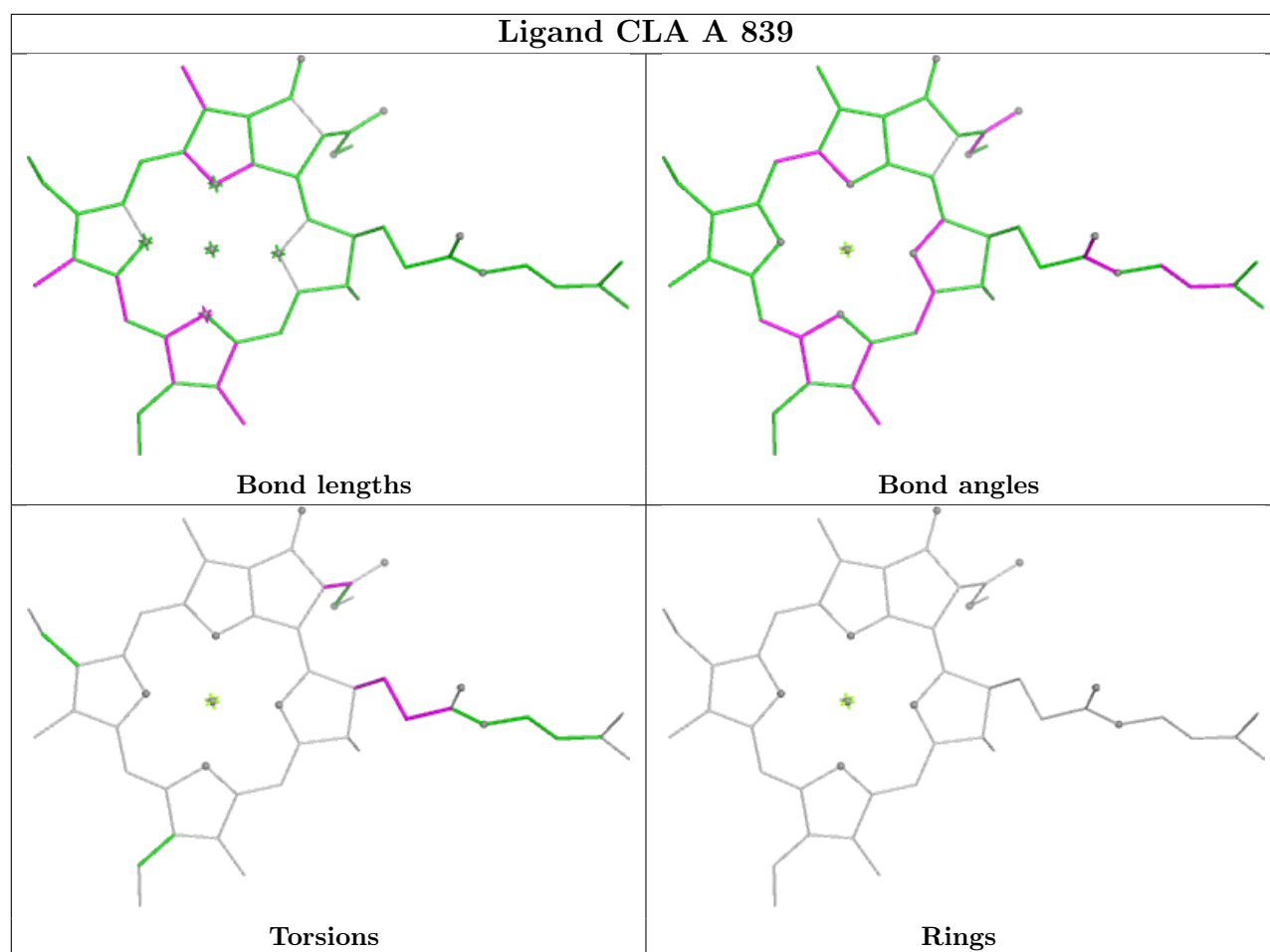


Ligand BCR e 851

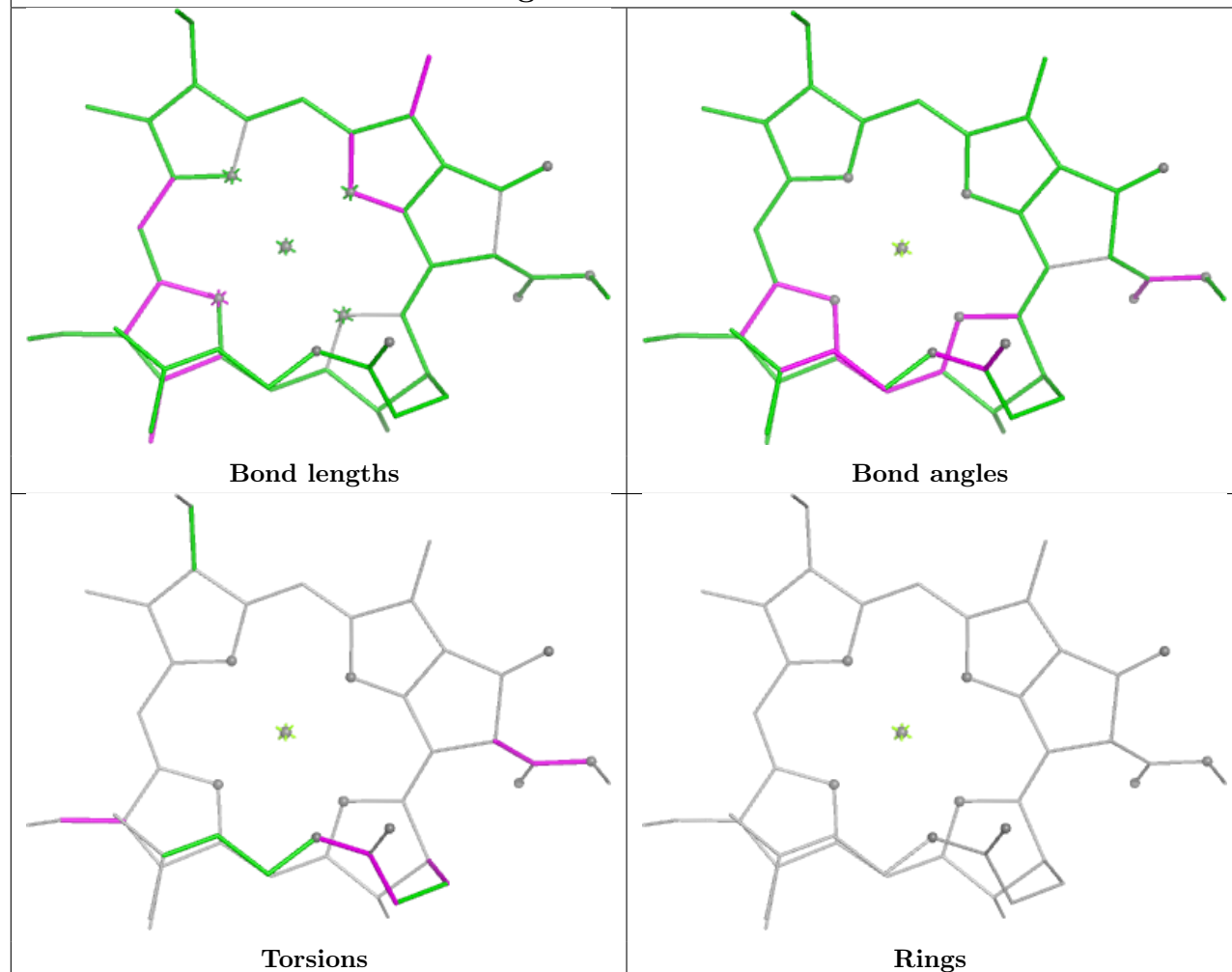


Ligand CLA a 841

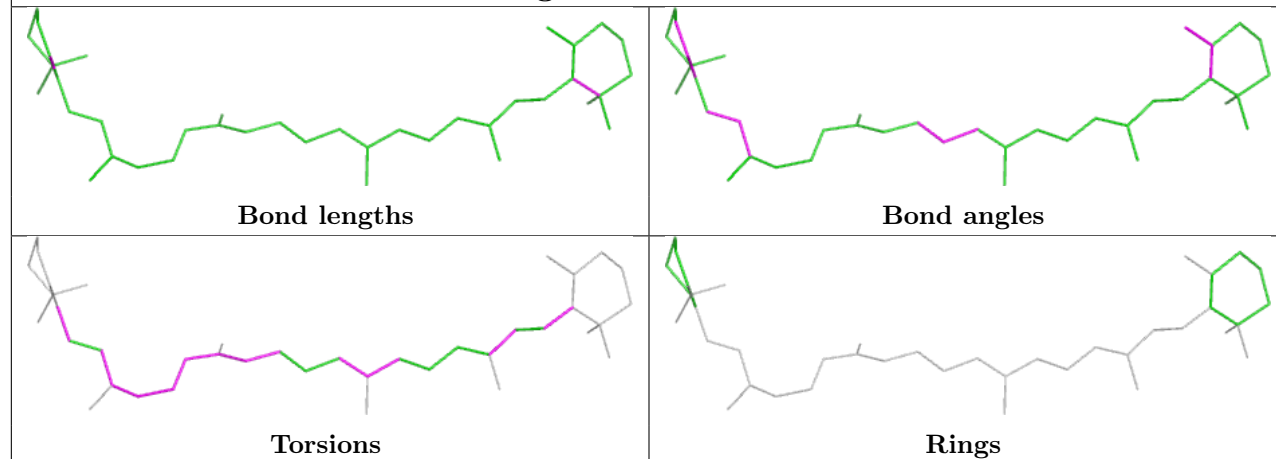




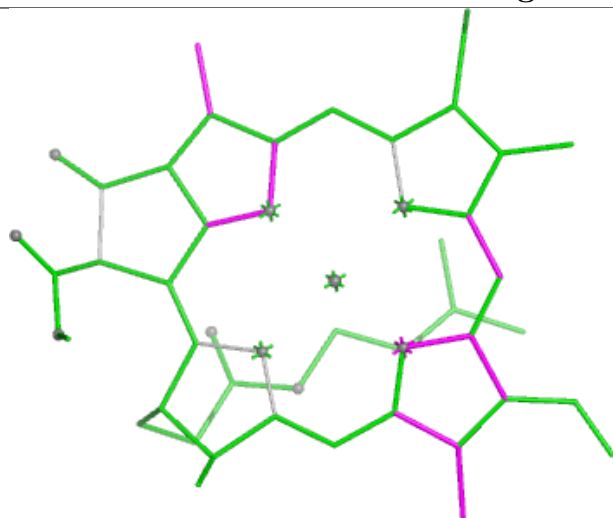
Ligand CLA a 824



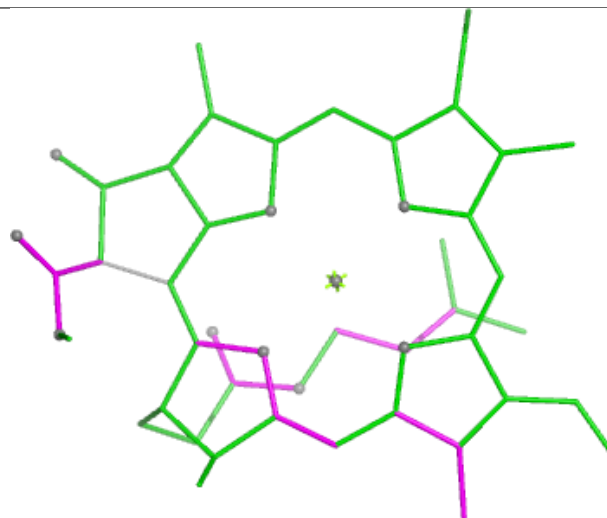
Ligand BCR s 201



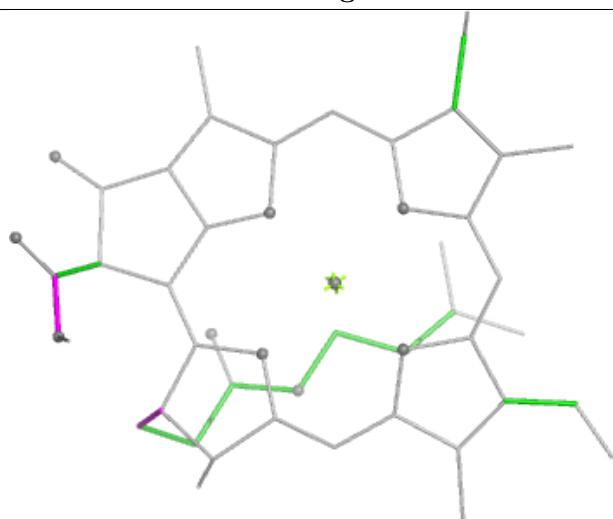
Ligand CLA b 809



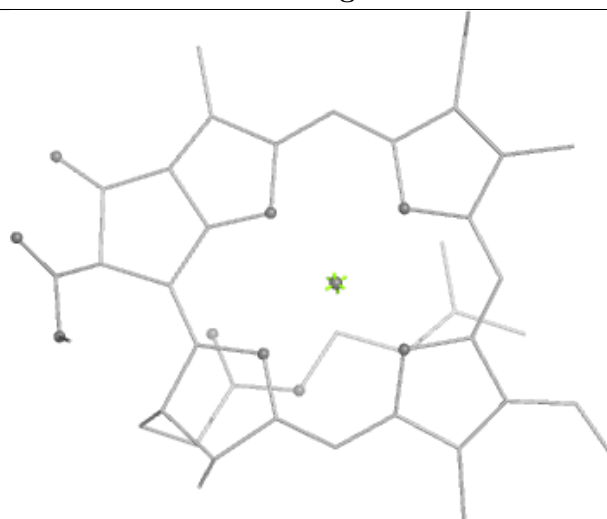
Bond lengths



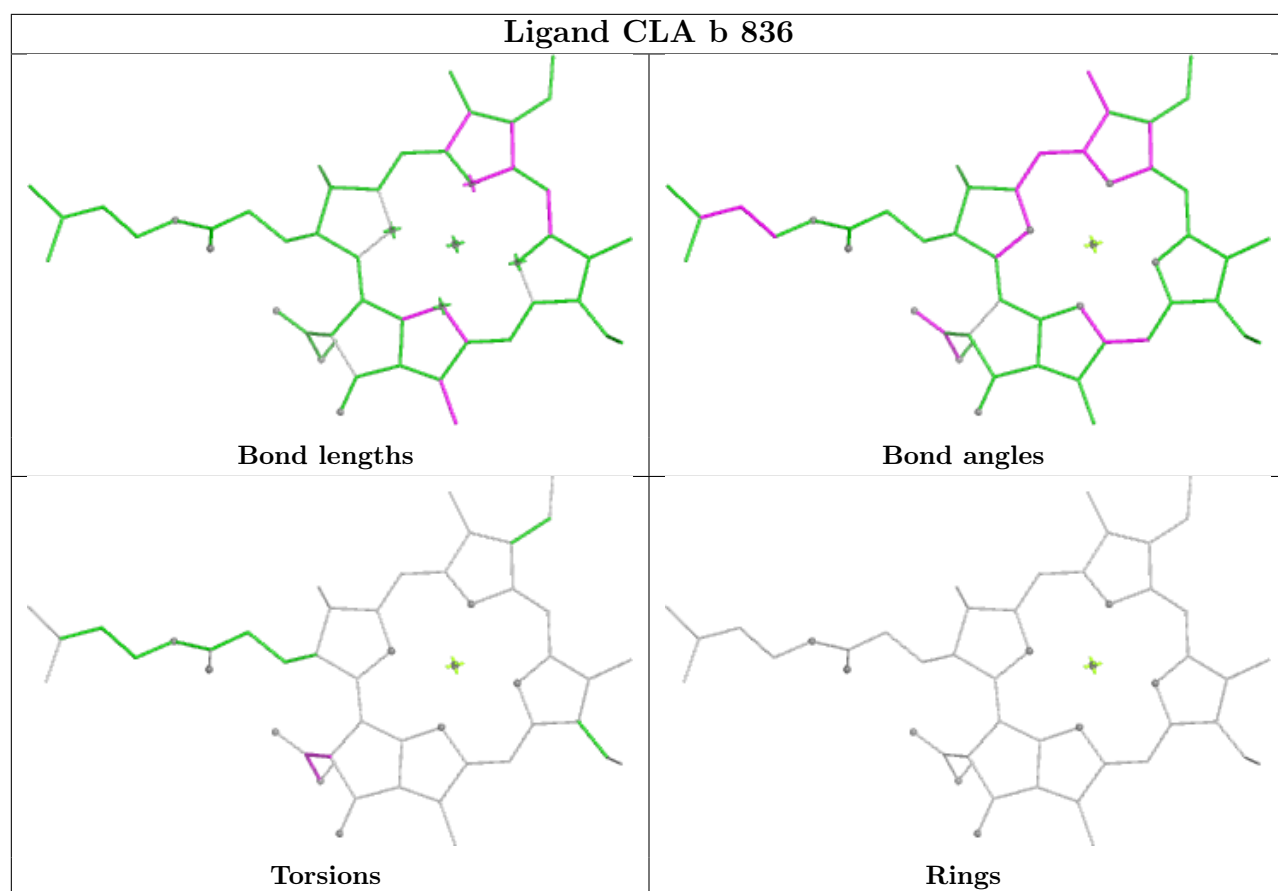
Bond angles

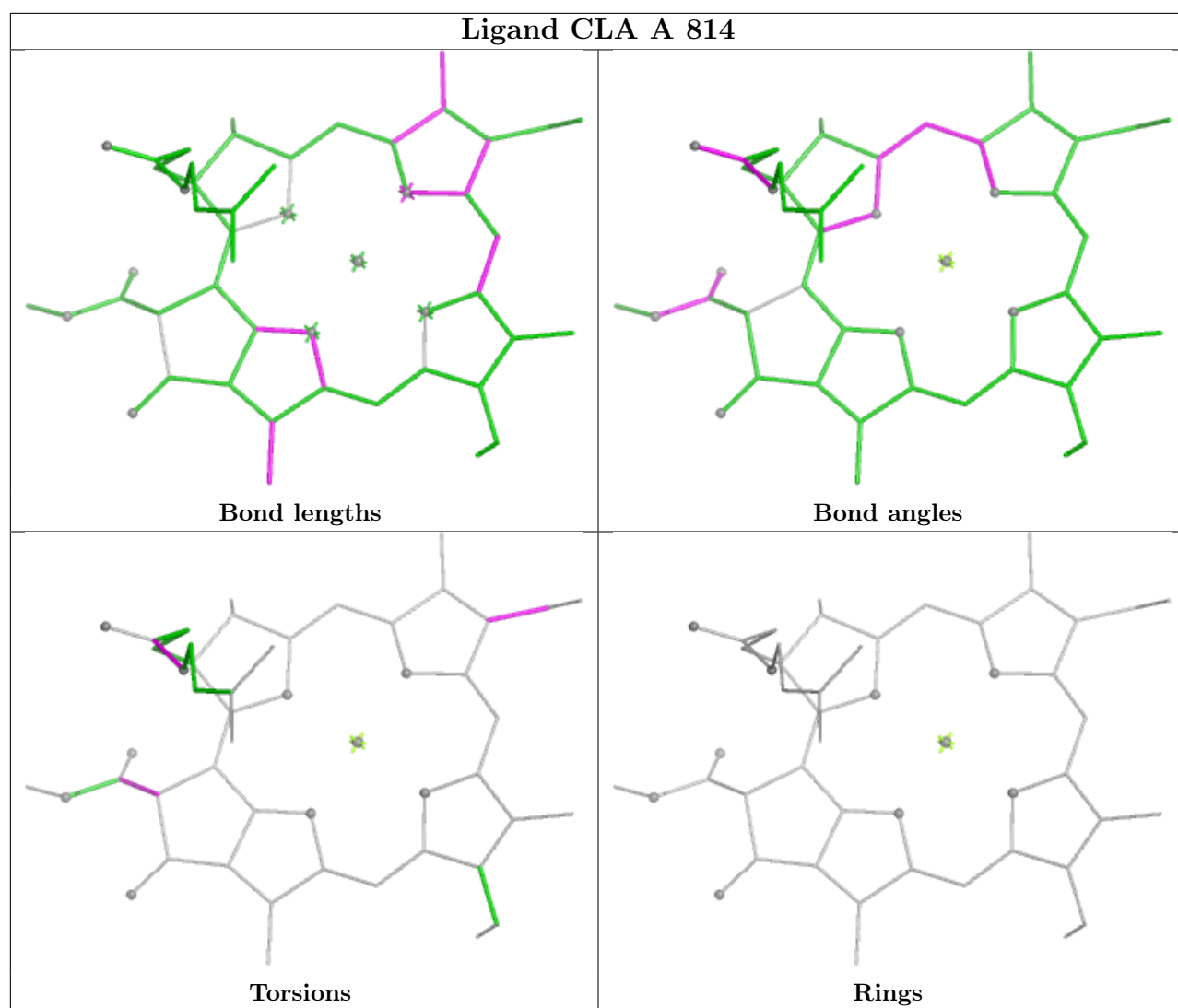


Torsions

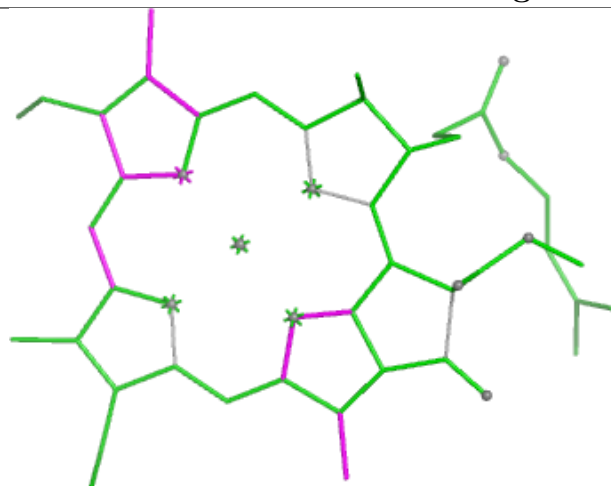


Rings

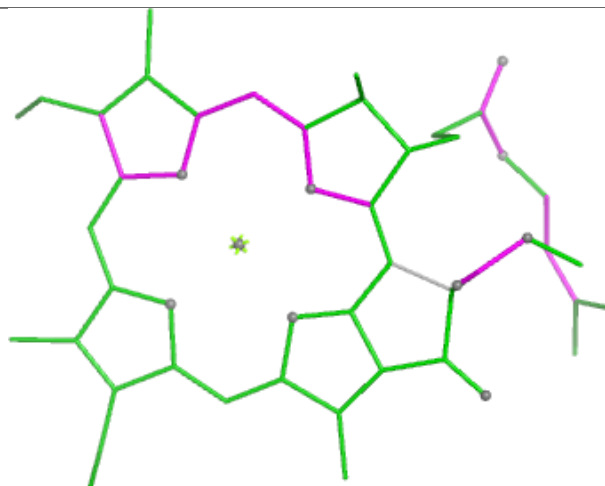




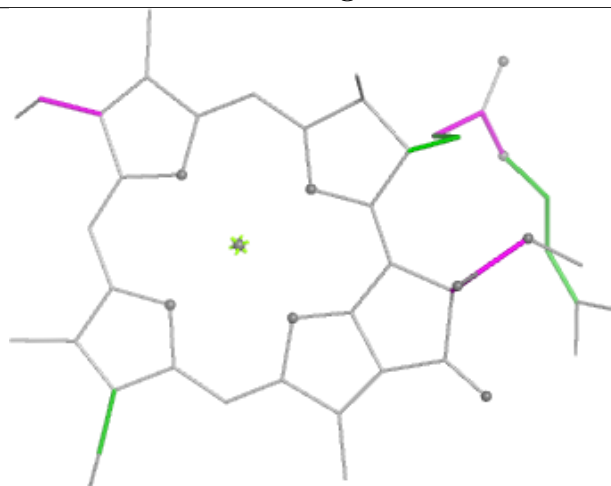
Ligand CLA G 817



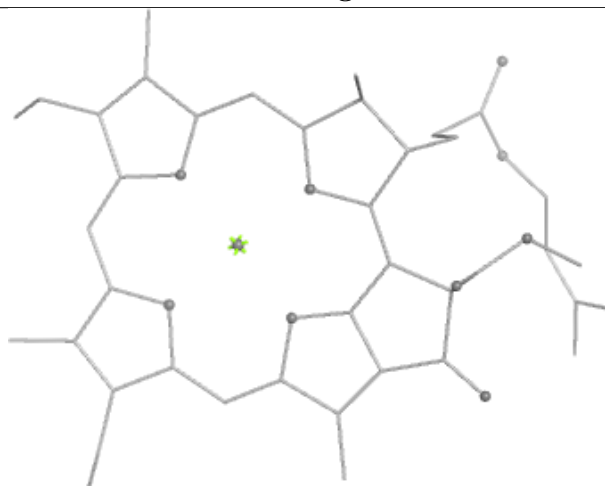
Bond lengths



Bond angles

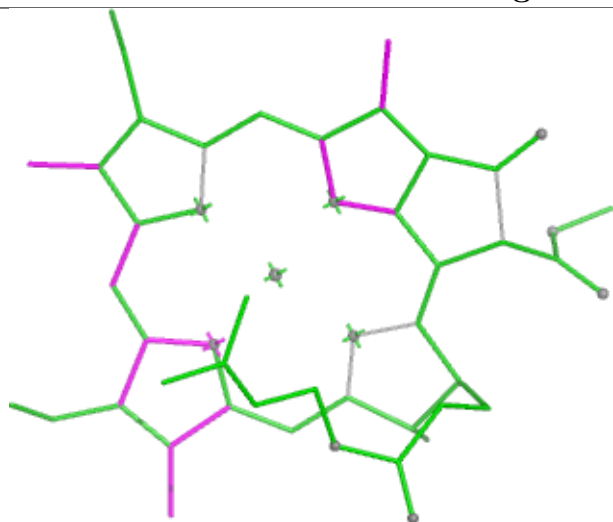


Torsions

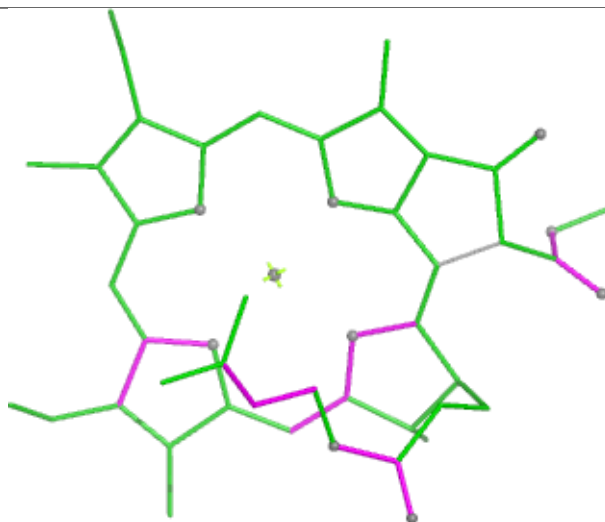


Rings

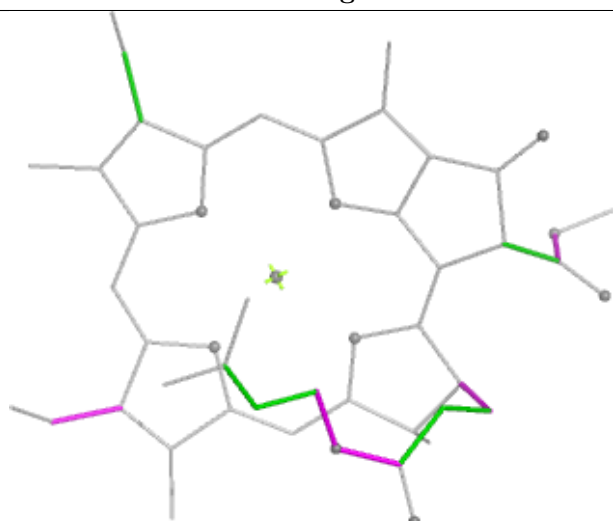
Ligand CLA G 828



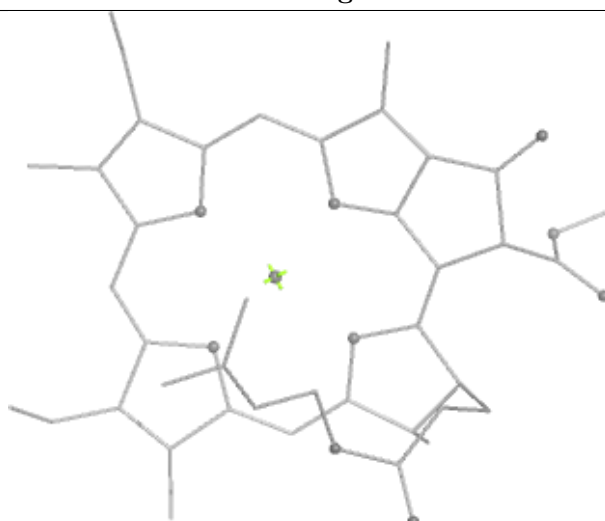
Bond lengths



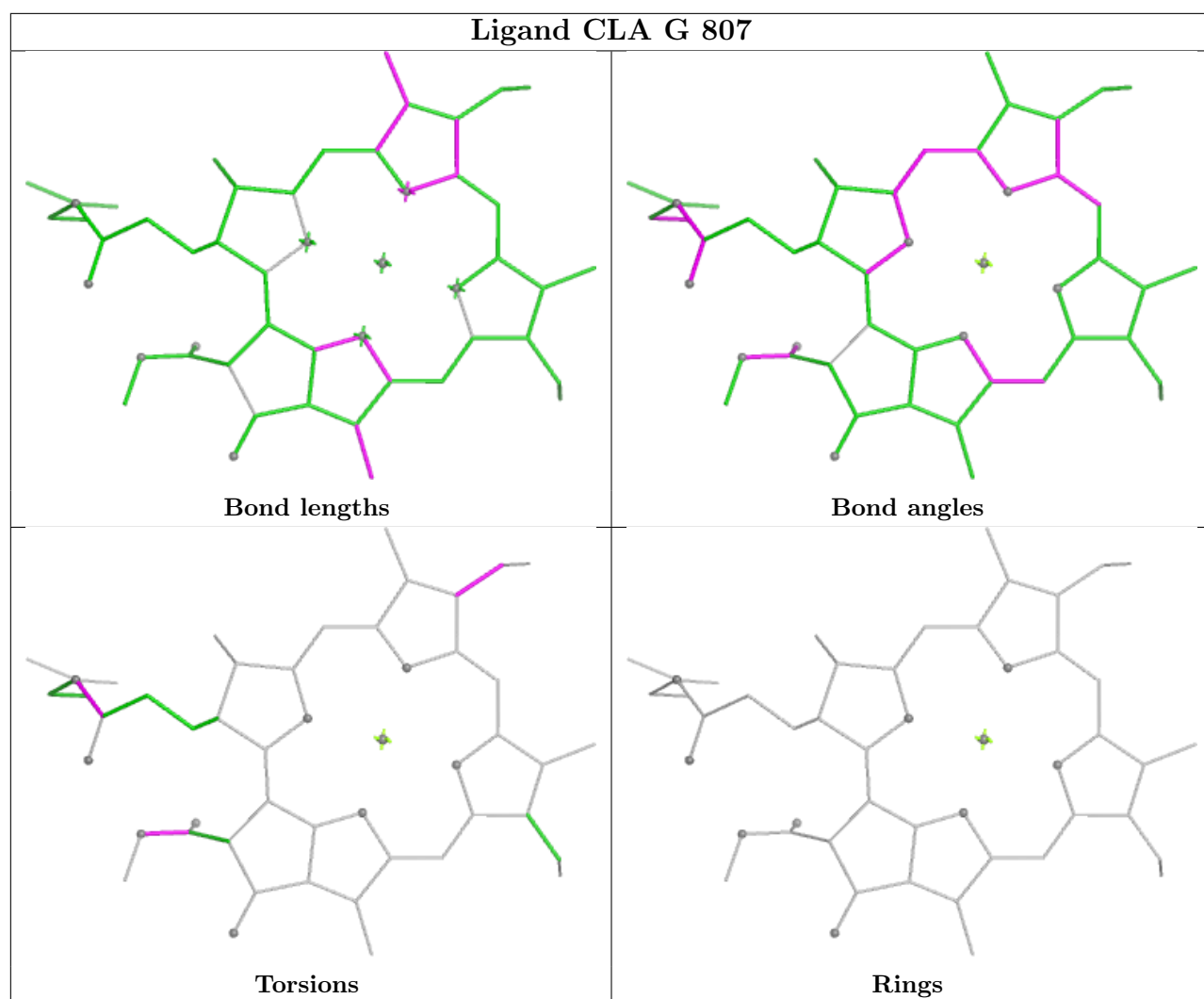
Bond angles



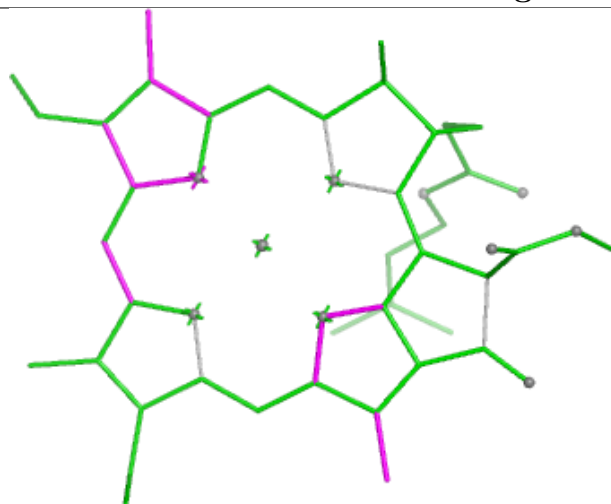
Torsions



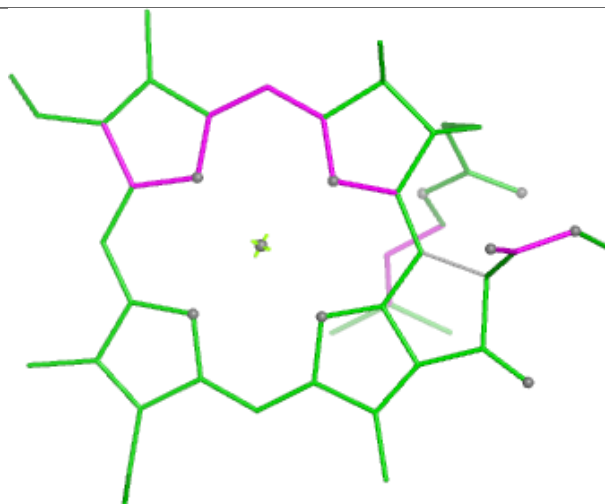
Rings



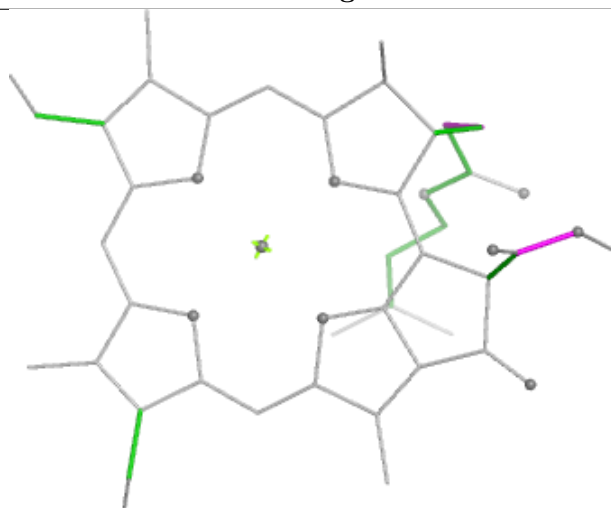
Ligand CLA B 815



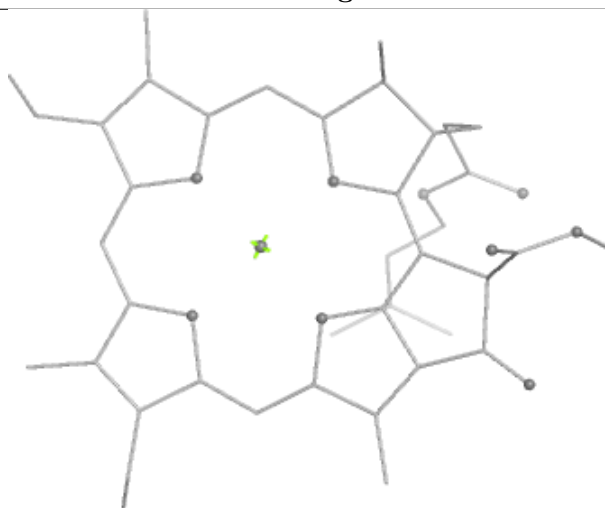
Bond lengths



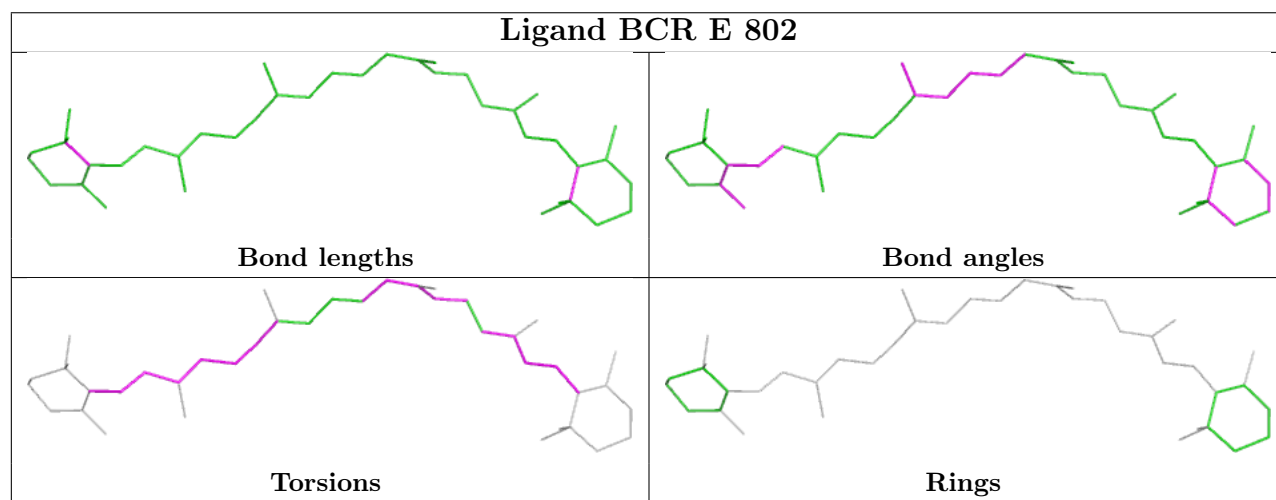
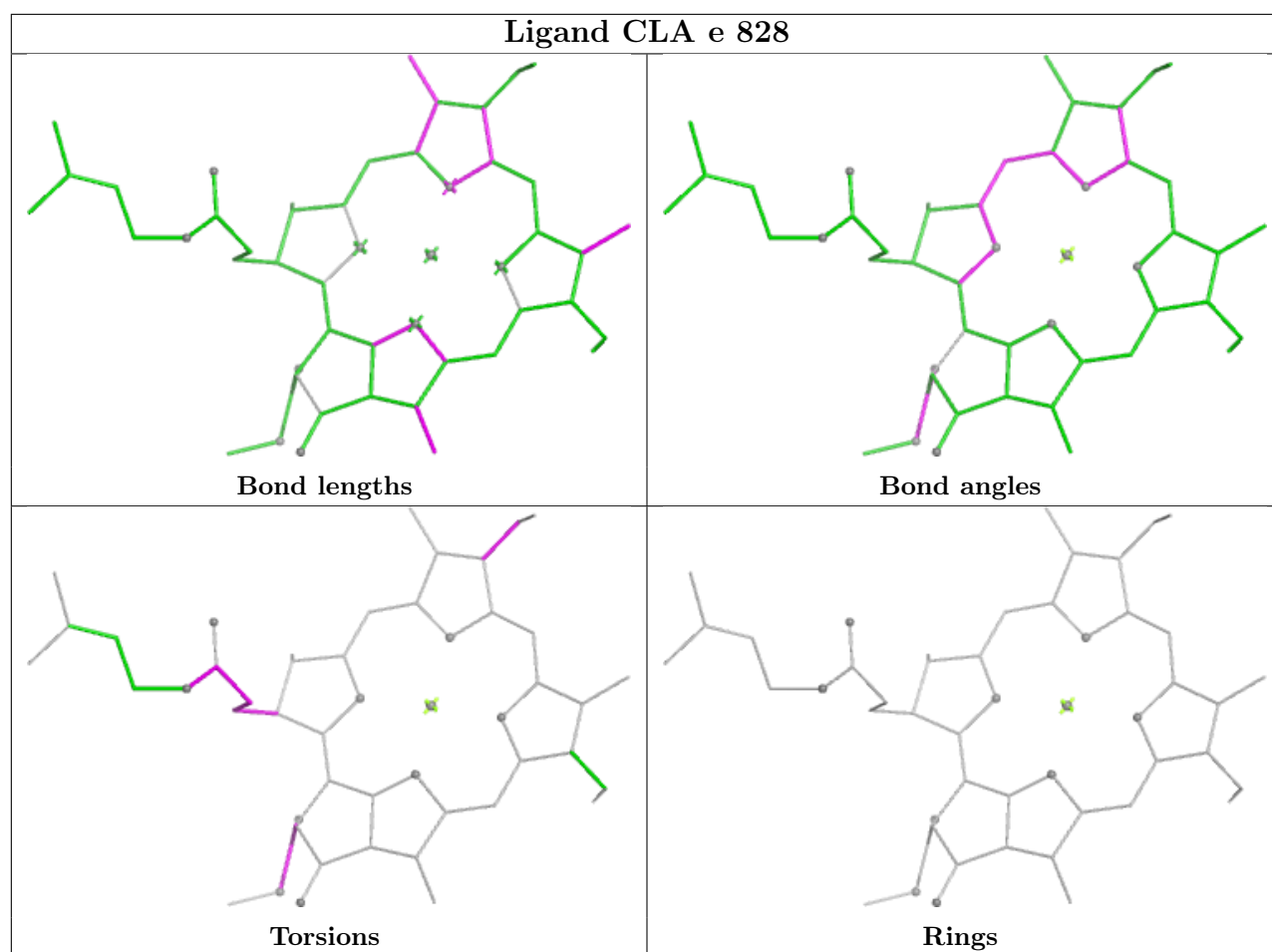
Bond angles



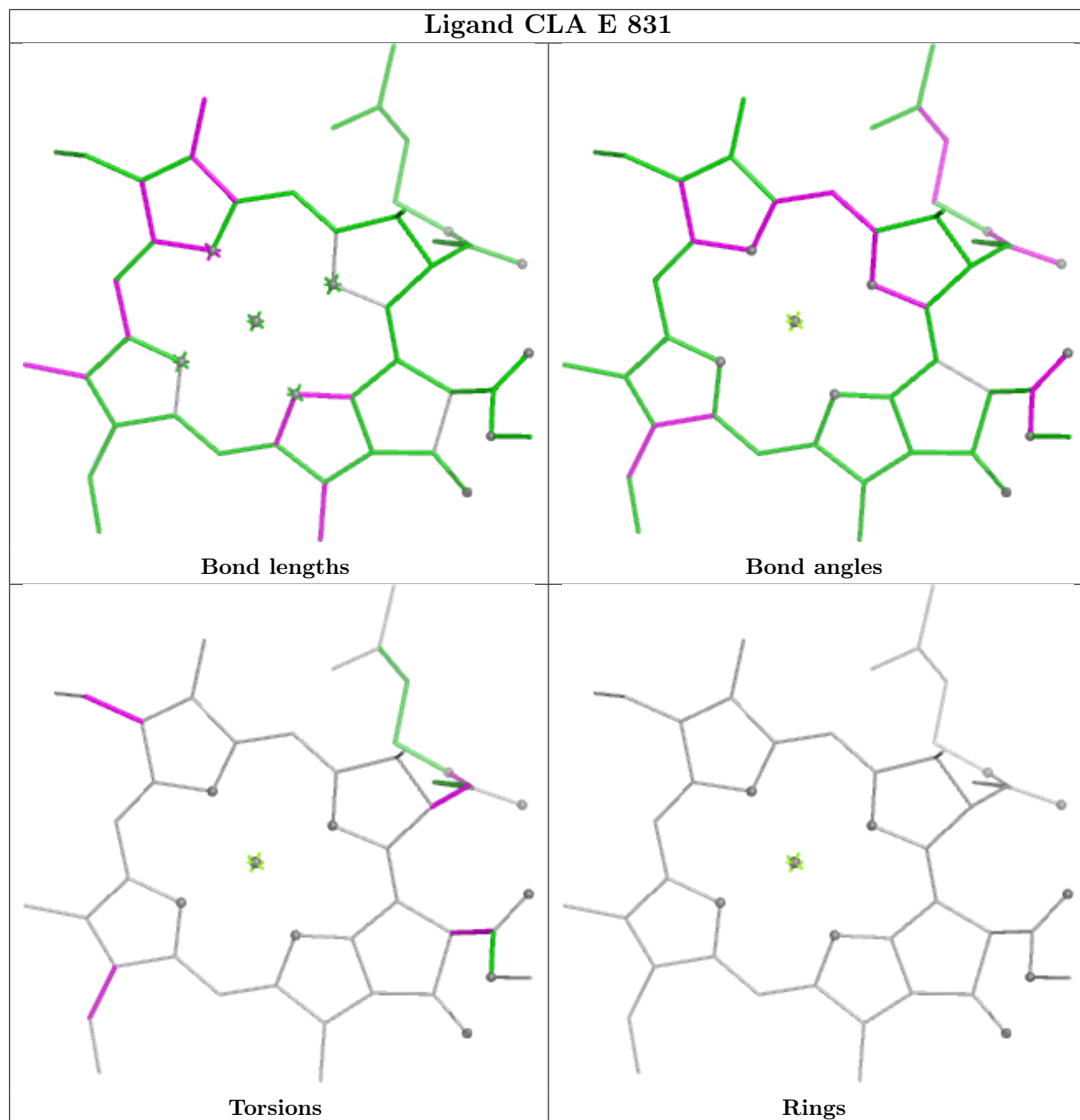
Torsions



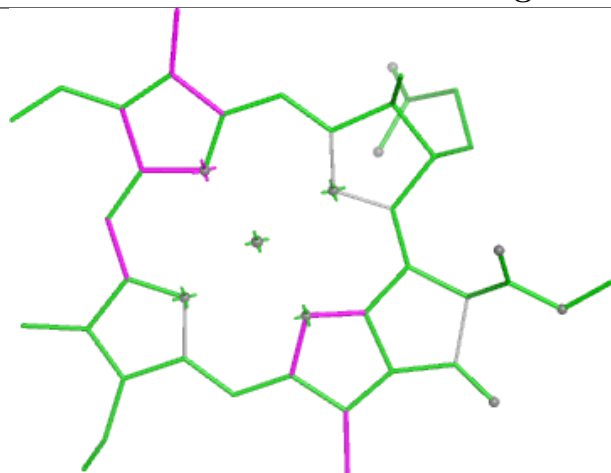
Rings



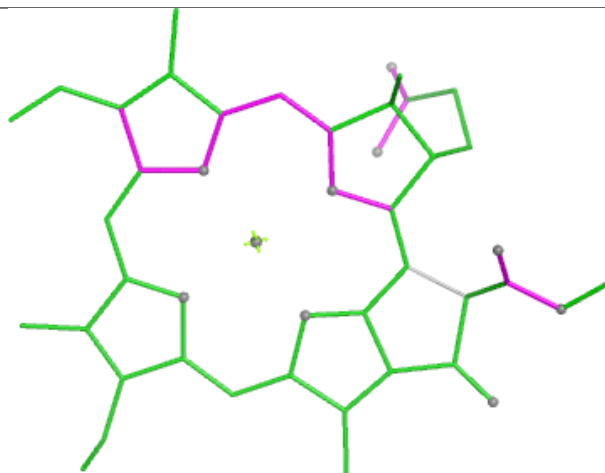
Ligand CLA E 831



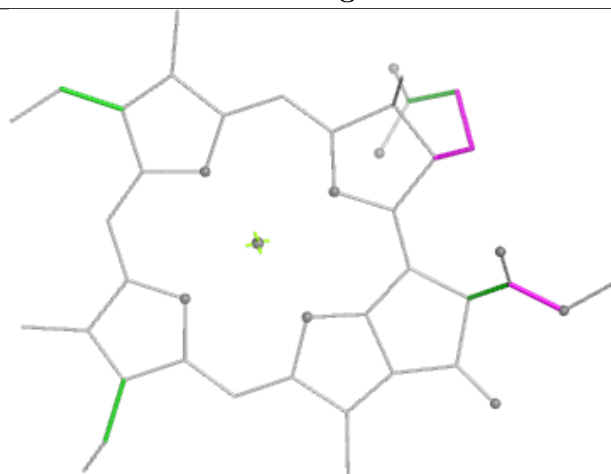
Ligand CLA B 813



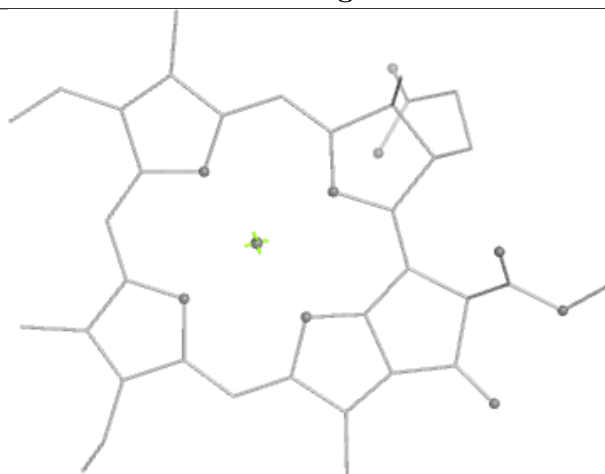
Bond lengths



Bond angles

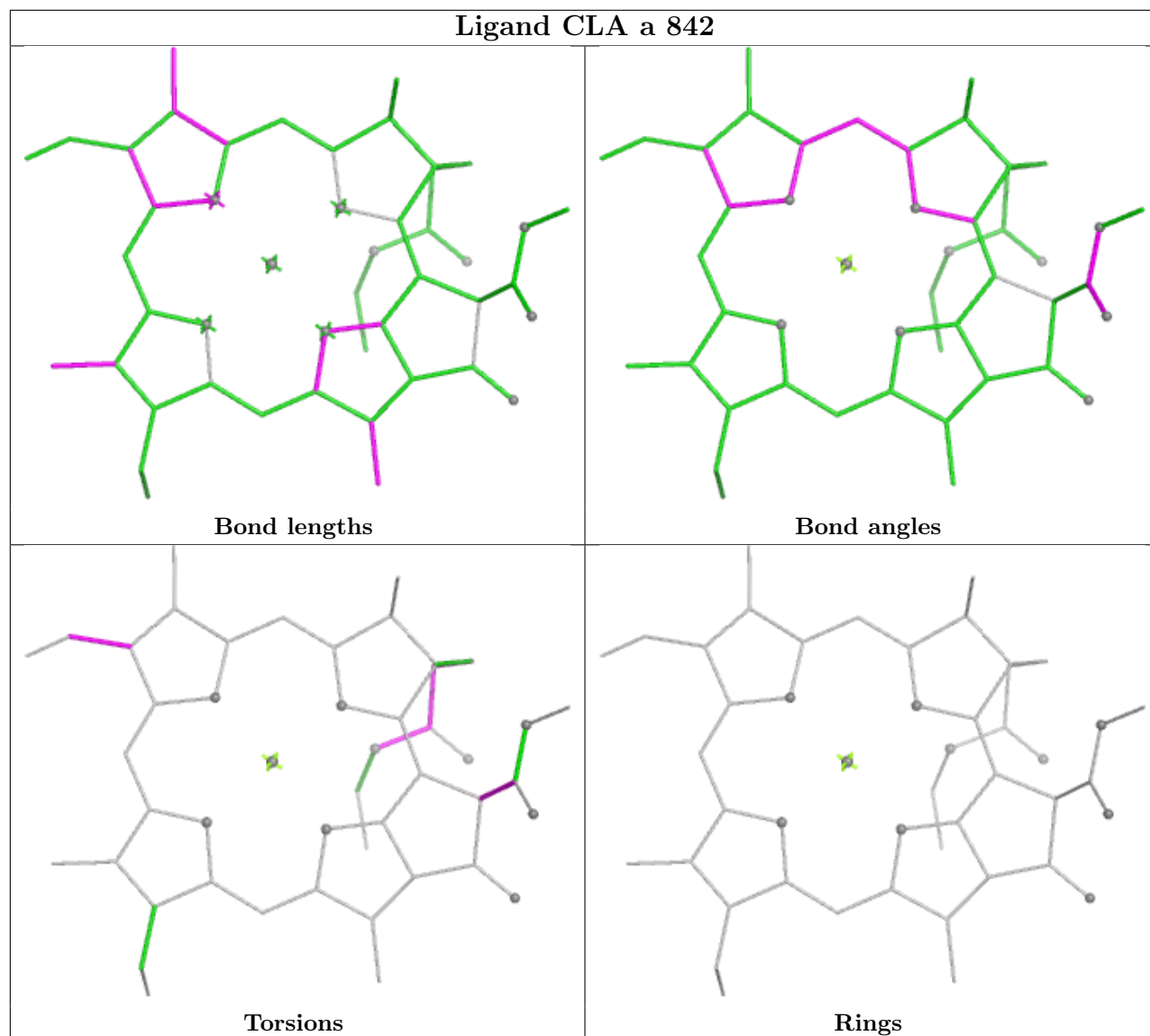


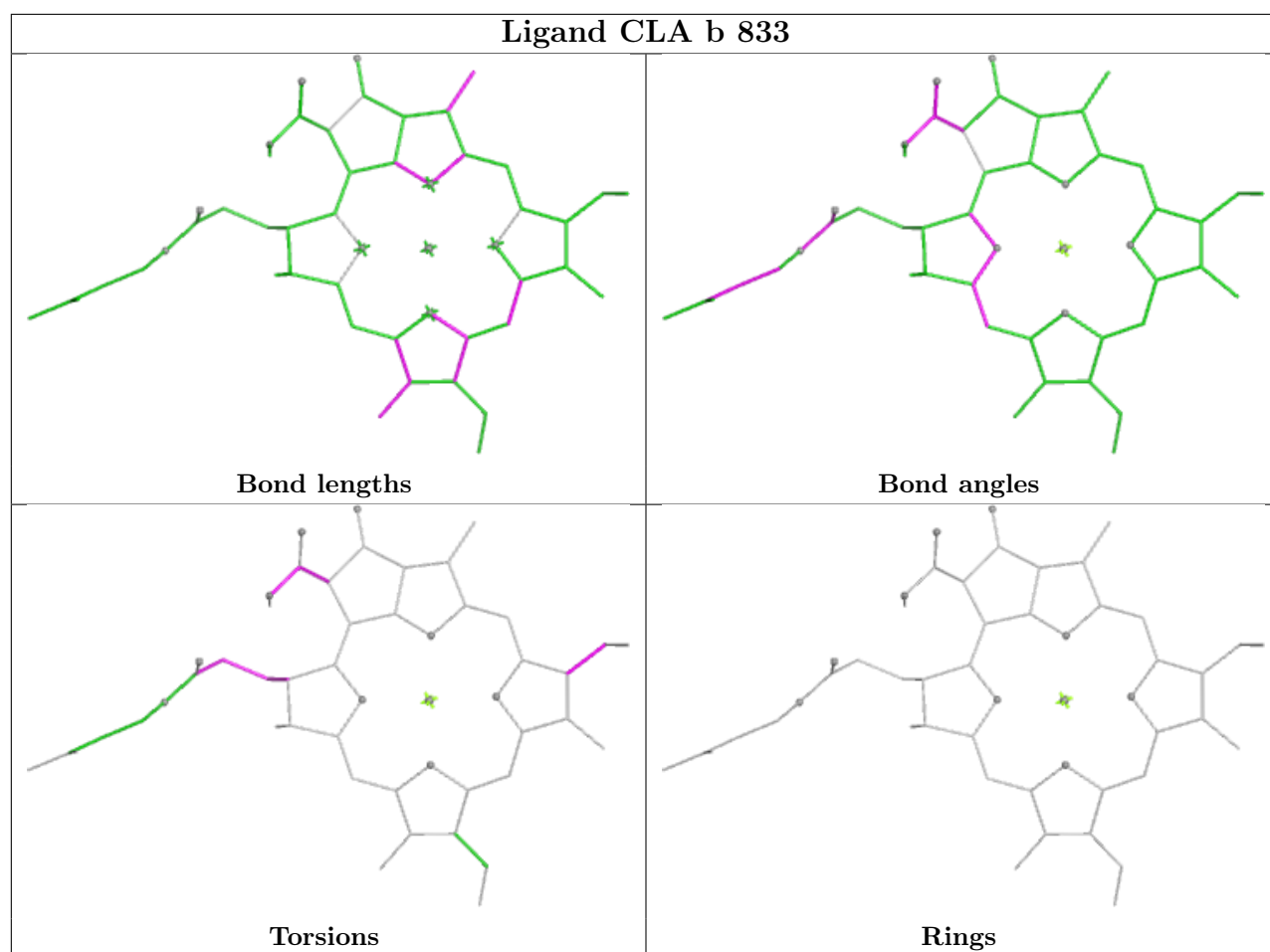
Torsions



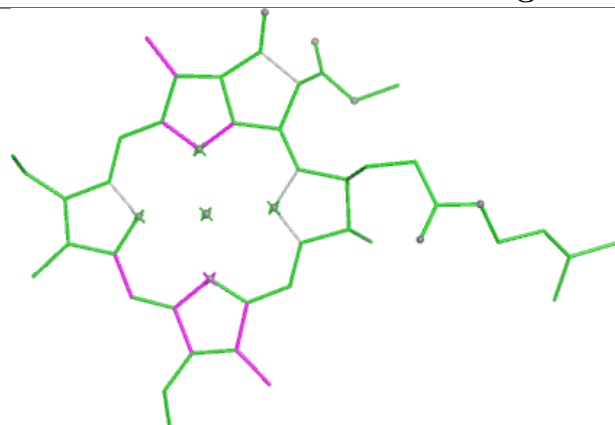
Rings

Ligand CLA a 842

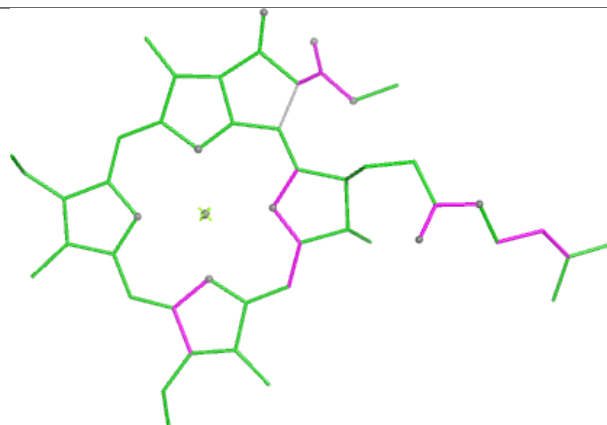




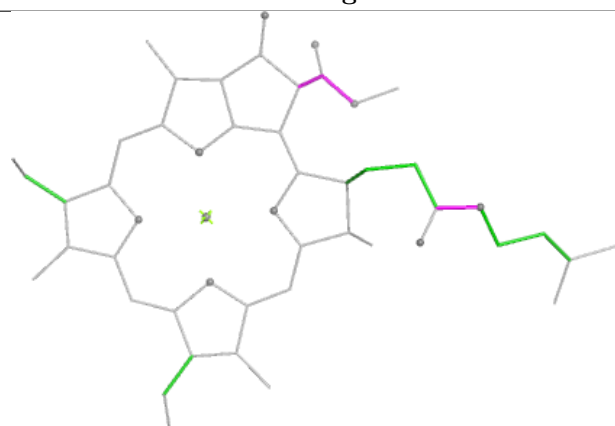
Ligand CLA E 816



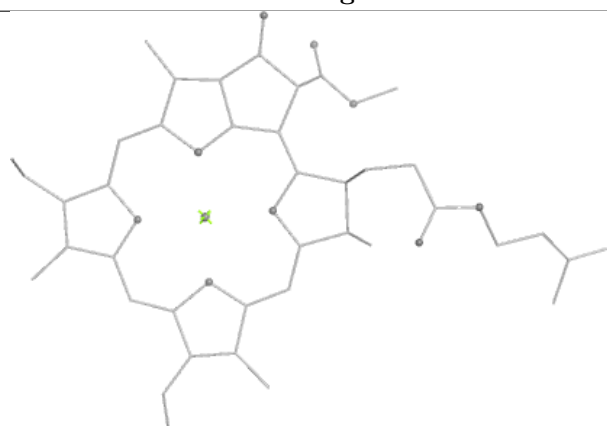
Bond lengths



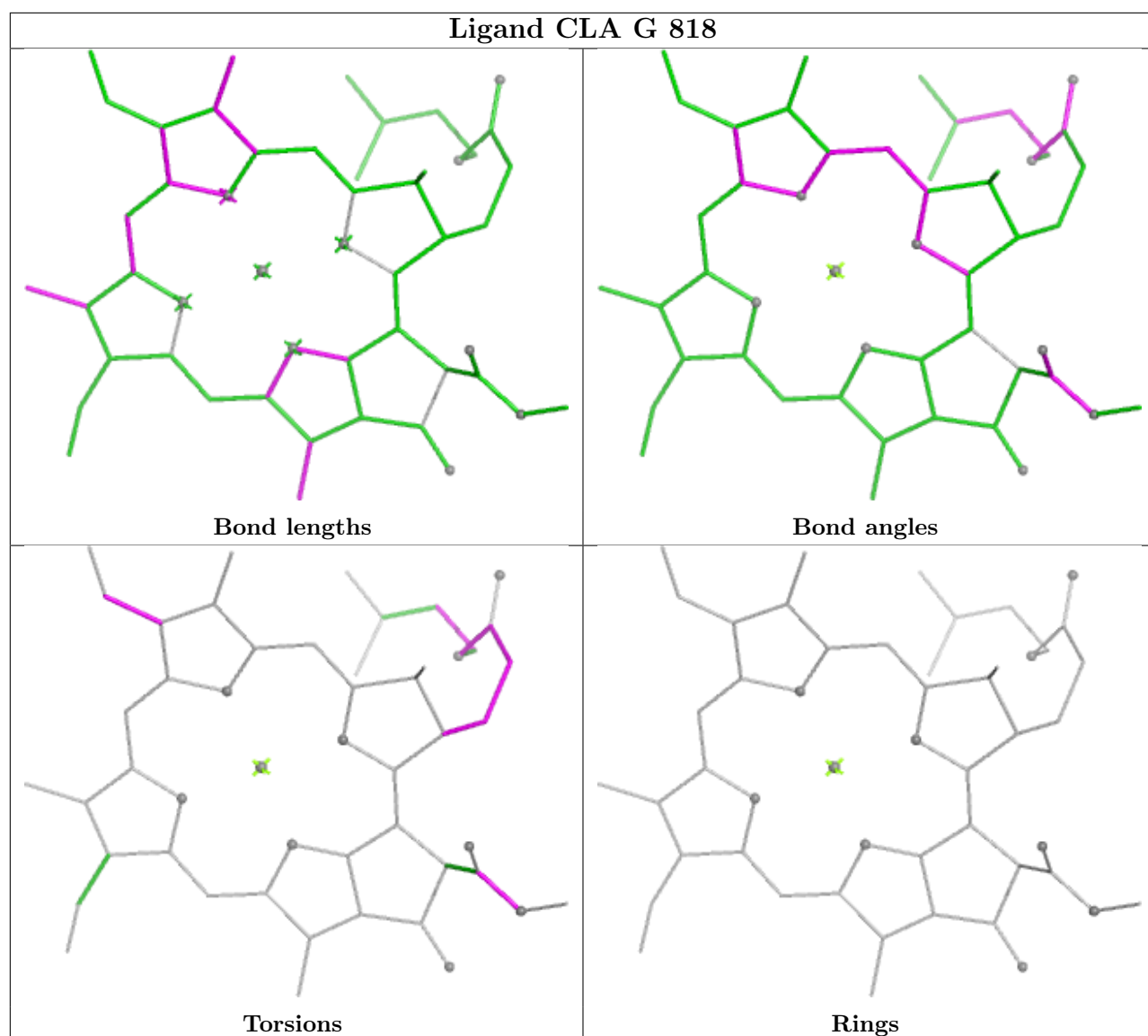
Bond angles



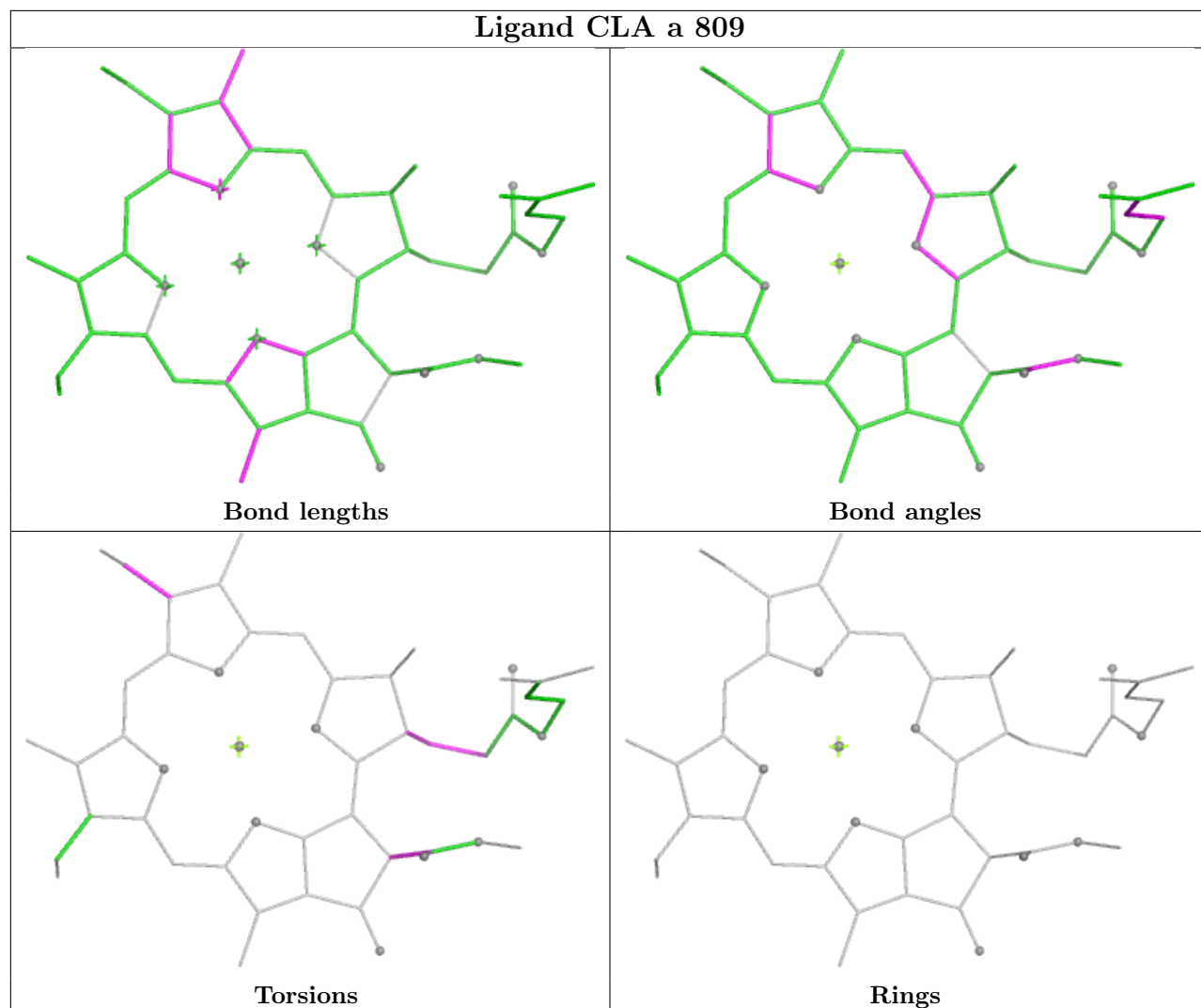
Torsions



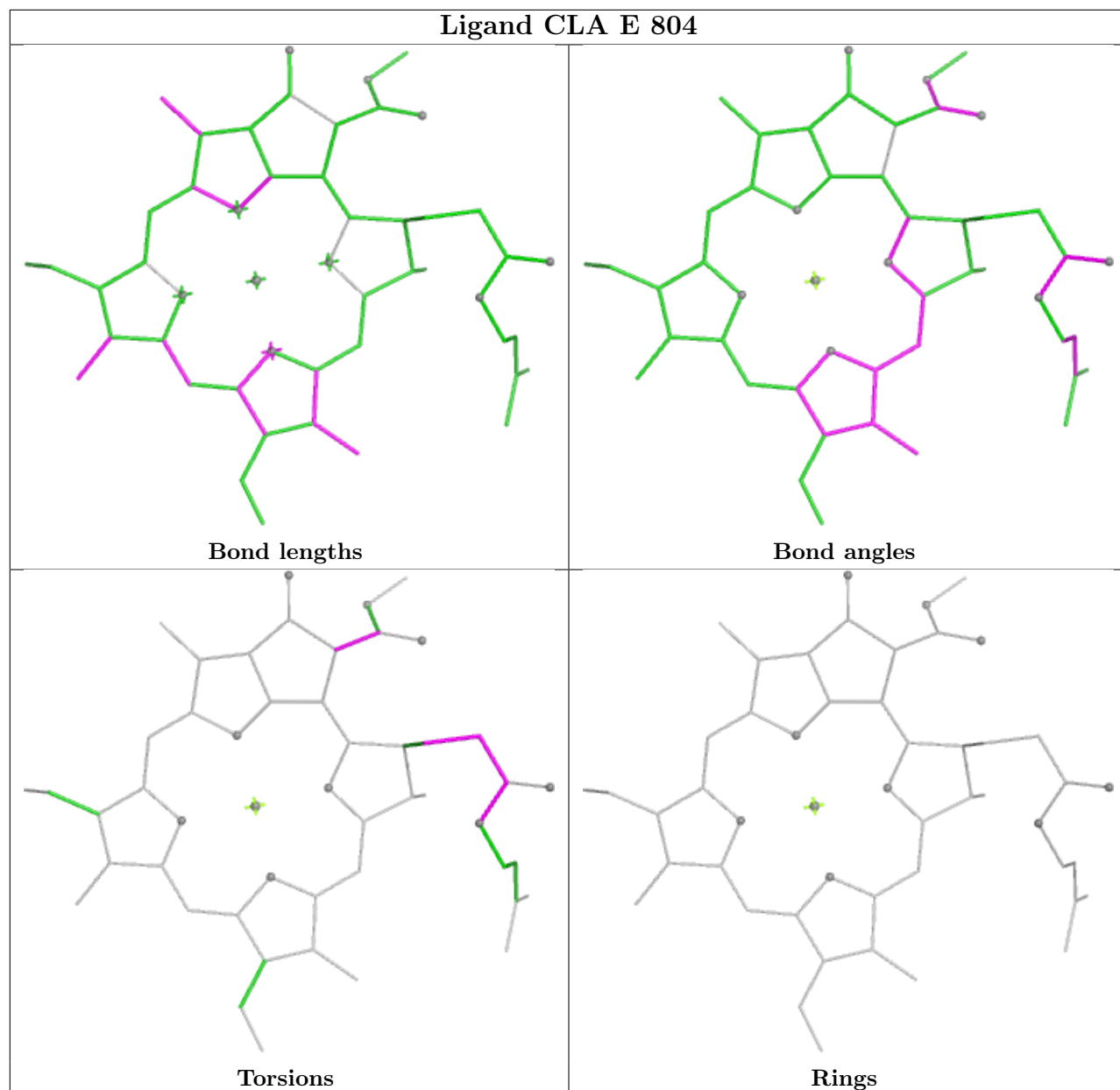
Rings



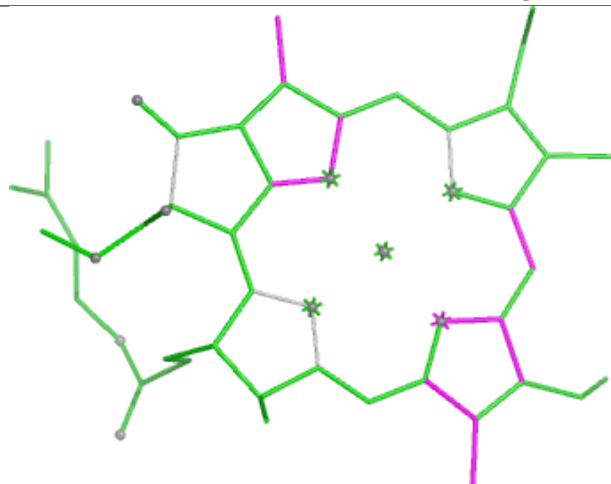
Ligand CLA a 809



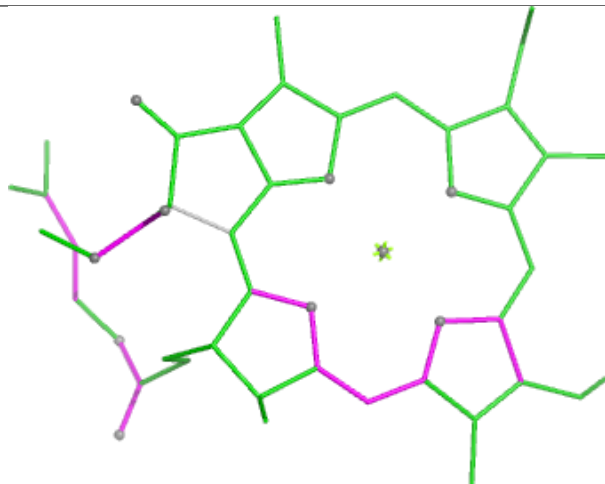
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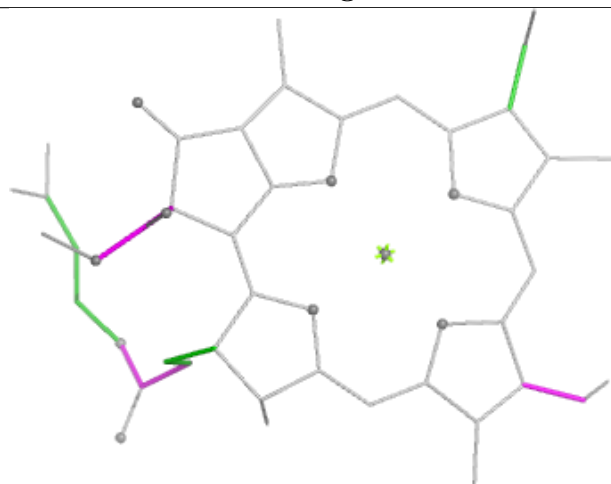
Ligand CLA b 816



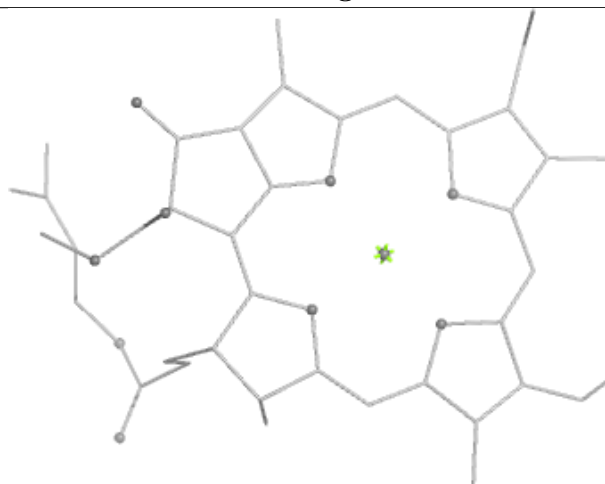
Bond lengths



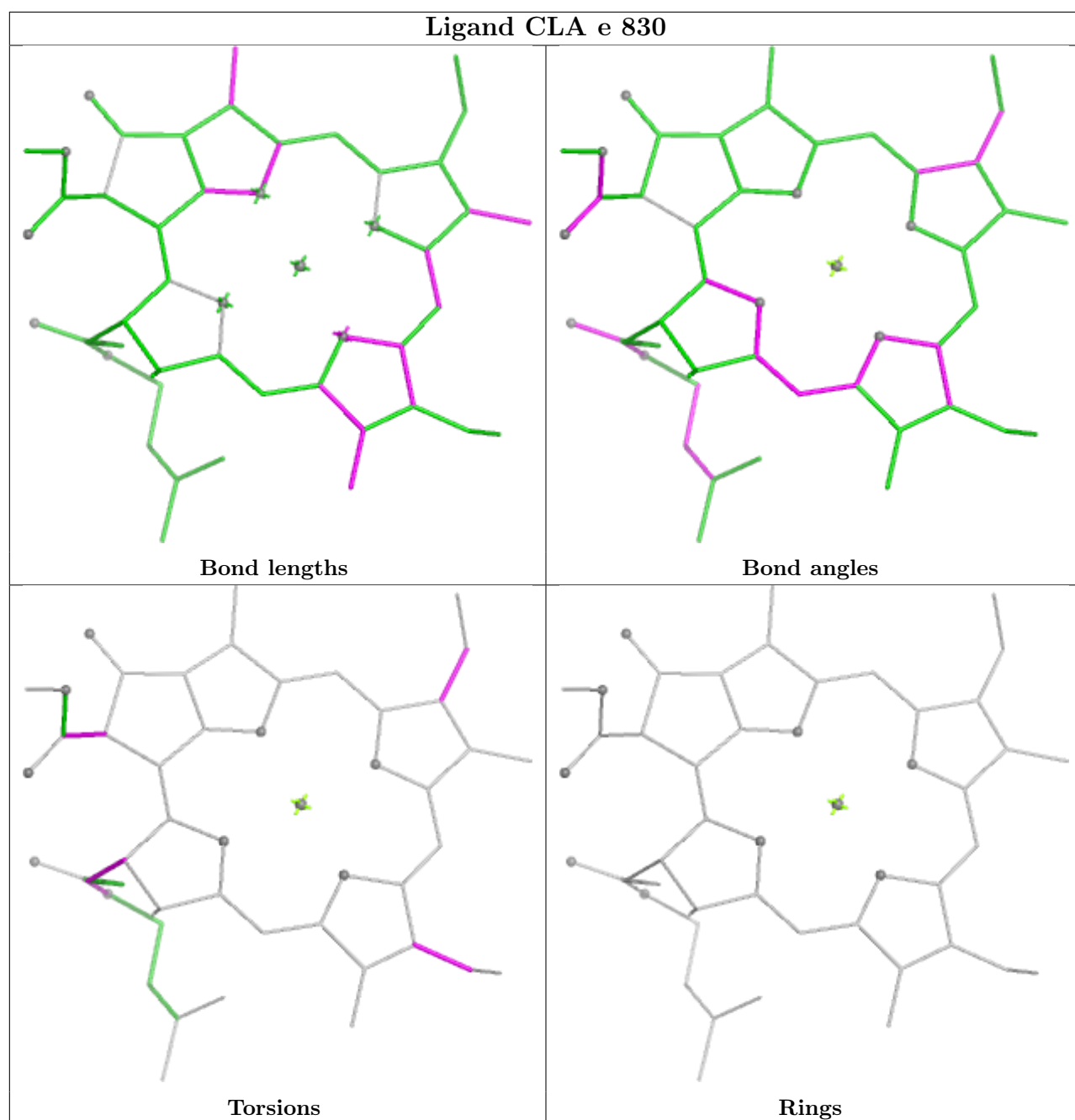
Bond angles



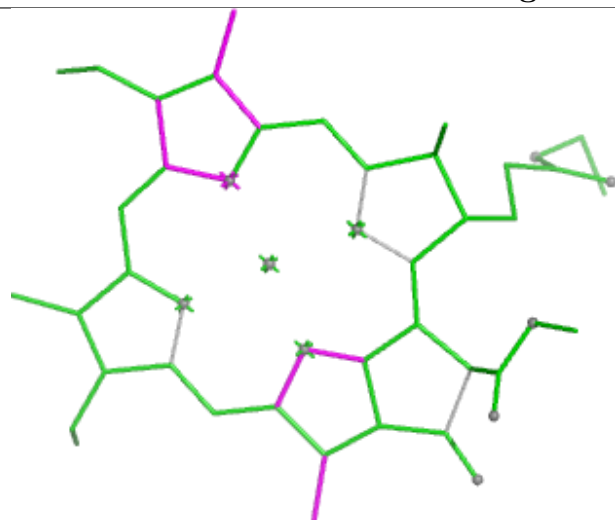
Torsions



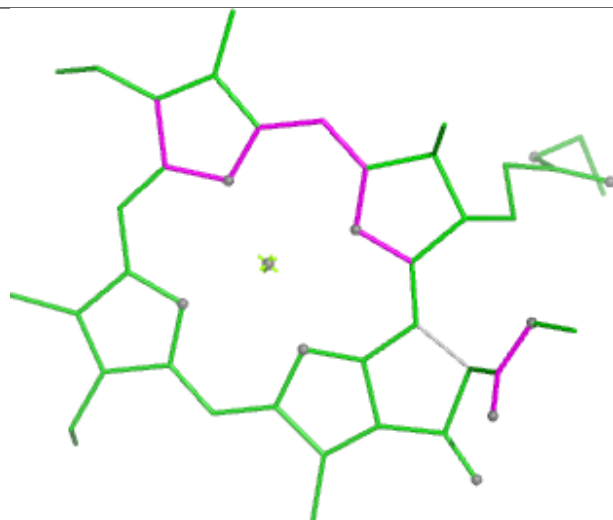
Rings



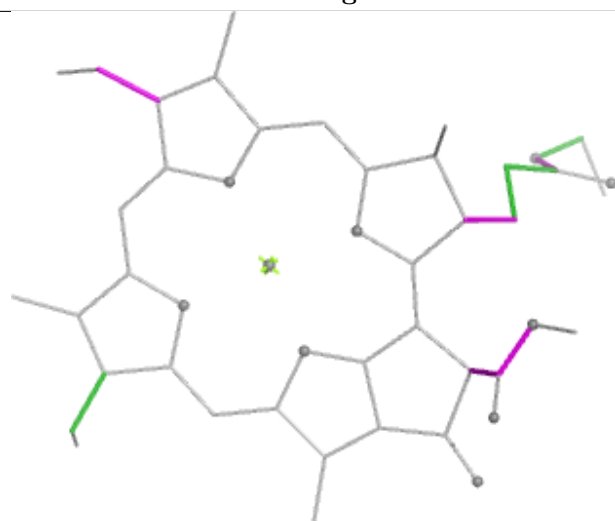
Ligand CLA b 838



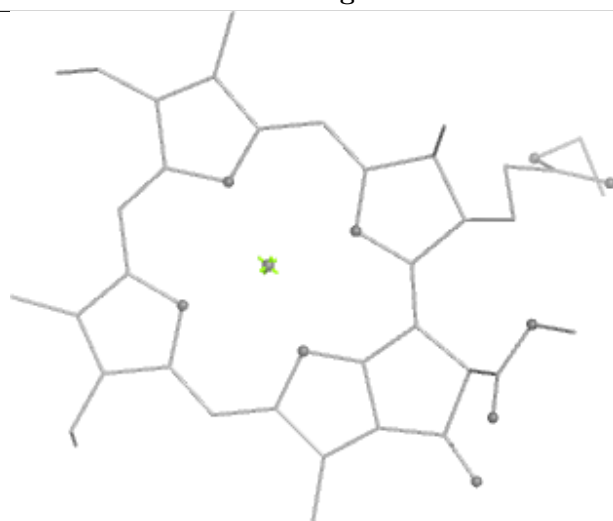
Bond lengths



Bond angles

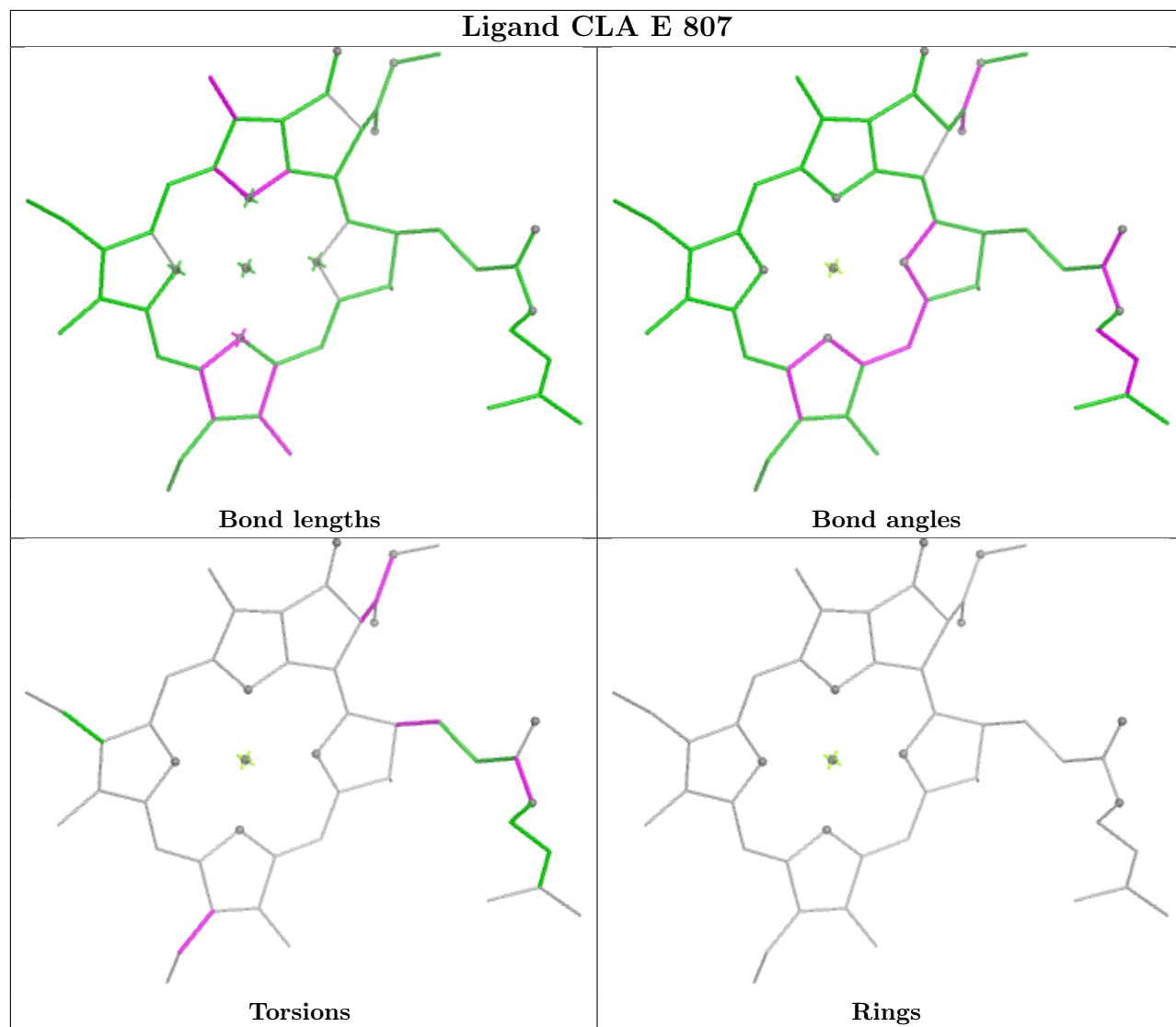


Torsions

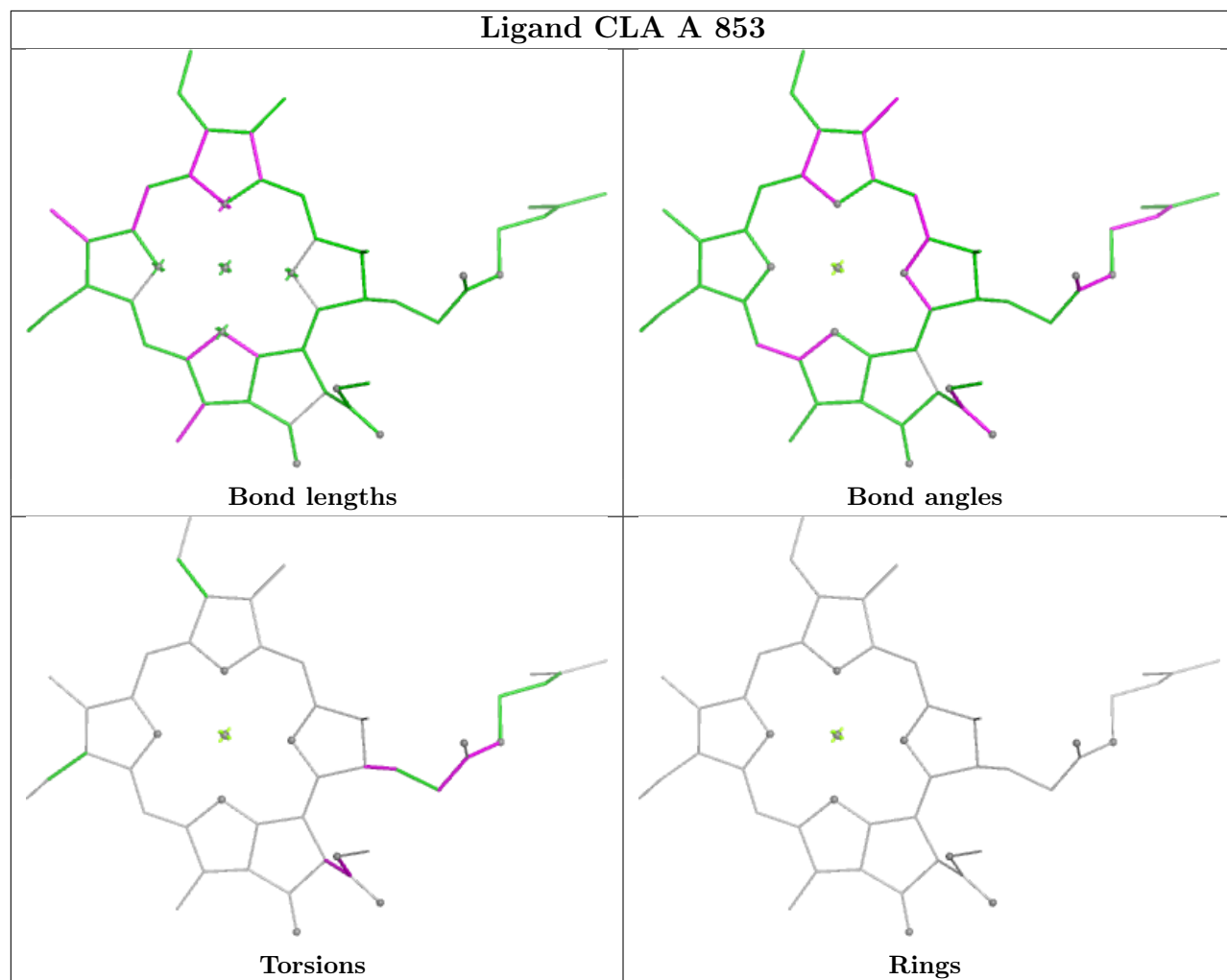


Rings

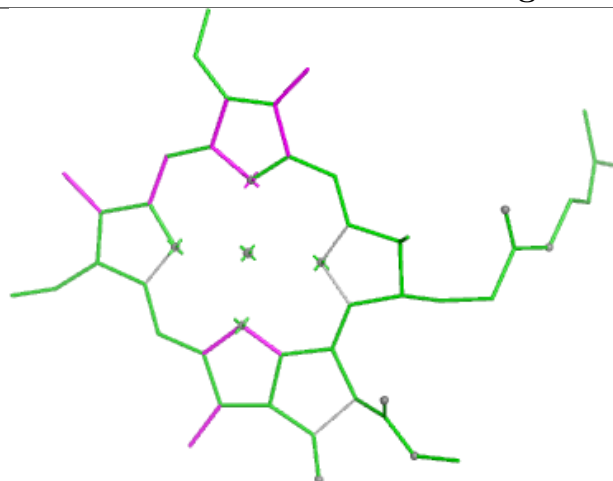
Ligand CLA E 807



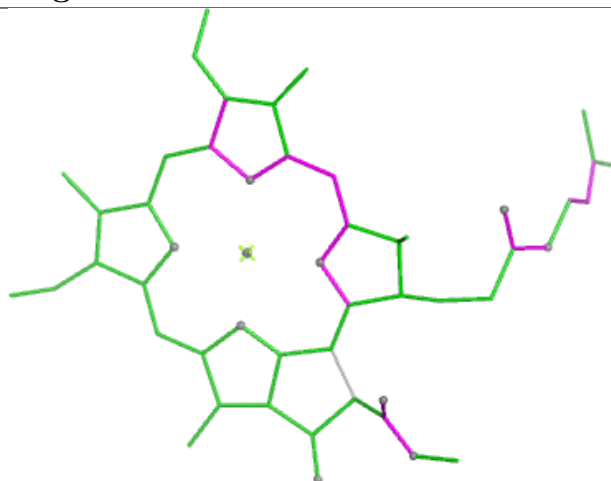
Ligand CLA A 853



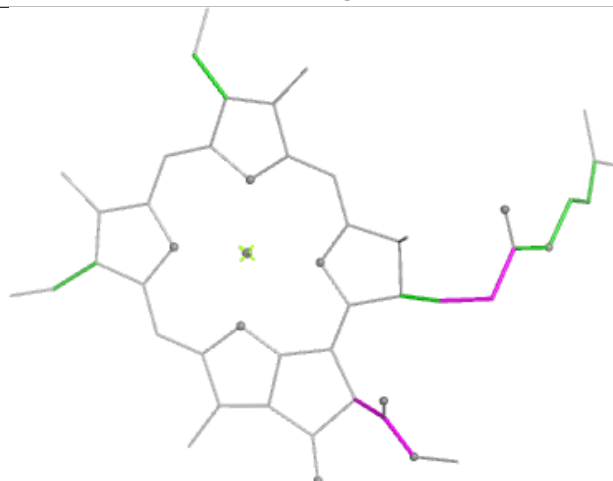
Ligand CLA g 812



Bond lengths



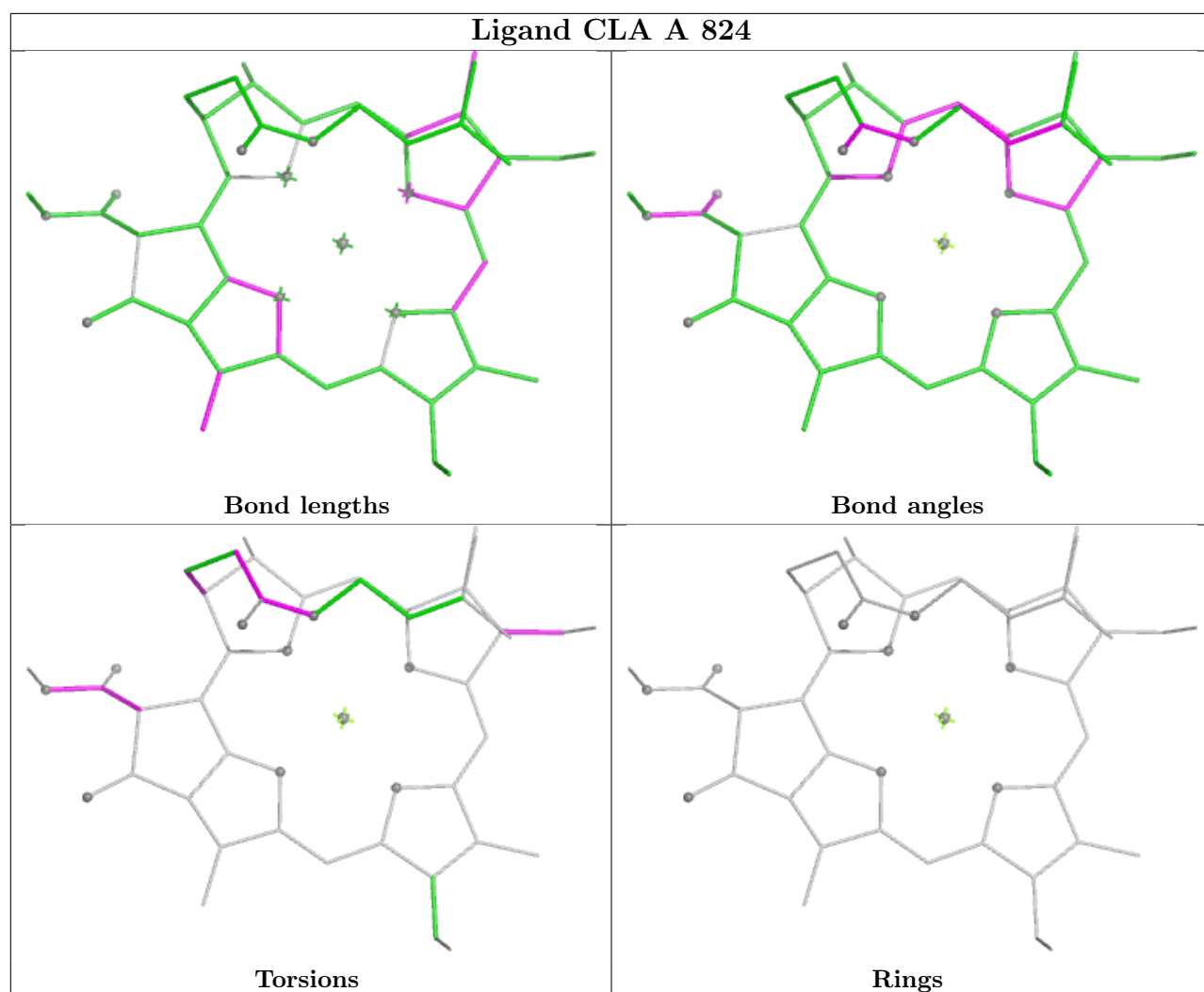
Bond angles



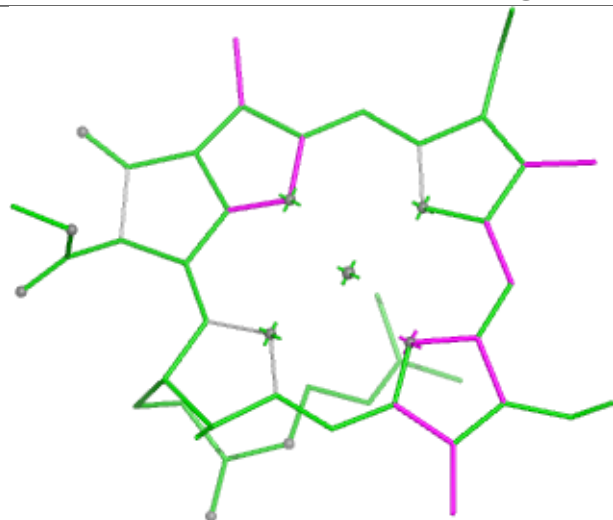
Torsions



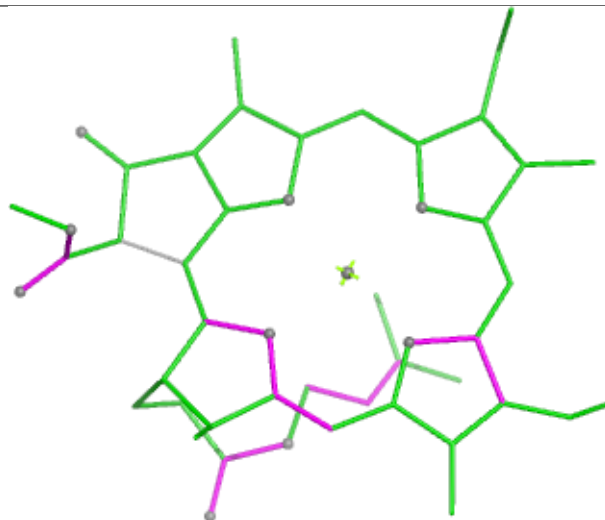
Rings



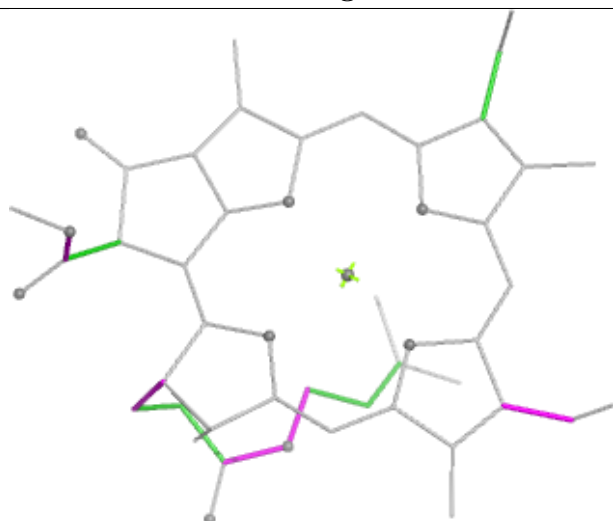
Ligand CLA b 827



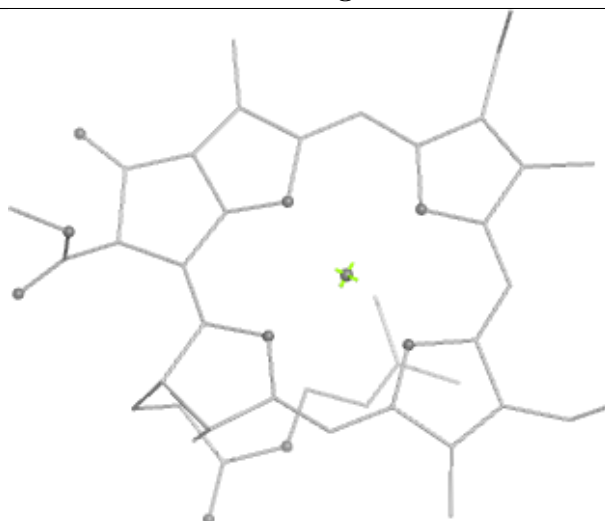
Bond lengths



Bond angles

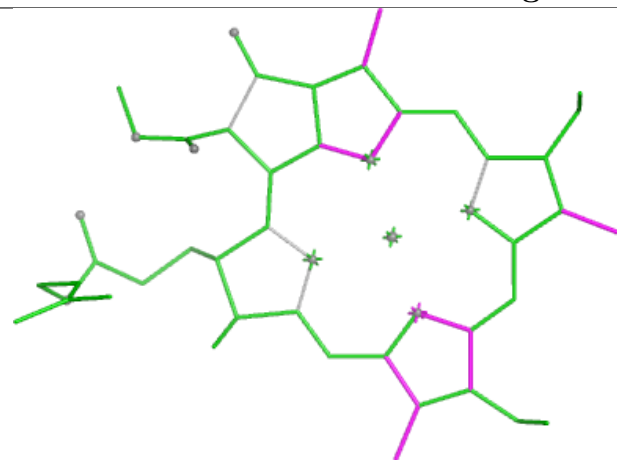


Torsions

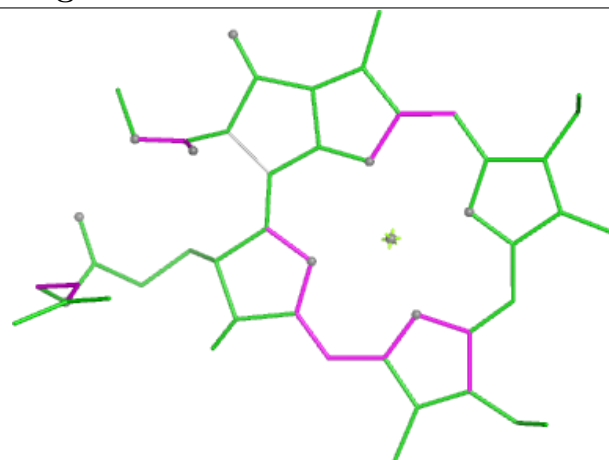


Rings

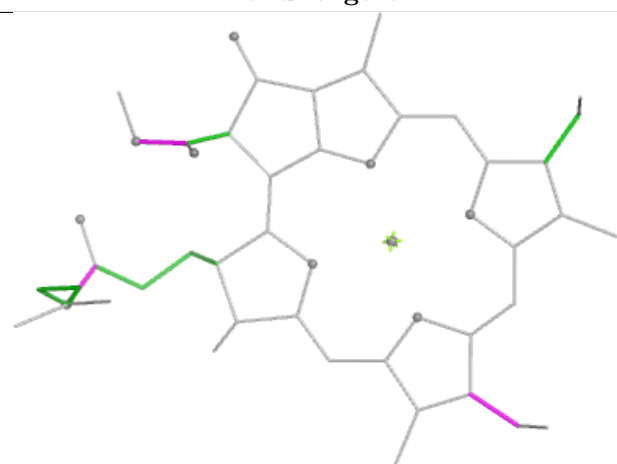
Ligand CLA g 809



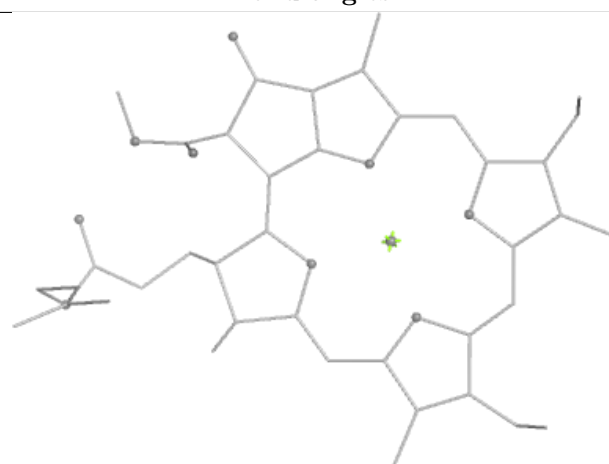
Bond lengths



Bond angles

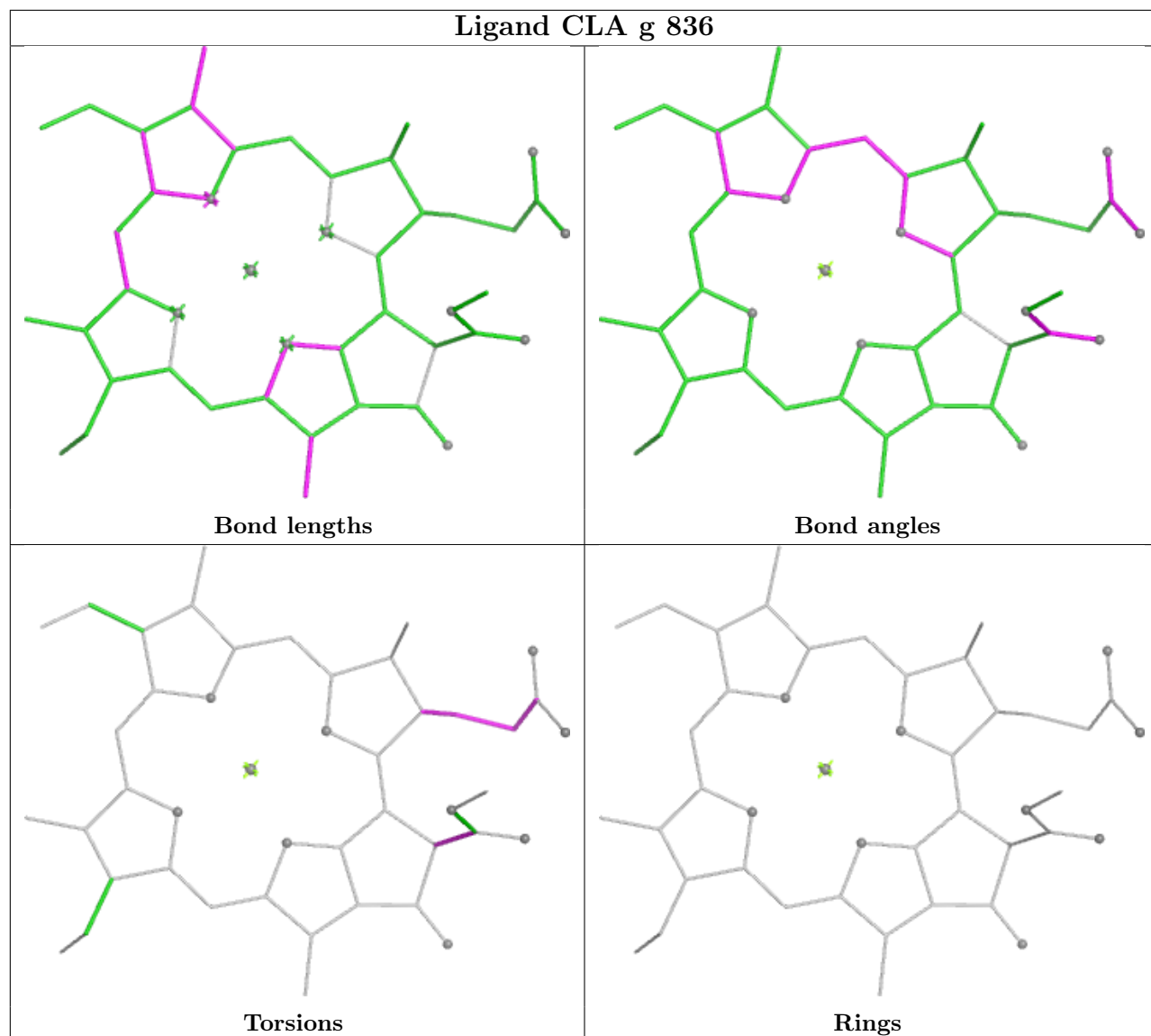


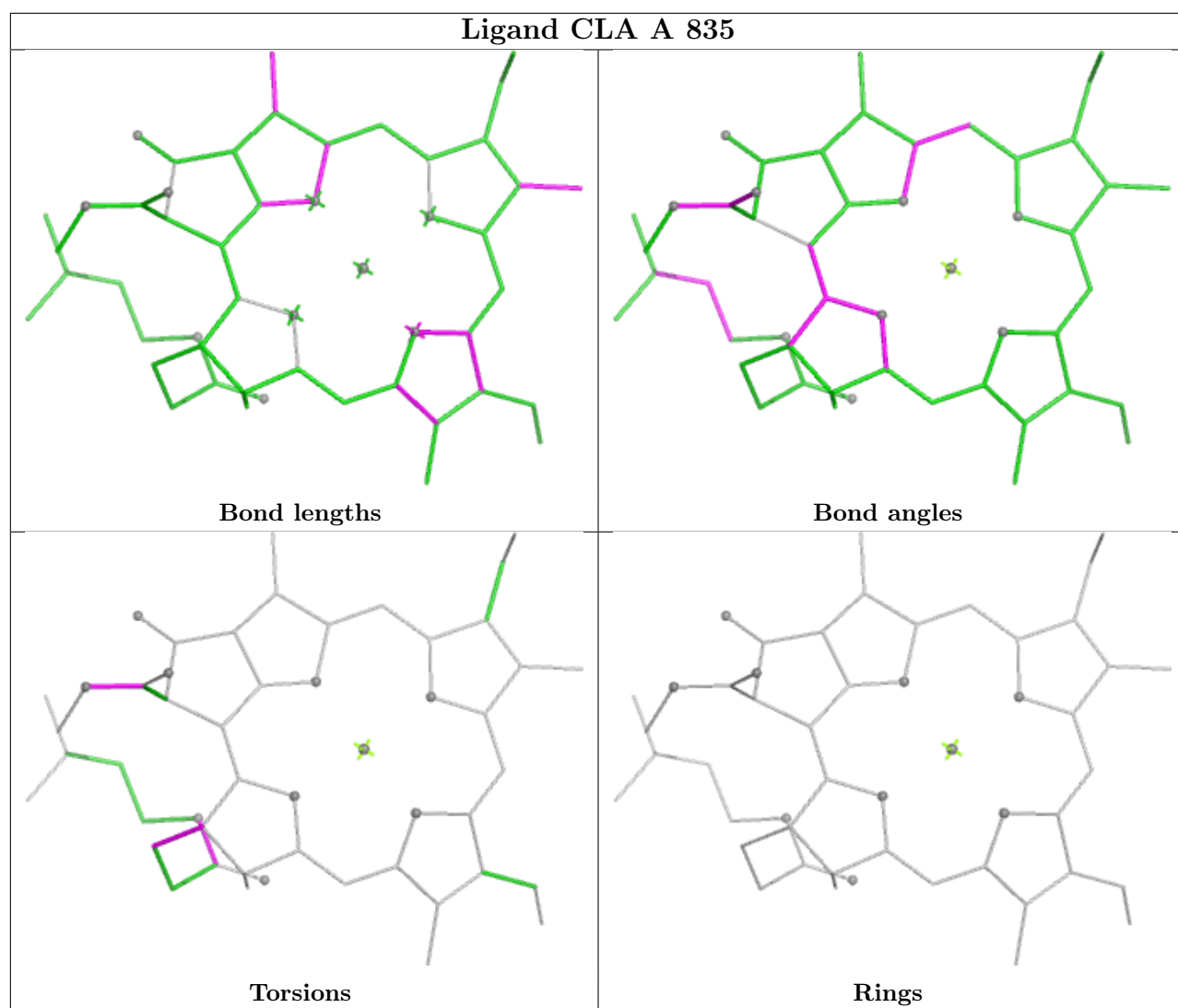
Torsions



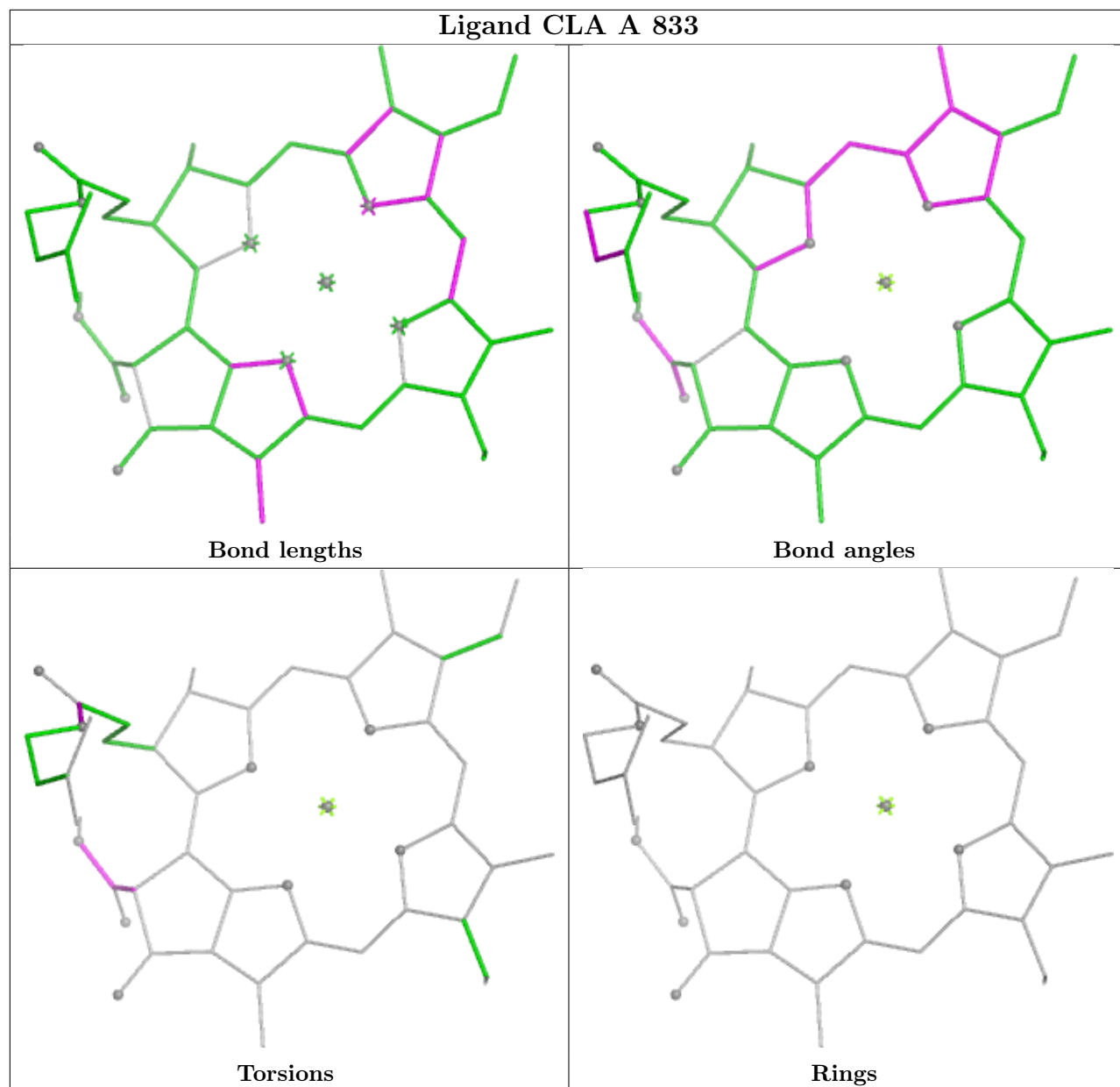
Rings

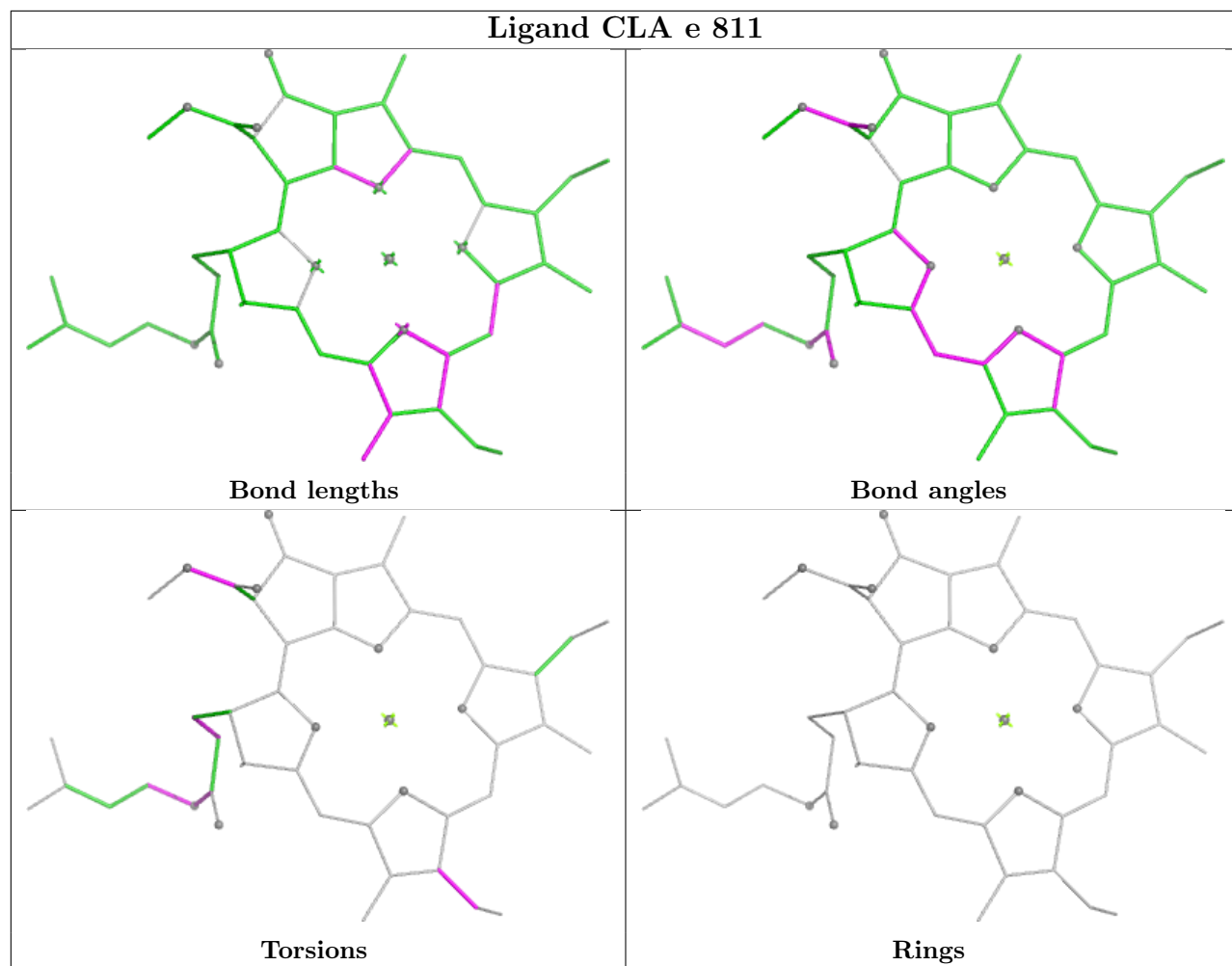
Ligand CLA g 836



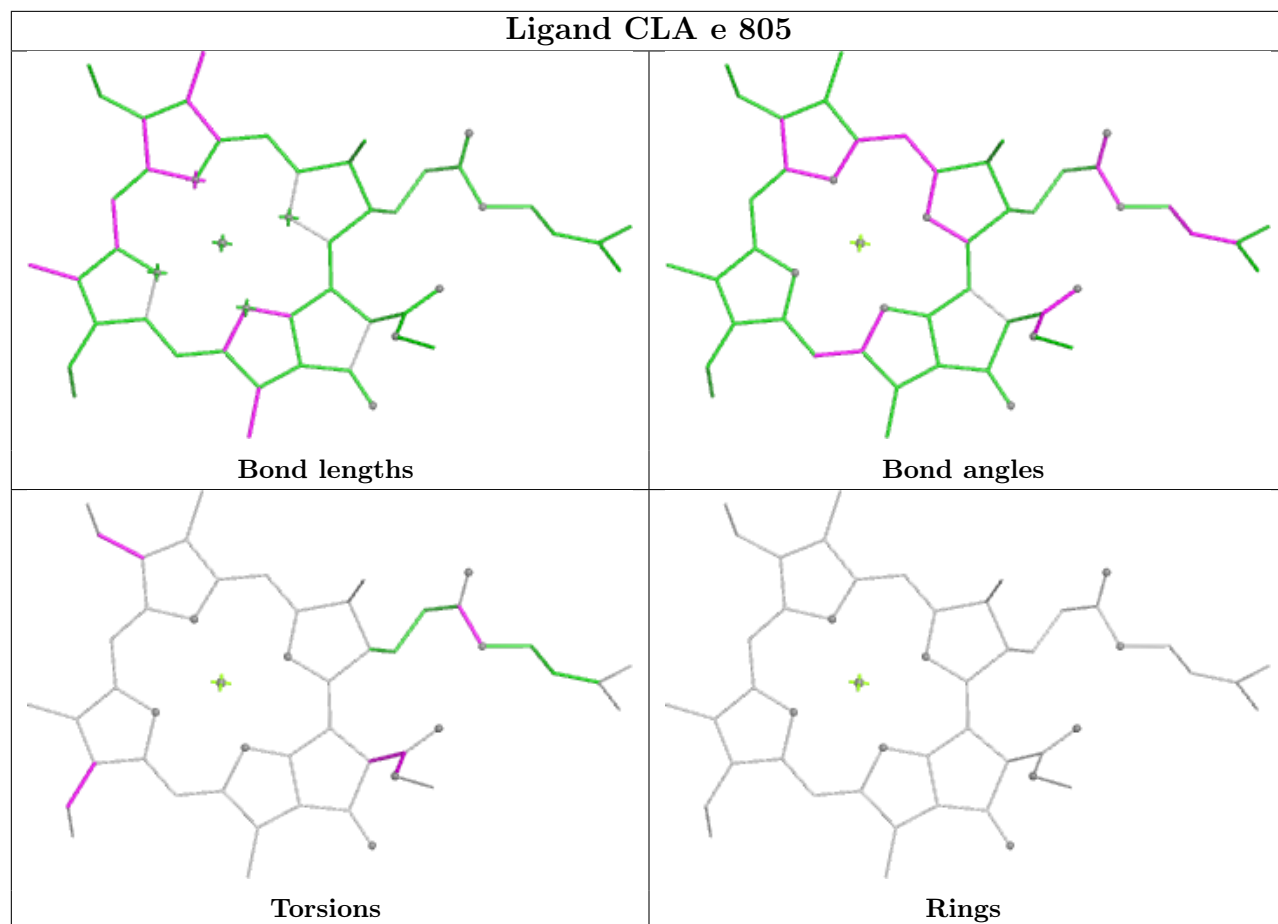


Ligand CLA A 833

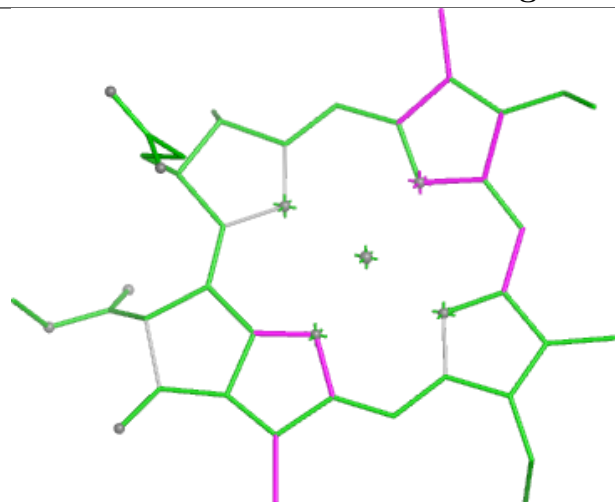




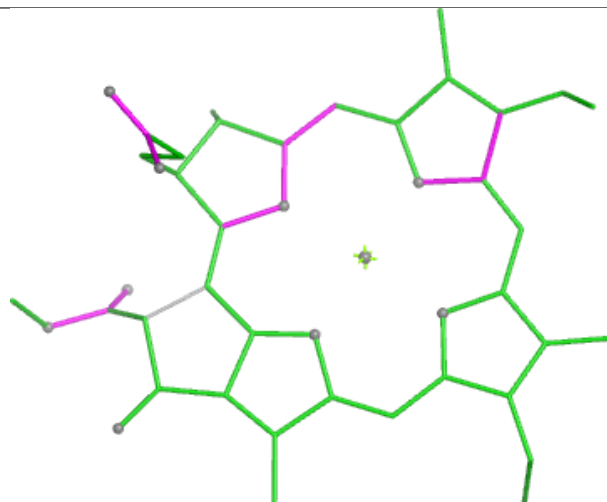
Ligand CLA e 805



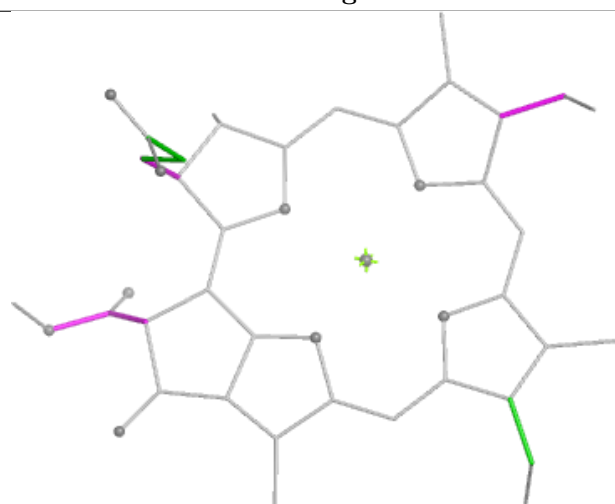
Ligand CLA b 811



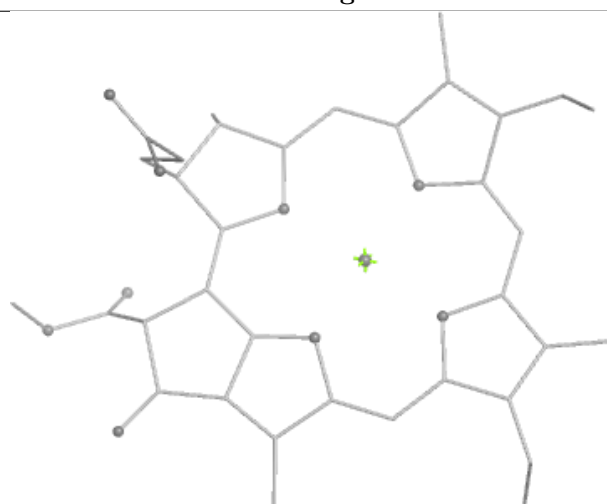
Bond lengths



Bond angles

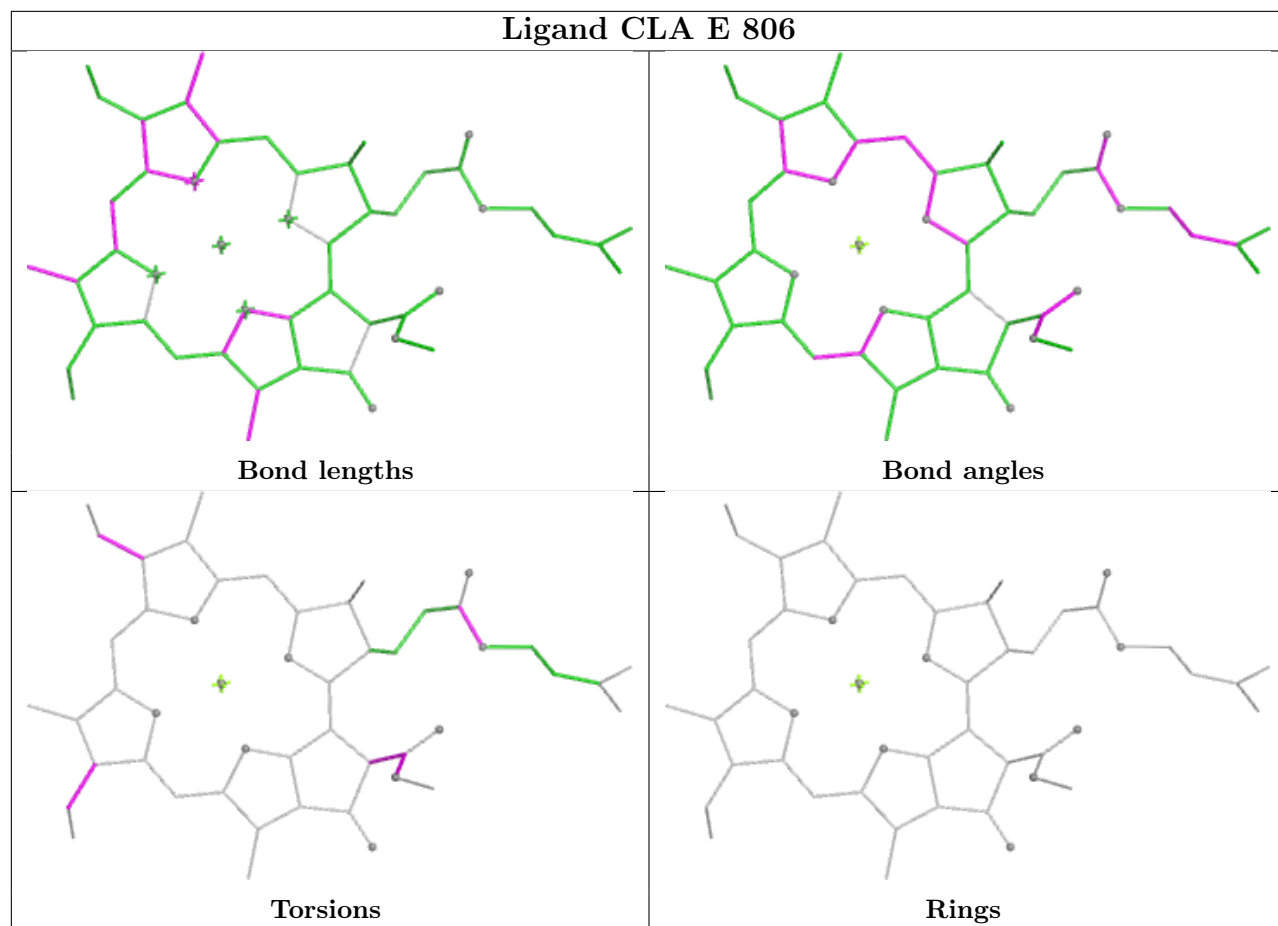


Torsions

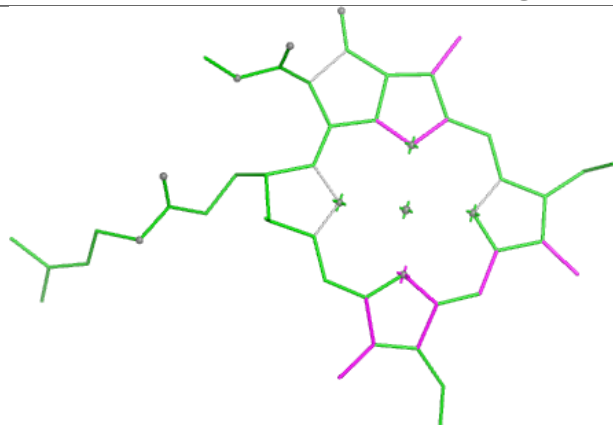


Rings

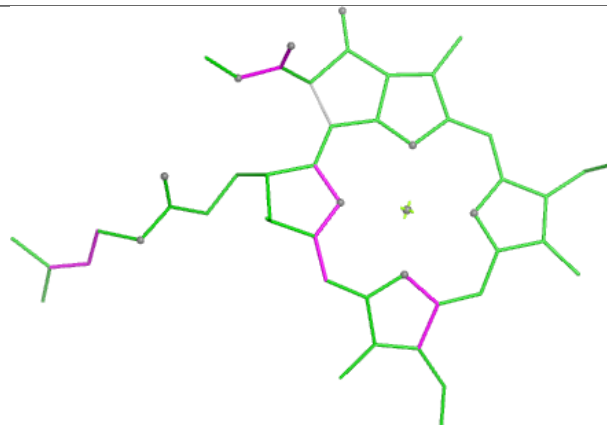
Ligand CLA E 806



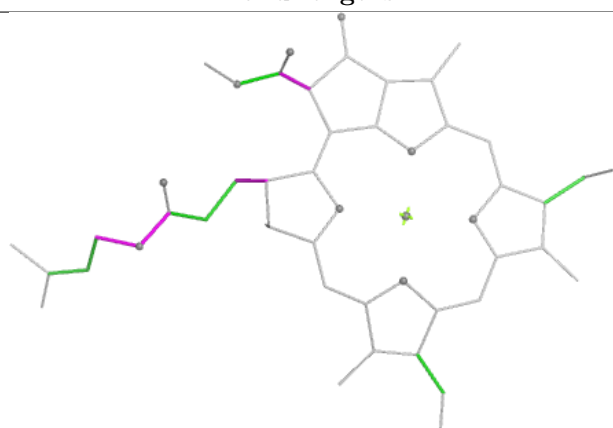
Ligand CLA E 805



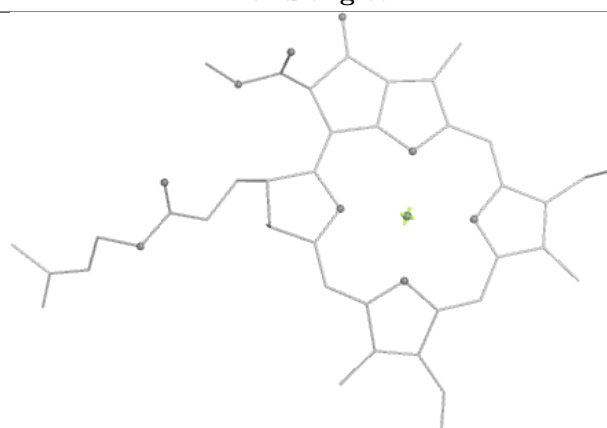
Bond lengths



Bond angles

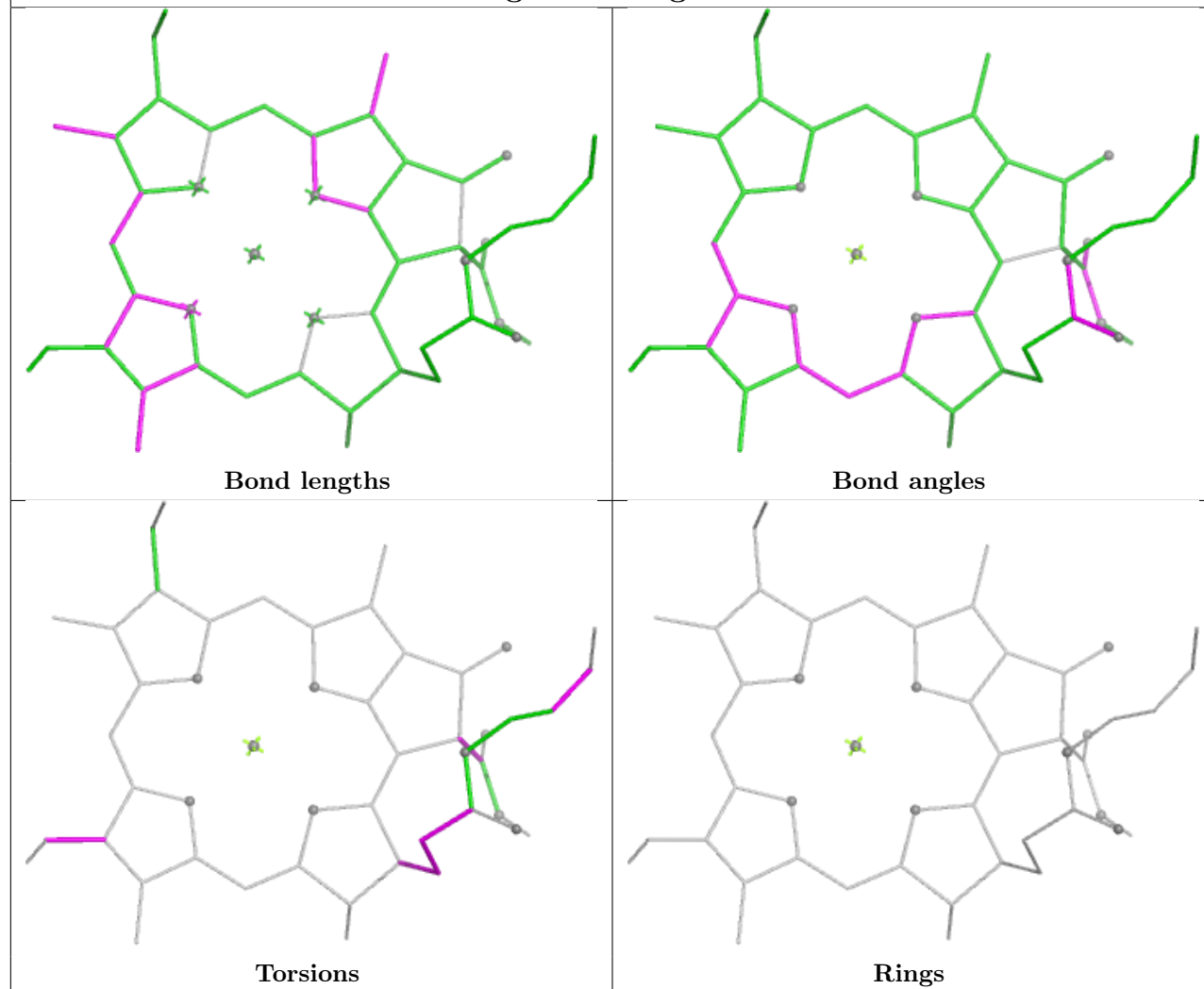


Torsions

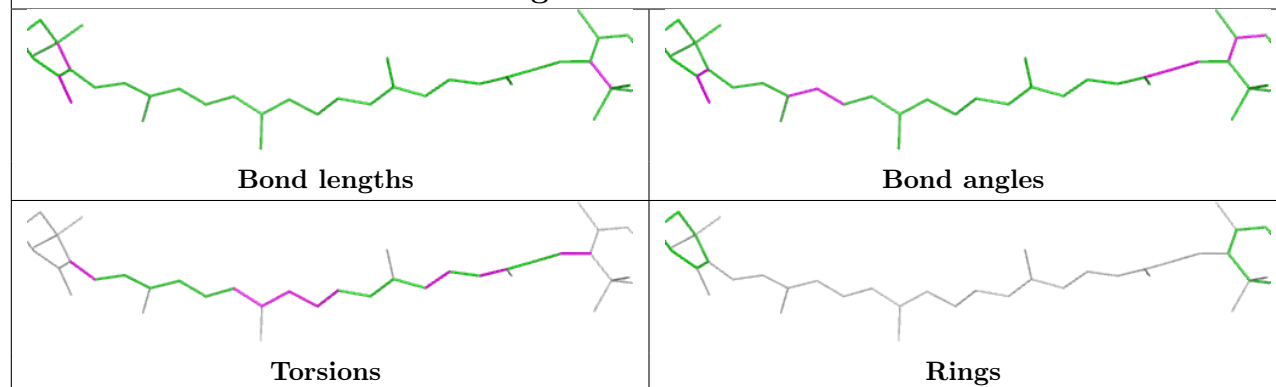


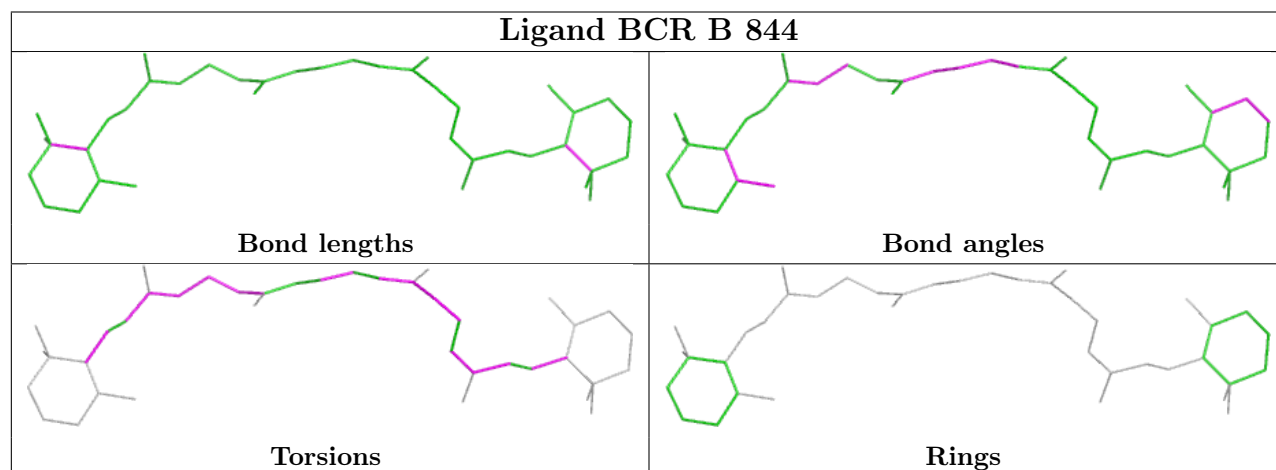
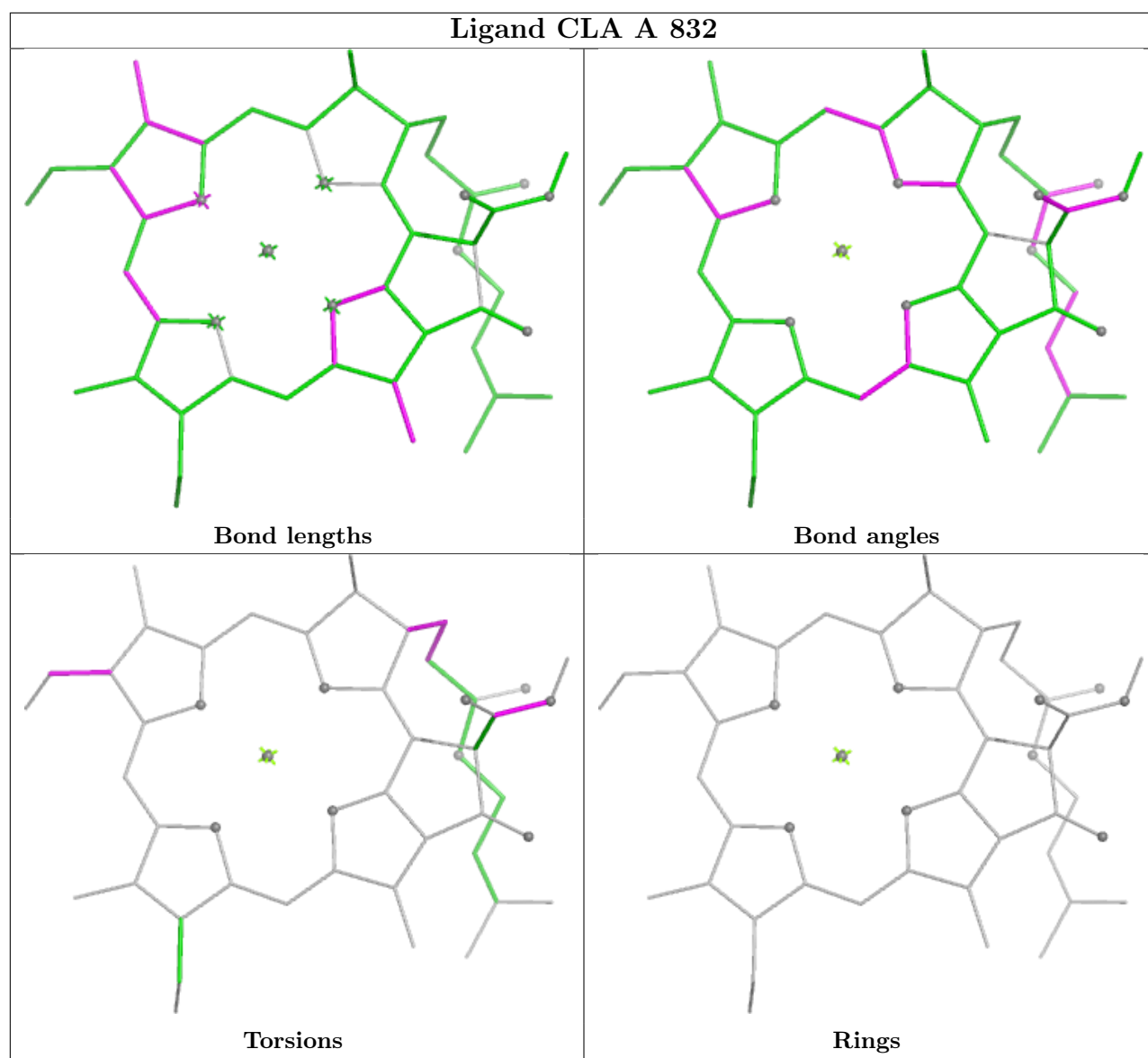
Rings

Ligand CLA g 833

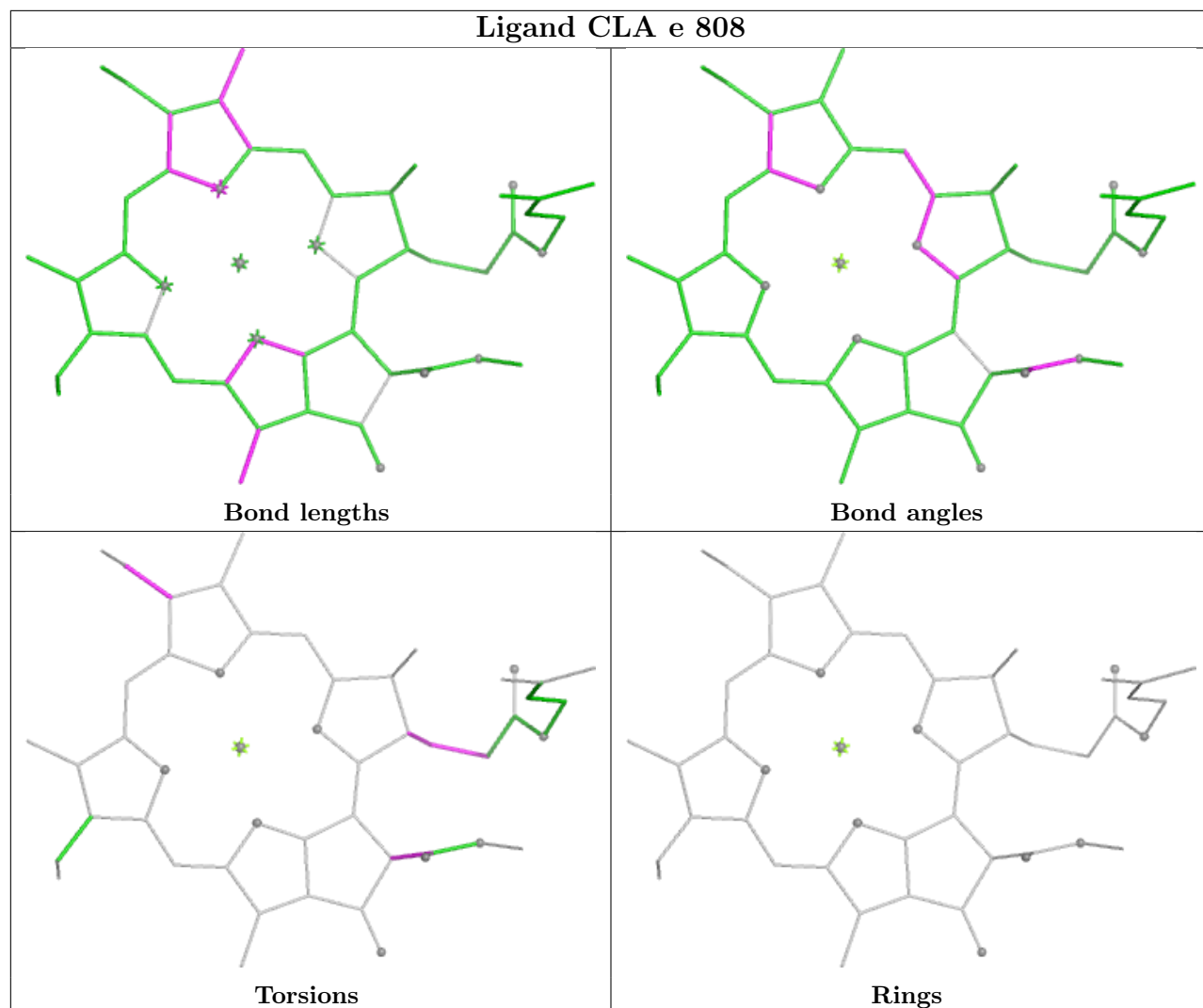


Ligand BCR T 101

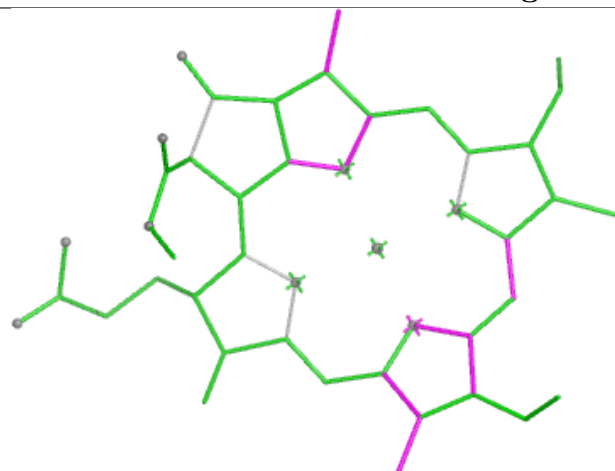




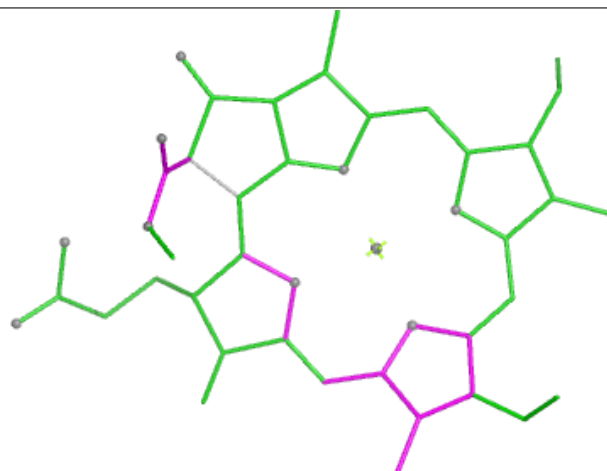
Ligand CLA e 808



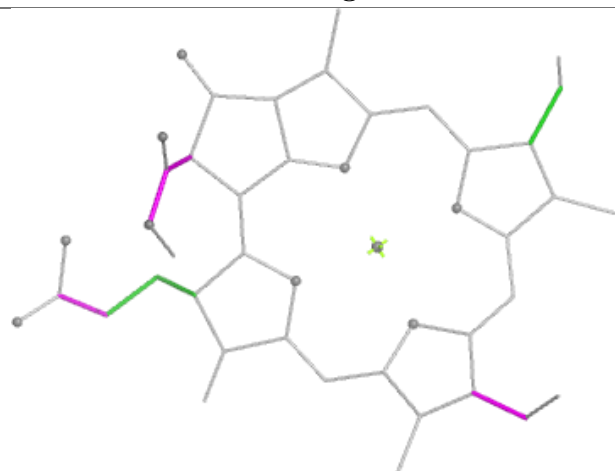
Ligand CLA e 817



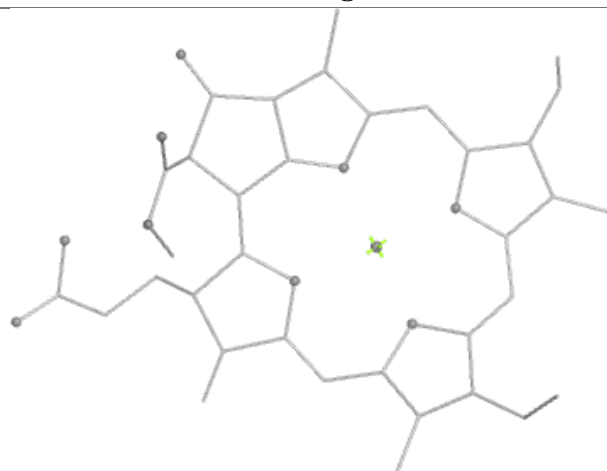
Bond lengths



Bond angles

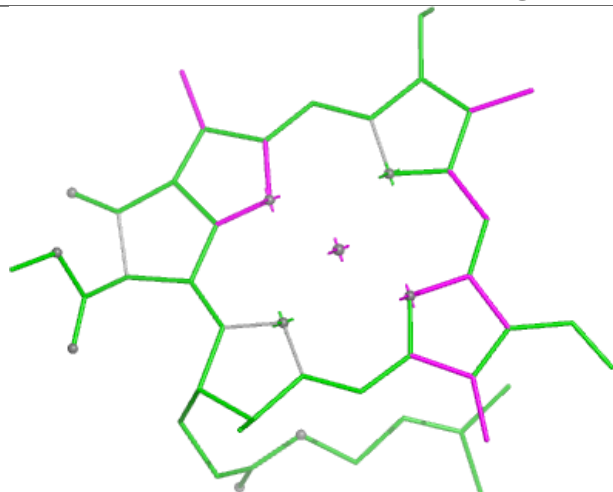


Torsions

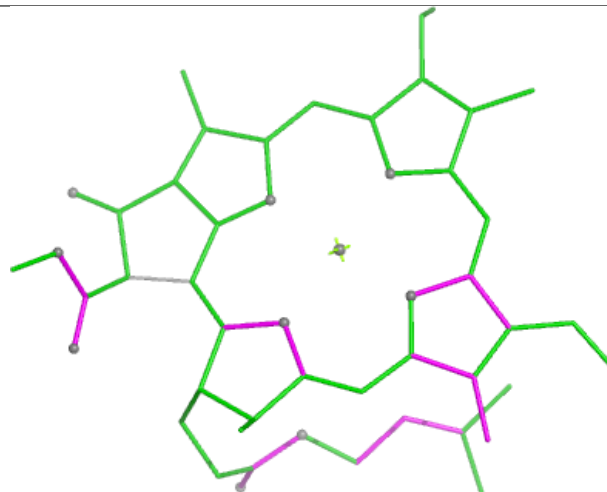


Rings

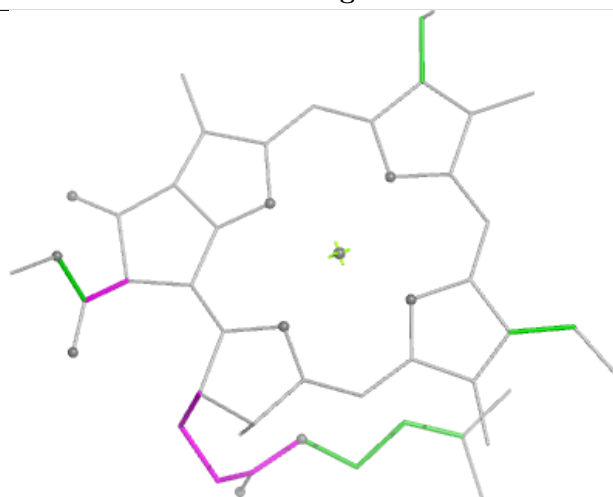
Ligand CLA A 823



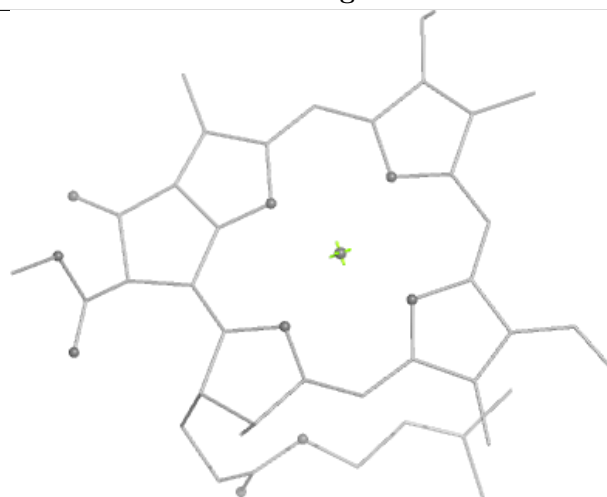
Bond lengths



Bond angles

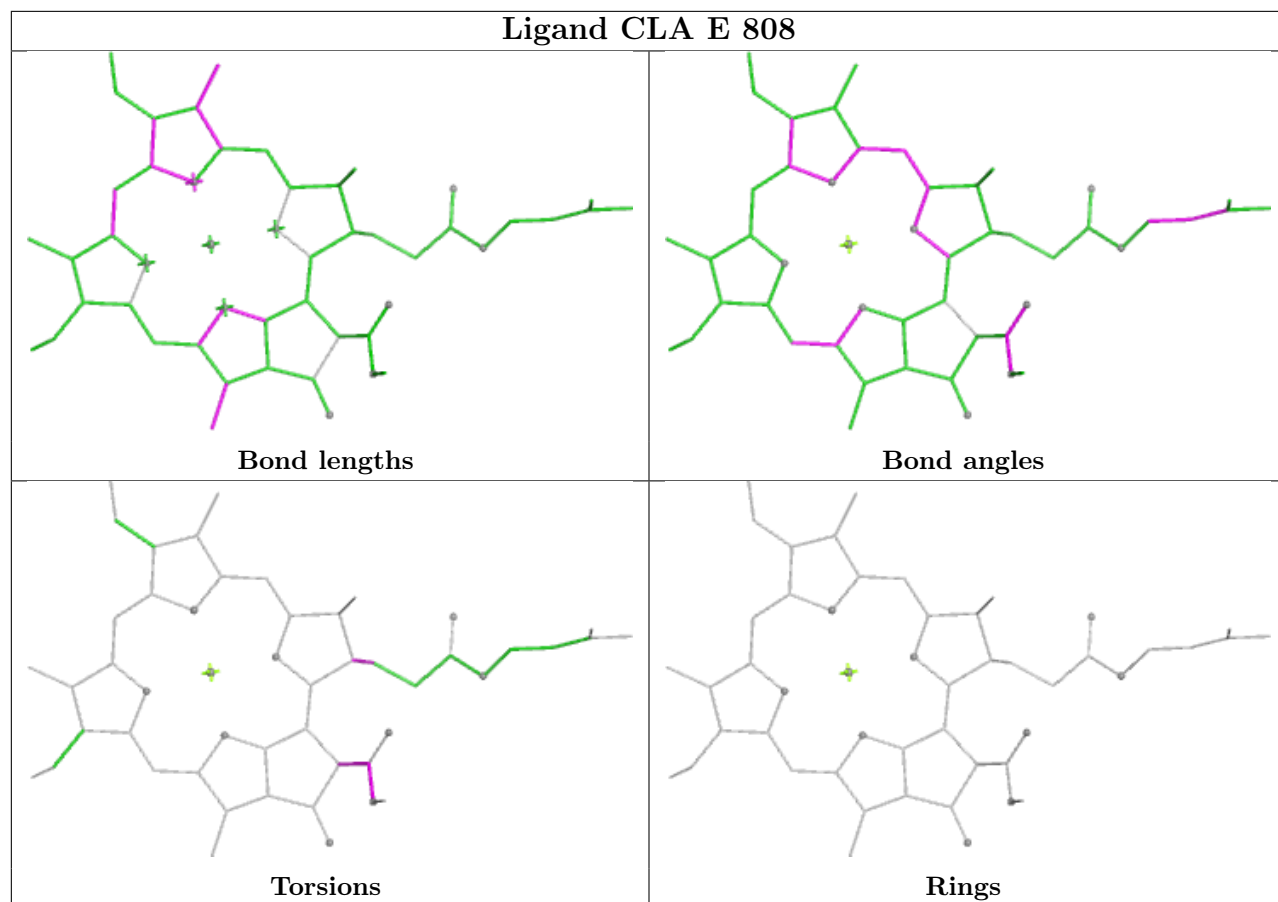


Torsions

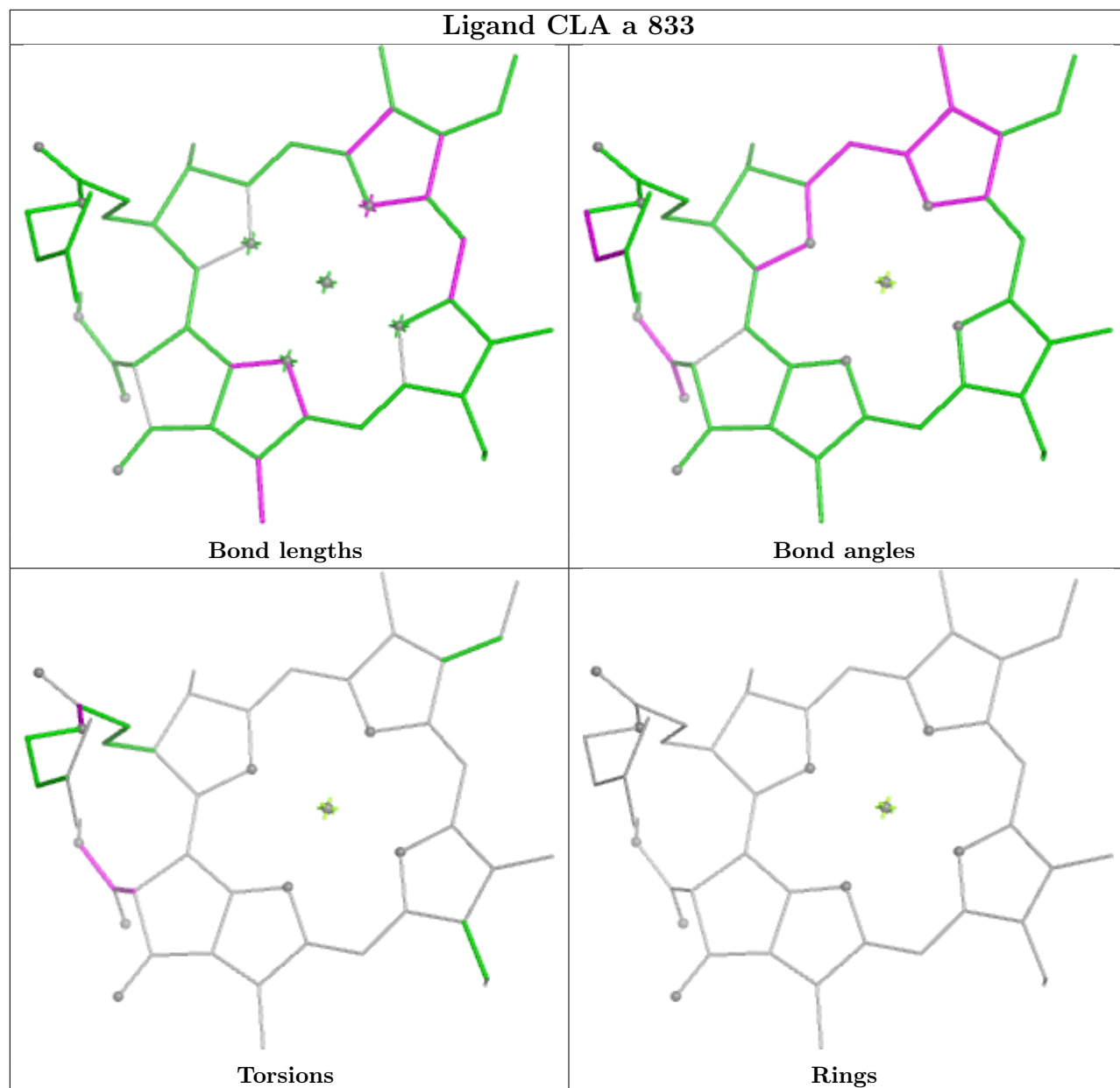


Rings

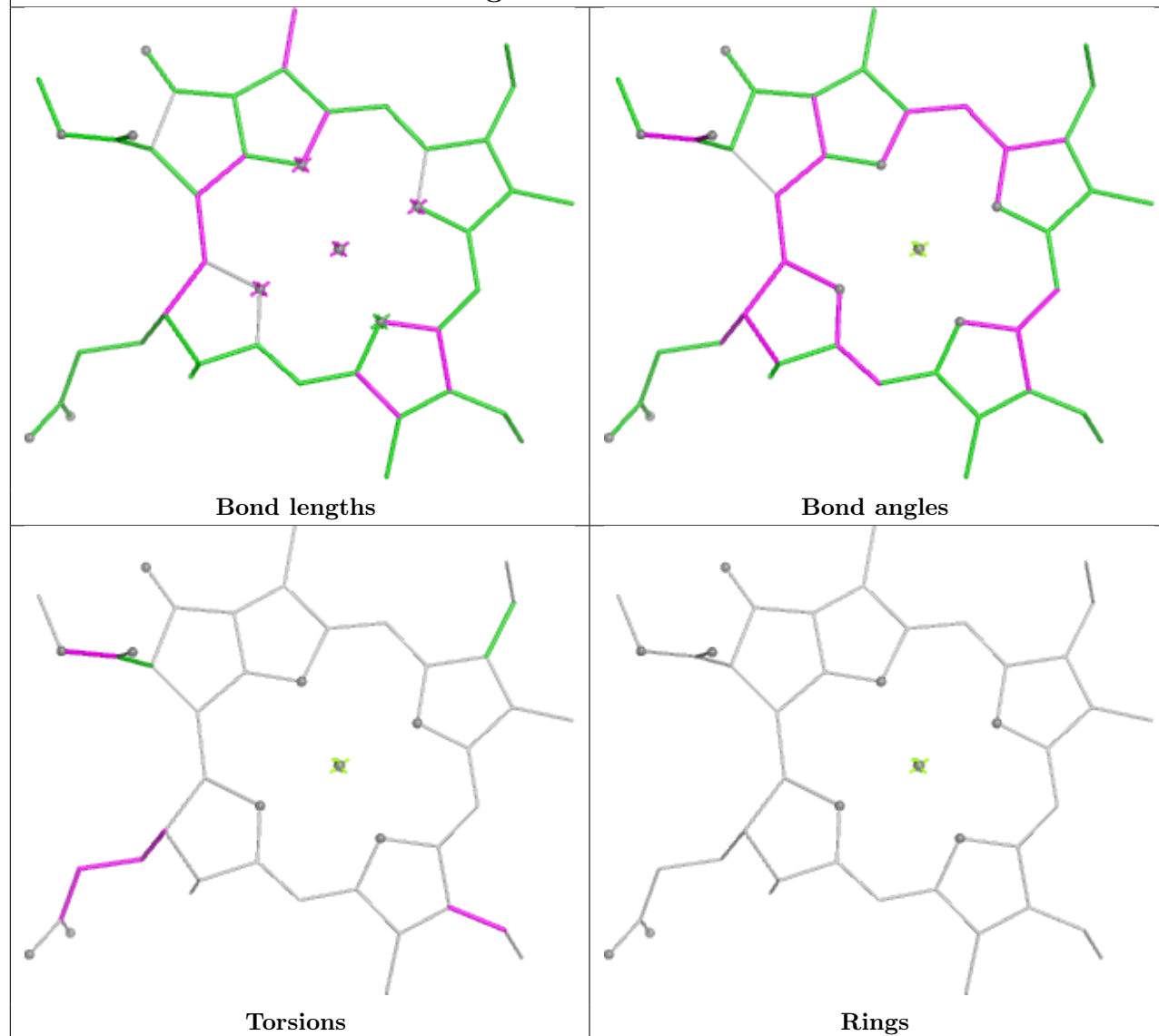
Ligand CLA E 808



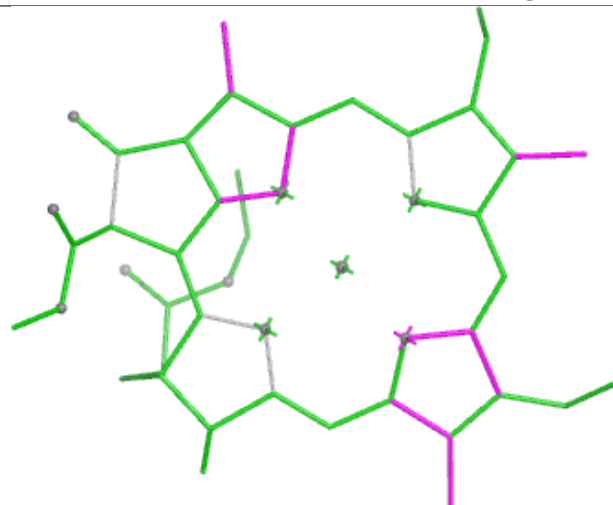
Ligand CLA a 833



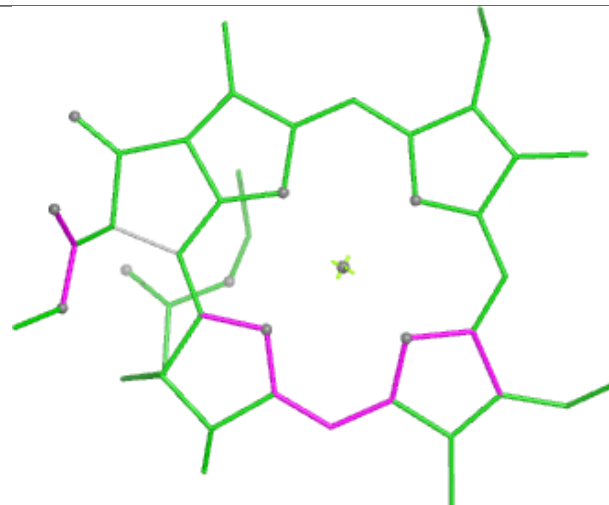
Ligand CLA S 204



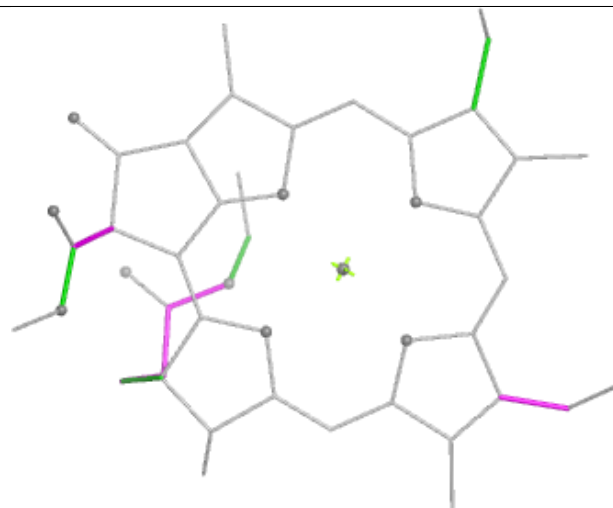
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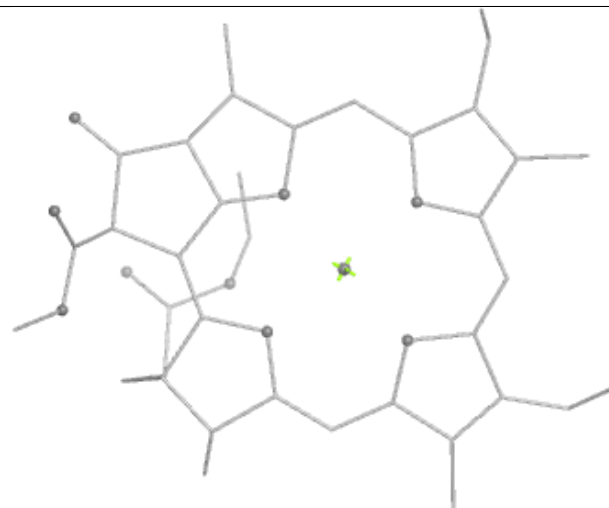
Bond lengths



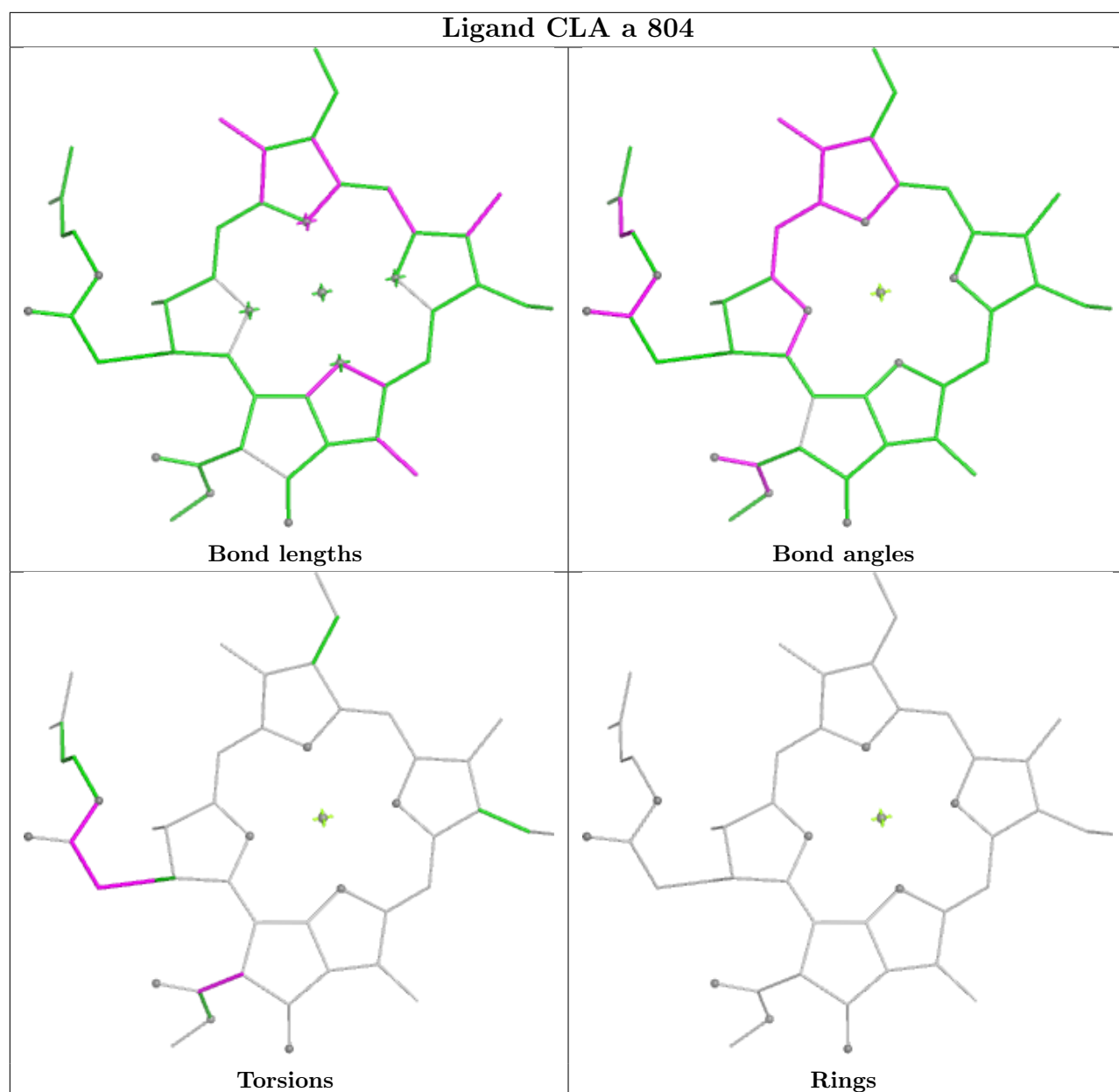
Bond angles



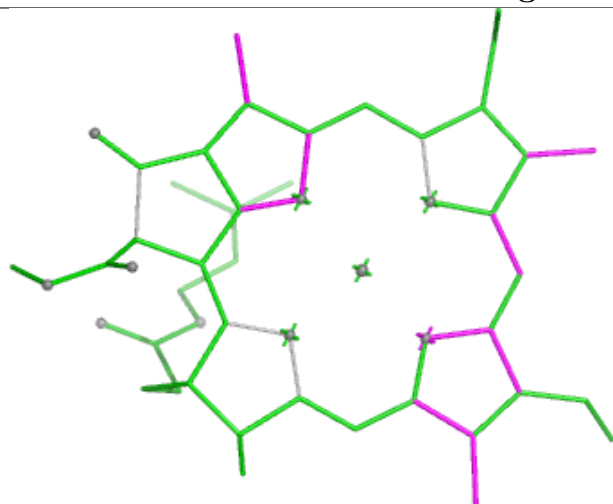
Torsions



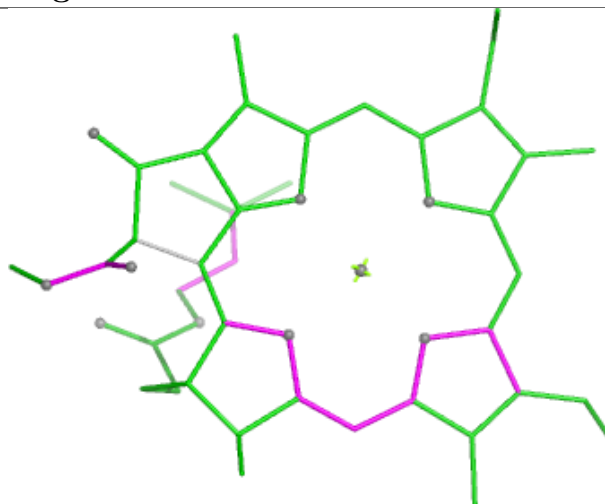
Rings



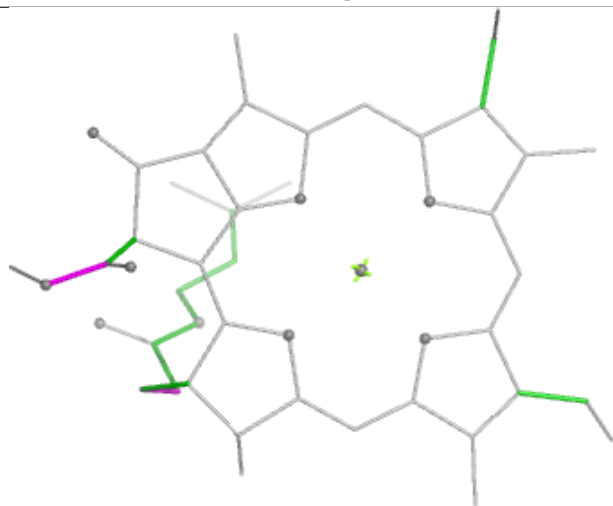
Ligand CLA g 816



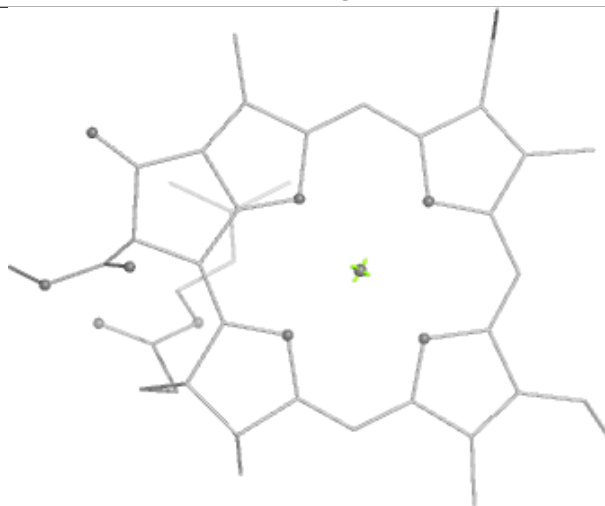
Bond lengths



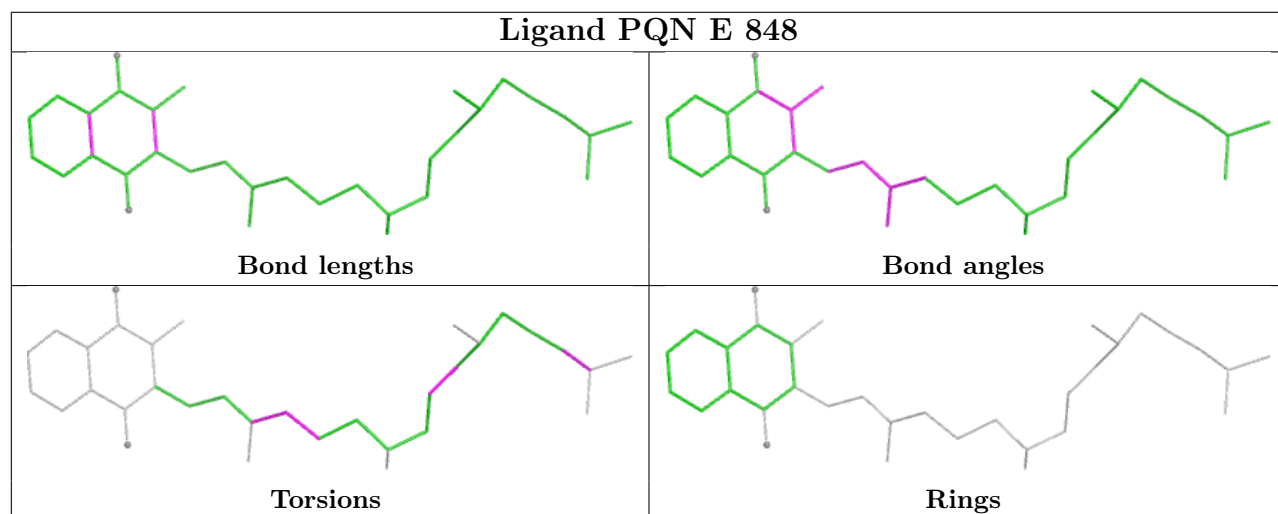
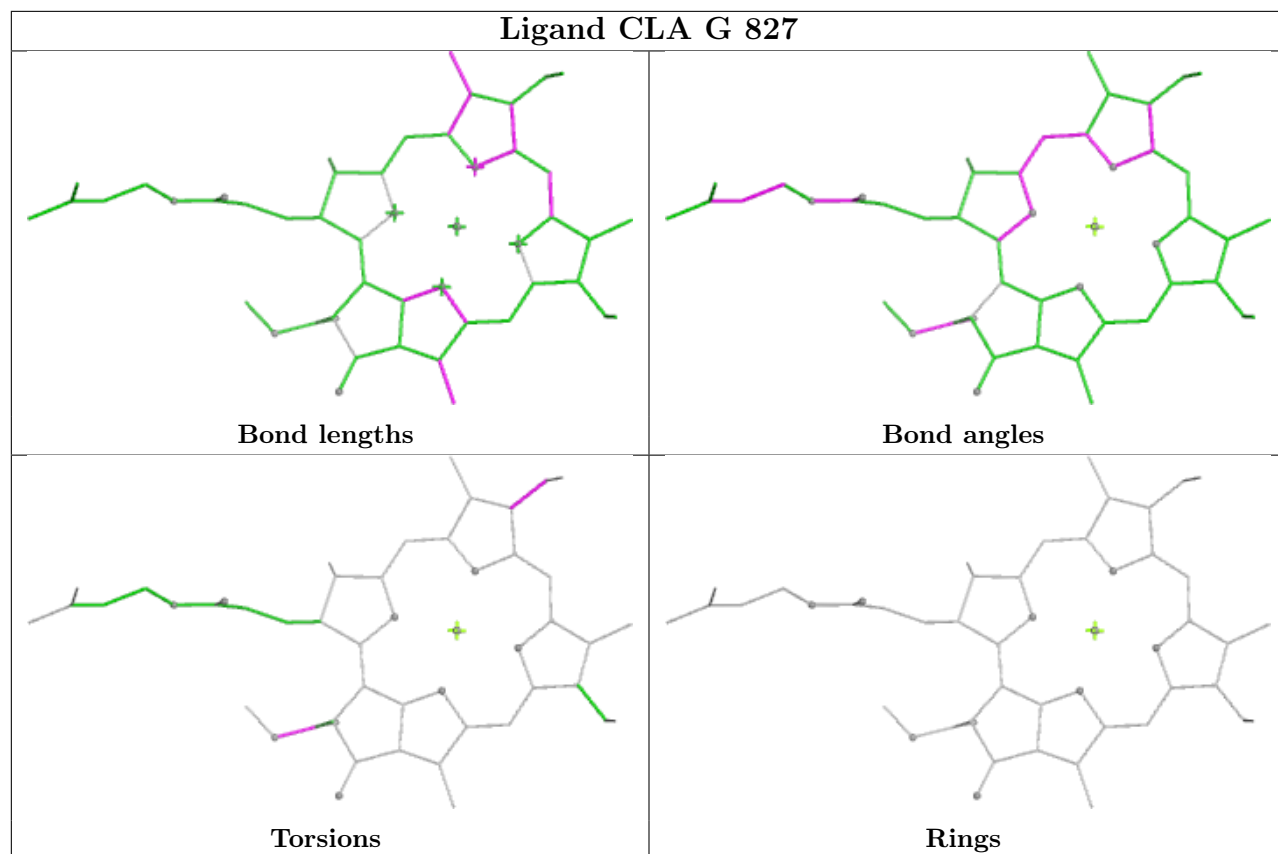
Bond angles



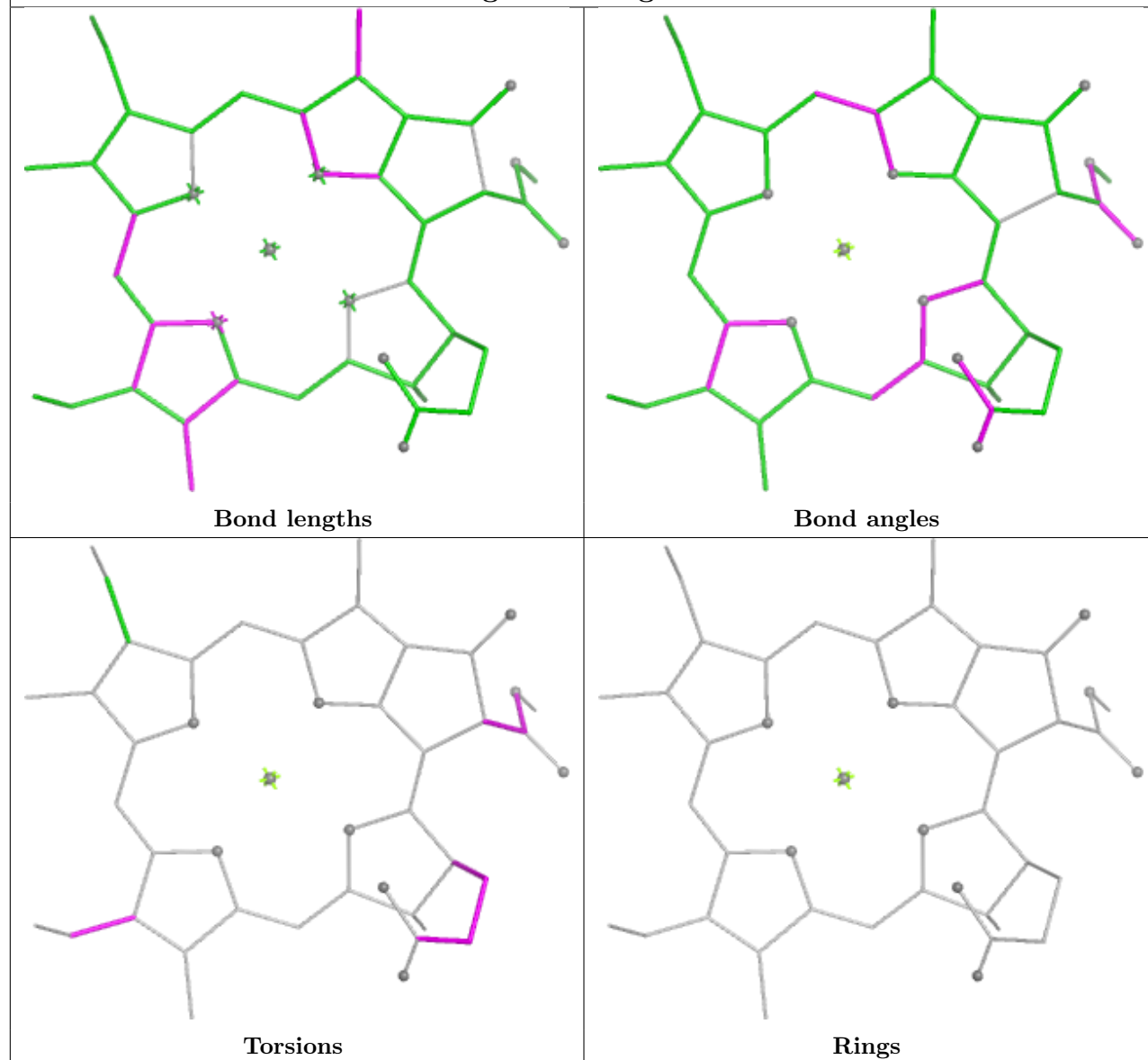
Torsions



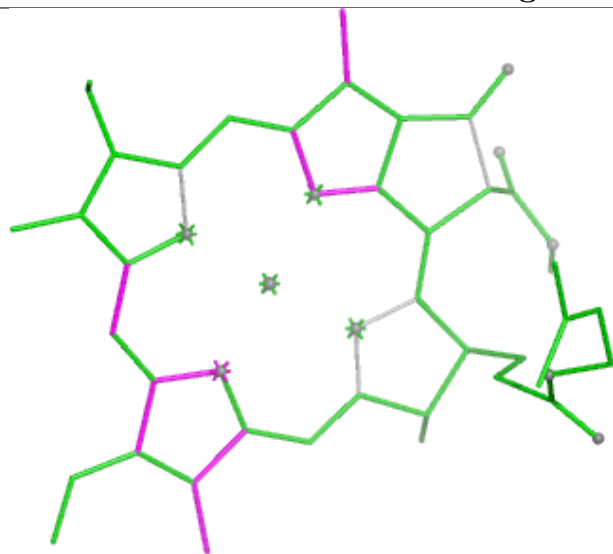
Rings



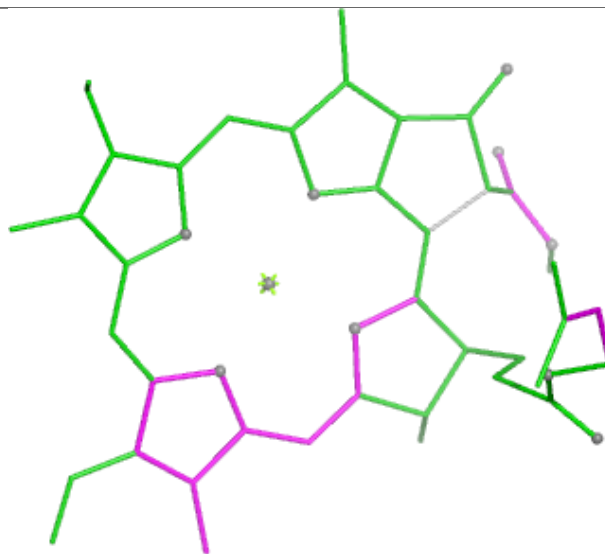
Ligand CLA g 832



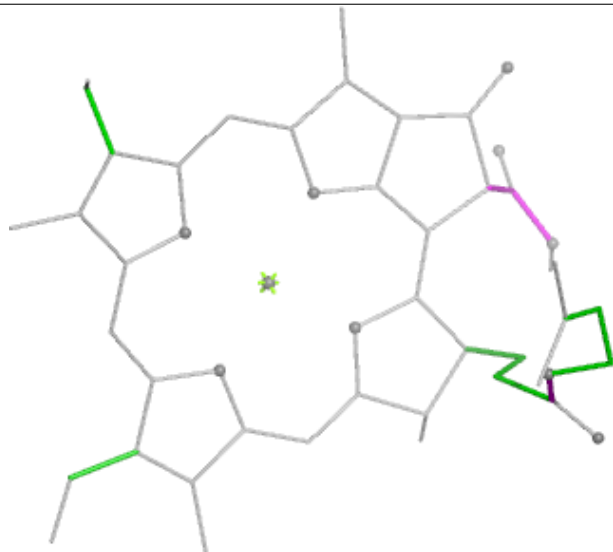
Ligand CLA e 832



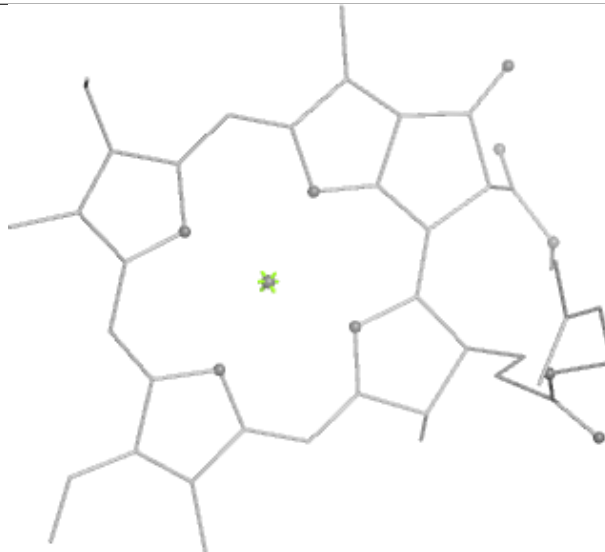
Bond lengths



Bond angles

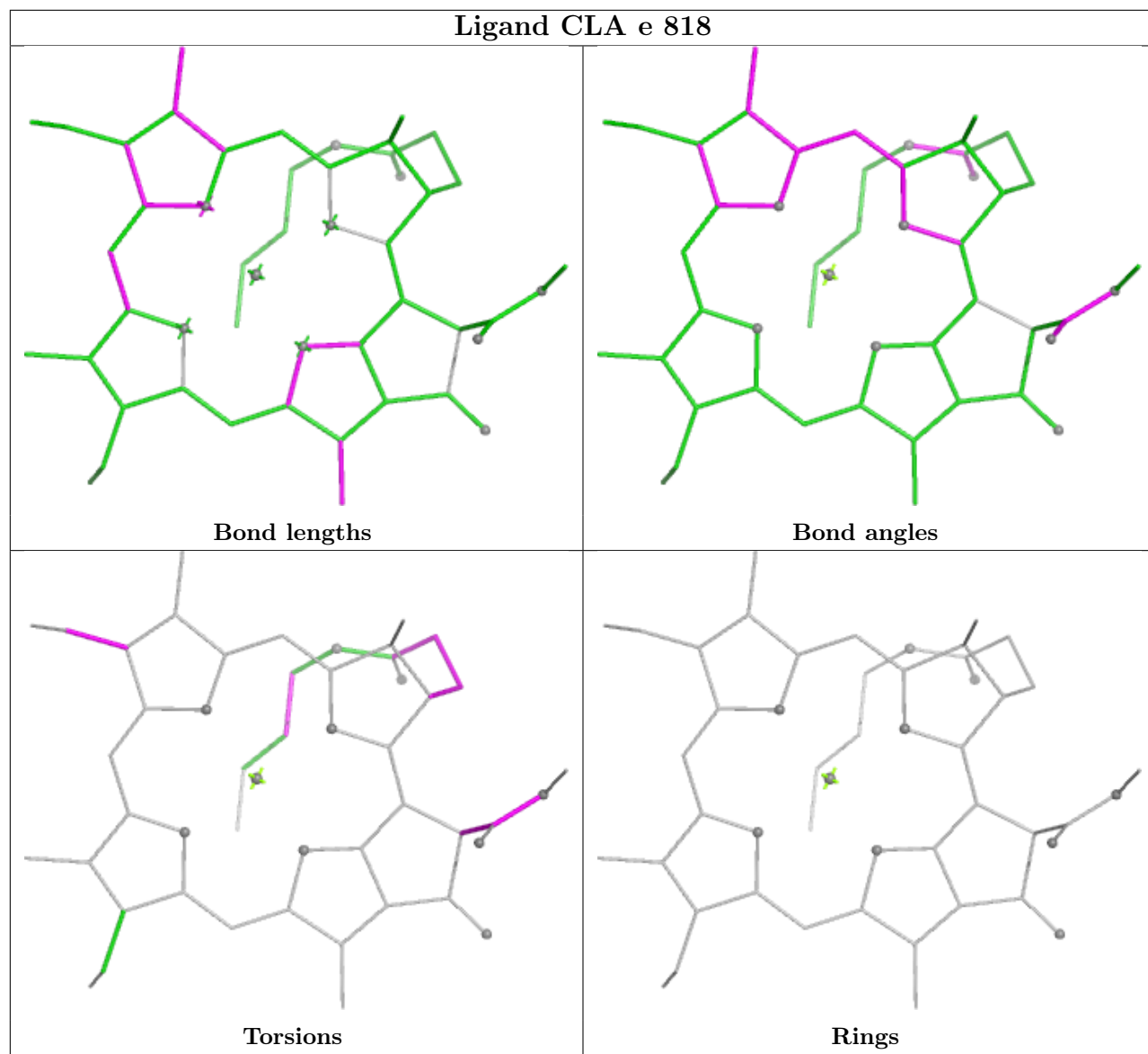


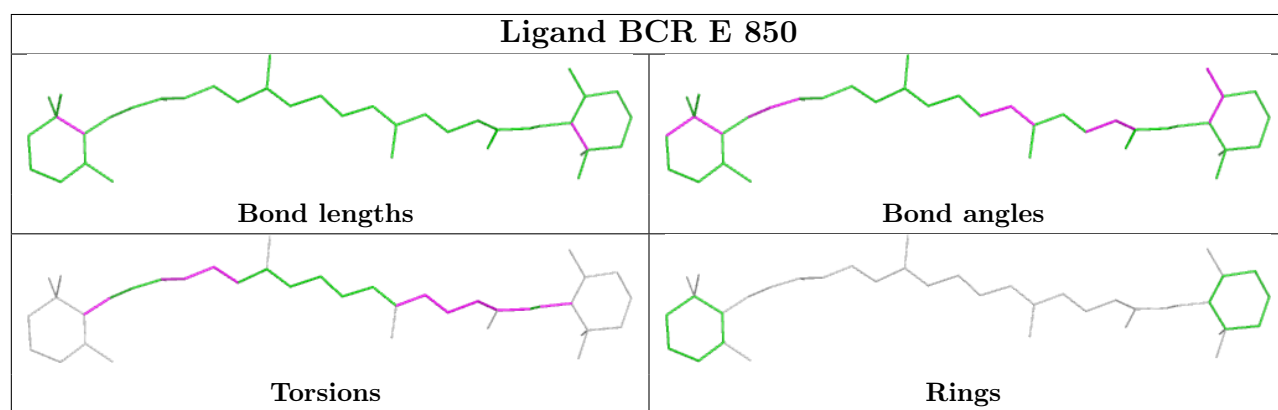
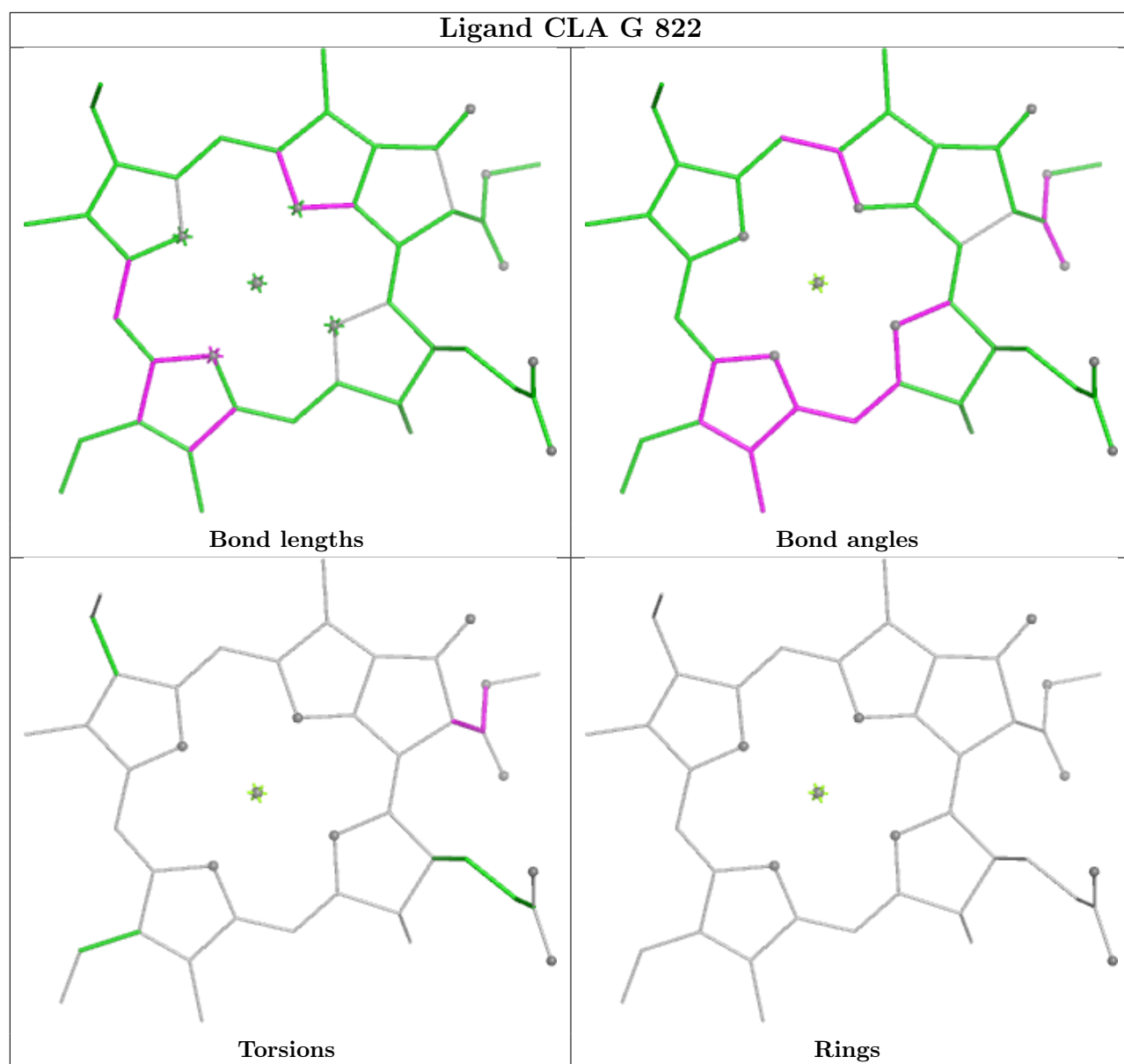
Torsions



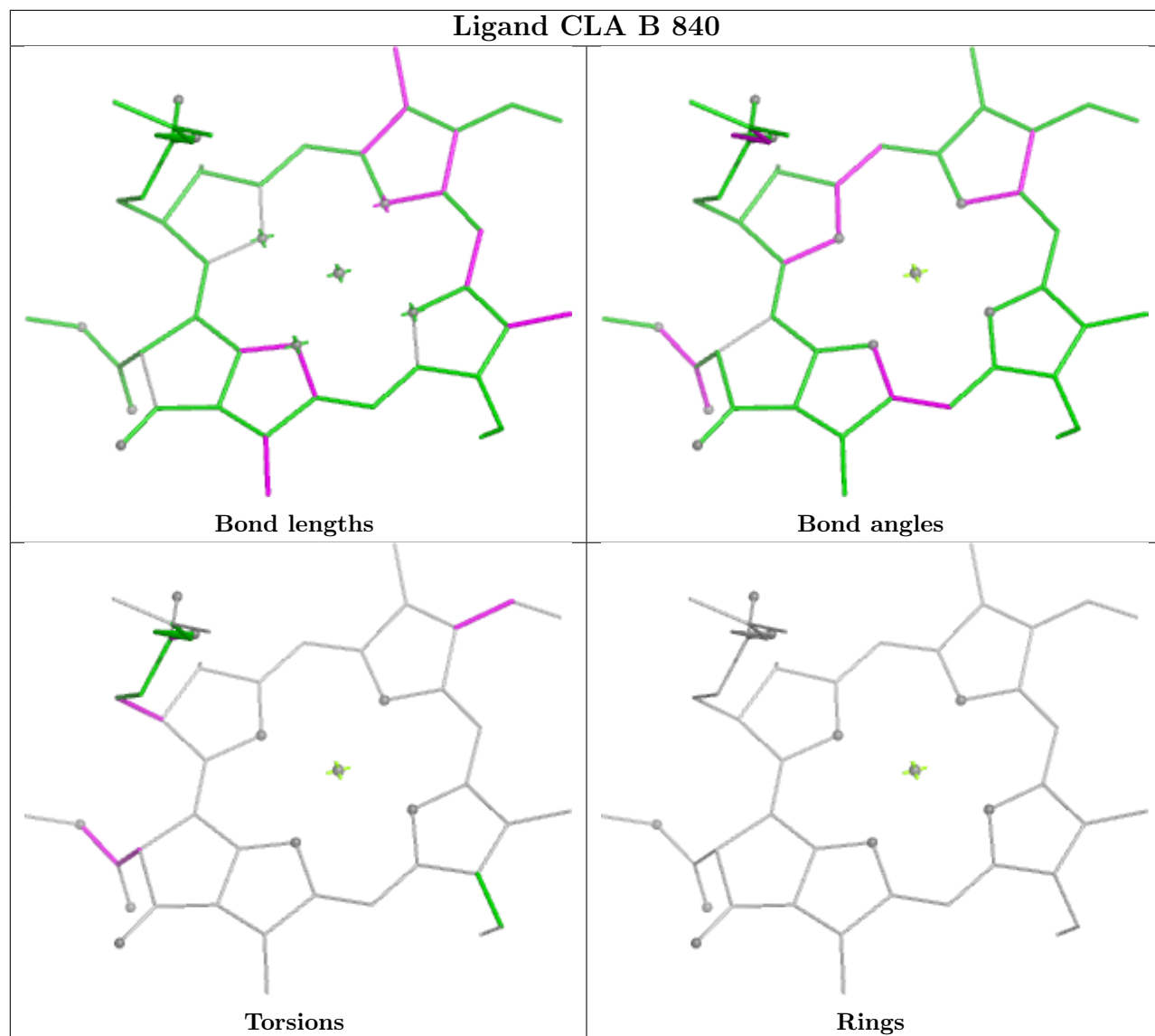
Rings

Ligand CLA e 818

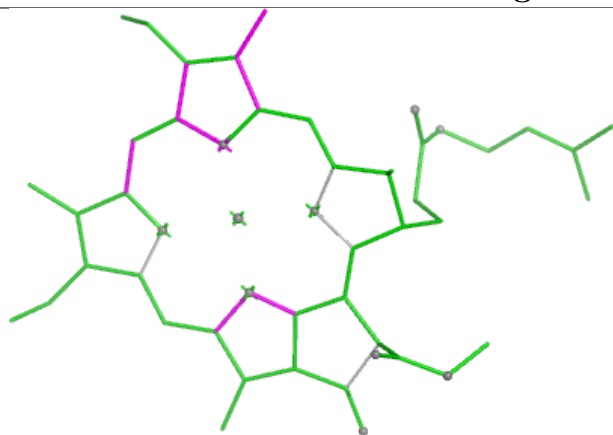




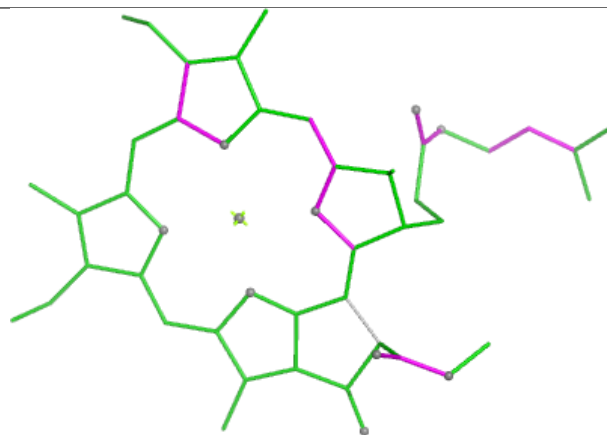
Ligand CLA B 840



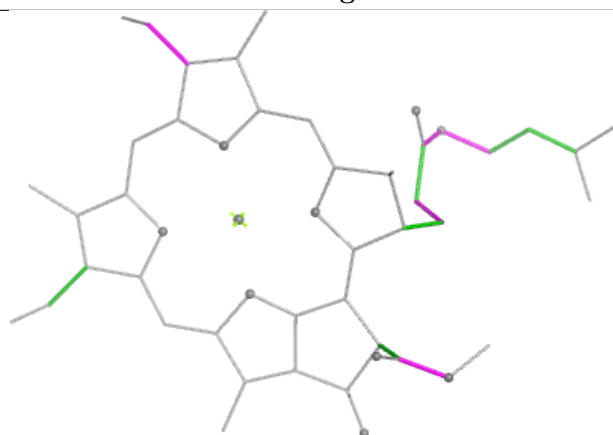
Ligand CLA A 812



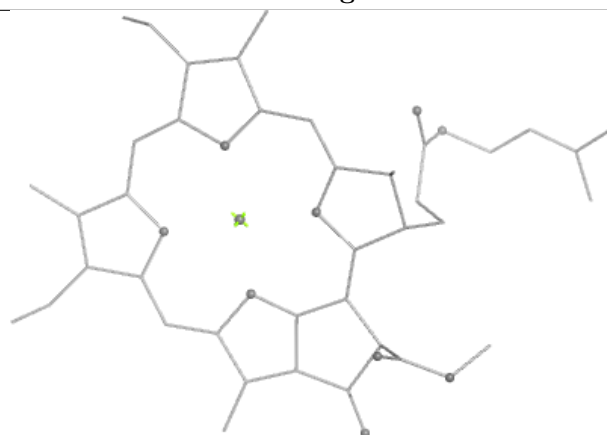
Bond lengths



Bond angles

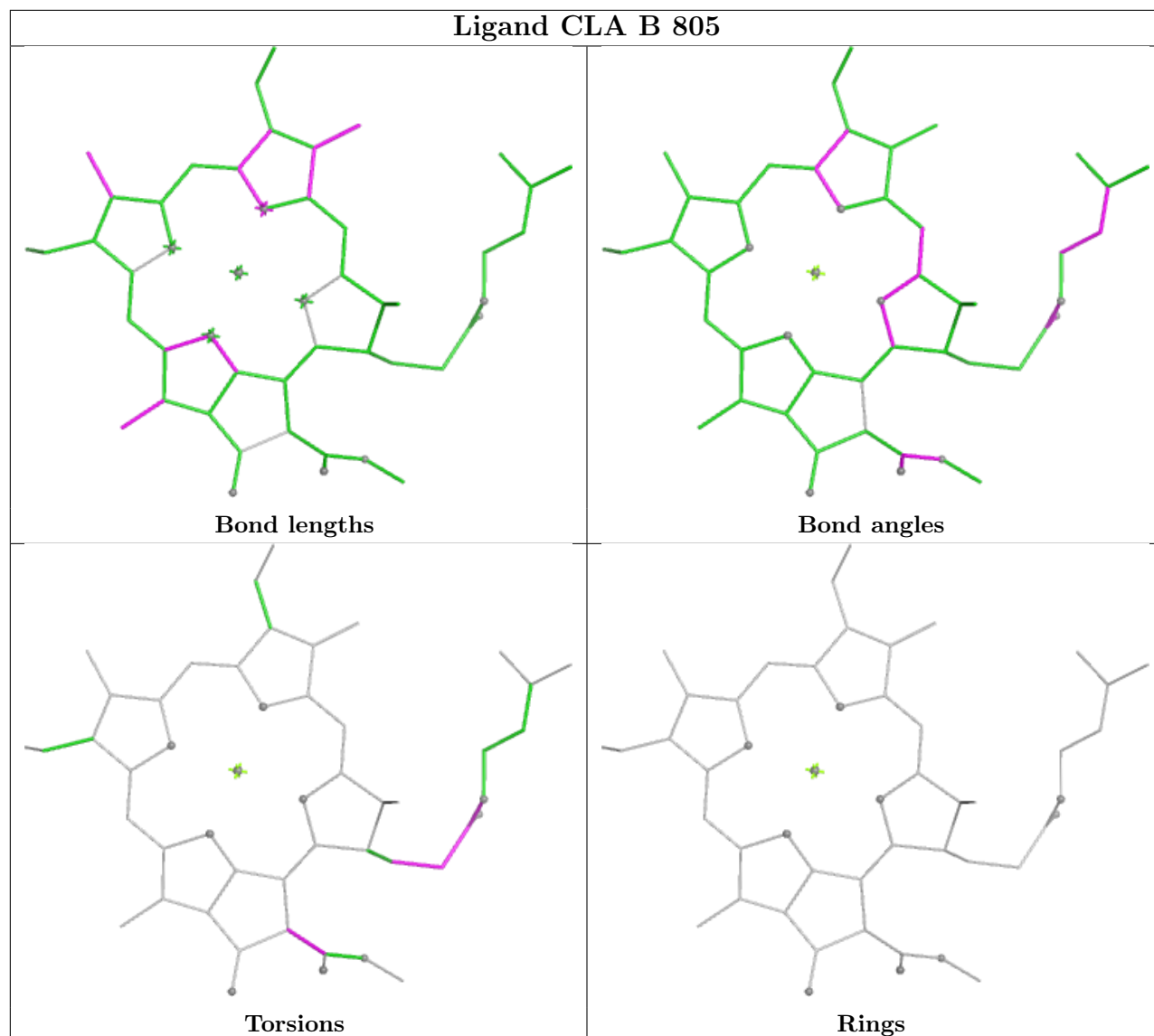


Torsions

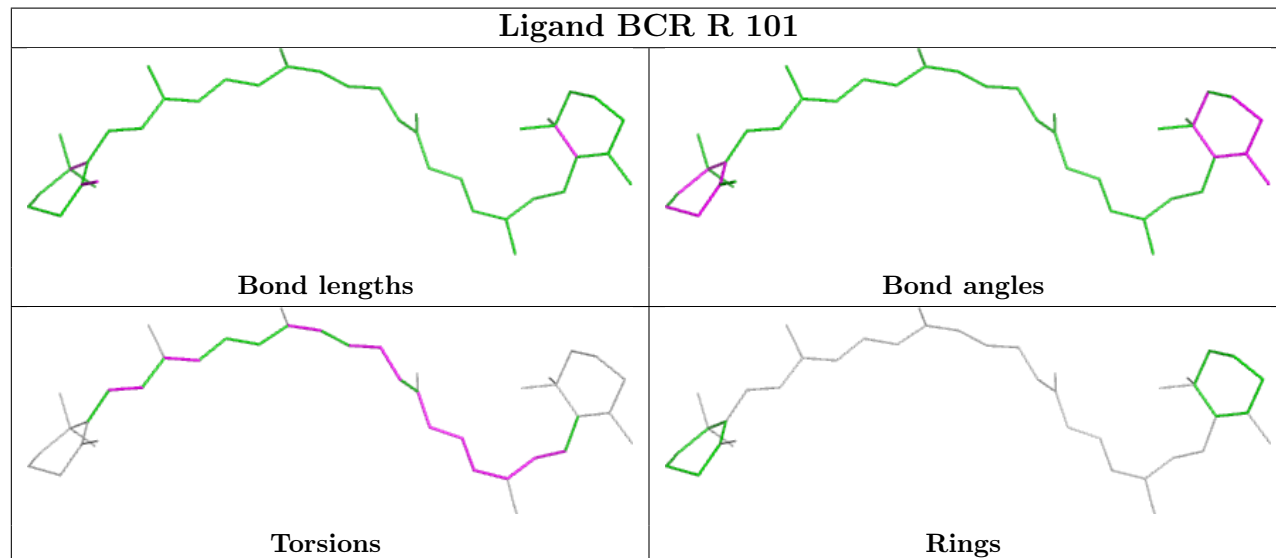


Rings

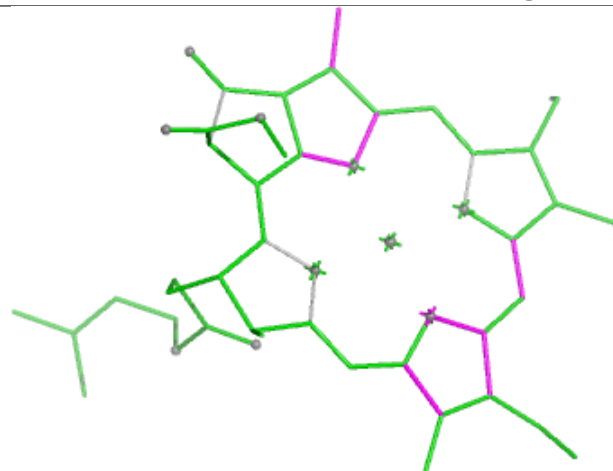
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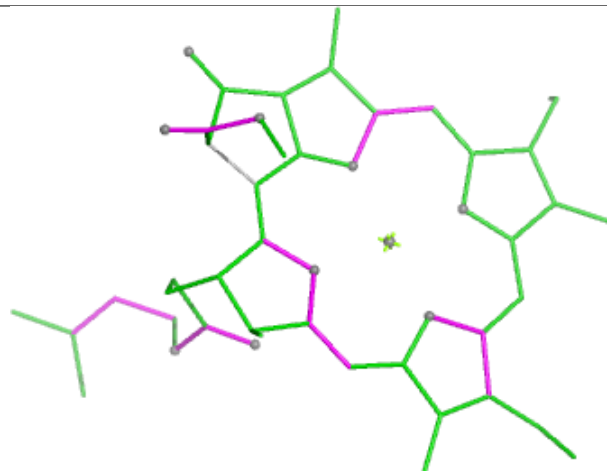
Ligand BCR R 101



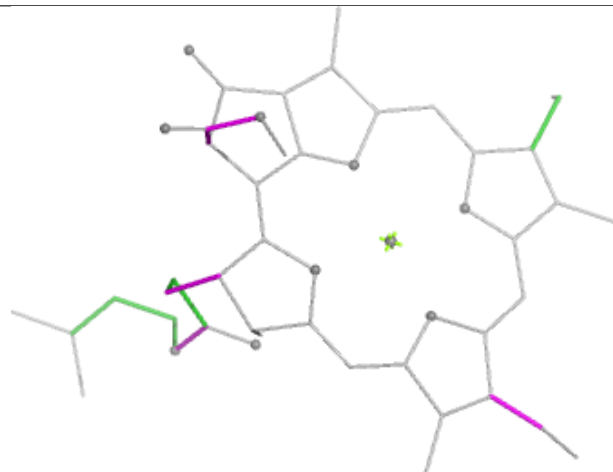
Ligand CLA a 838



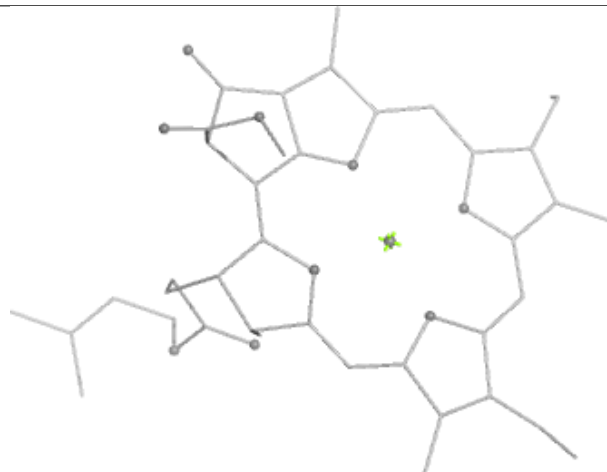
Bond lengths



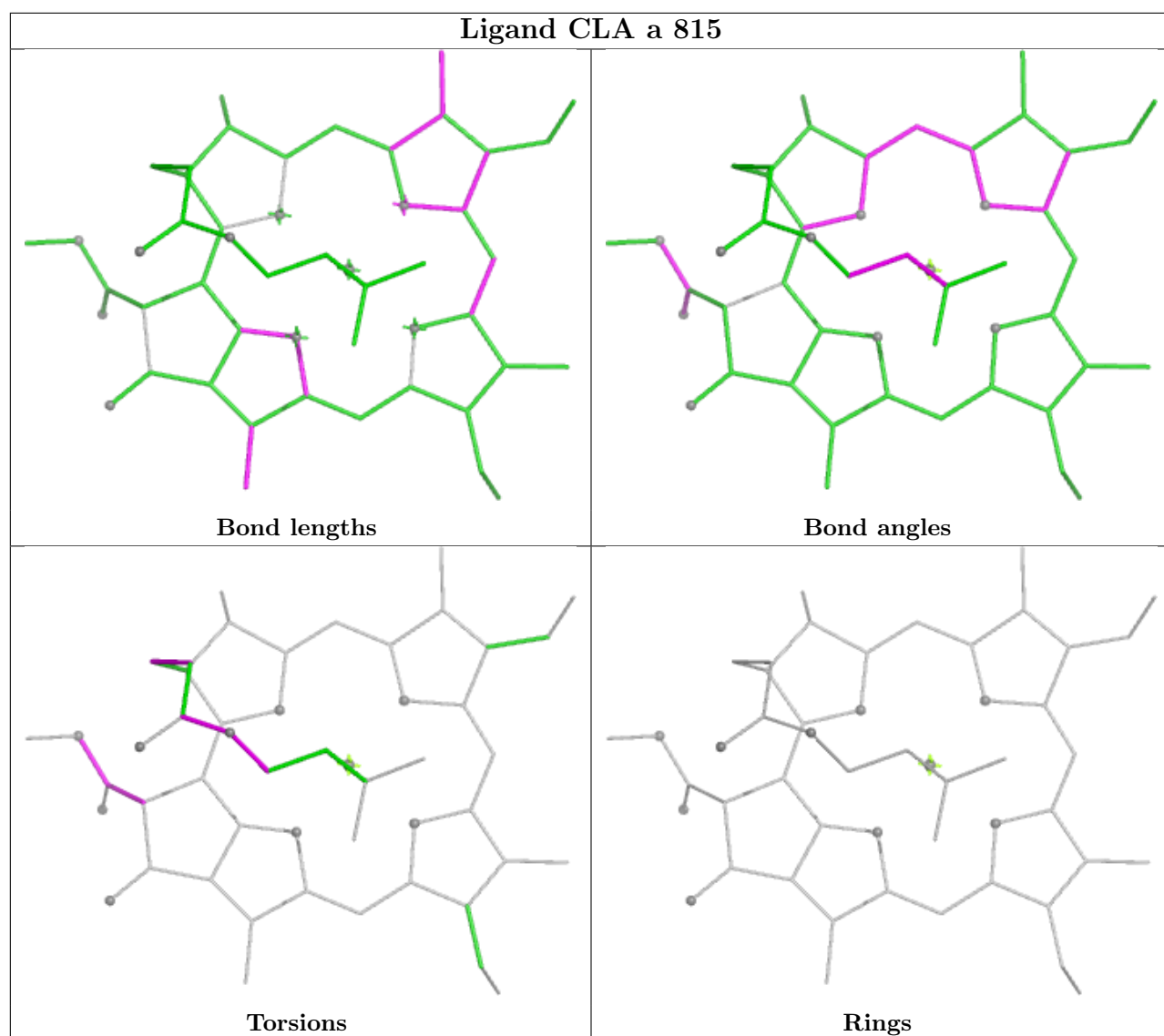
Bond angles



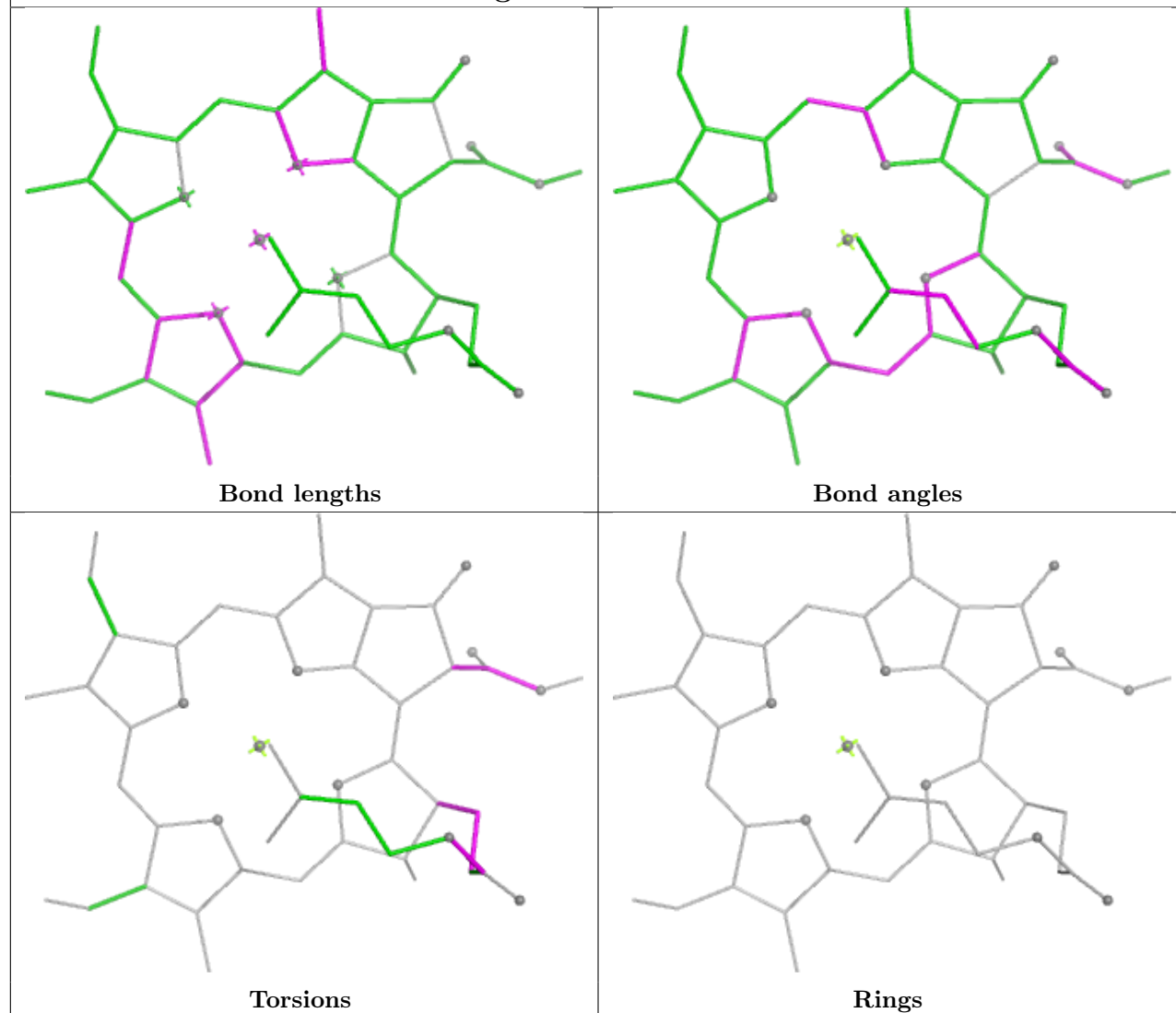
Torsions



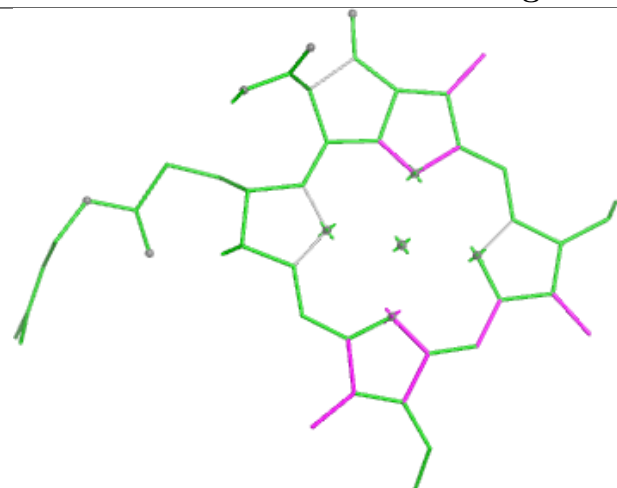
Rings



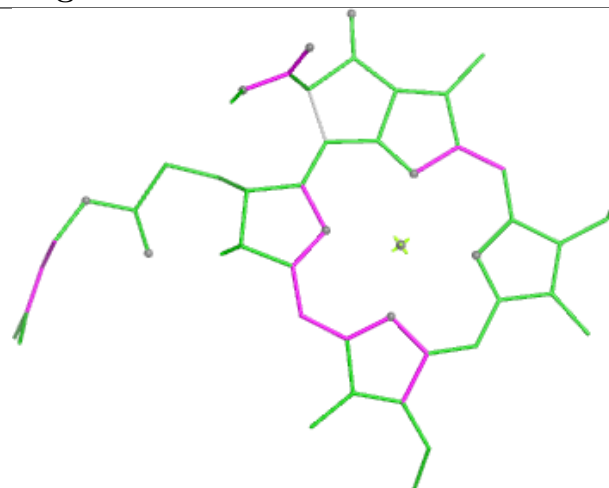
Ligand CLA e 820



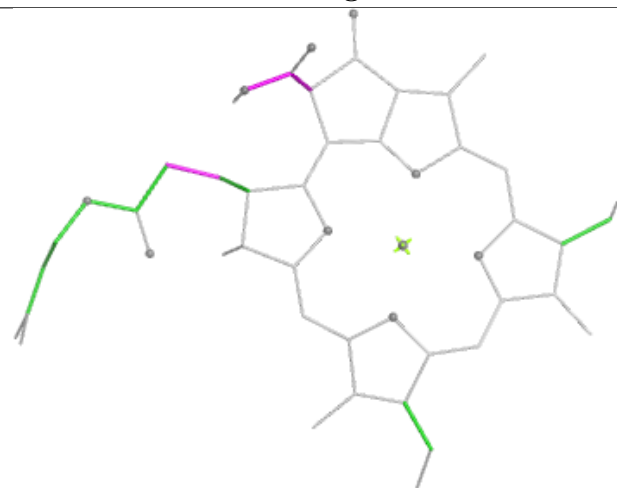
Ligand CLA g 815



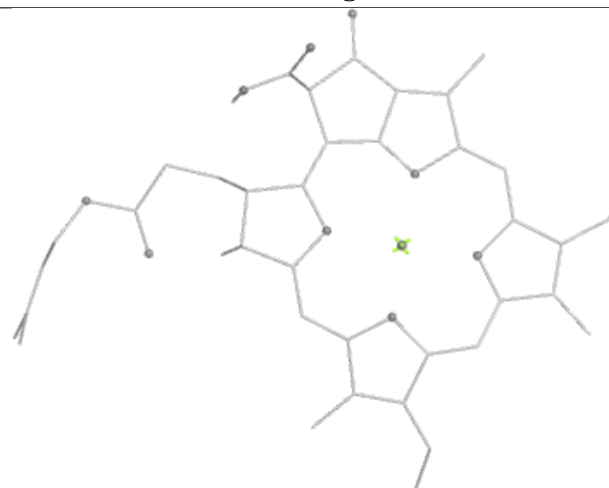
Bond lengths



Bond angles

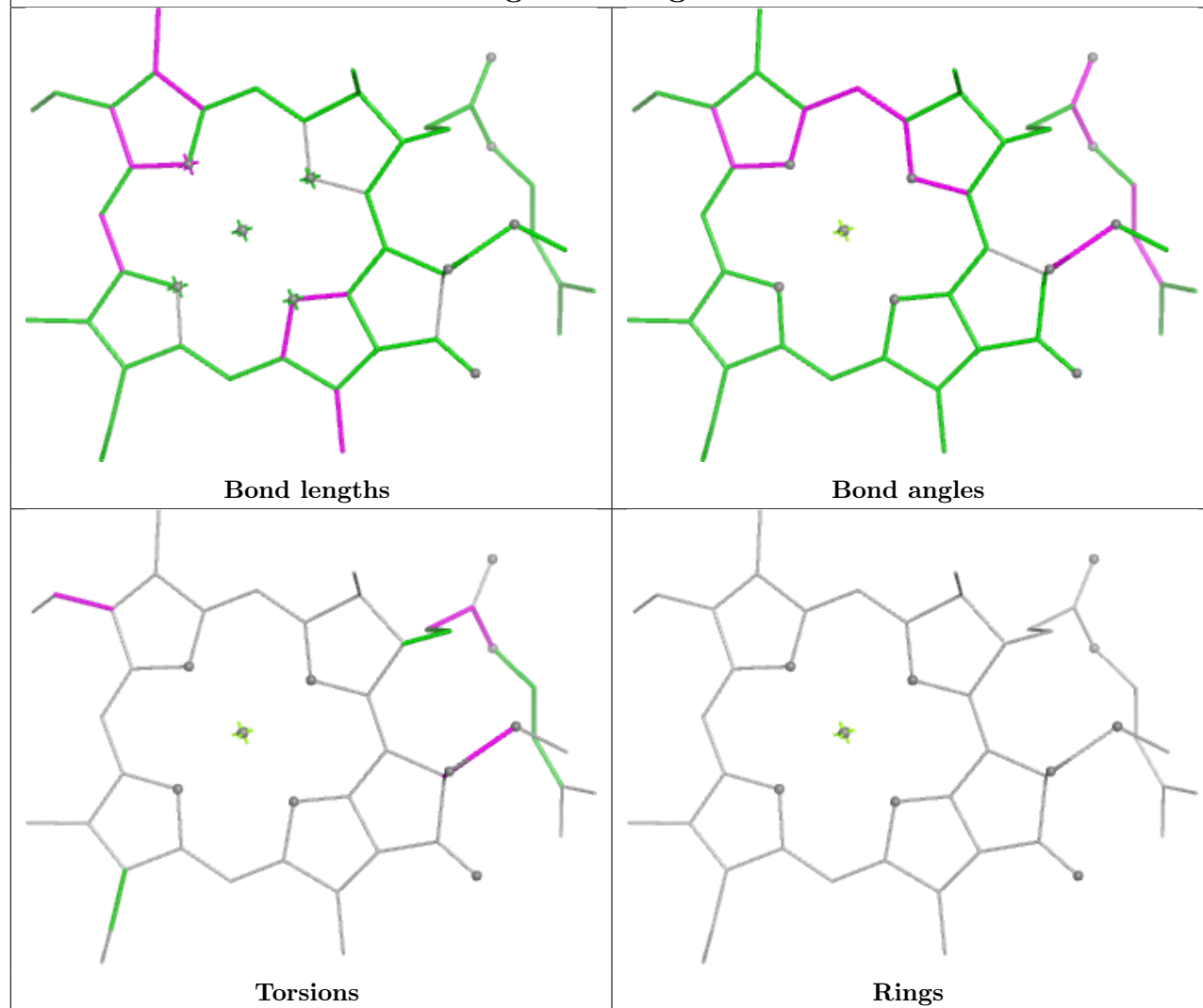


Torsions



Rings

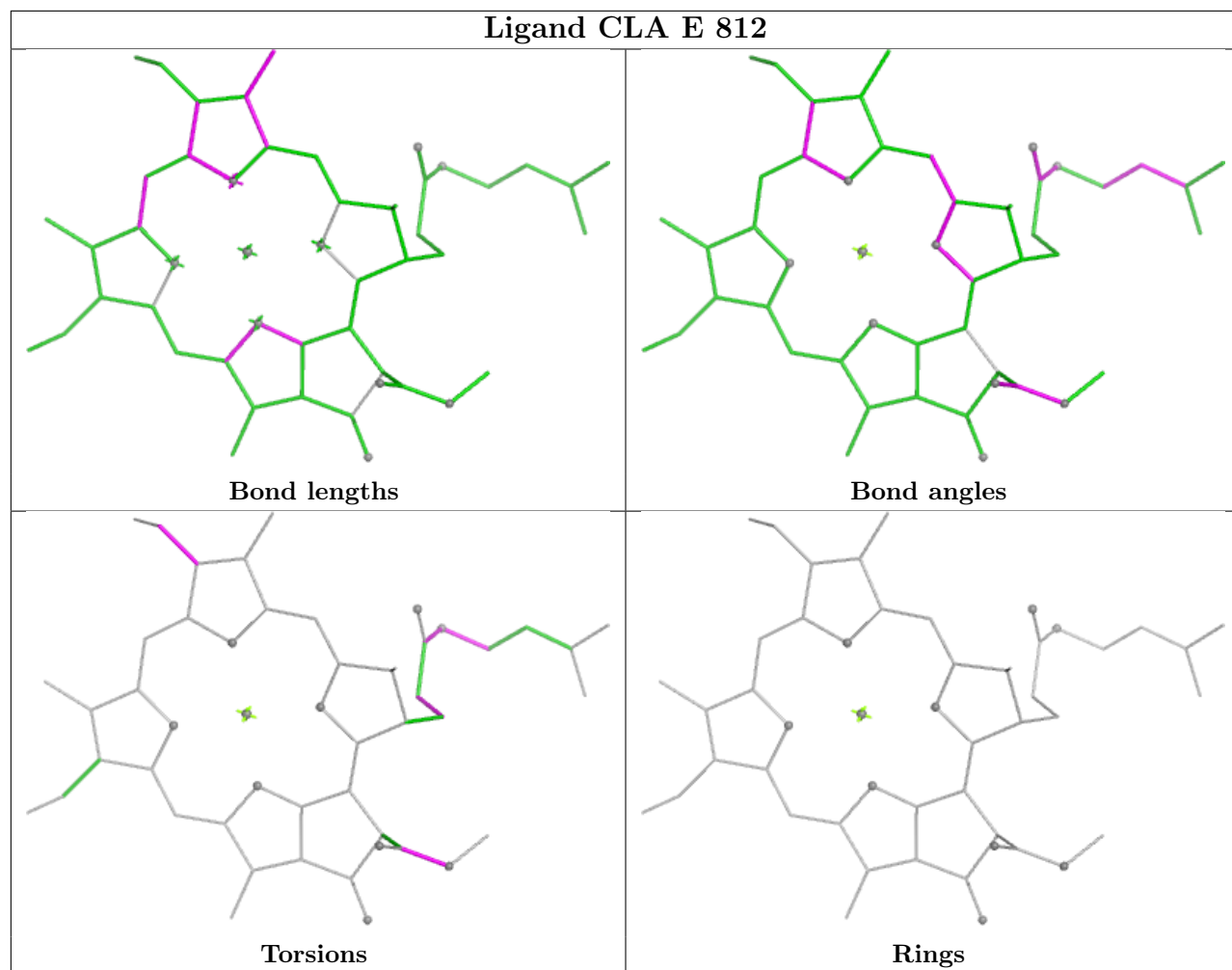
Ligand CLA g 818



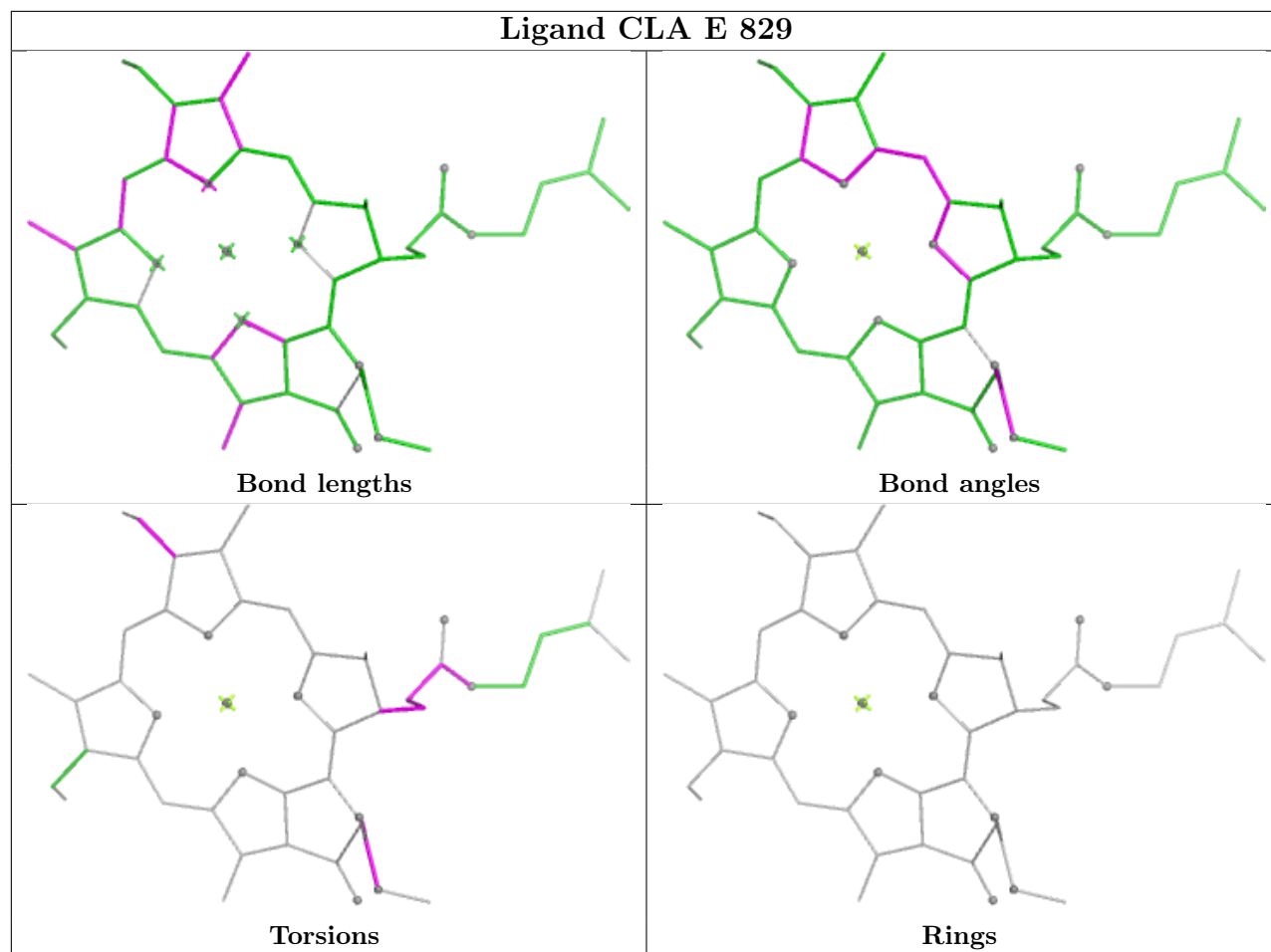
Ligand BCR J 101



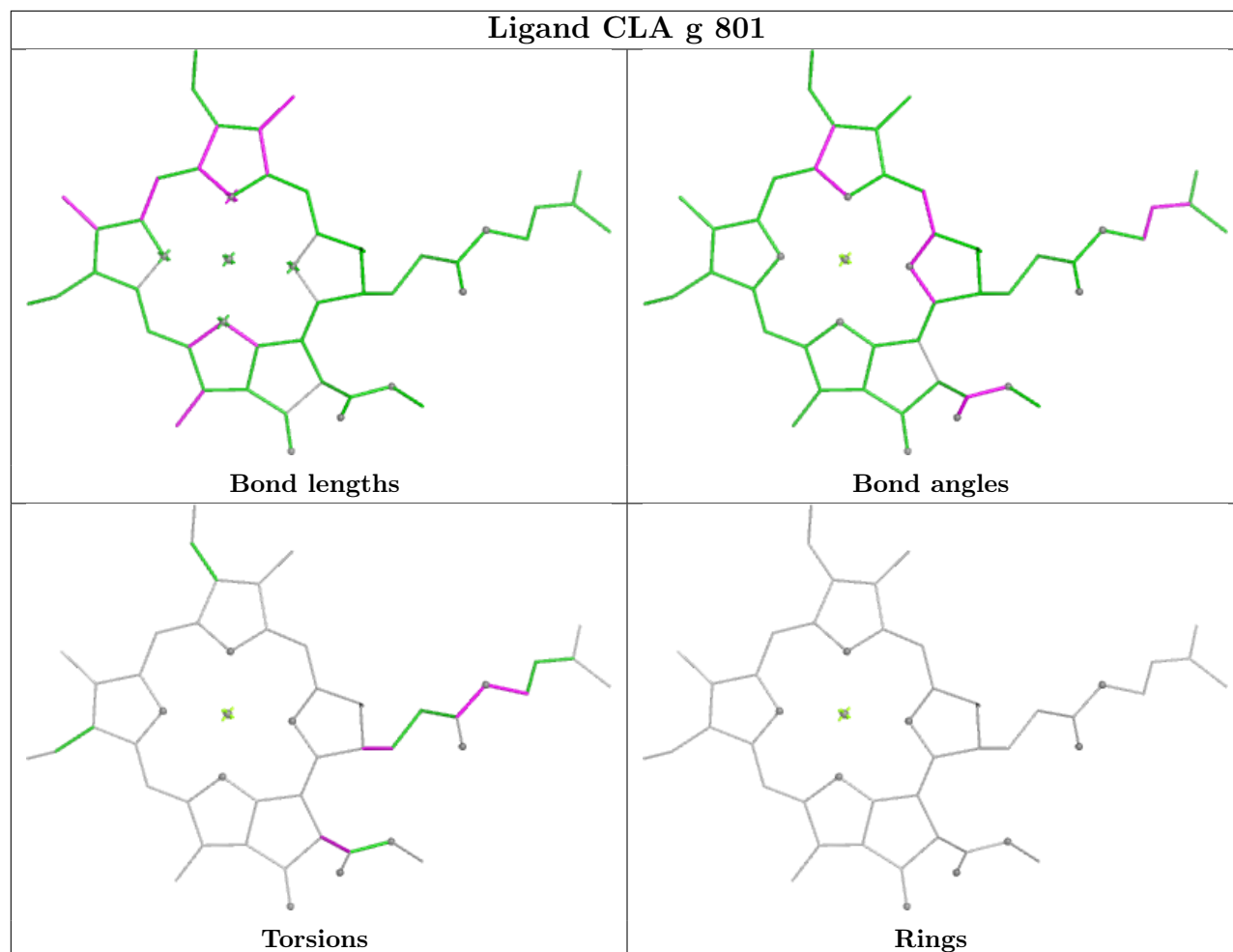
Ligand CLA E 812



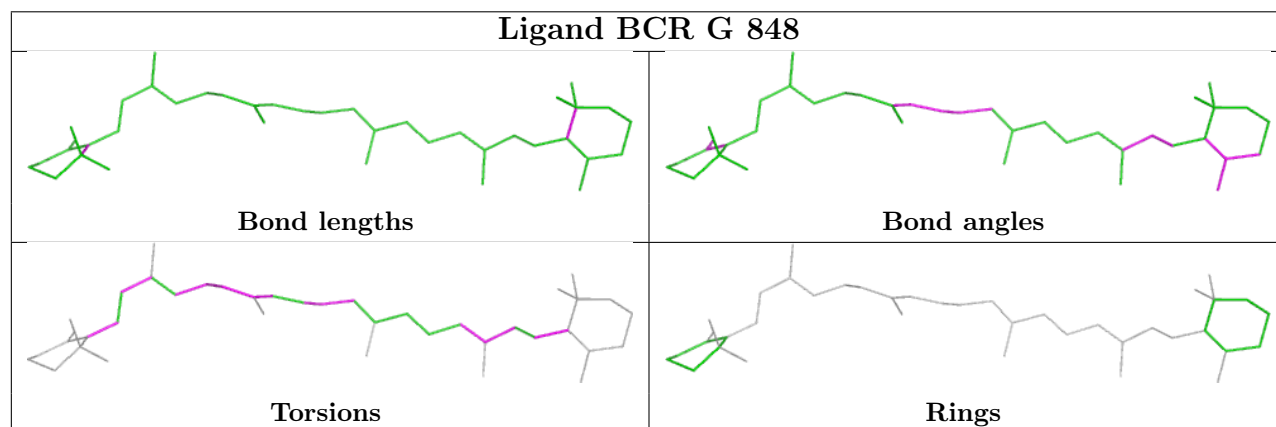
Ligand CLA E 829

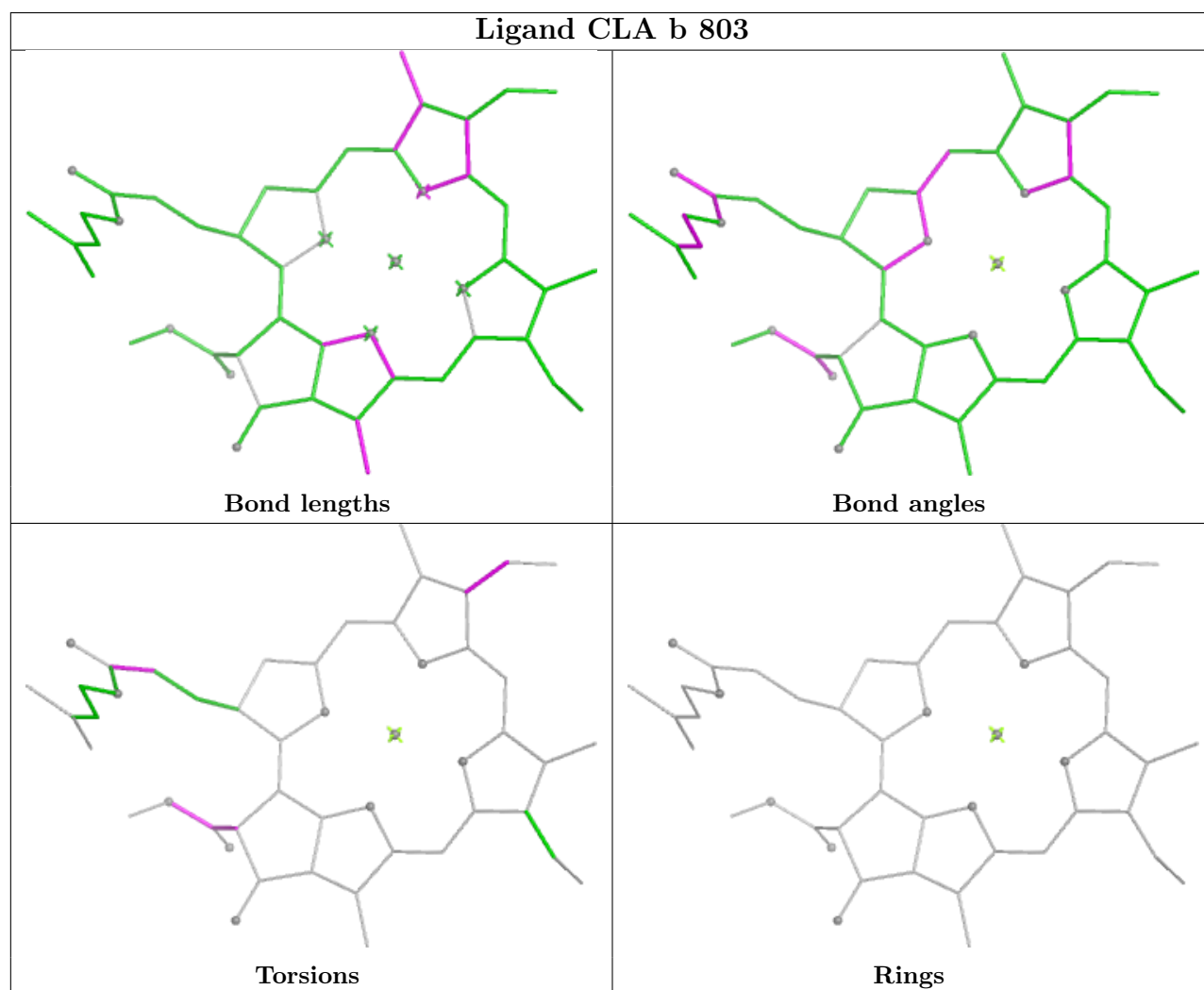
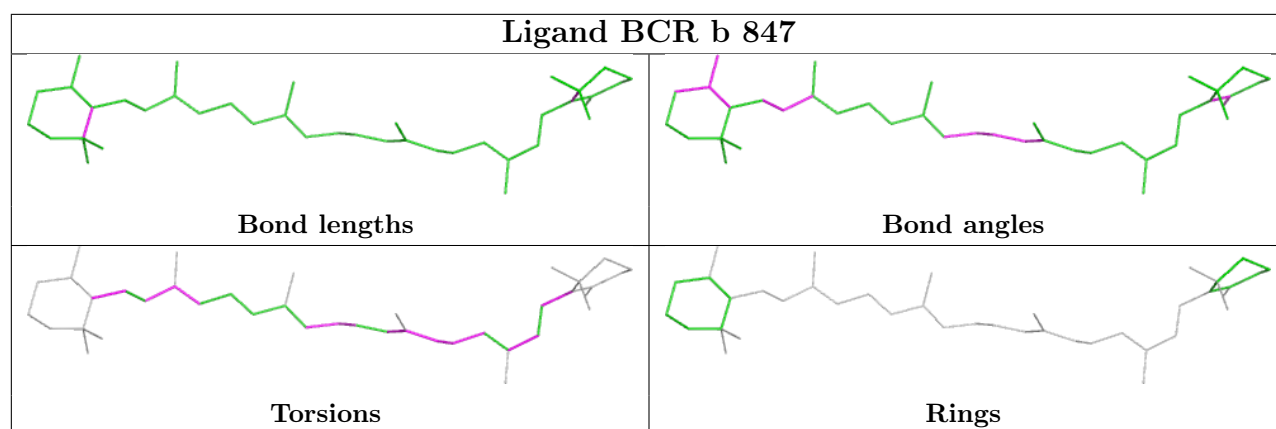


Ligand CLA g 801

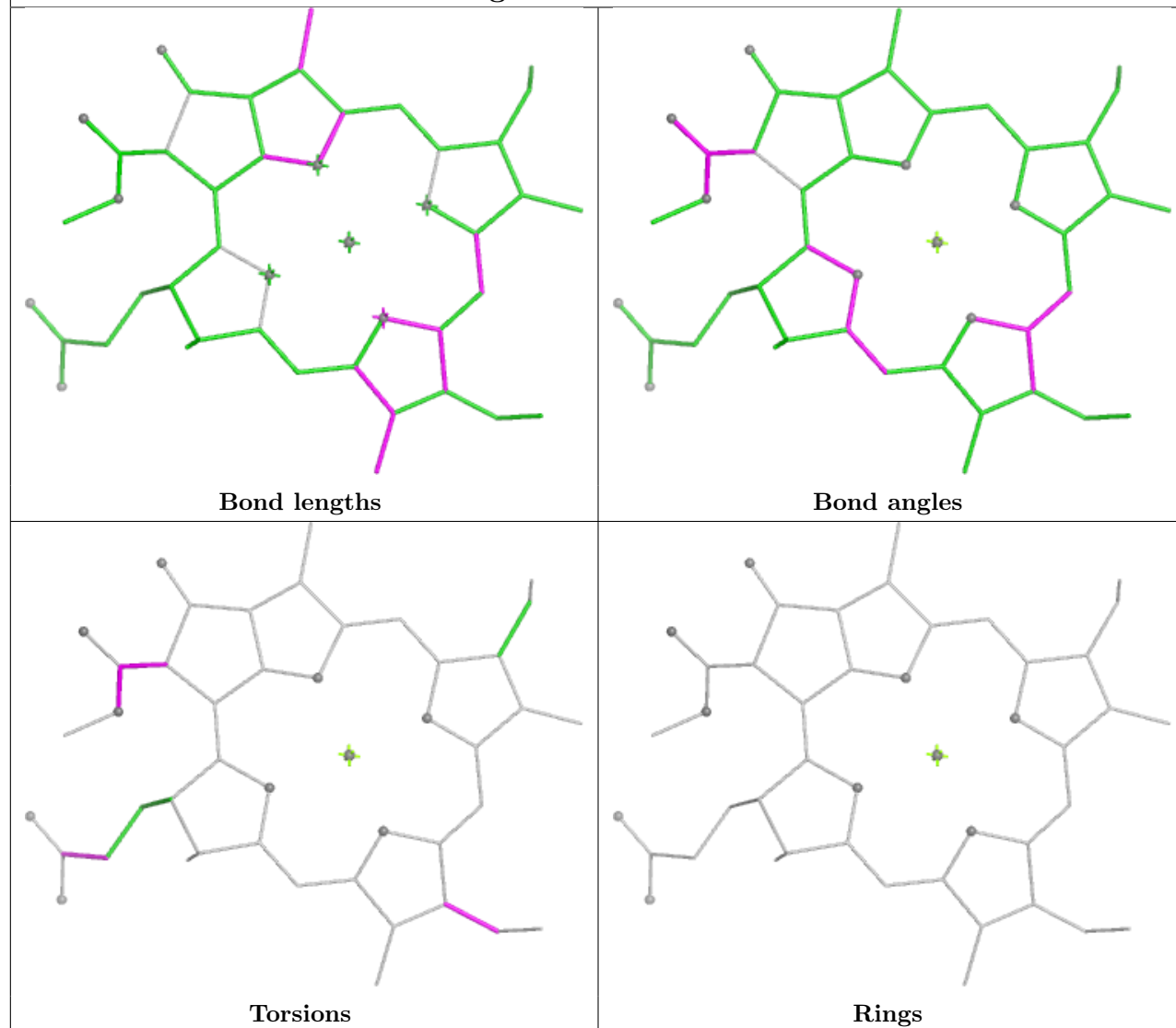


Ligand BCR G 848

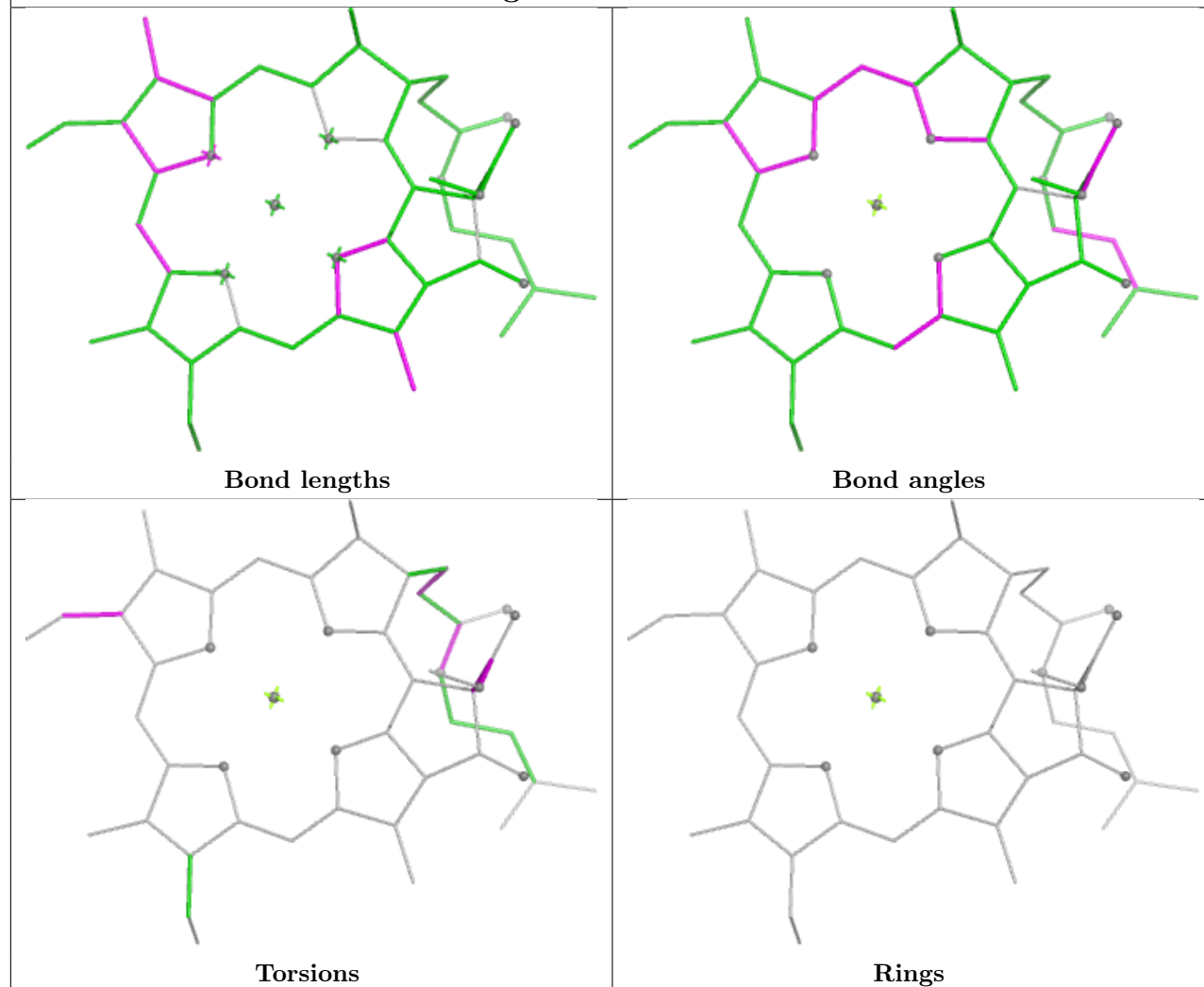




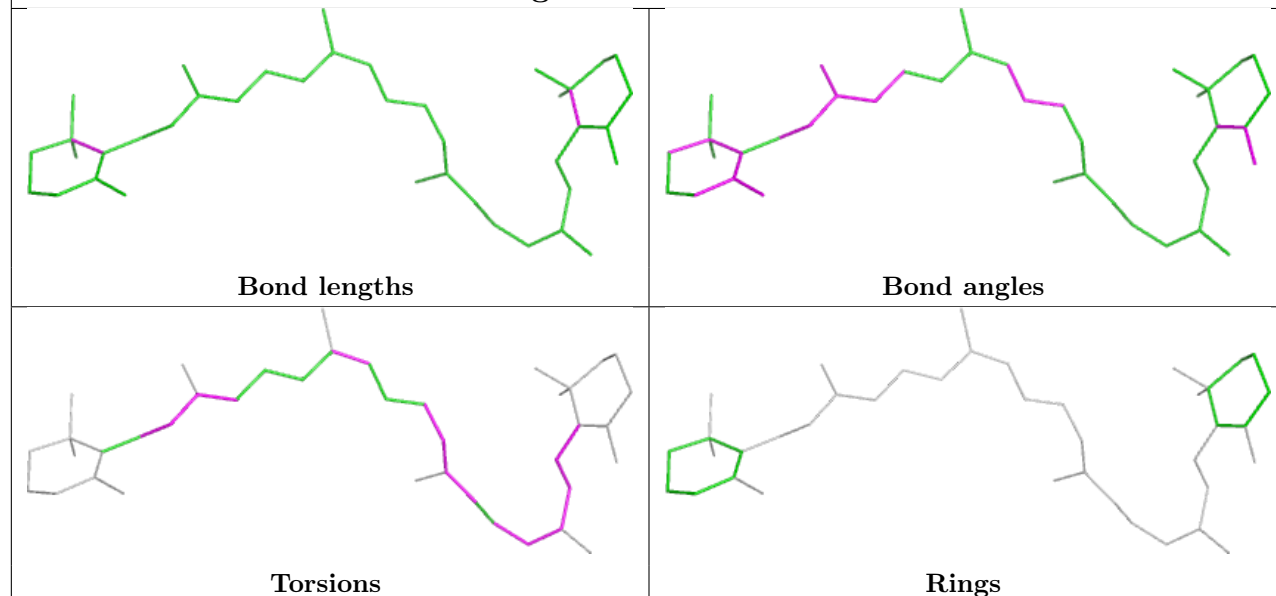
Ligand CLA G 824

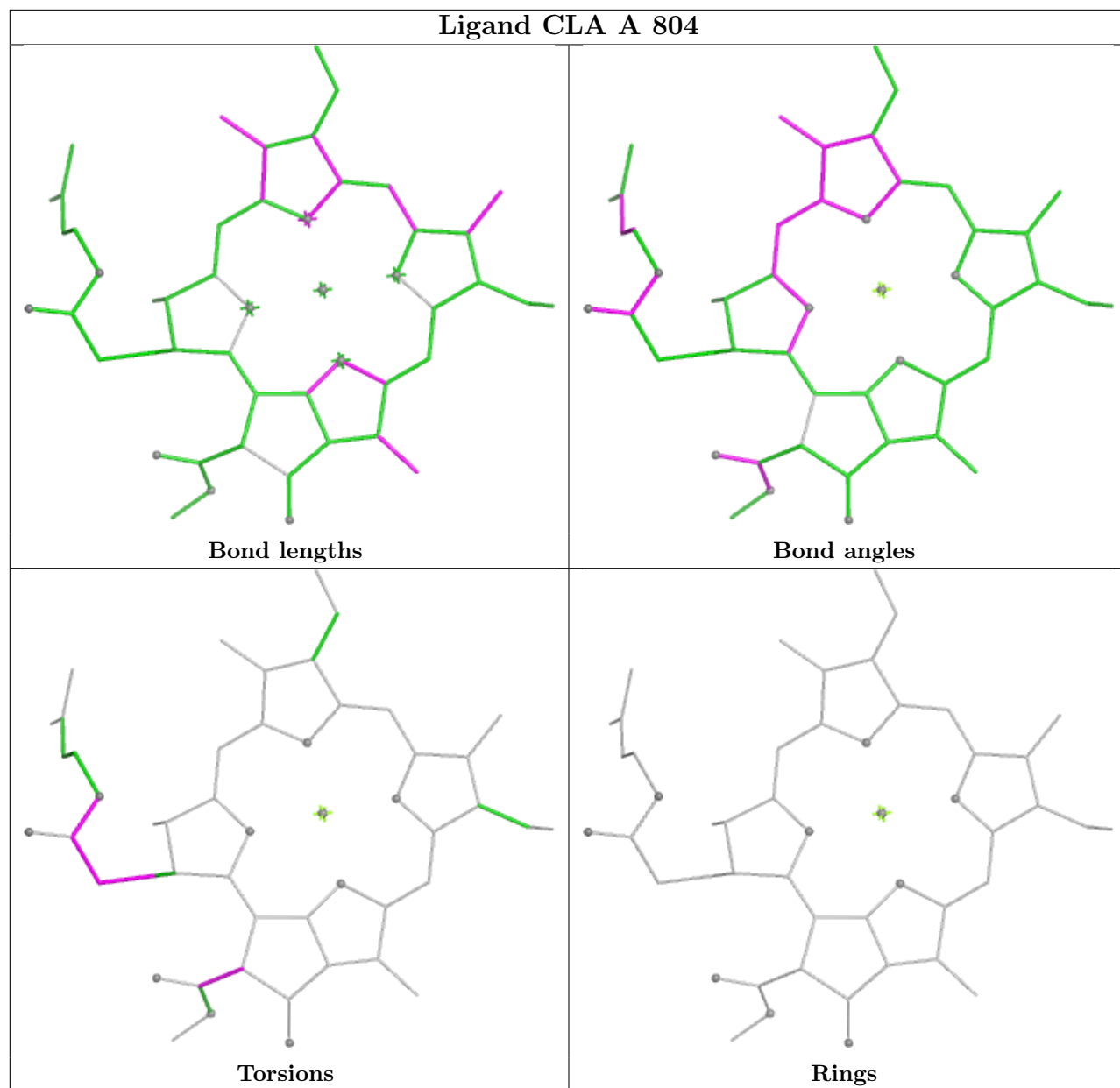


Ligand CLA E 810

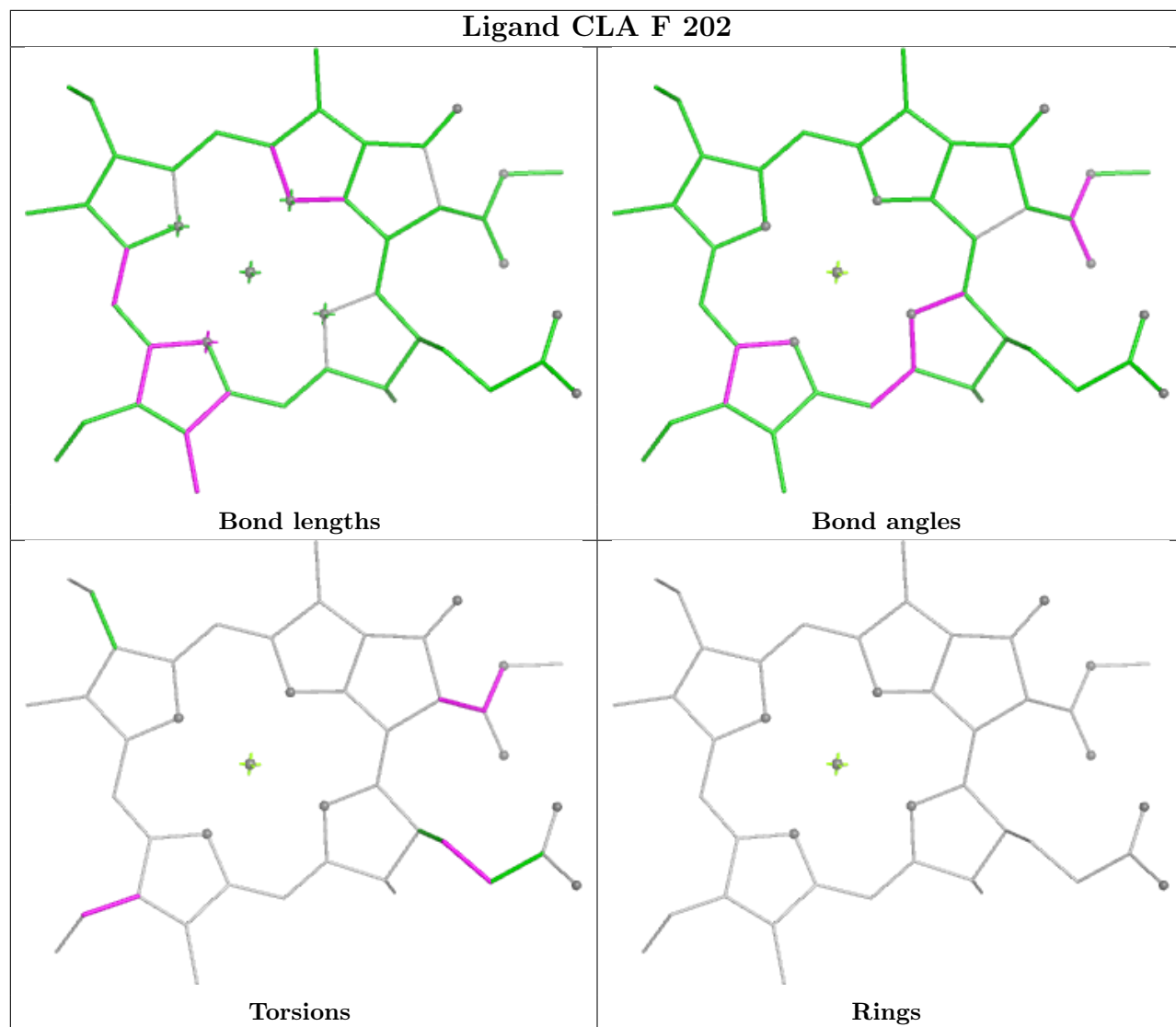


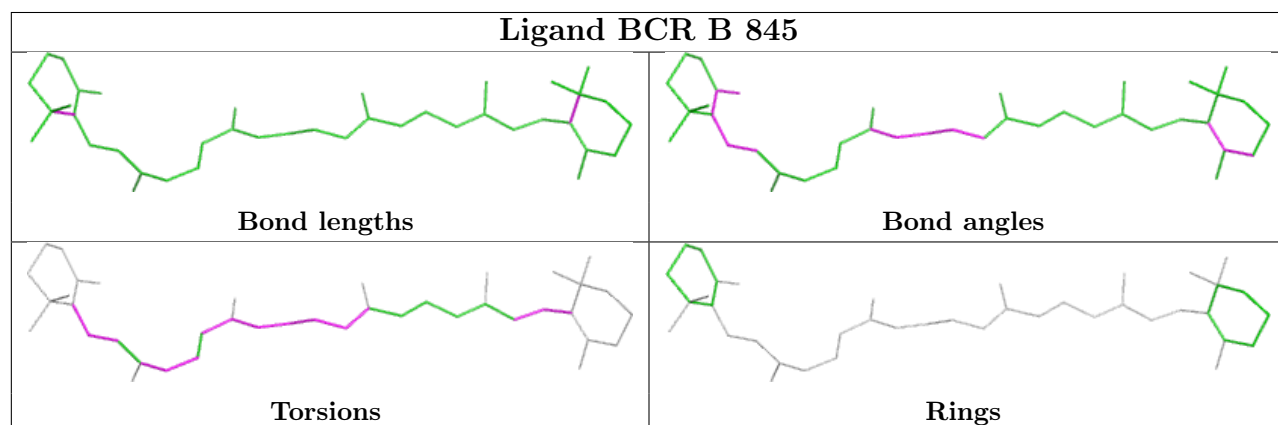
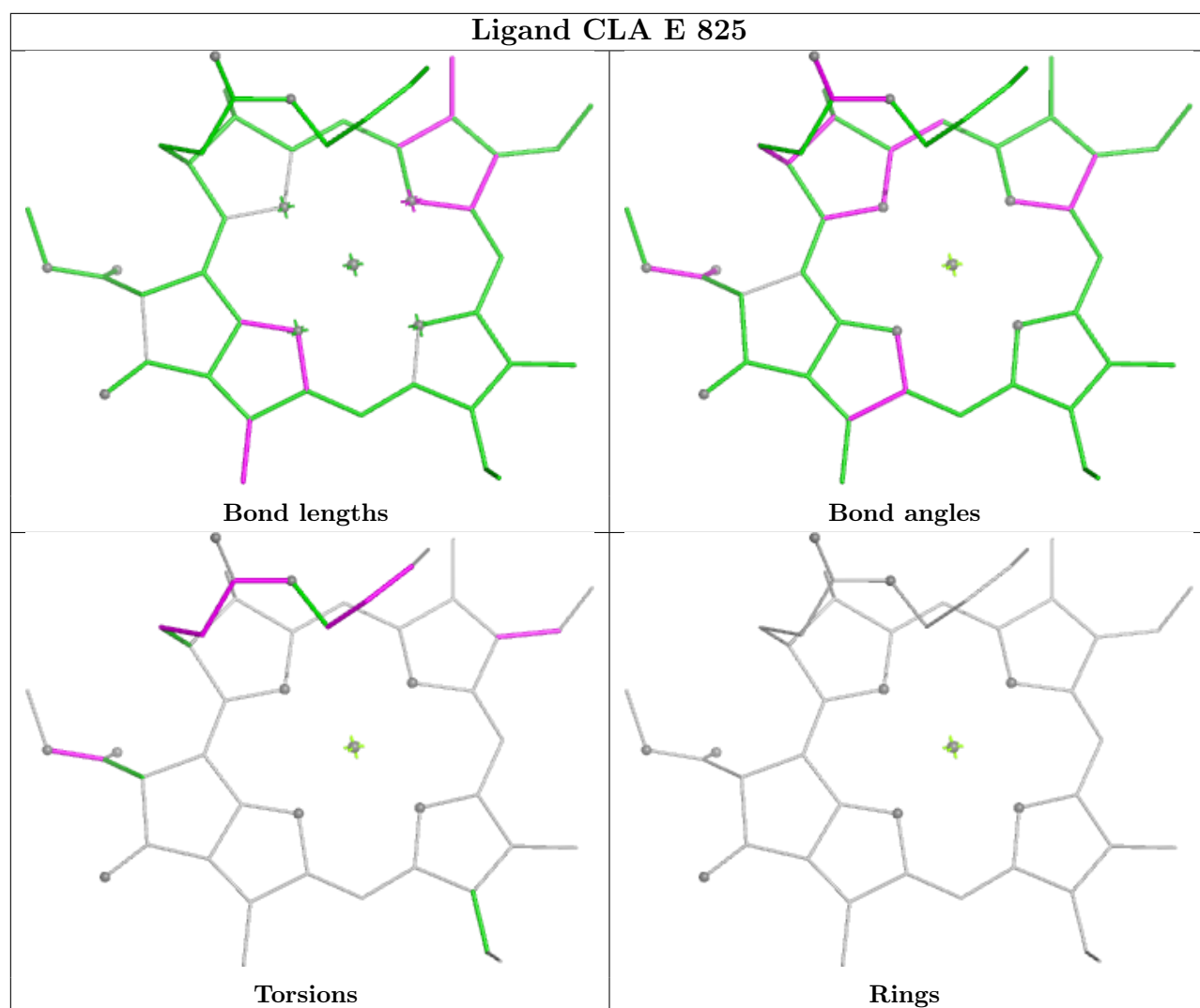
Ligand BCR E 849

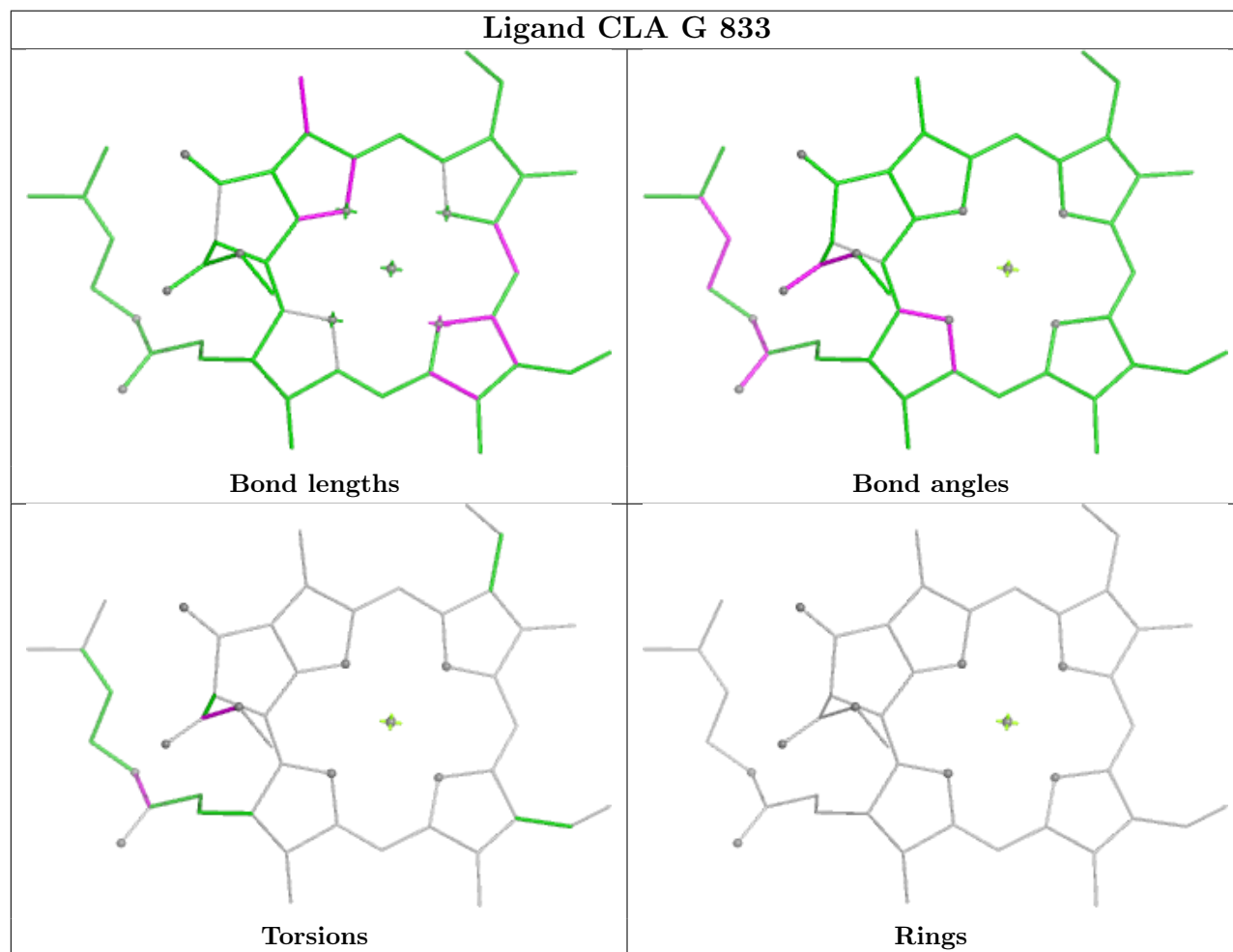
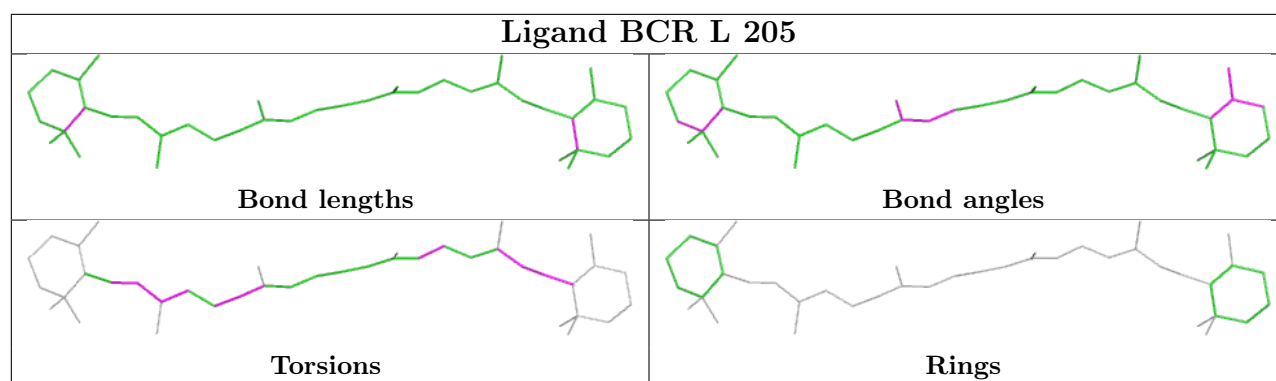




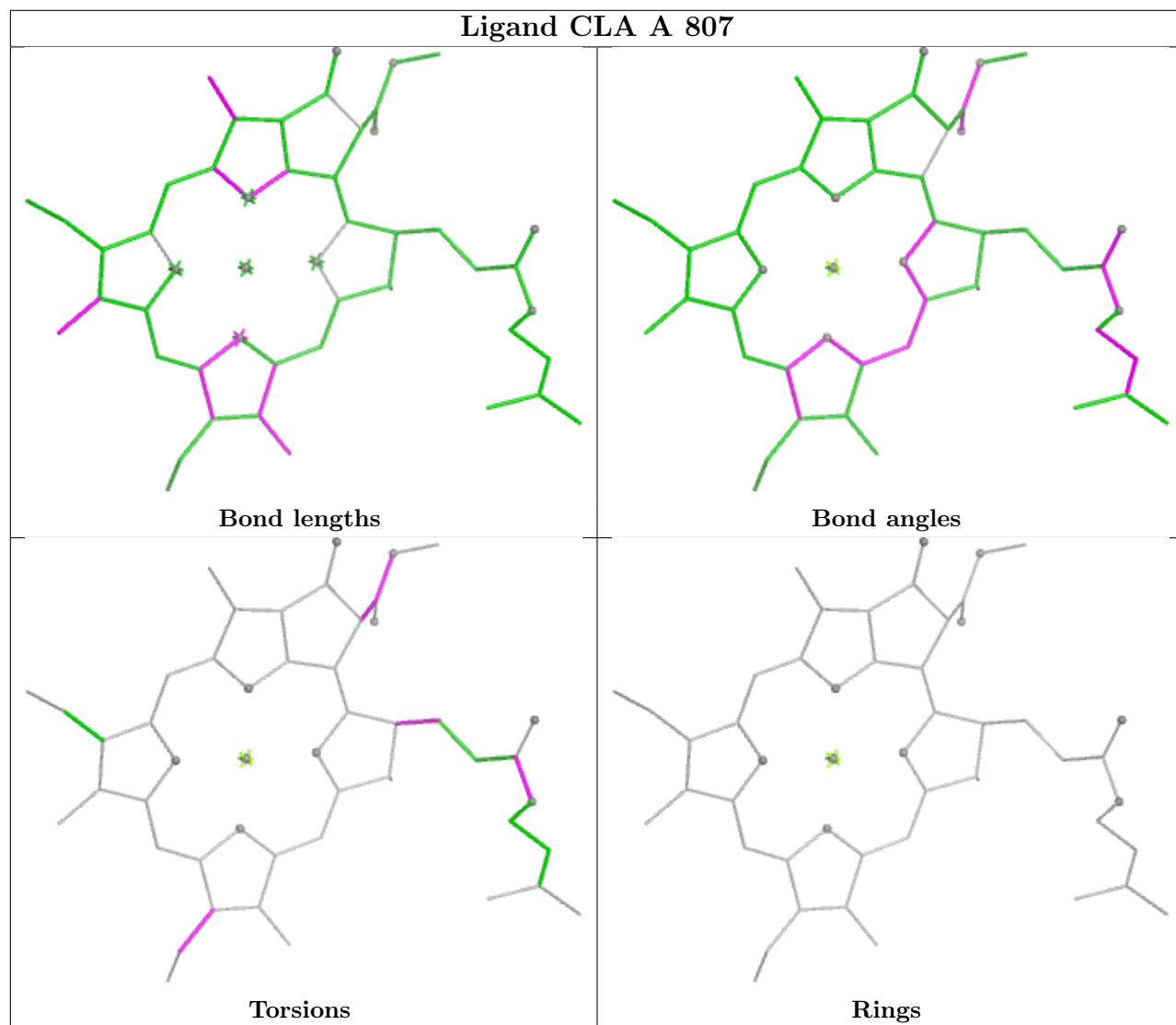
Ligand CLA F 202



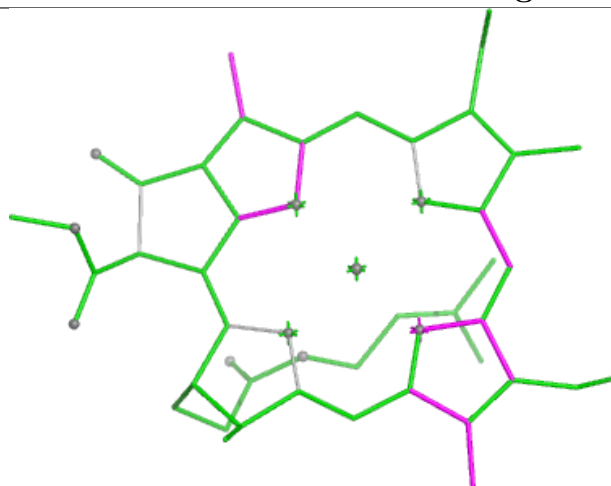




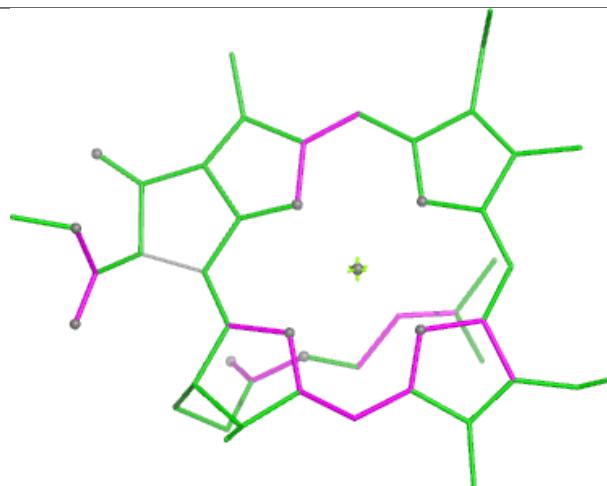
Ligand CLA A 807



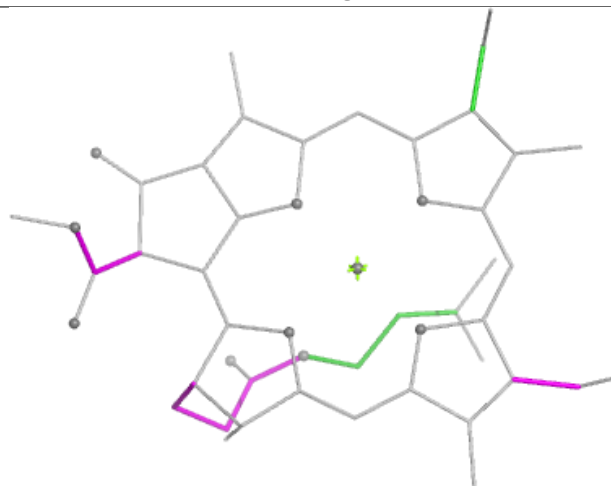
Ligand CLA E 826



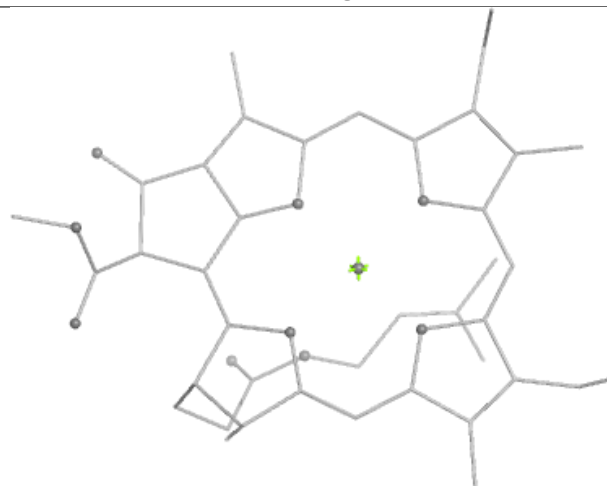
Bond lengths



Bond angles



Torsions

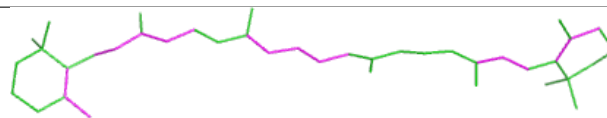


Rings

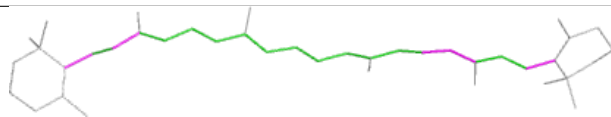
Ligand BCR E 851



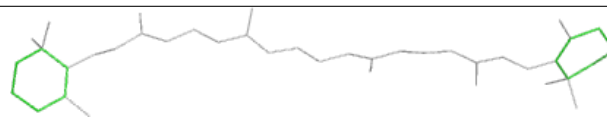
Bond lengths



Bond angles

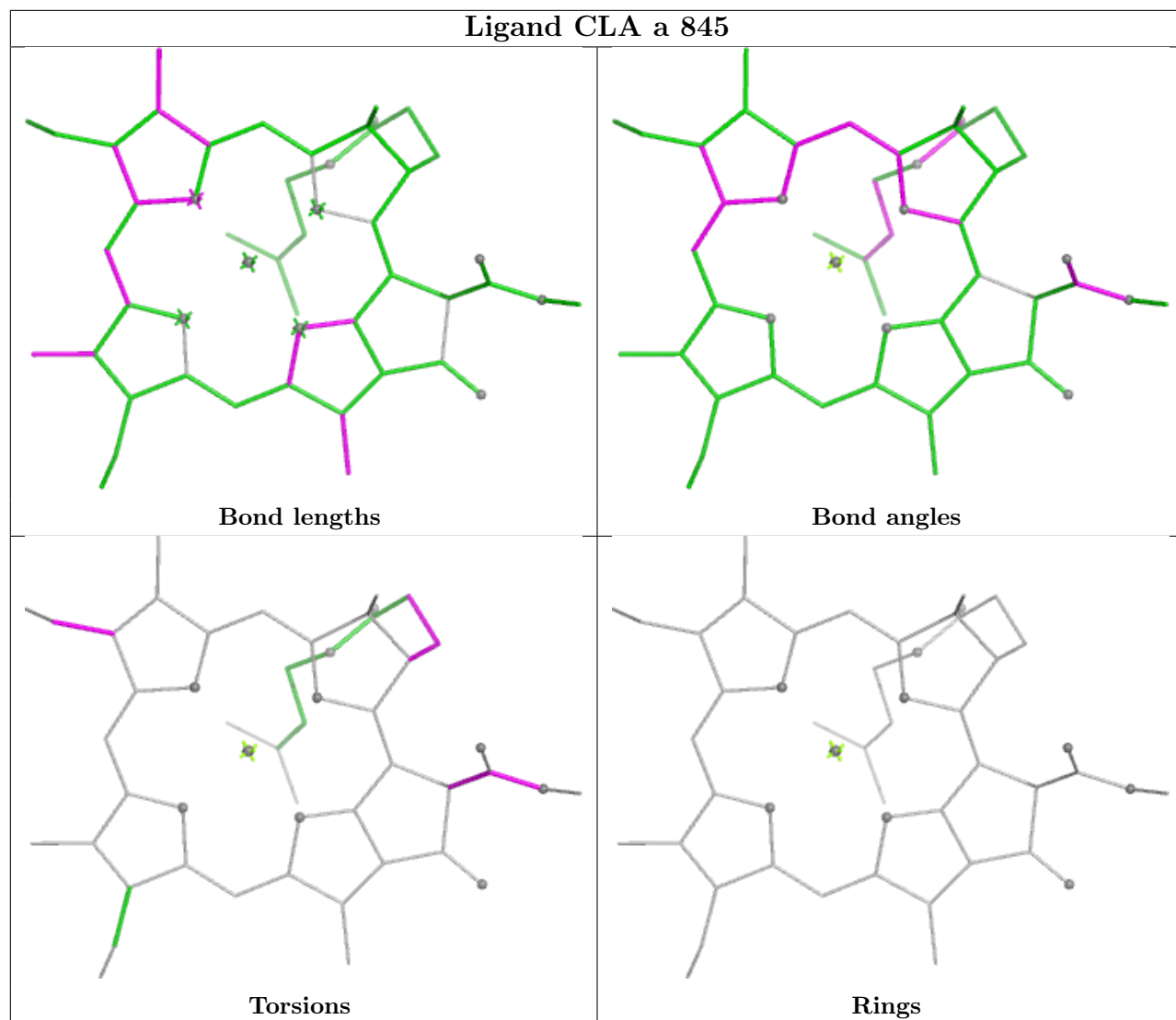


Torsions

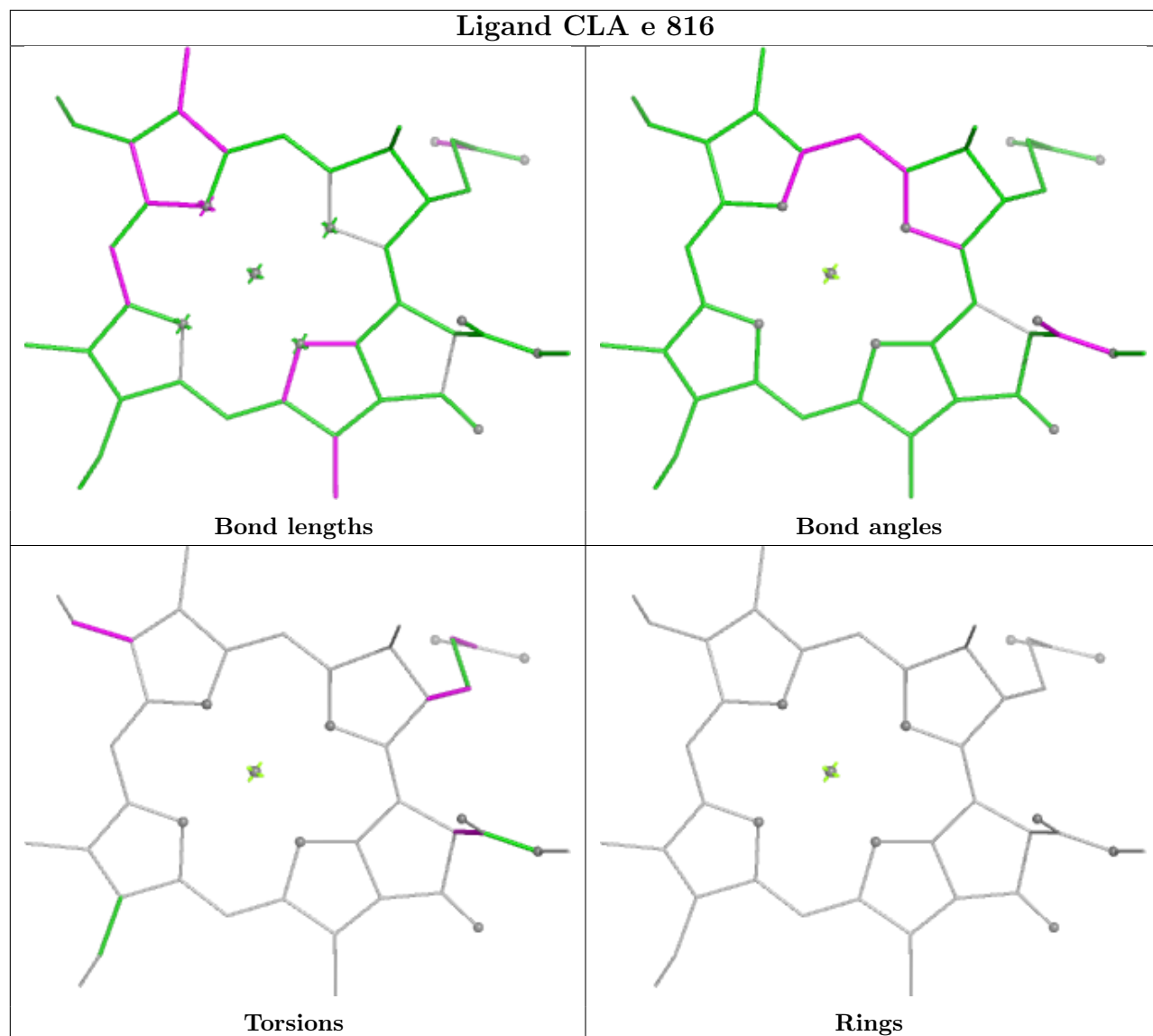


Rings

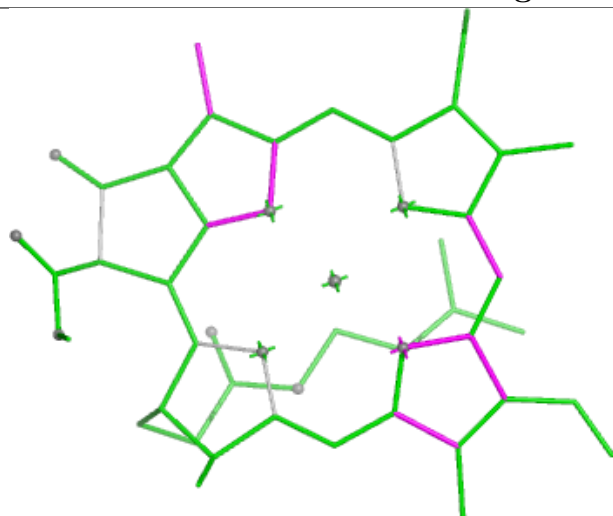
Ligand CLA a 845



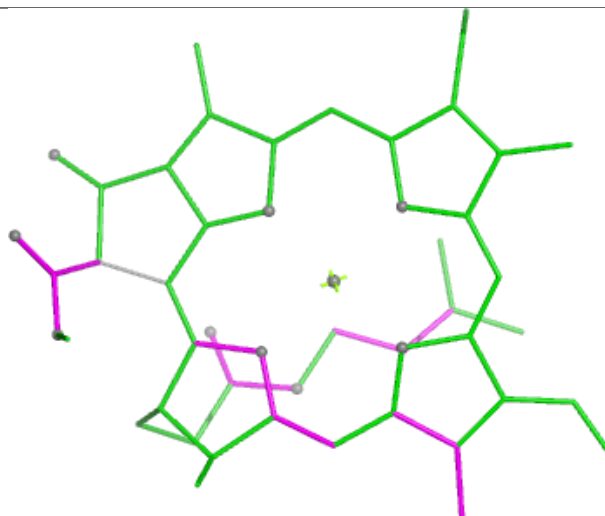
Ligand CLA e 816



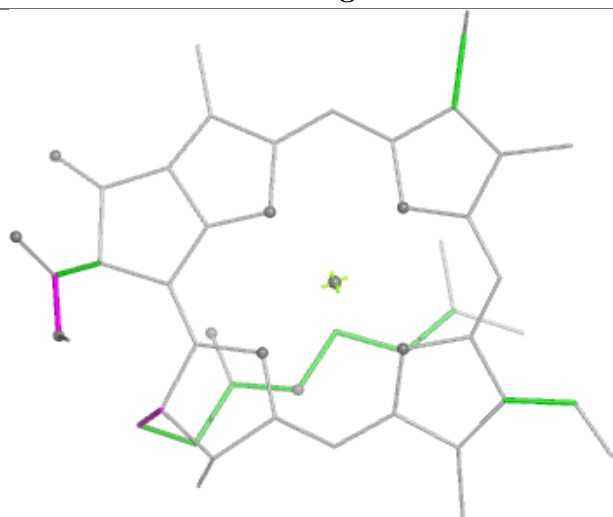
Ligand CLA B 810



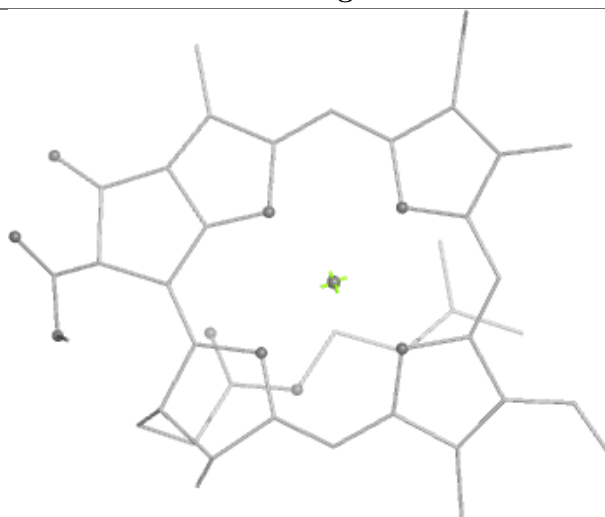
Bond lengths



Bond angles

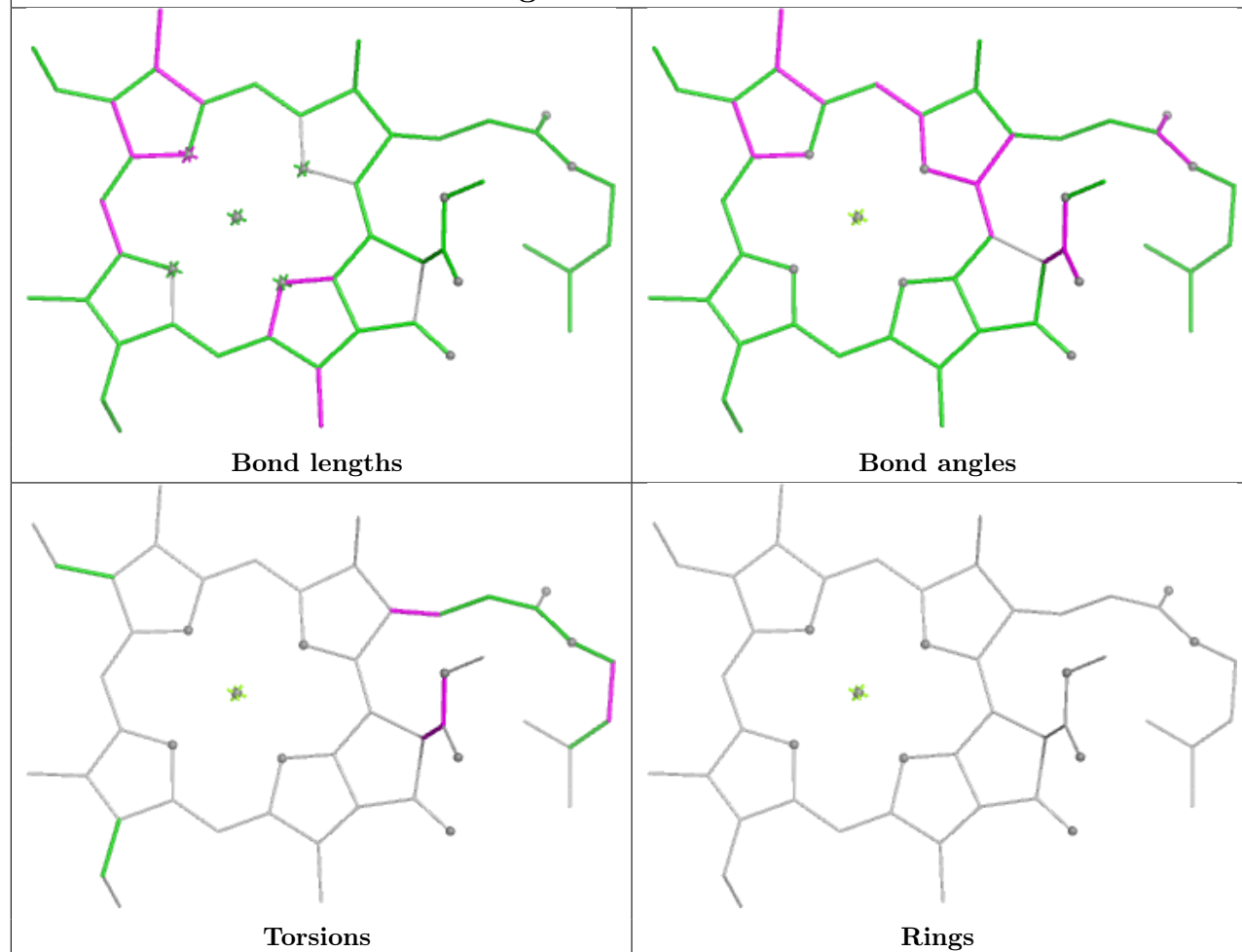


Torsions

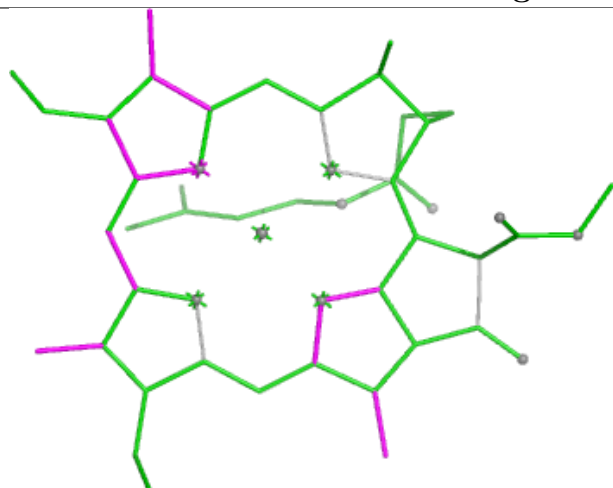


Rings

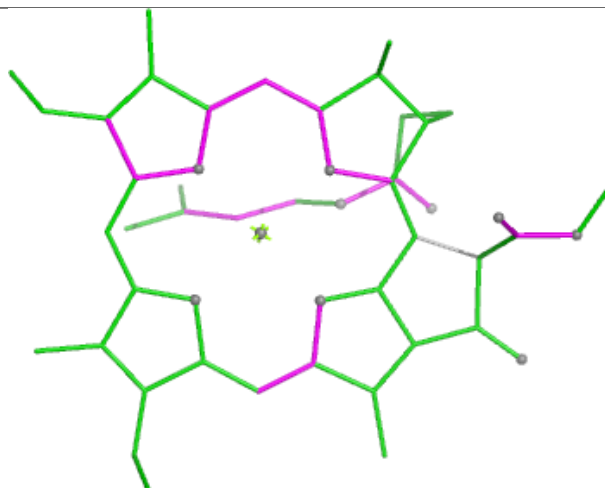
Ligand CLA E 828



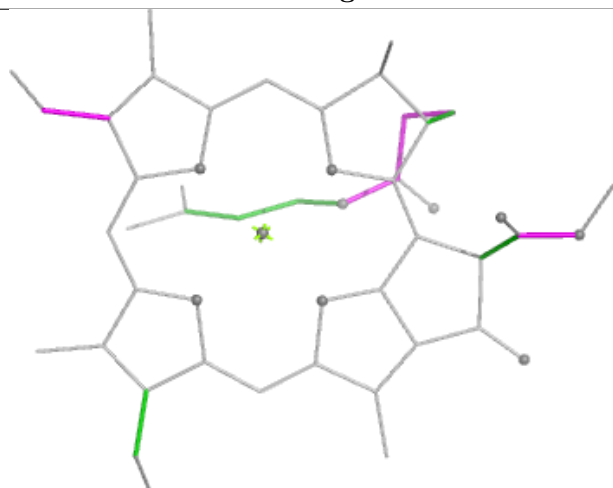
Ligand CLA G 838



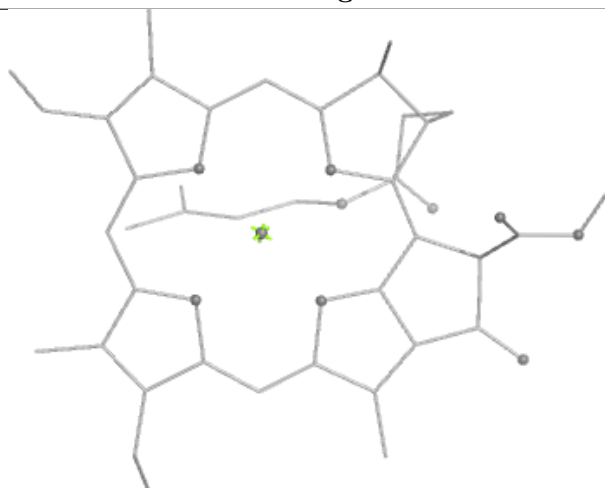
Bond lengths



Bond angles

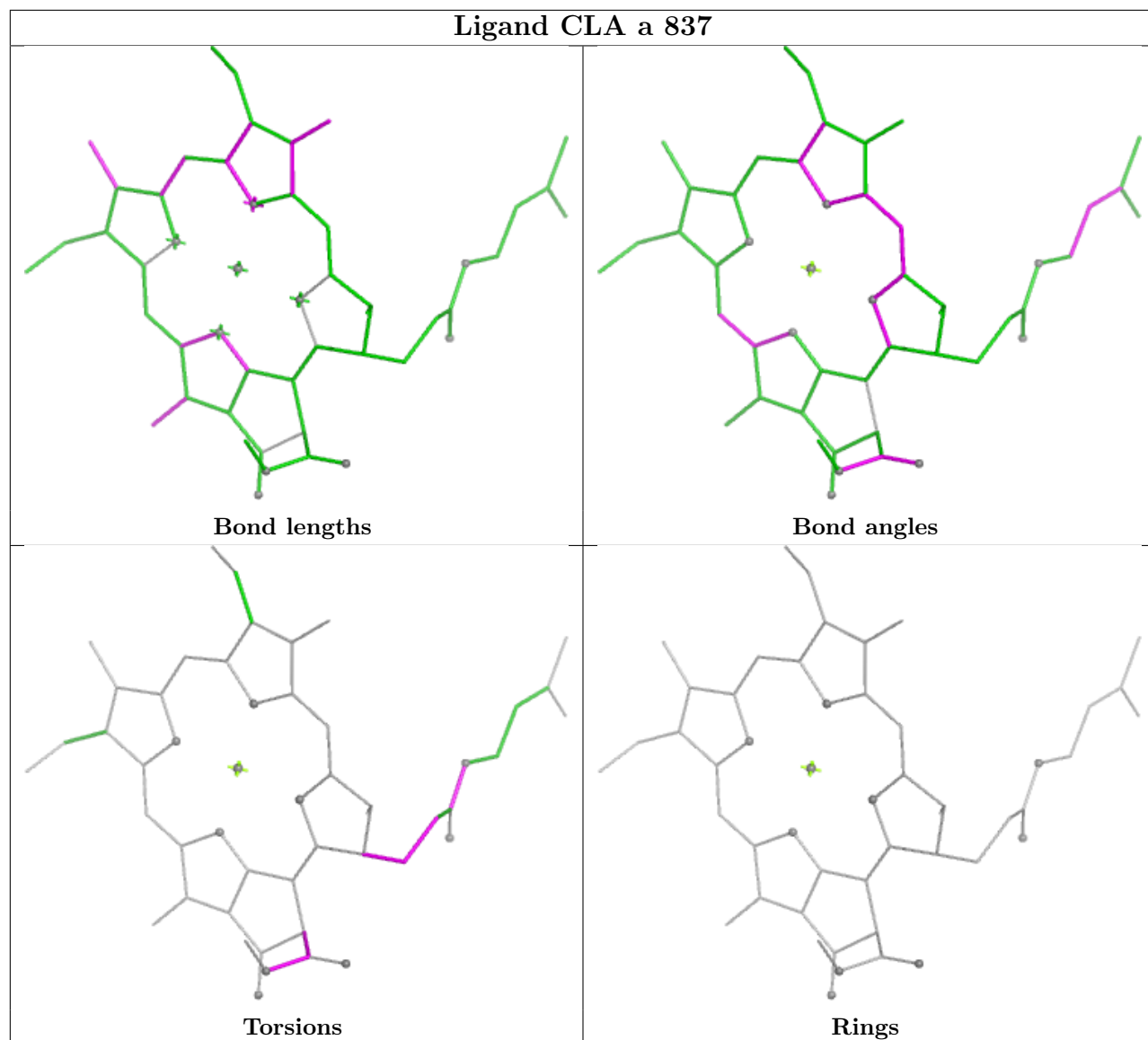


Torsions

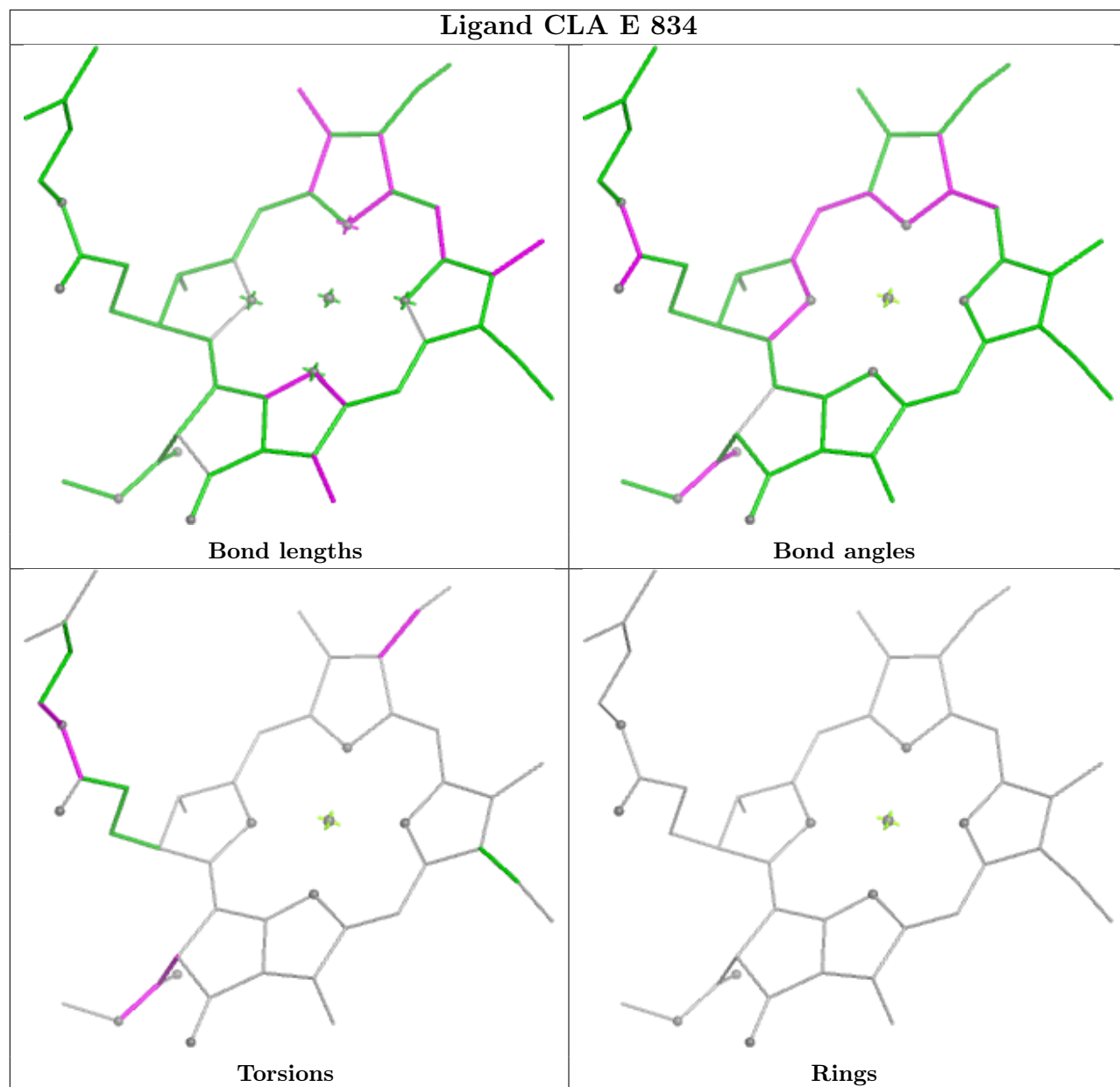


Rings

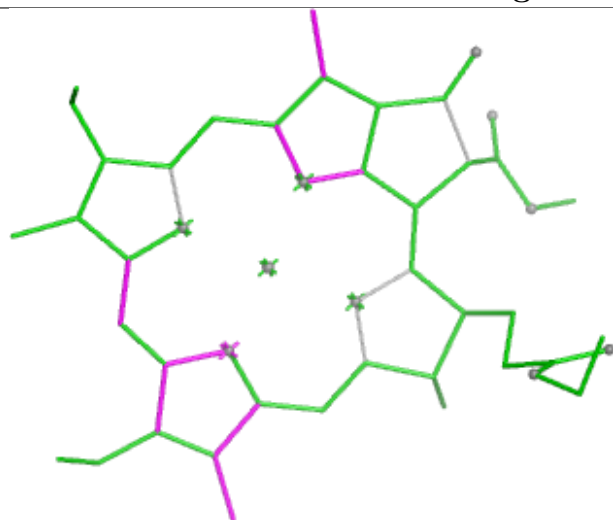
Ligand CLA a 837



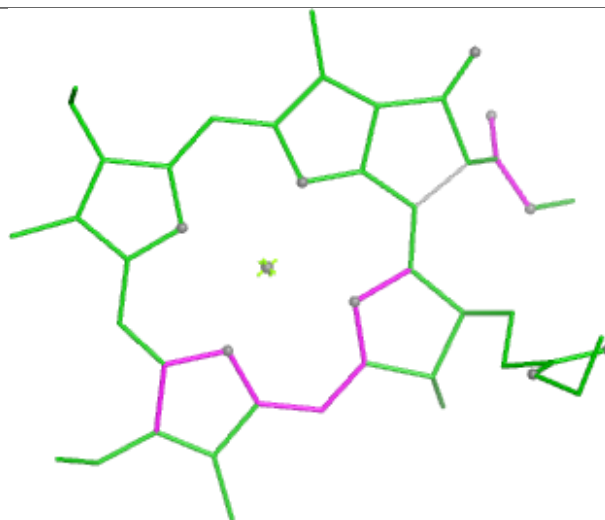
Ligand CLA E 834



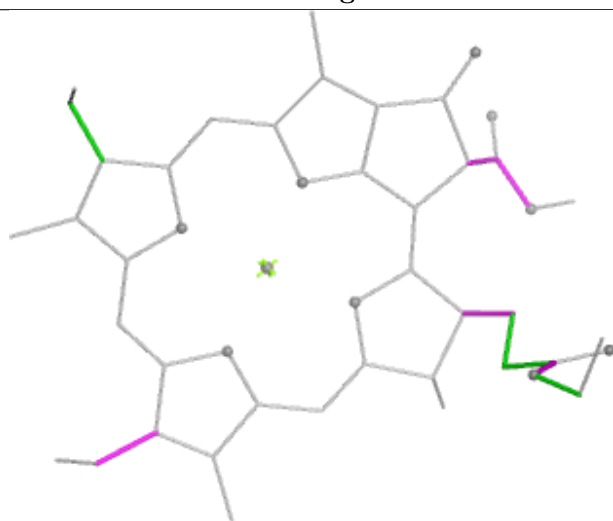
Ligand CLA G 839



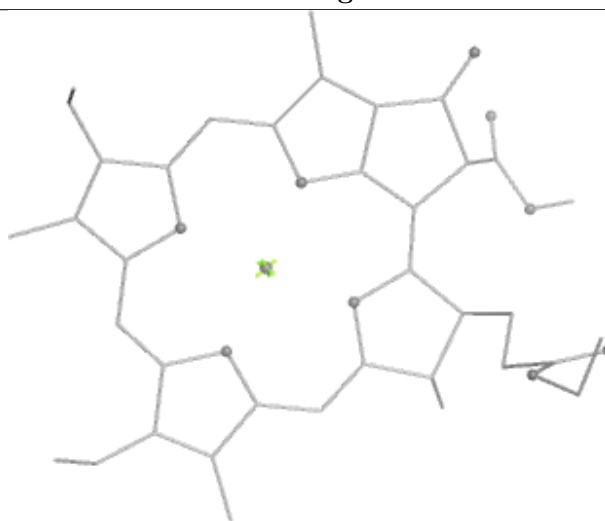
Bond lengths



Bond angles

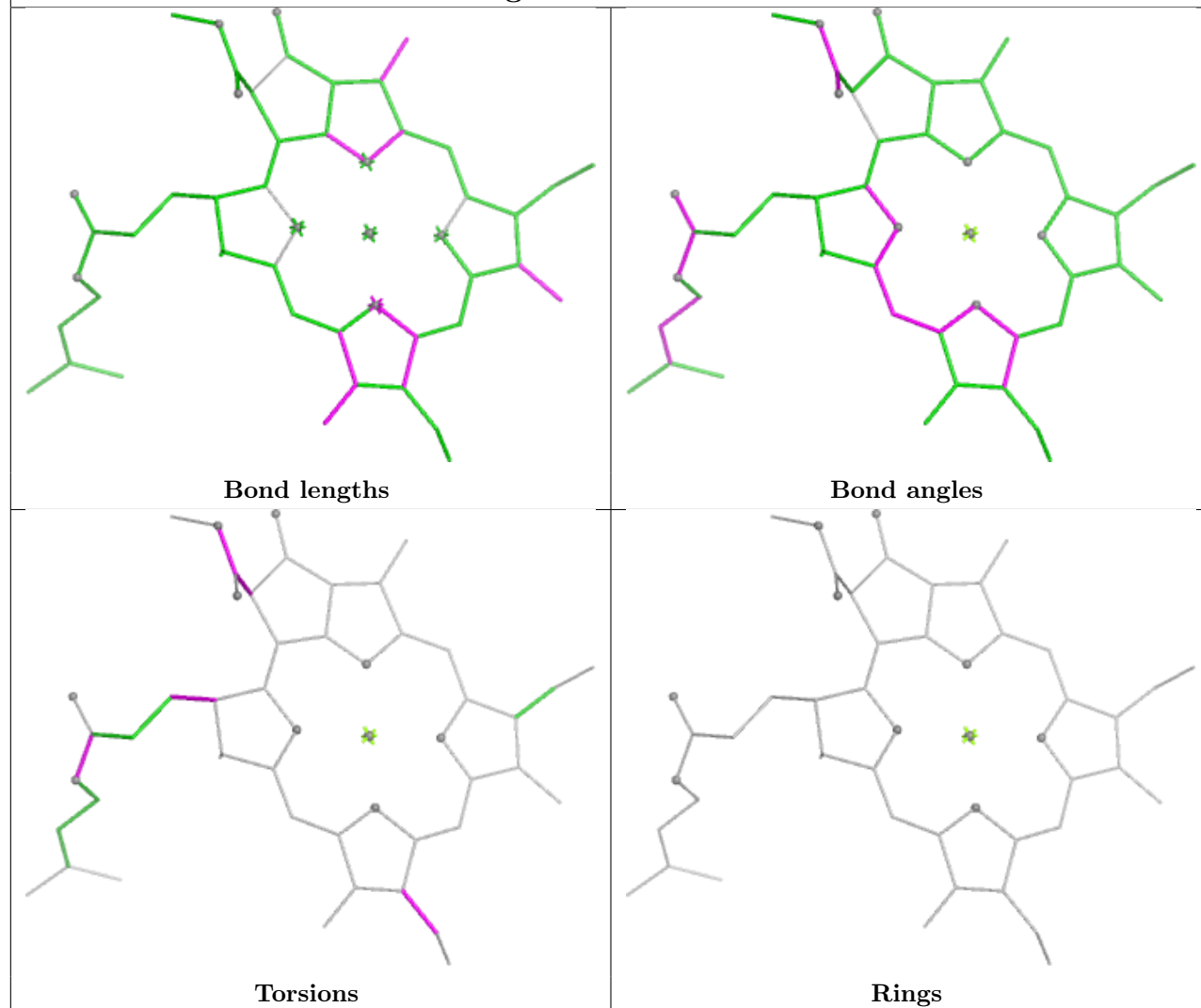


Torsions

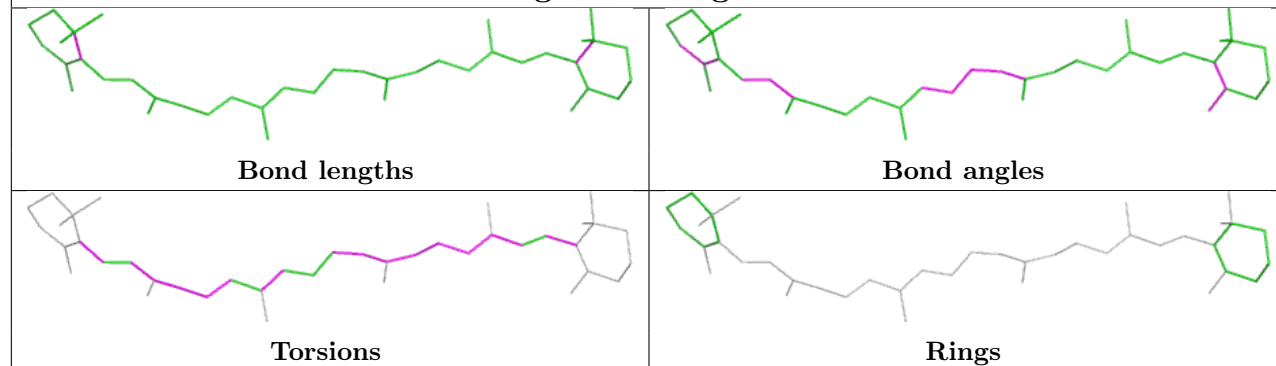


Rings

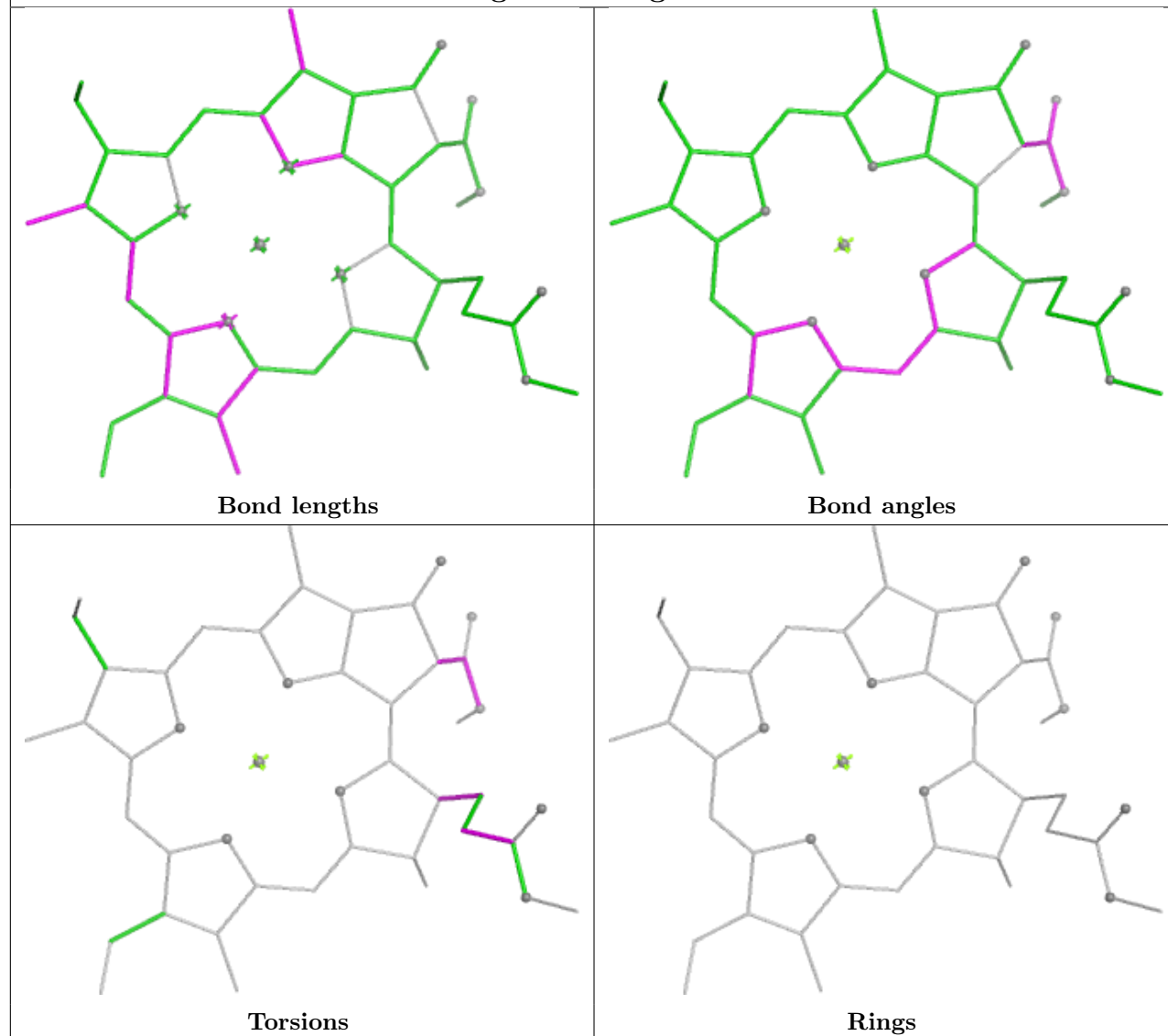
Ligand CLA e 806



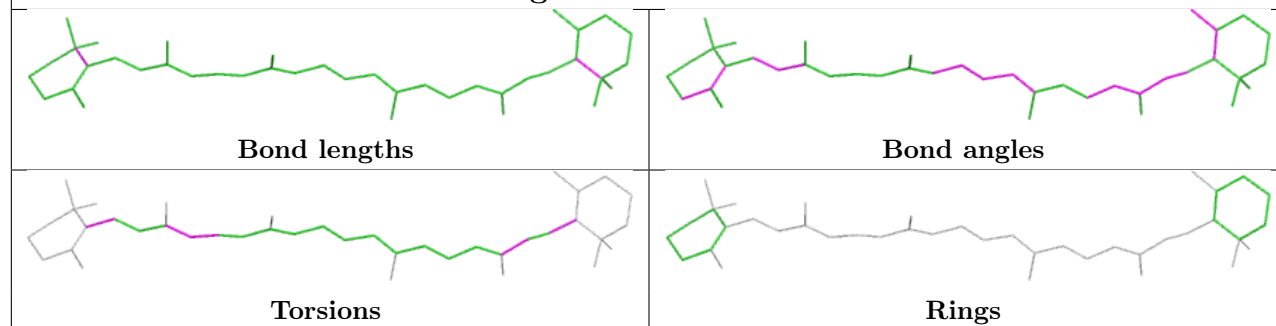
Ligand BCR g 847



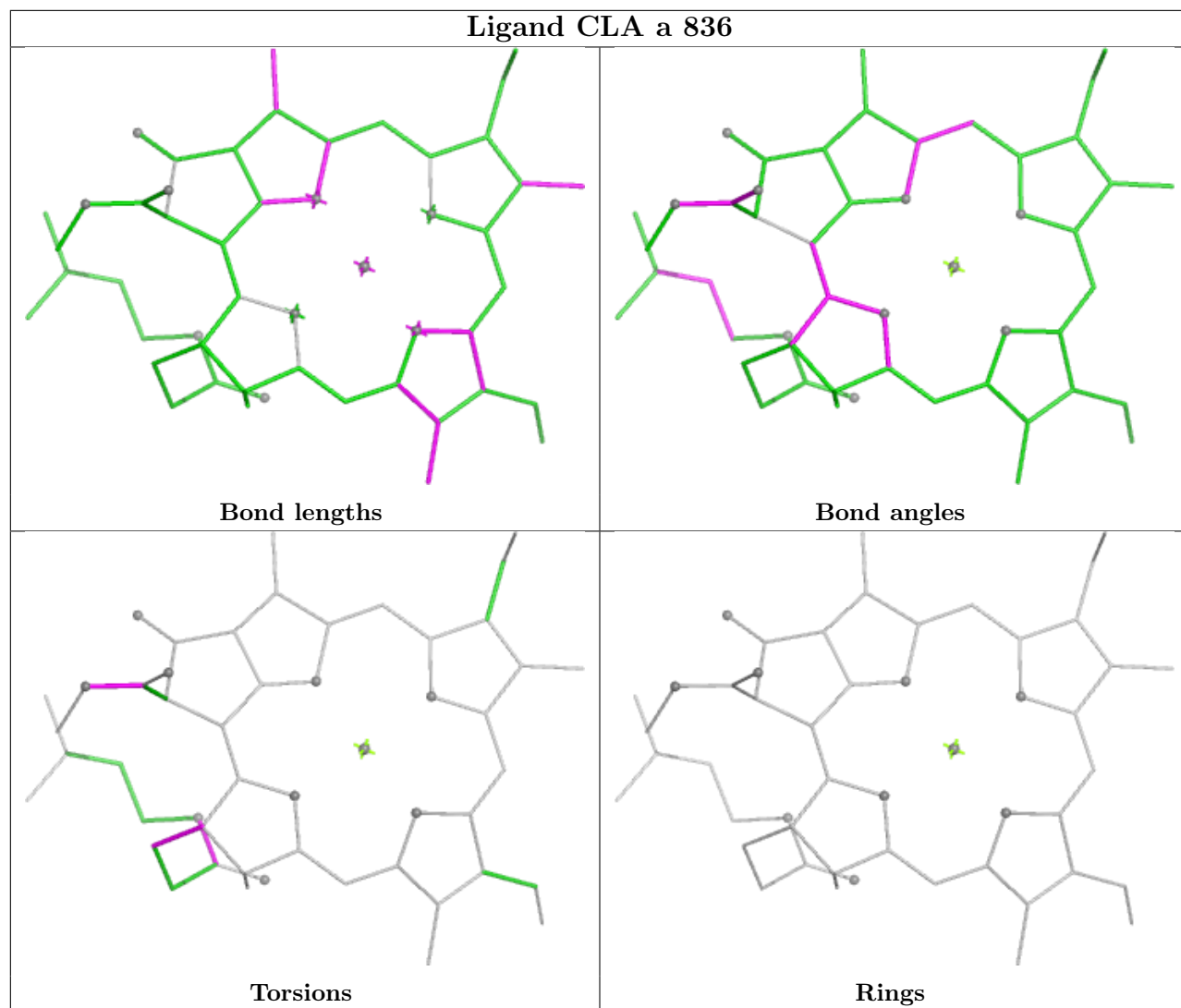
Ligand CLA g 827



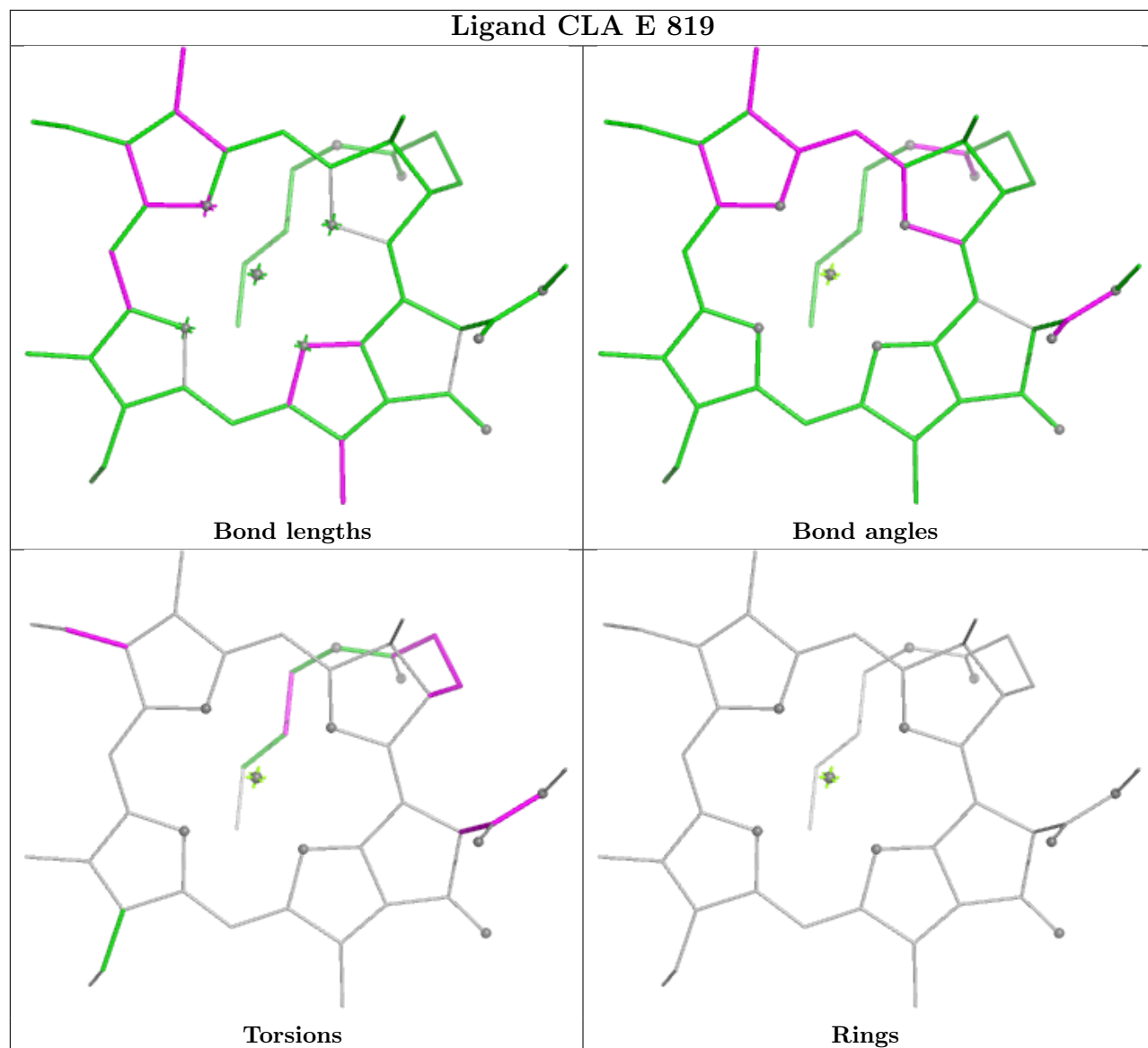
Ligand BCR A 849



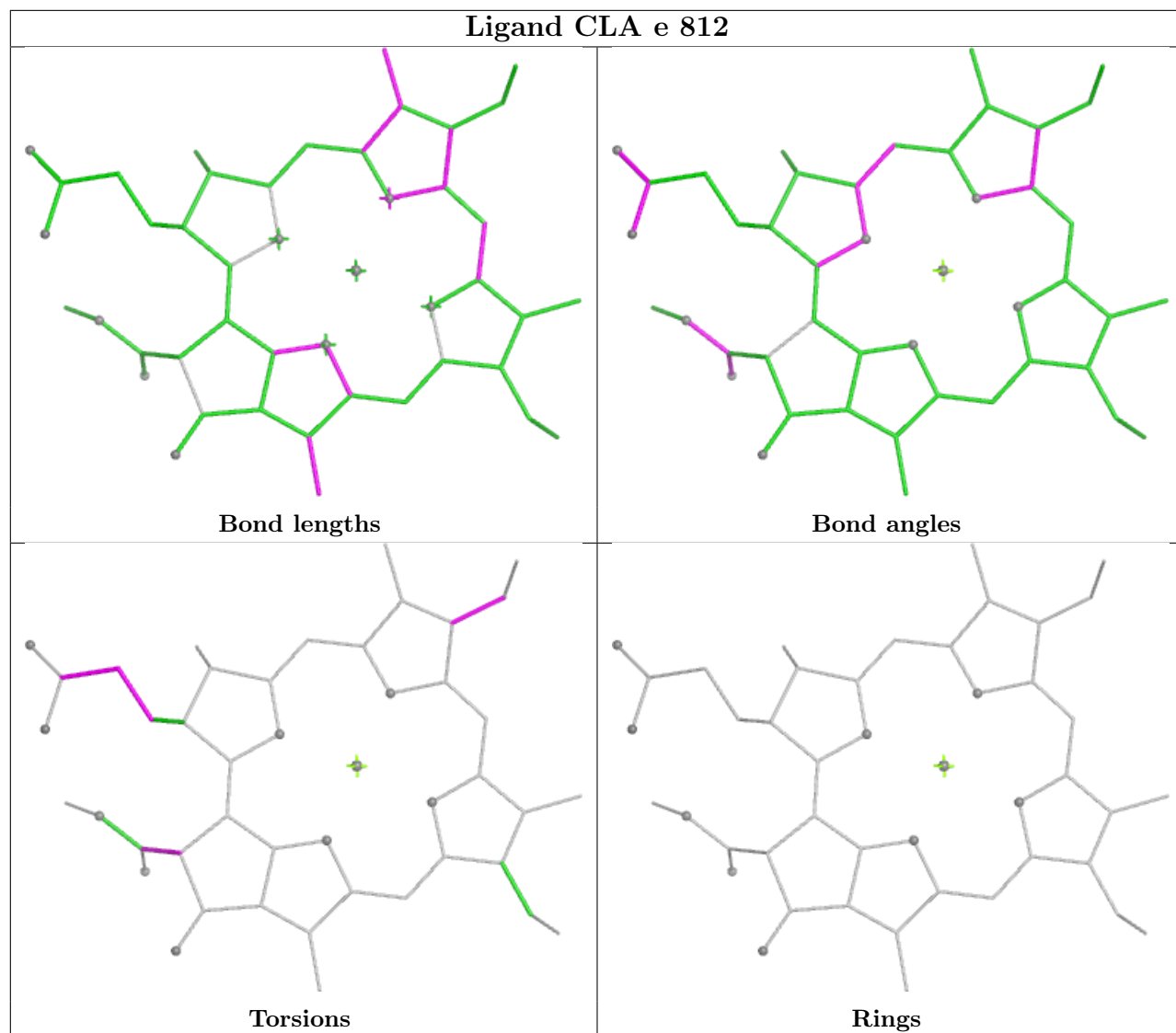
Ligand CLA a 836



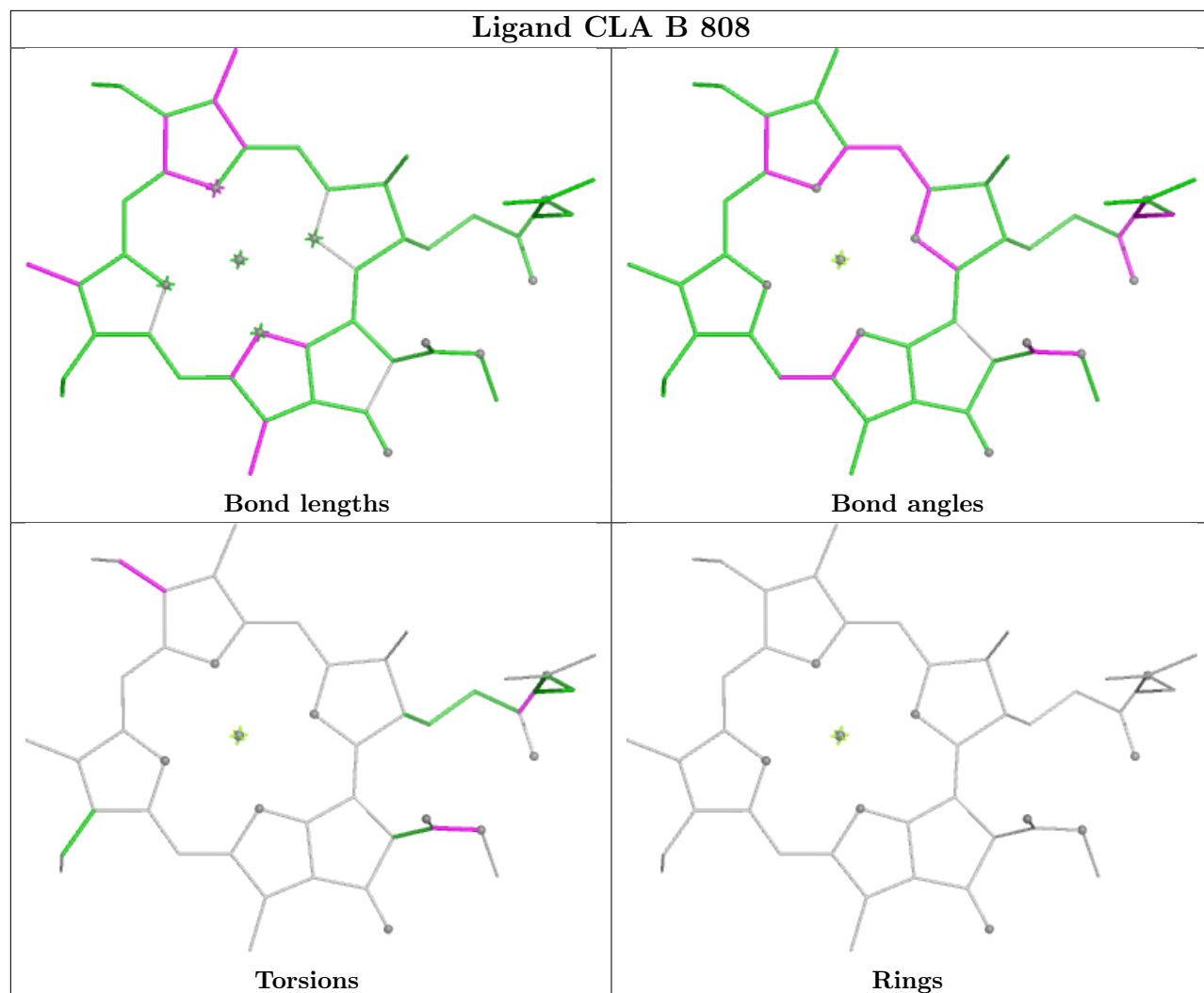
Ligand CLA E 819



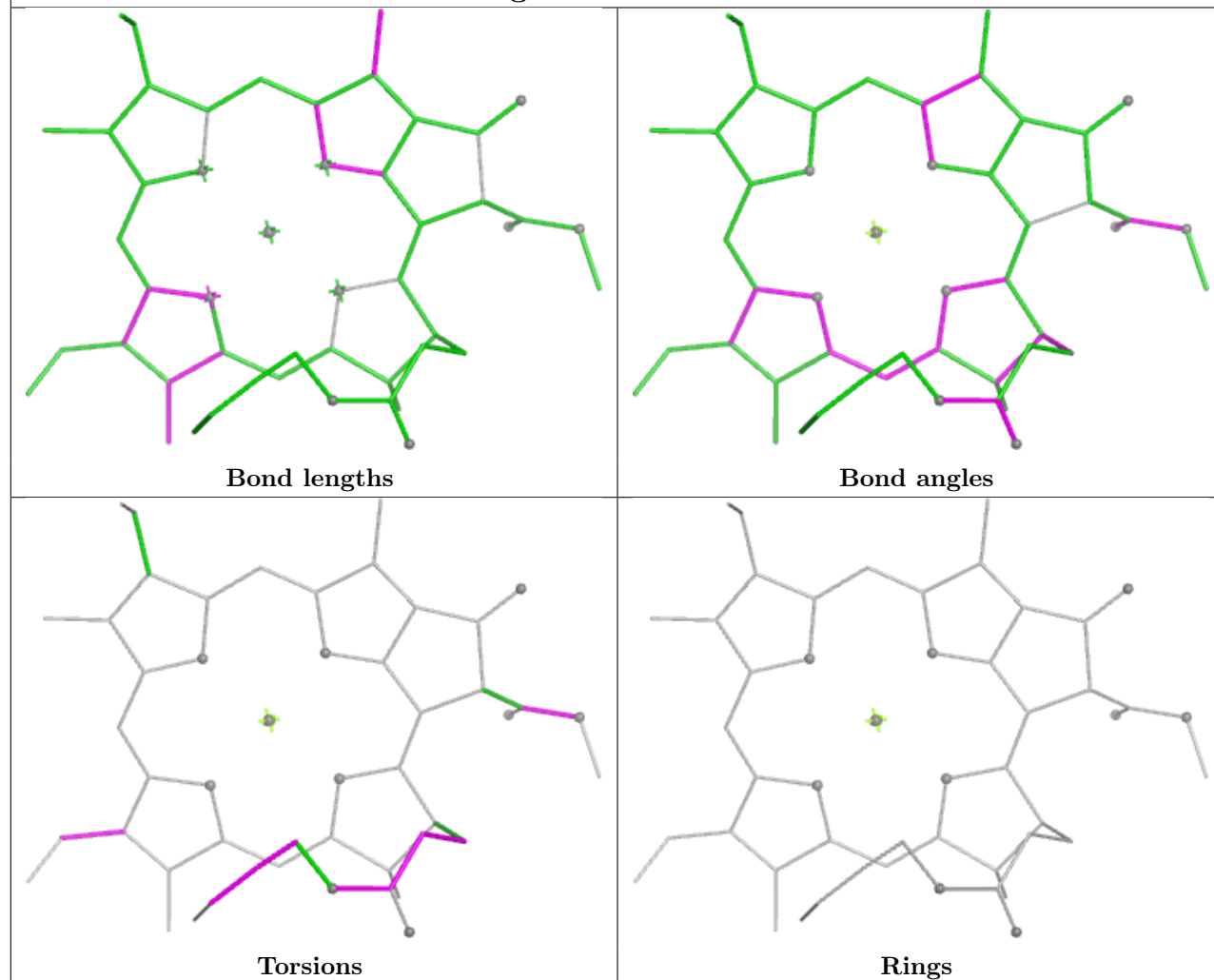
Ligand CLA e 812



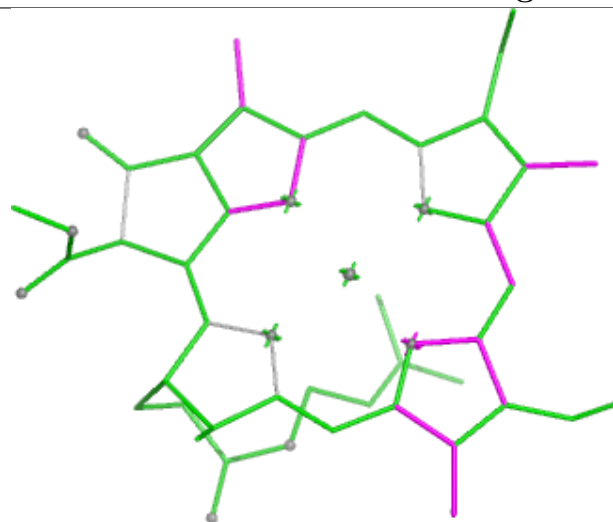
Ligand CLA B 808



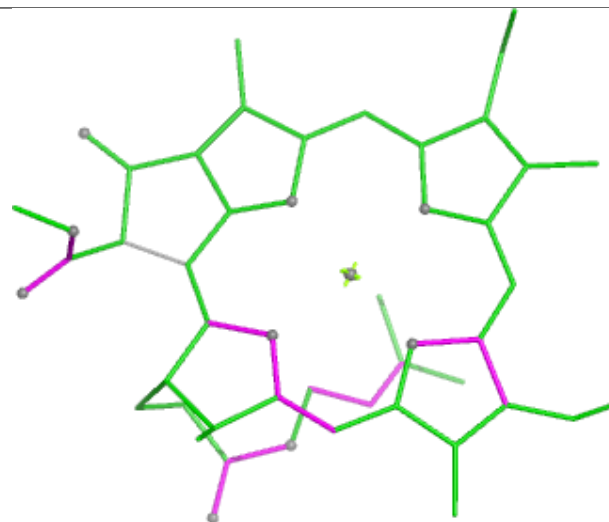
Ligand CLA a 825



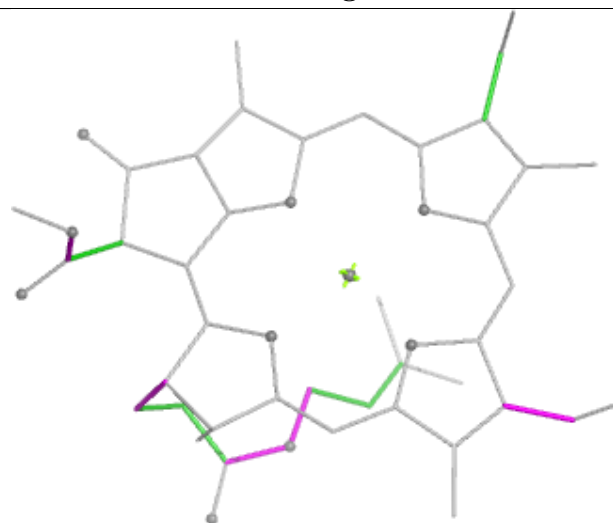
Ligand CLA B 828



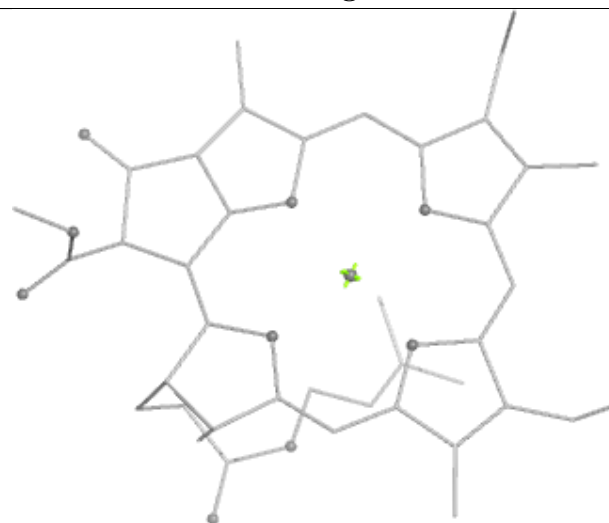
Bond lengths



Bond angles

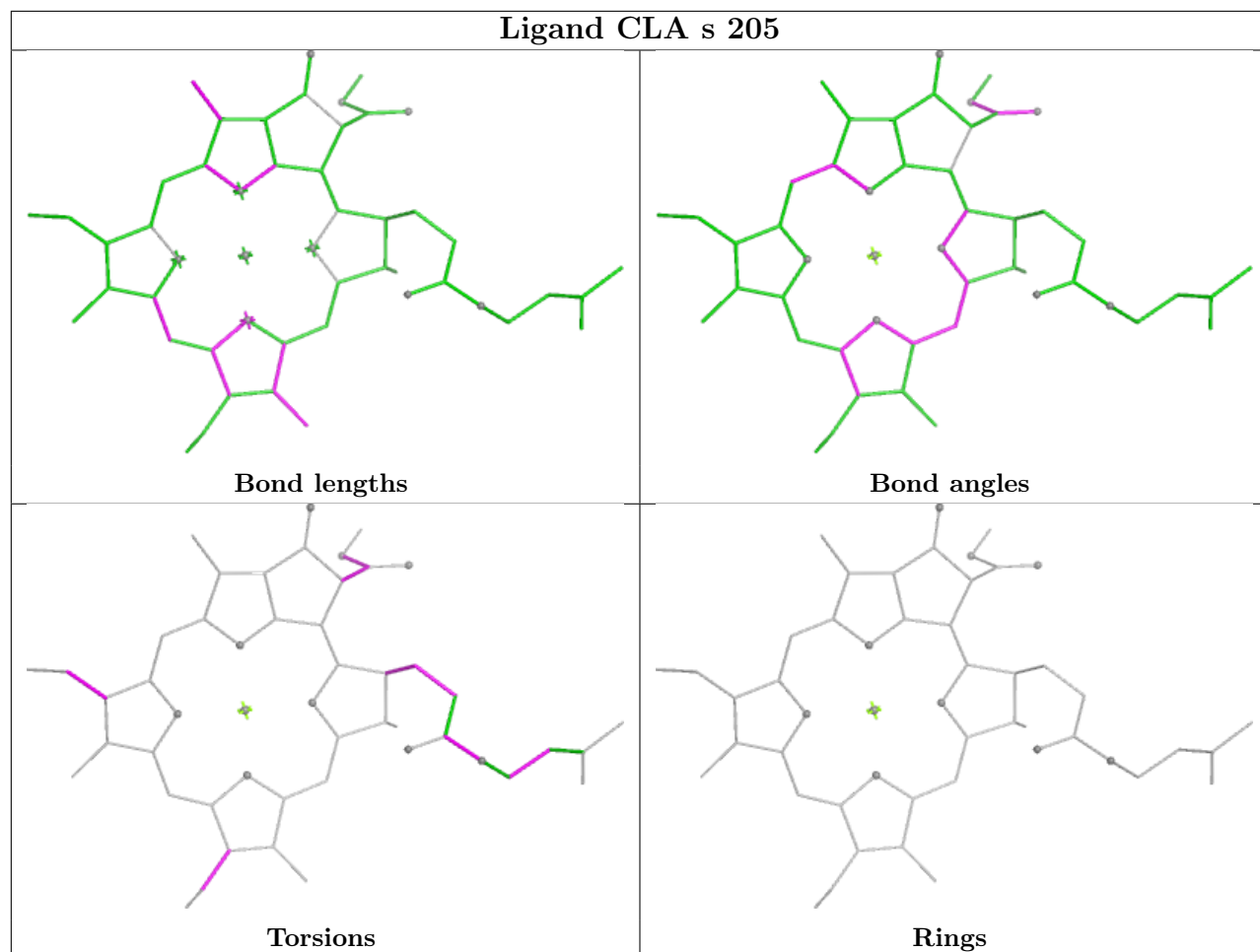


Torsions

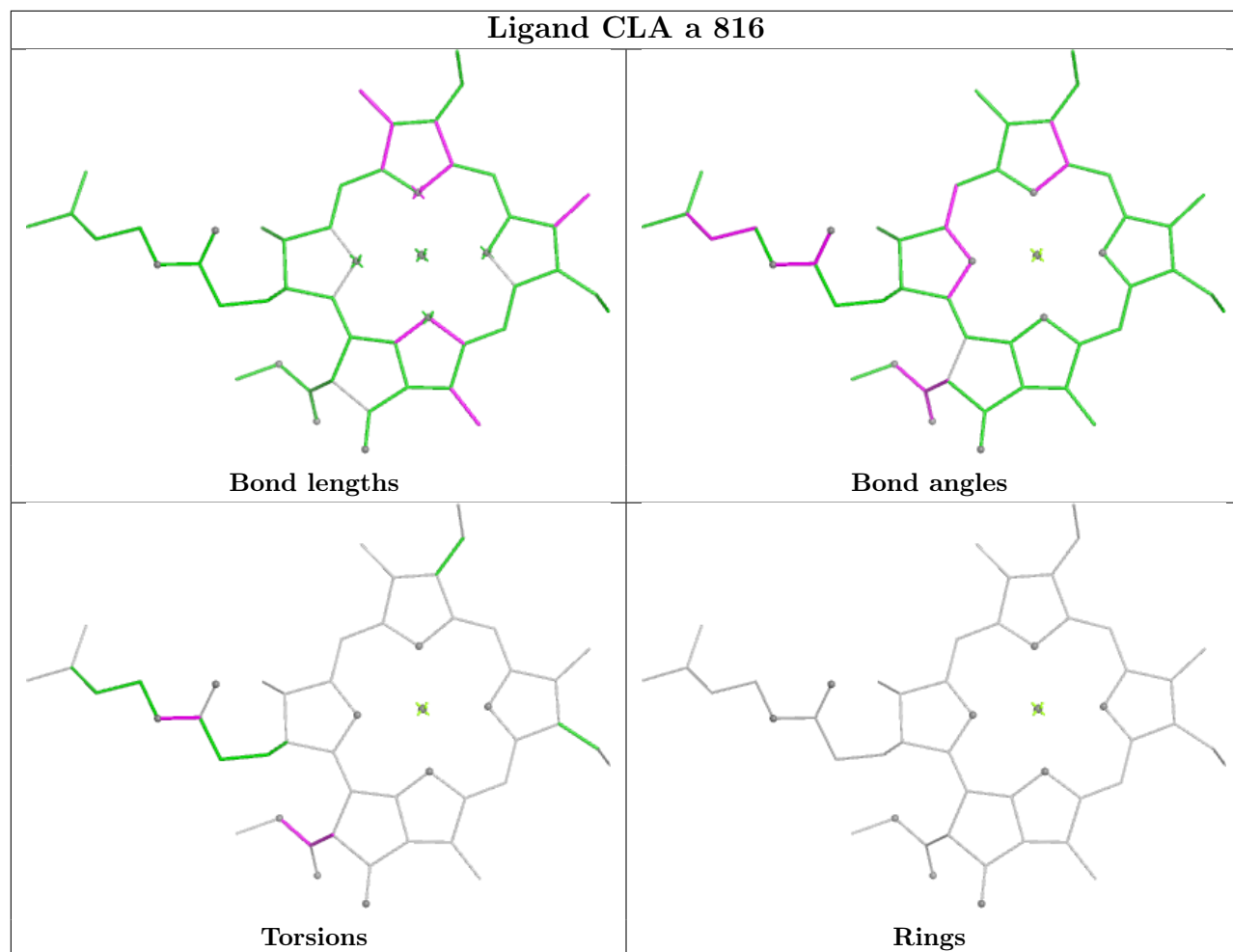


Rings

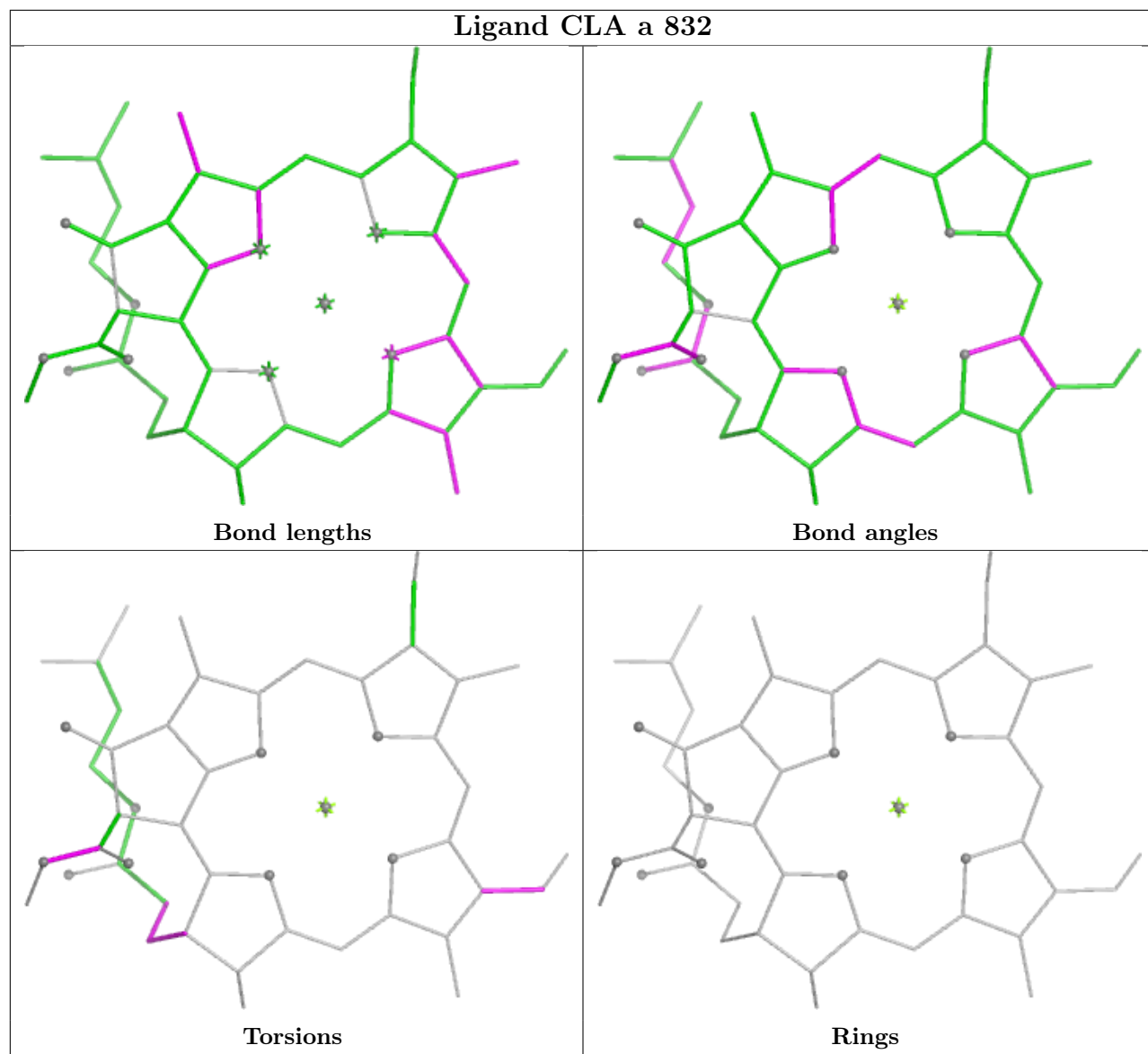
Ligand CLA s 205



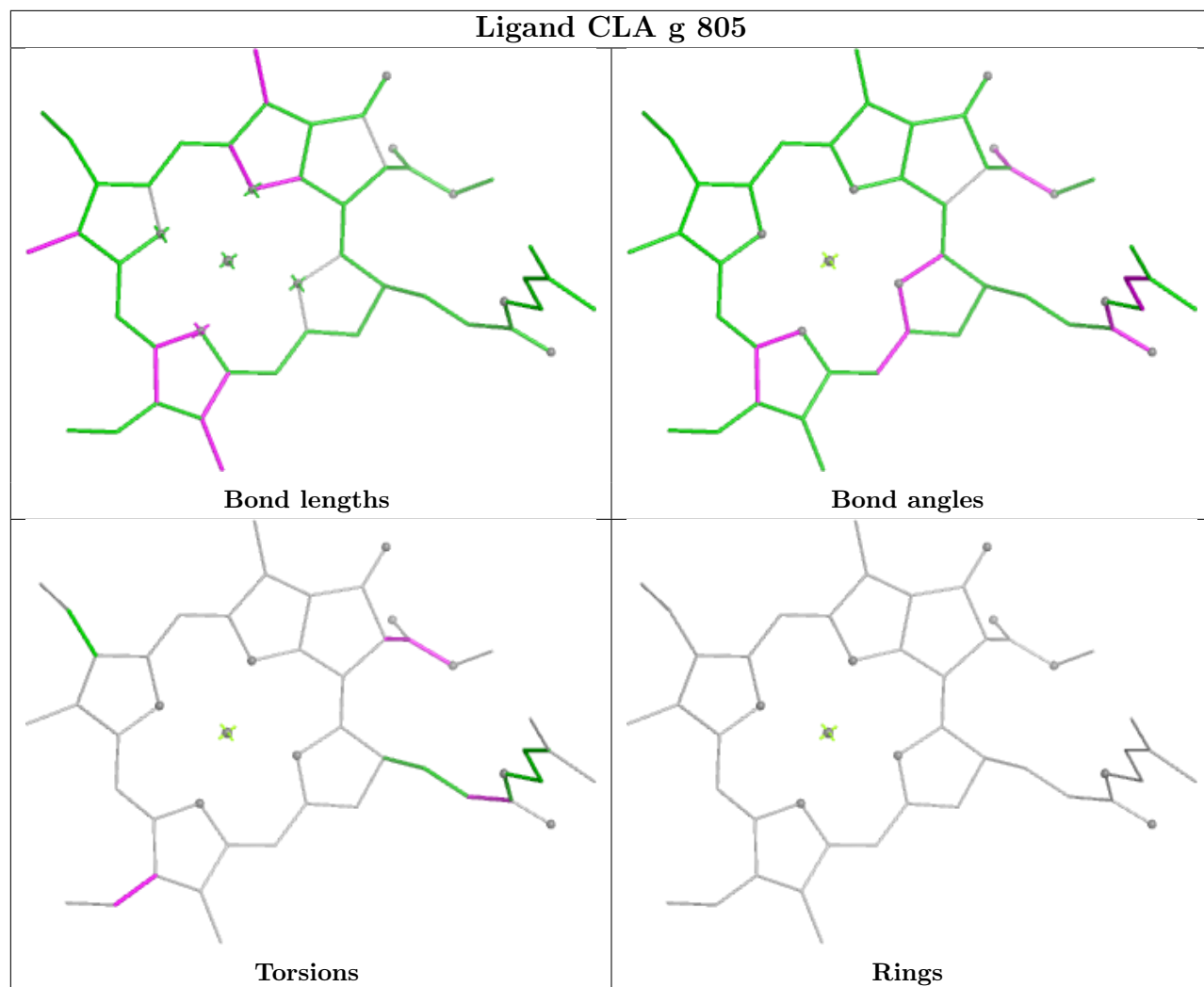
Ligand CLA a 816



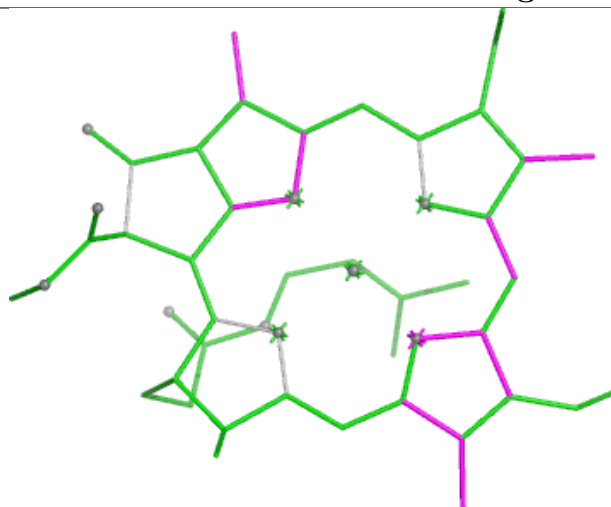
Ligand CLA a 832



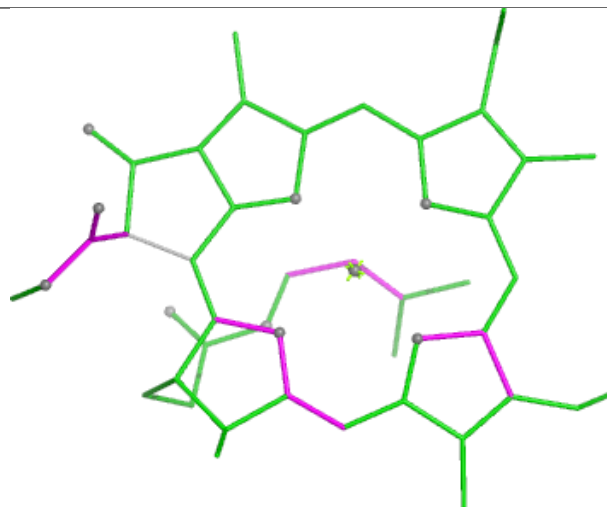
Ligand CLA g 805



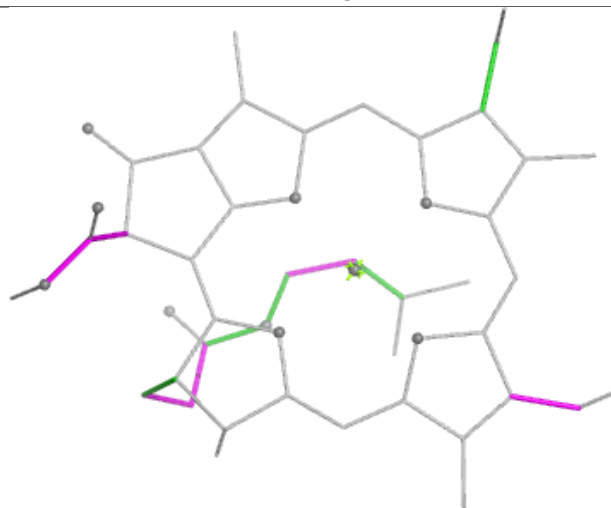
Ligand CLA b 822



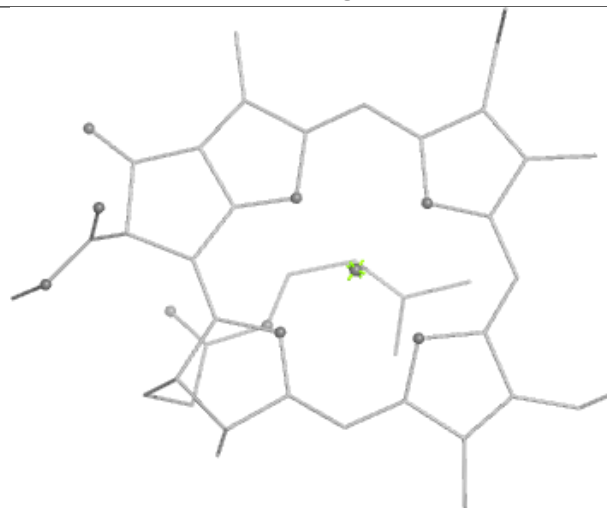
Bond lengths



Bond angles

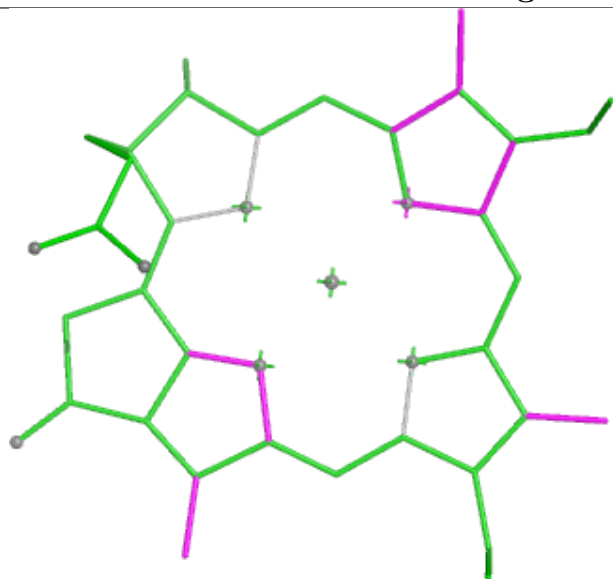


Torsions

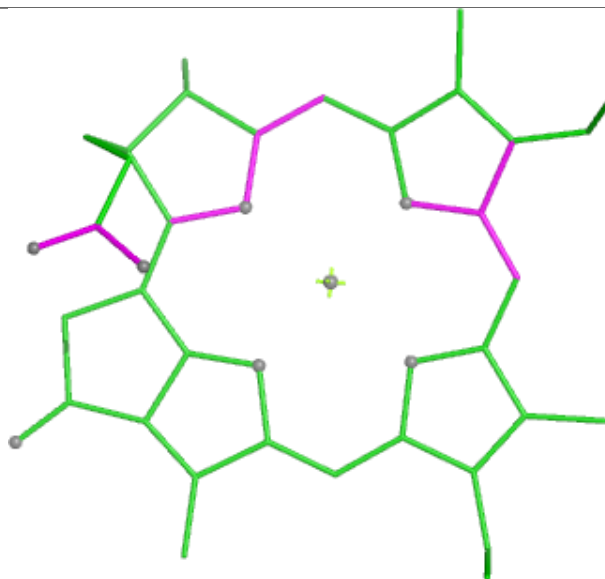


Rings

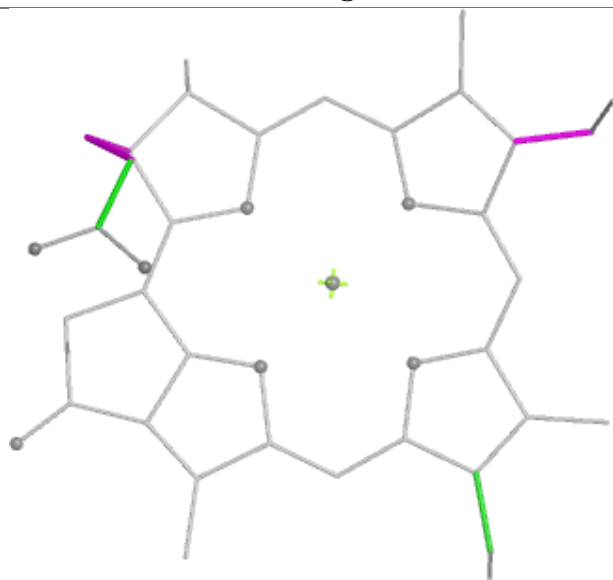
Ligand CLA b 801



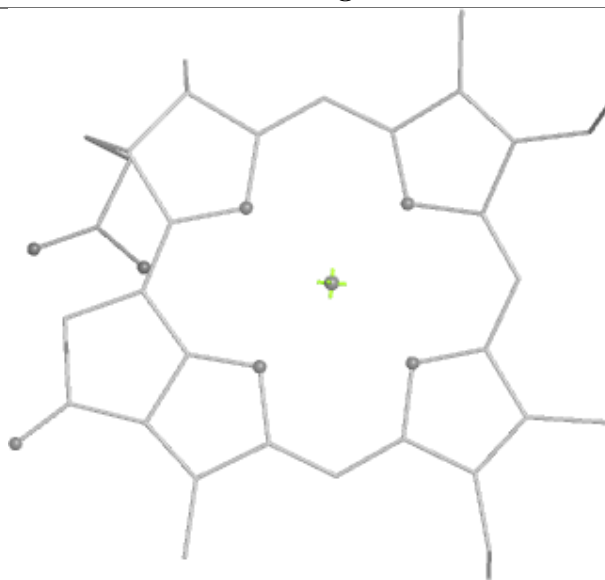
Bond lengths



Bond angles

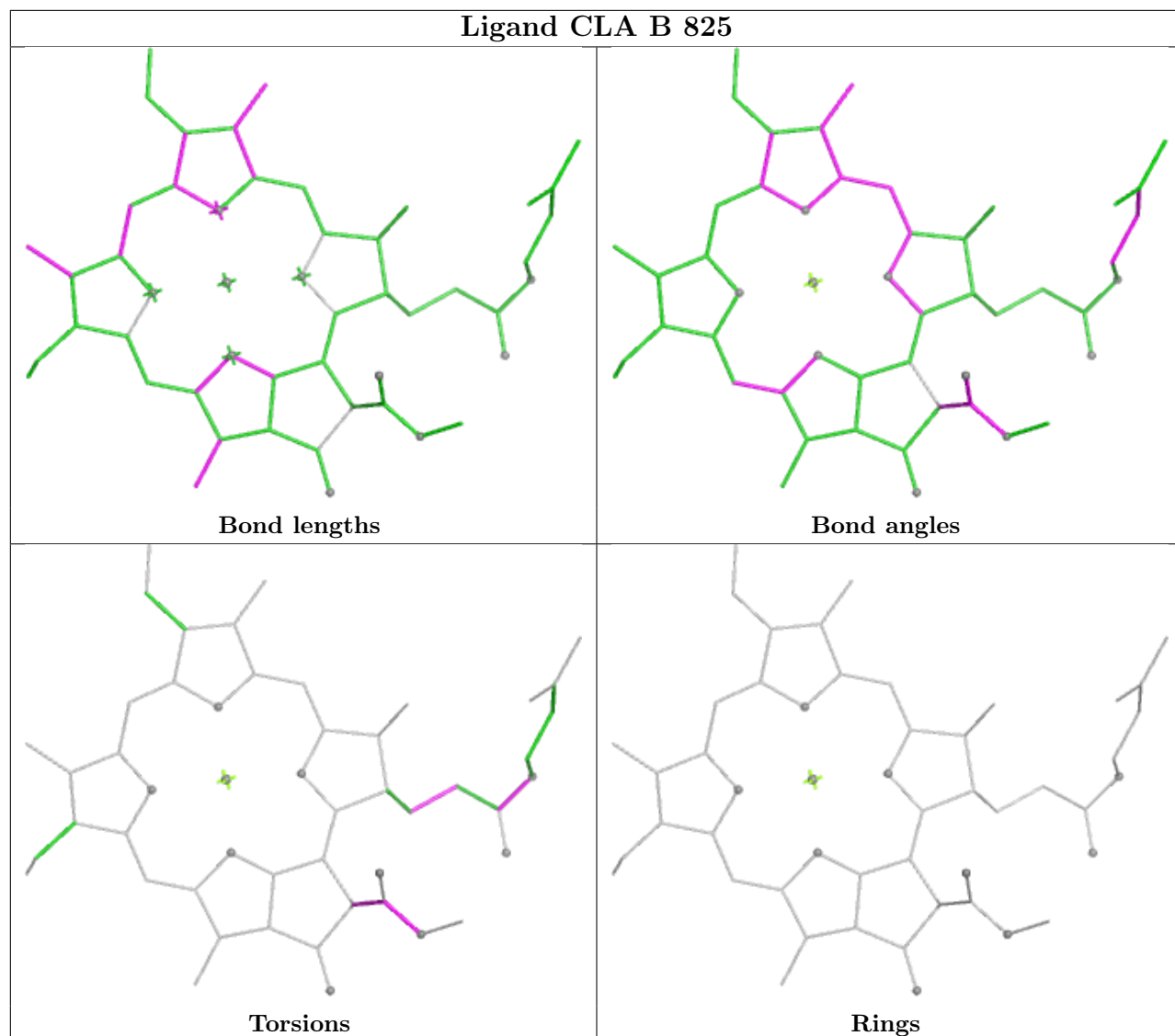


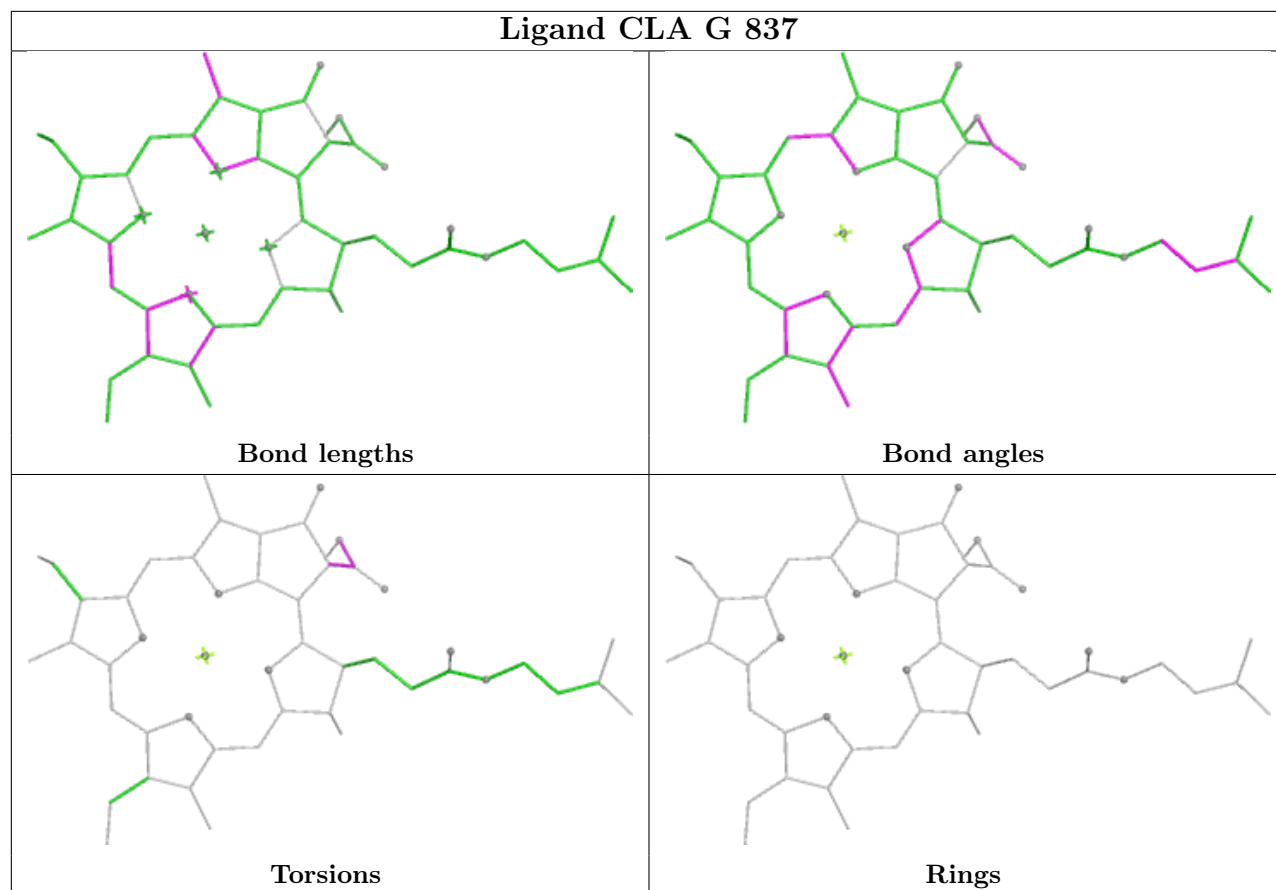
Torsions



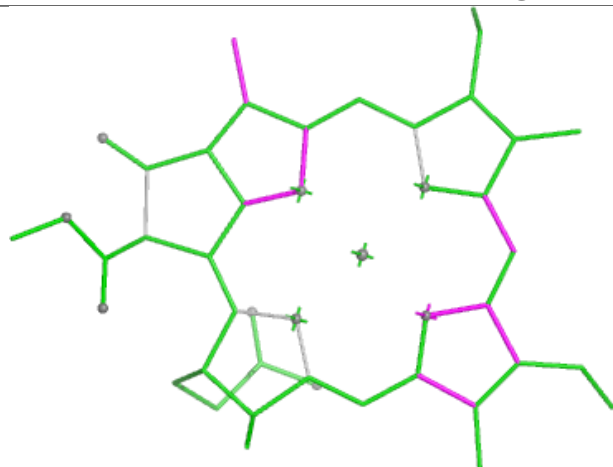
Rings

Ligand CLA B 825

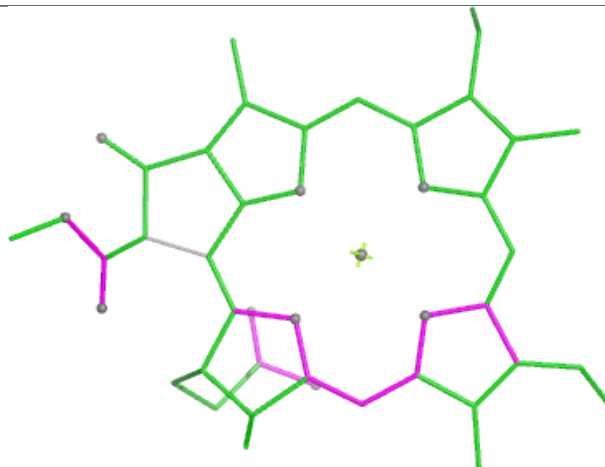




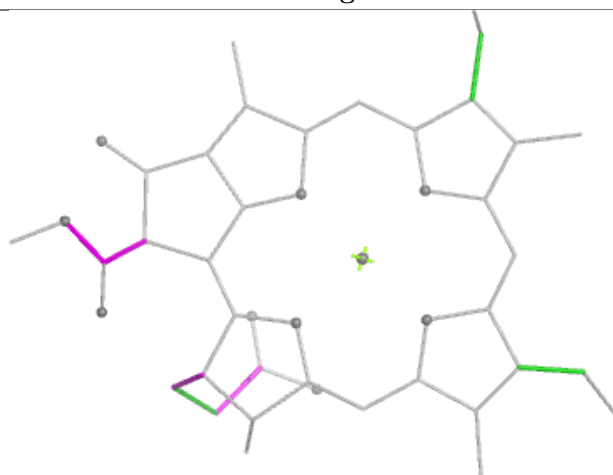
Ligand CLA G 836



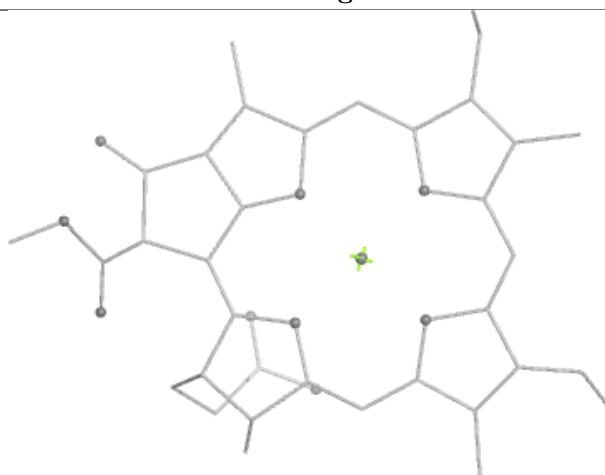
Bond lengths



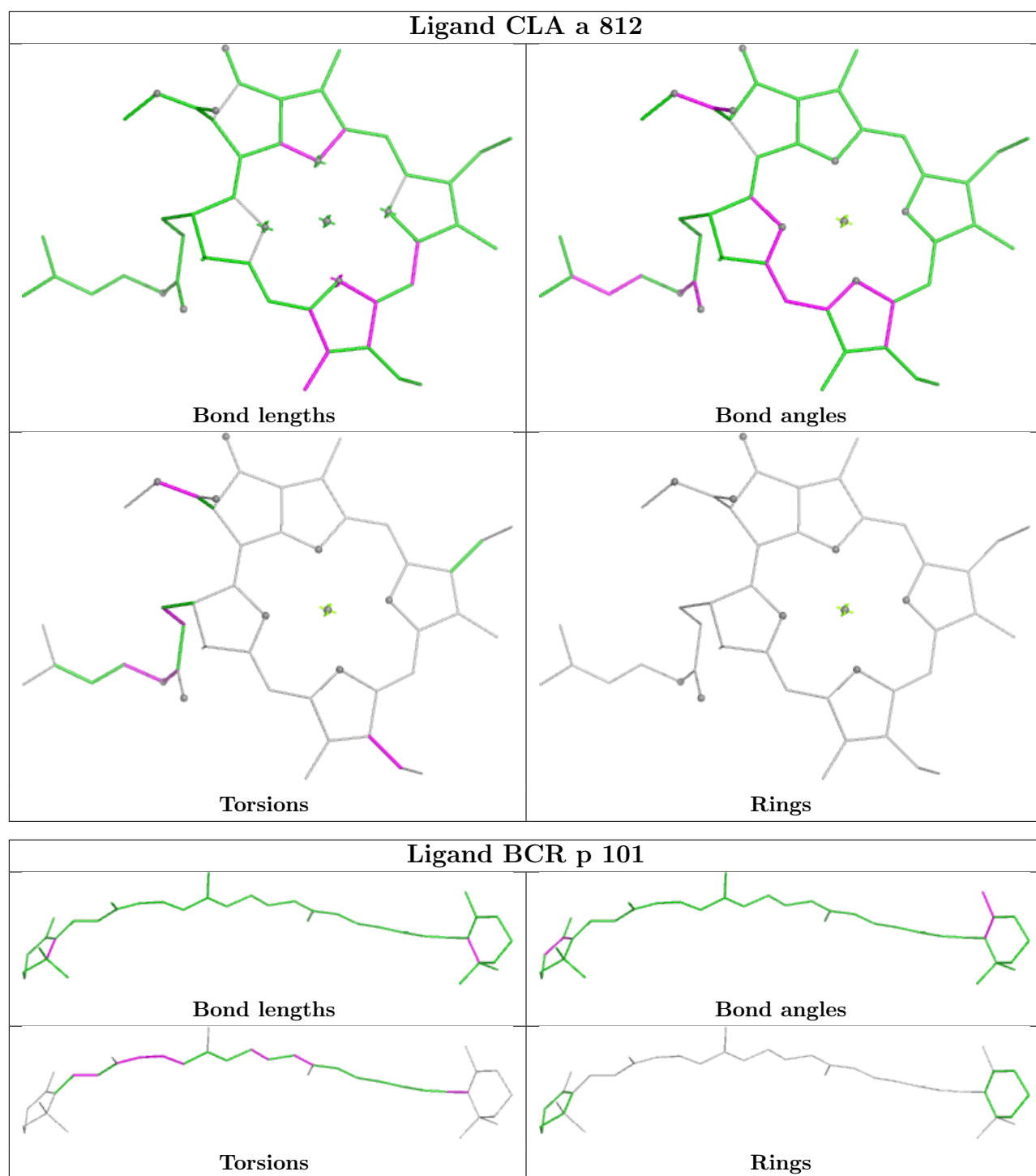
Bond angles



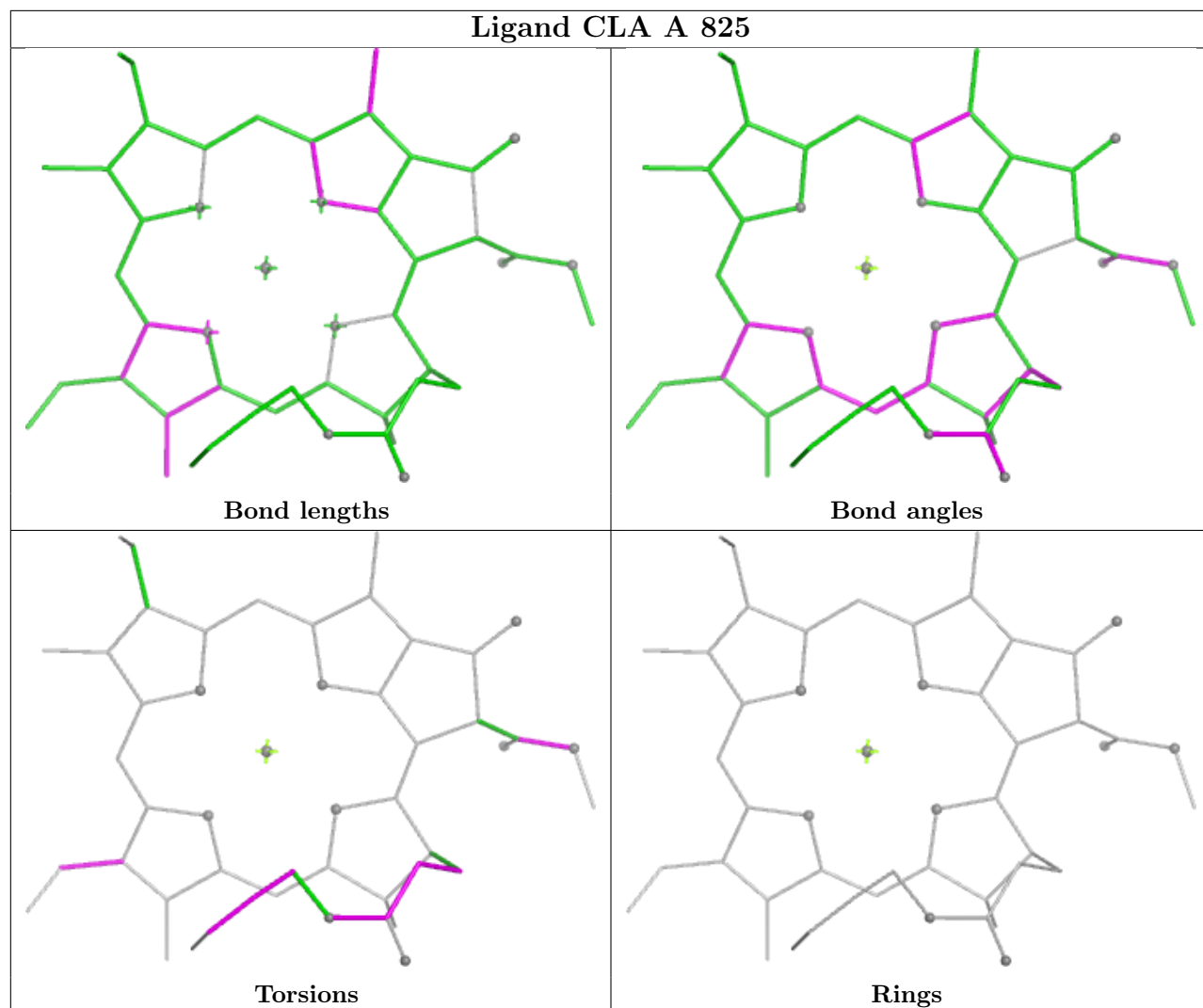
Torsions

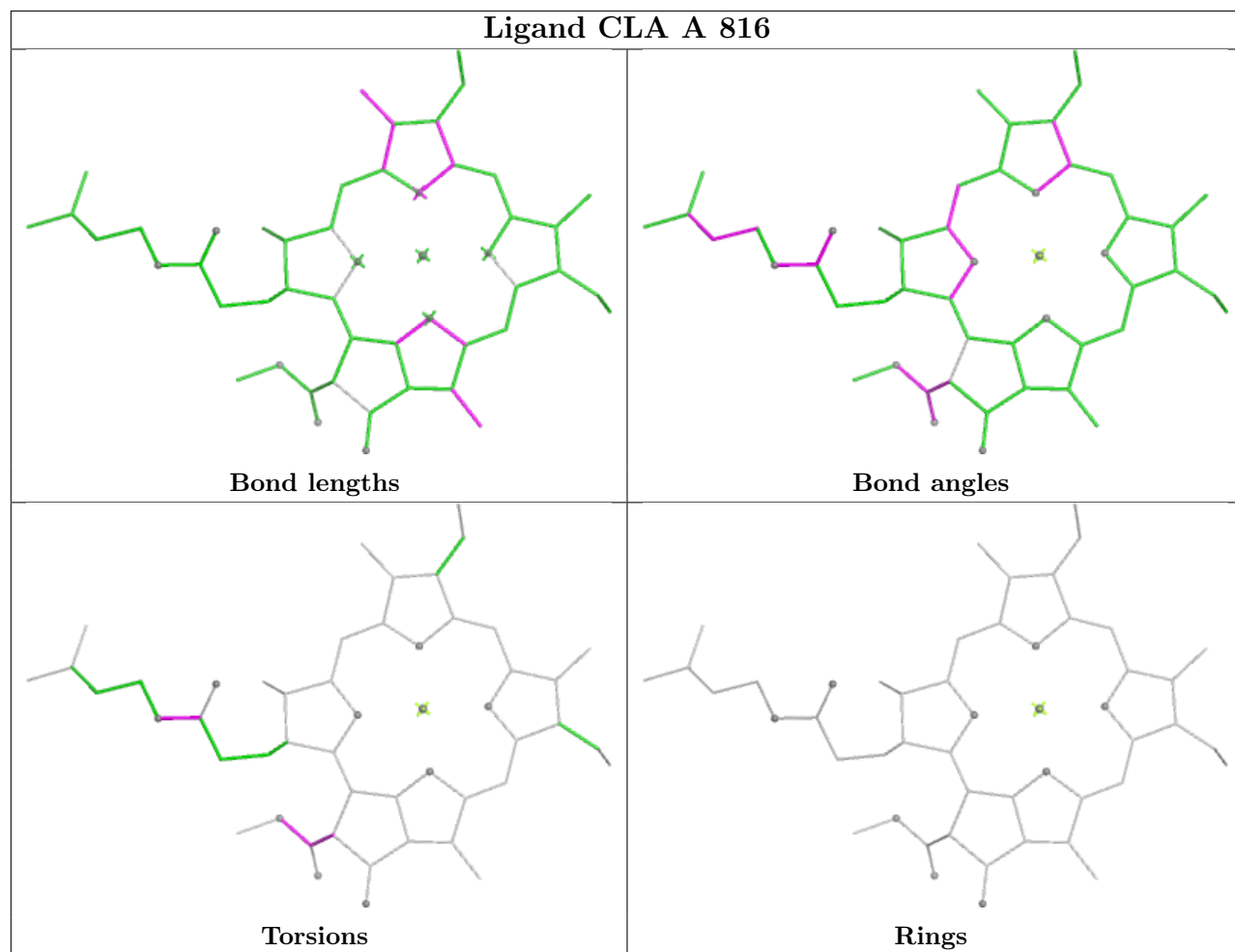


Rings

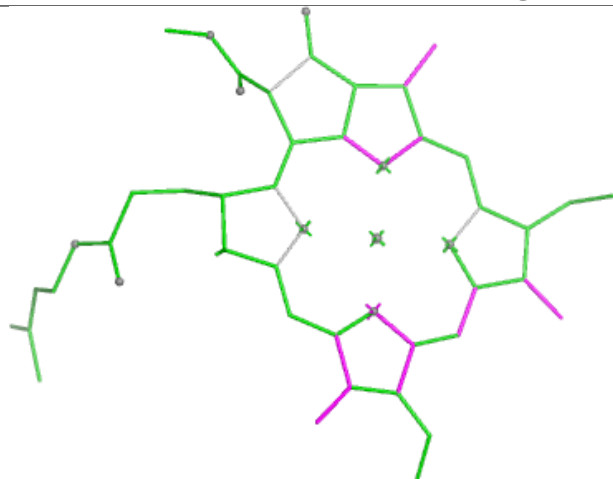


Ligand CLA A 825

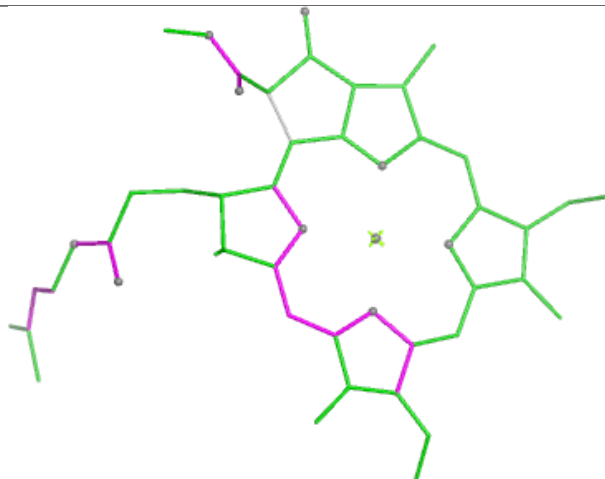




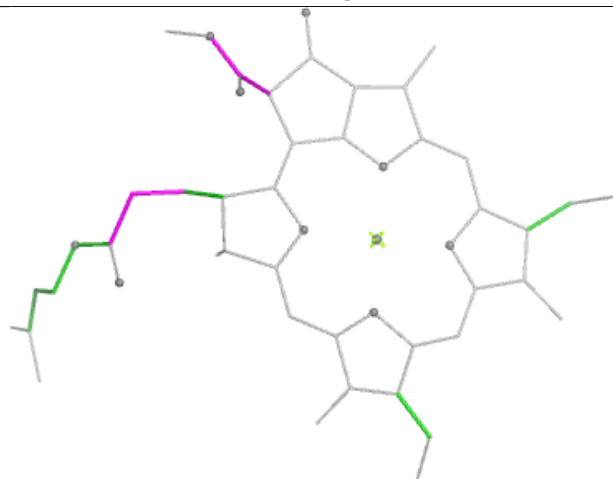
Ligand CLA B 811



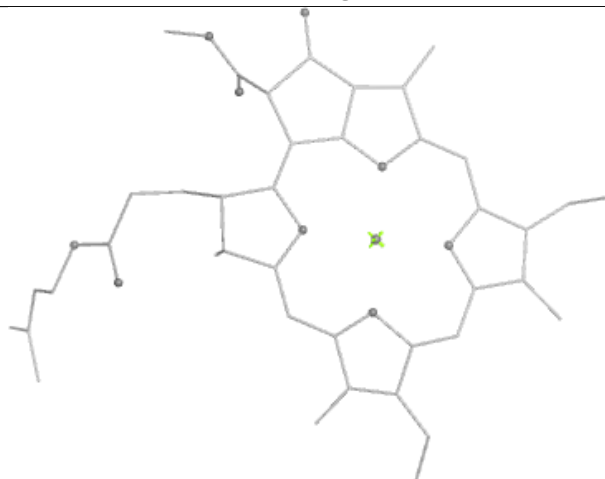
Bond lengths



Bond angles

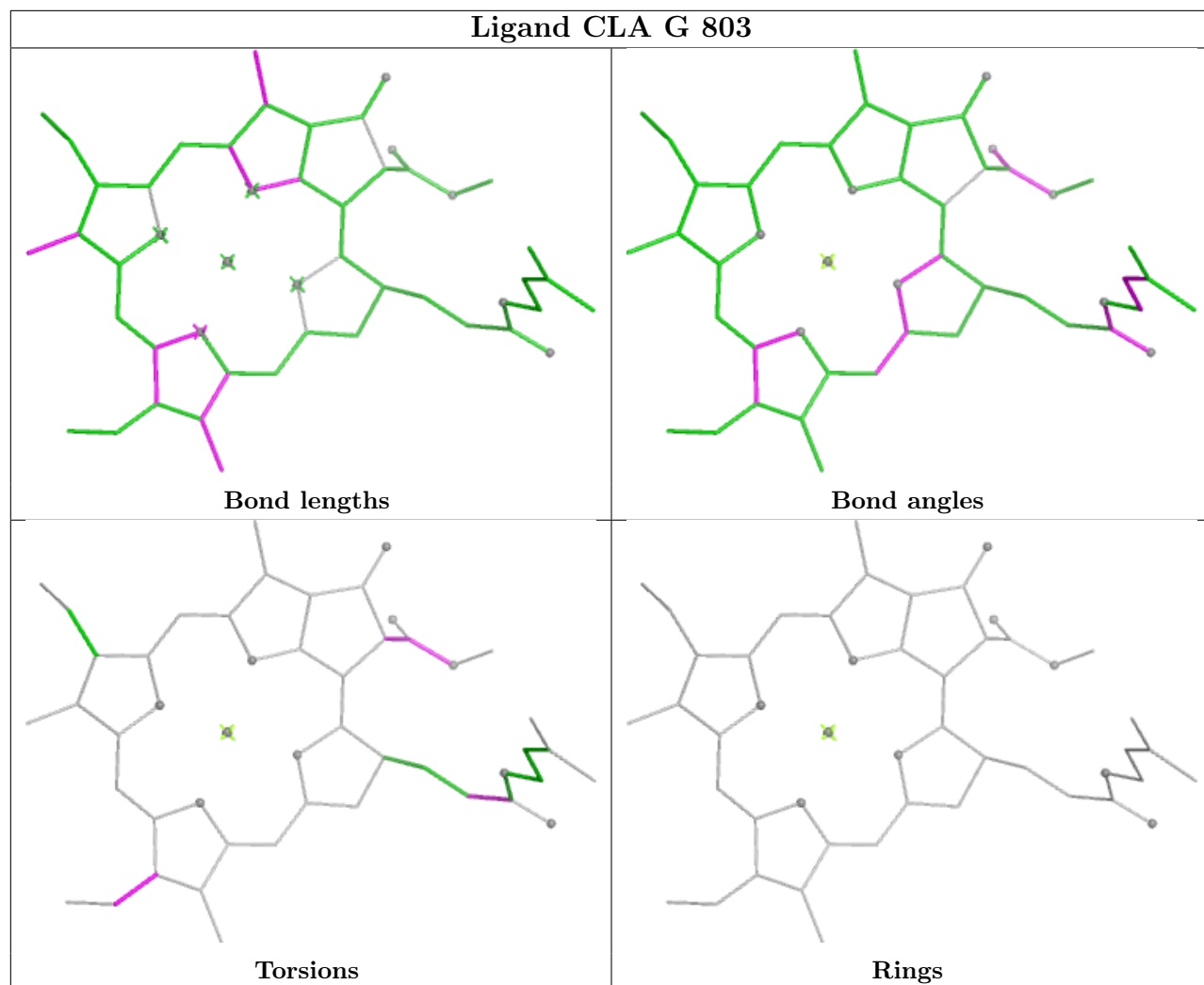


Torsions

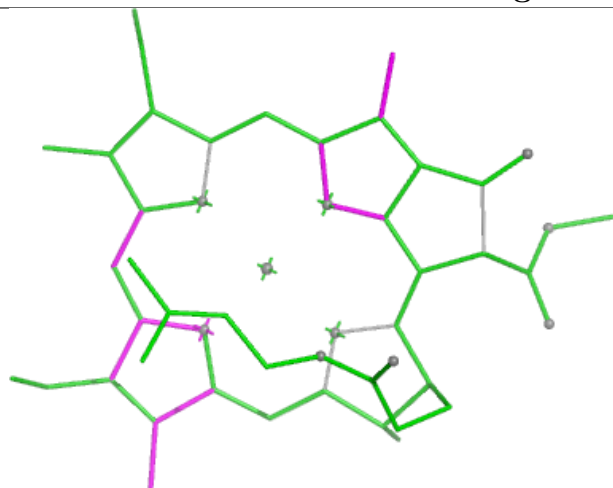


Rings

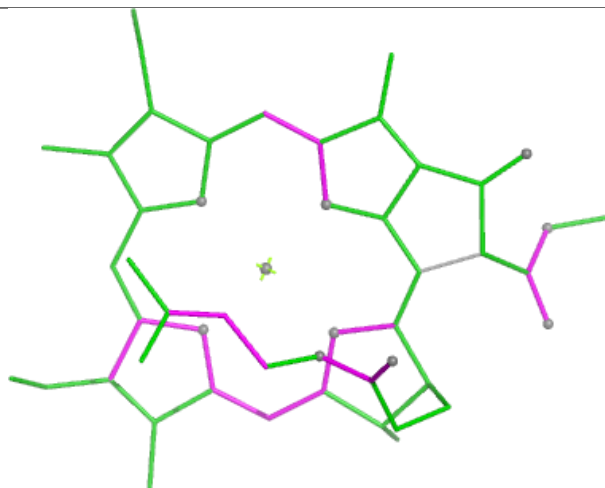
Ligand CLA G 803



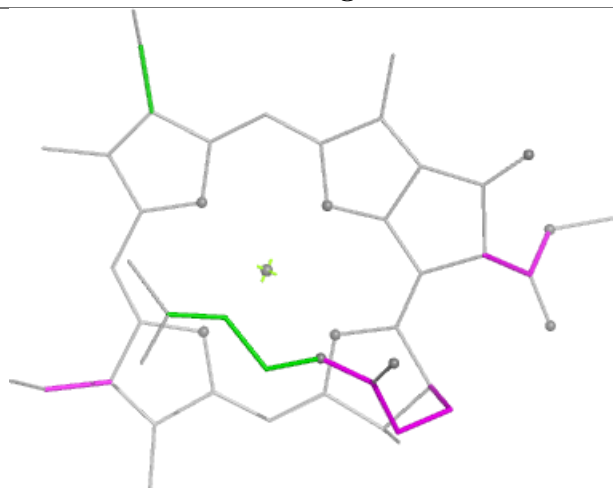
Ligand CLA A 826



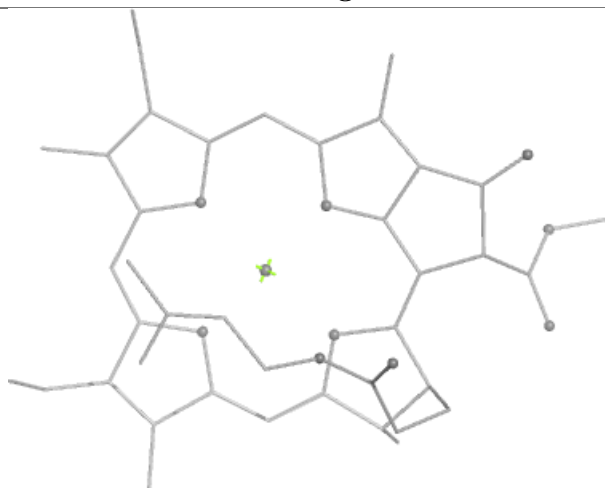
Bond lengths



Bond angles

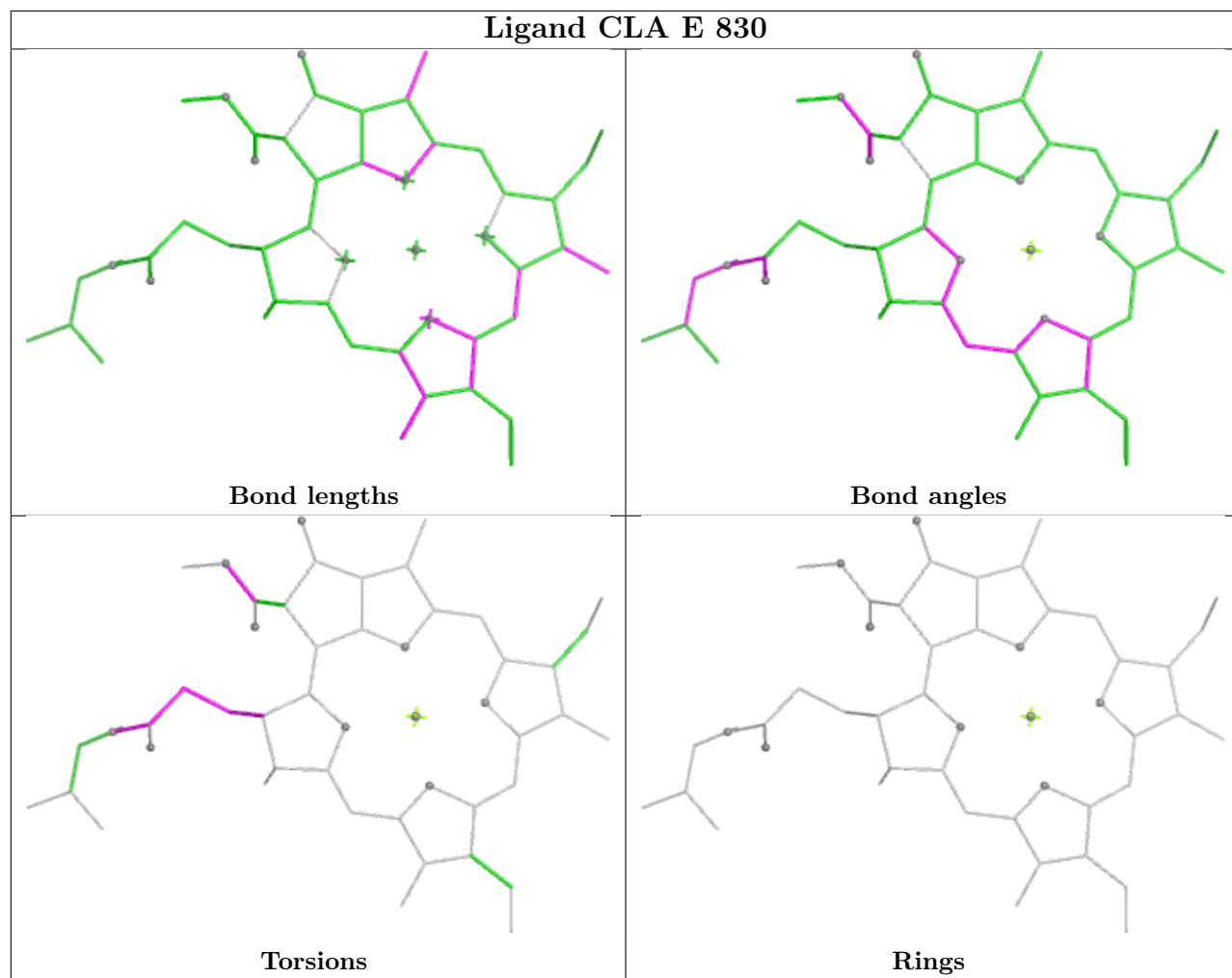


Torsions

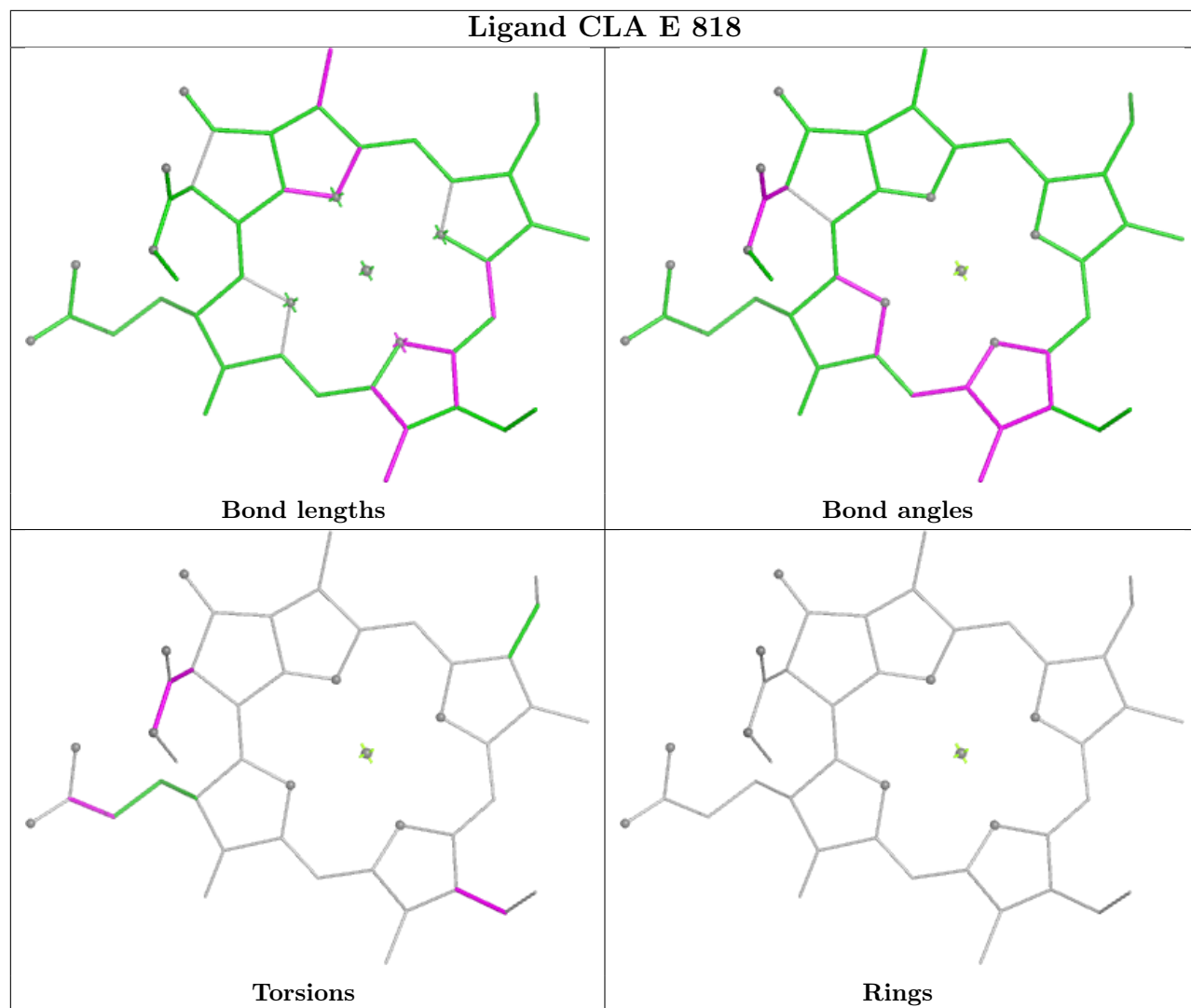


Rings

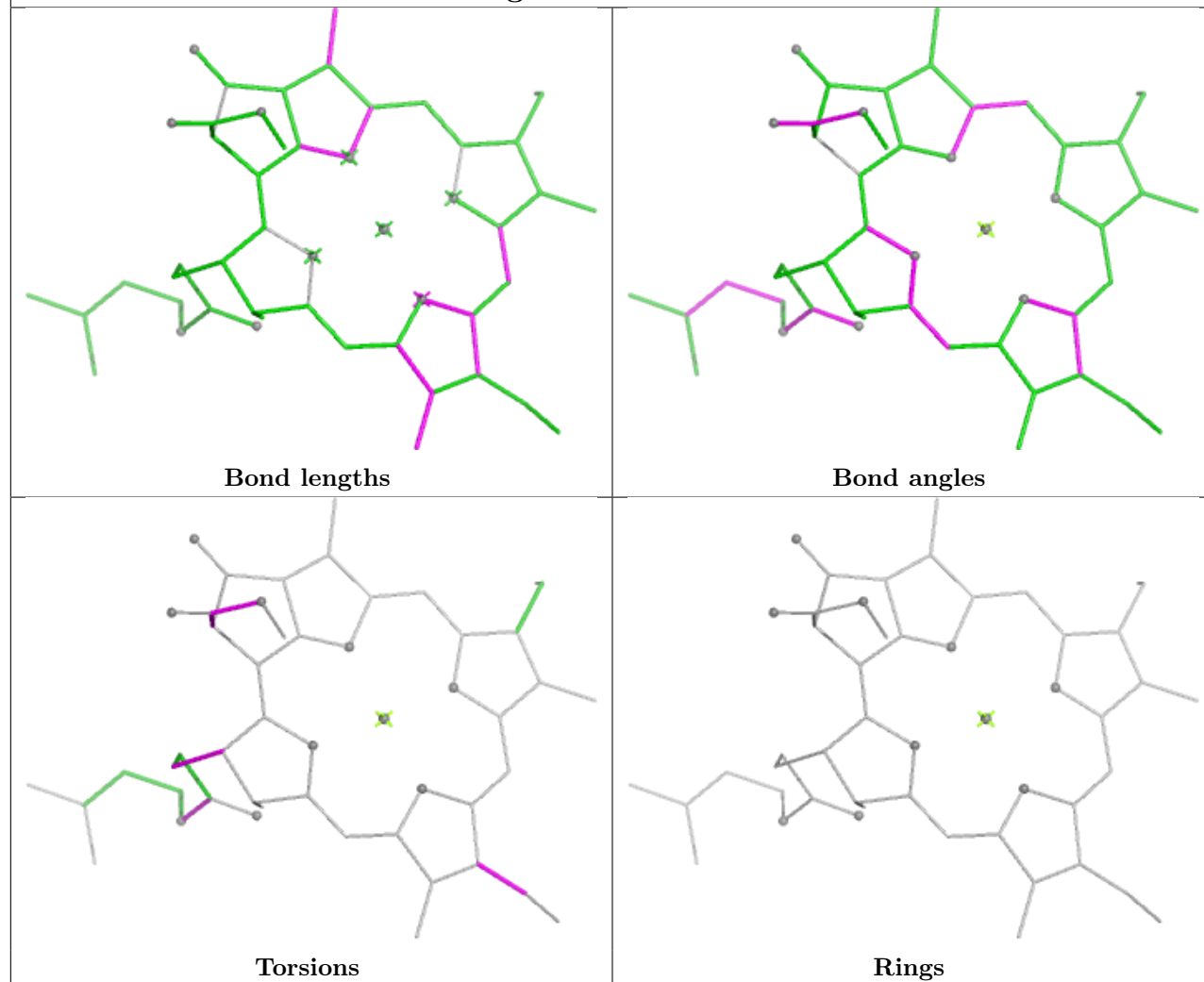
Ligand CLA E 830



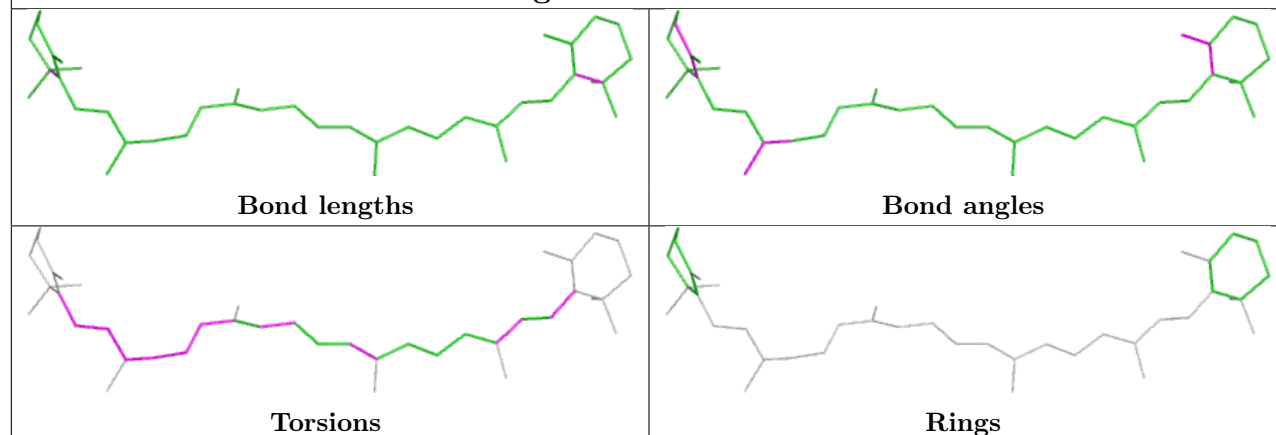
Ligand CLA E 818



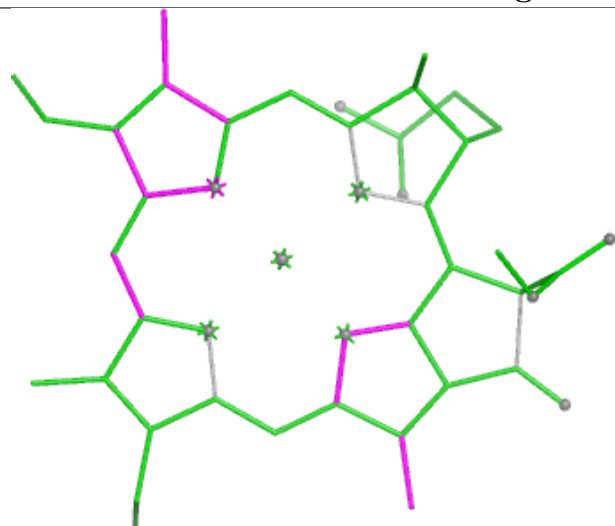
Ligand CLA e 836



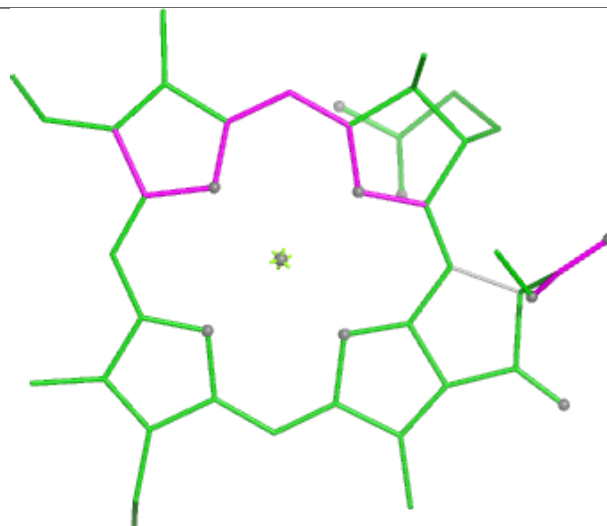
Ligand BCR S 201



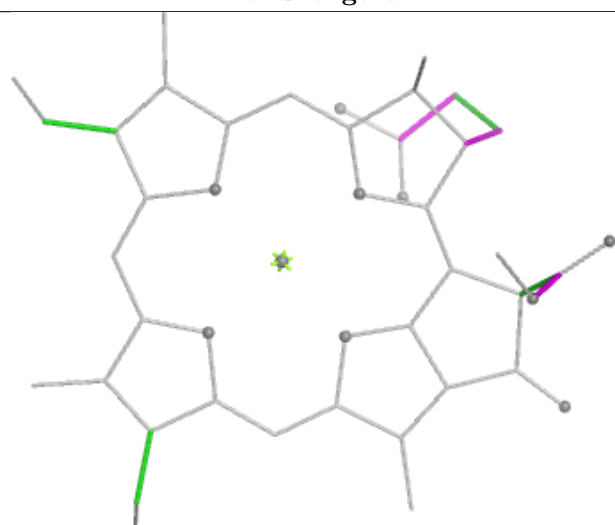
Ligand CLA G 816



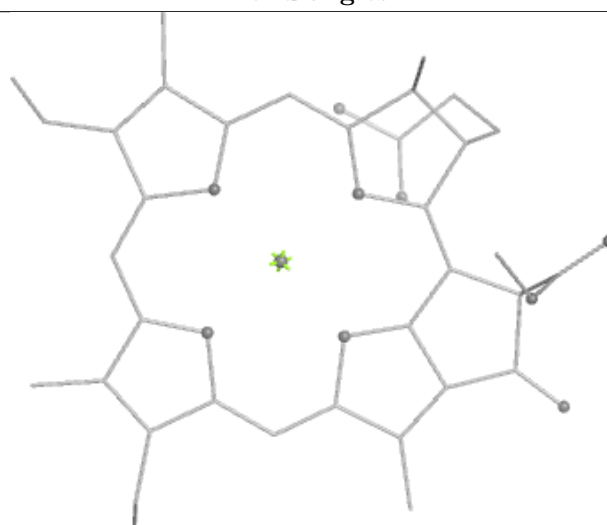
Bond lengths



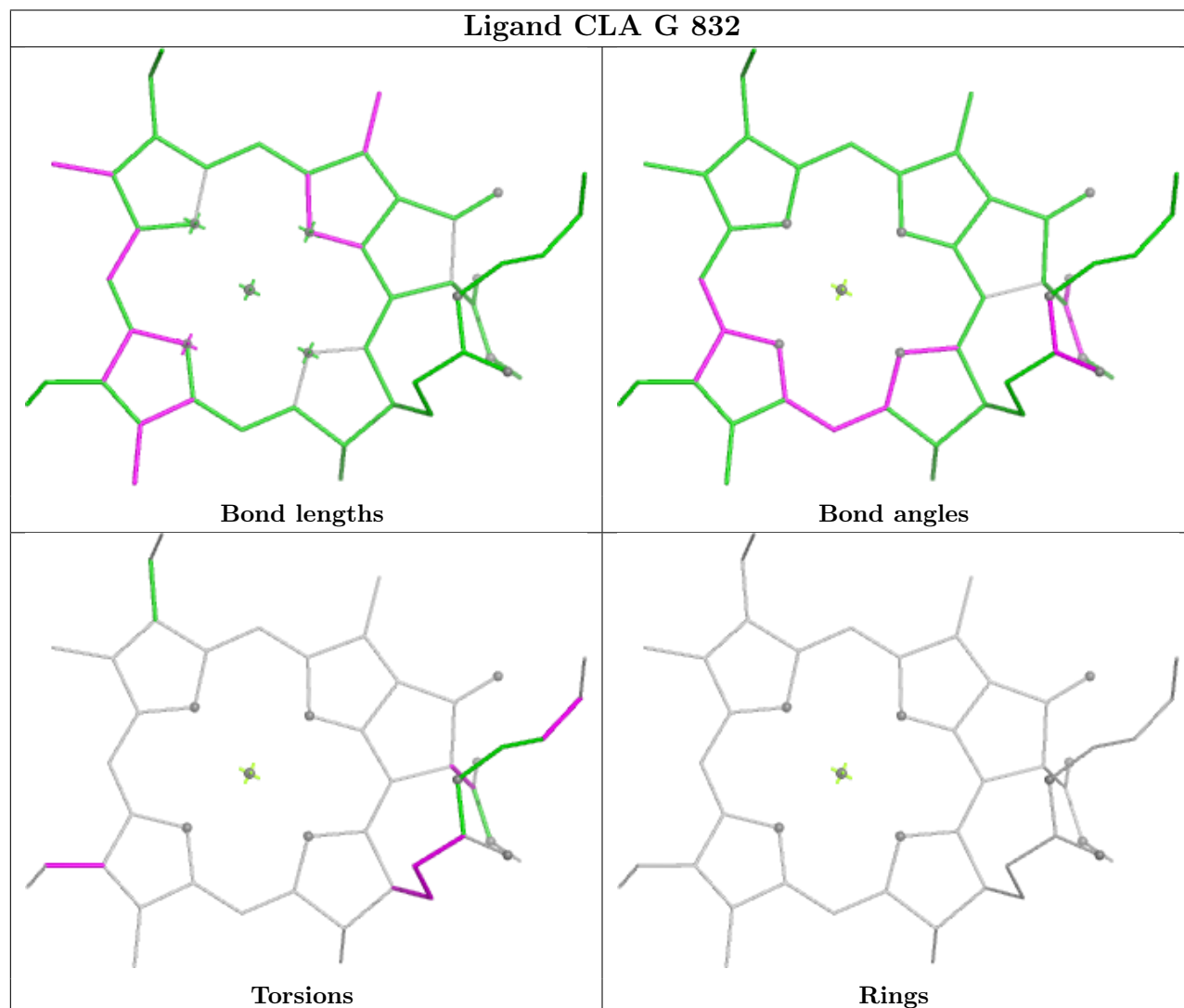
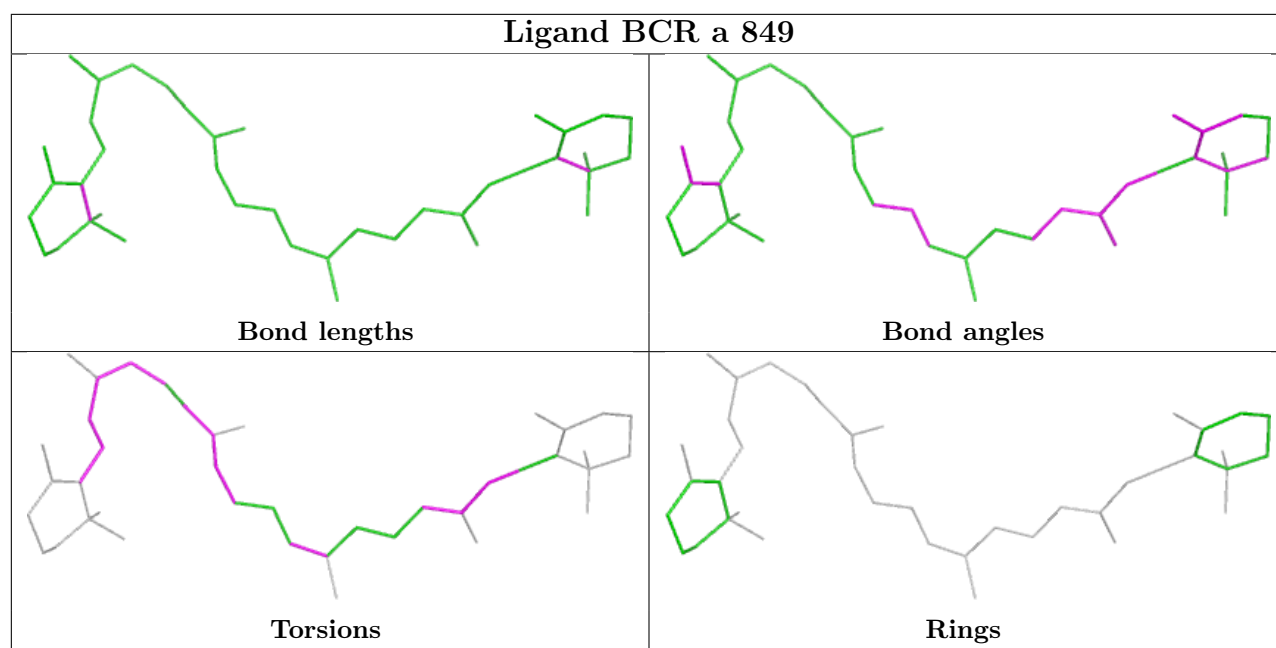
Bond angles



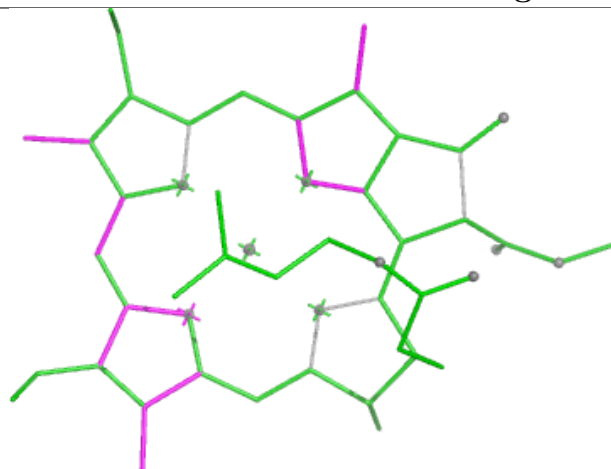
Torsions



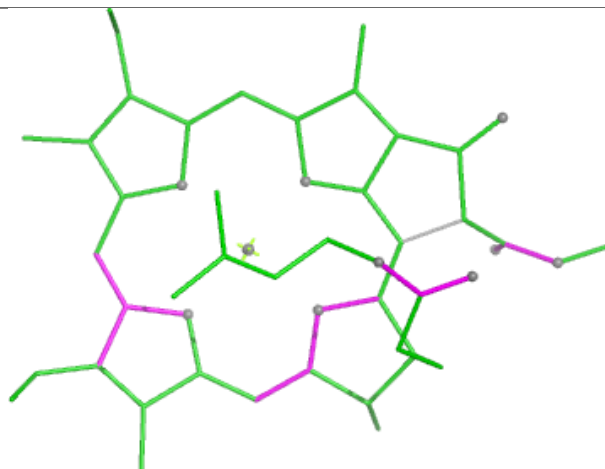
Rings



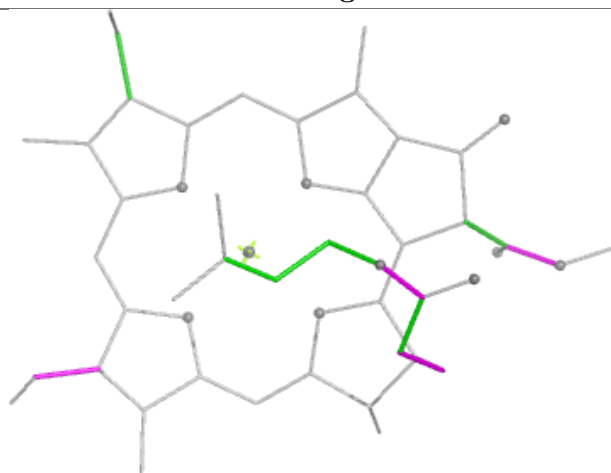
Ligand CLA B 802



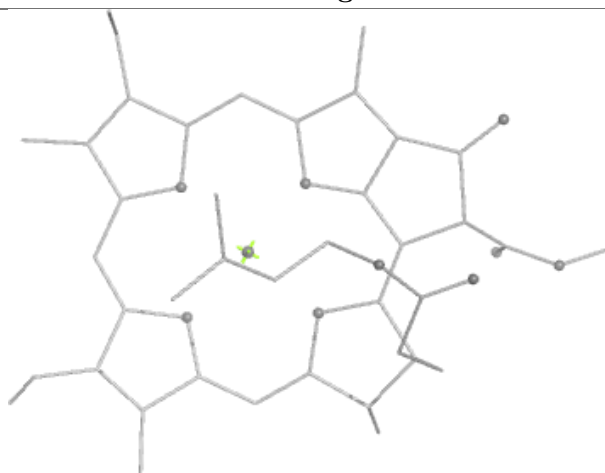
Bond lengths



Bond angles



Torsions

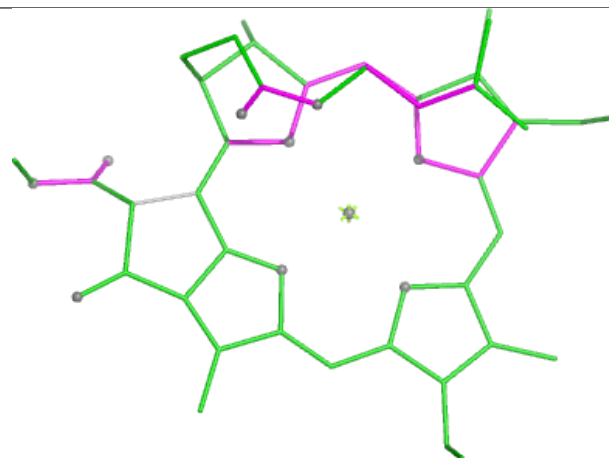


Rings

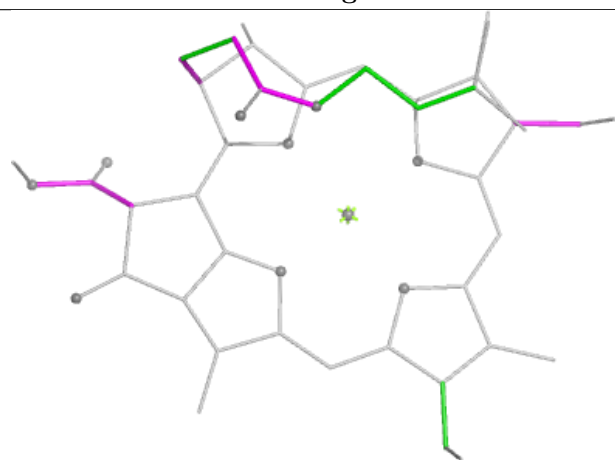
Ligand CLA E 824



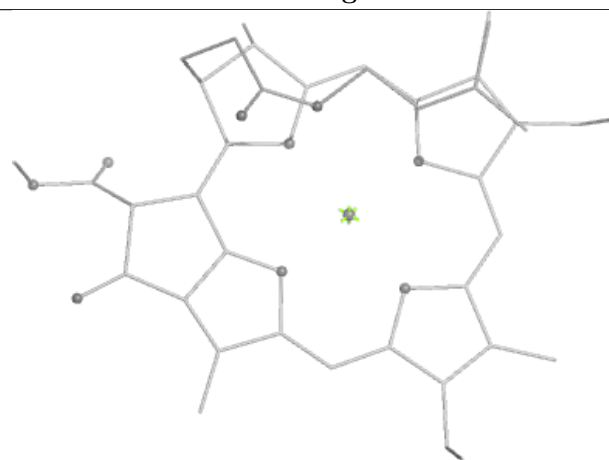
Bond lengths



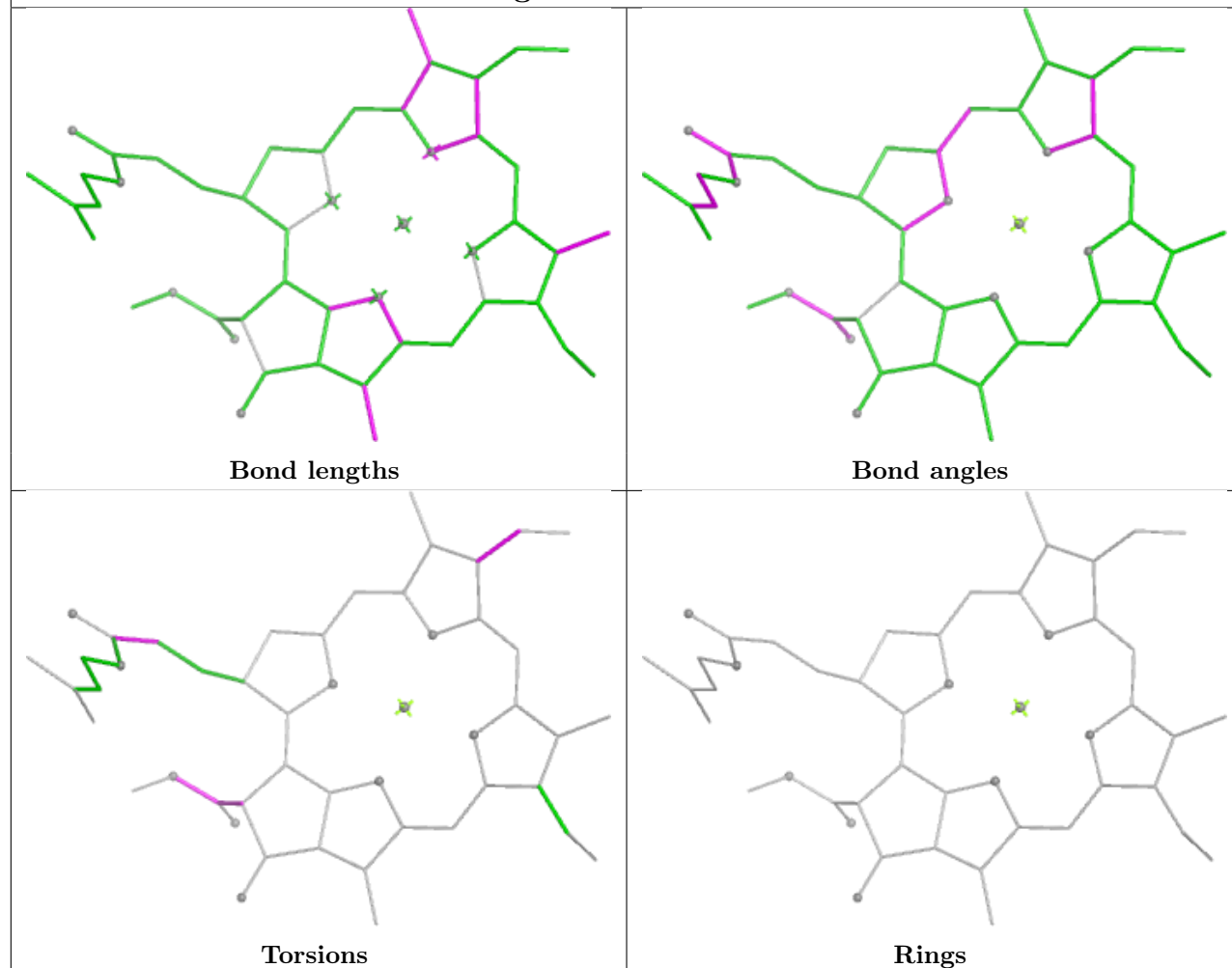
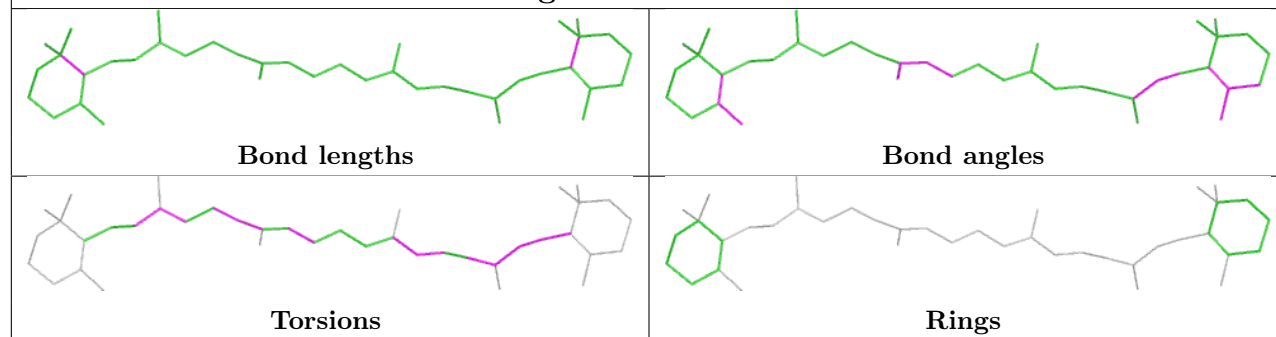
Bond angles



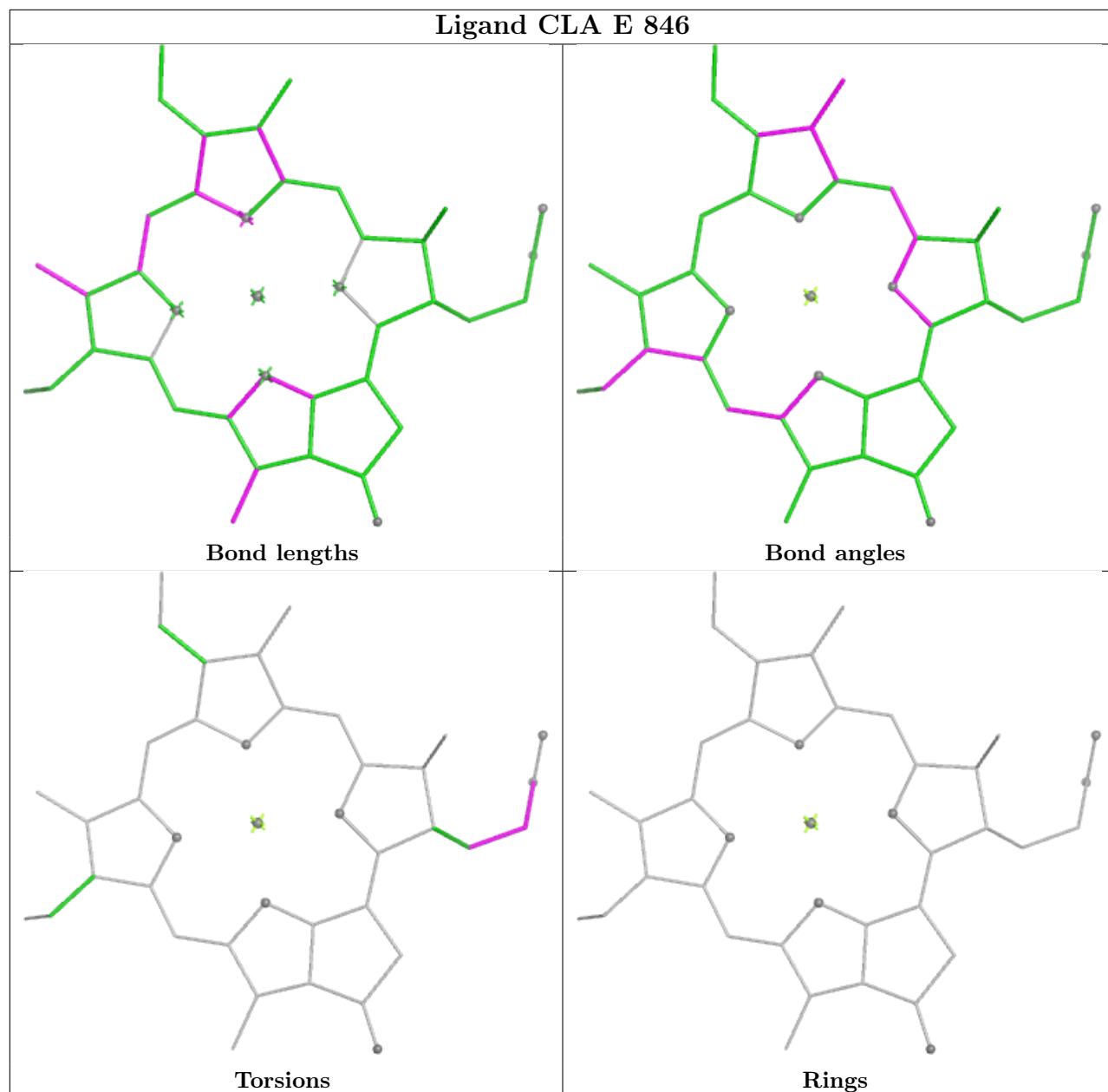
Torsions



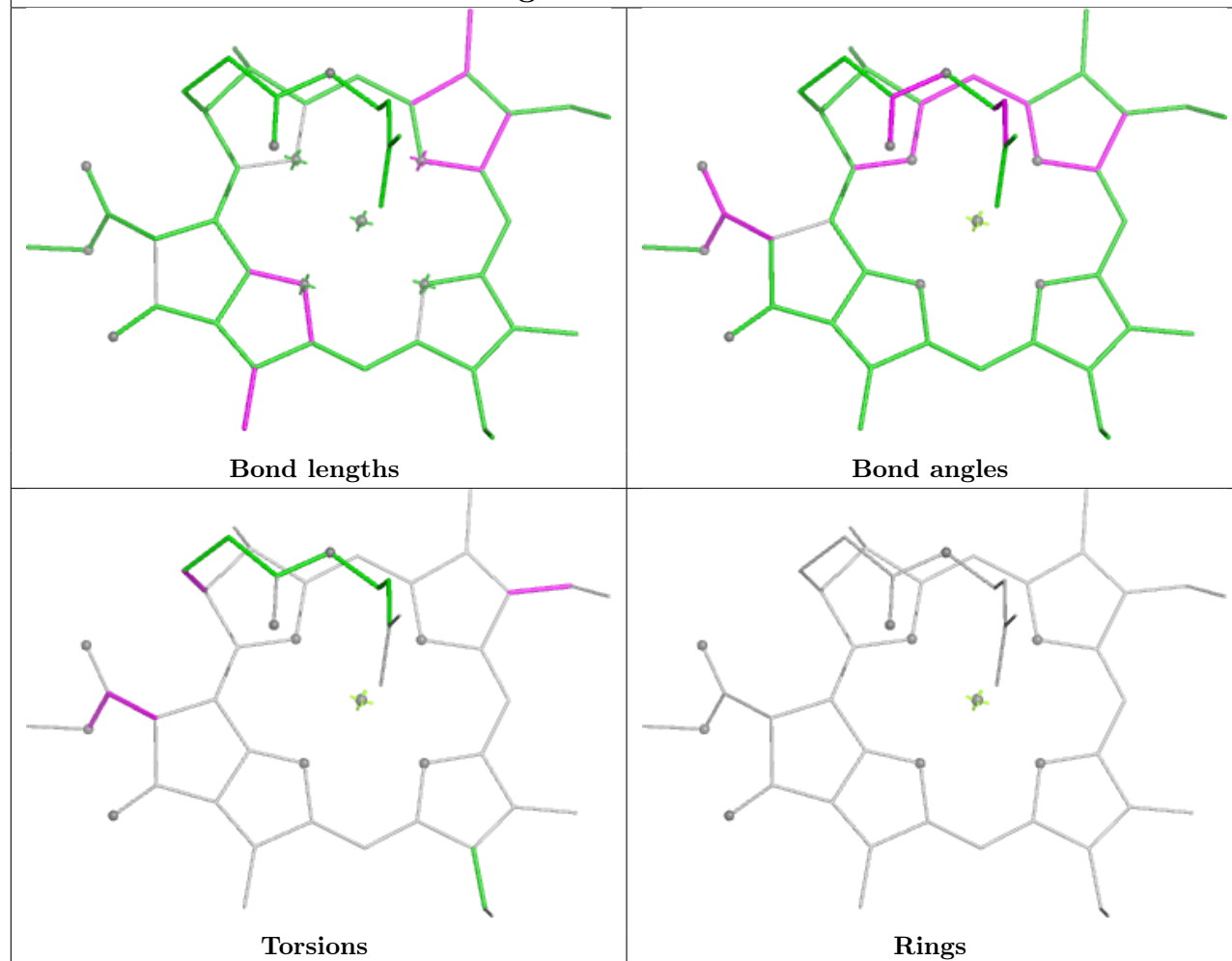
Rings

Ligand CLA B 804**Ligand BCR 1 206**

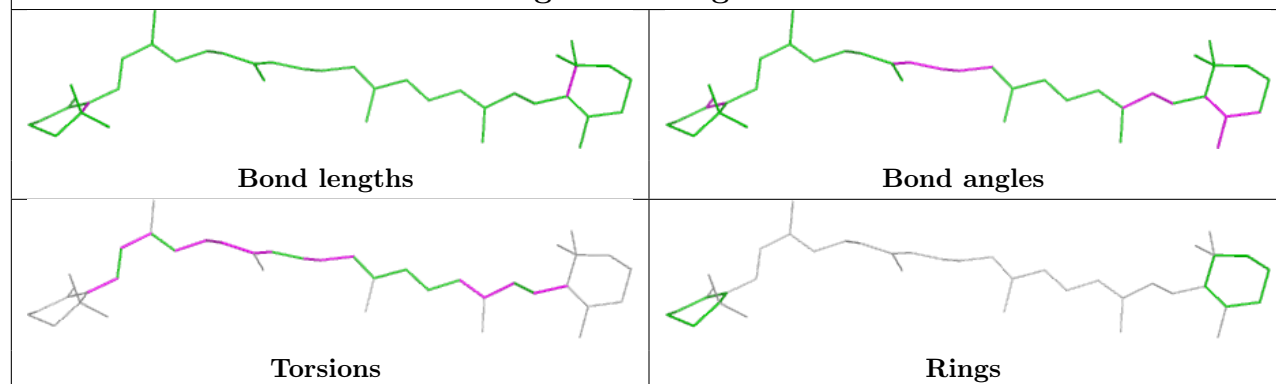
Ligand CLA E 846



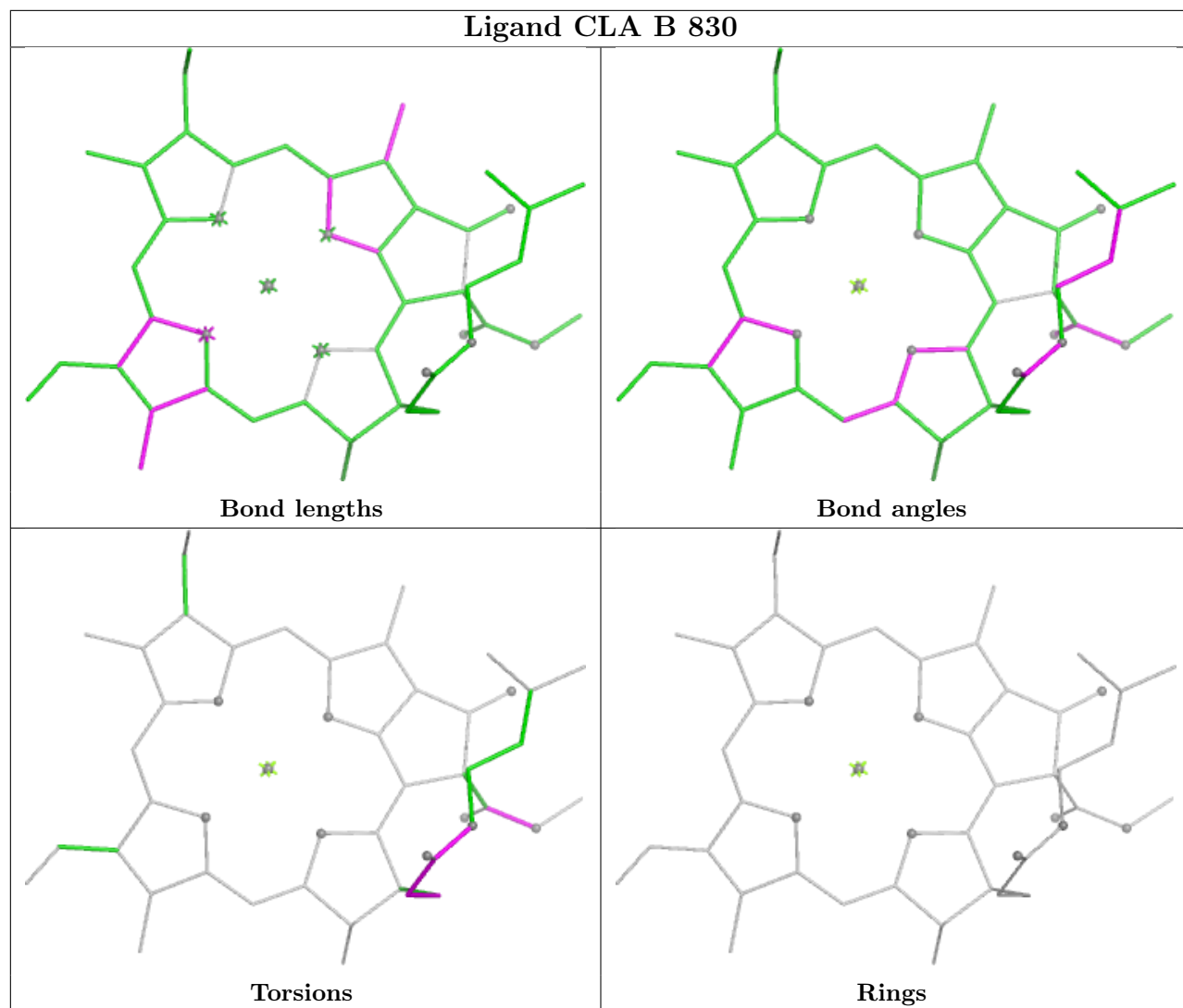
Ligand CLA e 844



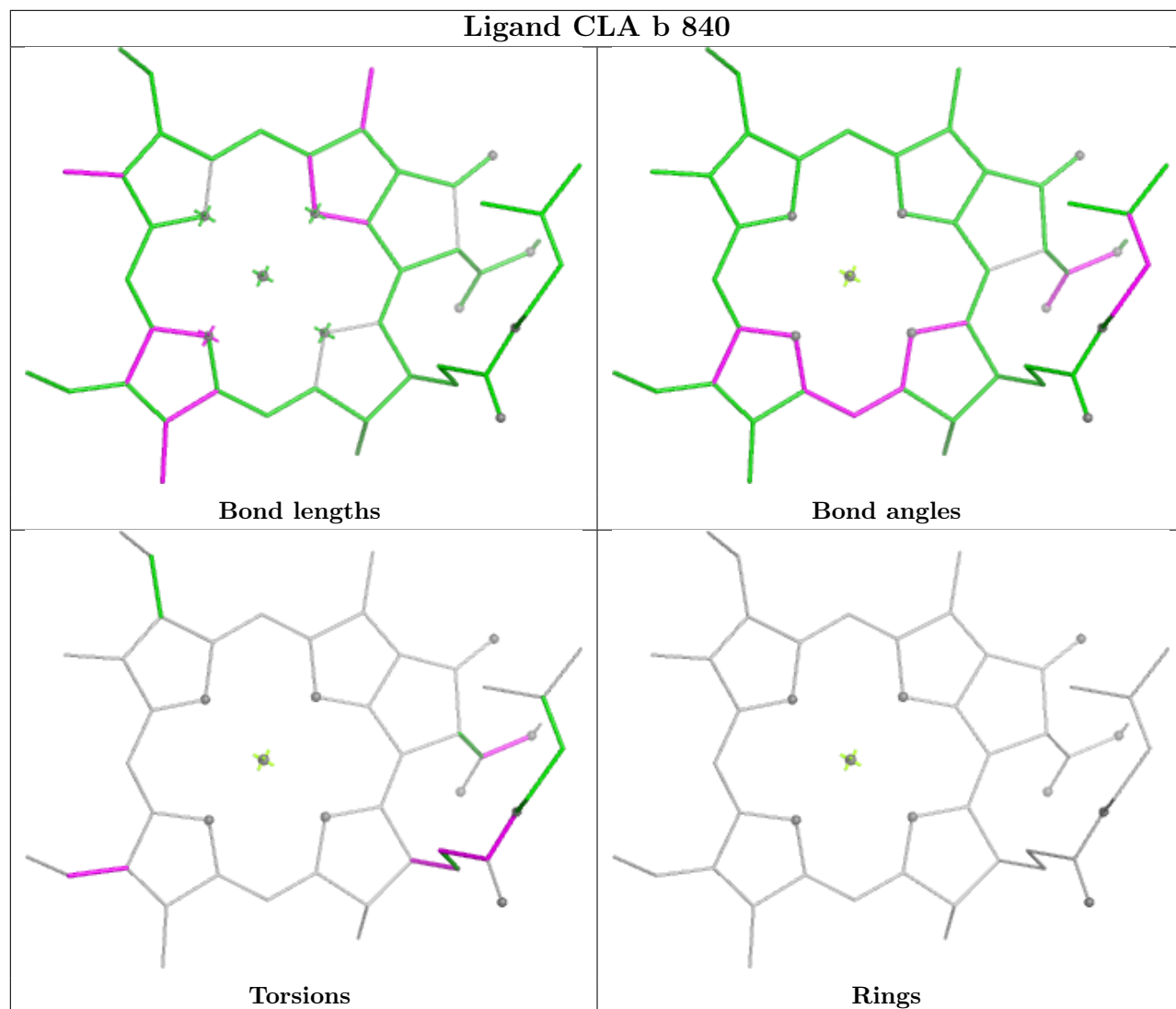
Ligand BCR g 849

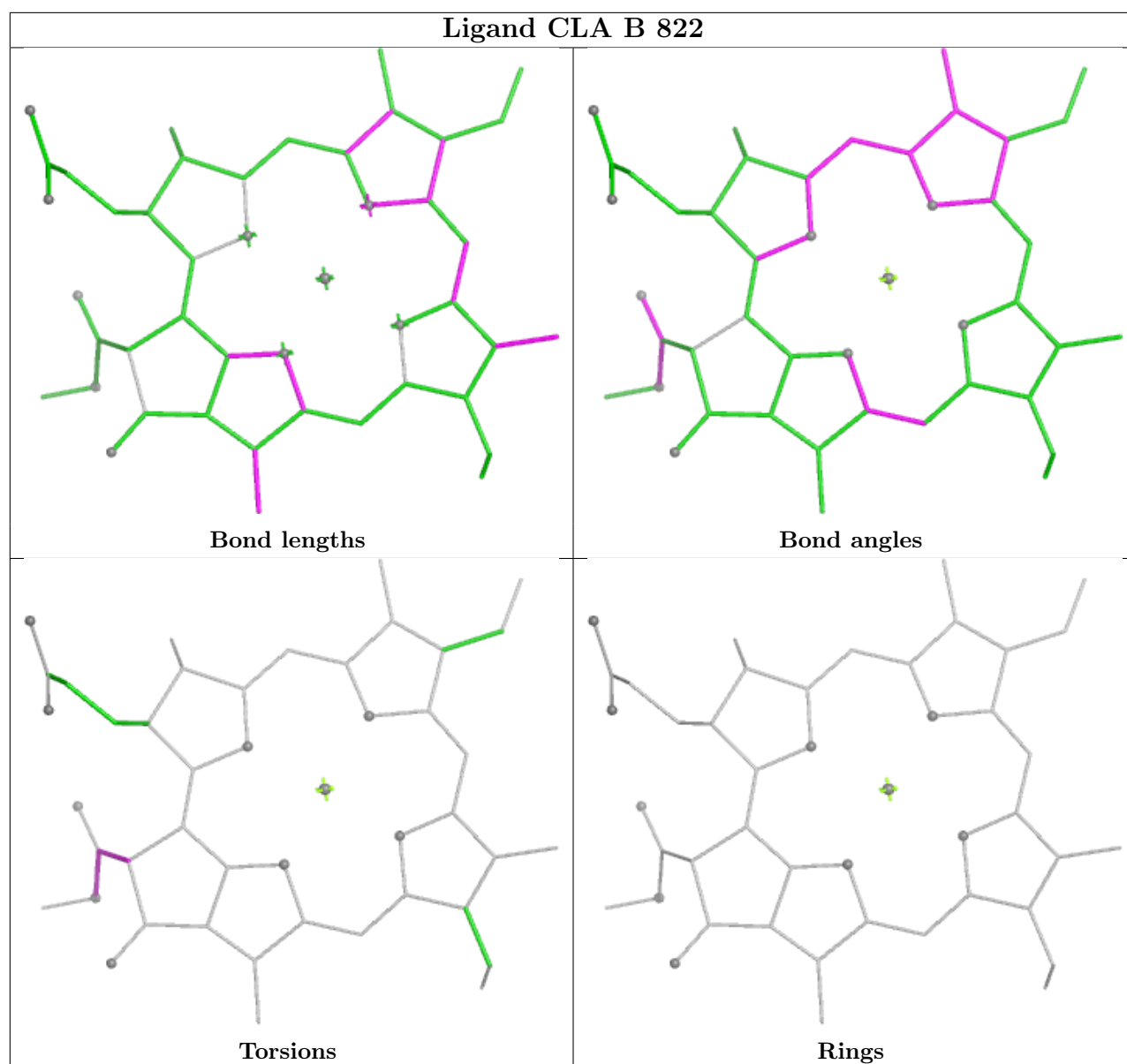


Ligand CLA B 830

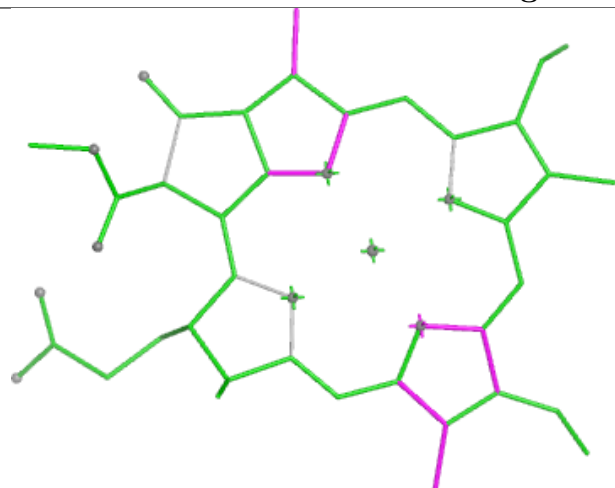


Ligand CLA b 840

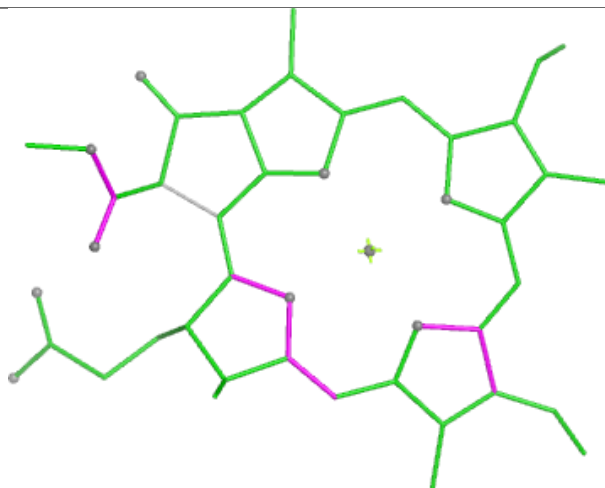




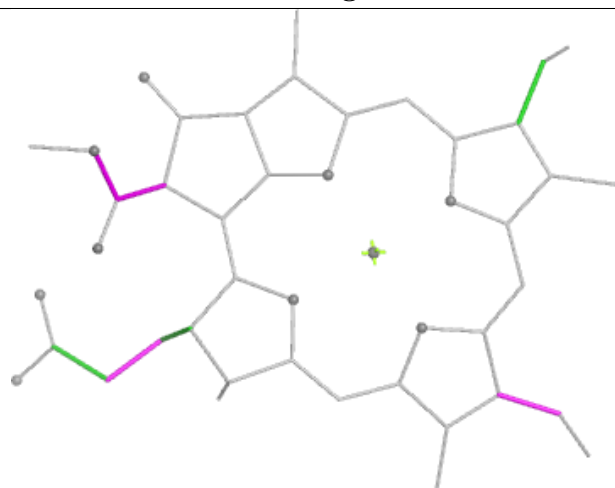
Ligand CLA o 202



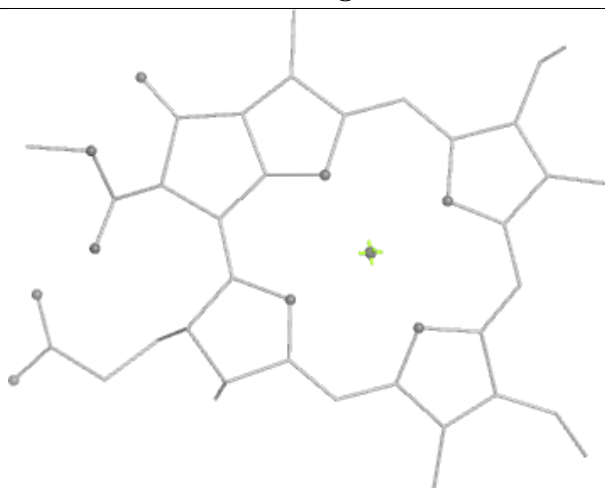
Bond lengths



Bond angles

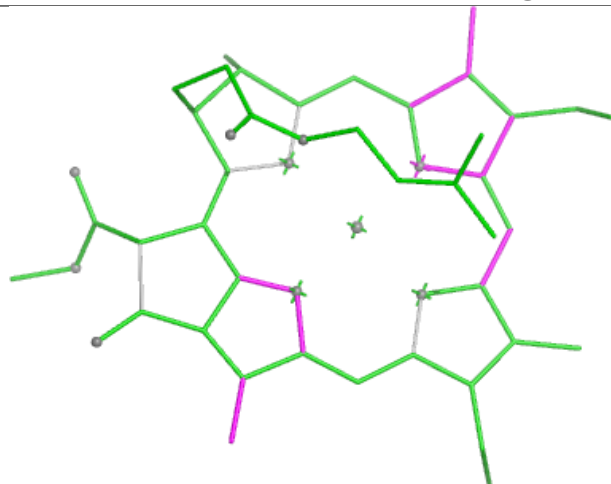


Torsions

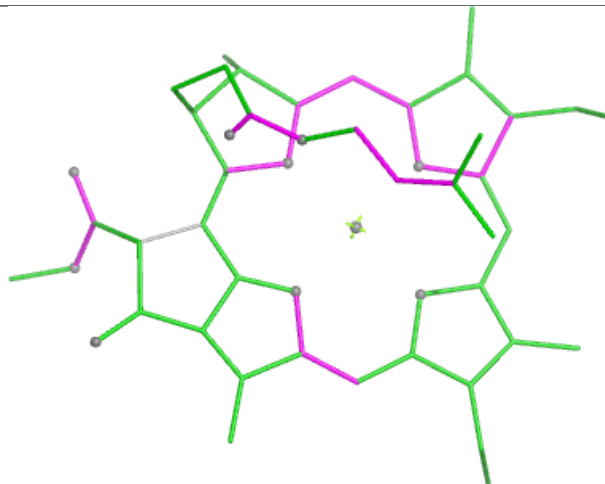


Rings

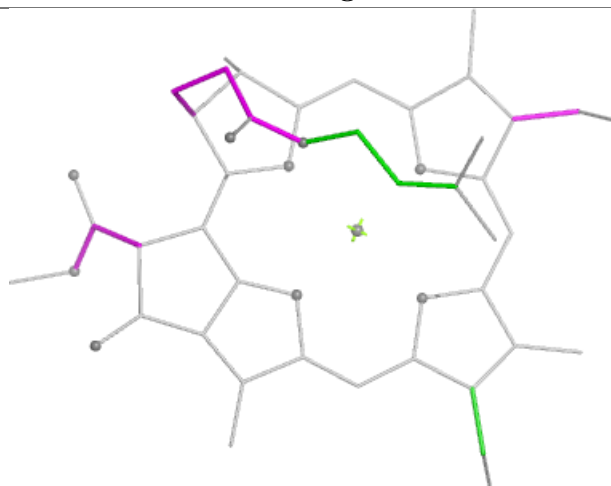
Ligand CLA e 825



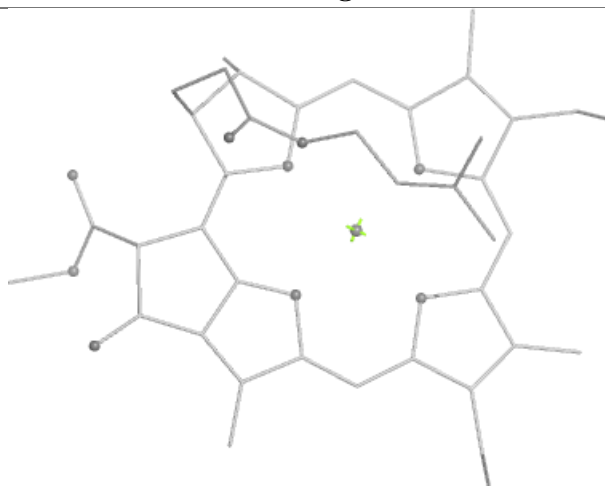
Bond lengths



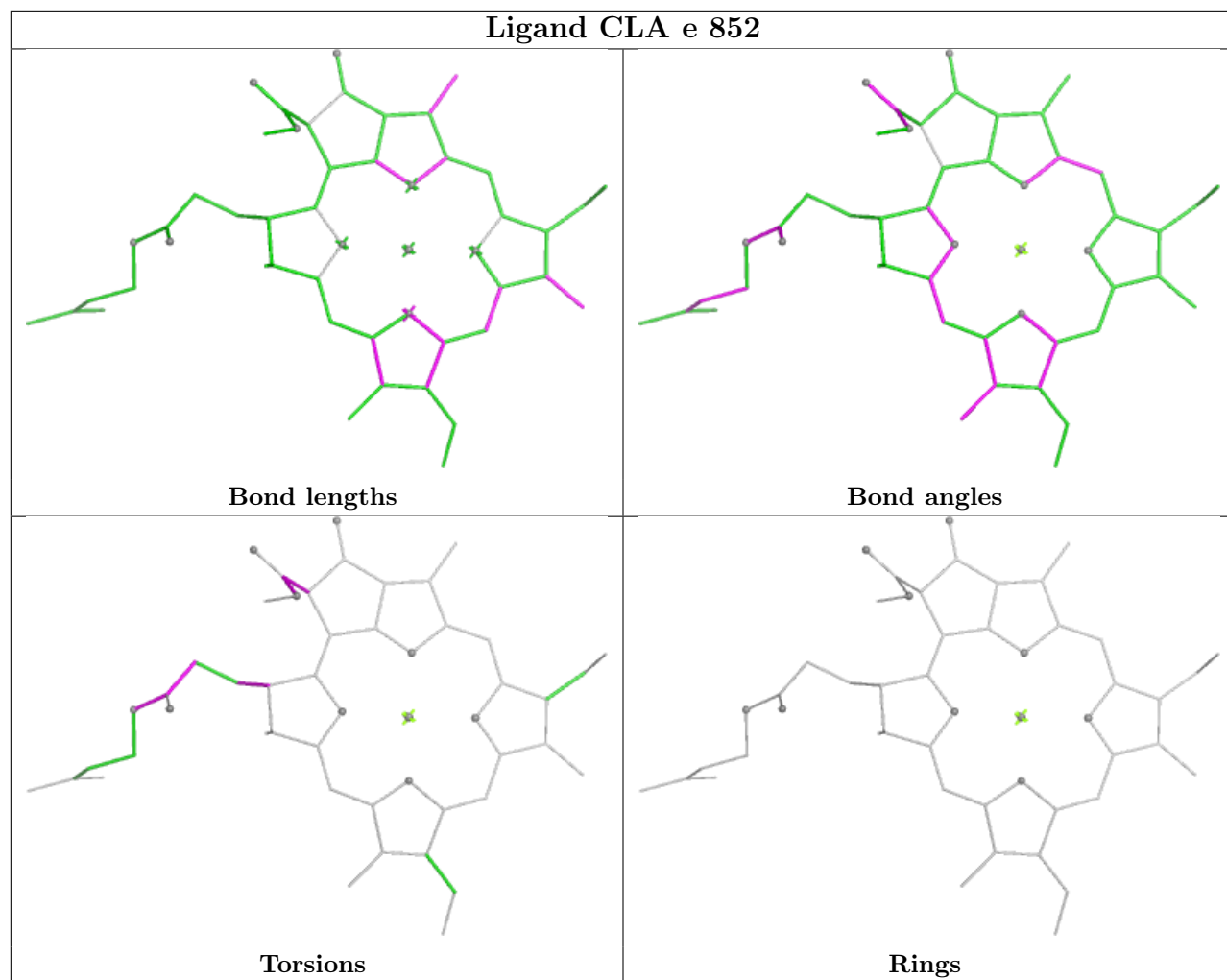
Bond angles



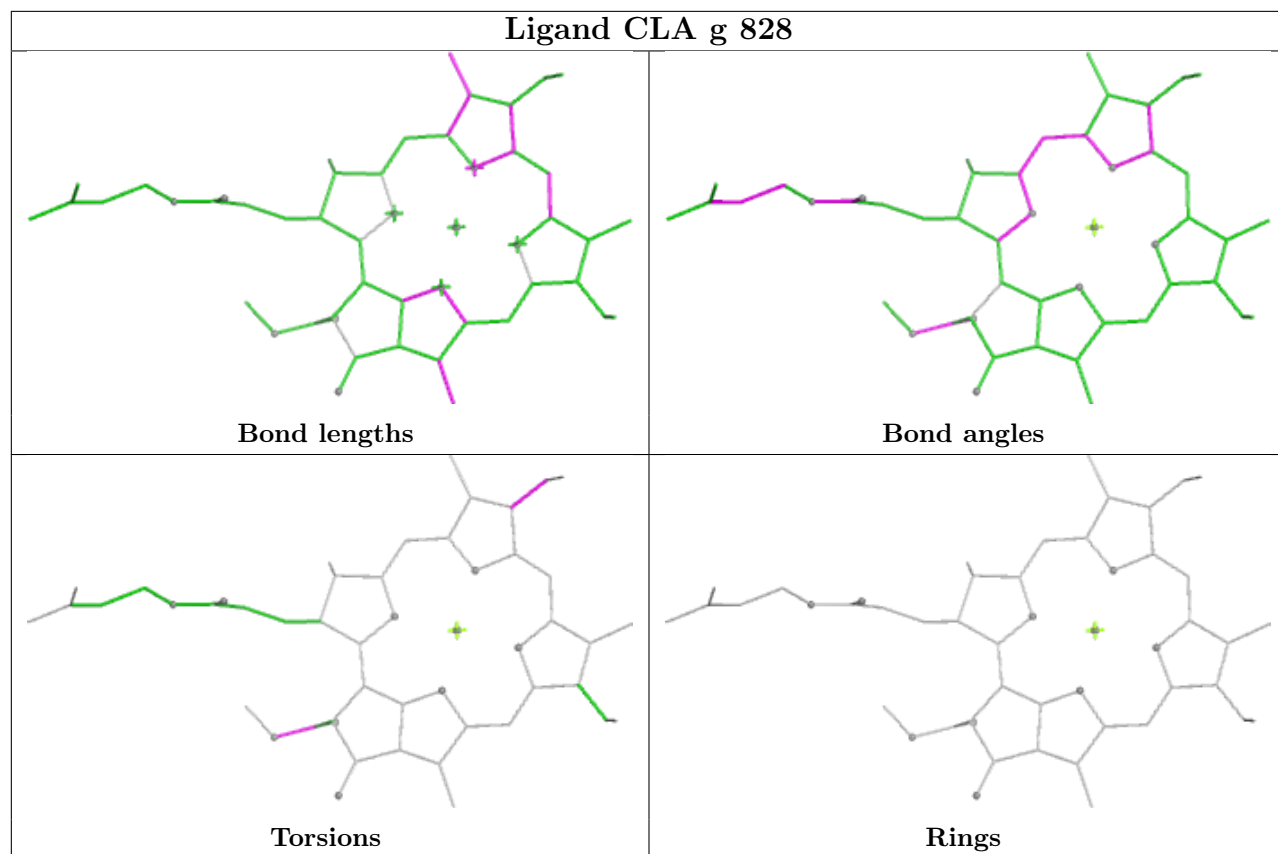
Torsions



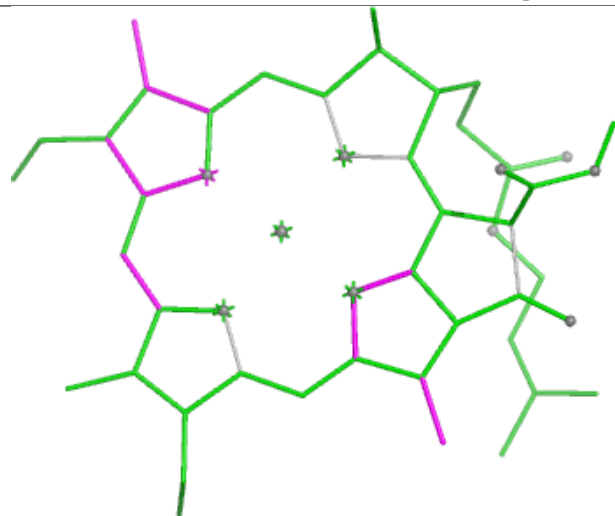
Rings



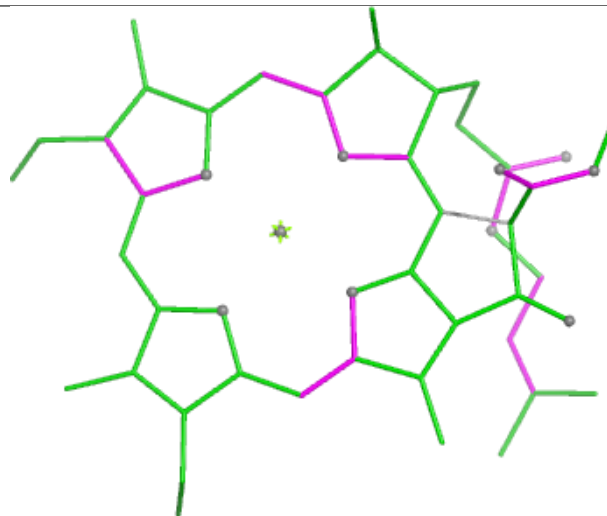
Ligand CLA g 828



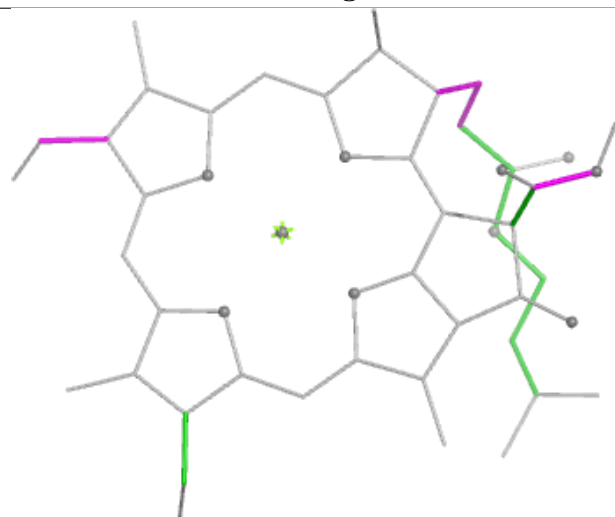
Ligand CLA E 832



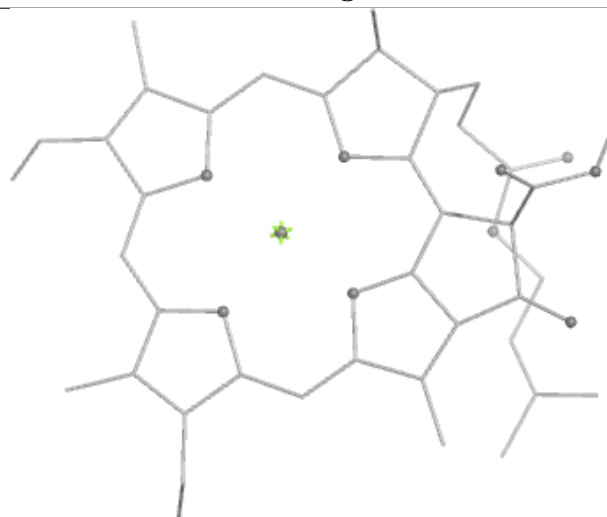
Bond lengths



Bond angles

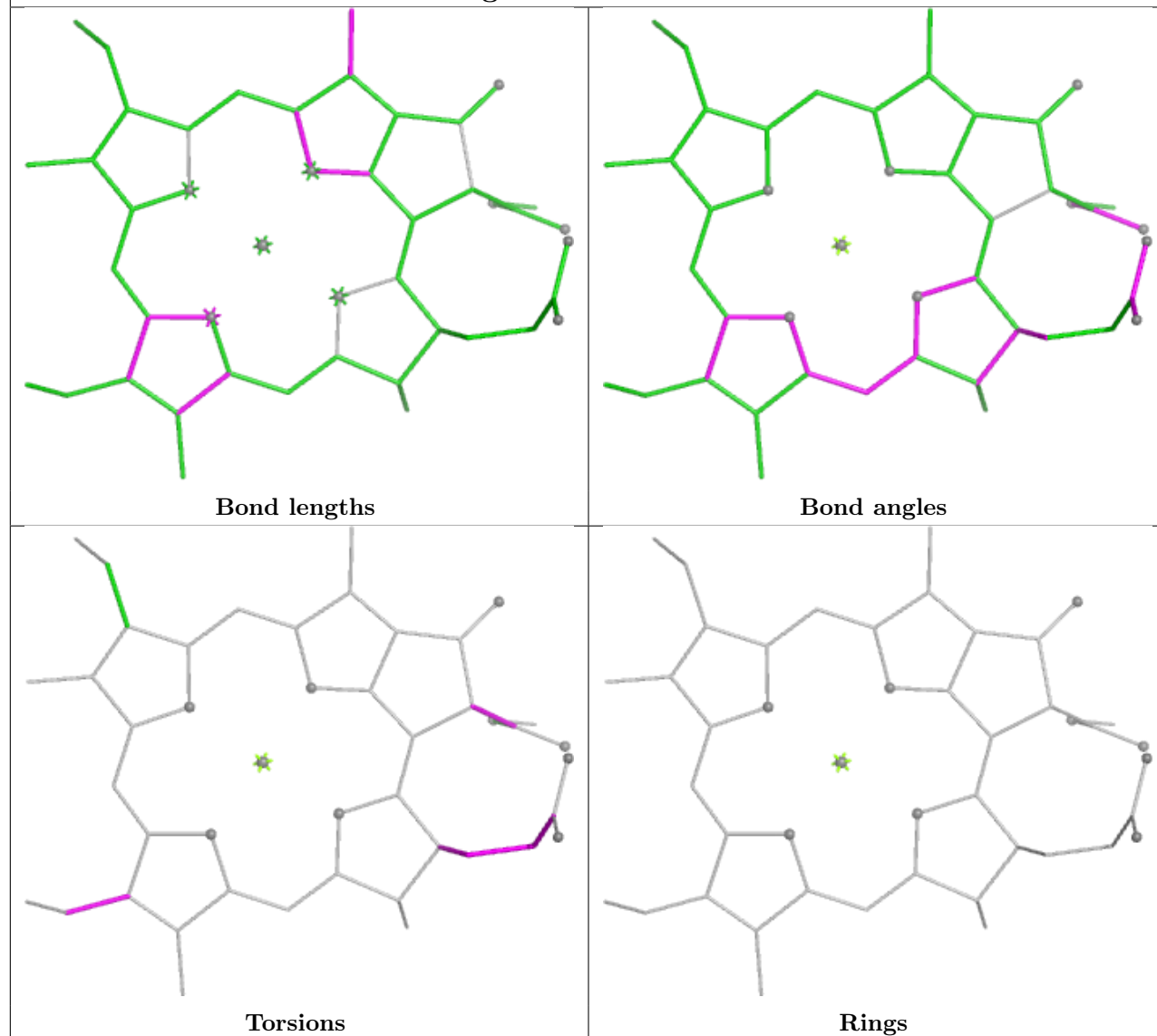


Torsions

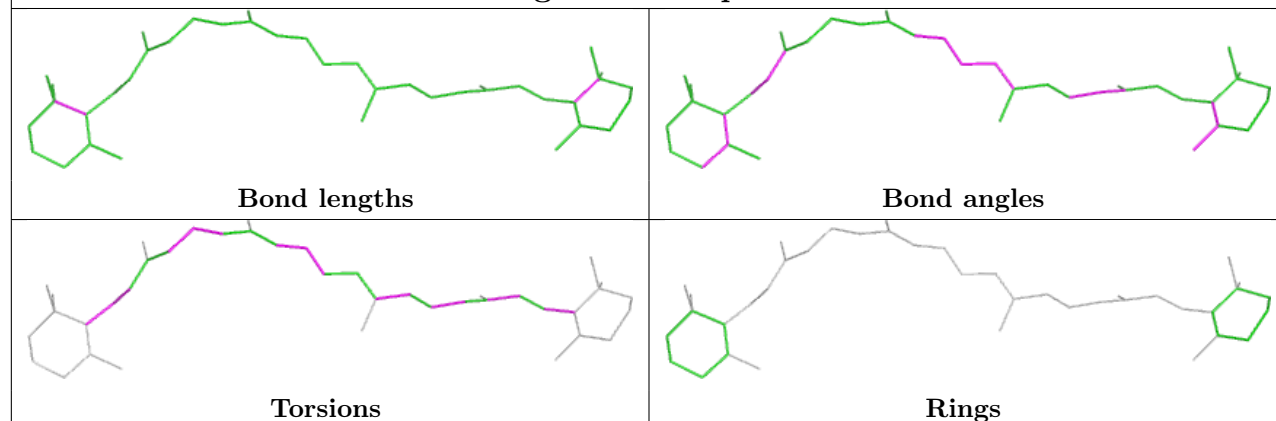


Rings

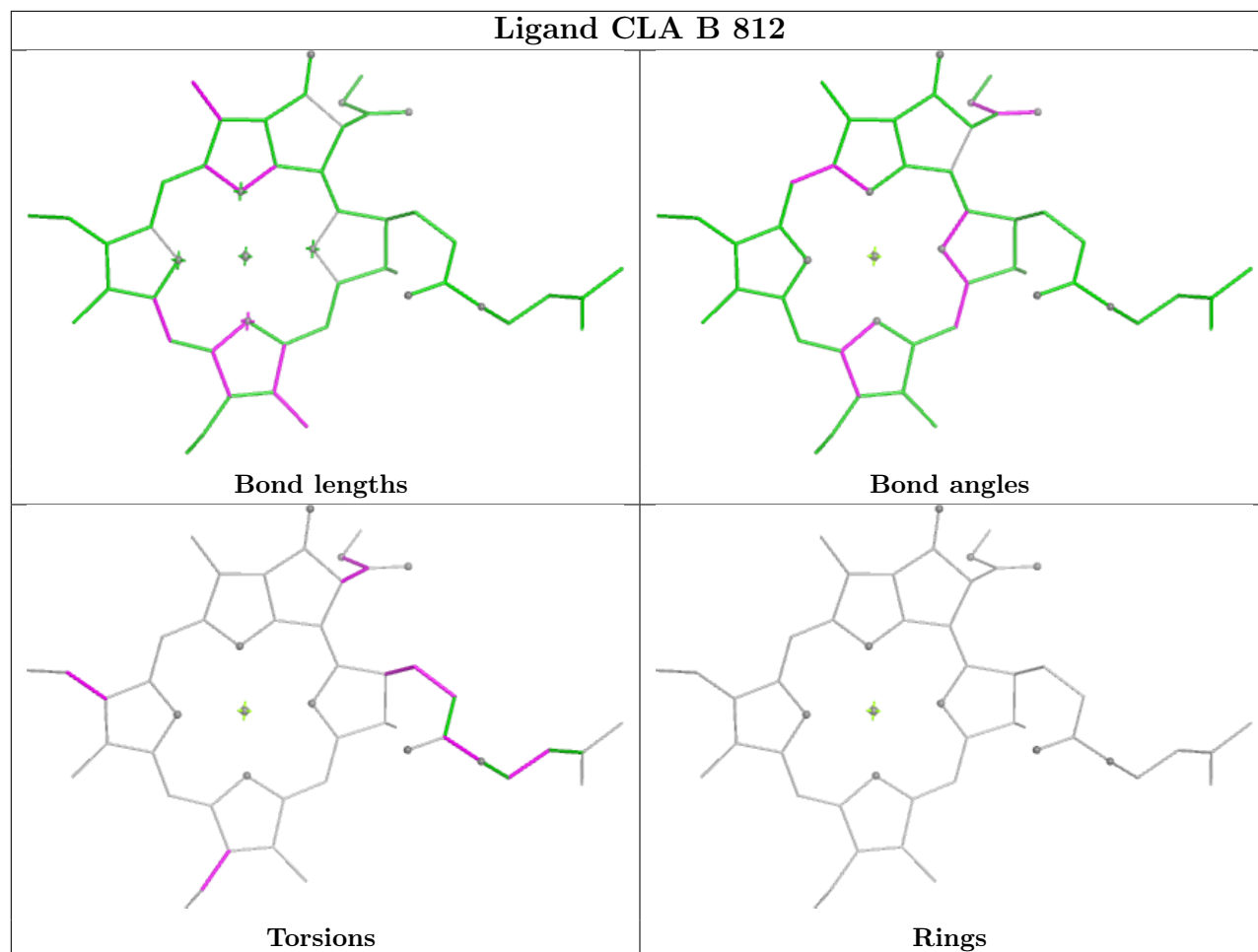
Ligand CLA R 102



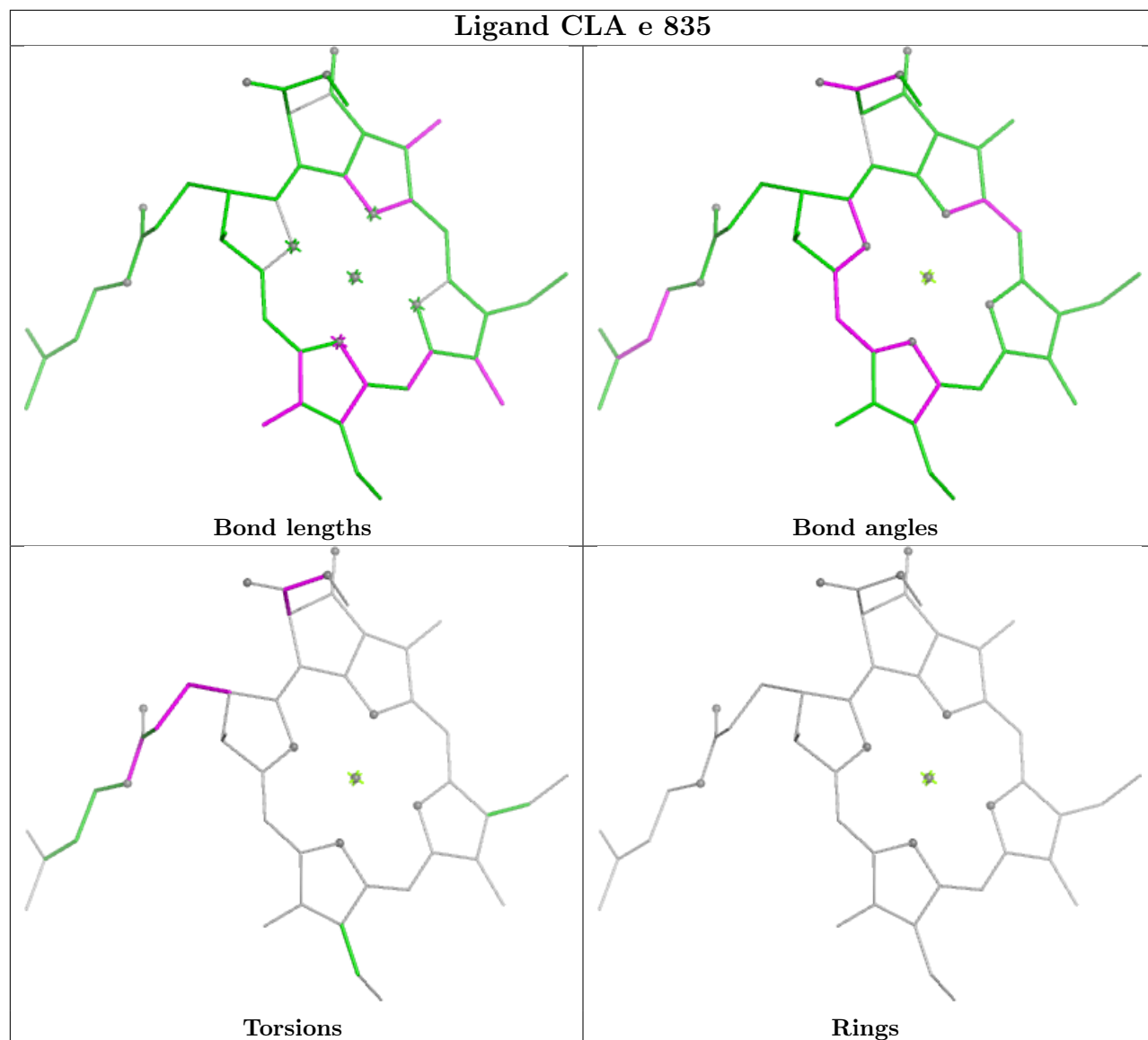
Ligand BCR q 101

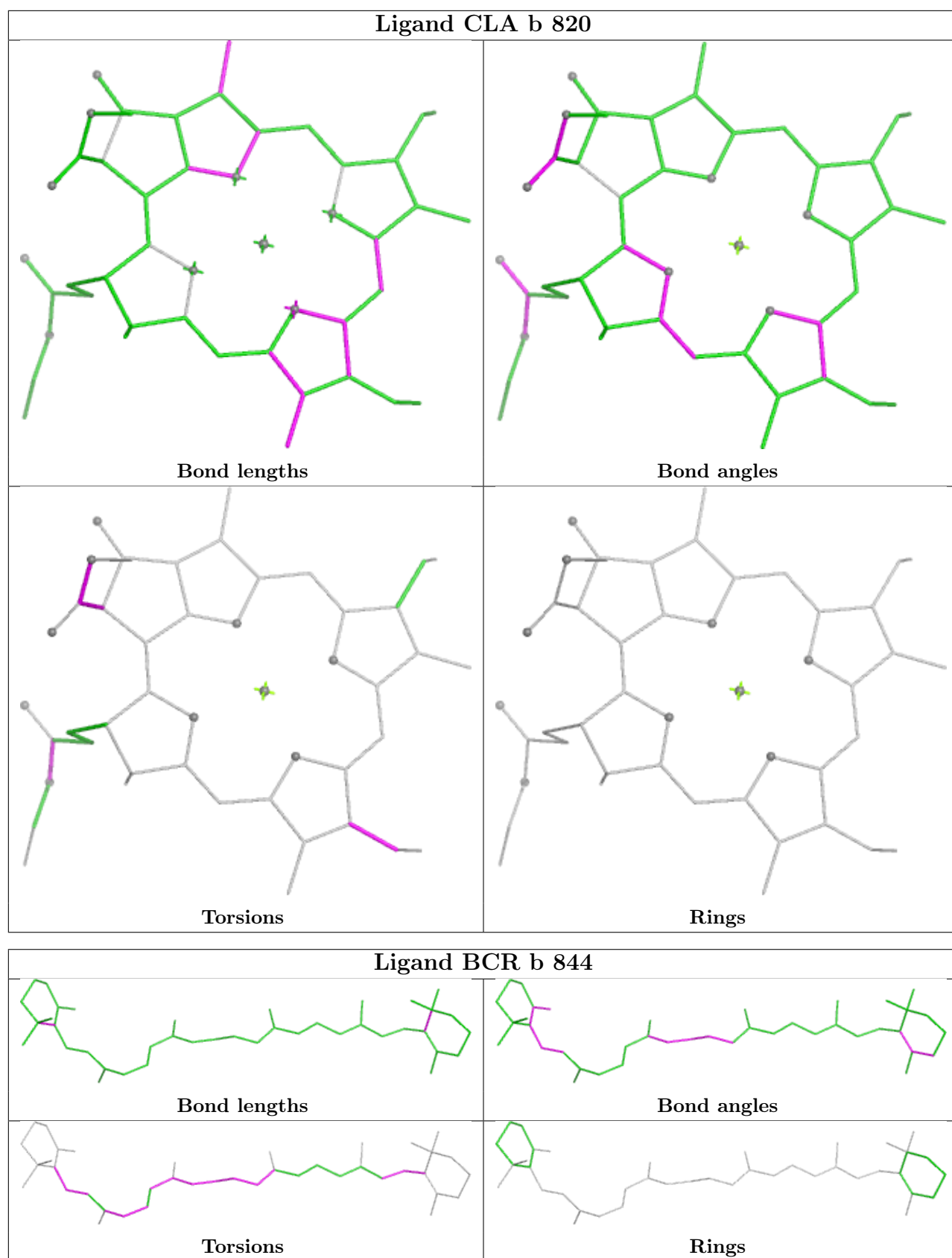


Ligand CLA B 812

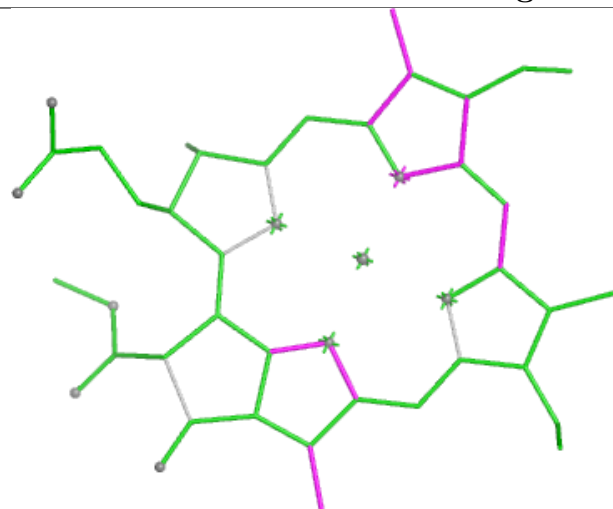


Ligand CLA e 835

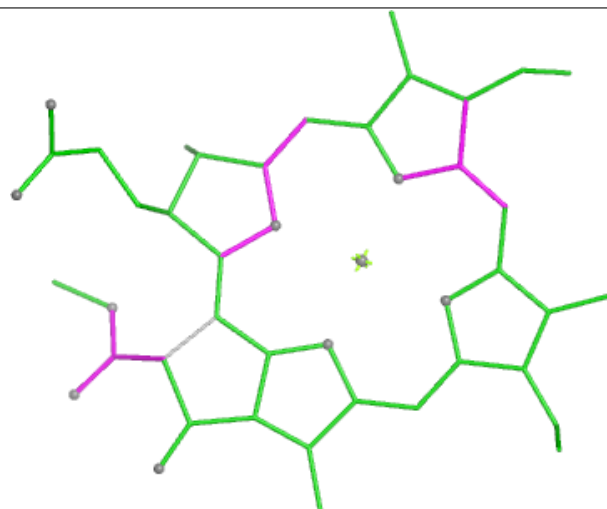




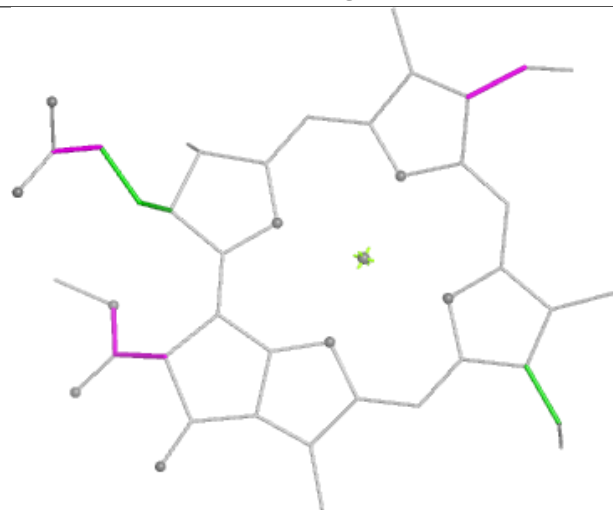
Ligand CLA B 824



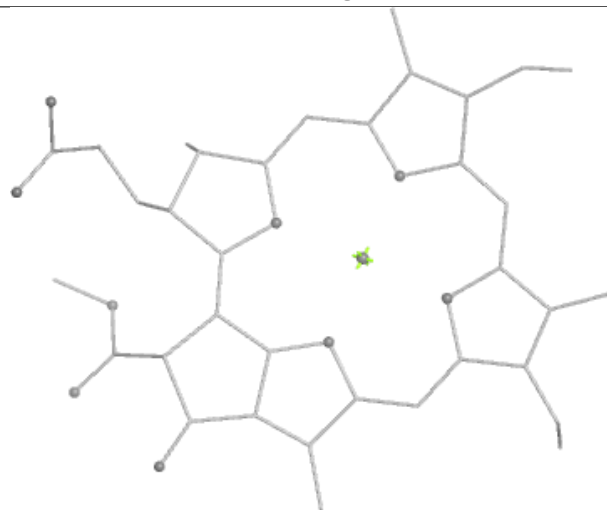
Bond lengths



Bond angles

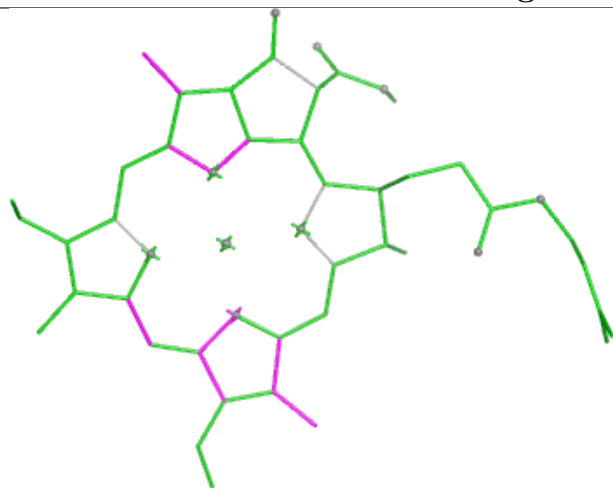


Torsions

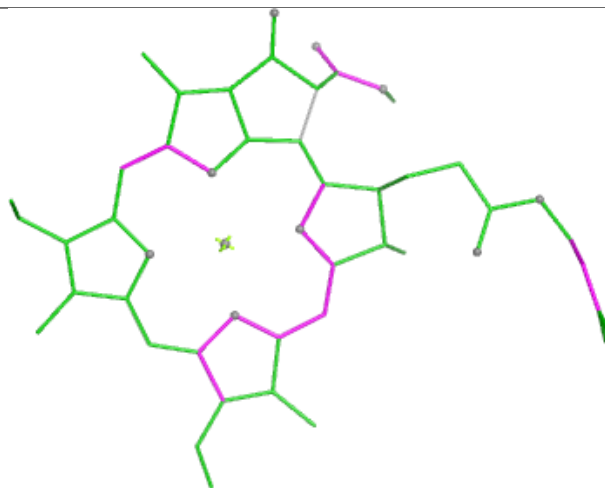


Rings

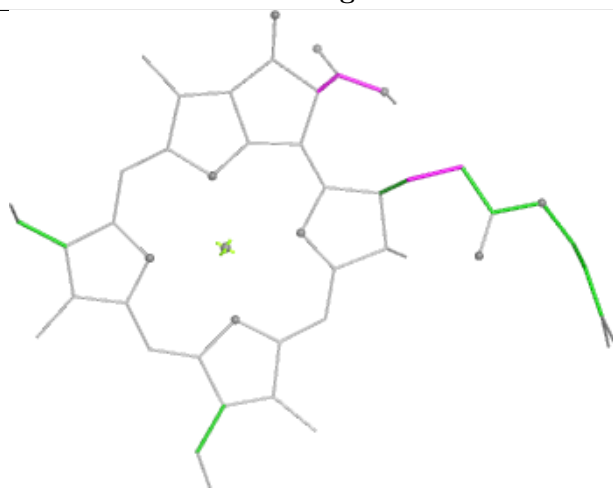
Ligand CLA b 813



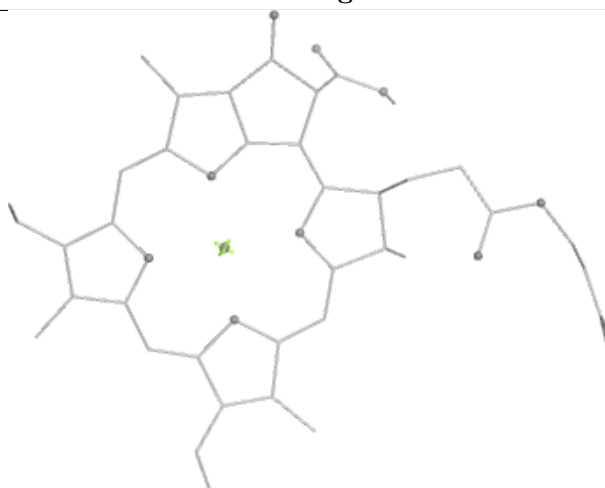
Bond lengths



Bond angles

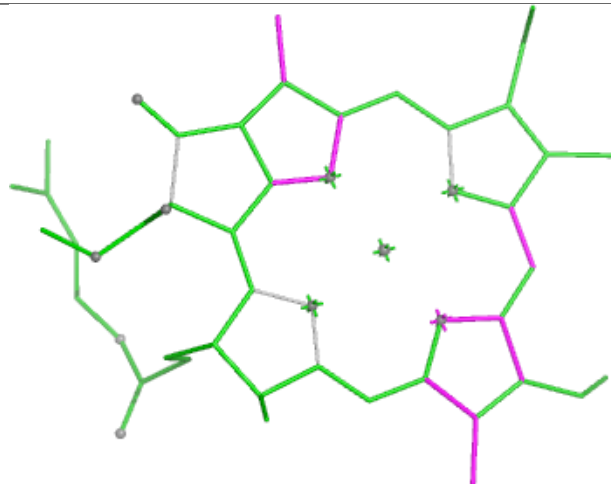


Torsions

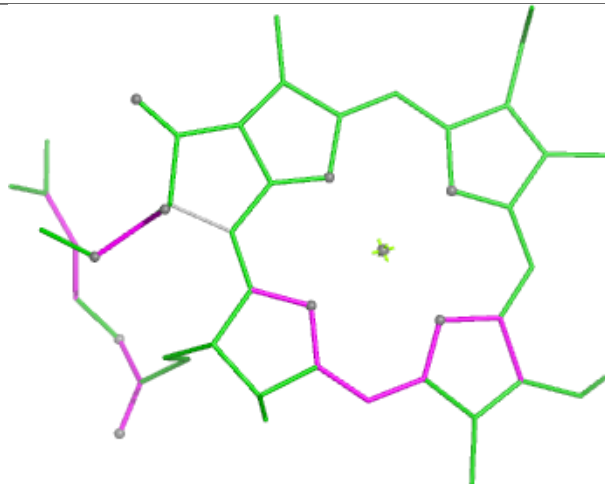


Rings

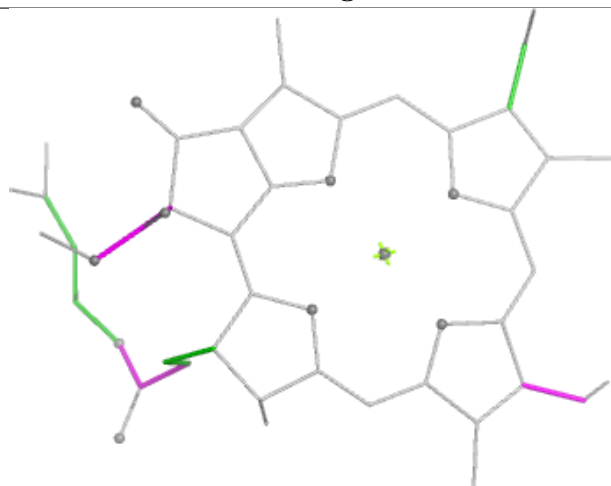
Ligand CLA B 817



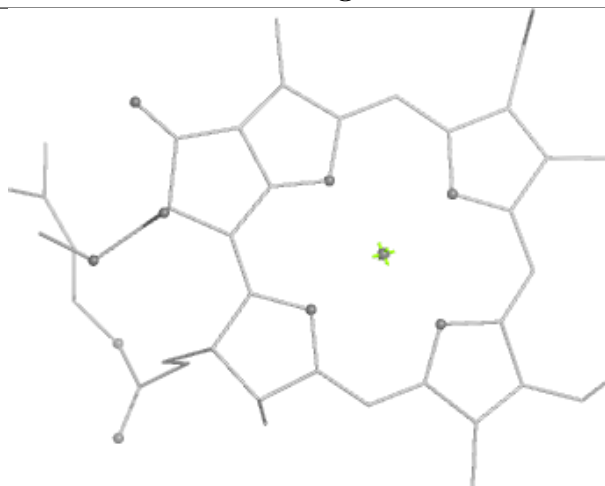
Bond lengths



Bond angles

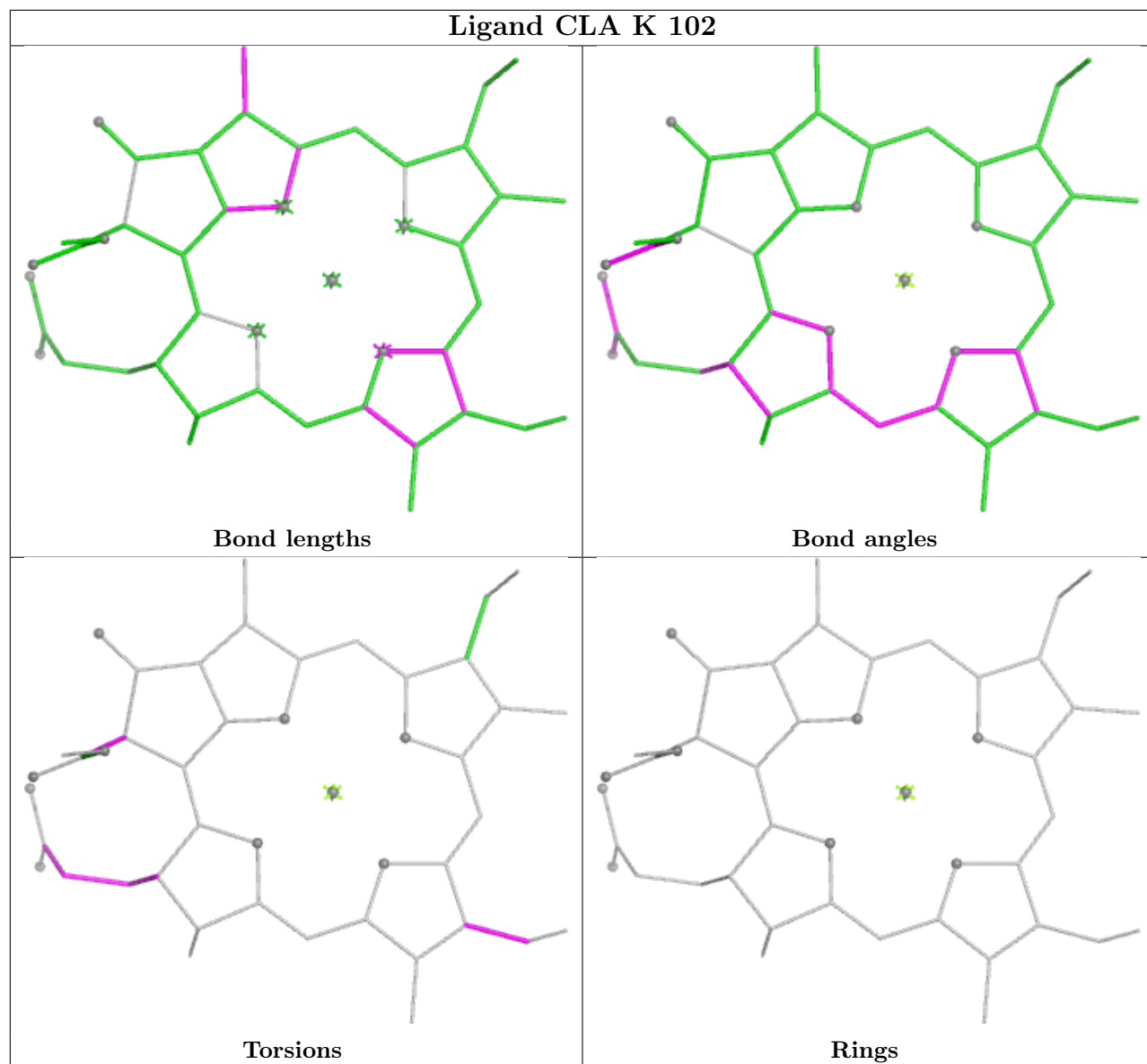


Torsions

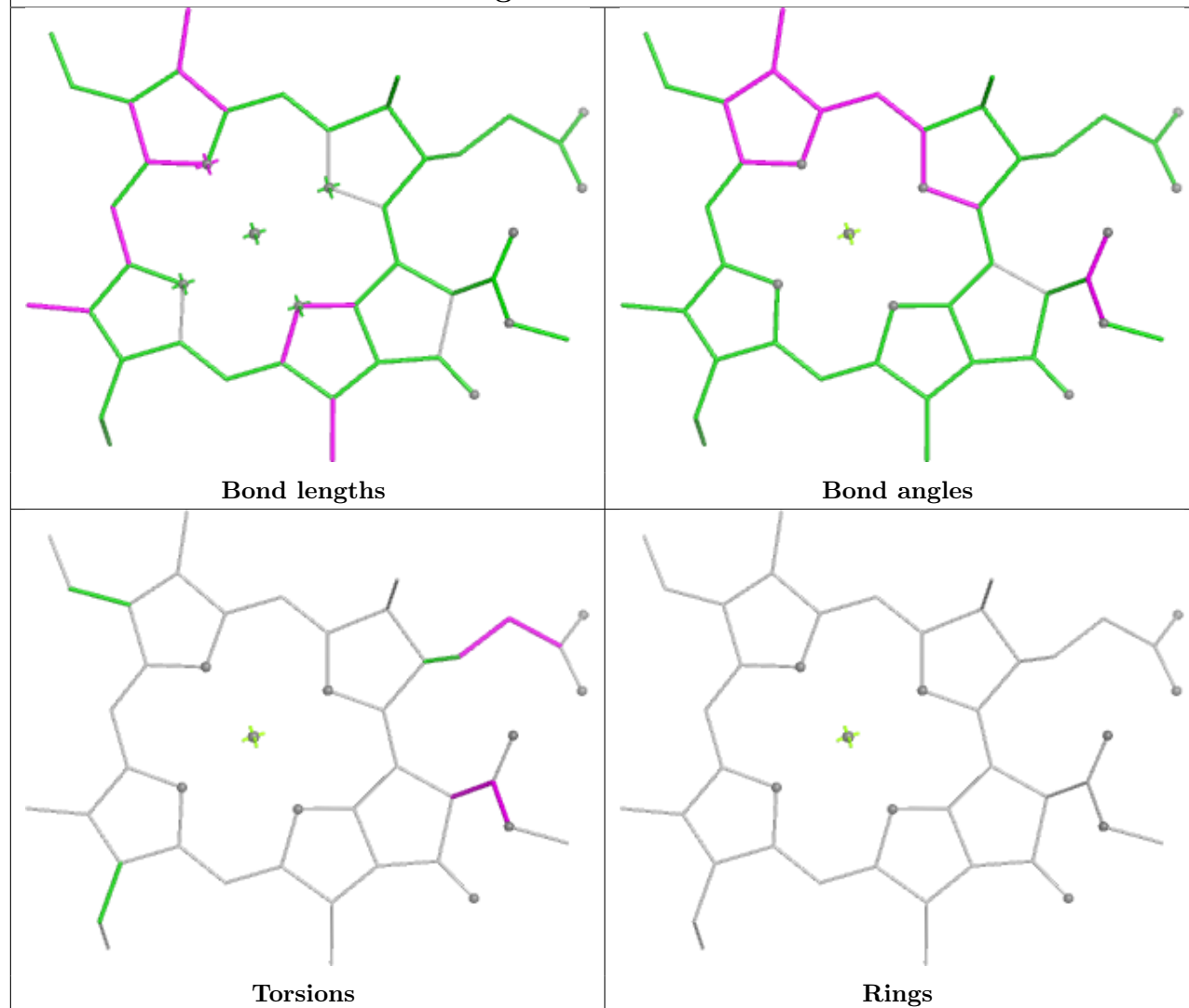


Rings

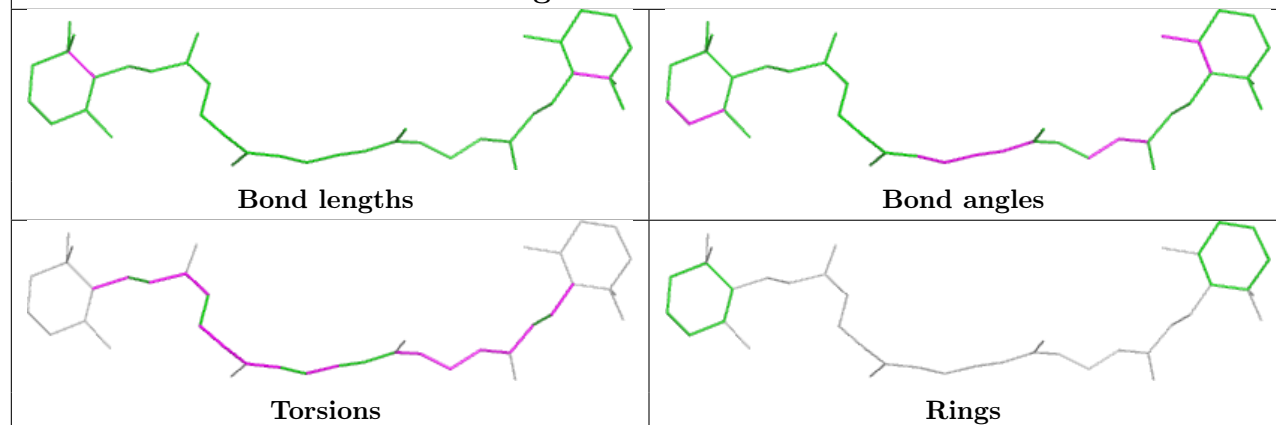
Ligand CLA K 102

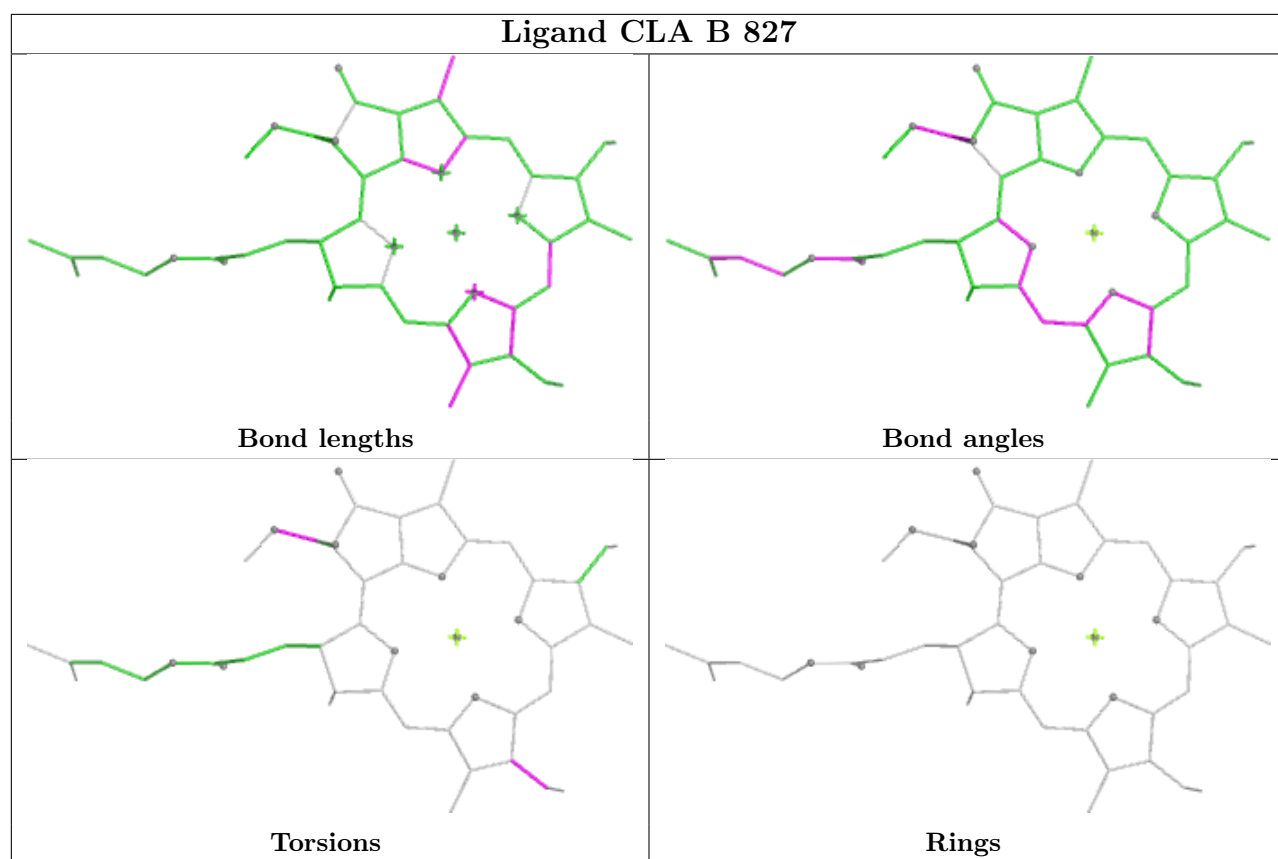


Ligand CLA O 203

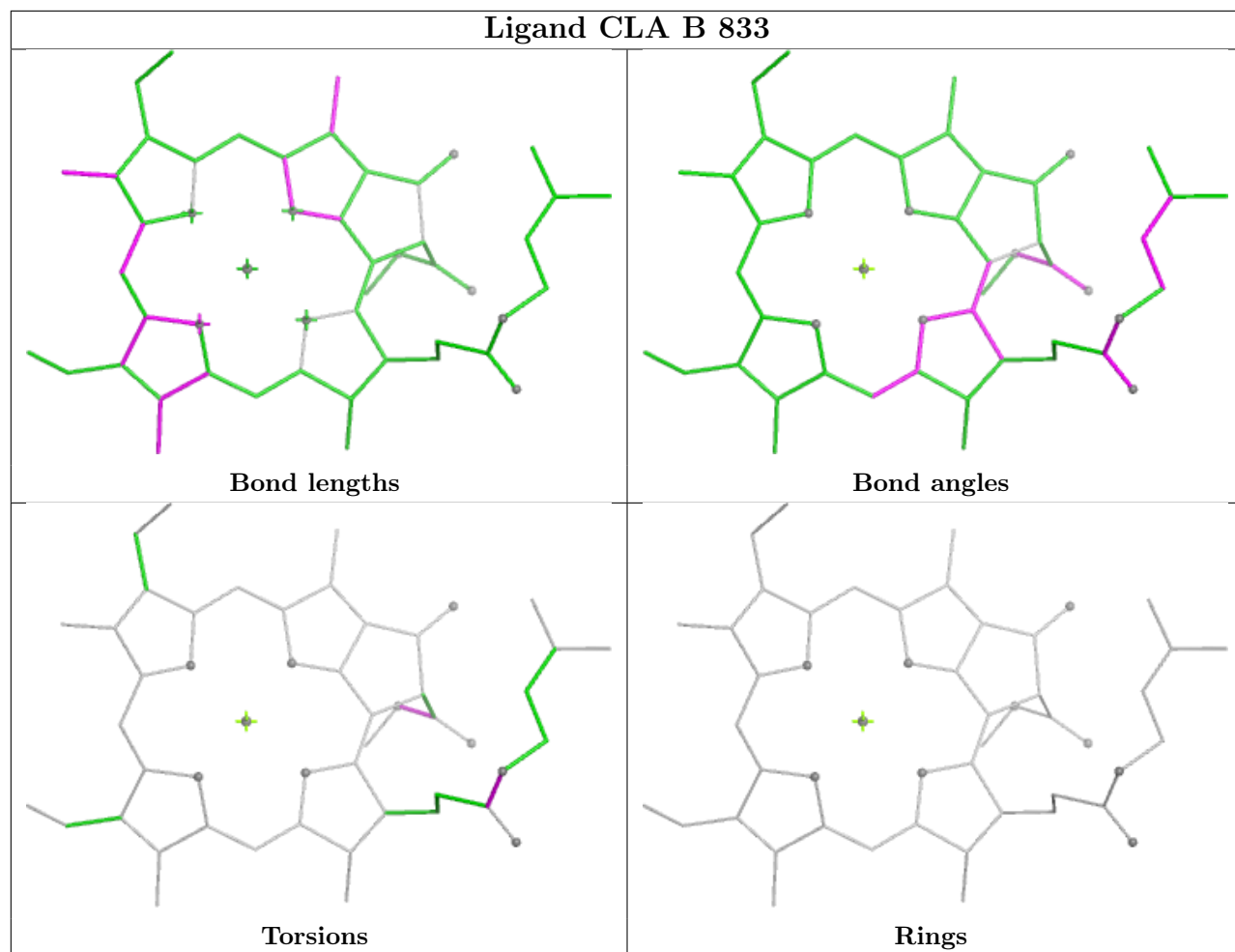


Ligand BCR b 843

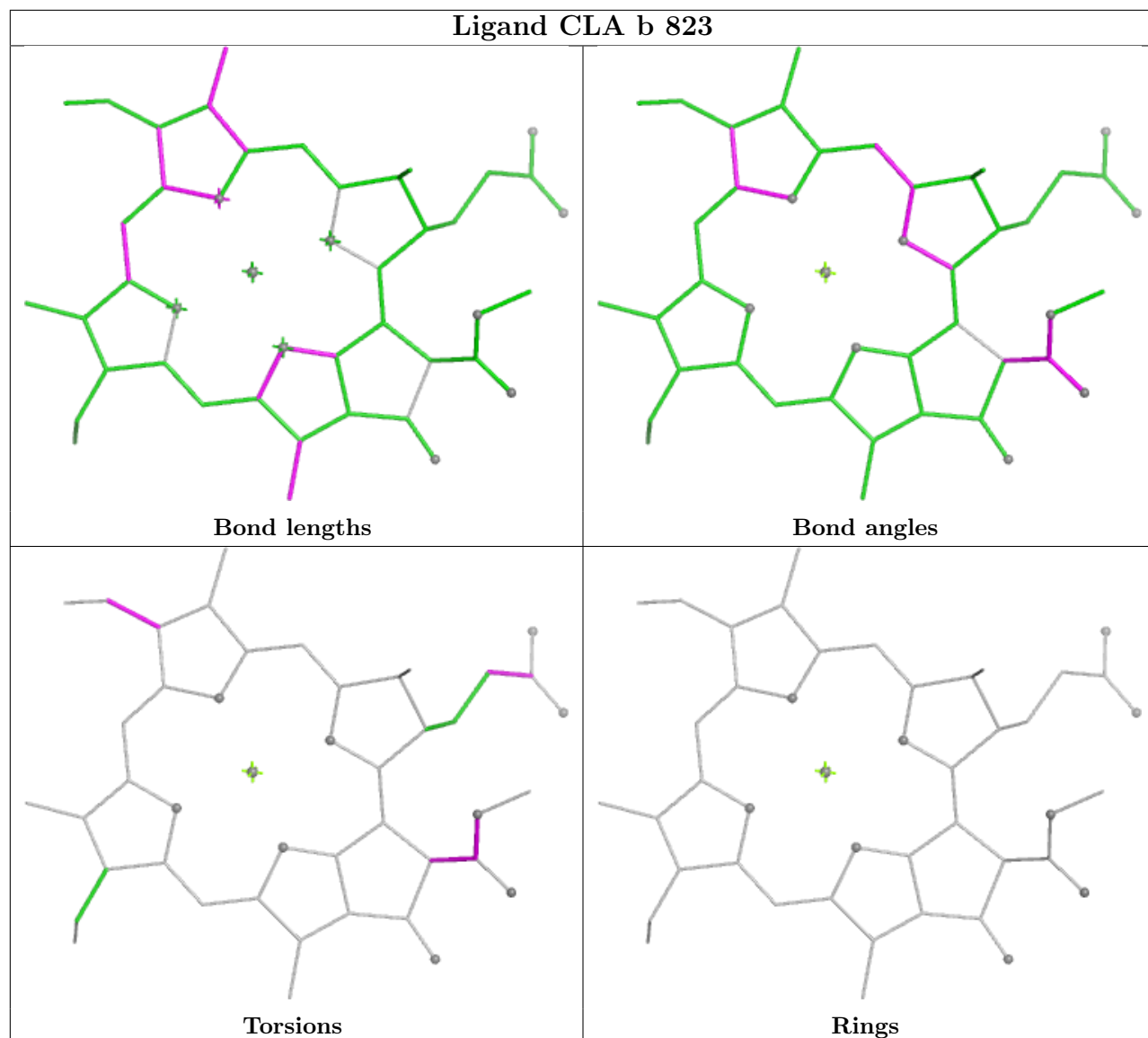




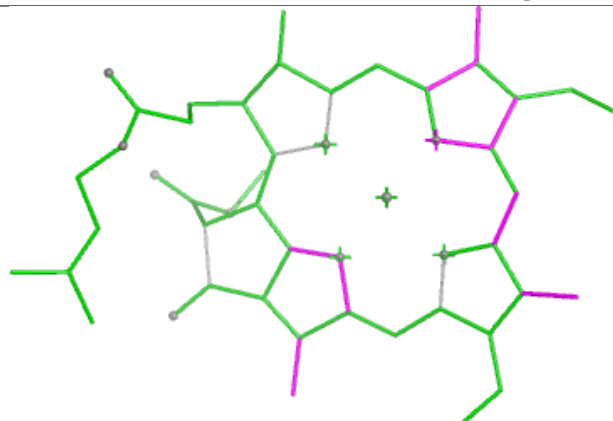
Ligand CLA B 833



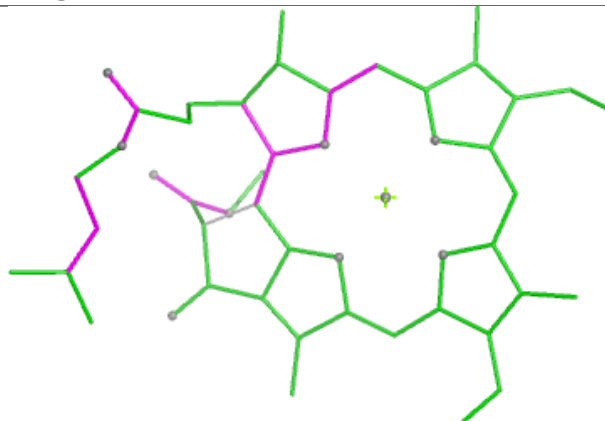
Ligand CLA b 823



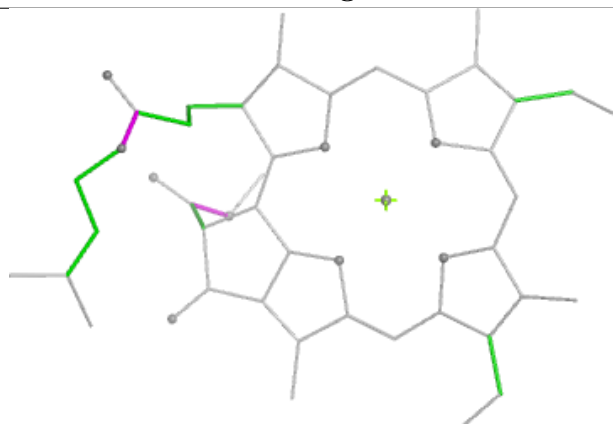
Ligand CLA g 834



Bond lengths



Bond angles

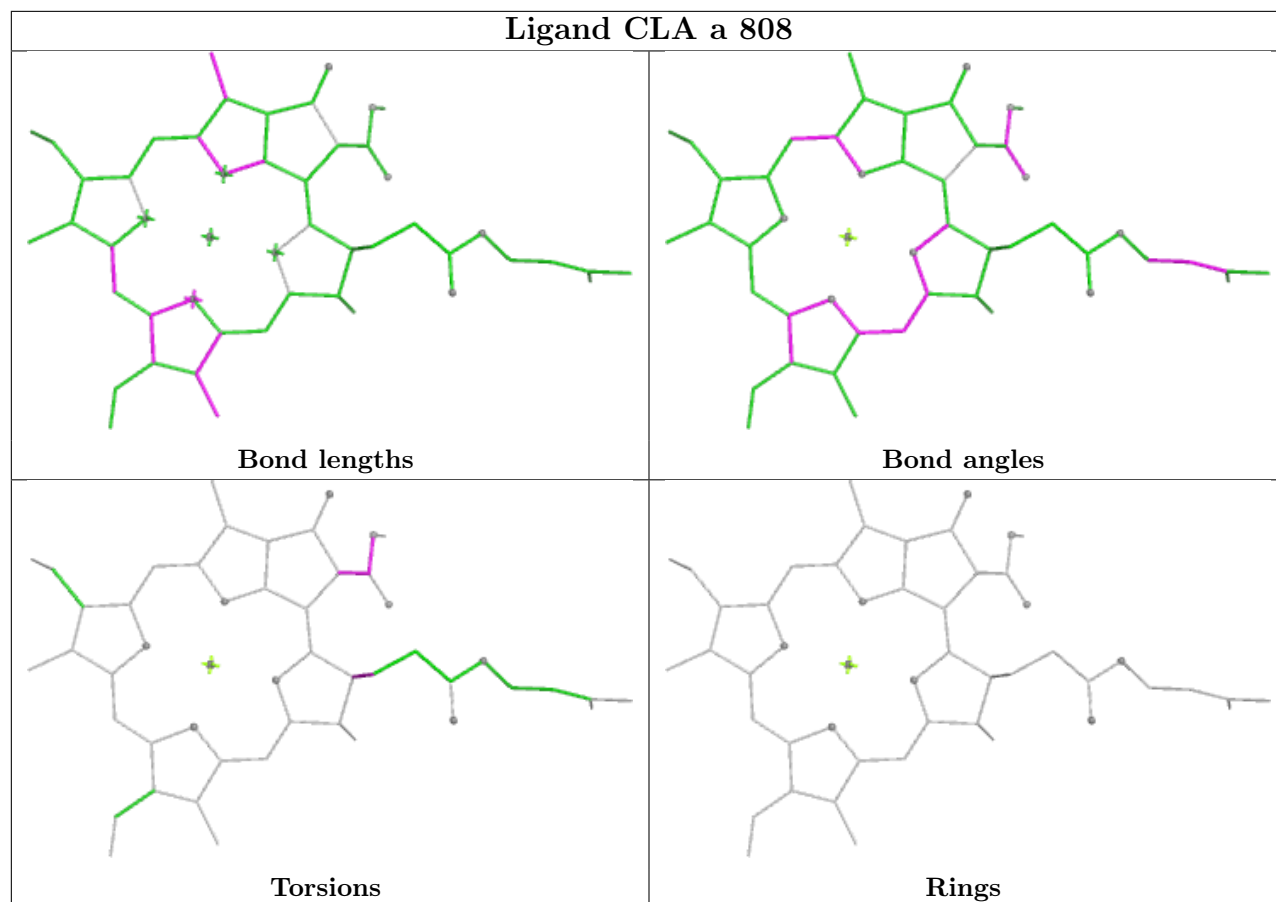


Torsions

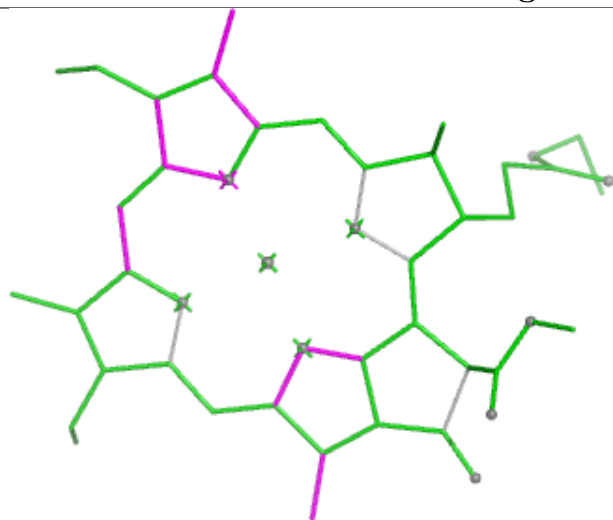


Rings

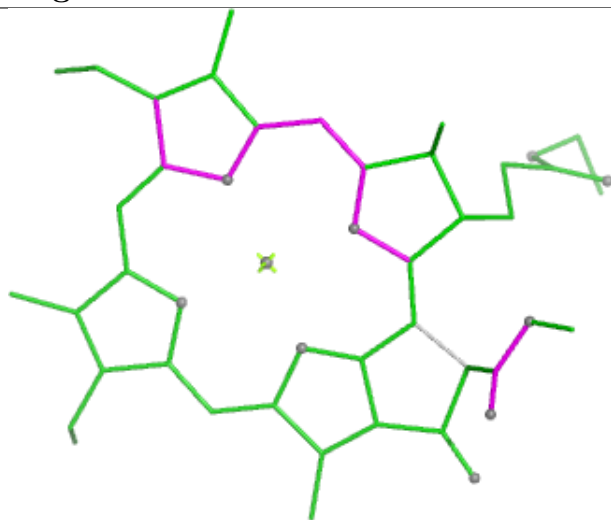
Ligand CLA a 808



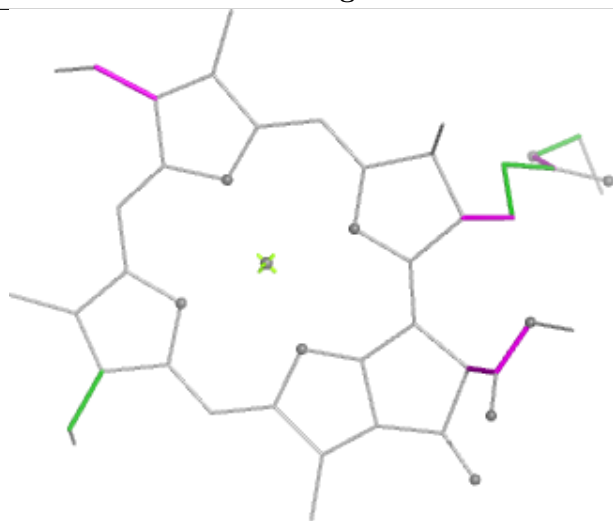
Ligand CLA g 840



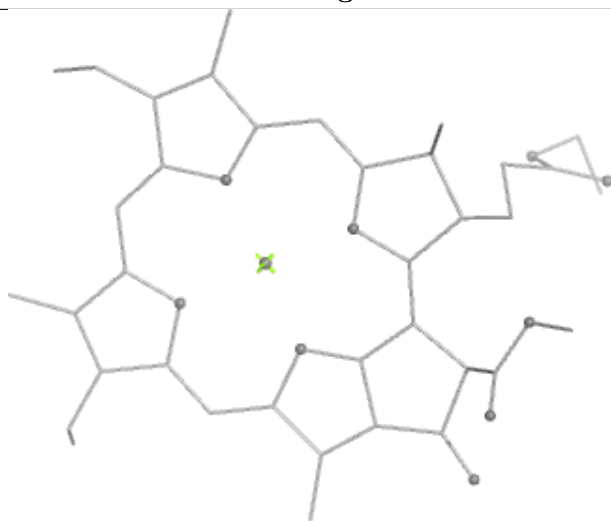
Bond lengths



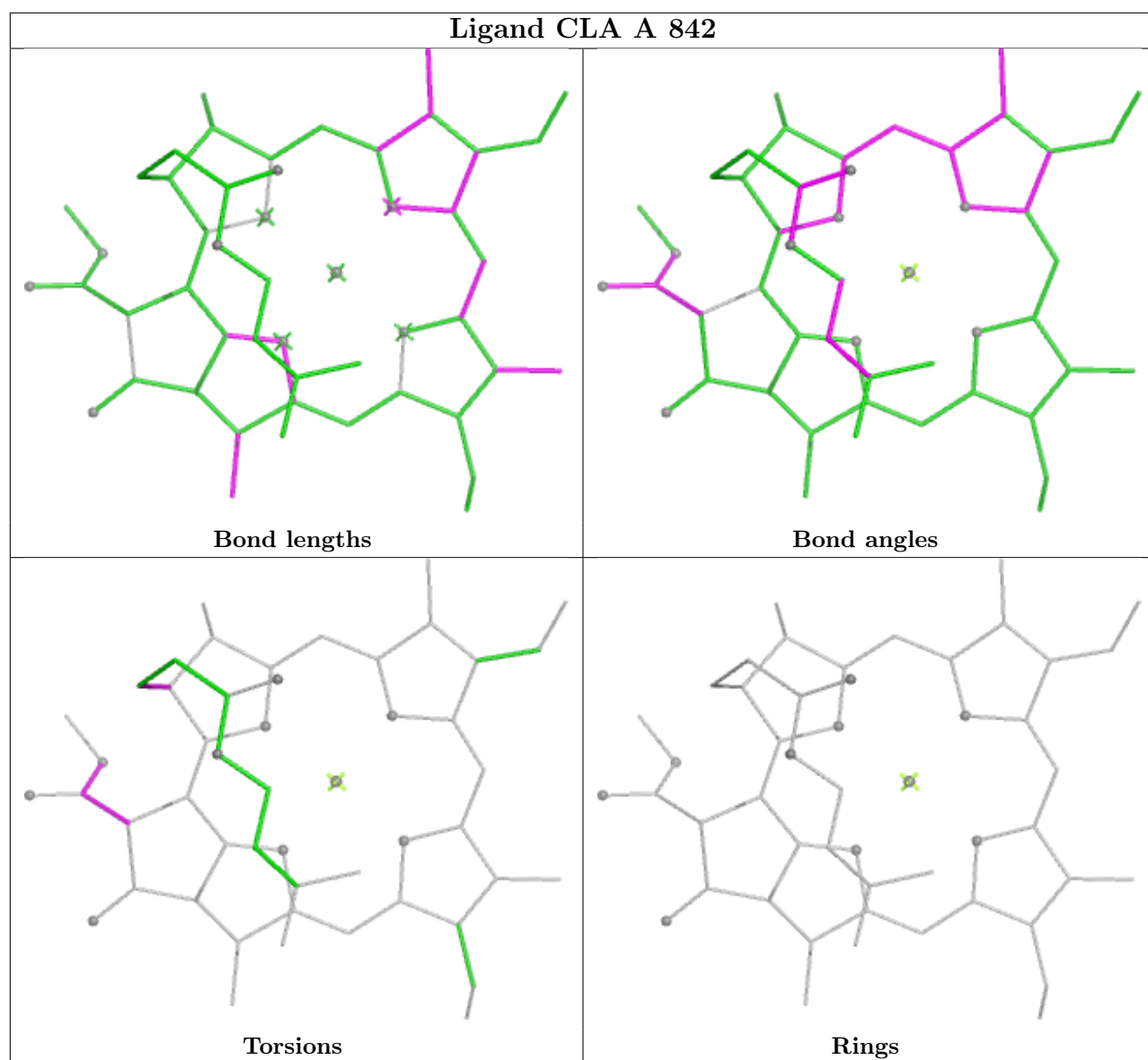
Bond angles



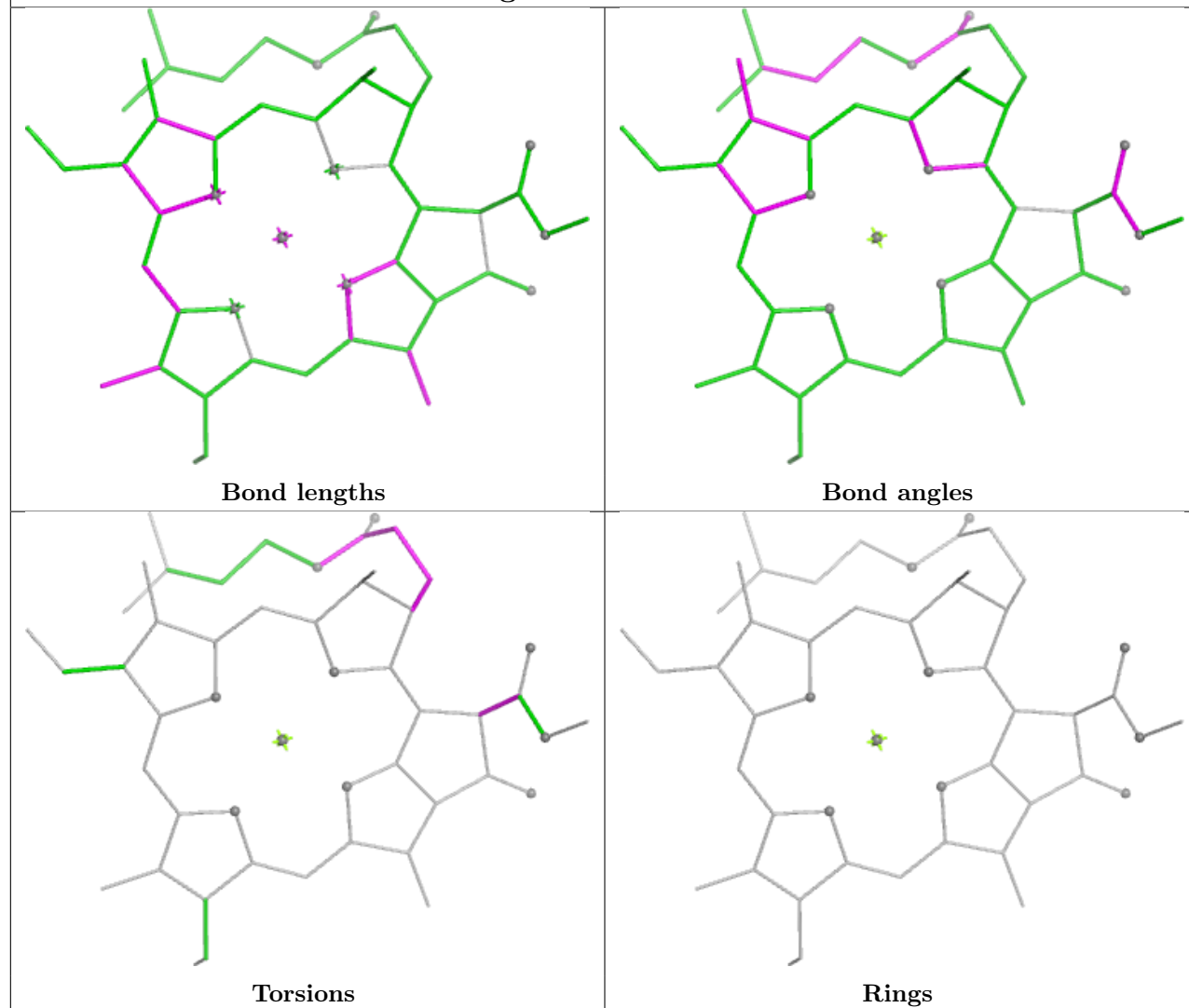
Torsions



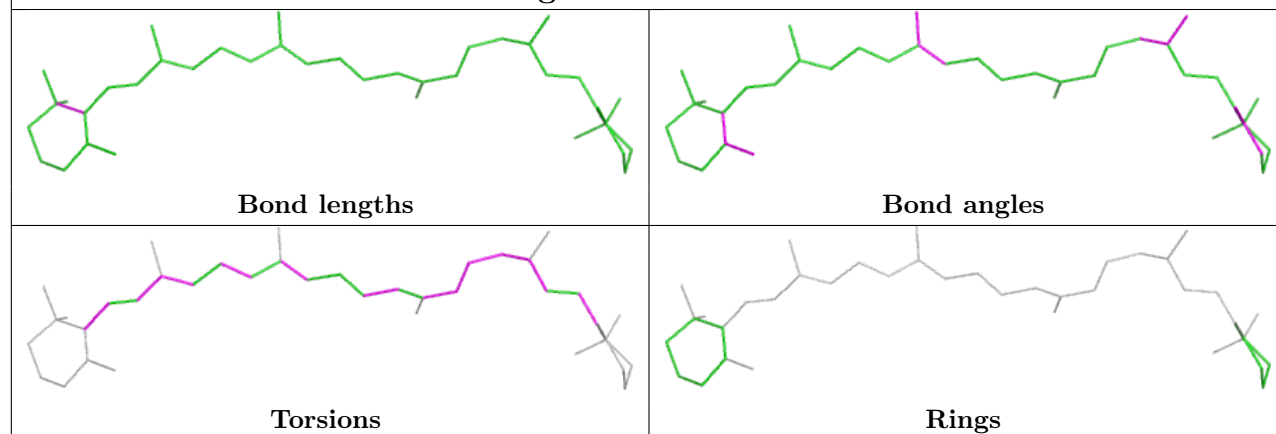
Rings



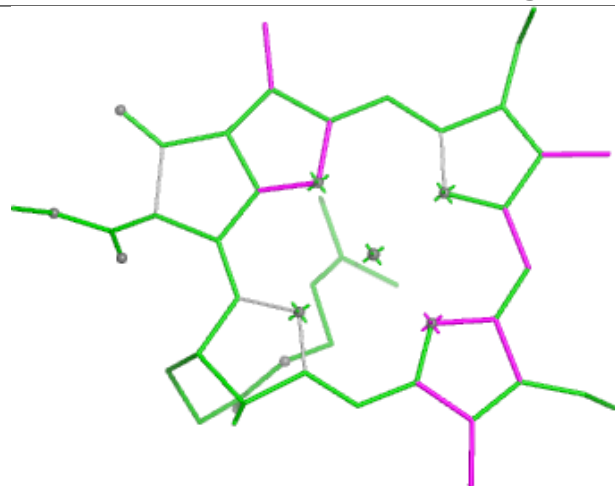
Ligand CLA a 823



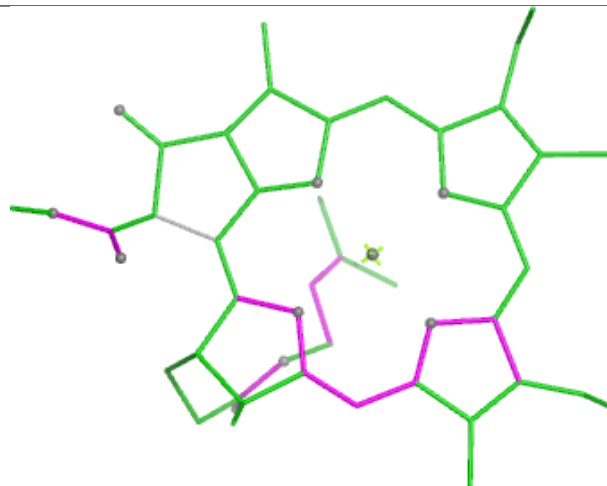
Ligand BCR 1 202



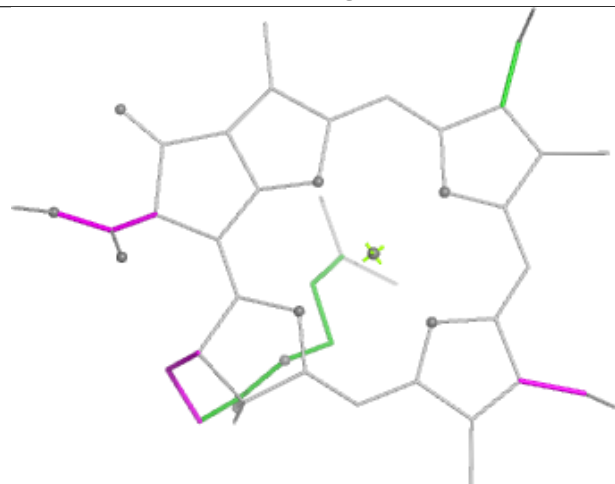
Ligand CLA e 843



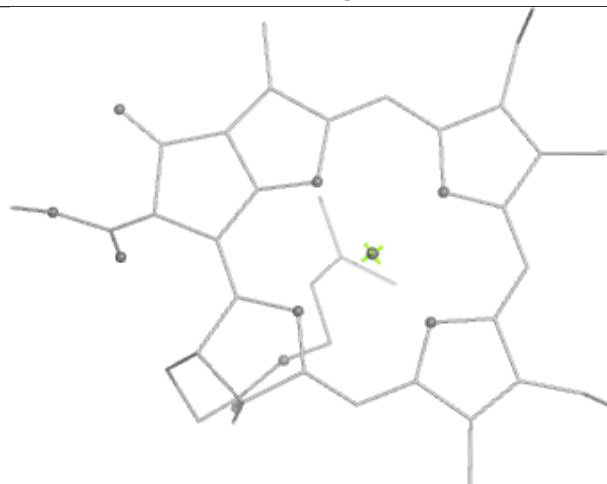
Bond lengths



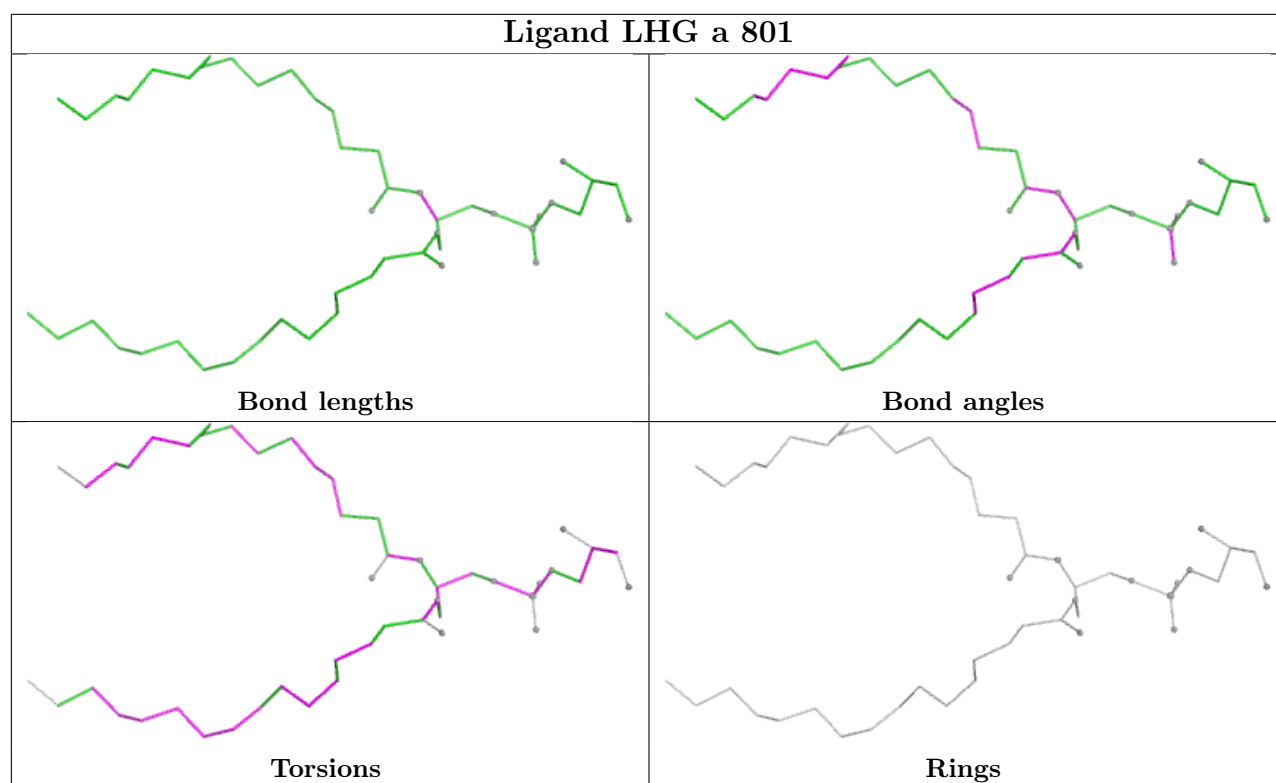
Bond angles



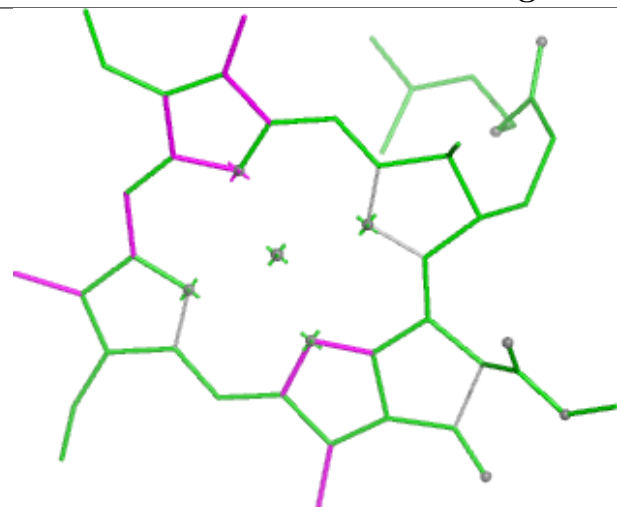
Torsions



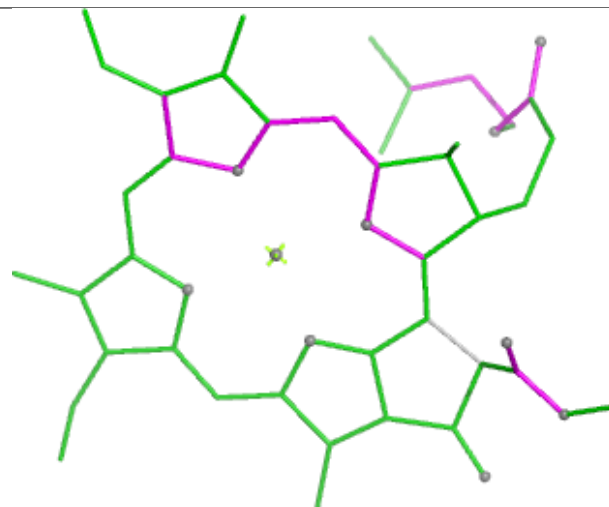
Rings



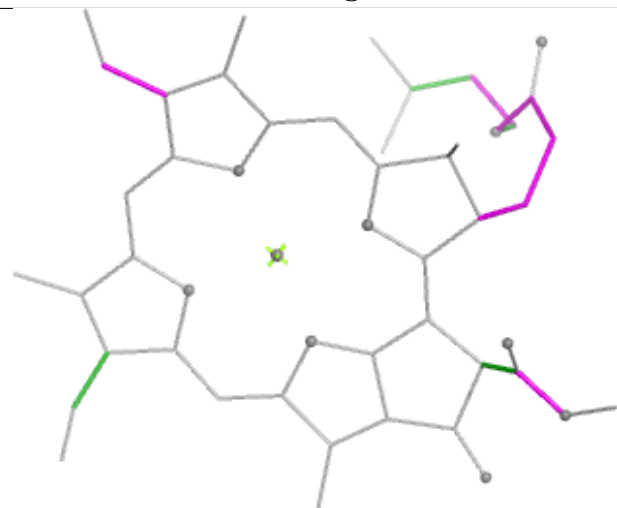
Ligand CLA B 818



Bond lengths



Bond angles

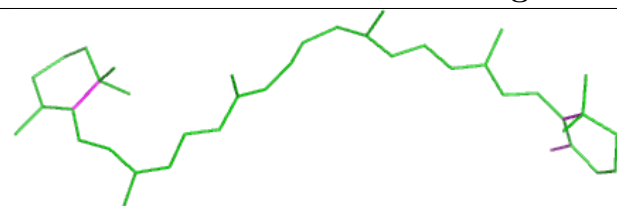


Torsions

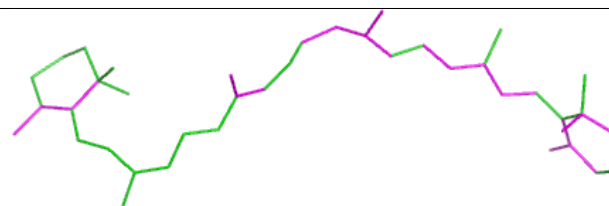


Rings

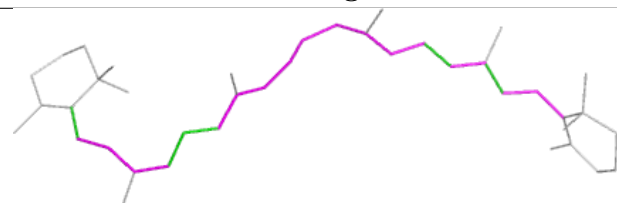
Ligand BCR k 4001



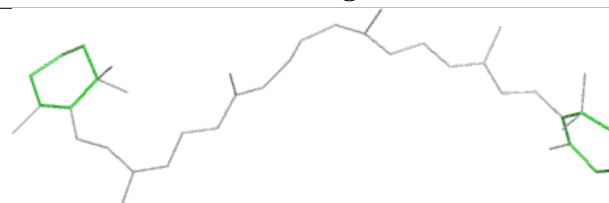
Bond lengths



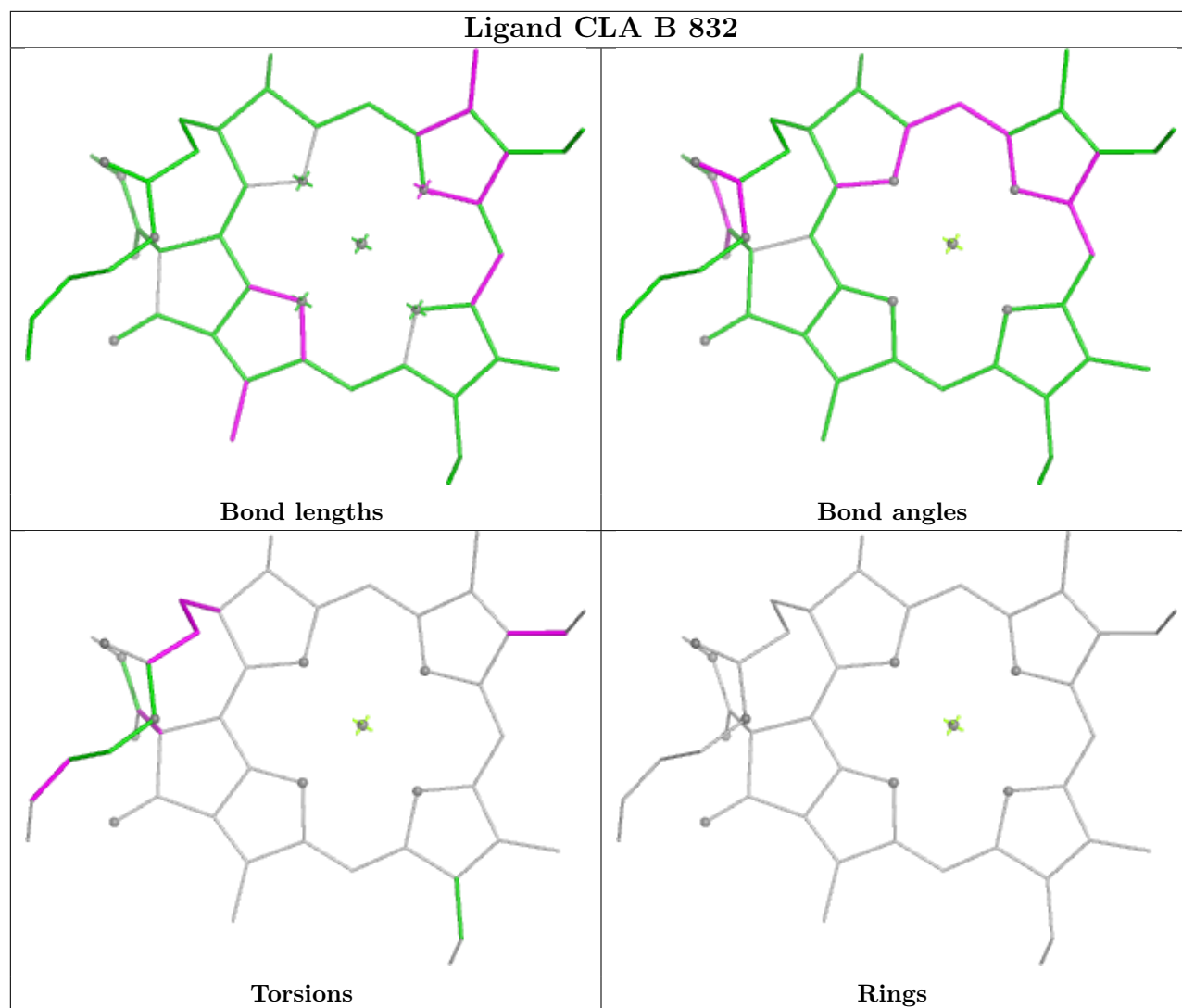
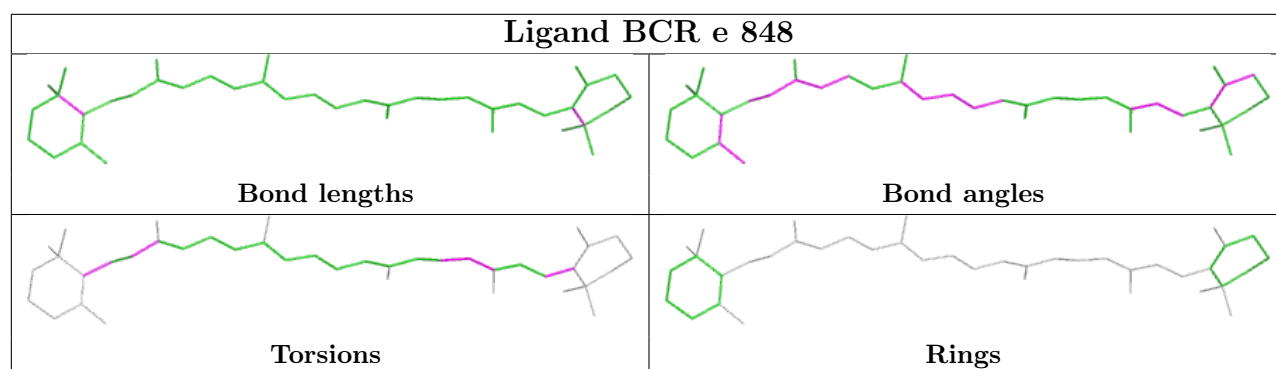
Bond angles

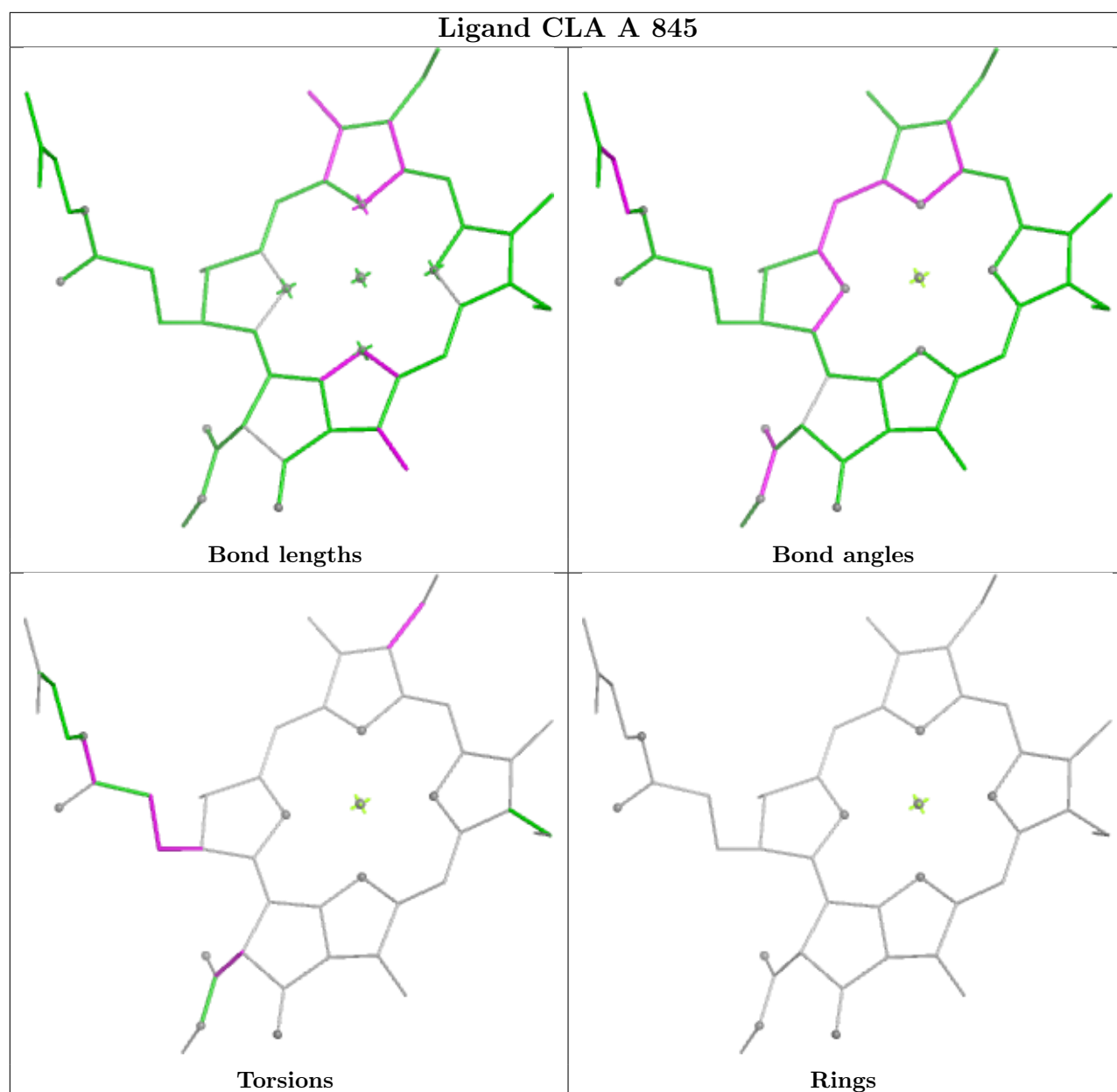


Torsions

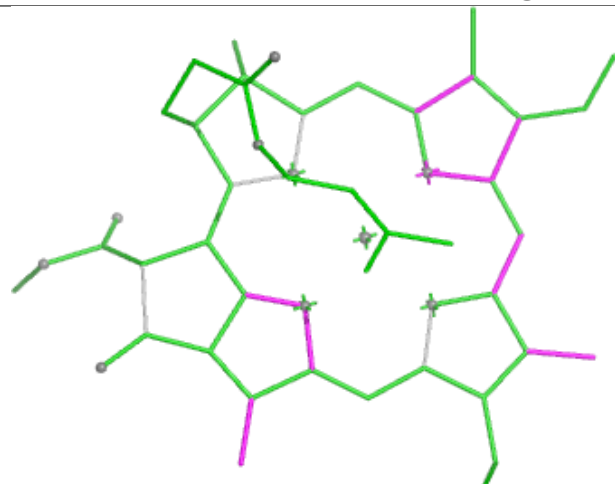


Rings

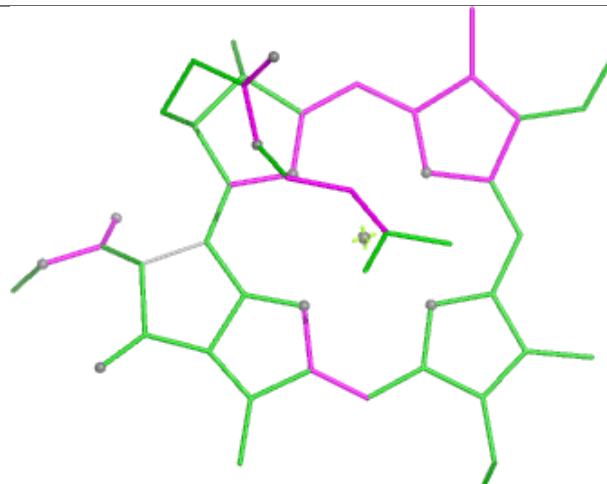




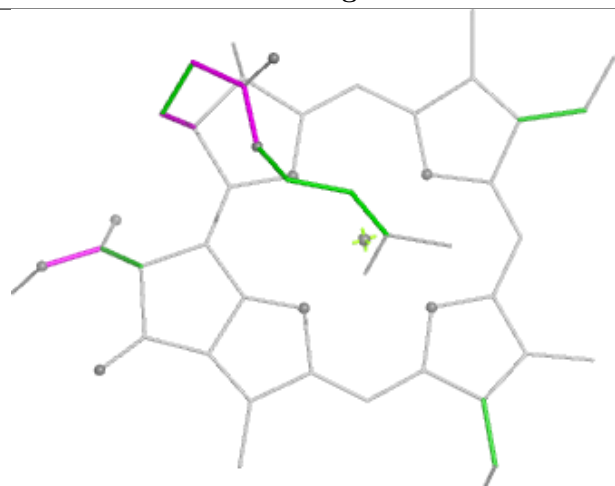
Ligand CLA L 202



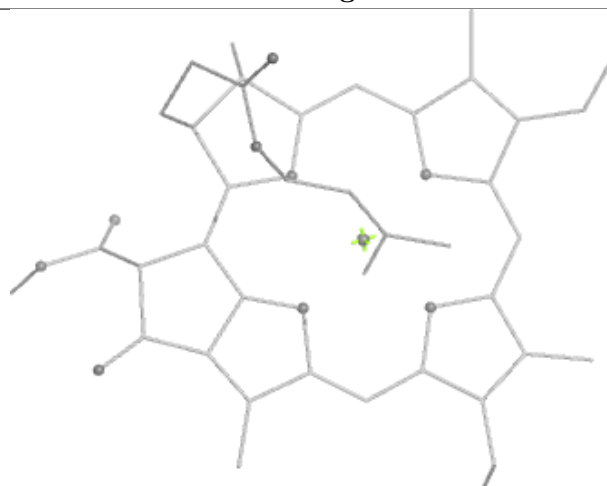
Bond lengths



Bond angles

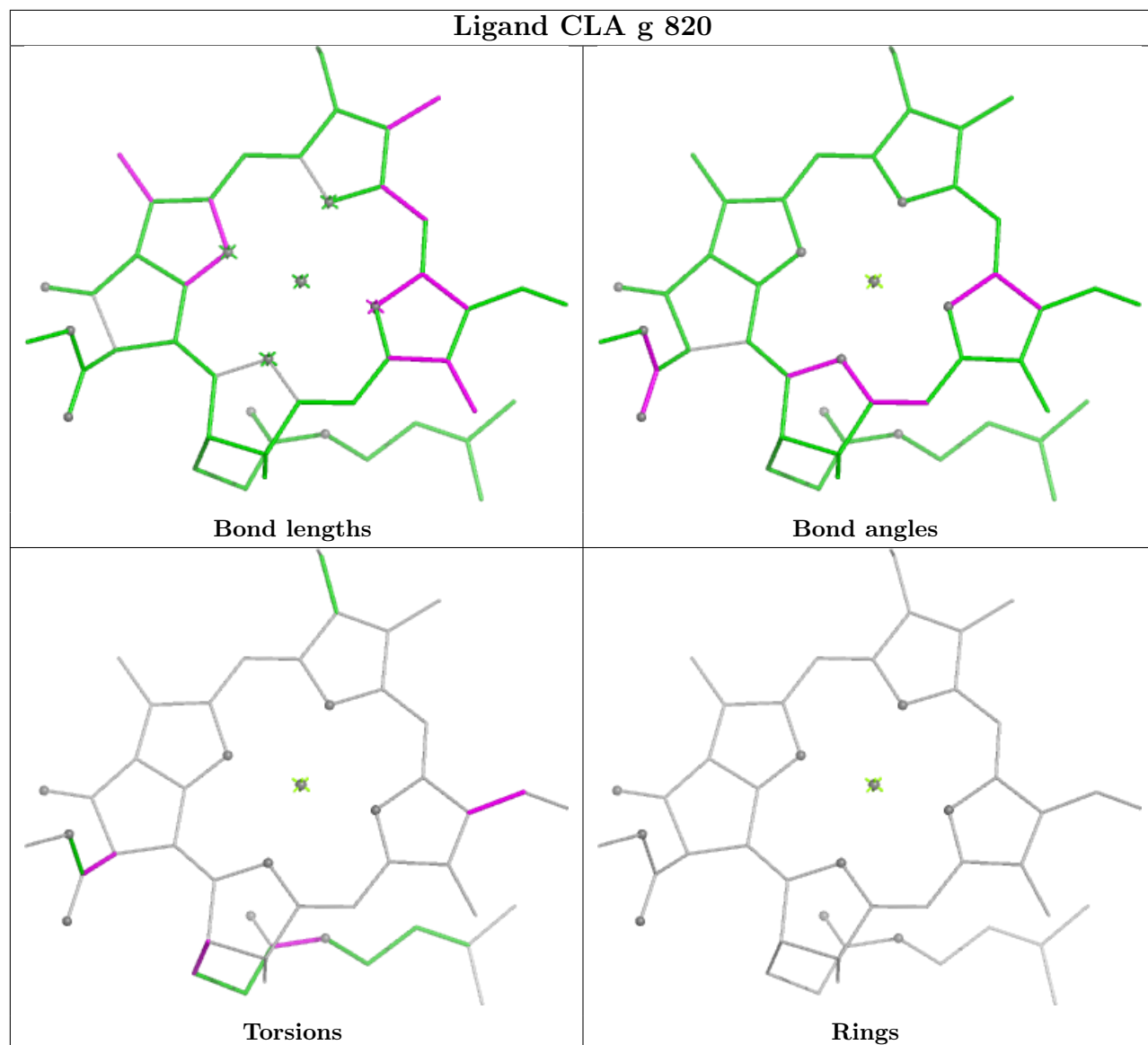


Torsions

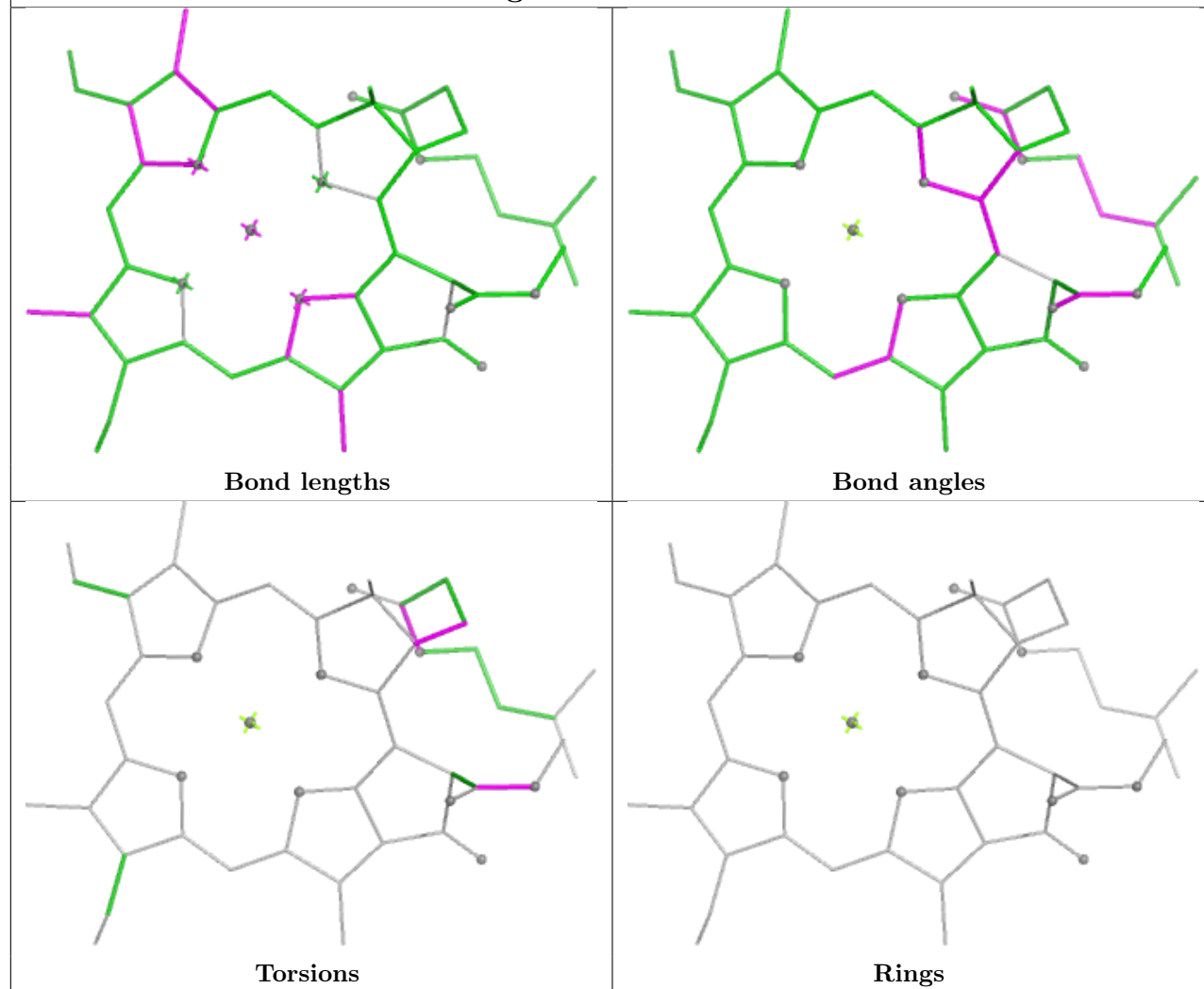


Rings

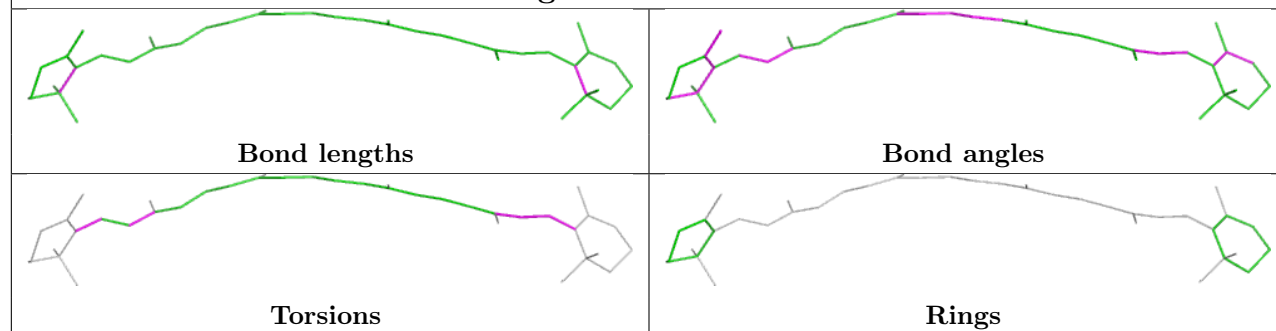
Ligand CLA g 820



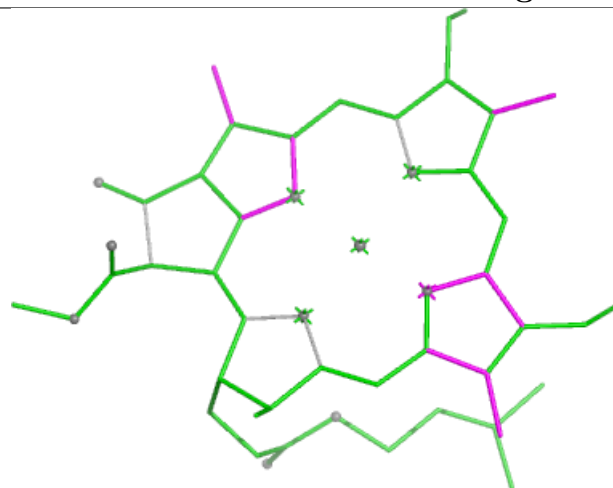
Ligand CLA e 834



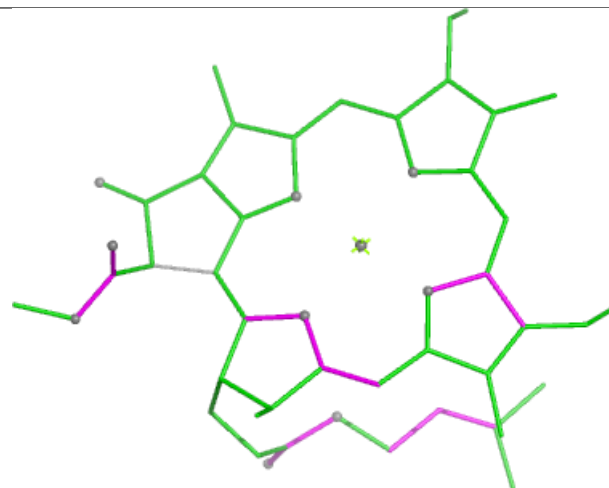
Ligand BCR f 201



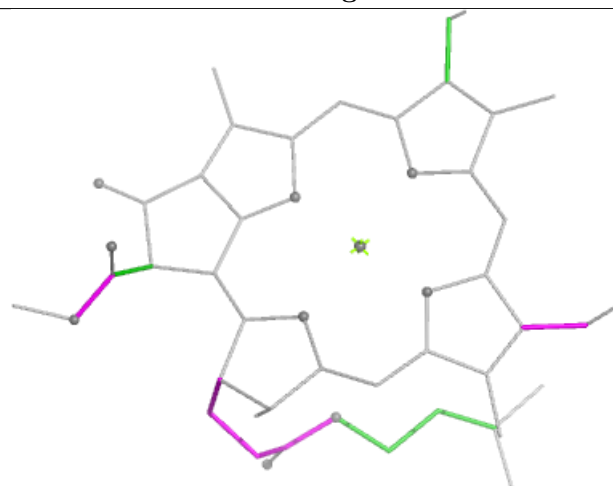
Ligand CLA A 822



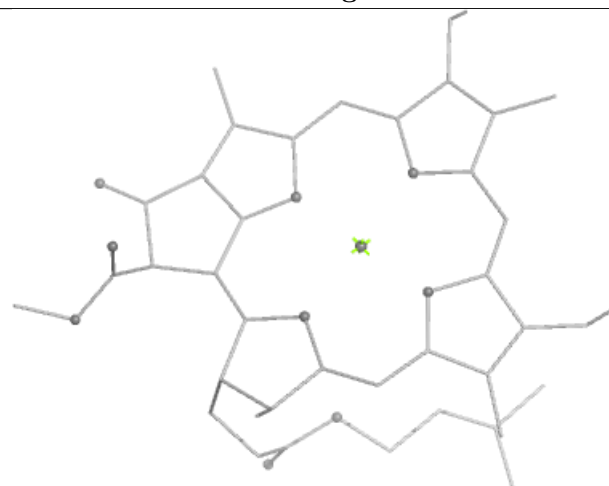
Bond lengths



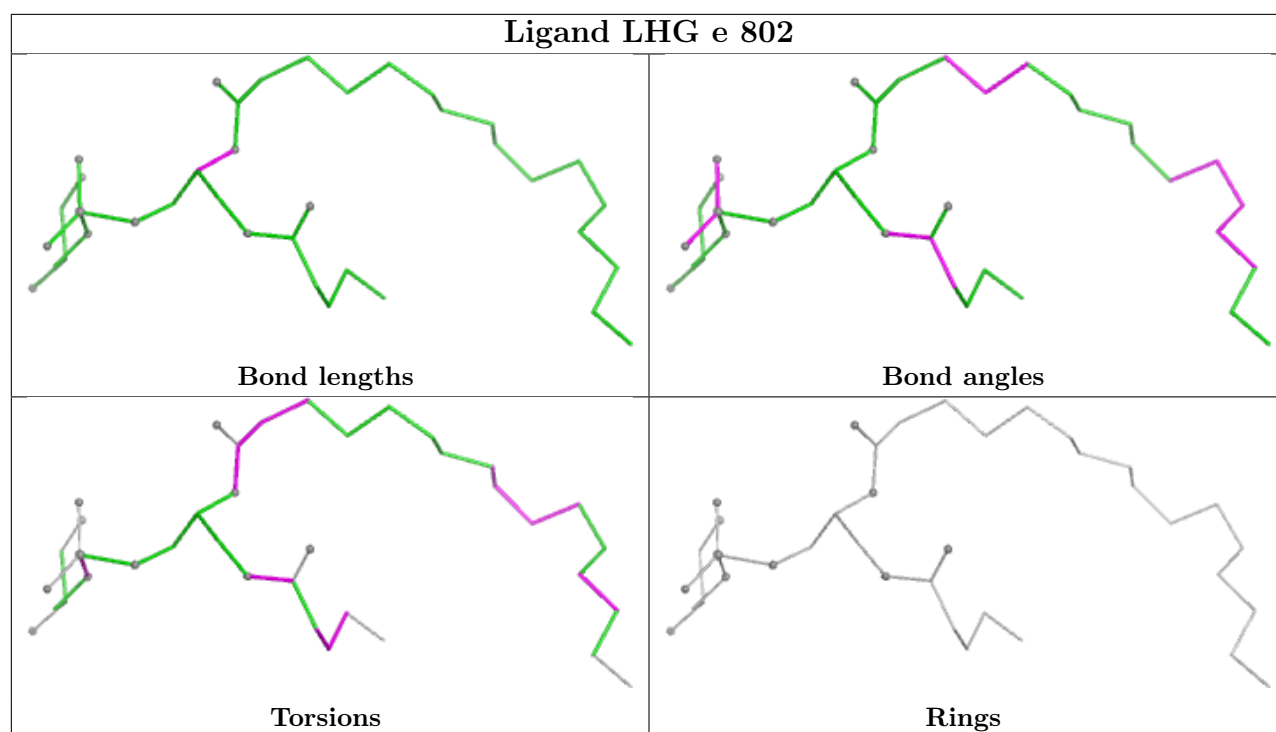
Bond angles



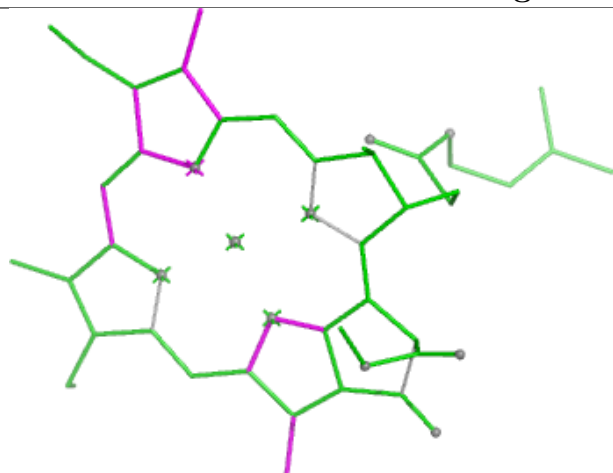
Torsions



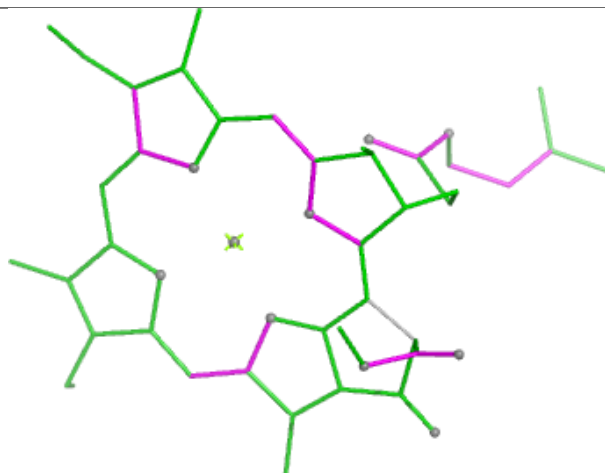
Rings



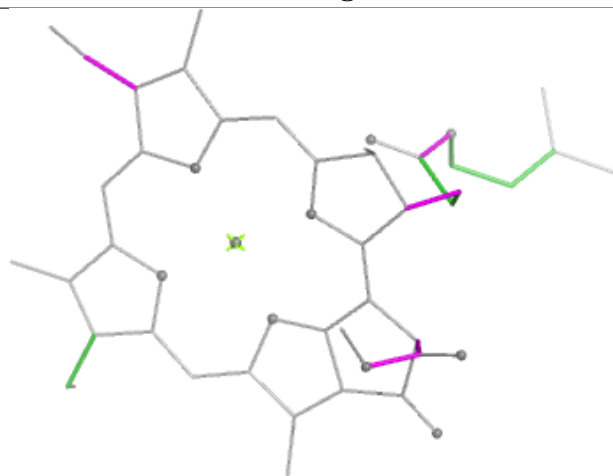
Ligand CLA A 837



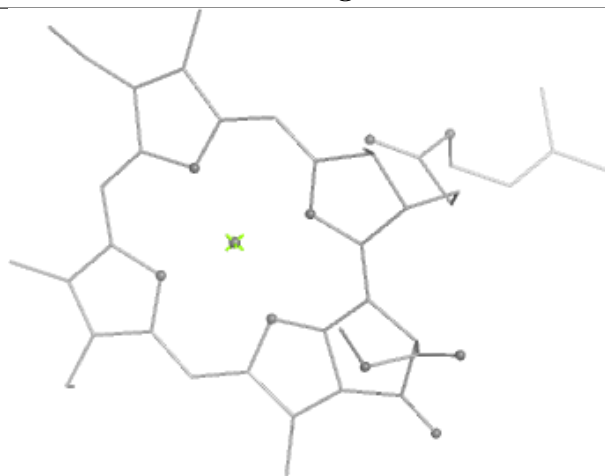
Bond lengths



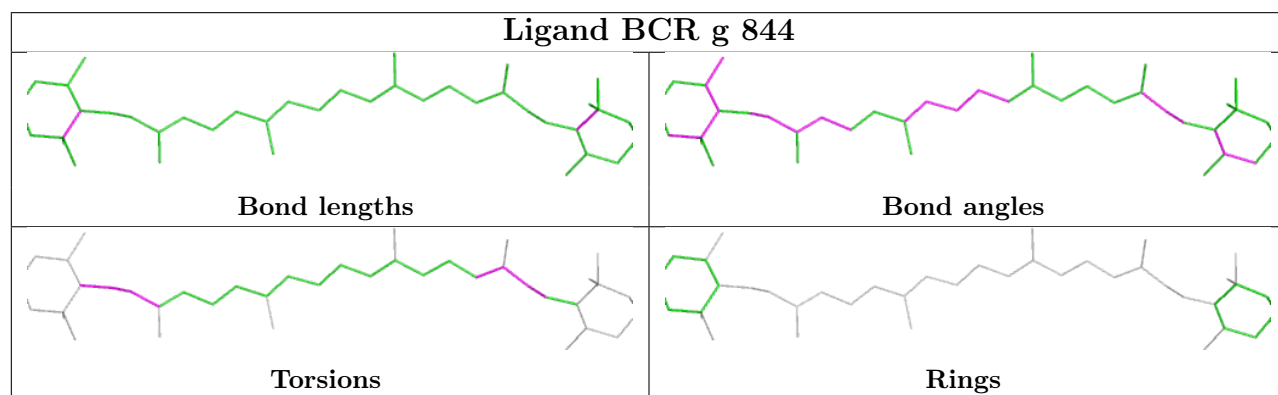
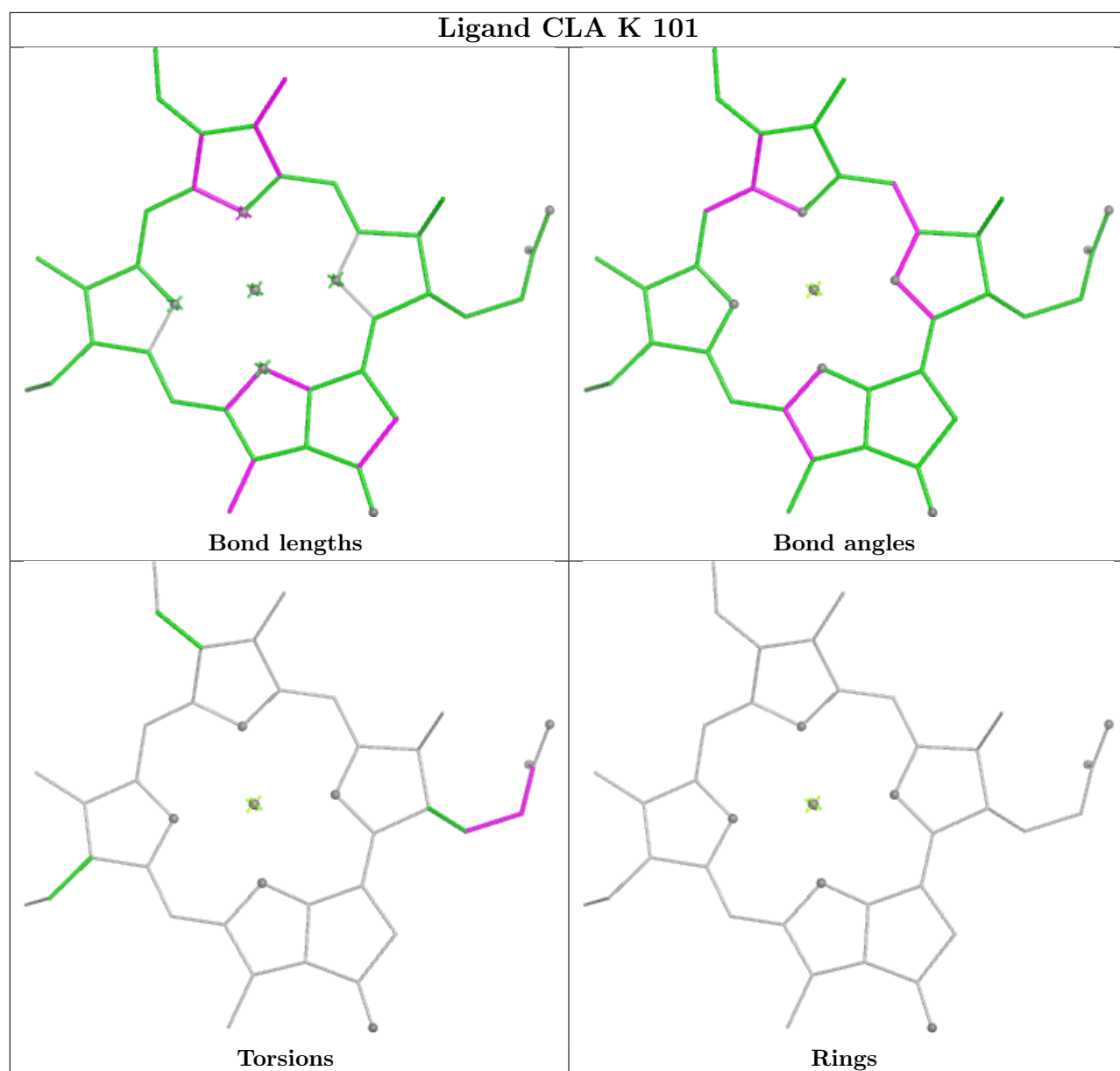
Bond angles



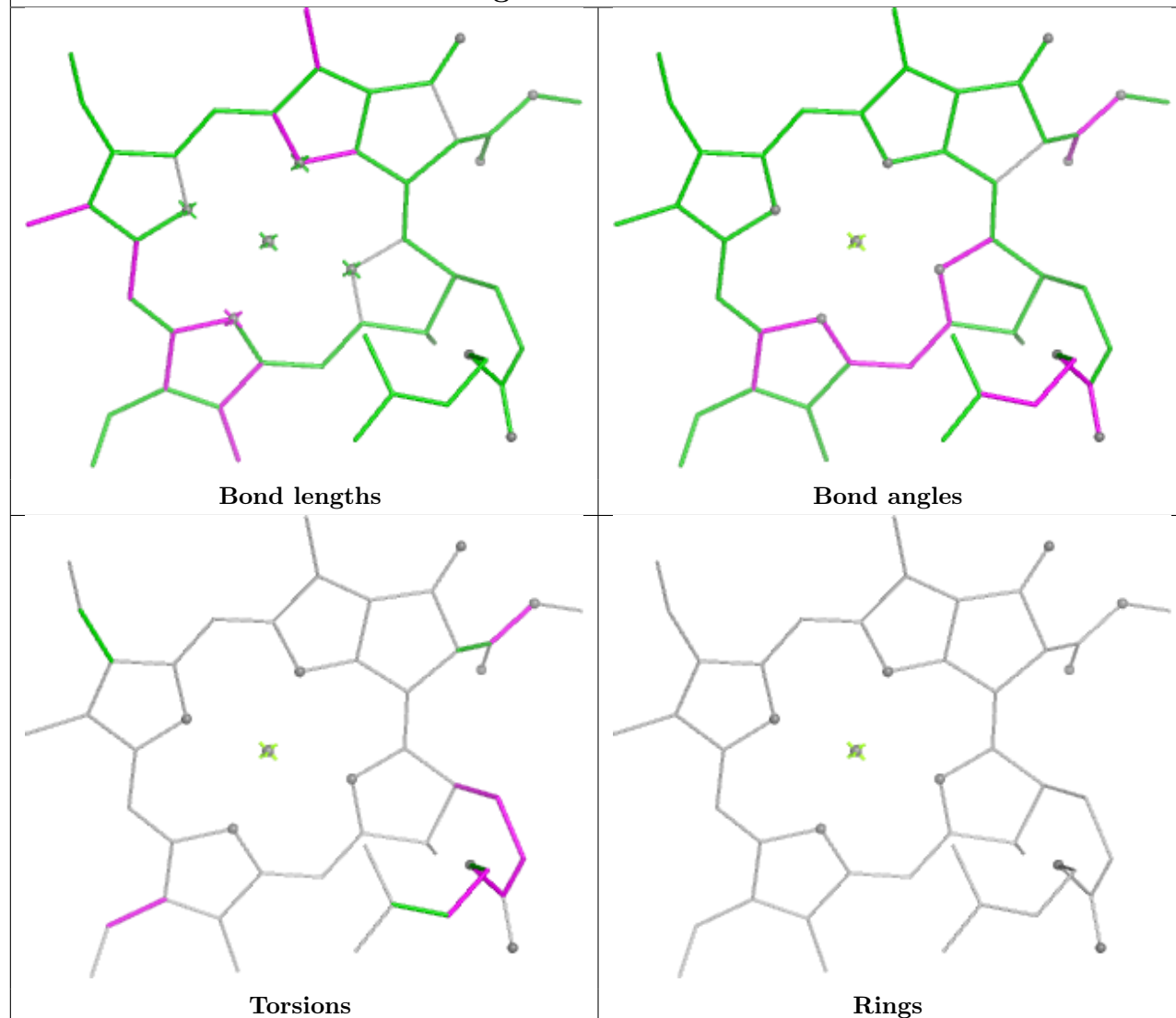
Torsions



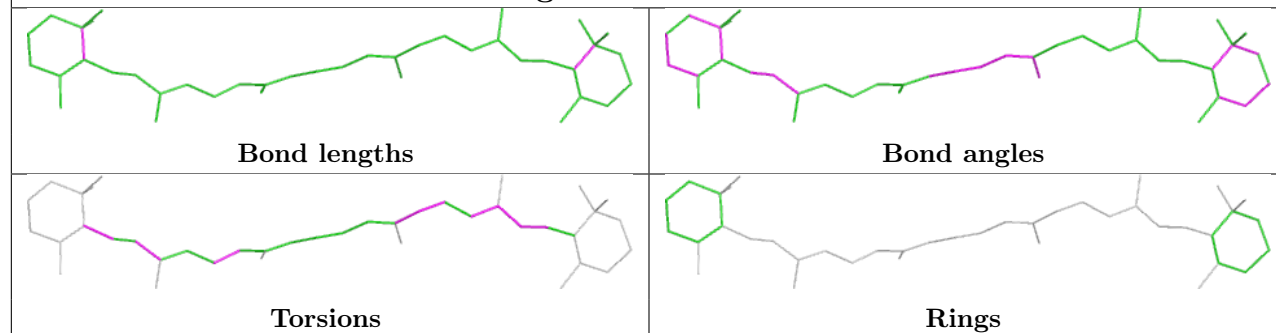
Rings

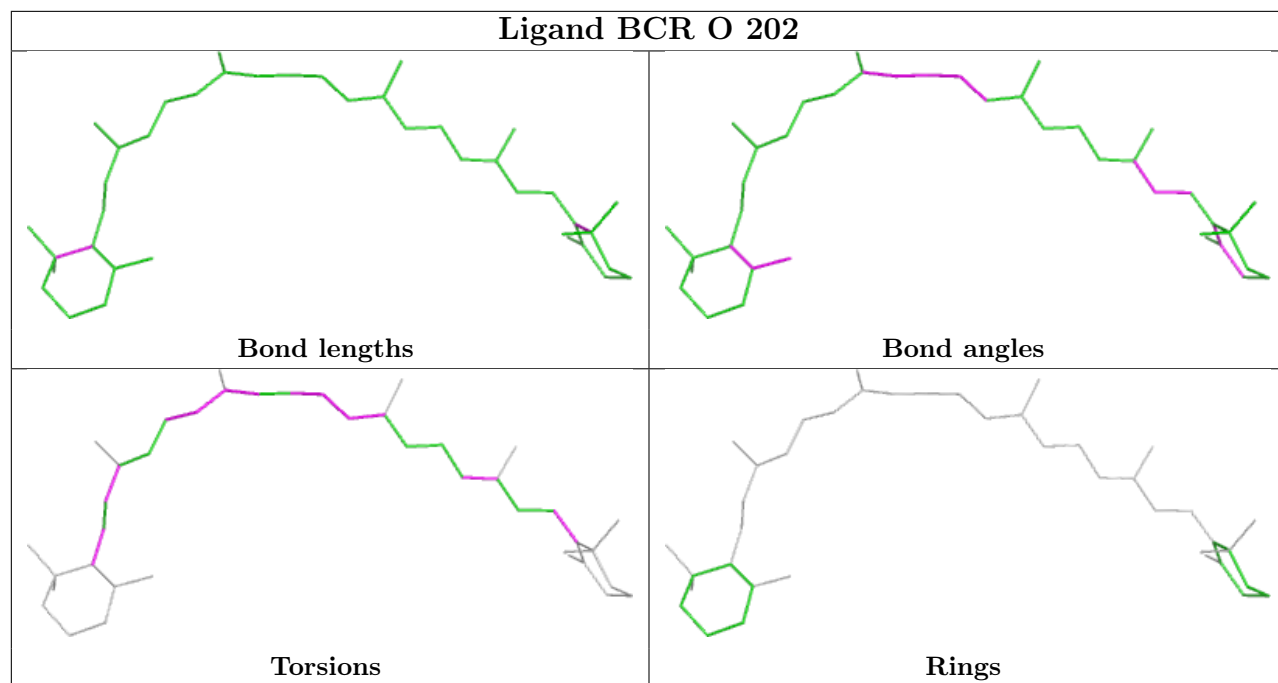


Ligand CLA b 817

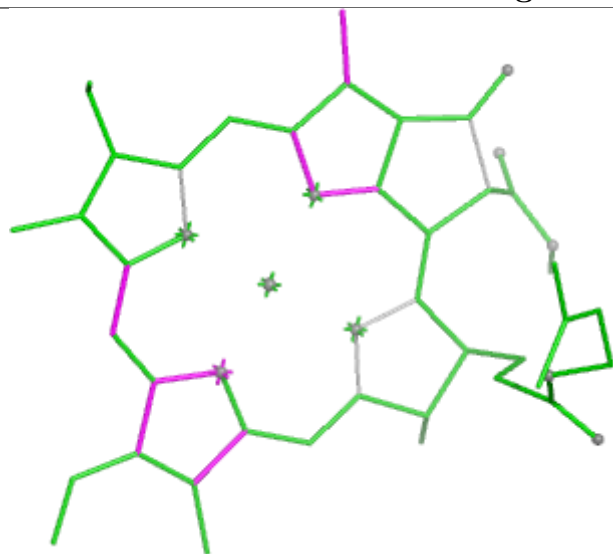


Ligand BCR s 204

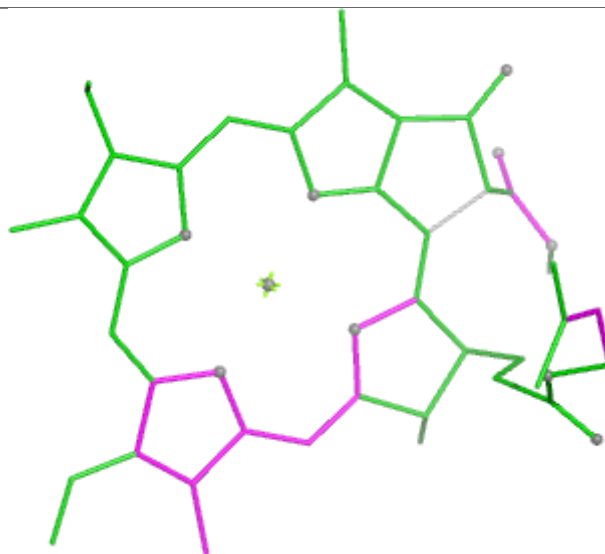




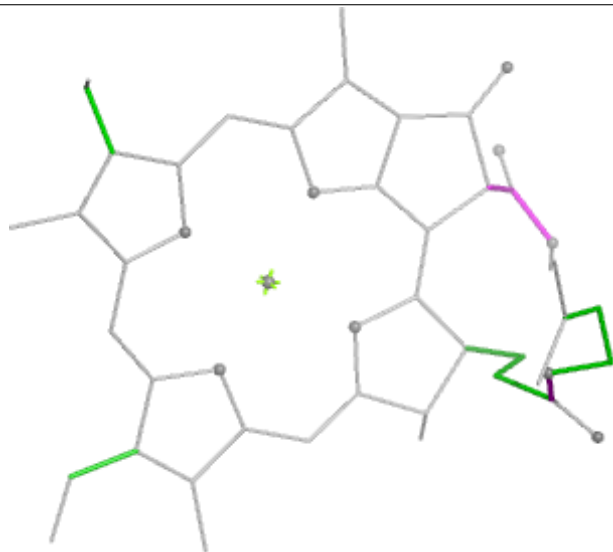
Ligand CLA E 833



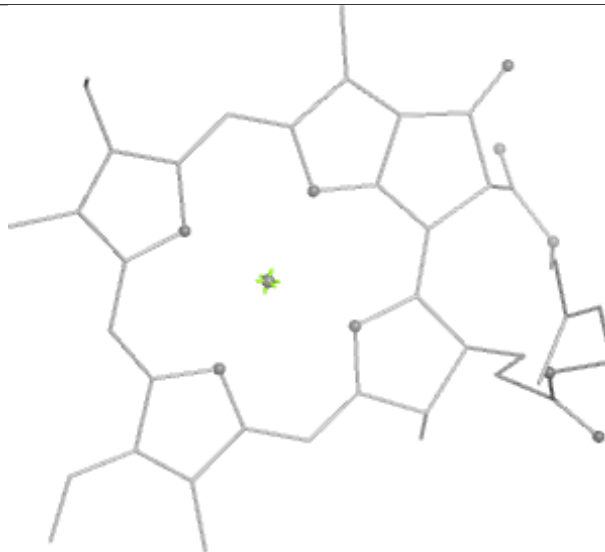
Bond lengths



Bond angles

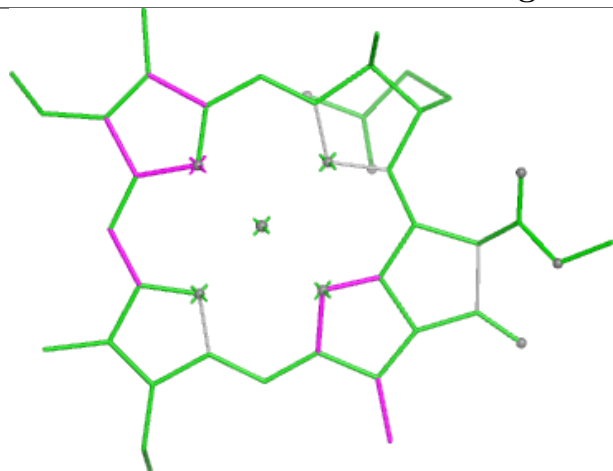


Torsions

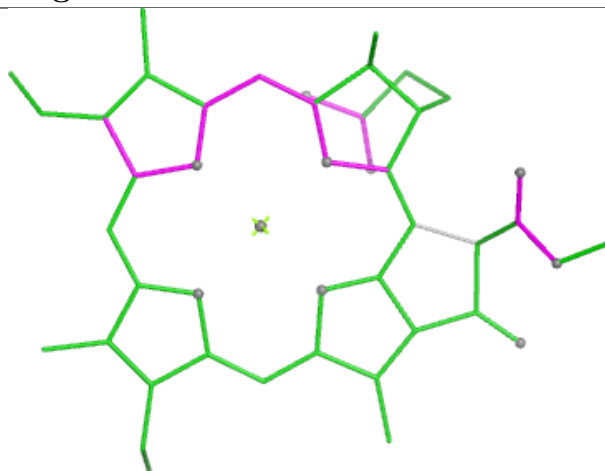


Rings

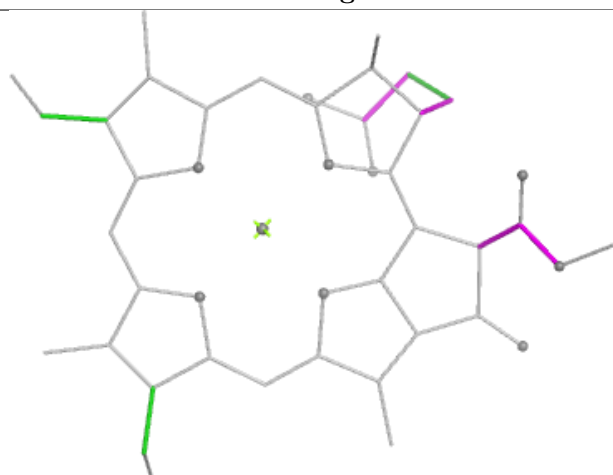
Ligand CLA g 837



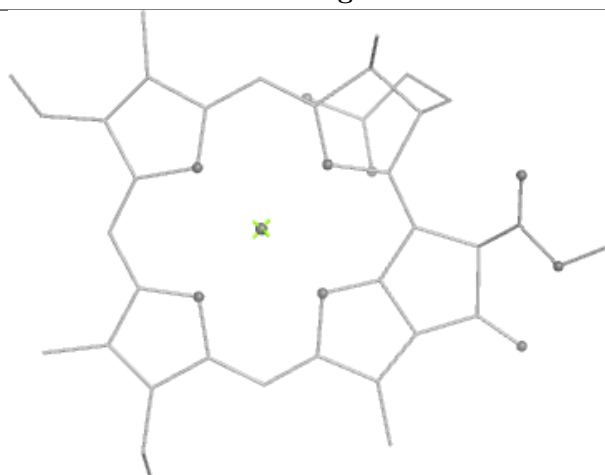
Bond lengths



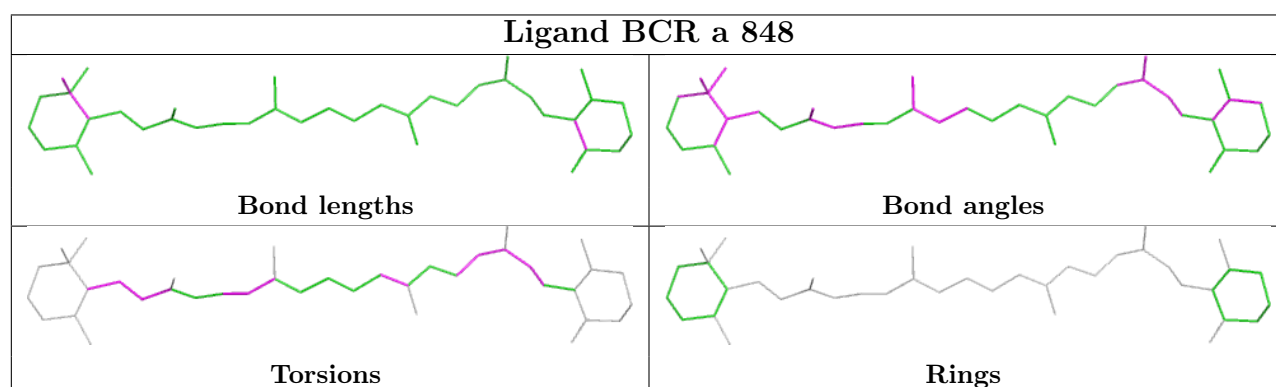
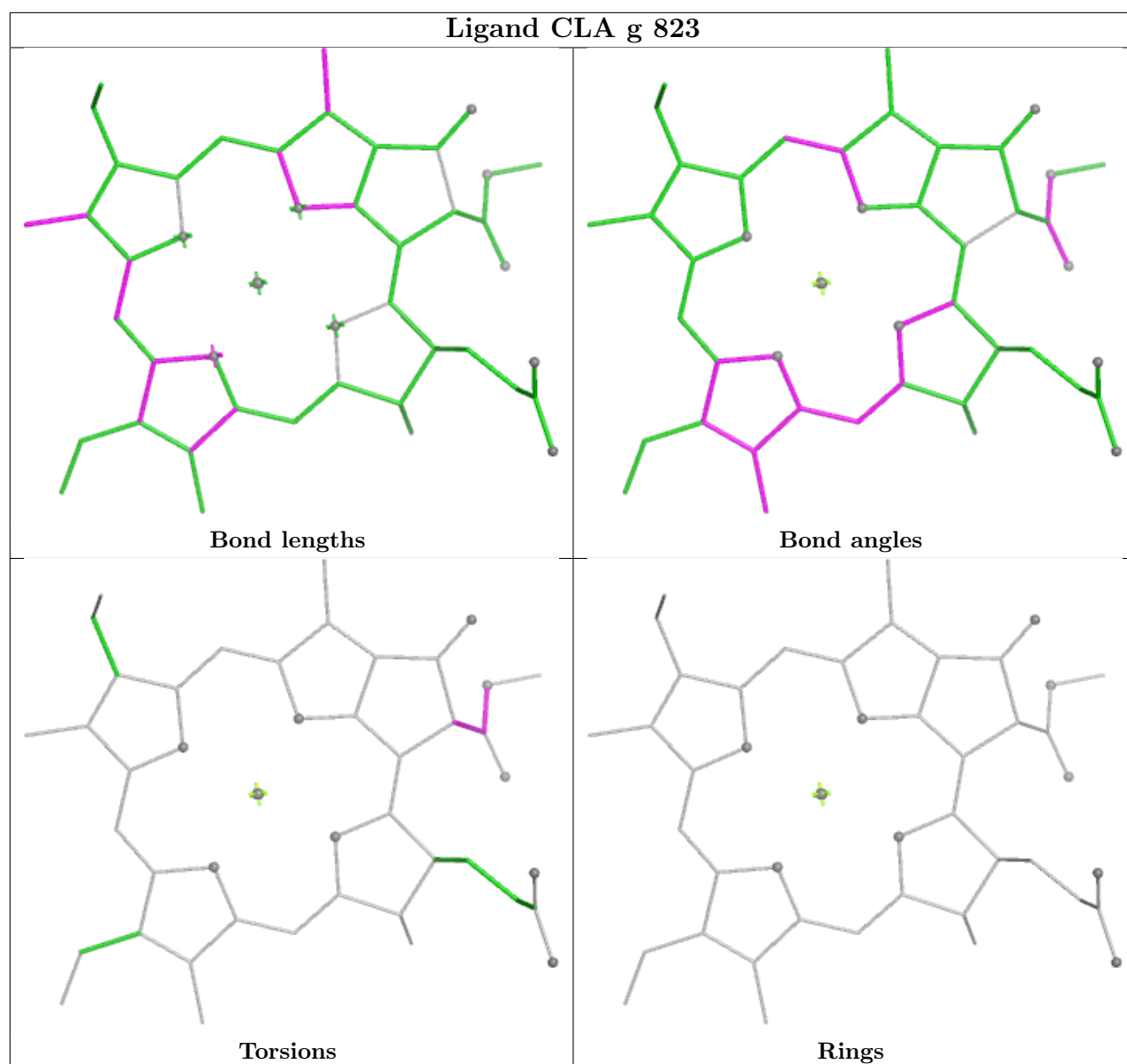
Bond angles



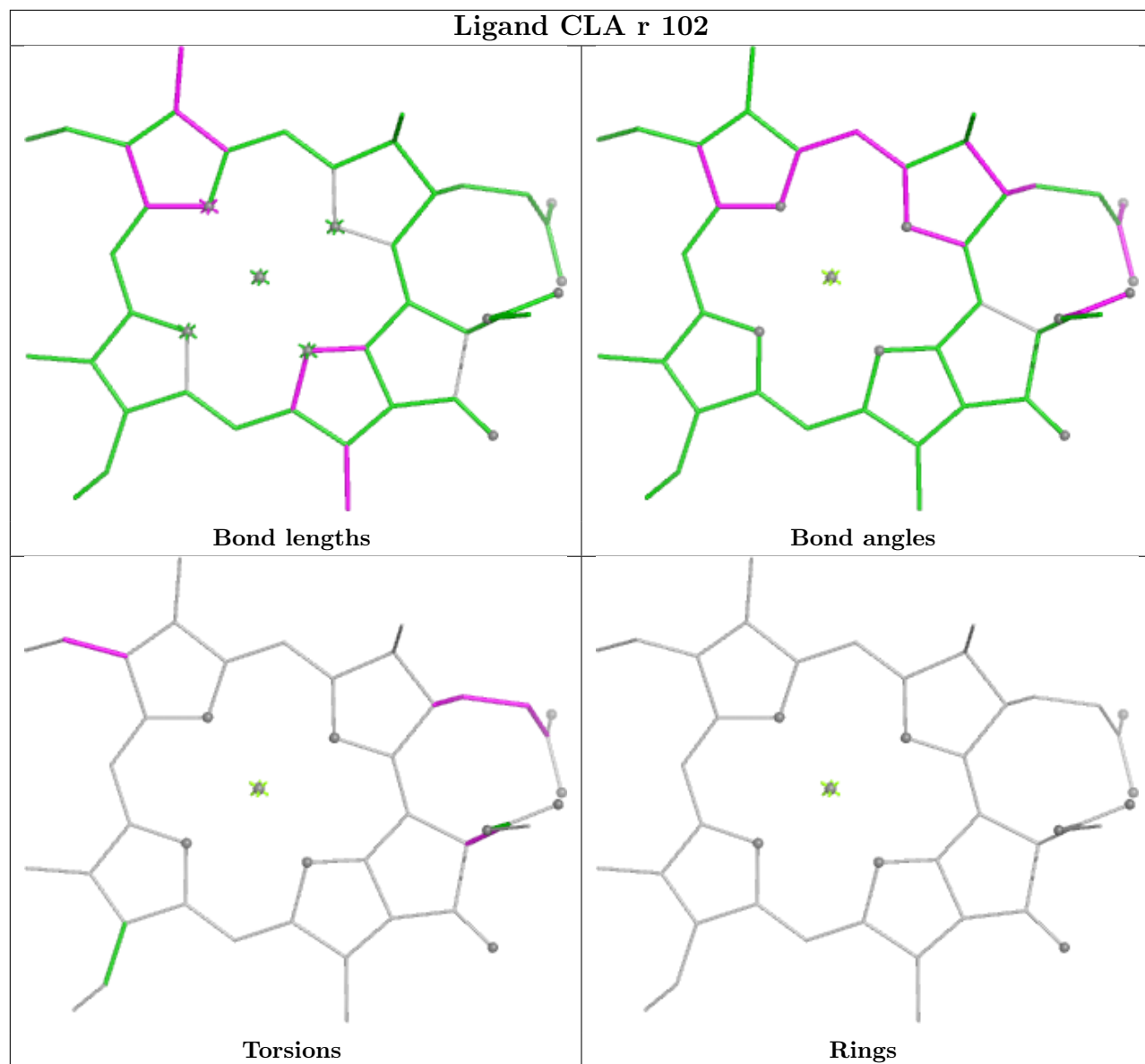
Torsions

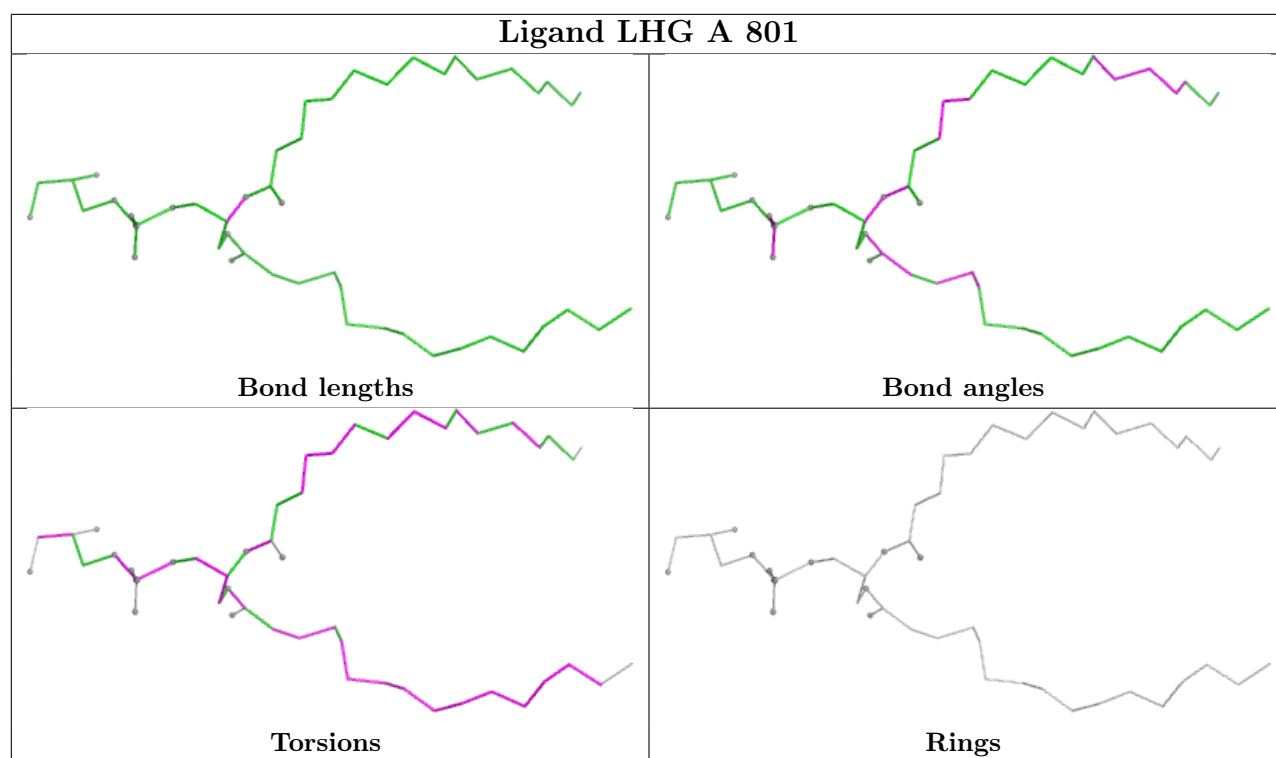


Rings

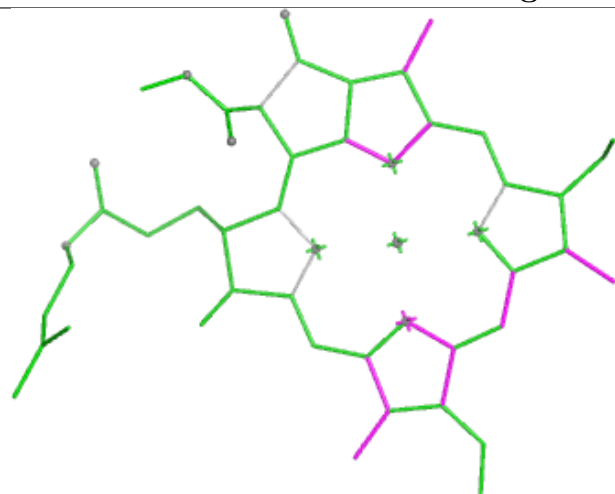


Ligand CLA r 102

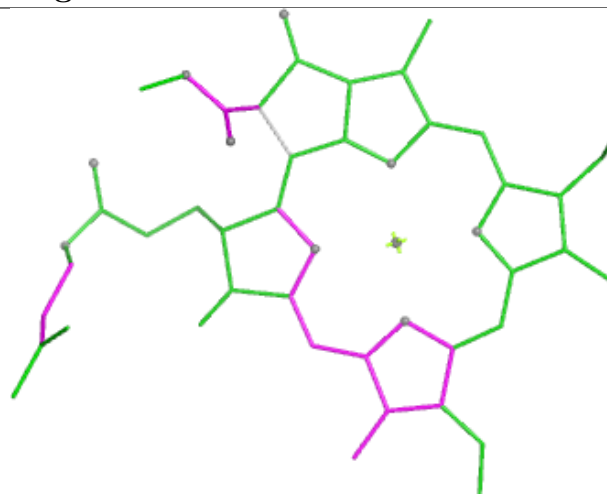




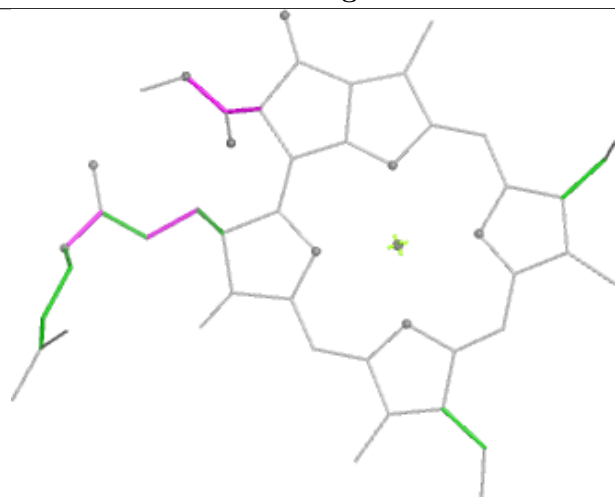
Ligand CLA g 826



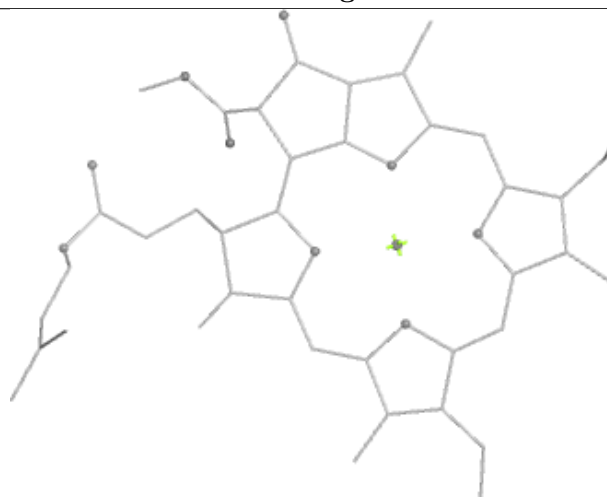
Bond lengths



Bond angles

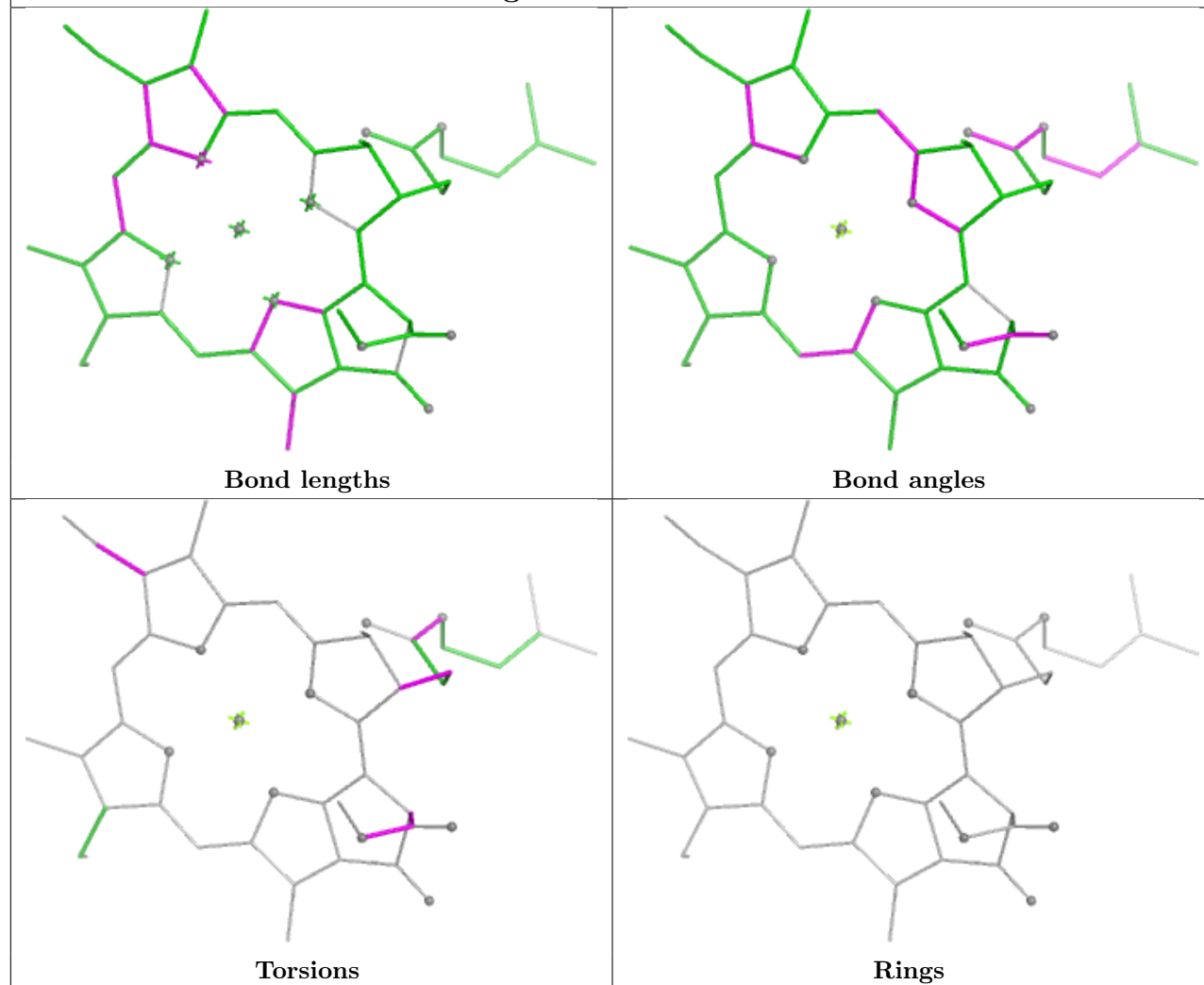


Torsions

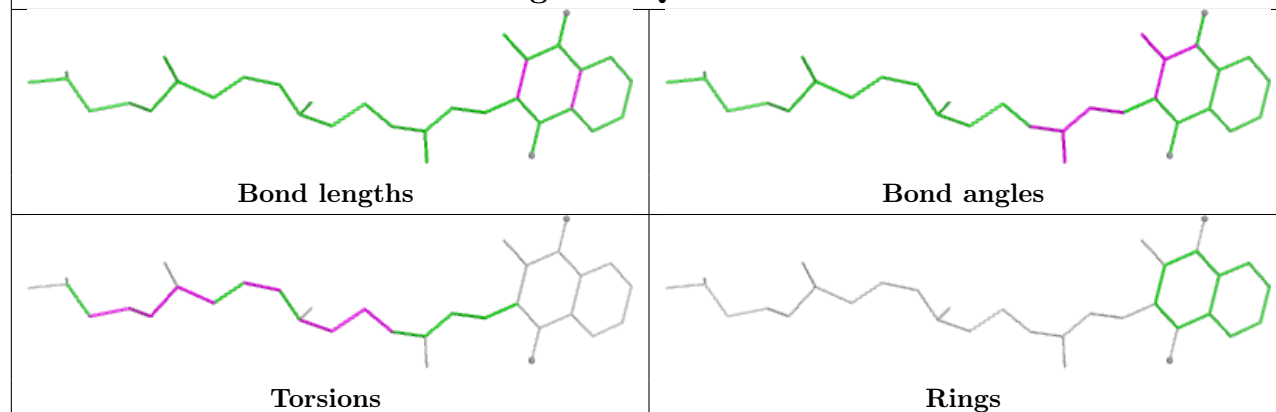


Rings

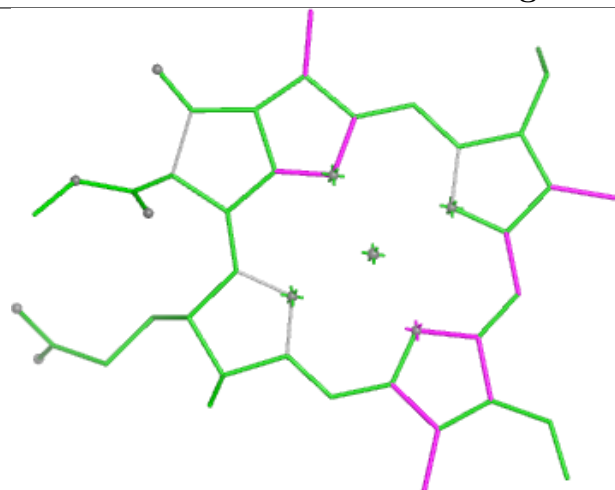
Ligand CLA E 838



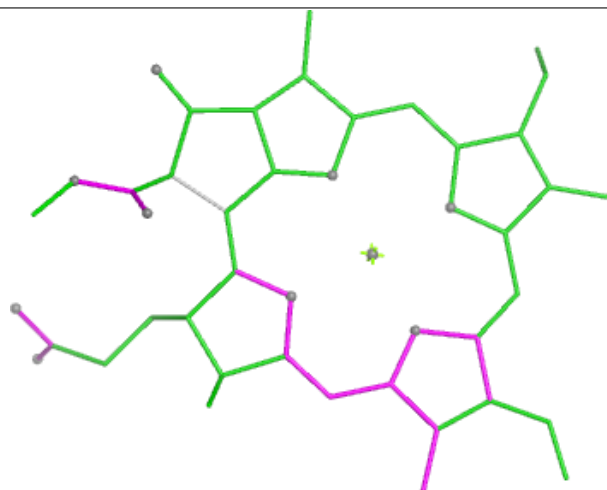
Ligand PQN B 842



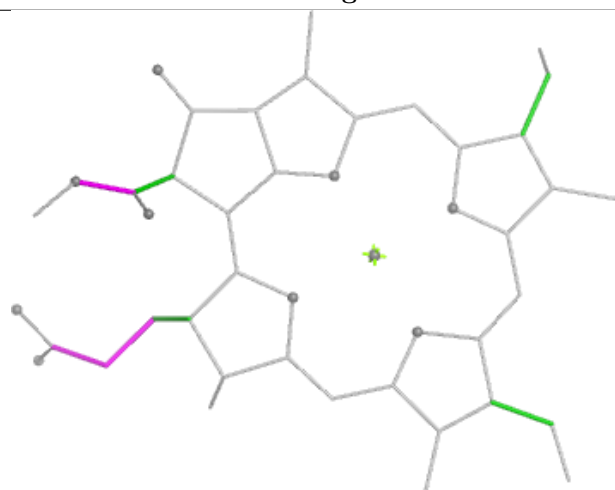
Ligand CLA S 203



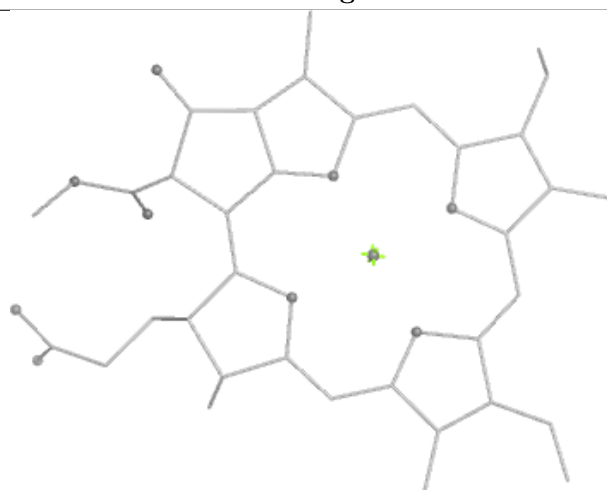
Bond lengths



Bond angles

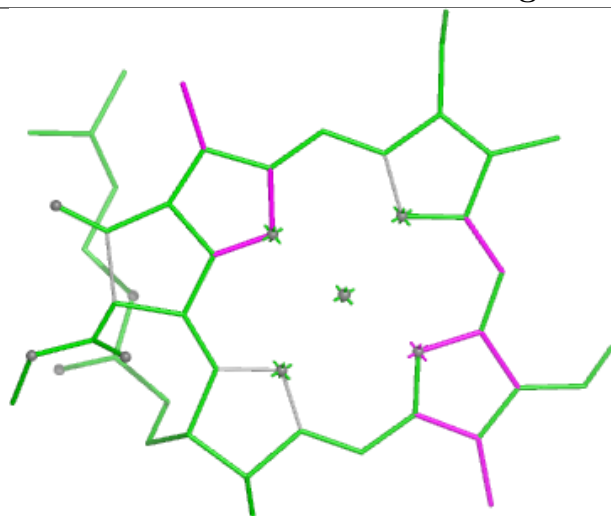


Torsions

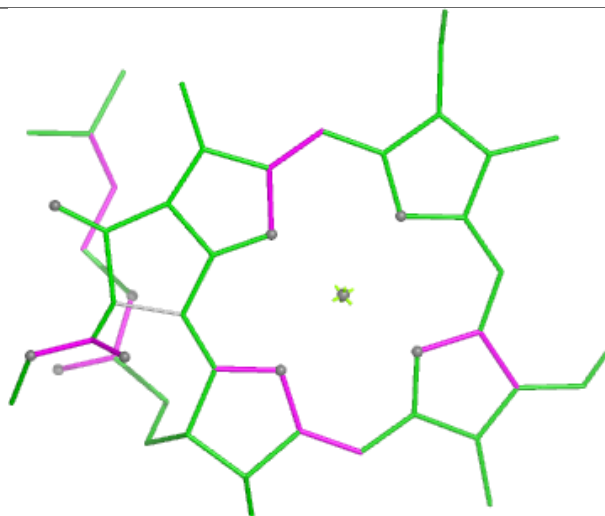


Rings

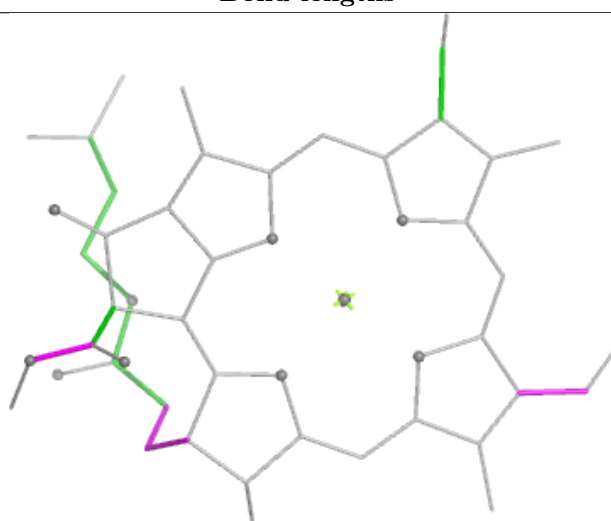
Ligand CLA e 831



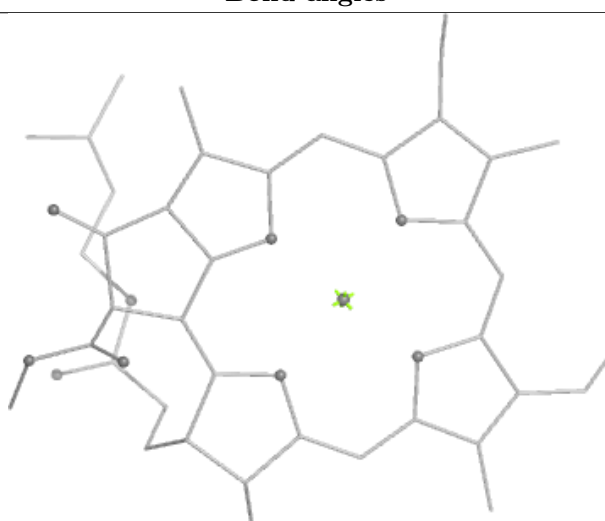
Bond lengths



Bond angles

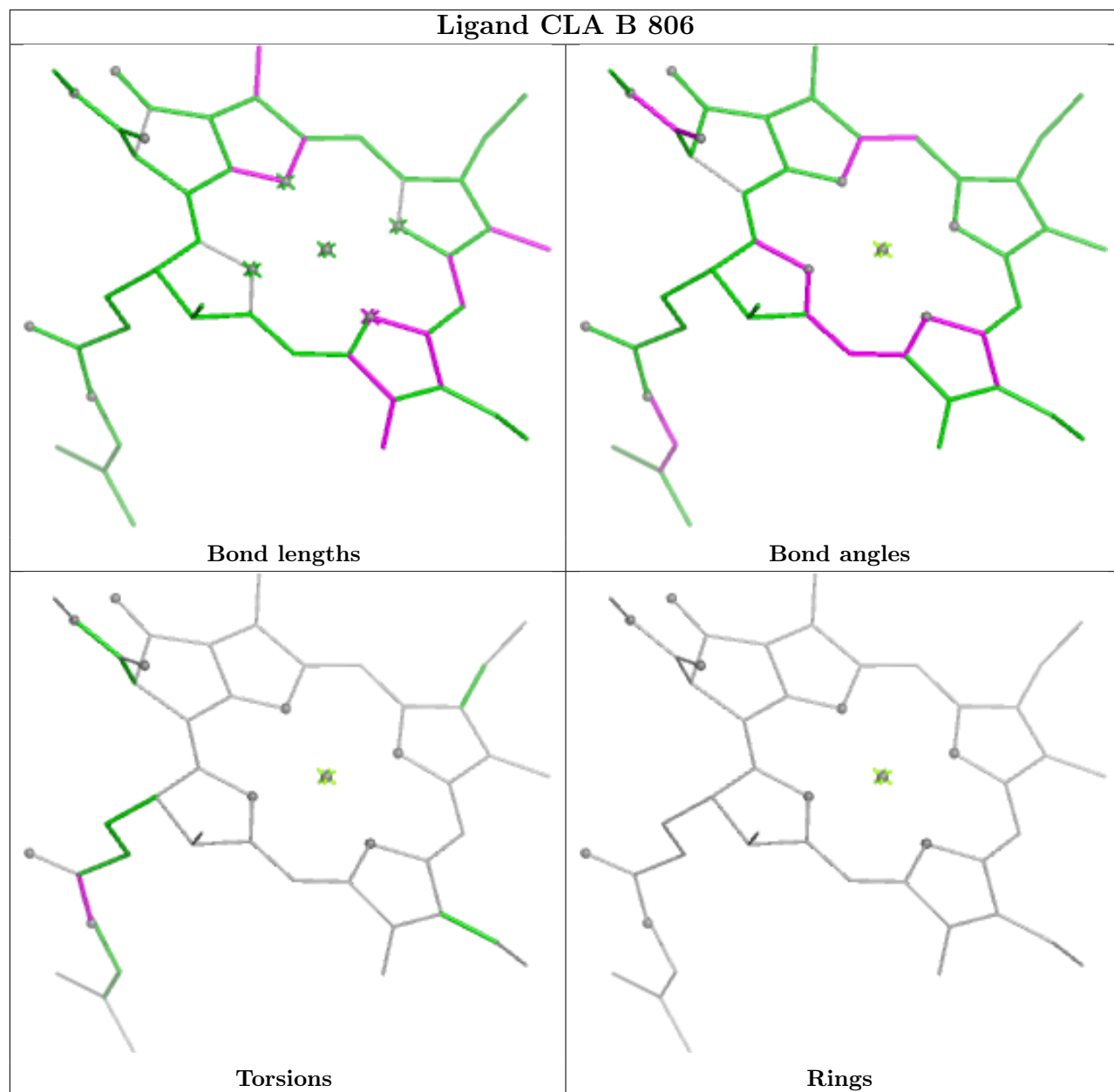


Torsions

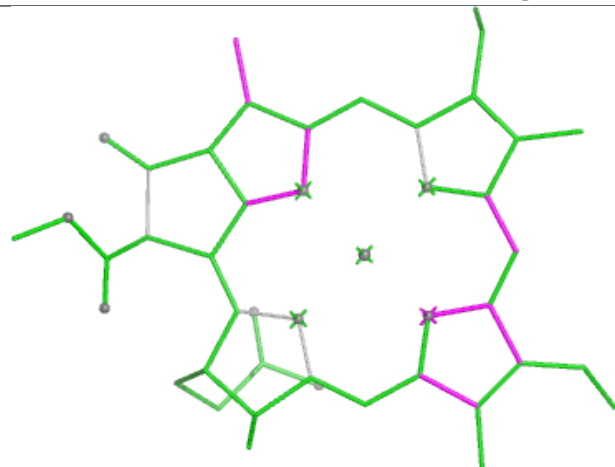


Rings

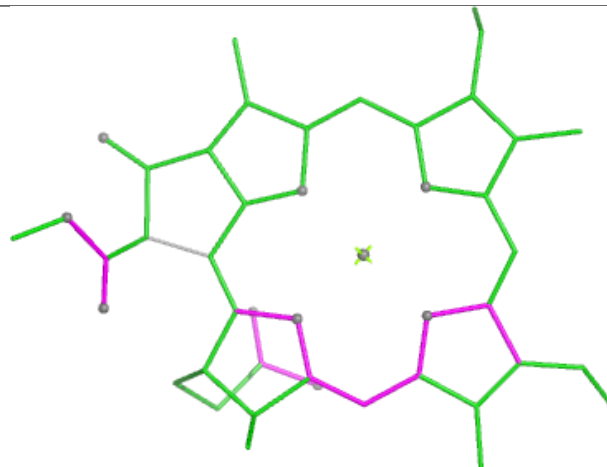
Ligand CLA B 806



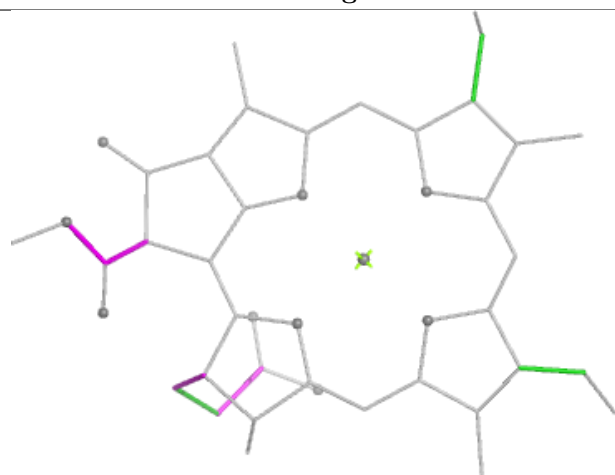
Ligand CLA B 836



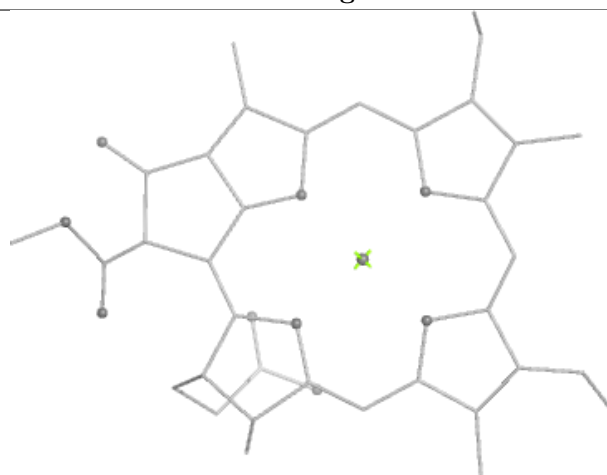
Bond lengths



Bond angles

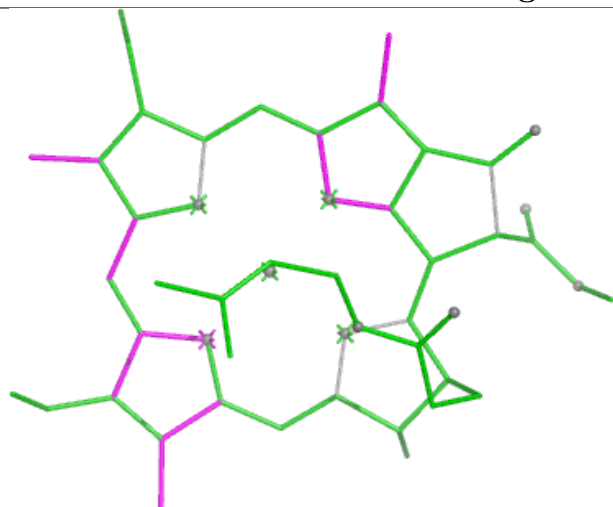


Torsions

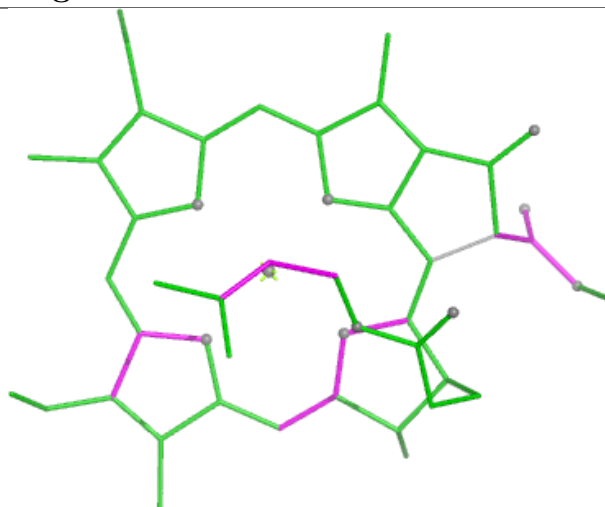


Rings

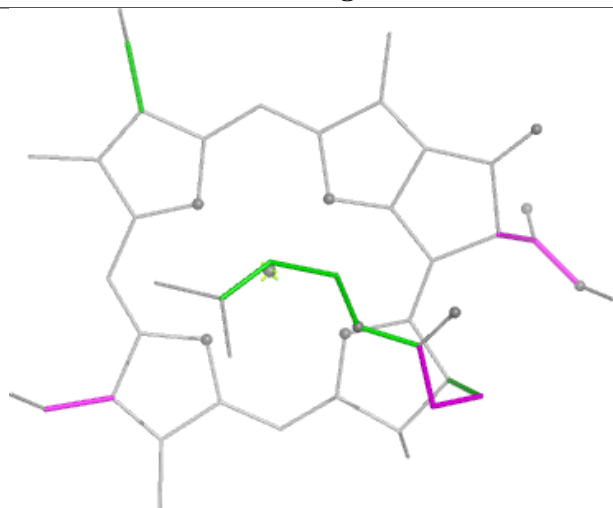
Ligand CLA g 824



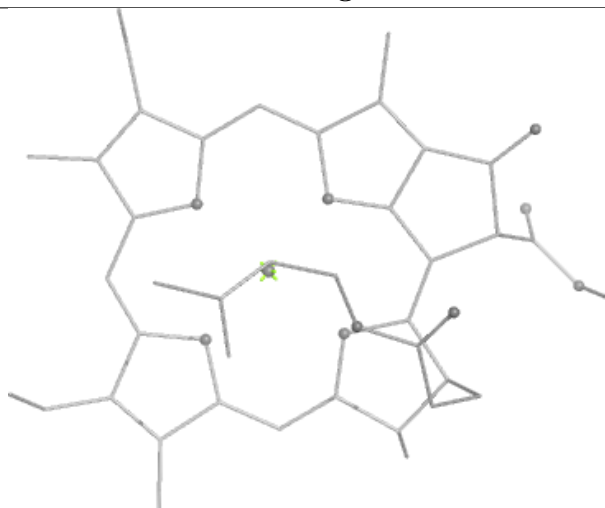
Bond lengths



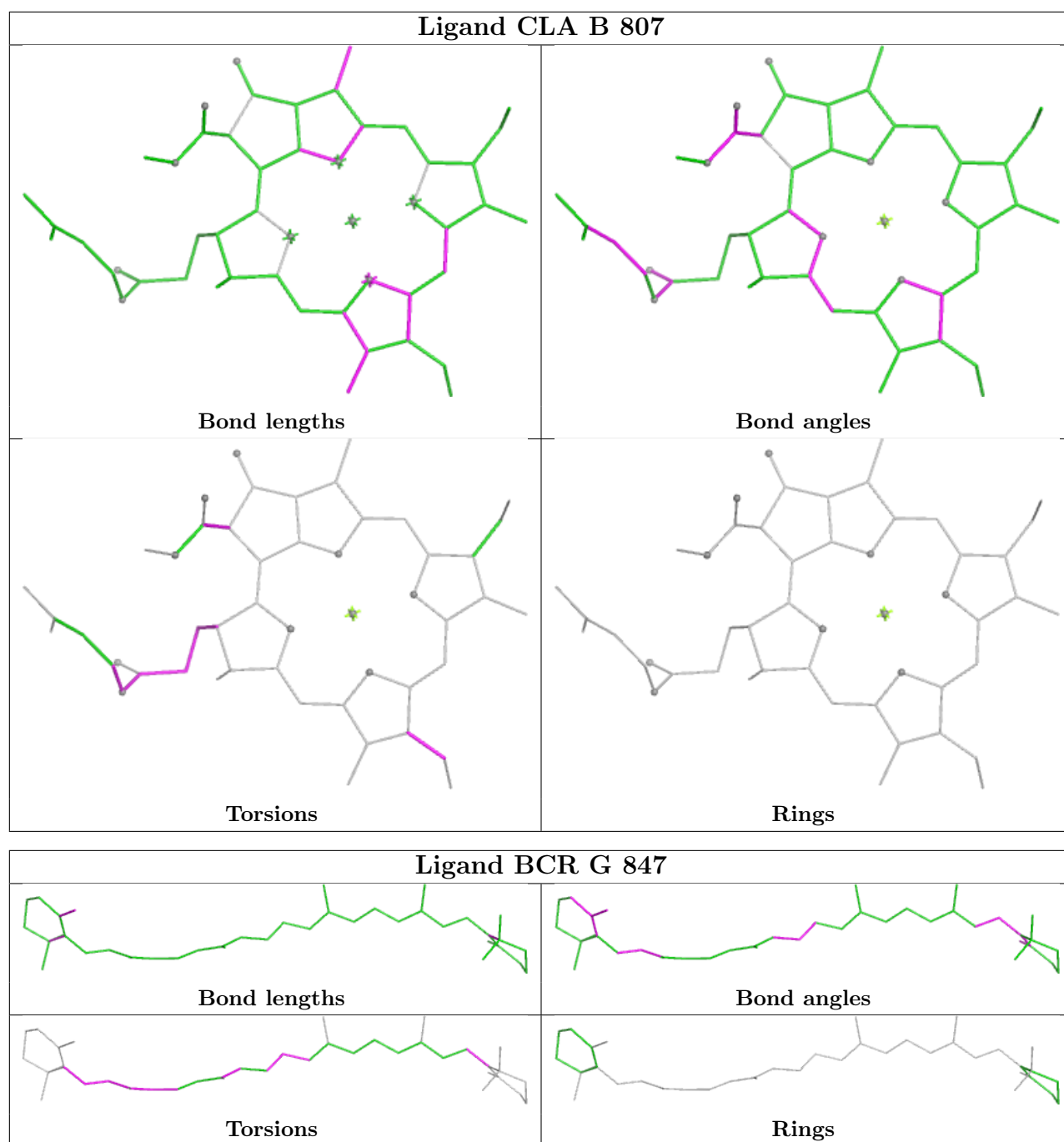
Bond angles



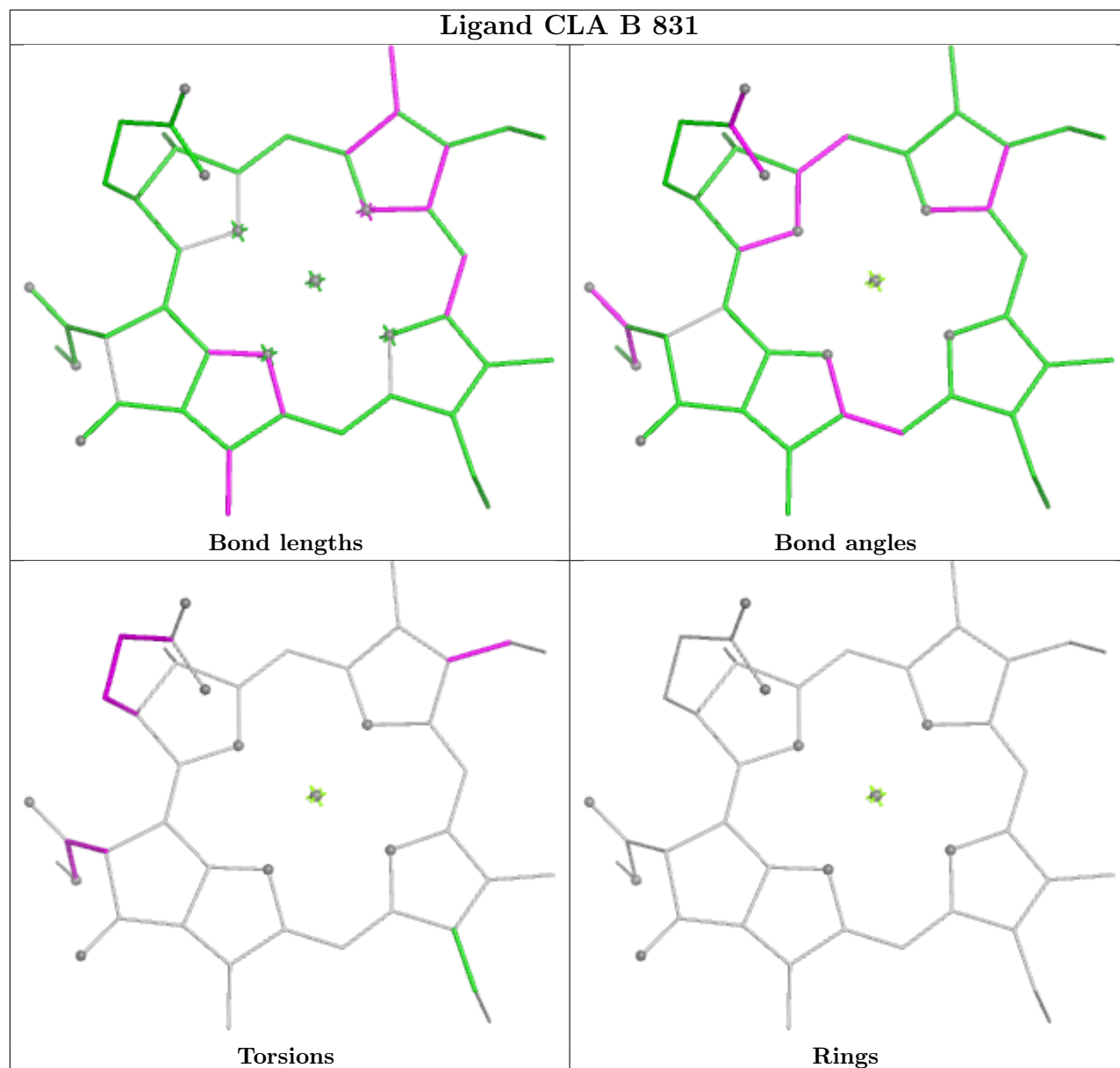
Torsions



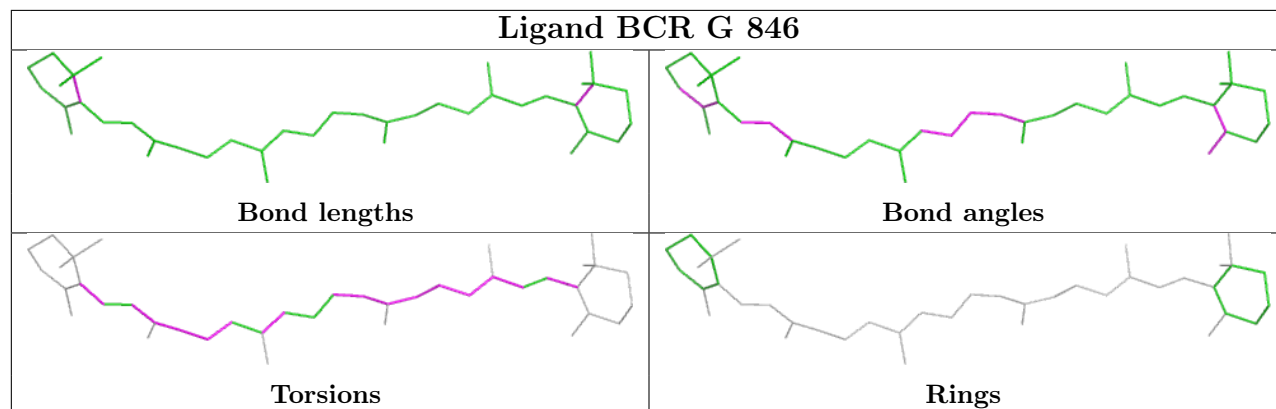
Rings

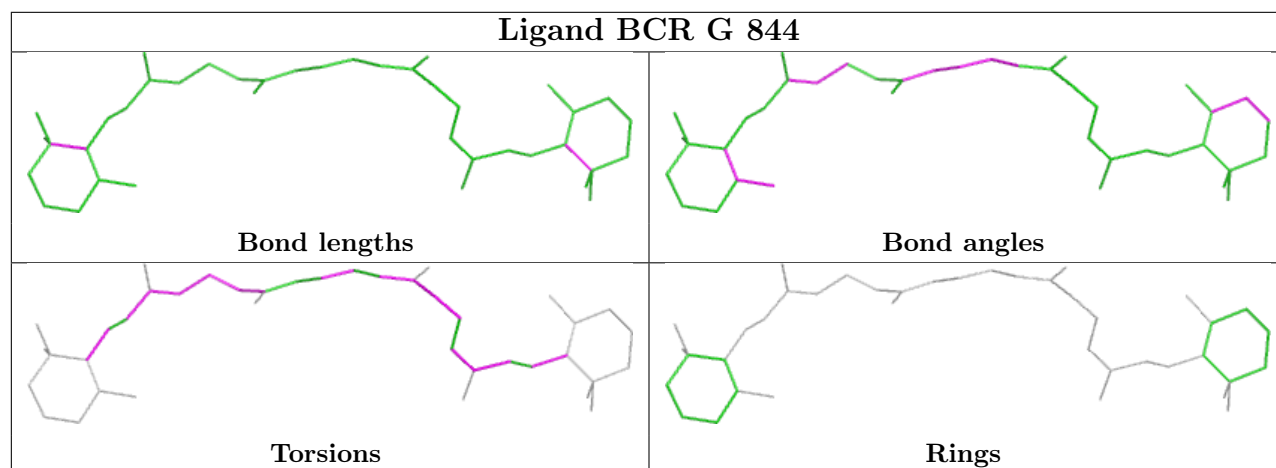
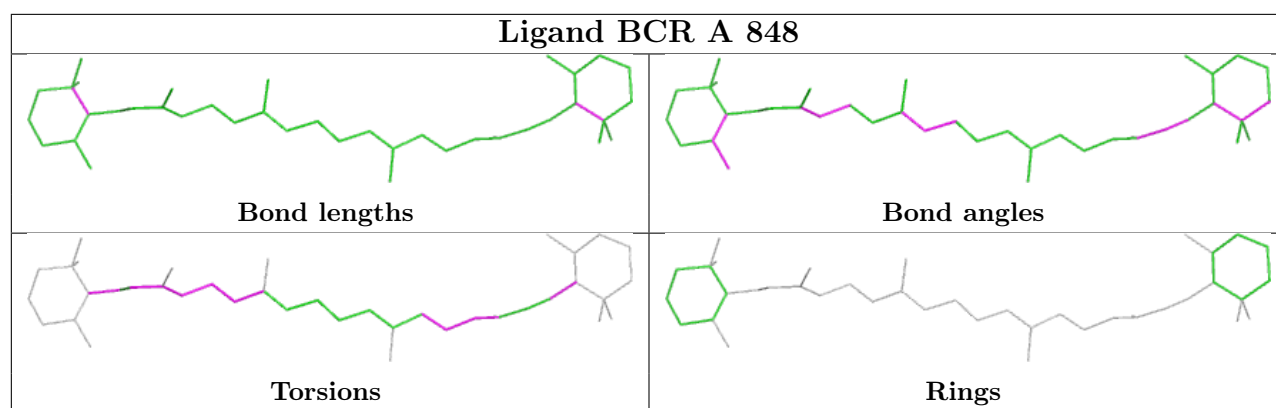


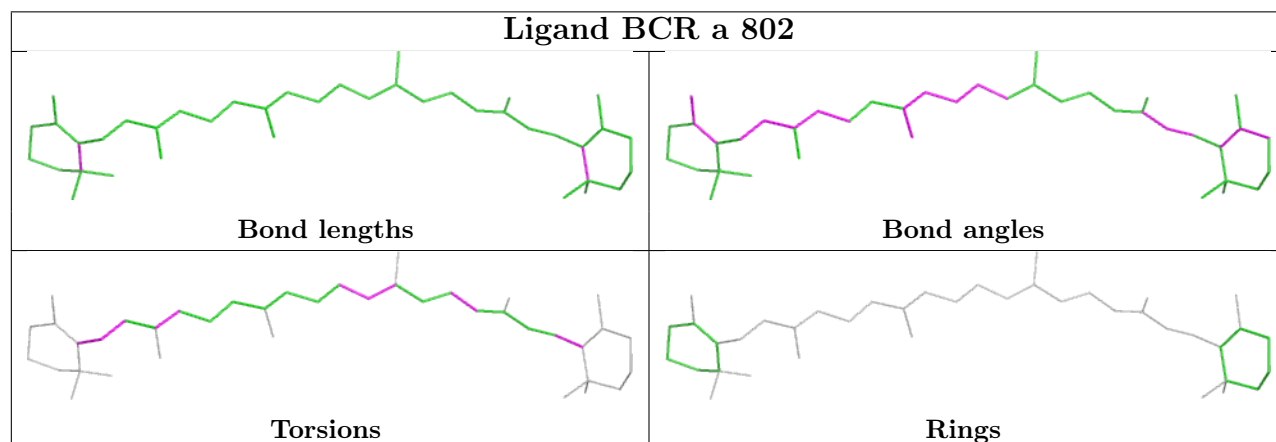
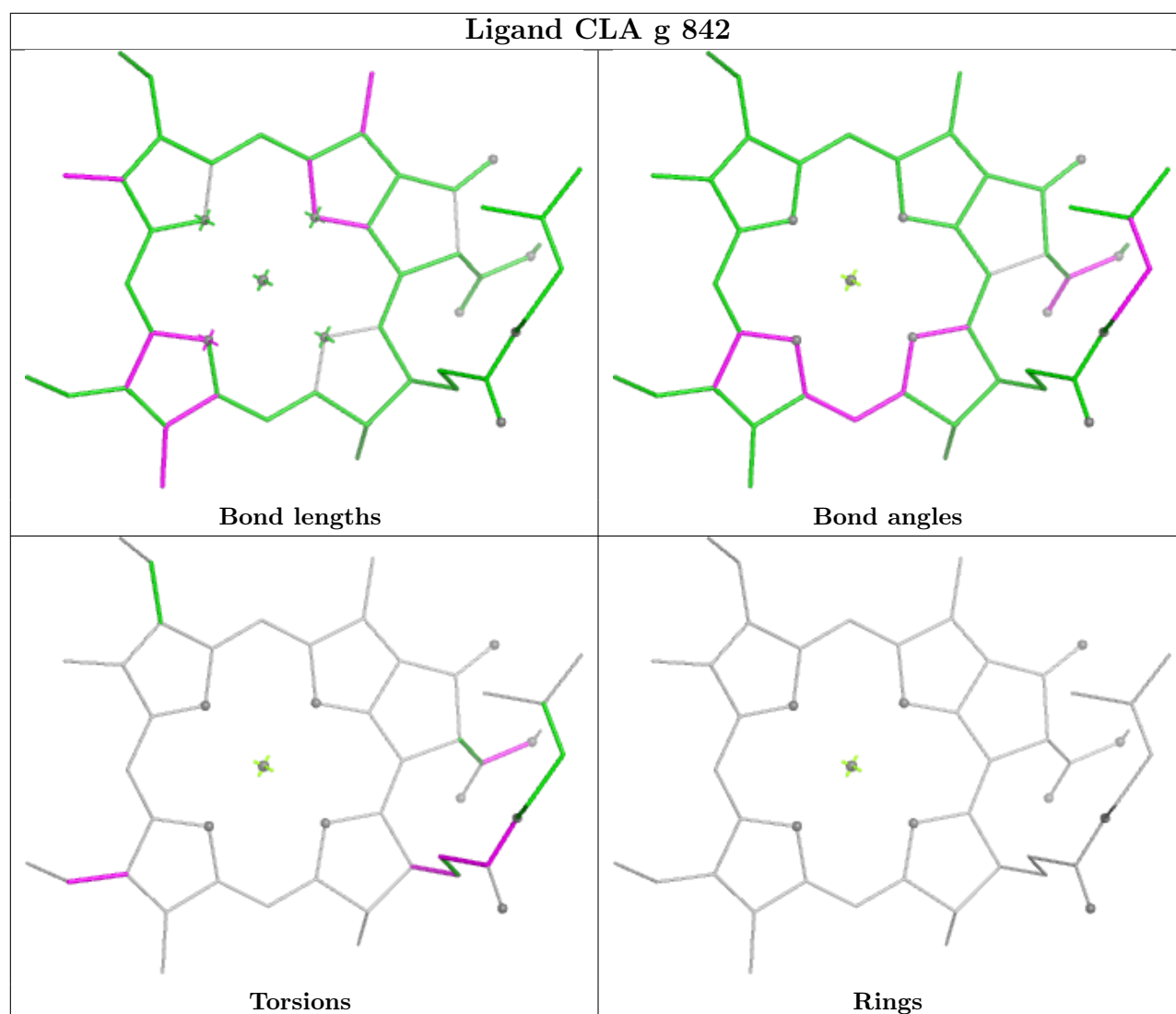
Ligand CLA B 831



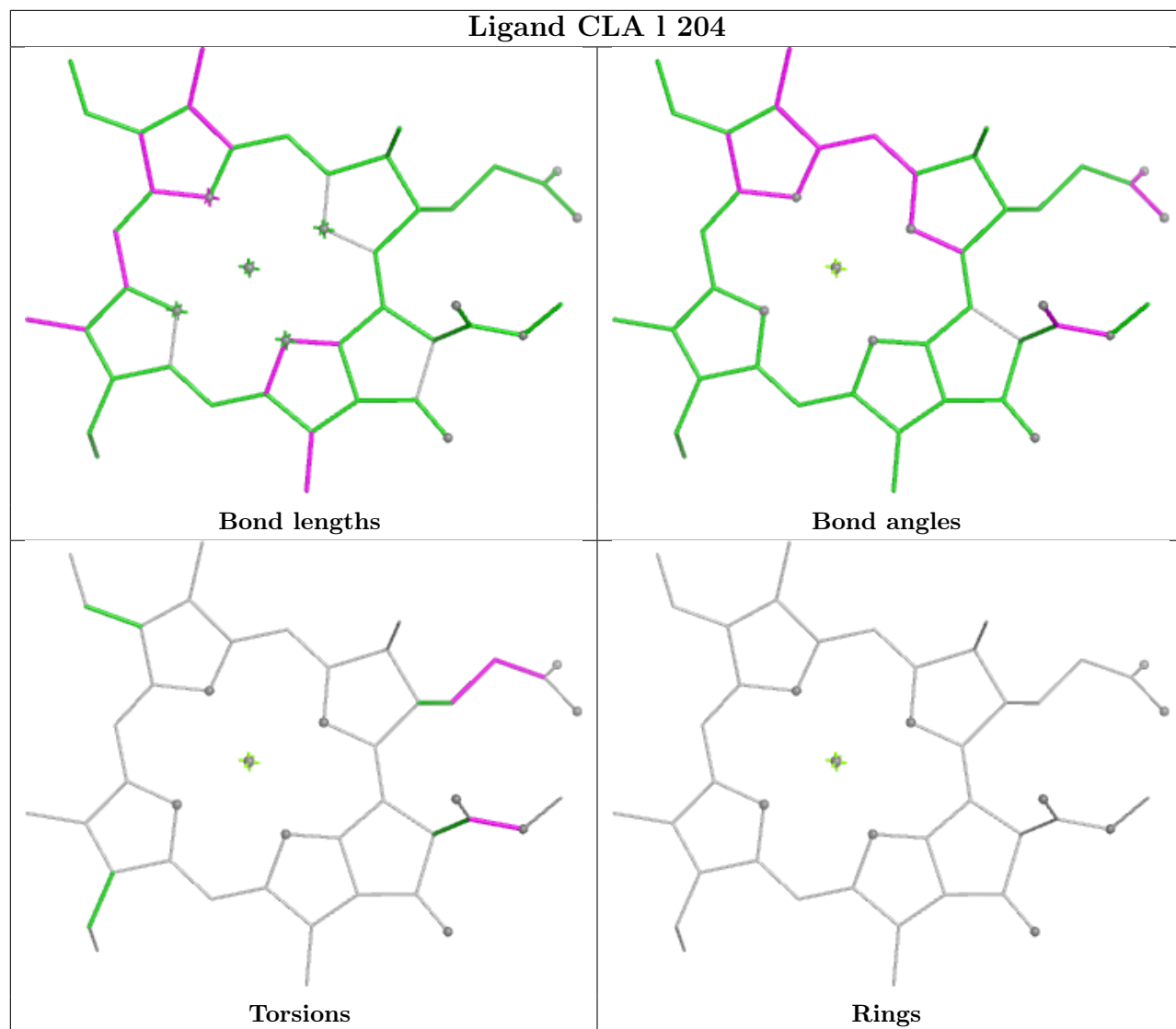
Ligand BCR G 846



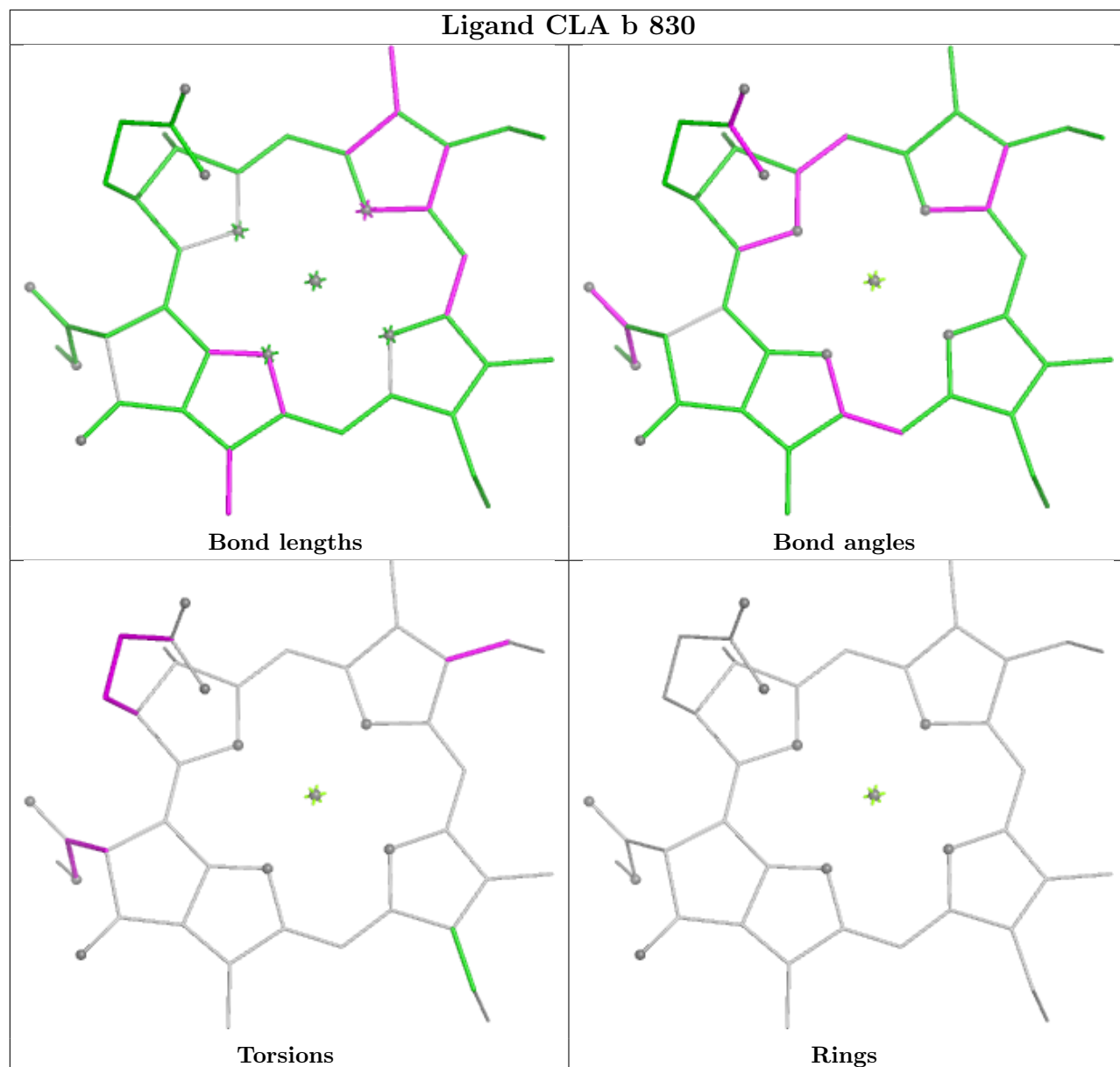




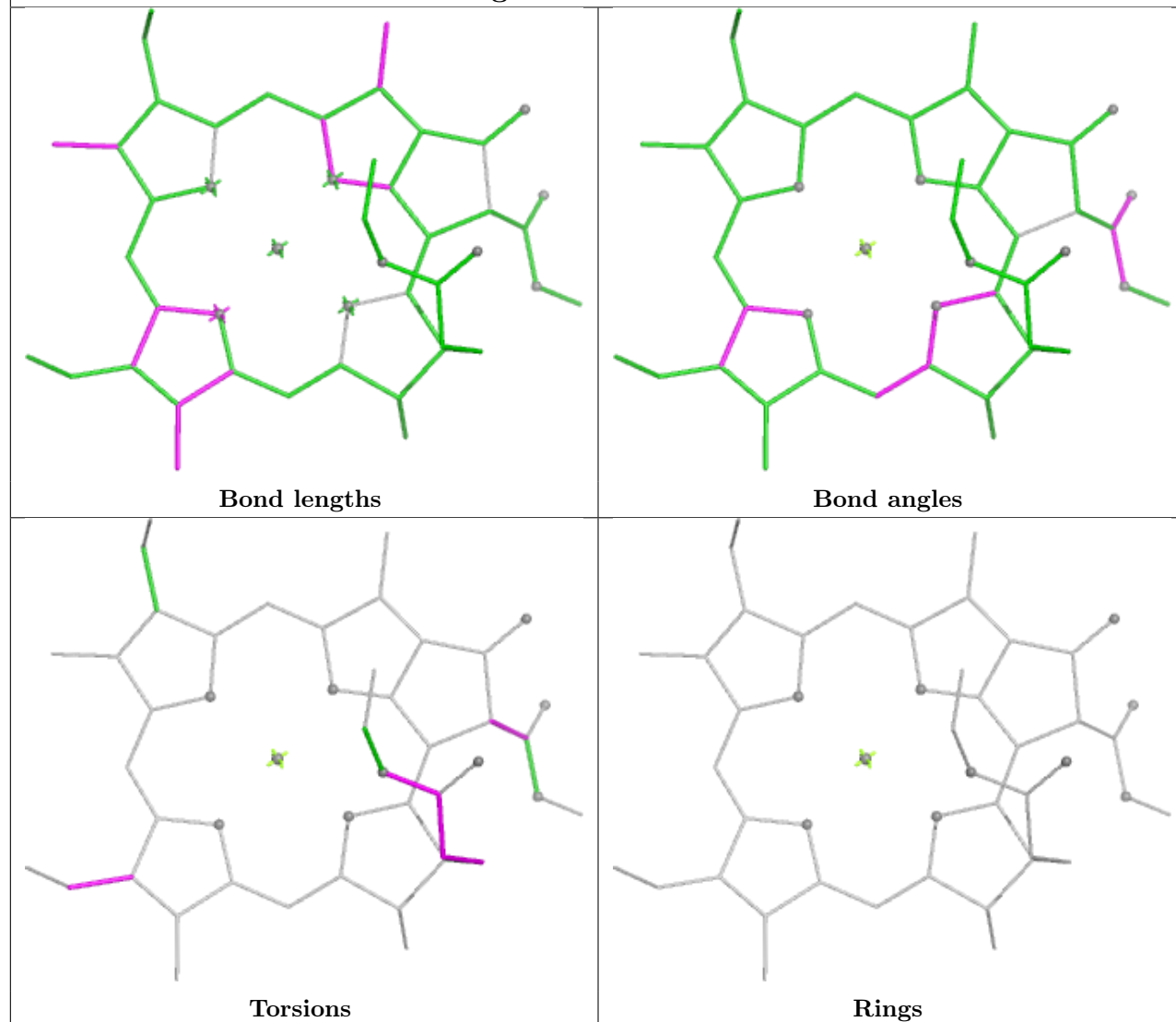
Ligand CLA 1 204



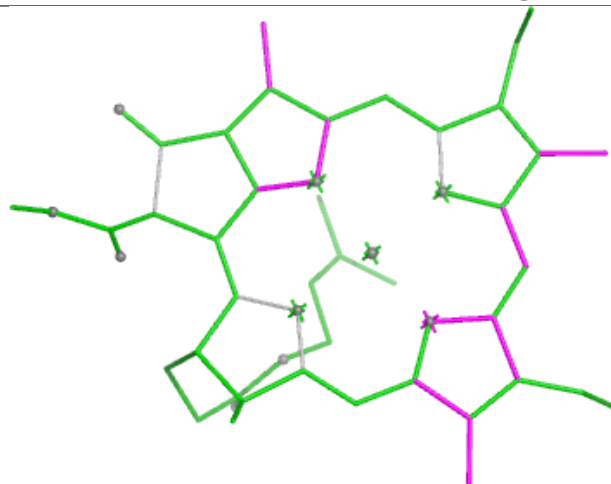
Ligand CLA b 830



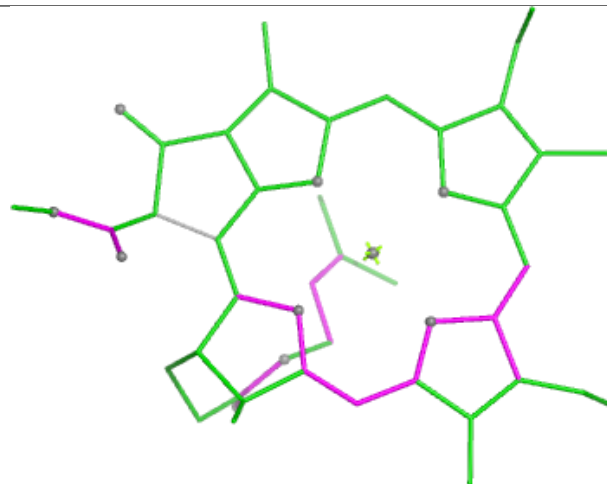
Ligand CLA E 842



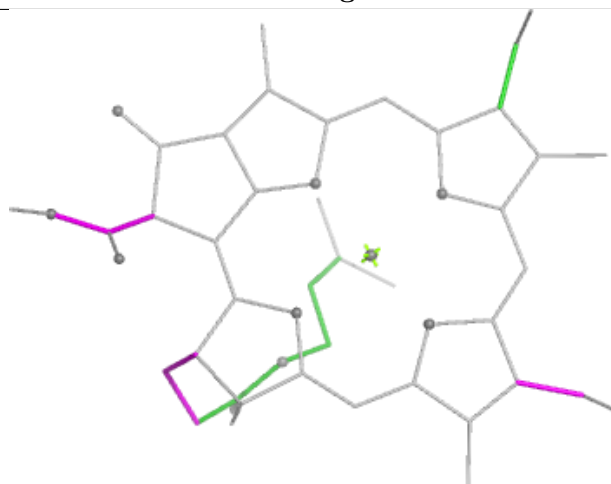
Ligand CLA E 845



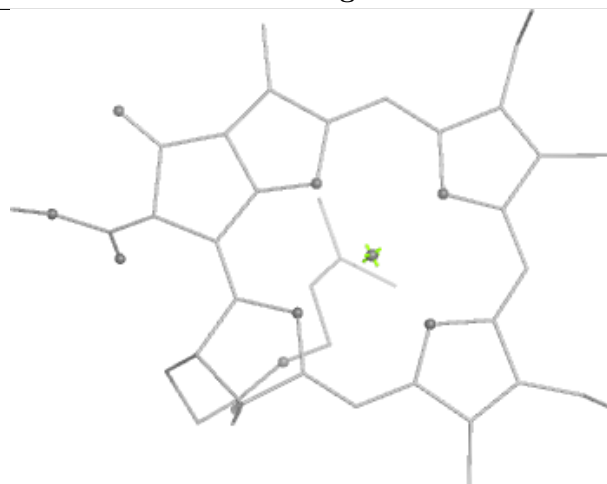
Bond lengths



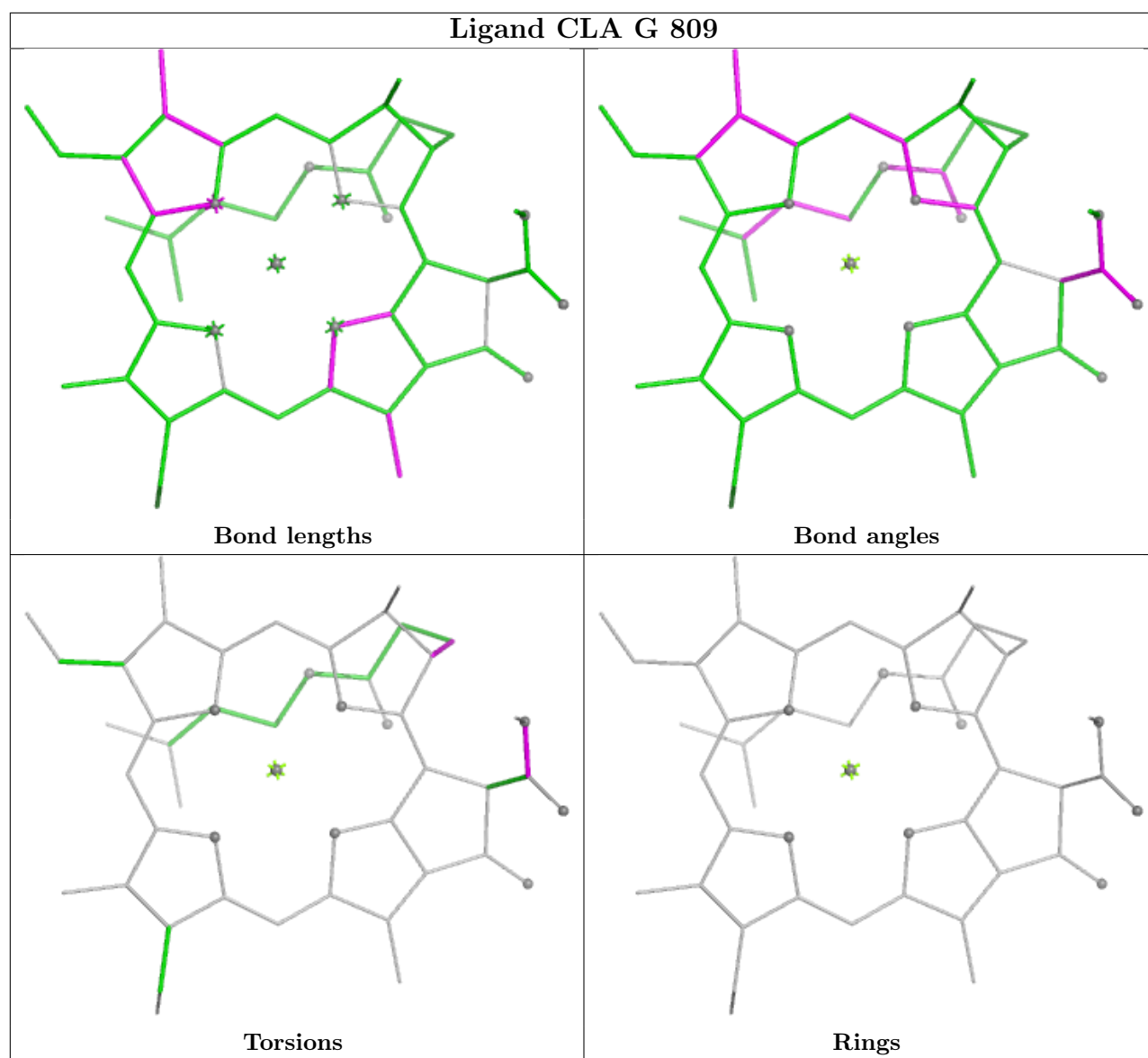
Bond angles



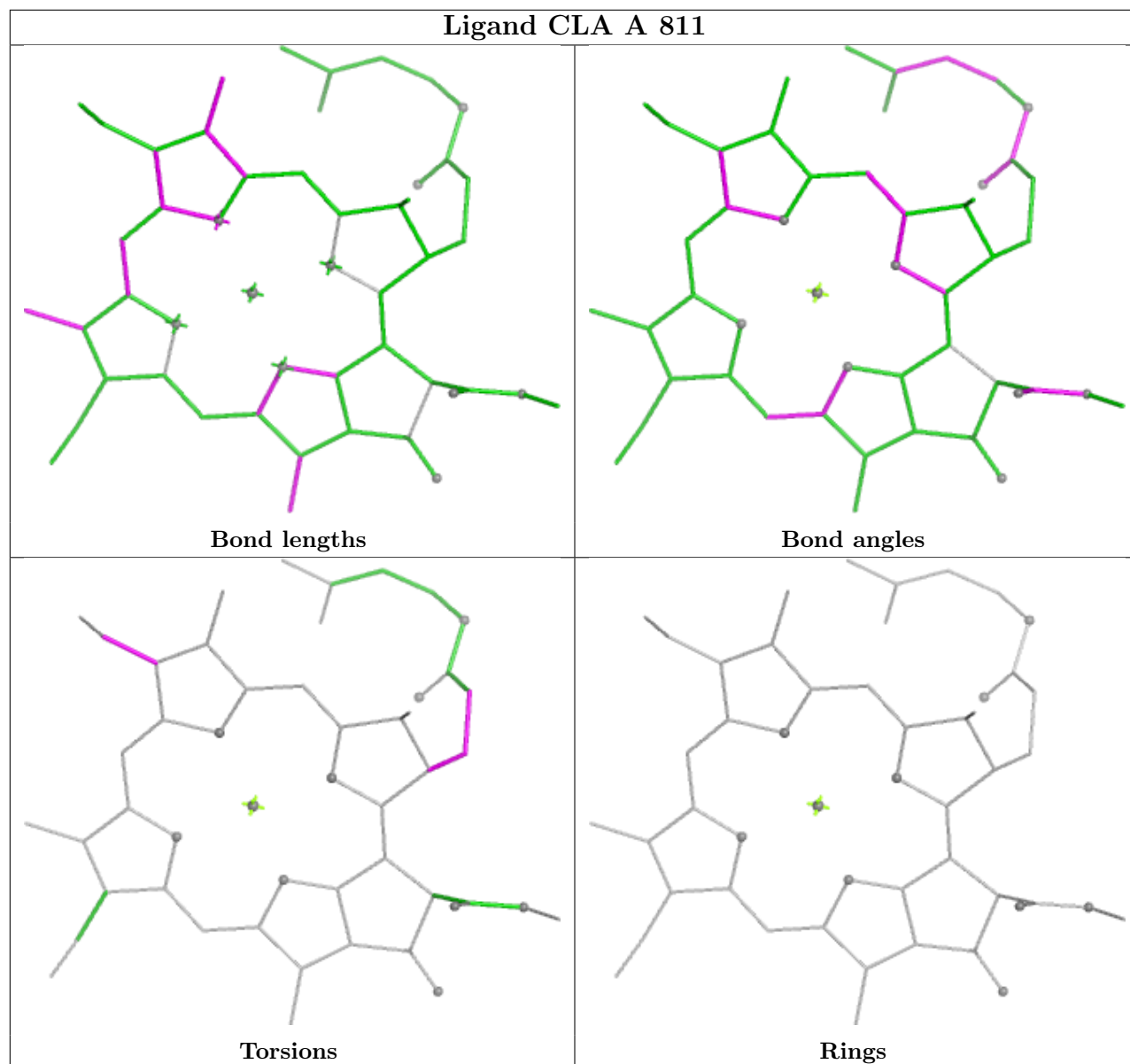
Torsions



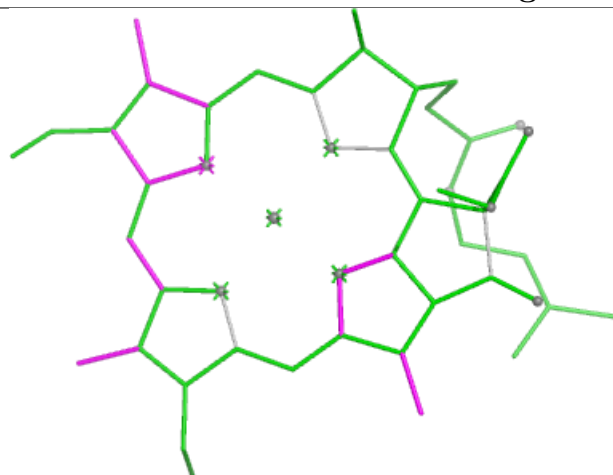
Rings



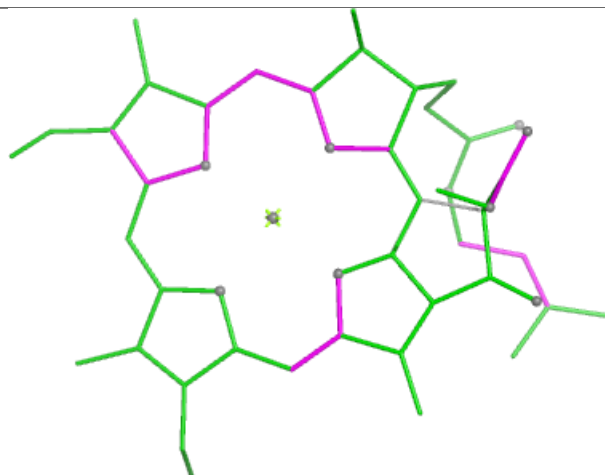
Ligand CLA A 811



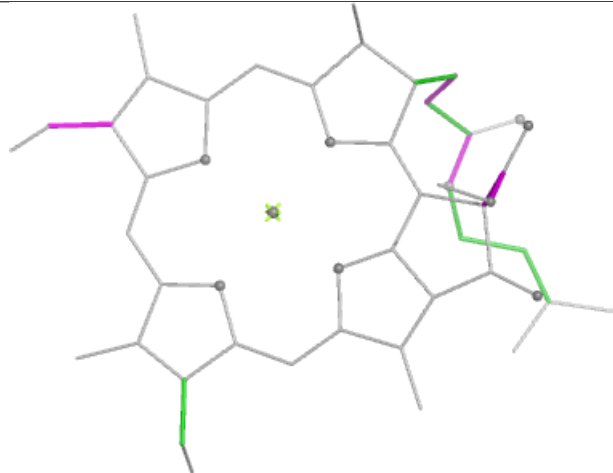
Ligand CLA e 809



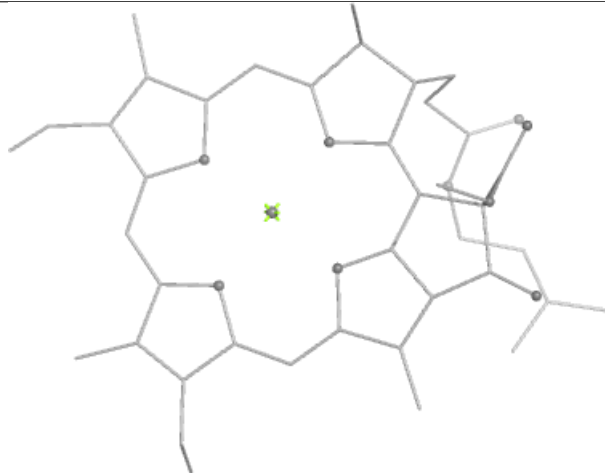
Bond lengths



Bond angles

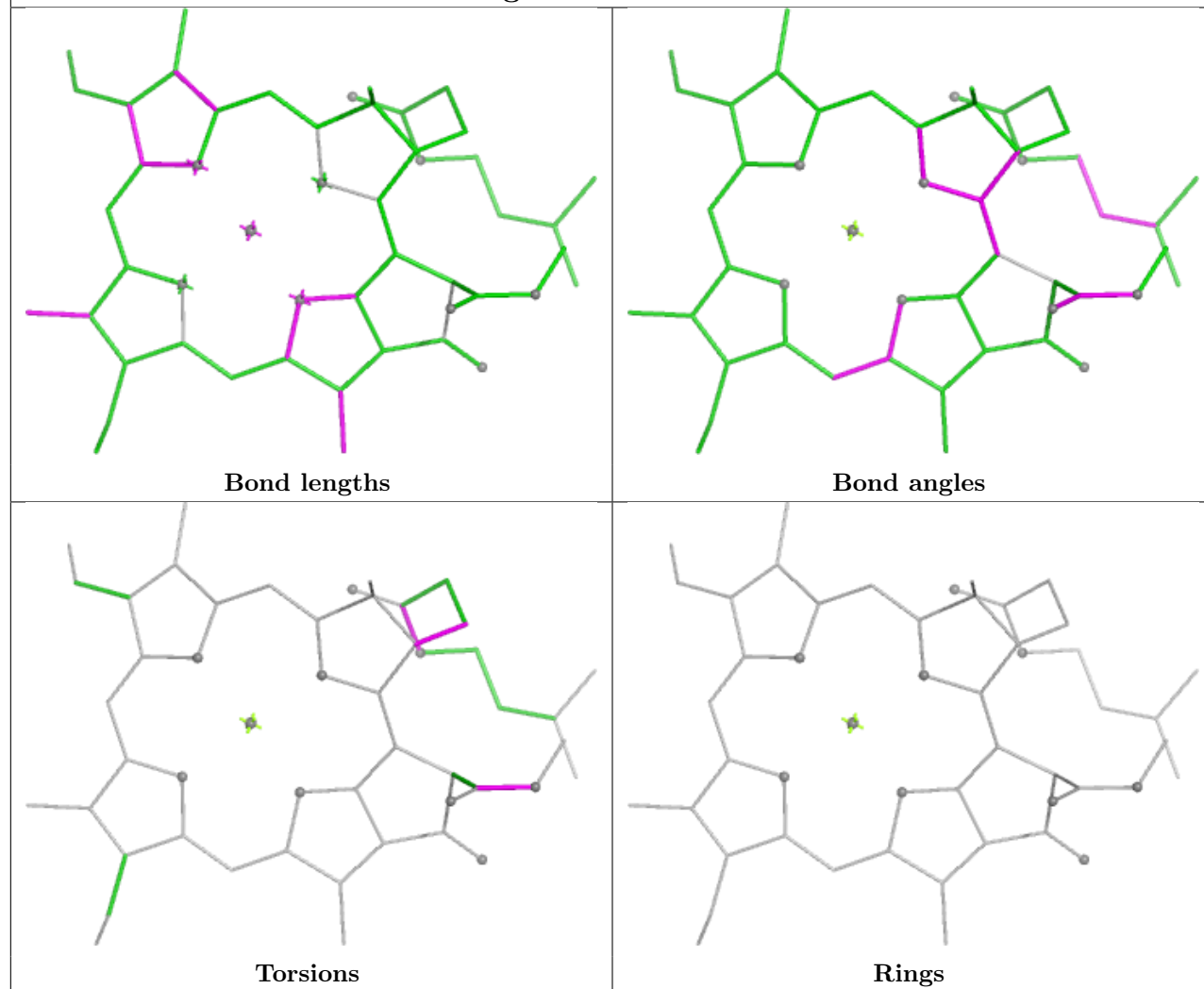


Torsions

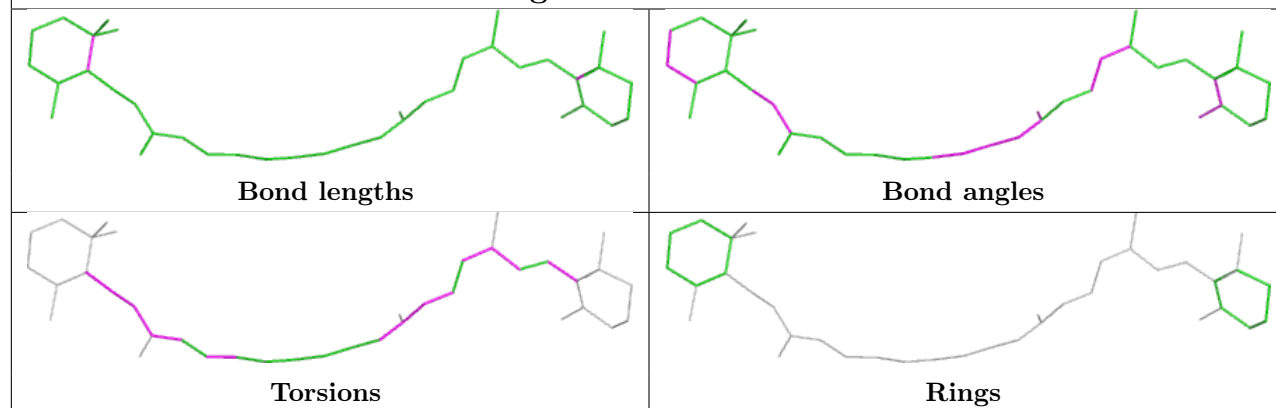


Rings

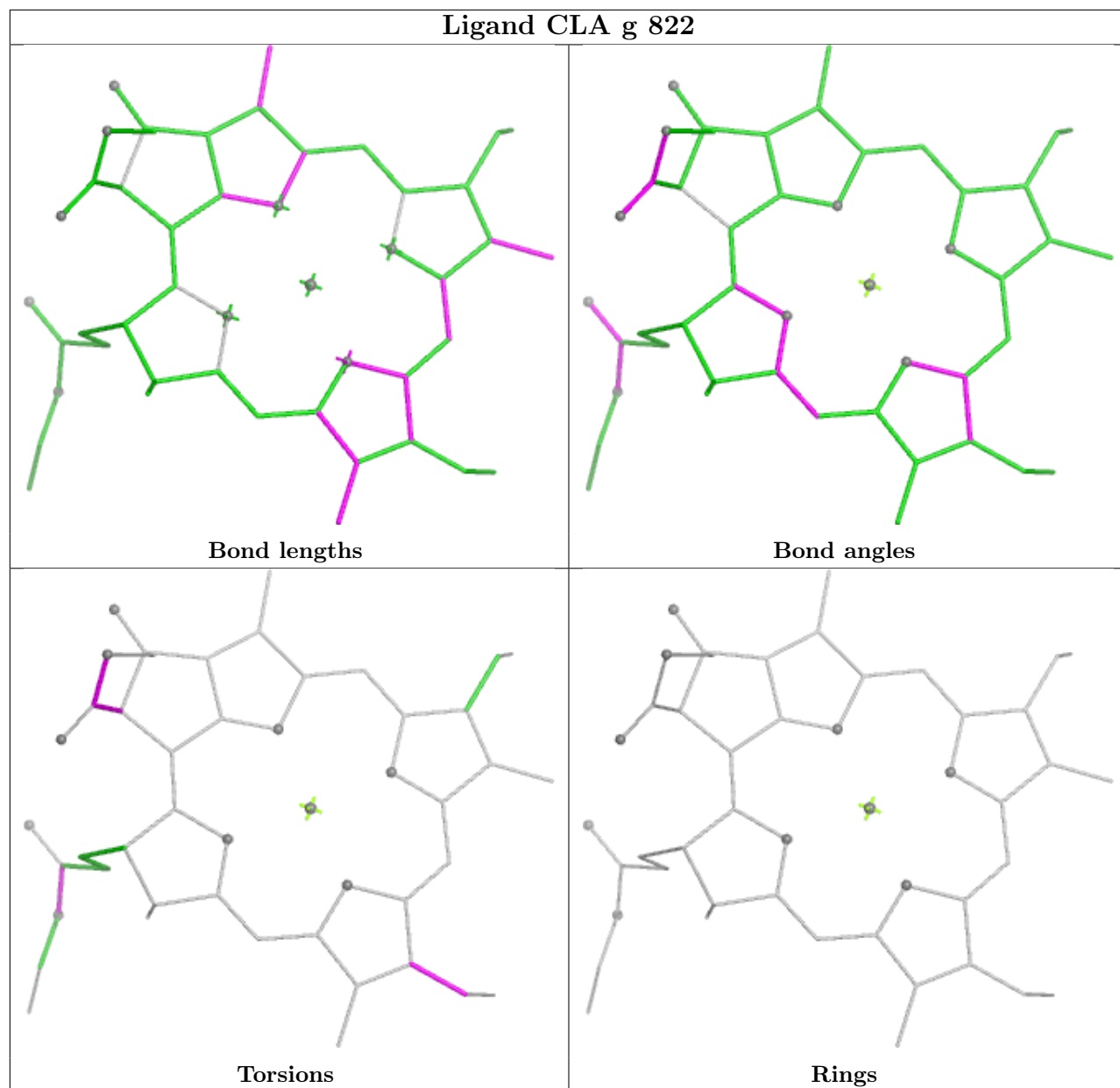
Ligand CLA E 836



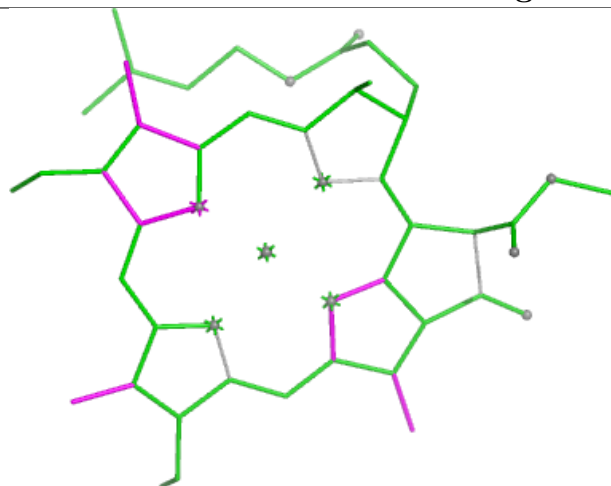
Ligand BCR A 852



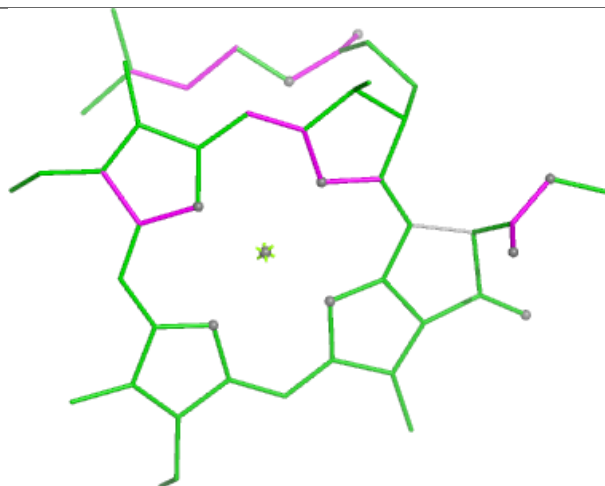
Ligand CLA g 822



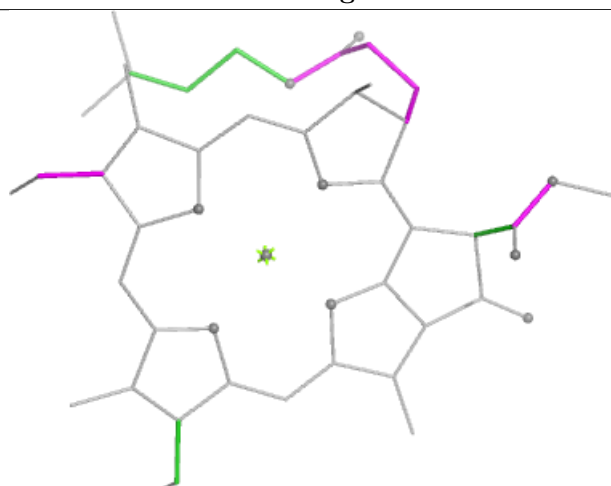
Ligand CLA E 822



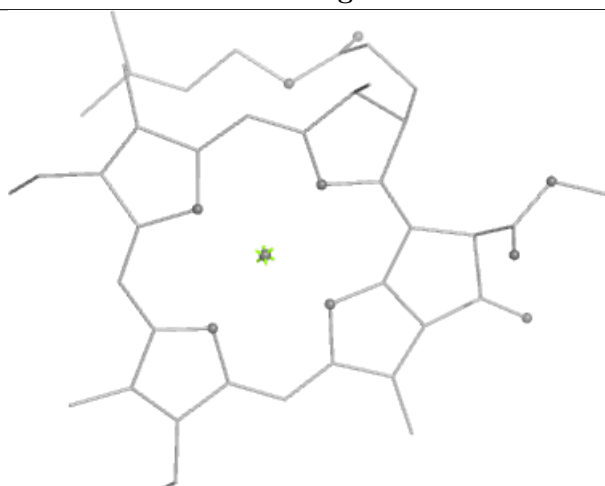
Bond lengths



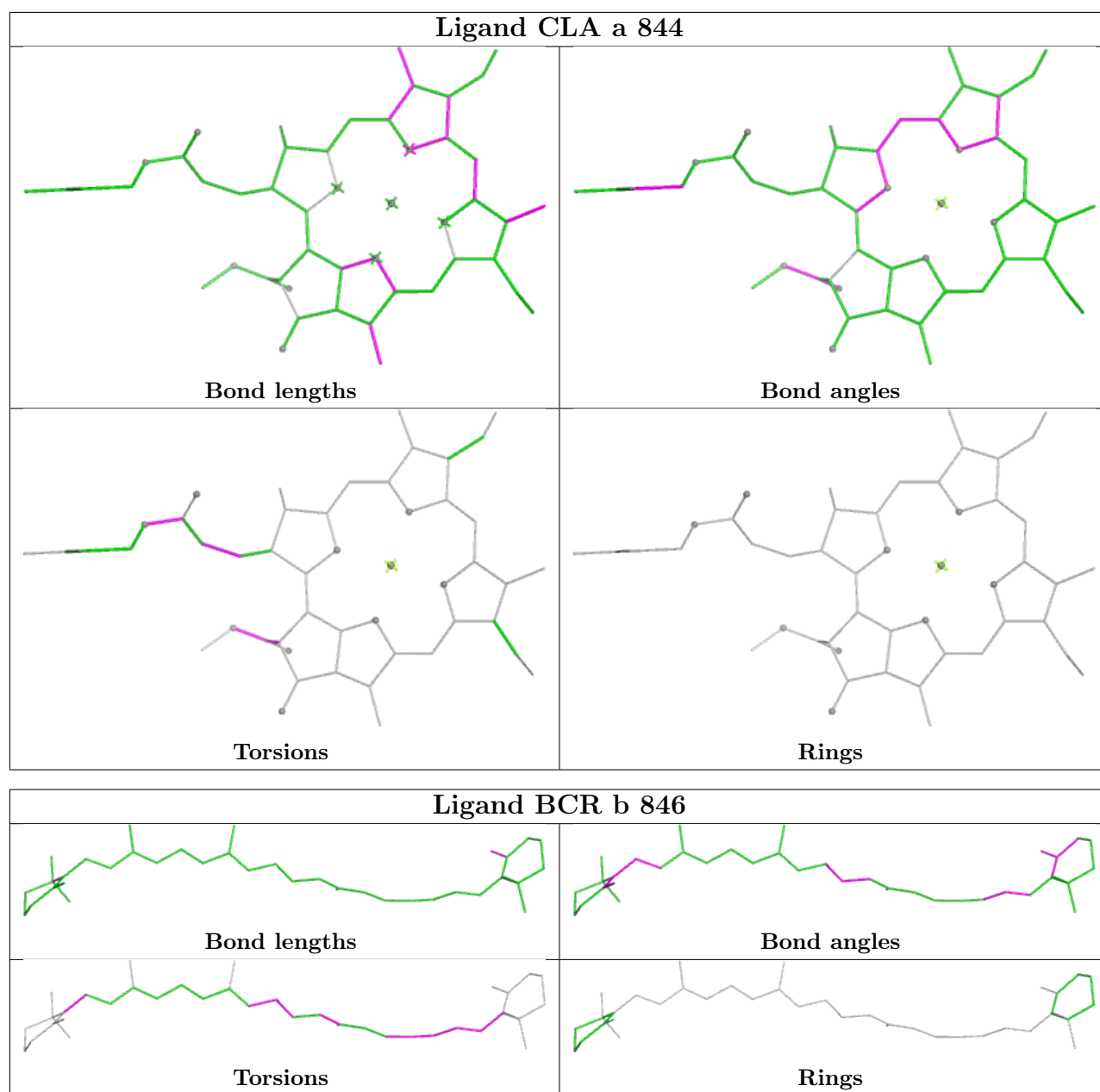
Bond angles

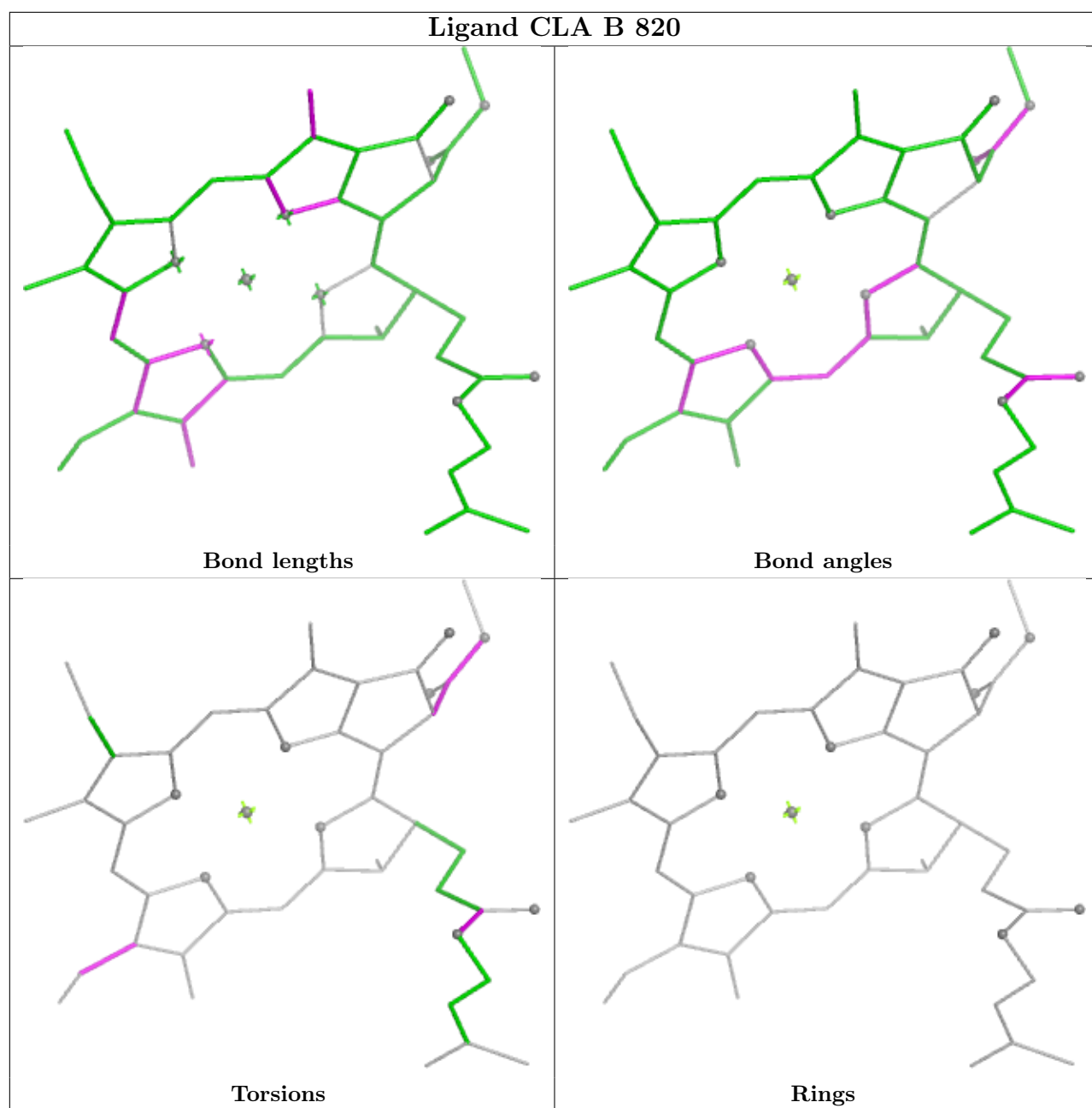


Torsions

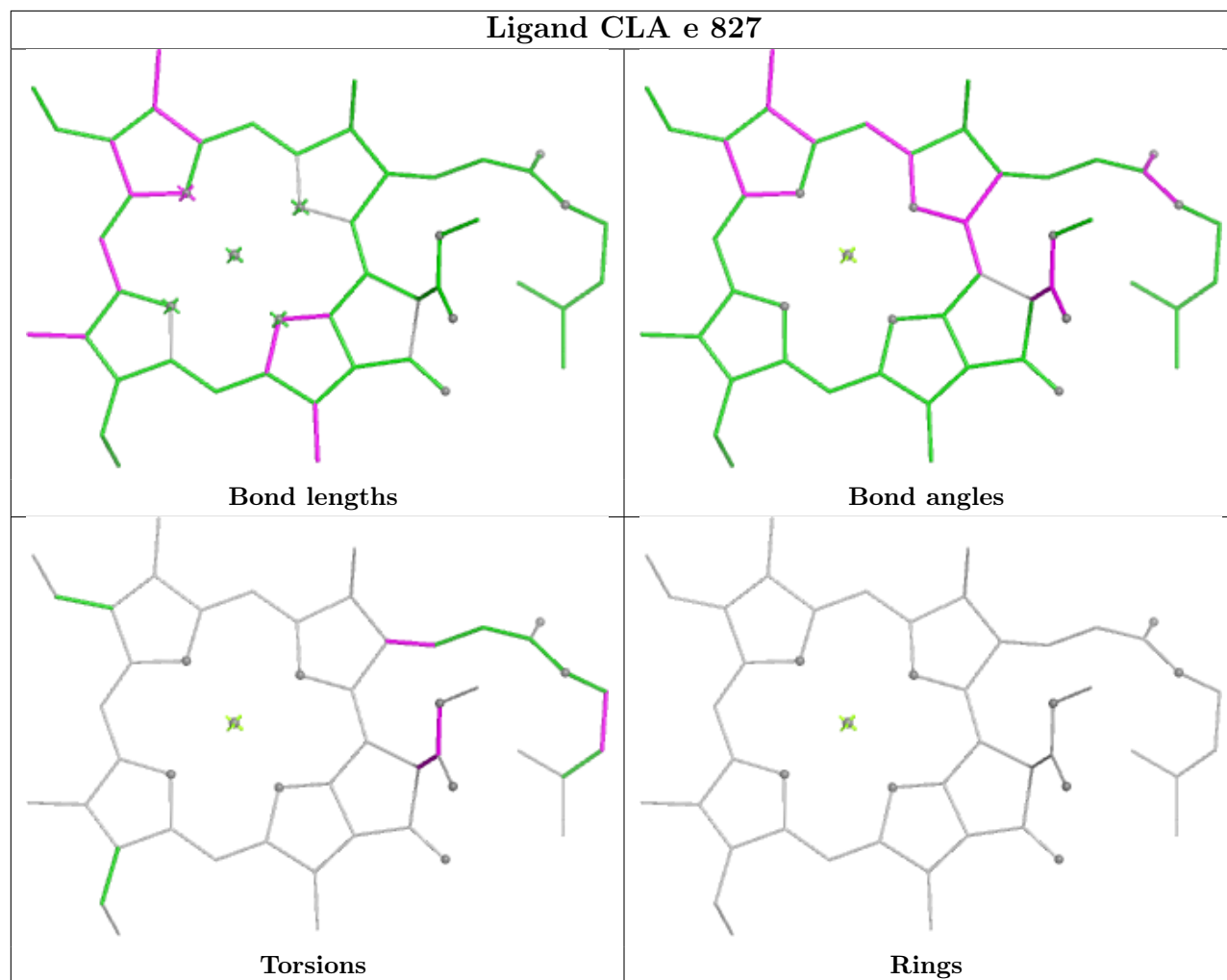


Rings

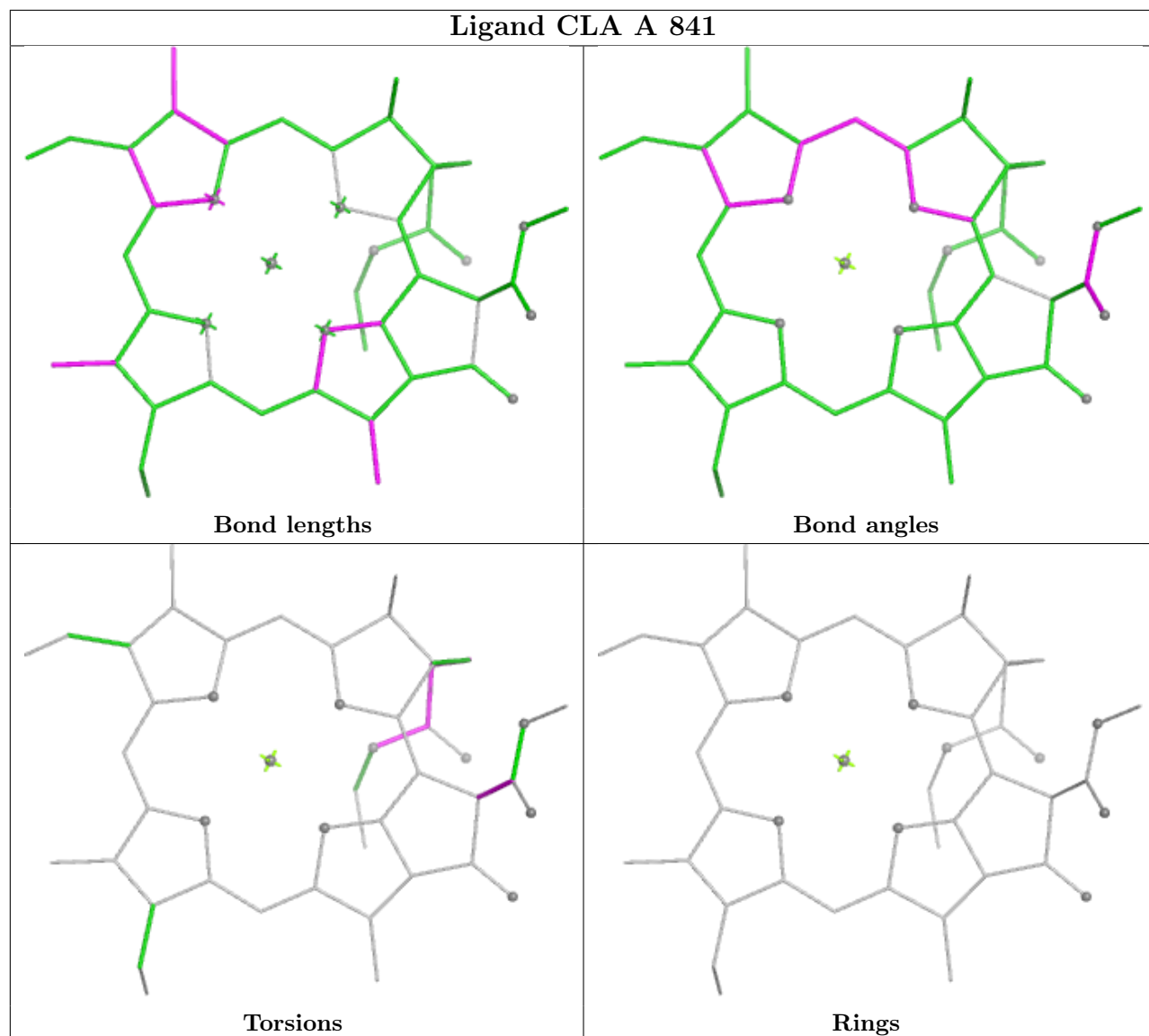


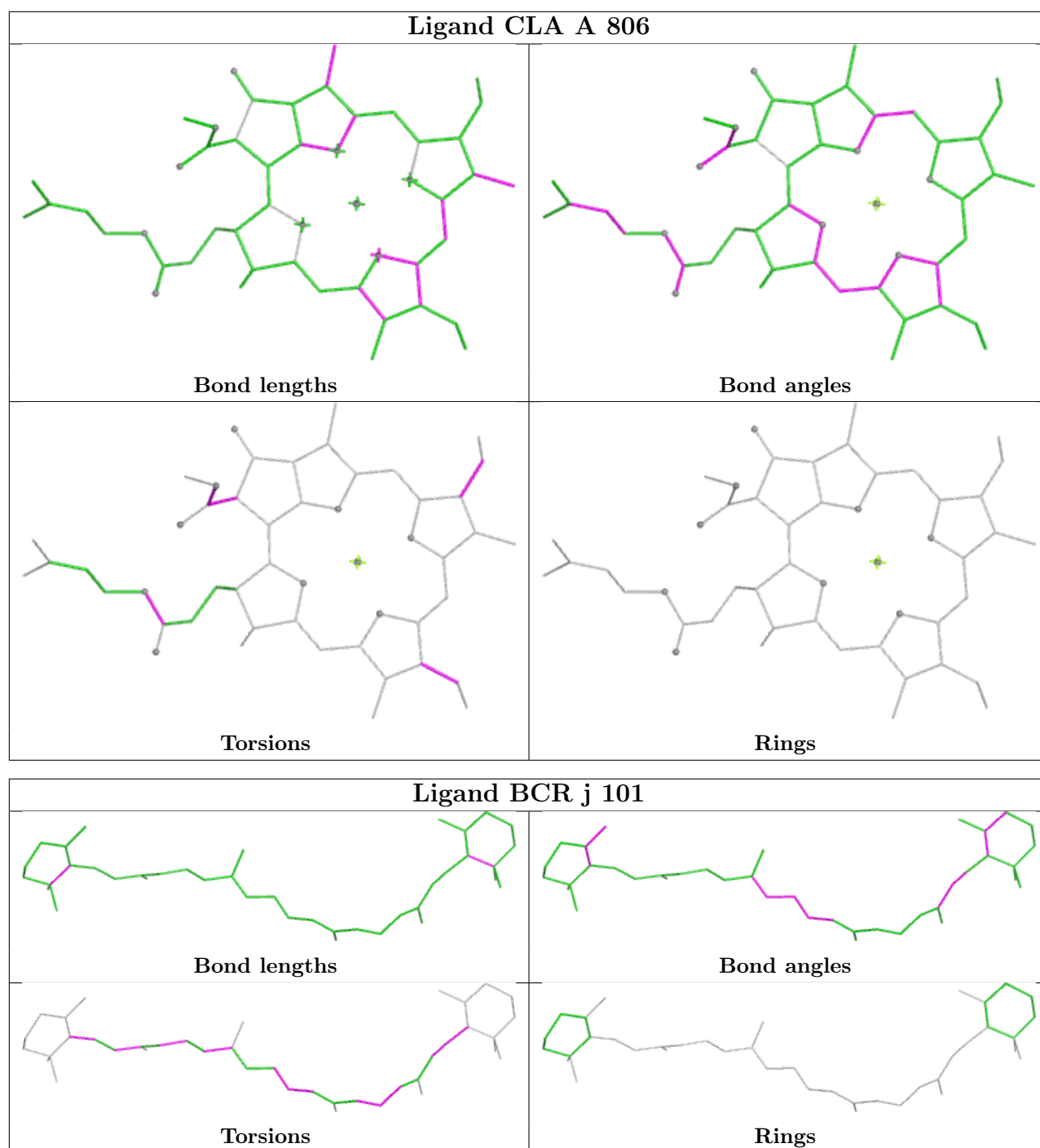


Ligand CLA e 827

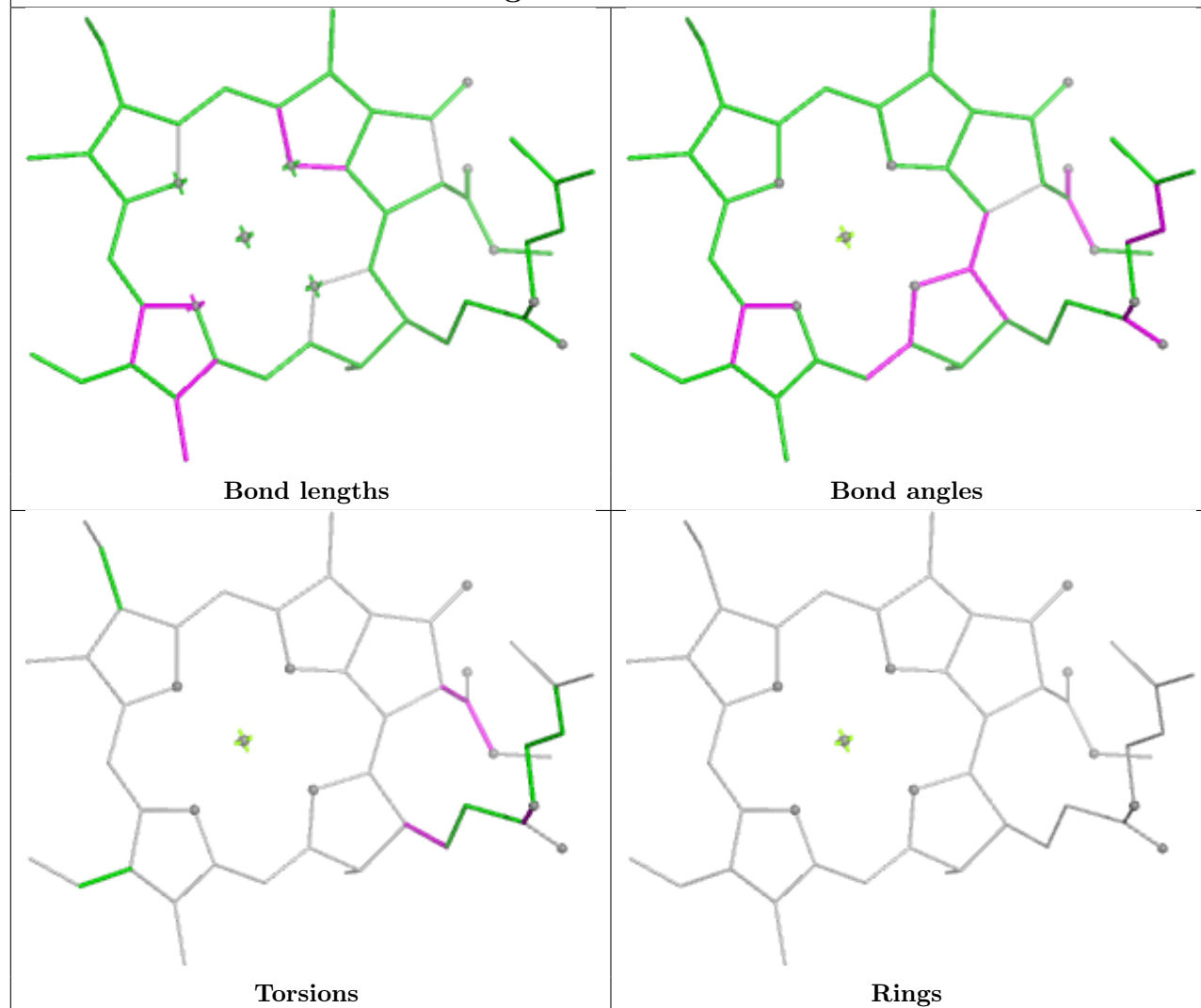


Ligand CLA A 841

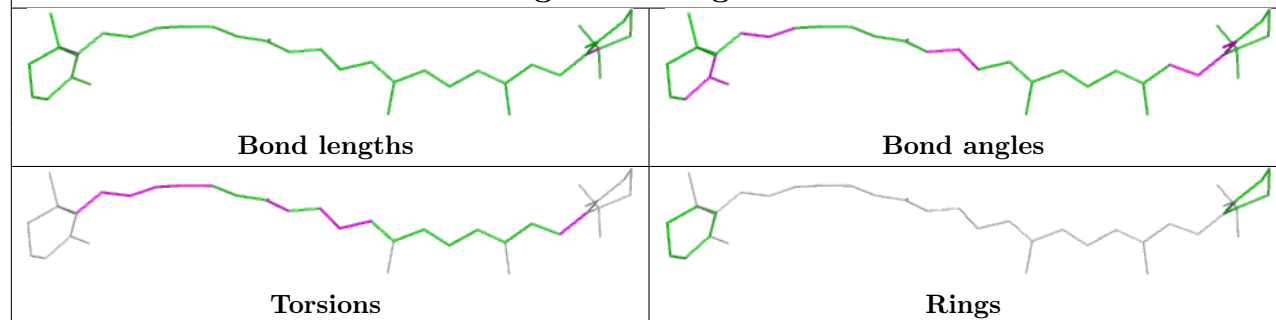




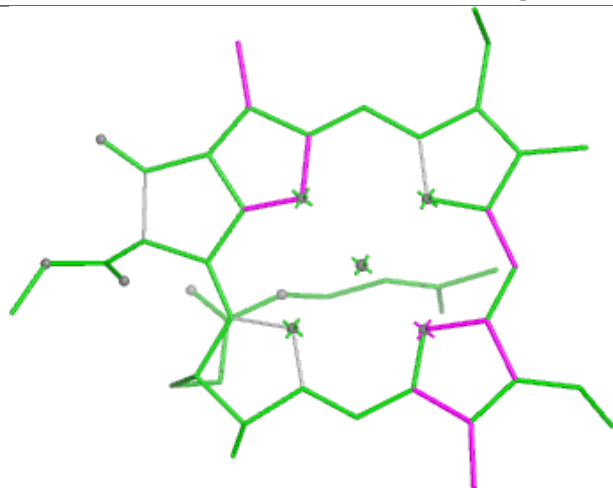
Ligand CLA a 852



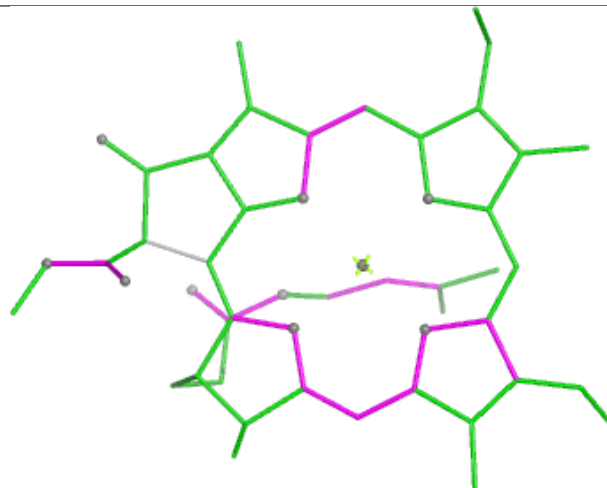
Ligand BCR g 848



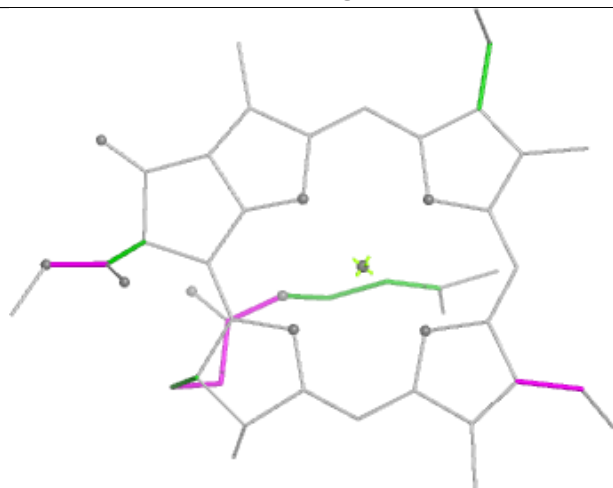
Ligand CLA B 838



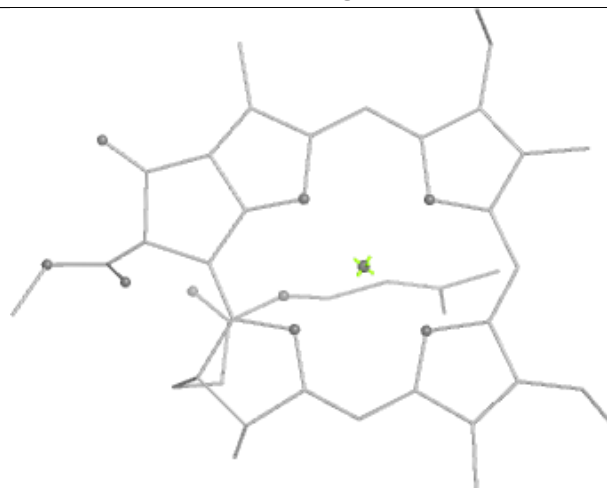
Bond lengths



Bond angles

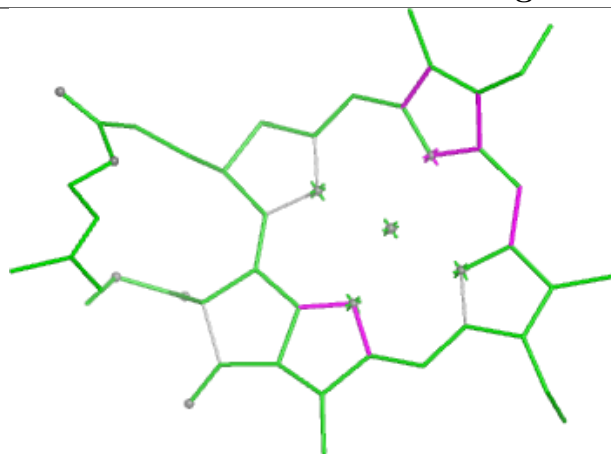


Torsions

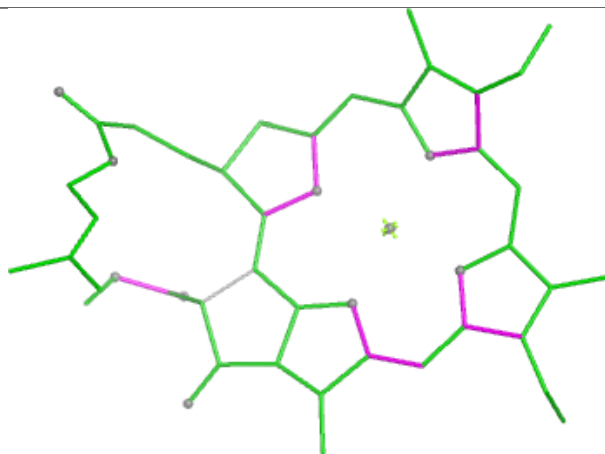


Rings

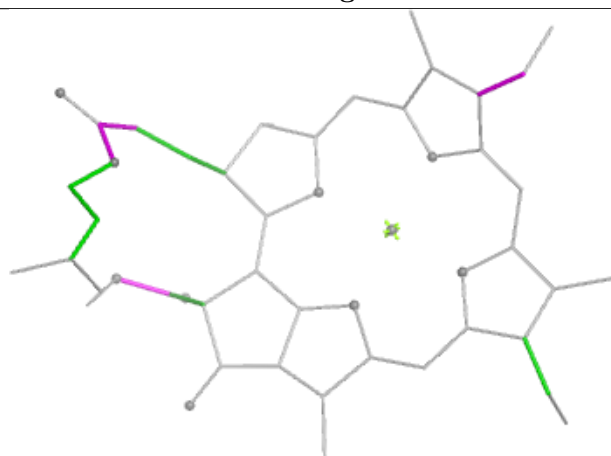
Ligand CLA E 803



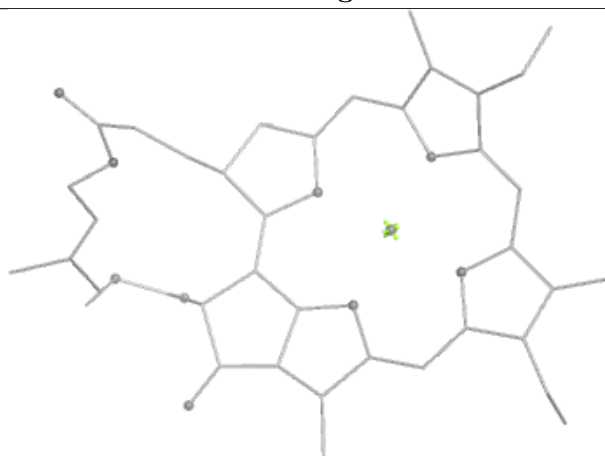
Bond lengths



Bond angles

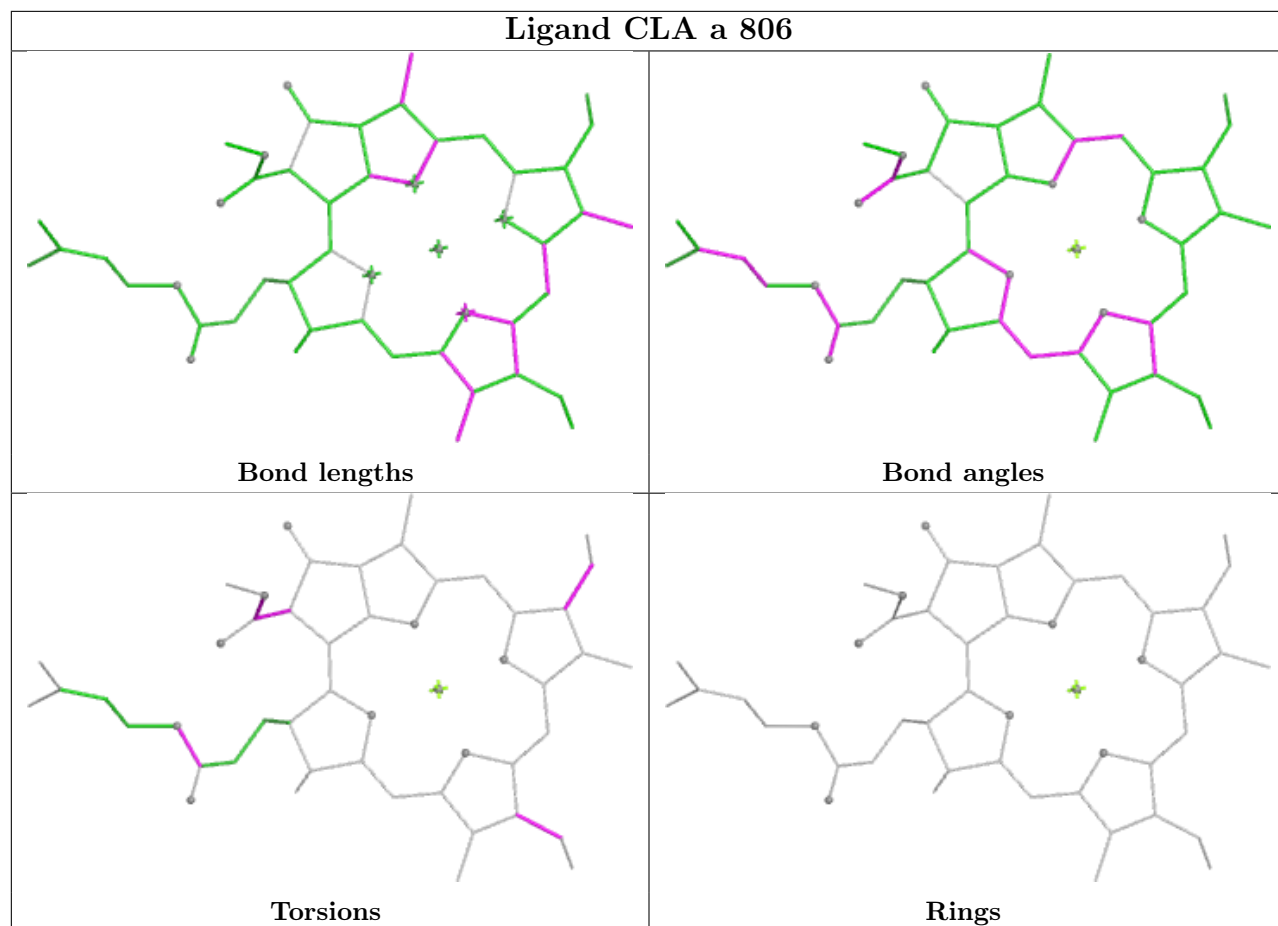


Torsions

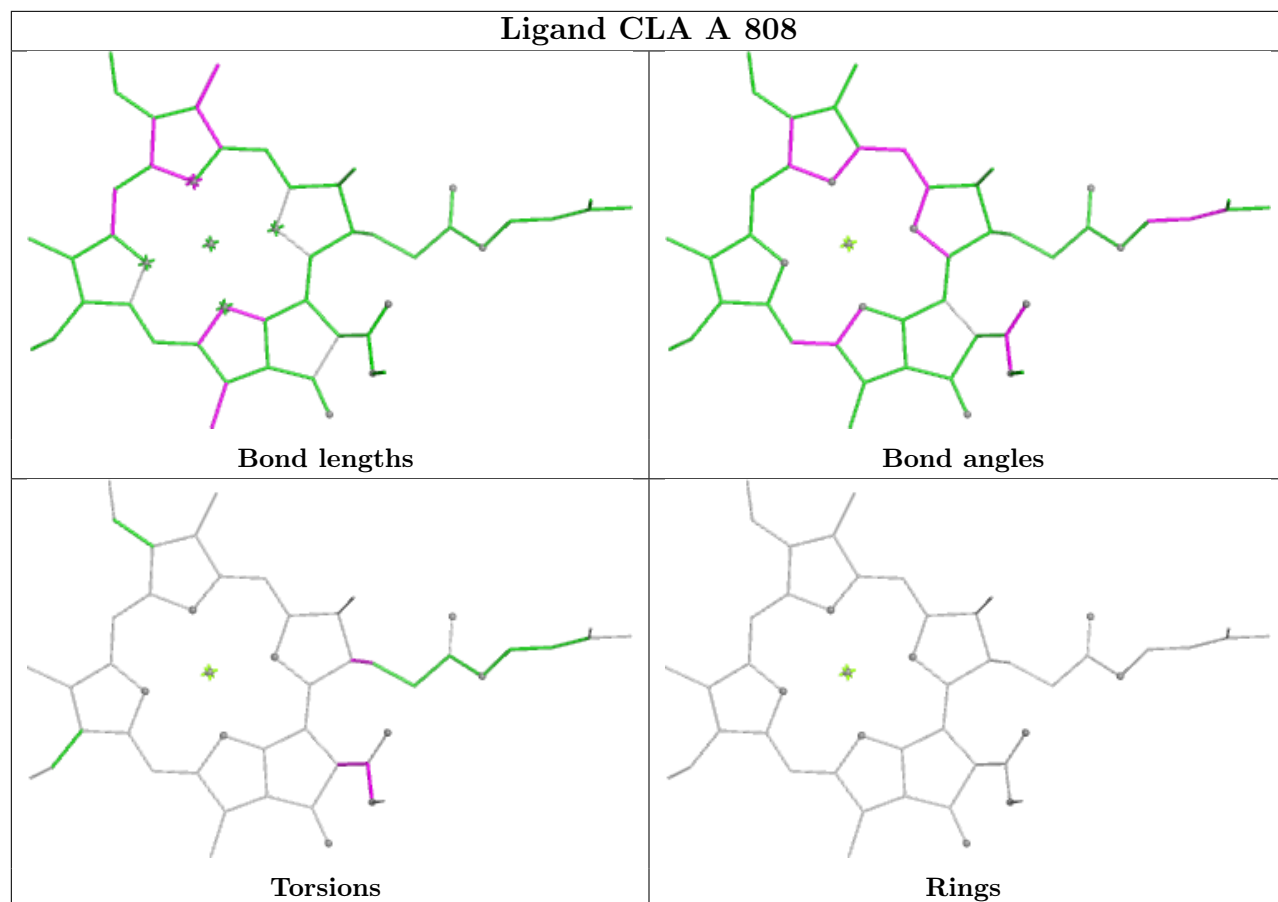


Rings

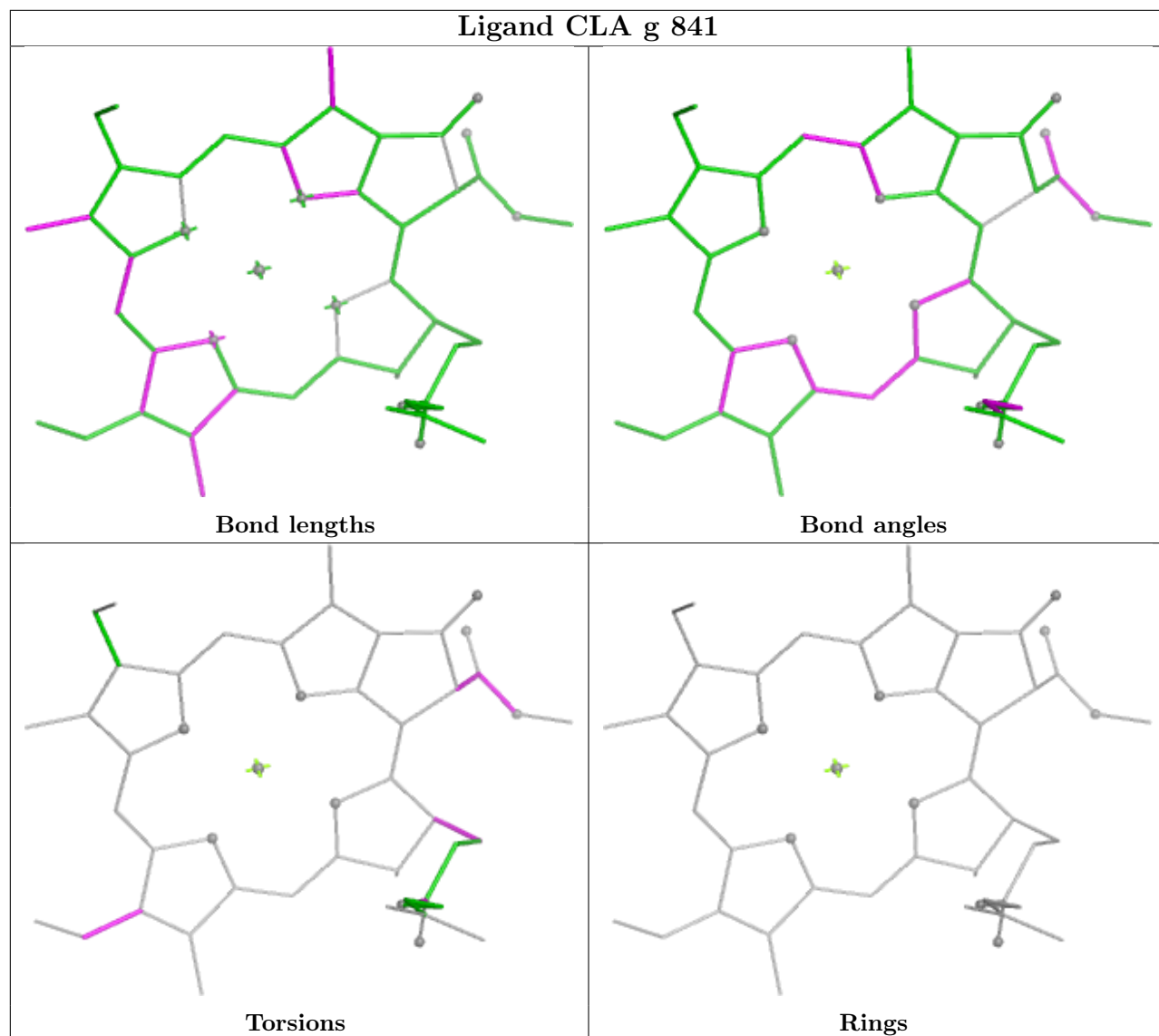
Ligand CLA a 806



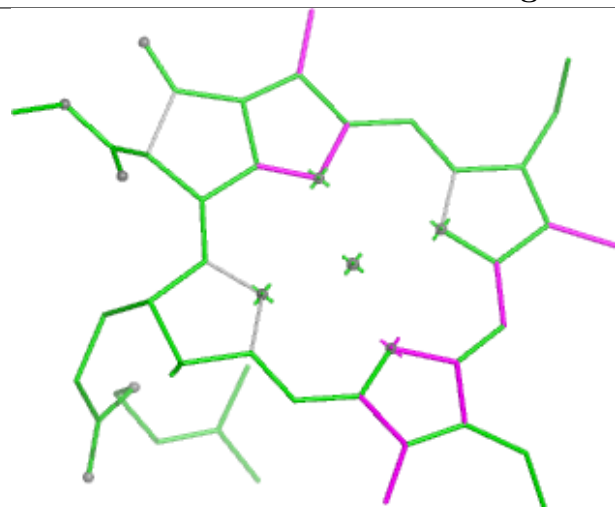
Ligand CLA A 808



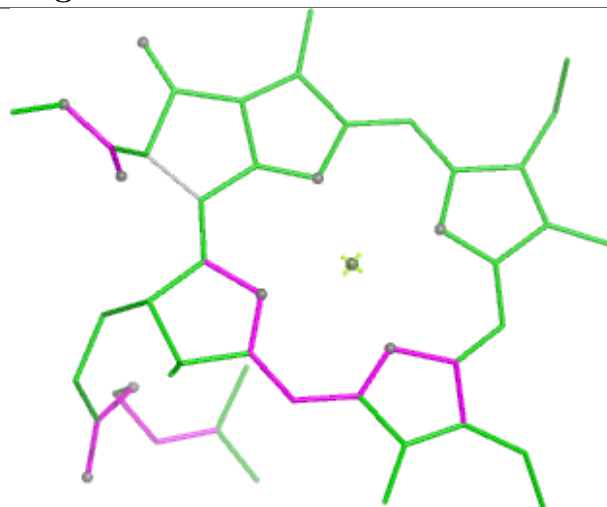
Ligand CLA g 841



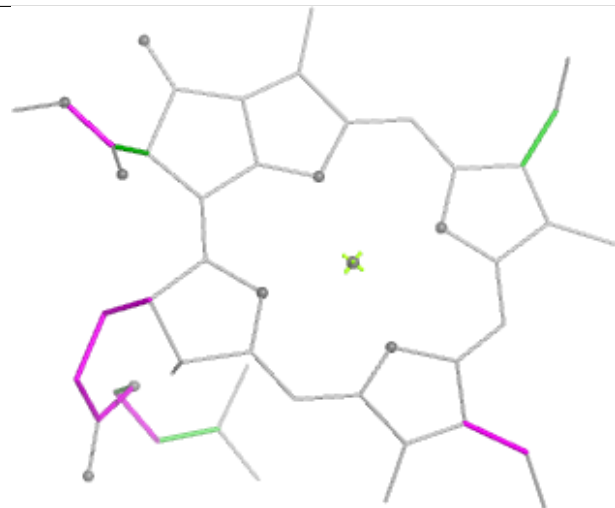
Ligand CLA g 819



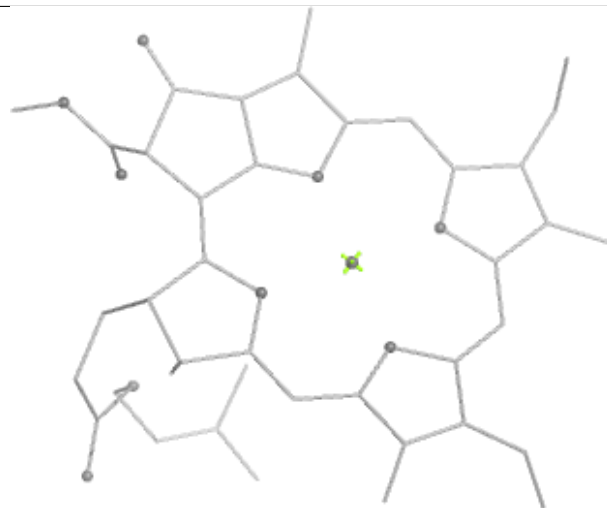
Bond lengths



Bond angles

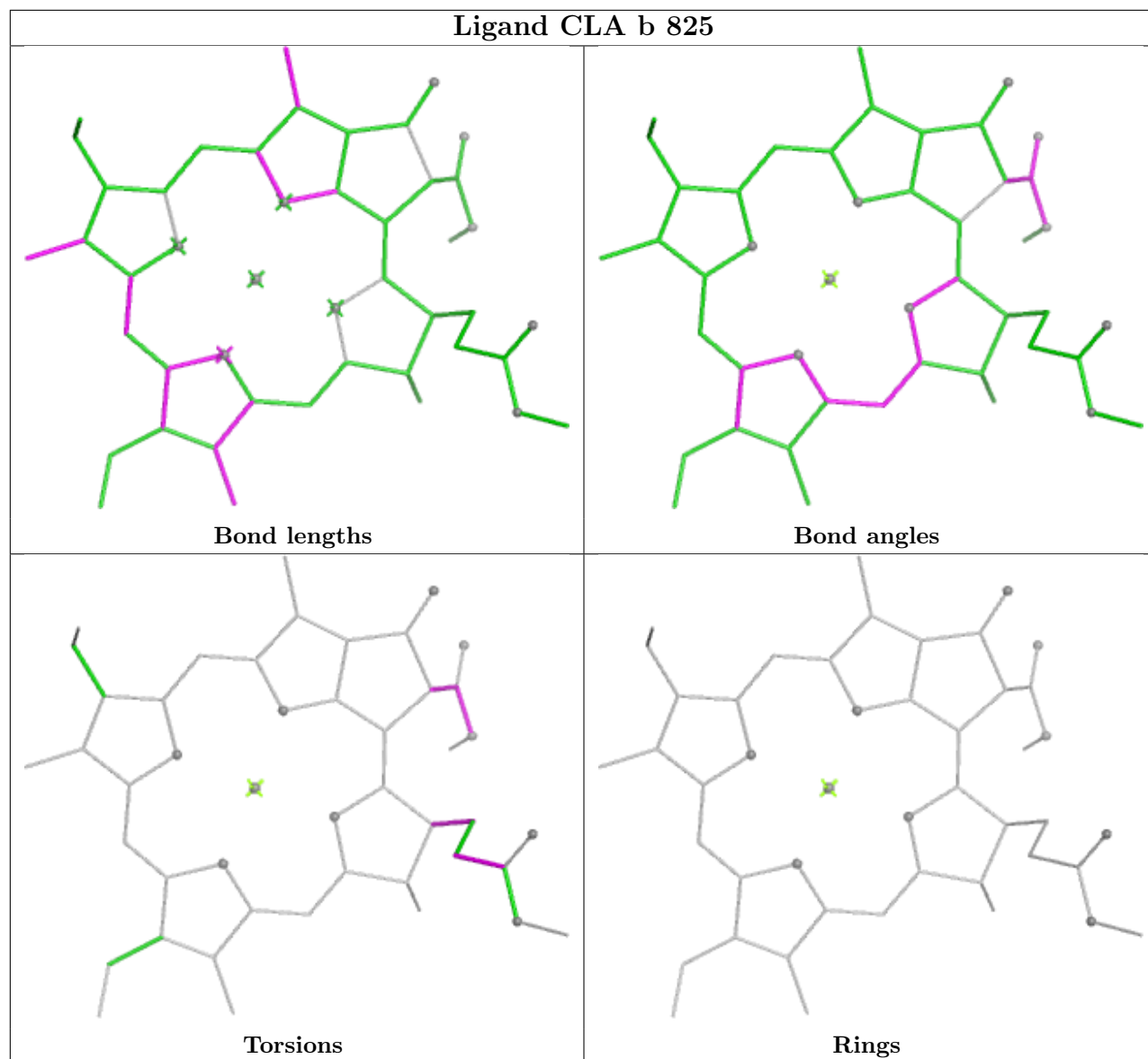


Torsions

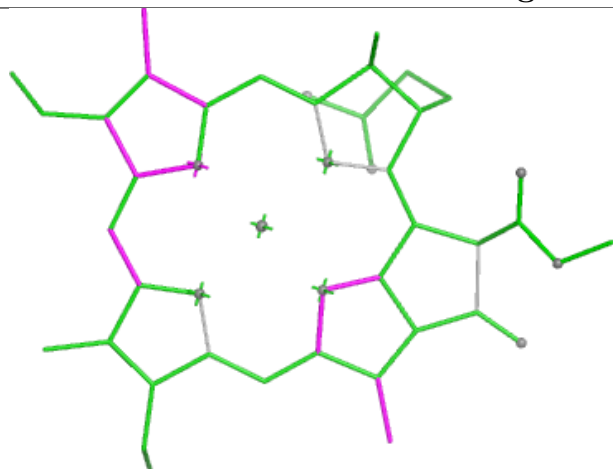


Rings

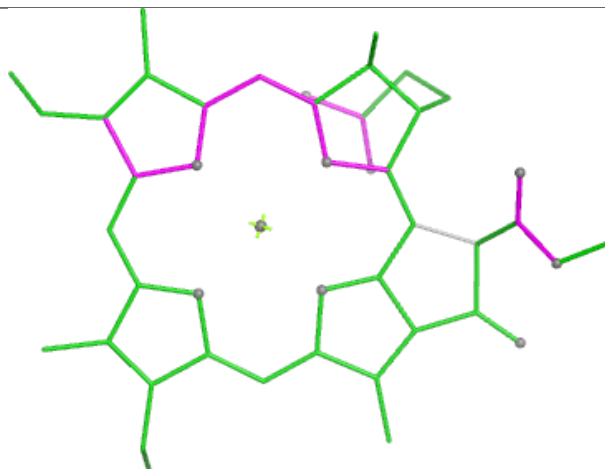
Ligand CLA b 825



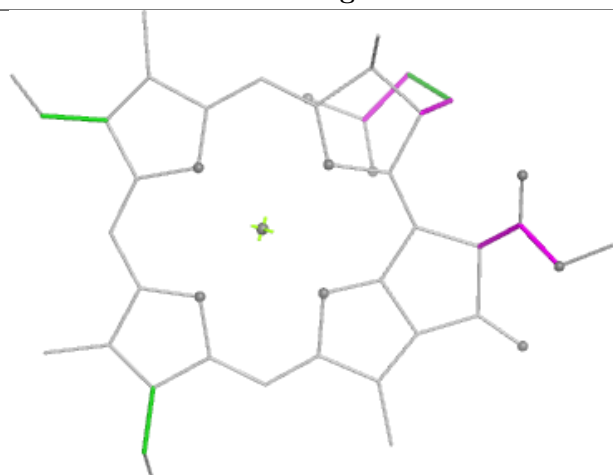
Ligand CLA b 835



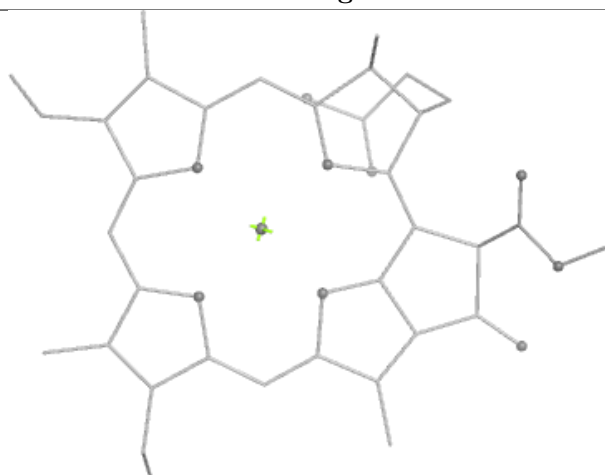
Bond lengths



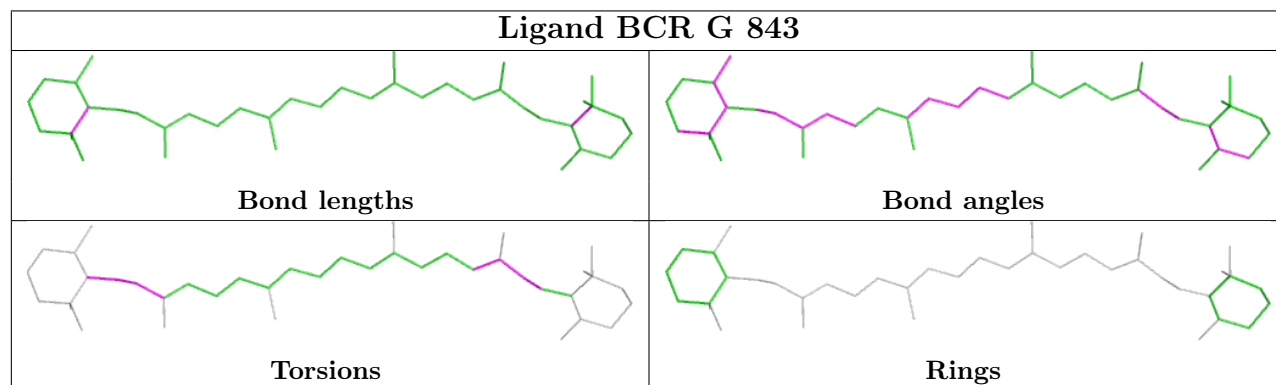
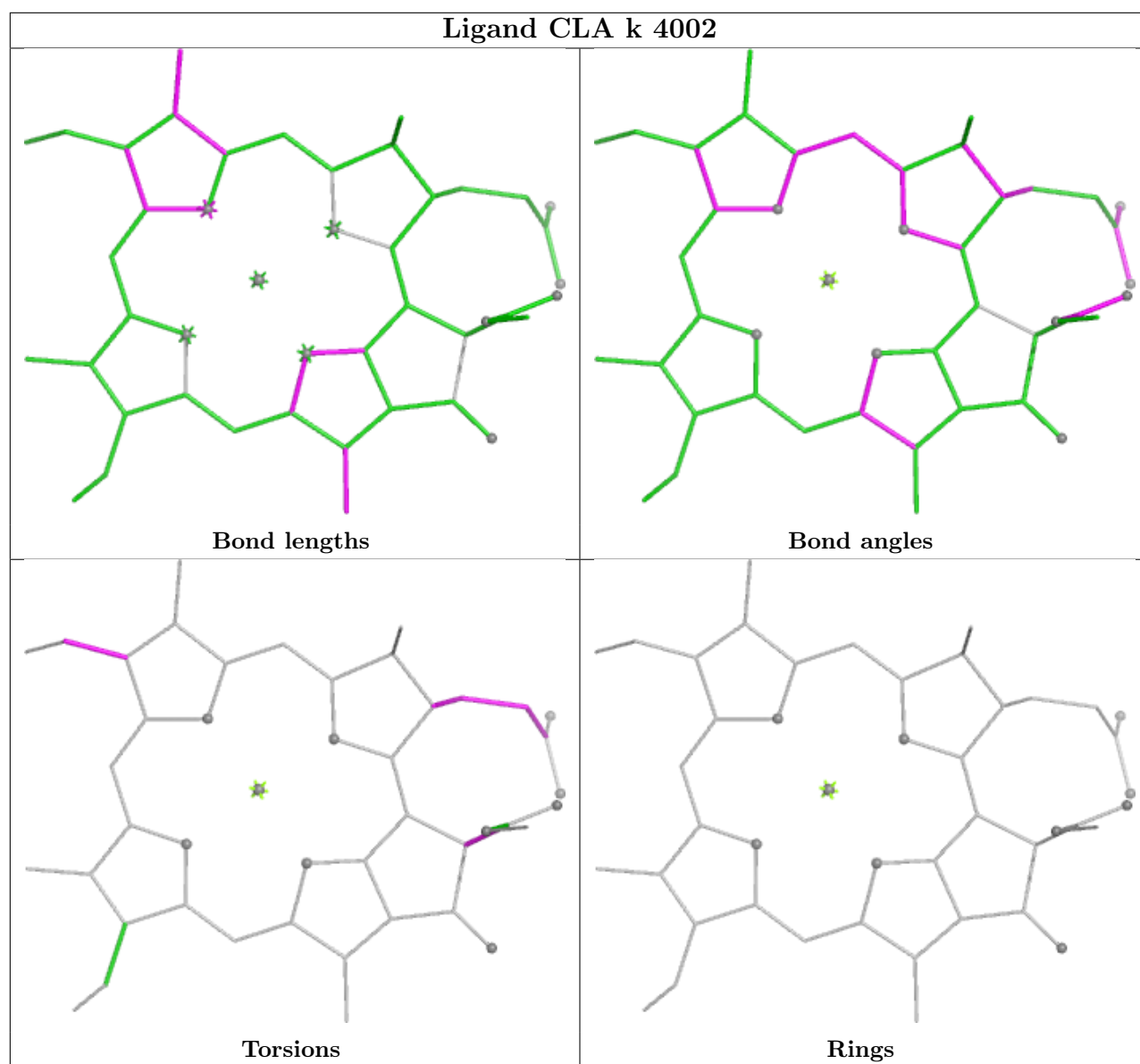
Bond angles



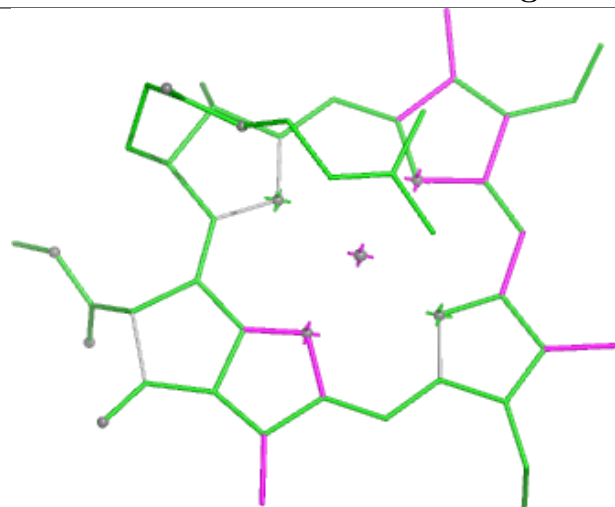
Torsions



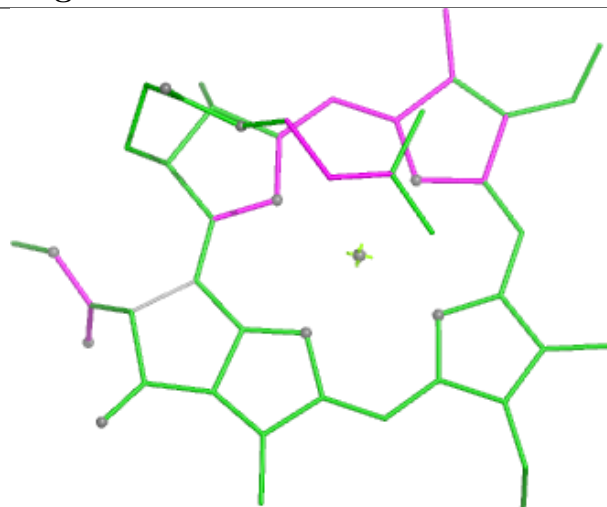
Rings



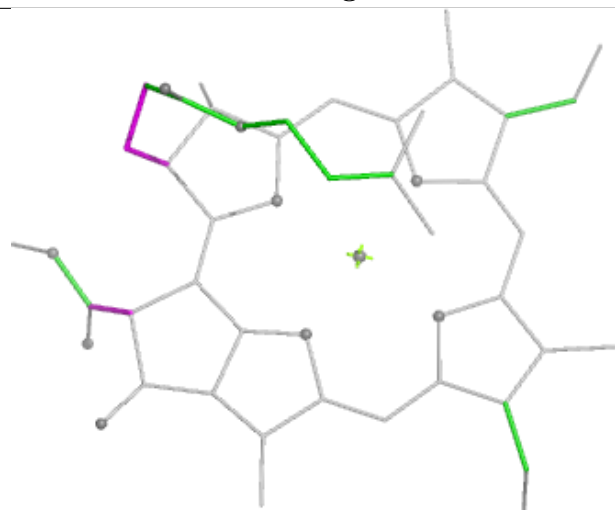
Ligand CLA g 802



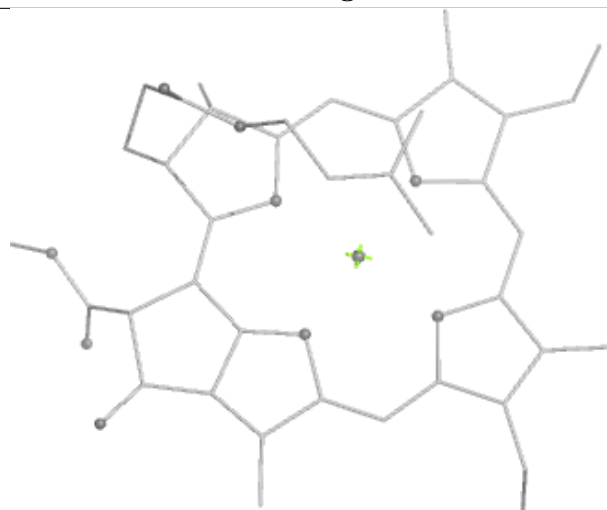
Bond lengths



Bond angles

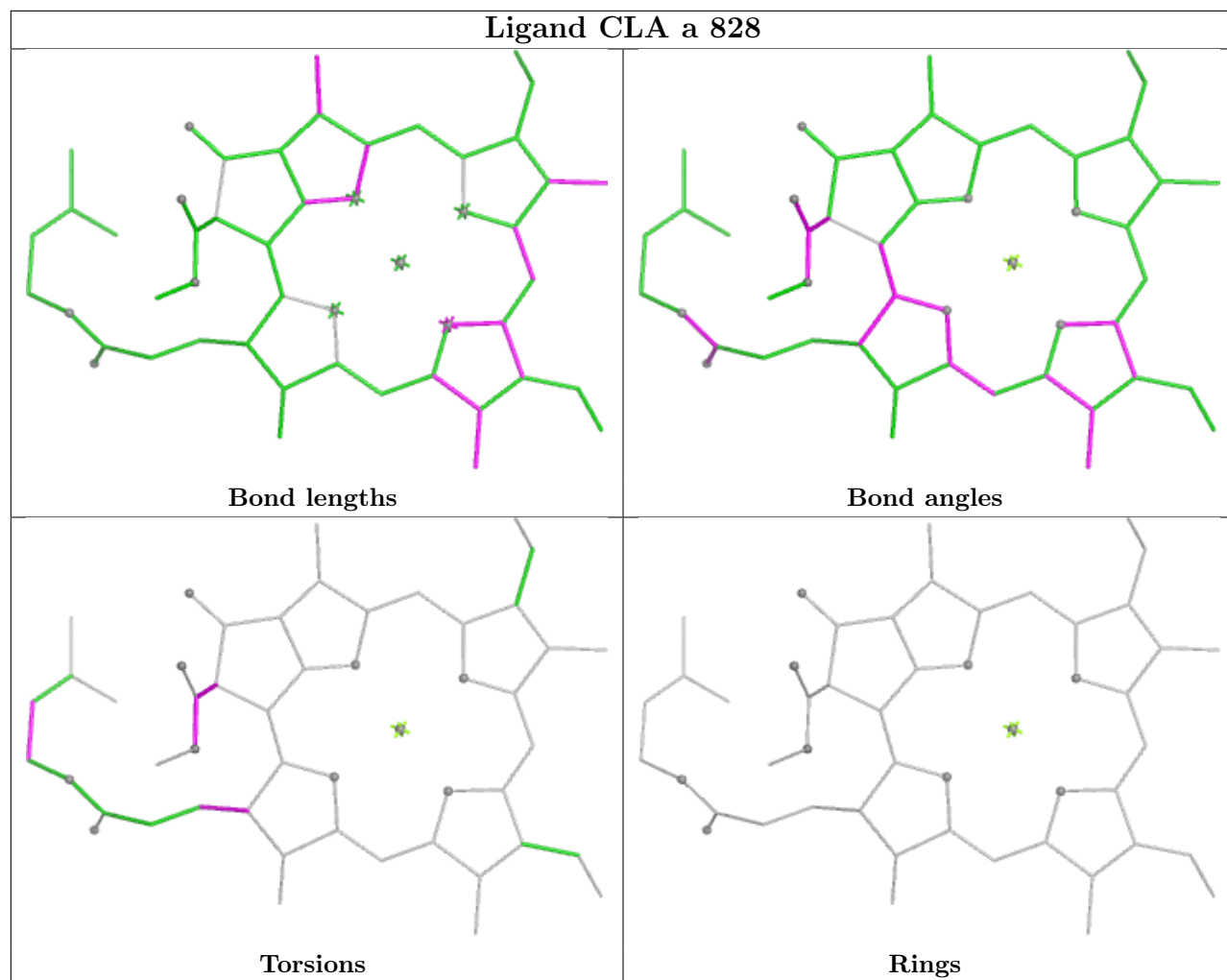


Torsions

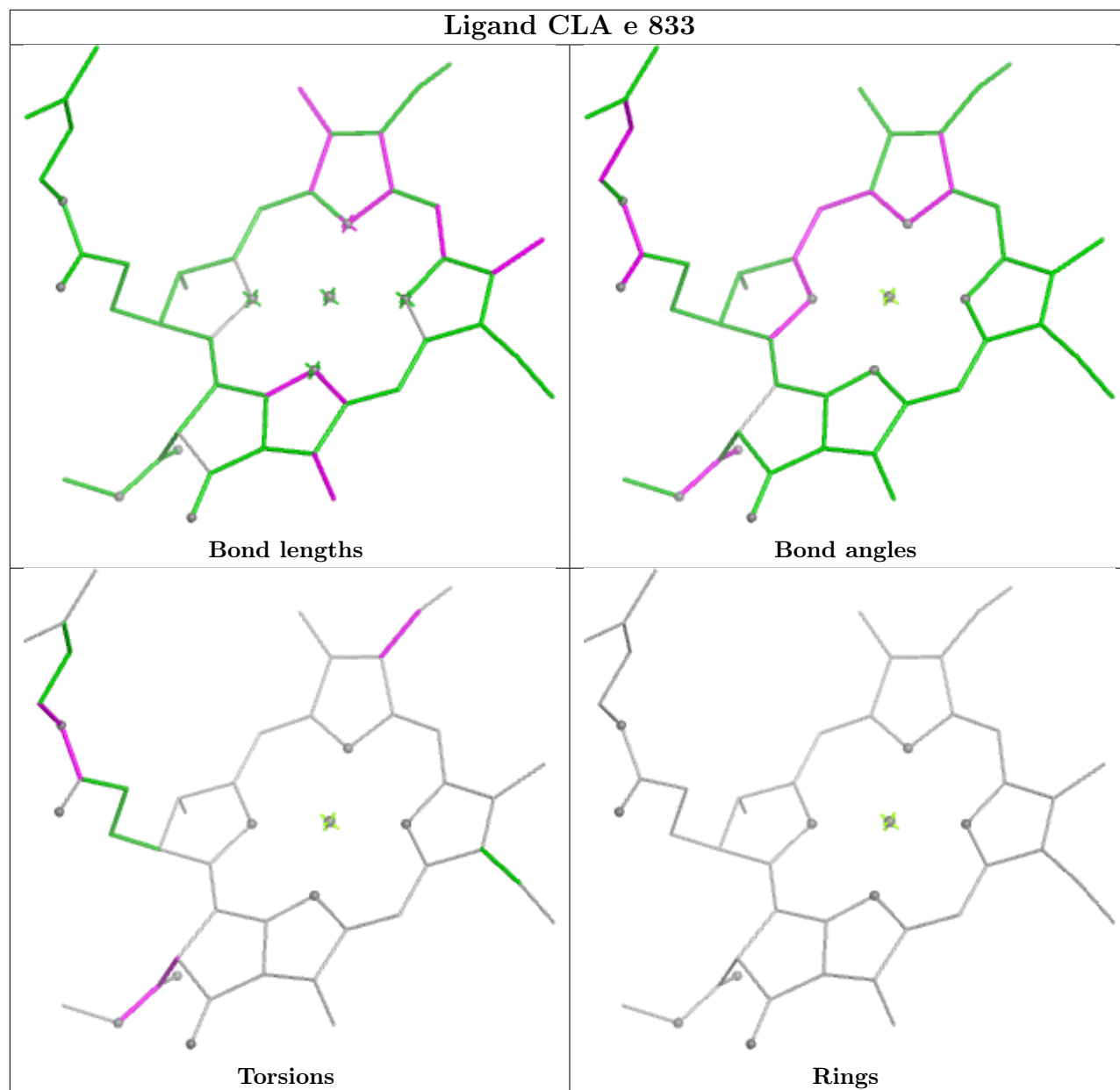


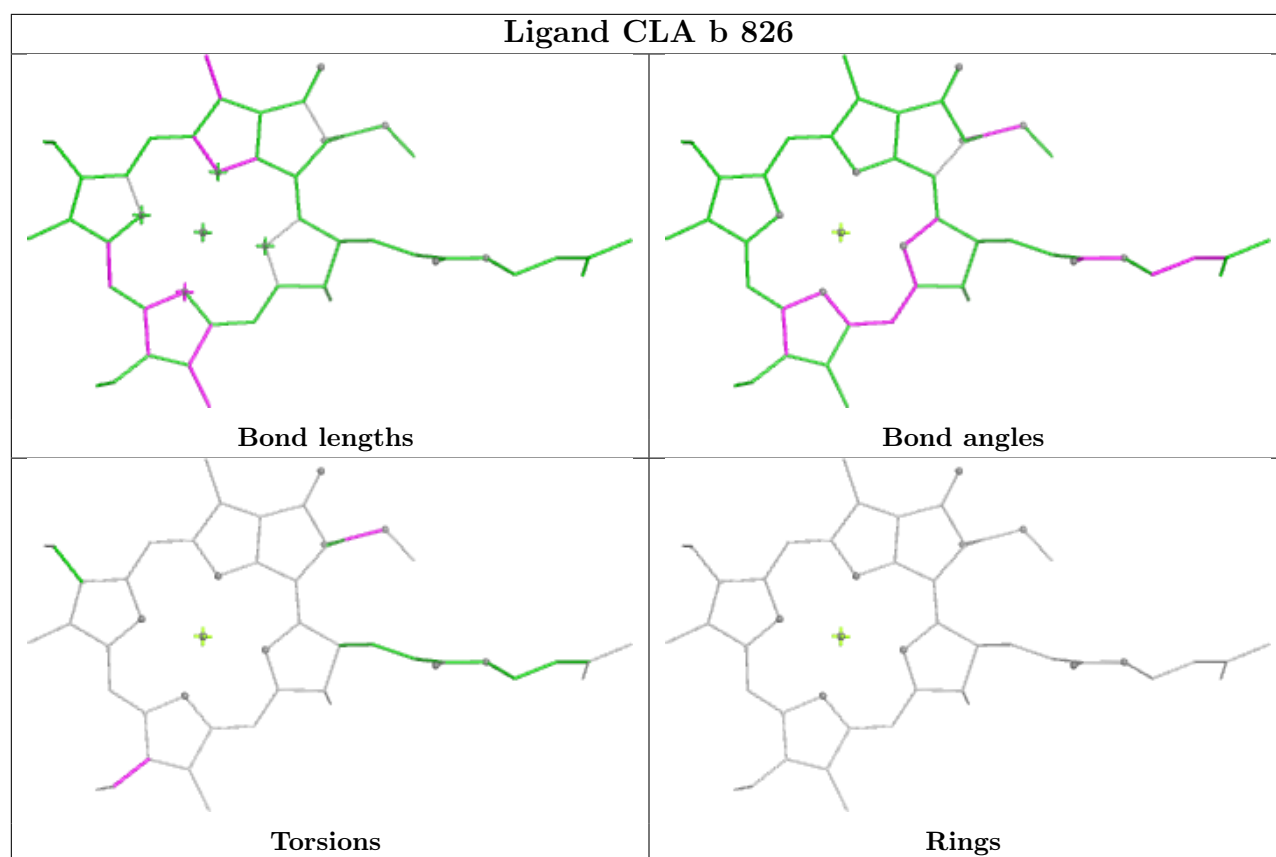
Rings

Ligand CLA a 828

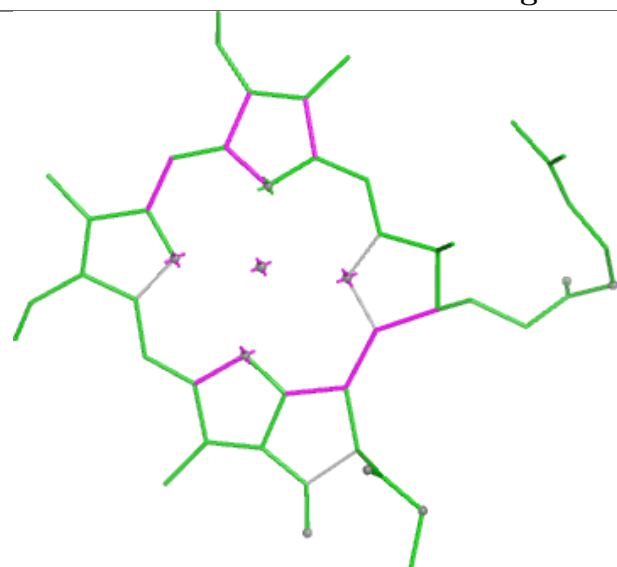


Ligand CLA e 833

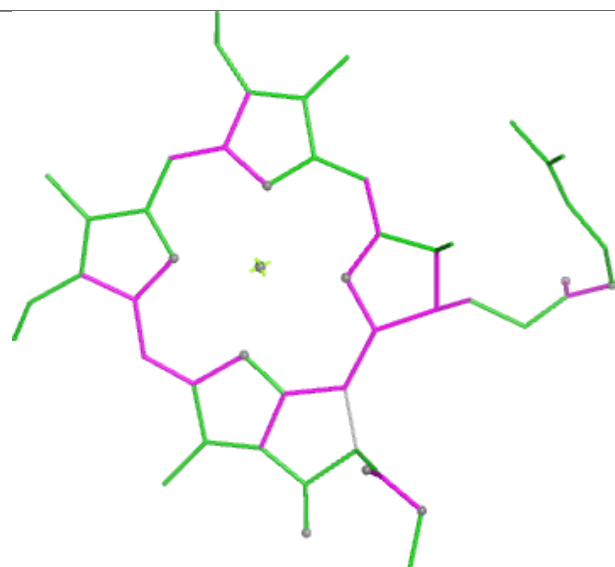




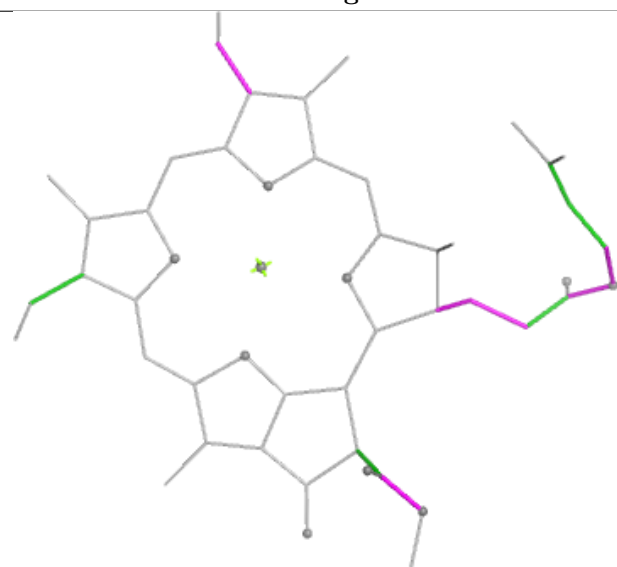
Ligand CLA L 204



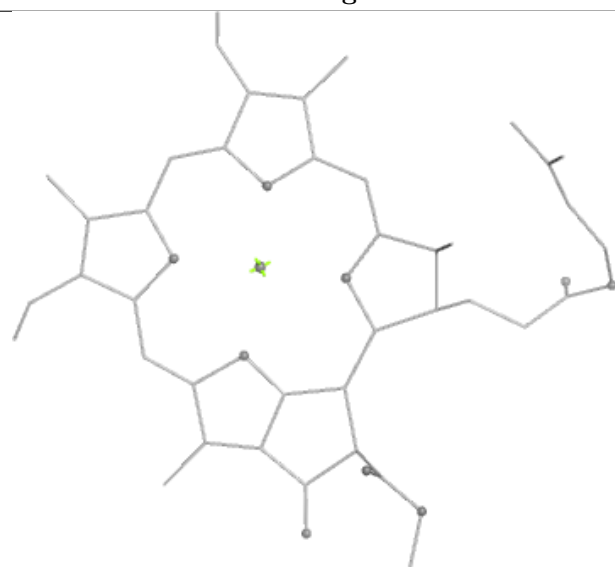
Bond lengths



Bond angles

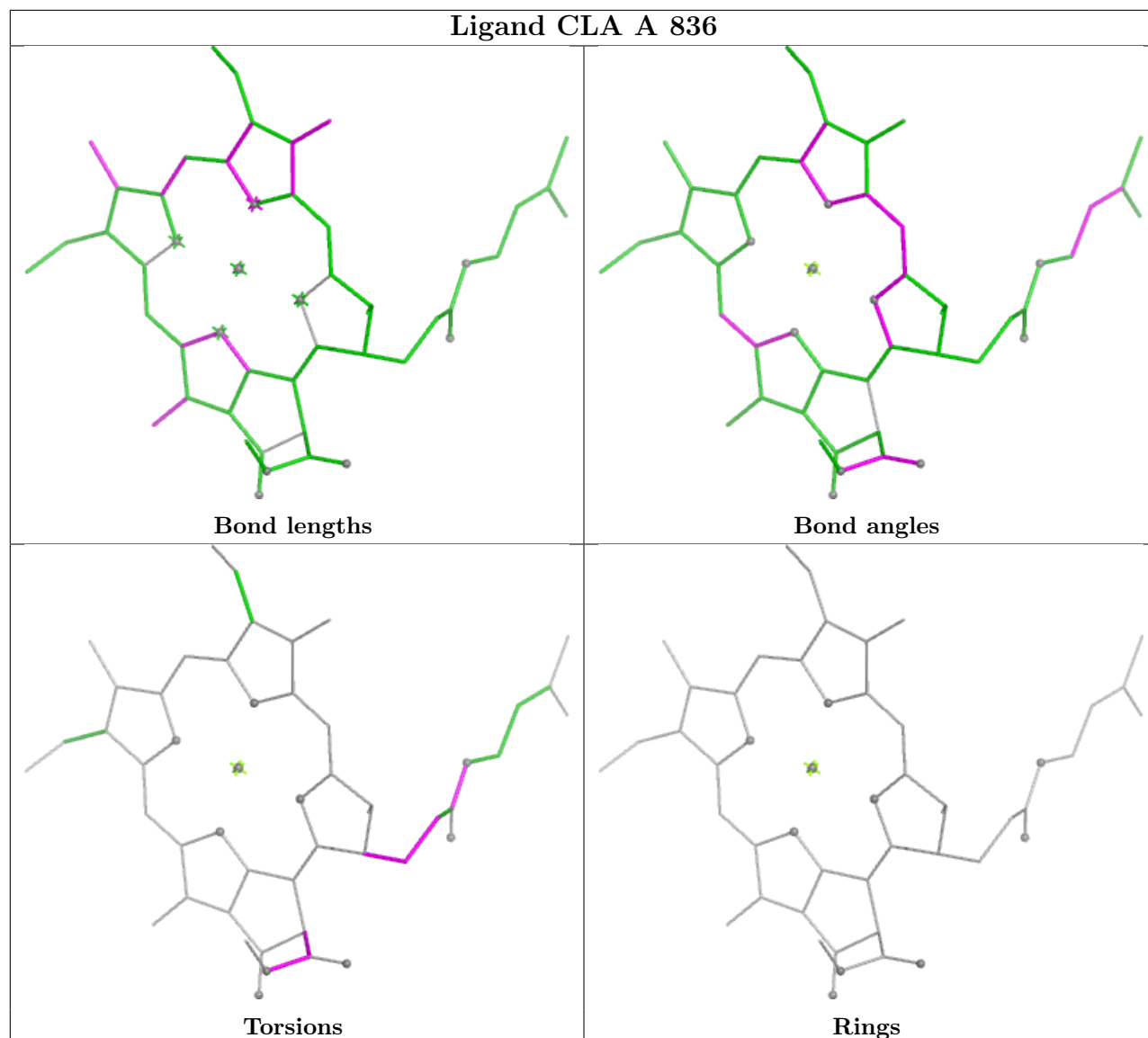


Torsions

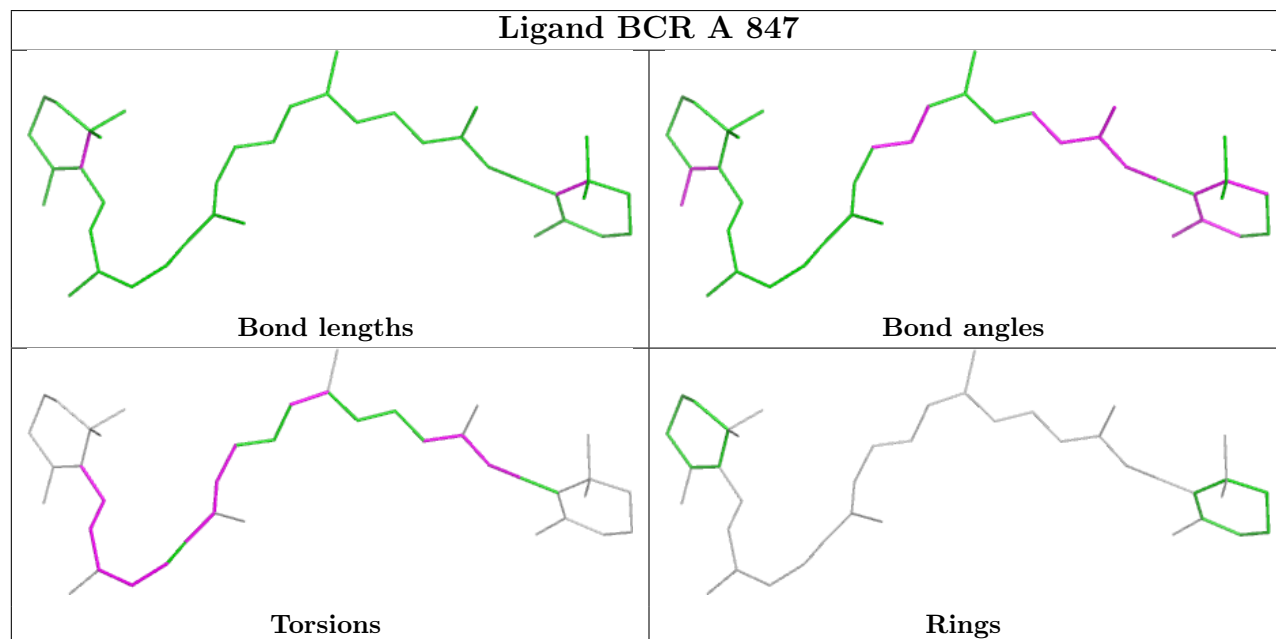


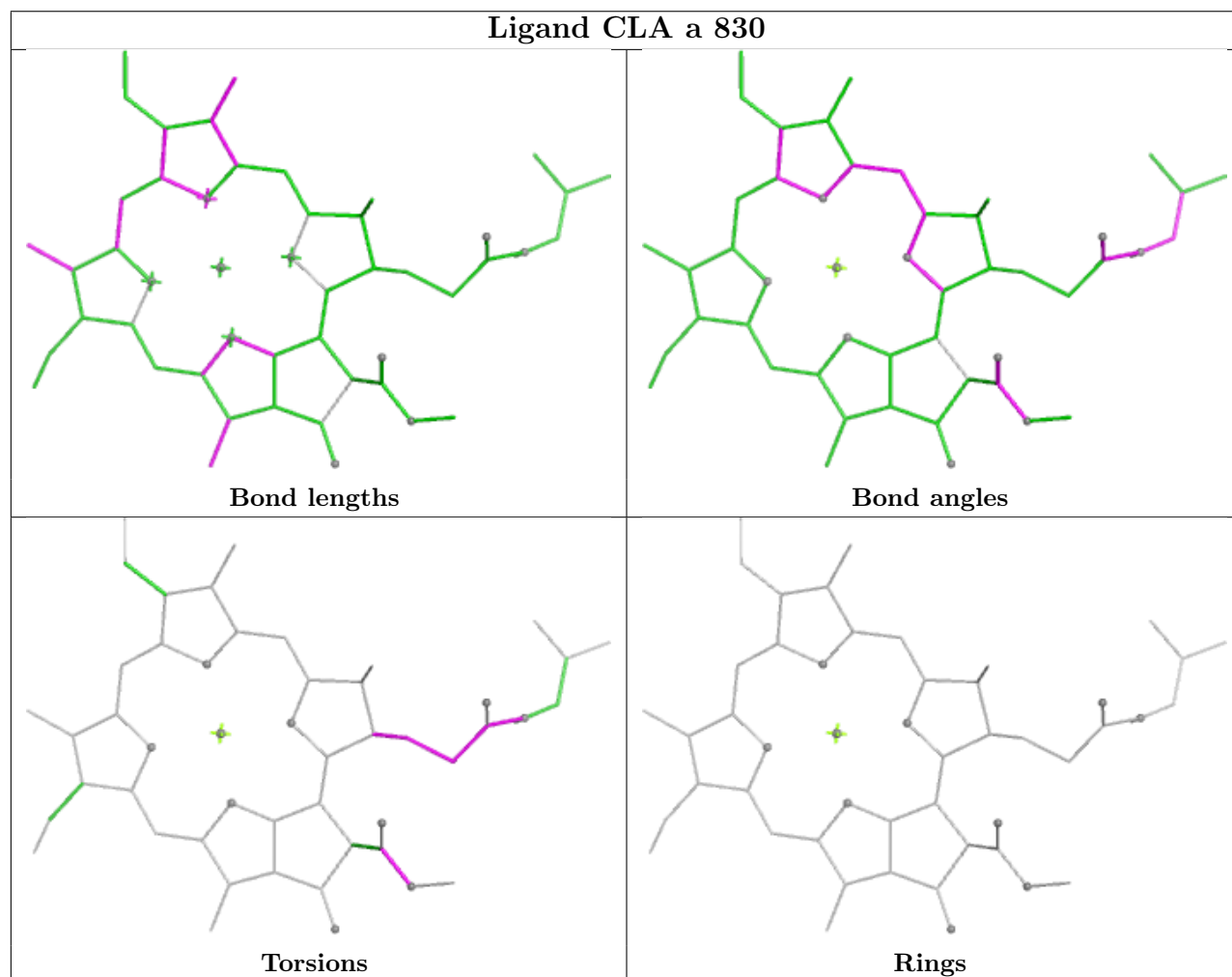
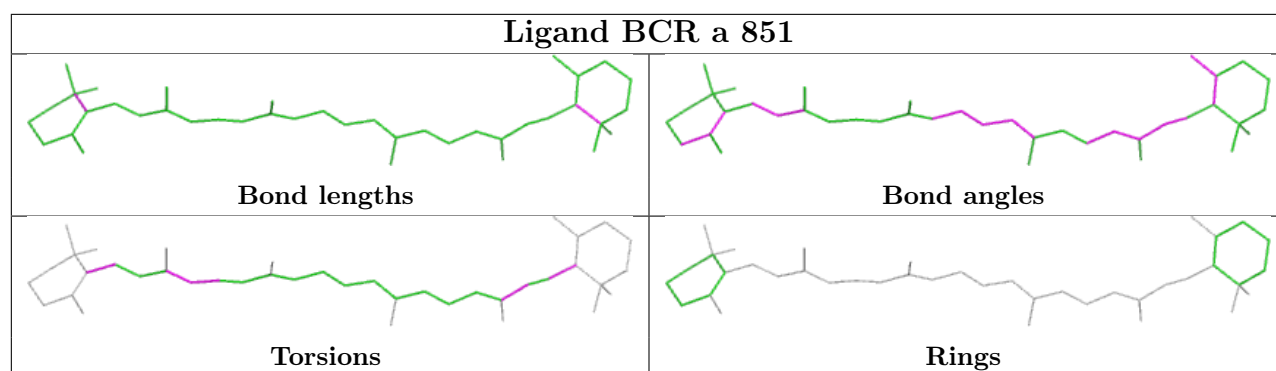
Rings

Ligand CLA A 836

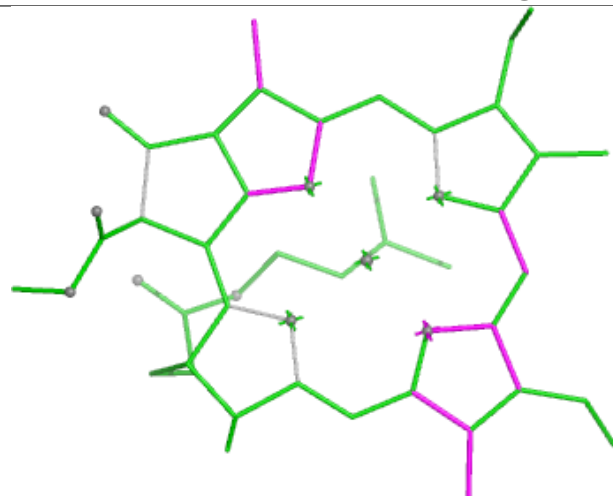


Ligand BCR A 847

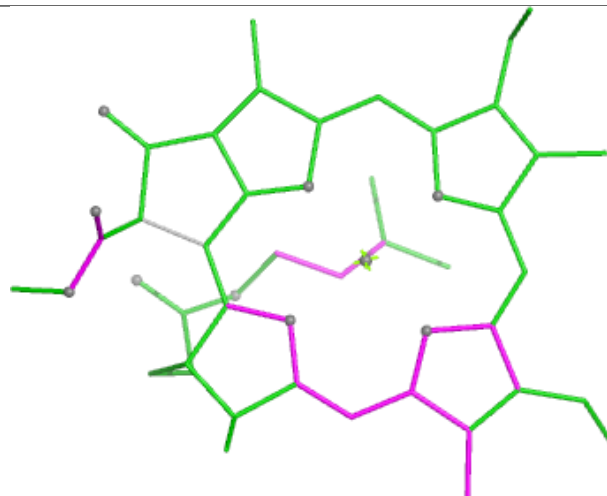




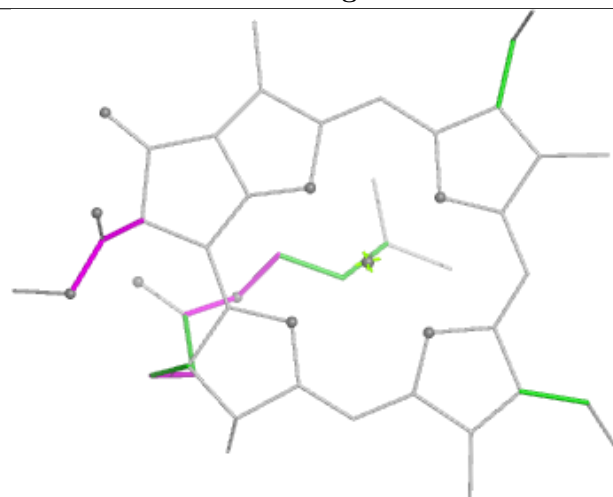
Ligand CLA A 815



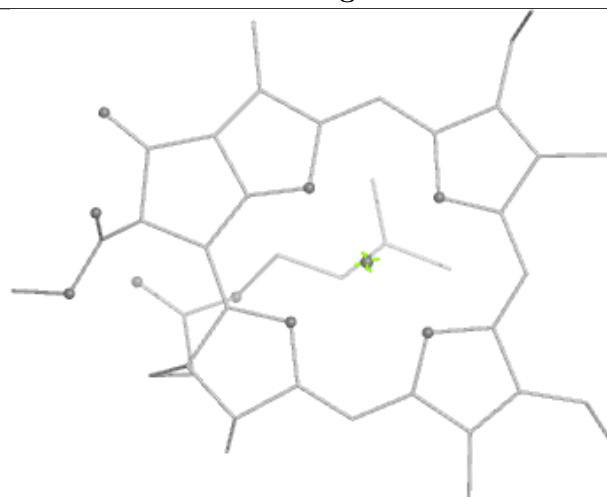
Bond lengths



Bond angles

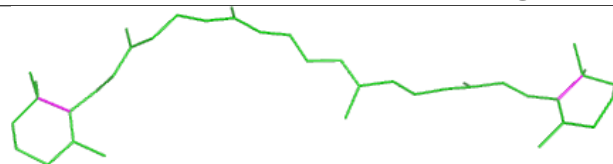


Torsions

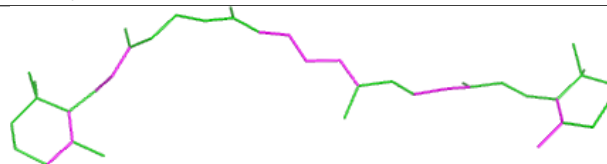


Rings

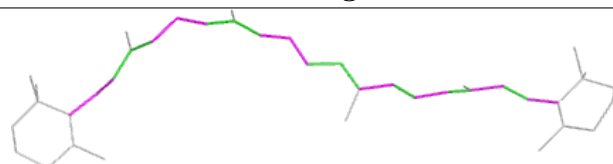
Ligand BCR Q 101



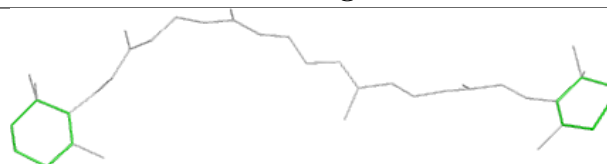
Bond lengths



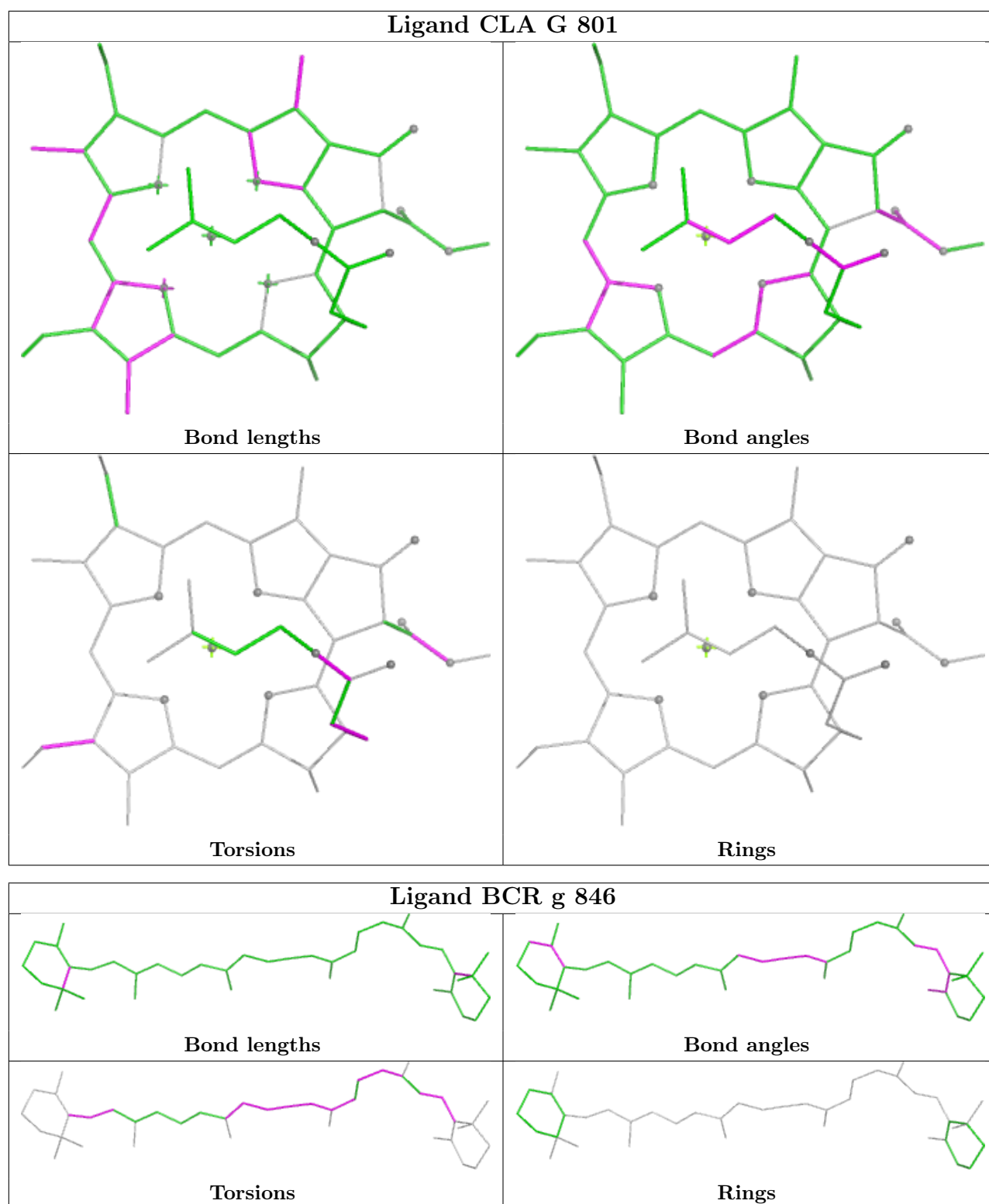
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

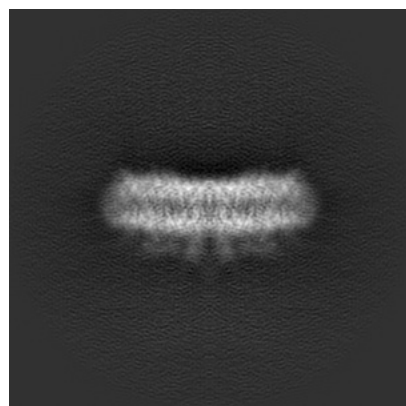
6 Map visualisation [i](#)

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

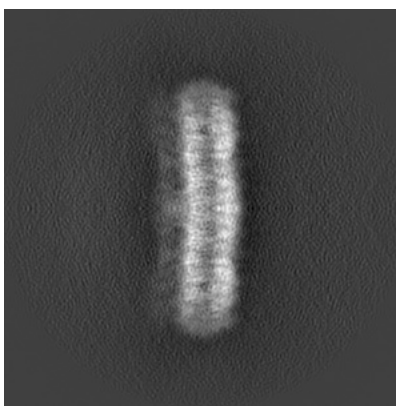
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

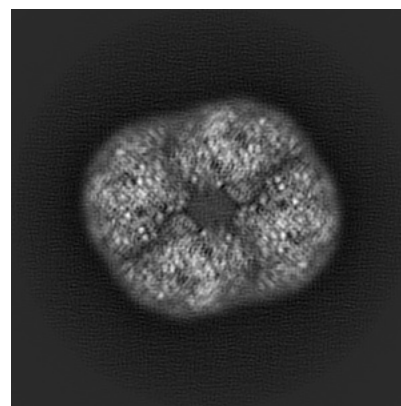
6.1.1 Primary map



X

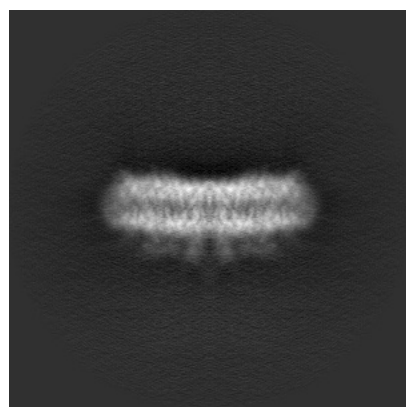


Y

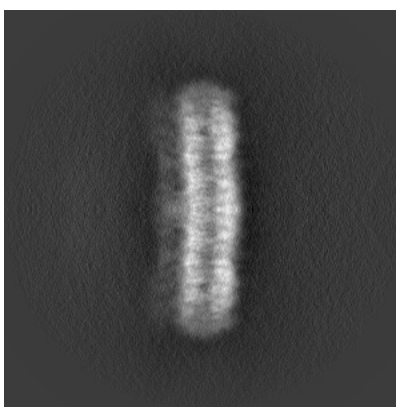


Z

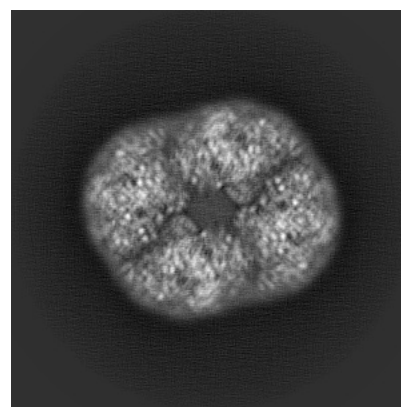
6.1.2 Raw map



X



Y

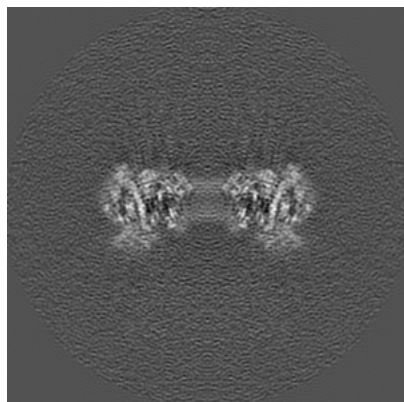


Z

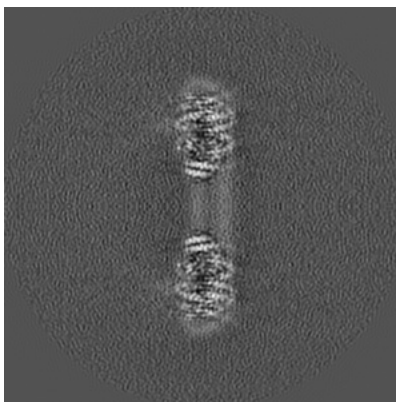
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

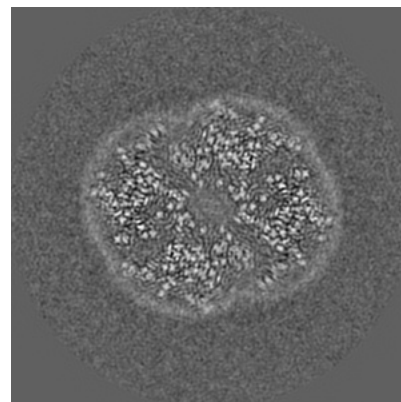
6.2.1 Primary map



X Index: 192

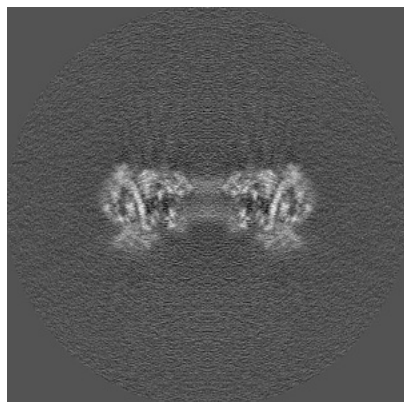


Y Index: 192

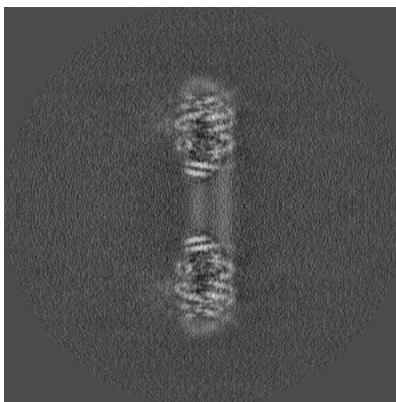


Z Index: 192

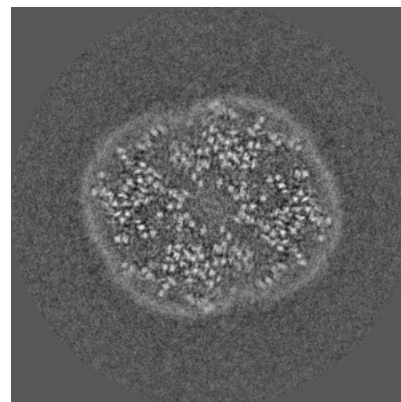
6.2.2 Raw map



X Index: 192



Y Index: 192

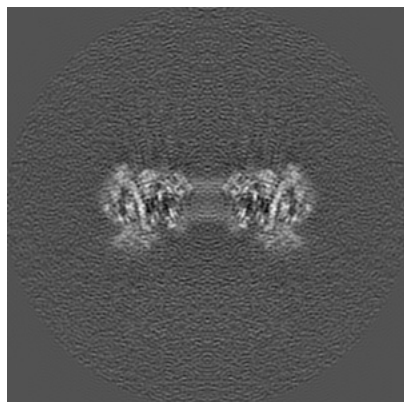


Z Index: 192

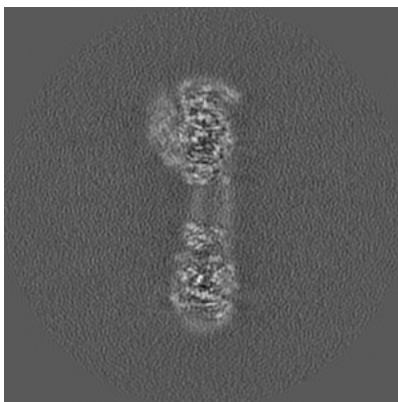
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

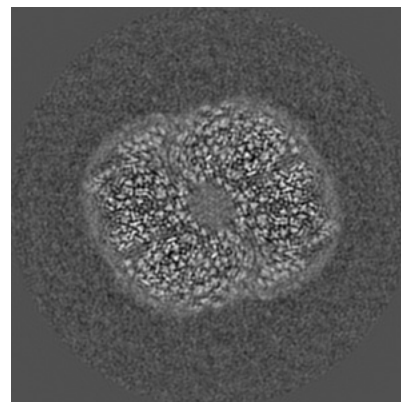
6.3.1 Primary map



X Index: 192

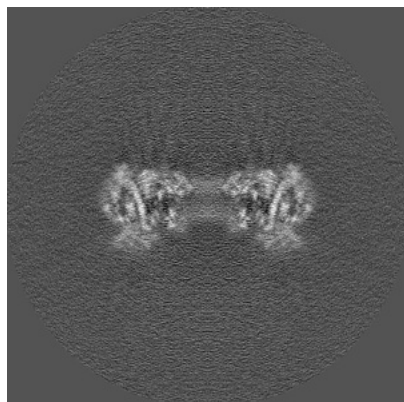


Y Index: 180

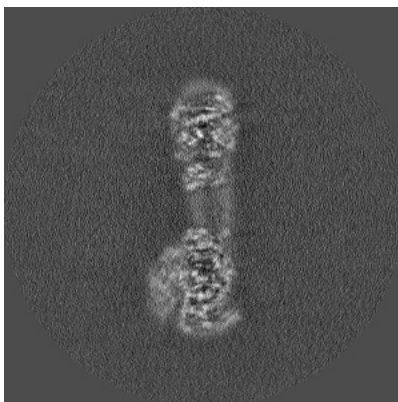


Z Index: 184

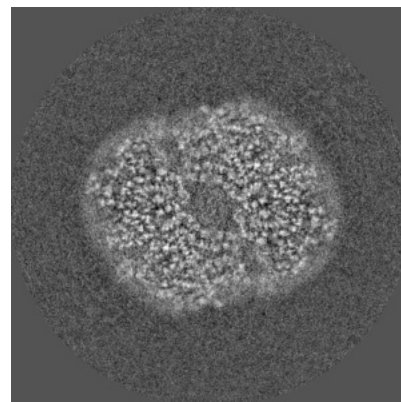
6.3.2 Raw map



X Index: 192



Y Index: 204

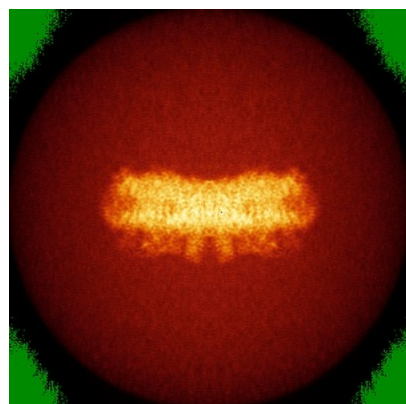


Z Index: 180

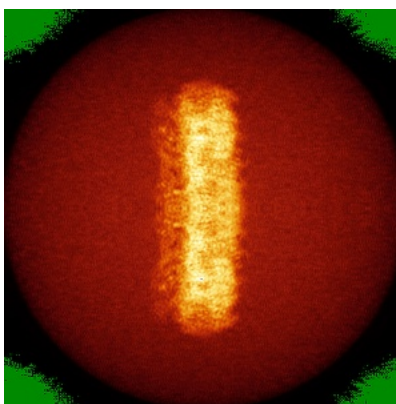
The images above show the largest variance slices of the map in three orthogonal directions.

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

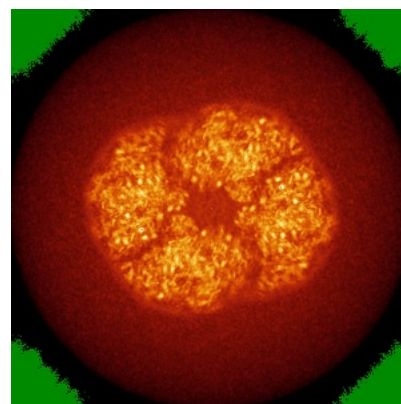
6.4.1 Primary map



X

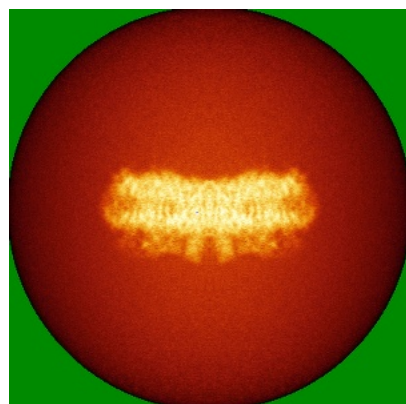


Y

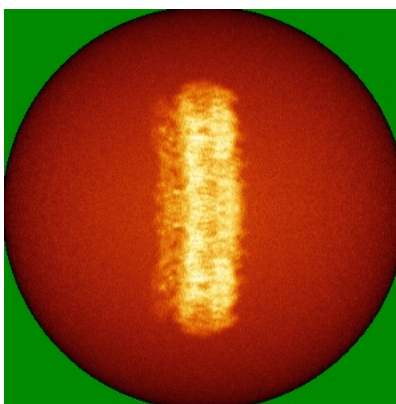


Z

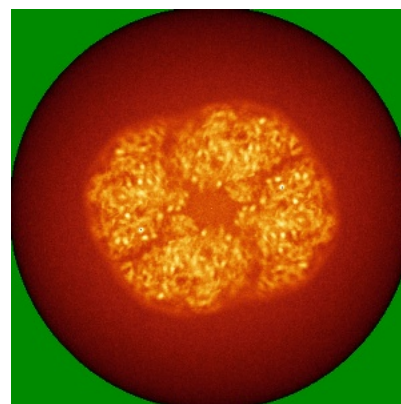
6.4.2 Raw map



X



Y

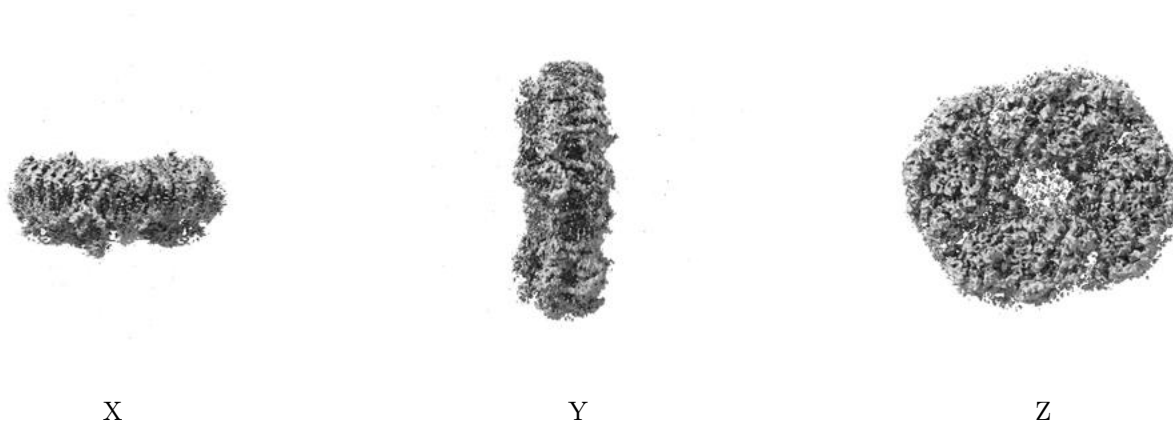


Z

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.

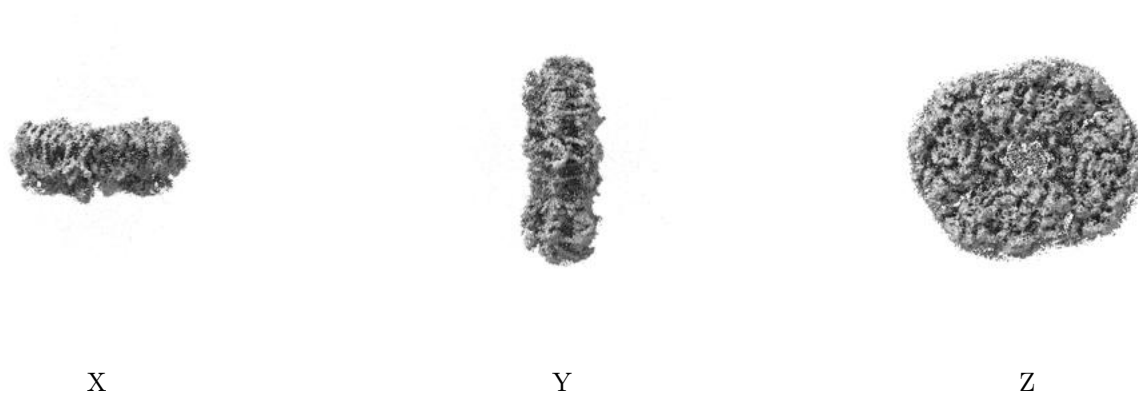
6.5 Orthogonal surface views [i](#)

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.

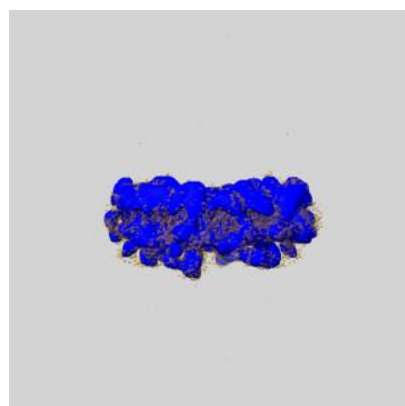
6.6 Mask visualisation [i](#)

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

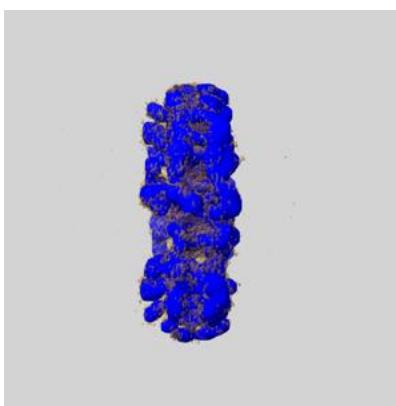
A mask typically either:

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

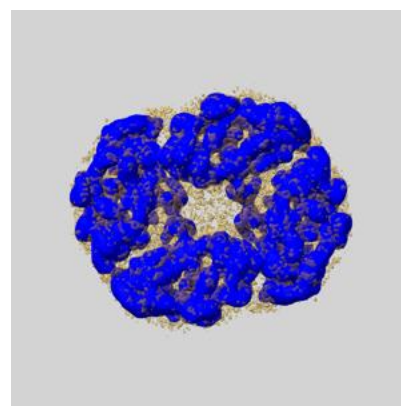
6.6.1 emd_13898_msk_1.map [i](#)



X



Y

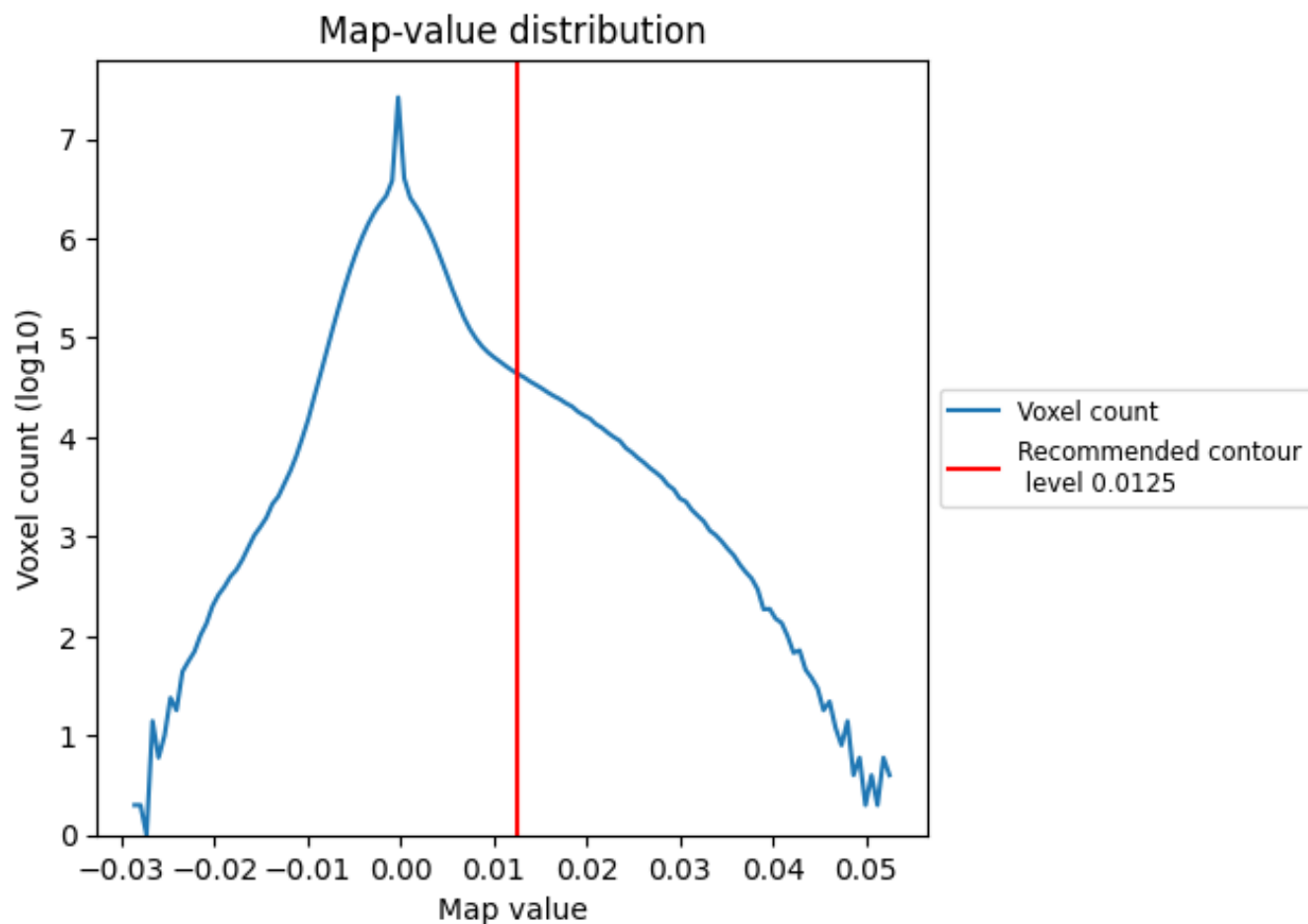


Z

7 Map analysis [i](#)

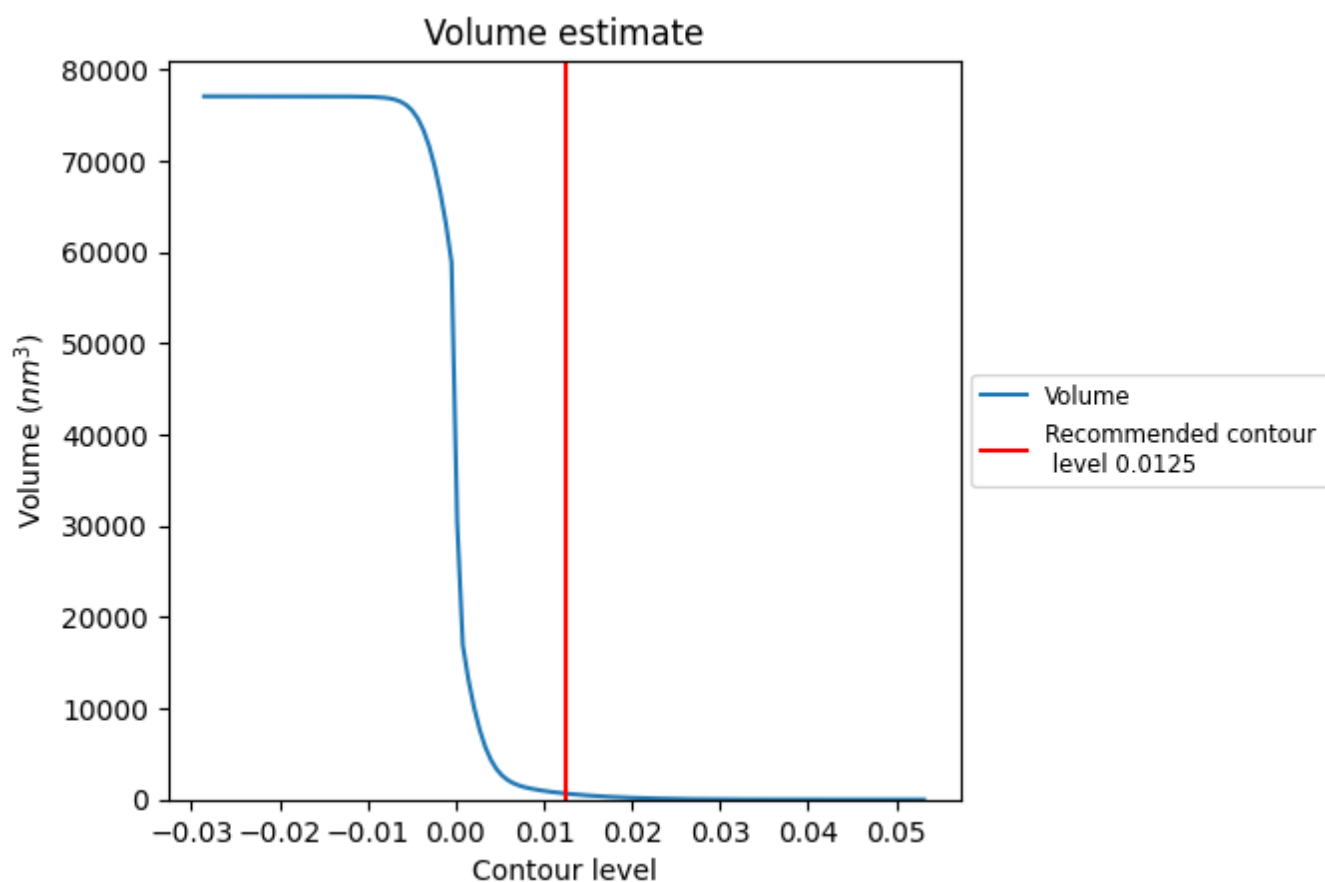
This section contains the results of statistical analysis of the map.

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.

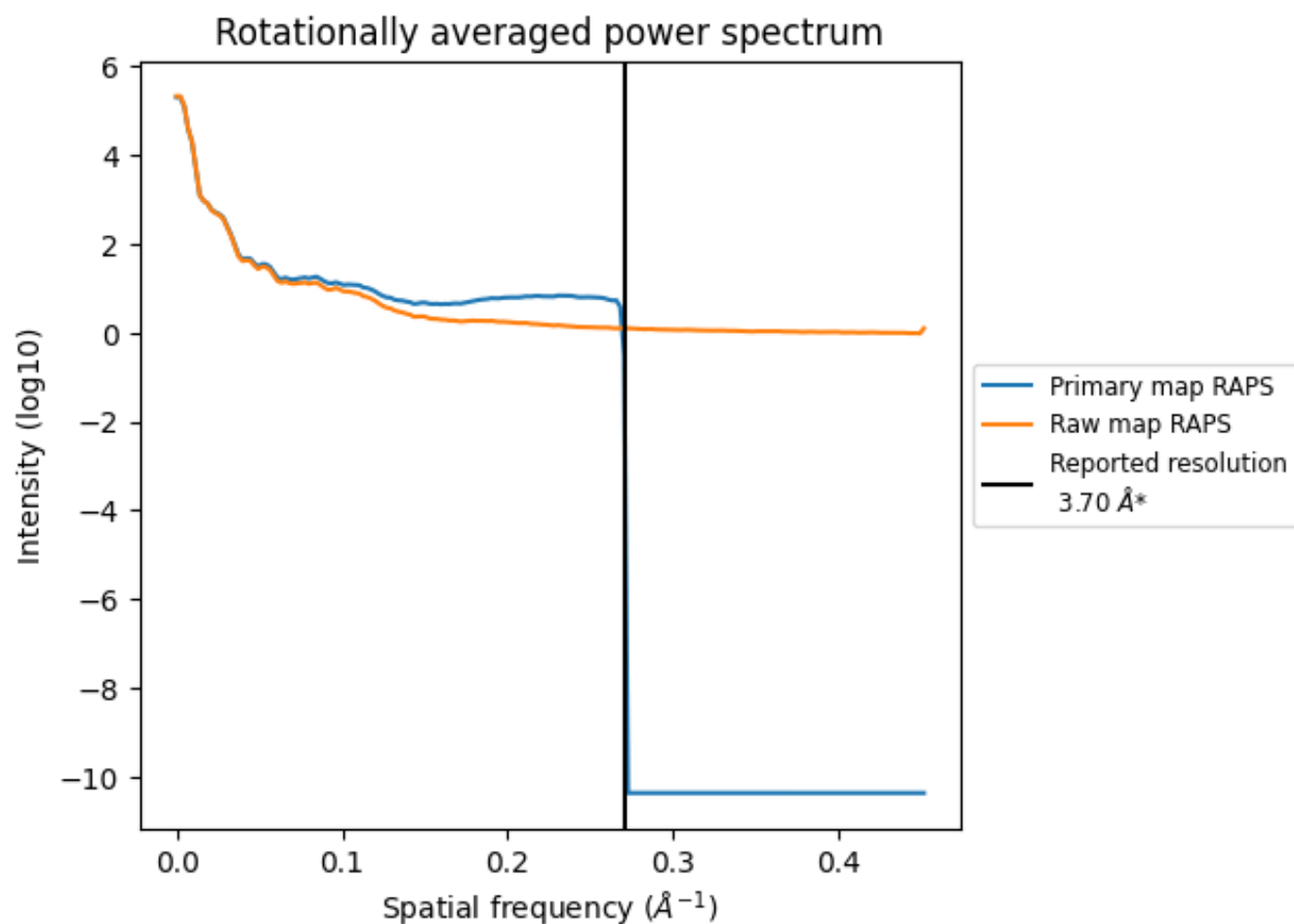
7.2 Volume estimate [i](#)



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 ⓘ

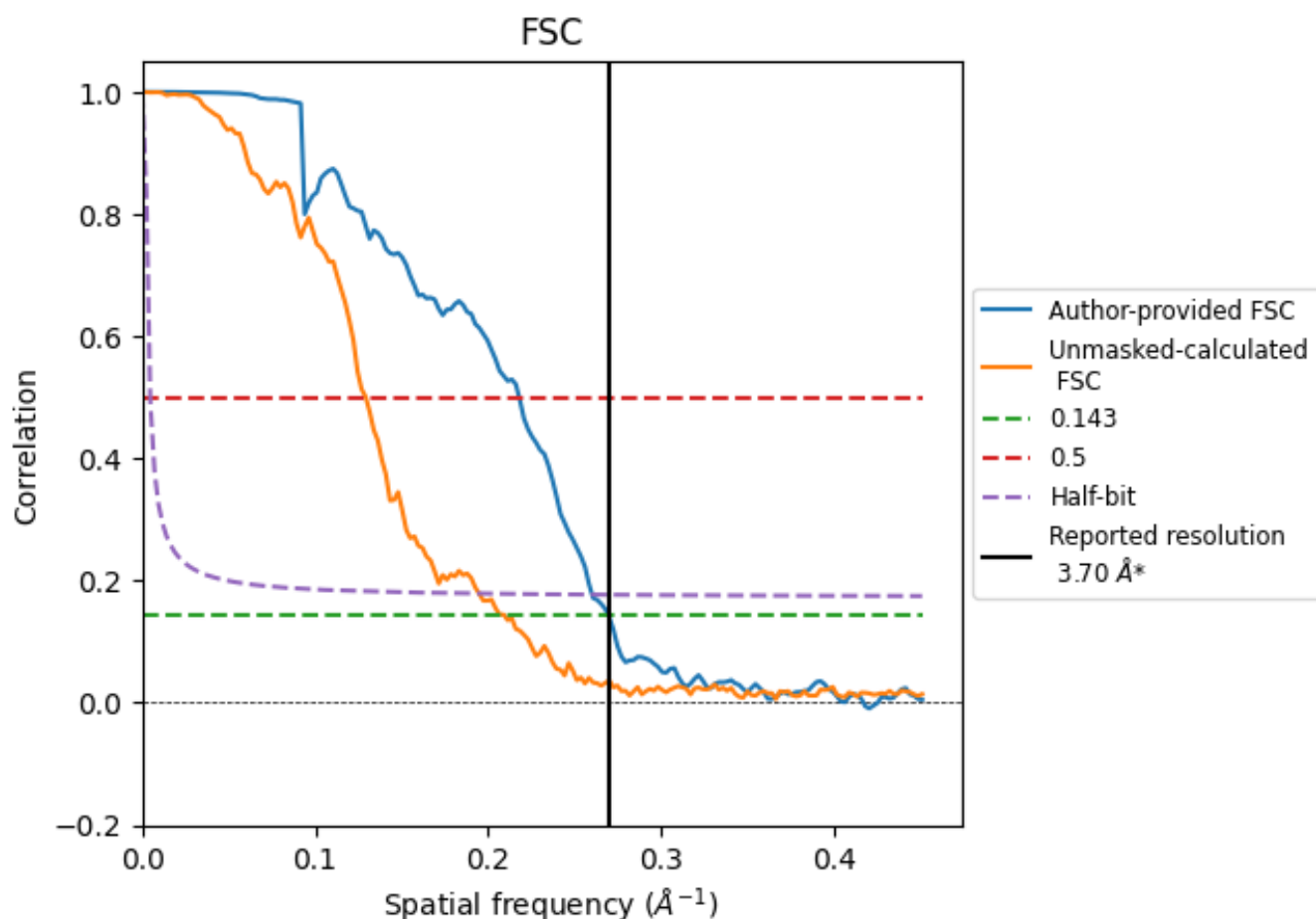


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

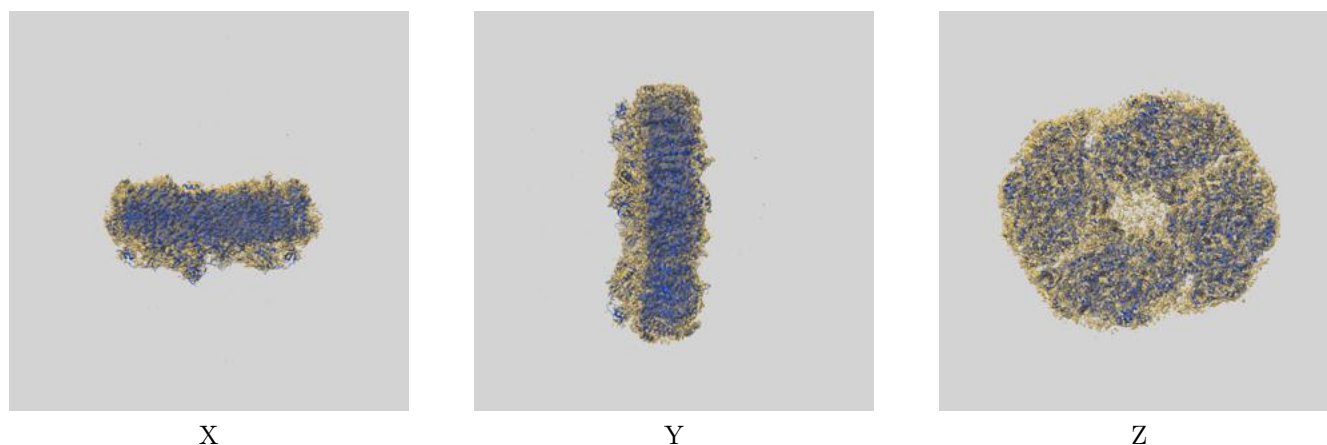
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.71	4.59	3.84
Unmasked-calculated*	4.77	7.73	5.13

*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](#)

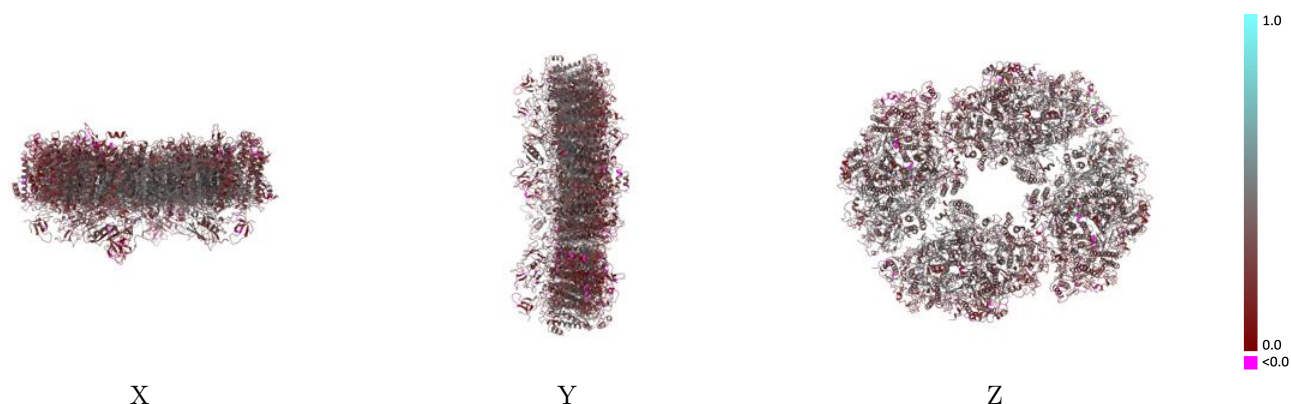
This section contains information regarding the fit between EMDB map EMD-13898 and PDB model 7QCO. Per-residue inclusion information can be found in section [3](#) on page [34](#).

9.1 Map-model overlay [i](#)



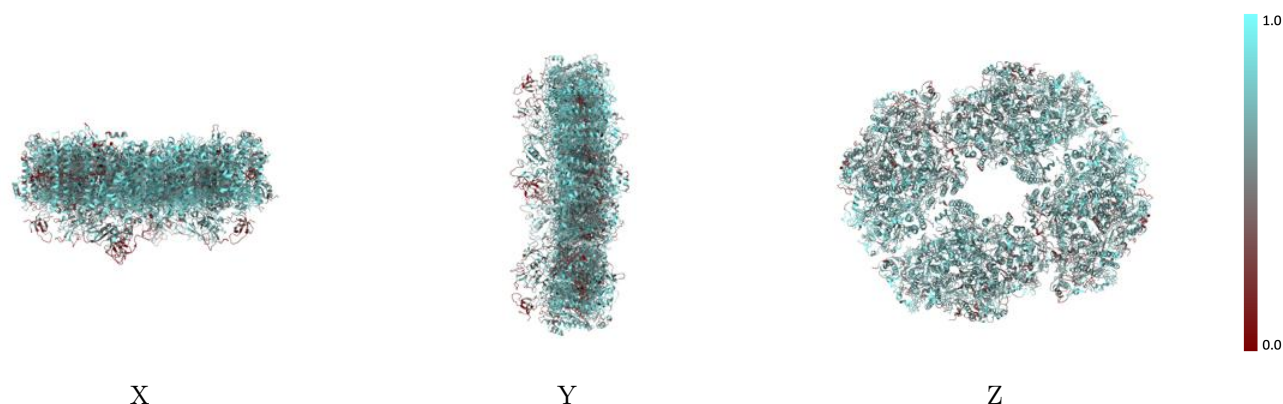
The images above show the 3D surface view of the map at the recommended contour level 0.0125 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



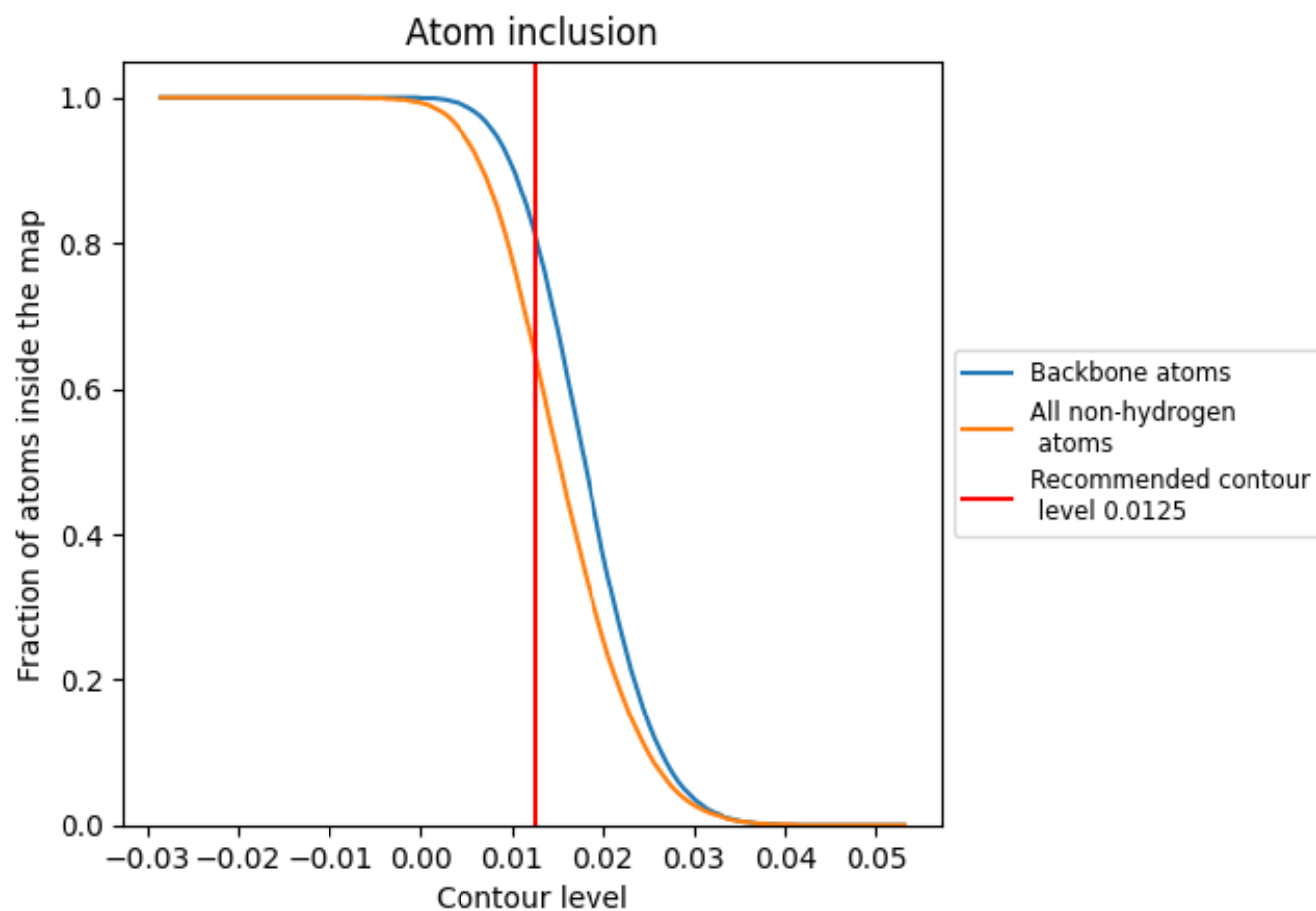
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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