



wwPDB EM Validation Summary Report ⓘ

Sep 10, 2026 – 01:48 am BST

PDB ID : 6TCL / pdb_00006tcl
EMDB ID : EMD-10461
Title : Photosystem I tetramer
Authors : Chen, M.; Perez-Boerema, A.; Li, S.; Amunts, A.
Deposited on : 2019-11-06
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

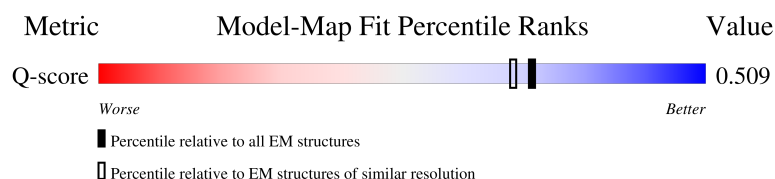
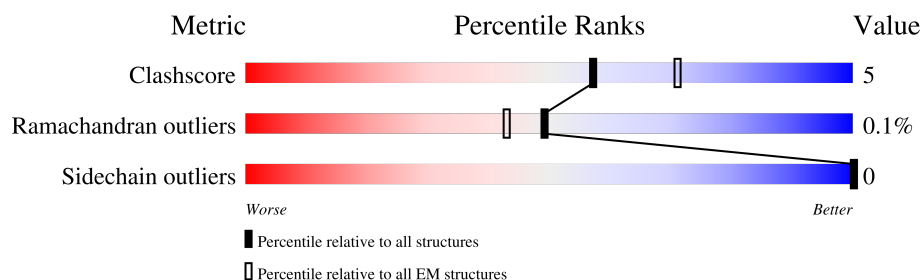
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.20 Å.

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



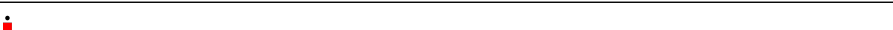
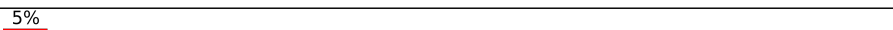
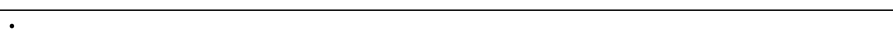
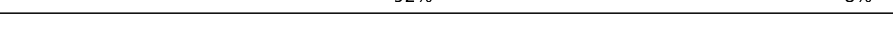
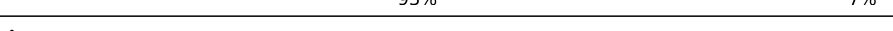
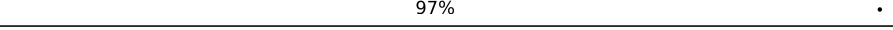
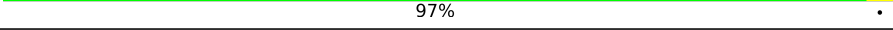
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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	740	 90% 10%
1	A1	740	 90% 10%
1	A2	740	 86% 14%
1	AA	740	 90% 10%

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Mol	Chain	Length	Quality of chain
2	B	739	
2	B1	739	
2	B2	739	
2	BB	739	
3	C	80	
3	C1	80	
3	C2	80	
3	CC	80	
4	D	134	
4	D1	134	
4	D2	134	
4	DD	134	
5	E1	60	
5	E2	60	
6	F	139	
6	F1	139	
6	FF	139	
7	I	31	
7	I1	31	
7	II	31	
8	J	48	
8	J1	48	
8	J2	48	
8	JJ	48	
9	K	74	

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Mol	Chain	Length	Quality of chain
9	K1	74	
9	KK	74	
10	L1	166	
11	M	31	
11	M1	31	
11	M2	31	
11	MM	31	
12	X	39	
12	X1	39	
12	X2	39	
12	XX	39	
13	F2	137	
14	I2	33	
15	K2	73	
16	L2	167	
17	E	63	
17	EE	63	
18	L	154	
18	LL	154	

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
20	CL0	A	803	X	-	-	-
20	CL0	A1	802	X	-	-	-
20	CL0	A2	803	X	-	-	-
20	CL0	AA	803	X	-	-	-
24	AJP	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	A	855	X	-	-	-
24	AJP	A1	854	X	-	-	-
24	AJP	A1	855	X	-	-	-
24	AJP	A2	854	X	-	-	-
24	AJP	AA	802	X	-	-	-
24	AJP	AA	856	X	-	-	-
24	AJP	B	849	X	-	-	-
24	AJP	B	850	X	-	-	-
24	AJP	B	857	X	-	-	-
24	AJP	BB	848	X	-	-	-
24	AJP	BB	849	X	-	-	-
24	AJP	I2	104	X	-	-	-
24	AJP	K	104	X	-	-	-
24	AJP	KK	104	X	-	-	-
24	AJP	L	208	X	-	-	-
24	AJP	L	209	X	-	-	-
24	AJP	L1	203	X	-	-	-
24	AJP	L1	204	X	-	-	-
24	AJP	L2	202	X	-	-	-
24	AJP	L2	203	X	-	-	-
24	AJP	M2	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 199181 atoms, of which 99577 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	A1	740	Total	C	H	N	O	S	0	0
			11478	3809	5672	1000	976	21		
1	A2	740	Total	C	H	N	O	S	0	0
			11486	3809	5680	1000	976	21		
1	A	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		
1	AA	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B1	739	Total	C	H	N	O	S	0	0
			11579	3905	5660	990	1006	18		
2	B2	739	Total	C	H	N	O	S	0	0
			11581	3905	5662	990	1006	18		
2	B	739	Total	C	H	N	O	S	0	0
			11586	3905	5667	990	1006	18		
2	BB	739	Total	C	H	N	O	S	0	0
			11595	3905	5676	990	1006	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	80	Total	C	H	N	O	S	0	0
			1183	367	584	103	118	11		
3	C2	80	Total	C	H	N	O	S	0	0
			1179	367	580	103	118	11		
3	C	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		
3	CC	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	134	Total	C	H	N	O	S	0	0
			2073	664	1037	178	193	1		
4	D2	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	D	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	DD	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
5	E1	60	Total	C	H	N	O		0	0
			958	308	477	83	90			
5	E2	60	Total	C	H	N	O		0	0
			958	308	477	83	90			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F1	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		
6	F	139	Total	C	H	N	O	S	0	0
			2111	678	1051	179	201	2		
6	FF	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
7	I1	31	Total	C	H	N	O		0	0
			508	177	255	35	41			
7	I	31	Total	C	H	N	O		0	0
			508	177	255	35	41			
7	II	31	Total	C	H	N	O		0	0
			508	177	255	35	41			

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

Mol	Chain	Residues	Atoms						AltConf	Trace
8	J1	43	Total	C	H	N	O		0	0
			701	237	355	52	57			

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J2	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	J	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	JJ	43	Total	C	H	N	O	0	0
			700	237	354	52	57		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K1	74	Total	C	H	N	O	S	0	0
			1091	356	555	87	92	1		
9	K	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		
9	KK	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	L1	166	Total	C	H	N	O	S	0	0
			2483	810	1239	213	220	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M2	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	MM	31	Total	C	H	N	O	0	0
			496	160	256	37	43		

- Molecule 12 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X1	39	Total	C	H	N	O	0	0
			627	212	318	49	48		
12	X2	39	Total	C	H	N	O	0	0
			627	212	318	49	48		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	39	Total	C	H	N	O	0	0
			628	212	319	49	48		
12	XX	39	Total	C	H	N	O	0	0
			628	212	319	49	48		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	F2	137	Total	C	H	N	O	S	0	0
			2087	670	1040	177	198	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I2	33	Total	C	H	N	O	0	0
			536	186	268	37	45		

- Molecule 15 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K2	73	Total	C	H	N	O	S	0	0
			1081	353	550	86	91	1		

- Molecule 16 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L2	167	Total	C	H	N	O	S	0	0
			2498	815	1245	215	222	1		

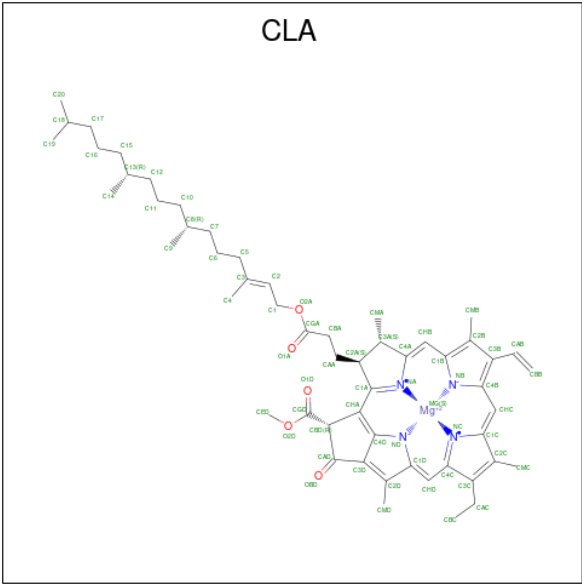
- Molecule 17 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	63	Total	C	H	N	O	0	0
			994	321	492	86	95		
17	EE	63	Total	C	H	N	O	0	0
			994	321	492	86	95		

- Molecule 18 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	154	Total	C	H	N	O	S	0	0
			2309	758	1153	196	201	1		
18	LL	154	Total	C	H	N	O	S	0	0
			2310	758	1154	196	201	1		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			104	46	48	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			133	55	68	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A1	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			135	55	70	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			105	46	49	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F1	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	F1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	J1	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	J1	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K1	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	K1	1	Total	C	H	Mg	N	O	0
			67	32	27	1	4	3	
19	L1	1	Total	C	H	Mg	N	O	0
			120	51	59	1	4	5	
19	L1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	L1	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	X1	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A2	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			135	55	70	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			105	46	49	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	F2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F2	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	J2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	J2	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K2	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	L2	1	Total	C	H	Mg	N	O	0
			119	51	58	1	4	5	
19	L2	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	L2	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	X2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	A	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	F	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	F	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	J	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	J	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	K	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			116	51	55	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	L	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	X	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			79	37	32	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			103	45	48	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			118	50	58	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			112	48	54	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			136	55	71	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			77	35	33	1	4	4	
19	AA	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			132	54	68	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	BB	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	

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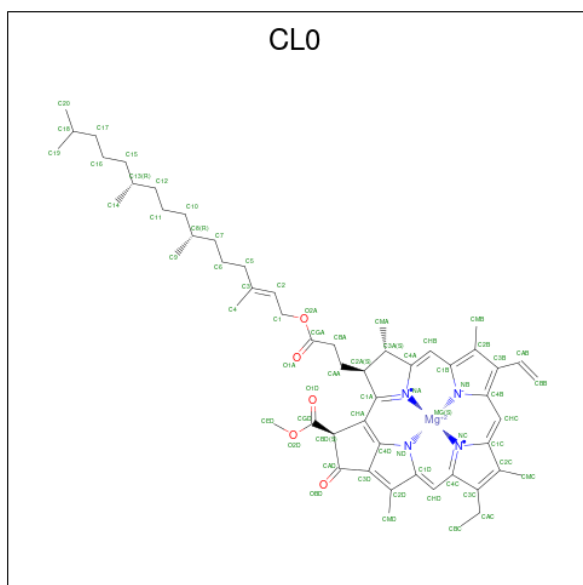
Mol	Chain	Residues	Atoms						AltConf
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			134	55	69	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			131	55	66	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			68	33	29	1	4	1	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	BB	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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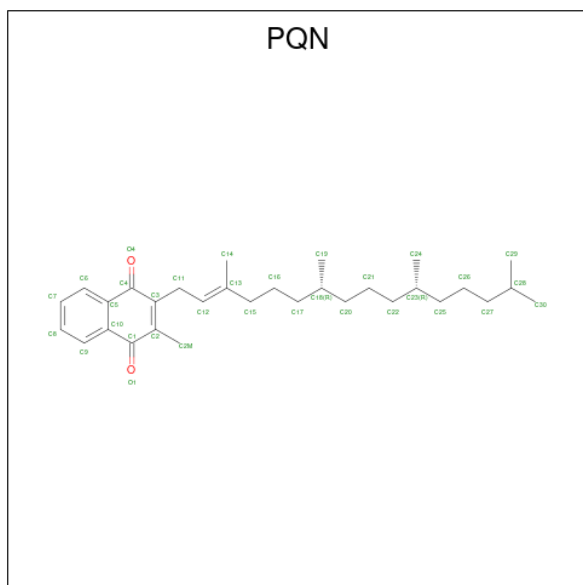
Mol	Chain	Residues	Atoms						AltConf
19	FF	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
19	FF	1	Total	C	H	Mg	N	O	0
			72	34	30	1	4	3	
19	FF	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	JJ	1	Total	C	H	Mg	N	O	0
			70	33	29	1	4	3	
19	JJ	1	Total	C	H	Mg	N	O	0
			69	33	28	1	4	3	
19	KK	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
19	KK	1	Total	C	H	Mg	N	O	0
			78	36	32	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			116	51	55	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
19	LL	1	Total	C	H	Mg	N	O	0
			70	34	28	1	4	3	
19	XX	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



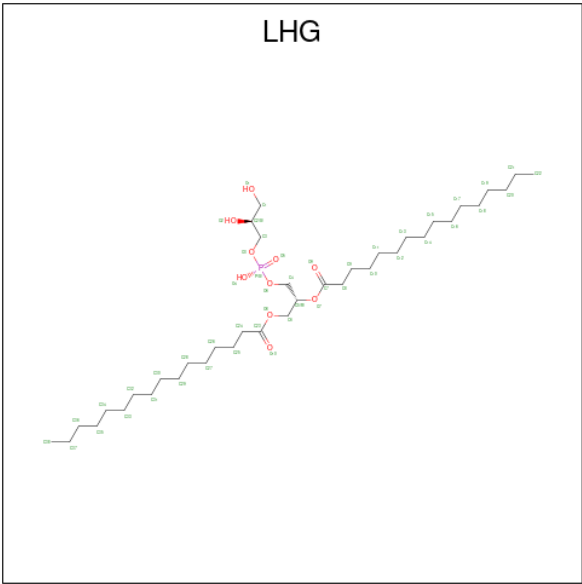
Mol	Chain	Residues	Atoms						AltConf
20	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
21	A1	1	Total	C	H	O	0
			79	31	46	2	
21	B1	1	Total	C	H	O	0
			79	31	46	2	
21	A2	1	Total	C	H	O	0
			79	31	46	2	
21	B2	1	Total	C	H	O	0
			79	31	46	2	
21	A	1	Total	C	H	O	0
			79	31	46	2	
21	B	1	Total	C	H	O	0
			79	31	46	2	
21	AA	1	Total	C	H	O	0
			79	31	46	2	
21	BB	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



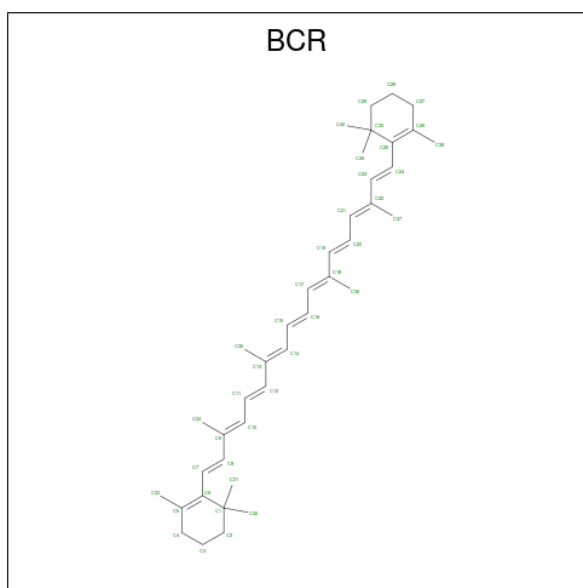
Mol	Chain	Residues	Atoms					AltConf
22	A1	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A1	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B1	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L1	1	Total	C	H	O	P	0
			68	22	35	10	1	
22	X1	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	X1	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A2	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A2	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B2	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L2	1	Total	C	H	O	P	0
			74	24	39	10	1	
22	X2	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	X2	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	A	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	B	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	B	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	L	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	X	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	AA	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	AA	1	Total	C	H	O	P	0
			86	27	48	10	1	
22	BB	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	BB	1	Total	C	H	O	P	0
			123	38	74	10	1	
22	LL	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	XX	1	Total	C	H	O	P	0
			89	29	49	10	1	

- Molecule 23 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms			AltConf
23	A1	1	Total	C	H	0
			92	39	53	
23	A1	1	Total	C	H	0
			96	40	56	
23	A1	1	Total	C	H	0
			96	40	56	
23	A1	1	Total	C	H	0
			96	40	56	
23	A1	1	Total	C	H	0
			96	40	56	
23	A1	1	Total	C	H	0
			96	40	56	
23	B1	1	Total	C	H	0
			96	40	56	
23	B1	1	Total	C	H	0
			96	40	56	
23	B1	1	Total	C	H	0
			96	40	56	
23	B1	1	Total	C	H	0
			96	40	56	
23	B1	1	Total	C	H	0
			96	40	56	
23	F1	1	Total	C	H	0
			96	40	56	
23	F1	1	Total	C	H	0
			96	40	56	
23	F1	1	Total	C	H	0
			91	40	51	
23	I1	1	Total	C	H	0
			96	40	56	
23	J1	1	Total	C	H	0
			96	40	56	
23	J1	1	Total	C	H	0
			96	40	56	
23	K1	1	Total	C	H	0
			96	40	56	
23	K1	1	Total	C	H	0
			96	40	56	
23	L1	1	Total	C	H	0
			96	40	56	
23	L1	1	Total	C	H	0
			96	40	56	
23	L1	1	Total	C	H	0
			96	40	56	

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Mol	Chain	Residues	Atoms			AltConf
23	M1	1	Total 96	C 40	H 56	0
23	A2	1	Total 92	C 39	H 53	0
23	A2	1	Total 96	C 40	H 56	0
23	A2	1	Total 96	C 40	H 56	0
23	A2	1	Total 96	C 40	H 56	0
23	A2	1	Total 96	C 40	H 56	0
23	A2	1	Total 96	C 40	H 56	0
23	B2	1	Total 96	C 40	H 56	0
23	B2	1	Total 96	C 40	H 56	0
23	B2	1	Total 91	C 40	H 51	0
23	B2	1	Total 96	C 40	H 56	0
23	B2	1	Total 96	C 40	H 56	0
23	F2	1	Total 96	C 40	H 56	0
23	F2	1	Total 96	C 40	H 56	0
23	F2	1	Total 91	C 40	H 51	0
23	I2	1	Total 96	C 40	H 56	0
23	I2	1	Total 96	C 40	H 56	0
23	I2	1	Total 96	C 40	H 56	0
23	J2	1	Total 96	C 40	H 56	0
23	J2	1	Total 96	C 40	H 56	0
23	K2	1	Total 96	C 40	H 56	0

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Mol	Chain	Residues	Atoms			AltConf
23	K2	1	Total 96	C 40	H 56	0
23	L2	1	Total 96	C 40	H 56	0
23	M2	1	Total 96	C 40	H 56	0
23	A	1	Total 92	C 39	H 53	0
23	A	1	Total 96	C 40	H 56	0
23	A	1	Total 96	C 40	H 56	0
23	A	1	Total 96	C 40	H 56	0
23	A	1	Total 96	C 40	H 56	0
23	A	1	Total 96	C 40	H 56	0
23	A	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	B	1	Total 96	C 40	H 56	0
23	F	1	Total 96	C 40	H 56	0
23	F	1	Total 96	C 40	H 56	0
23	F	1	Total 91	C 40	H 51	0
23	I	1	Total 96	C 40	H 56	0
23	I	1	Total 96	C 40	H 56	0

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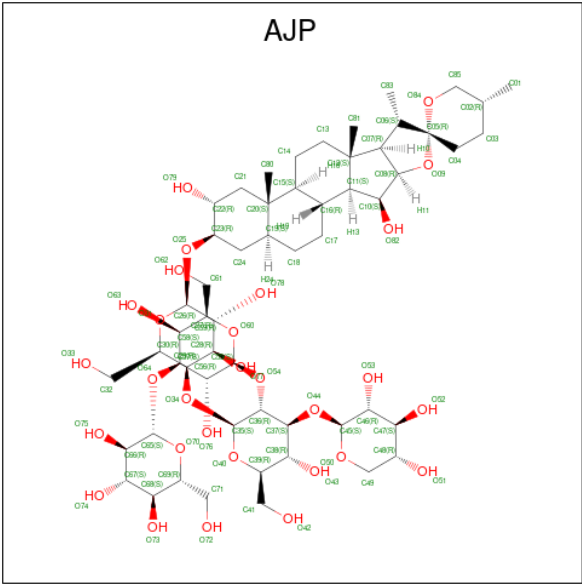
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total 96	C 40	H 56	0
23	J	1	Total 96	C 40	H 56	0
23	K	1	Total 96	C 40	H 56	0
23	L	1	Total 96	C 40	H 56	0
23	L	1	Total 96	C 40	H 56	0
23	M	1	Total 91	C 40	H 51	0
23	AA	1	Total 92	C 39	H 53	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	AA	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	BB	1	Total 96	C 40	H 56	0
23	FF	1	Total 96	C 40	H 56	0
23	FF	1	Total 96	C 40	H 56	0

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Mol	Chain	Residues	Atoms			AltConf
23	FF	1	Total	C	H	0
			91	40	51	
23	II	1	Total	C	H	0
			96	40	56	
23	II	1	Total	C	H	0
			96	40	56	
23	II	1	Total	C	H	0
			96	40	56	
23	JJ	1	Total	C	H	0
			96	40	56	
23	JJ	1	Total	C	H	0
			96	40	56	
23	KK	1	Total	C	H	0
			96	40	56	
23	LL	1	Total	C	H	0
			96	40	56	
23	MM	1	Total	C	H	0
			93	40	53	

- Molecule 24 is Digitonin (CCD ID: AJP) (formula: C₅₆H₉₂O₂₉).



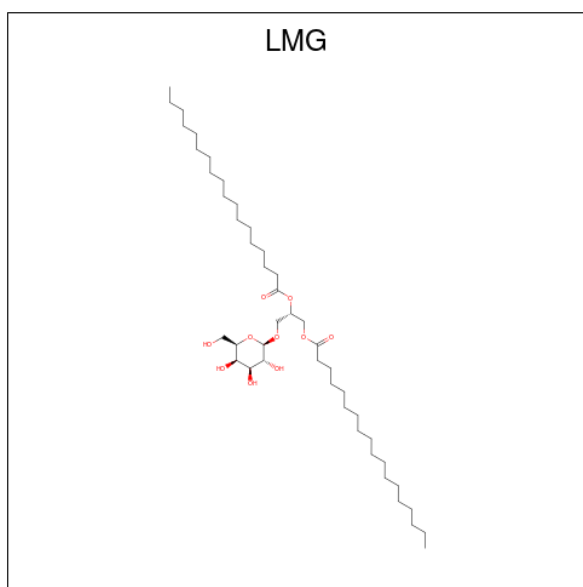
Mol	Chain	Residues	Atoms				AltConf
24	A1	1	Total	C	H	O	0
			96	33	53	10	
24	A1	1	Total	C	H	O	0
			75	27	43	5	

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Mol	Chain	Residues	Atoms				AltConf
24	L1	1	Total	C	H	O	0
			96	33	53	10	
24	L1	1	Total	C	H	O	0
			96	33	53	10	
24	A2	1	Total	C	H	O	0
			75	27	43	5	
24	I2	1	Total	C	H	O	0
			73	27	42	4	
24	L2	1	Total	C	H	O	0
			96	33	53	10	
24	L2	1	Total	C	H	O	0
			96	33	53	10	
24	M2	1	Total	C	H	O	0
			74	27	43	4	
24	A	1	Total	C	H	O	0
			72	27	42	3	
24	A	1	Total	C	H	O	0
			81	29	46	6	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	B	1	Total	C	H	O	0
			96	33	53	10	
24	K	1	Total	C	H	O	0
			91	32	50	9	
24	L	1	Total	C	H	O	0
			73	27	42	4	
24	L	1	Total	C	H	O	0
			74	27	43	4	
24	AA	1	Total	C	H	O	0
			72	27	42	3	
24	AA	1	Total	C	H	O	0
			81	29	46	6	
24	BB	1	Total	C	H	O	0
			96	33	53	10	
24	BB	1	Total	C	H	O	0
			96	33	53	10	
24	KK	1	Total	C	H	O	0
			91	32	50	9	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



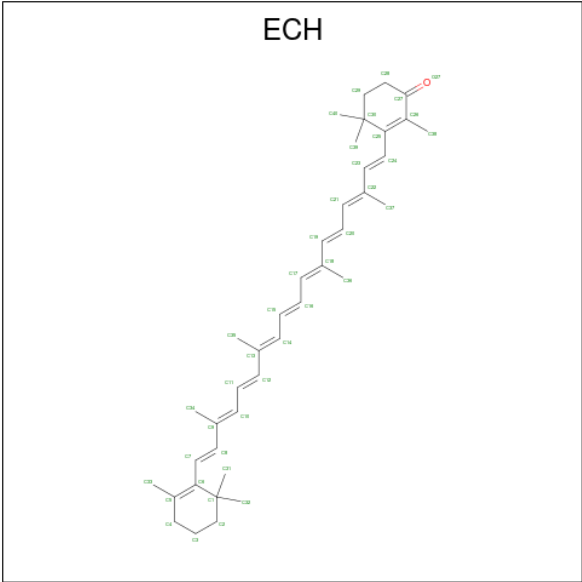
Mol	Chain	Residues	Atoms				AltConf
25	A1	1	Total	C	H	O	1
			88	28	50	10	
25	A1	1	Total	C	H	O	1
			64	20	34	10	
25	B1	1	Total	C	H	O	0
			140	45	85	10	
25	B1	1	Total	C	H	O	0
			65	22	33	10	
25	B1	1	Total	C	H	O	0
			60	20	30	10	
25	I1	1	Total	C	H	O	0
			75	25	40	10	
25	K1	1	Total	C	H	O	1
			68	22	36	10	
25	K1	1	Total	C	H	O	1
			52	16	26	10	
25	L1	1	Total	C	H	O	1
			82	26	46	10	
25	L1	1	Total	C	H	O	0
			141	45	86	10	
25	A2	1	Total	C	H	O	1
			107	34	63	10	
25	A2	1	Total	C	H	O	1
			64	20	34	10	
25	B2	1	Total	C	H	O	0
			140	45	85	10	
25	B2	1	Total	C	H	O	0
			65	22	33	10	

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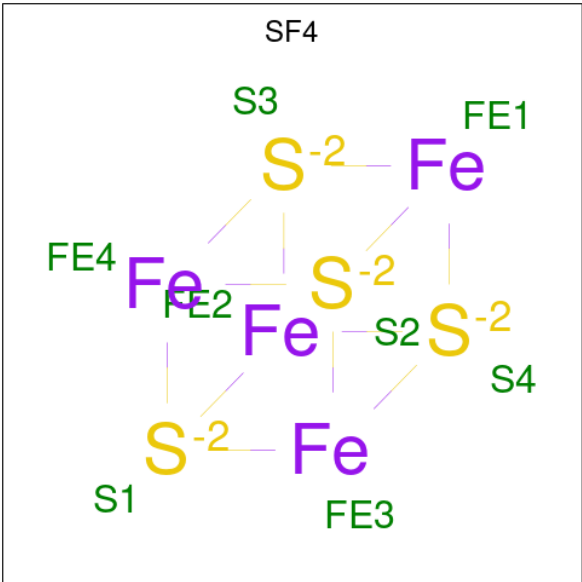
Mol	Chain	Residues	Atoms				AltConf
25	B2	1	Total	C	H	O	0
			60	20	30	10	
25	I2	1	Total	C	H	O	0
			75	25	40	10	
25	K2	1	Total	C	H	O	1
			62	20	32	10	
25	K2	1	Total	C	H	O	1
			52	16	26	10	
25	L2	1	Total	C	H	O	1
			82	26	46	10	
25	B	1	Total	C	H	O	0
			140	45	85	10	
25	B	1	Total	C	H	O	1
			79	25	44	10	
25	B	1	Total	C	H	O	0
			141	45	86	10	
25	B	1	Total	C	H	O	1
			67	21	36	10	
25	L	1	Total	C	H	O	1
			85	27	48	10	
25	M	1	Total	C	H	O	0
			105	36	59	10	
25	BB	1	Total	C	H	O	0
			140	45	85	10	
25	BB	1	Total	C	H	O	1
			82	26	46	10	
25	BB	1	Total	C	H	O	1
			67	21	36	10	
25	II	1	Total	C	H	O	1
			85	27	48	10	
25	II	1	Total	C	H	O	0
			96	32	54	10	

- Molecule 26 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).



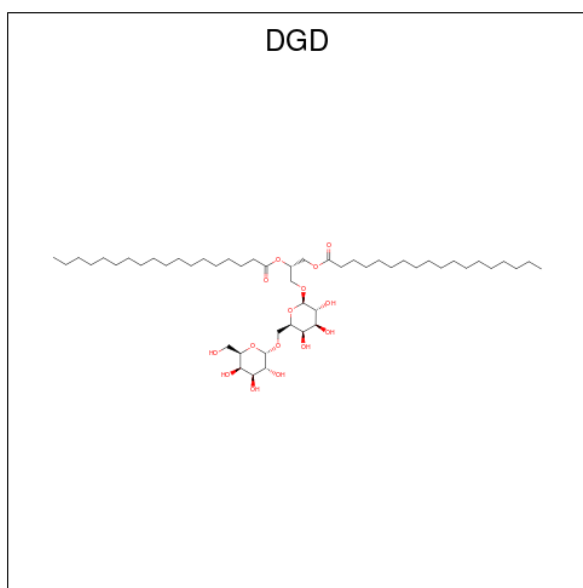
Mol	Chain	Residues	Atoms				AltConf
26	B1	1	Total	C	H	O	0
			95	40	54	1	
26	B2	1	Total	C	H	O	0
			95	40	54	1	
26	B	1	Total	C	H	O	0
			95	40	54	1	
26	BB	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 27 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
27	B1	1	Total	Fe	S	0
			8	4	4	
27	C1	1	Total	Fe	S	0
			8	4	4	
27	C1	1	Total	Fe	S	0
			8	4	4	
27	B2	1	Total	Fe	S	0
			8	4	4	
27	C2	1	Total	Fe	S	0
			8	4	4	
27	C2	1	Total	Fe	S	0
			8	4	4	
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			8	4	4	
27	BB	1	Total	Fe	S	0
			8	4	4	
27	CC	1	Total	Fe	S	0
			8	4	4	
27	CC	1	Total	Fe	S	0
			8	4	4	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).

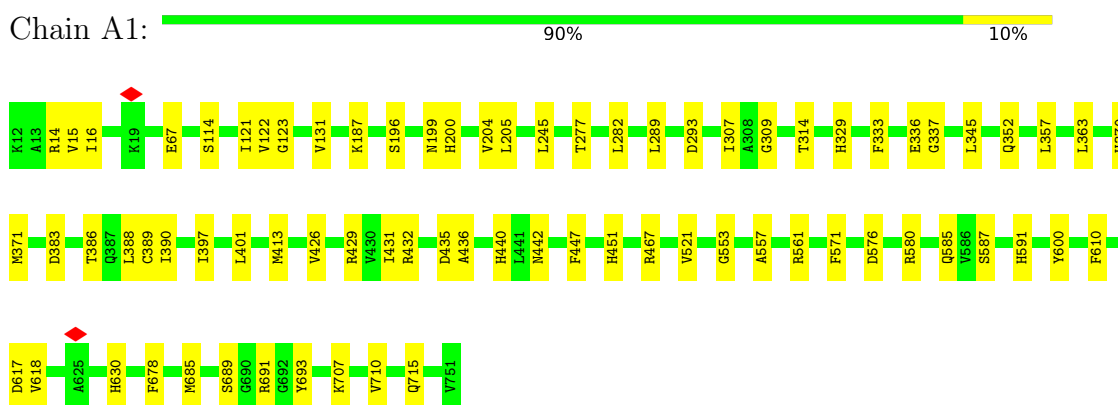


Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	H	O	0
			88	27	46	15	
28	BB	1	Total	C	H	O	0
			88	27	46	15	

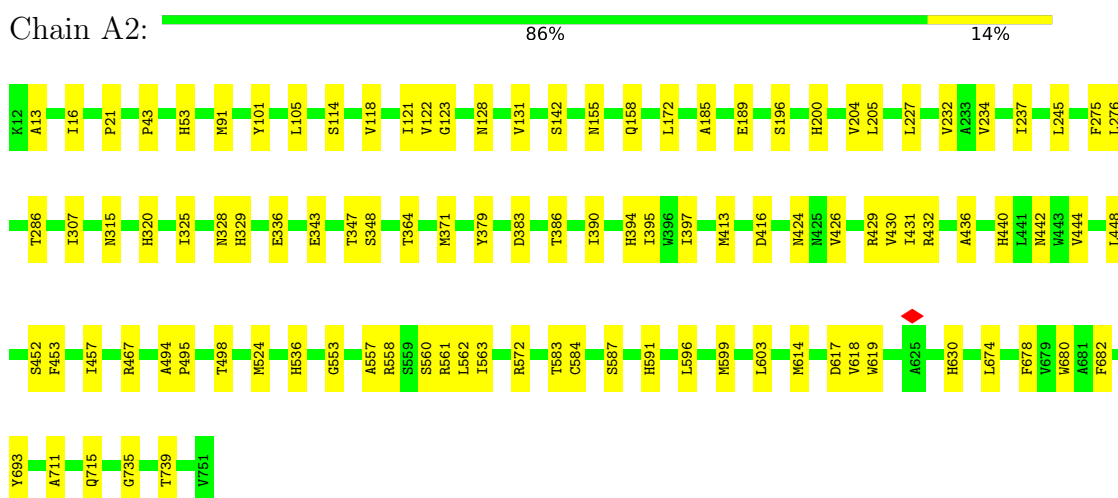
3 Residue-property plots [i](#)

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

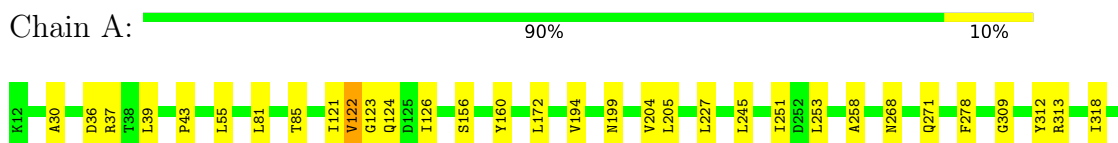
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

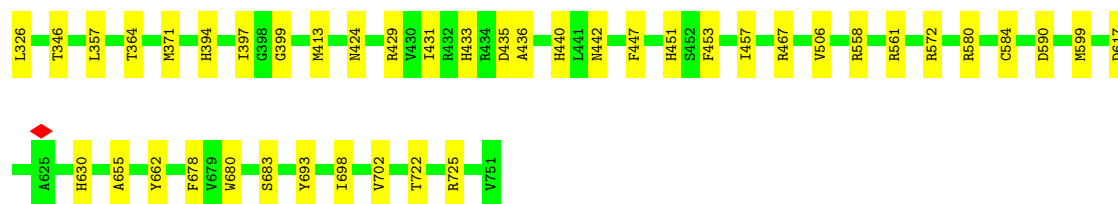


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



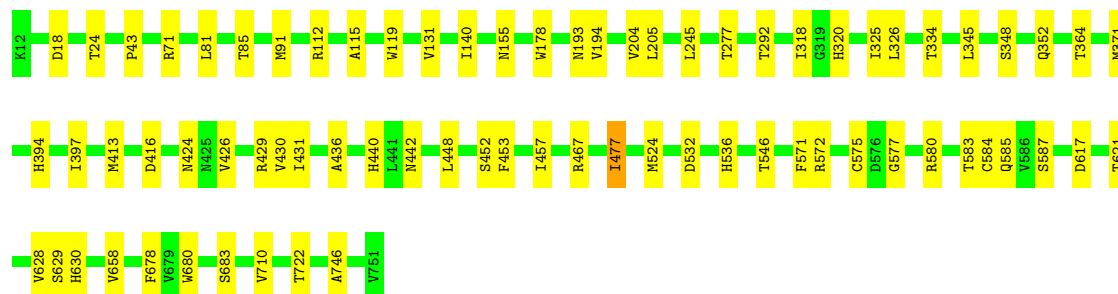
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





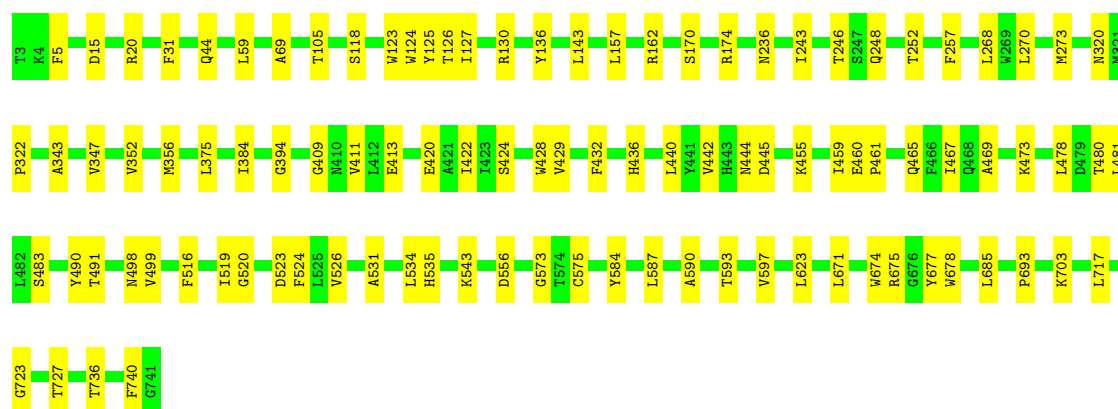
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA: 90% 10%



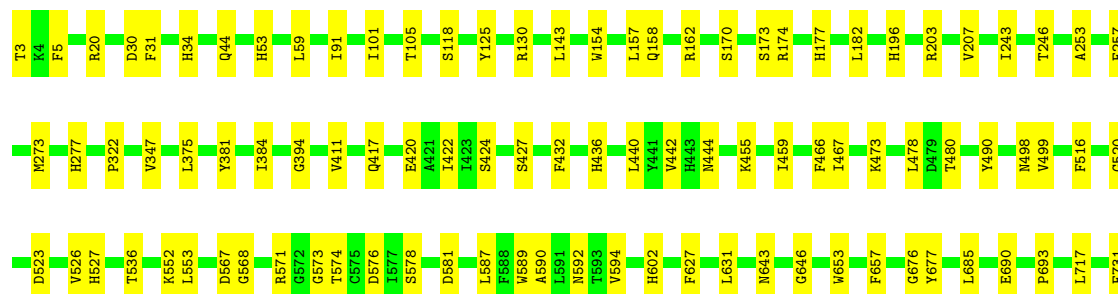
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B1: 86% 14%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

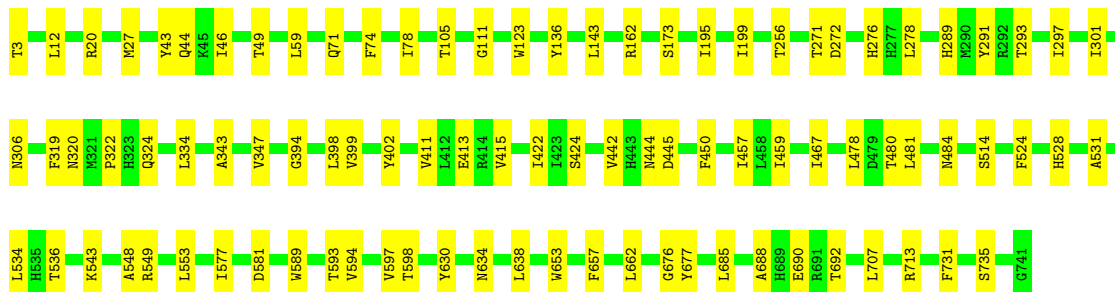
Chain B2: 87% 13%





- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B: 88% 12%



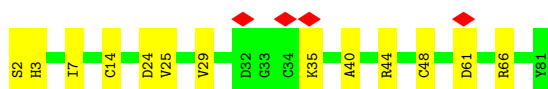
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain BB: 85% 15%



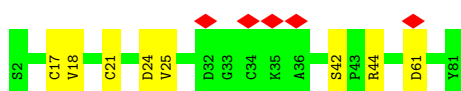
- Molecule 3: Photosystem I iron-sulfur center

Chain C1: 5% 84% 16%

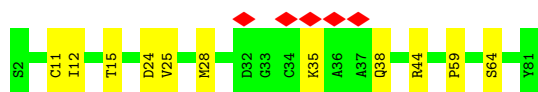
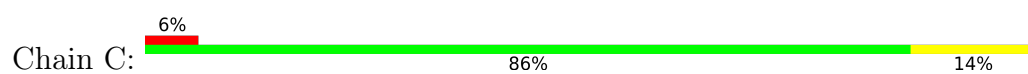


- Molecule 3: Photosystem I iron-sulfur center

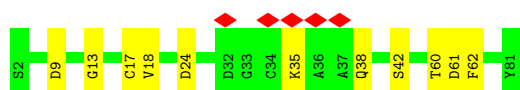
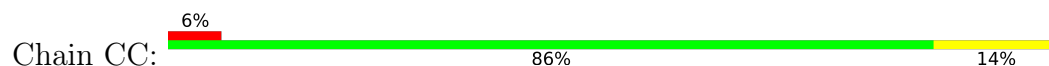
Chain C2: 6% 90% 10%



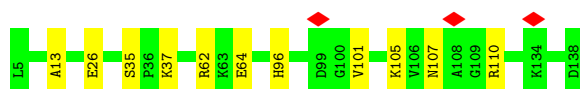
- Molecule 3: Photosystem I iron-sulfur center



- Molecule 3: Photosystem I iron-sulfur center



- Molecule 4: Photosystem I reaction center subunit II



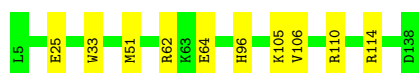
- Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II



- Molecule 4: Photosystem I reaction center subunit II

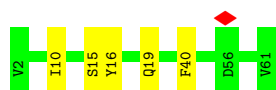


- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 5: Photosystem I reaction center subunit IV

Chain E2:  92% 8%



- Molecule 6: Photosystem I reaction center subunit III

Chain F1:  88% 12%



- Molecule 6: Photosystem I reaction center subunit III

Chain F:  93% 7%

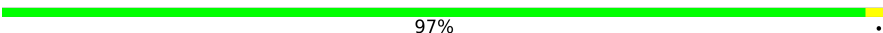


- Molecule 6: Photosystem I reaction center subunit III

Chain FF:  88% 12%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:  97%

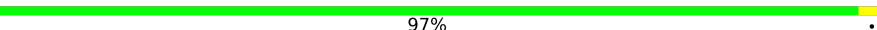


- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  90% 10%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain II:  97%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J1:  81% 8% 10%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J2:  79% 10% 10%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  83% 6% 10%



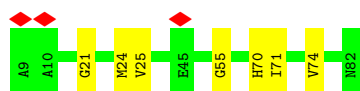
- Molecule 8: Photosystem I reaction center subunit IX

Chain JJ:  77% 12% 10%



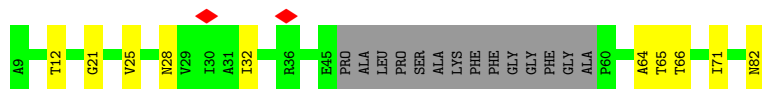
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K1:  91% 9%



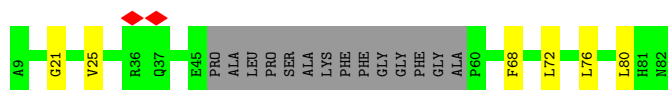
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K:  68% 14% 19%

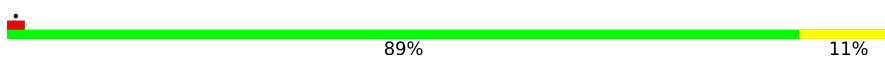


- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain KK:  73% 8% 19%

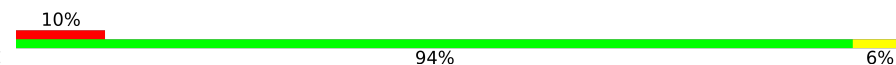


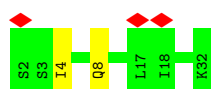
- Molecule 10: Photosystem I reaction center subunit XI

Chain L1:  89% 11%



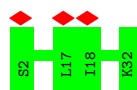
- Molecule 11: Photosystem I reaction center subunit XII

Chain M1:  10% 94% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M2:  10% 100%

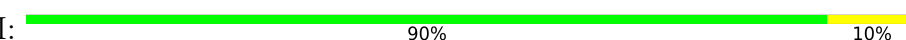


- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 16%

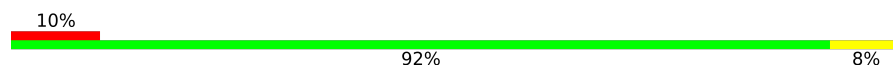


- Molecule 11: Photosystem I reaction center subunit XII

Chain MM:  90% 10%

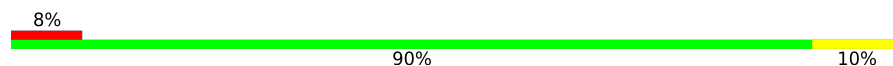


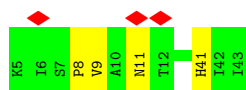
- Molecule 12: Photosystem I 4.8 kDa protein

Chain X1:  10% 92% 8%

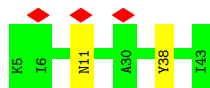


- Molecule 12: Photosystem I 4.8 kDa protein

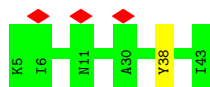
Chain X2:  8% 90% 10%



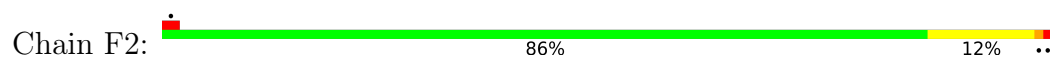
- Molecule 12: Photosystem I 4.8 kDa protein



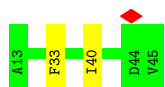
- Molecule 12: Photosystem I 4.8 kDa protein



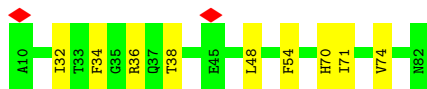
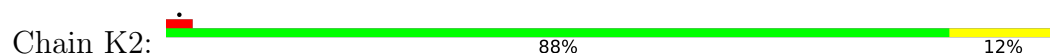
- Molecule 13: Photosystem I reaction center subunit III



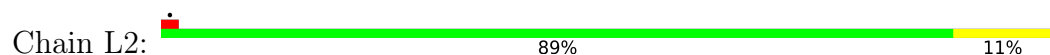
- Molecule 14: Photosystem I reaction center subunit VIII



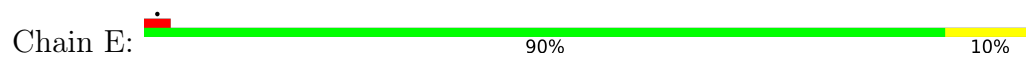
- Molecule 15: Photosystem I reaction center subunit PsaK 1



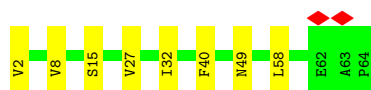
- Molecule 16: Photosystem I reaction center subunit XI



- Molecule 17: Photosystem I reaction center subunit IV



- Molecule 17: Photosystem I reaction center subunit IV



- Molecule 18: Photosystem I reaction center subunit XI



- Molecule 18: Photosystem I reaction center subunit XI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.390	Depositor
Minimum map value	-1.168	Depositor
Average map value	0.014	Depositor
Map value standard deviation	0.108	Depositor
Recommended contour level	0.434	Depositor
Map size ($\text{\AA}$)	392.19998, 392.19998, 392.19998	wwPDB
Map dimensions	370, 370, 370	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.20	0/6004	0.35	0/8193
1	A1	0.20	0/6004	0.36	0/8193
1	A2	0.20	0/6004	0.39	2/8193 (0.0%)
1	AA	0.20	0/6004	0.36	0/8193
2	B	0.23	0/6143	0.40	0/8396
2	B1	0.20	0/6143	0.37	0/8396
2	B2	0.20	0/6143	0.38	0/8396
2	BB	0.23	0/6143	0.39	0/8396
3	C	0.19	0/609	0.40	0/826
3	C1	0.21	0/609	0.41	0/826
3	C2	0.21	0/609	0.39	0/826
3	CC	0.20	0/609	0.38	0/826
4	D	0.19	0/1060	0.41	0/1431
4	D1	0.17	0/1060	0.39	0/1431
4	D2	0.18	0/1060	0.41	0/1431
4	DD	0.18	0/1060	0.42	0/1431
5	E1	0.17	0/490	0.41	0/665
5	E2	0.19	0/490	0.42	0/665
6	F	0.18	0/1084	0.38	0/1475
6	F1	0.15	0/1084	0.36	0/1475
6	FF	0.17	0/1084	0.34	0/1475
7	I	0.20	0/262	0.37	0/358
7	I1	0.21	0/262	0.31	0/358
7	II	0.19	0/262	0.37	0/358
8	J	0.18	0/358	0.35	0/491
8	J1	0.17	0/358	0.35	0/491
8	J2	0.16	0/358	0.32	0/491
8	JJ	0.18	0/358	0.35	0/491
9	K	0.14	0/448	0.33	0/613
9	K1	0.18	0/551	0.44	0/755
9	KK	0.16	0/448	0.36	0/613
10	L1	0.20	0/1281	0.39	0/1756

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	M	0.16	0/244	0.27	0/334
11	M1	0.16	0/244	0.32	0/334
11	M2	0.15	0/244	0.36	0/334
11	MM	0.17	0/244	0.30	0/334
12	X	0.22	0/320	0.41	0/439
12	X1	0.18	0/320	0.36	0/439
12	X2	0.18	0/320	0.38	0/439
12	XX	0.19	0/320	0.37	0/439
13	F2	0.19	0/1070	0.50	2/1455 (0.1%)
14	I2	0.20	0/277	0.36	0/379
15	K2	0.16	0/546	0.34	0/748
16	L2	0.21	0/1290	0.39	0/1768
17	E	0.18	0/512	0.43	0/696
17	EE	0.17	0/512	0.41	0/696
18	L	0.20	0/1191	0.39	0/1632
18	LL	0.21	0/1191	0.38	0/1632
All	All	0.20	0/73287	0.38	4/100012 (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
13	F2	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A2	536	HIS	CA-C-N	8.62	133.41	120.31
1	A2	536	HIS	C-N-CA	8.62	133.41	120.31
13	F2	158	GLU	CA-C-N	5.78	132.37	121.97
13	F2	158	GLU	C-N-CA	5.78	132.37	121.97

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F2	158	GLU	Peptide
13	F2	159	ILE	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	5806	5677	5682	53	0
1	A1	5806	5672	5682	63	0
1	A2	5806	5680	5682	72	0
1	AA	5806	5677	5682	54	0
2	B	5919	5667	5677	67	0
2	B1	5919	5660	5677	80	0
2	B2	5919	5662	5677	77	0
2	BB	5919	5676	5677	88	0
3	C	599	582	585	8	0
3	C1	599	584	585	10	0
3	C2	599	580	585	5	0
3	CC	599	582	585	9	0
4	D	1036	1042	1042	10	0
4	D1	1036	1037	1042	9	0
4	D2	1036	1042	1042	10	0
4	DD	1036	1042	1042	8	0
5	E1	481	477	478	4	0
5	E2	481	477	478	7	0
6	F	1060	1051	1054	7	0
6	F1	1060	1052	1054	12	0
6	FF	1060	1052	1054	11	0
7	I	253	255	255	2	0
7	I1	253	255	255	1	0
7	II	253	255	255	1	0
8	J	346	355	355	3	0
8	J1	346	355	355	4	0
8	J2	346	355	355	5	0
8	JJ	346	354	355	5	0
9	K	439	461	461	6	0
9	K1	536	555	555	5	0
9	KK	439	461	461	3	0
10	L1	1244	1239	1242	16	0
11	M	240	256	256	5	0
11	M1	240	256	256	3	0
11	M2	240	256	256	0	0
11	MM	240	256	256	5	0
12	X	309	319	319	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	X1	309	318	319	4	0
12	X2	309	318	319	5	0
12	XX	309	319	319	1	0
13	F2	1047	1040	1042	14	0
14	I2	268	268	268	2	0
15	K2	531	550	550	7	0
16	L2	1253	1245	1250	12	0
17	E	502	492	496	5	0
17	EE	502	492	496	6	0
18	L	1156	1153	1157	5	0
18	LL	1156	1154	1157	7	0
19	A	2339	2207	2215	35	0
19	A1	2394	2261	2275	39	0
19	A2	2375	2227	2236	35	0
19	AA	2404	2279	2287	31	0
19	B	2401	2357	2375	54	0
19	B1	2291	2253	2270	44	0
19	B2	2401	2358	2375	36	0
19	BB	2271	2219	2231	55	0
19	F	102	89	90	2	0
19	F1	147	122	123	5	0
19	F2	102	89	90	2	0
19	FF	167	161	162	4	0
19	J	82	58	58	2	0
19	J1	82	57	58	1	0
19	J2	82	58	58	1	0
19	JJ	82	57	58	1	0
19	K	91	65	66	0	0
19	K1	131	92	94	2	0
19	K2	86	61	62	1	0
19	KK	91	65	66	0	0
19	L	191	198	205	4	0
19	L1	191	202	205	5	0
19	L2	186	187	191	0	0
19	LL	168	155	164	4	0
19	X	45	32	33	0	0
19	X1	45	32	33	0	0
19	X2	45	32	33	1	0
19	XX	45	32	33	0	0
20	A	65	72	72	2	0
20	A1	65	72	71	4	0
20	A2	65	72	70	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	AA	65	72	71	1	0
21	A	33	46	46	1	0
21	A1	33	46	46	2	0
21	A2	33	46	46	1	0
21	AA	33	46	46	1	0
21	B	33	46	46	2	0
21	B1	33	46	46	0	0
21	B2	33	46	46	0	0
21	BB	33	46	46	2	0
22	A	87	122	123	2	0
22	A1	87	122	123	1	0
22	A2	87	122	123	2	0
22	AA	87	122	123	3	0
22	B	82	110	110	1	0
22	B1	33	36	36	1	0
22	B2	33	36	36	0	0
22	BB	82	110	110	0	0
22	L	34	42	38	0	0
22	L1	33	35	36	2	0
22	L2	35	39	40	1	0
22	LL	34	42	38	0	0
22	X	40	49	50	0	0
22	X1	89	123	124	0	0
22	X2	89	123	124	0	0
22	XX	40	49	50	0	0
23	A	279	389	389	7	0
23	A1	239	333	333	6	0
23	A2	239	333	333	7	0
23	AA	279	389	389	8	0
23	B	240	336	336	12	0
23	B1	200	280	280	7	0
23	B2	200	275	280	9	0
23	BB	240	336	336	11	0
23	F	120	163	168	6	0
23	F1	120	163	168	6	0
23	F2	120	163	168	6	0
23	FF	120	163	168	6	0
23	I	80	112	112	0	0
23	I1	40	56	56	1	0
23	I2	120	168	168	1	0
23	II	120	168	168	0	0
23	J	80	112	112	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	J1	80	112	112	2	0
23	J2	80	112	112	3	0
23	JJ	80	112	112	2	0
23	K	40	56	56	0	0
23	K1	80	112	112	3	0
23	K2	80	112	112	3	0
23	KK	40	56	56	0	0
23	L	80	112	112	1	0
23	L1	120	168	168	0	0
23	L2	40	56	56	0	0
23	LL	40	56	56	1	0
23	M	40	51	56	2	0
23	M1	40	56	56	0	0
23	M2	40	56	56	0	0
23	MM	40	53	56	1	0
24	A	65	88	0	0	0
24	A1	75	96	0	0	0
24	A2	32	43	0	0	0
24	AA	65	88	0	0	0
24	B	129	159	0	1	0
24	BB	86	106	0	1	0
24	I2	31	42	0	0	0
24	K	41	50	0	0	0
24	KK	41	50	0	0	0
24	L	62	85	0	0	0
24	L1	86	106	0	1	0
24	L2	86	106	0	1	0
24	M2	31	43	0	0	0
25	A1	68	84	0	0	0
25	A2	74	97	0	0	0
25	B	176	251	172	0	0
25	B1	117	148	150	0	0
25	B2	117	148	150	0	0
25	BB	122	167	86	0	0
25	I1	35	40	40	0	0
25	I2	35	40	40	1	0
25	II	79	102	54	0	0
25	K1	58	62	0	0	0
25	K2	56	58	0	0	0
25	L	37	48	0	0	0
25	L1	91	132	86	1	0
25	L2	36	46	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
25	M	46	59	62	1	0
26	B	41	54	54	2	0
26	B1	41	54	54	1	0
26	B2	41	54	54	1	0
26	BB	41	54	54	2	0
27	B	8	0	0	0	0
27	B1	8	0	0	0	0
27	B2	8	0	0	0	0
27	BB	8	0	0	0	0
27	C	16	0	0	1	0
27	C1	16	0	0	1	0
27	C2	16	0	0	0	0
27	CC	16	0	0	0	0
28	B	42	46	42	1	0
28	BB	42	46	42	0	0
All	All	99604	99577	98156	943	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 5.

The worst 5 of 943 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)
2:B2:587:LEU:HD23	2:B2:717:LEU:HD21	1.55	0.88
2:B:553:LEU:HD23	2:B:577:ILE:HD11	1.56	0.86
19:B2:822:CLA:H93	23:B2:843:BCR:H333	1.57	0.84
19:B1:822:CLA:H93	23:B1:842:BCR:H333	1.58	0.83
2:B1:534:LEU:HD12	19:B1:834:CLA:HED3	1.63	0.81

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	738/740 (100%)	713 (97%)	24 (3%)	1 (0%)	48	79
1	A1	738/740 (100%)	710 (96%)	27 (4%)	1 (0%)	48	79
1	A2	738/740 (100%)	714 (97%)	23 (3%)	1 (0%)	48	79
1	AA	738/740 (100%)	709 (96%)	28 (4%)	1 (0%)	48	79
2	B	737/739 (100%)	712 (97%)	25 (3%)	0	100	100
2	B1	737/739 (100%)	715 (97%)	22 (3%)	0	100	100
2	B2	737/739 (100%)	713 (97%)	24 (3%)	0	100	100
2	BB	737/739 (100%)	710 (96%)	27 (4%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	C1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	CC	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
4	D1	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
4	D2	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
4	DD	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
5	E1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
5	E2	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
6	F	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
6	F1	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	FF	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
7	I	29/31 (94%)	29 (100%)	0	0	100	100
7	I1	29/31 (94%)	29 (100%)	0	0	100	100
7	II	29/31 (94%)	29 (100%)	0	0	100	100
8	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
8	J1	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
8	J2	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
8	JJ	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
9	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
9	K1	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	KK	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
10	L1	164/166 (99%)	160 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	MM	29/31 (94%)	29 (100%)	0	0	100	100
12	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X1	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X2	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	XX	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
13	F2	135/137 (98%)	125 (93%)	7 (5%)	3 (2%)	5	29
14	I2	31/33 (94%)	31 (100%)	0	0	100	100
15	K2	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
16	L2	165/167 (99%)	160 (97%)	5 (3%)	0	100	100
17	E	61/63 (97%)	61 (100%)	0	0	100	100
17	EE	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	L	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	18	52
18	LL	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
All	All	8958/9106 (98%)	8634 (96%)	316 (4%)	8 (0%)	49	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	122	VAL
13	F2	159	ILE
1	A1	122	VAL
1	A	122	VAL
1	AA	477	ILE

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	594/594 (100%)	594 (100%)	0	100	100
1	A1	594/594 (100%)	594 (100%)	0	100	100
1	A2	594/594 (100%)	594 (100%)	0	100	100
1	AA	594/594 (100%)	594 (100%)	0	100	100
2	B	601/601 (100%)	601 (100%)	0	100	100
2	B1	601/601 (100%)	601 (100%)	0	100	100
2	B2	601/601 (100%)	601 (100%)	0	100	100
2	BB	601/601 (100%)	601 (100%)	0	100	100
3	C	68/68 (100%)	68 (100%)	0	100	100
3	C1	68/68 (100%)	68 (100%)	0	100	100
3	C2	68/68 (100%)	68 (100%)	0	100	100
3	CC	68/68 (100%)	68 (100%)	0	100	100
4	D	107/107 (100%)	107 (100%)	0	100	100
4	D1	107/107 (100%)	107 (100%)	0	100	100
4	D2	107/107 (100%)	107 (100%)	0	100	100
4	DD	107/107 (100%)	107 (100%)	0	100	100
5	E1	53/53 (100%)	53 (100%)	0	100	100
5	E2	53/53 (100%)	53 (100%)	0	100	100
6	F	108/108 (100%)	108 (100%)	0	100	100
6	F1	108/108 (100%)	108 (100%)	0	100	100
6	FF	108/108 (100%)	108 (100%)	0	100	100
7	I	28/28 (100%)	28 (100%)	0	100	100
7	I1	28/28 (100%)	28 (100%)	0	100	100
7	II	28/28 (100%)	28 (100%)	0	100	100
8	J	38/41 (93%)	38 (100%)	0	100	100
8	J1	38/41 (93%)	38 (100%)	0	100	100
8	J2	38/41 (93%)	38 (100%)	0	100	100
8	JJ	38/41 (93%)	38 (100%)	0	100	100
9	K	46/54 (85%)	46 (100%)	0	100	100
9	K1	54/54 (100%)	54 (100%)	0	100	100
9	KK	46/54 (85%)	46 (100%)	0	100	100
10	L1	127/127 (100%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	M	26/26 (100%)	26 (100%)	0	100	100
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	MM	26/26 (100%)	26 (100%)	0	100	100
12	X	31/31 (100%)	31 (100%)	0	100	100
12	X1	31/31 (100%)	31 (100%)	0	100	100
12	X2	31/31 (100%)	31 (100%)	0	100	100
12	XX	31/31 (100%)	31 (100%)	0	100	100
13	F2	106/106 (100%)	106 (100%)	0	100	100
14	I2	30/30 (100%)	30 (100%)	0	100	100
15	K2	54/54 (100%)	54 (100%)	0	100	100
16	L2	128/128 (100%)	128 (100%)	0	100	100
17	E	55/55 (100%)	55 (100%)	0	100	100
17	EE	55/55 (100%)	55 (100%)	0	100	100
18	L	117/117 (100%)	117 (100%)	0	100	100
18	LL	117/117 (100%)	117 (100%)	0	100	100
All	All	7309/7337 (100%)	7309 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 40 such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	182	HIS
2	BB	223	GLN
1	AA	344	ASN
1	AA	654	GLN
2	BB	294	ASN

5.3.3 RNA ⓘ

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](#)

594 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	$\# Z > 2$
24	AJP	BB	849	-	49,49,95	3.97	25 (51%)	74,80,149	4.32	47 (63%)
19	CLA	B1	817	-	46,50,73	1.51	8 (17%)	55,85,113	1.45	4 (7%)
23	BCR	L	206	-	41,41,41	1.17	2 (4%)	56,56,56	1.24	8 (14%)
19	CLA	B2	814	-	63,67,73	1.31	9 (14%)	75,105,113	1.31	7 (9%)
19	CLA	FF	305	-	69,73,73	1.27	9 (13%)	83,113,113	1.22	6 (7%)
23	BCR	JJ	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	8 (14%)
21	PQN	A2	843	-	34,34,34	0.63	0	42,45,45	1.09	3 (7%)
19	CLA	AA	834	-	45,49,73	1.51	10 (22%)	54,84,113	1.45	4 (7%)
24	AJP	A2	854	-	37,37,95	4.41	24 (64%)	58,62,149	3.48	22 (37%)
26	ECH	B	841	-	42,42,42	0.90	1 (2%)	55,58,58	2.48	22 (40%)
19	CLA	B1	821	2	69,73,73	1.23	8 (11%)	83,113,113	1.30	8 (9%)
19	CLA	B	819	-	45,49,73	1.51	9 (20%)	54,84,113	1.46	5 (9%)
19	CLA	B2	801	-	69,73,73	1.23	9 (13%)	83,113,113	1.43	9 (10%)
19	CLA	B	825	-	69,73,73	1.23	9 (13%)	83,113,113	1.29	8 (9%)
27	SF4	C1	102	-	0,12,12	-	-	-	-	-
19	CLA	B	835	-	49,53,73	1.47	8 (16%)	59,89,113	1.44	7 (11%)
24	AJP	I2	104	-	36,36,95	4.41	22 (61%)	56,60,149	4.44	33 (58%)
23	BCR	BB	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	BB	828	-	49,53,73	1.47	9 (18%)	59,89,113	1.43	5 (8%)
23	BCR	II	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	8 (14%)
19	CLA	A2	815	-	59,63,73	1.34	8 (13%)	71,101,113	1.29	5 (7%)
25	LMG	I2	105	-	35,35,55	0.92	1 (2%)	43,43,63	1.22	4 (9%)
19	CLA	AA	840	-	60,64,73	1.33	10 (16%)	72,102,113	1.30	5 (6%)
23	BCR	A	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
24	AJP	K	104	-	47,47,95	3.99	24 (51%)	71,77,149	4.30	39 (54%)
25	LMG	B1	852	-	30,30,55	1.00	0	38,38,63	1.23	4 (10%)
19	CLA	A	816	-	54,58,73	1.41	9 (16%)	65,95,113	1.38	6 (9%)
21	PQN	A	843	-	34,34,34	0.60	0	42,45,45	1.09	3 (7%)
19	CLA	AA	836	-	69,73,73	1.25	9 (13%)	83,113,113	1.27	5 (6%)
19	CLA	A1	852	-	69,73,73	1.25	9 (13%)	83,113,113	1.23	4 (4%)
19	CLA	B	809	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	6 (10%)
19	CLA	B	810	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
19	CLA	B	814	-	63,67,73	1.31	10 (15%)	75,105,113	1.38	7 (9%)
19	CLA	B	827	-	49,53,73	1.47	10 (20%)	59,89,113	1.47	8 (13%)
19	CLA	B	812	-	45,49,73	1.49	9 (20%)	54,84,113	1.56	6 (11%)
22	LHG	B	852	-	32,32,48	0.89	1 (3%)	35,38,54	1.02	3 (8%)
23	BCR	A2	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	10 (17%)
19	CLA	A	806	-	60,64,73	1.34	10 (16%)	72,102,113	1.47	9 (12%)
19	CLA	A1	844	-	45,49,73	1.50	9 (20%)	54,84,113	1.49	5 (9%)
19	CLA	B2	836	-	69,73,73	1.25	10 (14%)	83,113,113	1.26	6 (7%)
22	LHG	A2	845	-	48,48,48	0.76	1 (2%)	51,54,54	0.96	3 (5%)
19	CLA	B1	803	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
23	BCR	F2	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	9 (16%)
19	CLA	B	860	-	69,73,73	1.25	8 (11%)	83,113,113	1.49	9 (10%)
19	CLA	A	804	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	6 (7%)
19	CLA	A	815	-	59,63,73	1.34	8 (13%)	71,101,113	1.34	5 (7%)
19	CLA	F2	302	-	46,50,73	1.52	9 (19%)	55,85,113	1.54	6 (10%)
23	BCR	MM	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.36	10 (17%)
19	CLA	A	832	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
19	CLA	B1	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	7 (8%)
22	LHG	A1	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
19	CLA	A2	816	-	54,58,73	1.40	8 (14%)	65,95,113	1.38	6 (9%)
19	CLA	A2	821	-	69,73,73	1.23	9 (13%)	83,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	I	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	6 (10%)
19	CLA	B2	820	-	49,53,73	1.49	9 (18%)	59,89,113	1.57	8 (13%)
19	CLA	A2	804	-	69,73,73	1.24	9 (13%)	83,113,113	1.26	5 (6%)
23	BCR	K1	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	A	825	-	56,60,73	1.38	9 (16%)	67,97,113	1.38	5 (7%)
22	LHG	A	845	-	48,48,48	0.80	2 (4%)	51,54,54	0.98	3 (5%)
24	AJP	B	857	-	49,49,95	3.92	25 (51%)	74,80,149	3.32	21 (28%)
19	CLA	B2	846	-	44,47,73	1.53	9 (20%)	52,80,113	1.43	5 (9%)
19	CLA	AA	838	-	48,52,73	1.46	9 (18%)	56,87,113	1.47	6 (10%)
23	BCR	J1	104	-	41,41,41	1.13	2 (4%)	56,56,56	1.34	6 (10%)
19	CLA	F1	305	-	49,53,73	1.48	8 (16%)	59,89,113	1.38	5 (8%)
19	CLA	A1	811	-	50,54,73	1.44	9 (18%)	60,90,113	1.43	7 (11%)
27	SF4	C1	101	-	0,12,12	-	-	-	-	-
19	CLA	AA	837	-	49,53,73	1.49	9 (18%)	59,89,113	1.43	6 (10%)
19	CLA	BB	803	-	69,73,73	1.25	10 (14%)	83,113,113	1.29	8 (9%)
19	CLA	L2	205	-	63,67,73	1.30	10 (15%)	75,105,113	1.42	6 (8%)
22	LHG	L	207	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
19	CLA	B1	810	-	69,73,73	1.25	8 (11%)	83,113,113	1.27	7 (8%)
23	BCR	B2	839	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
23	BCR	B	843	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
19	CLA	L1	207	-	69,73,73	1.27	9 (13%)	83,113,113	1.25	5 (6%)
24	AJP	L	209	-	36,36,95	4.52	24 (66%)	56,60,149	4.59	34 (60%)
19	CLA	B1	827	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	7 (11%)
19	CLA	B1	812	-	45,49,73	1.51	8 (17%)	54,84,113	1.51	5 (9%)
19	CLA	LL	202	-	69,73,73	1.26	10 (14%)	83,113,113	1.36	7 (8%)
19	CLA	AA	853	-	69,73,73	1.25	10 (14%)	83,113,113	1.22	7 (8%)
19	CLA	B1	833	-	69,73,73	1.25	8 (11%)	83,113,113	1.55	18 (21%)
22	LHG	X1	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
19	CLA	AA	812	-	50,54,73	1.45	9 (18%)	60,90,113	1.44	5 (8%)
25	LMG	II	105	-	42,42,55	0.82	1 (2%)	50,50,63	1.24	6 (12%)
19	CLA	B	834	-	69,73,73	1.24	8 (11%)	83,113,113	1.53	18 (21%)
24	AJP	B	849	-	49,49,95	3.93	23 (46%)	74,80,149	4.32	43 (58%)
19	CLA	BB	817	-	46,50,73	1.50	9 (19%)	55,85,113	1.47	4 (7%)
19	CLA	A2	805	-	64,68,73	1.29	9 (14%)	77,107,113	1.32	6 (7%)
19	CLA	B1	834	-	49,53,73	1.47	8 (16%)	59,89,113	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	AA	831	-	69,73,73	1.25	8 (11%)	83,113,113	1.24	5 (6%)
19	CLA	B2	815	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	8 (9%)
19	CLA	BB	806	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	8 (9%)
19	CLA	B2	803	-	69,73,73	1.24	9 (13%)	83,113,113	1.32	7 (8%)
19	CLA	A2	835	-	69,73,73	1.26	10 (14%)	83,113,113	1.25	7 (8%)
19	CLA	LL	203	-	46,50,73	1.53	8 (17%)	55,85,113	1.63	9 (16%)
19	CLA	BB	822	-	69,73,73	1.25	8 (11%)	83,113,113	1.30	5 (6%)
19	CLA	B	820	-	49,53,73	1.49	9 (18%)	59,89,113	1.67	9 (15%)
19	CLA	A2	819	-	64,68,73	1.30	10 (15%)	77,107,113	1.31	8 (10%)
19	CLA	A1	817	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
19	CLA	B2	807	-	69,73,73	1.27	9 (13%)	83,113,113	1.47	11 (13%)
19	CLA	B	846	-	44,47,73	1.53	10 (22%)	52,80,113	1.46	7 (13%)
19	CLA	A2	814	-	46,50,73	1.50	9 (19%)	55,85,113	1.40	6 (10%)
19	CLA	BB	827	-	49,53,73	1.47	10 (20%)	59,89,113	1.46	7 (11%)
23	BCR	BB	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
25	LMG	I1	102	-	35,35,55	1.04	1 (2%)	43,43,63	1.27	3 (6%)
19	CLA	A	805	-	64,68,73	1.29	9 (14%)	77,107,113	1.34	7 (9%)
19	CLA	B	808	-	64,68,73	1.29	9 (14%)	77,107,113	1.25	6 (7%)
19	CLA	AA	833	-	54,58,73	1.41	10 (18%)	65,95,113	1.33	5 (7%)
19	CLA	A2	839	-	56,60,73	1.39	9 (16%)	67,97,113	1.37	5 (7%)
23	BCR	I	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	BB	838	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
19	CLA	L1	206	-	69,73,73	1.25	10 (14%)	83,113,113	1.34	7 (8%)
23	BCR	I2	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.27	9 (16%)
19	CLA	A2	833	-	54,58,73	1.41	10 (18%)	65,95,113	1.33	7 (10%)
19	CLA	B1	822	-	69,73,73	1.25	8 (11%)	83,113,113	1.26	5 (6%)
23	BCR	FF	306	-	41,41,41	1.15	3 (7%)	56,56,56	1.48	10 (17%)
19	CLA	KK	101	-	49,53,73	1.49	8 (16%)	59,89,113	1.51	7 (11%)
25	LMG	L1	210	-	55,55,55	0.68	0	63,63,63	1.28	6 (9%)
19	CLA	BB	825	-	69,73,73	1.23	9 (13%)	83,113,113	1.29	7 (8%)
19	CLA	BB	826	-	69,73,73	1.30	10 (14%)	83,113,113	1.44	12 (14%)
19	CLA	B1	850	-	64,68,73	1.29	9 (14%)	77,107,113	1.56	14 (18%)
19	CLA	A2	810	1	69,73,73	1.25	7 (10%)	83,113,113	1.37	9 (10%)
24	AJP	A1	855	-	37,37,95	4.41	24 (64%)	58,62,149	3.47	23 (39%)
27	SF4	C	101	-	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B2	818	-	45,49,73	1.53	8 (17%)	54,84,113	1.41	5 (9%)
19	CLA	A2	827	-	69,73,73	1.26	9 (13%)	83,113,113	1.34	6 (7%)
24	AJP	L2	203	-	49,49,95	3.89	24 (48%)	74,80,149	4.01	45 (60%)
24	AJP	AA	856	-	40,40,95	4.30	24 (60%)	60,65,149	3.51	21 (35%)
19	CLA	B2	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
19	CLA	AA	830	-	66,70,73	1.26	8 (12%)	79,109,113	1.26	6 (7%)
19	CLA	A	842	-	69,73,73	1.25	10 (14%)	83,113,113	1.36	11 (13%)
19	CLA	A2	834	-	45,49,73	1.50	10 (22%)	54,84,113	1.47	7 (12%)
19	CLA	B2	826	-	69,73,73	1.28	8 (11%)	83,113,113	1.38	9 (10%)
19	CLA	B2	829	-	69,73,73	1.27	9 (13%)	83,113,113	1.20	6 (7%)
19	CLA	KK	102	-	50,54,73	1.46	8 (16%)	60,90,113	1.40	5 (8%)
26	ECH	BB	840	-	42,42,42	0.89	0	55,58,58	2.44	18 (32%)
19	CLA	AA	828	-	60,64,73	1.33	9 (15%)	72,102,113	1.36	6 (8%)
27	SF4	B2	853	-	0,12,12	-	-	-	-	-
23	BCR	B	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	6 (10%)
19	CLA	BB	804	-	66,70,73	1.28	10 (15%)	79,109,113	1.31	8 (10%)
23	BCR	LL	204	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
23	BCR	F1	306	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	8 (14%)
19	CLA	B	836	-	69,73,73	1.25	10 (14%)	83,113,113	1.28	7 (8%)
19	CLA	A2	820	-	62,66,73	1.31	11 (17%)	74,104,113	1.40	8 (10%)
19	CLA	B2	821	-	69,73,73	1.23	7 (10%)	83,113,113	1.33	8 (9%)
19	CLA	B	811	-	65,69,73	1.29	9 (13%)	78,108,113	1.21	4 (5%)
19	CLA	AA	811	1	55,59,73	1.40	10 (18%)	66,96,113	1.50	9 (13%)
23	BCR	A1	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.37	9 (16%)
21	PQN	AA	844	-	34,34,34	0.66	0	42,45,45	1.06	4 (9%)
23	BCR	AA	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	BCR	A2	847	-	40,40,41	1.09	2 (5%)	54,54,56	1.26	7 (12%)
19	CLA	A1	818	-	64,68,73	1.30	9 (14%)	77,107,113	1.32	7 (9%)
21	PQN	B2	838	-	34,34,34	0.62	0	42,45,45	0.87	0
19	CLA	J	101	8	45,49,73	1.52	9 (20%)	54,84,113	1.46	5 (9%)
23	BCR	II	101	-	41,41,41	1.20	2 (4%)	56,56,56	1.22	8 (14%)
19	CLA	A1	829	-	66,70,73	1.28	7 (10%)	79,109,113	1.26	5 (6%)
19	CLA	B	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	7 (8%)
19	CLA	A1	842	-	69,73,73	1.25	10 (14%)	83,113,113	1.50	11 (13%)
19	CLA	B	807	-	69,73,73	1.27	9 (13%)	83,113,113	1.36	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	853	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	A1	840	-	50,54,73	1.44	8 (16%)	60,90,113	1.43	4 (6%)
19	CLA	A2	813	-	69,73,73	1.24	9 (13%)	83,113,113	1.30	7 (8%)
27	SF4	BB	857	-	0,12,12	-	-	-		
19	CLA	A	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.45	5 (8%)
24	AJP	AA	802	-	35,35,95	4.49	22 (62%)	54,58,149	4.38	29 (53%)
19	CLA	B2	817	-	46,50,73	1.50	8 (17%)	55,85,113	1.45	4 (7%)
19	CLA	A1	813	-	46,50,73	1.50	8 (17%)	55,85,113	1.40	6 (10%)
19	CLA	A1	816	-	48,52,73	1.48	9 (18%)	56,87,113	1.41	5 (8%)
19	CLA	A1	824	-	46,50,73	1.51	9 (19%)	55,85,113	1.43	5 (9%)
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
19	CLA	BB	816	-	61,65,73	1.34	9 (14%)	73,103,113	1.35	7 (9%)
19	CLA	B	821	2	69,73,73	1.24	7 (10%)	83,113,113	1.28	6 (7%)
19	CLA	BB	821	-	69,73,73	1.24	8 (11%)	83,113,113	1.23	6 (7%)
19	CLA	B1	813	-	46,50,73	1.50	9 (19%)	55,85,113	1.40	5 (9%)
19	CLA	K1	105	9	43,48,73	1.54	8 (18%)	52,82,113	1.52	6 (11%)
19	CLA	B2	827	-	49,53,73	1.48	10 (20%)	59,89,113	1.47	7 (11%)
19	CLA	B1	804	-	66,70,73	1.28	10 (15%)	79,109,113	1.32	7 (8%)
19	CLA	A2	840	-	60,64,73	1.32	9 (15%)	72,102,113	1.32	5 (6%)
19	CLA	A	823	-	64,68,73	1.30	9 (14%)	77,107,113	1.41	9 (11%)
19	CLA	K1	103	-	50,54,73	1.46	8 (16%)	60,90,113	1.40	5 (8%)
19	CLA	B	831	-	60,64,73	1.33	8 (13%)	72,102,113	1.31	6 (8%)
25	LMG	BB	844	-	55,55,55	0.69	1 (1%)	63,63,63	1.27	4 (6%)
19	CLA	A1	841	-	69,73,73	1.24	10 (14%)	83,113,113	1.36	8 (9%)
19	CLA	A	852	-	69,73,73	1.26	10 (14%)	83,113,113	1.30	7 (8%)
19	CLA	AA	804	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
23	BCR	FF	303	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
19	CLA	L1	205	10	65,69,73	1.29	9 (13%)	78,108,113	1.37	9 (11%)
28	DGD	BB	854	-	43,43,67	1.05	0	57,57,81	1.41	7 (12%)
23	BCR	F	305	-	41,41,41	1.15	3 (7%)	56,56,56	1.49	10 (17%)
26	ECH	B2	841	-	42,42,42	0.80	1 (2%)	55,58,58	2.41	18 (32%)
19	CLA	B1	819	-	45,49,73	1.51	8 (17%)	54,84,113	1.45	5 (9%)
19	CLA	A1	835	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	5 (6%)
19	CLA	A2	836	-	69,73,73	1.25	9 (13%)	83,113,113	1.35	6 (7%)
19	CLA	B	830	-	60,64,73	1.32	8 (13%)	72,102,113	1.38	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	844	-	45,49,73	1.50	9 (20%)	54,84,113	1.50	5 (9%)
23	BCR	JJ	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	10 (17%)
19	CLA	B1	830	-	60,64,73	1.33	7 (11%)	72,102,113	1.31	4 (5%)
19	CLA	B1	835	-	69,73,73	1.24	9 (13%)	83,113,113	1.25	6 (7%)
19	CLA	B	832	-	49,53,73	1.49	9 (18%)	59,89,113	1.40	5 (8%)
19	CLA	AA	843	-	69,73,73	1.24	8 (11%)	83,113,113	1.48	9 (10%)
19	CLA	BB	856	-	64,68,73	1.28	9 (14%)	77,107,113	1.60	14 (18%)
19	CLA	LL	201	18	65,69,73	1.28	9 (13%)	78,108,113	1.56	9 (11%)
25	LMG	B2	854	-	30,30,55	0.99	0	38,38,63	1.23	4 (10%)
19	CLA	B2	813	-	46,50,73	1.50	9 (19%)	55,85,113	1.38	6 (10%)
19	CLA	AA	805	-	64,68,73	1.28	10 (15%)	77,107,113	1.34	8 (10%)
19	CLA	B	828	-	49,53,73	1.47	9 (18%)	59,89,113	1.39	5 (8%)
19	CLA	B2	824	-	59,63,73	1.34	9 (15%)	71,101,113	1.32	5 (7%)
19	CLA	A	817	-	48,52,73	1.48	8 (16%)	56,87,113	1.43	4 (7%)
19	CLA	B1	814	-	63,67,73	1.32	9 (14%)	75,105,113	1.31	6 (8%)
19	CLA	A2	807	-	69,73,73	1.25	9 (13%)	83,113,113	1.25	6 (7%)
19	CLA	K2	102	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	7 (11%)
23	BCR	II	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)
19	CLA	BB	818	-	45,49,73	1.52	9 (20%)	54,84,113	1.40	5 (9%)
19	CLA	F1	302	-	46,50,73	1.51	9 (19%)	55,85,113	1.53	7 (12%)
23	BCR	F2	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
19	CLA	AA	819	-	64,68,73	1.29	9 (14%)	77,107,113	1.31	7 (9%)
23	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	4 (7%)
19	CLA	A	811	1	55,59,73	1.40	10 (18%)	66,96,113	1.48	8 (12%)
19	CLA	BB	835	-	69,73,73	1.25	10 (14%)	83,113,113	1.27	7 (8%)
19	CLA	JJ	103	-	45,49,73	1.52	8 (17%)	54,84,113	1.43	6 (11%)
23	BCR	K	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	BB	855	-	69,73,73	1.26	9 (13%)	83,113,113	1.24	3 (3%)
19	CLA	B	815	-	69,73,73	1.26	7 (10%)	83,113,113	1.34	11 (13%)
19	CLA	A2	811	-	55,59,73	1.39	10 (18%)	66,96,113	1.48	9 (13%)
19	CLA	F2	301	-	64,68,73	1.30	9 (14%)	77,107,113	1.37	8 (10%)
19	CLA	A1	826	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	5 (6%)
23	BCR	BB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	7 (12%)
19	CLA	B2	830	-	60,64,73	1.33	10 (16%)	72,102,113	1.38	7 (9%)
19	CLA	BB	823	-	69,73,73	1.28	10 (14%)	83,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B2	835	-	49,53,73	1.50	7 (14%)	59,89,113	1.41	6 (10%)
19	CLA	A1	801	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	A	829	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	AA	814	-	46,50,73	1.50	9 (19%)	55,85,113	1.41	6 (10%)
27	SF4	B1	851	-	0,12,12	-	-	-	-	-
19	CLA	B2	832	-	49,53,73	1.49	9 (18%)	59,89,113	1.39	6 (10%)
19	CLA	A	840	-	60,64,73	1.33	10 (16%)	72,102,113	1.33	6 (8%)
22	LHG	X2	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
19	CLA	A2	831	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	6 (7%)
19	CLA	BB	813	-	46,50,73	1.50	9 (19%)	55,85,113	1.43	5 (9%)
19	CLA	FF	302	-	46,50,73	1.51	9 (19%)	55,85,113	1.50	6 (10%)
19	CLA	X	101	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
22	LHG	BB	850	-	32,32,48	0.89	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	A2	808	-	69,73,73	1.25	9 (13%)	83,113,113	1.26	5 (6%)
19	CLA	A2	824	-	49,53,73	1.47	9 (18%)	59,89,113	1.46	6 (10%)
19	CLA	A1	823	-	49,53,73	1.47	9 (18%)	59,89,113	1.48	6 (10%)
19	CLA	A2	844	-	45,49,73	1.50	10 (22%)	54,84,113	1.48	4 (7%)
22	LHG	X1	102	-	39,39,48	0.82	2 (5%)	42,45,54	0.93	2 (4%)
23	BCR	K2	105	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	AA	801	-	69,73,73	1.24	9 (13%)	83,113,113	1.27	5 (6%)
19	CLA	AA	816	-	54,58,73	1.41	9 (16%)	65,95,113	1.41	8 (12%)
23	BCR	I2	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
21	PQN	A1	843	-	34,34,34	0.63	0	42,45,45	1.10	3 (7%)
19	CLA	A2	802	-	50,54,73	1.45	8 (16%)	60,90,113	1.41	5 (8%)
19	CLA	A2	830	-	66,70,73	1.25	7 (10%)	79,109,113	1.26	6 (7%)
22	LHG	XX	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	B1	809	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	7 (11%)
19	CLA	A2	822	-	55,59,73	1.41	9 (16%)	66,96,113	1.39	7 (10%)
19	CLA	A2	832	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	6 (7%)
19	CLA	BB	820	-	49,53,73	1.49	9 (18%)	59,89,113	1.69	11 (18%)
21	PQN	B	838	-	34,34,34	0.63	0	42,45,45	0.87	1 (2%)
19	CLA	B1	820	-	49,53,73	1.49	9 (18%)	59,89,113	1.37	5 (8%)
19	CLA	XX	101	-	49,53,73	1.49	8 (16%)	59,89,113	1.43	4 (6%)
19	CLA	BB	829	-	60,64,73	1.33	9 (15%)	72,102,113	1.33	9 (12%)
19	CLA	B1	845	-	44,47,73	1.53	8 (18%)	52,80,113	1.43	5 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	L2	208	-	34,34,48	0.87	1 (2%)	37,40,54	1.05	3 (8%)
19	CLA	B1	849	-	69,73,73	1.26	9 (13%)	83,113,113	1.17	5 (6%)
23	BCR	B1	841	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	AA	841	-	50,54,73	1.44	8 (16%)	60,90,113	1.41	5 (8%)
19	CLA	A2	812	-	50,54,73	1.44	9 (18%)	60,90,113	1.45	7 (11%)
19	CLA	A1	803	-	69,73,73	1.23	9 (13%)	83,113,113	1.28	5 (6%)
27	SF4	B	861	-	0,12,12	-	-	-	-	-
19	CLA	BB	802	-	69,73,73	1.25	9 (13%)	83,113,113	1.28	8 (9%)
23	BCR	A1	847	-	40,40,41	1.10	2 (5%)	54,54,56	1.26	7 (12%)
19	CLA	K1	102	-	49,53,73	1.48	9 (18%)	59,89,113	1.51	7 (11%)
23	BCR	B2	844	-	41,41,41	1.20	3 (7%)	56,56,56	1.19	6 (10%)
24	AJP	BB	848	-	49,49,95	3.92	25 (51%)	74,80,149	4.24	41 (55%)
23	BCR	B1	843	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
19	CLA	AA	835	-	69,73,73	1.26	9 (13%)	83,113,113	1.23	6 (7%)
19	CLA	AA	822	-	55,59,73	1.41	9 (16%)	66,96,113	1.38	4 (6%)
19	CLA	B2	811	-	65,69,73	1.30	8 (12%)	78,108,113	1.21	4 (5%)
19	CLA	A	838	-	48,52,73	1.46	9 (18%)	56,87,113	1.47	6 (10%)
19	CLA	B1	816	-	61,65,73	1.34	9 (14%)	73,103,113	1.31	7 (9%)
19	CLA	A1	812	-	69,73,73	1.25	9 (13%)	83,113,113	1.29	7 (8%)
23	BCR	A1	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	6 (10%)
19	CLA	B2	823	-	69,73,73	1.27	9 (13%)	83,113,113	1.30	5 (6%)
23	BCR	A	854	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	8 (14%)
19	CLA	A	801	-	69,73,73	1.24	9 (13%)	83,113,113	1.29	6 (7%)
21	PQN	B1	837	-	34,34,34	0.70	0	42,45,45	0.88	0
19	CLA	A2	809	-	54,58,73	1.39	9 (16%)	65,95,113	1.42	6 (9%)
23	BCR	J2	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	10 (17%)
19	CLA	BB	815	-	69,73,73	1.25	8 (11%)	83,113,113	1.33	10 (12%)
19	CLA	A	813	-	69,73,73	1.23	9 (13%)	83,113,113	1.27	6 (7%)
23	BCR	KK	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	10 (17%)
23	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	9 (16%)
19	CLA	A2	828	-	60,64,73	1.34	9 (15%)	72,102,113	1.36	5 (6%)
19	CLA	B2	812	-	45,49,73	1.51	8 (17%)	54,84,113	1.51	5 (9%)
19	CLA	X2	101	-	49,53,73	1.49	8 (16%)	59,89,113	1.41	4 (6%)
19	CLA	AA	806	-	60,64,73	1.34	10 (16%)	72,102,113	1.47	8 (11%)
23	BCR	F2	304	-	41,41,41	1.20	3 (7%)	56,56,56	1.25	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	LMG	B2	847	-	32,32,55	0.94	1 (3%)	40,40,63	1.22	2 (5%)
23	BCR	L2	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	A1	838	-	56,60,73	1.39	9 (16%)	67,97,113	1.39	5 (7%)
19	CLA	J2	101	8	45,49,73	1.53	8 (17%)	54,84,113	1.43	5 (9%)
19	CLA	FF	301	-	64,68,73	1.30	9 (14%)	77,107,113	1.30	7 (9%)
23	BCR	B1	842	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
19	CLA	A2	818	-	49,53,73	1.49	9 (18%)	59,89,113	1.45	5 (8%)
22	LHG	B1	847	-	32,32,48	0.87	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	B	826	-	69,73,73	1.28	10 (14%)	83,113,113	1.37	10 (12%)
19	CLA	B1	836	-	64,68,73	1.30	9 (14%)	77,107,113	1.38	7 (9%)
19	CLA	AA	826	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
23	BCR	M1	101	-	41,41,41	1.14	3 (7%)	56,56,56	1.24	8 (14%)
19	CLA	B	823	-	69,73,73	1.28	10 (14%)	83,113,113	1.30	6 (7%)
19	CLA	A1	825	-	49,53,73	1.47	10 (20%)	59,89,113	1.45	6 (10%)
19	CLA	B	805	-	68,72,73	1.24	10 (14%)	81,111,113	1.36	7 (8%)
19	CLA	B	837	-	64,68,73	1.30	7 (10%)	77,107,113	1.30	7 (9%)
19	CLA	BB	810	-	69,73,73	1.25	8 (11%)	83,113,113	1.25	5 (6%)
23	BCR	M2	102	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	9 (16%)
19	CLA	K	101	-	49,53,73	1.48	8 (16%)	59,89,113	1.51	7 (11%)
19	CLA	B2	833	-	69,73,73	1.27	6 (8%)	83,113,113	1.46	10 (12%)
23	BCR	I2	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	AA	823	-	64,68,73	1.30	9 (14%)	77,107,113	1.40	9 (11%)
19	CLA	A1	807	-	69,73,73	1.26	9 (13%)	83,113,113	1.33	5 (6%)
23	BCR	B2	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	6 (10%)
23	BCR	AA	855	-	41,41,41	1.14	2 (4%)	56,56,56	1.28	8 (14%)
19	CLA	A1	810	-	55,59,73	1.40	10 (18%)	66,96,113	1.47	8 (12%)
19	CLA	A	841	-	50,54,73	1.44	8 (16%)	60,90,113	1.41	5 (8%)
24	AJP	B	850	-	49,49,95	3.94	25 (51%)	74,80,149	4.28	45 (60%)
19	CLA	BB	807	-	69,73,73	1.27	9 (13%)	83,113,113	1.37	6 (7%)
19	CLA	A2	842	-	69,73,73	1.24	10 (14%)	83,113,113	1.39	8 (9%)
23	BCR	A1	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
19	CLA	B1	807	-	69,73,73	1.27	9 (13%)	83,113,113	1.46	11 (13%)
19	CLA	A1	827	-	60,64,73	1.34	9 (15%)	72,102,113	1.35	5 (6%)
23	BCR	A1	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	8 (14%)
19	CLA	B2	834	-	69,73,73	1.27	8 (11%)	83,113,113	1.55	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	AA	818	-	49,53,73	1.48	9 (18%)	59,89,113	1.46	5 (8%)
19	CLA	B1	808	-	64,68,73	1.30	9 (14%)	77,107,113	1.26	5 (6%)
19	CLA	A2	852	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	B2	851	-	64,68,73	1.29	9 (14%)	77,107,113	1.56	14 (18%)
27	SF4	C2	102	-	0,12,12	-	-	-	-	-
19	CLA	BB	801	-	69,73,73	1.24	7 (10%)	83,113,113	1.52	7 (8%)
19	CLA	A1	833	-	45,49,73	1.51	10 (22%)	54,84,113	1.46	6 (11%)
19	CLA	B1	823	-	69,73,73	1.27	9 (13%)	83,113,113	1.29	4 (4%)
19	CLA	B1	811	-	65,69,73	1.29	8 (12%)	78,108,113	1.20	4 (5%)
19	CLA	A	835	-	69,73,73	1.26	9 (13%)	83,113,113	1.24	6 (7%)
19	CLA	B2	849	-	69,73,73	1.26	9 (13%)	83,113,113	1.32	6 (7%)
19	CLA	B2	852	-	69,73,73	1.25	8 (11%)	83,113,113	1.47	9 (10%)
19	CLA	A	828	-	60,64,73	1.32	9 (15%)	72,102,113	1.34	6 (8%)
19	CLA	BB	845	-	44,47,73	1.52	10 (22%)	52,80,113	1.47	7 (13%)
19	CLA	B	801	-	69,73,73	1.23	9 (13%)	83,113,113	1.54	11 (13%)
19	CLA	A1	831	-	69,73,73	1.25	9 (13%)	83,113,113	1.31	6 (7%)
19	CLA	L	202	18	65,69,73	1.28	9 (13%)	78,108,113	1.52	9 (11%)
22	LHG	X2	103	-	48,48,48	0.77	1 (2%)	51,54,54	0.96	4 (7%)
23	BCR	B2	842	-	41,41,41	1.02	2 (4%)	56,56,56	1.35	7 (12%)
27	SF4	CC	102	-	0,12,12	-	-	-	-	-
19	CLA	B1	831	-	49,53,73	1.49	8 (16%)	59,89,113	1.40	6 (10%)
19	CLA	K2	104	-	46,49,73	1.52	9 (19%)	55,83,113	1.46	4 (7%)
20	CL0	AA	803	-	69,73,73	2.01	19 (27%)	83,113,113	2.89	30 (36%)
19	CLA	B2	810	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	6 (7%)
23	BCR	L	205	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	BB	808	-	64,68,73	1.30	9 (14%)	77,107,113	1.28	6 (7%)
19	CLA	A	812	-	50,54,73	1.44	9 (18%)	60,90,113	1.46	5 (8%)
19	CLA	J	103	-	45,49,73	1.52	7 (15%)	54,84,113	1.42	5 (9%)
23	BCR	AA	850	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
21	PQN	BB	837	-	34,34,34	0.66	0	42,45,45	0.85	0
19	CLA	L2	206	-	69,73,73	1.27	8 (11%)	83,113,113	1.27	5 (6%)
19	CLA	B1	802	-	69,73,73	1.24	9 (13%)	83,113,113	1.27	7 (8%)
19	CLA	B	806	-	69,73,73	1.24	9 (13%)	83,113,113	1.37	8 (9%)
24	AJP	L	208	-	36,36,95	4.50	24 (66%)	56,60,149	4.65	34 (60%)
19	CLA	A2	837	-	49,53,73	1.50	9 (18%)	59,89,113	1.44	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B1	832	-	69,73,73	1.27	7 (10%)	83,113,113	1.36	9 (10%)
19	CLA	B	803	-	69,73,73	1.24	10 (14%)	83,113,113	1.30	8 (9%)
19	CLA	B	817	-	46,50,73	1.50	9 (19%)	55,85,113	1.50	5 (9%)
19	CLA	A1	820	-	69,73,73	1.22	9 (13%)	83,113,113	1.34	8 (9%)
19	CLA	BB	852	-	69,73,73	1.24	8 (11%)	83,113,113	1.33	5 (6%)
19	CLA	A1	828	-	69,73,73	1.24	10 (14%)	83,113,113	1.29	6 (7%)
23	BCR	B	839	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
19	CLA	B1	848	-	69,73,73	1.26	9 (13%)	83,113,113	1.36	6 (7%)
23	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
19	CLA	A1	822	-	64,68,73	1.29	10 (15%)	77,107,113	1.37	8 (10%)
19	CLA	B2	837	-	64,68,73	1.30	9 (14%)	77,107,113	1.36	7 (9%)
23	BCR	B1	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.15	3 (5%)
25	LMG	B	845	-	55,55,55	0.69	0	63,63,63	1.27	4 (6%)
27	SF4	C2	101	-	0,12,12	-	-	-	-	-
25	LMG	B2	845	-	55,55,55	0.69	0	63,63,63	1.27	5 (7%)
19	CLA	A	839	-	56,60,73	1.39	9 (16%)	67,97,113	1.38	7 (10%)
19	CLA	B	854	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	4 (4%)
19	CLA	A	826	-	49,53,73	1.47	10 (20%)	59,89,113	1.43	6 (10%)
19	CLA	AA	832	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	7 (8%)
19	CLA	B1	824	-	59,63,73	1.36	9 (15%)	71,101,113	1.30	7 (9%)
19	CLA	AA	817	-	48,52,73	1.48	8 (16%)	56,87,113	1.42	4 (7%)
24	AJP	L2	202	-	49,49,95	3.93	23 (46%)	74,80,149	4.41	46 (62%)
19	CLA	A	833	-	54,58,73	1.40	10 (18%)	65,95,113	1.36	5 (7%)
22	LHG	A	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
19	CLA	A1	808	-	54,58,73	1.39	9 (16%)	65,95,113	1.43	6 (9%)
26	ECH	B1	840	-	42,42,42	0.82	1 (2%)	55,58,58	2.43	19 (34%)
19	CLA	B	818	-	45,49,73	1.56	7 (15%)	54,84,113	1.41	5 (9%)
23	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
19	CLA	A2	826	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
19	CLA	J1	101	-	45,49,73	1.53	8 (17%)	54,84,113	1.44	6 (11%)
24	AJP	A1	854	-	49,49,95	3.93	25 (51%)	74,80,149	3.33	21 (28%)
23	BCR	L1	209	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	9 (16%)
28	DGD	B	856	-	43,43,67	1.06	0	57,57,81	1.40	6 (10%)
27	SF4	CC	101	-	0,12,12	-	-	-	-	-
19	CLA	A2	823	-	64,68,73	1.29	9 (14%)	77,107,113	1.45	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B1	815	-	69,73,73	1.25	8 (11%)	83,113,113	1.40	11 (13%)
20	CL0	A1	802	-	69,73,73	2.05	19 (27%)	83,113,113	2.82	33 (39%)
19	CLA	B2	831	-	60,64,73	1.33	8 (13%)	72,102,113	1.31	5 (6%)
19	CLA	B	829	-	69,73,73	1.27	9 (13%)	83,113,113	1.23	6 (7%)
23	BCR	BB	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	6 (10%)
19	CLA	AA	807	-	69,73,73	1.25	9 (13%)	83,113,113	1.22	5 (6%)
24	AJP	M2	101	-	36,36,95	4.51	24 (66%)	56,60,149	4.49	30 (53%)
25	LMG	B1	846	-	32,32,55	0.93	0	40,40,63	1.21	4 (10%)
19	CLA	AA	810	-	69,73,73	1.24	8 (11%)	83,113,113	1.37	10 (12%)
19	CLA	L	204	-	69,73,73	1.25	9 (13%)	83,113,113	1.36	7 (8%)
19	CLA	A2	801	-	69,73,73	1.24	9 (13%)	83,113,113	1.31	5 (6%)
22	LHG	B2	848	-	32,32,48	0.90	2 (6%)	35,38,54	0.98	2 (5%)
19	CLA	BB	811	-	65,69,73	1.28	9 (13%)	78,108,113	1.22	4 (5%)
24	AJP	A	855	-	40,40,95	4.29	24 (60%)	60,65,149	3.51	21 (35%)
19	CLA	BB	833	-	69,73,73	1.24	7 (10%)	83,113,113	1.52	18 (21%)
19	CLA	B	833	-	69,73,73	1.28	8 (11%)	83,113,113	1.40	9 (10%)
23	BCR	M	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	10 (17%)
19	CLA	B1	828	-	69,73,73	1.27	9 (13%)	83,113,113	1.20	6 (7%)
20	CL0	A2	803	-	69,73,73	1.98	18 (26%)	83,113,113	2.87	31 (37%)
19	CLA	A	814	-	46,50,73	1.51	9 (19%)	55,85,113	1.37	6 (10%)
24	AJP	L1	203	-	49,49,95	3.92	24 (48%)	74,80,149	3.79	37 (50%)
19	CLA	B2	822	-	69,73,73	1.26	9 (13%)	83,113,113	1.31	7 (8%)
19	CLA	AA	825	-	56,60,73	1.38	9 (16%)	67,97,113	1.37	5 (7%)
23	BCR	A	847	-	40,40,41	1.09	2 (5%)	54,54,56	1.28	11 (20%)
23	BCR	J2	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	8 (14%)
19	CLA	A2	806	-	60,64,73	1.34	9 (15%)	72,102,113	1.46	8 (11%)
19	CLA	J1	103	-	45,49,73	1.53	7 (15%)	54,84,113	1.43	5 (9%)
24	AJP	L1	204	-	49,49,95	3.89	24 (48%)	74,80,149	4.01	46 (62%)
19	CLA	A	819	-	64,68,73	1.29	10 (15%)	77,107,113	1.32	6 (7%)
23	BCR	FF	304	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	B1	818	-	45,49,73	1.53	8 (17%)	54,84,113	1.41	5 (9%)
19	CLA	BB	819	-	45,49,73	1.51	8 (17%)	54,84,113	1.45	5 (9%)
23	BCR	BB	843	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	6 (10%)
19	CLA	A1	806	-	69,73,73	1.25	9 (13%)	83,113,113	1.25	6 (7%)
19	CLA	A1	836	-	49,53,73	1.49	9 (18%)	59,89,113	1.43	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	816	-	61,65,73	1.34	9 (14%)	73,103,113	1.37	7 (9%)
19	CLA	A	810	1	69,73,73	1.25	8 (11%)	83,113,113	1.37	10 (12%)
19	CLA	A	821	-	69,73,73	1.23	9 (13%)	83,113,113	1.34	7 (8%)
19	CLA	AA	813	-	69,73,73	1.24	9 (13%)	83,113,113	1.27	6 (7%)
23	BCR	F1	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
19	CLA	A1	815	-	54,58,73	1.41	8 (14%)	65,95,113	1.40	7 (10%)
24	AJP	KK	104	-	47,47,95	3.98	24 (51%)	71,77,149	4.34	40 (56%)
19	CLA	AA	824	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
19	CLA	A1	809	-	69,73,73	1.24	8 (11%)	83,113,113	1.31	9 (10%)
19	CLA	AA	827	-	69,73,73	1.26	8 (11%)	83,113,113	1.25	6 (7%)
19	CLA	F	301	-	64,68,73	1.29	9 (14%)	77,107,113	1.42	8 (10%)
19	CLA	BB	832	-	69,73,73	1.28	8 (11%)	83,113,113	1.38	8 (9%)
19	CLA	L	203	-	69,73,73	1.27	10 (14%)	83,113,113	1.32	8 (9%)
23	BCR	AA	852	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	7 (12%)
24	AJP	A	802	-	35,35,95	4.49	22 (62%)	54,58,149	4.38	29 (53%)
22	LHG	BB	851	-	48,48,48	0.77	2 (4%)	51,54,54	0.98	4 (7%)
22	LHG	A2	846	-	37,37,48	0.82	1 (2%)	40,43,54	1.02	3 (7%)
19	CLA	A	827	-	69,73,73	1.26	9 (13%)	83,113,113	1.25	5 (6%)
19	CLA	B2	808	-	64,68,73	1.30	9 (14%)	77,107,113	1.28	5 (6%)
23	BCR	A1	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.46	8 (14%)
19	CLA	B2	828	-	49,53,73	1.48	8 (16%)	59,89,113	1.39	5 (8%)
19	CLA	B	822	-	69,73,73	1.24	8 (11%)	83,113,113	1.28	4 (4%)
19	CLA	A	807	-	69,73,73	1.25	9 (13%)	83,113,113	1.23	6 (7%)
19	CLA	A1	832	-	54,58,73	1.41	10 (18%)	65,95,113	1.37	6 (9%)
23	BCR	F1	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	9 (16%)
19	CLA	BB	824	-	59,63,73	1.35	10 (16%)	71,101,113	1.29	5 (7%)
19	CLA	AA	820	-	62,66,73	1.32	10 (16%)	74,104,113	1.40	8 (10%)
19	CLA	A	837	-	49,53,73	1.50	9 (18%)	59,89,113	1.42	6 (10%)
22	LHG	A1	845	-	48,48,48	0.78	2 (4%)	51,54,54	0.96	3 (5%)
23	BCR	AA	854	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	12 (21%)
19	CLA	A1	821	-	55,59,73	1.40	9 (16%)	66,96,113	1.39	7 (10%)
19	CLA	L2	204	16	65,69,73	1.29	8 (12%)	78,108,113	1.35	8 (10%)
19	CLA	A2	838	-	48,52,73	1.46	9 (18%)	56,87,113	1.49	5 (8%)
19	CLA	AA	842	-	69,73,73	1.25	10 (14%)	83,113,113	1.35	10 (12%)
25	LMG	M	102	-	46,46,55	0.82	0	54,54,63	1.28	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	K	102	-	50,54,73	1.45	8 (16%)	60,90,113	1.40	5 (8%)
19	CLA	A1	804	-	64,68,73	1.28	8 (12%)	77,107,113	1.27	6 (7%)
19	CLA	A1	819	-	62,66,73	1.31	11 (17%)	74,104,113	1.36	9 (12%)
22	LHG	AA	846	-	48,48,48	0.79	2 (4%)	51,54,54	0.97	3 (5%)
23	BCR	I1	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	8 (14%)
22	LHG	LL	205	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
19	CLA	B2	809	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	7 (11%)
19	CLA	BB	814	-	63,67,73	1.31	11 (17%)	75,105,113	1.37	9 (12%)
23	BCR	J	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	10 (17%)
19	CLA	A1	839	-	60,64,73	1.33	10 (16%)	72,102,113	1.31	5 (6%)
19	CLA	B1	829	-	60,64,73	1.33	10 (16%)	72,102,113	1.35	7 (9%)
19	CLA	AA	808	-	69,73,73	1.25	9 (13%)	83,113,113	1.24	5 (6%)
19	CLA	BB	830	-	60,64,73	1.32	8 (13%)	72,102,113	1.29	5 (6%)
25	LMG	B1	844	-	55,55,55	0.68	0	63,63,63	1.28	4 (6%)
19	CLA	A2	825	-	46,50,73	1.51	10 (21%)	55,85,113	1.47	5 (9%)
19	CLA	F	302	-	46,50,73	1.51	9 (19%)	55,85,113	1.51	6 (10%)
22	LHG	AA	847	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
19	CLA	A1	814	-	59,63,73	1.35	8 (13%)	71,101,113	1.31	5 (7%)
23	BCR	K1	106	-	41,41,41	1.14	2 (4%)	56,56,56	1.35	10 (17%)
25	LMG	B	851	-	55,55,55	0.68	0	63,63,63	1.28	7 (11%)
19	CLA	A1	805	-	60,64,73	1.35	10 (16%)	72,102,113	1.33	6 (8%)
19	CLA	A1	837	1	48,52,73	1.47	9 (18%)	56,87,113	1.48	6 (10%)
23	BCR	A2	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
19	CLA	A	822	-	55,59,73	1.42	8 (14%)	66,96,113	1.38	6 (9%)
19	CLA	A1	830	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	7 (8%)
19	CLA	BB	805	-	68,72,73	1.24	10 (14%)	81,111,113	1.35	8 (9%)
19	CLA	B1	805	-	68,72,73	1.24	10 (14%)	81,111,113	1.34	8 (9%)
23	BCR	B	844	-	41,41,41	1.24	4 (9%)	56,56,56	1.22	7 (12%)
19	CLA	AA	829	-	69,73,73	1.25	9 (13%)	83,113,113	1.30	6 (7%)
23	BCR	B1	838	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	10 (17%)
23	BCR	L1	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	AA	839	-	56,60,73	1.39	8 (14%)	67,97,113	1.37	6 (8%)
23	BCR	L1	201	-	41,41,41	1.17	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	A2	849	-	41,41,41	1.05	2 (4%)	56,56,56	1.25	8 (14%)
22	LHG	X	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	AA	845	-	45,49,73	1.50	9 (20%)	54,84,113	1.51	6 (11%)
19	CLA	BB	809	-	49,53,73	1.47	9 (18%)	59,89,113	1.47	6 (10%)
19	CLA	BB	836	-	64,68,73	1.30	9 (14%)	77,107,113	1.62	10 (12%)
19	CLA	B2	816	-	61,65,73	1.34	9 (14%)	73,103,113	1.32	6 (8%)
19	CLA	BB	812	-	45,49,73	1.50	8 (17%)	54,84,113	1.47	4 (7%)
23	BCR	B2	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
22	LHG	L1	211	-	32,32,48	0.96	3 (9%)	35,38,54	1.02	3 (8%)
23	BCR	F	303	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
19	CLA	A	831	-	69,73,73	1.25	8 (11%)	83,113,113	1.23	4 (4%)
23	BCR	B	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
19	CLA	B2	806	2	69,73,73	1.24	8 (11%)	83,113,113	1.34	7 (8%)
19	CLA	B	858	-	69,73,73	1.26	8 (11%)	83,113,113	1.23	5 (6%)
19	CLA	A	808	-	69,73,73	1.25	9 (13%)	83,113,113	1.32	8 (9%)
19	CLA	A	824	-	49,53,73	1.48	9 (18%)	59,89,113	1.47	6 (10%)
23	BCR	A2	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	J1	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	AA	815	-	59,63,73	1.34	8 (13%)	71,101,113	1.34	5 (7%)
19	CLA	B2	804	-	66,70,73	1.28	10 (15%)	79,109,113	1.33	7 (8%)
19	CLA	B1	826	-	69,73,73	1.28	9 (13%)	83,113,113	1.38	8 (9%)
19	CLA	JJ	101	8	45,49,73	1.52	9 (20%)	54,84,113	1.46	5 (9%)
19	CLA	A	836	-	69,73,73	1.24	9 (13%)	83,113,113	1.28	5 (6%)
22	LHG	B	853	-	48,48,48	0.75	1 (2%)	51,54,54	0.98	4 (7%)
23	BCR	AA	848	-	40,40,41	1.09	2 (5%)	54,54,56	1.28	10 (18%)
19	CLA	AA	809	-	54,58,73	1.39	8 (14%)	65,95,113	1.43	7 (10%)
19	CLA	A1	834	-	69,73,73	1.26	10 (14%)	83,113,113	1.23	7 (8%)
19	CLA	A	834	-	45,49,73	1.51	10 (22%)	54,84,113	1.46	6 (11%)
19	CLA	J2	103	-	45,49,73	1.53	7 (15%)	54,84,113	1.42	6 (11%)
19	CLA	B	859	-	64,68,73	1.28	9 (14%)	77,107,113	1.61	14 (18%)
23	BCR	K2	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
23	BCR	AA	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	5 (8%)
19	CLA	B1	801	-	69,73,73	1.23	9 (13%)	83,113,113	1.41	8 (9%)
19	CLA	A	830	-	66,70,73	1.25	8 (12%)	79,109,113	1.27	6 (7%)
19	CLA	B2	825	-	69,73,73	1.24	8 (11%)	83,113,113	1.30	7 (8%)
19	CLA	B2	850	-	69,73,73	1.26	9 (13%)	83,113,113	1.21	5 (6%)
19	CLA	A2	829	-	69,73,73	1.26	11 (15%)	83,113,113	1.25	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A2	841	-	50,54,73	1.44	8 (16%)	60,90,113	1.42	4 (6%)
19	CLA	A	820	-	62,66,73	1.31	10 (16%)	74,104,113	1.38	9 (12%)
19	CLA	F1	301	-	64,68,73	1.30	9 (14%)	77,107,113	1.41	9 (11%)
19	CLA	X1	101	-	49,53,73	1.49	8 (16%)	59,89,113	1.42	4 (6%)
19	CLA	B2	819	-	45,49,73	1.51	9 (20%)	54,84,113	1.49	4 (7%)
23	BCR	A2	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
19	CLA	B2	805	-	68,72,73	1.24	10 (14%)	81,111,113	1.35	8 (9%)
19	CLA	BB	834	-	49,53,73	1.48	9 (18%)	59,89,113	1.42	5 (8%)
20	CL0	A	803	-	69,73,73	2.04	18 (26%)	83,113,113	2.80	31 (37%)
19	CLA	B	813	-	46,50,73	1.50	9 (19%)	55,85,113	1.40	5 (9%)
19	CLA	A2	817	-	48,52,73	1.48	10 (20%)	56,87,113	1.42	5 (8%)
19	CLA	AA	821	-	69,73,73	1.23	9 (13%)	83,113,113	1.32	7 (8%)
19	CLA	B1	806	-	69,73,73	1.24	8 (11%)	83,113,113	1.38	8 (9%)
19	CLA	B	824	-	59,63,73	1.35	9 (15%)	71,101,113	1.27	5 (7%)
19	CLA	B	804	-	66,70,73	1.28	9 (13%)	79,109,113	1.30	8 (10%)
23	BCR	F	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
27	SF4	C	102	3	0,12,12	-	-	-	-	-
19	CLA	A	809	-	54,58,73	1.39	9 (16%)	65,95,113	1.43	8 (12%)
19	CLA	BB	831	-	49,53,73	1.48	9 (18%)	59,89,113	1.44	7 (11%)

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
24	AJP	BB	849	-	17/17/19/38	3/6/121/220	0/7/7/11
19	CLA	B1	817	-	-	4/12/88/115	-
23	BCR	L	206	-	-	18/29/63/63	0/2/2/2
19	CLA	B2	814	-	-	14/32/108/115	-
19	CLA	FF	305	-	-	11/39/115/115	-
23	BCR	JJ	104	-	-	16/29/63/63	0/2/2/2
21	PQN	A2	843	-	-	8/23/43/43	0/2/2/2
19	CLA	AA	834	-	-	4/10/86/115	-
24	AJP	A2	854	-	12/12/14/38	-	0/6/6/11
26	ECH	B	841	-	-	16/29/66/66	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	821	2	-	14/39/115/115	-
19	CLA	B	819	-	-	2/10/86/115	-
19	CLA	B2	801	-	-	18/39/115/115	-
19	CLA	B	825	-	-	20/39/115/115	-
27	SF4	C1	102	-	-	-	0/6/5/5
19	CLA	B	835	-	-	1/15/91/115	-
24	AJP	I2	104	-	12/12/14/38	-	0/6/6/11
23	BCR	BB	842	-	-	16/29/63/63	0/2/2/2
19	CLA	BB	828	-	-	1/15/91/115	-
23	BCR	II	104	-	-	18/29/63/63	0/2/2/2
19	CLA	A2	815	-	-	9/27/103/115	-
25	LMG	I2	105	-	-	10/29/49/70	0/1/1/1
19	CLA	AA	840	-	-	7/29/105/115	-
24	AJP	K	104	-	16/16/19/38	2/4/116/220	0/7/7/11
23	BCR	A	851	-	-	19/29/63/63	0/2/2/2
25	LMG	B1	852	-	-	5/25/45/70	0/1/1/1
19	CLA	A	816	-	-	7/21/97/115	-
21	PQN	A	843	-	-	8/23/43/43	0/2/2/2
19	CLA	AA	836	-	-	18/39/115/115	-
19	CLA	A1	852	-	-	18/39/115/115	-
19	CLA	B	809	-	-	6/15/91/115	-
19	CLA	B	810	-	-	15/39/115/115	-
19	CLA	B	814	-	-	12/32/108/115	-
19	CLA	B	827	-	-	10/15/91/115	-
19	CLA	B	812	-	-	4/10/86/115	-
22	LHG	B	852	-	-	14/37/37/53	-
23	BCR	A2	851	-	-	17/29/63/63	0/2/2/2
19	CLA	A	806	-	-	10/29/105/115	-
19	CLA	A1	844	-	-	3/10/86/115	-
19	CLA	B2	836	-	-	13/39/115/115	-
22	LHG	A2	845	-	-	16/53/53/53	-
19	CLA	B1	803	-	-	15/39/115/115	-
23	BCR	F2	305	-	-	26/29/63/63	0/2/2/2
19	CLA	B	860	-	-	15/39/115/115	-
19	CLA	A	804	-	-	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	815	-	-	9/27/103/115	-
19	CLA	F2	302	-	-	4/12/88/115	-
23	BCR	MM	101	-	-	23/29/63/63	0/2/2/2
19	CLA	A	832	-	-	9/39/115/115	-
19	CLA	B1	825	-	-	18/39/115/115	-
22	LHG	A1	846	-	-	12/42/42/53	-
19	CLA	A2	816	-	-	6/21/97/115	-
19	CLA	A2	821	-	-	13/39/115/115	-
23	BCR	I	102	-	-	10/29/63/63	0/2/2/2
19	CLA	B2	820	-	-	11/15/91/115	-
19	CLA	A2	804	-	-	19/39/115/115	-
23	BCR	K1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	A	825	-	-	5/24/100/115	-
22	LHG	A	845	-	-	19/53/53/53	-
24	AJP	B	857	-	16/16/19/38	0/6/121/220	0/7/7/11
19	CLA	B2	846	-	-	0/7/79/115	-
19	CLA	AA	838	-	-	4/13/90/115	-
23	BCR	J1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	F1	305	-	-	4/15/91/115	-
19	CLA	A1	811	-	-	7/17/93/115	-
27	SF4	C1	101	-	-	-	0/6/5/5
19	CLA	AA	837	-	-	1/15/91/115	-
19	CLA	BB	803	-	-	14/39/115/115	-
19	CLA	L2	205	-	-	8/32/108/115	-
22	LHG	L	207	-	-	13/38/38/53	-
19	CLA	B1	810	-	-	16/39/115/115	-
23	BCR	B2	839	-	-	19/29/63/63	0/2/2/2
23	BCR	B	843	-	-	16/29/63/63	0/2/2/2
19	CLA	L1	207	-	-	12/39/115/115	-
24	AJP	L	209	-	13/13/14/38	-	0/6/6/11
19	CLA	B1	827	-	-	8/15/91/115	-
19	CLA	B1	812	-	-	6/10/86/115	-
19	CLA	LL	202	-	-	8/39/115/115	-
19	CLA	AA	853	-	-	18/39/115/115	-
19	CLA	B1	833	-	-	20/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	LHG	X1	103	-	-	20/53/53/53	-
19	CLA	AA	812	-	-	9/17/93/115	-
25	LMG	II	105	-	-	20/37/57/70	0/1/1/1
19	CLA	B	834	-	-	20/39/115/115	-
24	AJP	B	849	-	18/18/19/38	3/6/121/220	0/7/7/11
19	CLA	BB	817	-	-	3/12/88/115	-
19	CLA	A2	805	-	-	8/33/109/115	-
19	CLA	B1	834	-	-	1/15/91/115	-
19	CLA	AA	831	-	-	14/39/115/115	-
19	CLA	B2	815	-	-	15/39/115/115	-
19	CLA	BB	806	-	-	15/39/115/115	-
19	CLA	B2	803	-	-	13/39/115/115	-
19	CLA	A2	835	-	-	9/39/115/115	-
19	CLA	LL	203	-	-	8/12/88/115	-
19	CLA	BB	822	-	-	8/39/115/115	-
19	CLA	B	820	-	-	11/15/91/115	-
19	CLA	A2	819	-	-	10/33/109/115	-
19	CLA	A1	817	-	-	5/15/91/115	-
19	CLA	B2	807	-	-	15/39/115/115	-
19	CLA	B	846	-	-	1/7/79/115	-
19	CLA	A2	814	-	-	5/12/88/115	-
19	CLA	BB	827	-	-	4/15/91/115	-
23	BCR	BB	839	-	-	9/29/63/63	0/2/2/2
25	LMG	I1	102	-	-	18/30/50/70	0/1/1/1
19	CLA	A	805	-	-	8/33/109/115	-
19	CLA	B	808	-	-	12/33/109/115	-
19	CLA	AA	833	-	-	4/21/97/115	-
19	CLA	A2	839	-	-	8/24/100/115	-
23	BCR	I	101	-	-	20/29/63/63	0/2/2/2
23	BCR	BB	838	-	-	15/29/63/63	0/2/2/2
19	CLA	L1	206	-	-	5/39/115/115	-
23	BCR	I2	101	-	-	17/29/63/63	0/2/2/2
19	CLA	A2	833	-	-	5/21/97/115	-
19	CLA	B1	822	-	-	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	FF	306	-	-	22/29/63/63	0/2/2/2
19	CLA	KK	101	-	-	1/15/91/115	-
25	LMG	L1	210	-	-	16/50/70/70	0/1/1/1
19	CLA	BB	825	-	-	20/39/115/115	-
19	CLA	BB	826	-	-	17/39/115/115	-
19	CLA	B1	850	-	-	13/33/109/115	-
24	AJP	A1	855	-	12/12/14/38	-	0/6/6/11
19	CLA	A2	810	1	-	10/39/115/115	-
27	SF4	C	101	-	-	-	0/6/5/5
19	CLA	B2	818	-	-	2/10/86/115	-
19	CLA	A2	827	-	-	16/39/115/115	-
24	AJP	L2	203	-	16/16/19/38	4/6/121/220	0/7/7/11
24	AJP	AA	856	-	12/12/16/38	2/4/99/220	0/6/6/11
19	CLA	B2	802	-	-	9/39/115/115	-
19	CLA	AA	830	-	-	14/36/112/115	-
19	CLA	A	842	-	-	11/39/115/115	-
19	CLA	A2	834	-	-	4/10/86/115	-
19	CLA	B2	826	-	-	16/39/115/115	-
19	CLA	B2	829	-	-	13/39/115/115	-
19	CLA	KK	102	-	-	10/17/93/115	-
26	ECH	BB	840	-	-	16/29/66/66	0/2/2/2
19	CLA	AA	828	-	-	11/29/105/115	-
27	SF4	B2	853	-	-	-	0/6/5/5
23	BCR	B	842	-	-	18/29/63/63	0/2/2/2
19	CLA	BB	804	-	-	9/36/112/115	-
23	BCR	LL	204	-	-	18/29/63/63	0/2/2/2
23	BCR	F1	306	-	-	25/29/63/63	0/2/2/2
19	CLA	B	836	-	-	11/39/115/115	-
19	CLA	A2	820	-	-	13/31/107/115	-
19	CLA	B2	821	-	-	14/39/115/115	-
19	CLA	B	811	-	-	16/35/111/115	-
19	CLA	AA	811	1	-	8/23/99/115	-
23	BCR	A1	853	-	-	16/29/63/63	0/2/2/2
21	PQN	AA	844	-	-	4/23/43/43	0/2/2/2
23	BCR	AA	849	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A2	847	-	-	12/27/61/63	0/2/2/2
19	CLA	A1	818	-	-	13/33/109/115	-
21	PQN	B2	838	-	-	7/23/43/43	0/2/2/2
19	CLA	J	101	8	-	5/10/86/115	-
23	BCR	II	101	-	-	17/29/63/63	0/2/2/2
19	CLA	A1	829	-	-	16/36/112/115	-
19	CLA	B	802	-	-	13/39/115/115	-
19	CLA	A1	842	-	-	15/39/115/115	-
19	CLA	B	807	-	-	11/39/115/115	-
23	BCR	A	853	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	840	-	-	6/17/93/115	-
19	CLA	A2	813	-	-	13/39/115/115	-
27	SF4	BB	857	-	-	-	0/6/5/5
19	CLA	A	818	-	-	5/15/91/115	-
24	AJP	AA	802	-	11/11/14/38	-	0/6/6/11
19	CLA	B2	817	-	-	4/12/88/115	-
19	CLA	A1	813	-	-	5/12/88/115	-
19	CLA	A1	816	-	-	2/13/90/115	-
19	CLA	A1	824	-	-	4/12/88/115	-
23	BCR	J	104	-	-	16/29/63/63	0/2/2/2
19	CLA	BB	816	-	-	10/30/106/115	-
19	CLA	B	821	2	-	14/39/115/115	-
19	CLA	BB	821	-	-	17/39/115/115	-
19	CLA	B1	813	-	-	8/12/88/115	-
19	CLA	K1	105	9	-	6/10/82/115	-
19	CLA	B2	827	-	-	6/15/91/115	-
19	CLA	B1	804	-	-	11/36/112/115	-
19	CLA	A2	840	-	-	4/29/105/115	-
19	CLA	A	823	-	-	16/33/109/115	-
19	CLA	K1	103	-	-	8/17/93/115	-
19	CLA	B	831	-	-	5/29/105/115	-
25	LMG	BB	844	-	-	18/50/70/70	0/1/1/1
19	CLA	A1	841	-	-	9/39/115/115	-
19	CLA	A	852	-	-	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	804	-	-	16/39/115/115	-
23	BCR	FF	303	-	-	19/29/63/63	0/2/2/2
19	CLA	L1	205	10	-	11/35/111/115	-
28	DGD	BB	854	-	-	21/31/71/95	0/2/2/2
23	BCR	F	305	-	-	23/29/63/63	0/2/2/2
26	ECH	B2	841	-	-	16/29/66/66	0/2/2/2
19	CLA	B1	819	-	-	3/10/86/115	-
19	CLA	A1	835	-	-	13/39/115/115	-
19	CLA	A2	836	-	-	16/39/115/115	-
19	CLA	B	830	-	-	4/29/105/115	-
19	CLA	A	844	-	-	4/10/86/115	-
23	BCR	JJ	102	-	-	20/29/63/63	0/2/2/2
19	CLA	B1	830	-	-	8/29/105/115	-
19	CLA	B1	835	-	-	12/39/115/115	-
19	CLA	B	832	-	-	6/15/91/115	-
19	CLA	AA	843	-	-	15/39/115/115	-
19	CLA	BB	856	-	-	15/33/109/115	-
19	CLA	LL	201	18	-	13/35/111/115	-
25	LMG	B2	854	-	-	5/25/45/70	0/1/1/1
19	CLA	B2	813	-	-	8/12/88/115	-
19	CLA	AA	805	-	-	8/33/109/115	-
19	CLA	B	828	-	-	4/15/91/115	-
19	CLA	B2	824	-	-	13/27/103/115	-
19	CLA	A	817	-	-	5/13/90/115	-
19	CLA	B1	814	-	-	14/32/108/115	-
19	CLA	A2	807	-	-	18/39/115/115	-
19	CLA	K2	102	-	-	1/15/91/115	-
23	BCR	II	102	-	-	9/29/63/63	0/2/2/2
19	CLA	BB	818	-	-	4/10/86/115	-
19	CLA	F1	302	-	-	5/12/88/115	-
23	BCR	F2	303	-	-	21/29/63/63	0/2/2/2
19	CLA	AA	819	-	-	15/33/109/115	-
23	BCR	A	850	-	-	15/29/63/63	0/2/2/2
19	CLA	A	811	1	-	8/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	835	-	-	11/39/115/115	-
19	CLA	JJ	103	-	-	2/10/86/115	-
23	BCR	K	103	-	-	19/29/63/63	0/2/2/2
19	CLA	BB	855	-	-	6/39/115/115	-
19	CLA	B	815	-	-	18/39/115/115	-
19	CLA	A2	811	-	-	8/23/99/115	-
19	CLA	F2	301	-	-	10/33/109/115	-
19	CLA	A1	826	-	-	16/39/115/115	-
23	BCR	BB	847	-	-	17/29/63/63	0/2/2/2
19	CLA	B2	830	-	-	4/29/105/115	-
19	CLA	BB	823	-	-	15/39/115/115	-
19	CLA	B2	835	-	-	2/15/91/115	-
19	CLA	A1	801	-	-	13/39/115/115	-
19	CLA	A	829	-	-	14/39/115/115	-
19	CLA	AA	814	-	-	5/12/88/115	-
27	SF4	B1	851	-	-	-	0/6/5/5
19	CLA	B2	832	-	-	8/15/91/115	-
19	CLA	A	840	-	-	5/29/105/115	-
22	LHG	X2	102	-	-	15/44/44/53	-
19	CLA	A2	831	-	-	13/39/115/115	-
19	CLA	BB	813	-	-	6/12/88/115	-
19	CLA	FF	302	-	-	4/12/88/115	-
19	CLA	X	101	-	-	4/15/91/115	-
22	LHG	BB	850	-	-	13/37/37/53	-
19	CLA	A2	808	-	-	15/39/115/115	-
19	CLA	A2	824	-	-	4/15/91/115	-
19	CLA	A1	823	-	-	6/15/91/115	-
19	CLA	A2	844	-	-	3/10/86/115	-
22	LHG	X1	102	-	-	17/44/44/53	-
23	BCR	K2	105	-	-	17/29/63/63	0/2/2/2
19	CLA	AA	801	-	-	13/39/115/115	-
19	CLA	AA	816	-	-	9/21/97/115	-
23	BCR	I2	102	-	-	11/29/63/63	0/2/2/2
21	PQN	A1	843	-	-	8/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A2	802	-	-	9/17/93/115	-
19	CLA	A2	830	-	-	18/36/112/115	-
22	LHG	XX	102	-	-	18/44/44/53	-
19	CLA	B1	809	-	-	7/15/91/115	-
19	CLA	A2	822	-	-	7/23/99/115	-
19	CLA	A2	832	-	-	6/39/115/115	-
19	CLA	BB	820	-	-	12/15/91/115	-
21	PQN	B	838	-	-	7/23/43/43	0/2/2/2
19	CLA	B1	820	-	-	11/15/91/115	-
19	CLA	XX	101	-	-	9/15/91/115	-
19	CLA	BB	829	-	-	7/29/105/115	-
19	CLA	B1	845	-	-	0/7/79/115	-
22	LHG	L2	208	-	-	17/39/39/53	-
19	CLA	B1	849	-	-	4/39/115/115	-
23	BCR	B1	841	-	-	20/29/63/63	0/2/2/2
19	CLA	AA	841	-	-	5/17/93/115	-
19	CLA	A2	812	-	-	7/17/93/115	-
19	CLA	A1	803	-	-	17/39/115/115	-
27	SF4	B	861	-	-	-	0/6/5/5
19	CLA	BB	802	-	-	18/39/115/115	-
23	BCR	A1	847	-	-	12/27/61/63	0/2/2/2
19	CLA	K1	102	-	-	1/15/91/115	-
23	BCR	B2	844	-	-	13/29/63/63	0/2/2/2
24	AJP	BB	848	-	17/17/19/38	3/6/121/220	0/7/7/11
23	BCR	B1	843	-	-	13/29/63/63	0/2/2/2
19	CLA	AA	835	-	-	10/39/115/115	-
19	CLA	AA	822	-	-	10/23/99/115	-
19	CLA	B2	811	-	-	15/35/111/115	-
19	CLA	A	838	-	-	5/13/90/115	-
19	CLA	B1	816	-	-	11/30/106/115	-
19	CLA	A1	812	-	-	11/39/115/115	-
23	BCR	A1	850	-	-	14/29/63/63	0/2/2/2
19	CLA	B2	823	-	-	18/39/115/115	-
23	BCR	A	854	-	-	18/29/63/63	0/2/2/2
19	CLA	A	801	-	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	PQN	B1	837	-	-	7/23/43/43	0/2/2/2
19	CLA	A2	809	-	-	4/21/97/115	-
23	BCR	J2	104	-	-	16/29/63/63	0/2/2/2
19	CLA	BB	815	-	-	17/39/115/115	-
19	CLA	A	813	-	-	11/39/115/115	-
23	BCR	KK	103	-	-	19/29/63/63	0/2/2/2
23	BCR	A	849	-	-	18/29/63/63	0/2/2/2
19	CLA	A2	828	-	-	11/29/105/115	-
19	CLA	B2	812	-	-	4/10/86/115	-
19	CLA	X2	101	-	-	5/15/91/115	-
19	CLA	AA	806	-	-	10/29/105/115	-
23	BCR	F2	304	-	-	15/29/63/63	0/2/2/2
25	LMG	B2	847	-	-	9/27/47/70	0/1/1/1
23	BCR	L2	207	-	-	19/29/63/63	0/2/2/2
19	CLA	A1	838	-	-	8/24/100/115	-
19	CLA	J2	101	8	-	5/10/86/115	-
19	CLA	FF	301	-	-	15/33/109/115	-
23	BCR	B1	842	-	-	16/29/63/63	0/2/2/2
19	CLA	A2	818	-	-	5/15/91/115	-
22	LHG	B1	847	-	-	14/37/37/53	-
19	CLA	B	826	-	-	14/39/115/115	-
19	CLA	B1	836	-	-	10/33/109/115	-
19	CLA	AA	826	-	-	9/15/91/115	-
23	BCR	M1	101	-	-	17/29/63/63	0/2/2/2
19	CLA	B	823	-	-	14/39/115/115	-
19	CLA	A1	825	-	-	9/15/91/115	-
19	CLA	B	805	-	-	11/38/114/115	-
19	CLA	B	837	-	-	10/33/109/115	-
19	CLA	BB	810	-	-	16/39/115/115	-
23	BCR	M2	102	-	-	19/29/63/63	0/2/2/2
19	CLA	K	101	-	-	2/15/91/115	-
19	CLA	B2	833	-	-	13/39/115/115	-
23	BCR	I2	103	-	-	18/29/63/63	0/2/2/2
19	CLA	AA	823	-	-	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A1	807	-	-	14/39/115/115	-
23	BCR	B2	843	-	-	18/29/63/63	0/2/2/2
23	BCR	AA	855	-	-	18/29/63/63	0/2/2/2
24	AJP	B	850	-	17/17/19/38	2/6/121/220	0/7/7/11
19	CLA	A1	810	-	-	9/23/99/115	-
19	CLA	A	841	-	-	5/17/93/115	-
19	CLA	BB	807	-	-	11/39/115/115	-
19	CLA	A2	842	-	-	12/39/115/115	-
23	BCR	A1	848	-	-	14/29/63/63	0/2/2/2
19	CLA	B1	807	-	-	11/39/115/115	-
19	CLA	A1	827	-	-	11/29/105/115	-
23	BCR	A1	849	-	-	13/29/63/63	0/2/2/2
19	CLA	B2	834	-	-	20/39/115/115	-
19	CLA	AA	818	-	-	5/15/91/115	-
19	CLA	B1	808	-	-	13/33/109/115	-
19	CLA	A2	852	-	-	13/39/115/115	-
19	CLA	B2	851	-	-	13/33/109/115	-
27	SF4	C2	102	-	-	-	0/6/5/5
19	CLA	BB	801	-	-	21/39/115/115	-
19	CLA	A1	833	-	-	4/10/86/115	-
19	CLA	B1	823	-	-	18/39/115/115	-
19	CLA	B1	811	-	-	15/35/111/115	-
19	CLA	A	835	-	-	10/39/115/115	-
19	CLA	B2	849	-	-	14/39/115/115	-
19	CLA	B2	852	-	-	15/39/115/115	-
19	CLA	A	828	-	-	11/29/105/115	-
19	CLA	BB	845	-	-	1/7/79/115	-
19	CLA	B	801	-	-	17/39/115/115	-
19	CLA	A1	831	-	-	8/39/115/115	-
19	CLA	L	202	18	-	14/35/111/115	-
22	LHG	X2	103	-	-	22/53/53/53	-
23	BCR	B2	842	-	-	21/29/63/63	0/2/2/2
27	SF4	CC	102	-	-	-	0/6/5/5
19	CLA	B1	831	-	-	8/15/91/115	-
20	CL0	AA	803	-	1/1/20/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	K2	104	-	-	6/9/81/115	-
19	CLA	B2	810	-	-	17/39/115/115	-
23	BCR	L	205	-	-	17/29/63/63	0/2/2/2
19	CLA	BB	808	-	-	15/33/109/115	-
19	CLA	A	812	-	-	9/17/93/115	-
19	CLA	J	103	-	-	8/10/86/115	-
23	BCR	AA	850	-	-	16/29/63/63	0/2/2/2
21	PQN	BB	837	-	-	7/23/43/43	0/2/2/2
19	CLA	L2	206	-	-	14/39/115/115	-
19	CLA	B1	802	-	-	15/39/115/115	-
19	CLA	B	806	-	-	15/39/115/115	-
24	AJP	L	208	-	13/13/14/38	-	0/6/6/11
19	CLA	A2	837	-	-	7/15/91/115	-
19	CLA	B1	832	-	-	14/39/115/115	-
19	CLA	B	803	-	-	13/39/115/115	-
19	CLA	B	817	-	-	6/12/88/115	-
19	CLA	A1	820	-	-	18/39/115/115	-
19	CLA	BB	852	-	-	13/39/115/115	-
19	CLA	A1	828	-	-	20/39/115/115	-
23	BCR	B	839	-	-	16/29/63/63	0/2/2/2
19	CLA	B1	848	-	-	16/39/115/115	-
23	BCR	A	848	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	822	-	-	15/33/109/115	-
19	CLA	B2	837	-	-	11/33/109/115	-
23	BCR	B1	839	-	-	9/29/63/63	0/2/2/2
25	LMG	B	845	-	-	21/50/70/70	0/1/1/1
27	SF4	C2	101	-	-	-	0/6/5/5
25	LMG	B2	845	-	-	21/50/70/70	0/1/1/1
19	CLA	A	839	-	-	8/24/100/115	-
19	CLA	B	854	-	-	13/39/115/115	-
19	CLA	A	826	-	-	9/15/91/115	-
19	CLA	AA	832	-	-	6/39/115/115	-
19	CLA	B1	824	-	-	15/27/103/115	-
19	CLA	AA	817	-	-	4/13/90/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	L2	202	-	17/17/19/38	3/6/121/220	0/7/7/11
19	CLA	A	833	-	-	5/21/97/115	-
22	LHG	A	846	-	-	12/42/42/53	-
19	CLA	A1	808	-	-	3/21/97/115	-
26	ECH	B1	840	-	-	16/29/66/66	0/2/2/2
19	CLA	B	818	-	-	4/10/86/115	-
24	AJP	A1	854	-	16/16/19/38	2/6/121/220	0/7/7/11
19	CLA	A2	826	-	-	9/15/91/115	-
19	CLA	J1	101	-	-	5/10/86/115	-
23	BCR	B	840	-	-	9/29/63/63	0/2/2/2
23	BCR	L1	209	-	-	18/29/63/63	0/2/2/2
28	DGD	B	856	-	-	22/31/71/95	0/2/2/2
27	SF4	CC	101	-	-	-	0/6/5/5
19	CLA	A2	823	-	-	14/33/109/115	-
19	CLA	B1	815	-	-	16/39/115/115	-
20	CL0	A1	802	-	1/1/20/20	13/39/115/115	-
19	CLA	B2	831	-	-	9/29/105/115	-
19	CLA	B	829	-	-	14/39/115/115	-
23	BCR	BB	841	-	-	20/29/63/63	0/2/2/2
24	AJP	M2	101	-	12/12/14/38	-	0/6/6/11
19	CLA	AA	807	-	-	18/39/115/115	-
25	LMG	B1	846	-	-	10/27/47/70	0/1/1/1
19	CLA	AA	810	-	-	10/39/115/115	-
19	CLA	L	204	-	-	17/39/115/115	-
19	CLA	A2	801	-	-	13/39/115/115	-
22	LHG	B2	848	-	-	8/37/37/53	-
19	CLA	BB	811	-	-	18/35/111/115	-
24	AJP	A	855	-	12/12/16/38	2/4/99/220	1/6/6/11
19	CLA	BB	833	-	-	18/39/115/115	-
19	CLA	B	833	-	-	14/39/115/115	-
23	BCR	M	101	-	-	22/29/63/63	0/2/2/2
19	CLA	B1	828	-	-	11/39/115/115	-
20	CL0	A2	803	-	1/1/20/20	16/39/115/115	-
19	CLA	A	814	-	-	5/12/88/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	L1	203	-	16/16/19/38	4/6/121/220	0/7/7/11
19	CLA	B2	822	-	-	7/39/115/115	-
19	CLA	AA	825	-	-	4/24/100/115	-
23	BCR	A	847	-	-	14/27/61/63	0/2/2/2
23	BCR	J2	102	-	-	18/29/63/63	0/2/2/2
19	CLA	A2	806	-	-	11/29/105/115	-
24	AJP	L1	204	-	16/16/19/38	3/6/121/220	0/7/7/11
19	CLA	J1	103	-	-	2/10/86/115	-
19	CLA	A	819	-	-	13/33/109/115	-
23	BCR	FF	304	-	-	14/29/63/63	0/2/2/2
19	CLA	B1	818	-	-	2/10/86/115	-
19	CLA	BB	819	-	-	2/10/86/115	-
23	BCR	BB	843	-	-	13/29/63/63	0/2/2/2
19	CLA	A1	806	-	-	18/39/115/115	-
19	CLA	A1	836	-	-	7/15/91/115	-
19	CLA	B	816	-	-	11/30/106/115	-
19	CLA	A	810	1	-	11/39/115/115	-
19	CLA	A	821	-	-	13/39/115/115	-
19	CLA	AA	813	-	-	10/39/115/115	-
23	BCR	F1	303	-	-	17/29/63/63	0/2/2/2
19	CLA	A1	815	-	-	9/21/97/115	-
24	AJP	KK	104	-	16/16/19/38	2/4/116/220	0/7/7/11
19	CLA	AA	824	-	-	9/15/91/115	-
19	CLA	A1	809	-	-	11/39/115/115	-
19	CLA	AA	827	-	-	18/39/115/115	-
19	CLA	F	301	-	-	12/33/109/115	-
19	CLA	BB	832	-	-	13/39/115/115	-
19	CLA	L	203	-	-	8/39/115/115	-
23	BCR	AA	852	-	-	19/29/63/63	0/2/2/2
24	AJP	A	802	-	11/11/14/38	-	0/6/6/11
22	LHG	BB	851	-	-	20/53/53/53	-
22	LHG	A2	846	-	-	12/42/42/53	-
19	CLA	A	827	-	-	17/39/115/115	-
19	CLA	B2	808	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A1	851	-	-	19/29/63/63	0/2/2/2
19	CLA	B2	828	-	-	1/15/91/115	-
19	CLA	B	822	-	-	4/39/115/115	-
19	CLA	A	807	-	-	19/39/115/115	-
19	CLA	A1	832	-	-	9/21/97/115	-
23	BCR	F1	304	-	-	15/29/63/63	0/2/2/2
19	CLA	BB	824	-	-	12/27/103/115	-
19	CLA	AA	820	-	-	13/31/107/115	-
19	CLA	A	837	-	-	5/15/91/115	-
22	LHG	A1	845	-	-	20/53/53/53	-
23	BCR	AA	854	-	-	18/29/63/63	0/2/2/2
19	CLA	A1	821	-	-	6/23/99/115	-
19	CLA	L2	204	16	-	16/35/111/115	-
19	CLA	A2	838	-	-	4/13/90/115	-
19	CLA	AA	842	-	-	10/39/115/115	-
25	LMG	M	102	-	-	15/41/61/70	0/1/1/1
19	CLA	K	102	-	-	11/17/93/115	-
19	CLA	A1	804	-	-	11/33/109/115	-
19	CLA	A1	819	-	-	11/31/107/115	-
22	LHG	AA	846	-	-	19/53/53/53	-
23	BCR	I1	101	-	-	17/29/63/63	0/2/2/2
22	LHG	LL	205	-	-	13/38/38/53	-
19	CLA	B2	809	-	-	7/15/91/115	-
19	CLA	BB	814	-	-	13/32/108/115	-
23	BCR	J	102	-	-	19/29/63/63	0/2/2/2
19	CLA	A1	839	-	-	7/29/105/115	-
19	CLA	B1	829	-	-	5/29/105/115	-
19	CLA	AA	808	-	-	14/39/115/115	-
19	CLA	BB	830	-	-	8/29/105/115	-
25	LMG	B1	844	-	-	20/50/70/70	0/1/1/1
19	CLA	A2	825	-	-	5/12/88/115	-
19	CLA	F	302	-	-	4/12/88/115	-
22	LHG	AA	847	-	-	12/42/42/53	-
19	CLA	A1	814	-	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	K1	106	-	-	18/29/63/63	0/2/2/2
25	LMG	B	851	-	-	17/50/70/70	0/1/1/1
19	CLA	A1	805	-	-	8/29/105/115	-
19	CLA	A1	837	1	-	4/13/90/115	-
23	BCR	A2	848	-	-	15/29/63/63	0/2/2/2
19	CLA	A	822	-	-	9/23/99/115	-
19	CLA	A1	830	-	-	14/39/115/115	-
19	CLA	BB	805	-	-	10/38/114/115	-
19	CLA	B1	805	-	-	10/38/114/115	-
23	BCR	B	844	-	-	15/29/63/63	0/2/2/2
19	CLA	AA	829	-	-	14/39/115/115	-
23	BCR	B1	838	-	-	19/29/63/63	0/2/2/2
23	BCR	L1	208	-	-	17/29/63/63	0/2/2/2
19	CLA	AA	839	-	-	8/24/100/115	-
23	BCR	L1	201	-	-	12/29/63/63	0/2/2/2
23	BCR	A2	849	-	-	13/29/63/63	0/2/2/2
22	LHG	X	102	-	-	19/44/44/53	-
19	CLA	AA	845	-	-	3/10/86/115	-
19	CLA	BB	809	-	-	8/15/91/115	-
19	CLA	BB	836	-	-	11/33/109/115	-
19	CLA	B2	816	-	-	10/30/106/115	-
19	CLA	BB	812	-	-	6/10/86/115	-
23	BCR	B2	840	-	-	8/29/63/63	0/2/2/2
22	LHG	L1	211	-	-	14/37/37/53	-
23	BCR	F	303	-	-	18/29/63/63	0/2/2/2
19	CLA	A	831	-	-	13/39/115/115	-
23	BCR	B	848	-	-	16/29/63/63	0/2/2/2
19	CLA	B2	806	2	-	15/39/115/115	-
19	CLA	B	858	-	-	5/39/115/115	-
19	CLA	A	808	-	-	13/39/115/115	-
19	CLA	A	824	-	-	9/15/91/115	-
23	BCR	A2	850	-	-	13/29/63/63	0/2/2/2
23	BCR	J1	102	-	-	19/29/63/63	0/2/2/2
19	CLA	AA	815	-	-	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	804	-	-	11/36/112/115	-
19	CLA	B1	826	-	-	15/39/115/115	-
19	CLA	JJ	101	8	-	5/10/86/115	-
19	CLA	A	836	-	-	15/39/115/115	-
22	LHG	B	853	-	-	23/53/53/53	-
23	BCR	AA	848	-	-	13/27/61/63	0/2/2/2
19	CLA	AA	809	-	-	4/21/97/115	-
19	CLA	A1	834	-	-	9/39/115/115	-
19	CLA	A	834	-	-	4/10/86/115	-
19	CLA	J2	103	-	-	2/10/86/115	-
19	CLA	B	859	-	-	15/33/109/115	-
23	BCR	K2	103	-	-	12/29/63/63	0/2/2/2
23	BCR	AA	851	-	-	15/29/63/63	0/2/2/2
19	CLA	B1	801	-	-	20/39/115/115	-
19	CLA	A	830	-	-	15/36/112/115	-
19	CLA	B2	825	-	-	20/39/115/115	-
19	CLA	B2	850	-	-	4/39/115/115	-
19	CLA	A2	829	-	-	17/39/115/115	-
19	CLA	A2	841	-	-	6/17/93/115	-
19	CLA	A	820	-	-	13/31/107/115	-
19	CLA	F1	301	-	-	10/33/109/115	-
19	CLA	X1	101	-	-	6/15/91/115	-
19	CLA	B2	819	-	-	3/10/86/115	-
23	BCR	A2	853	-	-	17/29/63/63	0/2/2/2
19	CLA	B2	805	-	-	11/38/114/115	-
19	CLA	BB	834	-	-	1/15/91/115	-
20	CL0	A	803	-	1/1/20/20	18/39/115/115	-
19	CLA	B	813	-	-	8/12/88/115	-
19	CLA	A2	817	-	-	3/13/90/115	-
19	CLA	AA	821	-	-	15/39/115/115	-
19	CLA	B1	806	-	-	15/39/115/115	-
19	CLA	B	824	-	-	12/27/103/115	-
19	CLA	B	804	-	-	8/36/112/115	-
23	BCR	F	304	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	SF4	C	102	3	-	-	0/6/5/5
19	CLA	A	809	-	-	4/21/97/115	-
19	CLA	BB	831	-	-	6/15/91/115	-

The worst 5 of 4204 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	AJP	C14-C15	-11.11	1.35	1.53
24	AA	802	AJP	C14-C15	-11.05	1.35	1.53
24	L	208	AJP	C14-C15	-10.91	1.35	1.53
24	BB	849	AJP	C14-C15	-10.86	1.35	1.53
24	AA	856	AJP	C16-C11	-10.78	1.39	1.54

The worst 5 of 4335 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A1	854	AJP	C80-C20-C21	-13.26	88.84	108.97
24	B	857	AJP	C80-C20-C21	-13.18	88.97	108.97
24	L1	203	AJP	C80-C20-C21	-13.09	89.10	108.97
24	L2	202	AJP	C80-C20-C21	-12.73	89.64	108.97
24	L	208	AJP	C80-C20-C21	-12.67	89.73	108.97

5 of 322 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A1	802	CL0	C8
20	A2	803	CL0	C8
20	A	803	CL0	C8
20	AA	803	CL0	C8
24	A1	854	AJP	C27

5 of 6157 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	CBD-CGD-O2D-CED
19	A1	804	CLA	C1A-C2A-CAA-CBA
19	A1	804	CLA	C3A-C2A-CAA-CBA
19	A1	804	CLA	CHA-CBD-CGD-O1D
19	A1	804	CLA	CHA-CBD-CGD-O2D

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	855	AJP	C19-C20-C21-C22-C23-C24

314 monomers are involved in 452 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	FF	305	CLA	2	0
23	JJ	104	BCR	1	0
21	A2	843	PQN	1	0
19	AA	834	CLA	1	0
26	B	841	ECH	2	0
19	B1	821	CLA	1	0
27	C1	102	SF4	1	0
19	B	835	CLA	8	0
23	BB	842	BCR	2	0
19	BB	828	CLA	3	0
19	A2	815	CLA	3	0
25	I2	105	LMG	1	0
23	A	851	BCR	4	0
19	A	816	CLA	1	0
21	A	843	PQN	1	0
19	AA	836	CLA	1	0
19	A1	852	CLA	6	0
19	B	810	CLA	3	0
19	B	827	CLA	1	0
19	B	812	CLA	2	0
22	B	852	LHG	1	0
23	A2	851	BCR	5	0
19	A	806	CLA	1	0
19	A1	844	CLA	1	0
19	B2	836	CLA	1	0
22	A2	845	LHG	1	0
23	F2	305	BCR	4	0
19	B	860	CLA	2	0
19	A	804	CLA	1	0
19	A	815	CLA	3	0
19	F2	302	CLA	1	0
23	MM	101	BCR	1	0
19	A	832	CLA	2	0
19	B1	825	CLA	1	0
22	A1	846	LHG	1	0
19	A2	816	CLA	1	0
19	A2	821	CLA	1	0
19	B2	820	CLA	1	0
19	A2	804	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	K1	104	BCR	1	0
22	A	845	LHG	2	0
23	J1	104	BCR	1	0
19	F1	305	CLA	2	0
19	A1	811	CLA	1	0
19	B1	810	CLA	3	0
23	B2	839	BCR	1	0
23	B	843	BCR	4	0
19	L1	207	CLA	1	0
19	B1	827	CLA	2	0
19	AA	853	CLA	3	0
19	B1	833	CLA	13	0
19	B	834	CLA	12	0
24	B	849	AJP	1	0
19	BB	817	CLA	1	0
19	A2	805	CLA	3	0
19	B1	834	CLA	9	0
19	AA	831	CLA	1	0
19	BB	806	CLA	2	0
19	A2	835	CLA	1	0
19	BB	822	CLA	2	0
19	B	820	CLA	3	0
19	A1	817	CLA	2	0
23	BB	839	BCR	1	0
19	A	805	CLA	3	0
23	BB	838	BCR	2	0
19	L1	206	CLA	1	0
19	A2	833	CLA	1	0
19	B1	822	CLA	1	0
23	FF	306	BCR	3	0
25	L1	210	LMG	1	0
19	BB	826	CLA	2	0
19	B1	850	CLA	2	0
19	A2	810	CLA	1	0
24	L2	203	AJP	1	0
19	B2	802	CLA	2	0
19	AA	830	CLA	3	0
19	A	842	CLA	2	0
19	A2	834	CLA	1	0
19	B2	826	CLA	2	0
19	B2	829	CLA	2	0
26	BB	840	ECH	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	AA	828	CLA	3	0
23	B	842	BCR	5	0
19	BB	804	CLA	2	0
23	LL	204	BCR	1	0
23	F1	306	BCR	4	0
19	B	836	CLA	2	0
19	A2	820	CLA	1	0
19	B2	821	CLA	1	0
19	B	811	CLA	1	0
21	AA	844	PQN	1	0
23	A2	847	BCR	1	0
19	A1	829	CLA	2	0
19	B	802	CLA	1	0
19	A1	842	CLA	1	0
19	A1	840	CLA	1	0
19	A	818	CLA	1	0
19	A1	824	CLA	1	0
23	J	104	BCR	1	0
19	B	821	CLA	1	0
19	BB	821	CLA	1	0
19	K1	105	CLA	1	0
19	B2	827	CLA	1	0
19	B1	804	CLA	1	0
19	A2	840	CLA	1	0
19	K1	103	CLA	1	0
19	B	831	CLA	1	0
19	A1	841	CLA	3	0
19	A	852	CLA	6	0
19	AA	804	CLA	2	0
23	FF	303	BCR	3	0
19	L1	205	CLA	3	0
23	F	305	BCR	4	0
26	B2	841	ECH	1	0
19	A1	835	CLA	1	0
19	A2	836	CLA	1	0
19	B	830	CLA	1	0
23	JJ	102	BCR	1	0
19	B1	835	CLA	1	0
19	B	832	CLA	1	0
19	AA	843	CLA	1	0
19	BB	856	CLA	2	0
19	LL	201	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	AA	805	CLA	2	0
19	B	828	CLA	3	0
19	F1	302	CLA	1	0
23	F2	303	BCR	2	0
19	BB	835	CLA	2	0
19	JJ	103	CLA	1	0
19	B	815	CLA	1	0
19	F2	301	CLA	2	0
19	B2	830	CLA	1	0
19	BB	823	CLA	2	0
19	B2	835	CLA	3	0
19	A1	801	CLA	1	0
19	A	840	CLA	1	0
19	A2	831	CLA	1	0
19	FF	302	CLA	1	0
19	A2	844	CLA	1	0
23	K2	105	BCR	2	0
19	AA	801	CLA	1	0
19	AA	816	CLA	1	0
21	A1	843	PQN	2	0
19	A2	802	CLA	1	0
19	A2	830	CLA	1	0
19	B1	809	CLA	1	0
19	A2	832	CLA	2	0
19	BB	820	CLA	4	0
21	B	838	PQN	2	0
19	B1	820	CLA	1	0
19	BB	829	CLA	2	0
22	L2	208	LHG	1	0
23	B1	841	BCR	2	0
19	AA	841	CLA	1	0
19	A2	812	CLA	1	0
19	A1	803	CLA	1	0
19	BB	802	CLA	1	0
23	A1	847	BCR	2	0
24	BB	848	AJP	1	0
19	AA	822	CLA	1	0
19	B2	811	CLA	1	0
23	A1	850	BCR	1	0
19	B2	823	CLA	1	0
23	A	854	BCR	2	0
19	A	801	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J2	104	BCR	2	0
19	BB	815	CLA	2	0
19	A2	828	CLA	1	0
19	X2	101	CLA	1	0
19	AA	806	CLA	1	0
19	FF	301	CLA	2	0
23	B1	842	BCR	3	0
19	A2	818	CLA	2	0
22	B1	847	LHG	1	0
19	B	826	CLA	2	0
19	B1	836	CLA	1	0
19	AA	826	CLA	1	0
19	B	823	CLA	1	0
19	B	837	CLA	1	0
19	BB	810	CLA	5	0
19	B2	833	CLA	3	0
23	I2	103	BCR	1	0
19	A1	807	CLA	1	0
23	B2	843	BCR	3	0
23	AA	855	BCR	1	0
19	A	841	CLA	2	0
19	A2	842	CLA	4	0
19	B1	807	CLA	1	0
19	A1	827	CLA	1	0
19	B2	834	CLA	4	0
19	AA	818	CLA	2	0
19	A2	852	CLA	5	0
19	B2	851	CLA	2	0
19	BB	801	CLA	1	0
19	A1	833	CLA	2	0
19	B1	823	CLA	1	0
19	B1	811	CLA	1	0
19	B2	849	CLA	2	0
19	B2	852	CLA	2	0
19	A	828	CLA	2	0
19	B	801	CLA	1	0
19	A1	831	CLA	1	0
19	L	202	CLA	3	0
23	B2	842	BCR	4	0
19	K2	104	CLA	1	0
20	AA	803	CL0	1	0
19	B2	810	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	L	205	BCR	1	0
19	A	812	CLA	1	0
19	J	103	CLA	2	0
21	BB	837	PQN	2	0
19	B1	802	CLA	1	0
19	B	806	CLA	3	0
19	A2	837	CLA	1	0
19	B1	832	CLA	4	0
19	BB	852	CLA	4	0
19	A1	828	CLA	3	0
23	B	839	BCR	2	0
19	B1	848	CLA	2	0
19	B2	837	CLA	1	0
23	B1	839	BCR	1	0
19	B	854	CLA	1	0
19	A	826	CLA	1	0
19	AA	832	CLA	1	0
19	A	833	CLA	1	0
26	B1	840	ECH	1	0
19	B	818	CLA	2	0
23	B	840	BCR	1	0
28	B	856	DGD	1	0
19	B1	815	CLA	2	0
20	A1	802	CL0	4	0
19	B	829	CLA	1	0
23	BB	841	BCR	6	0
19	AA	810	CLA	1	0
19	A2	801	CLA	1	0
19	BB	811	CLA	1	0
19	BB	833	CLA	12	0
19	B	833	CLA	6	0
23	M	101	BCR	2	0
19	B1	828	CLA	2	0
20	A2	803	CL0	4	0
19	B2	822	CLA	1	0
23	A	847	BCR	1	0
23	J2	102	BCR	1	0
19	A2	806	CLA	2	0
19	J1	103	CLA	1	0
24	L1	204	AJP	1	0
19	A1	836	CLA	1	0
19	A	821	CLA	1	0

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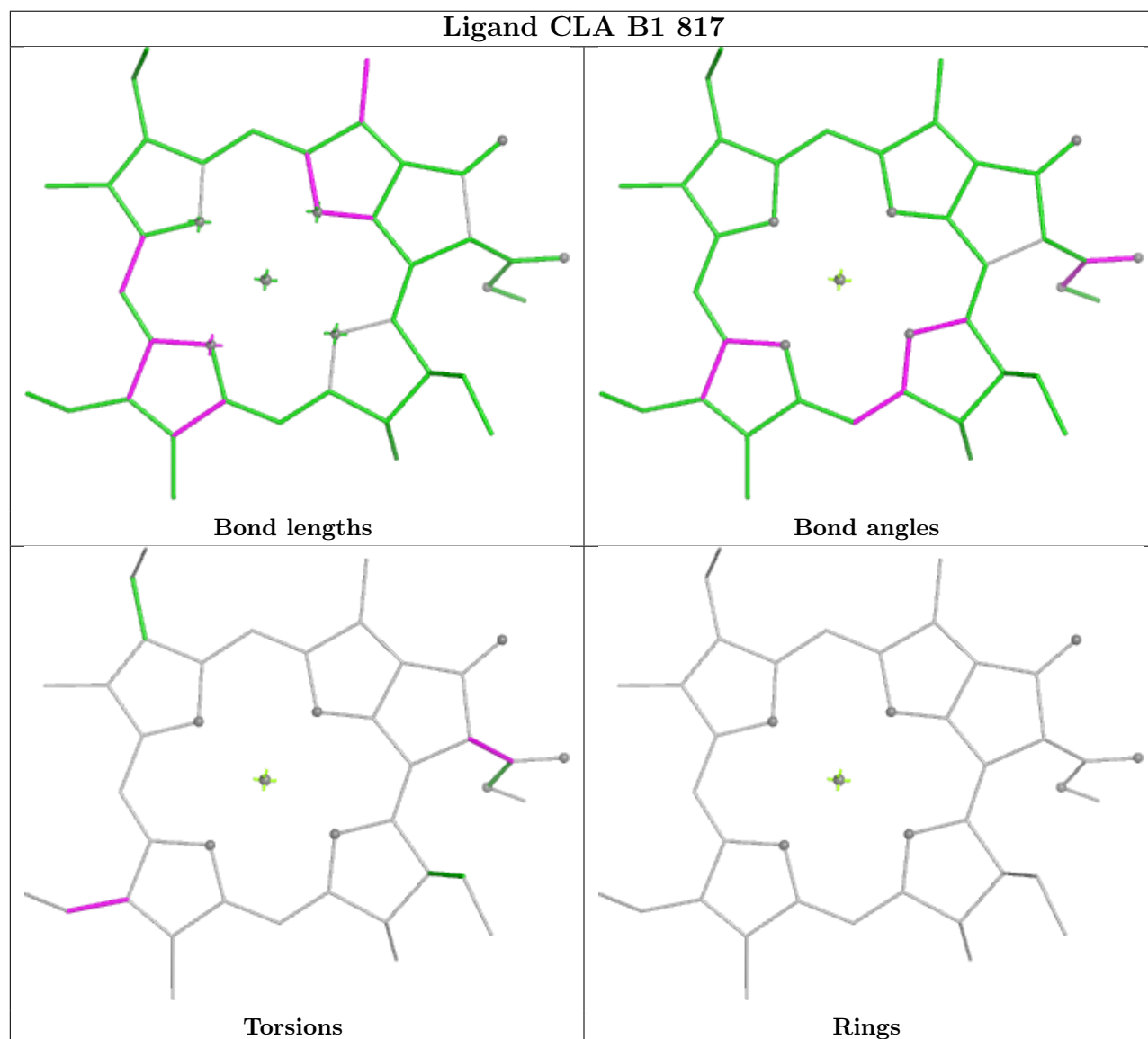
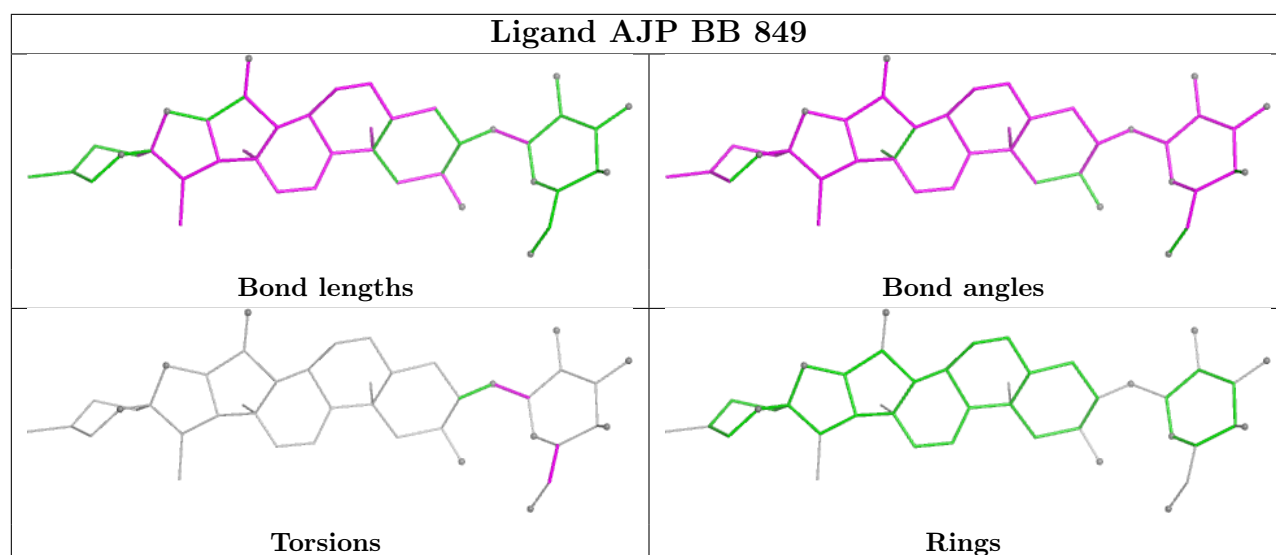
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	F1	303	BCR	2	0
19	A1	815	CLA	2	0
19	AA	827	CLA	1	0
19	F	301	CLA	2	0
19	BB	832	CLA	6	0
19	L	203	CLA	1	0
23	AA	852	BCR	4	0
22	A2	846	LHG	1	0
23	A1	851	BCR	3	0
19	B2	828	CLA	1	0
19	B	822	CLA	2	0
19	A1	832	CLA	1	0
19	AA	820	CLA	2	0
19	A	837	CLA	2	0
23	AA	854	BCR	1	0
19	AA	842	CLA	2	0
25	M	102	LMG	1	0
19	A1	804	CLA	2	0
19	A1	819	CLA	2	0
22	AA	846	LHG	2	0
23	I1	101	BCR	1	0
19	B2	809	CLA	1	0
23	J	102	BCR	1	0
19	A1	839	CLA	2	0
19	A2	825	CLA	1	0
19	F	302	CLA	1	0
22	AA	847	LHG	1	0
19	A1	814	CLA	3	0
23	K1	106	BCR	2	0
19	A1	805	CLA	1	0
19	A	822	CLA	3	0
19	A1	830	CLA	1	0
19	BB	805	CLA	1	0
23	B1	838	BCR	1	0
19	BB	812	CLA	2	0
23	B2	840	BCR	2	0
22	L1	211	LHG	2	0
23	F	303	BCR	2	0
19	A	831	CLA	1	0
19	B2	806	CLA	2	0
19	B	858	CLA	1	0
23	A2	850	BCR	1	0

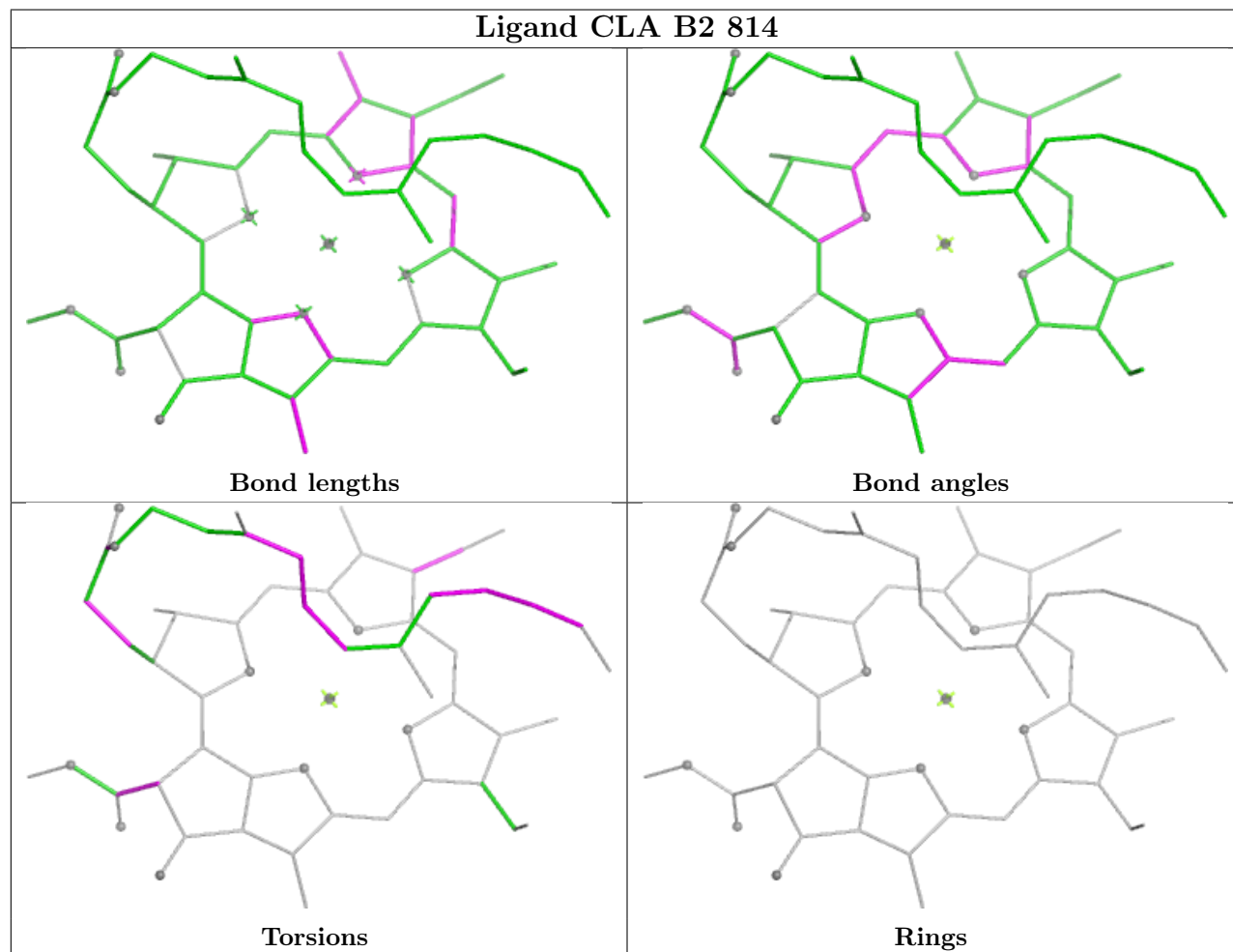
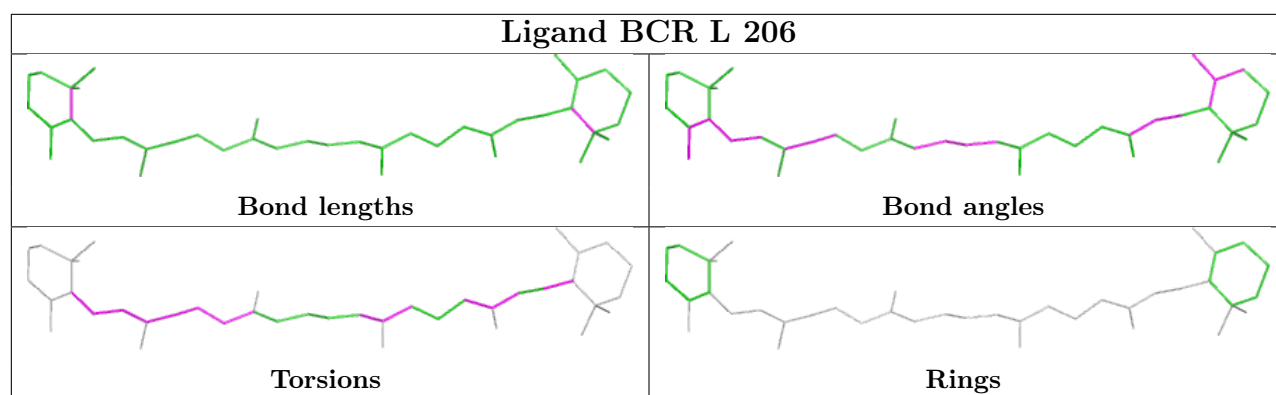
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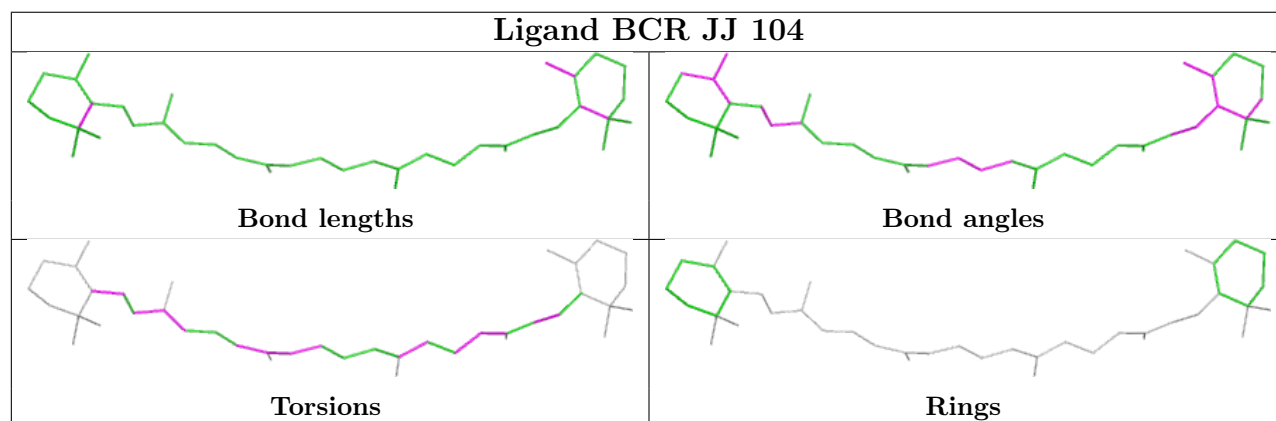
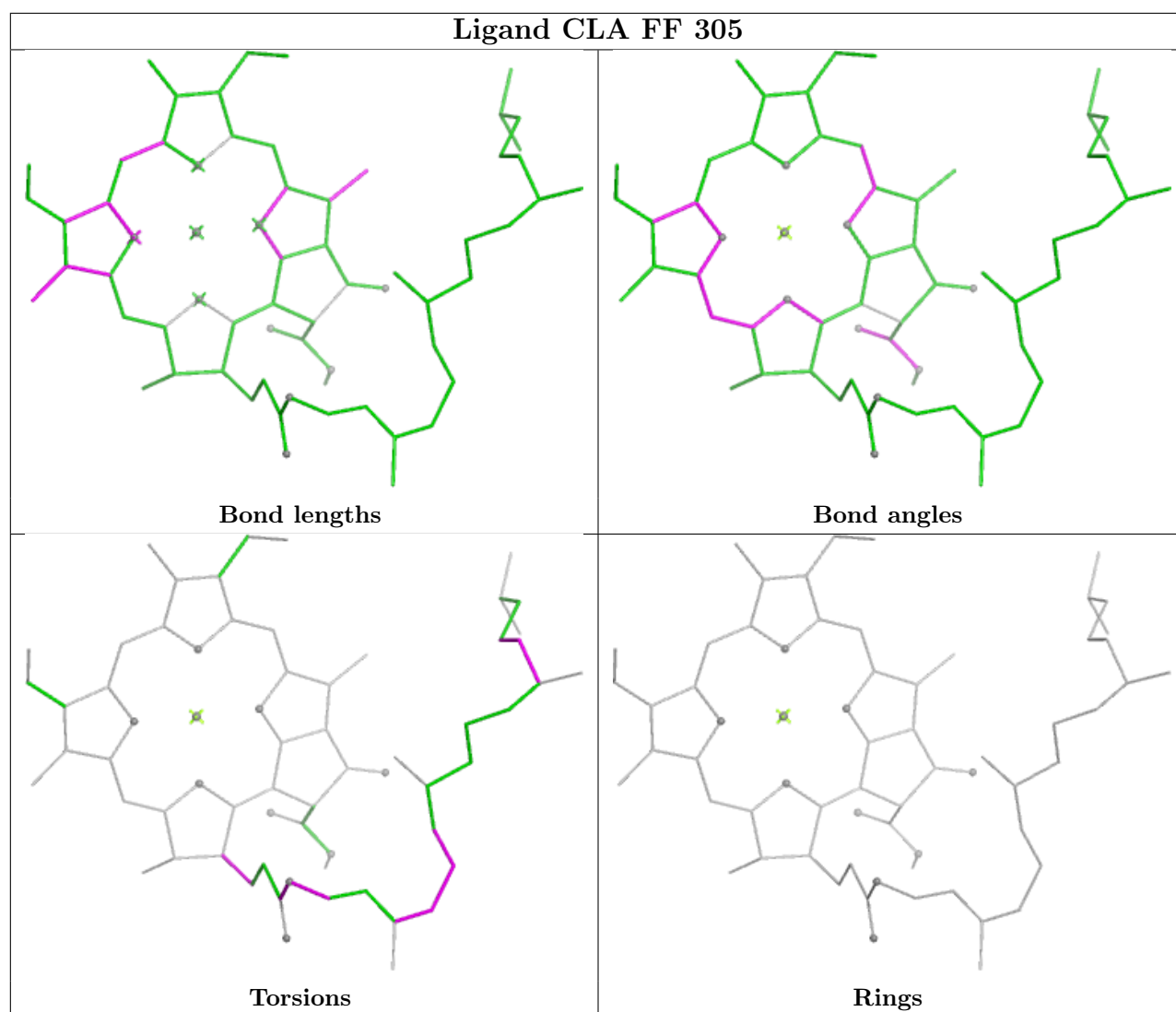
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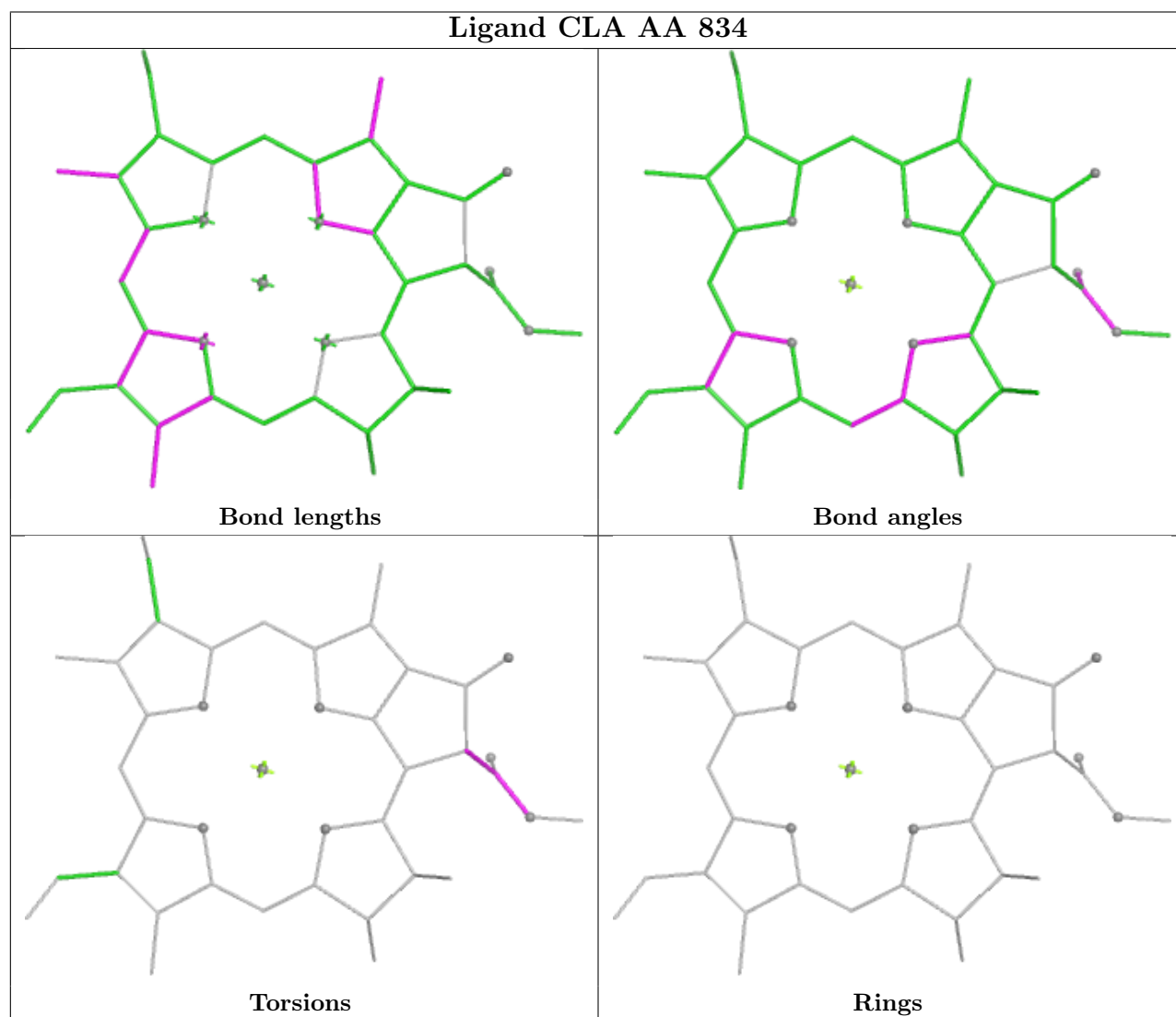
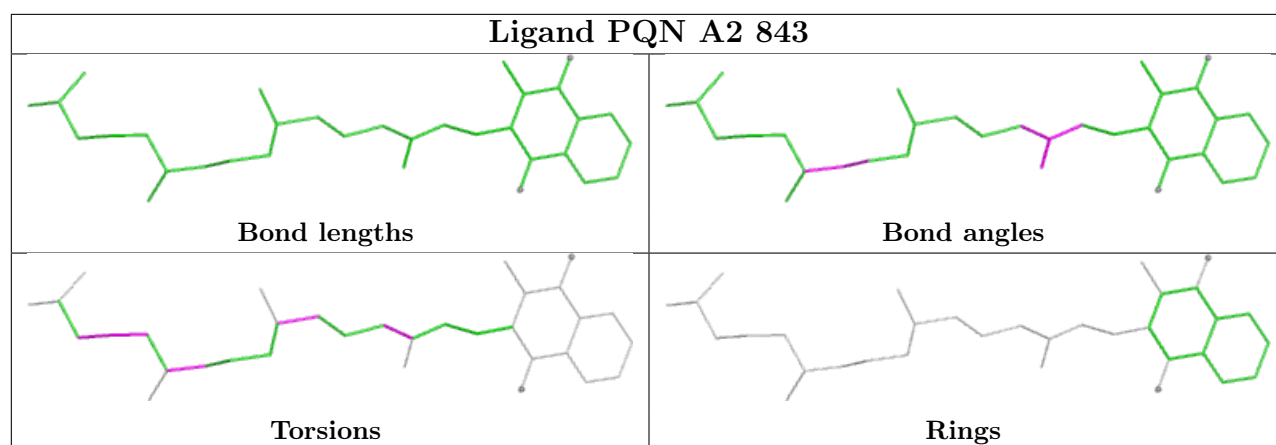
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	J1	102	BCR	1	0
19	AA	815	CLA	3	0
19	B1	826	CLA	1	0
19	A	836	CLA	1	0
23	AA	848	BCR	1	0
19	A1	834	CLA	2	0
19	A	834	CLA	2	0
19	J2	103	CLA	1	0
19	B	859	CLA	2	0
23	K2	103	BCR	1	0
23	AA	851	BCR	1	0
19	A	830	CLA	1	0
19	B2	850	CLA	1	0
19	A2	841	CLA	1	0
19	A	820	CLA	3	0
19	F1	301	CLA	3	0
19	BB	834	CLA	6	0
20	A	803	CL0	2	0
19	AA	821	CLA	2	0
19	B1	806	CLA	1	0
19	B	804	CLA	2	0
27	C	102	SF4	1	0
19	BB	831	CLA	1	0

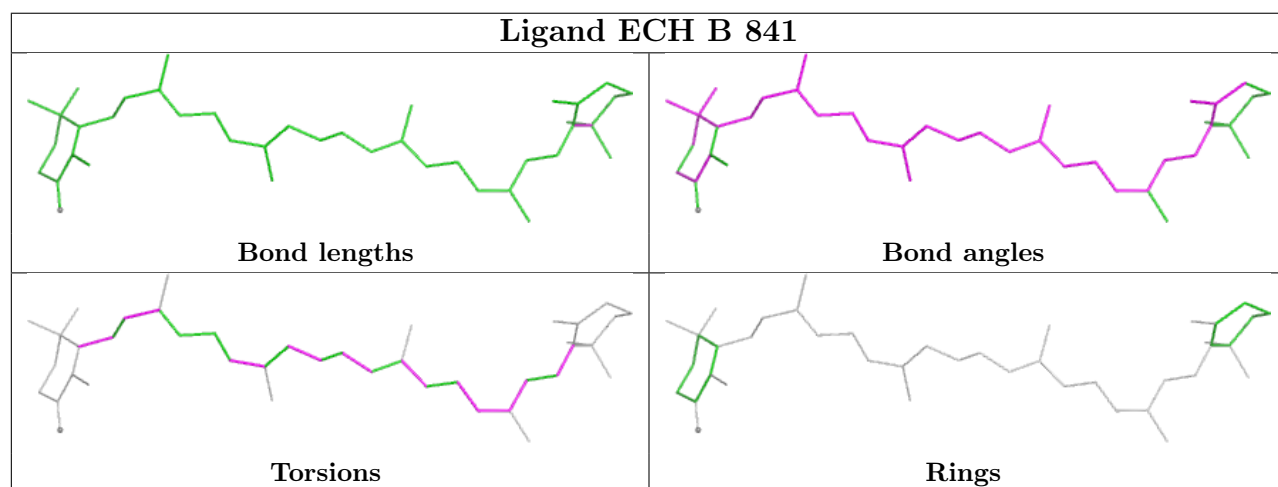
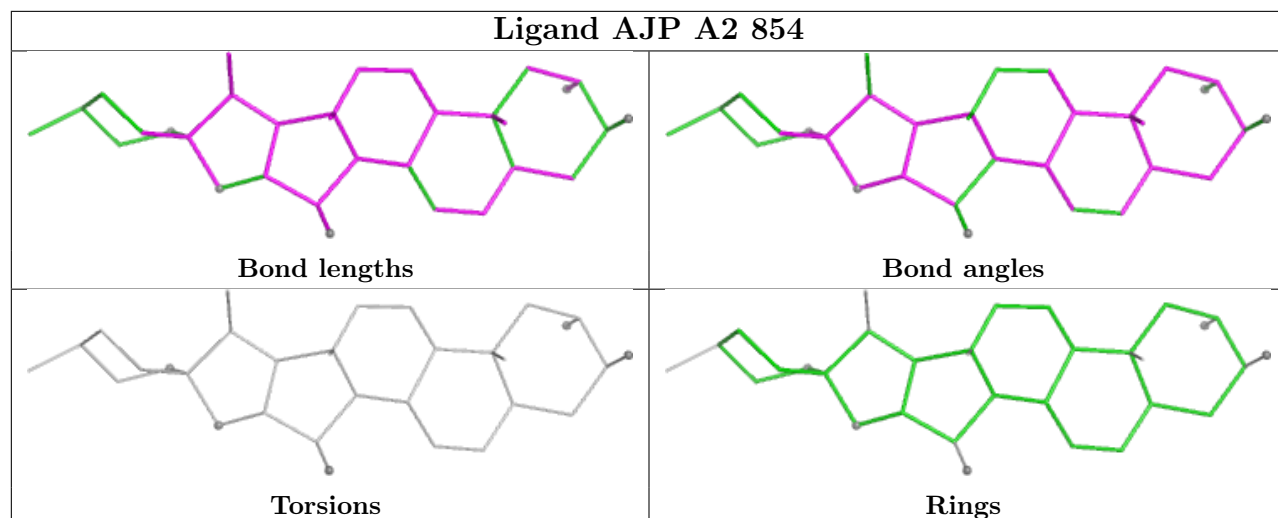
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

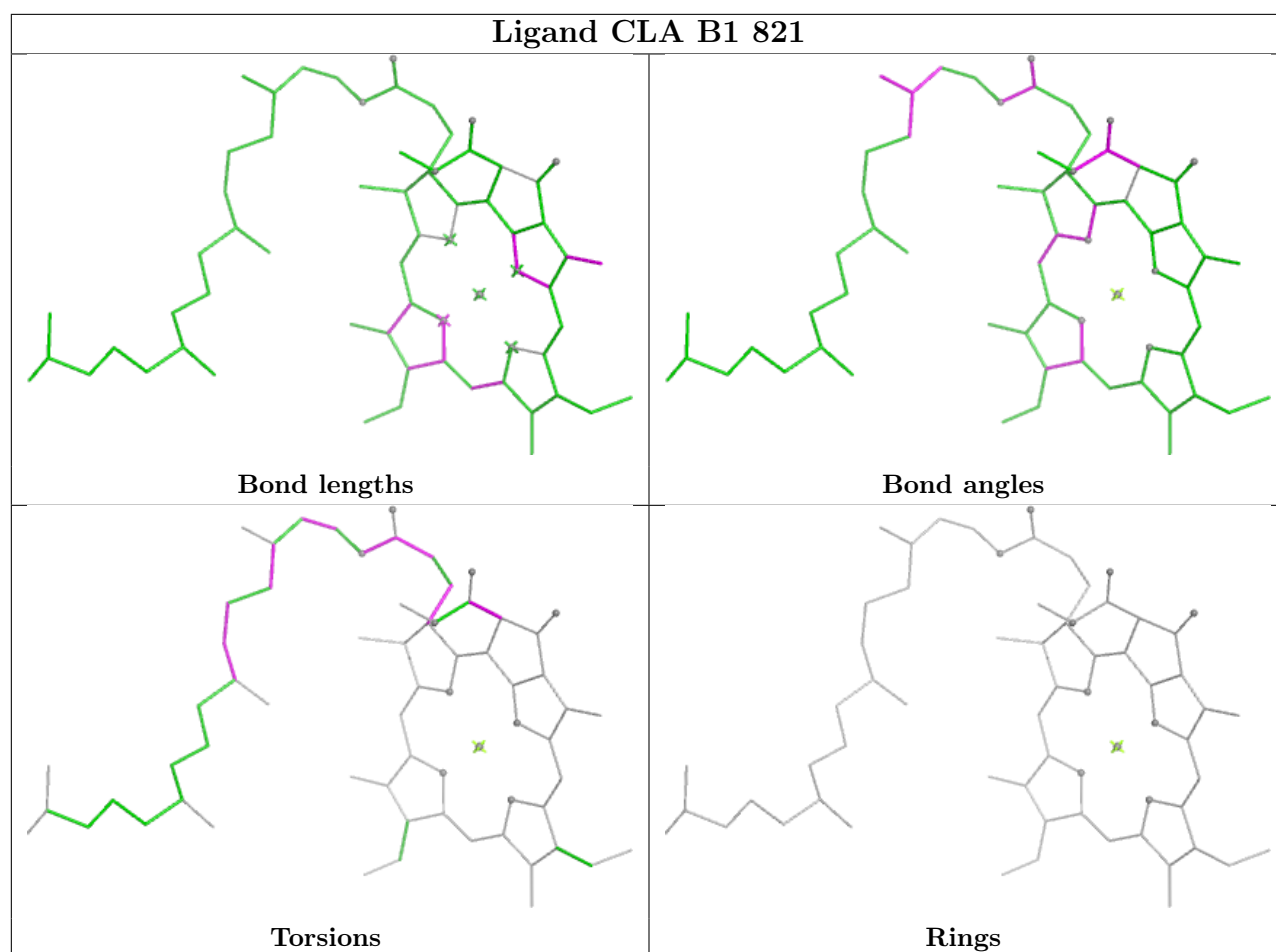




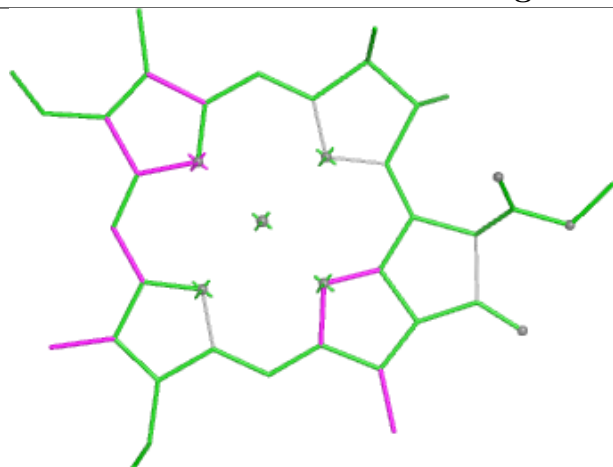




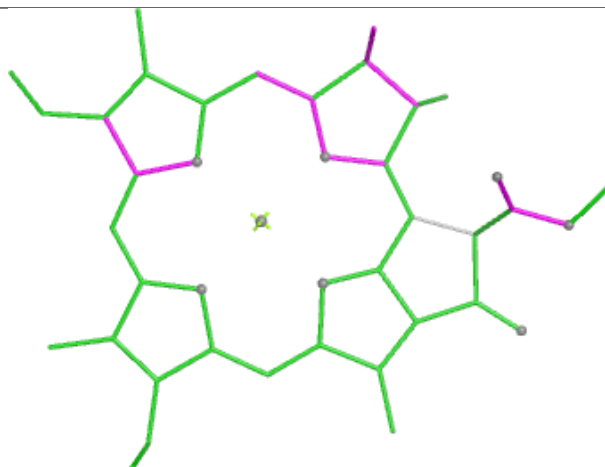




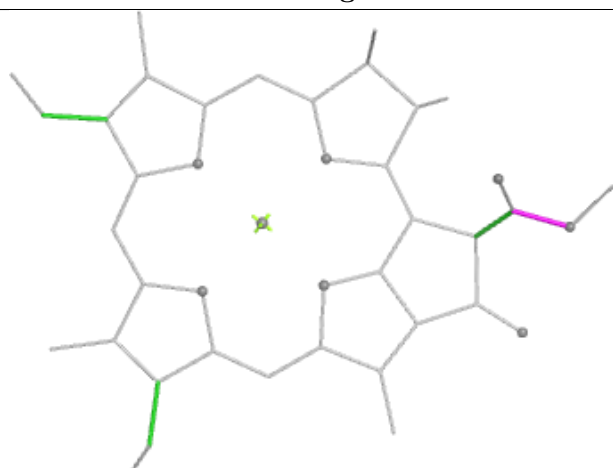
Ligand CLA B 819



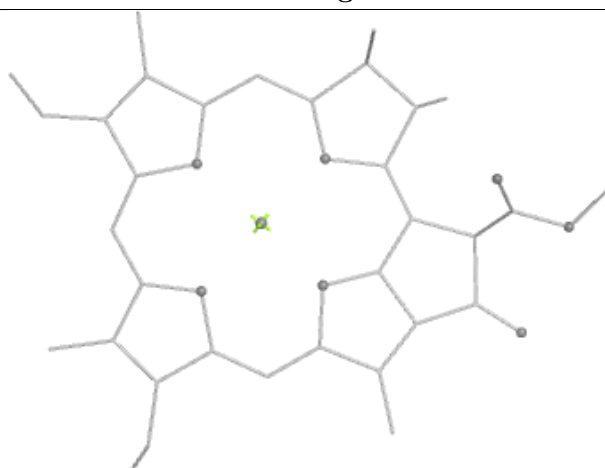
Bond lengths



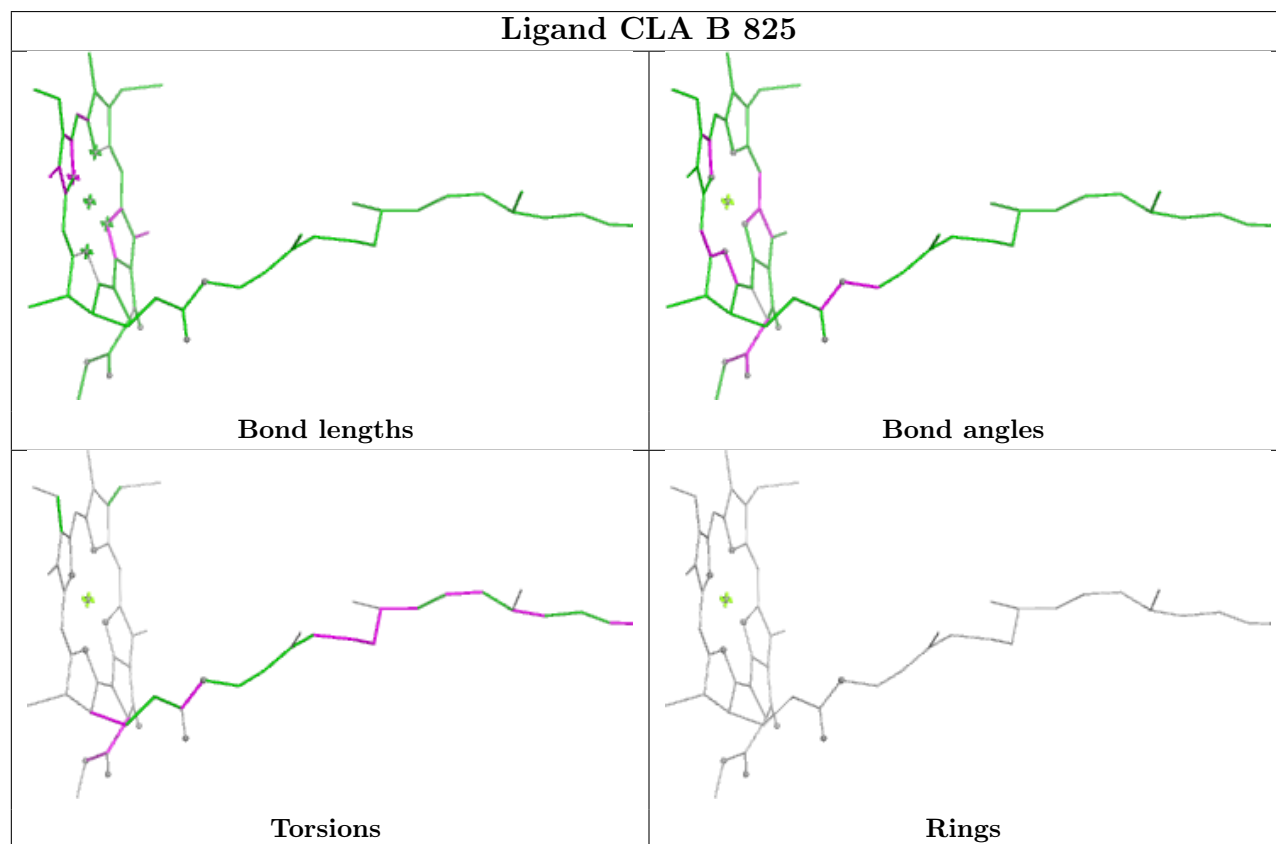
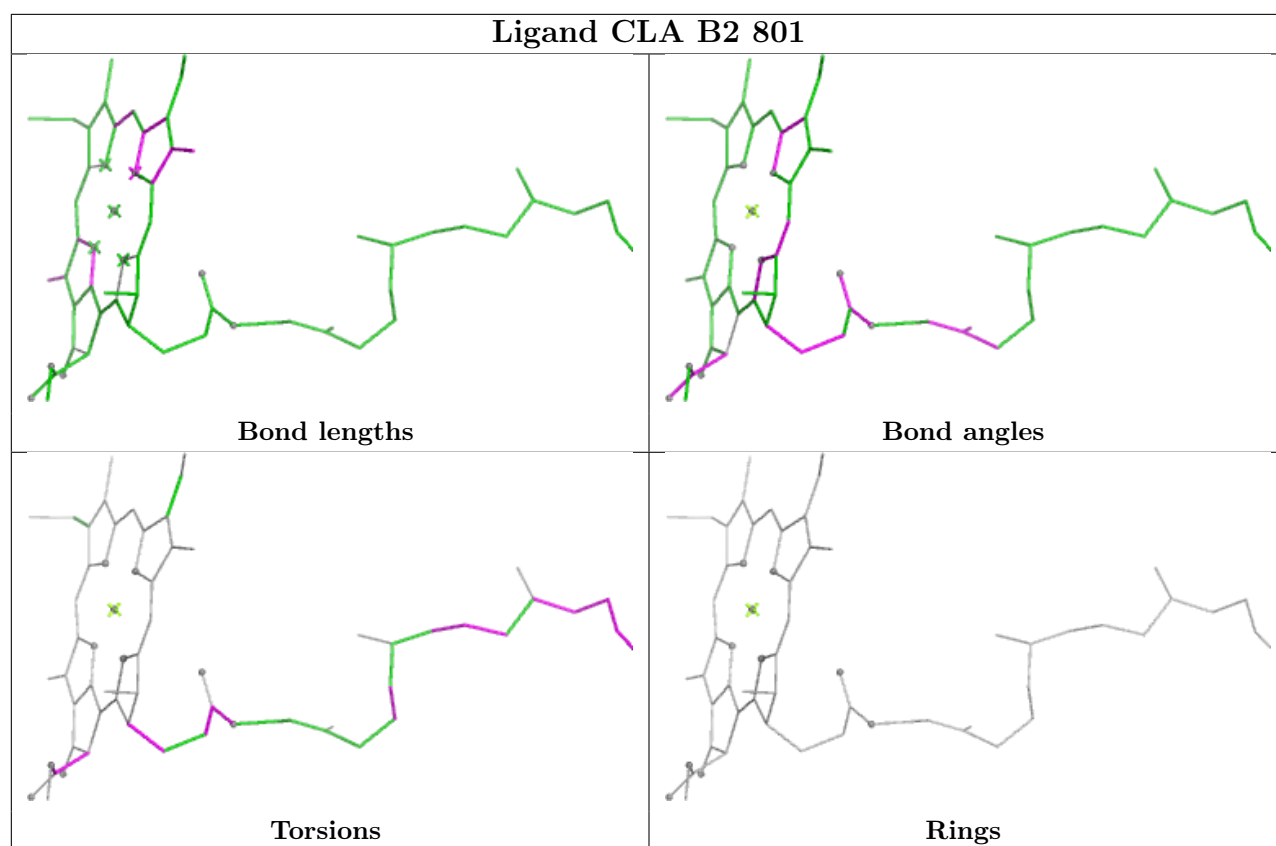
Bond angles



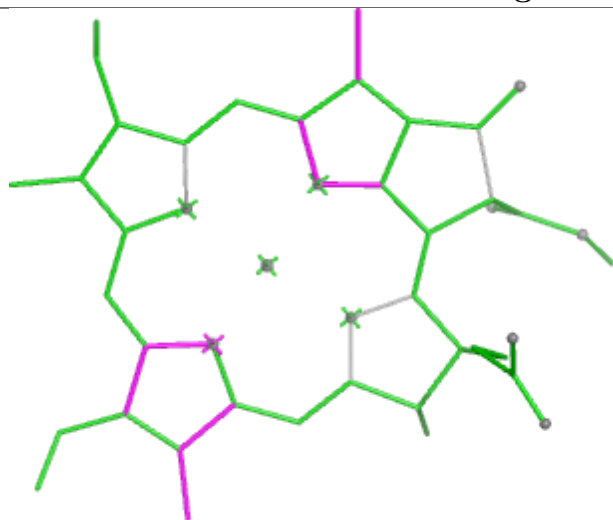
Torsions



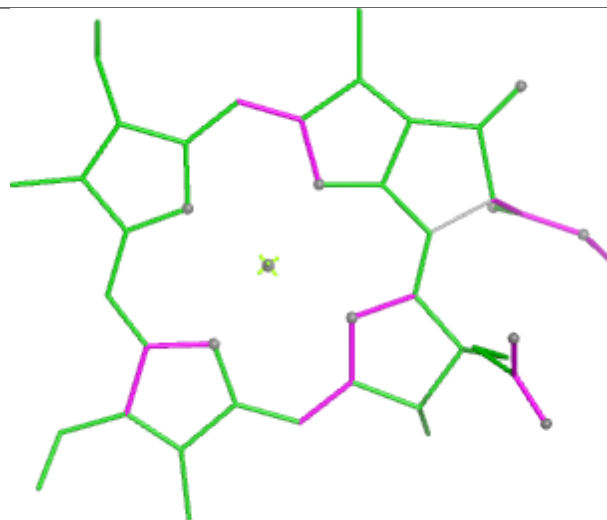
Rings



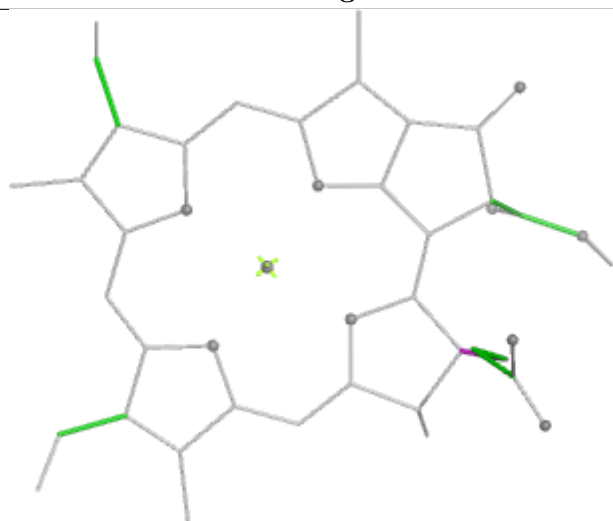
Ligand CLA B 835



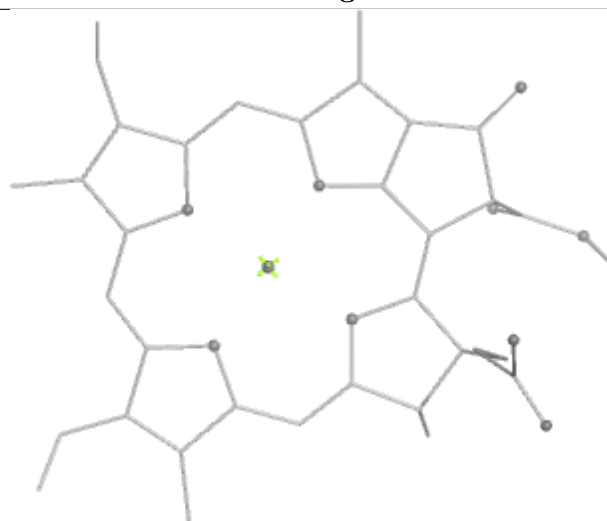
Bond lengths



Bond angles

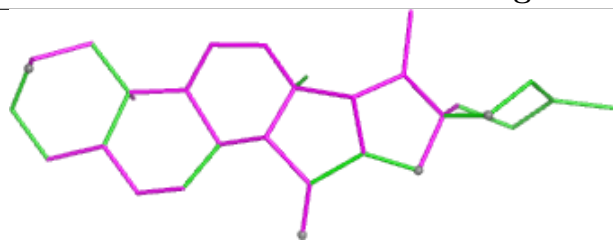


Torsions

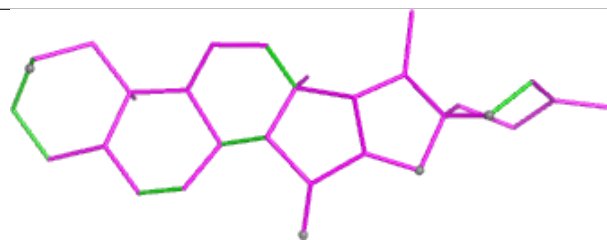


Rings

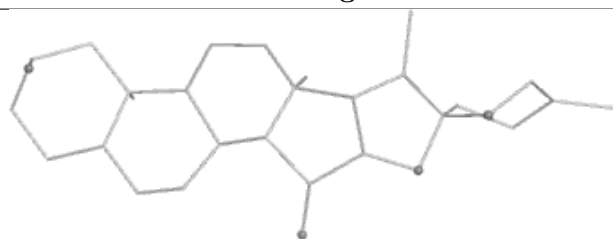
Ligand AJP I2 104



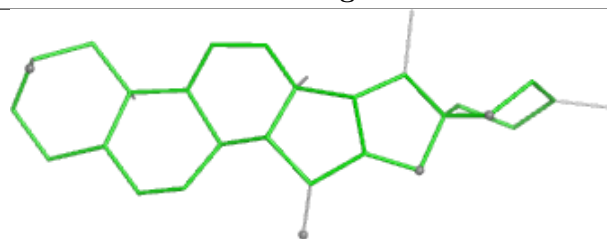
Bond lengths



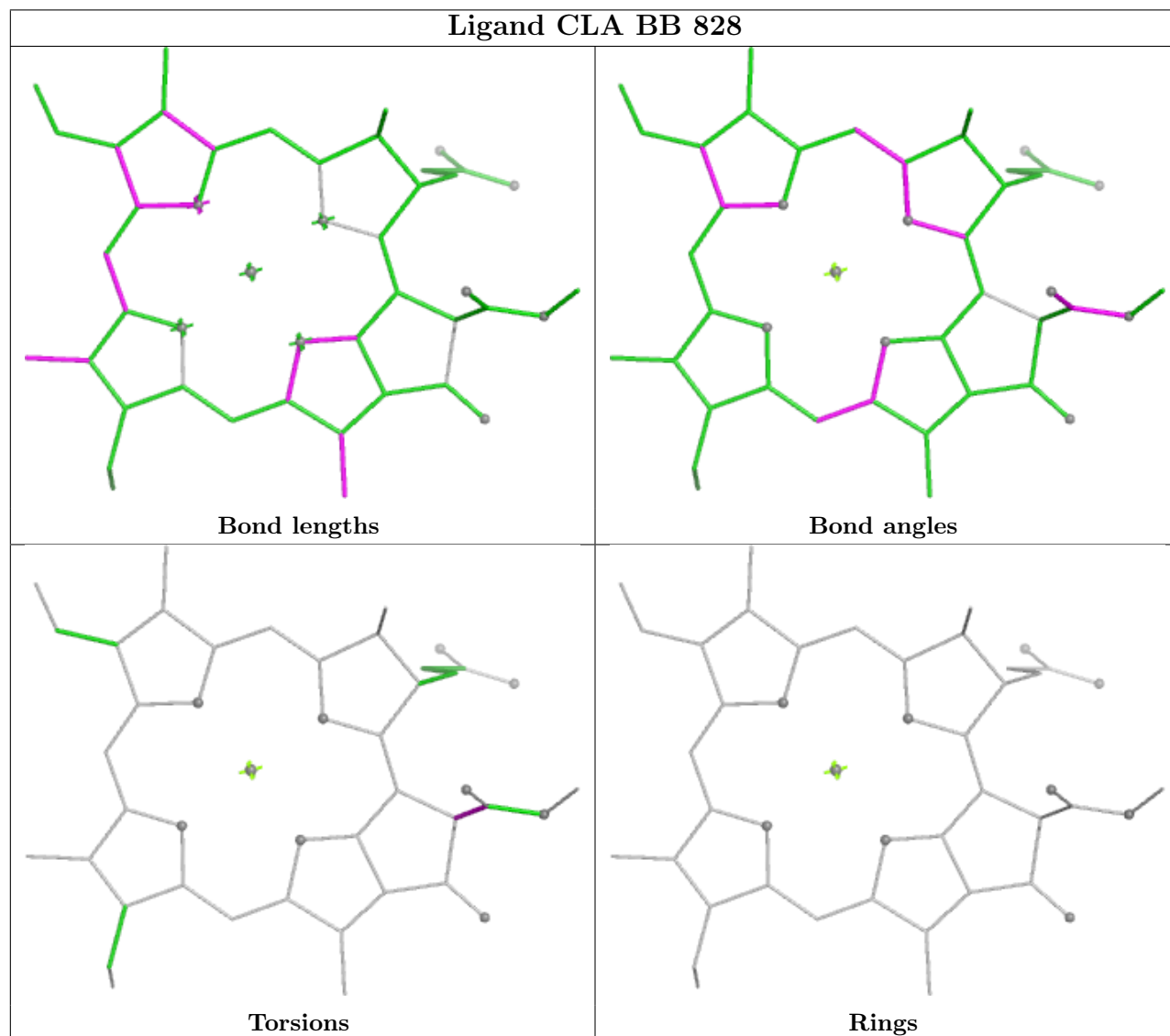
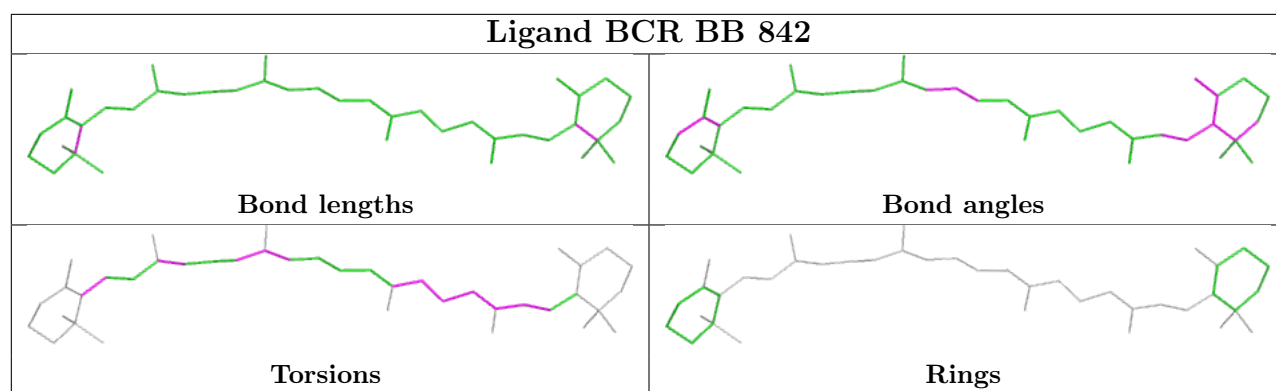
Bond angles

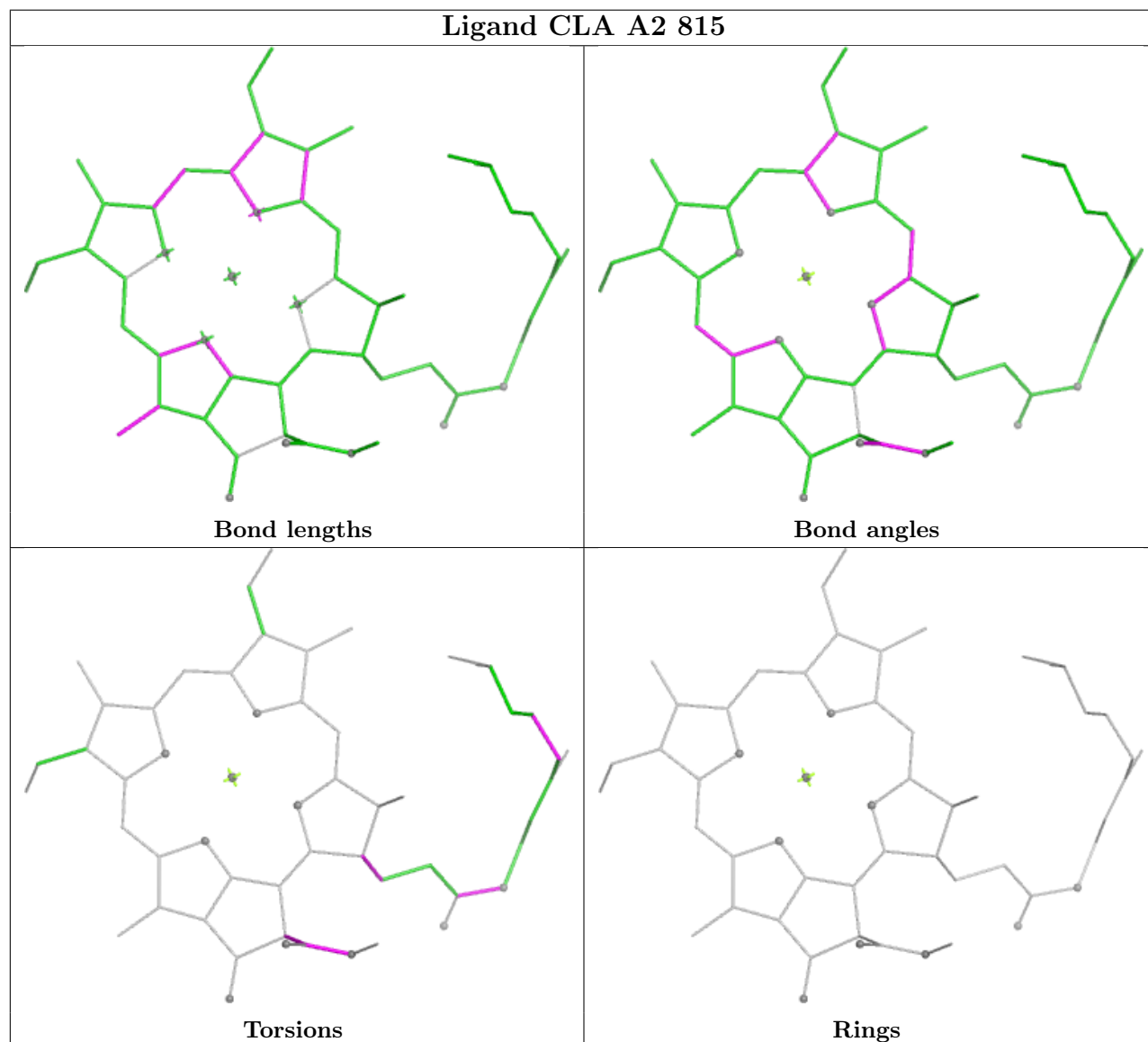
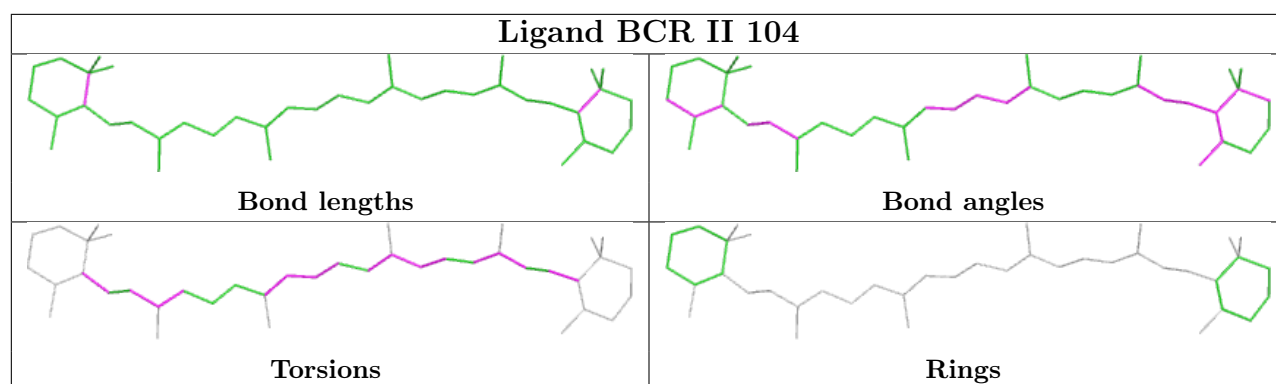


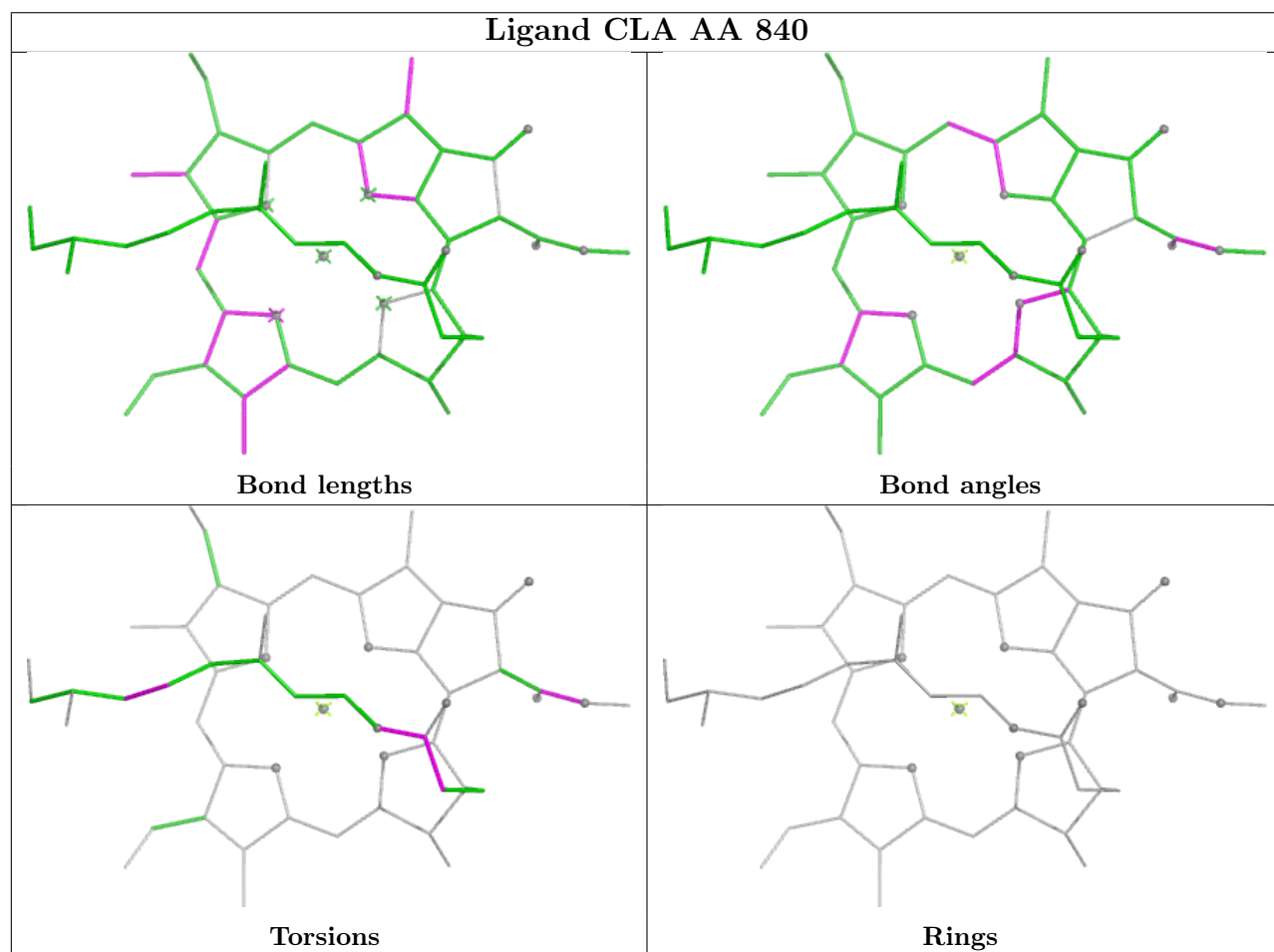
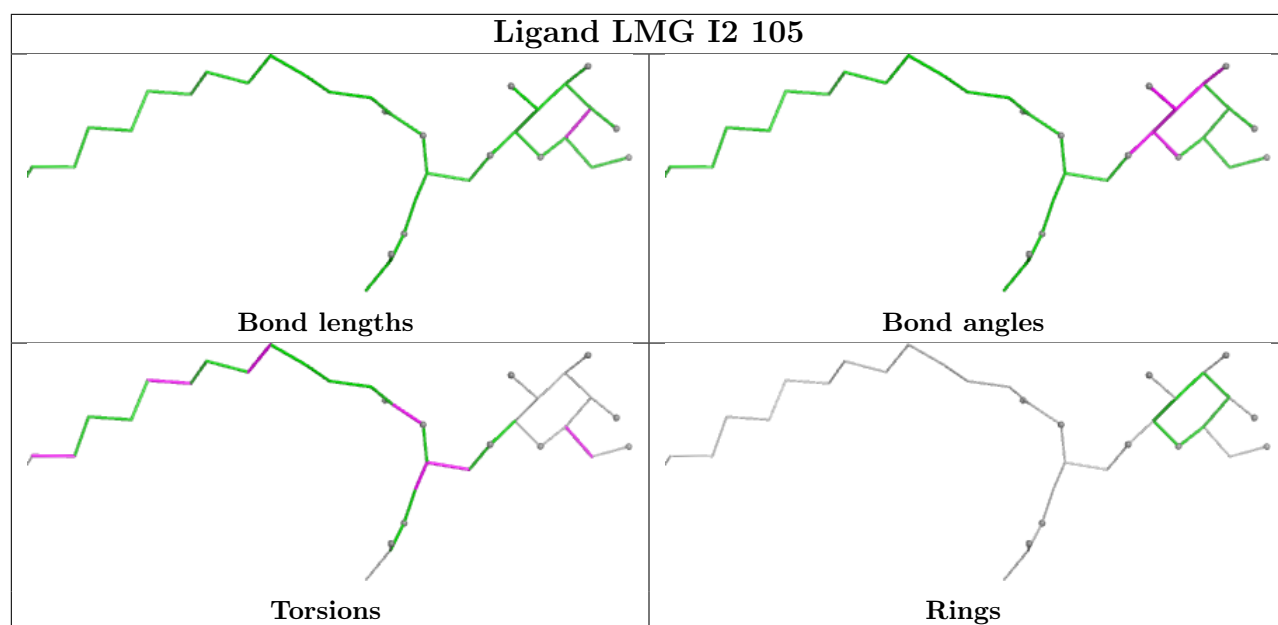
Torsions

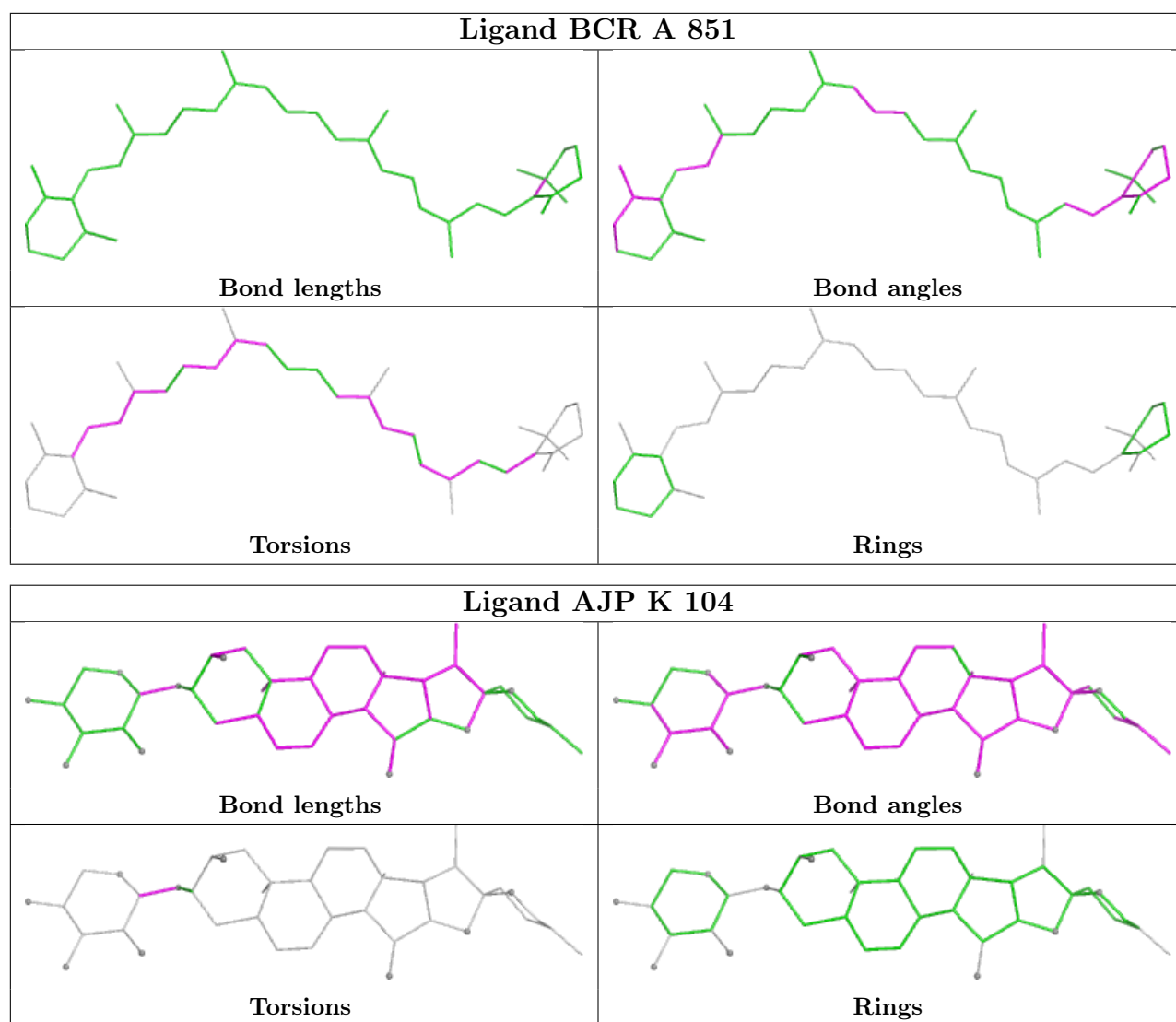


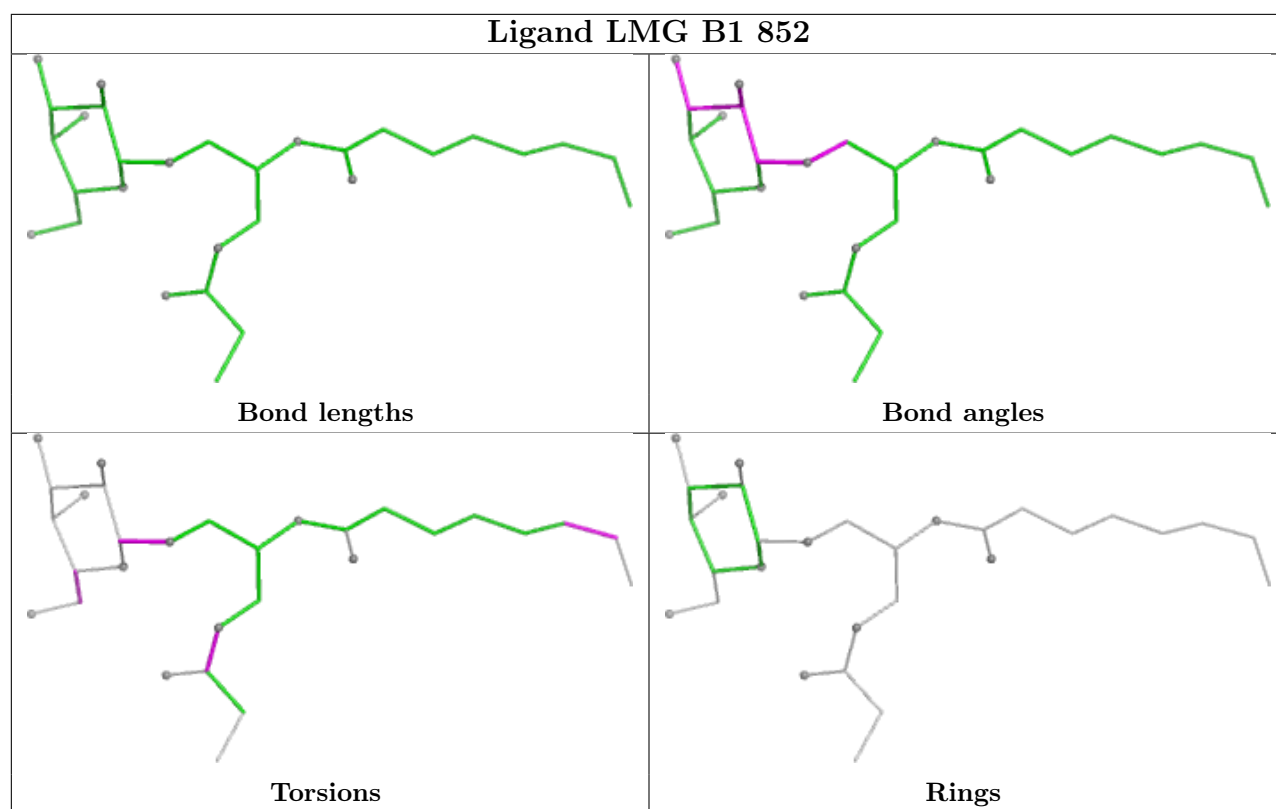
Rings

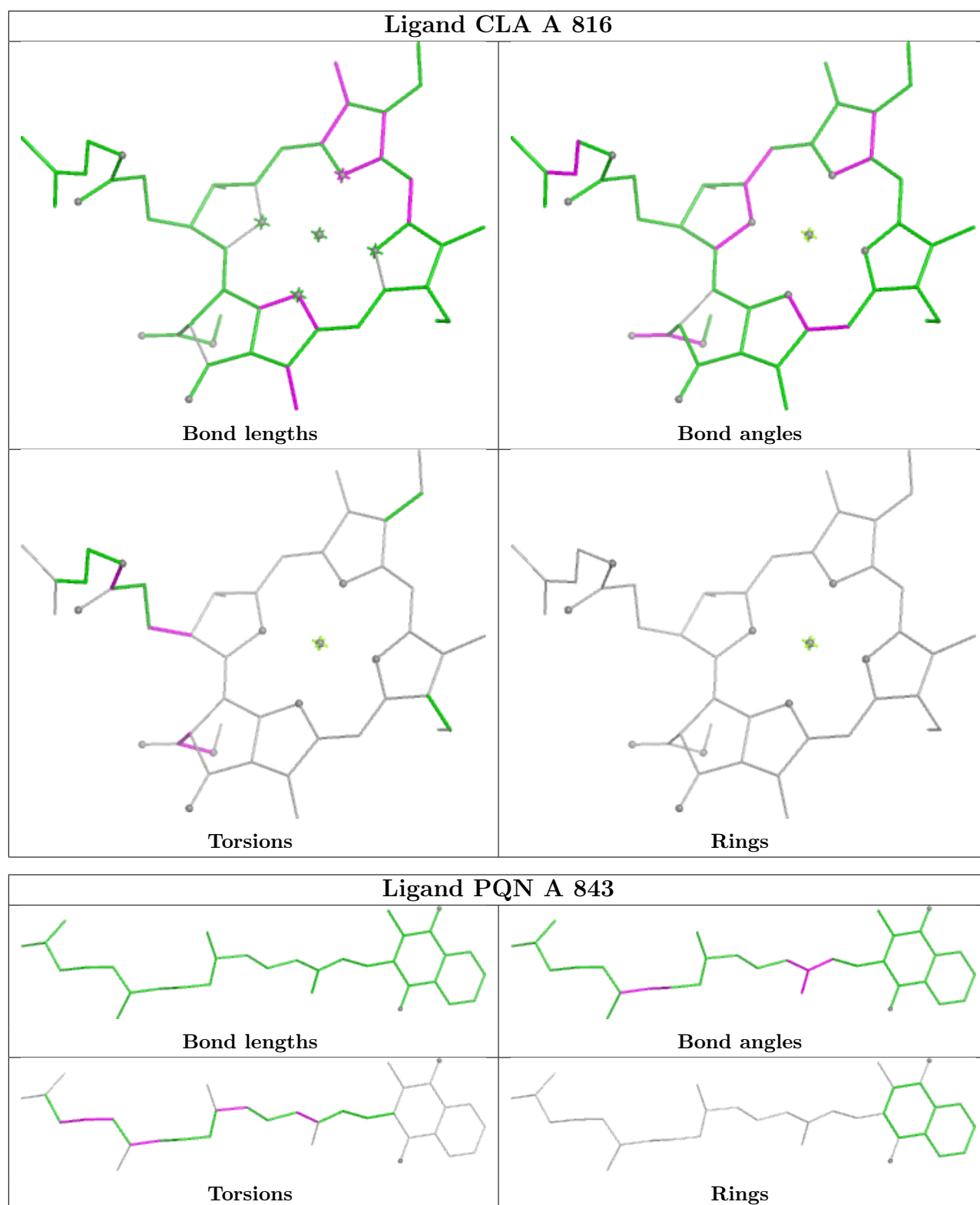


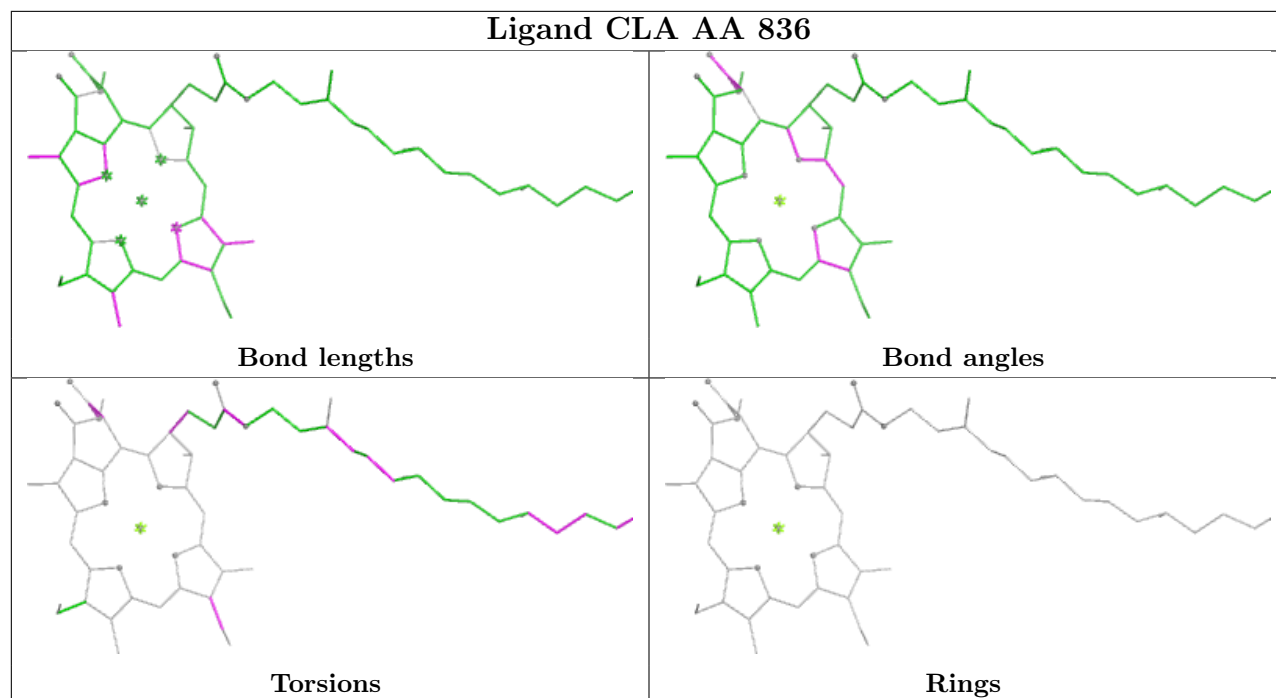
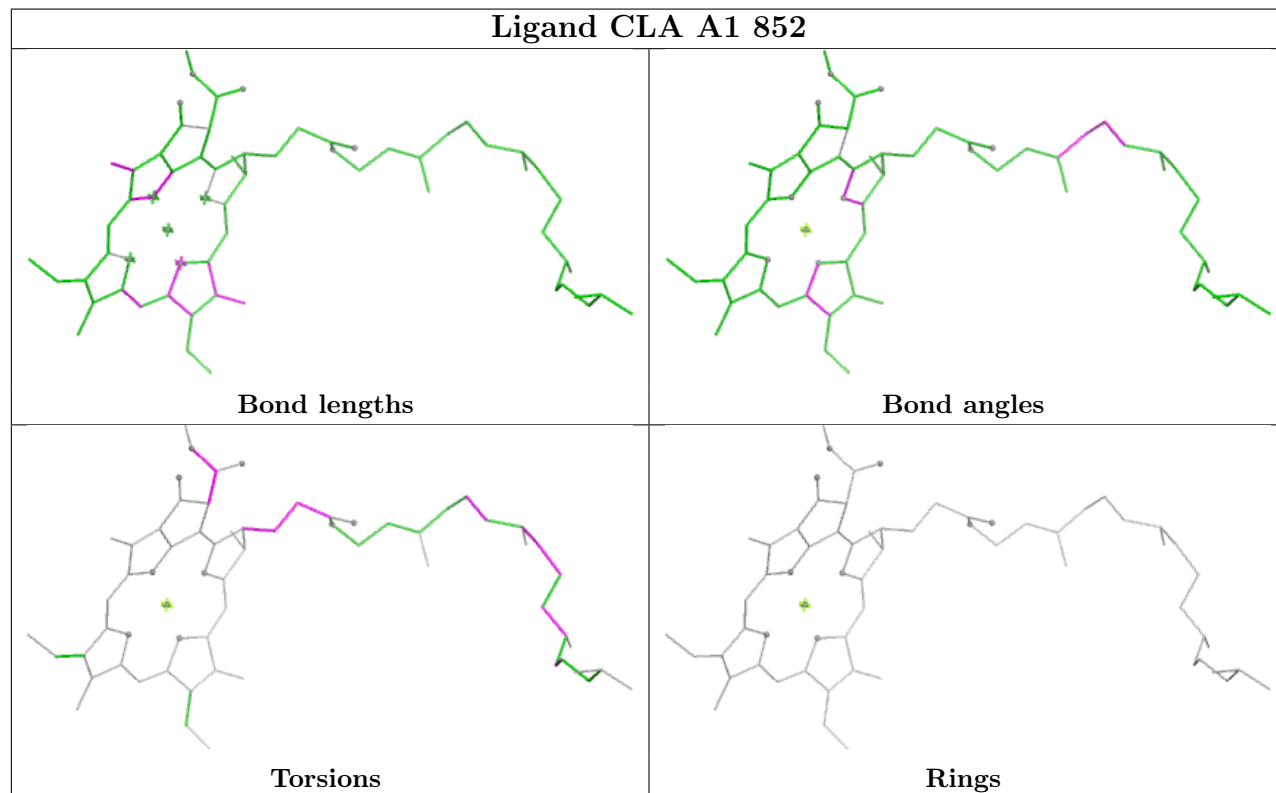




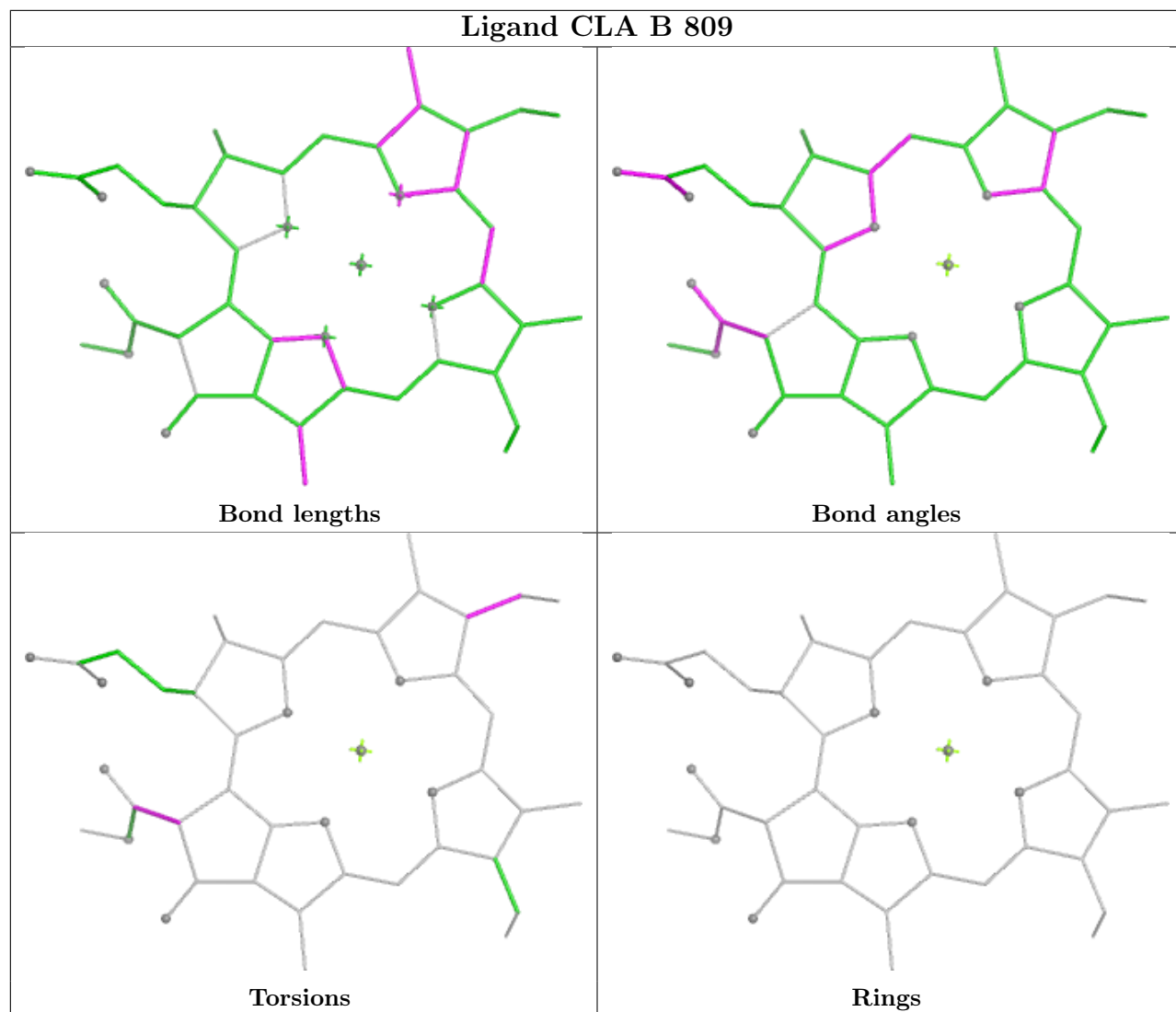


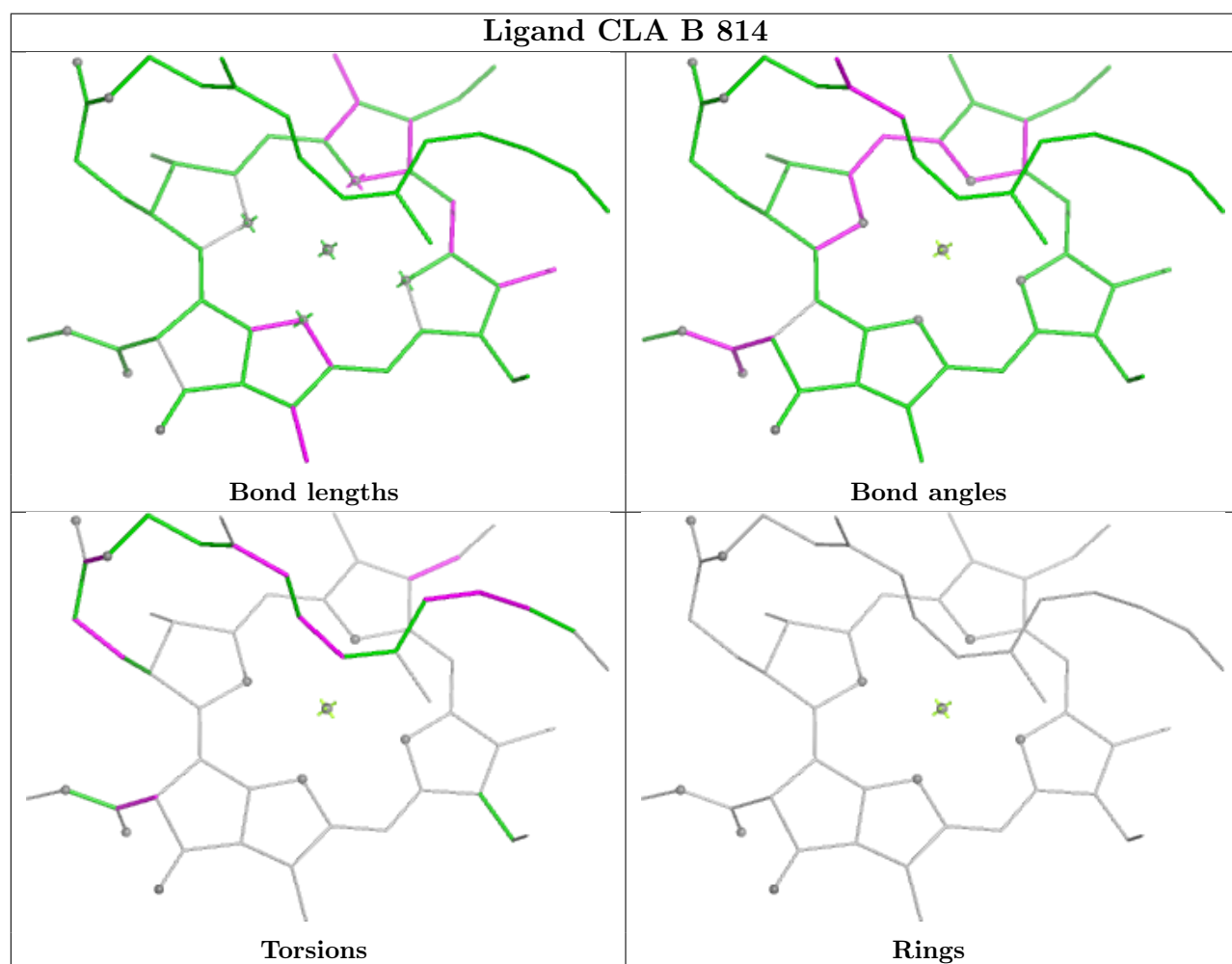
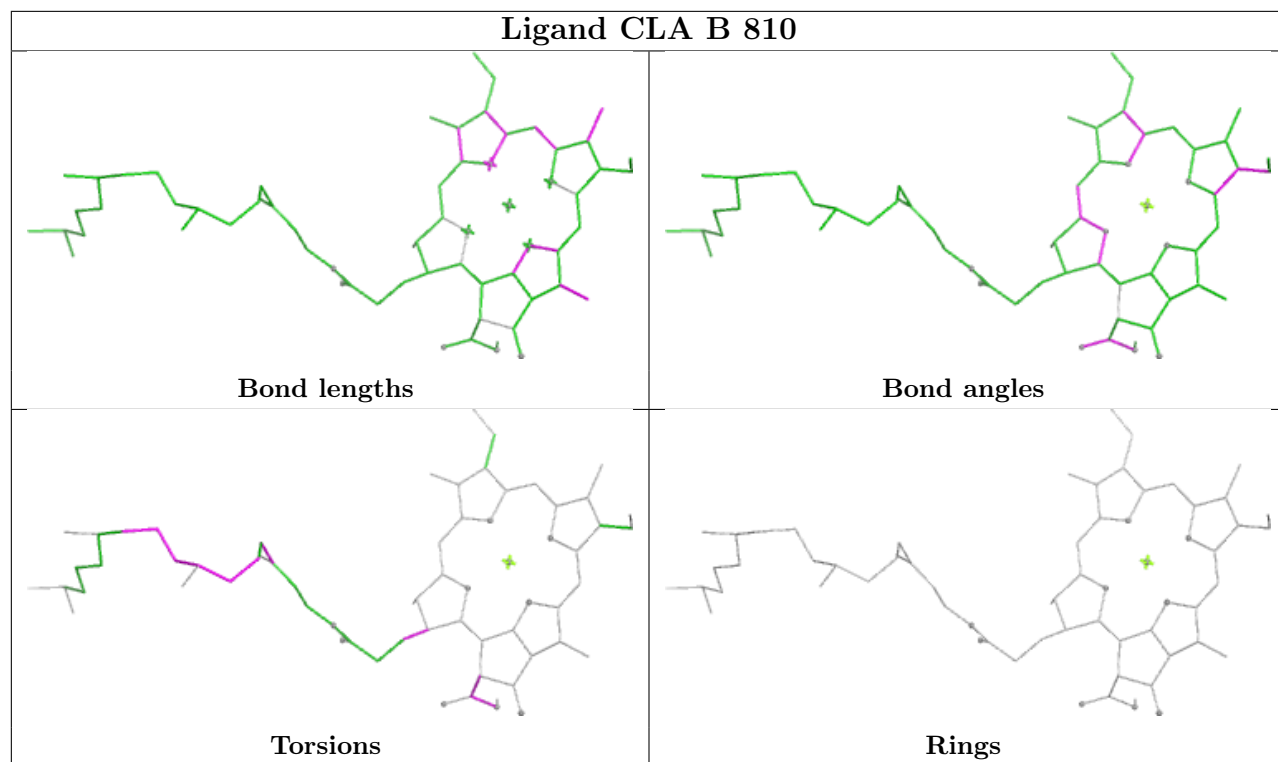




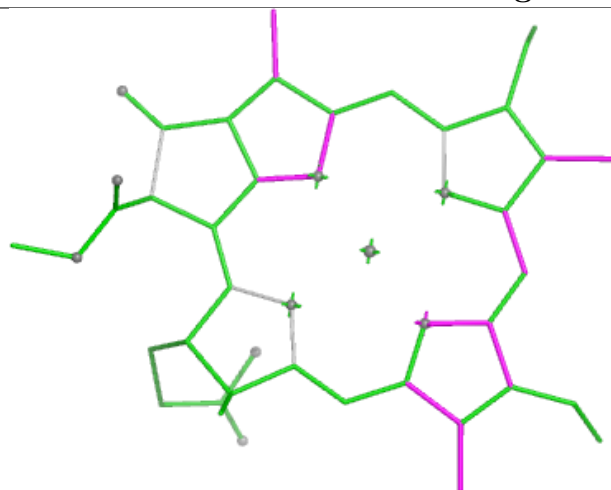
Ligand CLA AA 836**Ligand CLA A1 852**

Ligand CLA B 809

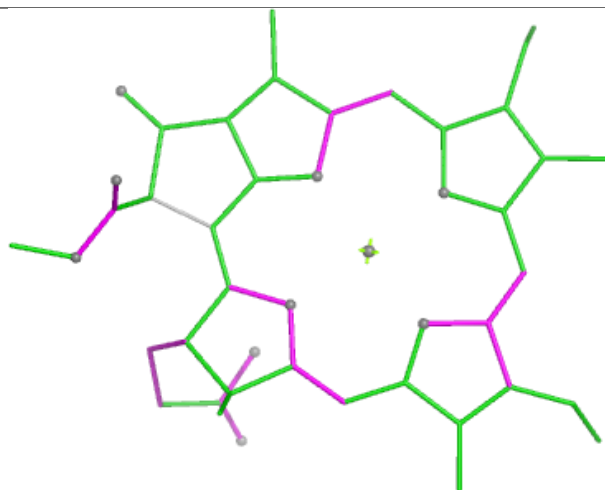




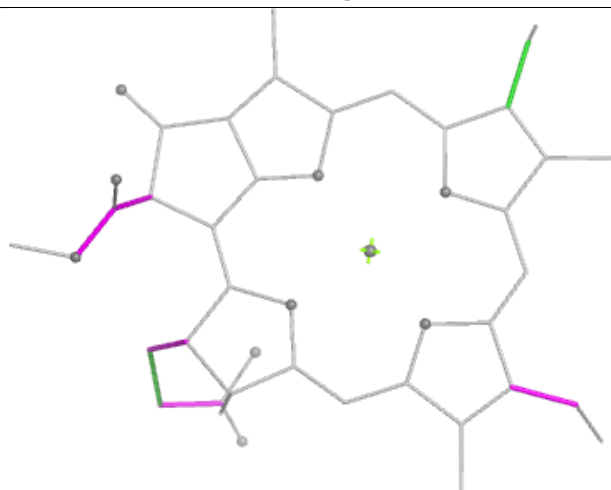
Ligand CLA B 827



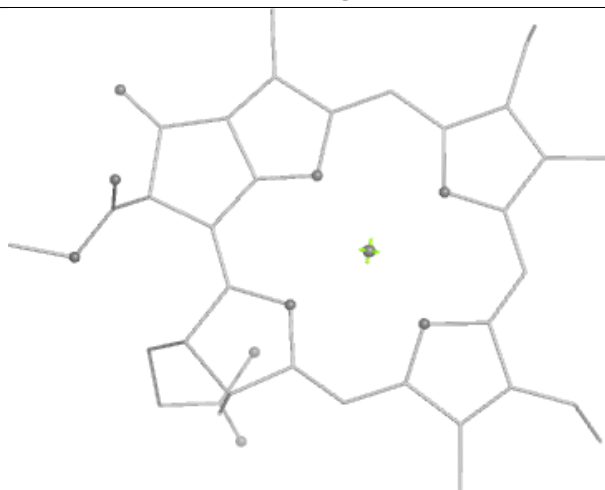
Bond lengths



Bond angles

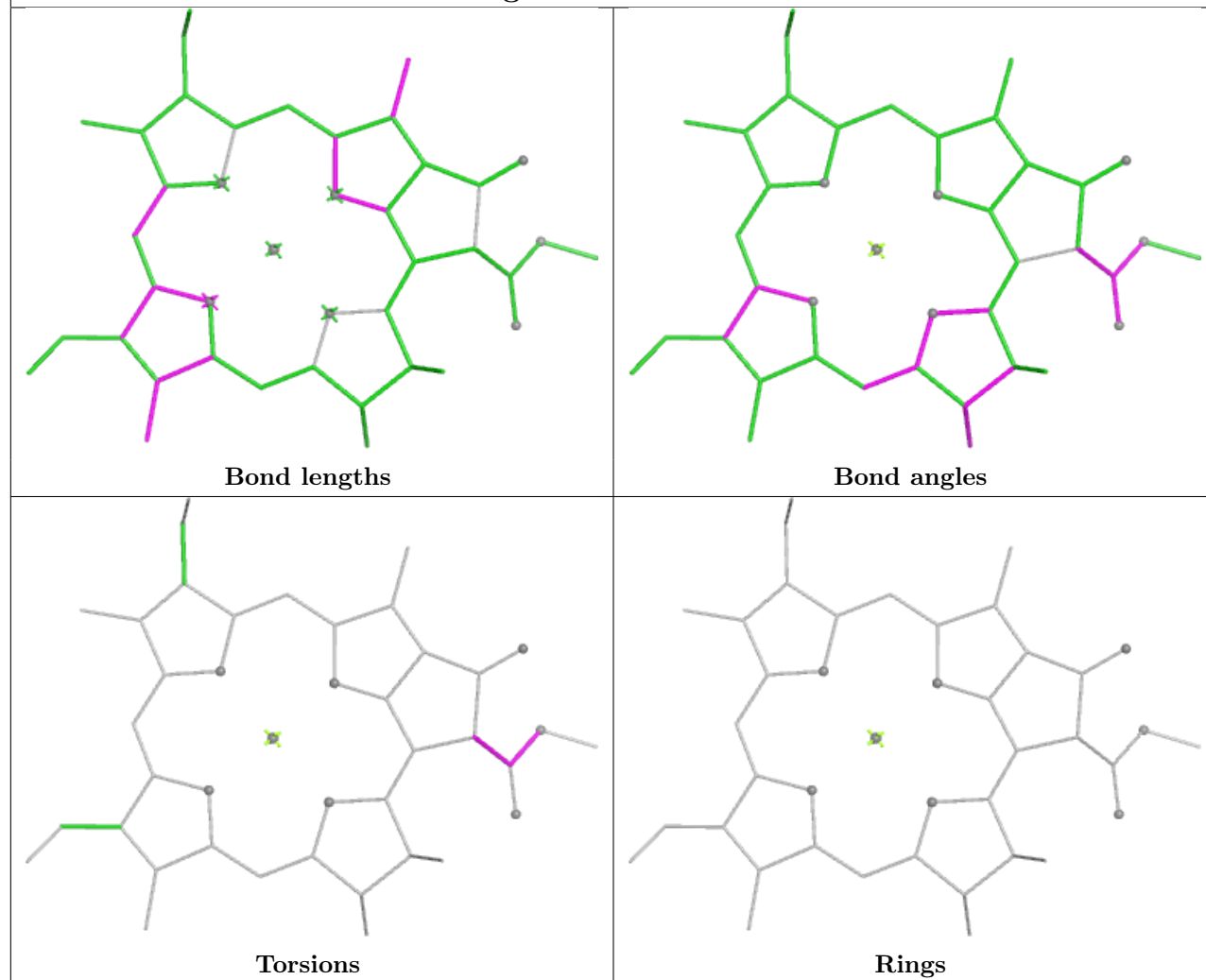


Torsions

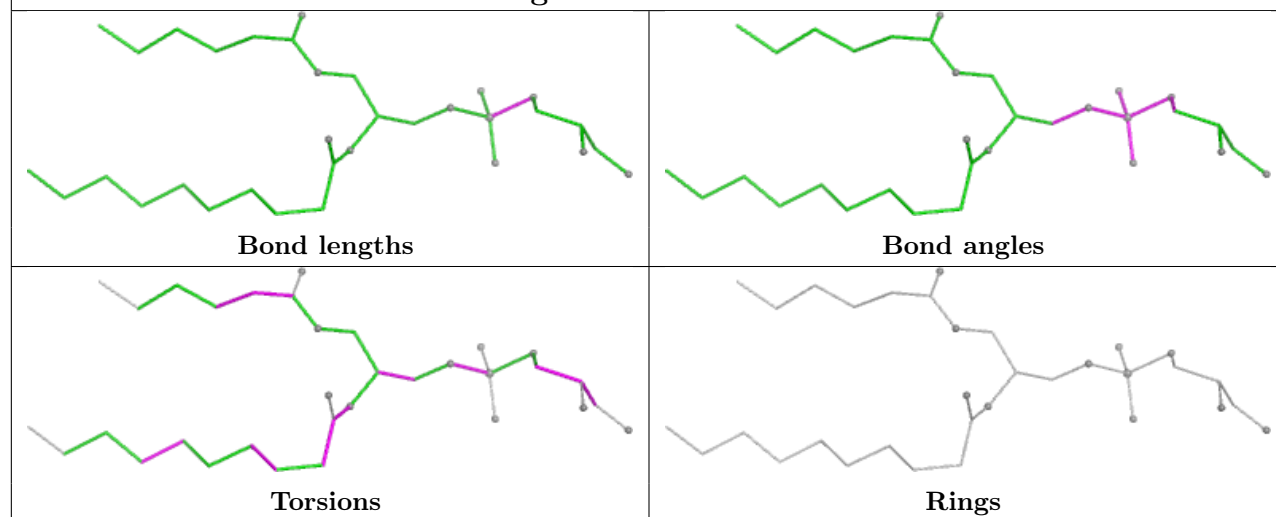


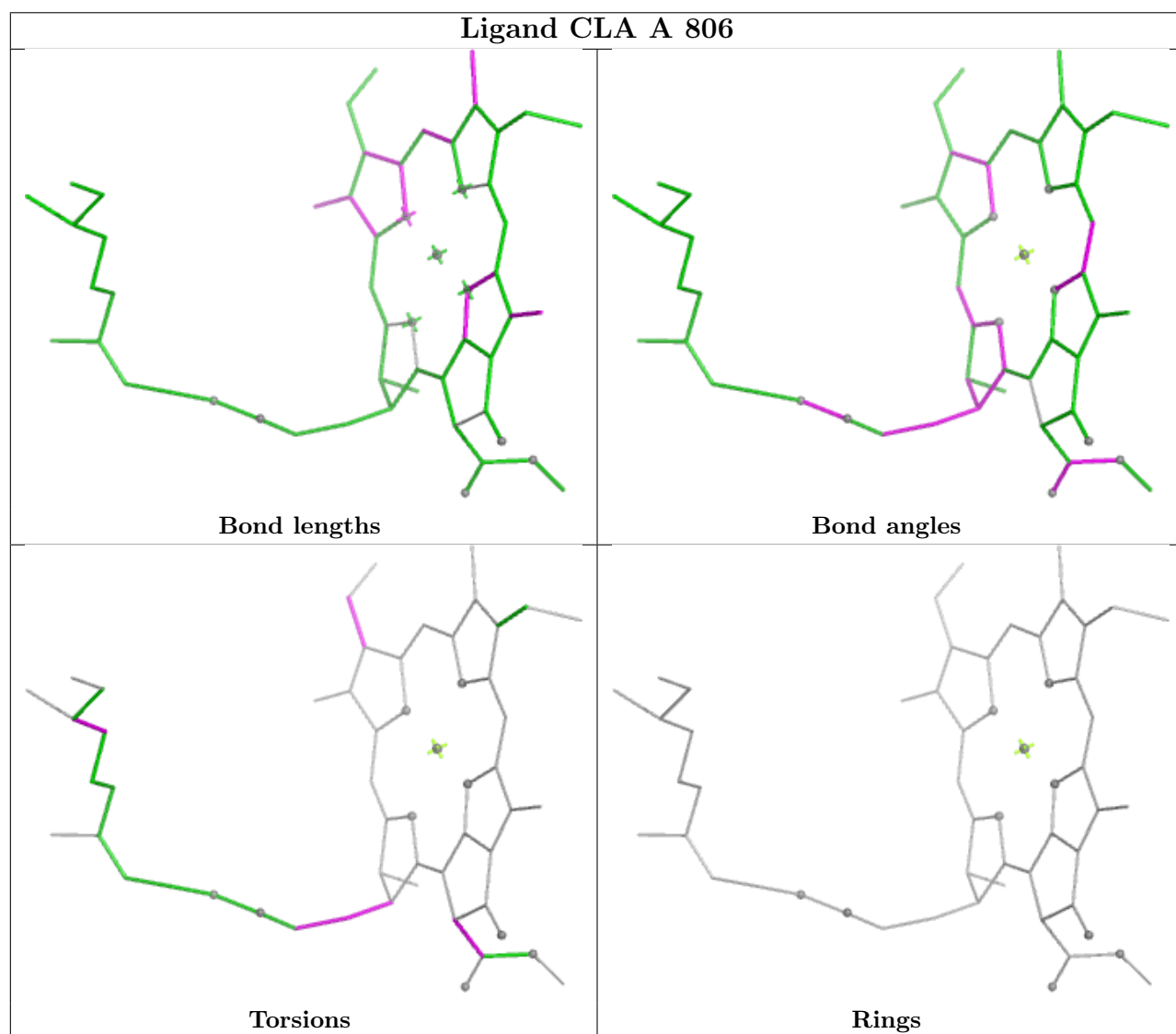
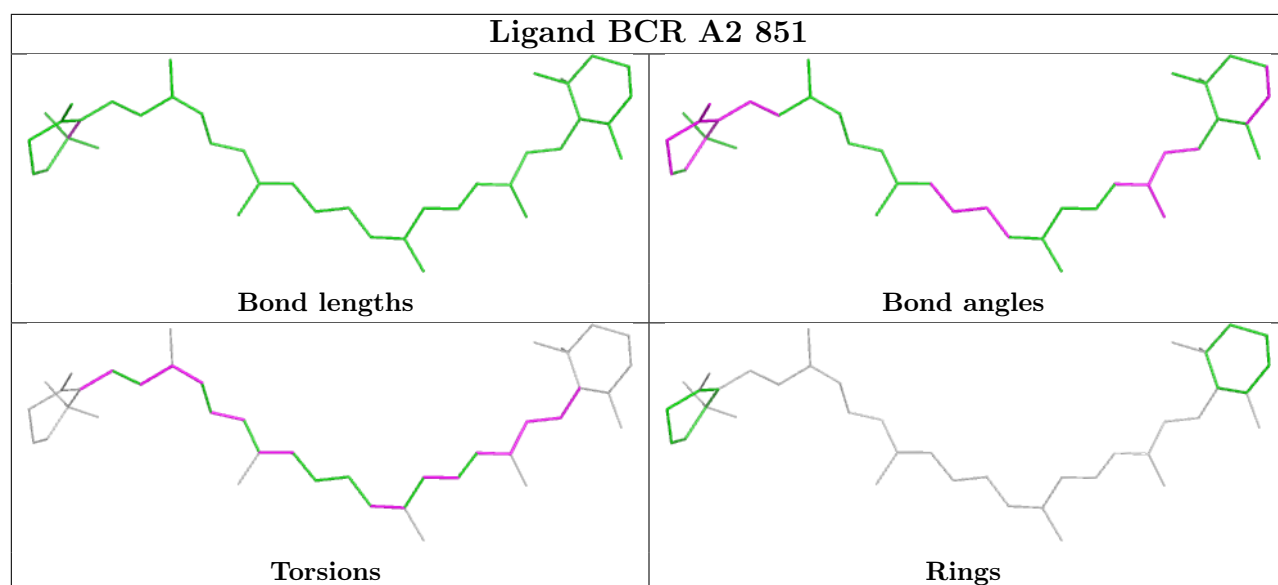
Rings

Ligand CLA B 812

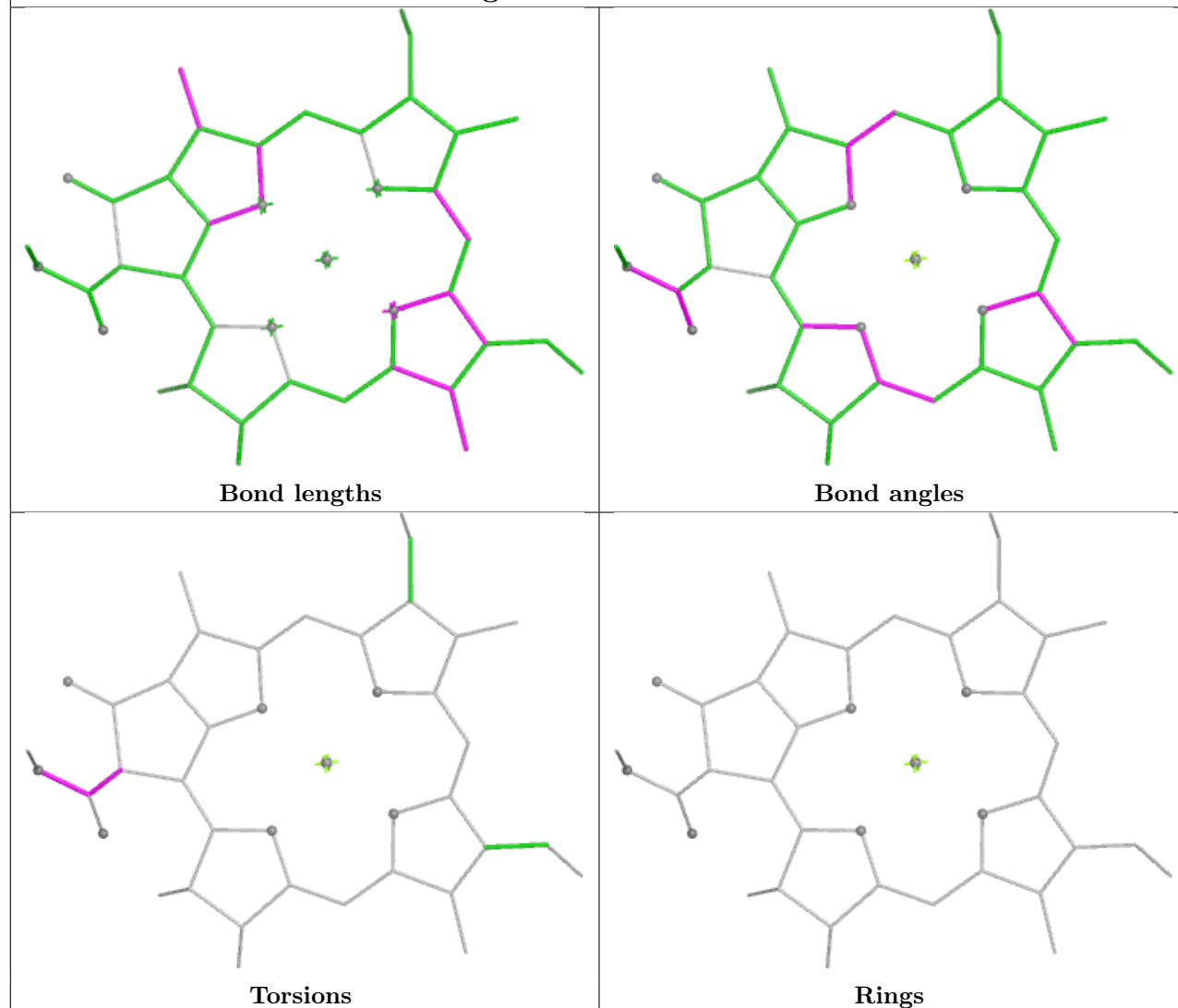


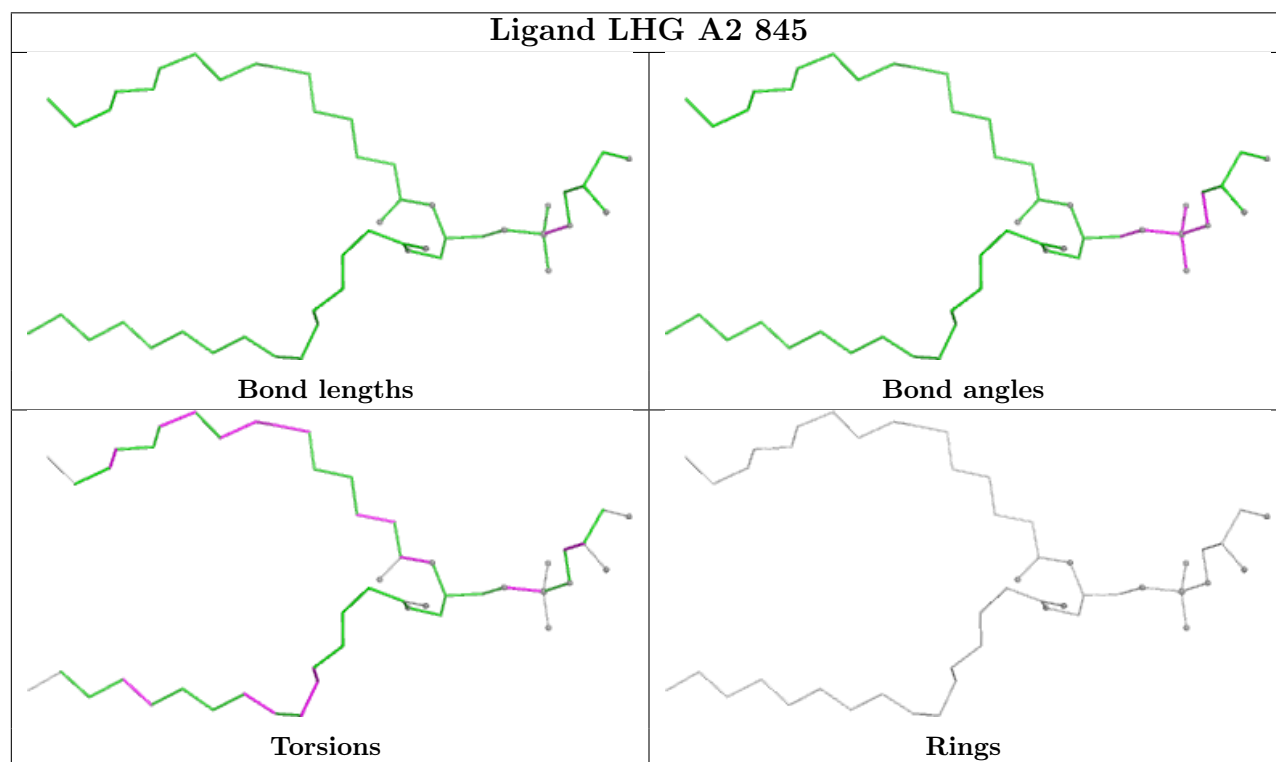
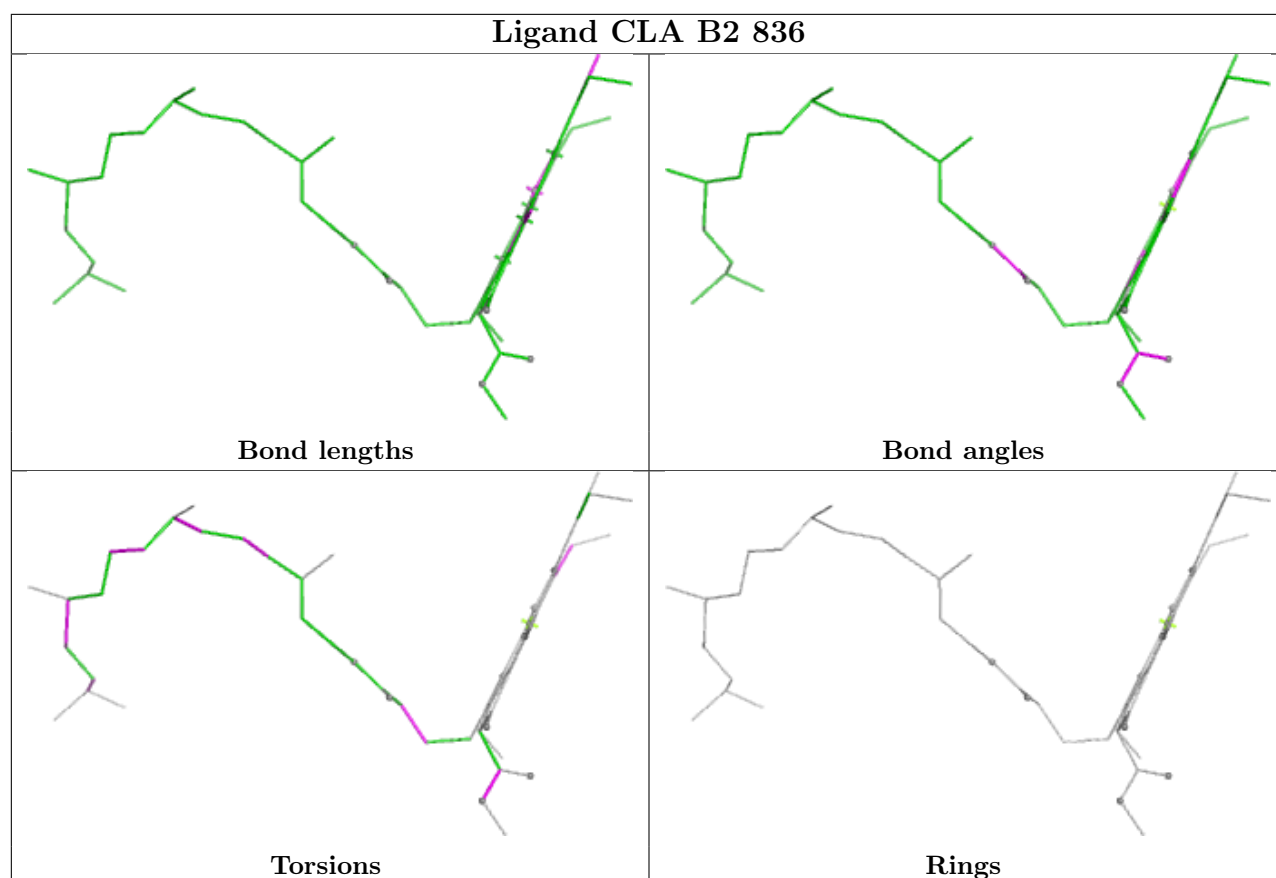
Ligand LHG B 852

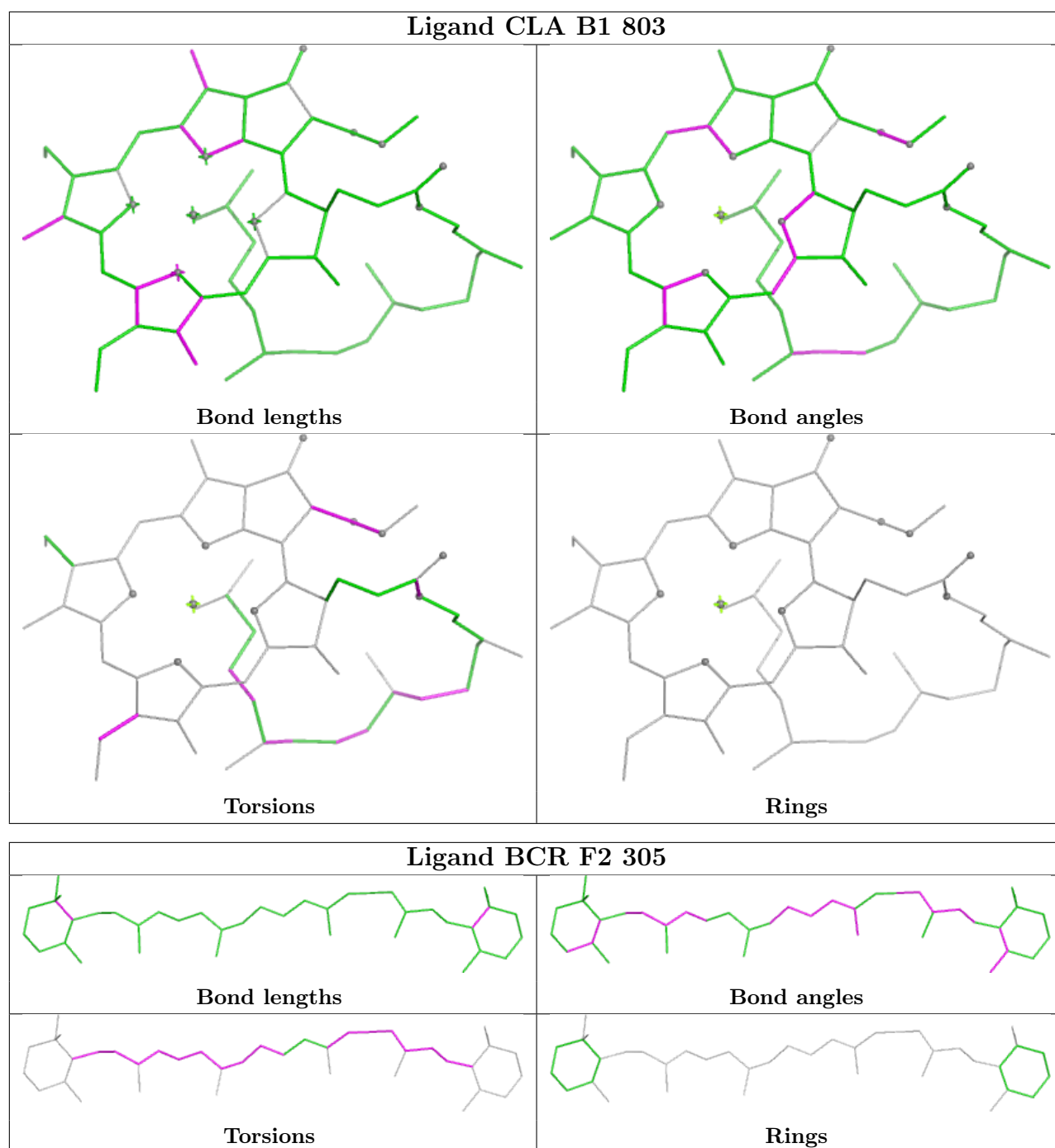


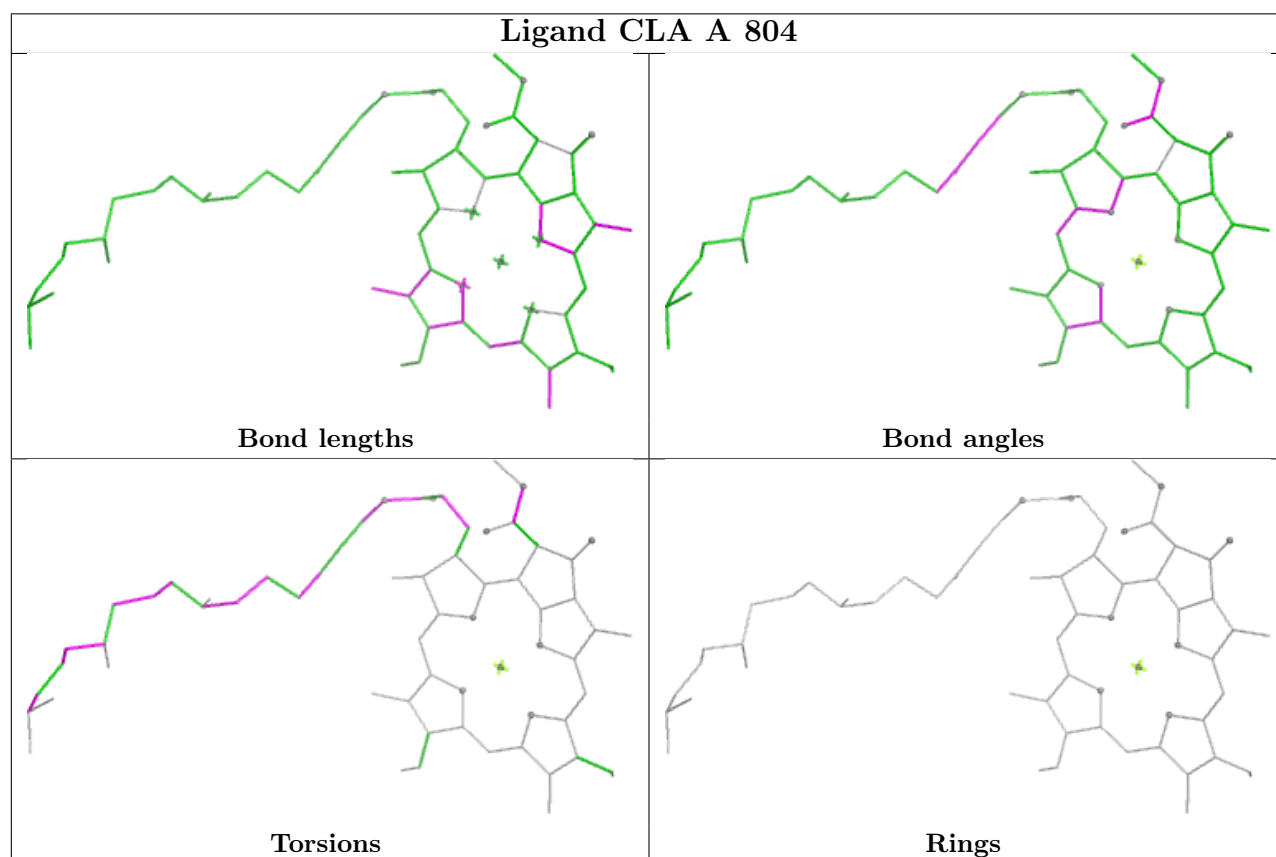
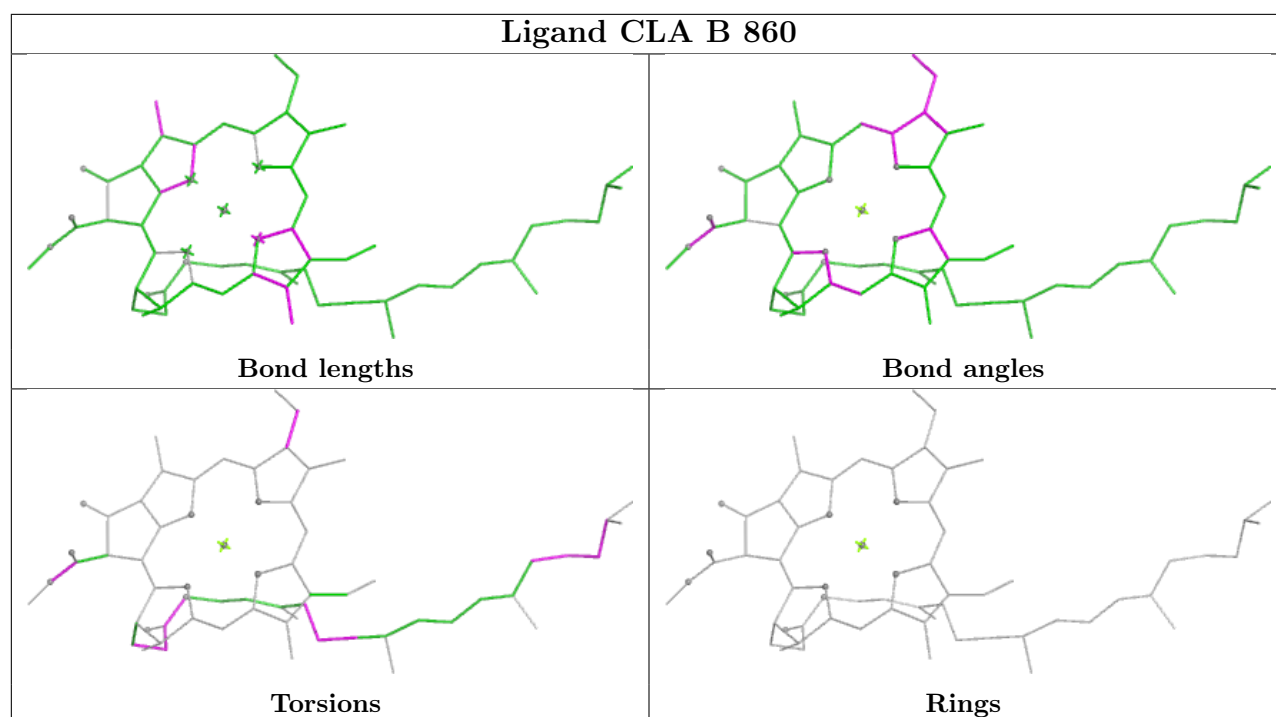


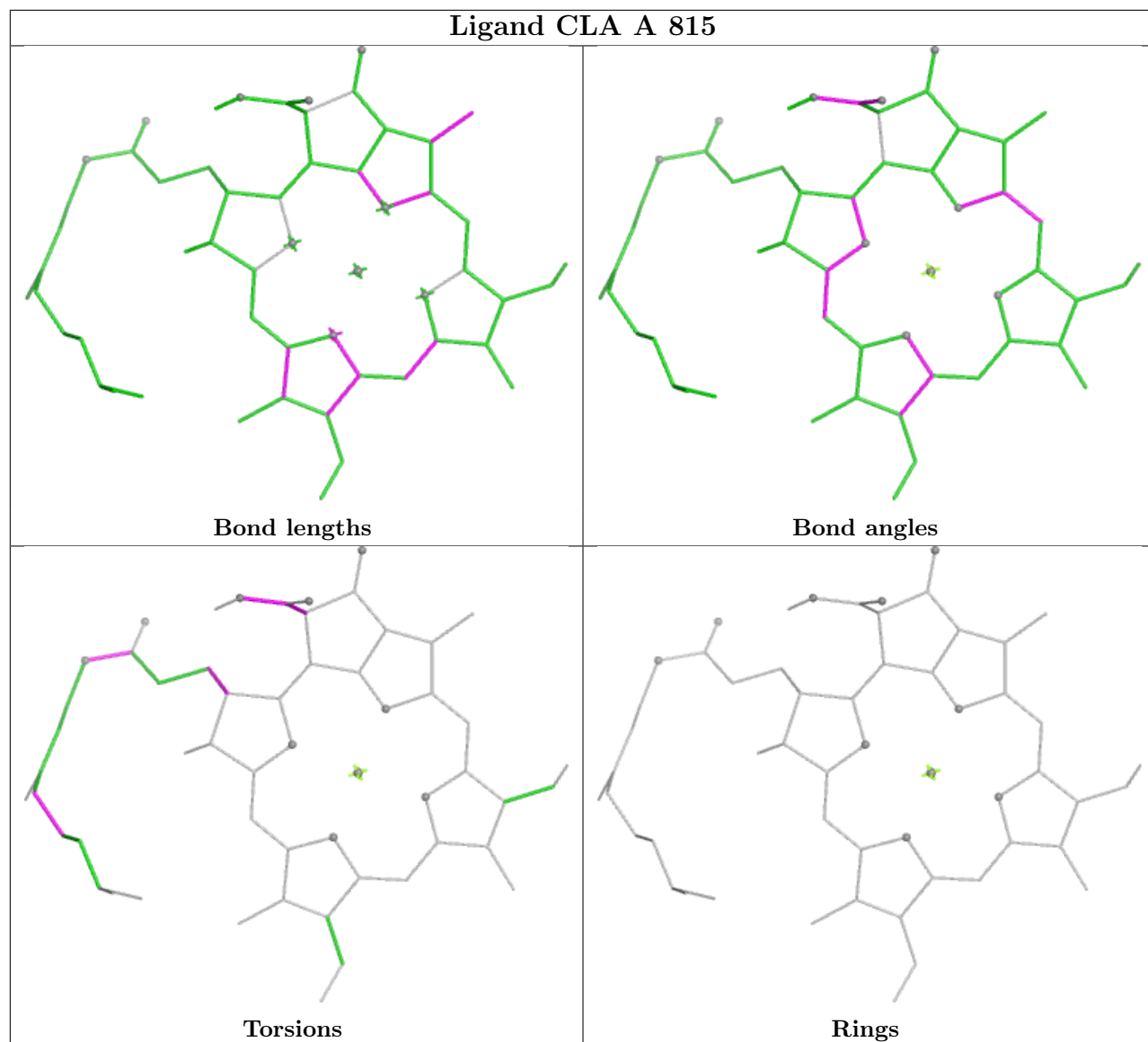
Ligand CLA A1 844

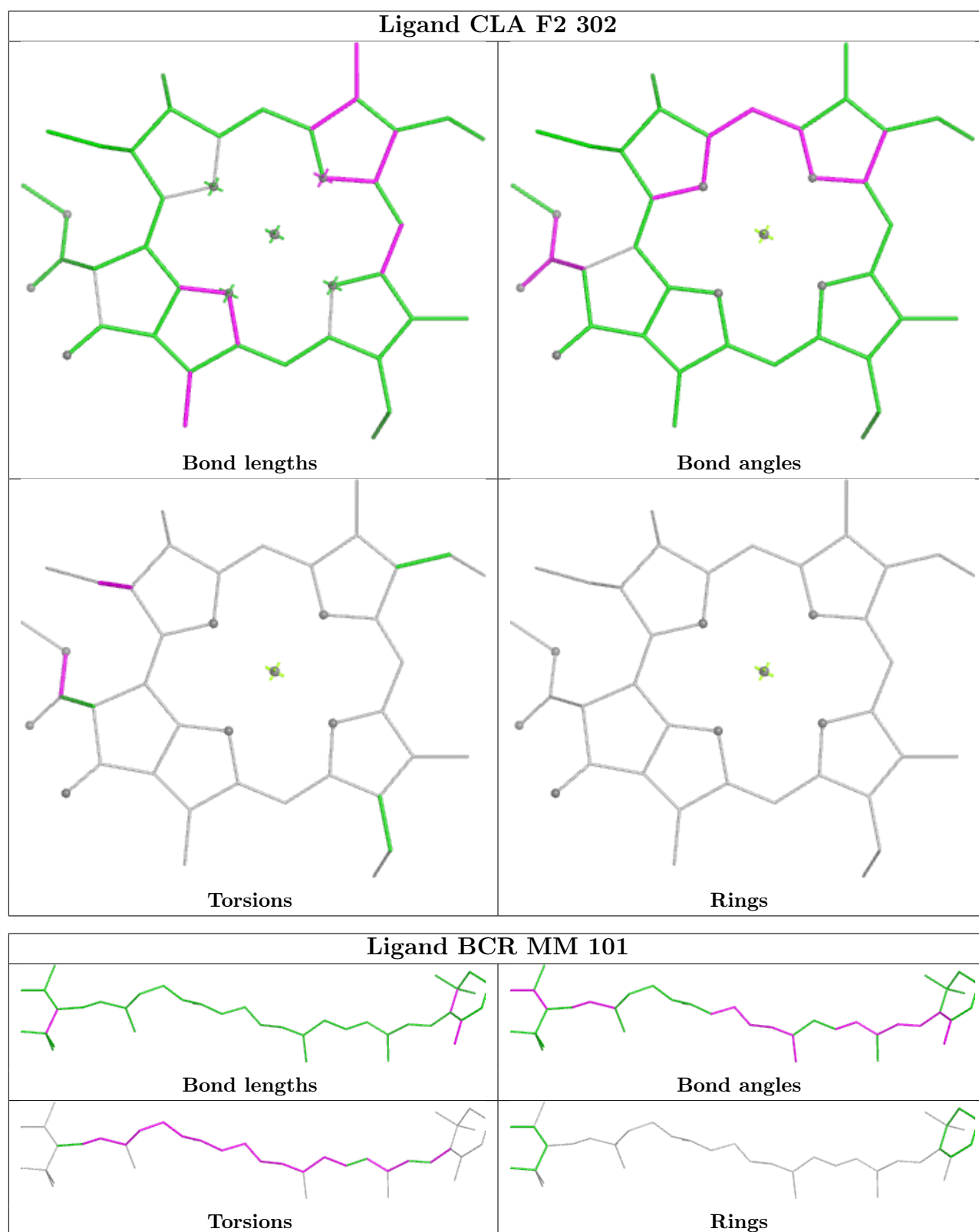


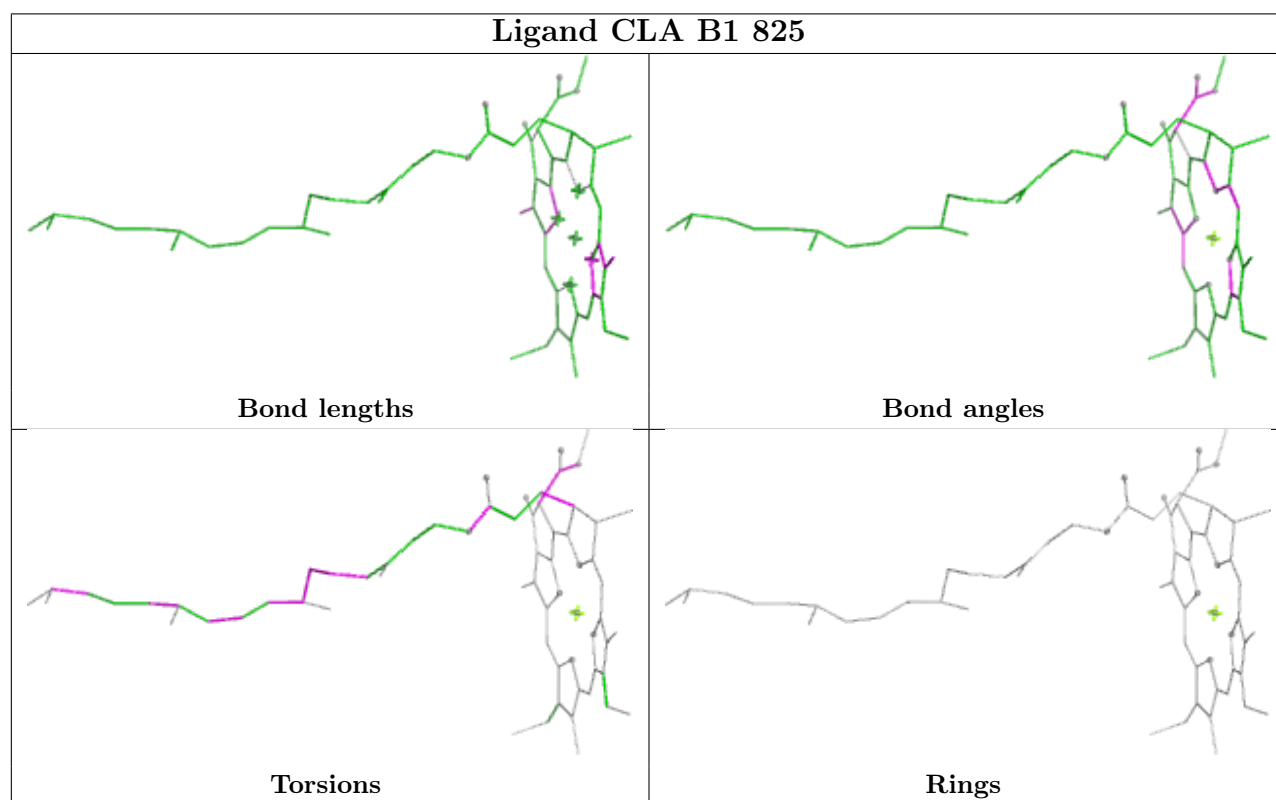
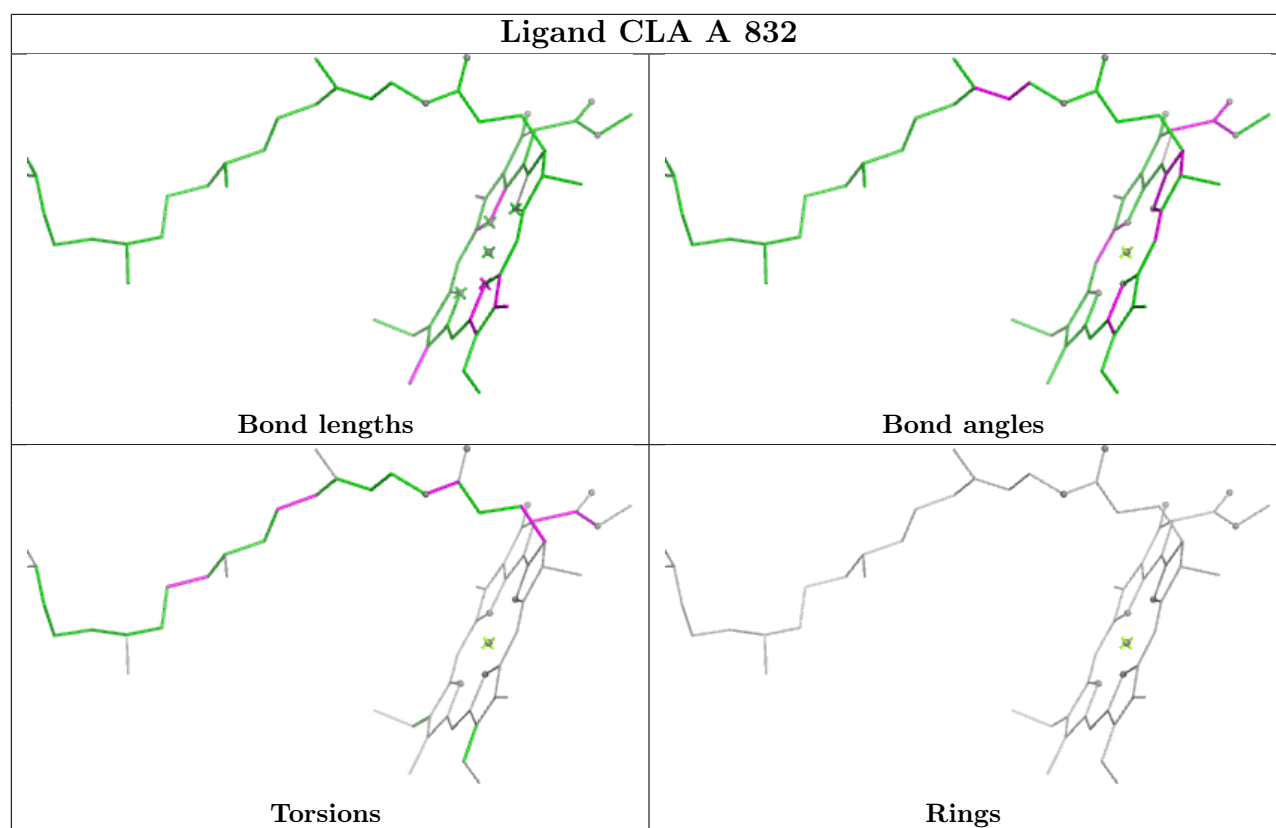


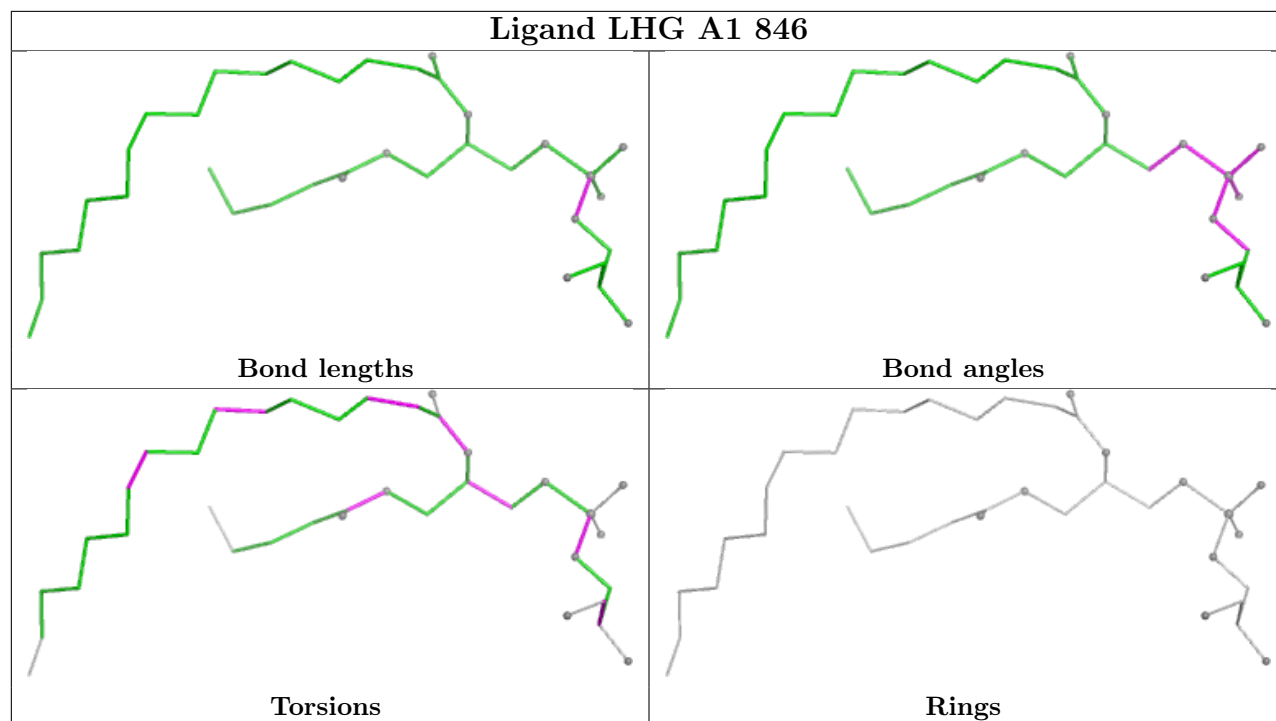




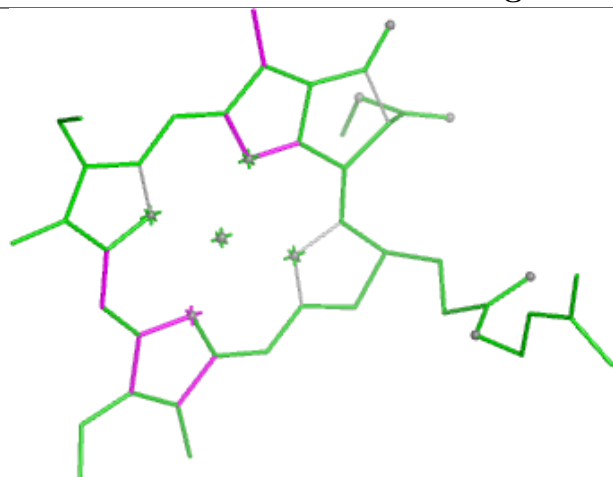




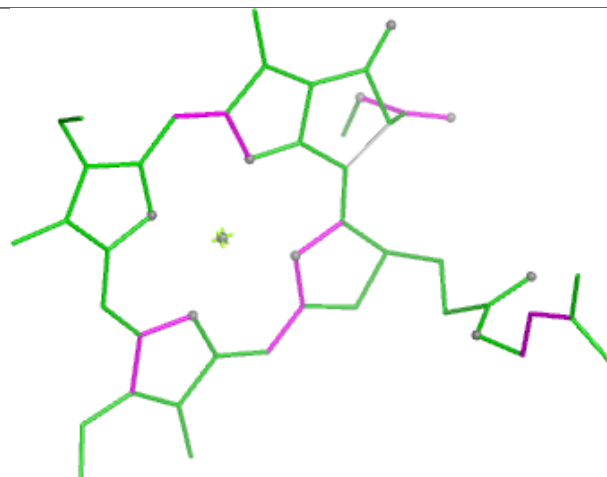




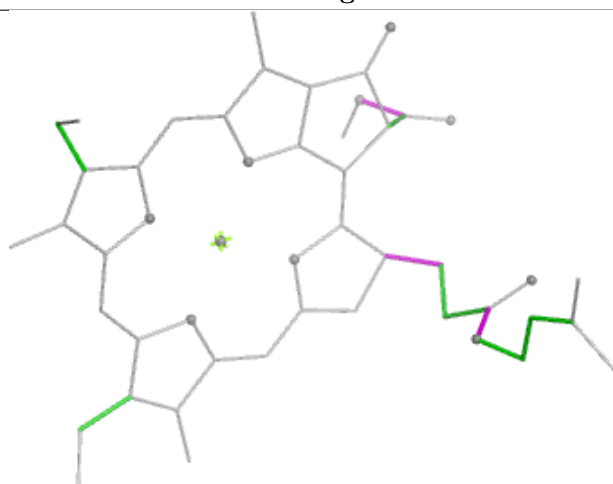
Ligand CLA A2 816



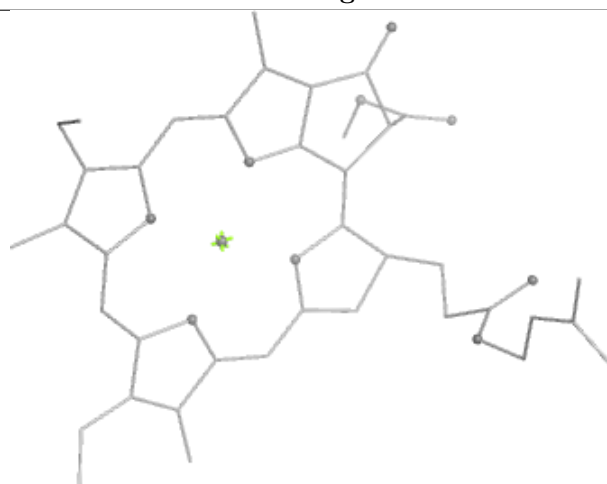
Bond lengths



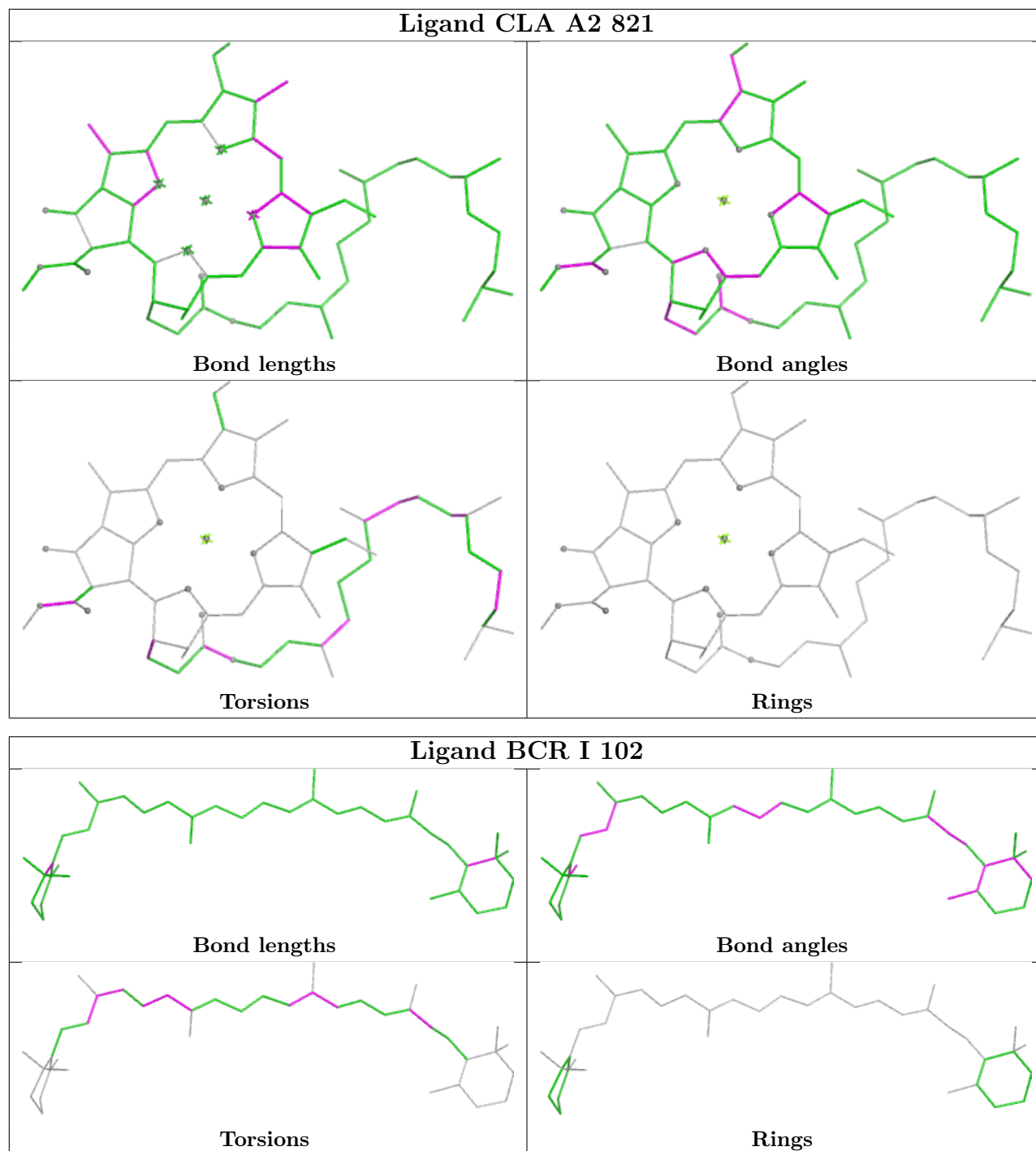
Bond angles



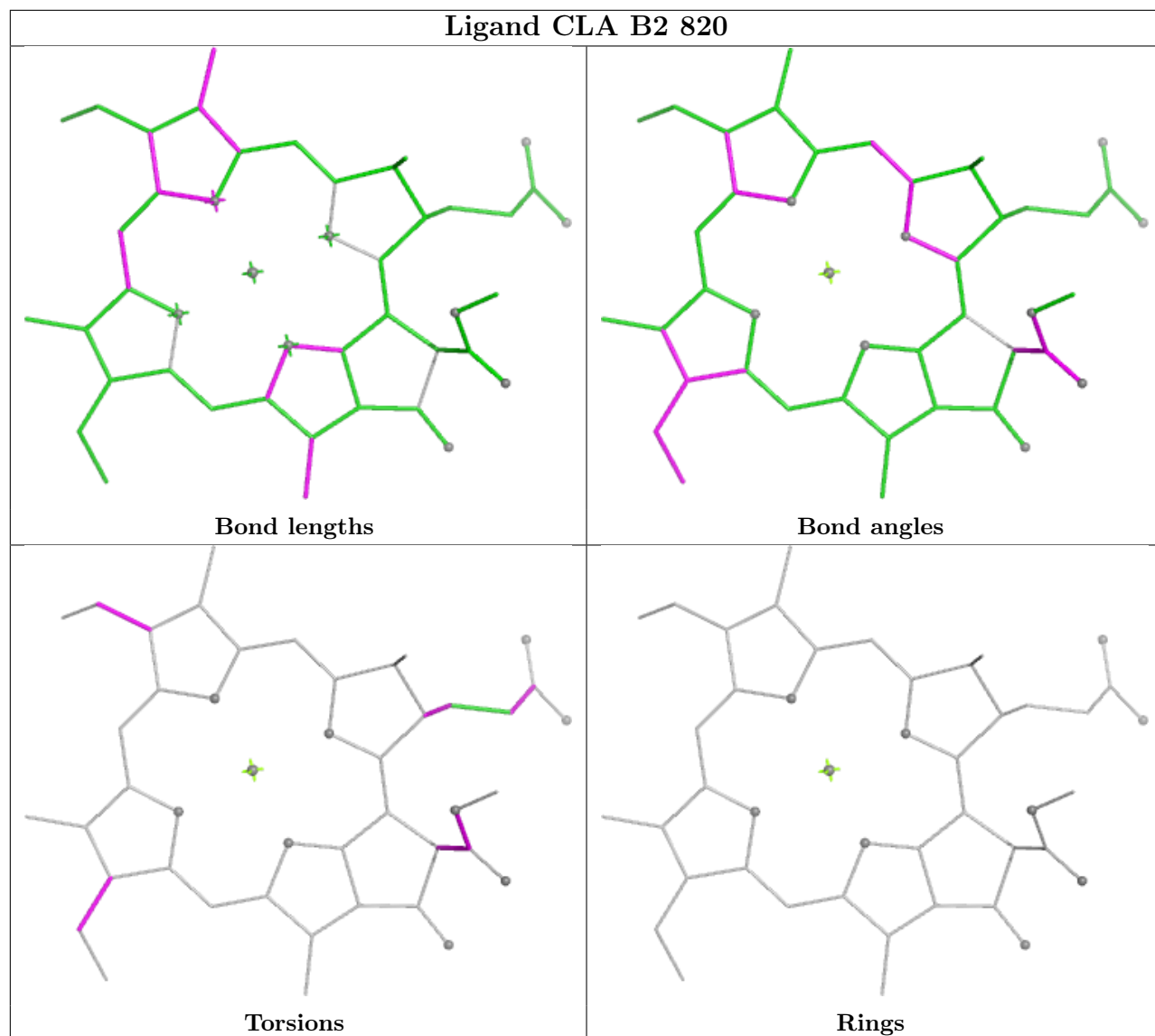
Torsions

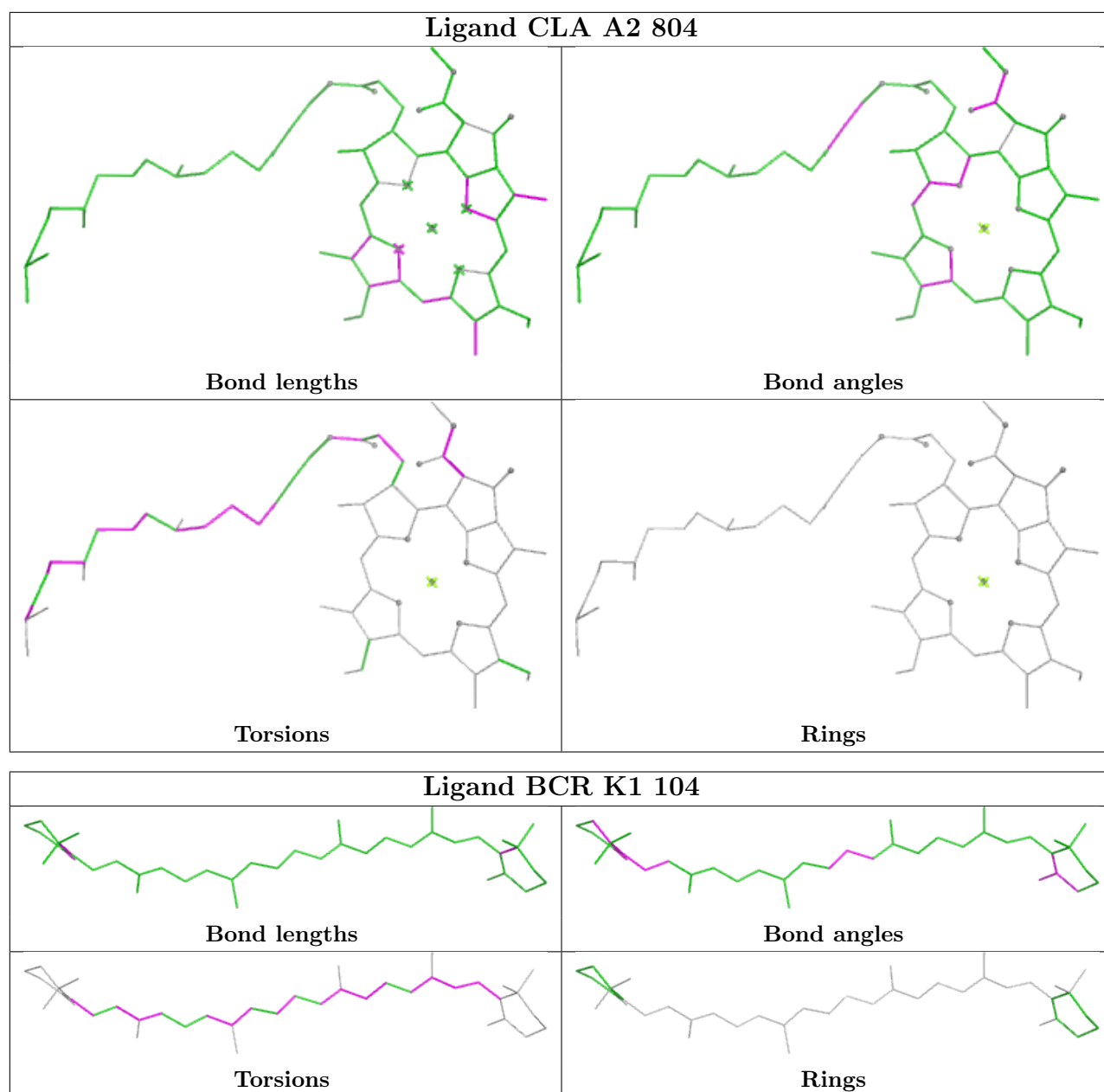


Rings

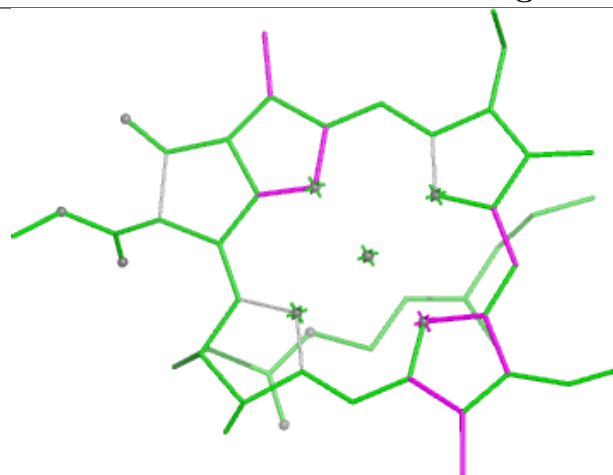


Ligand CLA B2 820

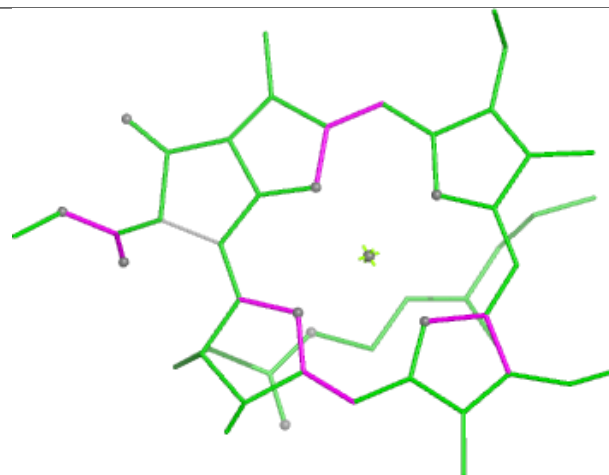




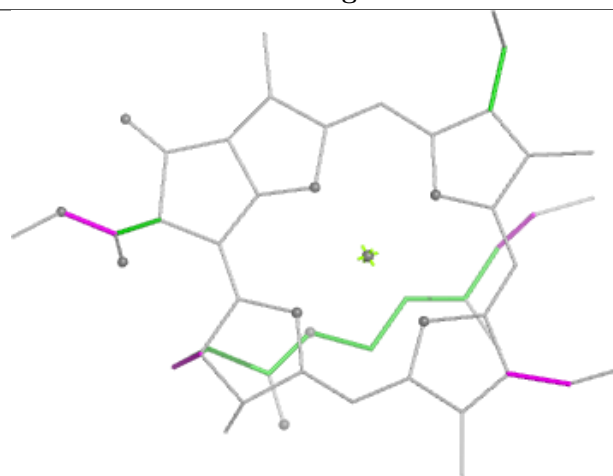
Ligand CLA A 825



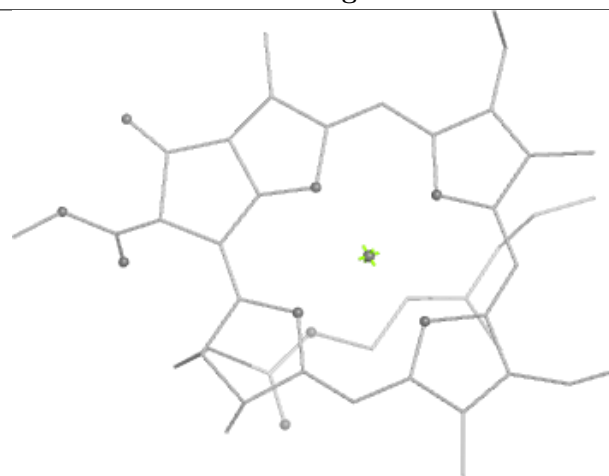
Bond lengths



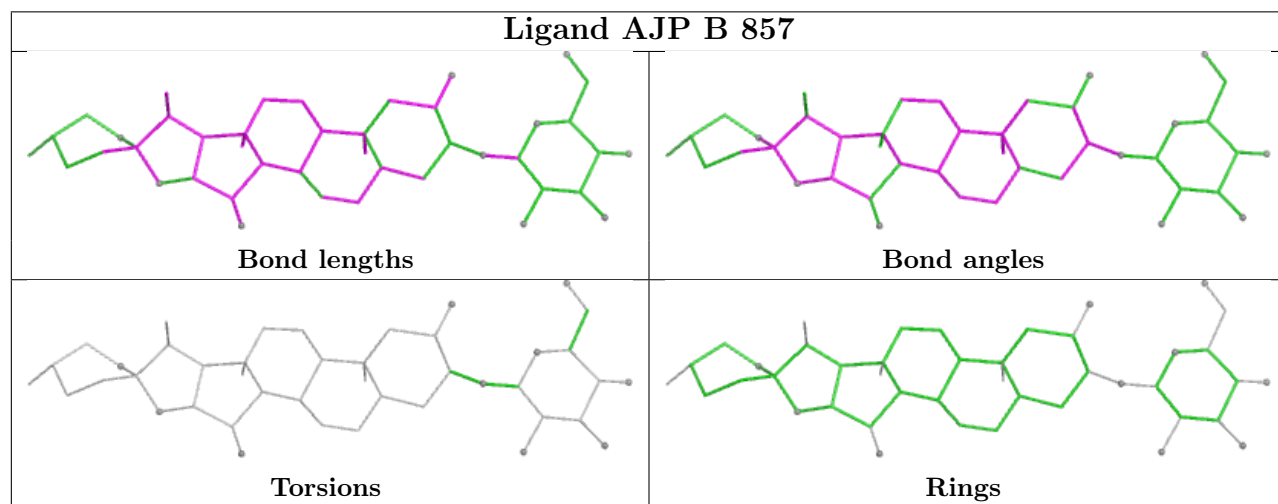
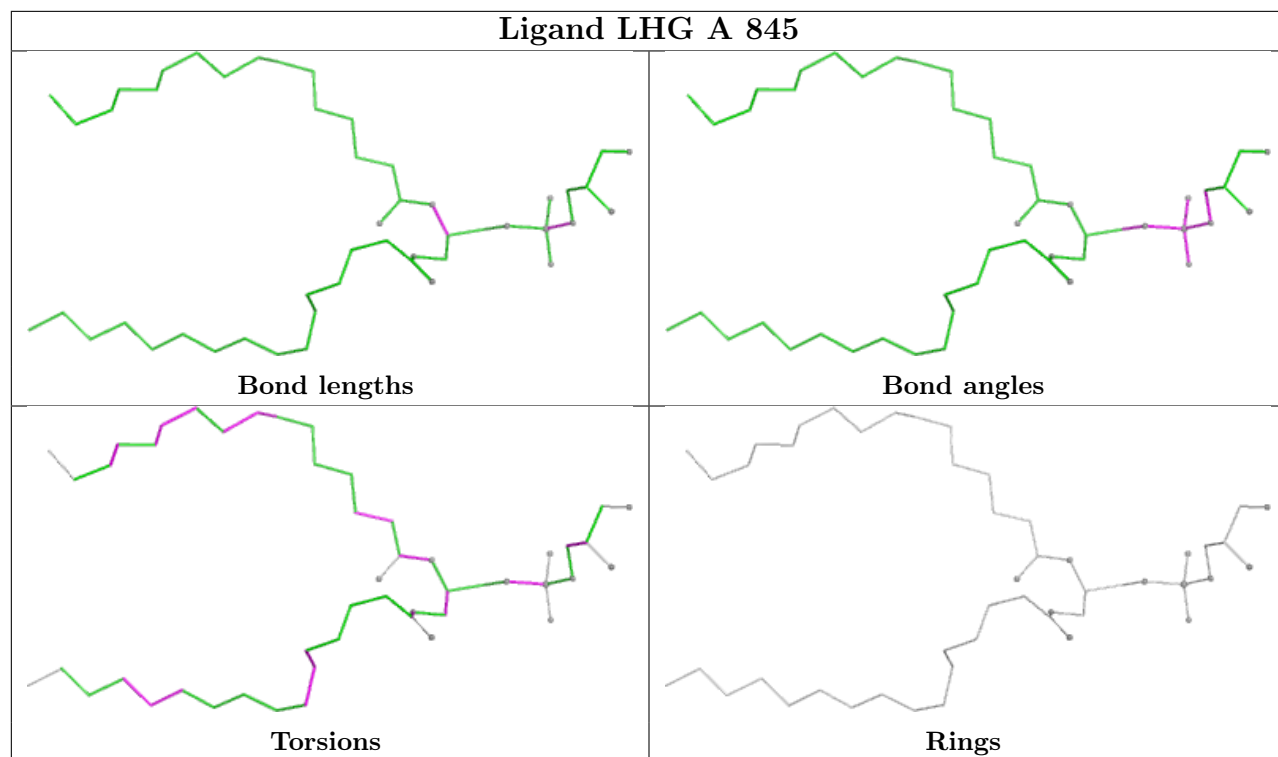
Bond angles

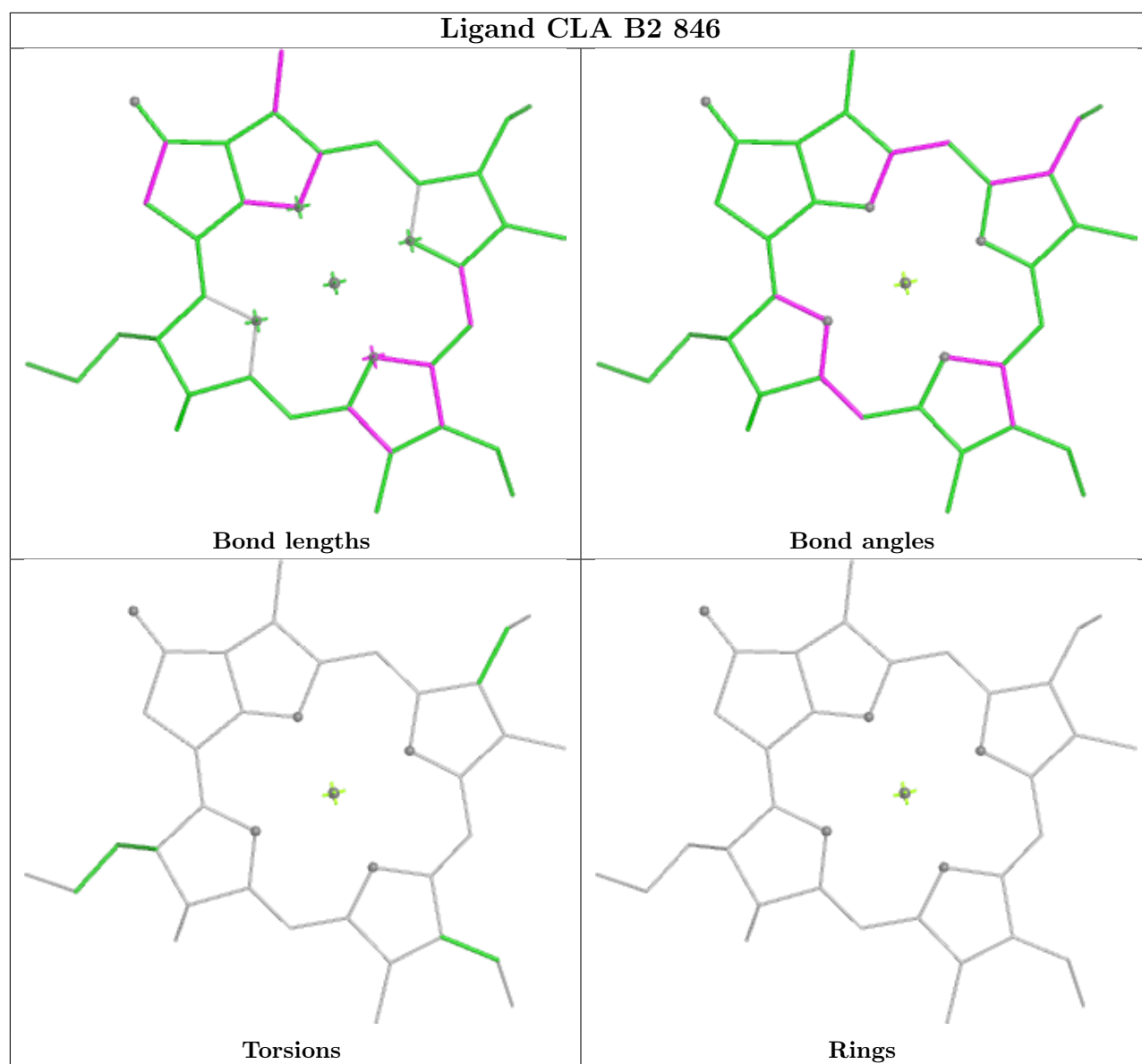


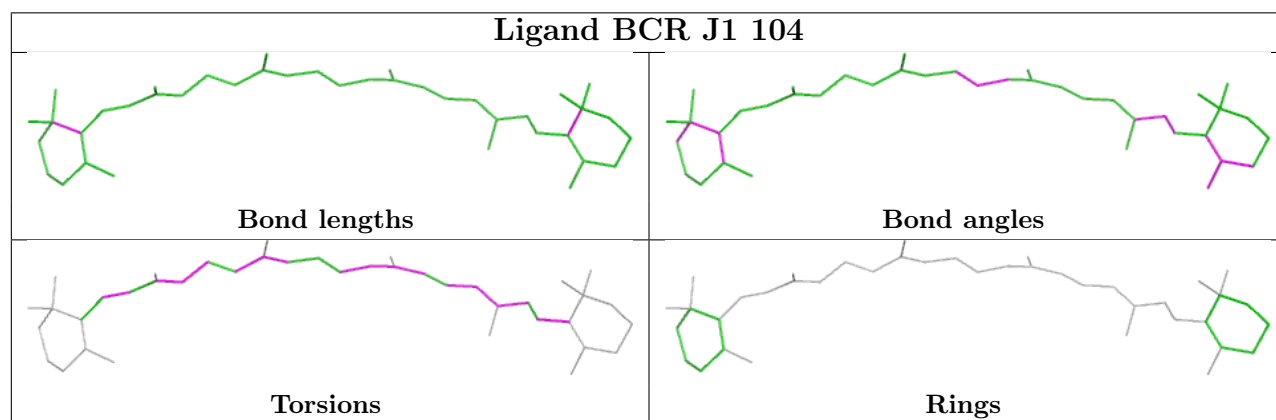
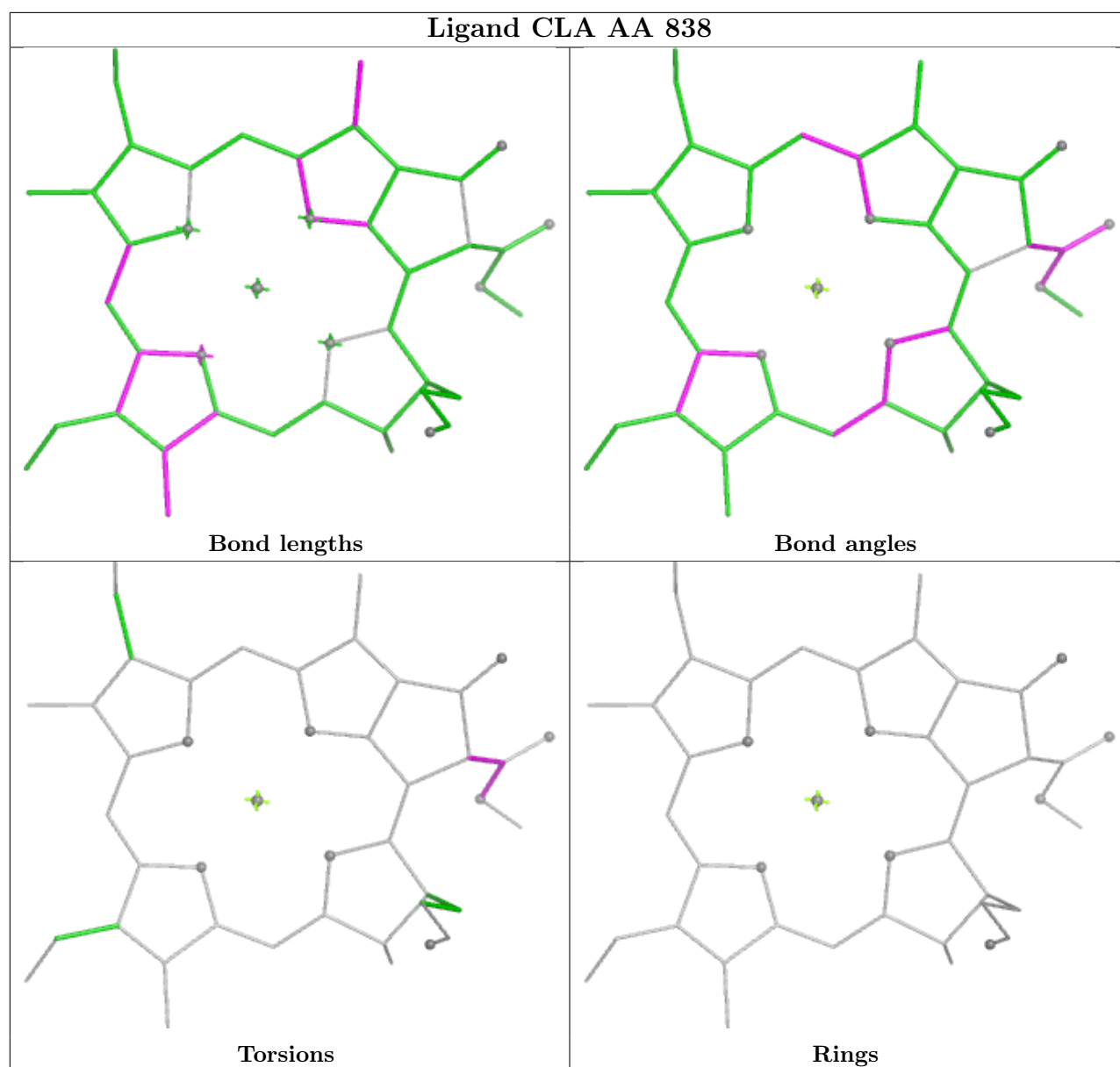
Torsions

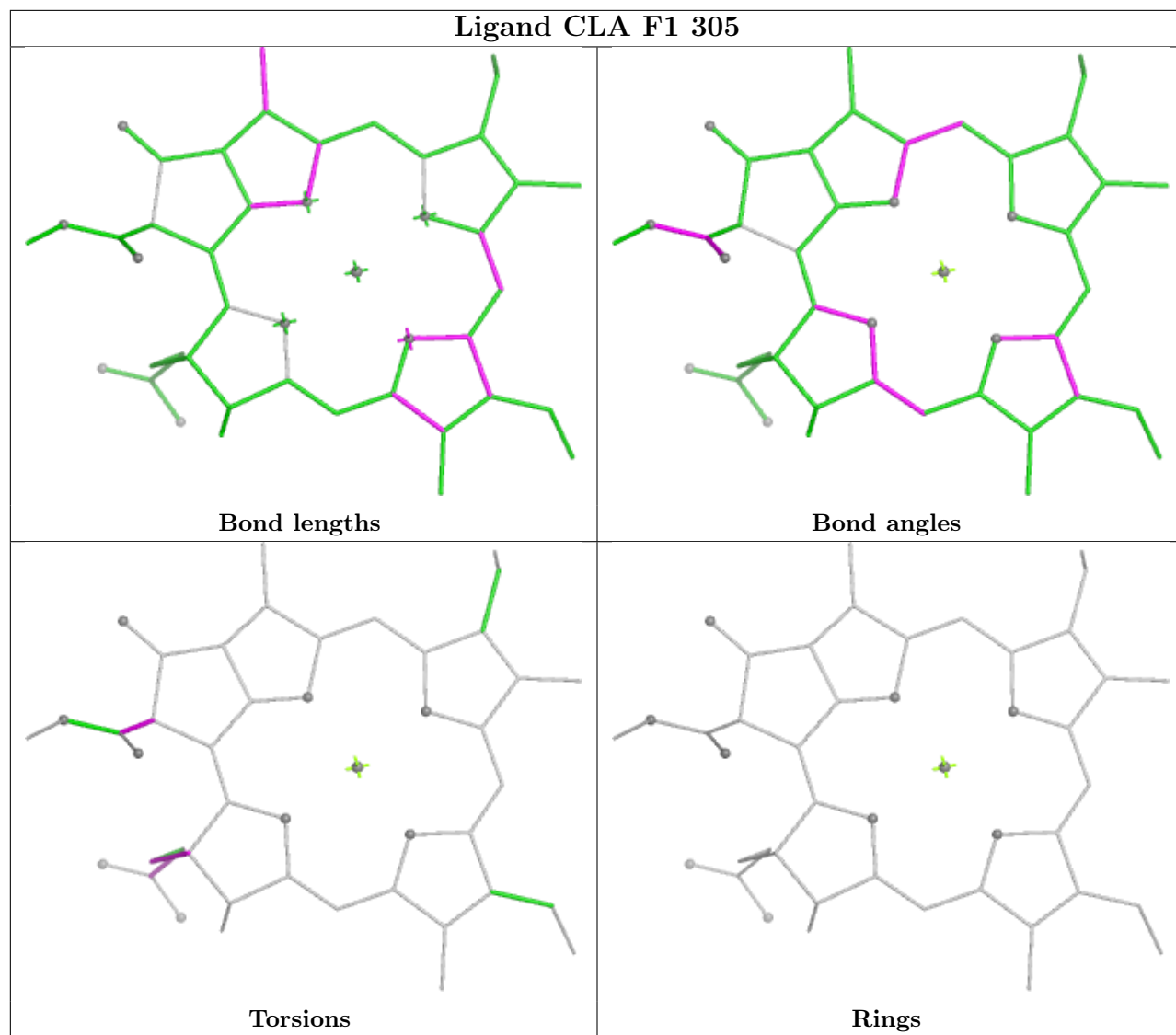


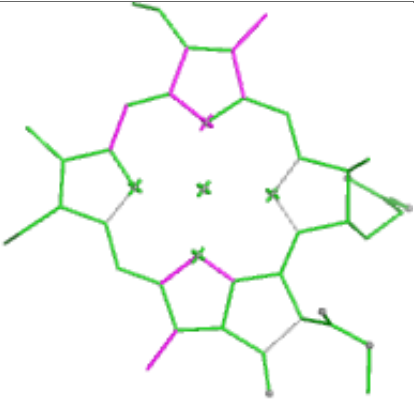
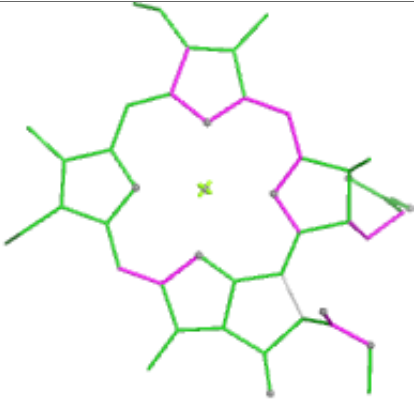
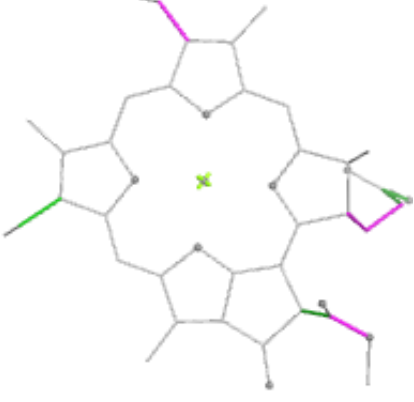
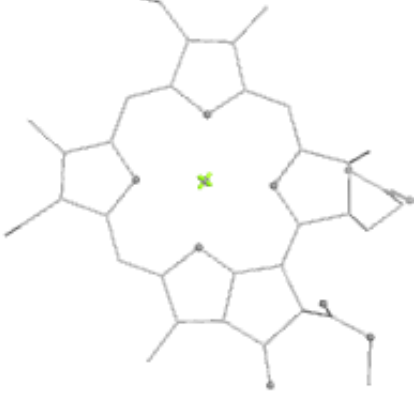
Rings



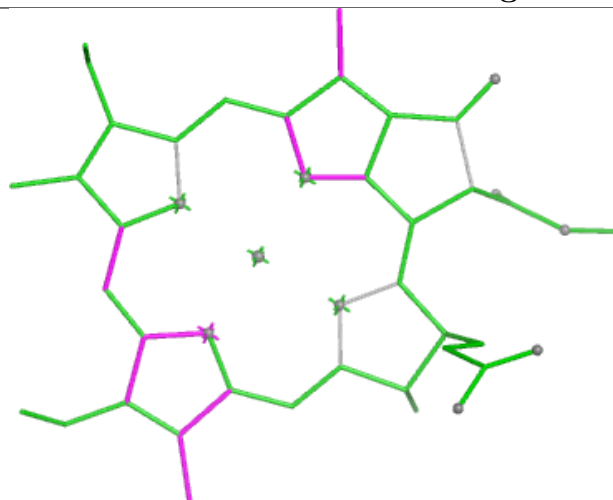




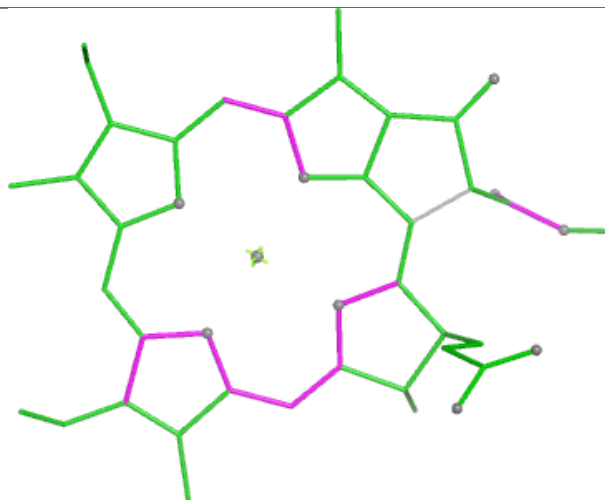


Ligand CLA A1 811	
 ✖	 ✖
Bond lengths	Bond angles
 ✖	 ✖
Torsions	Rings

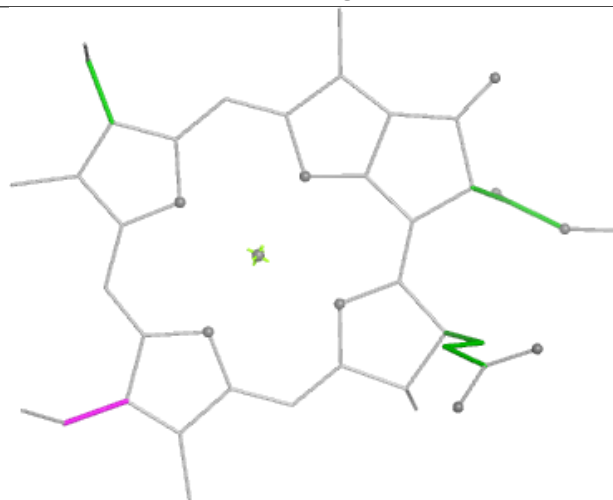
Ligand CLA AA 837



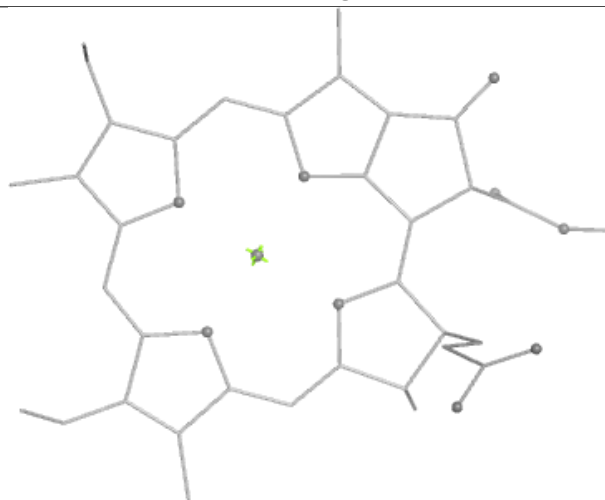
Bond lengths



Bond angles

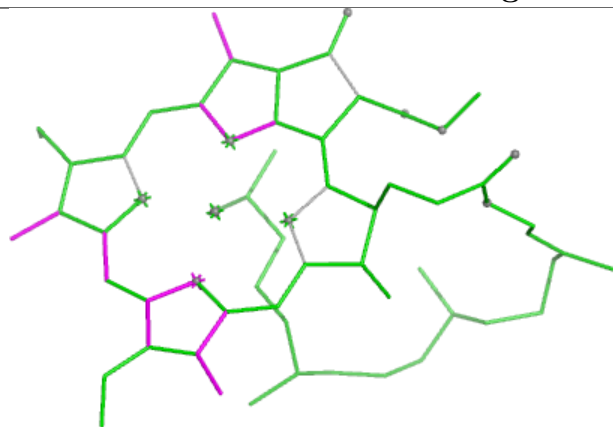


Torsions

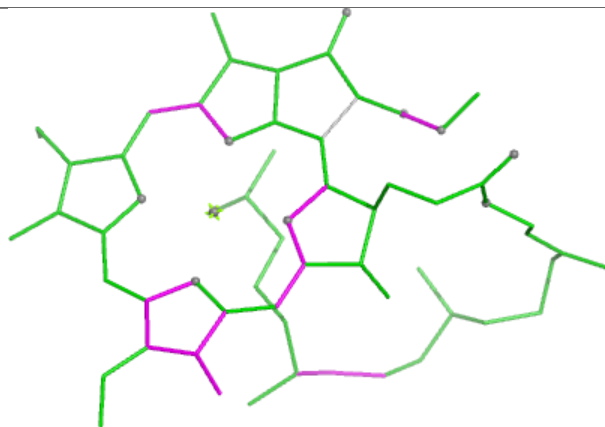


Rings

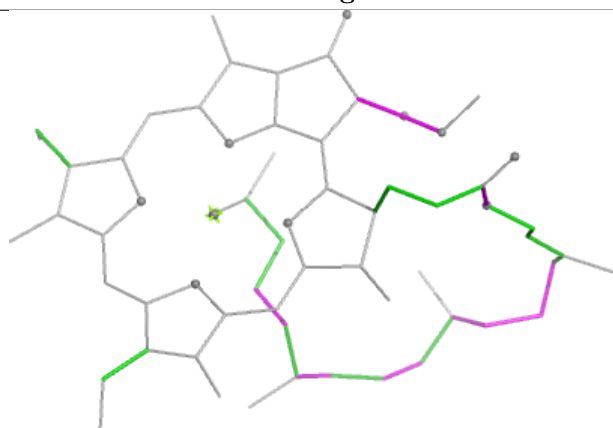
Ligand CLA BB 803



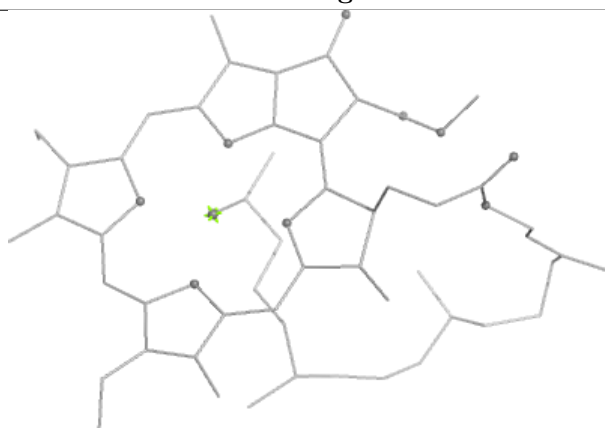
Bond lengths



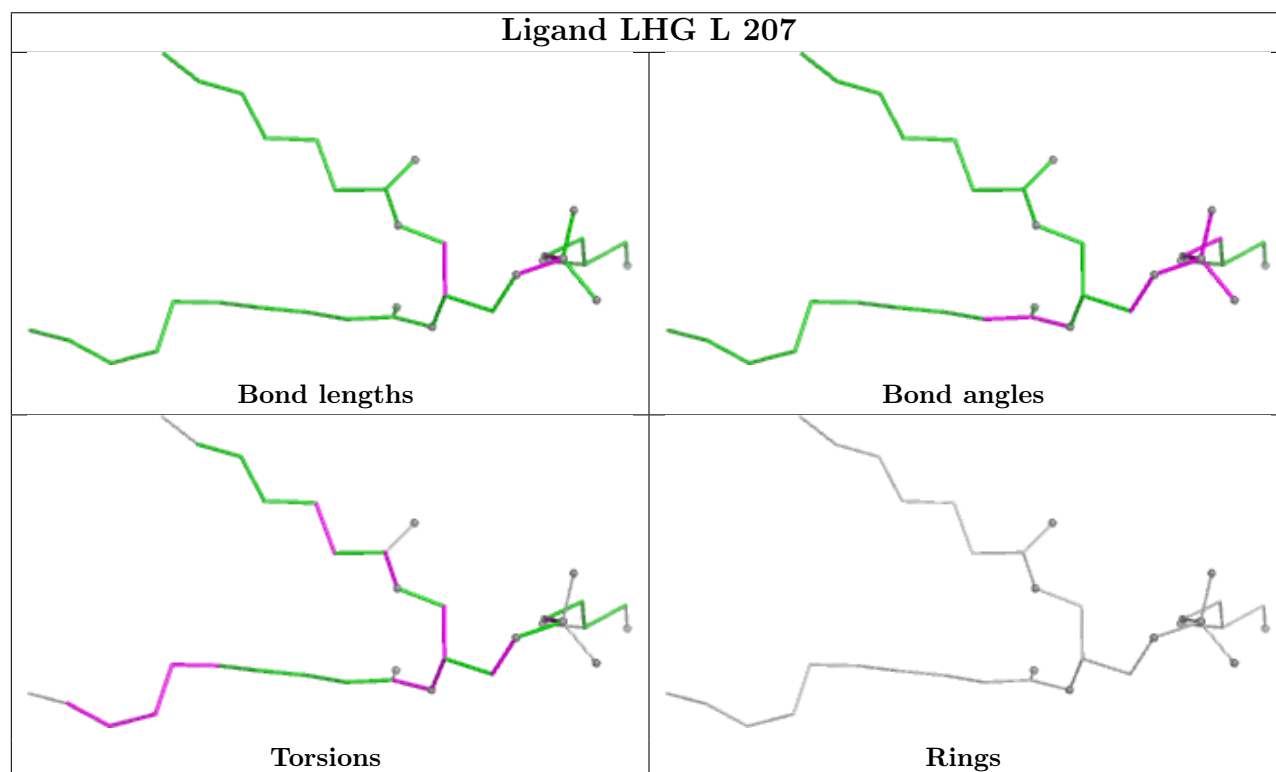
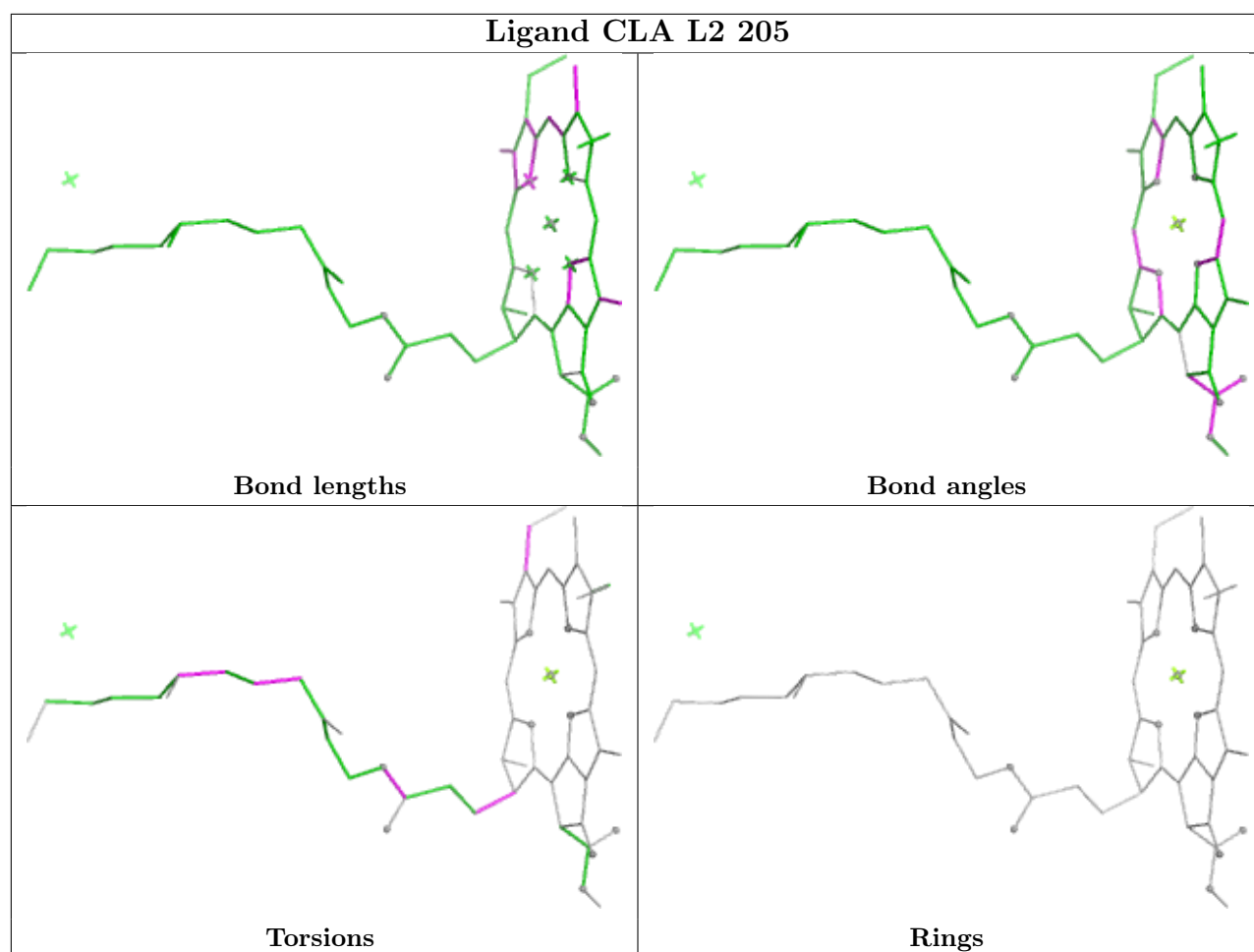
Bond angles

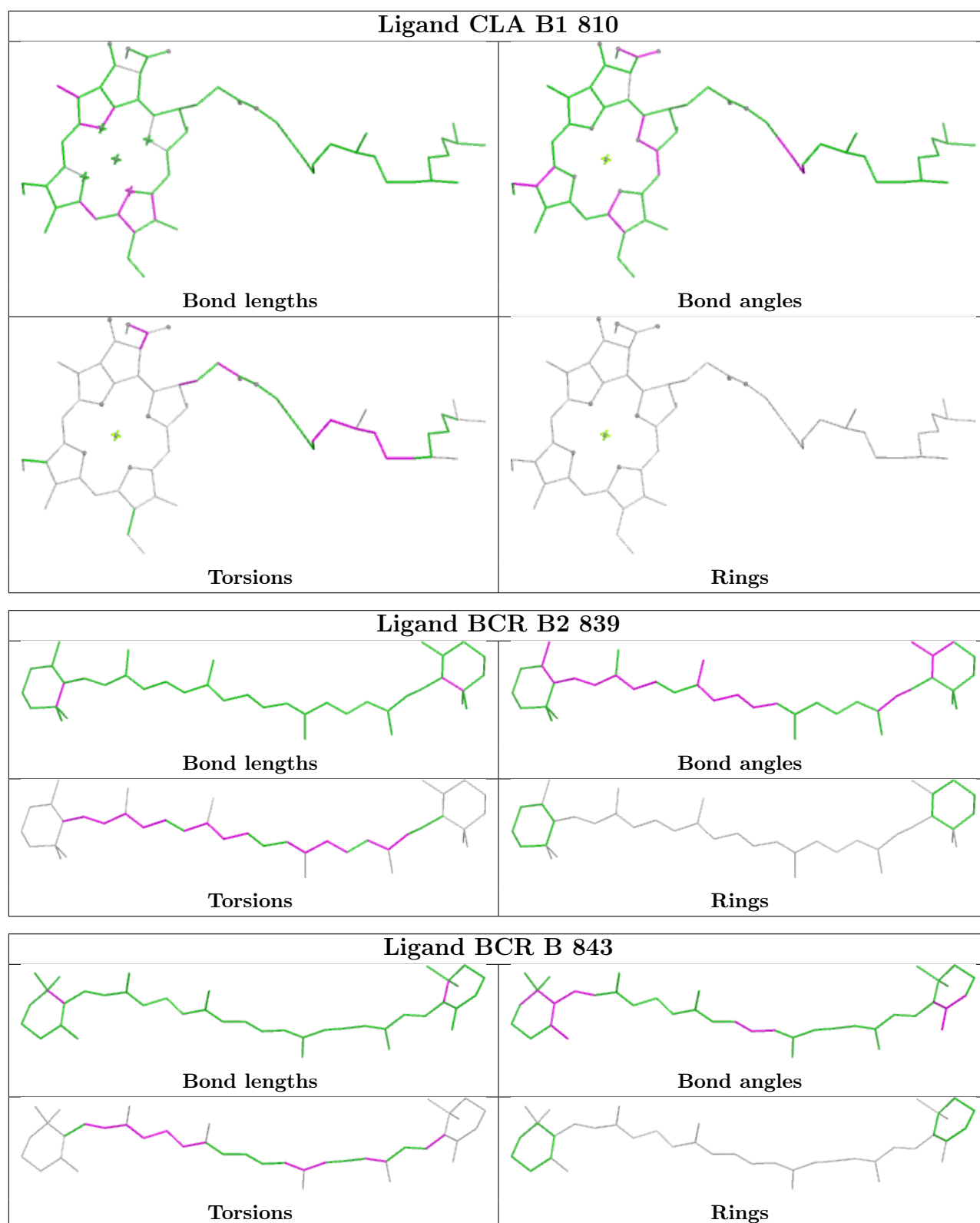


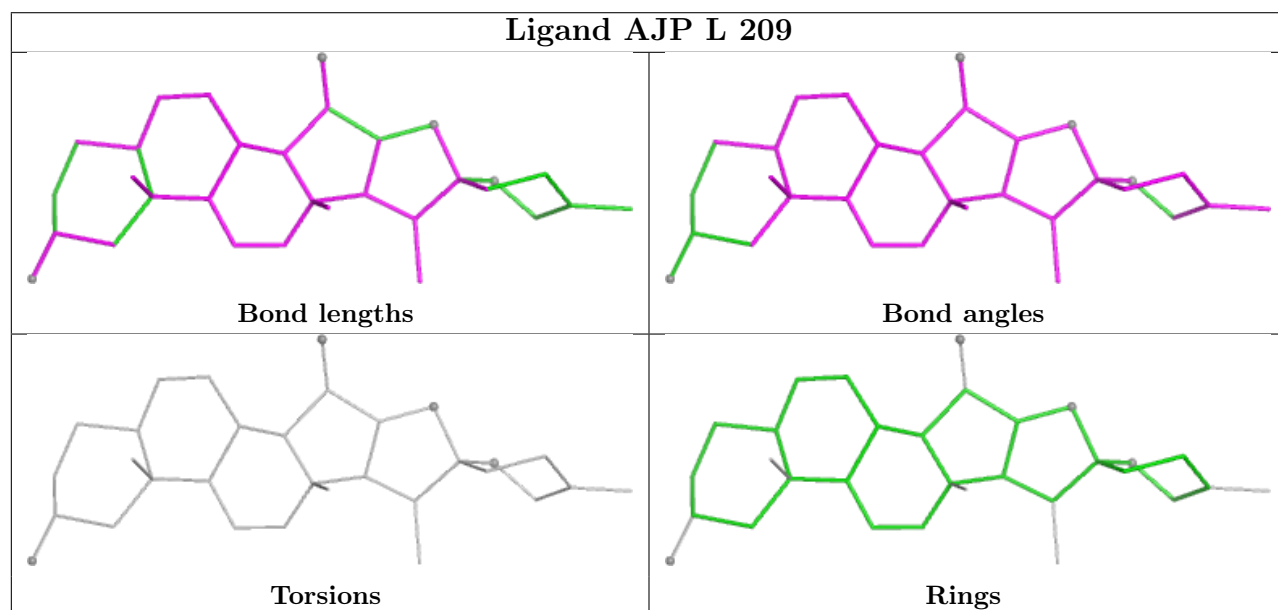
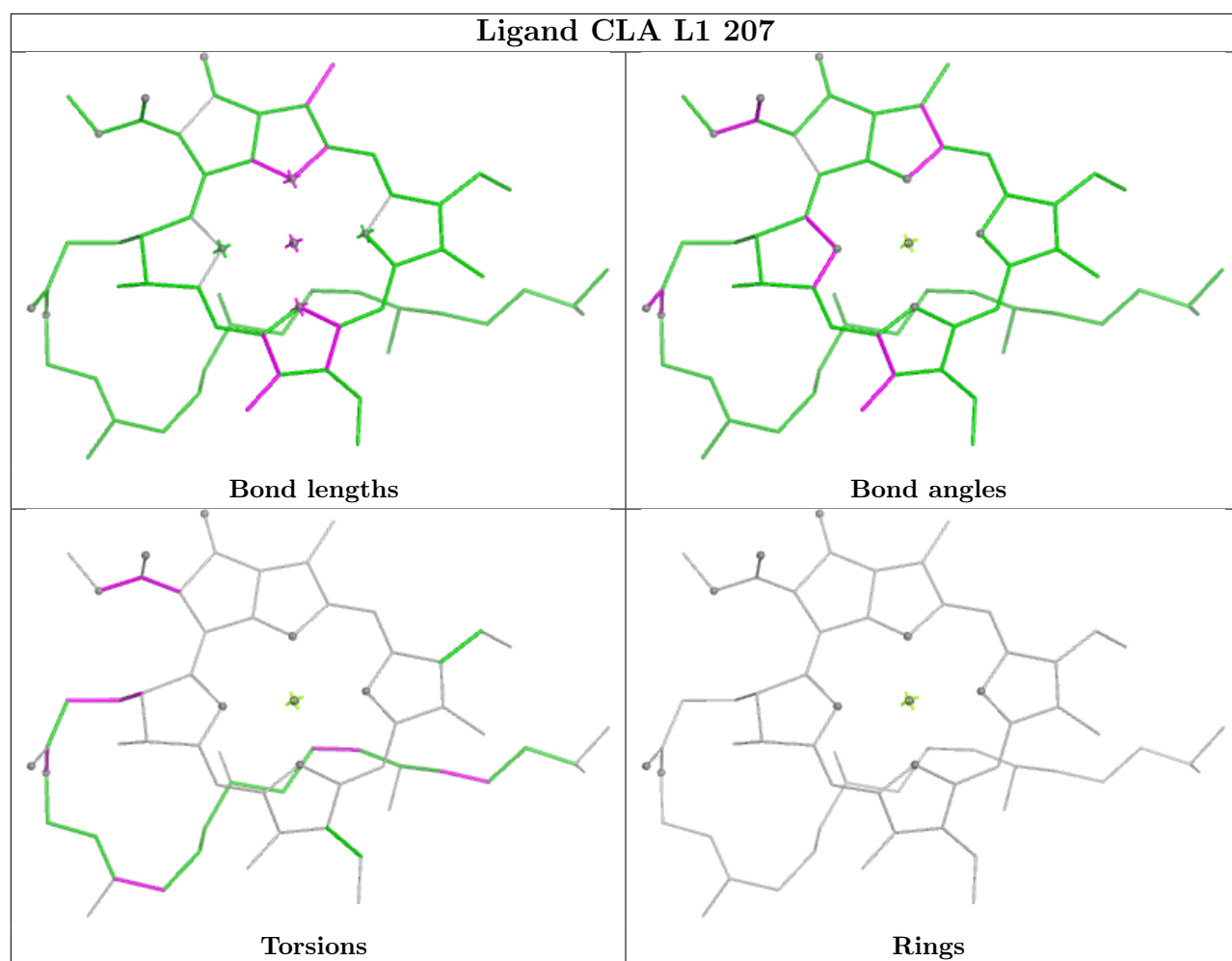
Torsions

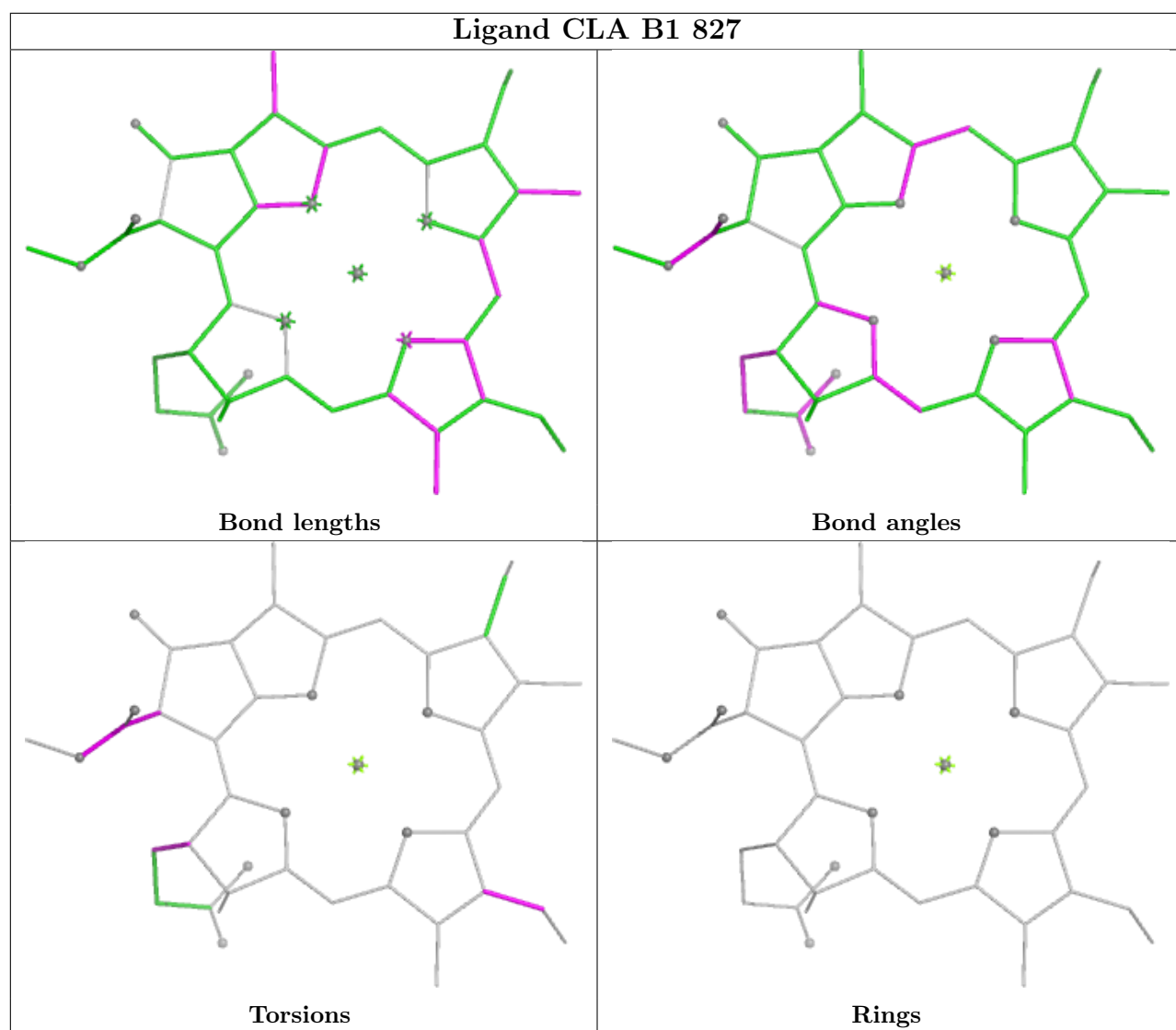


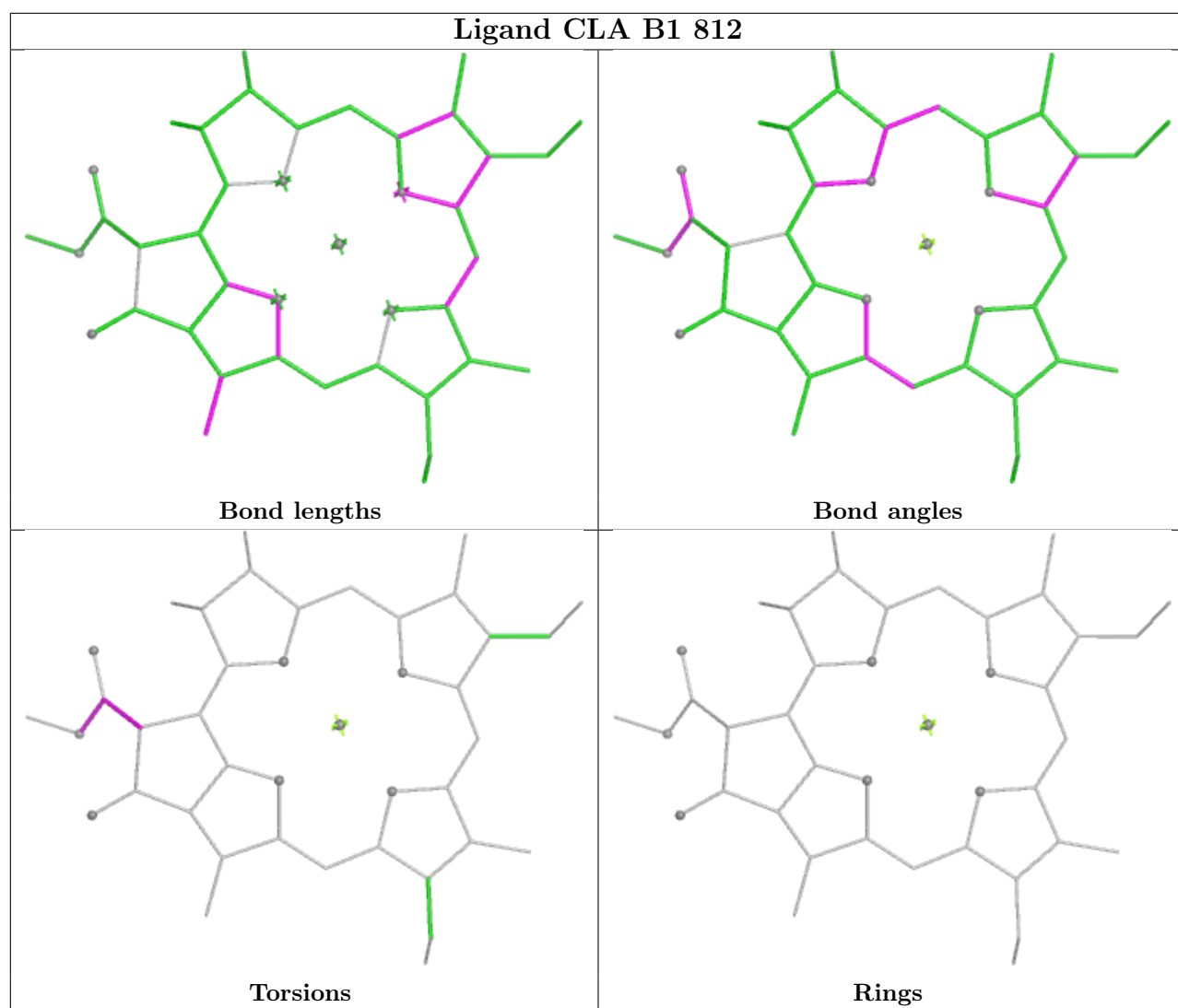
Rings

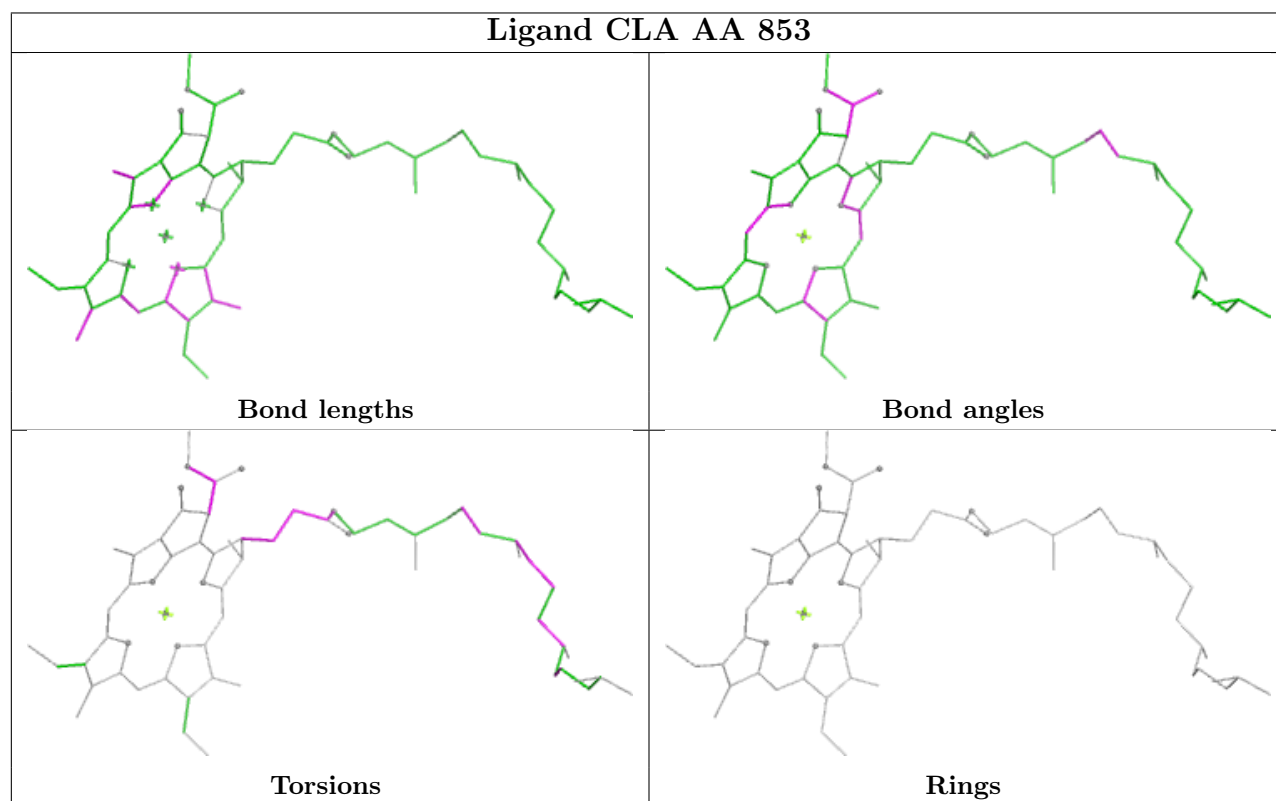
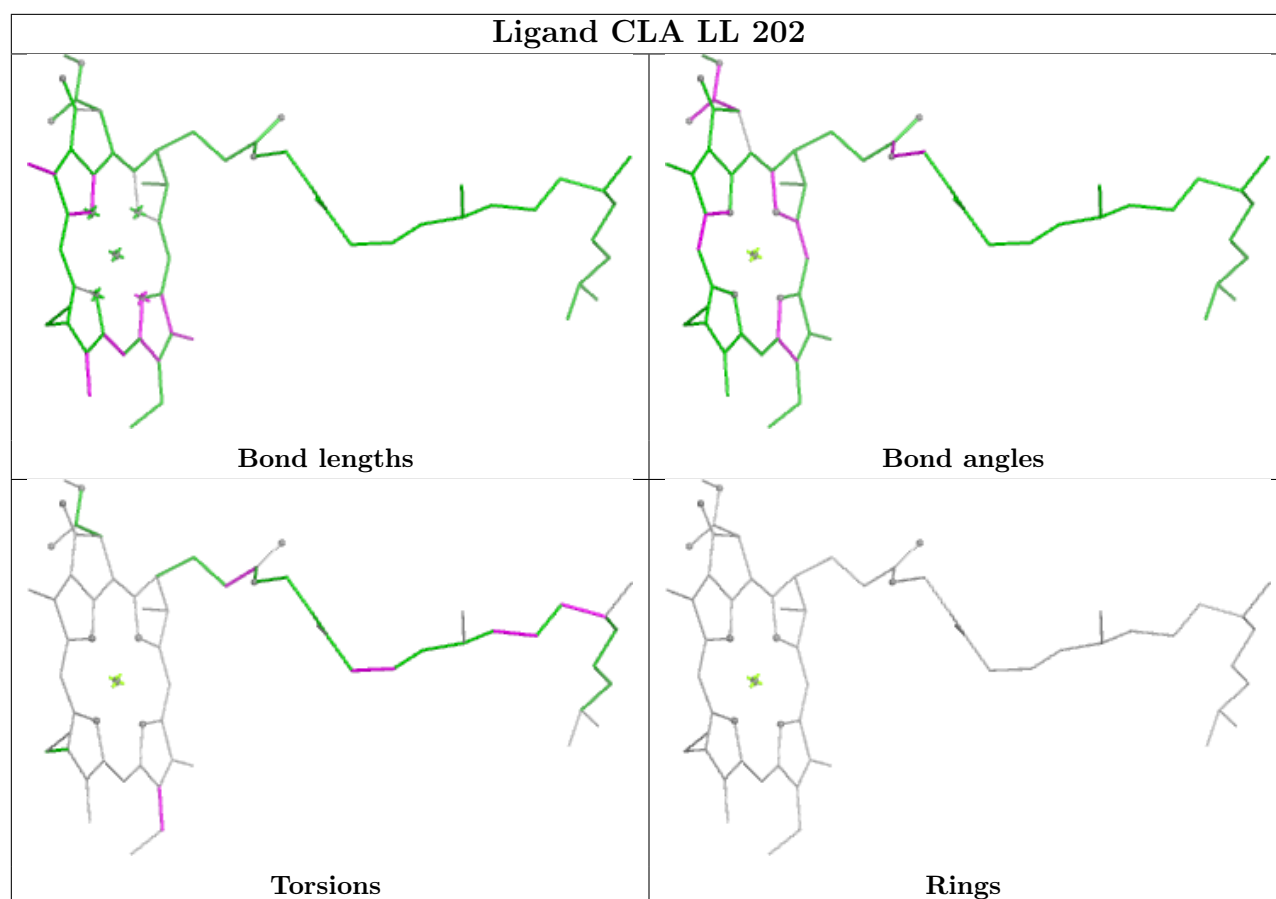


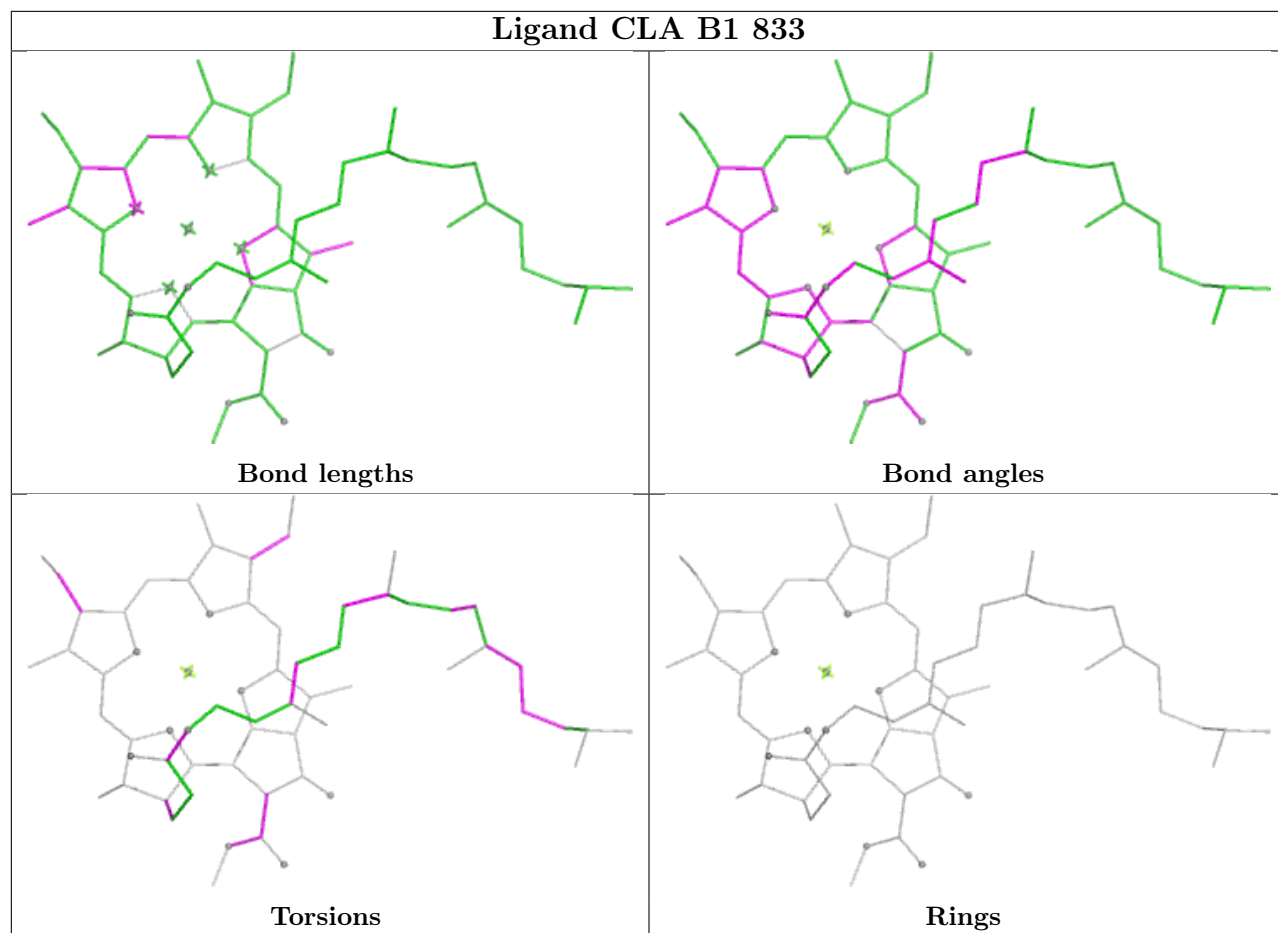


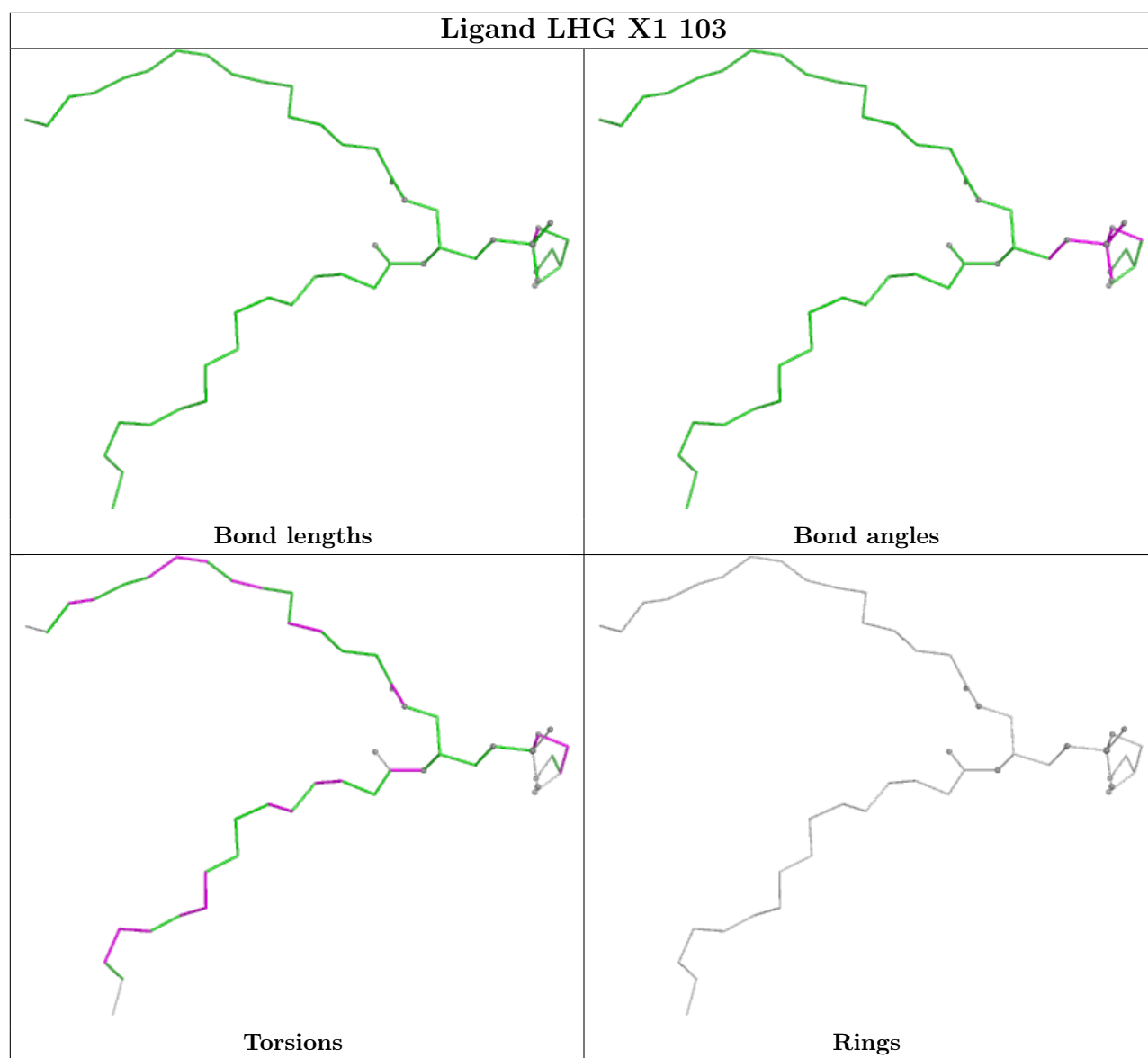


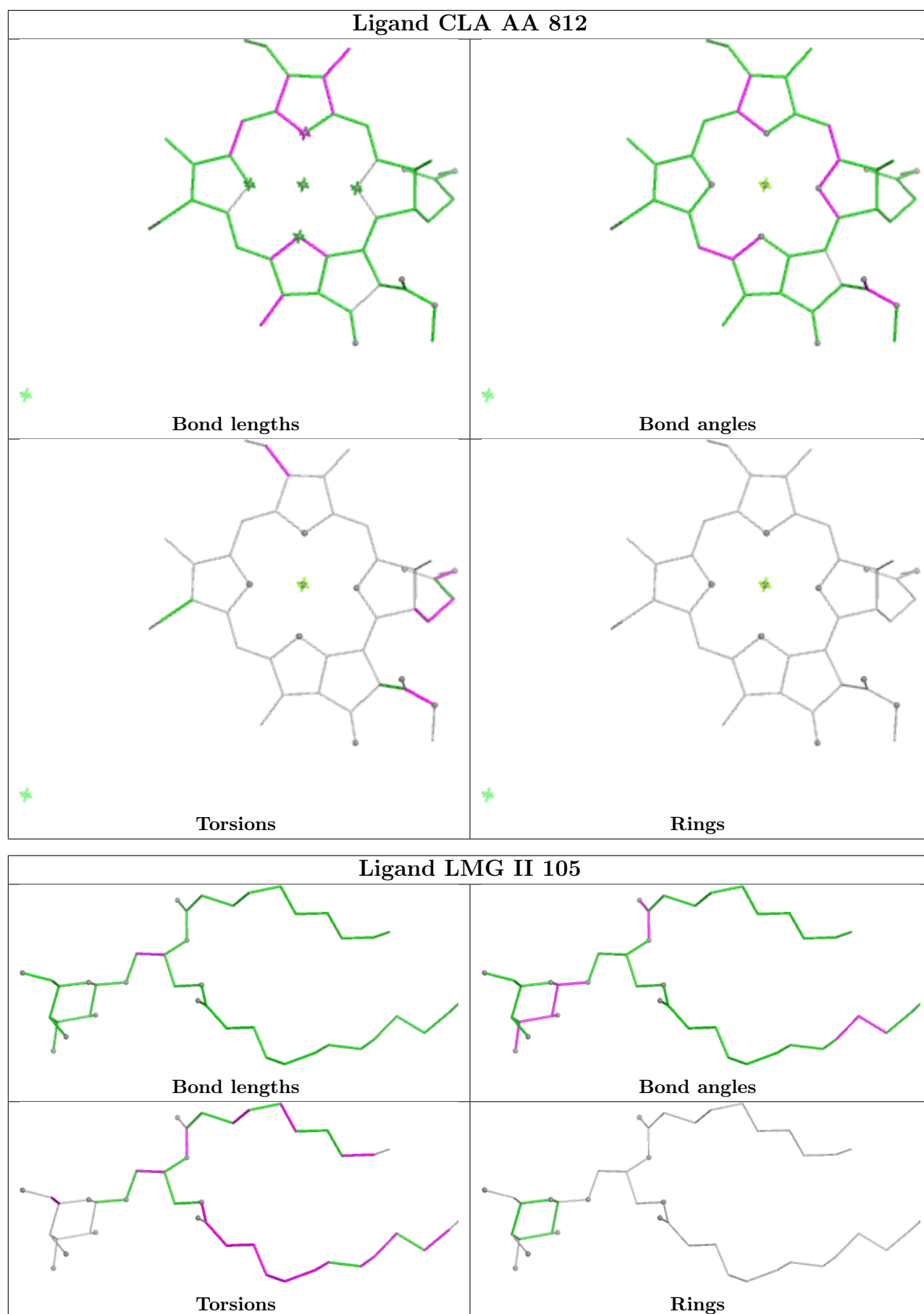


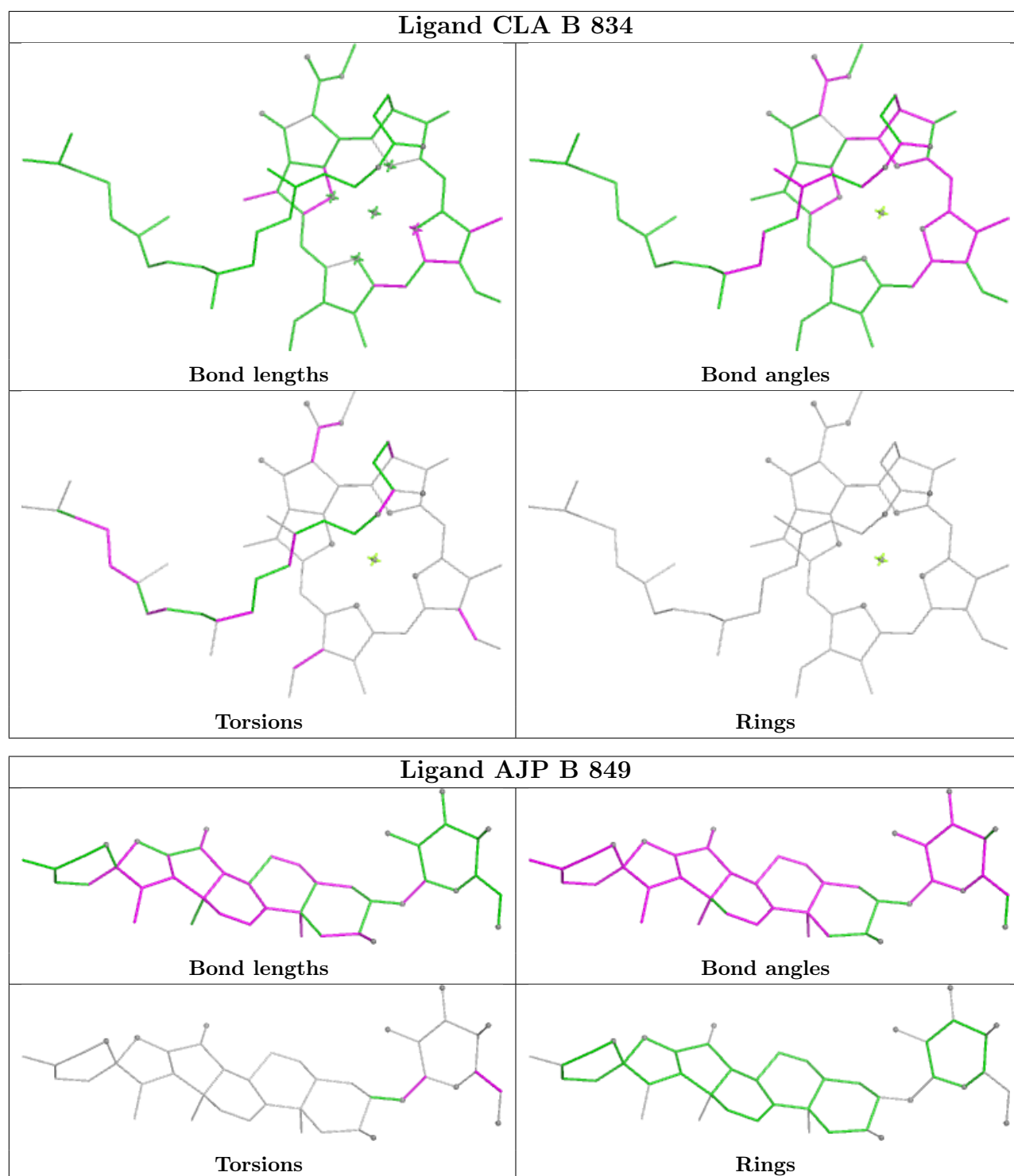




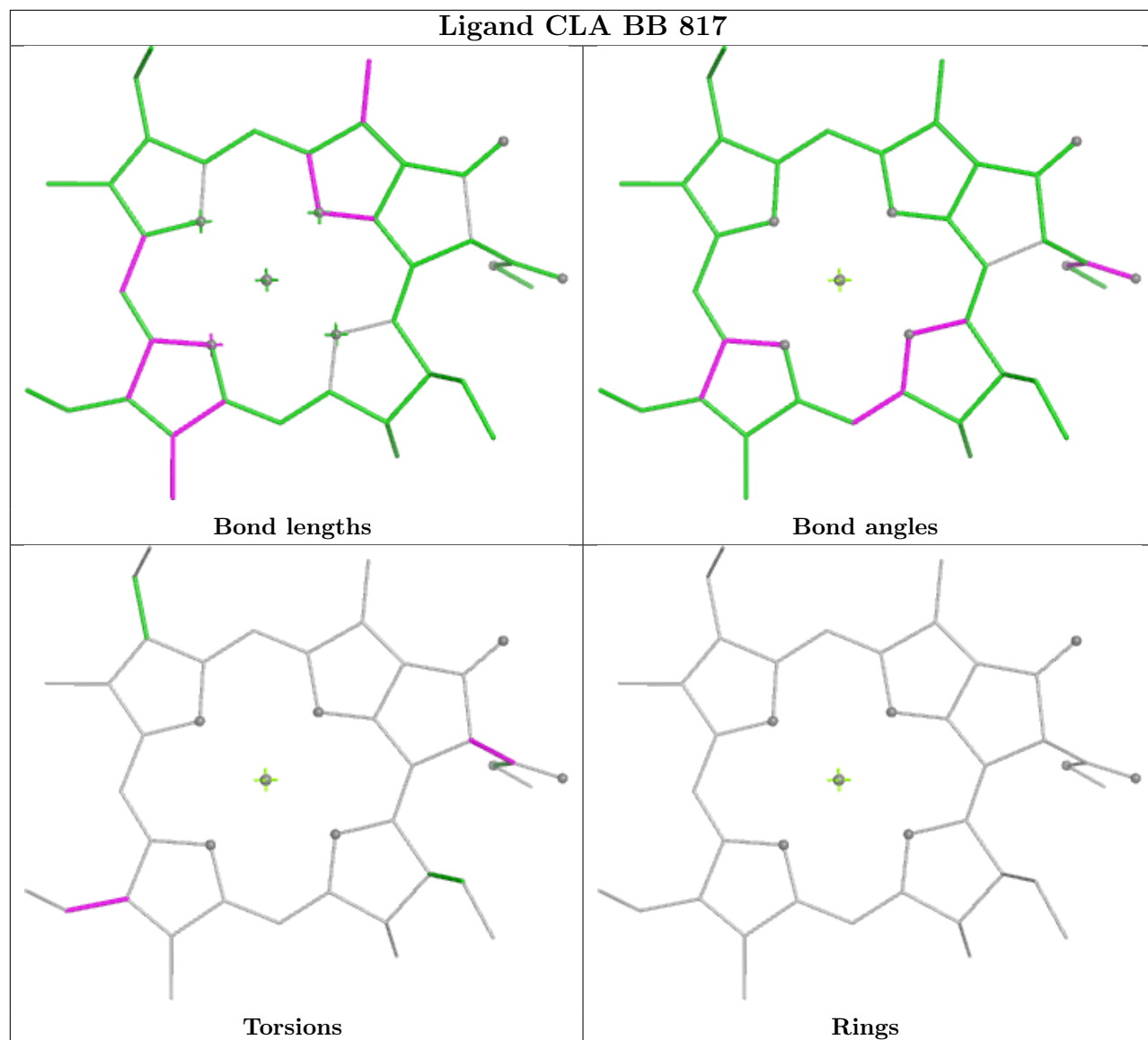


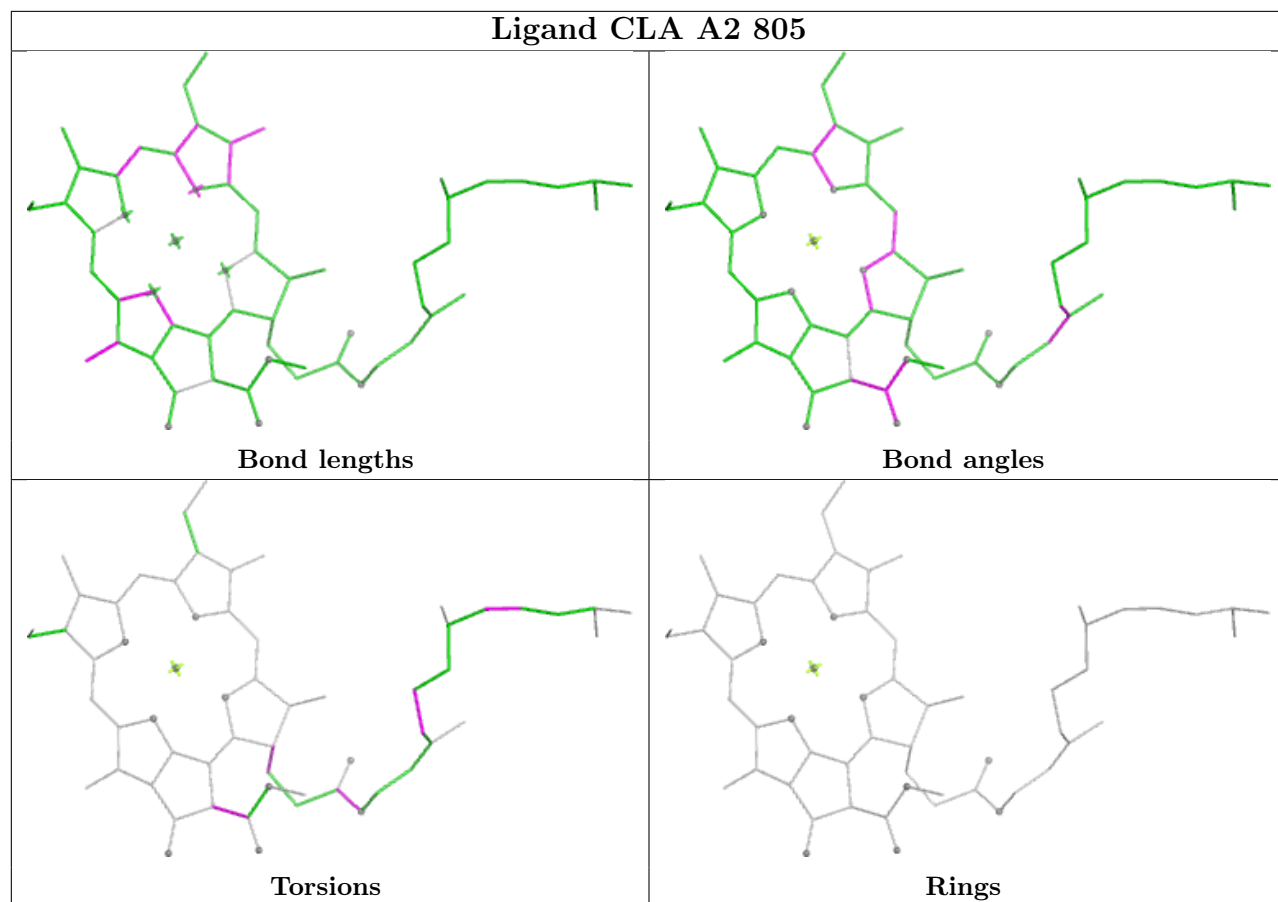


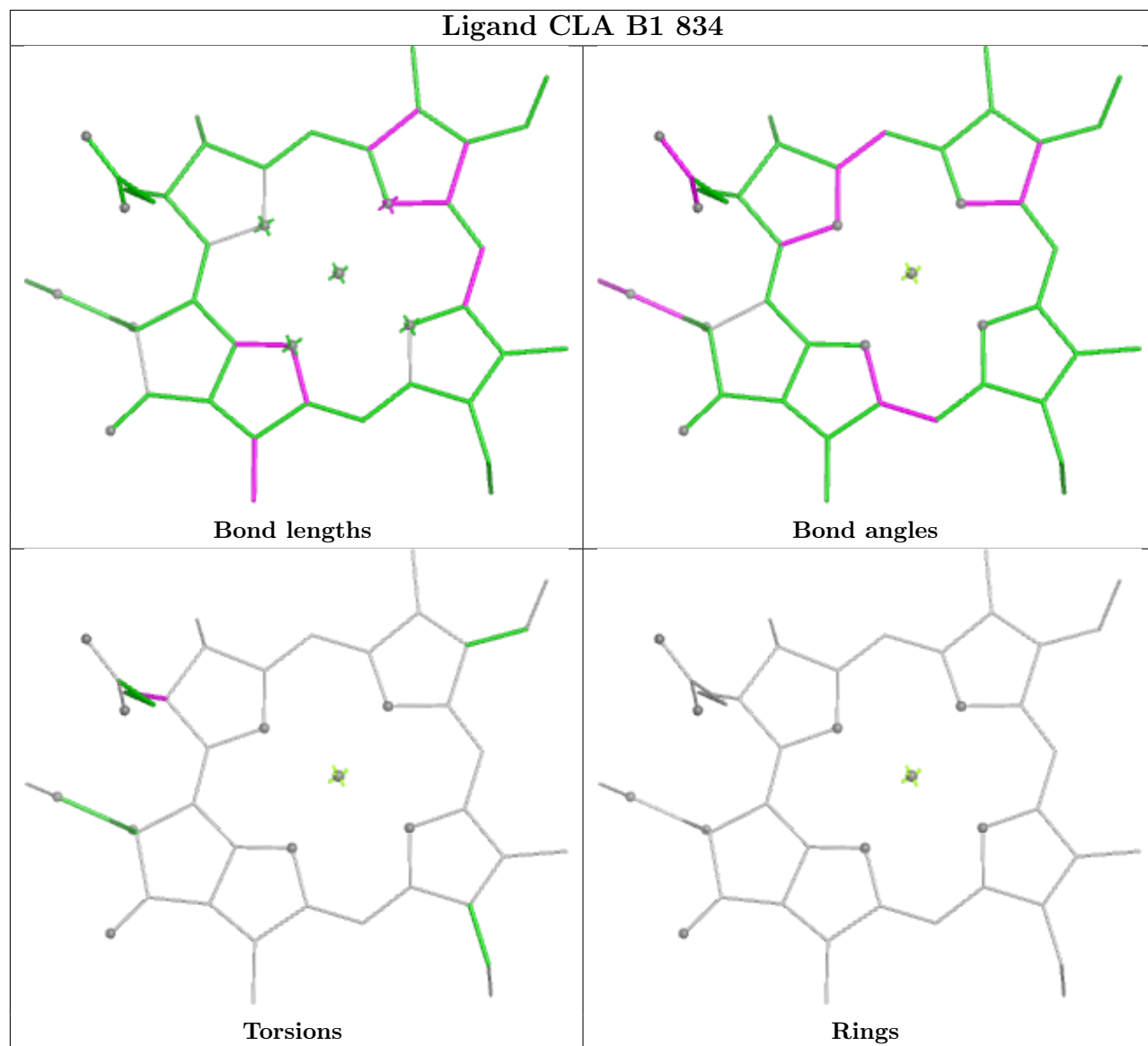




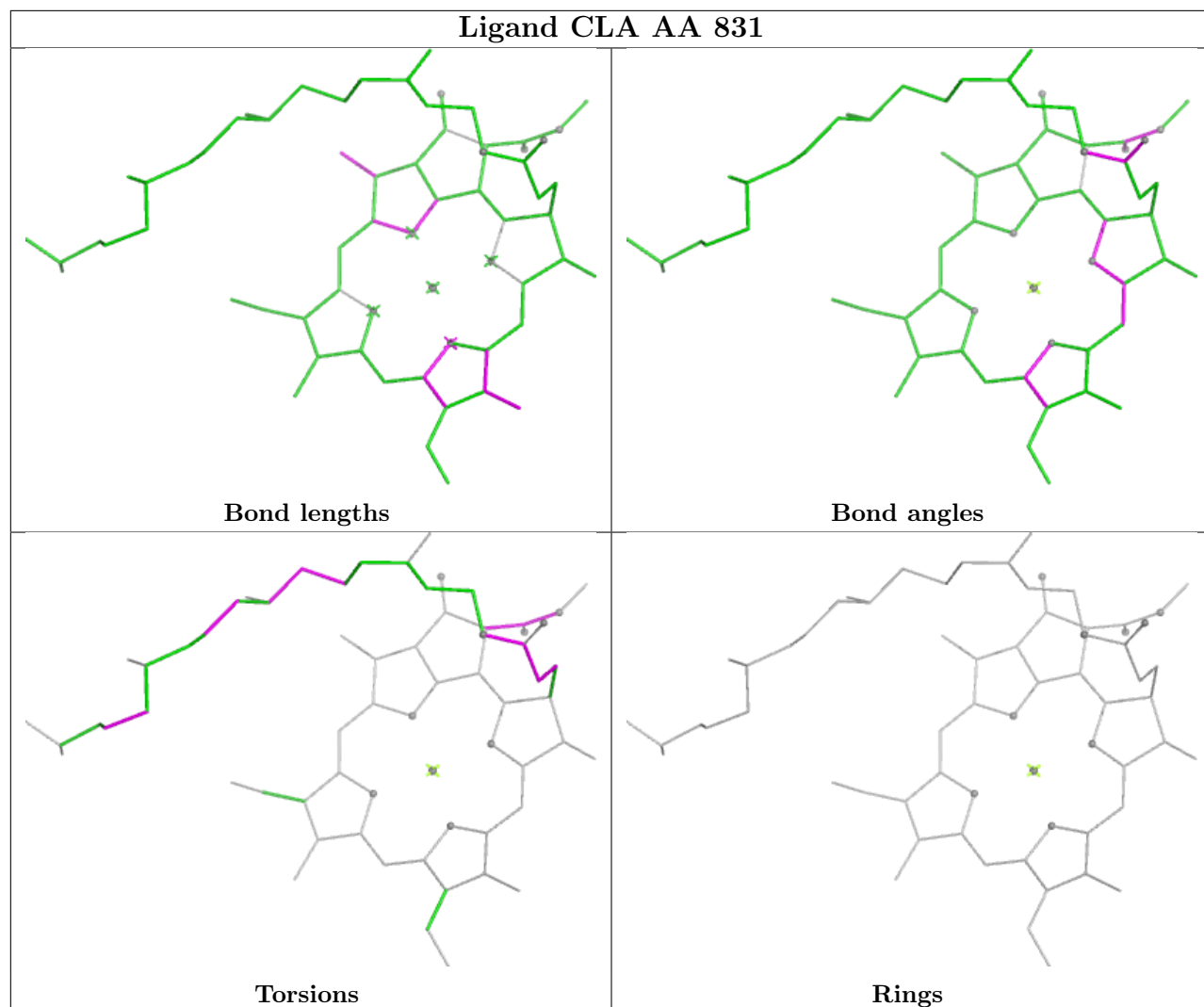
Ligand CLA BB 817

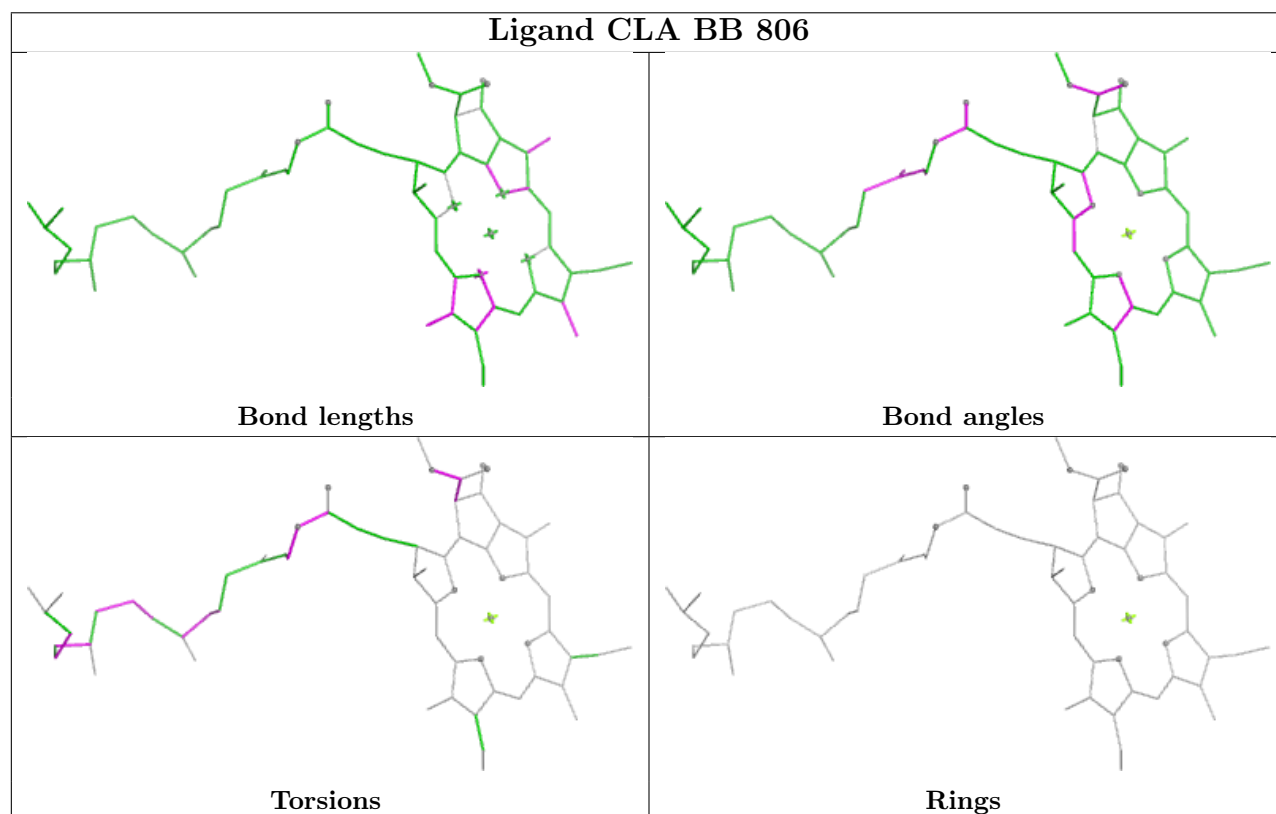
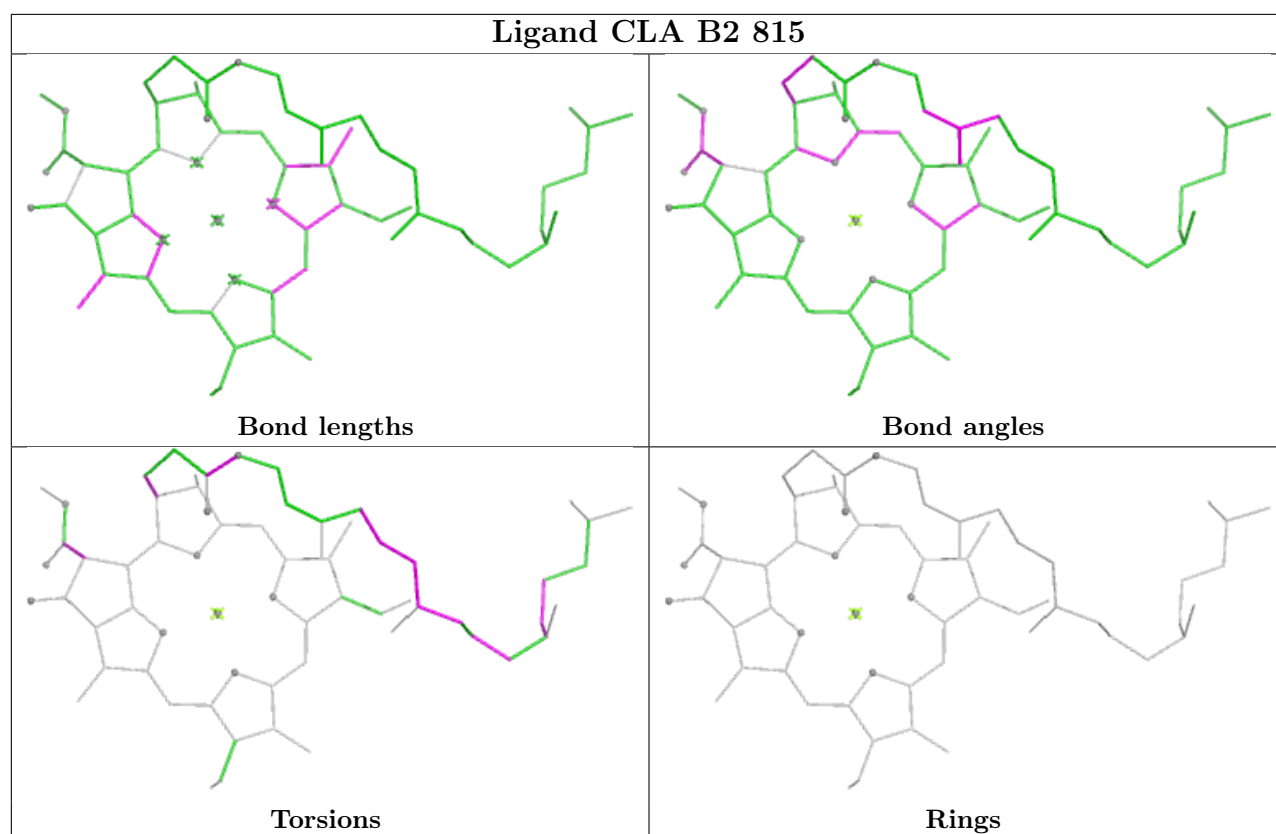




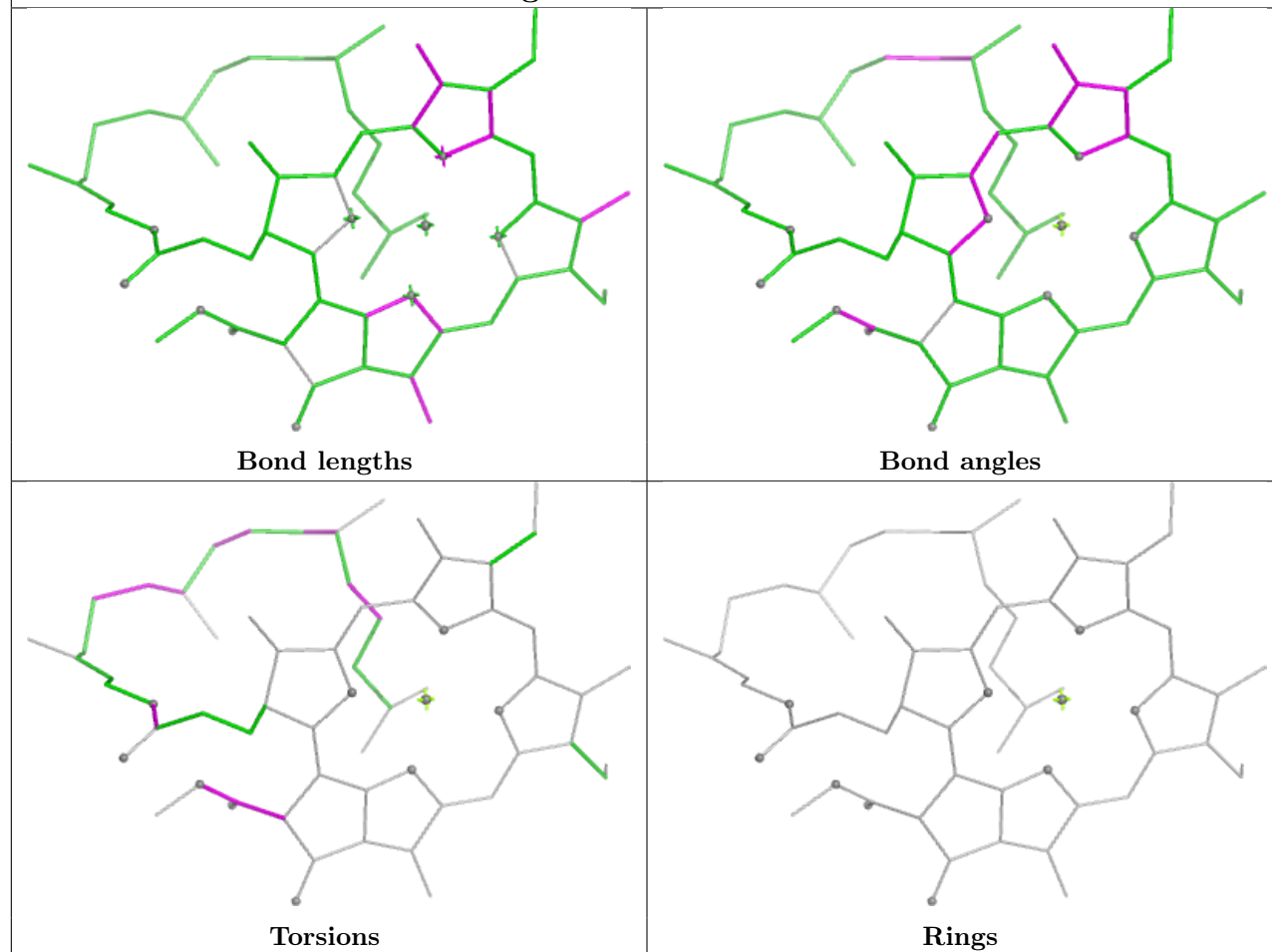


Ligand CLA AA 831

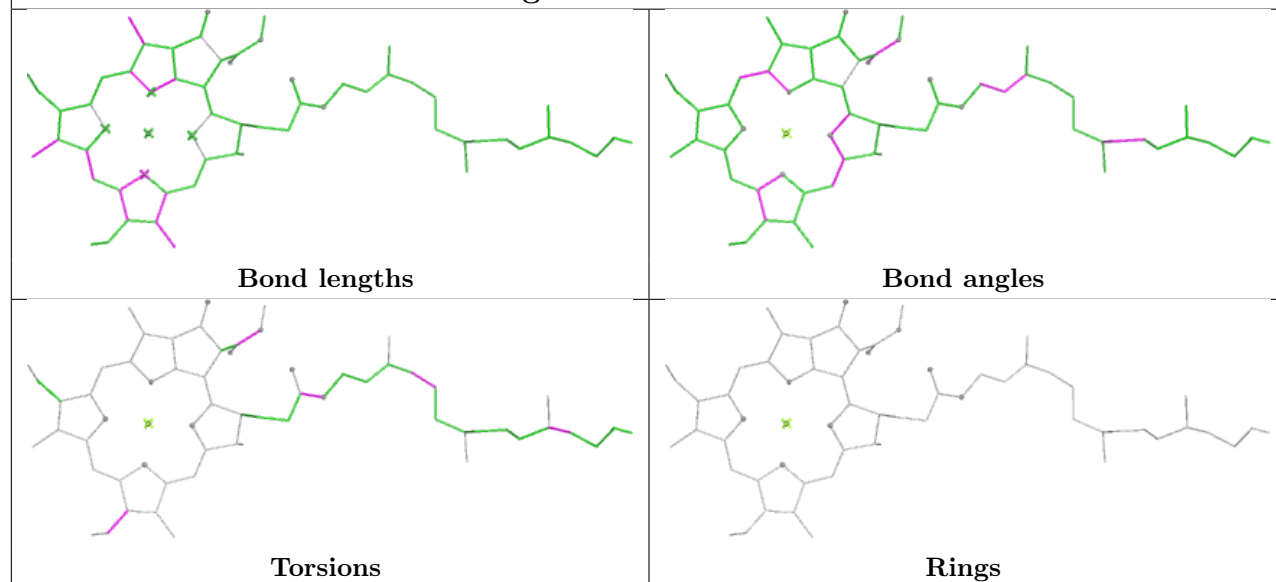




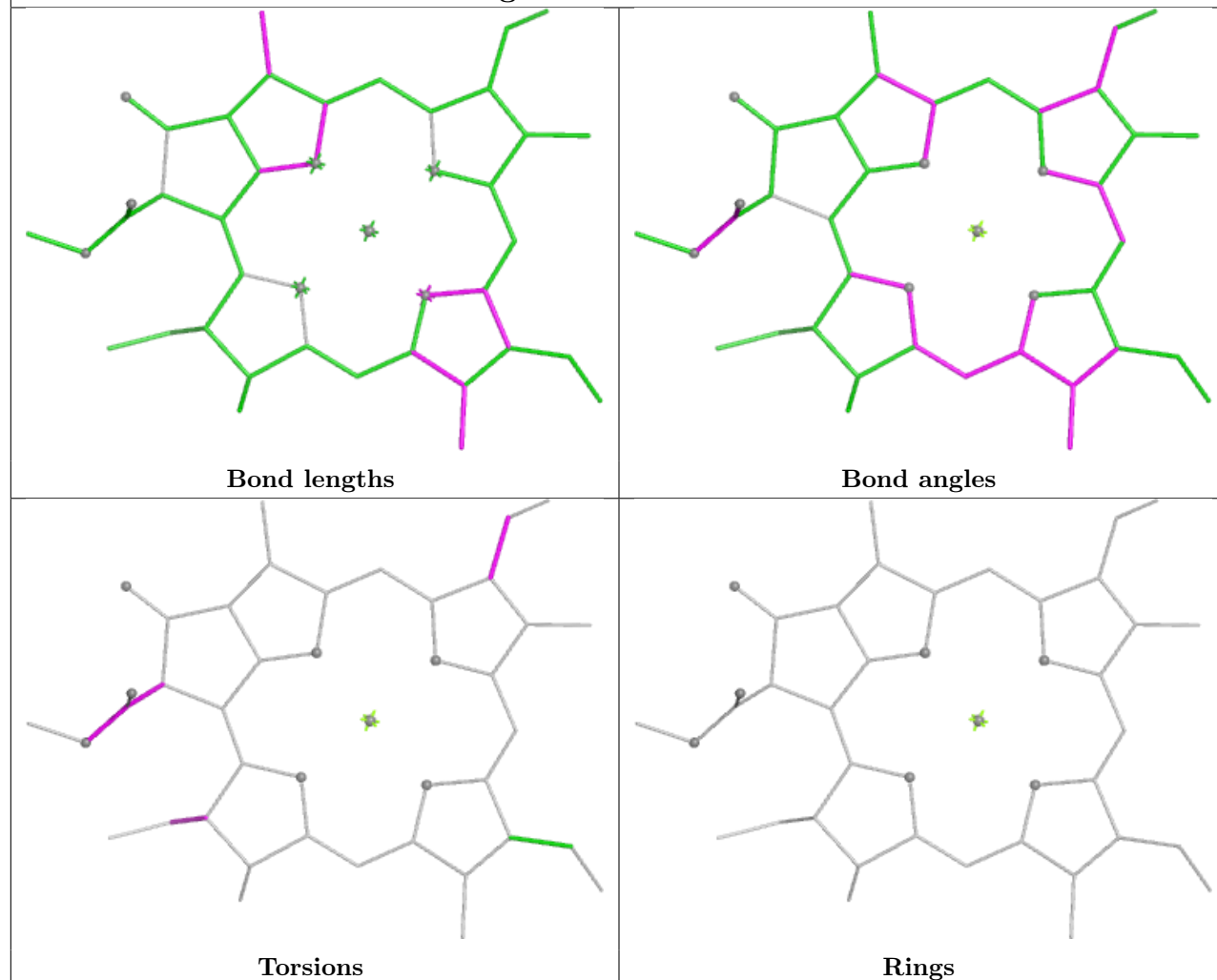
Ligand CLA B2 803



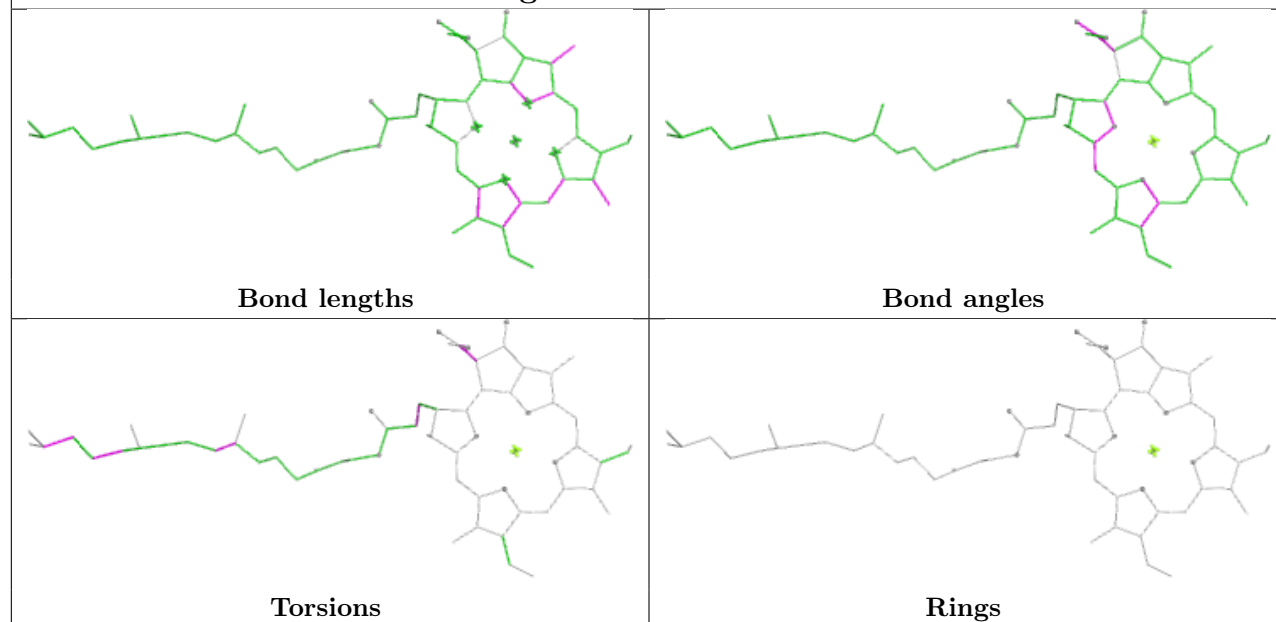
Ligand CLA A2 835



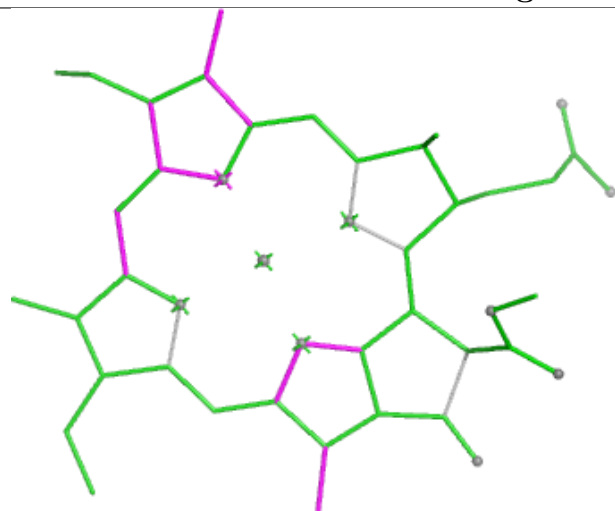
Ligand CLA LL 203



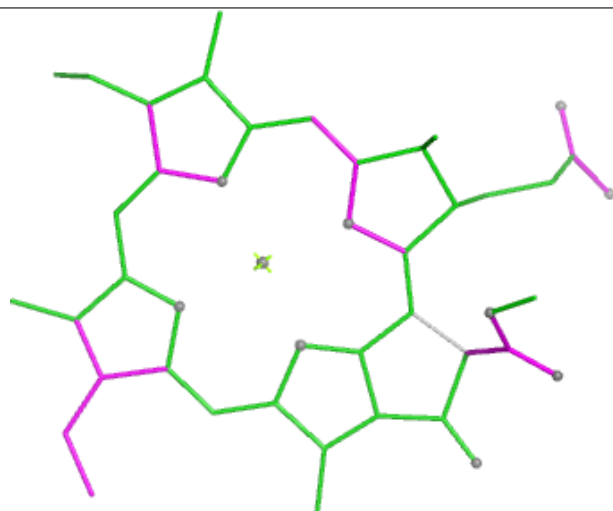
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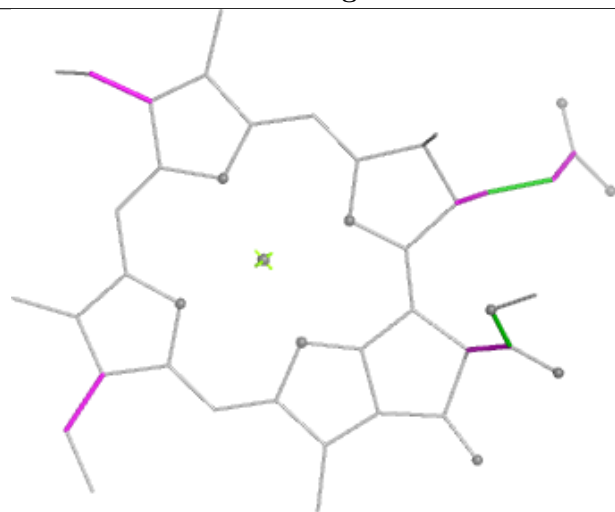
Ligand CLA B 820



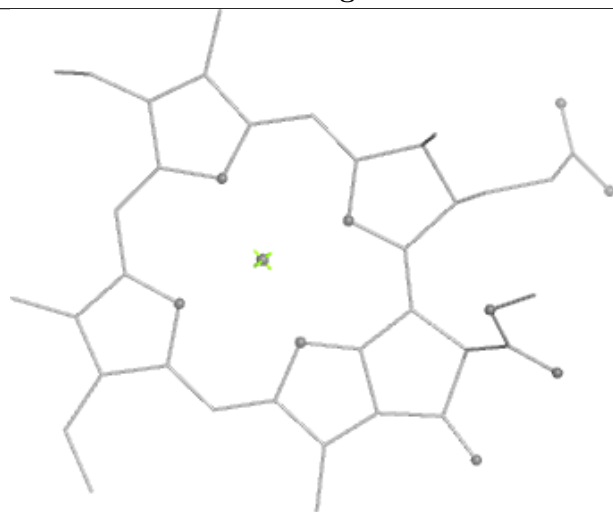
Bond lengths



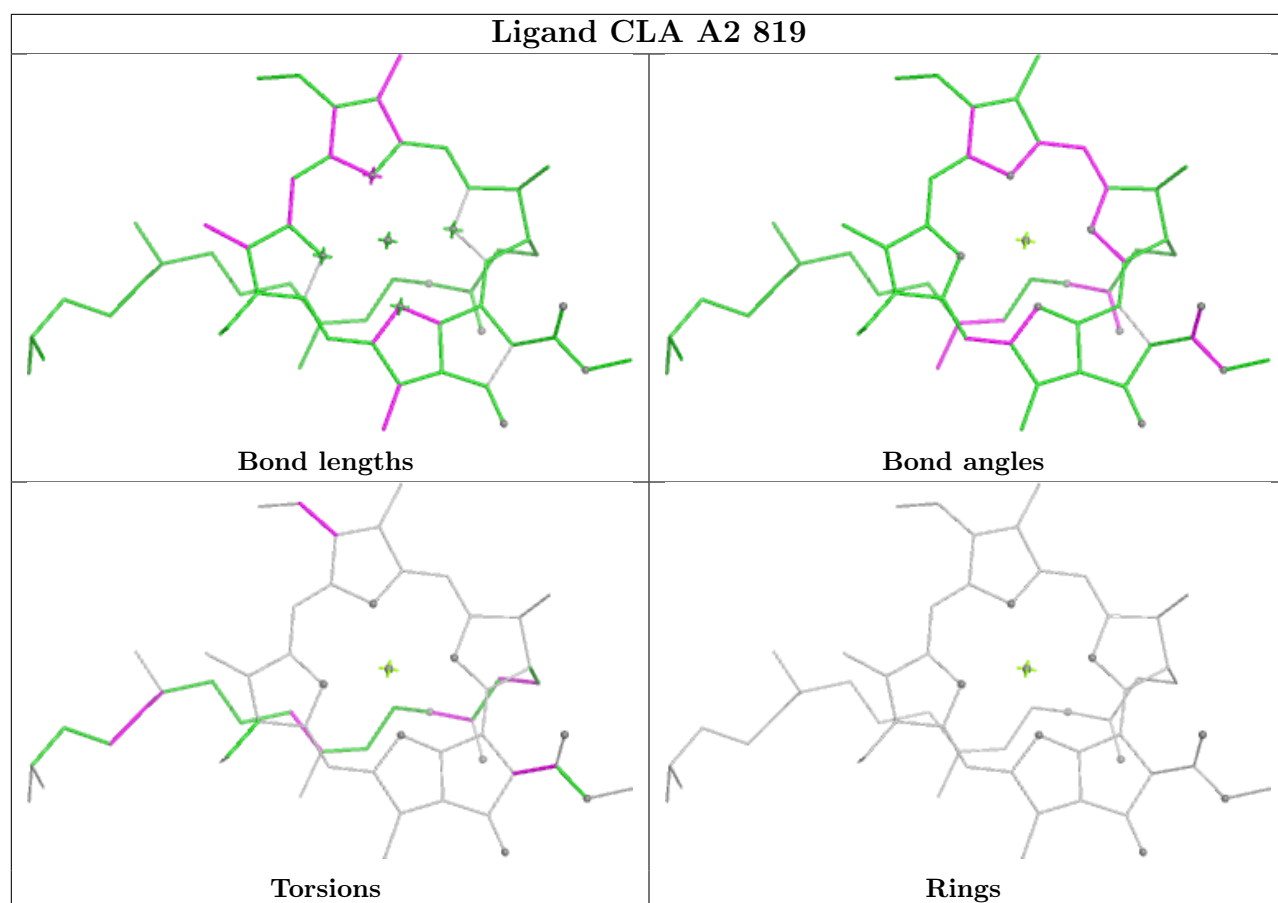
Bond angles



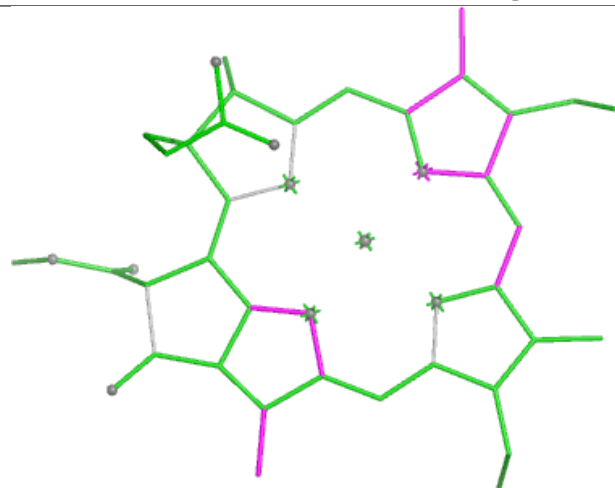
Torsions



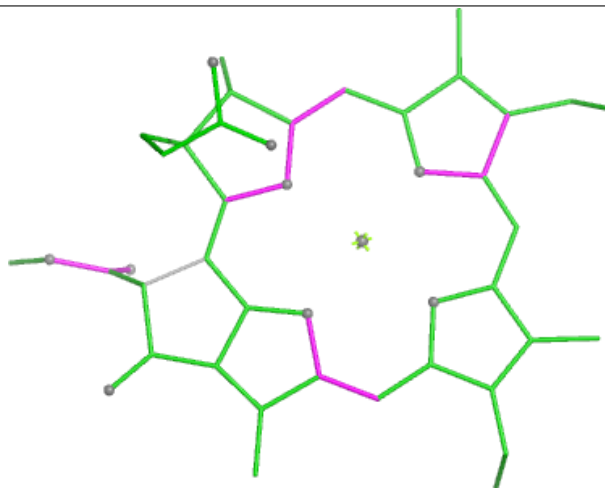
Rings



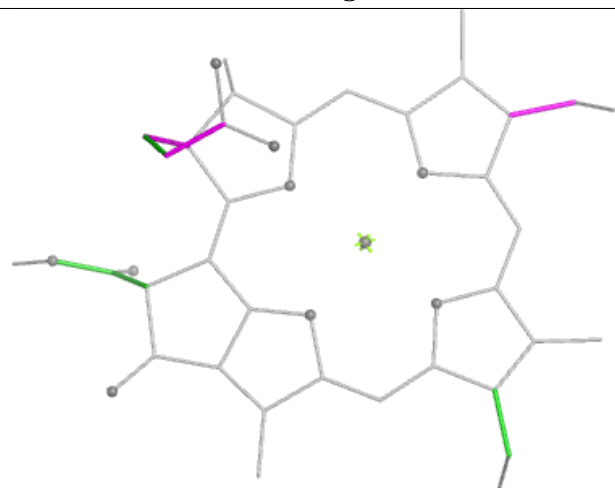
Ligand CLA A1 817



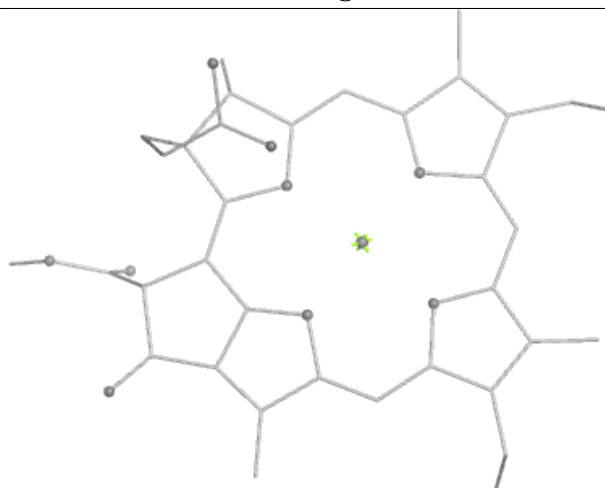
Bond lengths



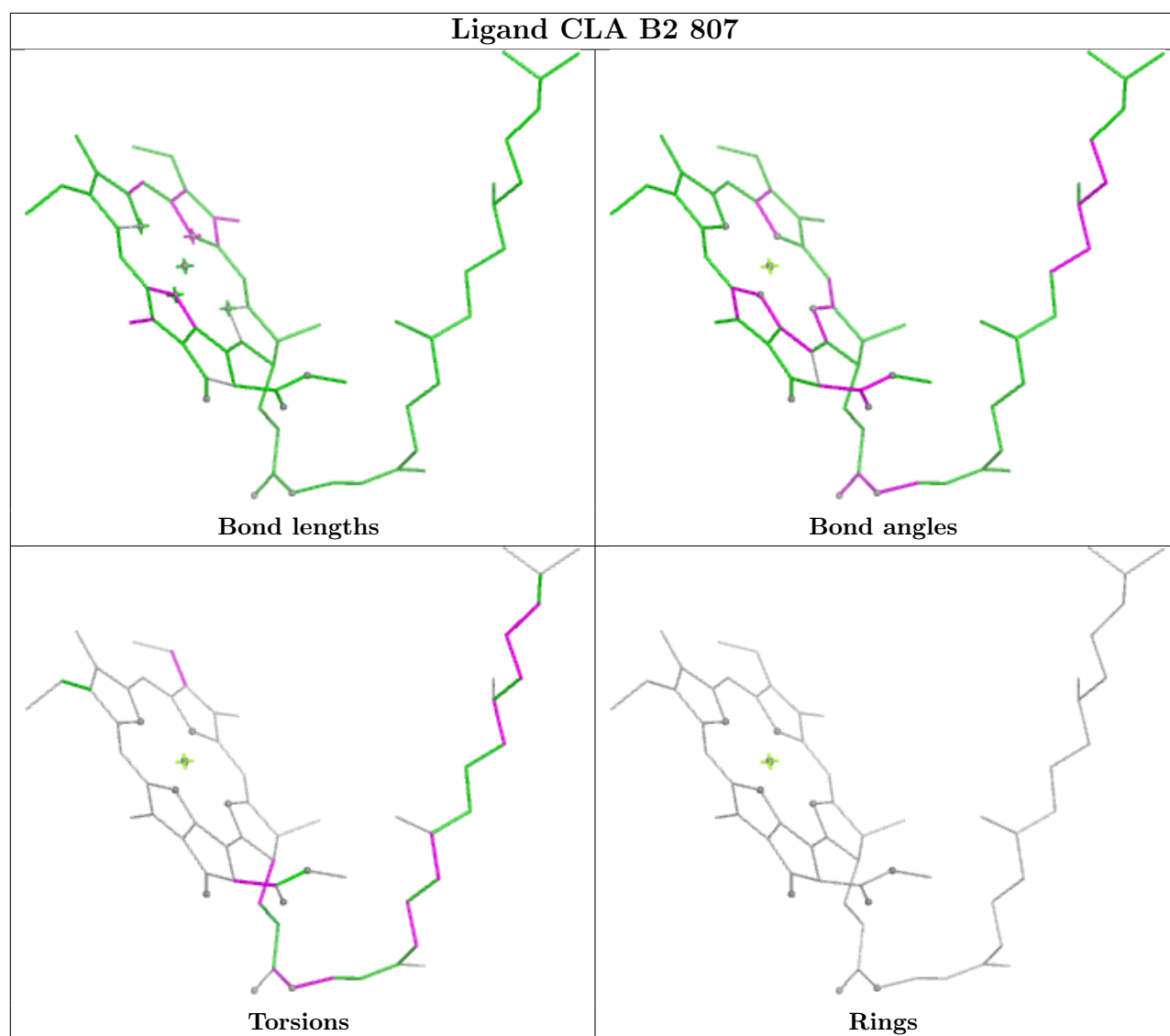
Bond angles



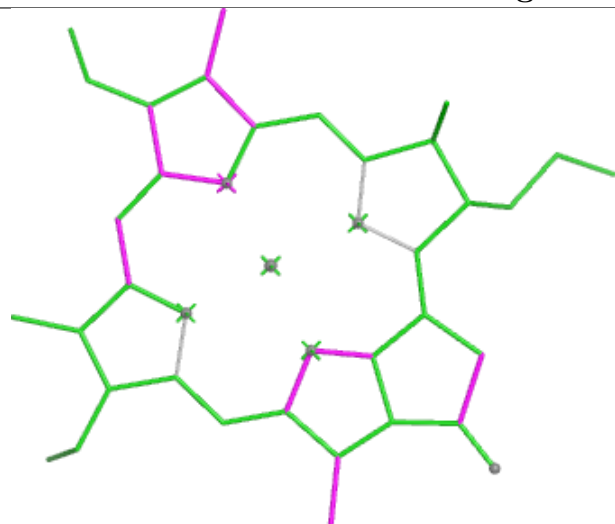
Torsions



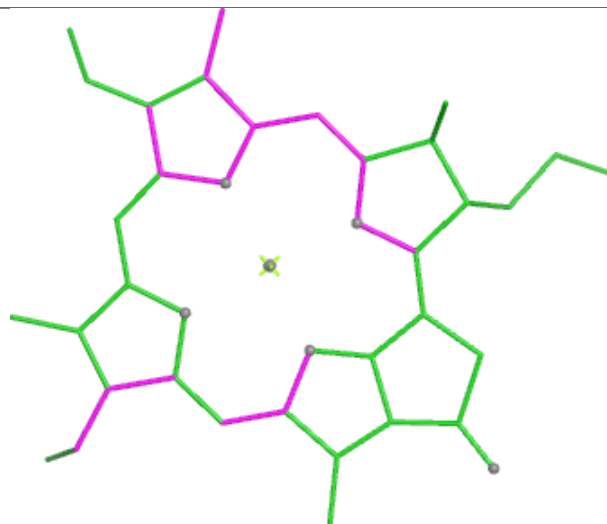
Rings



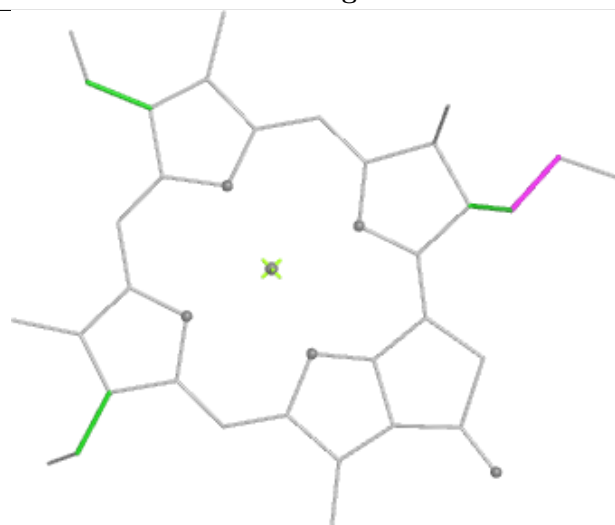
Ligand CLA B 846



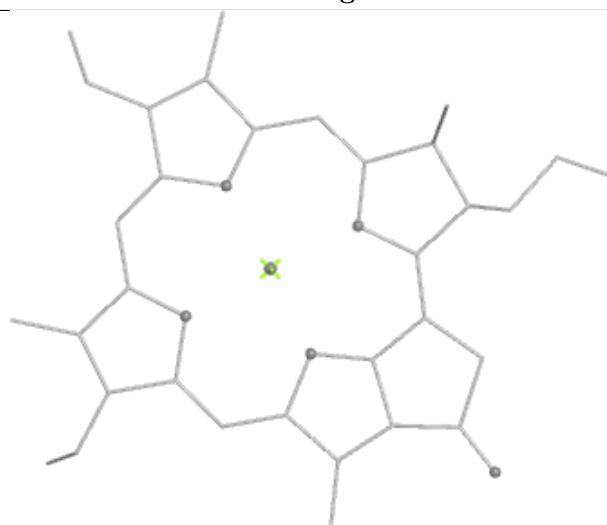
Bond lengths



Bond angles

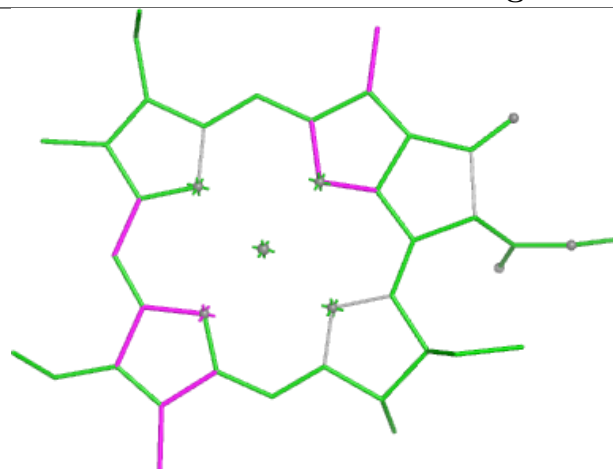


Torsions

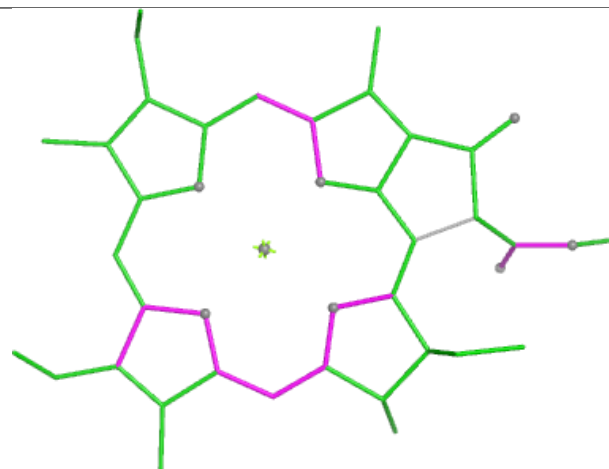


Rings

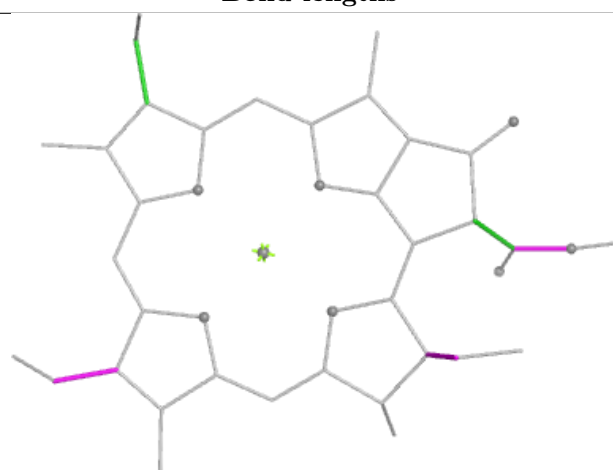
Ligand CLA A2 814



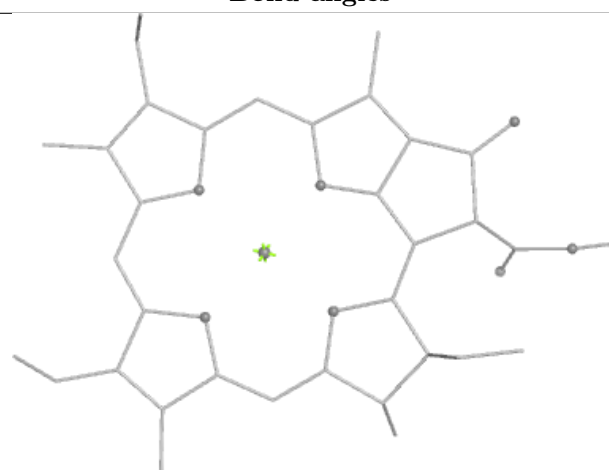
Bond lengths



Bond angles

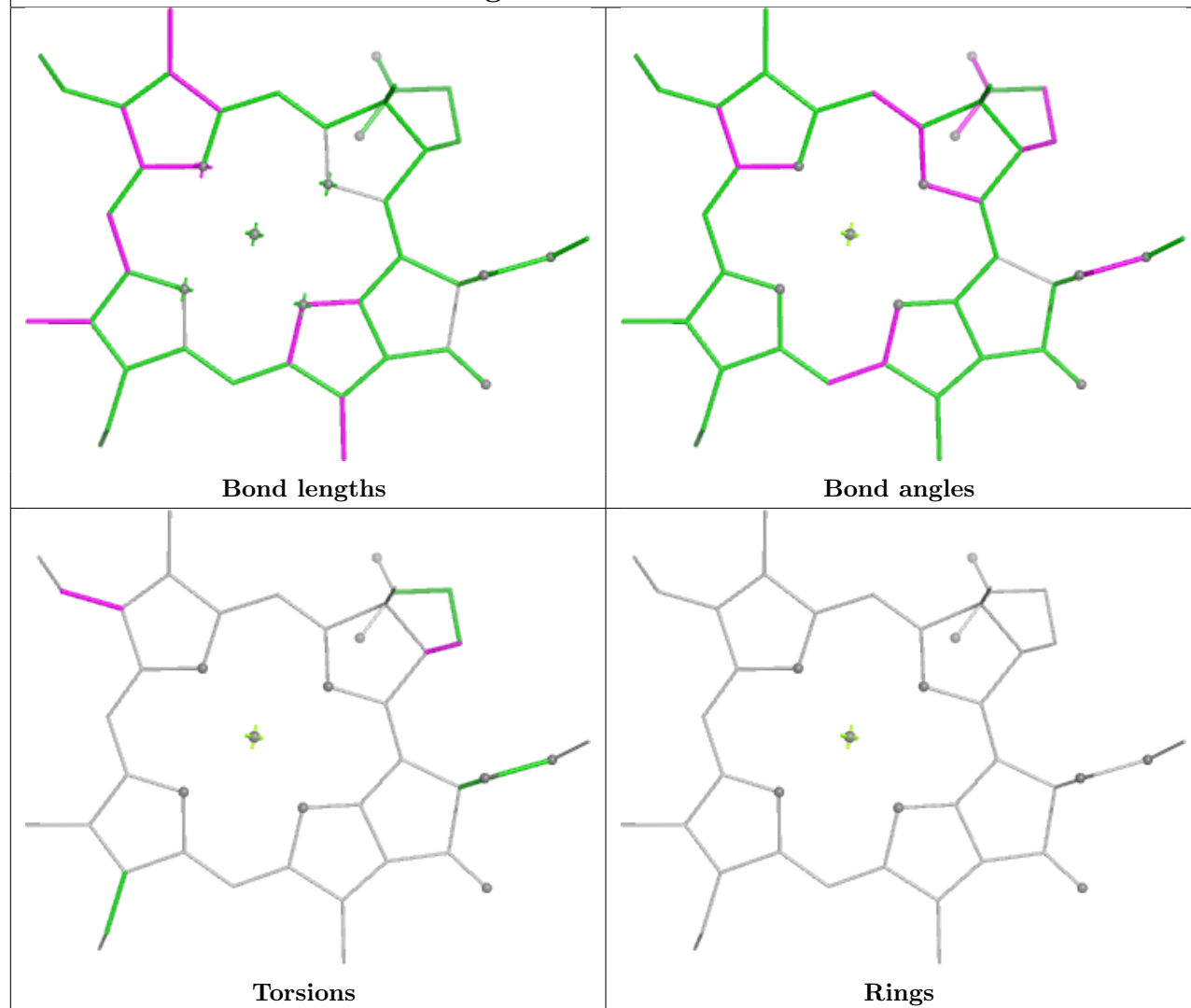


Torsions



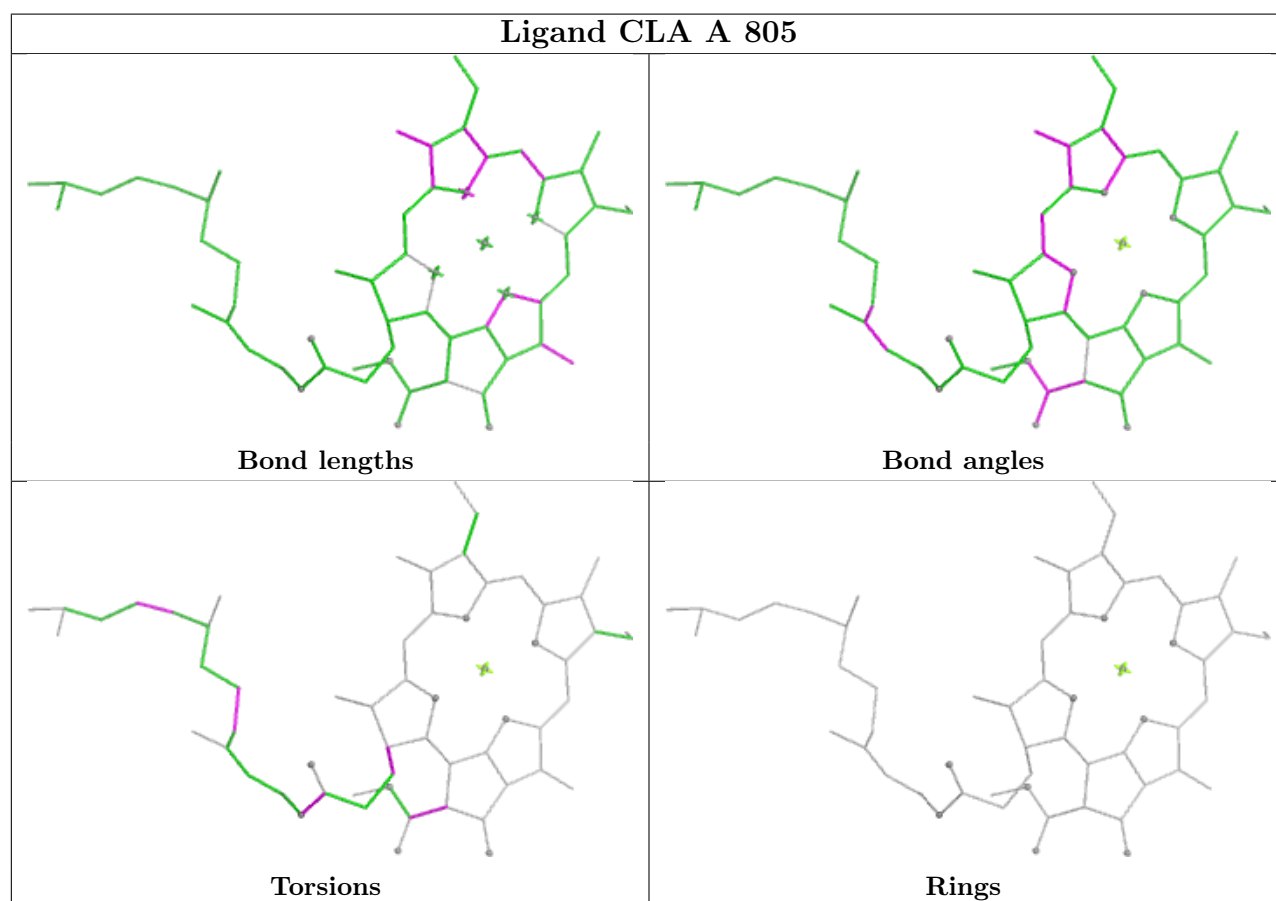
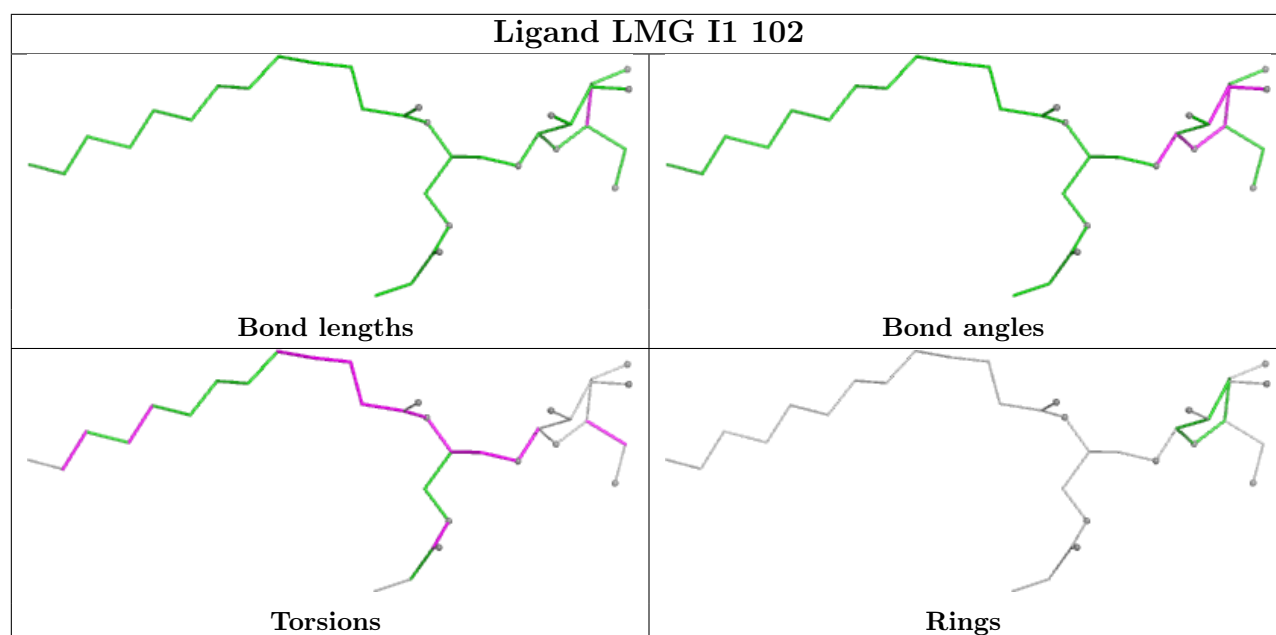
Rings

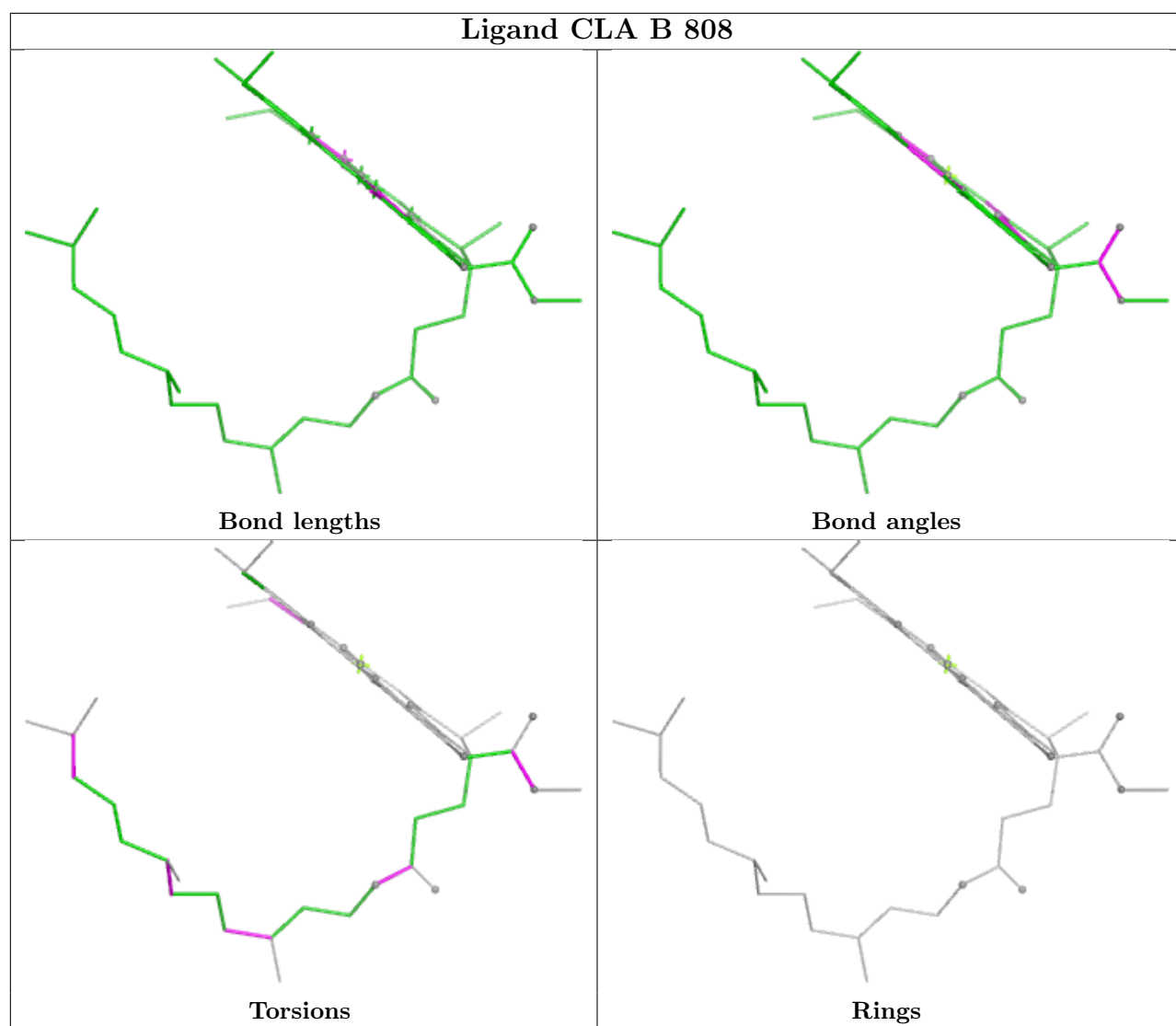
Ligand CLA BB 827

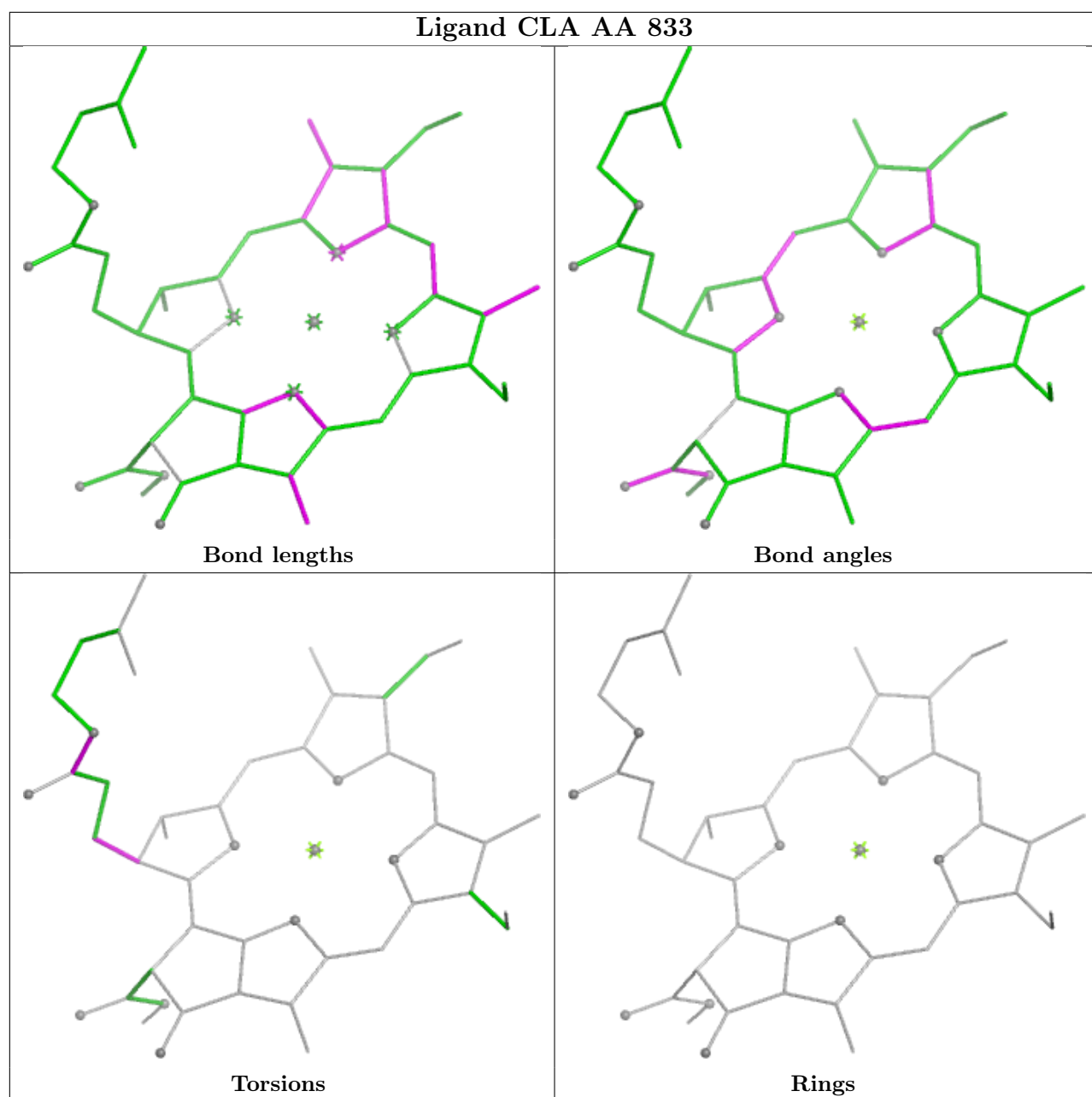


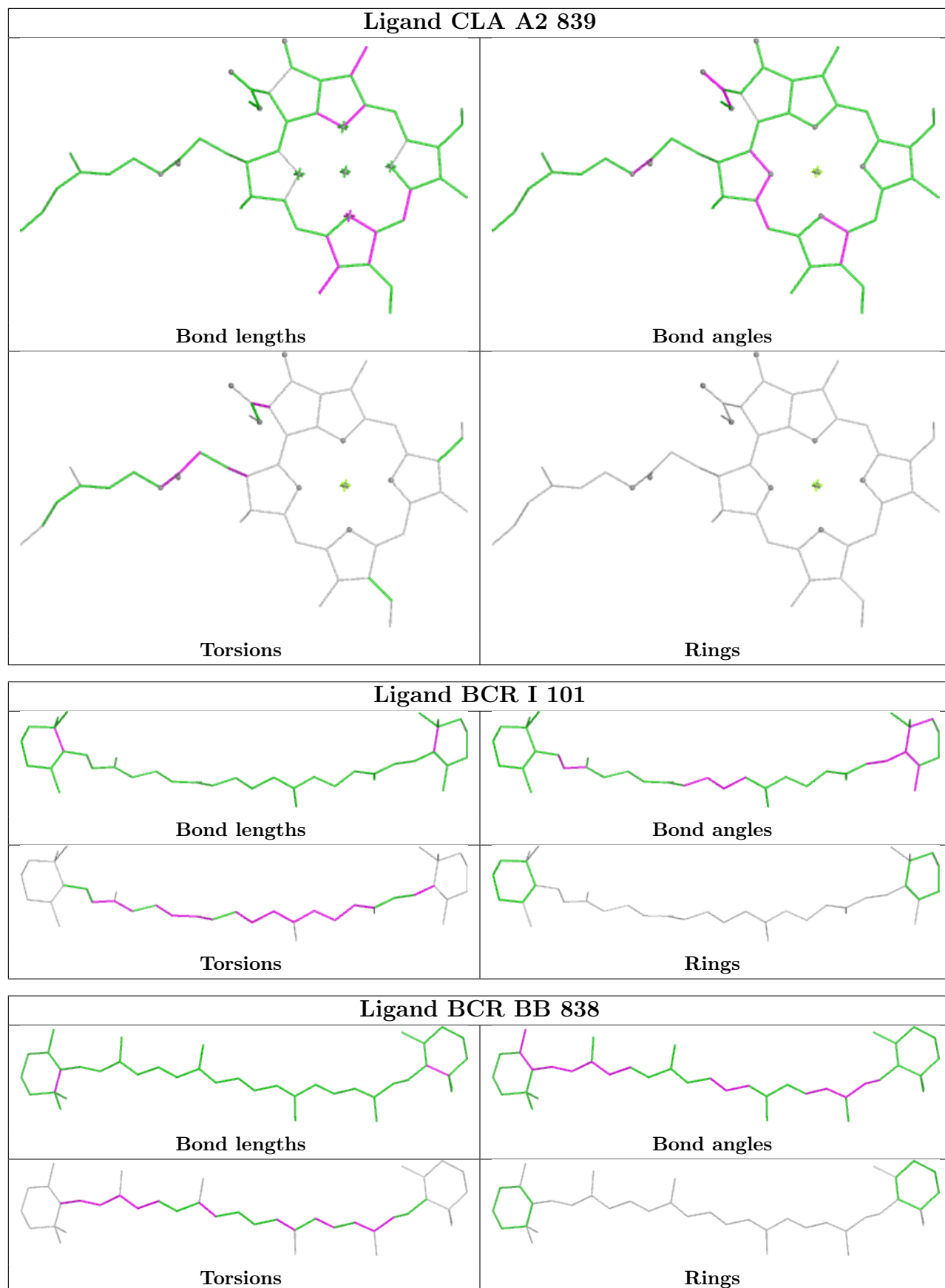
Ligand BCR BB 839

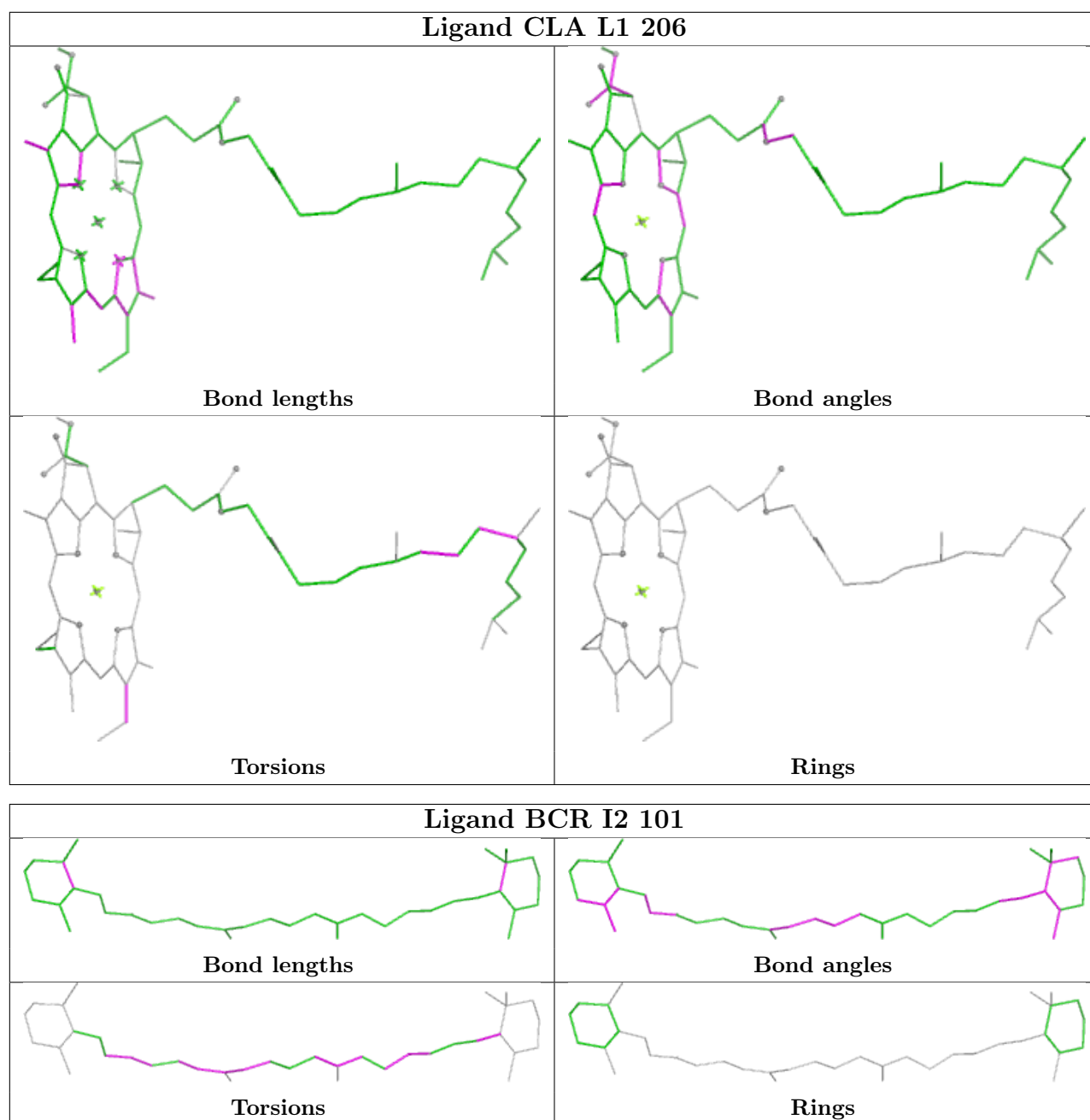


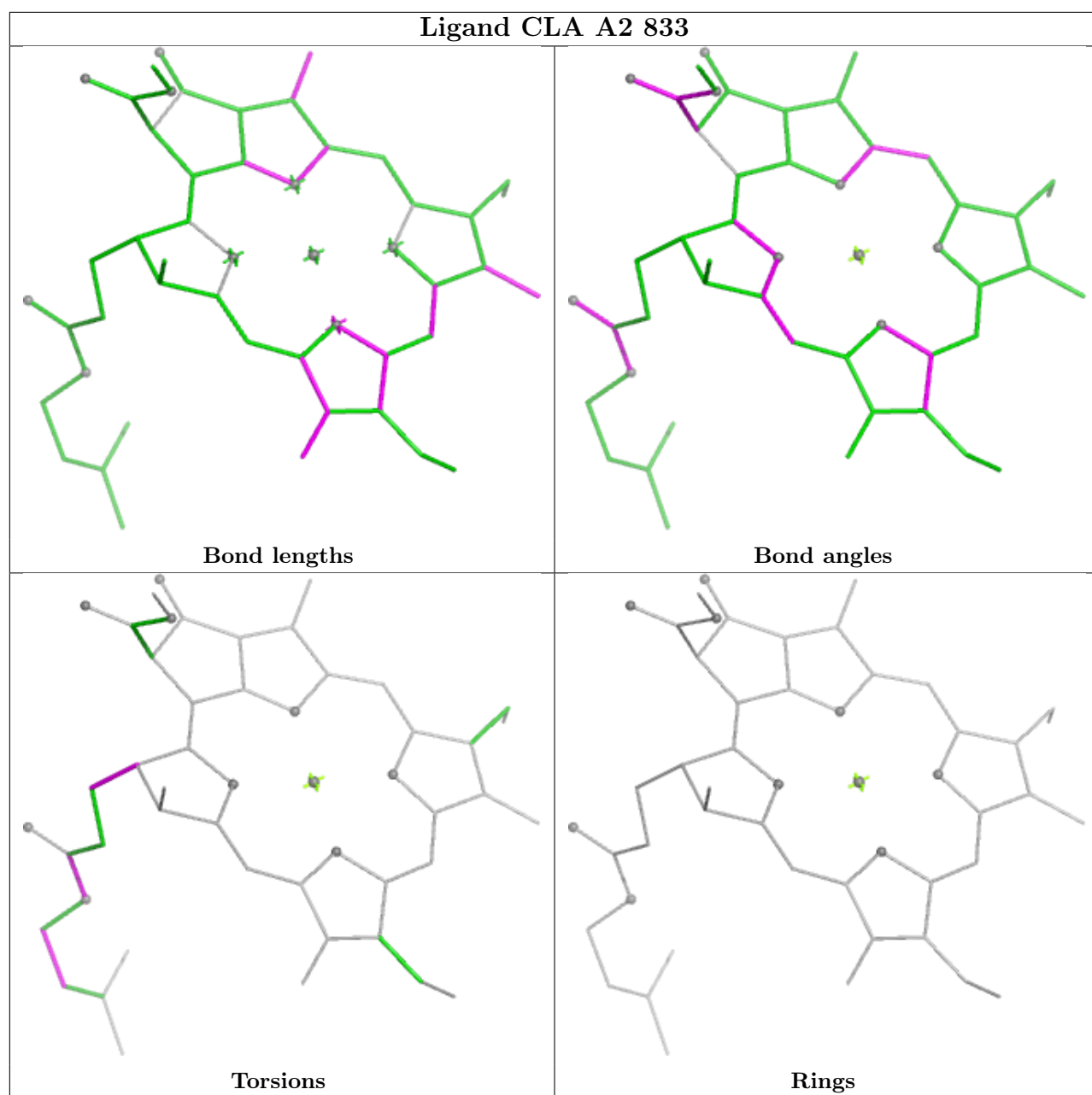


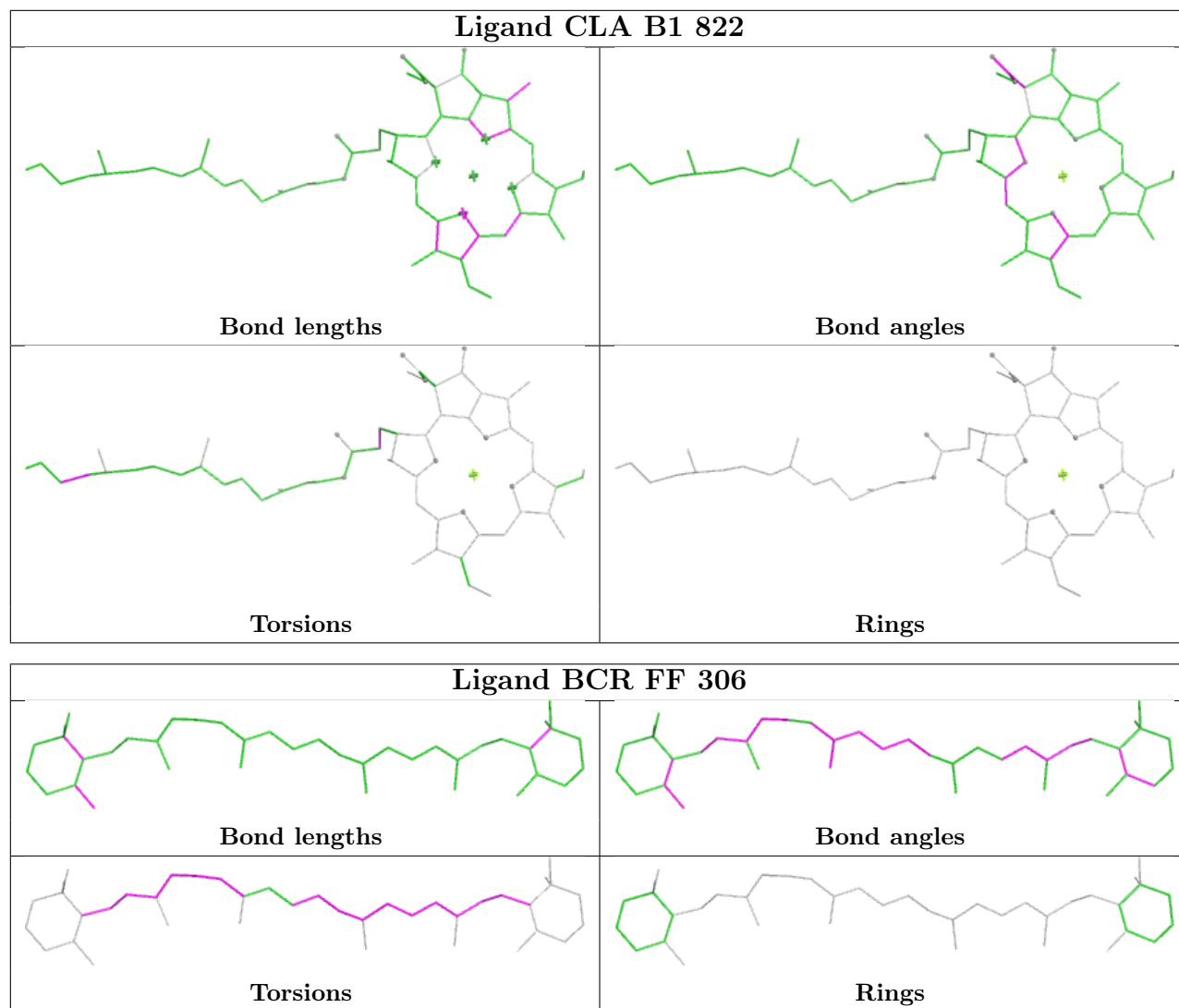




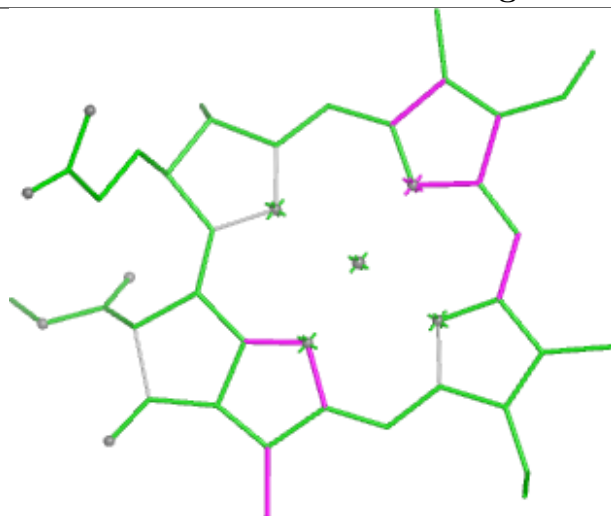




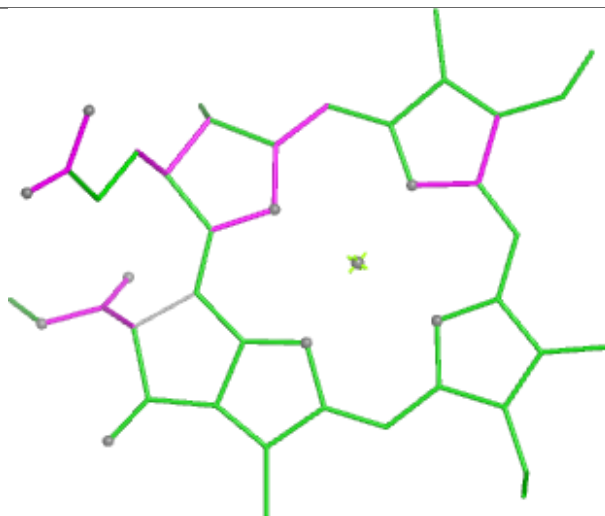




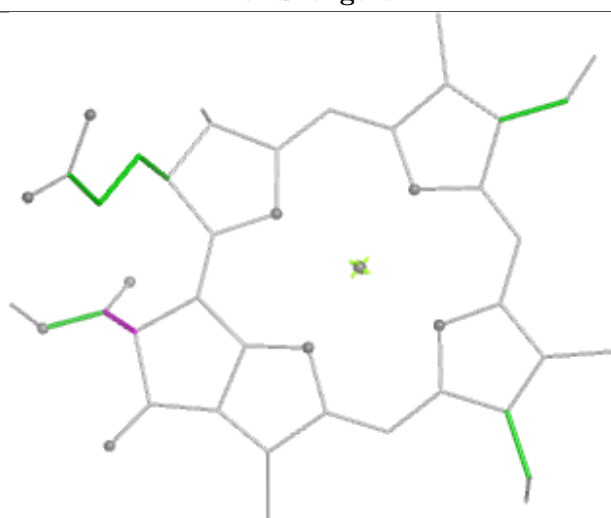
Ligand CLA KK 101



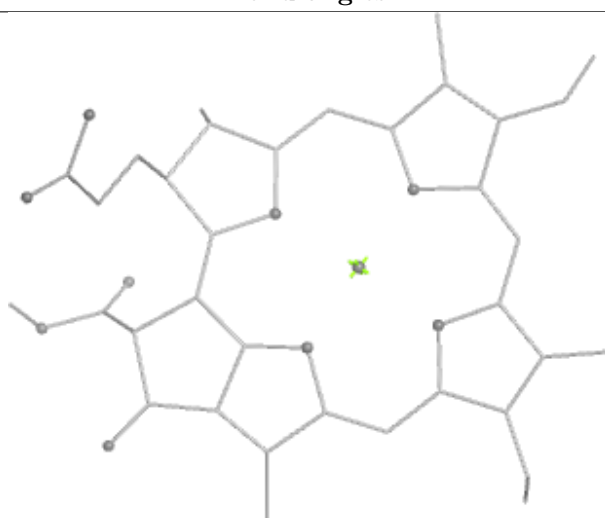
Bond lengths



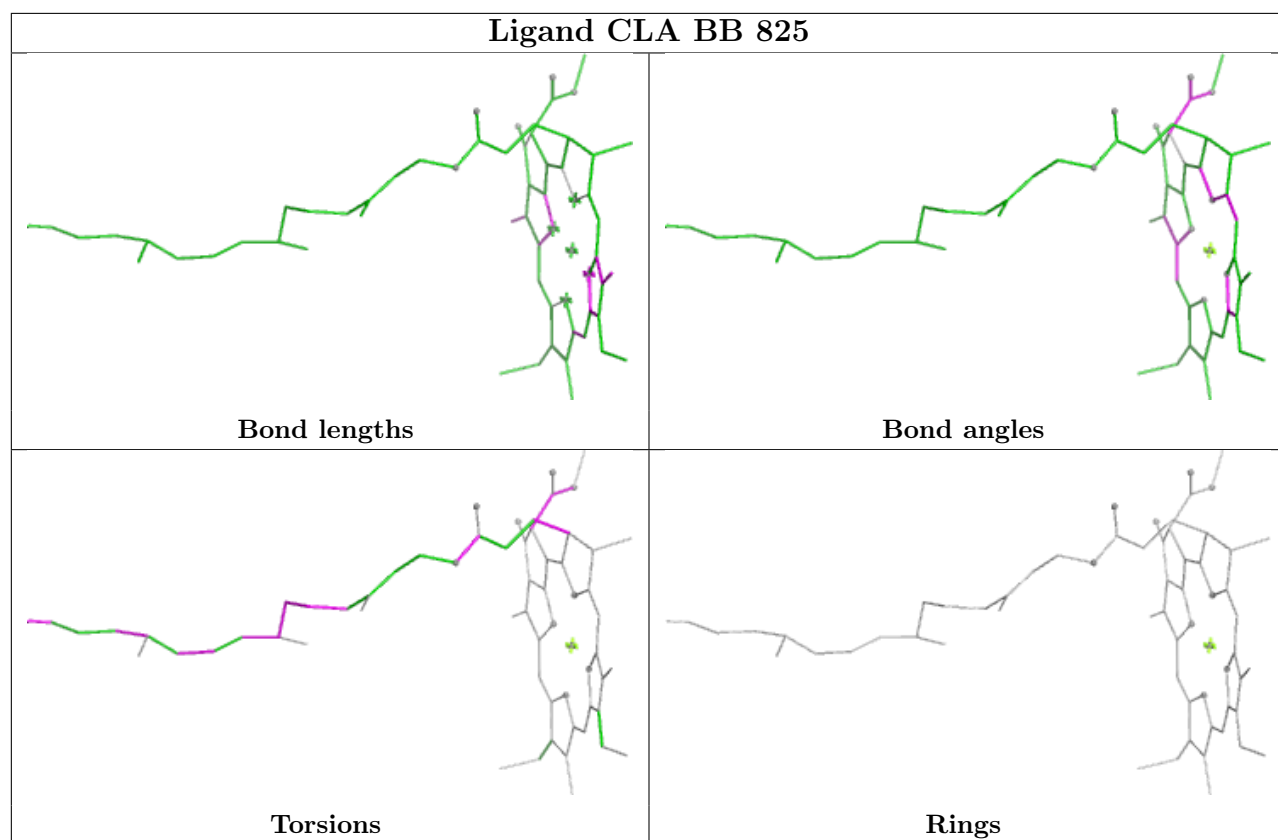
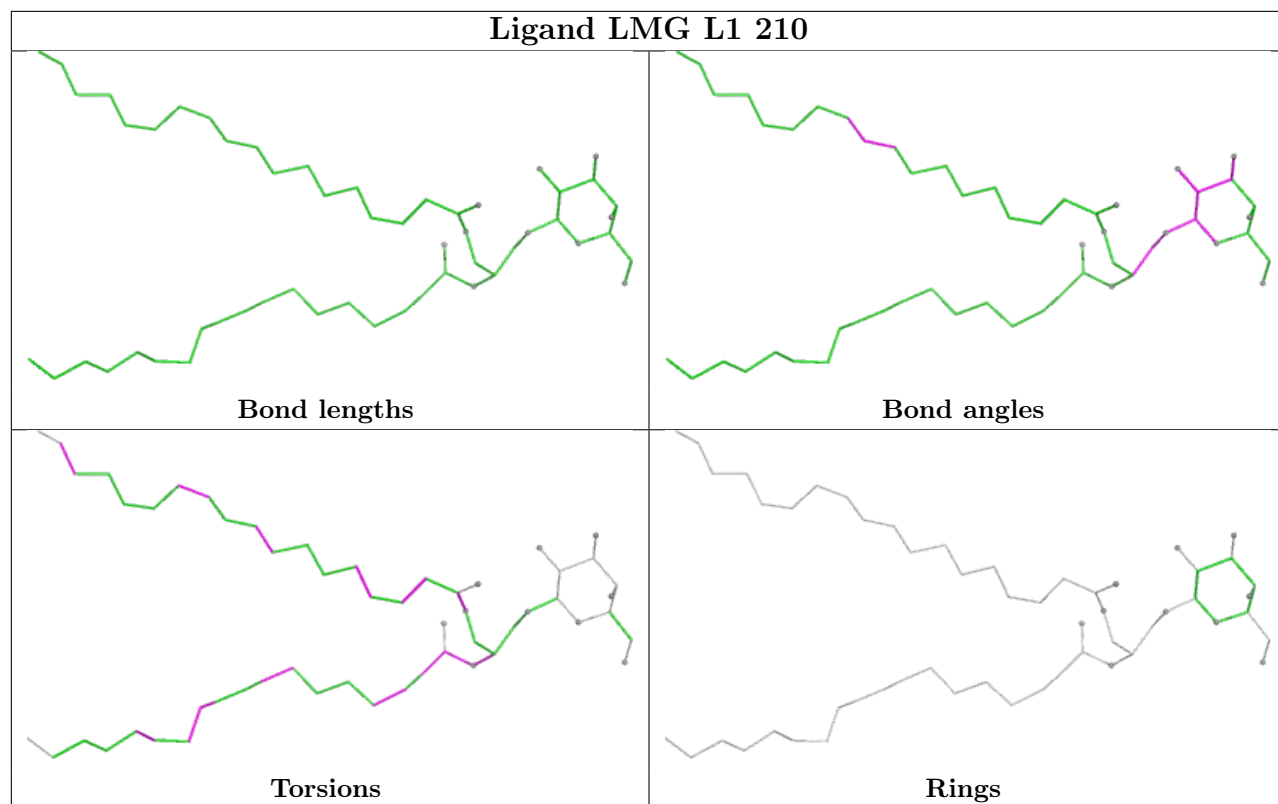
Bond angles

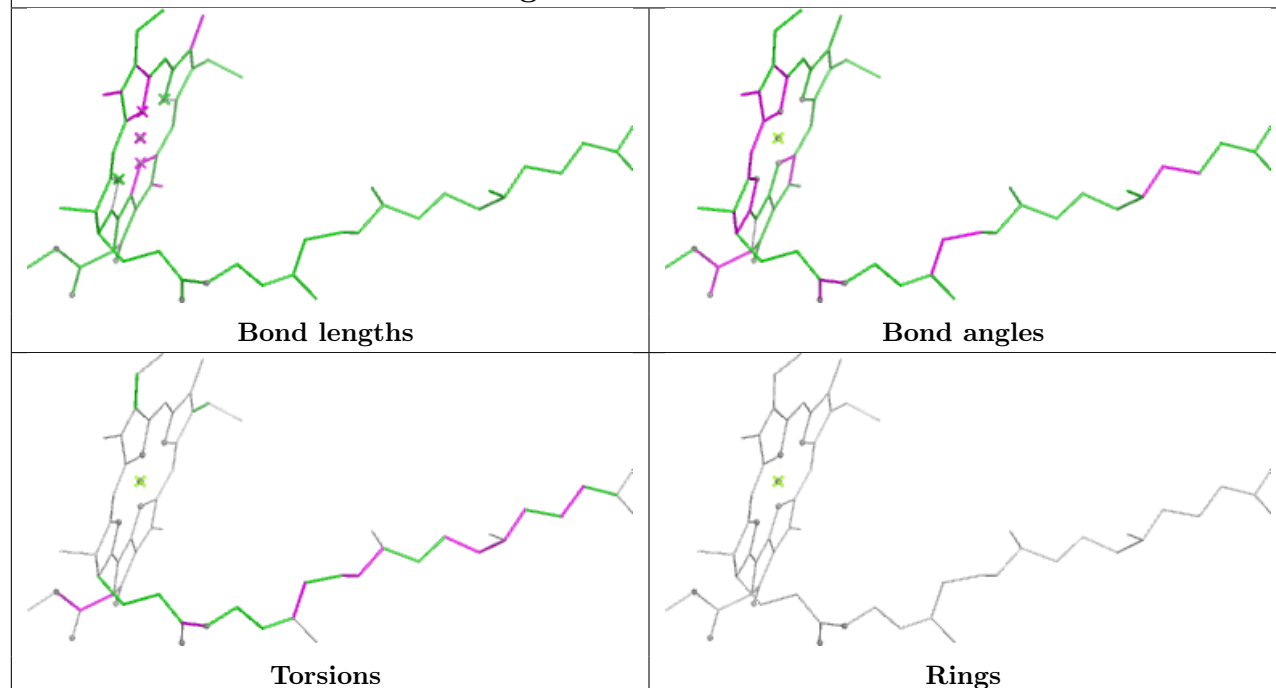
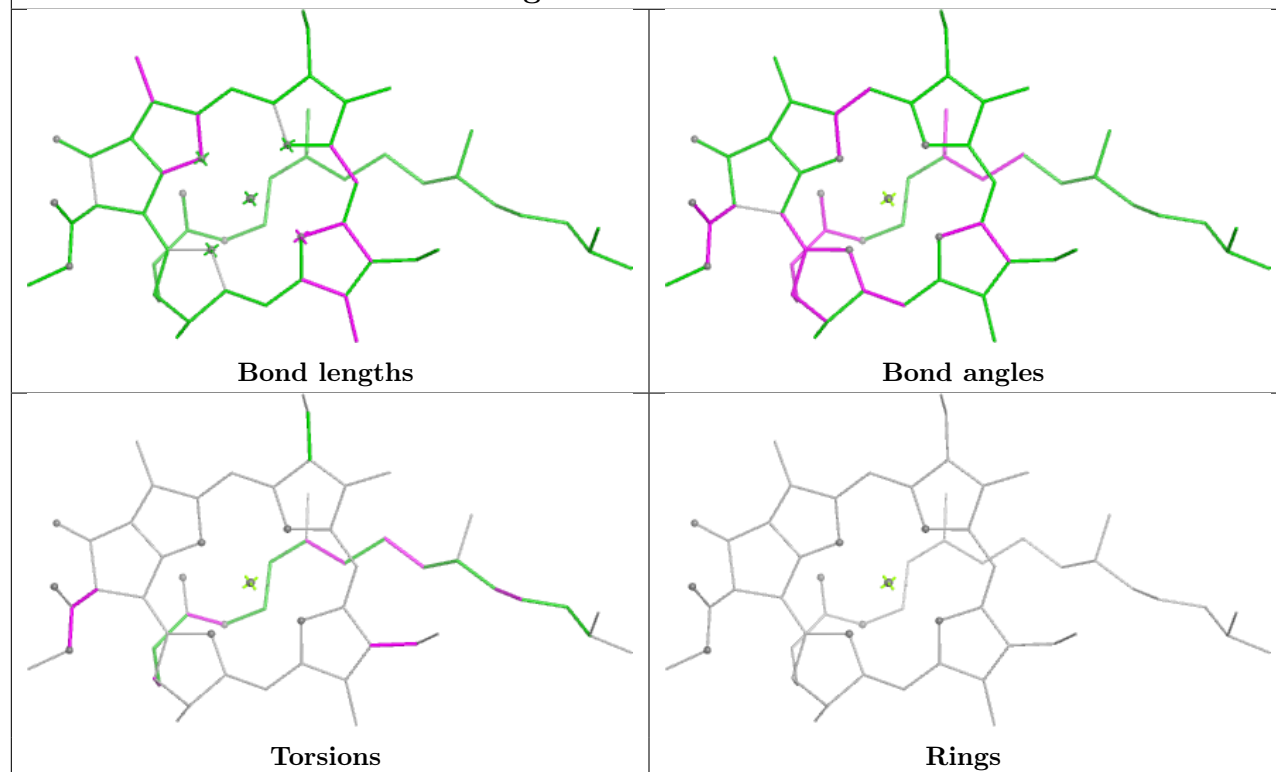


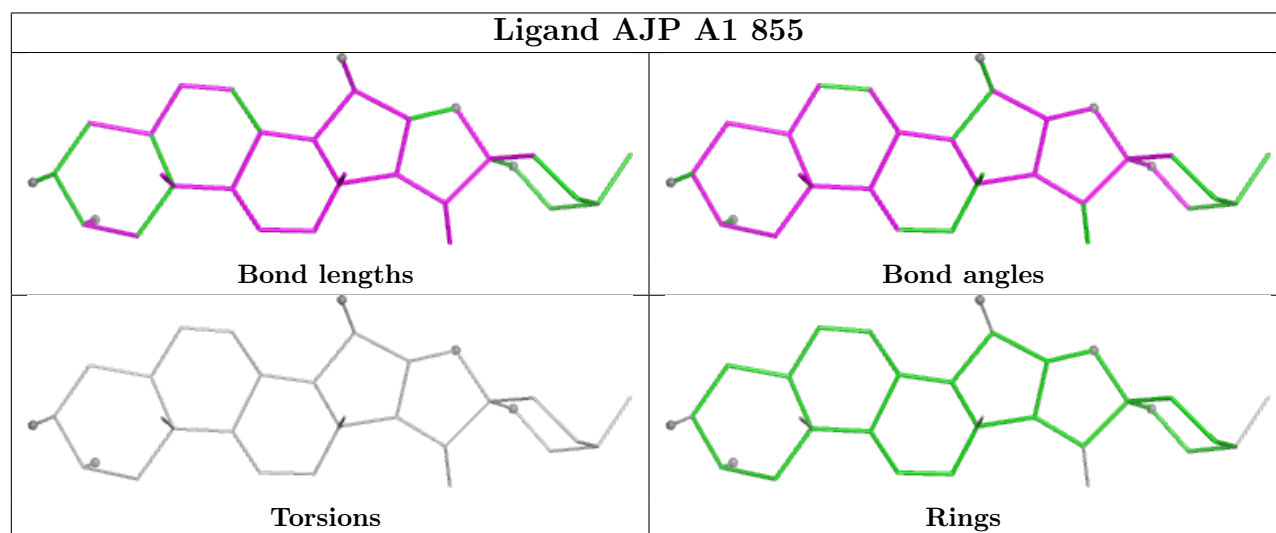
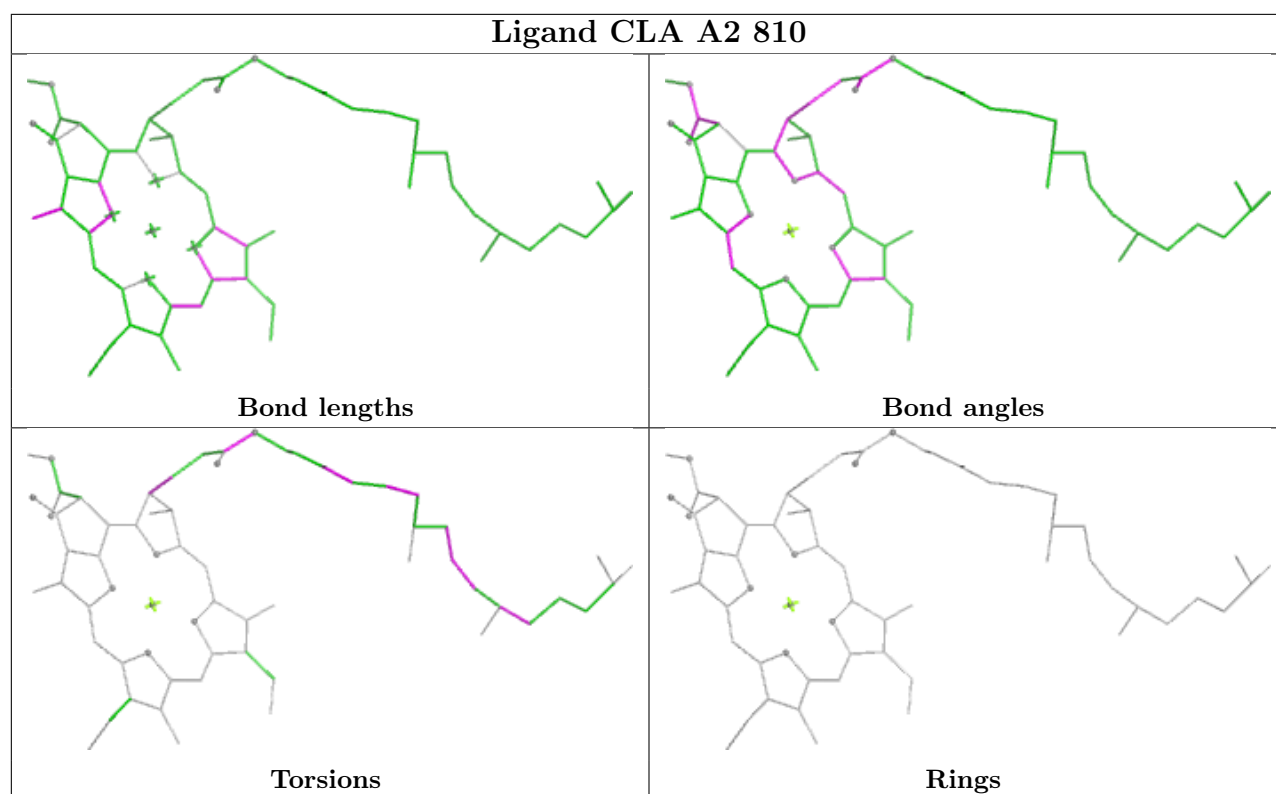
Torsions



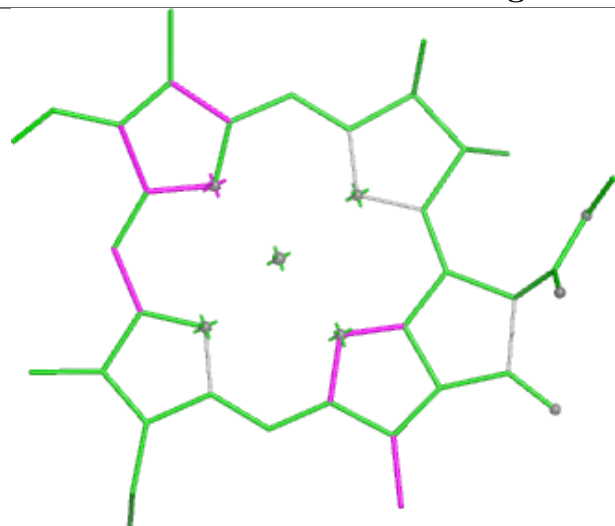
Rings



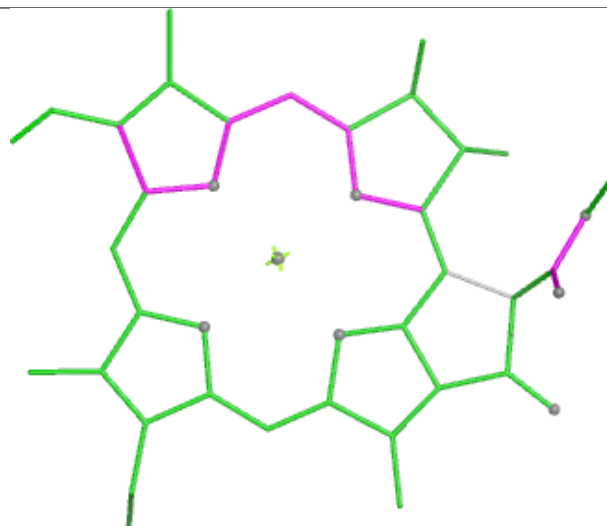
Ligand CLA BB 826**Ligand CLA B1 850**



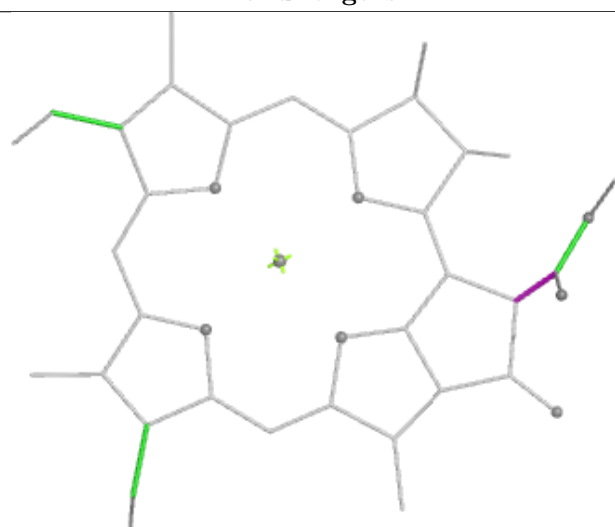
Ligand CLA B2 818



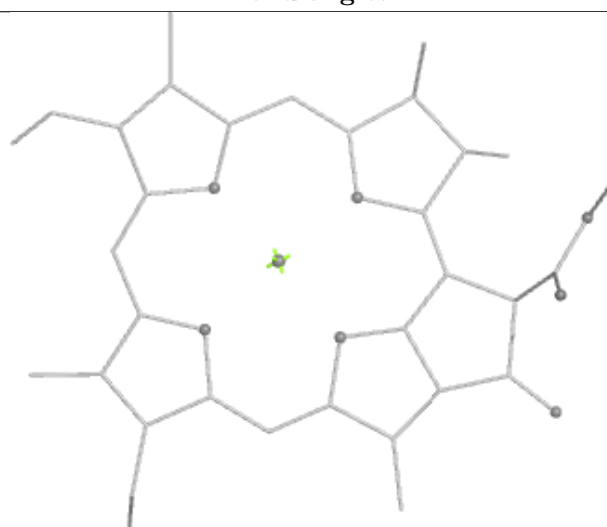
Bond lengths



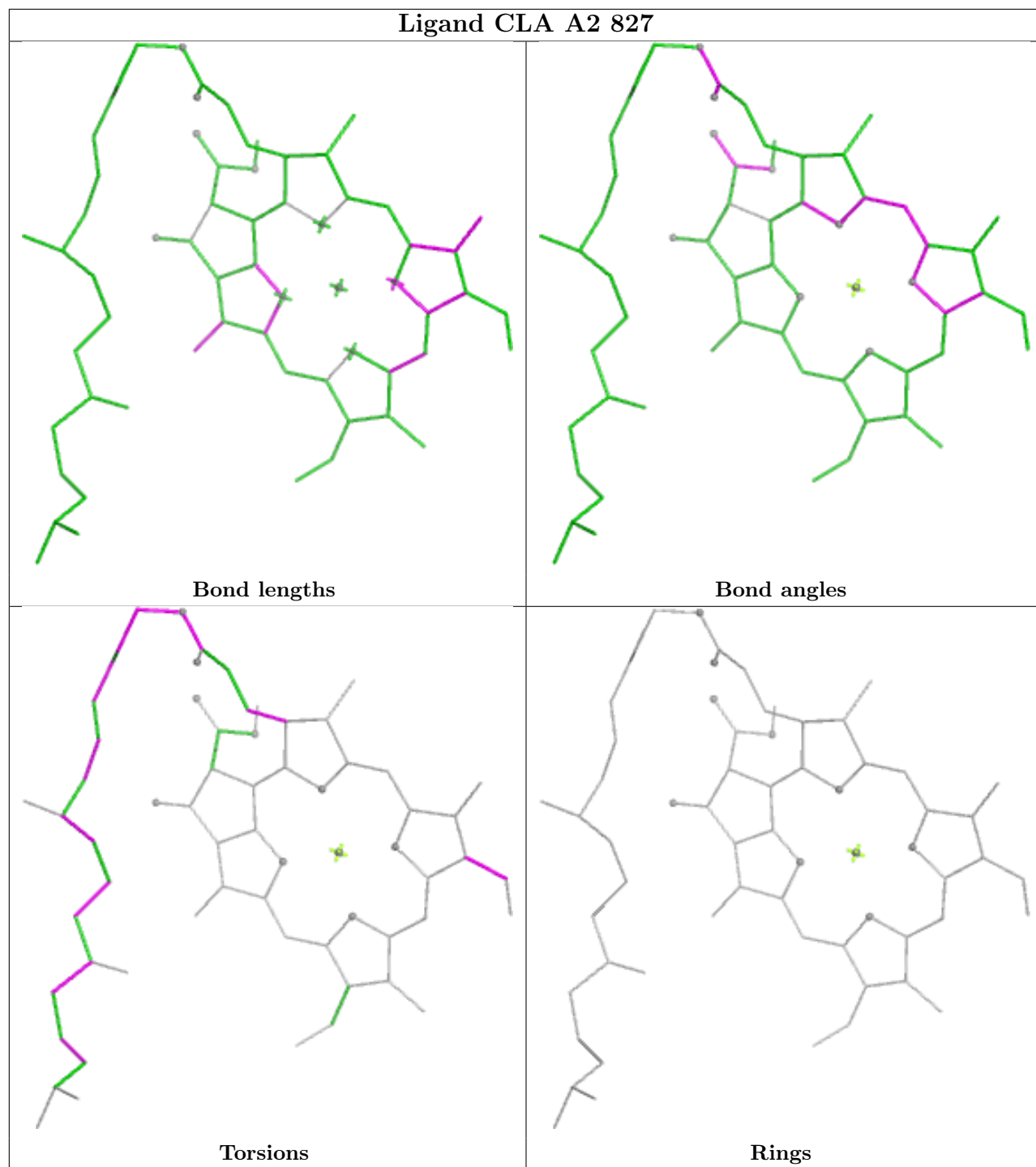
Bond angles

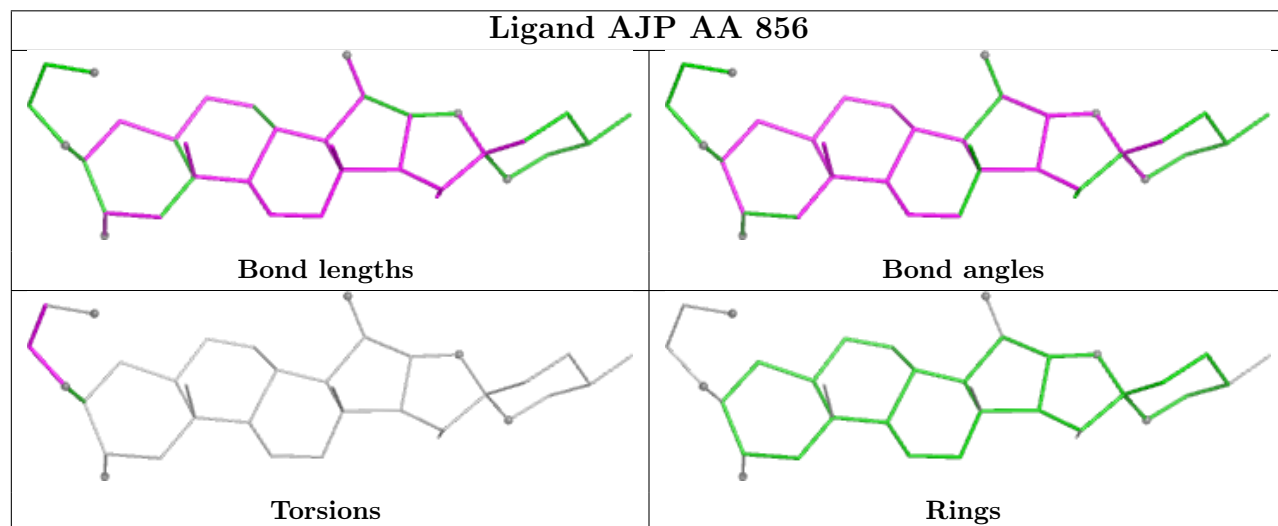
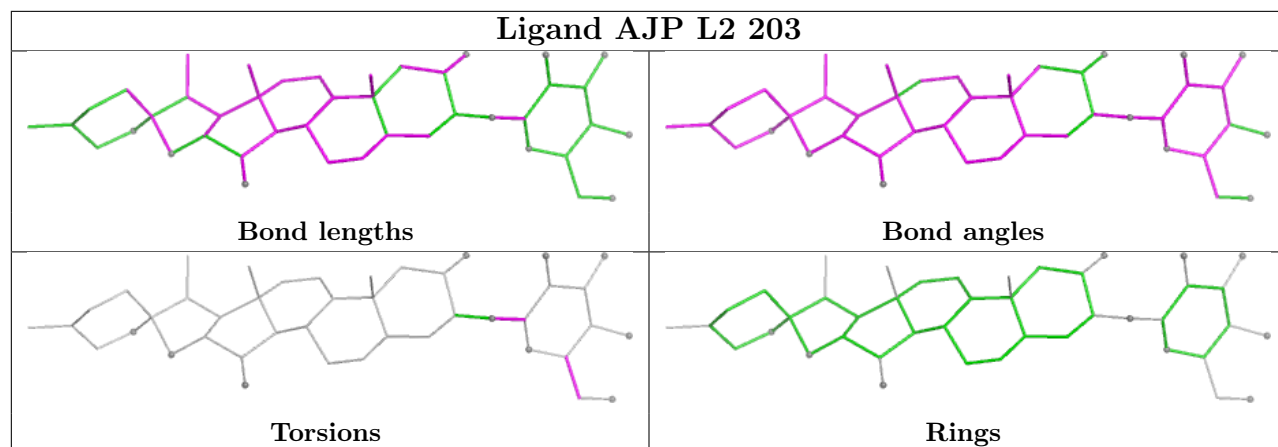


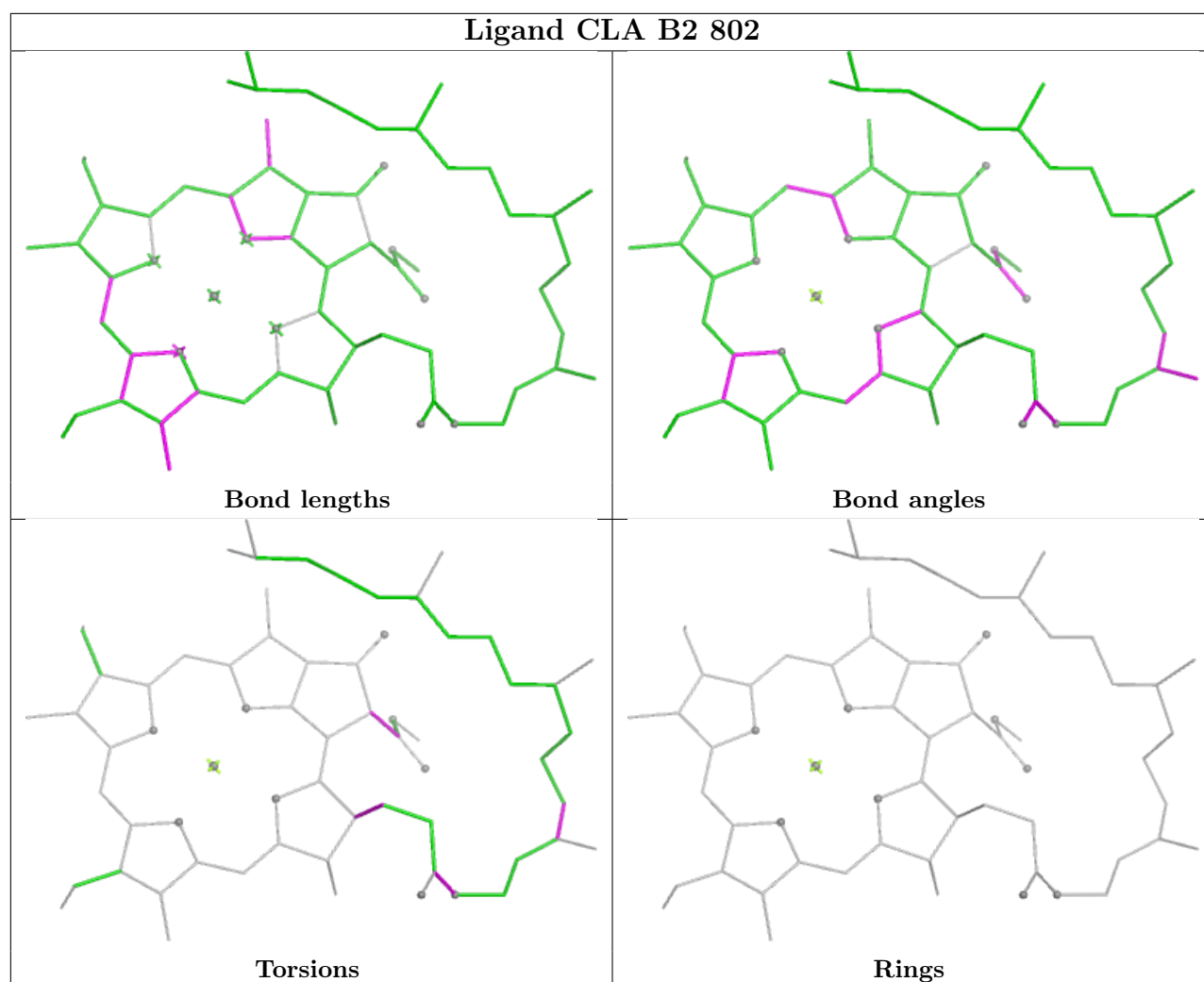
Torsions



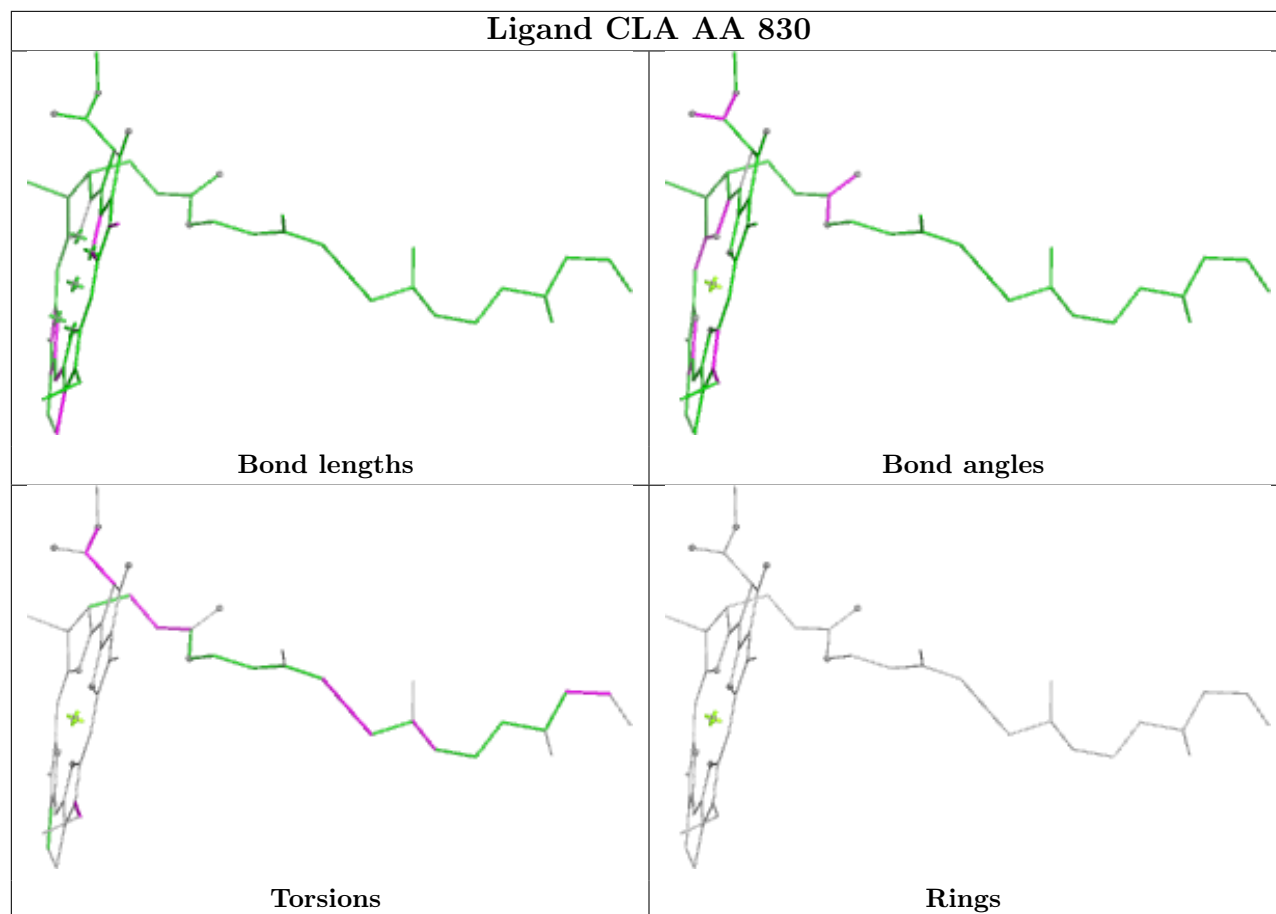
Rings



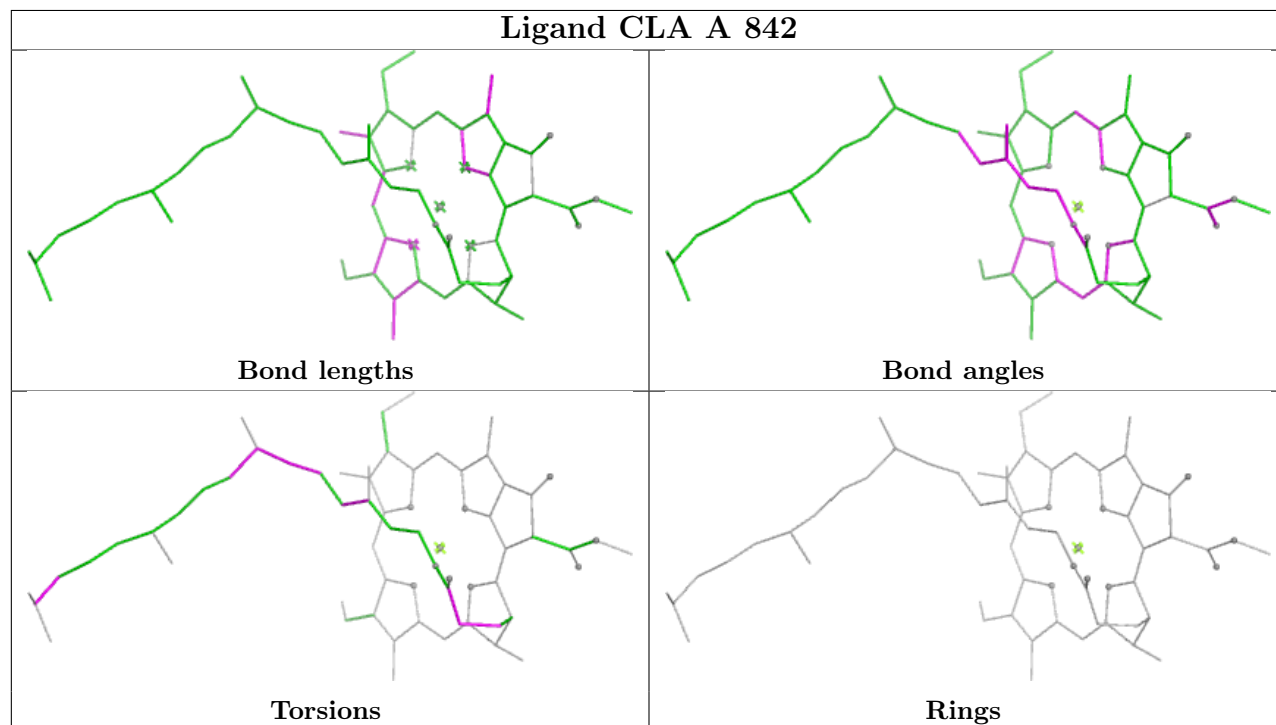




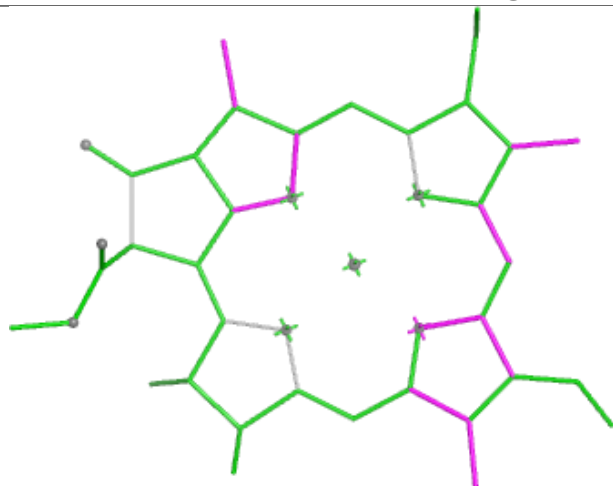
Ligand CLA AA 830



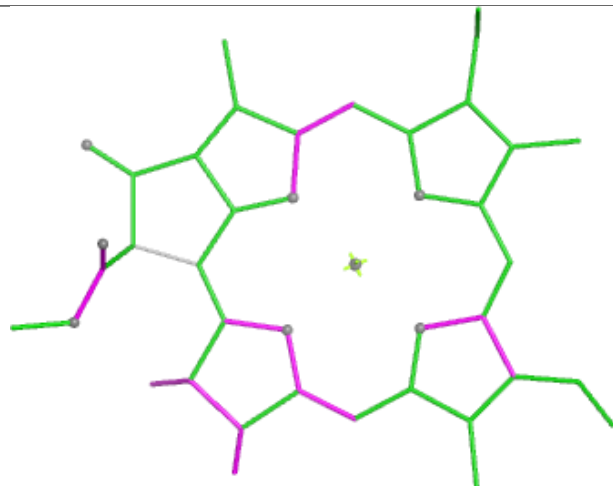
Ligand CLA A 842



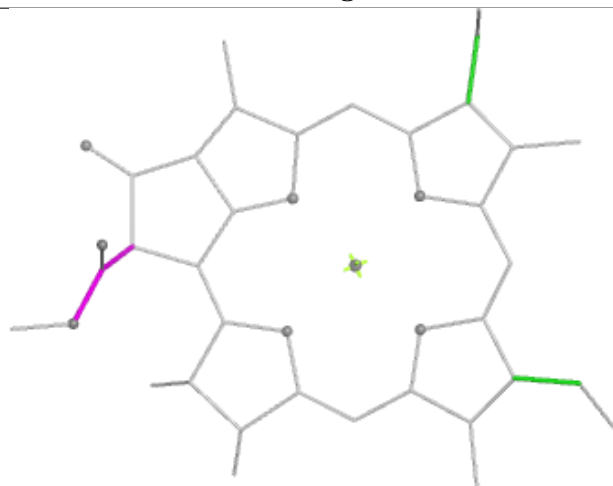
Ligand CLA A2 834



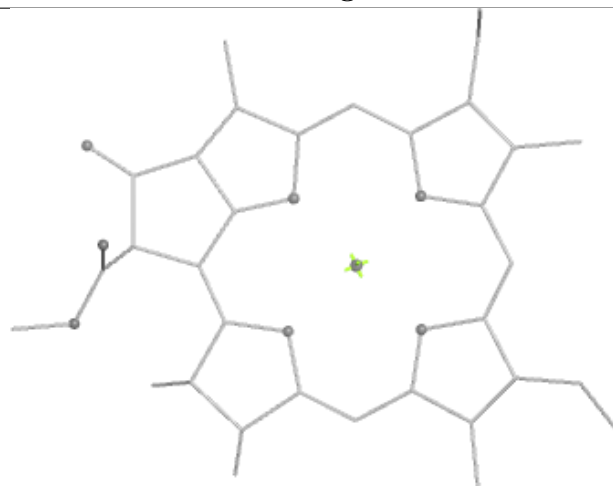
Bond lengths



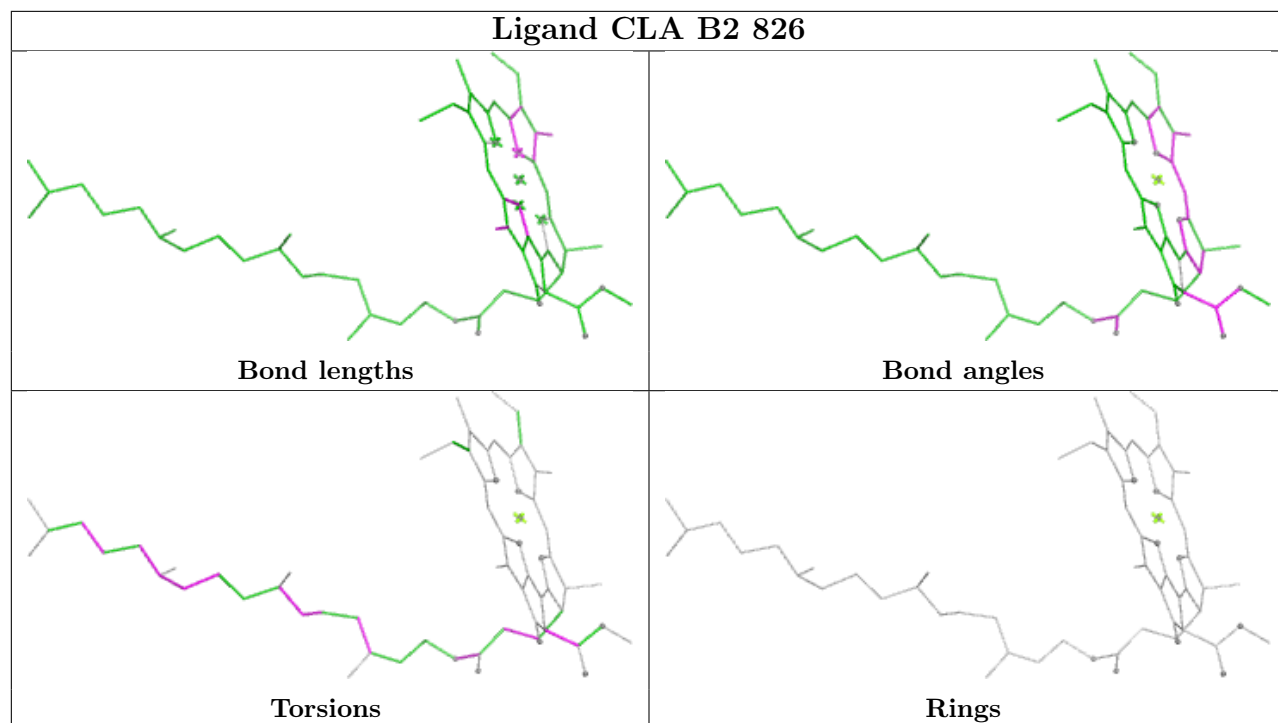
Bond angles

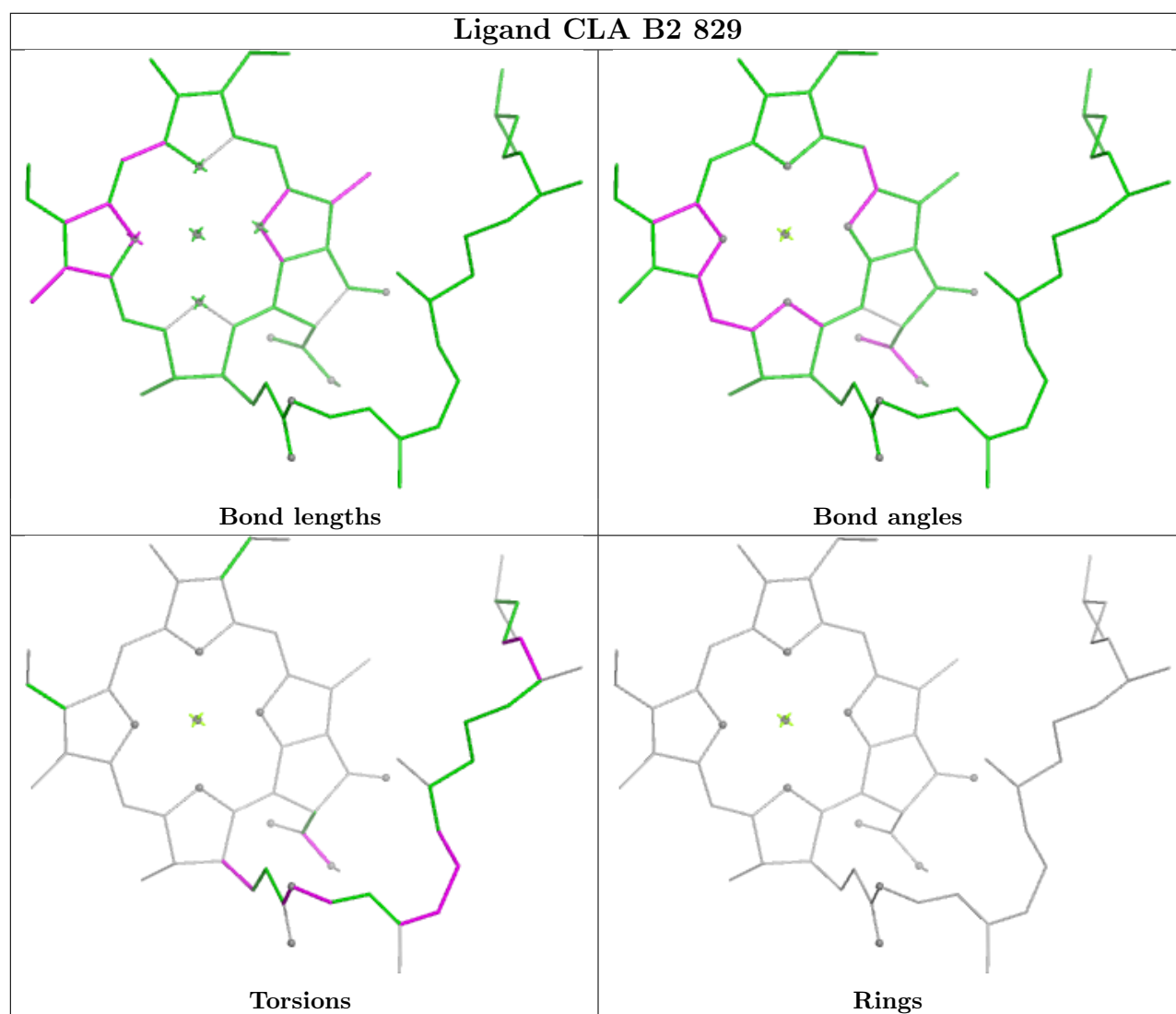


Torsions

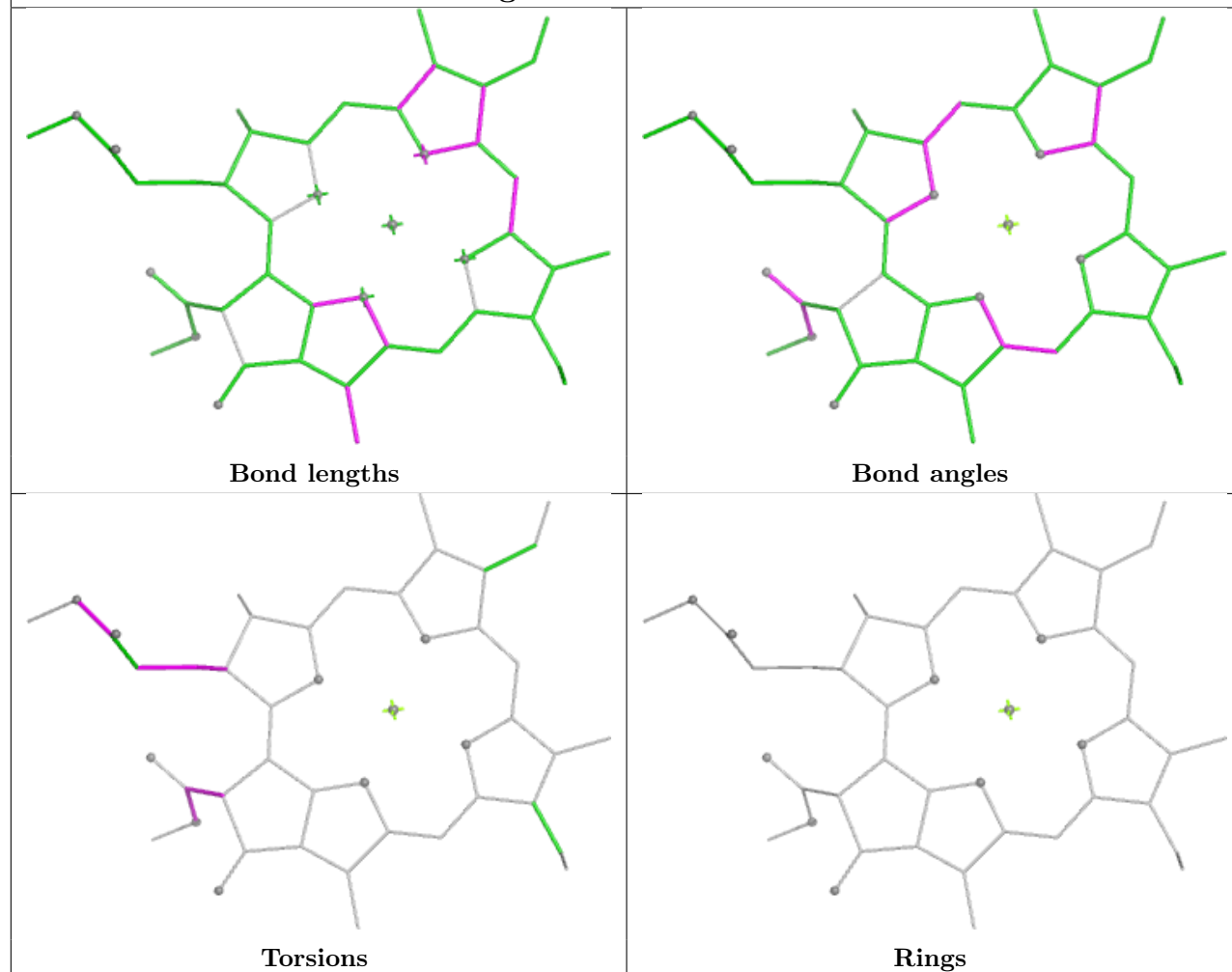


Rings

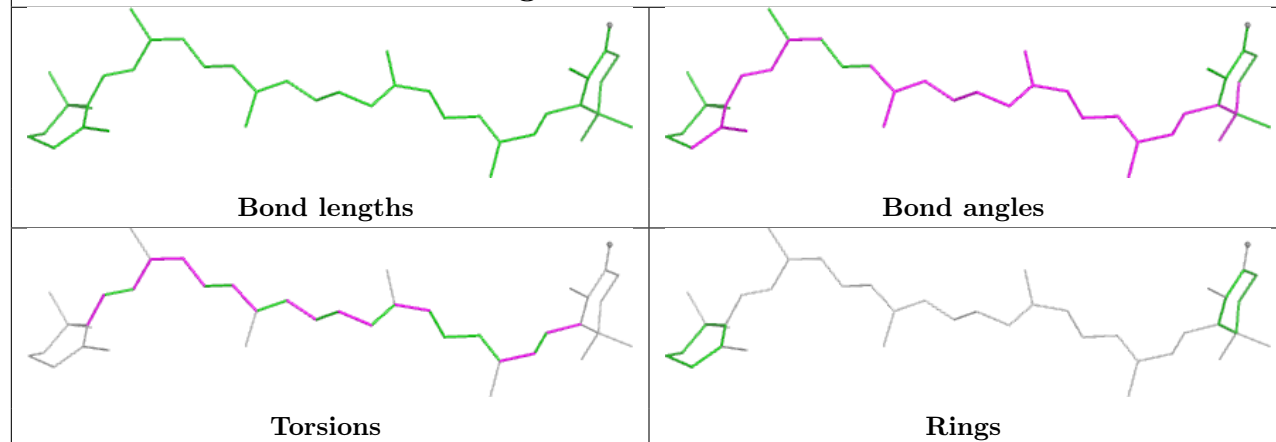


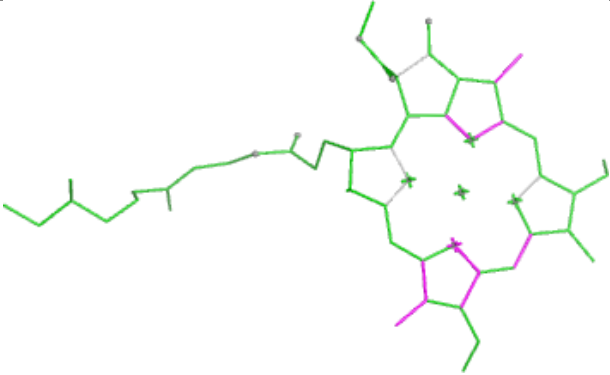
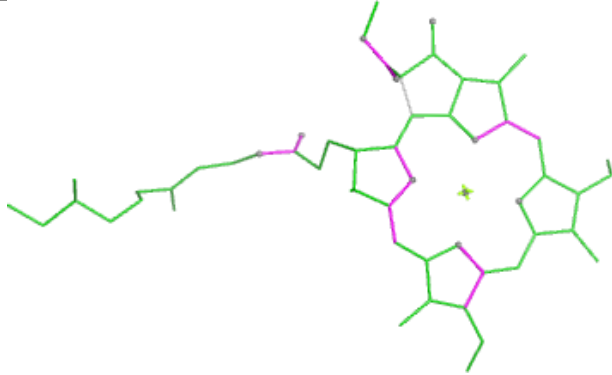
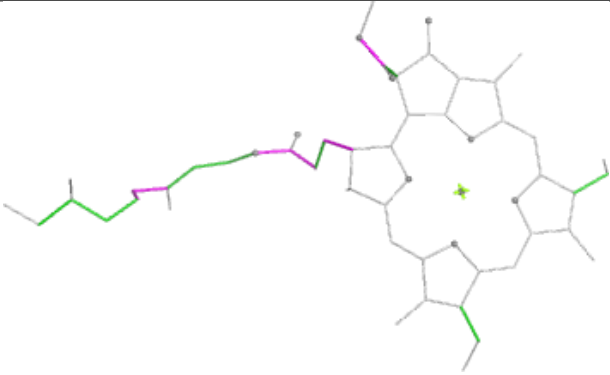
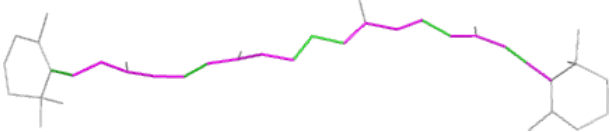


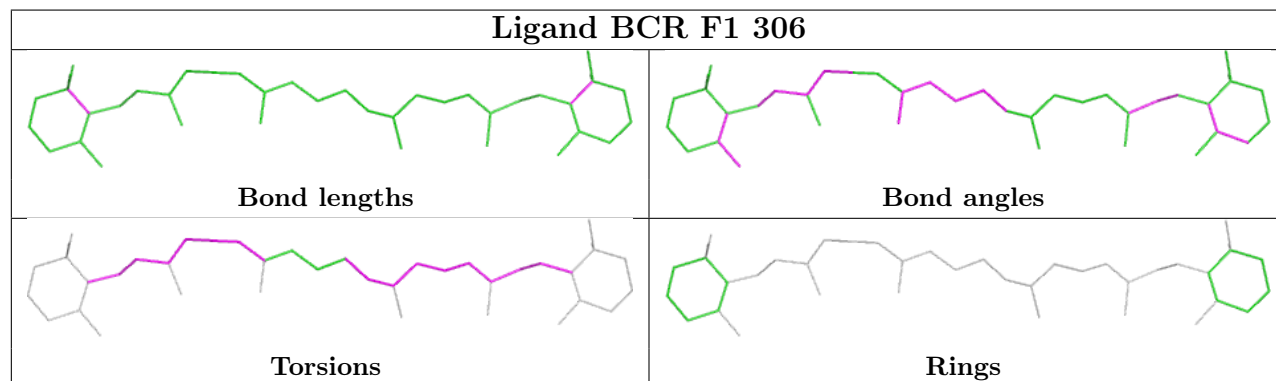
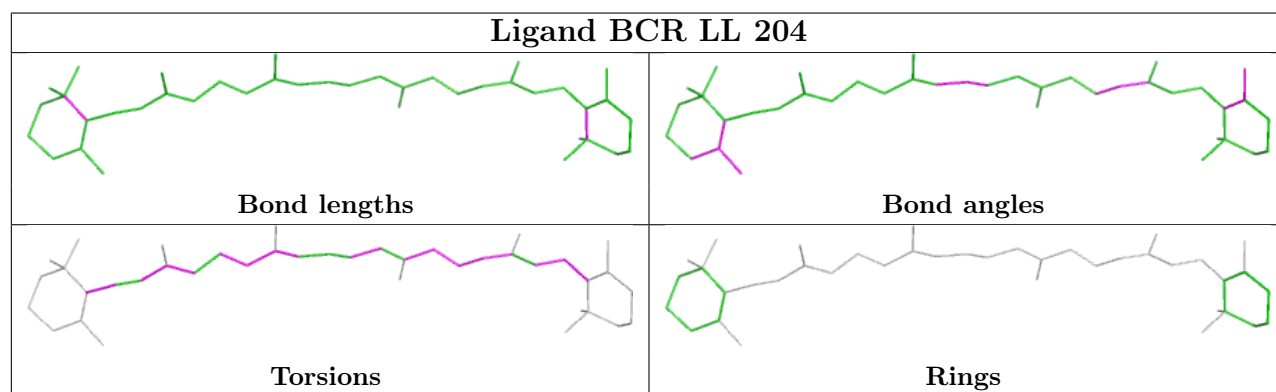
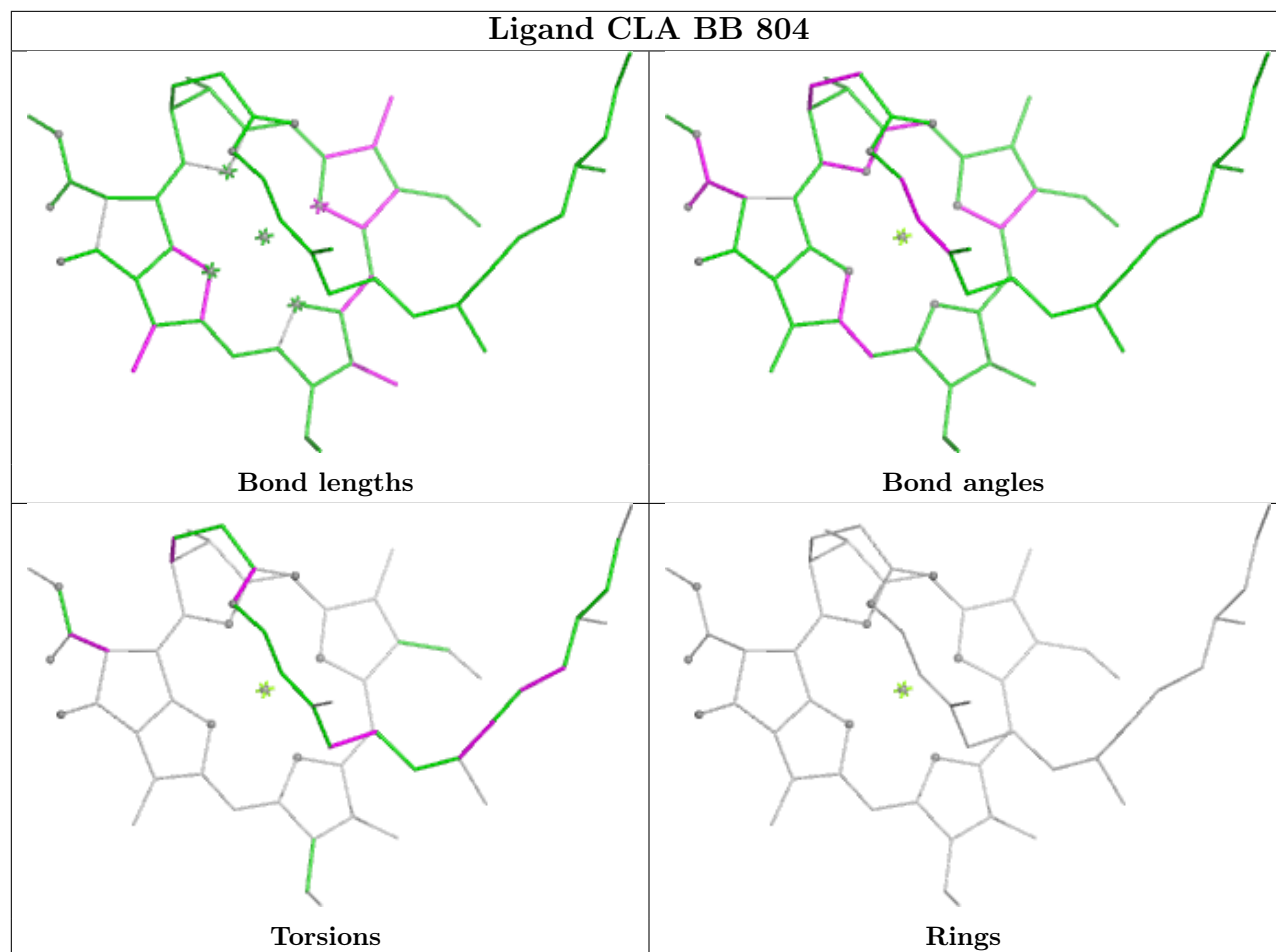
Ligand CLA KK 102



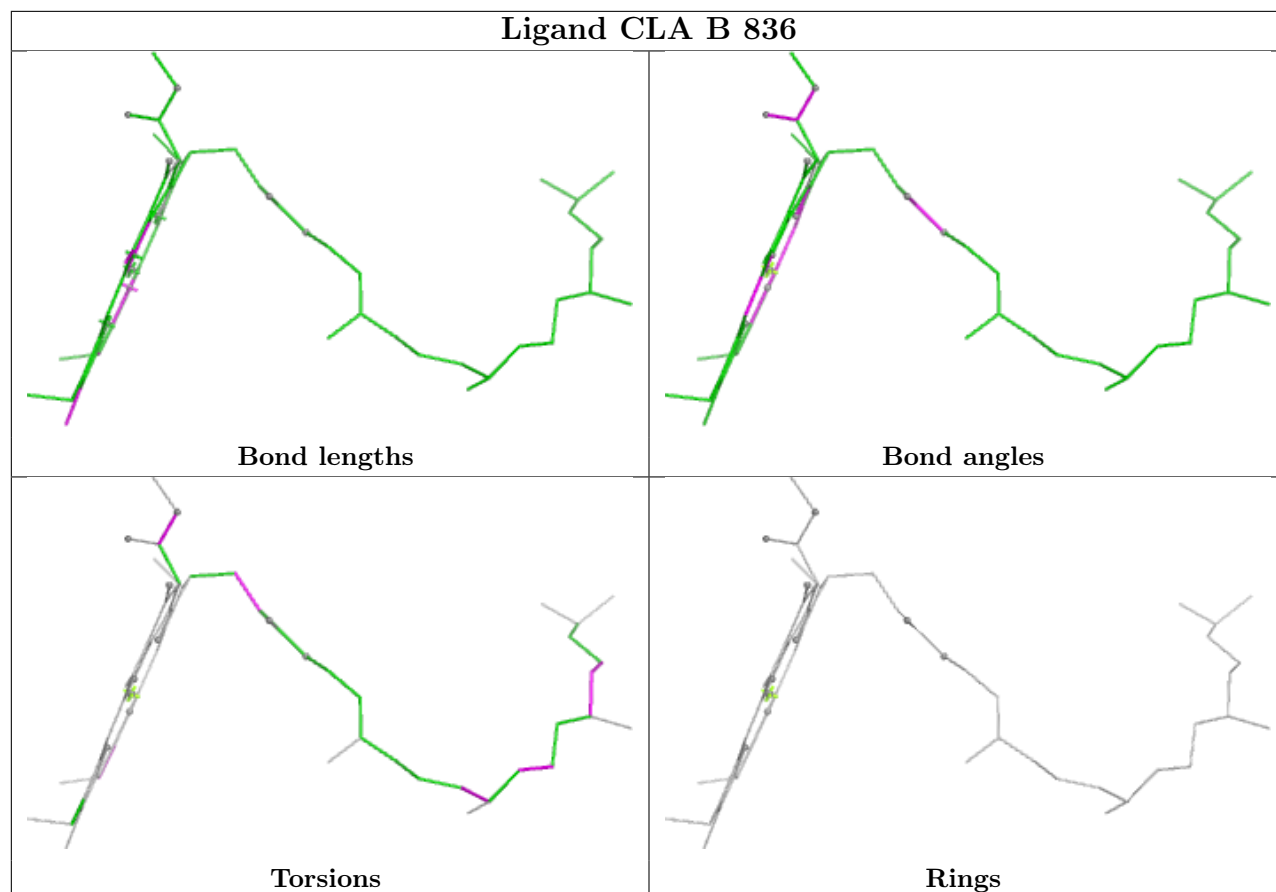
Ligand ECH BB 840



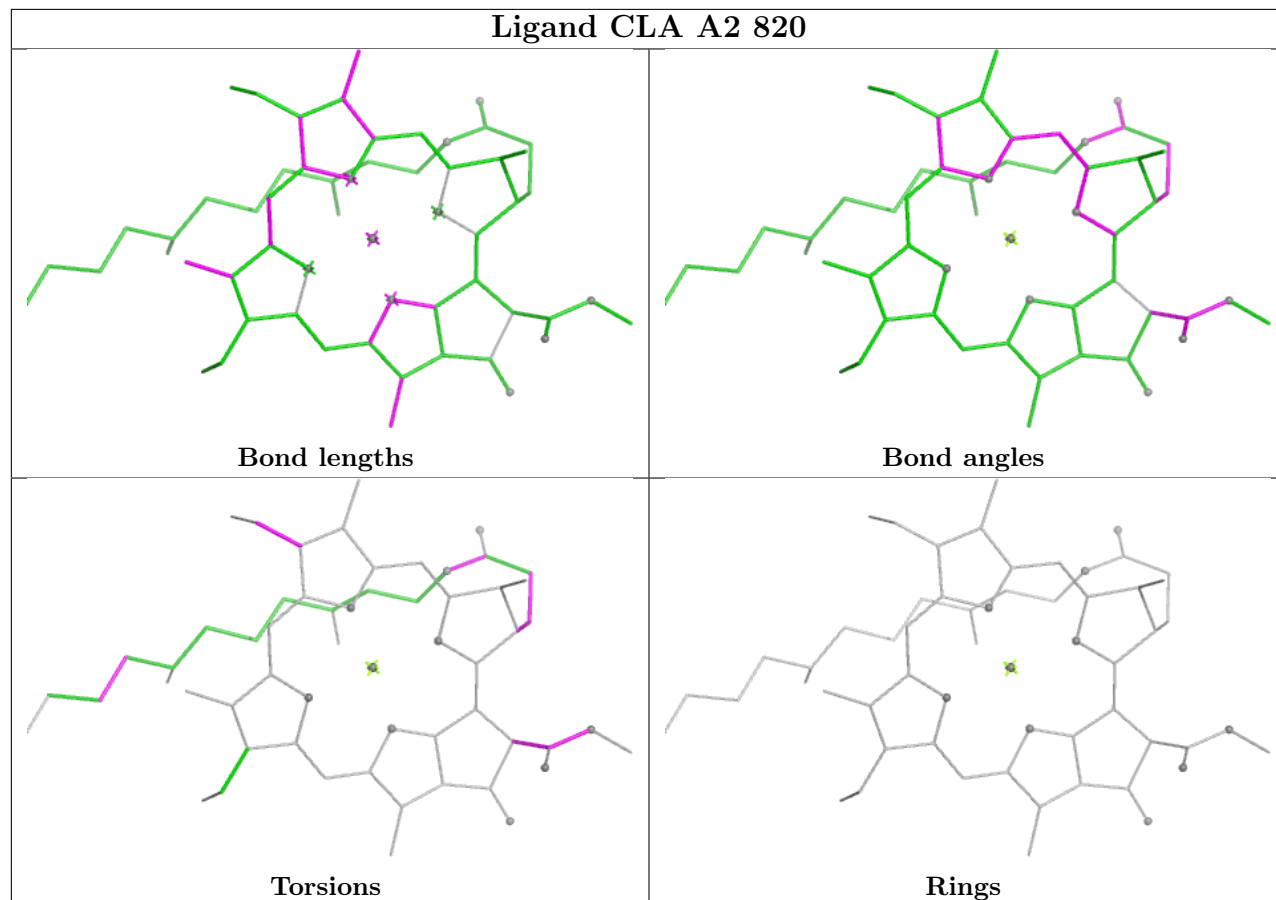
Ligand CLA AA 828	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 842	
 Bond lengths	 Bond angles
 Torsions	 Rings

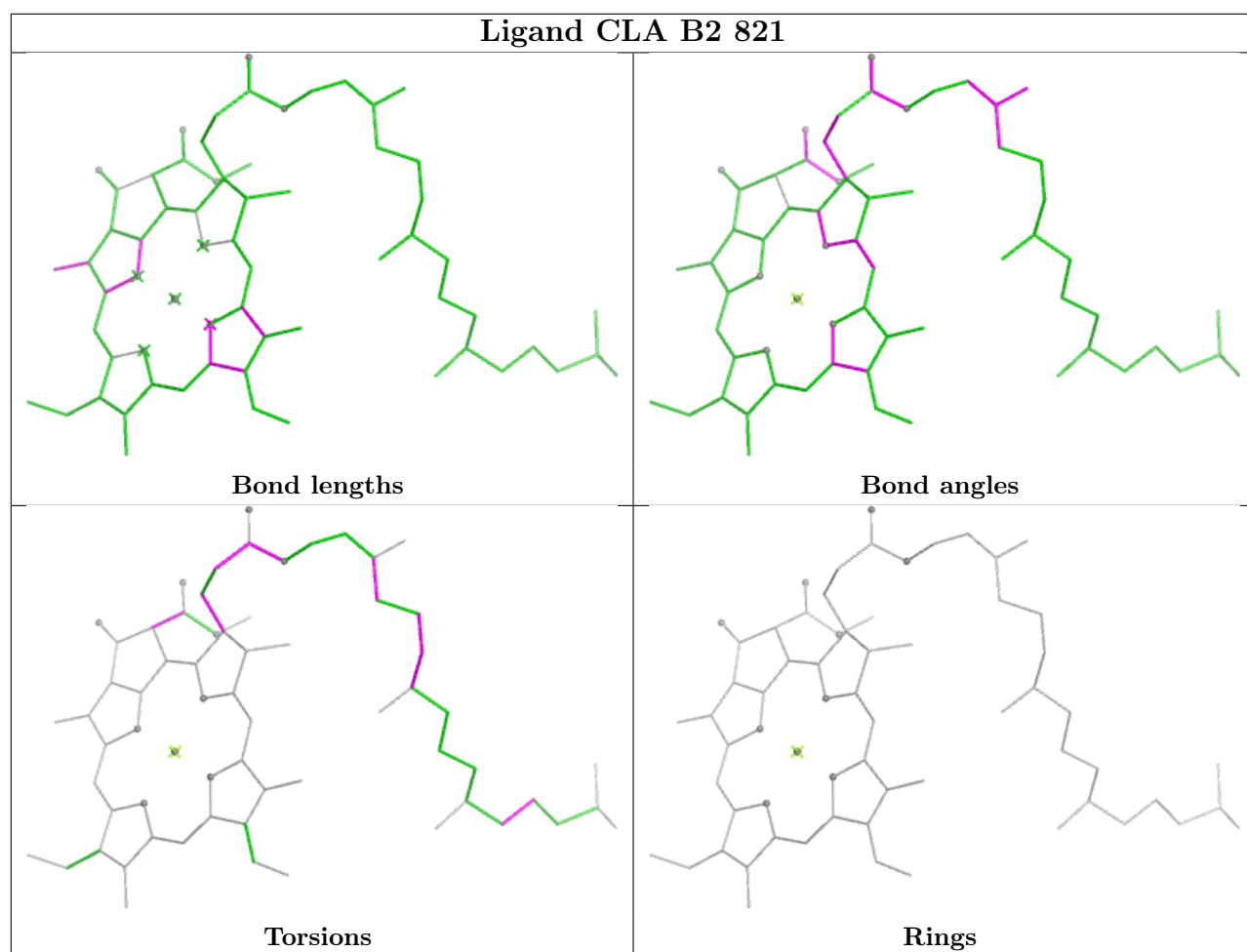


Ligand CLA B 836

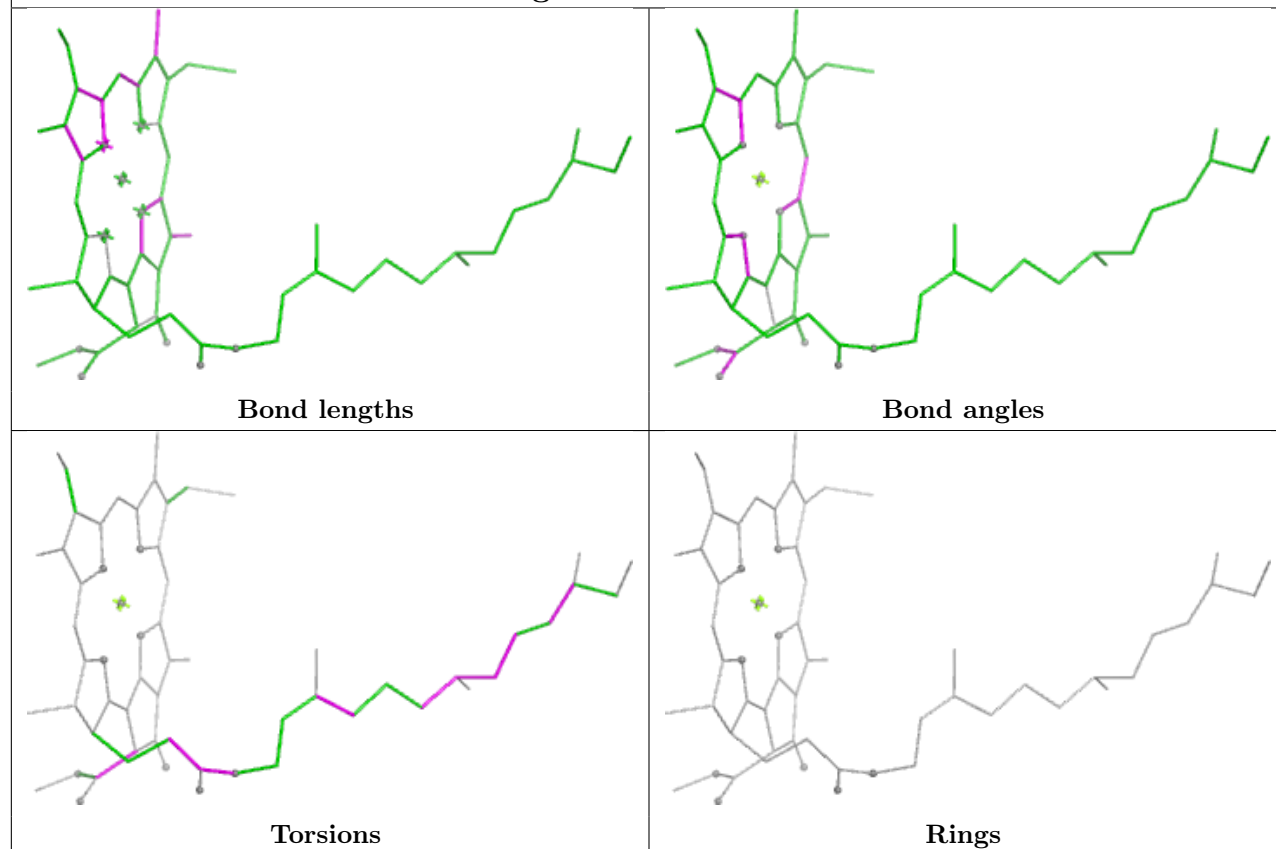


Ligand CLA A2 820

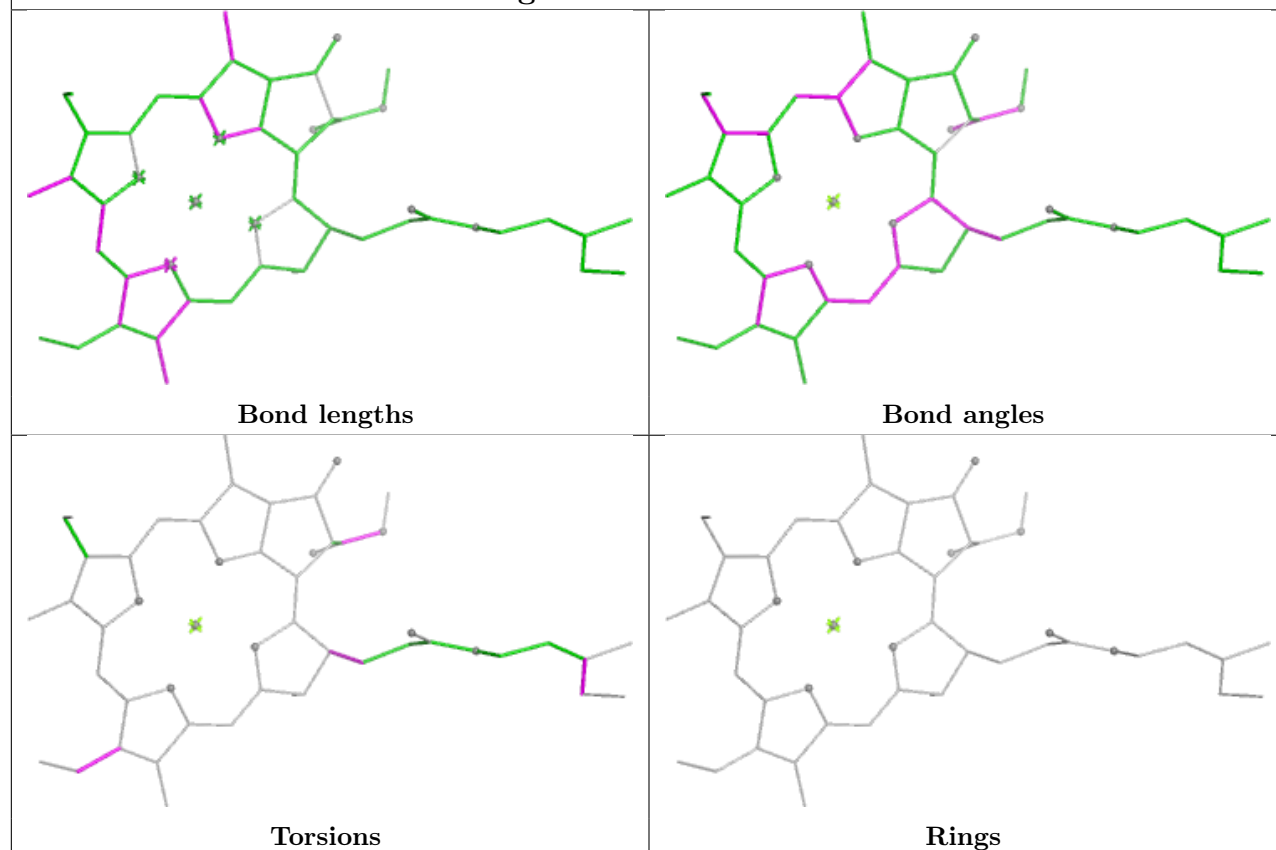


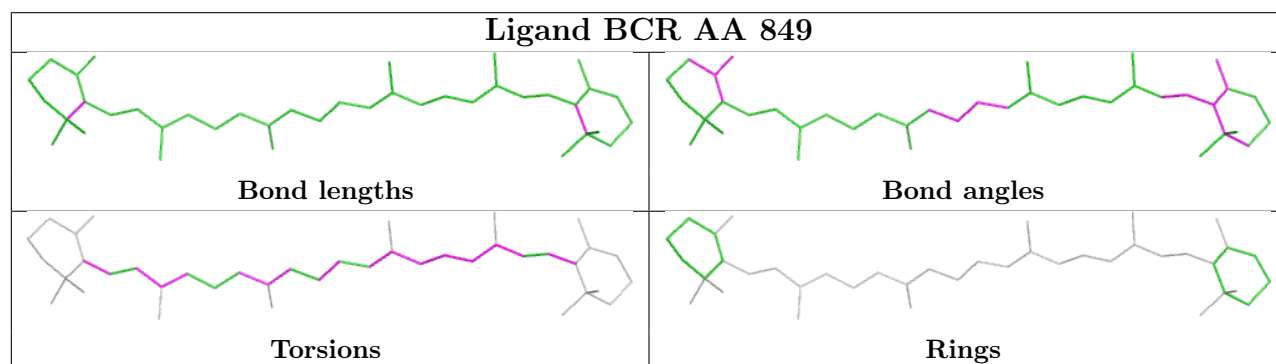
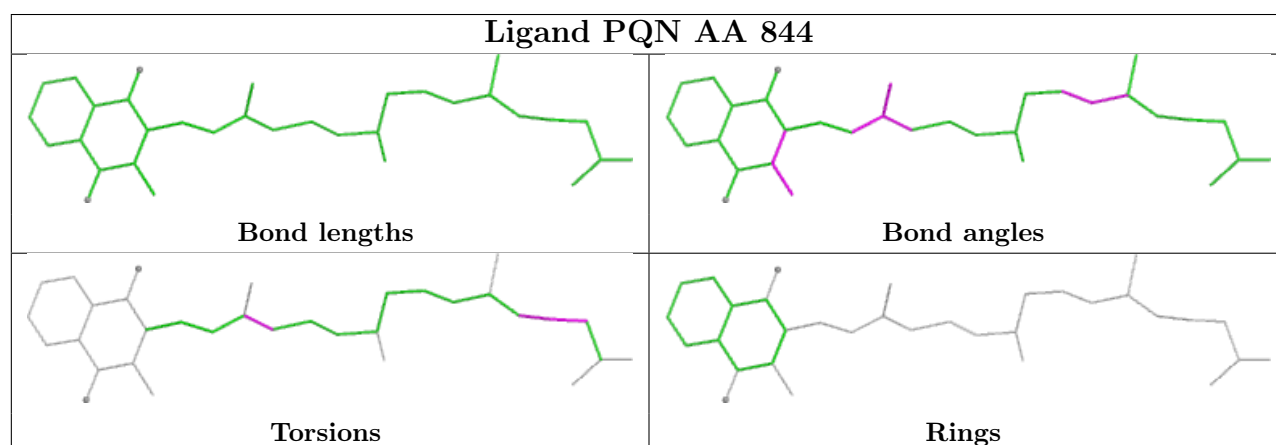
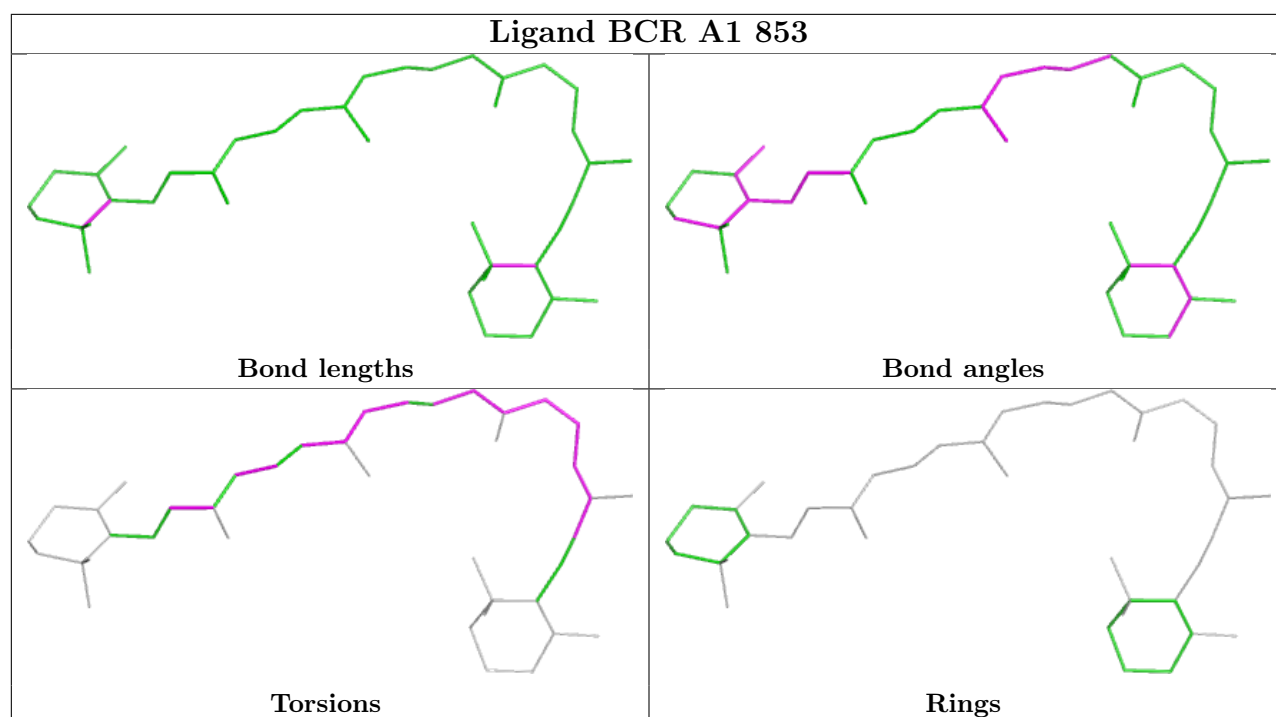


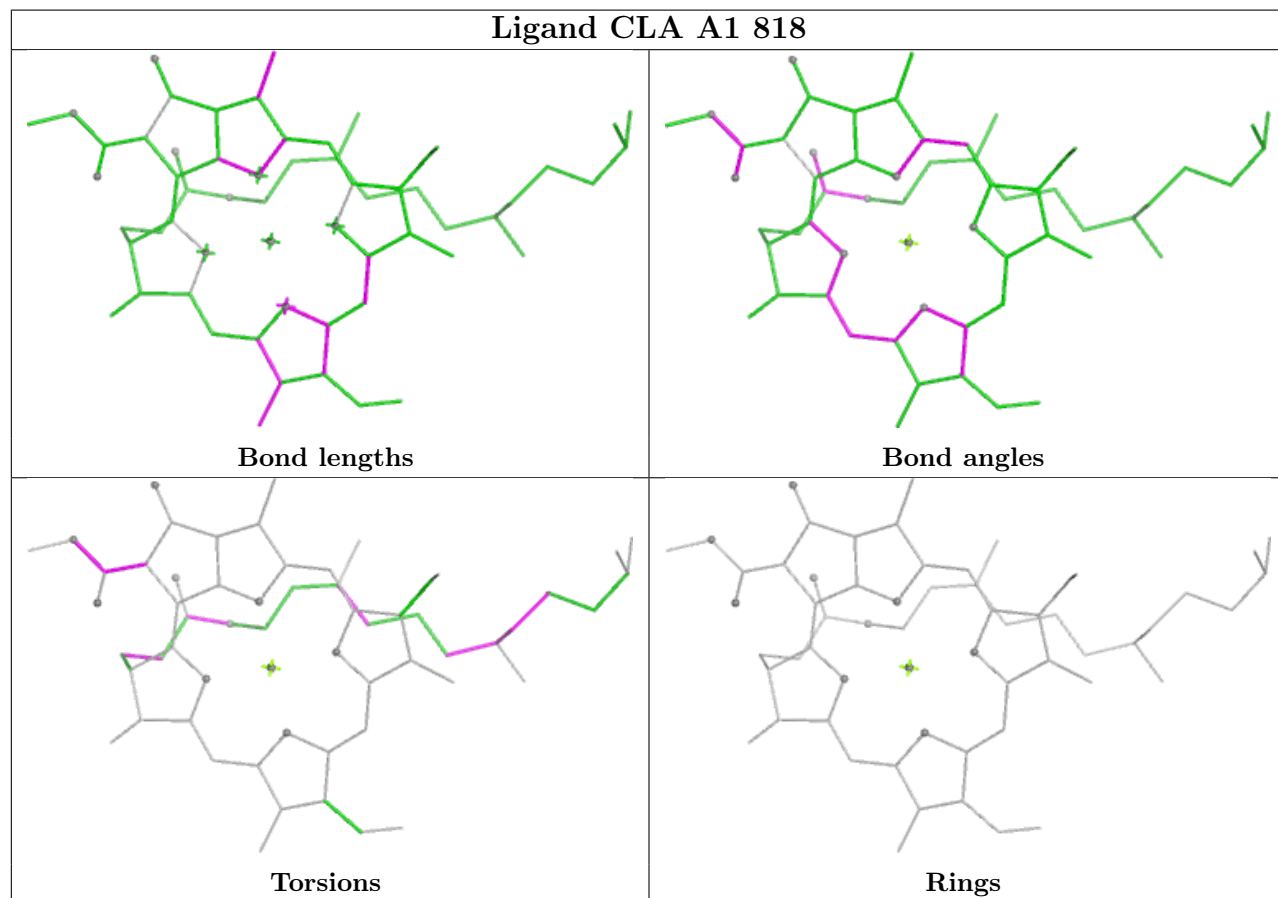
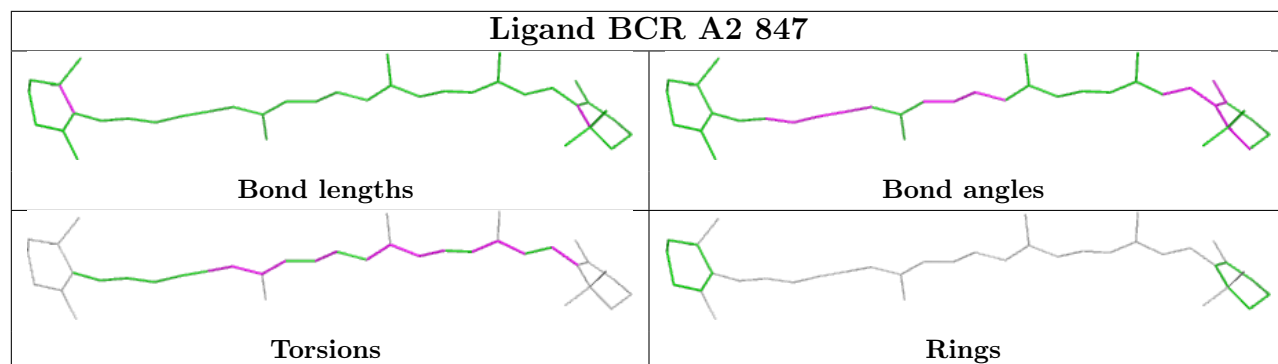
Ligand CLA B 811

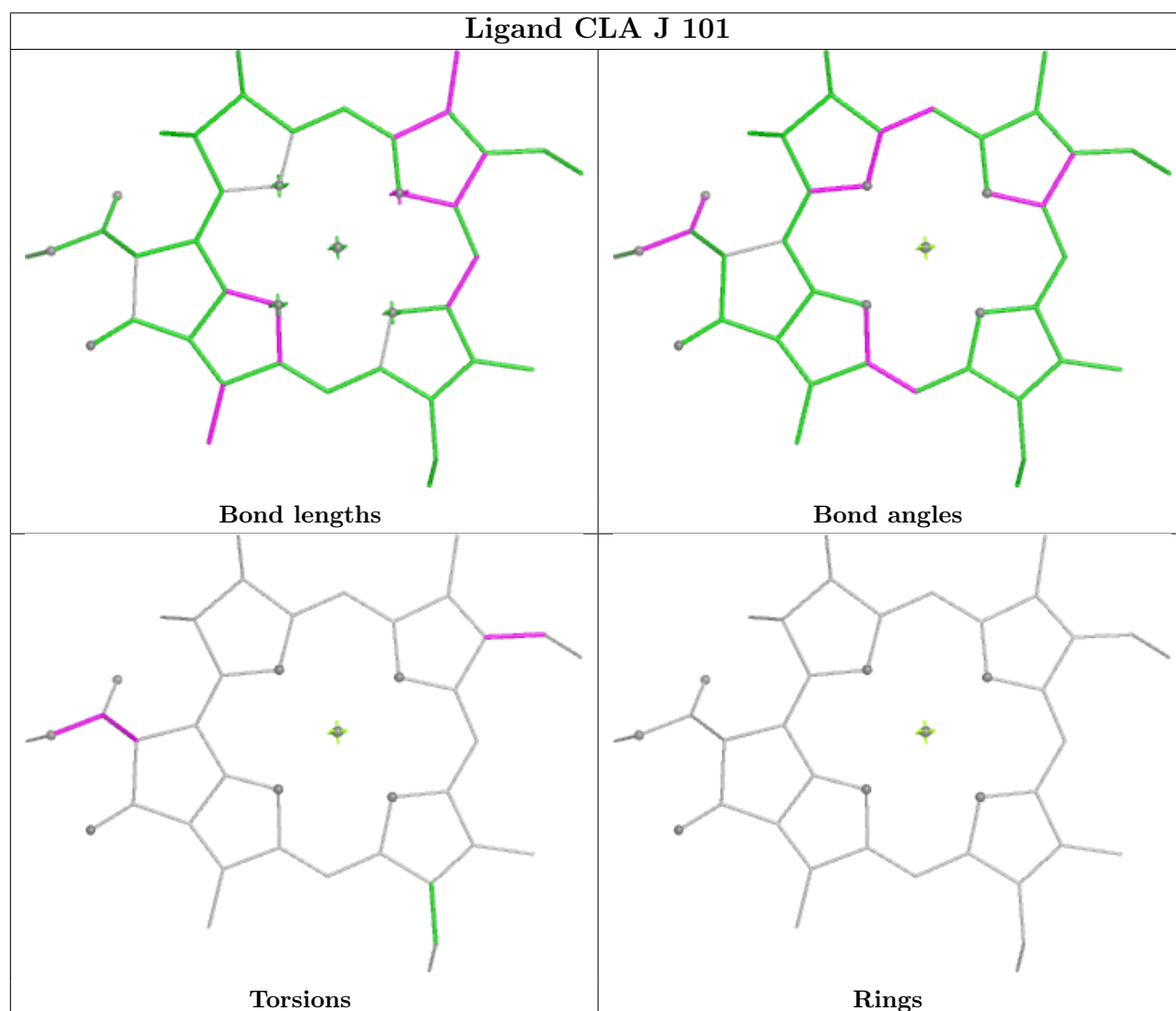
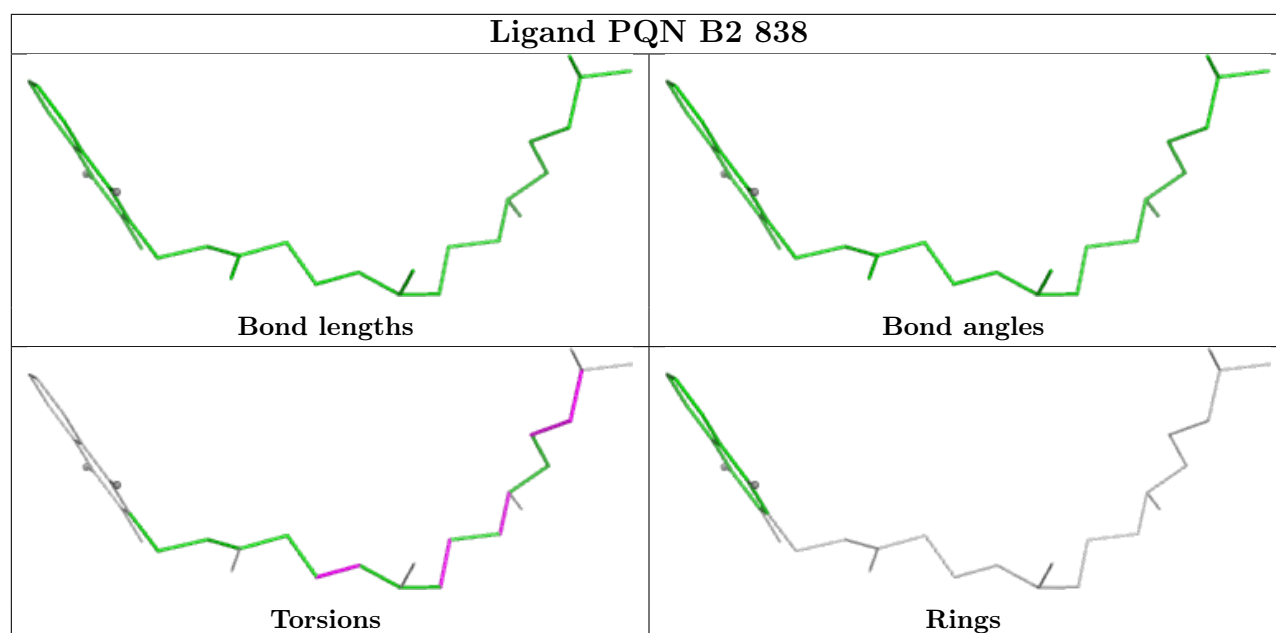


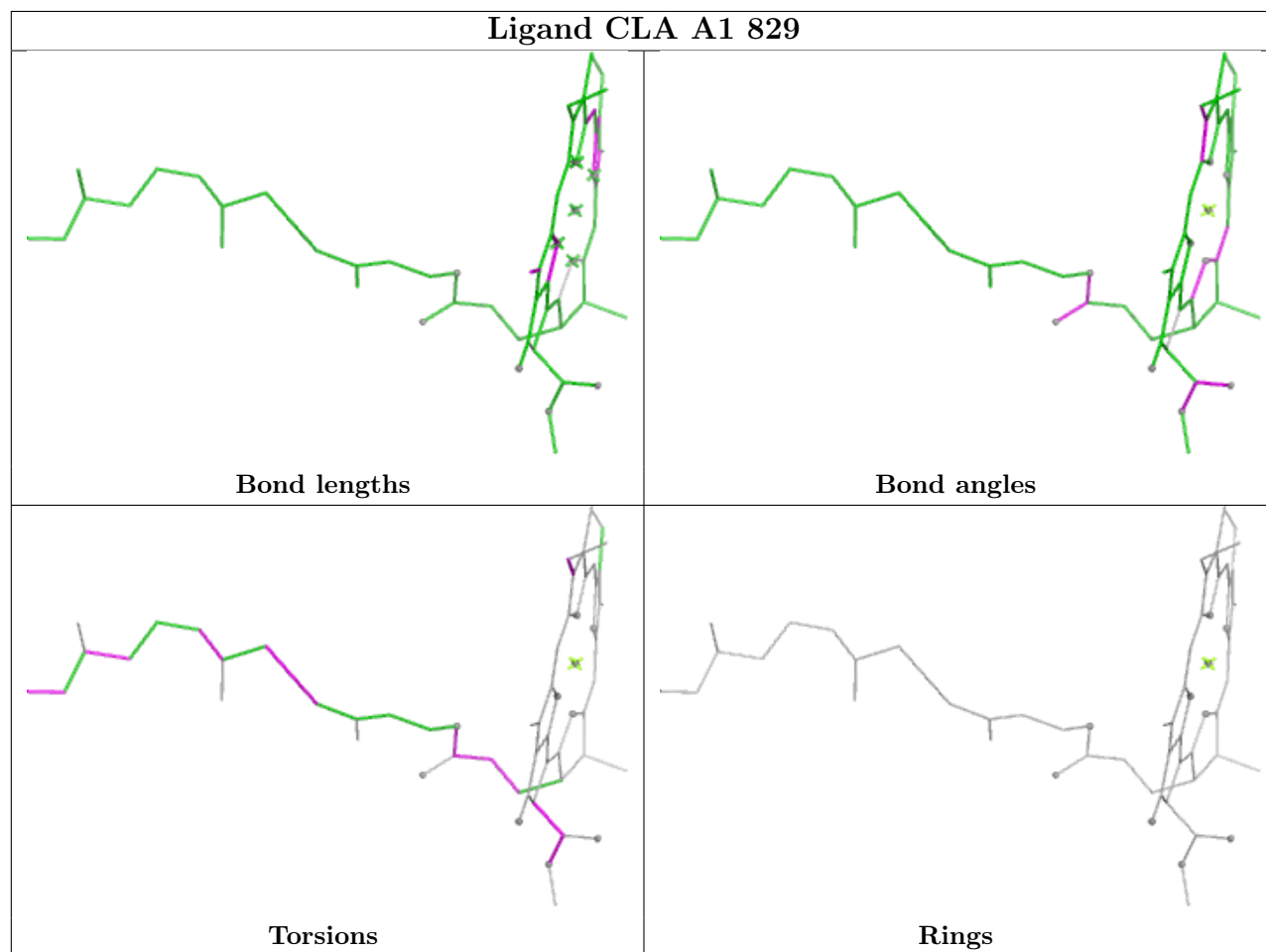
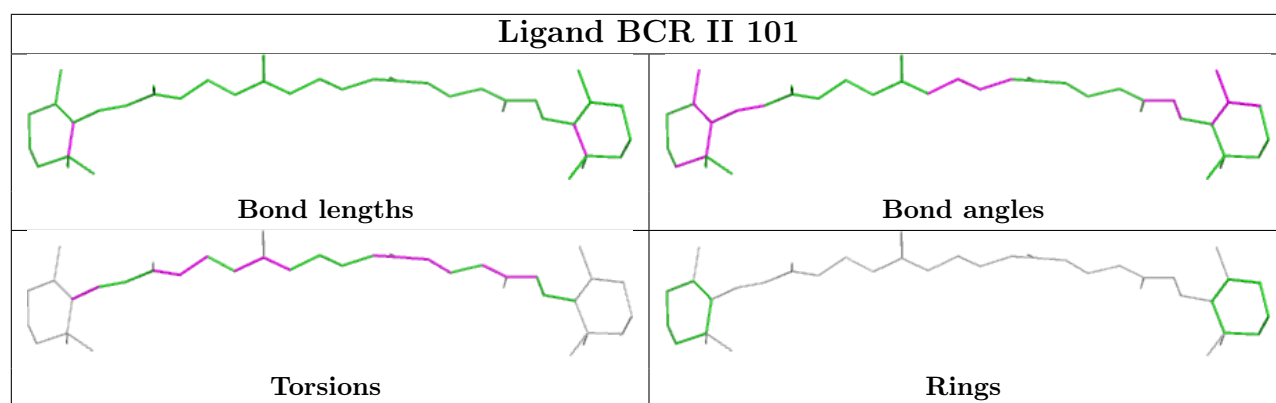
Ligand CLA AA 811



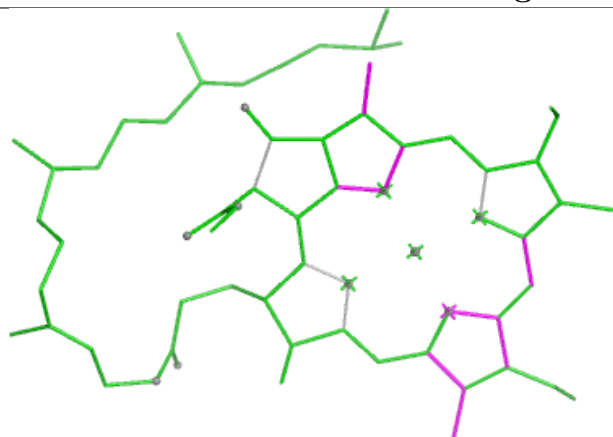




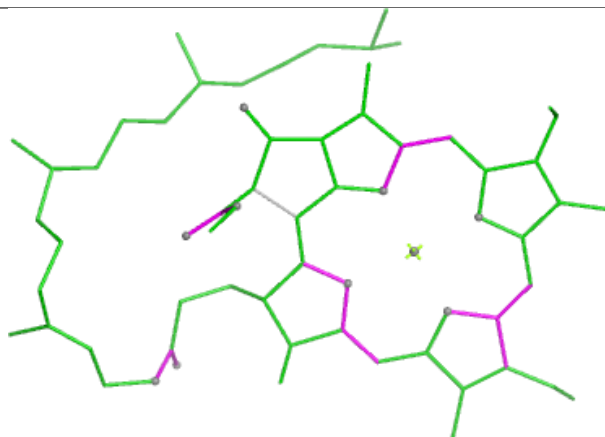




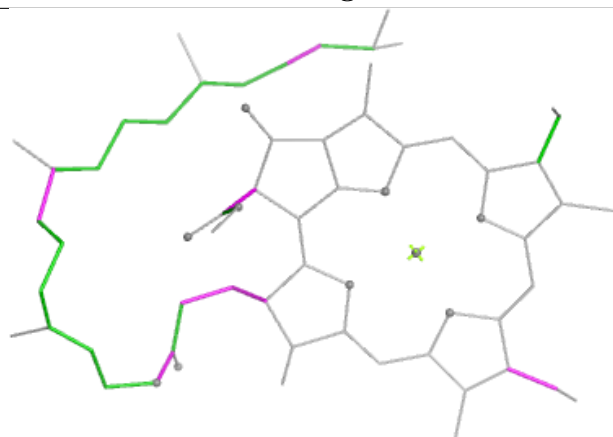
Ligand CLA B 802



Bond lengths



Bond angles

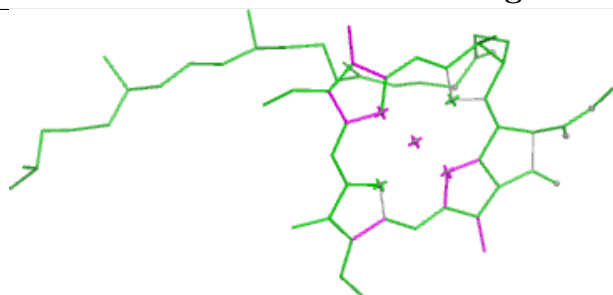


Torsions

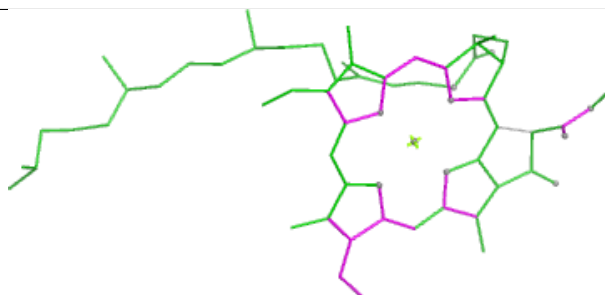


Rings

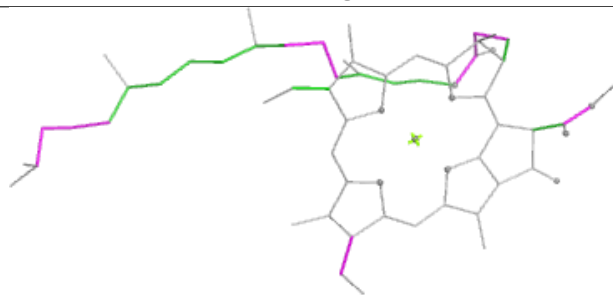
Ligand CLA A1 842



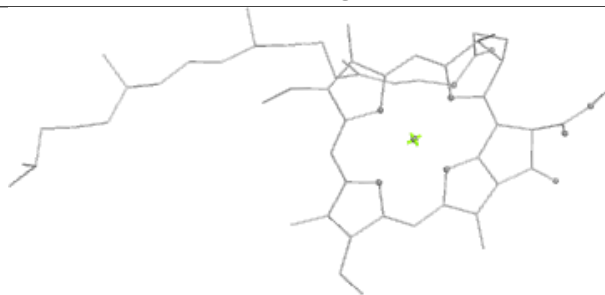
Bond lengths



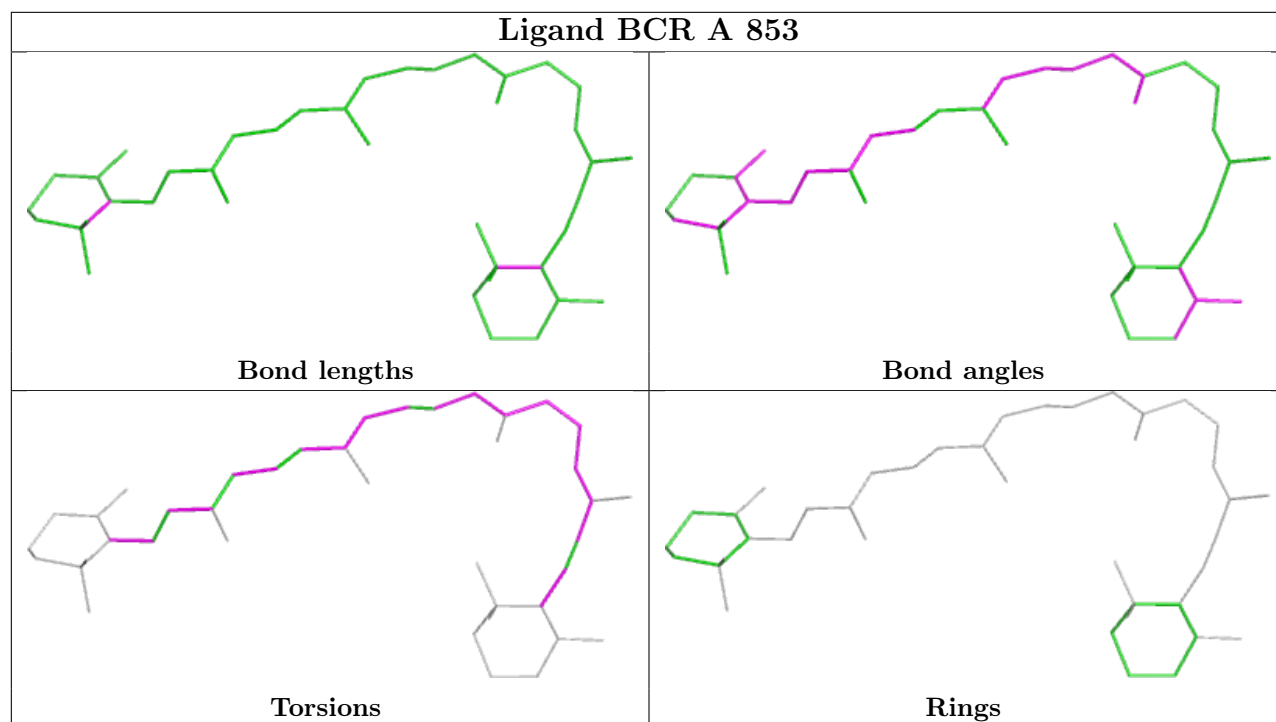
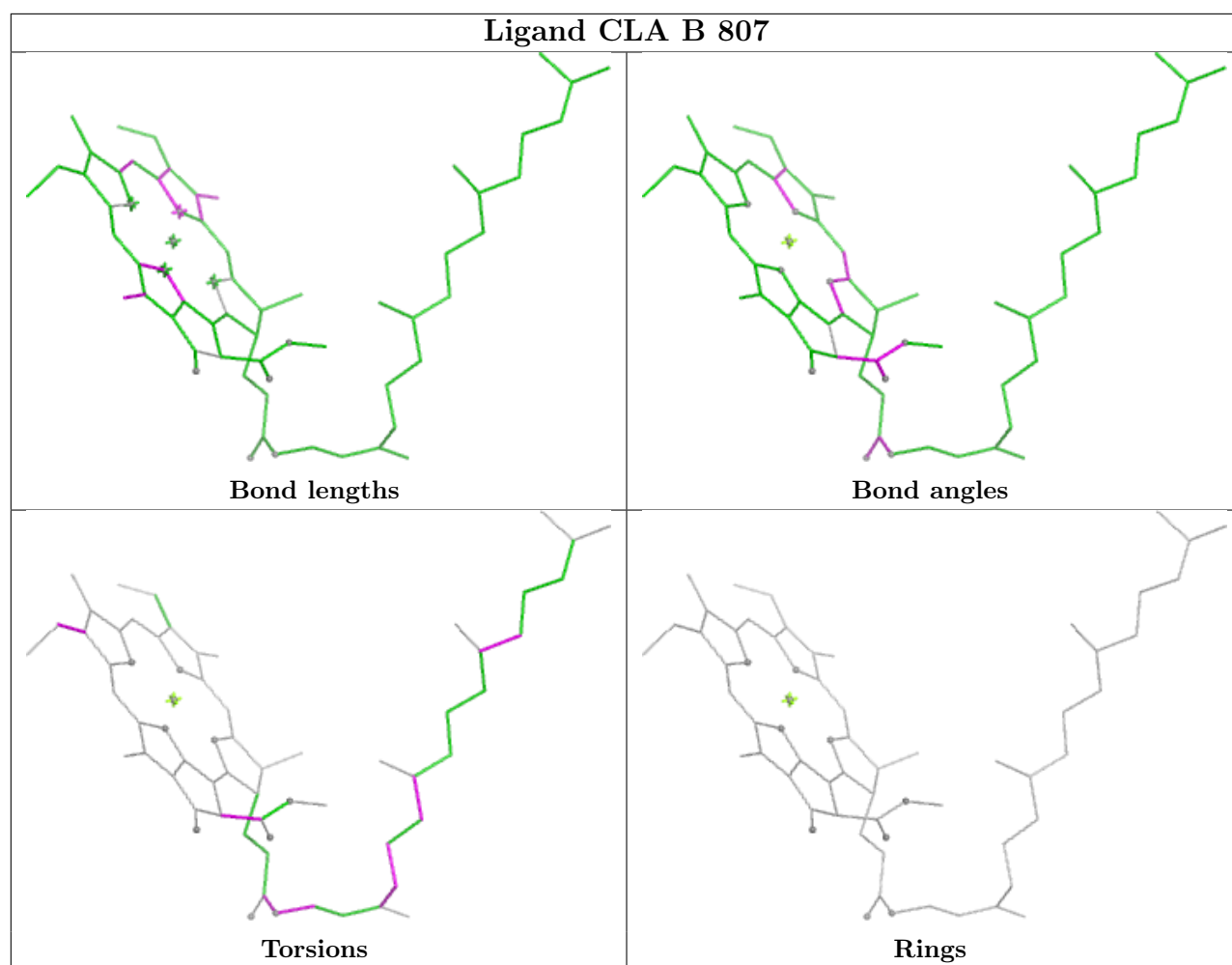
Bond angles

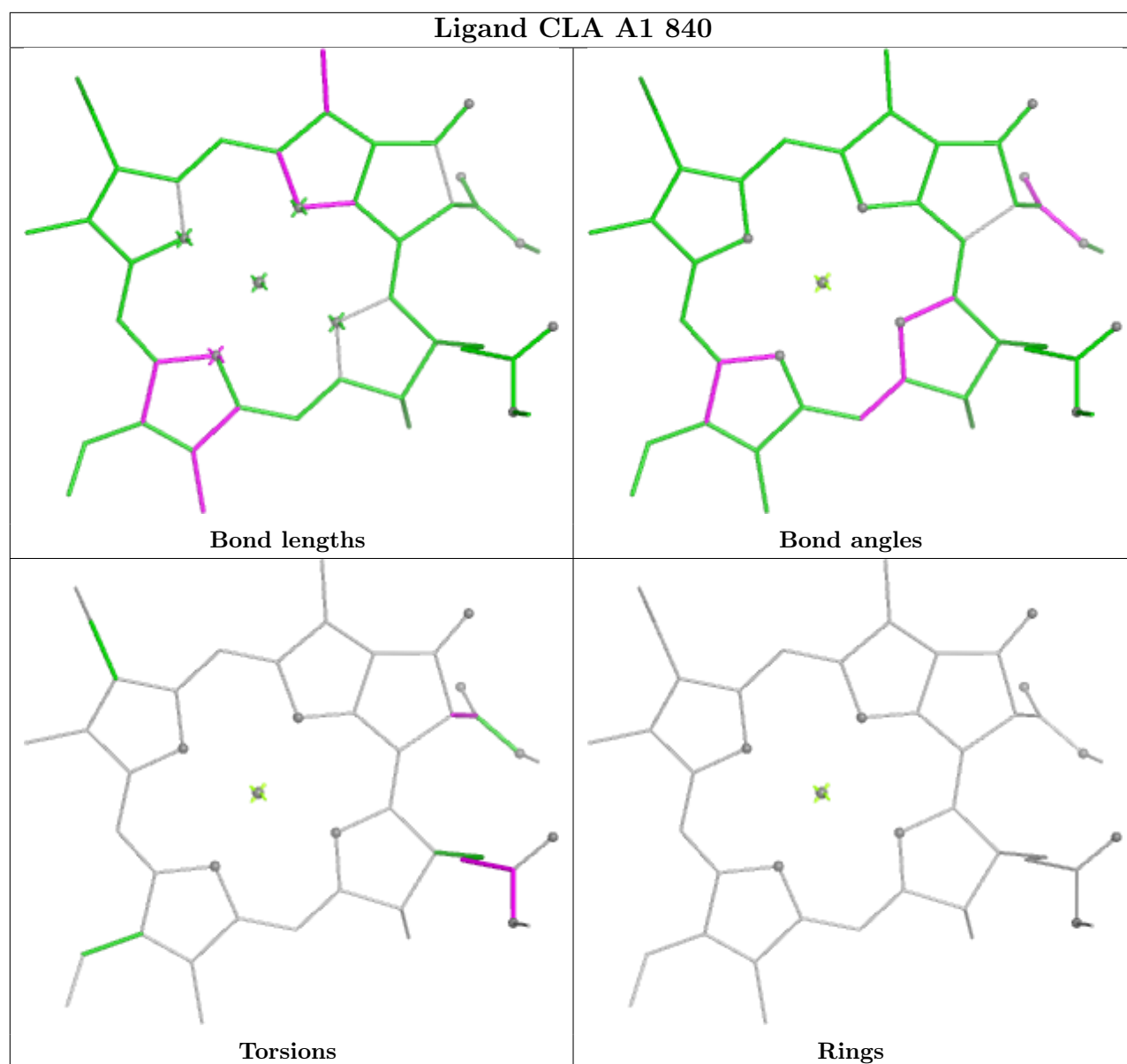


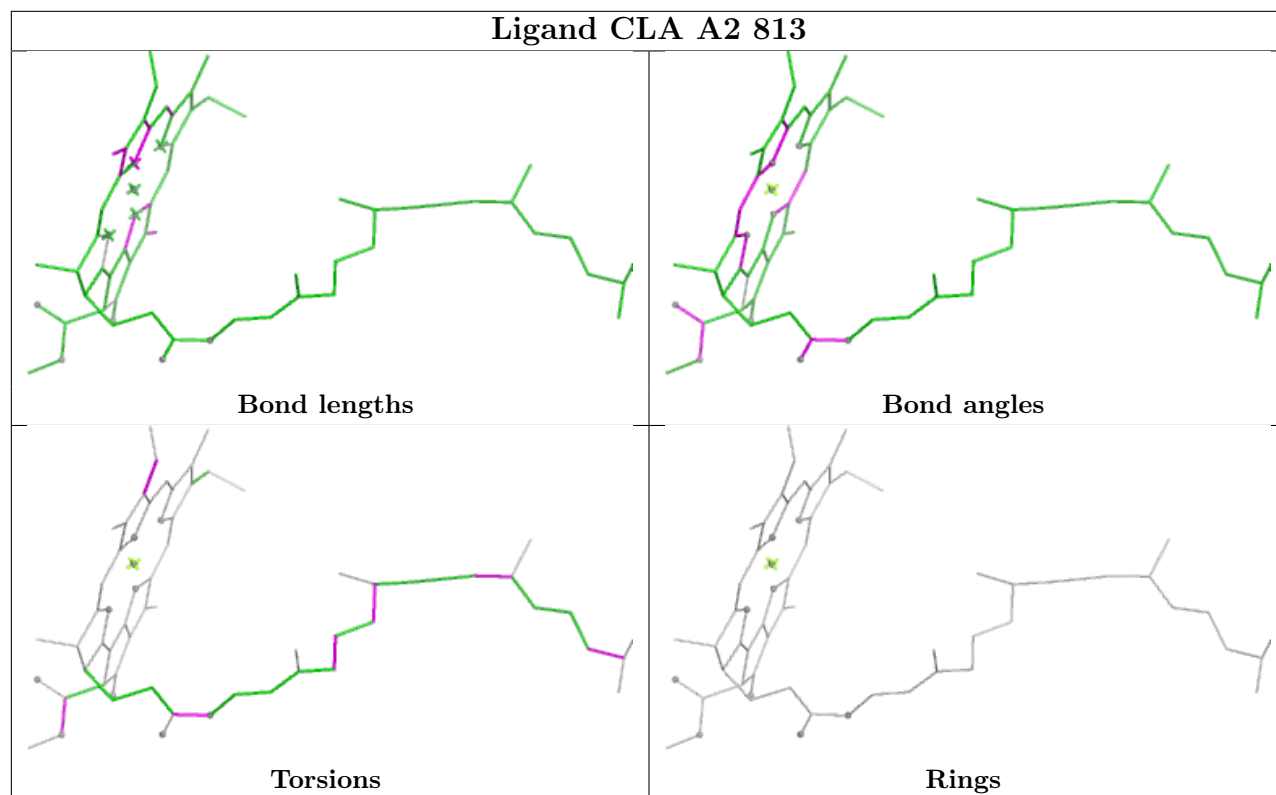
Torsions



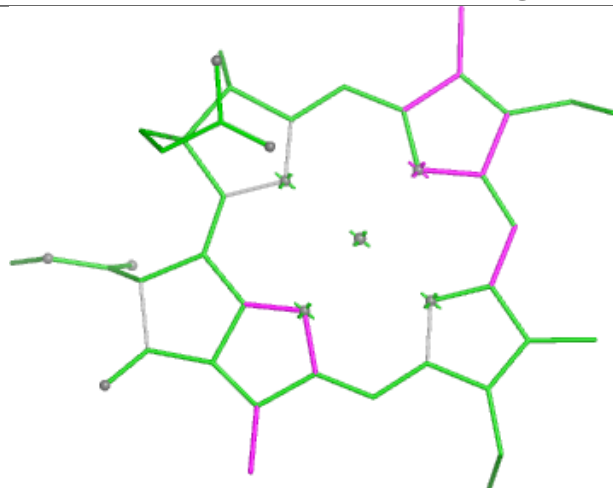
Rings



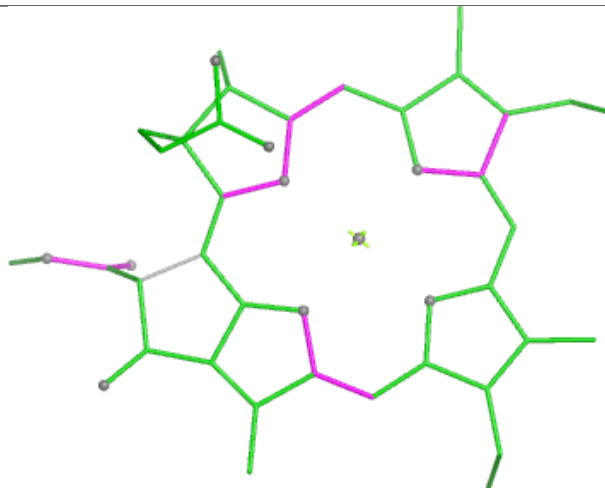




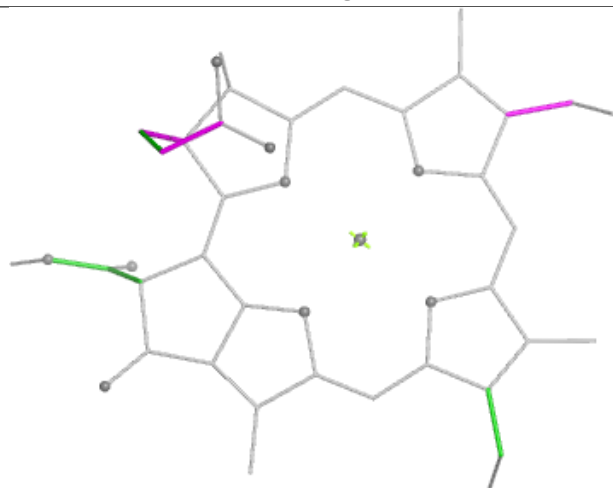
Ligand CLA A 818



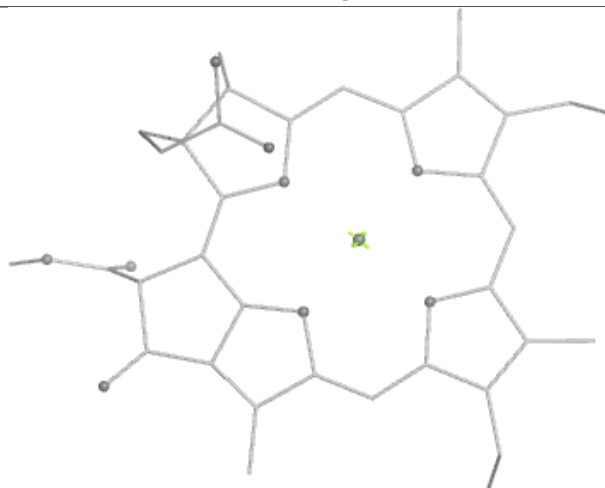
Bond lengths



Bond angles

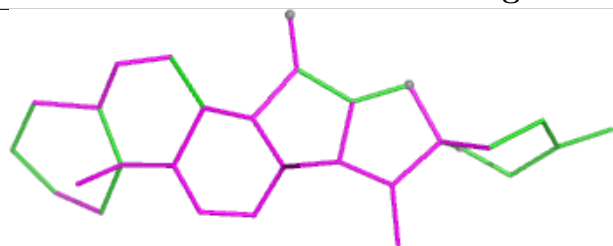


Torsions

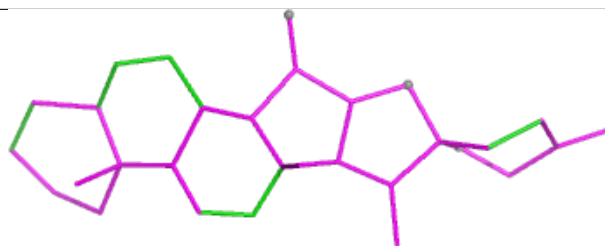


Rings

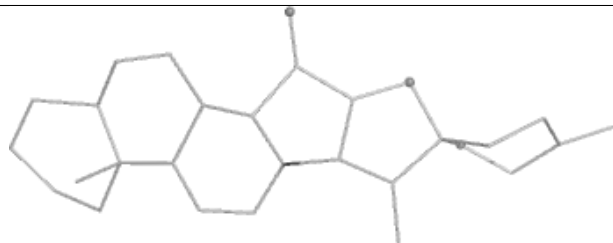
Ligand AJP AA 802



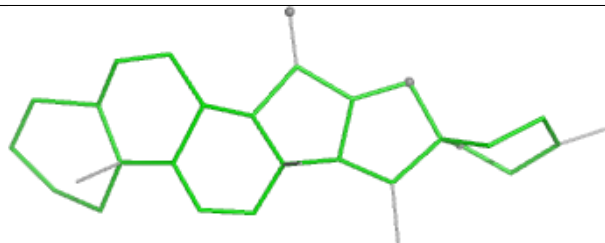
Bond lengths



Bond angles

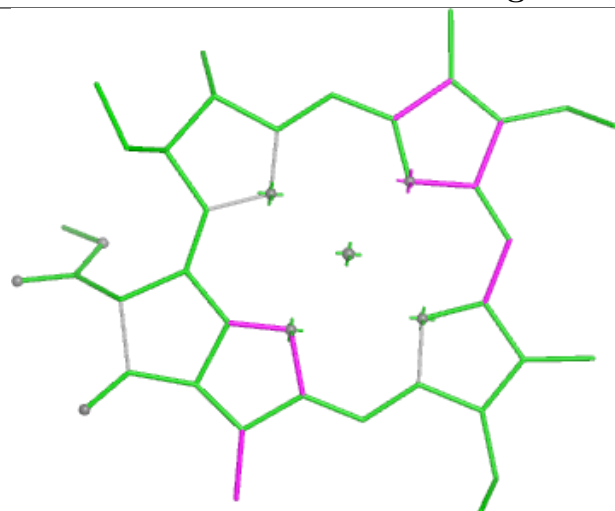


Torsions

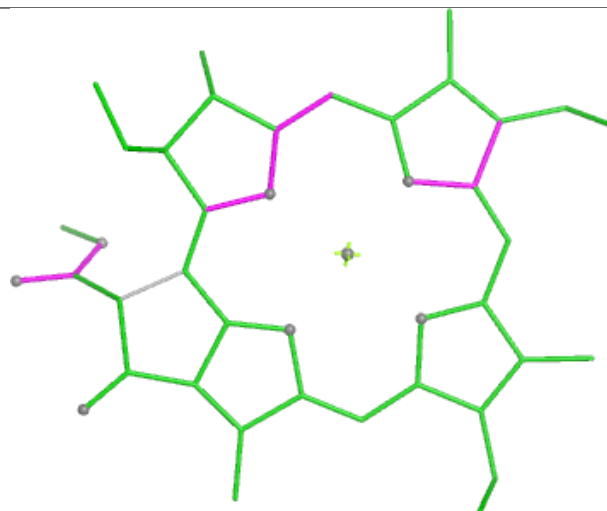


Rings

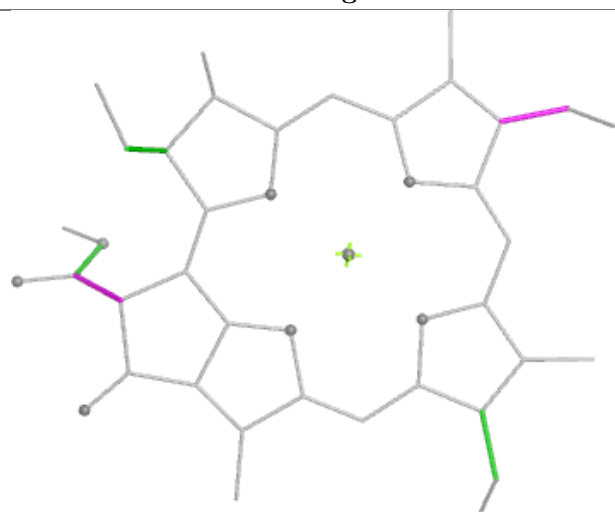
Ligand CLA B2 817



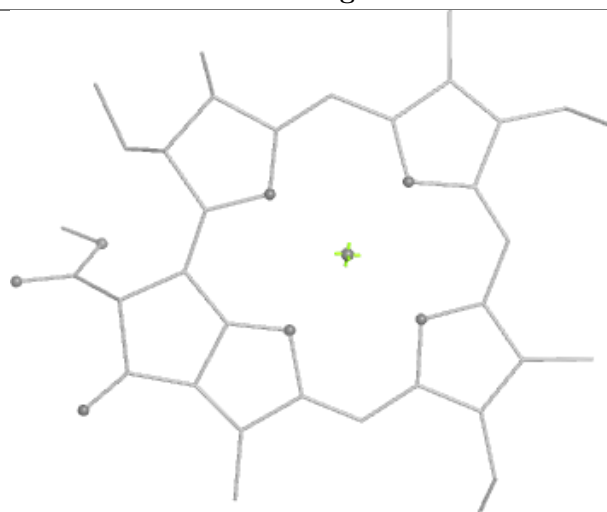
Bond lengths



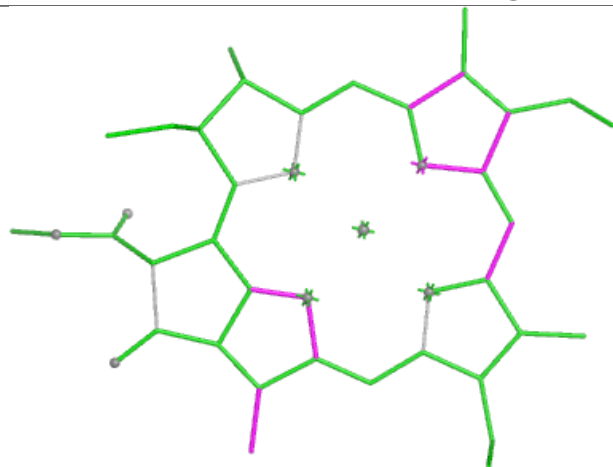
Bond angles



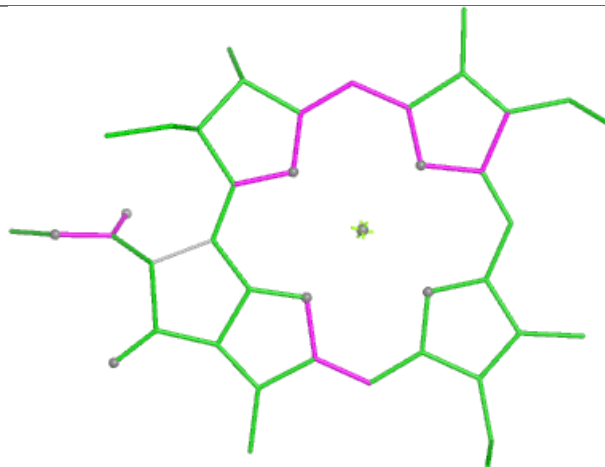
Torsions



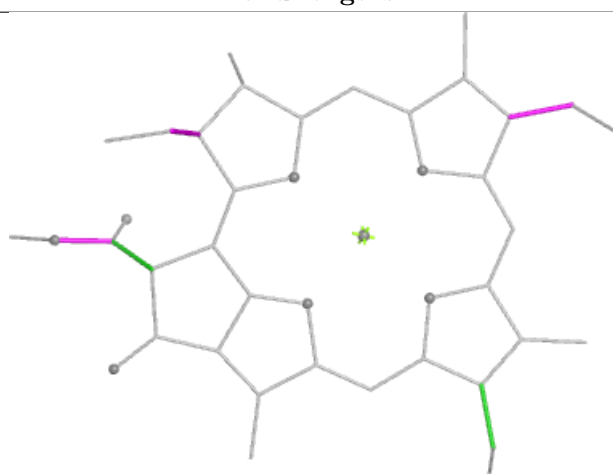
Rings

Ligand CLA A1 813

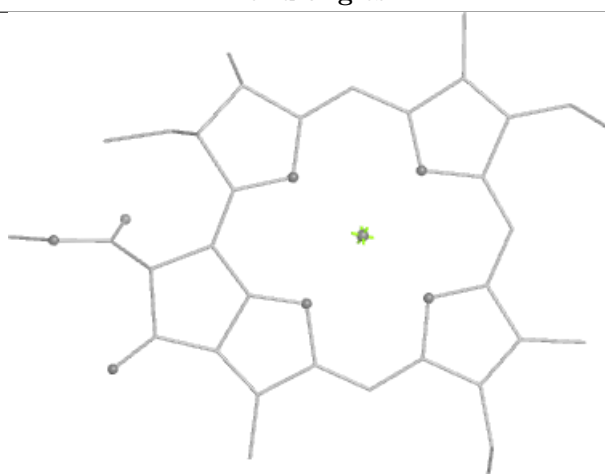
Bond lengths



Bond angles

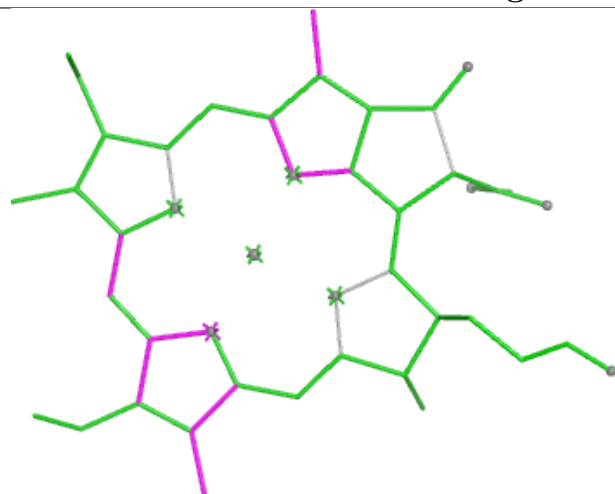


Torsions

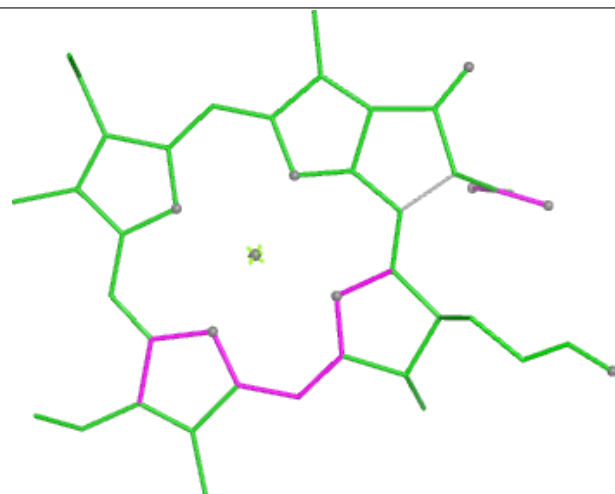


Rings

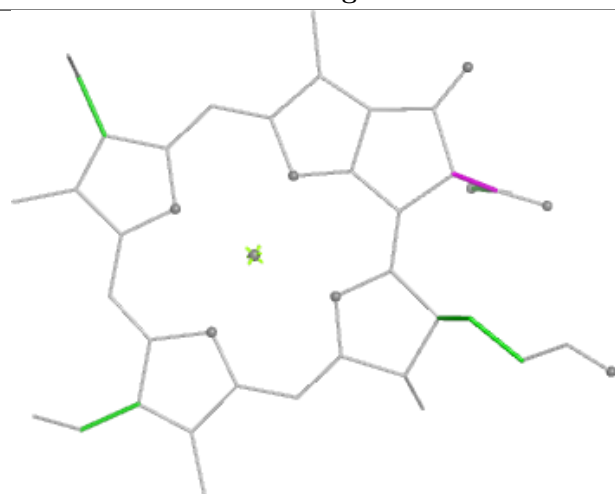
Ligand CLA A1 816



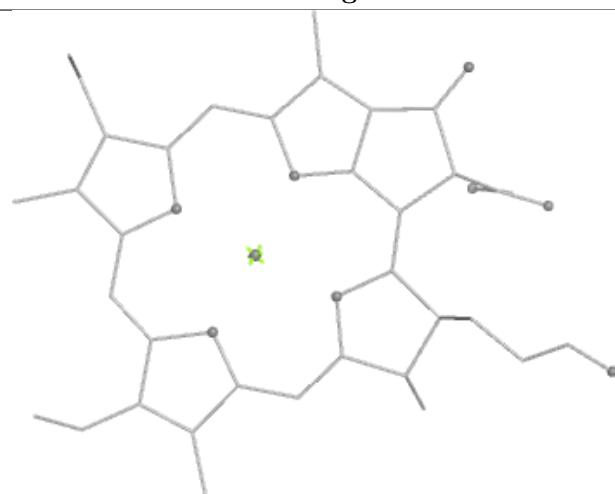
Bond lengths



Bond angles

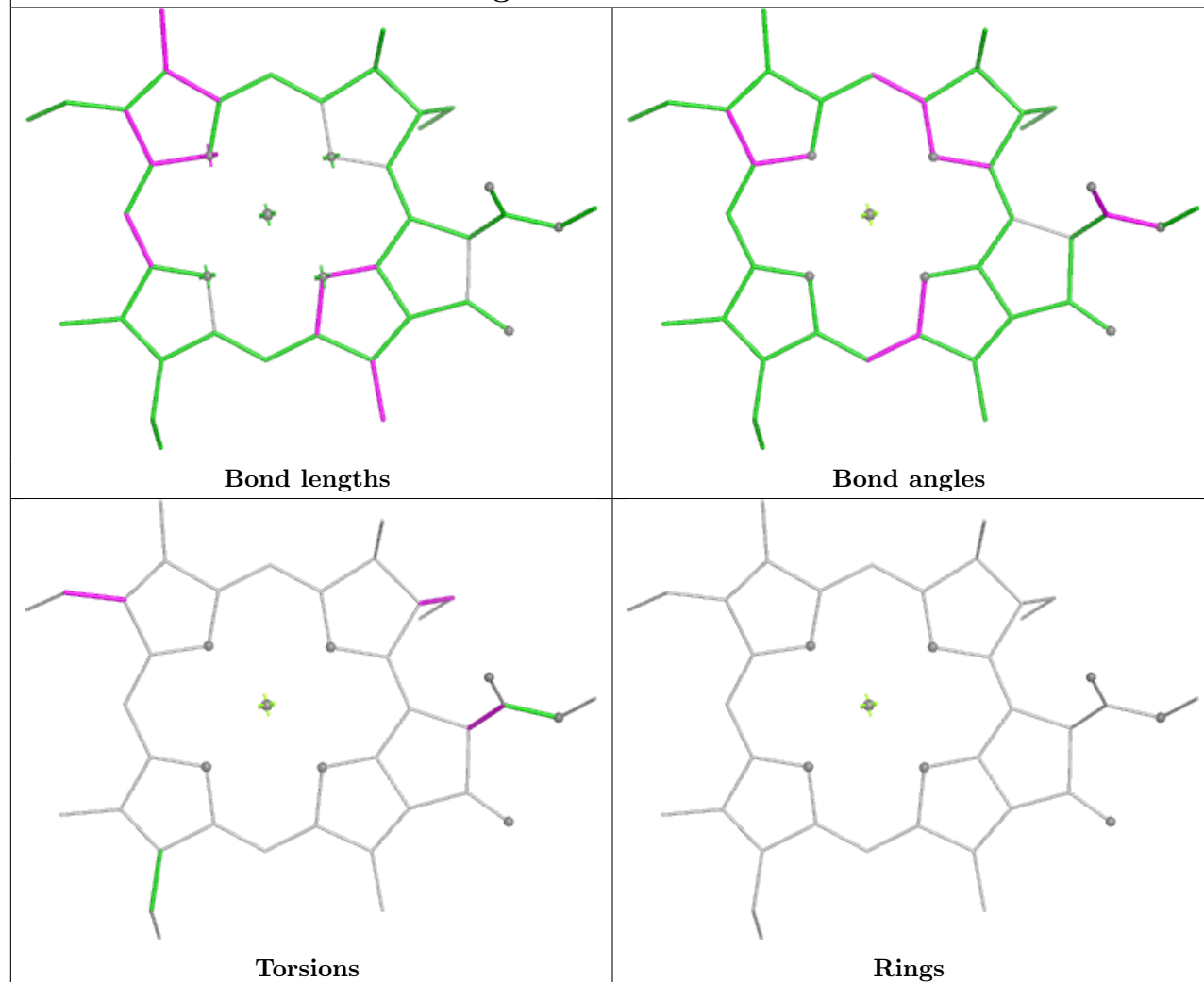


Torsions

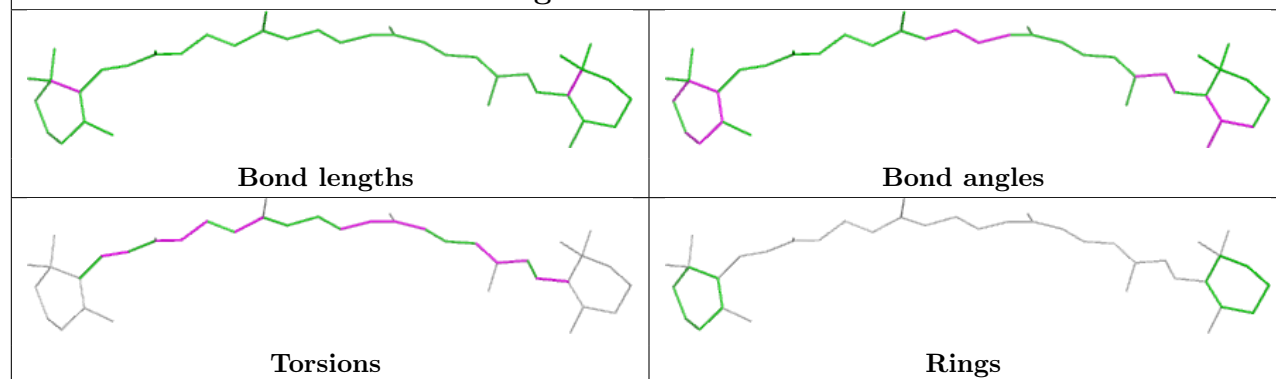


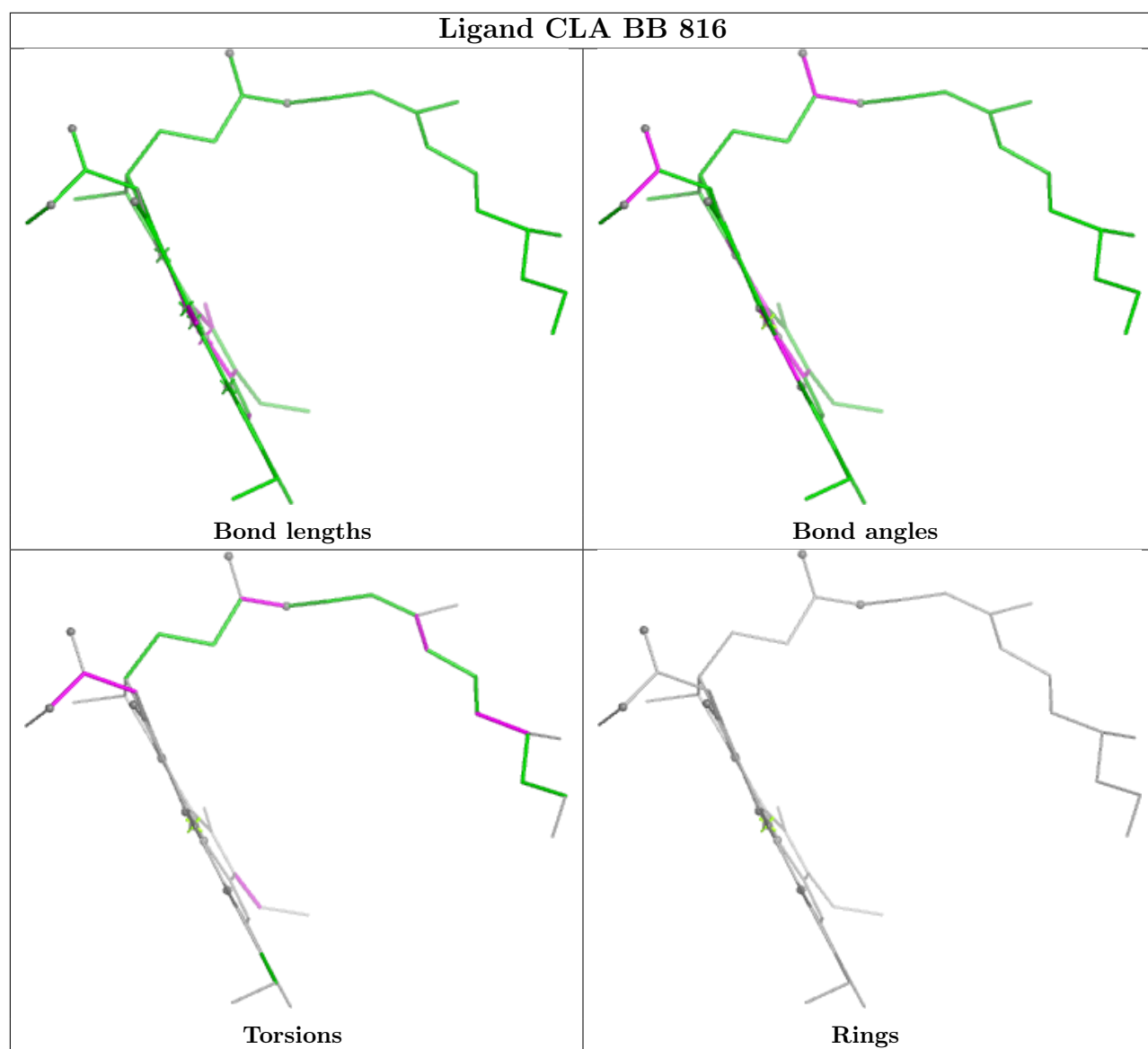
Rings

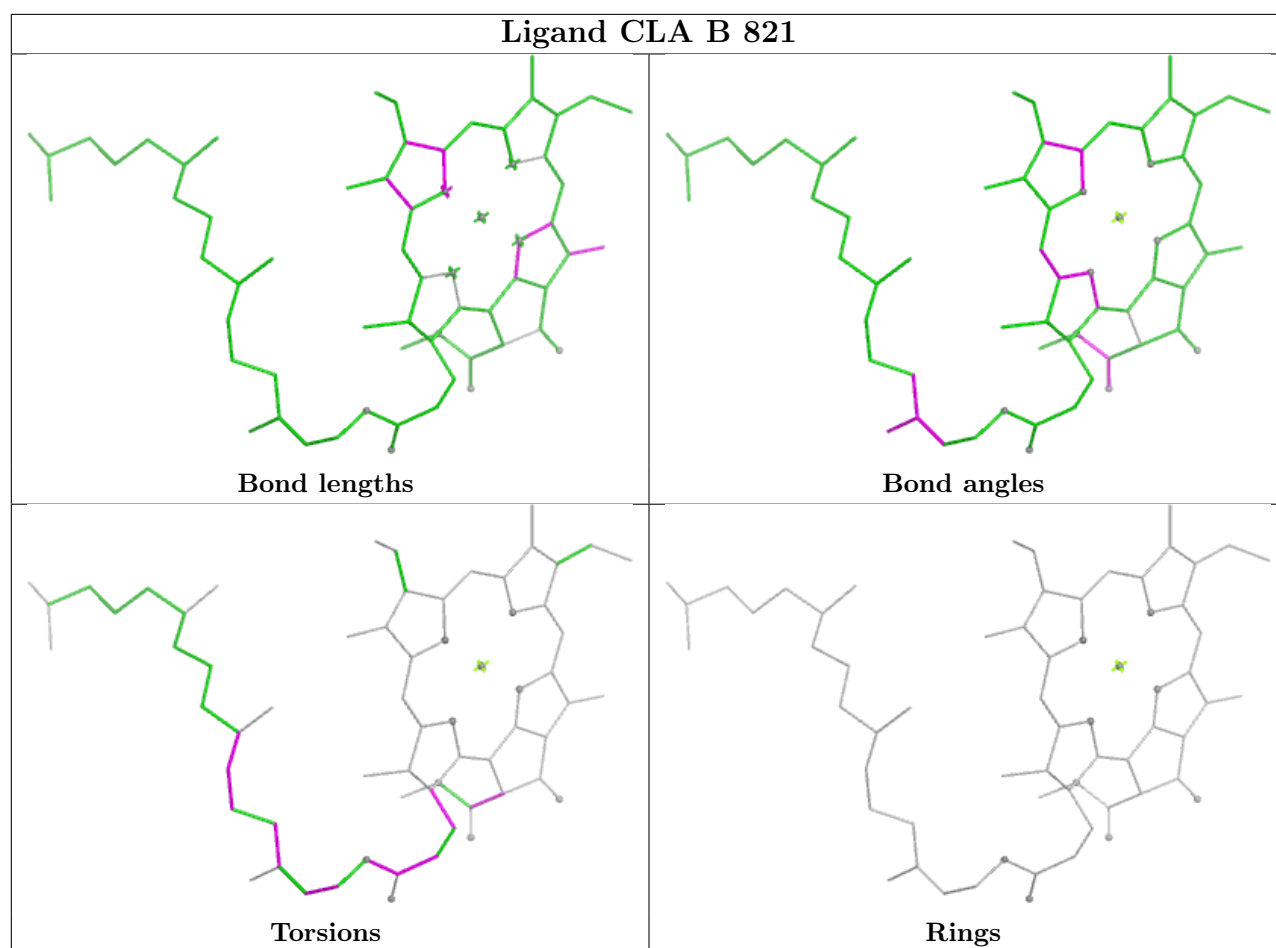
Ligand CLA A1 824

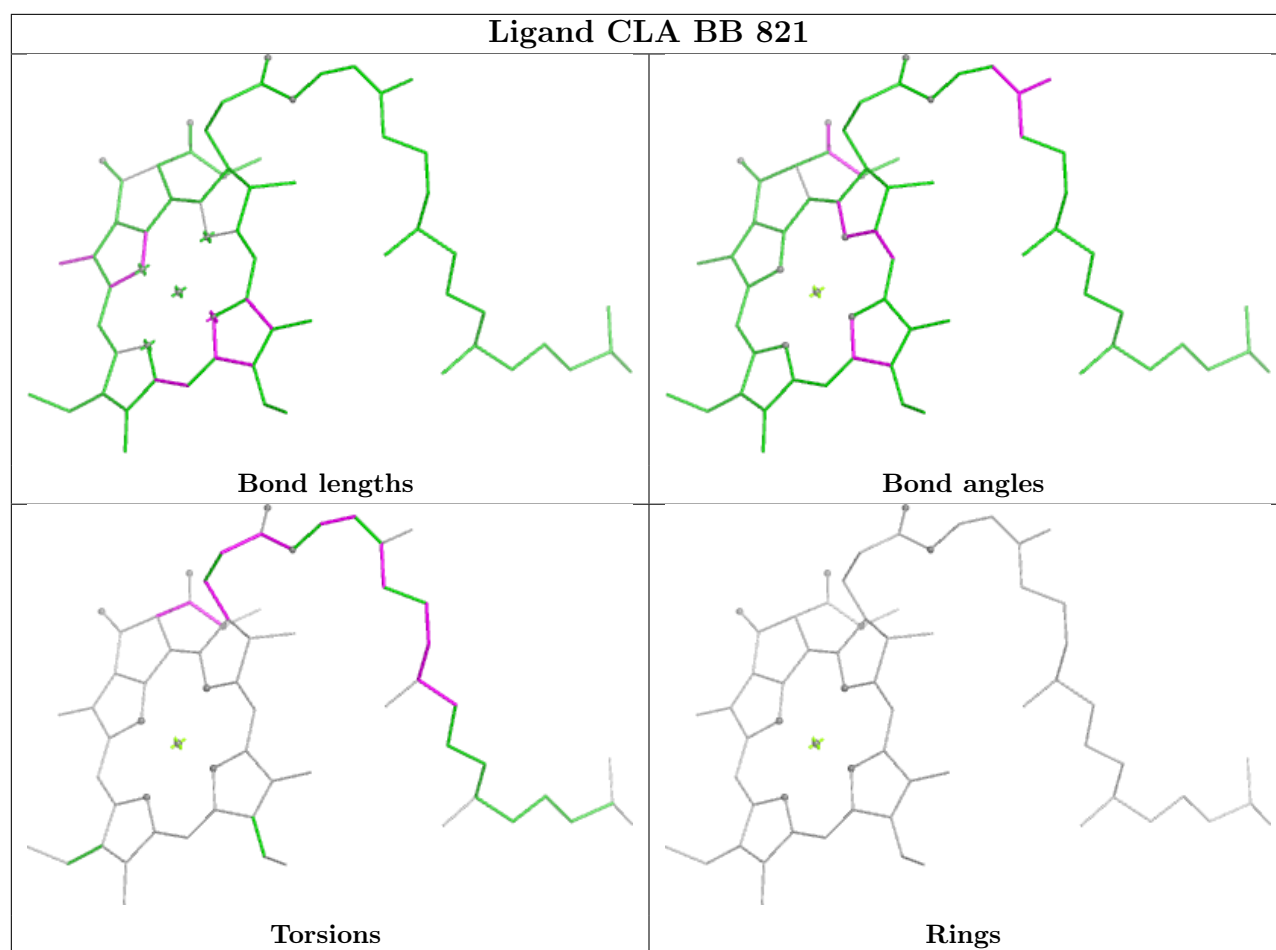


Ligand BCR J 104

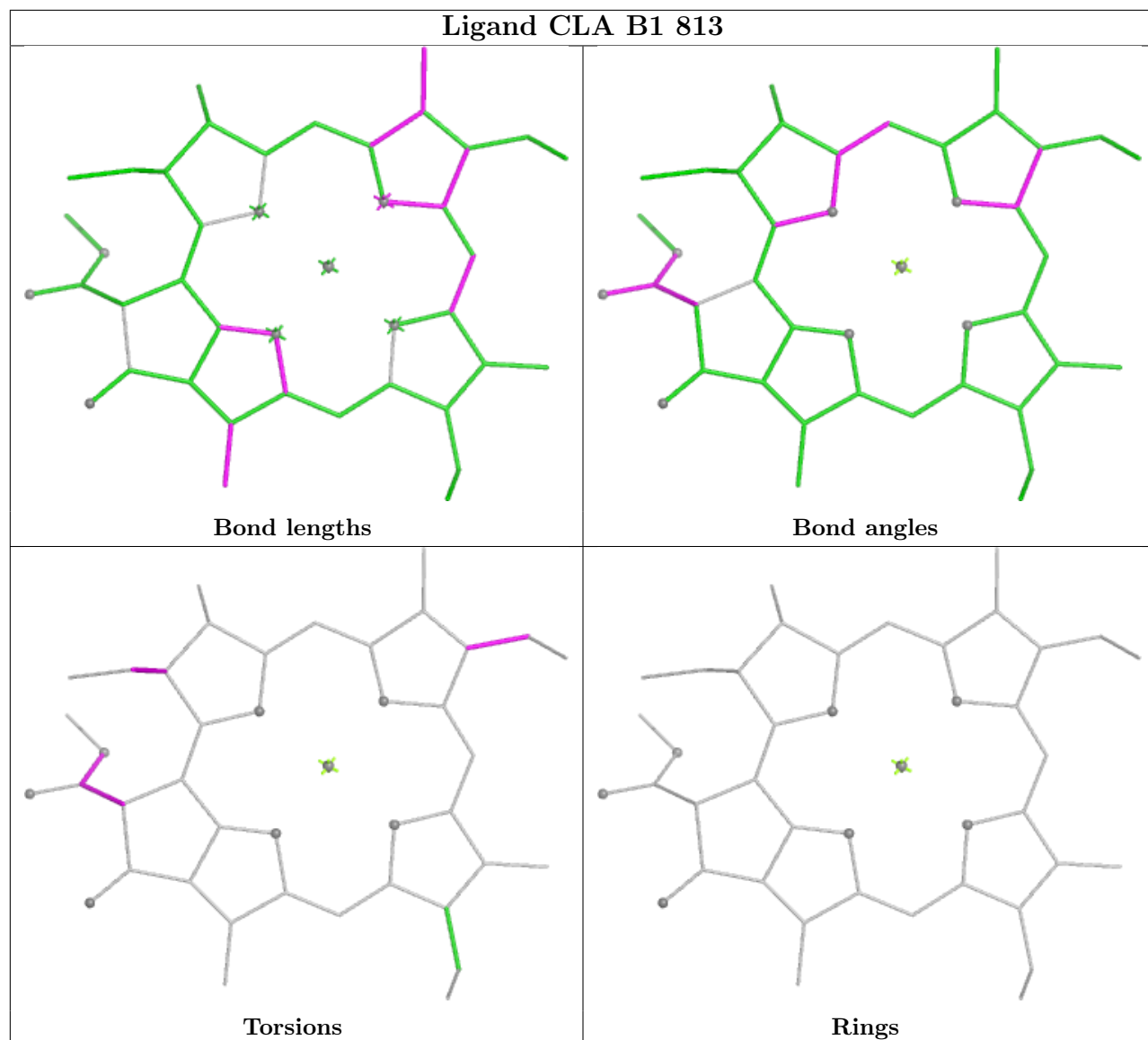




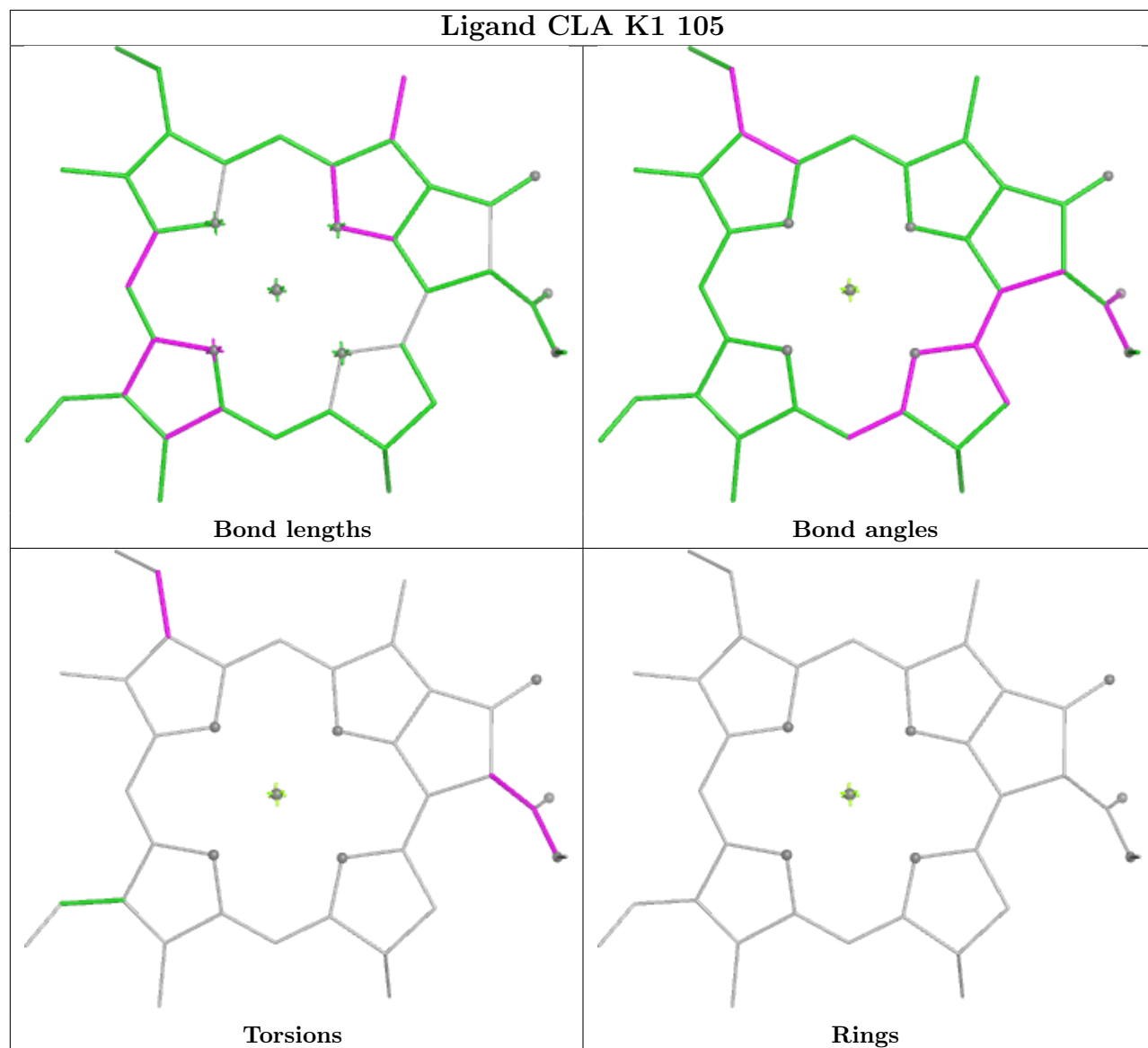




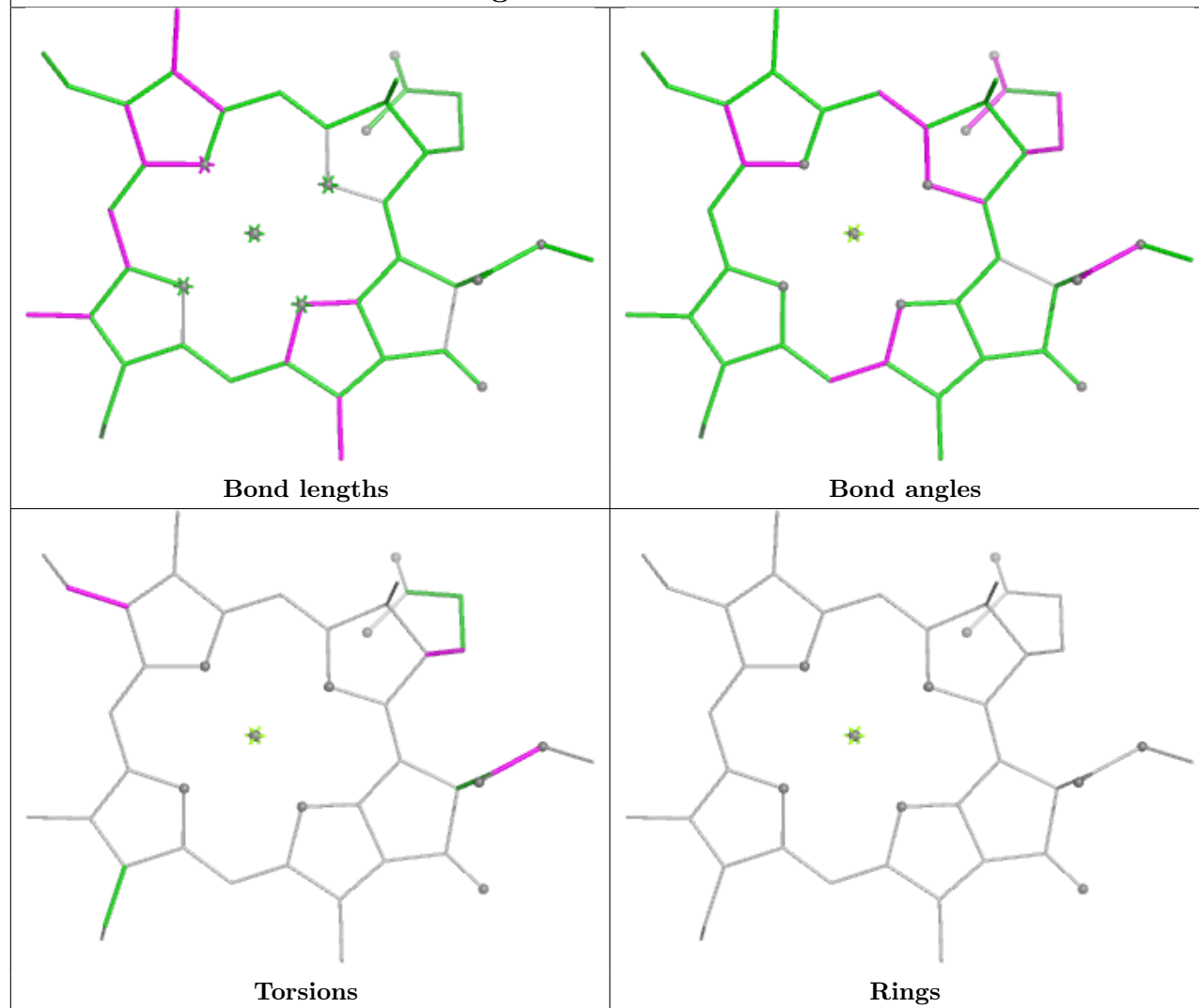
Ligand CLA B1 813

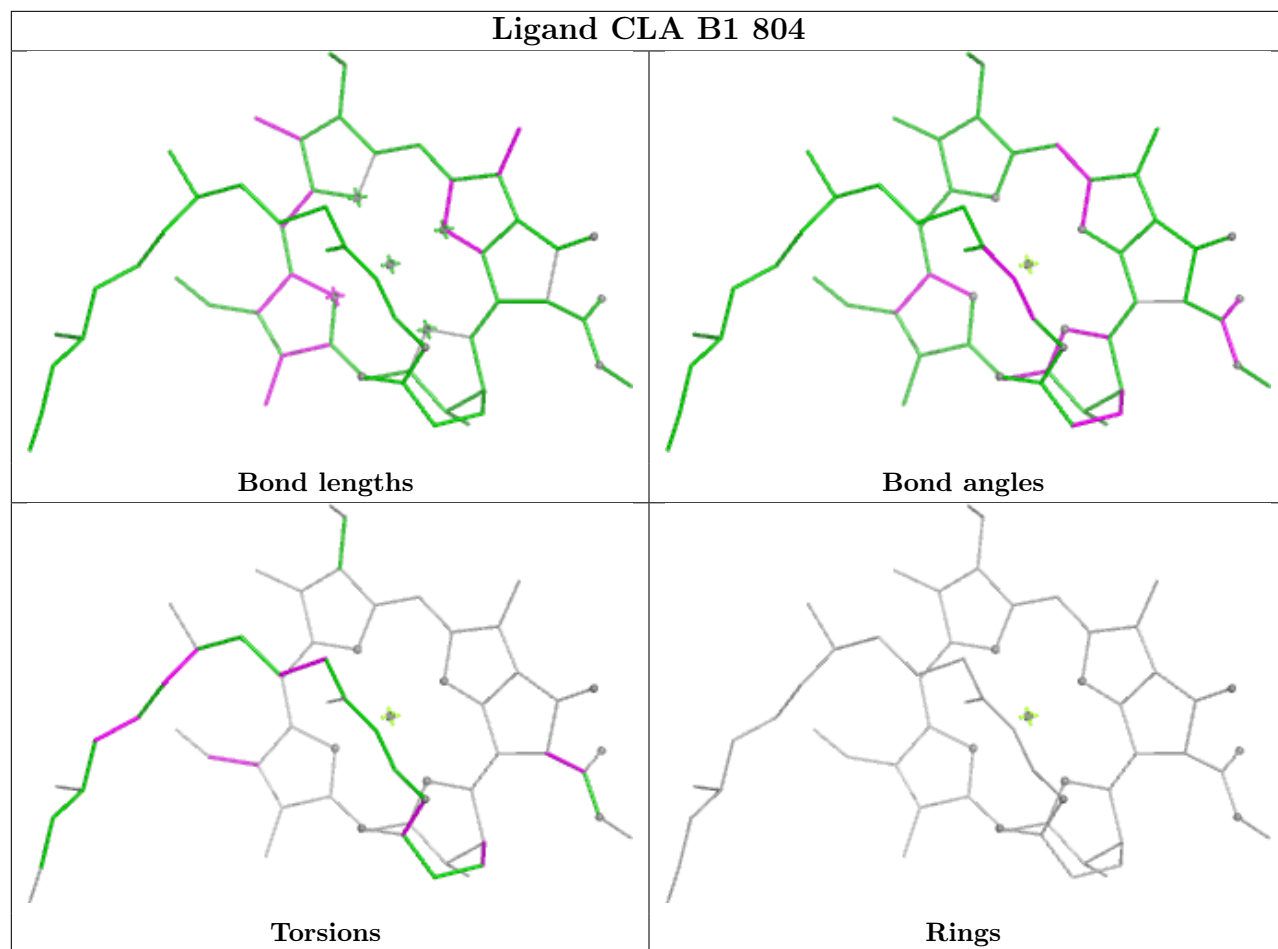


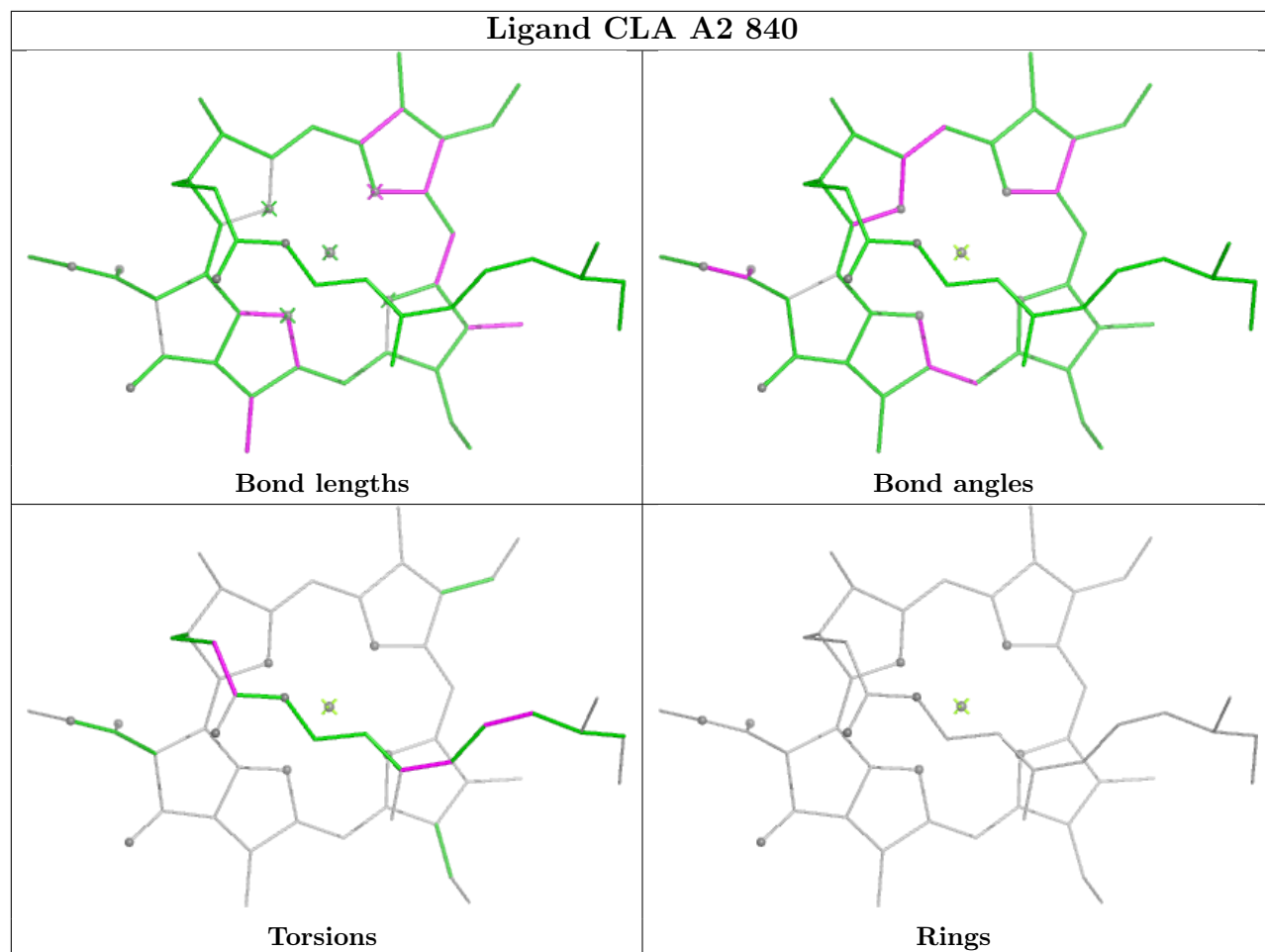
Ligand CLA K1 105

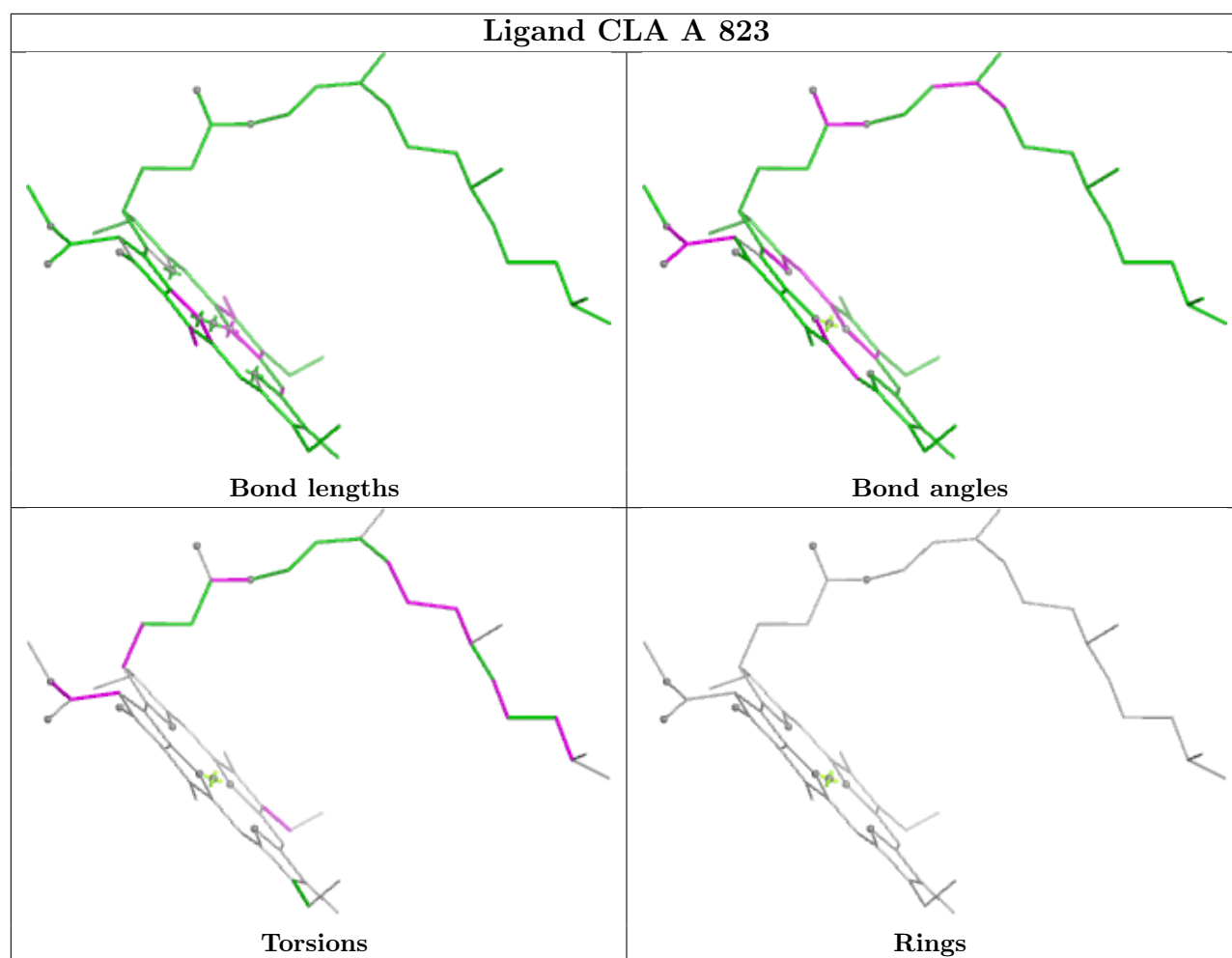


Ligand CLA B2 827

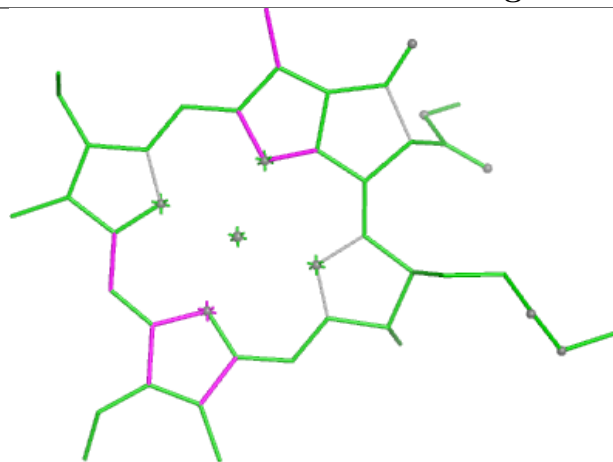




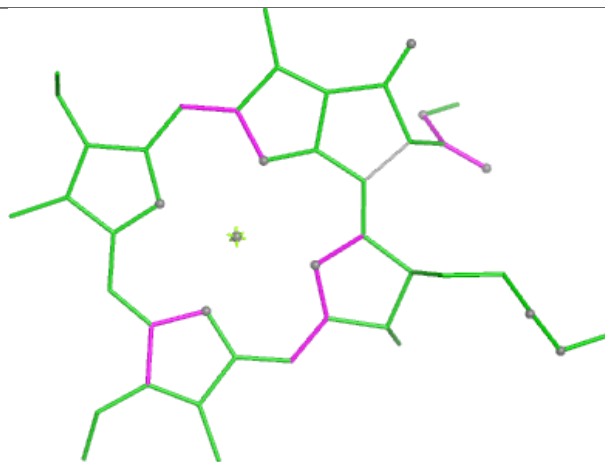




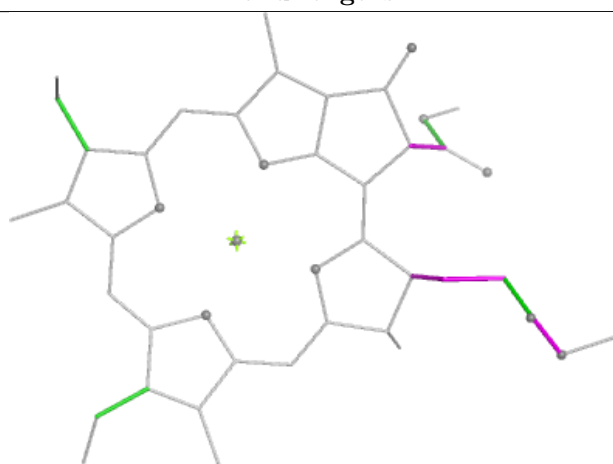
Ligand CLA K1 103



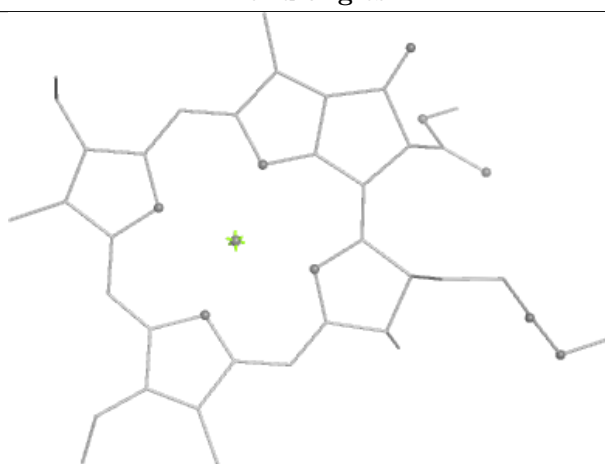
Bond lengths



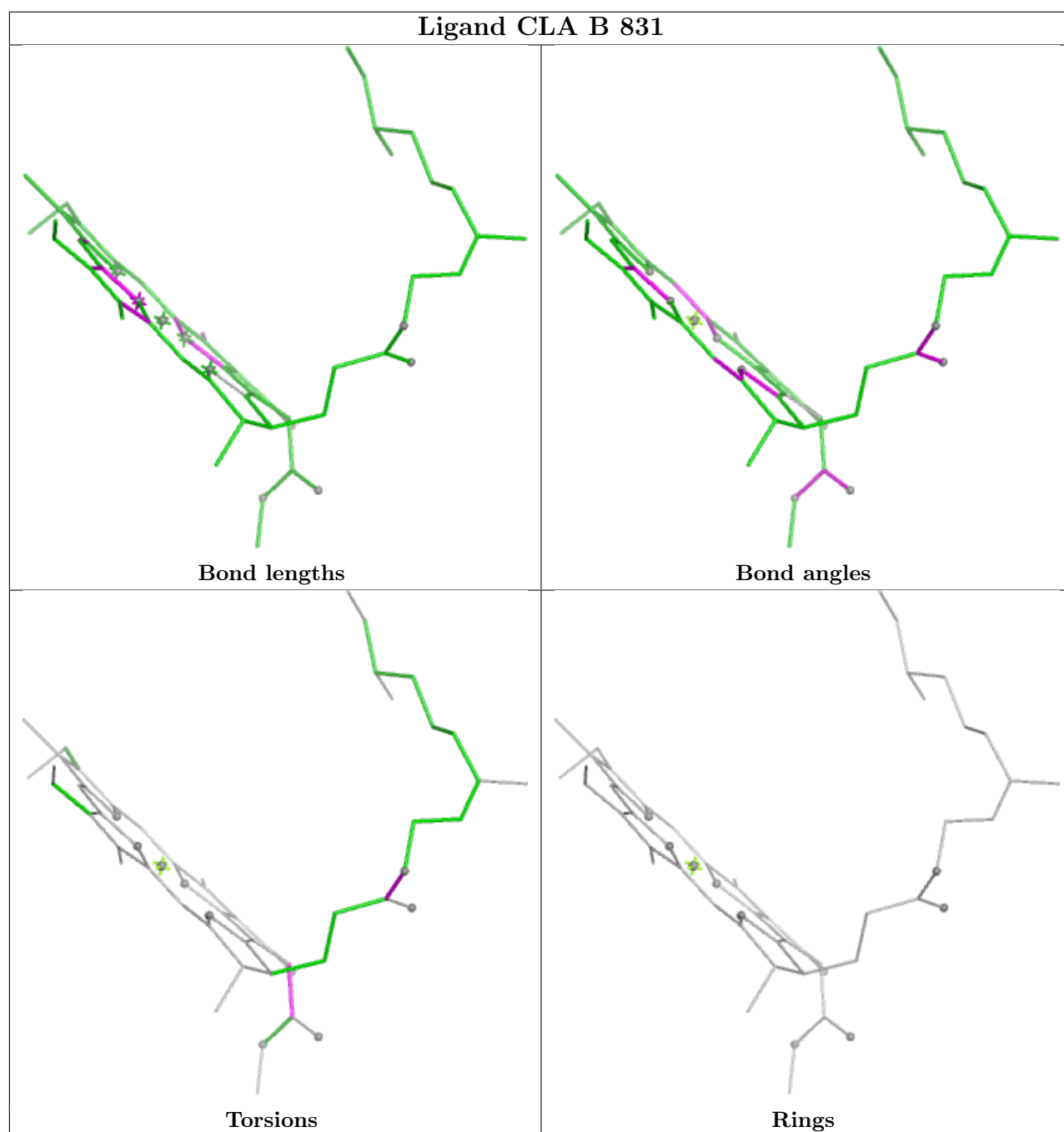
Bond angles

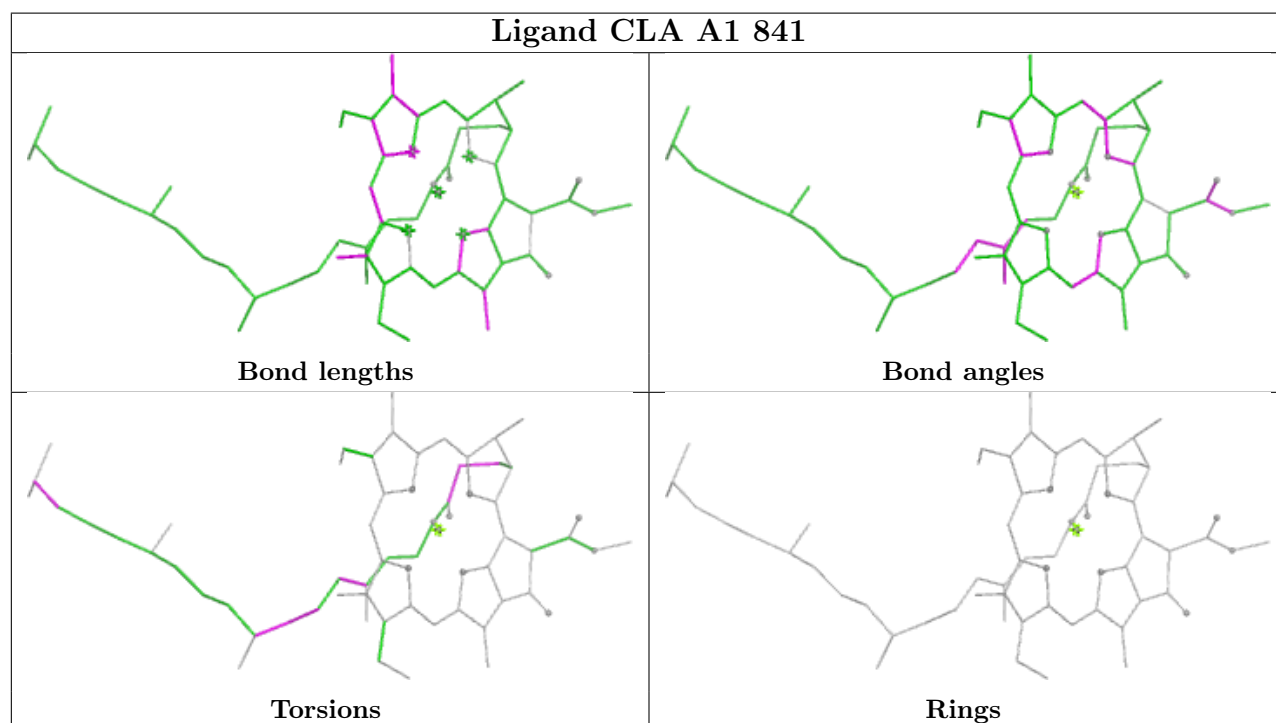
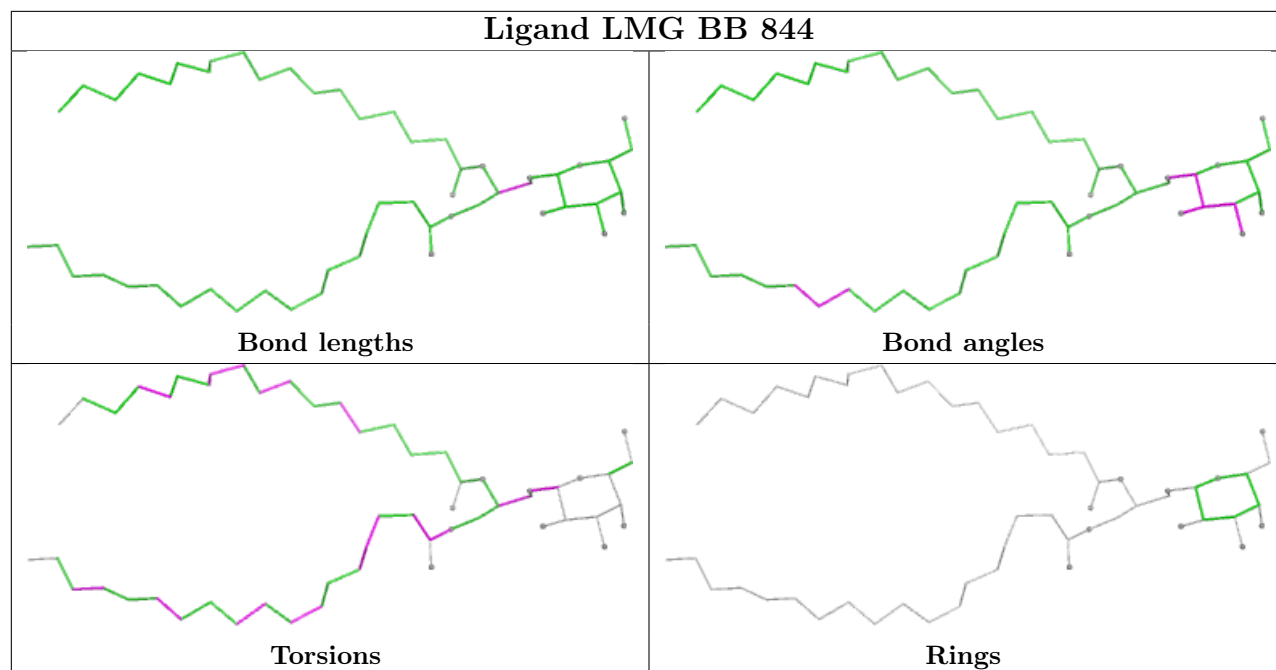


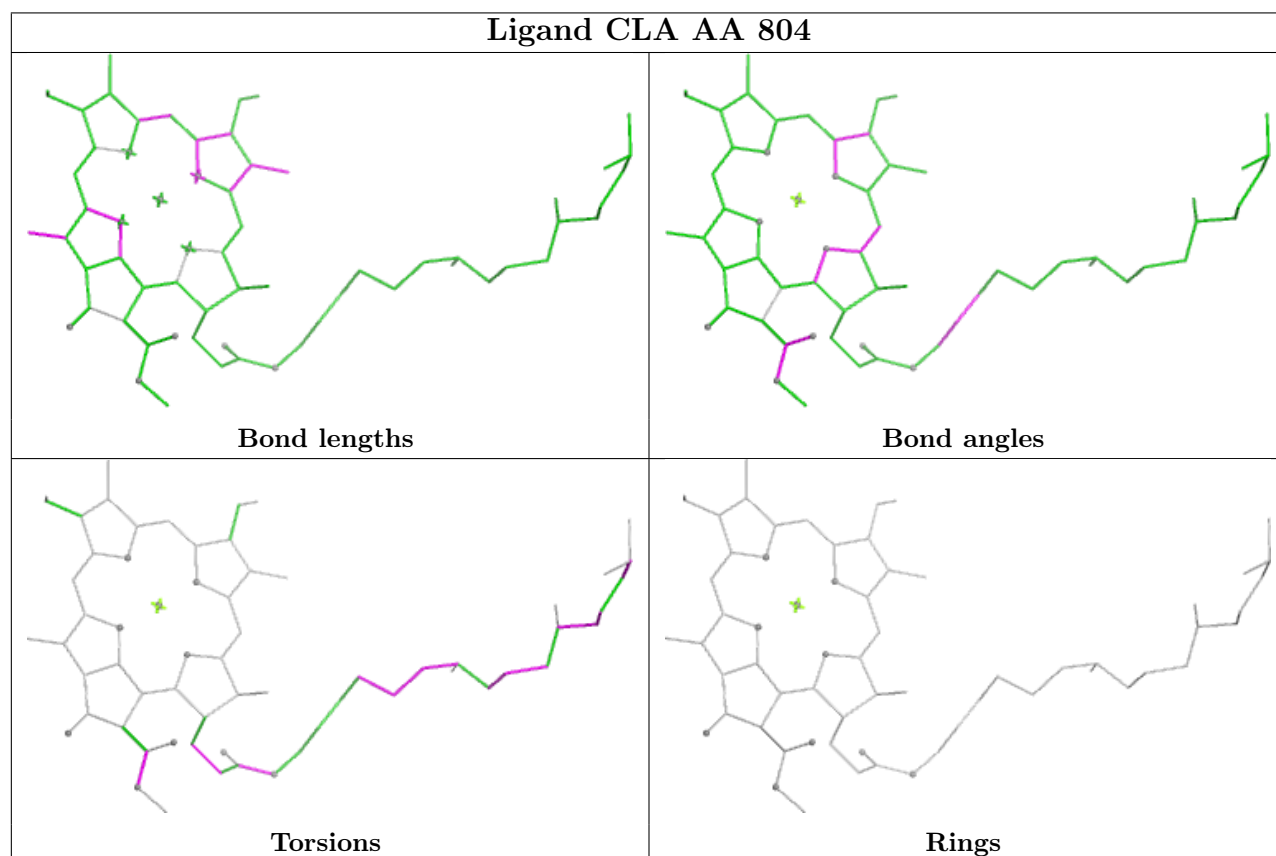
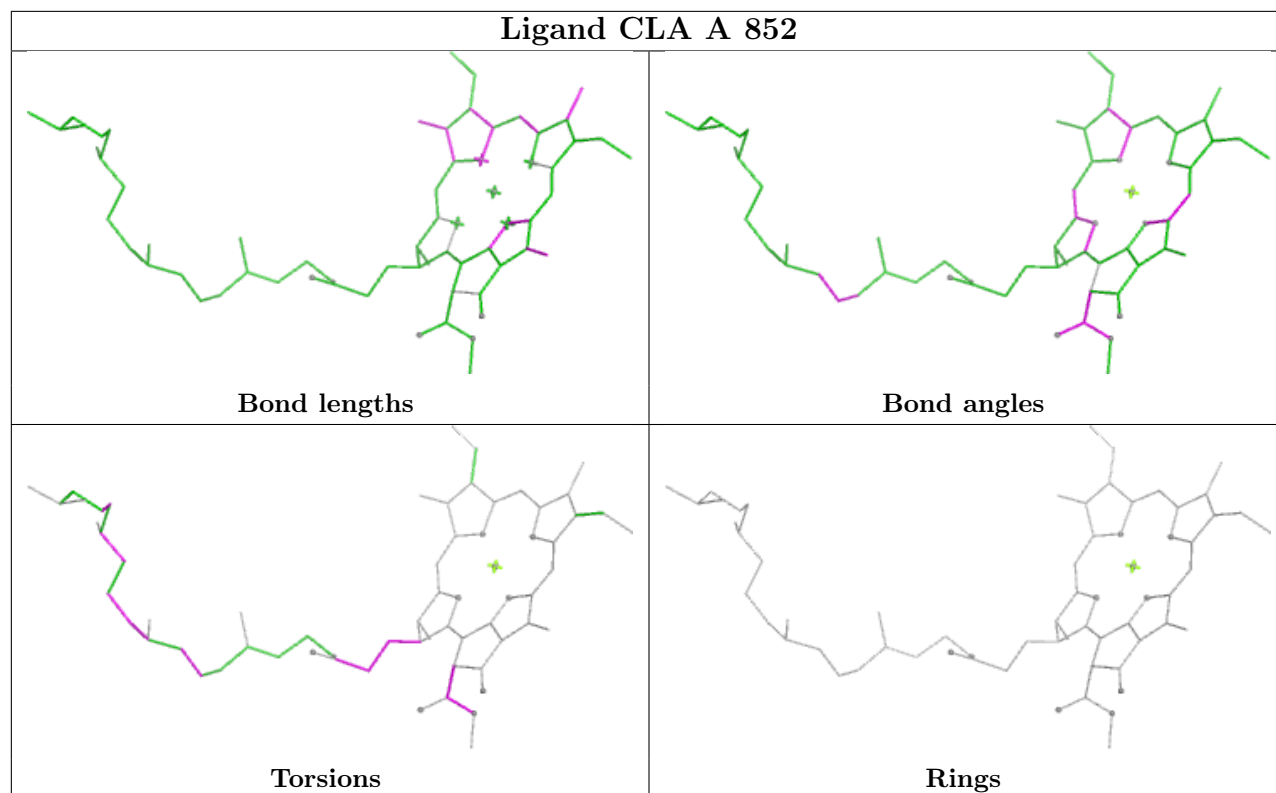
Torsions

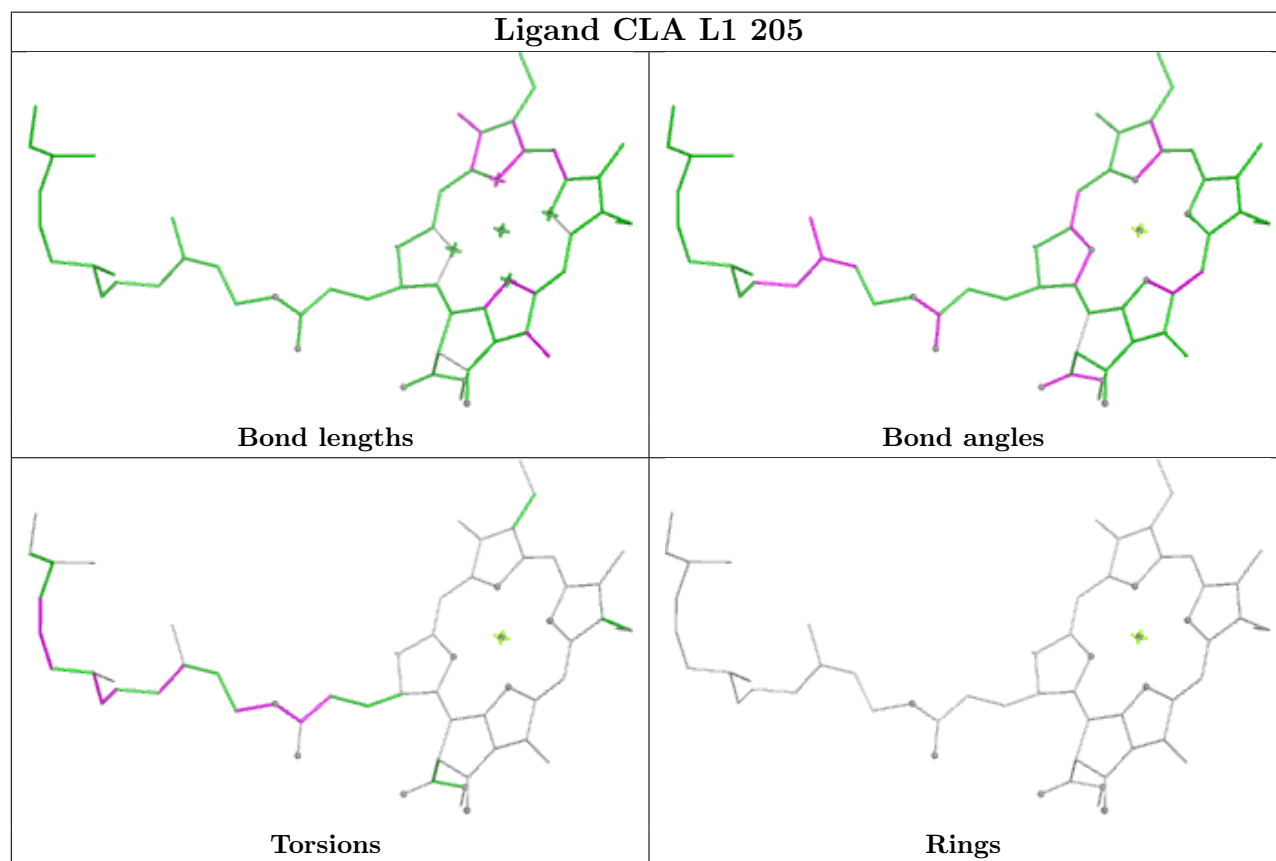
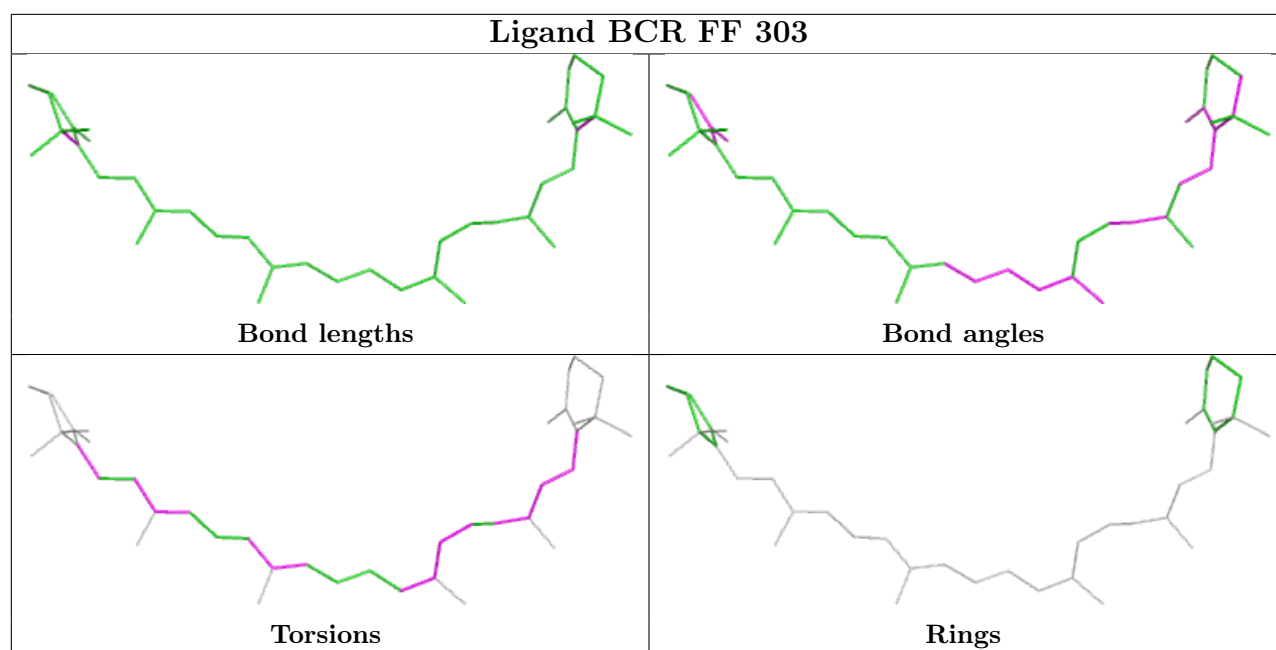


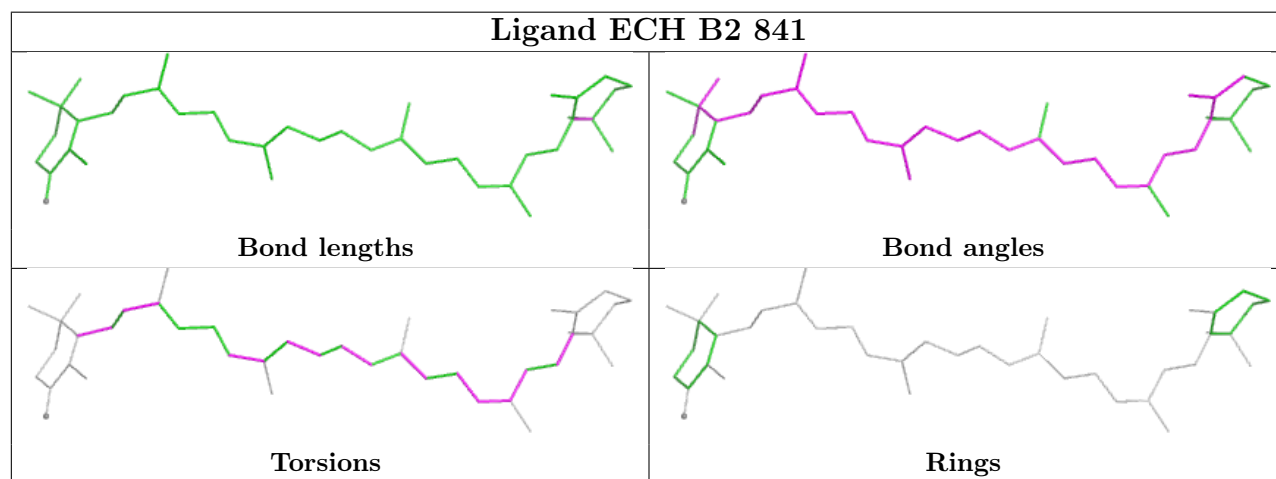
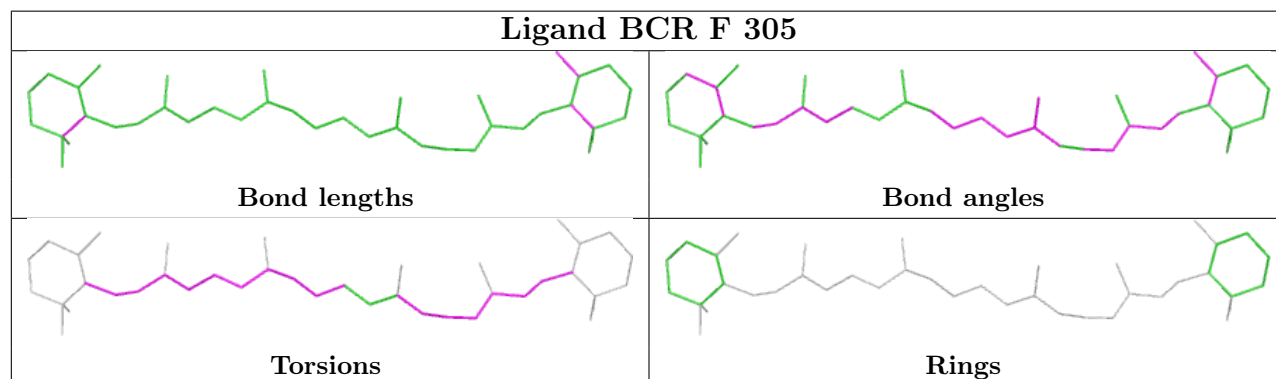
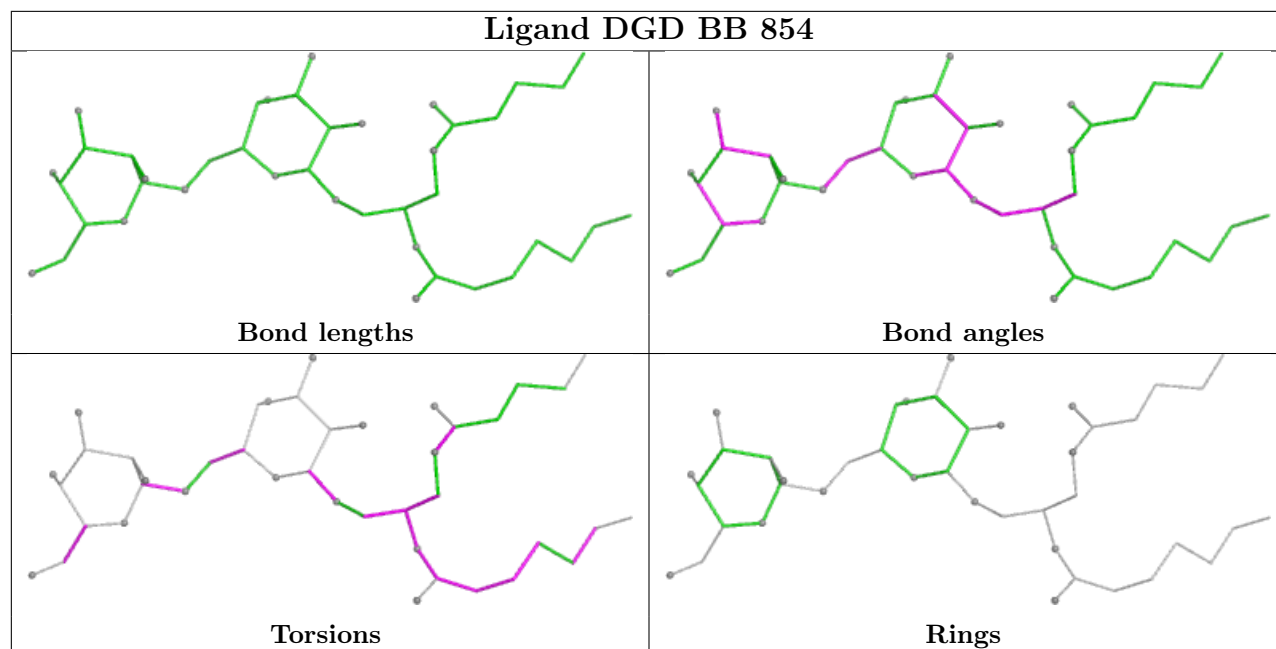
Rings



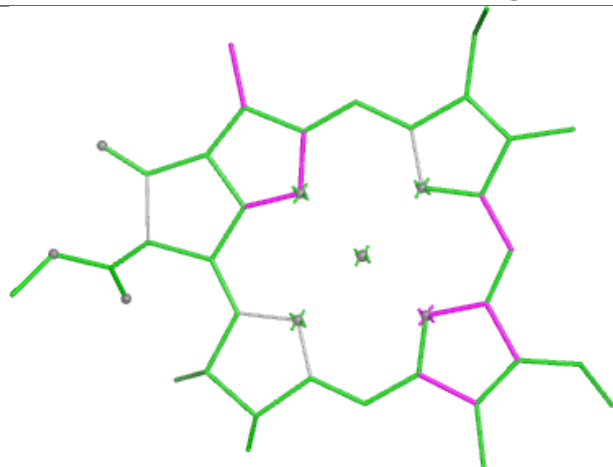




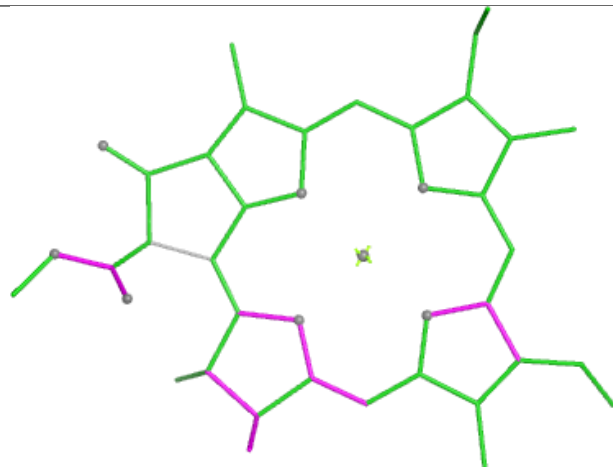




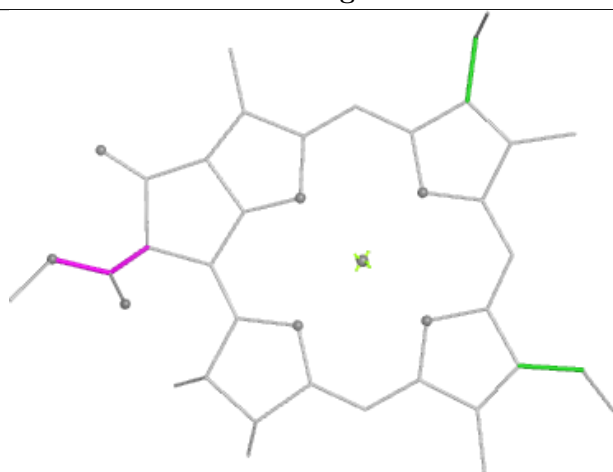
Ligand CLA B1 819



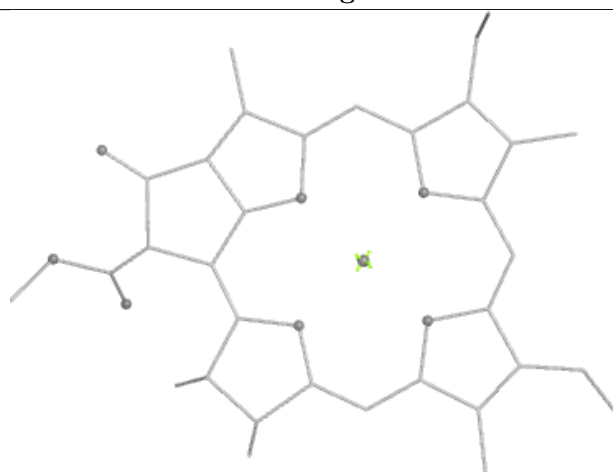
Bond lengths



Bond angles

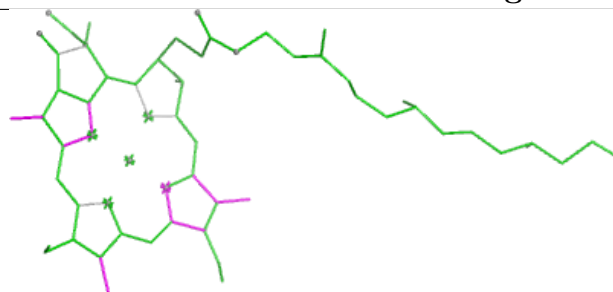


Torsions

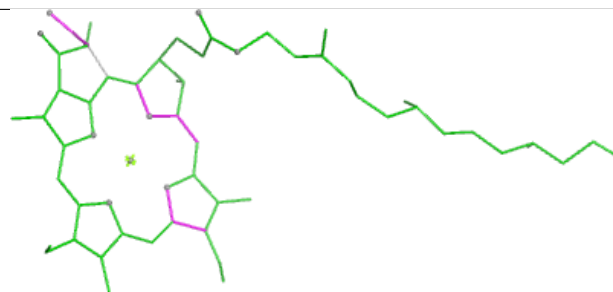


Rings

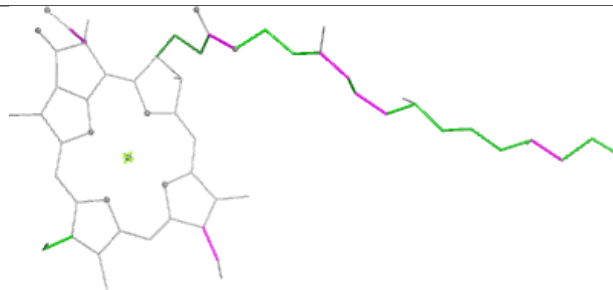
Ligand CLA A1 835



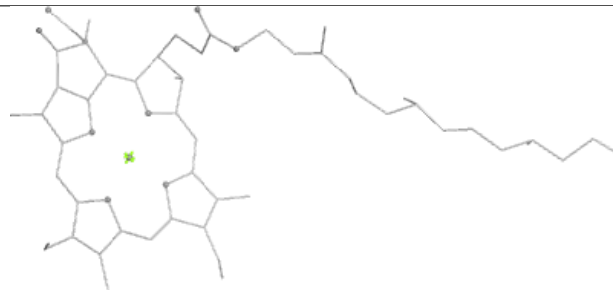
Bond lengths



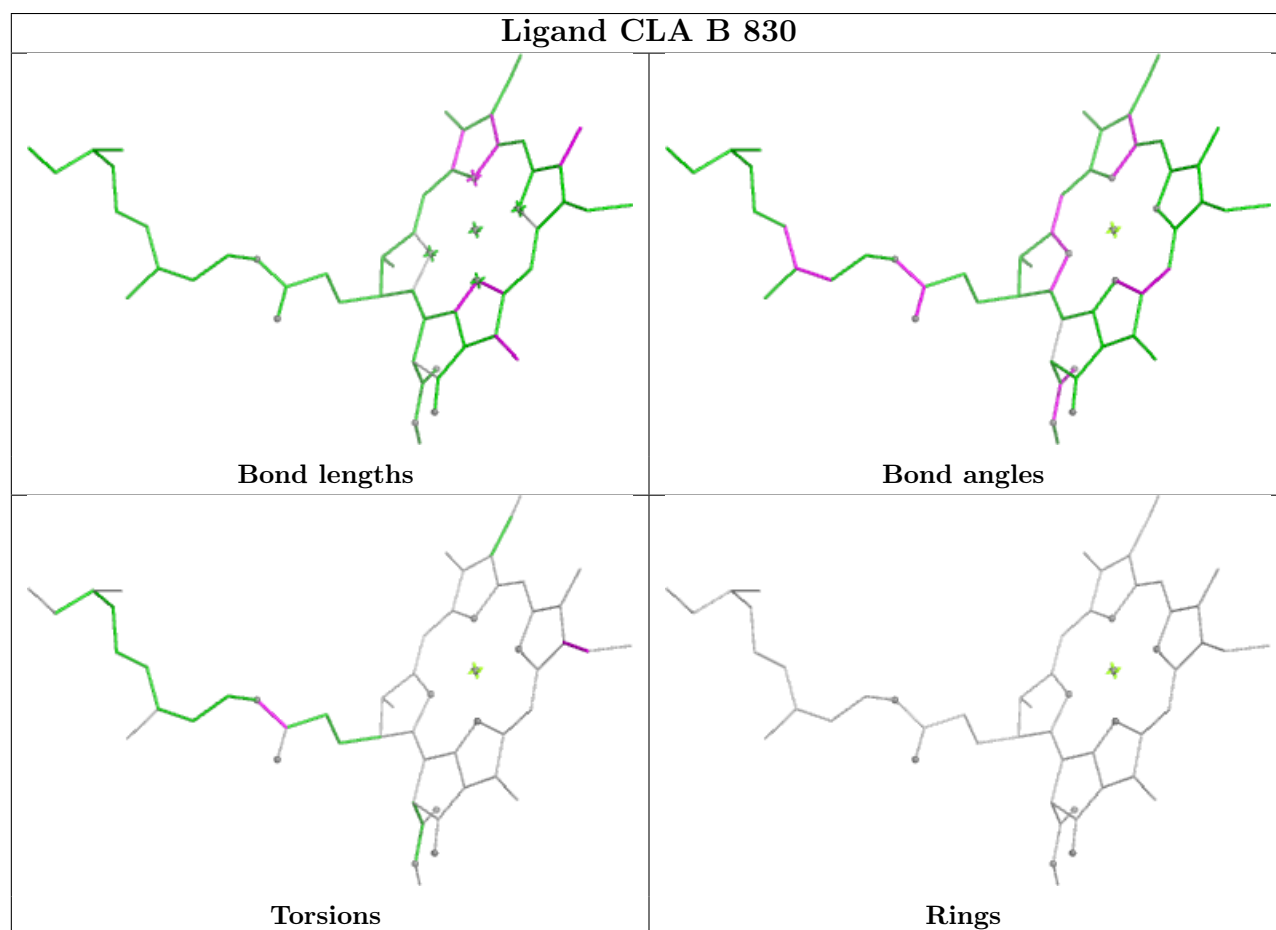
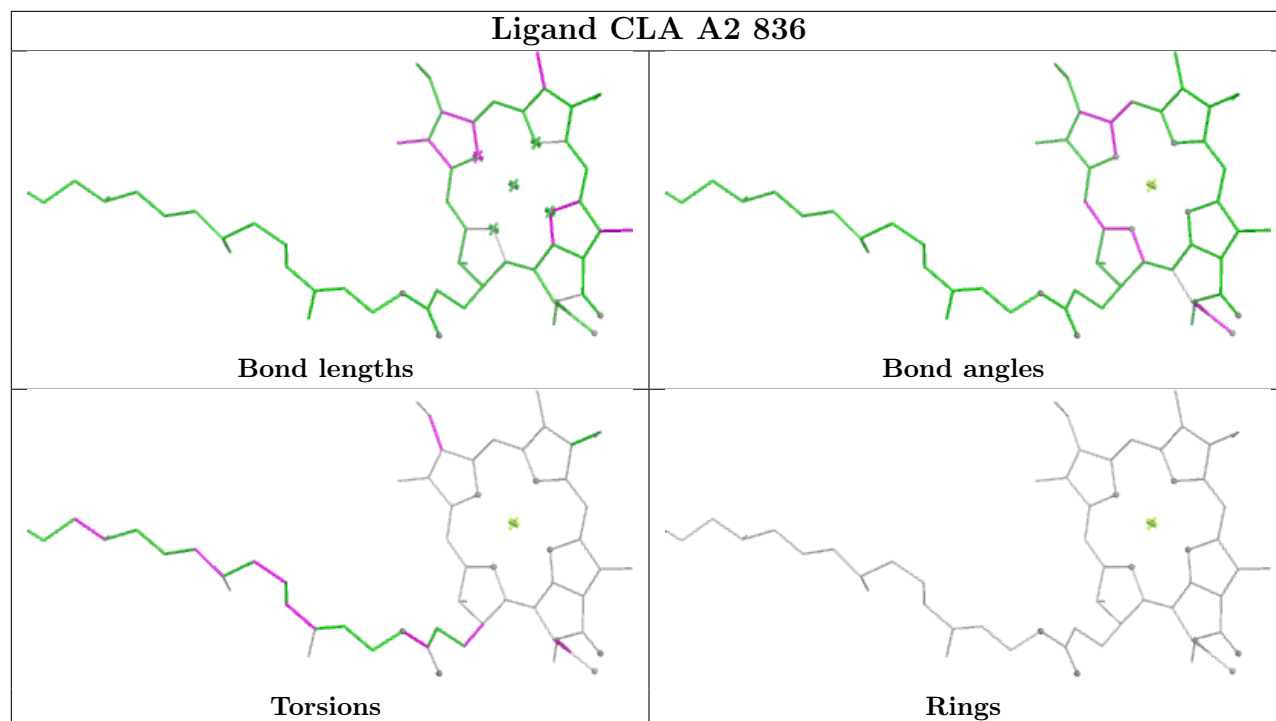
Bond angles

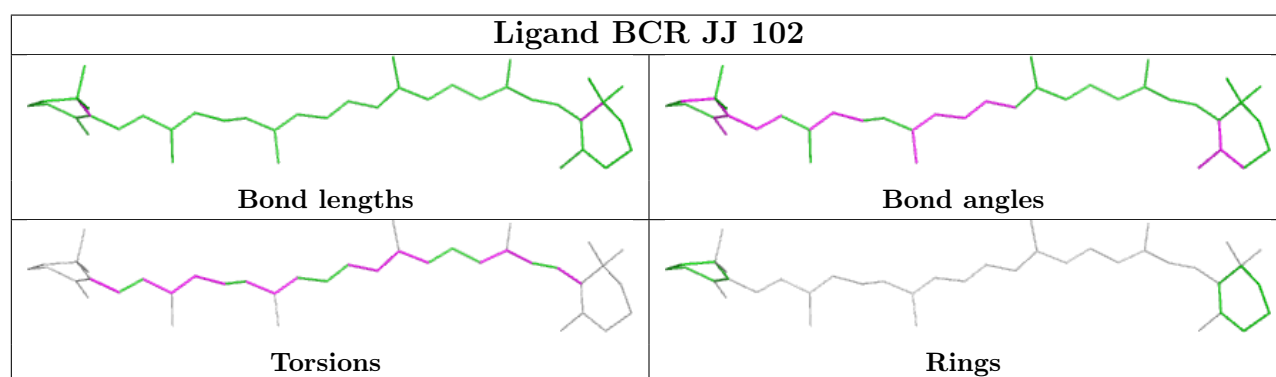
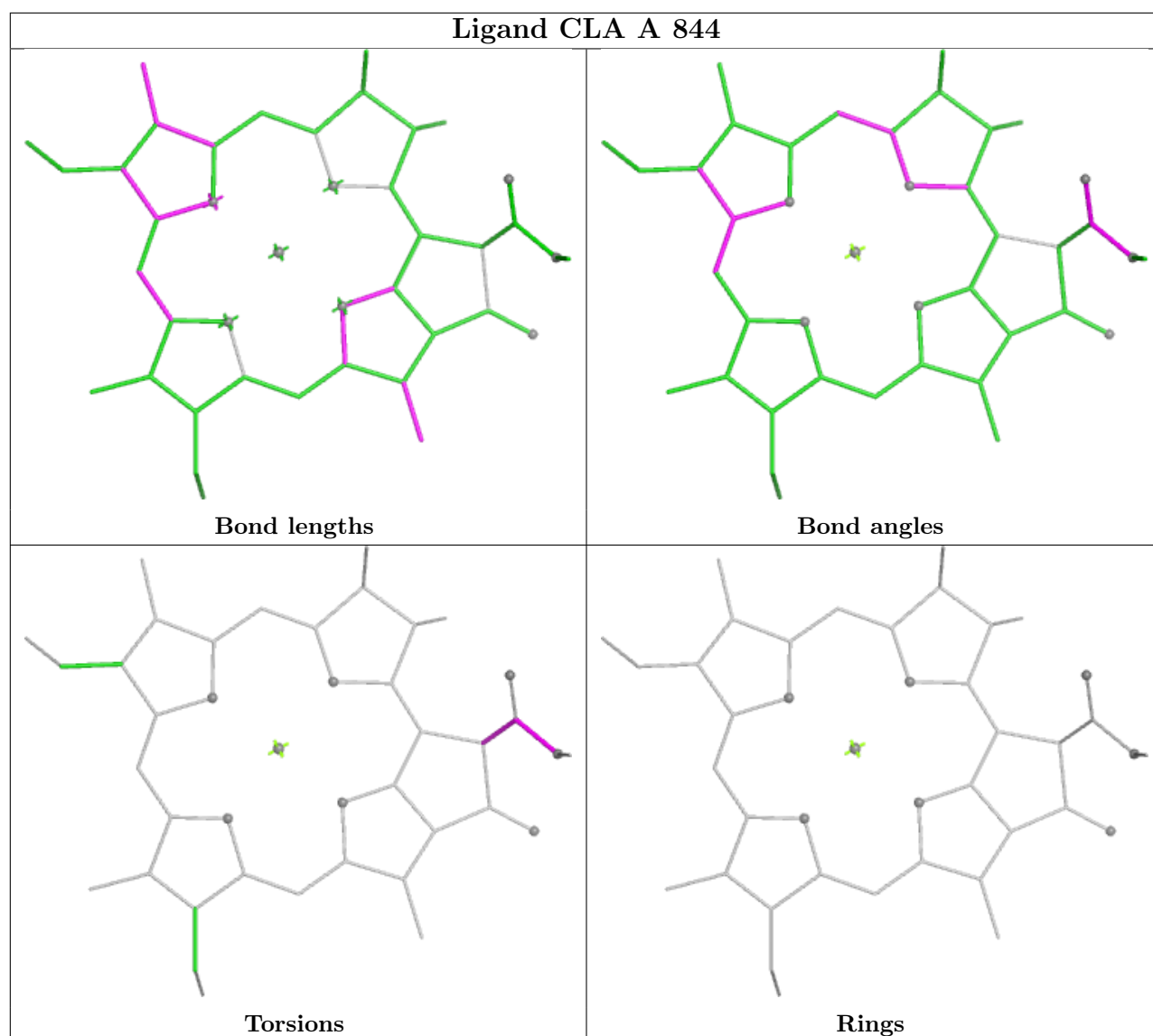


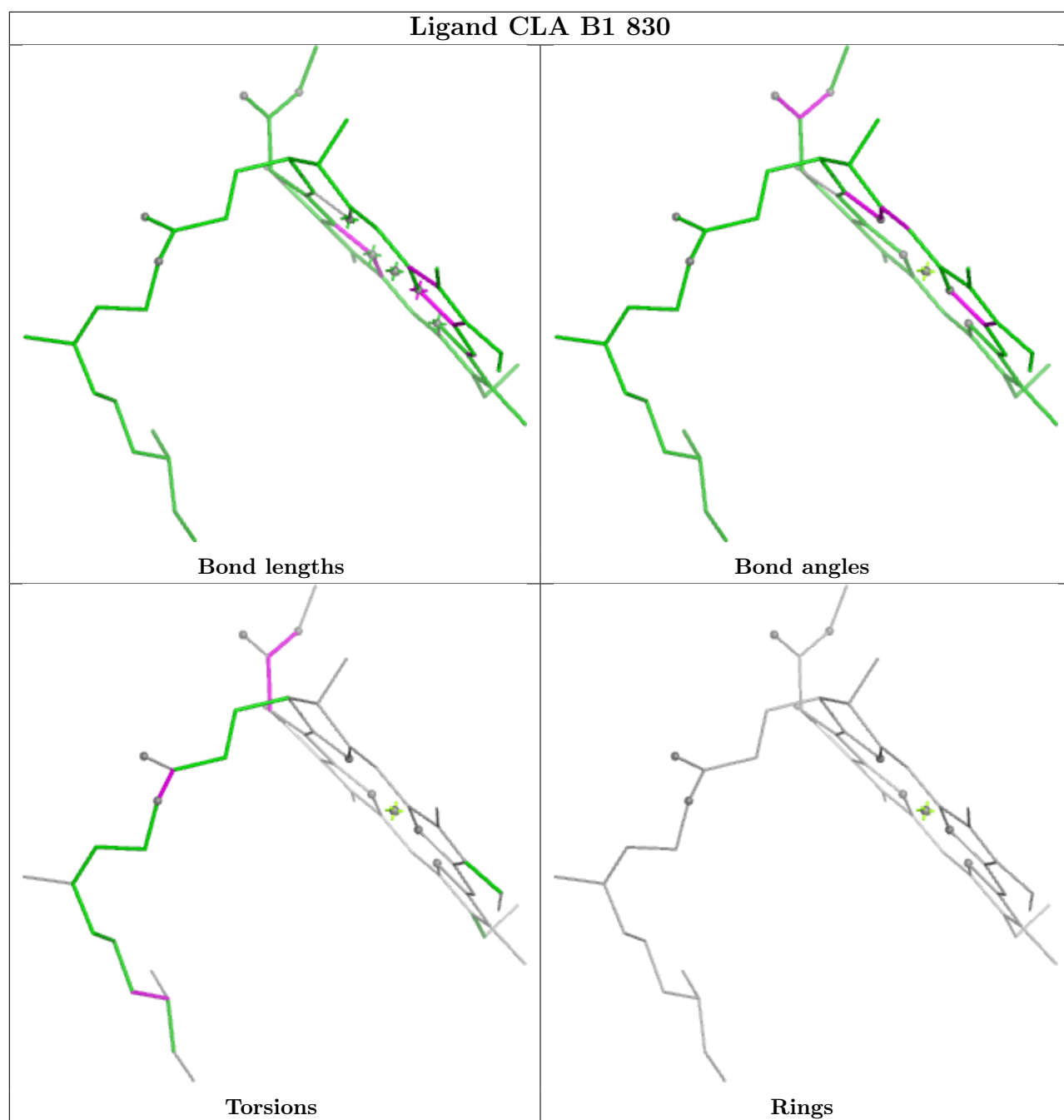
Torsions

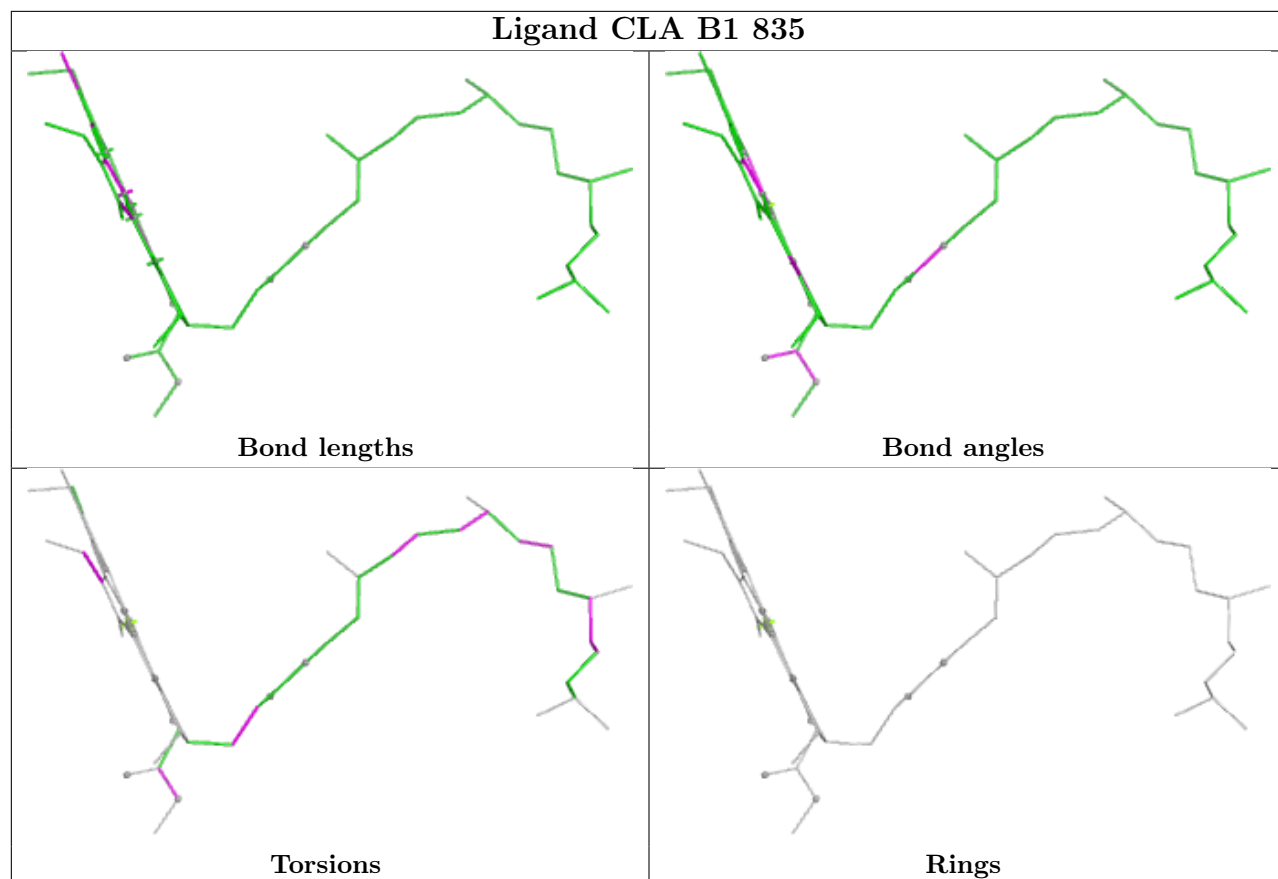


Rings

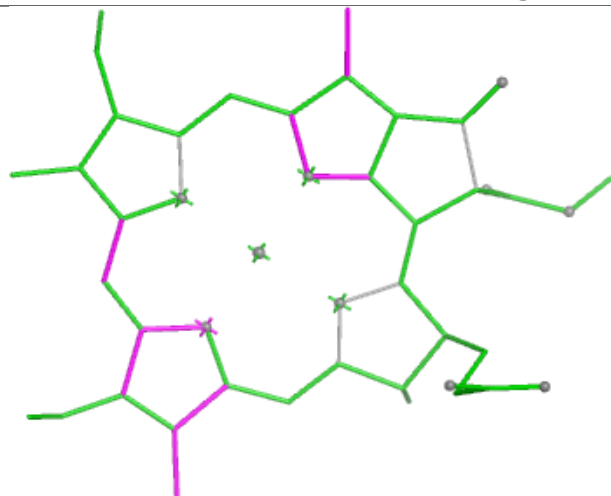




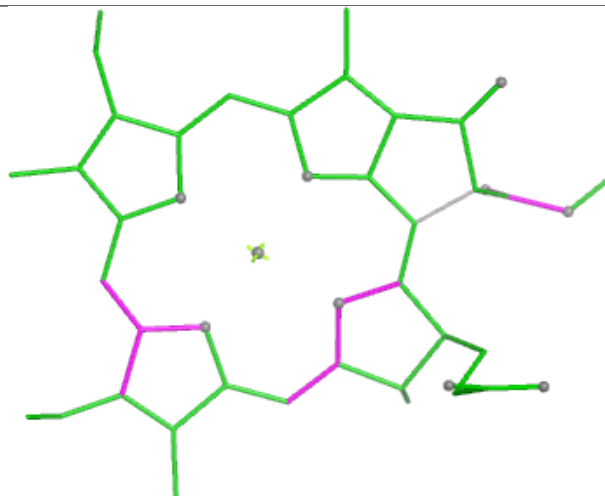




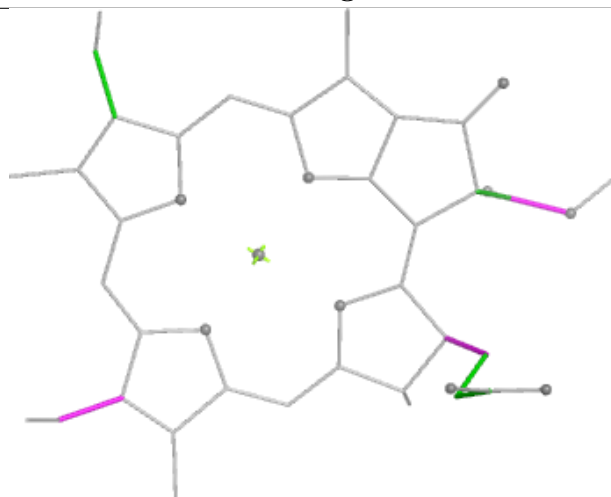
Ligand CLA B 832



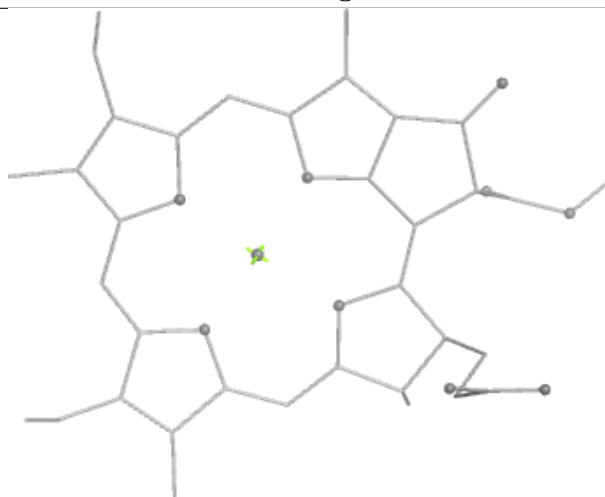
Bond lengths



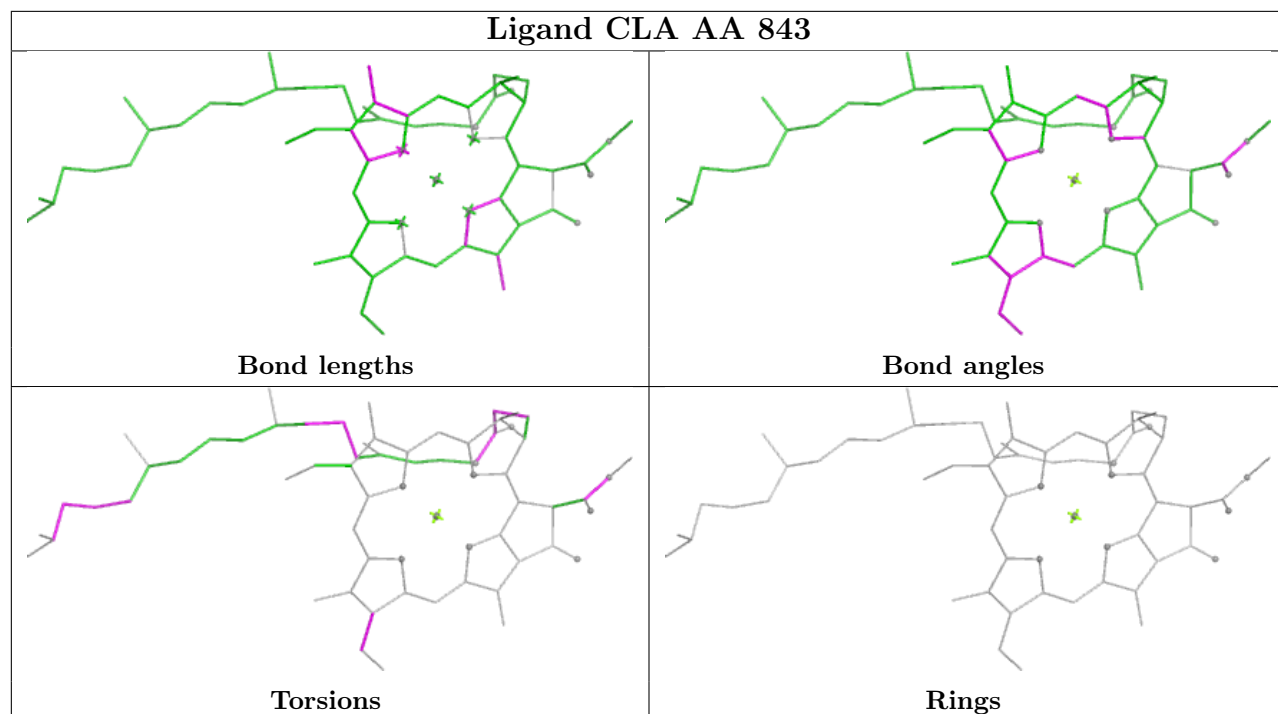
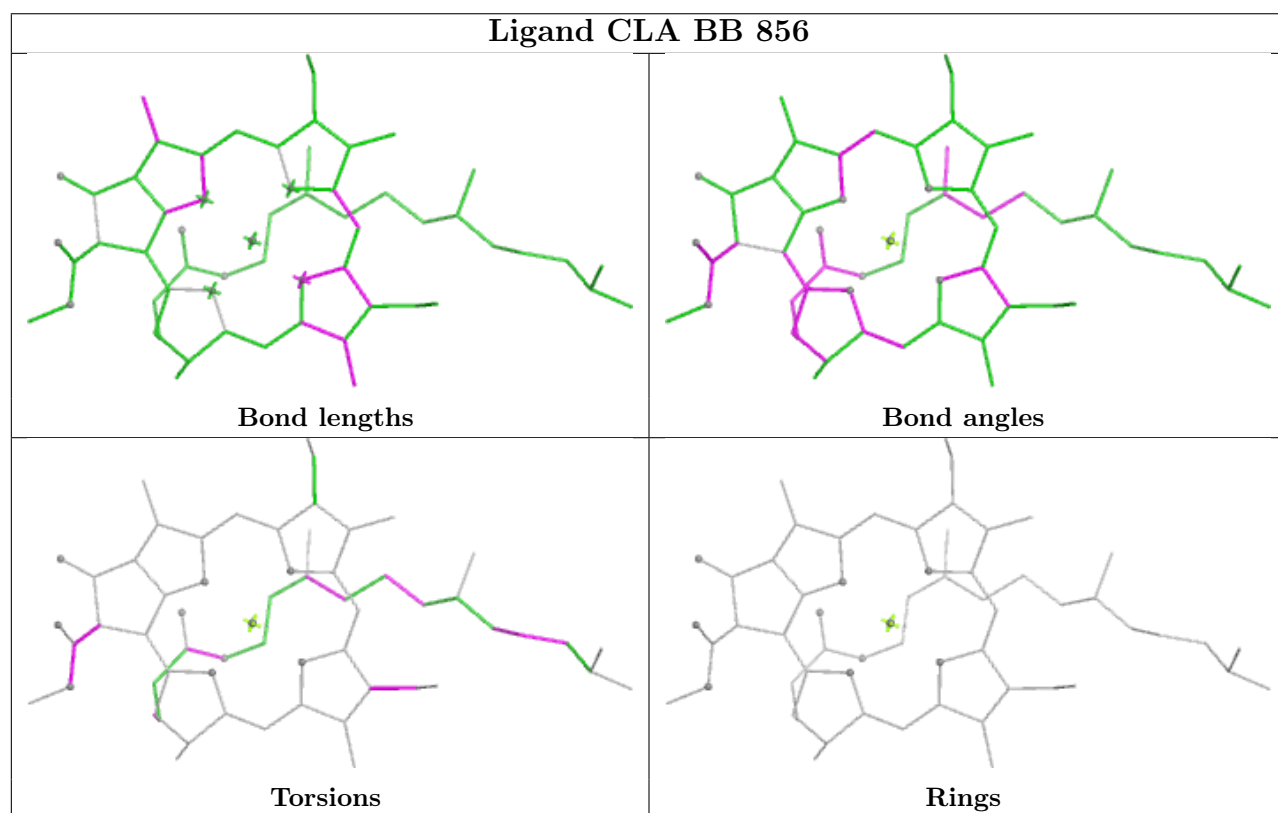
Bond angles

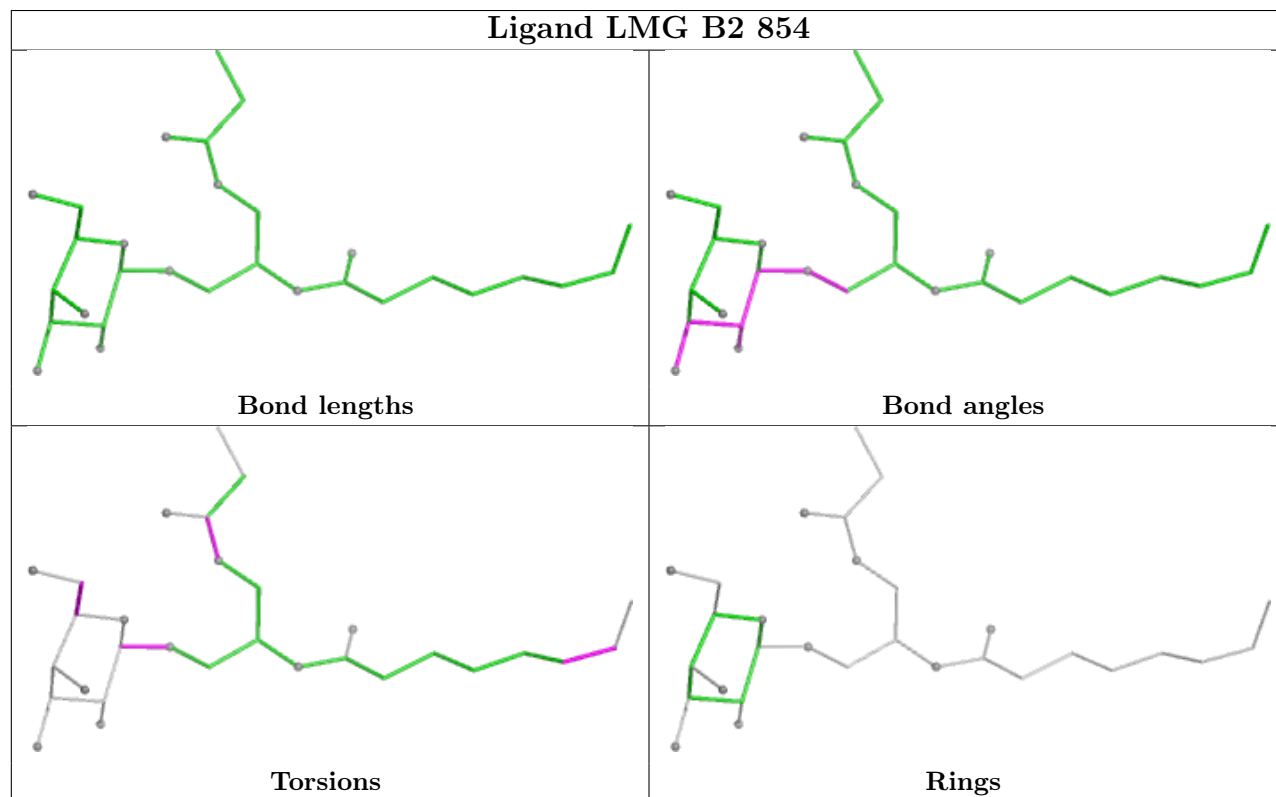
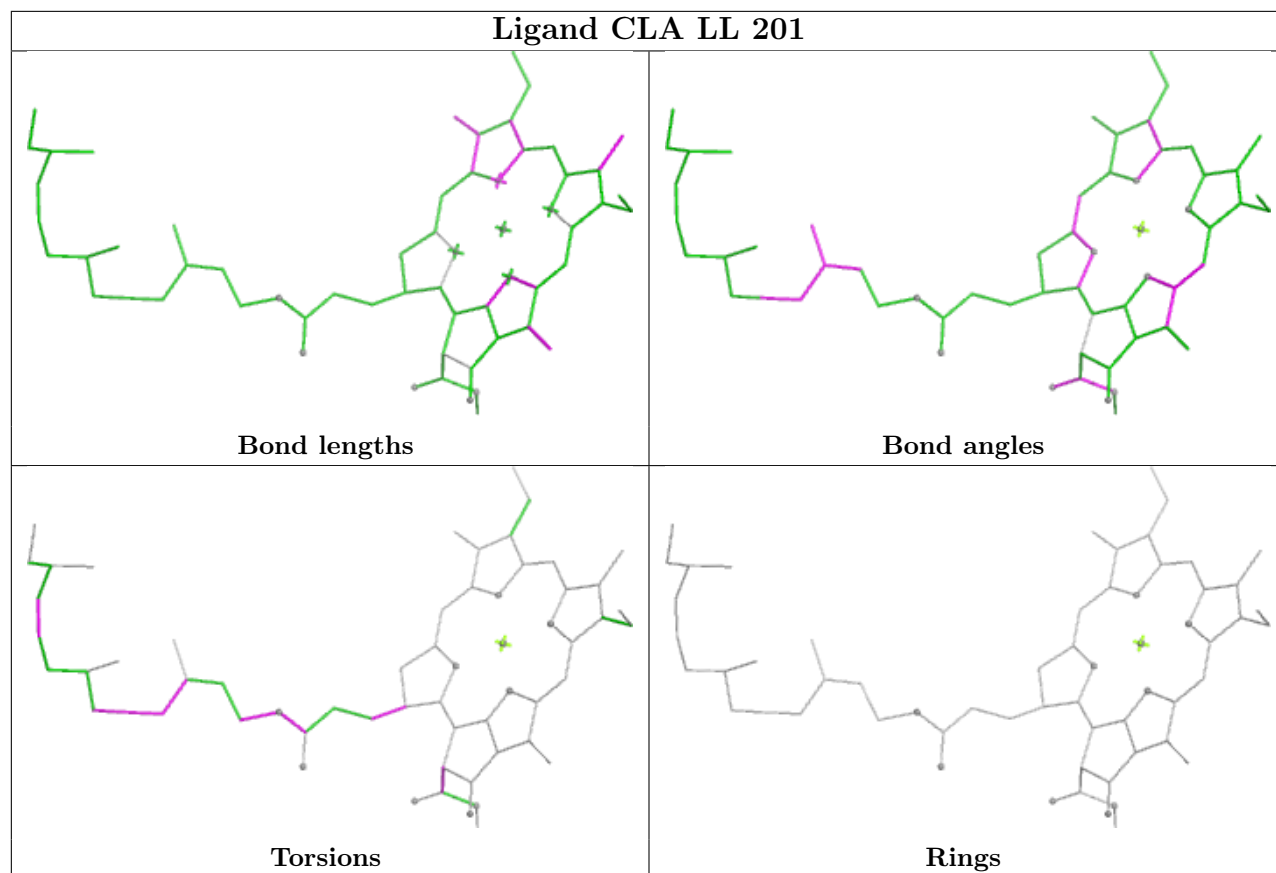


Torsions

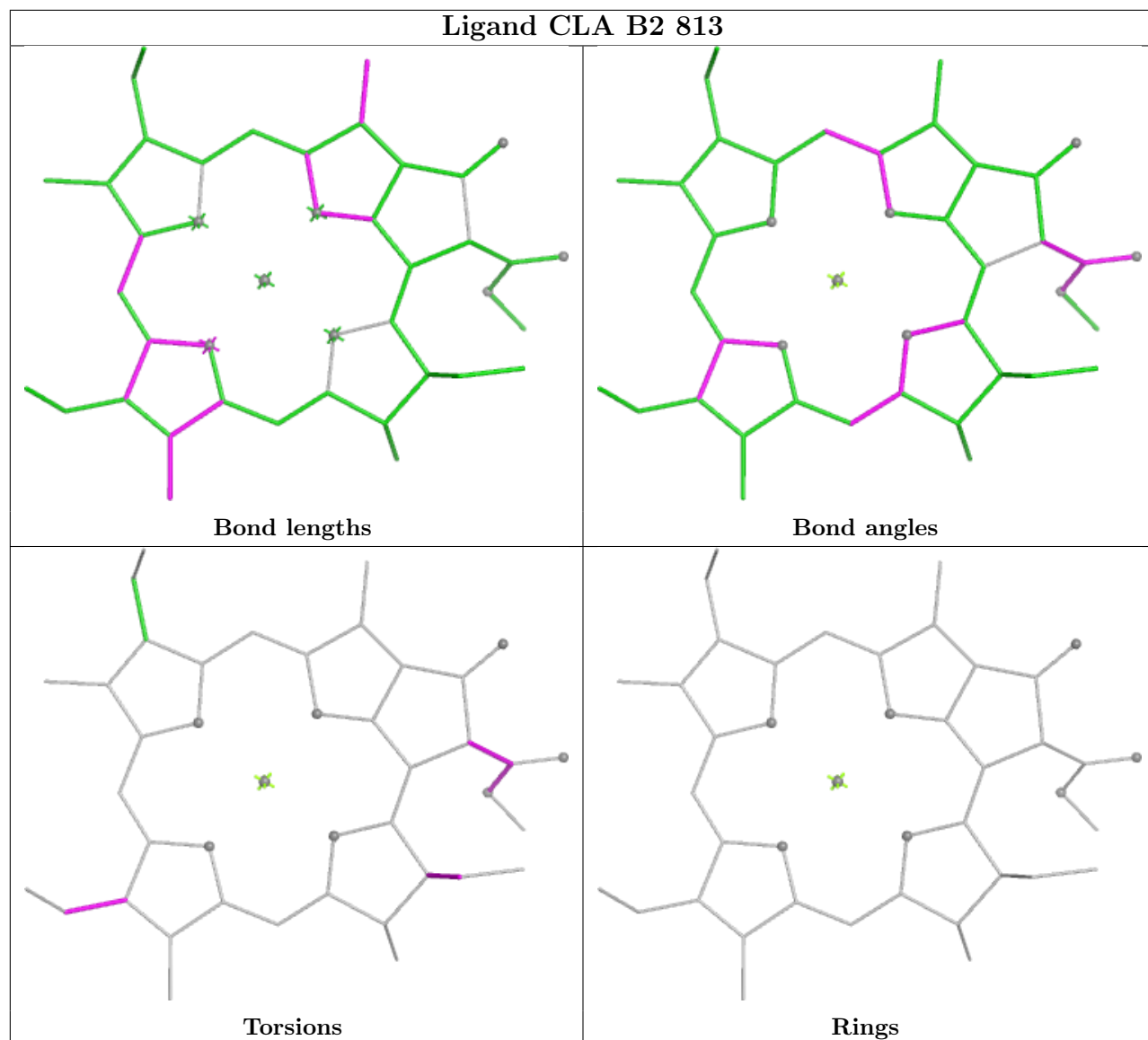


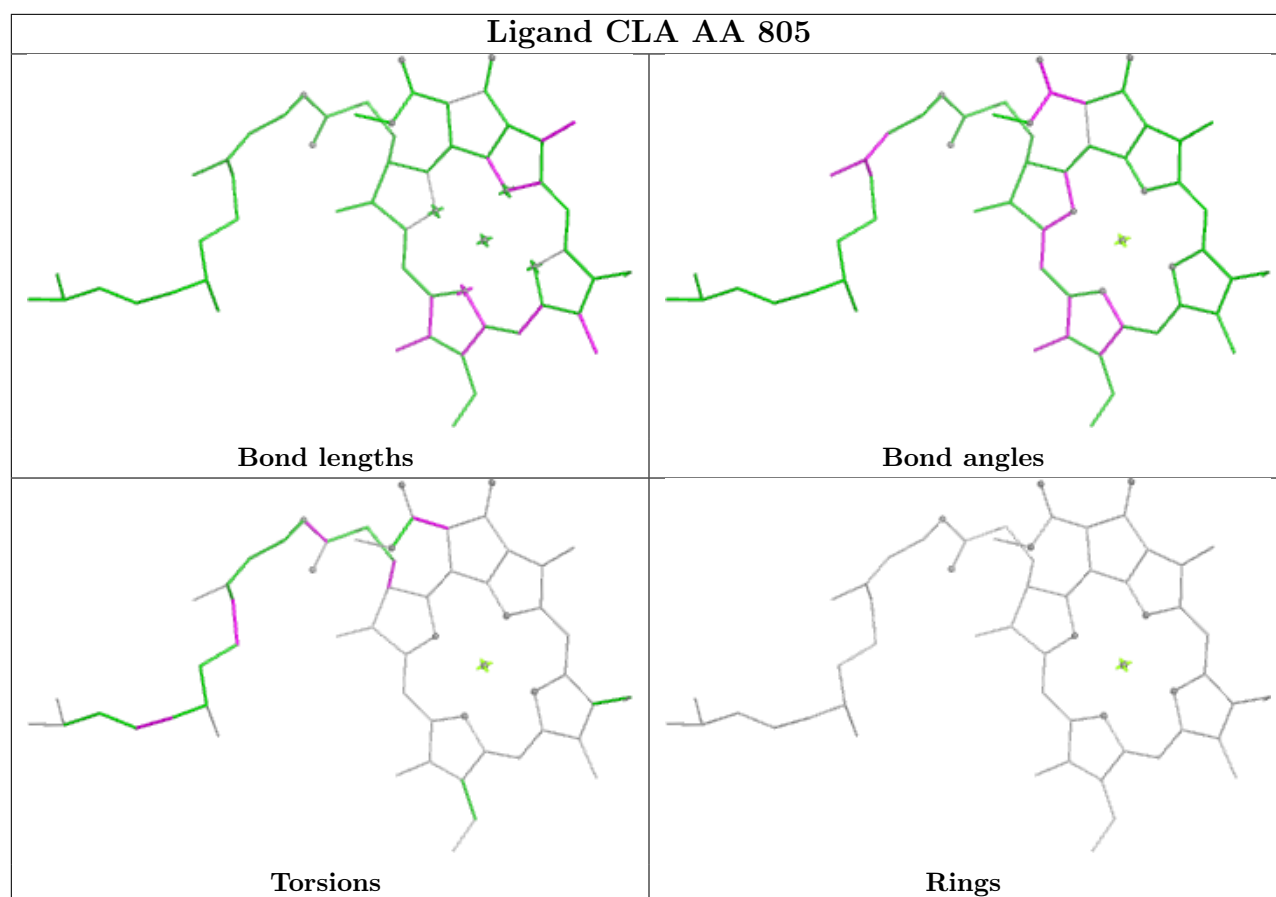
Rings

Ligand CLA AA 843**Ligand CLA BB 856**

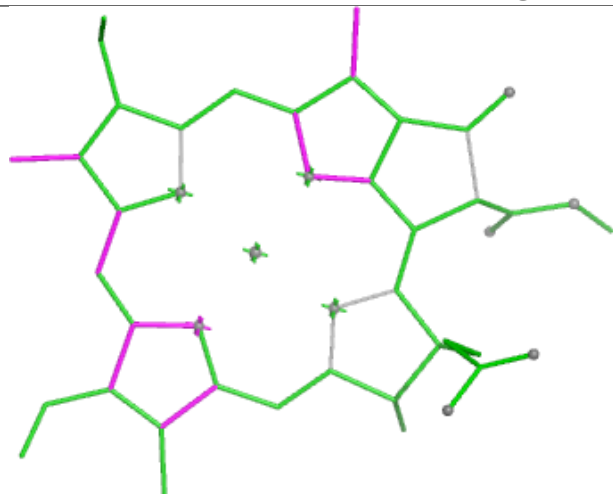


Ligand CLA B2 813

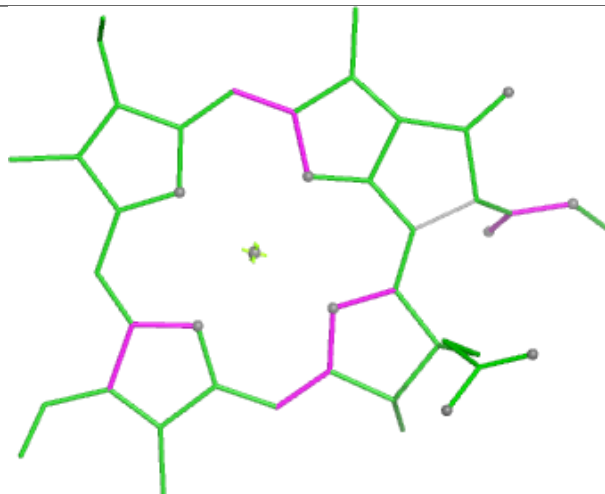




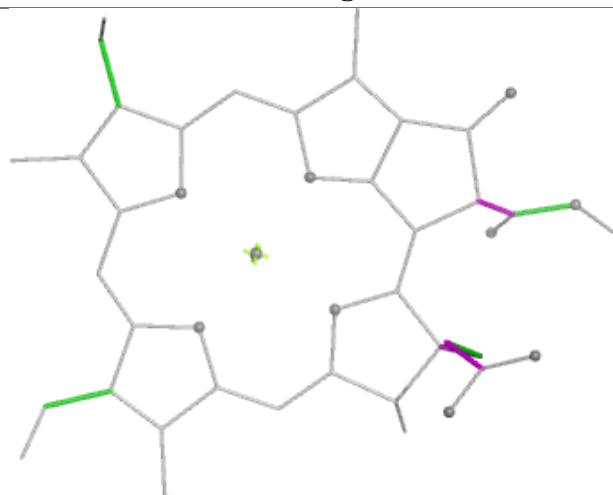
Ligand CLA B 828



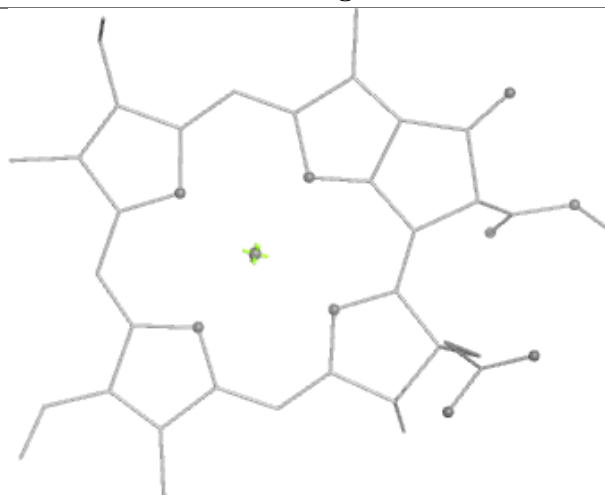
Bond lengths



Bond angles

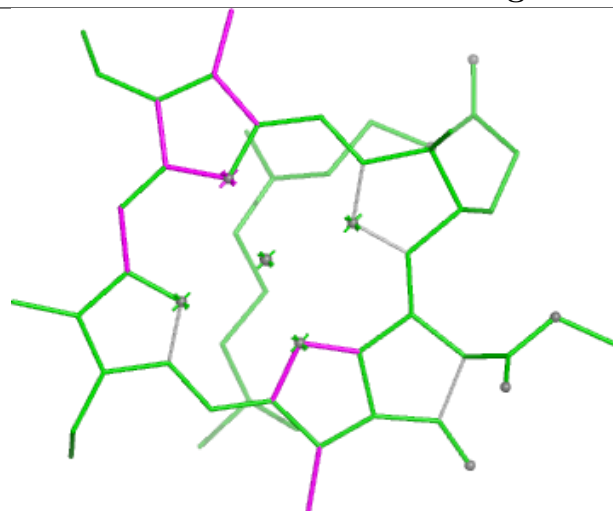


Torsions

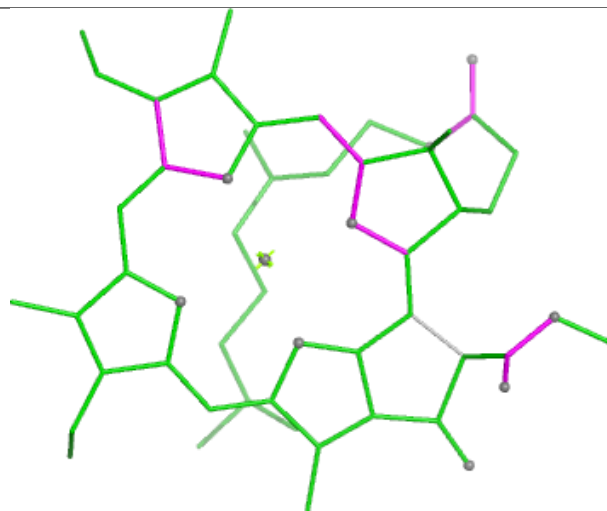


Rings

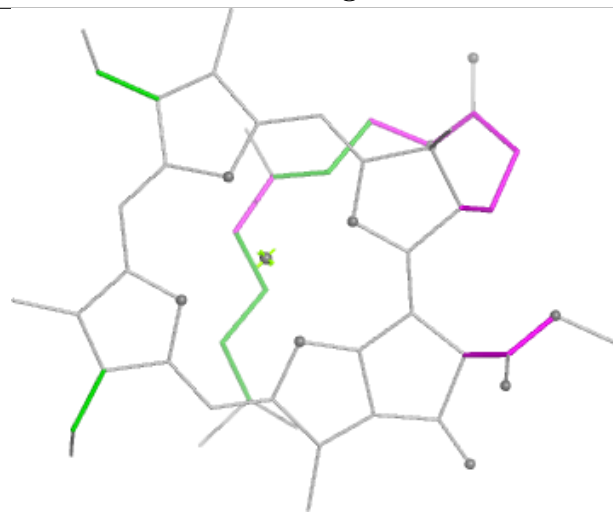
Ligand CLA B2 824



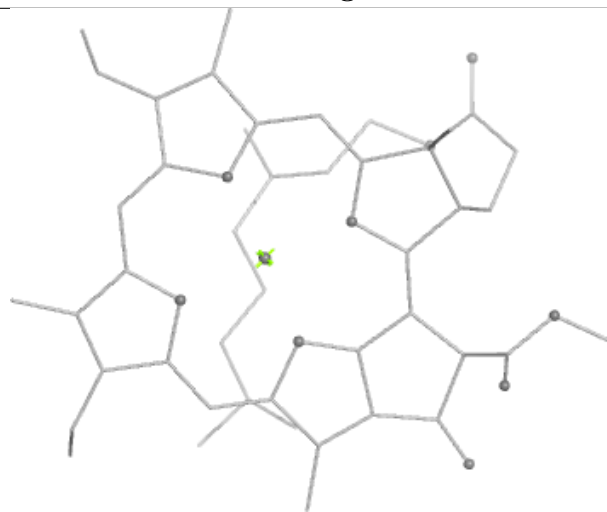
Bond lengths



Bond angles

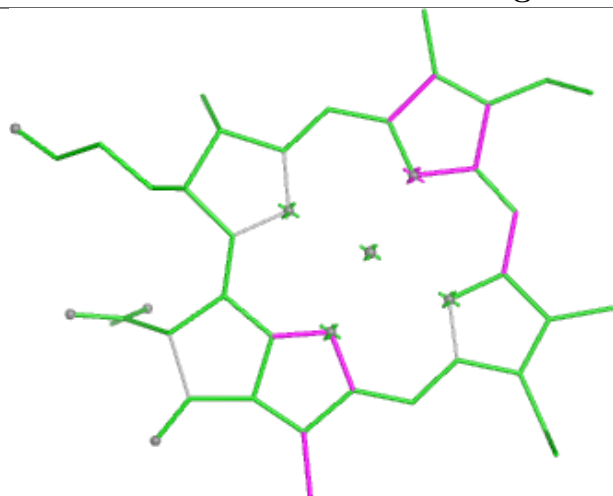


Torsions

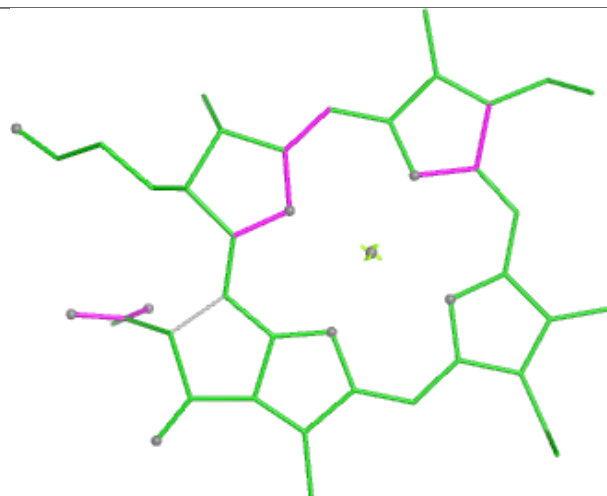


Rings

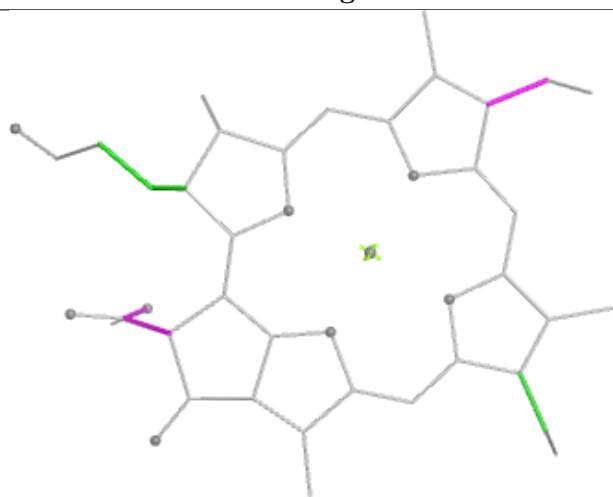
Ligand CLA A 817



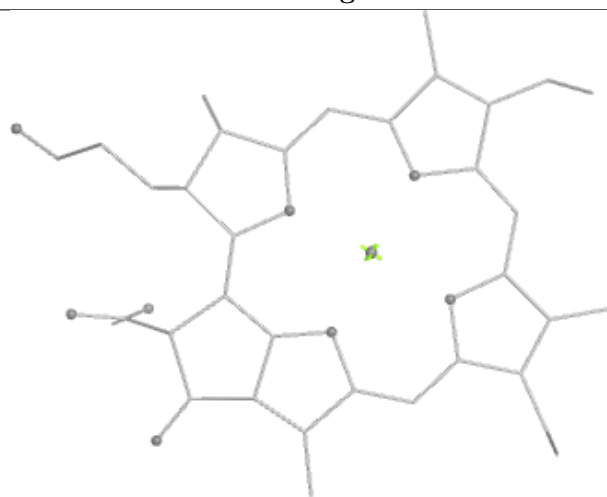
Bond lengths



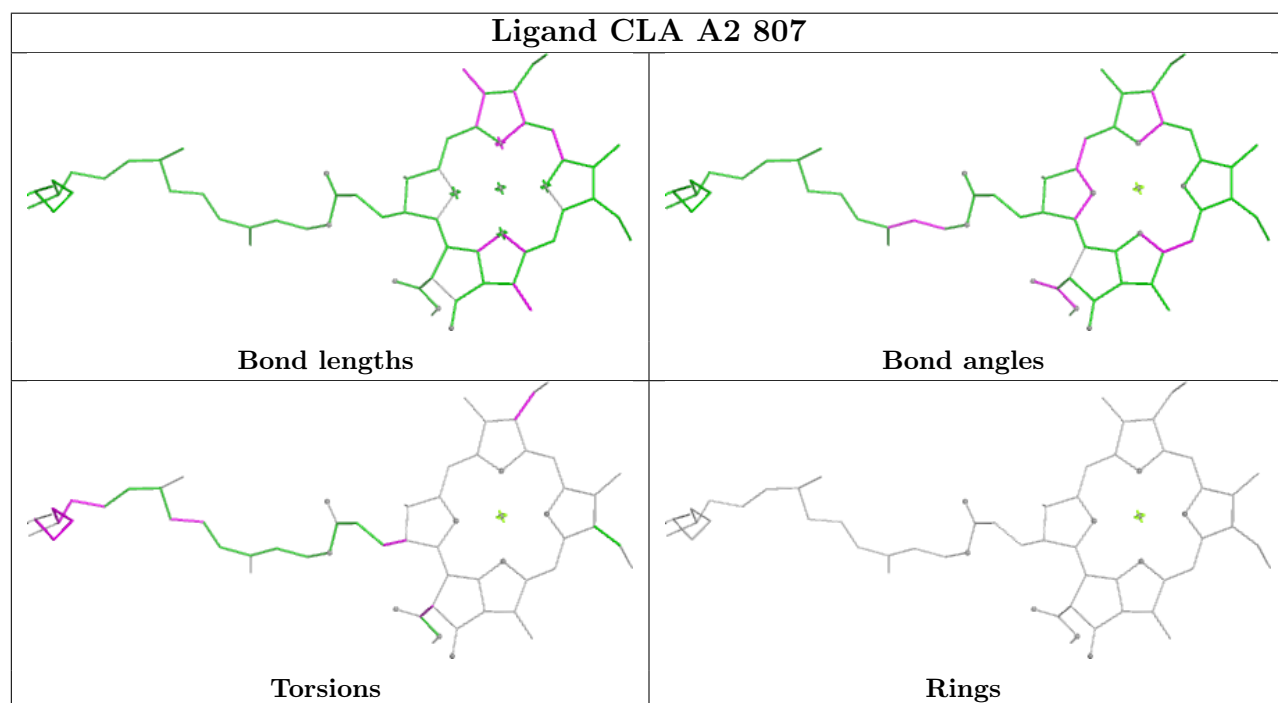
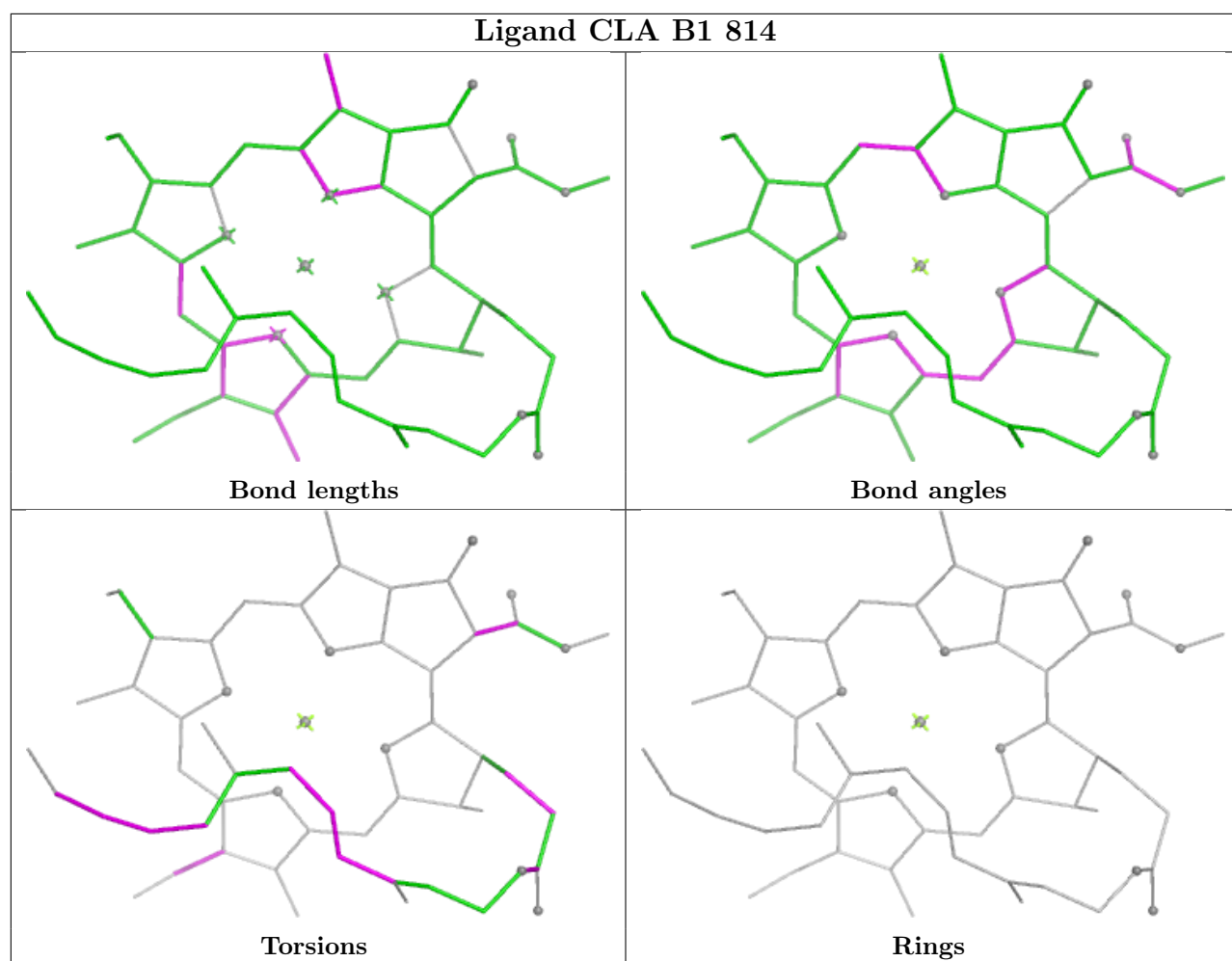
Bond angles



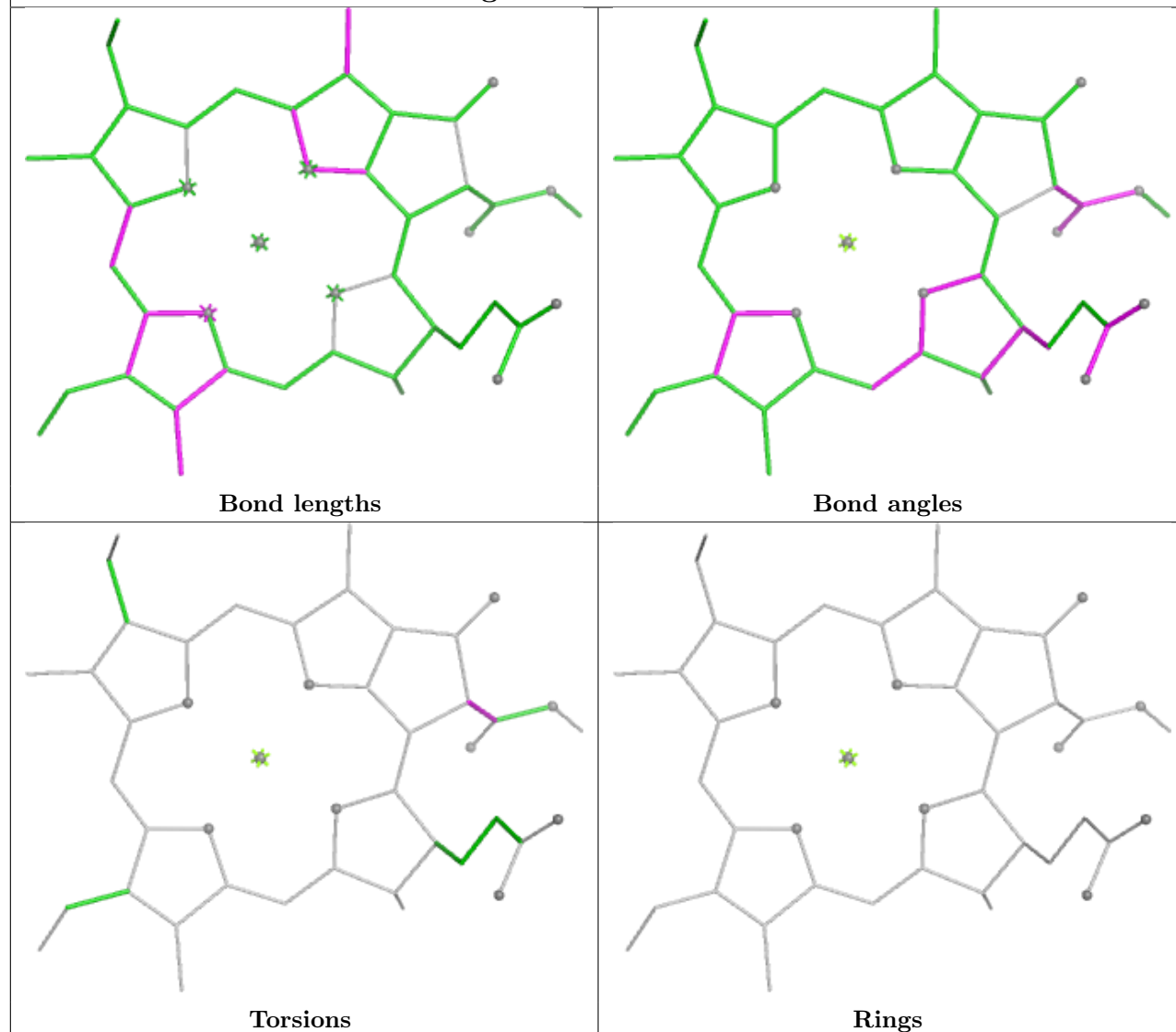
Torsions



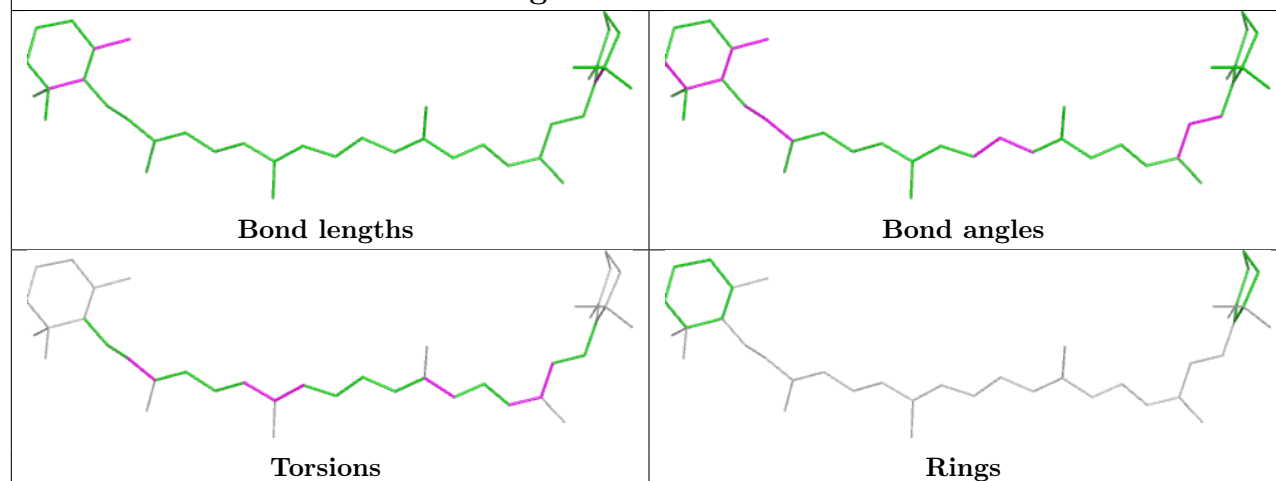
Rings



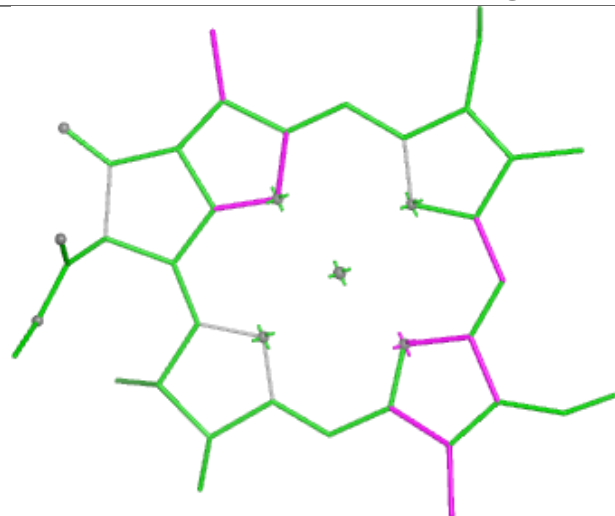
Ligand CLA K2 102



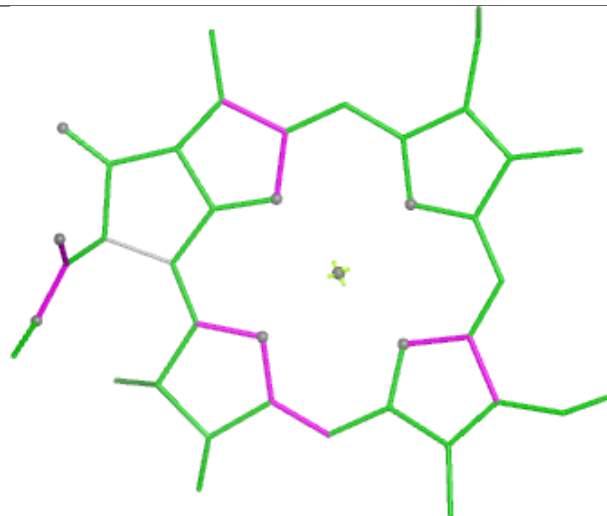
Ligand BCR II 102



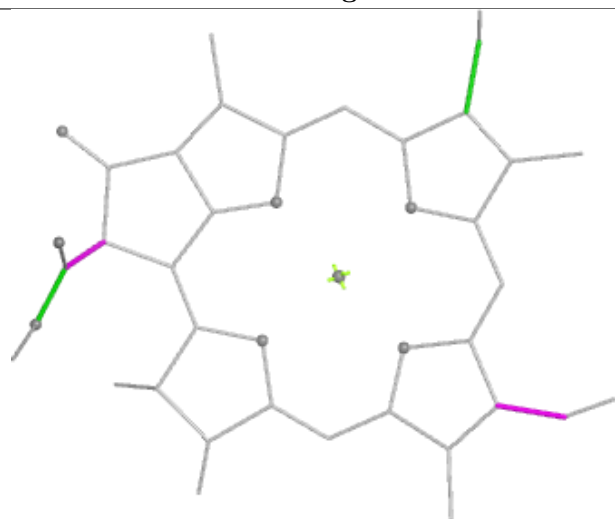
Ligand CLA BB 818



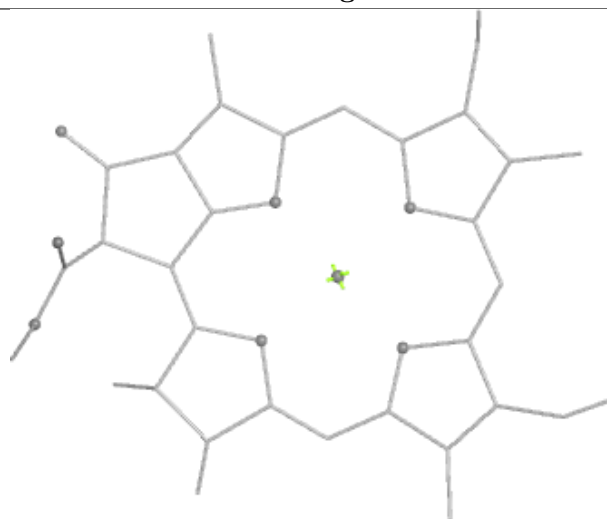
Bond lengths



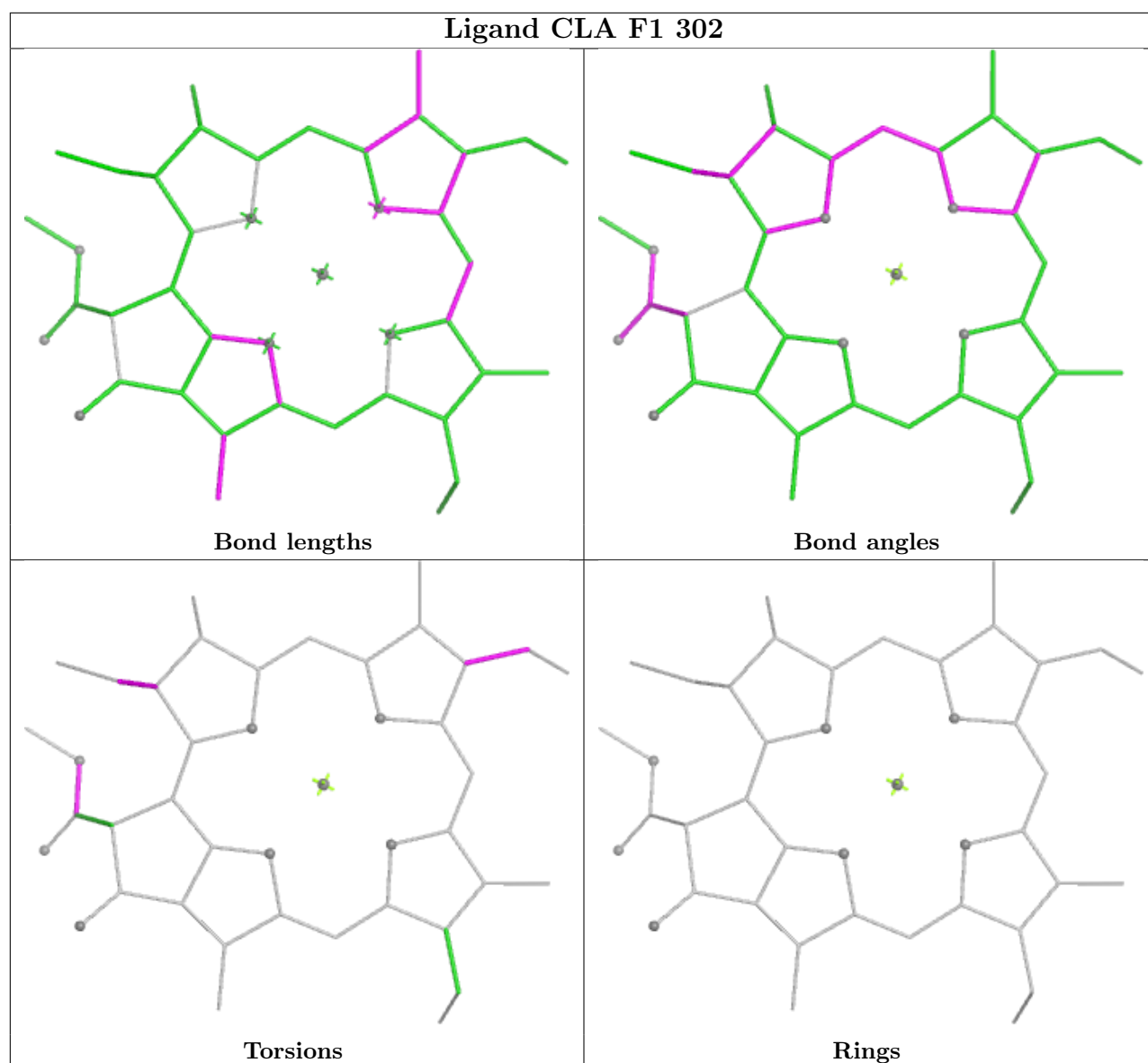
Bond angles

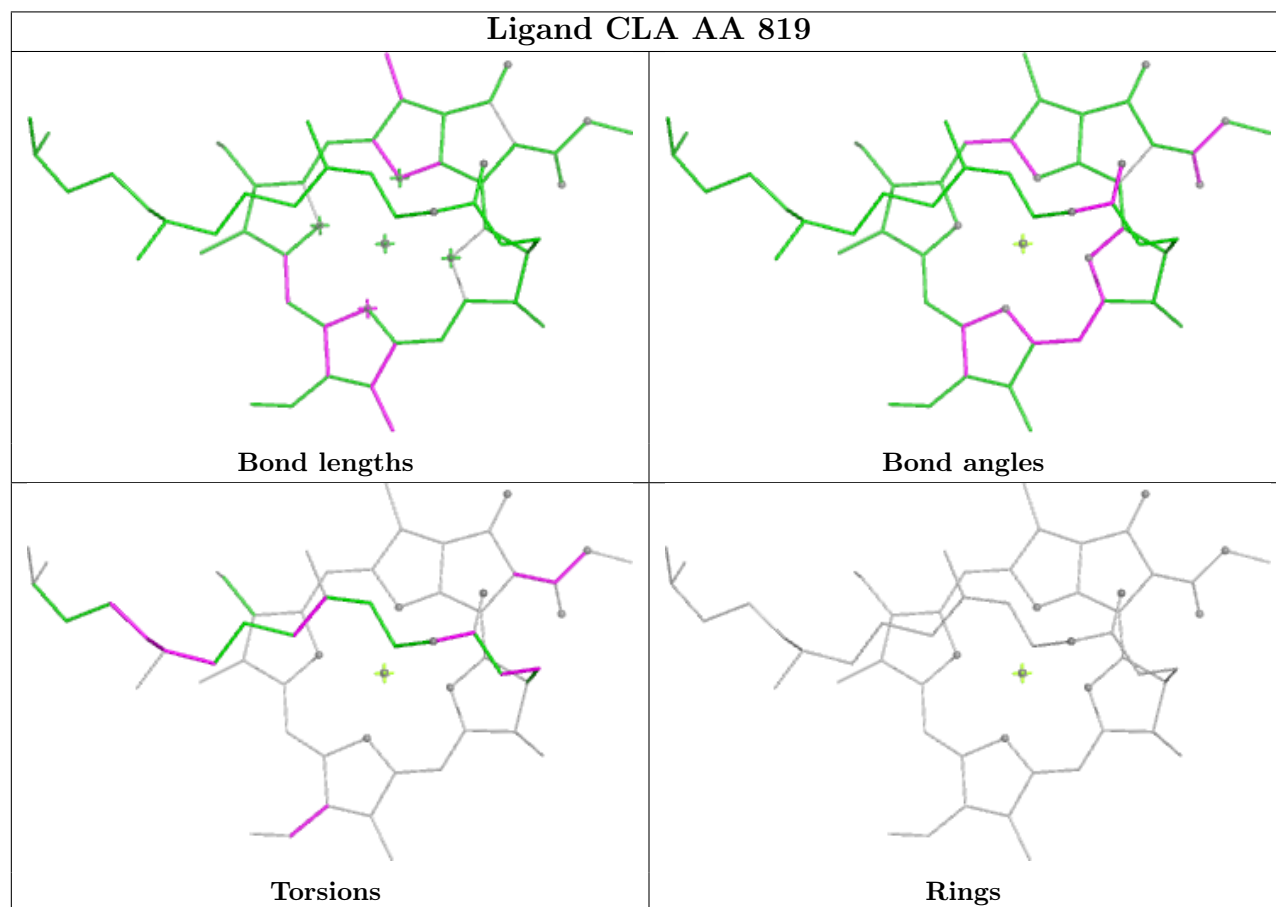
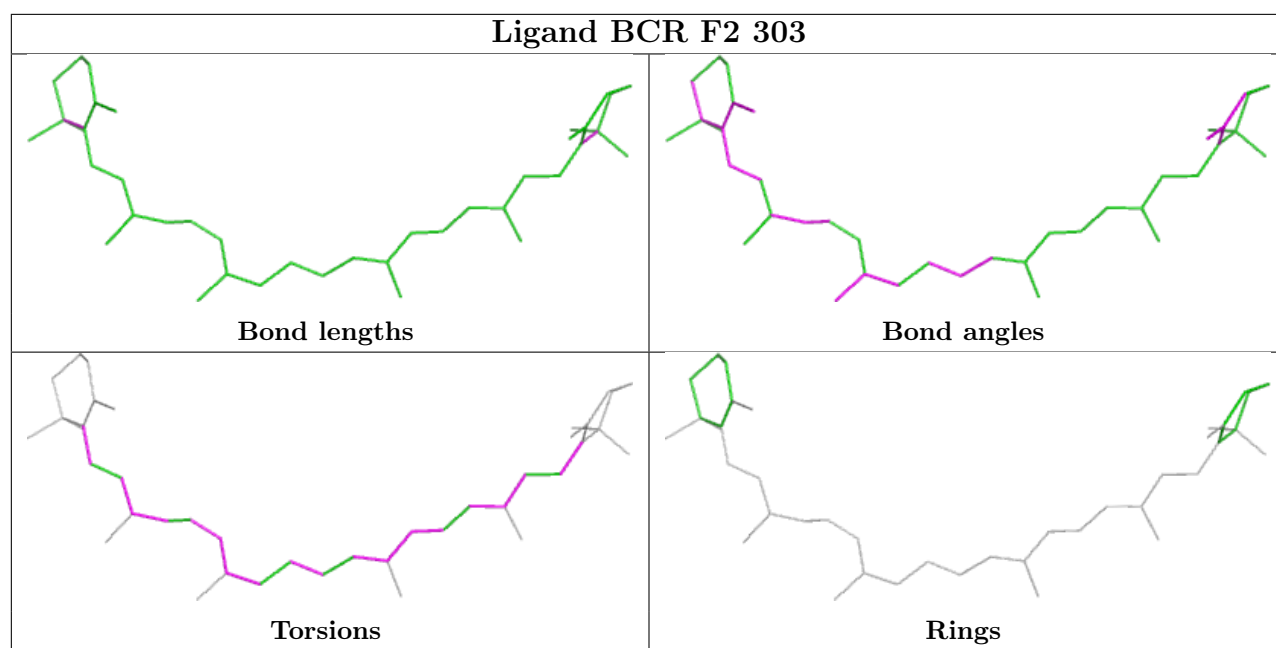


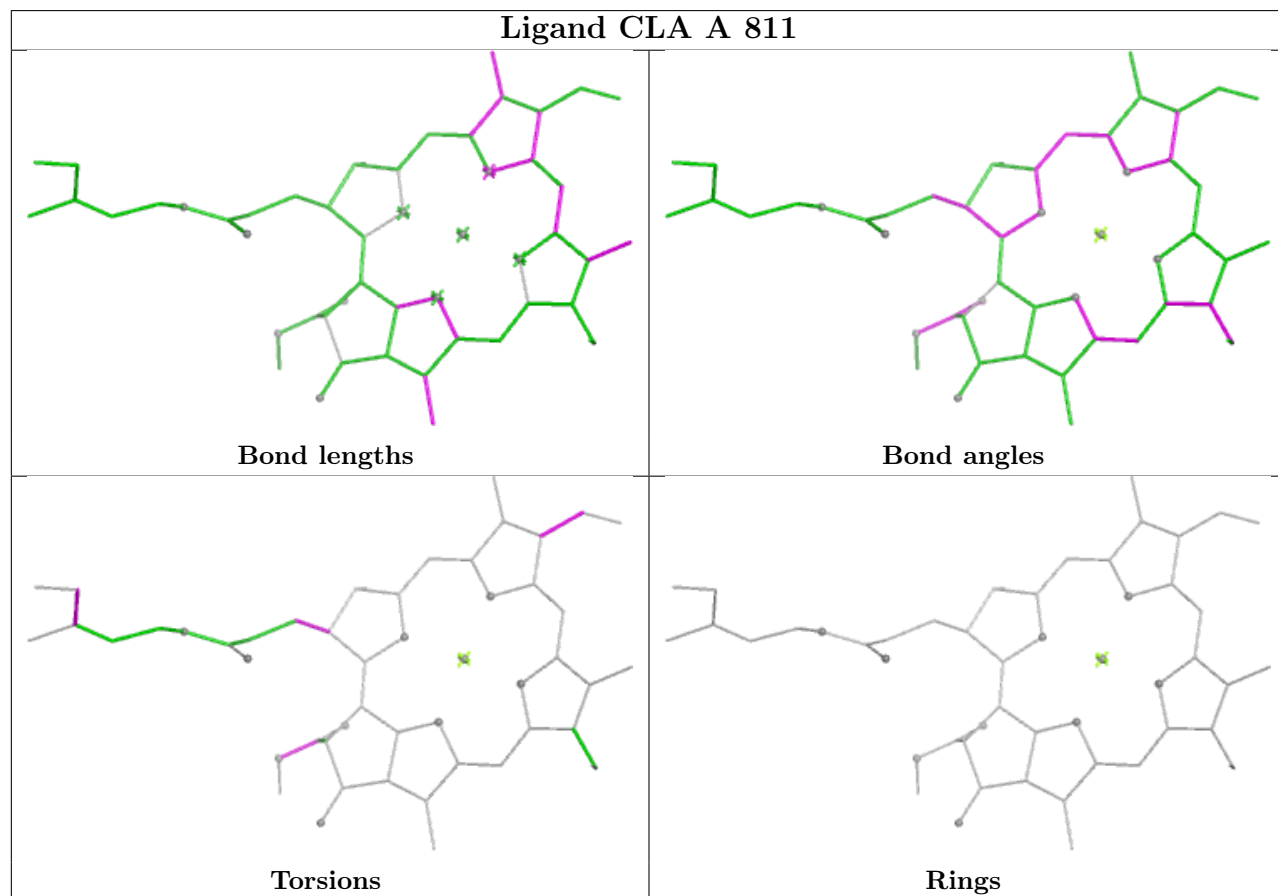
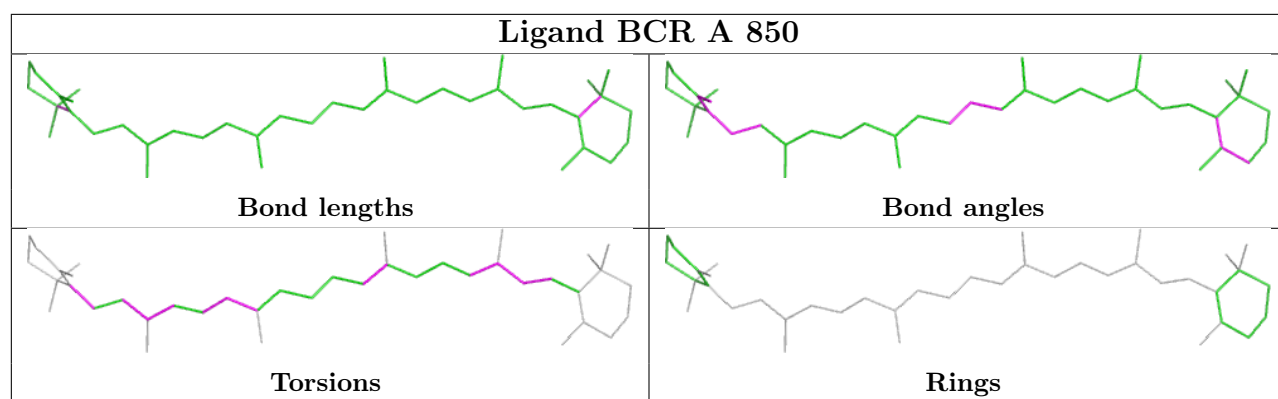
Torsions

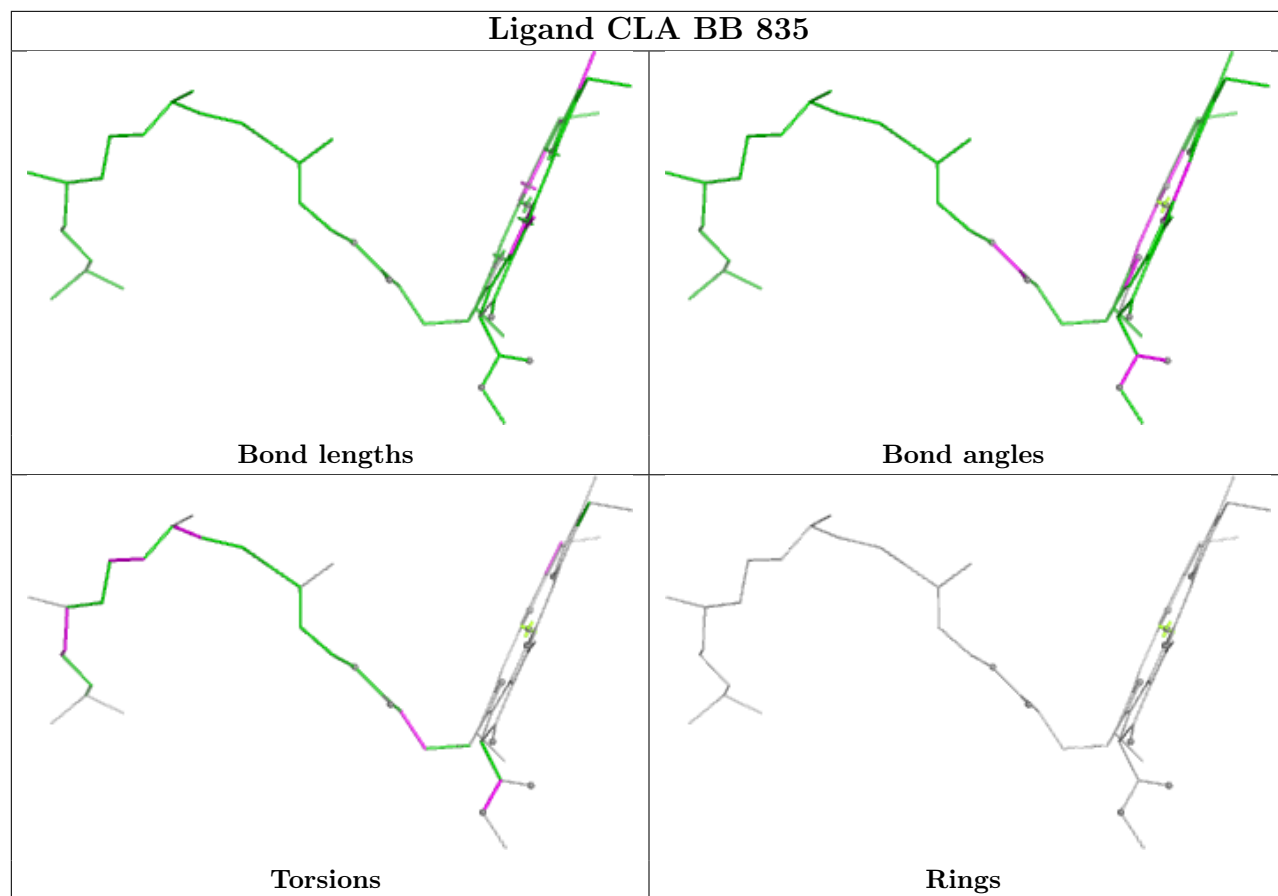


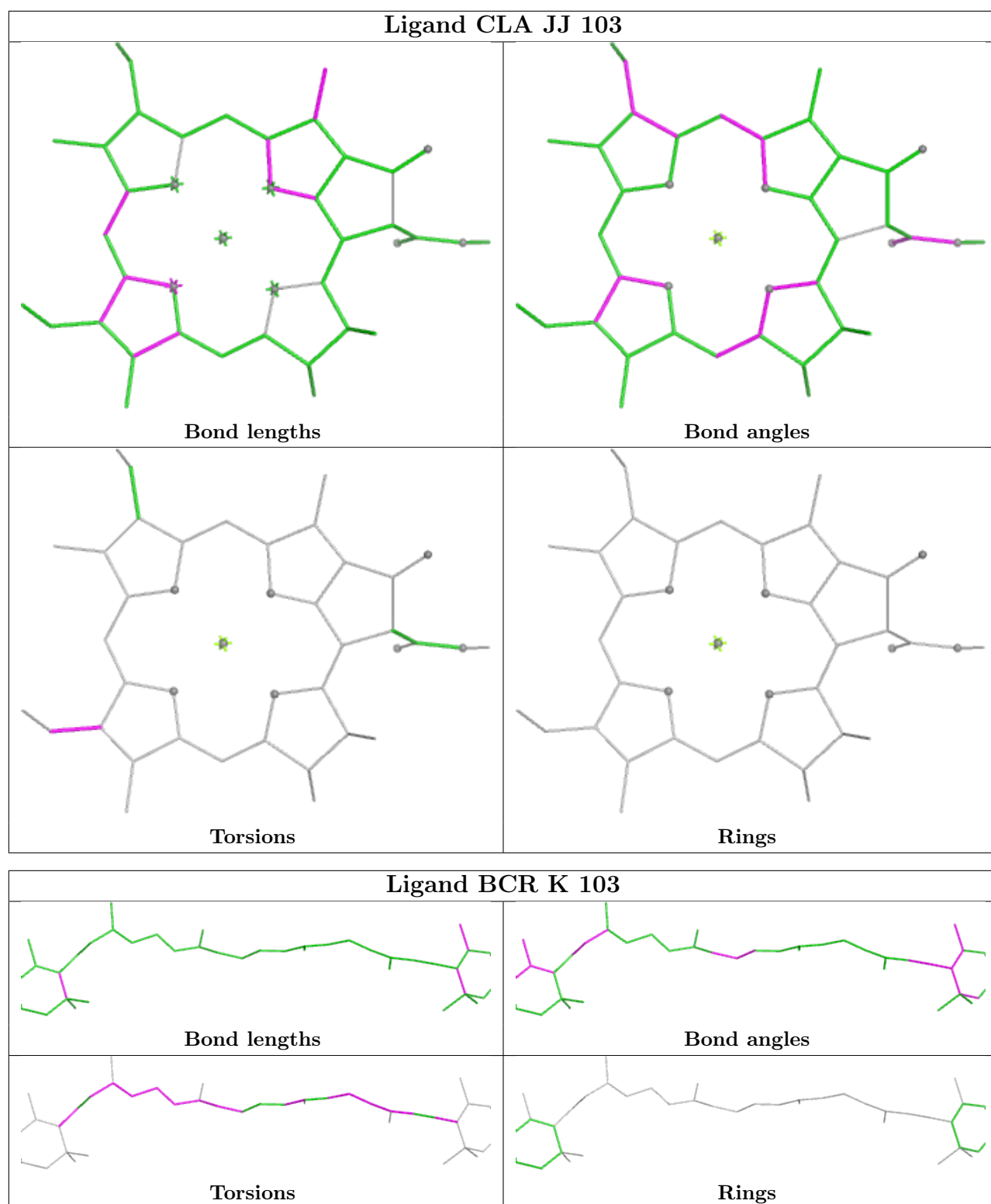
Rings

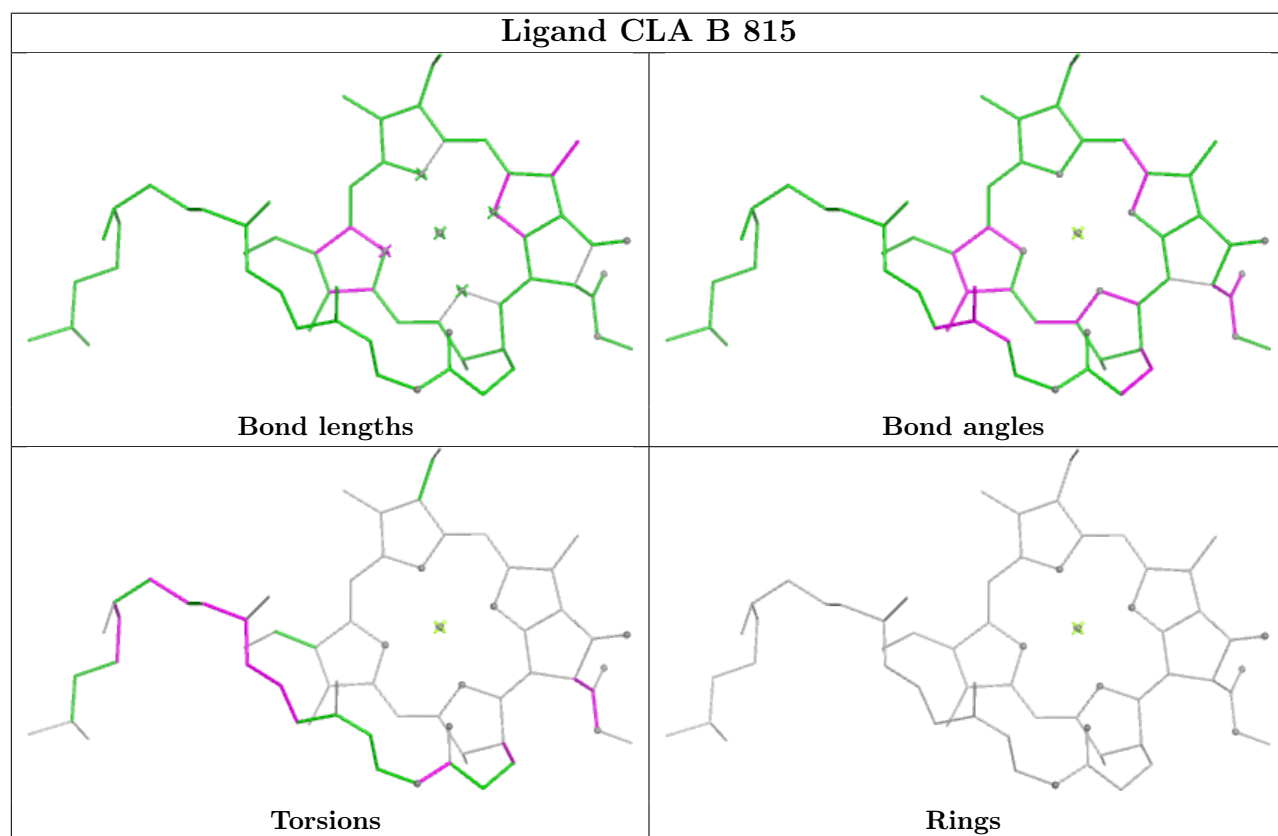
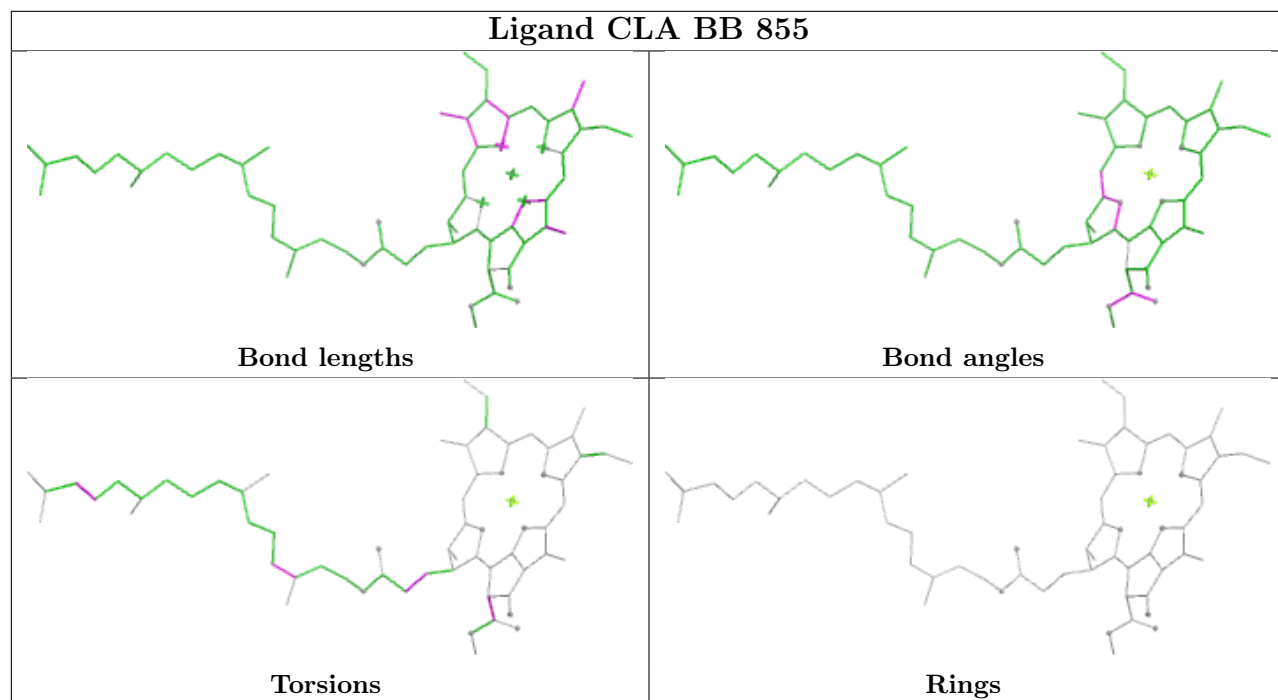


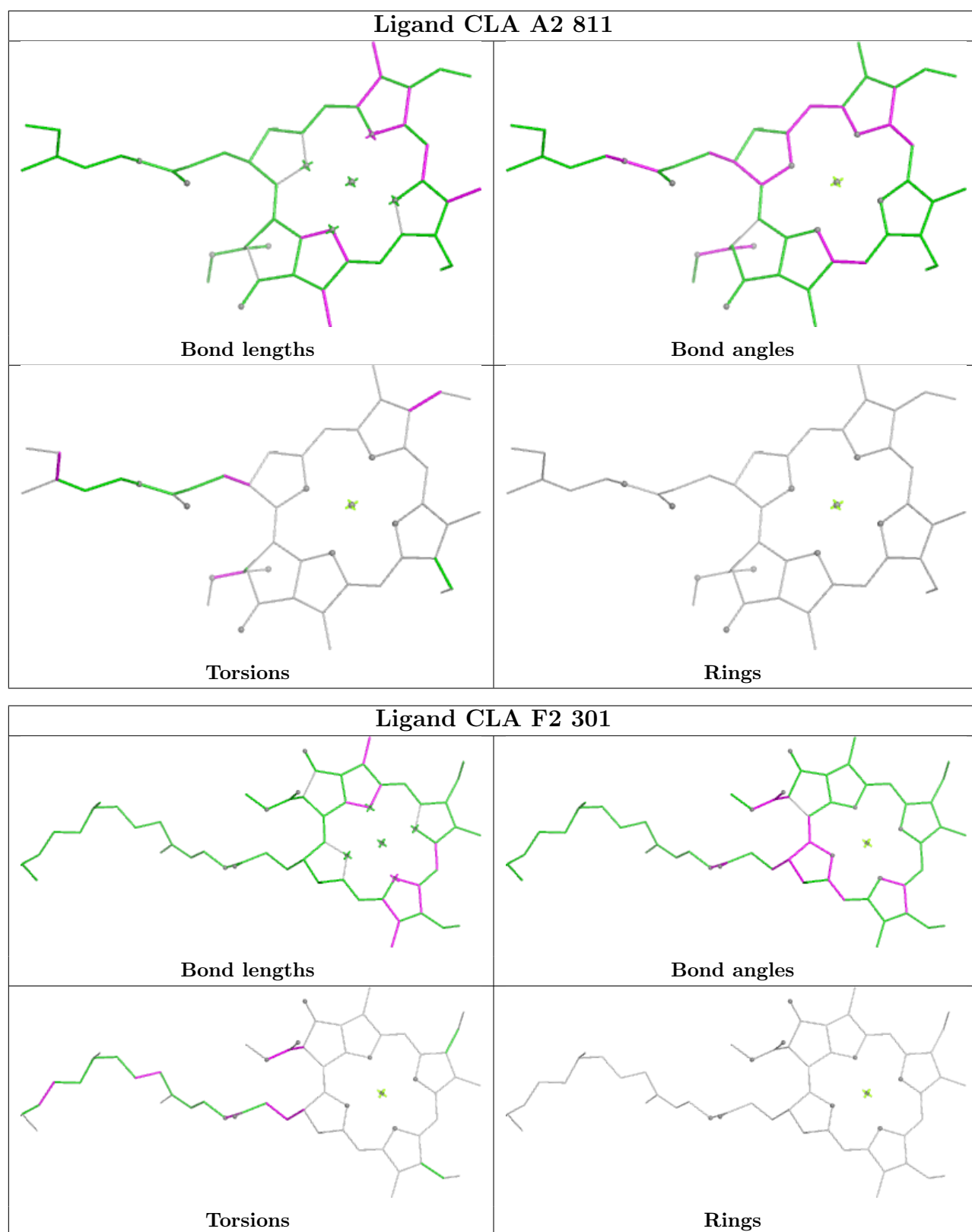


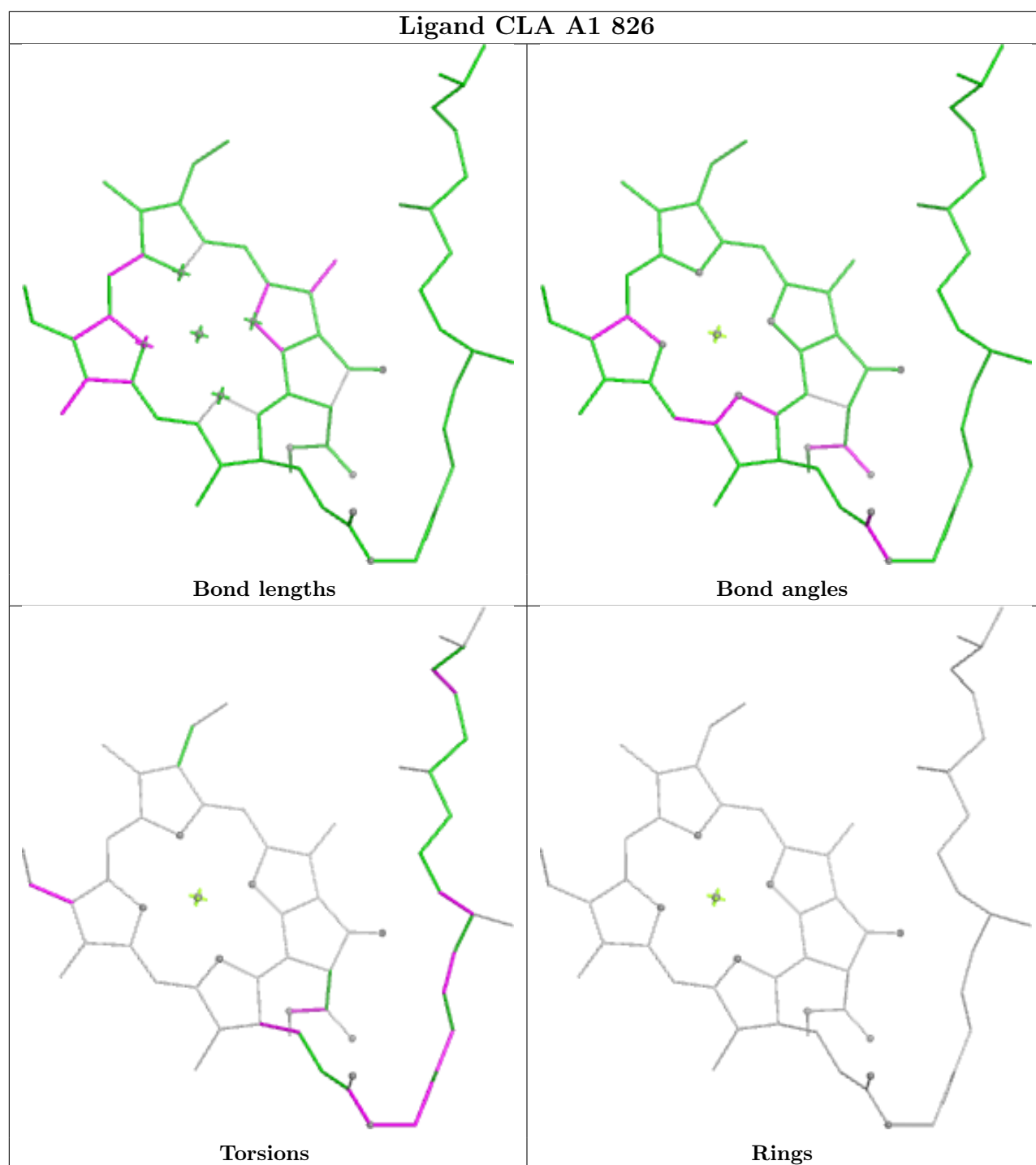


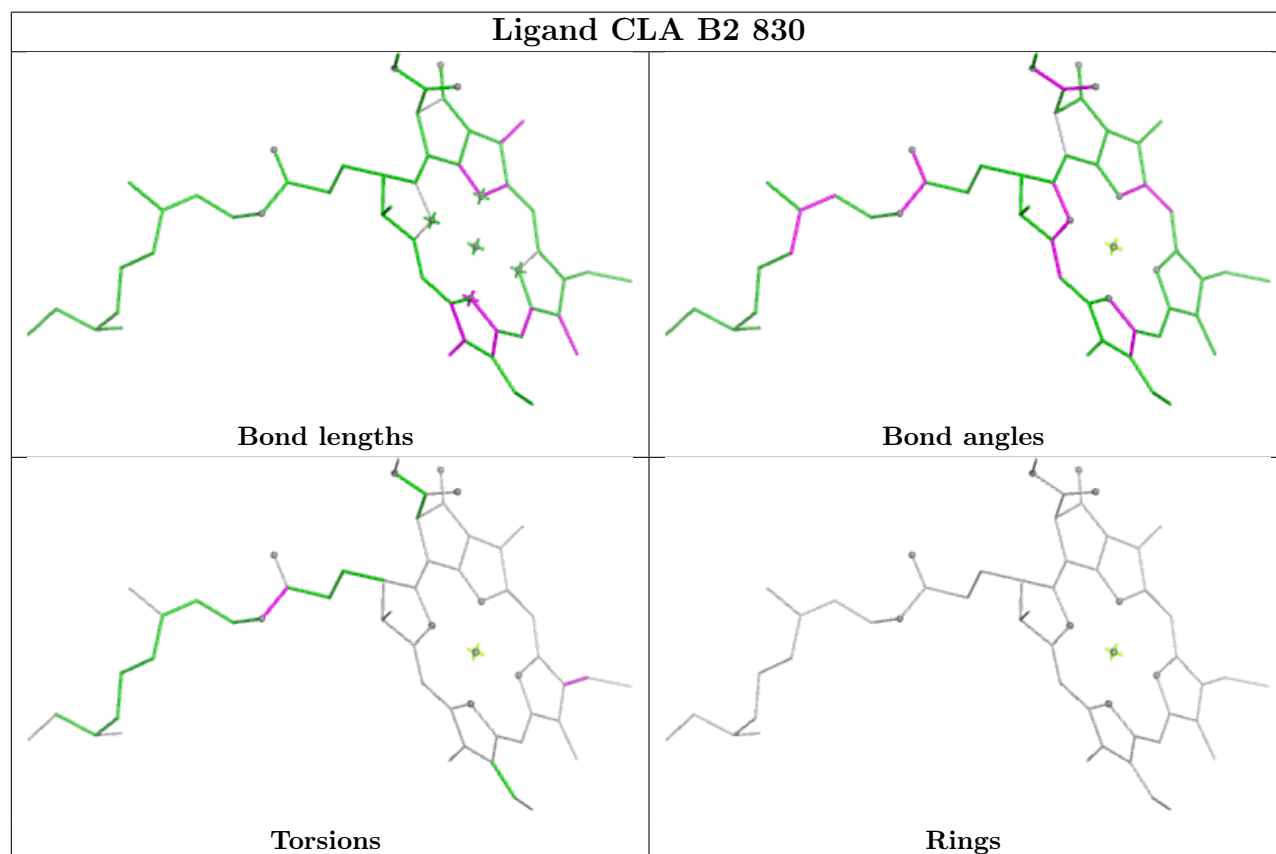
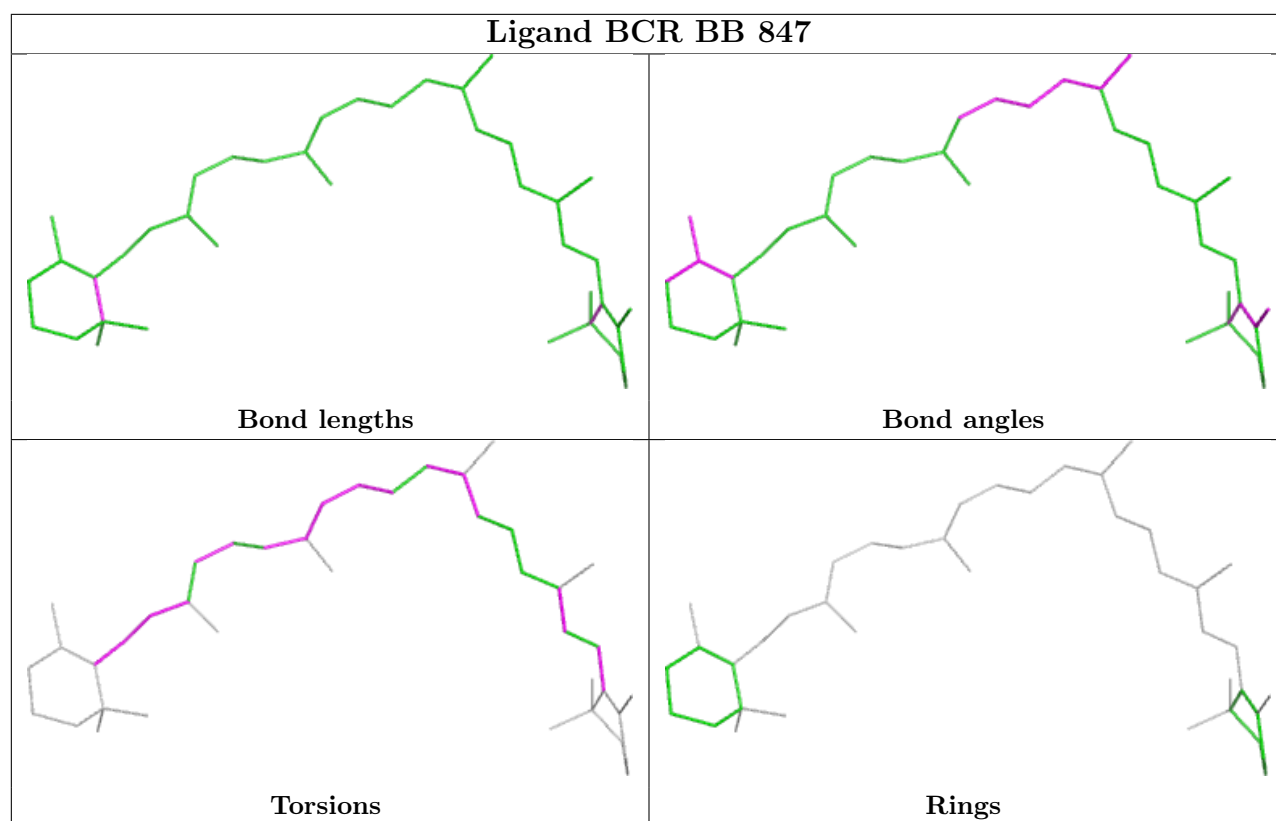


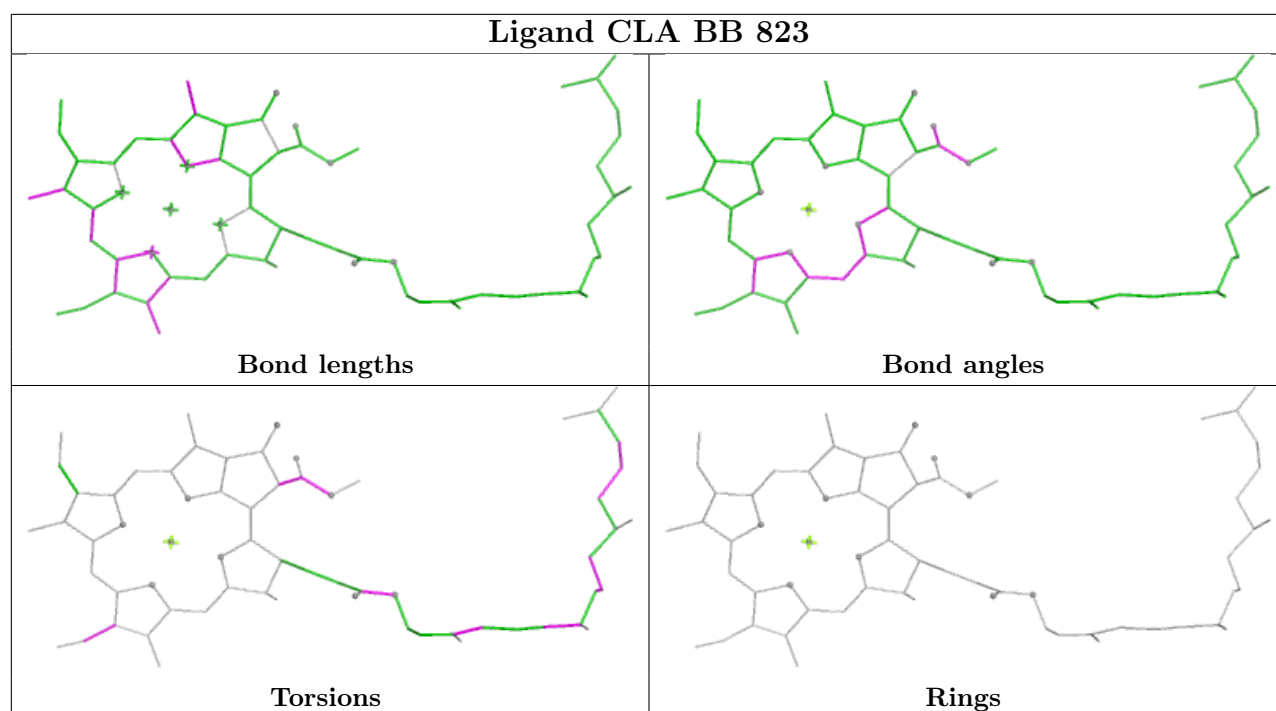




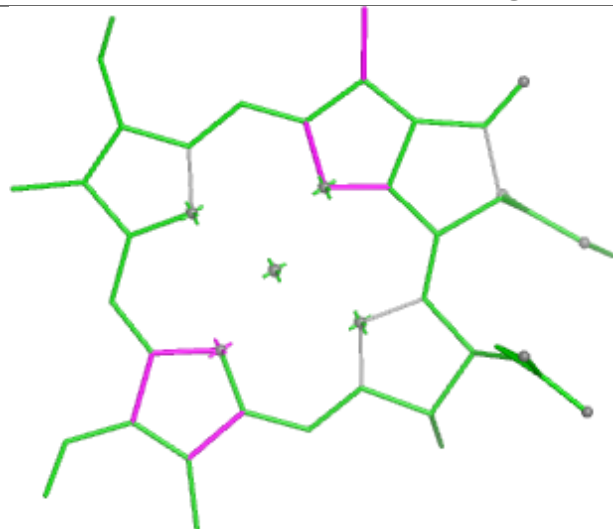




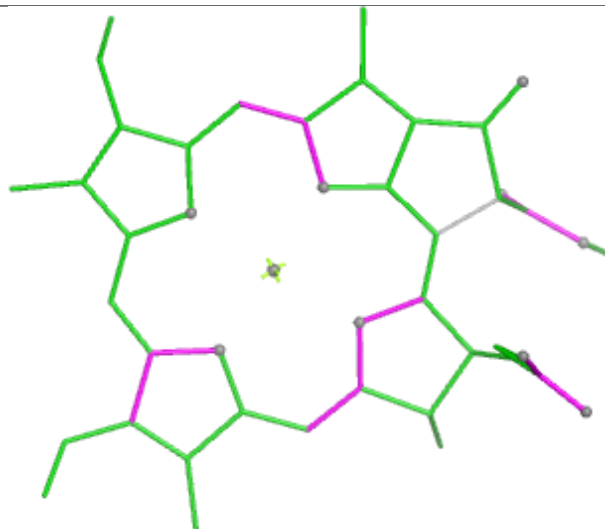




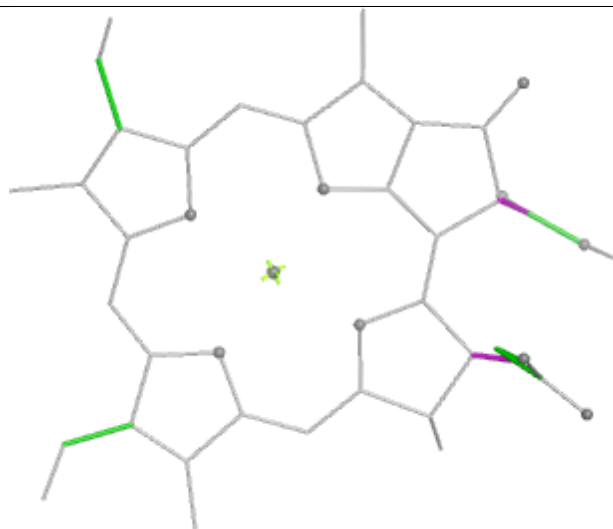
Ligand CLA B2 835



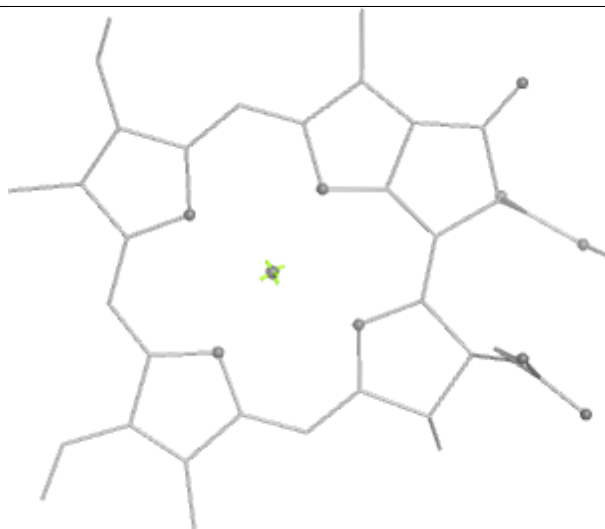
Bond lengths



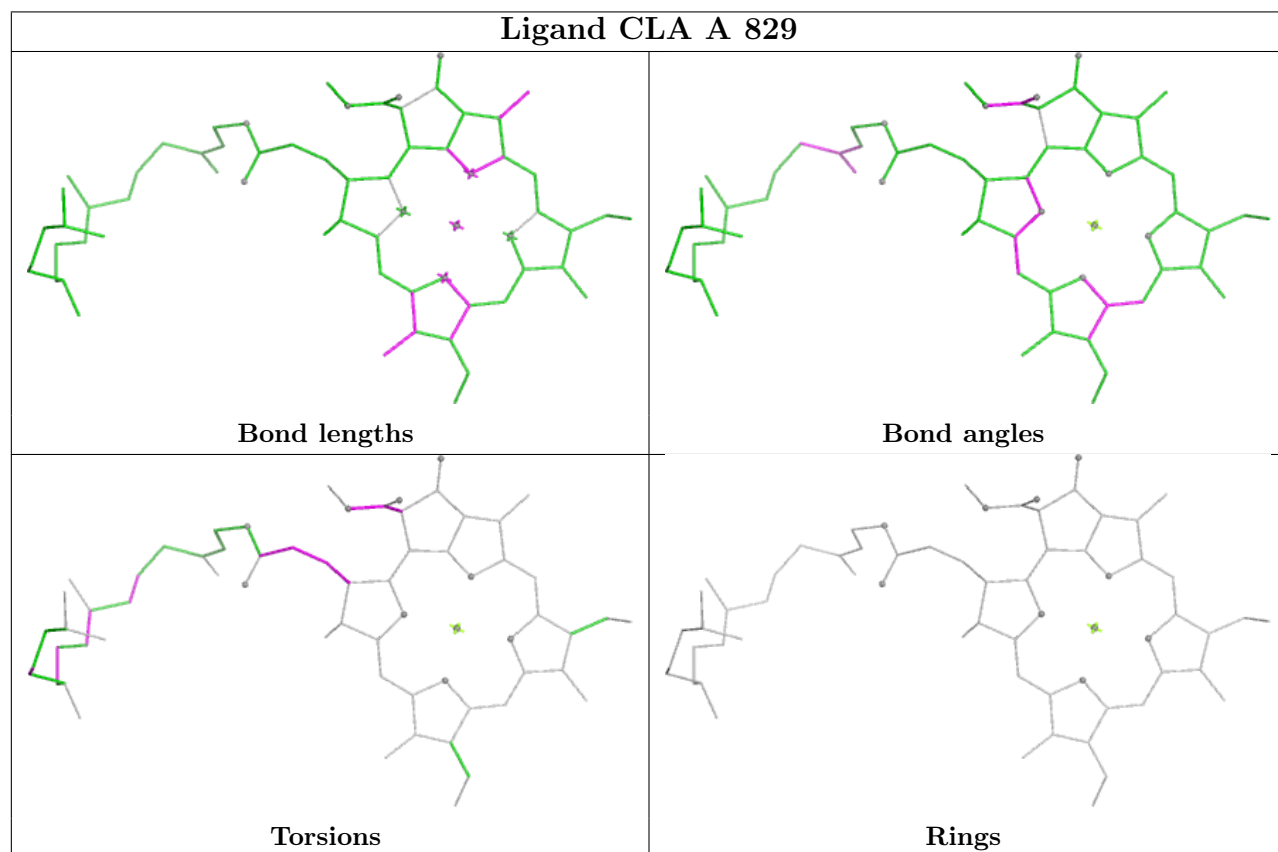
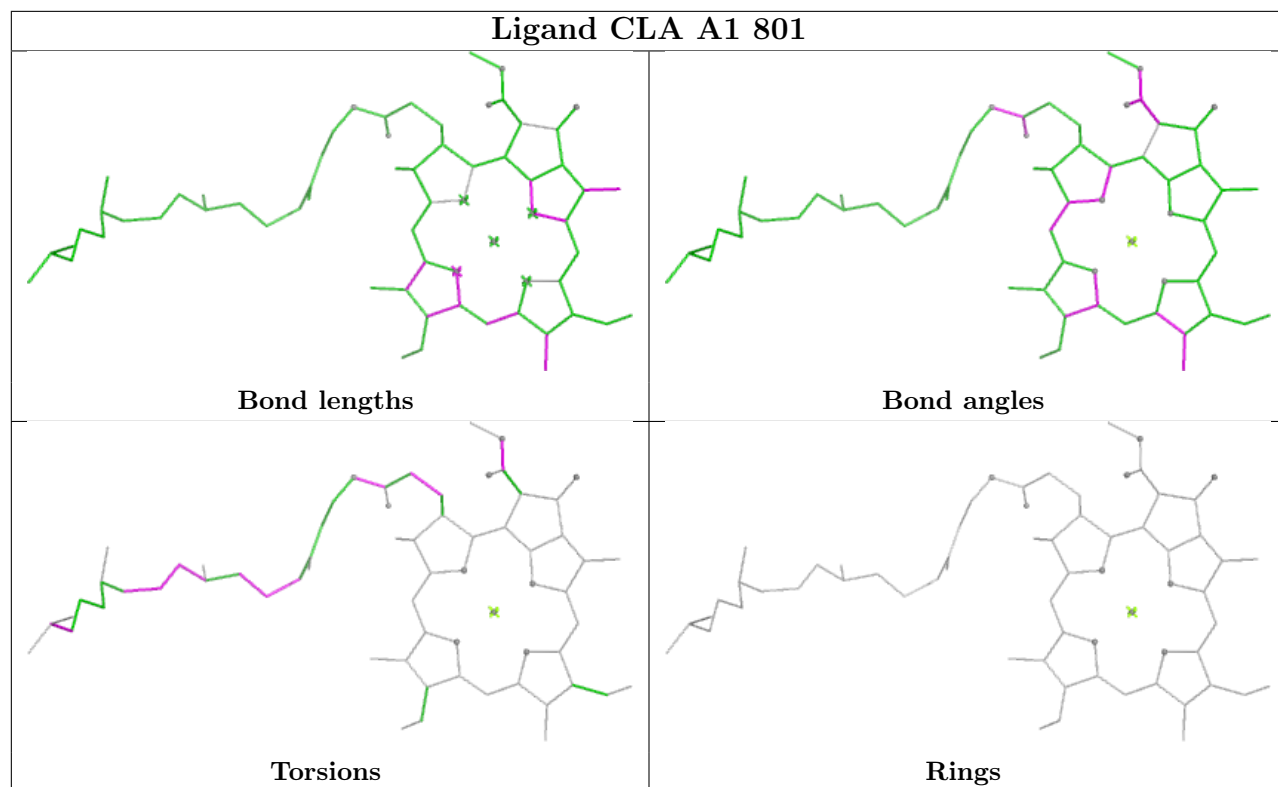
Bond angles



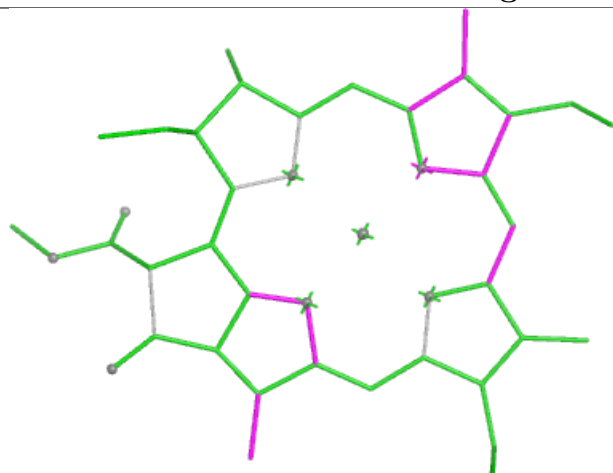
Torsions



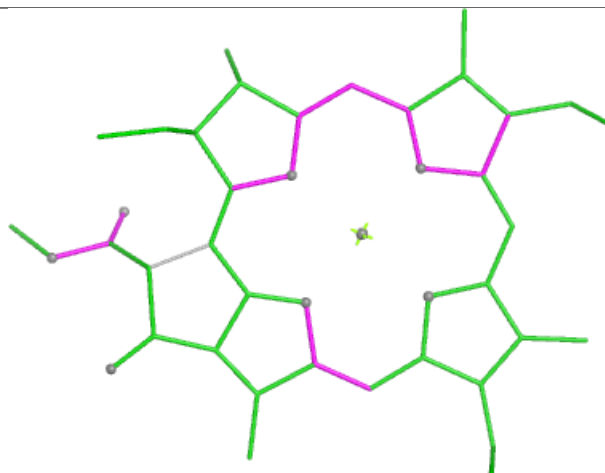
Rings



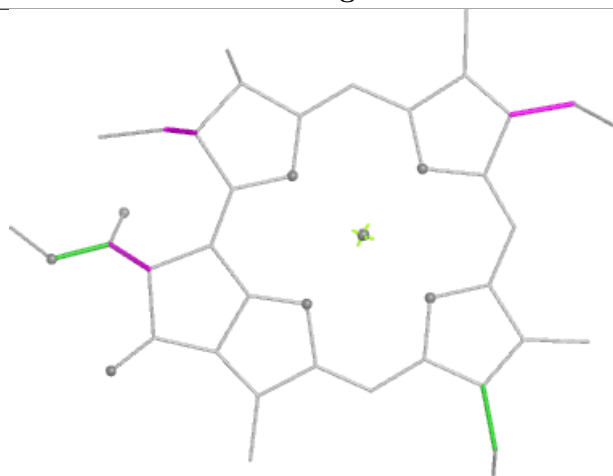
Ligand CLA AA 814



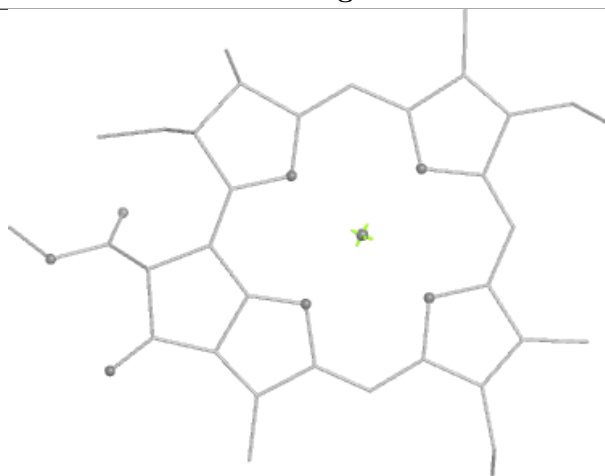
Bond lengths



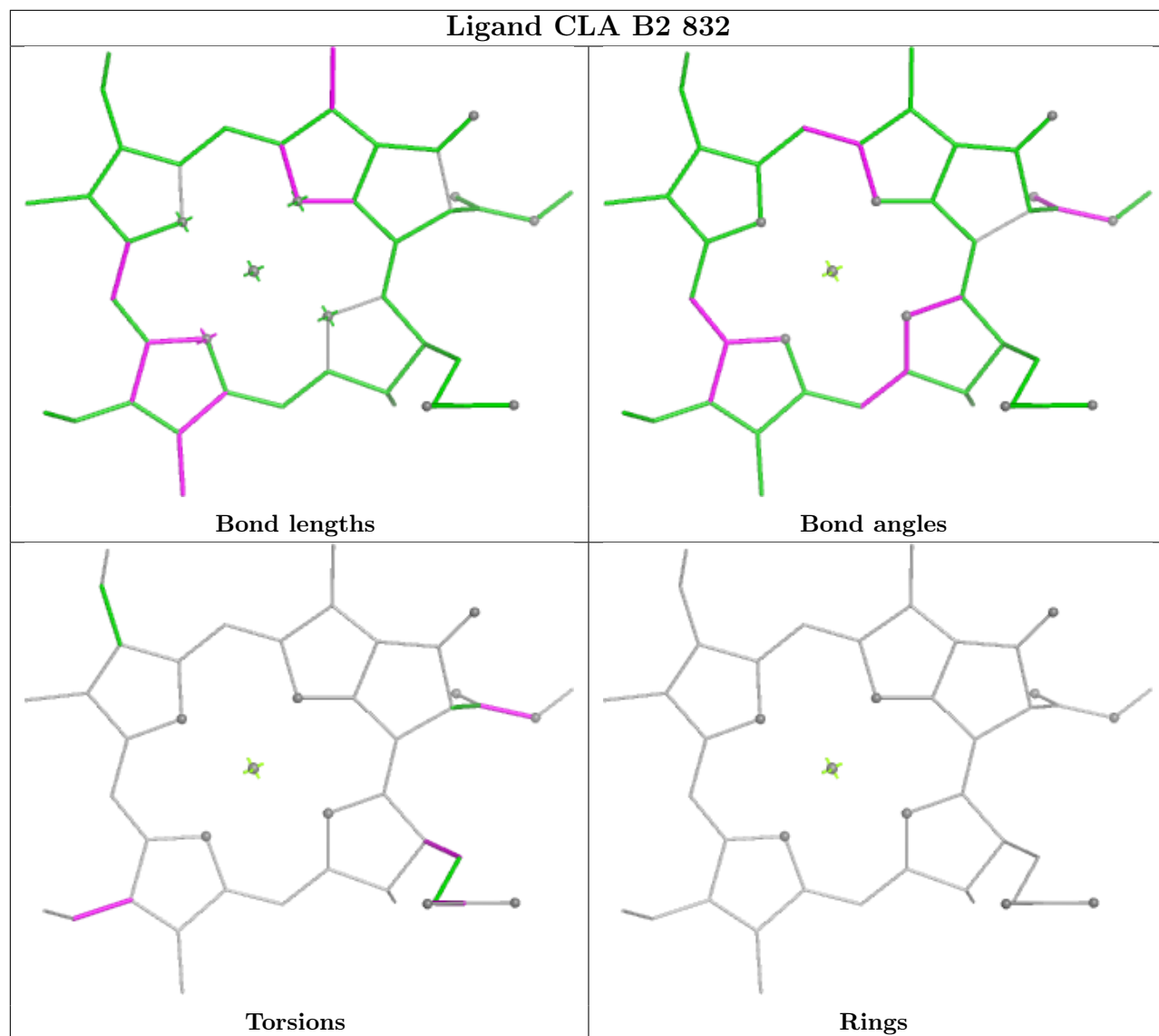
Bond angles

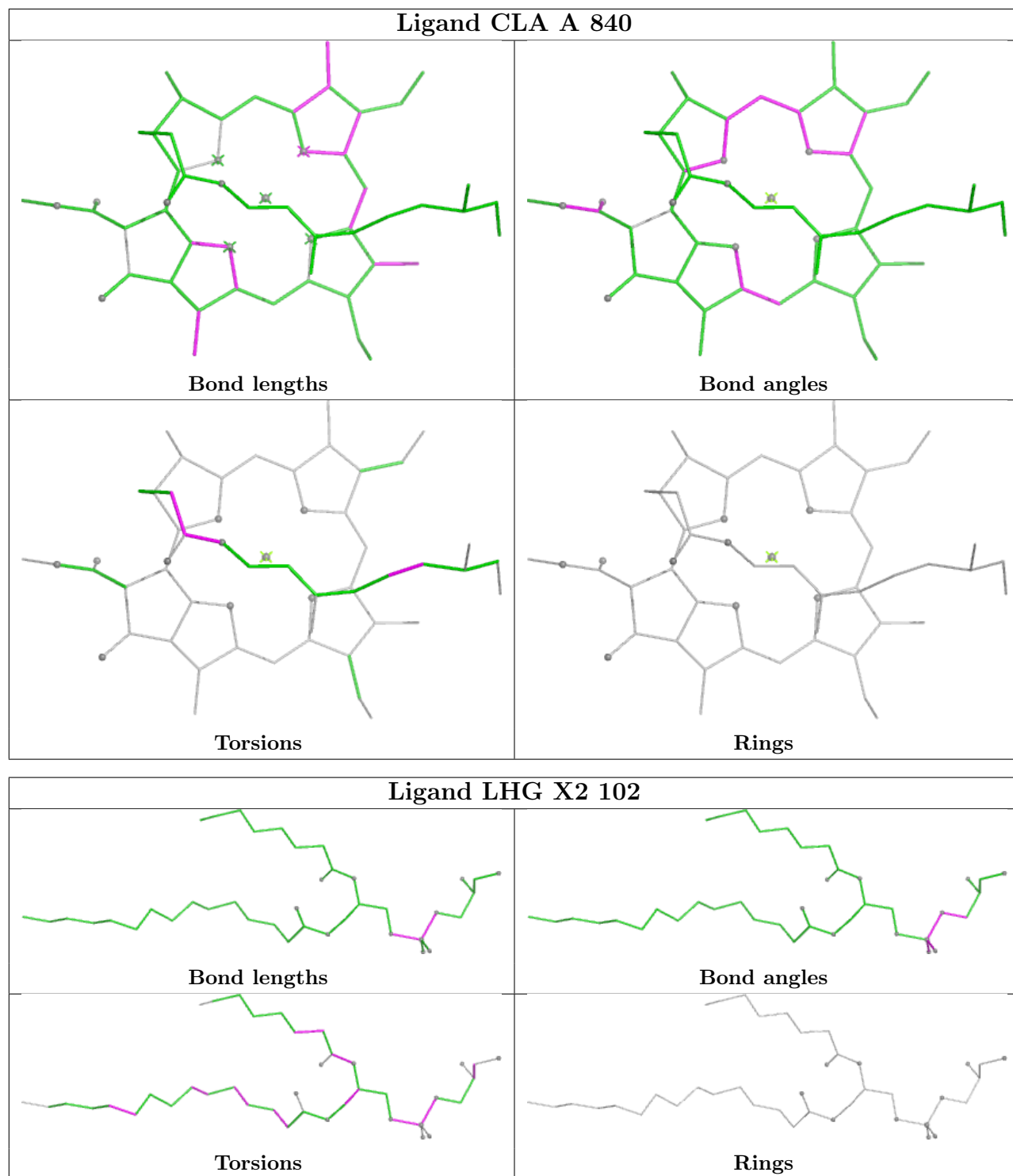


Torsions

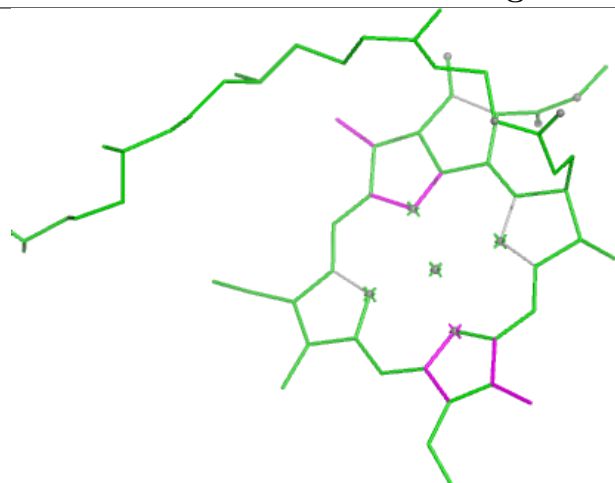


Rings

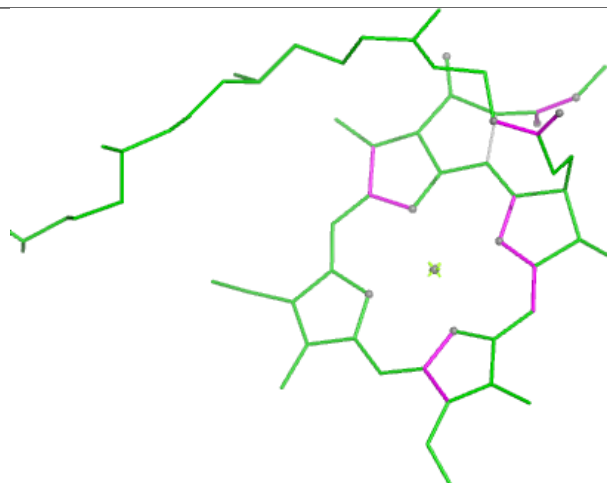




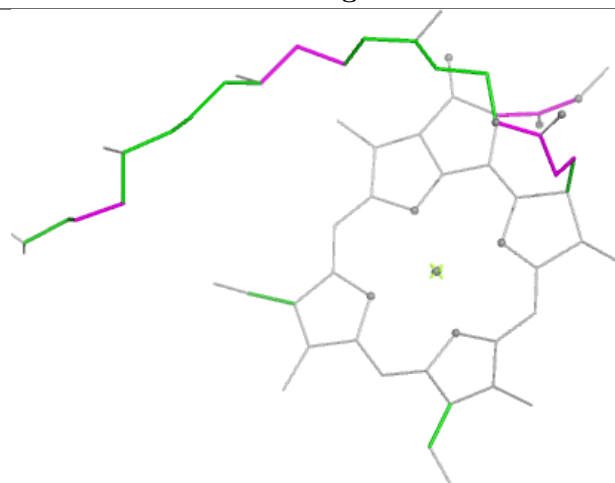
Ligand CLA A2 831



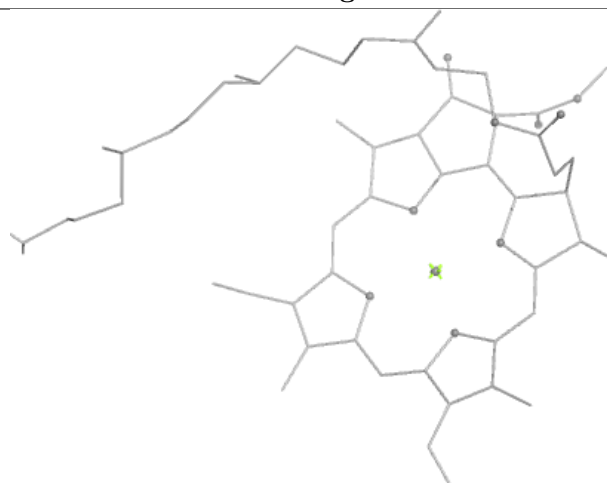
Bond lengths



Bond angles

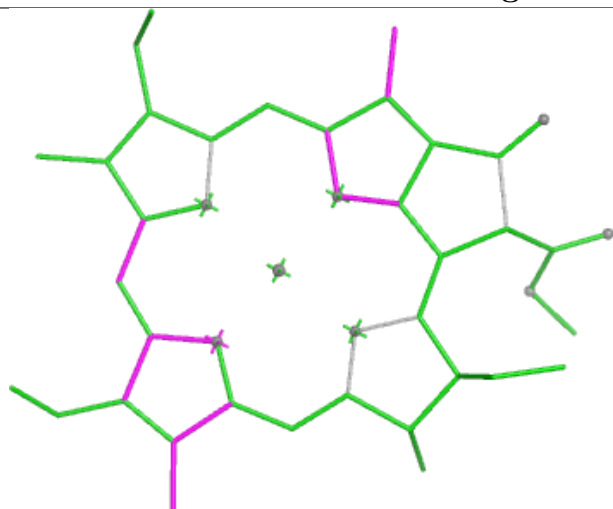


Torsions

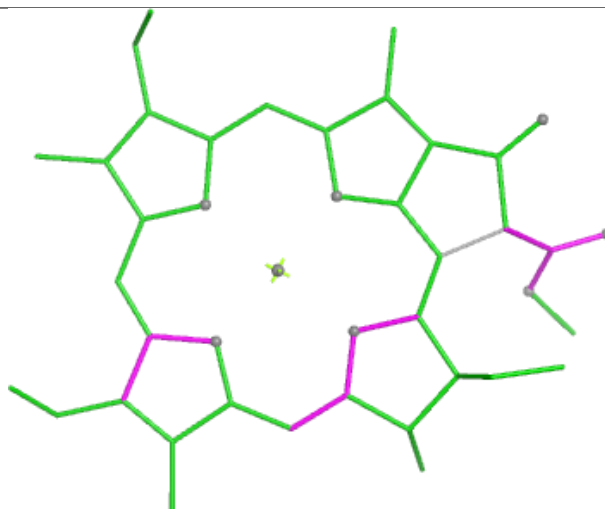


Rings

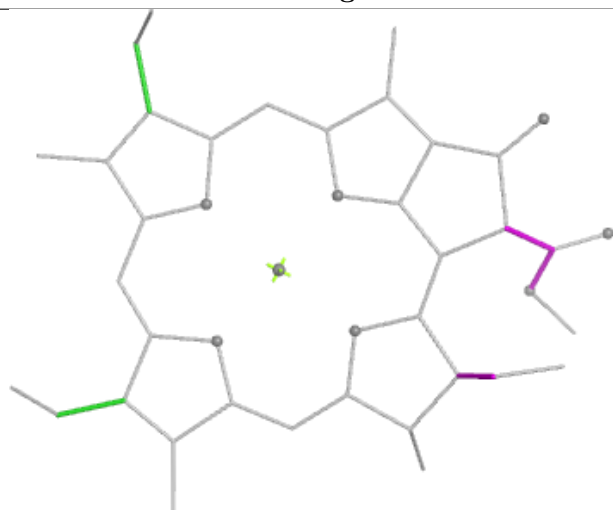
Ligand CLA BB 813



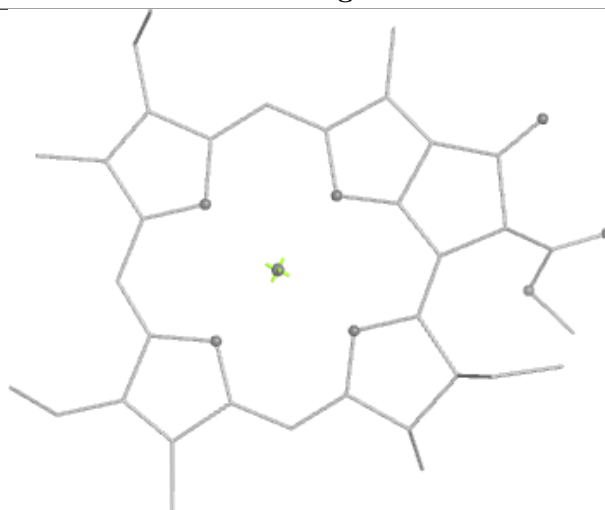
Bond lengths



Bond angles

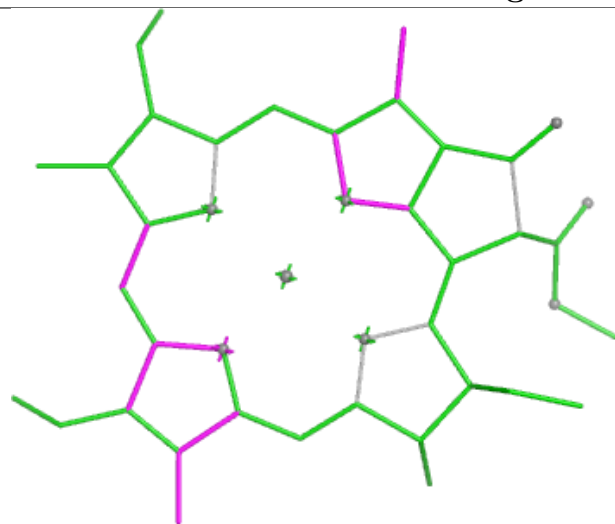


Torsions

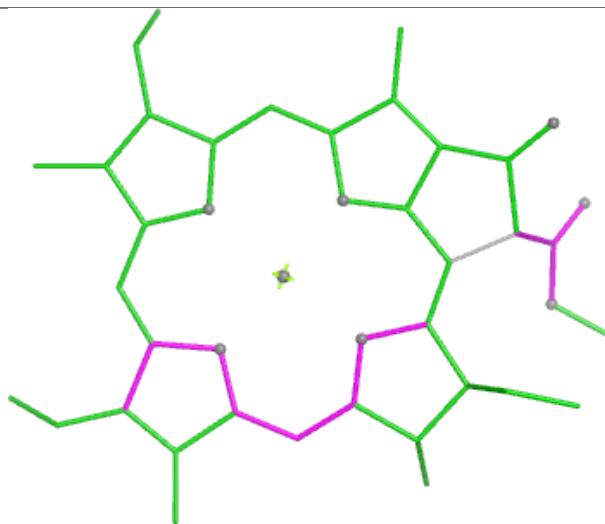


Rings

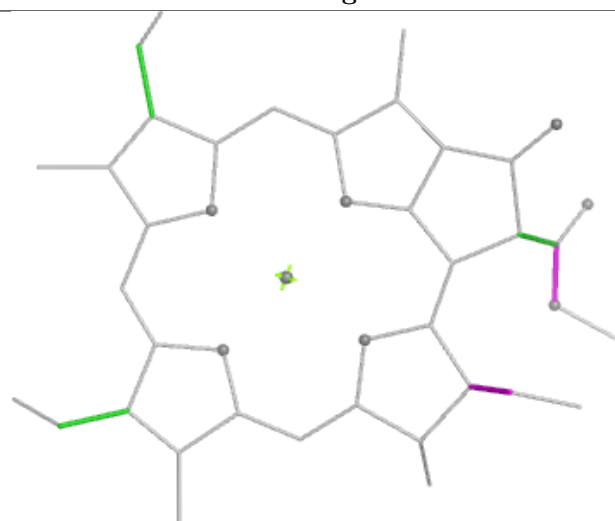
Ligand CLA FF 302



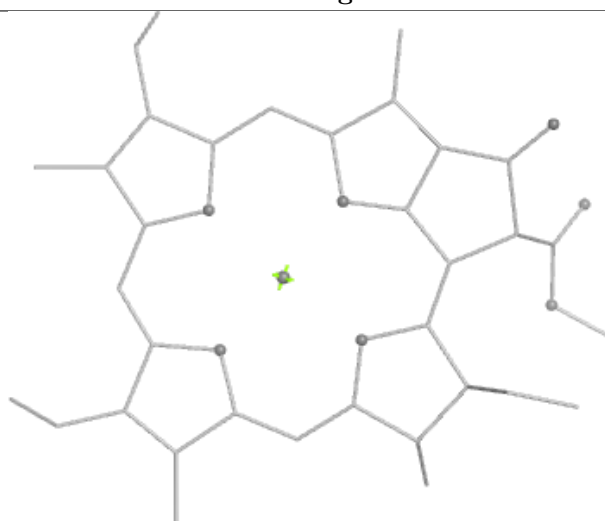
Bond lengths



Bond angles

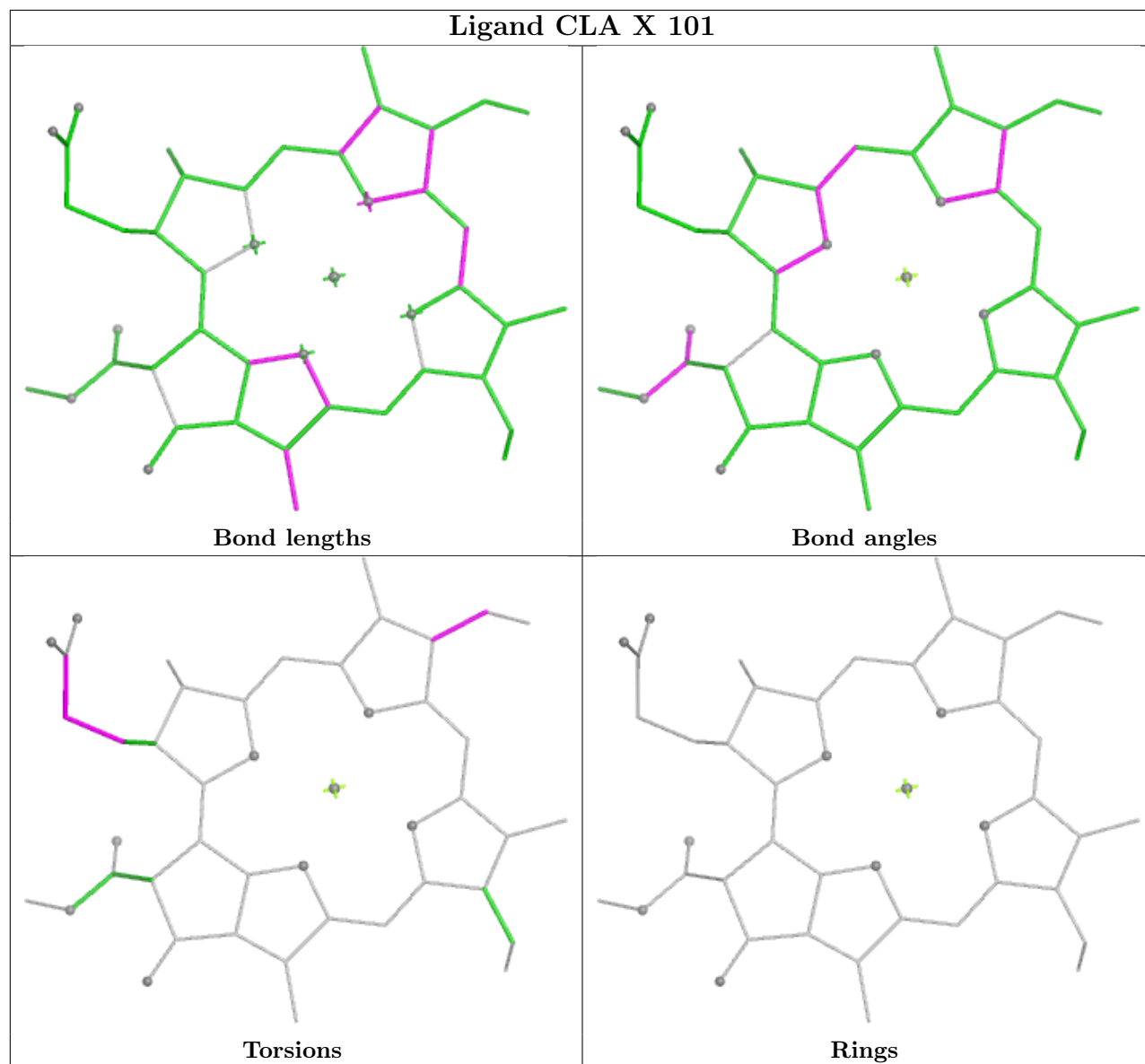


Torsions

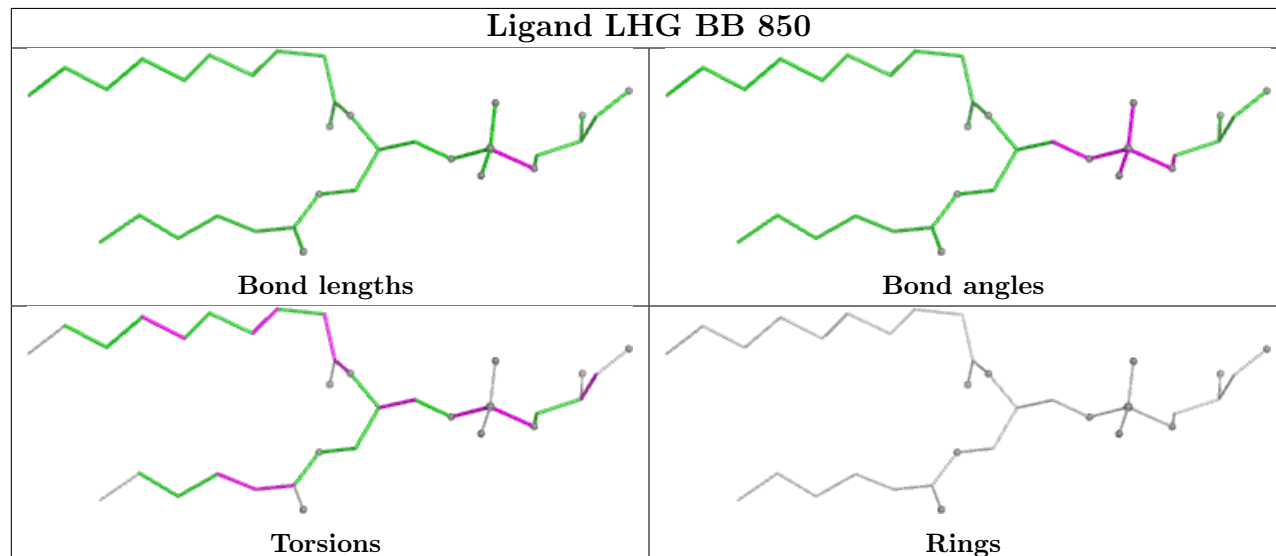


Rings

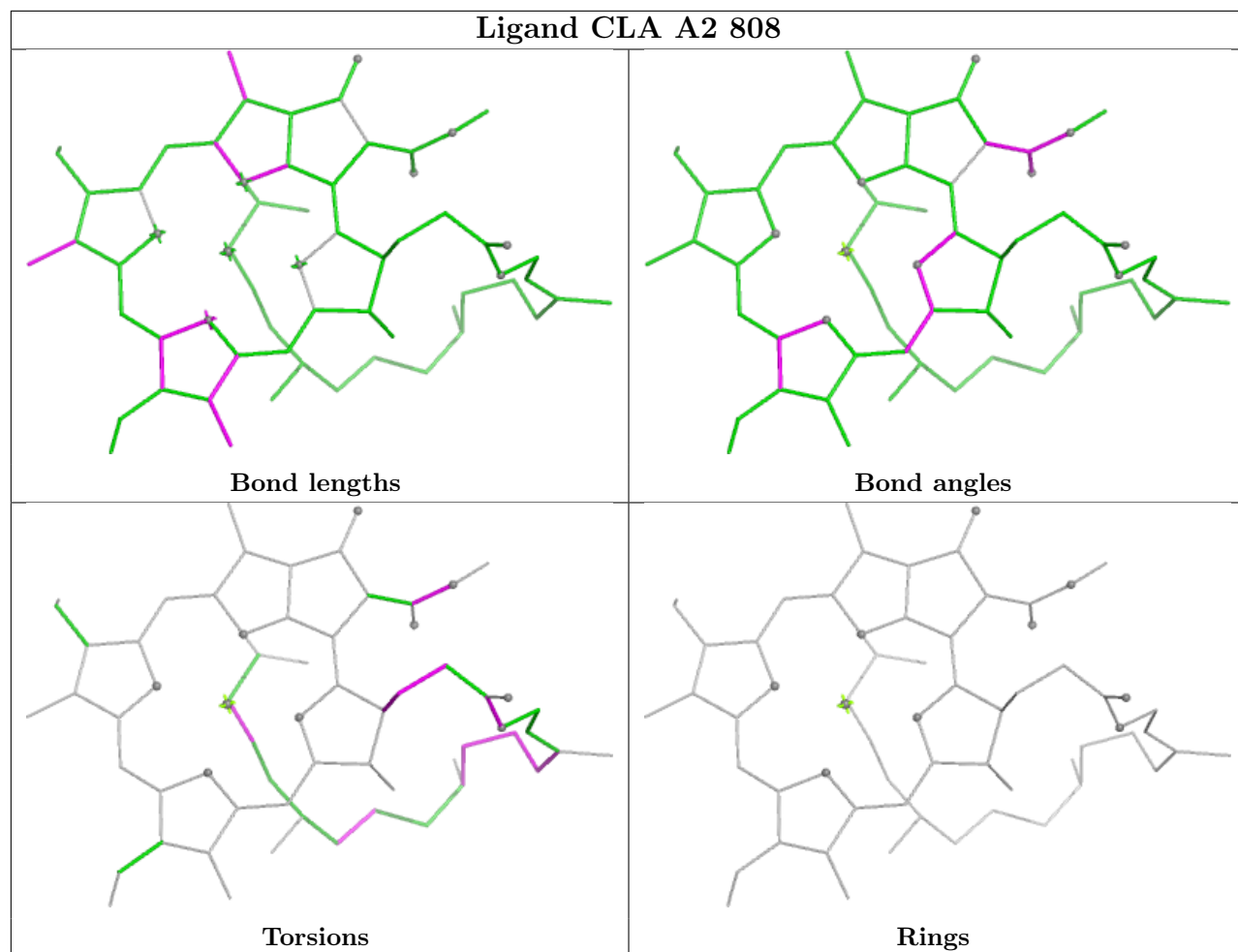
Ligand CLA X 101



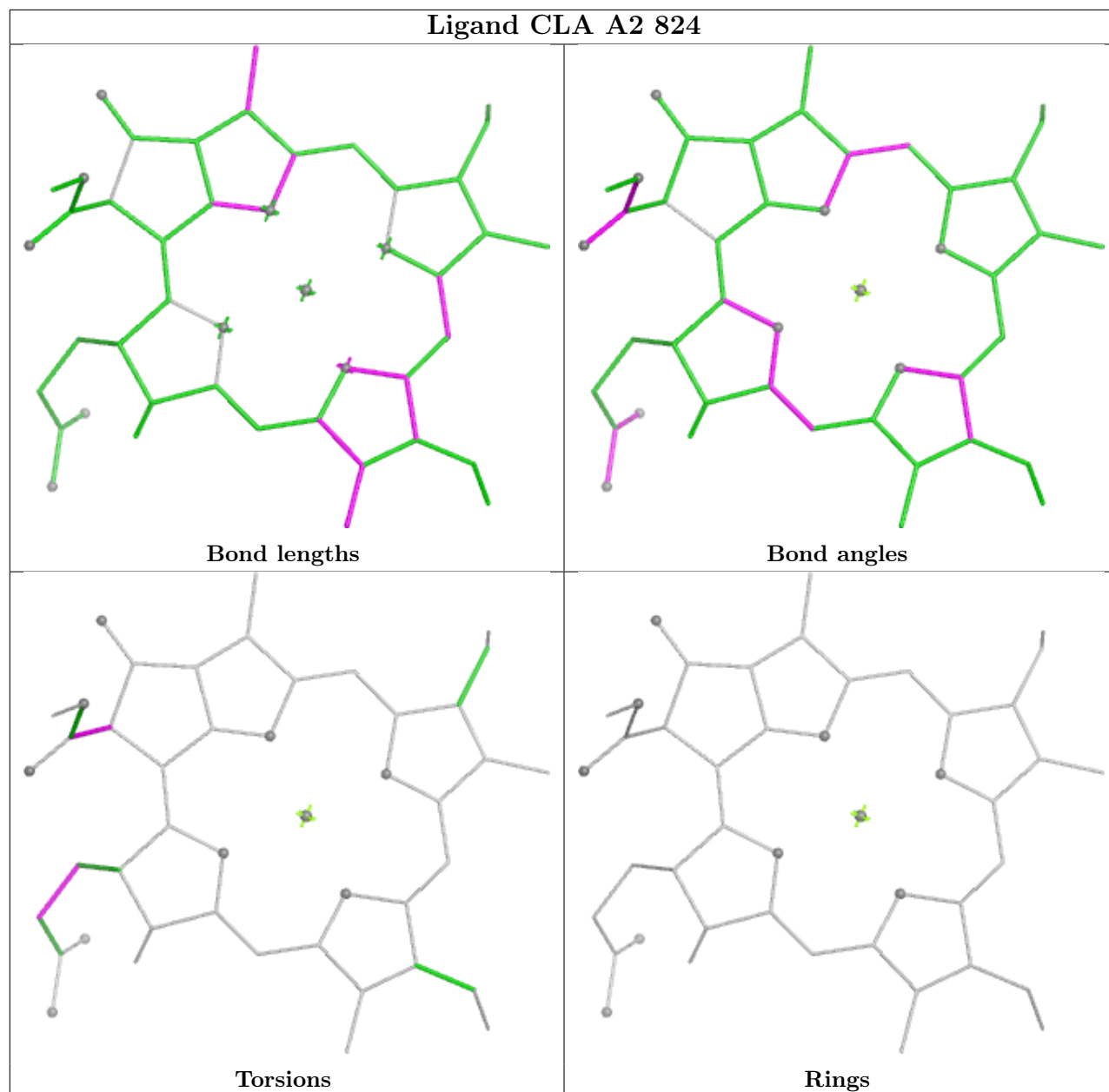
Ligand LHG BB 850

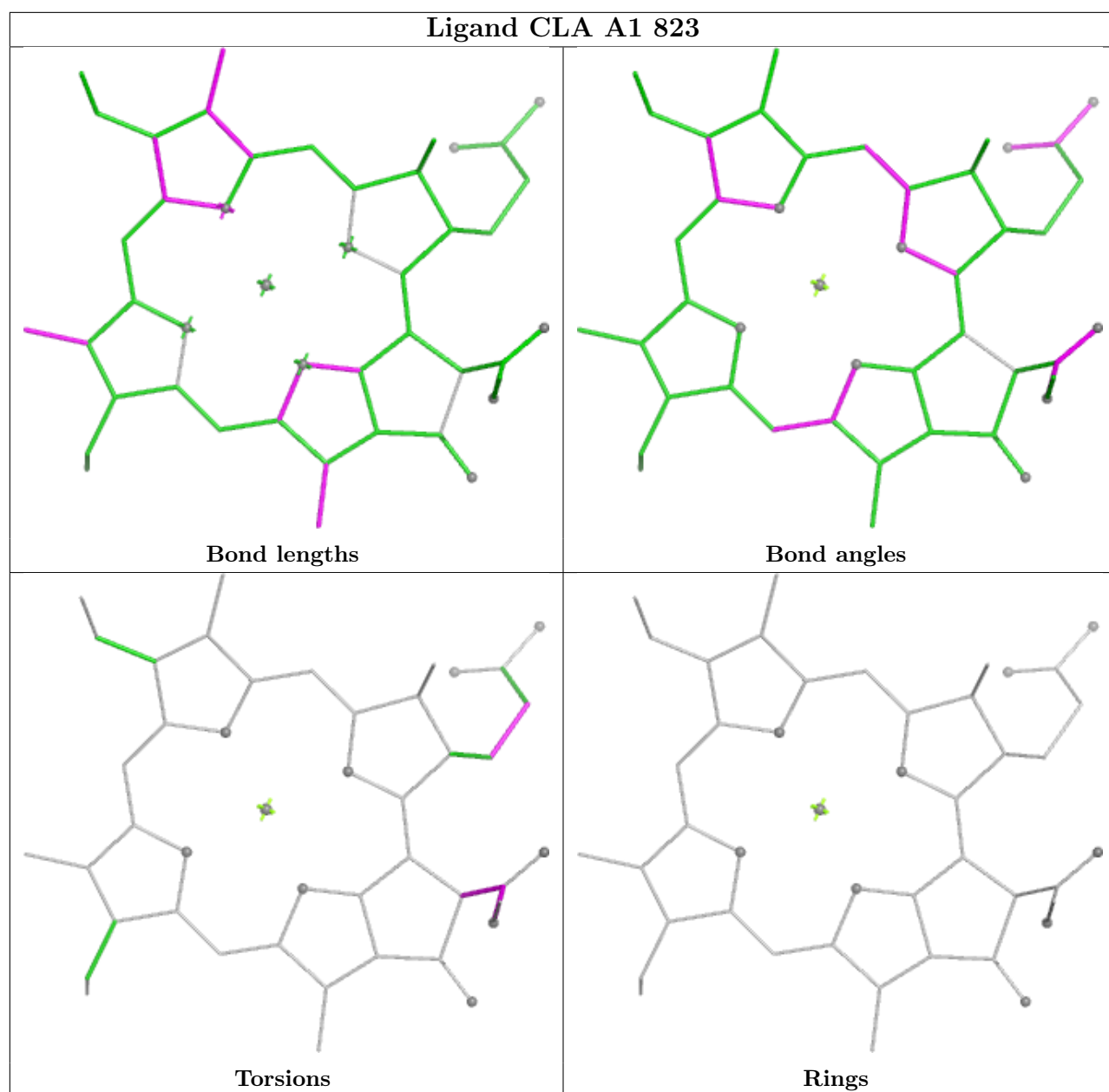


Ligand CLA A2 808

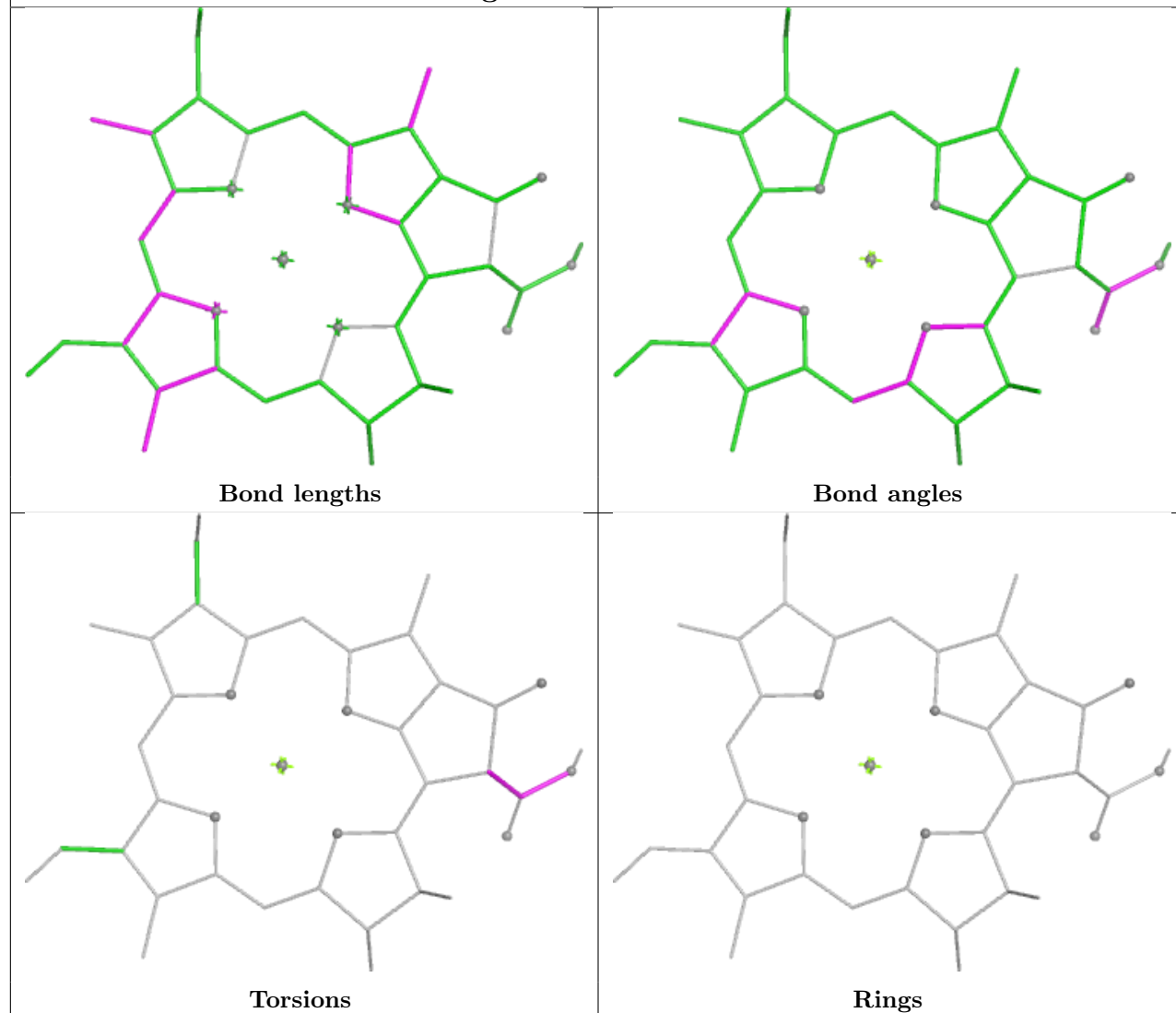


Ligand CLA A2 824

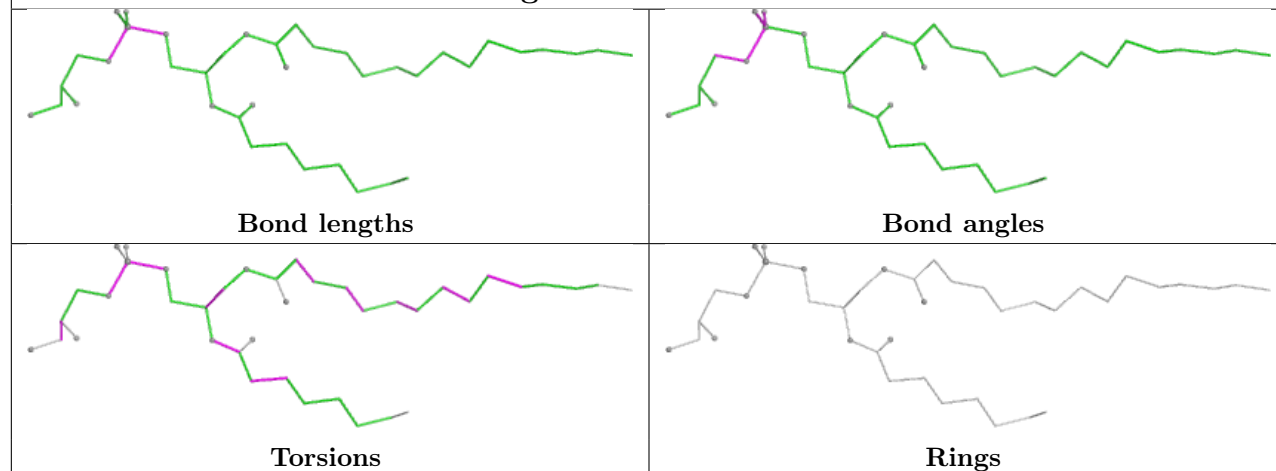


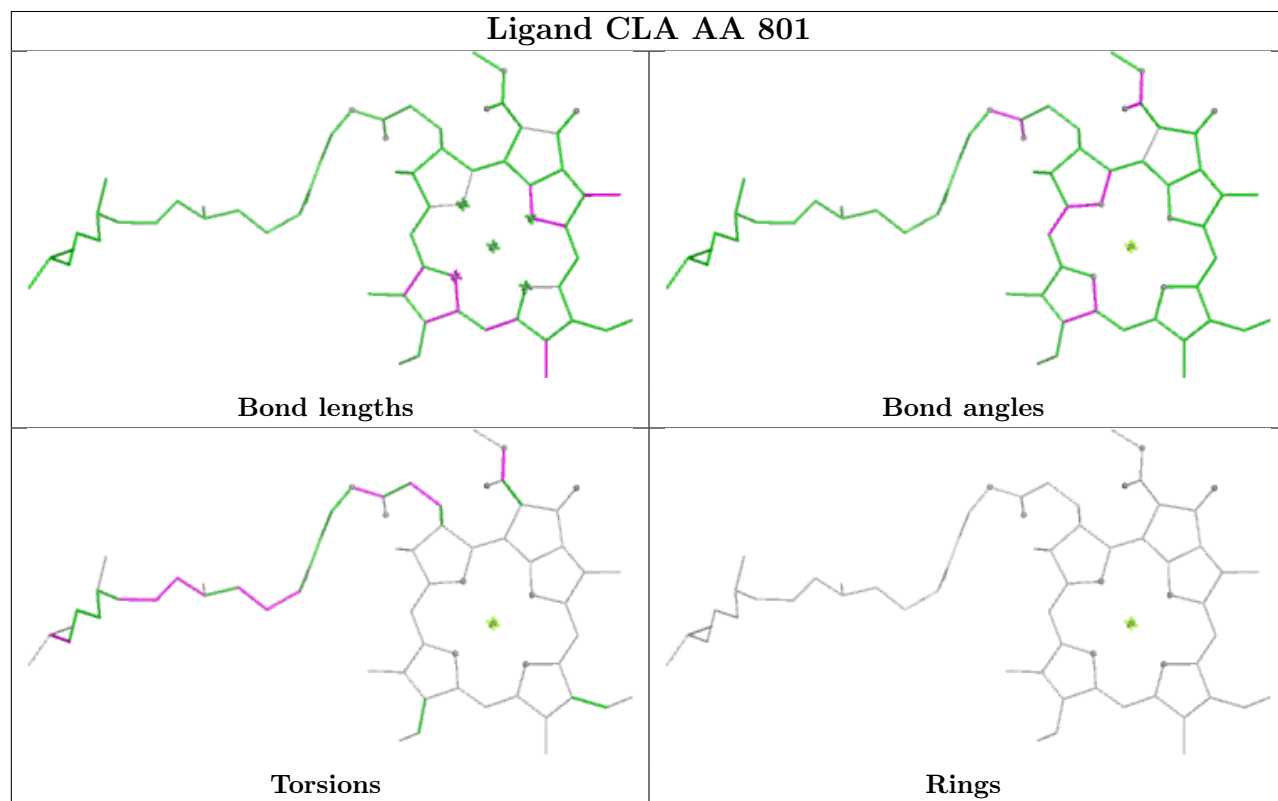
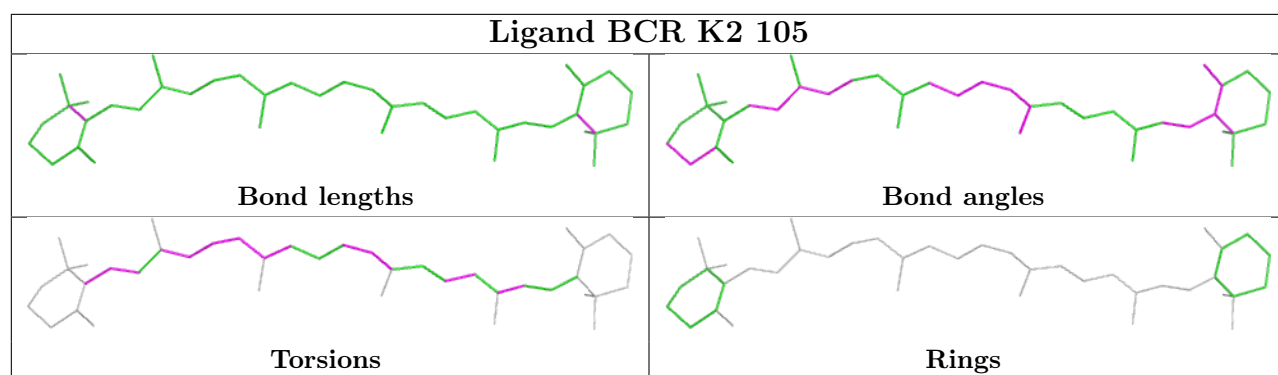


Ligand CLA A2 844

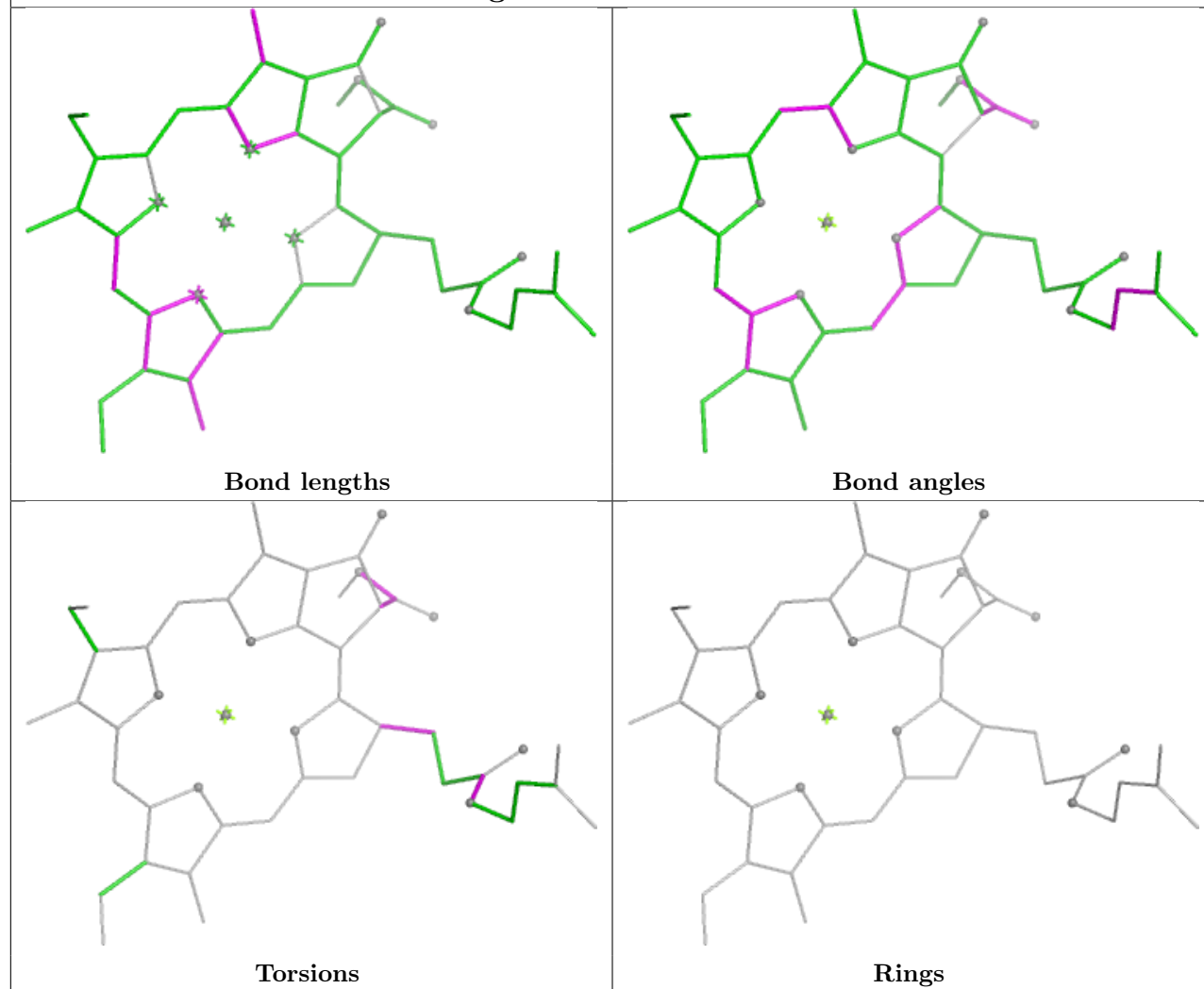


Ligand LHG X1 102

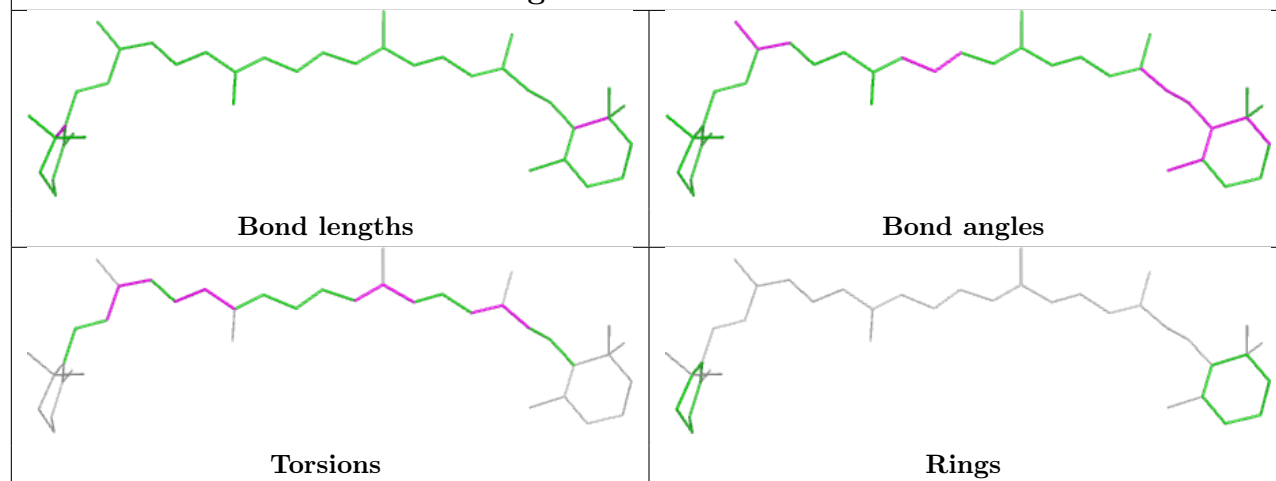


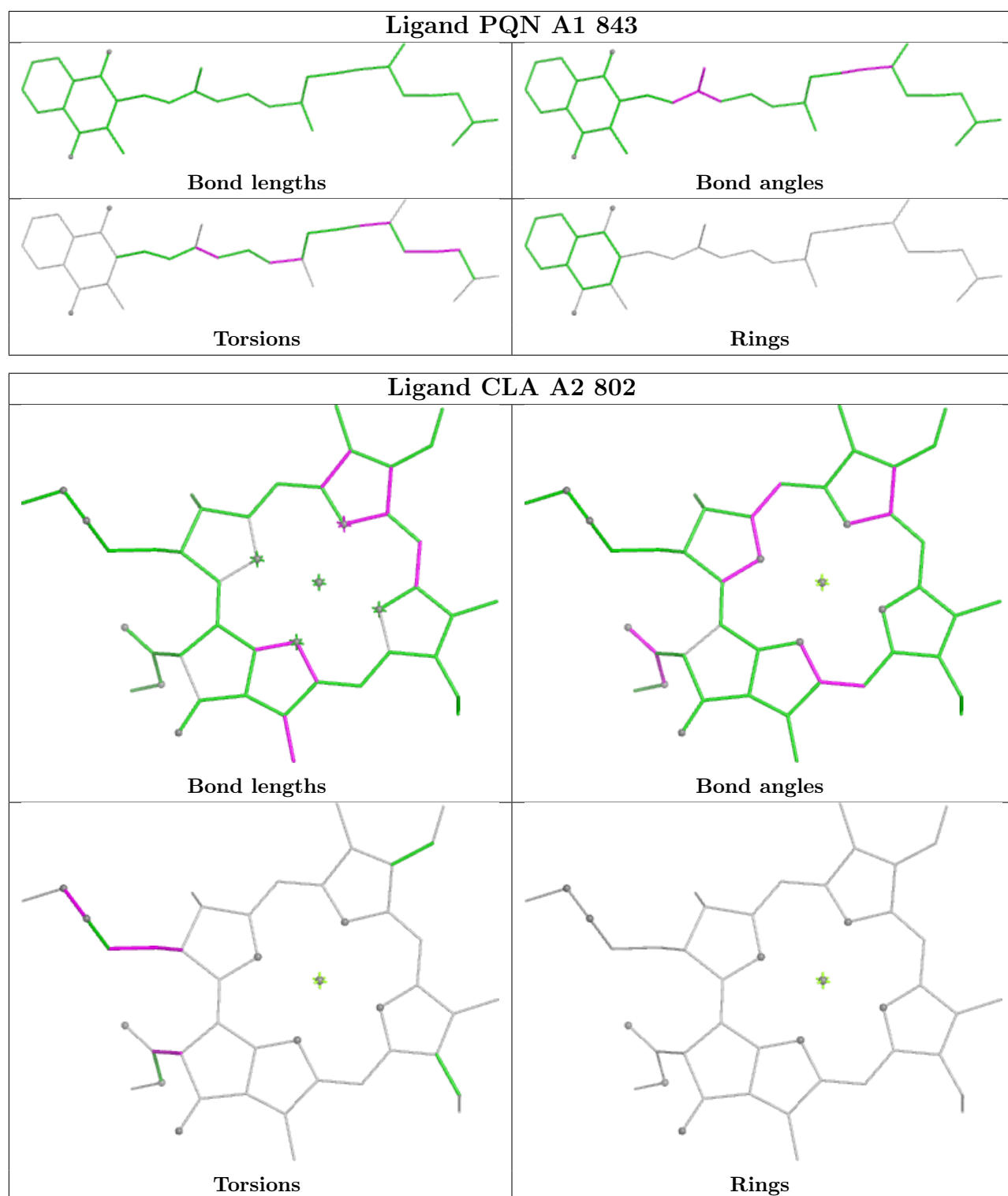


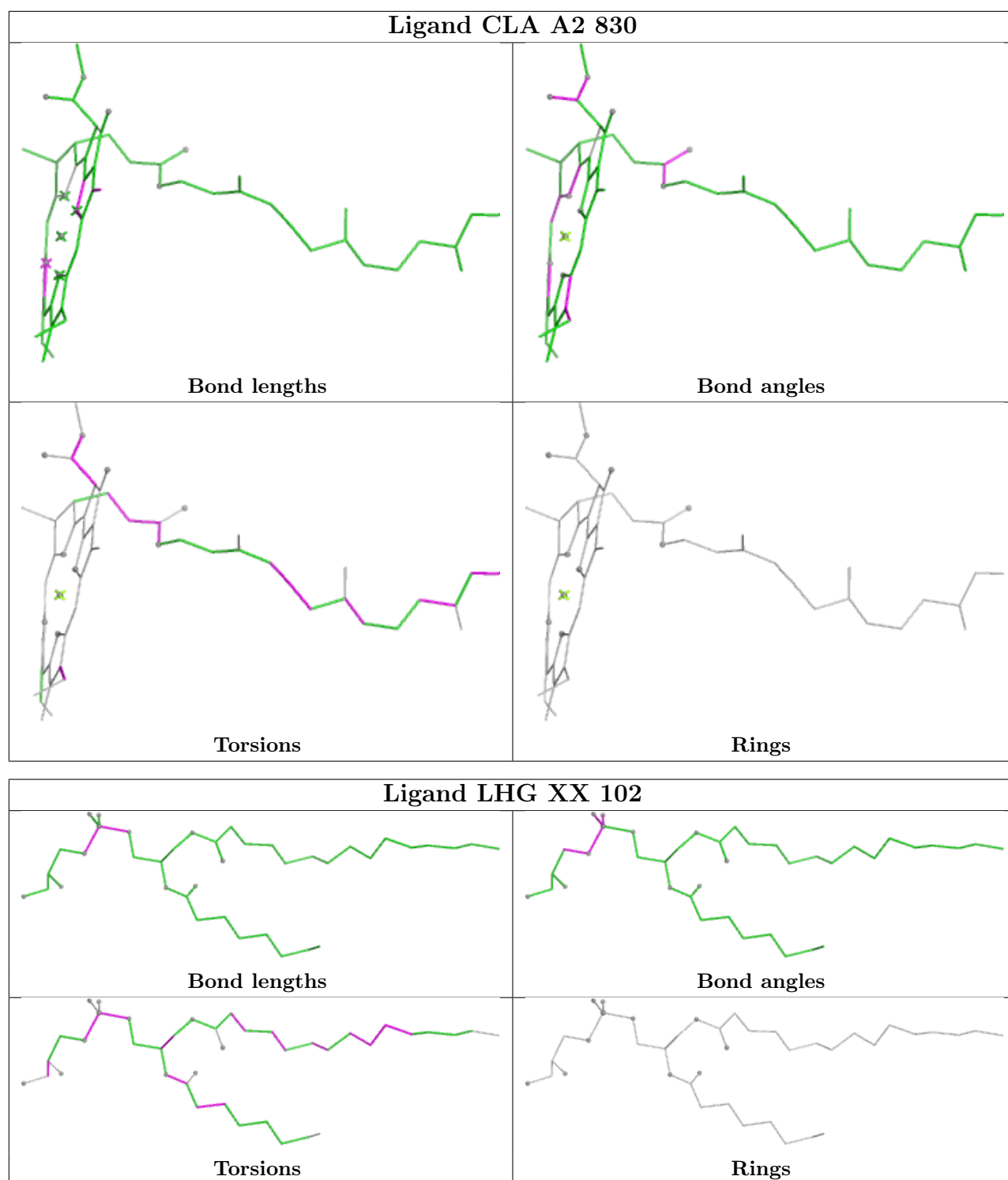
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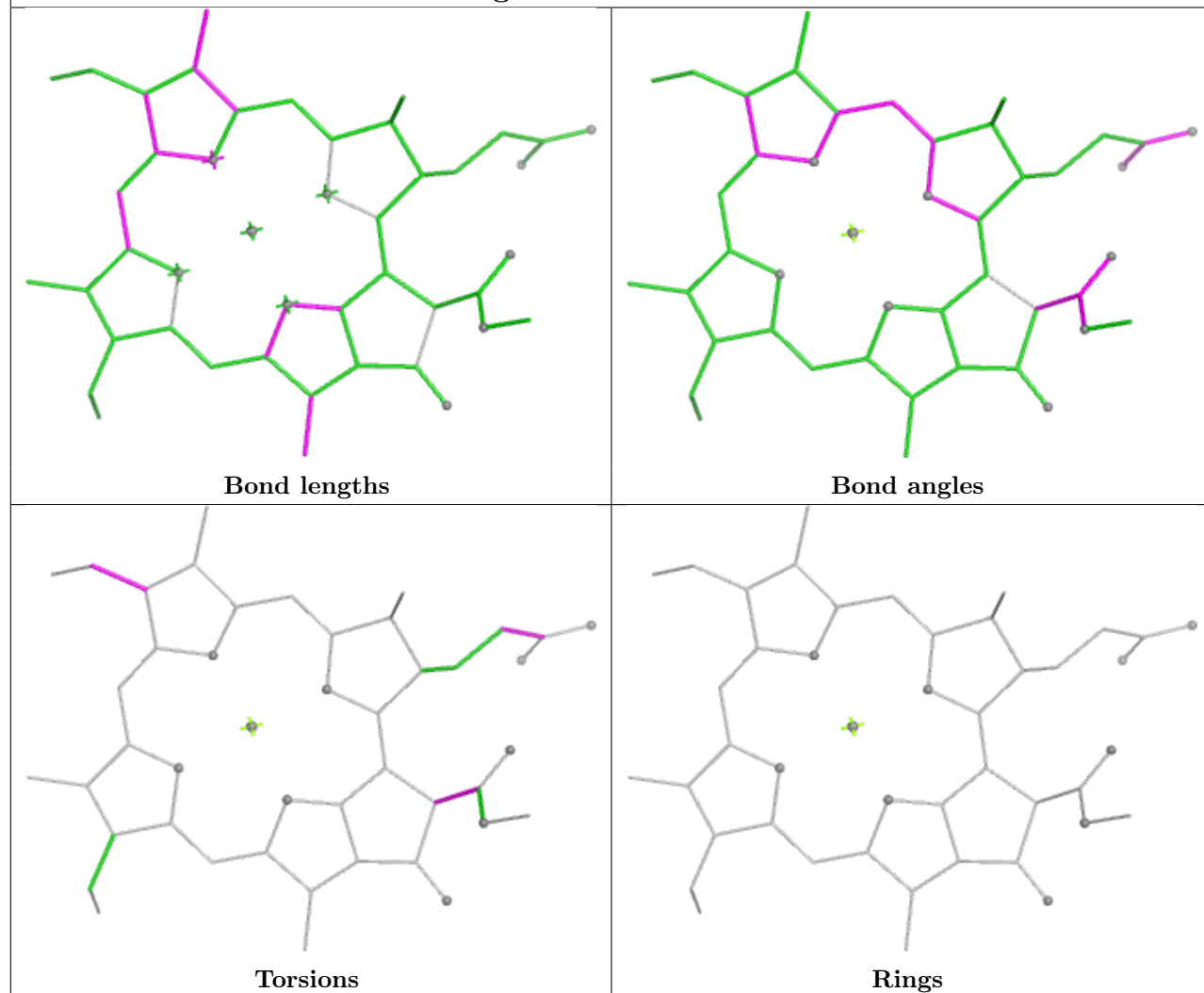
Ligand BCR I2 102



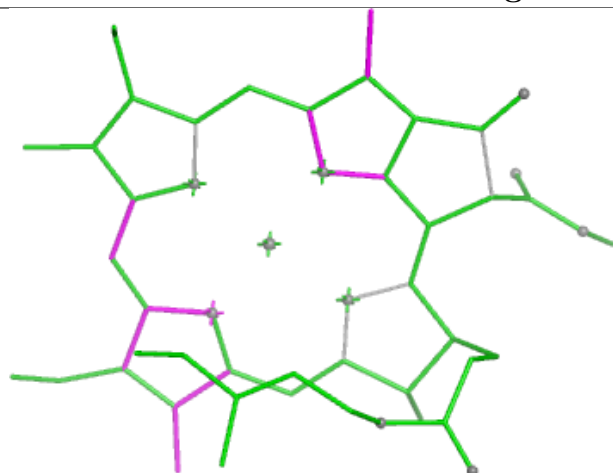




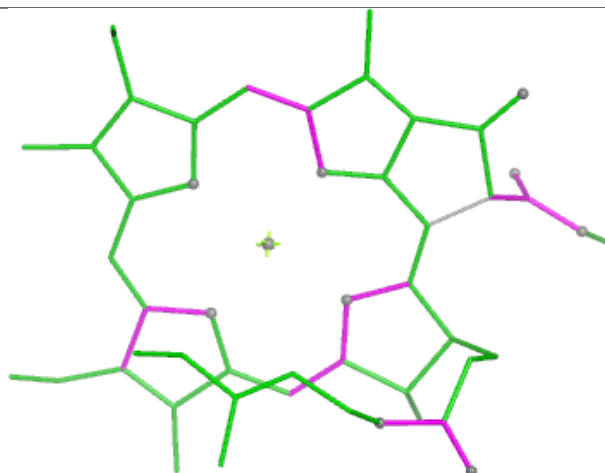
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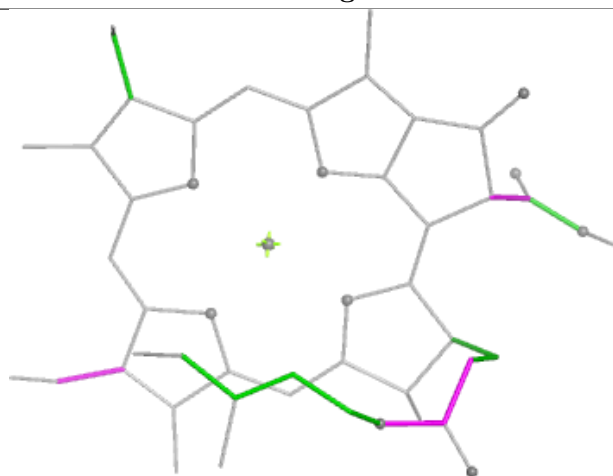
Ligand CLA A2 822



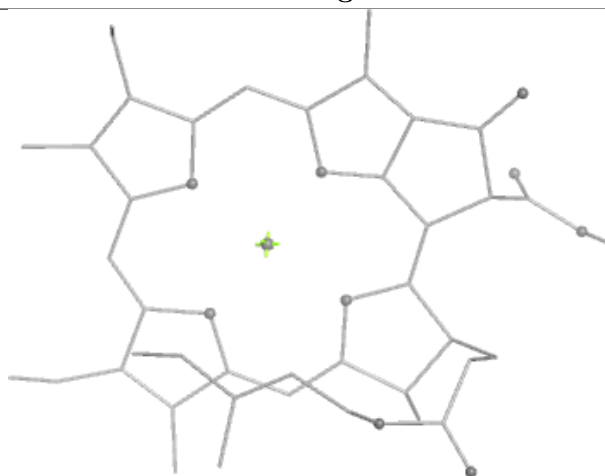
Bond lengths



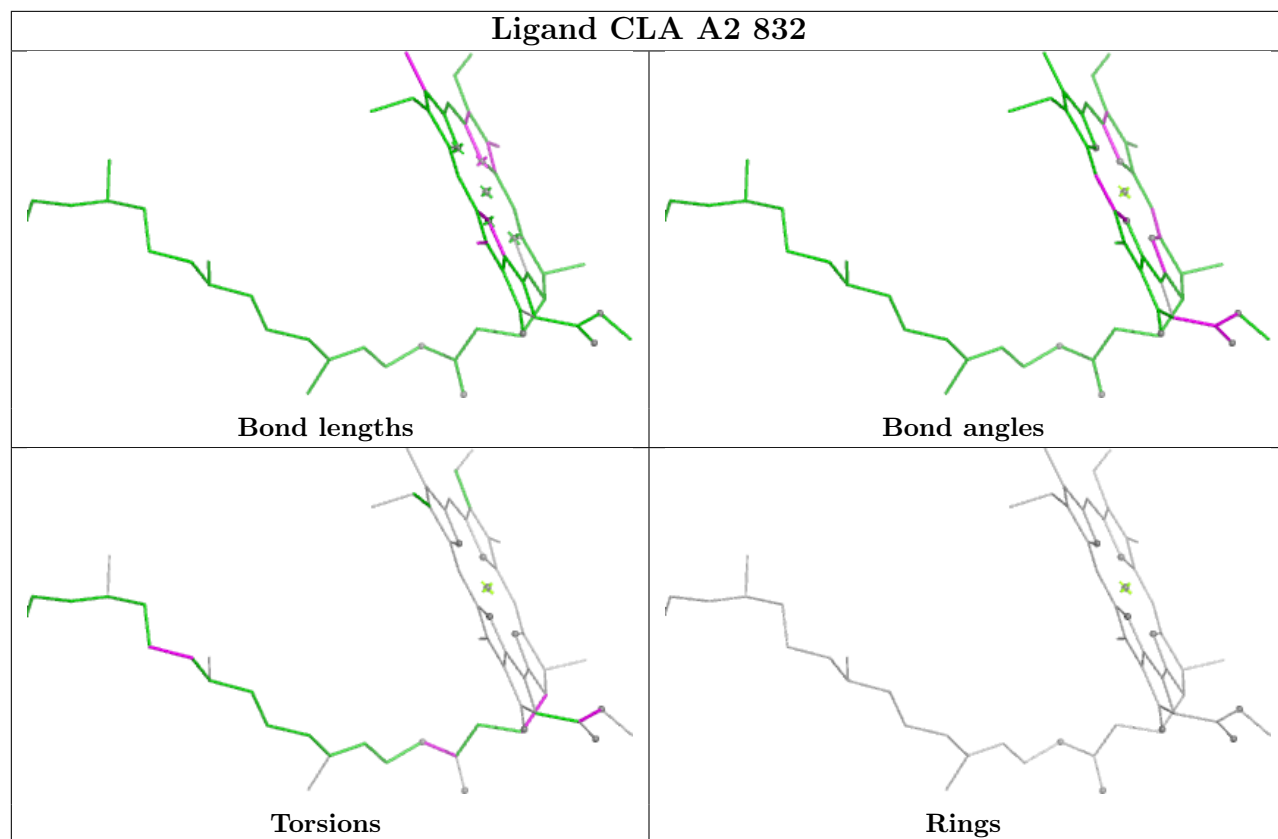
Bond angles

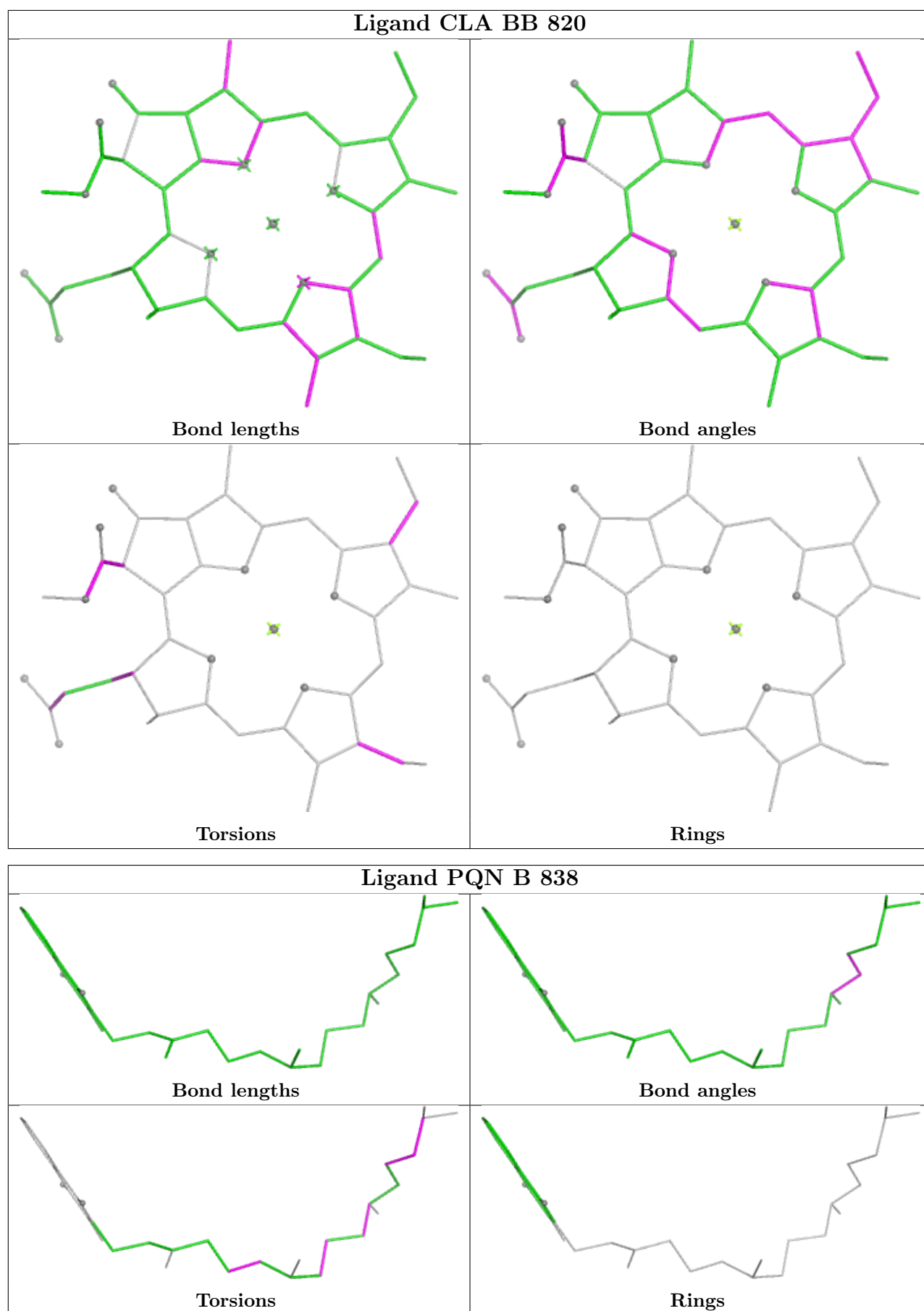


Torsions

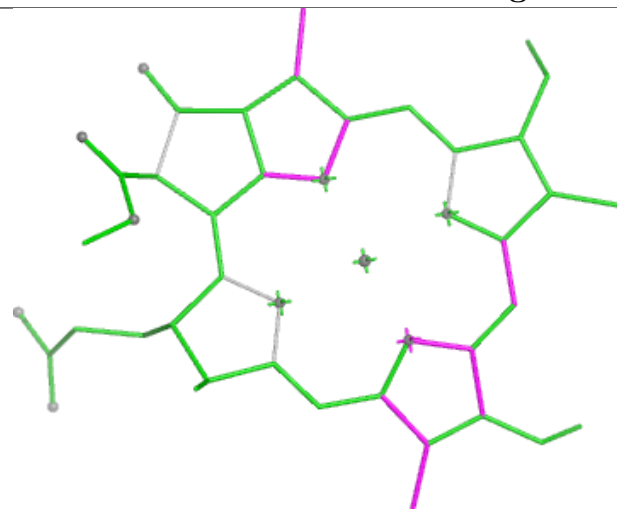


Rings

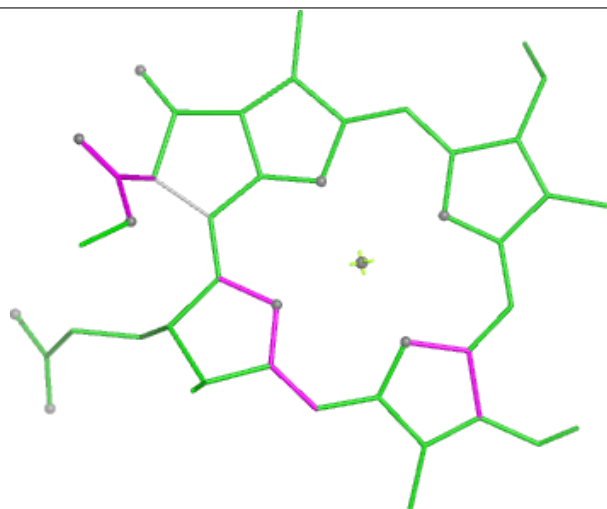




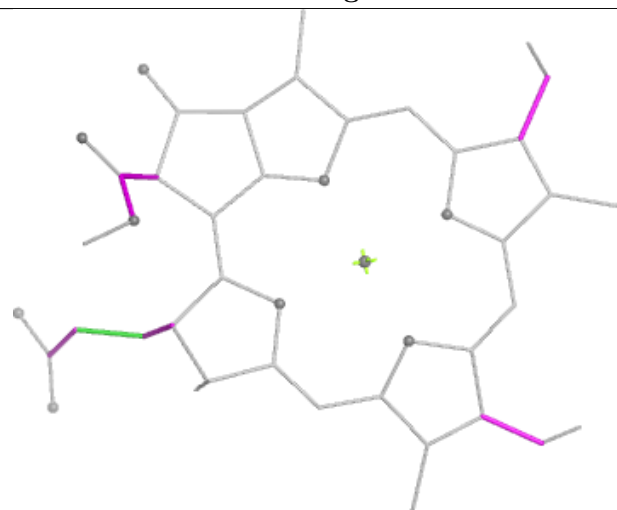
Ligand CLA B1 820



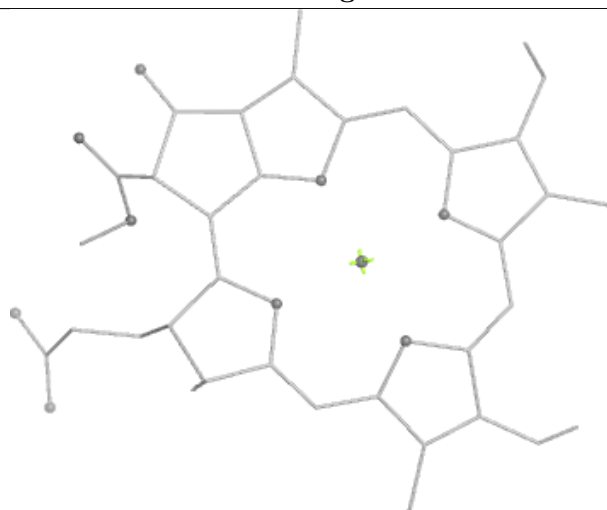
Bond lengths



Bond angles

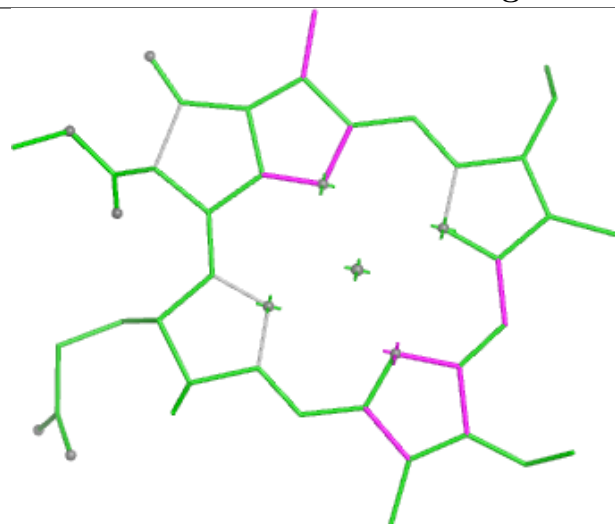


Torsions

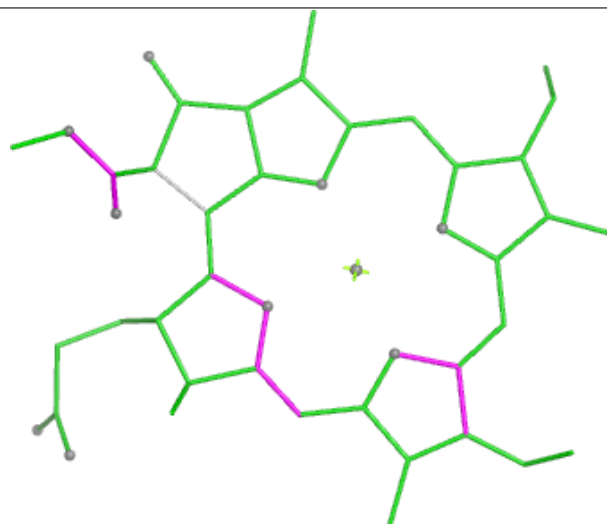


Rings

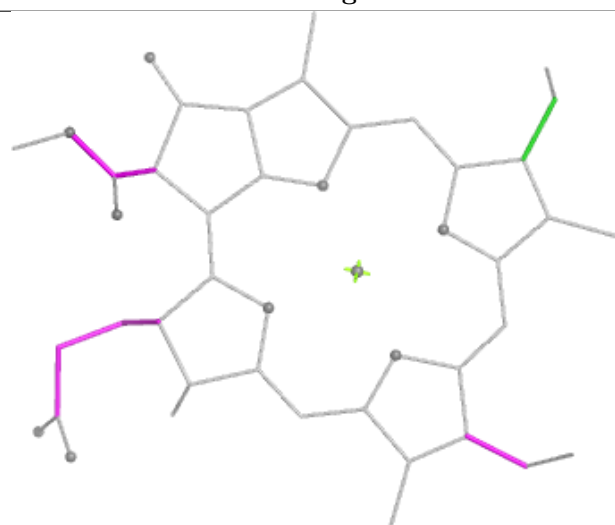
Ligand CLA XX 101



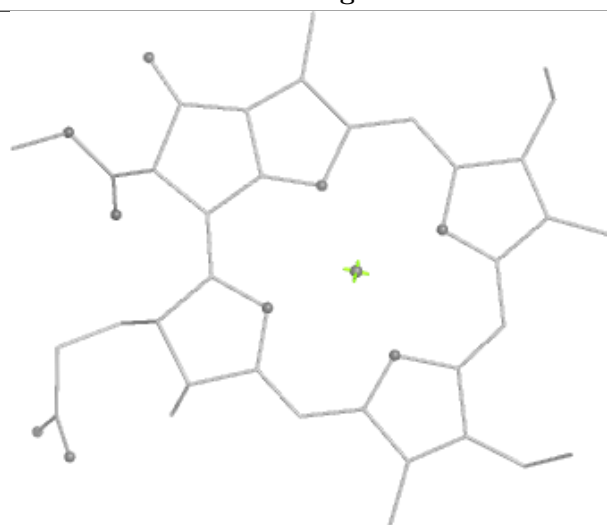
Bond lengths



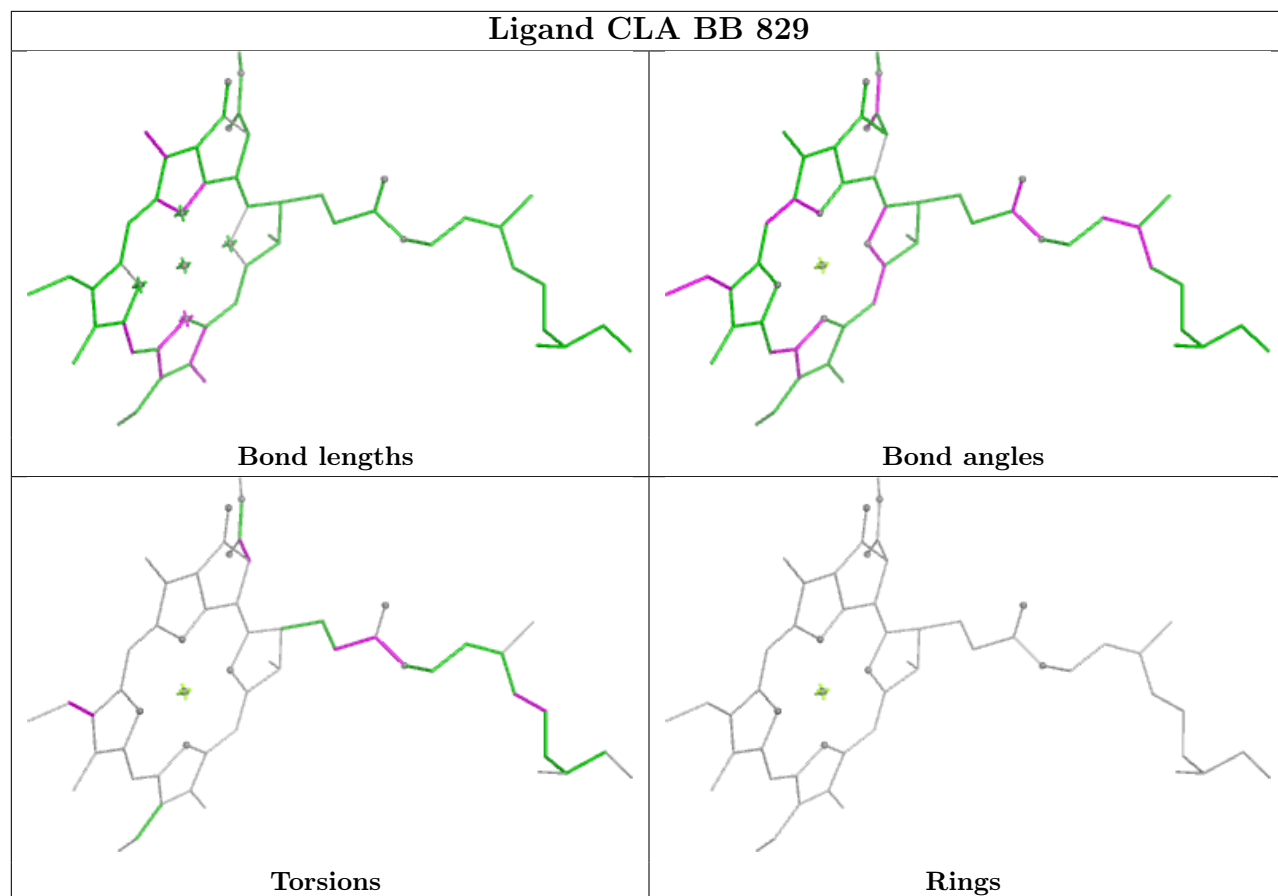
Bond angles

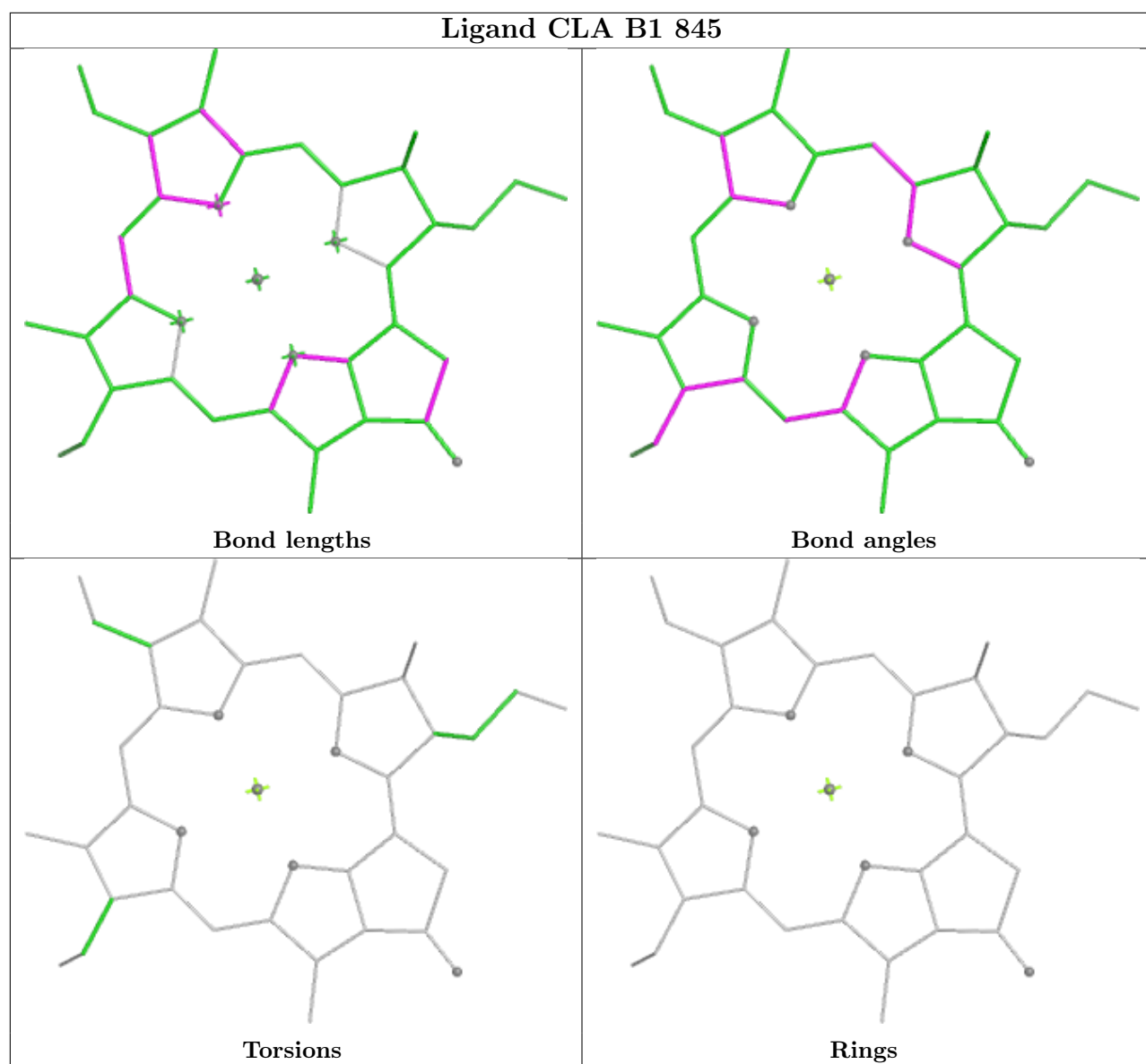


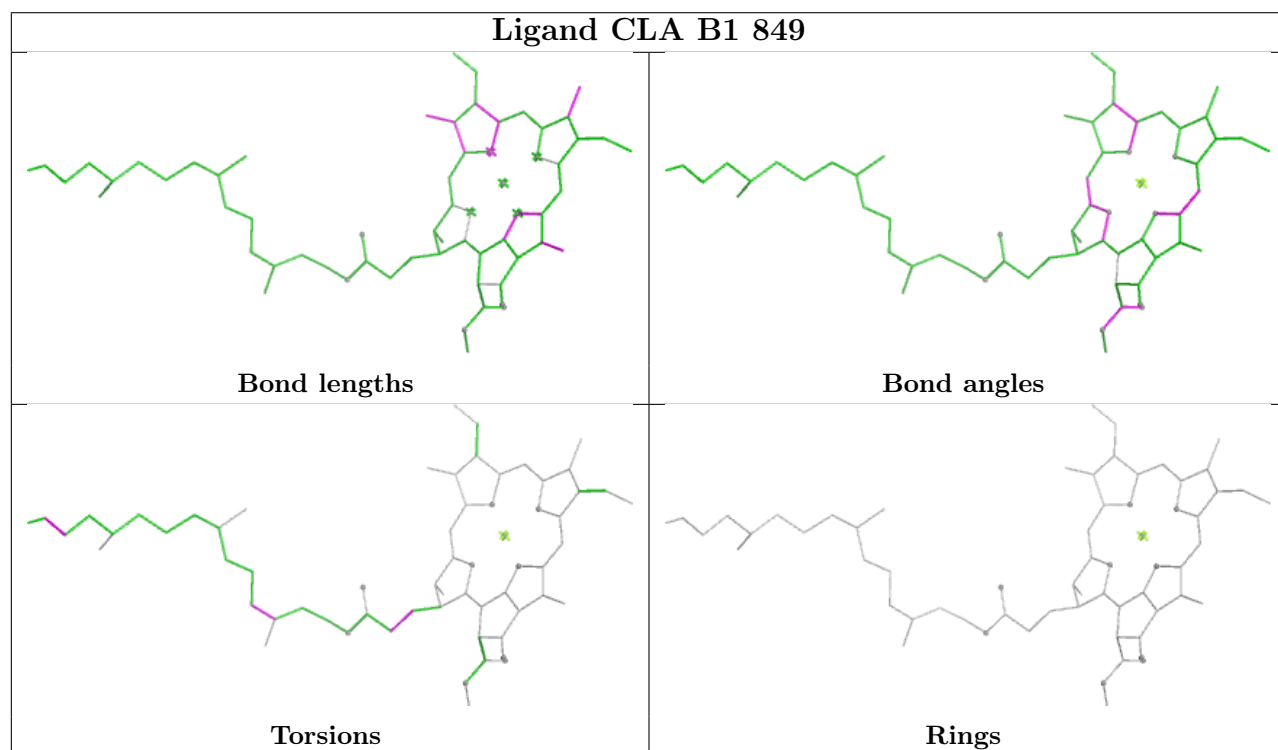
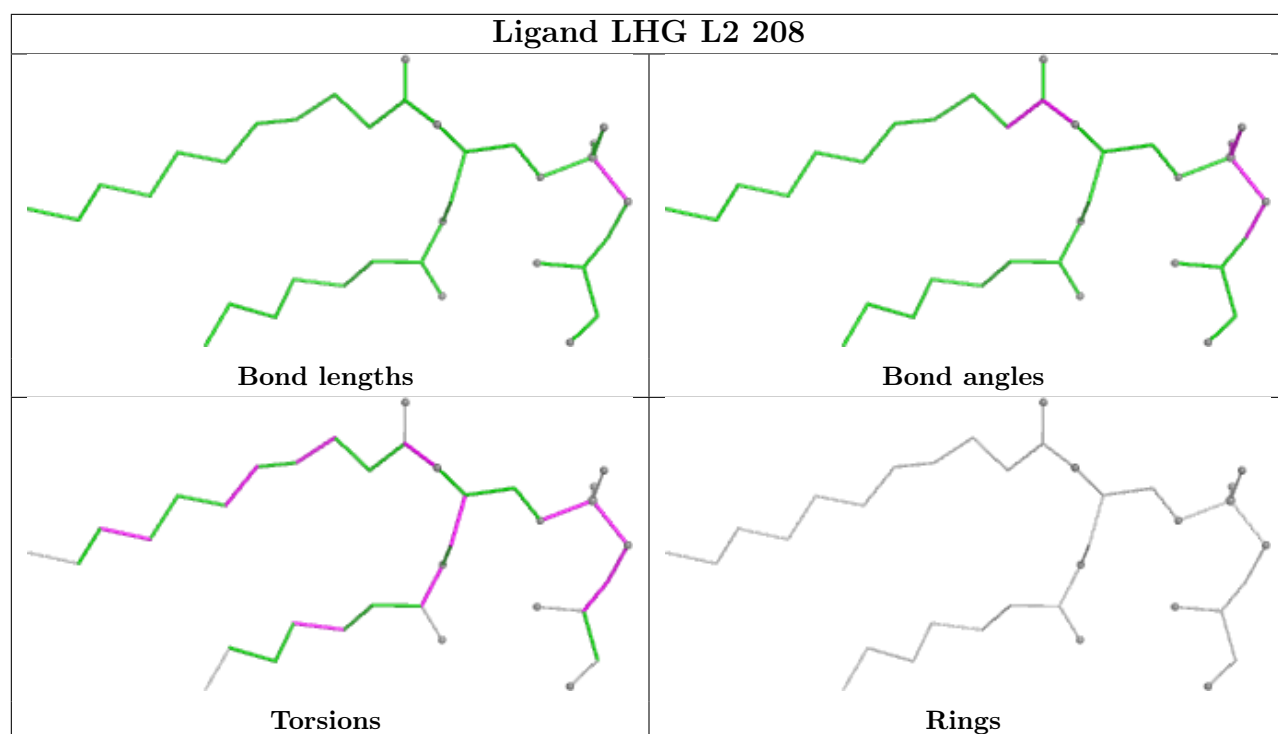
Torsions

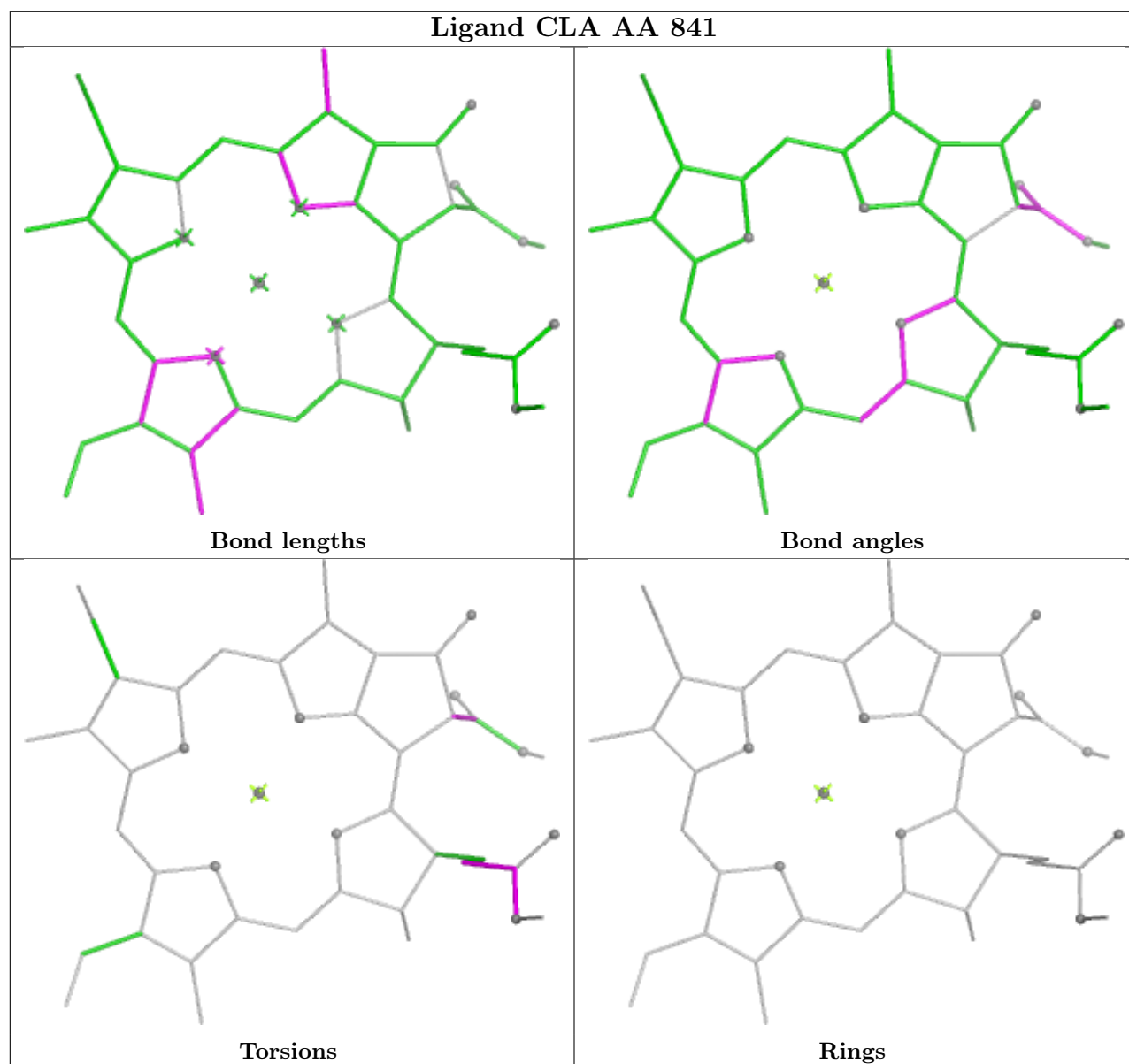
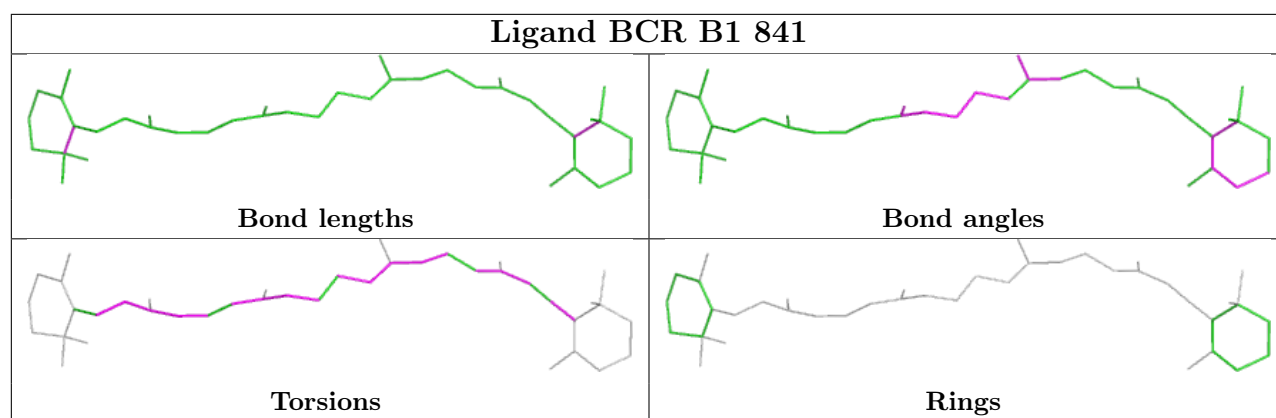


Rings

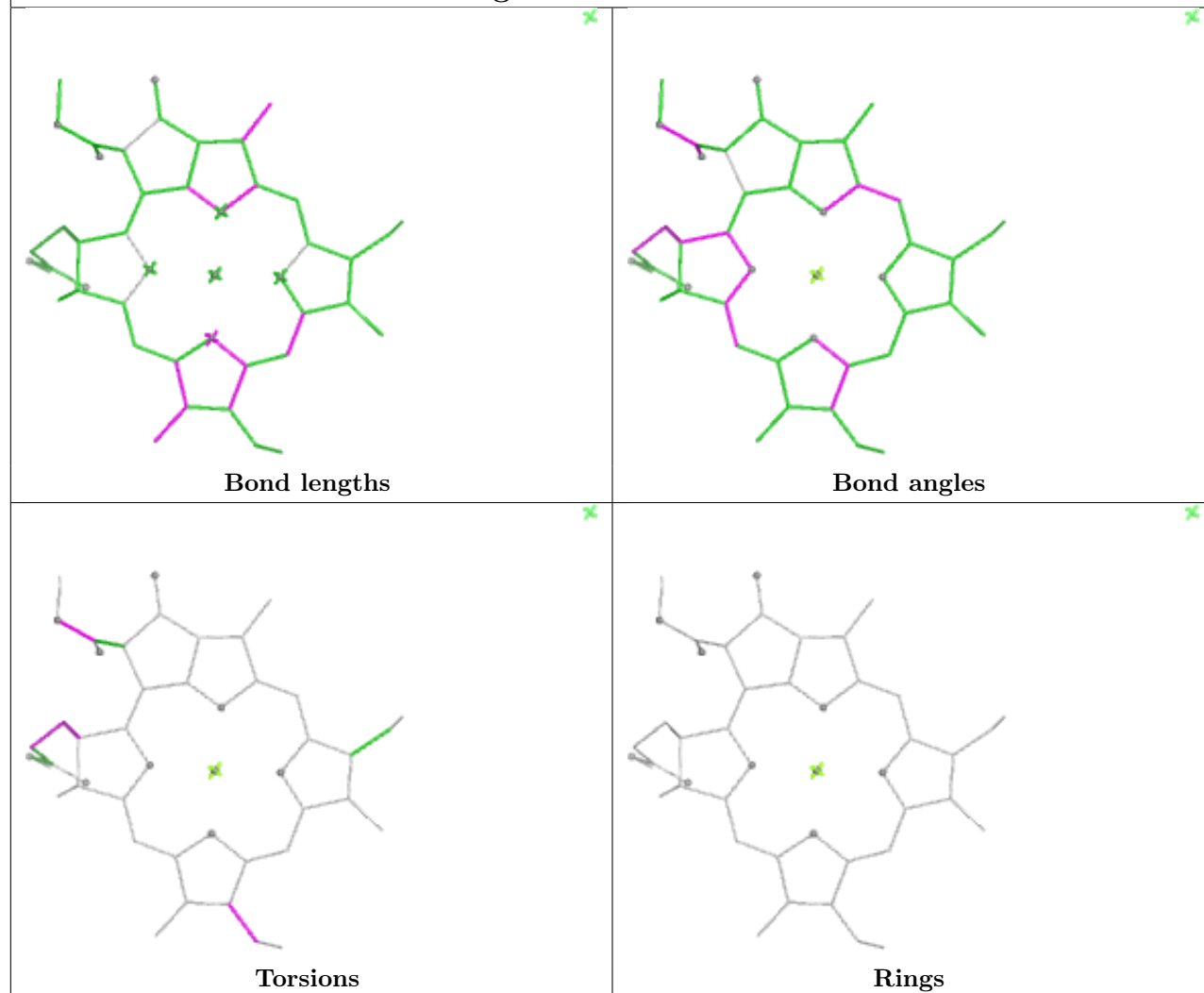


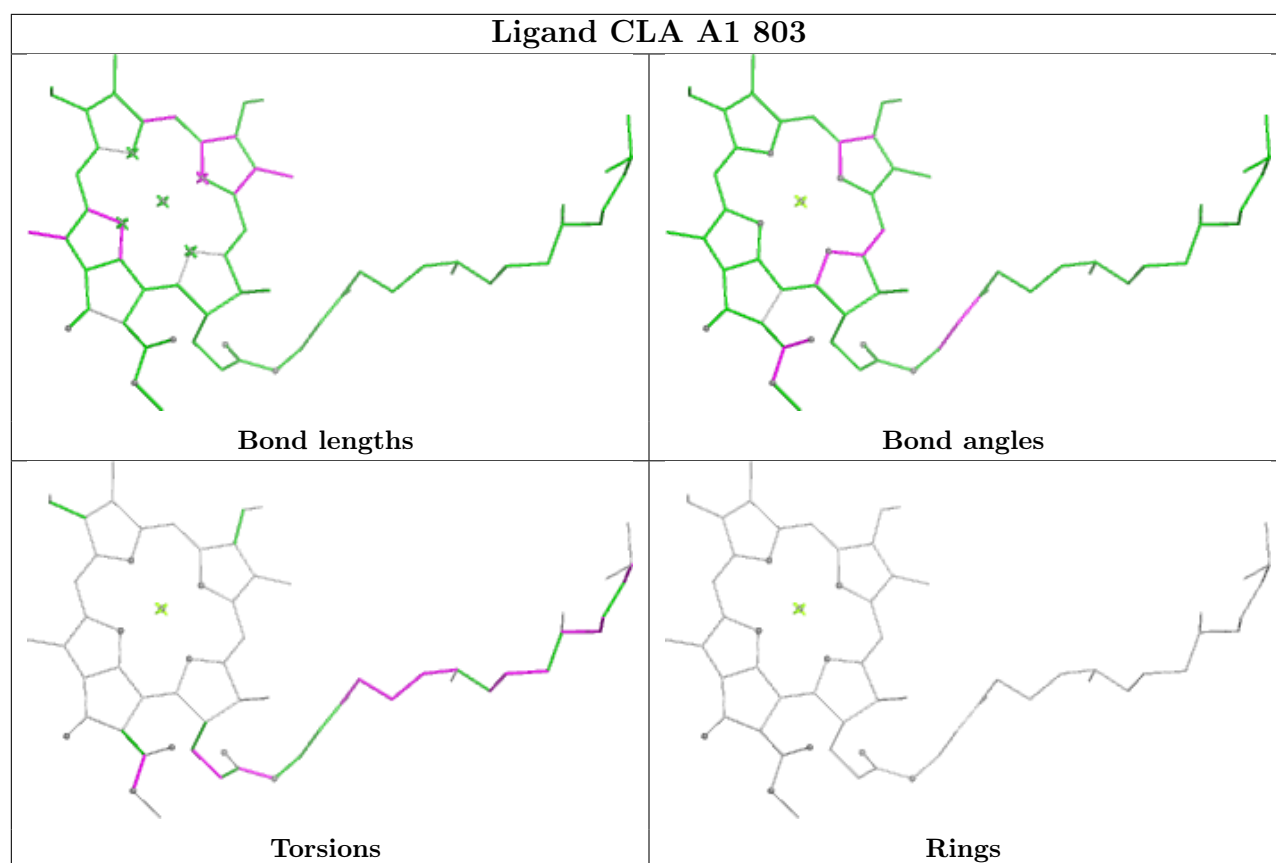


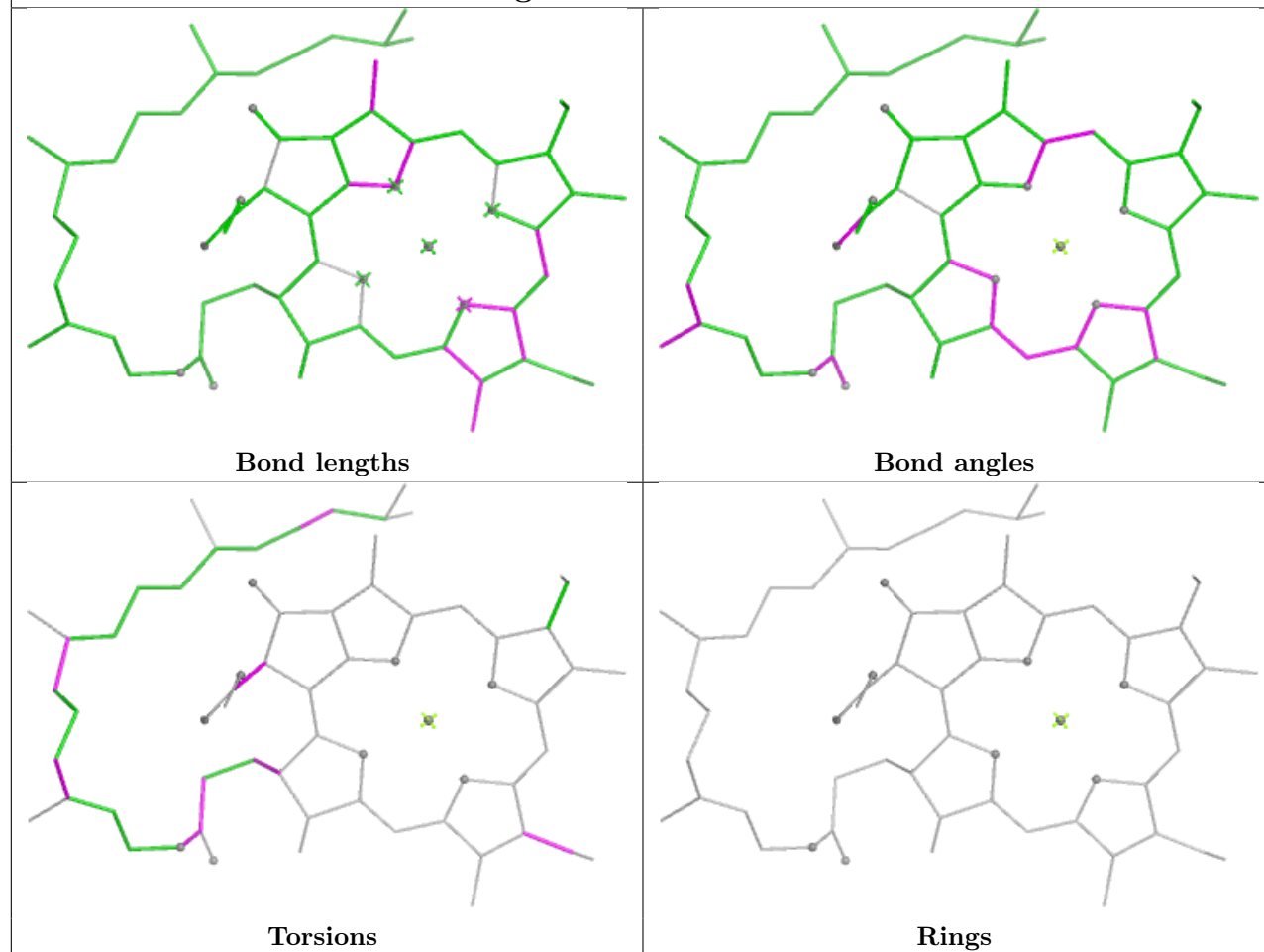
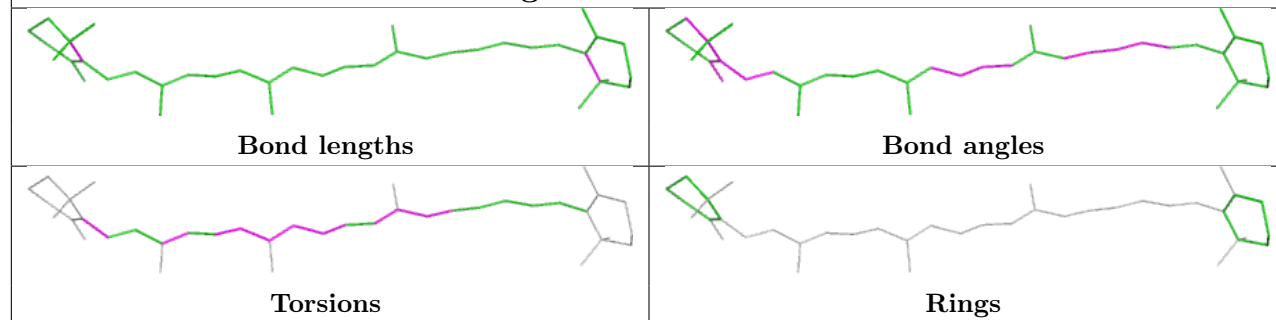




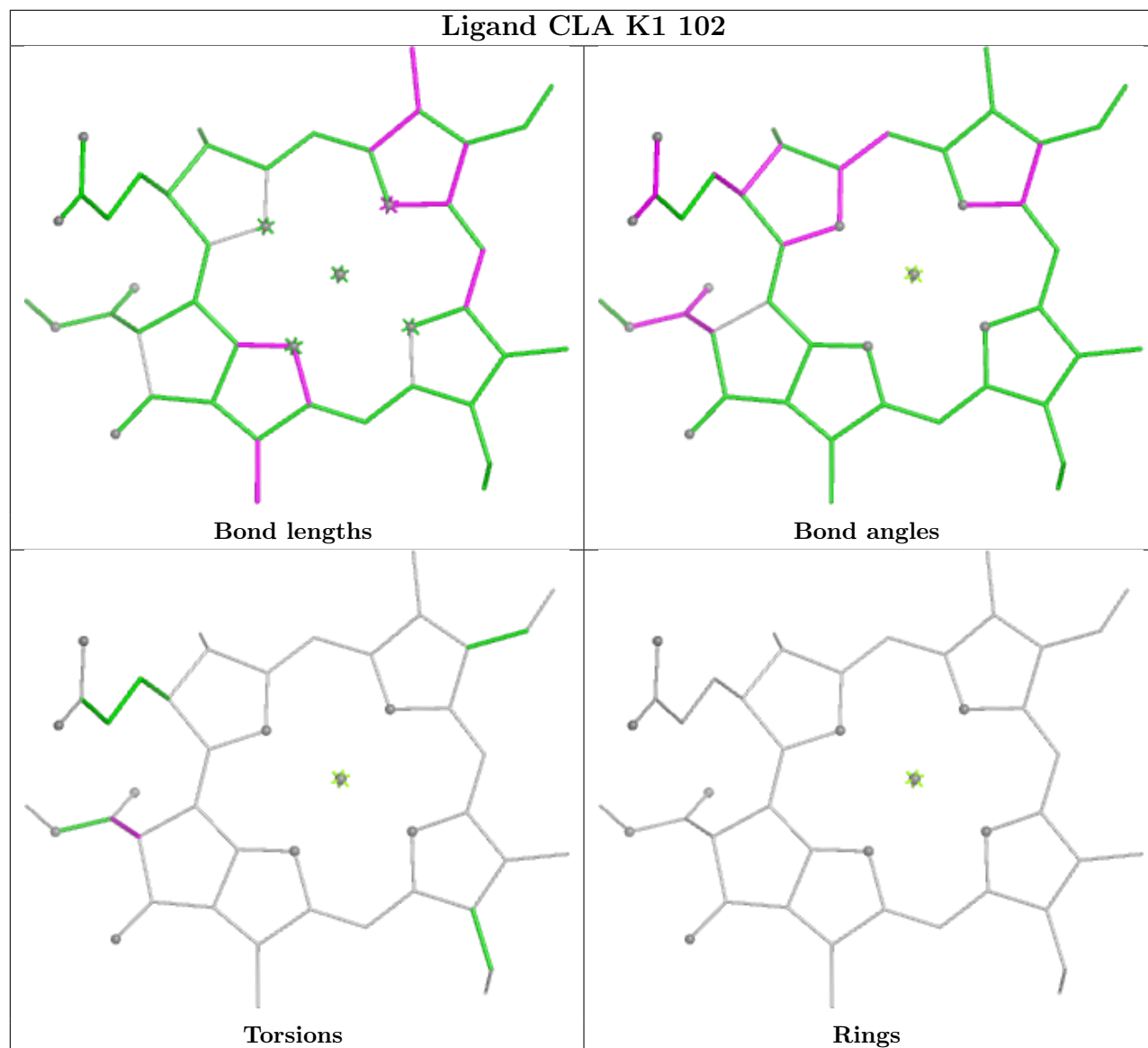
Ligand CLA A2 812



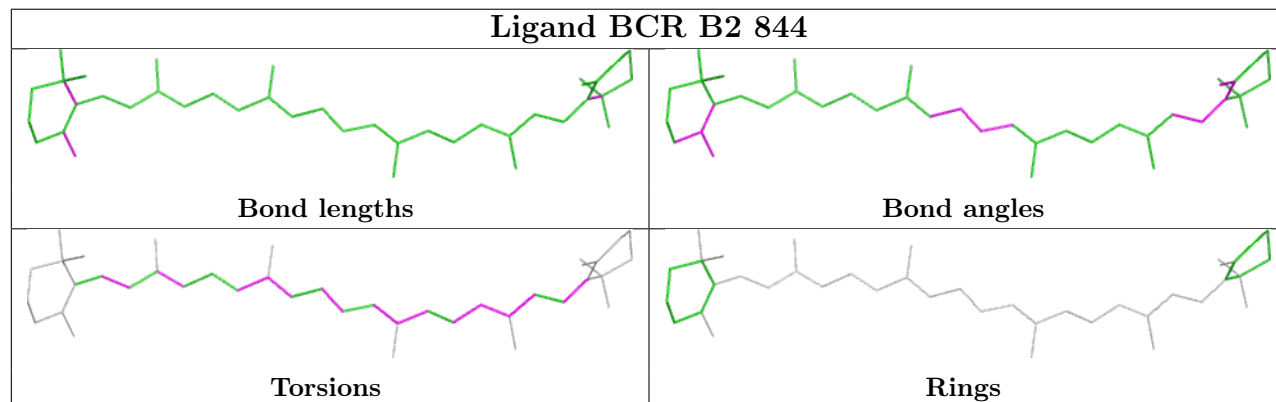


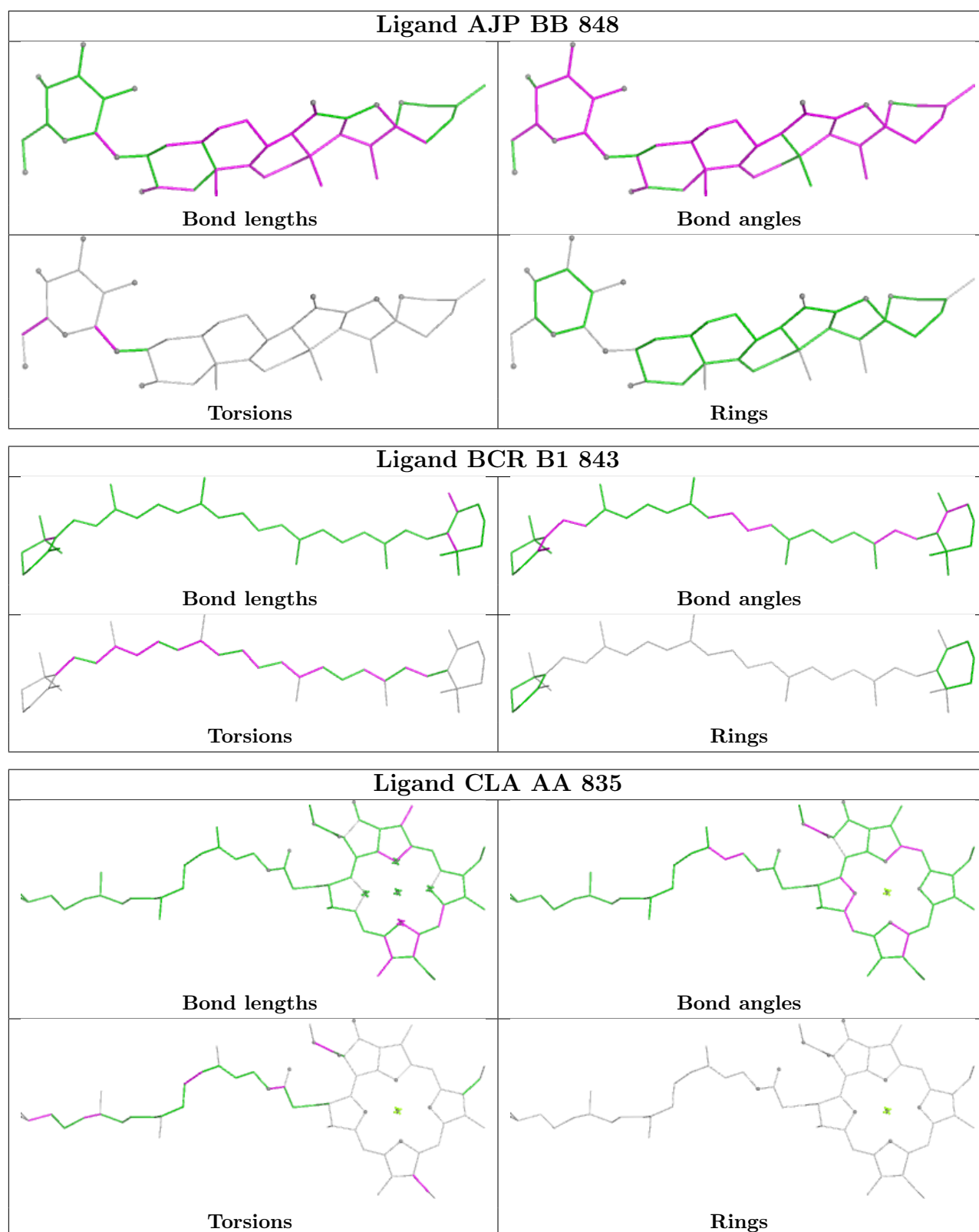
Ligand CLA BB 802**Ligand BCR A1 847**

Ligand CLA K1 102

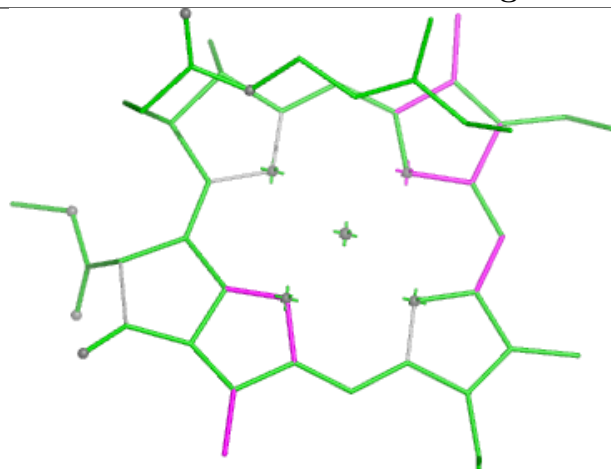


Ligand BCR B2 844

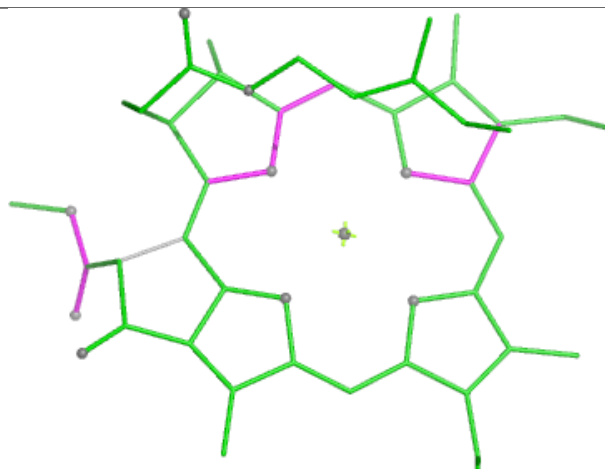




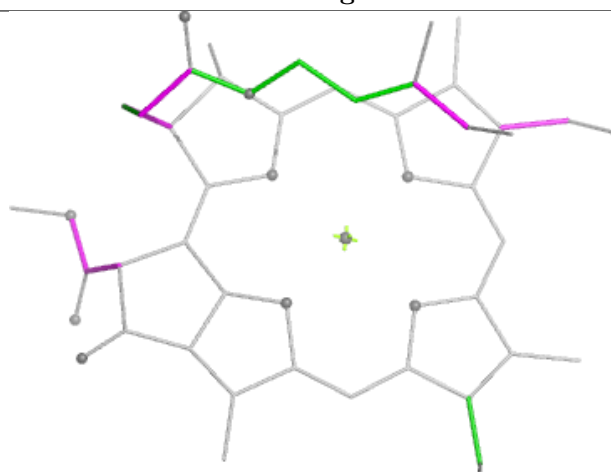
Ligand CLA AA 822



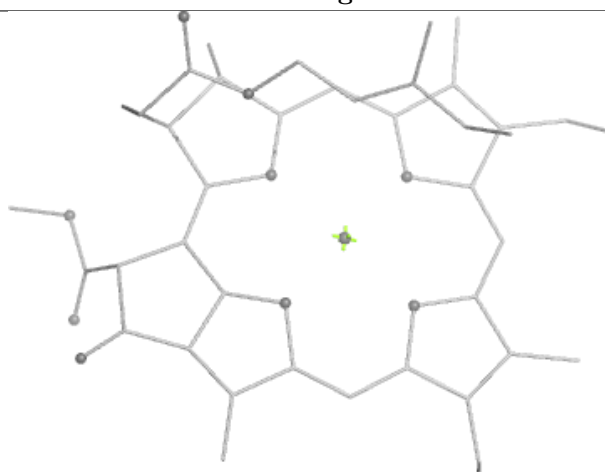
Bond lengths



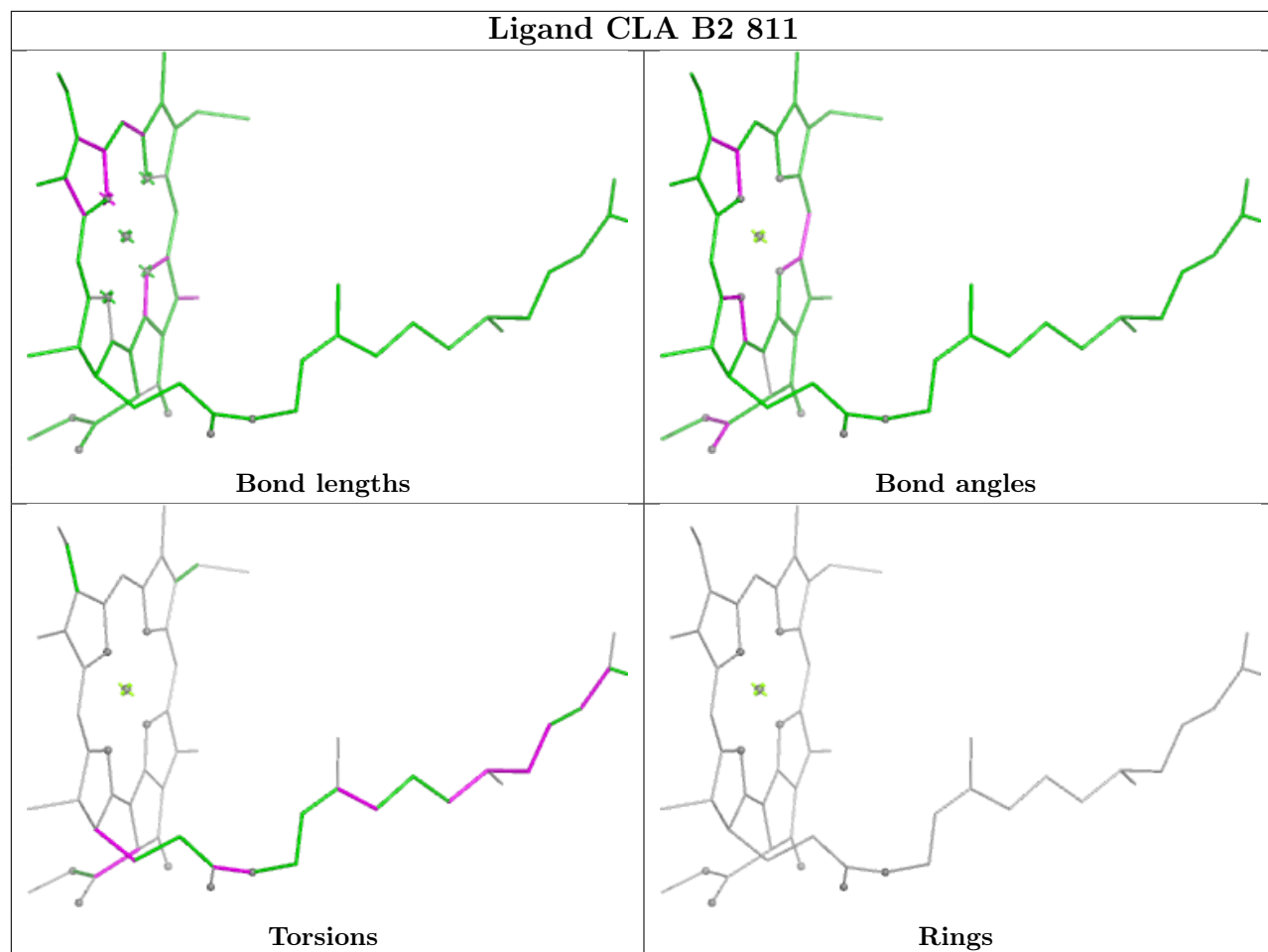
Bond angles



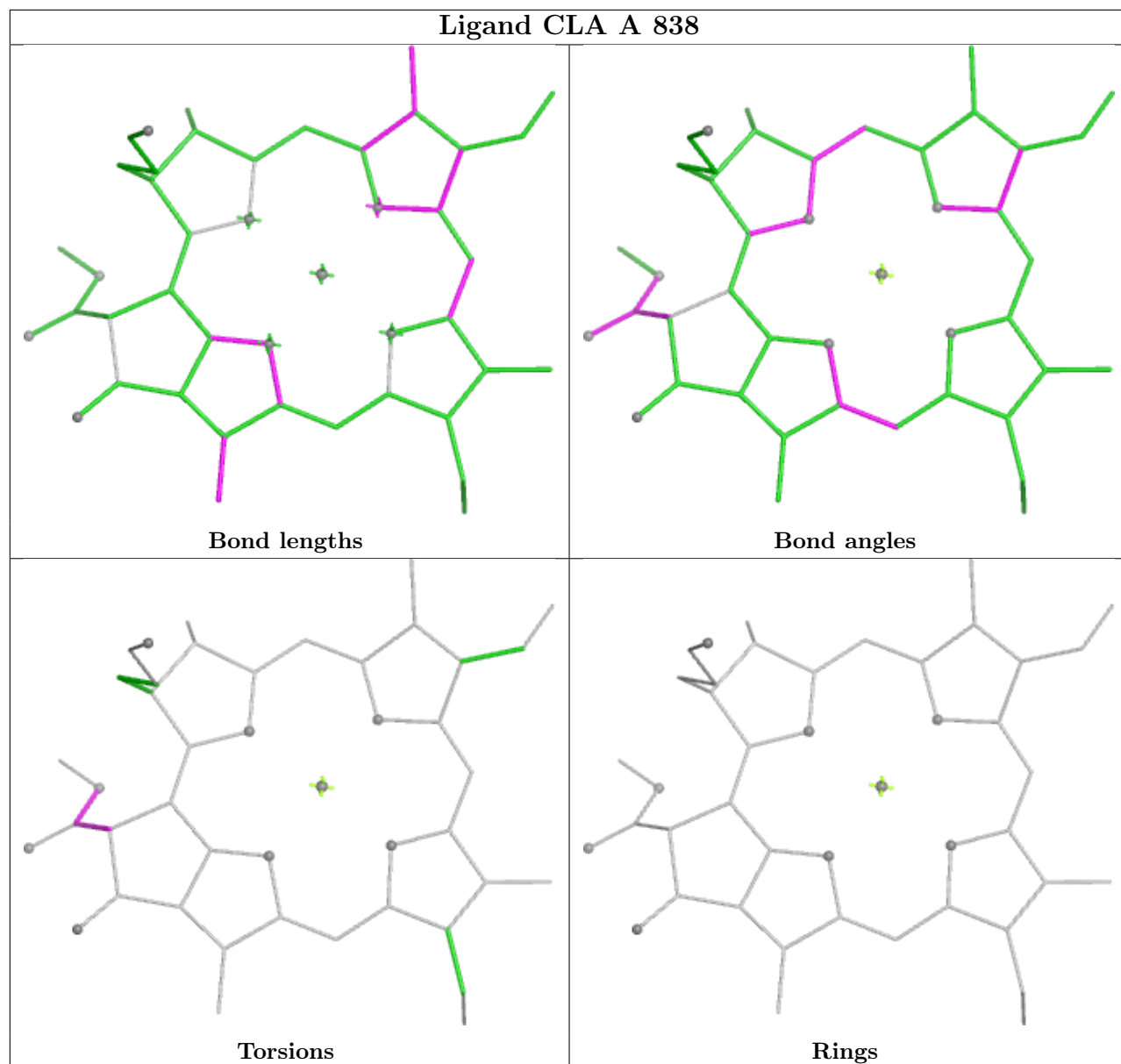
Torsions

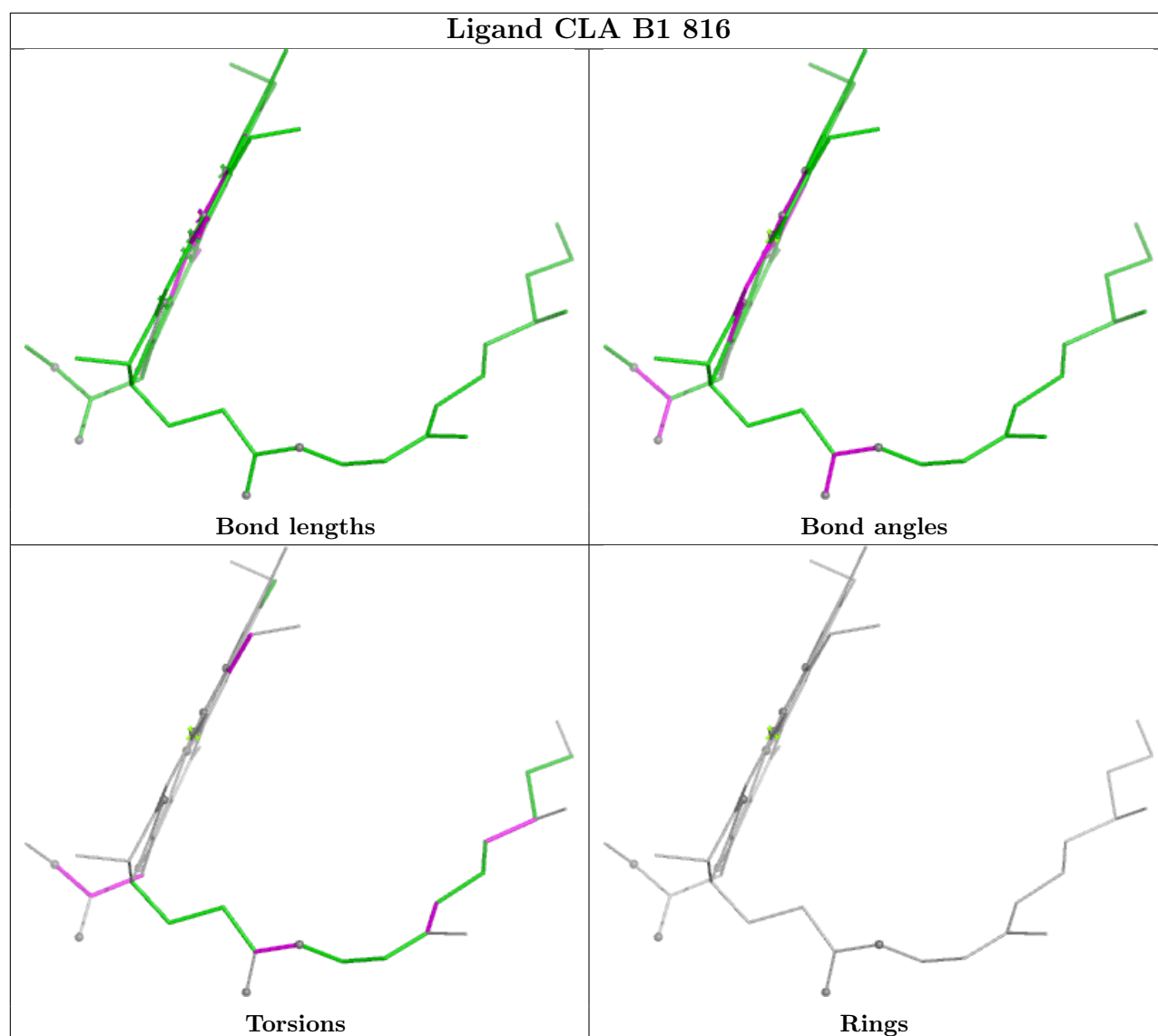


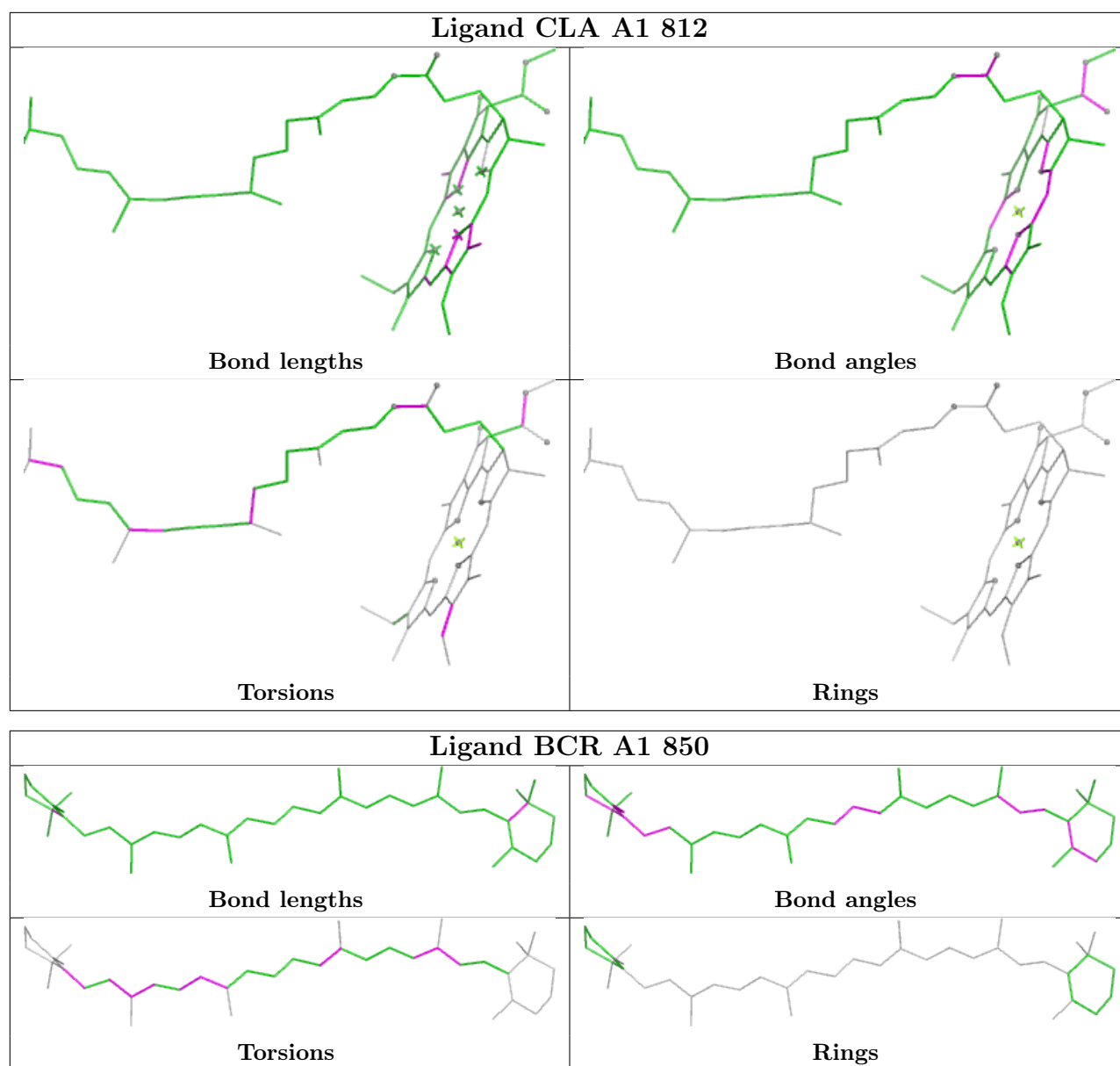
Rings

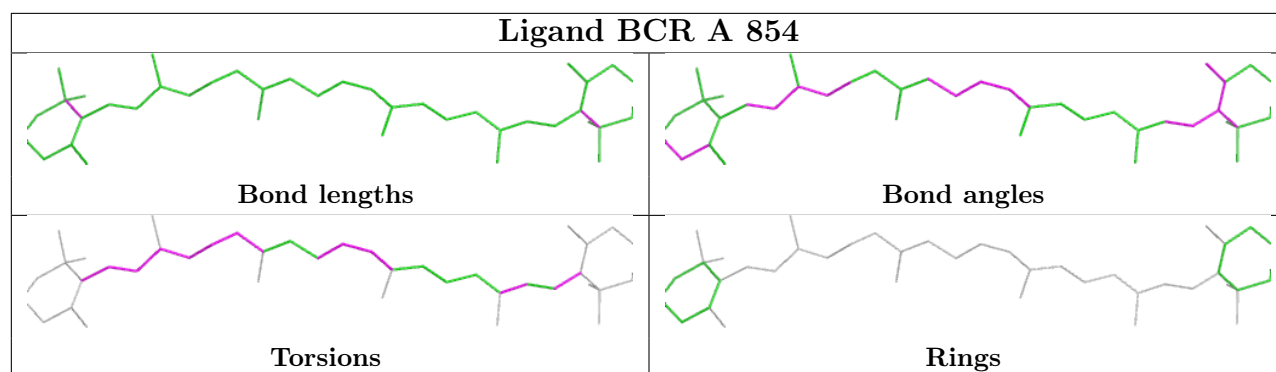
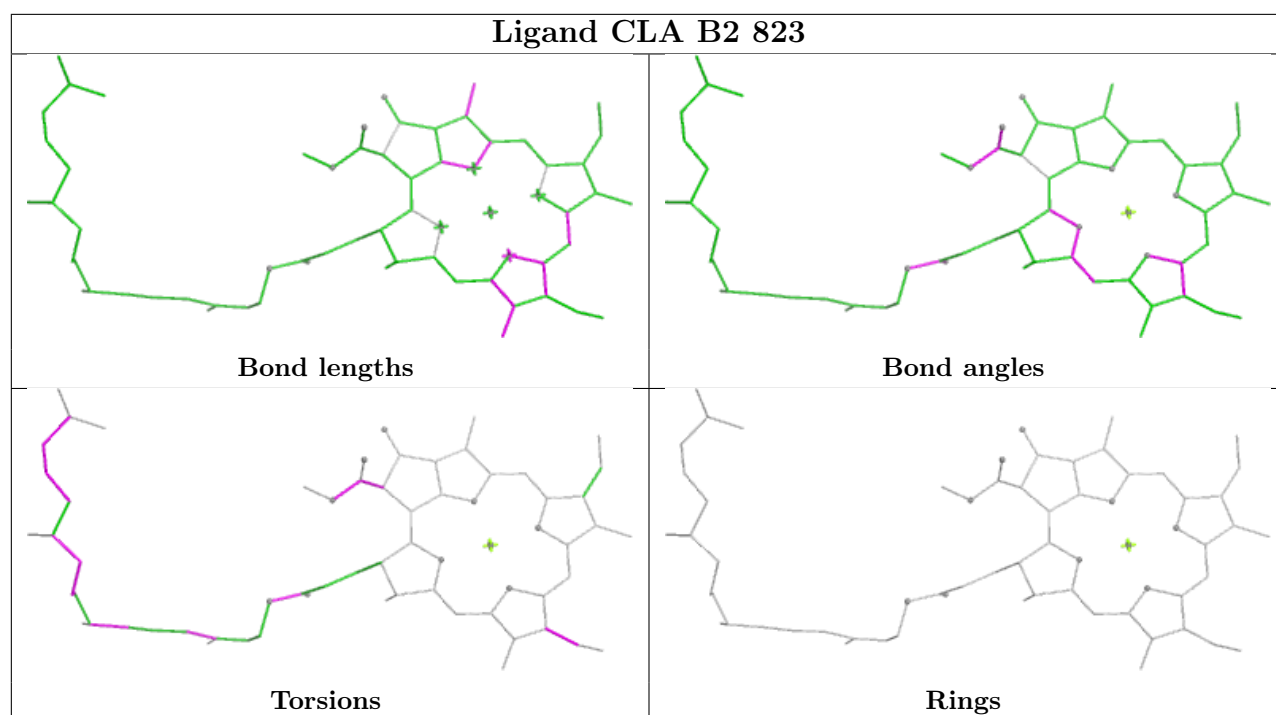


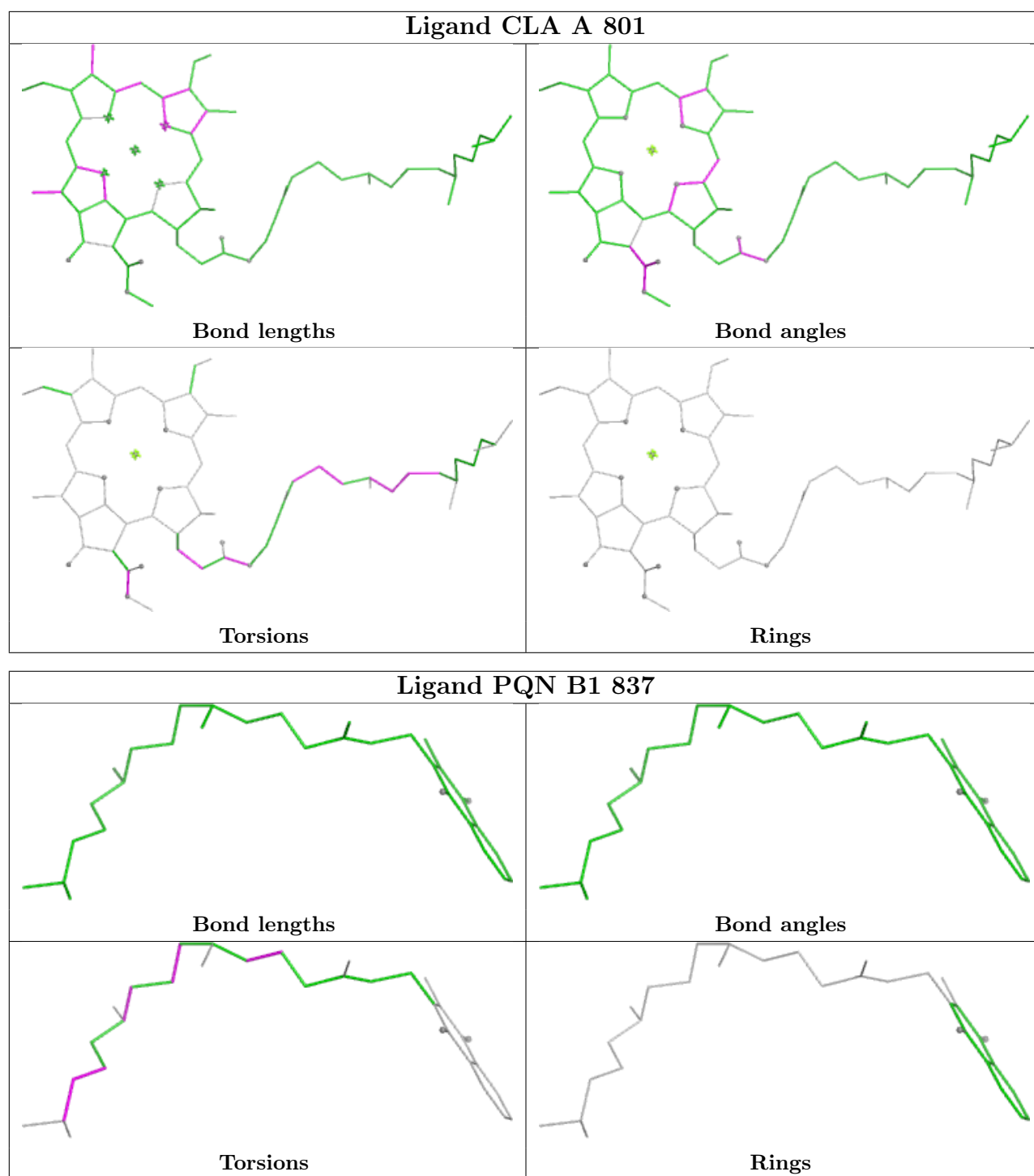
Ligand CLA A 838

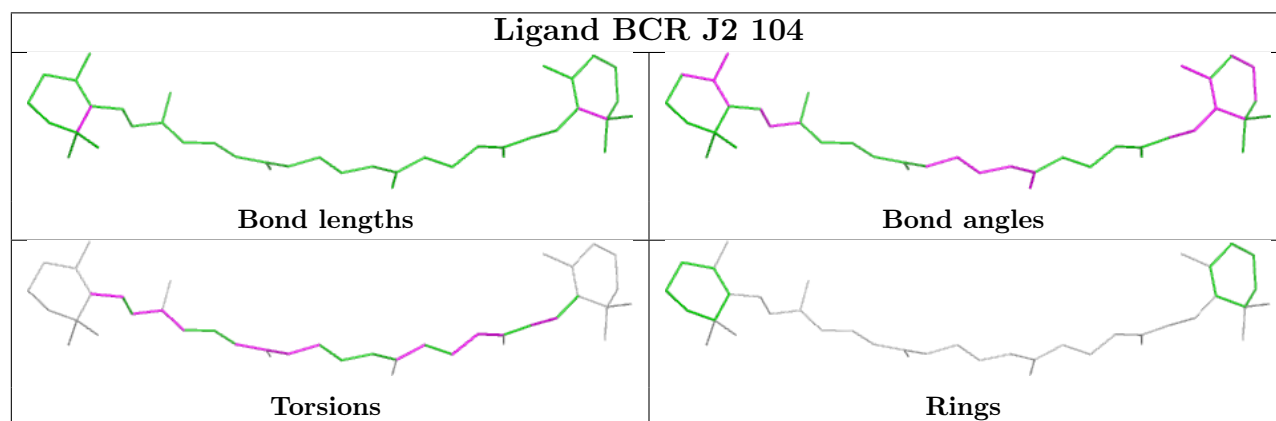
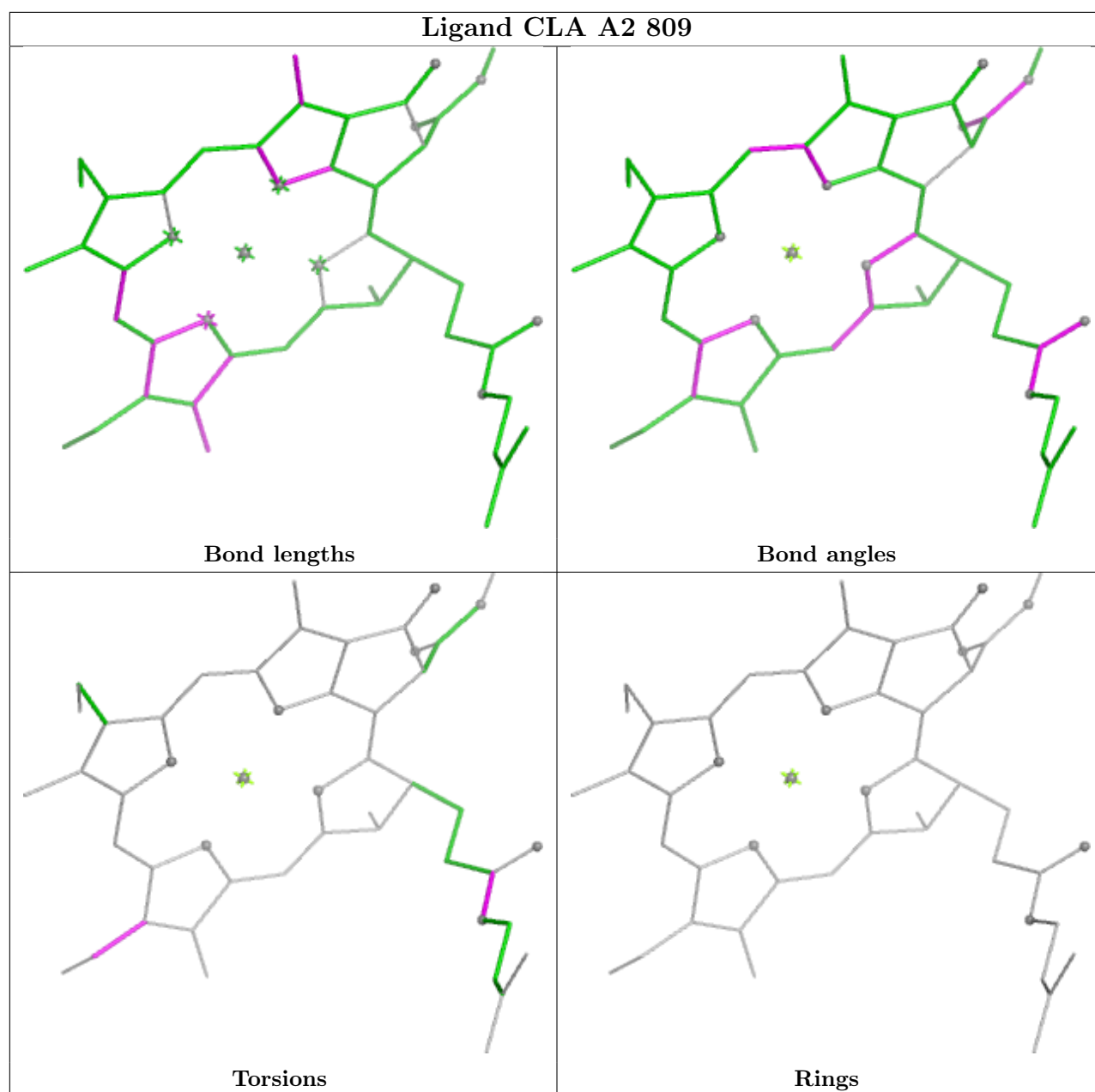


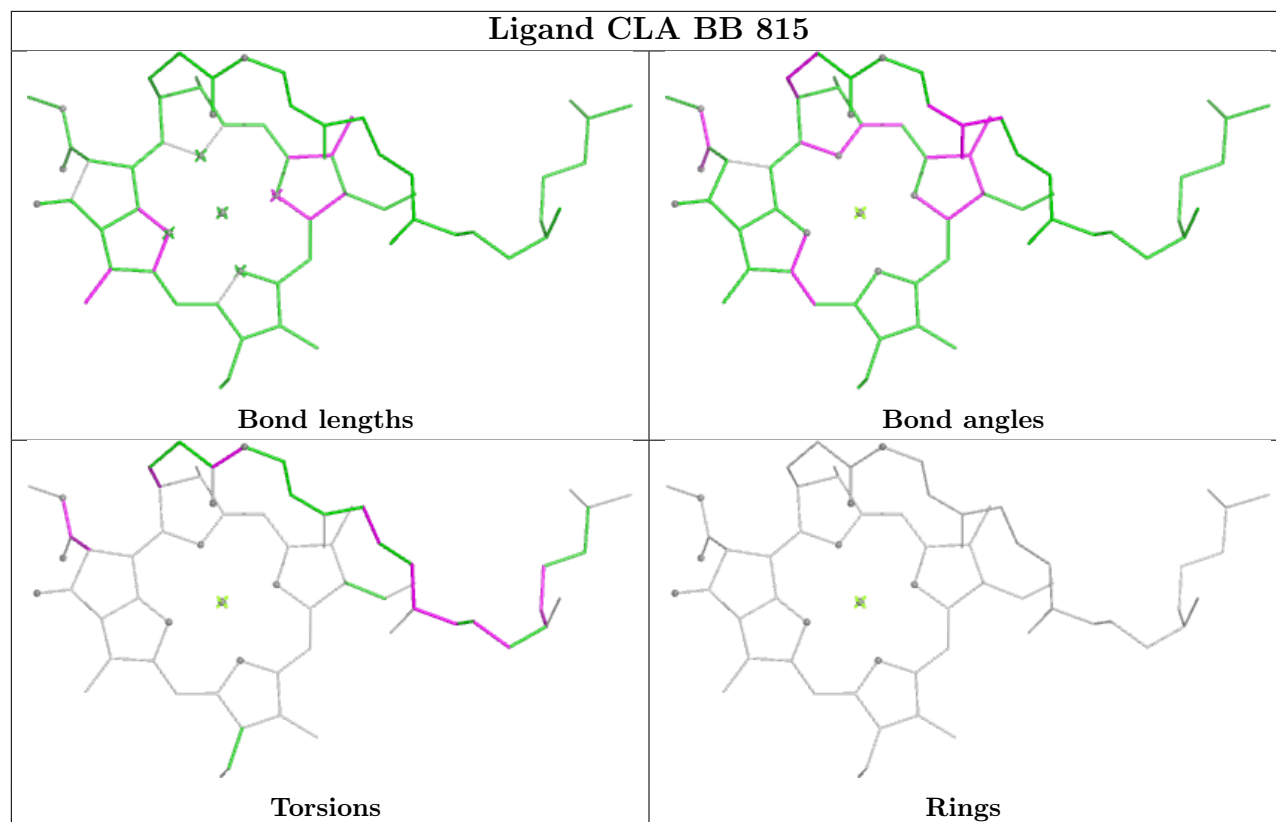
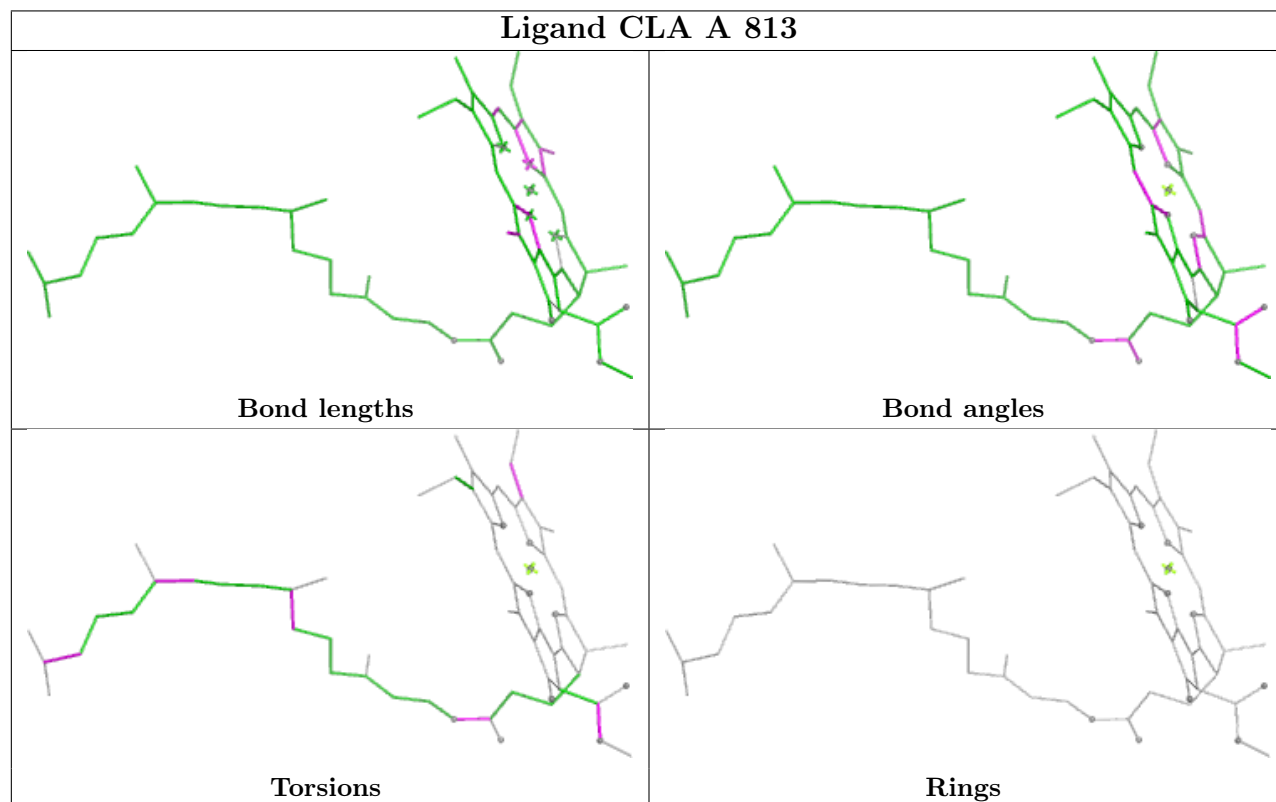


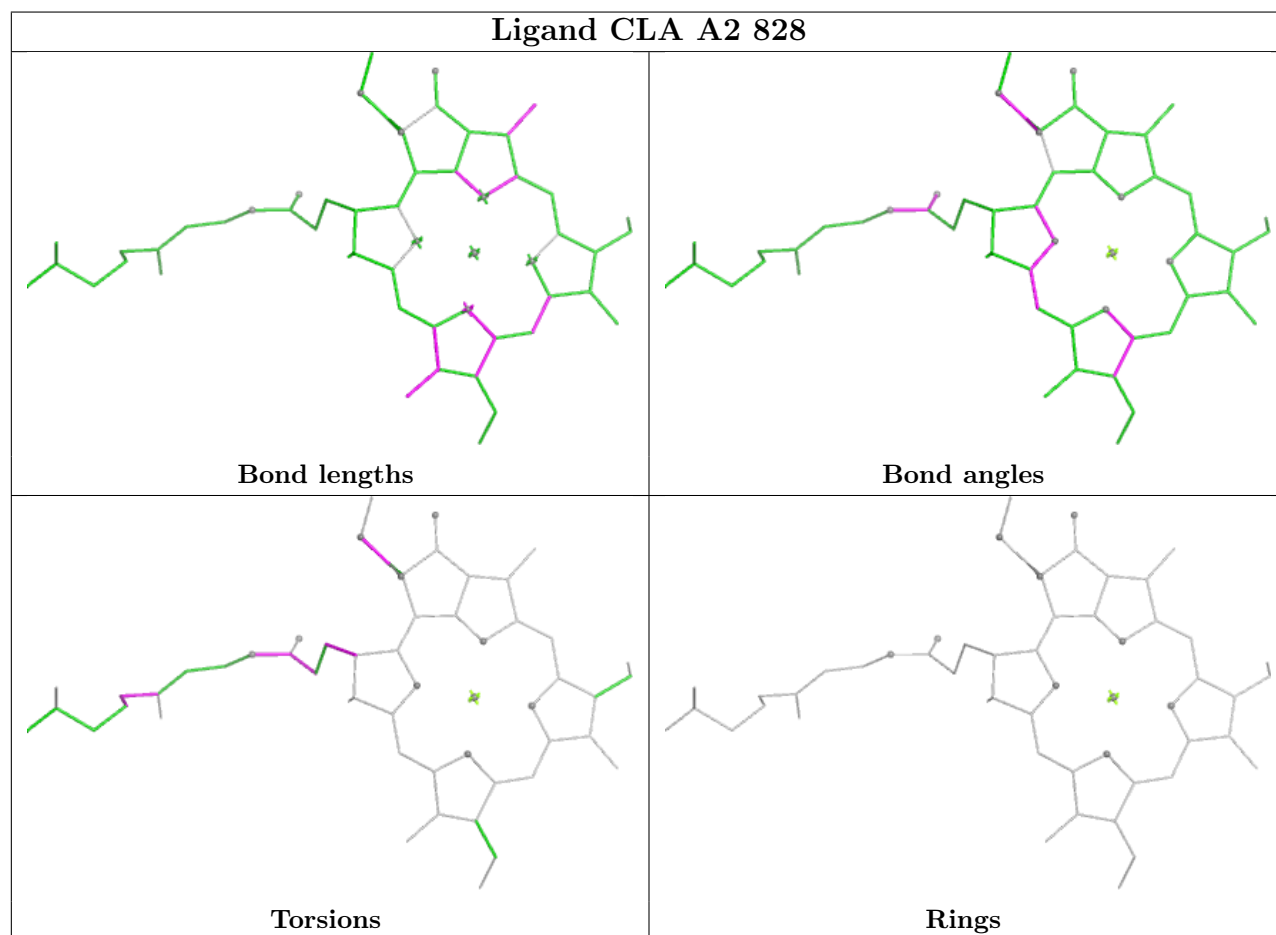
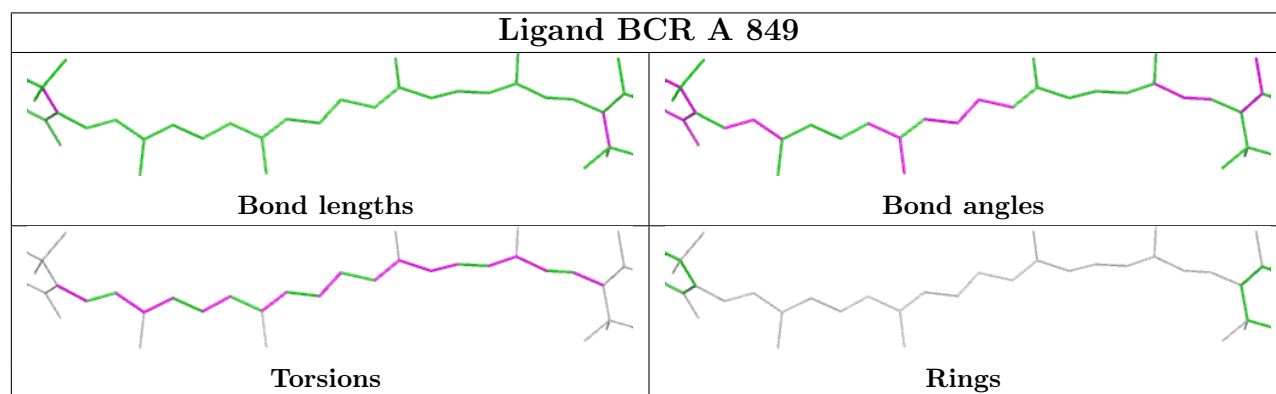
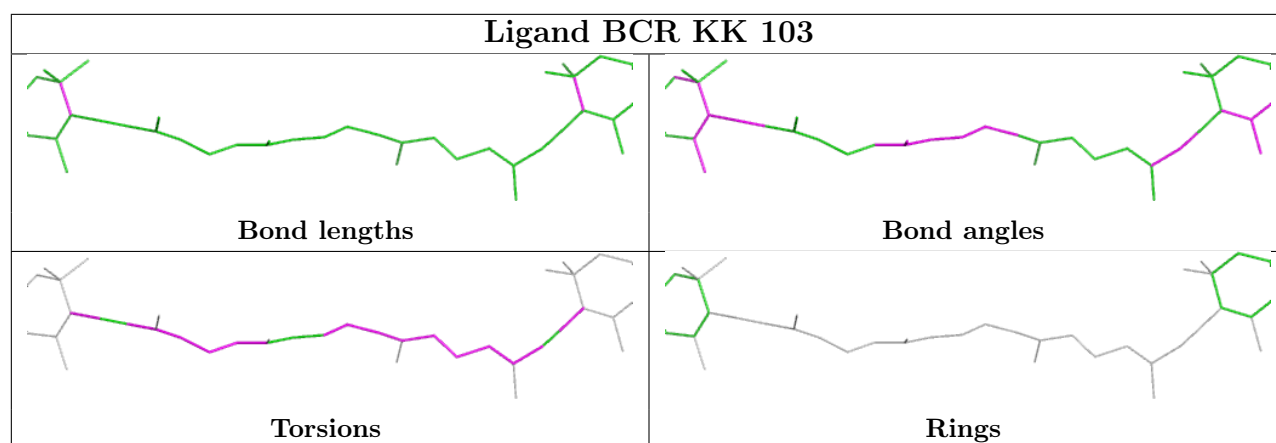


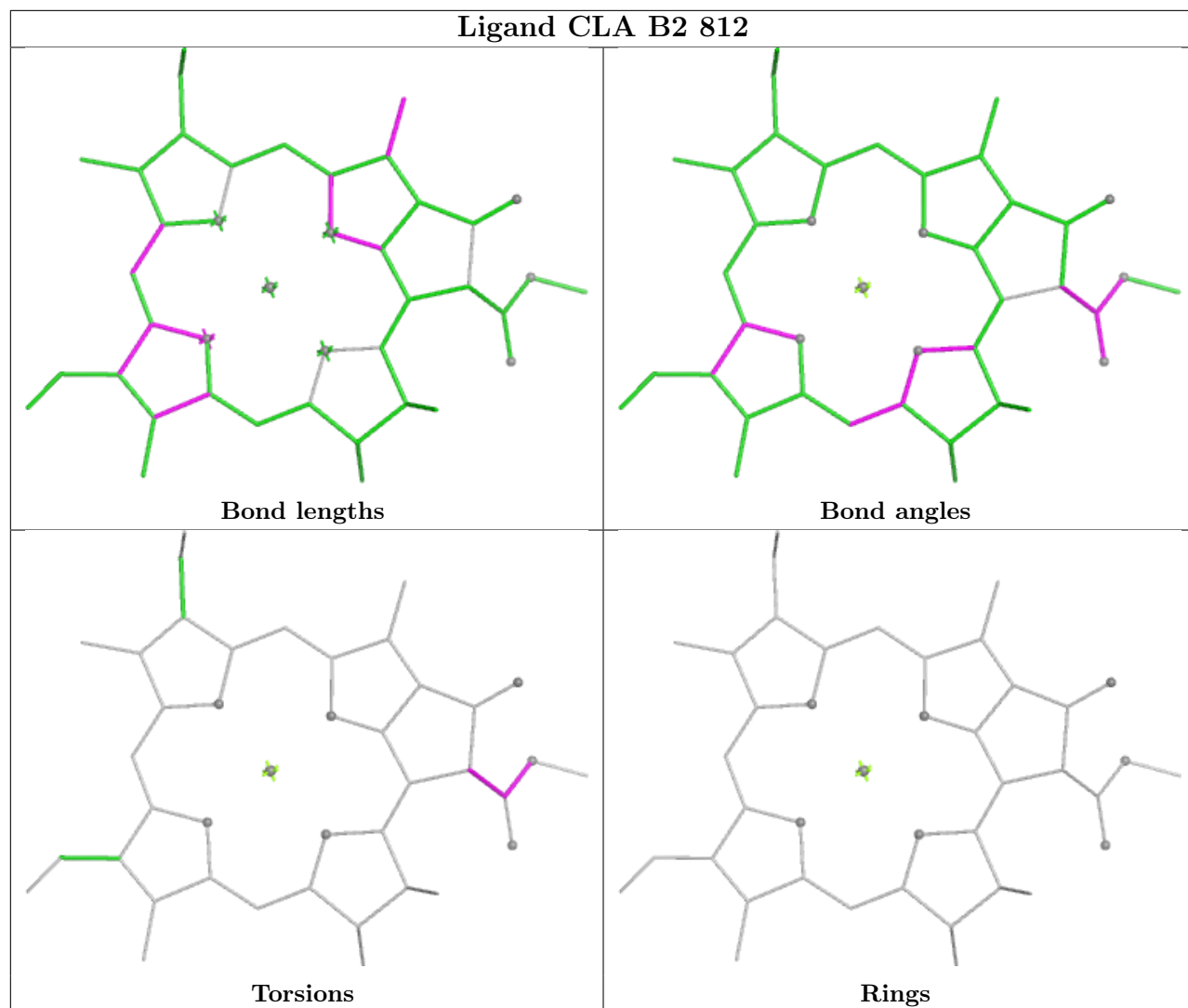




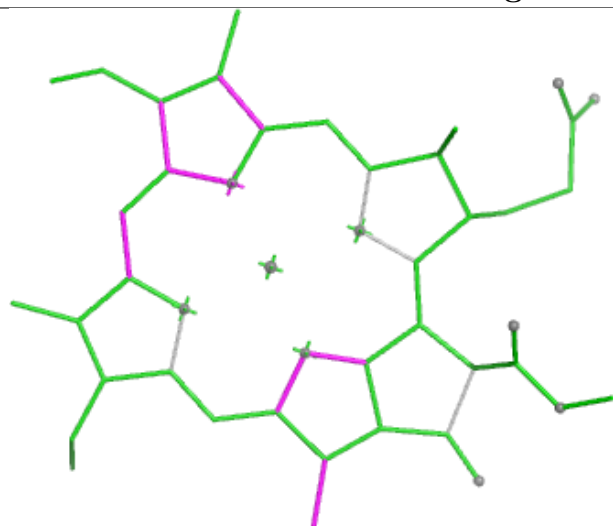


Ligand CLA BB 815**Ligand CLA A 813**

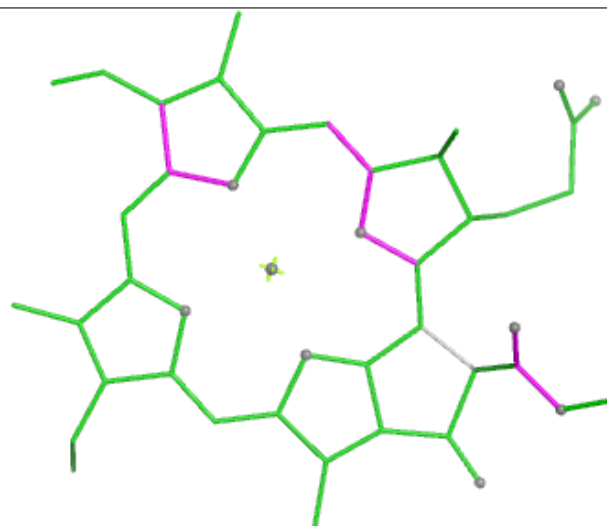




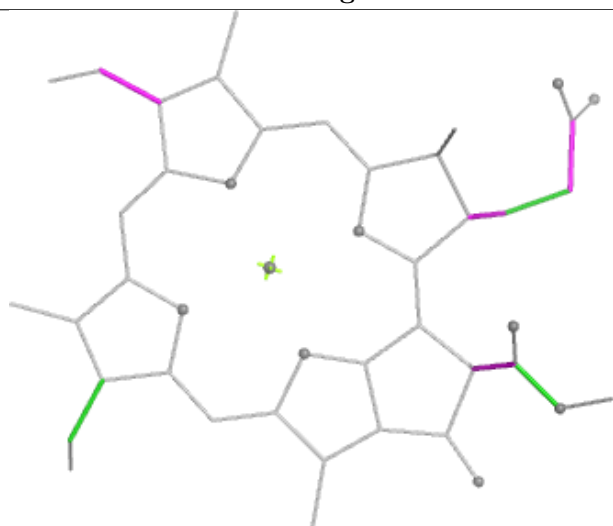
Ligand CLA X2 101



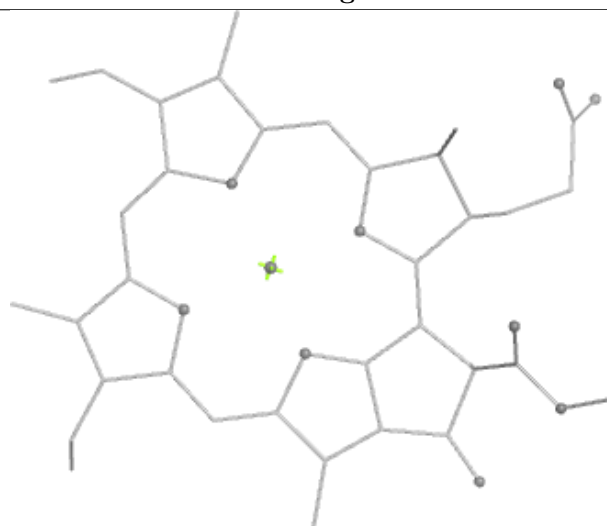
Bond lengths



Bond angles

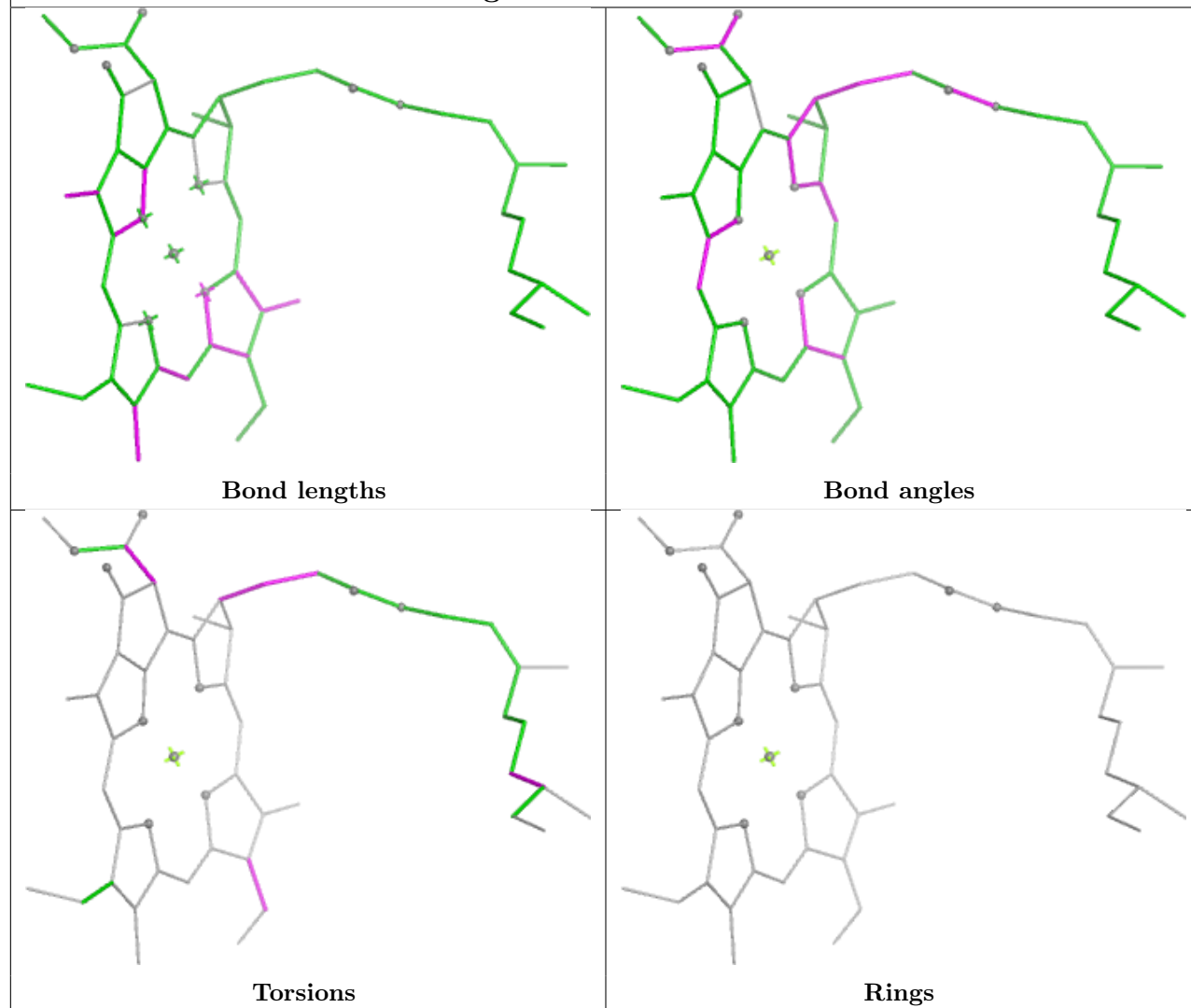


Torsions

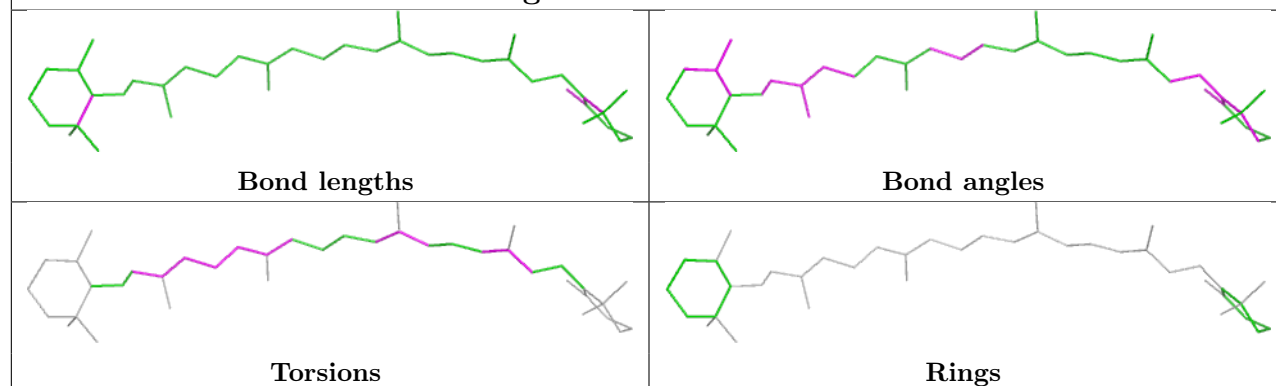


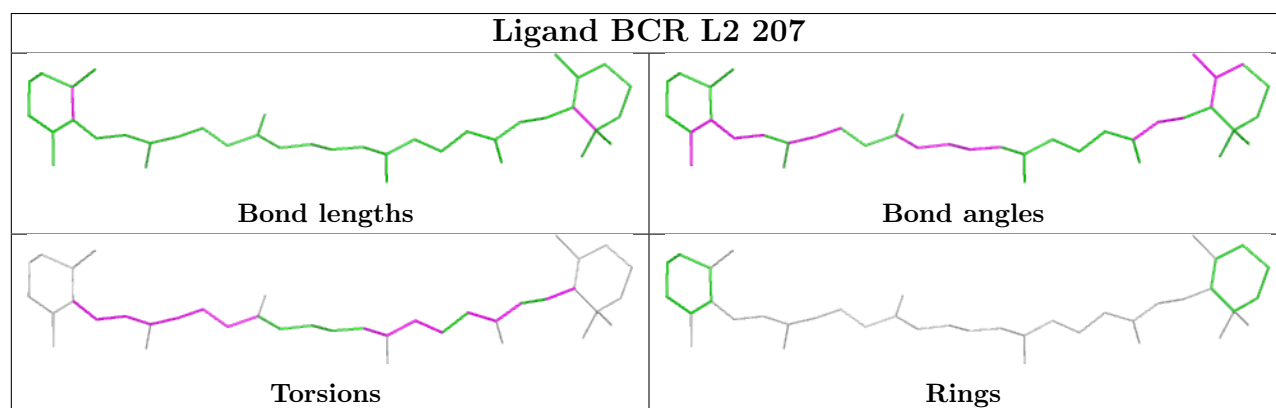
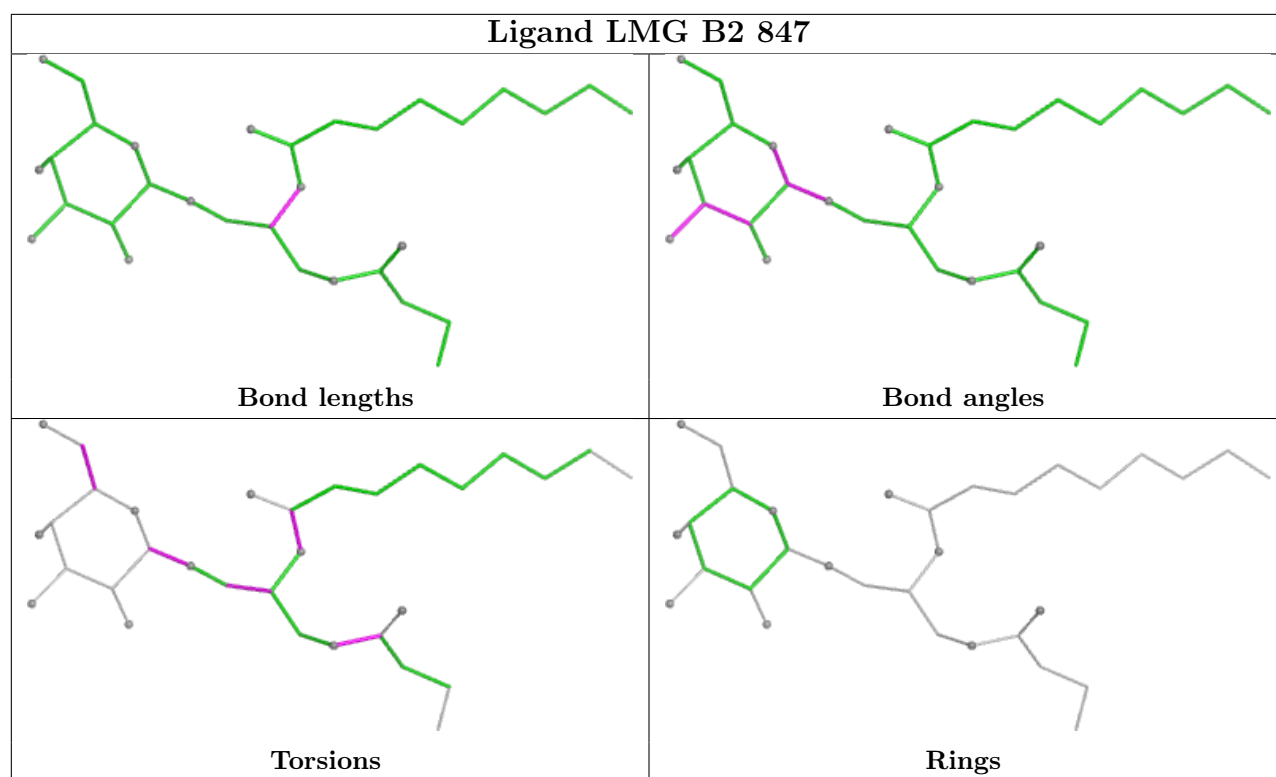
Rings

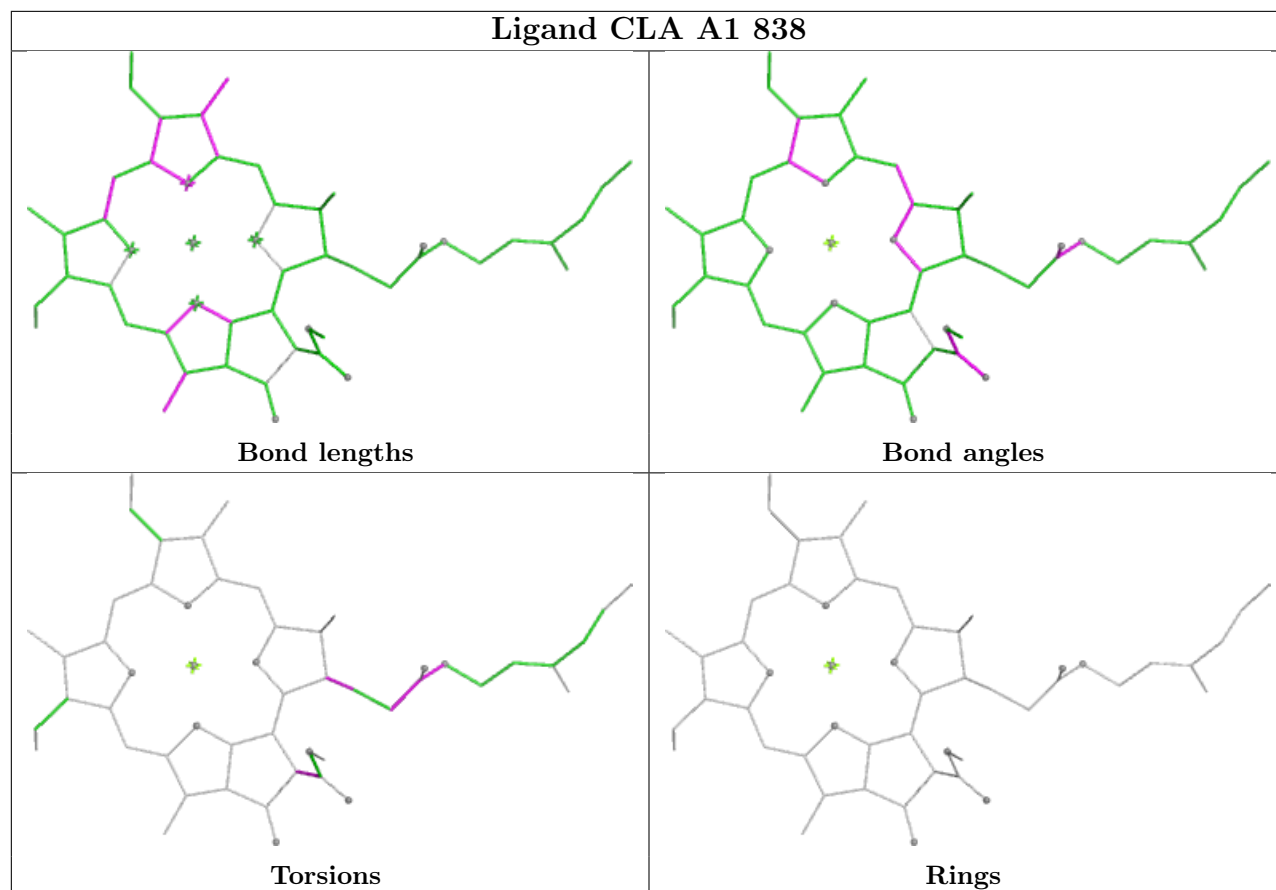
Ligand CLA AA 806

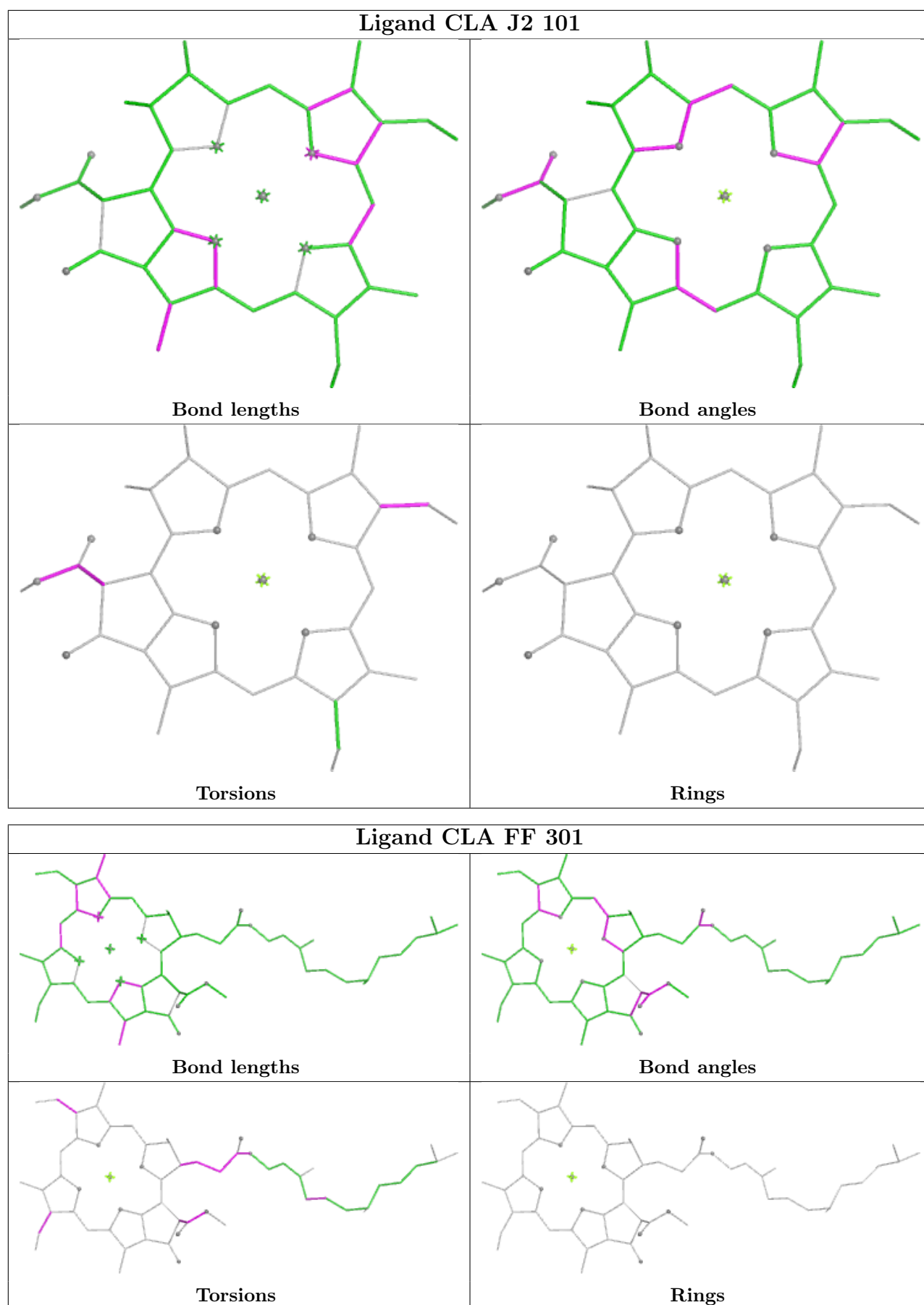


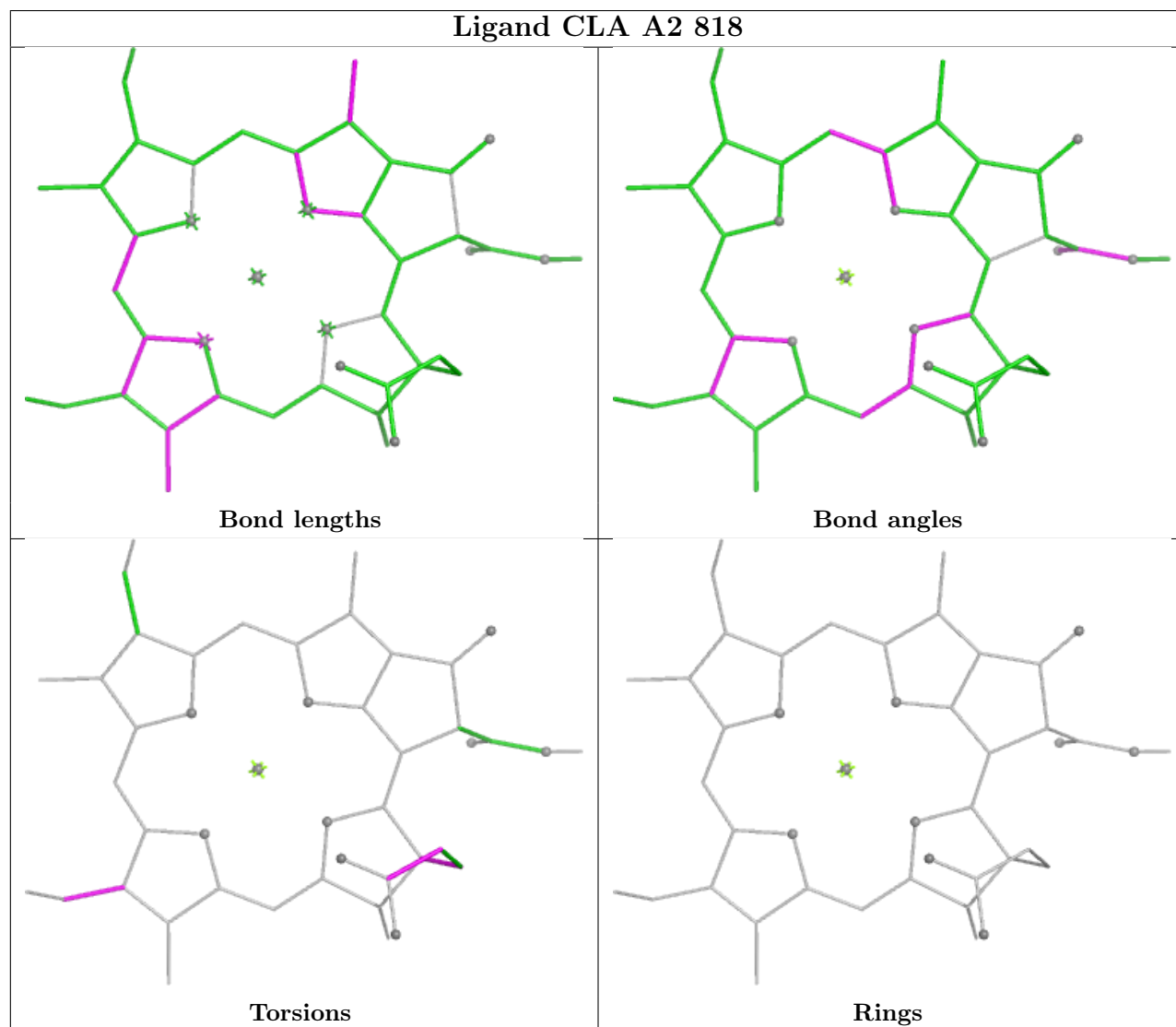
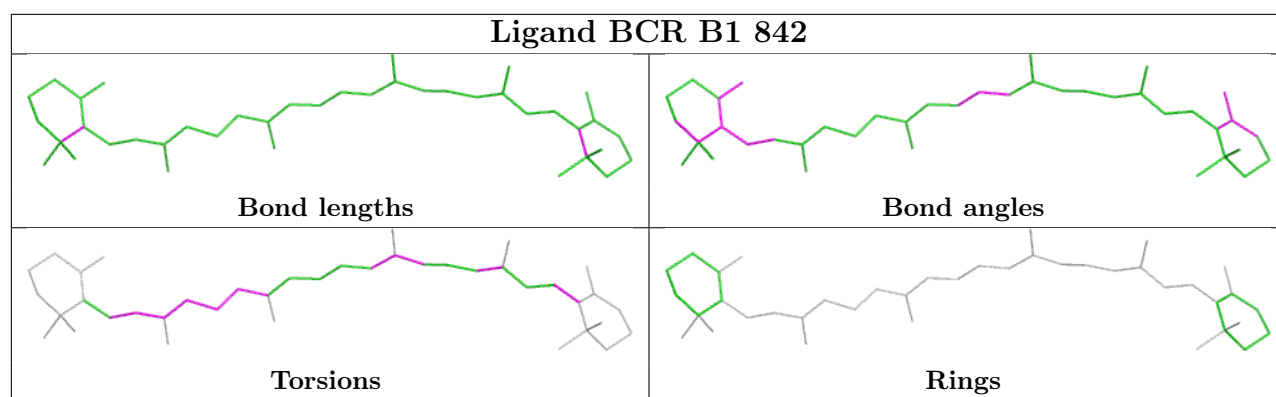
Ligand BCR F2 304

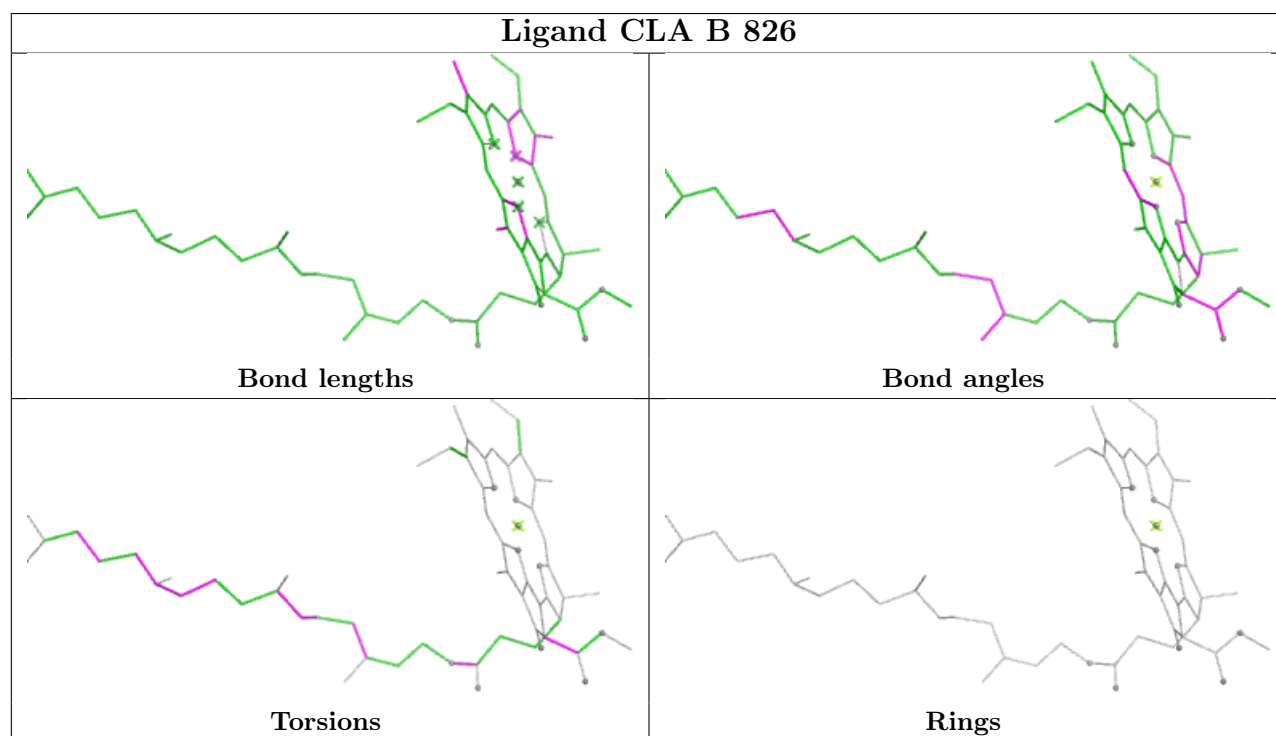
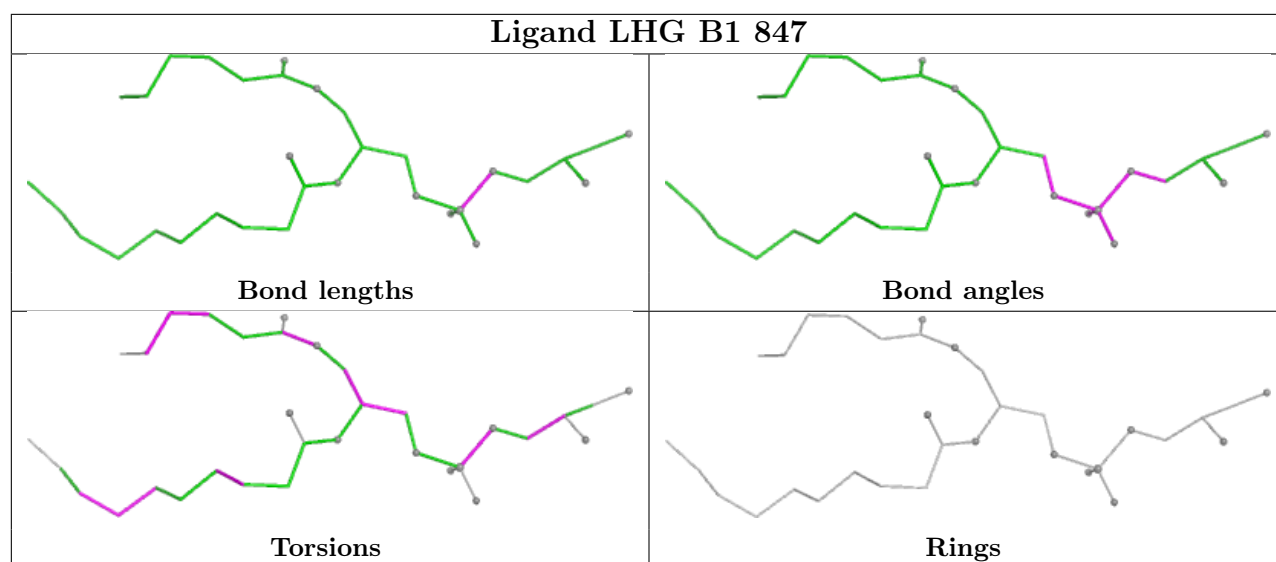


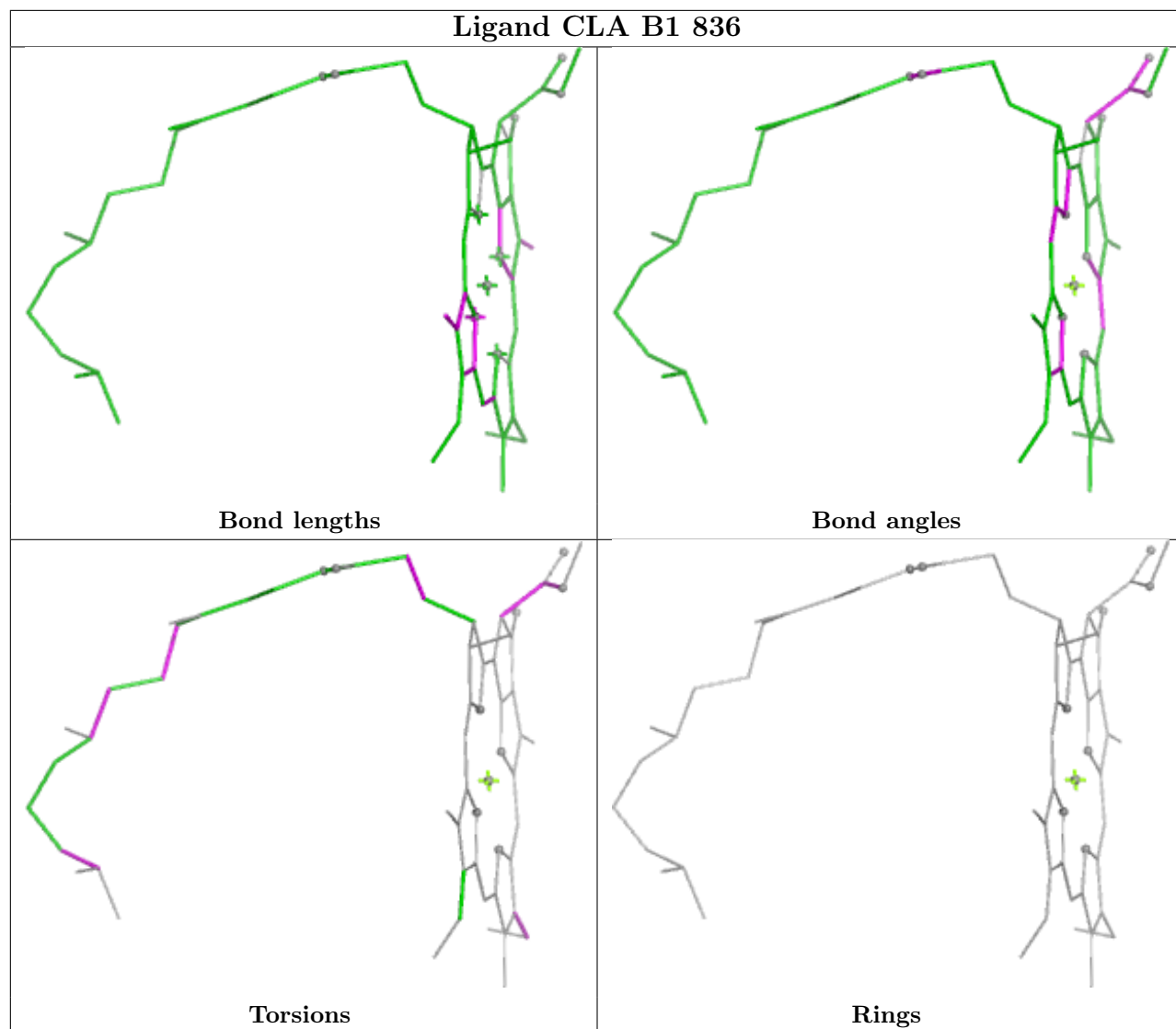




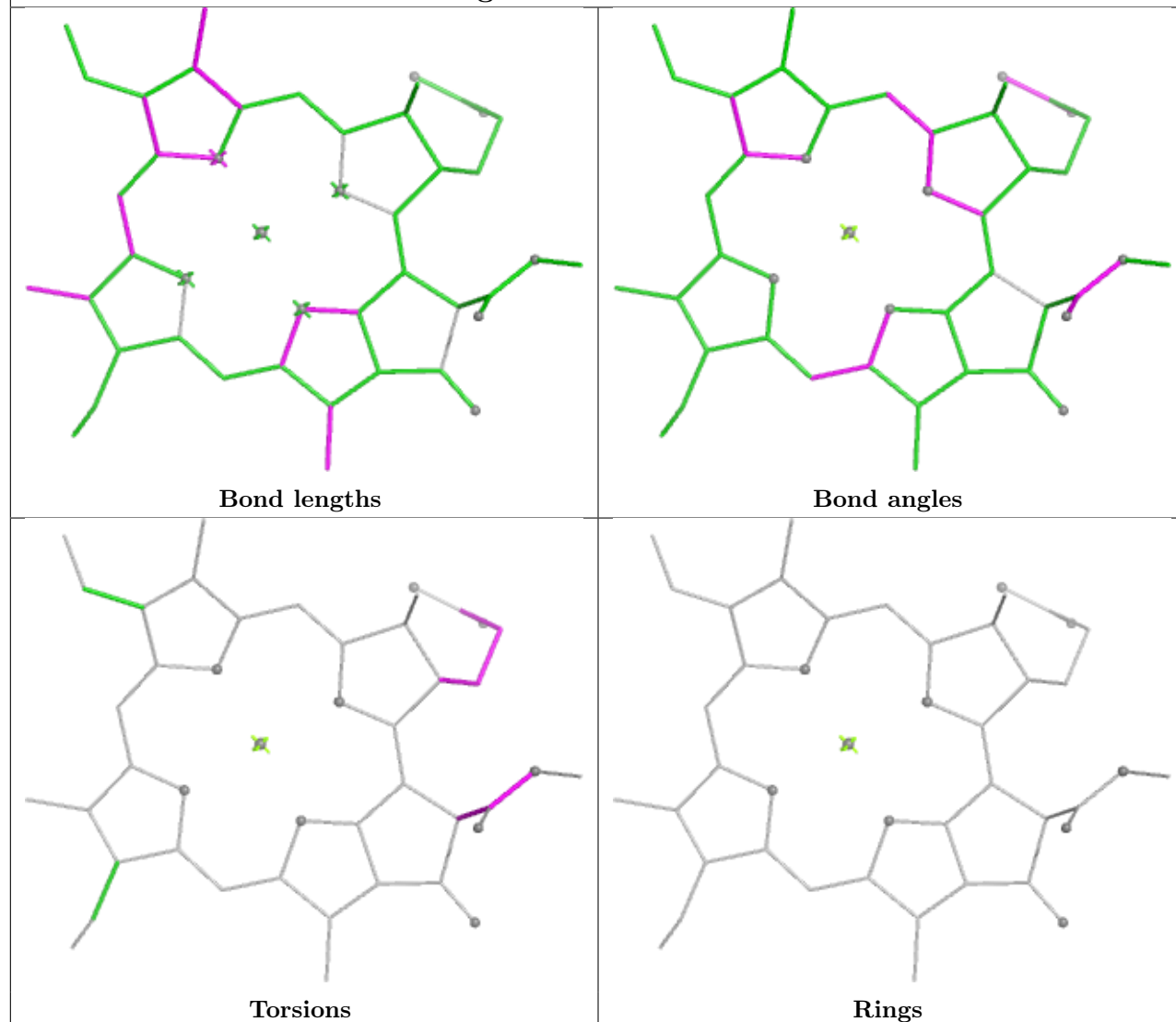




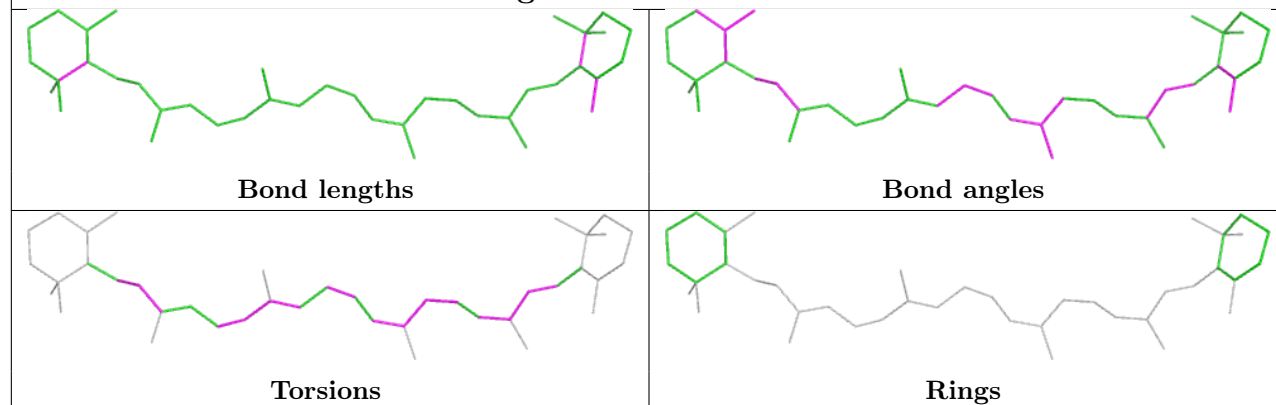


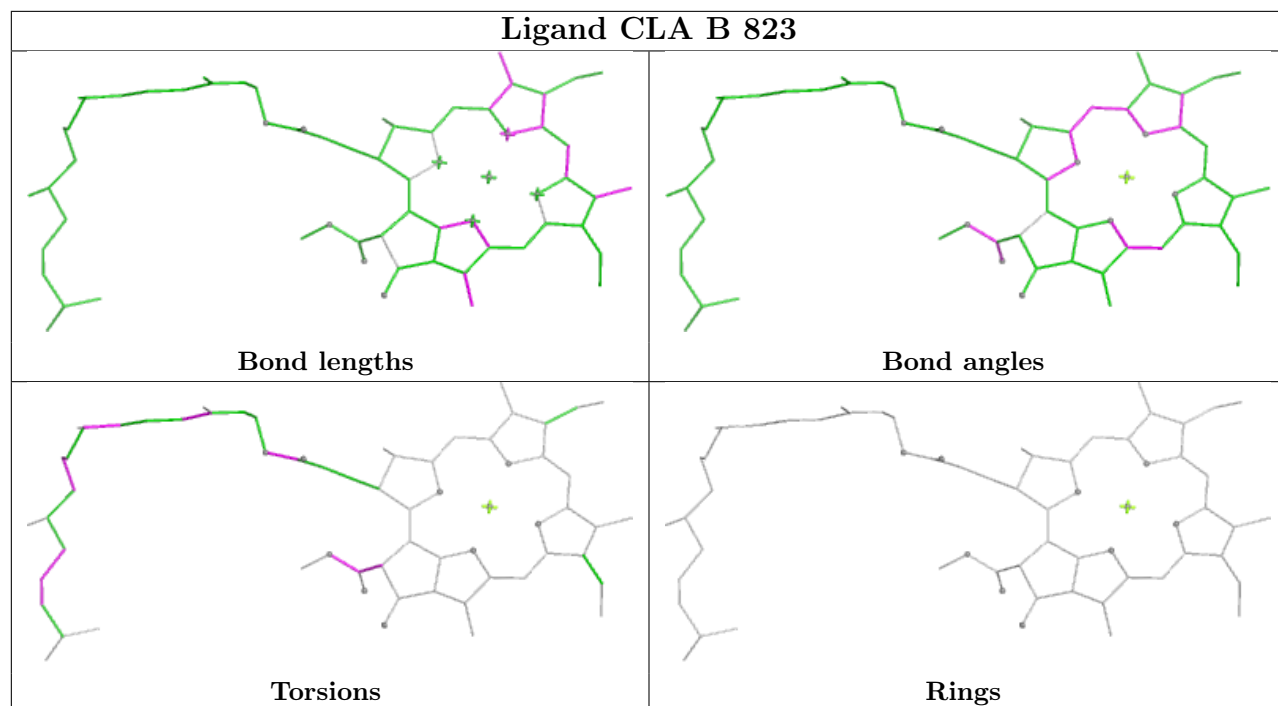


Ligand CLA AA 826

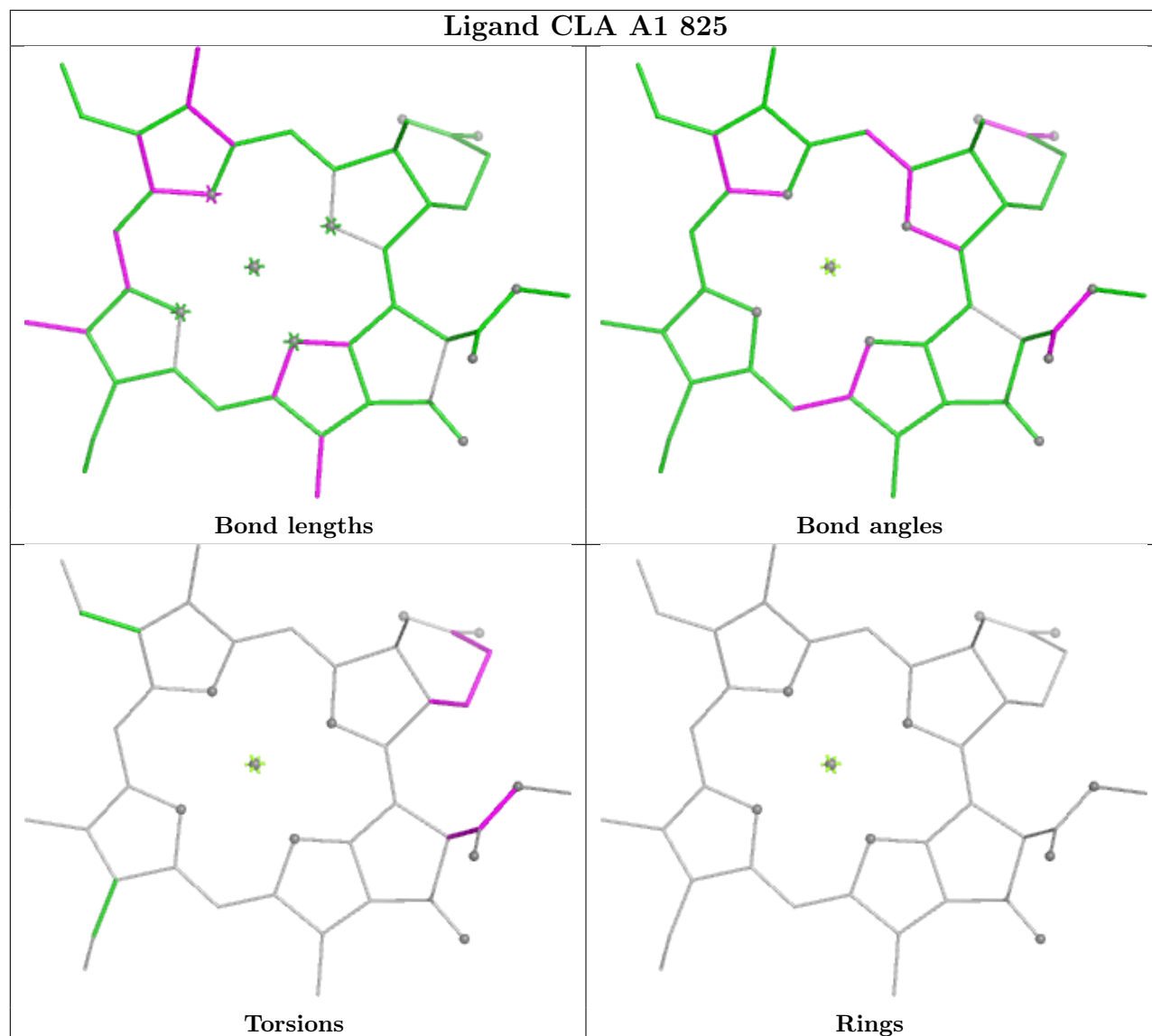


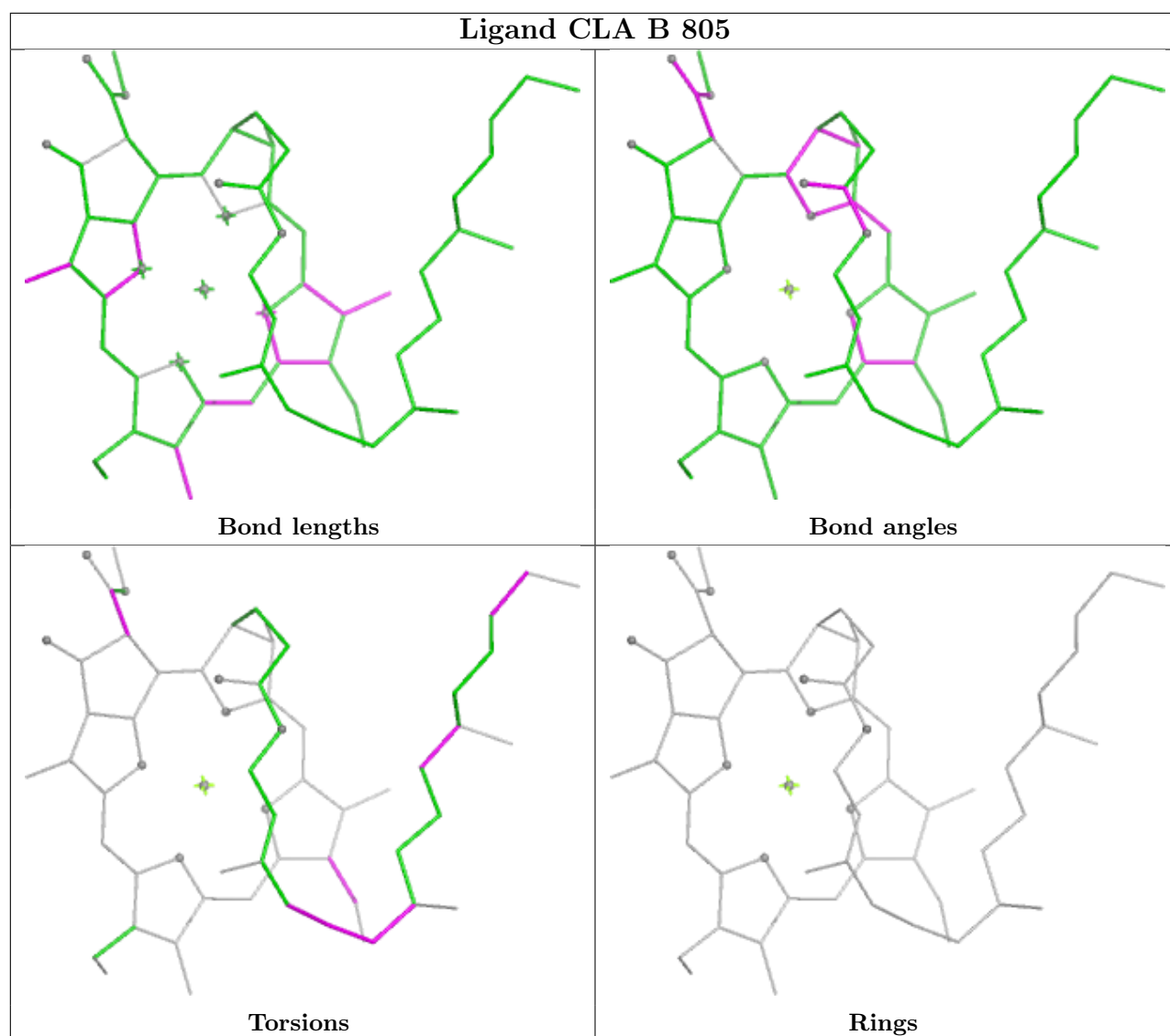
Ligand BCR M1 101

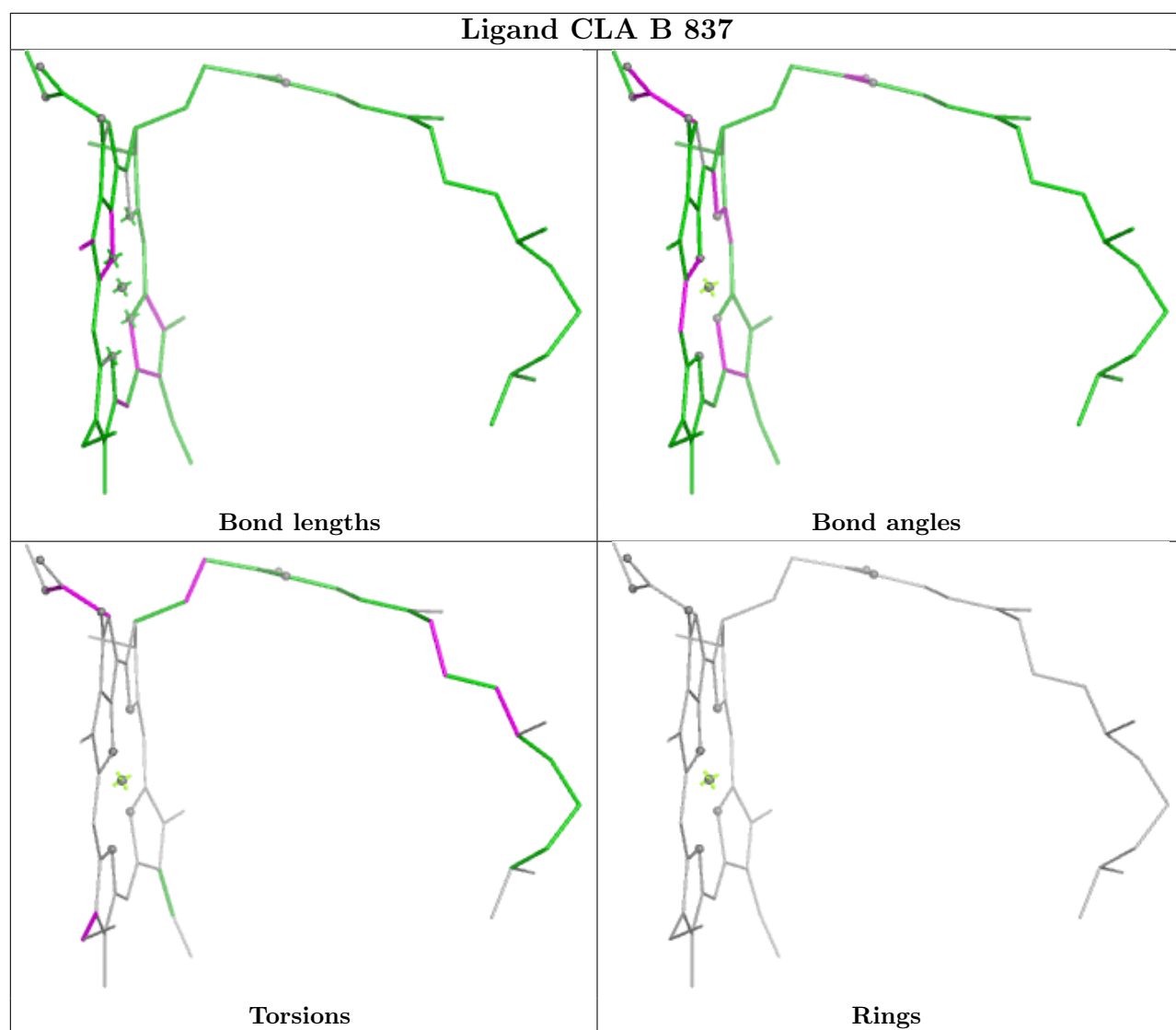


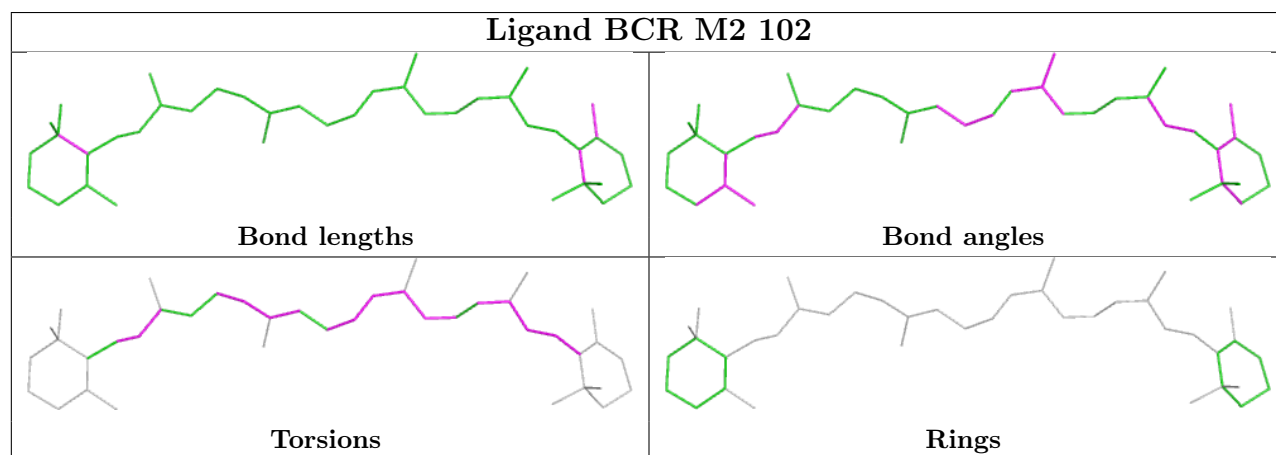
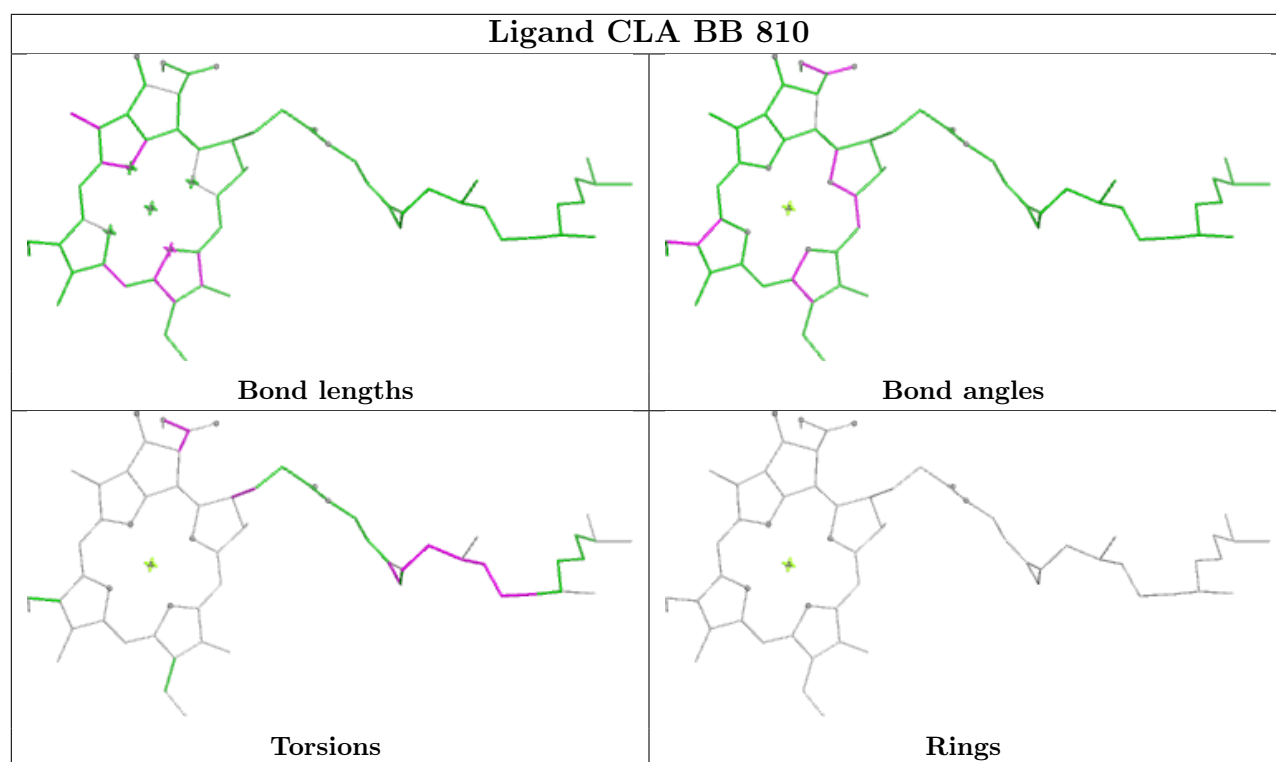


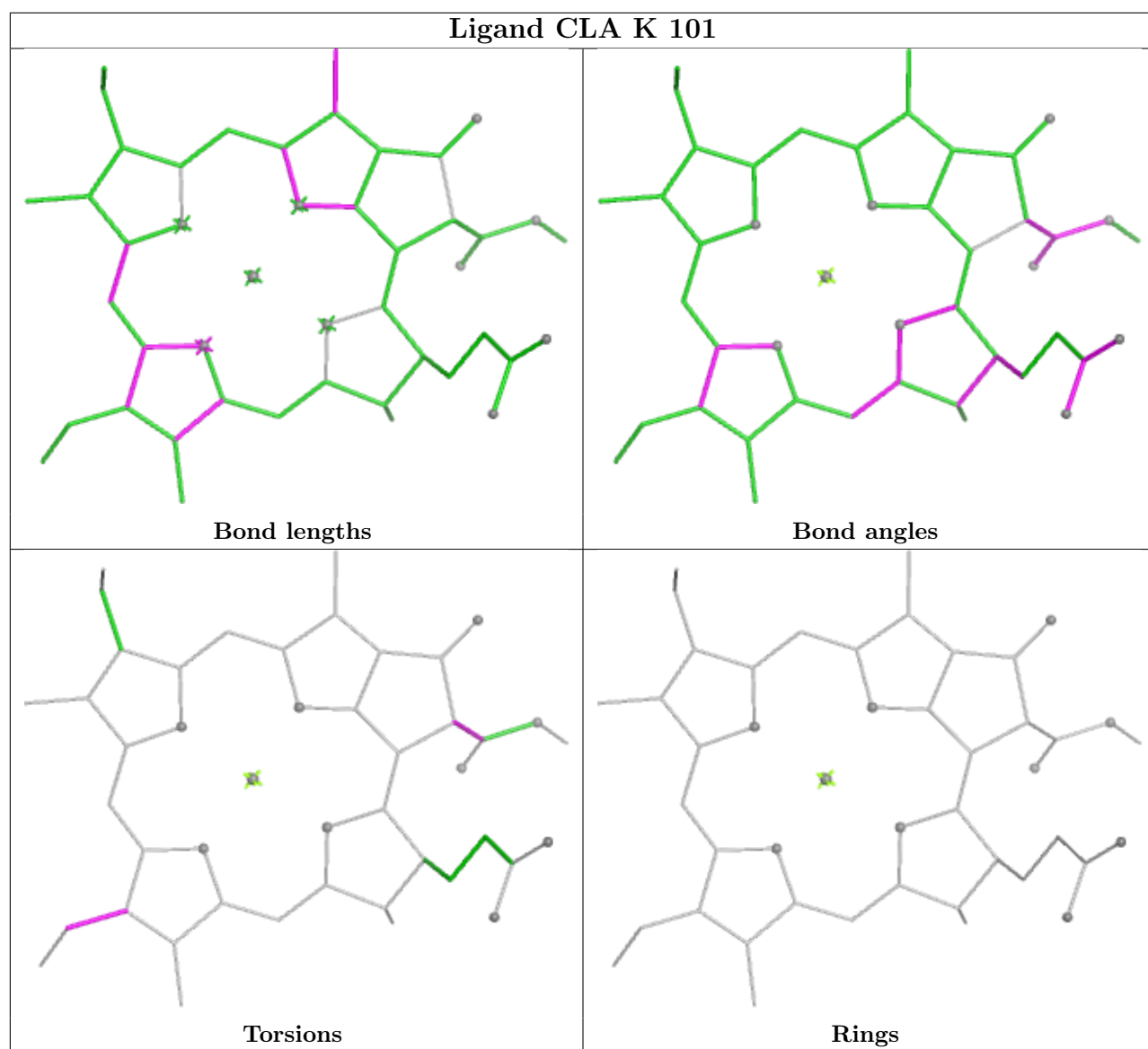
Ligand CLA A1 825

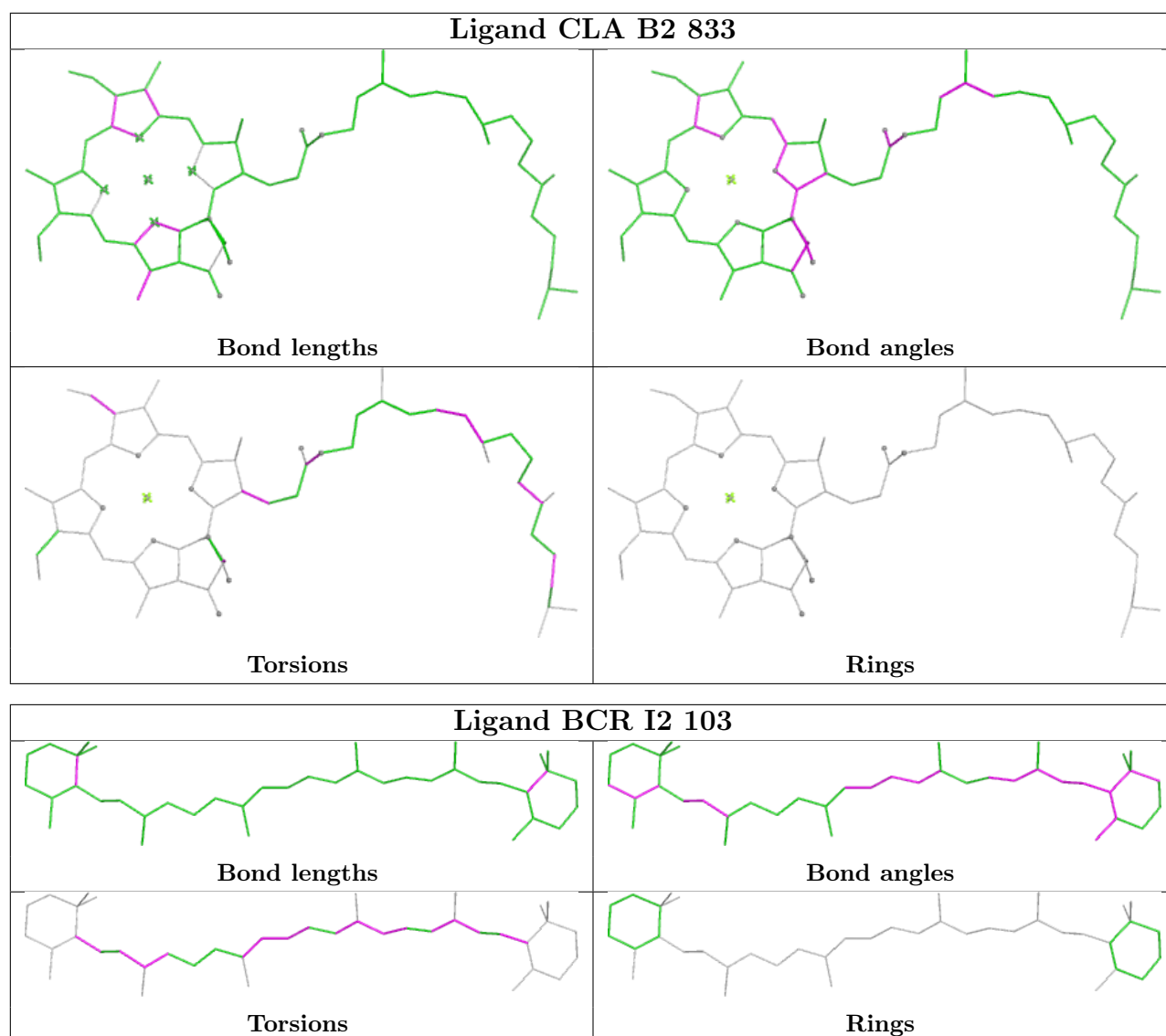


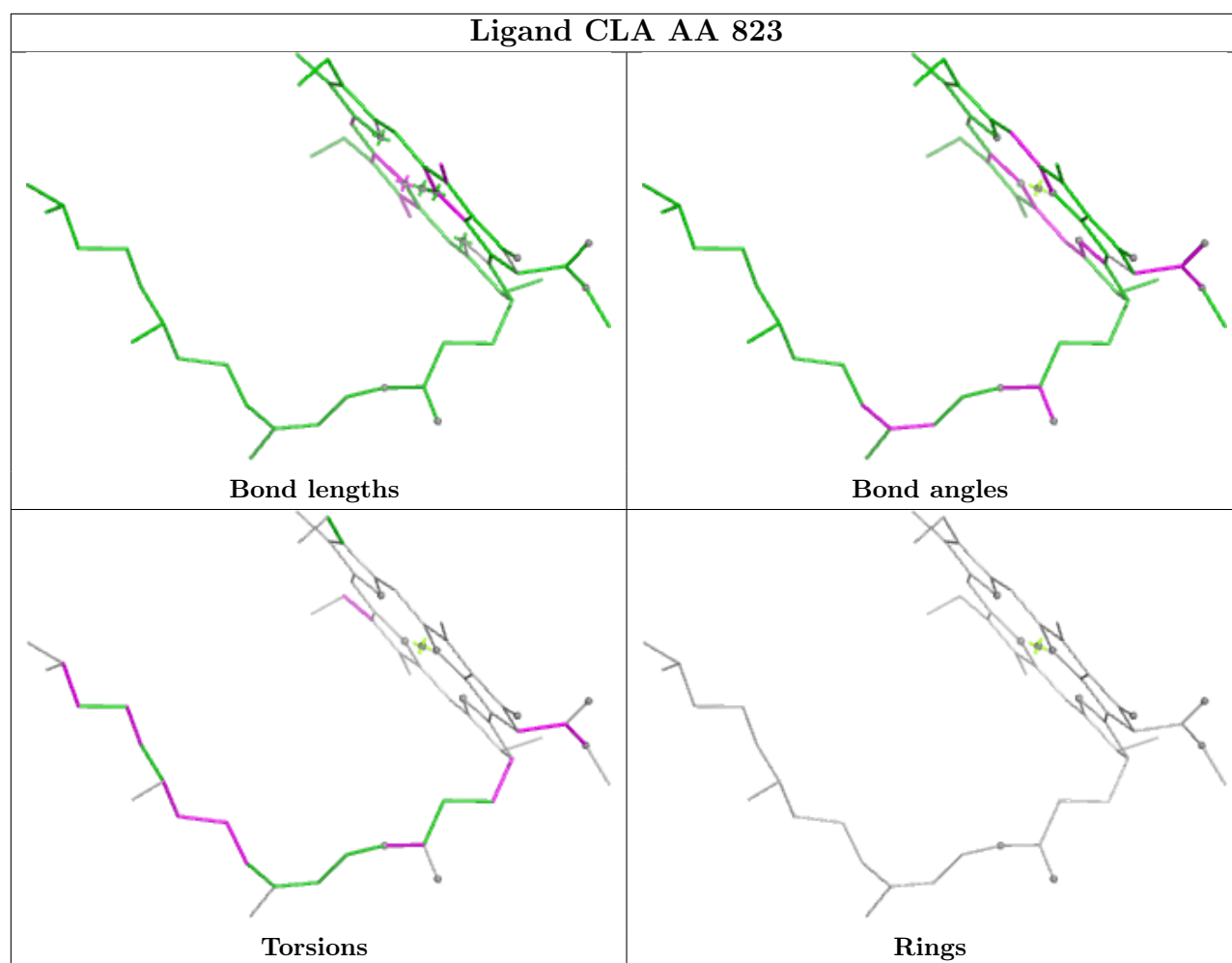


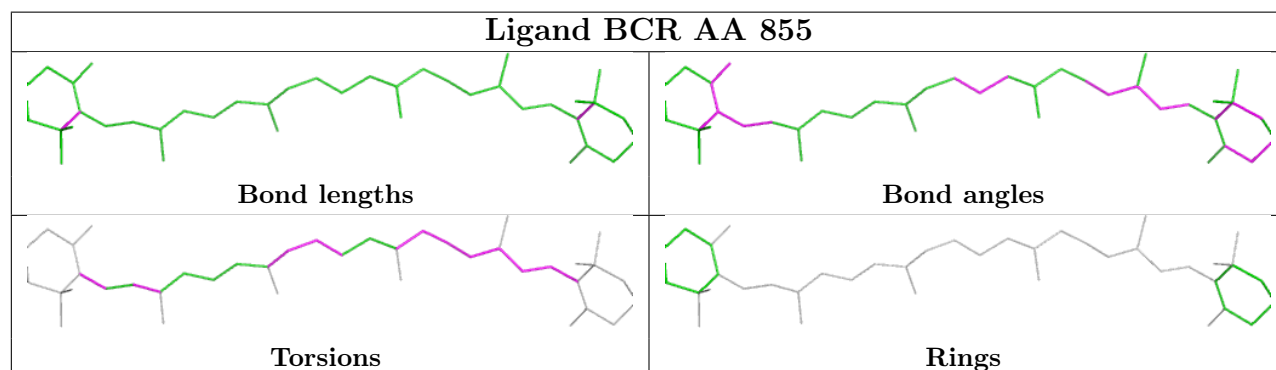
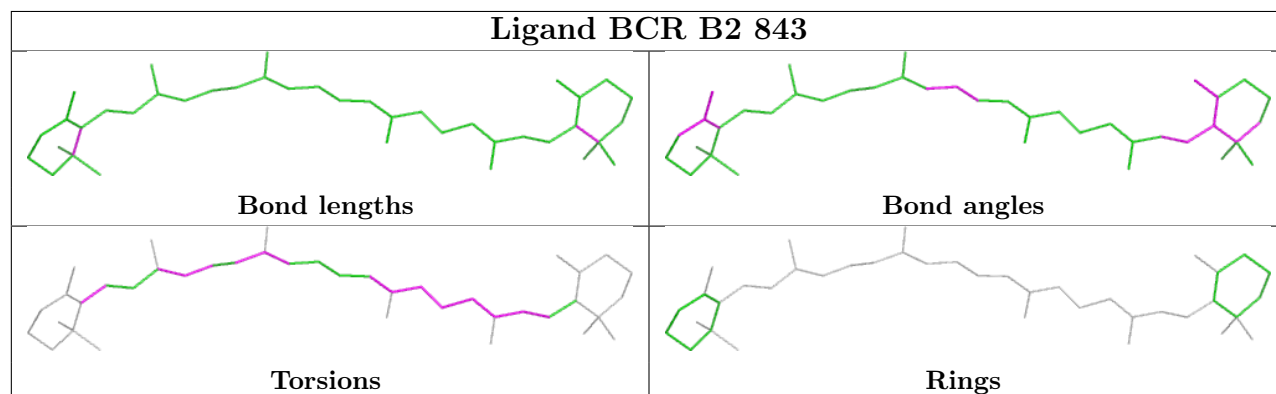
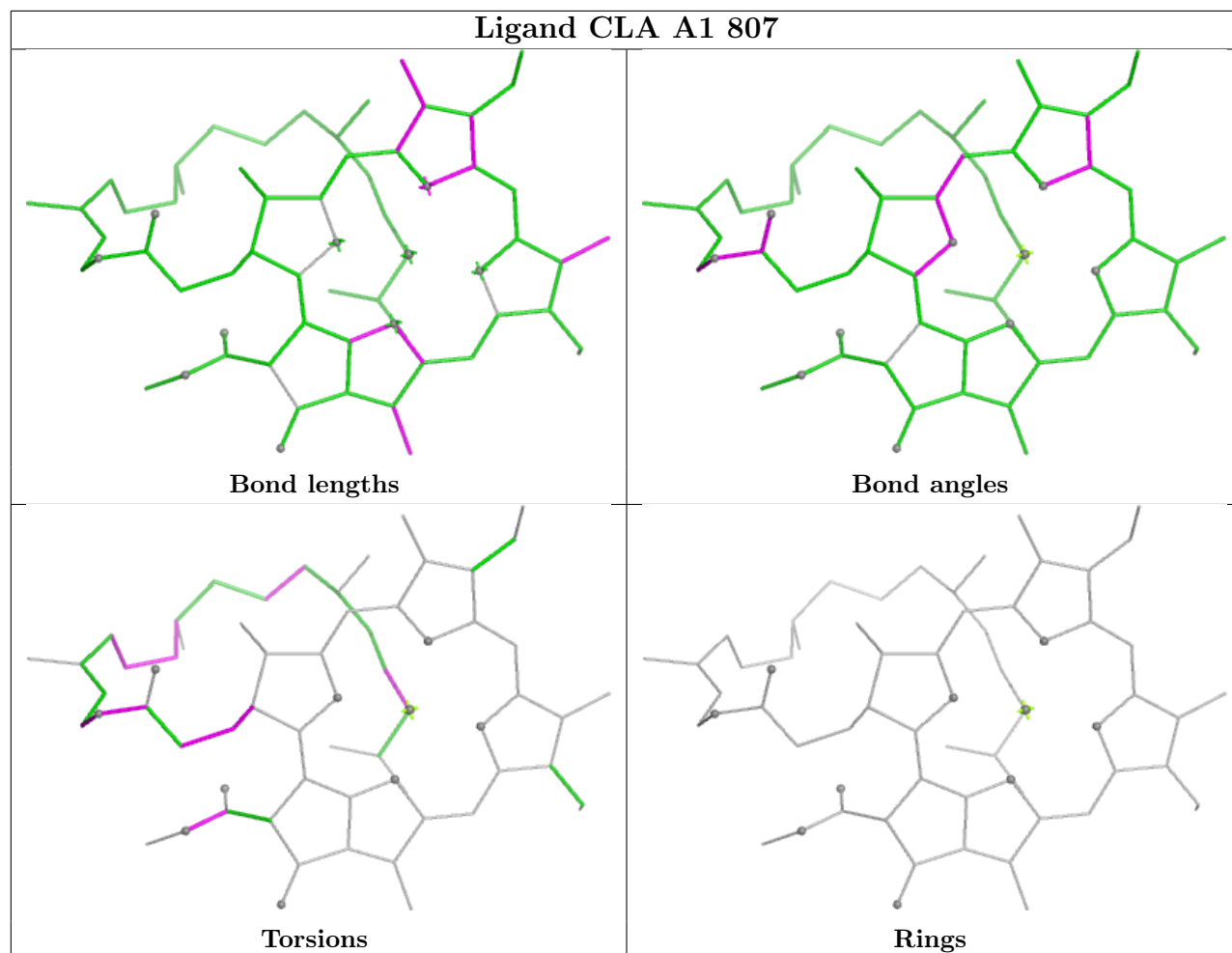




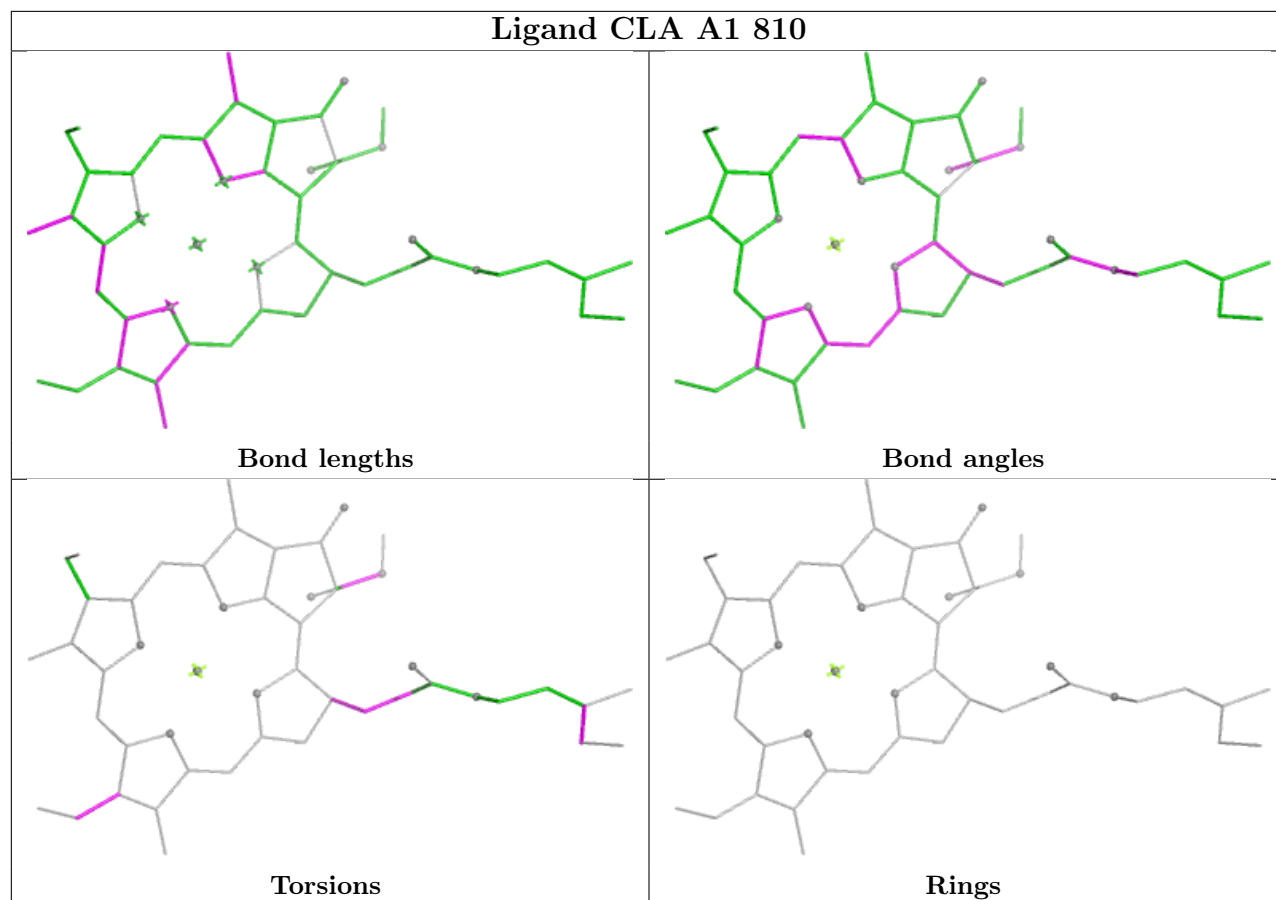


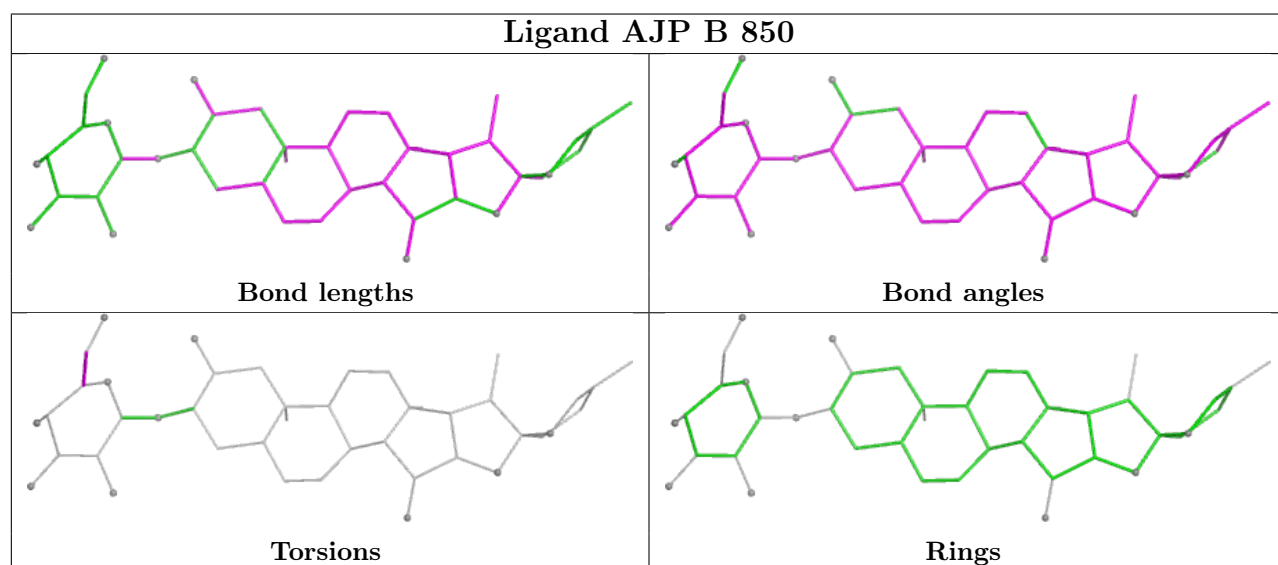
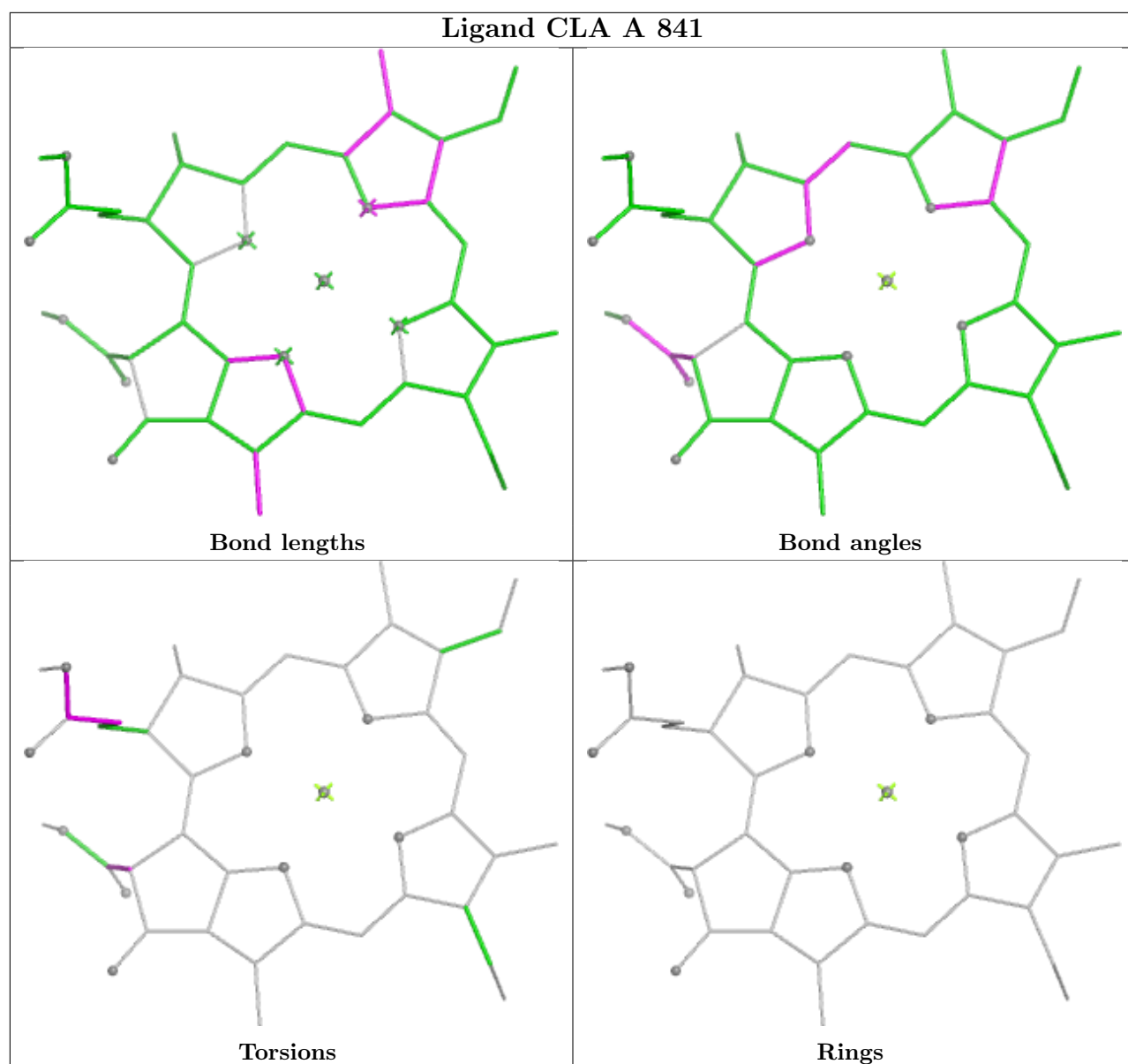


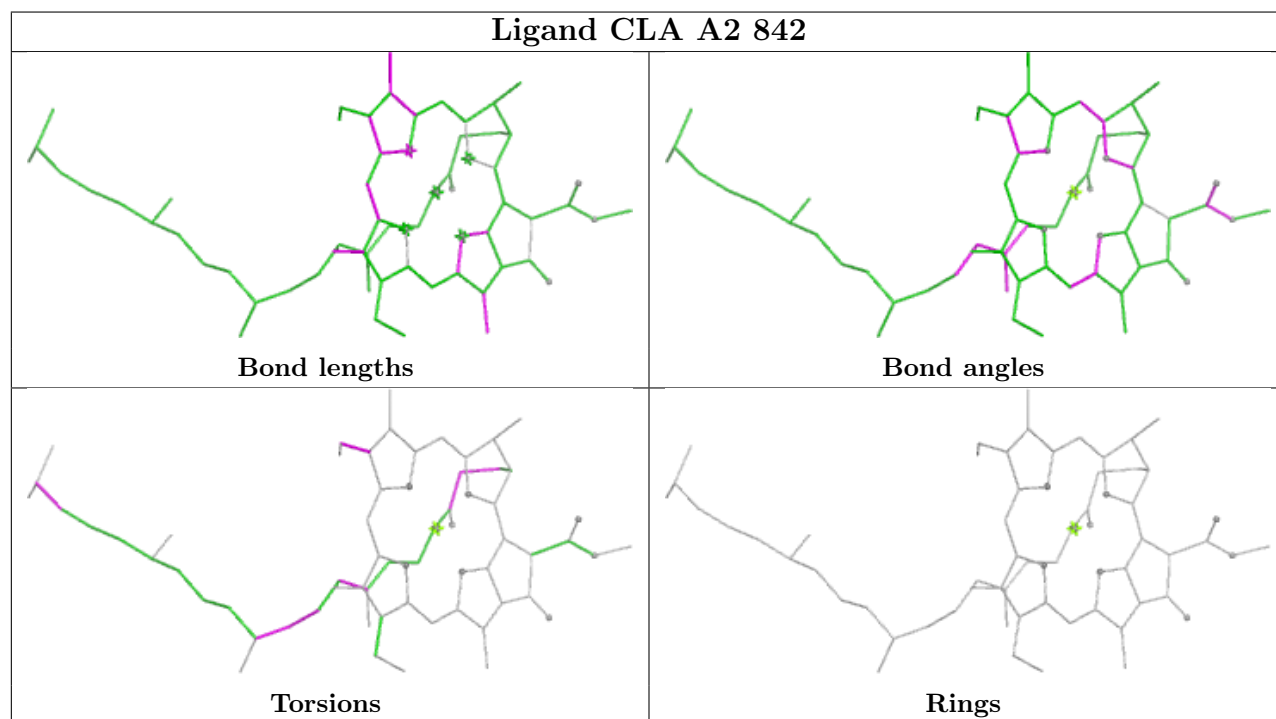
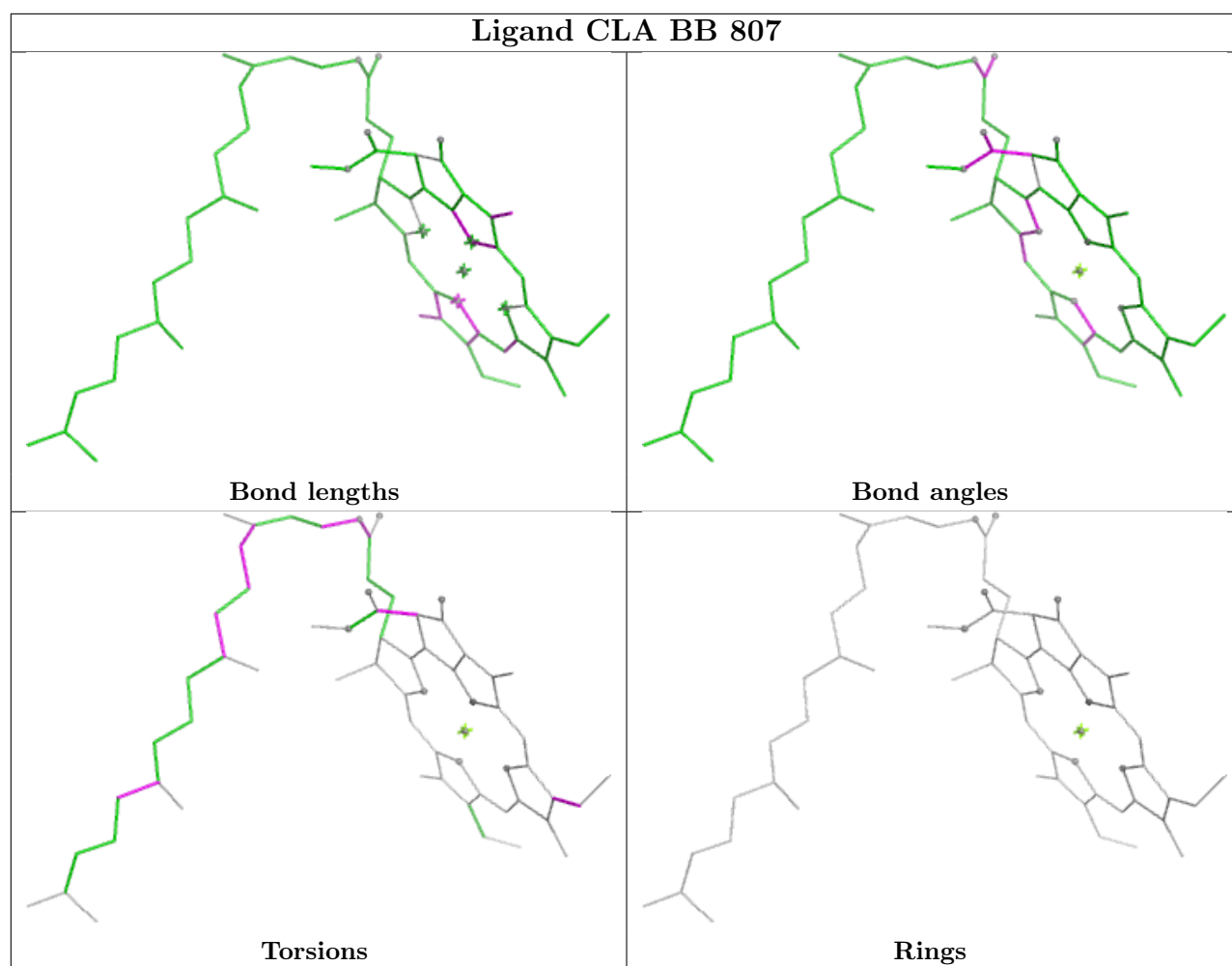


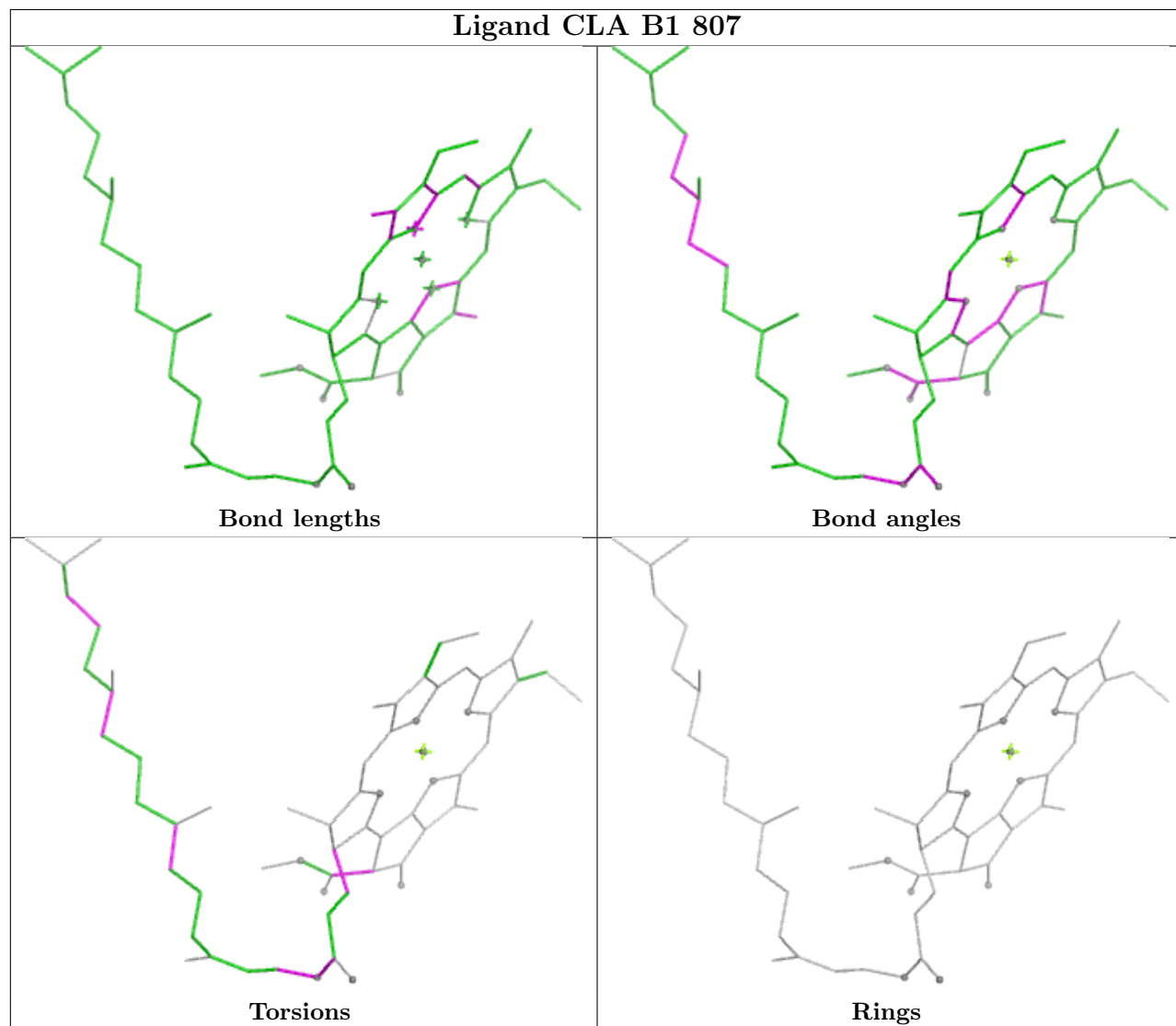
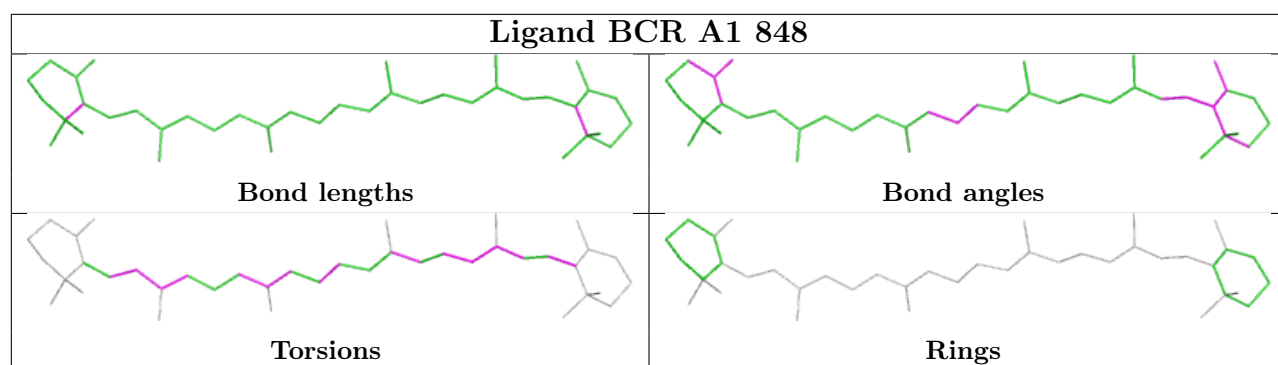


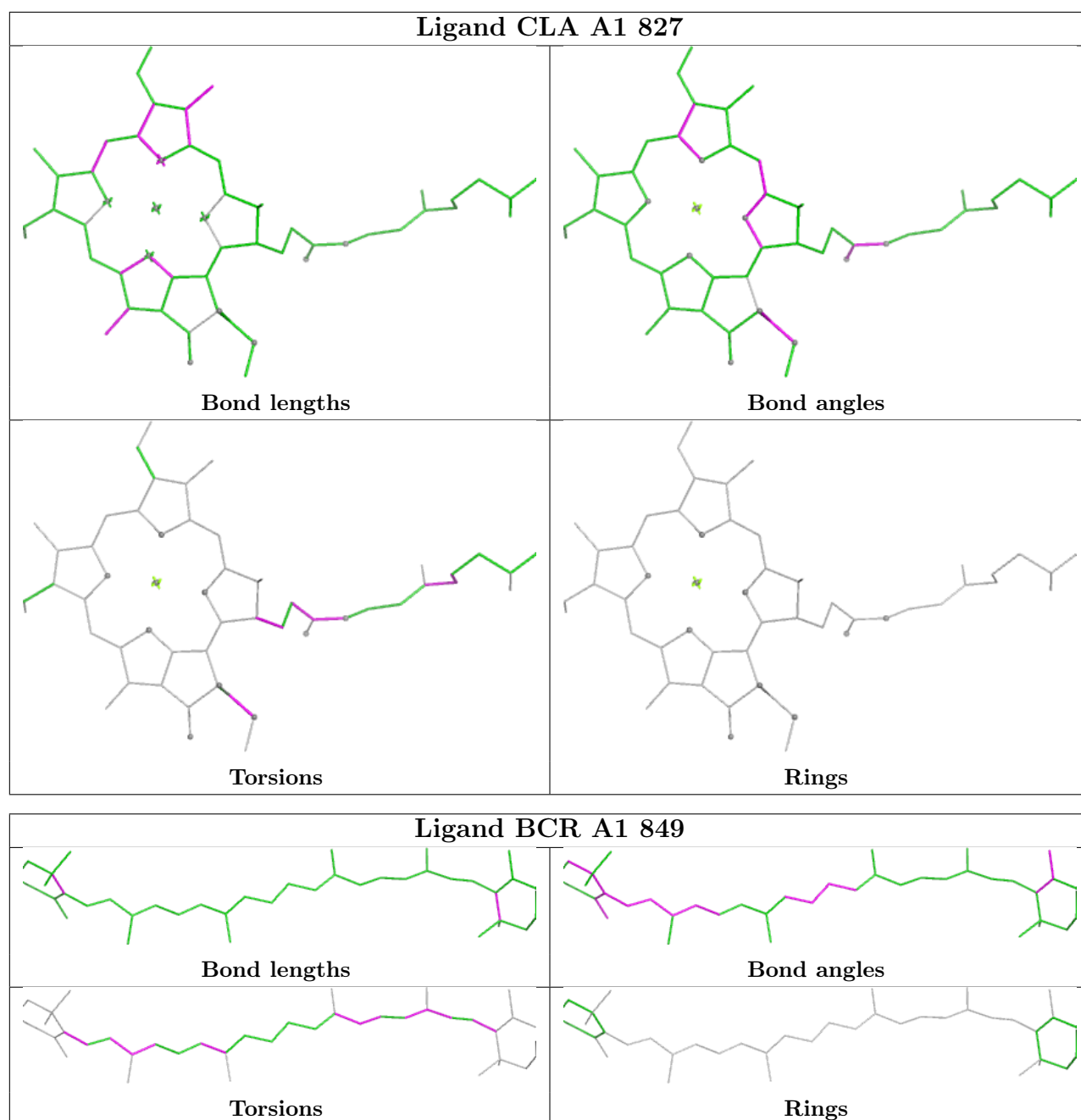
Ligand CLA A1 810

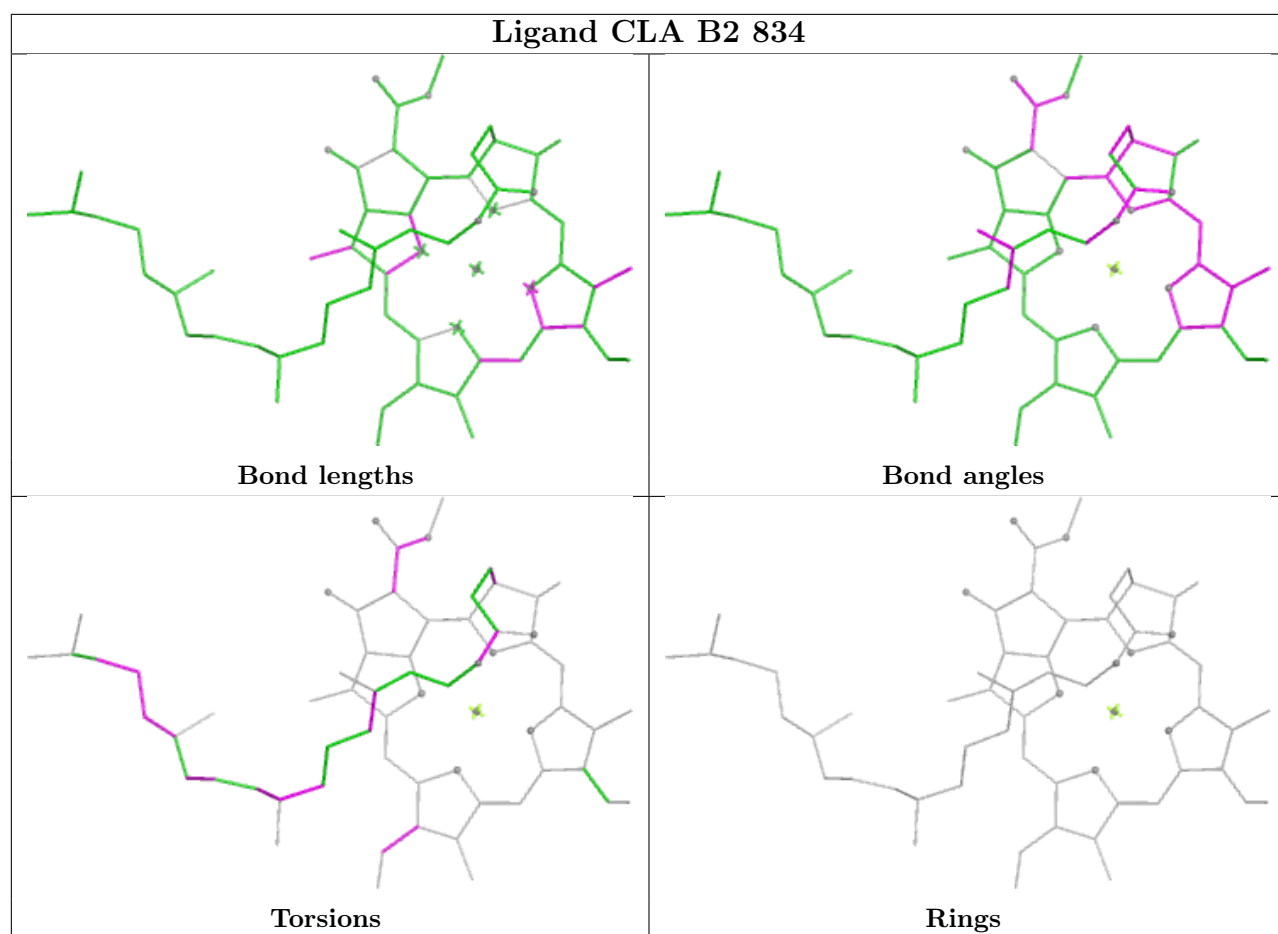




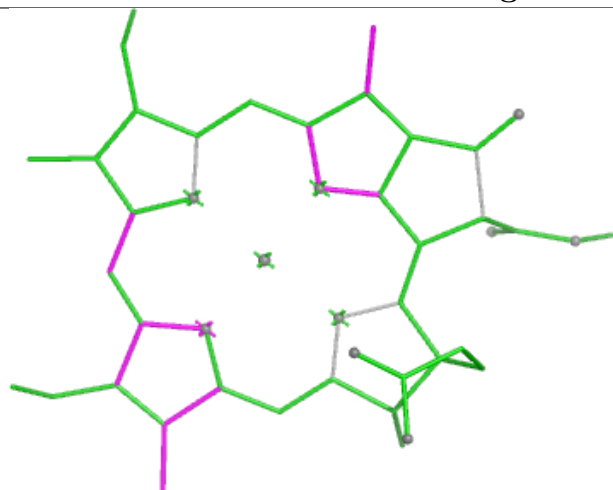




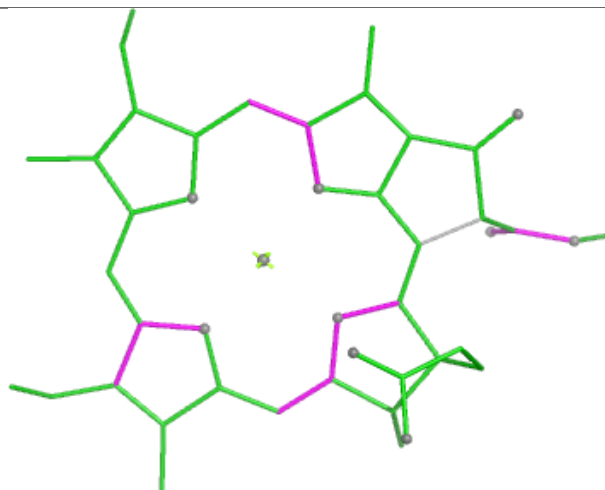




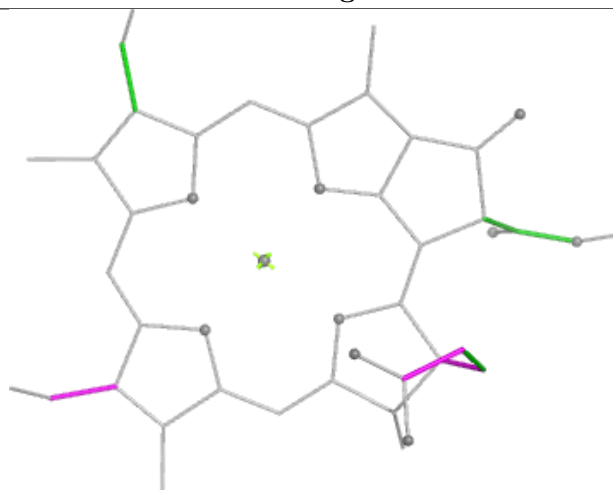
Ligand CLA AA 818



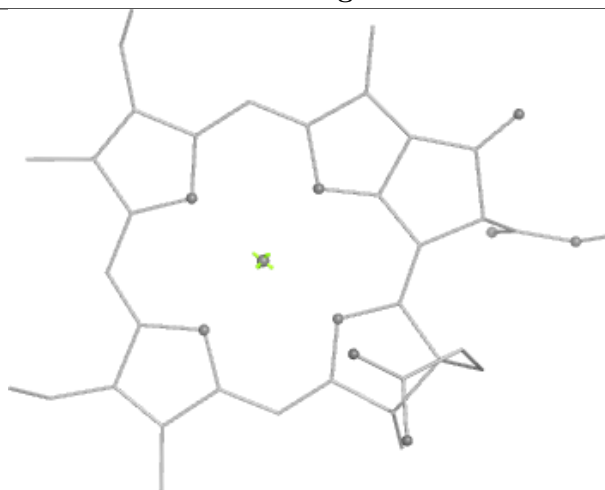
Bond lengths



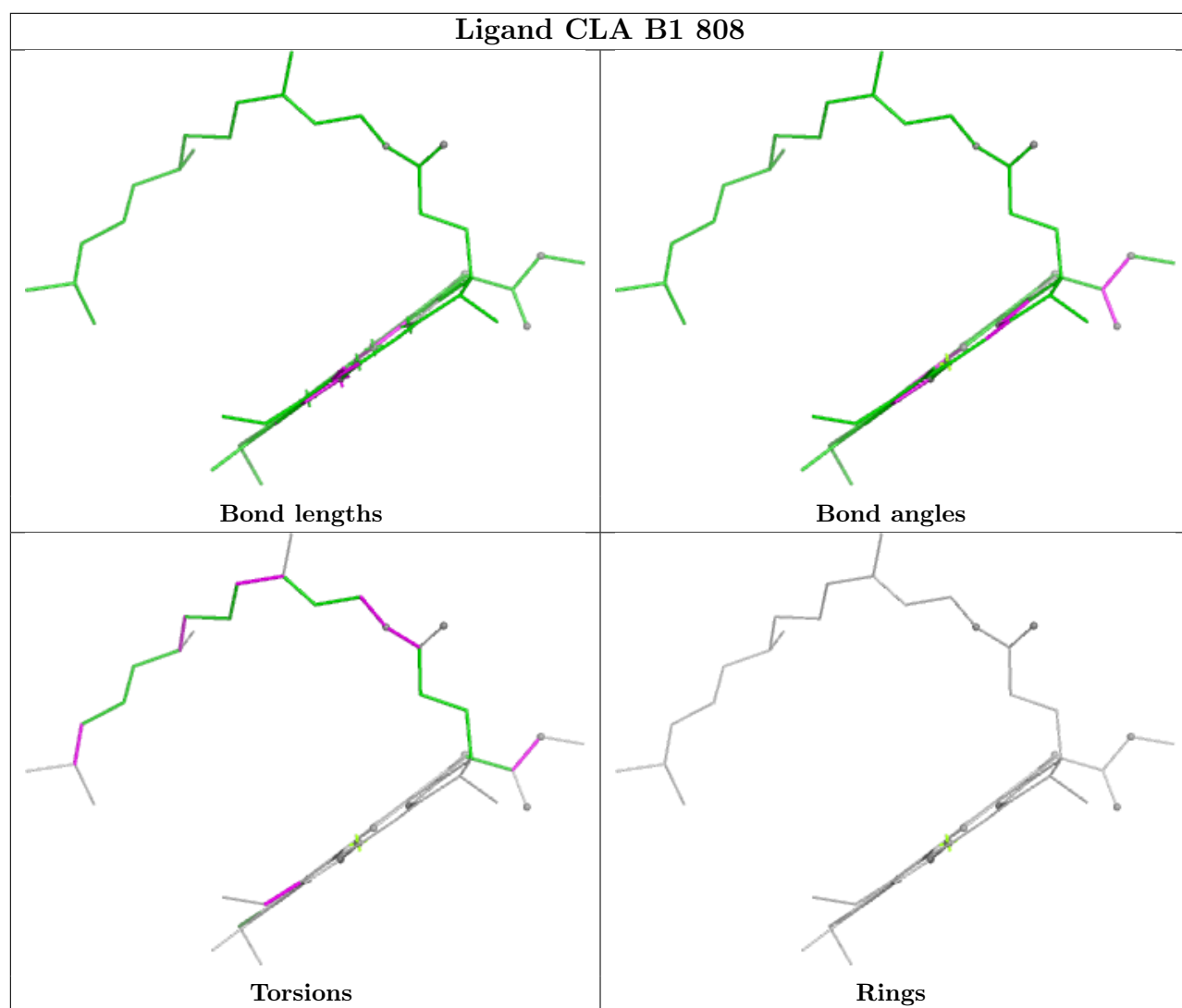
Bond angles

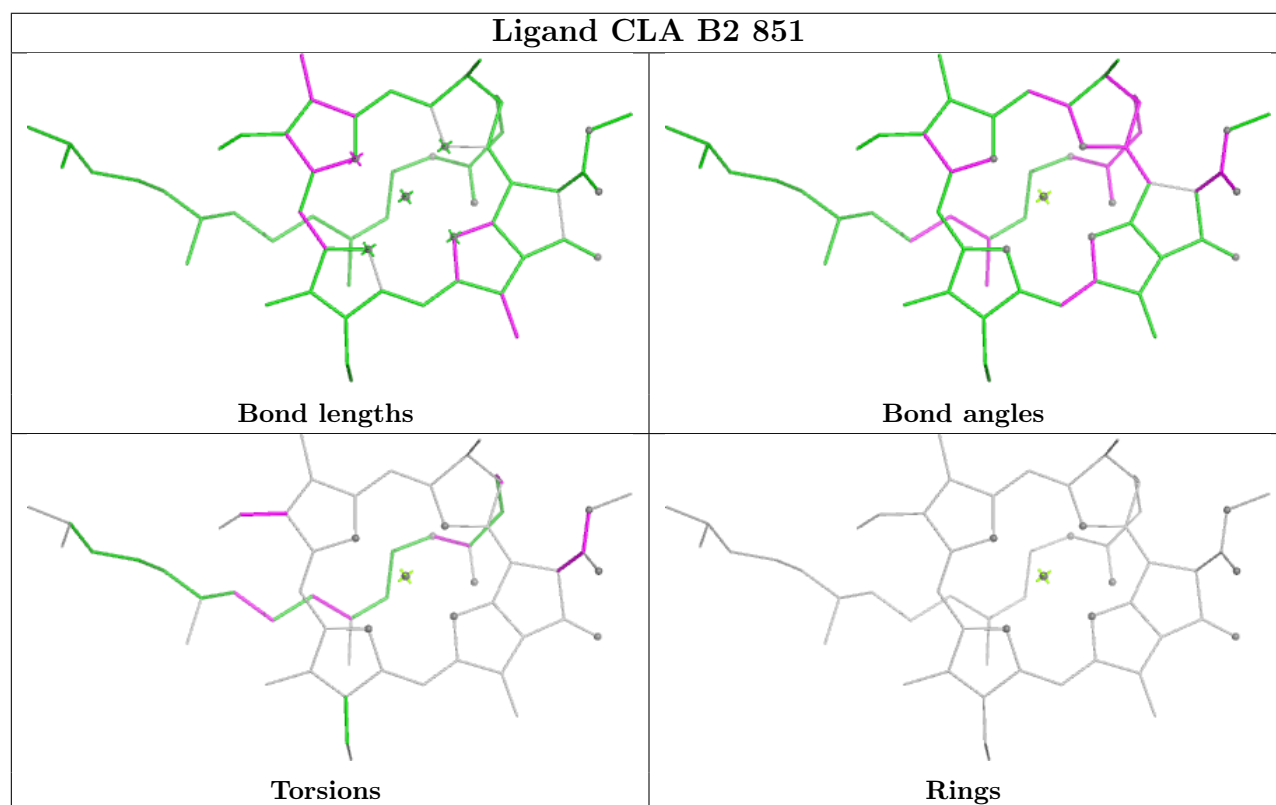
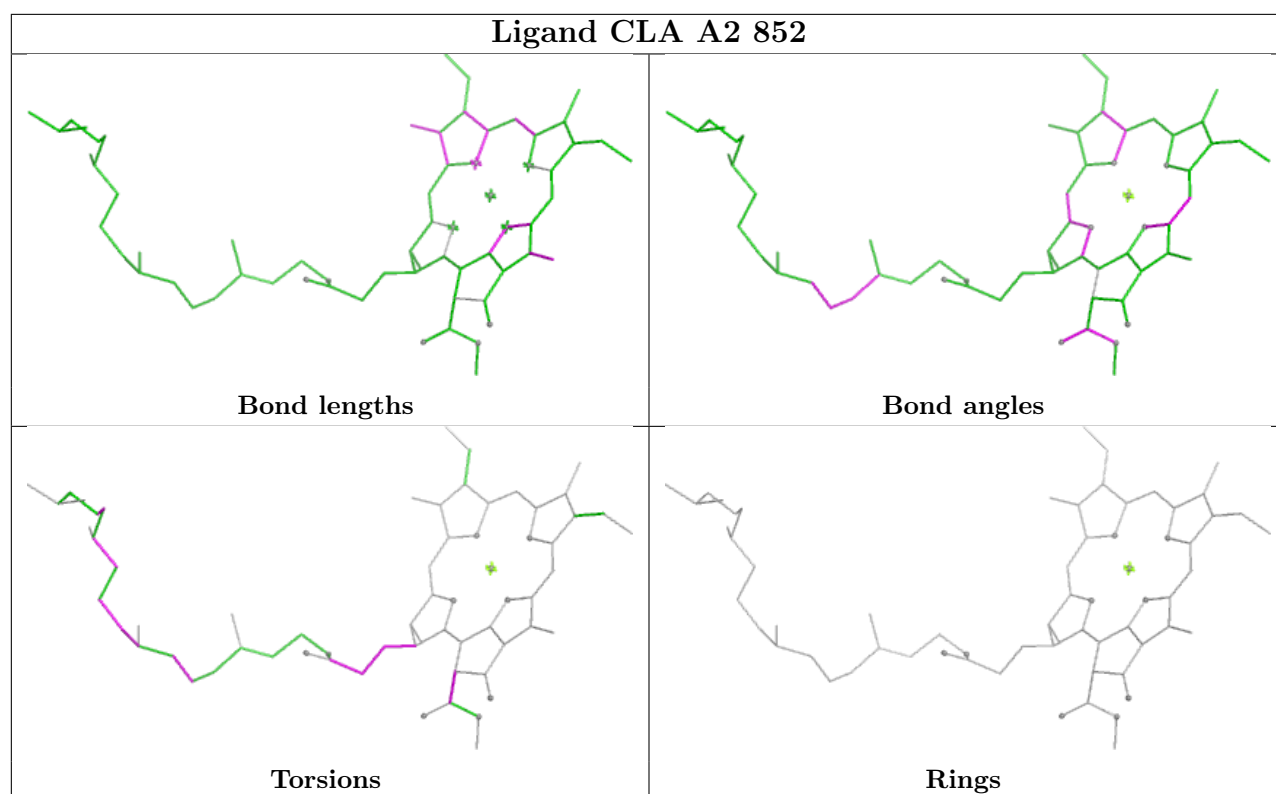


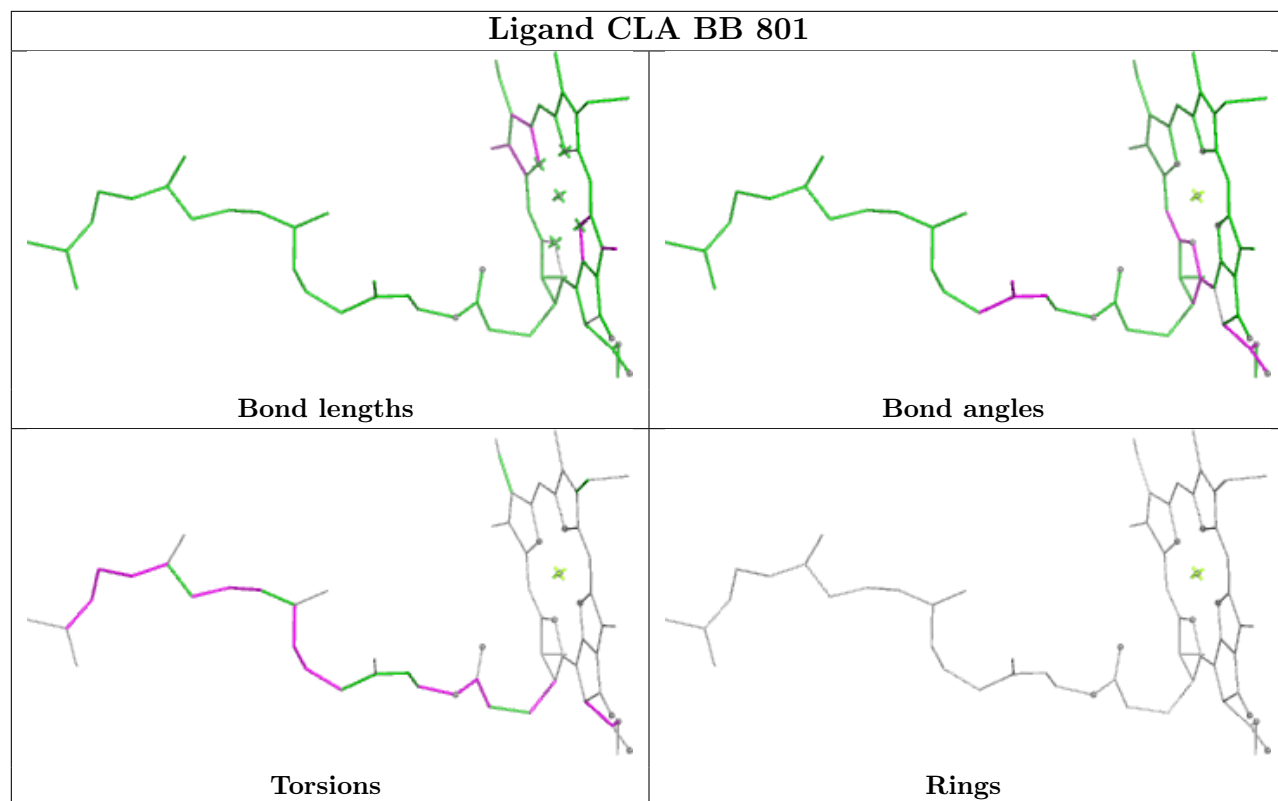
Torsions



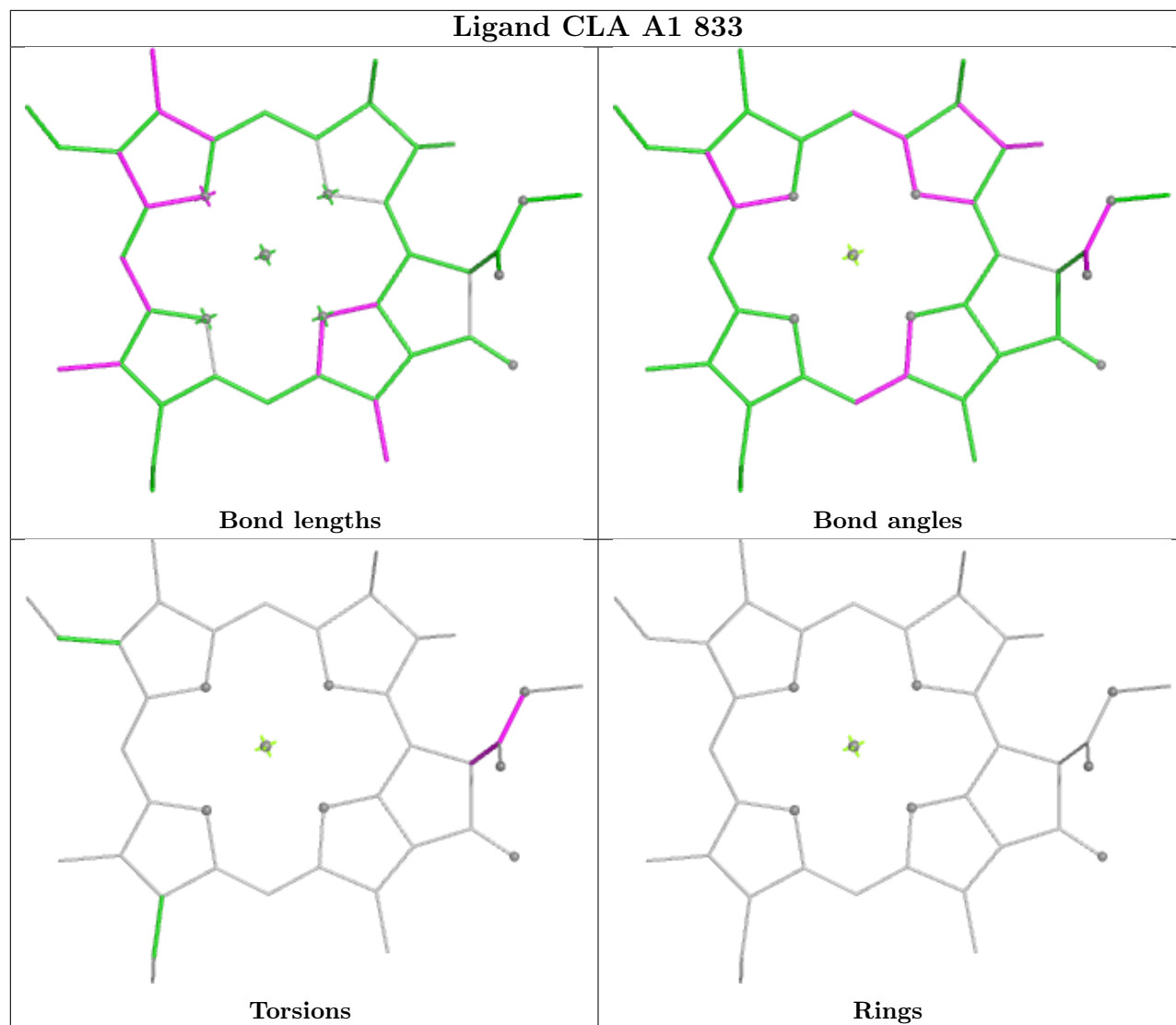
Rings

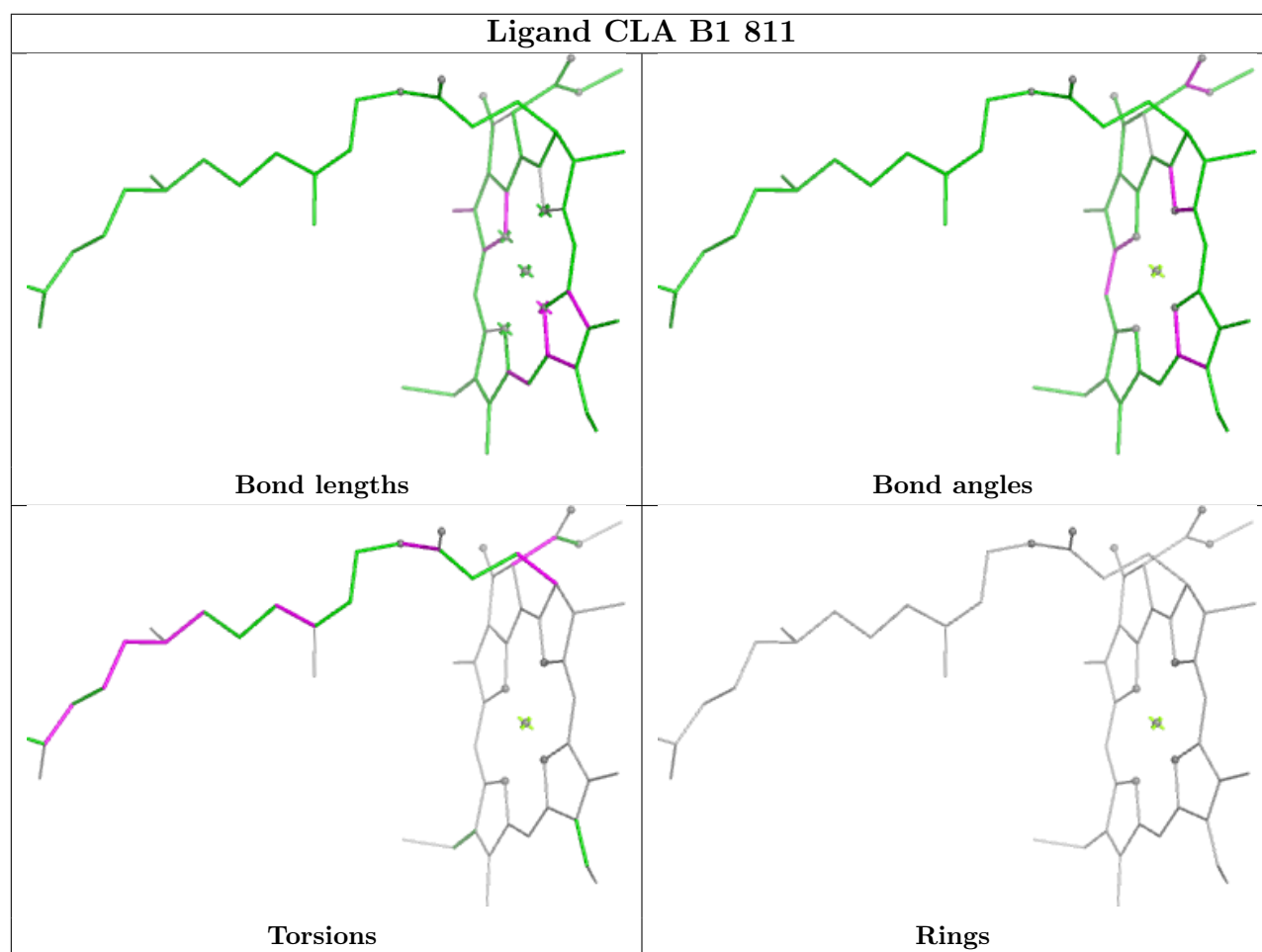
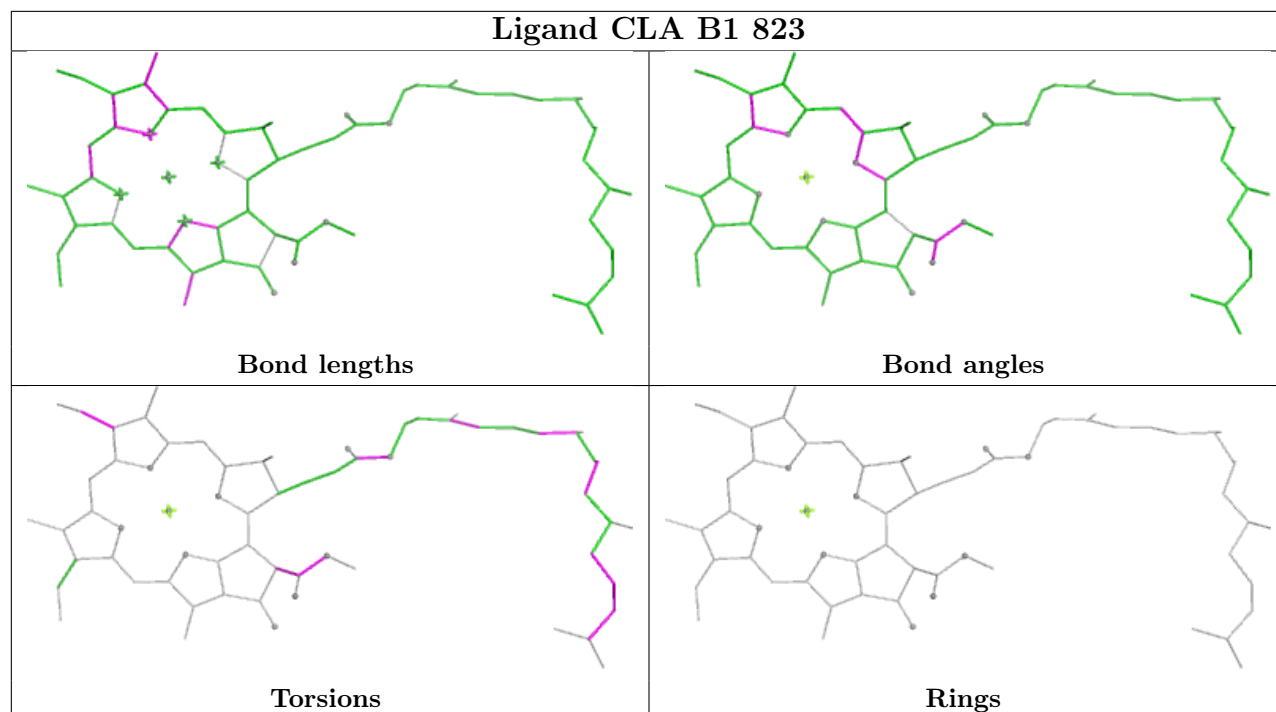


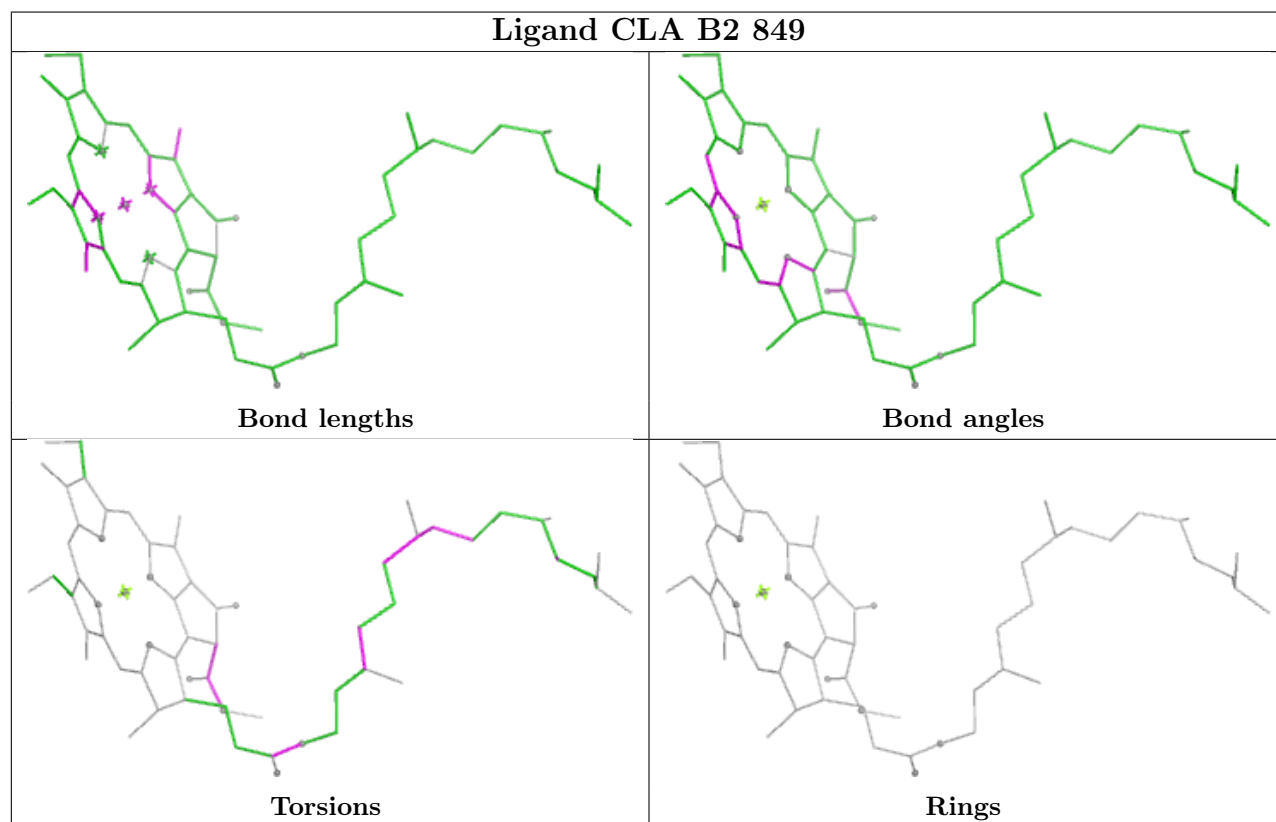
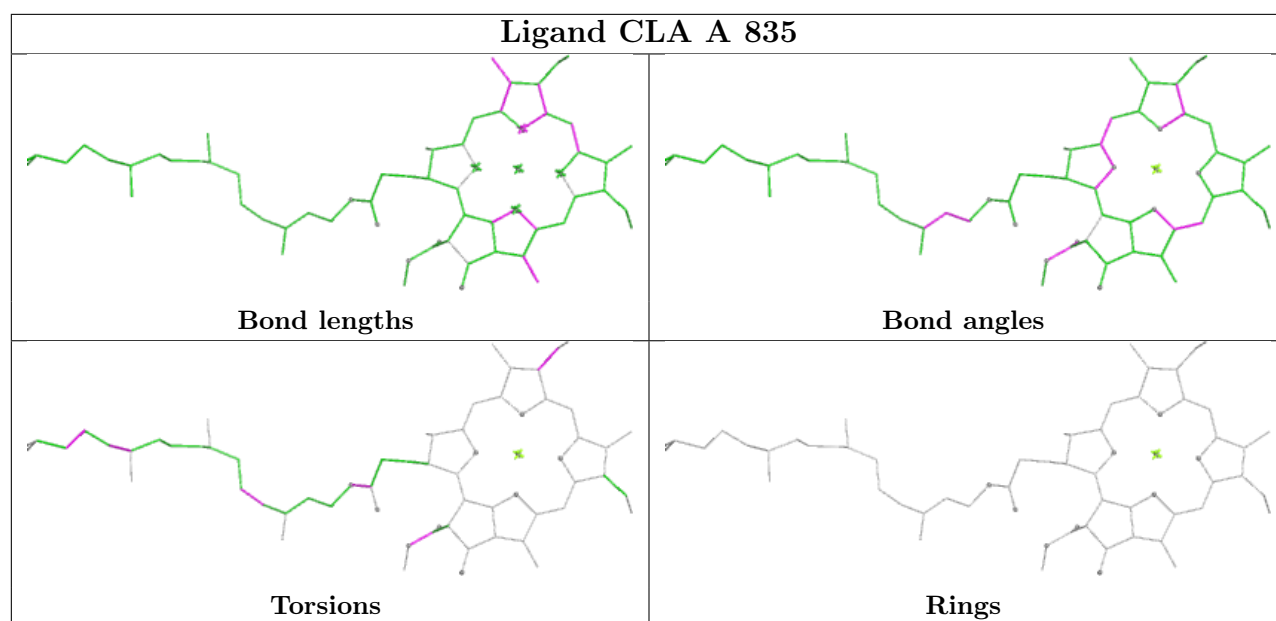


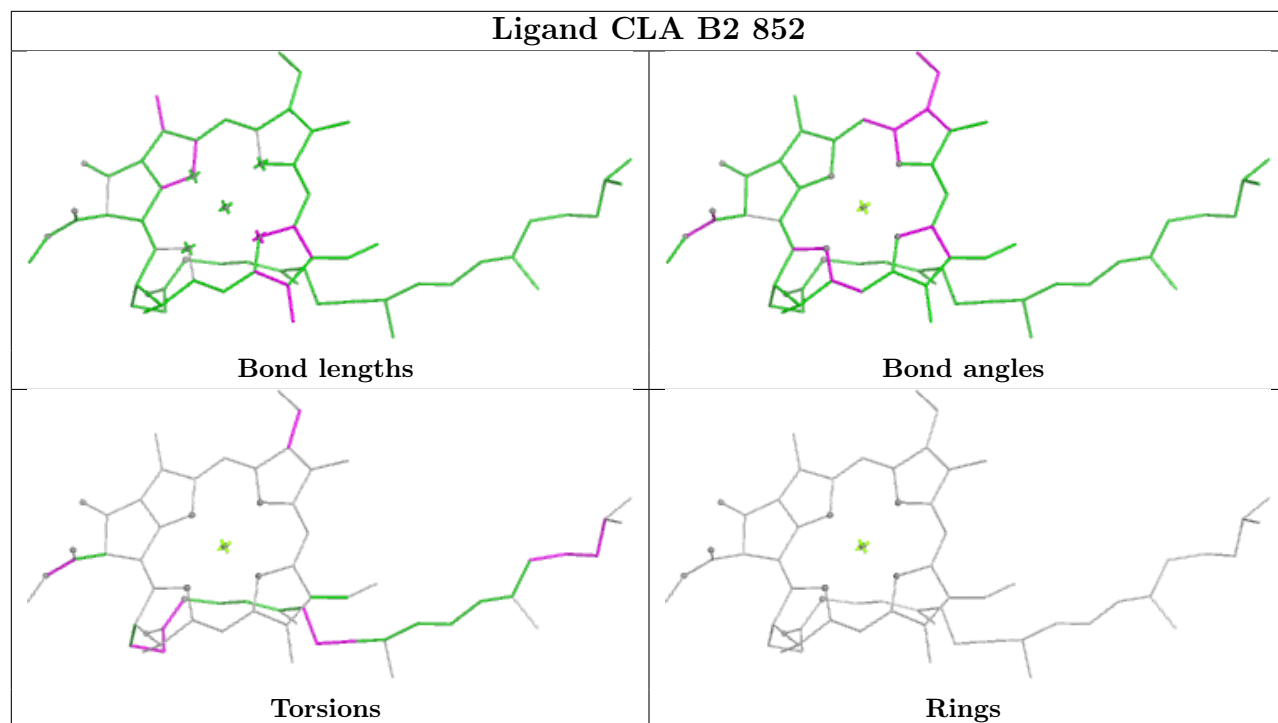
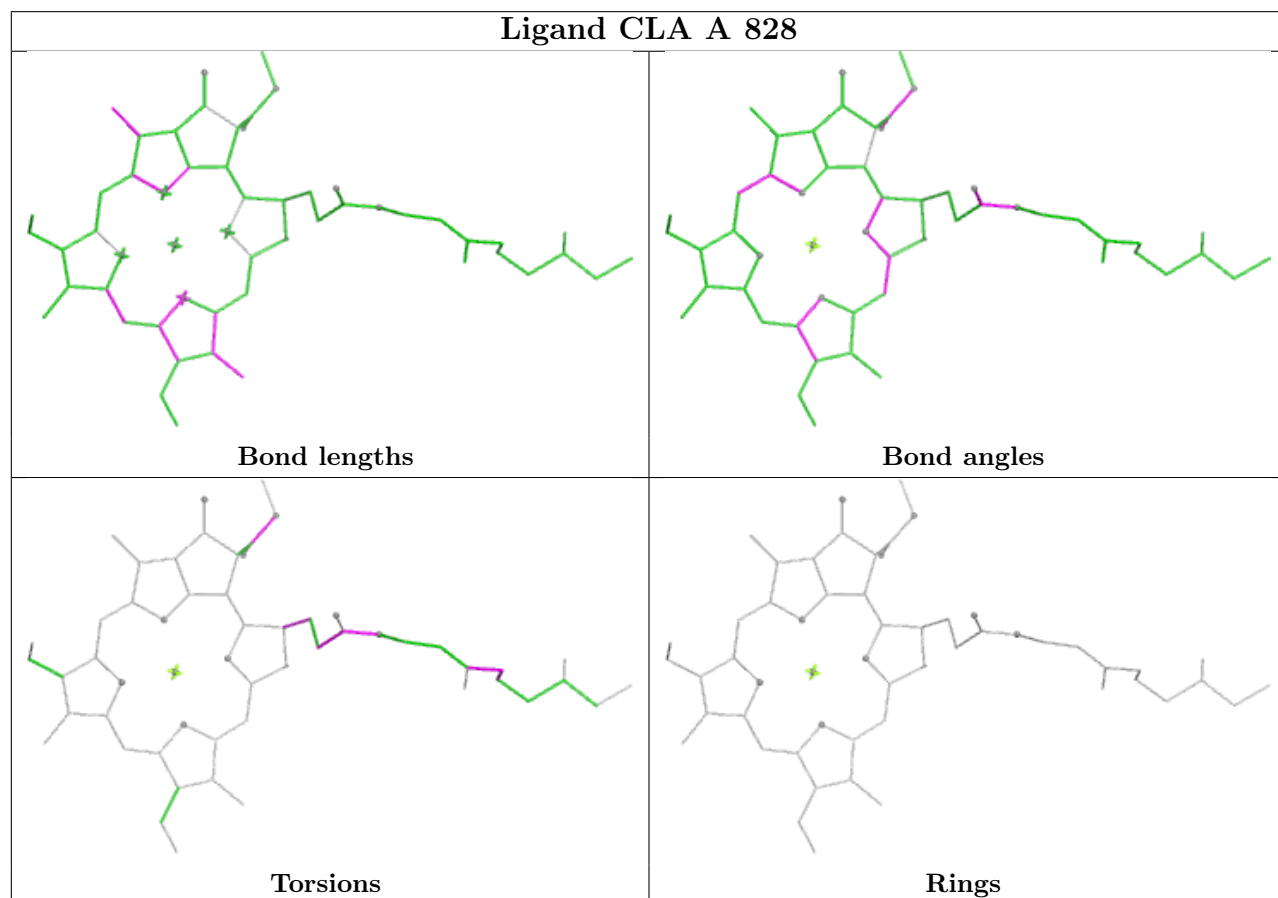


Ligand CLA A1 833

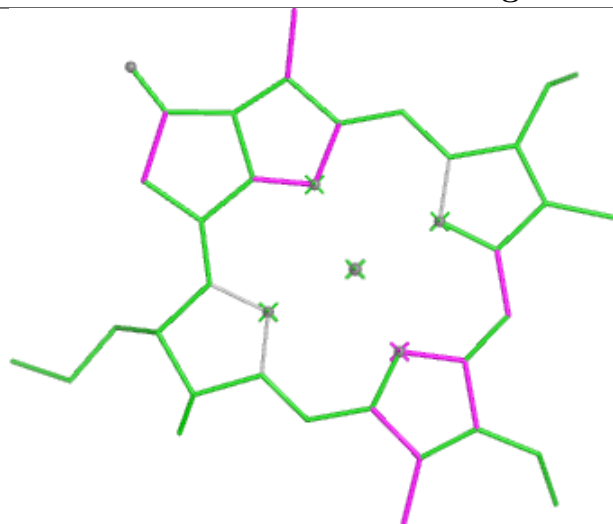




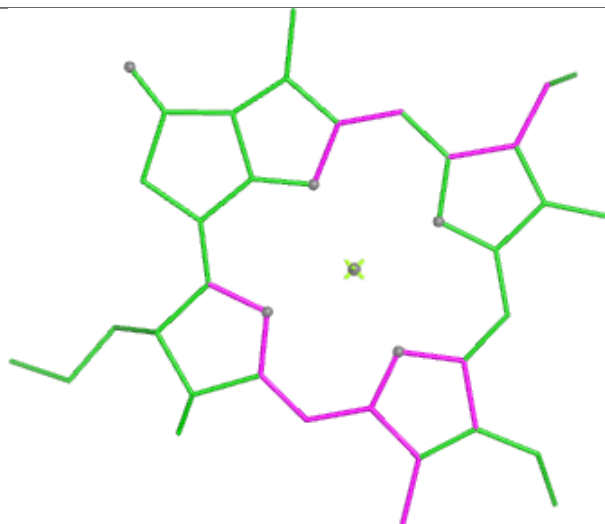


Ligand CLA B2 852**Ligand CLA A 828**

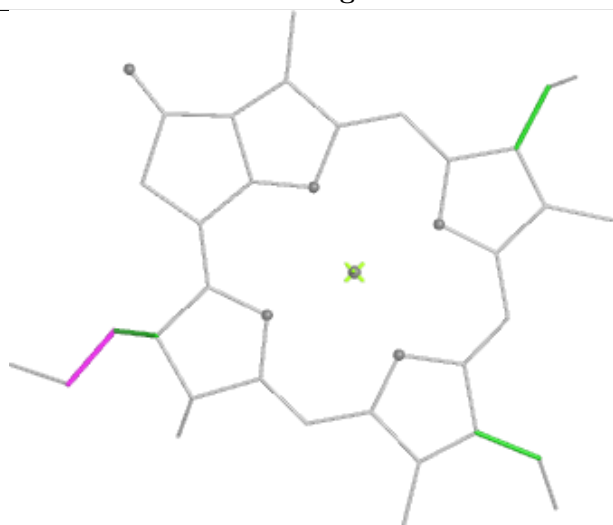
Ligand CLA BB 845



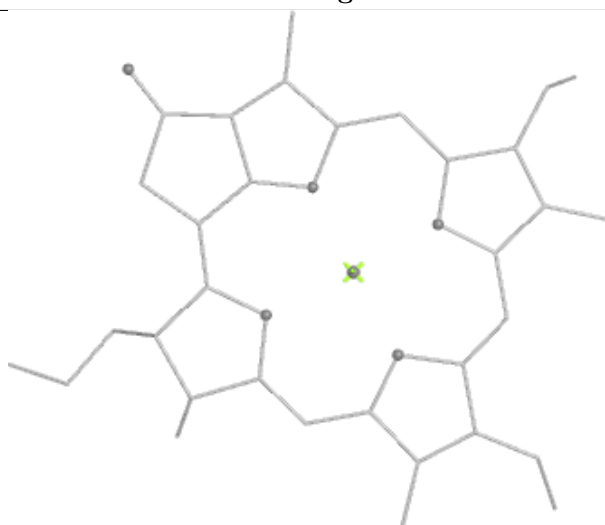
Bond lengths



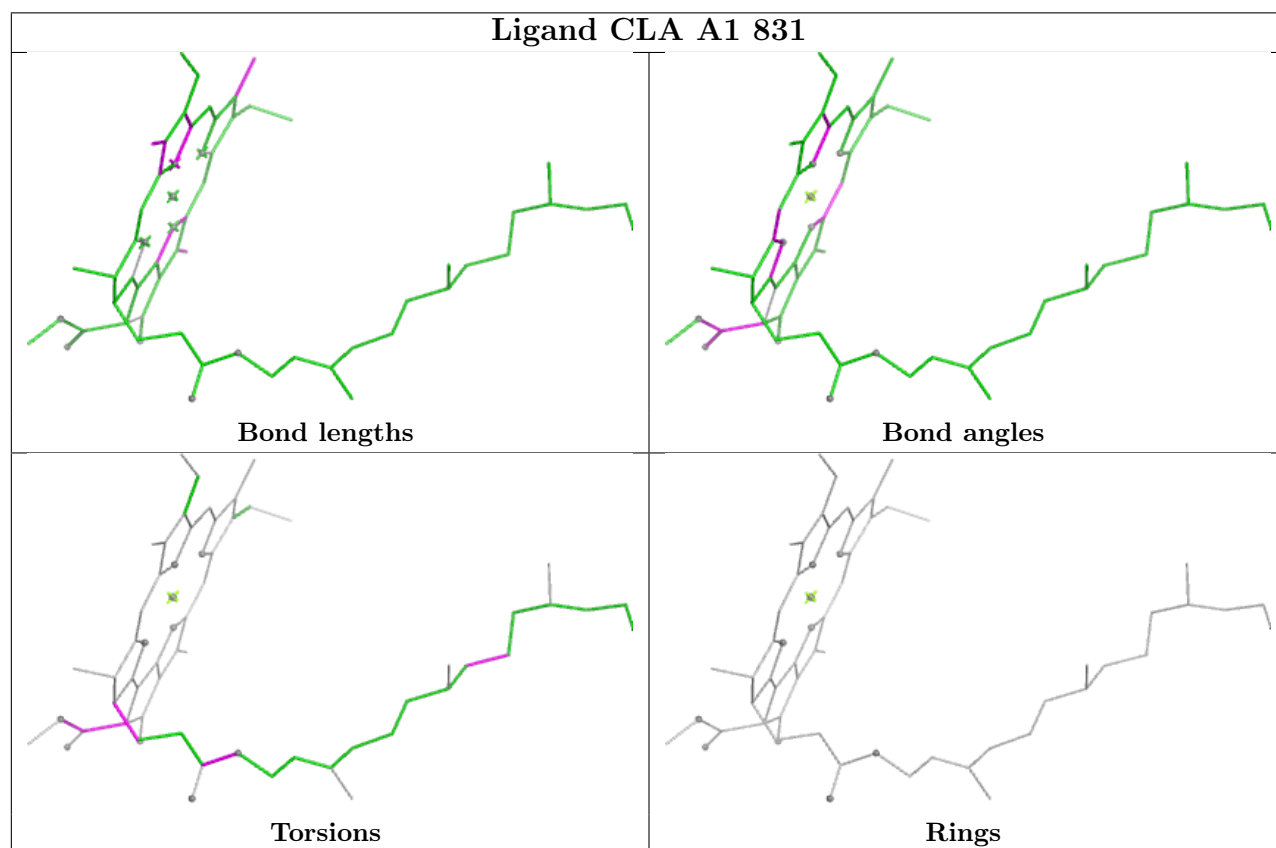
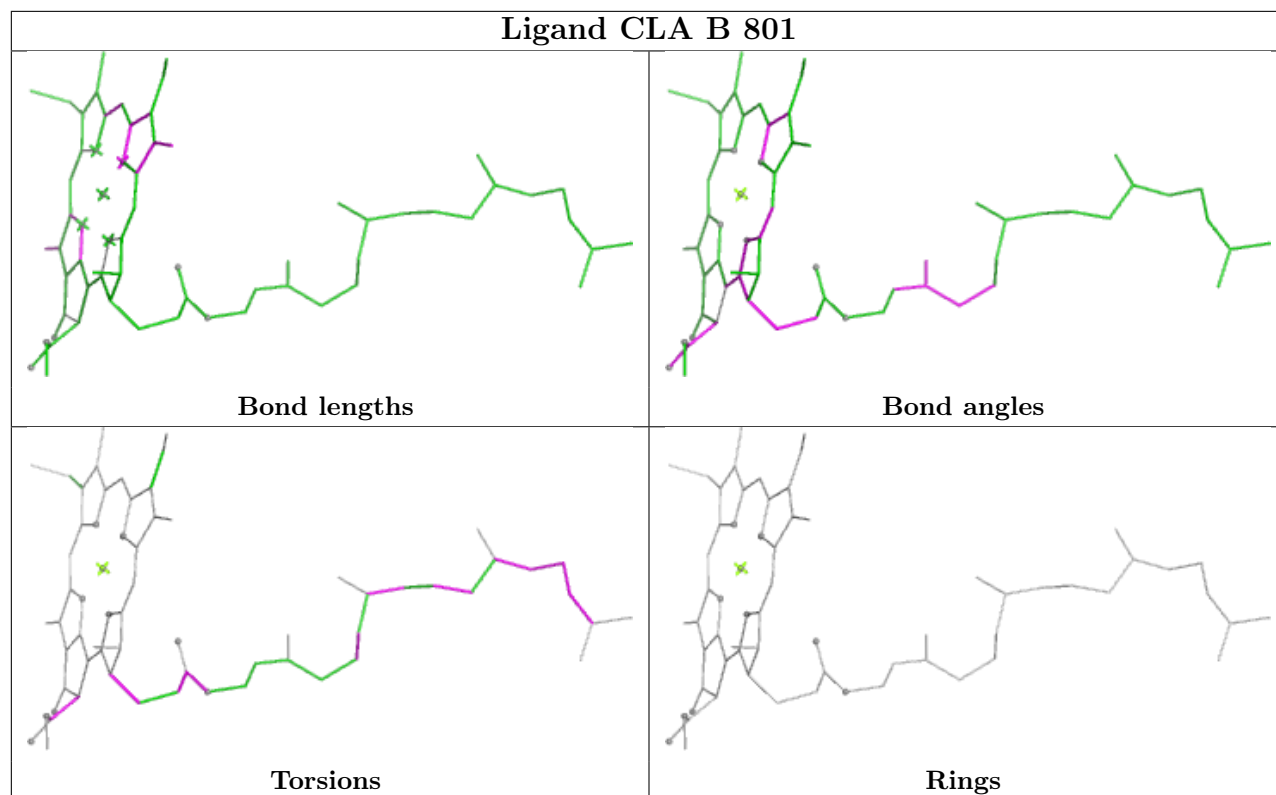
Bond angles

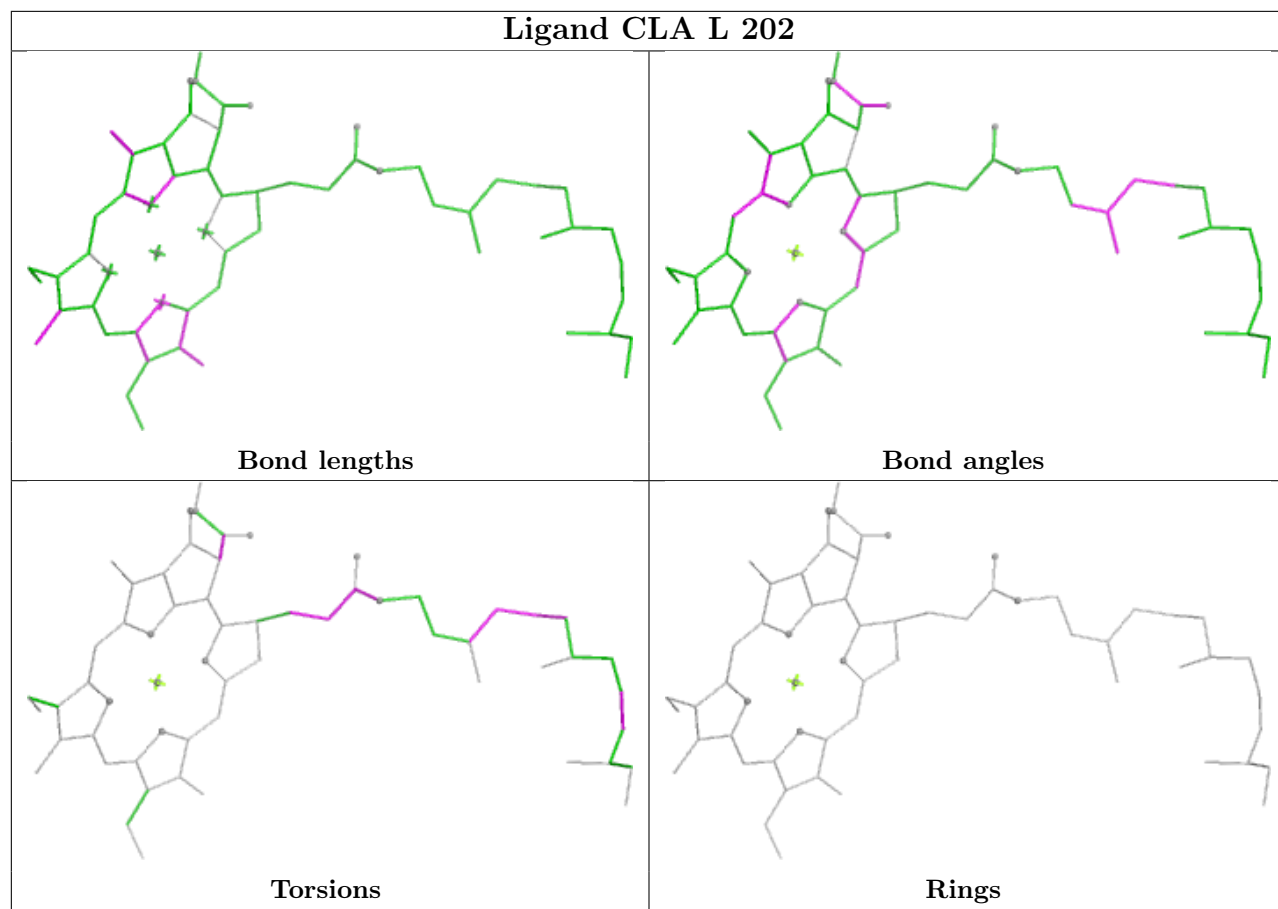


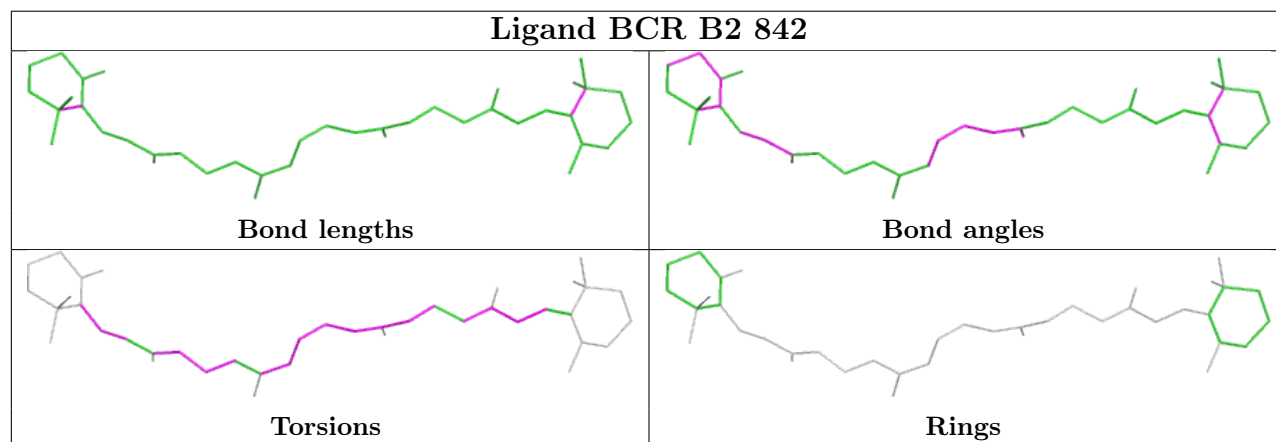
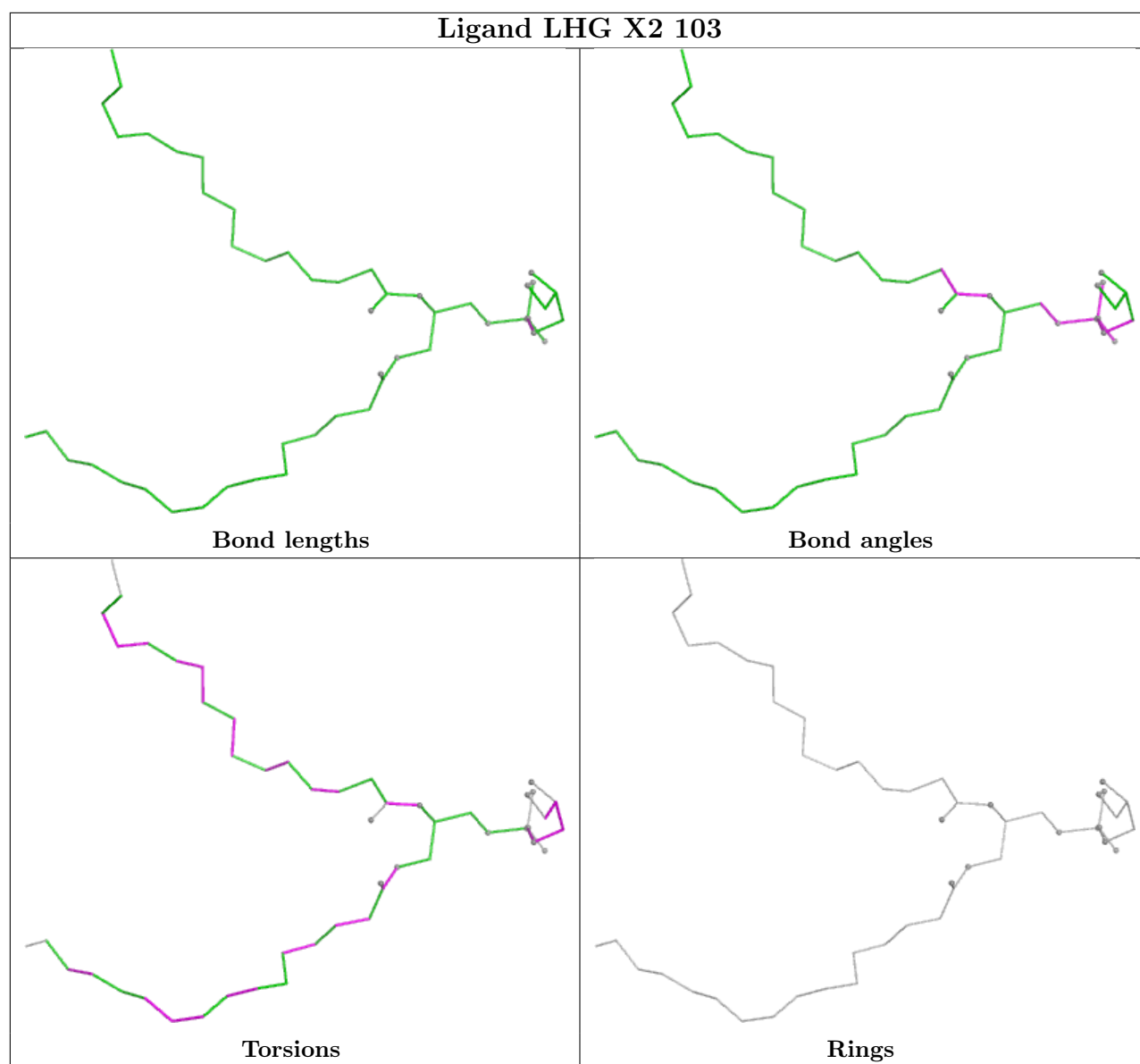
Torsions



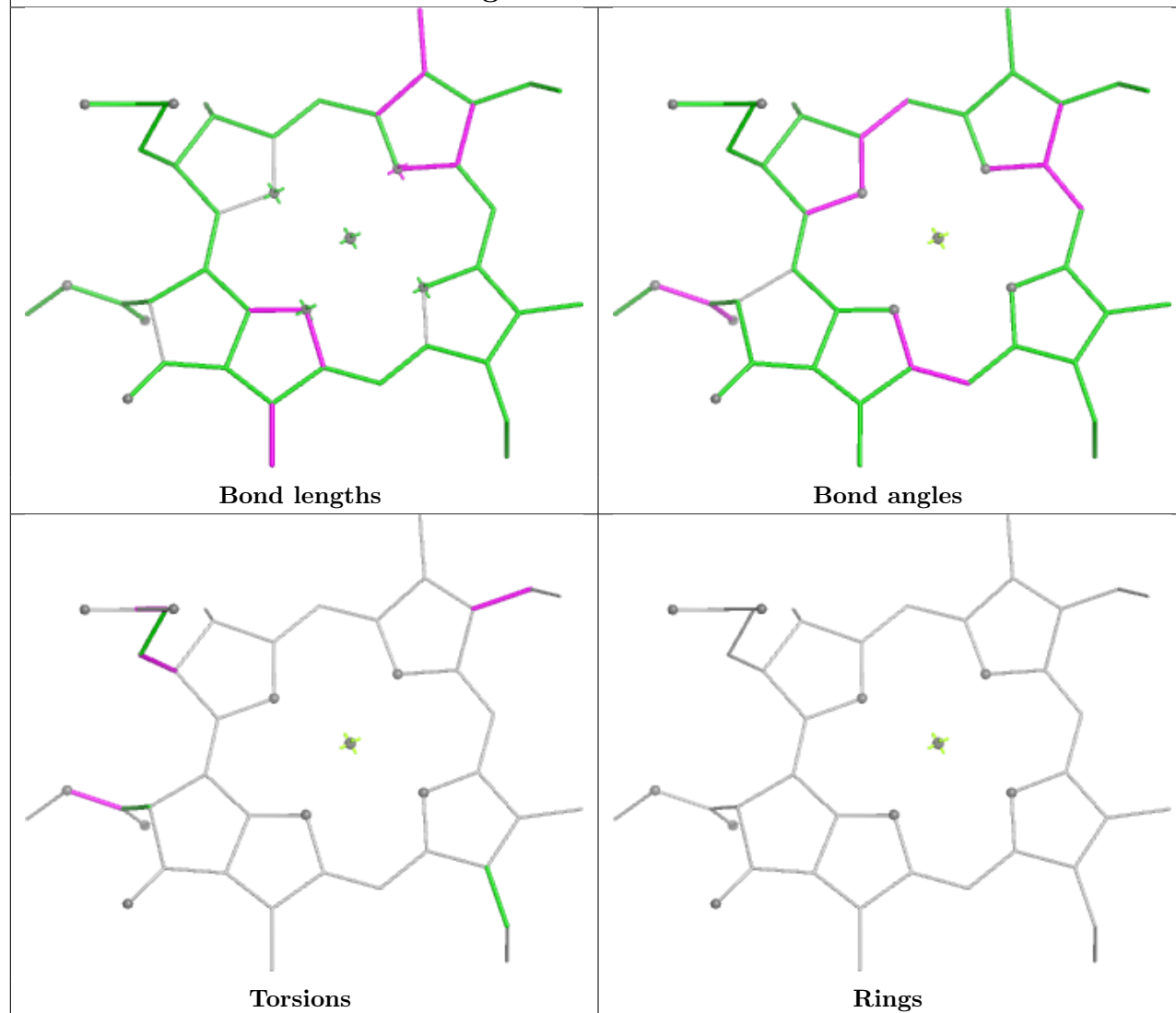
Rings



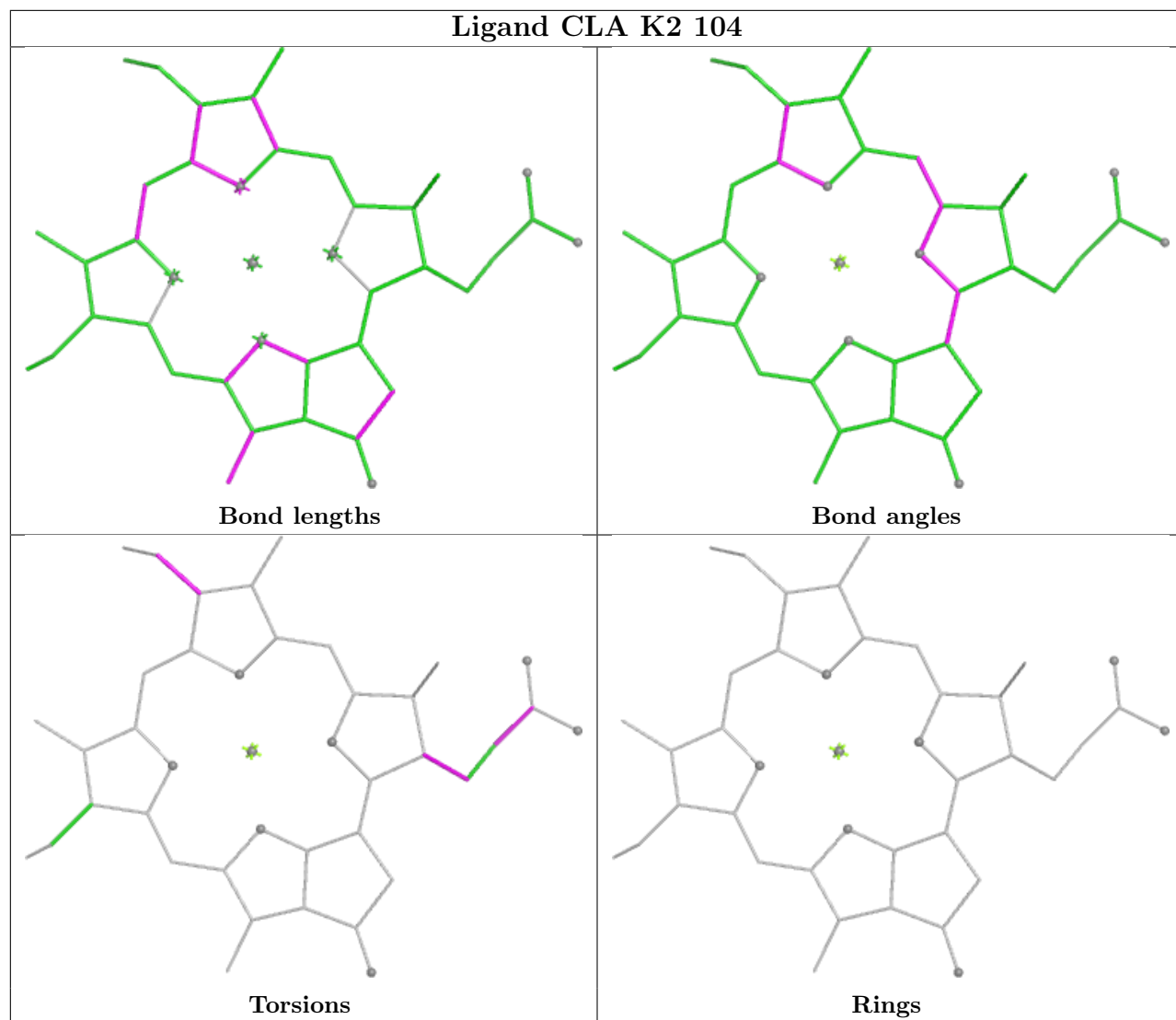


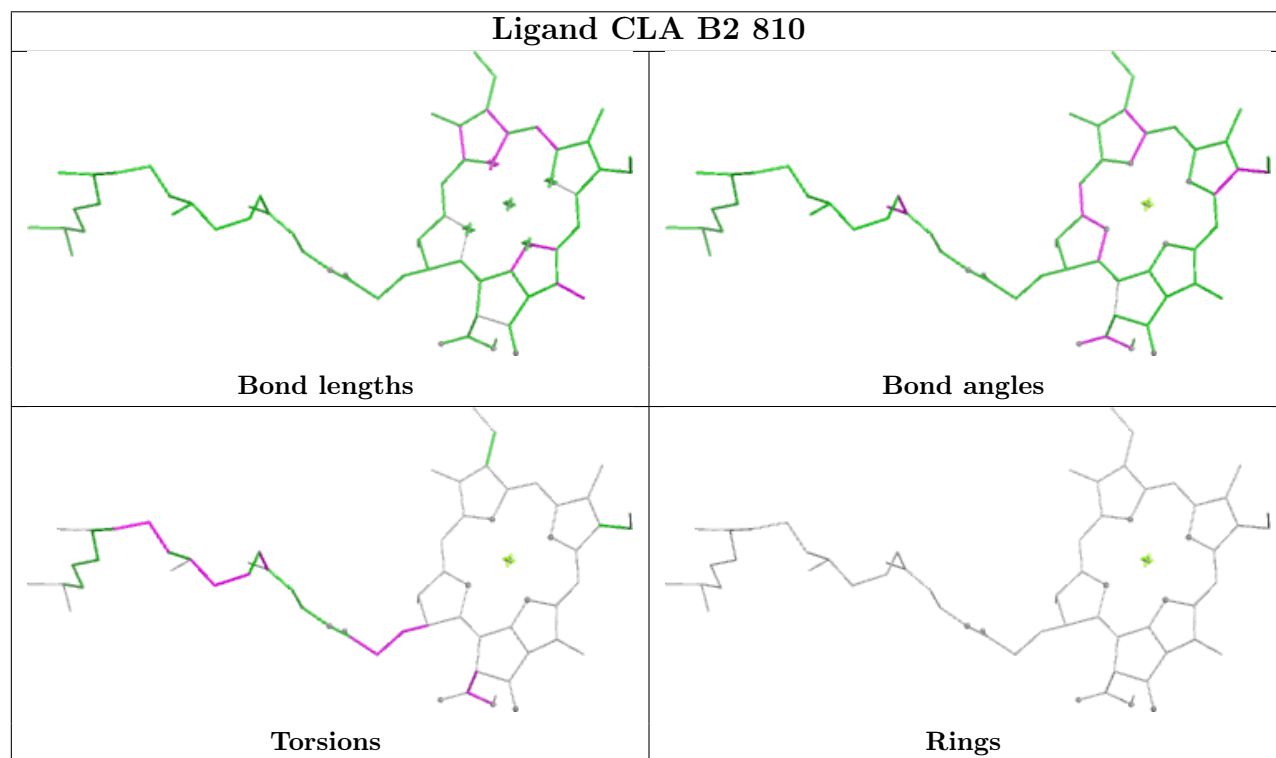
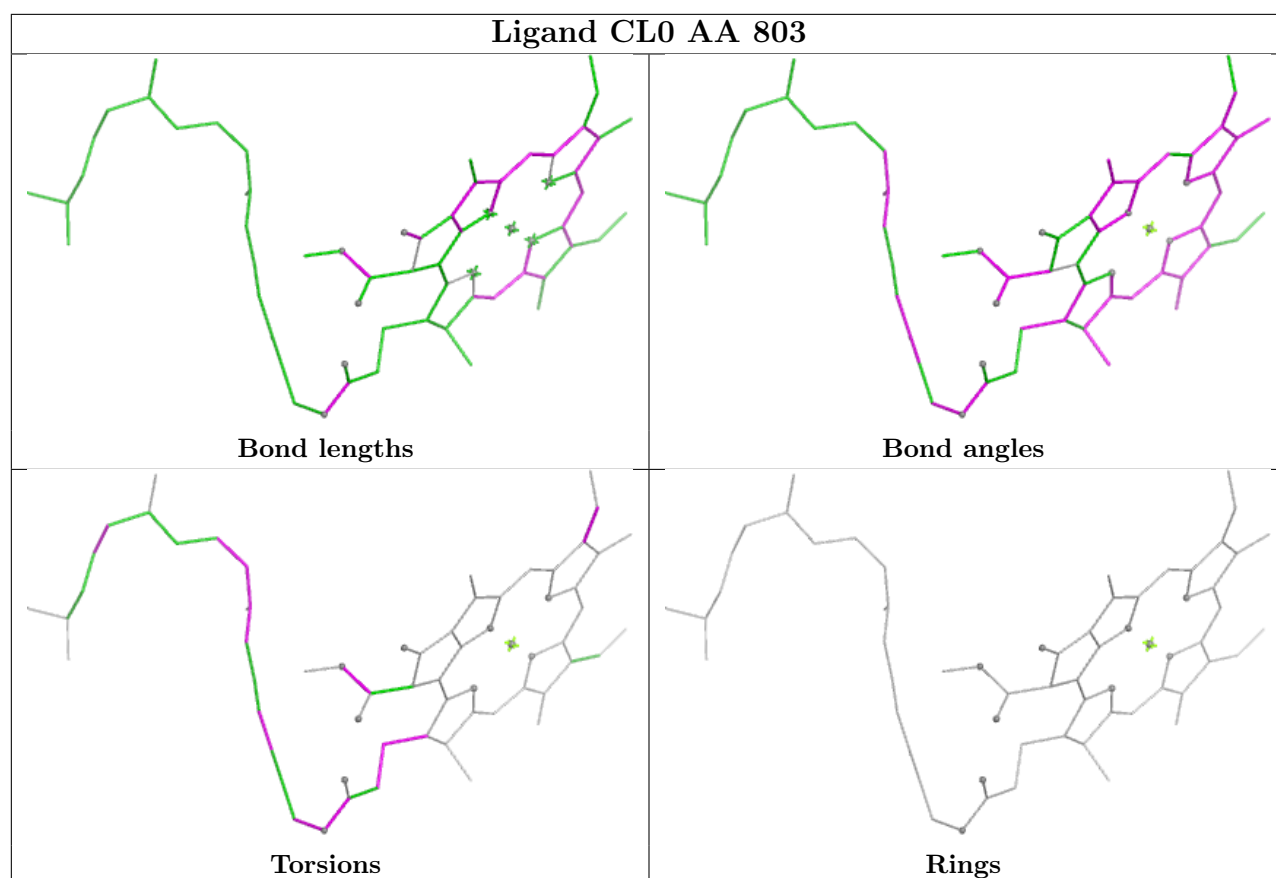


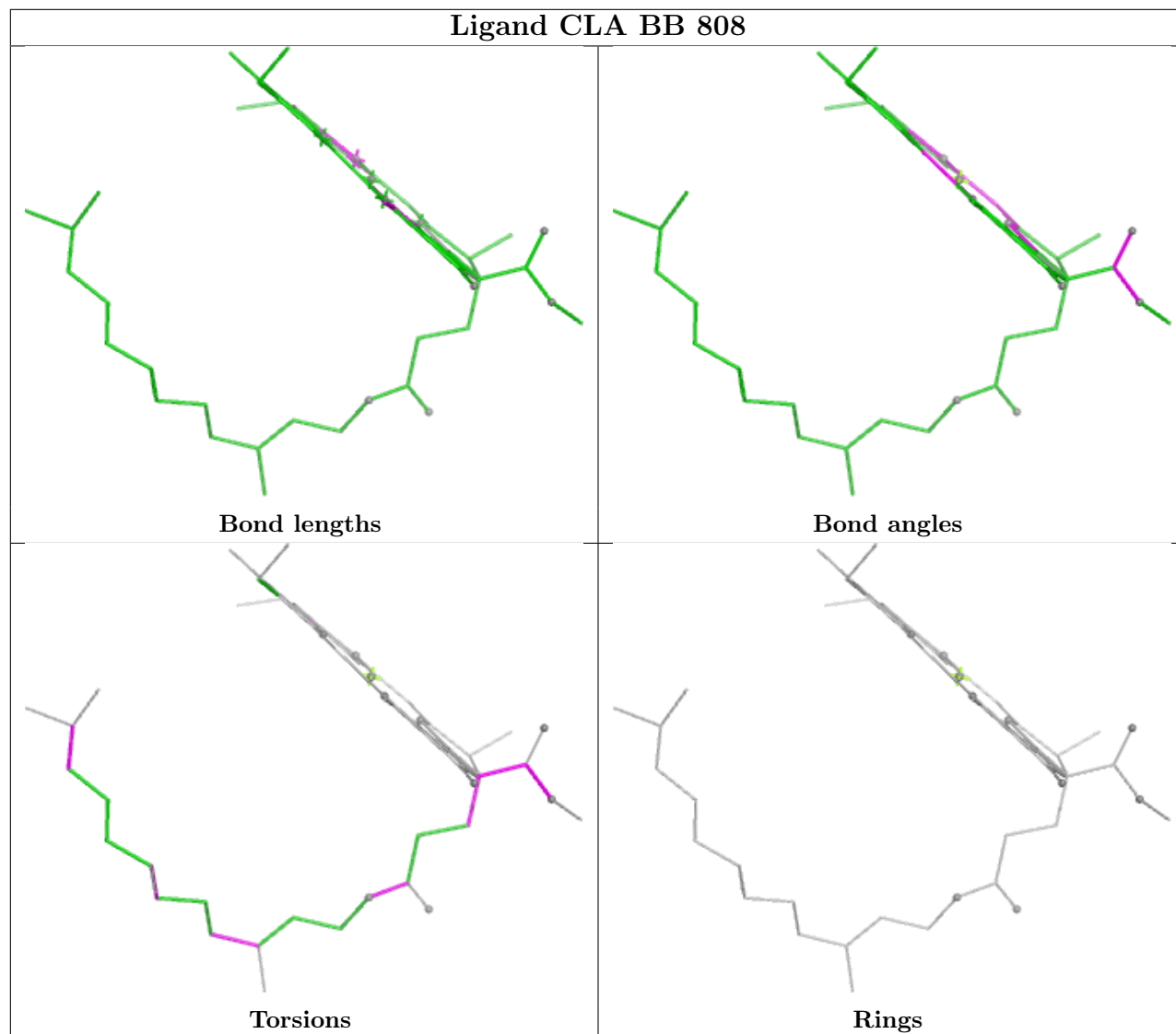
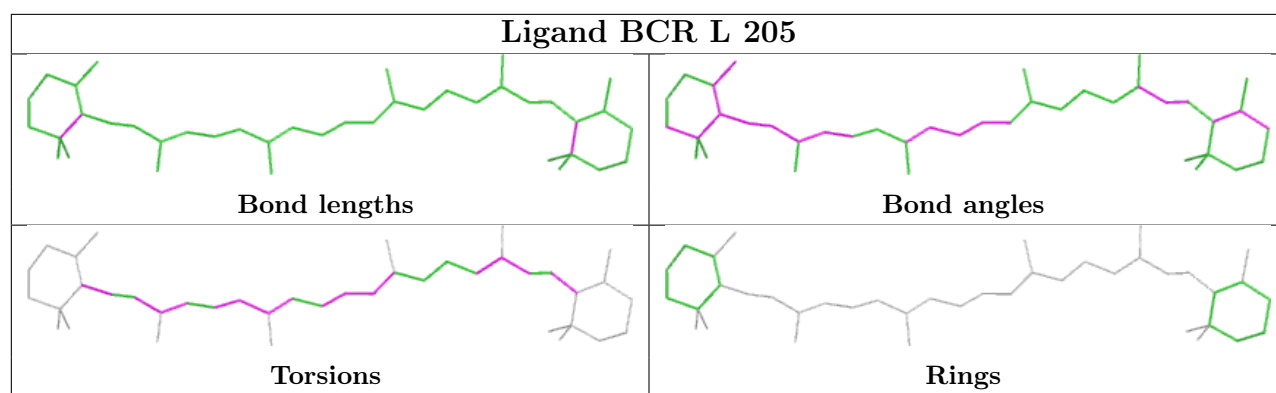
Ligand CLA B1 831



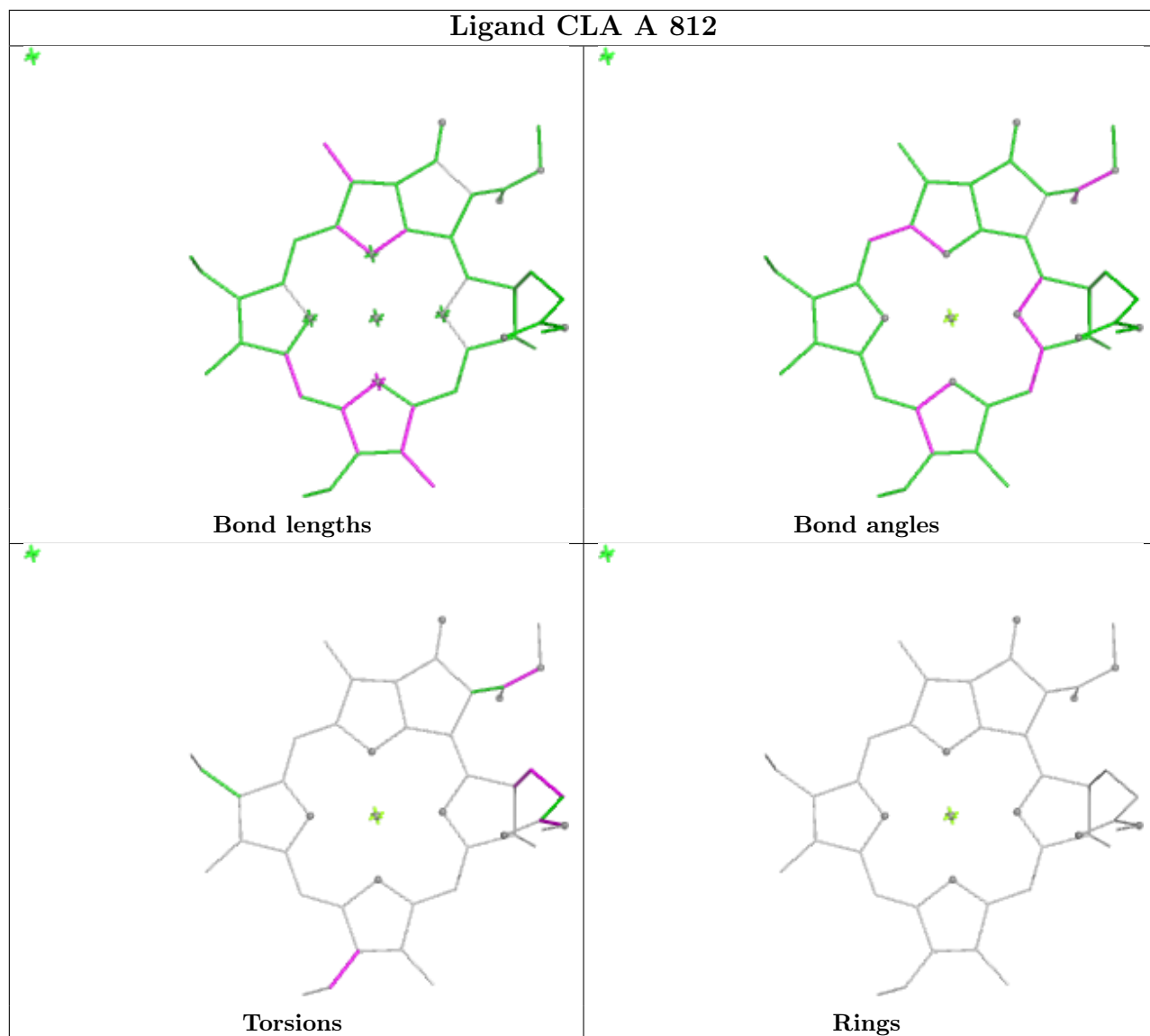
Ligand CLA K2 104



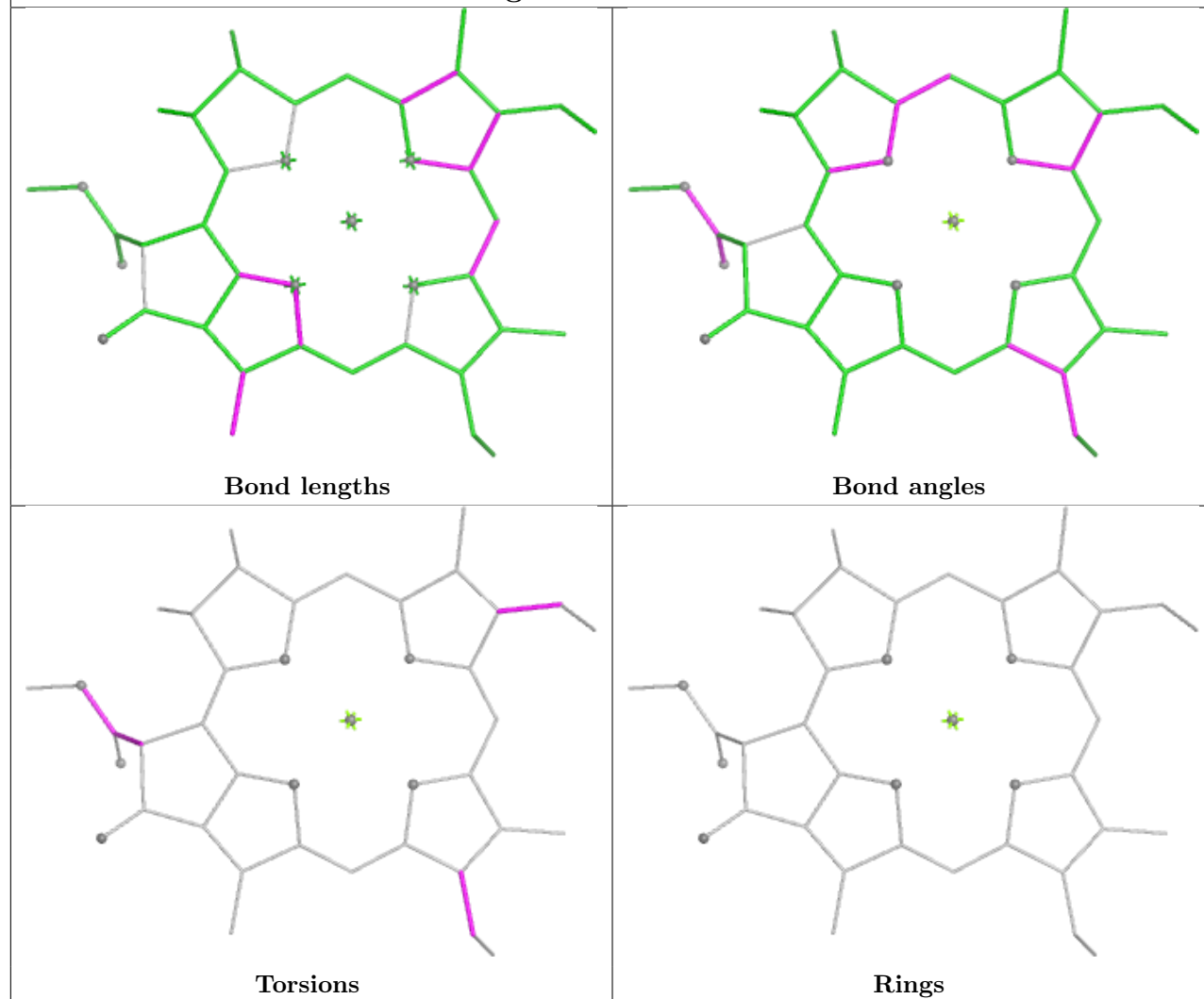




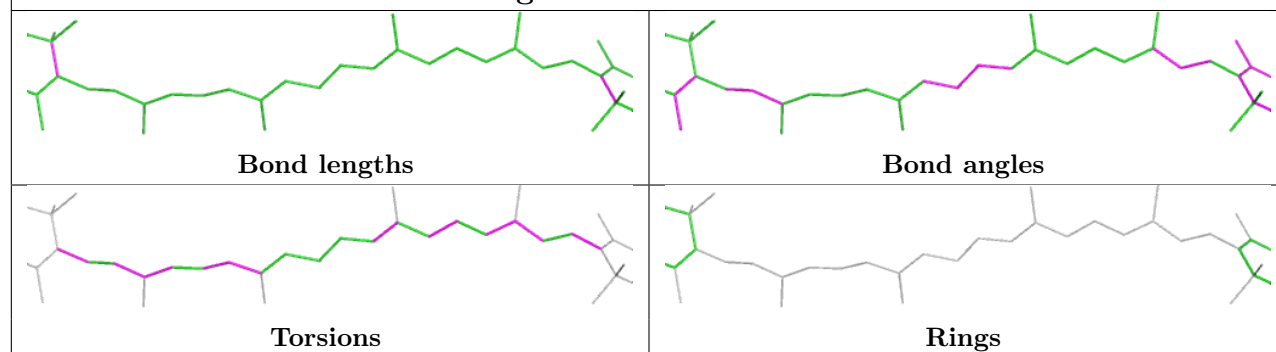
Ligand CLA A 812

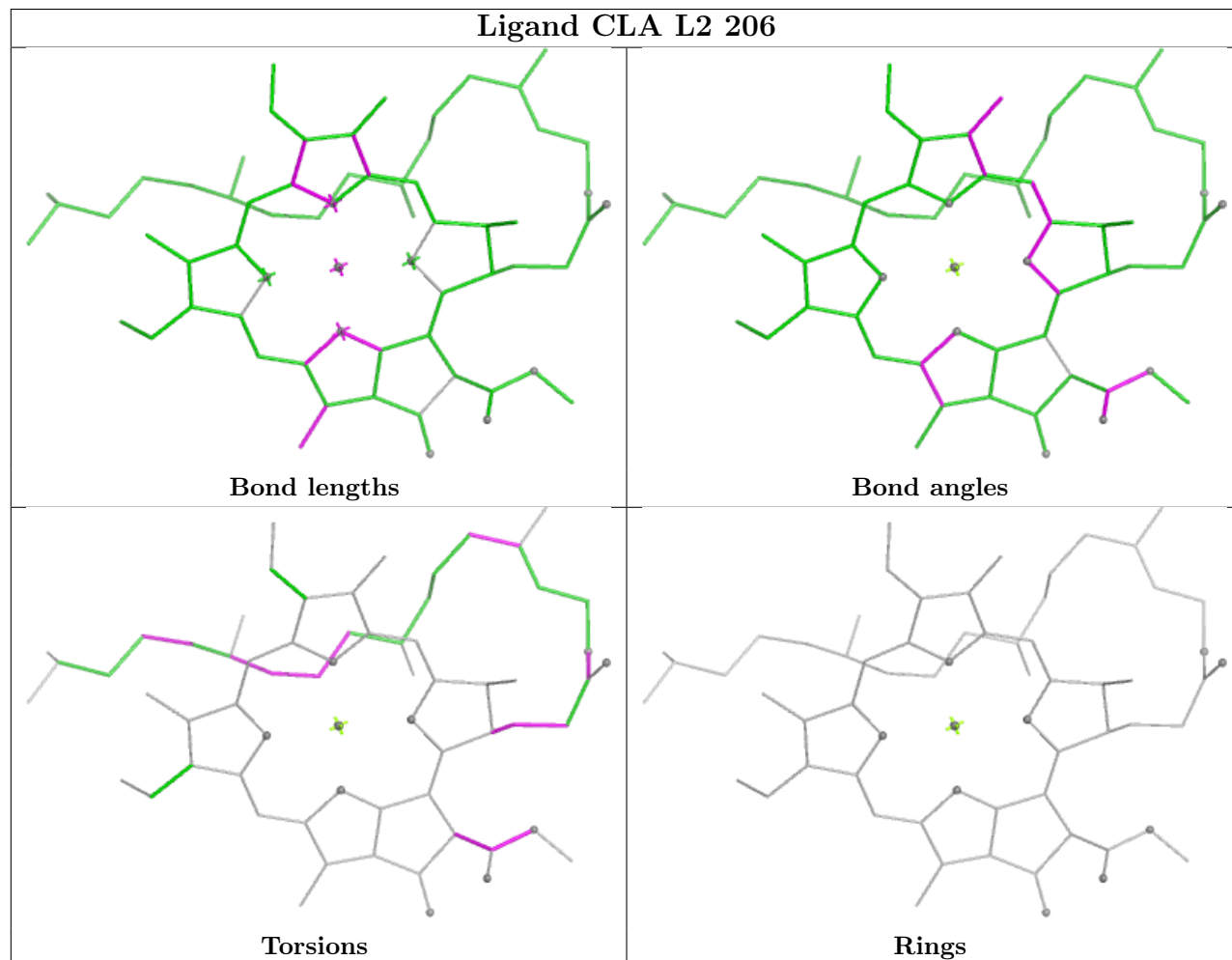
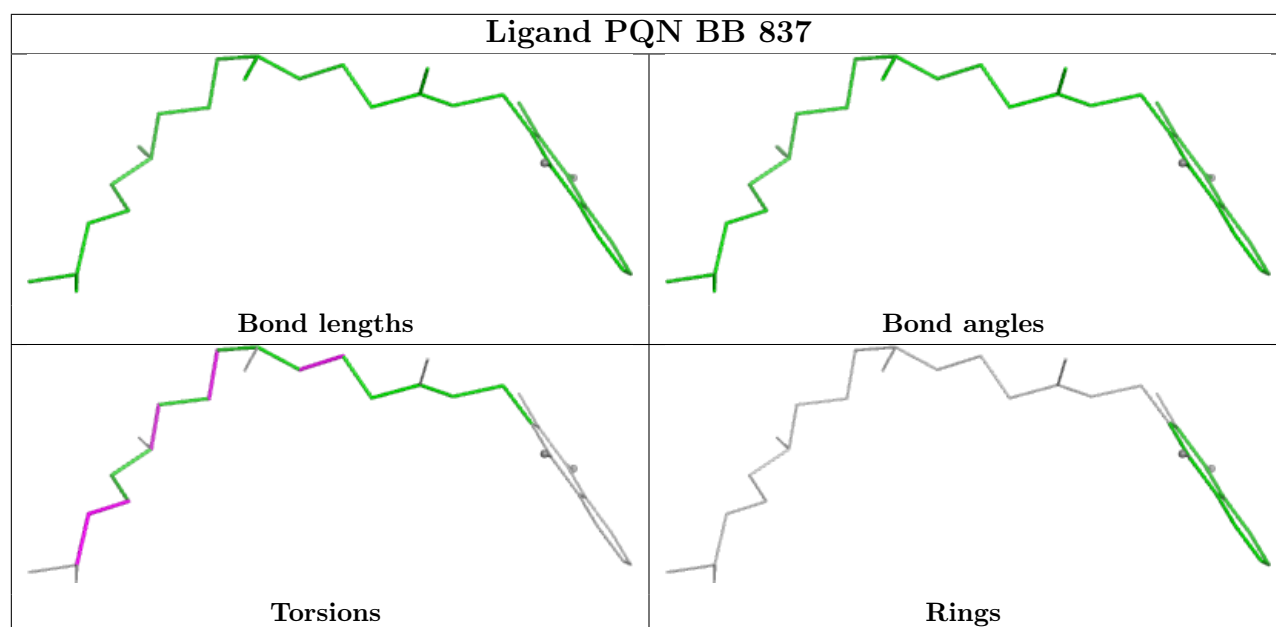


Ligand CLA J 103

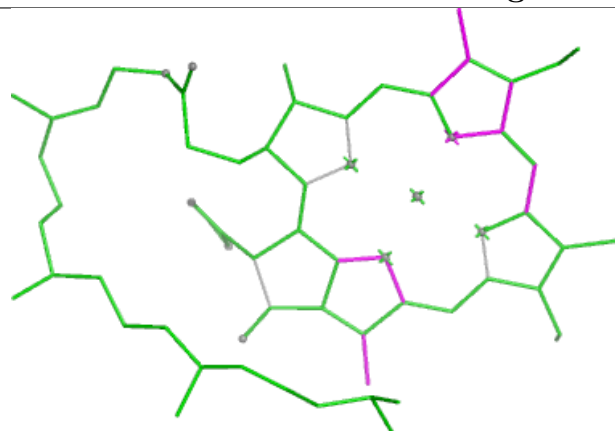


Ligand BCR AA 850

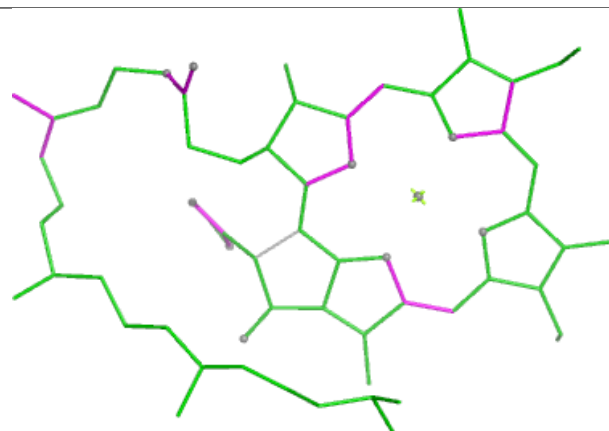




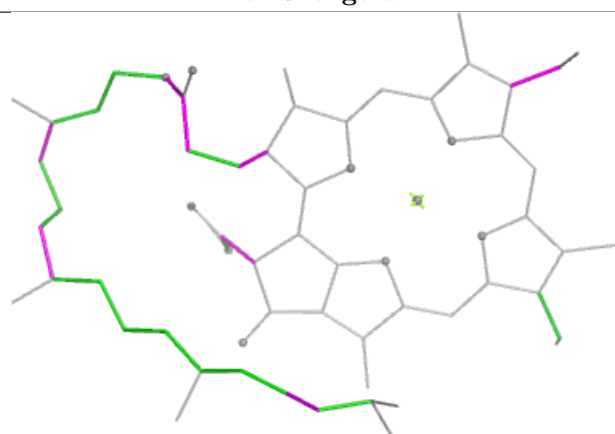
Ligand CLA B1 802



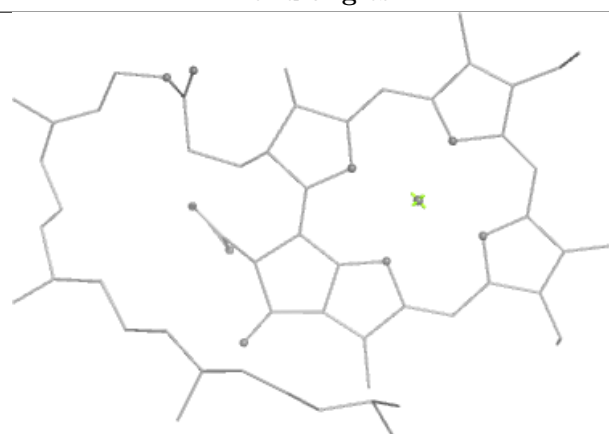
Bond lengths



Bond angles

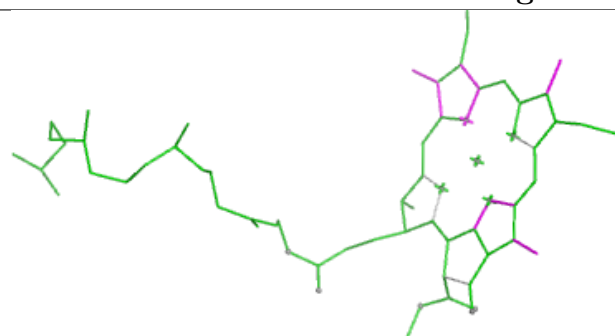


Torsions

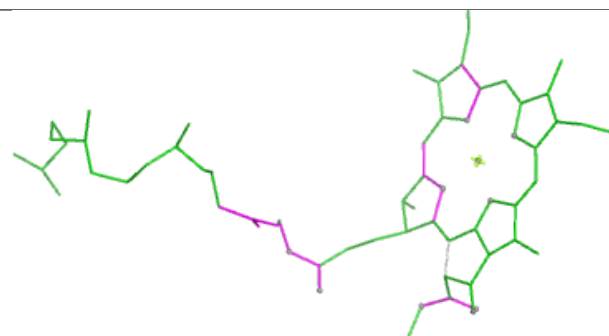


Rings

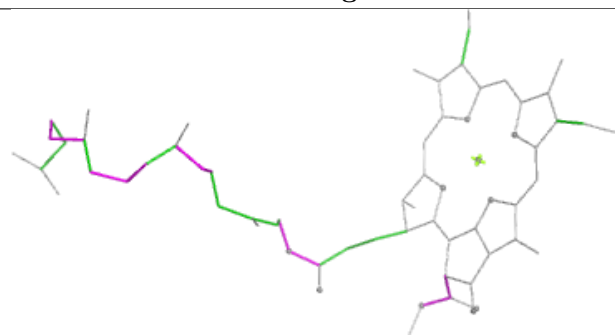
Ligand CLA B 806



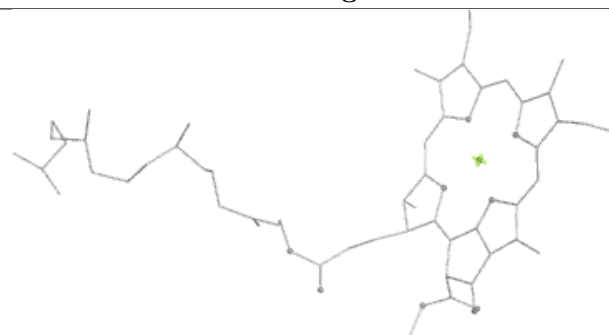
Bond lengths



Bond angles

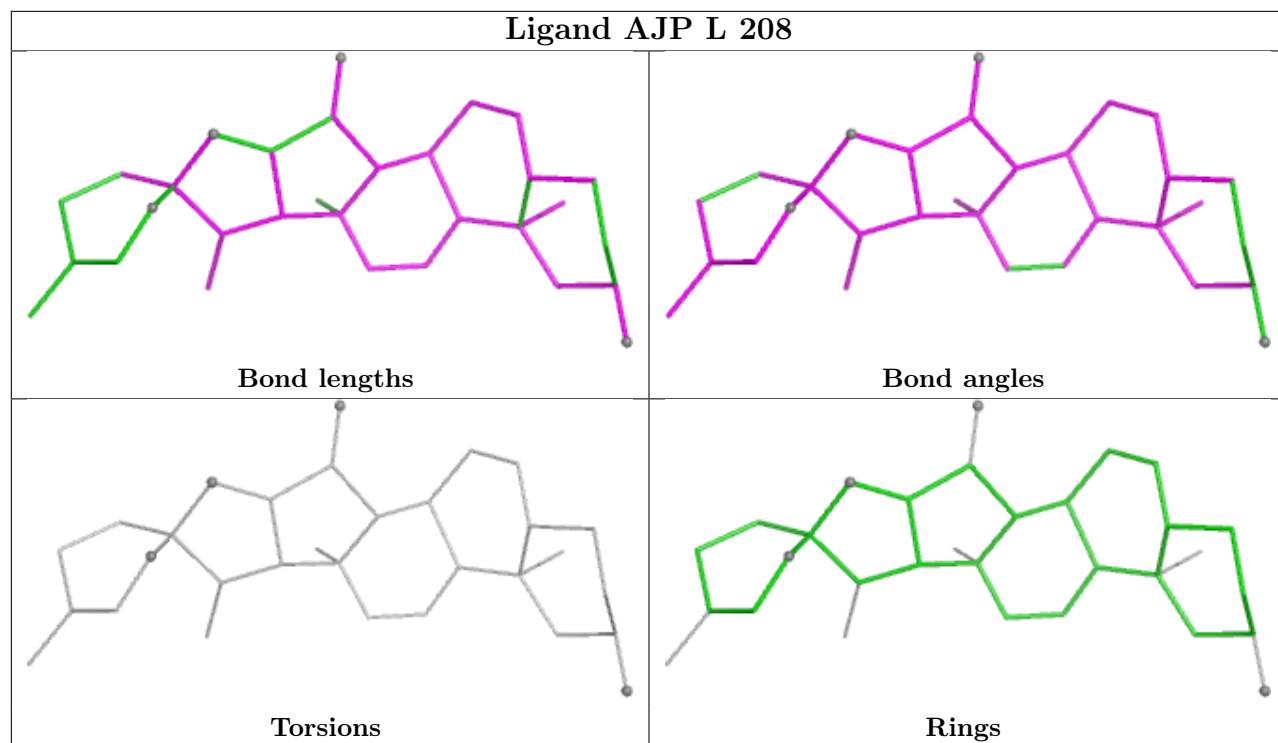


Torsions

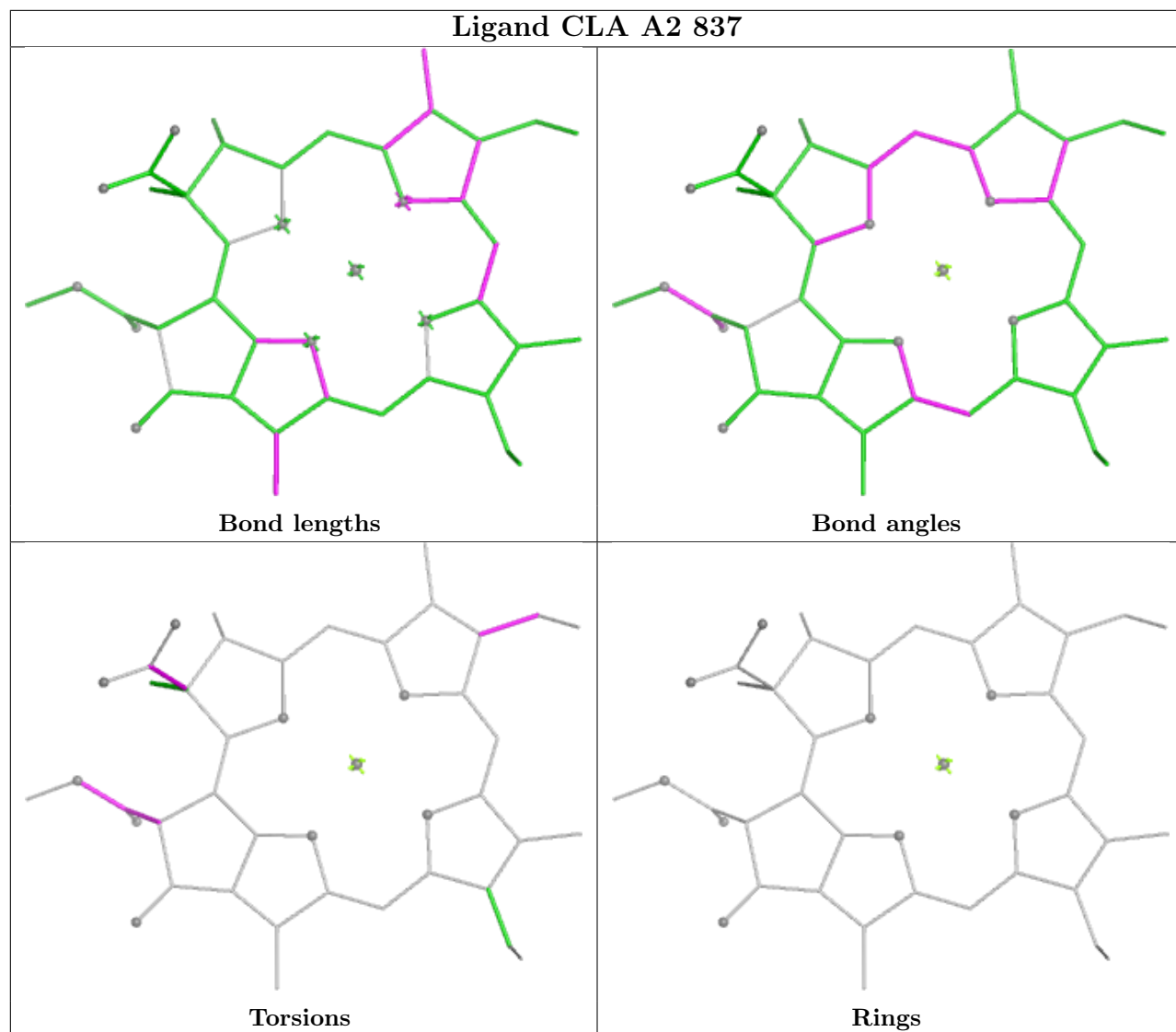


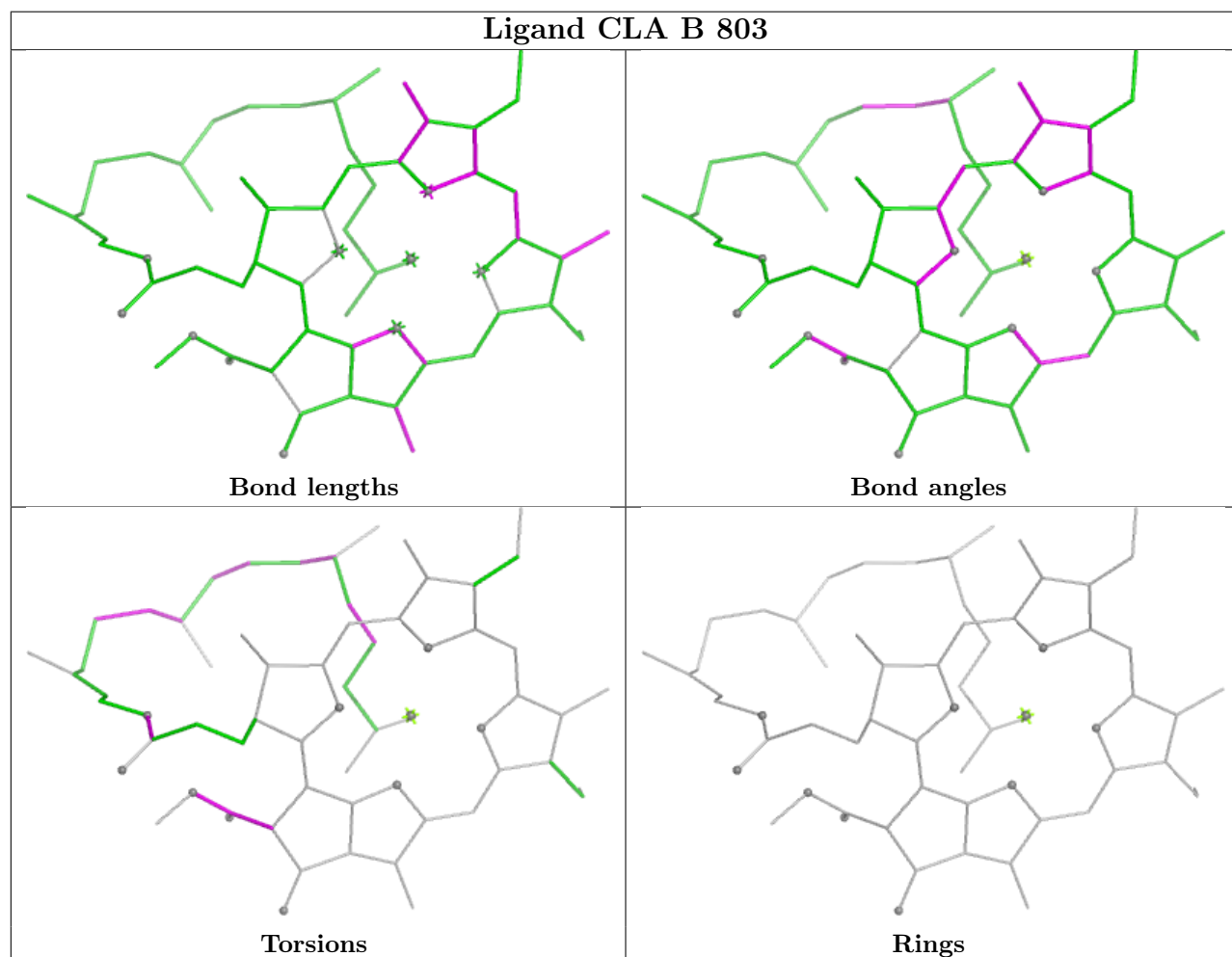
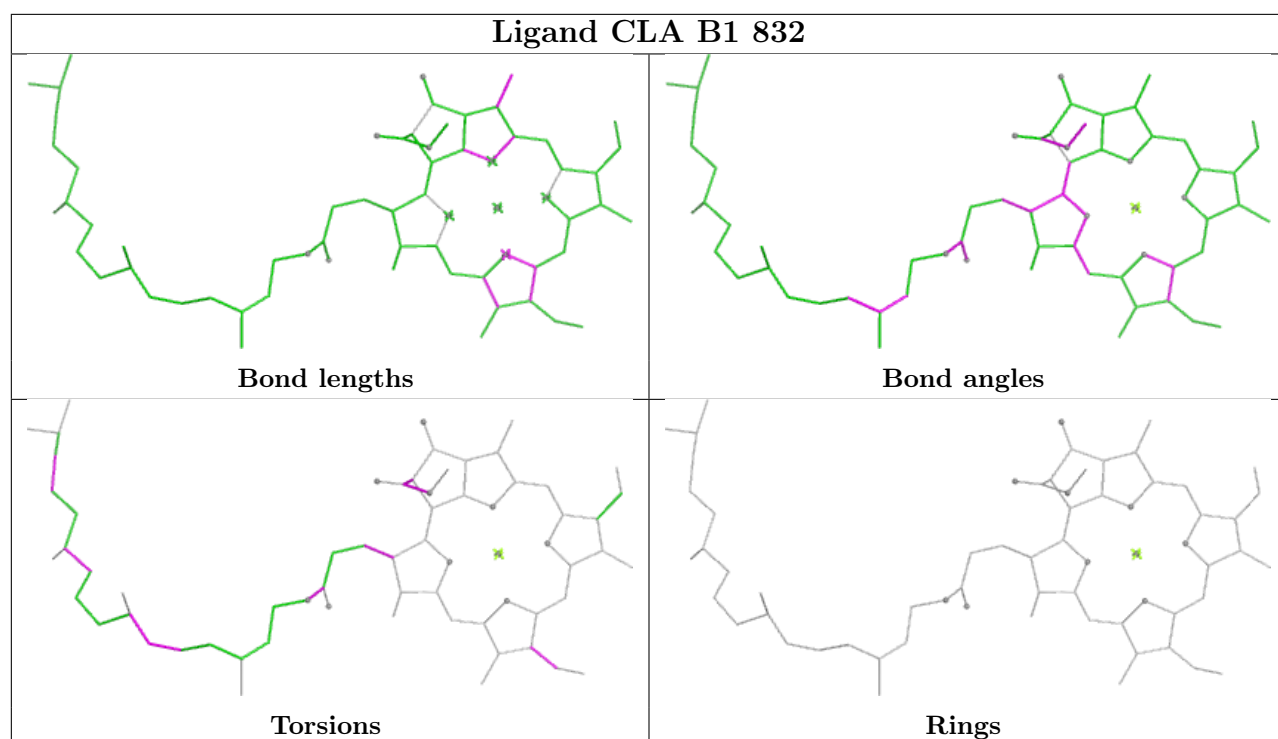
Rings

Ligand AJP L 208

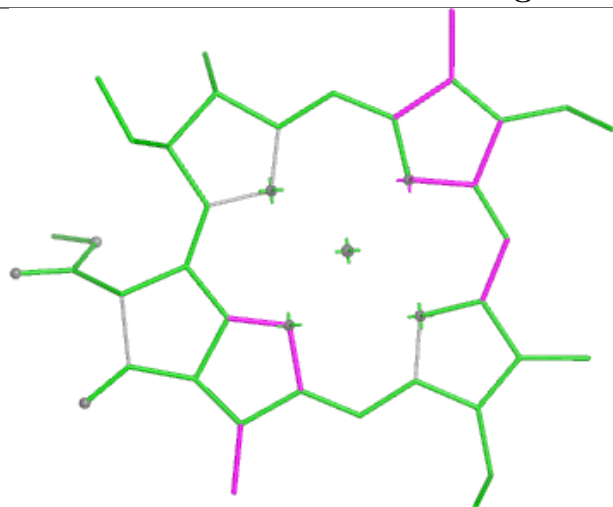


Ligand CLA A2 837

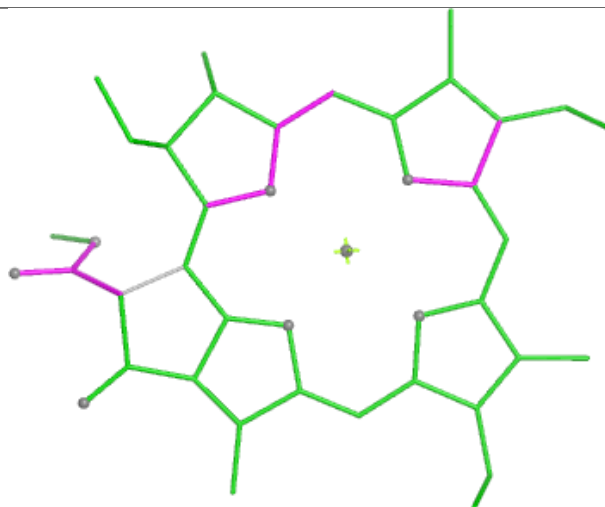




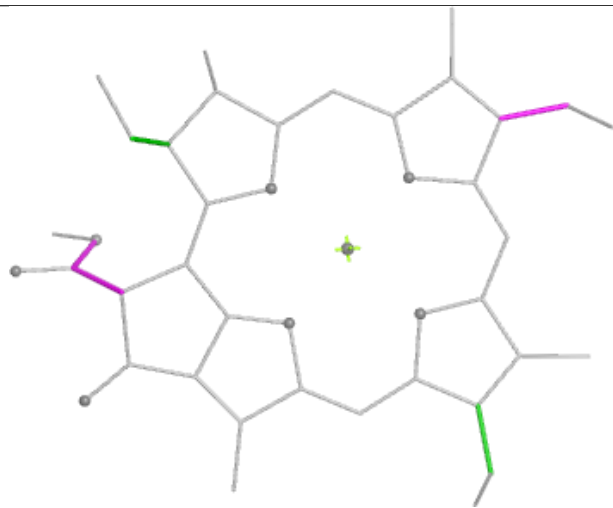
Ligand CLA B 817



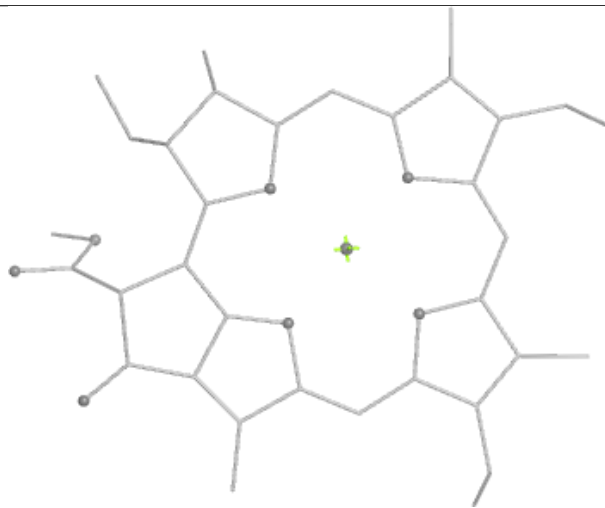
Bond lengths



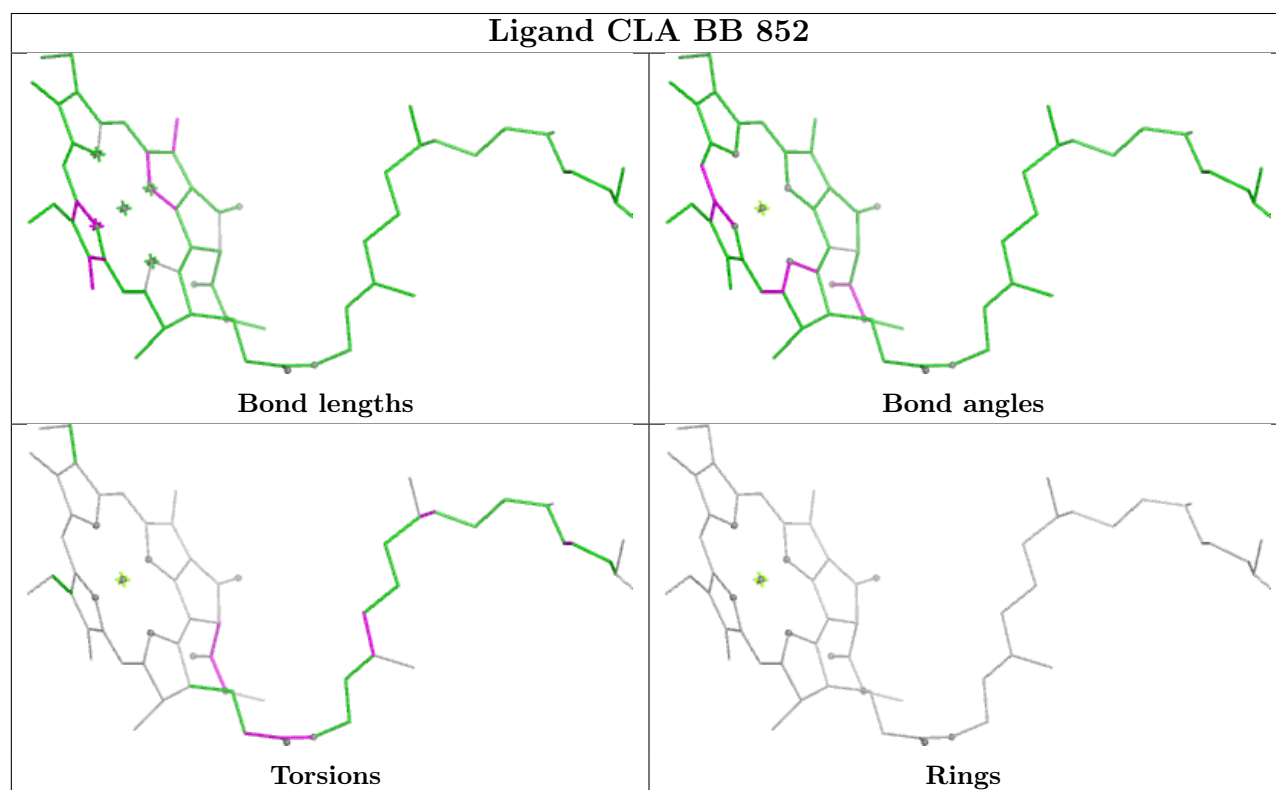
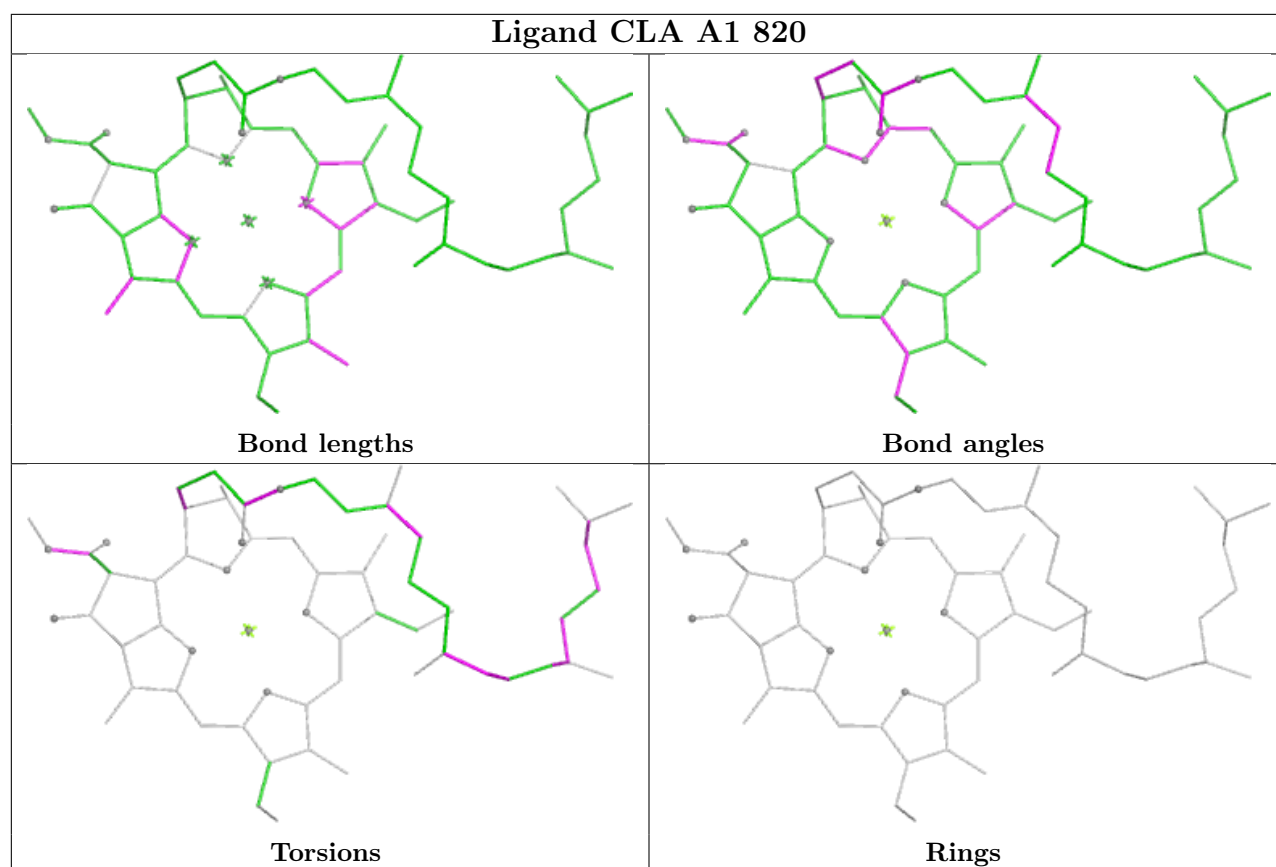
Bond angles

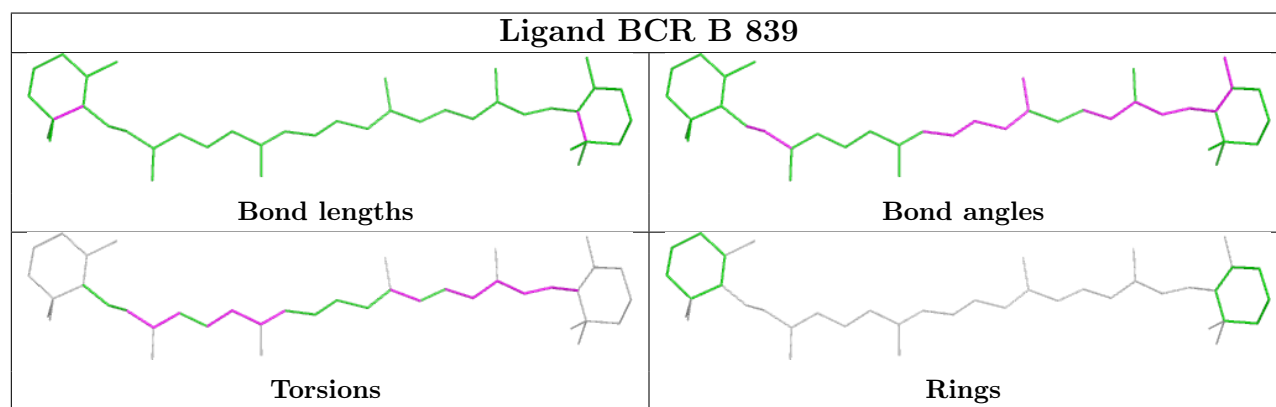
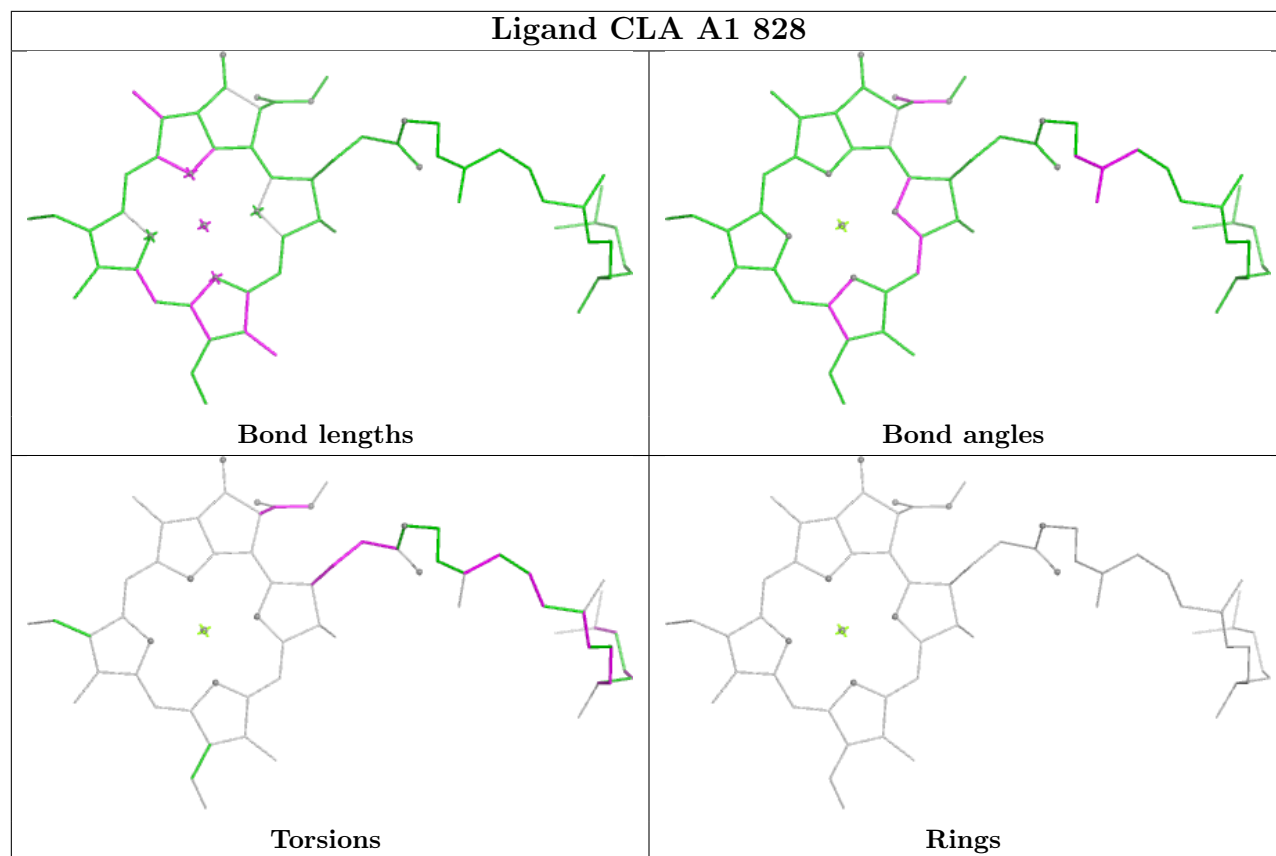


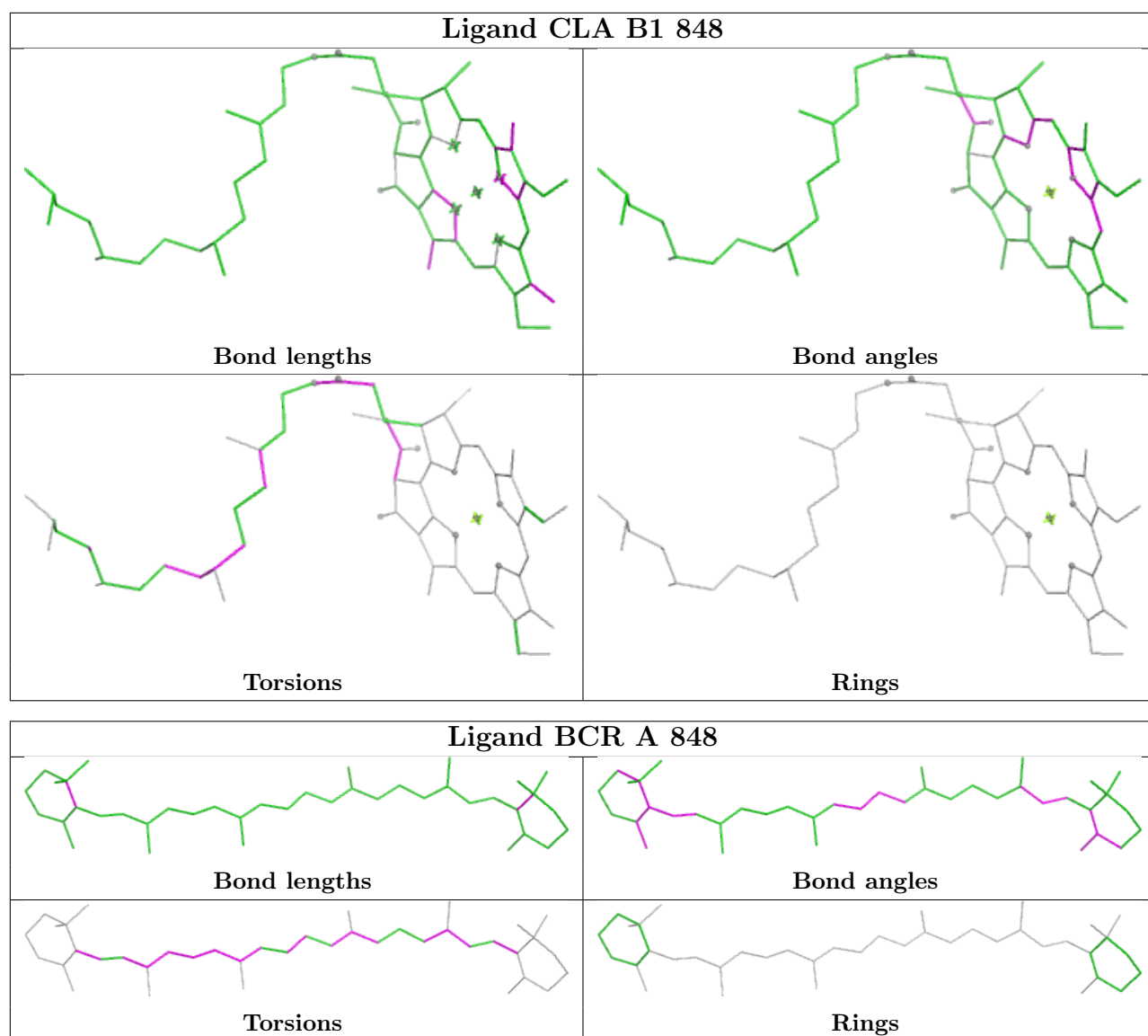
Torsions

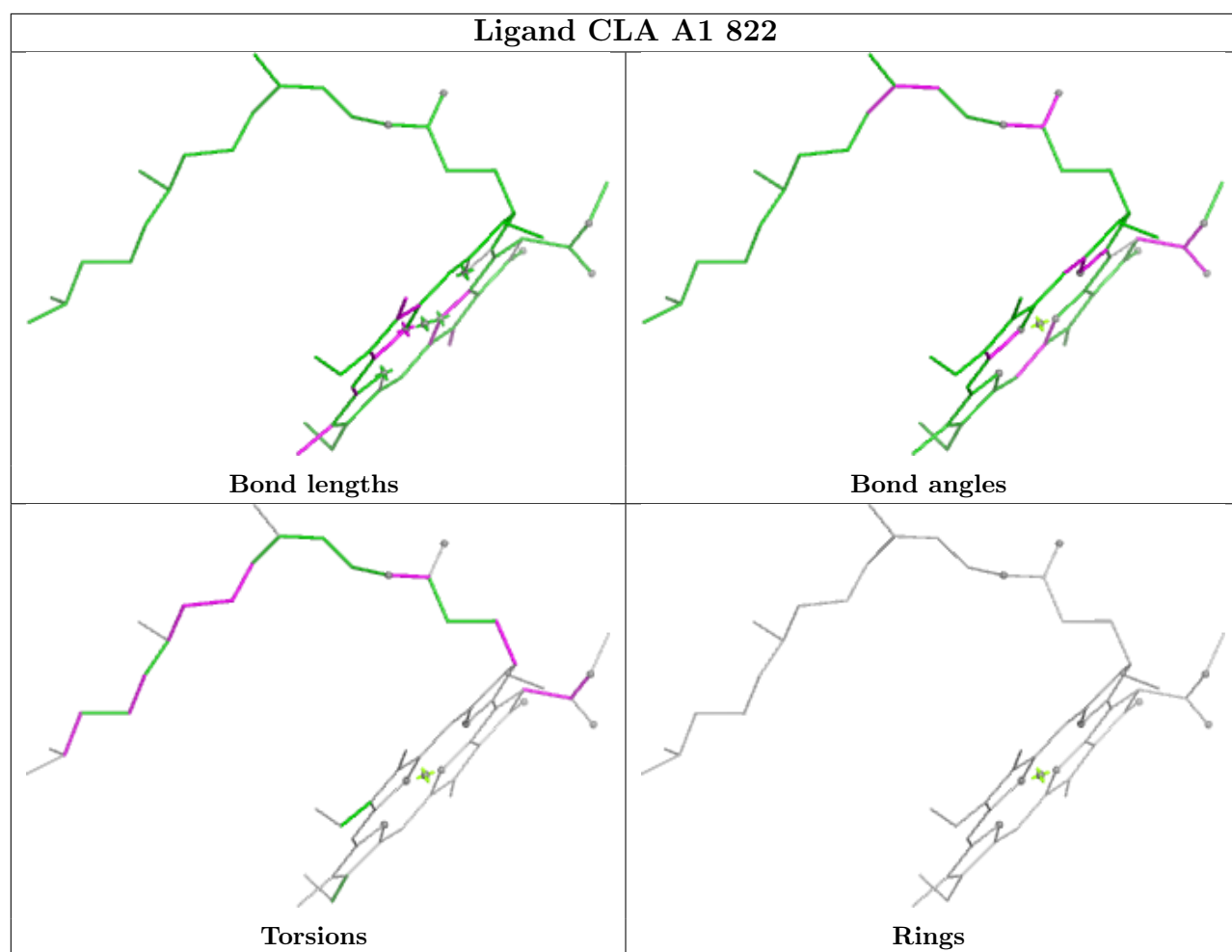


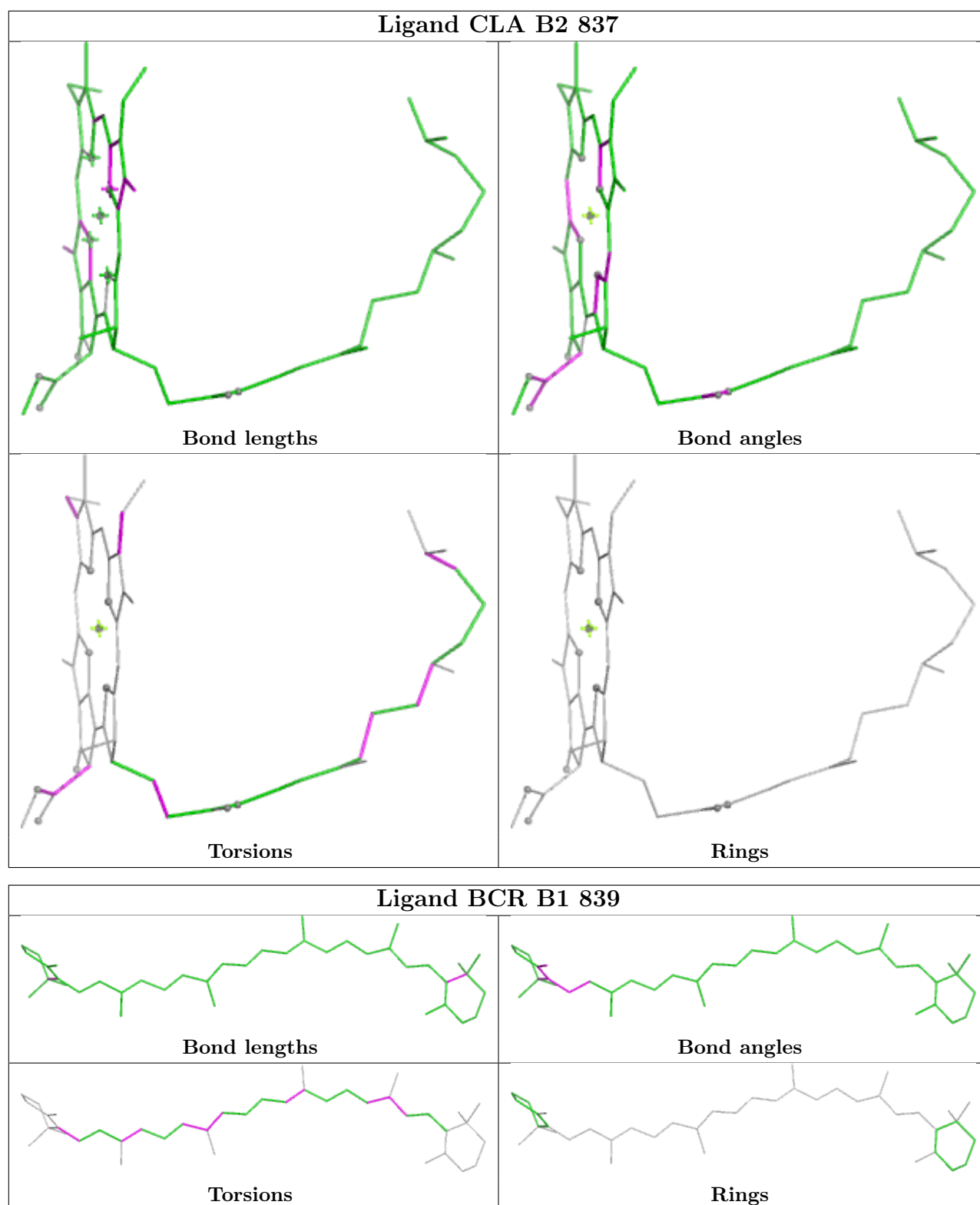
Rings

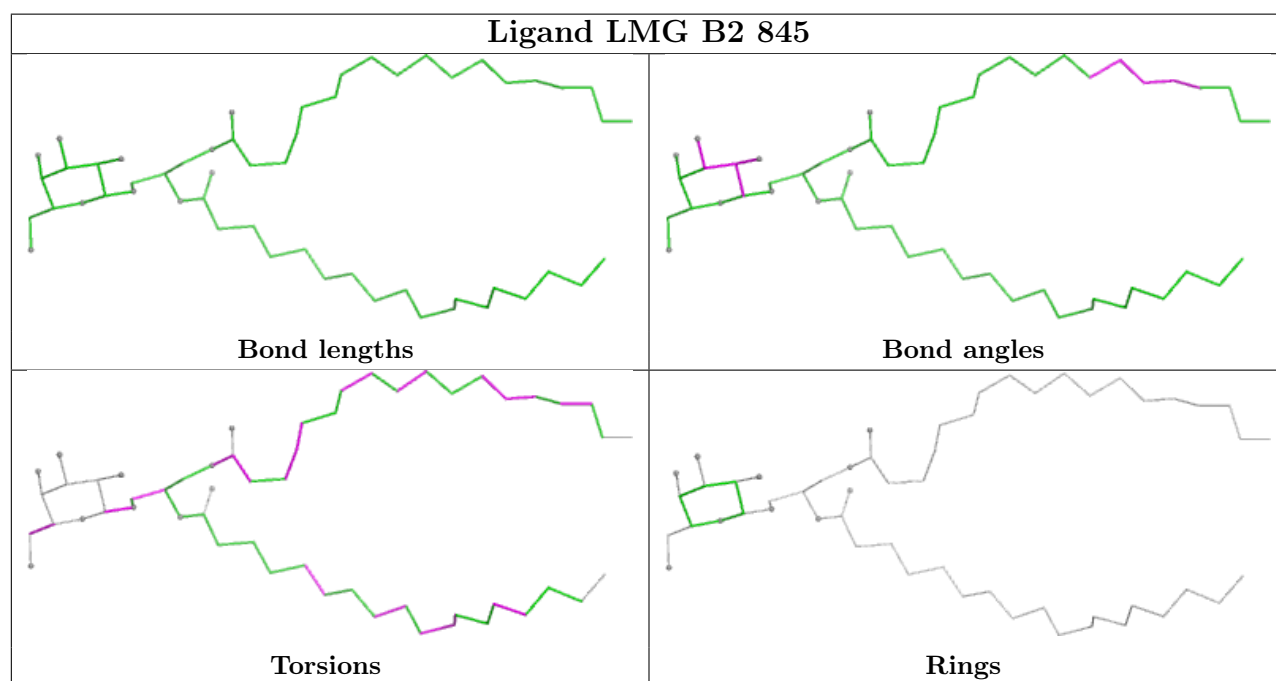
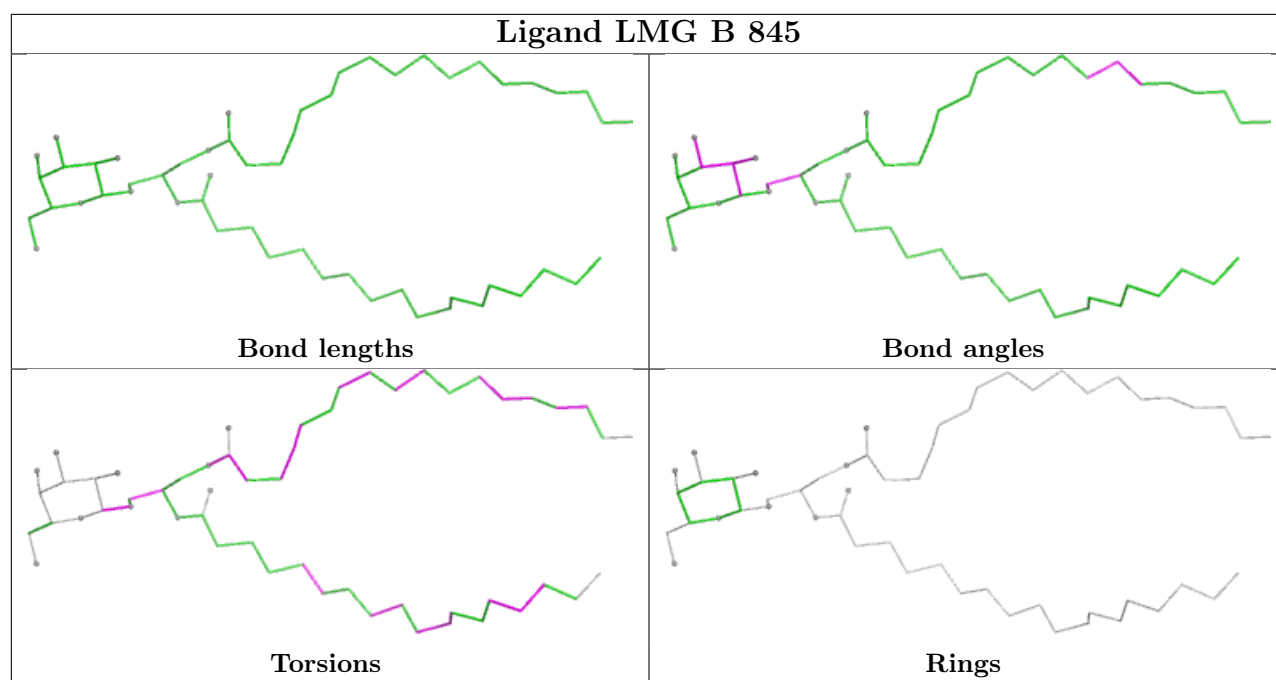




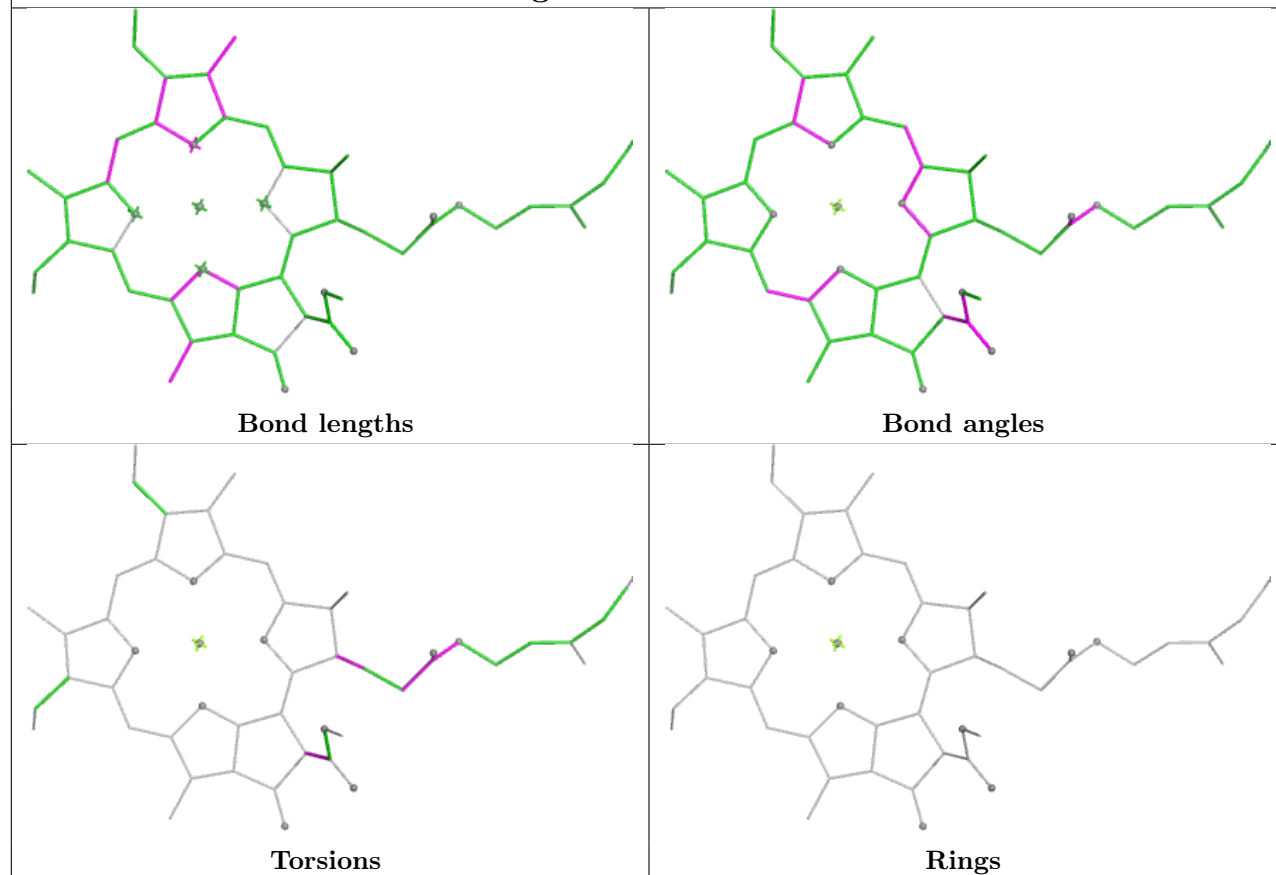




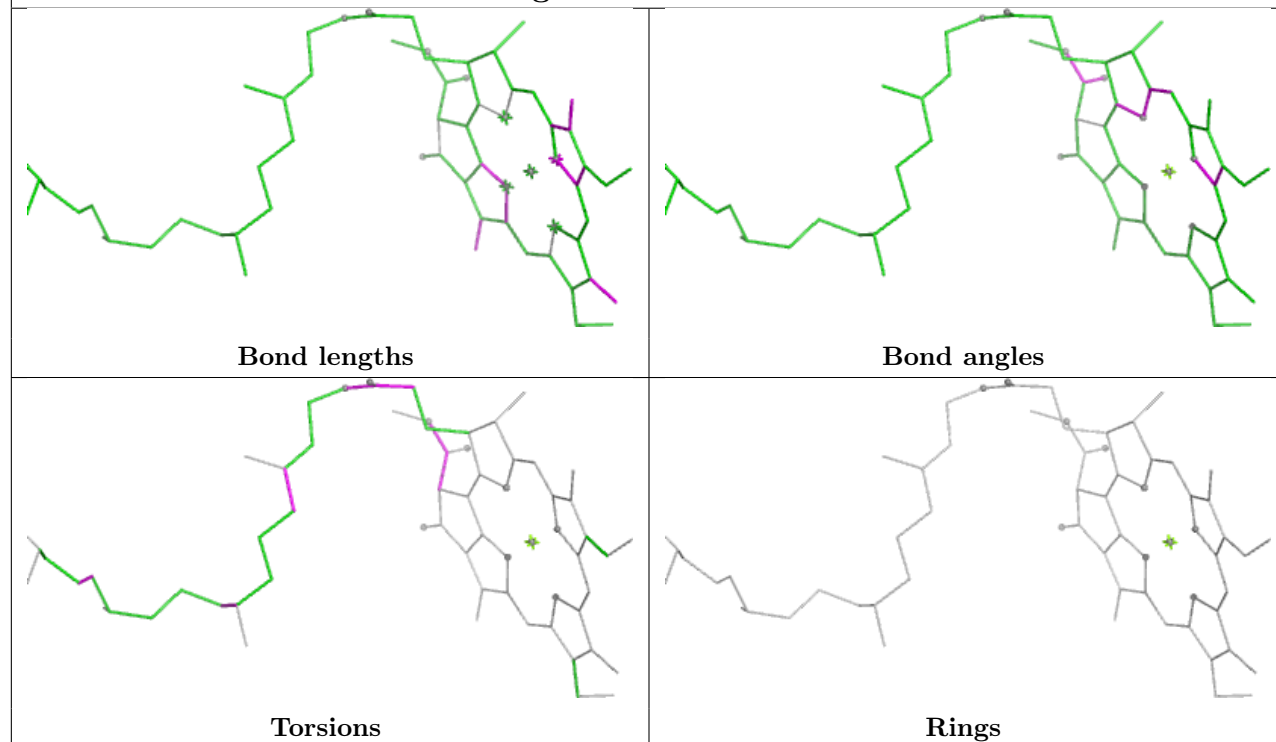




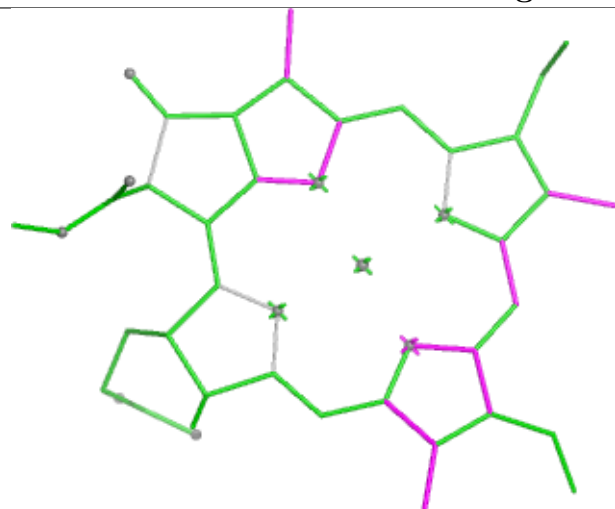
Ligand CLA A 839



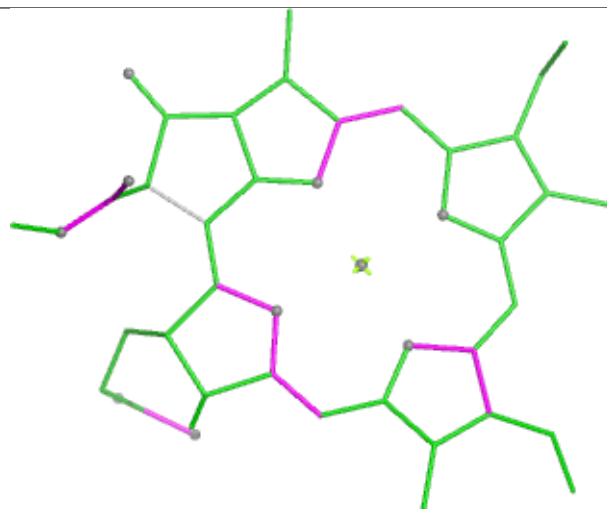
Ligand CLA B 854



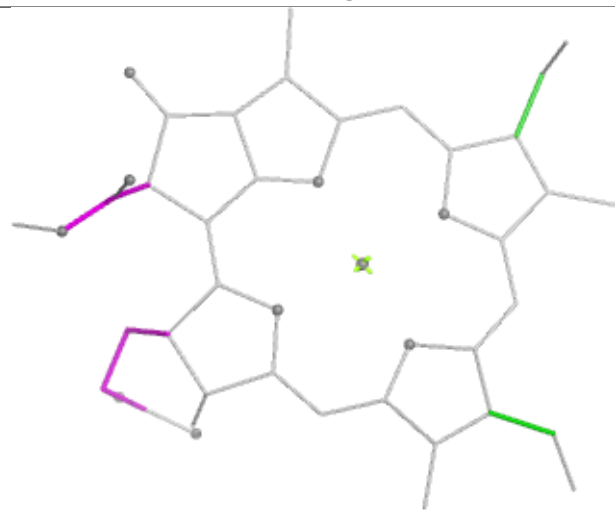
Ligand CLA A 826



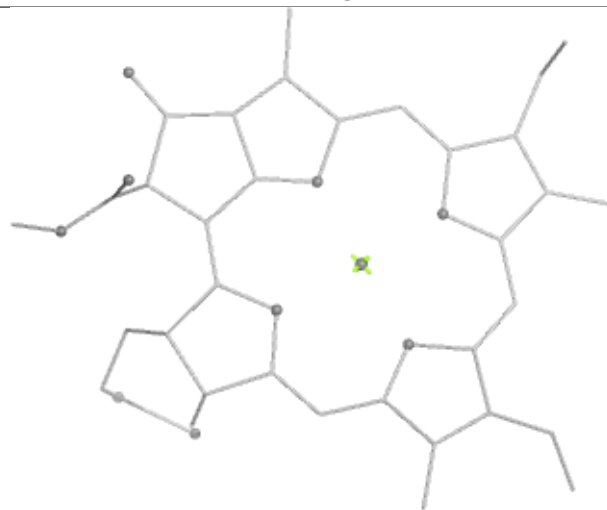
Bond lengths



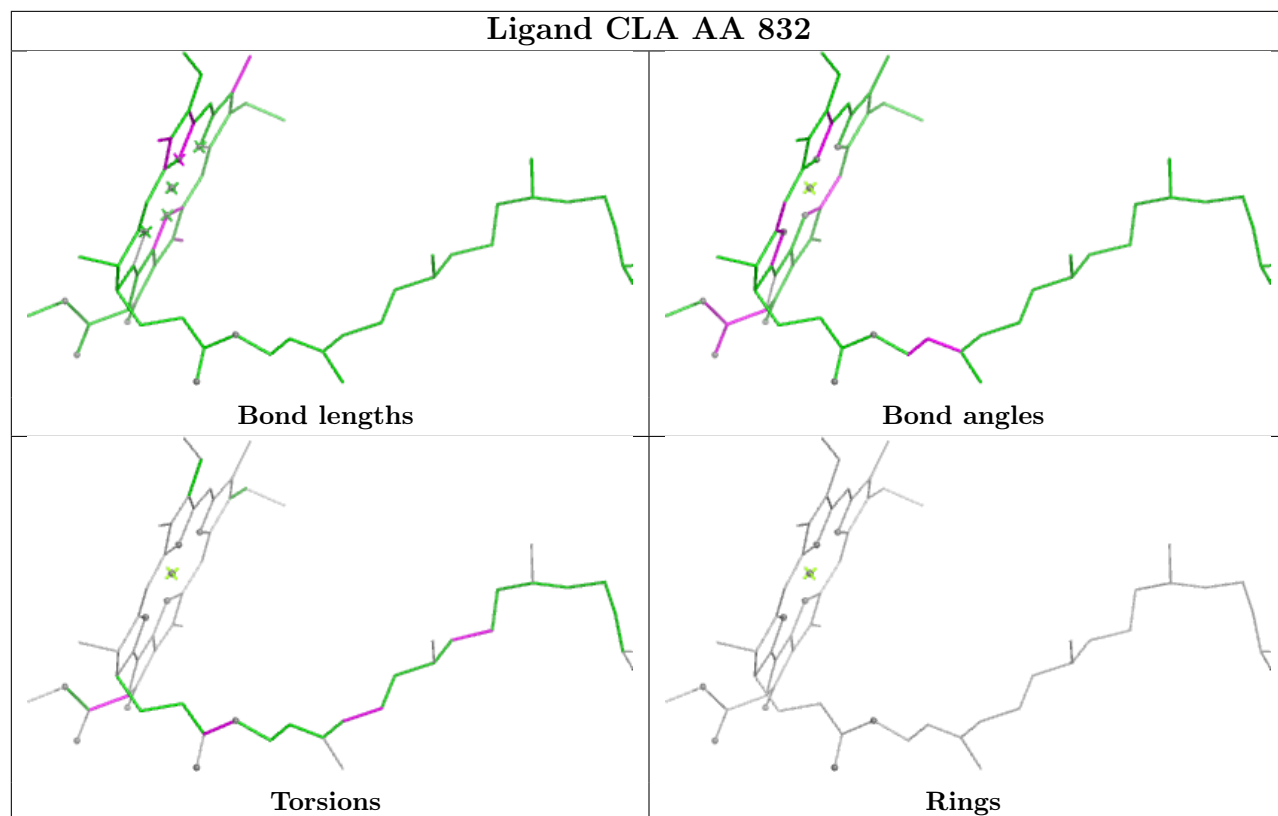
Bond angles



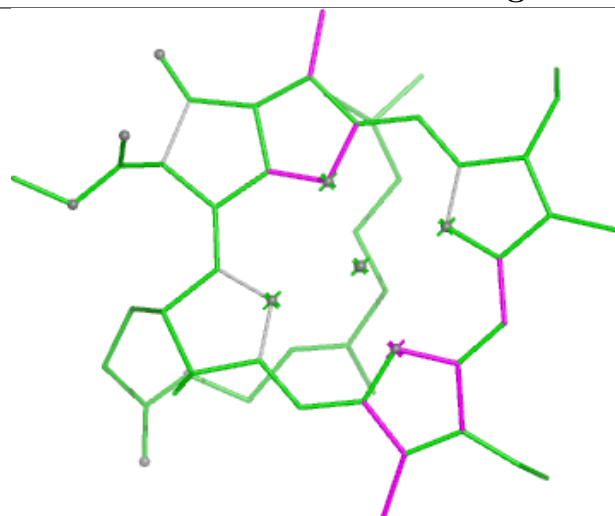
Torsions



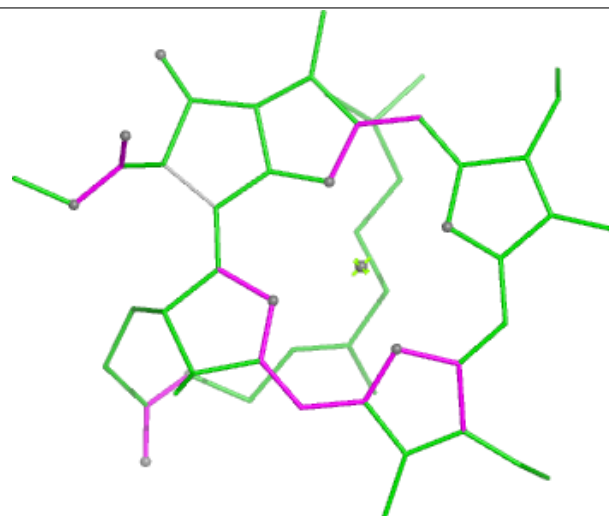
Rings



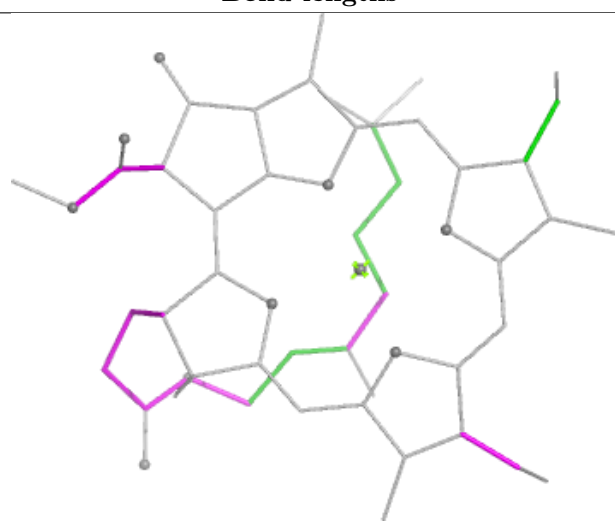
Ligand CLA B1 824



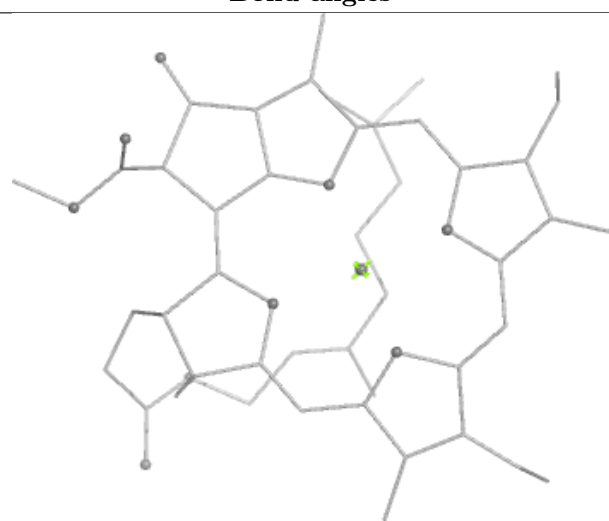
Bond lengths



Bond angles

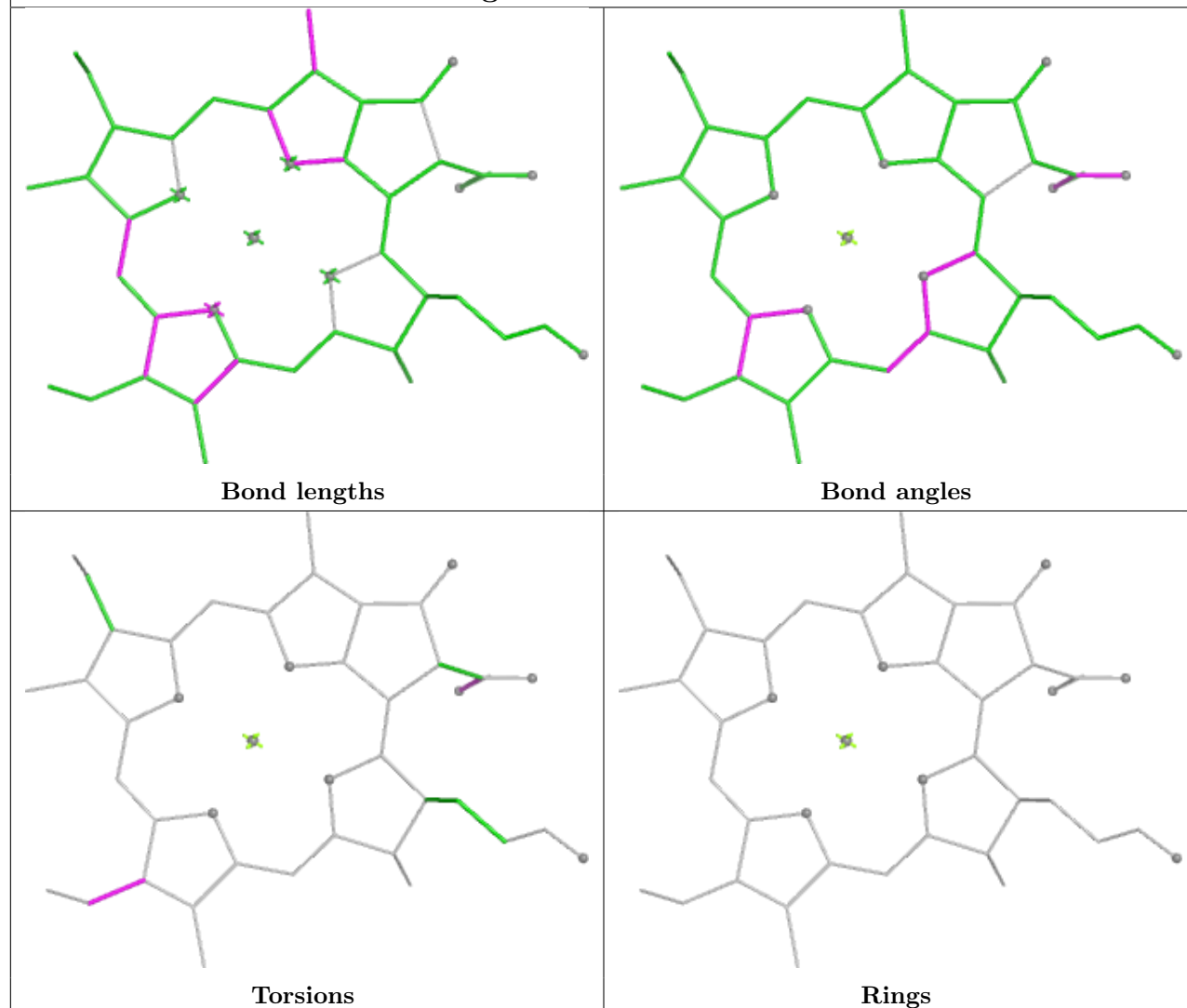


Torsions

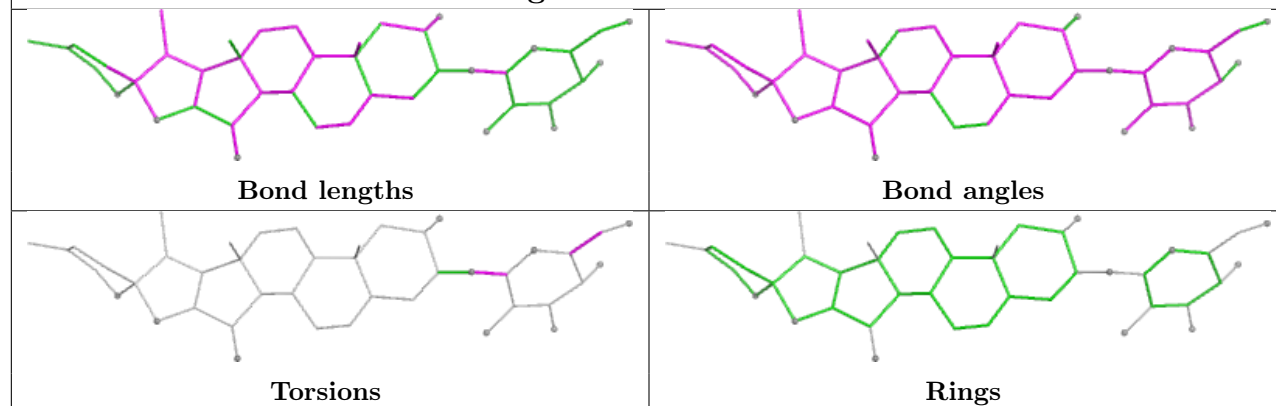


Rings

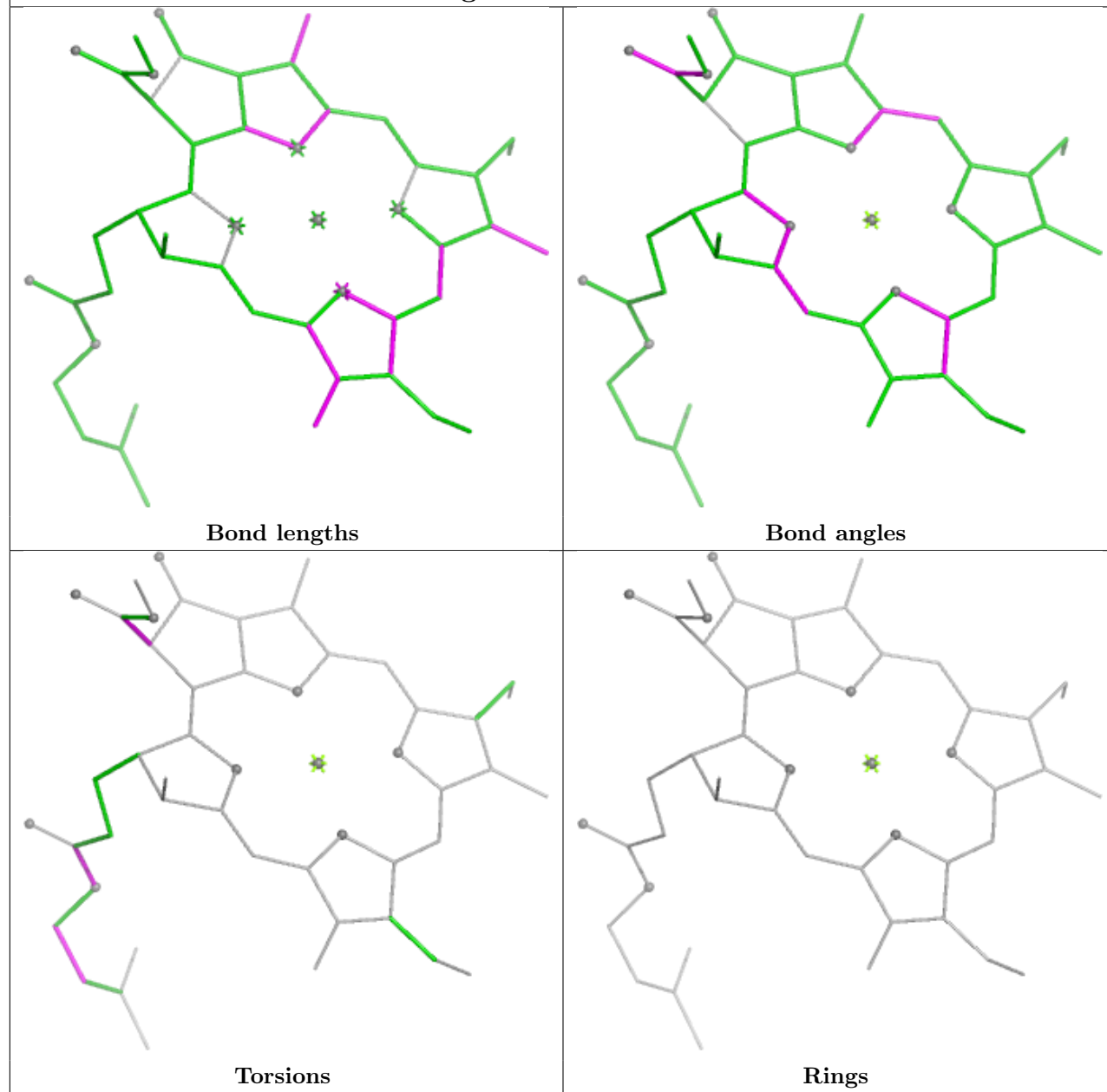
Ligand CLA AA 817

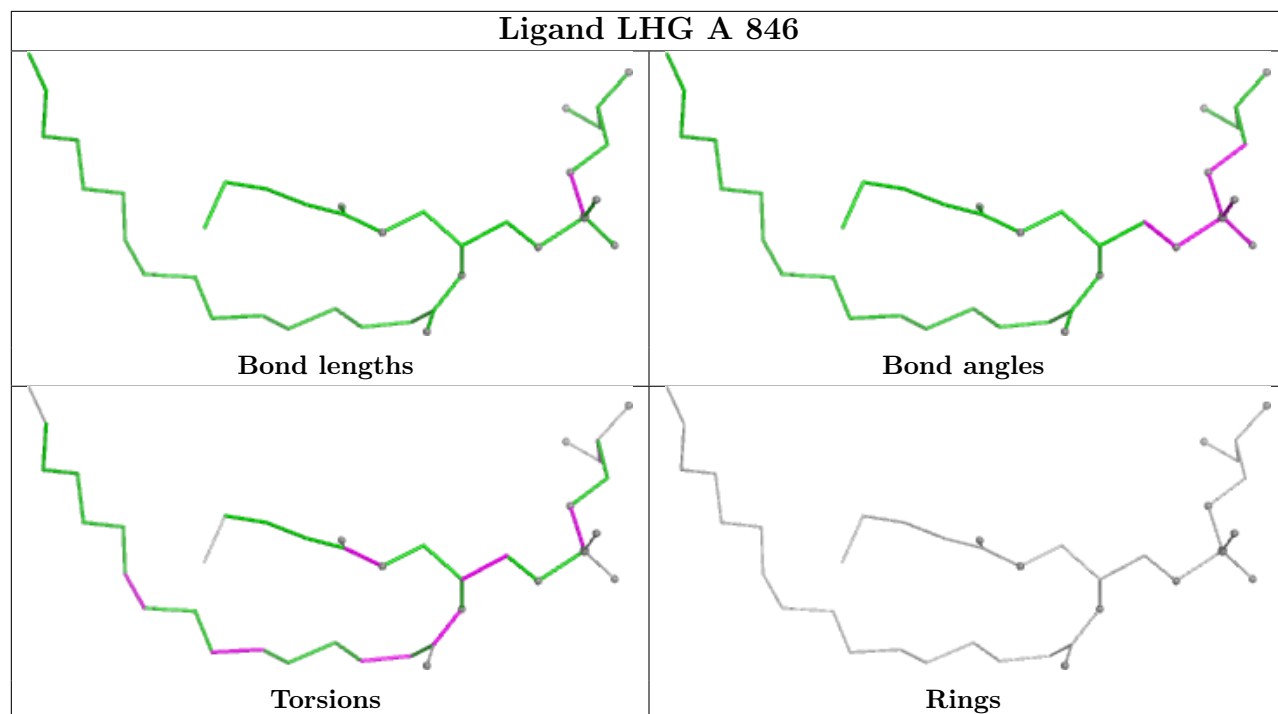


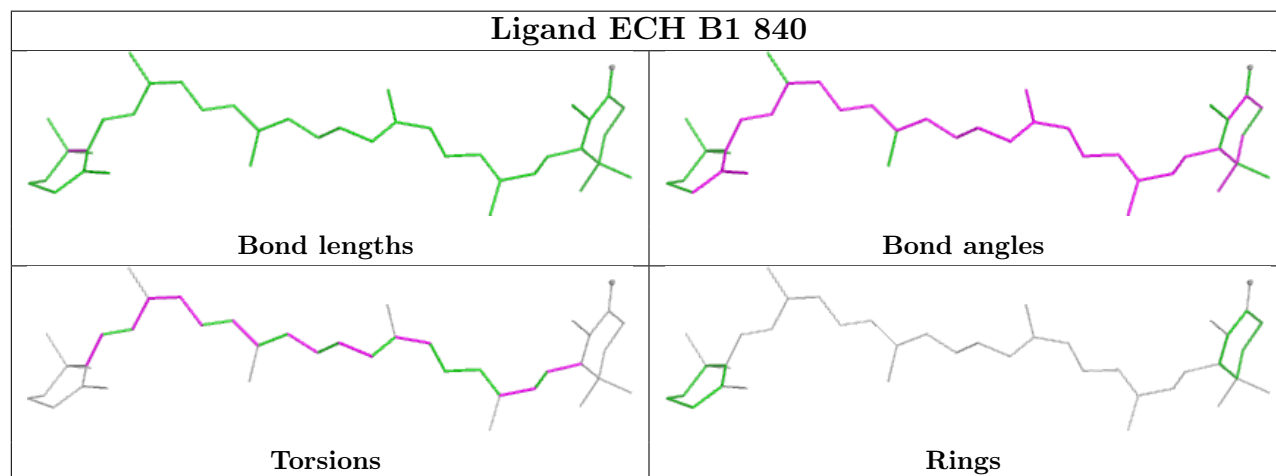
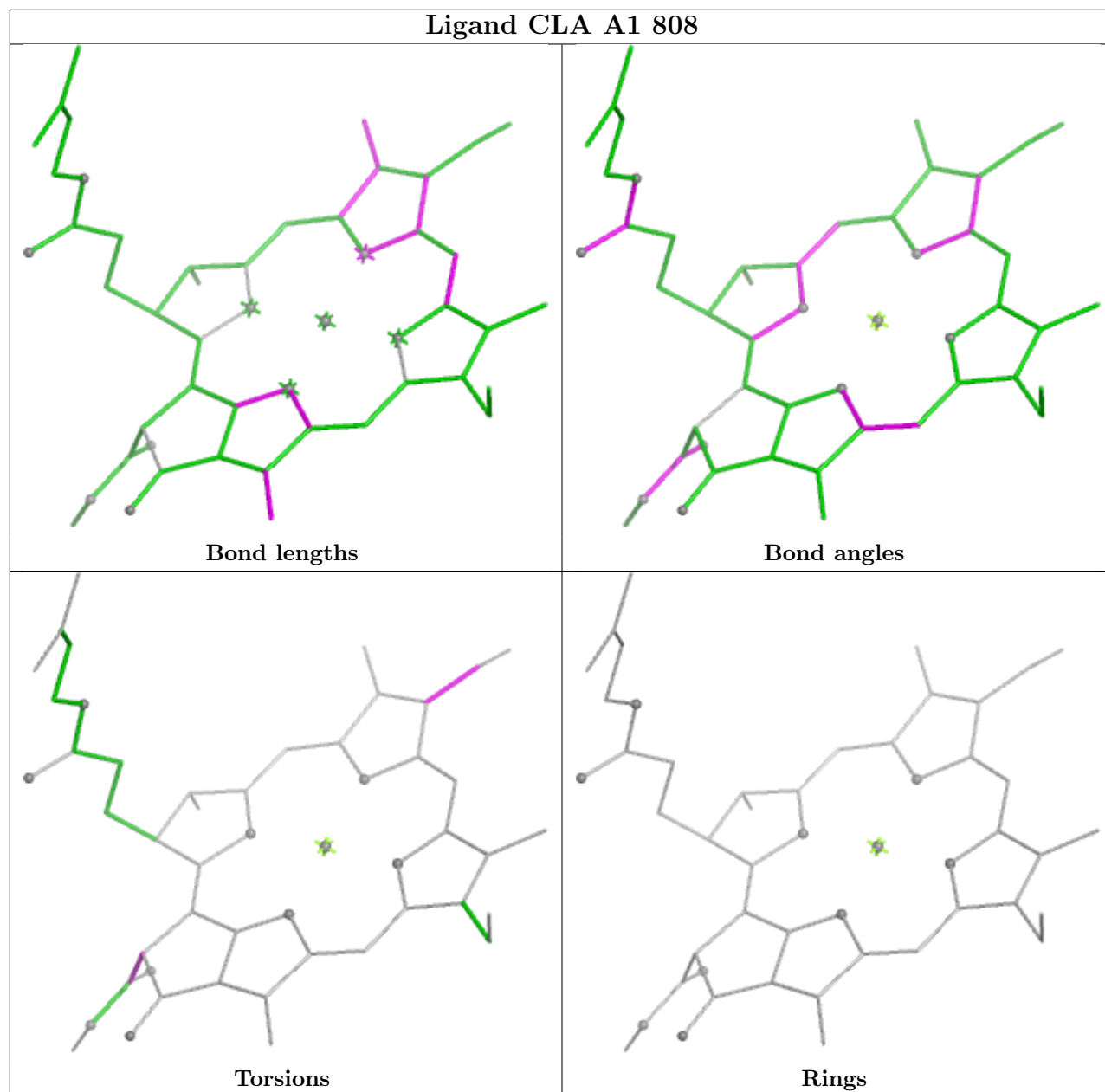
Ligand AJP L2 202



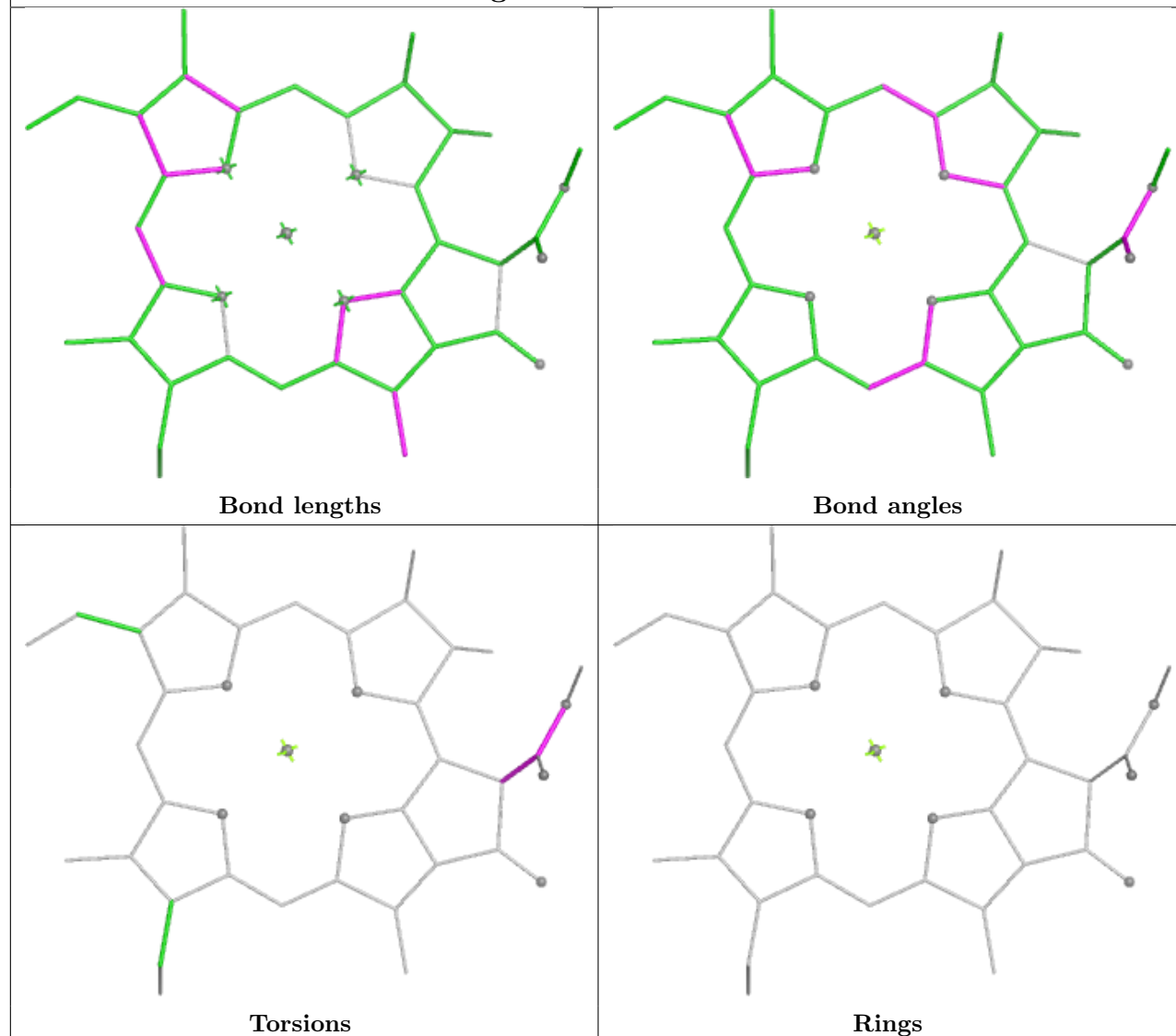
Ligand CLA A 833



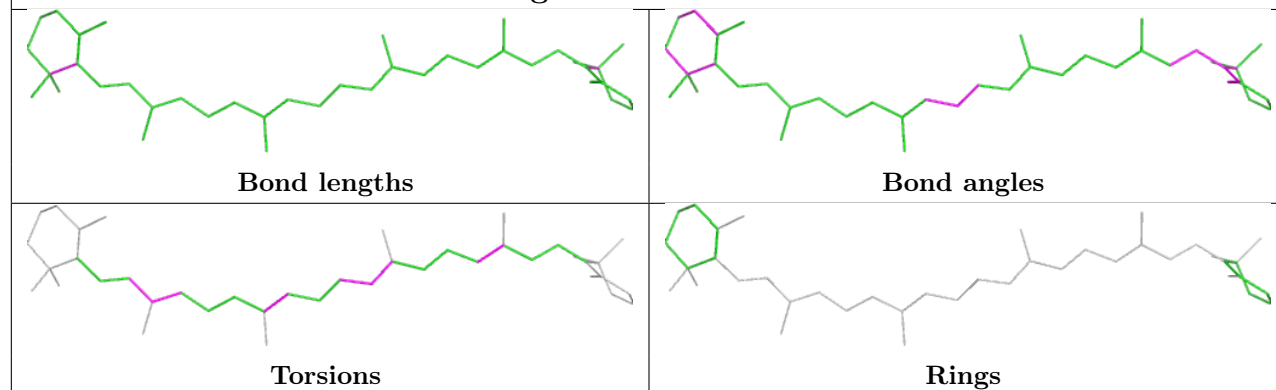




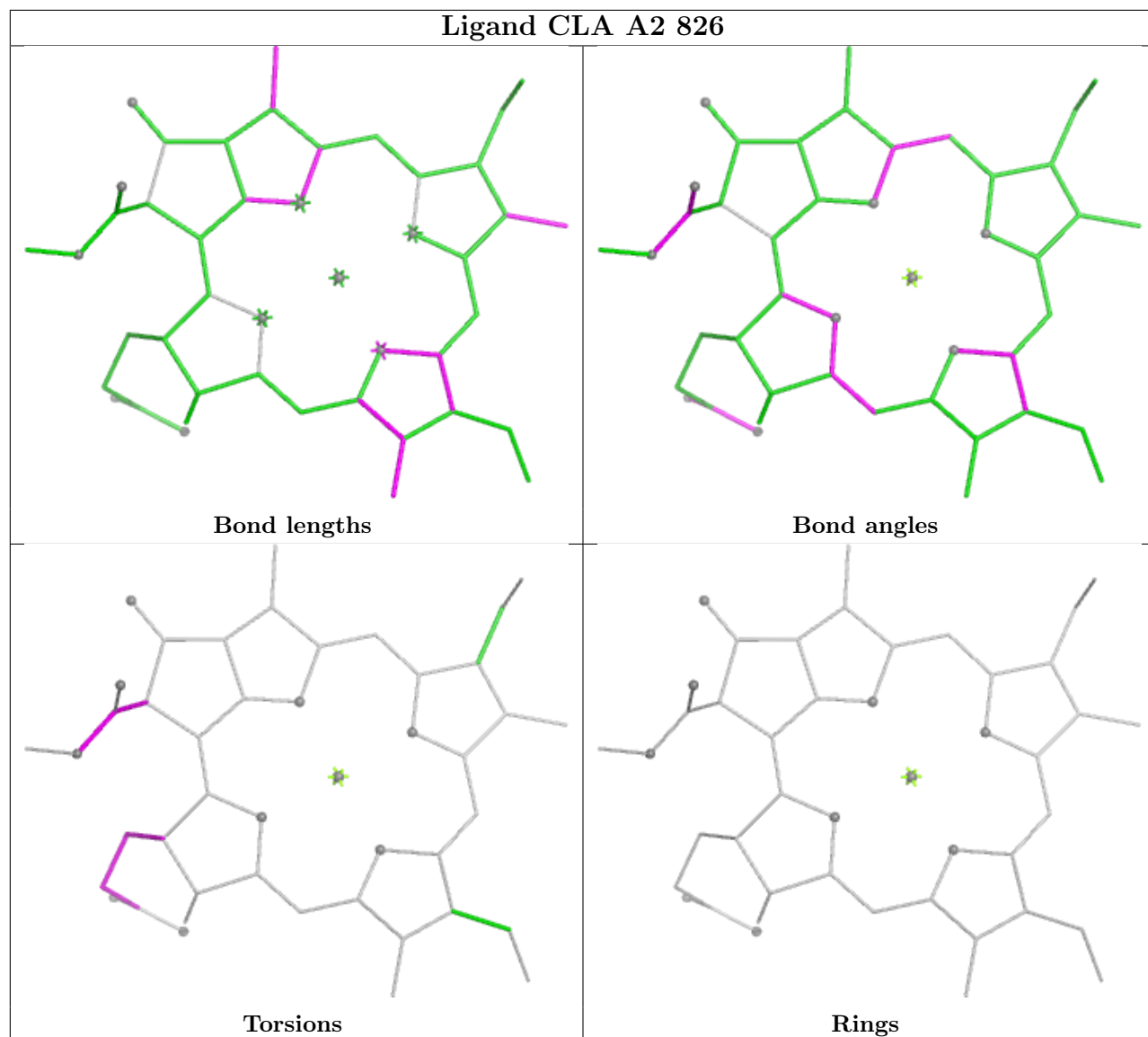
Ligand CLA B 818



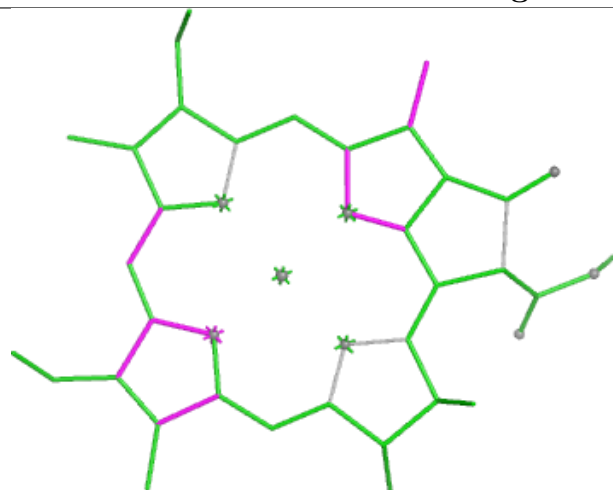
Ligand BCR B 840



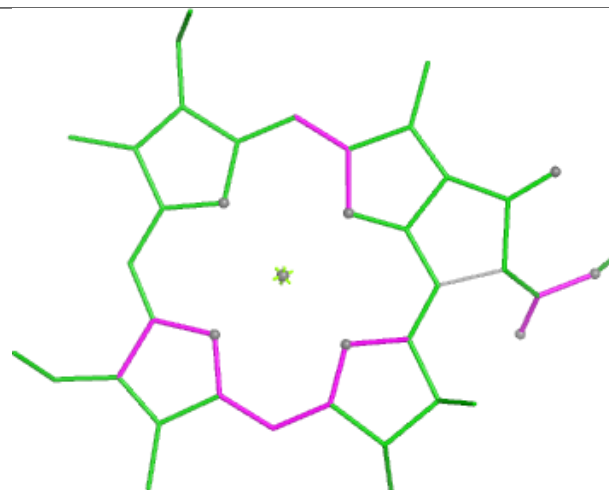
Ligand CLA A2 826



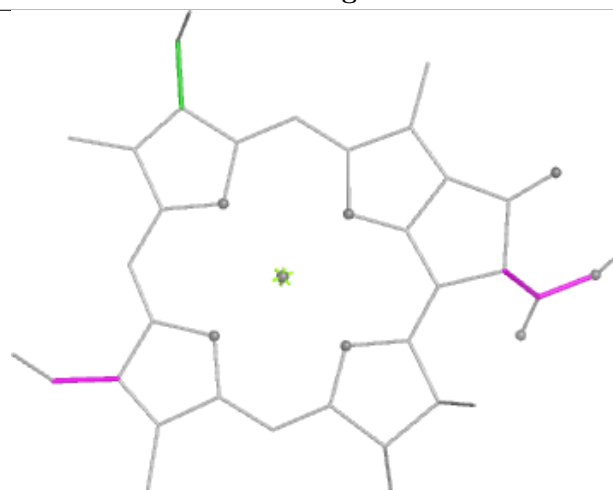
Ligand CLA J1 101



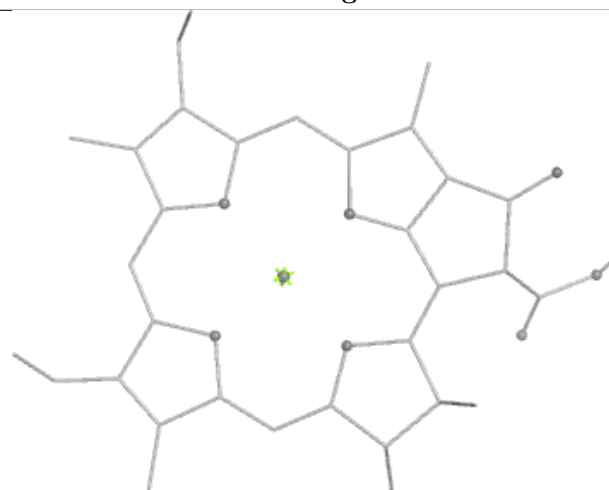
Bond lengths



Bond angles

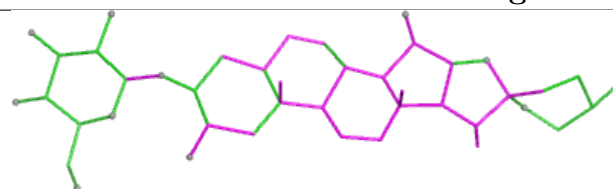


Torsions

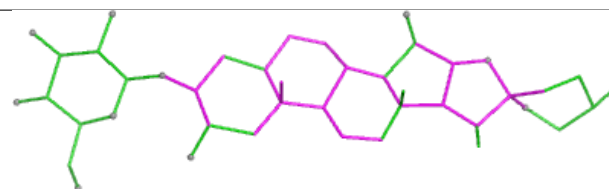


Rings

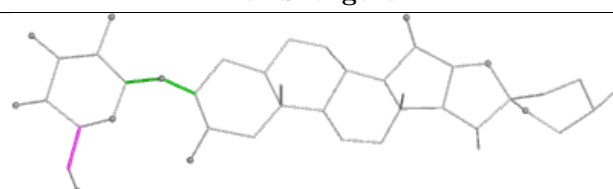
Ligand AJP A1 854



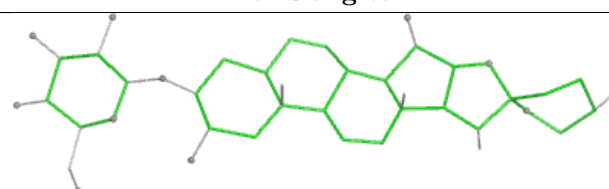
Bond lengths



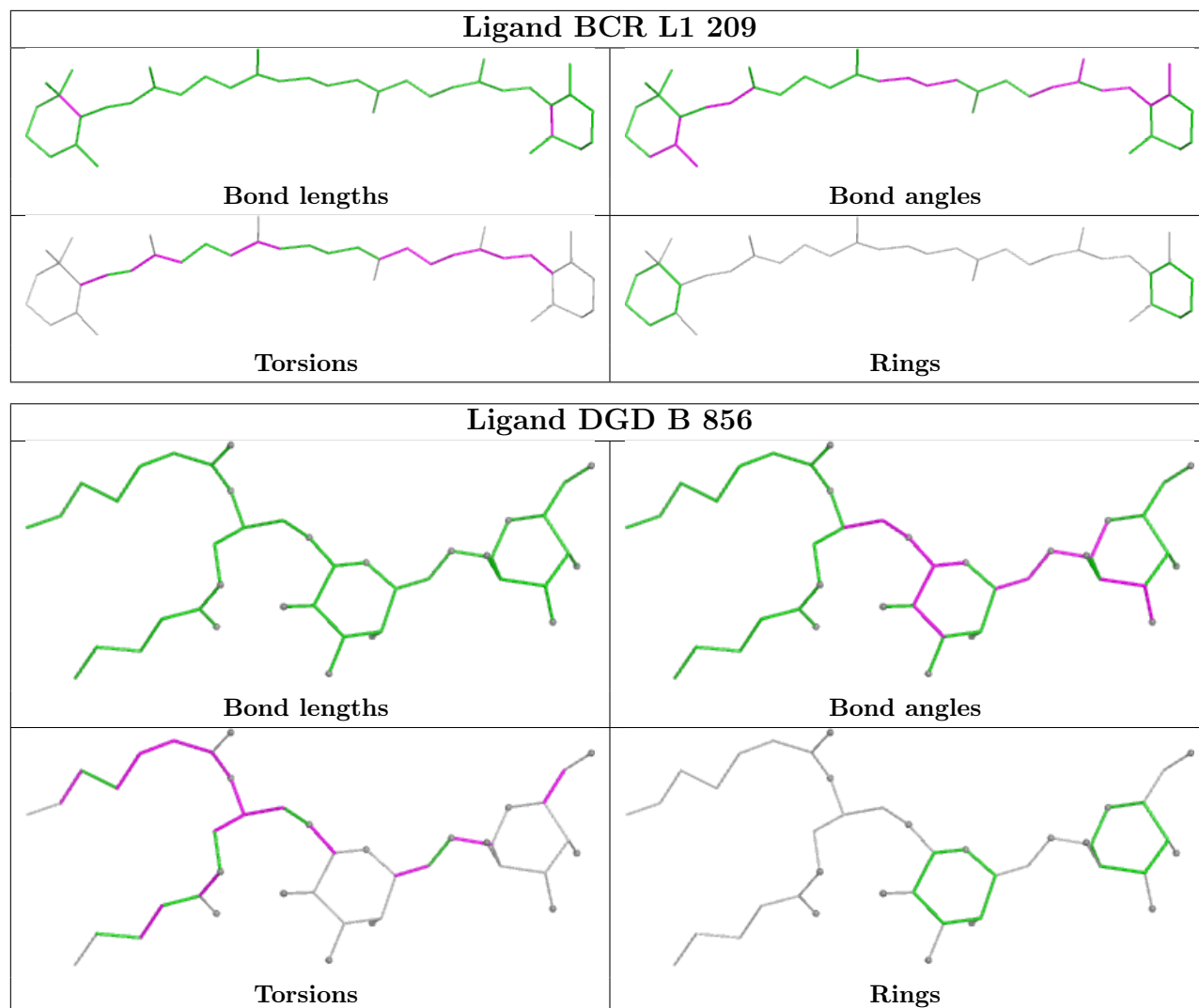
Bond angles



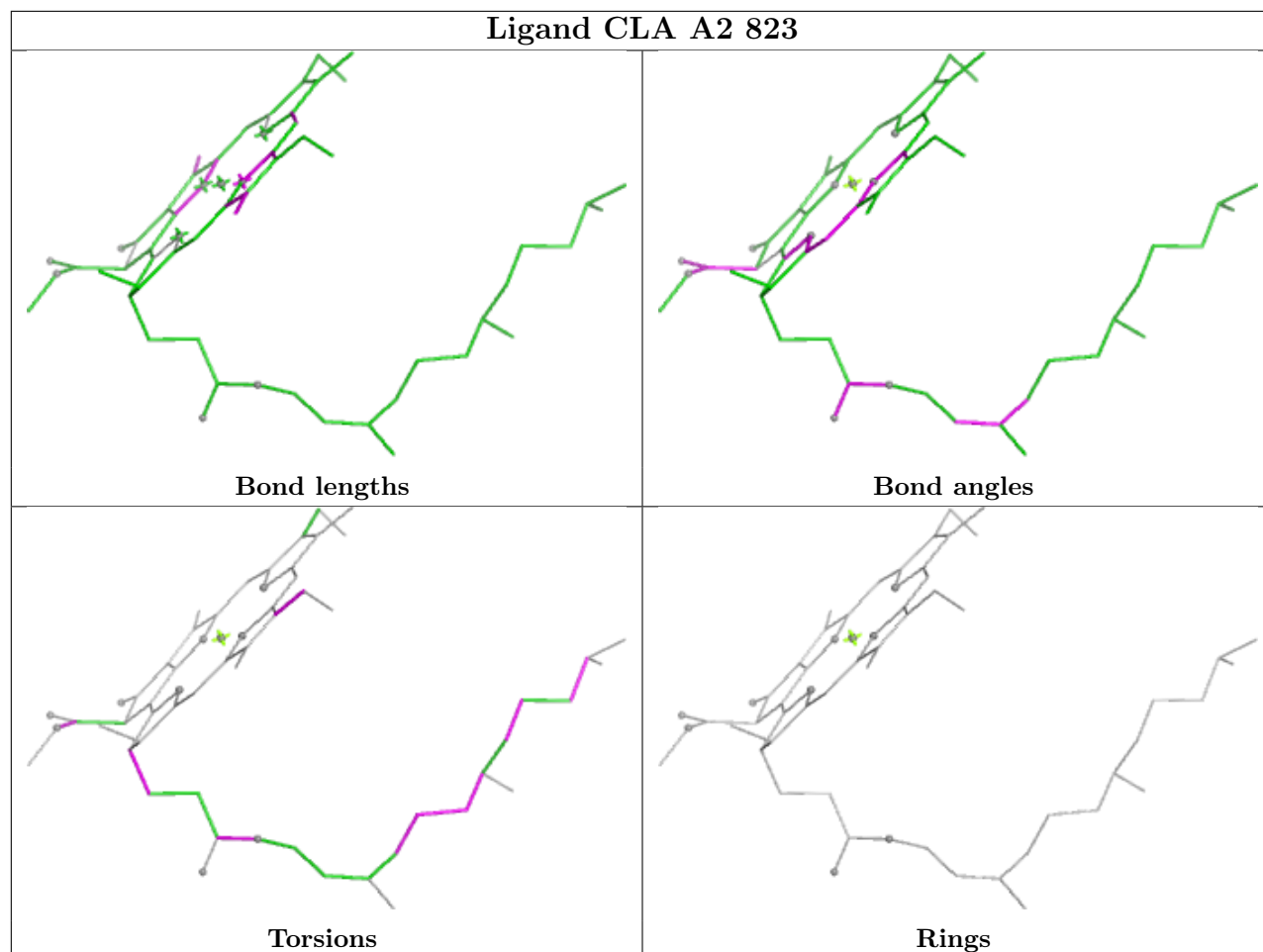
Torsions



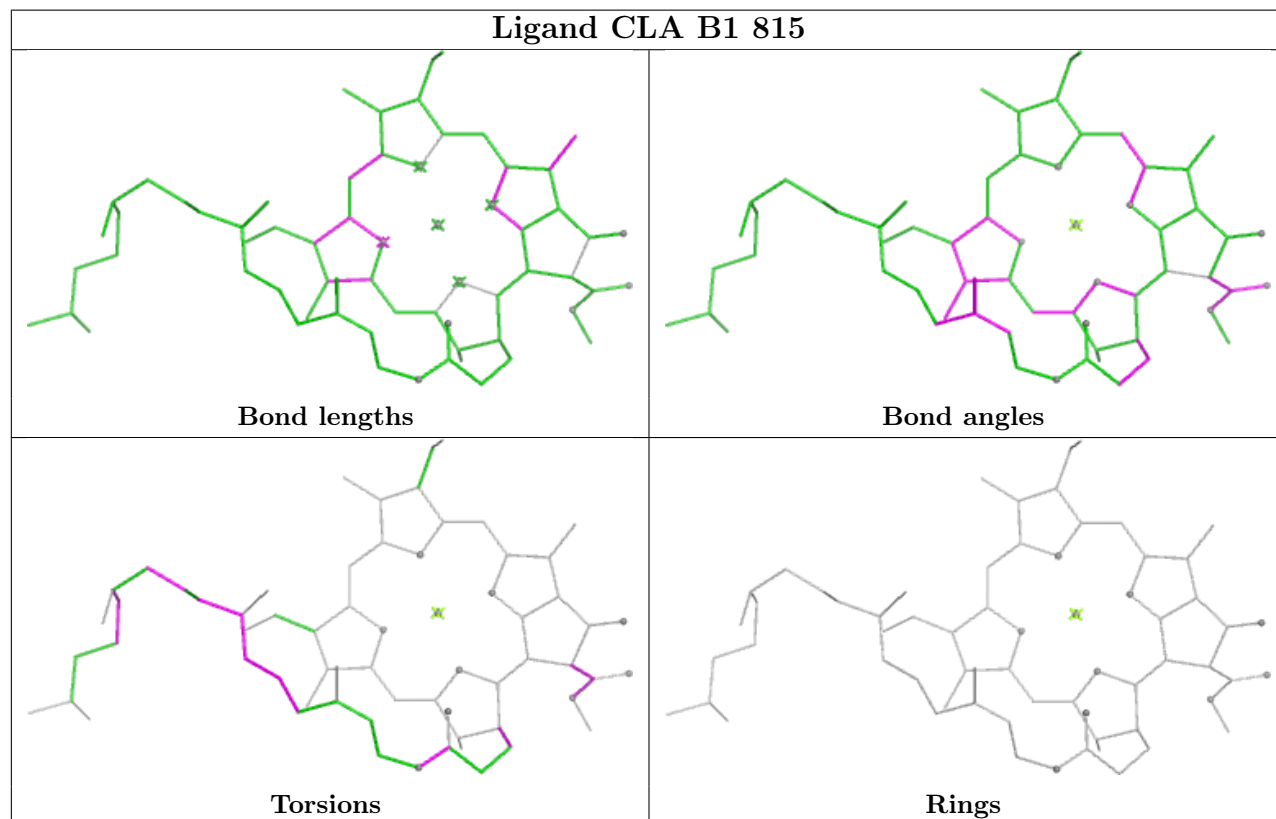
Rings

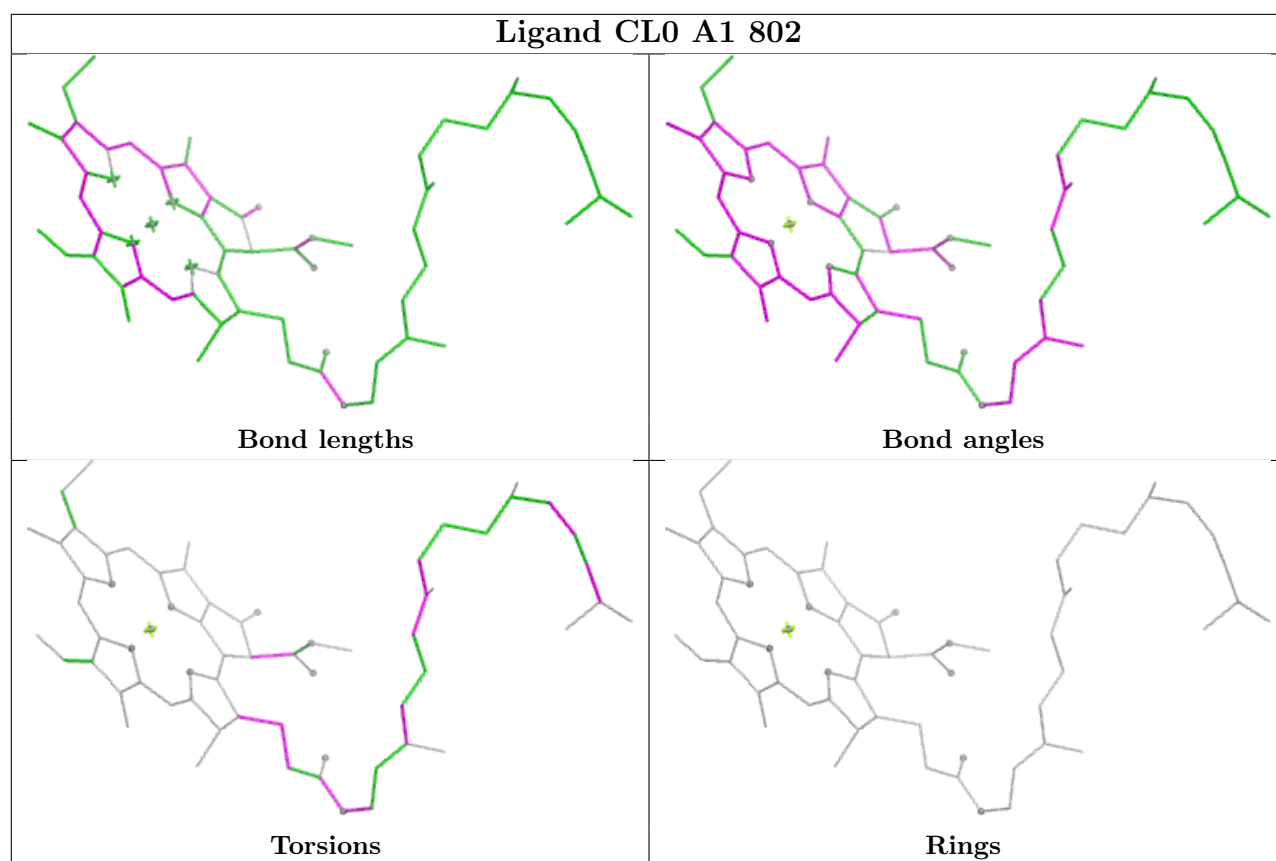


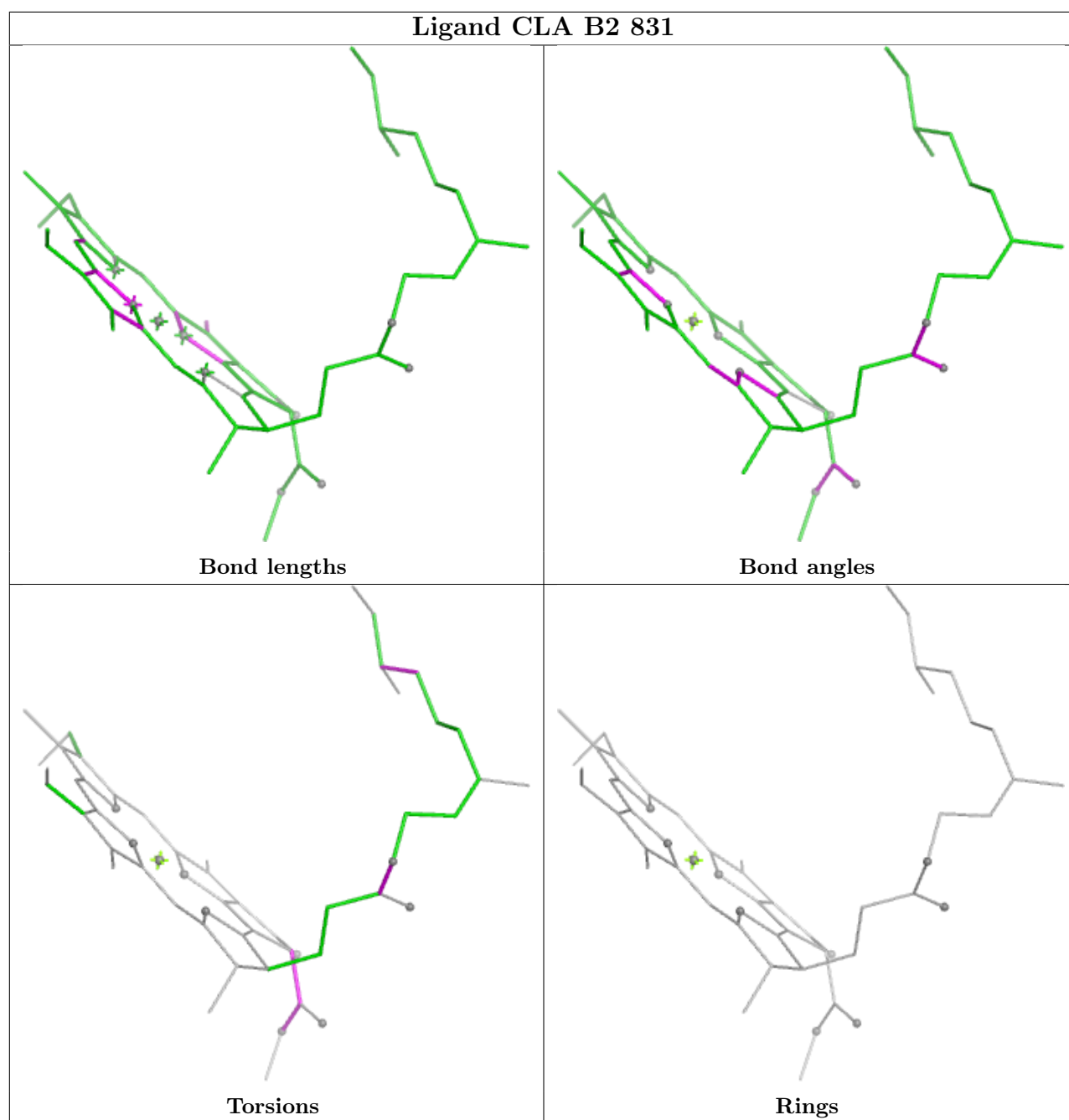
Ligand CLA A2 823



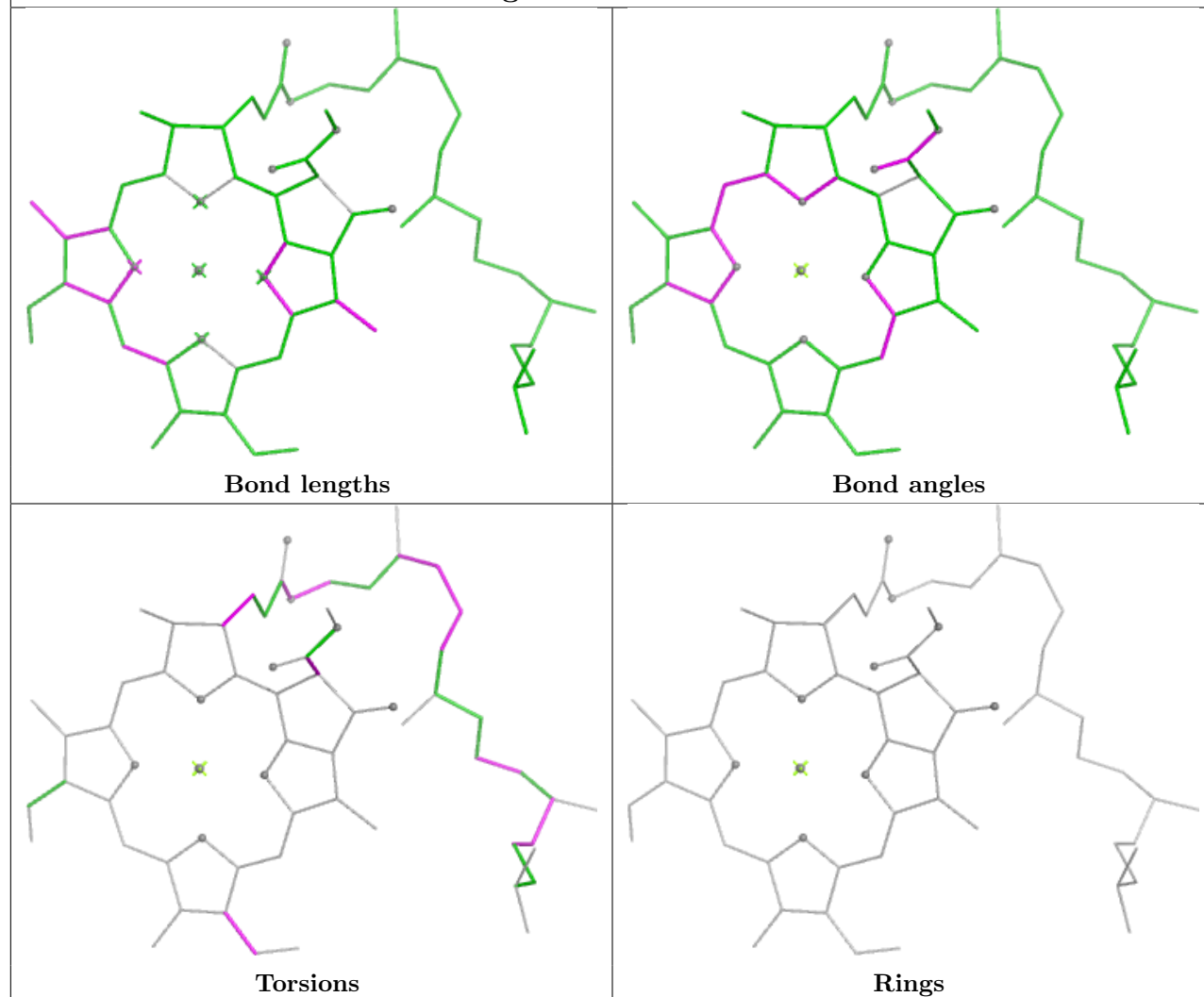
Ligand CLA B1 815



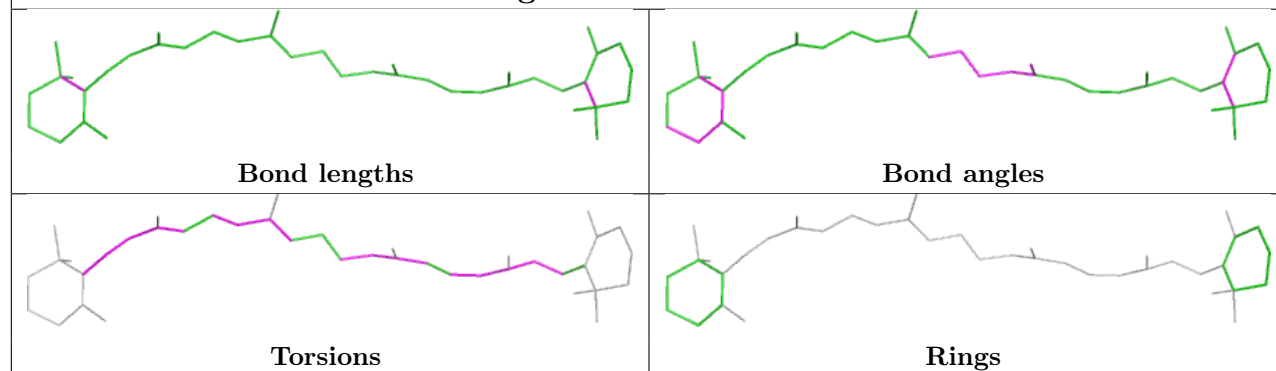


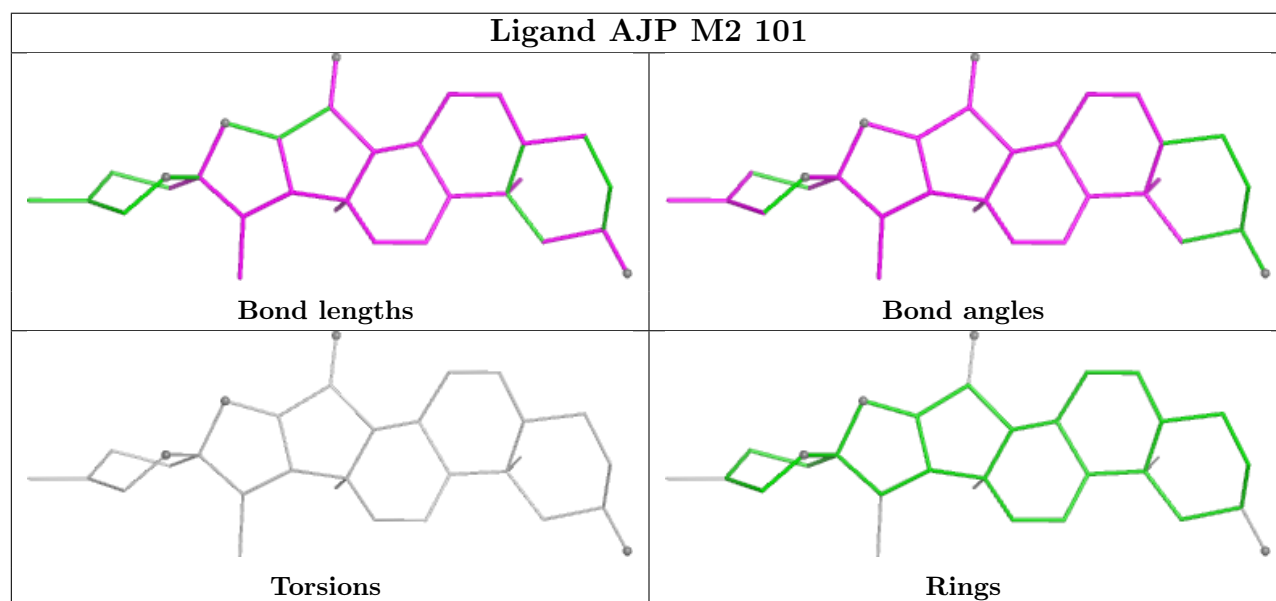
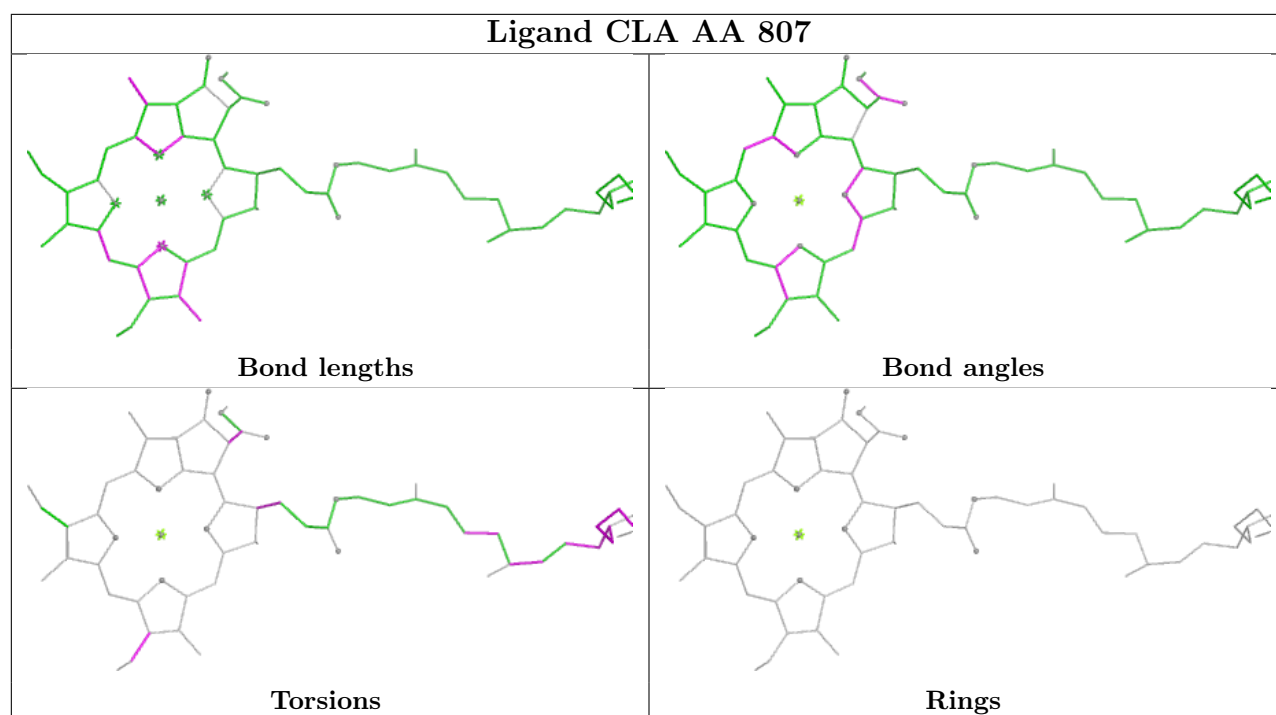


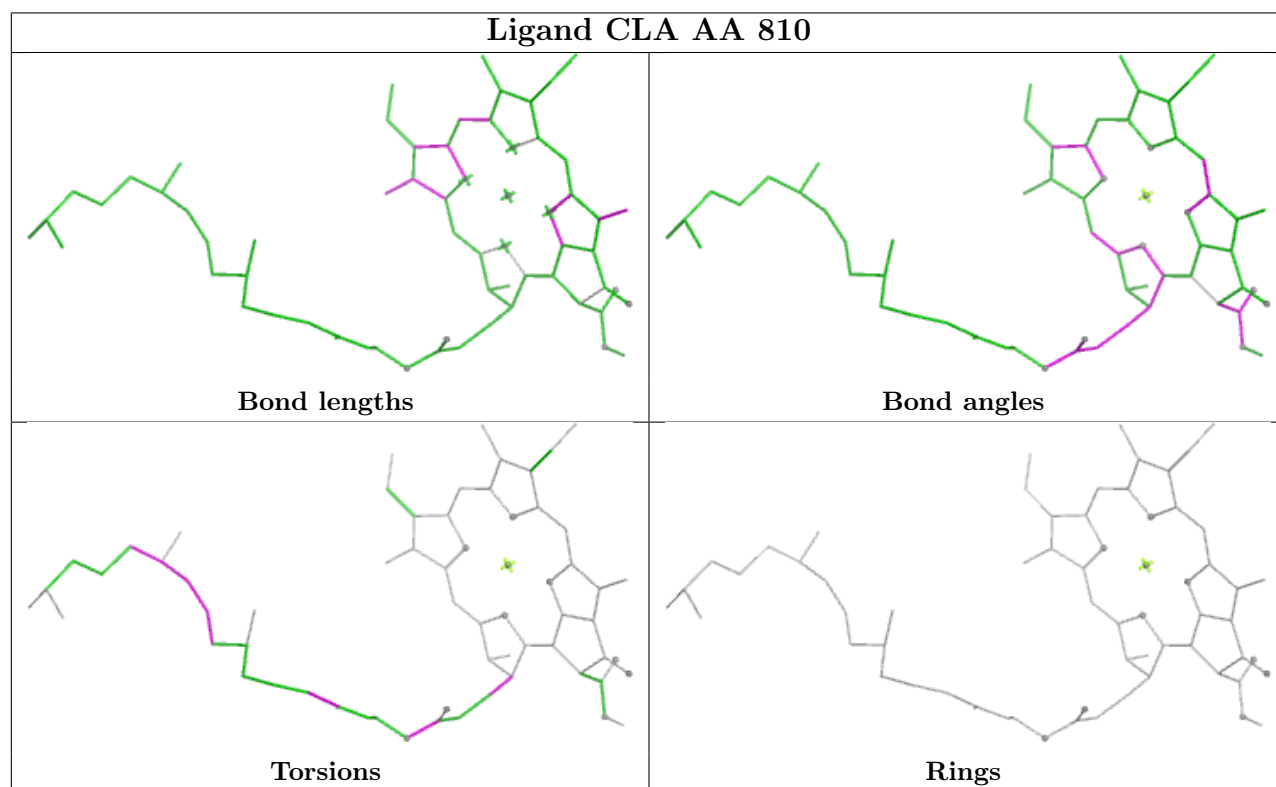
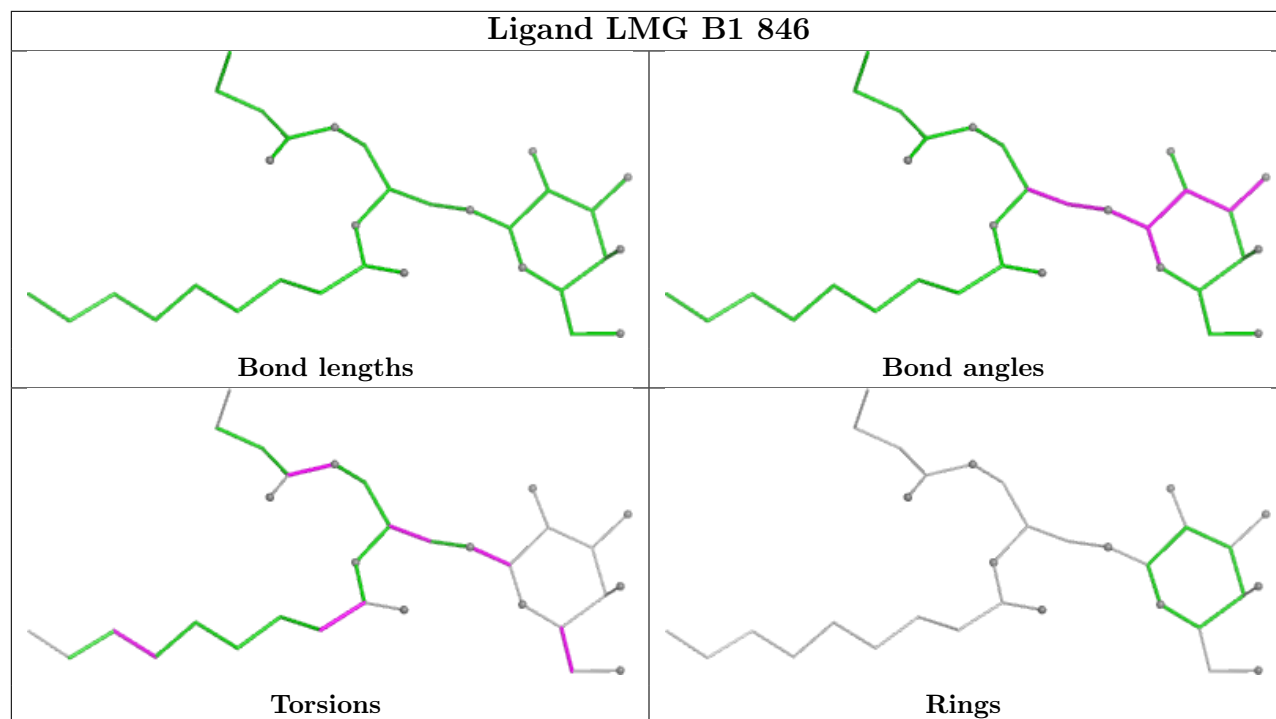
Ligand CLA B 829



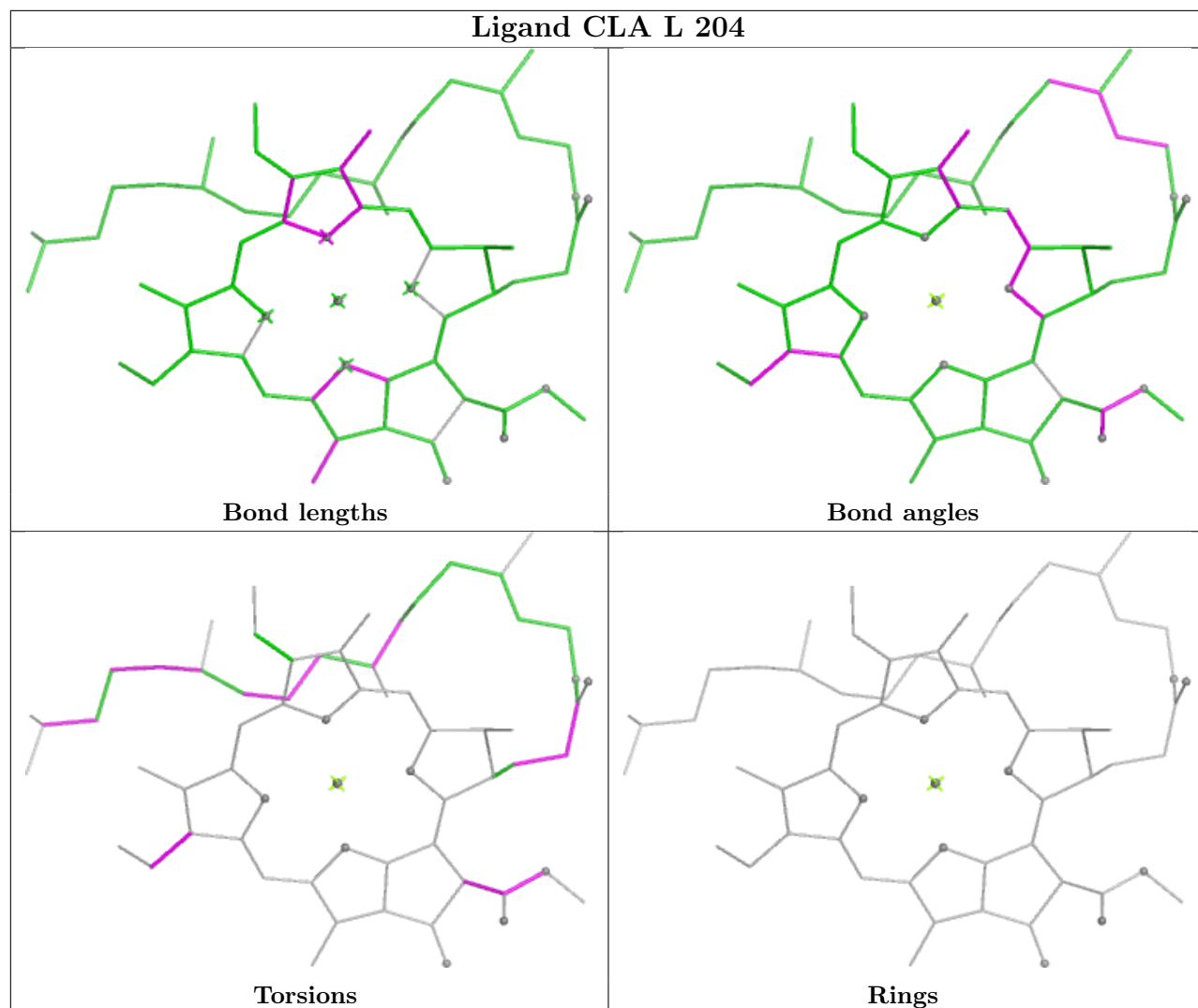
Ligand BCR BB 841

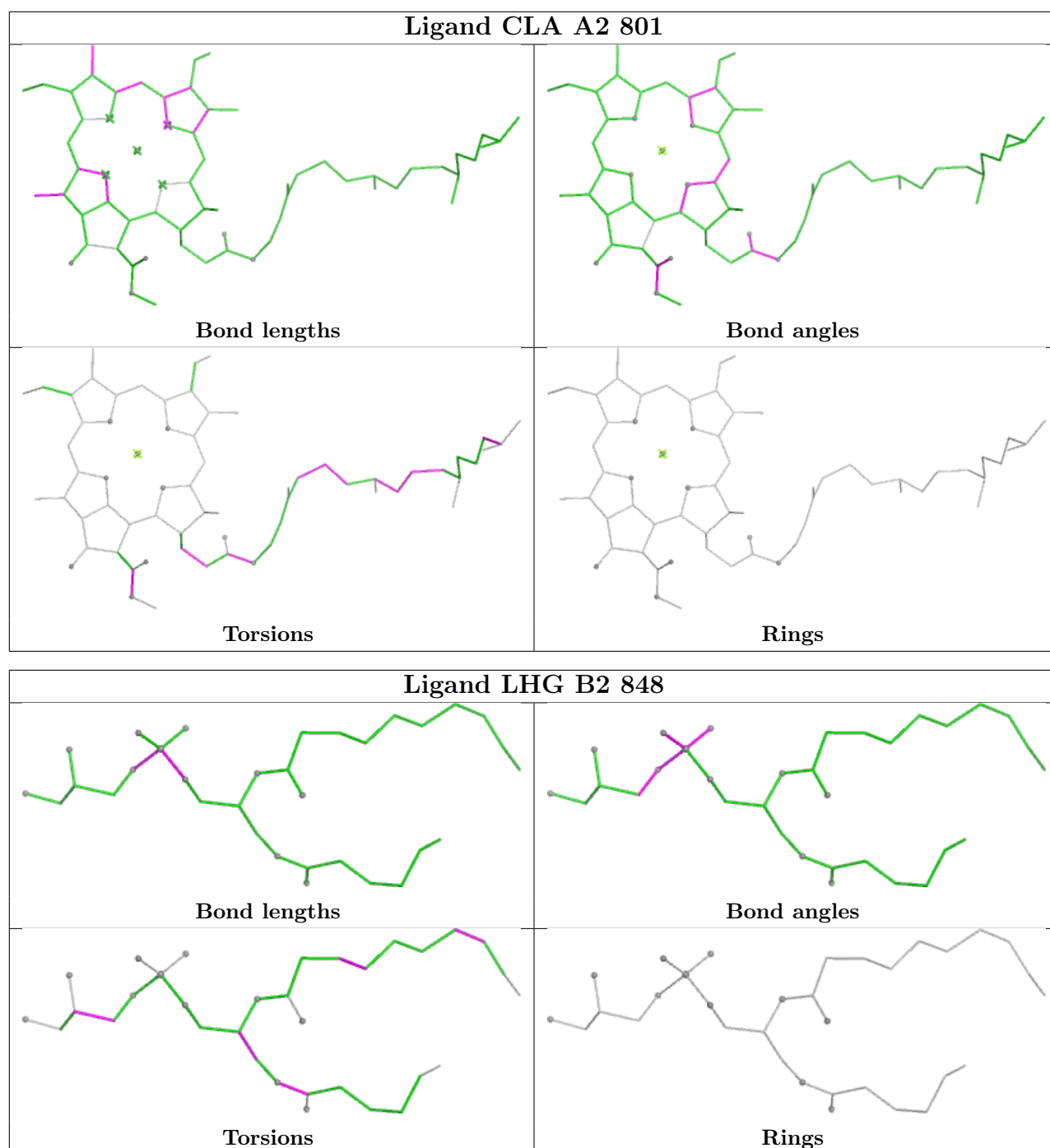


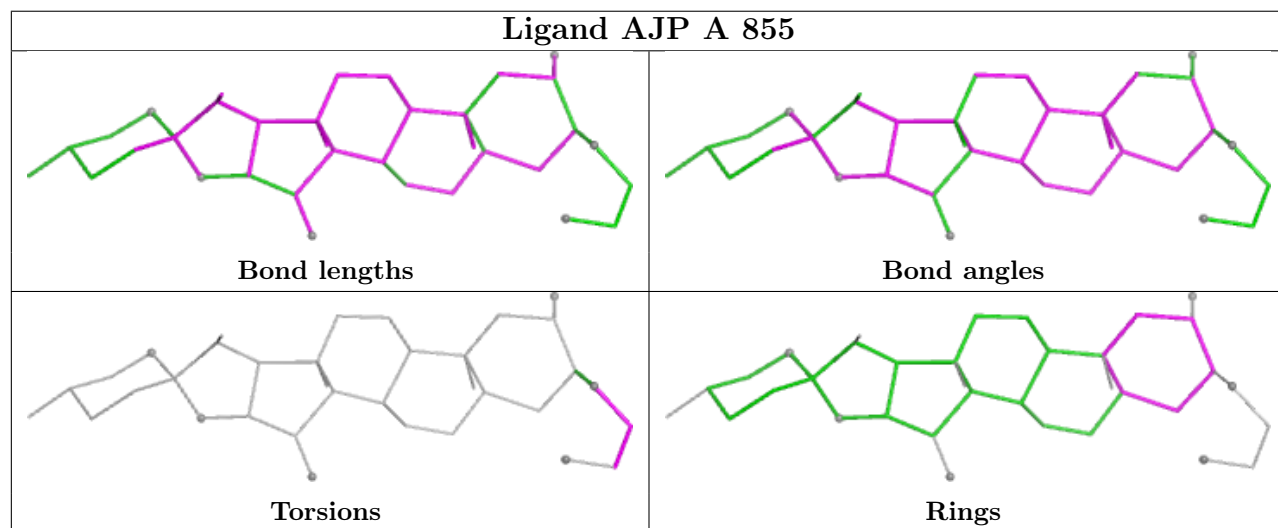
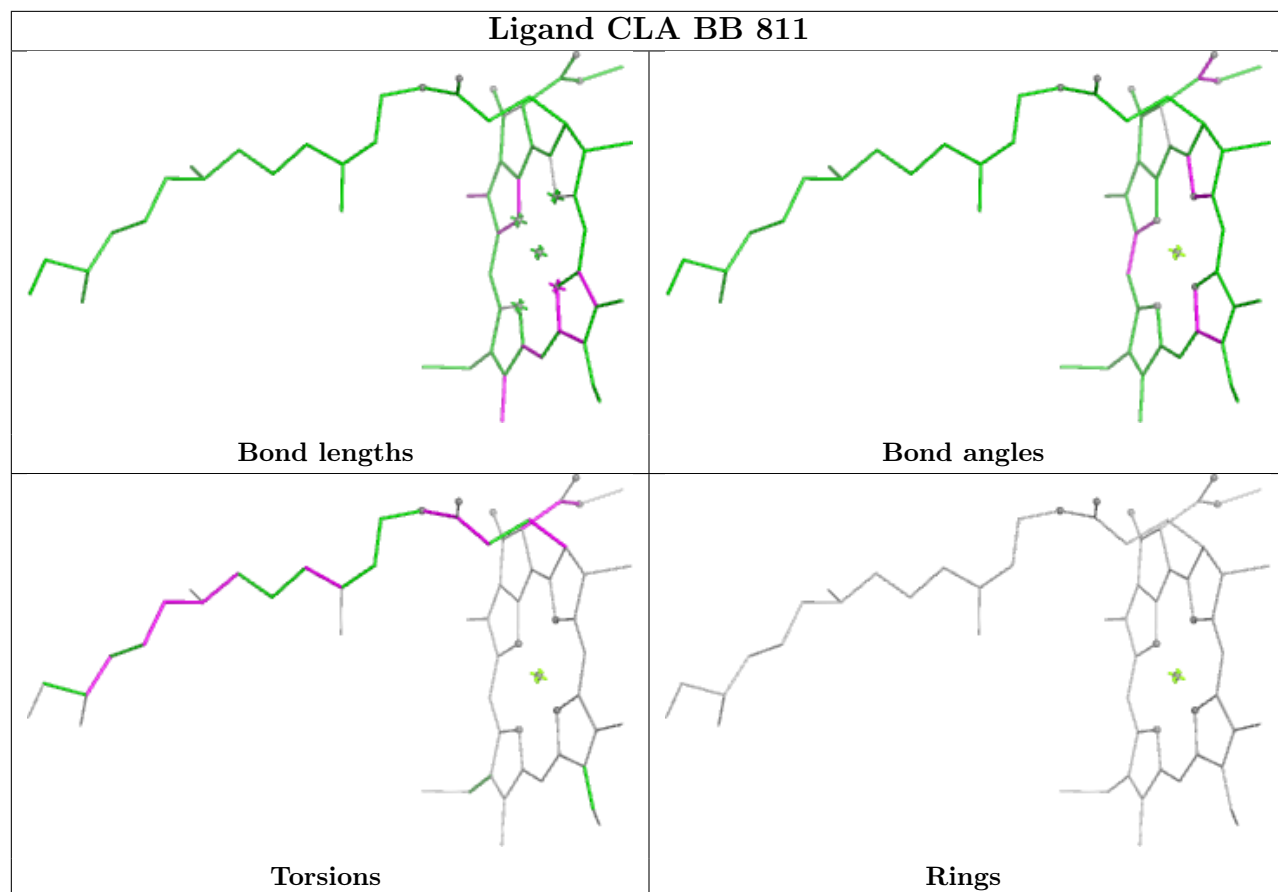


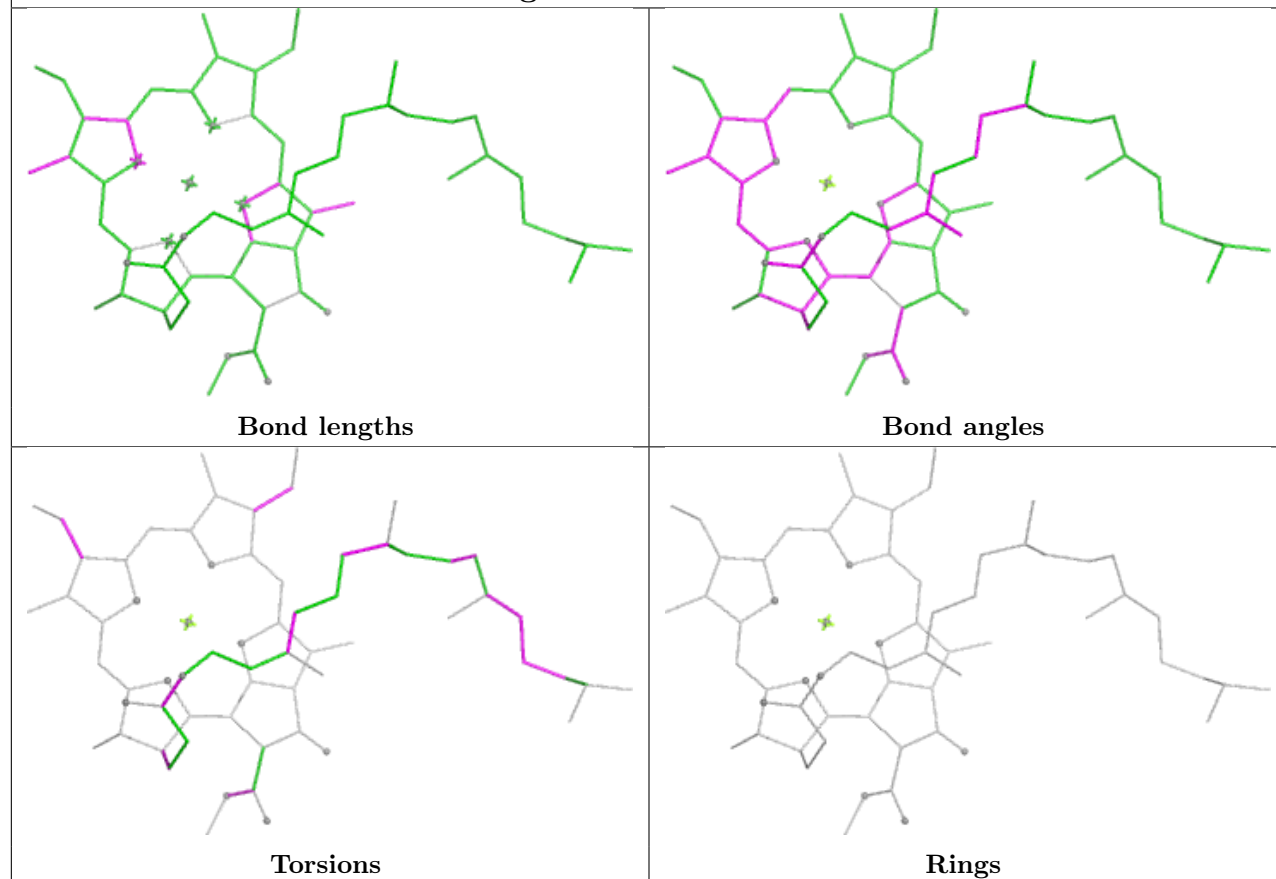
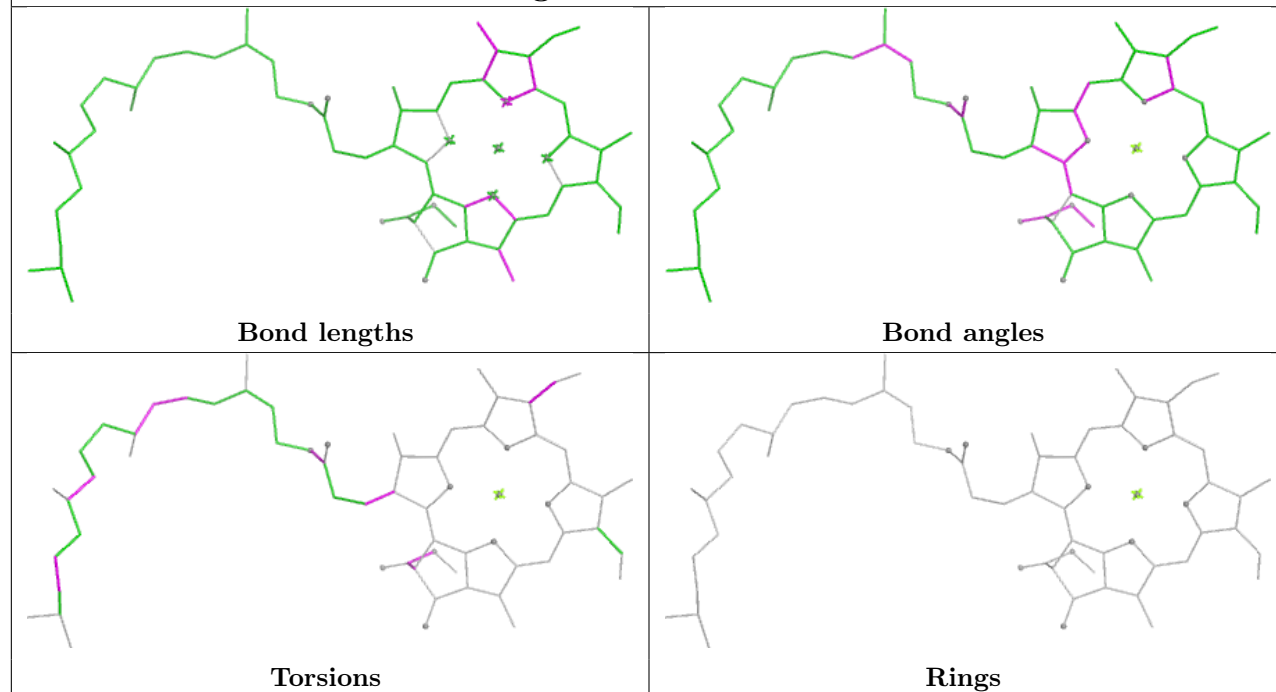


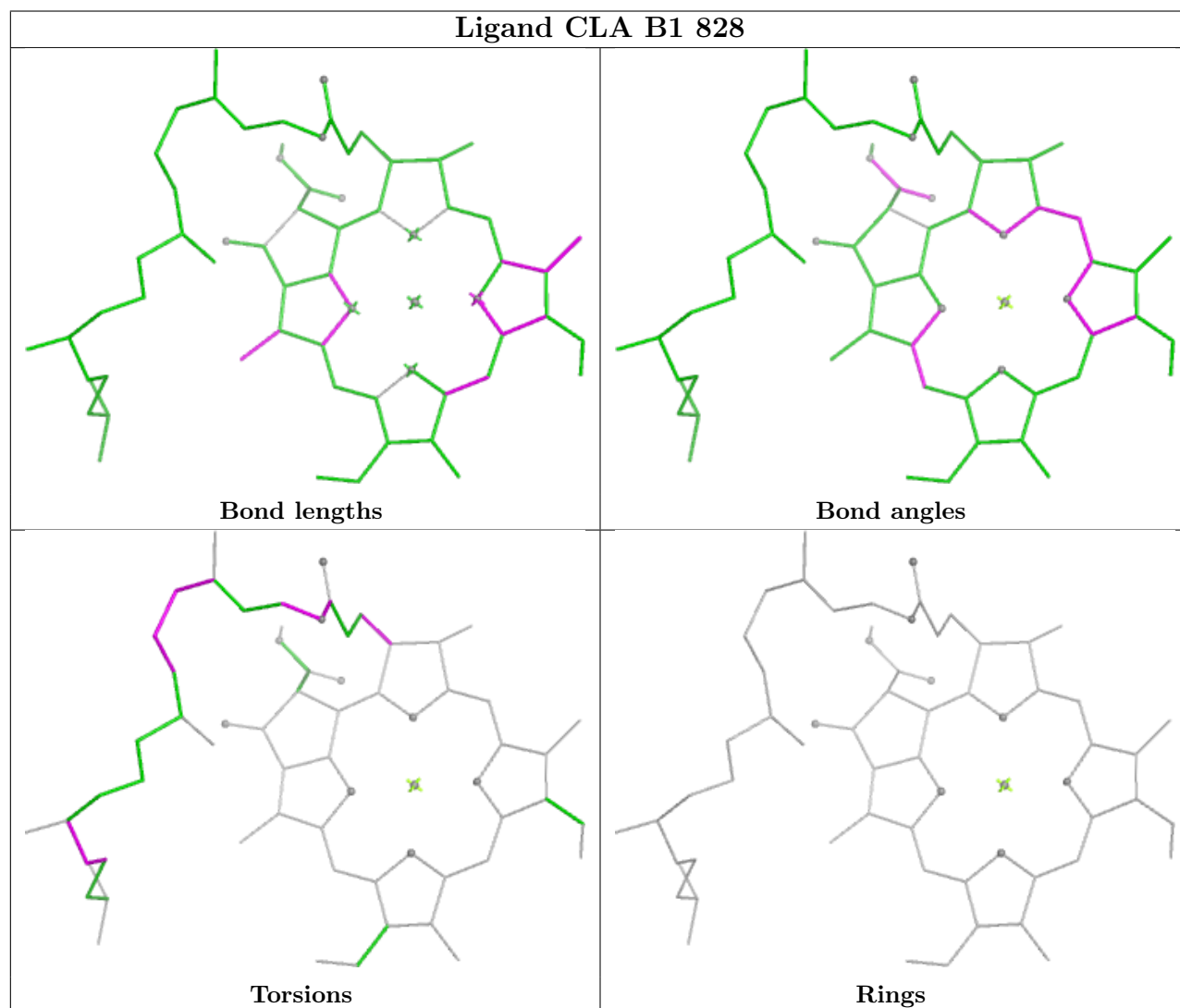
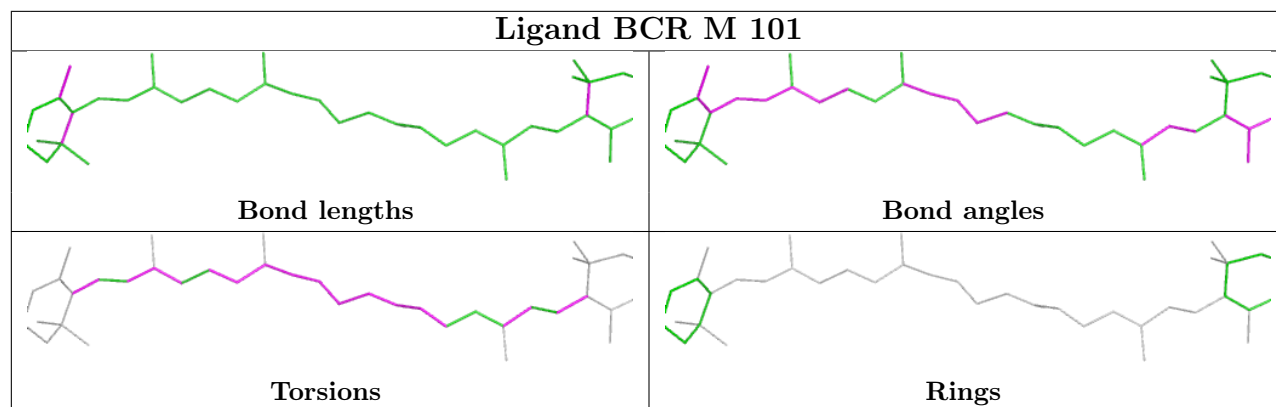
Ligand CLA L 204

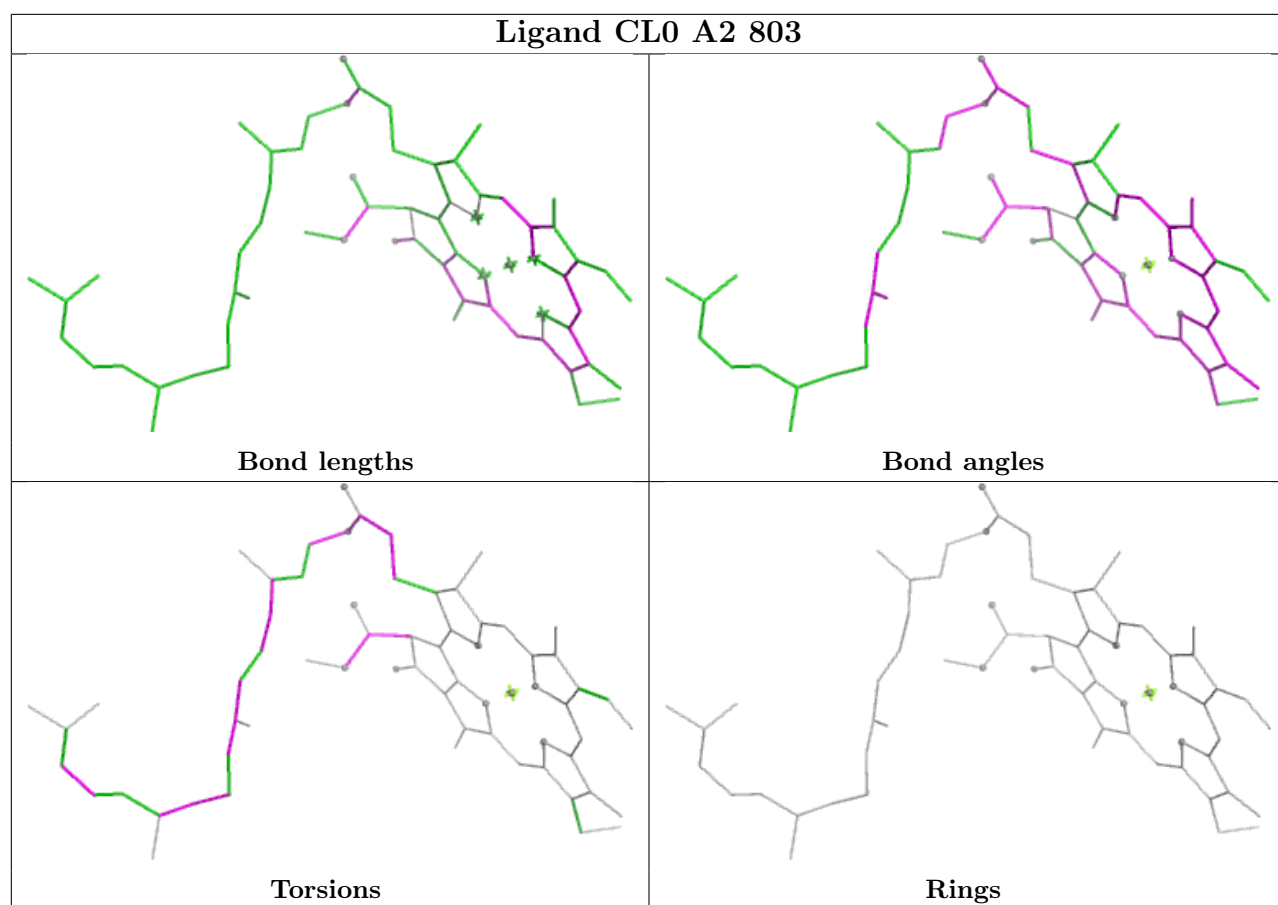




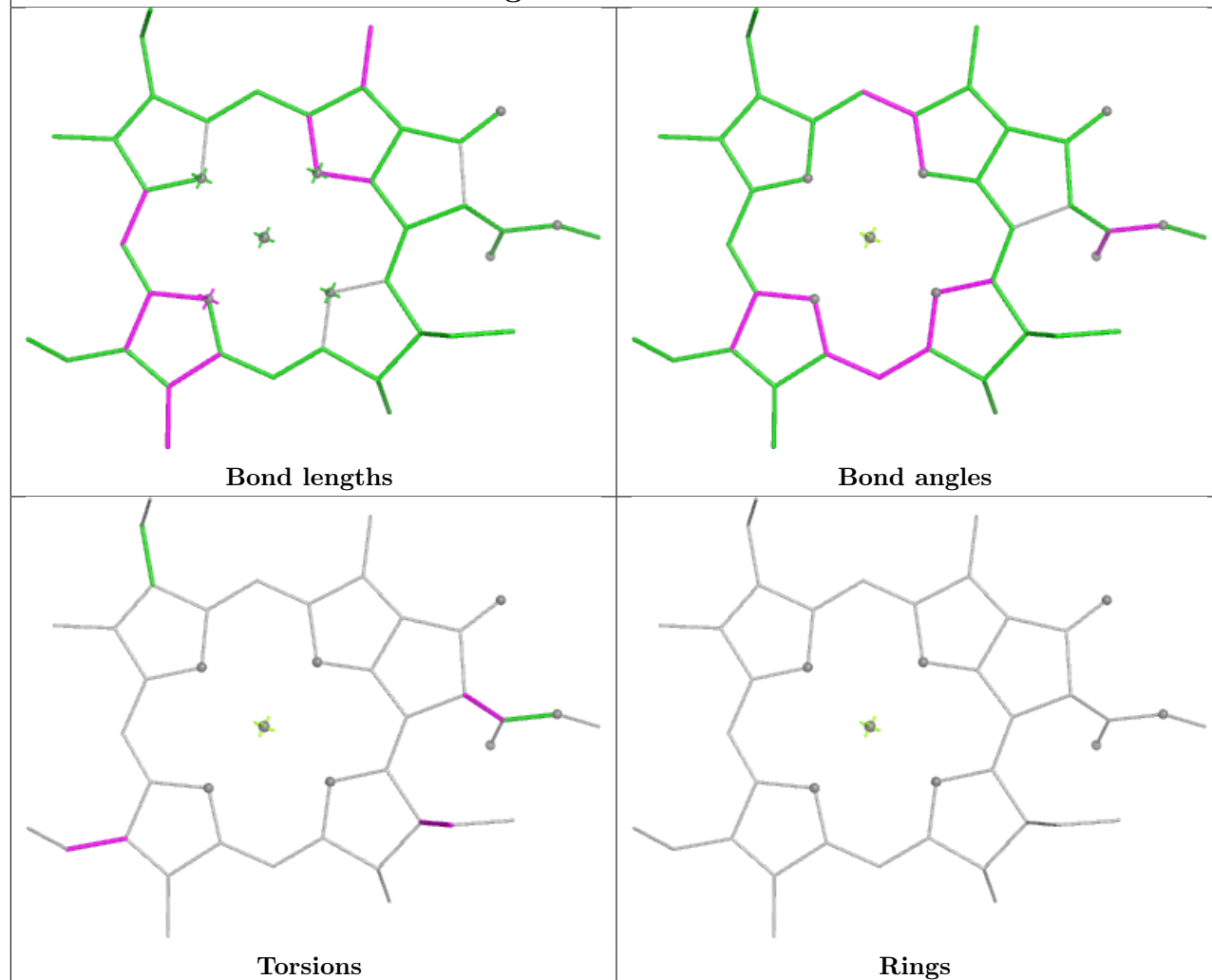


Ligand CLA BB 833**Ligand CLA B 833**

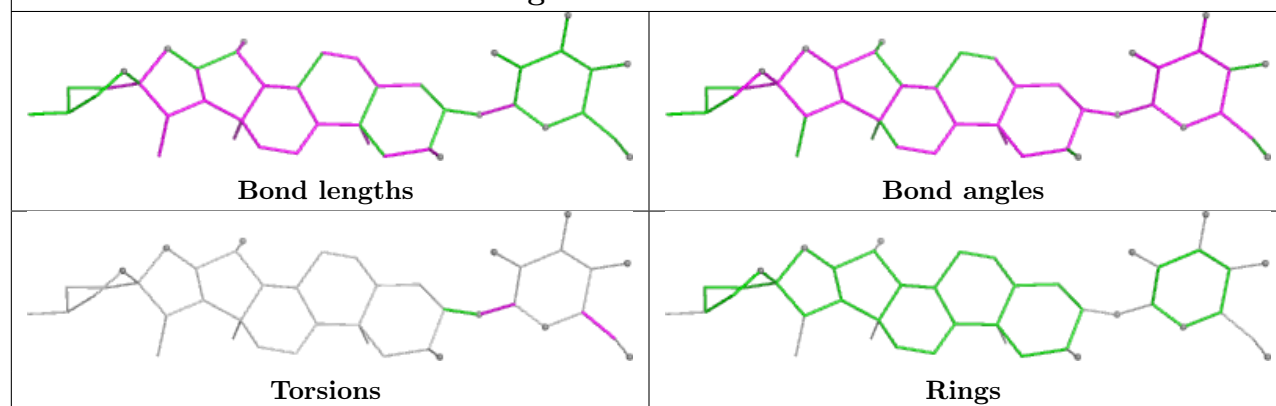




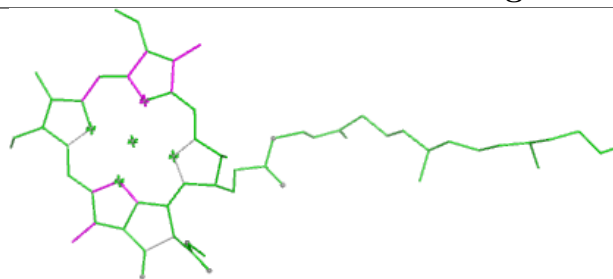
Ligand CLA A 814



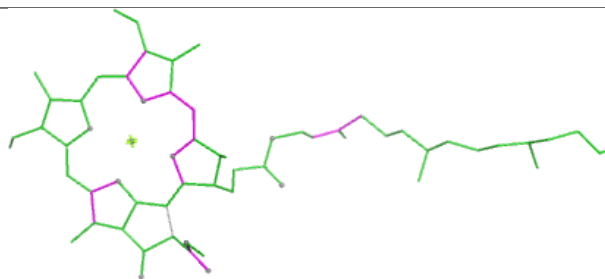
Ligand AJP L1 203



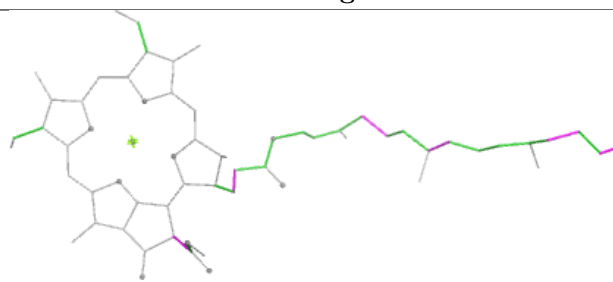
Ligand CLA B2 822



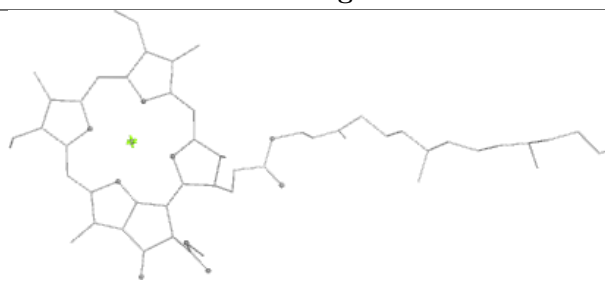
Bond lengths



Bond angles

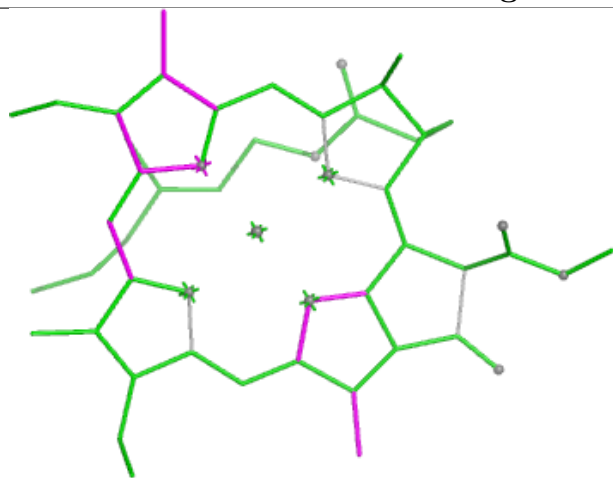


Torsions

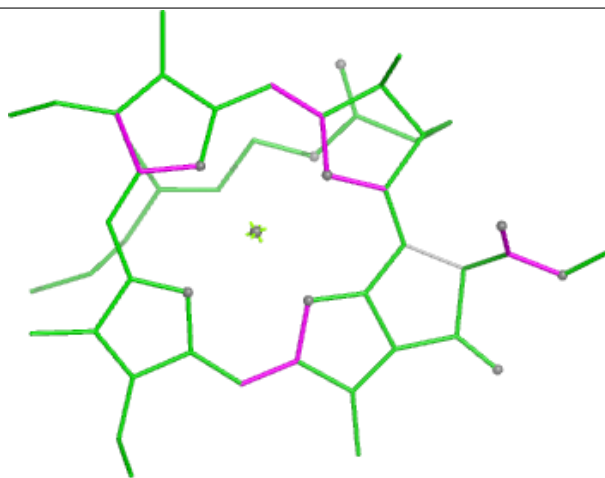


Rings

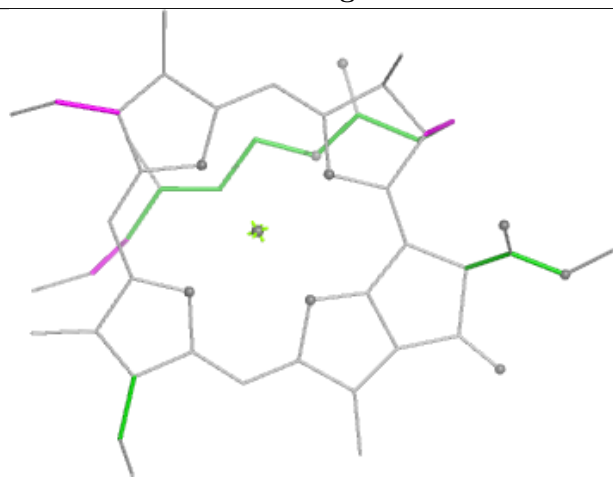
Ligand CLA AA 825



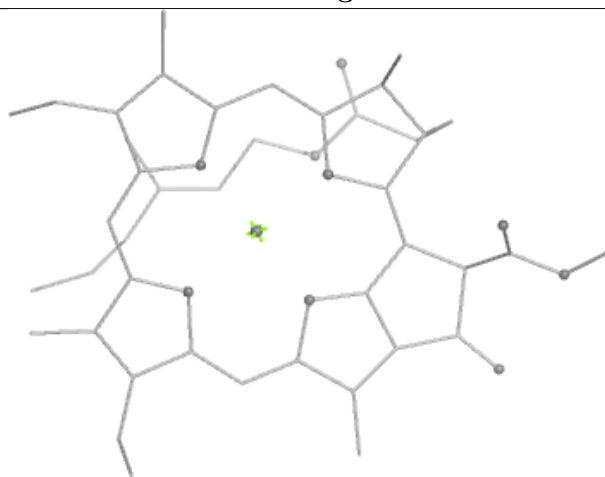
Bond lengths



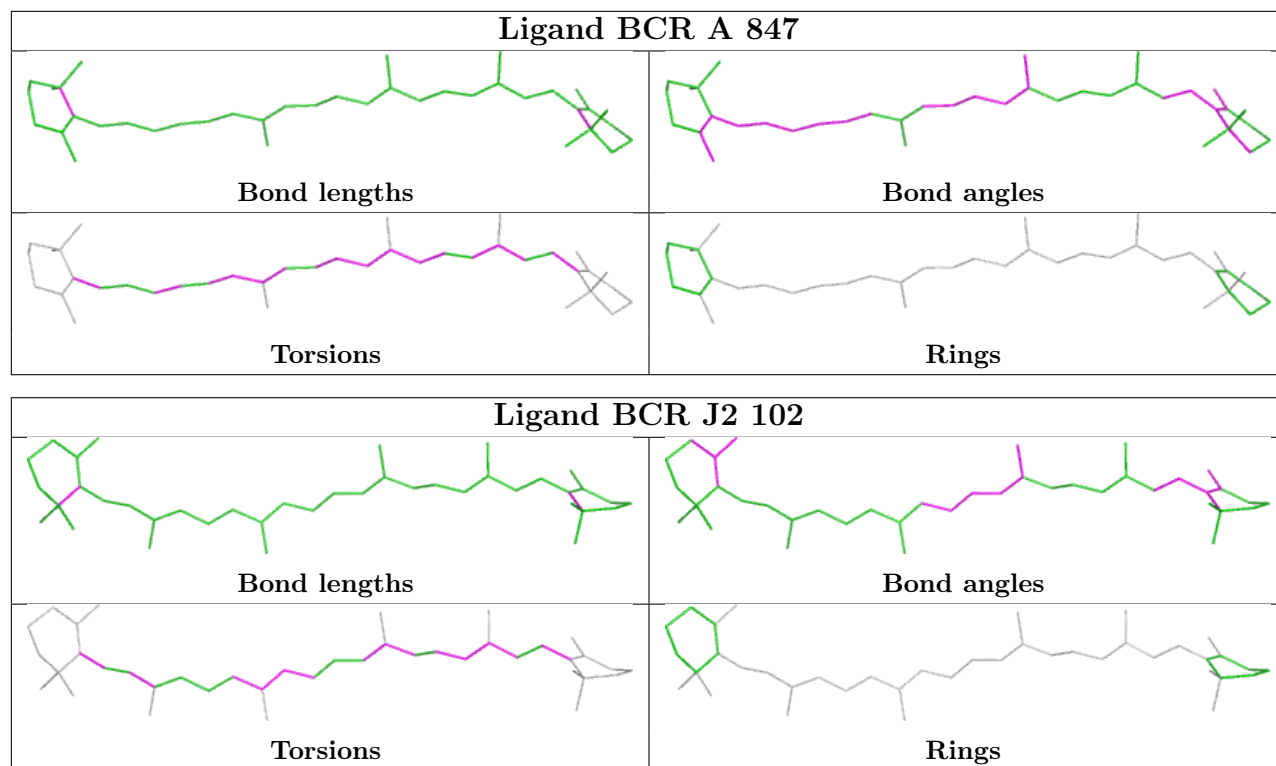
Bond angles

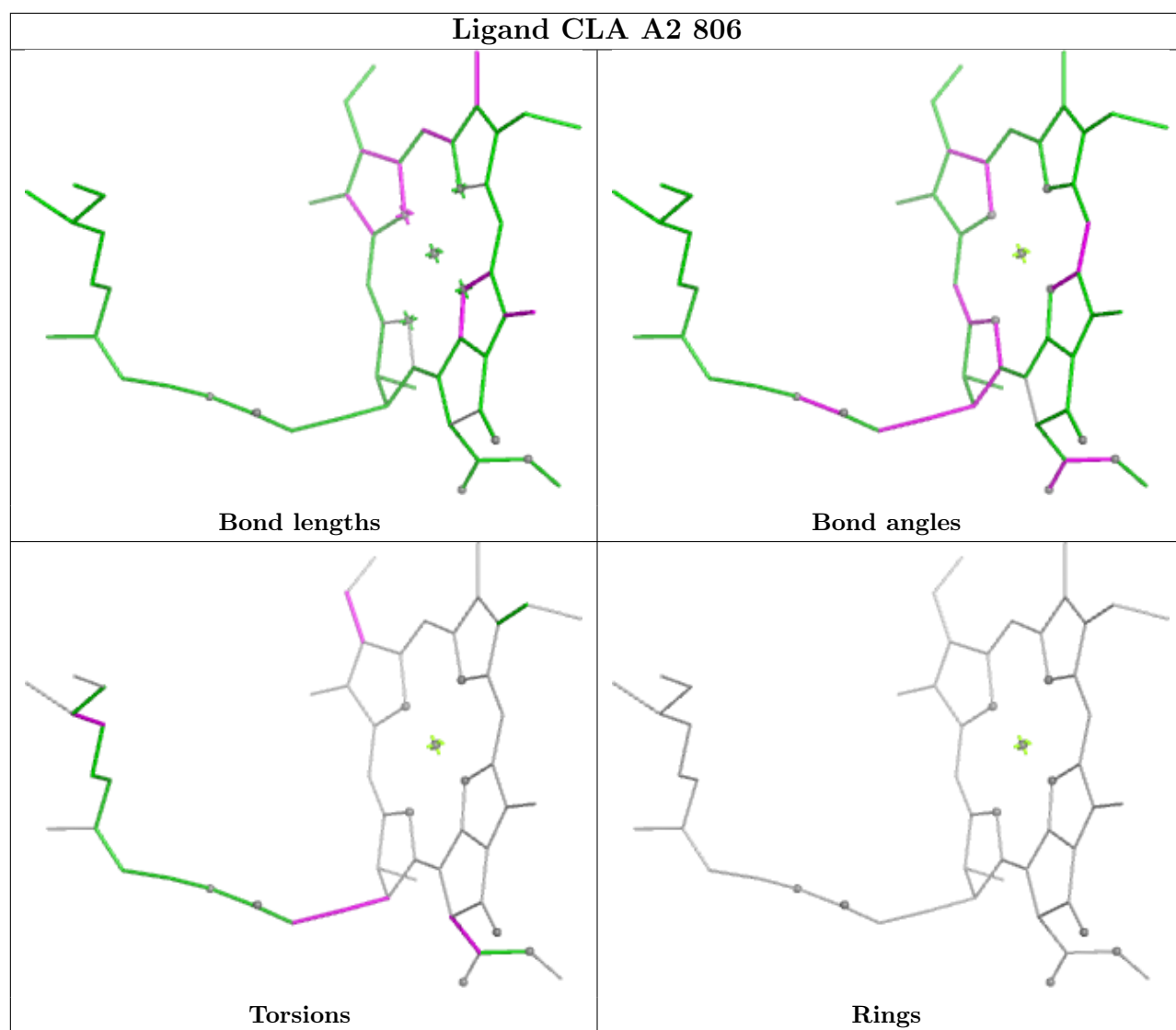


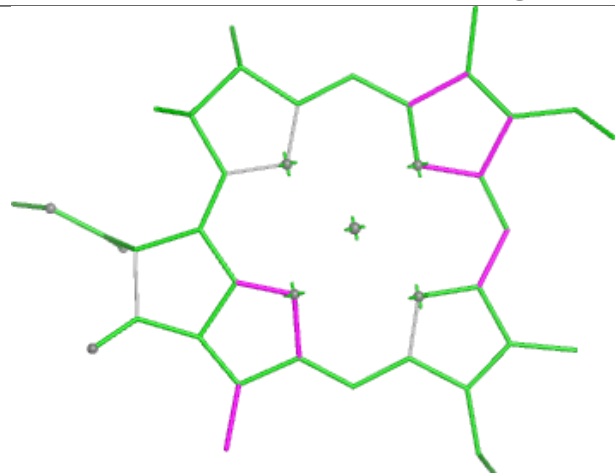
Torsions



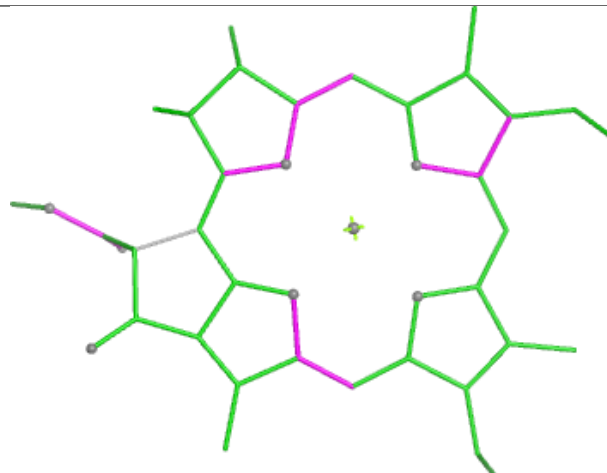
Rings



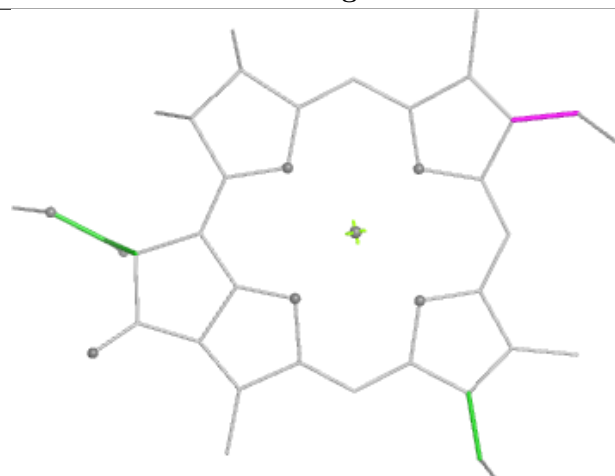


Ligand CLA J1 103

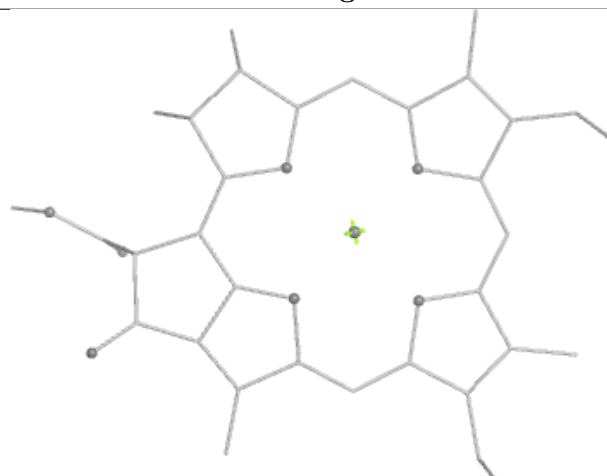
Bond lengths



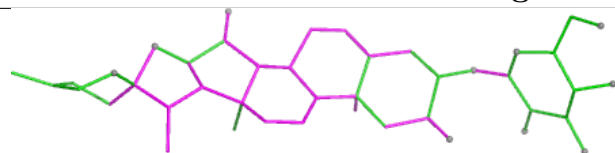
Bond angles



Torsions



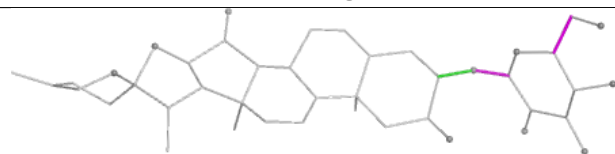
Rings

Ligand AJP L1 204

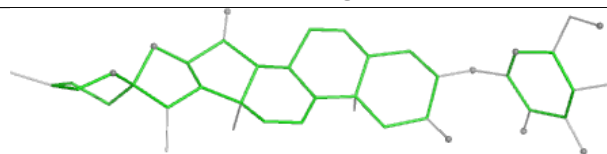
Bond lengths



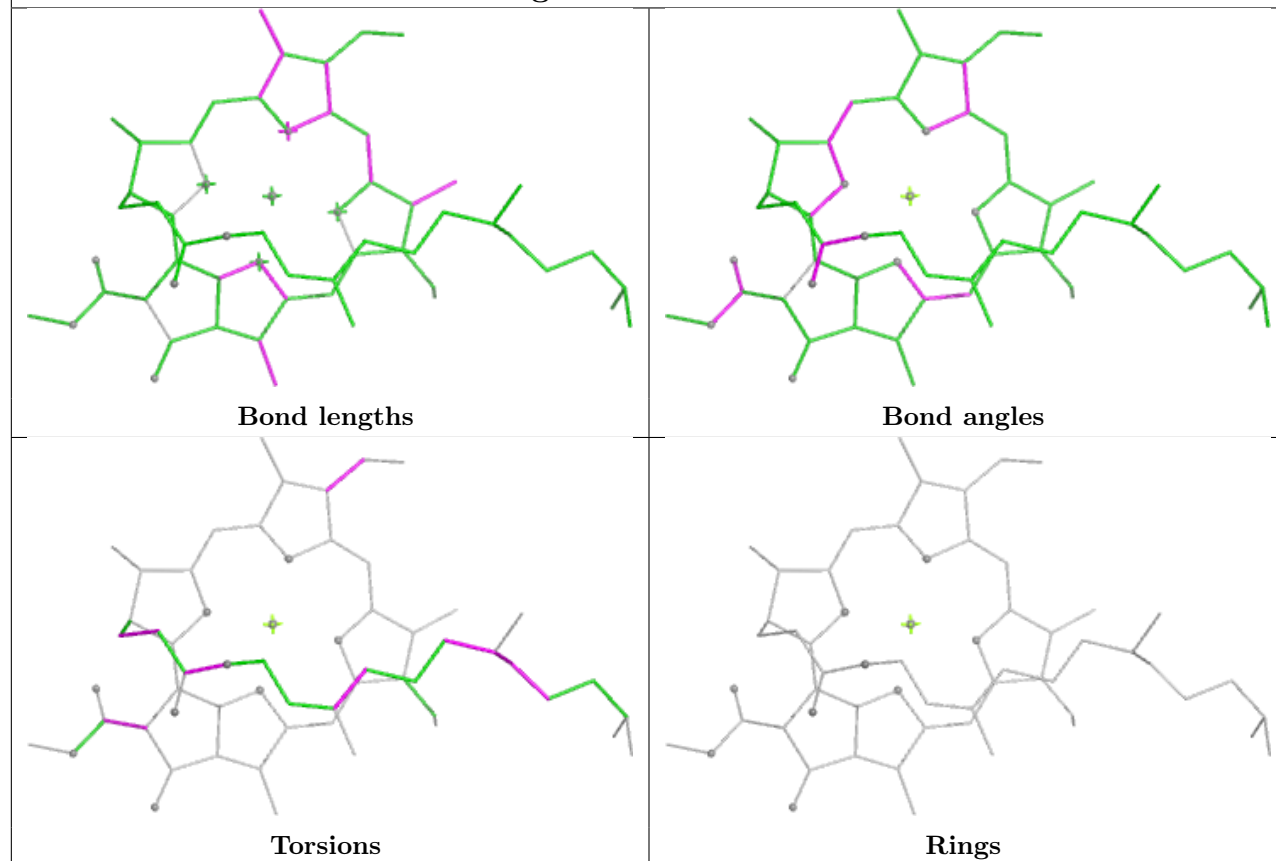
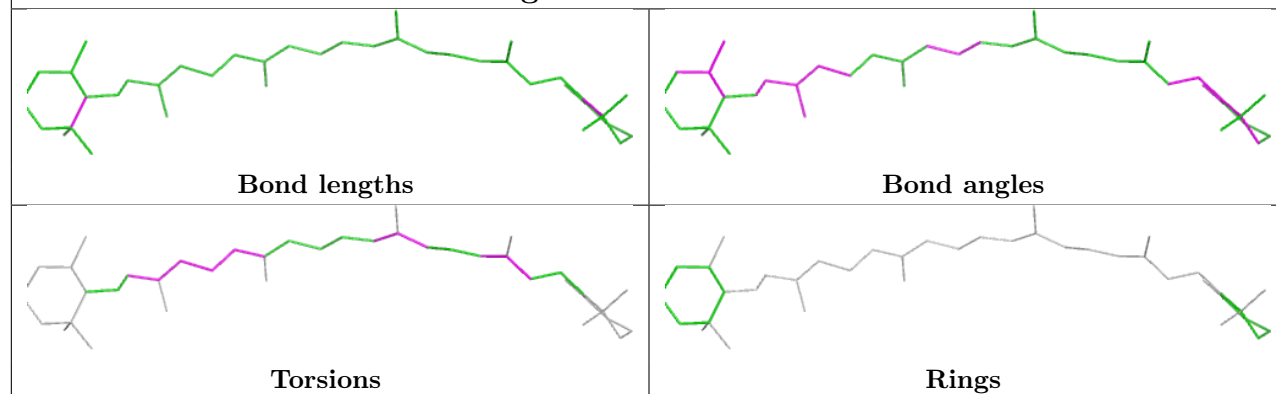
Bond angles



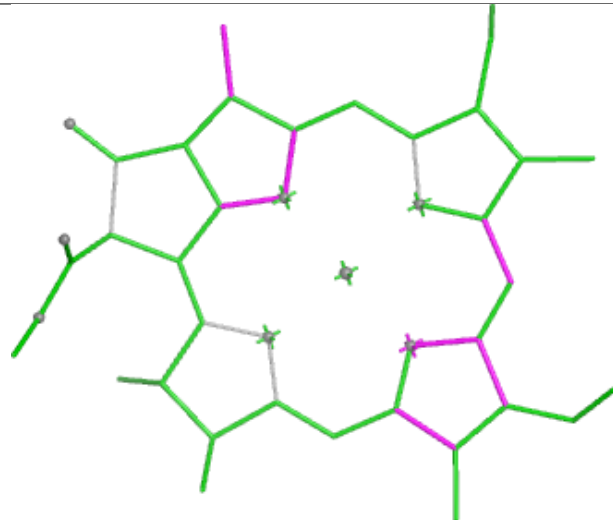
Torsions



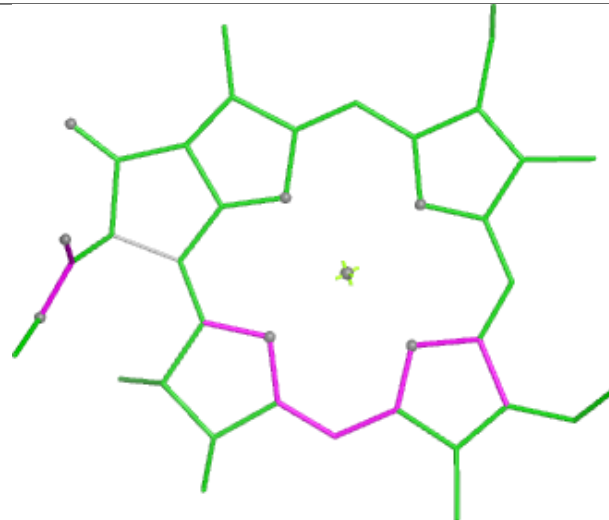
Rings

Ligand CLA A 819**Ligand BCR FF 304**

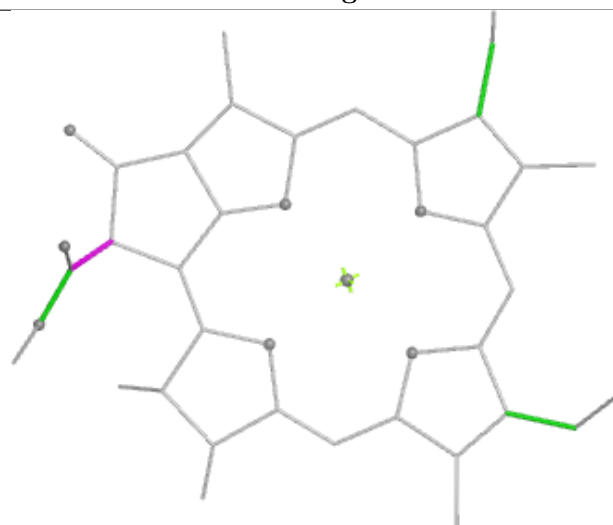
Ligand CLA B1 818



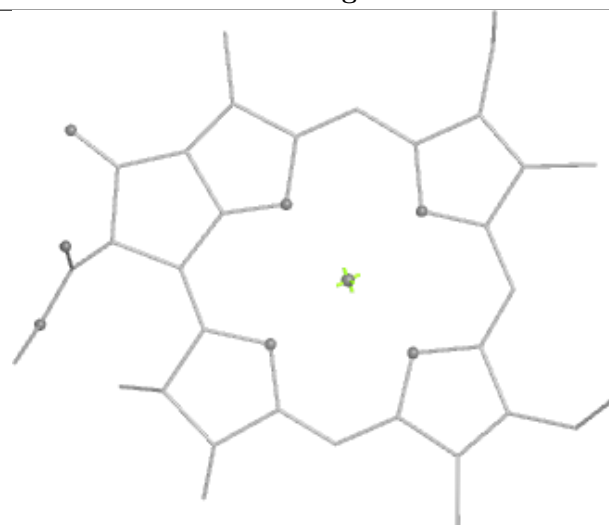
Bond lengths



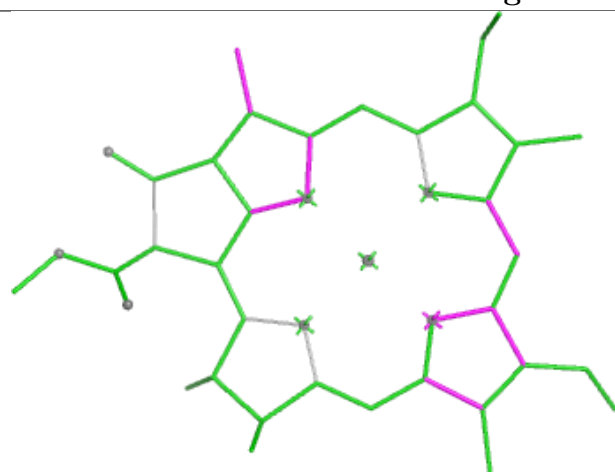
Bond angles



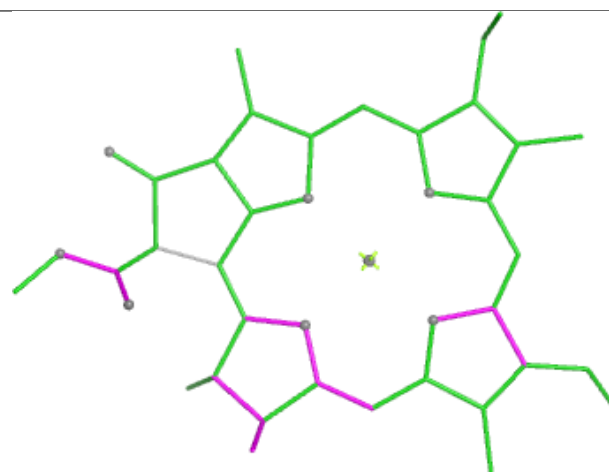
Torsions



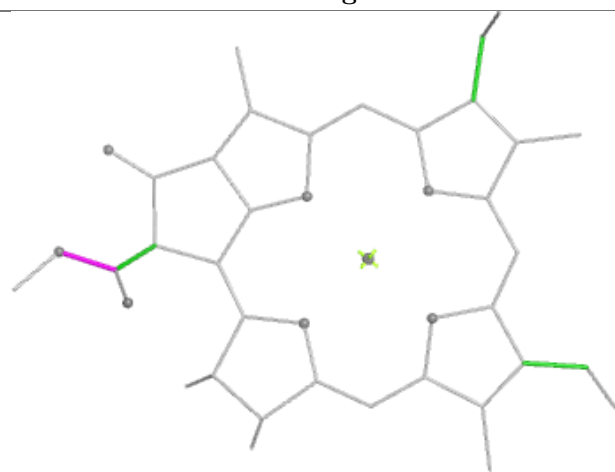
Rings

Ligand CLA BB 819

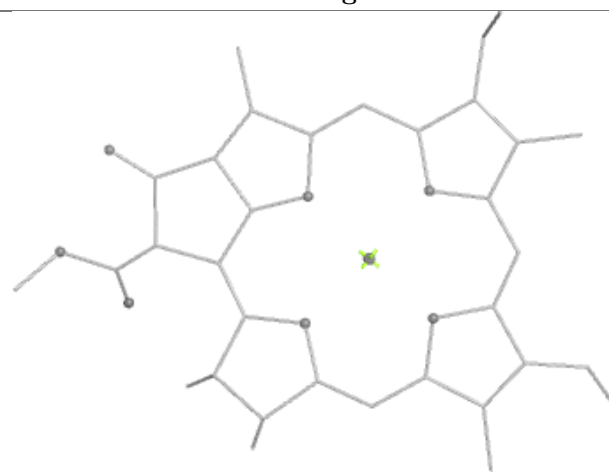
Bond lengths



Bond angles



Torsions



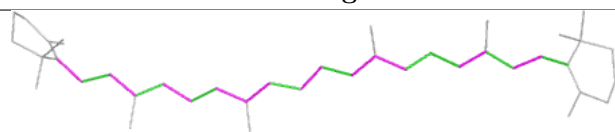
Rings

Ligand BCR BB 843

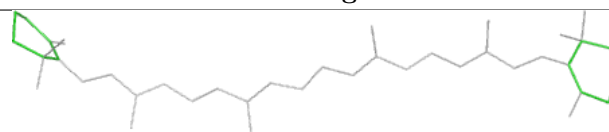
Bond lengths



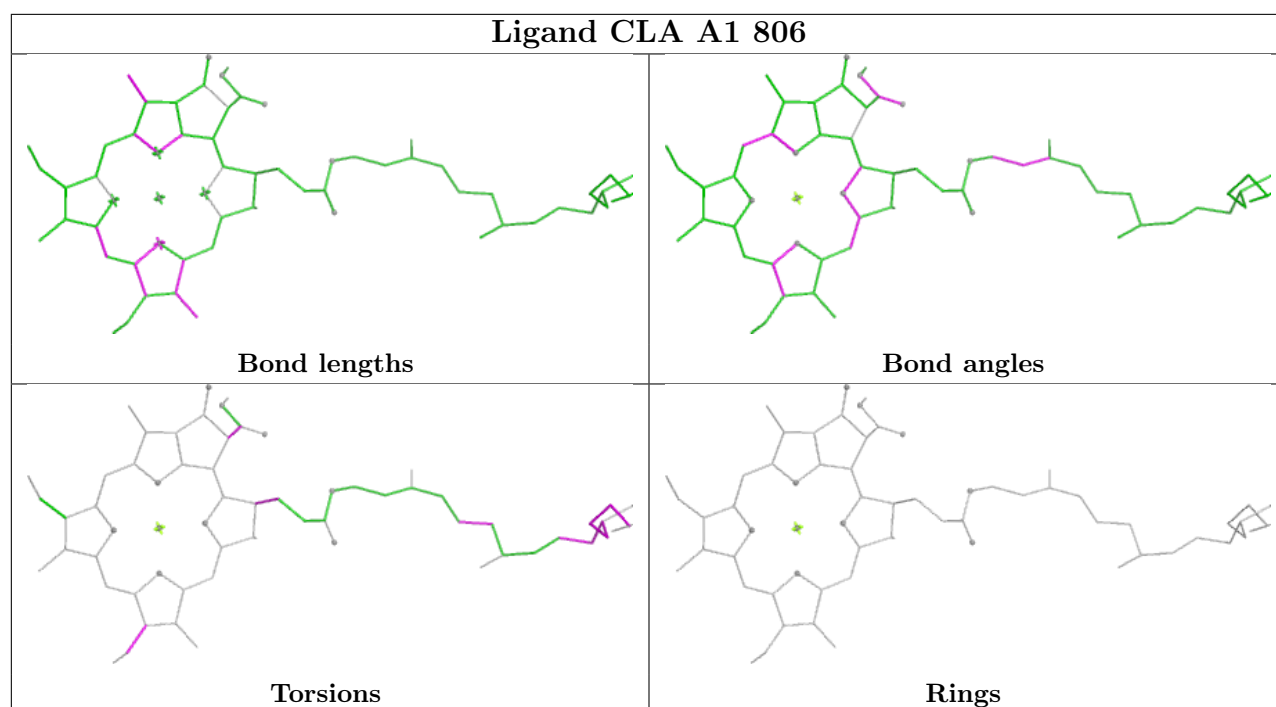
Bond angles



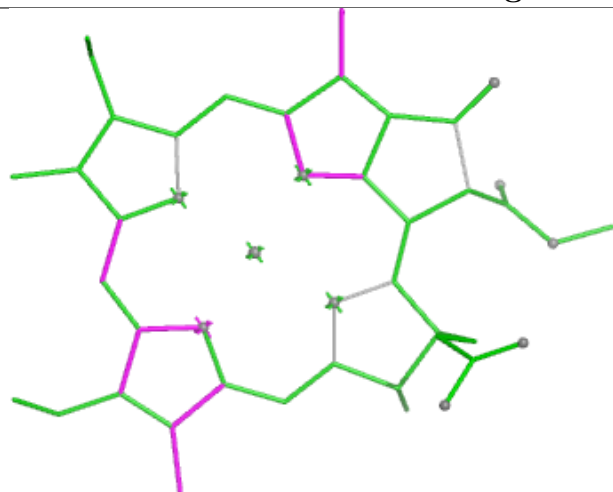
Torsions



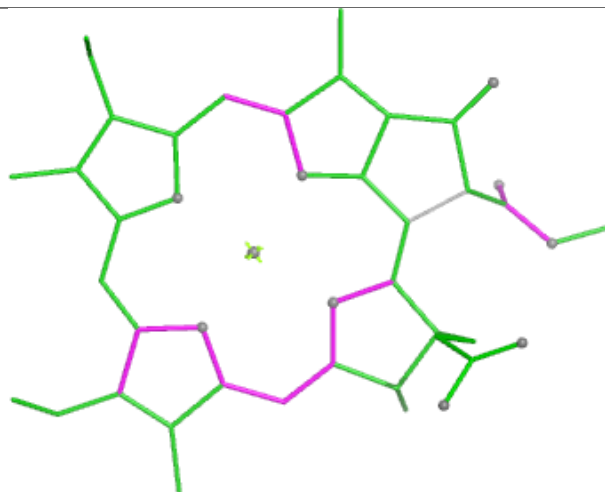
Rings



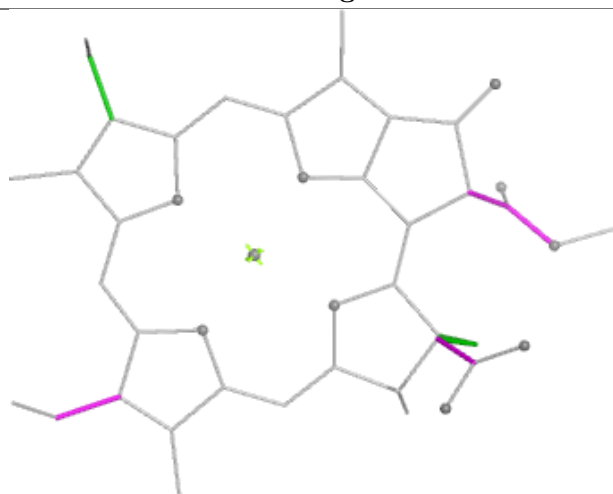
Ligand CLA A1 836



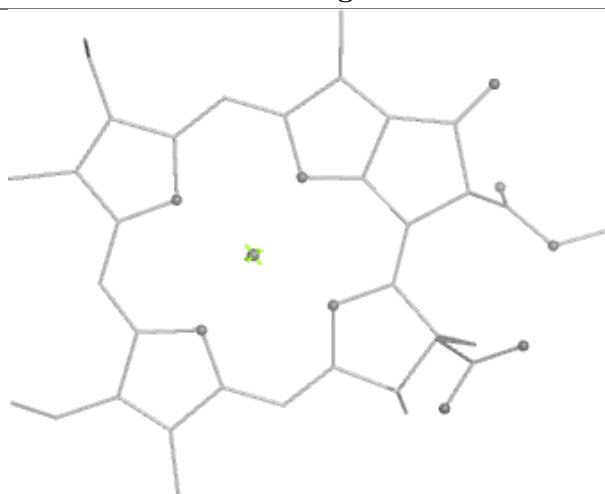
Bond lengths



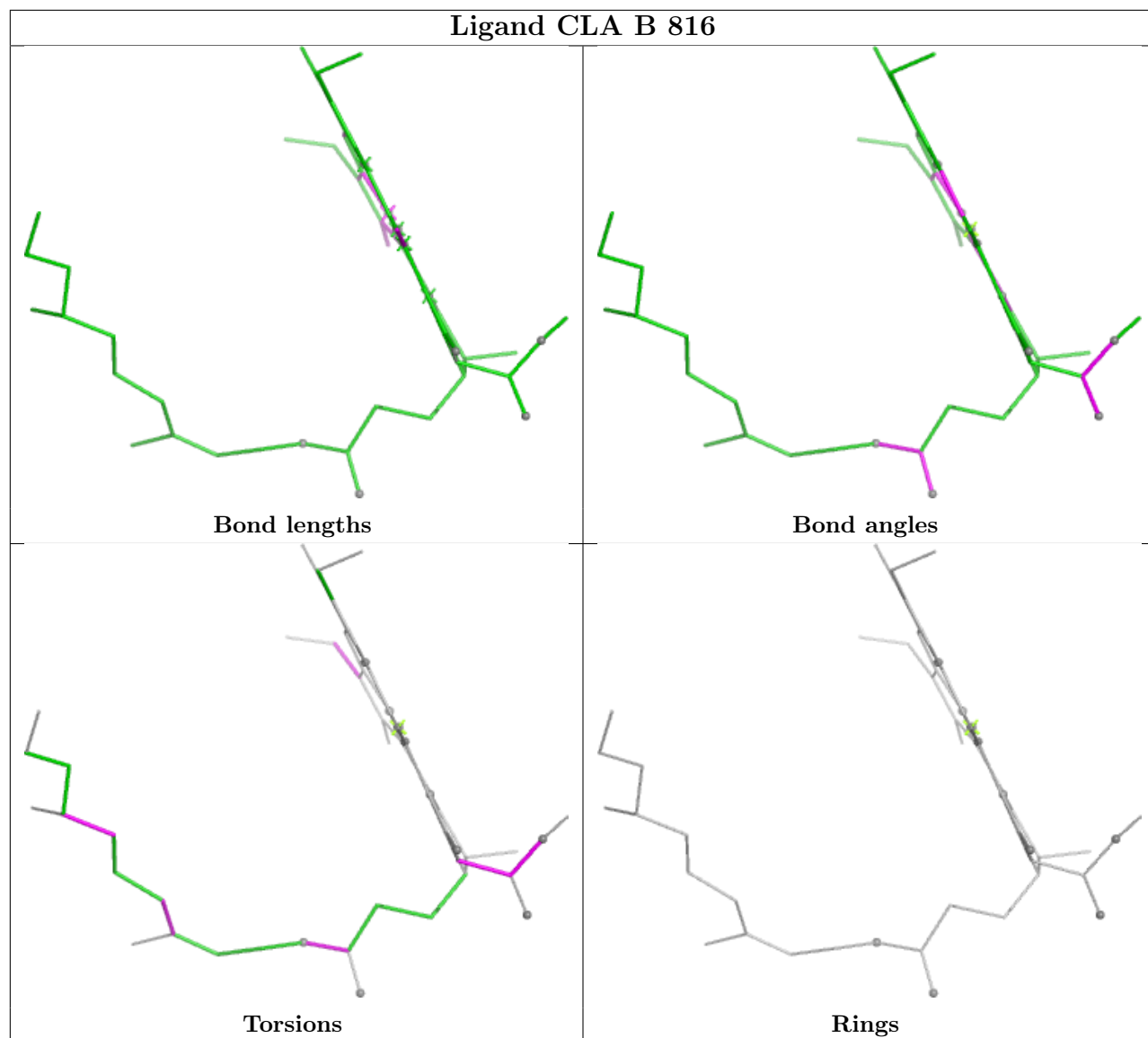
Bond angles

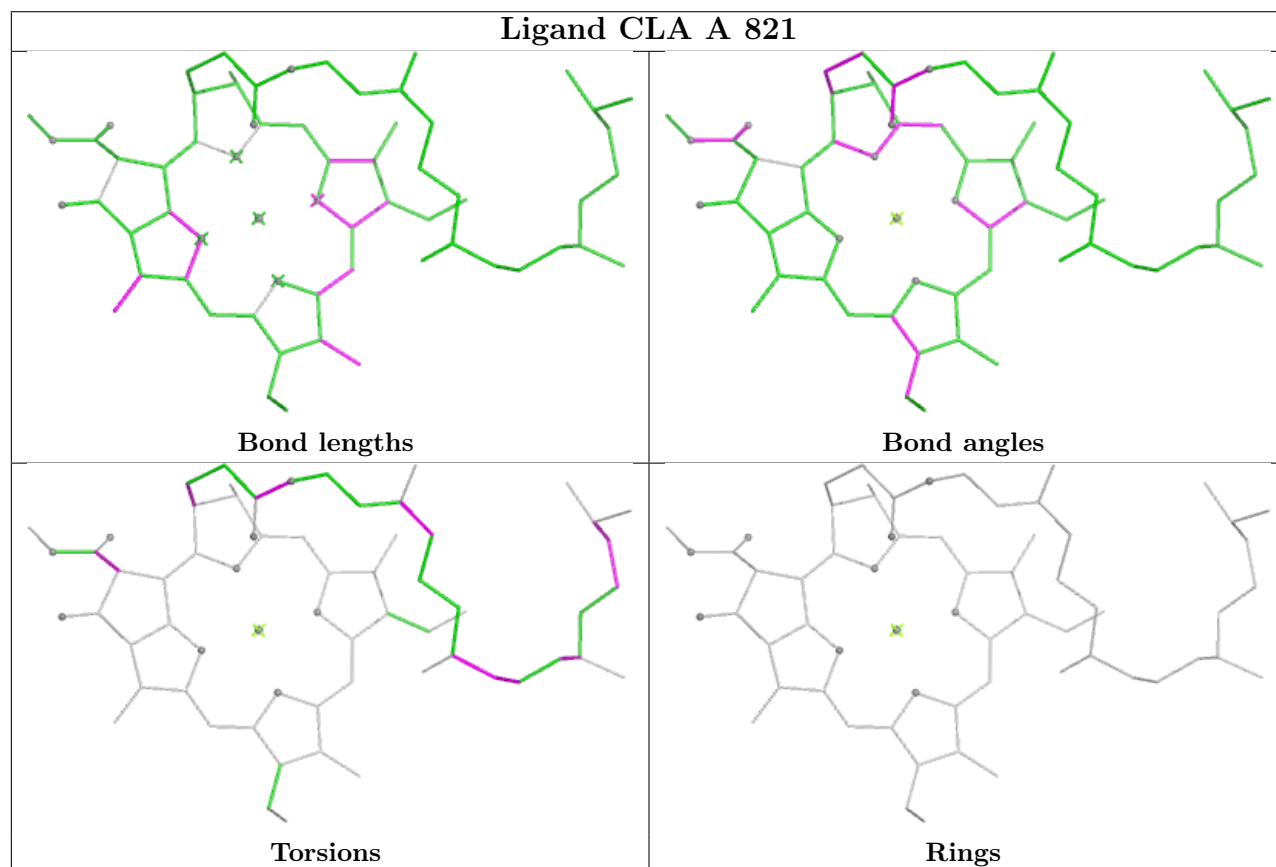
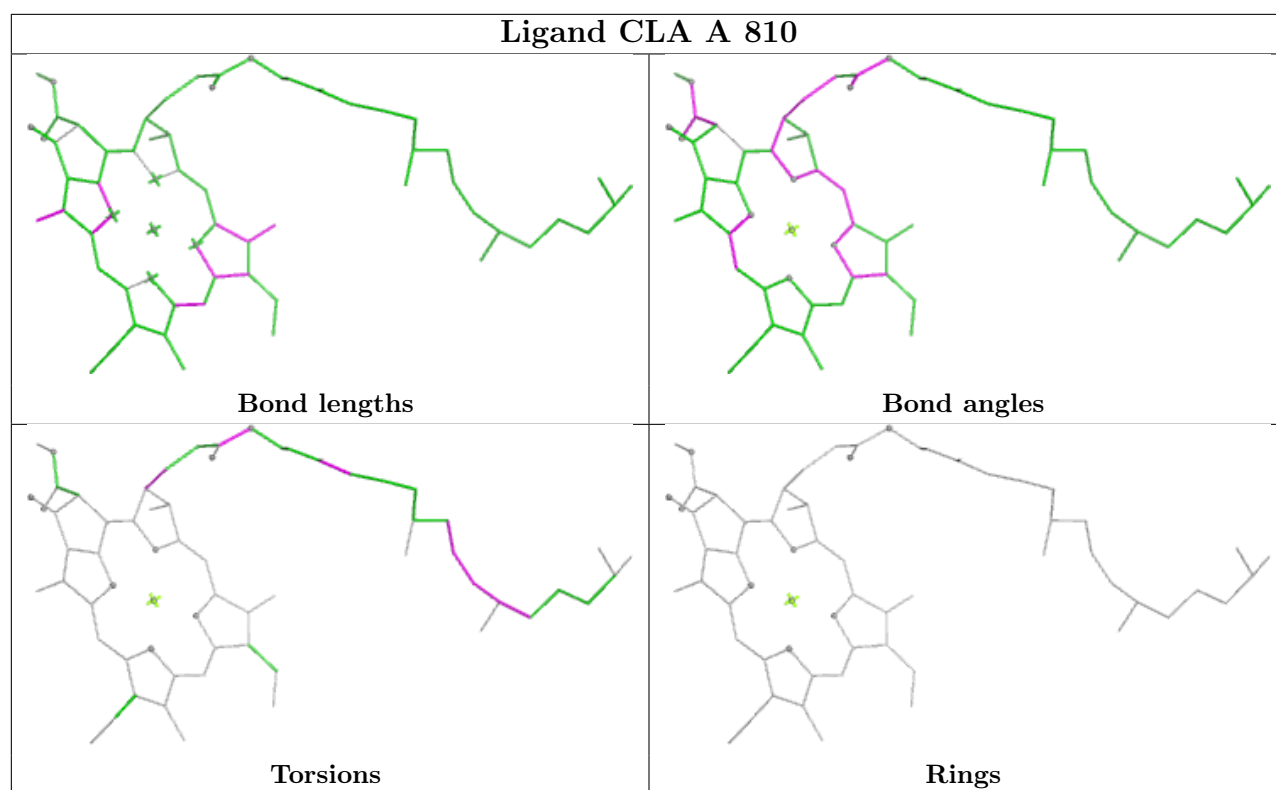


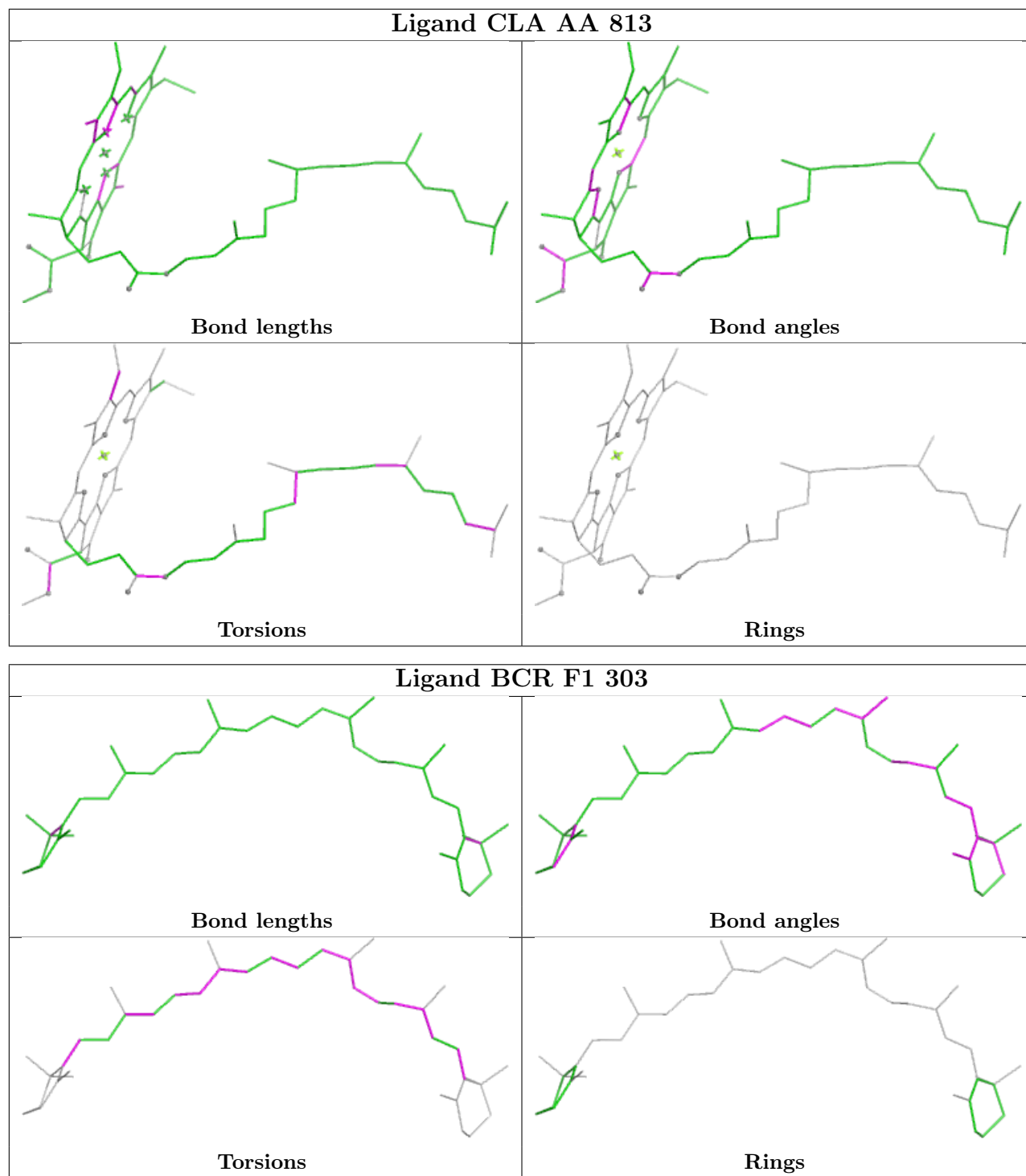
Torsions

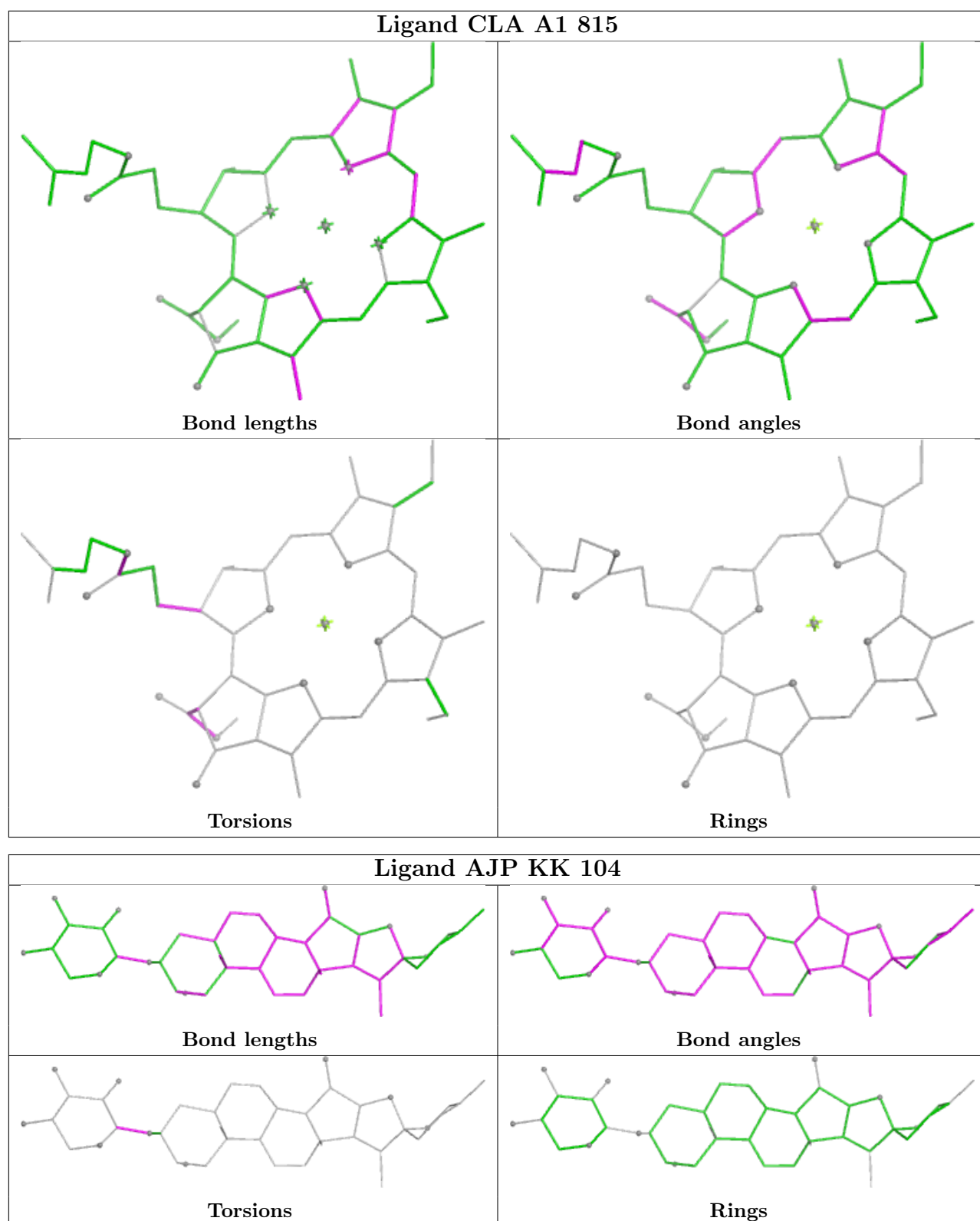


Rings

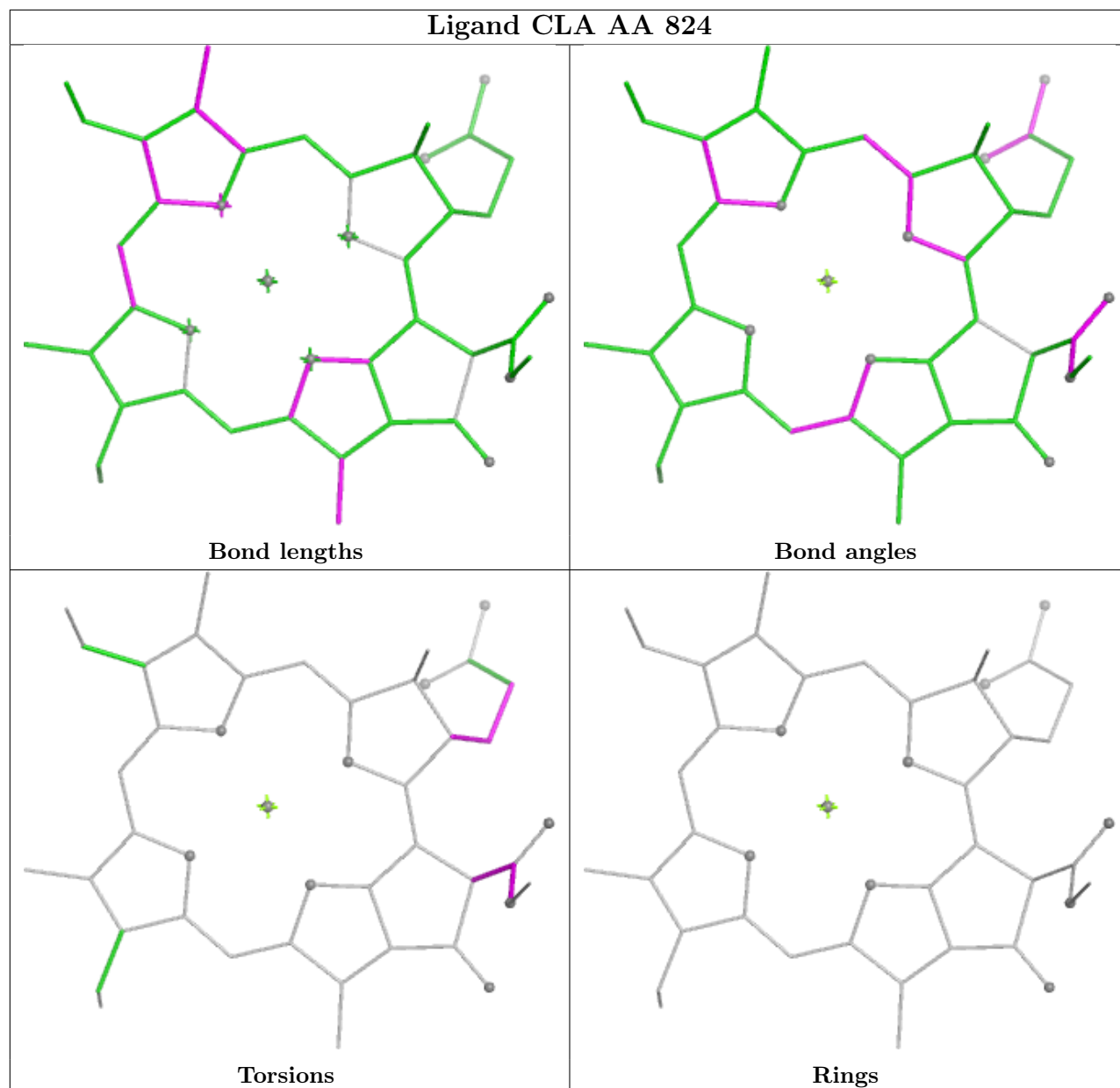


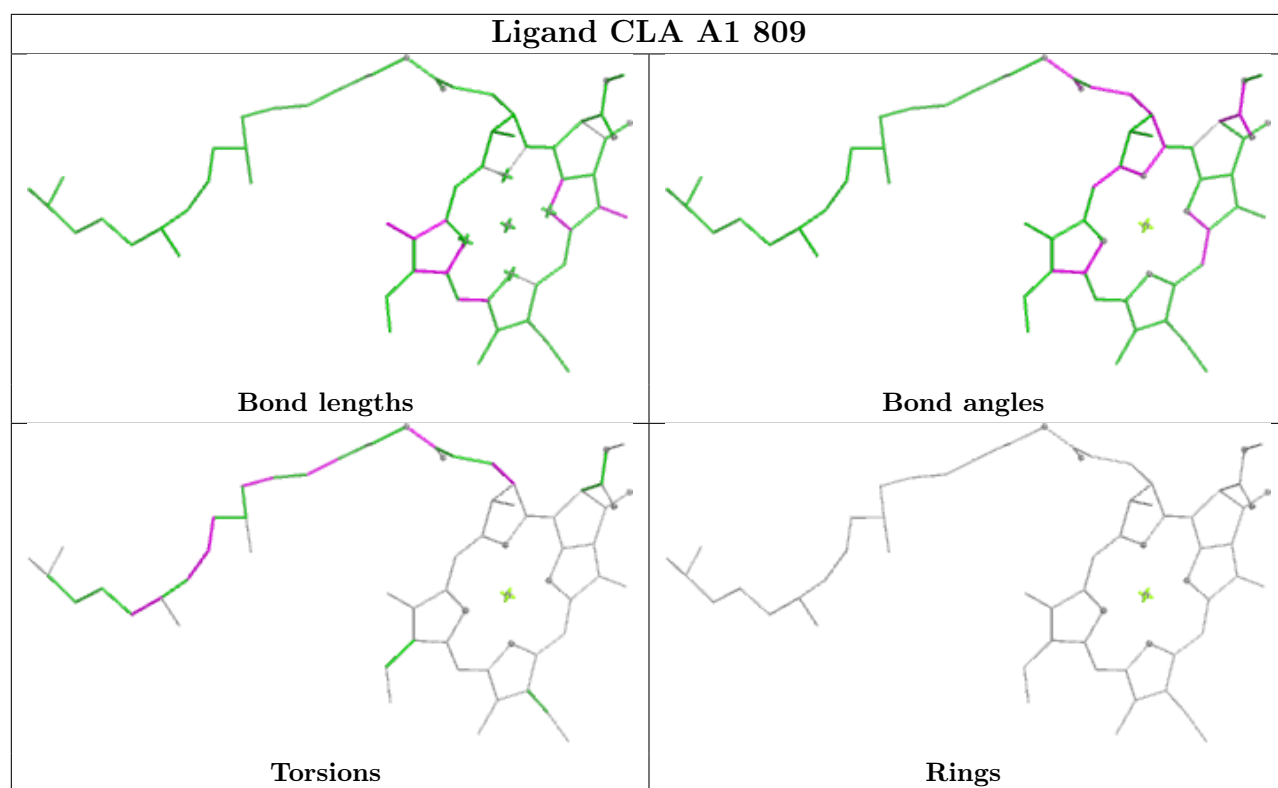


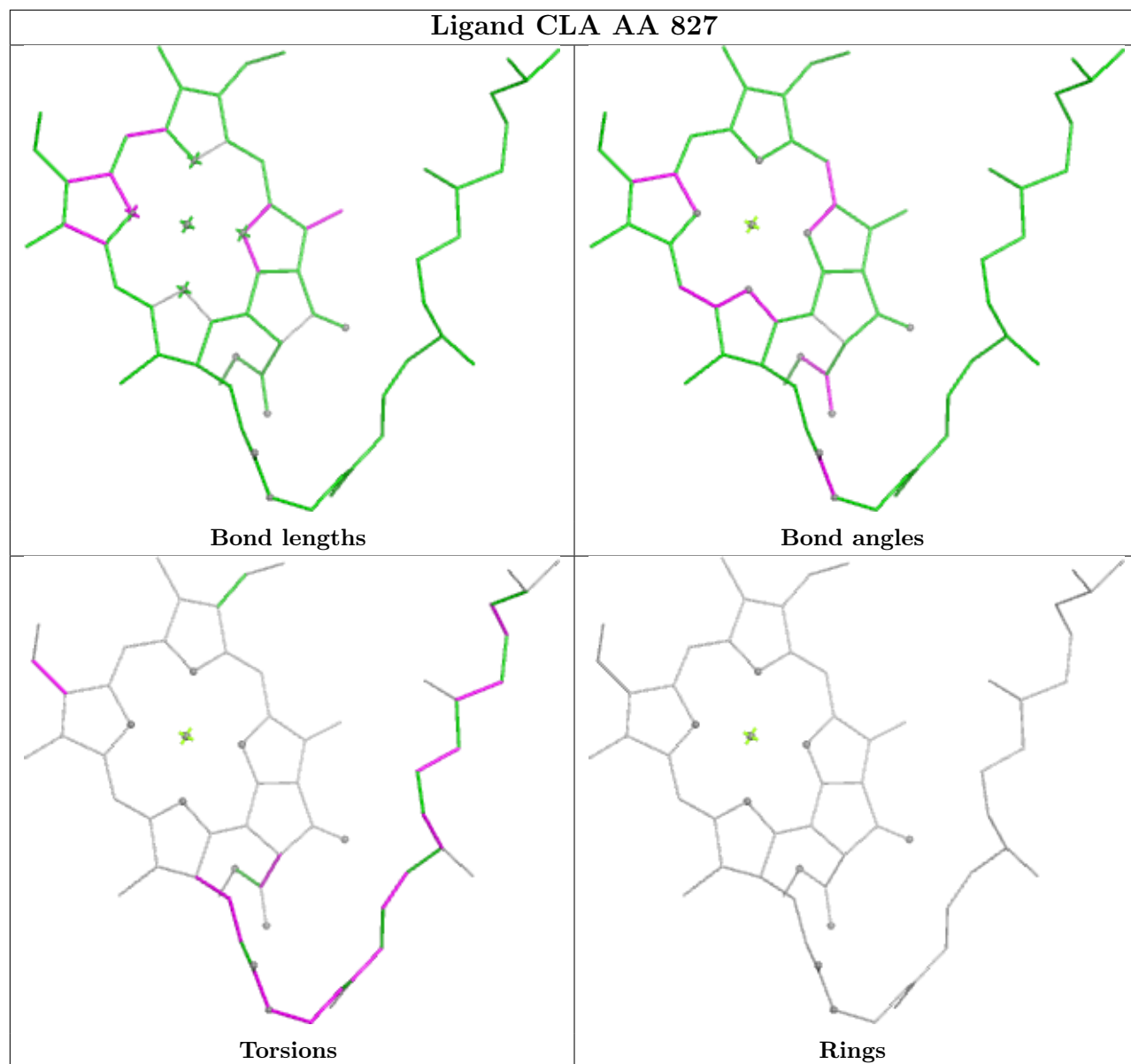


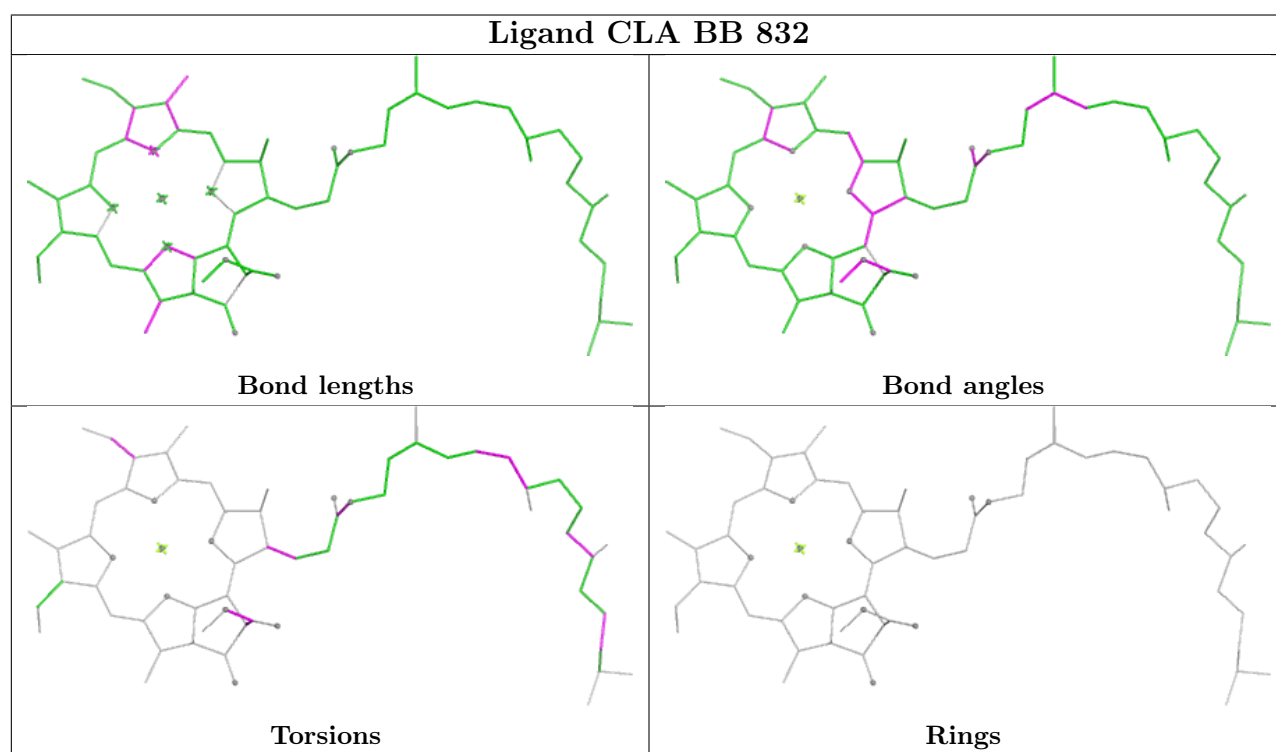
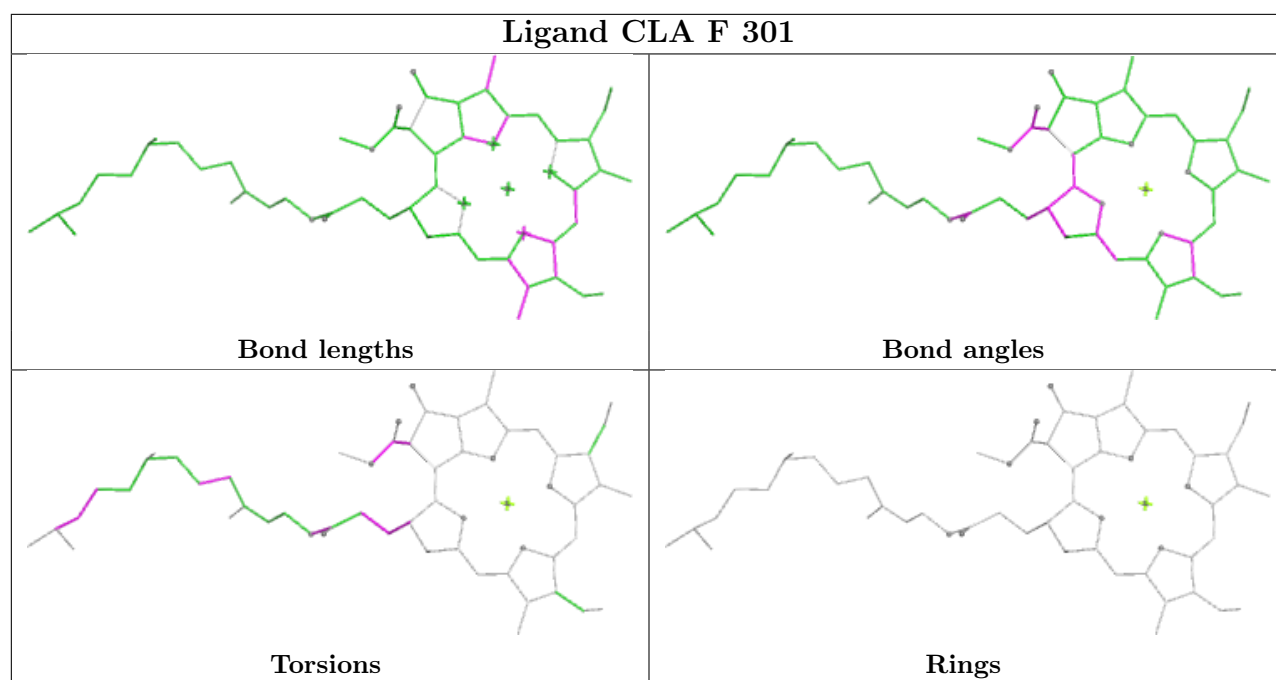


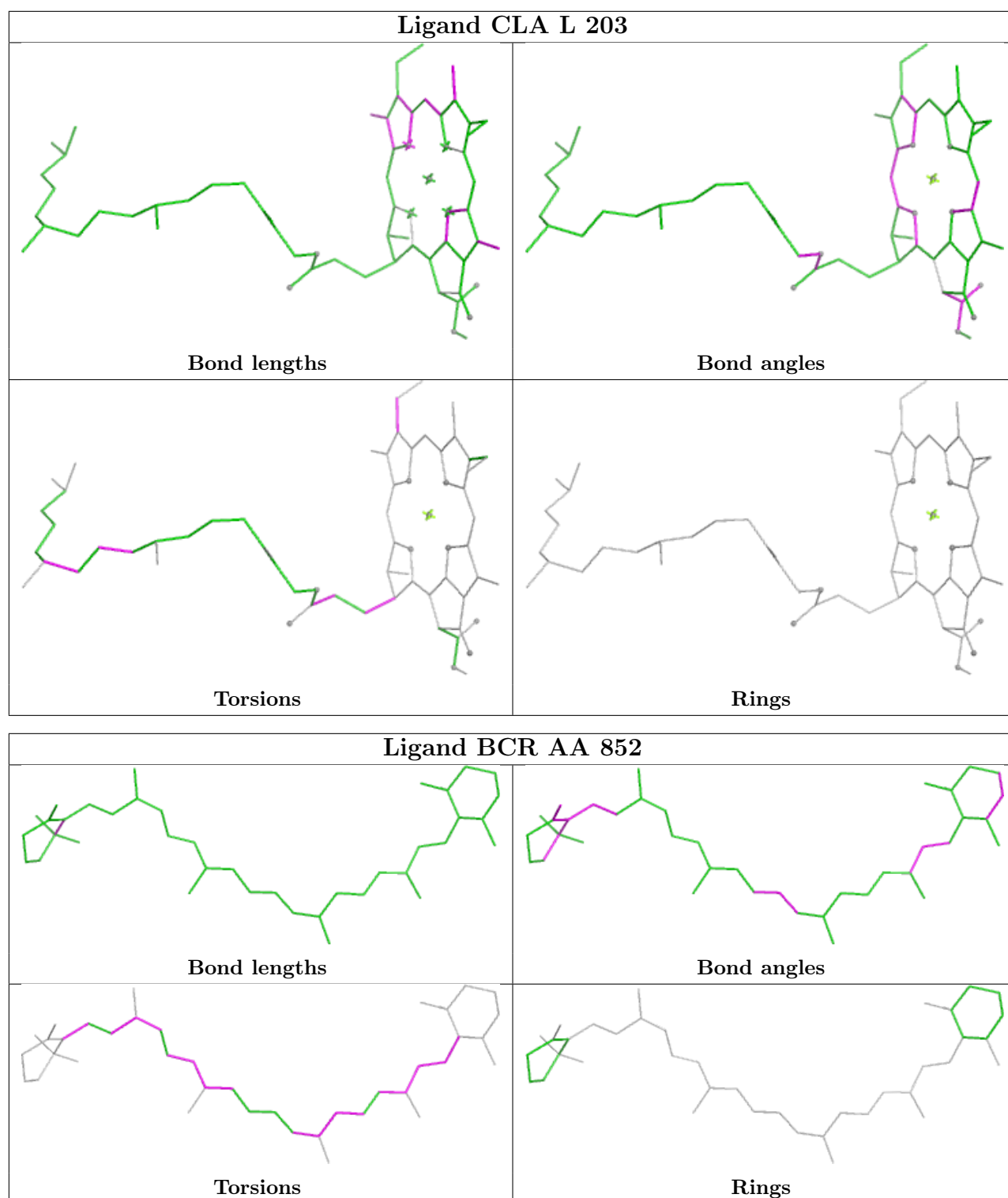
Ligand CLA AA 824

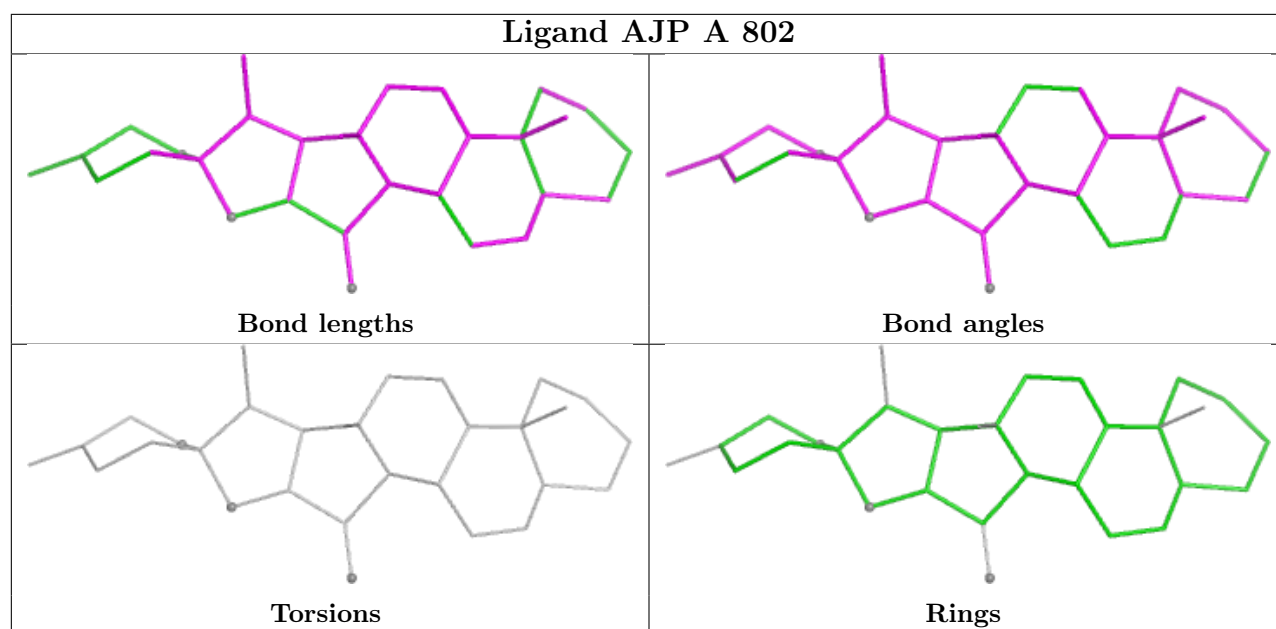


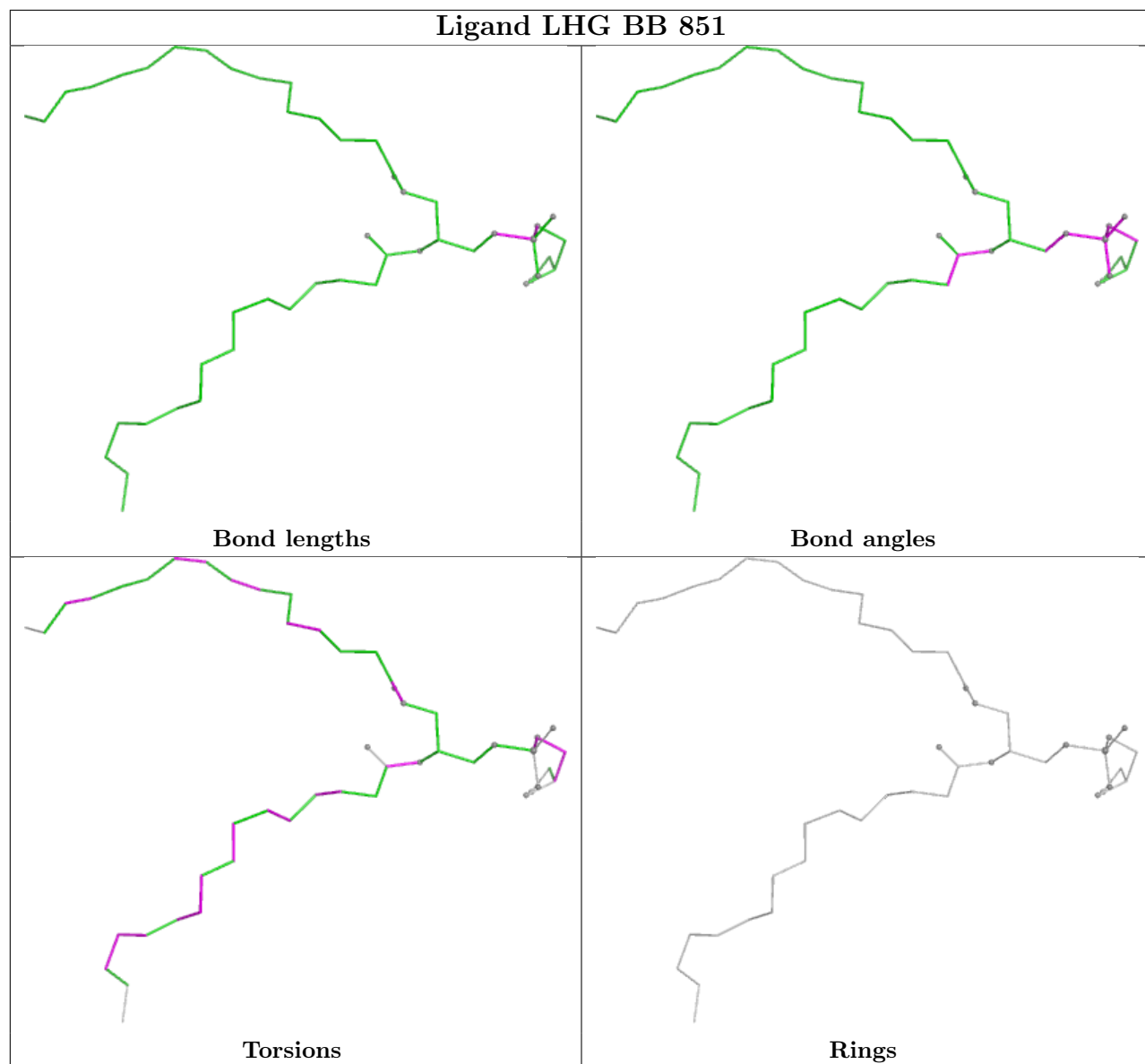


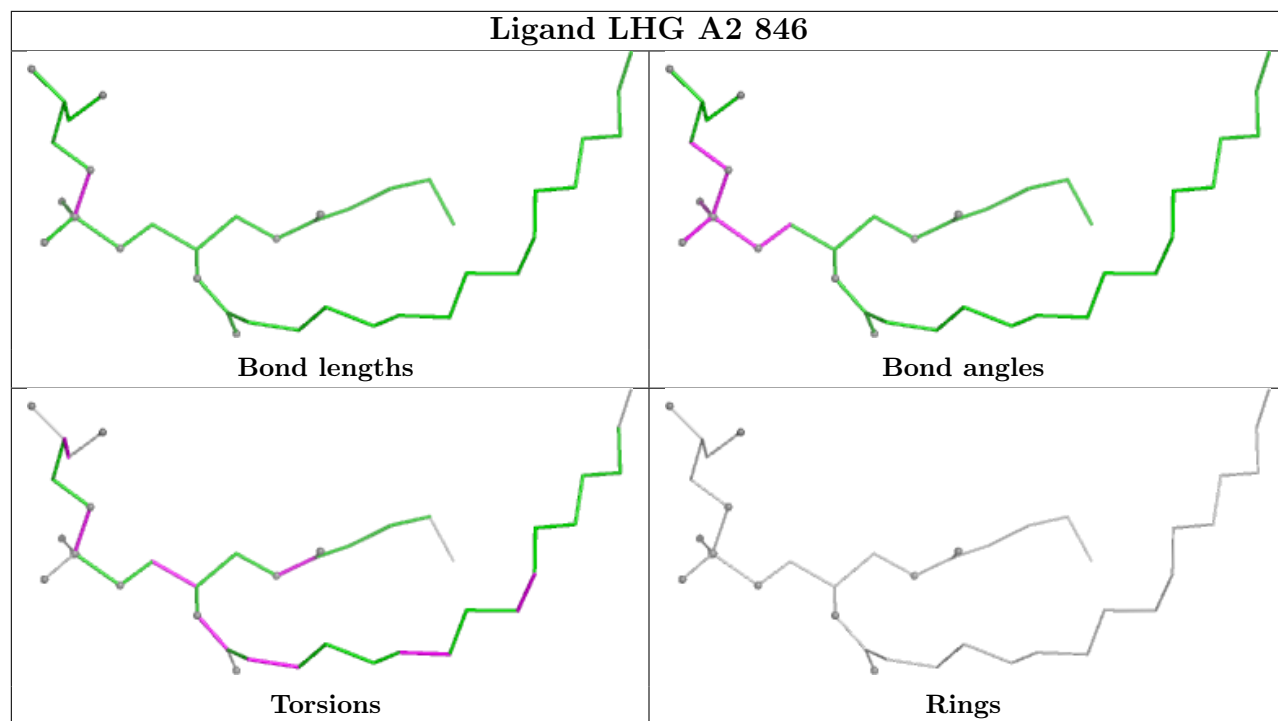


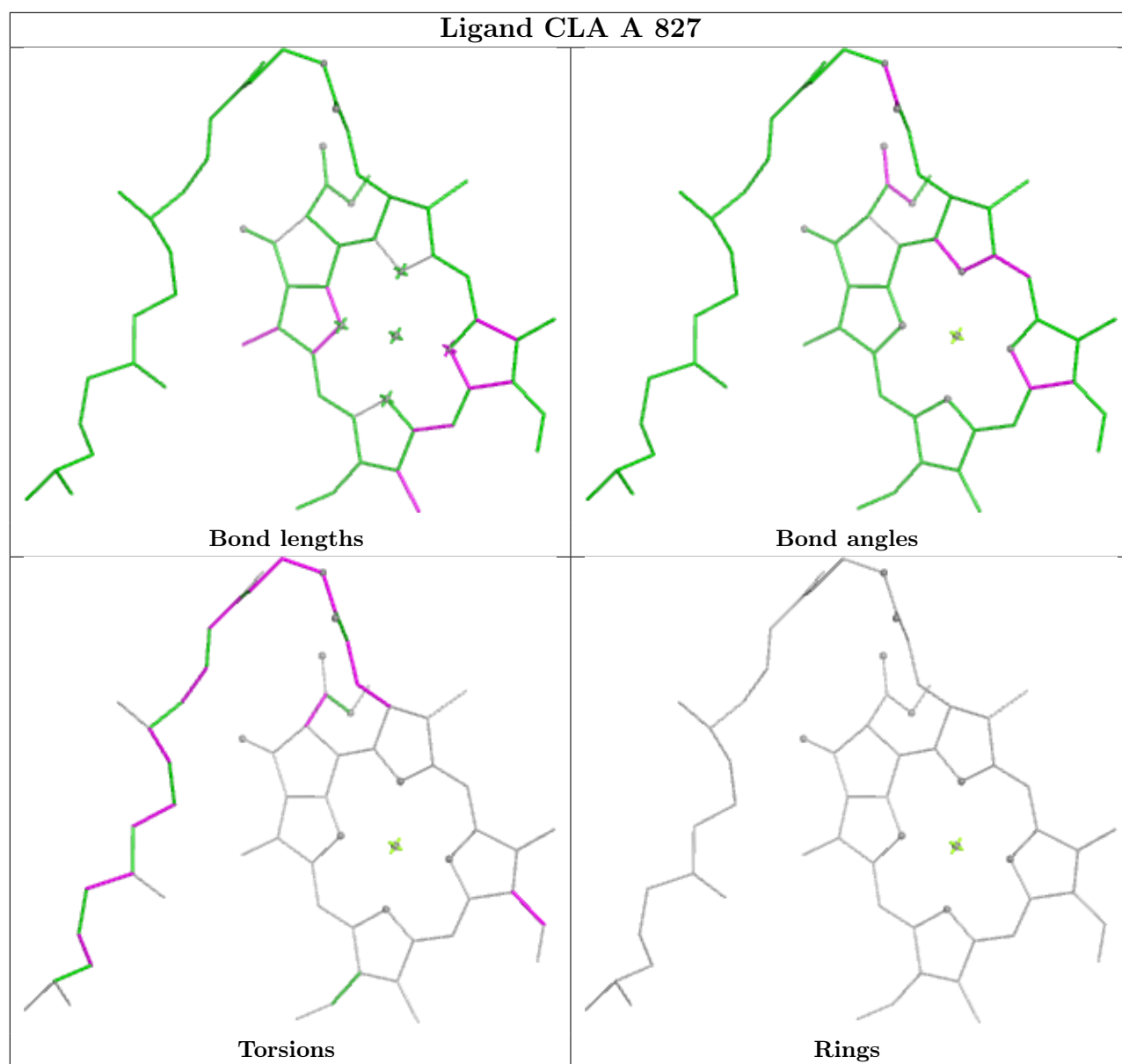


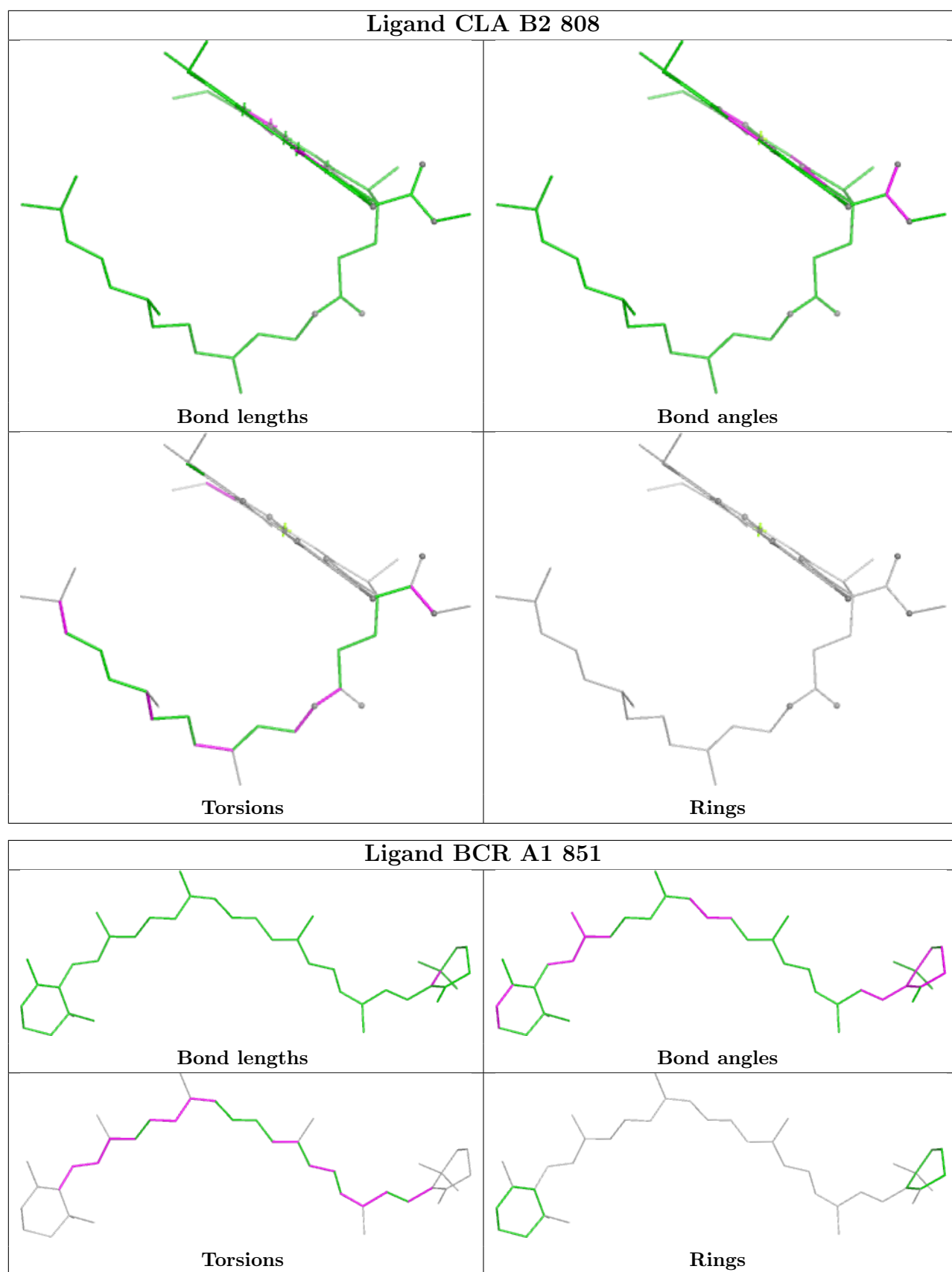




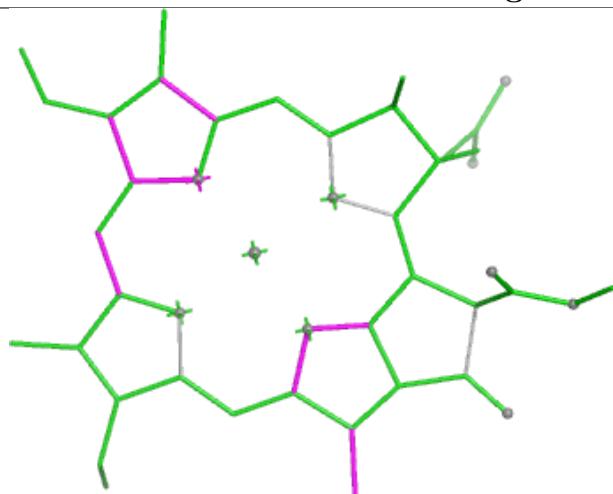




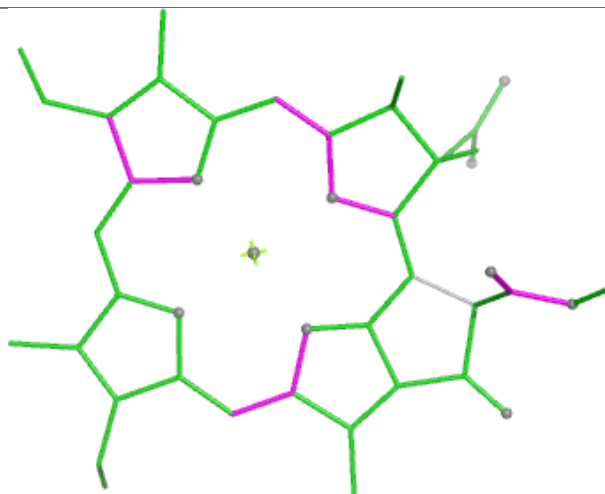




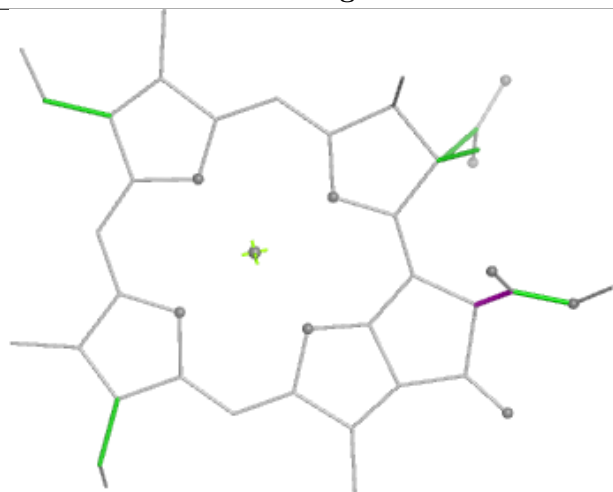
Ligand CLA B2 828



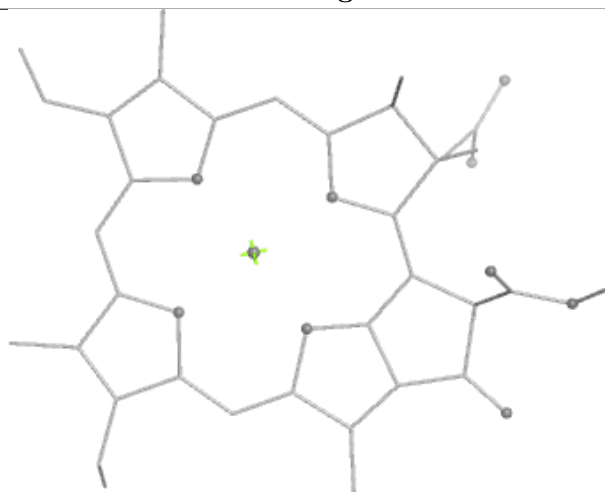
Bond lengths



Bond angles

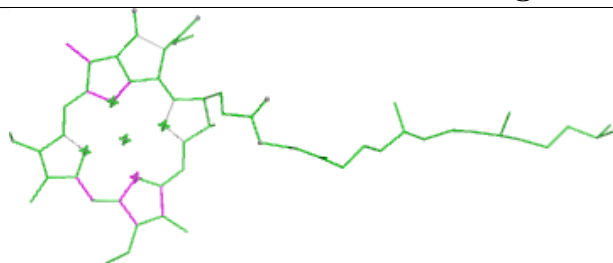


Torsions

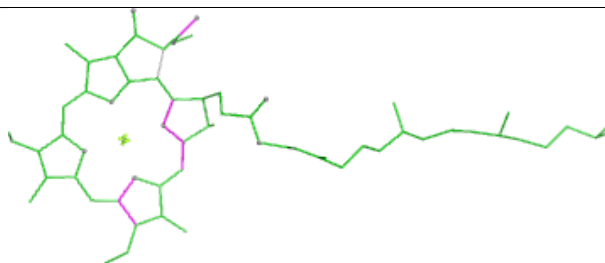


Rings

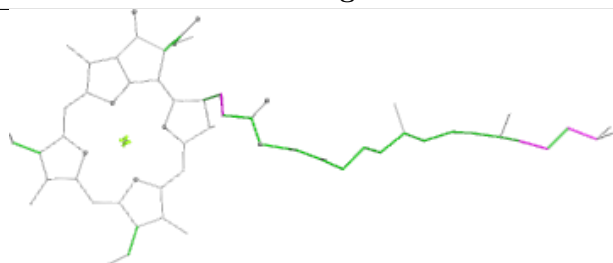
Ligand CLA B 822



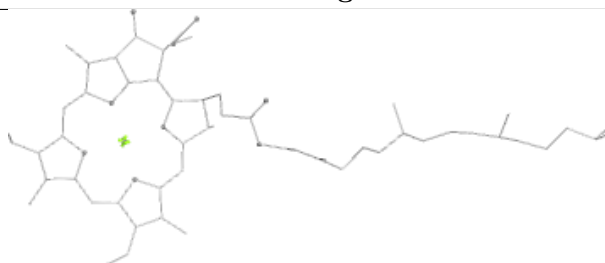
Bond lengths



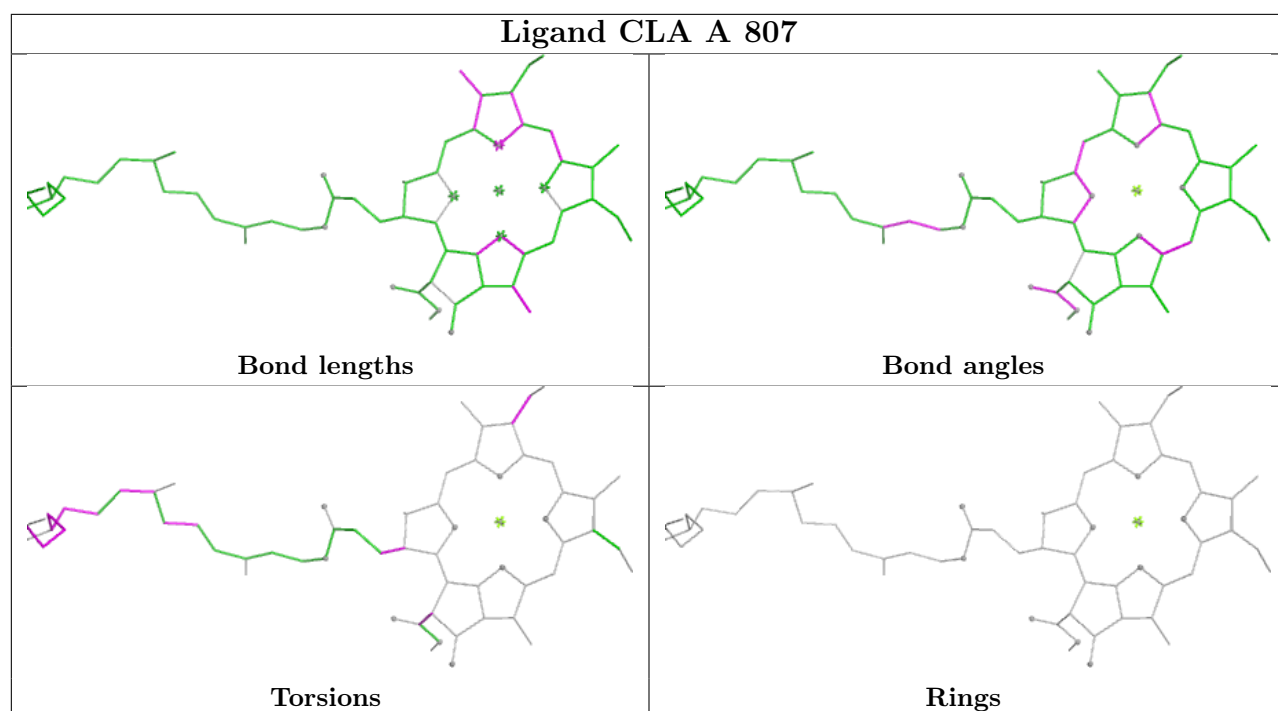
Bond angles



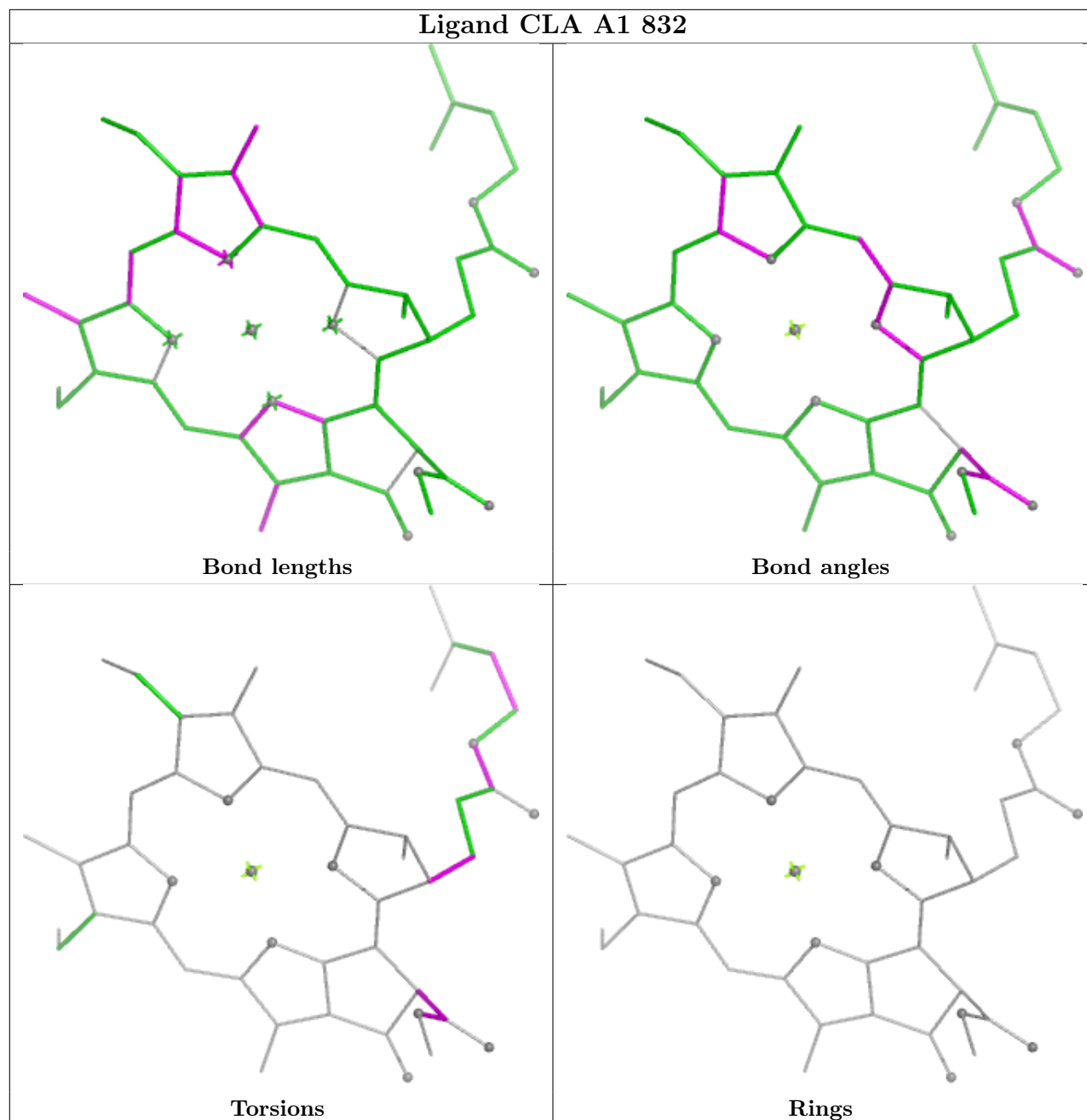
Torsions



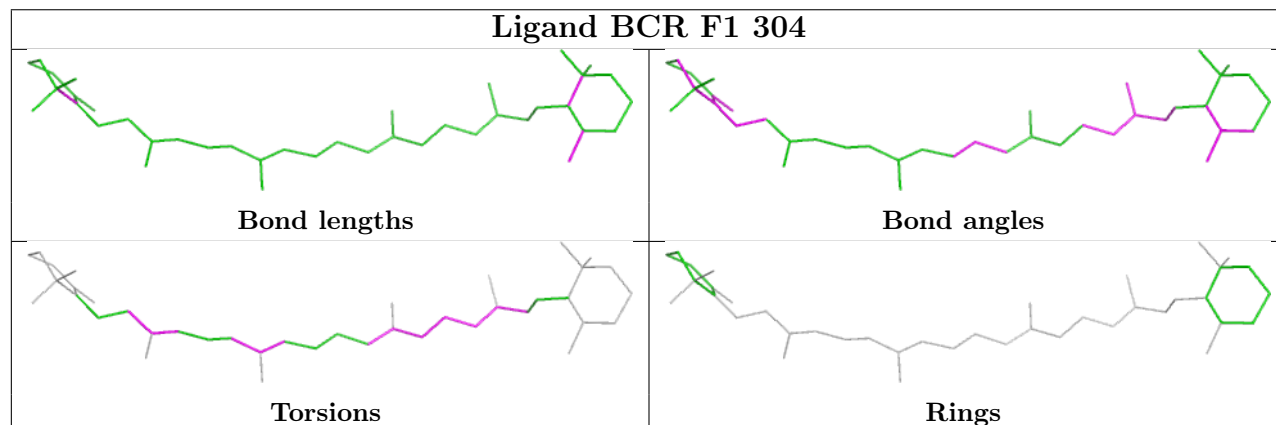
Rings



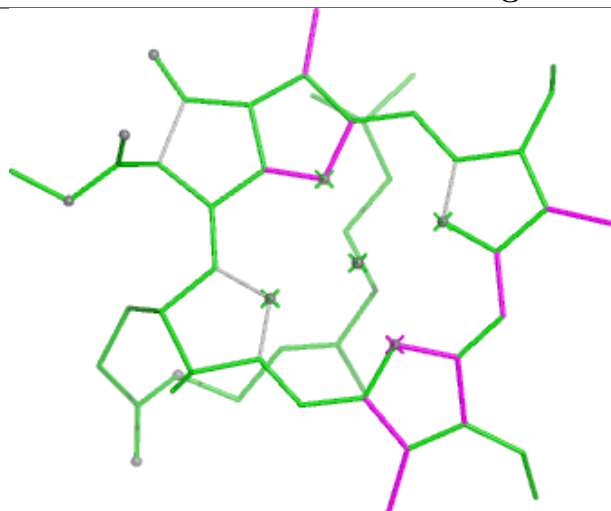
Ligand CLA A1 832



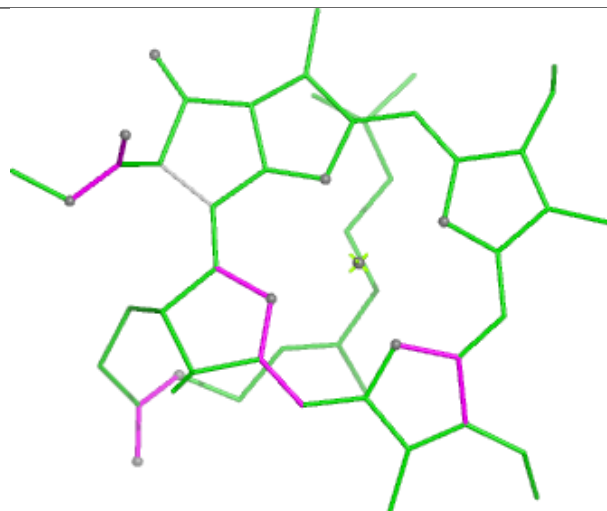
Ligand BCR F1 304



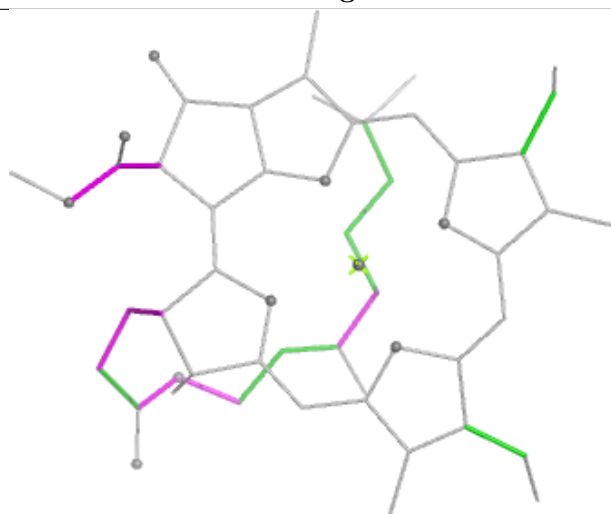
Ligand CLA BB 824



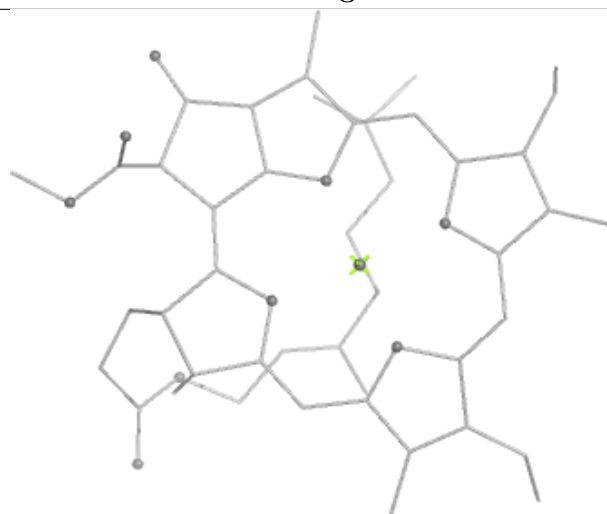
Bond lengths



Bond angles

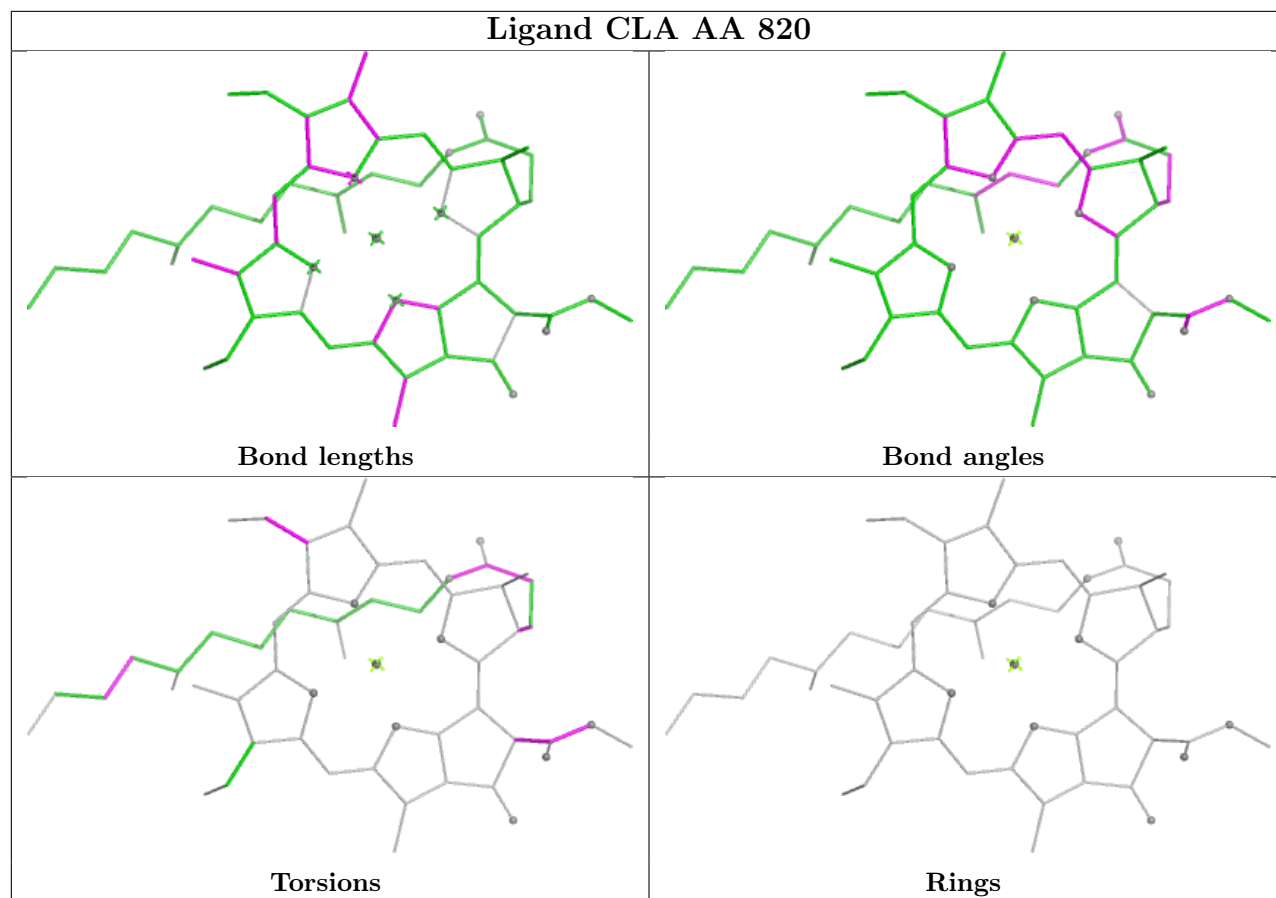


Torsions

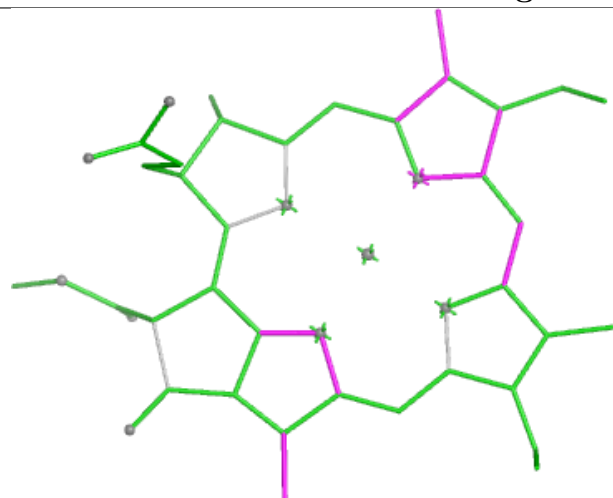


Rings

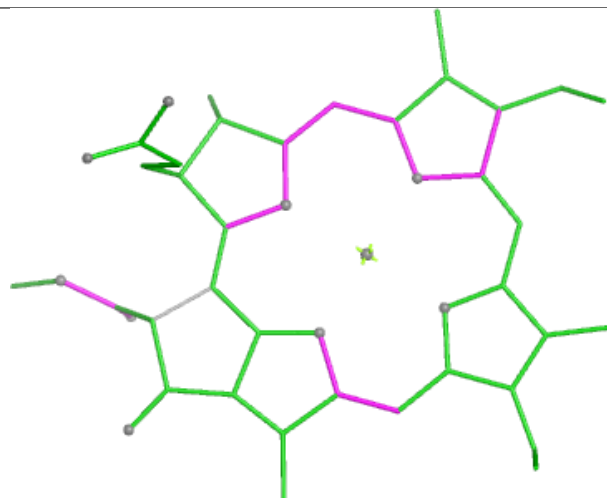
Ligand CLA AA 820



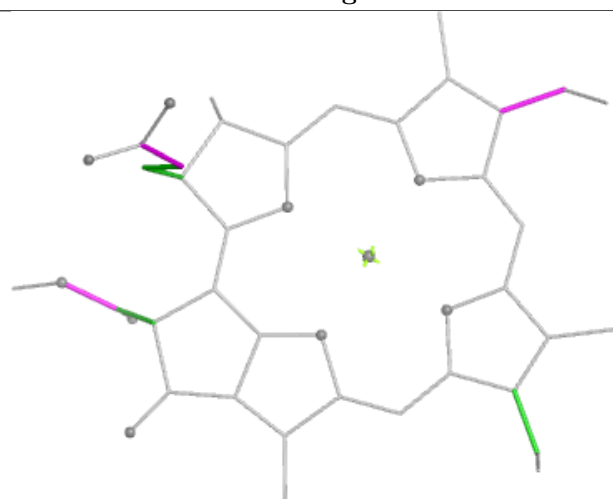
Ligand CLA A 837



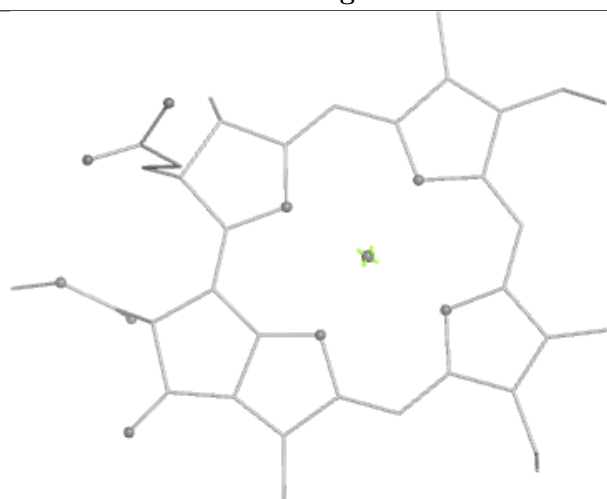
Bond lengths



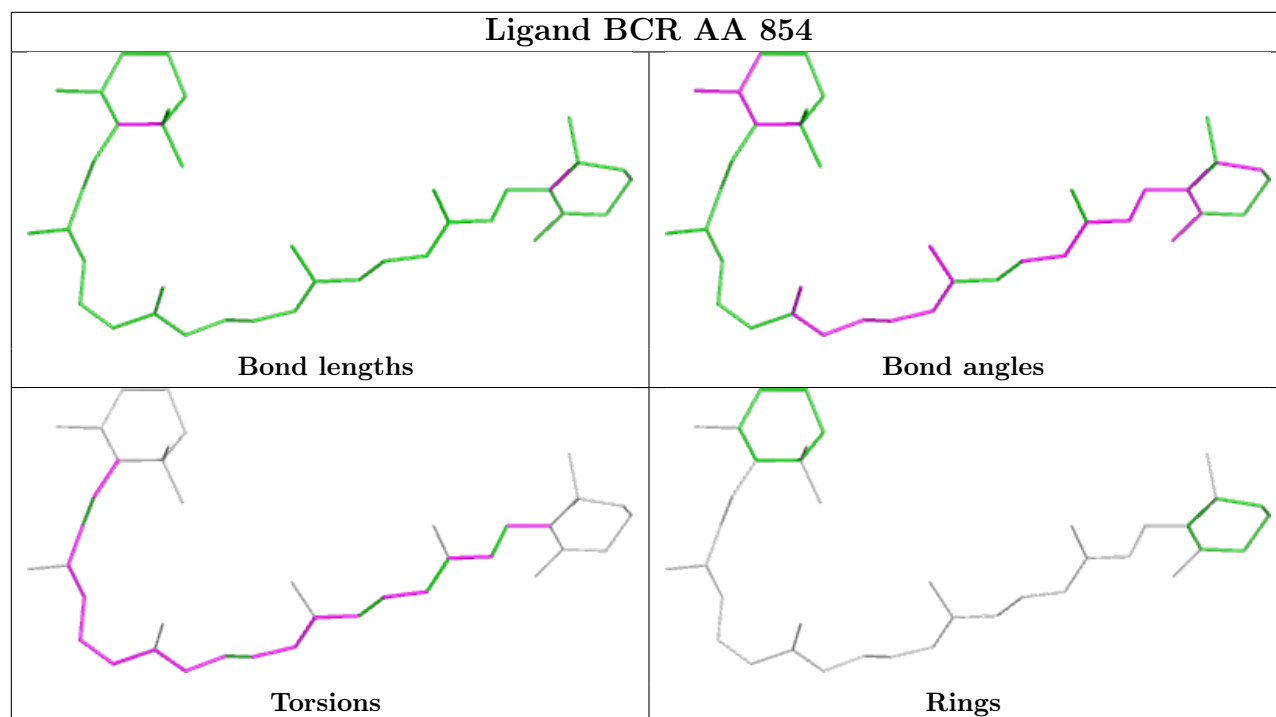
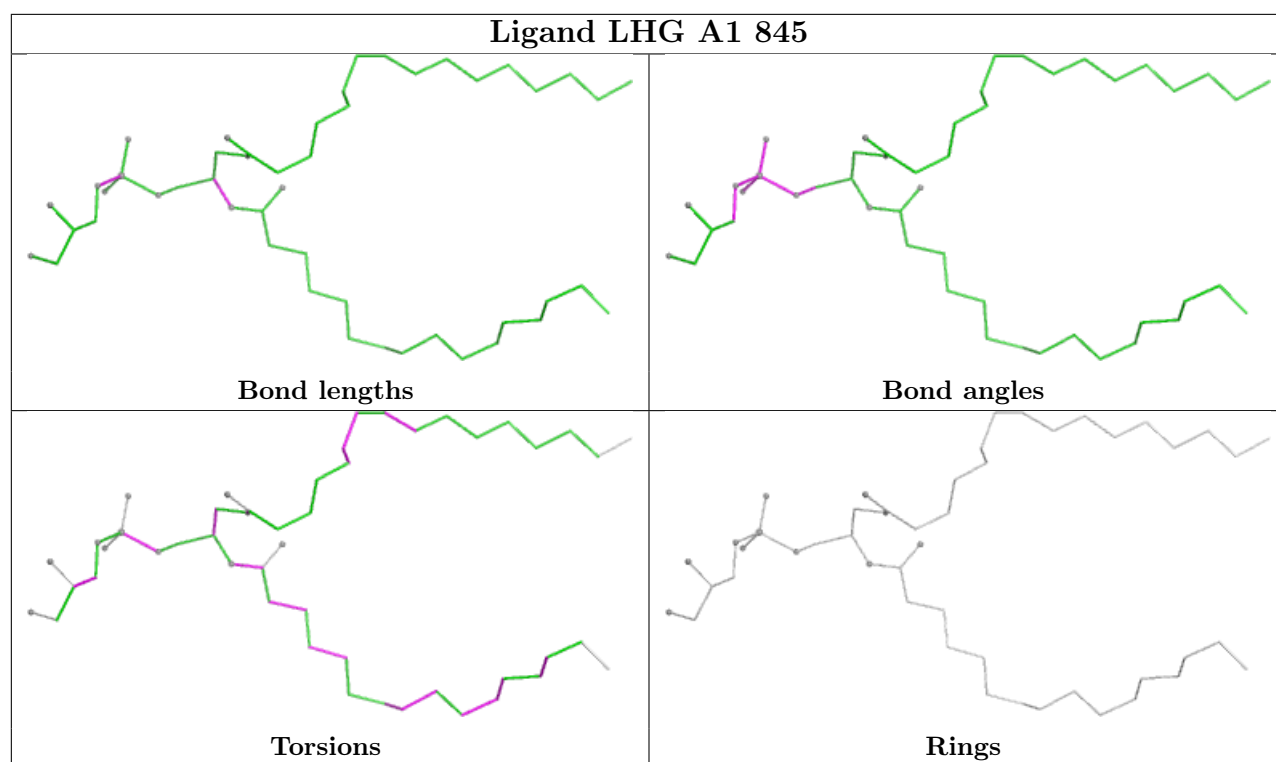
Bond angles

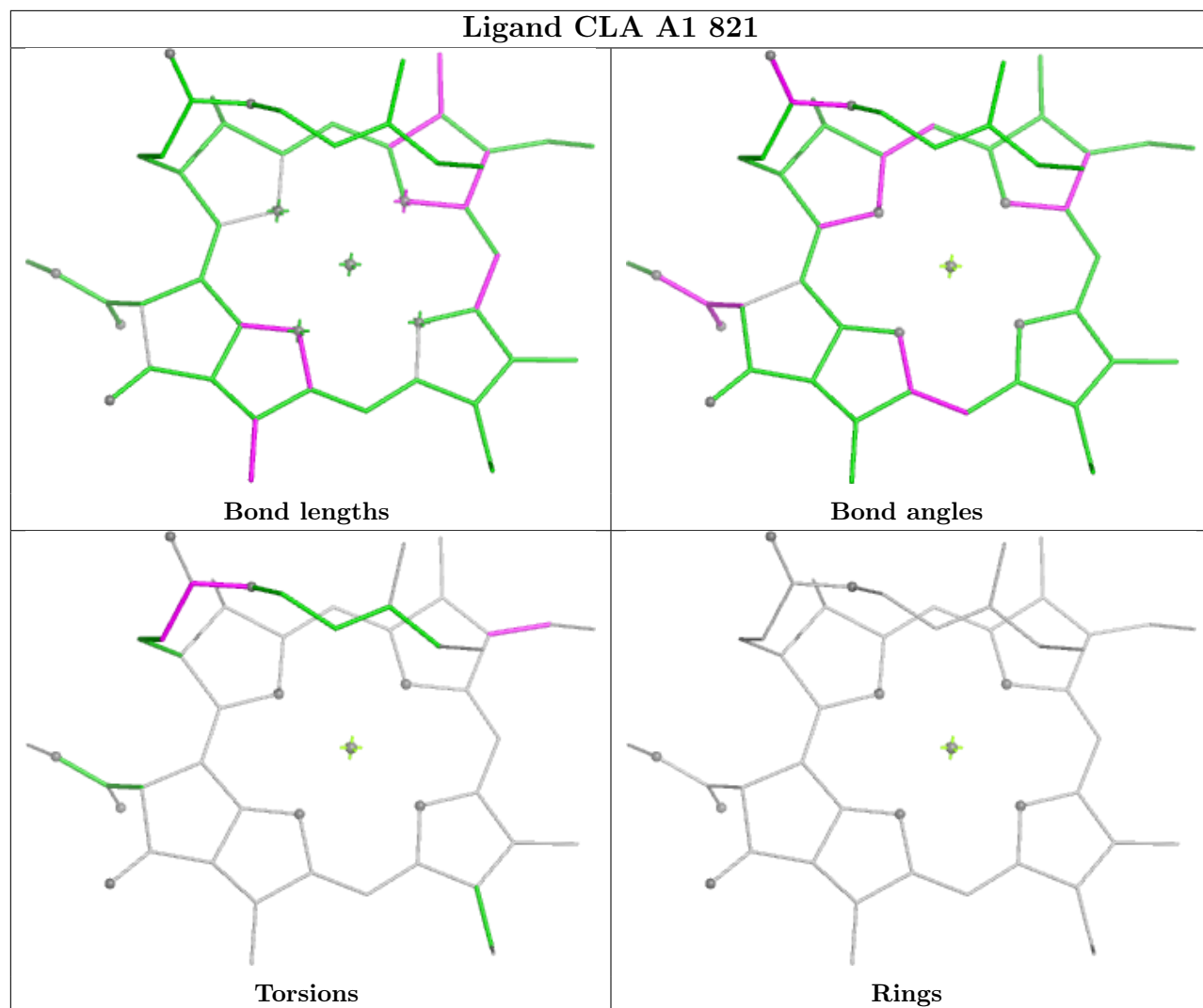


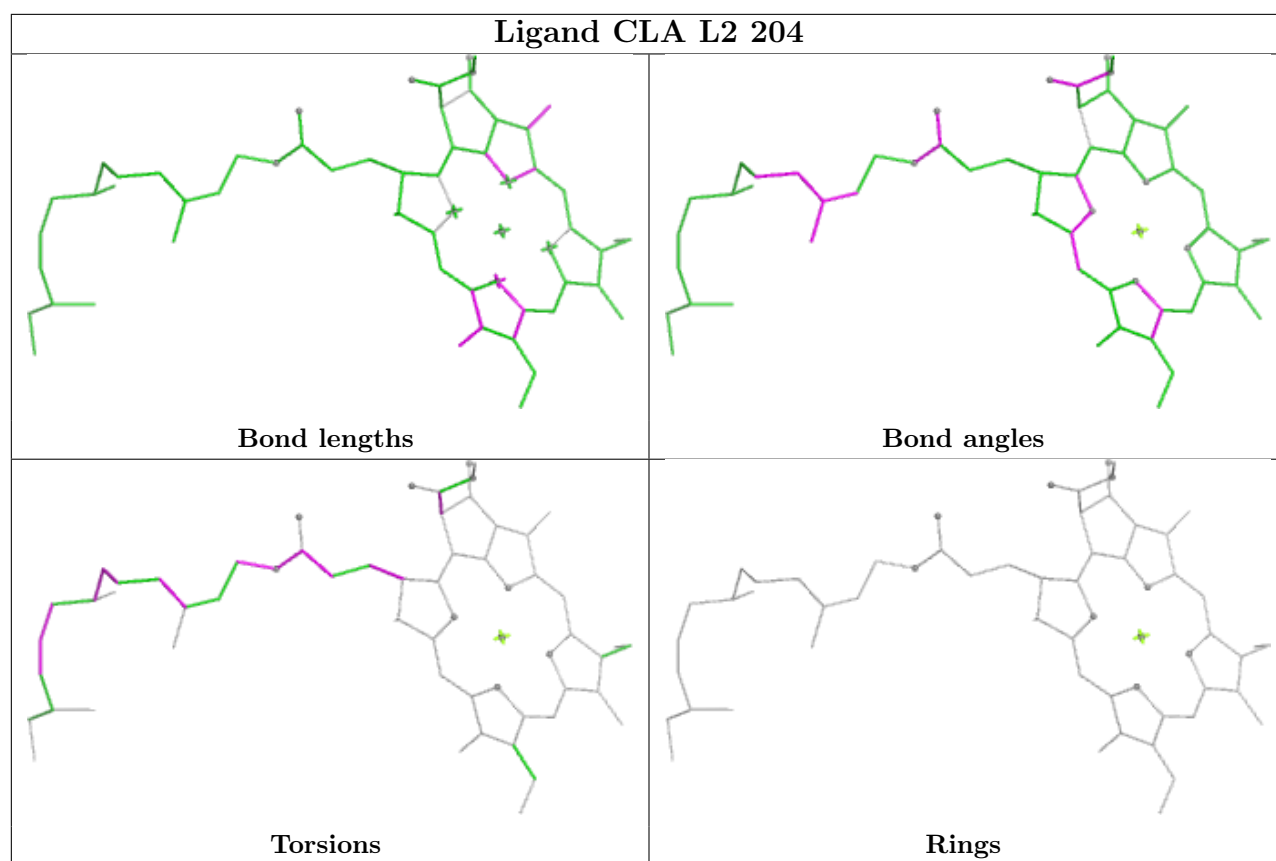
Torsions



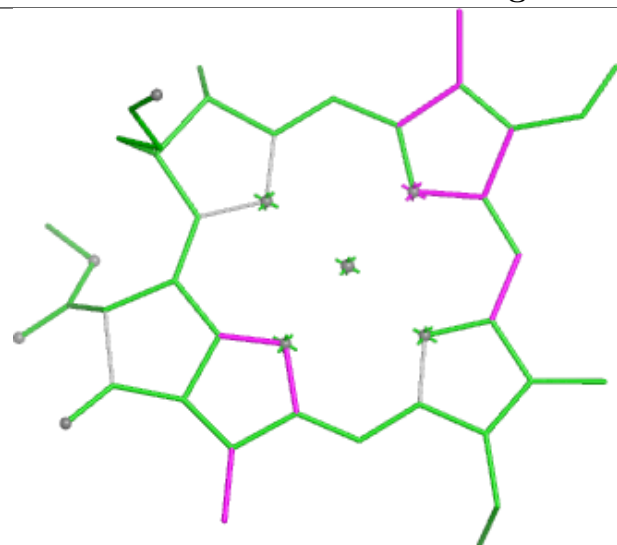
Rings



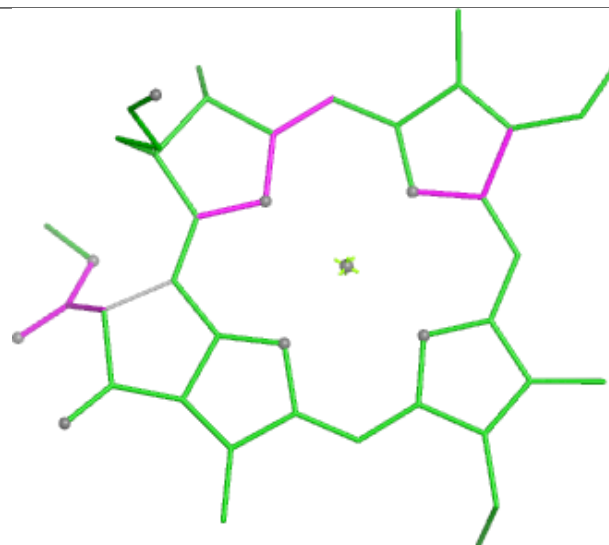




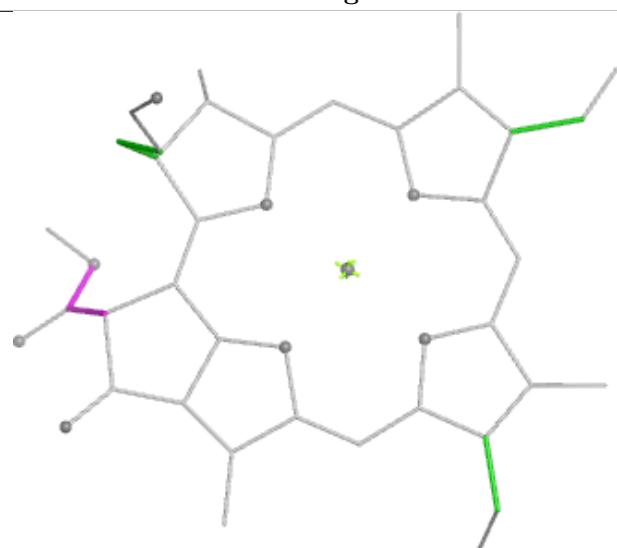
Ligand CLA A2 838



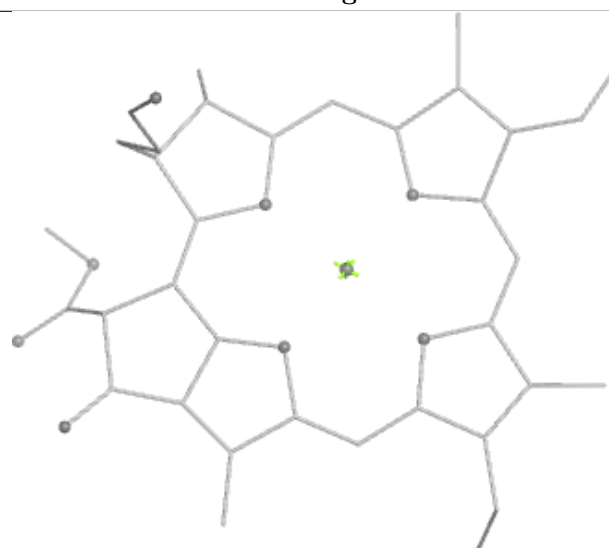
Bond lengths



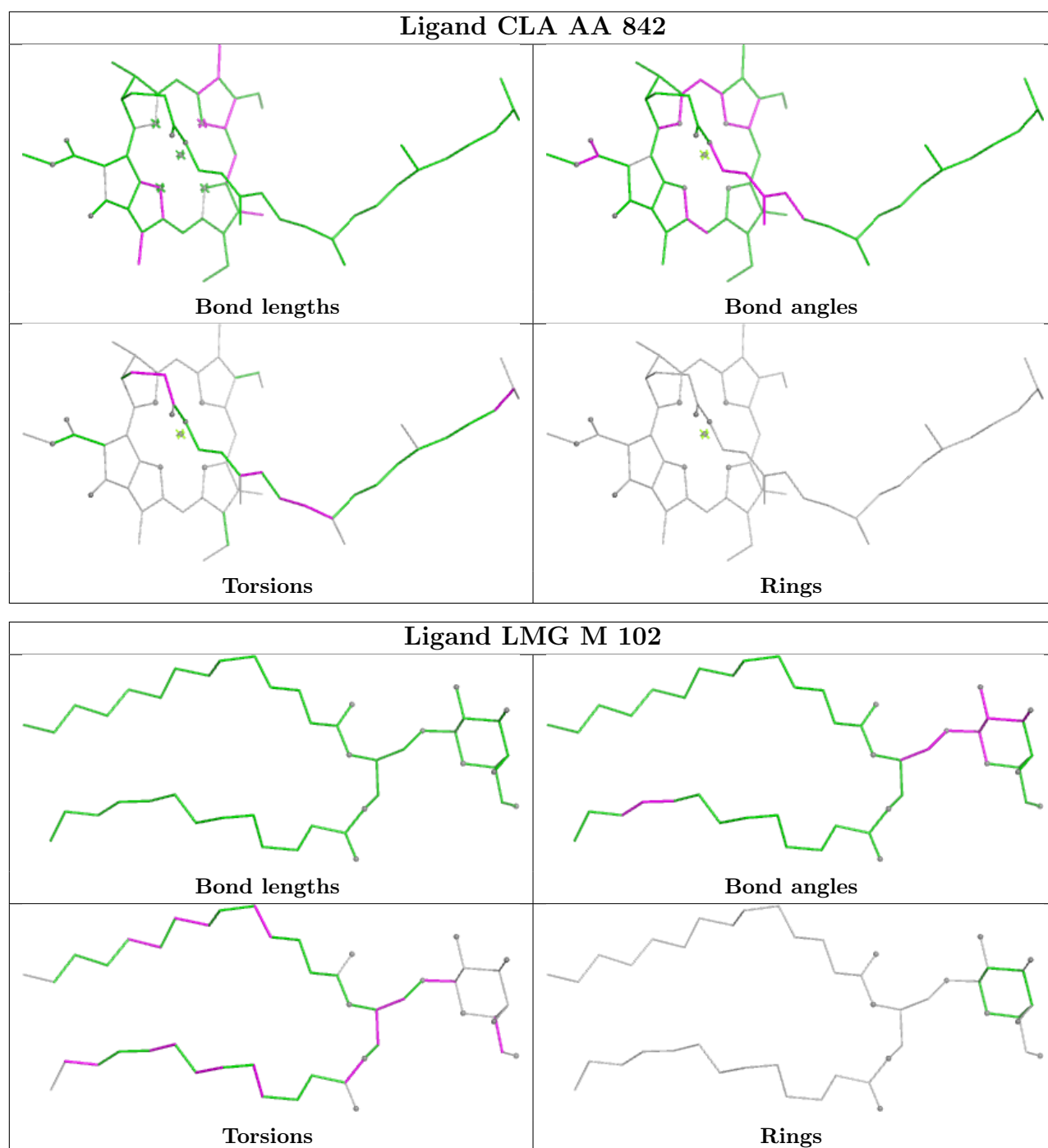
Bond angles



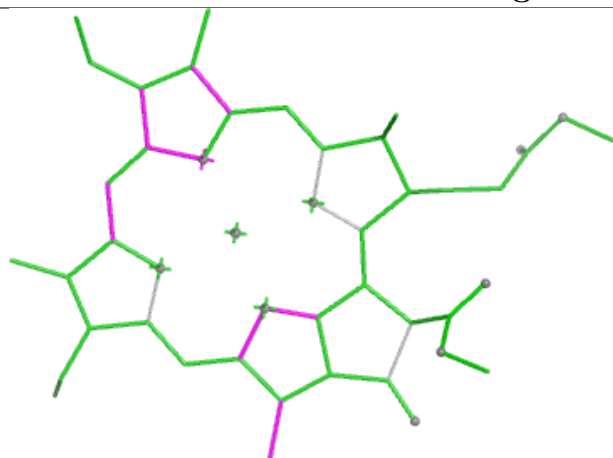
Torsions



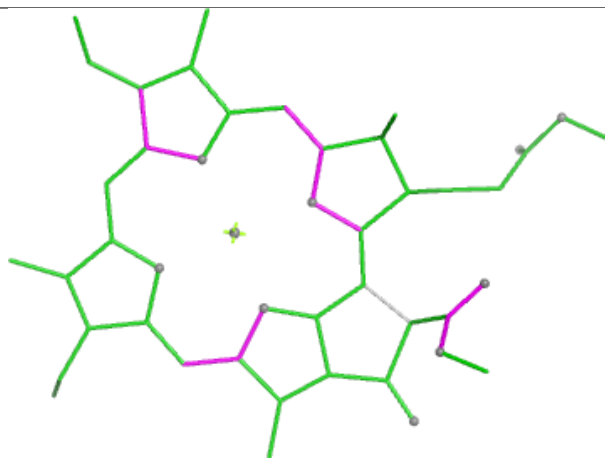
Rings



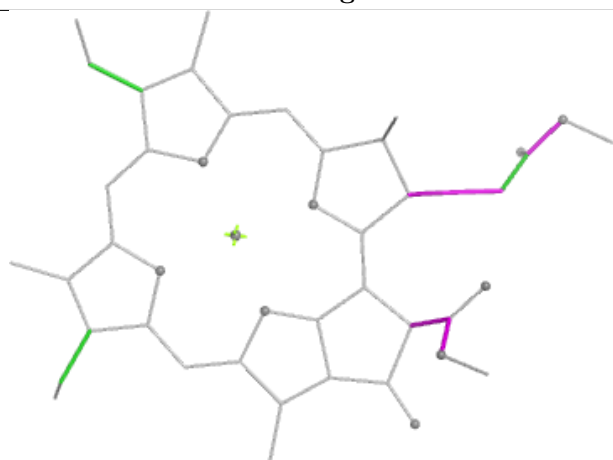
Ligand CLA K 102



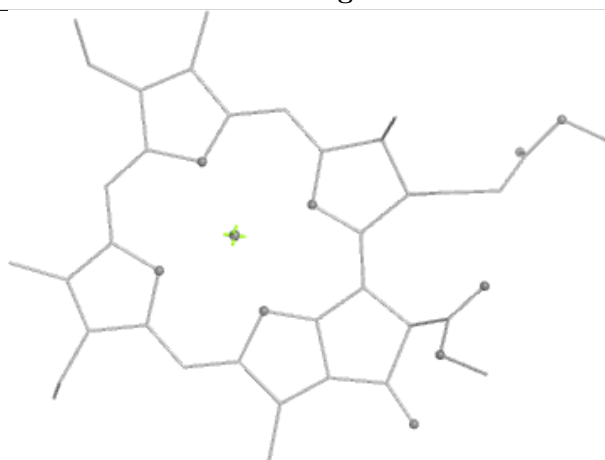
Bond lengths



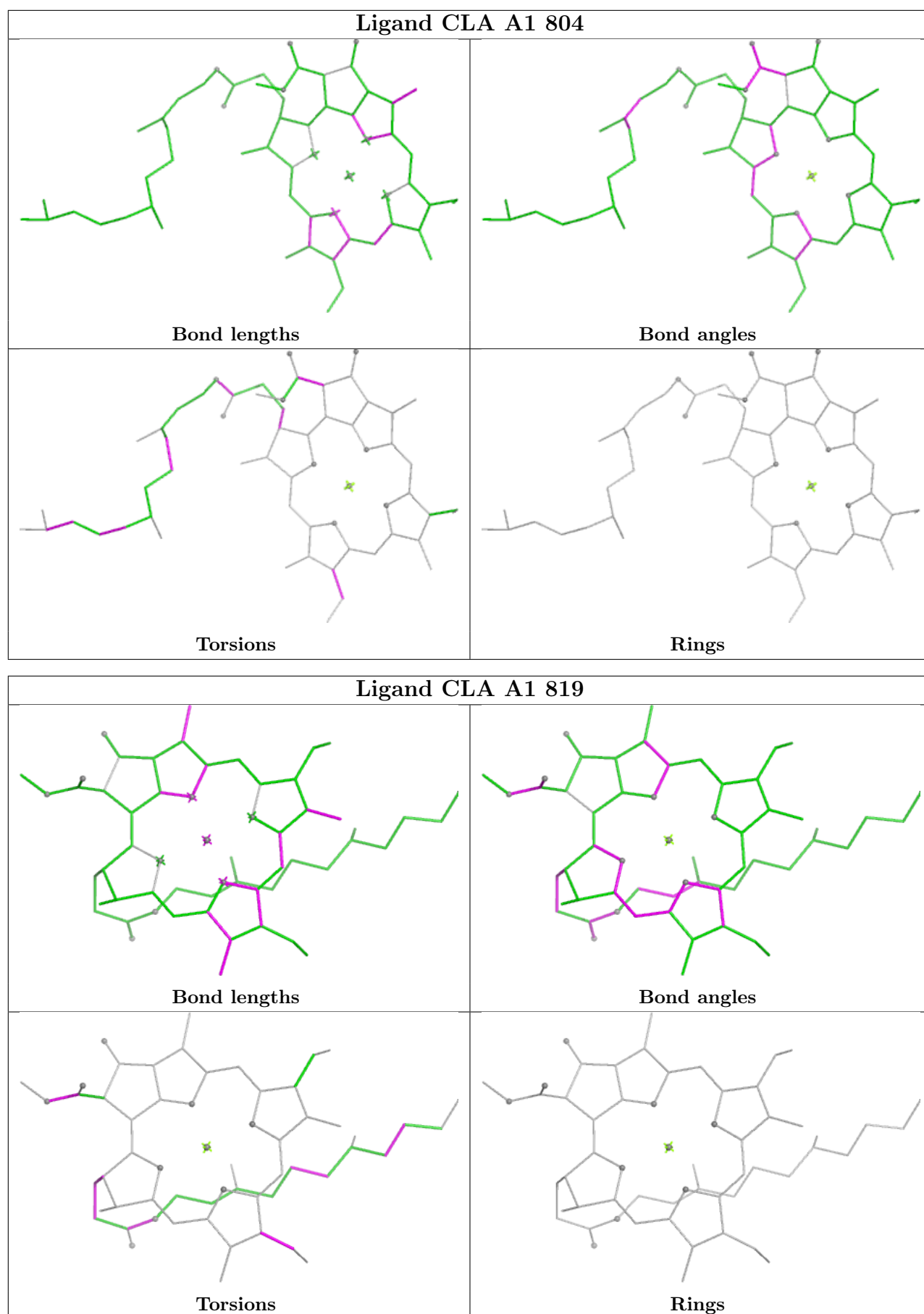
Bond angles

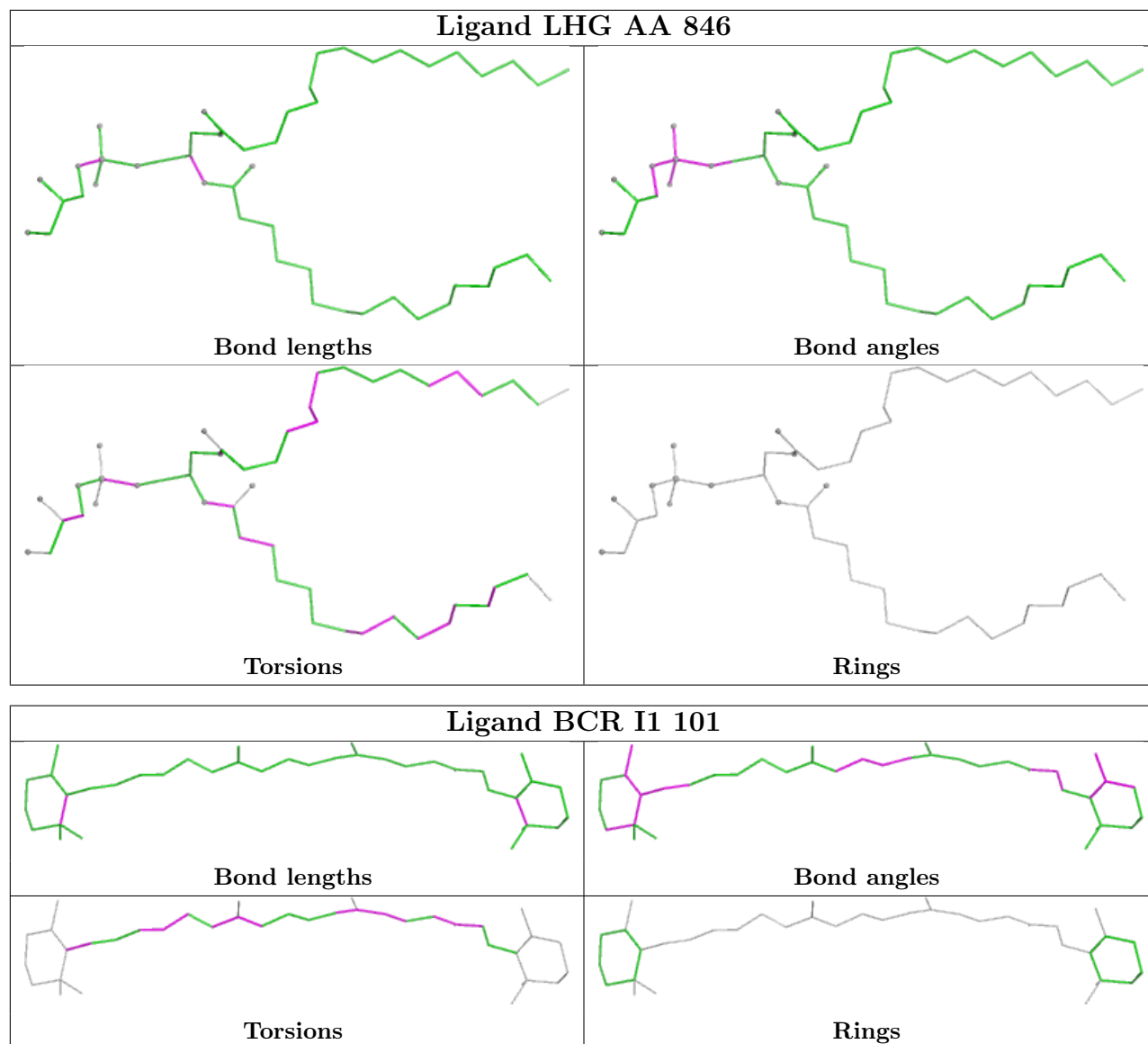


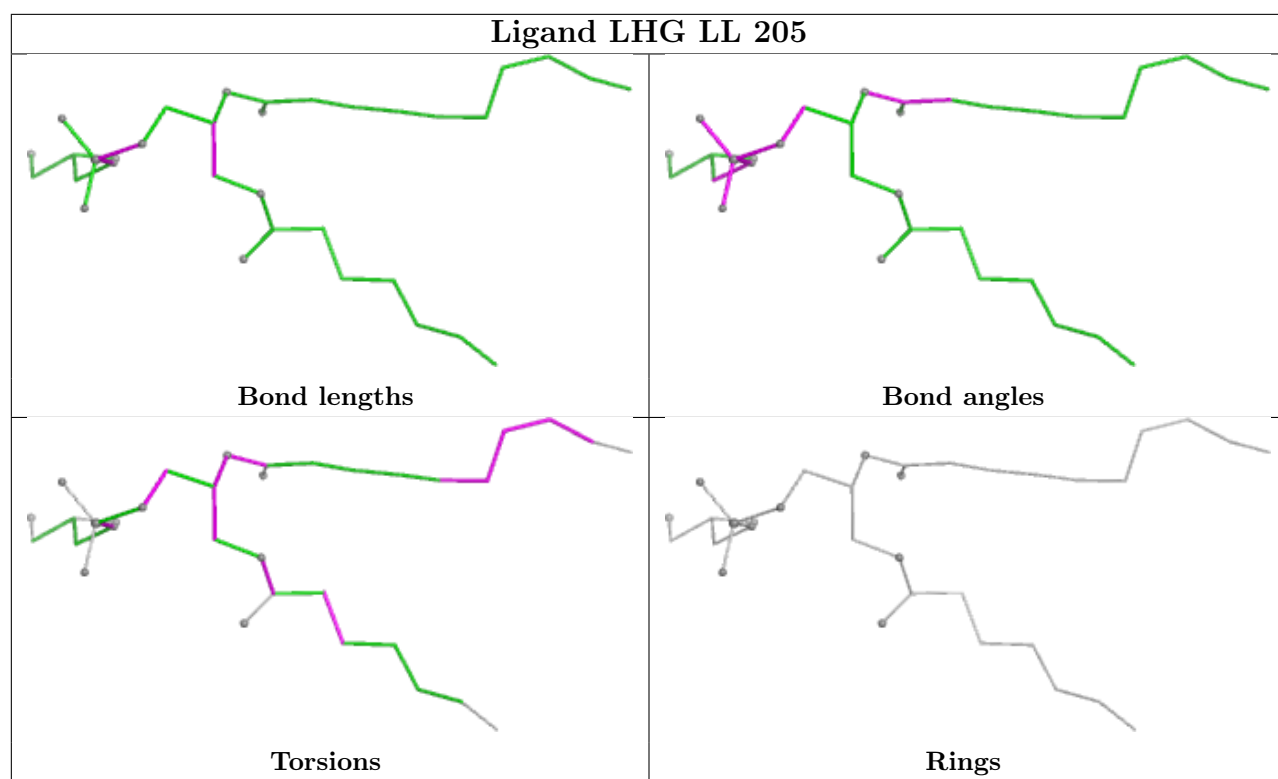
Torsions



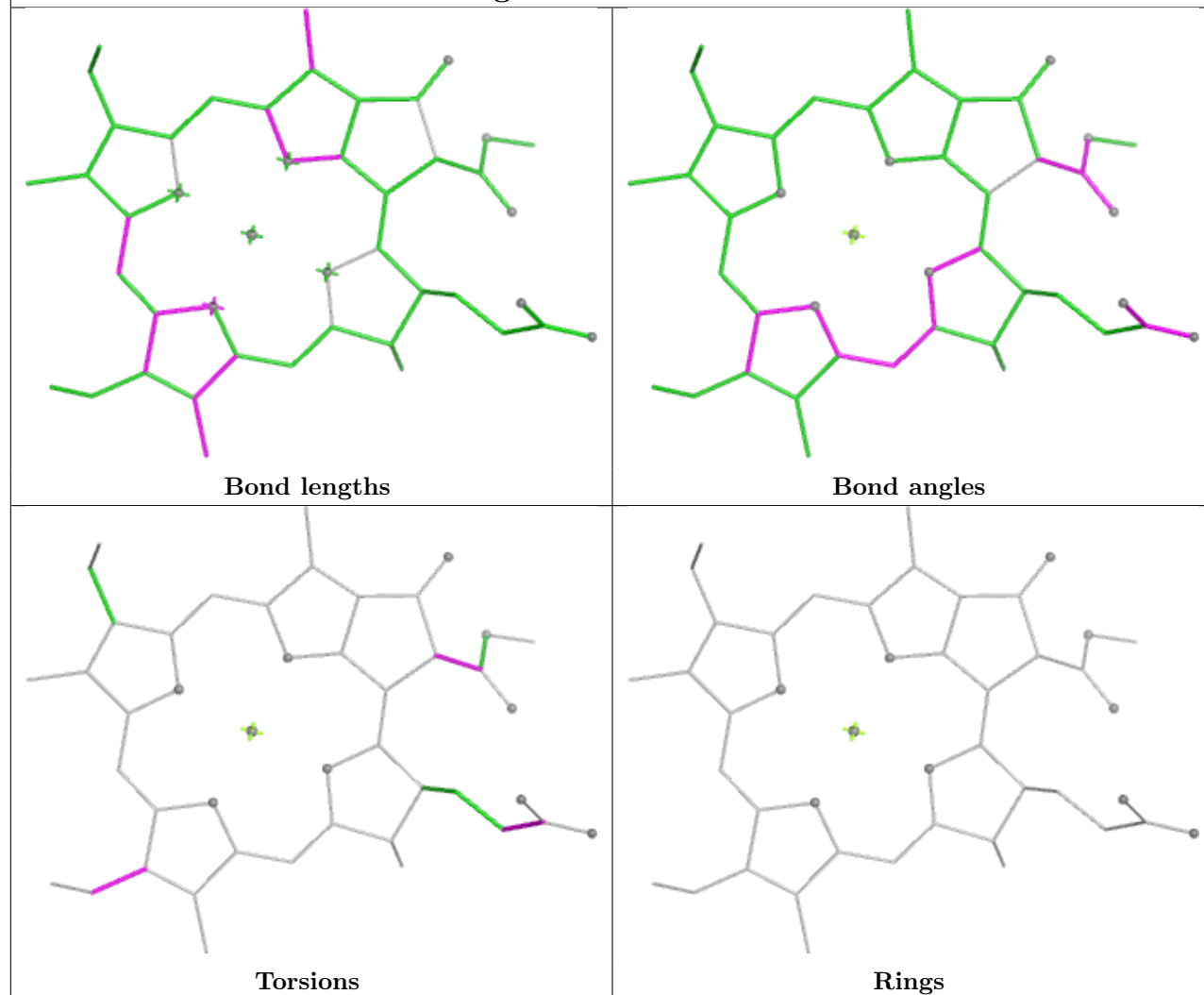
Rings

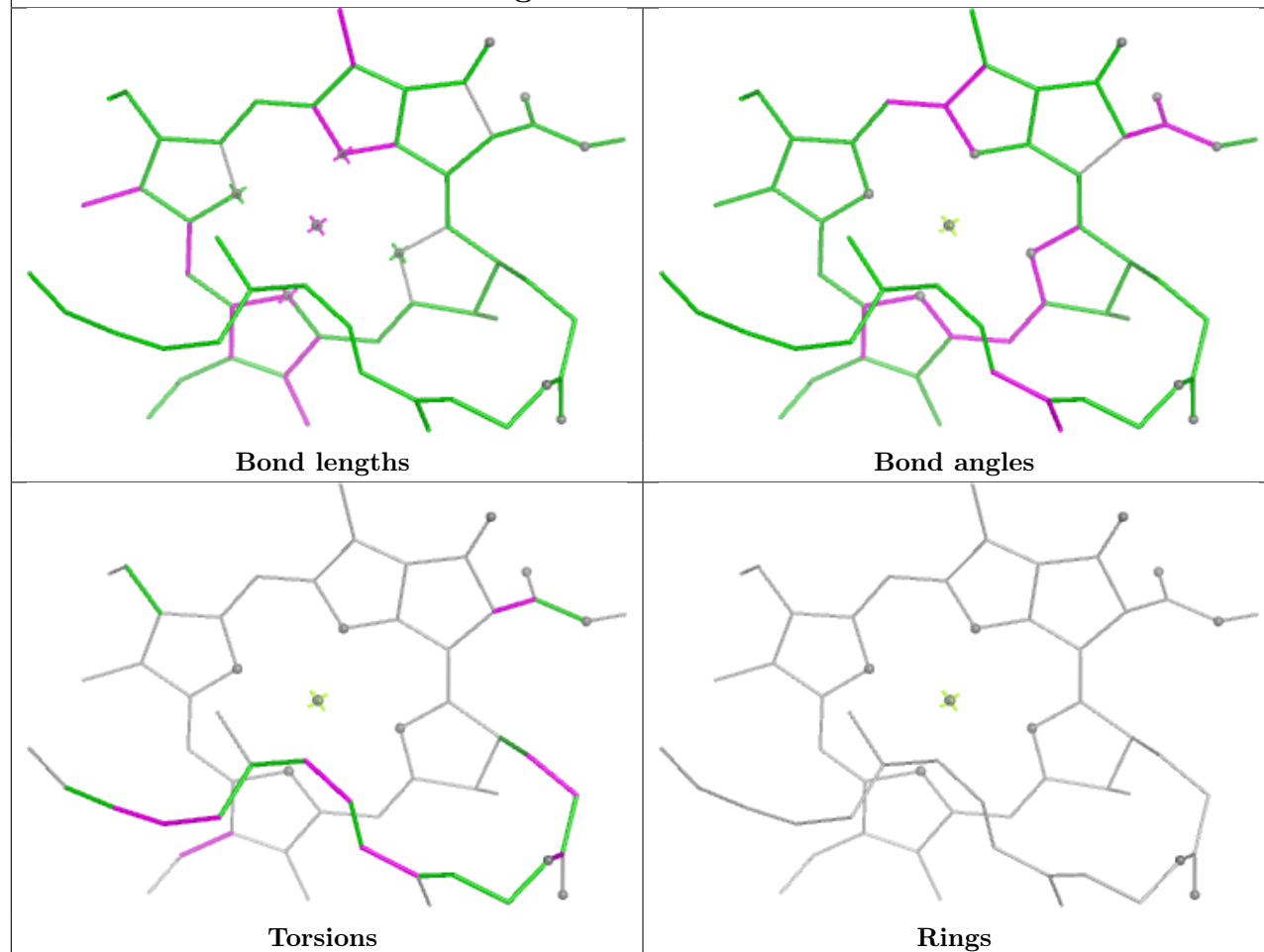
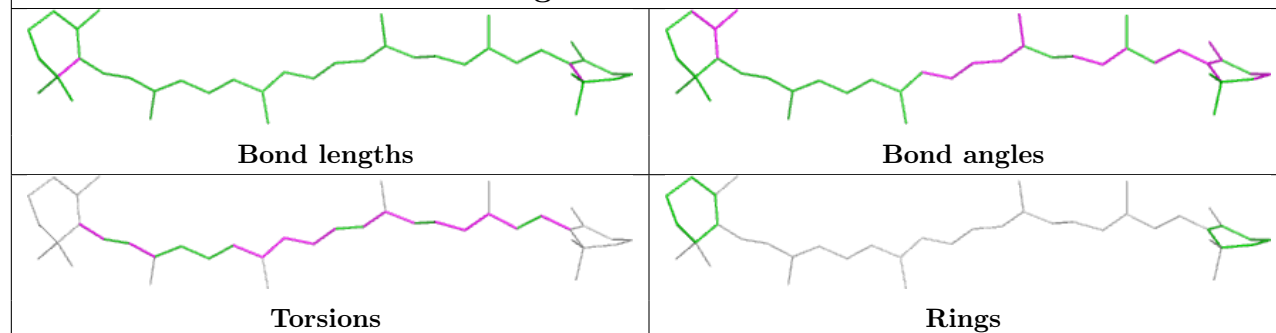


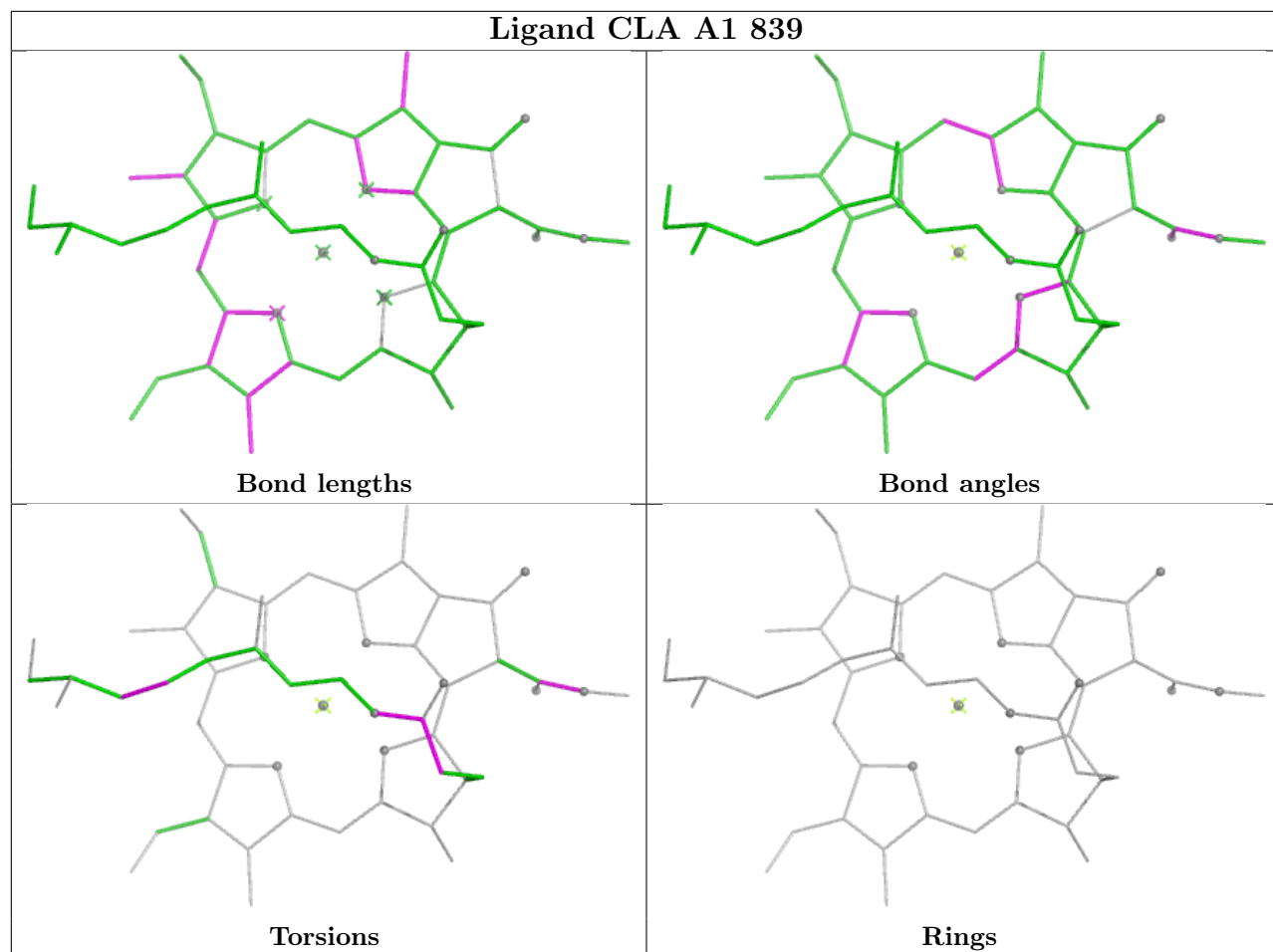


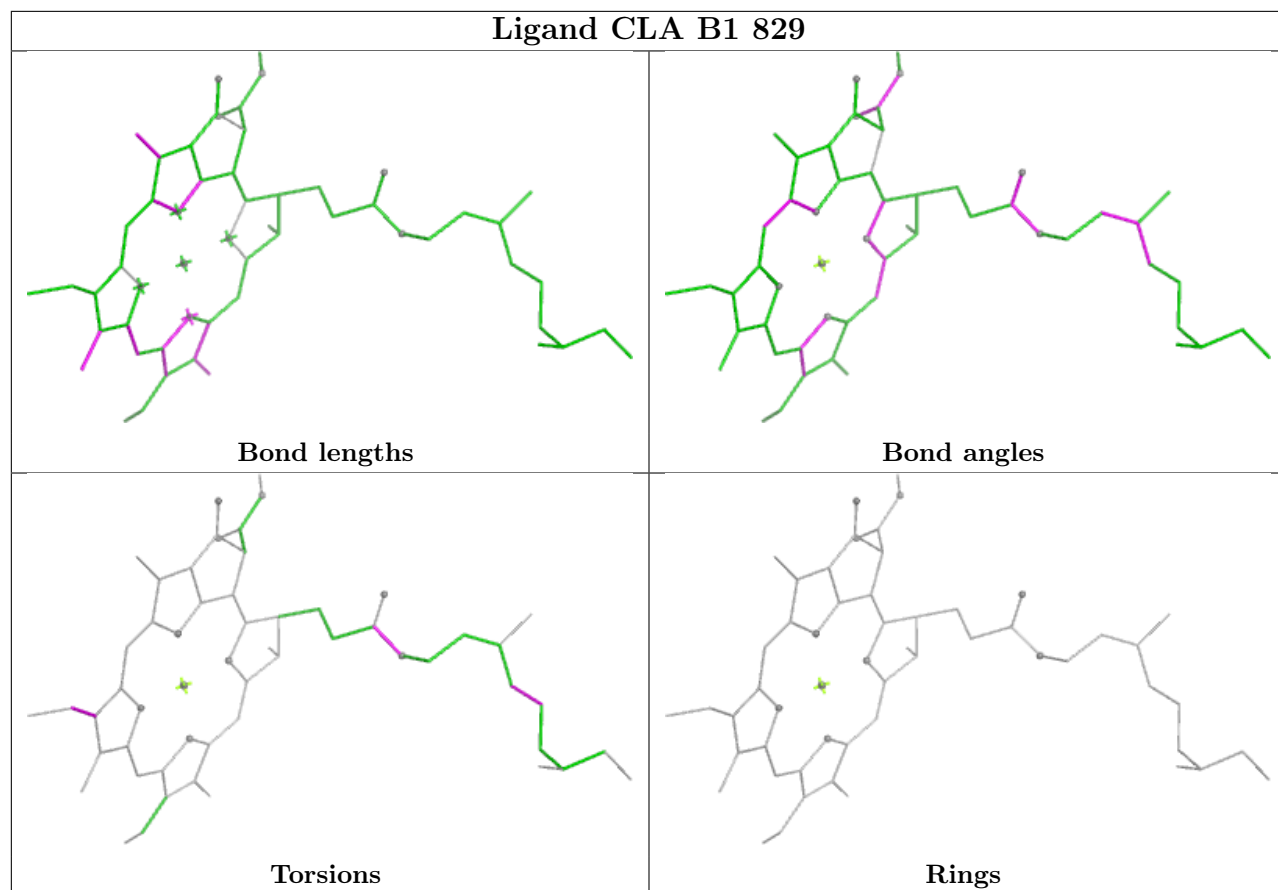


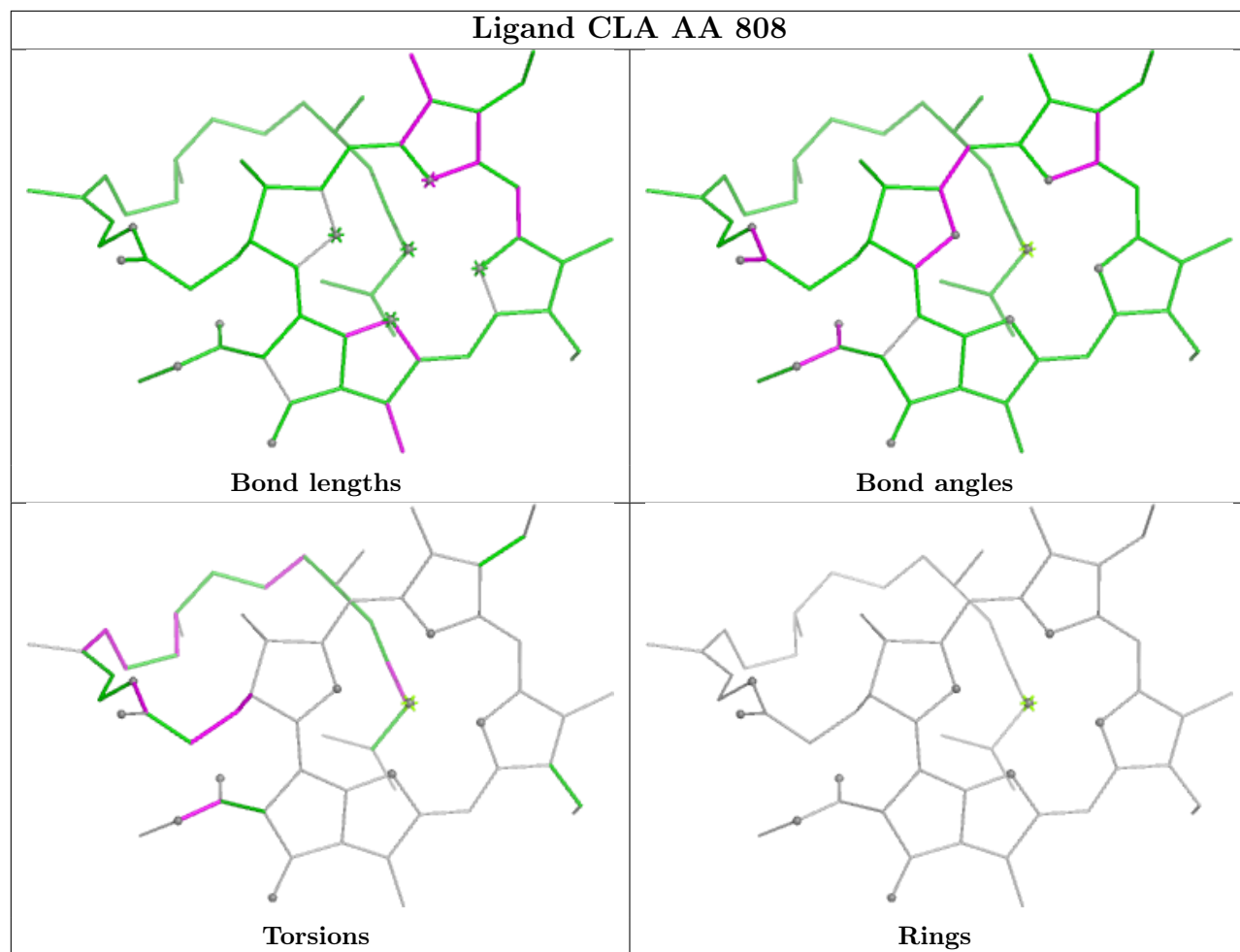
Ligand CLA B2 809

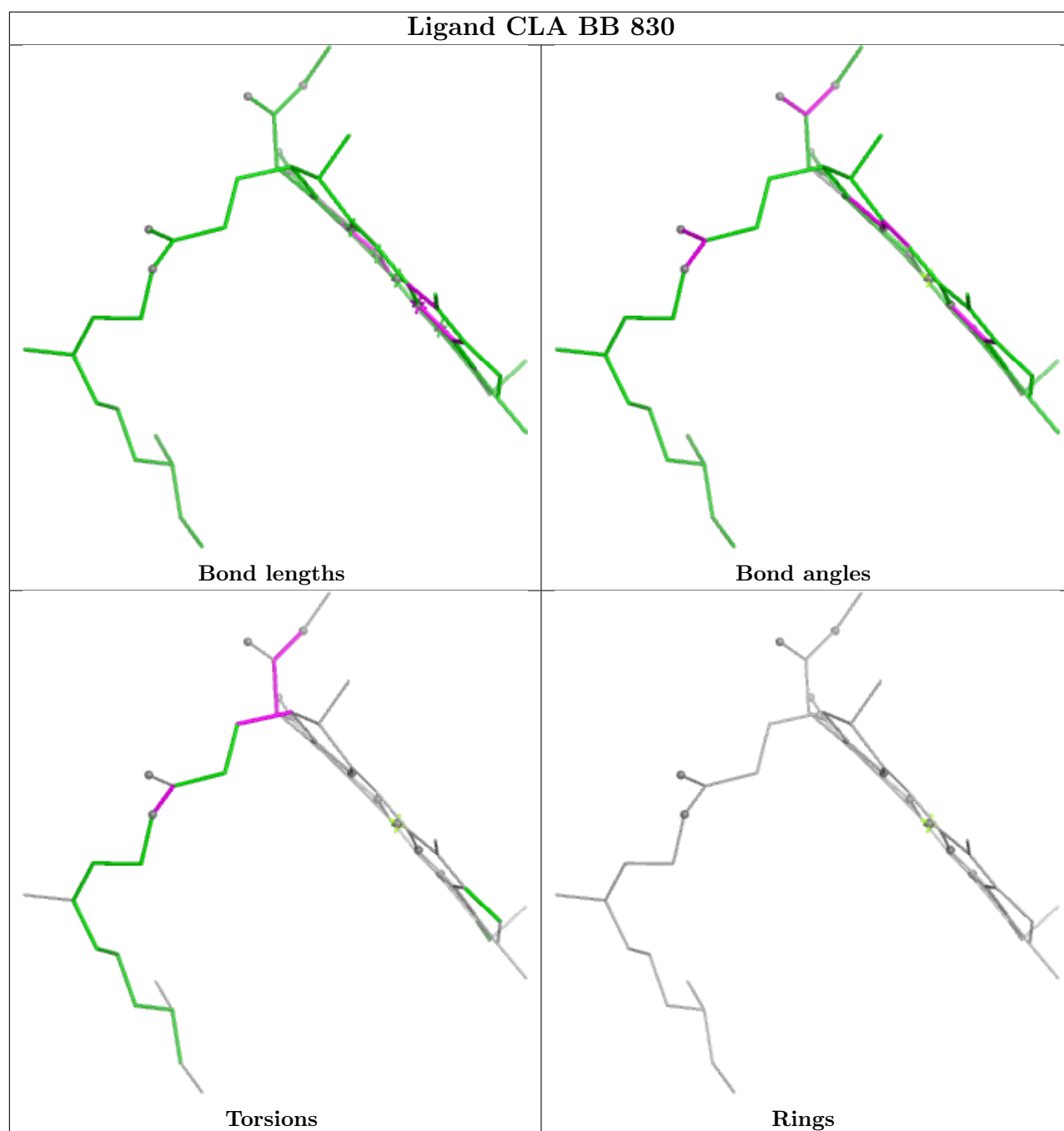


Ligand CLA BB 814**Ligand BCR J 102**

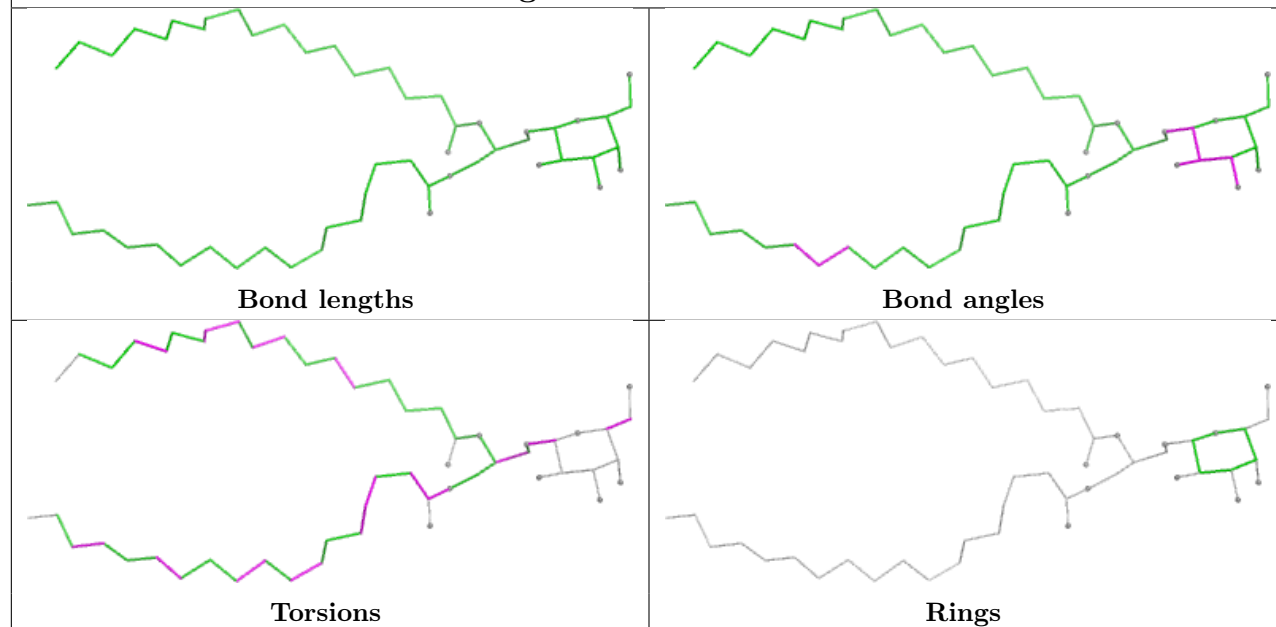




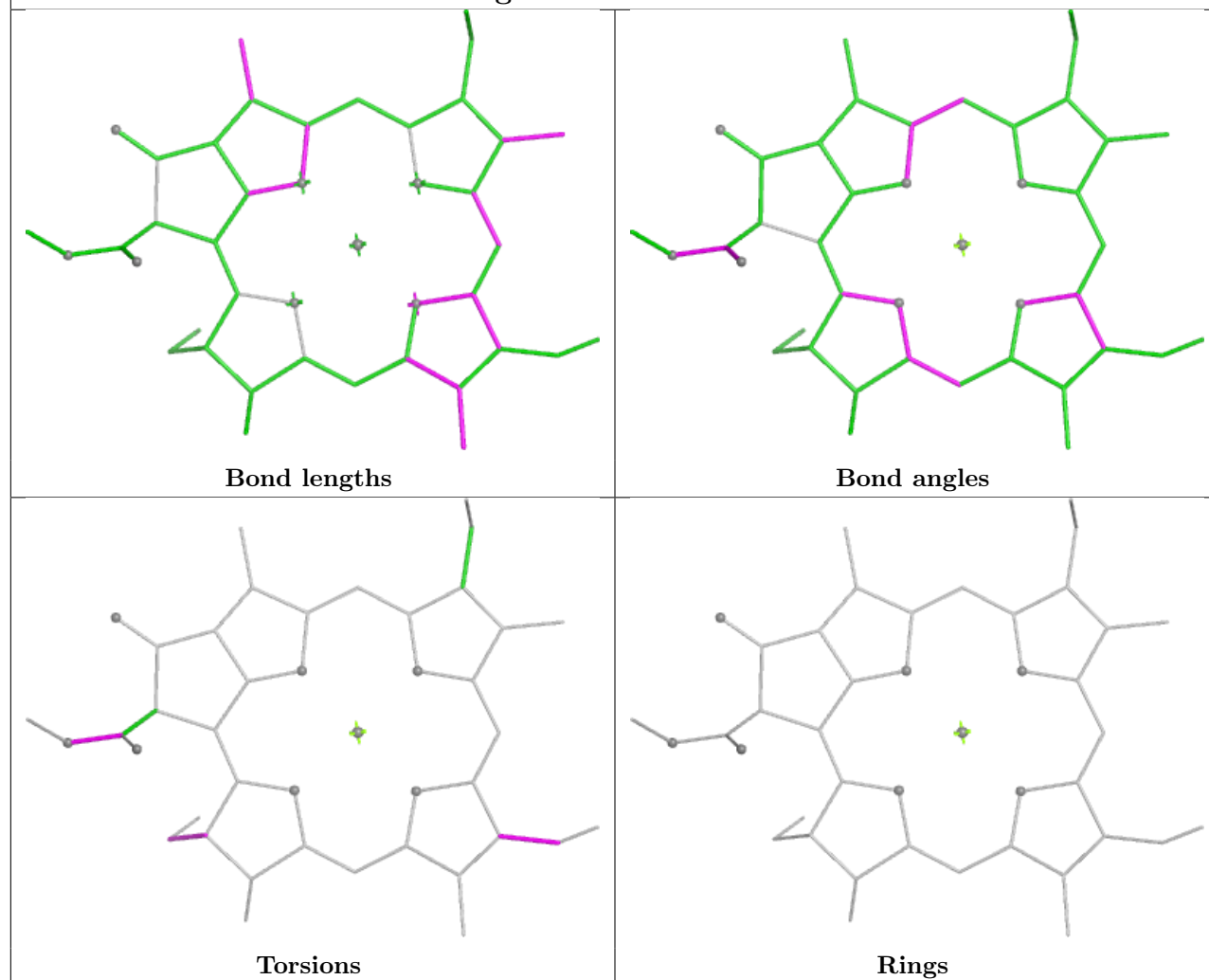




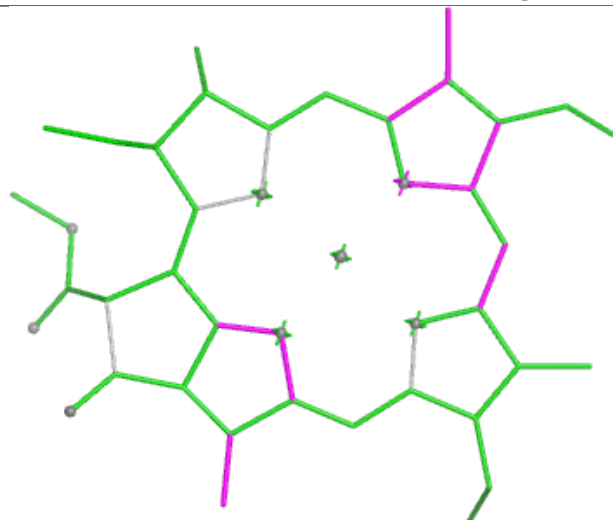
Ligand LMG B1 844



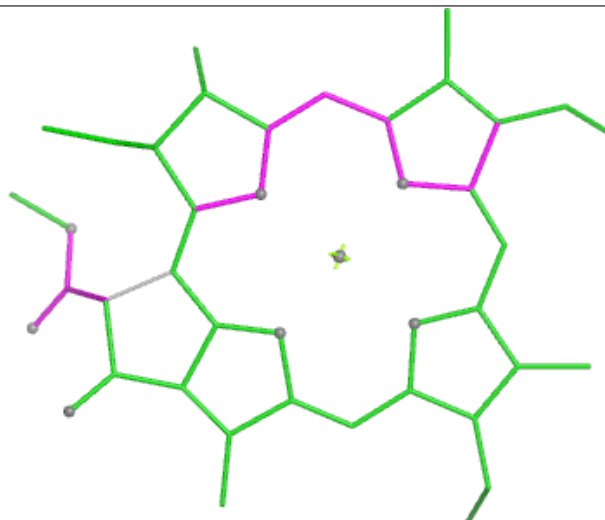
Ligand CLA A2 825



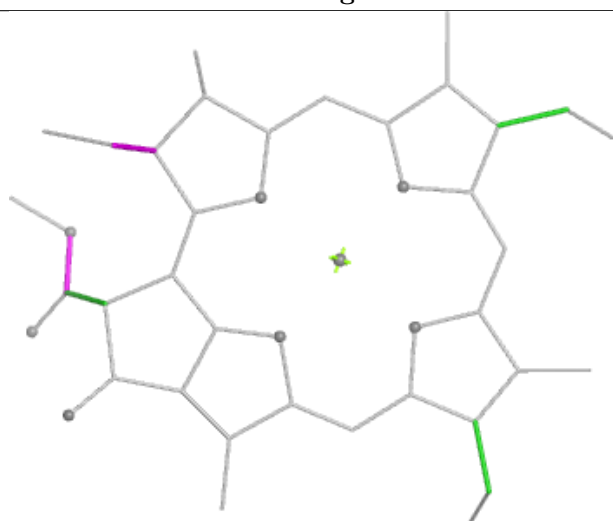
Ligand CLA F 302



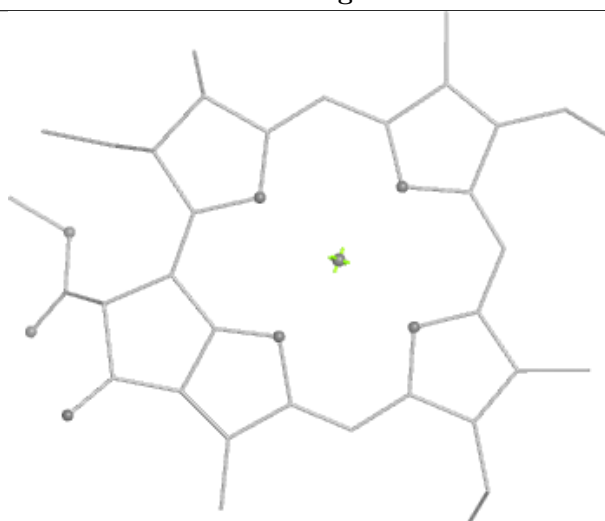
Bond lengths



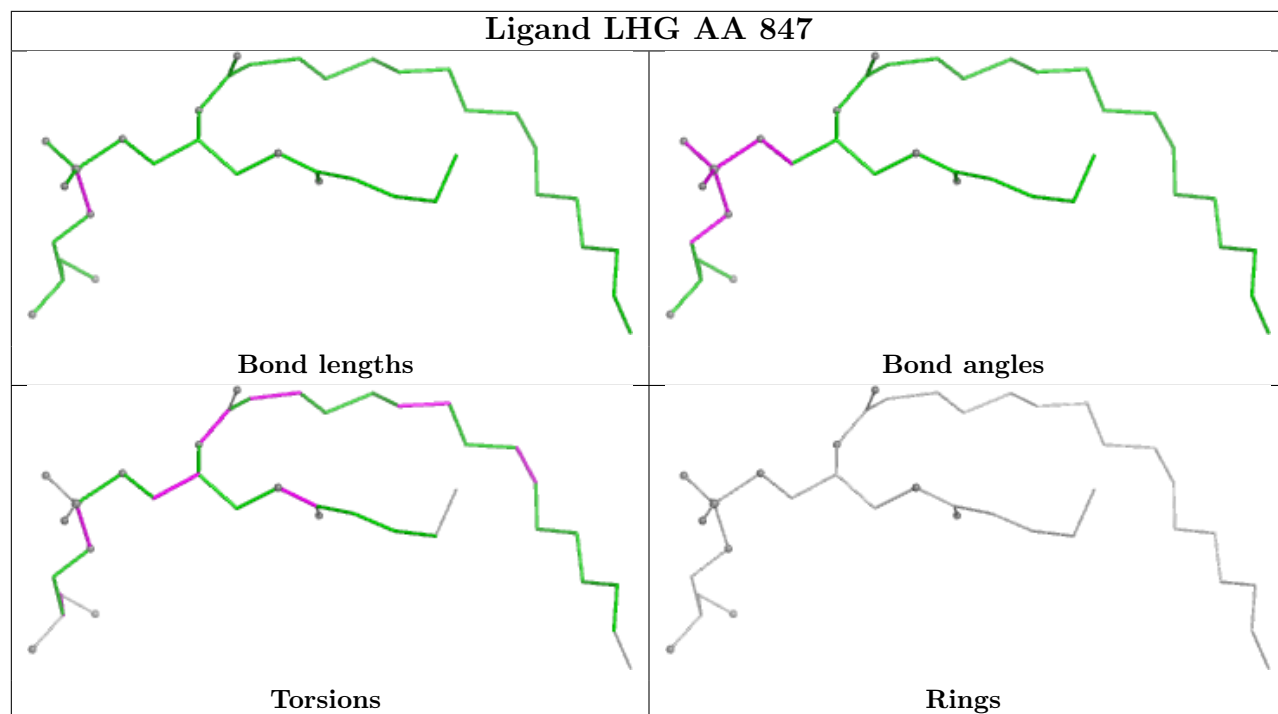
Bond angles

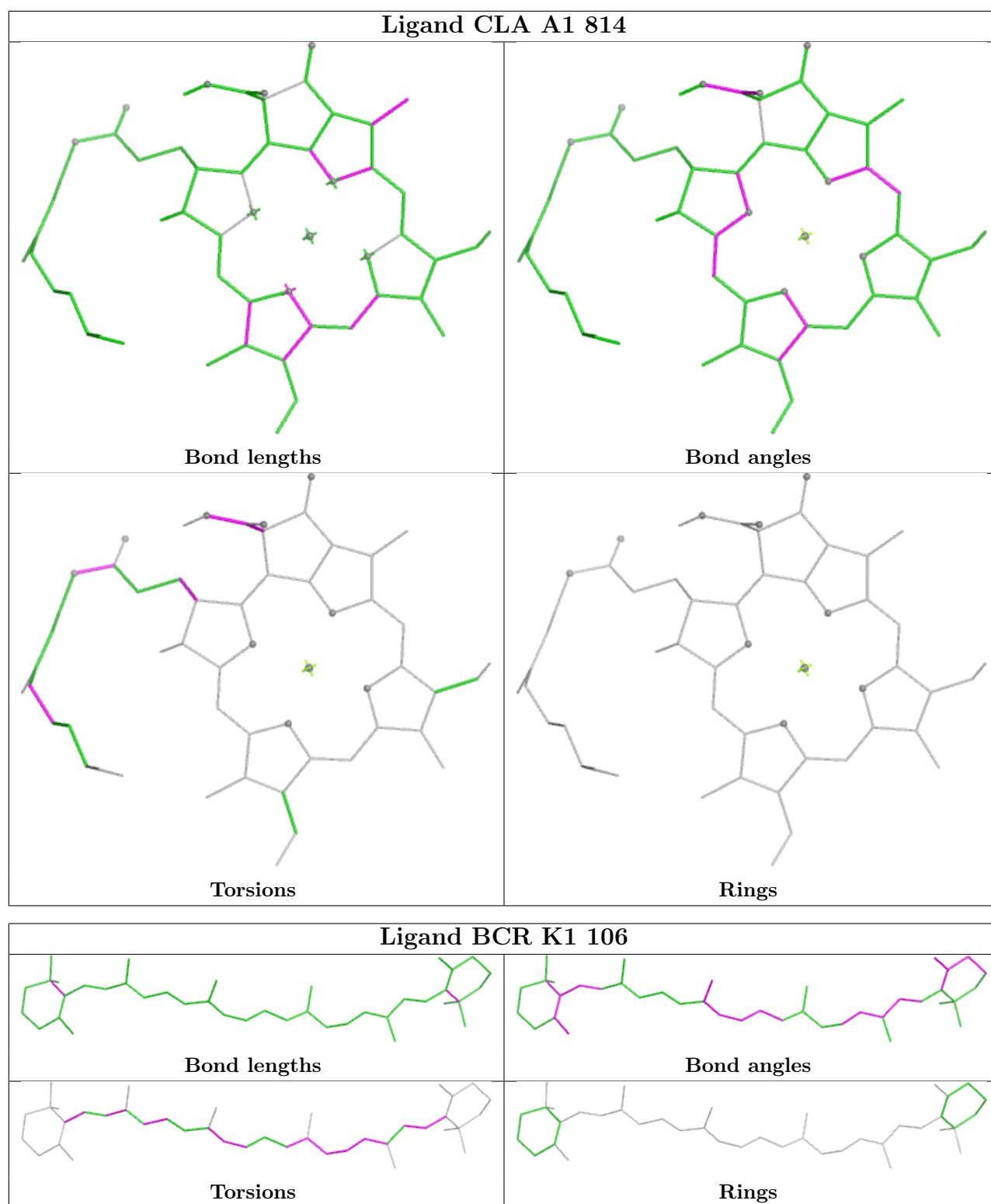


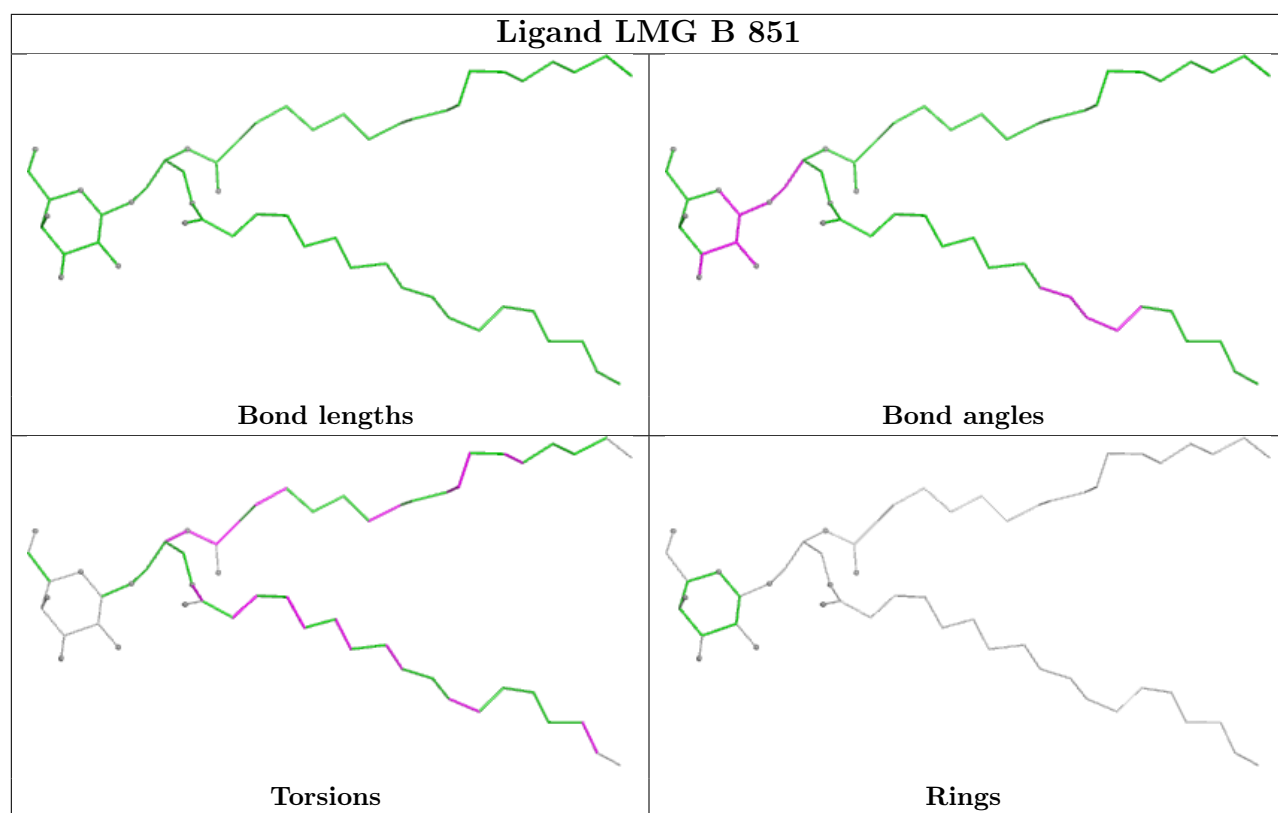
Torsions



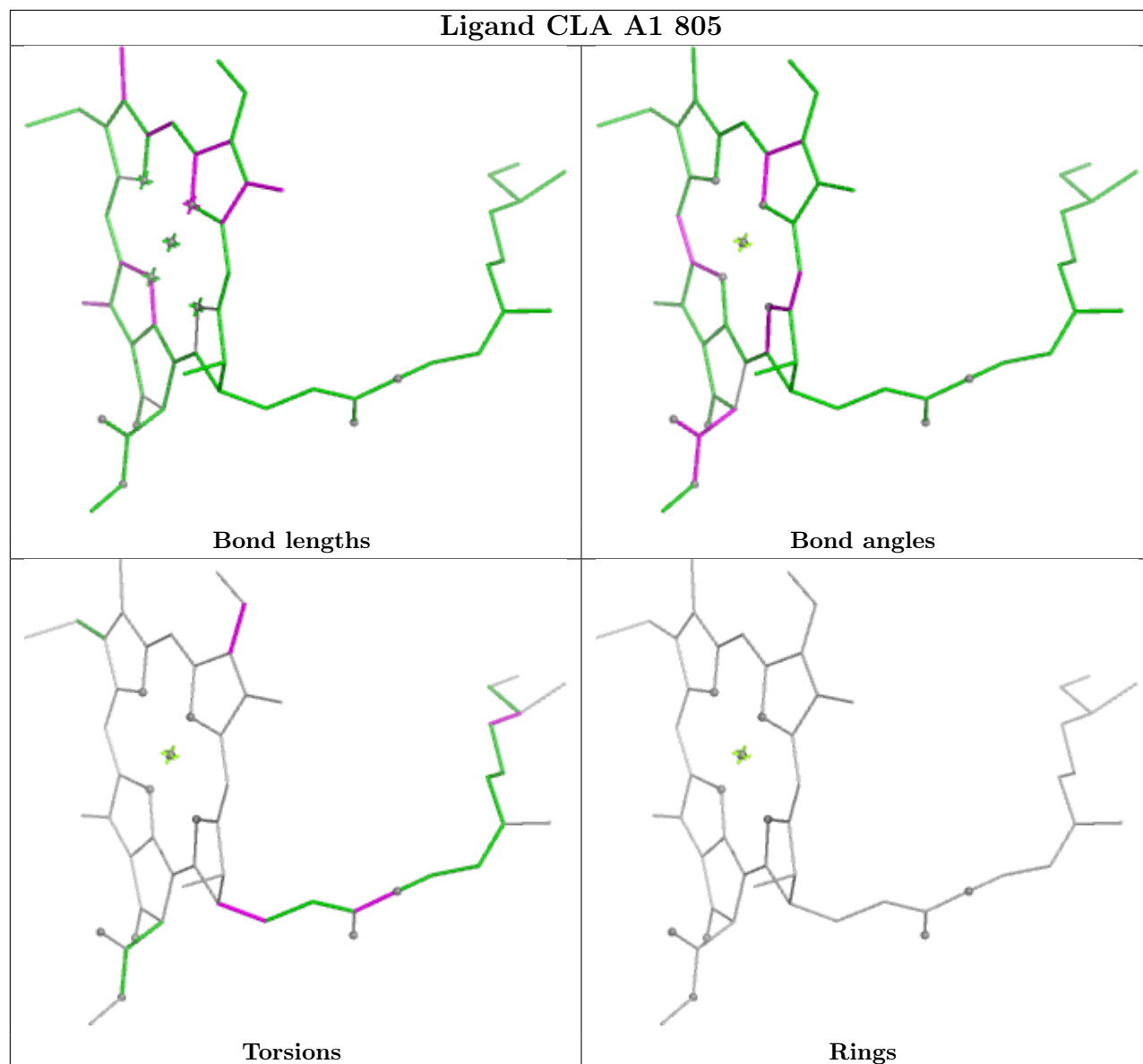
Rings

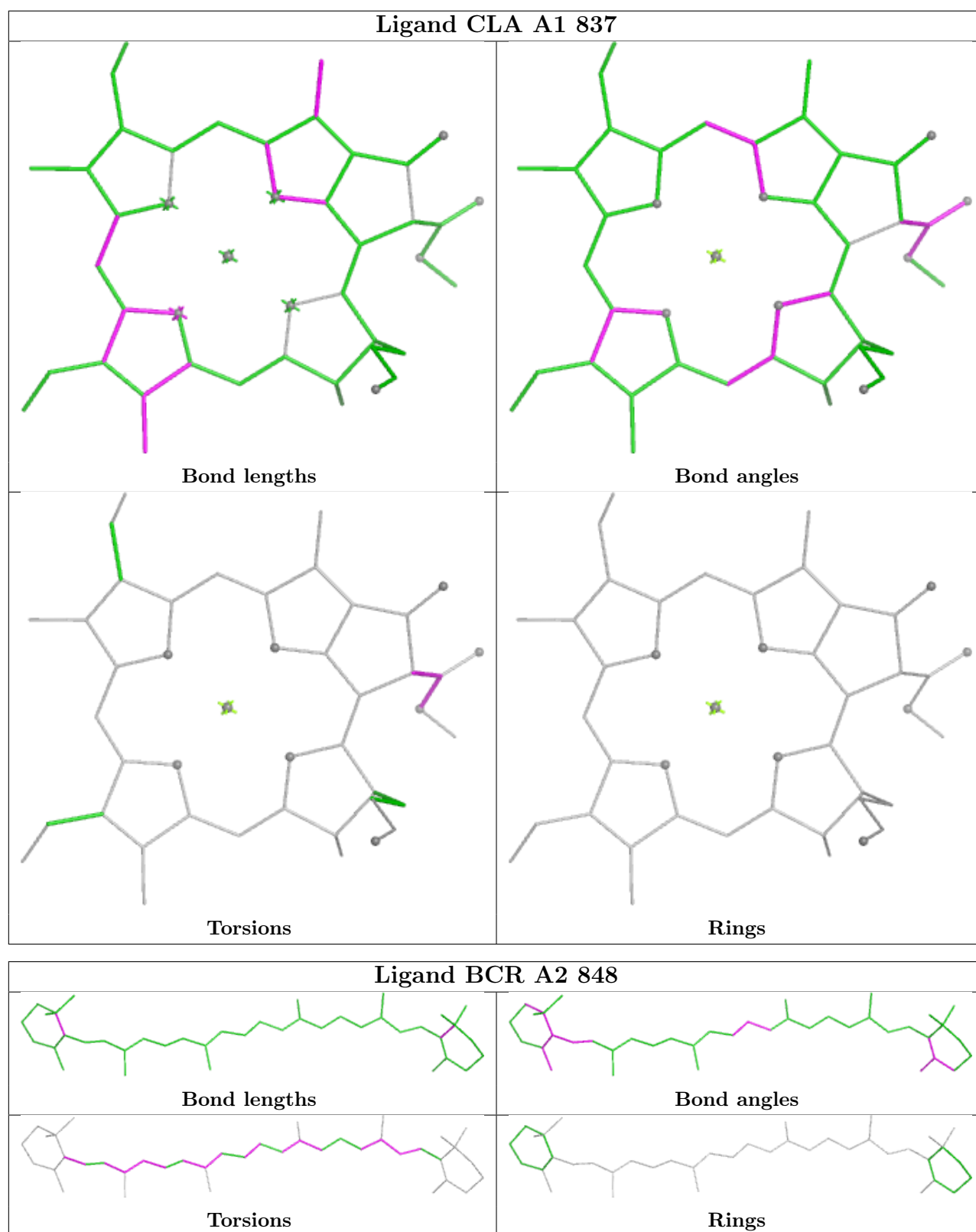




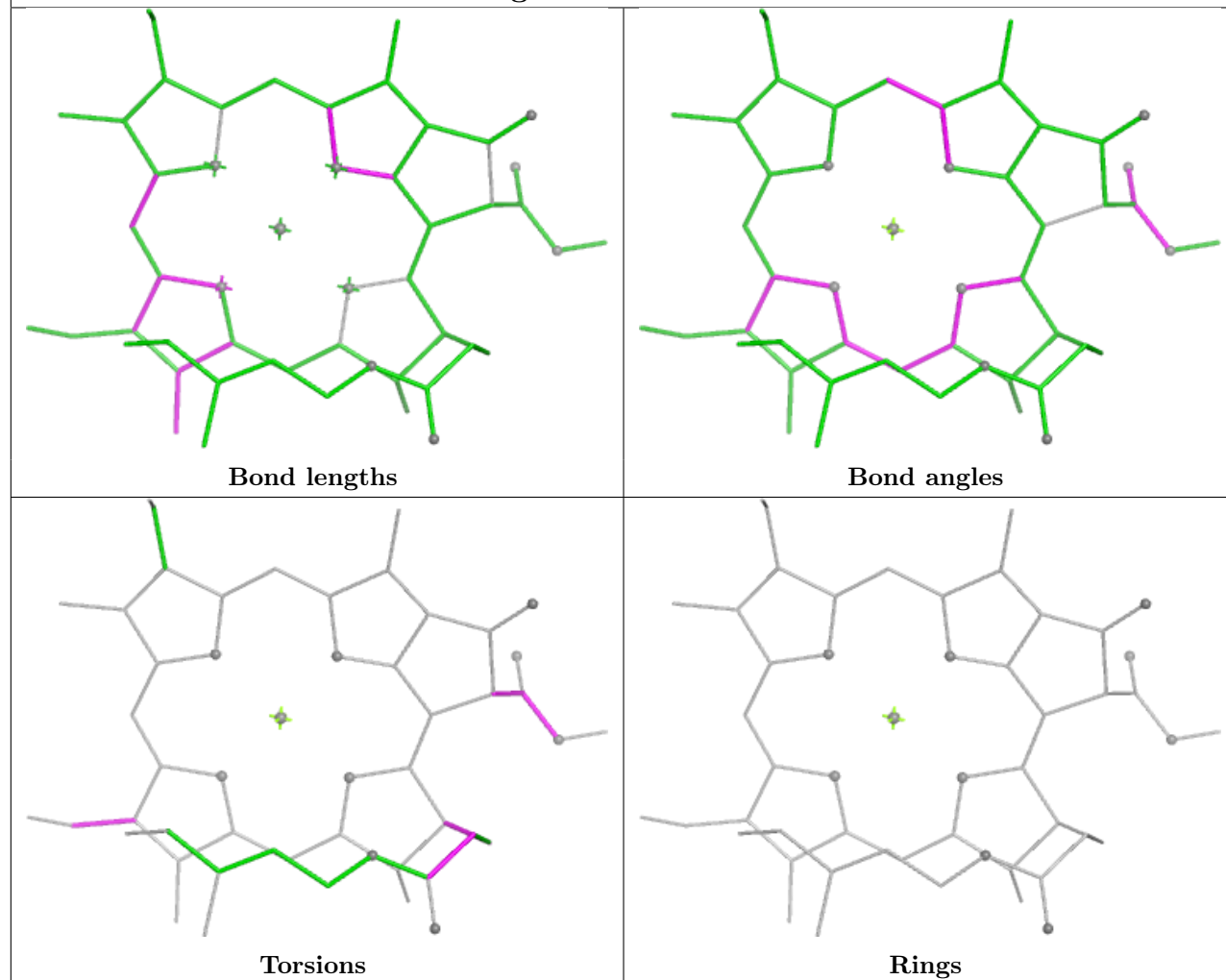


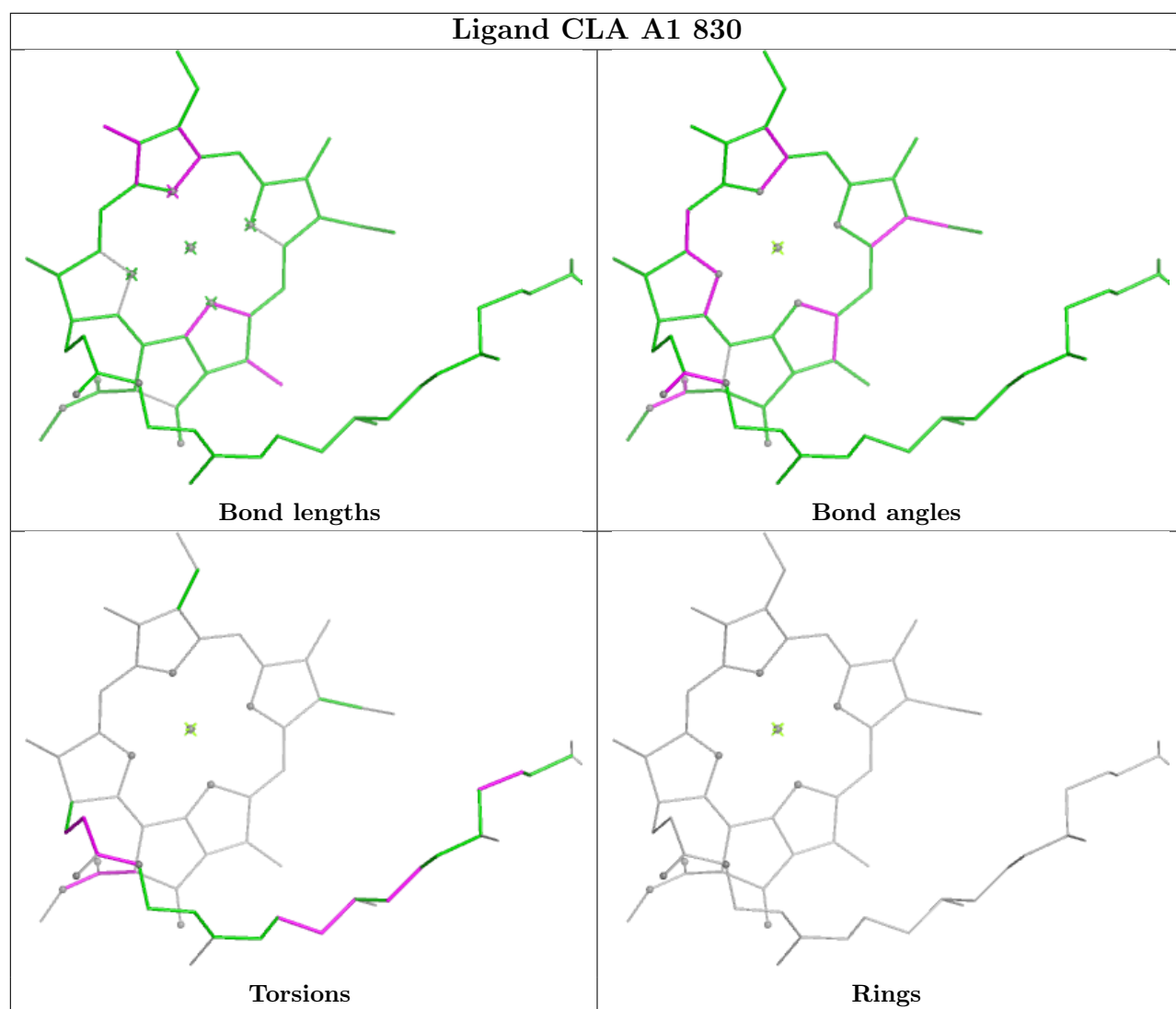
Ligand CLA A1 805



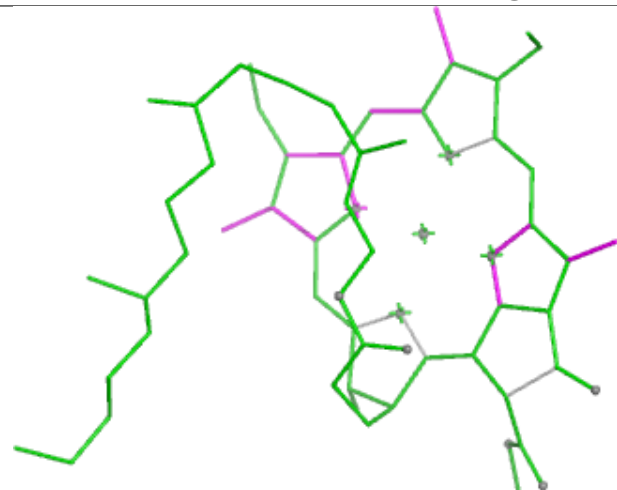


Ligand CLA A 822

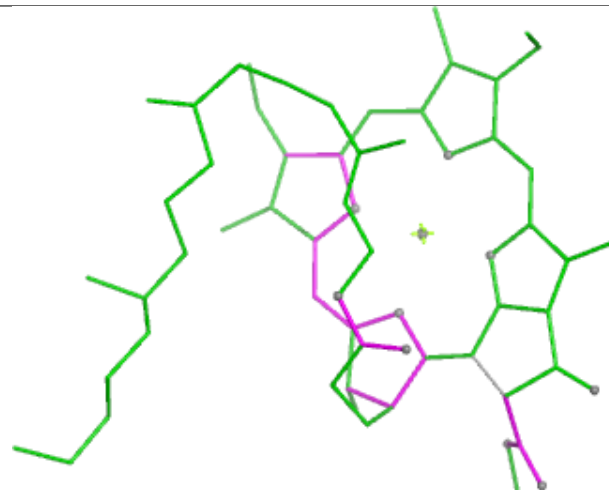




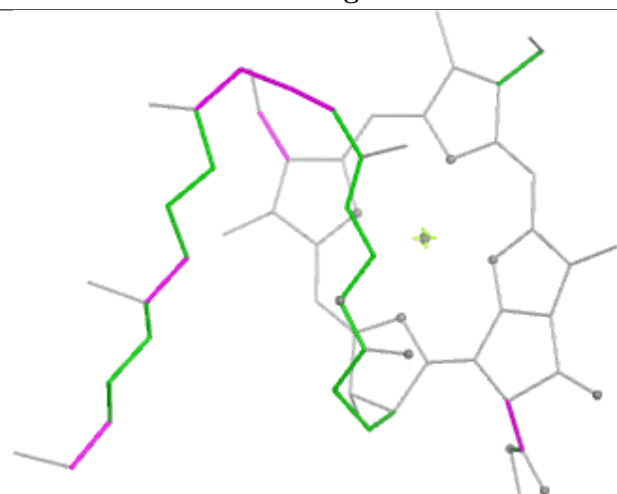
Ligand CLA BB 805



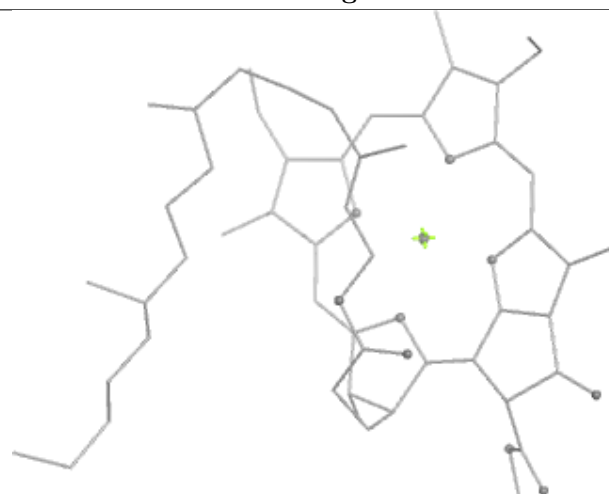
Bond lengths



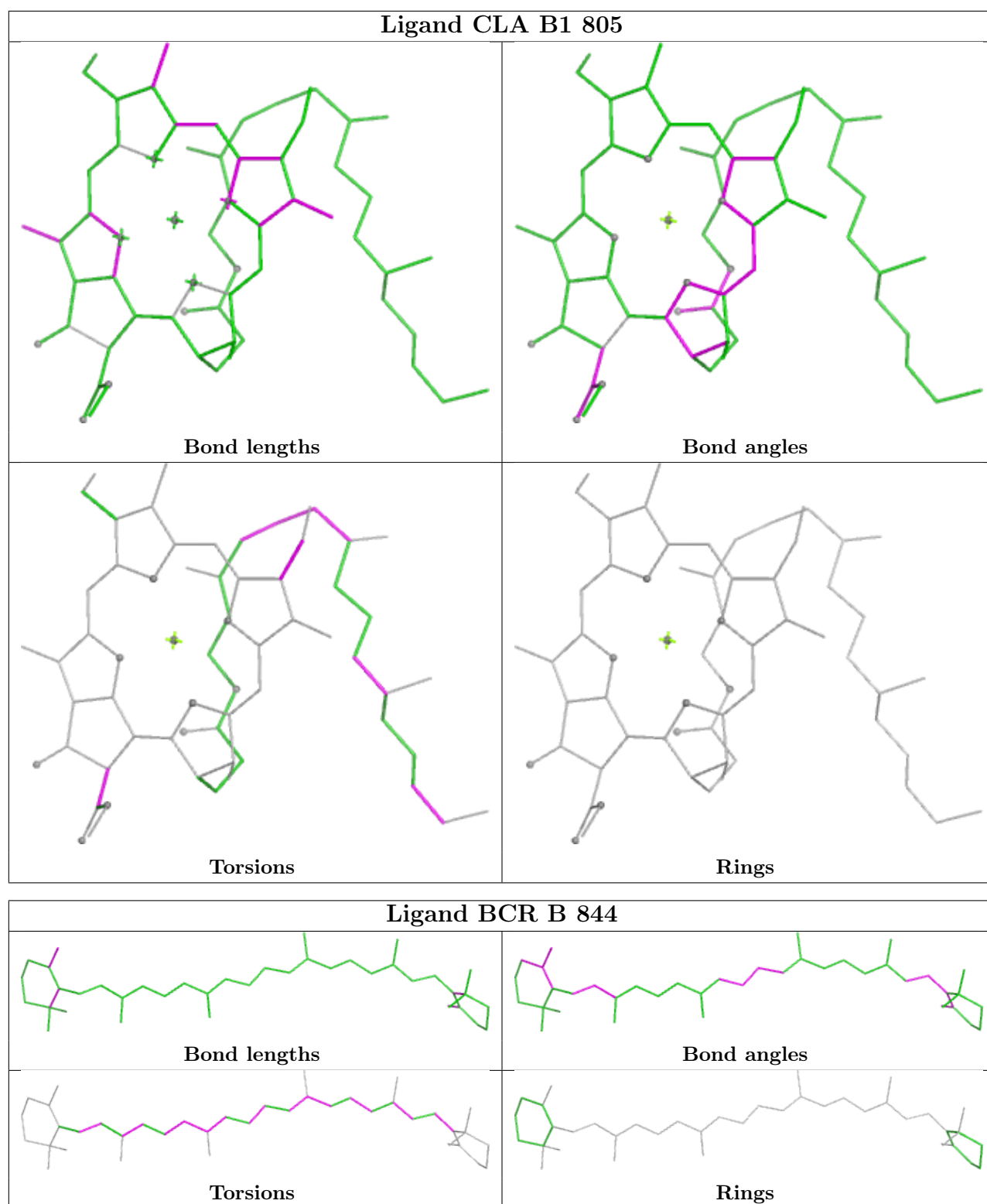
Bond angles

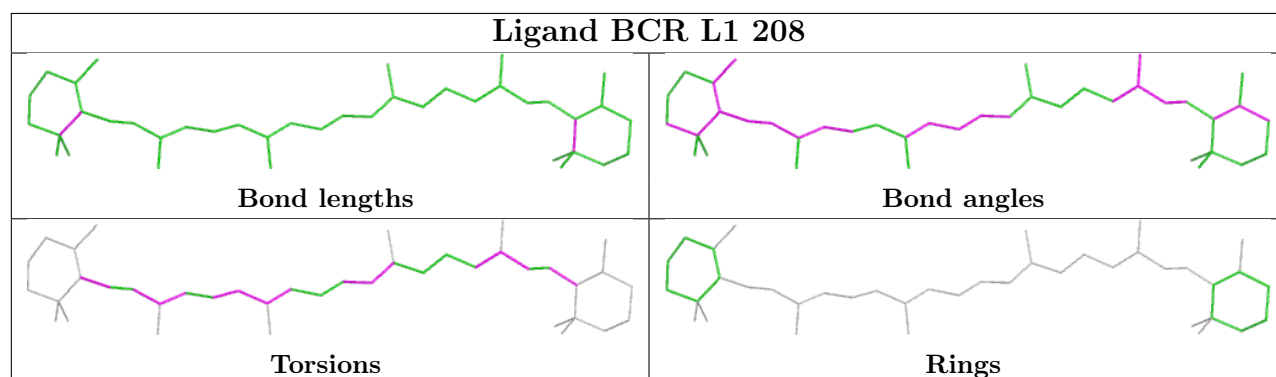
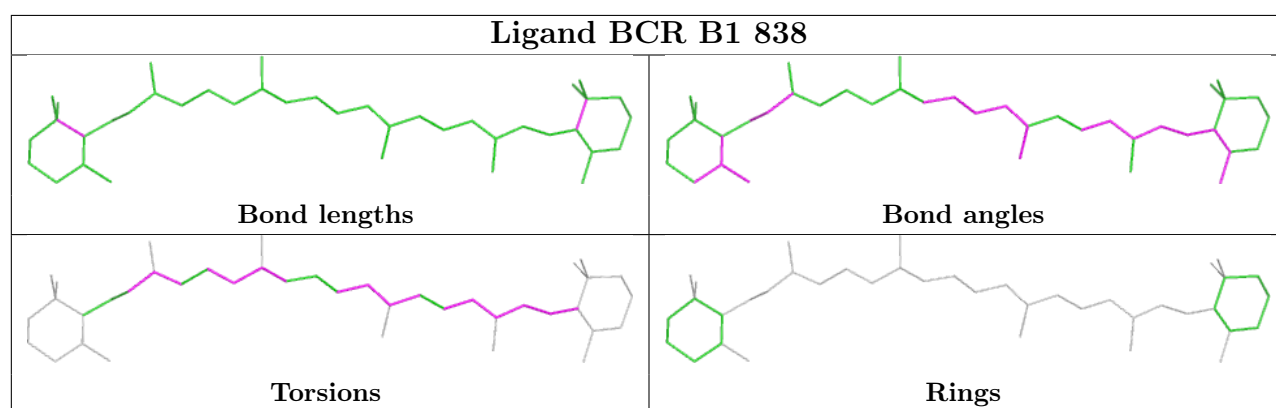
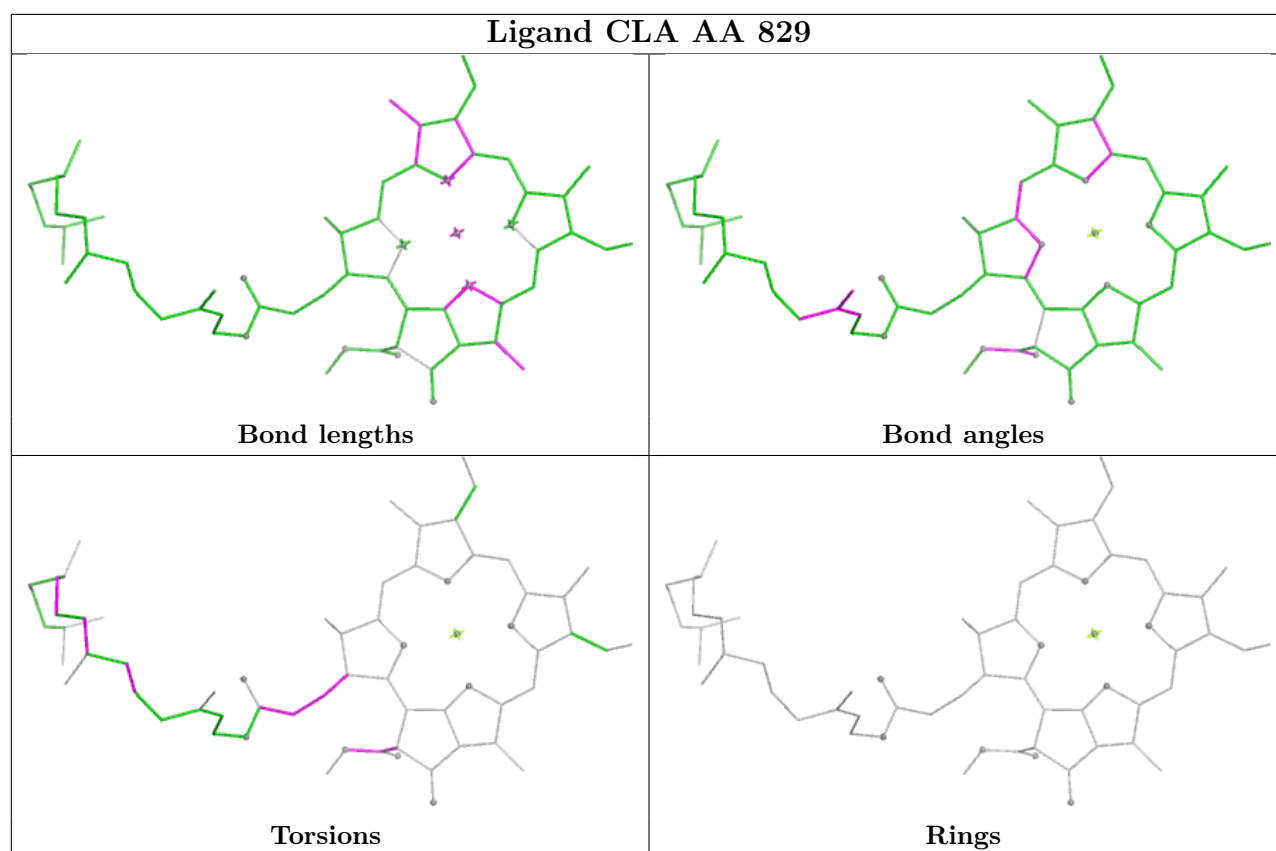


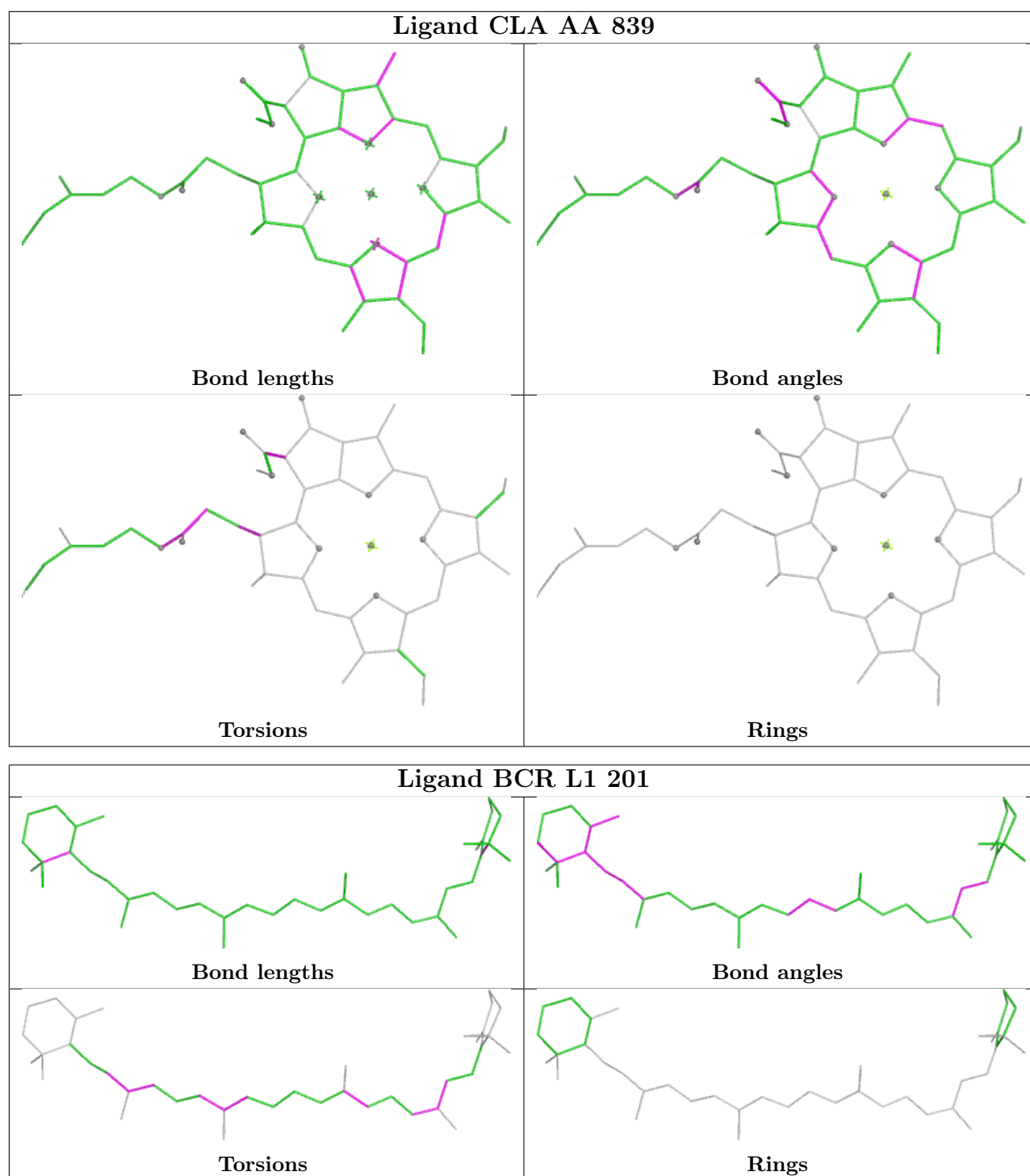
Torsions

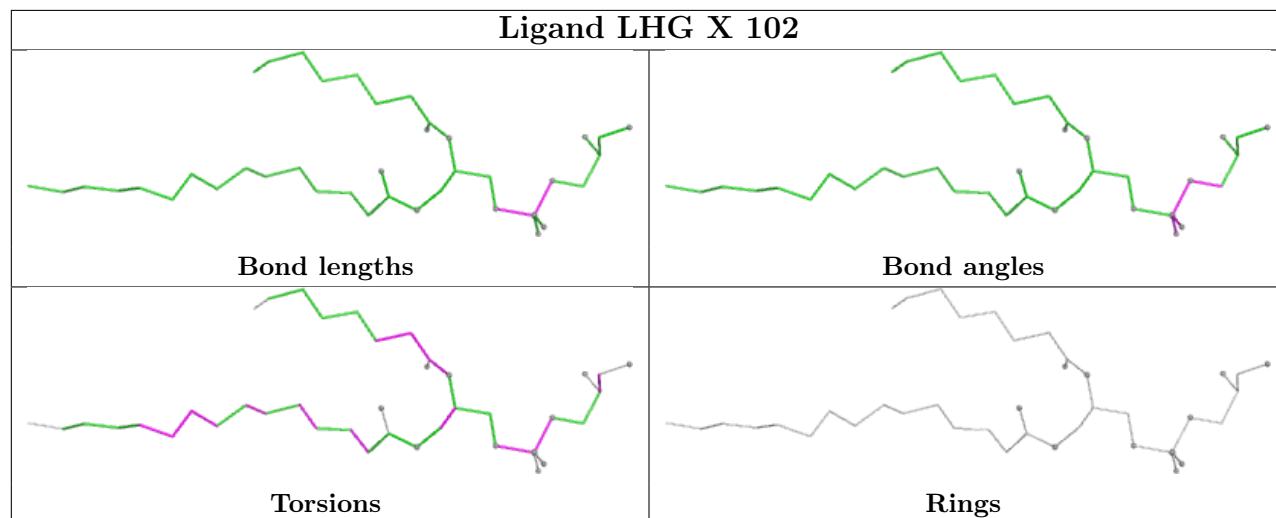
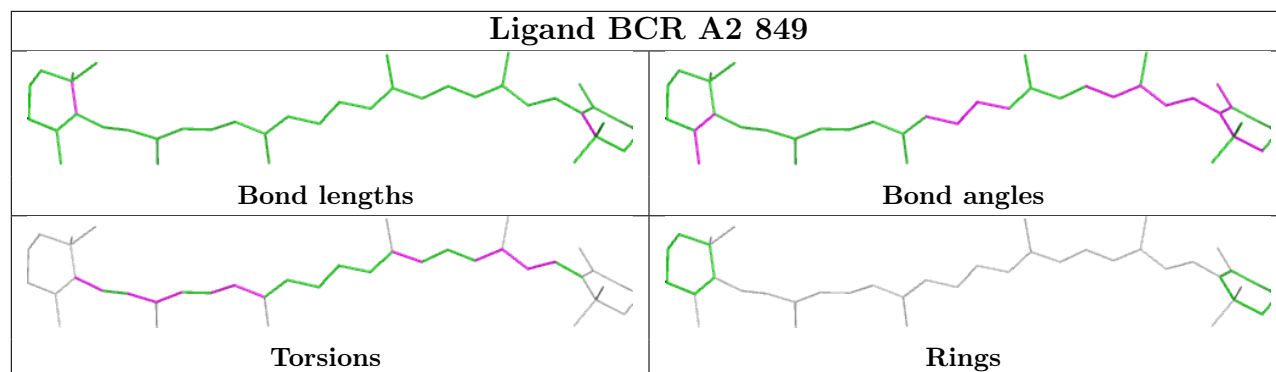


Rings

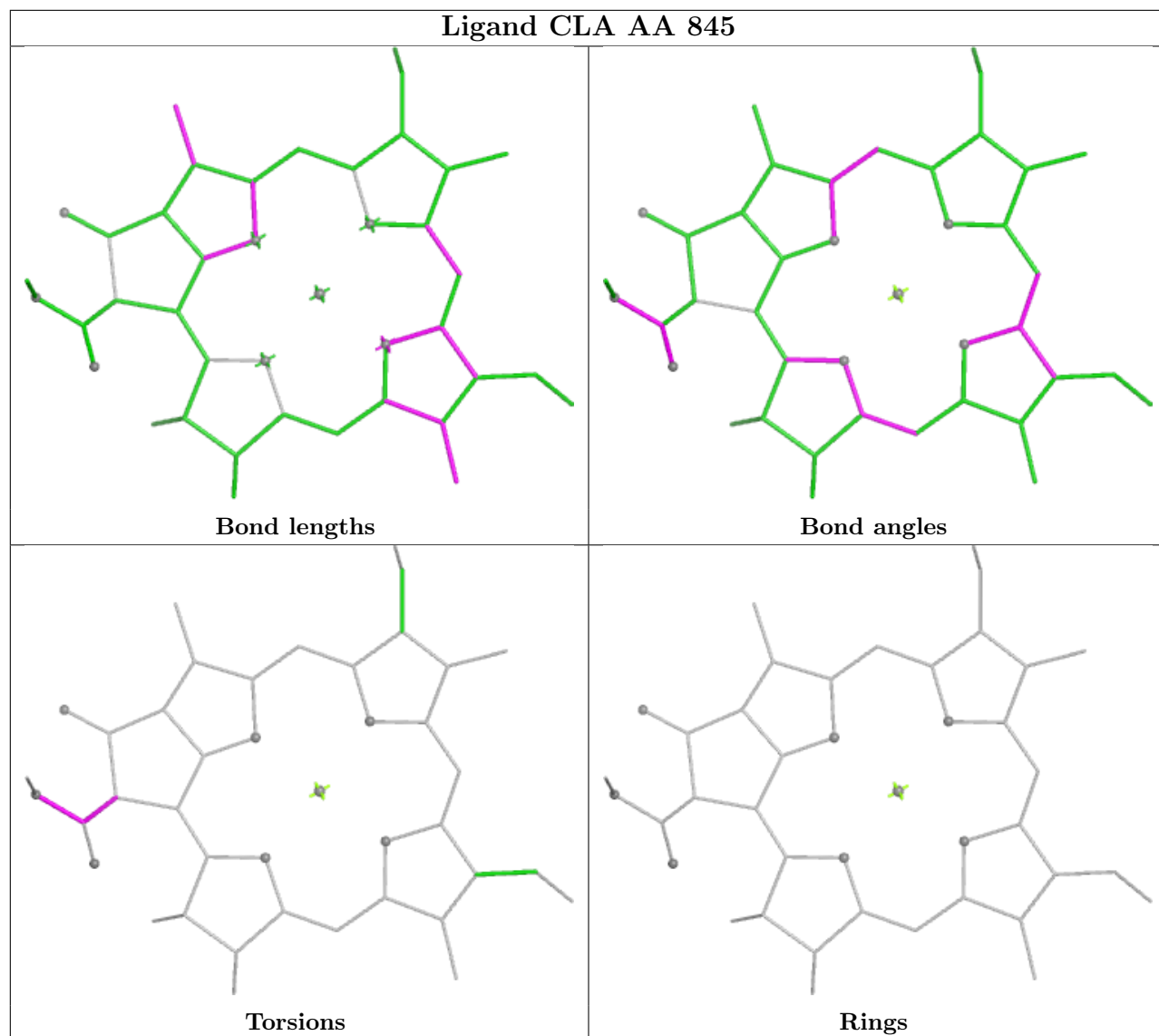




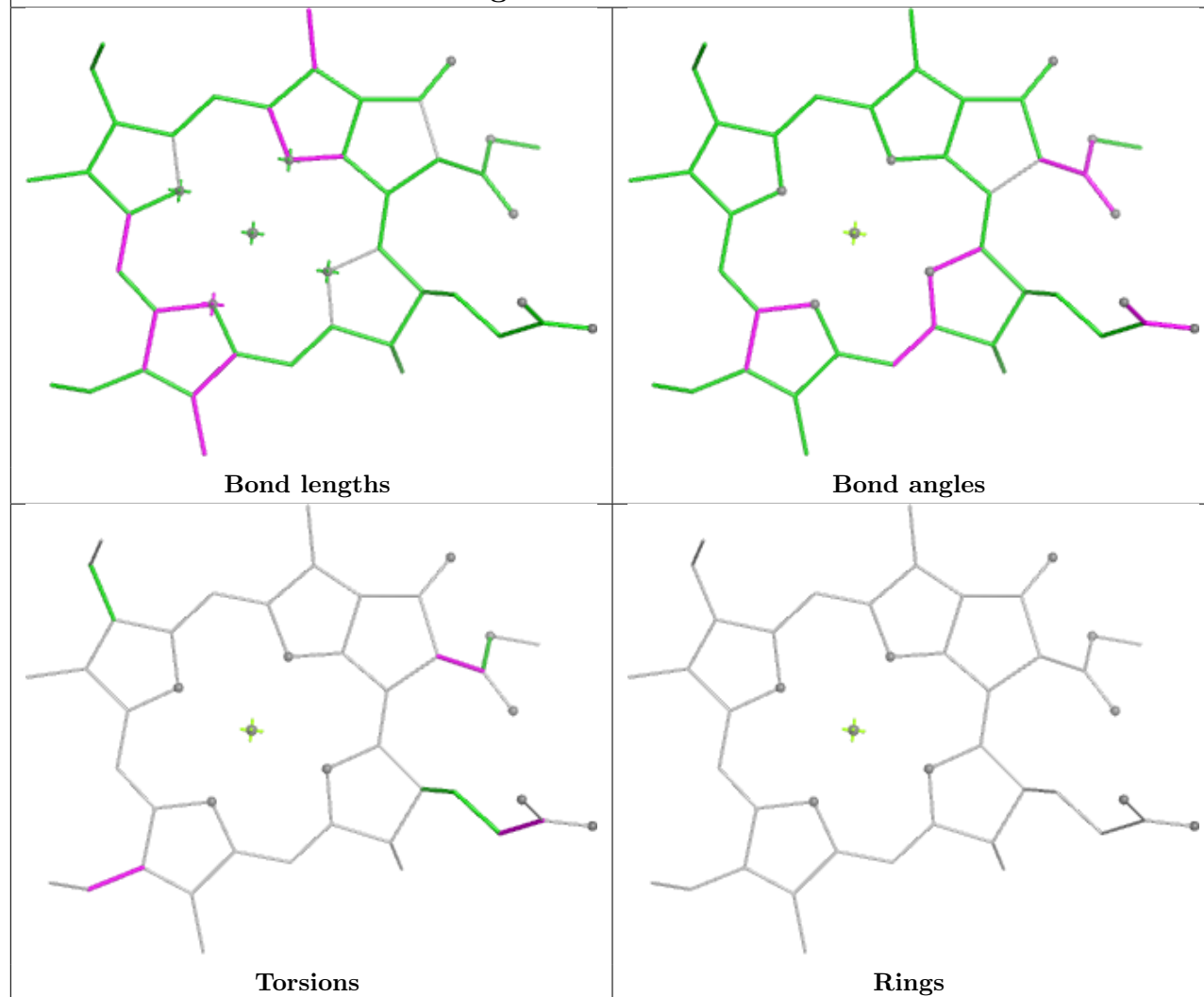


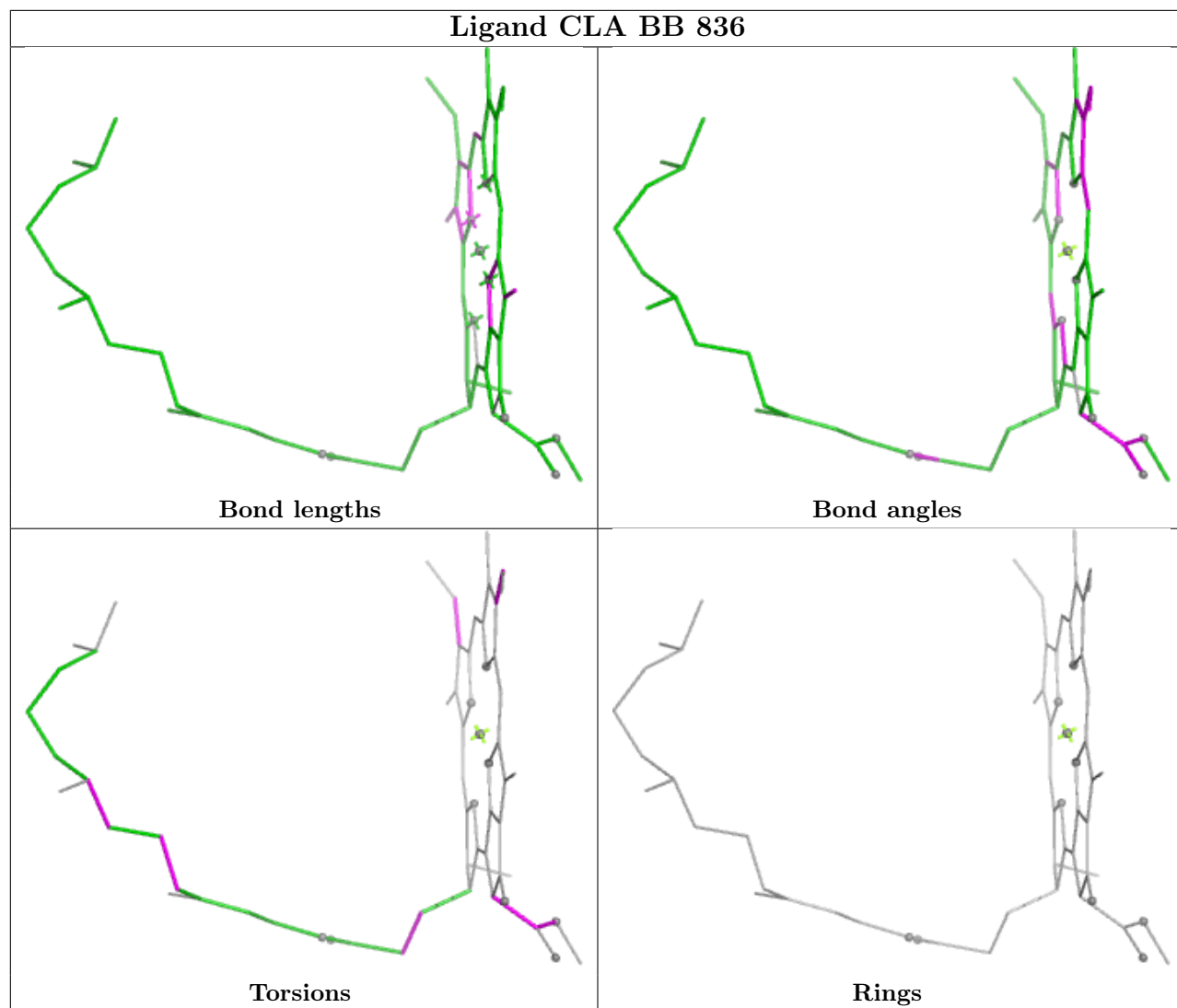


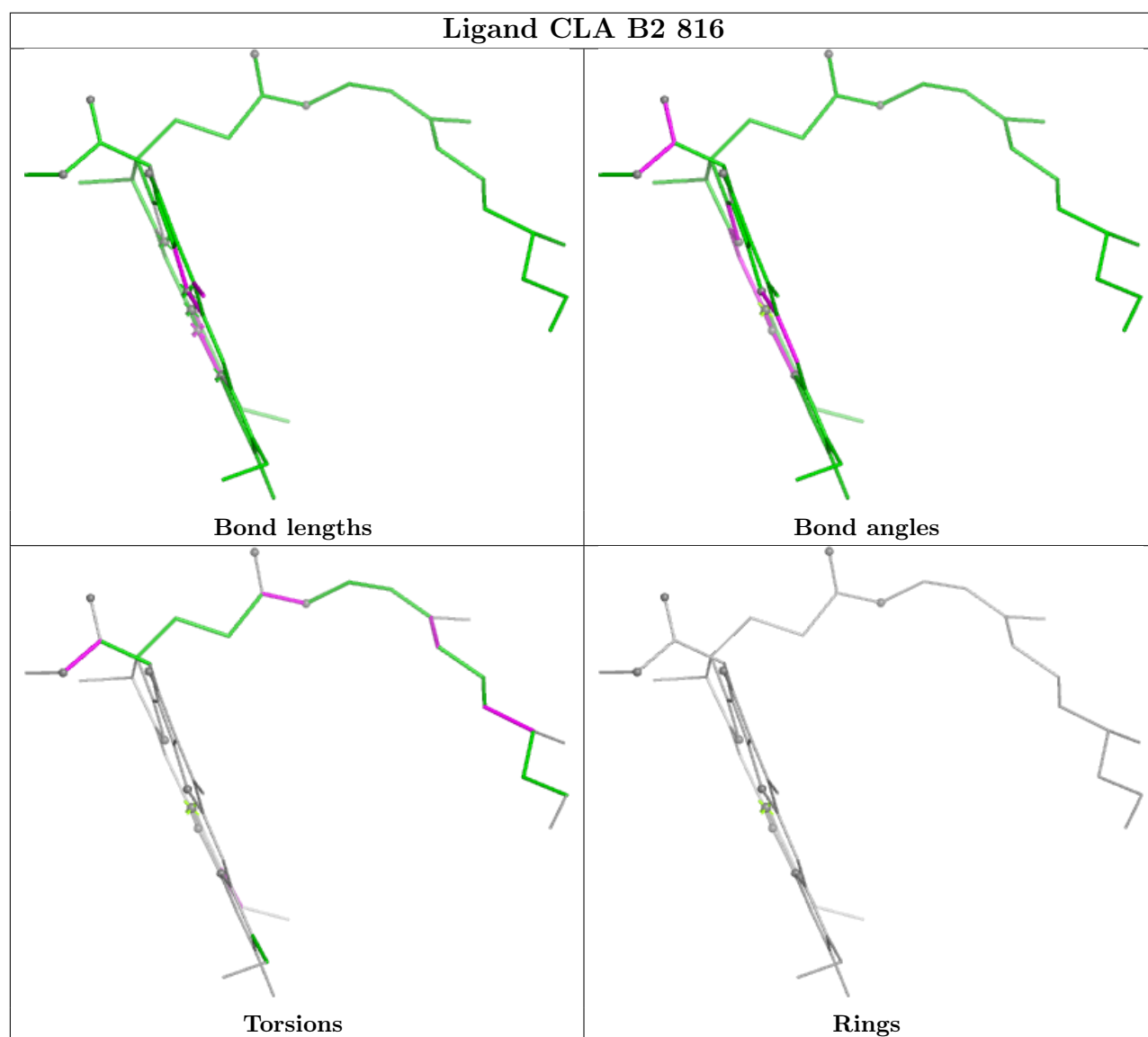
Ligand CLA AA 845

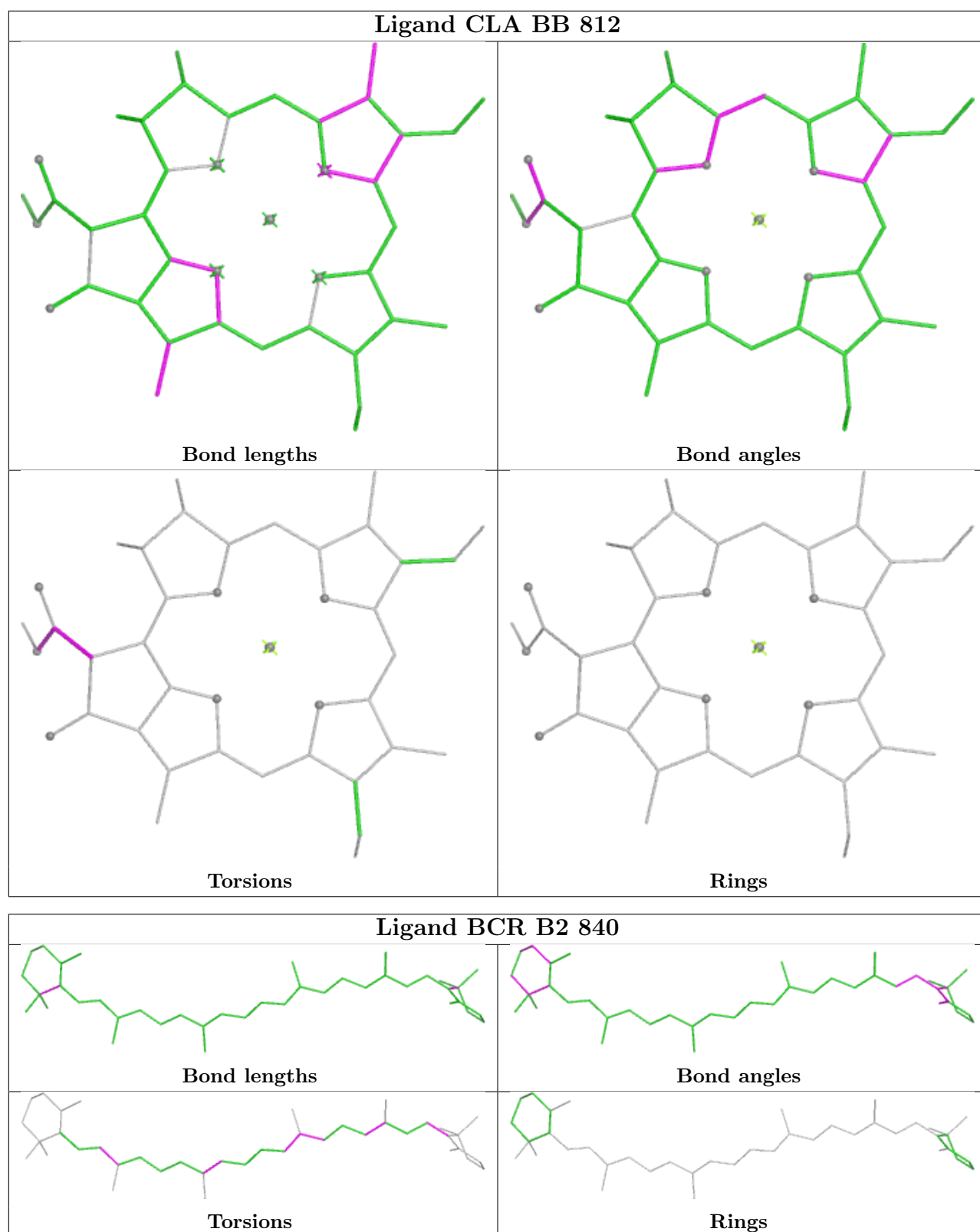


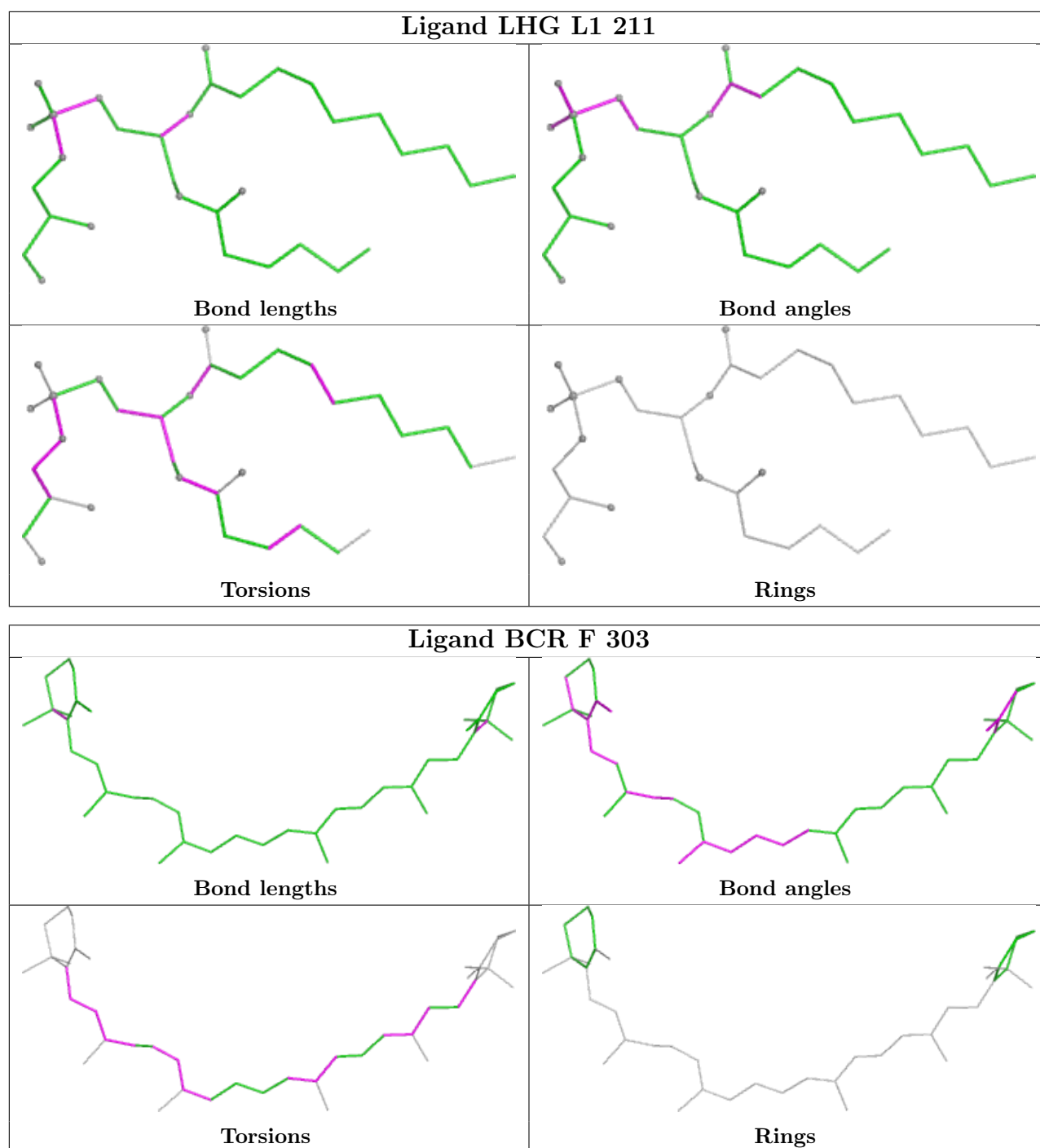
Ligand CLA BB 809



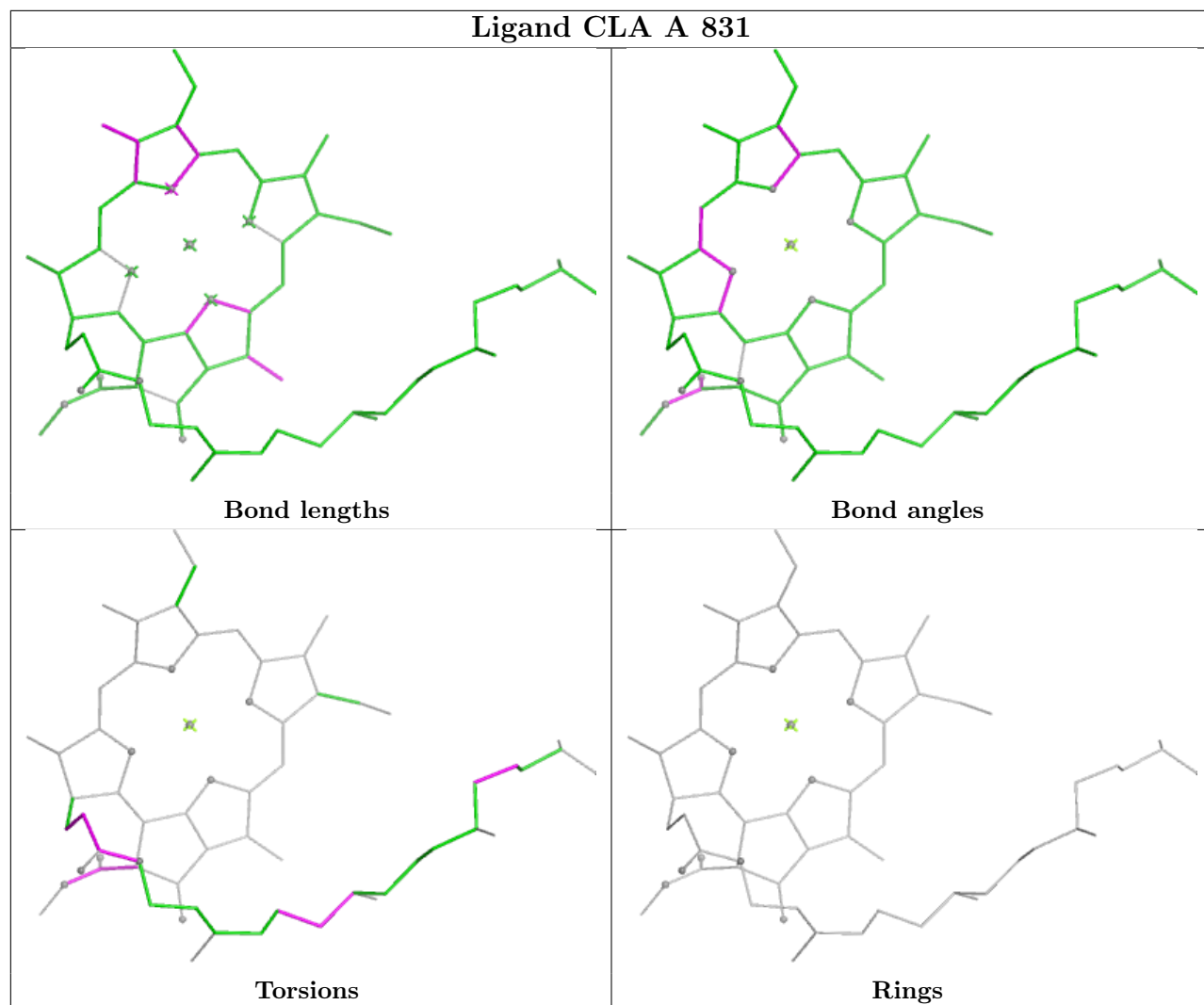


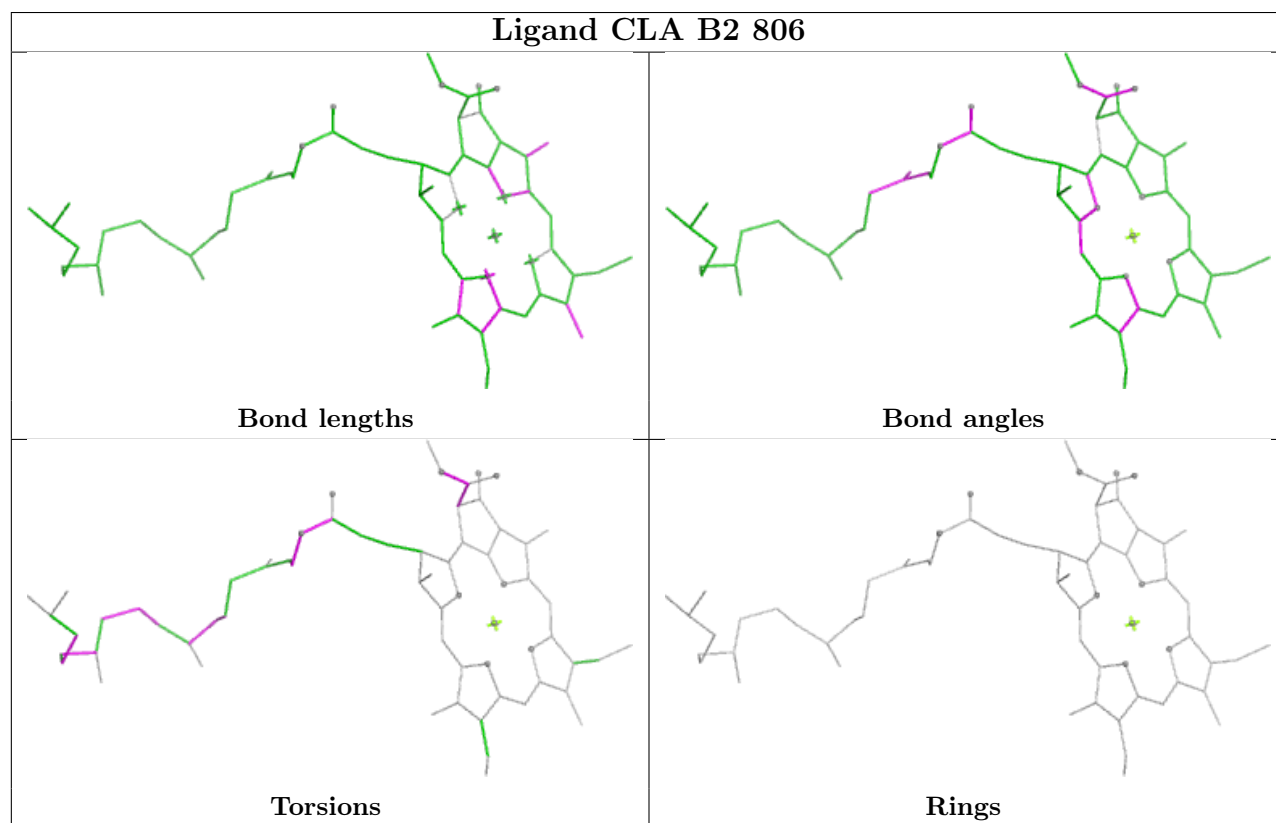
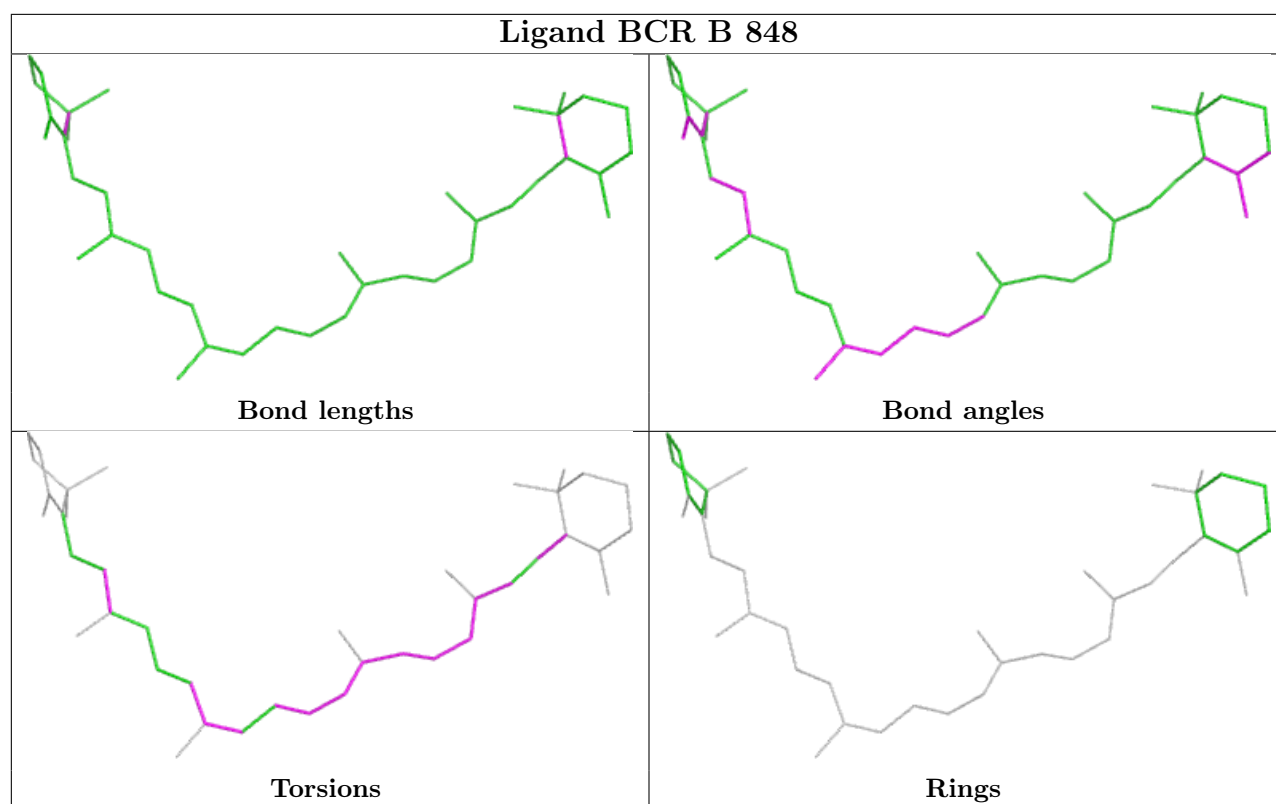


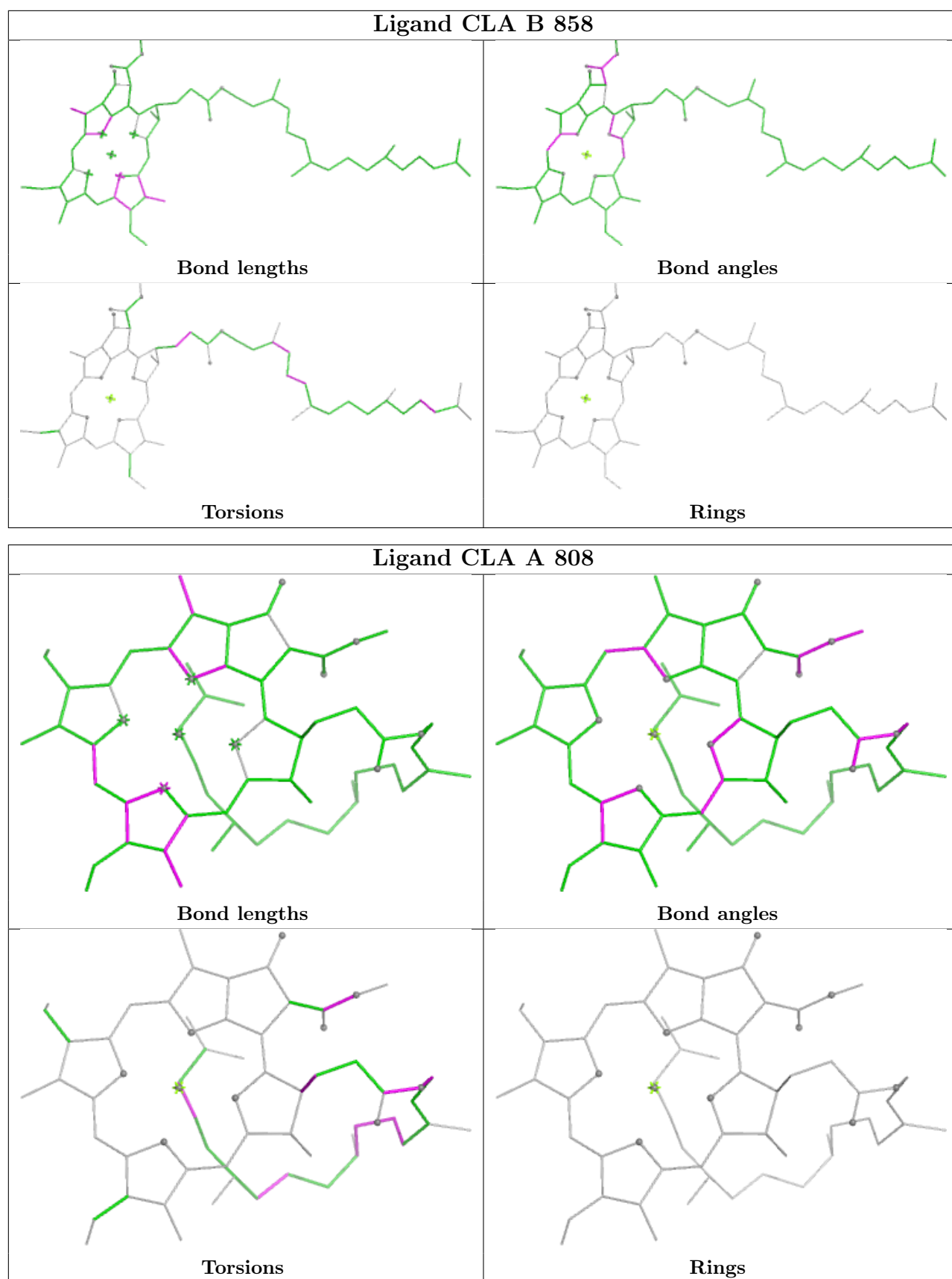




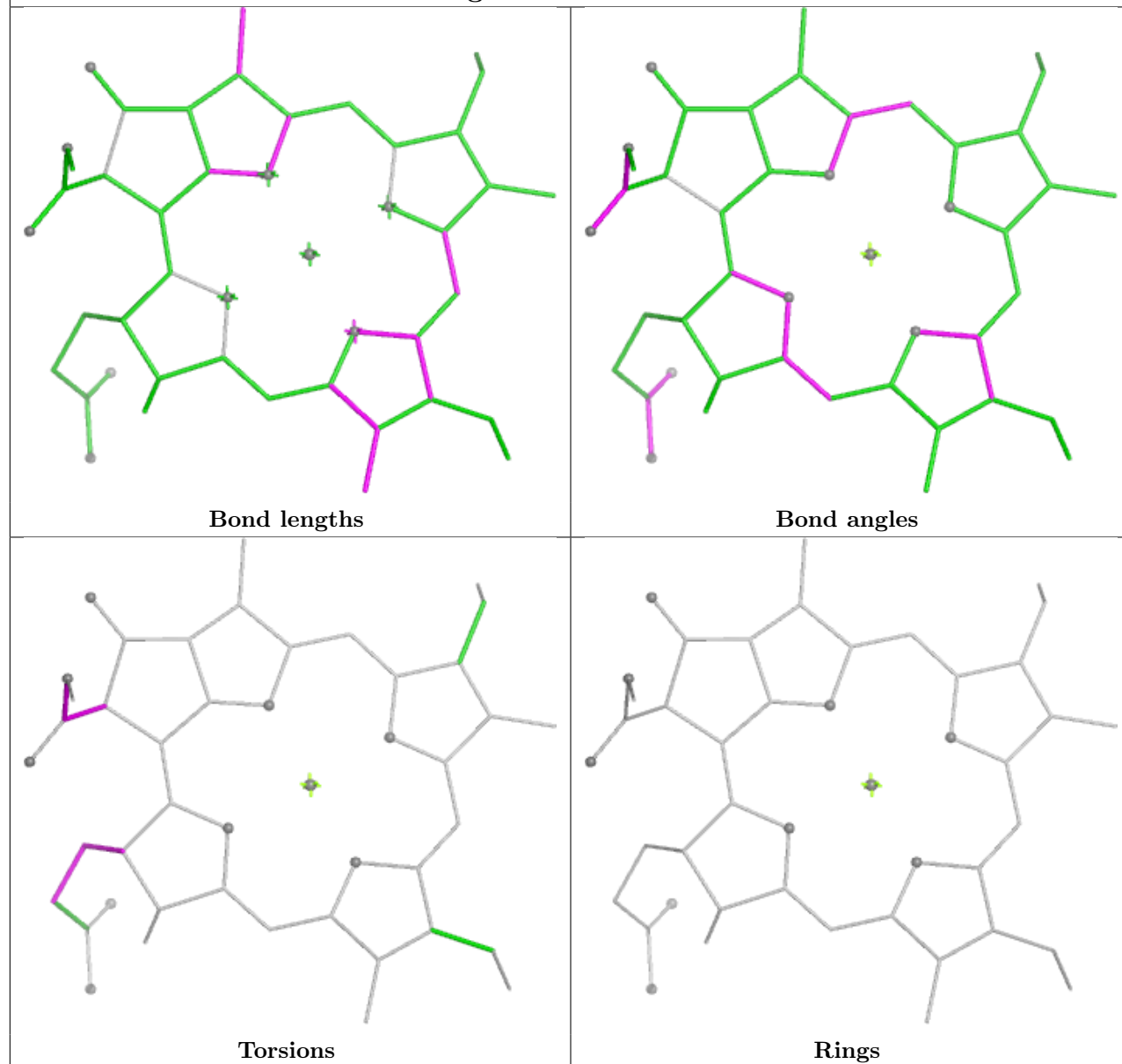
Ligand CLA A 831



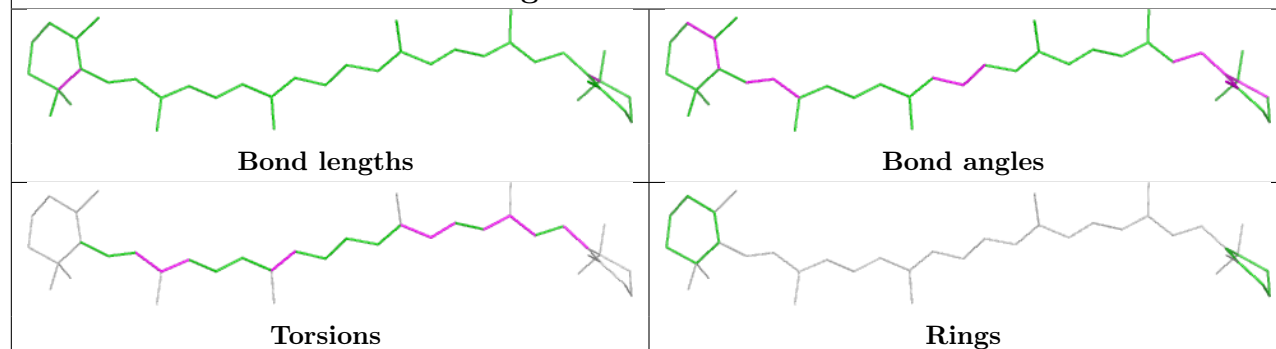


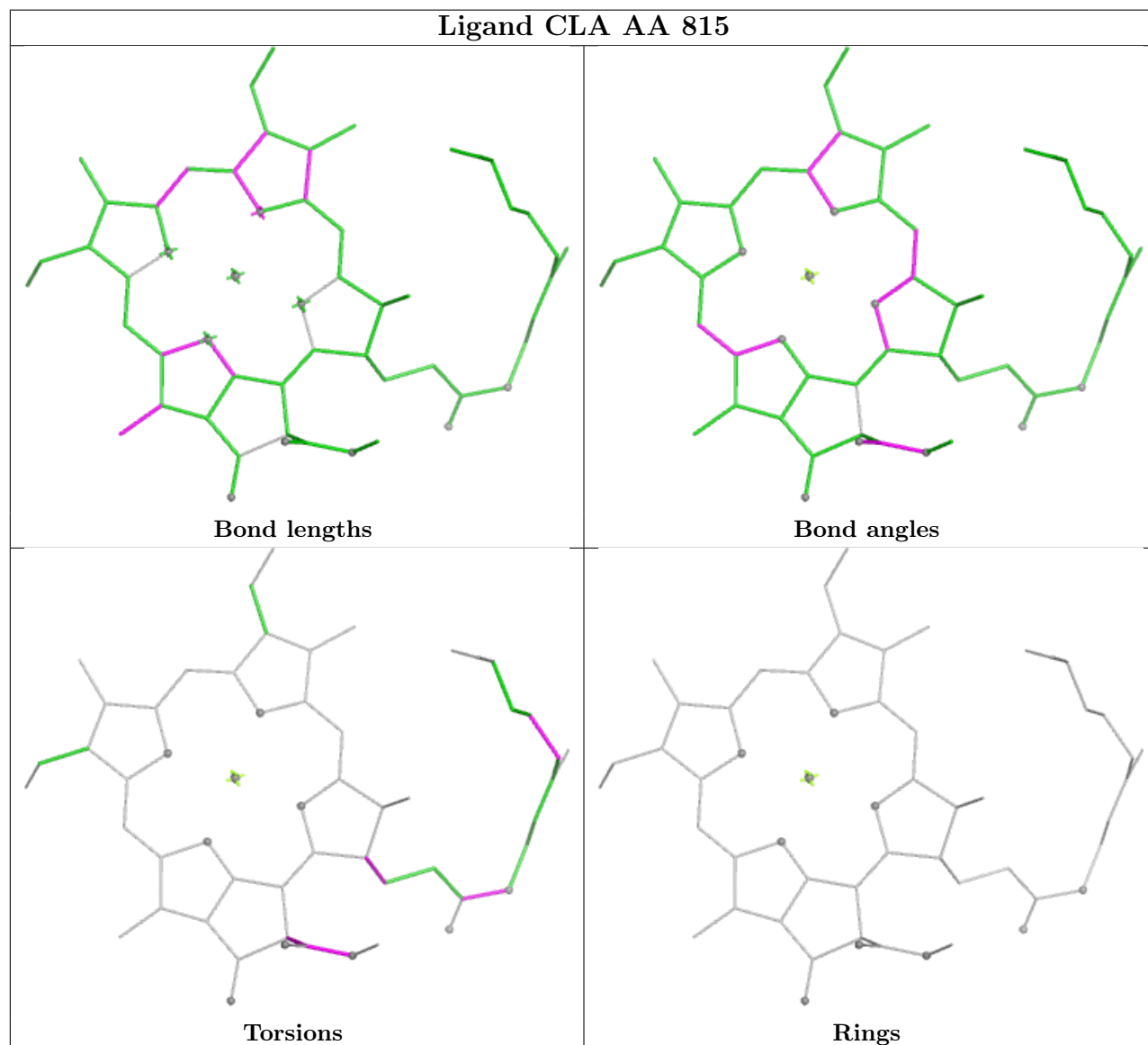
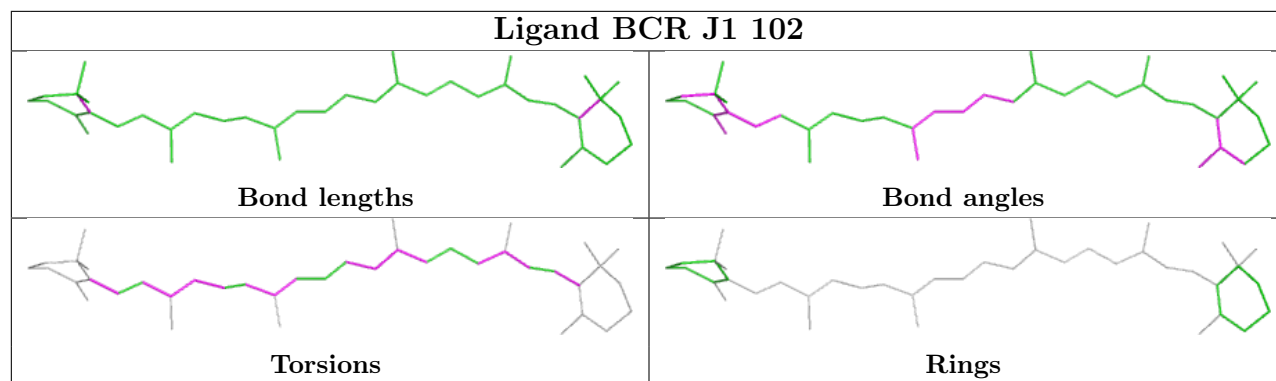


Ligand CLA A 824

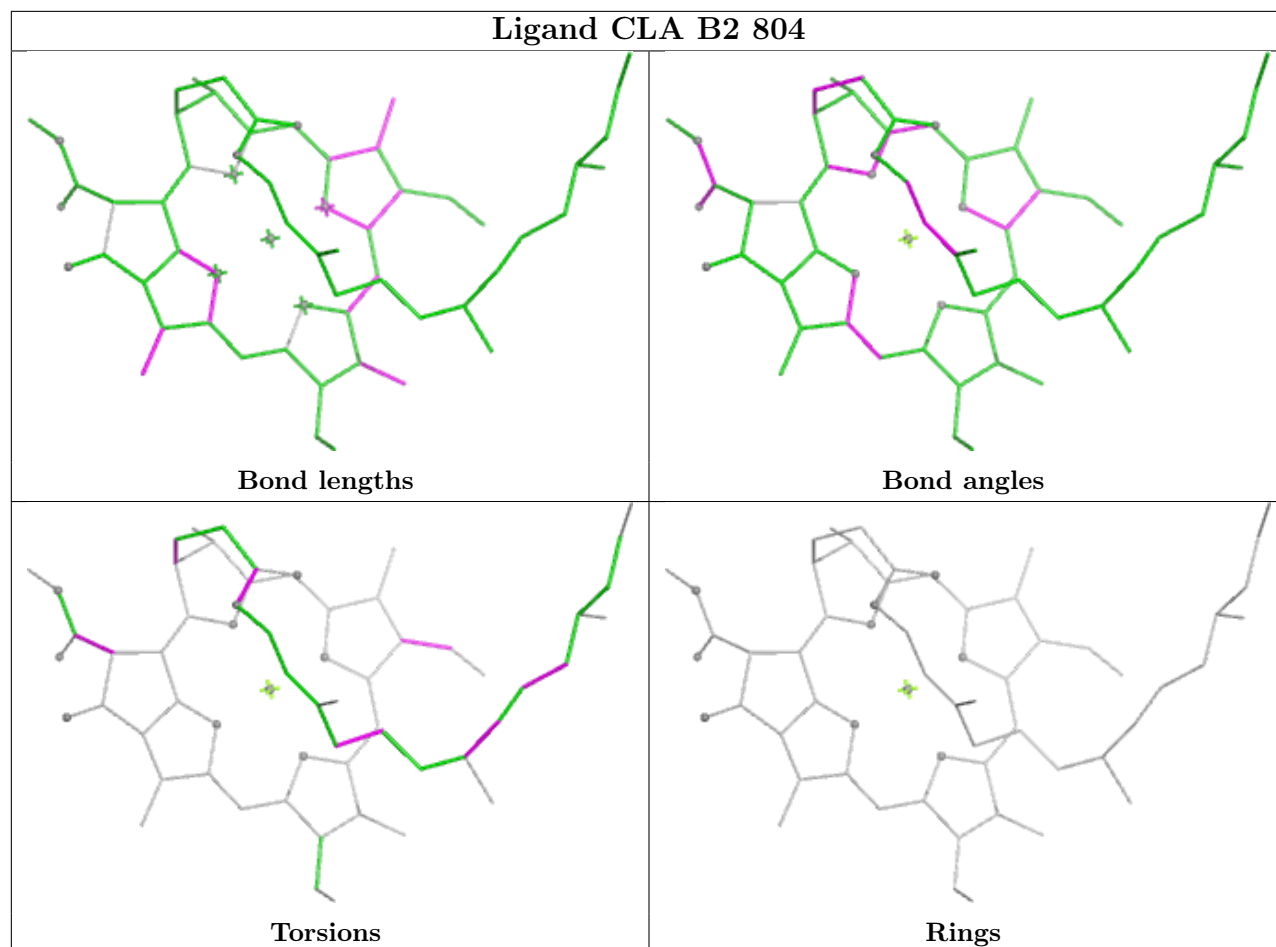


Ligand BCR A2 850

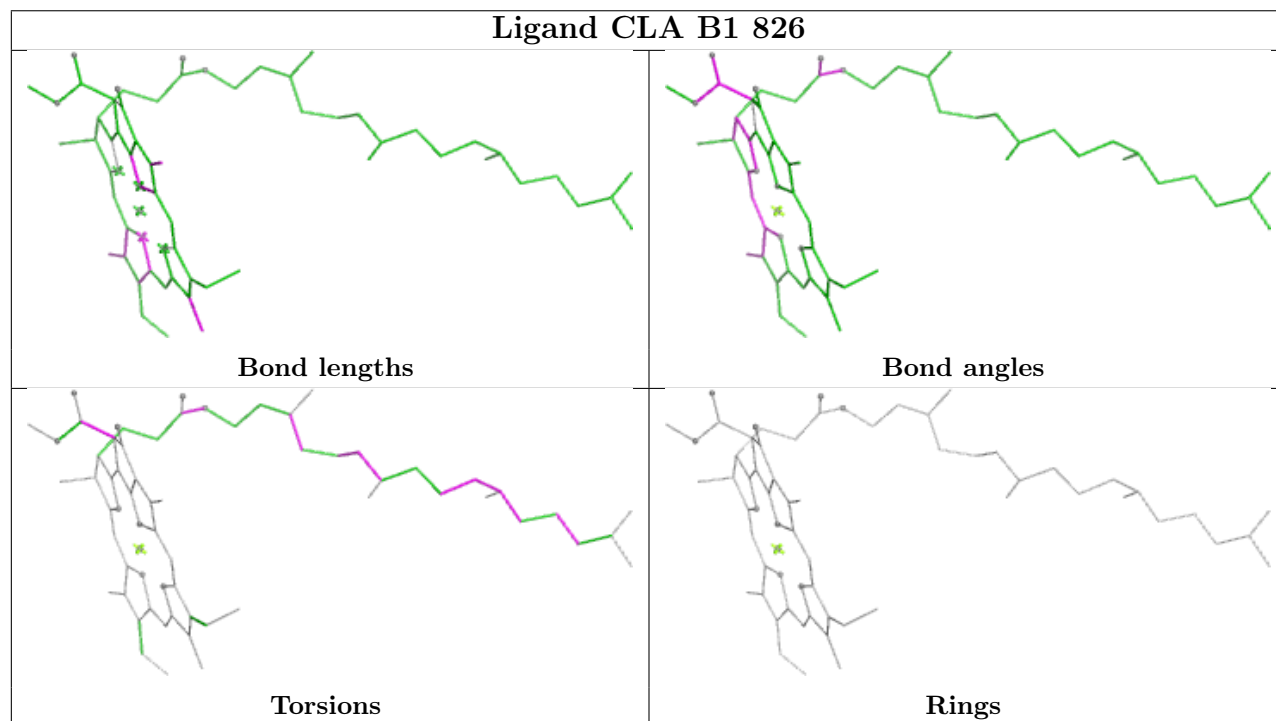




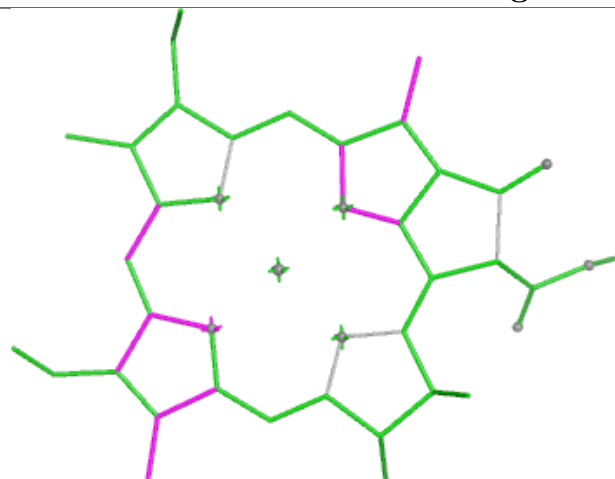
Ligand CLA B2 804



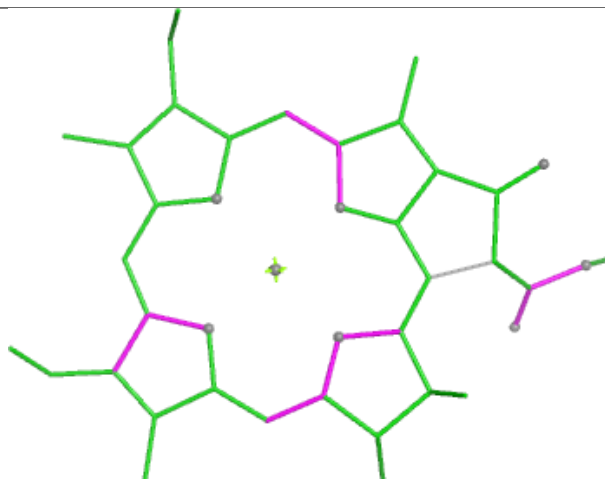
Ligand CLA B1 826



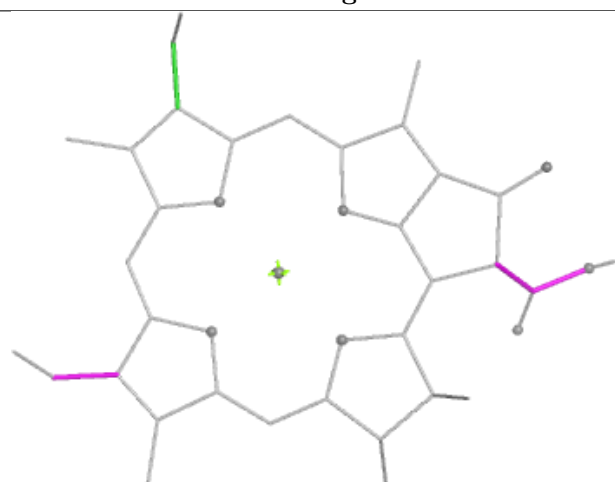
Ligand CLA JJ 101



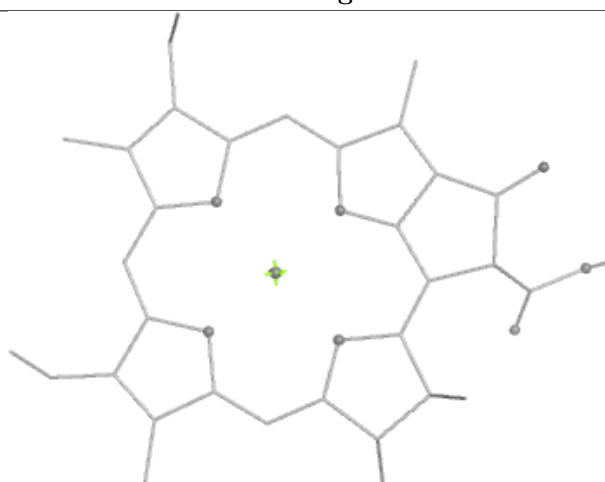
Bond lengths



Bond angles

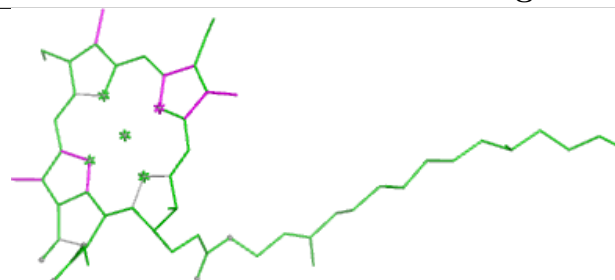


Torsions

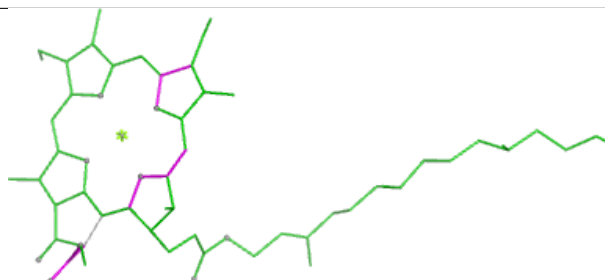


Rings

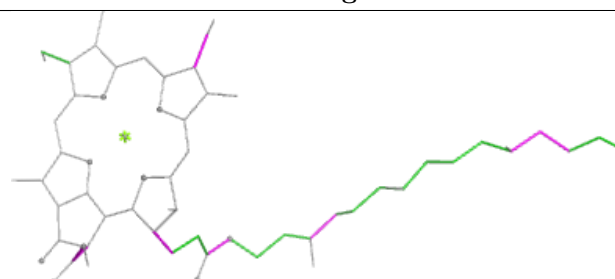
Ligand CLA A 836



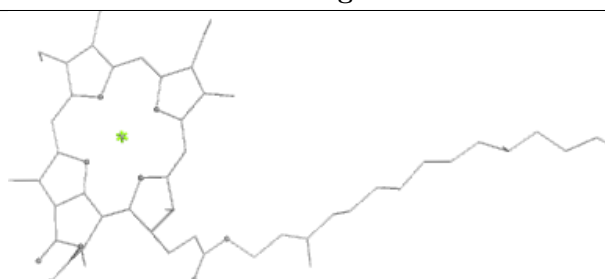
Bond lengths



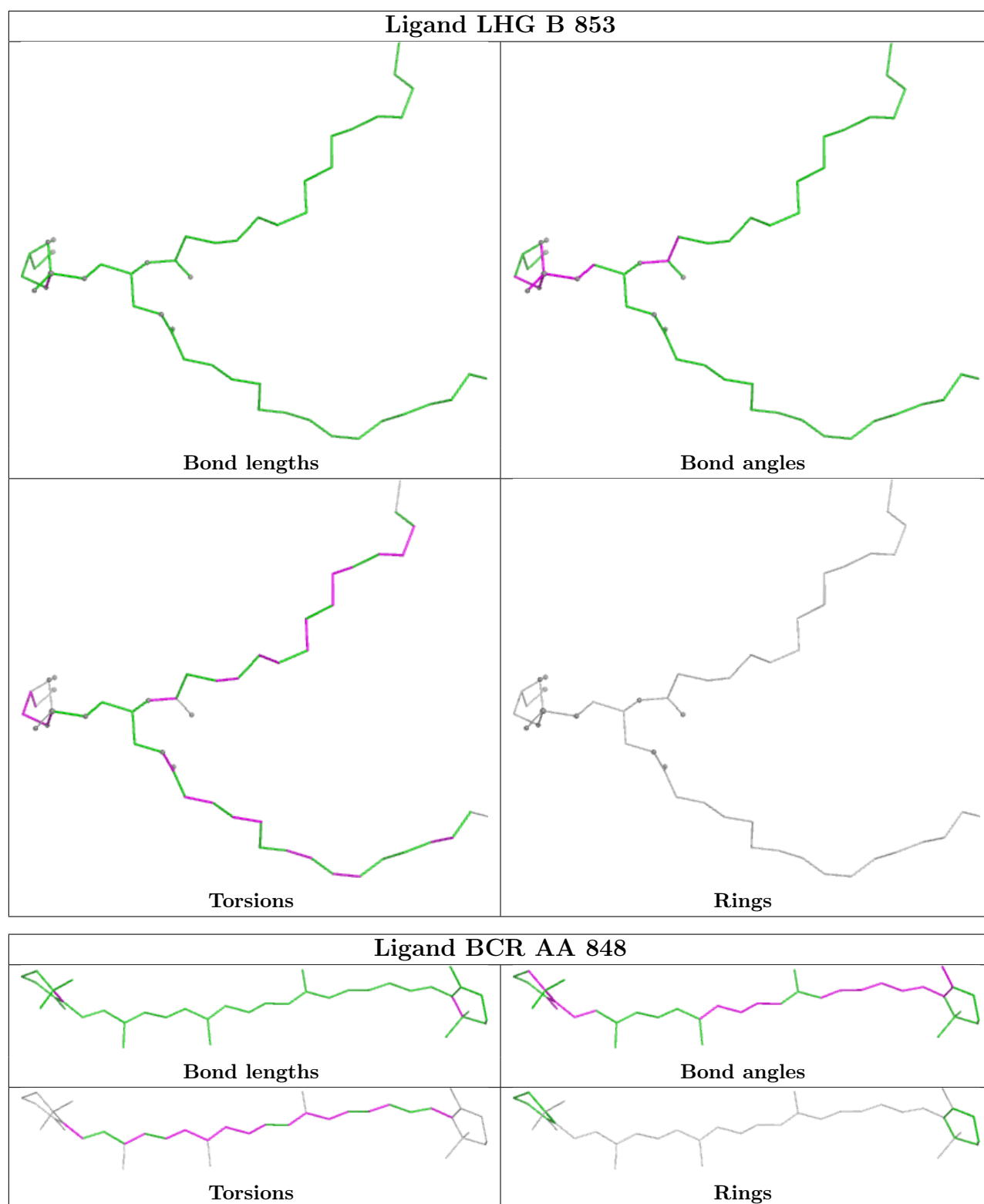
Bond angles



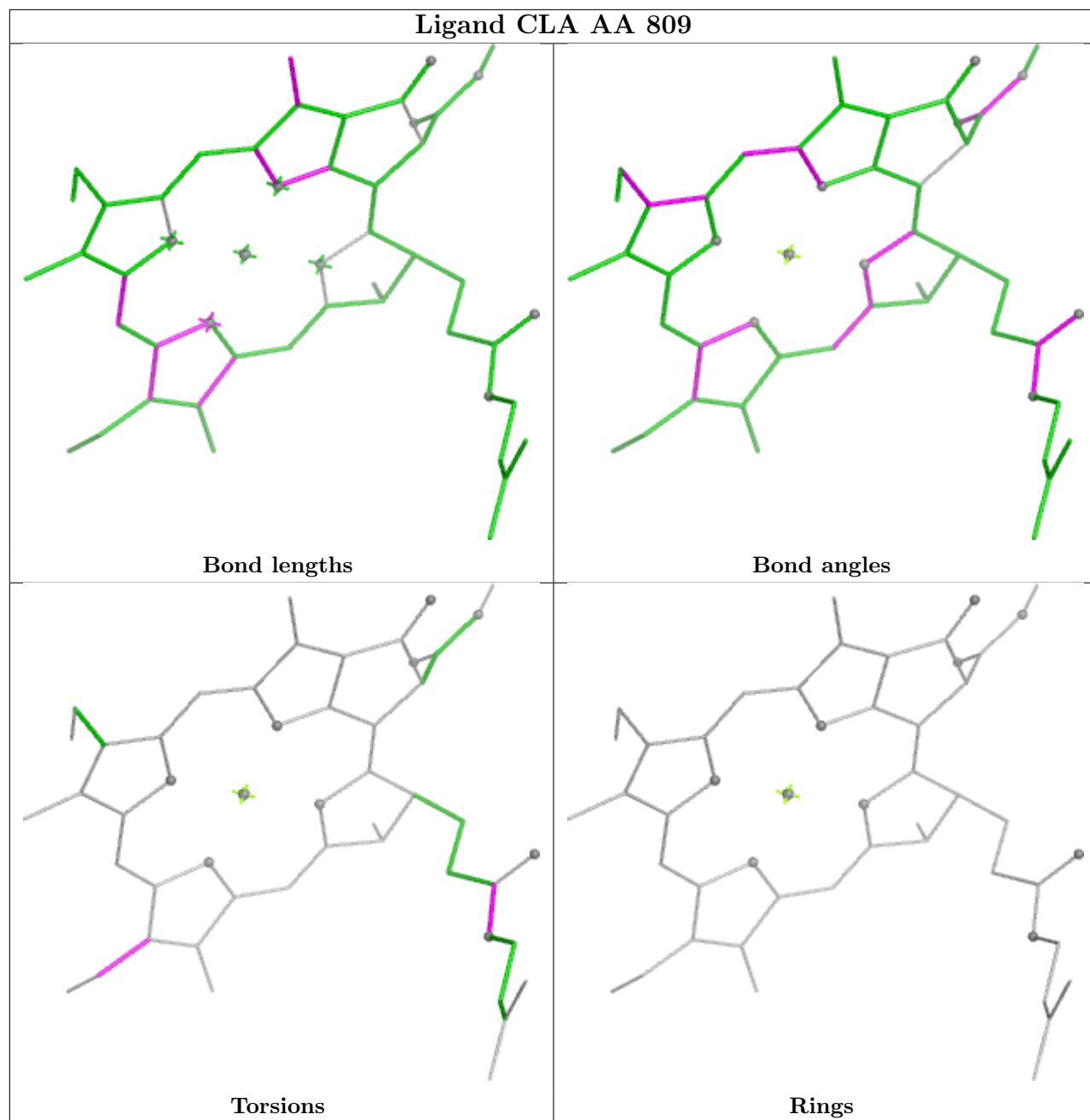
Torsions

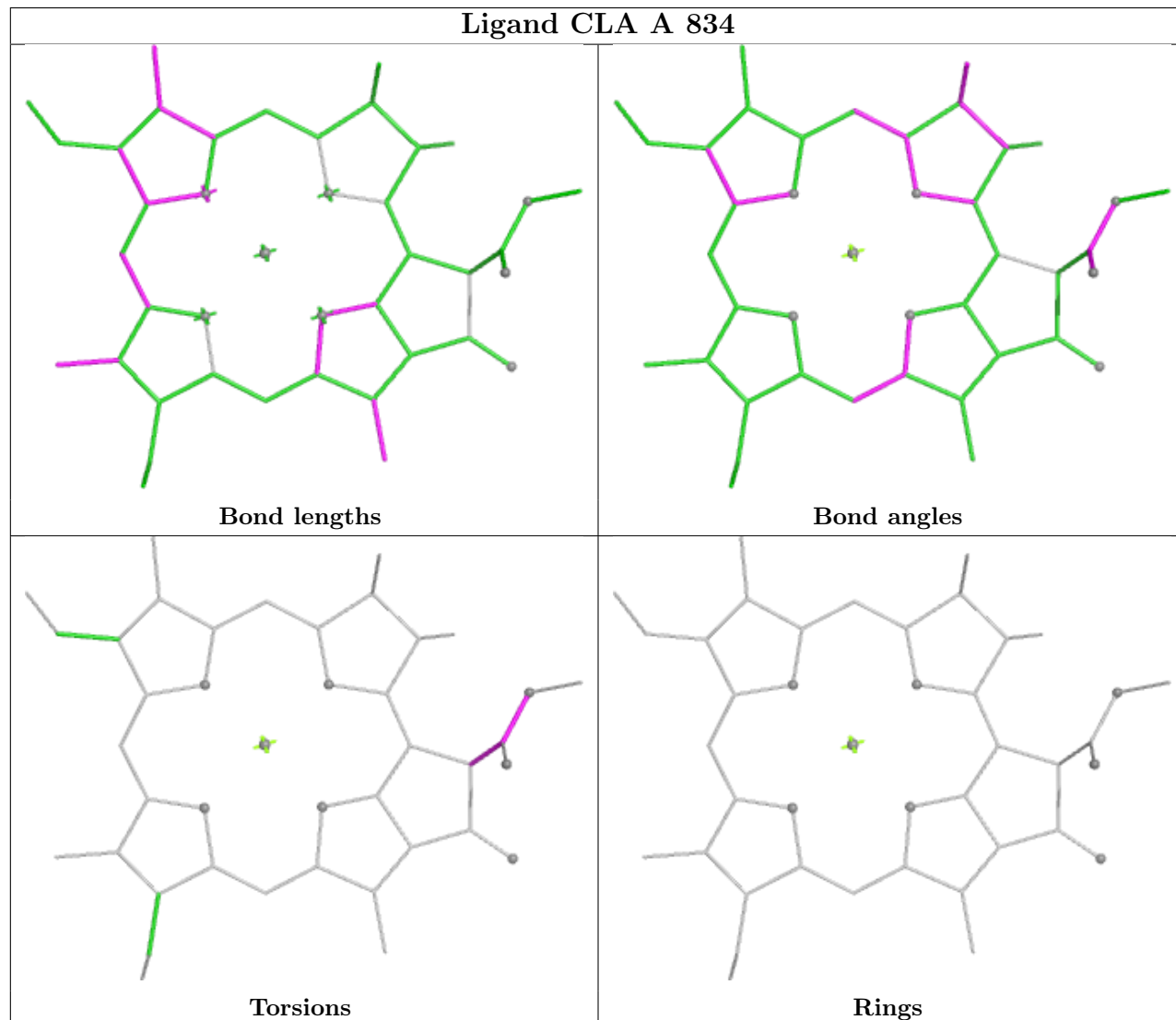
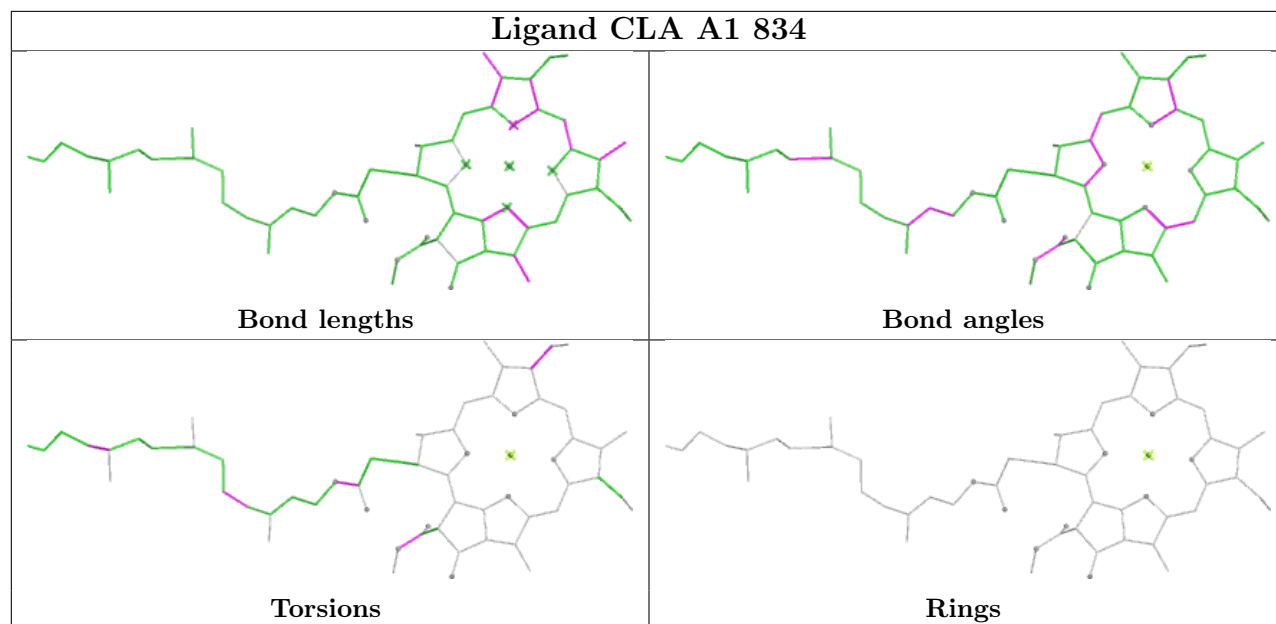


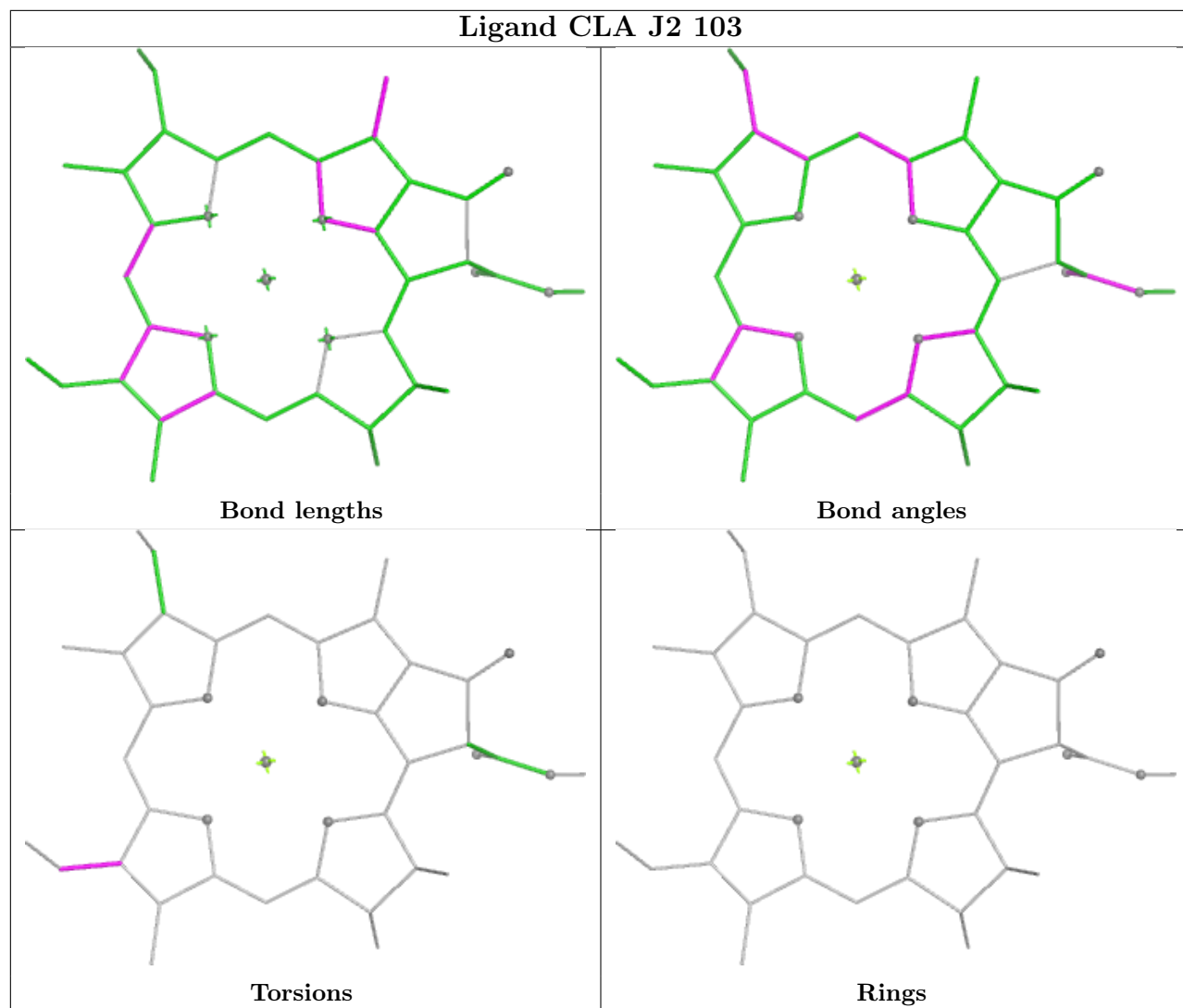
Rings

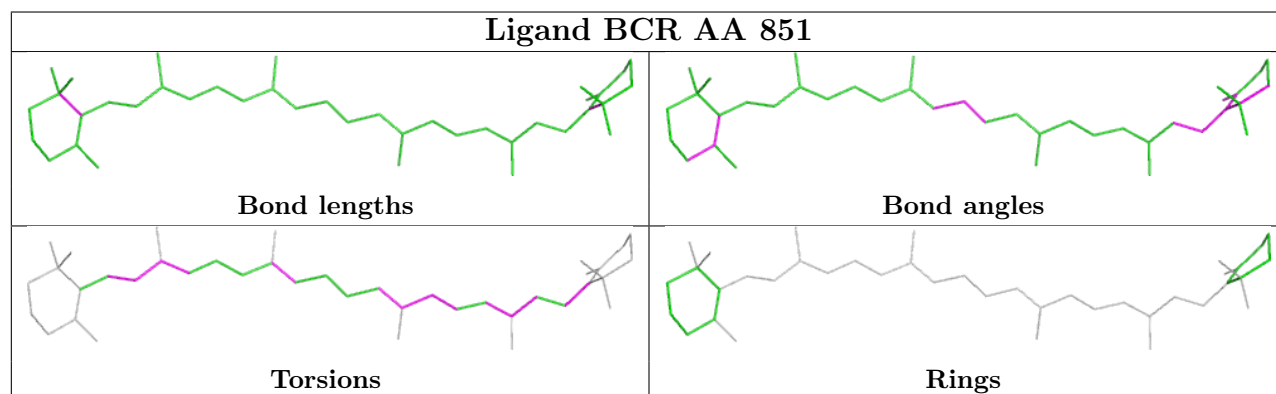
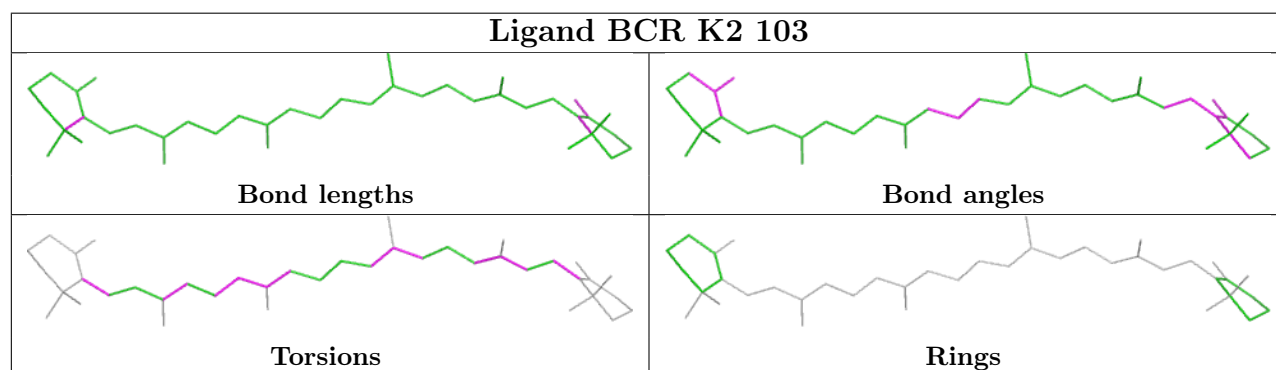
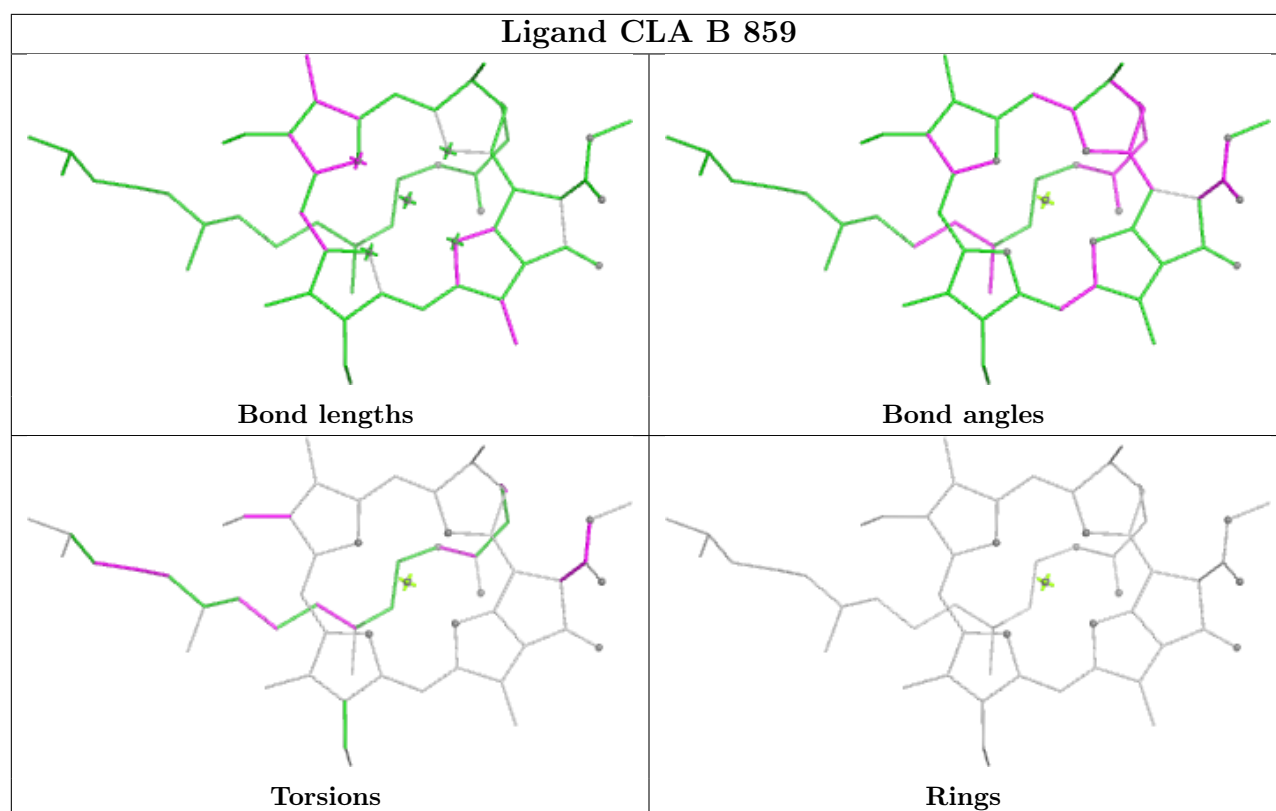


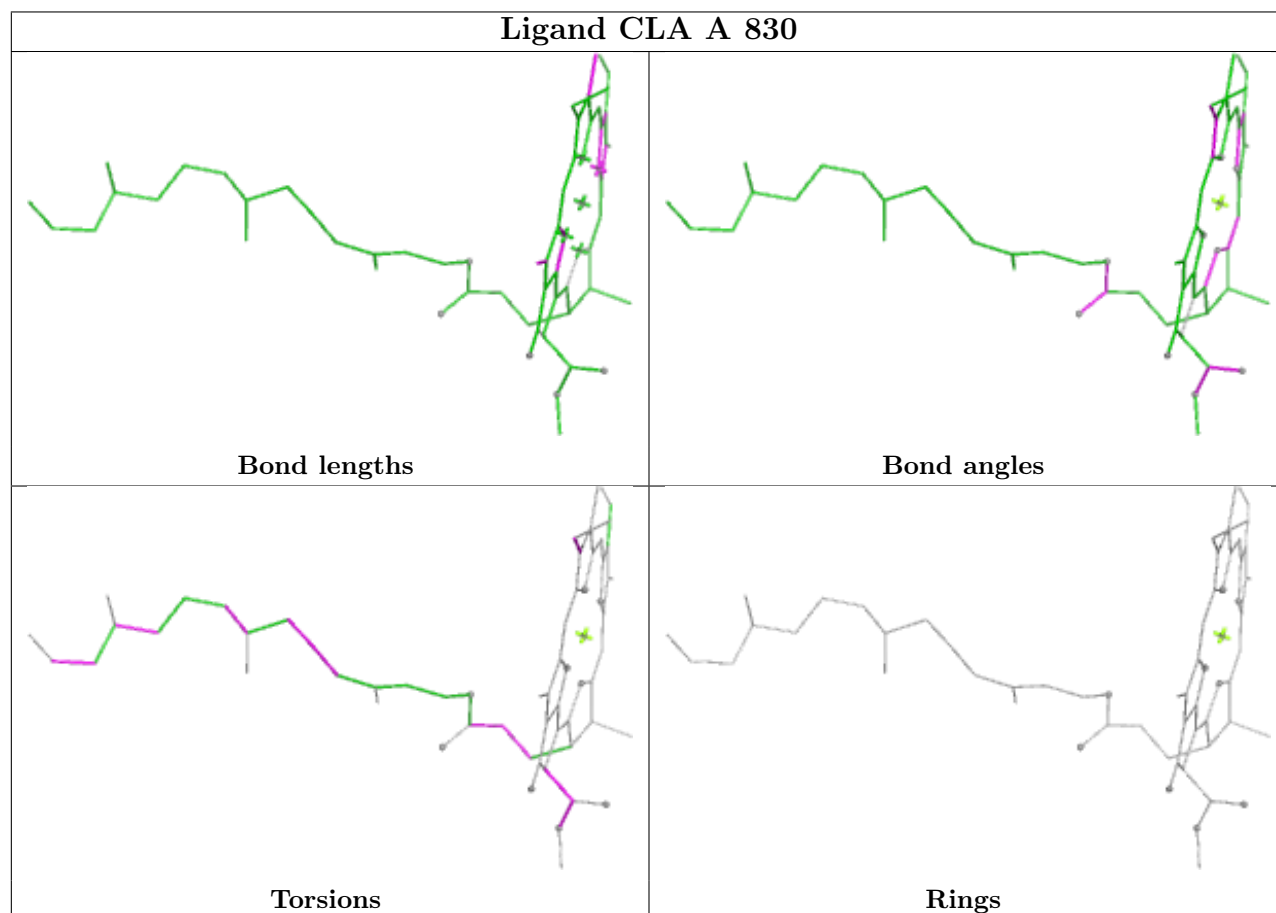
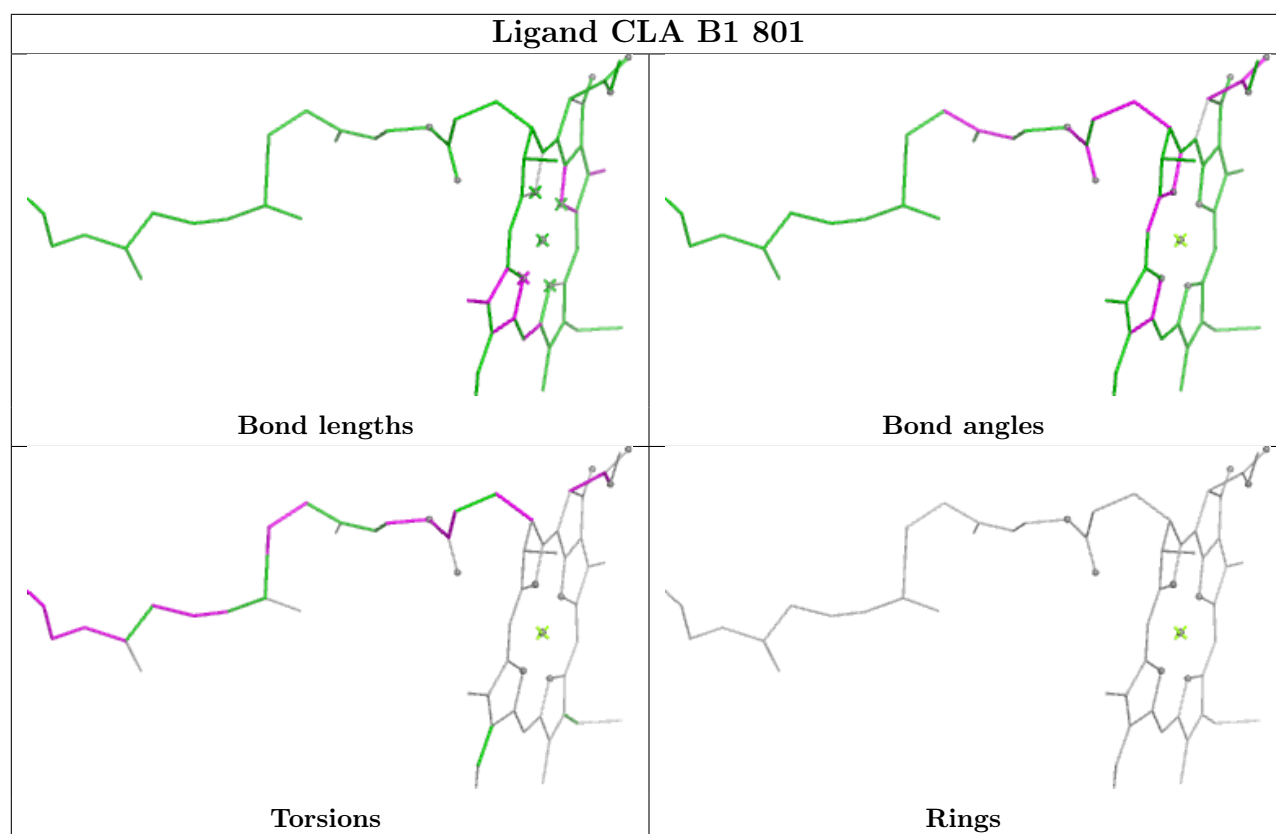
Ligand CLA AA 809

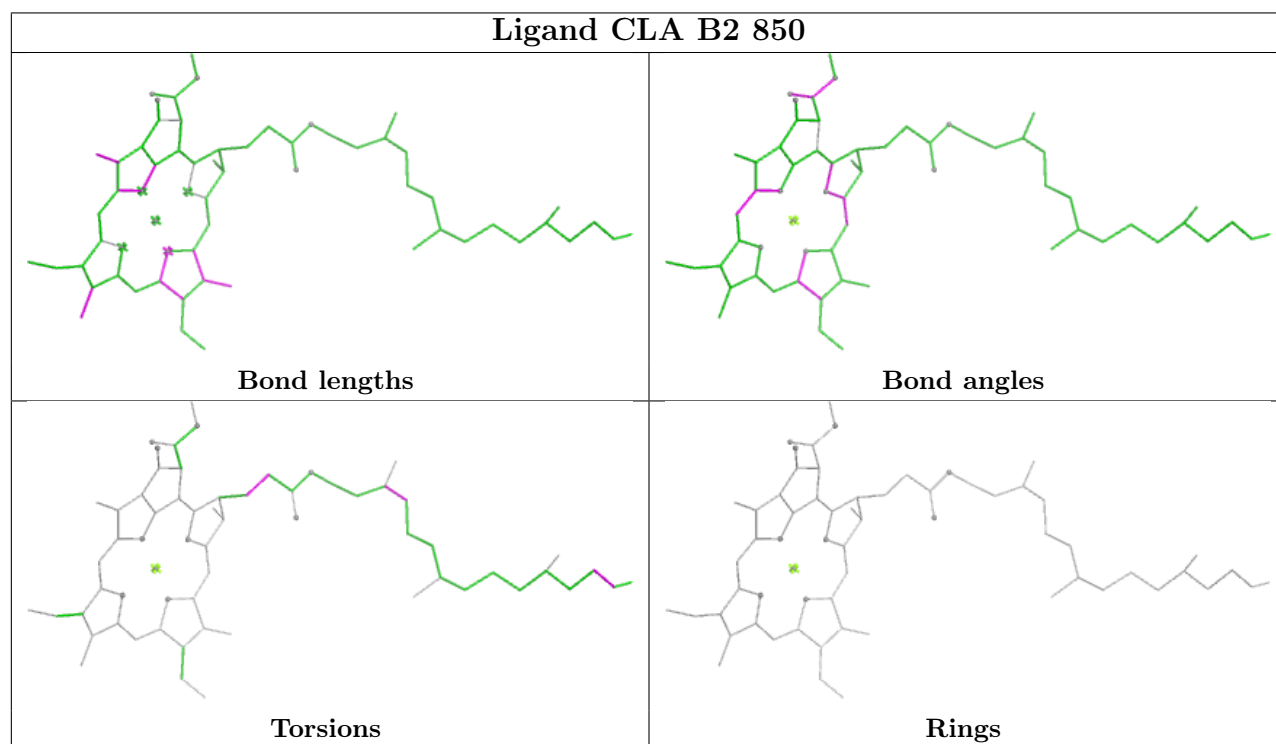
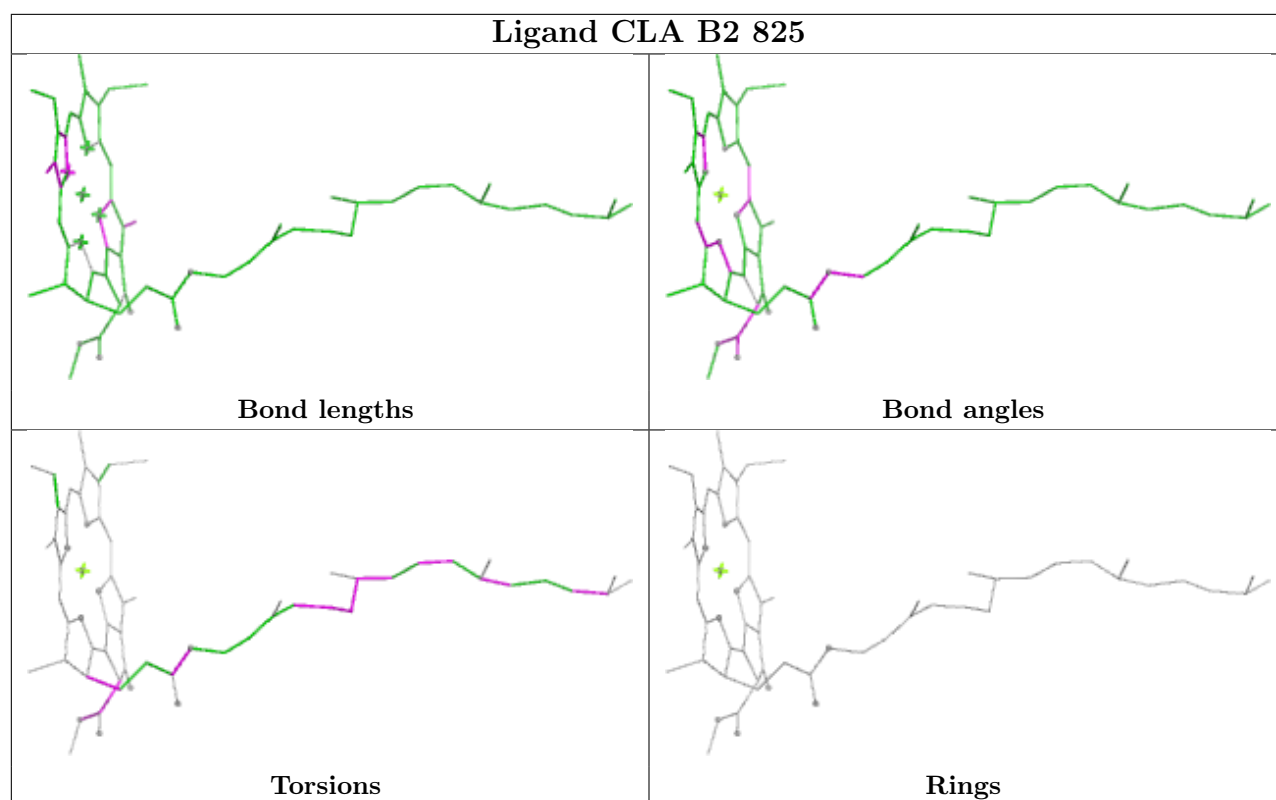


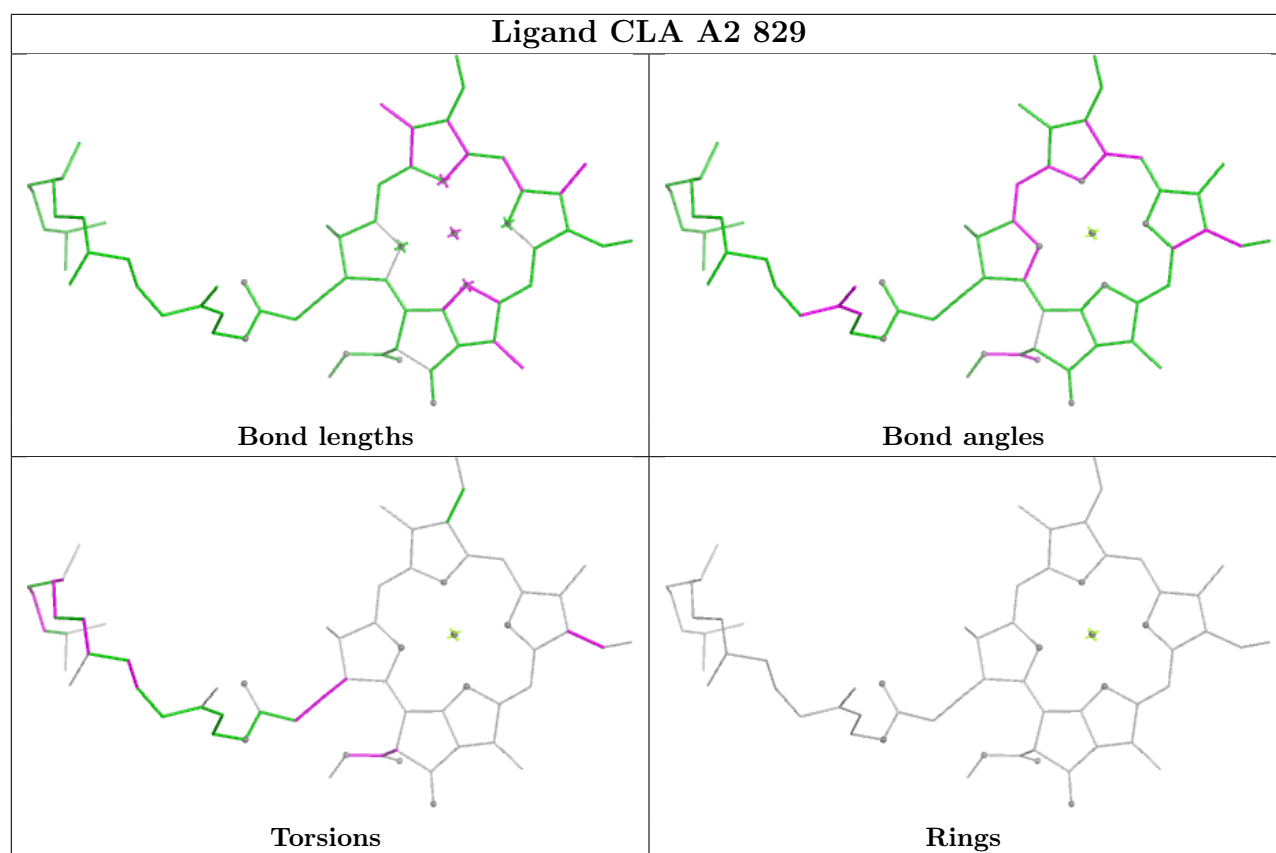




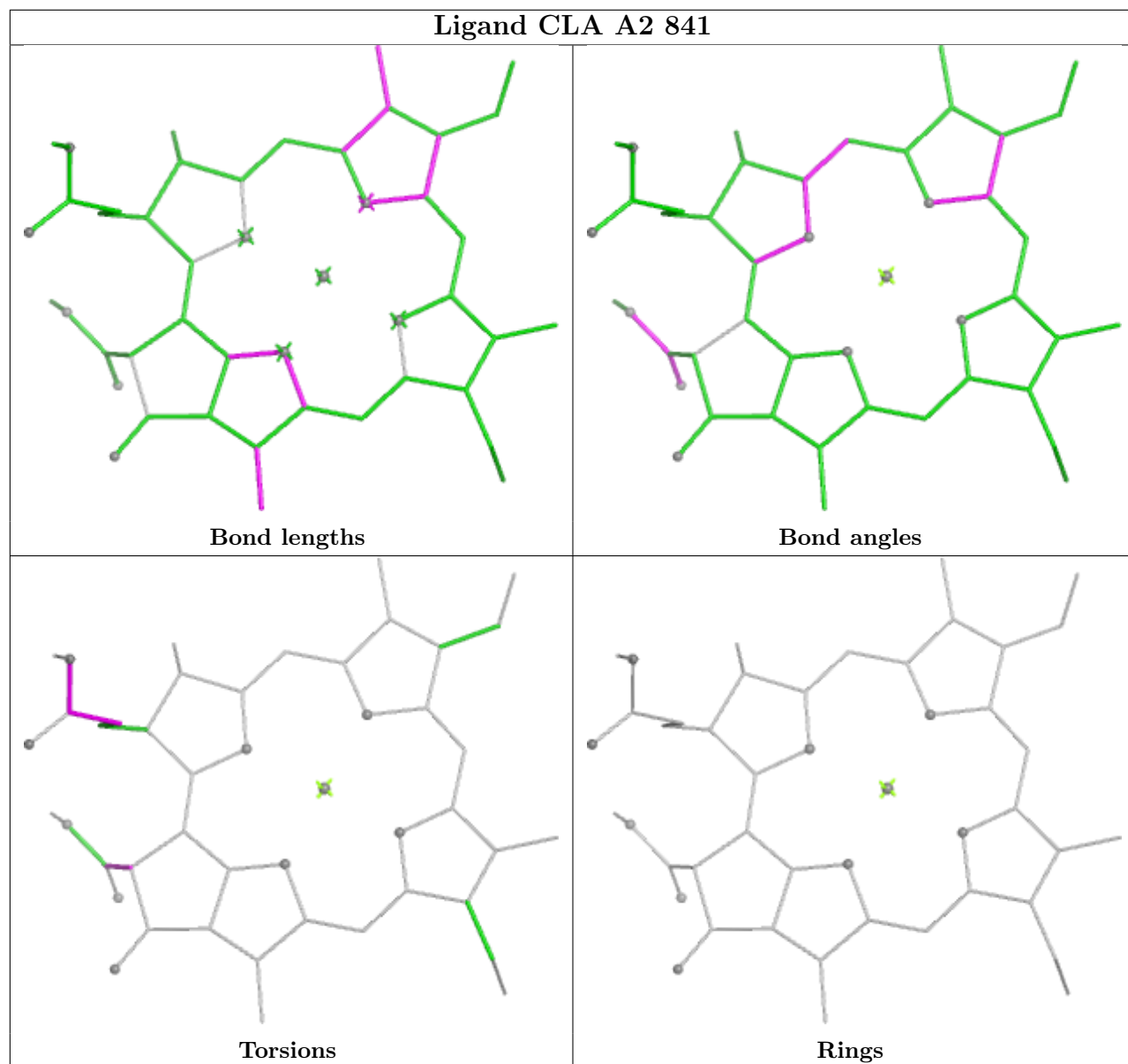


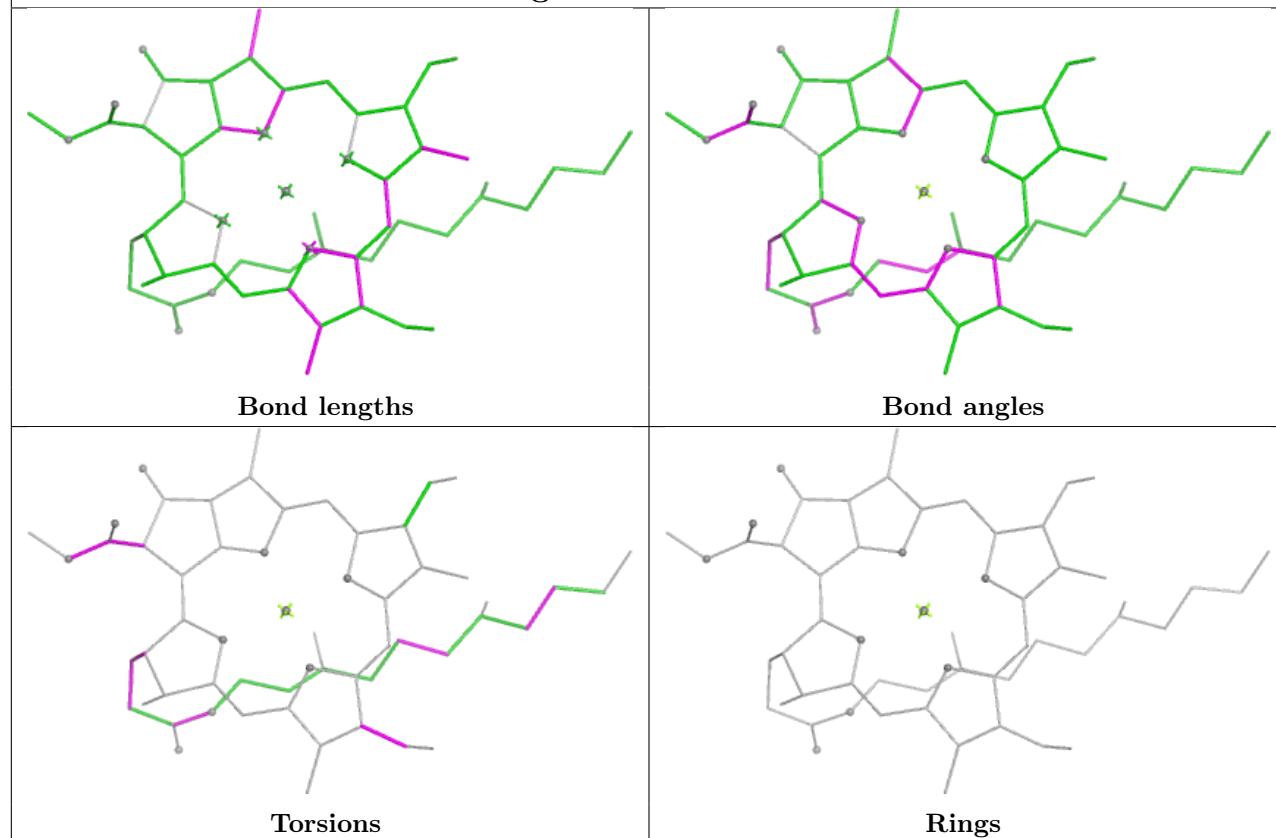
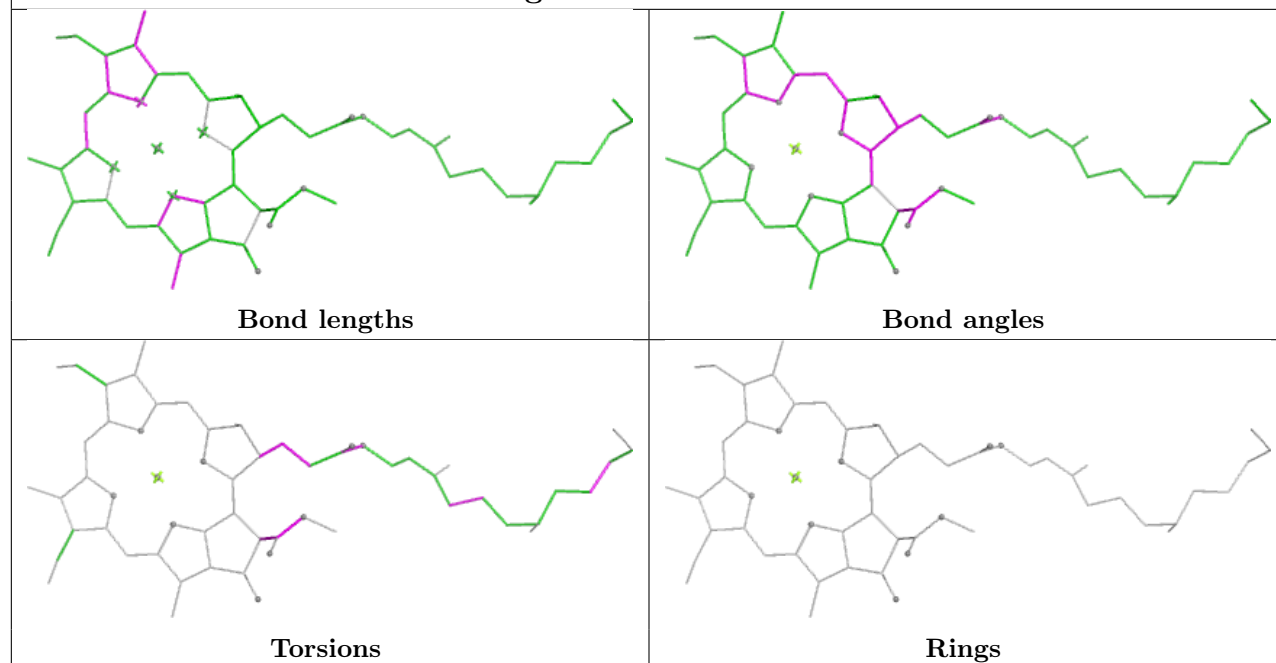




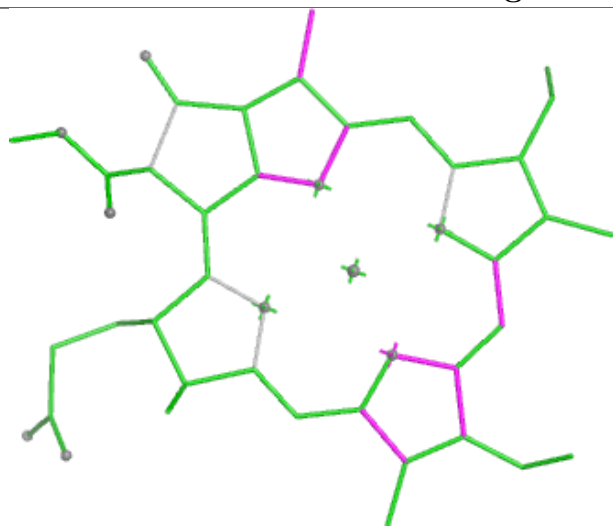


Ligand CLA A2 841

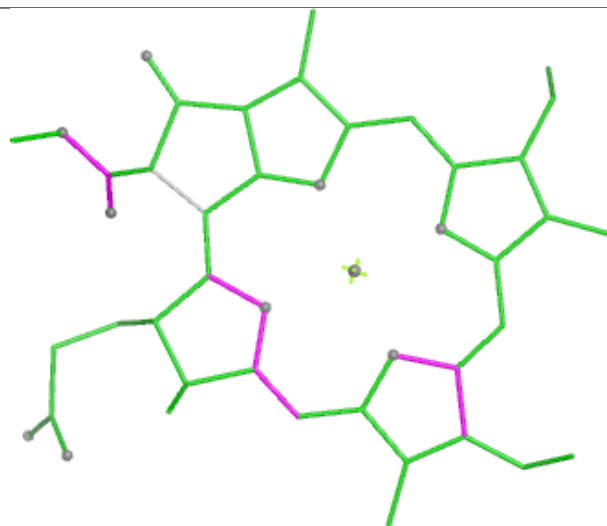


Ligand CLA A 820**Ligand CLA F1 301**

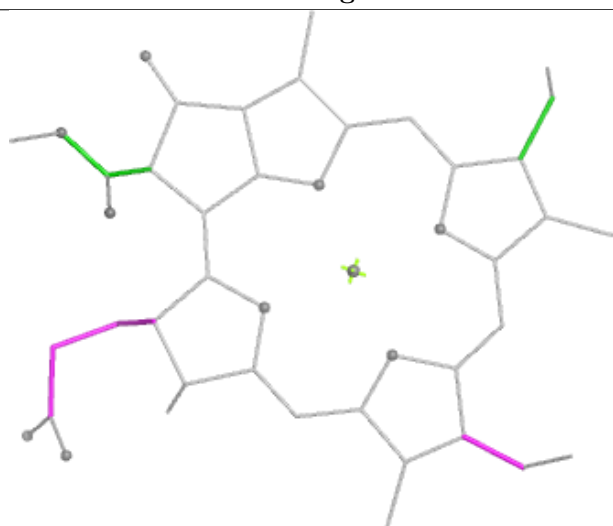
Ligand CLA X1 101



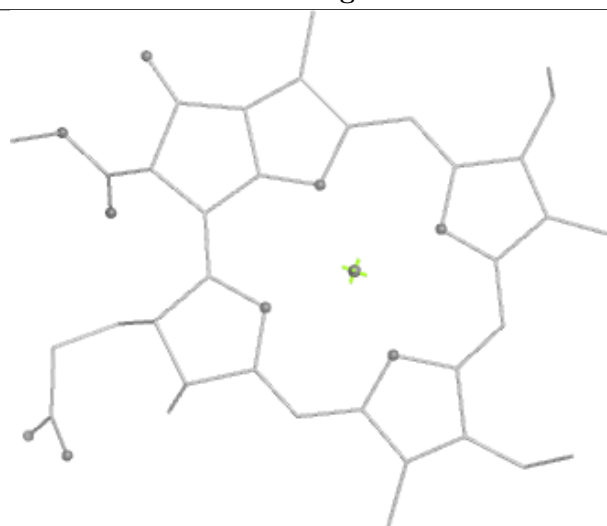
Bond lengths



Bond angles

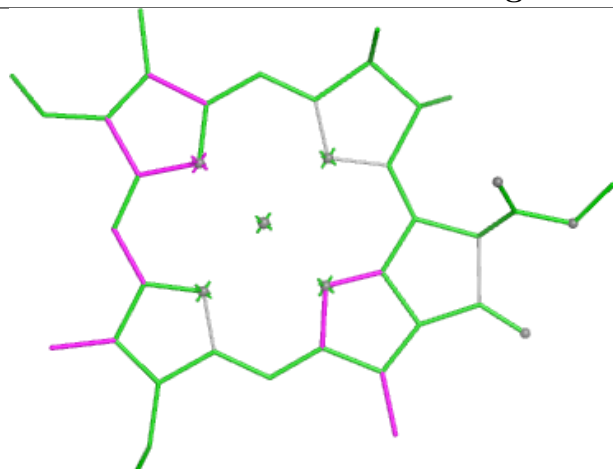


Torsions

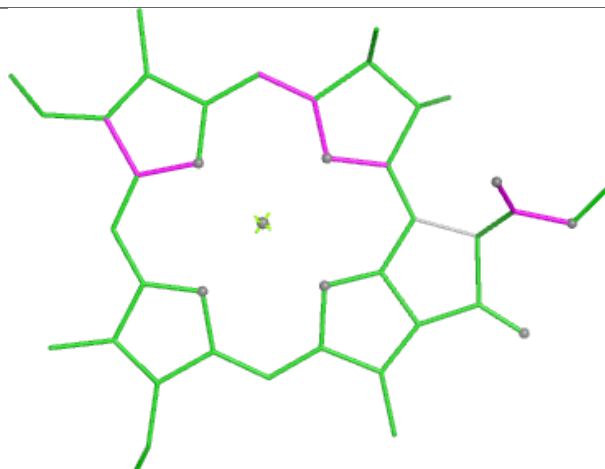


Rings

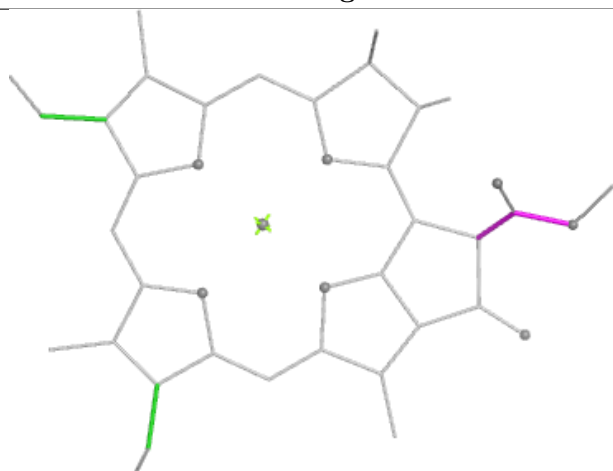
Ligand CLA B2 819



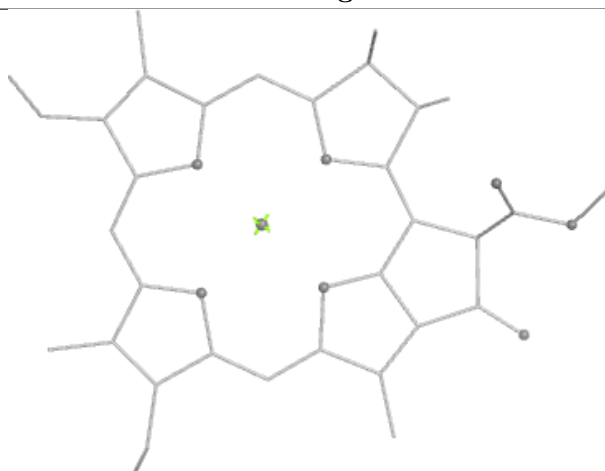
Bond lengths



Bond angles

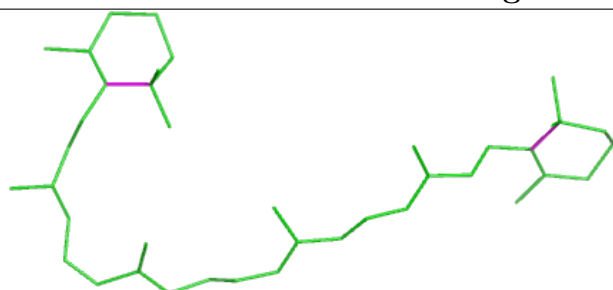


Torsions

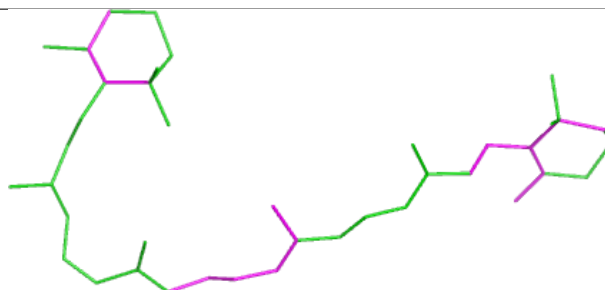


Rings

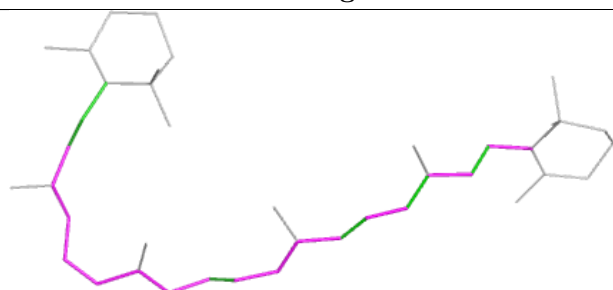
Ligand BCR A2 853



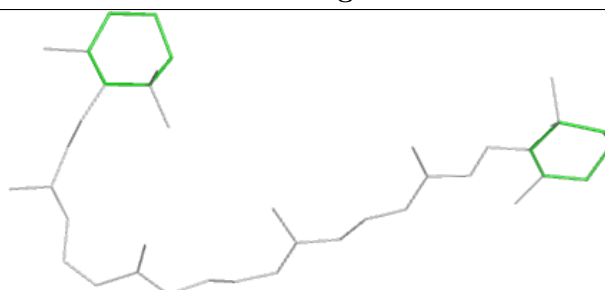
Bond lengths



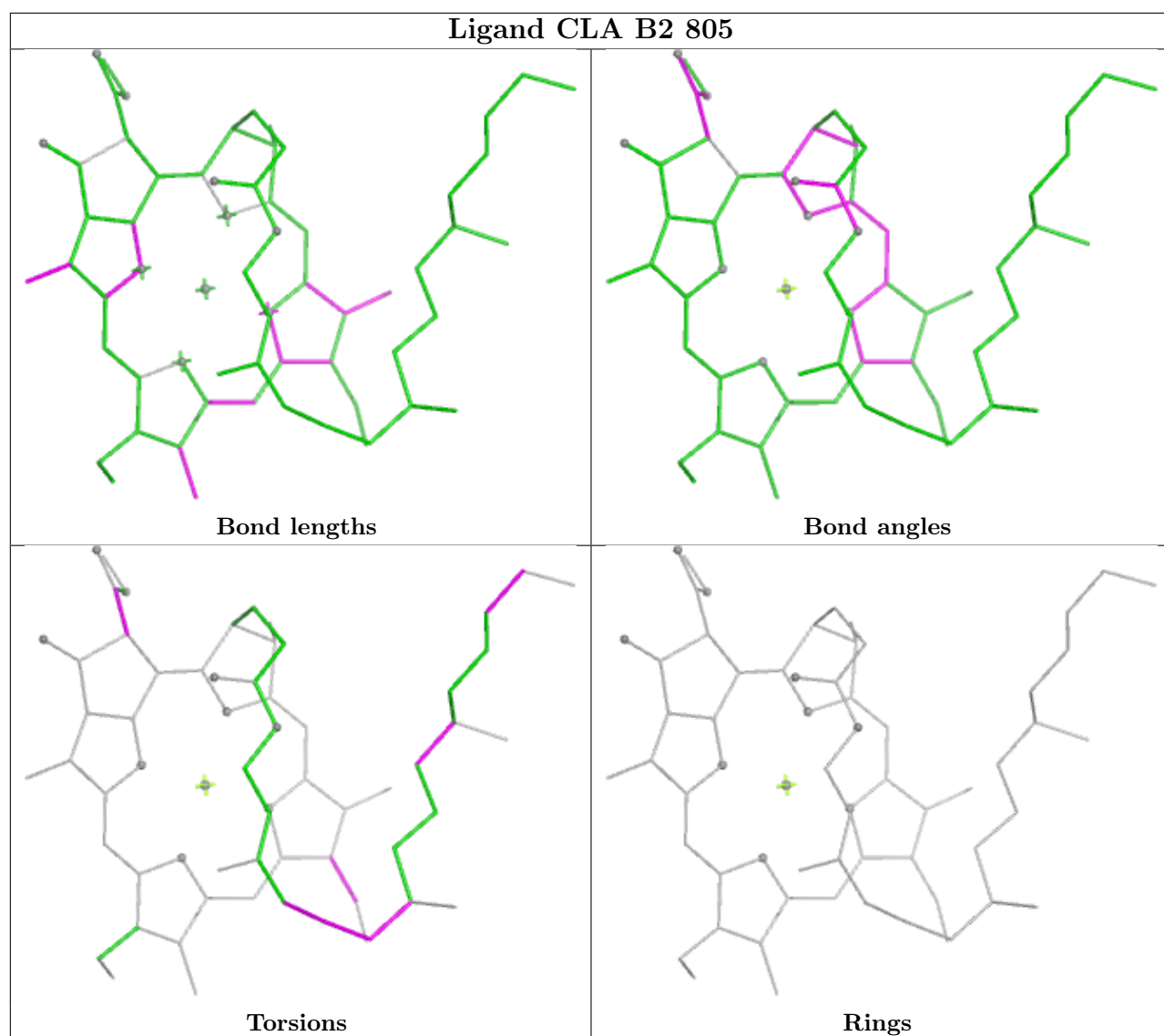
Bond angles

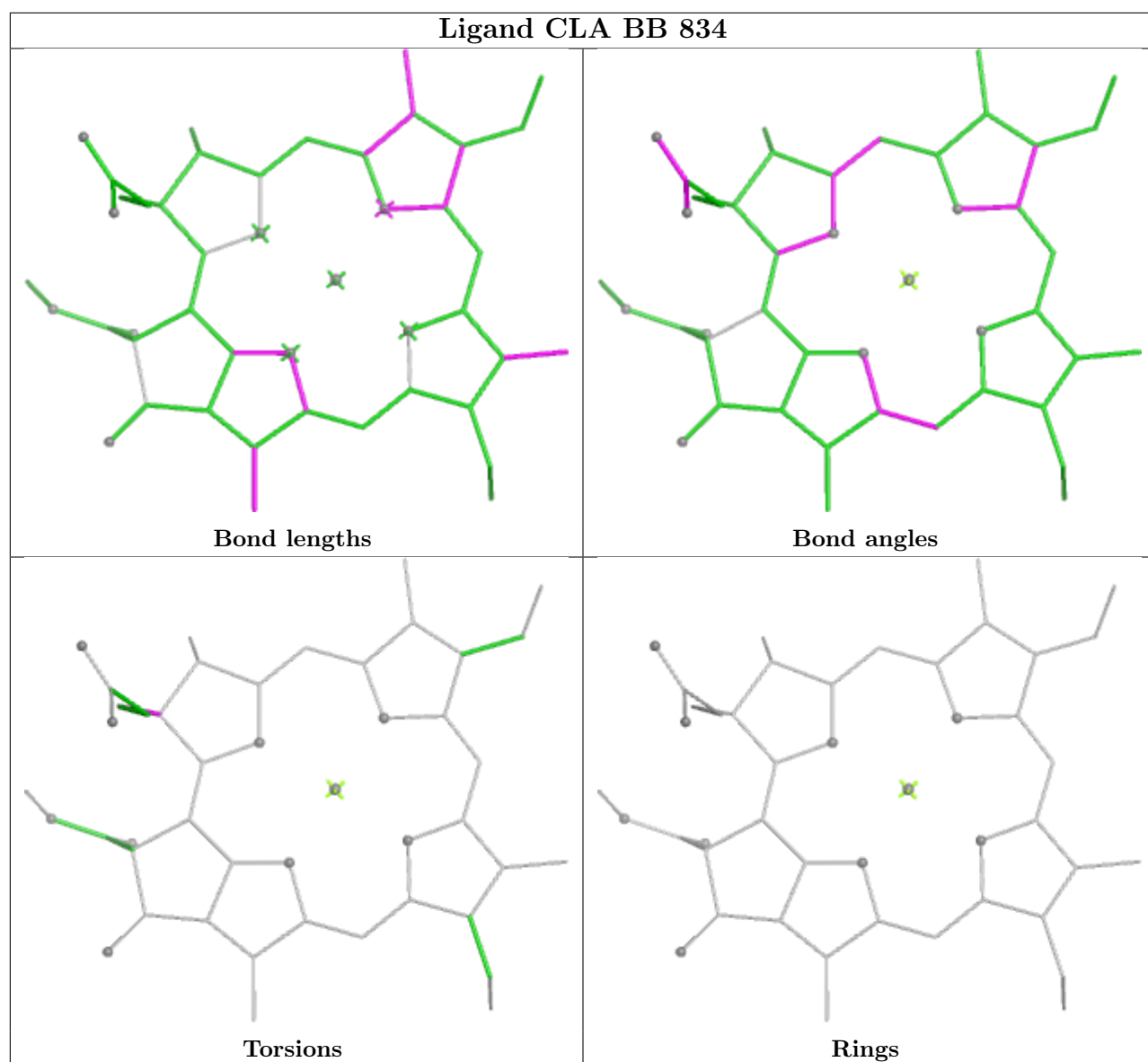


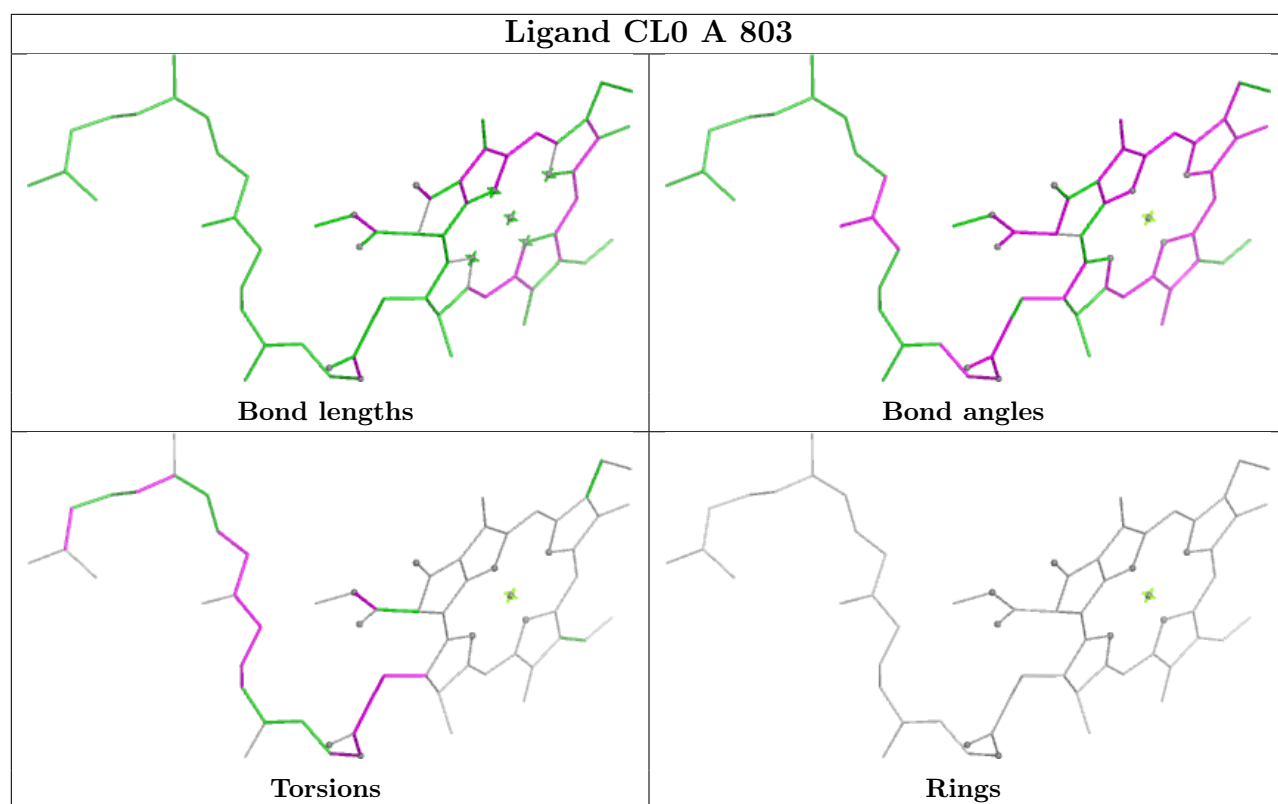
Torsions



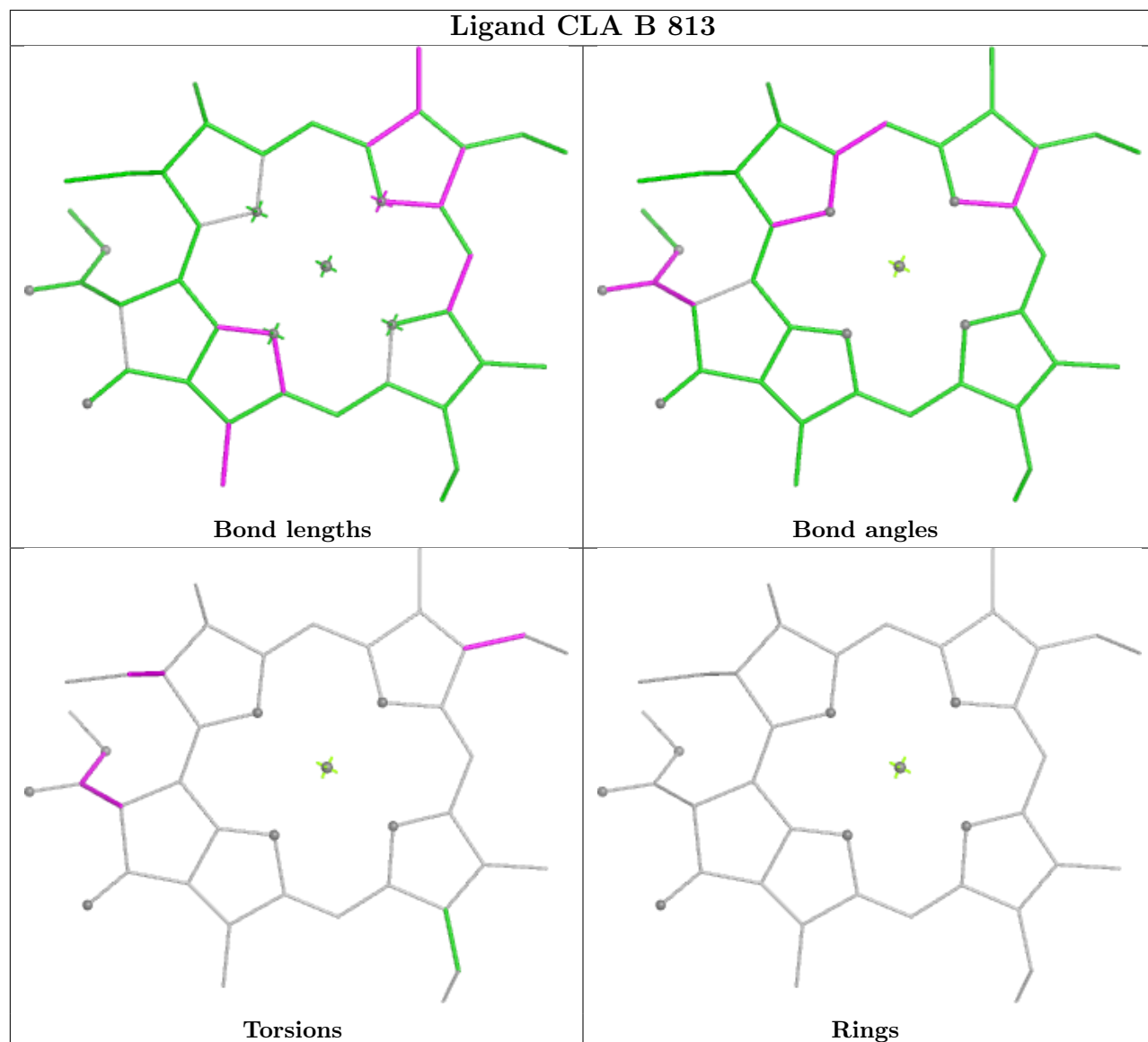
Rings



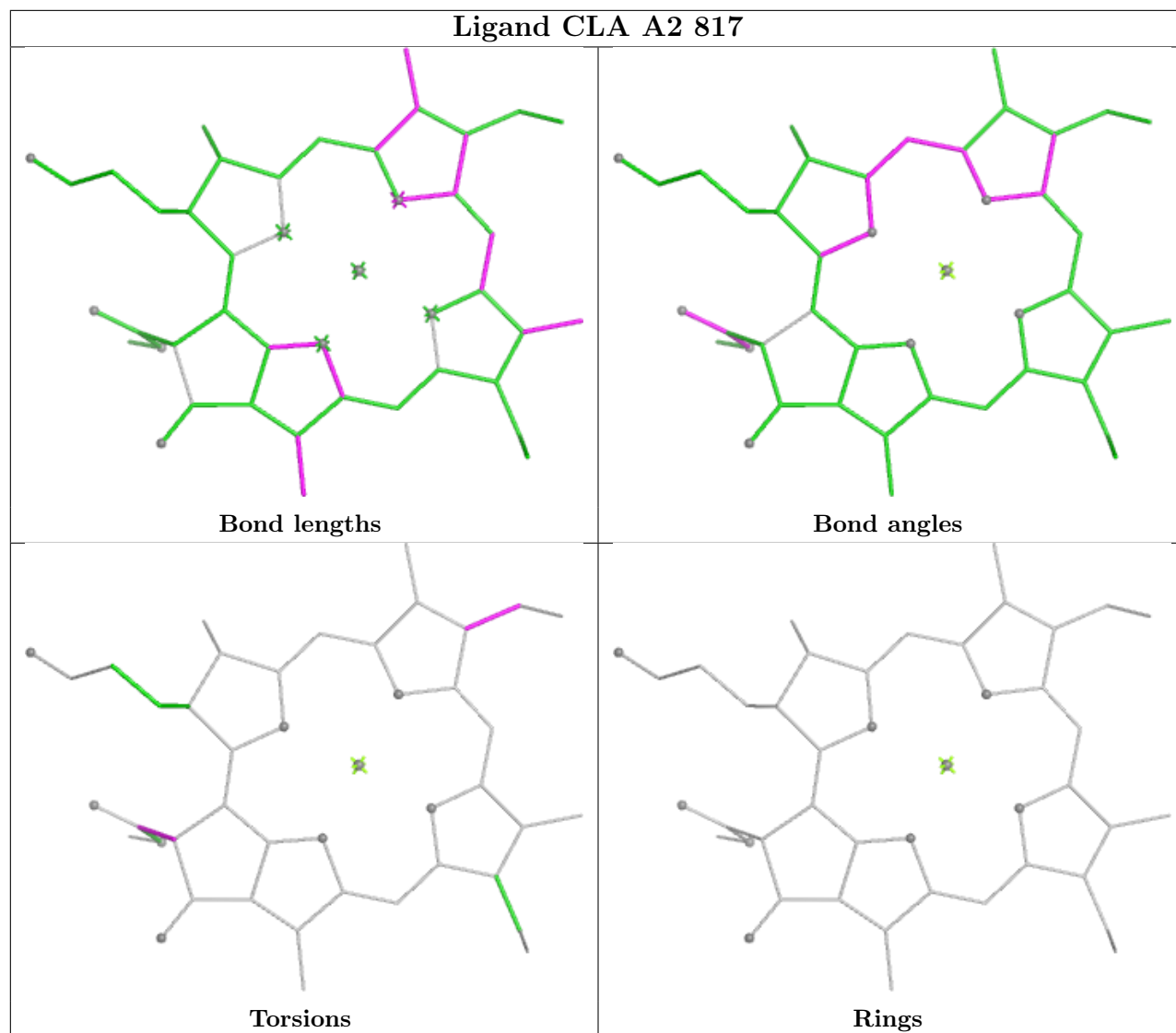




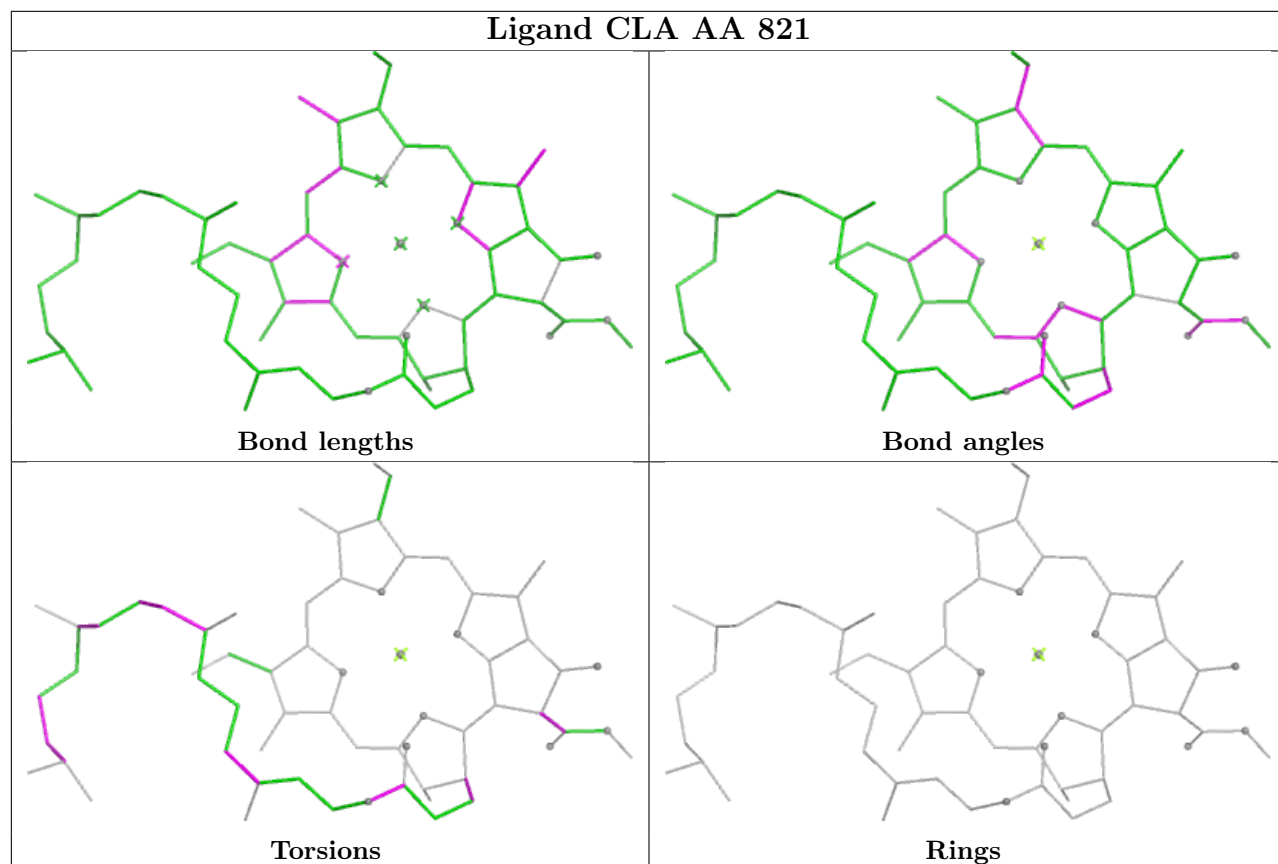
Ligand CLA B 813



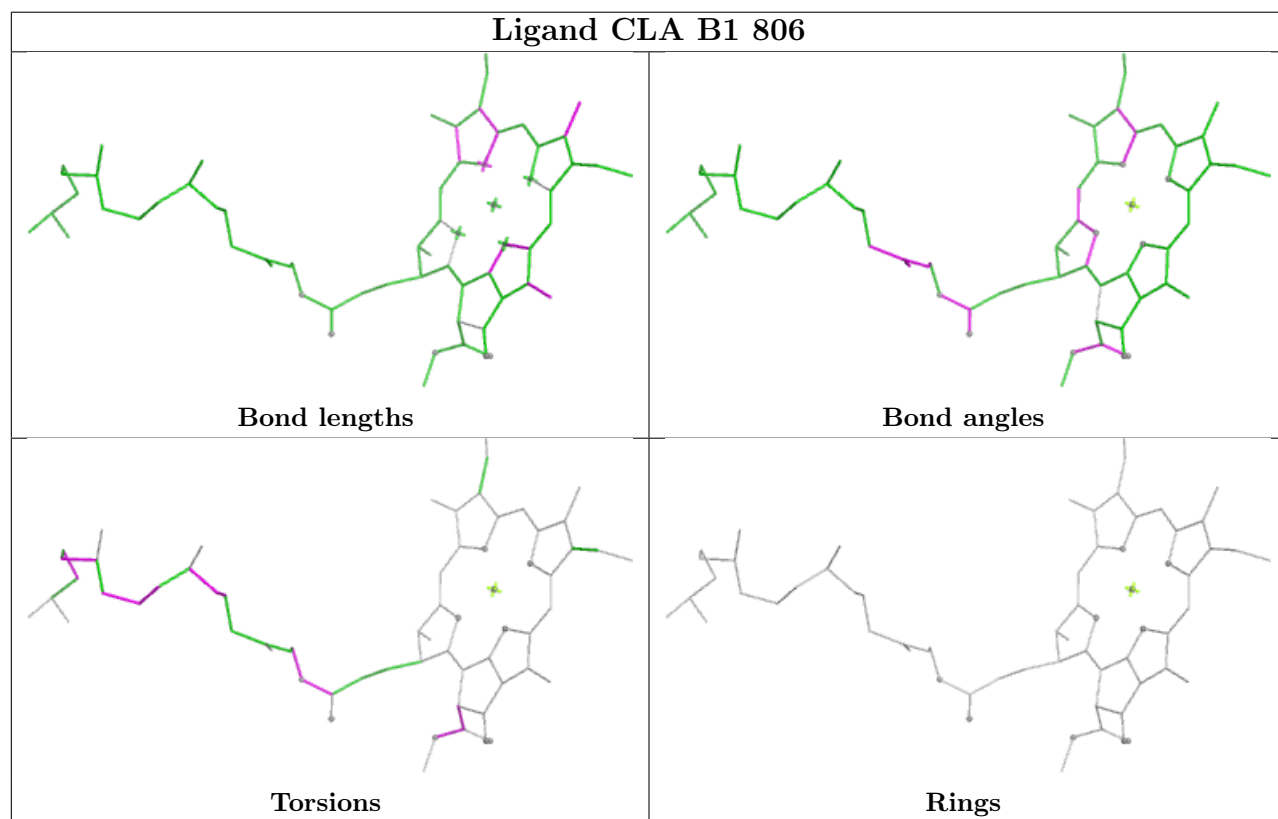
Ligand CLA A2 817



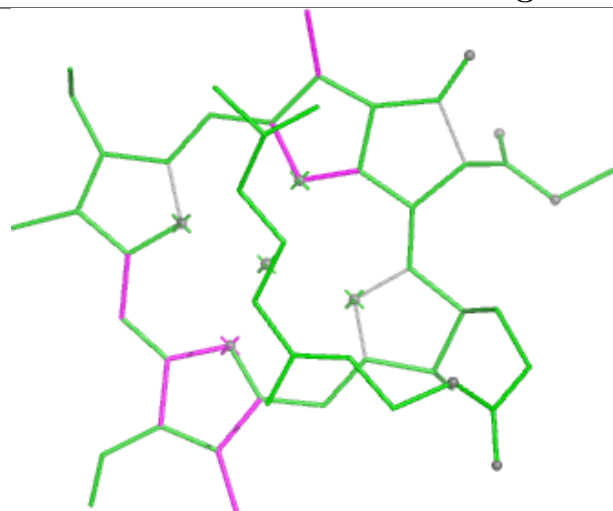
Ligand CLA AA 821



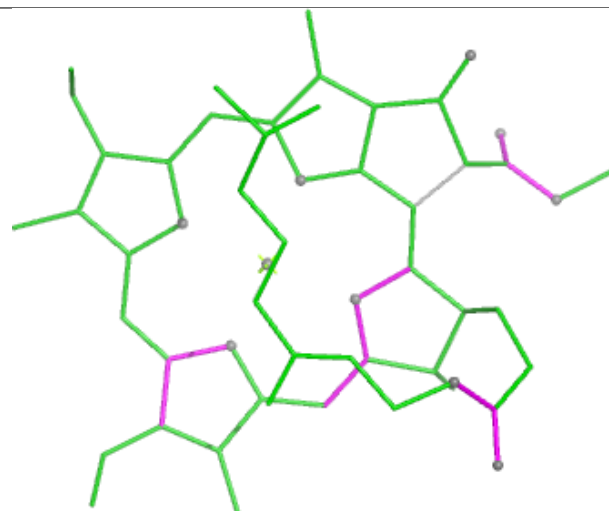
Ligand CLA B1 806



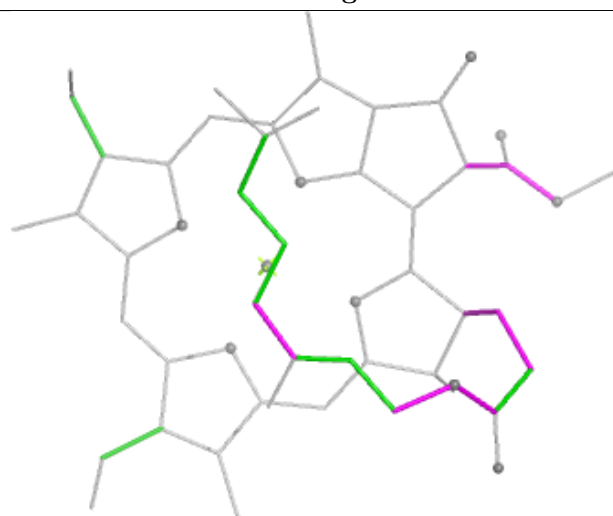
Ligand CLA B 824



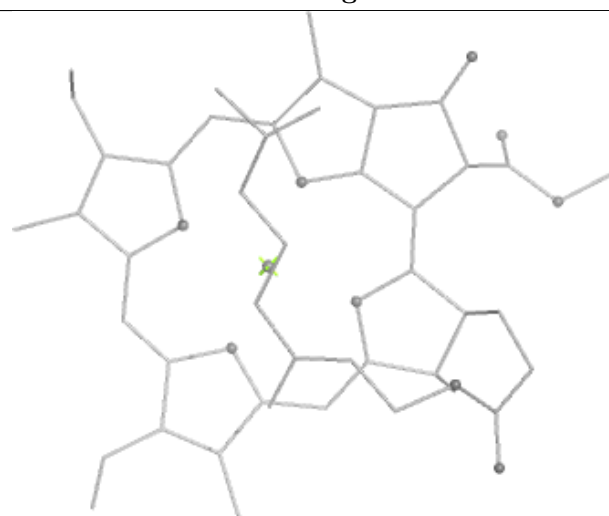
Bond lengths



Bond angles

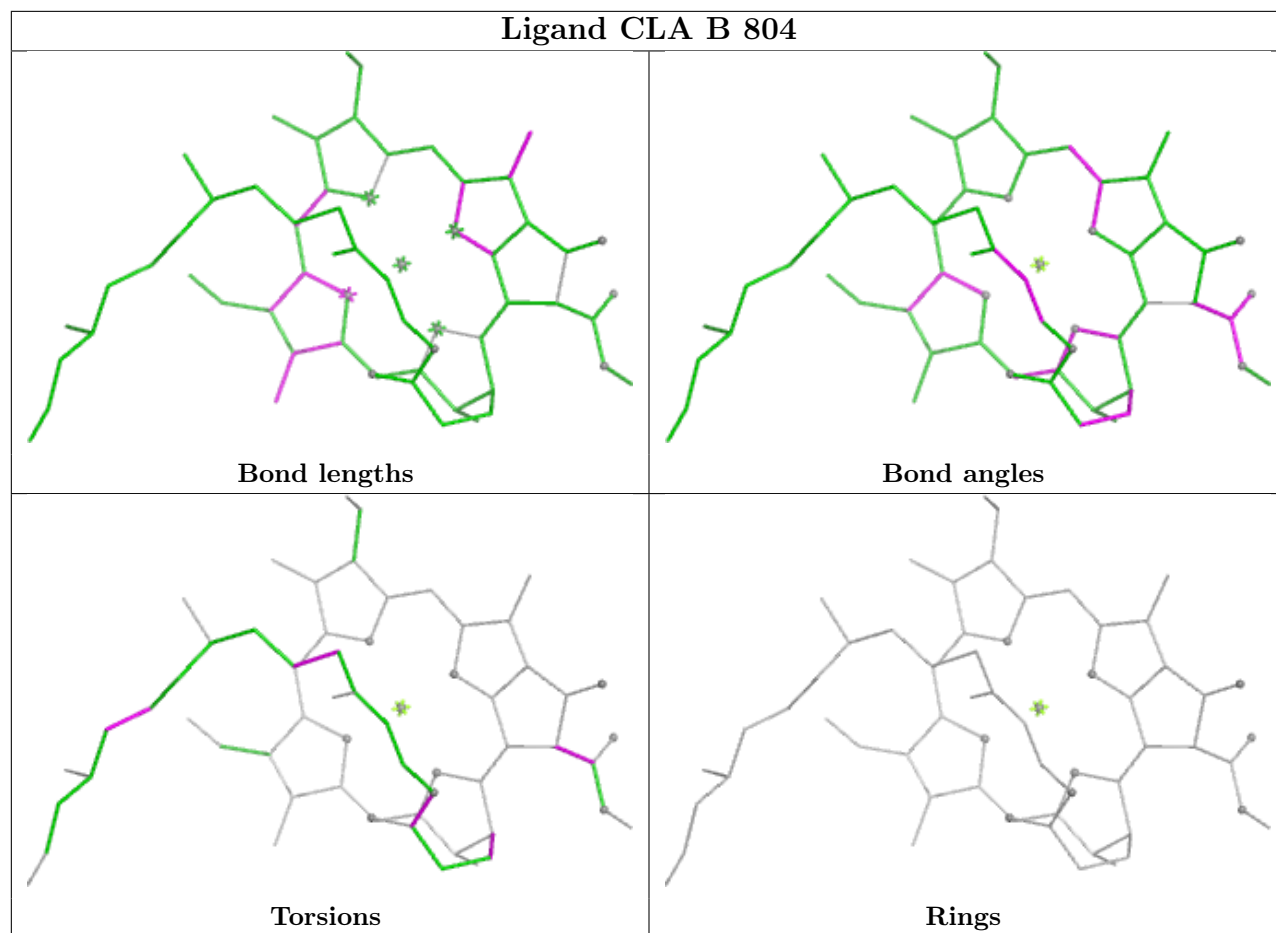


Torsions

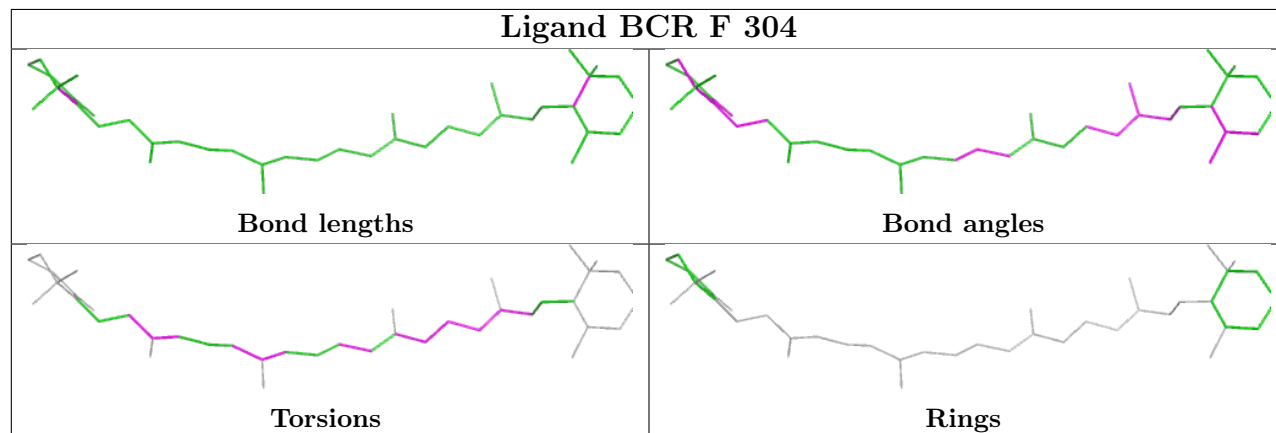


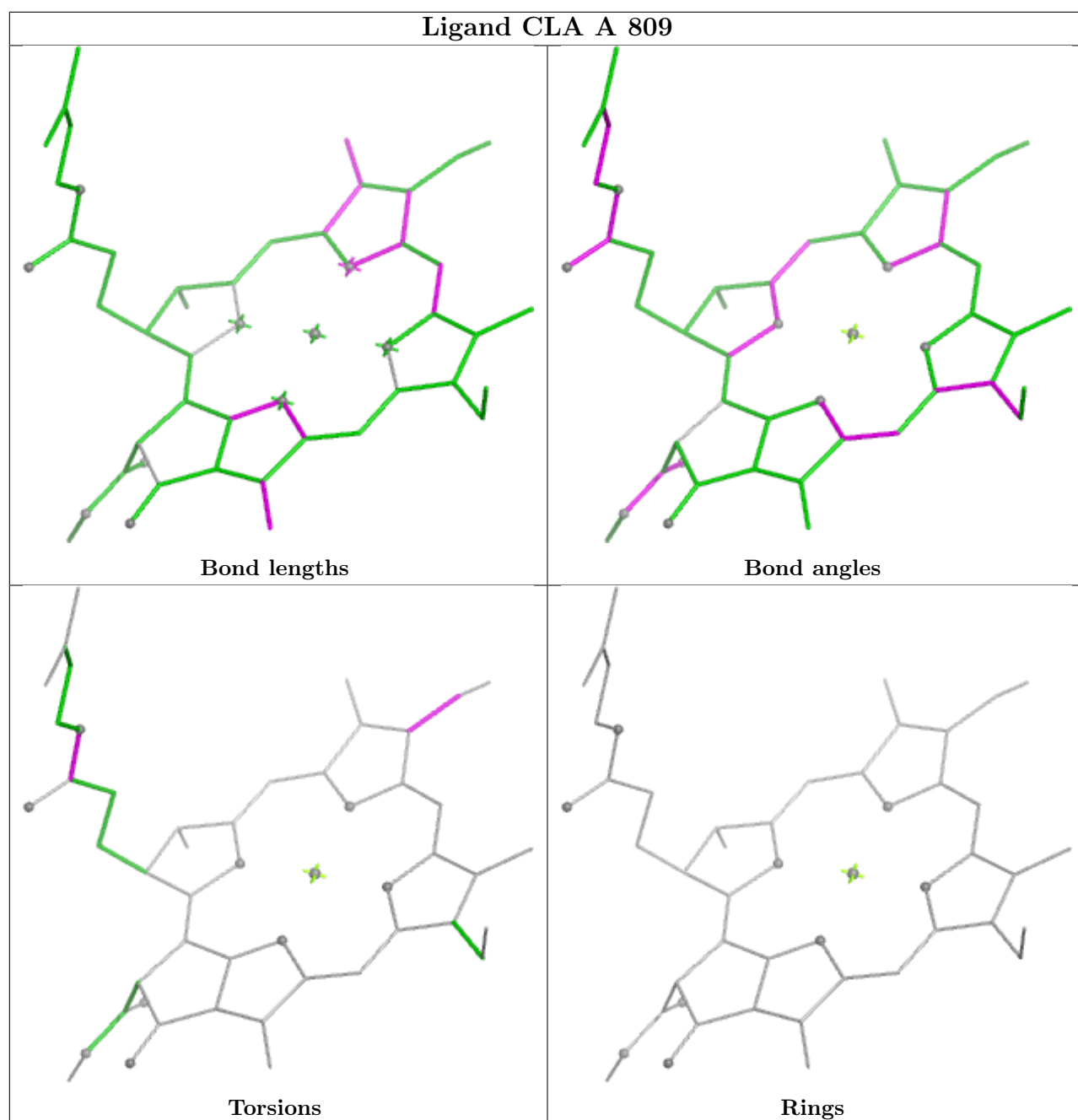
Rings

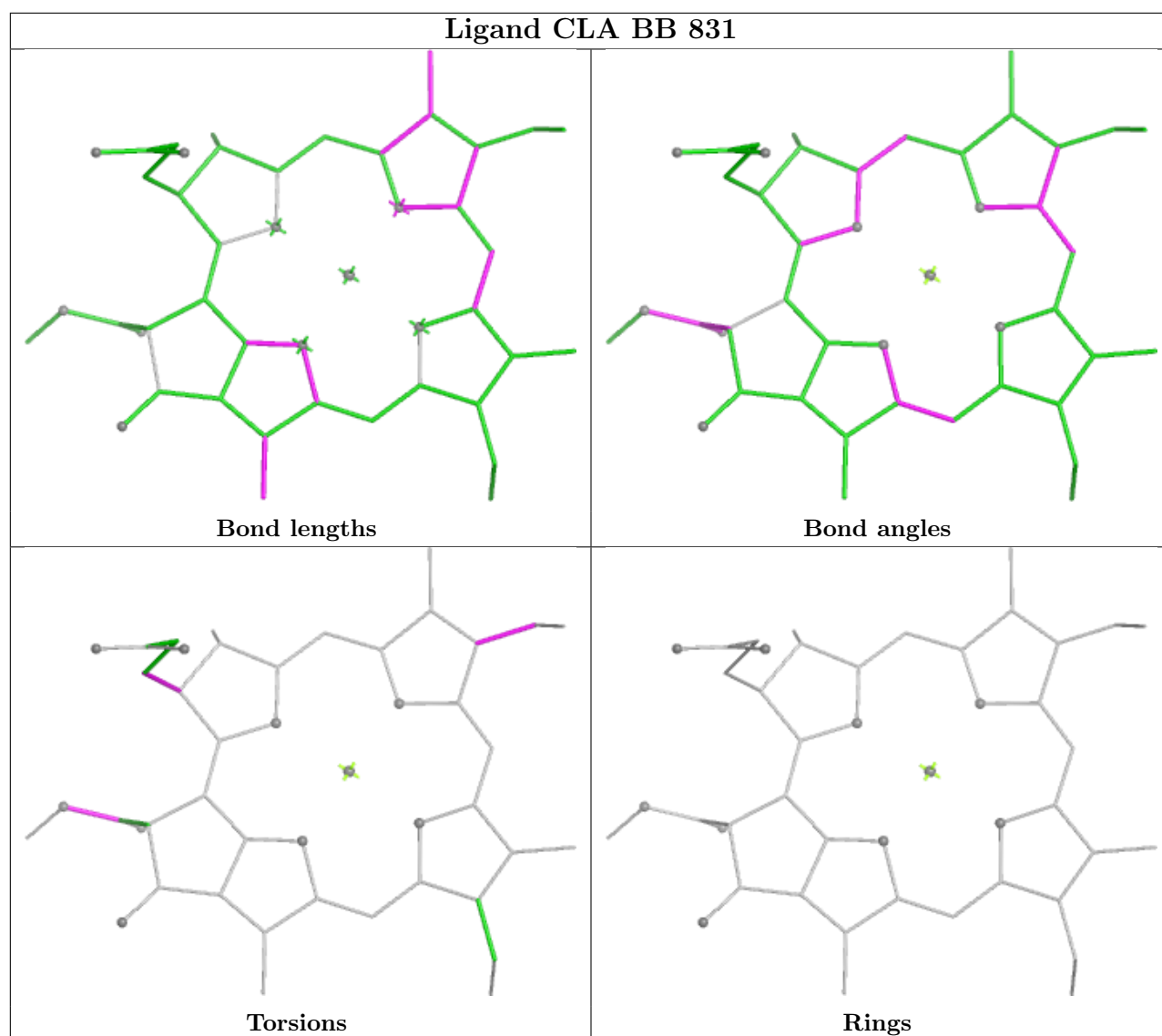
Ligand CLA B 804



Ligand BCR F 304







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

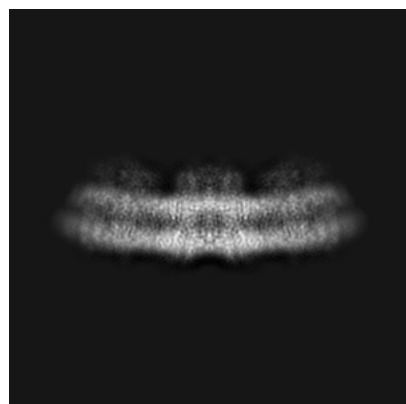
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10461. These allow visual inspection of the internal detail of the map and identification of artifacts.

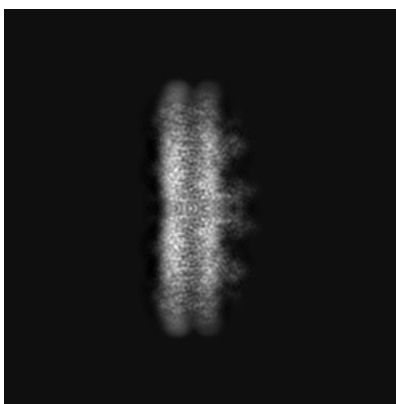
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

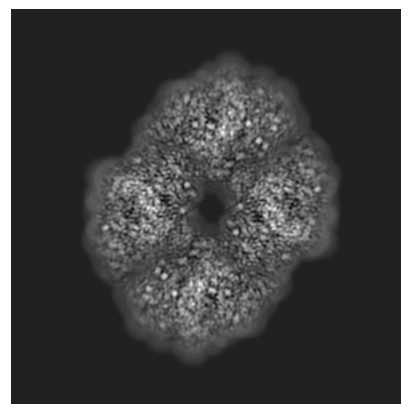
6.1.1 Primary map



X

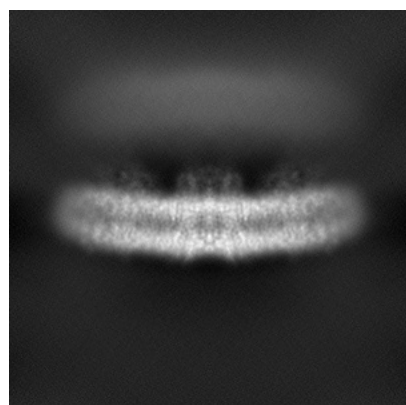


Y

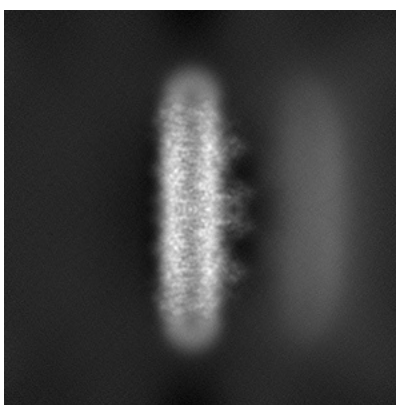


Z

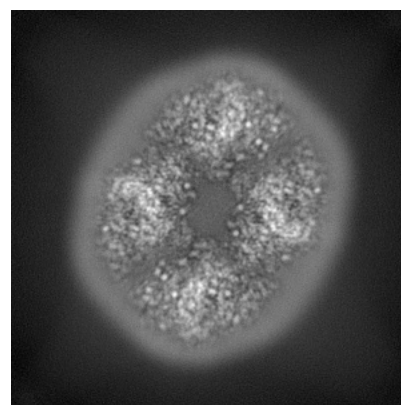
6.1.2 Raw map



X



Y

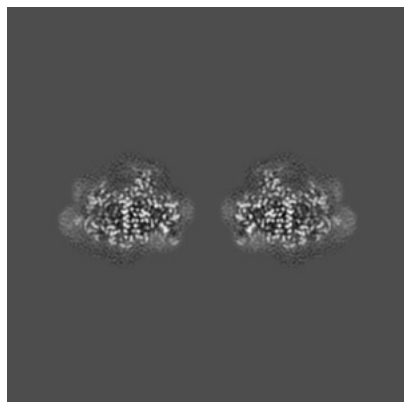


Z

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

6.2 Central slices [i](#)

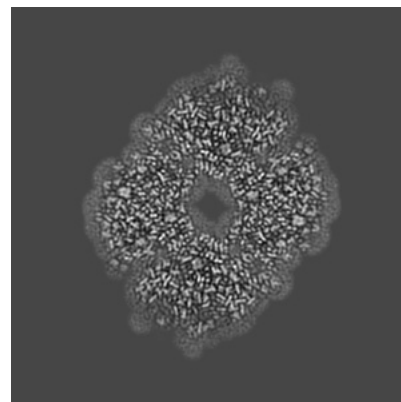
6.2.1 Primary map



X Index: 185

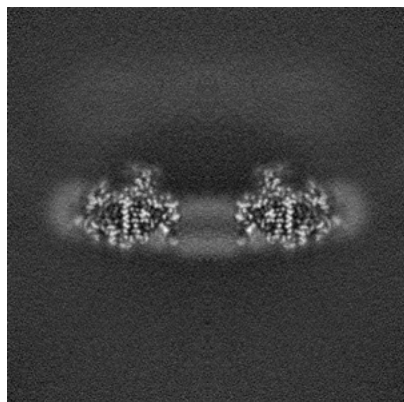


Y Index: 185

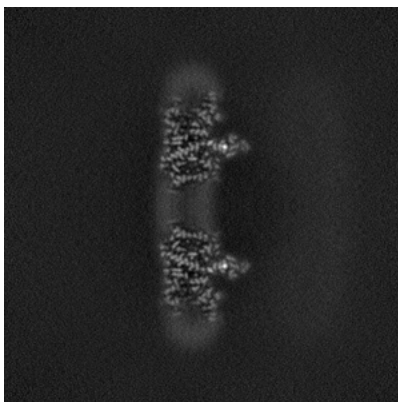


Z Index: 185

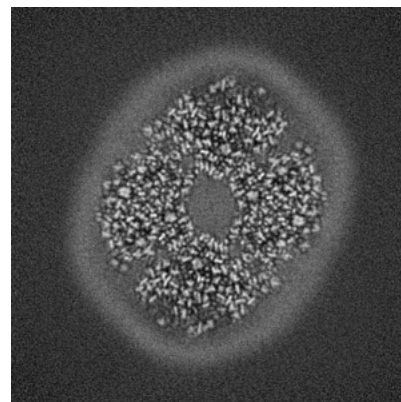
6.2.2 Raw map



X Index: 185



Y Index: 185

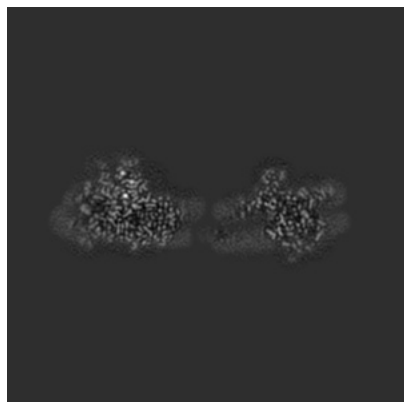


Z Index: 185

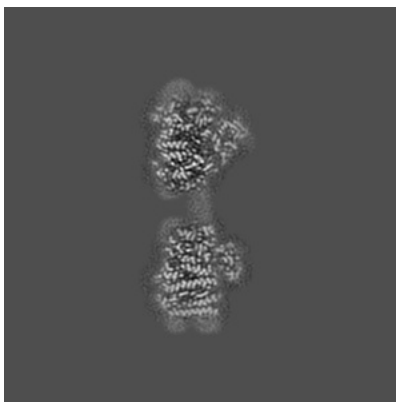
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

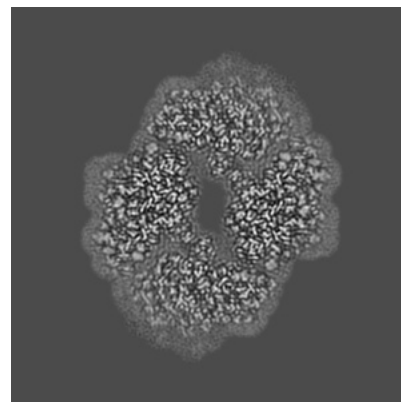
6.3.1 Primary map



X Index: 173

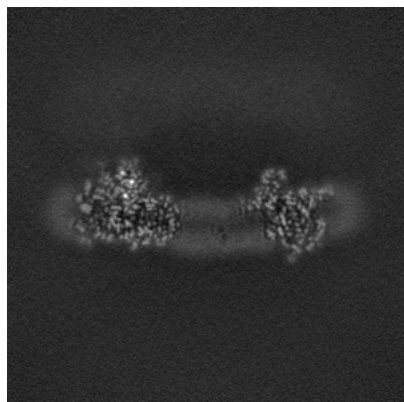


Y Index: 168

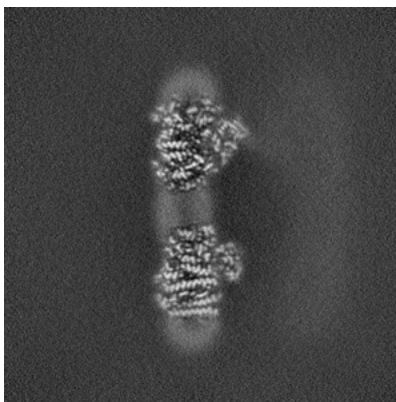


Z Index: 160

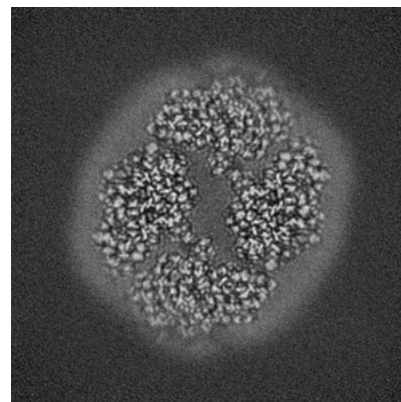
6.3.2 Raw map



X Index: 174



Y Index: 168

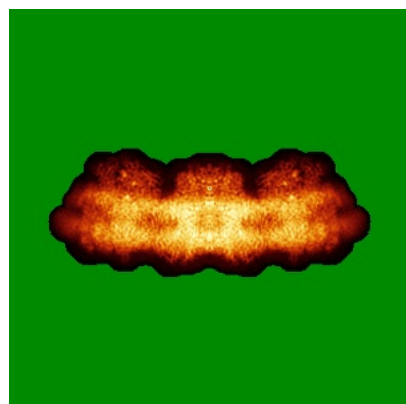


Z Index: 160

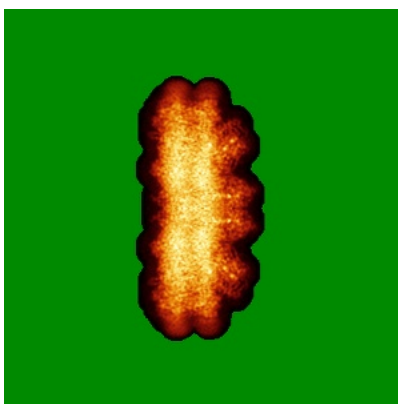
The images above show the largest variance slices of the map in three orthogonal directions.

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

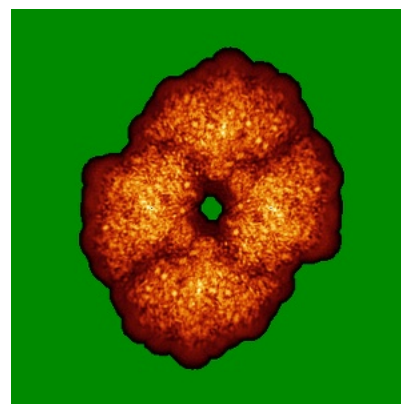
6.4.1 Primary map



X

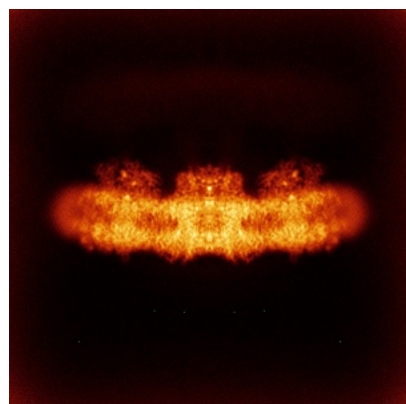


Y

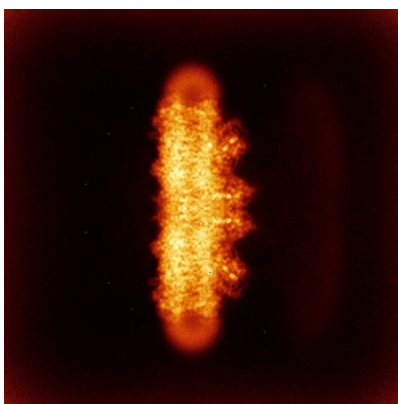


Z

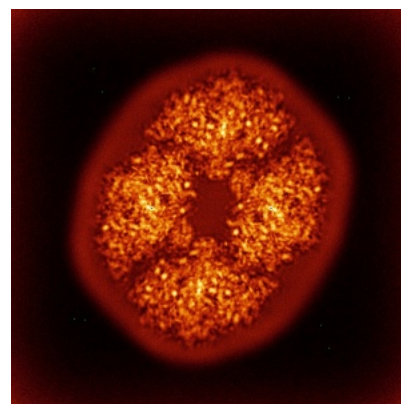
6.4.2 Raw map



X



Y

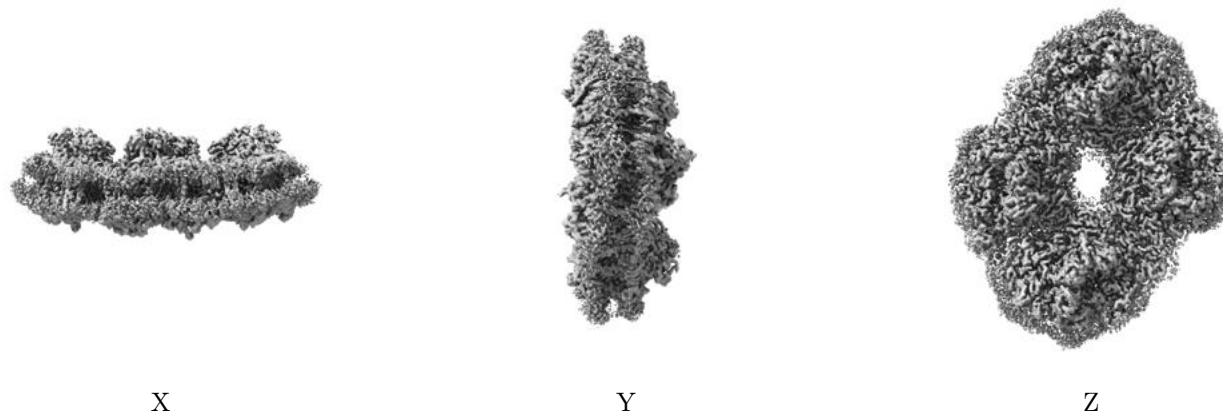


Z

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.

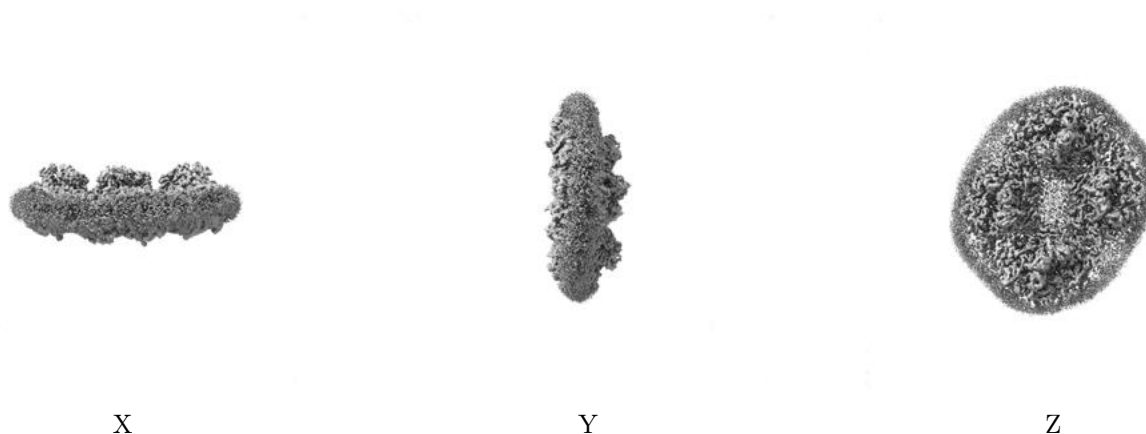
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.434. 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.

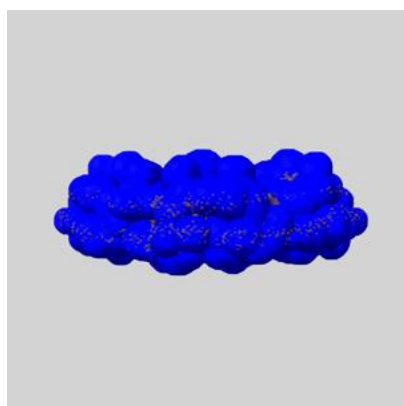
6.6 Mask visualisation [i](#)

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

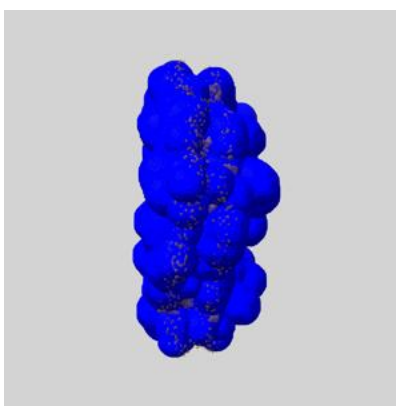
A mask typically either:

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

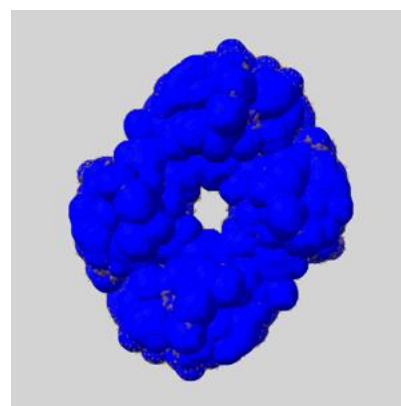
6.6.1 emd_10461_msk_1.map [i](#)



X



Y

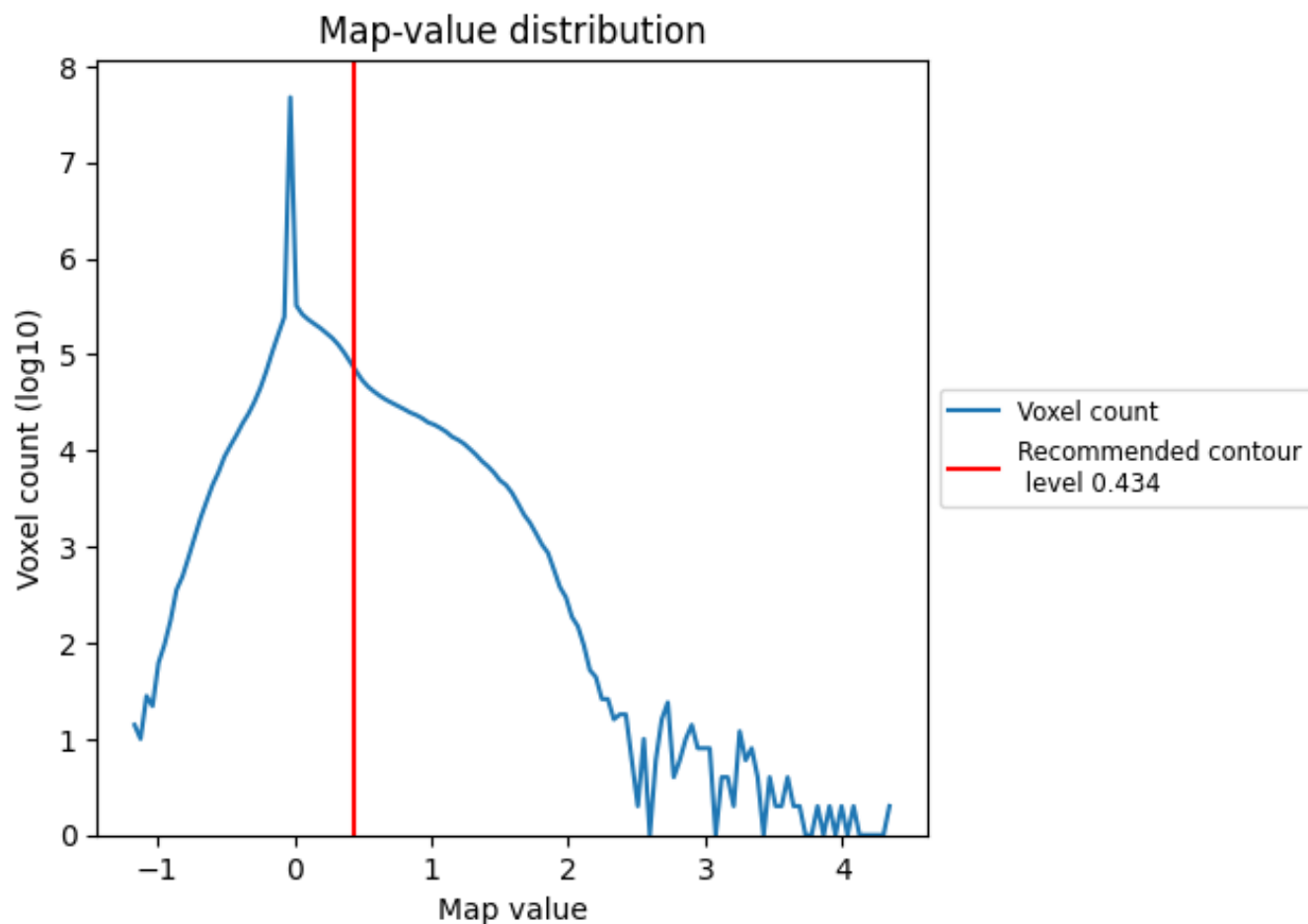


Z

7 Map analysis [i](#)

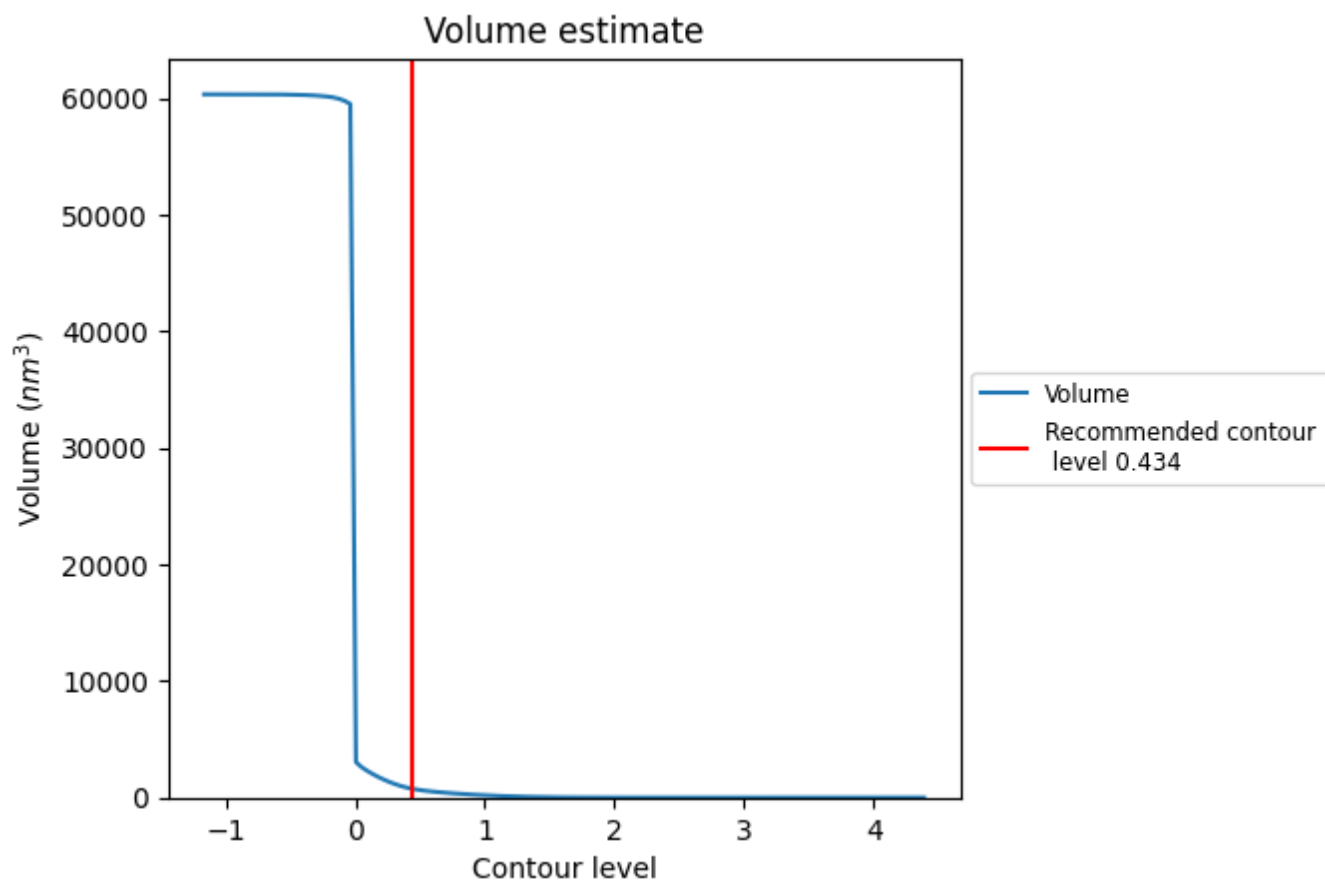
This section contains the results of statistical analysis of the map.

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.

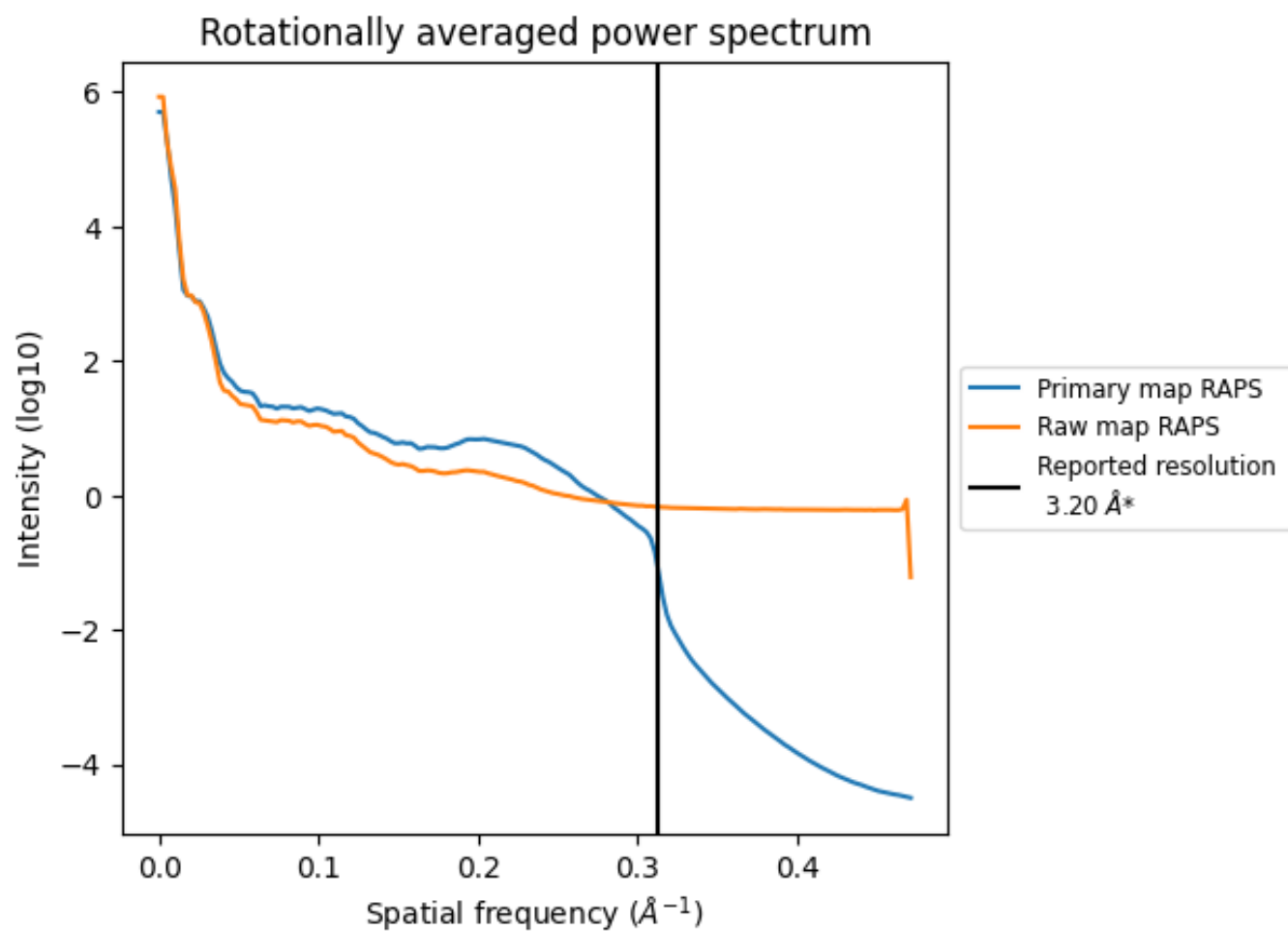
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 765 nm³; this corresponds to an approximate mass of 691 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 ⓘ

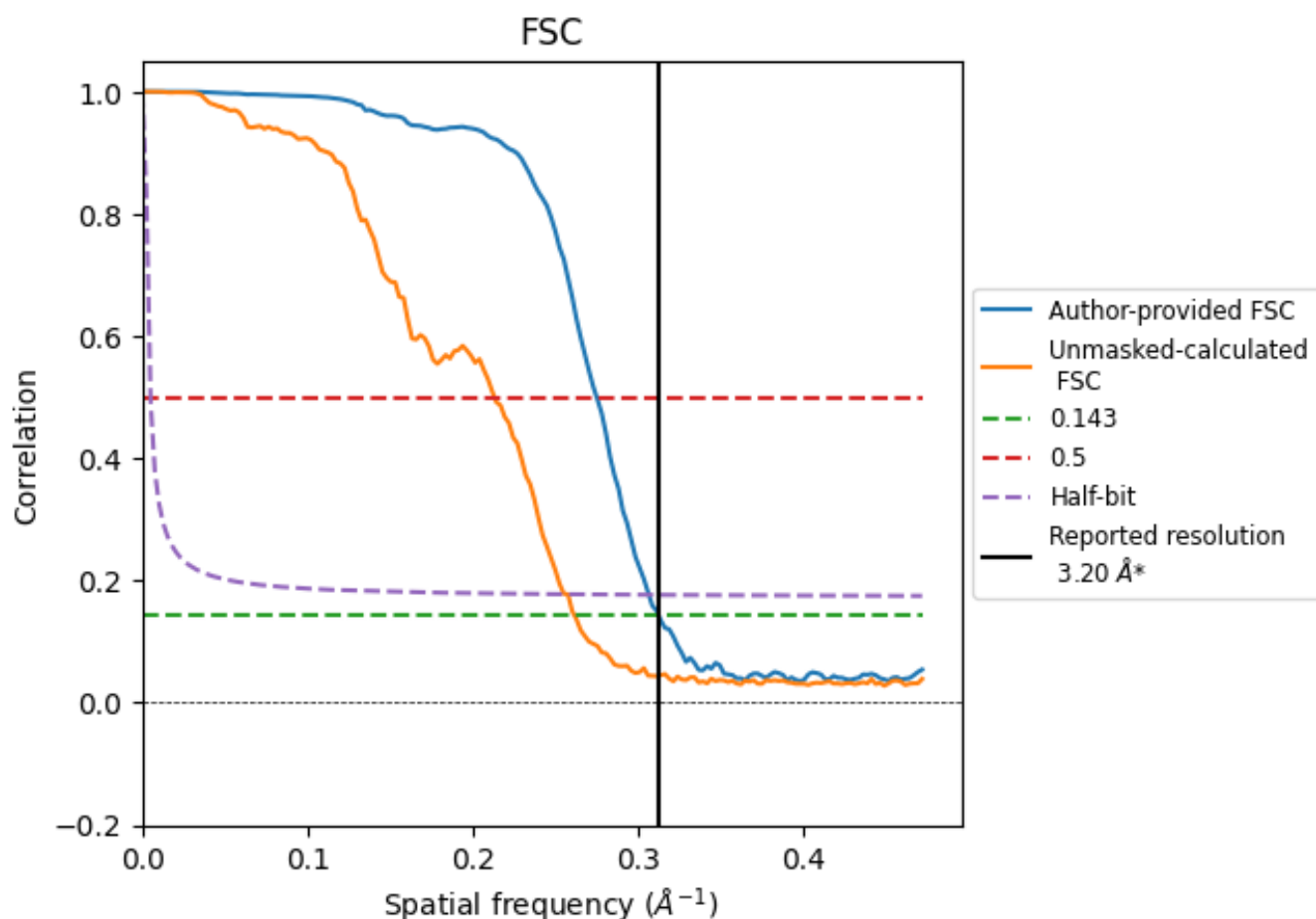


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

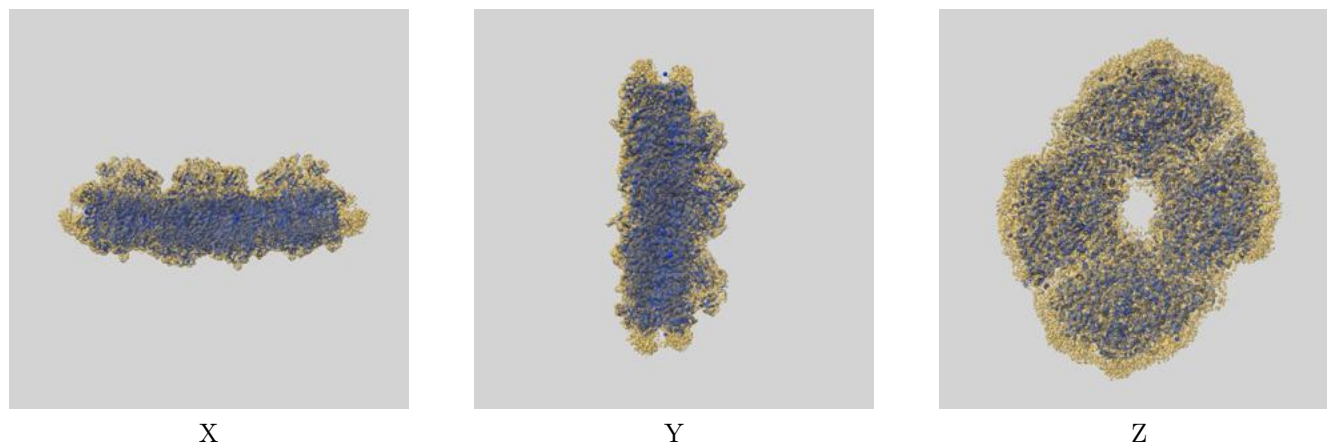
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.20	3.64	3.26
Unmasked-calculated*	3.83	4.69	3.89

*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 3.83 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

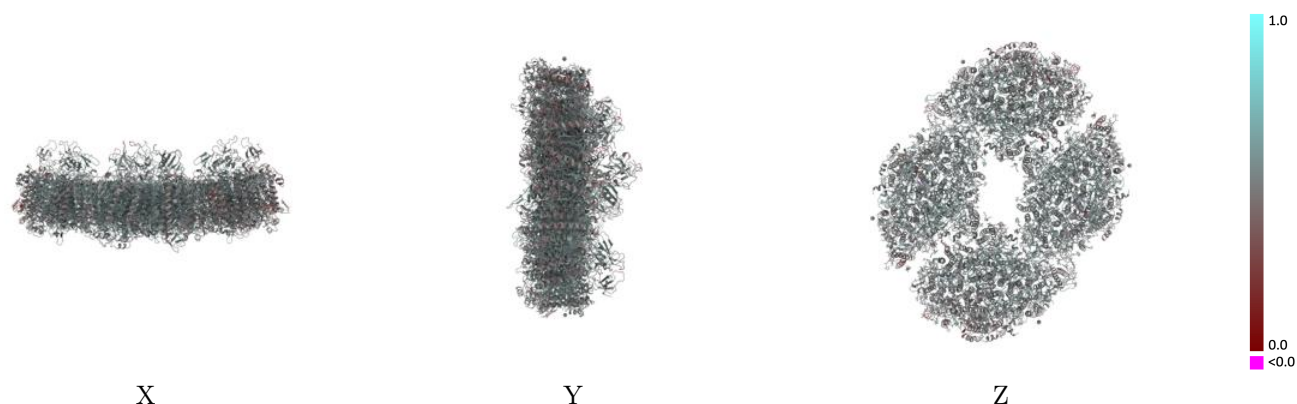
This section contains information regarding the fit between EMDB map EMD-10461 and PDB model 6TCL. Per-residue inclusion information can be found in section [3](#) on page [43](#).

9.1 Map-model overlay [i](#)



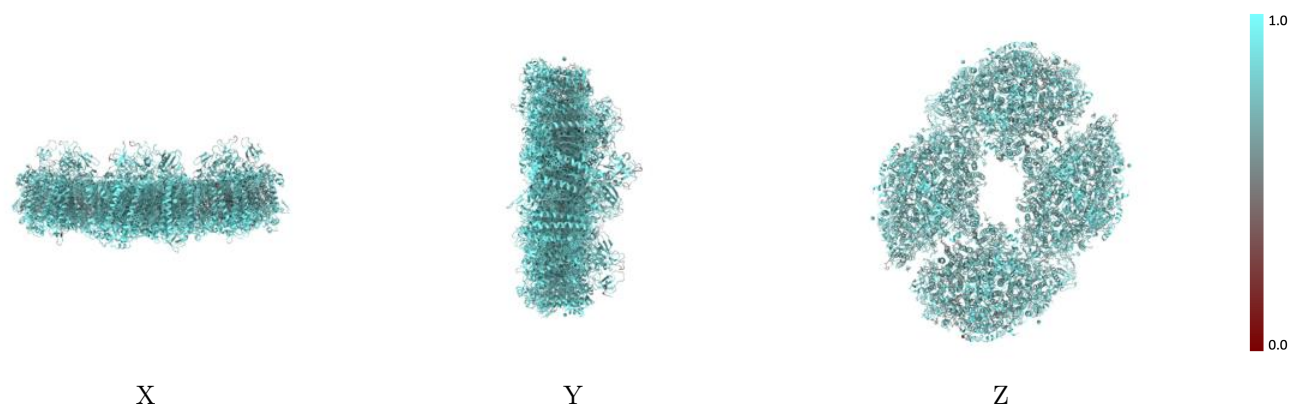
The images above show the 3D surface view of the map at the recommended contour level 0.434 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



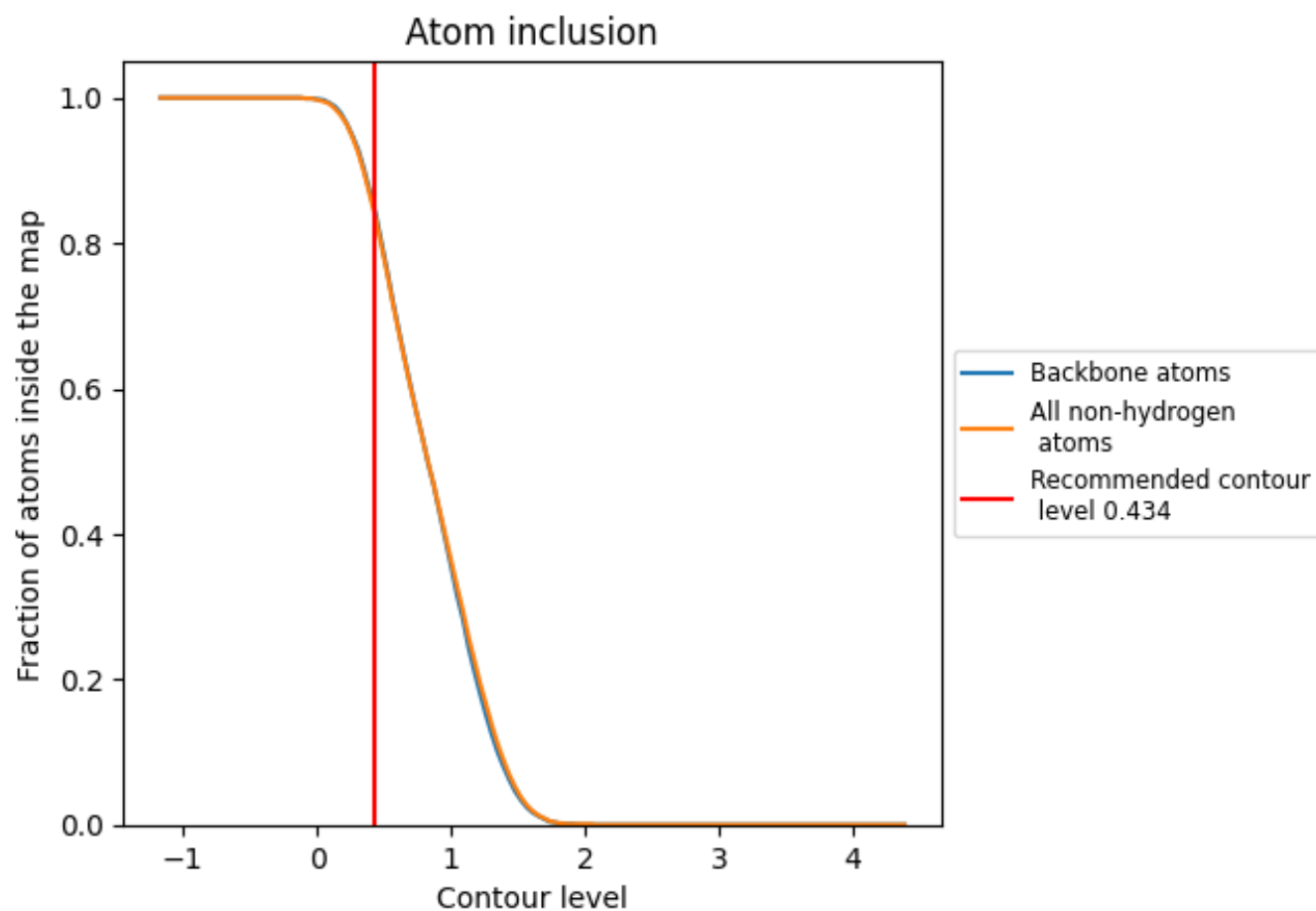
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.434).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 84% 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 (0.434) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8380	 0.5090
A	 0.8610	 0.5210
A1	 0.8530	 0.5190
A2	 0.8530	 0.5170
AA	 0.8600	 0.5210
B	 0.8670	 0.5280
B1	 0.8290	 0.5000
B2	 0.8310	 0.5000
BB	 0.8730	 0.5310
C	 0.8500	 0.4900
C1	 0.8340	 0.4840
C2	 0.8250	 0.5000
CC	 0.8340	 0.4910
D	 0.8260	 0.5140
D1	 0.7880	 0.5010
D2	 0.7910	 0.5050
DD	 0.8140	 0.5130
E	 0.7800	 0.4770
E1	 0.7570	 0.4530
E2	 0.7500	 0.4610
EE	 0.7840	 0.4900
F	 0.8440	 0.4940
F1	 0.7870	 0.4560
F2	 0.7880	 0.4470
FF	 0.8380	 0.4990
I	 0.8570	 0.5390
I1	 0.8490	 0.5220
I2	 0.8110	 0.5110
II	 0.8330	 0.5380
J	 0.8570	 0.4860
J1	 0.7840	 0.4490
J2	 0.8020	 0.4530
JJ	 0.8510	 0.4850
K	 0.7080	 0.4170
K1	 0.8090	 0.4850



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Chain	Atom inclusion	Q-score
K2	 0.8070	 0.4820
KK	 0.7200	 0.4200
L	 0.8190	 0.5020
L1	 0.8190	 0.5050
L2	 0.8360	 0.5040
LL	 0.8360	 0.5080
M	 0.8100	 0.5100
M1	 0.7310	 0.4640
M2	 0.7160	 0.4600
MM	 0.8260	 0.5060
X	 0.7890	 0.4990
X1	 0.6720	 0.4540
X2	 0.6770	 0.4530
XX	 0.7840	 0.4930