



wwPDB EM Validation Summary Report ⓘ

Apr 1, 2025 – 10:34 pm BST

PDB ID : 6TRD / pdb_00006trd
EMDB ID : EMD-10559
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 3.16 Å(reported)
Based on initial model : 1JB0

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

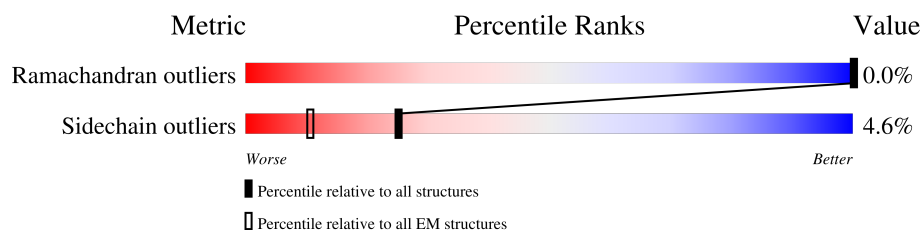
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.16 Å.

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




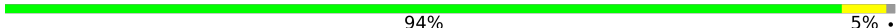






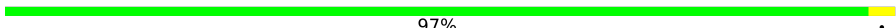
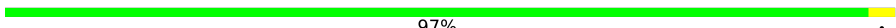
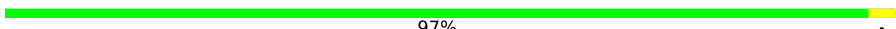






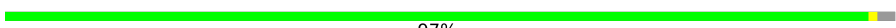
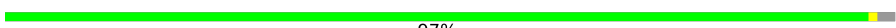
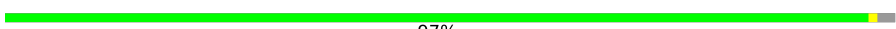





Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	1	755	95% . .
1	A	755	95% . .
1	a	755	95% . .
2	2	741	97% .
2	B	741	97% .
2	b	741	97% .
3	3	81	99% .
3	C	81	99% .
3	c	81	99% .
4	4	139	94% 5% .


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Mol	Chain	Length	Quality of chain
4	D	139	 94% 5% .
4	d	139	 94% 5% .
5	5	76	 83% 9% 8%
5	E	76	 83% 9% 8%
5	e	76	 83% 9% 8%
6	6	141	 89% 11%
6	F	141	 89% 11%
6	f	141	 89% 11%
7	7	38	 97% .
7	I	38	 97% .
7	i	38	 97% .
8	8	41	 90% 7% .
8	J	41	 90% 7% .
8	j	41	 90% 7% .
9	9	83	 83% 10% . 5%
9	K	83	 83% 10% . 5%
9	k	83	 83% 10% . 5%
10	0	155	 97% ..
10	L	155	 97% ..
10	l	155	 97% ..
11	M	31	 90% 6% .
11	m	31	 90% 6% .
11	y	31	 90% 6% .
12	X	36	 64% 11% 25%
12	x	36	 64% 11% 25%

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Mol	Chain	Length	Quality of chain
12	z	36	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	1	1602	X	-	-	-
13	CL0	A	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	0	205	X	-	-	-
14	CLA	0	206	X	-	-	-
14	CLA	0	207	X	-	-	-
14	CLA	1	1601	X	-	-	-
14	CLA	1	1603	X	-	-	-
14	CLA	1	1604	X	-	-	-
14	CLA	1	1605	X	-	-	-
14	CLA	1	1606	X	-	-	-
14	CLA	1	1607	X	-	-	-
14	CLA	1	1608	X	-	-	-
14	CLA	1	1609	X	-	-	-
14	CLA	1	1610	X	-	-	-
14	CLA	1	1611	X	-	-	-
14	CLA	1	1612	X	-	-	-
14	CLA	1	1613	X	-	-	-
14	CLA	1	1614	X	-	-	-
14	CLA	1	1615	X	-	-	-
14	CLA	1	1616	X	-	-	-
14	CLA	1	1617	X	-	-	-
14	CLA	1	1618	X	-	-	-
14	CLA	1	1619	X	-	-	-
14	CLA	1	1620	X	-	-	-
14	CLA	1	1621	X	-	-	-
14	CLA	1	1622	X	-	-	-
14	CLA	1	1623	X	-	-	-
14	CLA	1	1624	X	-	-	-
14	CLA	1	1625	X	-	-	-
14	CLA	1	1626	X	-	-	-
14	CLA	1	1627	X	-	-	-
14	CLA	1	1628	X	-	-	-
14	CLA	1	1629	X	-	-	-
14	CLA	1	1630	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	1631	X	-	-	-
14	CLA	1	1632	X	-	-	-
14	CLA	1	1633	X	-	-	-
14	CLA	1	1634	X	-	-	-
14	CLA	1	1635	X	-	-	-
14	CLA	1	1636	X	-	-	-
14	CLA	1	1637	X	-	-	-
14	CLA	1	1638	X	-	-	-
14	CLA	1	1639	X	-	-	-
14	CLA	1	1640	X	-	-	-
14	CLA	1	1641	X	-	-	-
14	CLA	1	1642	X	-	-	-
14	CLA	1	1643	X	-	-	-
14	CLA	1	1644	X	-	-	-
14	CLA	1	1645	X	-	-	-
14	CLA	2	802	X	-	-	-
14	CLA	2	803	X	-	-	-
14	CLA	2	804	X	-	-	-
14	CLA	2	805	X	-	-	-
14	CLA	2	806	X	-	-	-
14	CLA	2	807	X	-	-	-
14	CLA	2	808	X	-	-	-
14	CLA	2	809	X	-	-	-
14	CLA	2	810	X	-	-	-
14	CLA	2	811	X	-	-	-
14	CLA	2	812	X	-	-	-
14	CLA	2	813	X	-	-	-
14	CLA	2	814	X	-	-	-
14	CLA	2	815	X	-	-	-
14	CLA	2	816	X	-	-	-
14	CLA	2	817	X	-	-	-
14	CLA	2	818	X	-	-	-
14	CLA	2	819	X	-	-	-
14	CLA	2	820	X	-	-	-
14	CLA	2	821	X	-	-	-
14	CLA	2	822	X	-	-	-
14	CLA	2	823	X	-	-	-
14	CLA	2	824	X	-	-	-
14	CLA	2	825	X	-	-	-
14	CLA	2	826	X	-	-	-
14	CLA	2	827	X	-	-	-
14	CLA	2	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	2	829	X	-	-	-
14	CLA	2	830	X	-	-	-
14	CLA	2	831	X	-	-	-
14	CLA	2	832	X	-	-	-
14	CLA	2	833	X	-	-	-
14	CLA	2	834	X	-	-	-
14	CLA	2	835	X	-	-	-
14	CLA	2	836	X	-	-	-
14	CLA	2	837	X	-	-	-
14	CLA	2	838	X	-	-	-
14	CLA	2	839	X	-	-	-
14	CLA	2	841	X	-	-	-
14	CLA	2	842	X	-	-	-
14	CLA	6	201	X	-	-	-
14	CLA	6	203	X	-	-	-
14	CLA	8	1301	X	-	-	-
14	CLA	8	1302	X	-	-	-
14	CLA	8	1303	X	-	-	-
14	CLA	9	101	X	-	-	-
14	CLA	9	103	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	855	X	-	-	-
14	CLA	A	857	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	103	X	-	-	-
14	CLA	L	203	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	M	102	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	842	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	a	844	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	803	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-
14	CLA	b	806	X	-	-	-
14	CLA	b	807	X	-	-	-
14	CLA	b	808	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	816	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	819	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	822	X	-	-	-
14	CLA	b	823	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	825	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	827	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	841	X	-	-	-
14	CLA	b	842	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	j	1301	X	-	-	-
14	CLA	j	1302	X	-	-	-
14	CLA	j	1303	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	103	X	-	-	-
14	CLA	l	204	X	-	-	-
14	CLA	l	205	X	-	-	-
14	CLA	l	206	X	-	-	-
14	CLA	x	1701	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	z	102	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 74991 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	a	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	1	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	b	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	2	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	4	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	70	Total	C	N	O		0	0
			546	347	94	105			
5	e	70	Total	C	N	O		0	0
			546	347	94	105			
5	5	70	Total	C	N	O		0	0
			546	347	94	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	6	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	i	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	7	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		
8	j	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	k	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	9	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	l	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	0	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4
0	143	LEU	SER	conflict	UNP Q8DGB4

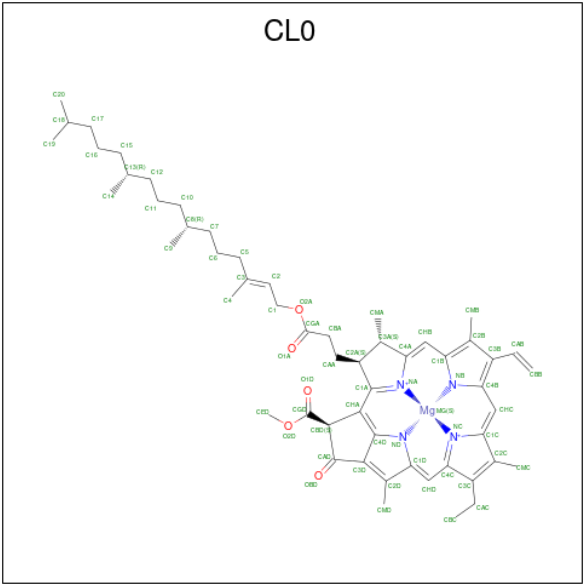
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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

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

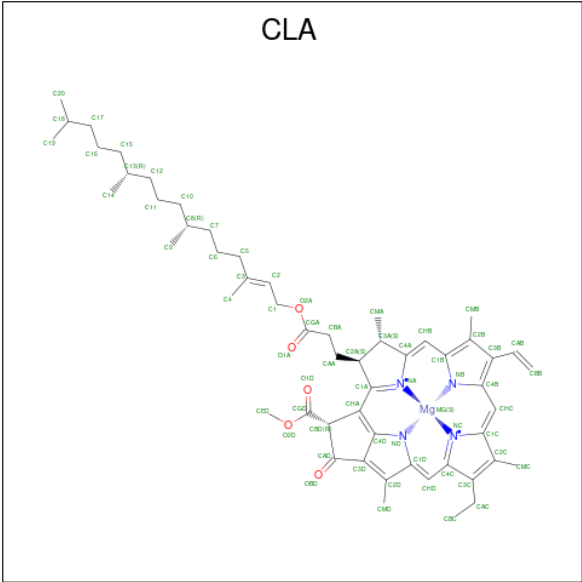
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		
12	x	27	Total	C	N	O	0	0
			228	163	33	32		
12	z	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	K	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	M	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 58	C 48	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	j	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	x	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0

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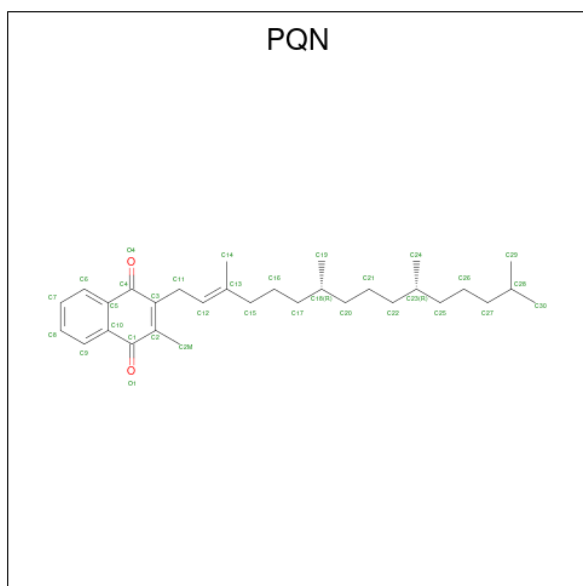
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	8	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	9	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0

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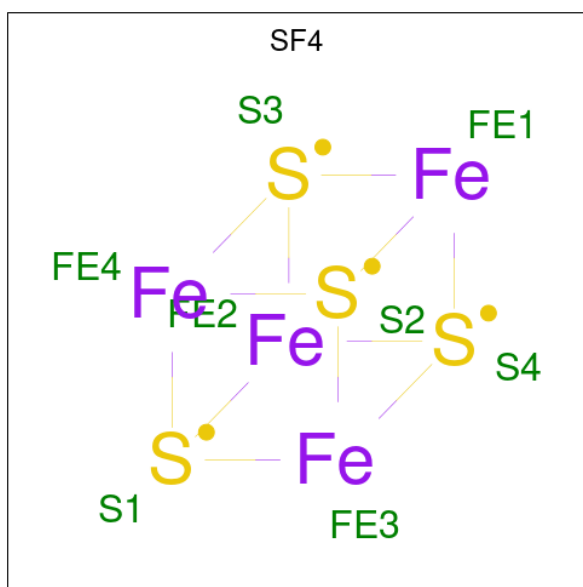
Mol	Chain	Residues	Atoms					AltConf
14	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



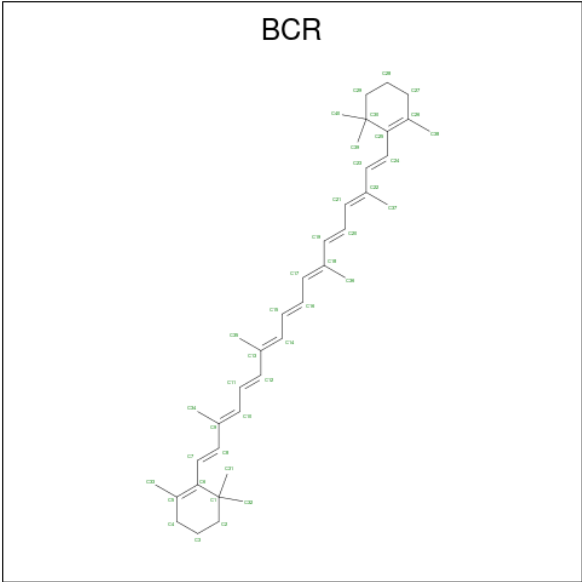
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	a	1	Total	Fe	S	0
			8	4	4	
16	c	1	Total	Fe	S	0
			8	4	4	
16	c	1	Total	Fe	S	0
			8	4	4	
16	1	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			25	25	
17	A	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	F	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 25 25	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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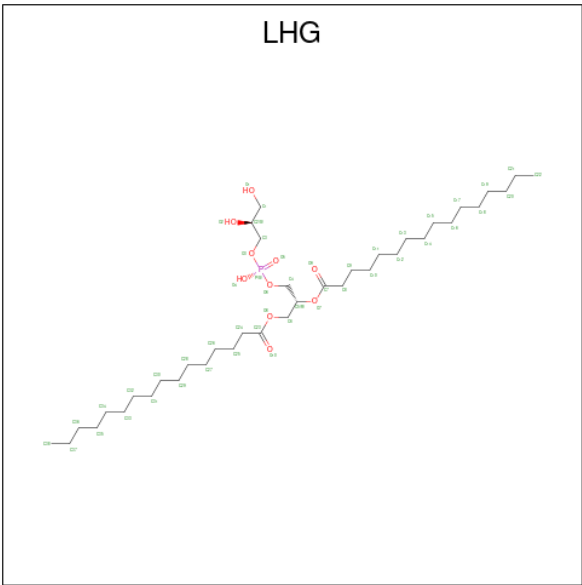
Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 25 25	0
17	l	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	m	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	9	1	Total C 40 40	0
17	9	1	Total C 25 25	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	y	1	Total C 40 40	0

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	
18	A	1	Total	C	O	P	0
			41	30	10	1	
18	B	1	Total	C	O	P	0
			49	38	10	1	
18	L	1	Total	C	O	P	0
			39	28	10	1	
18	M	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			41	30	10	1	
18	b	1	Total	C	O	P	0
			49	38	10	1	
18	l	1	Total	C	O	P	0
			39	28	10	1	
18	m	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			49	38	10	1	
18	1	1	Total	C	O	P	0
			41	30	10	1	
18	0	1	Total	C	O	P	0
			39	28	10	1	
18	y	1	Total	C	O	P	0
			49	38	10	1	

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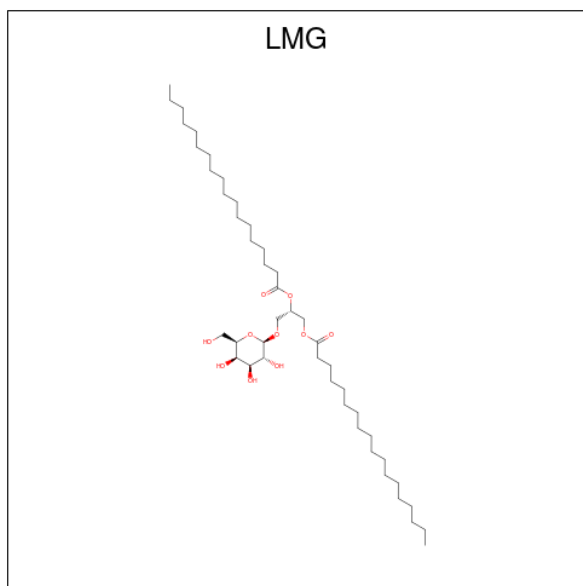
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Mol	Chain	Residues	Atoms				AltConf
18	z	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 19 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	
19	b	1	Total	Ca	0
			1	1	
19	1	1	Total	Ca	0
			1	1	
19	2	1	Total	Ca	0
			1	1	
19	0	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



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

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Mol	Chain	Residues	Atoms			AltConf
20	2	1	Total	C	O	0
			55	45	10	

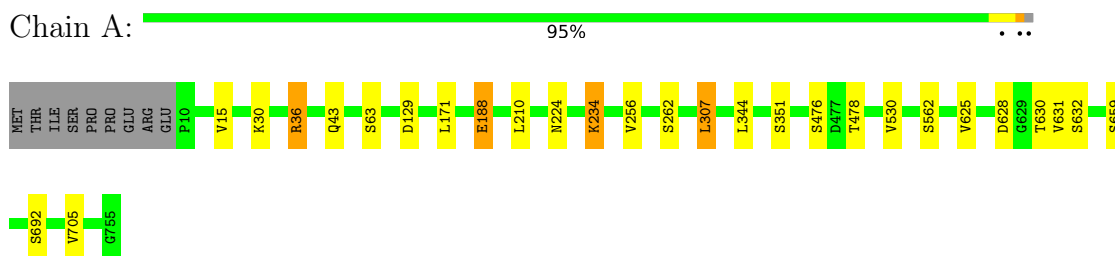
- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	5	Total	O	0
			5	5	
21	B	8	Total	O	0
			8	8	
21	F	1	Total	O	0
			1	1	
21	J	1	Total	O	0
			1	1	
21	K	1	Total	O	0
			1	1	
21	L	1	Total	O	0
			1	1	
21	a	5	Total	O	0
			5	5	
21	b	8	Total	O	0
			8	8	
21	f	1	Total	O	0
			1	1	
21	j	1	Total	O	0
			1	1	
21	k	1	Total	O	0
			1	1	
21	l	1	Total	O	0
			1	1	
21	1	5	Total	O	0
			5	5	
21	2	8	Total	O	0
			8	8	
21	6	1	Total	O	0
			1	1	
21	8	1	Total	O	0
			1	1	
21	9	1	Total	O	0
			1	1	
21	0	1	Total	O	0
			1	1	

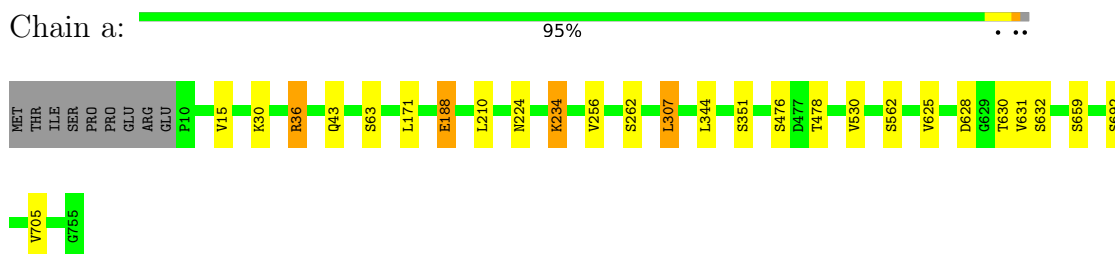
3 Residue-property plots [i](#)

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. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

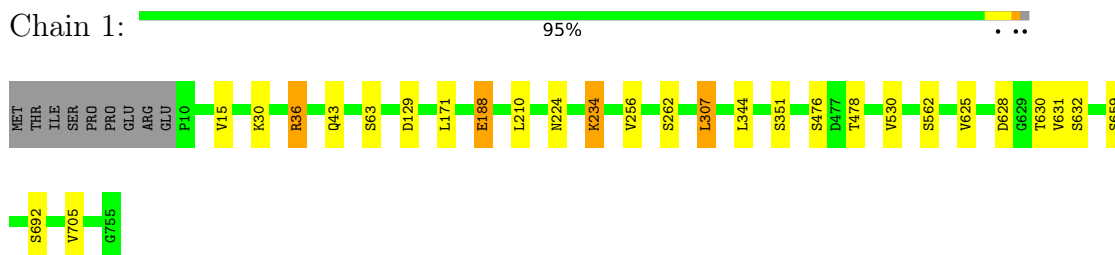
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



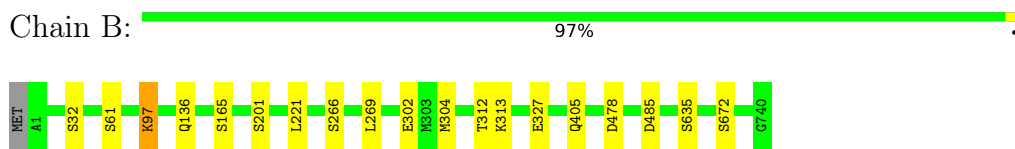
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b:  97%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  97%



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  99%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  99%



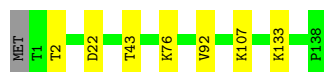
- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  99%



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  94% 5%



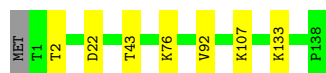
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  94% 5%




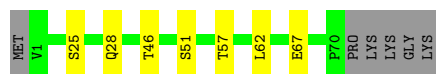
- Molecule 4: Photosystem I reaction center subunit II

Chain 4:  94% 5%




- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  83% 9% 8%




- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  83% 9% 8%




- Molecule 5: Photosystem I reaction center subunit IV

Chain 5:  83% 9% 8%




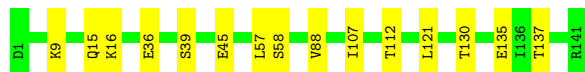
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  89% 11%




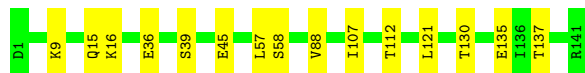
- Molecule 6: Photosystem I reaction center subunit III

Chain f:  89% 11%



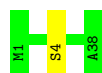
- Molecule 6: Photosystem I reaction center subunit III

Chain 6:  89% 11%



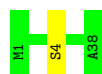
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  97% .



- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  97% .




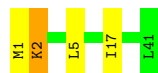
- Molecule 7: Photosystem I reaction center subunit VIII

Chain 7:  97% .




- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  90% 7% .



- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  90% 7% .




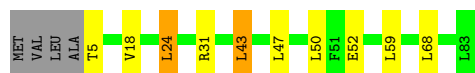
- Molecule 8: Photosystem I reaction center subunit IX

Chain 8:  90% 7% .




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  83% 10% 5% .




- Molecule 9: Photosystem I reaction center subunit PsaK

Chain k:  83% 10% • 5%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain 9:  83% 10% • 5%



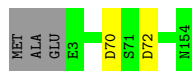
- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  97% ..



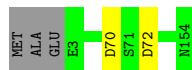
- Molecule 10: Photosystem I reaction center subunit XI

Chain l:  97% ..



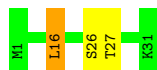
- Molecule 10: Photosystem I reaction center subunit XI

Chain 0:  97% ..



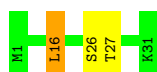
- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  90% 6% •




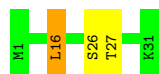
- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  90% 6% •



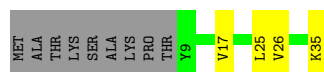
- Molecule 11: Photosystem I reaction center subunit XII

Chain y:  90% 6% .



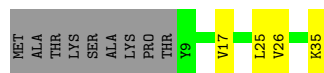
- Molecule 12: Photosystem I 4.8K protein

Chain X:  64% 11% 25%



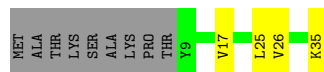
- Molecule 12: Photosystem I 4.8K protein

Chain x:  64% 11% 25%



- Molecule 12: Photosystem I 4.8K protein

Chain z:  64% 11% 25%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.44	0/6027	0.54	6/8220 (0.1%)
1	A	0.44	0/6027	0.54	6/8220 (0.1%)
1	a	0.44	0/6027	0.54	6/8220 (0.1%)
2	2	0.44	0/6112	0.51	4/8350 (0.0%)
2	B	0.44	0/6112	0.51	4/8350 (0.0%)
2	b	0.44	0/6112	0.51	4/8350 (0.0%)
3	3	0.45	0/608	0.50	0/824
3	C	0.45	0/608	0.49	0/824
3	c	0.45	0/608	0.50	0/824
4	4	0.43	0/1101	0.70	2/1492 (0.1%)
4	D	0.43	0/1101	0.70	2/1492 (0.1%)
4	d	0.43	0/1101	0.70	2/1492 (0.1%)
5	5	0.39	0/559	0.60	1/762 (0.1%)
5	E	0.39	0/559	0.60	1/762 (0.1%)
5	e	0.39	0/559	0.60	1/762 (0.1%)
6	6	0.44	0/1087	0.99	6/1476 (0.4%)
6	F	0.44	0/1087	0.99	6/1476 (0.4%)
6	f	0.44	0/1087	0.99	6/1476 (0.4%)
7	7	0.50	0/304	0.56	0/415
7	I	0.50	0/304	0.55	0/415
7	i	0.50	0/304	0.55	0/415
8	8	0.37	0/342	0.65	1/467 (0.2%)
8	J	0.37	0/342	0.65	1/467 (0.2%)
8	j	0.37	0/342	0.65	1/467 (0.2%)
9	9	0.36	0/585	1.01	7/800 (0.9%)
9	K	0.36	0/585	1.02	7/800 (0.9%)
9	k	0.36	0/585	1.02	7/800 (0.9%)
10	0	0.50	0/1153	0.49	0/1565
10	L	0.50	0/1153	0.49	0/1565
10	l	0.50	0/1153	0.49	0/1565
11	M	0.42	0/244	0.54	1/332 (0.3%)
11	m	0.42	0/244	0.54	1/332 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	y	0.42	0/244	0.54	1/332 (0.3%)
12	X	0.47	0/236	1.77	5/321 (1.6%)
12	x	0.47	0/236	1.77	5/321 (1.6%)
12	z	0.48	0/236	1.77	5/321 (1.6%)
All	All	0.44	0/55074	0.63	99/75072 (0.1%)

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
9	9	0	1
9	K	0	1
9	k	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 99 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	z	25	LEU	CA-CB-CG	17.61	155.81	115.30
12	X	25	LEU	CA-CB-CG	17.61	155.79	115.30
12	x	25	LEU	CA-CB-CG	17.60	155.77	115.30
6	f	121	LEU	CA-CB-CG	16.85	154.04	115.30
6	F	121	LEU	CA-CB-CG	16.84	154.03	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
9	9	47	LEU	Peptide
9	K	47	LEU	Peptide
9	k	47	LEU	Peptide

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
1	A	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
1	a	744/755 (98%)	684 (92%)	60 (8%)	0	100	100
2	2	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	B	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
2	b	738/741 (100%)	679 (92%)	59 (8%)	0	100	100
3	3	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	C	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
3	c	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	4	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	D	136/139 (98%)	121 (89%)	15 (11%)	0	100	100
4	d	136/139 (98%)	120 (88%)	16 (12%)	0	100	100
5	5	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	E	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
5	e	68/76 (90%)	62 (91%)	6 (9%)	0	100	100
6	6	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
6	F	139/141 (99%)	112 (81%)	27 (19%)	0	100	100
6	f	139/141 (99%)	113 (81%)	26 (19%)	0	100	100
7	7	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
8	8	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	22
8	J	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	22
8	j	39/41 (95%)	35 (90%)	3 (8%)	1 (3%)	4	22
9	9	77/83 (93%)	68 (88%)	9 (12%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	K	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
9	k	77/83 (93%)	68 (88%)	9 (12%)	0	100	100
10	0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	L	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	l	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	y	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	x	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
12	z	25/36 (69%)	23 (92%)	2 (8%)	0	100	100
All	All	6777/6951 (98%)	6181 (91%)	593 (9%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	J	2	LYS
8	j	2	LYS
8	8	2	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	594/603 (98%)	568 (96%)	26 (4%)	24	52
1	A	594/603 (98%)	568 (96%)	26 (4%)	24	52
1	a	594/603 (98%)	569 (96%)	25 (4%)	25	53
2	2	597/598 (100%)	579 (97%)	18 (3%)	36	63
2	B	597/598 (100%)	579 (97%)	18 (3%)	36	63
2	b	597/598 (100%)	579 (97%)	18 (3%)	36	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	67/68 (98%)	67 (100%)	0	100	100
3	C	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	67 (100%)	0	100	100
4	4	115/116 (99%)	110 (96%)	5 (4%)	25	53
4	D	115/116 (99%)	110 (96%)	5 (4%)	25	53
4	d	115/116 (99%)	110 (96%)	5 (4%)	25	53
5	5	60/65 (92%)	54 (90%)	6 (10%)	6	23
5	E	60/65 (92%)	54 (90%)	6 (10%)	6	23
5	e	60/65 (92%)	54 (90%)	6 (10%)	6	23
6	6	109/109 (100%)	97 (89%)	12 (11%)	5	20
6	F	109/109 (100%)	97 (89%)	12 (11%)	5	20
6	f	109/109 (100%)	97 (89%)	12 (11%)	5	20
7	7	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	I	31/31 (100%)	30 (97%)	1 (3%)	34	61
7	i	31/31 (100%)	30 (97%)	1 (3%)	34	61
8	8	35/35 (100%)	33 (94%)	2 (6%)	17	45
8	J	35/35 (100%)	33 (94%)	2 (6%)	17	45
8	j	35/35 (100%)	33 (94%)	2 (6%)	17	45
9	9	58/61 (95%)	51 (88%)	7 (12%)	4	17
9	K	58/61 (95%)	51 (88%)	7 (12%)	4	17
9	k	58/61 (95%)	51 (88%)	7 (12%)	4	17
10	0	117/120 (98%)	115 (98%)	2 (2%)	56	75
10	L	117/120 (98%)	115 (98%)	2 (2%)	56	75
10	l	117/120 (98%)	115 (98%)	2 (2%)	56	75
11	M	26/26 (100%)	23 (88%)	3 (12%)	4	19
11	m	26/26 (100%)	23 (88%)	3 (12%)	4	19
11	y	26/26 (100%)	23 (88%)	3 (12%)	4	19
12	X	21/28 (75%)	19 (90%)	2 (10%)	7	25
12	x	21/28 (75%)	19 (90%)	2 (10%)	7	25
12	z	21/28 (75%)	19 (90%)	2 (10%)	7	25
All	All	5490/5580 (98%)	5239 (95%)	251 (5%)	25	52

5 of 251 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	266	SER
5	5	67	GLU
6	f	58	SER
5	5	51	SER
8	8	17	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	642	ASN
4	4	71	GLN
10	0	75	ASN
10	L	75	ASN
9	K	23	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
7	FME	7	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	J	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)
7	FME	I	1	7	8,9,10	0.98	0	7,9,11	0.83	0
8	FME	8	1	8	8,9,10	1.02	0	7,9,11	1.37	2 (28%)
7	FME	i	1	7	8,9,10	1.00	0	7,9,11	0.82	0
8	FME	j	1	8	8,9,10	1.01	0	7,9,11	1.37	2 (28%)

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
7	FME	7	1	7	-	1/7/9/11	-
8	FME	J	1	8	-	1/7/9/11	-
7	FME	I	1	7	-	1/7/9/11	-
8	FME	8	1	8	-	1/7/9/11	-
7	FME	i	1	7	-	1/7/9/11	-
8	FME	j	1	8	-	1/7/9/11	-

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	1	FME	C-CA-N	2.57	114.36	109.73
8	8	1	FME	C-CA-N	2.56	114.36	109.73
8	J	1	FME	C-CA-N	2.56	114.34	109.73
8	j	1	FME	O-C-CA	-2.06	119.38	124.78
8	J	1	FME	O-C-CA	-2.06	119.38	124.78

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	J	1	FME	CB-CA-N-CN
8	j	1	FME	CB-CA-N-CN
8	8	1	FME	CB-CA-N-CN
7	I	1	FME	N-CA-CB-CG
7	i	1	FME	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	a	848	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	a	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.50	9 (11%)
14	CLA	A	833	-	65,73,73	1.45	10 (15%)	76,113,113	1.38	6 (7%)
14	CLA	1	1615	-	65,73,73	1.49	9 (13%)	76,113,113	1.34	7 (9%)
14	CLA	1	1625	-	65,73,73	1.52	8 (12%)	76,113,113	1.39	9 (11%)
14	CLA	1	206	21	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	2	826	21	65,73,73	1.50	9 (13%)	76,113,113	1.53	10 (13%)
14	CLA	6	201	21	58,66,73	1.58	7 (12%)	67,104,113	1.47	8 (11%)
14	CLA	2	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
14	CLA	A	835	-	65,73,73	1.44	9 (13%)	76,113,113	1.44	6 (7%)
17	BCR	1	1653	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	2	837	21	45,53,73	1.81	7 (15%)	52,89,113	1.51	5 (9%)
17	BCR	J	103	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	6 (10%)
14	CLA	a	816	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
14	CLA	b	802	21	65,73,73	1.42	7 (10%)	76,113,113	1.60	8 (10%)
14	CLA	k	101	-	46,54,73	1.74	7 (15%)	53,90,113	1.57	7 (13%)
14	CLA	1	1606	14	59,67,73	1.51	7 (11%)	68,105,113	1.54	8 (11%)
14	CLA	1	1641	-	65,73,73	1.49	9 (13%)	76,113,113	1.44	8 (10%)
15	PQN	A	845	-	34,34,34	0.39	0	42,45,45	0.35	0
14	CLA	2	825	2	65,73,73	1.46	8 (12%)	76,113,113	1.47	8 (10%)
14	CLA	1	1629	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
14	CLA	1	205	-	65,73,73	1.46	10 (15%)	76,113,113	1.53	9 (11%)
17	BCR	L	206	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
17	BCR	j	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	a	804	-	65,73,73	1.41	7 (10%)	76,113,113	1.50	7 (9%)
14	CLA	2	823	21	55,63,73	1.62	7 (12%)	64,101,113	1.46	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	PQN	1	1646	-	34,34,34	0.40	0	42,45,45	0.36	0
14	CLA	a	817	21	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	1	1603	-	65,73,73	1.44	8 (12%)	76,113,113	1.54	8 (10%)
15	PQN	2	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1627	21	65,73,73	1.45	9 (13%)	76,113,113	1.50	9 (11%)
14	CLA	a	843	21	65,73,73	1.50	9 (13%)	76,113,113	1.42	7 (9%)
17	BCR	A	850	-	41,41,41	1.33	3 (7%)	56,56,56	1.29	7 (12%)
17	BCR	k	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	0	205	10	65,73,73	1.52	9 (13%)	76,113,113	1.37	8 (10%)
13	CL0	A	801	-	65,73,73	1.45	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	f	203	-	50,58,73	1.72	5 (10%)	58,95,113	1.53	8 (13%)
17	BCR	6	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
18	LHG	B	850	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	F	204	-	50,58,73	1.72	5 (10%)	58,95,113	1.52	8 (13%)
16	SF4	A	846	2,1	0,12,12	-	-	-	-	-
17	BCR	a	851	-	41,41,41	1.27	3 (7%)	56,56,56	1.29	7 (12%)
15	PQN	B	842	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	b	839	-	65,73,73	1.47	9 (13%)	76,113,113	1.39	5 (6%)
14	CLA	B	818	-	65,73,73	1.44	8 (12%)	76,113,113	1.51	9 (11%)
14	CLA	a	813	-	45,53,73	1.77	8 (17%)	52,89,113	1.63	7 (13%)
18	LHG	y	101	-	48,48,48	0.71	2 (4%)	51,54,54	1.22	3 (5%)
18	LHG	a	853	-	48,48,48	0.74	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	b	808	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
14	CLA	L	205	21	65,73,73	1.45	10 (15%)	76,113,113	1.49	10 (13%)
14	CLA	A	843	21	65,73,73	1.49	9 (13%)	76,113,113	1.42	7 (9%)
14	CLA	b	825	2	65,73,73	1.47	7 (10%)	76,113,113	1.48	8 (10%)
14	CLA	2	831	-	55,63,73	1.60	9 (16%)	64,101,113	1.50	9 (14%)
14	CLA	a	810	1	65,73,73	1.47	7 (10%)	76,113,113	1.45	7 (9%)
14	CLA	1	1621	-	65,73,73	1.44	7 (10%)	76,113,113	1.58	9 (11%)
17	BCR	K	104	-	25,25,41	1.15	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	2	817	-	65,73,73	1.45	6 (9%)	76,113,113	1.48	8 (10%)
14	CLA	B	813	-	65,73,73	1.46	8 (12%)	76,113,113	1.44	9 (11%)
14	CLA	b	818	-	65,73,73	1.51	9 (13%)	76,113,113	1.49	9 (11%)
14	CLA	A	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.58	9 (11%)
14	CLA	a	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.47	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMG	B	849	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
17	BCR	B	845	-	41,41,41	1.26	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	857	-	36,44,73	1.96	7 (19%)	40,76,113	1.65	5 (12%)
14	CLA	b	832	-	49,57,73	1.65	7 (14%)	55,93,113	1.65	6 (10%)
14	CLA	1	1623	21	65,73,73	1.48	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	1	1607	-	65,73,73	1.45	10 (15%)	76,113,113	1.58	12 (15%)
14	CLA	8	1302	-	45,53,73	1.79	6 (13%)	52,89,113	1.58	8 (15%)
14	CLA	a	835	-	65,73,73	1.44	9 (13%)	76,113,113	1.45	7 (9%)
17	BCR	1	1652	-	41,41,41	1.27	2 (4%)	56,56,56	1.29	7 (12%)
14	CLA	a	806	-	65,73,73	1.46	10 (15%)	76,113,113	1.59	12 (15%)
14	CLA	2	805	-	65,73,73	1.50	9 (13%)	76,113,113	1.46	11 (14%)
14	CLA	b	815	-	65,73,73	1.44	8 (12%)	76,113,113	1.43	8 (10%)
17	BCR	I	101	-	41,41,41	1.28	4 (9%)	56,56,56	1.25	3 (5%)
17	BCR	b	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	B	823	-	45,53,73	1.75	7 (15%)	52,89,113	1.71	7 (13%)
14	CLA	a	838	-	65,73,73	1.42	7 (10%)	76,113,113	1.61	7 (9%)
14	CLA	1	1644	21	65,73,73	1.50	9 (13%)	76,113,113	1.42	7 (9%)
14	CLA	2	814	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	9 (11%)
14	CLA	a	805	14	59,67,73	1.51	7 (11%)	68,105,113	1.54	8 (11%)
18	LHG	m	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	j	1302	-	45,53,73	1.78	5 (11%)	52,89,113	1.59	8 (15%)
14	CLA	1	1640	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	9 (11%)
18	LHG	b	851	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	B	820	-	65,73,73	1.50	7 (10%)	76,113,113	1.33	7 (9%)
14	CLA	2	830	-	65,73,73	1.43	12 (18%)	76,113,113	1.57	10 (13%)
14	CLA	b	823	21	55,63,73	1.62	7 (12%)	64,101,113	1.48	6 (9%)
14	CLA	b	834	-	65,73,73	1.47	9 (13%)	76,113,113	1.45	7 (9%)
17	BCR	f	202	-	41,41,41	1.24	3 (7%)	56,56,56	1.26	6 (10%)
14	CLA	1	1645	18	45,53,73	1.73	7 (15%)	52,89,113	1.69	7 (13%)
14	CLA	a	814	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)
16	SF4	3	101	3	0,12,12	-	-	-	-	-
14	CLA	1	1636	-	65,73,73	1.44	9 (13%)	76,113,113	1.45	6 (7%)
14	CLA	a	832	-	60,68,73	1.52	10 (16%)	70,107,113	1.44	6 (8%)
14	CLA	A	806	-	65,73,73	1.46	10 (15%)	76,113,113	1.58	12 (15%)
14	CLA	A	838	-	65,73,73	1.41	7 (10%)	76,113,113	1.61	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	810	2	65,73,73	1.46	11 (16%)	76,113,113	1.60	9 (11%)
14	CLA	A	805	14	59,67,73	1.51	7 (11%)	68,105,113	1.55	8 (11%)
14	CLA	b	841	21	65,73,73	1.47	9 (13%)	76,113,113	1.43	10 (13%)
18	LHG	l	201	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	1	1624	-	45,53,73	1.76	7 (15%)	52,89,113	1.67	8 (15%)
17	BCR	2	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.22	4 (7%)
20	LMG	b	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	10 (15%)
14	CLA	B	815	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
14	CLA	B	811	-	65,73,73	1.44	7 (10%)	76,113,113	1.54	9 (11%)
14	CLA	b	833	-	65,73,73	1.49	8 (12%)	76,113,113	1.44	8 (10%)
14	CLA	A	811	-	49,57,73	1.70	9 (18%)	55,93,113	1.48	8 (14%)
14	CLA	b	836	21	50,58,73	1.69	9 (18%)	58,95,113	1.52	8 (13%)
14	CLA	1	1617	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
14	CLA	2	839	-	65,73,73	1.46	9 (13%)	76,113,113	1.40	6 (7%)
14	CLA	b	821	-	65,73,73	1.50	7 (10%)	76,113,113	1.34	8 (10%)
14	CLA	B	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.52	8 (10%)
14	CLA	1	1633	-	60,68,73	1.52	10 (16%)	70,107,113	1.44	6 (8%)
14	CLA	L	203	10	65,73,73	1.51	9 (13%)	76,113,113	1.38	8 (10%)
14	CLA	a	809	1	65,73,73	1.46	9 (13%)	76,113,113	1.51	9 (11%)
14	CLA	1	1604	21	65,73,73	1.54	9 (13%)	76,113,113	1.30	8 (10%)
14	CLA	2	819	-	65,73,73	1.44	8 (12%)	76,113,113	1.52	10 (13%)
13	CL0	1	1602	-	65,73,73	1.45	10 (15%)	76,113,113	1.47	8 (10%)
17	BCR	0	209	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	b	807	-	65,73,73	1.47	9 (13%)	76,113,113	1.41	8 (10%)
14	CLA	a	830	-	65,73,73	1.41	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	a	841	-	65,73,73	1.46	8 (12%)	76,113,113	1.46	8 (10%)
14	CLA	2	840	-	47,55,73	1.80	9 (19%)	54,91,113	1.48	8 (14%)
14	CLA	2	804	-	65,73,73	1.42	10 (15%)	76,113,113	1.50	8 (10%)
14	CLA	a	828	-	65,73,73	1.47	7 (10%)	76,113,113	1.38	8 (10%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	1	1642	-	65,73,73	1.46	8 (12%)	76,113,113	1.46	8 (10%)
14	CLA	1	1626	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	9 (11%)
17	BCR	F	205	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
17	BCR	l	207	-	41,41,41	1.21	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	b	810	2	65,73,73	1.46	11 (16%)	76,113,113	1.61	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	1635	-	65,73,73	1.45	8 (12%)	76,113,113	1.59	12 (15%)
17	BCR	2	848	-	41,41,41	1.28	3 (7%)	56,56,56	1.31	8 (14%)
17	BCR	1	1651	-	41,41,41	1.35	4 (9%)	56,56,56	1.28	7 (12%)
14	CLA	2	841	21	65,73,73	1.47	9 (13%)	76,113,113	1.43	10 (13%)
14	CLA	X	1701	12	45,53,73	1.81	6 (13%)	52,89,113	1.60	6 (11%)
14	CLA	b	824	-	45,53,73	1.74	7 (15%)	52,89,113	1.71	7 (13%)
17	BCR	b	847	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	8 (14%)
14	CLA	1	1638	1	45,53,73	1.78	7 (15%)	52,89,113	1.53	8 (15%)
17	BCR	A	852	-	25,25,41	1.13	1 (4%)	33,33,56	1.28	4 (12%)
14	CLA	A	842	-	65,73,73	1.47	9 (13%)	76,113,113	1.50	9 (11%)
14	CLA	2	836	21	50,58,73	1.70	9 (18%)	58,95,113	1.53	8 (13%)
18	LHG	A	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.22	4 (9%)
17	BCR	B	844	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	2	821	-	65,73,73	1.49	7 (10%)	76,113,113	1.32	7 (9%)
17	BCR	A	848	-	41,41,41	1.18	3 (7%)	56,56,56	1.23	6 (10%)
18	LHG	0	202	-	38,38,48	0.73	1 (2%)	41,44,54	1.26	3 (7%)
17	BCR	b	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
16	SF4	3	102	3	0,12,12	-	-	-	-	-
14	CLA	b	820	21	65,73,73	1.54	7 (10%)	76,113,113	1.35	9 (11%)
17	BCR	a	849	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	B	835	21	50,58,73	1.70	9 (18%)	58,95,113	1.53	8 (13%)
14	CLA	a	808	-	51,59,73	1.66	9 (17%)	59,96,113	1.53	8 (13%)
14	CLA	a	825	-	65,73,73	1.46	8 (12%)	76,113,113	1.45	8 (10%)
14	CLA	B	819	21	65,73,73	1.55	8 (12%)	76,113,113	1.35	9 (11%)
14	CLA	A	819	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	9 (11%)
14	CLA	a	823	-	45,53,73	1.75	6 (13%)	52,89,113	1.68	8 (15%)
14	CLA	8	1301	21	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	A	837	1	45,53,73	1.79	7 (15%)	52,89,113	1.54	8 (15%)
14	CLA	b	831	-	55,63,73	1.60	9 (16%)	64,101,113	1.49	9 (14%)
14	CLA	2	812	-	65,73,73	1.44	7 (10%)	76,113,113	1.55	9 (11%)
14	CLA	B	808	-	65,73,73	1.43	8 (12%)	76,113,113	1.54	10 (13%)
14	CLA	B	804	-	65,73,73	1.49	9 (13%)	76,113,113	1.46	11 (14%)
14	CLA	b	827	-	65,73,73	1.48	8 (12%)	76,113,113	1.43	8 (10%)
14	CLA	M	102	-	36,44,73	1.96	7 (19%)	40,76,113	1.64	5 (12%)
14	CLA	A	804	-	65,73,73	1.42	7 (10%)	76,113,113	1.50	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	802	-	65,73,73	1.45	8 (12%)	76,113,113	1.54	8 (10%)
15	PQN	b	843	-	34,34,34	0.45	0	42,45,45	0.38	0
14	CLA	1	1639	-	65,73,73	1.42	8 (12%)	76,113,113	1.61	7 (9%)
14	CLA	A	831	-	65,73,73	1.51	11 (16%)	76,113,113	1.49	9 (11%)
17	BCR	8	1306	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
17	BCR	l	202	-	41,41,41	1.39	4 (9%)	56,56,56	1.32	7 (12%)
17	BCR	m	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	A	818	-	65,73,73	1.46	6 (9%)	76,113,113	1.44	7 (9%)
14	CLA	1	1628	21	65,73,73	1.46	9 (13%)	76,113,113	1.52	10 (13%)
14	CLA	F	201	21	58,66,73	1.59	7 (12%)	67,104,113	1.47	8 (11%)
14	CLA	a	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.52	7 (9%)
14	CLA	A	826	21	65,73,73	1.46	9 (13%)	76,113,113	1.49	9 (11%)
14	CLA	2	838	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	7 (10%)
14	CLA	B	836	21	45,53,73	1.82	7 (15%)	52,89,113	1.52	5 (9%)
14	CLA	a	827	21	65,73,73	1.45	9 (13%)	76,113,113	1.52	10 (13%)
14	CLA	2	803	-	65,73,73	1.45	10 (15%)	76,113,113	1.45	8 (10%)
14	CLA	A	810	1	65,73,73	1.47	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	a	826	21	65,73,73	1.46	9 (13%)	76,113,113	1.50	9 (11%)
14	CLA	x	1701	12	45,53,73	1.79	6 (13%)	52,89,113	1.61	6 (11%)
17	BCR	0	201	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	2	824	-	45,53,73	1.75	7 (15%)	52,89,113	1.71	7 (13%)
17	BCR	1	1649	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	6 (10%)
17	BCR	0	208	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	7 (12%)
14	CLA	1	1605	-	65,73,73	1.42	7 (10%)	76,113,113	1.49	7 (9%)
14	CLA	B	827	-	65,73,73	1.50	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	A	809	1	65,73,73	1.45	8 (12%)	76,113,113	1.51	8 (10%)
14	CLA	B	829	-	65,73,73	1.44	12 (18%)	76,113,113	1.57	10 (13%)
17	BCR	a	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.29	7 (12%)
14	CLA	A	825	-	65,73,73	1.46	9 (13%)	76,113,113	1.47	9 (11%)
14	CLA	A	829	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	9	103	21	58,66,73	1.56	7 (12%)	67,104,113	1.50	9 (13%)
14	CLA	b	803	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	8 (10%)
14	CLA	2	833	-	65,73,73	1.49	8 (12%)	76,113,113	1.44	8 (10%)
14	CLA	2	827	-	65,73,73	1.48	8 (12%)	76,113,113	1.42	8 (10%)
14	CLA	a	834	-	65,73,73	1.45	7 (10%)	76,113,113	1.59	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	a	852	-	25,25,41	1.12	1 (4%)	33,33,56	1.29	4 (12%)
18	LHG	M	101	-	48,48,48	0.70	2 (4%)	51,54,54	1.22	3 (5%)
14	CLA	b	822	-	45,53,73	1.73	7 (15%)	52,89,113	1.78	9 (17%)
14	CLA	2	818	-	65,73,73	1.50	9 (13%)	76,113,113	1.49	9 (11%)
14	CLA	B	839	-	47,55,73	1.80	9 (19%)	54,91,113	1.48	8 (14%)
17	BCR	A	856	-	41,41,41	1.23	3 (7%)	56,56,56	1.28	8 (14%)
14	CLA	a	836	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
17	BCR	b	844	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
16	SF4	c	101	3	0,12,12	-	-	-	-	-
17	BCR	B	843	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	2	822	-	45,53,73	1.72	7 (15%)	52,89,113	1.78	9 (17%)
14	CLA	K	103	21	58,66,73	1.56	7 (12%)	67,104,113	1.50	9 (13%)
14	CLA	B	810	2	65,73,73	1.44	9 (13%)	76,113,113	1.52	9 (11%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
17	BCR	F	202	-	41,41,41	1.25	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	b	811	2	65,73,73	1.44	9 (13%)	76,113,113	1.52	8 (10%)
14	CLA	A	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	8 (10%)
14	CLA	a	815	-	65,73,73	1.50	7 (10%)	76,113,113	1.40	7 (9%)
14	CLA	A	844	18	45,53,73	1.72	7 (15%)	52,89,113	1.69	7 (13%)
14	CLA	b	835	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	9 (11%)
14	CLA	B	816	-	65,73,73	1.44	6 (9%)	76,113,113	1.48	8 (10%)
14	CLA	2	809	-	65,73,73	1.44	8 (12%)	76,113,113	1.54	10 (13%)
14	CLA	a	803	21	65,73,73	1.54	9 (13%)	76,113,113	1.29	6 (7%)
14	CLA	2	807	-	65,73,73	1.48	9 (13%)	76,113,113	1.40	8 (10%)
14	CLA	B	837	-	60,68,73	1.56	9 (15%)	70,107,113	1.46	7 (10%)
14	CLA	1	1632	-	65,73,73	1.51	9 (13%)	76,113,113	1.50	9 (11%)
14	CLA	a	822	21	65,73,73	1.47	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	z	102	12	45,53,73	1.80	6 (13%)	52,89,113	1.61	6 (11%)
14	CLA	1	1611	1	65,73,73	1.47	7 (10%)	76,113,113	1.44	7 (9%)
14	CLA	b	805	-	65,73,73	1.49	9 (13%)	76,113,113	1.46	12 (15%)
14	CLA	B	838	-	65,73,73	1.47	9 (13%)	76,113,113	1.40	6 (7%)
14	CLA	A	814	-	65,73,73	1.49	9 (13%)	76,113,113	1.33	8 (10%)
14	CLA	f	201	21	58,66,73	1.58	7 (12%)	67,104,113	1.47	8 (11%)
14	CLA	1	1643	-	65,73,73	1.47	8 (12%)	76,113,113	1.50	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	M	103	-	41,41,41	1.23	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	B	805	-	65,73,73	1.44	7 (10%)	76,113,113	1.57	8 (10%)
14	CLA	a	807	-	65,73,73	1.44	8 (12%)	76,113,113	1.53	5 (6%)
14	CLA	B	822	21	55,63,73	1.63	7 (12%)	64,101,113	1.47	6 (9%)
17	BCR	a	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	a	833	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	6 (7%)
14	CLA	B	807	-	65,73,73	1.48	9 (13%)	76,113,113	1.43	10 (13%)
14	CLA	2	808	-	65,73,73	1.48	9 (13%)	76,113,113	1.43	9 (11%)
14	CLA	B	814	-	65,73,73	1.44	7 (10%)	76,113,113	1.44	8 (10%)
14	CLA	B	809	2	65,73,73	1.45	10 (15%)	76,113,113	1.61	10 (13%)
14	CLA	B	833	-	65,73,73	1.48	9 (13%)	76,113,113	1.45	7 (9%)
17	BCR	B	851	-	41,41,41	1.21	2 (4%)	56,56,56	1.34	9 (16%)
17	BCR	f	204	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	B	830	-	55,63,73	1.60	9 (16%)	64,101,113	1.50	9 (14%)
16	SF4	1	1647	2,1	0,12,12	-	-	-	-	-
14	CLA	b	819	-	65,73,73	1.43	7 (10%)	76,113,113	1.51	9 (11%)
14	CLA	b	809	-	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	B	806	-	65,73,73	1.48	9 (13%)	76,113,113	1.40	8 (10%)
17	BCR	1	1648	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	8	1303	-	38,45,73	1.91	8 (21%)	43,78,113	1.68	7 (16%)
14	CLA	A	830	-	65,73,73	1.41	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	1	1613	14	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
14	CLA	2	815	-	65,73,73	1.45	8 (12%)	76,113,113	1.44	8 (10%)
14	CLA	A	839	-	65,73,73	1.44	9 (13%)	76,113,113	1.47	9 (11%)
14	CLA	1	1612	-	49,57,73	1.71	9 (18%)	55,93,113	1.49	8 (14%)
14	CLA	A	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.51	7 (9%)
14	CLA	A	840	-	65,73,73	1.49	9 (13%)	76,113,113	1.43	8 (10%)
14	CLA	1	1622	-	65,73,73	1.45	6 (9%)	76,113,113	1.52	7 (9%)
14	CLA	F	203	21	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	b	830	-	65,73,73	1.44	12 (18%)	76,113,113	1.57	10 (13%)
14	CLA	A	808	-	51,59,73	1.66	8 (15%)	59,96,113	1.54	8 (13%)
14	CLA	0	207	21	65,73,73	1.45	10 (15%)	76,113,113	1.50	9 (11%)
17	BCR	9	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.32	7 (12%)
13	CL0	a	801	-	65,73,73	1.44	10 (15%)	76,113,113	1.46	8 (10%)
14	CLA	B	828	-	65,73,73	1.51	8 (12%)	76,113,113	1.30	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	1610	1	65,73,73	1.46	8 (12%)	76,113,113	1.51	9 (11%)
17	BCR	2	845	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	a	824	-	65,73,73	1.52	8 (12%)	76,113,113	1.39	9 (11%)
14	CLA	2	816	-	65,73,73	1.46	7 (10%)	76,113,113	1.39	7 (9%)
14	CLA	A	816	-	65,73,73	1.47	6 (9%)	76,113,113	1.39	7 (9%)
17	BCR	j	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.19	7 (12%)
14	CLA	2	802	21	65,73,73	1.42	8 (12%)	76,113,113	1.60	8 (10%)
17	BCR	L	201	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	A	832	-	60,68,73	1.53	10 (16%)	70,107,113	1.43	6 (8%)
15	PQN	a	845	-	34,34,34	0.40	0	42,45,45	0.35	0
17	BCR	B	846	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	A	803	21	65,73,73	1.54	9 (13%)	76,113,113	1.30	8 (10%)
17	BCR	A	851	-	41,41,41	1.27	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	b	813	-	45,53,73	1.80	8 (17%)	52,89,113	1.62	7 (13%)
17	BCR	8	1305	-	41,41,41	1.22	2 (4%)	56,56,56	1.28	8 (14%)
14	CLA	k	103	21	58,66,73	1.57	7 (12%)	67,104,113	1.50	9 (13%)
14	CLA	2	806	-	65,73,73	1.44	7 (10%)	76,113,113	1.58	8 (10%)
14	CLA	L	204	-	65,73,73	1.46	10 (15%)	76,113,113	1.53	9 (11%)
14	CLA	1	1637	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
17	BCR	8	1304	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	7 (12%)
14	CLA	2	813	-	45,53,73	1.80	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	B	840	21	65,73,73	1.47	9 (13%)	76,113,113	1.43	10 (13%)
17	BCR	B	848	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	J	102	-	38,45,73	1.92	8 (21%)	43,78,113	1.68	7 (16%)
14	CLA	B	817	-	65,73,73	1.52	9 (13%)	76,113,113	1.49	9 (11%)
14	CLA	1	1608	-	65,73,73	1.43	7 (10%)	76,113,113	1.53	5 (6%)
17	BCR	i	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
17	BCR	b	846	-	41,41,41	1.25	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	A	817	21	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	1	1614	-	45,53,73	1.78	8 (17%)	52,89,113	1.64	8 (15%)
14	CLA	1	1619	-	65,73,73	1.45	6 (9%)	76,113,113	1.45	7 (9%)
14	CLA	b	812	-	65,73,73	1.45	7 (10%)	76,113,113	1.54	10 (13%)
14	CLA	b	840	-	47,55,73	1.79	9 (19%)	54,91,113	1.48	7 (12%)
14	CLA	A	834	-	65,73,73	1.45	7 (10%)	76,113,113	1.58	13 (17%)
14	CLA	A	802	-	65,73,73	1.45	8 (12%)	76,113,113	1.54	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LHG	a	854	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
17	BCR	b	852	-	41,41,41	1.21	2 (4%)	56,56,56	1.33	9 (16%)
14	CLA	K	101	-	46,54,73	1.74	7 (15%)	53,90,113	1.57	7 (13%)
17	BCR	b	848	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)
14	CLA	a	839	-	65,73,73	1.45	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	b	842	-	65,73,73	1.48	9 (13%)	76,113,113	1.47	7 (9%)
14	CLA	2	829	-	65,73,73	1.51	8 (12%)	76,113,113	1.30	7 (9%)
14	CLA	1	1609	-	51,59,73	1.66	9 (17%)	59,96,113	1.55	8 (13%)
14	CLA	1	1618	21	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
14	CLA	A	823	-	45,53,73	1.75	6 (13%)	52,89,113	1.67	8 (15%)
14	CLA	1	1616	-	65,73,73	1.50	8 (12%)	76,113,113	1.40	7 (9%)
14	CLA	A	841	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	8 (10%)
14	CLA	a	831	-	65,73,73	1.51	10 (15%)	76,113,113	1.49	9 (11%)
14	CLA	b	816	-	65,73,73	1.45	7 (10%)	76,113,113	1.39	7 (9%)
14	CLA	l	204	10	65,73,73	1.52	9 (13%)	76,113,113	1.38	8 (10%)
20	LMG	2	850	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	A	824	-	65,73,73	1.52	8 (12%)	76,113,113	1.38	9 (11%)
14	CLA	A	815	-	65,73,73	1.50	8 (12%)	76,113,113	1.40	7 (9%)
14	CLA	B	825	21	65,73,73	1.51	9 (13%)	76,113,113	1.53	10 (13%)
17	BCR	y	102	-	41,41,41	1.24	3 (7%)	56,56,56	1.22	5 (8%)
18	LHG	A	853	-	48,48,48	0.75	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	2	828	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	1	1631	-	65,73,73	1.41	9 (13%)	76,113,113	1.54	6 (7%)
18	LHG	1	1654	-	48,48,48	0.75	1 (2%)	51,54,54	1.23	4 (7%)
14	CLA	A	836	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	7 (9%)
18	LHG	L	208	-	38,38,48	0.73	0	41,44,54	1.26	3 (7%)
14	CLA	J	101	-	45,53,73	1.78	5 (11%)	52,89,113	1.58	8 (15%)
14	CLA	B	821	-	45,53,73	1.73	7 (15%)	52,89,113	1.78	9 (17%)
14	CLA	1	1620	-	65,73,73	1.50	8 (12%)	76,113,113	1.47	9 (11%)
14	CLA	a	812	14	65,73,73	1.47	7 (10%)	76,113,113	1.36	6 (7%)
14	CLA	2	811	2	65,73,73	1.45	9 (13%)	76,113,113	1.51	9 (11%)
14	CLA	b	837	21	45,53,73	1.82	7 (15%)	52,89,113	1.53	5 (9%)
14	CLA	a	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.58	9 (11%)
17	BCR	A	849	-	41,41,41	1.23	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	j	1301	21	45,53,73	1.77	7 (15%)	52,89,113	1.68	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	802	-	65,73,73	1.43	10 (15%)	76,113,113	1.44	8 (10%)
14	CLA	1	1634	-	65,73,73	1.45	10 (15%)	76,113,113	1.39	6 (7%)
14	CLA	A	827	21	65,73,73	1.46	10 (15%)	76,113,113	1.53	10 (13%)
14	CLA	1	1630	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	b	804	-	65,73,73	1.43	11 (16%)	76,113,113	1.51	8 (10%)
14	CLA	B	826	-	65,73,73	1.48	8 (12%)	76,113,113	1.43	8 (10%)
14	CLA	A	807	-	65,73,73	1.44	8 (12%)	76,113,113	1.53	6 (7%)
14	CLA	2	832	-	49,57,73	1.65	7 (14%)	55,93,113	1.65	6 (10%)
14	CLA	a	811	-	49,57,73	1.70	8 (16%)	55,93,113	1.49	8 (14%)
17	BCR	6	204	-	41,41,41	1.18	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	1	1601	-	36,44,73	1.95	7 (19%)	40,76,113	1.64	5 (12%)
16	SF4	a	846	2,1	0,12,12	-	-	-	-	-
18	LHG	1	1655	14	40,40,48	0.77	1 (2%)	43,46,54	1.21	4 (9%)
14	CLA	a	818	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
14	CLA	B	812	-	45,53,73	1.78	8 (17%)	52,89,113	1.62	7 (13%)
14	CLA	2	820	21	65,73,73	1.55	8 (12%)	76,113,113	1.35	9 (11%)
17	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.25	7 (12%)
17	BCR	9	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	A	812	14	65,73,73	1.46	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	2	842	-	65,73,73	1.48	9 (13%)	76,113,113	1.47	7 (9%)
14	CLA	b	806	-	65,73,73	1.44	7 (10%)	76,113,113	1.57	8 (10%)
14	CLA	b	814	-	65,73,73	1.45	8 (12%)	76,113,113	1.45	9 (11%)
17	BCR	K	102	-	41,41,41	1.18	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	B	832	-	65,73,73	1.50	8 (12%)	76,113,113	1.44	8 (10%)
14	CLA	a	837	1	45,53,73	1.79	7 (15%)	52,89,113	1.54	8 (15%)
14	CLA	b	826	21	65,73,73	1.51	9 (13%)	76,113,113	1.53	10 (13%)
17	BCR	L	207	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	0	206	-	65,73,73	1.45	10 (15%)	76,113,113	1.52	9 (11%)
14	CLA	b	838	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	7 (10%)
14	CLA	B	831	-	49,57,73	1.66	7 (14%)	55,93,113	1.66	7 (12%)
17	BCR	2	849	-	41,41,41	1.39	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	2	834	-	65,73,73	1.47	9 (13%)	76,113,113	1.45	7 (9%)
14	CLA	9	101	-	46,54,73	1.73	7 (15%)	53,90,113	1.58	7 (13%)
17	BCR	A	847	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	7 (12%)
14	CLA	b	829	-	65,73,73	1.51	8 (12%)	76,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	817	-	65,73,73	1.45	6 (9%)	76,113,113	1.47	8 (10%)
17	BCR	7	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.24	3 (5%)
14	CLA	A	813	-	45,53,73	1.78	8 (17%)	52,89,113	1.63	8 (15%)
14	CLA	B	834	-	65,73,73	1.47	6 (9%)	76,113,113	1.45	9 (11%)
17	BCR	2	846	-	41,41,41	1.26	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	A	822	21	65,73,73	1.47	7 (10%)	76,113,113	1.46	7 (9%)
17	BCR	k	104	-	25,25,41	1.14	1 (4%)	33,33,56	1.15	4 (12%)
14	CLA	B	824	2	65,73,73	1.46	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	6	203	-	50,58,73	1.72	5 (10%)	58,95,113	1.52	8 (13%)
18	LHG	z	101	-	48,48,48	0.61	1 (2%)	51,54,54	1.20	5 (9%)
14	CLA	B	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.47	7 (9%)
14	CLA	b	828	-	65,73,73	1.50	8 (12%)	76,113,113	1.43	7 (9%)
14	CLA	j	1303	-	38,45,73	1.92	8 (21%)	43,78,113	1.67	7 (16%)
17	BCR	0	203	-	41,41,41	1.39	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	a	819	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	10 (13%)
17	BCR	1	1650	-	41,41,41	1.22	2 (4%)	56,56,56	1.20	6 (10%)
14	CLA	a	840	-	65,73,73	1.49	9 (13%)	76,113,113	1.44	8 (10%)
14	CLA	A	855	21	65,73,73	1.43	7 (10%)	76,113,113	1.61	8 (10%)
14	CLA	a	844	18	45,53,73	1.73	7 (15%)	52,89,113	1.70	7 (13%)
17	BCR	B	847	-	41,41,41	1.27	3 (7%)	56,56,56	1.31	9 (16%)

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
17	BCR	a	848	-	-	15/29/63/63	0/2/2/2
14	CLA	a	842	-	1/1/15/20	12/37/115/115	-
14	CLA	A	833	-	1/1/15/20	12/37/115/115	-
14	CLA	1	1615	-	1/1/15/20	15/37/115/115	-
14	CLA	1	1625	-	1/1/15/20	12/37/115/115	-
14	CLA	l	206	21	1/1/15/20	11/37/115/115	-
14	CLA	2	826	21	1/1/15/20	11/37/115/115	-
14	CLA	6	201	21	1/1/13/20	6/29/107/115	-
14	CLA	2	835	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	835	-	1/1/15/20	8/37/115/115	-
17	BCR	1	1653	-	-	11/18/35/63	0/1/1/2
14	CLA	2	837	21	1/1/11/20	3/13/91/115	-
17	BCR	J	103	-	-	11/29/63/63	0/2/2/2
14	CLA	a	816	-	1/1/15/20	19/37/115/115	-
14	CLA	b	802	21	1/1/15/20	18/37/115/115	-
14	CLA	k	101	-	1/1/11/20	10/15/93/115	-
14	CLA	1	1606	14	1/1/13/20	10/30/108/115	-
14	CLA	1	1641	-	1/1/15/20	17/37/115/115	-
15	PQN	A	845	-	-	1/23/43/43	0/2/2/2
14	CLA	2	825	2	1/1/15/20	14/37/115/115	-
14	CLA	1	1629	-	1/1/15/20	7/37/115/115	-
14	CLA	l	205	-	1/1/15/20	11/37/115/115	-
17	BCR	L	206	-	-	10/29/63/63	0/2/2/2
17	BCR	j	1305	-	-	13/29/63/63	0/2/2/2
14	CLA	a	804	-	1/1/15/20	16/37/115/115	-
14	CLA	2	823	21	1/1/13/20	5/25/103/115	-
15	PQN	1	1646	-	-	1/23/43/43	0/2/2/2
14	CLA	a	817	21	1/1/15/20	12/37/115/115	-
14	CLA	1	1603	-	1/1/15/20	15/37/115/115	-
15	PQN	2	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1627	21	1/1/15/20	13/37/115/115	-
14	CLA	a	843	21	1/1/15/20	16/37/115/115	-
17	BCR	A	850	-	-	8/29/63/63	0/2/2/2
17	BCR	k	102	-	-	6/29/63/63	0/2/2/2
14	CLA	0	205	10	1/1/15/20	17/37/115/115	-
13	CL0	A	801	-	3/3/20/25	10/37/135/135	-
14	CLA	f	203	-	1/1/12/20	6/19/97/115	-
17	BCR	6	202	-	-	12/29/63/63	0/2/2/2
18	LHG	B	850	-	-	18/53/53/53	-
14	CLA	F	204	-	1/1/12/20	6/19/97/115	-
16	SF4	A	846	2,1	-	-	0/6/5/5
17	BCR	a	851	-	-	18/29/63/63	0/2/2/2
15	PQN	B	842	-	-	1/23/43/43	0/2/2/2
14	CLA	b	839	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	818	-	1/1/15/20	17/37/115/115	-
14	CLA	a	813	-	1/1/11/20	4/13/91/115	-
18	LHG	y	101	-	-	27/53/53/53	-
18	LHG	a	853	-	-	21/53/53/53	-
14	CLA	b	808	-	1/1/15/20	6/37/115/115	-
14	CLA	L	205	21	1/1/15/20	11/37/115/115	-
14	CLA	A	843	21	1/1/15/20	16/37/115/115	-
14	CLA	b	825	2	1/1/15/20	14/37/115/115	-
14	CLA	2	831	-	1/1/13/20	13/25/103/115	-
14	CLA	a	810	1	1/1/15/20	12/37/115/115	-
14	CLA	1	1621	-	1/1/15/20	10/37/115/115	-
17	BCR	K	104	-	-	4/18/35/63	0/1/1/2
14	CLA	2	817	-	1/1/15/20	12/37/115/115	-
14	CLA	B	813	-	1/1/15/20	16/37/115/115	-
14	CLA	b	818	-	1/1/15/20	13/37/115/115	-
14	CLA	A	820	-	1/1/15/20	10/37/115/115	-
14	CLA	a	829	-	1/1/15/20	14/37/115/115	-
20	LMG	B	849	-	-	27/50/70/70	0/1/1/1
17	BCR	B	845	-	-	11/29/63/63	0/2/2/2
14	CLA	A	857	-	1/1/7/20	0/2/72/115	-
14	CLA	b	832	-	1/1/11/20	10/18/96/115	-
14	CLA	1	1623	21	1/1/15/20	12/37/115/115	-
14	CLA	1	1607	-	1/1/15/20	21/37/115/115	-
14	CLA	8	1302	-	1/1/11/20	5/13/91/115	-
14	CLA	a	835	-	1/1/15/20	8/37/115/115	-
17	BCR	1	1652	-	-	18/29/63/63	0/2/2/2
14	CLA	a	806	-	1/1/15/20	21/37/115/115	-
14	CLA	2	805	-	1/1/15/20	17/37/115/115	-
14	CLA	b	815	-	1/1/15/20	13/37/115/115	-
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
17	BCR	b	845	-	-	8/29/63/63	0/2/2/2
14	CLA	B	823	-	1/1/11/20	5/13/91/115	-
14	CLA	a	838	-	1/1/15/20	16/37/115/115	-
14	CLA	1	1644	21	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	814	-	1/1/15/20	16/37/115/115	-
14	CLA	a	805	14	1/1/13/20	10/30/108/115	-
18	LHG	m	101	-	-	27/53/53/53	-
14	CLA	j	1302	-	1/1/11/20	5/13/91/115	-
14	CLA	1	1640	-	1/1/15/20	20/37/115/115	-
18	LHG	b	851	-	-	18/53/53/53	-
14	CLA	B	820	-	1/1/15/20	19/37/115/115	-
14	CLA	2	830	-	1/1/15/20	7/37/115/115	-
14	CLA	b	823	21	1/1/13/20	5/25/103/115	-
14	CLA	b	834	-	1/1/15/20	11/37/115/115	-
17	BCR	f	202	-	-	12/29/63/63	0/2/2/2
14	CLA	1	1645	18	1/1/11/20	5/13/91/115	-
14	CLA	a	814	-	1/1/15/20	15/37/115/115	-
14	CLA	1	1636	-	1/1/15/20	8/37/115/115	-
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	a	832	-	1/1/14/20	6/31/109/115	-
14	CLA	A	806	-	1/1/15/20	21/37/115/115	-
14	CLA	A	838	-	1/1/15/20	16/37/115/115	-
14	CLA	2	810	2	1/1/15/20	11/37/115/115	-
14	CLA	A	805	14	1/1/13/20	10/30/108/115	-
14	CLA	b	841	21	1/1/15/20	7/37/115/115	-
18	LHG	l	201	-	-	27/43/43/53	-
14	CLA	1	1624	-	1/1/11/20	8/13/91/115	-
17	BCR	2	844	-	-	11/29/63/63	0/2/2/2
20	LMG	b	850	-	-	27/50/70/70	0/1/1/1
14	CLA	B	815	-	1/1/15/20	13/37/115/115	-
14	CLA	B	811	-	1/1/15/20	10/37/115/115	-
14	CLA	b	833	-	1/1/15/20	16/37/115/115	-
14	CLA	A	811	-	1/1/11/20	8/18/96/115	-
14	CLA	b	836	21	1/1/12/20	9/19/97/115	-
14	CLA	1	1617	-	1/1/15/20	19/37/115/115	-
14	CLA	2	839	-	1/1/15/20	9/37/115/115	-
14	CLA	b	821	-	1/1/15/20	19/37/115/115	-
14	CLA	B	803	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	1633	-	1/1/14/20	6/31/109/115	-
14	CLA	L	203	10	1/1/15/20	17/37/115/115	-
14	CLA	a	809	1	1/1/15/20	11/37/115/115	-
14	CLA	1	1604	21	1/1/15/20	6/37/115/115	-
14	CLA	2	819	-	1/1/15/20	17/37/115/115	-
13	CL0	1	1602	-	3/3/20/25	10/37/135/135	-
17	BCR	0	209	-	-	5/29/63/63	0/2/2/2
14	CLA	b	807	-	1/1/15/20	9/37/115/115	-
14	CLA	a	830	-	1/1/15/20	15/37/115/115	-
14	CLA	a	841	-	1/1/15/20	14/37/115/115	-
14	CLA	2	840	-	-	2/16/94/115	-
14	CLA	2	804	-	1/1/15/20	12/37/115/115	-
14	CLA	a	828	-	1/1/15/20	7/37/115/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	1	1642	-	1/1/15/20	14/37/115/115	-
14	CLA	1	1626	-	1/1/15/20	12/37/115/115	-
17	BCR	F	205	-	-	8/29/63/63	0/2/2/2
17	BCR	l	207	-	-	10/29/63/63	0/2/2/2
14	CLA	b	810	2	1/1/15/20	11/37/115/115	-
14	CLA	1	1635	-	1/1/15/20	10/37/115/115	-
17	BCR	2	848	-	-	11/29/63/63	0/2/2/2
17	BCR	1	1651	-	-	8/29/63/63	0/2/2/2
14	CLA	2	841	21	1/1/15/20	7/37/115/115	-
14	CLA	X	1701	12	1/1/11/20	7/13/91/115	-
14	CLA	b	824	-	1/1/11/20	5/13/91/115	-
17	BCR	b	847	-	-	12/29/63/63	0/2/2/2
14	CLA	1	1638	1	1/1/11/20	5/13/91/115	-
17	BCR	A	852	-	-	11/18/35/63	0/1/1/2
14	CLA	A	842	-	1/1/15/20	12/37/115/115	-
14	CLA	2	836	21	1/1/12/20	9/19/97/115	-
18	LHG	A	854	14	-	13/45/45/53	-
17	BCR	B	844	-	-	8/29/63/63	0/2/2/2
14	CLA	2	821	-	1/1/15/20	19/37/115/115	-
17	BCR	A	848	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	0	202	-	-	27/43/43/53	-
17	BCR	b	849	-	-	5/29/63/63	0/2/2/2
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	b	820	21	1/1/15/20	15/37/115/115	-
17	BCR	a	849	-	-	5/29/63/63	0/2/2/2
14	CLA	B	835	21	1/1/12/20	9/19/97/115	-
14	CLA	a	808	-	1/1/12/20	4/21/99/115	-
14	CLA	a	825	-	1/1/15/20	12/37/115/115	-
14	CLA	B	819	21	1/1/15/20	15/37/115/115	-
14	CLA	A	819	-	1/1/15/20	17/37/115/115	-
14	CLA	a	823	-	1/1/11/20	8/13/91/115	-
14	CLA	8	1301	21	1/1/11/20	2/13/91/115	-
14	CLA	A	837	1	1/1/11/20	5/13/91/115	-
14	CLA	b	831	-	1/1/13/20	13/25/103/115	-
14	CLA	2	812	-	1/1/15/20	10/37/115/115	-
14	CLA	B	808	-	1/1/15/20	8/37/115/115	-
14	CLA	B	804	-	1/1/15/20	17/37/115/115	-
14	CLA	b	827	-	1/1/15/20	6/37/115/115	-
14	CLA	M	102	-	1/1/7/20	0/2/72/115	-
14	CLA	A	804	-	1/1/15/20	16/37/115/115	-
14	CLA	a	802	-	1/1/15/20	15/37/115/115	-
15	PQN	b	843	-	-	1/23/43/43	0/2/2/2
14	CLA	1	1639	-	1/1/15/20	16/37/115/115	-
14	CLA	A	831	-	1/1/15/20	7/37/115/115	-
17	BCR	8	1306	-	-	15/29/63/63	0/2/2/2
17	BCR	l	202	-	-	8/29/63/63	0/2/2/2
17	BCR	m	102	-	-	9/29/63/63	0/2/2/2
14	CLA	A	818	-	1/1/15/20	10/37/115/115	-
14	CLA	1	1628	21	1/1/15/20	9/37/115/115	-
14	CLA	F	201	21	1/1/13/20	6/29/107/115	-
14	CLA	a	821	-	1/1/15/20	16/37/115/115	-
14	CLA	A	826	21	1/1/15/20	13/37/115/115	-
14	CLA	2	838	-	1/1/14/20	5/31/109/115	-
14	CLA	B	836	21	1/1/11/20	3/13/91/115	-
14	CLA	a	827	21	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	803	-	1/1/15/20	18/37/115/115	-
14	CLA	A	810	1	1/1/15/20	12/37/115/115	-
14	CLA	a	826	21	1/1/15/20	13/37/115/115	-
14	CLA	x	1701	12	1/1/11/20	7/13/91/115	-
17	BCR	0	201	-	-	5/29/63/63	0/2/2/2
14	CLA	2	824	-	1/1/11/20	5/13/91/115	-
17	BCR	1	1649	-	-	15/29/63/63	0/2/2/2
17	BCR	0	208	-	-	10/29/63/63	0/2/2/2
14	CLA	1	1605	-	1/1/15/20	16/37/115/115	-
14	CLA	B	827	-	1/1/15/20	15/37/115/115	-
14	CLA	A	809	1	1/1/15/20	11/37/115/115	-
14	CLA	B	829	-	1/1/15/20	7/37/115/115	-
17	BCR	a	850	-	-	8/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/15/20	12/37/115/115	-
14	CLA	A	829	-	1/1/15/20	14/37/115/115	-
14	CLA	9	103	21	1/1/13/20	9/29/107/115	-
14	CLA	b	803	-	1/1/15/20	18/37/115/115	-
14	CLA	2	833	-	1/1/15/20	16/37/115/115	-
14	CLA	2	827	-	1/1/15/20	6/37/115/115	-
14	CLA	a	834	-	1/1/15/20	10/37/115/115	-
17	BCR	a	852	-	-	11/18/35/63	0/1/1/2
18	LHG	M	101	-	-	27/53/53/53	-
14	CLA	b	822	-	1/1/11/20	5/13/91/115	-
14	CLA	2	818	-	1/1/15/20	13/37/115/115	-
14	CLA	B	839	-	-	2/16/94/115	-
17	BCR	A	856	-	-	13/29/63/63	0/2/2/2
14	CLA	a	836	-	1/1/15/20	6/37/115/115	-
17	BCR	b	844	-	-	11/29/63/63	0/2/2/2
16	SF4	c	102	3	-	-	0/6/5/5
17	BCR	B	843	-	-	11/29/63/63	0/2/2/2
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	2	822	-	1/1/11/20	5/13/91/115	-
14	CLA	K	103	21	1/1/13/20	9/29/107/115	-
14	CLA	B	810	2	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	F	202	-	-	12/29/63/63	0/2/2/2
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	b	811	2	1/1/15/20	15/37/115/115	-
14	CLA	A	828	-	1/1/15/20	7/37/115/115	-
14	CLA	a	815	-	1/1/15/20	12/37/115/115	-
14	CLA	A	844	18	1/1/11/20	5/13/91/115	-
14	CLA	b	835	-	1/1/15/20	9/37/115/115	-
14	CLA	B	816	-	1/1/15/20	12/37/115/115	-
14	CLA	2	809	-	1/1/15/20	8/37/115/115	-
14	CLA	a	803	21	1/1/15/20	6/37/115/115	-
14	CLA	2	807	-	1/1/15/20	9/37/115/115	-
14	CLA	B	837	-	1/1/14/20	4/31/109/115	-
14	CLA	1	1632	-	1/1/15/20	7/37/115/115	-
14	CLA	a	822	21	1/1/15/20	12/37/115/115	-
14	CLA	z	102	12	1/1/11/20	7/13/91/115	-
14	CLA	1	1611	1	1/1/15/20	12/37/115/115	-
14	CLA	b	805	-	1/1/15/20	17/37/115/115	-
14	CLA	B	838	-	1/1/15/20	9/37/115/115	-
14	CLA	A	814	-	1/1/15/20	15/37/115/115	-
14	CLA	f	201	21	1/1/13/20	6/29/107/115	-
14	CLA	1	1643	-	1/1/15/20	12/37/115/115	-
17	BCR	M	103	-	-	9/29/63/63	0/2/2/2
14	CLA	B	805	-	1/1/15/20	16/37/115/115	-
14	CLA	a	807	-	1/1/15/20	15/37/115/115	-
14	CLA	B	822	21	1/1/13/20	5/25/103/115	-
17	BCR	a	847	-	-	9/29/63/63	0/2/2/2
14	CLA	a	833	-	1/1/15/20	12/37/115/115	-
14	CLA	B	807	-	1/1/15/20	6/37/115/115	-
14	CLA	2	808	-	1/1/15/20	6/37/115/115	-
14	CLA	B	814	-	1/1/15/20	13/37/115/115	-
14	CLA	B	809	2	1/1/15/20	11/37/115/115	-
14	CLA	B	833	-	1/1/15/20	11/37/115/115	-
17	BCR	B	851	-	-	15/29/63/63	0/2/2/2
17	BCR	f	204	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	830	-	1/1/13/20	13/25/103/115	-
16	SF4	1	1647	2,1	-	-	0/6/5/5
14	CLA	b	819	-	1/1/15/20	17/37/115/115	-
14	CLA	b	809	-	1/1/15/20	8/37/115/115	-
14	CLA	B	806	-	1/1/15/20	9/37/115/115	-
17	BCR	1	1648	-	-	9/29/63/63	0/2/2/2
14	CLA	8	1303	-	1/1/8/20	0/2/76/115	-
14	CLA	A	830	-	1/1/15/20	15/37/115/115	-
14	CLA	1	1613	14	1/1/15/20	13/37/115/115	-
14	CLA	2	815	-	1/1/15/20	13/37/115/115	-
14	CLA	A	839	-	1/1/15/20	20/37/115/115	-
14	CLA	1	1612	-	1/1/11/20	8/18/96/115	-
14	CLA	A	821	-	1/1/15/20	16/37/115/115	-
14	CLA	A	840	-	1/1/15/20	17/37/115/115	-
14	CLA	1	1622	-	1/1/15/20	16/37/115/115	-
14	CLA	F	203	21	1/1/11/20	2/13/91/115	-
14	CLA	b	830	-	1/1/15/20	7/37/115/115	-
14	CLA	A	808	-	1/1/12/20	4/21/99/115	-
14	CLA	0	207	21	1/1/15/20	11/37/115/115	-
17	BCR	9	102	-	-	6/29/63/63	0/2/2/2
13	CL0	a	801	-	3/3/20/25	10/37/135/135	-
14	CLA	B	828	-	1/1/15/20	11/37/115/115	-
14	CLA	1	1610	1	1/1/15/20	11/37/115/115	-
17	BCR	2	845	-	-	8/29/63/63	0/2/2/2
14	CLA	a	824	-	1/1/15/20	12/37/115/115	-
14	CLA	2	816	-	1/1/15/20	13/37/115/115	-
14	CLA	A	816	-	1/1/15/20	19/37/115/115	-
17	BCR	j	1304	-	-	11/29/63/63	0/2/2/2
14	CLA	2	802	21	1/1/15/20	18/37/115/115	-
17	BCR	L	201	-	-	8/29/63/63	0/2/2/2
14	CLA	A	832	-	1/1/14/20	6/31/109/115	-
15	PQN	a	845	-	-	1/23/43/43	0/2/2/2
17	BCR	B	846	-	-	12/29/63/63	0/2/2/2
14	CLA	A	803	21	1/1/15/20	6/37/115/115	-
17	BCR	A	851	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	813	-	1/1/11/20	0/13/91/115	-
17	BCR	8	1305	-	-	13/29/63/63	0/2/2/2
14	CLA	k	103	21	1/1/13/20	9/29/107/115	-
14	CLA	2	806	-	1/1/15/20	16/37/115/115	-
14	CLA	L	204	-	1/1/15/20	11/37/115/115	-
14	CLA	1	1637	-	1/1/15/20	6/37/115/115	-
17	BCR	8	1304	-	-	11/29/63/63	0/2/2/2
14	CLA	2	813	-	1/1/11/20	0/13/91/115	-
14	CLA	B	840	21	1/1/15/20	7/37/115/115	-
17	BCR	B	848	-	-	5/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	B	817	-	1/1/15/20	13/37/115/115	-
14	CLA	1	1608	-	1/1/15/20	15/37/115/115	-
17	BCR	i	101	-	-	7/29/63/63	0/2/2/2
17	BCR	b	846	-	-	11/29/63/63	0/2/2/2
14	CLA	A	817	21	1/1/15/20	12/37/115/115	-
14	CLA	1	1614	-	1/1/11/20	4/13/91/115	-
14	CLA	1	1619	-	1/1/15/20	10/37/115/115	-
14	CLA	b	812	-	1/1/15/20	10/37/115/115	-
14	CLA	b	840	-	-	2/16/94/115	-
14	CLA	A	834	-	1/1/15/20	10/37/115/115	-
14	CLA	A	802	-	1/1/15/20	15/37/115/115	-
18	LHG	a	854	14	-	13/45/45/53	-
17	BCR	b	852	-	-	15/29/63/63	0/2/2/2
14	CLA	K	101	-	1/1/11/20	10/15/93/115	-
17	BCR	b	848	-	-	11/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/15/20	20/37/115/115	-
14	CLA	b	842	-	1/1/15/20	10/37/115/115	-
14	CLA	2	829	-	1/1/15/20	11/37/115/115	-
14	CLA	1	1609	-	1/1/12/20	4/21/99/115	-
14	CLA	1	1618	21	1/1/15/20	12/37/115/115	-
14	CLA	A	823	-	1/1/11/20	8/13/91/115	-
14	CLA	1	1616	-	1/1/15/20	12/37/115/115	-
14	CLA	A	841	-	1/1/15/20	14/37/115/115	-
14	CLA	a	831	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	816	-	1/1/15/20	13/37/115/115	-
14	CLA	l	204	10	1/1/15/20	17/37/115/115	-
20	LMG	2	850	-	-	27/50/70/70	0/1/1/1
14	CLA	A	824	-	1/1/15/20	12/37/115/115	-
14	CLA	A	815	-	1/1/15/20	12/37/115/115	-
14	CLA	B	825	21	1/1/15/20	11/37/115/115	-
17	BCR	y	102	-	-	9/29/63/63	0/2/2/2
18	LHG	A	853	-	-	21/53/53/53	-
14	CLA	2	828	-	1/1/15/20	15/37/115/115	-
14	CLA	1	1631	-	1/1/15/20	15/37/115/115	-
18	LHG	1	1654	-	-	21/53/53/53	-
14	CLA	A	836	-	1/1/15/20	6/37/115/115	-
18	LHG	L	208	-	-	27/43/43/53	-
14	CLA	J	101	-	1/1/11/20	5/13/91/115	-
14	CLA	B	821	-	1/1/11/20	5/13/91/115	-
14	CLA	1	1620	-	1/1/15/20	17/37/115/115	-
14	CLA	a	812	14	1/1/15/20	13/37/115/115	-
14	CLA	2	811	2	1/1/15/20	15/37/115/115	-
14	CLA	b	837	21	1/1/11/20	3/13/91/115	-
14	CLA	a	820	-	1/1/15/20	10/37/115/115	-
17	BCR	A	849	-	-	5/29/63/63	0/2/2/2
14	CLA	j	1301	21	1/1/11/20	2/13/91/115	-
14	CLA	B	802	-	1/1/15/20	18/37/115/115	-
14	CLA	1	1634	-	1/1/15/20	12/37/115/115	-
14	CLA	A	827	21	1/1/15/20	9/37/115/115	-
14	CLA	1	1630	-	1/1/15/20	14/37/115/115	-
14	CLA	b	804	-	1/1/15/20	12/37/115/115	-
14	CLA	B	826	-	1/1/15/20	6/37/115/115	-
14	CLA	A	807	-	1/1/15/20	15/37/115/115	-
14	CLA	2	832	-	1/1/11/20	10/18/96/115	-
14	CLA	a	811	-	1/1/11/20	8/18/96/115	-
17	BCR	6	204	-	-	8/29/63/63	0/2/2/2
14	CLA	1	1601	-	1/1/7/20	0/2/72/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LHG	1	1655	14	-	13/45/45/53	-
14	CLA	a	818	-	1/1/15/20	10/37/115/115	-
14	CLA	B	812	-	1/1/11/20	0/13/91/115	-
14	CLA	2	820	21	1/1/15/20	15/37/115/115	-
17	BCR	2	847	-	-	12/29/63/63	0/2/2/2
17	BCR	9	104	-	-	4/18/35/63	0/1/1/2
14	CLA	A	812	14	1/1/15/20	13/37/115/115	-
14	CLA	2	842	-	1/1/15/20	10/37/115/115	-
14	CLA	b	806	-	1/1/15/20	16/37/115/115	-
14	CLA	b	814	-	1/1/15/20	16/37/115/115	-
17	BCR	K	102	-	-	6/29/63/63	0/2/2/2
14	CLA	B	832	-	1/1/15/20	16/37/115/115	-
14	CLA	a	837	1	1/1/11/20	5/13/91/115	-
14	CLA	b	826	21	1/1/15/20	11/37/115/115	-
17	BCR	L	207	-	-	5/29/63/63	0/2/2/2
14	CLA	0	206	-	1/1/15/20	11/37/115/115	-
14	CLA	b	838	-	1/1/14/20	5/31/109/115	-
14	CLA	B	831	-	1/1/11/20	10/18/96/115	-
17	BCR	2	849	-	-	5/29/63/63	0/2/2/2
14	CLA	2	834	-	1/1/15/20	11/37/115/115	-
14	CLA	9	101	-	1/1/11/20	10/15/93/115	-
17	BCR	A	847	-	-	9/29/63/63	0/2/2/2
14	CLA	b	829	-	1/1/15/20	11/37/115/115	-
14	CLA	b	817	-	1/1/15/20	12/37/115/115	-
17	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	A	813	-	1/1/11/20	4/13/91/115	-
14	CLA	B	834	-	1/1/15/20	9/37/115/115	-
17	BCR	2	846	-	-	11/29/63/63	0/2/2/2
14	CLA	A	822	21	1/1/15/20	12/37/115/115	-
17	BCR	k	104	-	-	4/18/35/63	0/1/1/2
14	CLA	B	824	2	1/1/15/20	14/37/115/115	-
14	CLA	6	203	-	1/1/12/20	6/19/97/115	-
18	LHG	z	101	-	-	18/53/53/53	-
14	CLA	B	841	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	828	-	1/1/15/20	15/37/115/115	-
14	CLA	j	1303	-	1/1/8/20	0/2/76/115	-
17	BCR	0	203	-	-	8/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/15/20	17/37/115/115	-
17	BCR	1	1650	-	-	5/29/63/63	0/2/2/2
14	CLA	a	840	-	1/1/15/20	17/37/115/115	-
14	CLA	A	855	21	1/1/15/20	18/37/115/115	-
14	CLA	a	844	18	1/1/11/20	5/13/91/115	-
17	BCR	B	847	-	-	11/29/63/63	0/2/2/2

The worst 5 of 2563 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	f	203	CLA	C4B-NB	7.82	1.42	1.35
14	A	824	CLA	C4B-NB	7.79	1.42	1.35
14	F	204	CLA	C4B-NB	7.74	1.42	1.35
14	1	1625	CLA	C4B-NB	7.74	1.42	1.35
14	6	203	CLA	C4B-NB	7.72	1.42	1.35

The worst 5 of 2850 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	808	CLA	C4A-NA-C1A	8.39	110.48	106.71
14	2	809	CLA	C4A-NA-C1A	8.34	110.46	106.71
14	b	809	CLA	C4A-NA-C1A	8.29	110.43	106.71
14	B	803	CLA	C4A-NA-C1A	8.28	110.43	106.71
14	a	835	CLA	C4A-NA-C1A	8.24	110.41	106.71

5 of 294 chirality outliers are listed below:

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

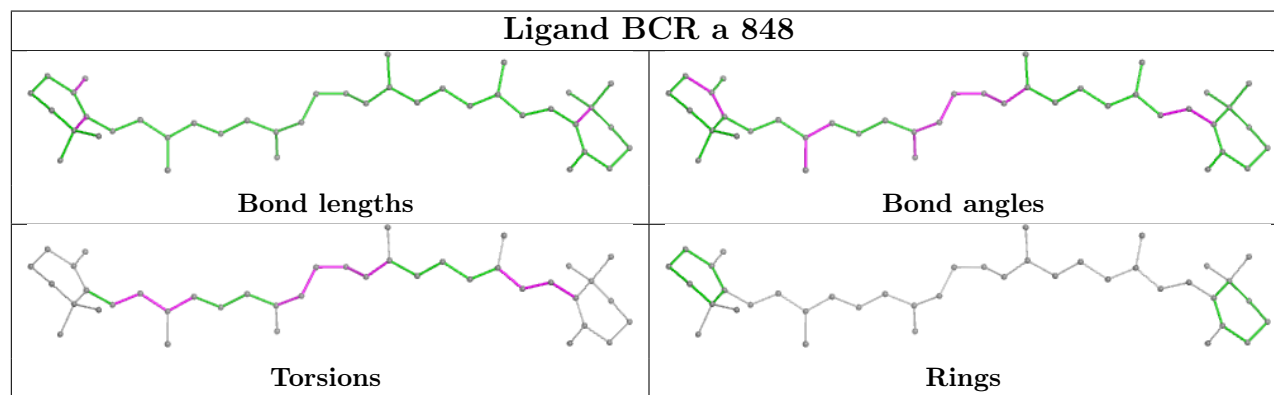
5 of 4211 torsion outliers are listed below:

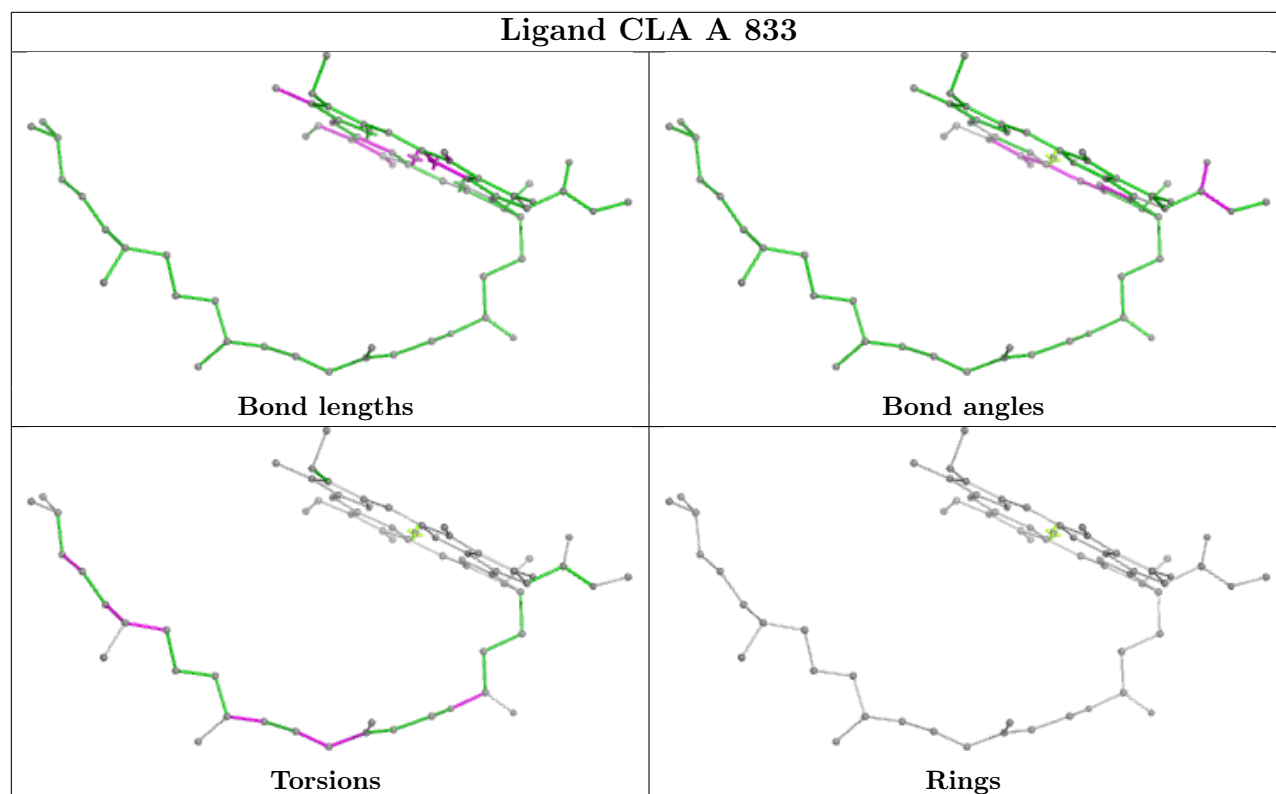
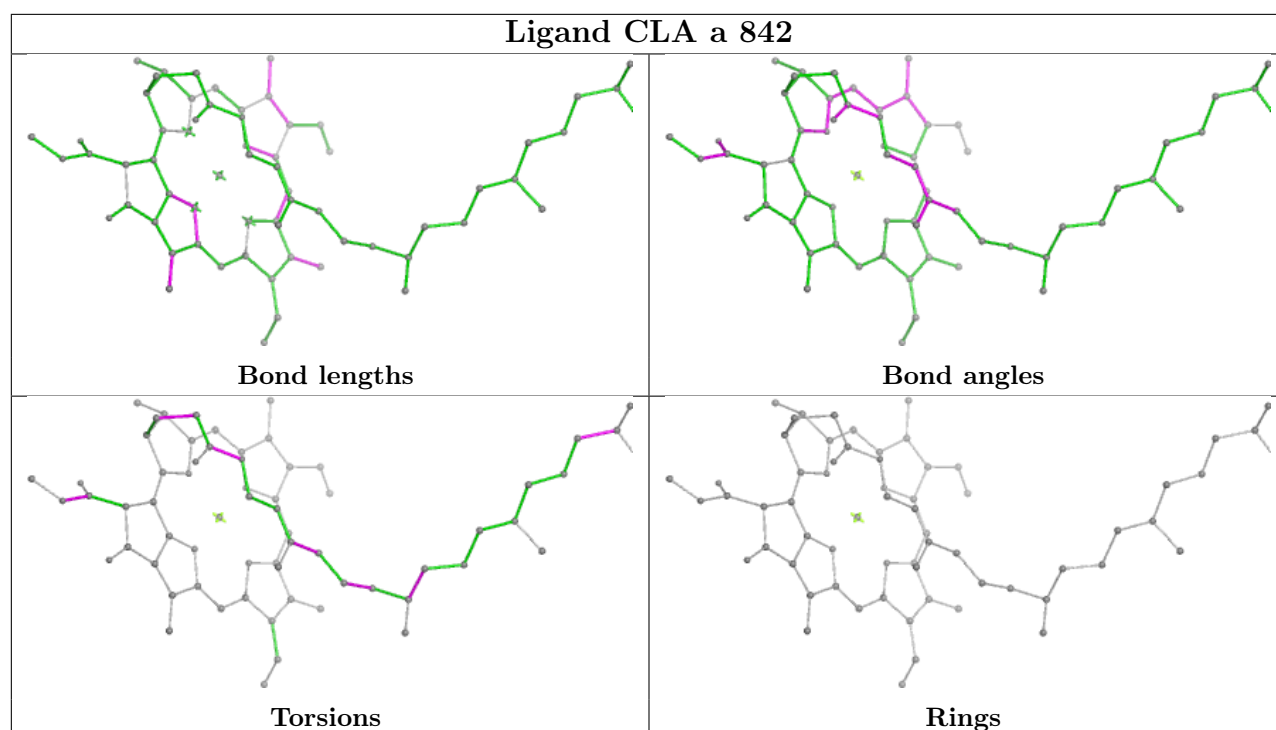
Mol	Chain	Res	Type	Atoms
14	A	802	CLA	CBD-CGD-O2D-CED
14	A	803	CLA	C6-C7-C8-C9
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D
14	A	805	CLA	C1A-C2A-CAA-CBA

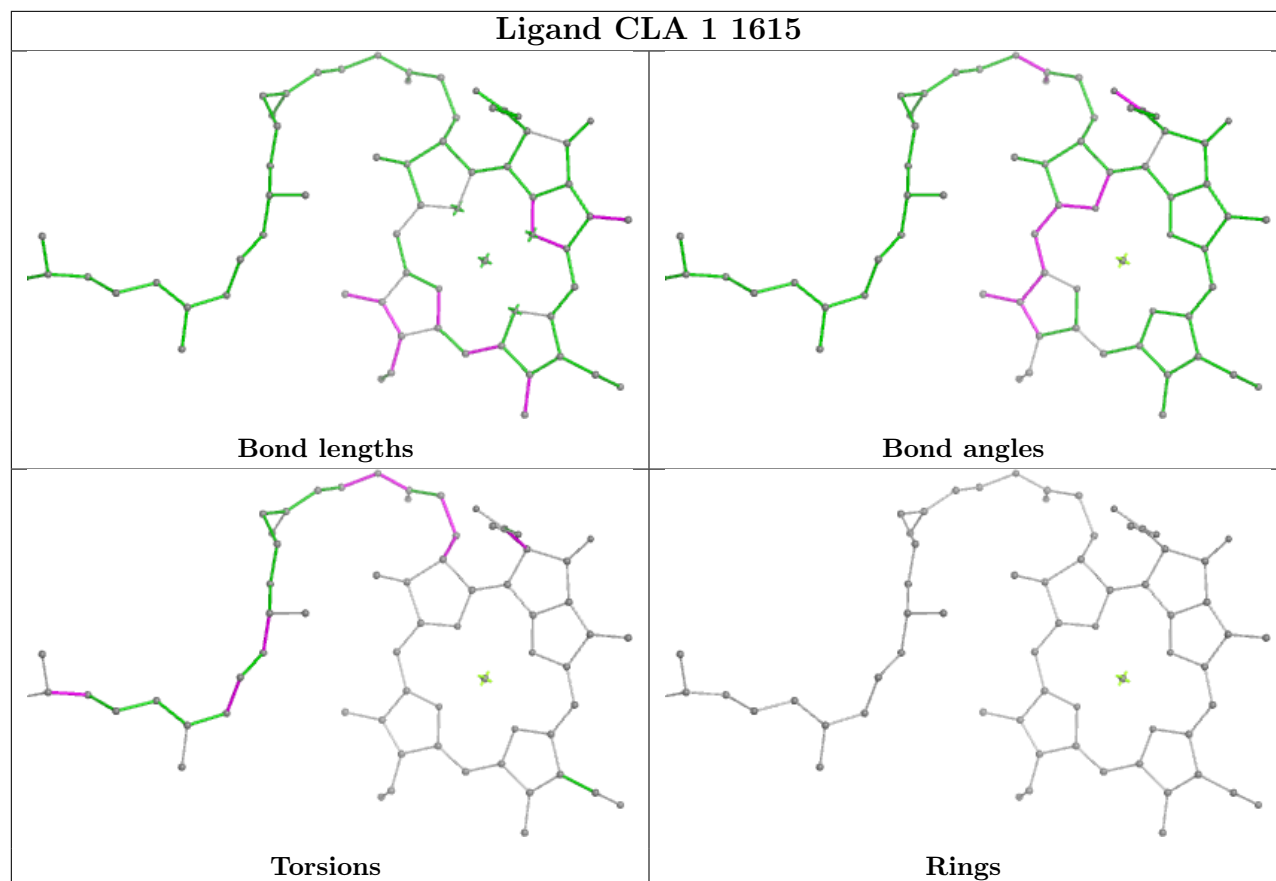
There are no ring outliers.

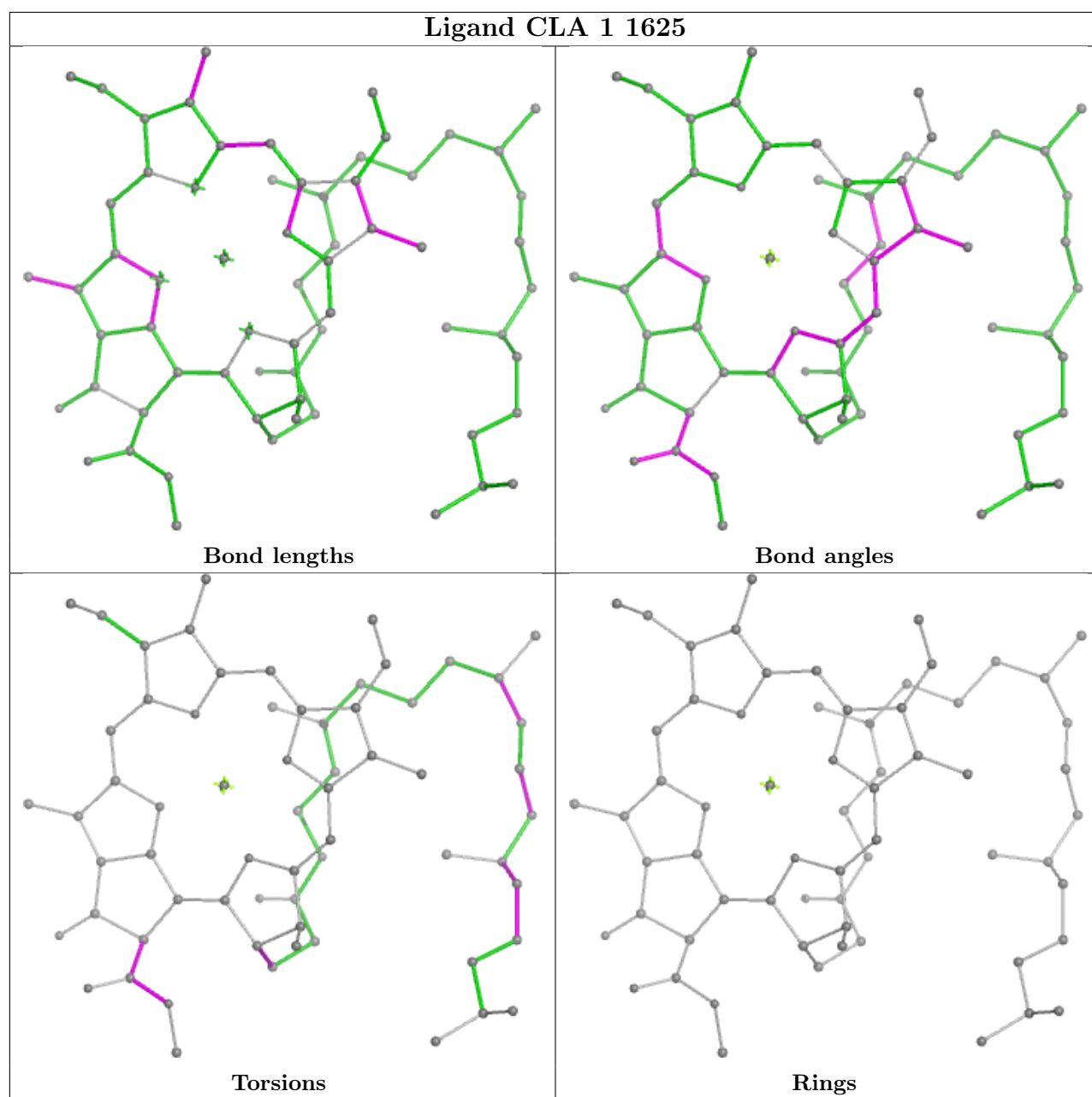
No monomer is involved in short contacts.

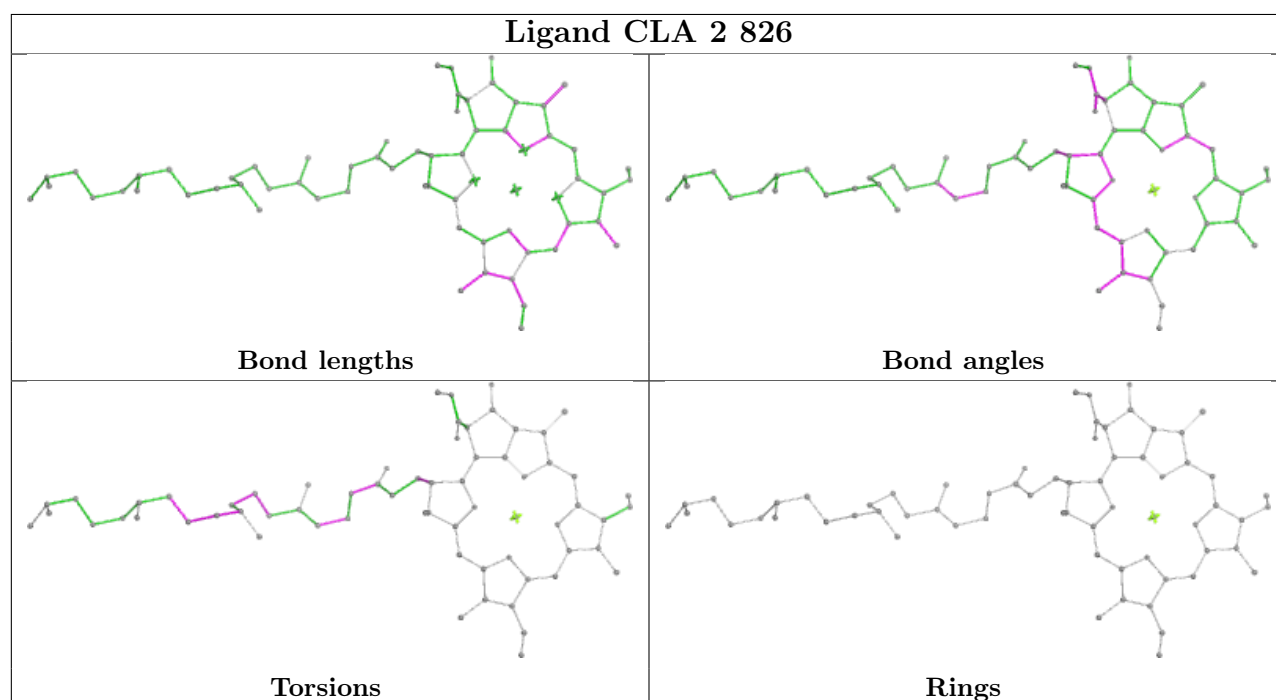
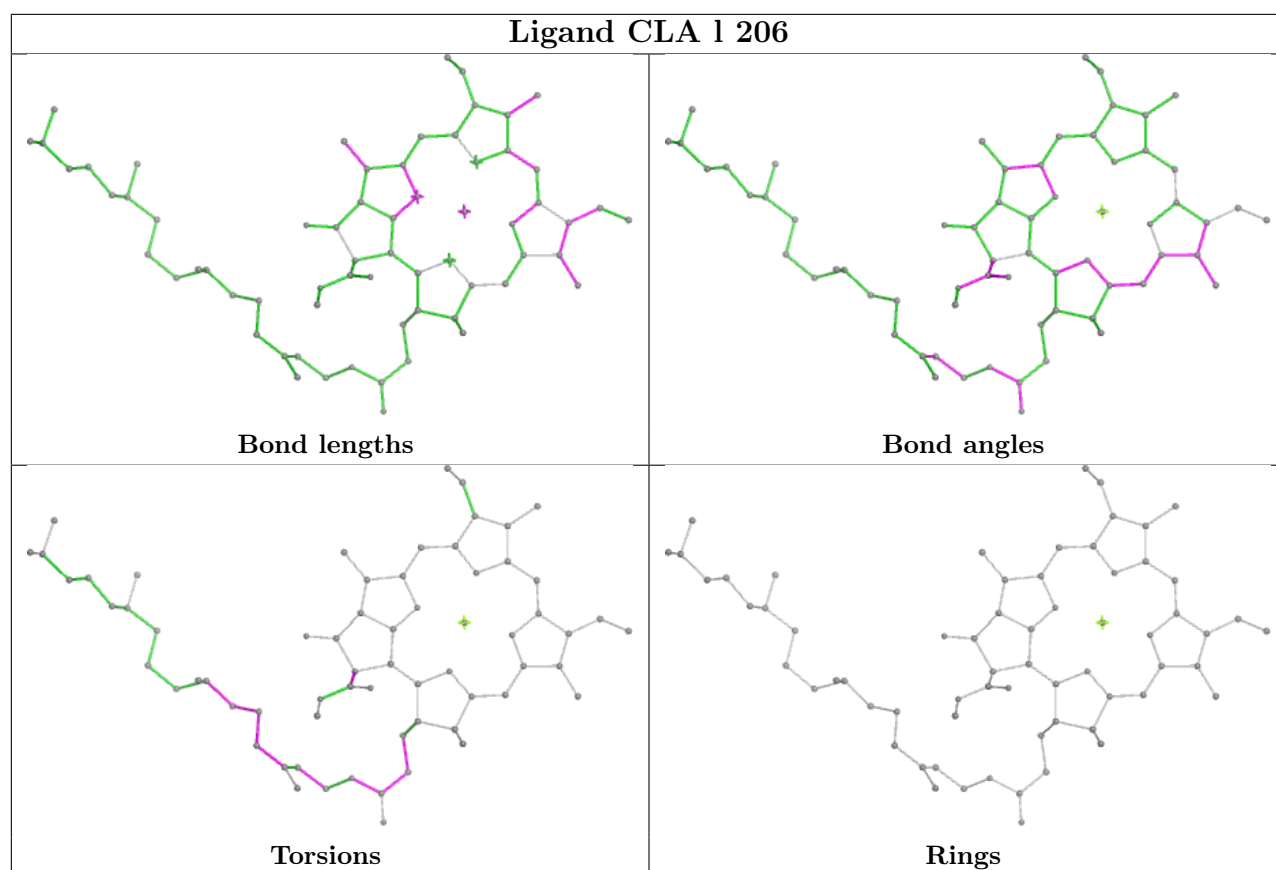
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

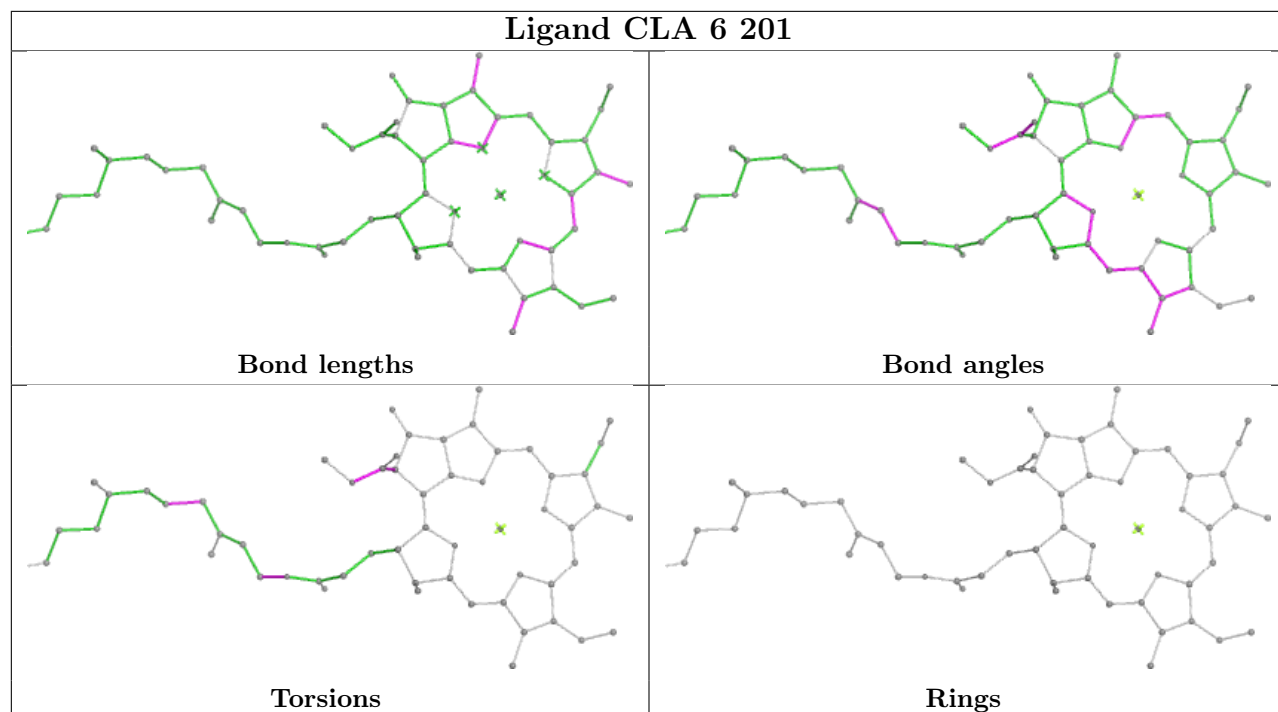


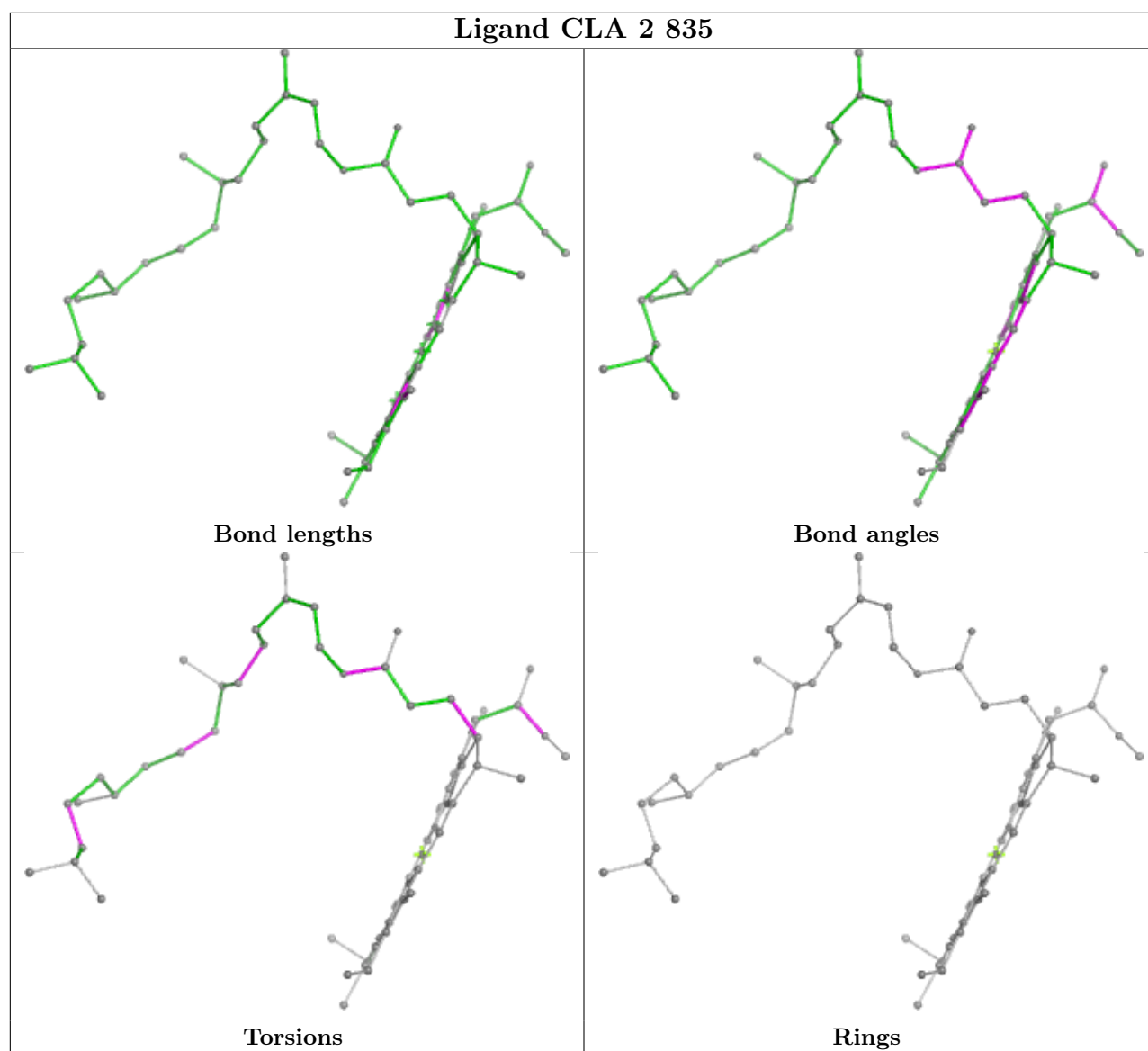


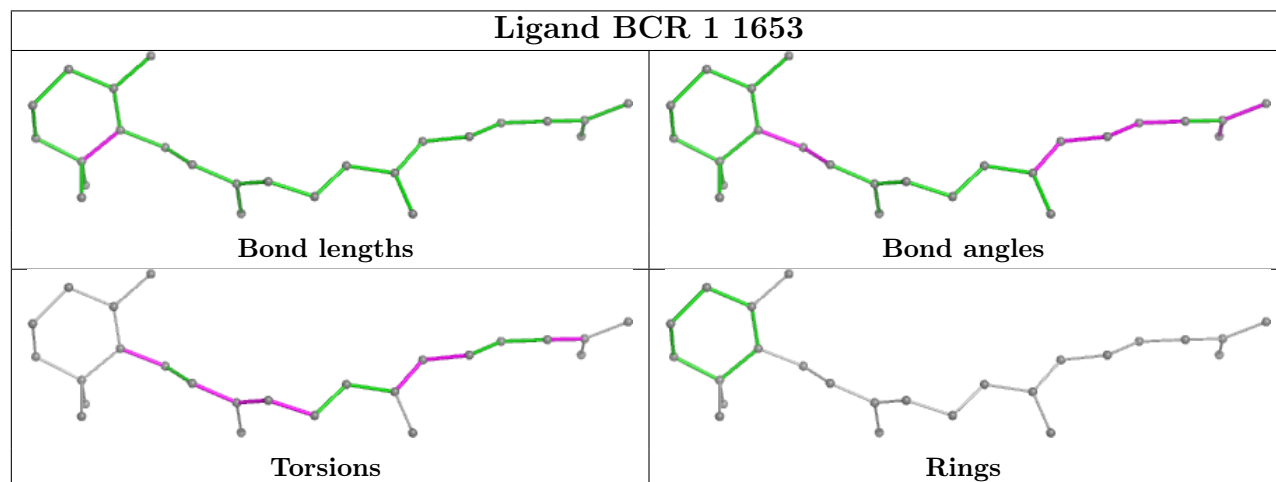
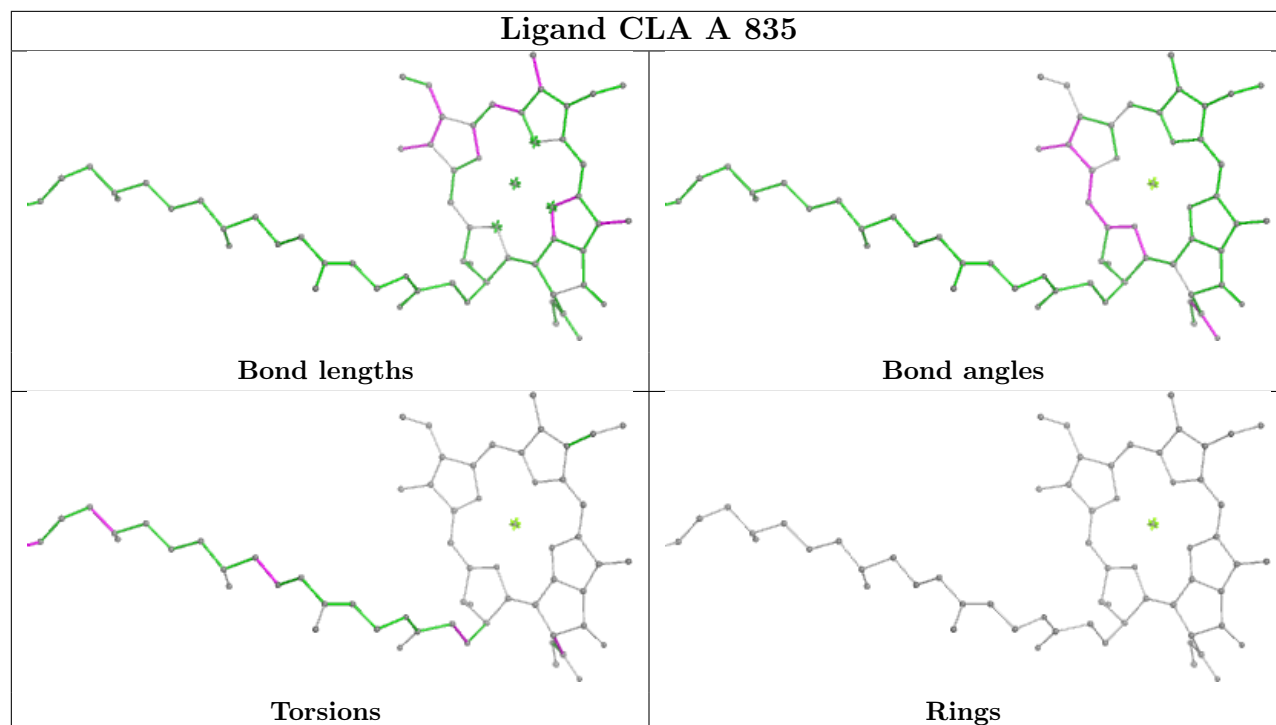




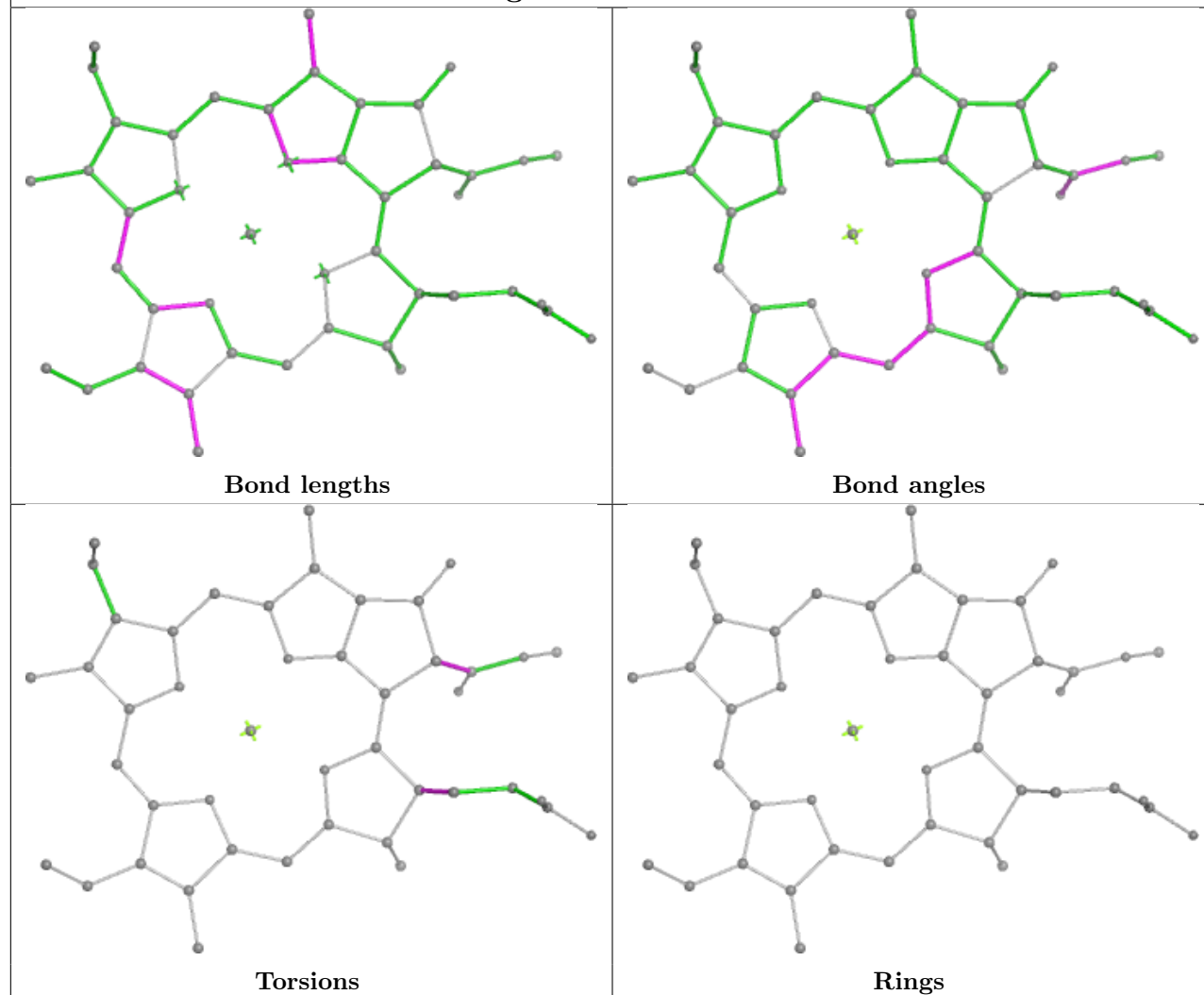




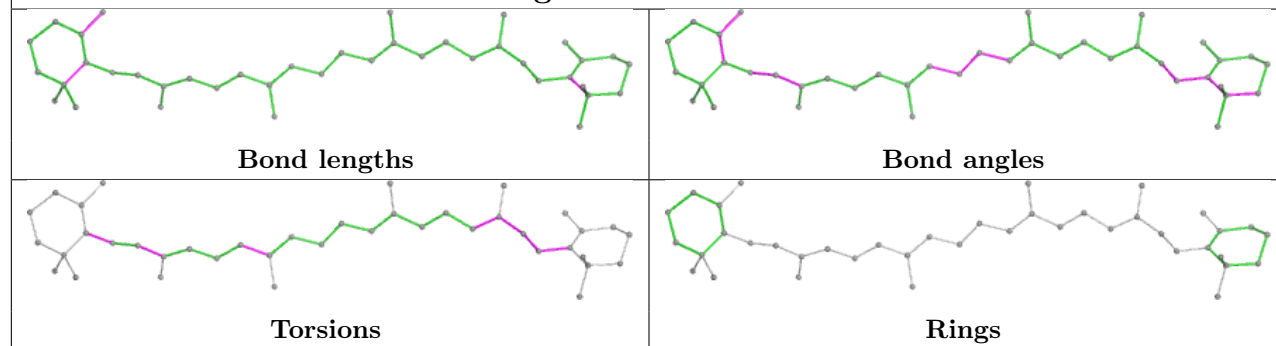




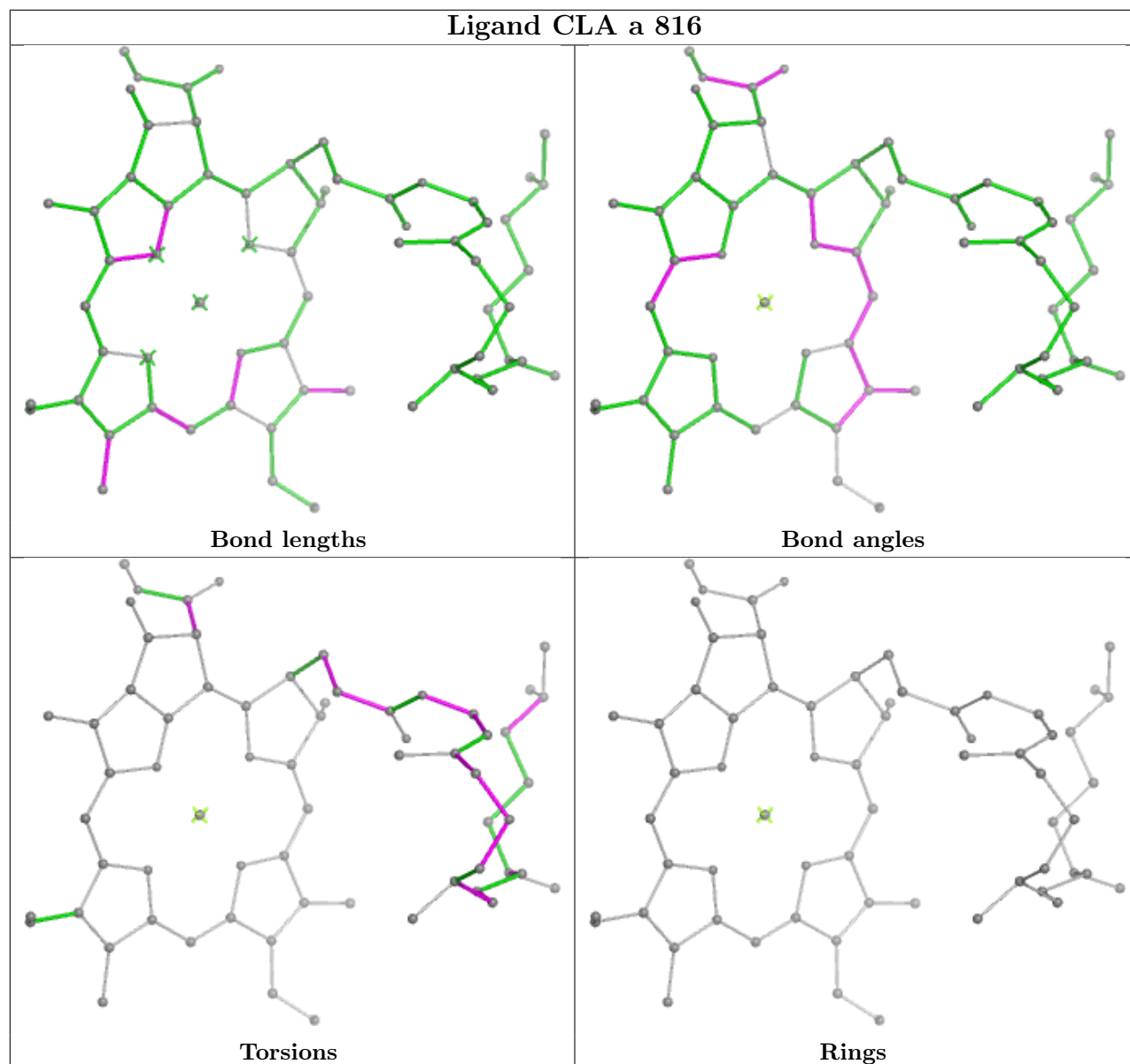
Ligand CLA 2 837

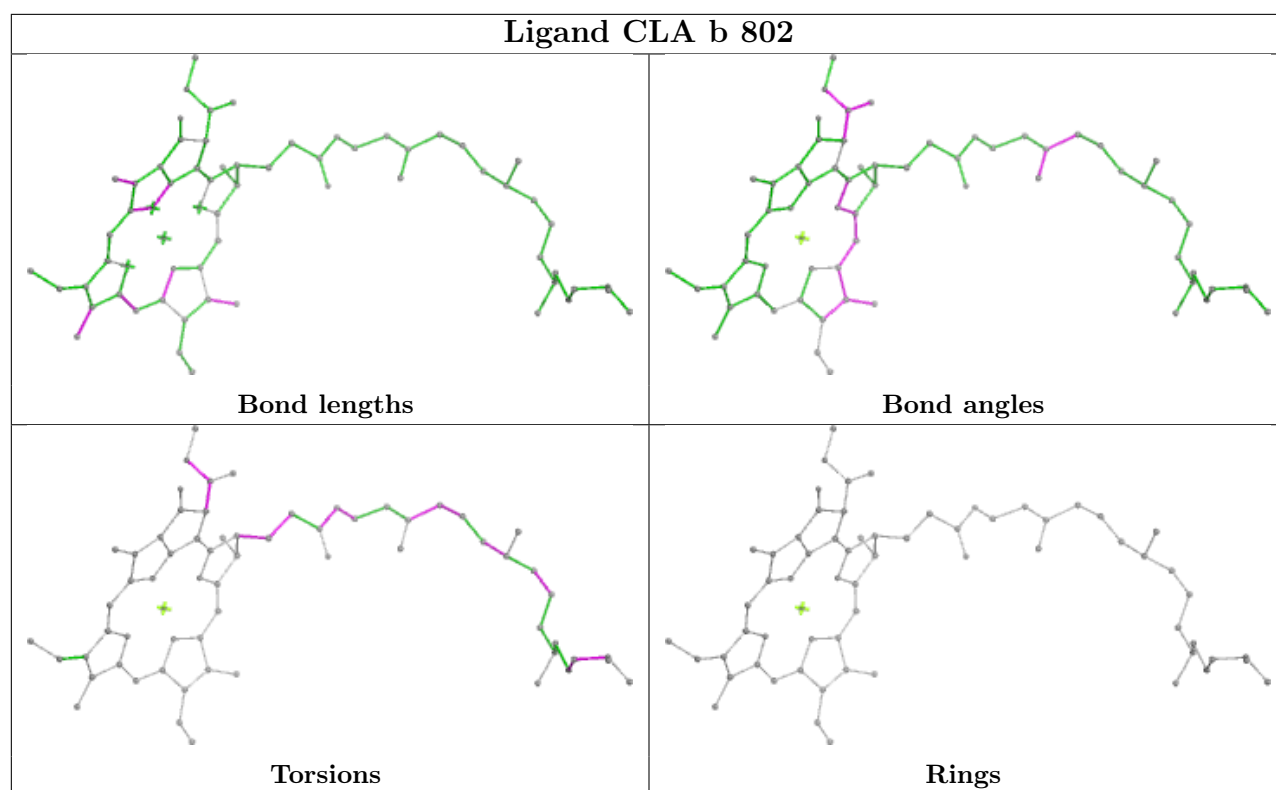


Ligand BCR J 103

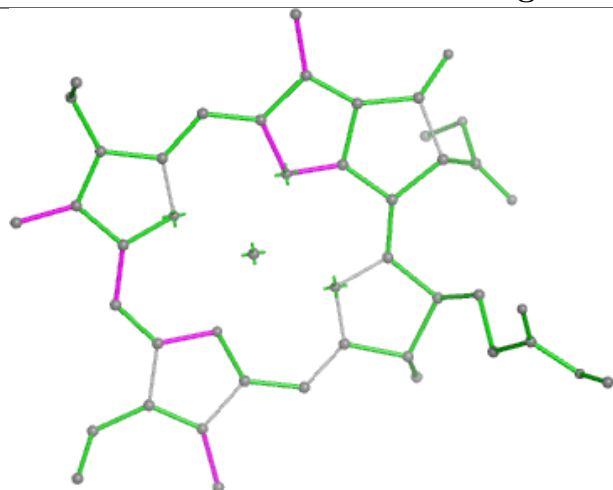


Ligand CLA a 816

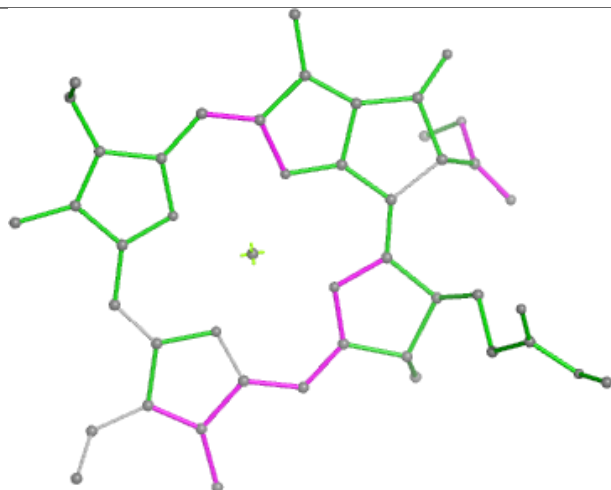




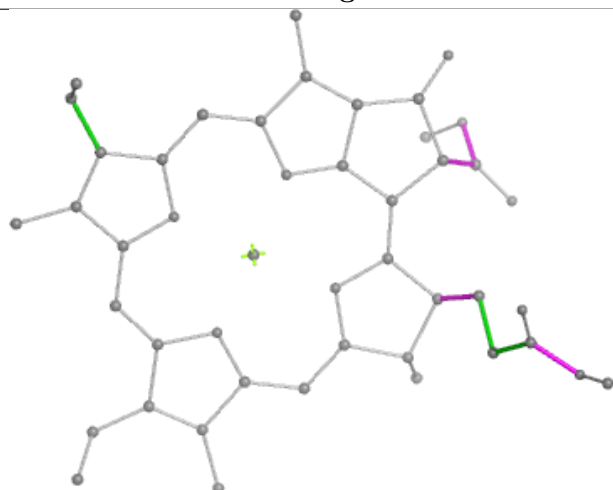
Ligand CLA k 101



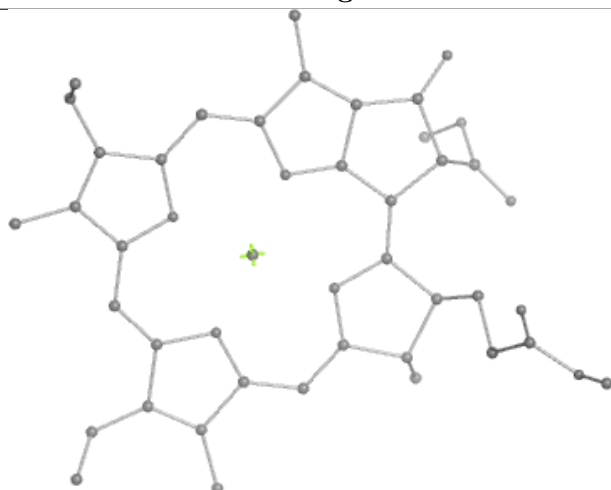
Bond lengths



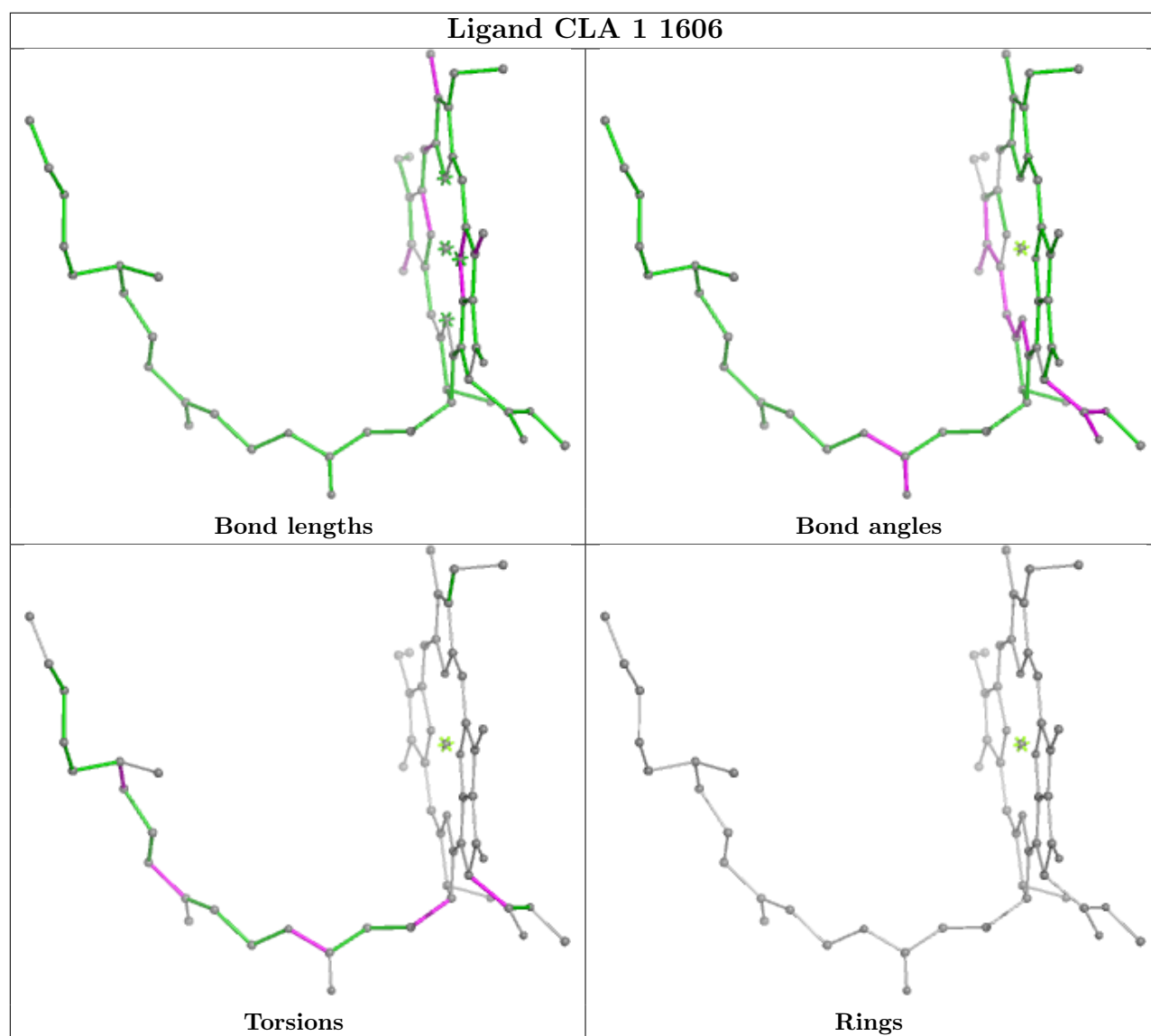
Bond angles

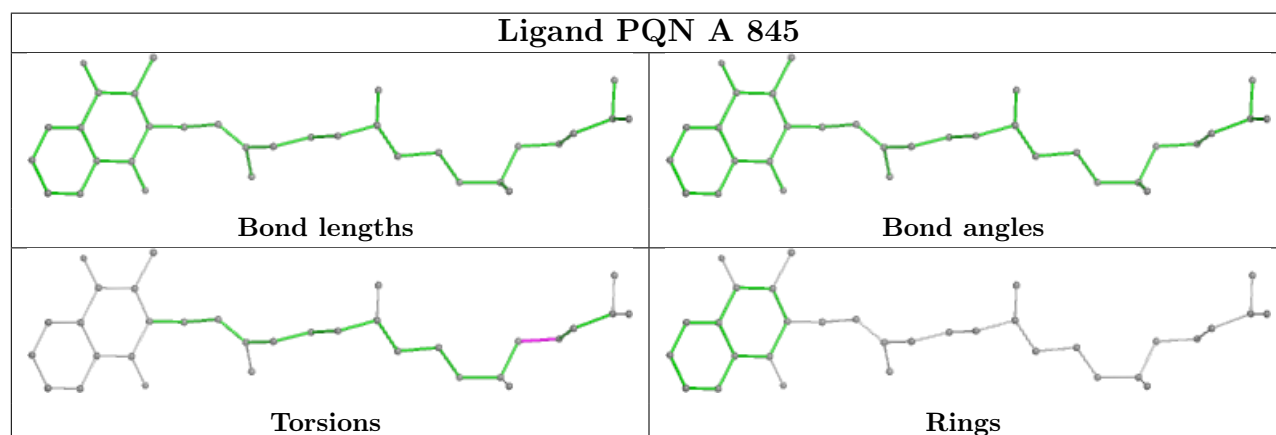
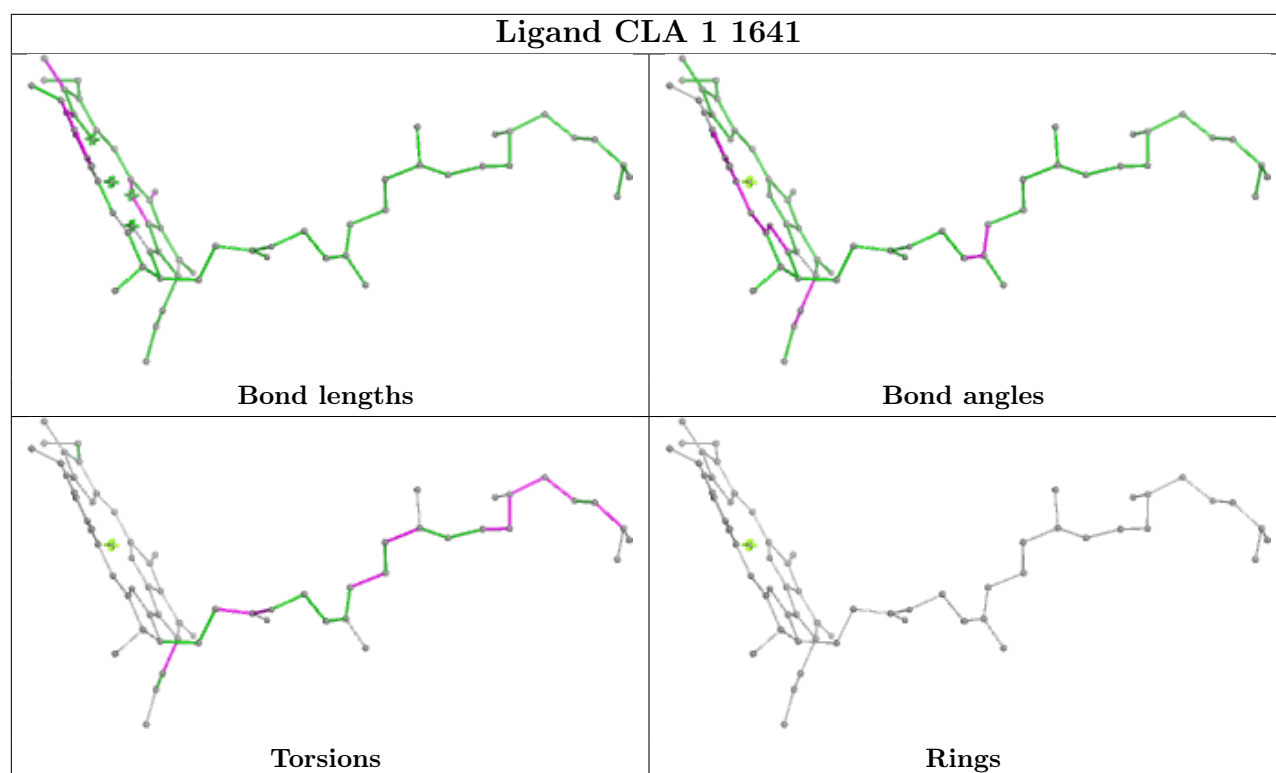


Torsions

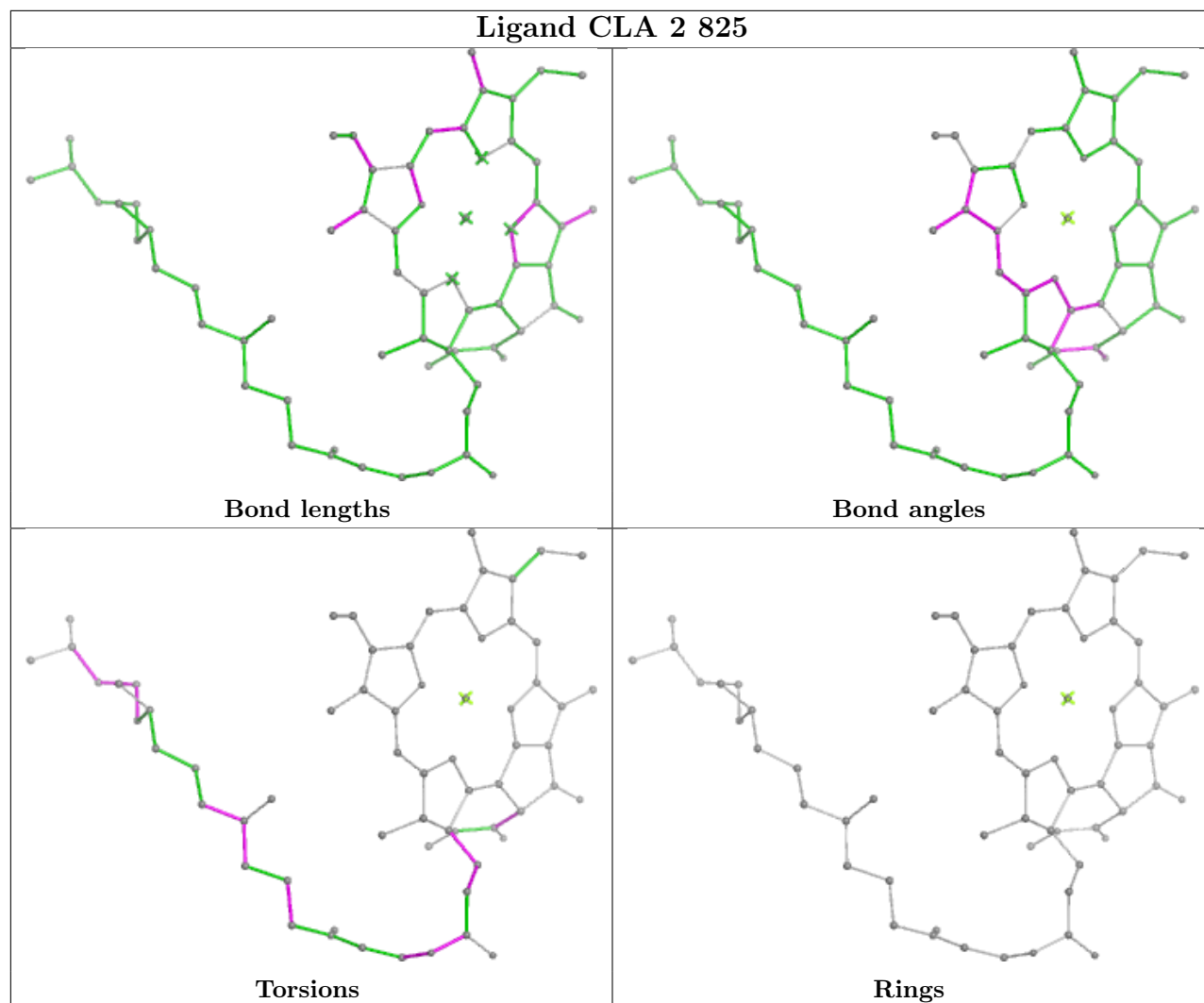


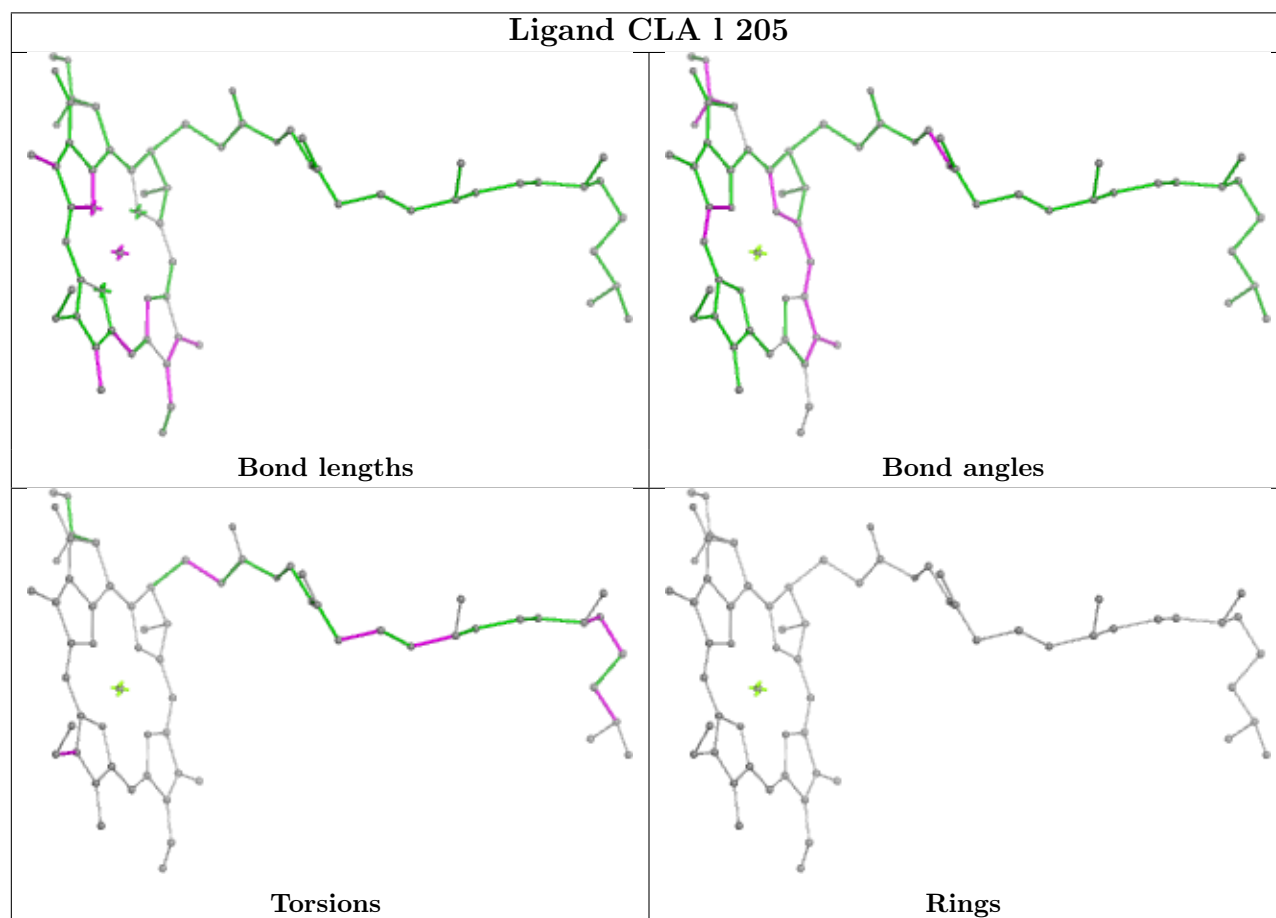
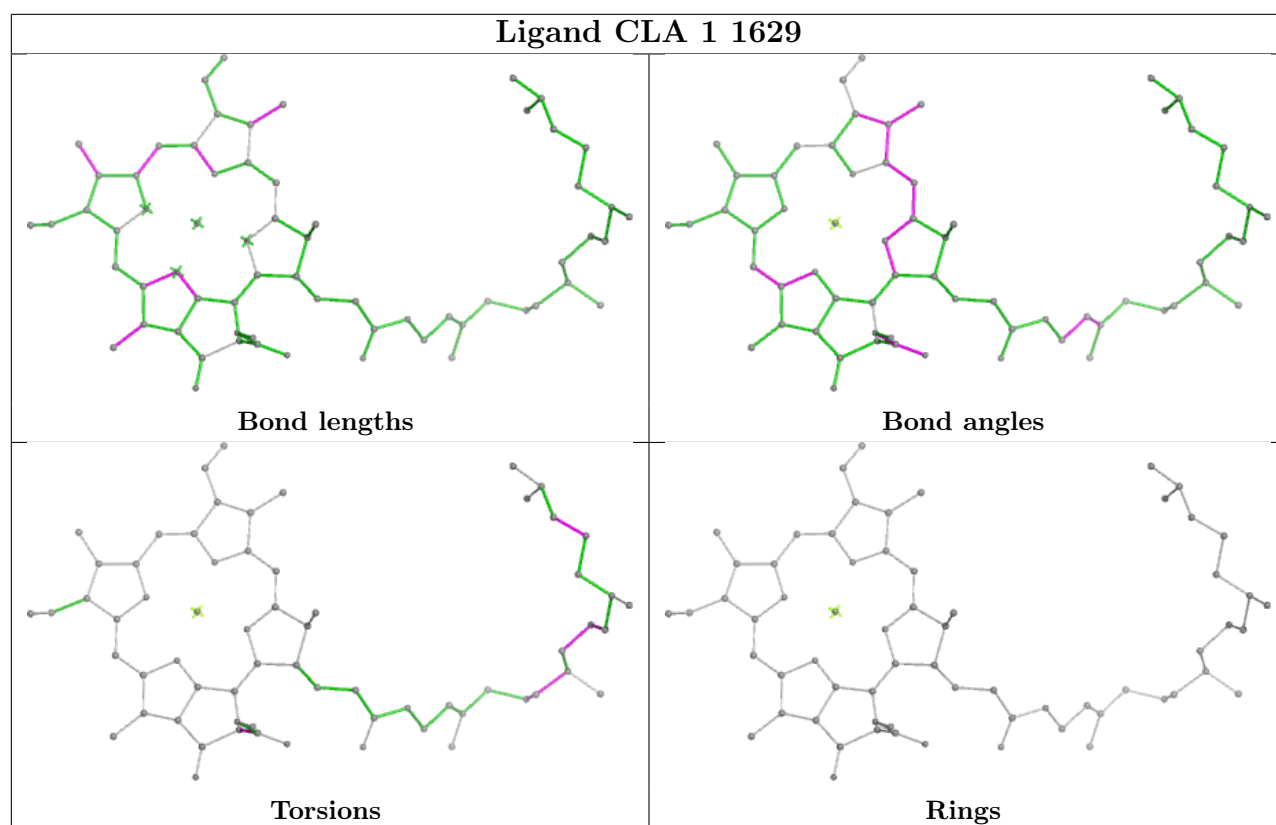
Rings

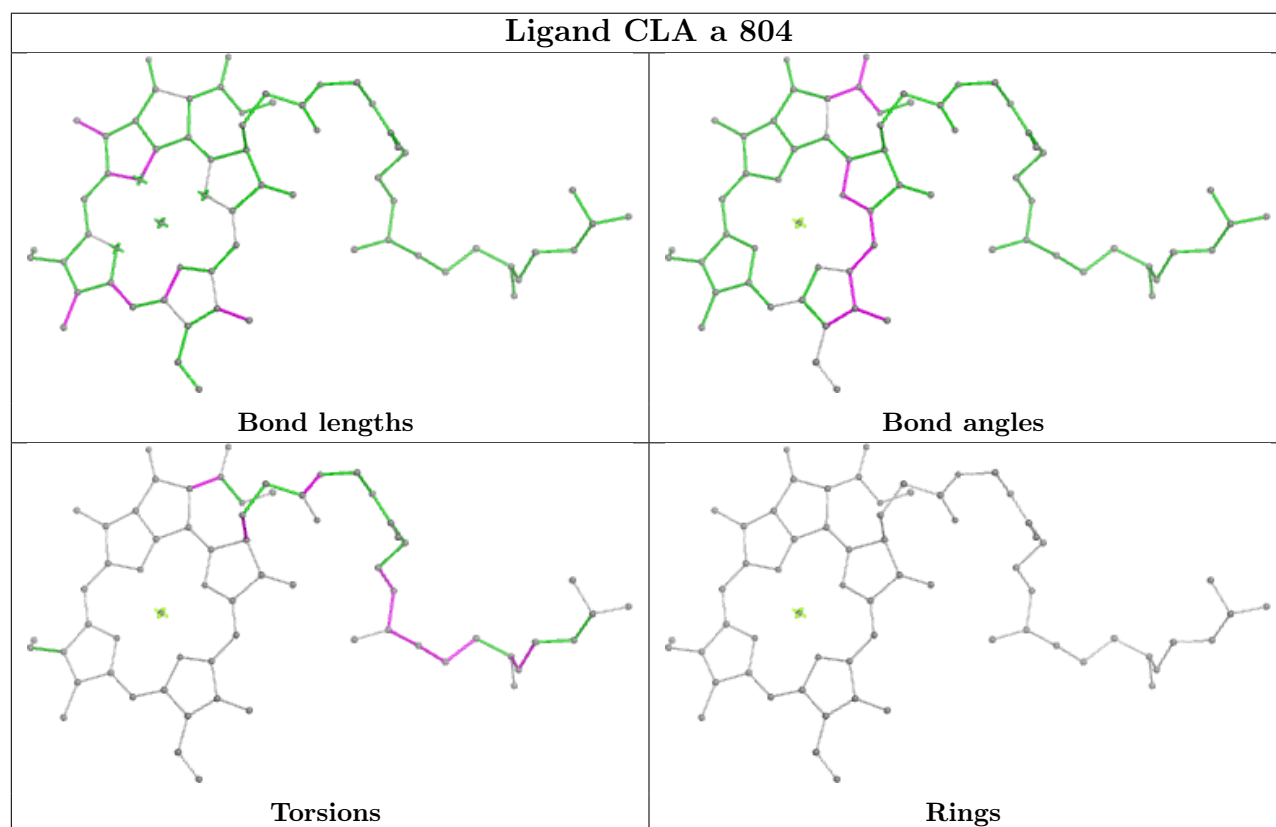
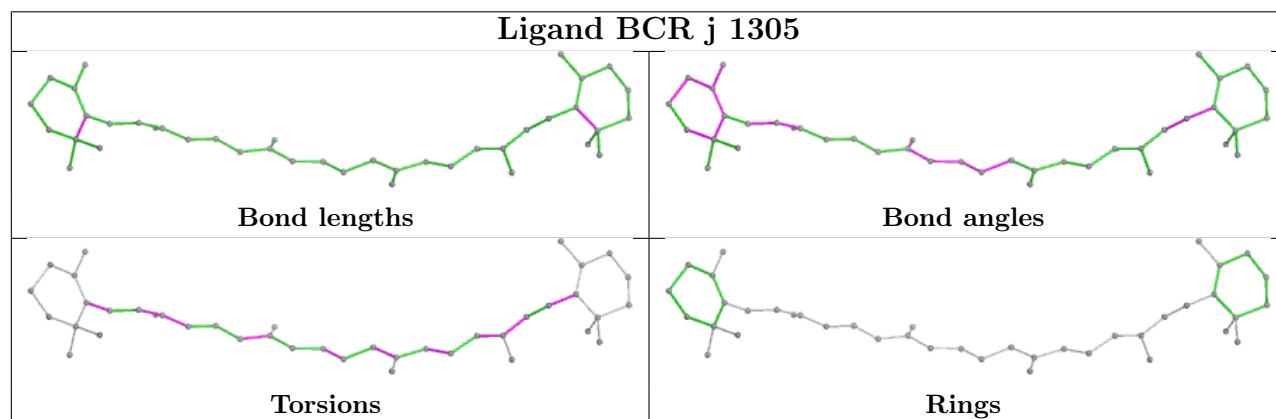
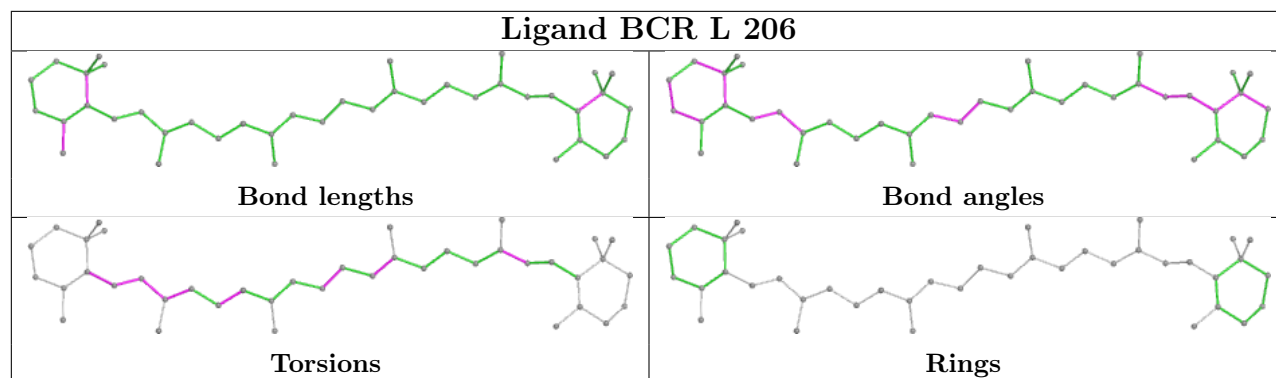




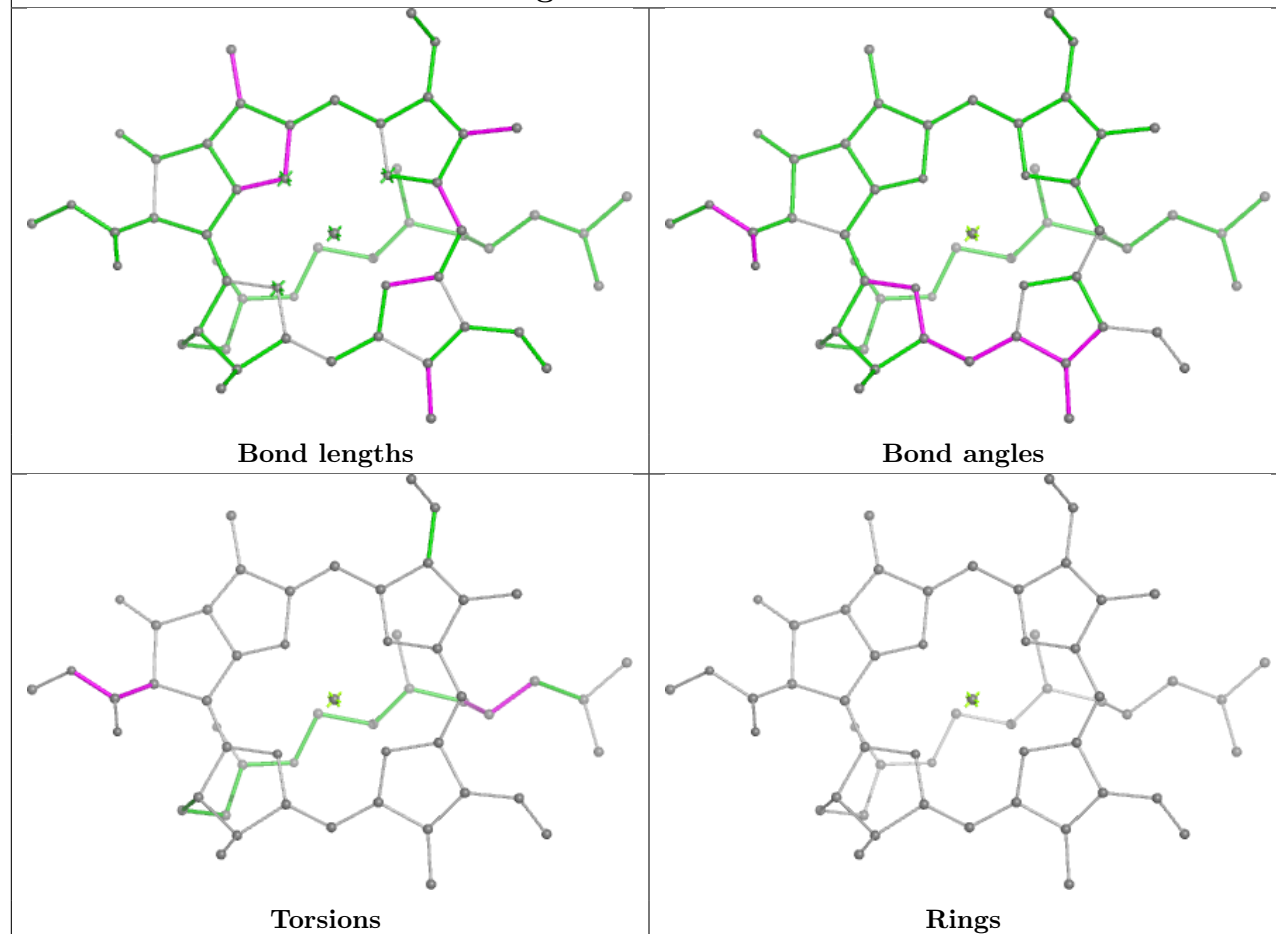
Ligand CLA 2 825



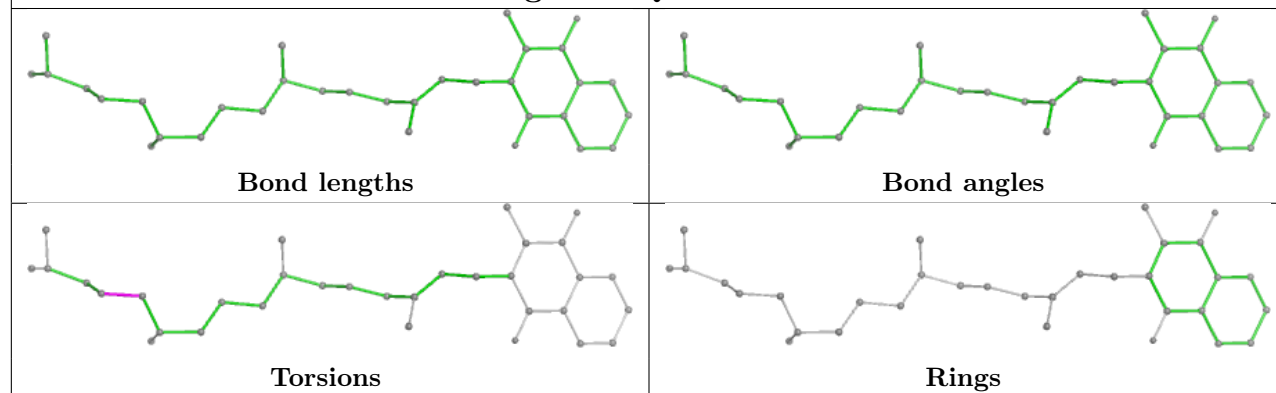




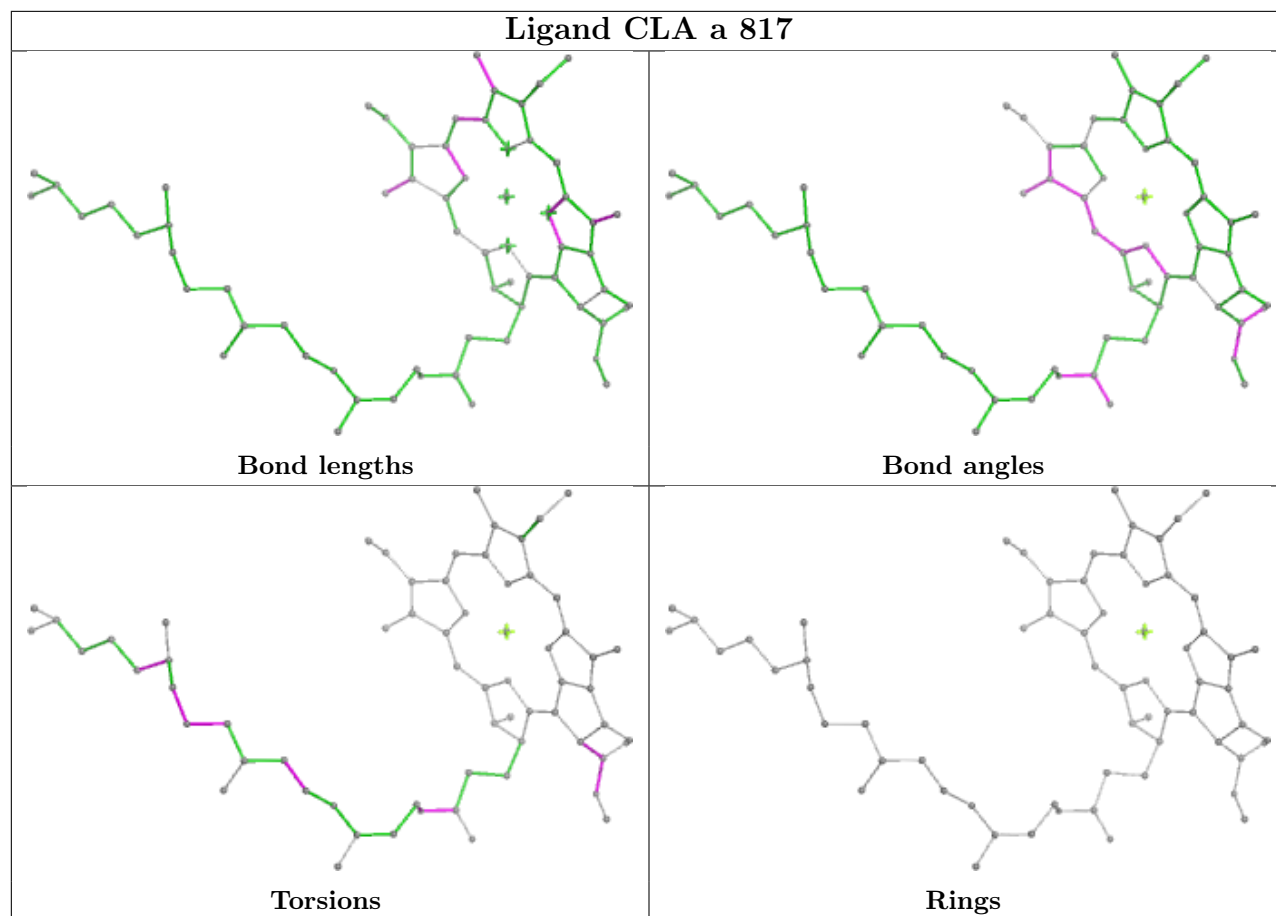
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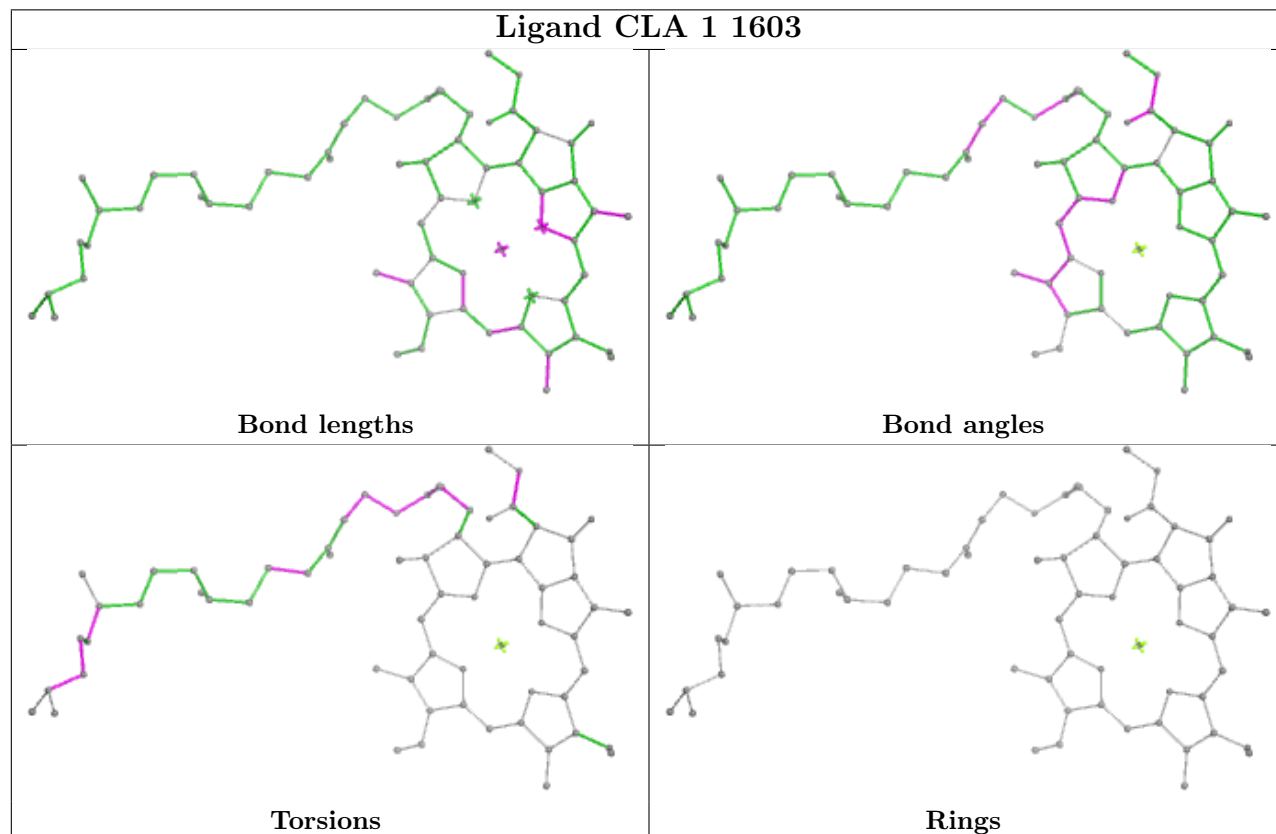
Ligand PQN 1 1646

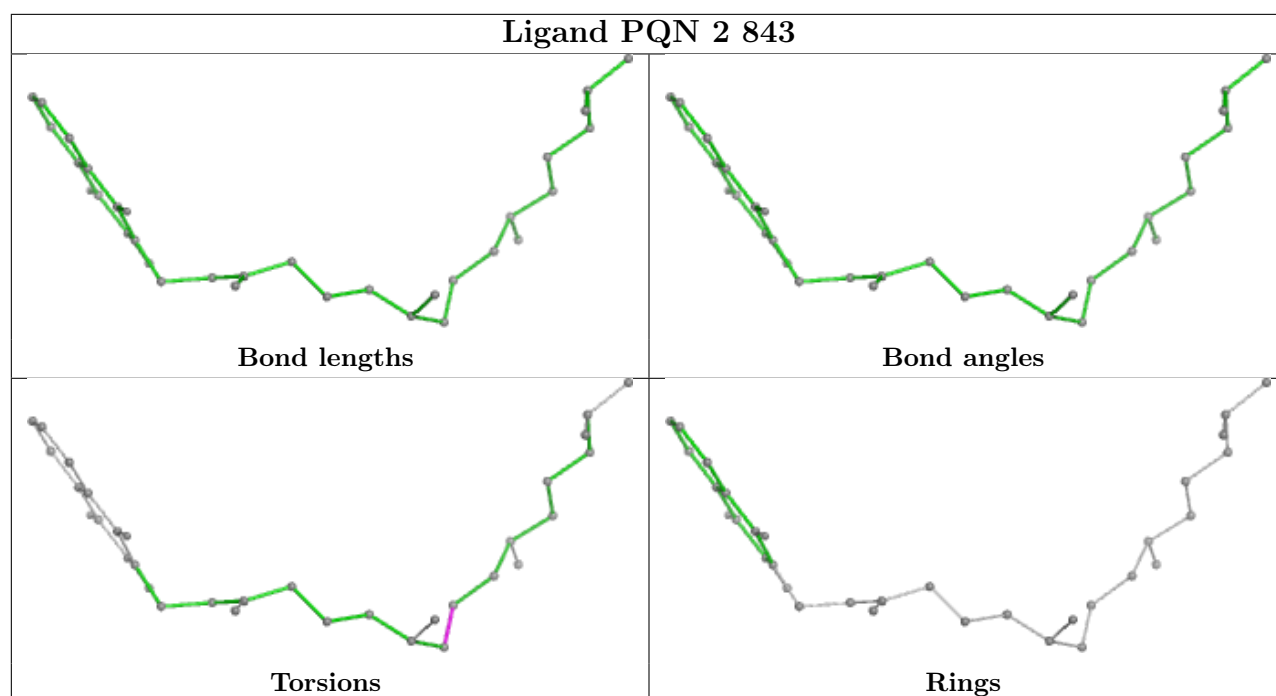


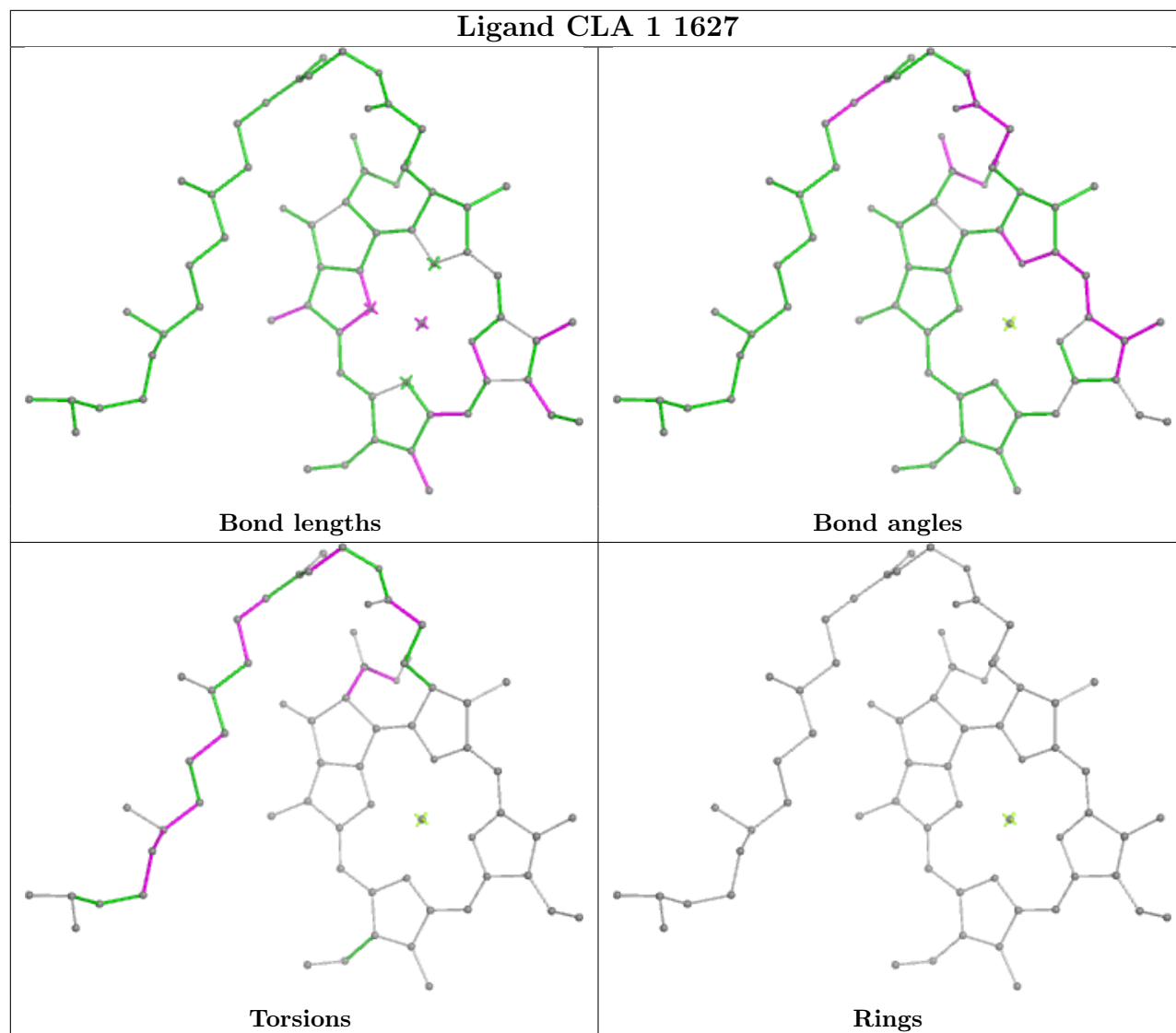
Ligand CLA a 817

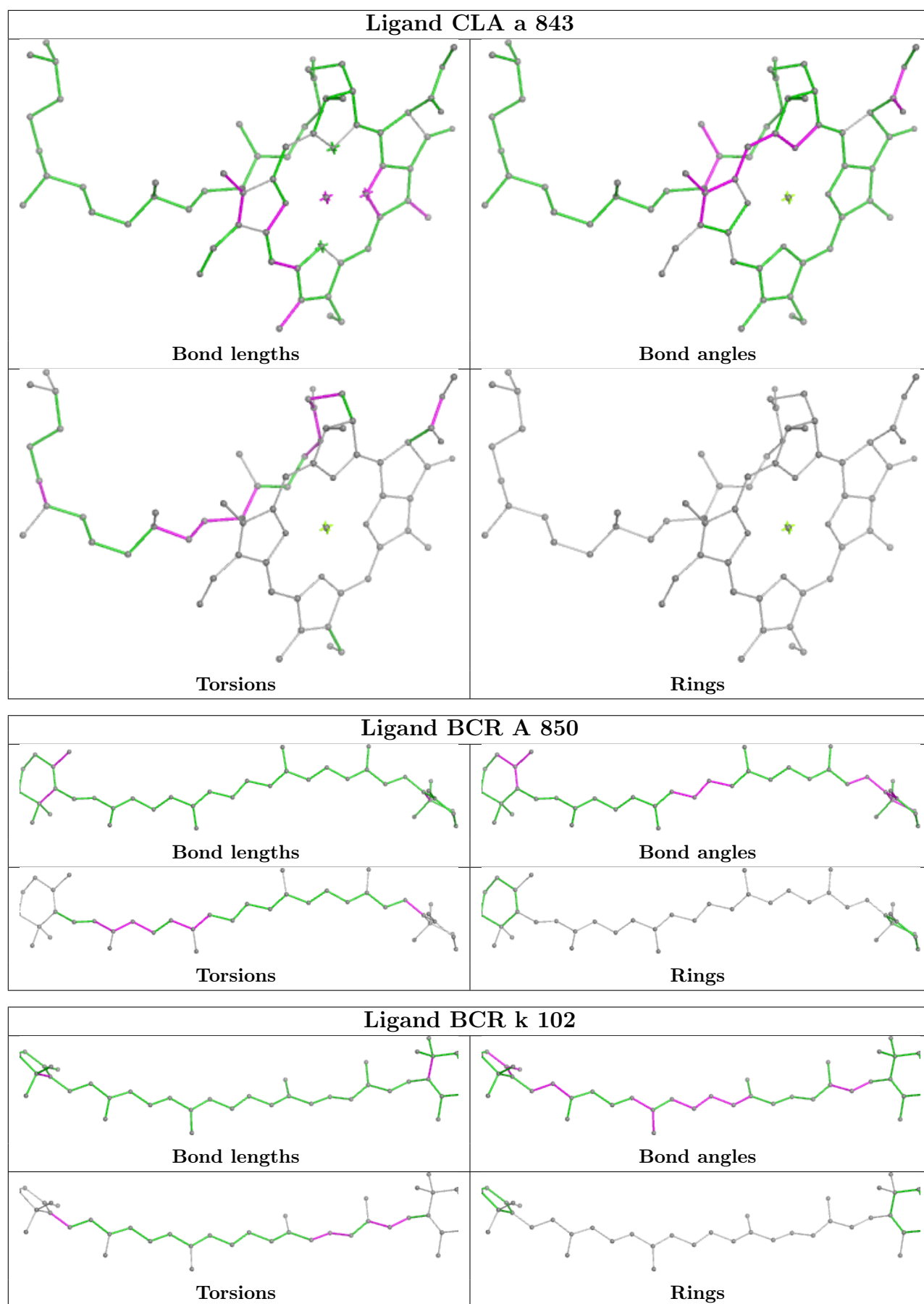


Ligand CLA 1 1603

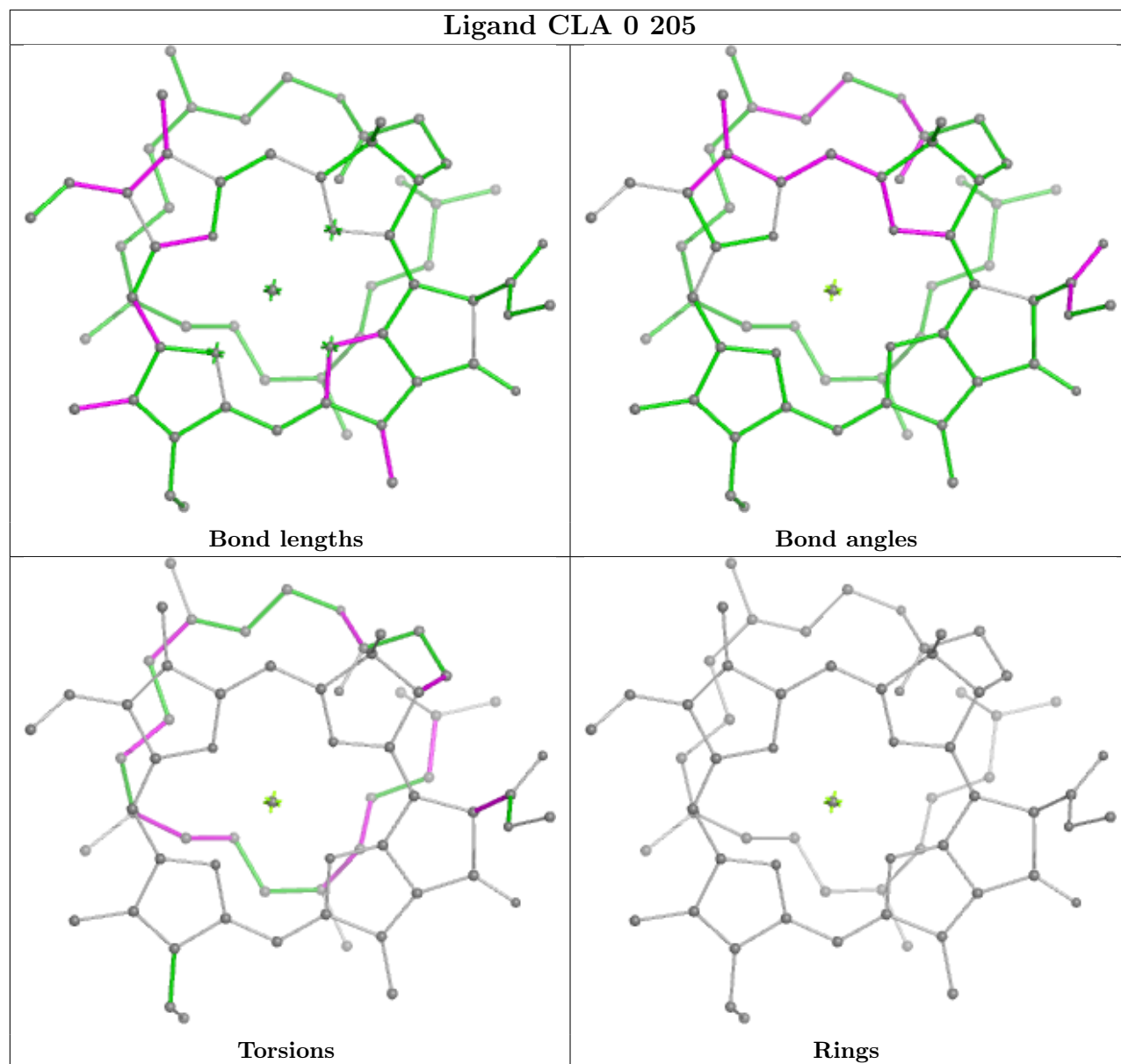




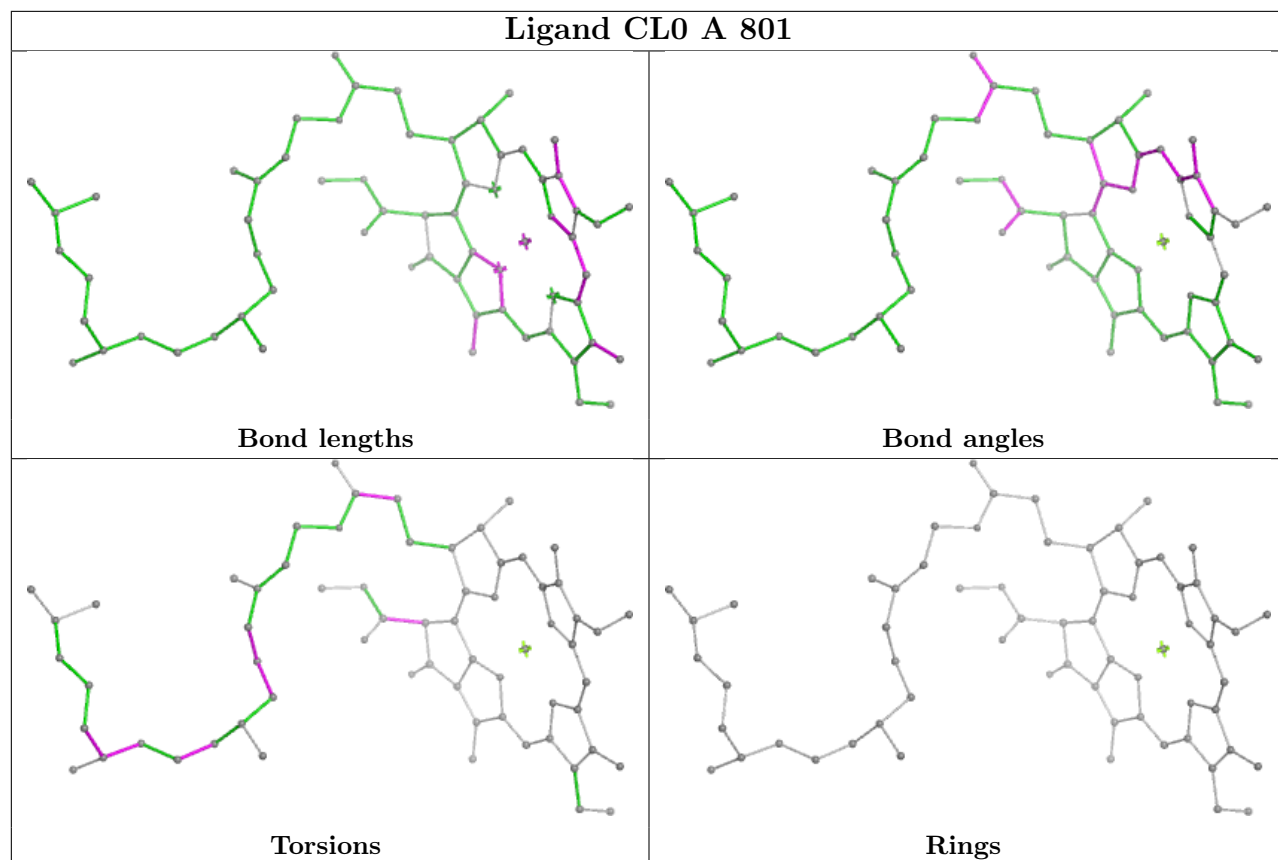




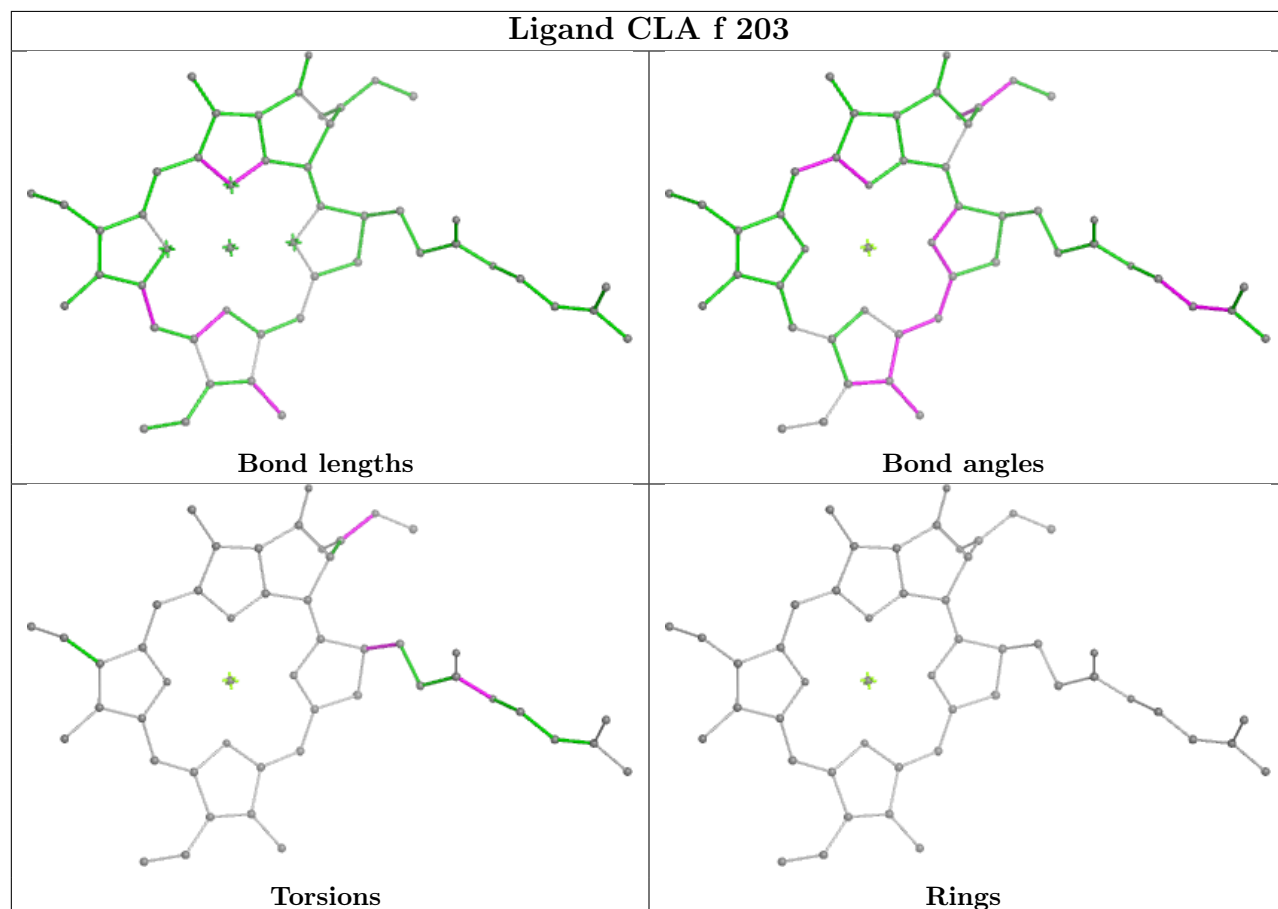
Ligand CLA 0 205

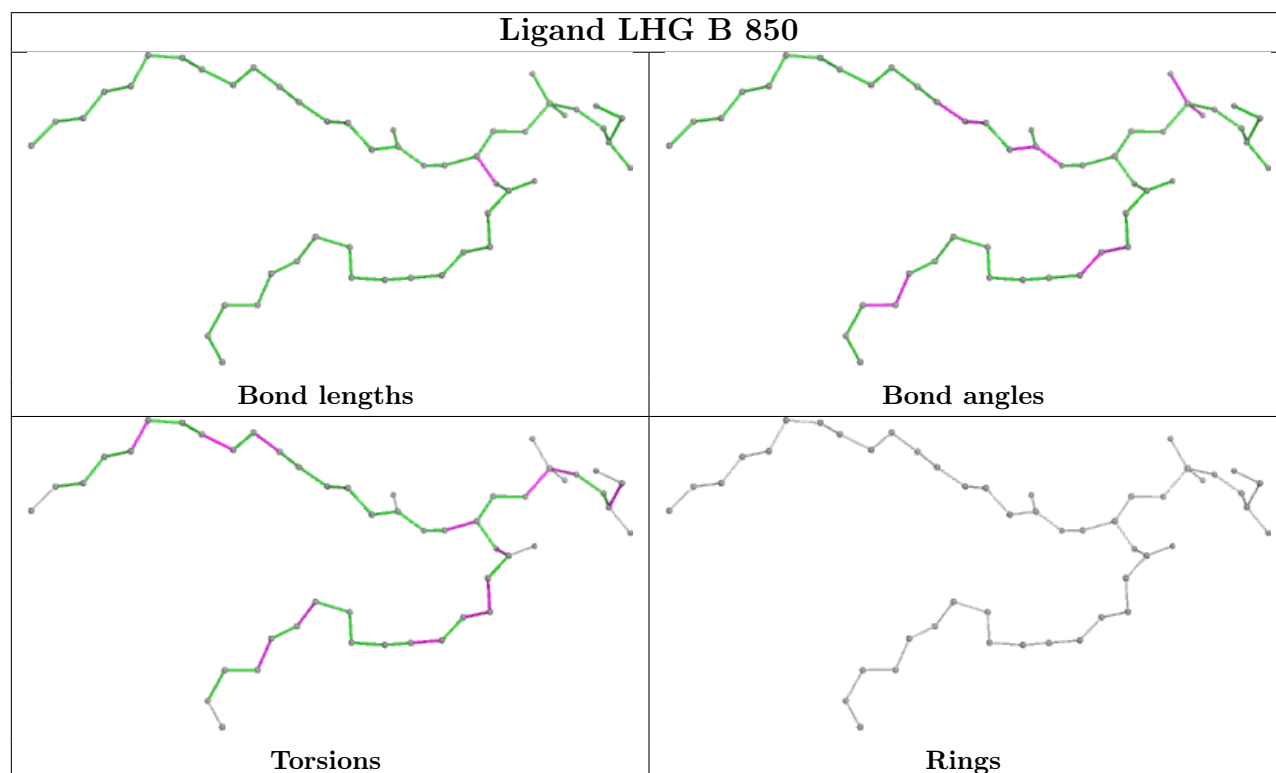
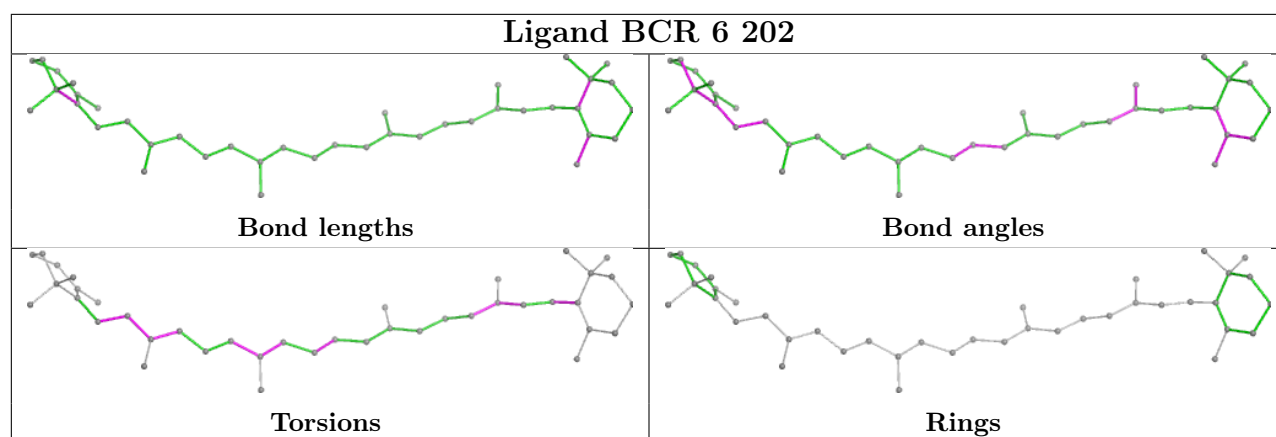


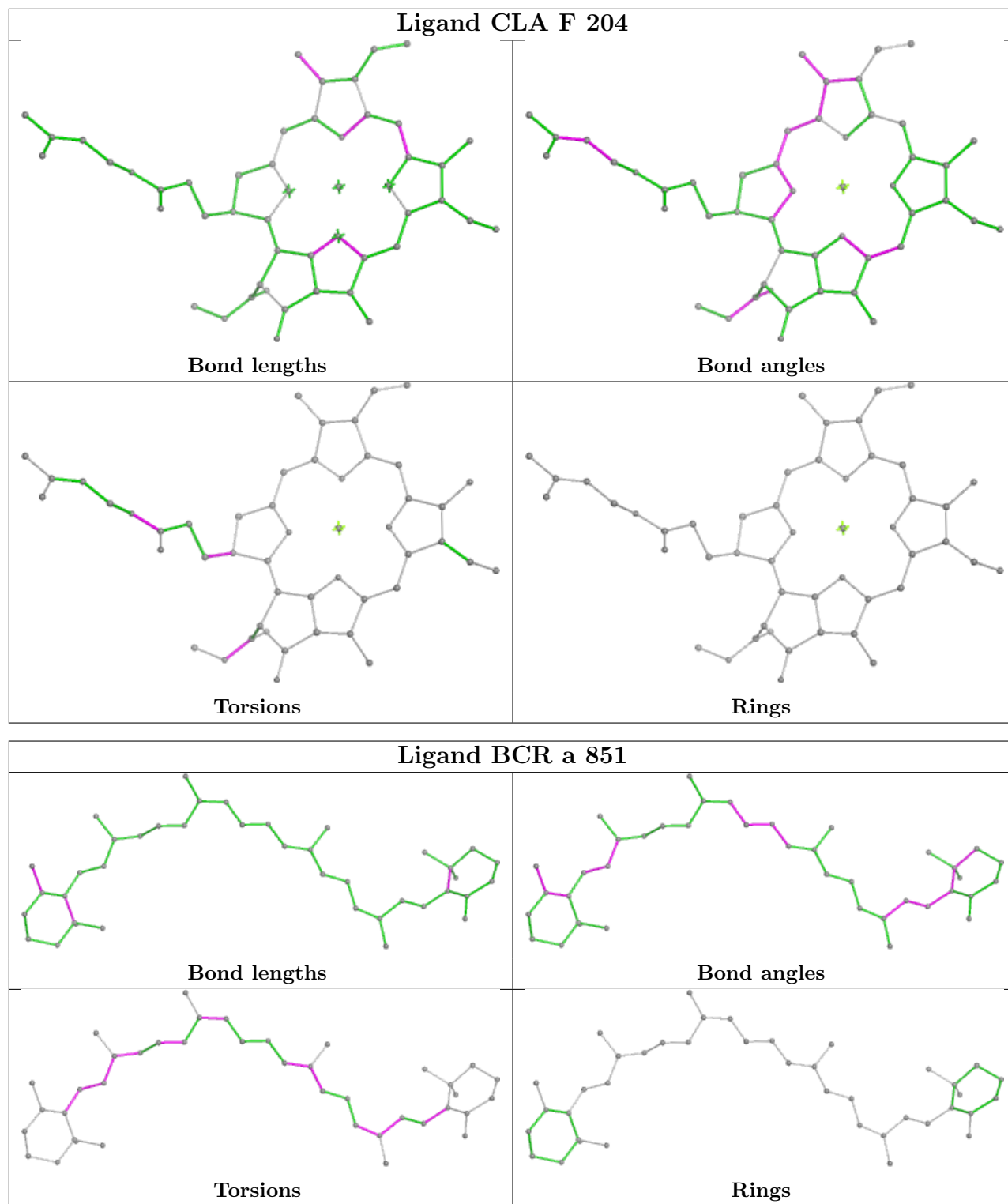
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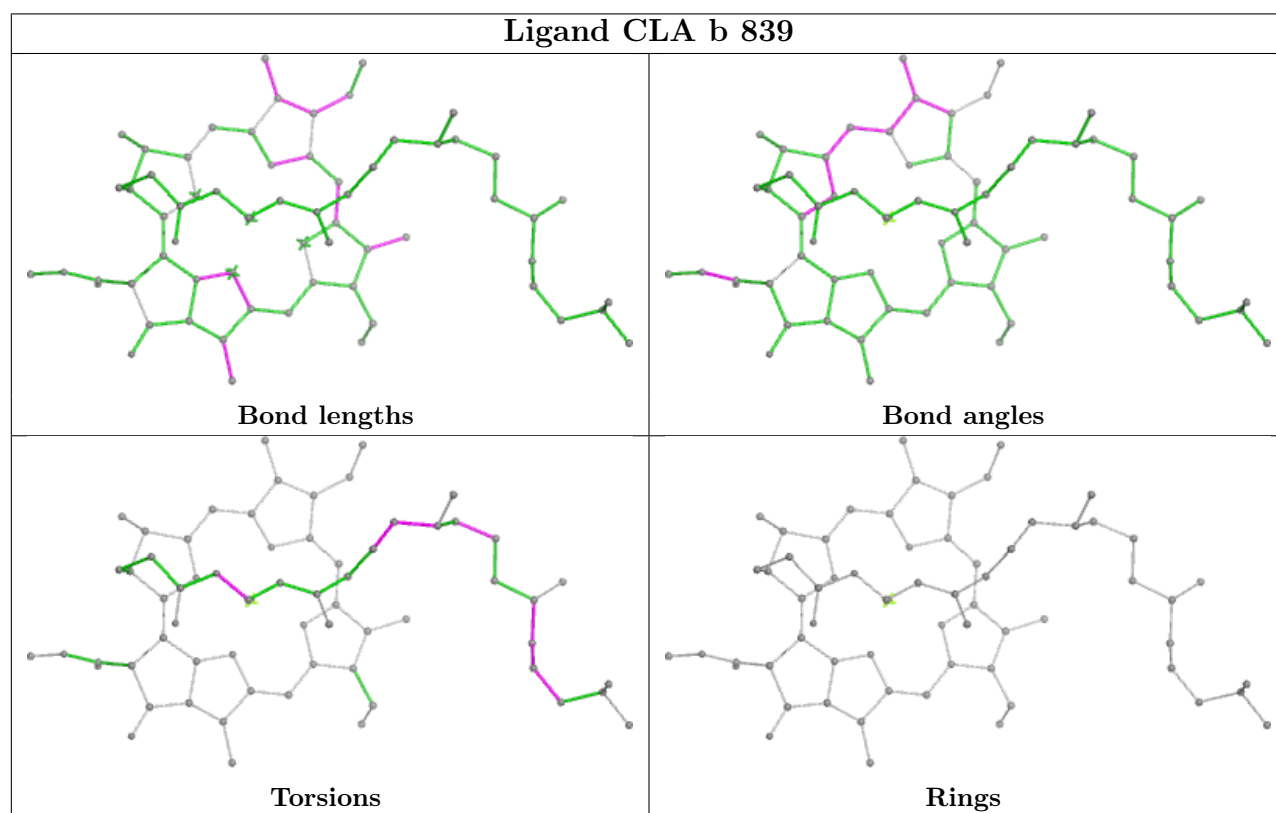
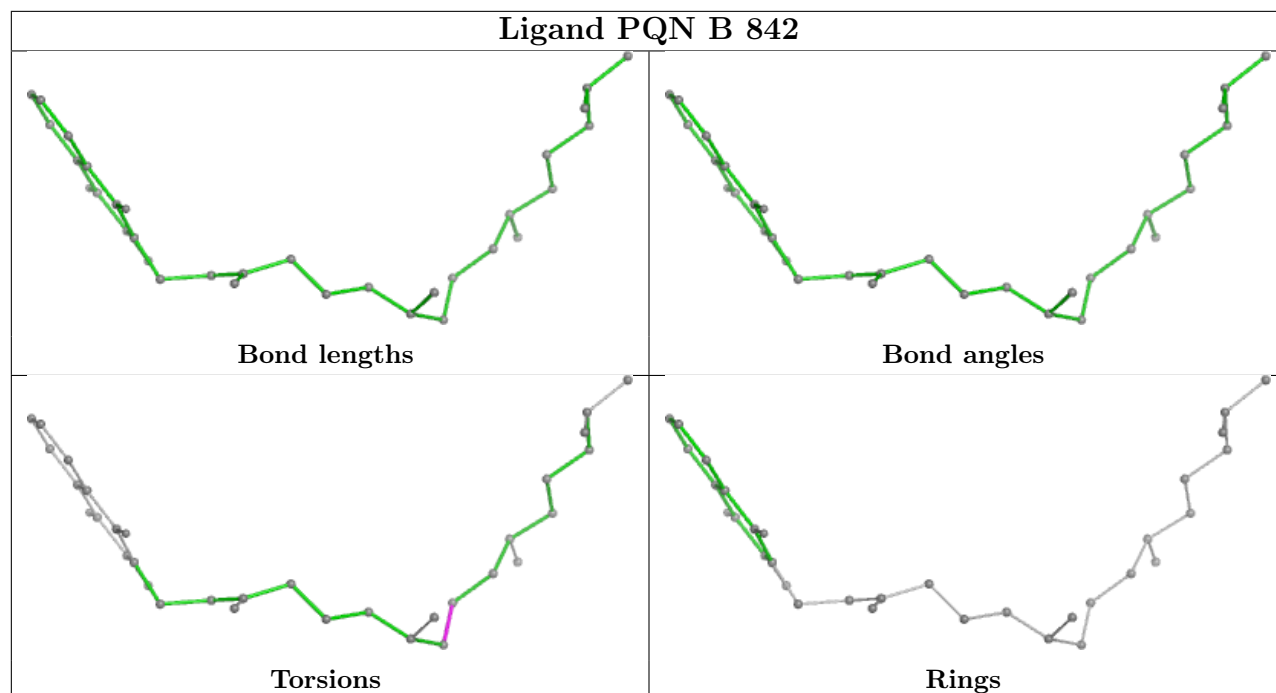


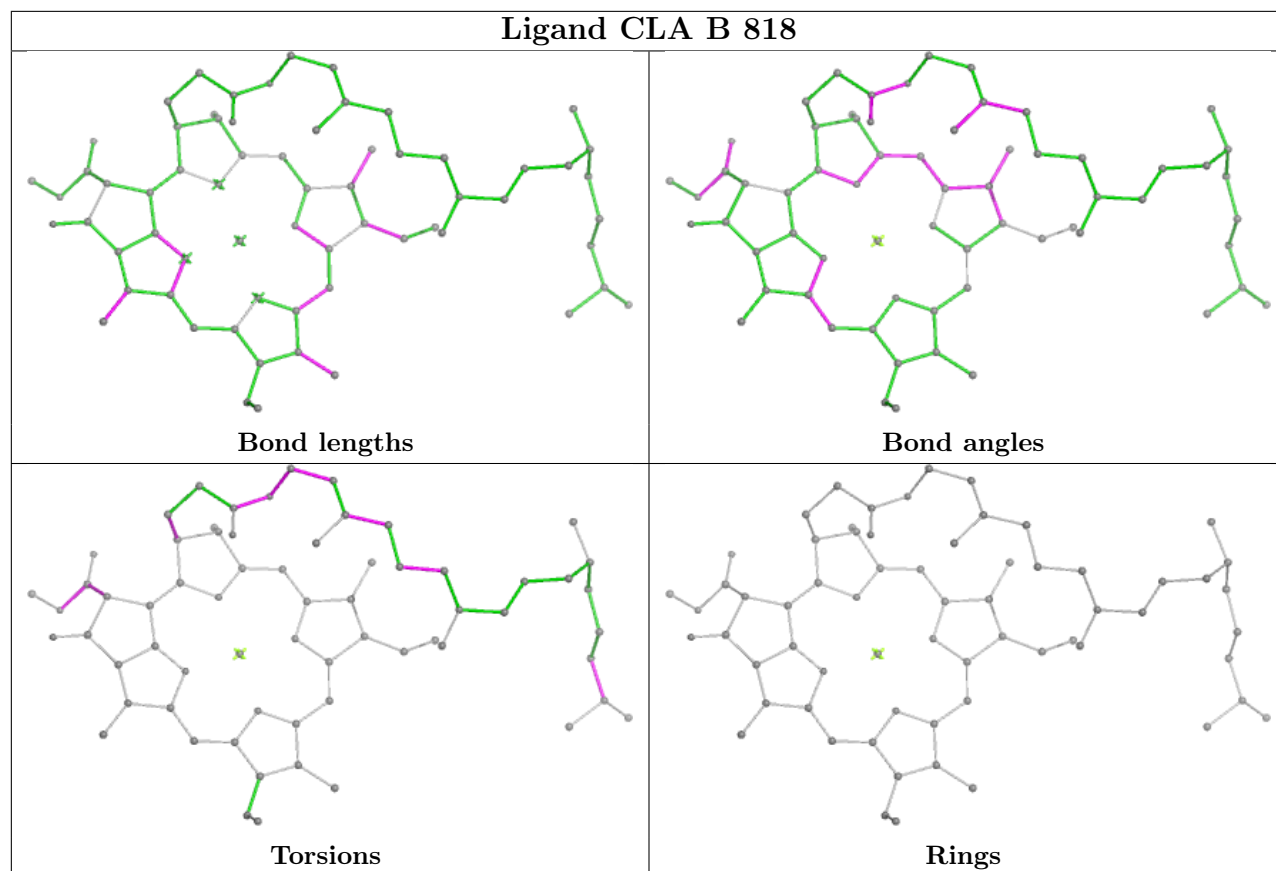
Ligand CLA f 203



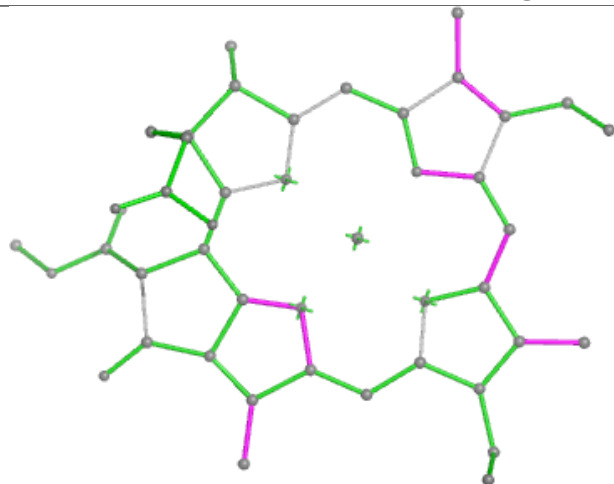




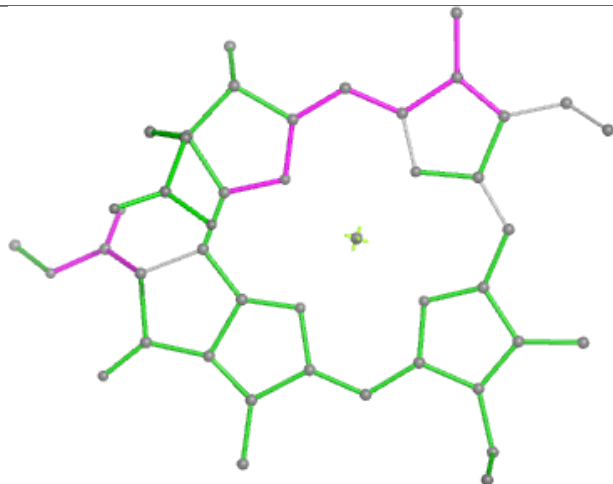


Ligand CLA B 818

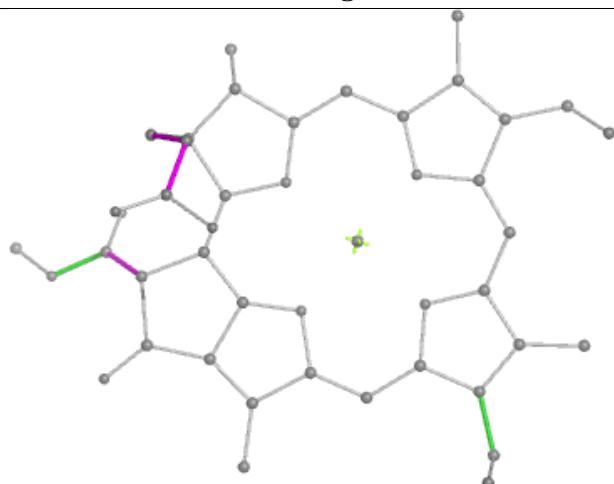
Ligand CLA a 813



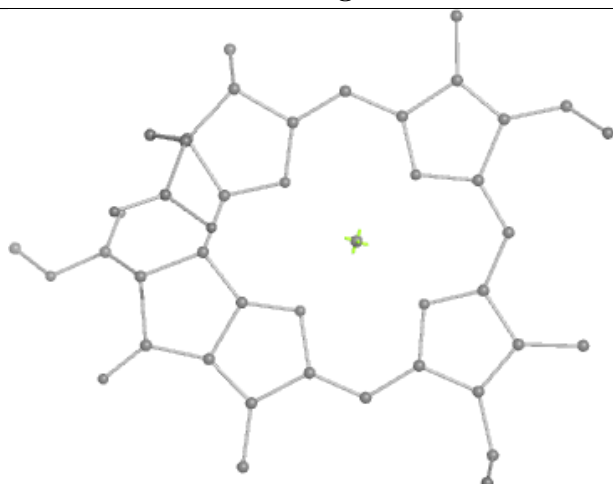
Bond lengths



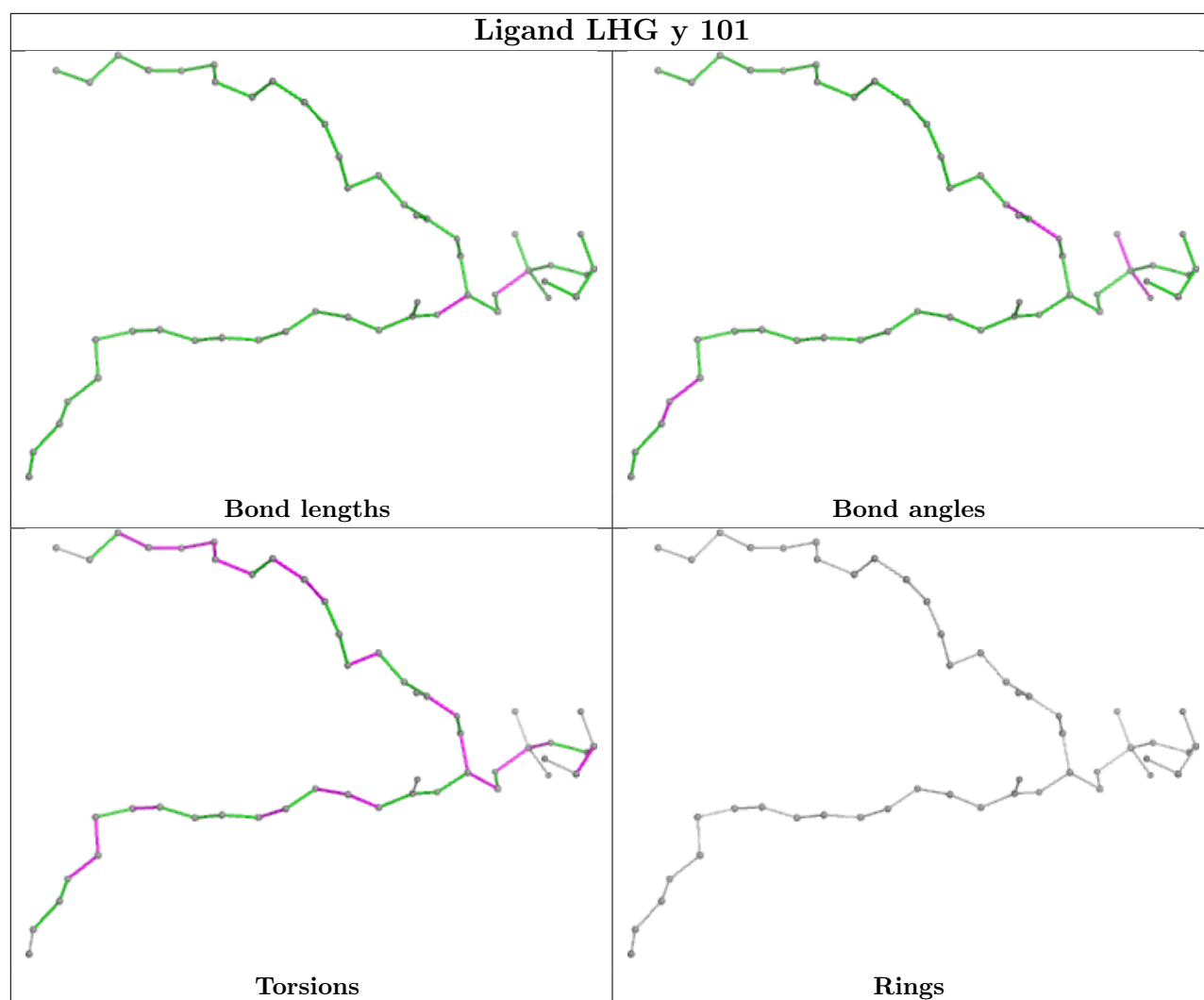
Bond angles

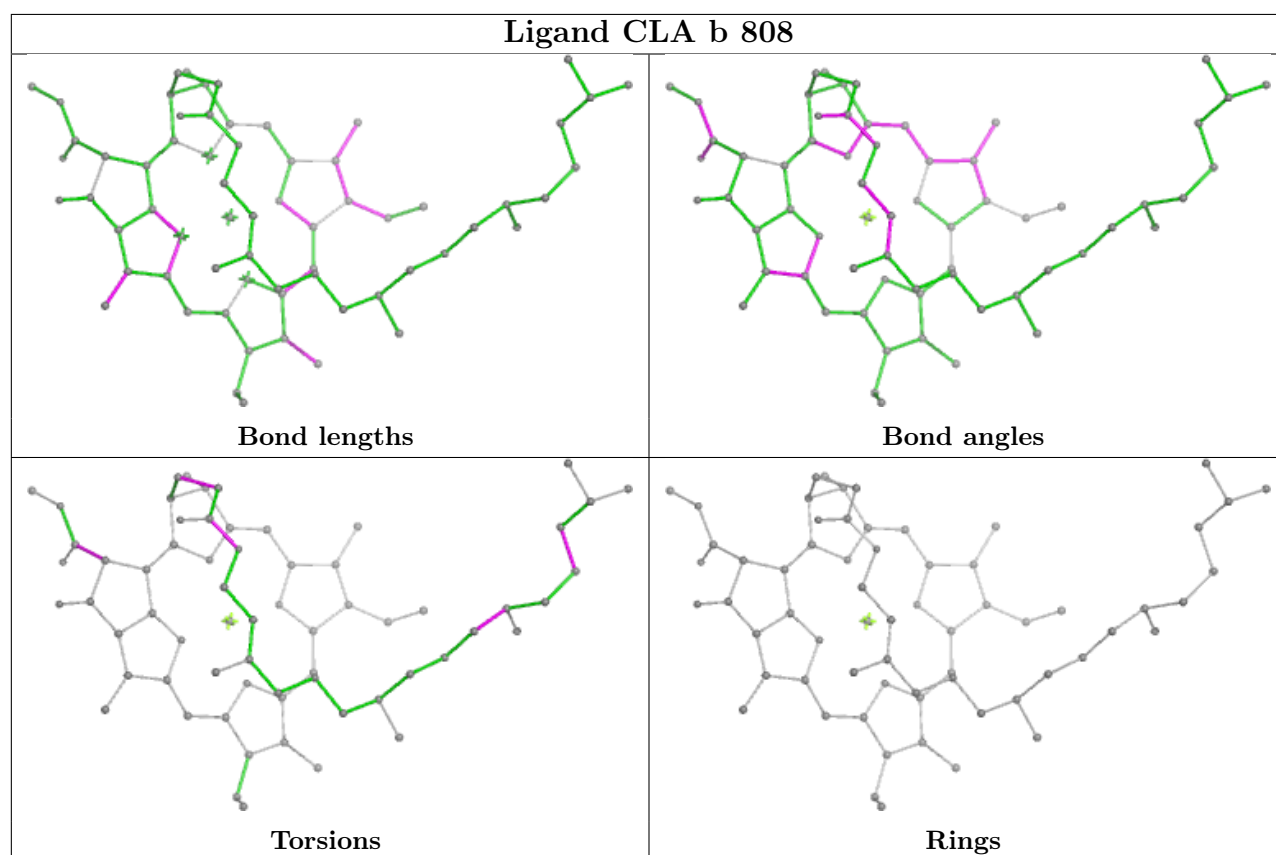
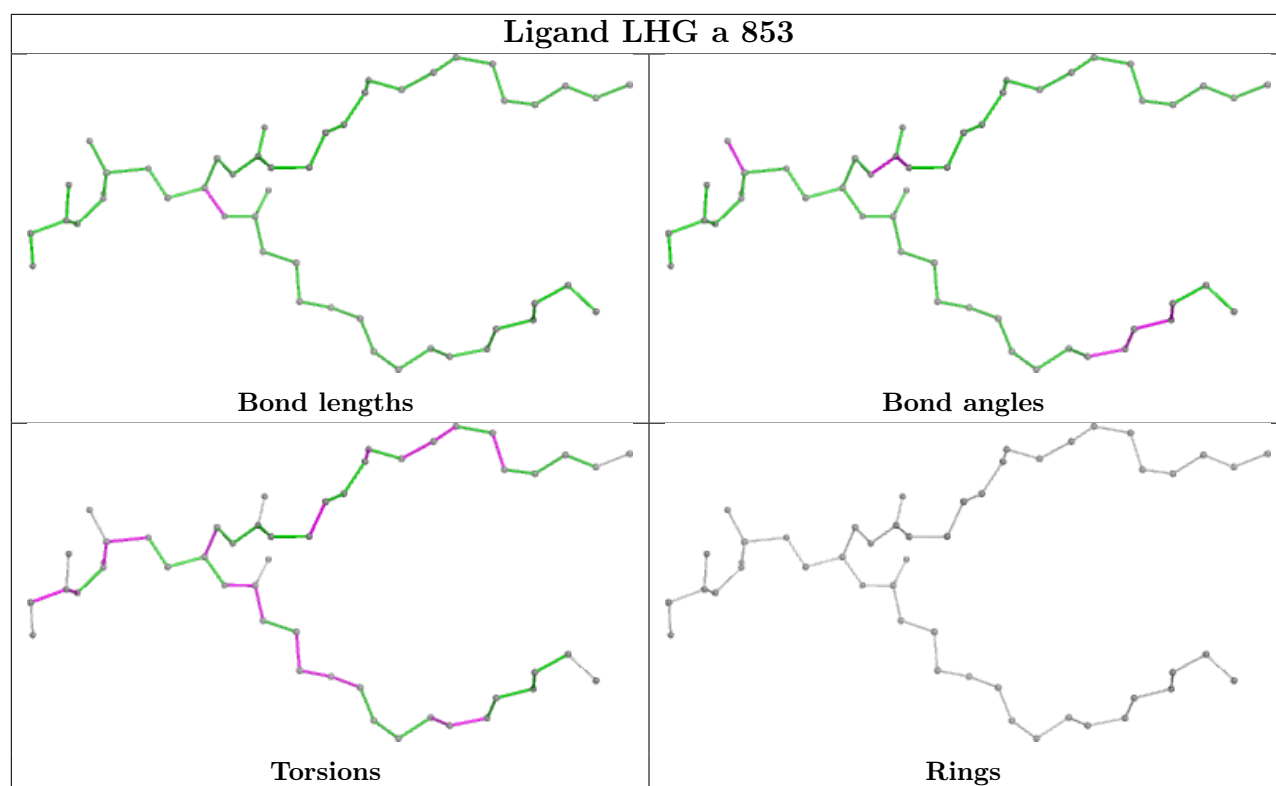


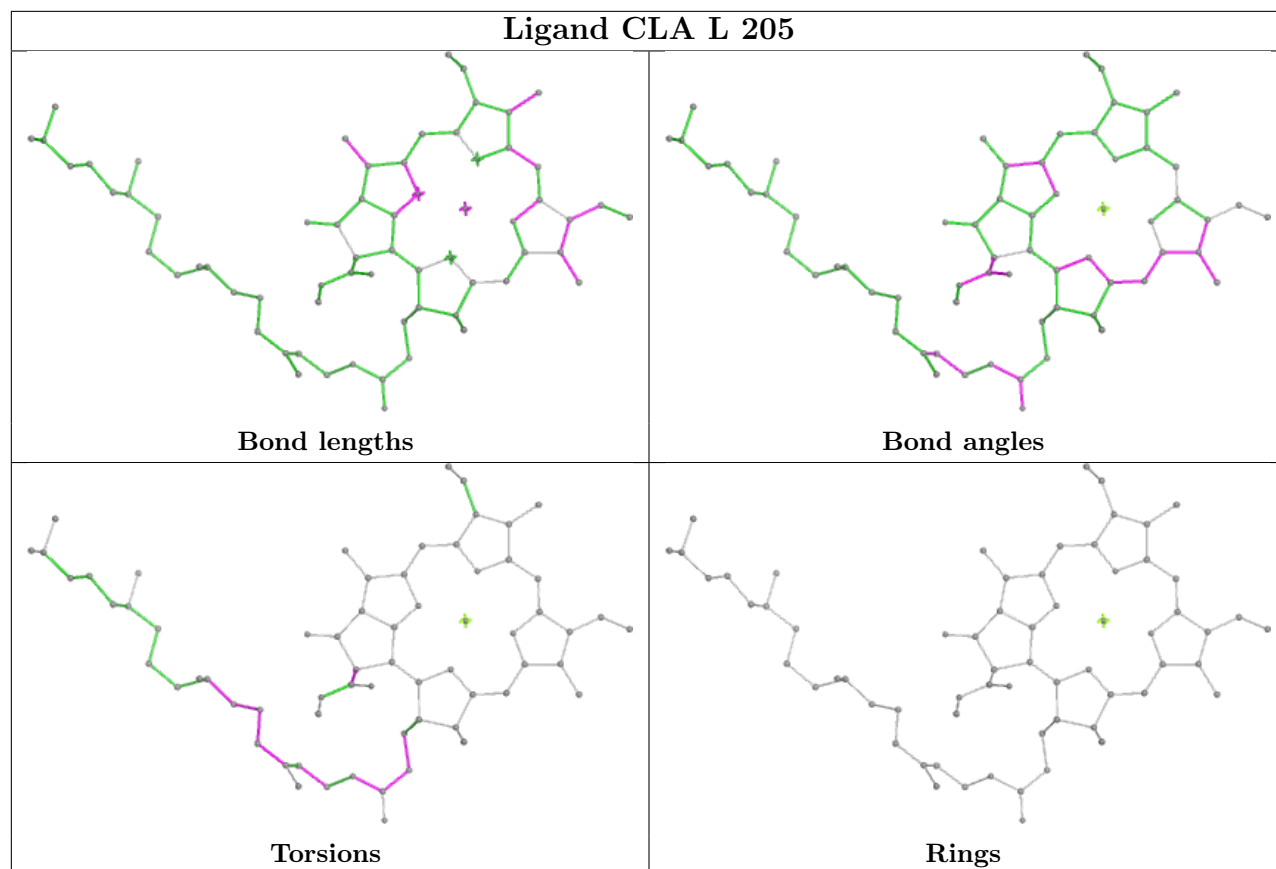
Torsions



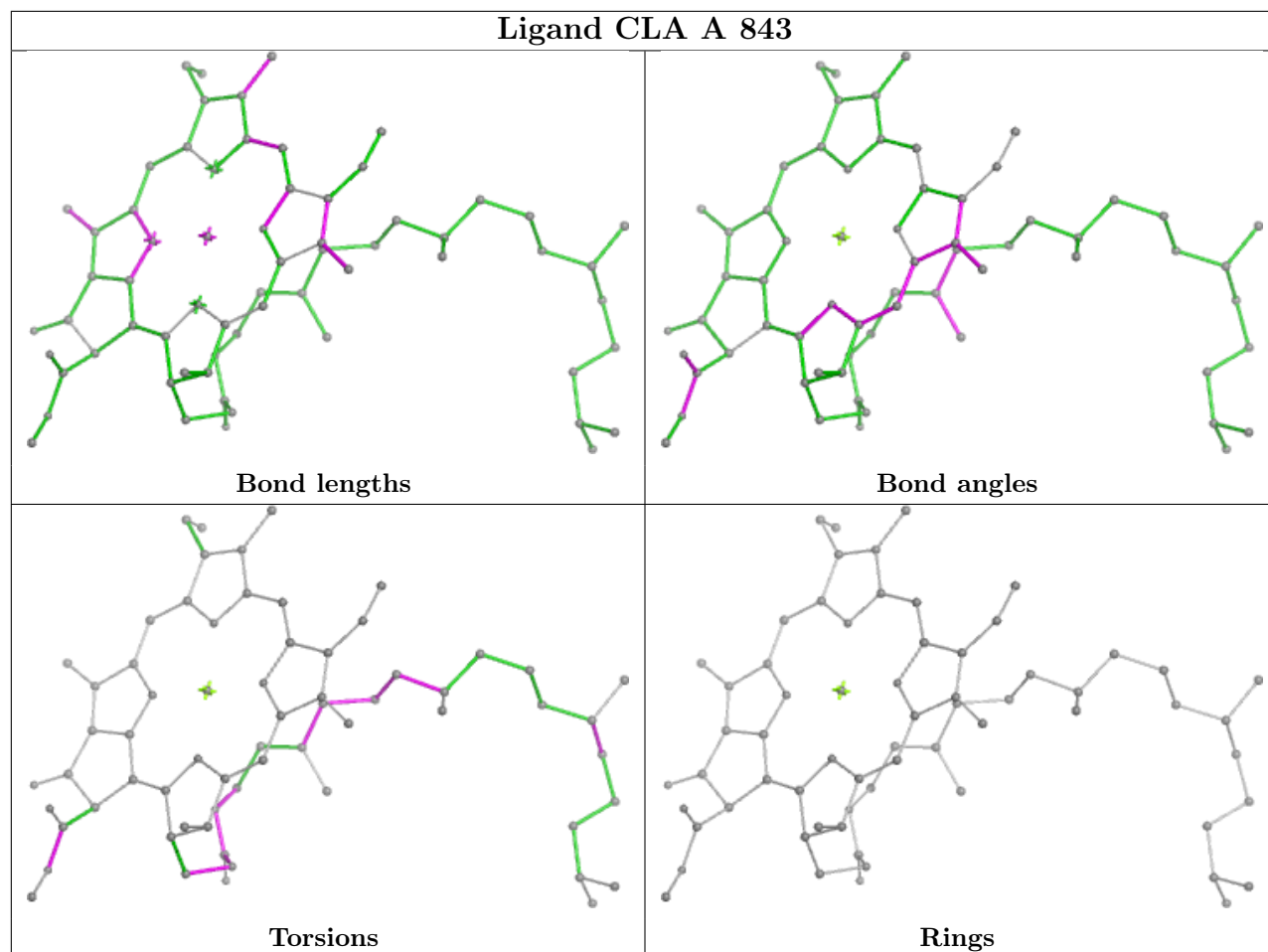
Rings



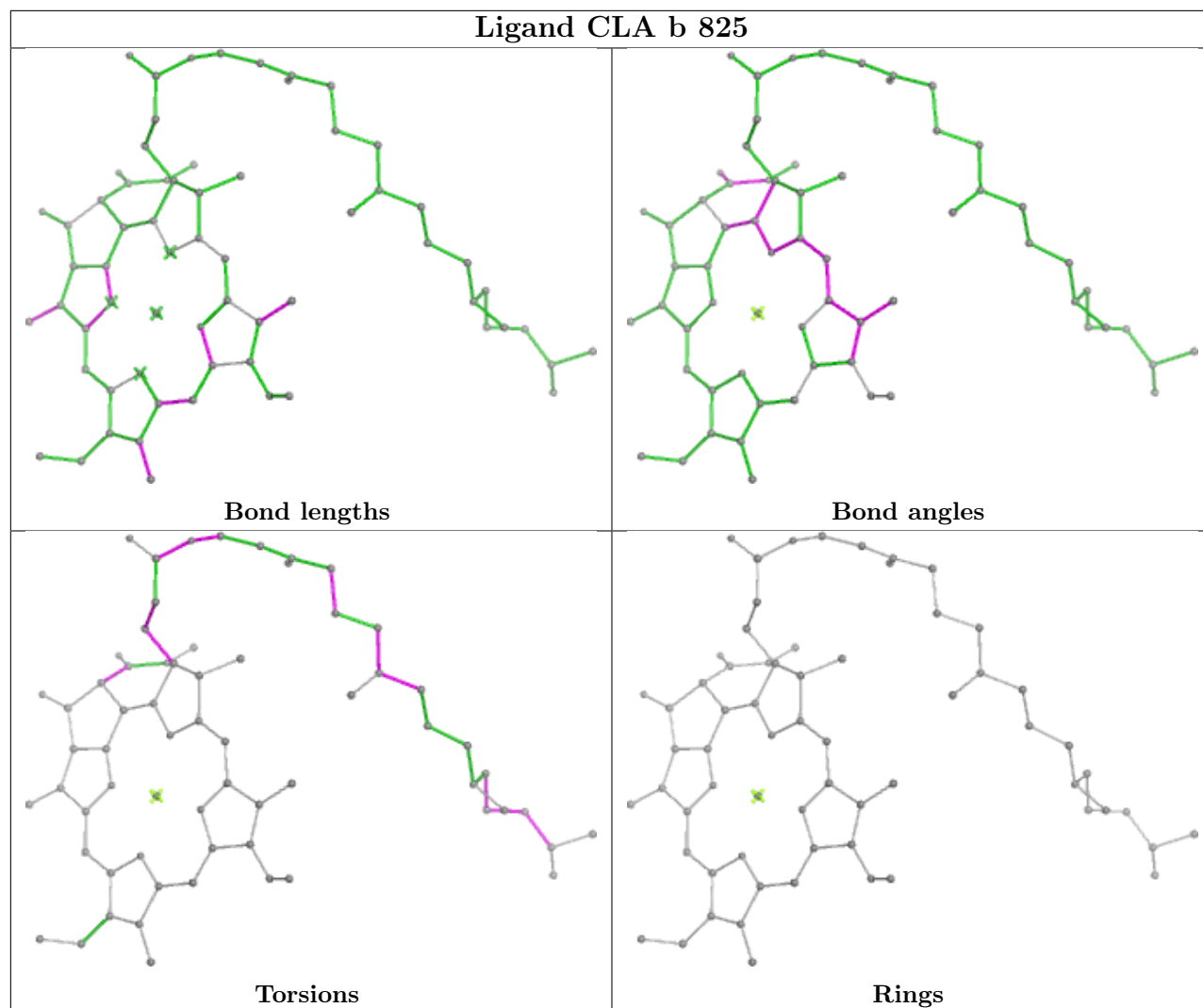


Ligand CLA L 205

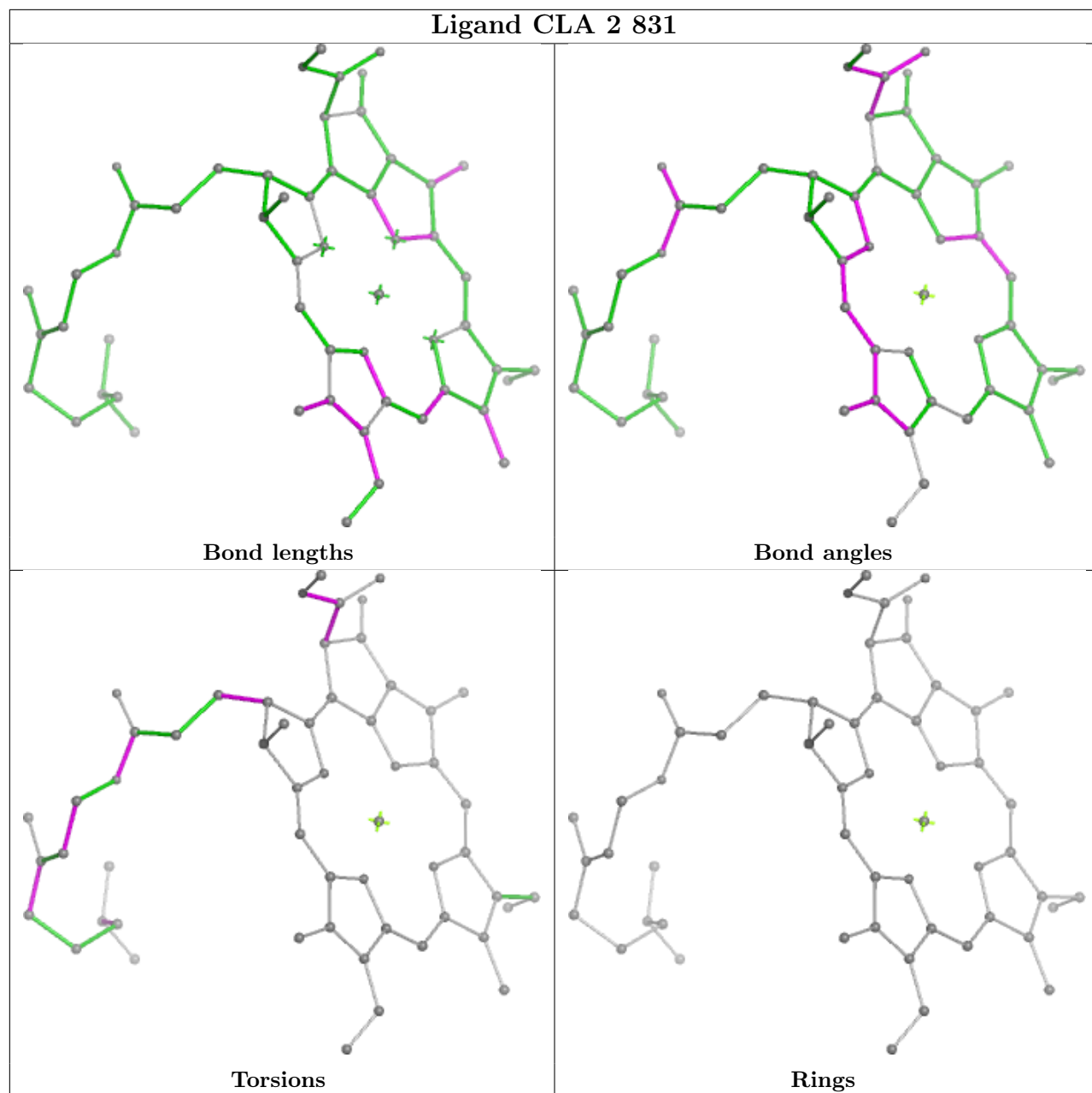
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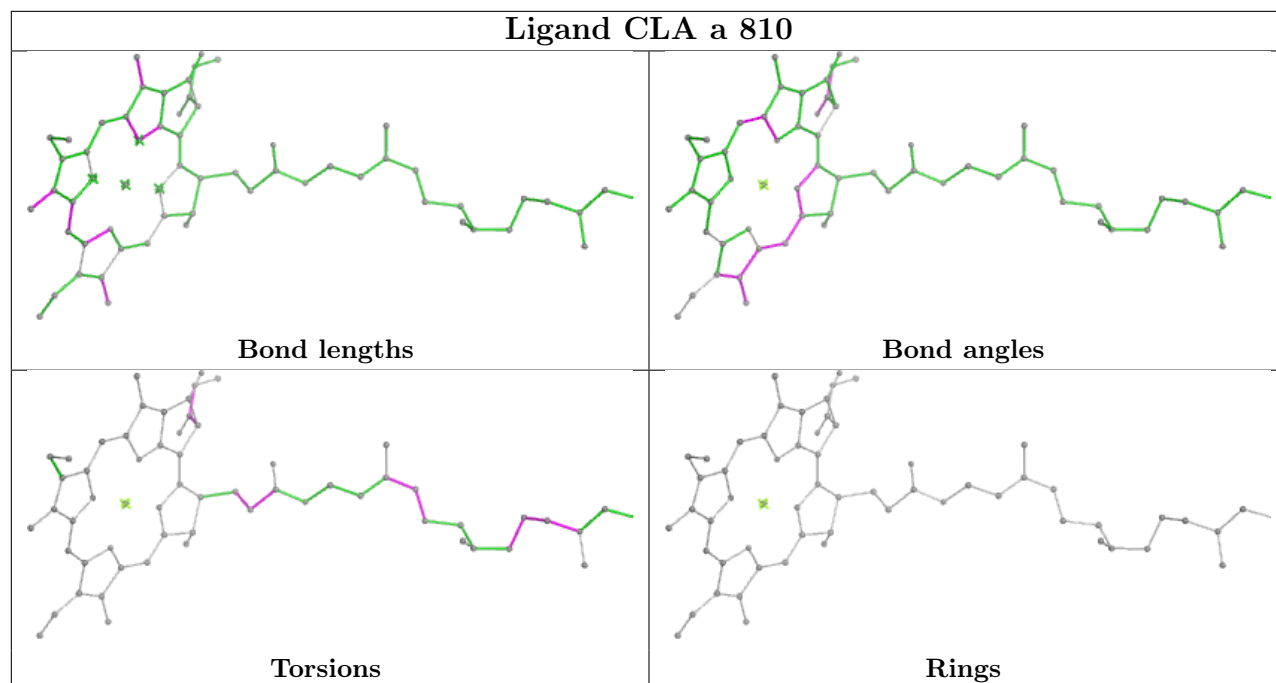
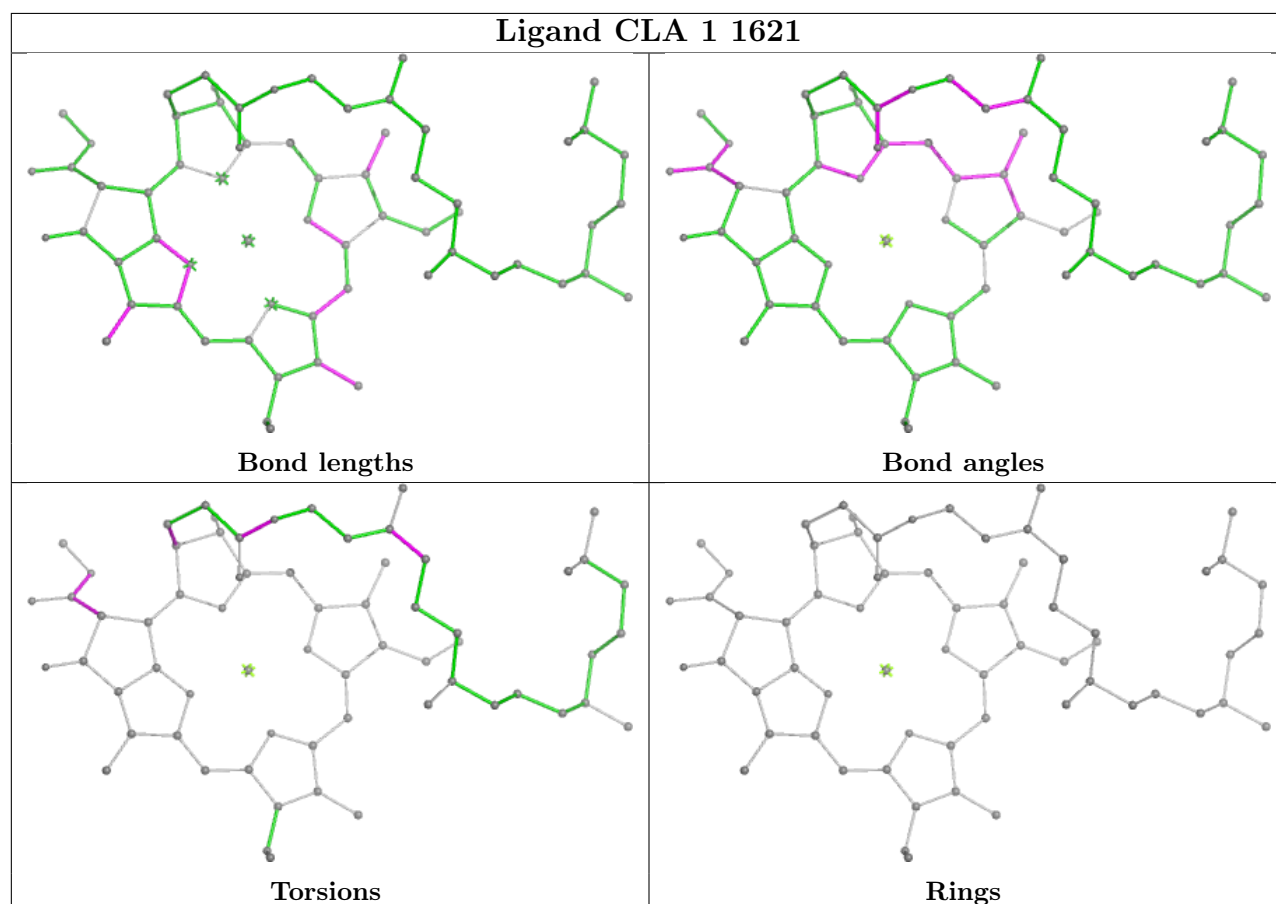


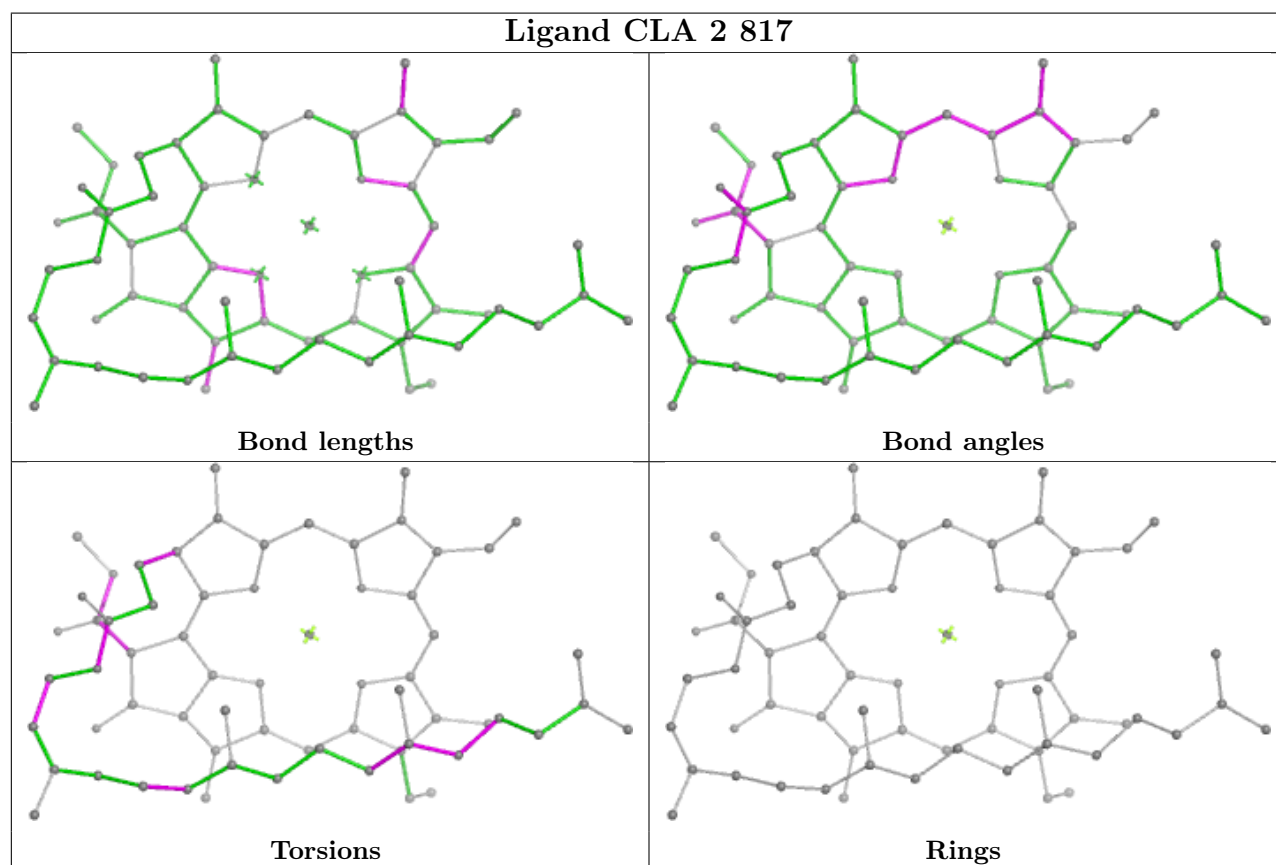
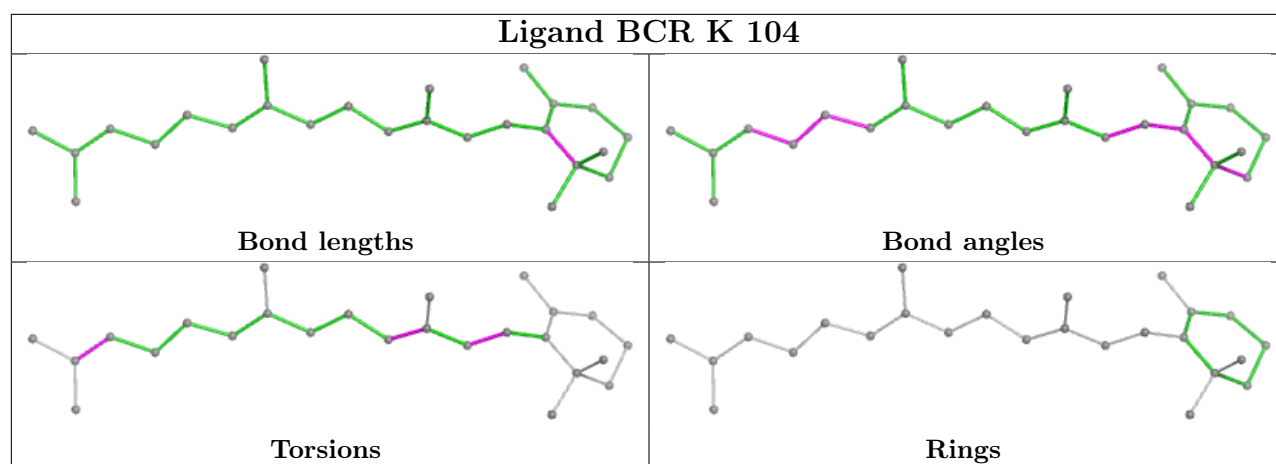
Ligand CLA b 825

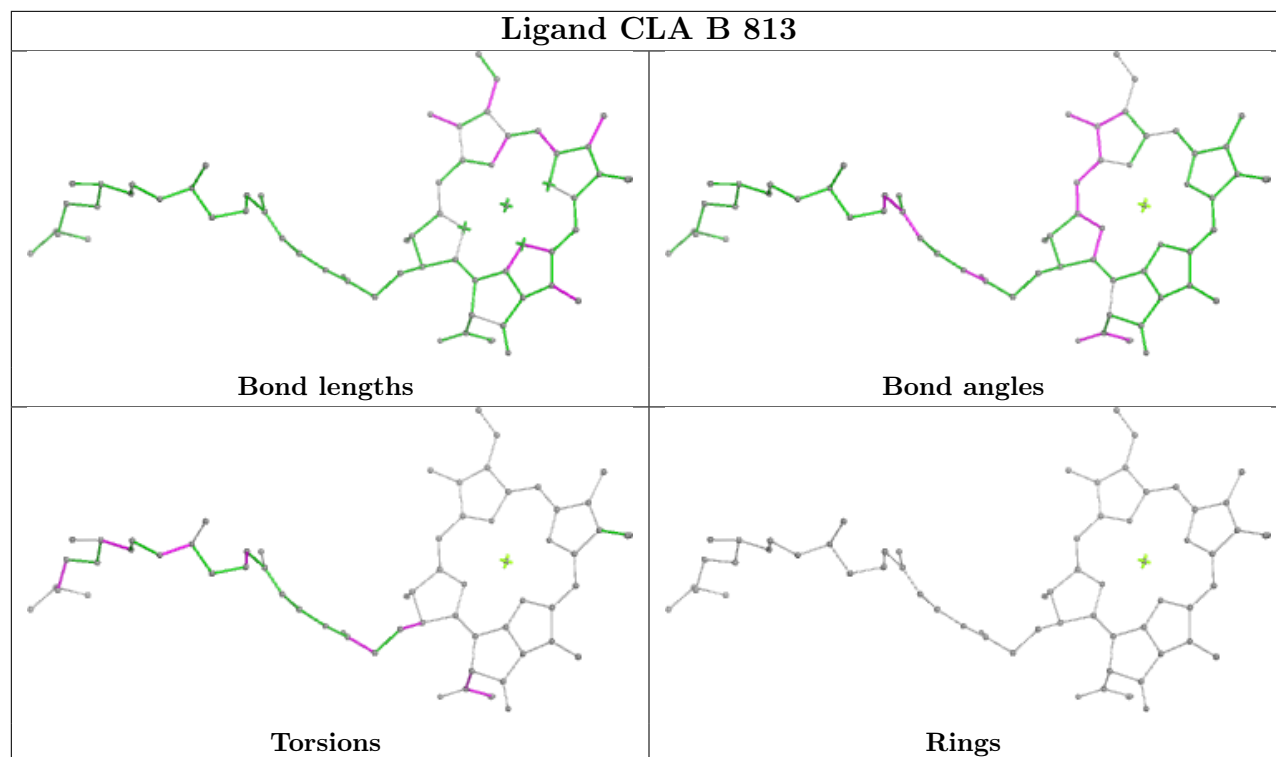
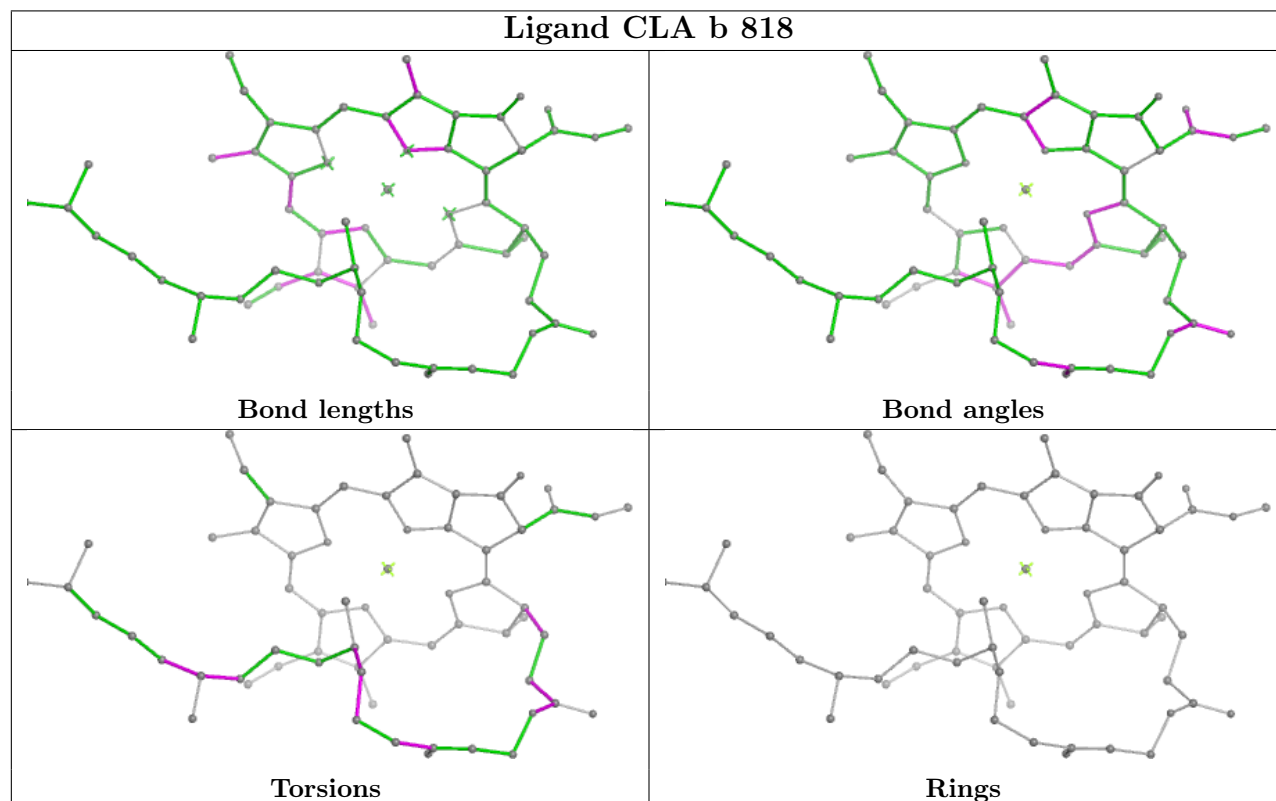


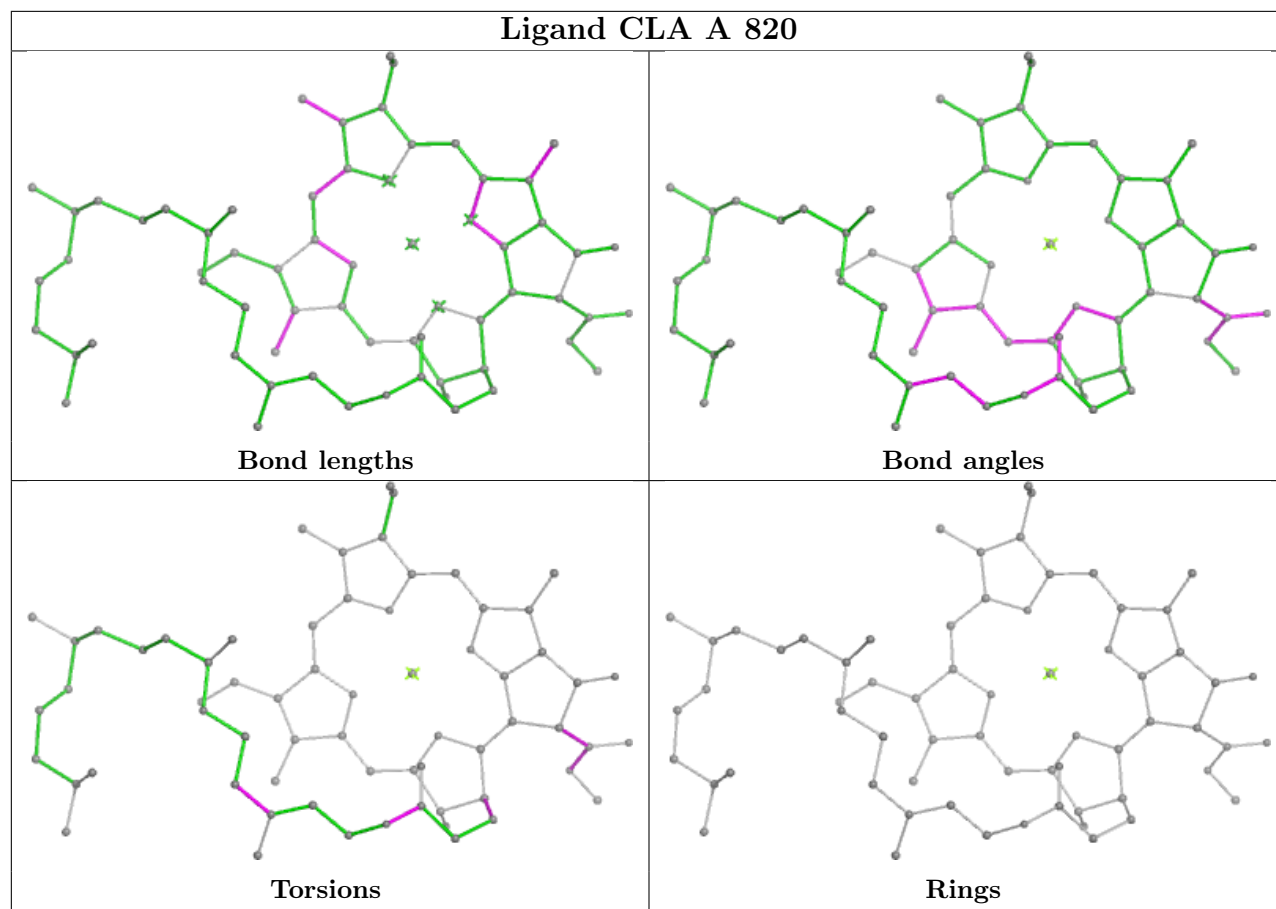
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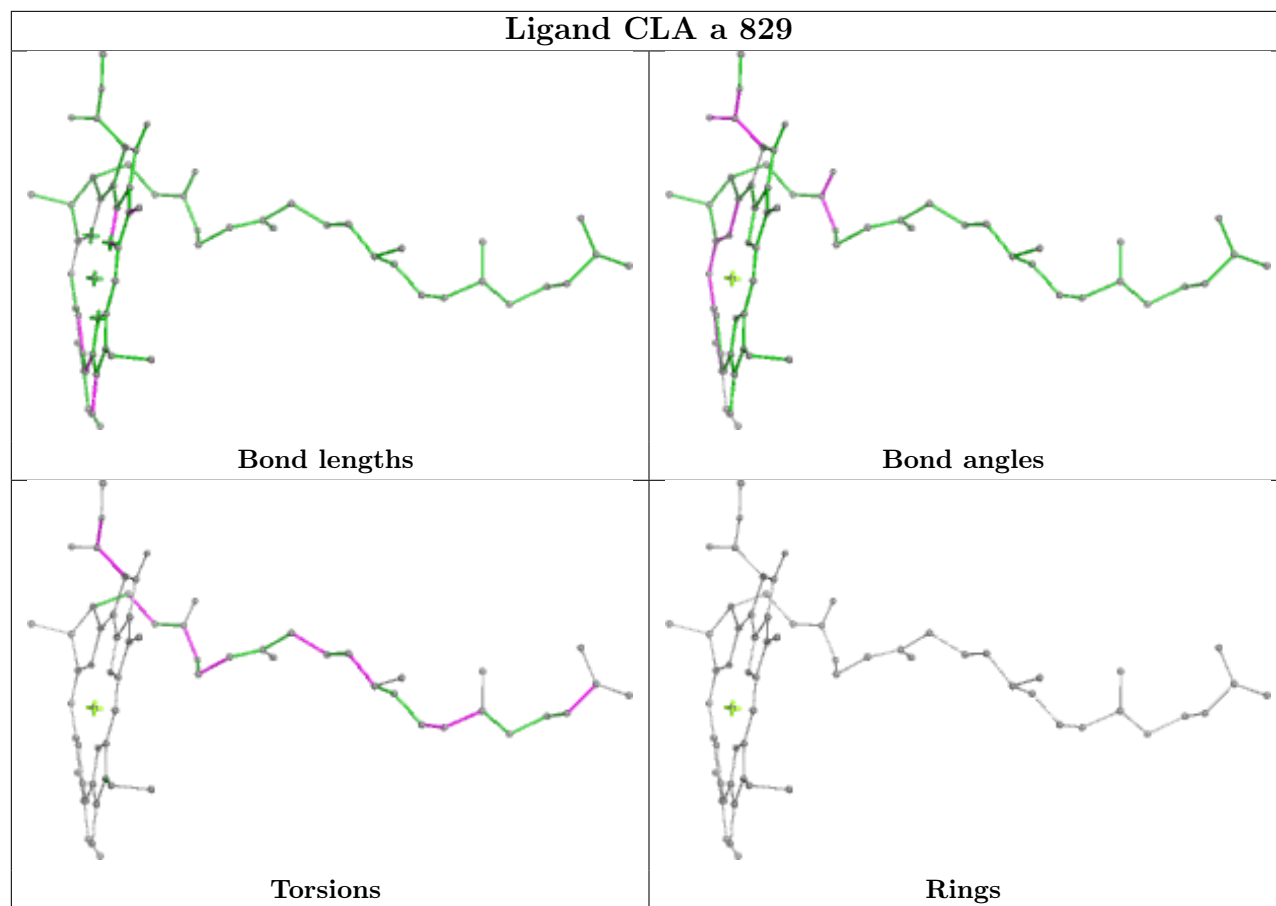
Ligand CLA a 810**Ligand CLA 1 1621**



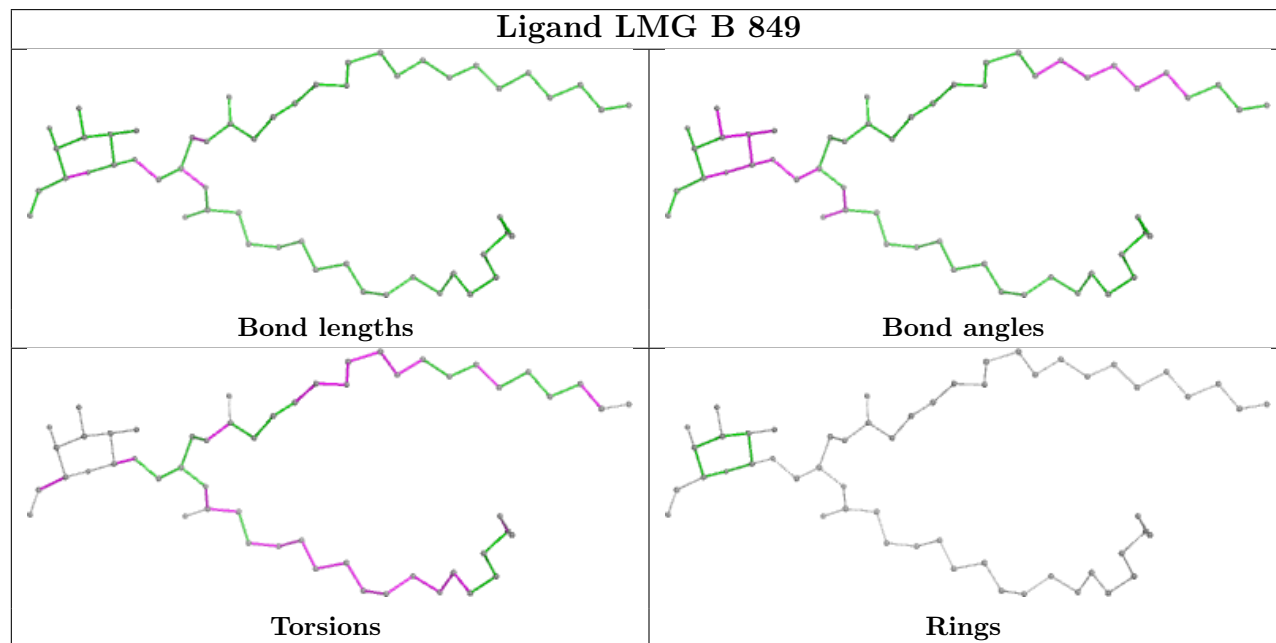
Ligand CLA B 813**Ligand CLA b 818**

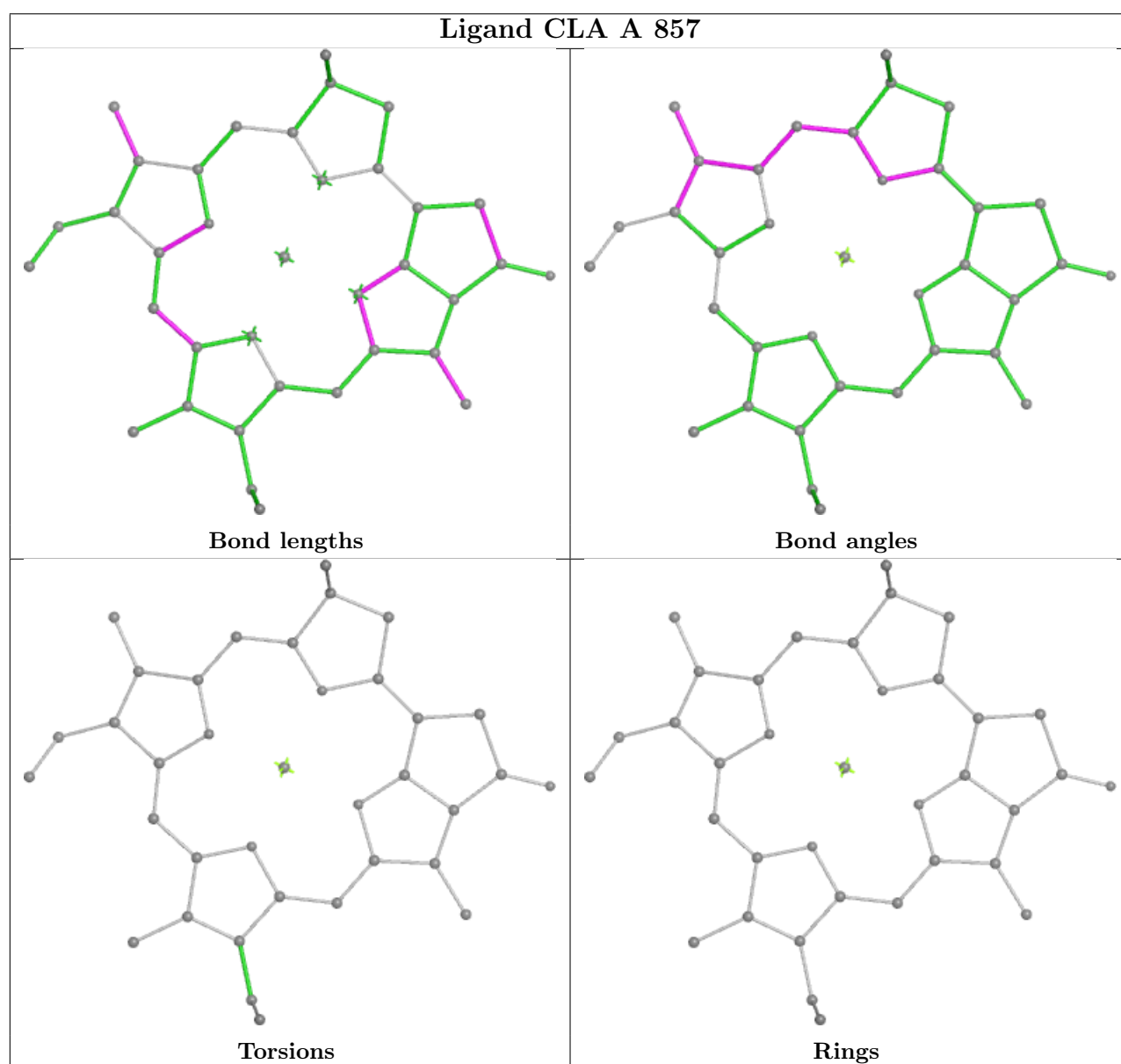
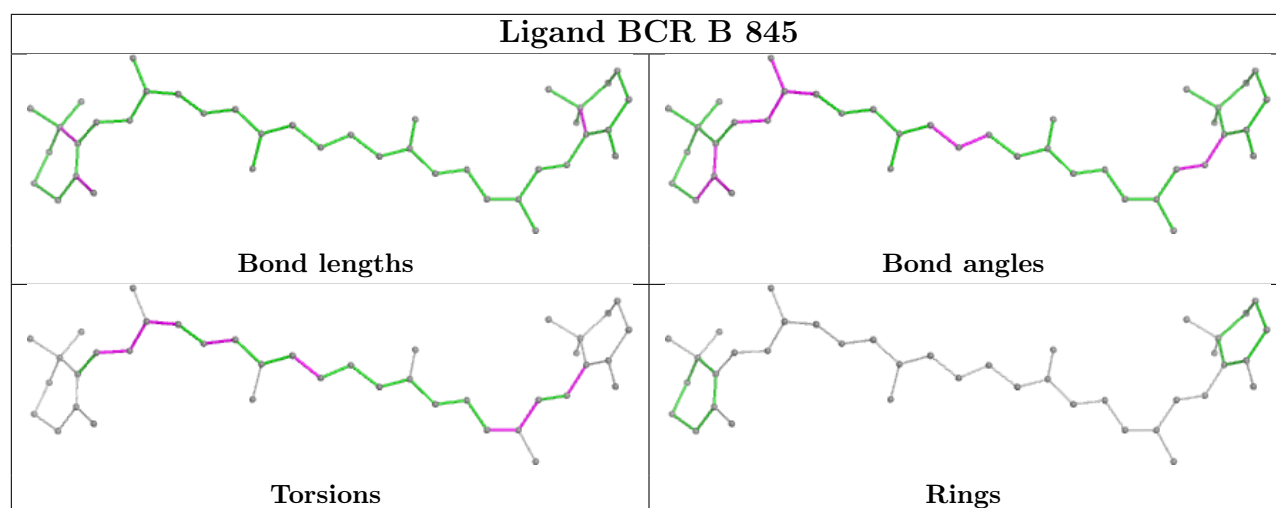


Ligand CLA a 829

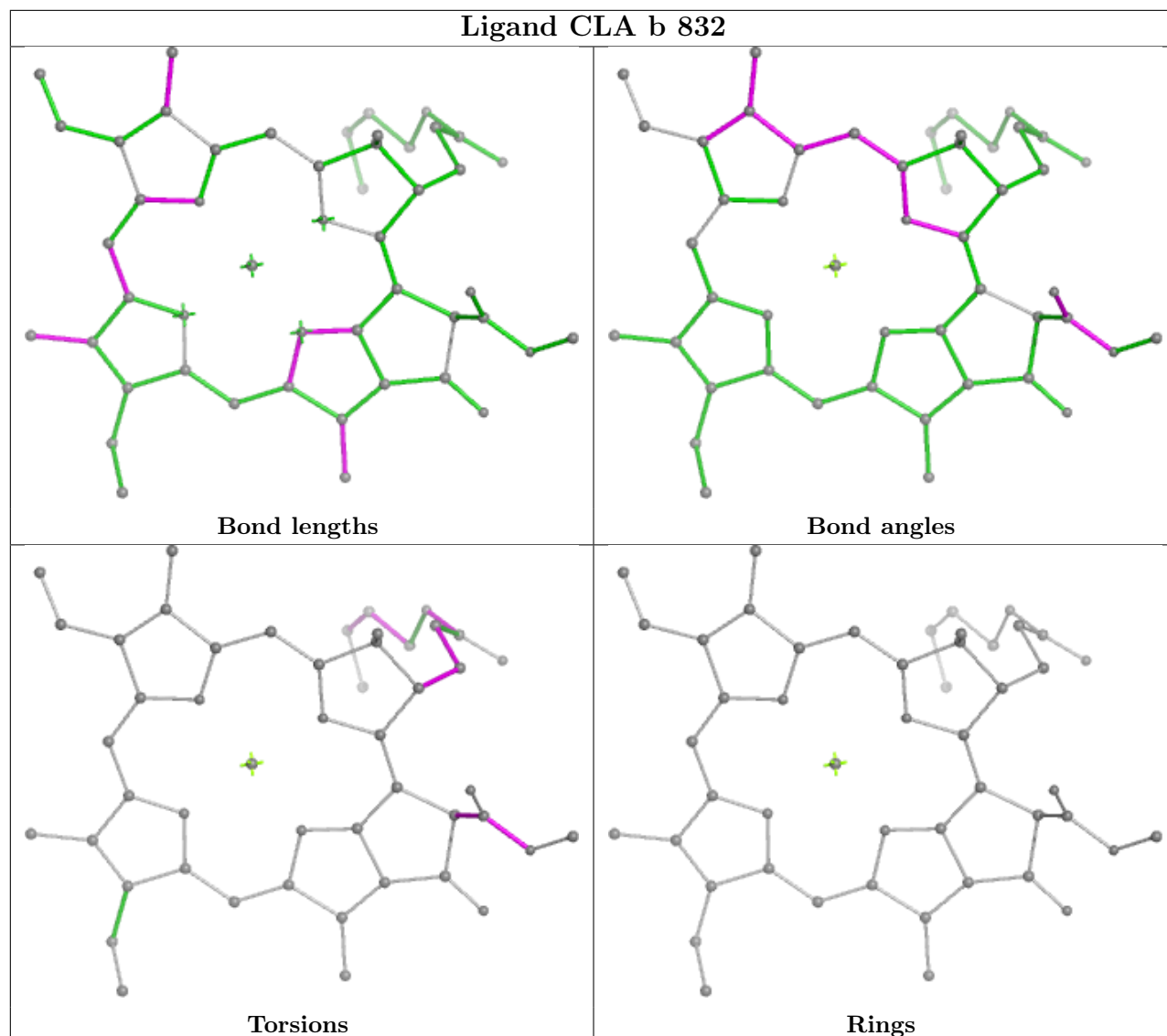


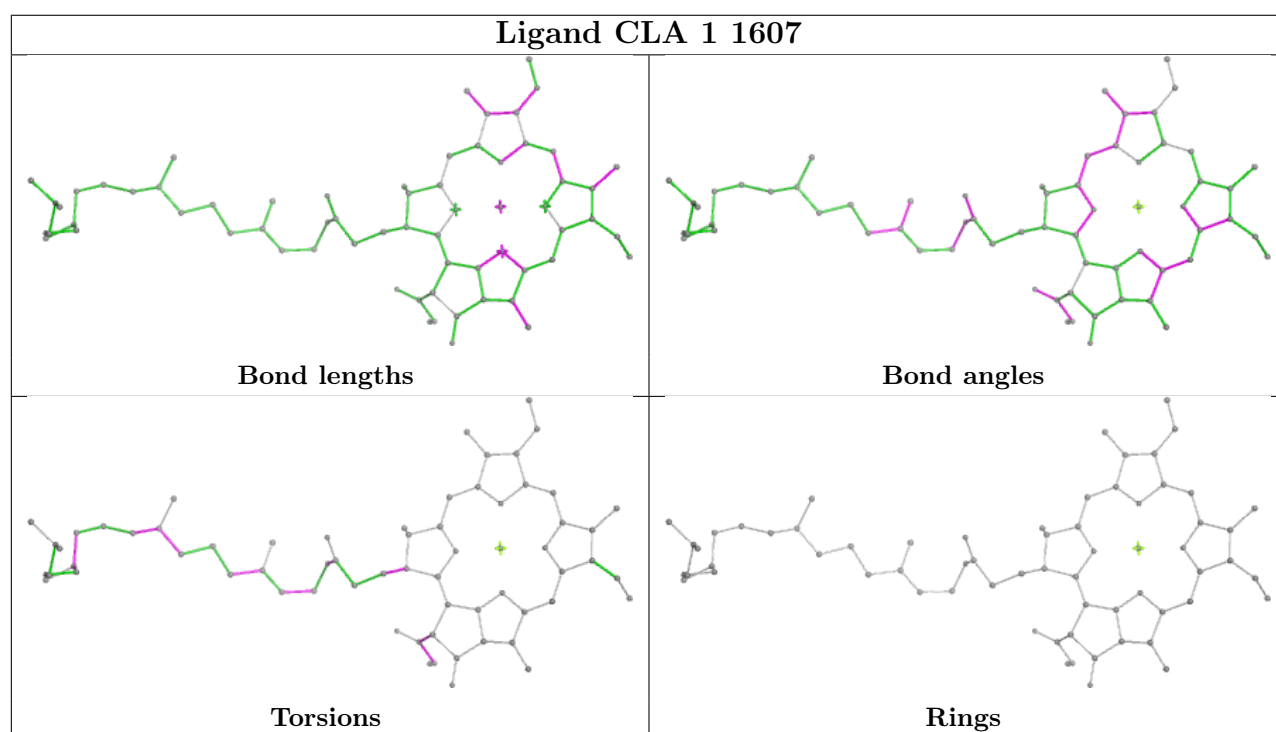
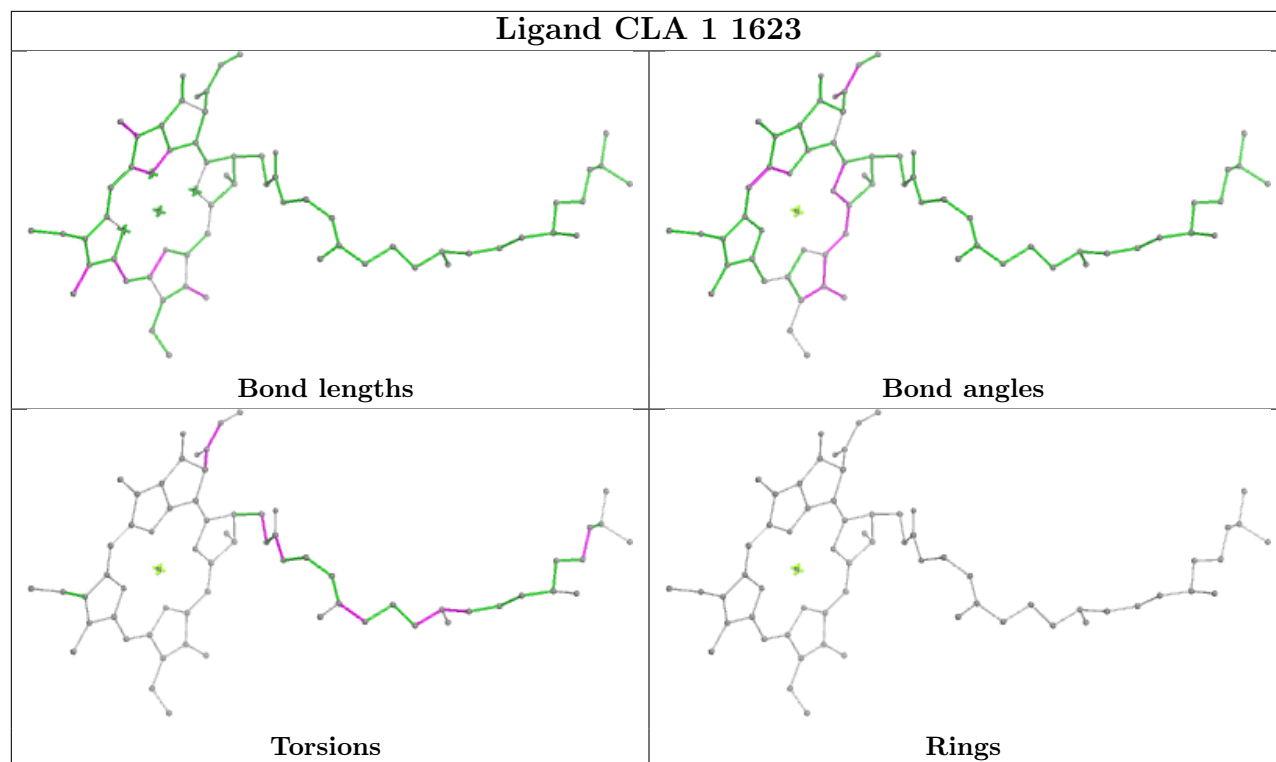
Ligand LMG B 849

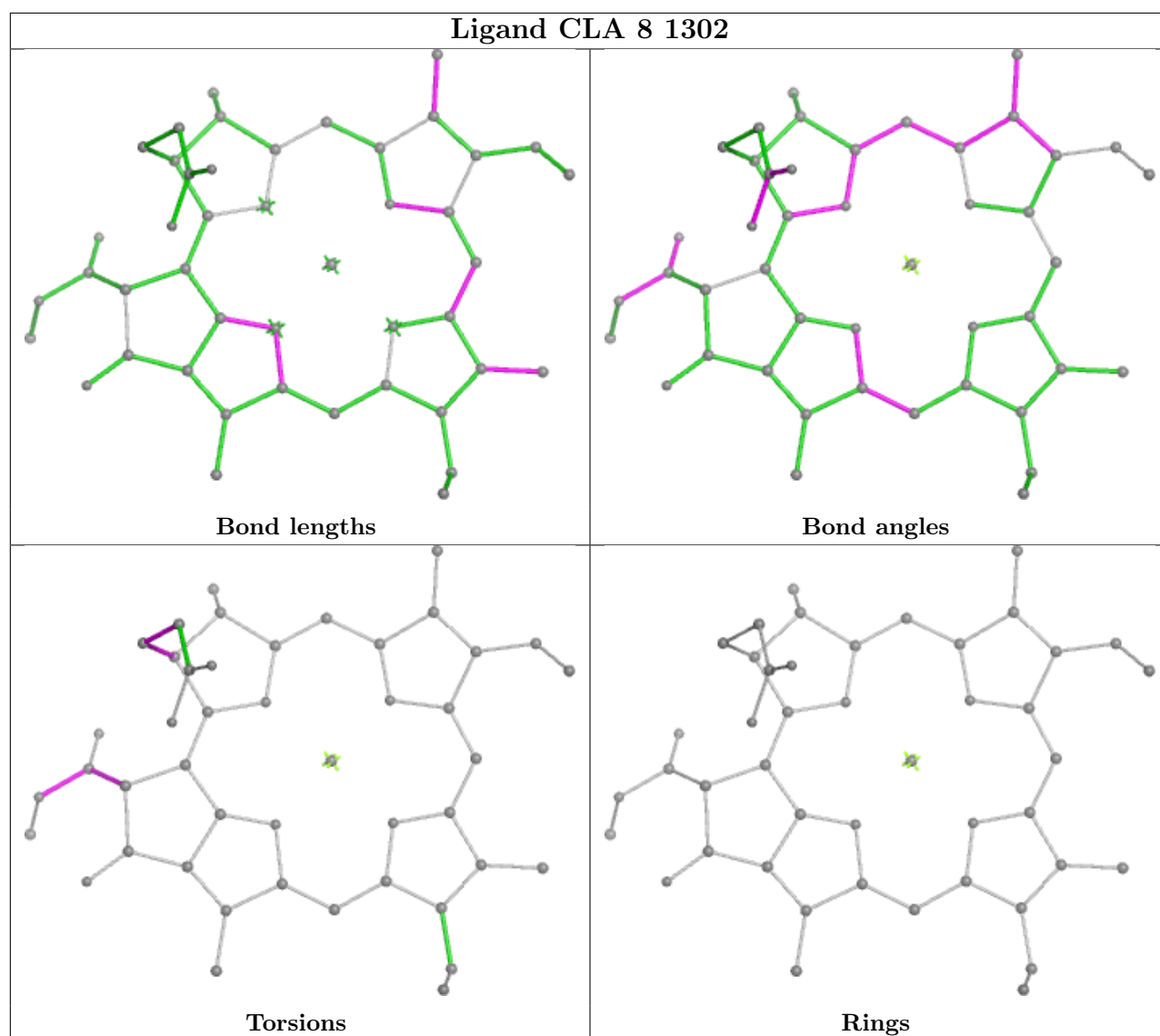


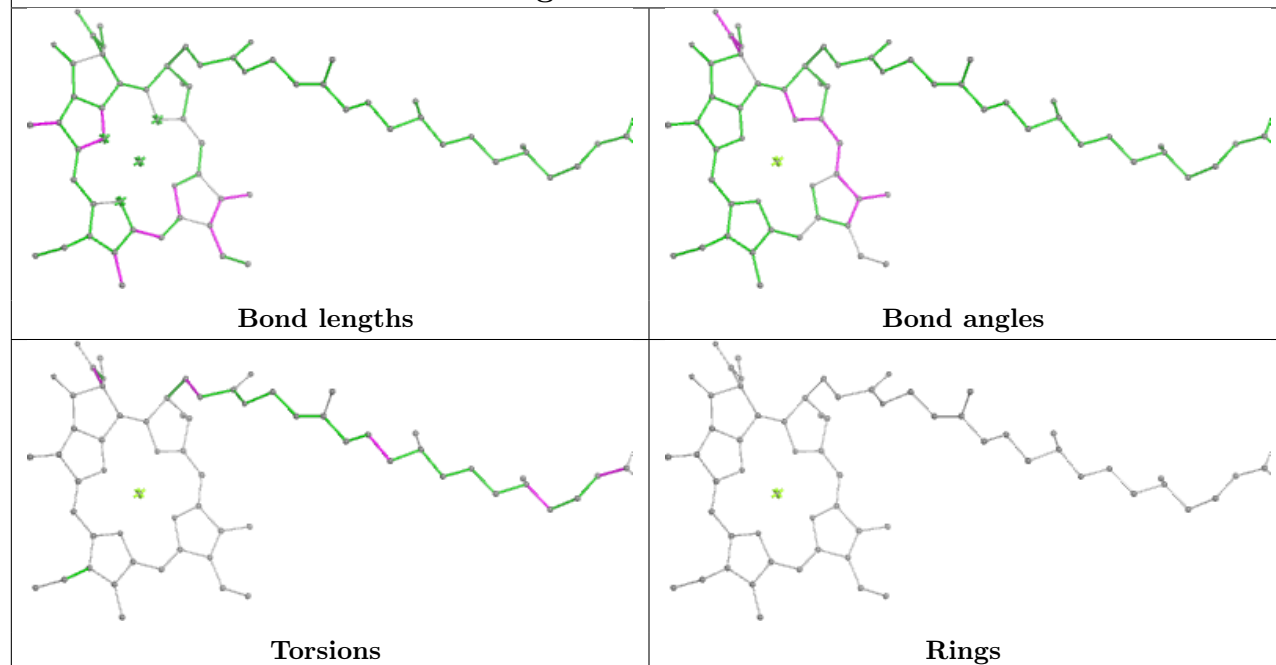
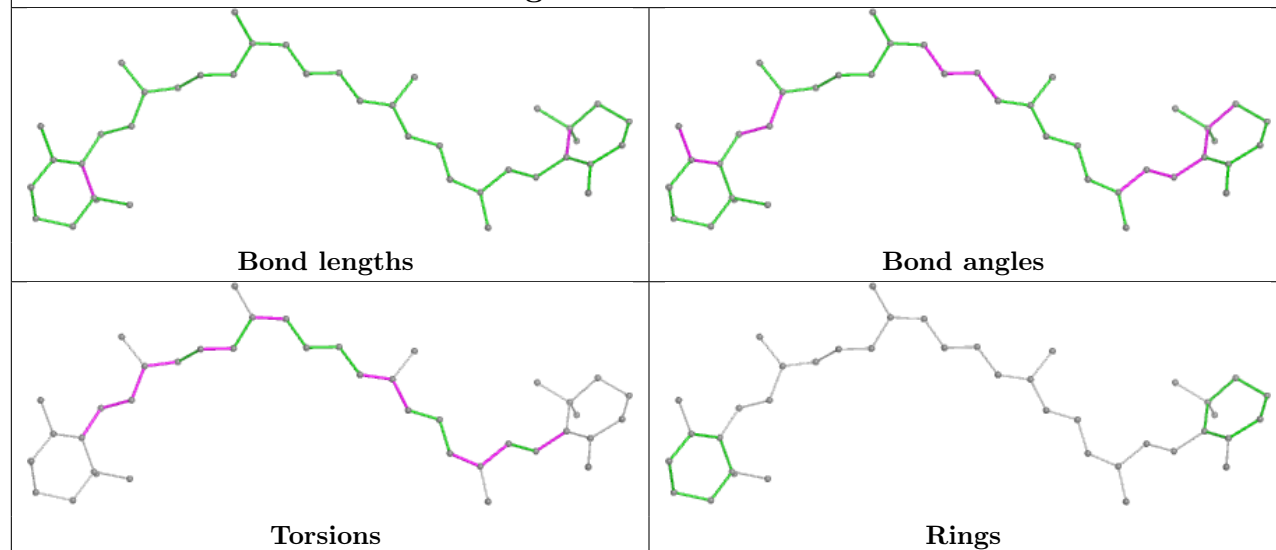


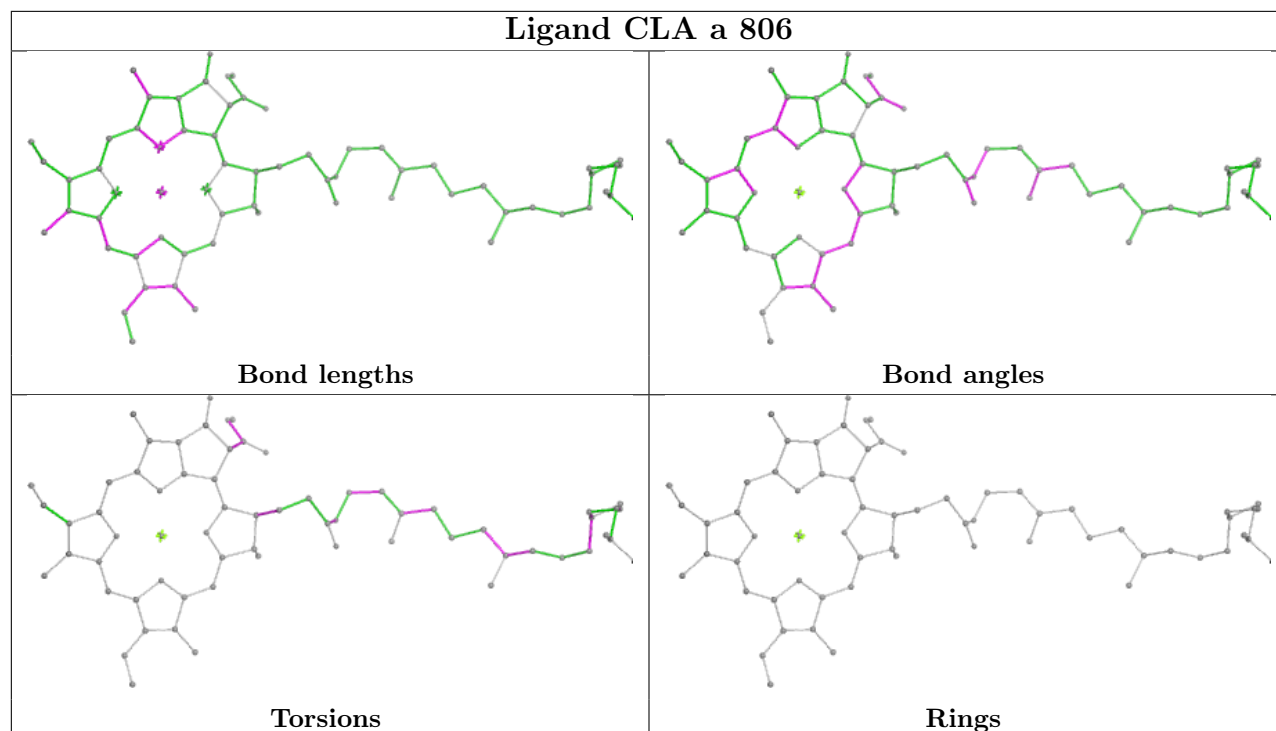
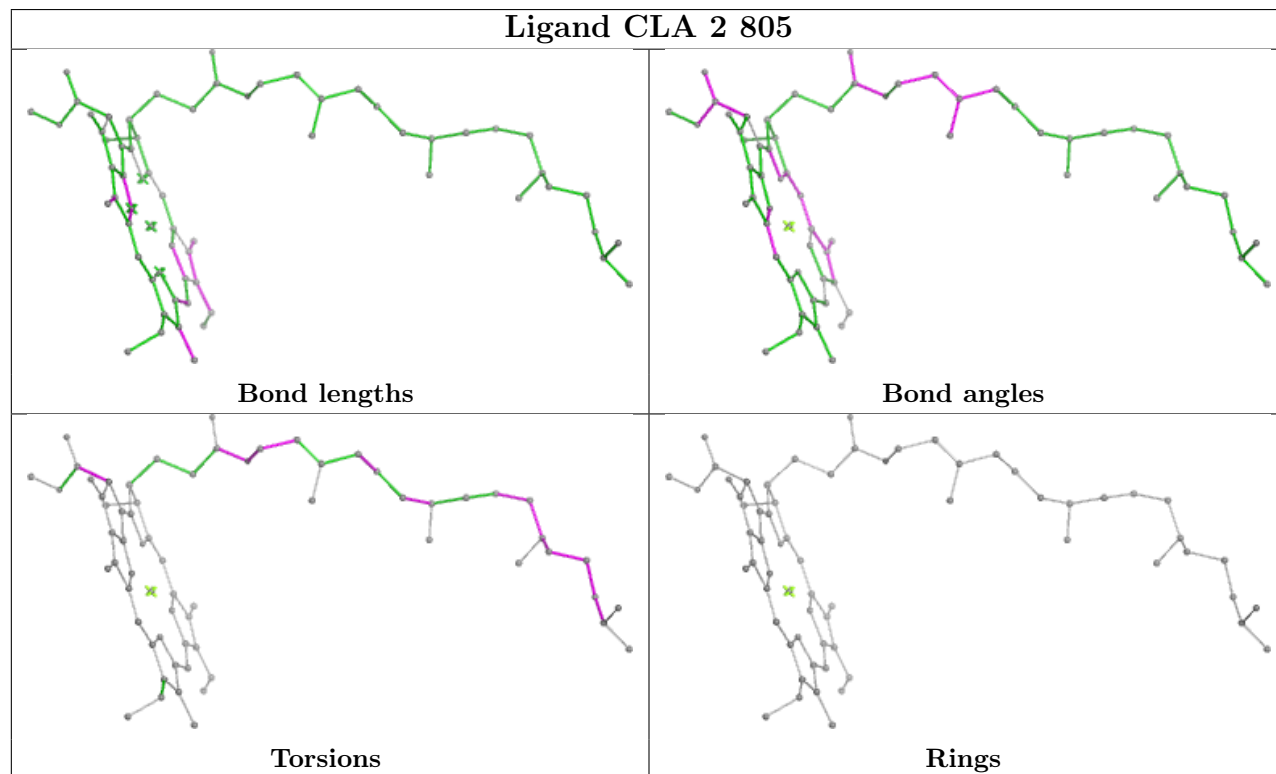
Ligand CLA b 832

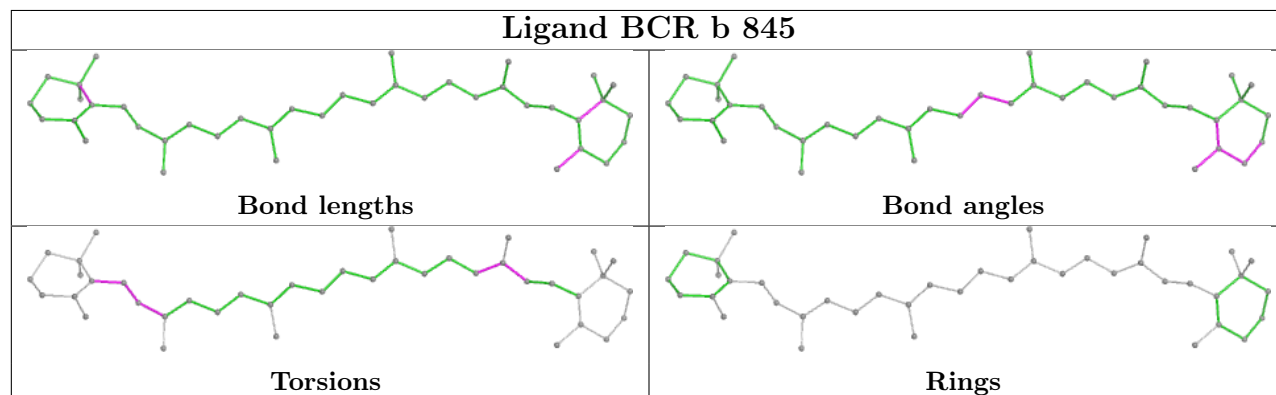
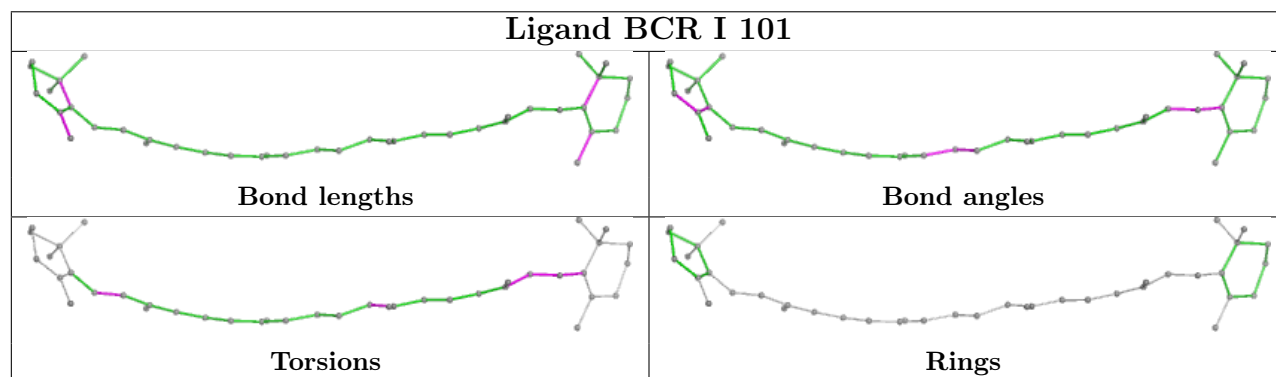
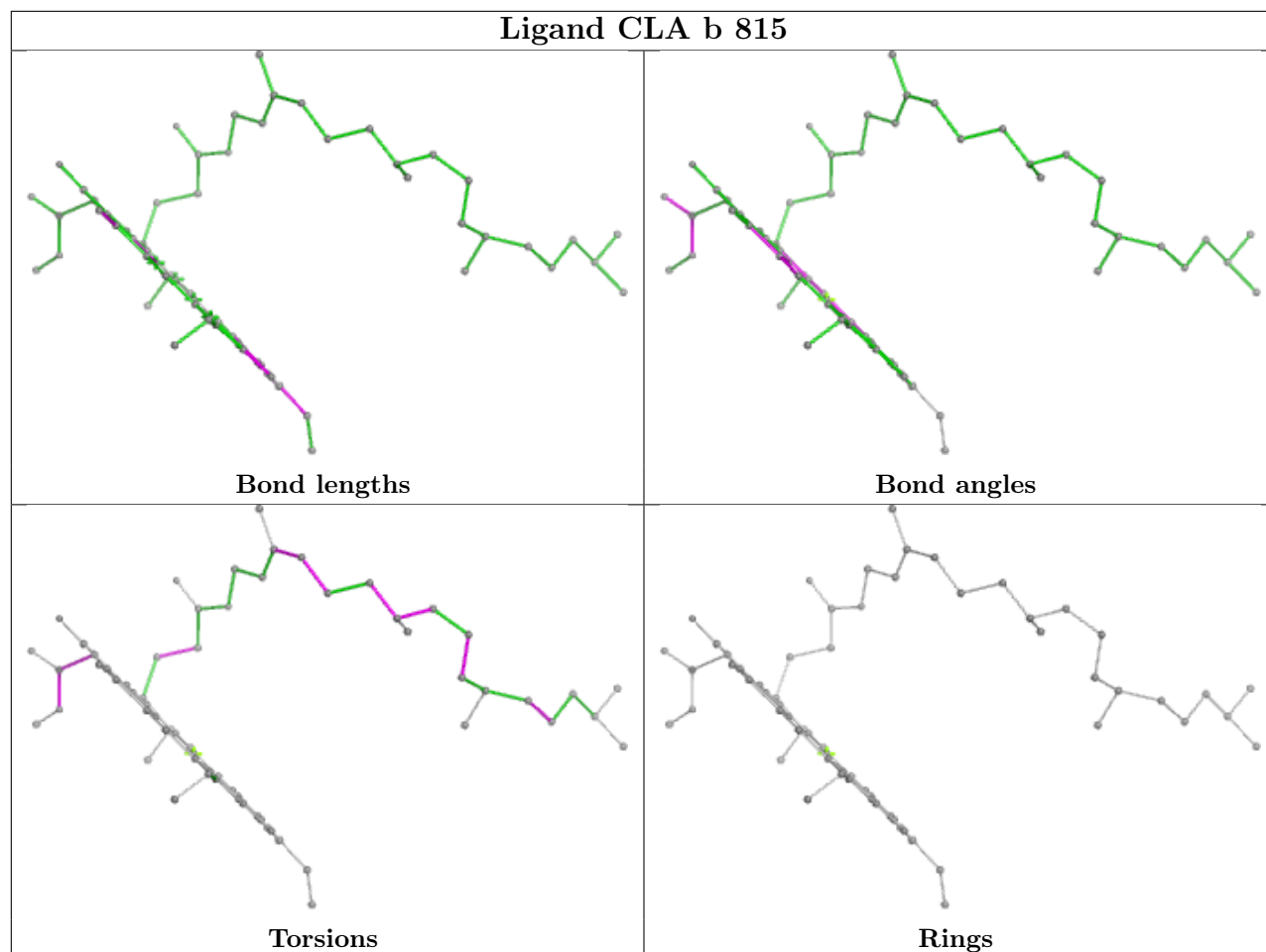




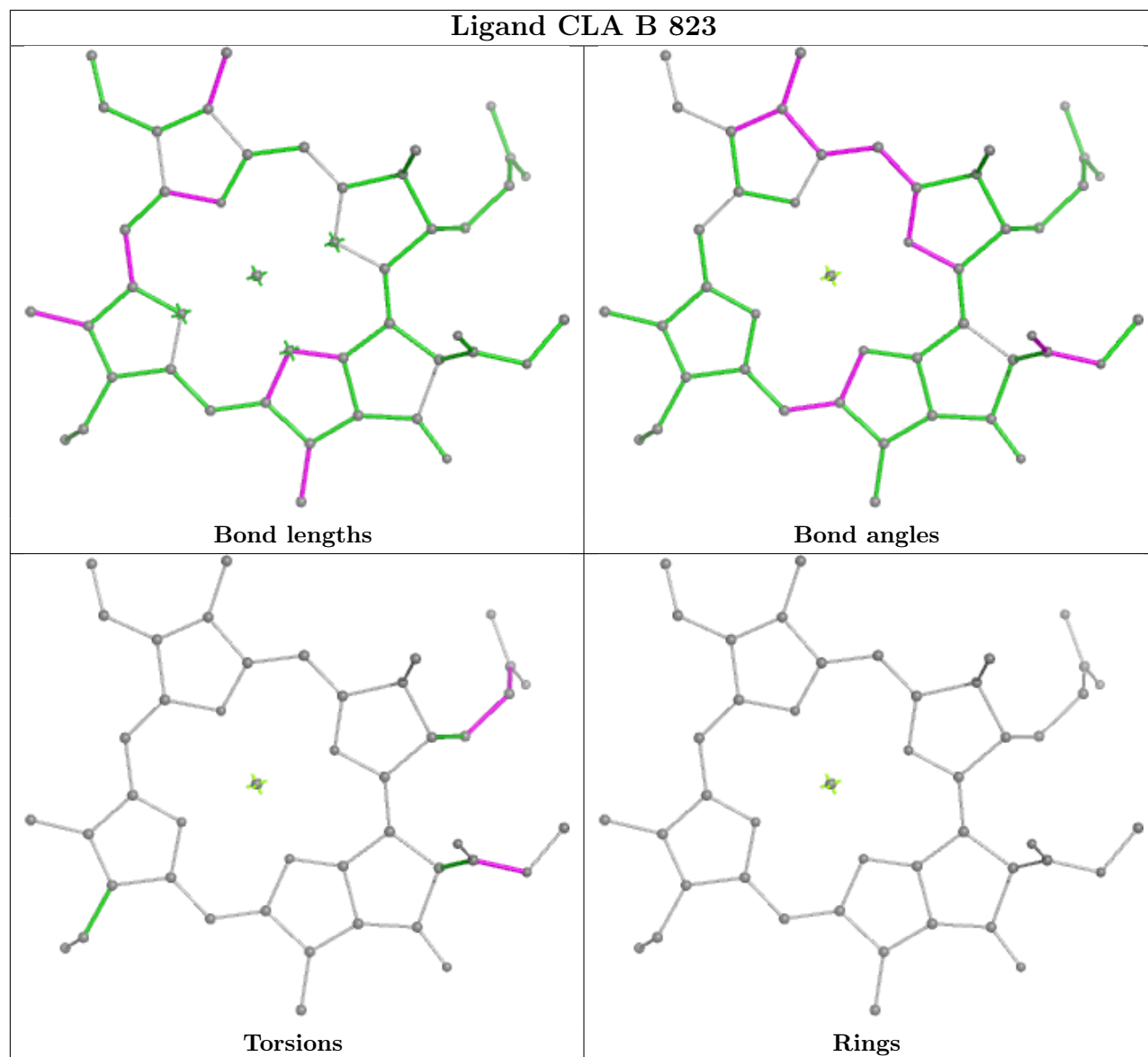


Ligand CLA a 835**Ligand BCR 1 1652**

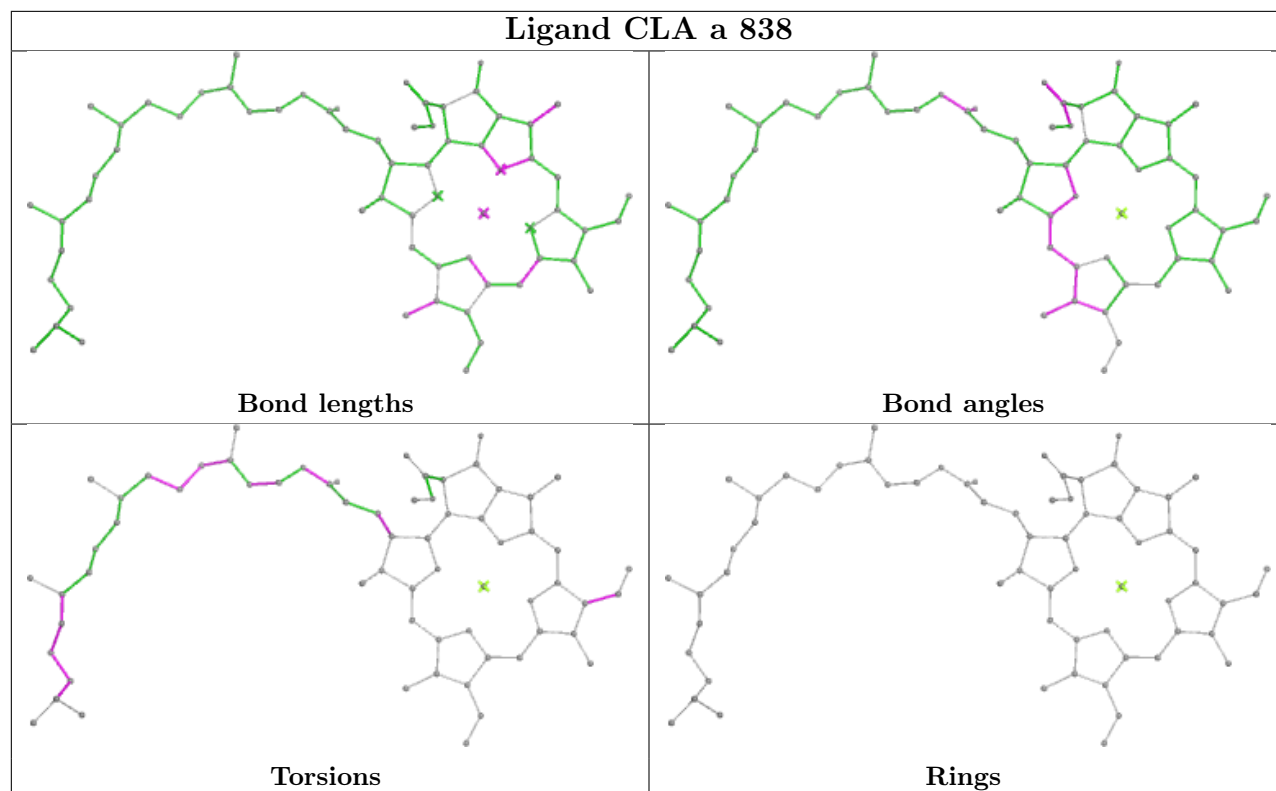
Ligand CLA a 806**Ligand CLA 2 805**



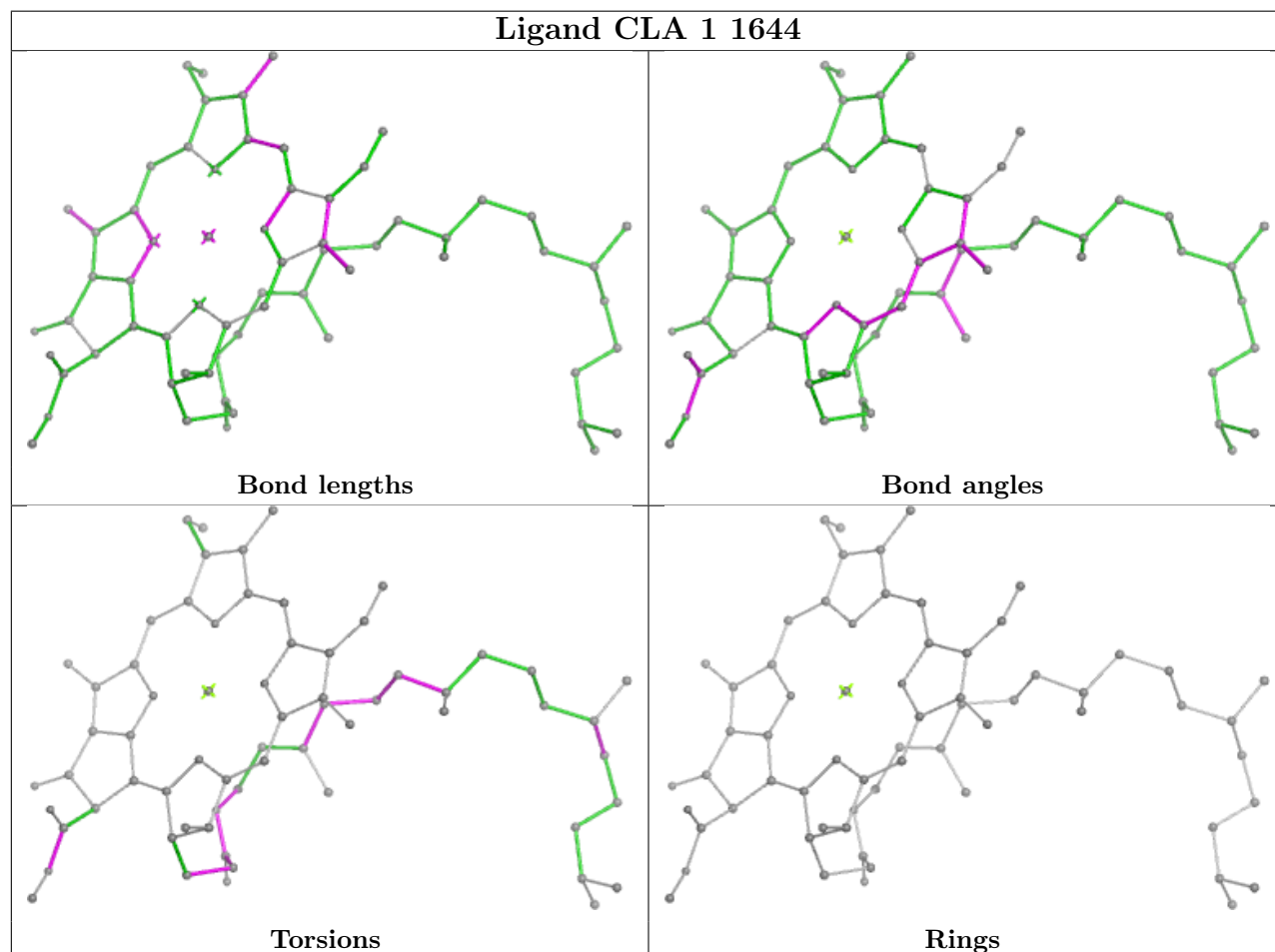
Ligand CLA B 823

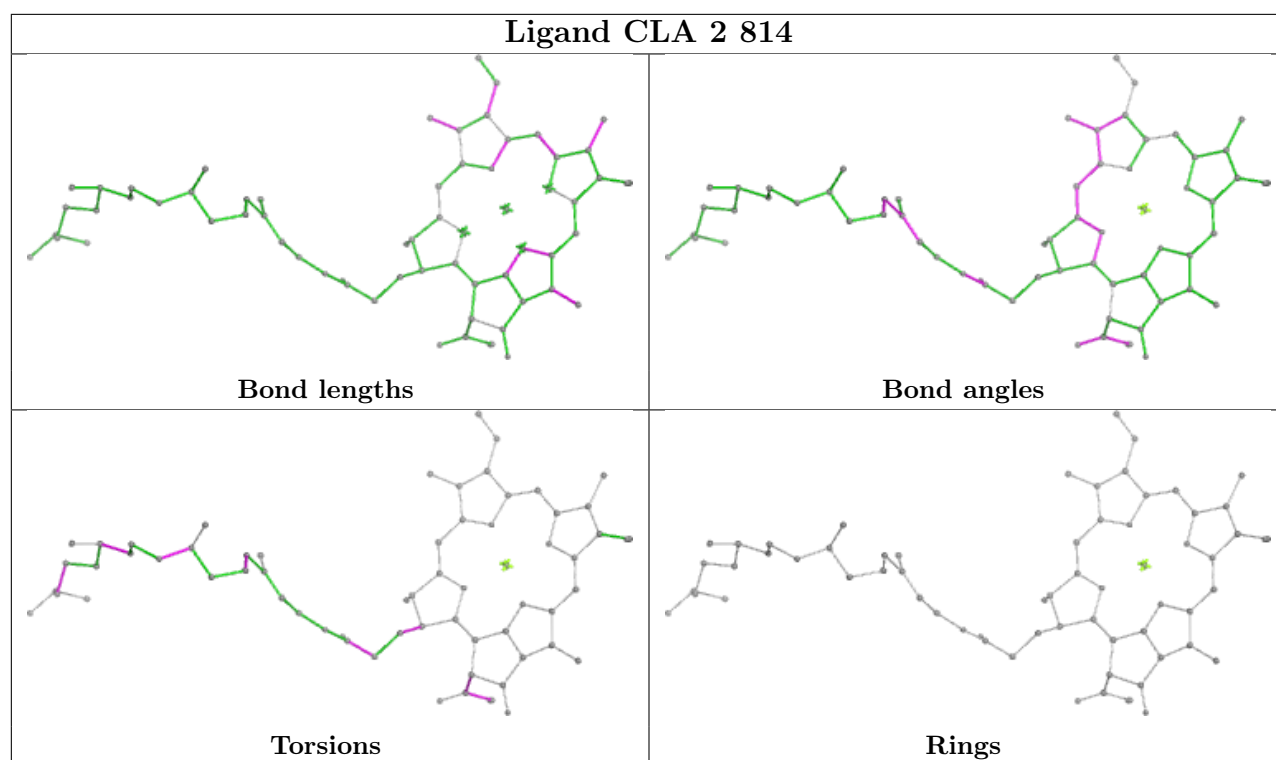


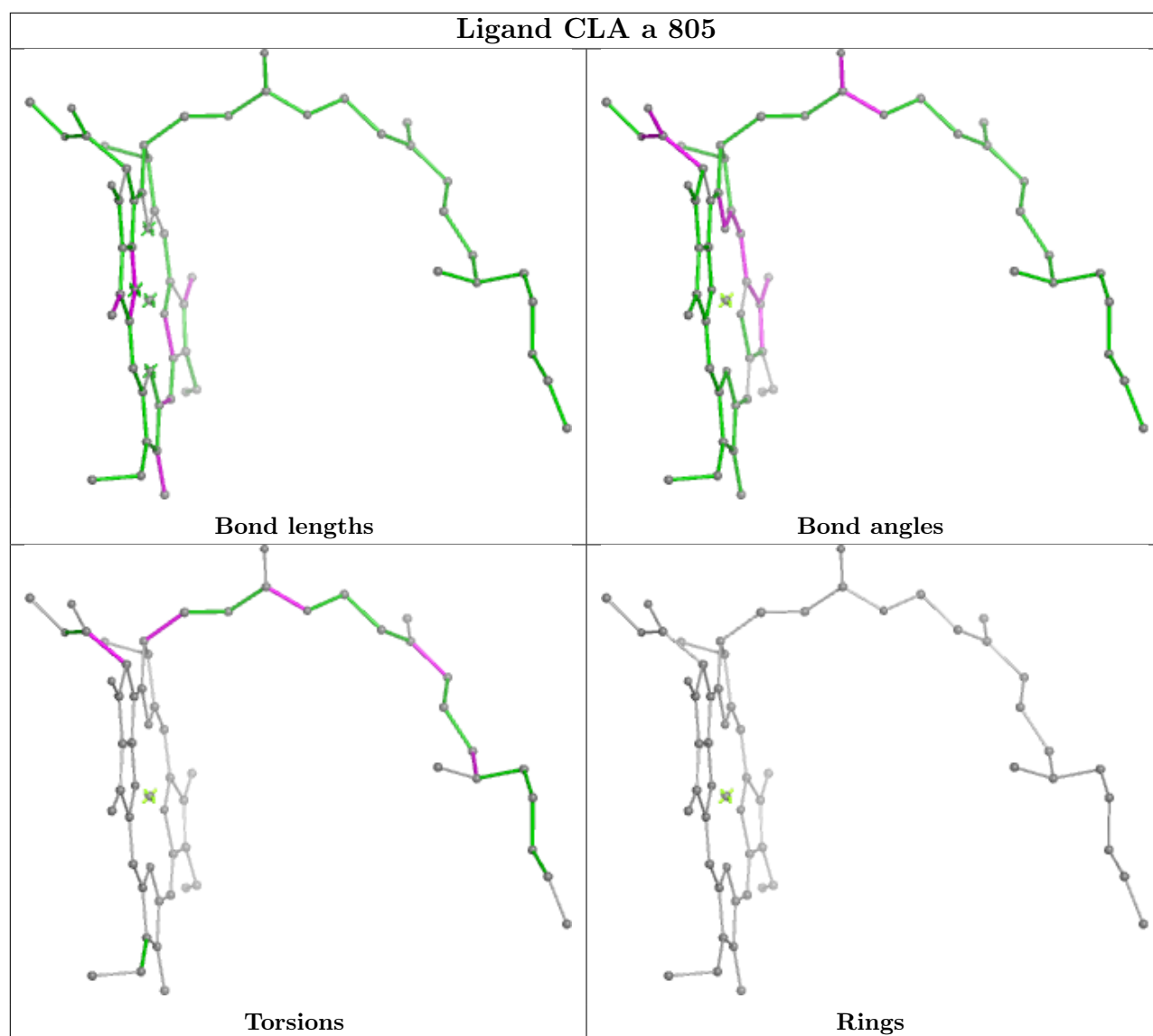
Ligand CLA a 838

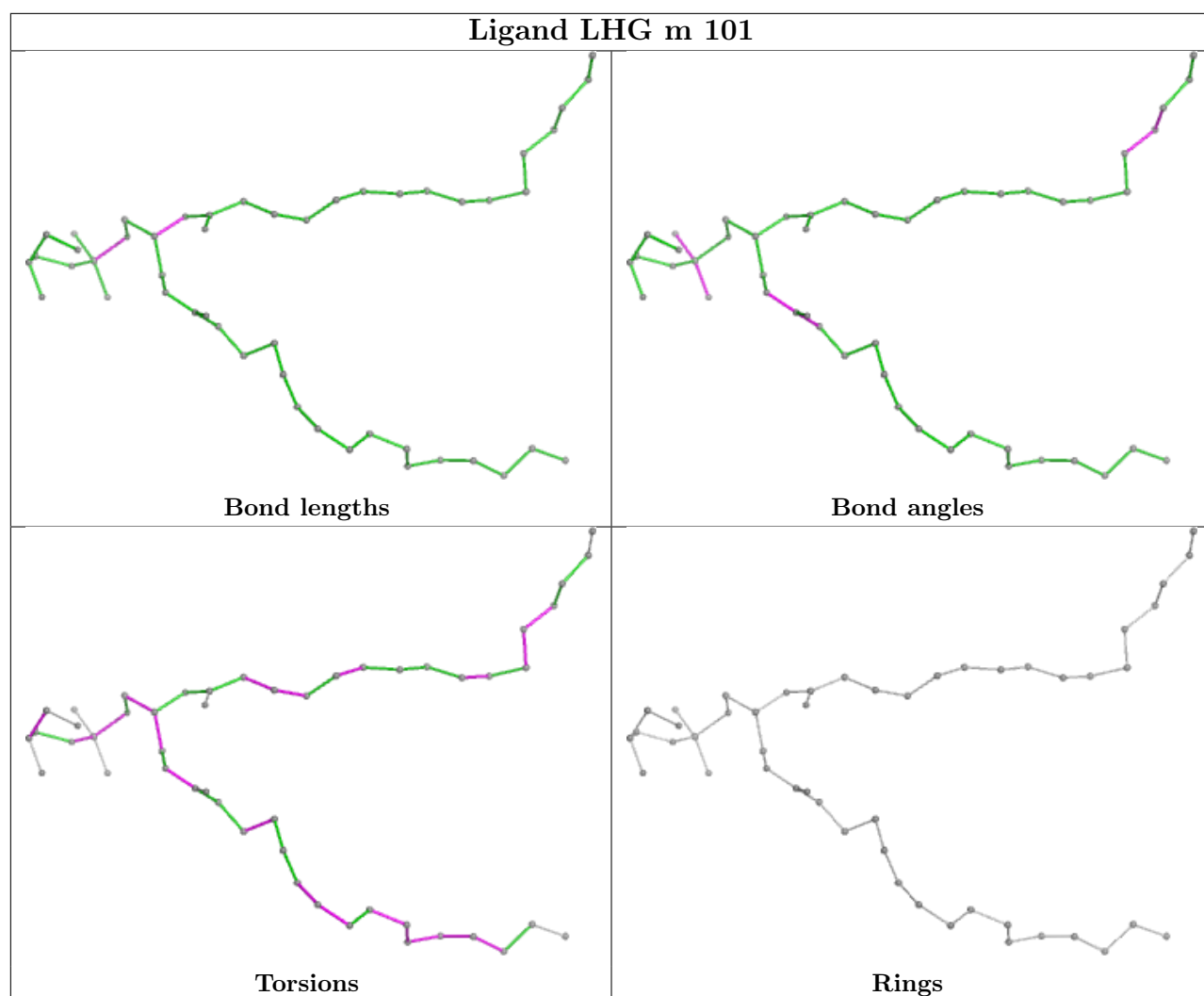


Ligand CLA 1 1644

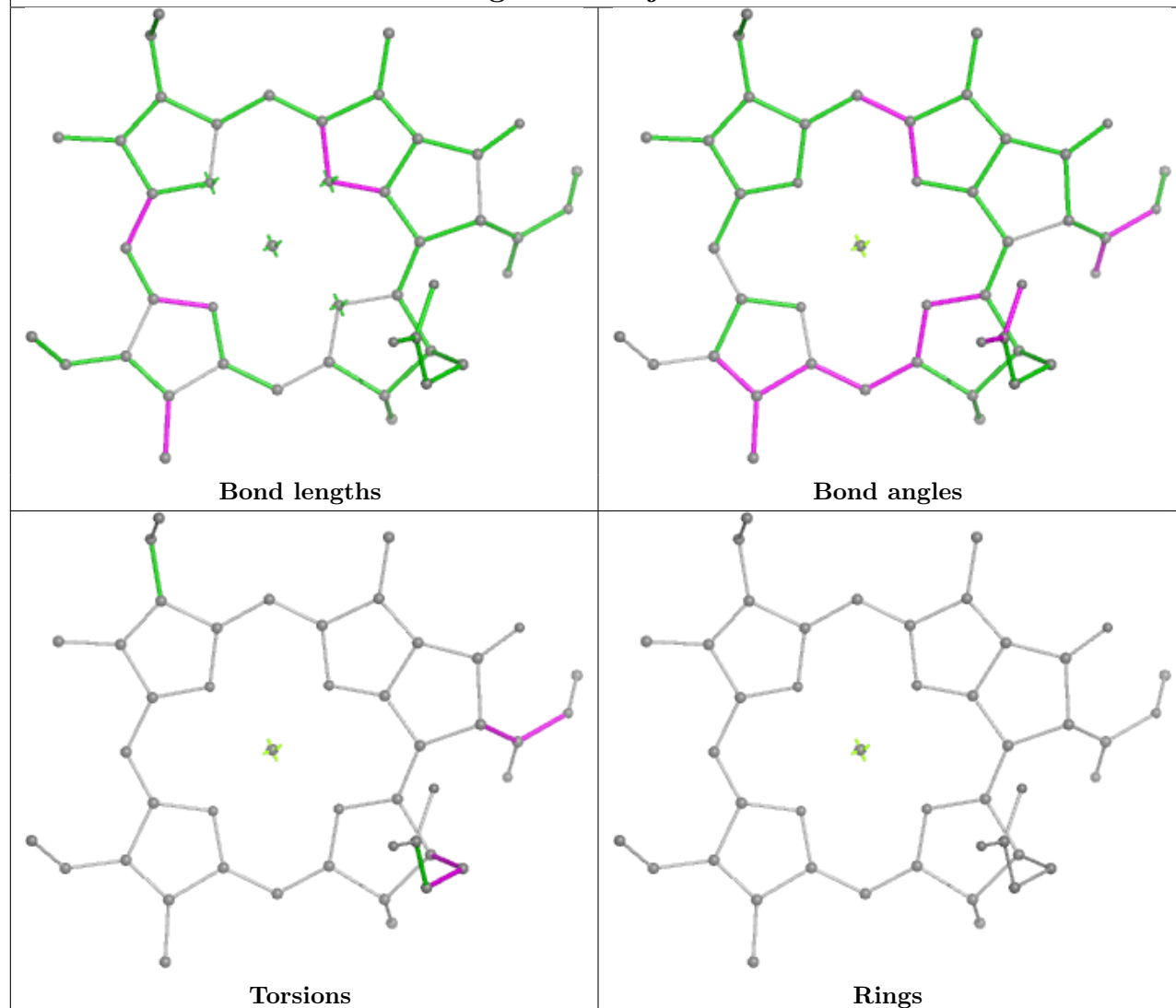


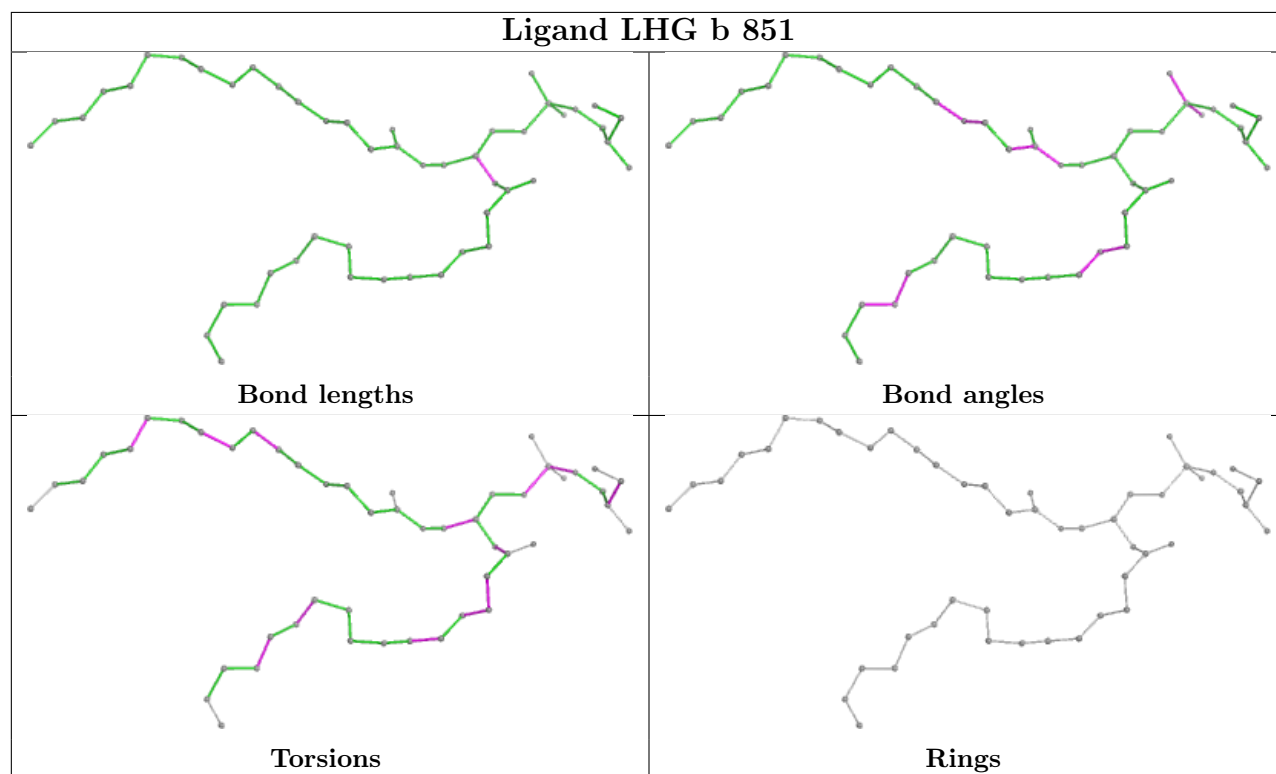
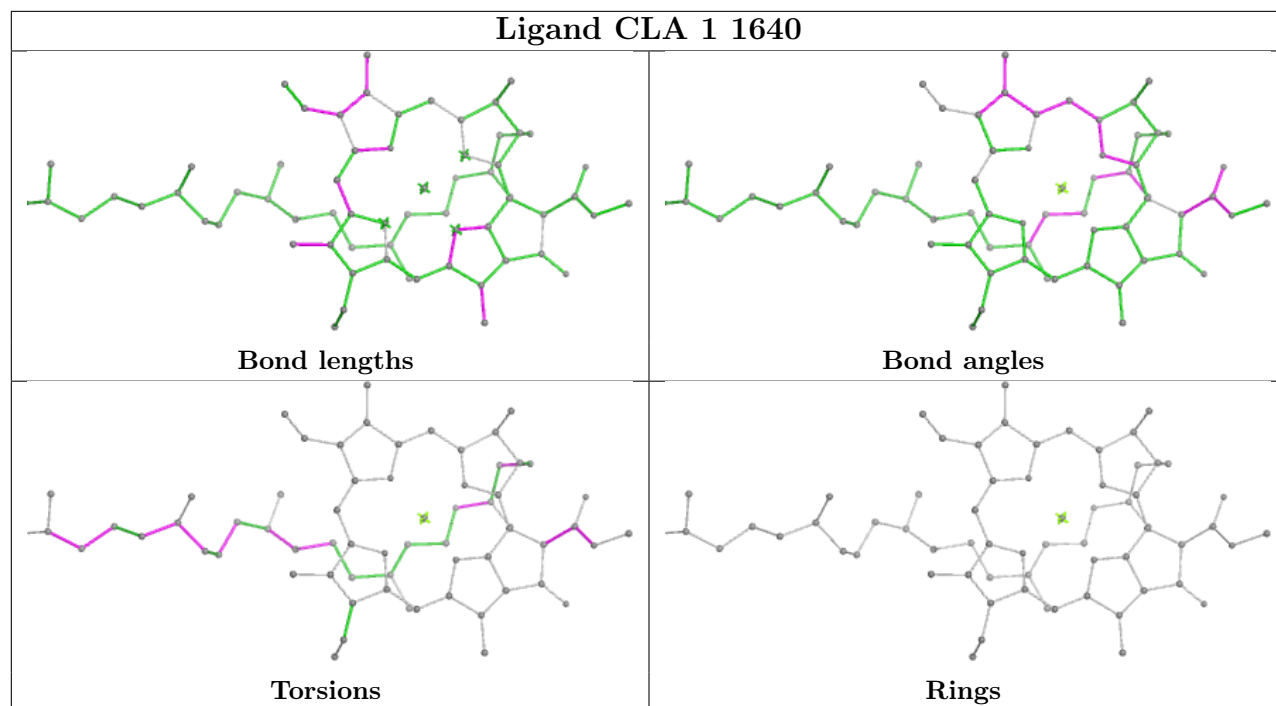


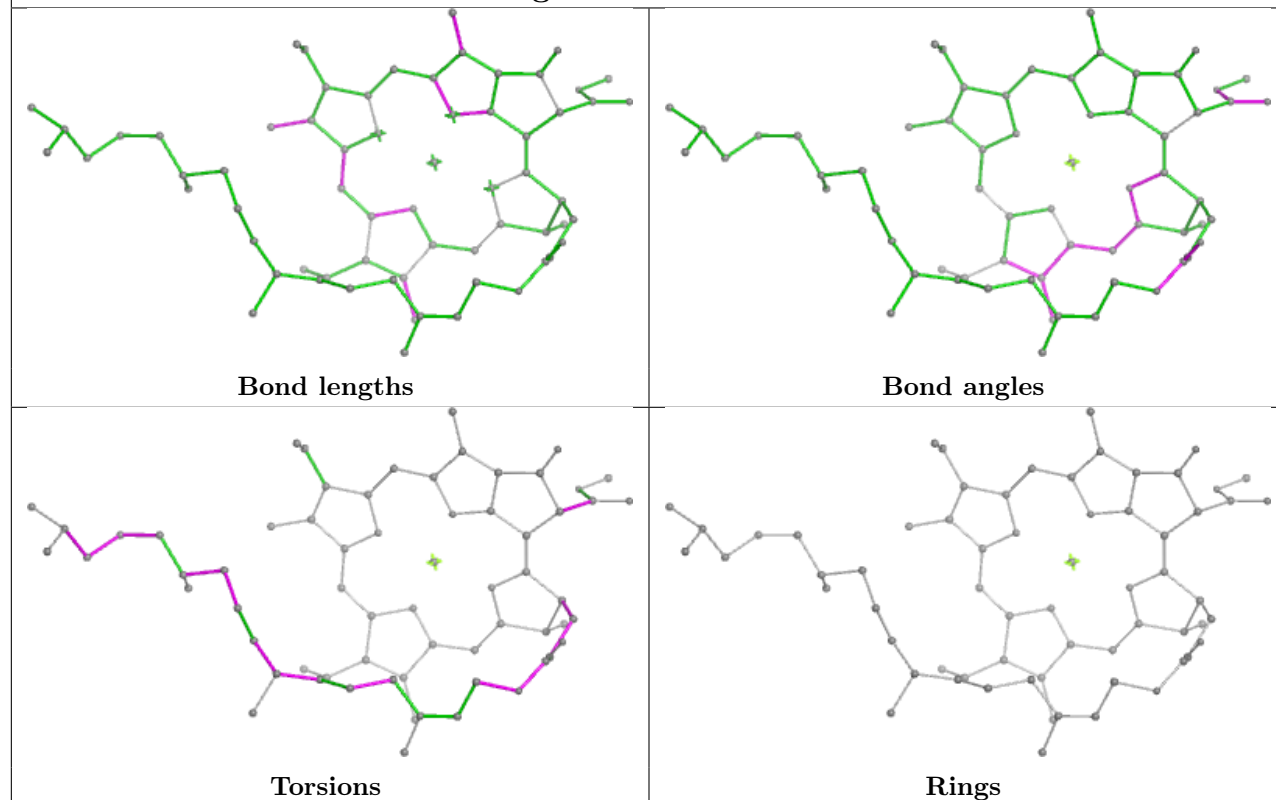
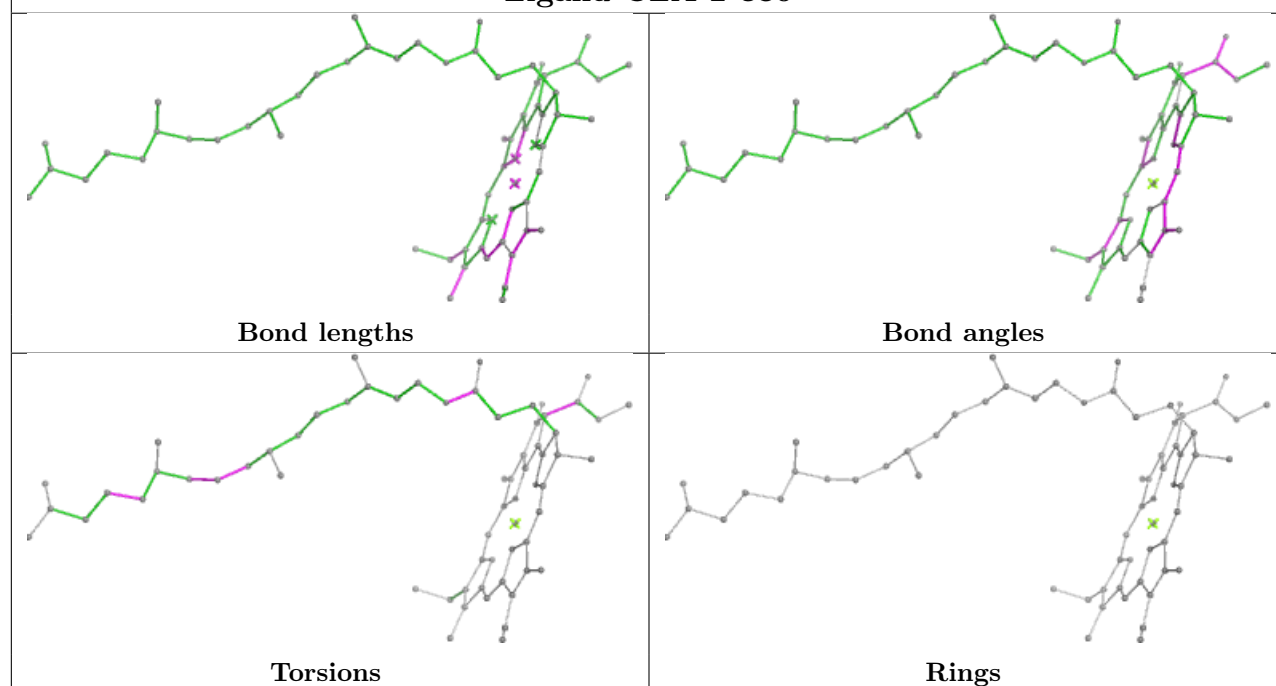




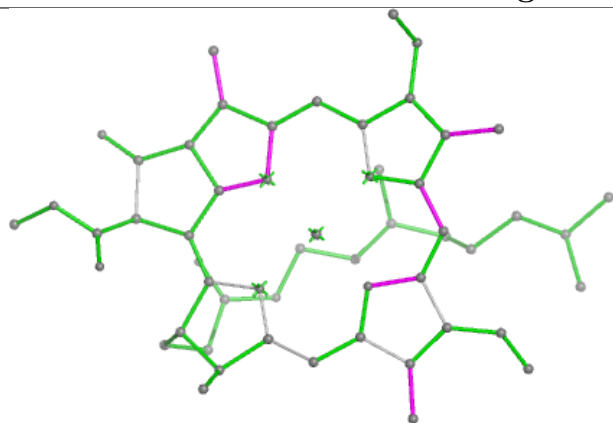
Ligand CLA j 1302



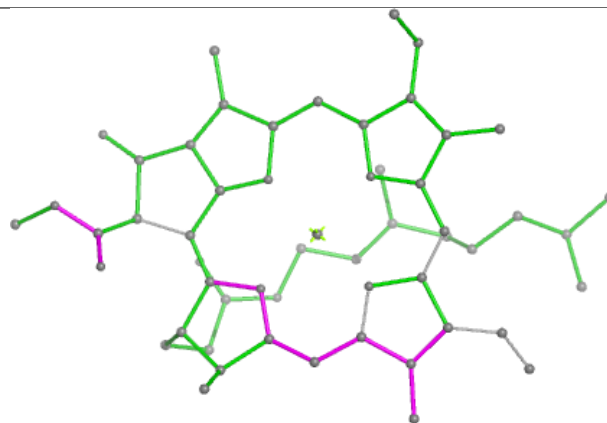


Ligand CLA B 820**Ligand CLA 2 830**

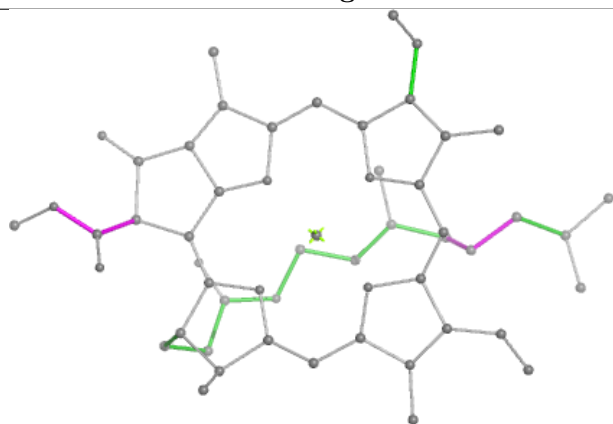
Ligand CLA b 823



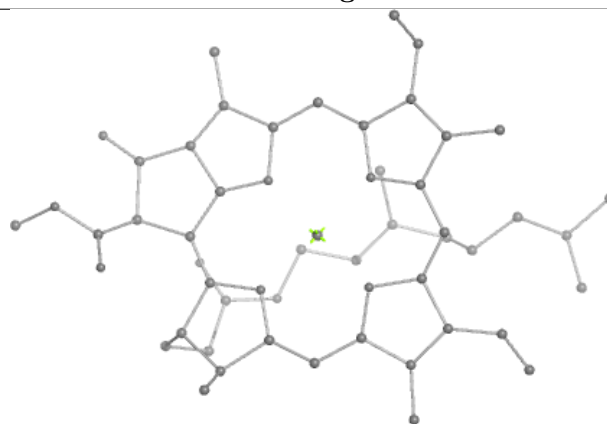
Bond lengths



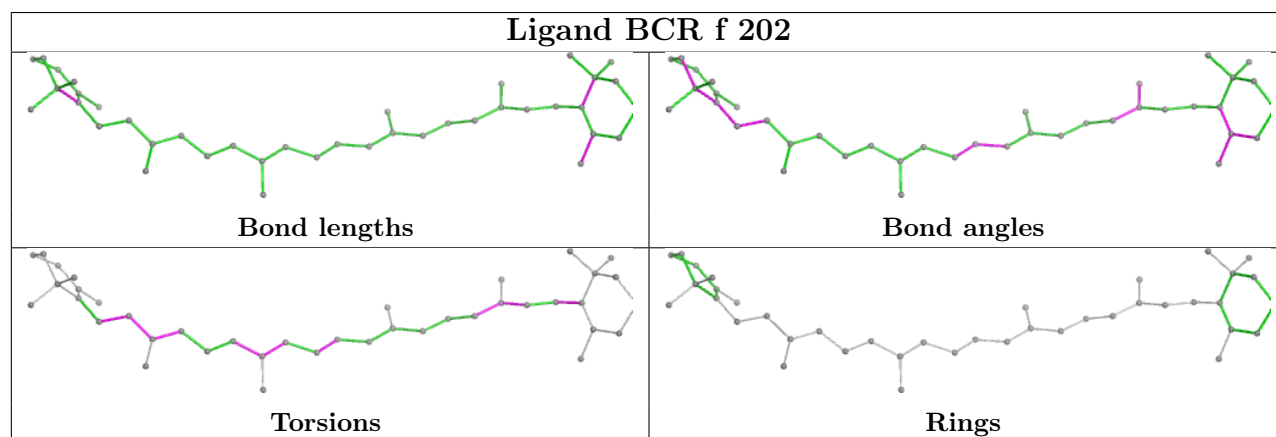
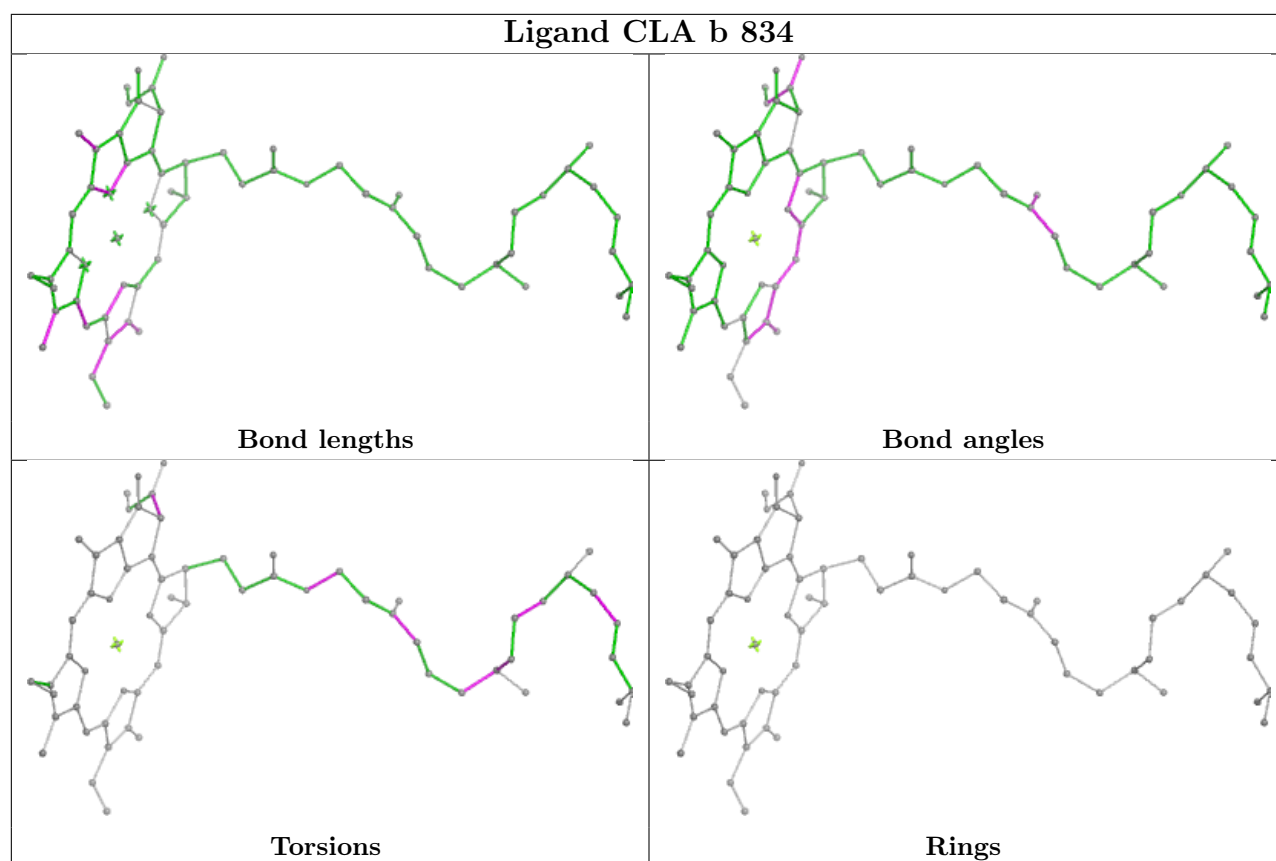
Bond angles

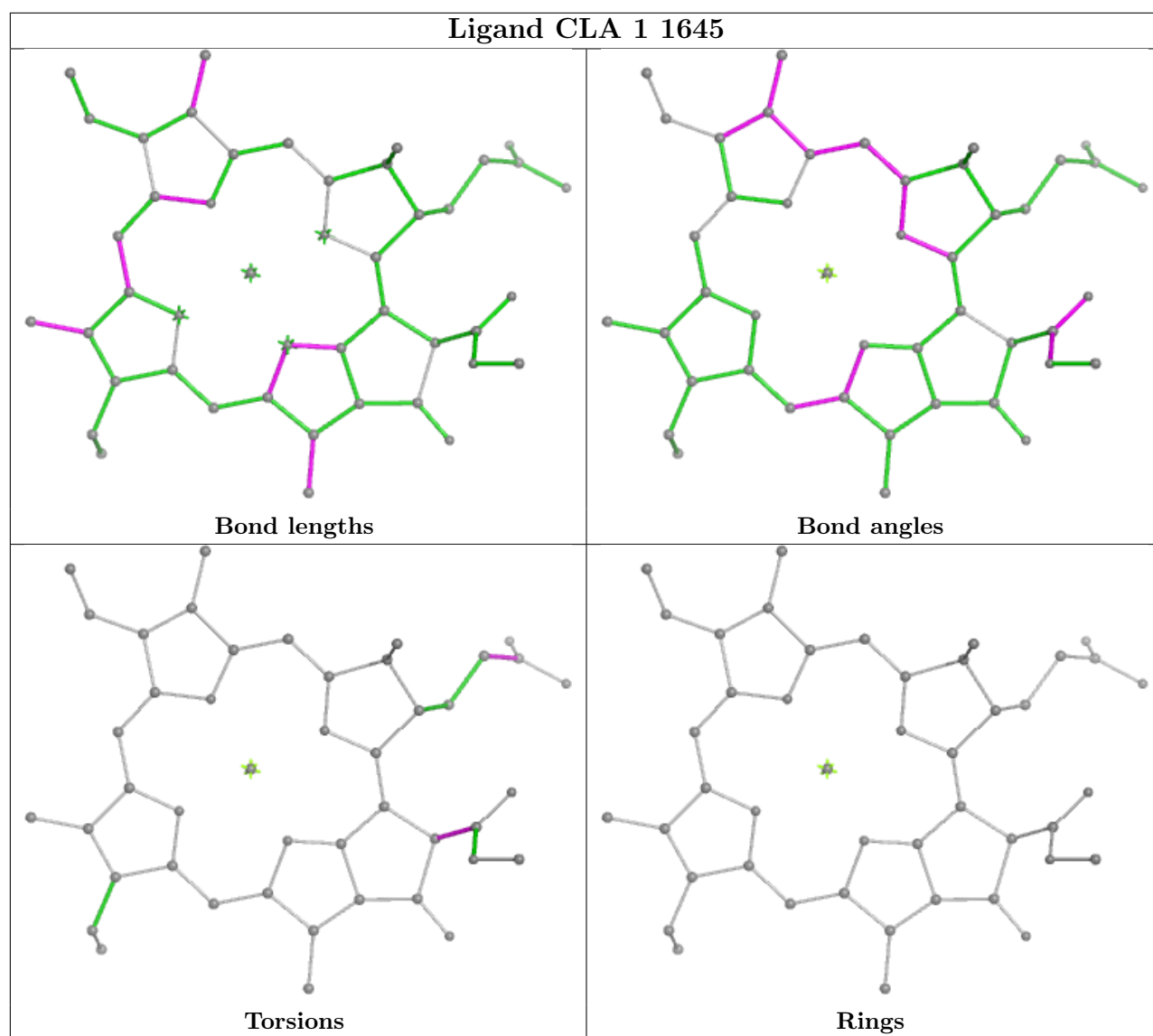


Torsions

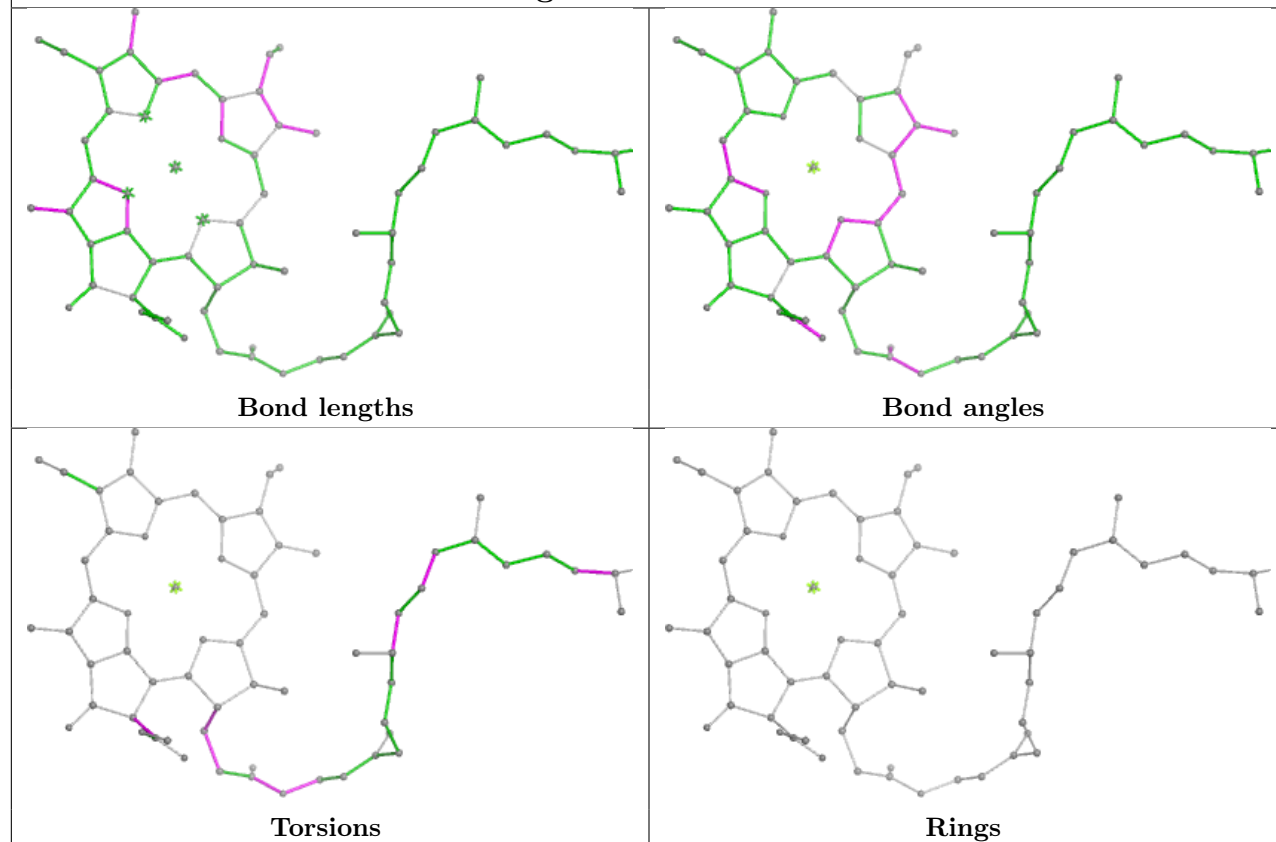


Rings

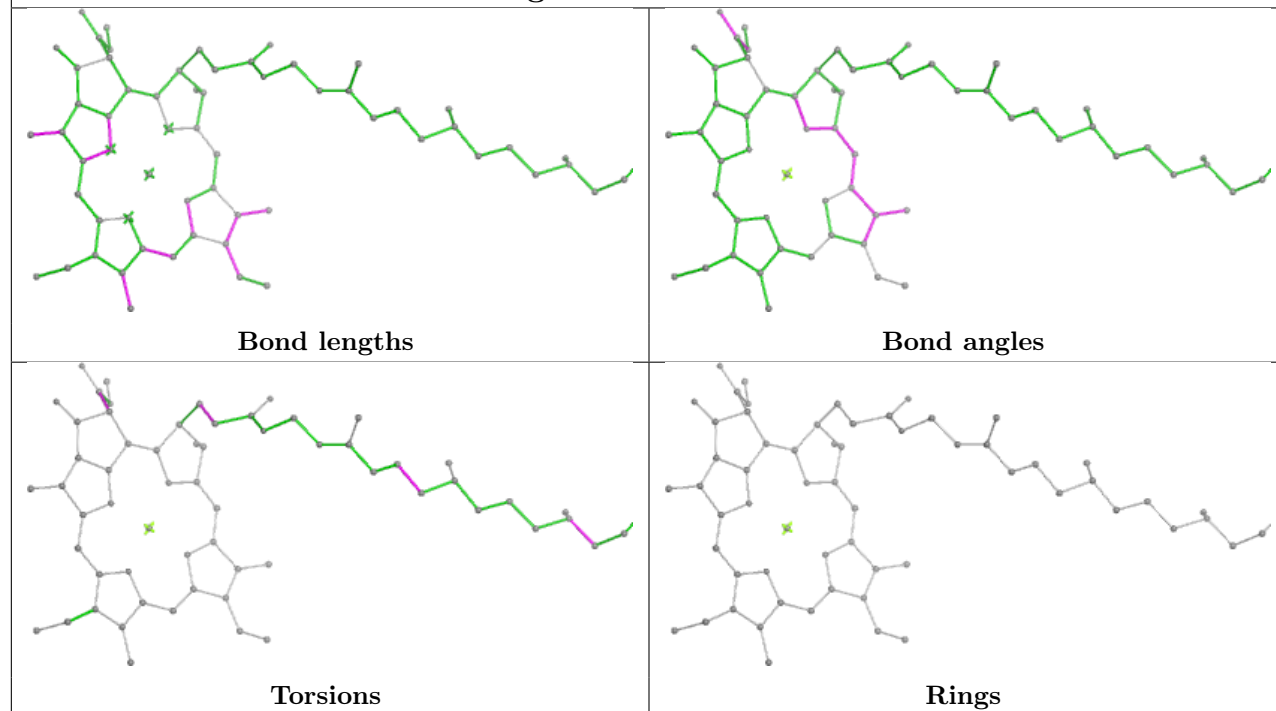


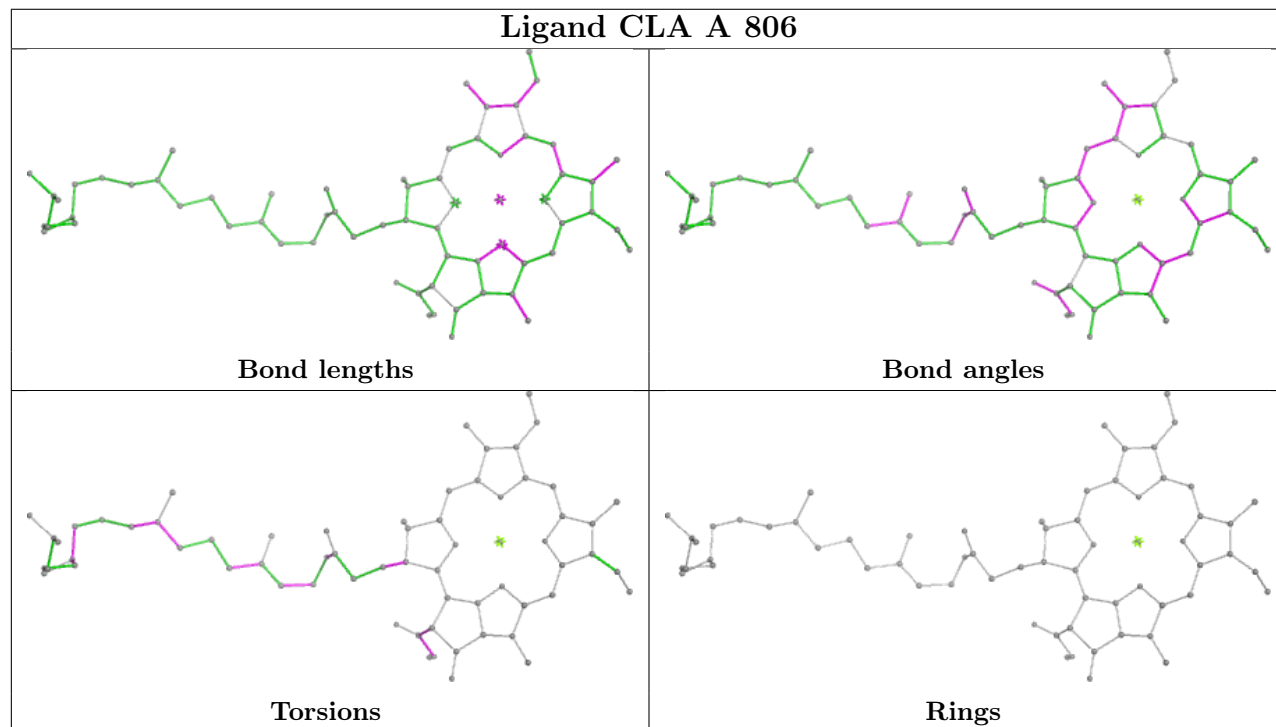
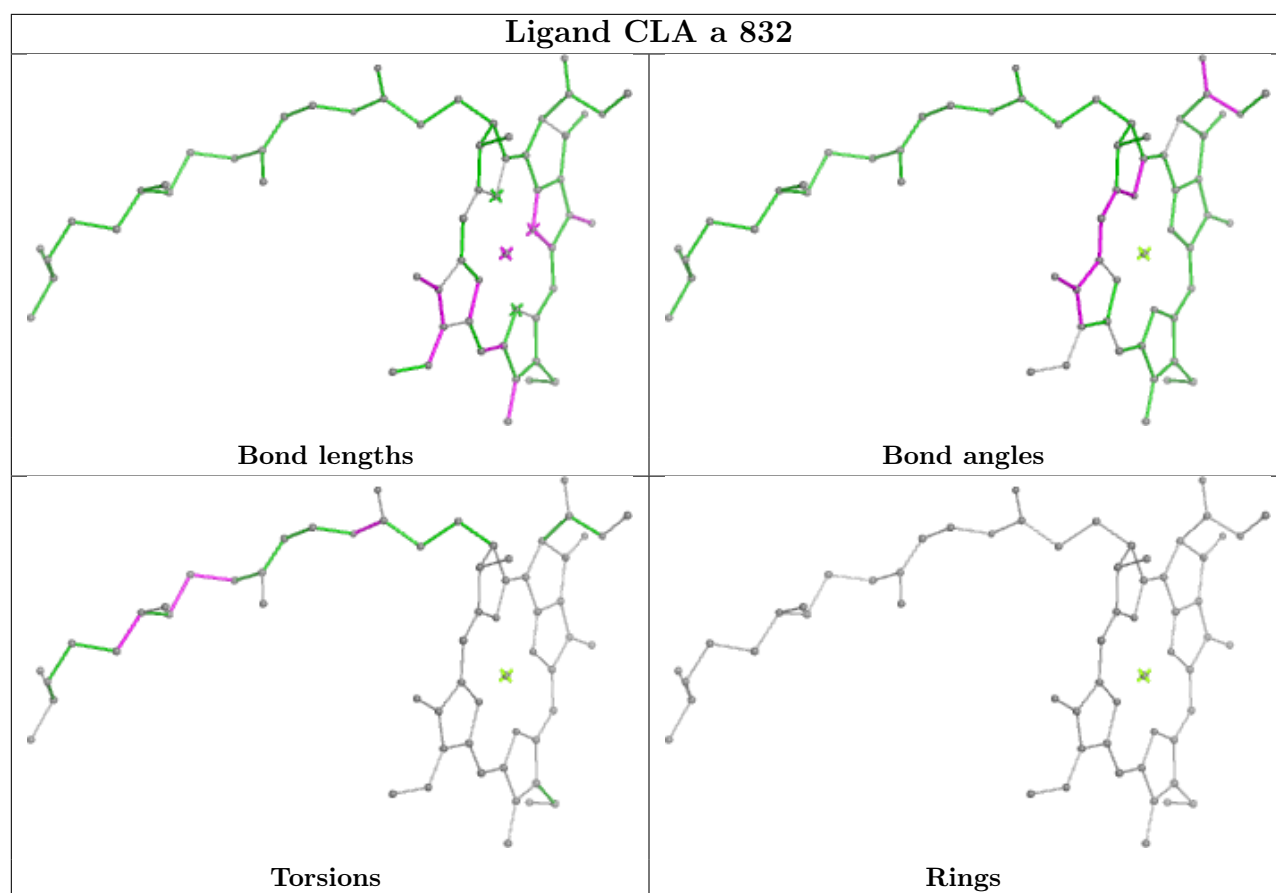


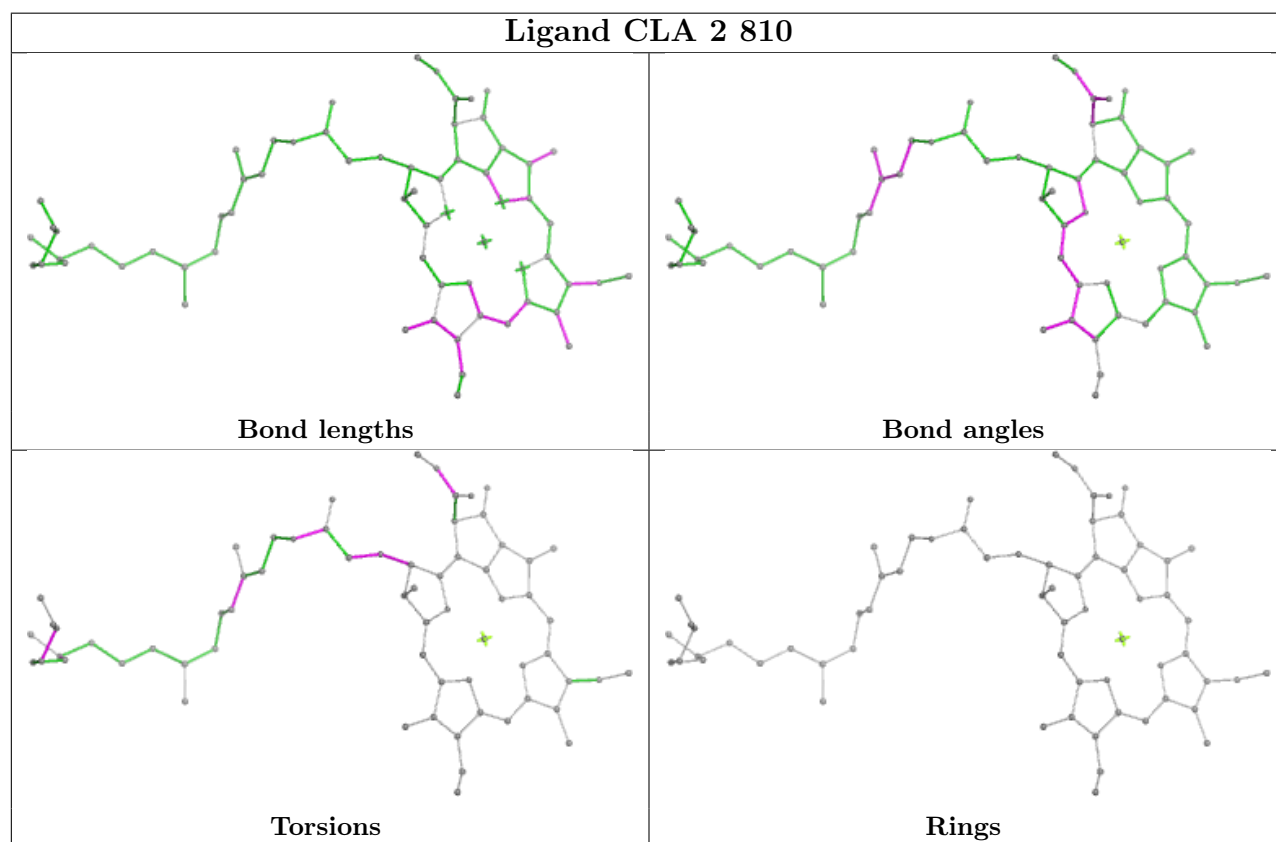
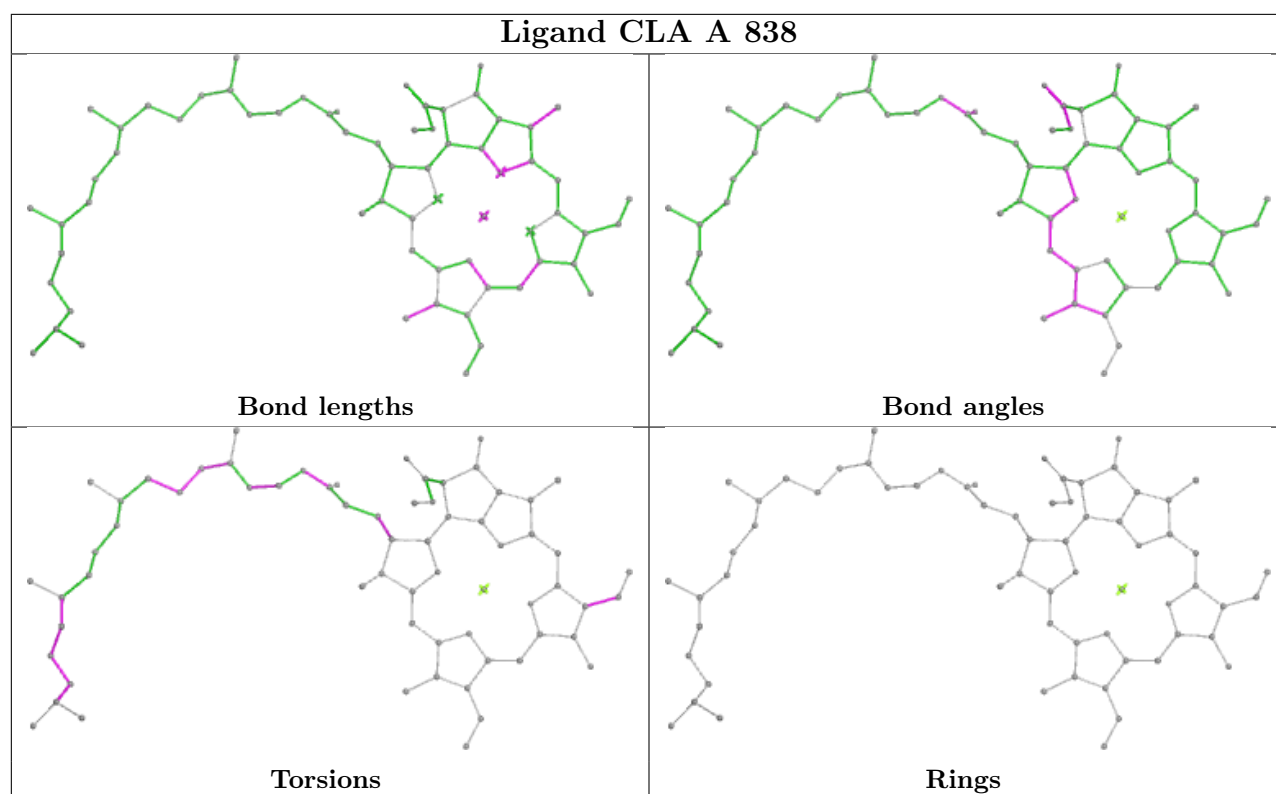
Ligand CLA a 814

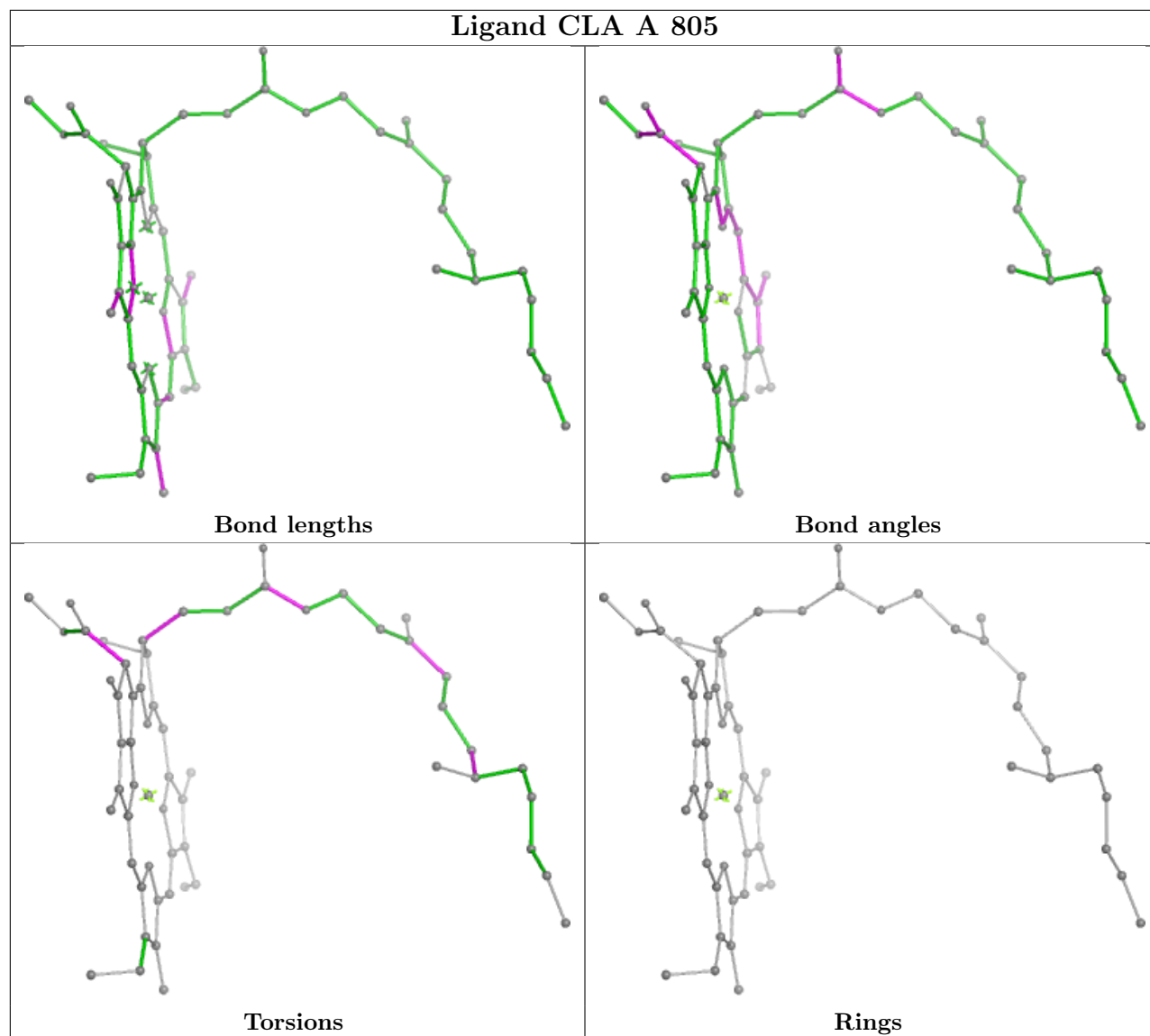


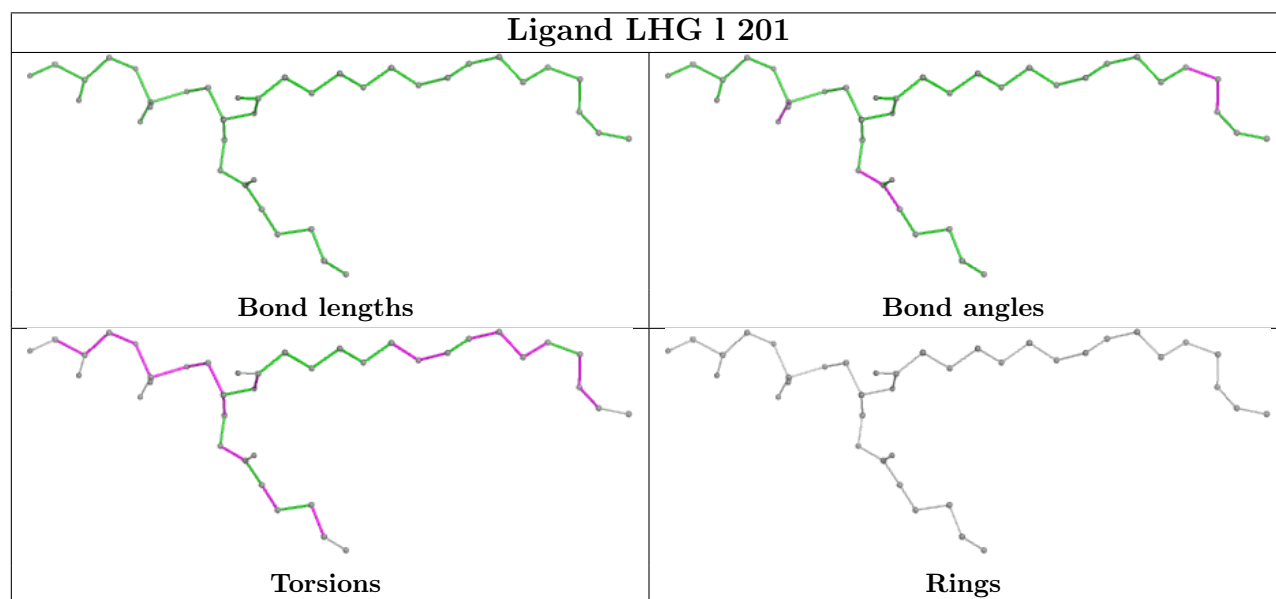
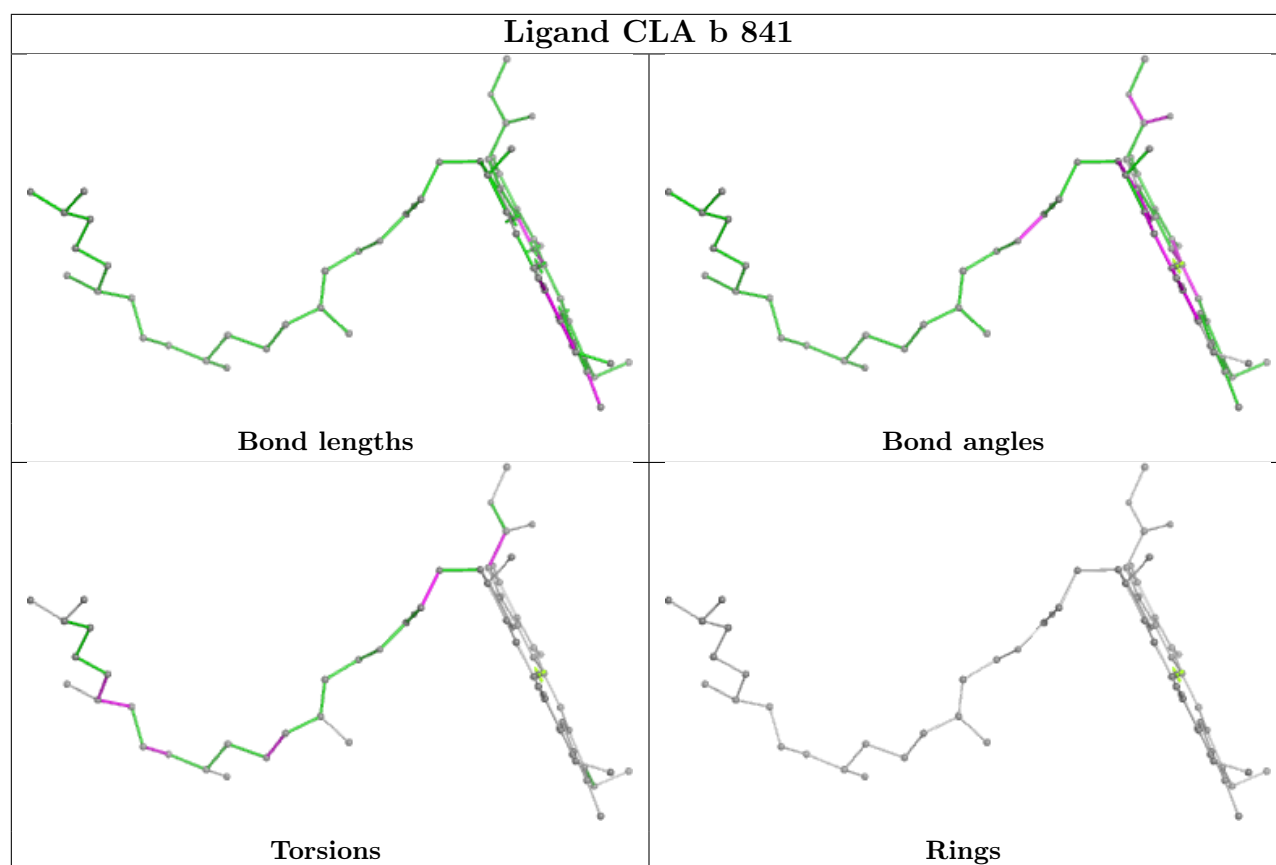
Ligand CLA 1 1636

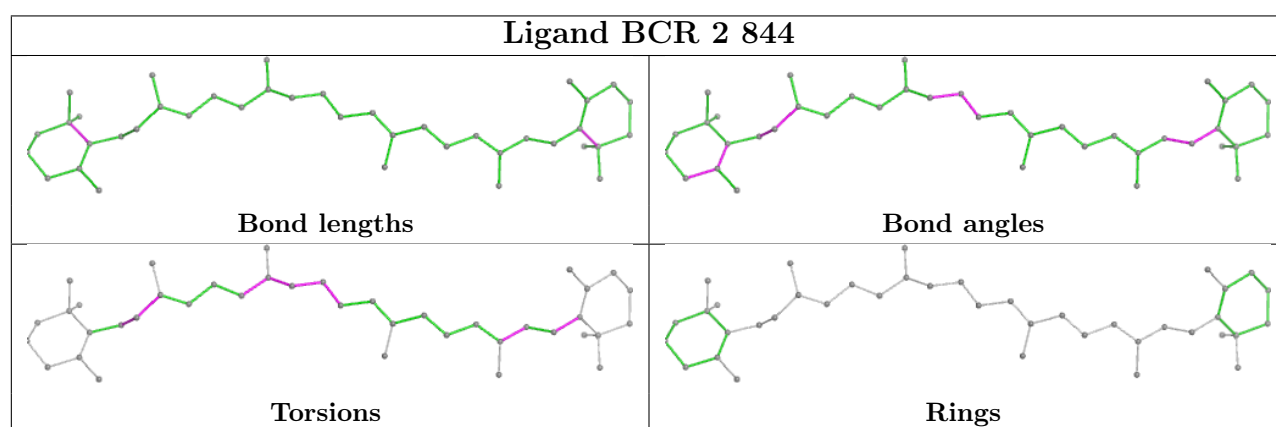
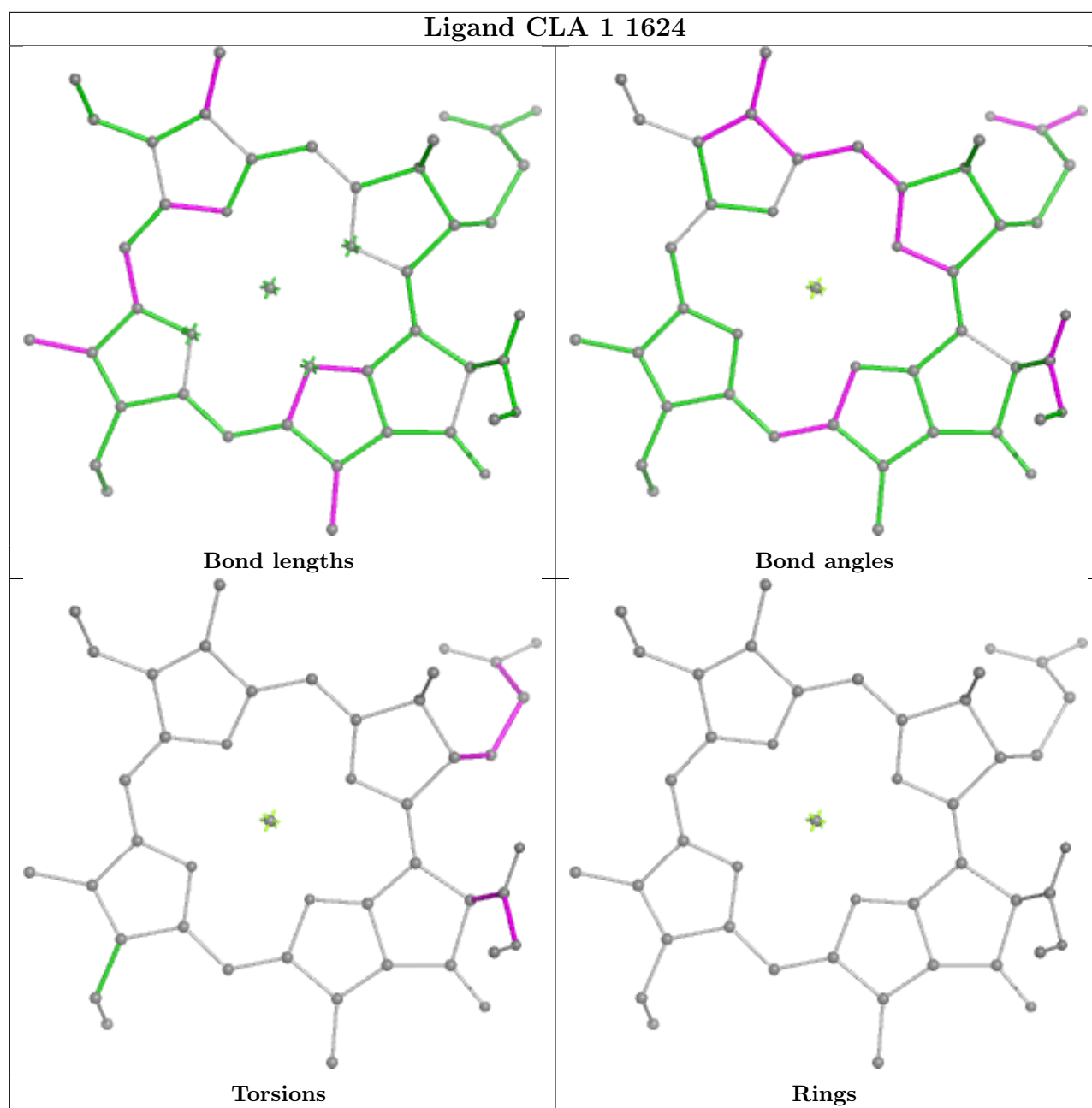


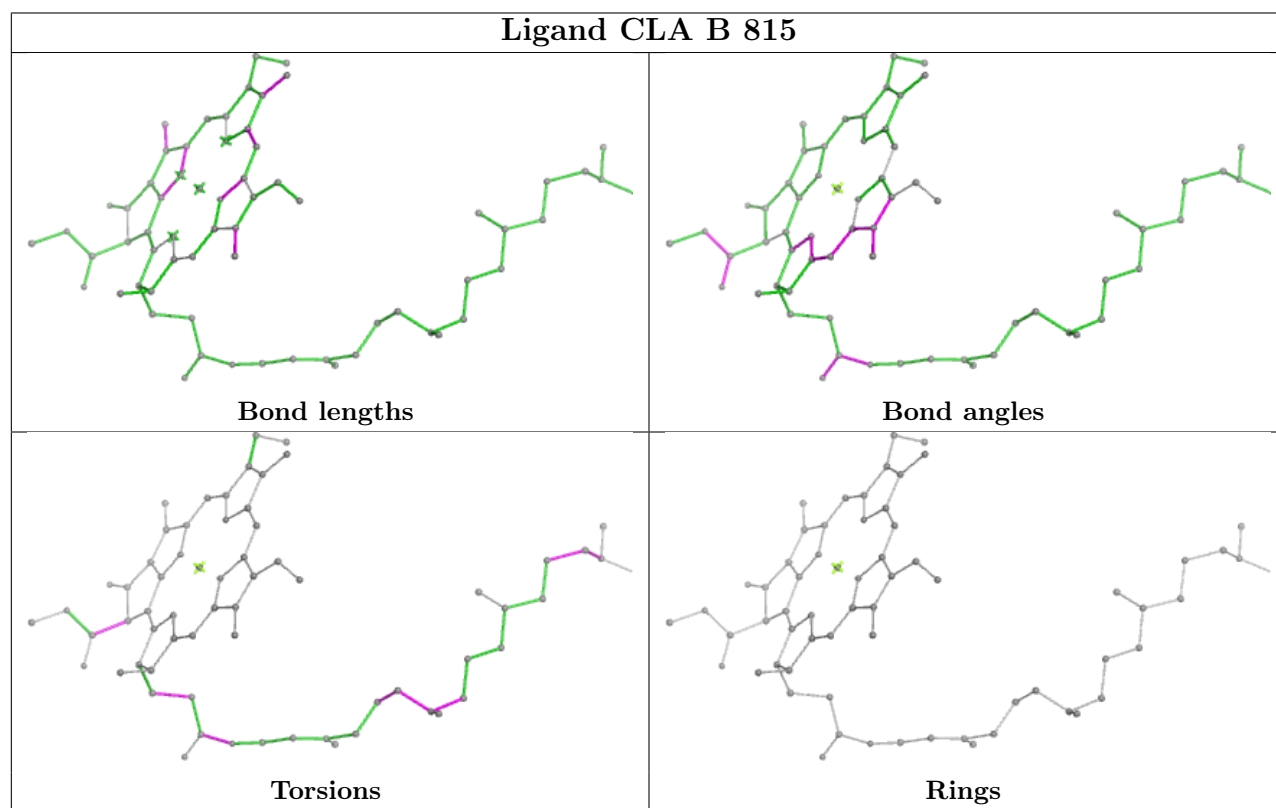
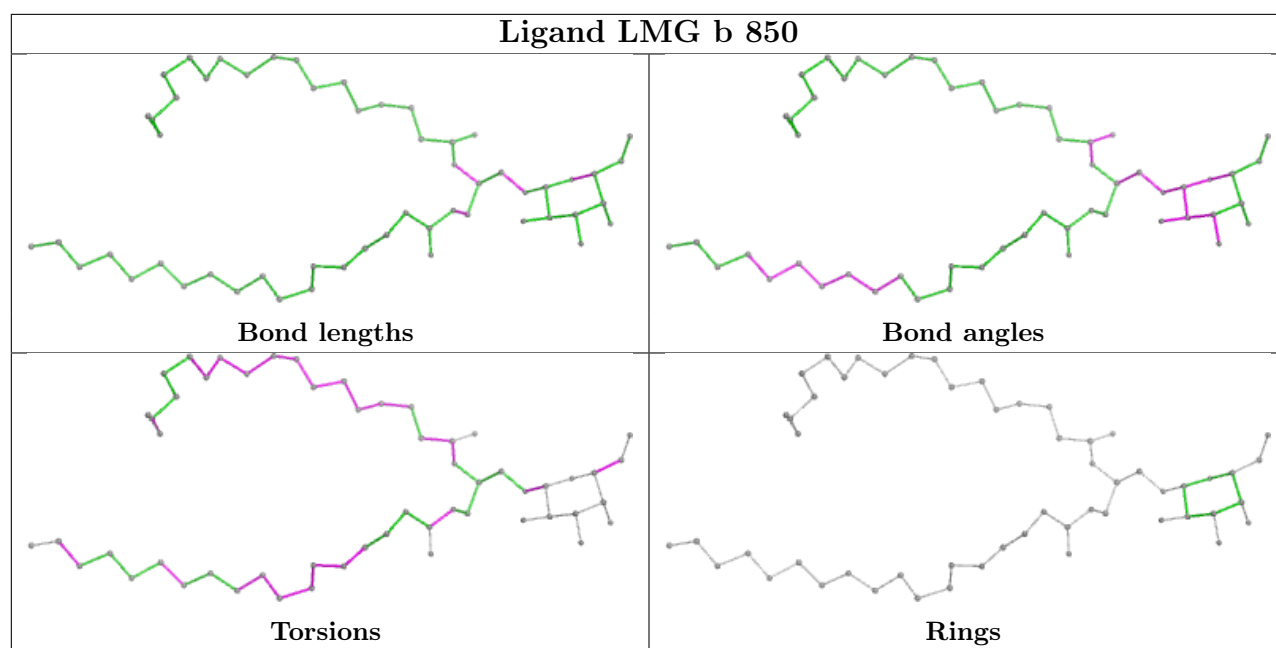


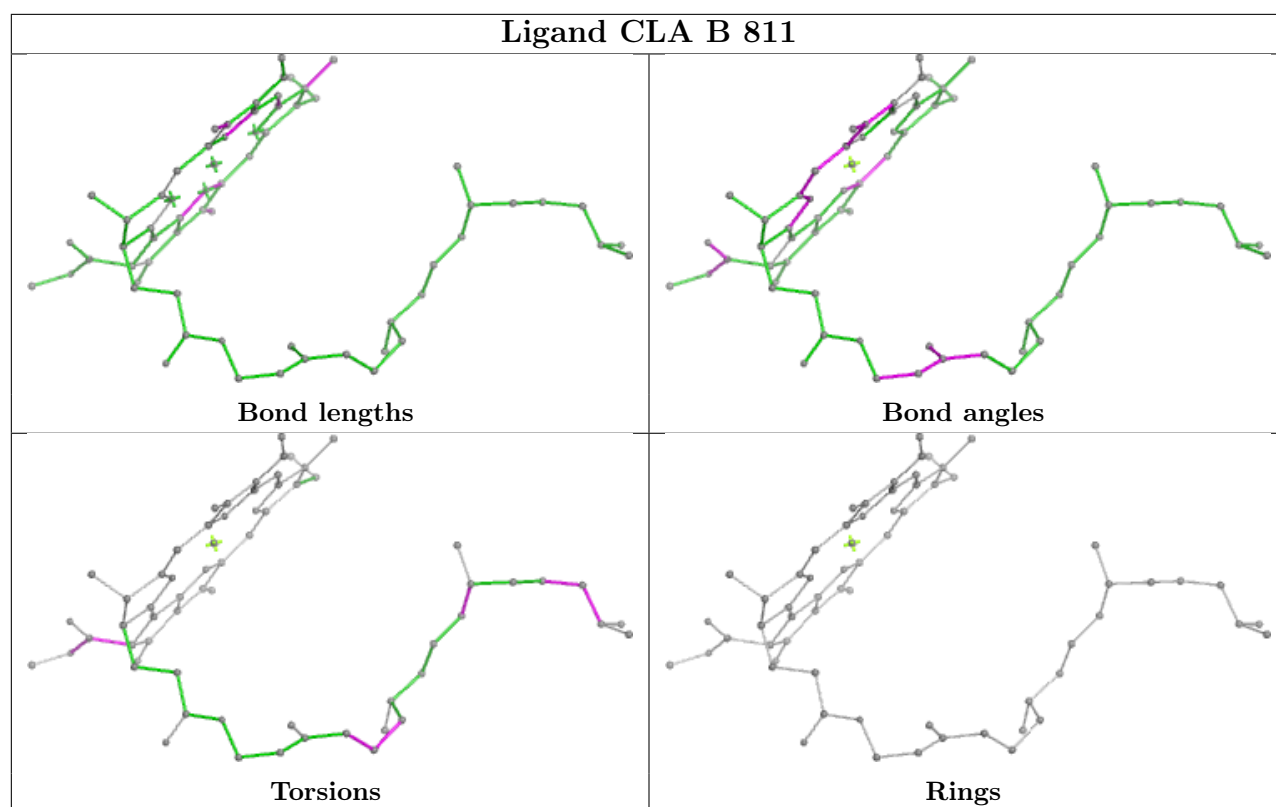




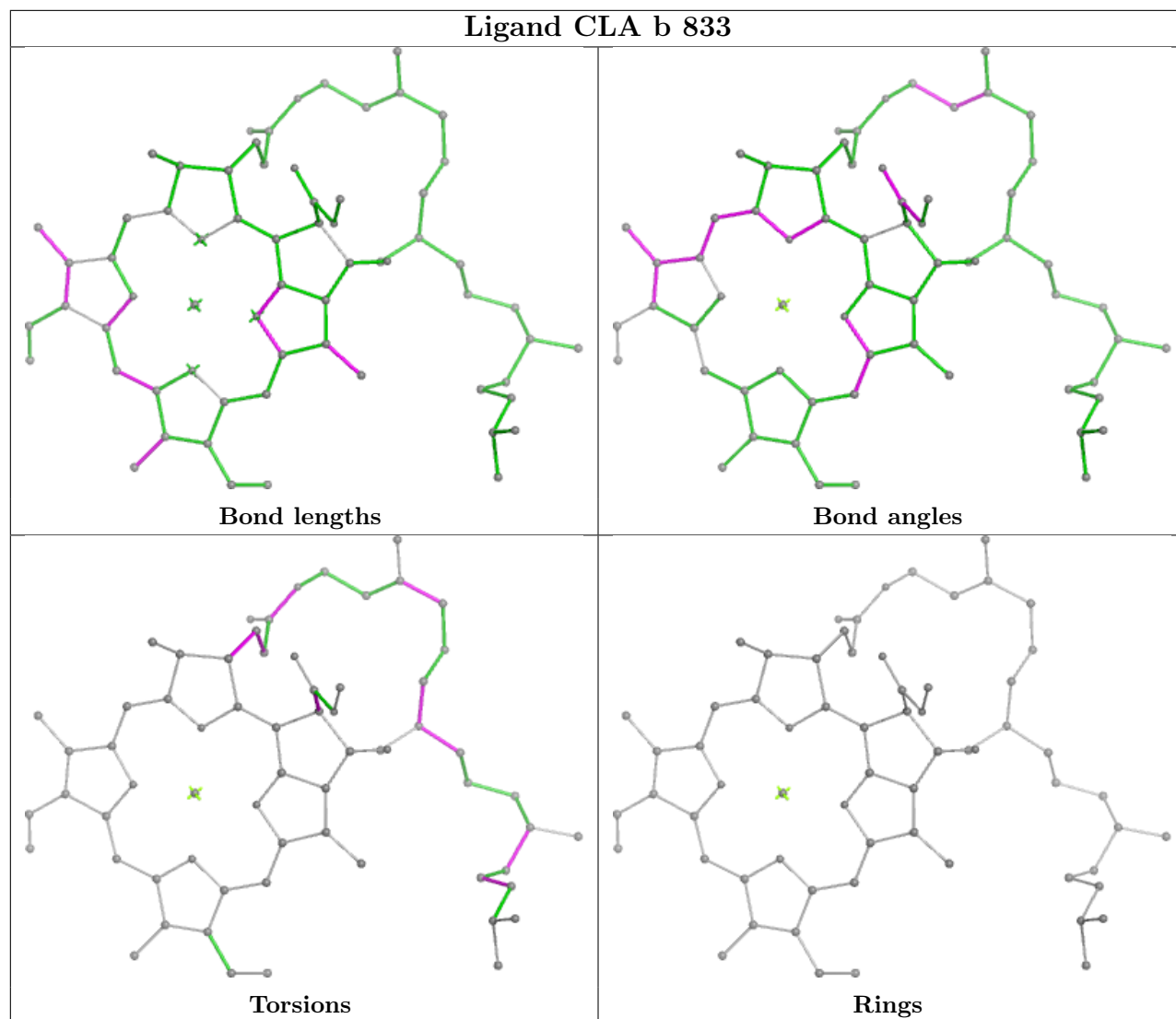




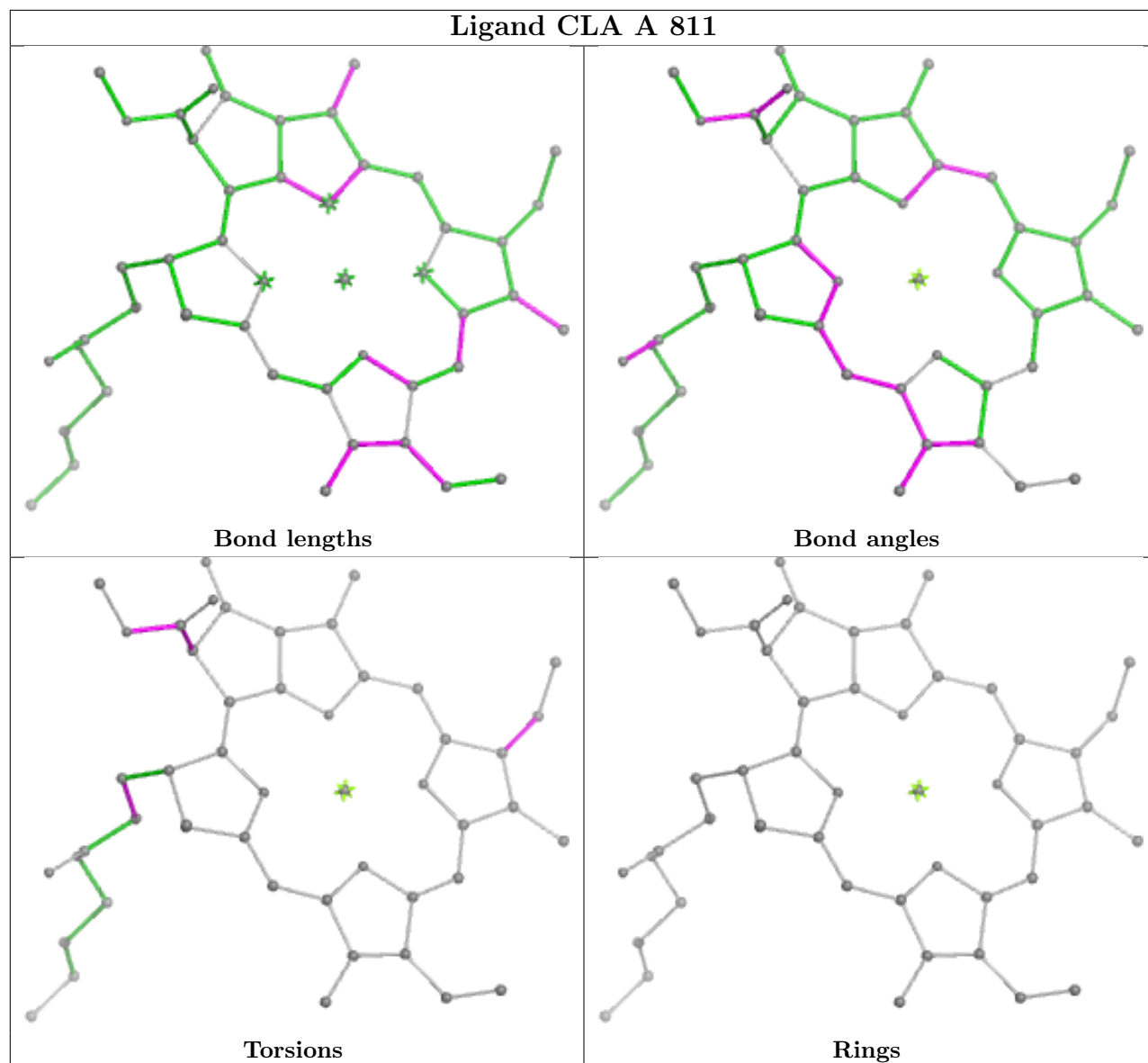




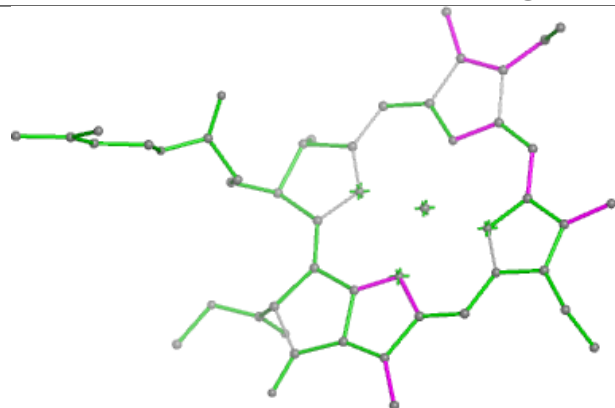
Ligand CLA b 833



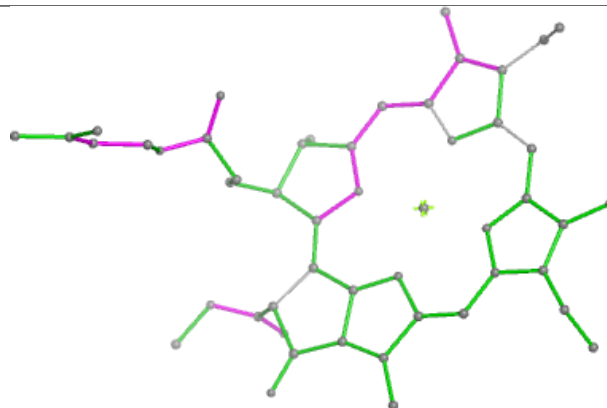
Ligand CLA A 811



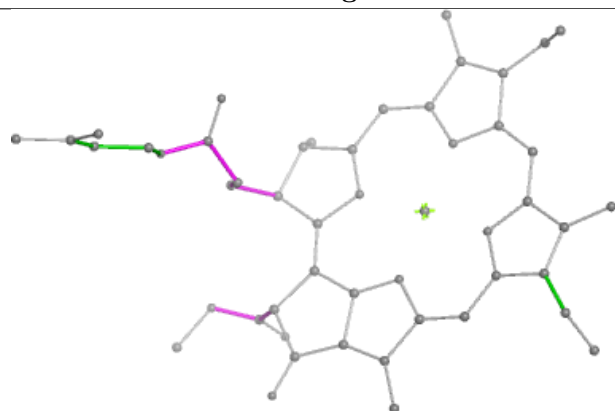
Ligand CLA b 836



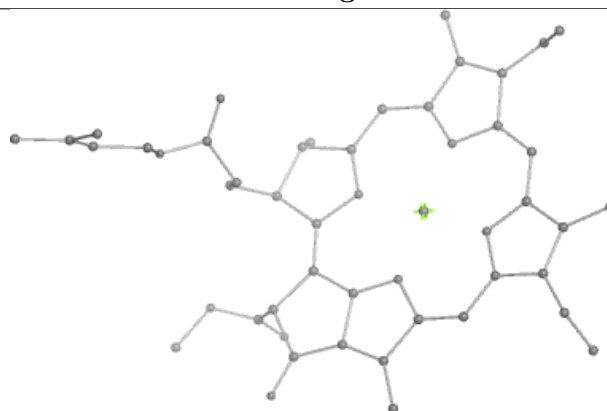
Bond lengths



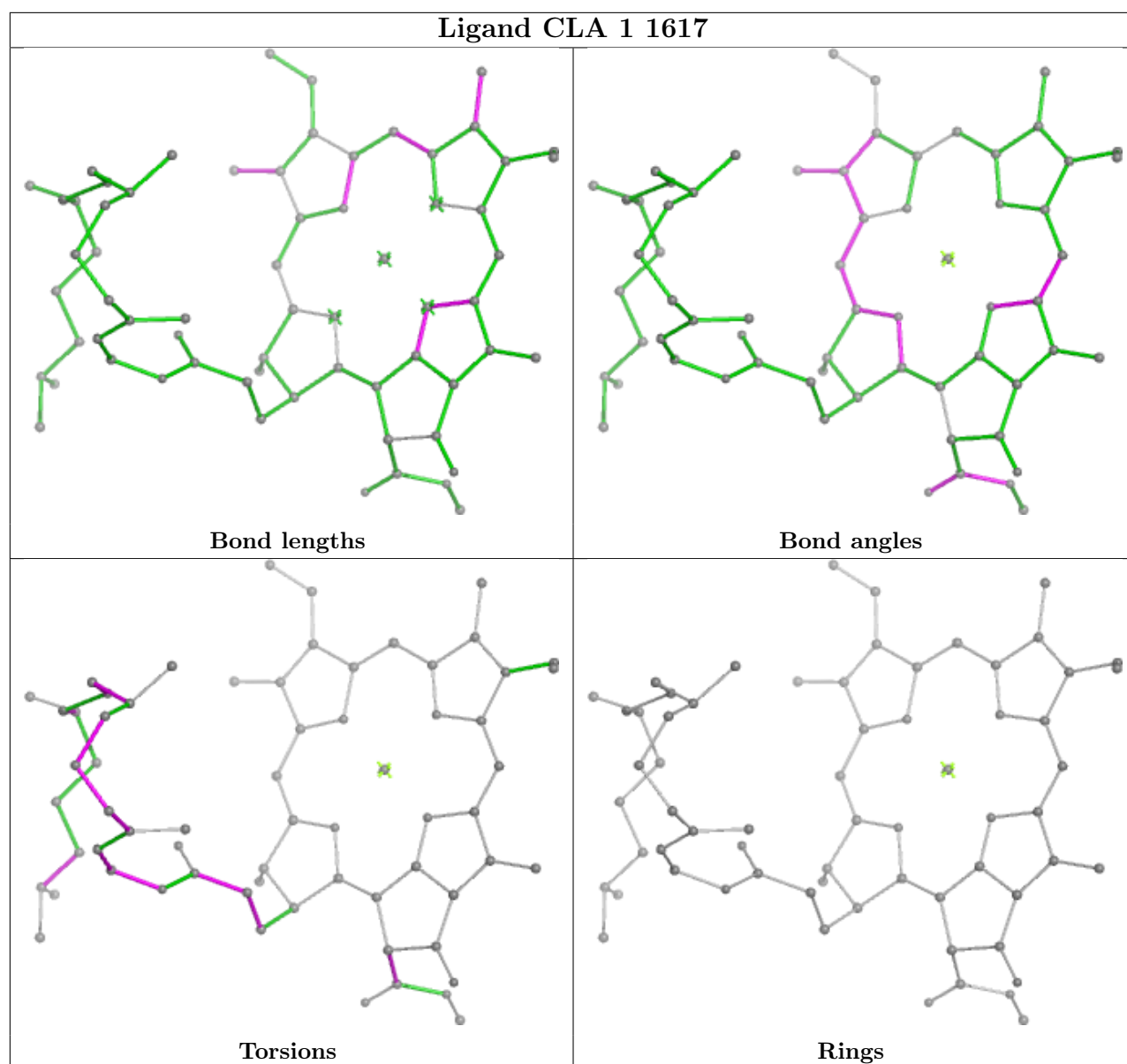
Bond angles



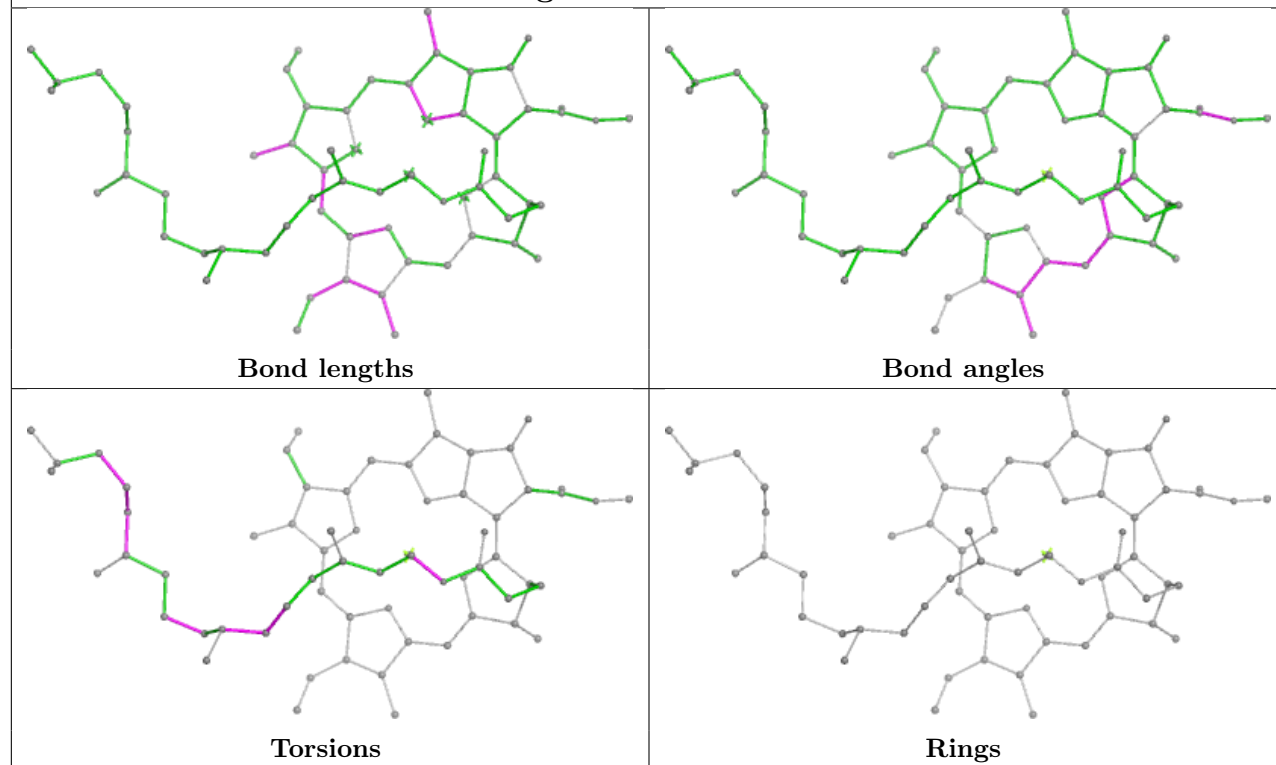
Torsions



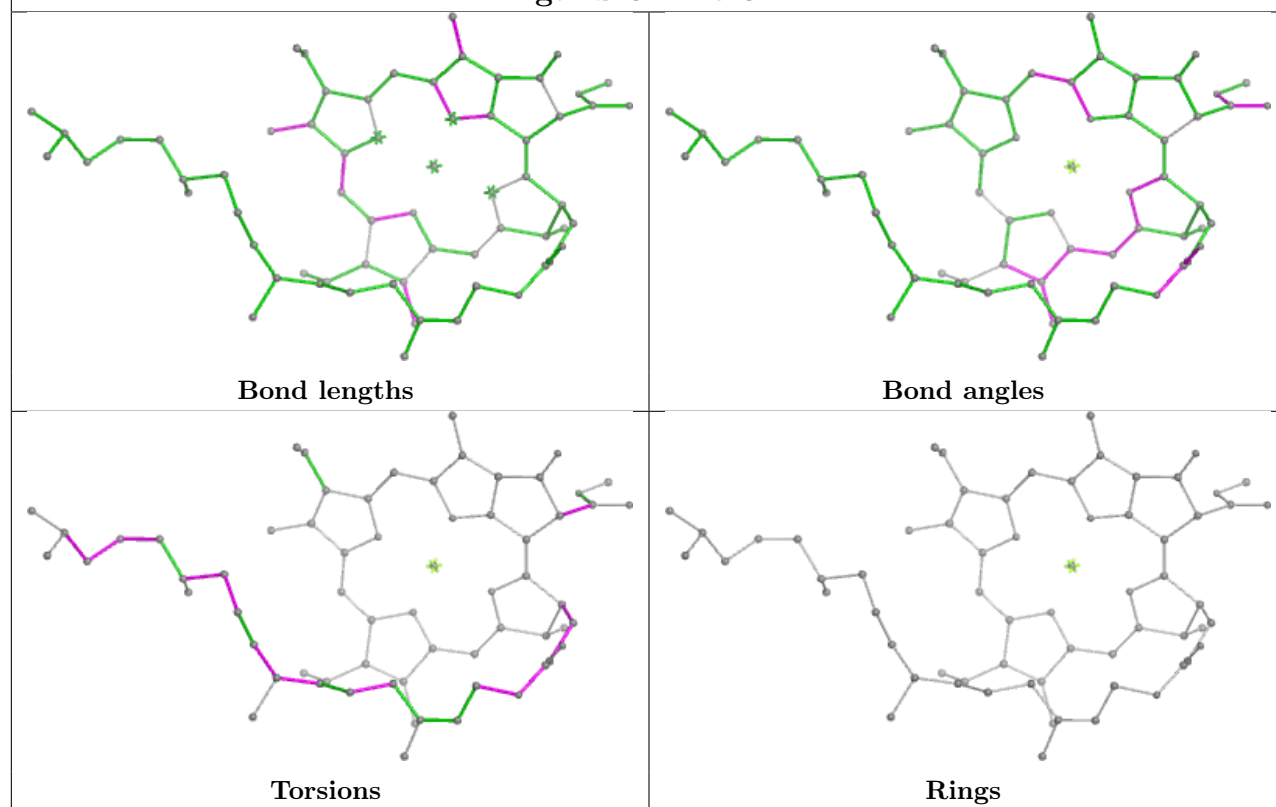
Rings



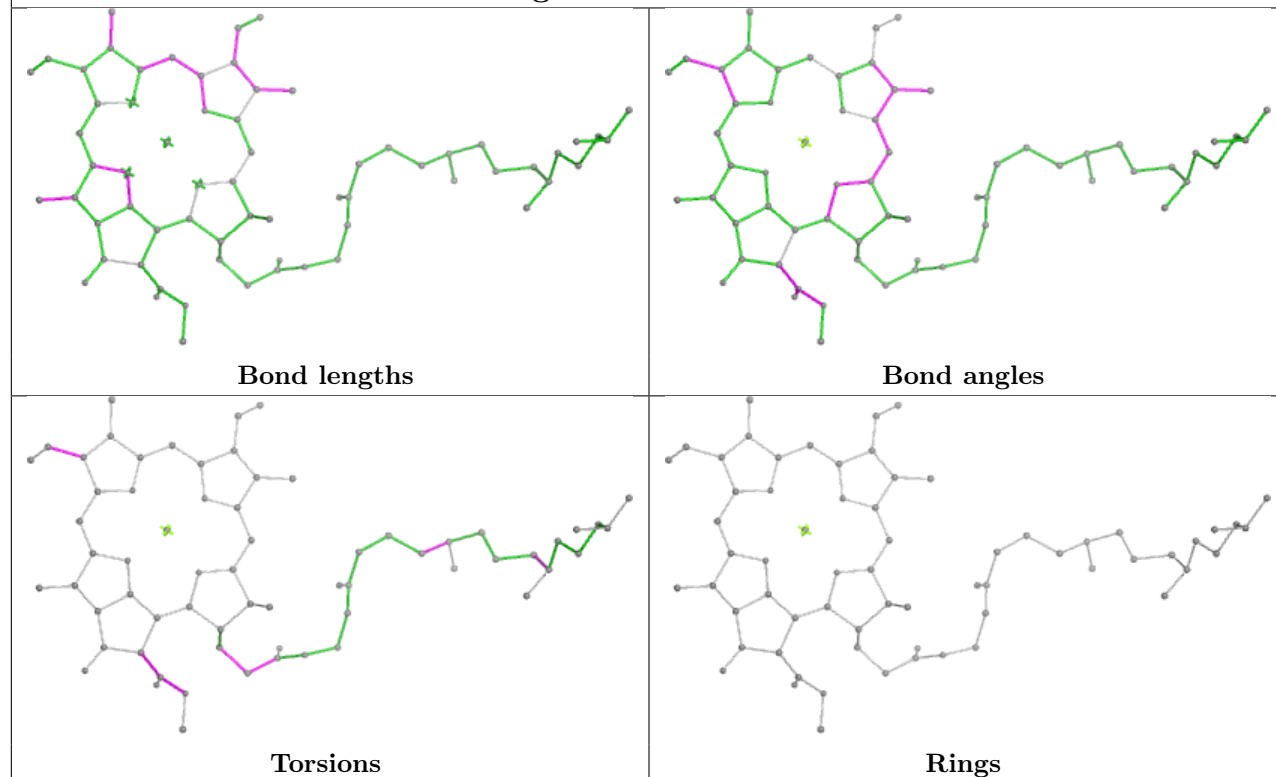
Ligand CLA 2 839



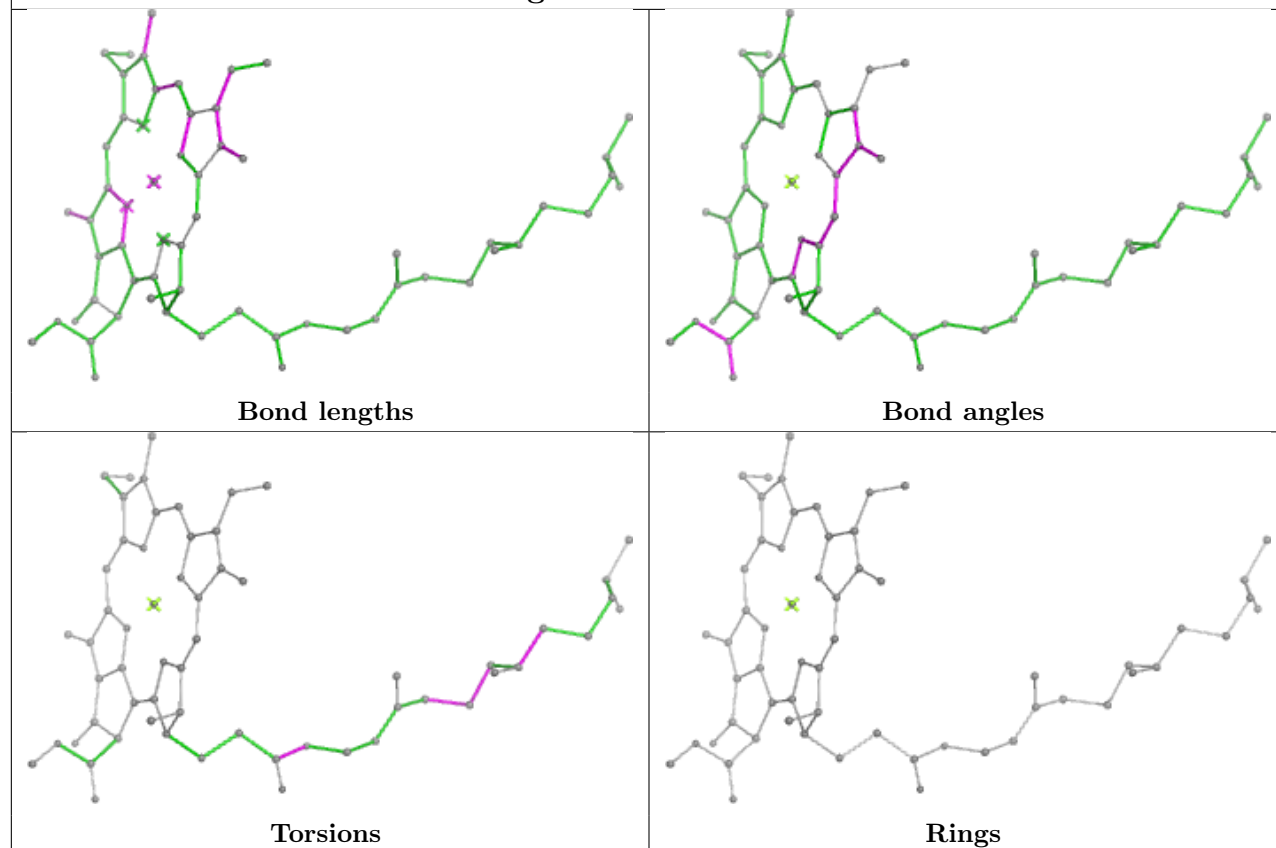
Ligand CLA b 821



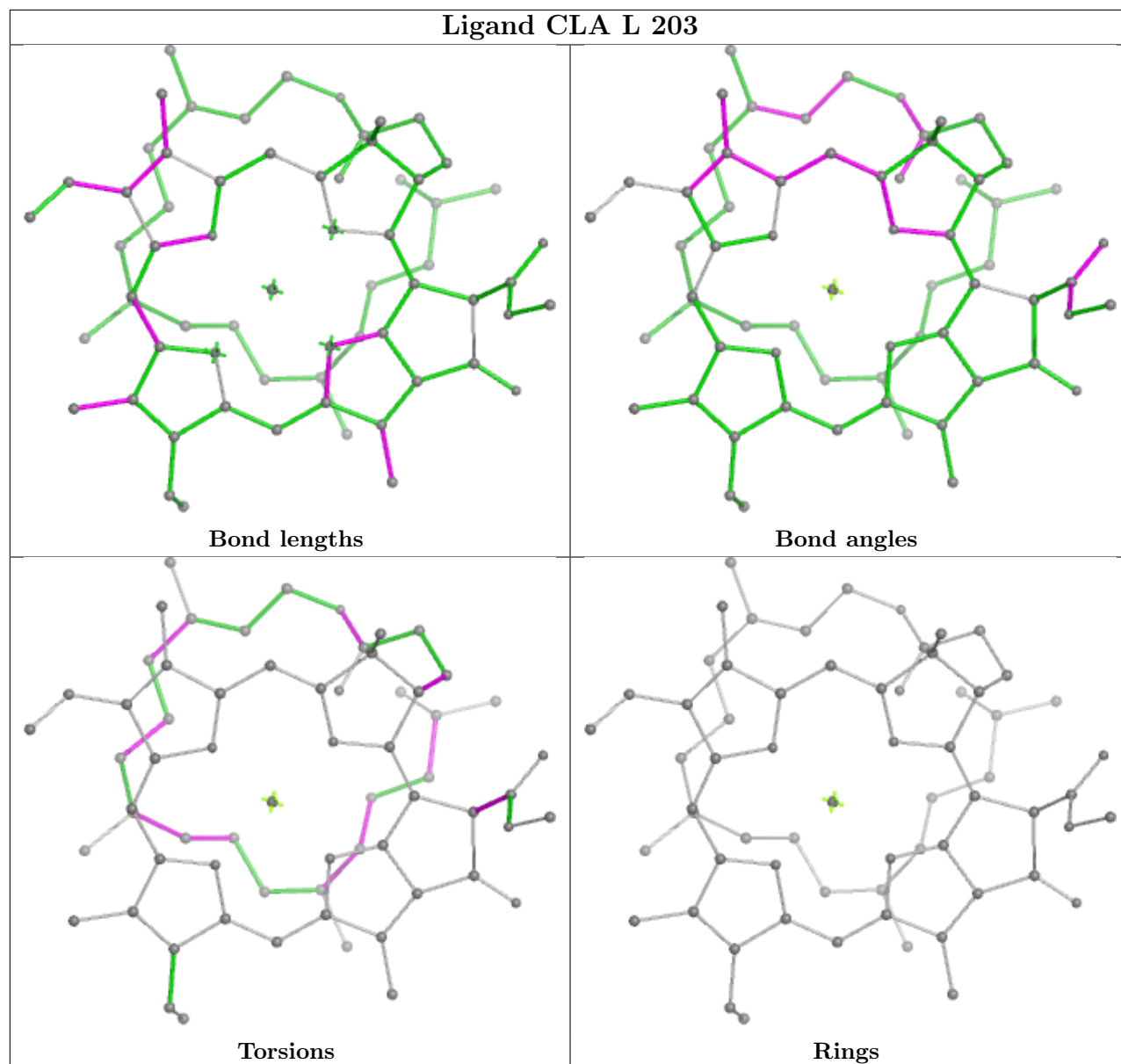
Ligand CLA B 803

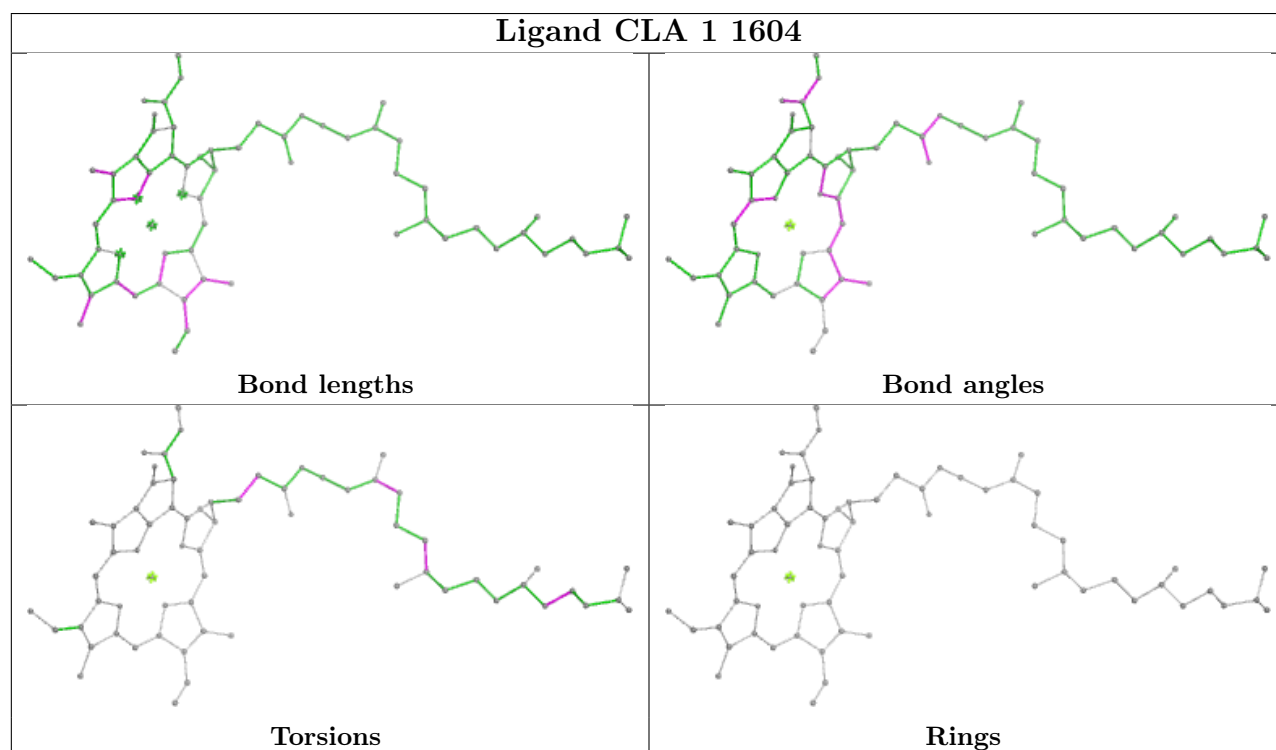
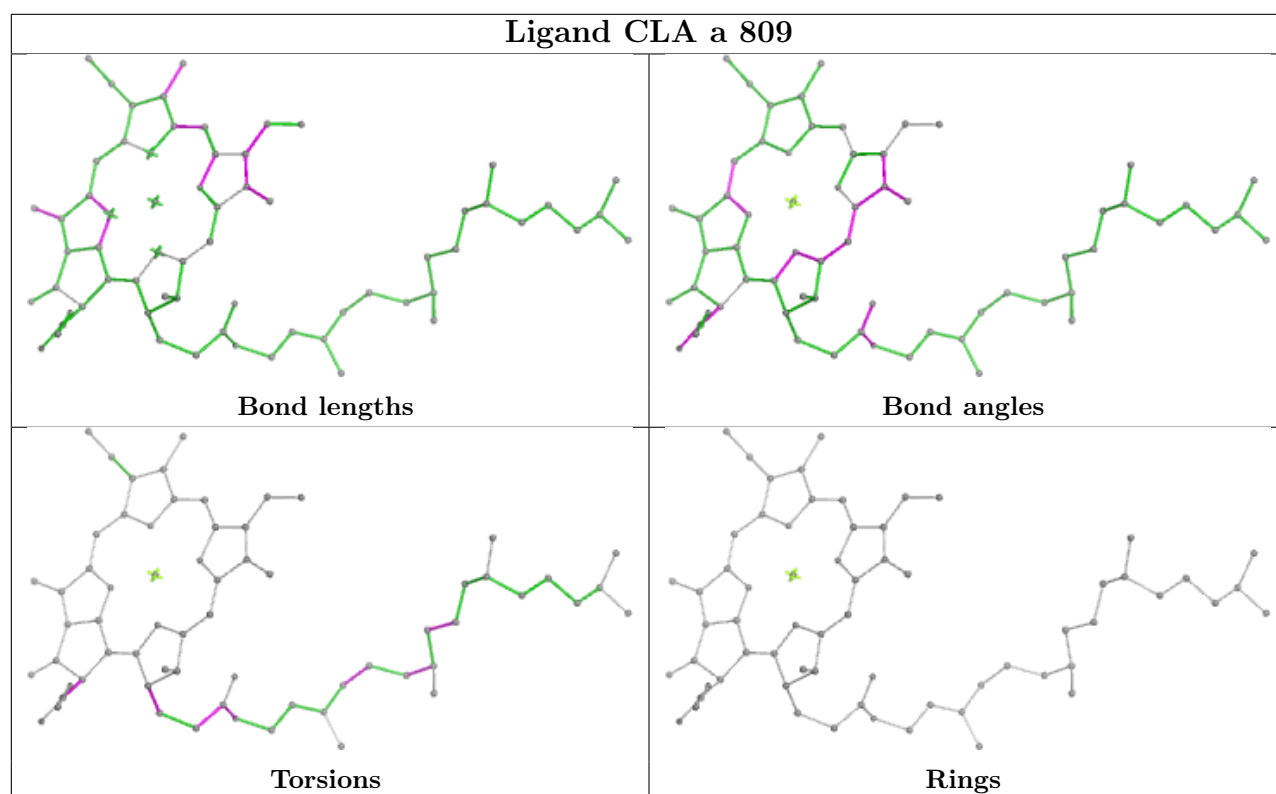


Ligand CLA 1 1633

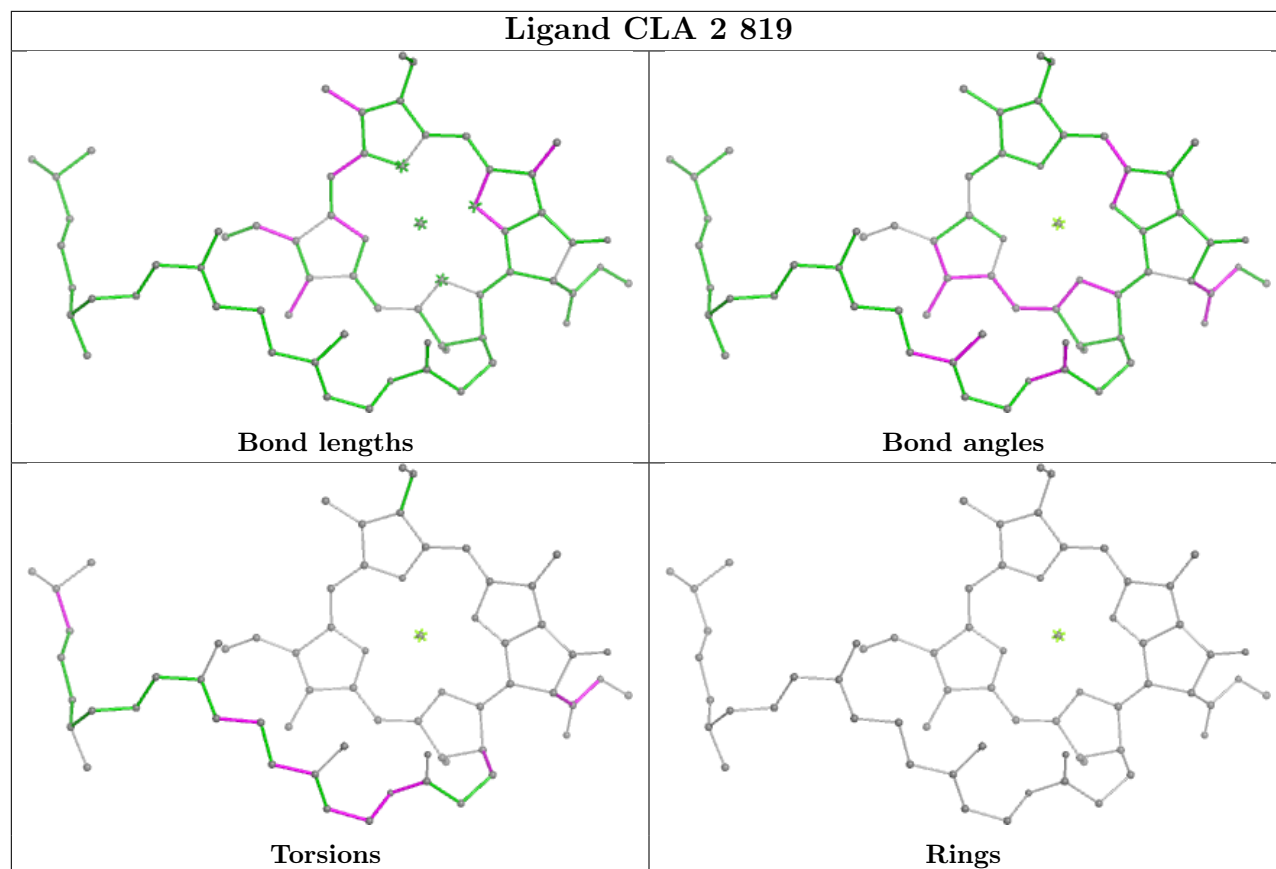


Ligand CLA L 203

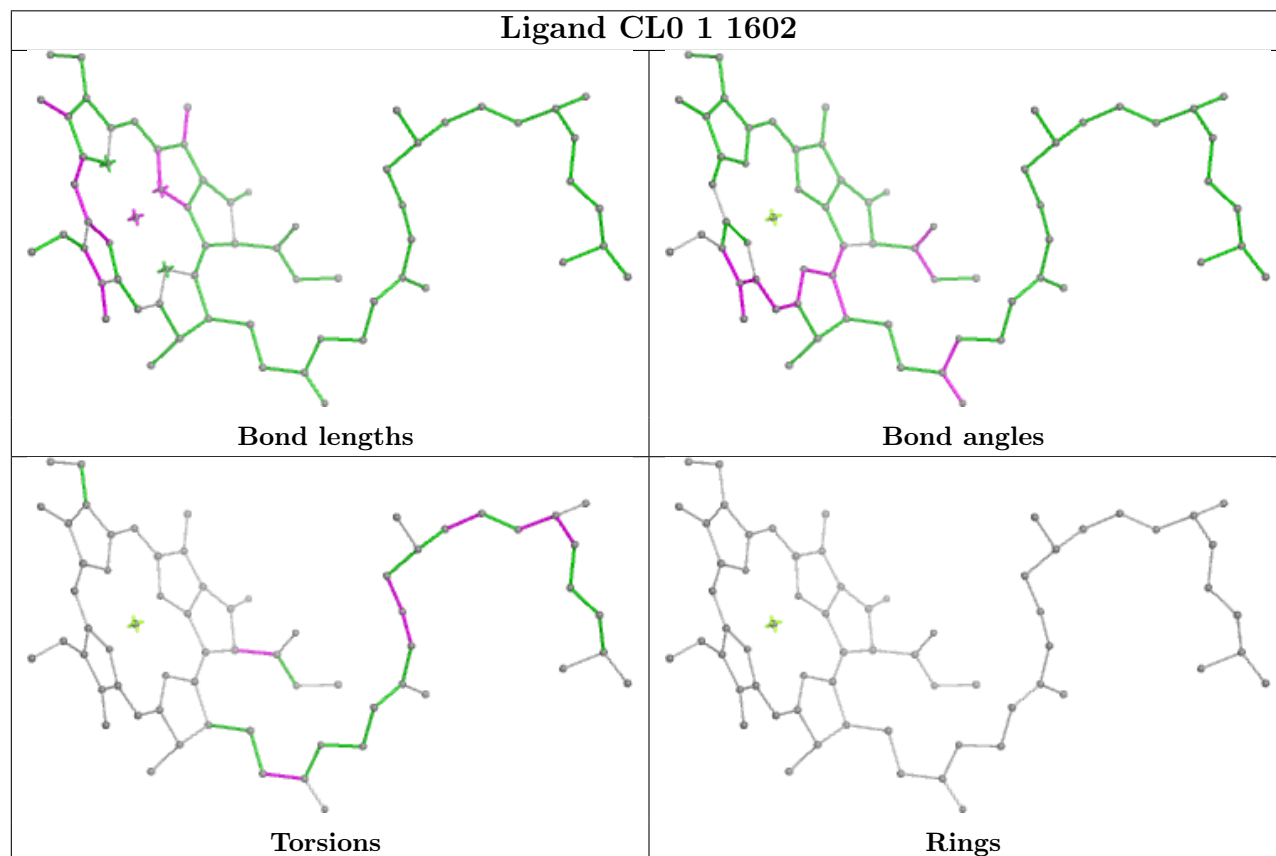


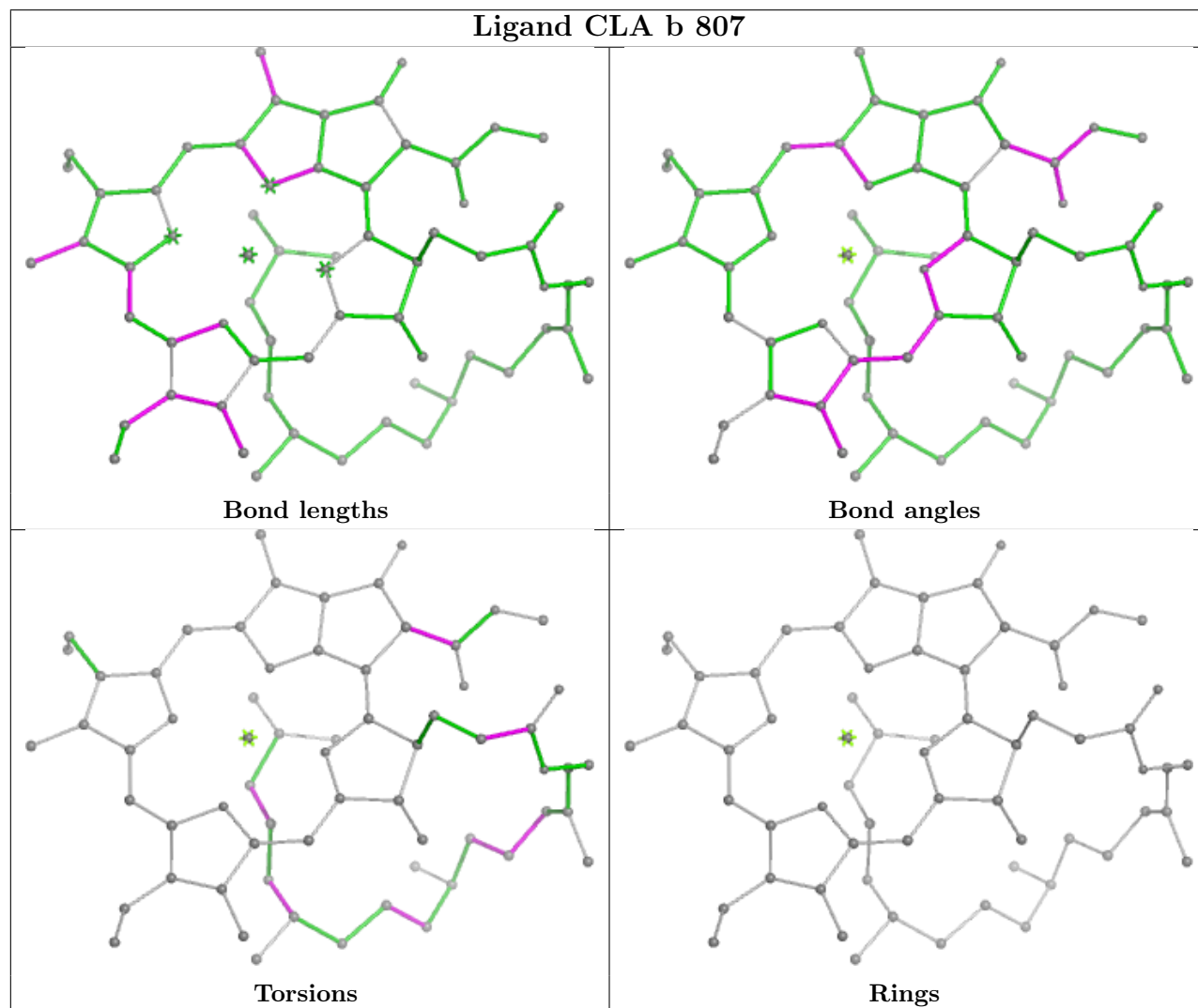
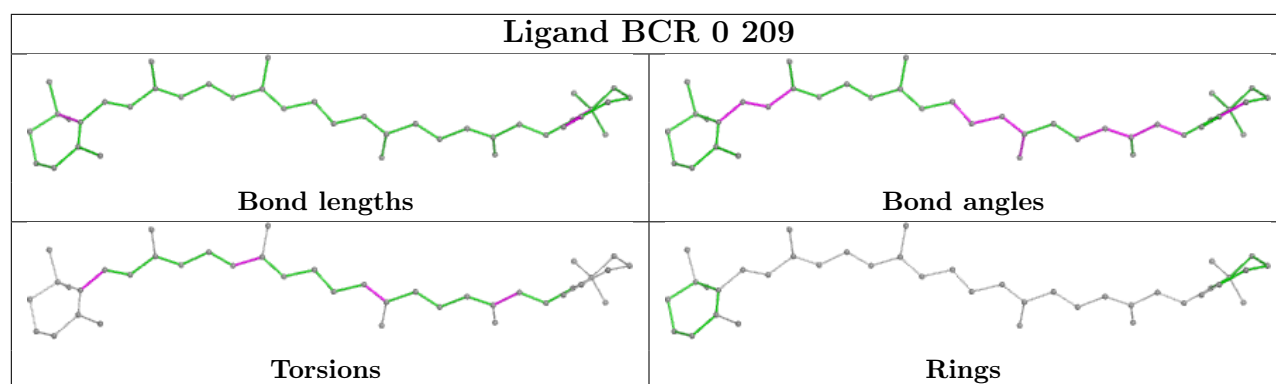


Ligand CLA 2 819

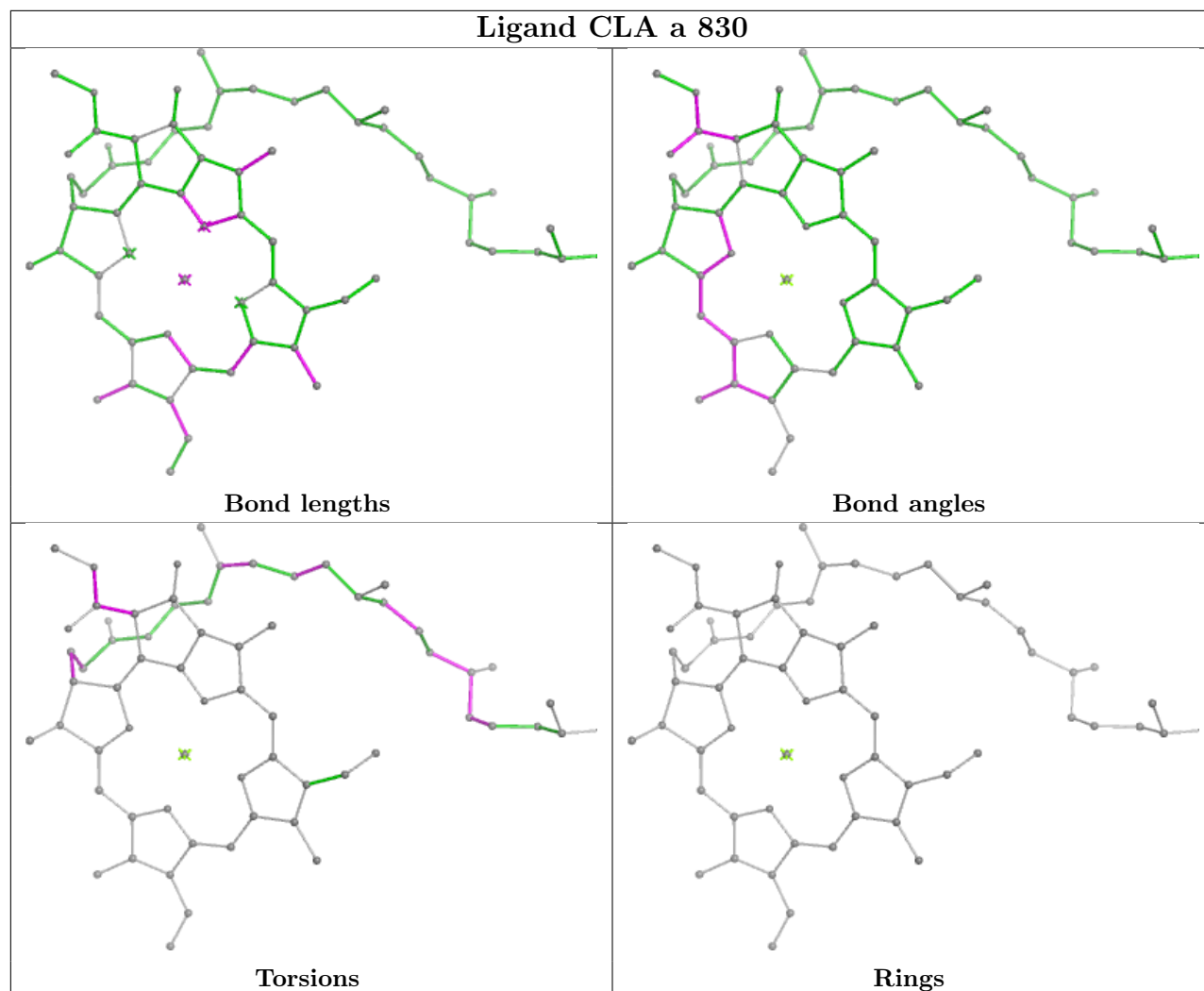


Ligand CL0 1 1602

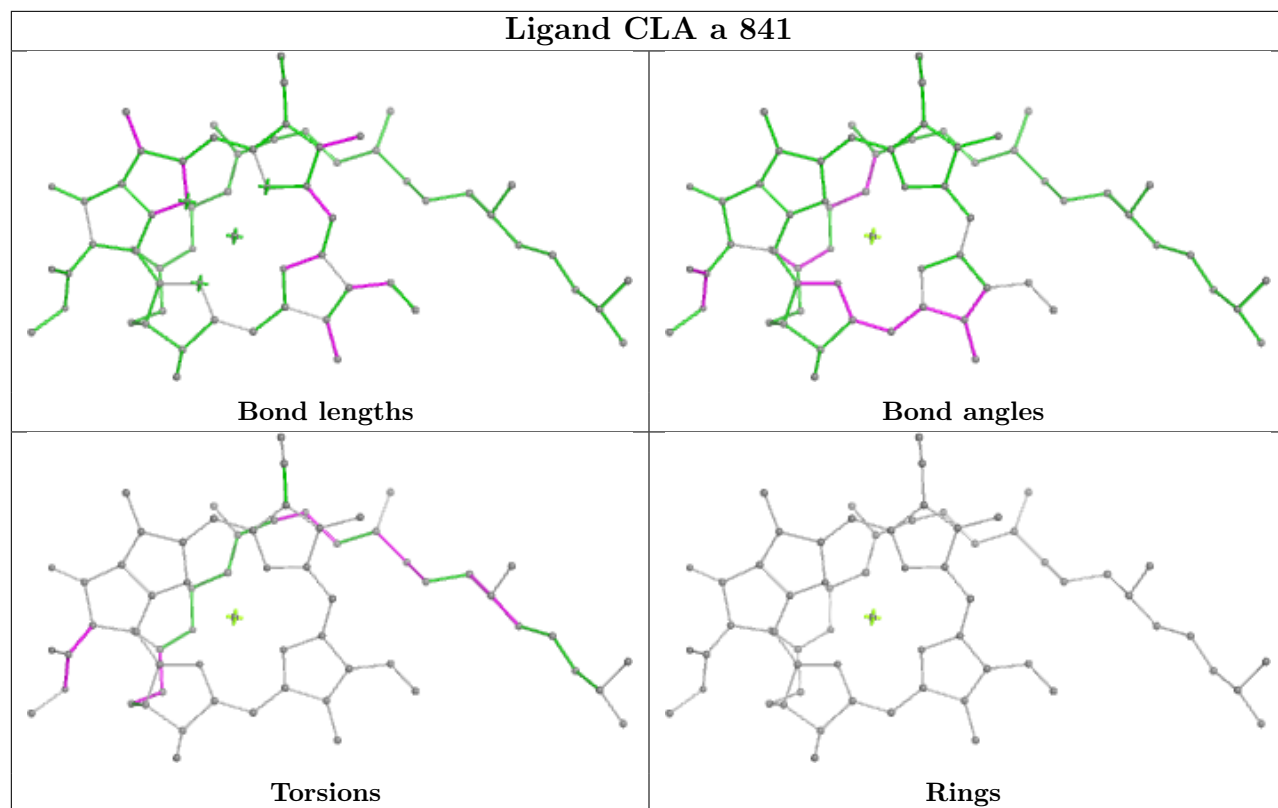




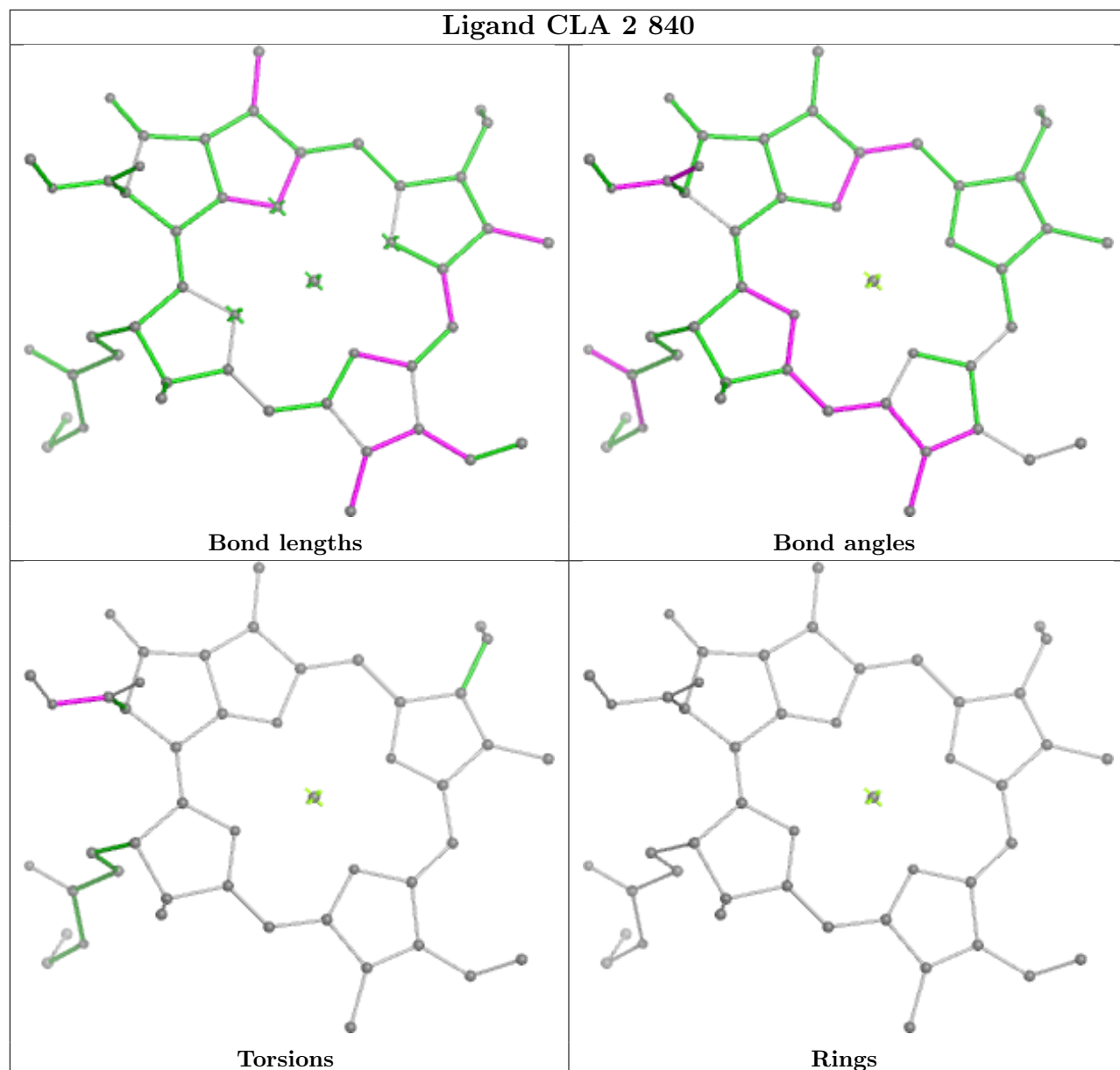
Ligand CLA a 830



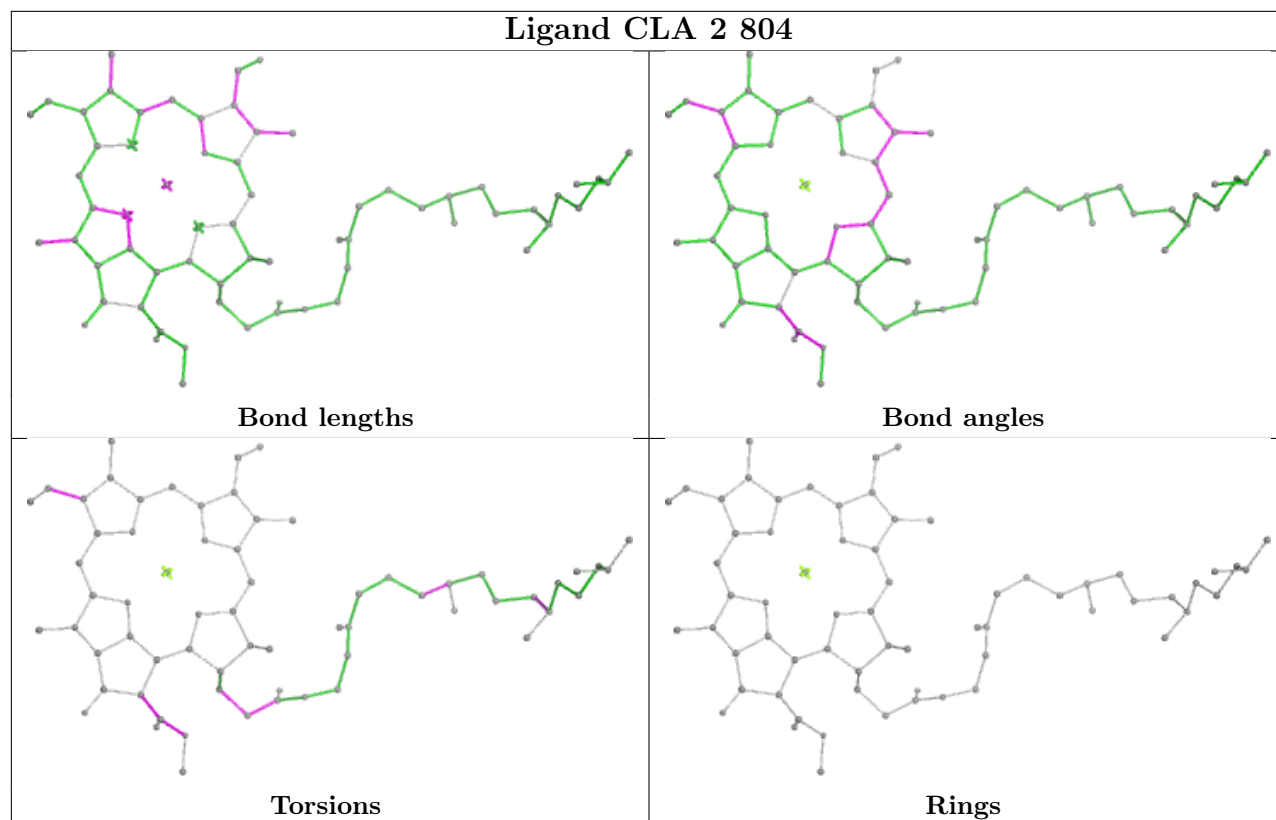
Ligand CLA a 841



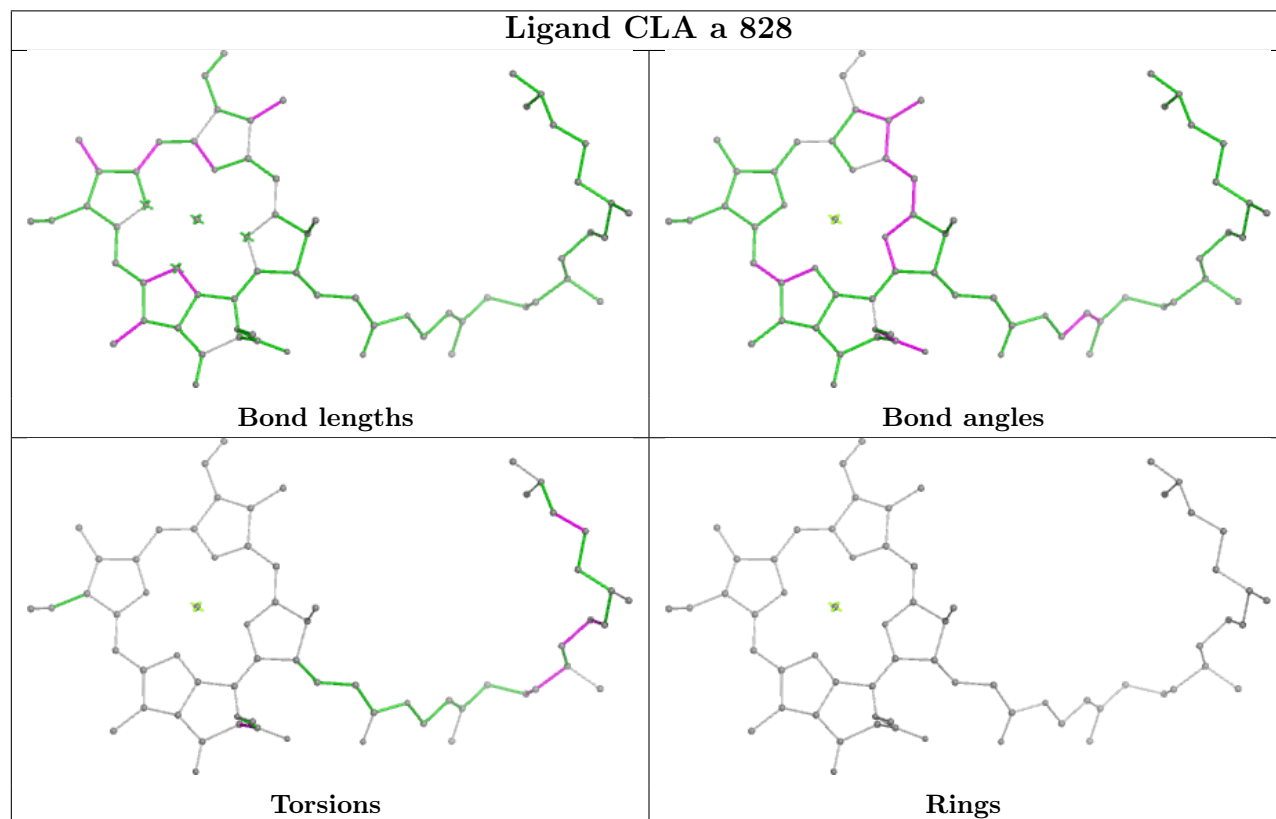
Ligand CLA 2 840

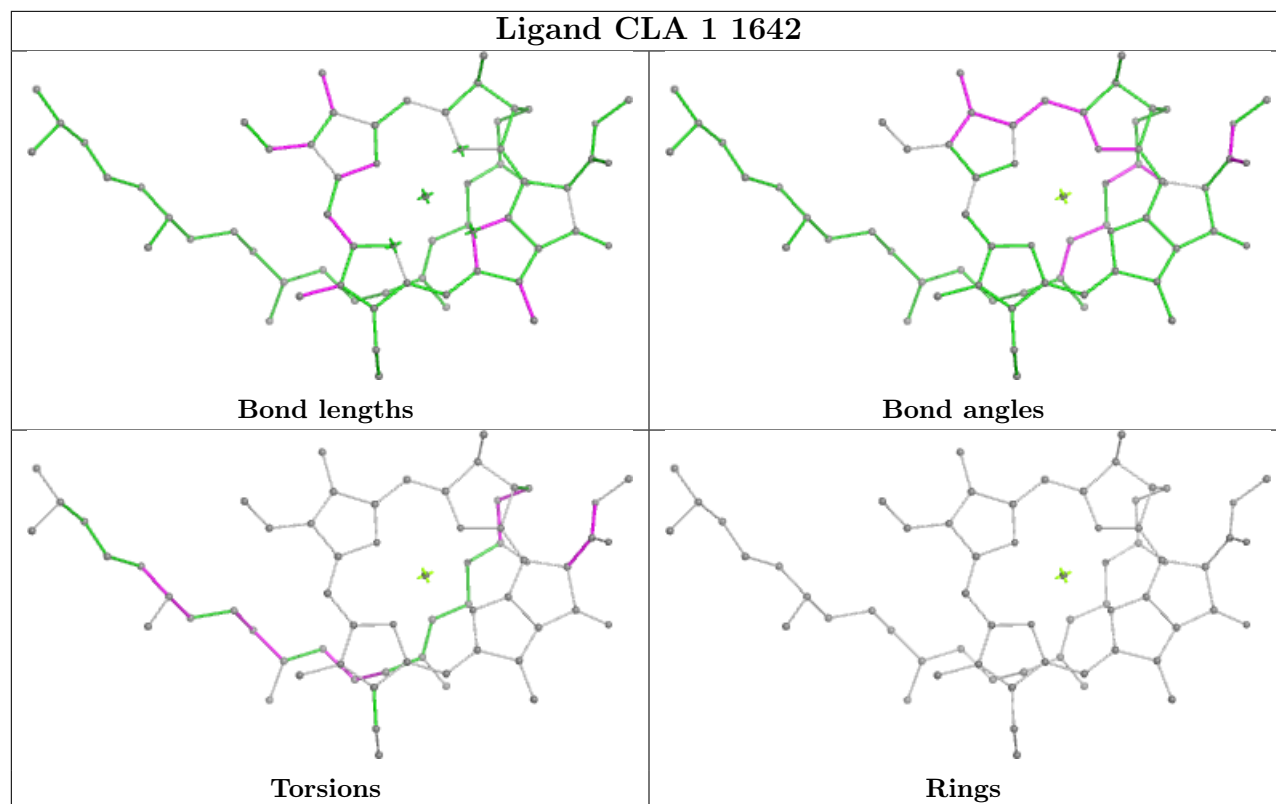


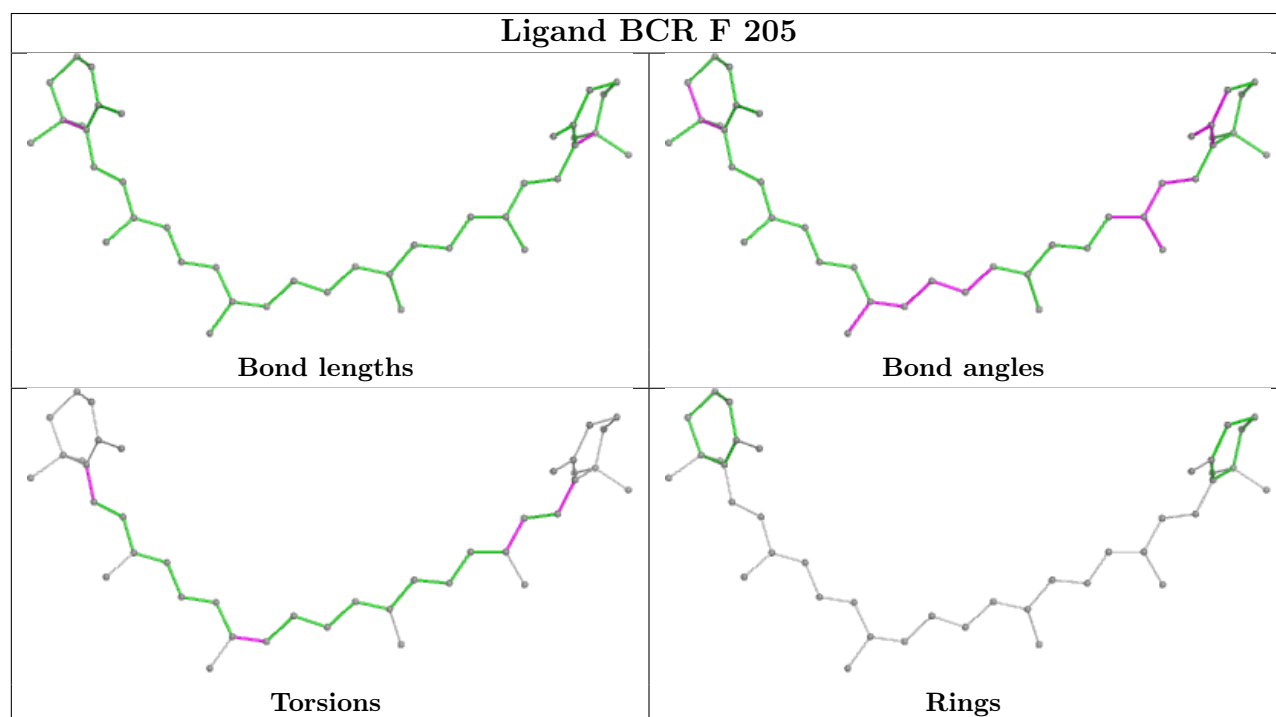
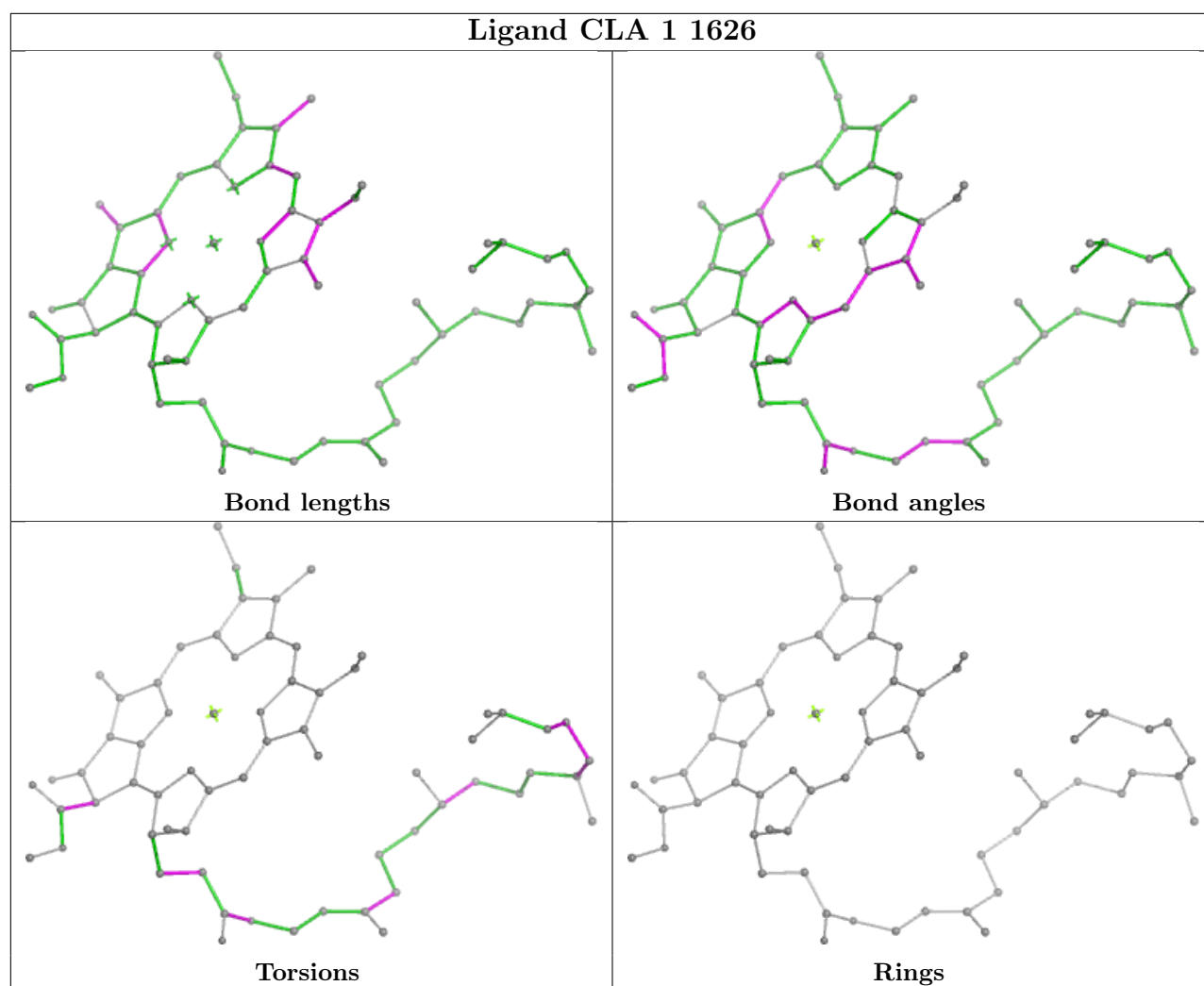
Ligand CLA 2 804

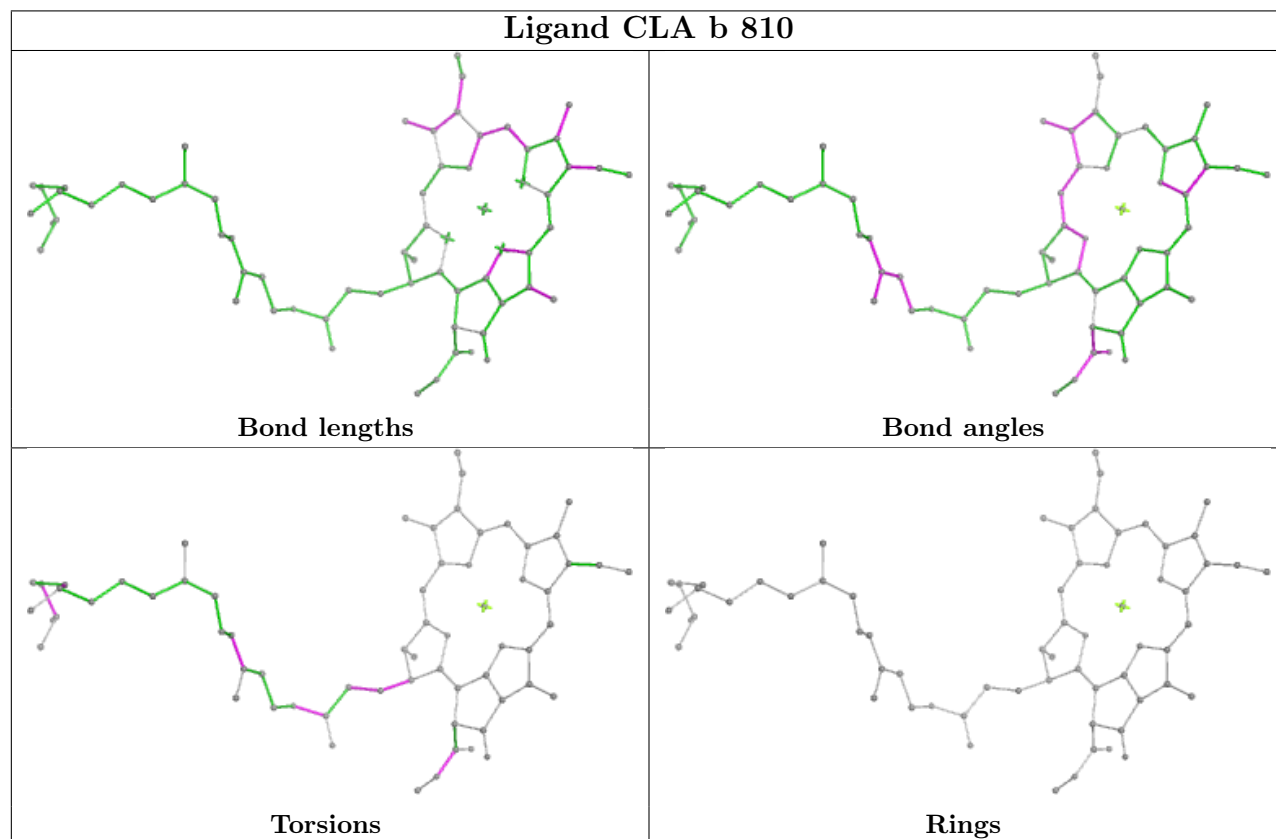
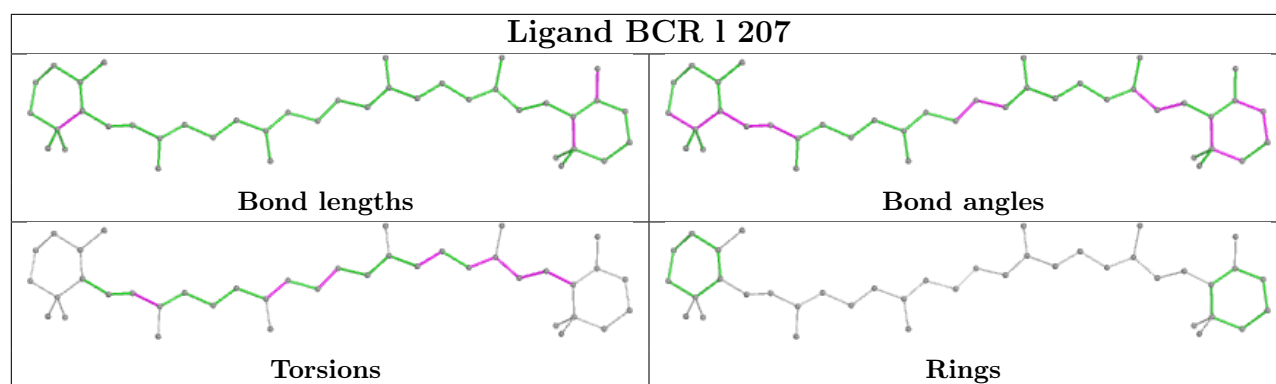


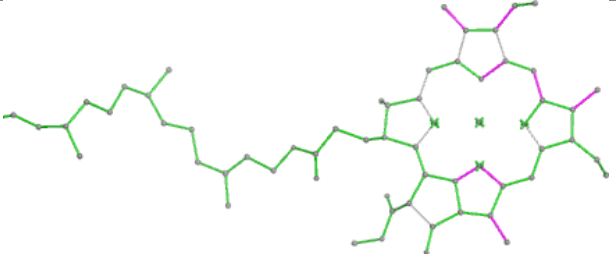
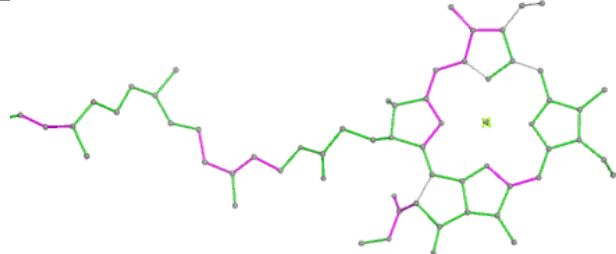
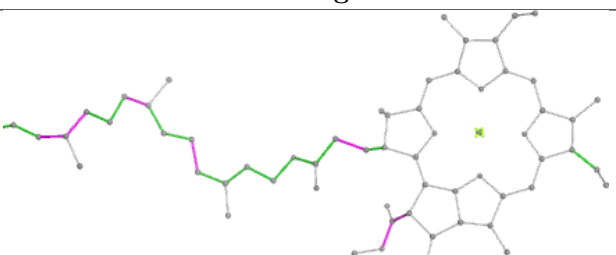
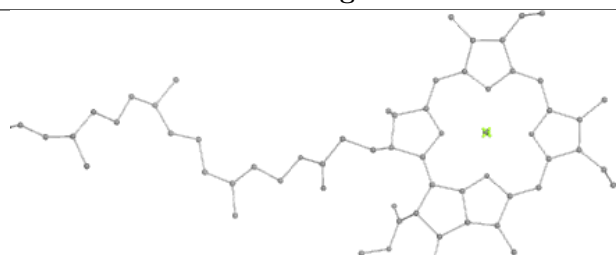
Ligand CLA a 828

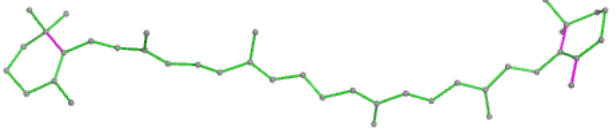
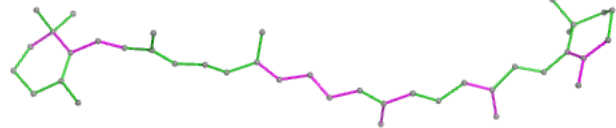
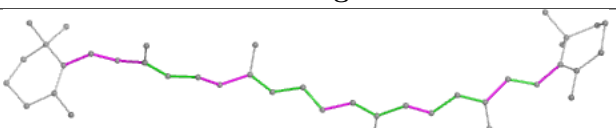
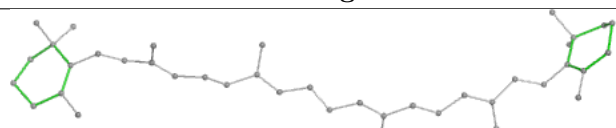


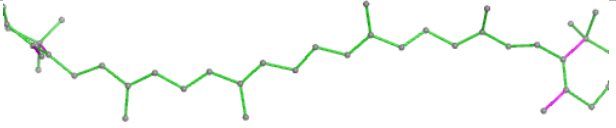
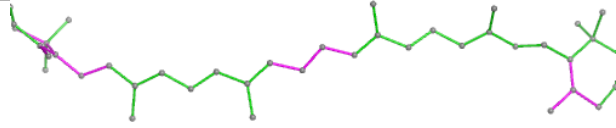
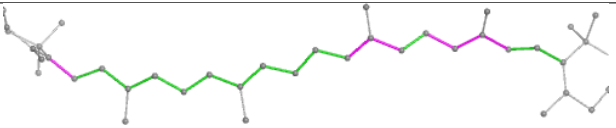
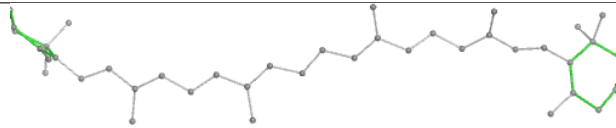


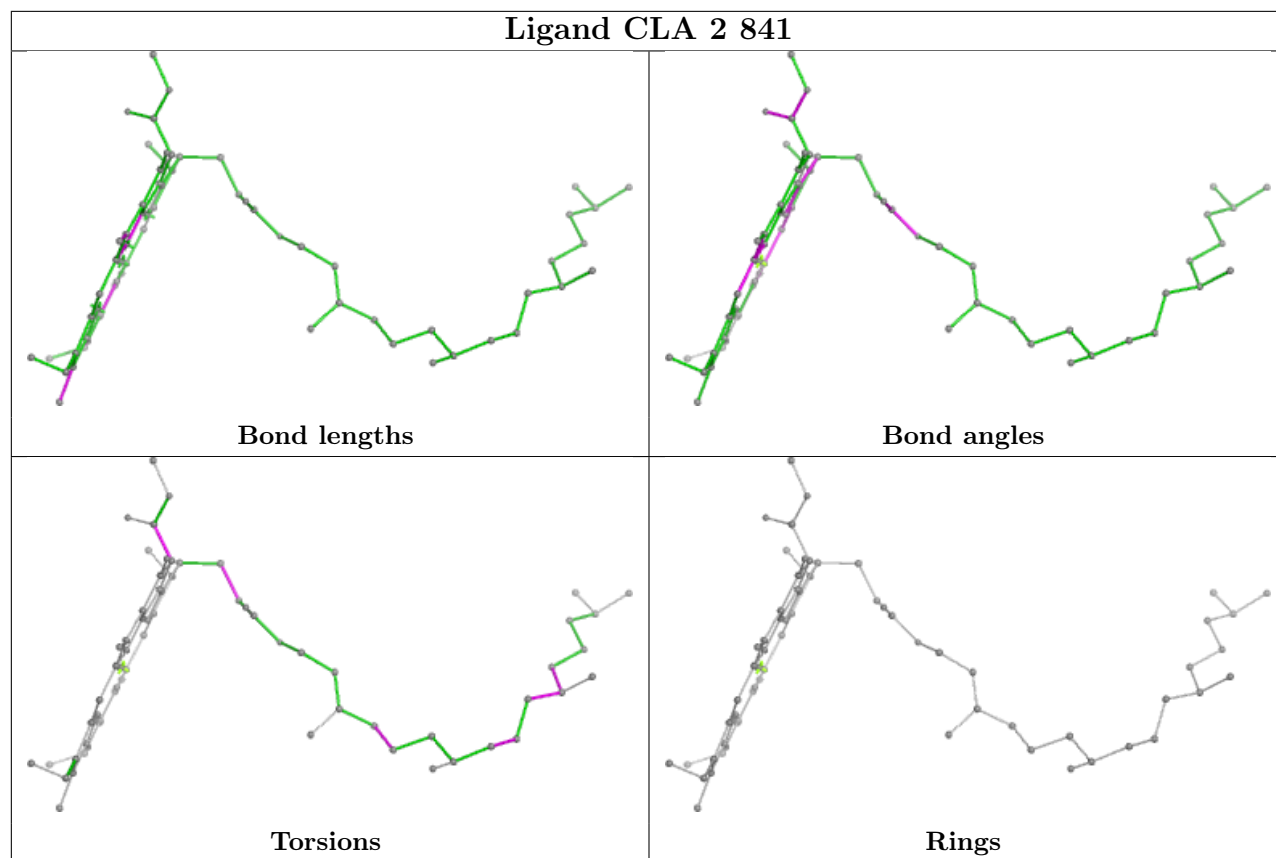




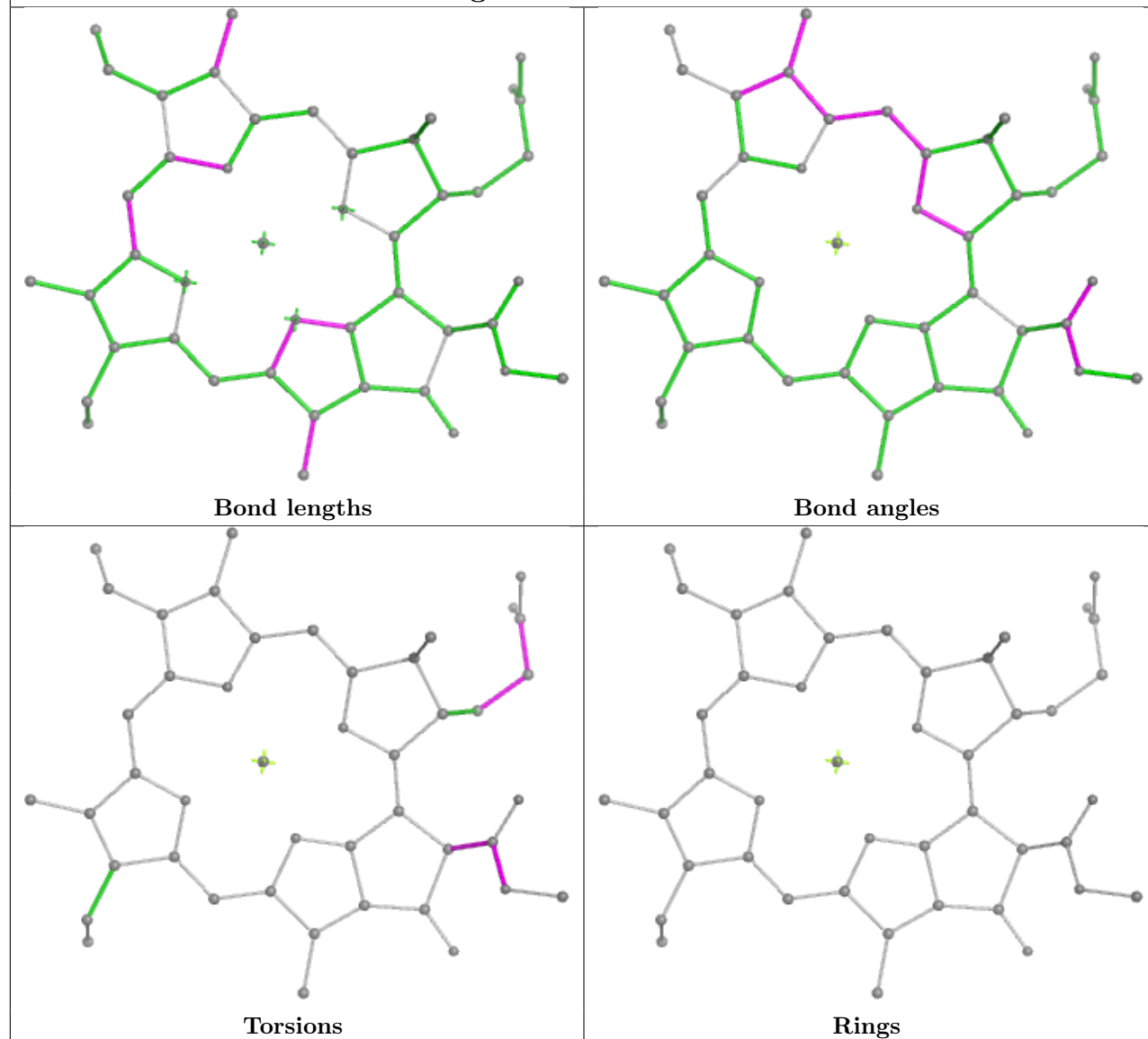
Ligand CLA 1 1635	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 2 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

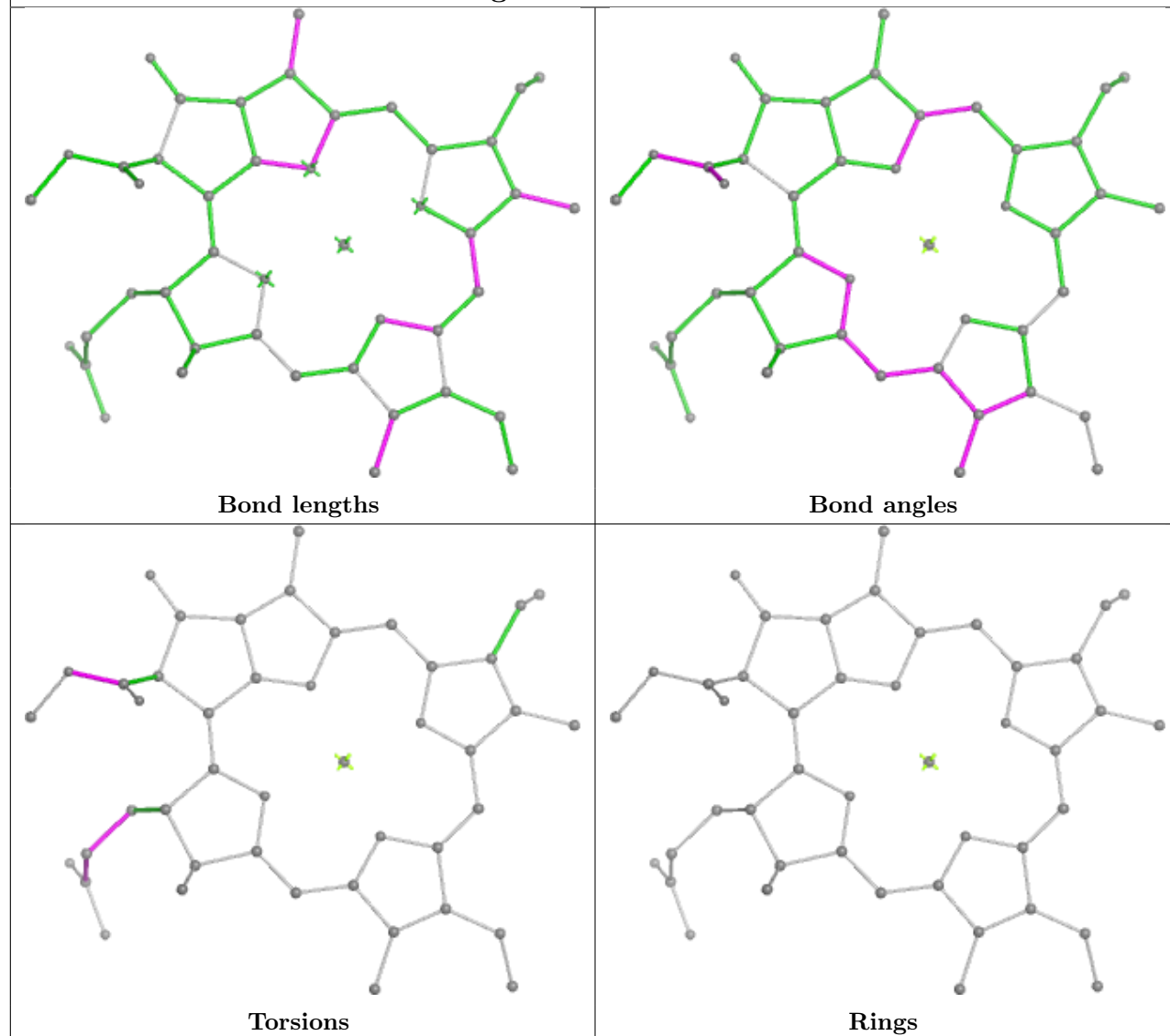
Ligand BCR 1 1651	
	
Bond lengths	Bond angles
	
Torsions	Rings



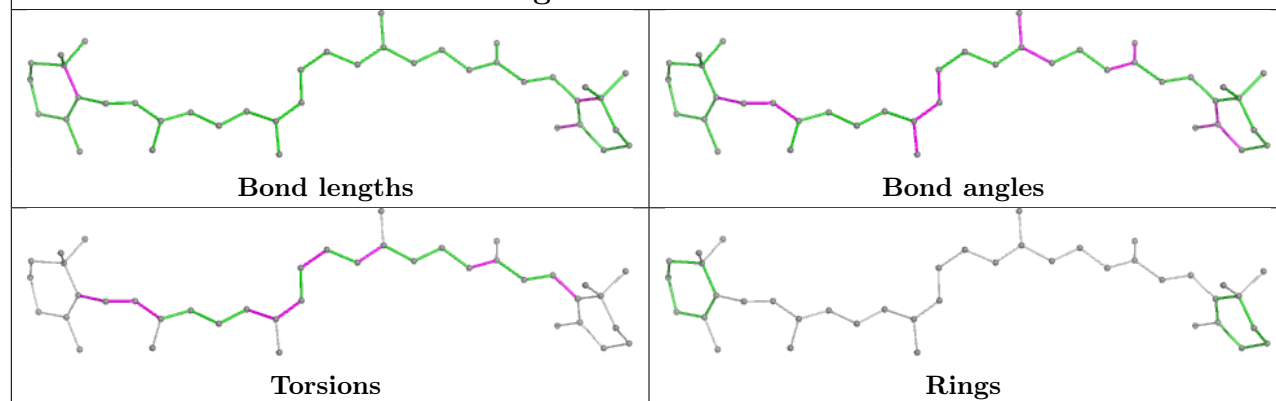
Ligand CLA X 1701

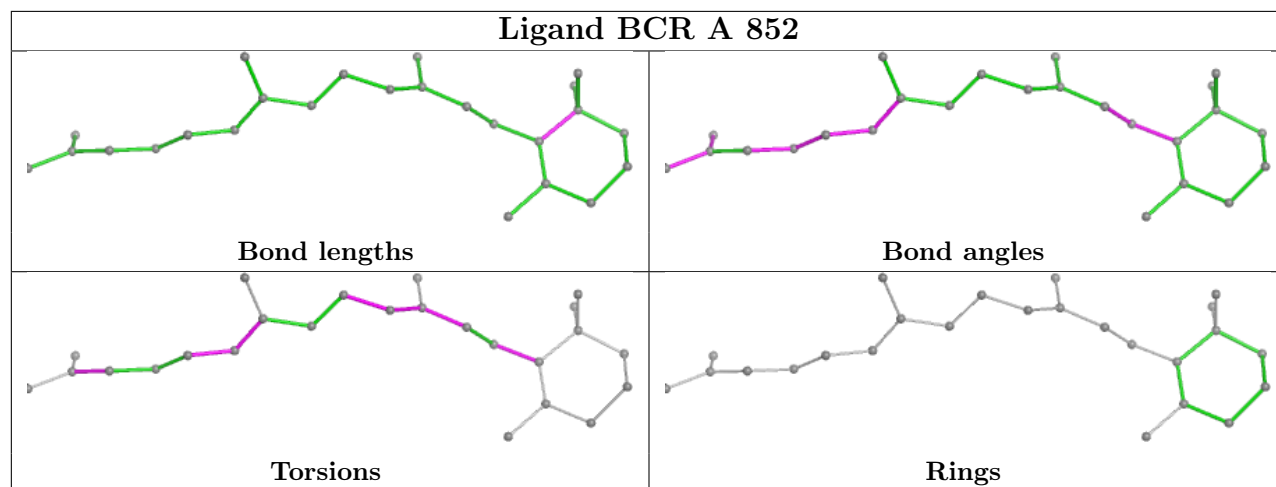
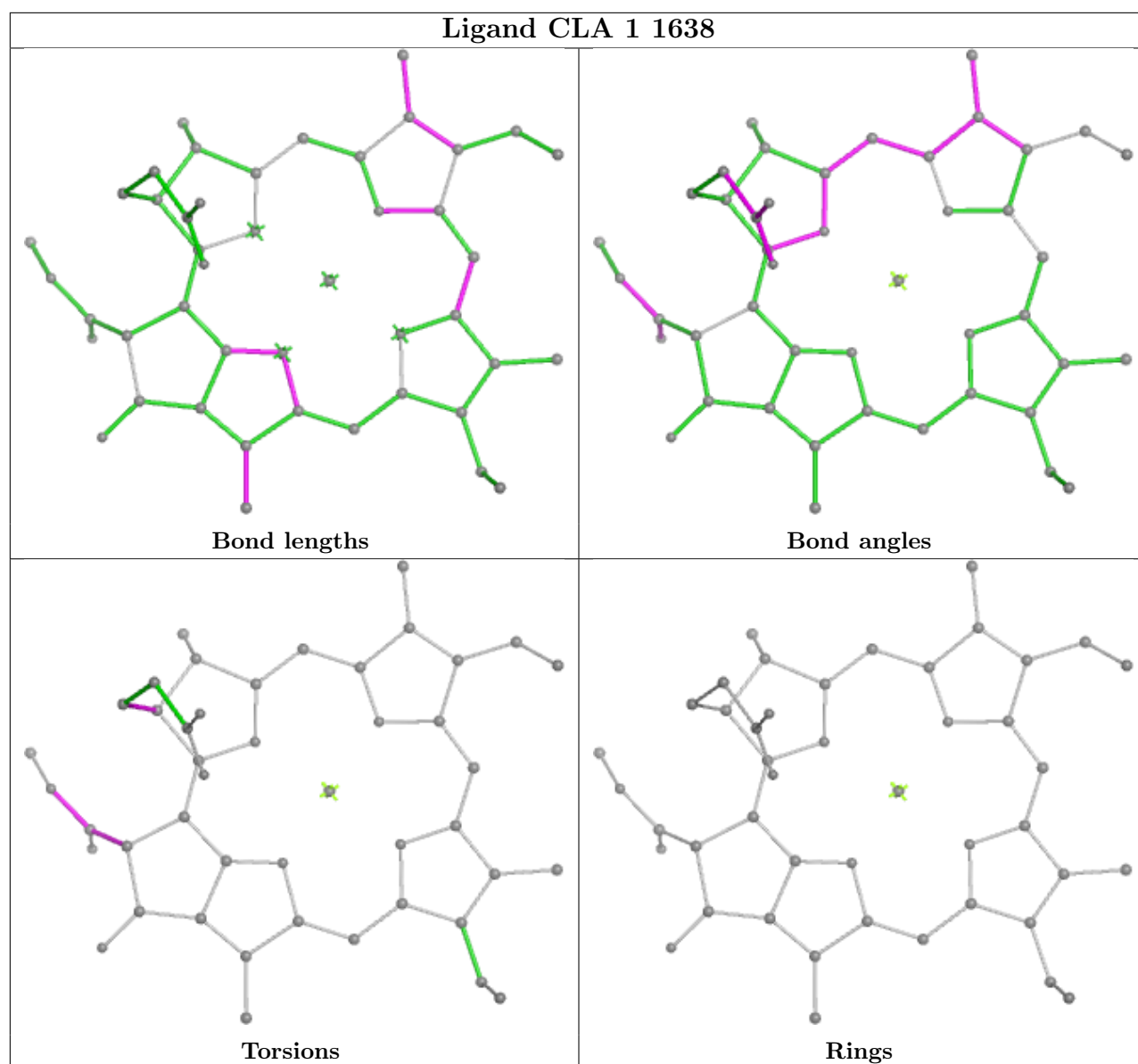


Ligand CLA b 824

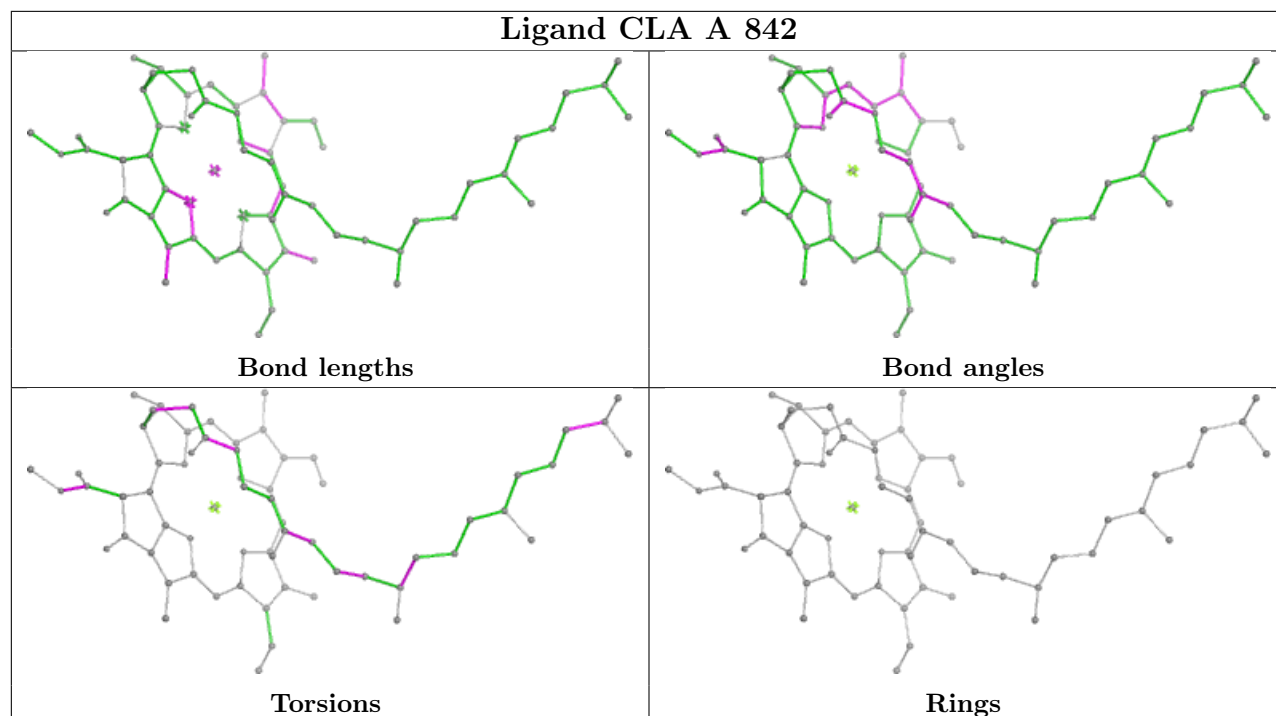


Ligand BCR b 847

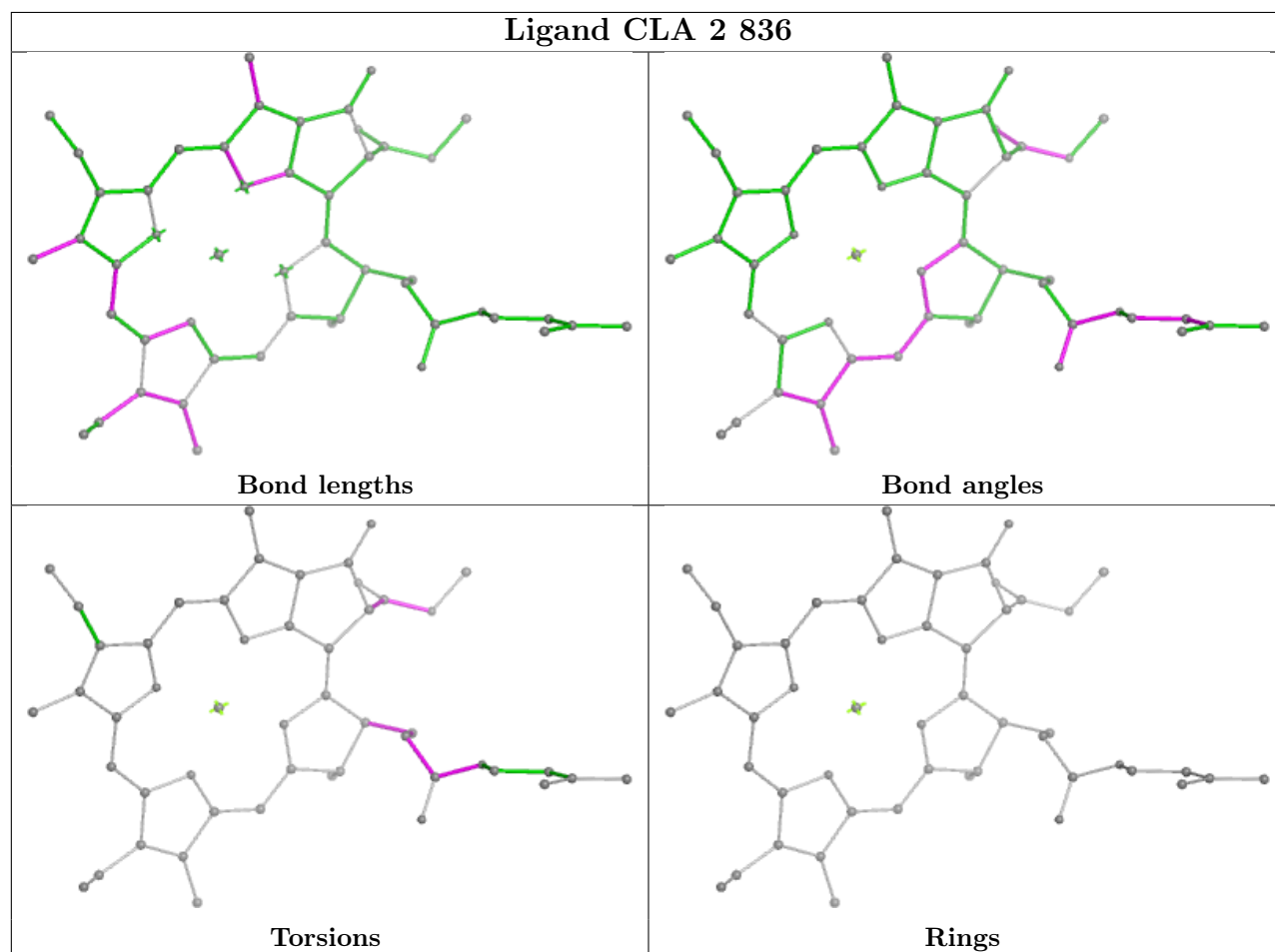


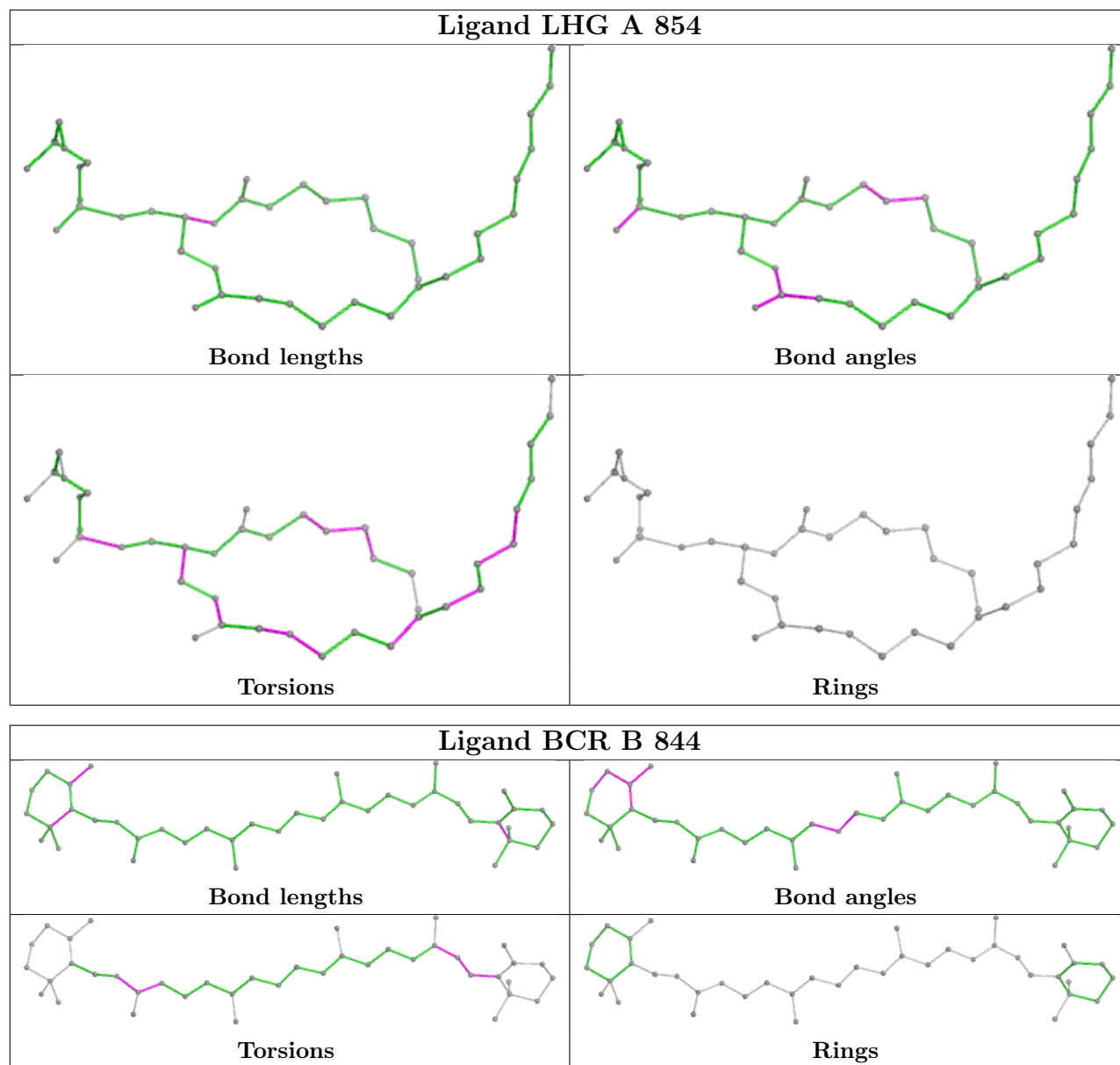


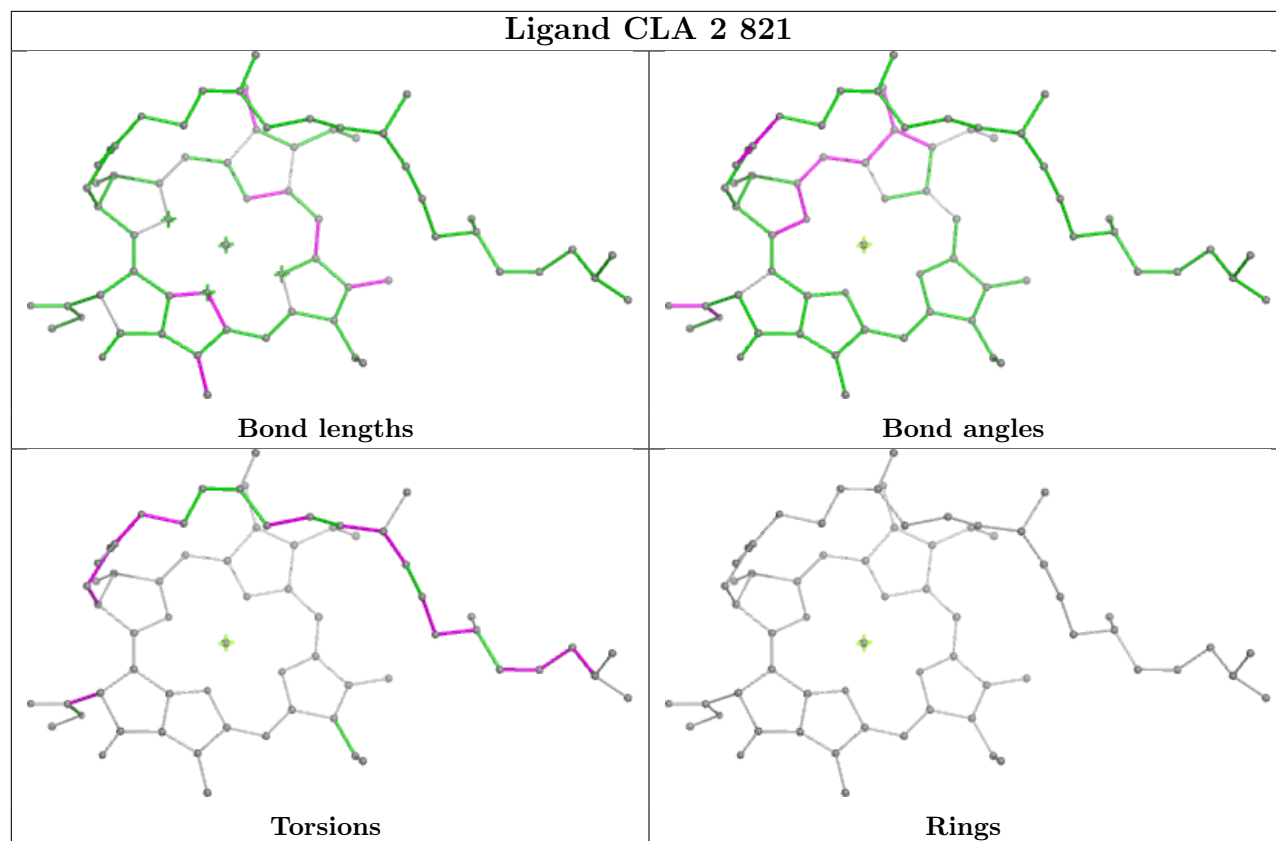
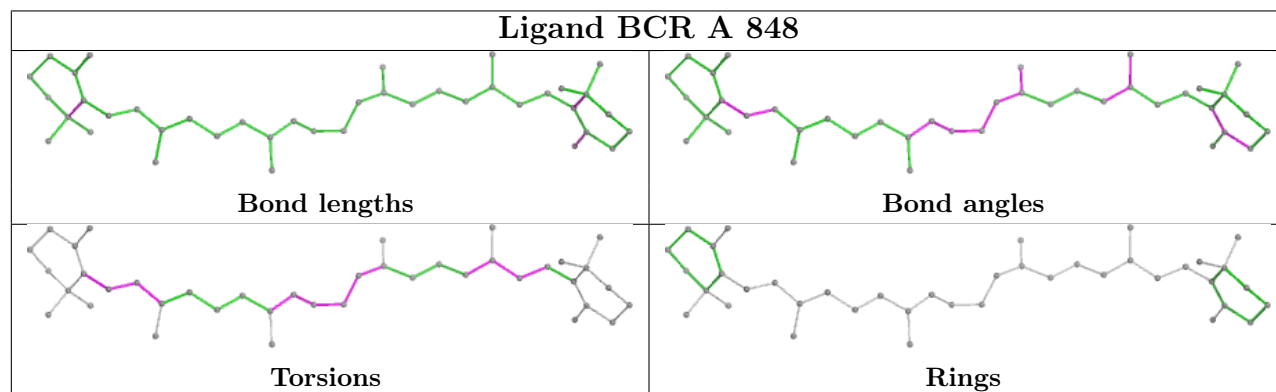
Ligand CLA A 842

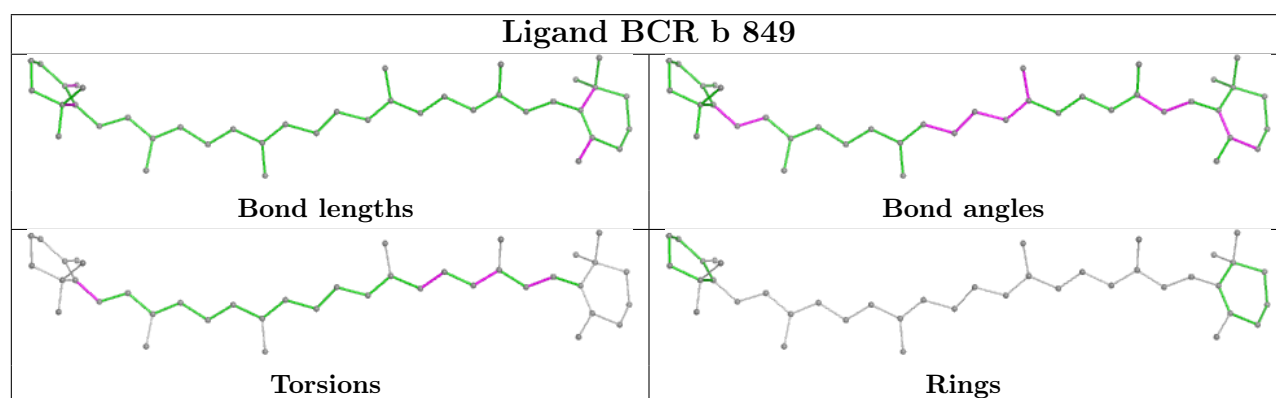
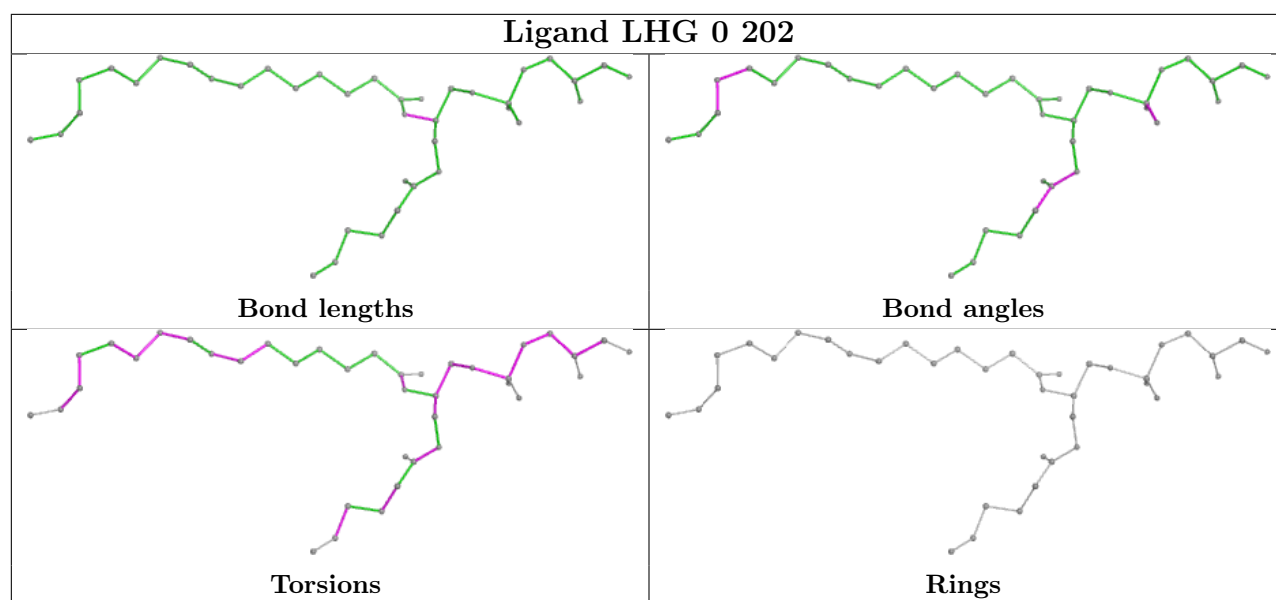


Ligand CLA 2 836

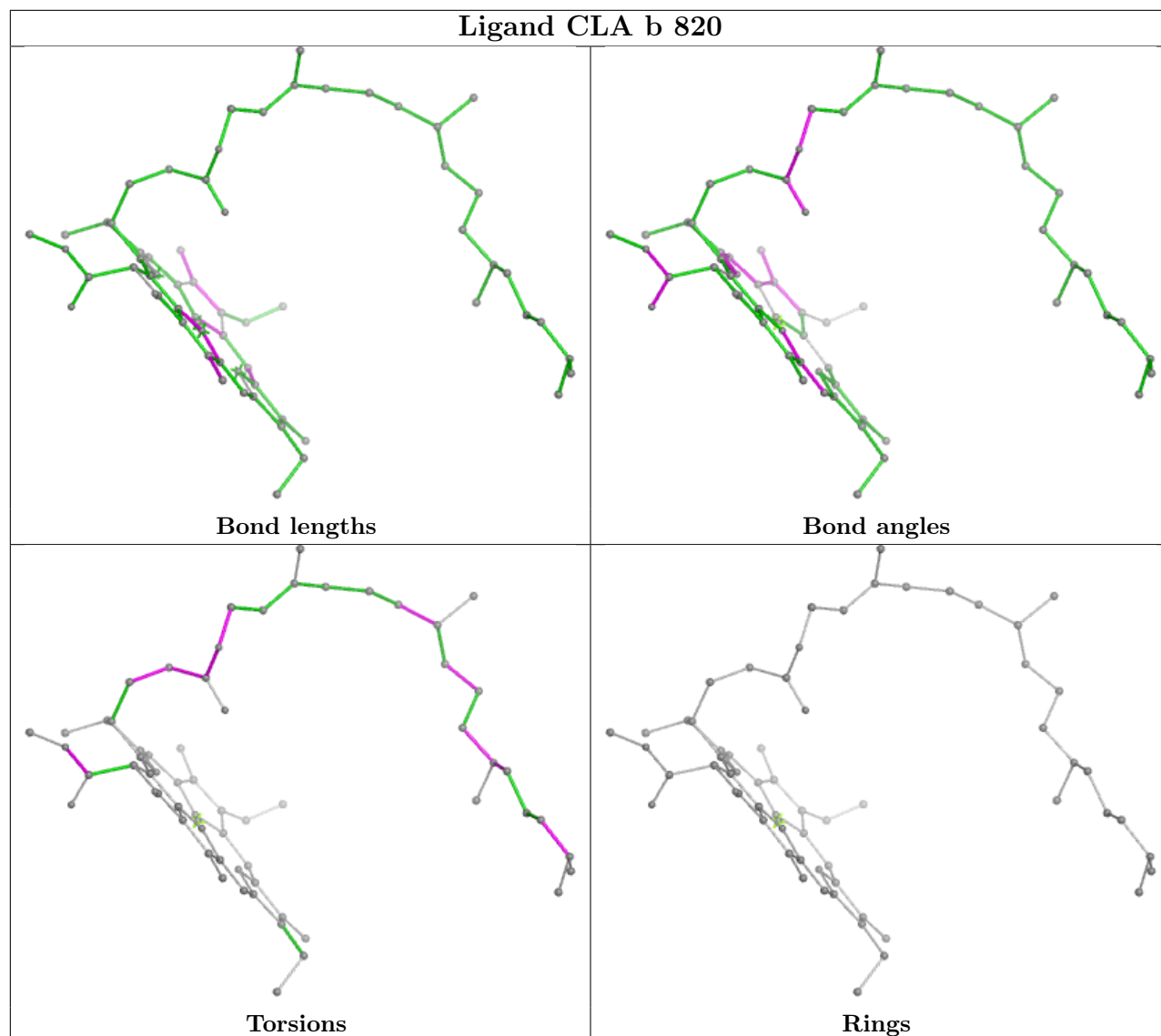




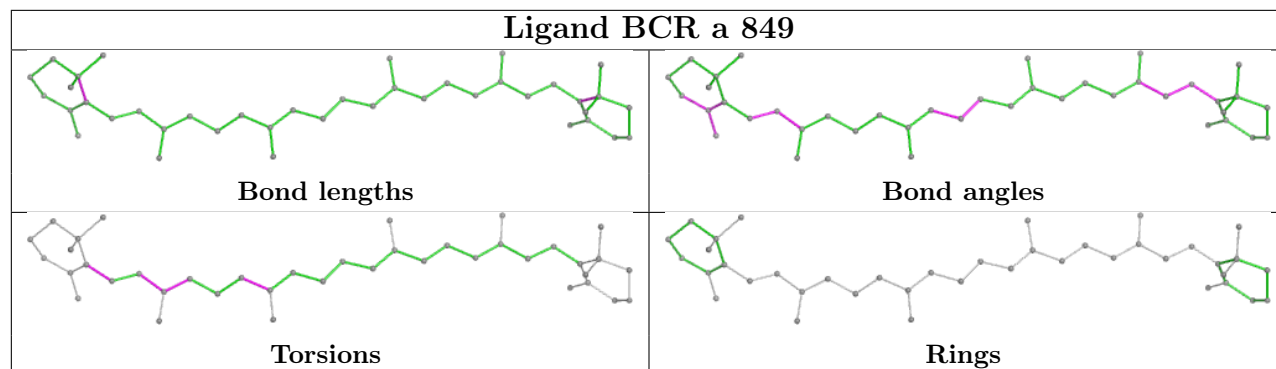
Ligand CLA 2 821**Ligand BCR A 848**



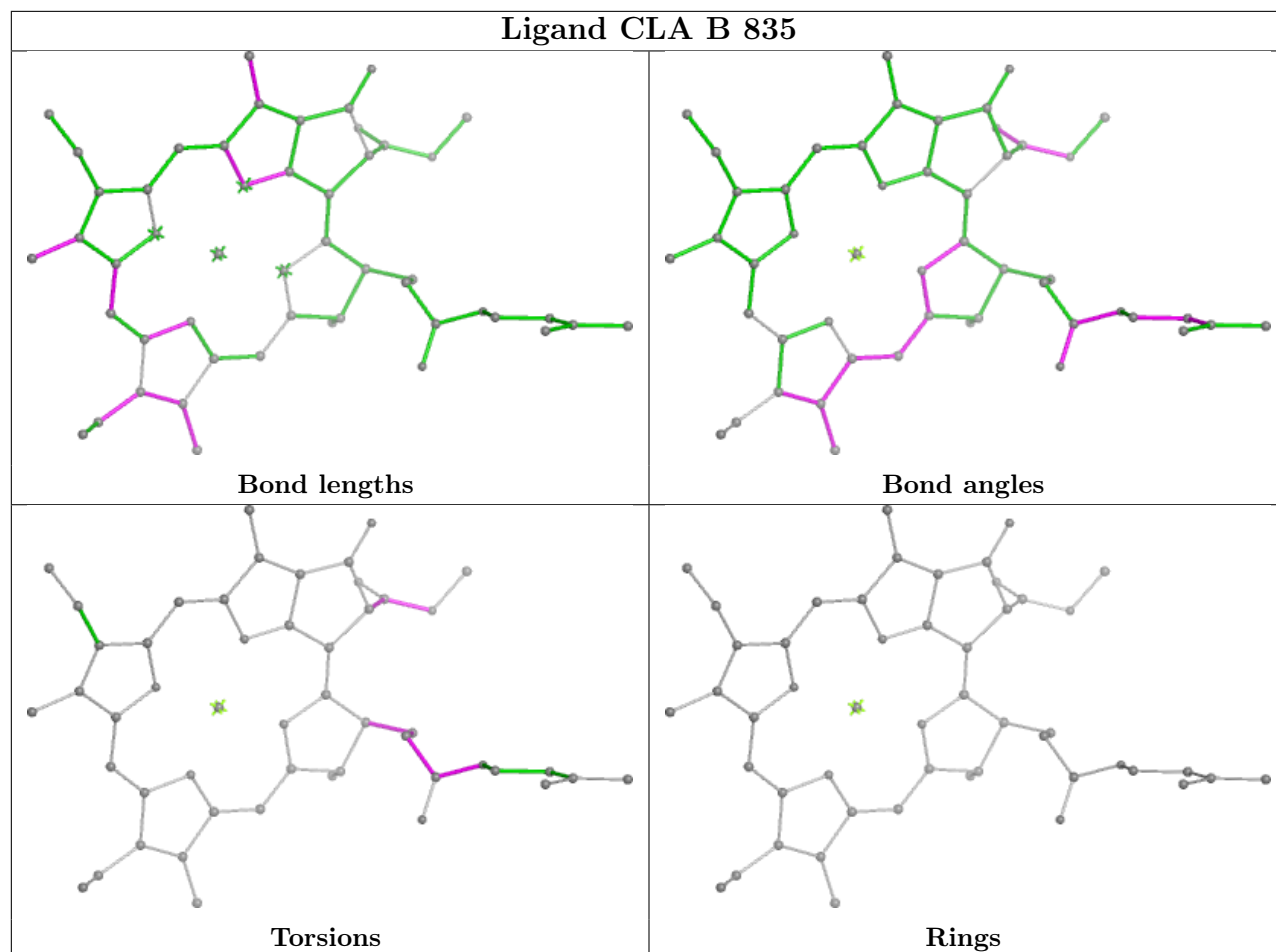
Ligand CLA b 820



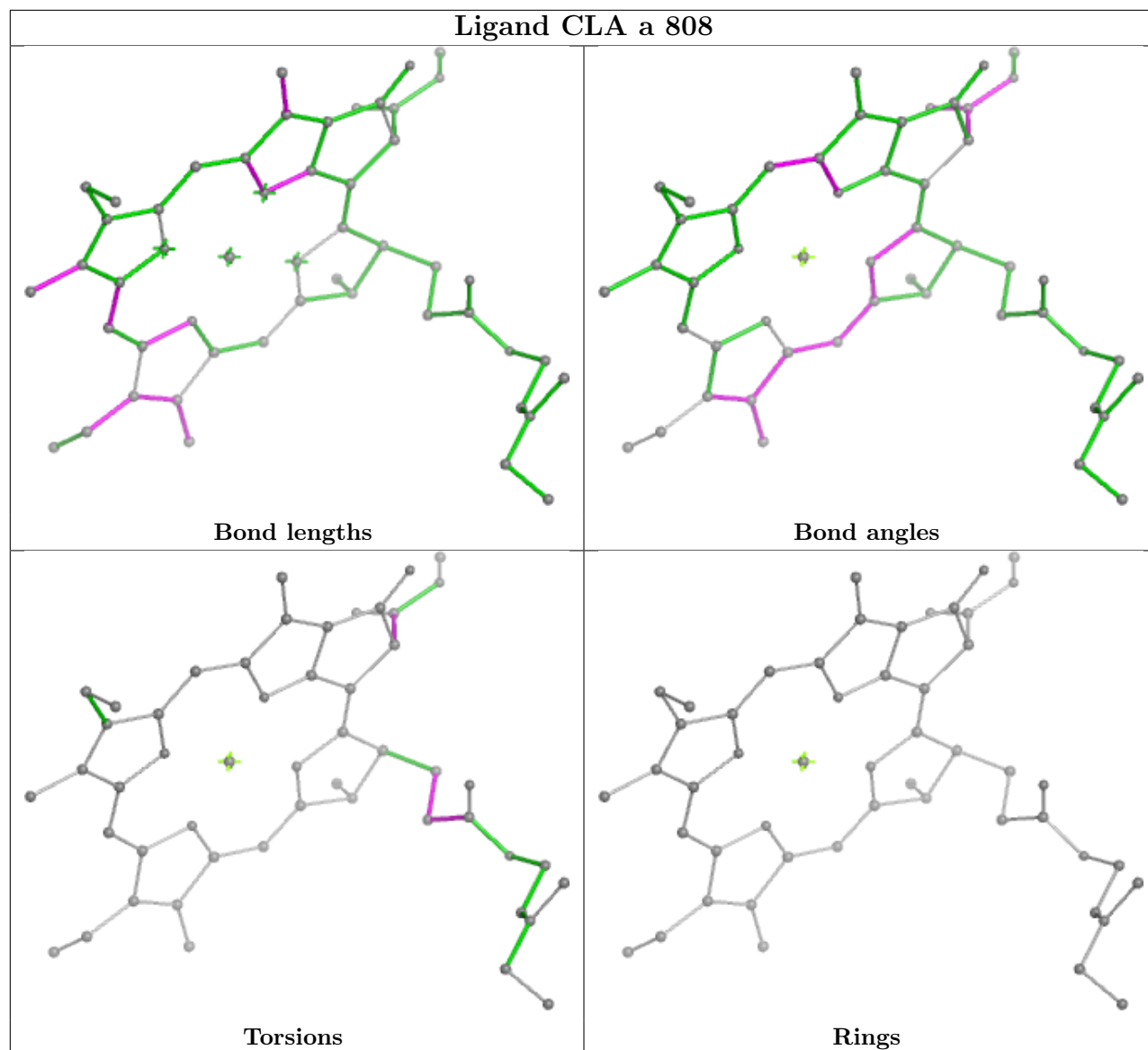
Ligand BCR a 849

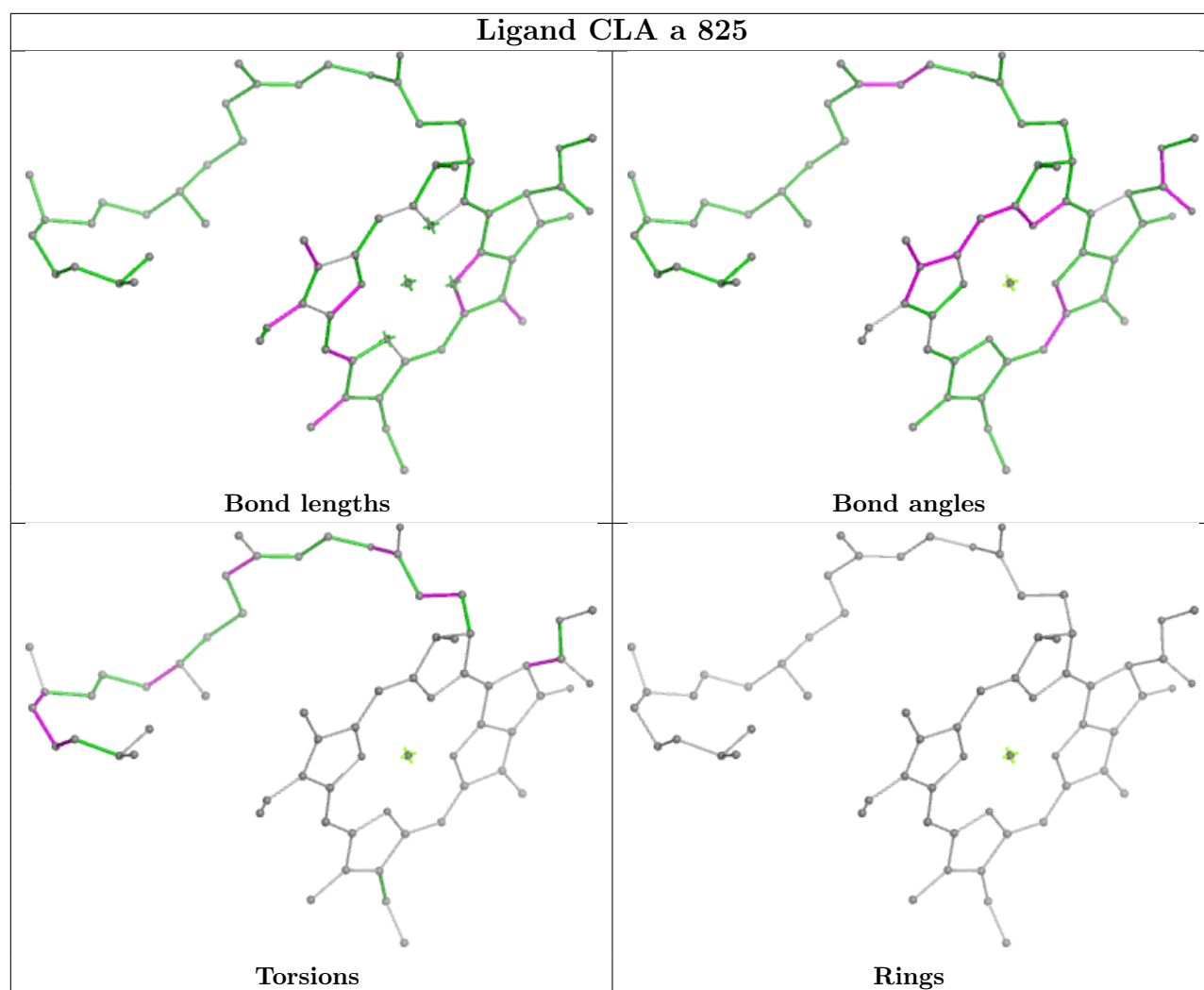


Ligand CLA B 835

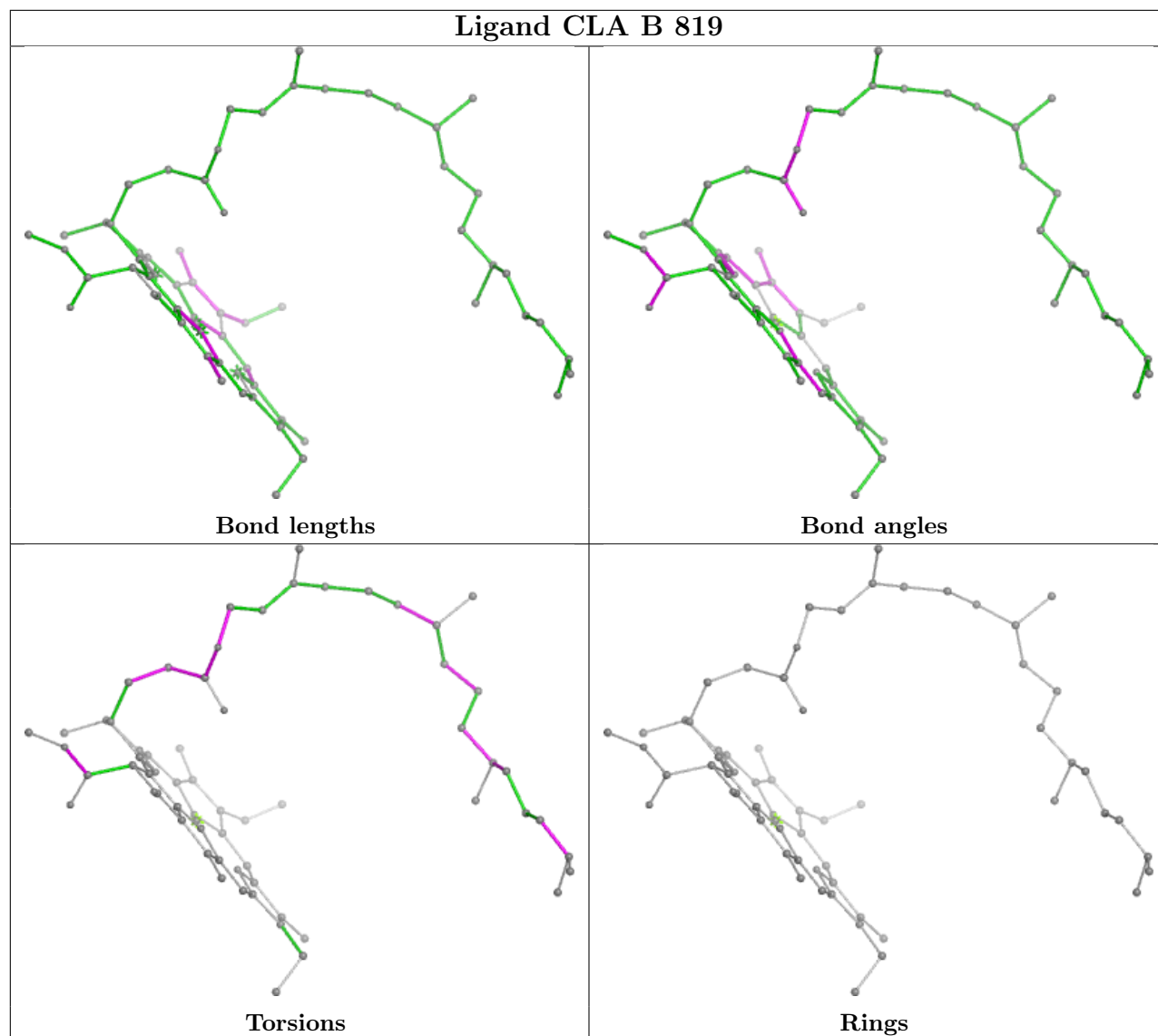


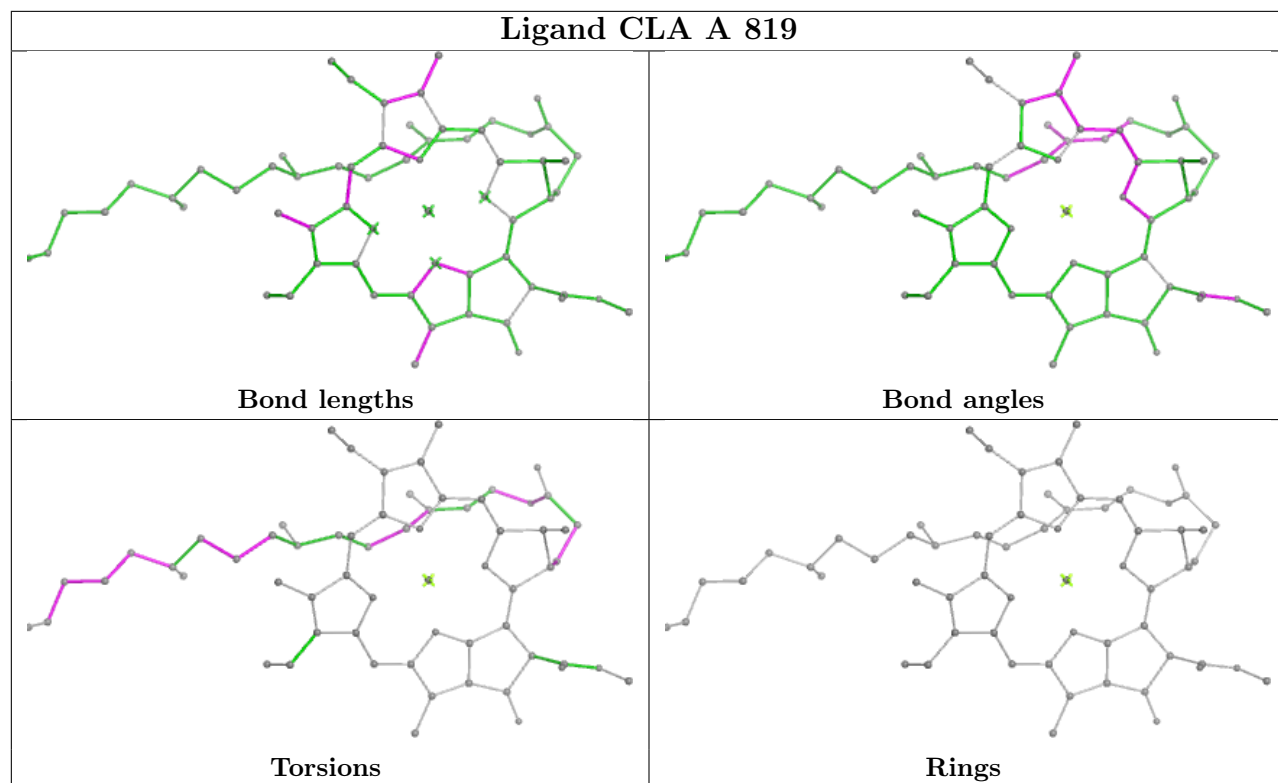
Ligand CLA a 808



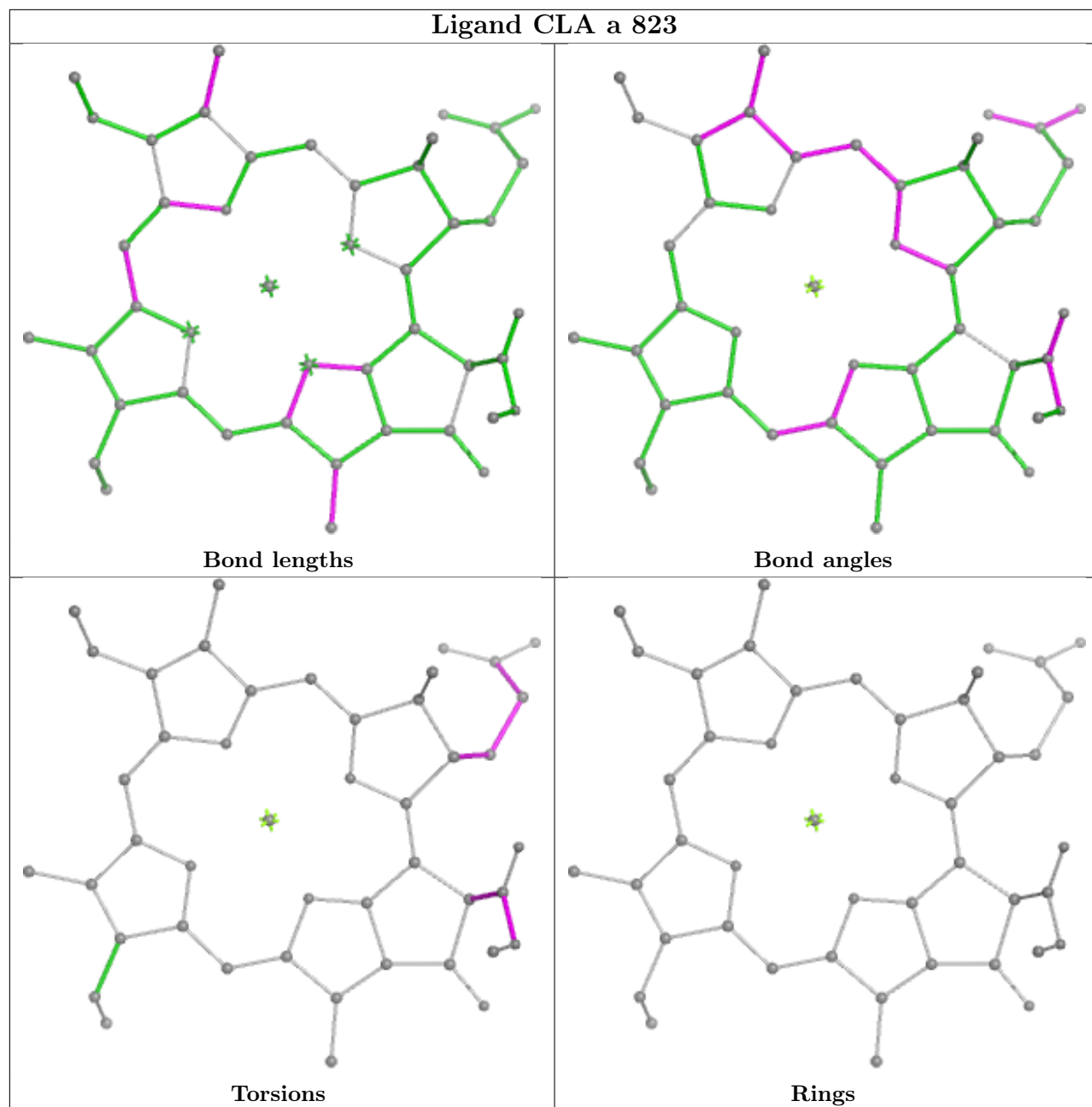


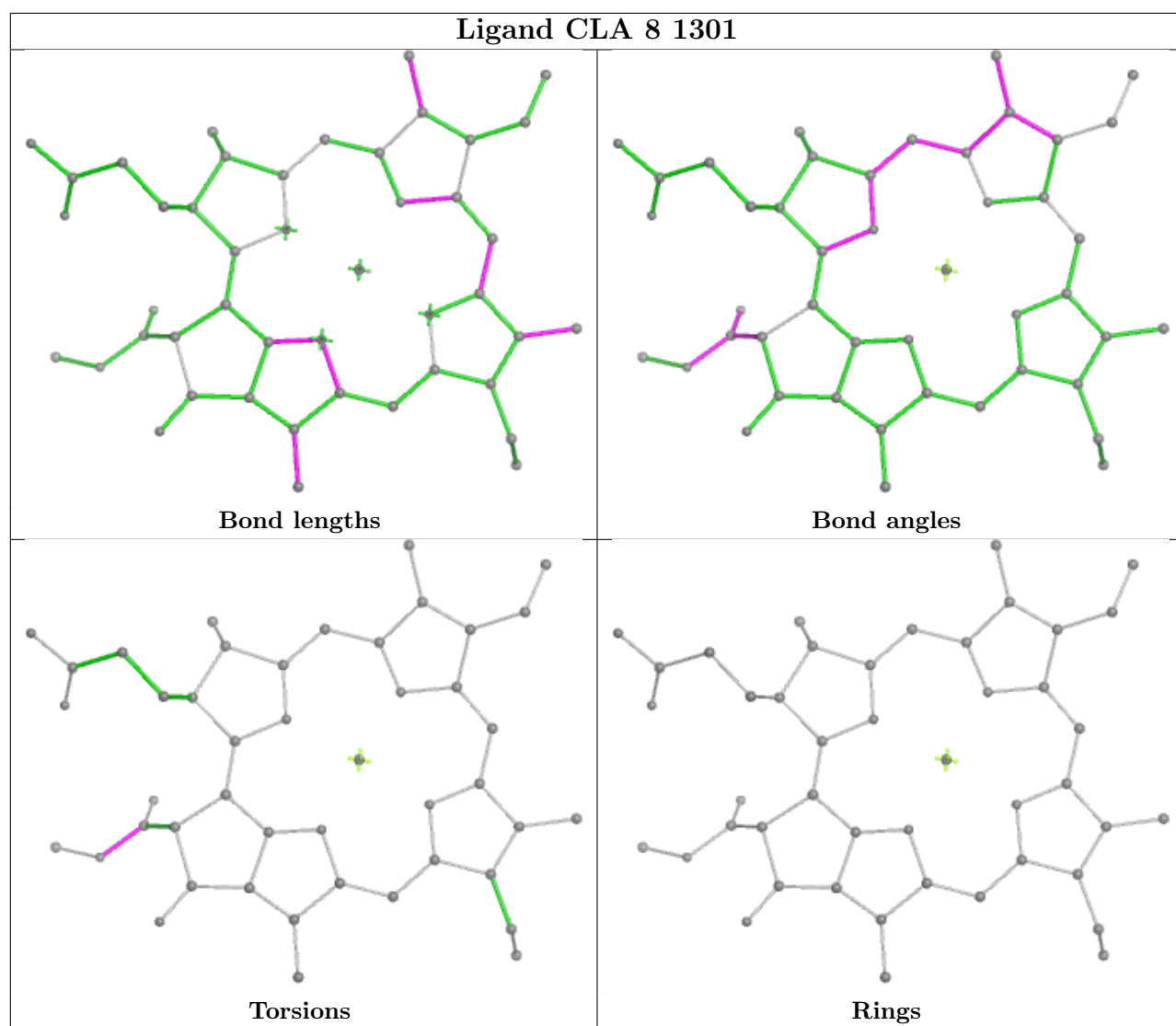
Ligand CLA B 819



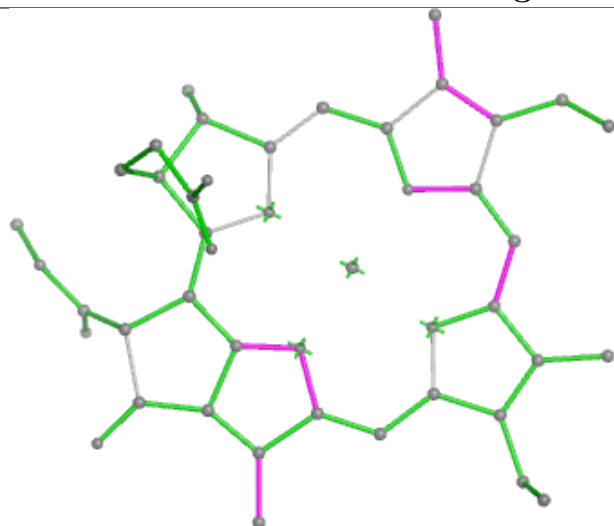


Ligand CLA a 823

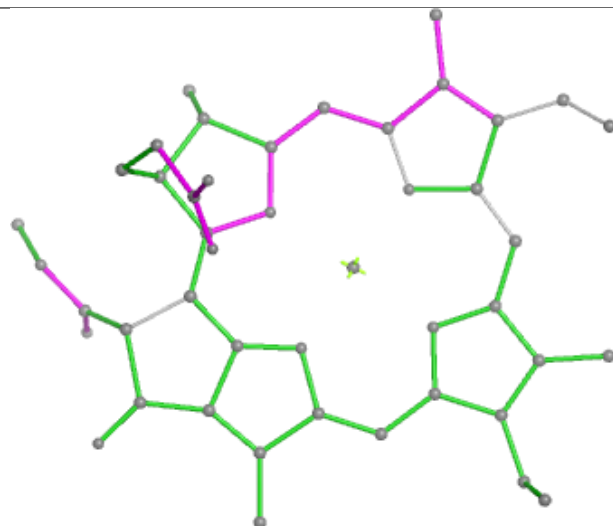




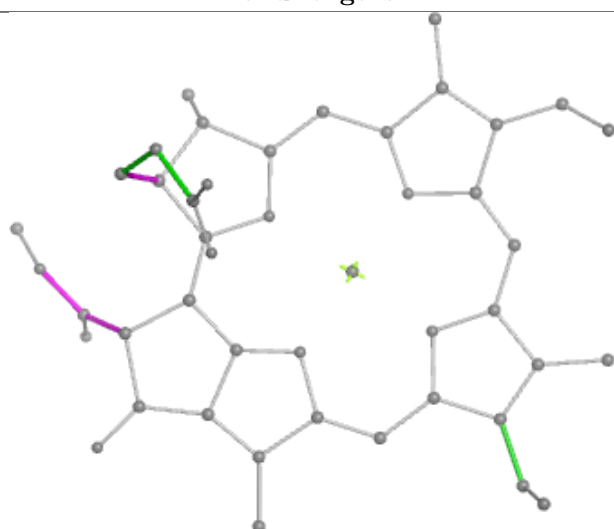
Ligand CLA A 837



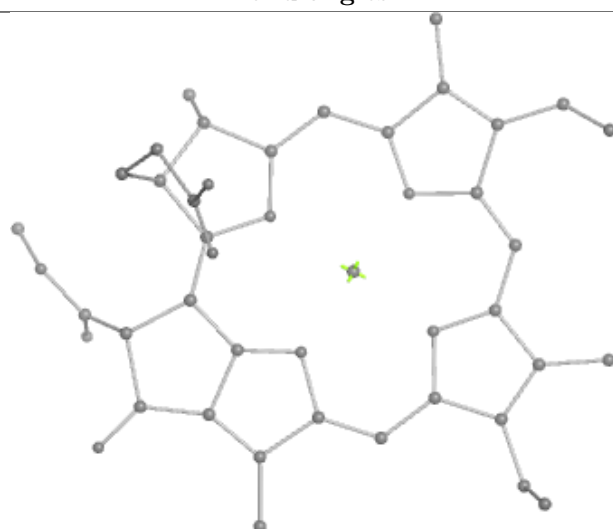
Bond lengths



Bond angles

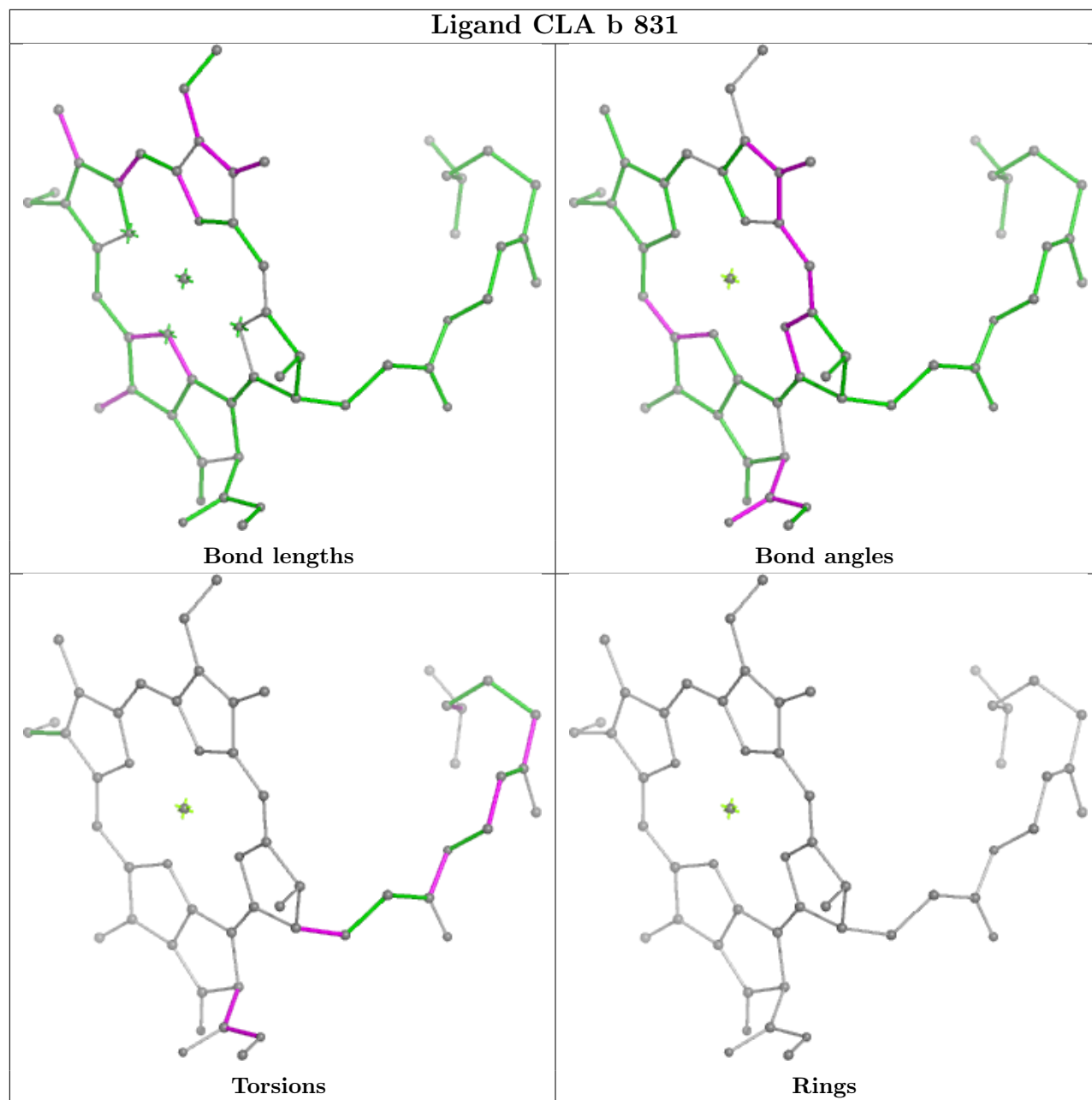


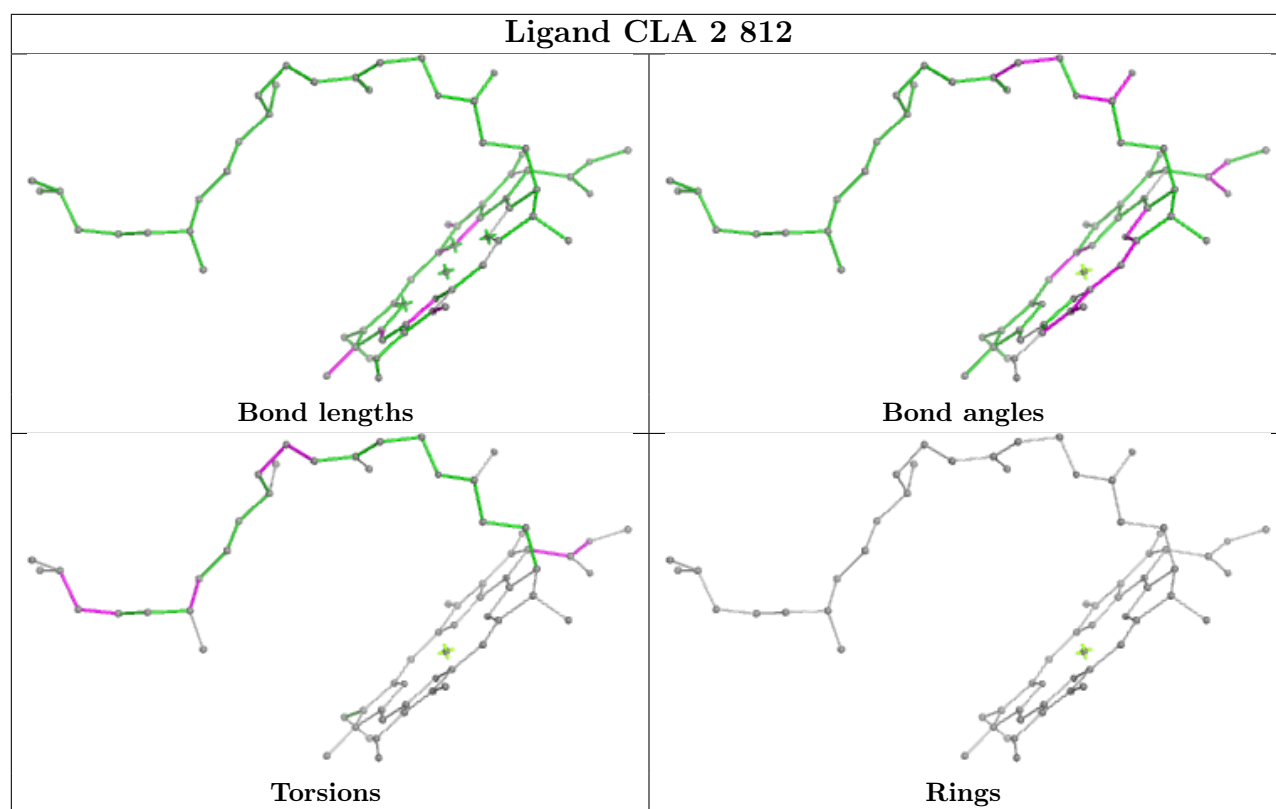
Torsions



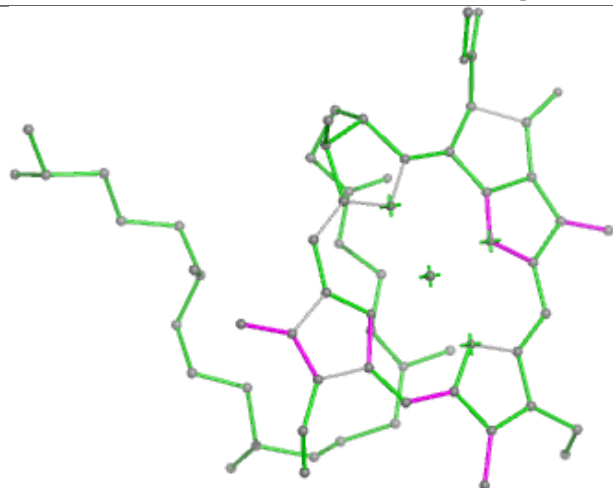
Rings

Ligand CLA b 831

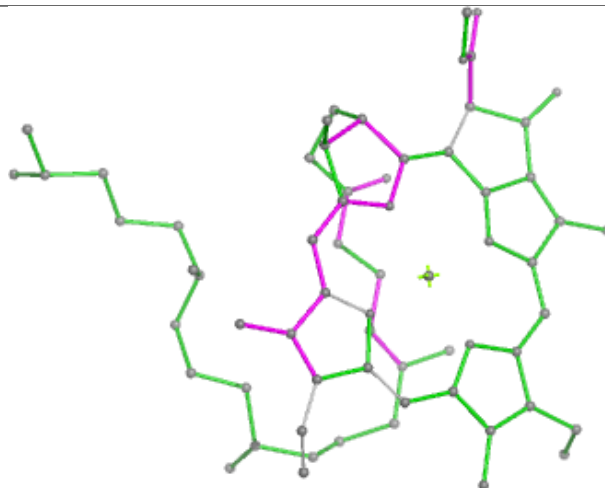




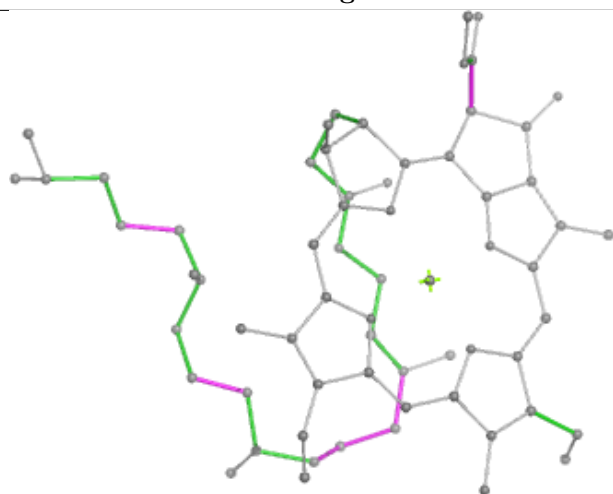
Ligand CLA B 808



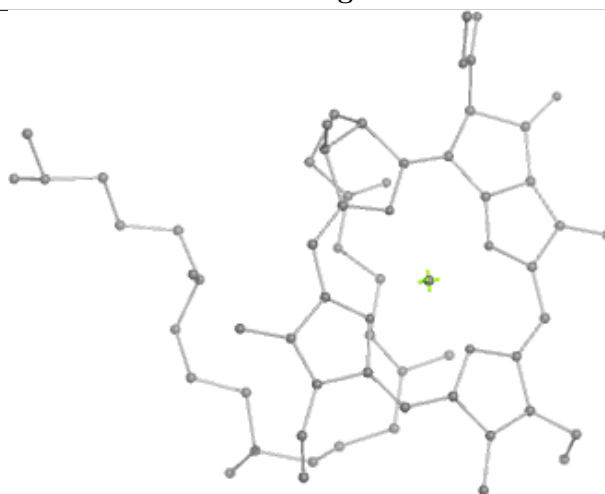
Bond lengths



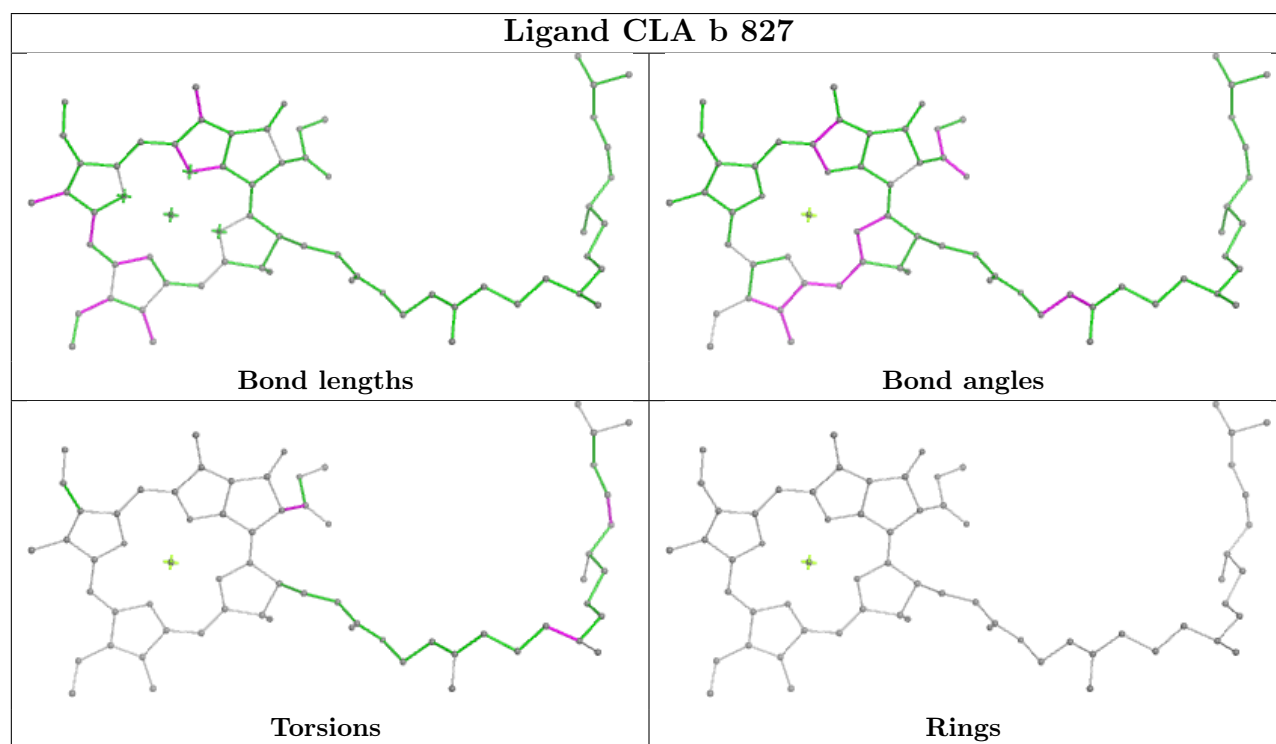
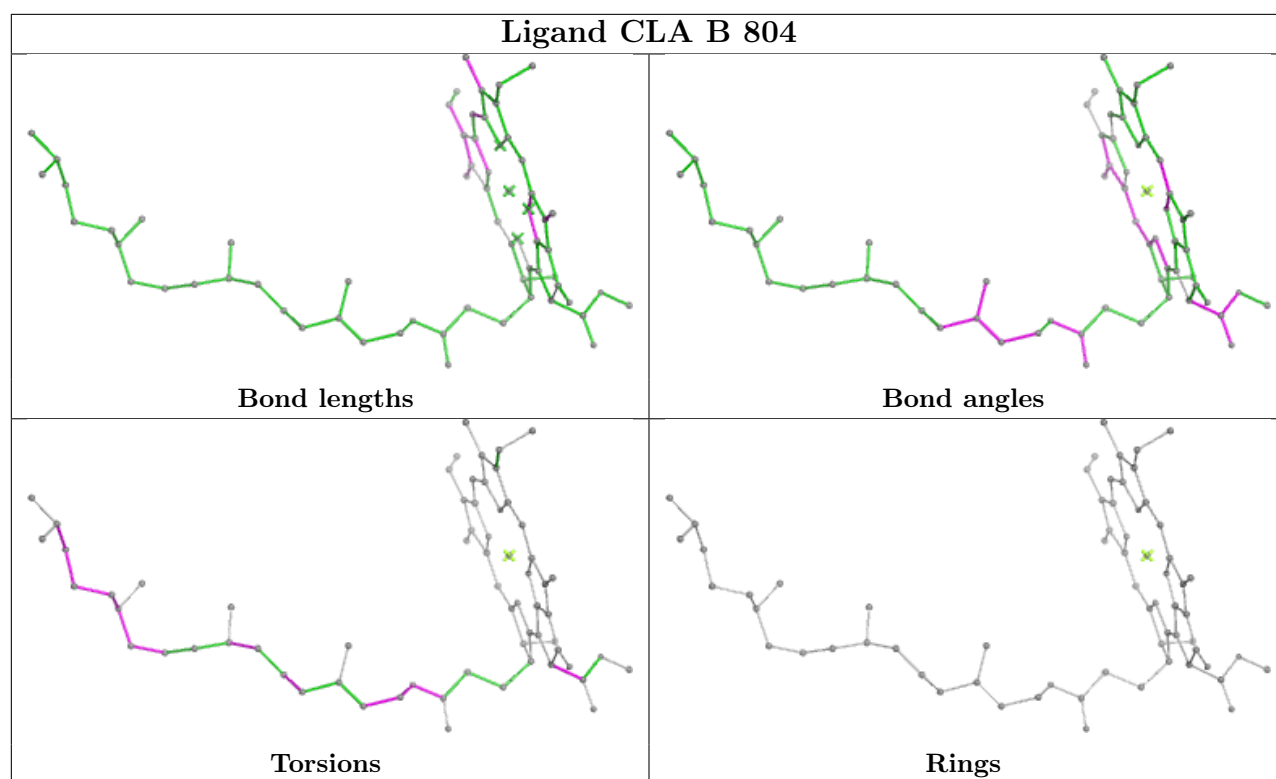
Bond angles

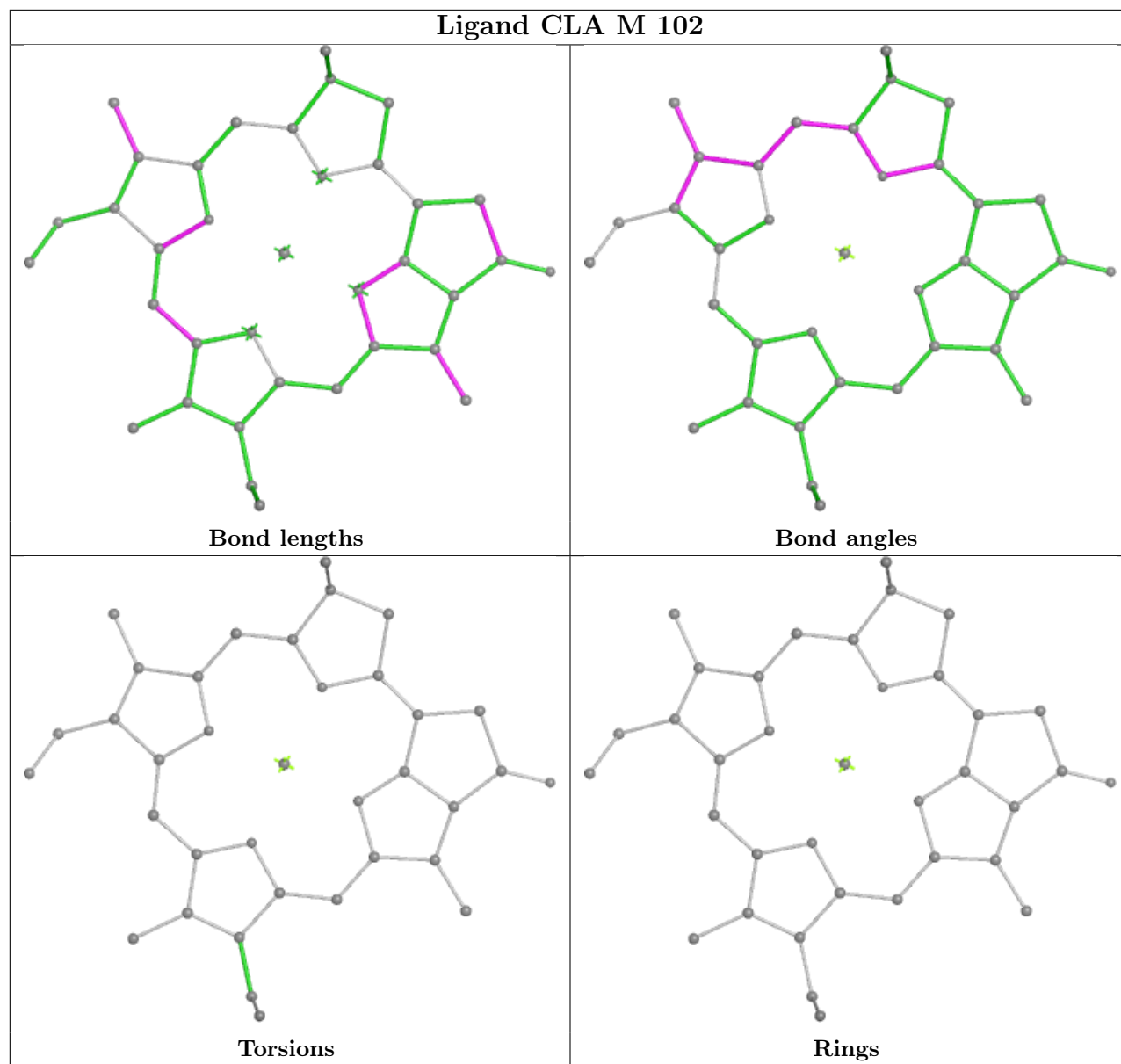


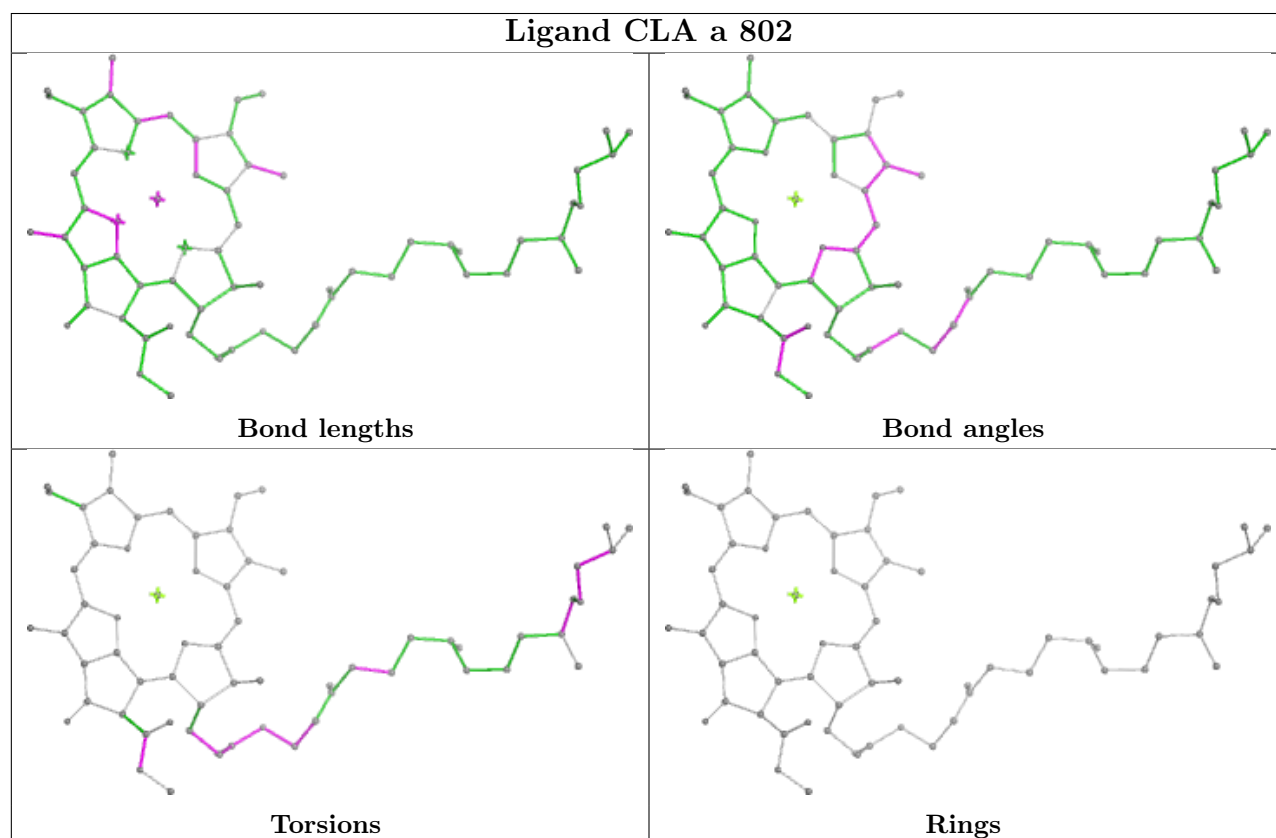
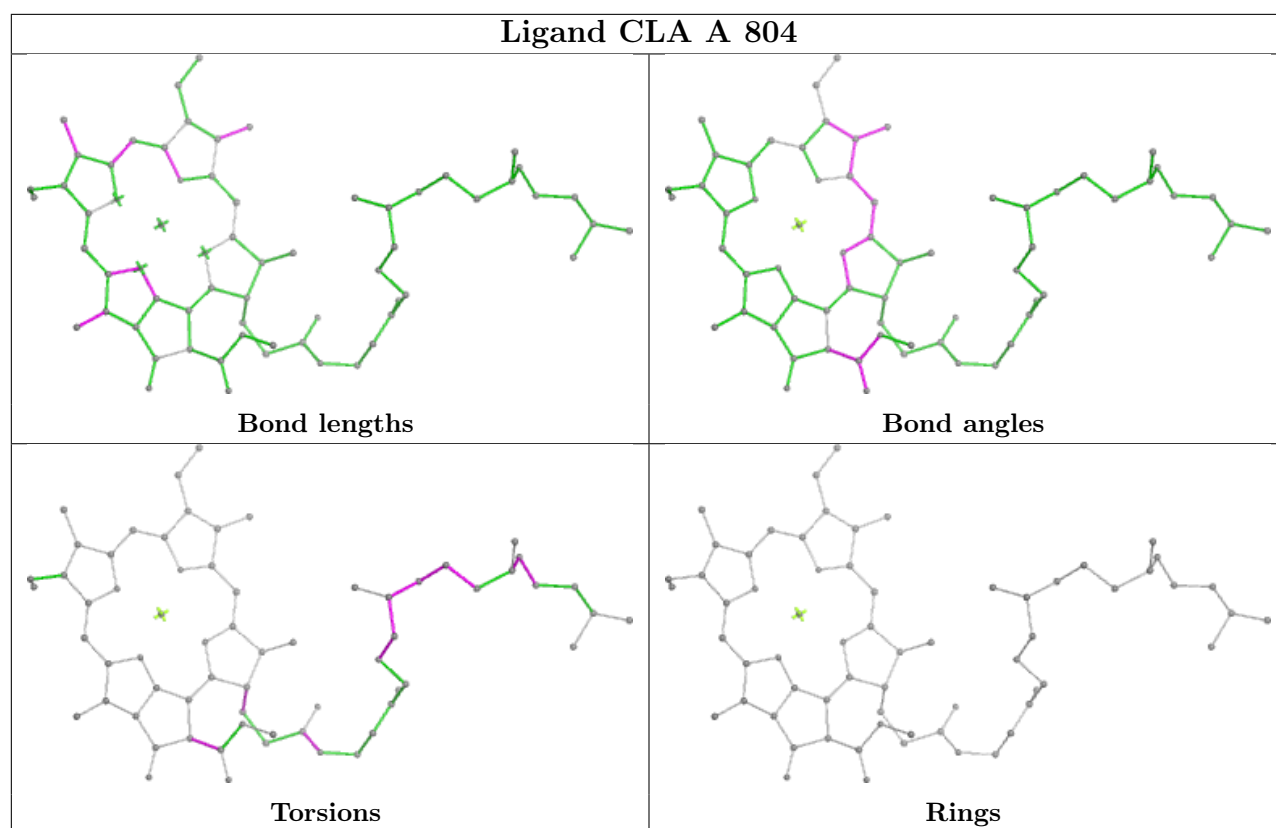
Torsions

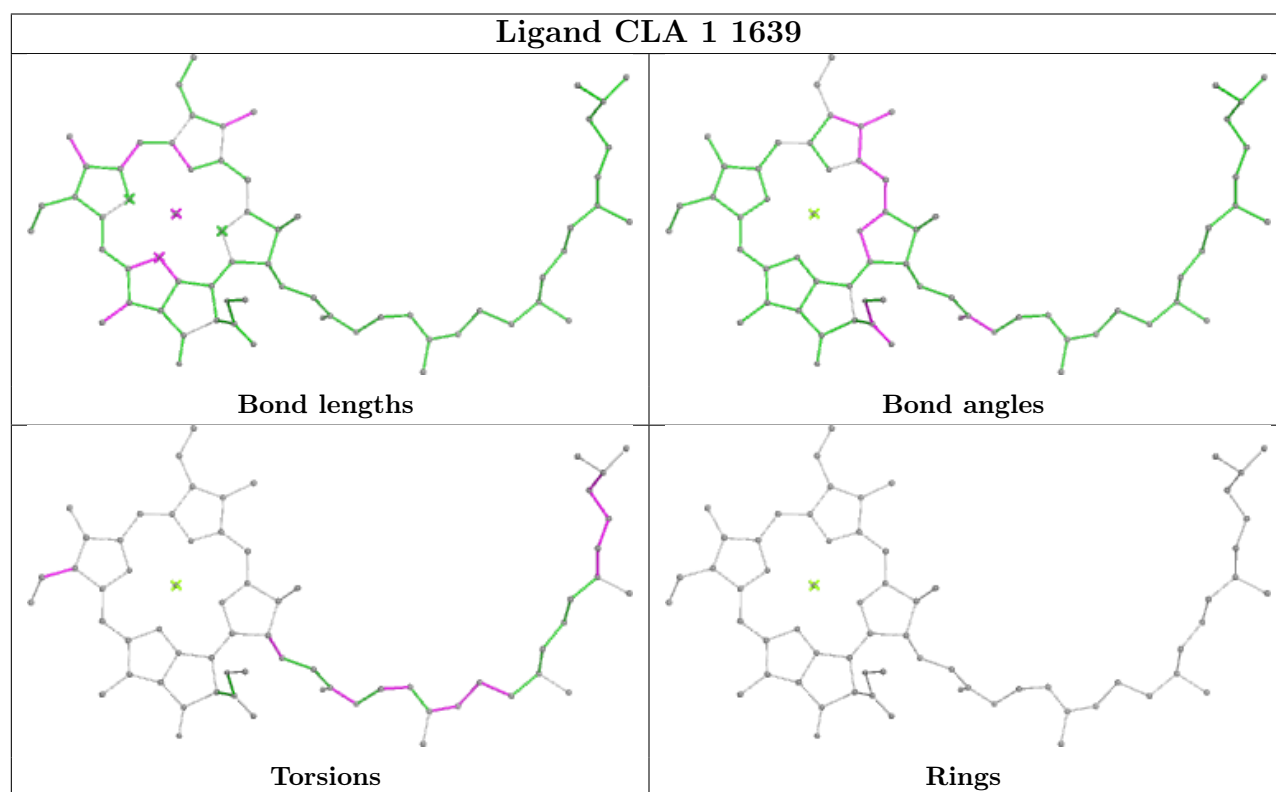
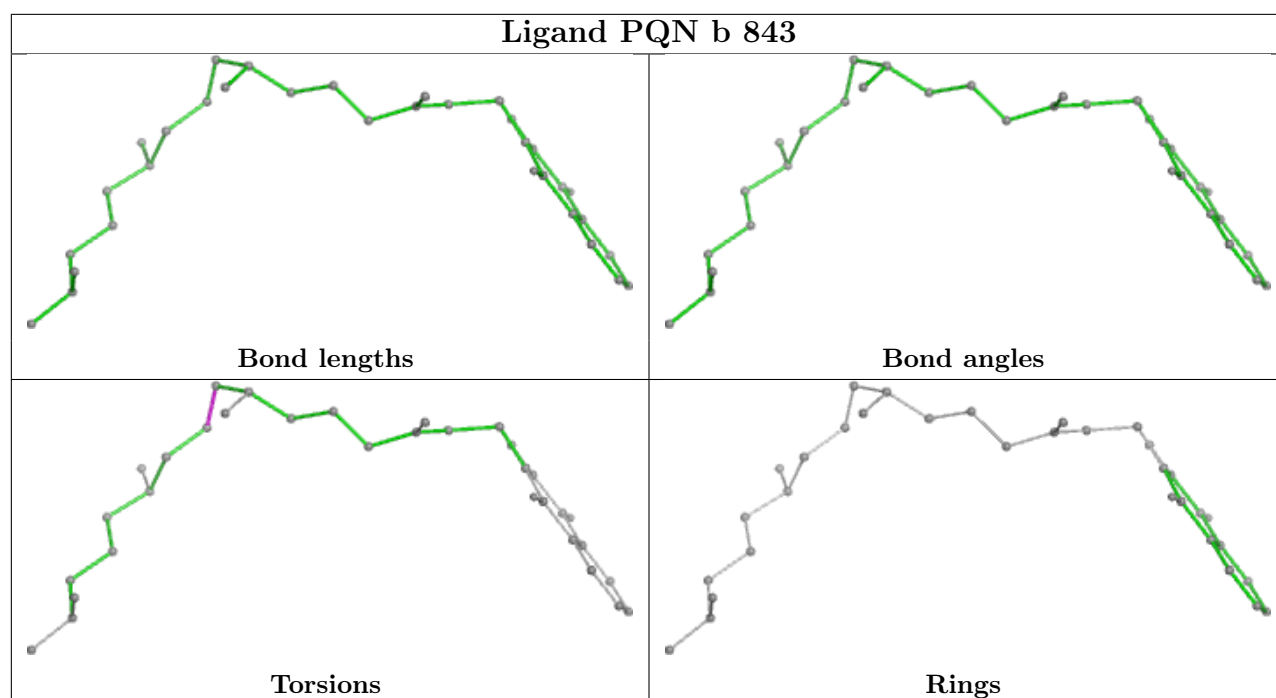


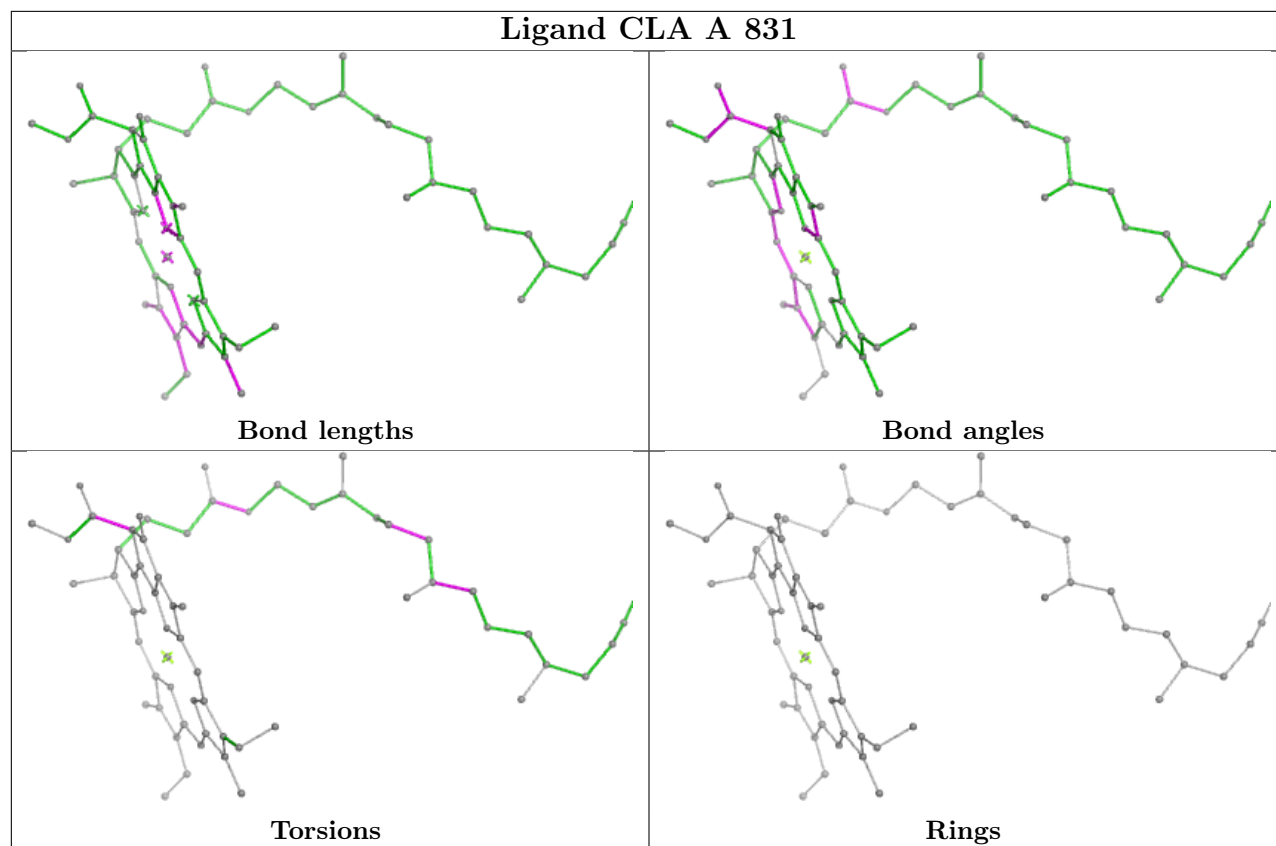
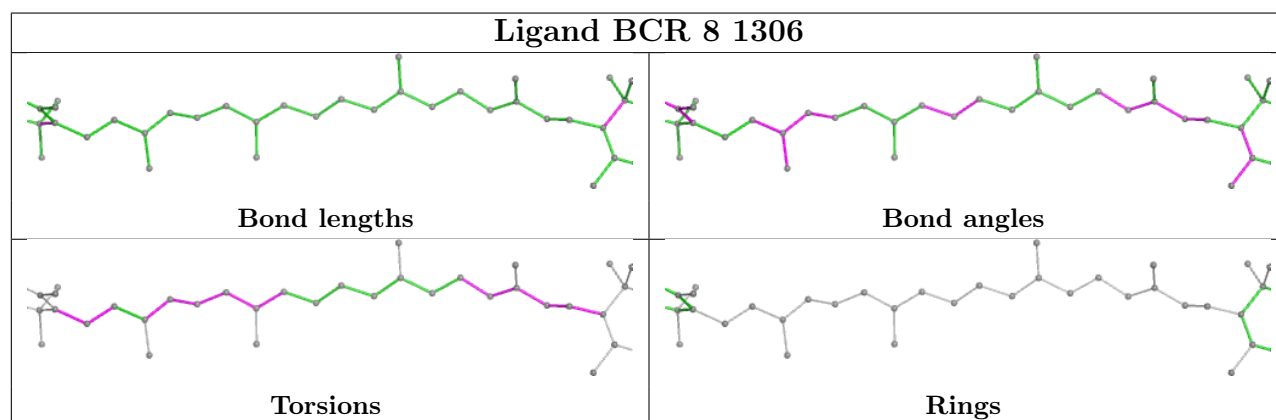
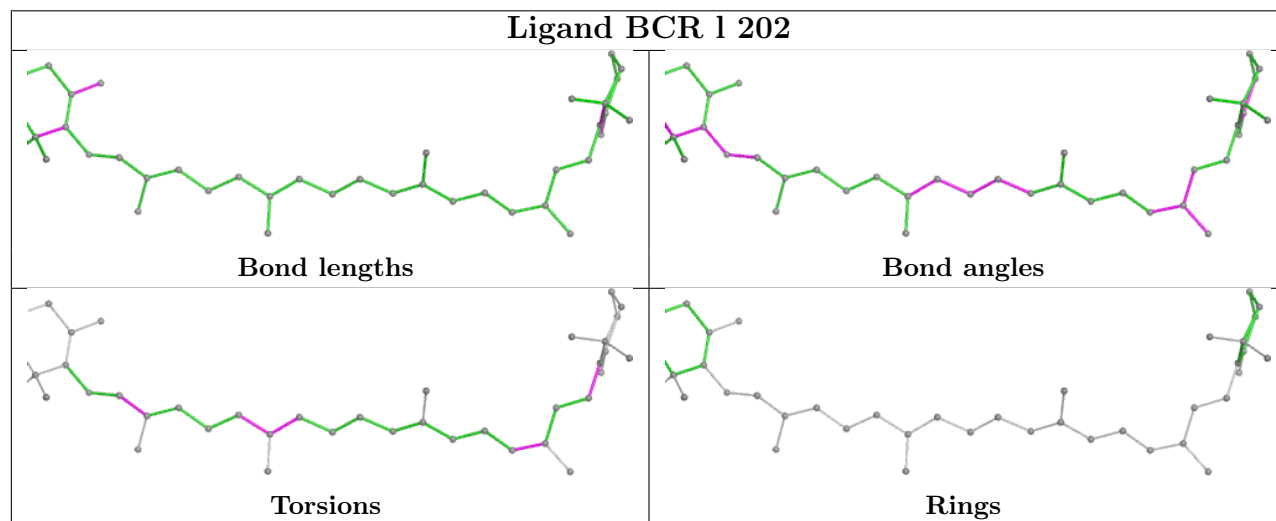
Rings

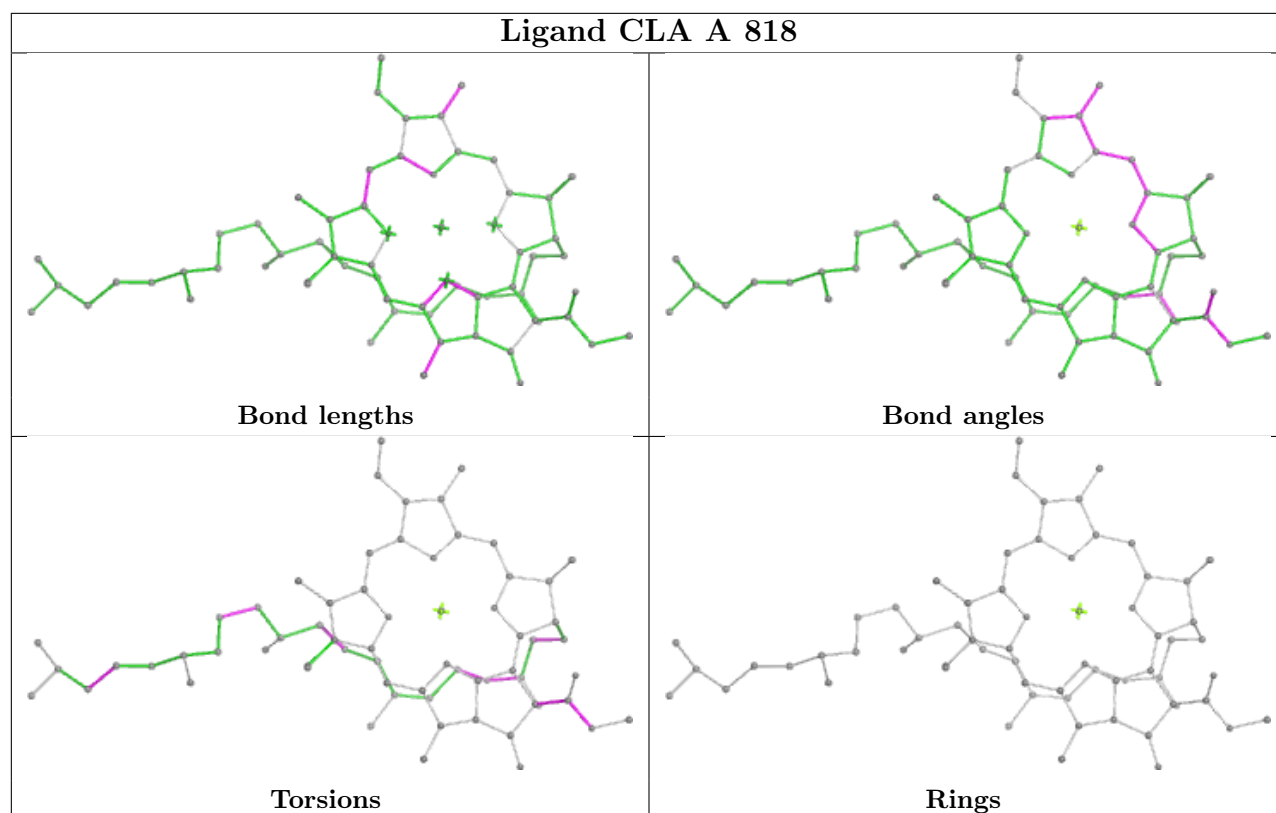
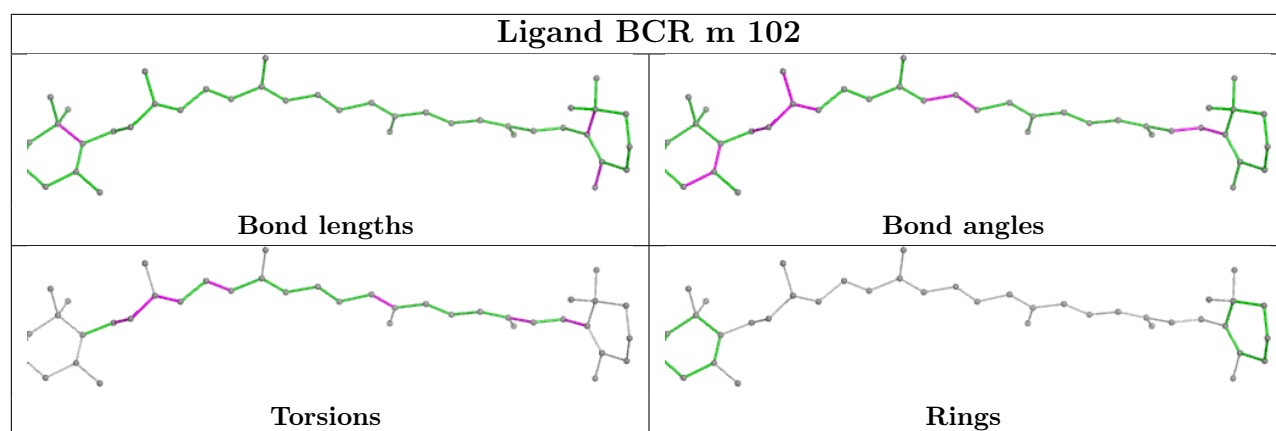


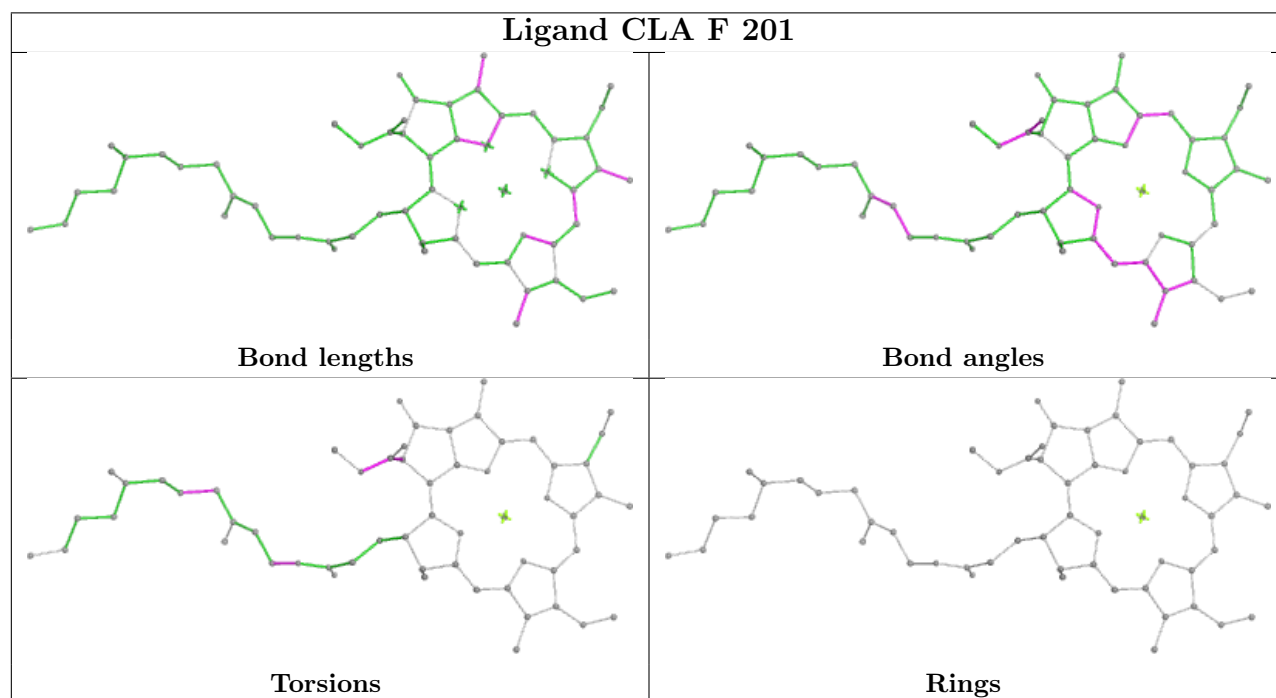
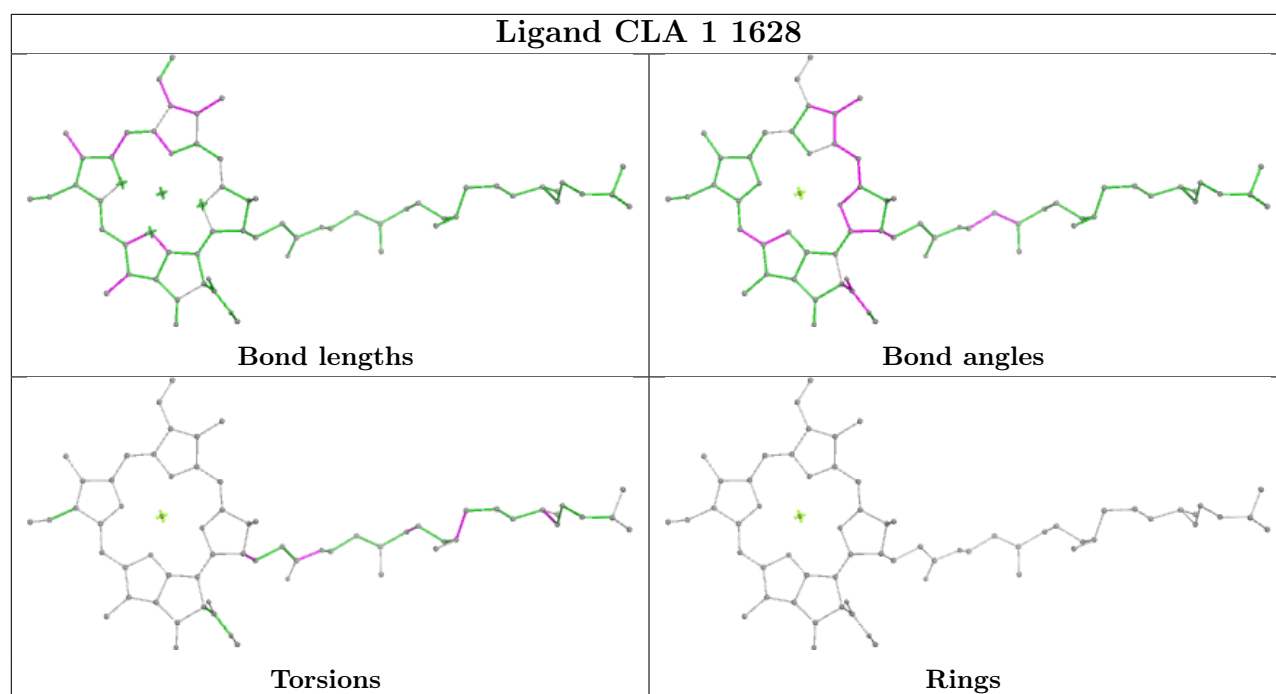




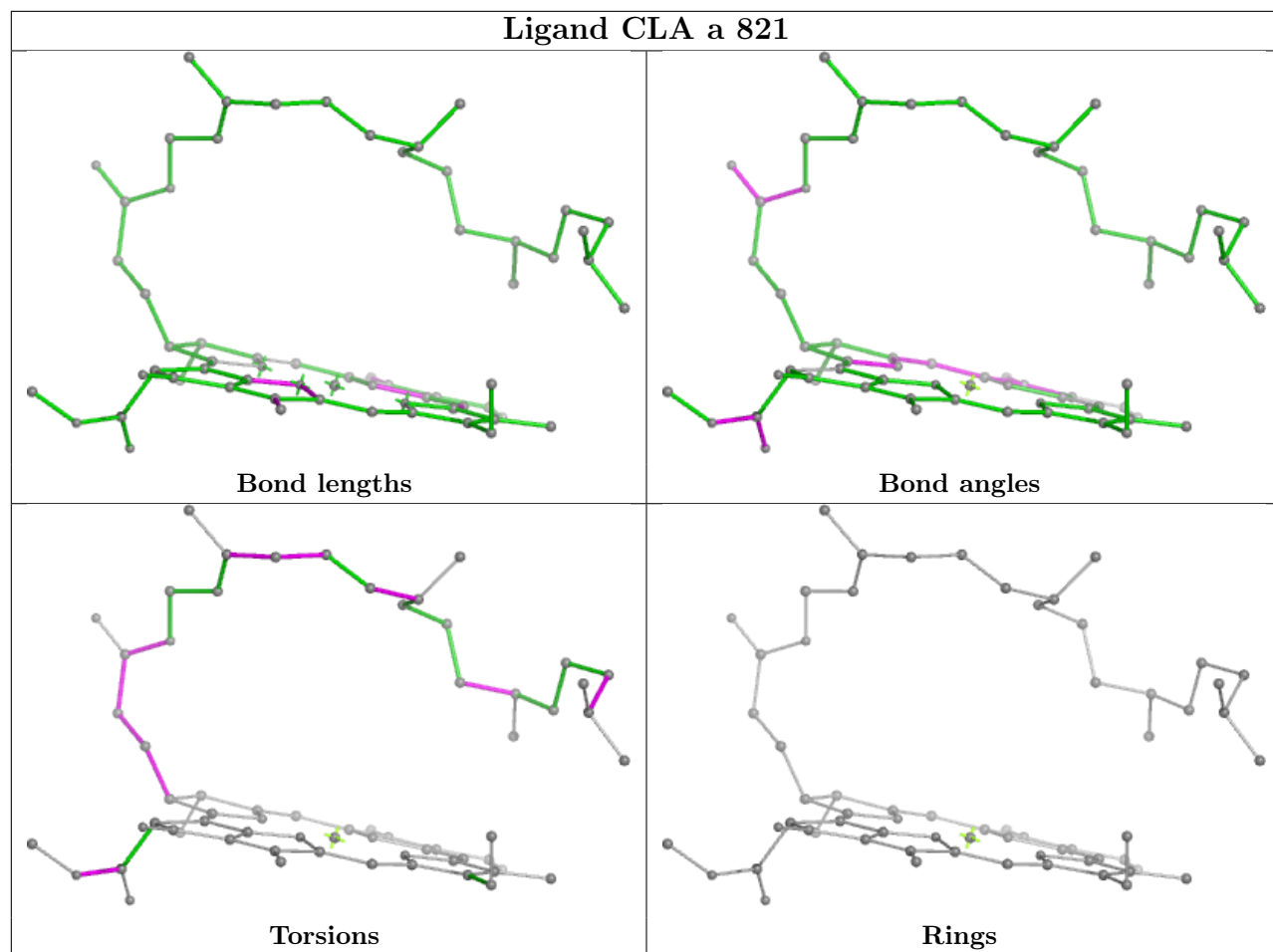


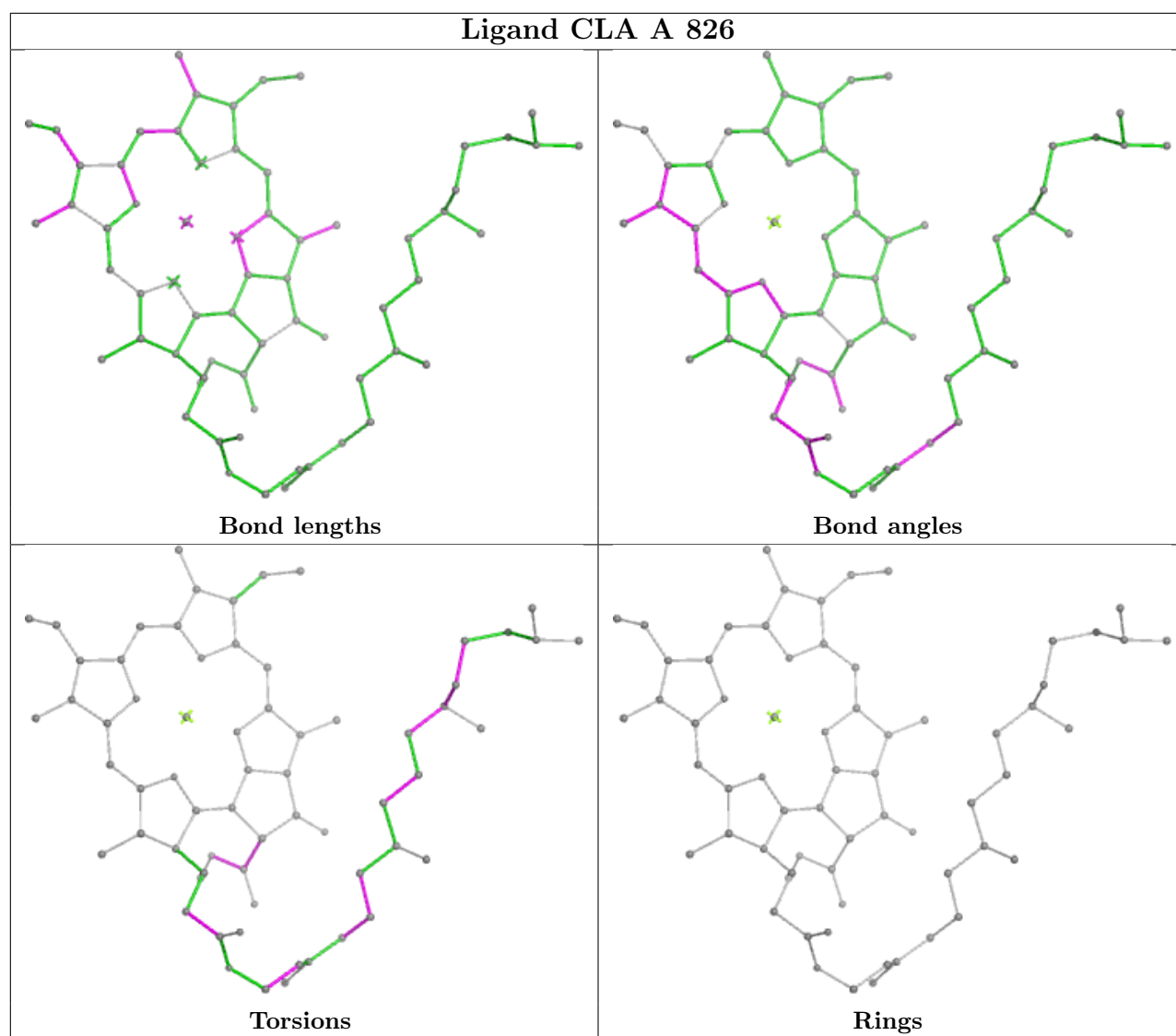
Ligand CLA A 831**Ligand BCR 8 1306****Ligand BCR 1 202**

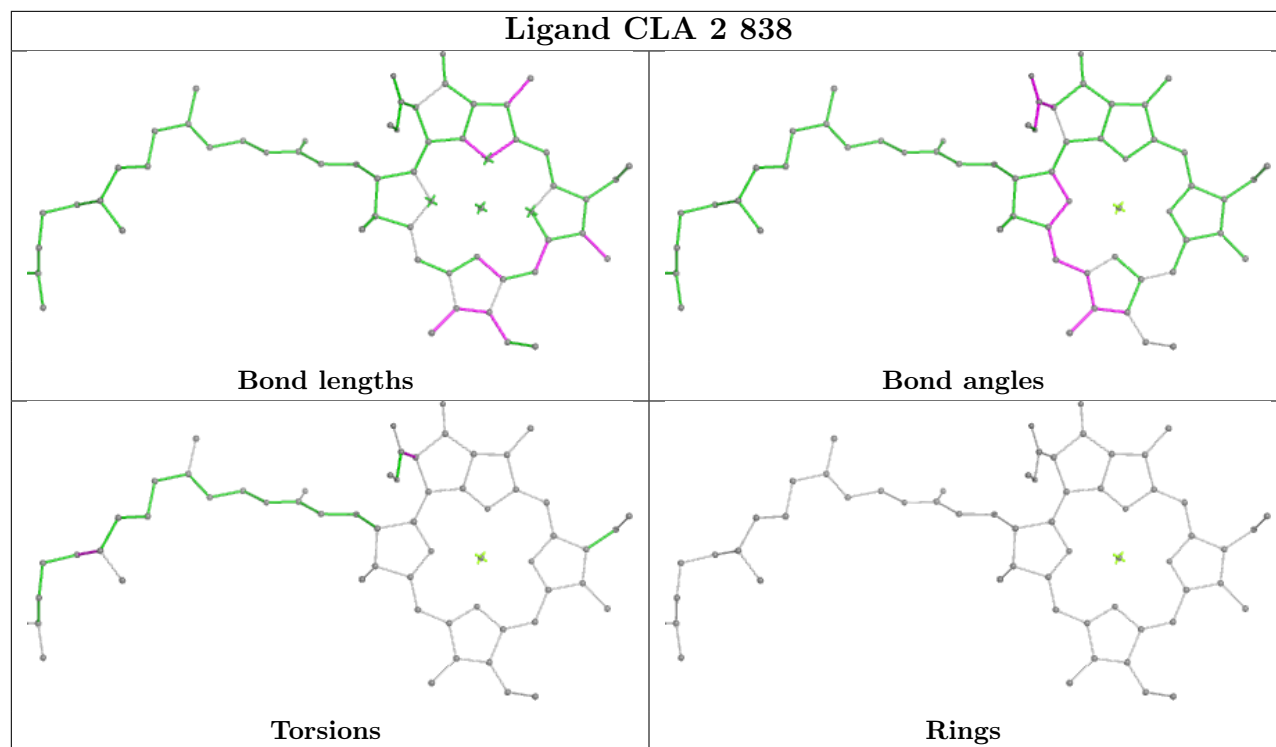




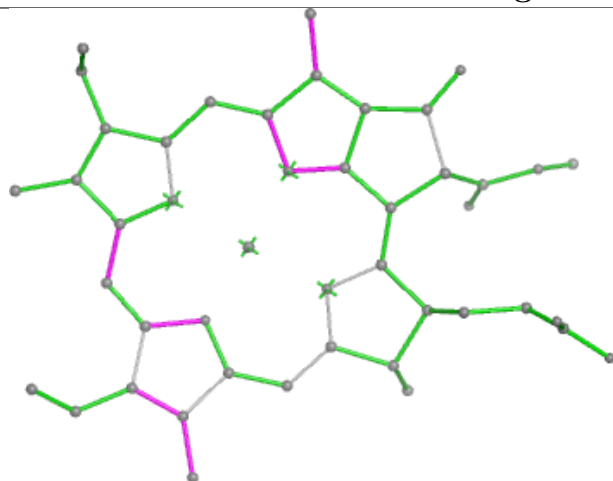
Ligand CLA a 821



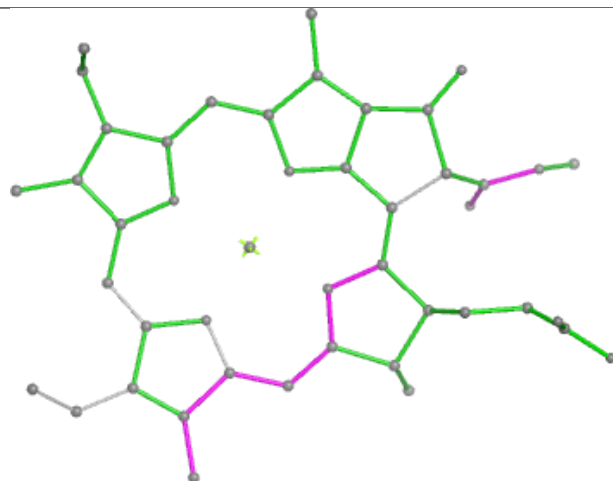




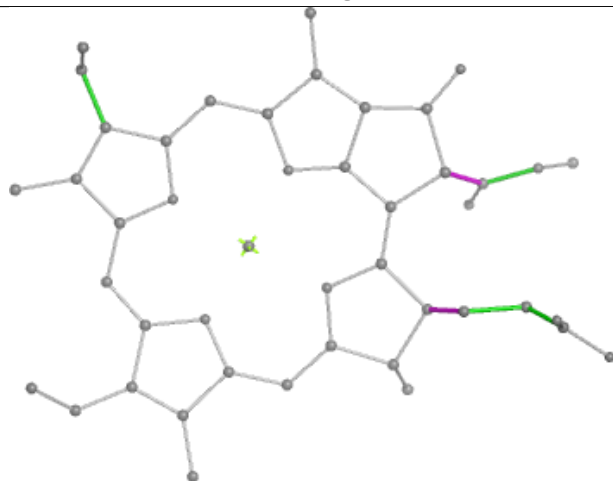
Ligand CLA B 836



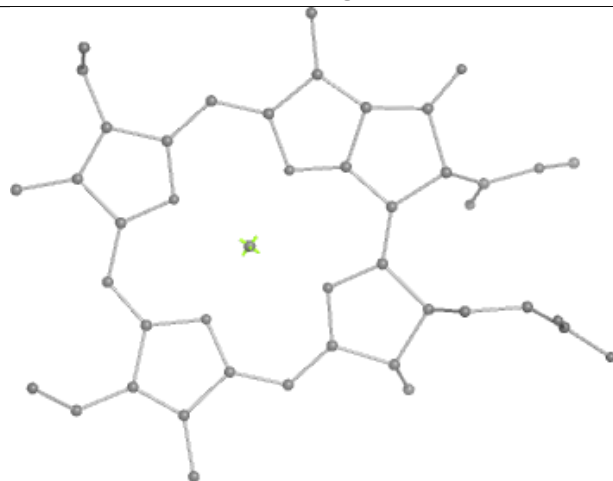
Bond lengths



Bond angles

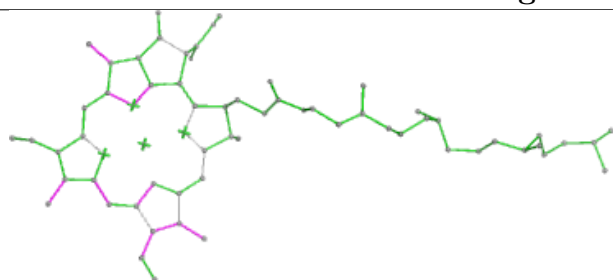


Torsions

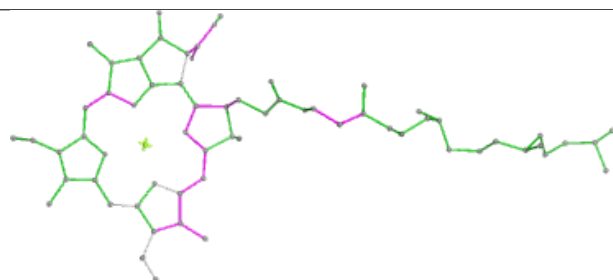


Rings

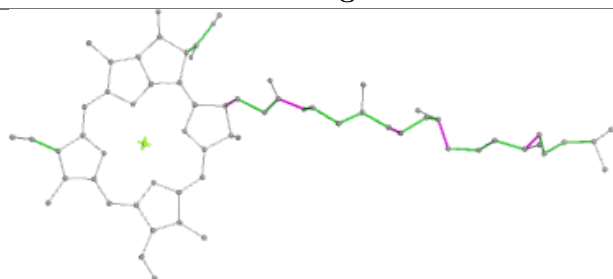
Ligand CLA a 827



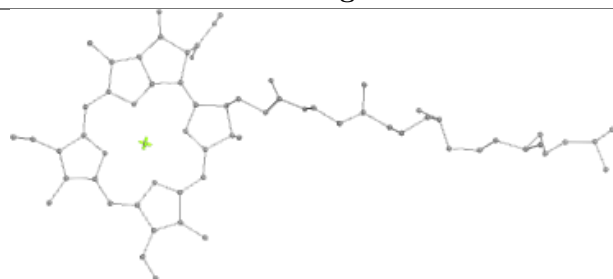
Bond lengths



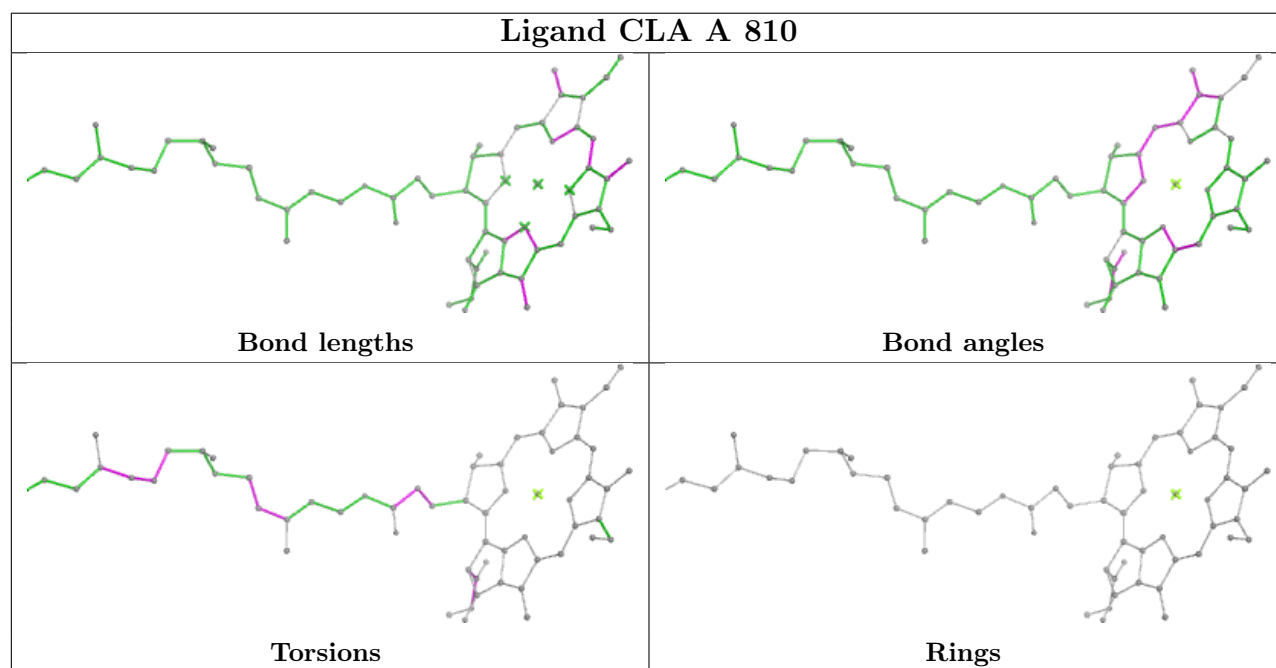
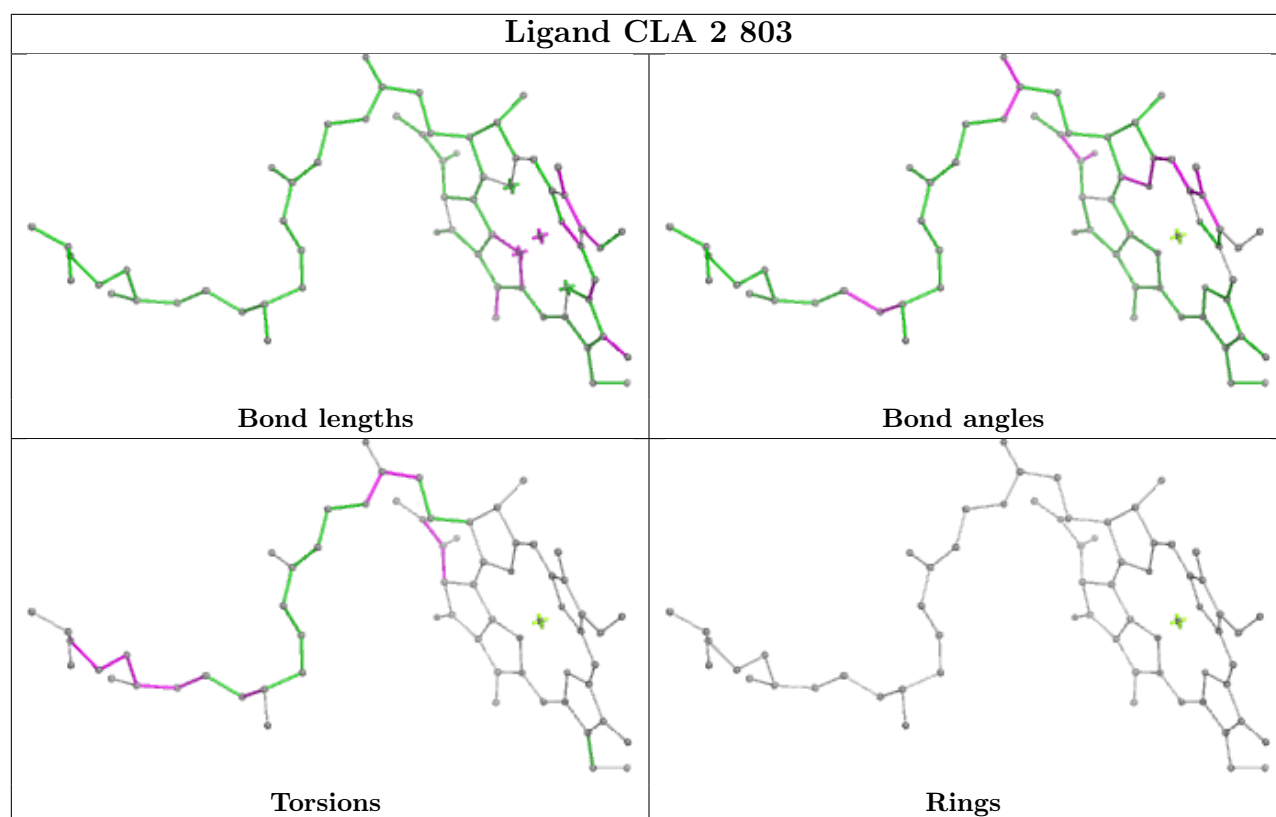
Bond angles



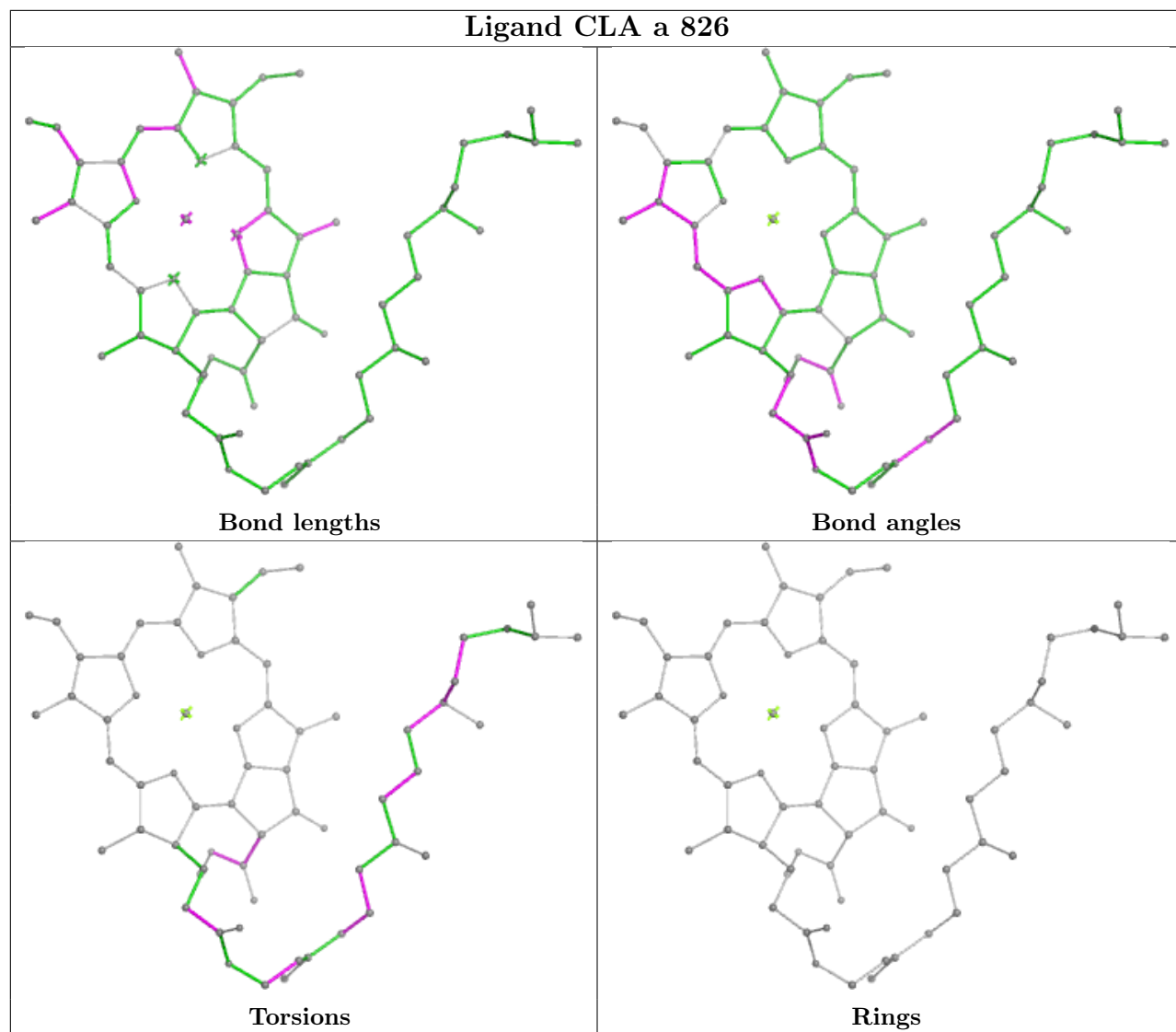
Torsions

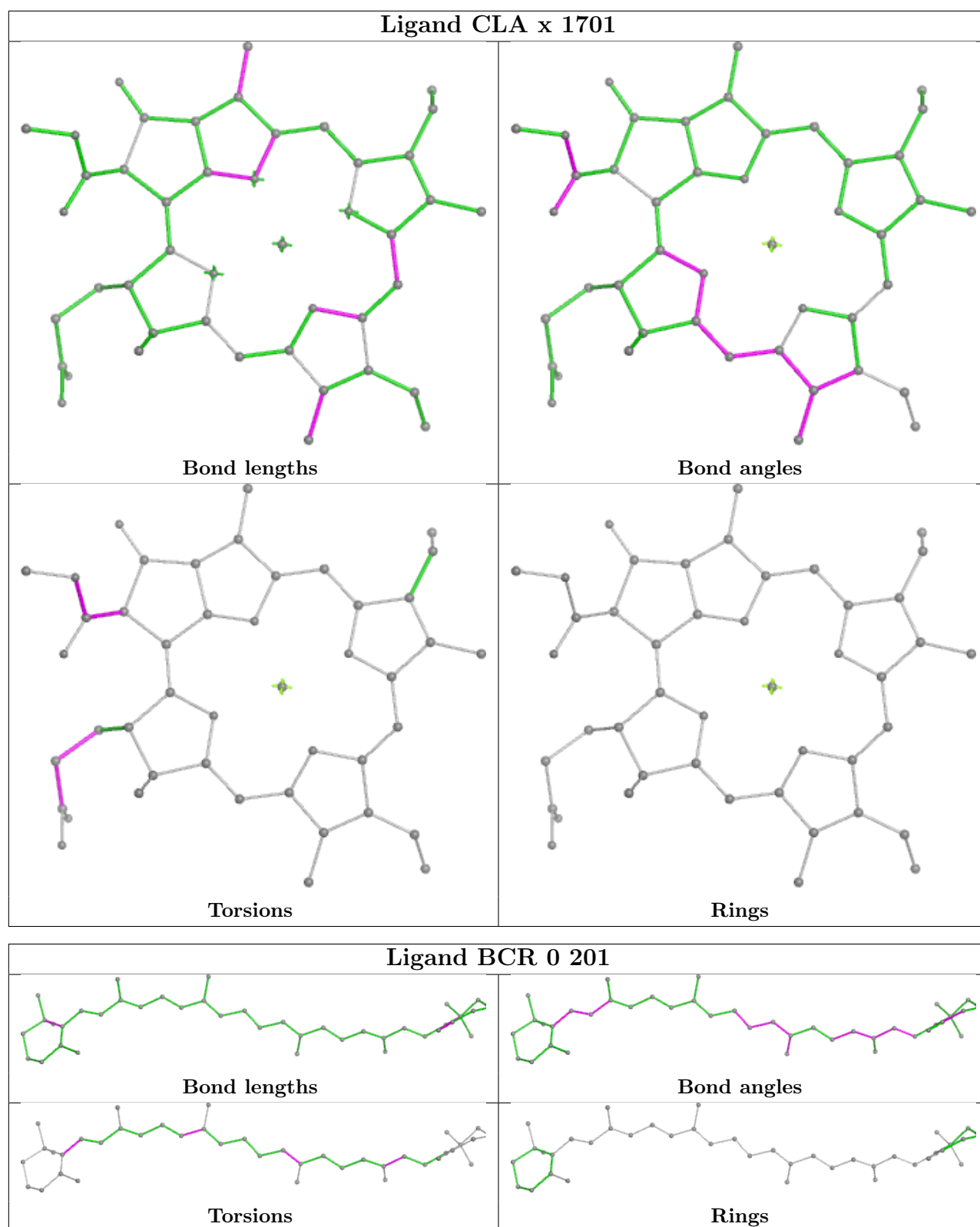


Rings

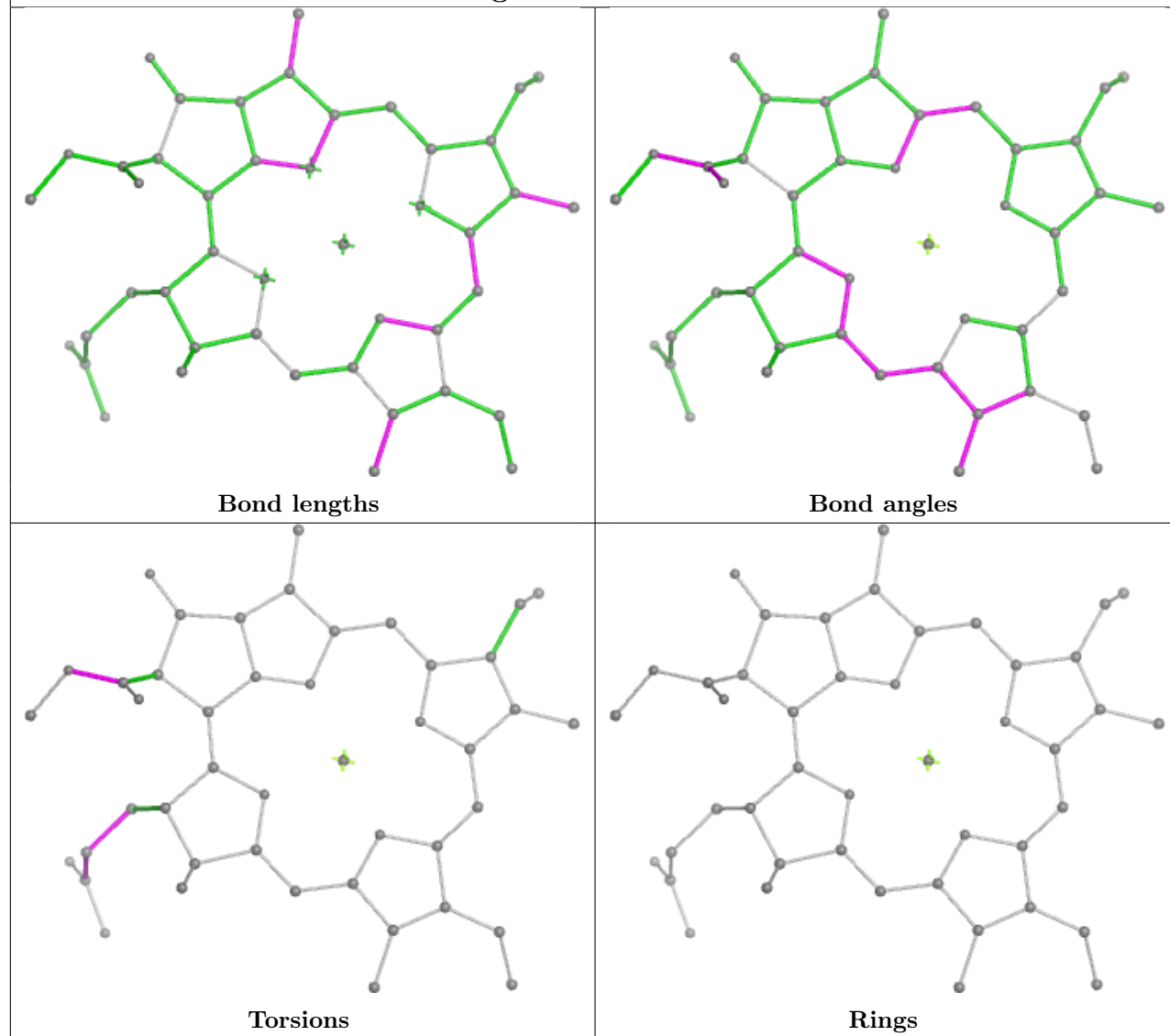


Ligand CLA a 826

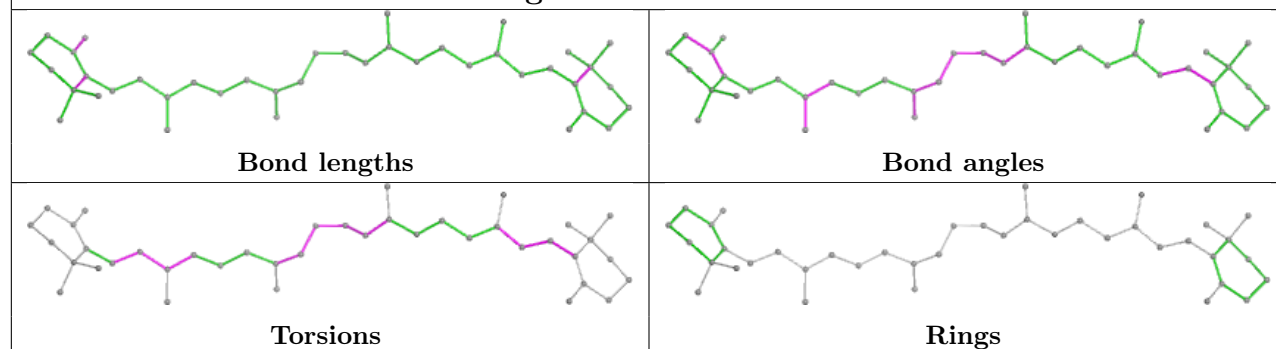


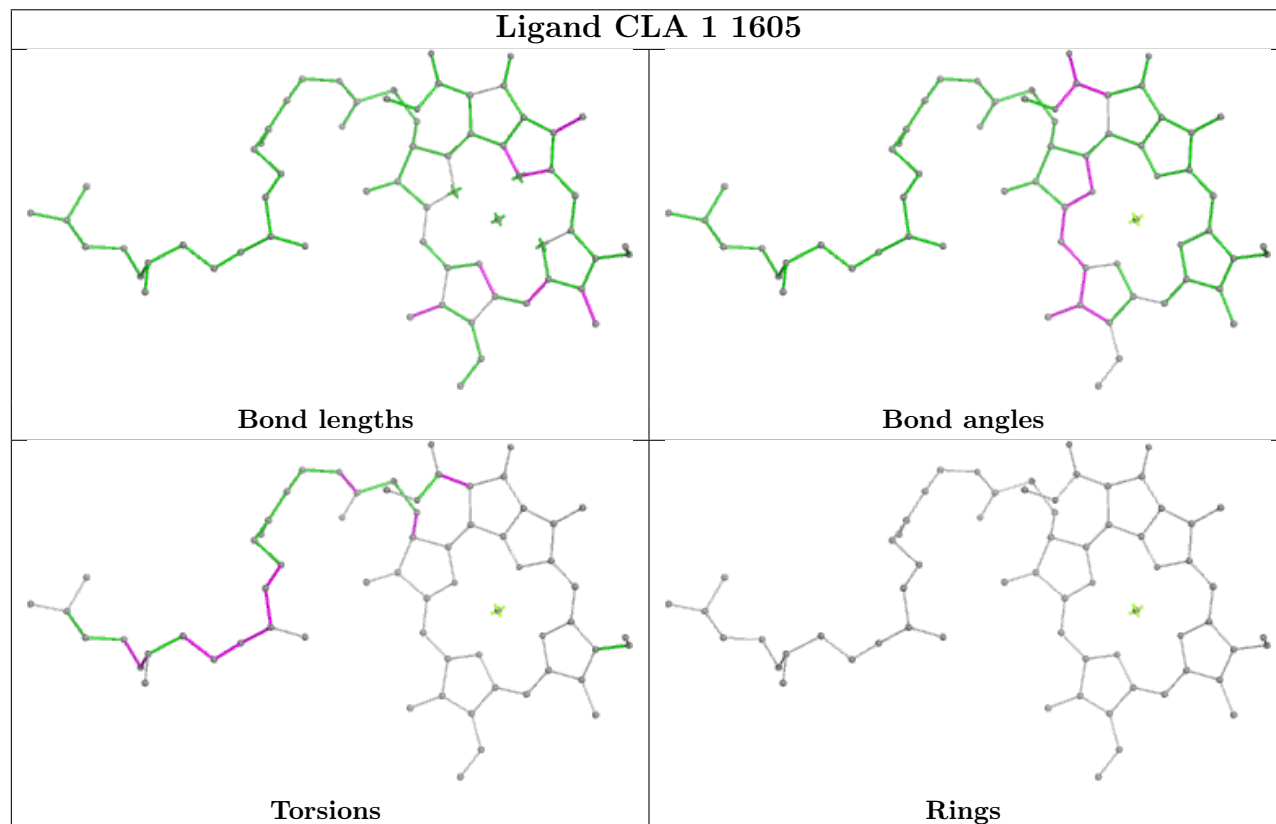
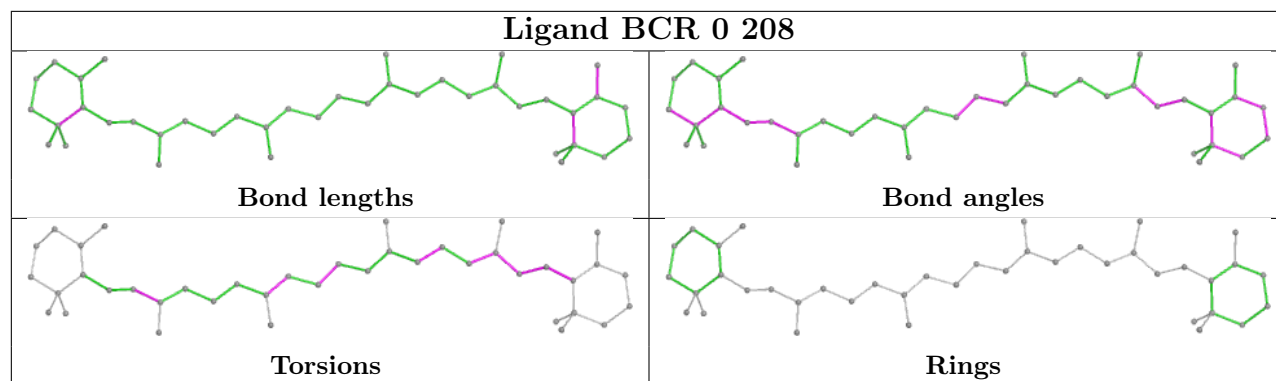


Ligand CLA 2 824

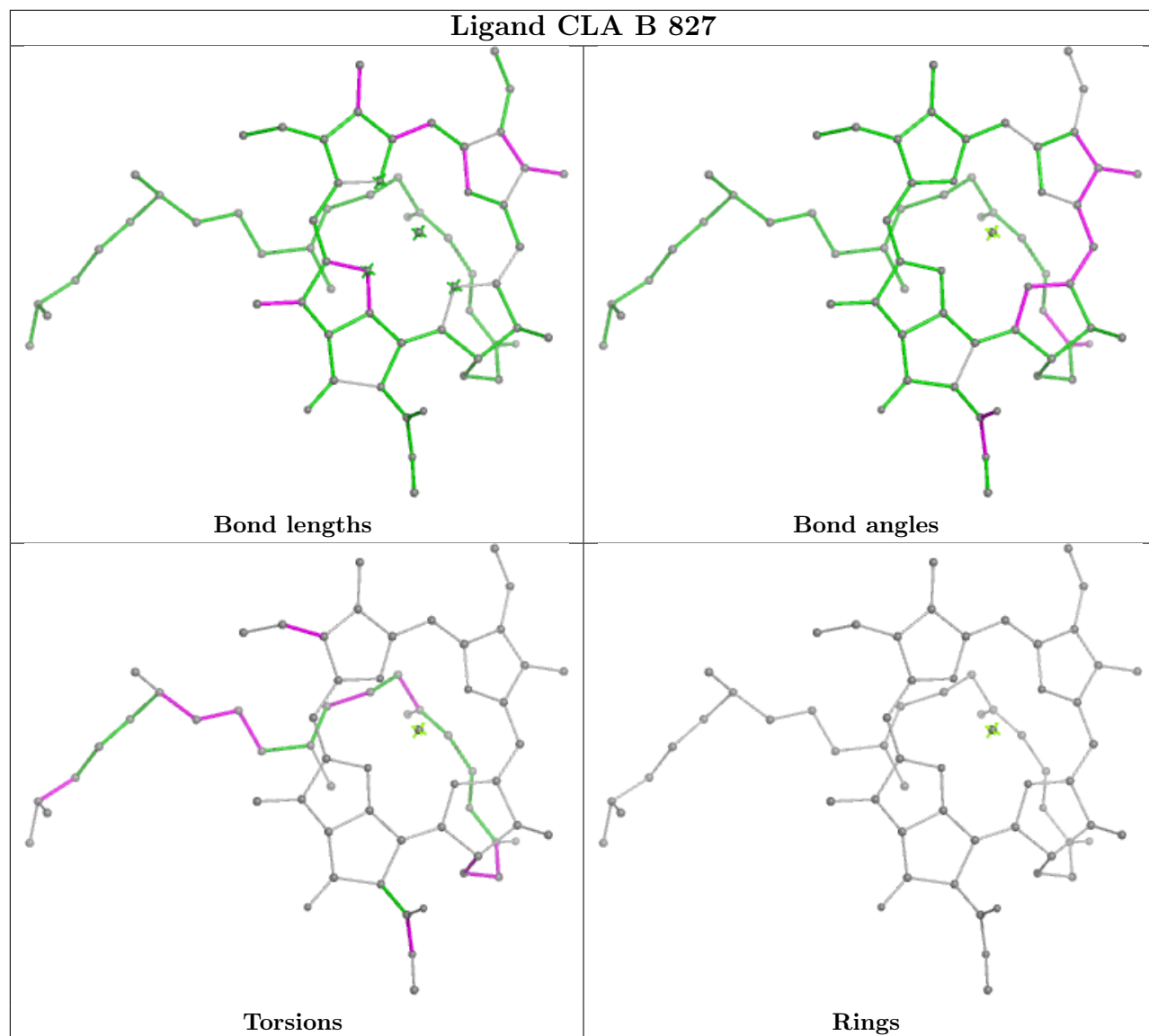


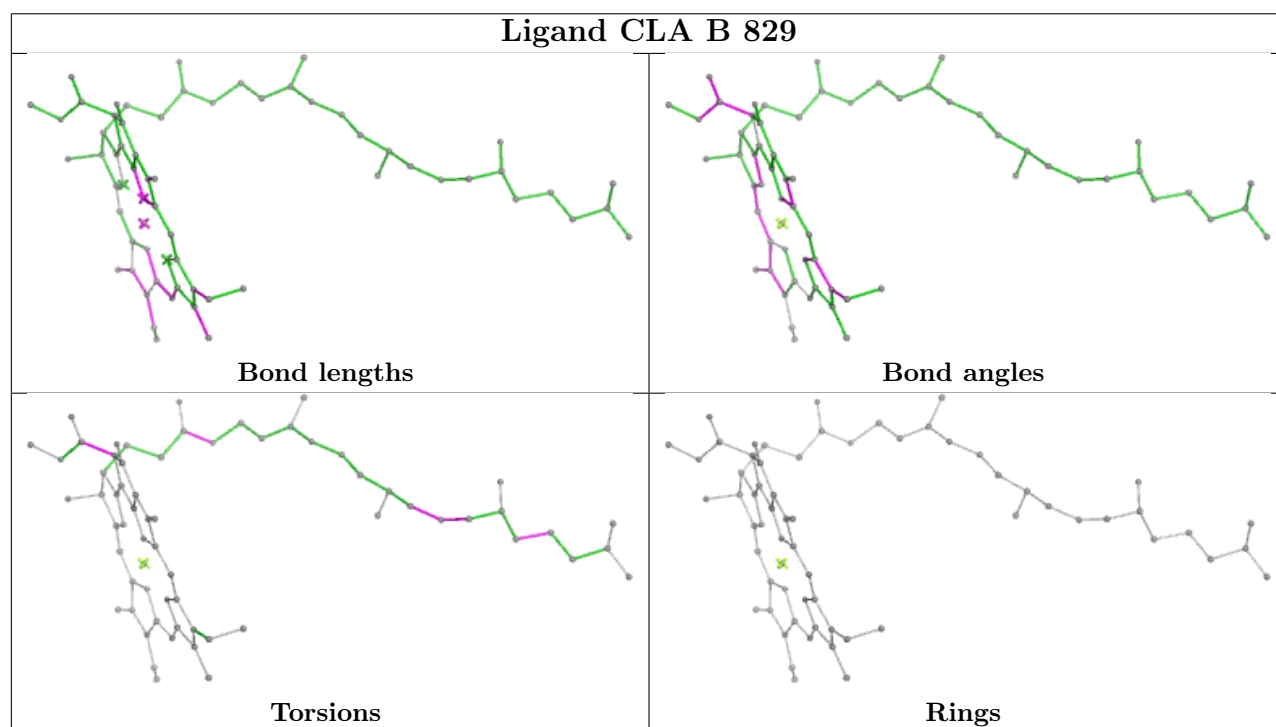
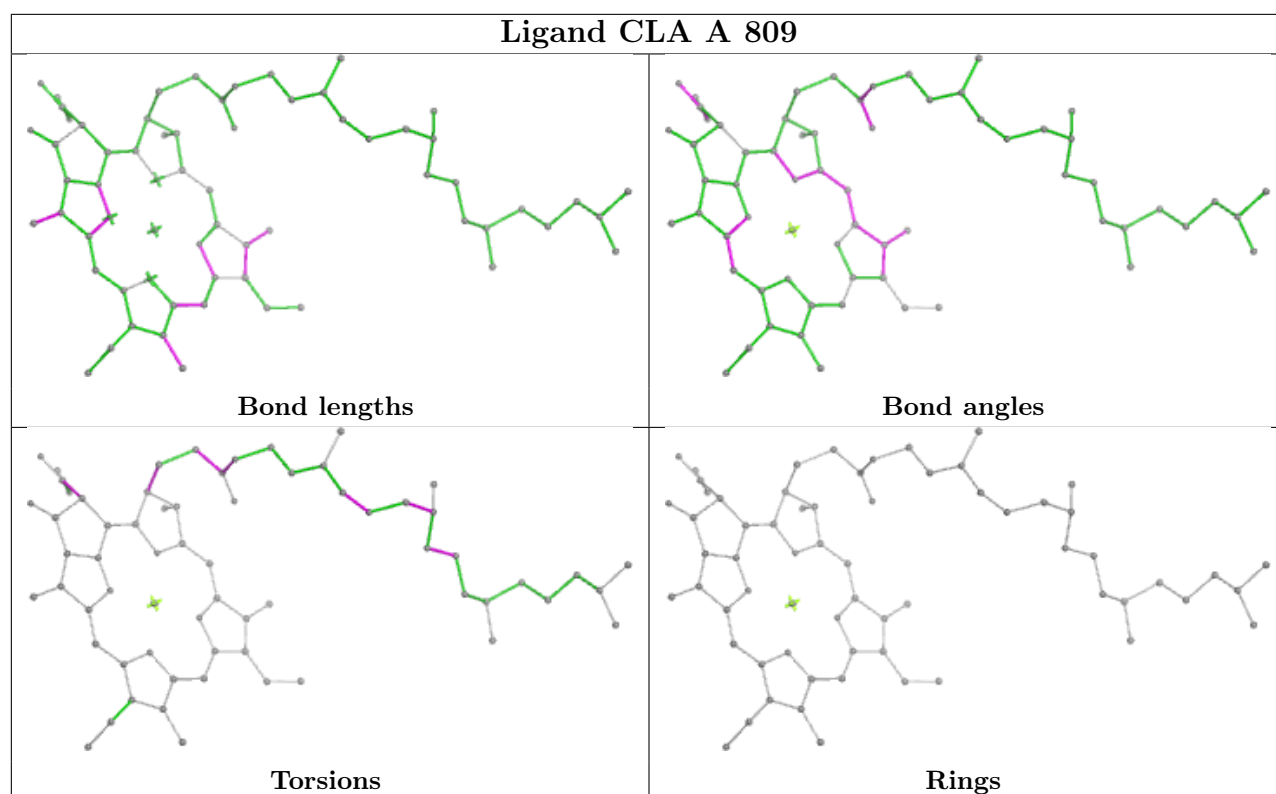
Ligand BCR 1 1649

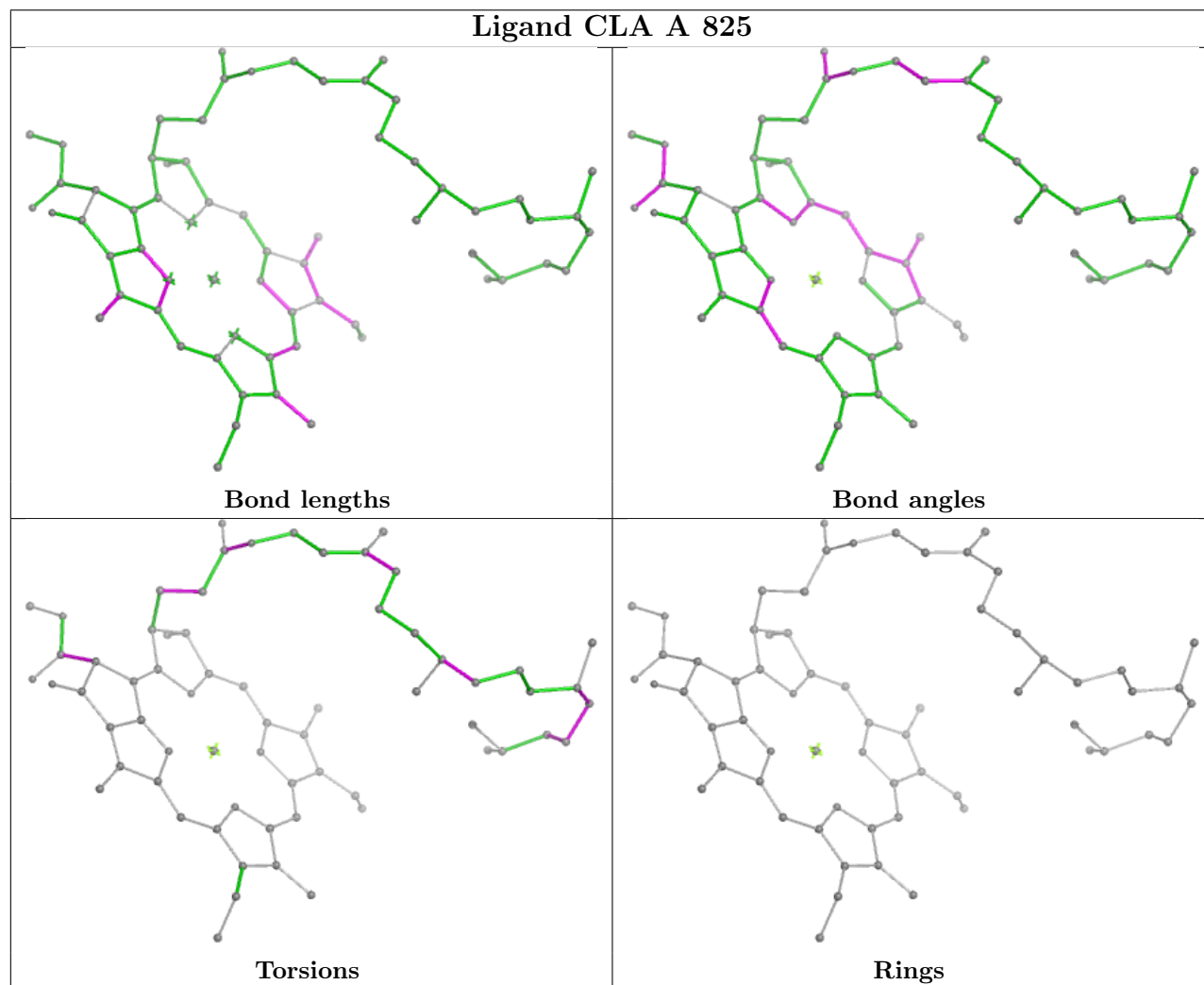
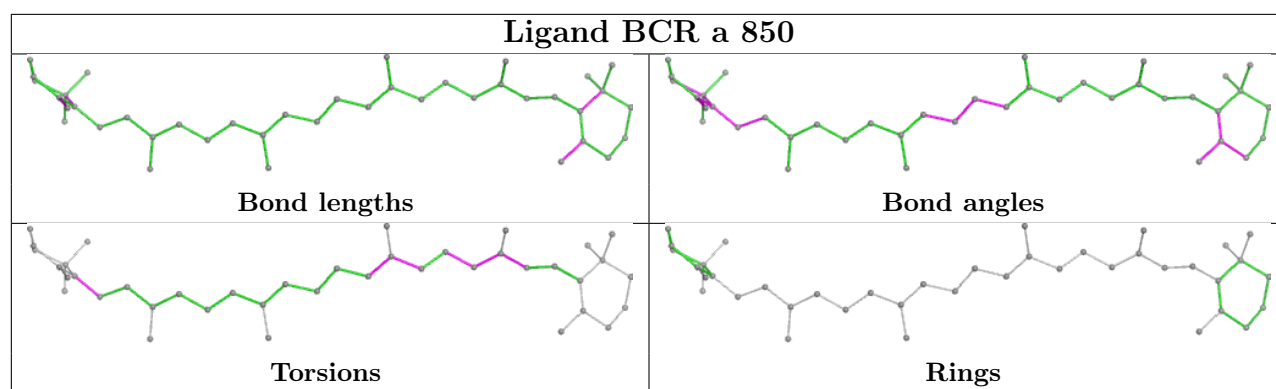




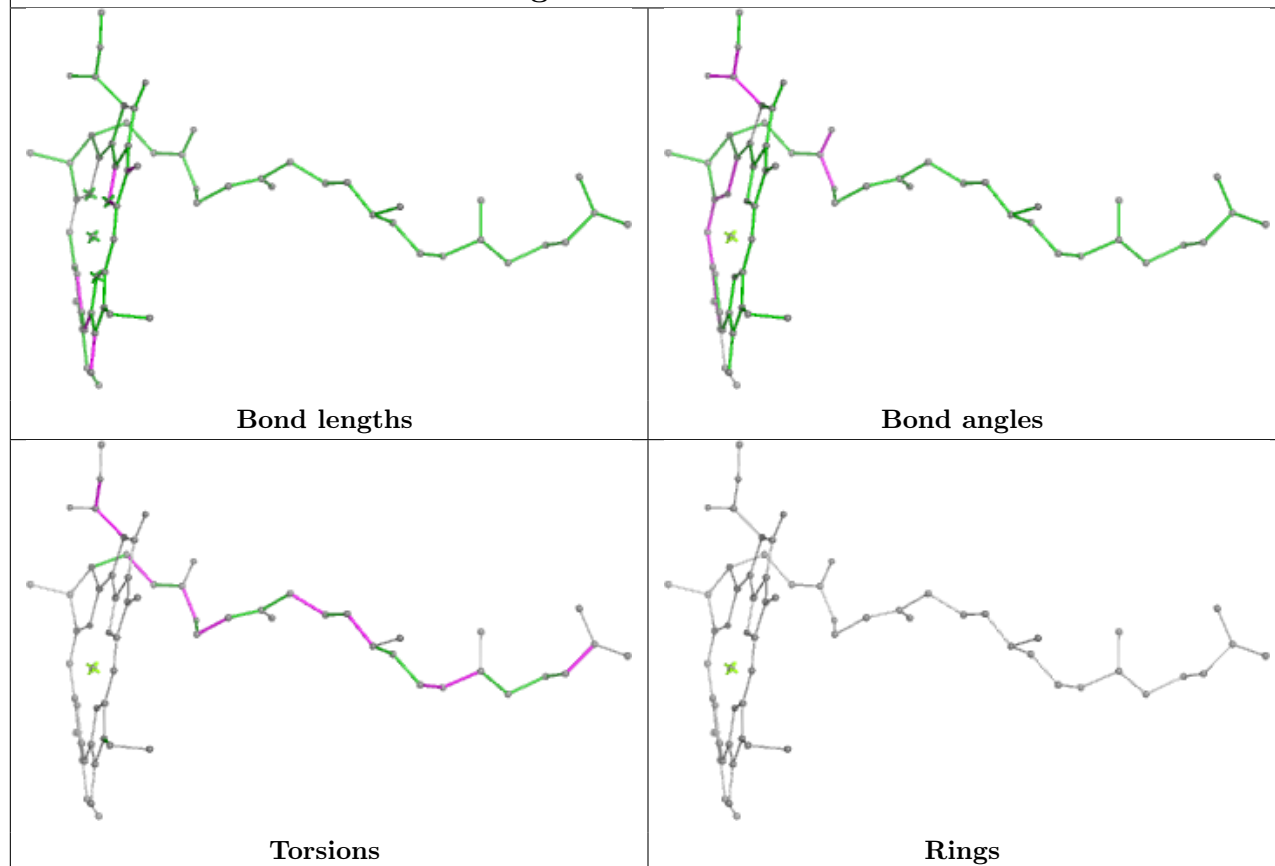
Ligand CLA B 827



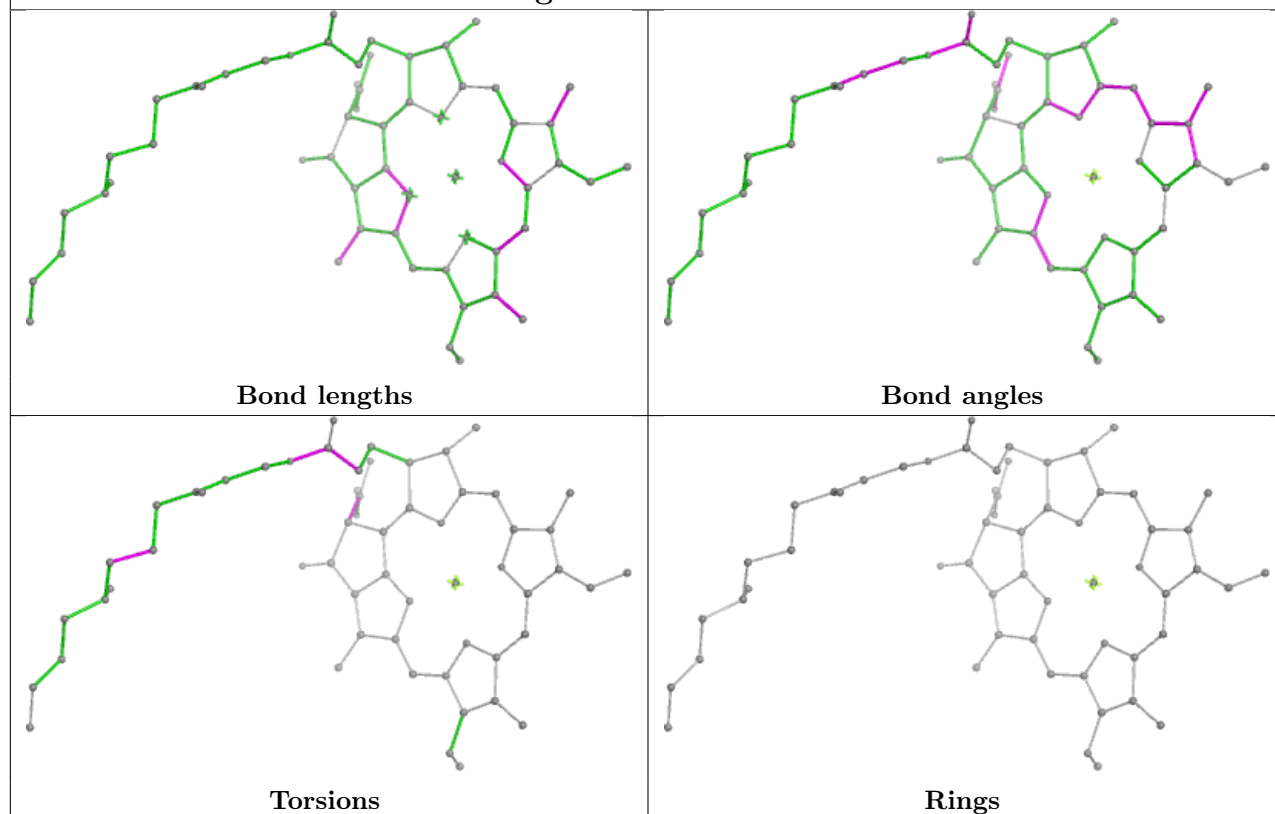


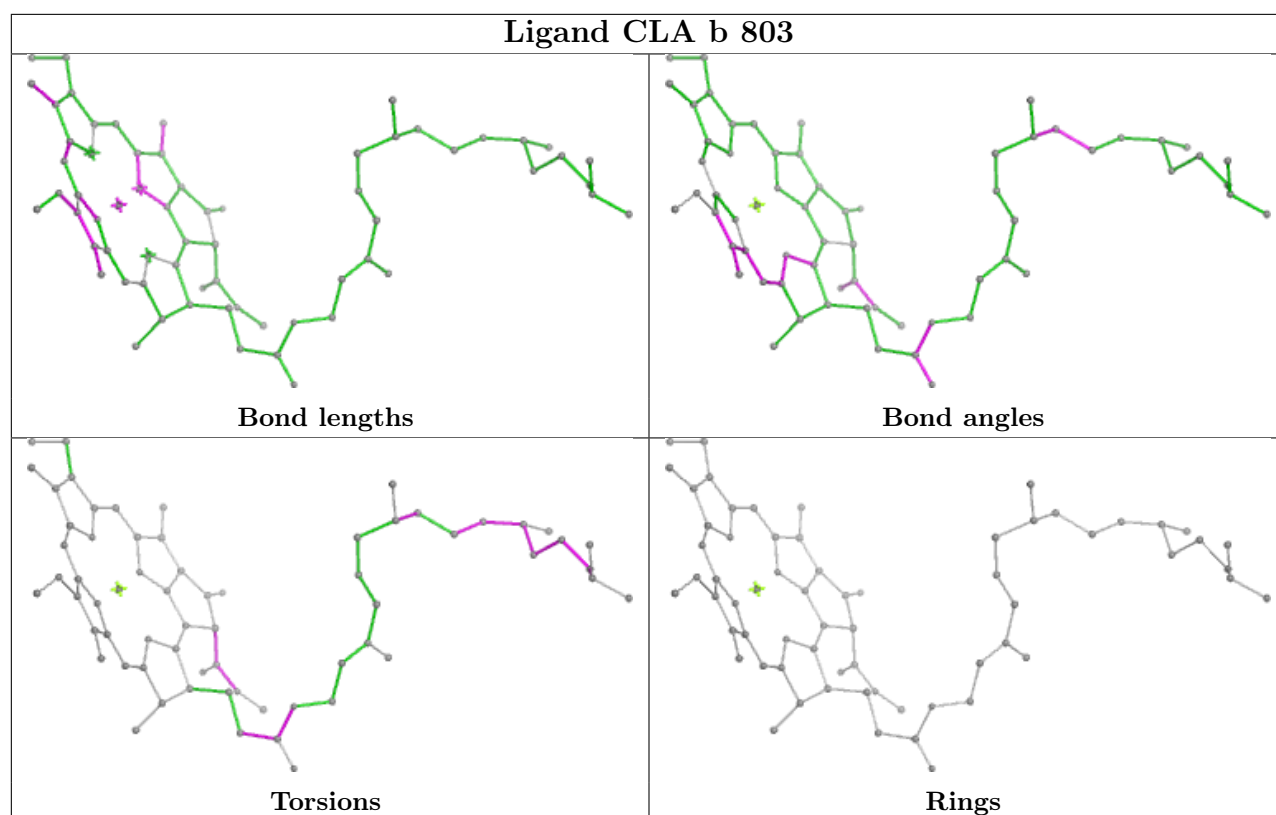


Ligand CLA A 829

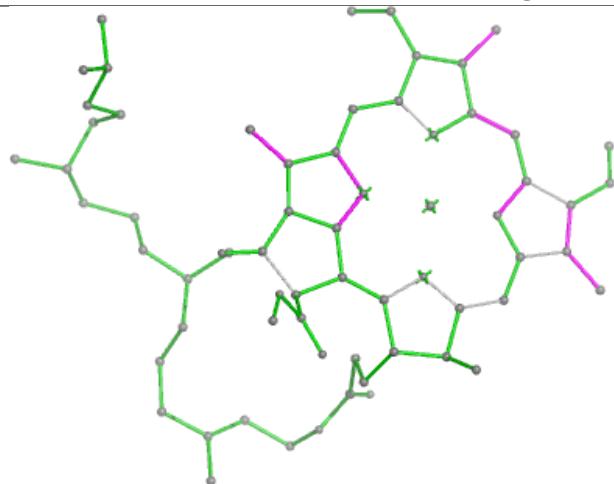


Ligand CLA 9 103

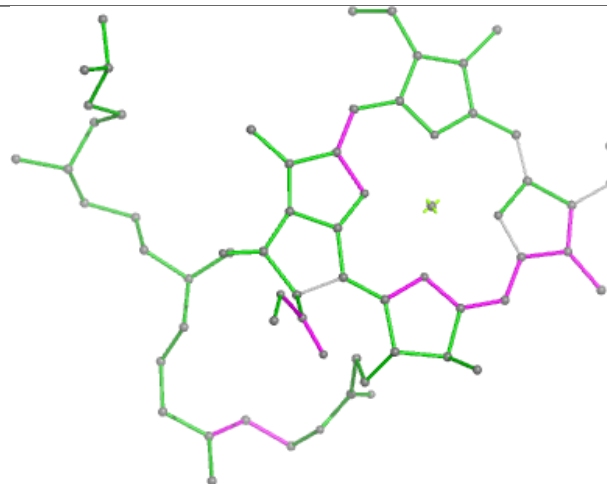




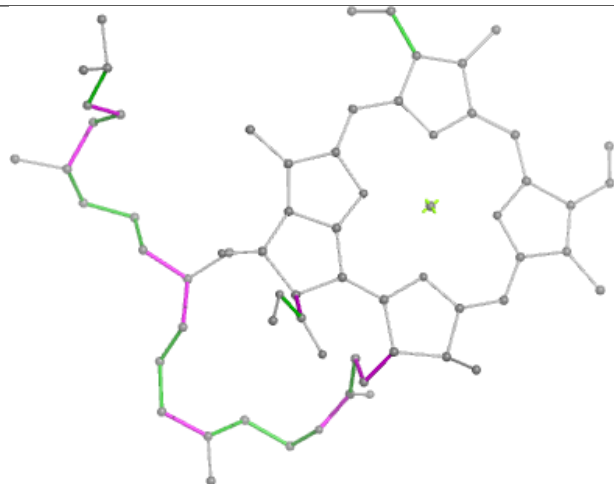
Ligand CLA 2 833



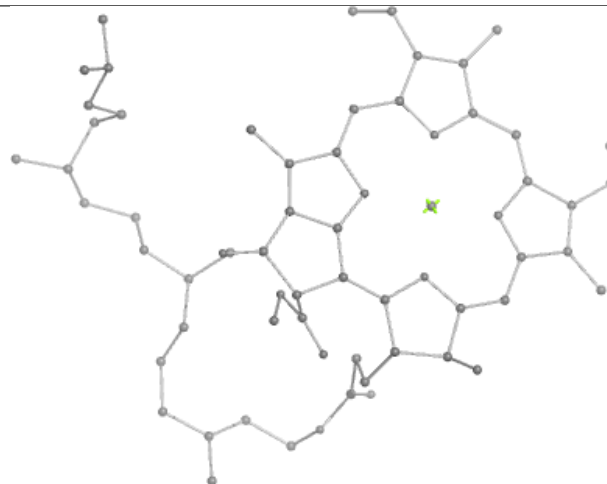
Bond lengths



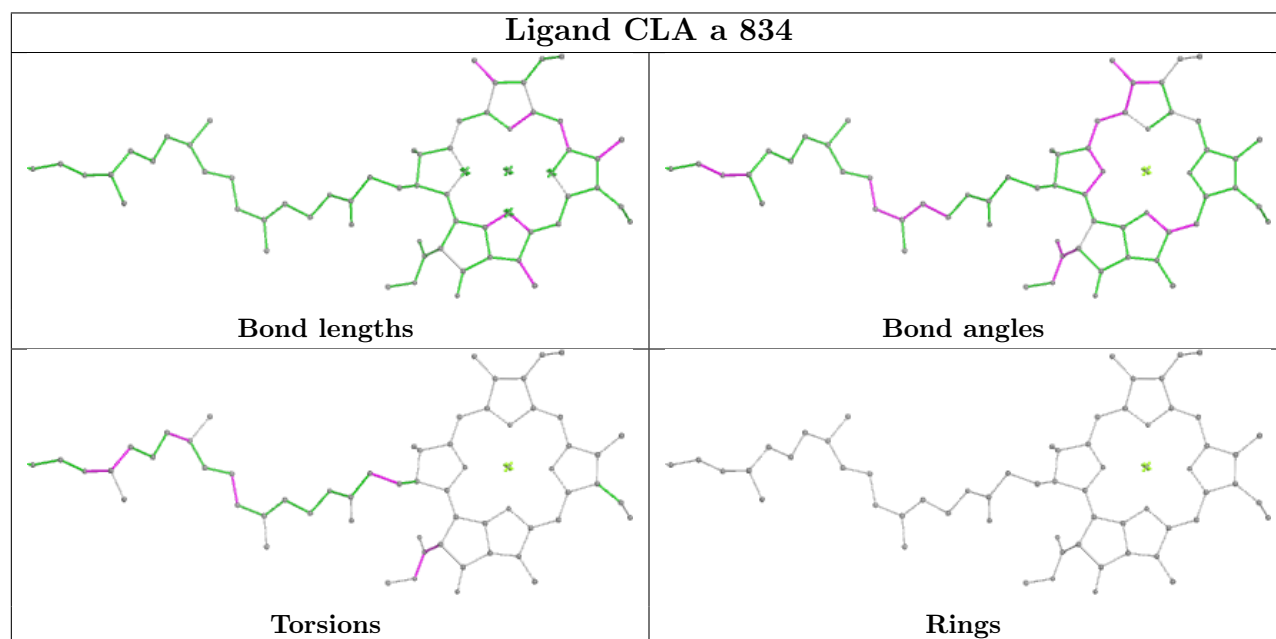
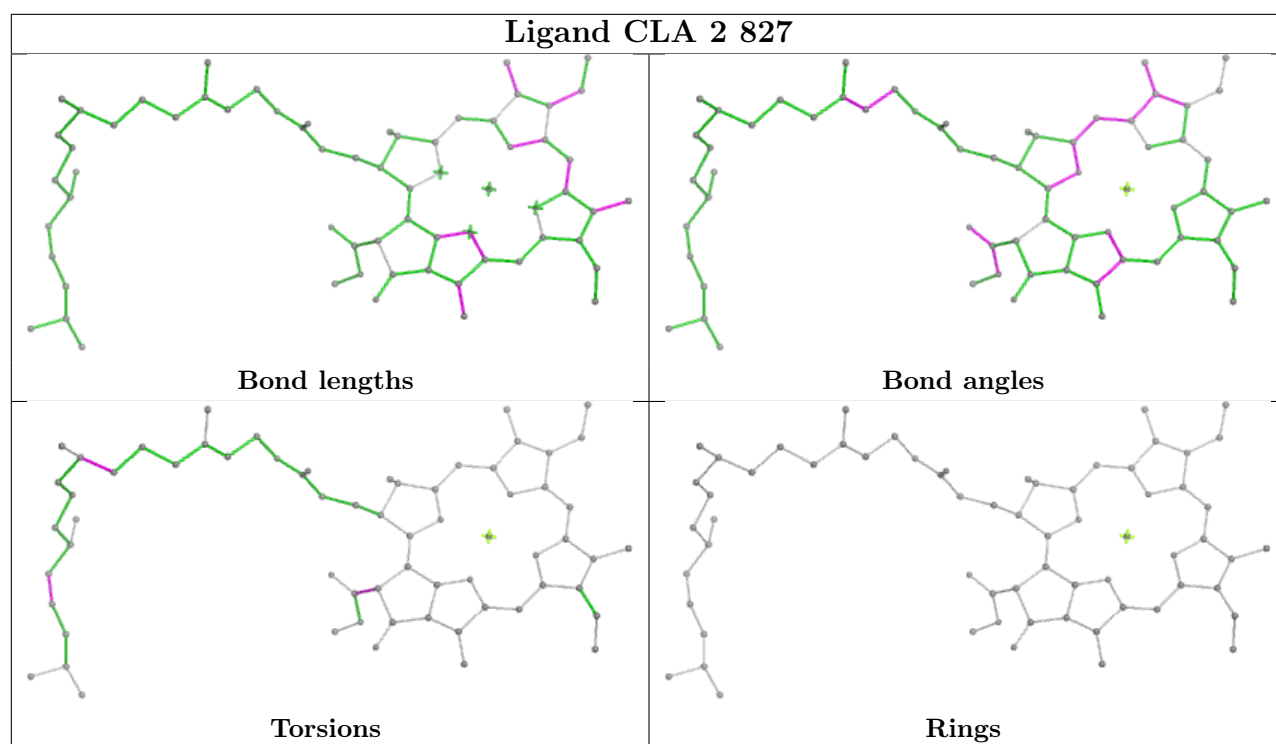
Bond angles

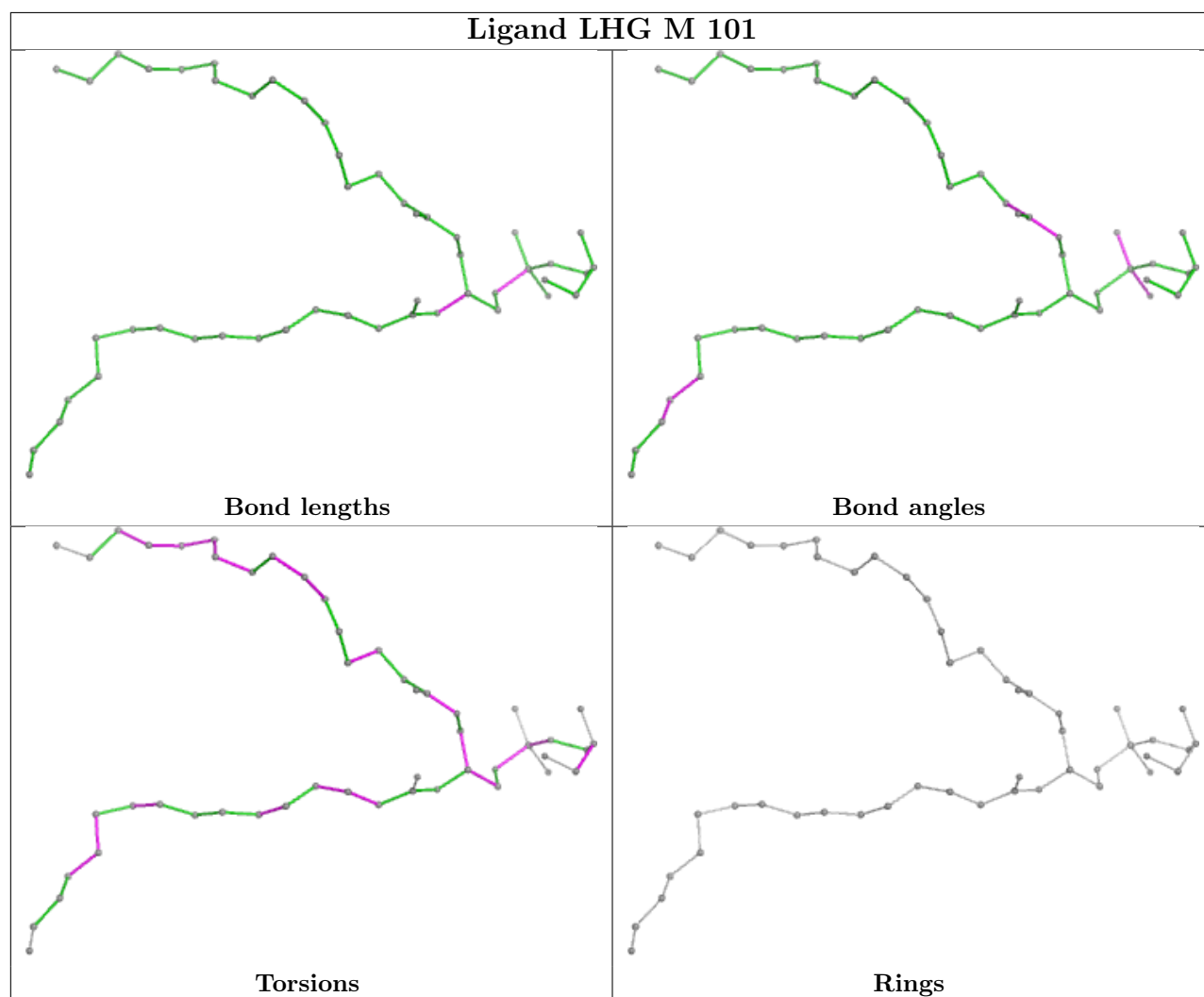
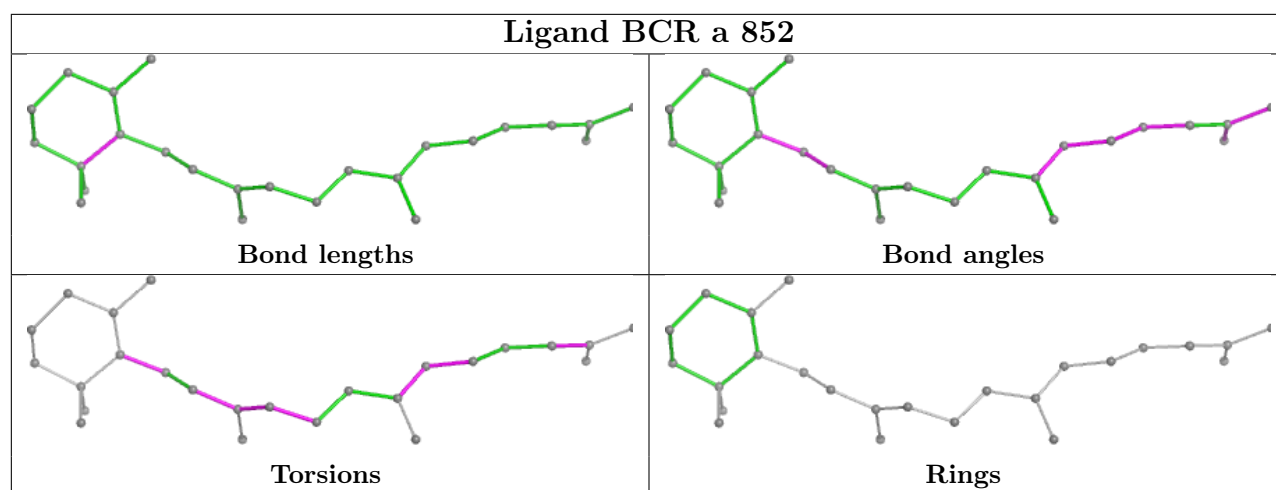


Torsions

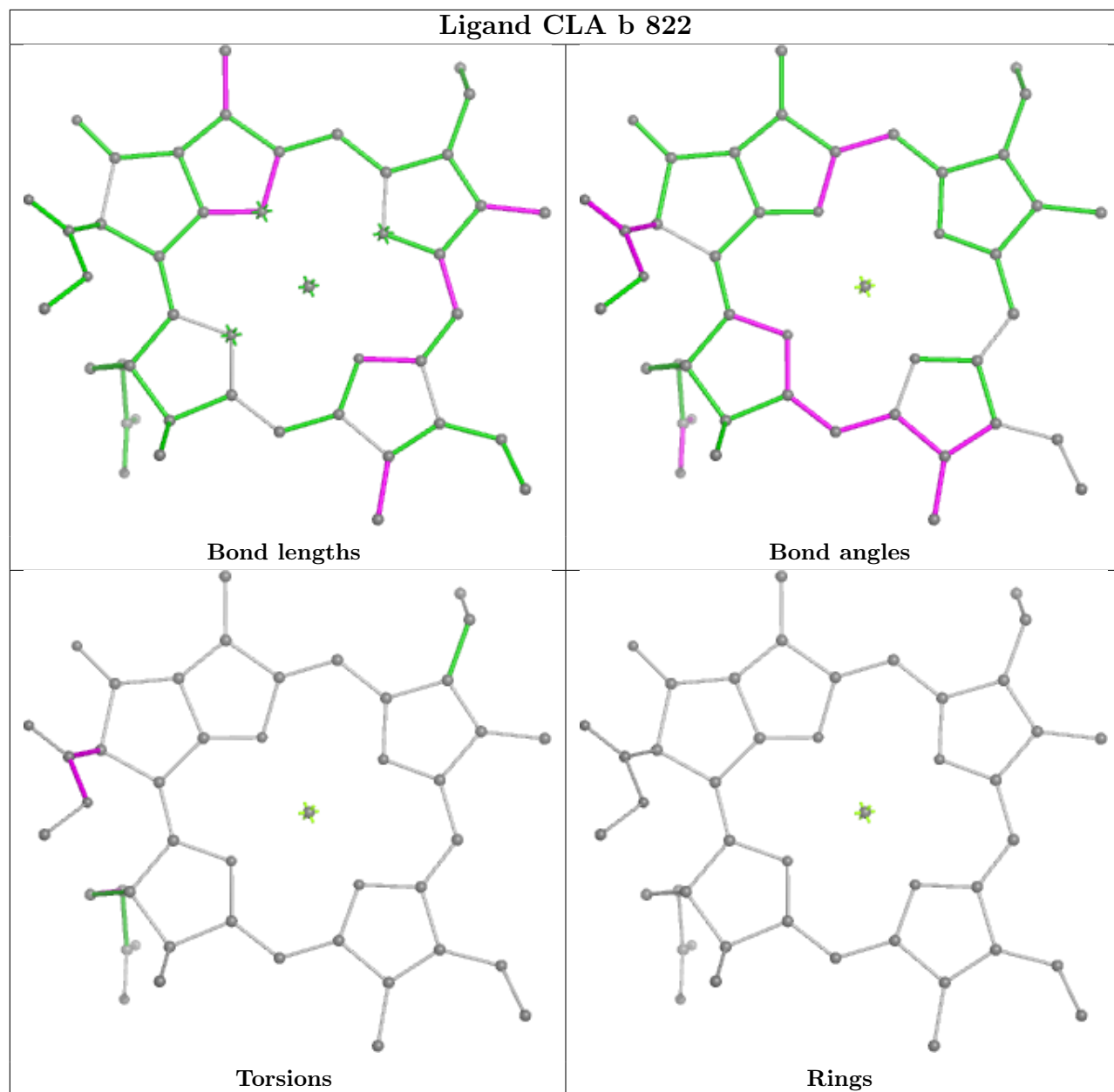


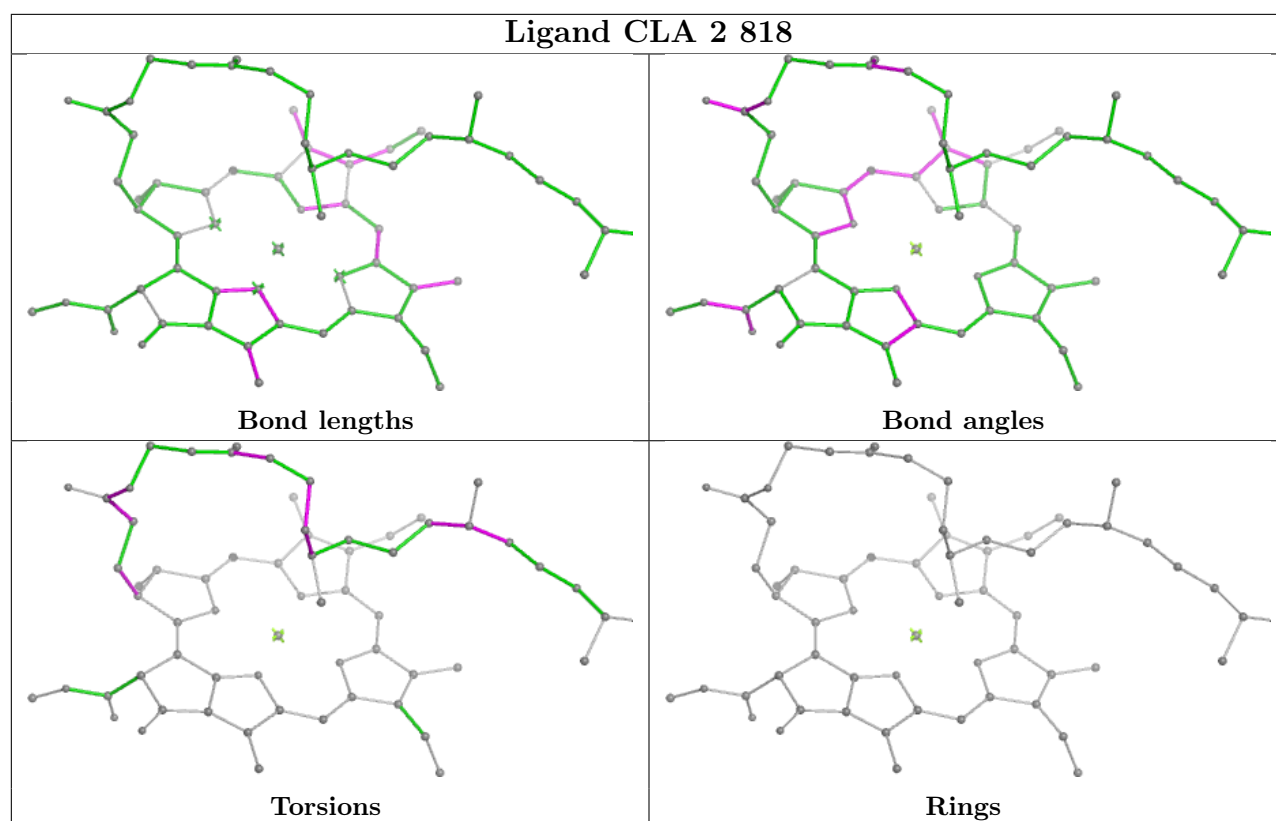
Rings



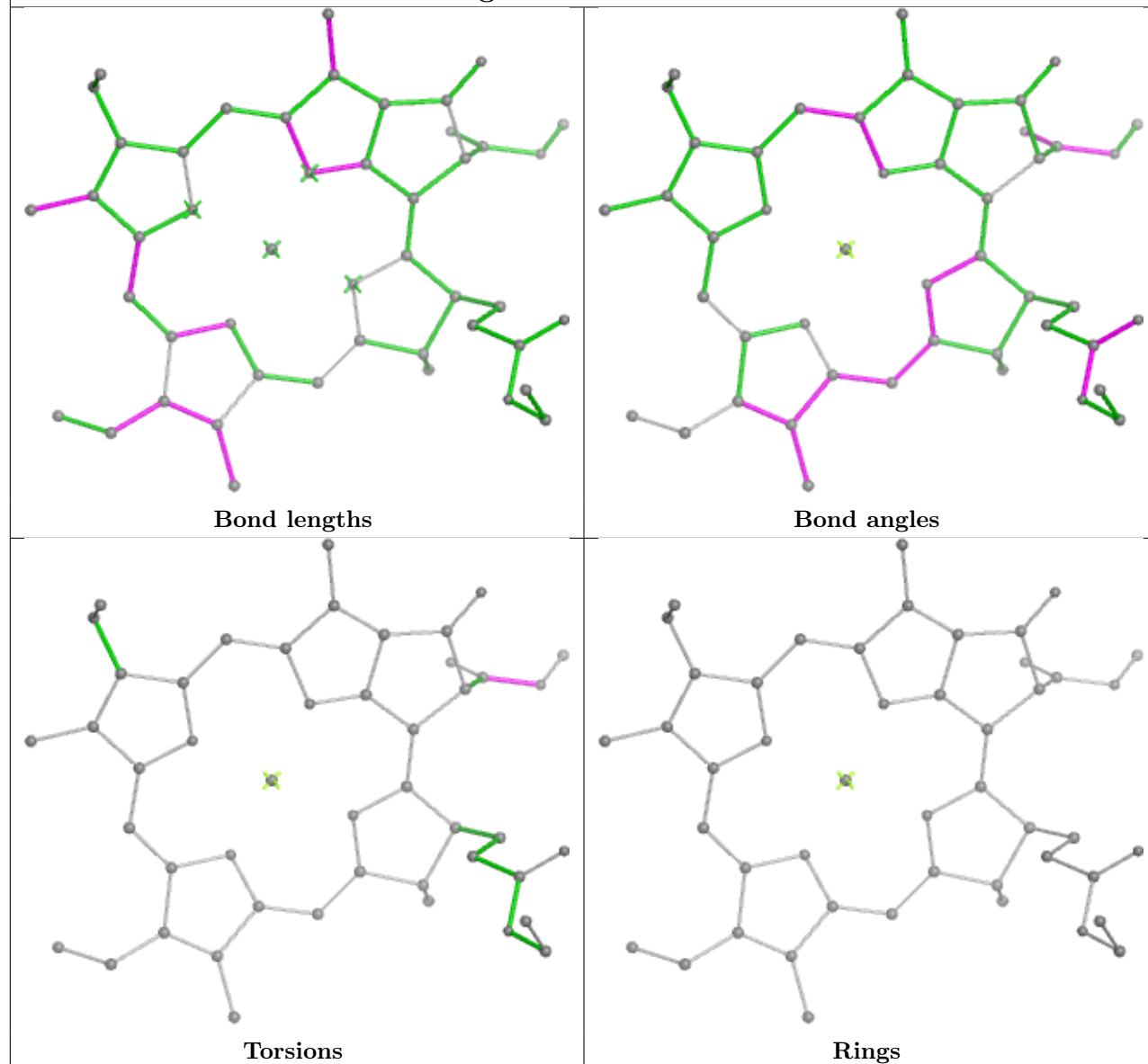


Ligand CLA b 822

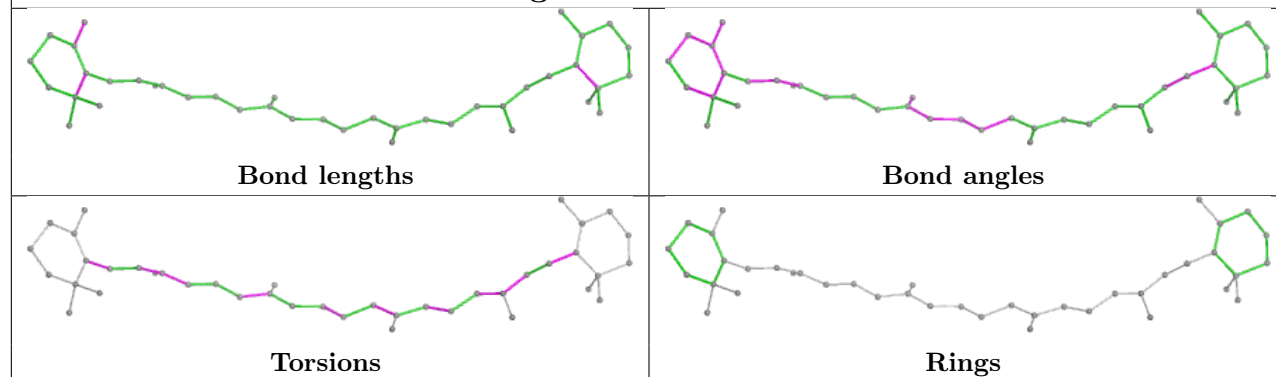


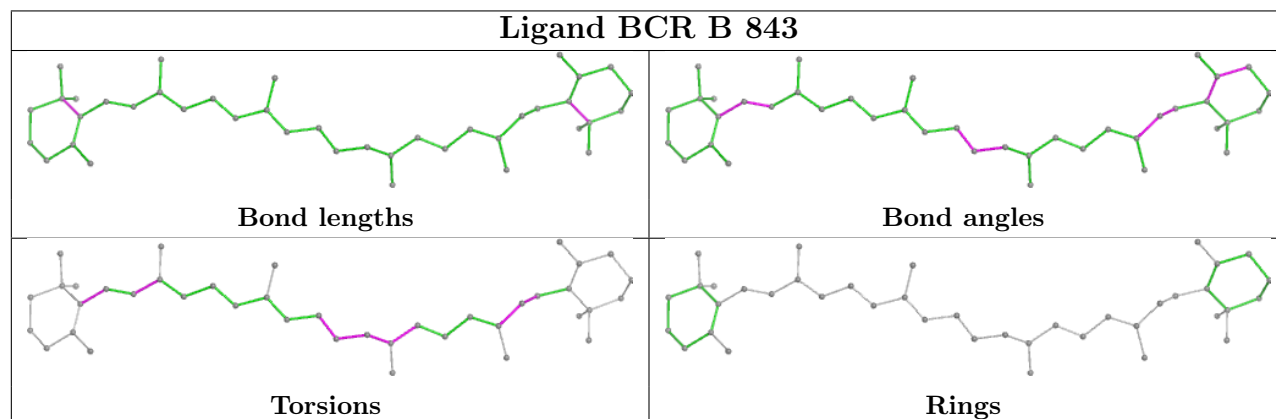
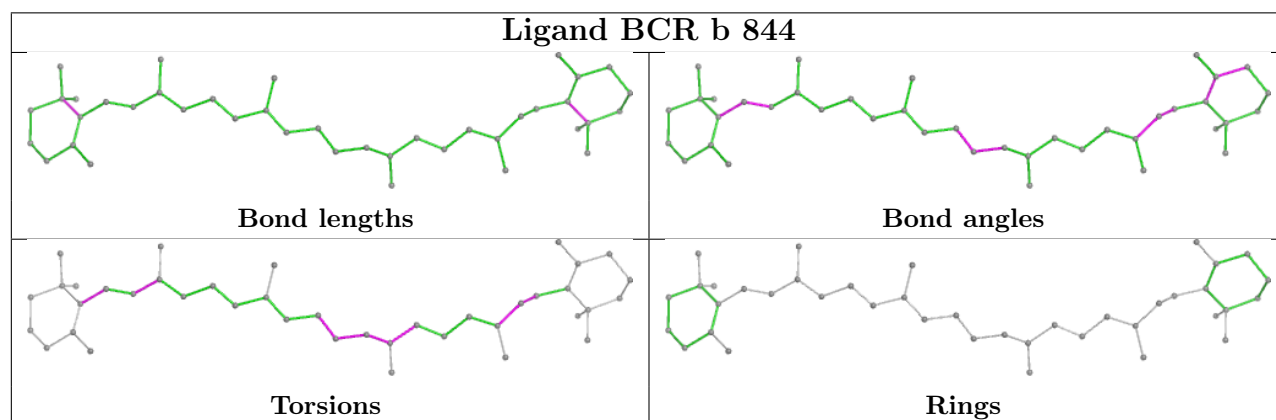
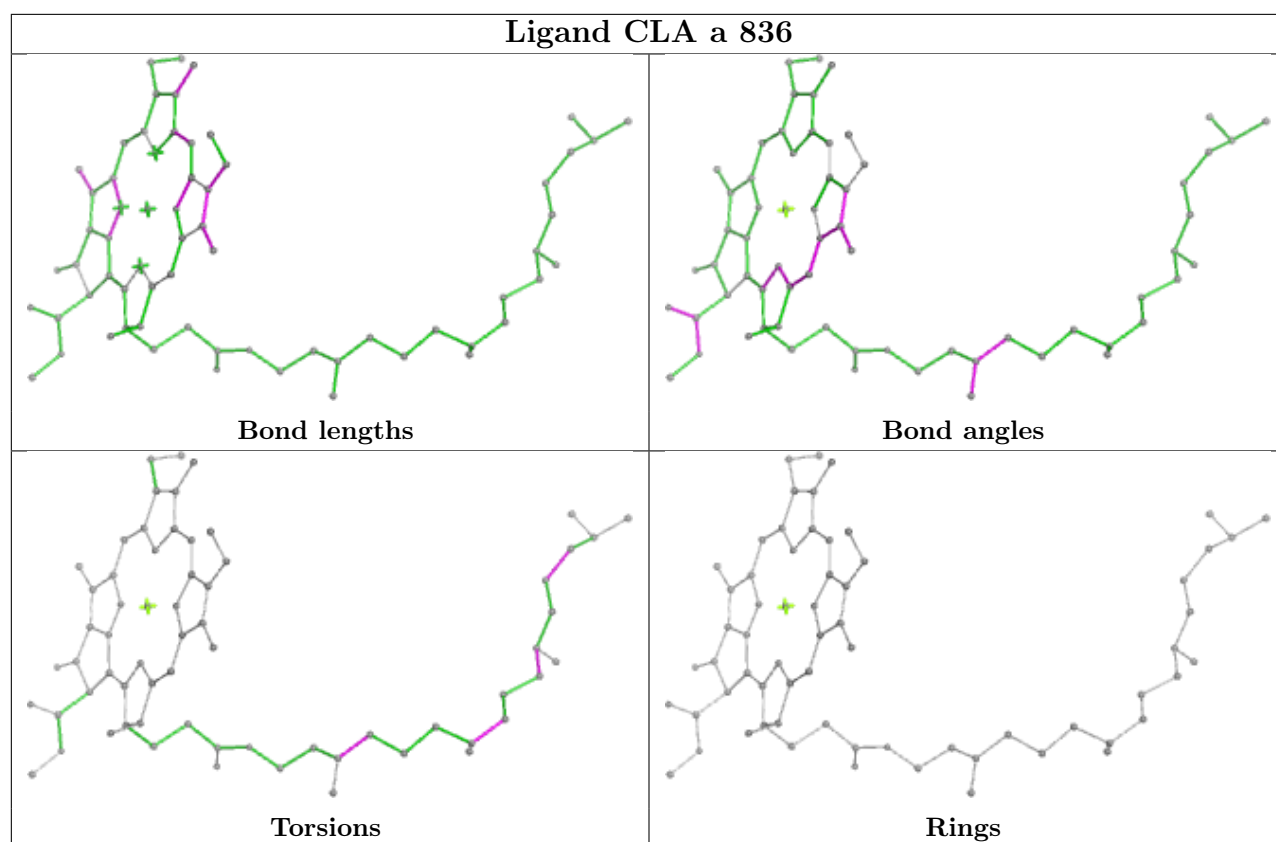


Ligand CLA B 839

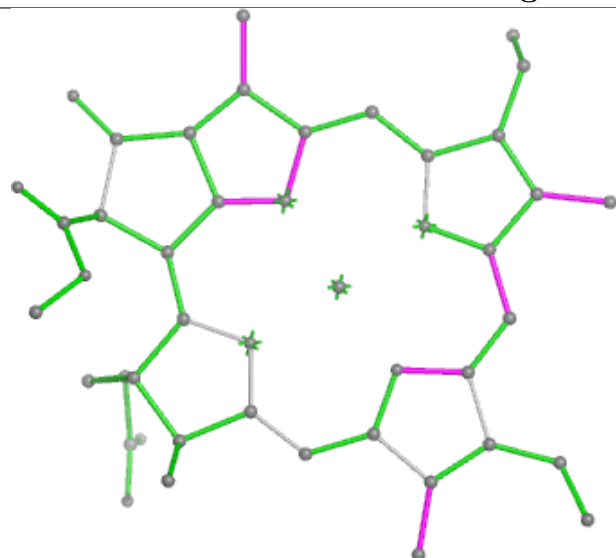


Ligand BCR A 856

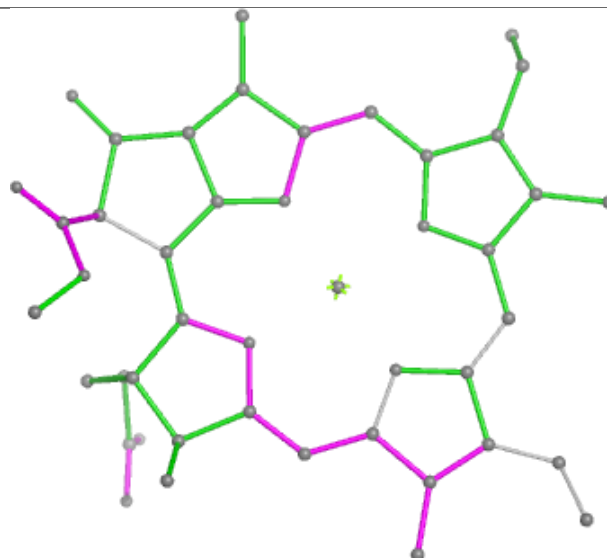




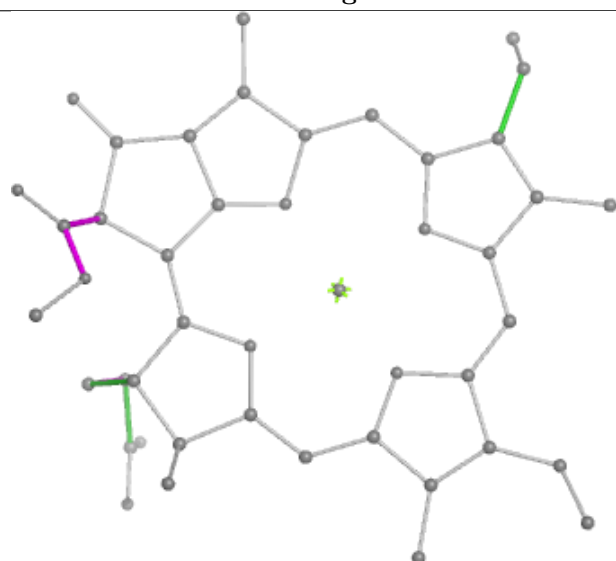
Ligand CLA 2 822



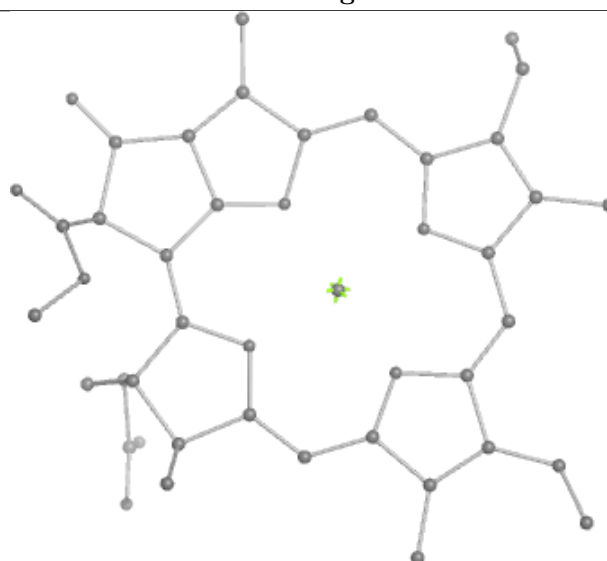
Bond lengths



Bond angles

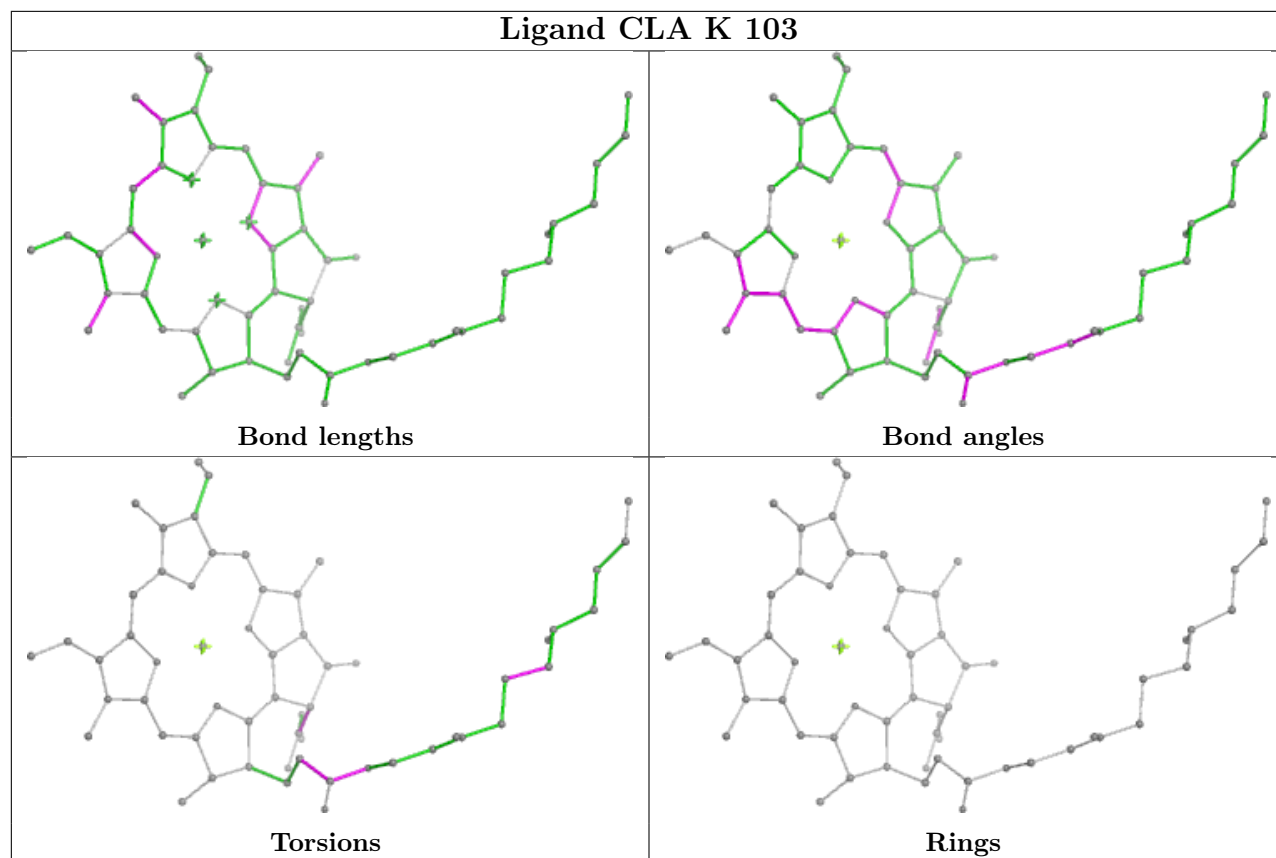


Torsions

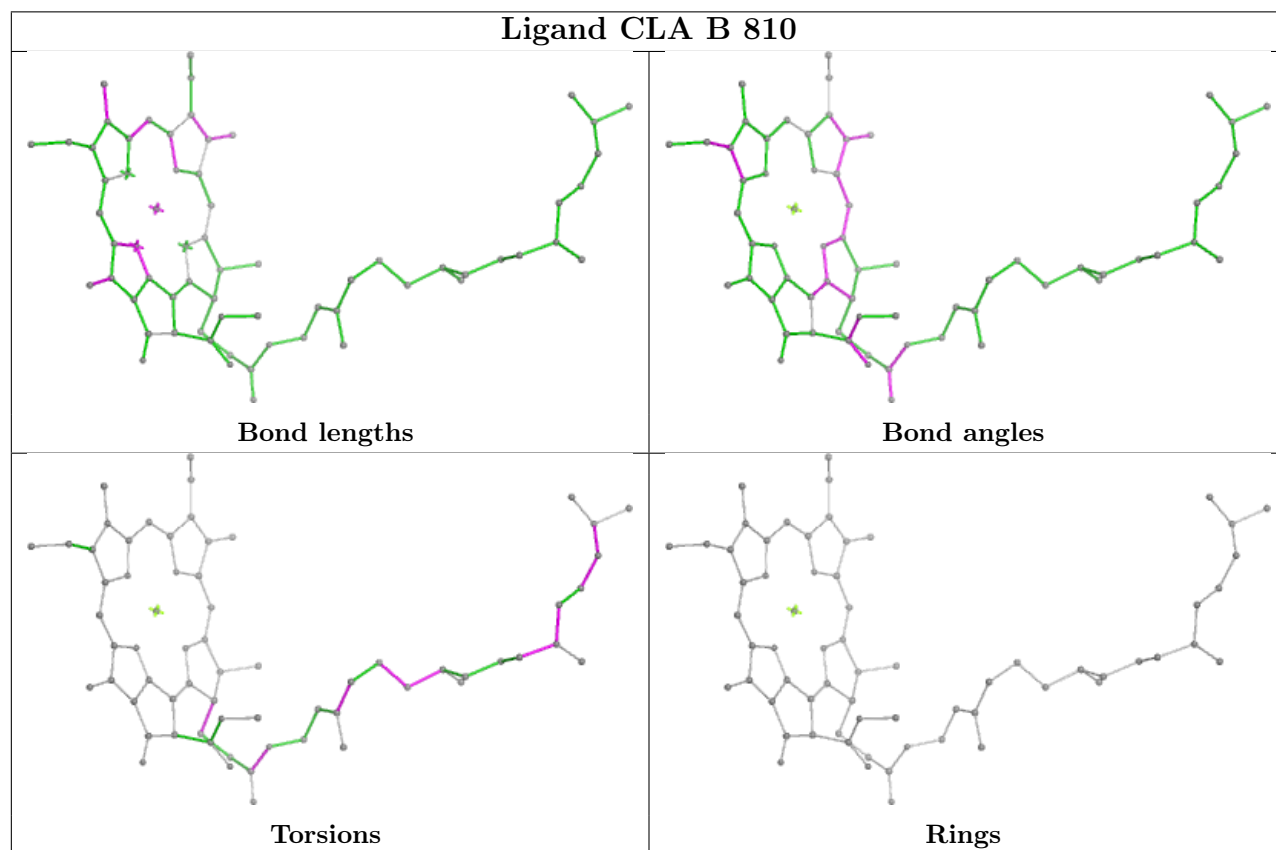


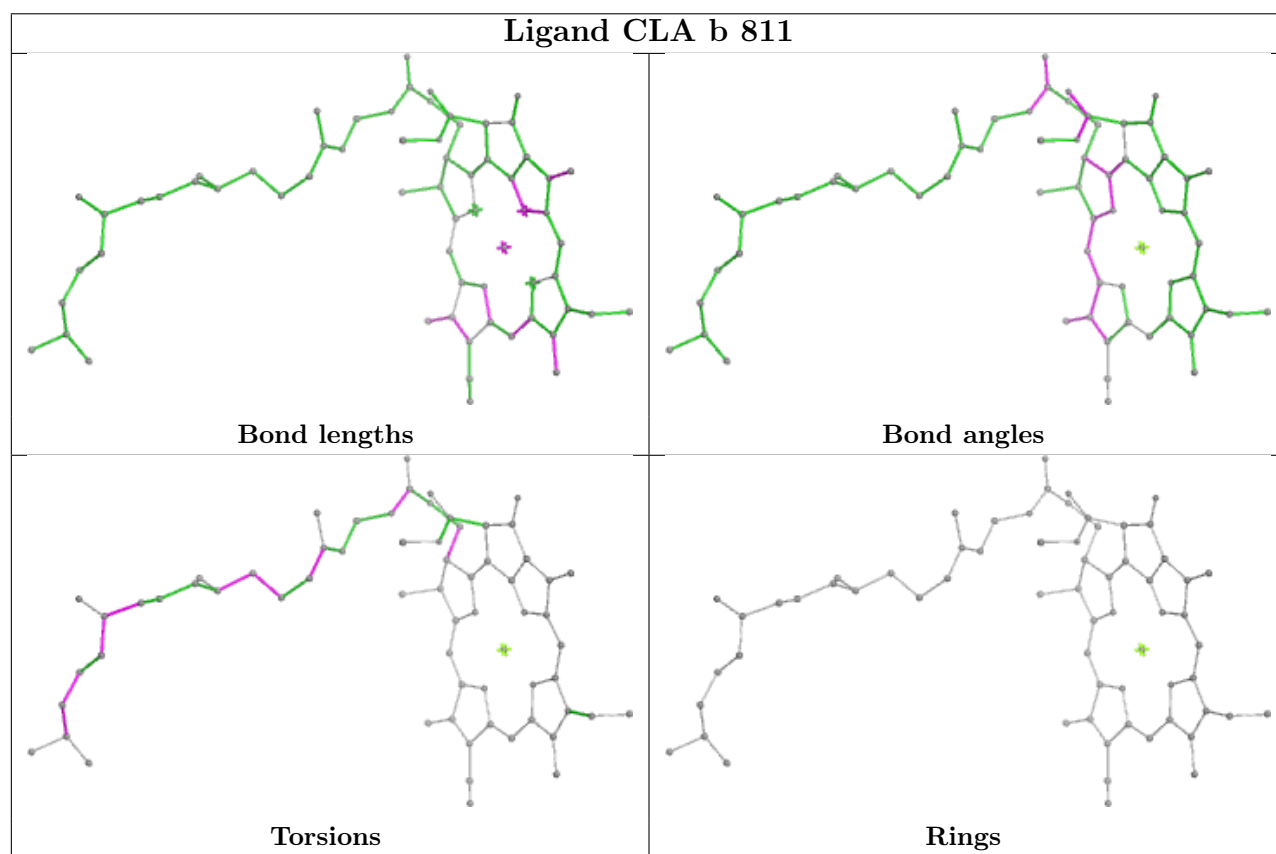
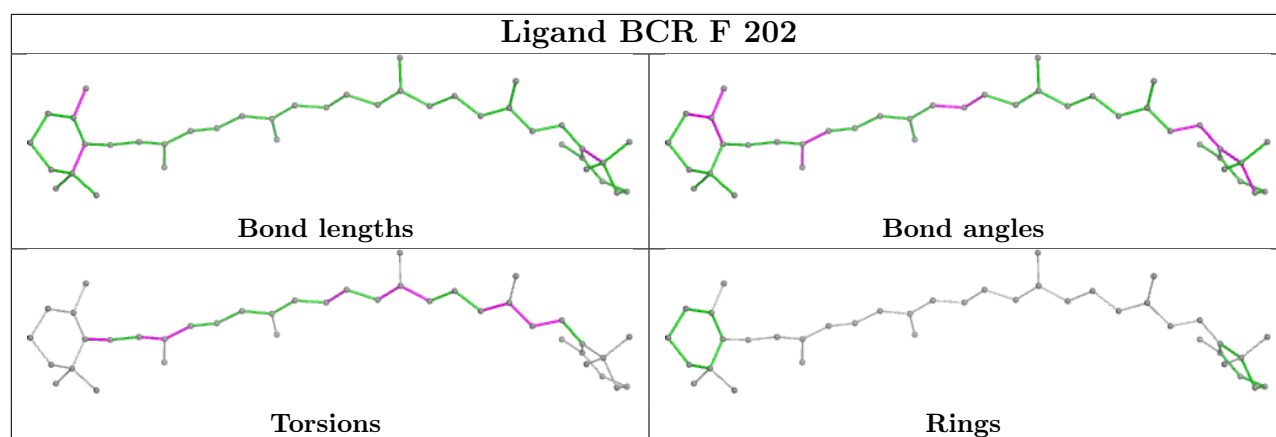
Rings

Ligand CLA K 103

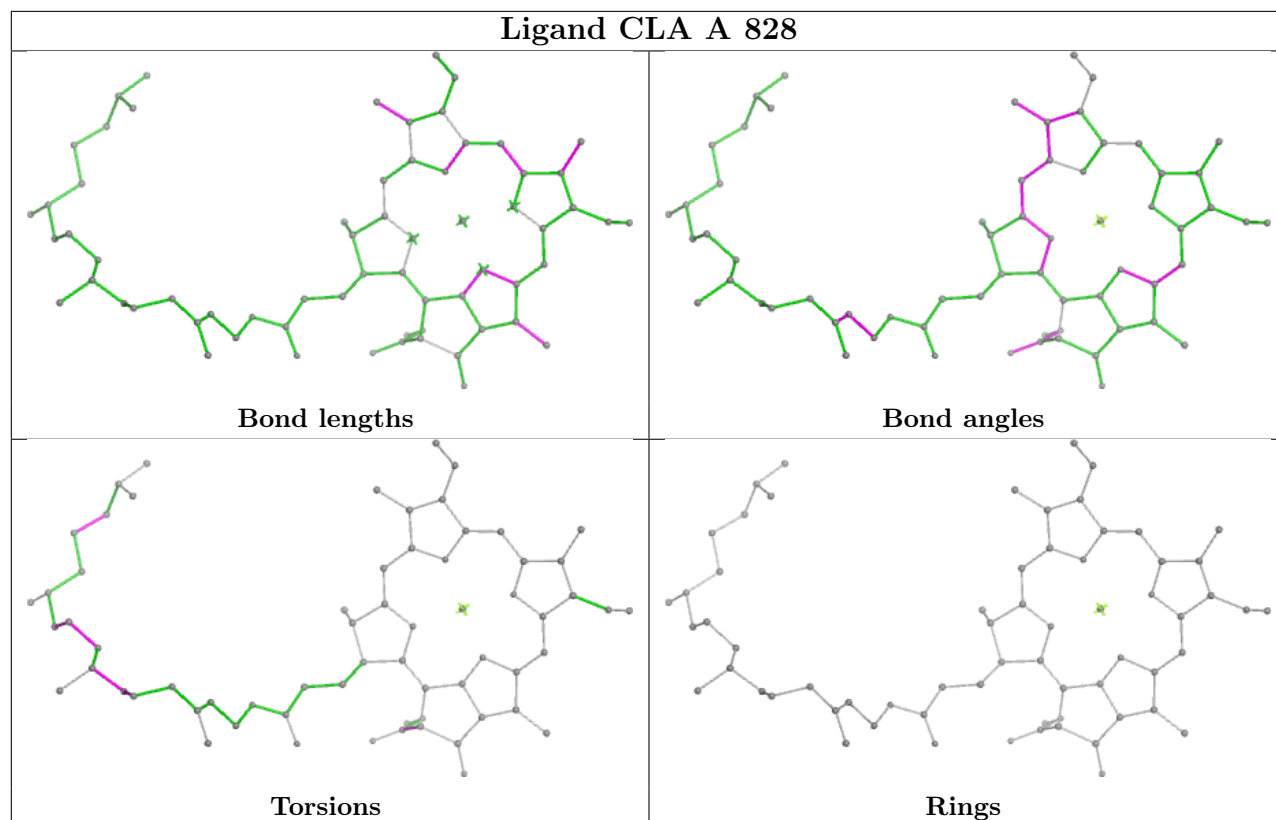


Ligand CLA B 810

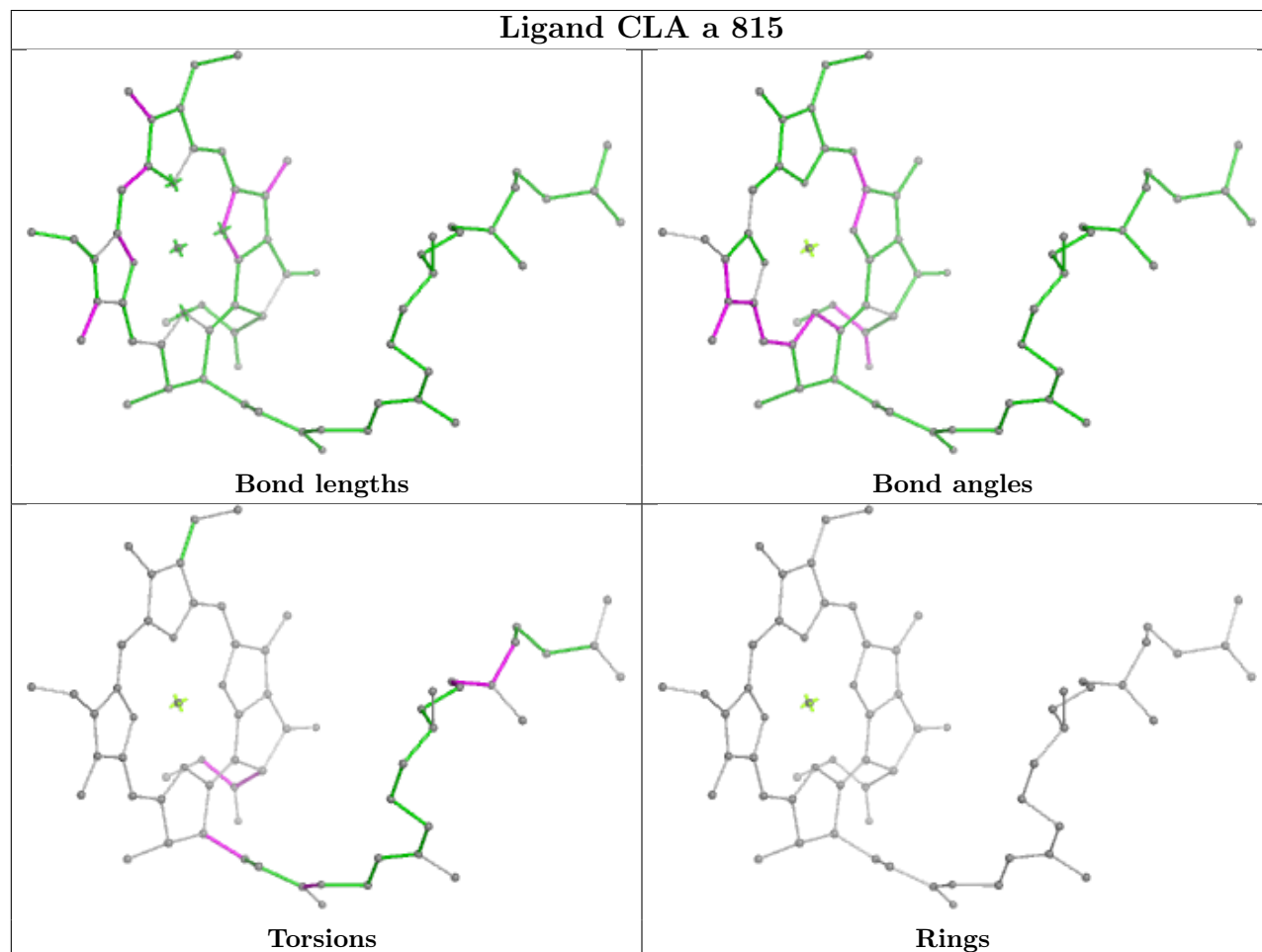




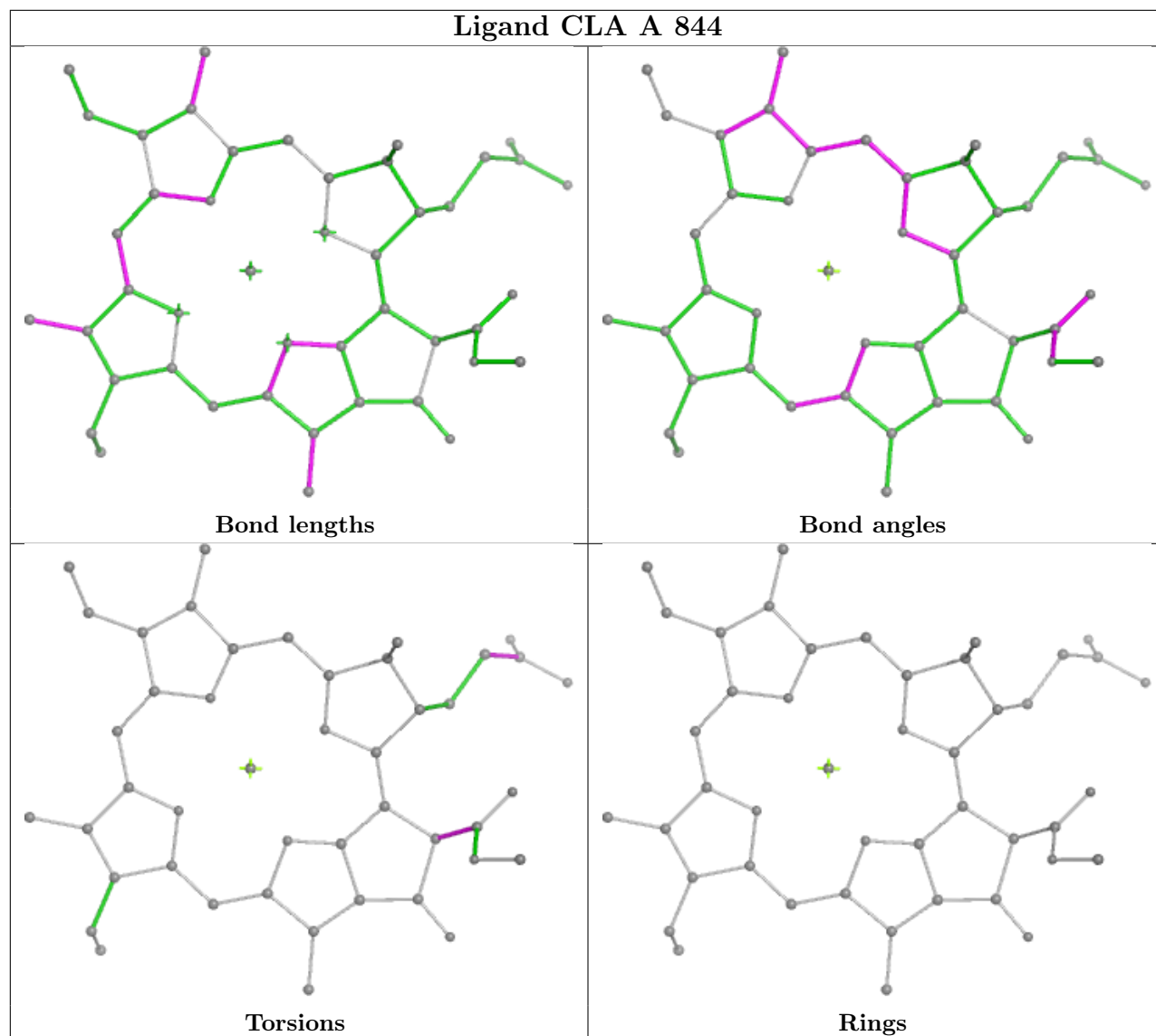
Ligand CLA A 828



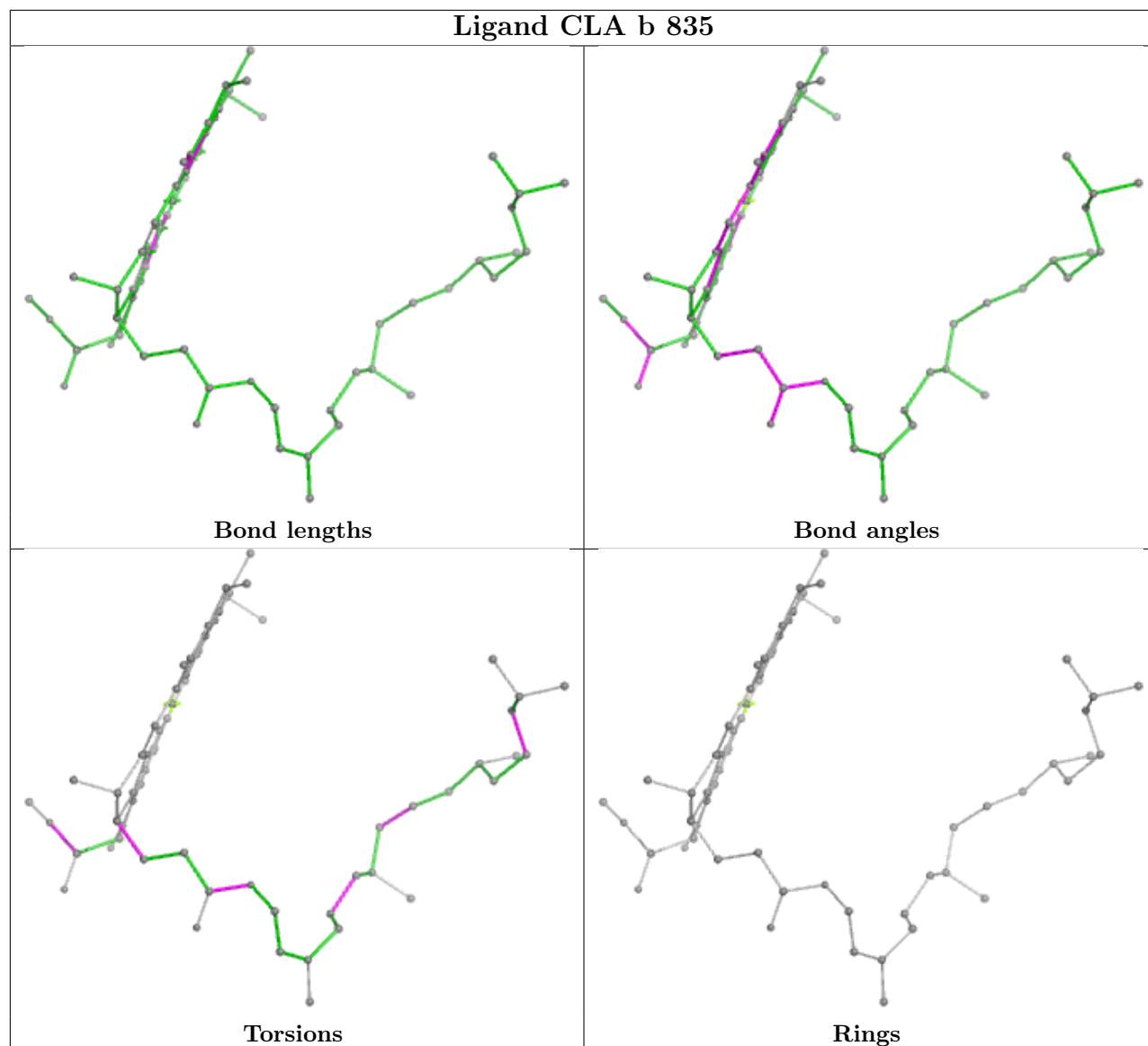
Ligand CLA a 815

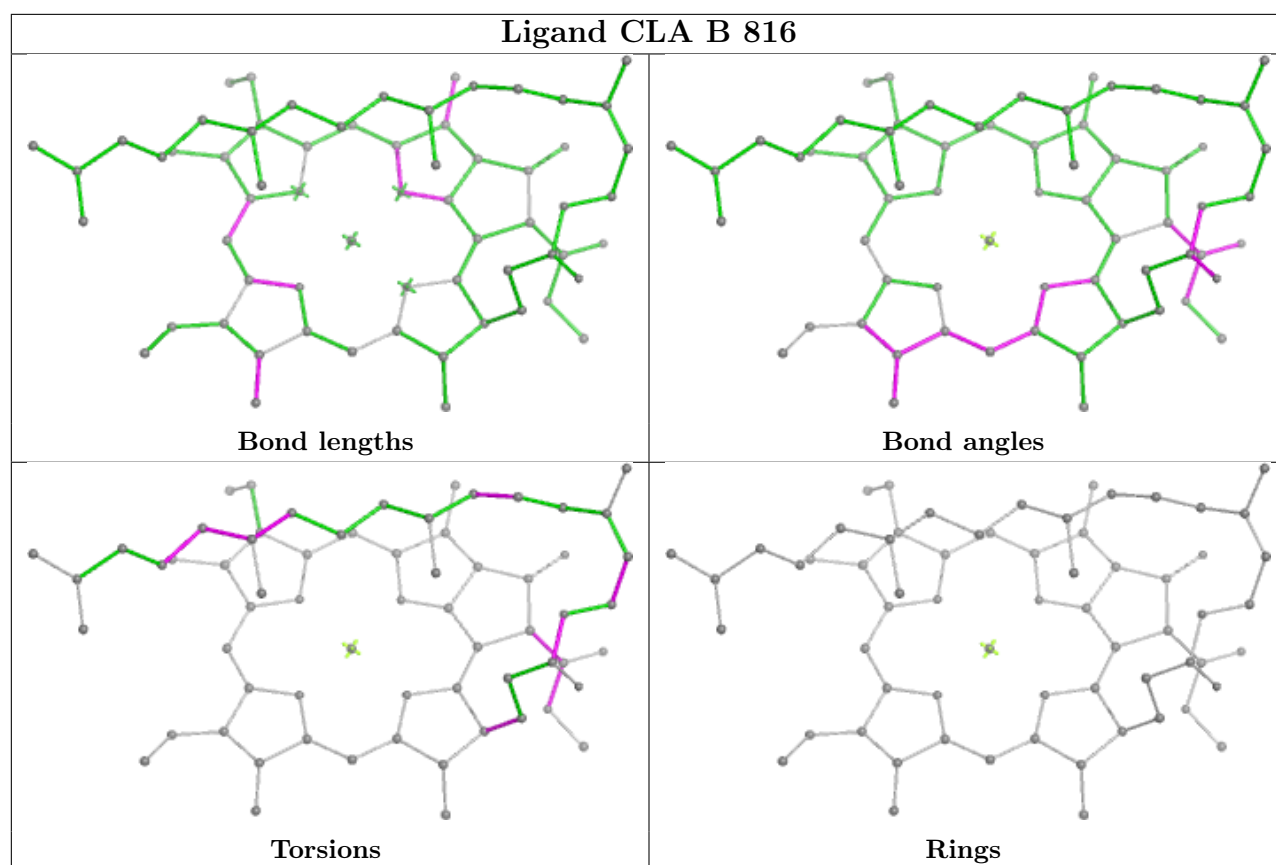


Ligand CLA A 844

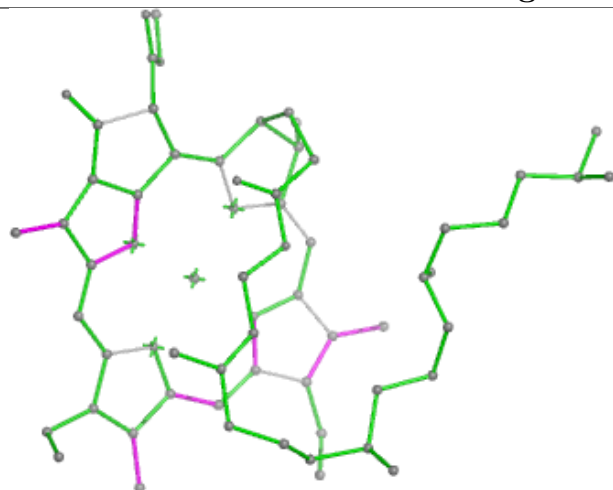


Ligand CLA b 835

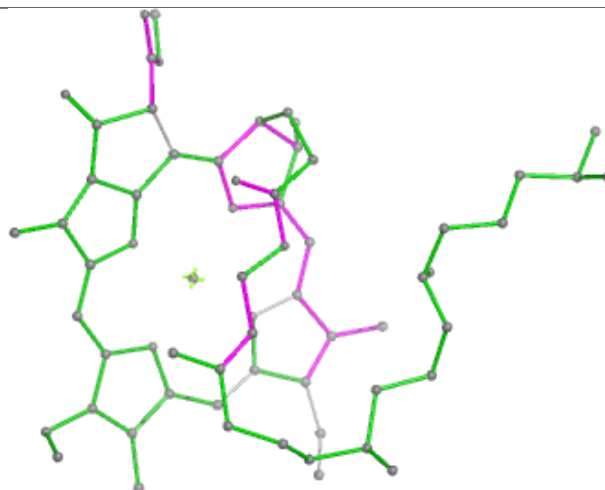




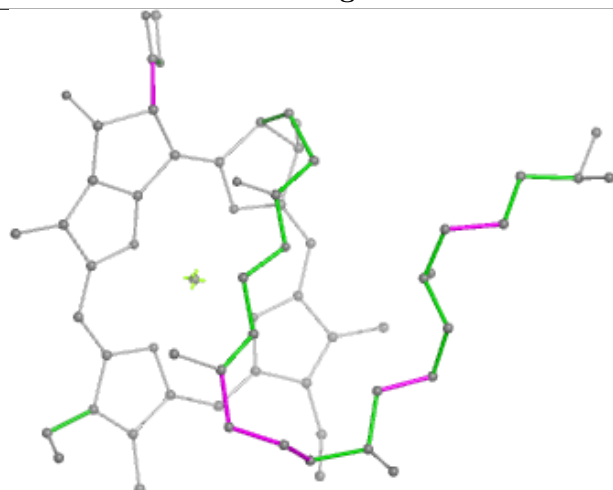
Ligand CLA 2 809



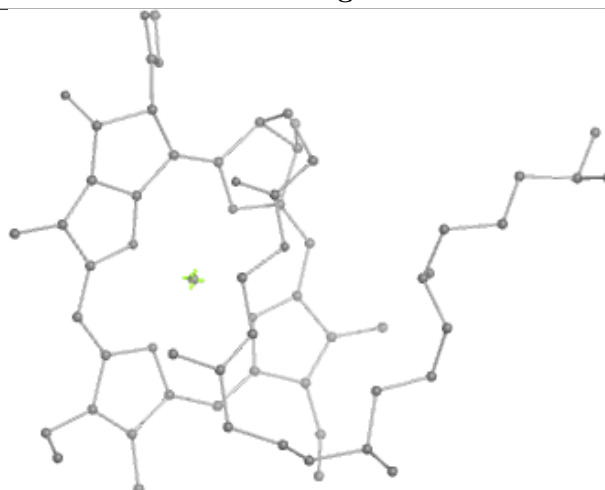
Bond lengths



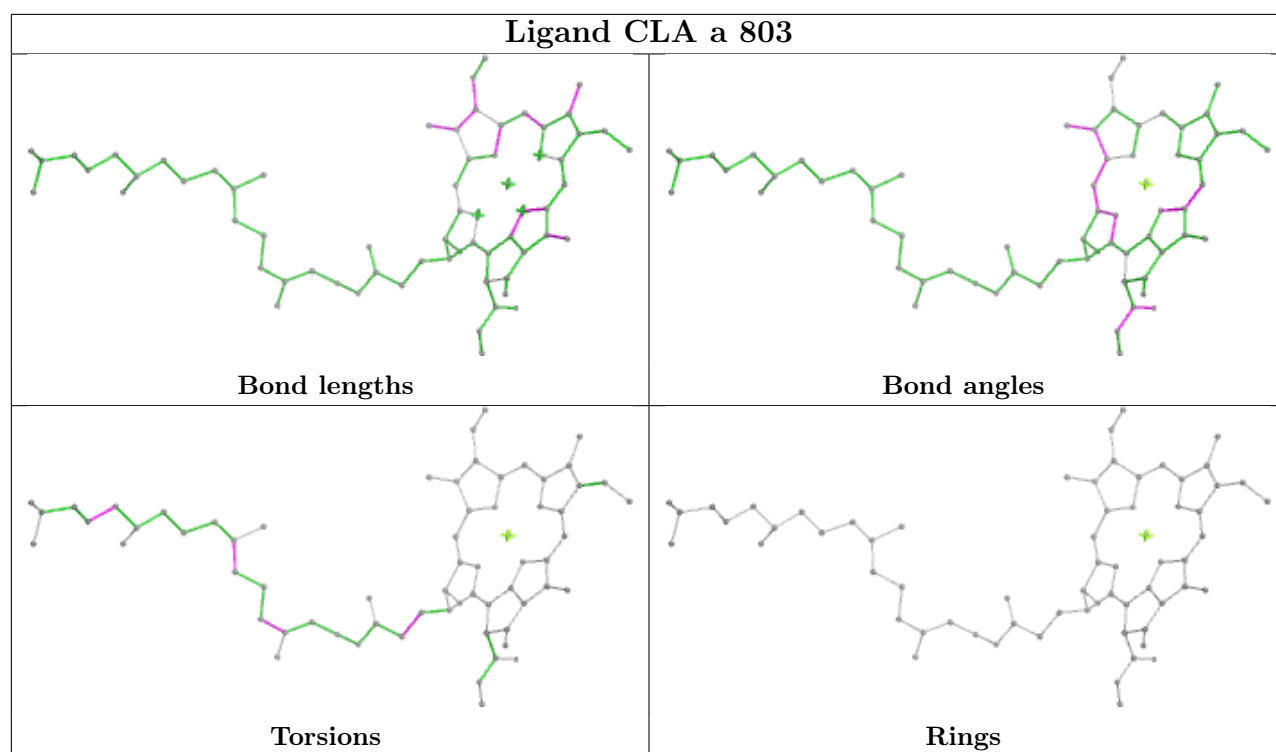
Bond angles



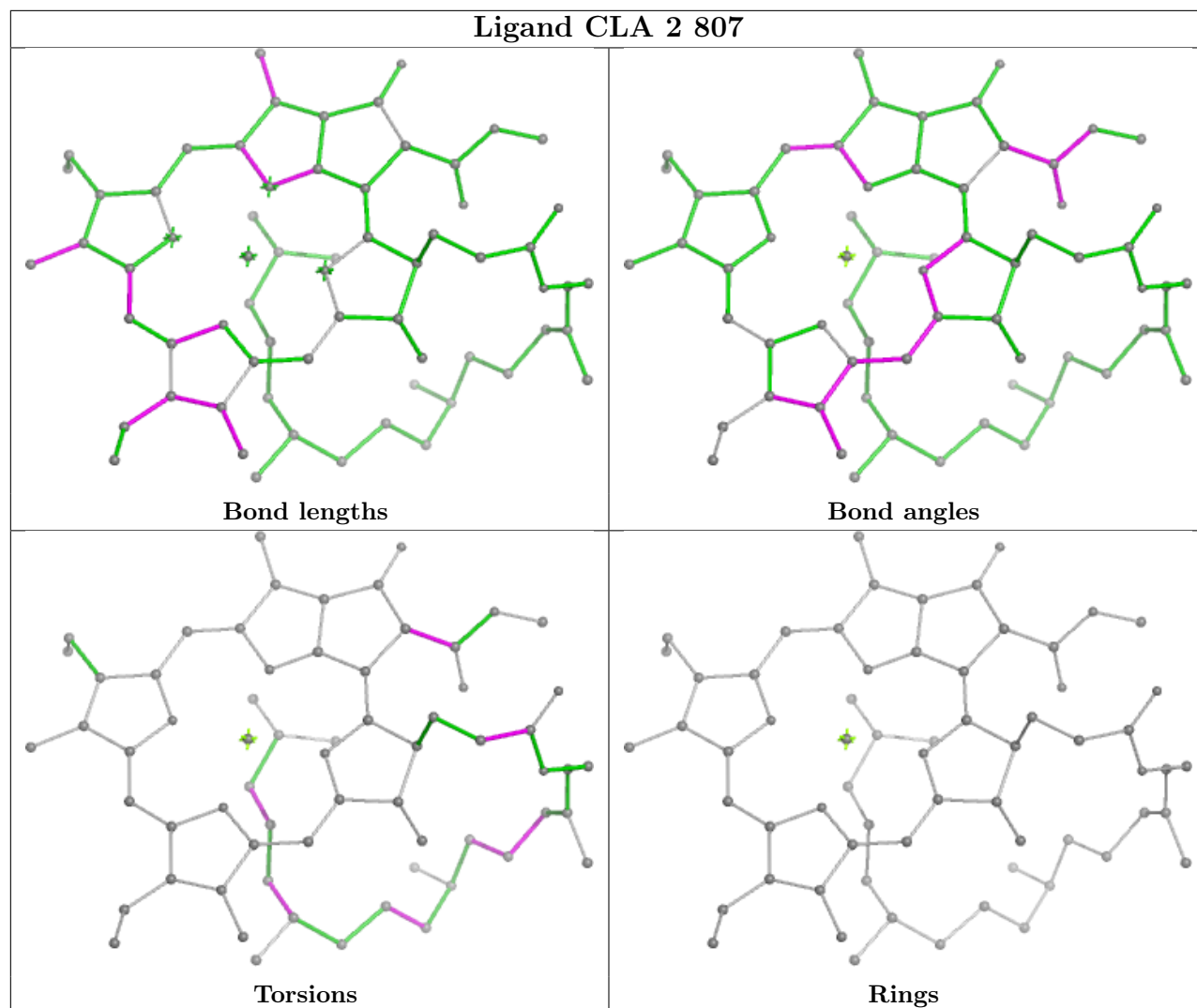
Torsions

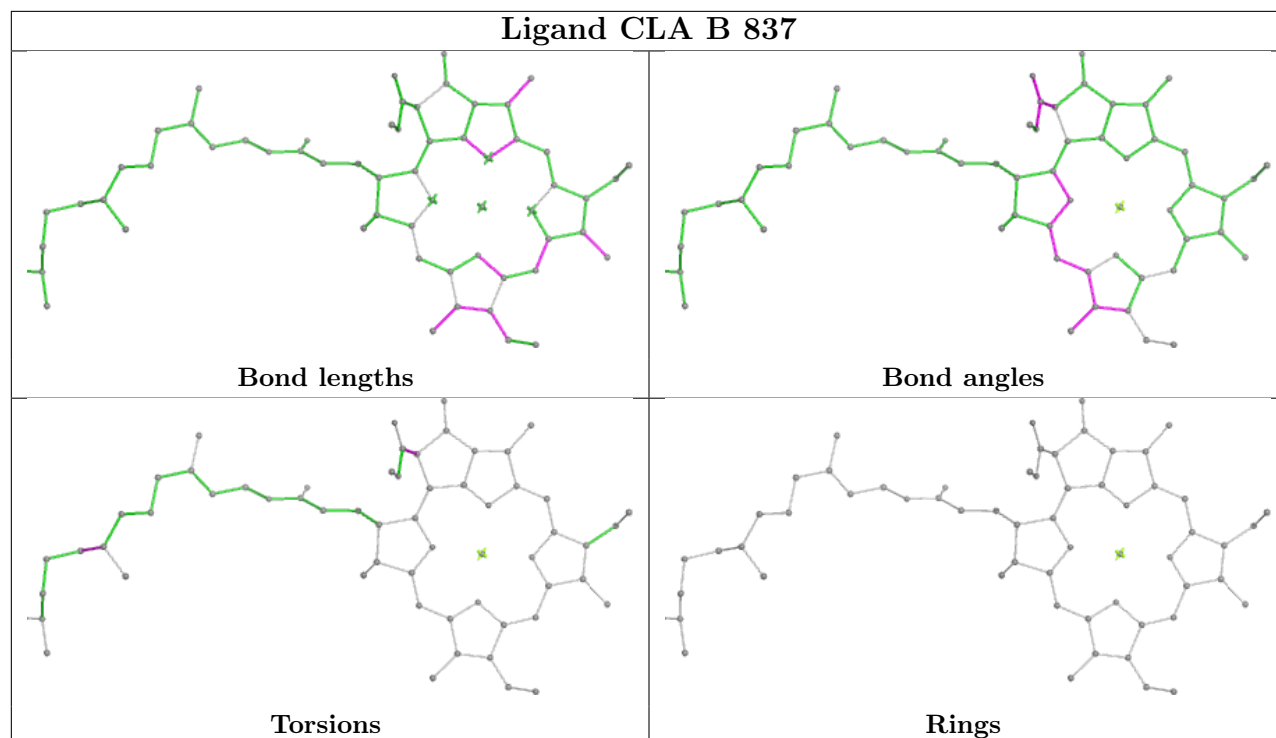
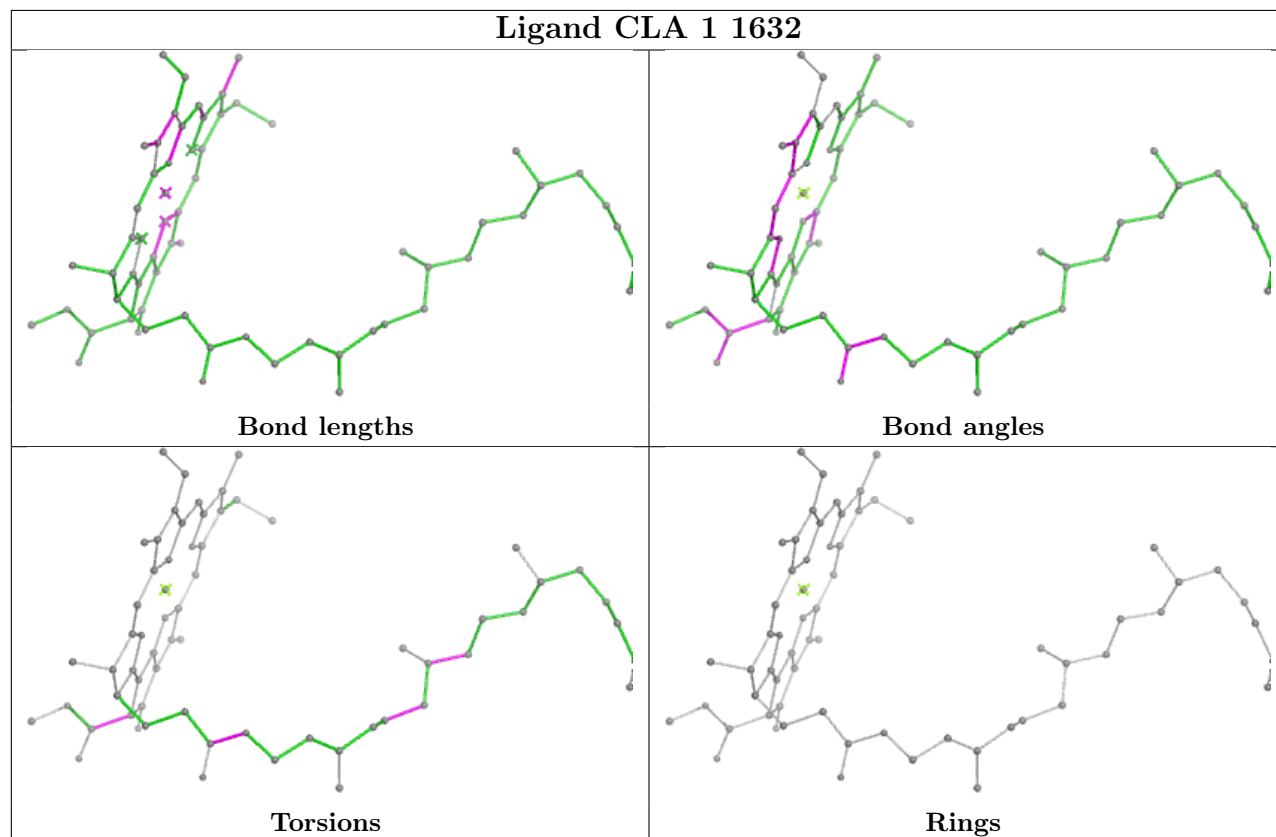


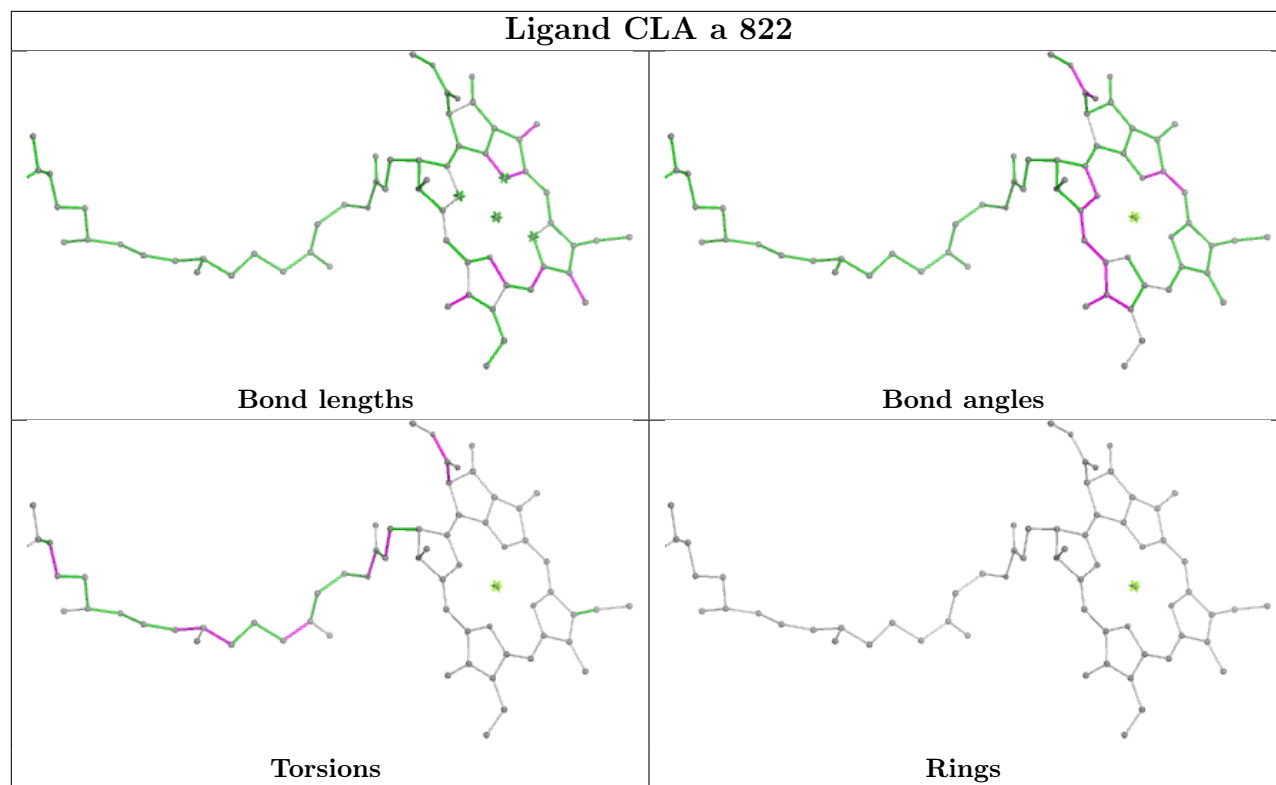
Rings



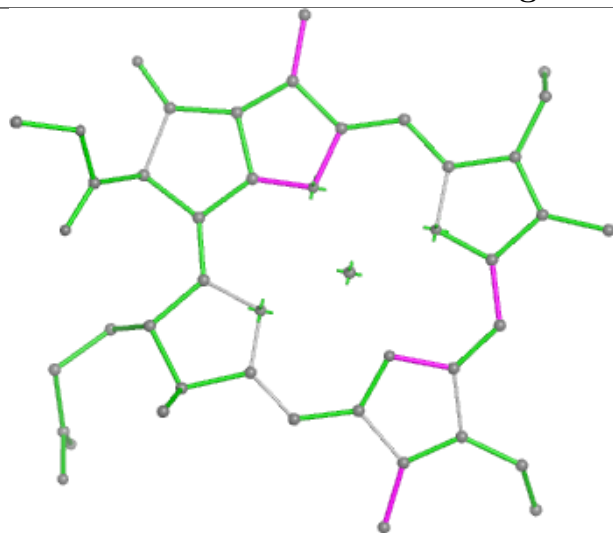
Ligand CLA 2 807



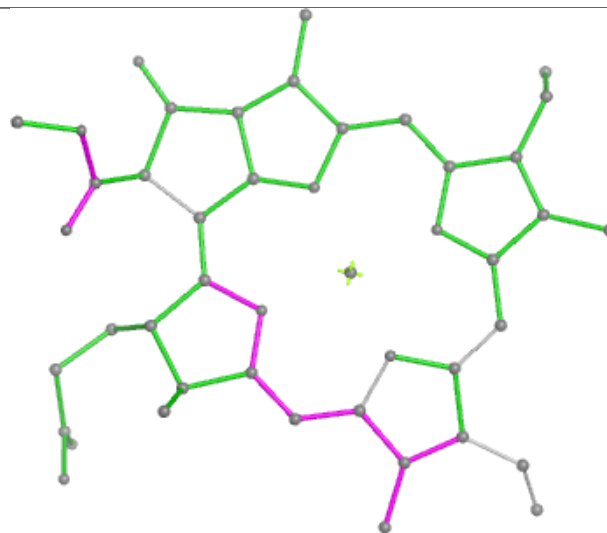
Ligand CLA B 837**Ligand CLA 1 1632**



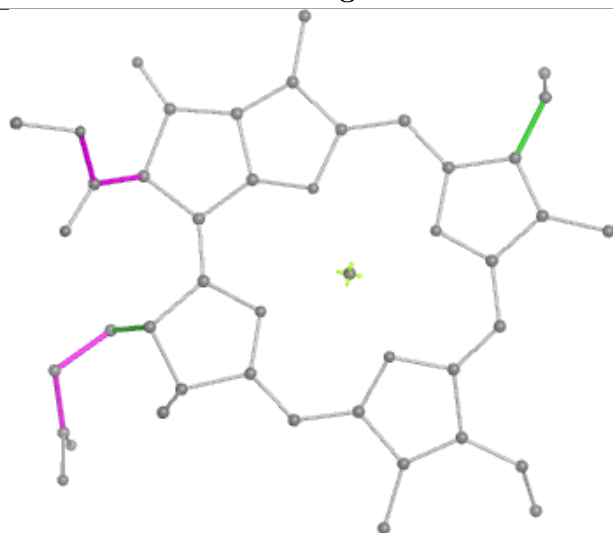
Ligand CLA z 102



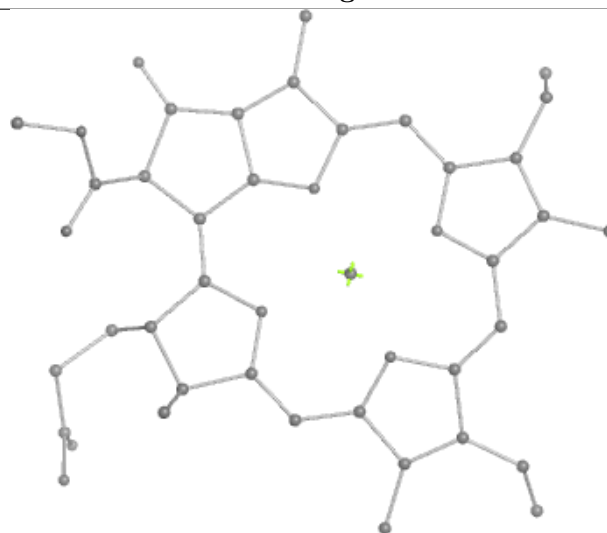
Bond lengths



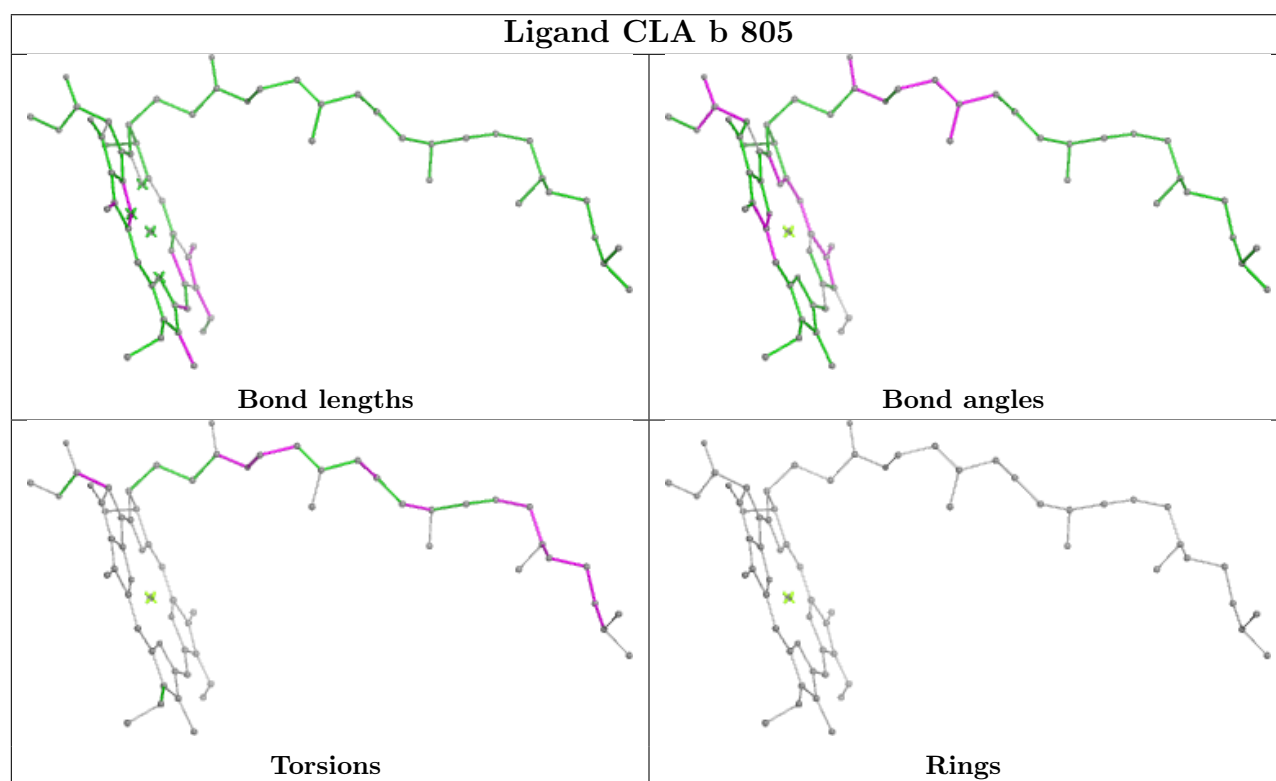
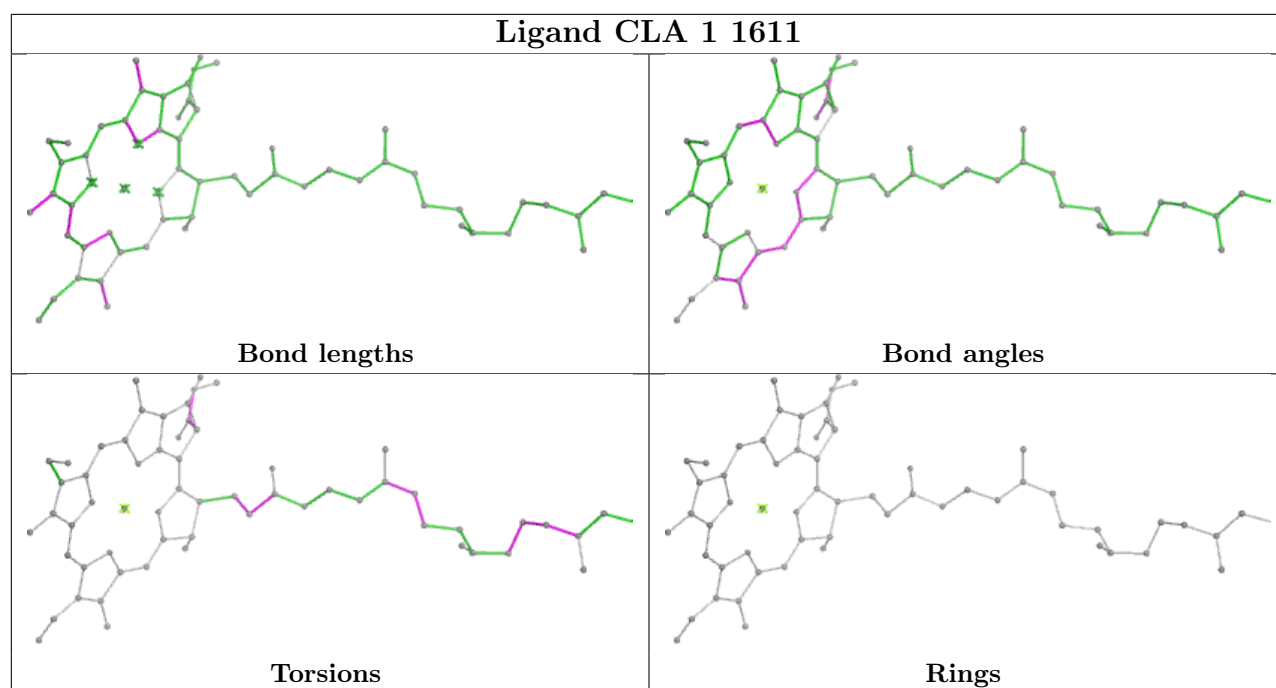
Bond angles

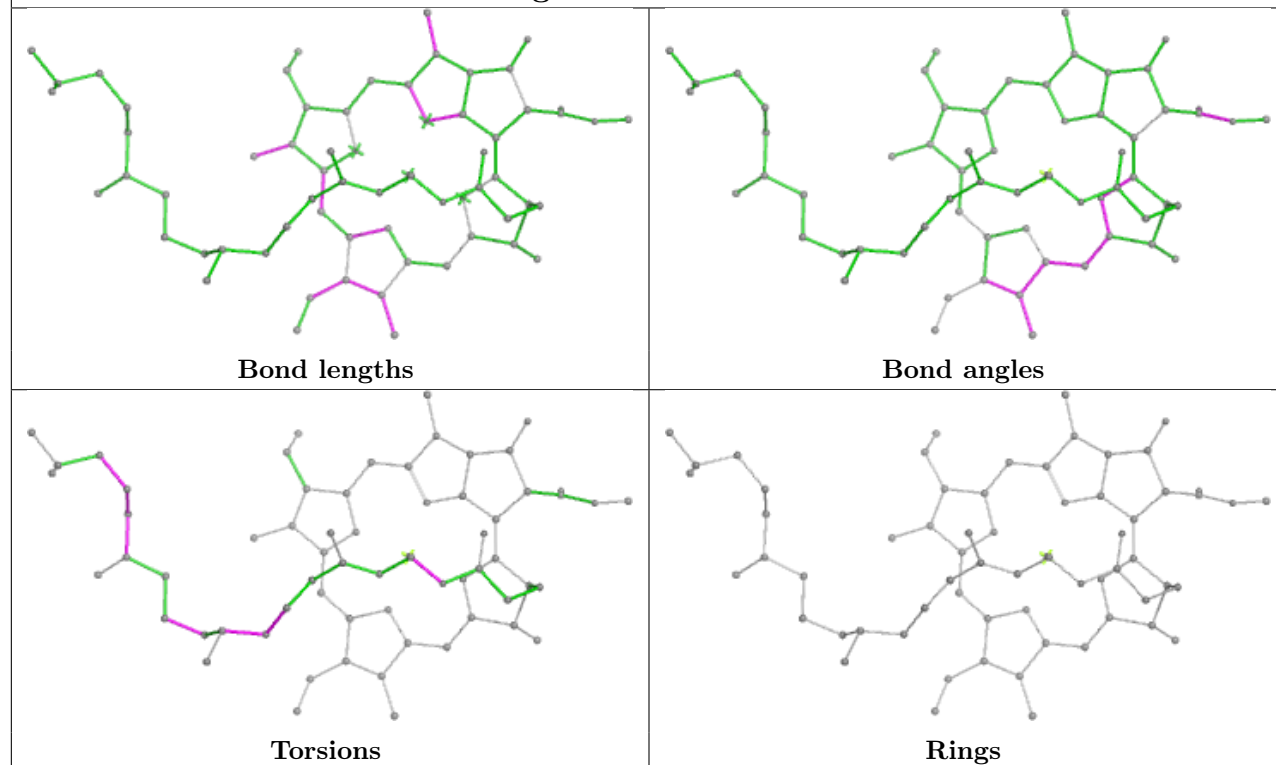
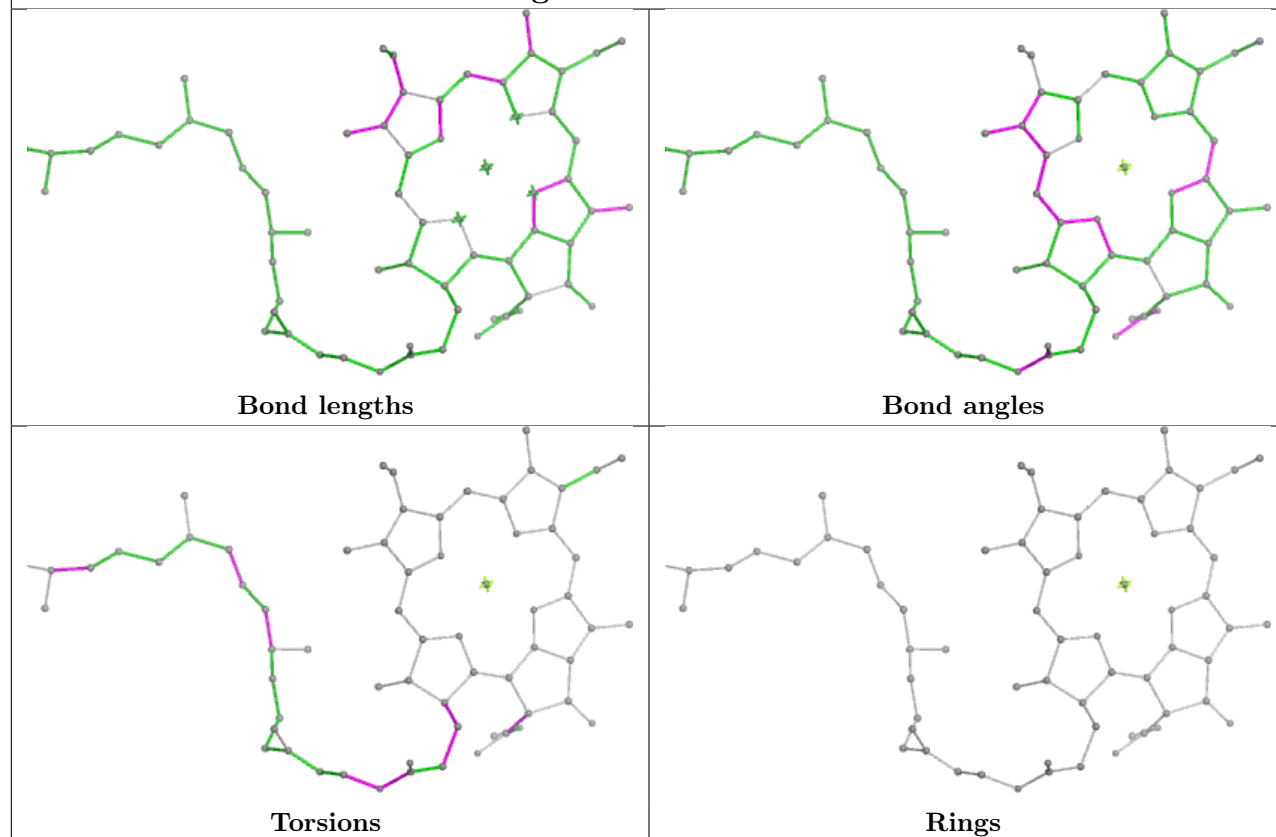


Torsions

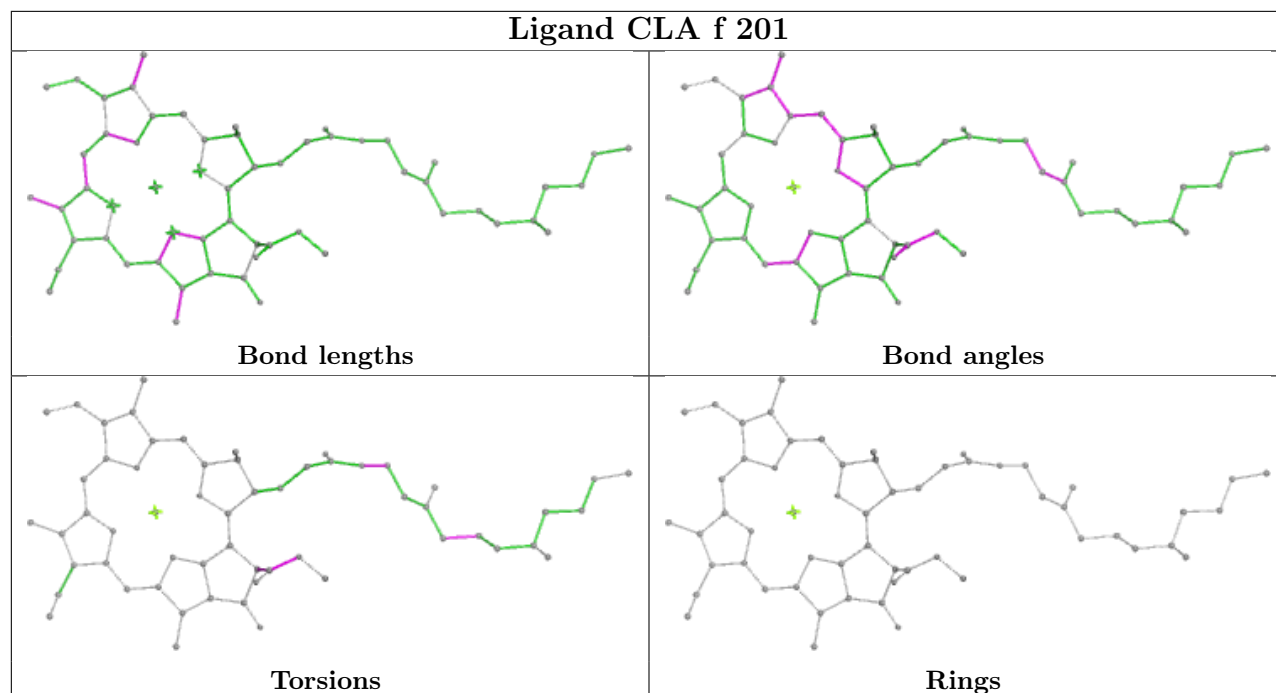


Rings

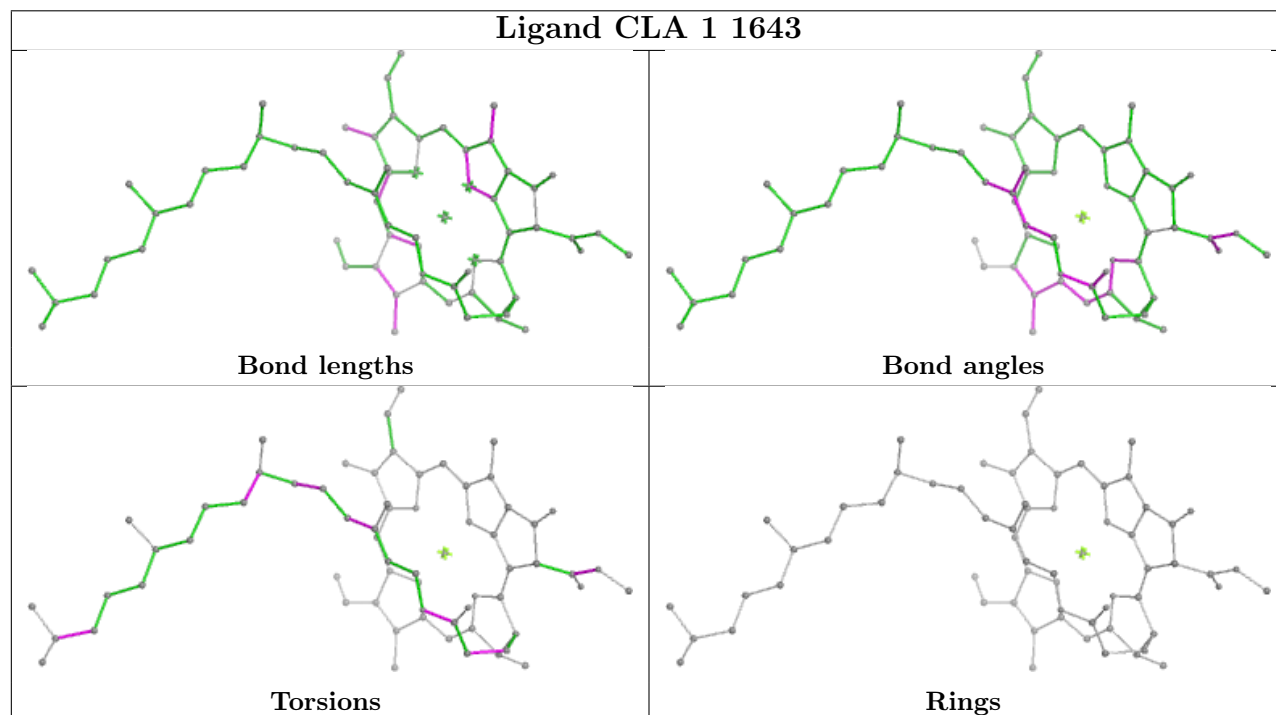


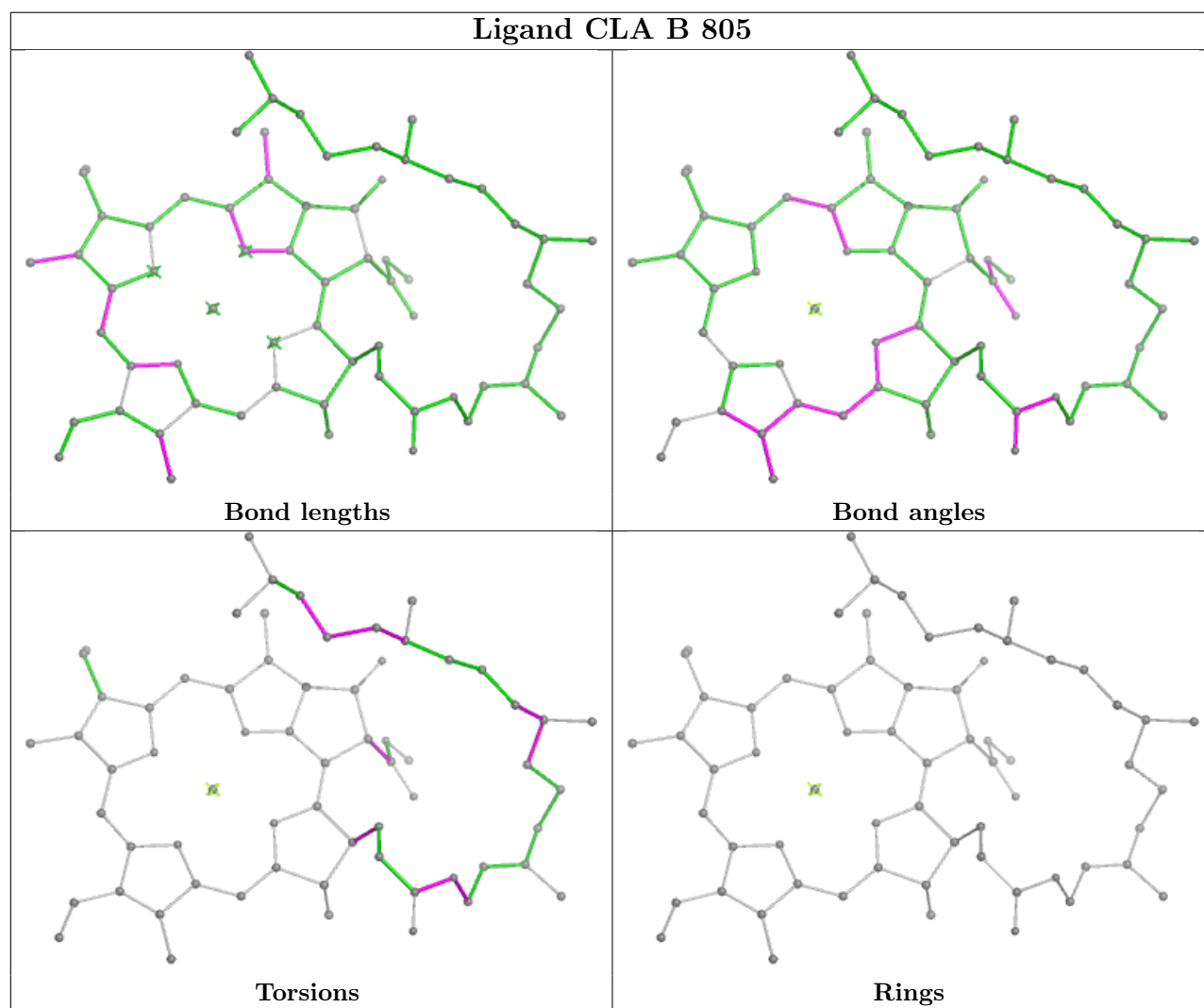
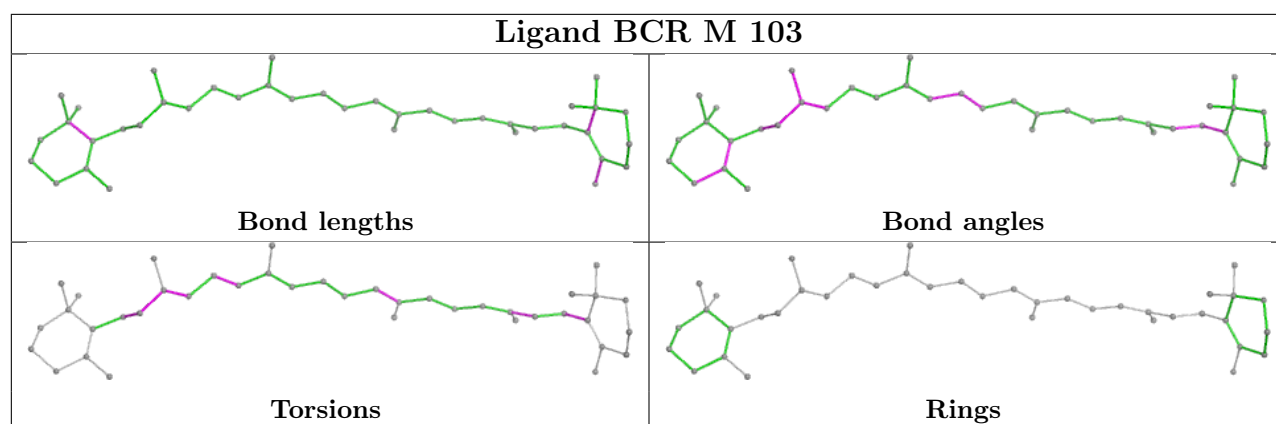
Ligand CLA B 838**Ligand CLA A 814**

Ligand CLA f 201

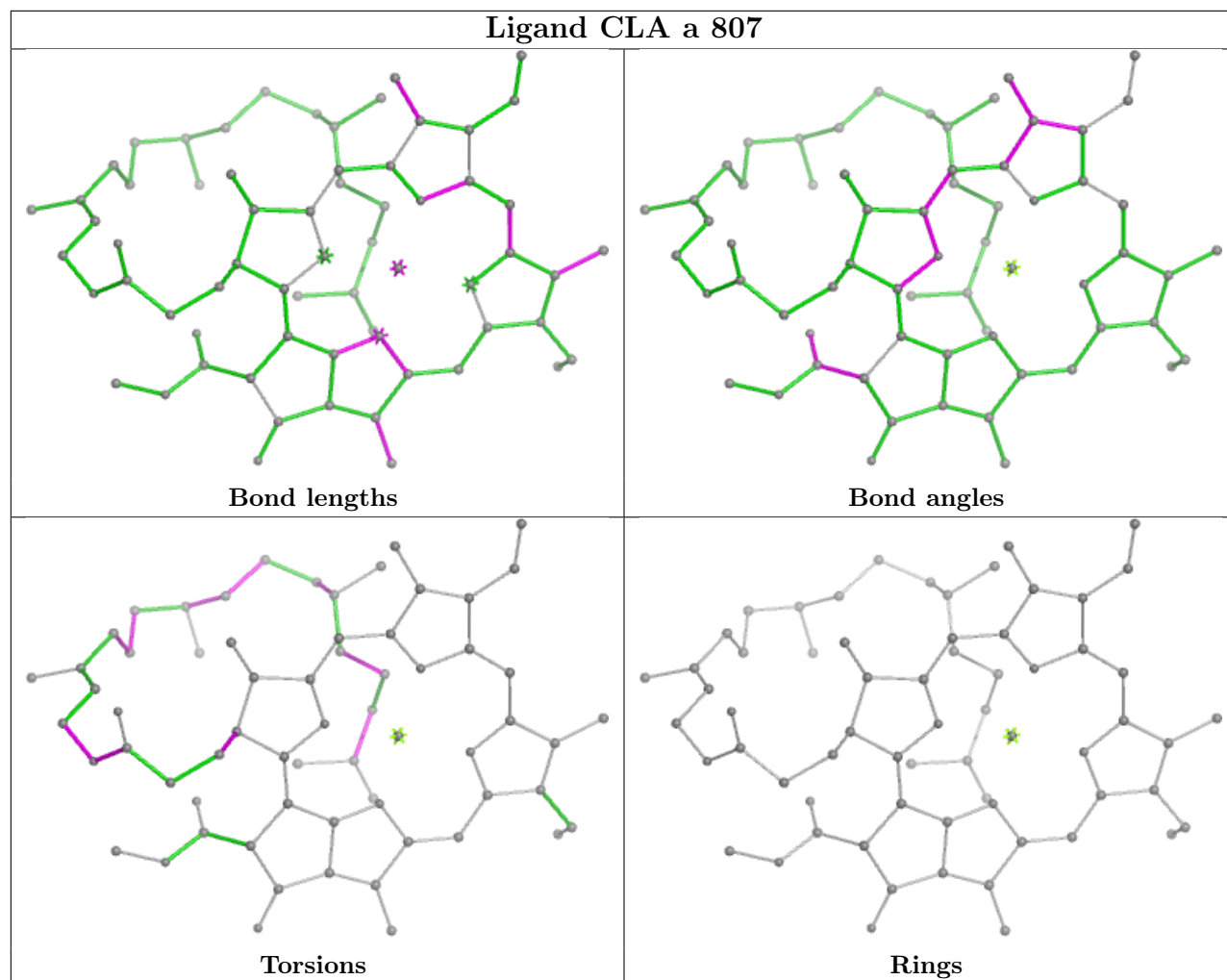


Ligand CLA 1 1643

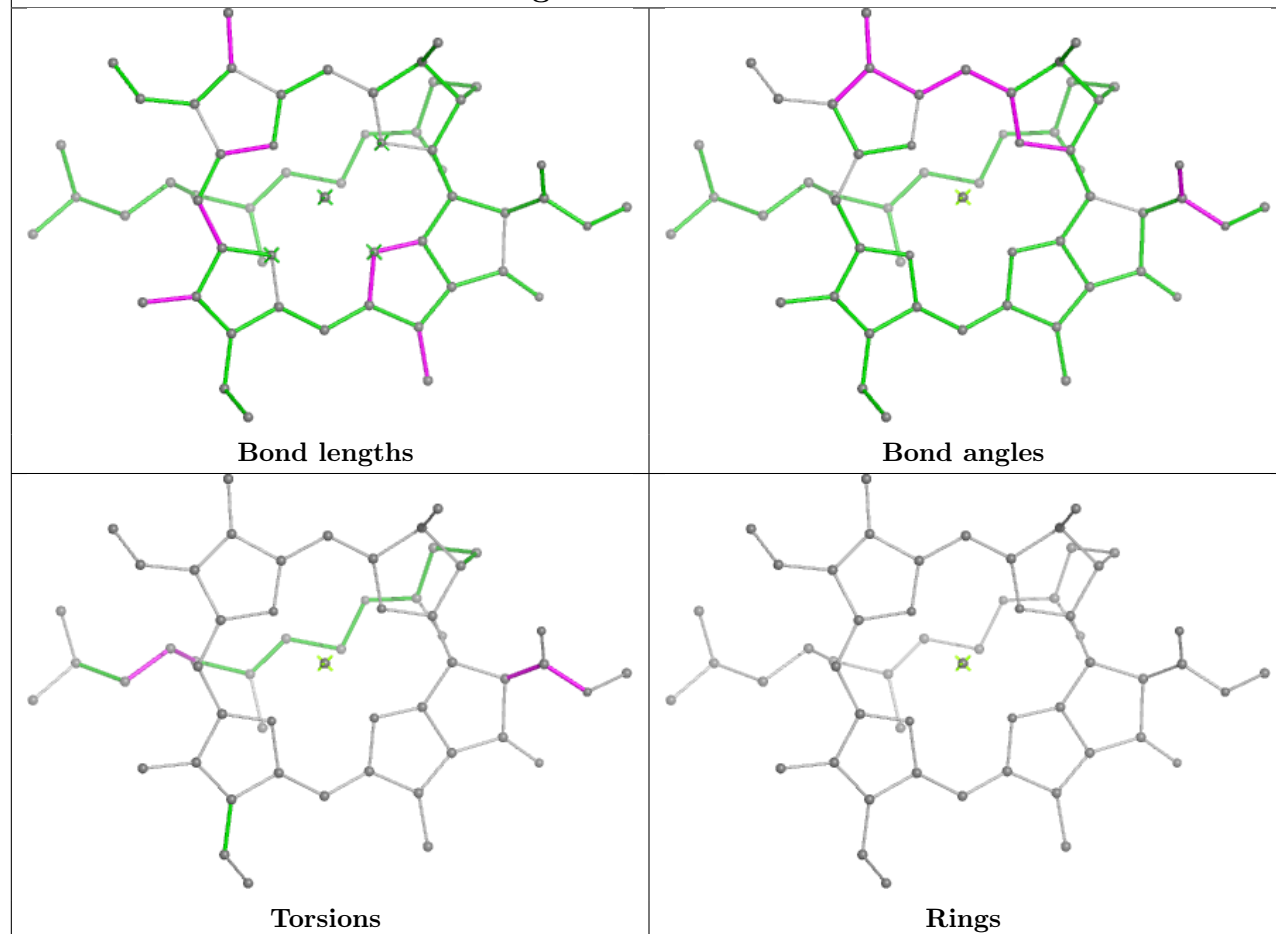




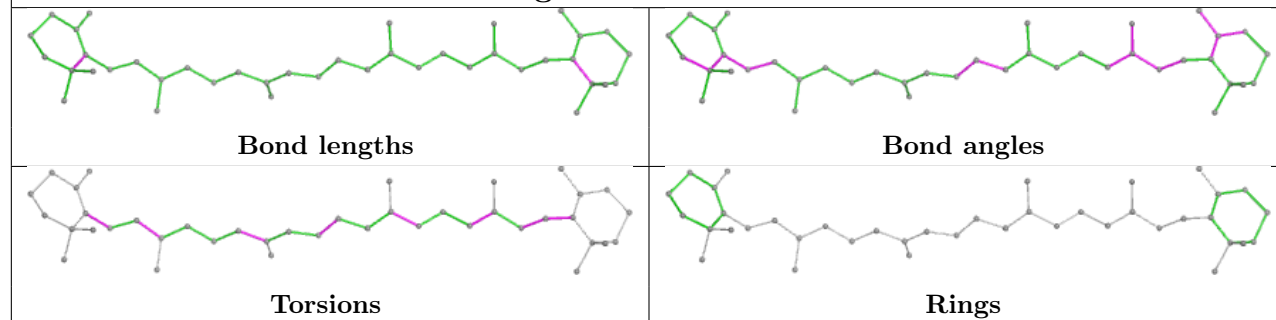
Ligand CLA a 807

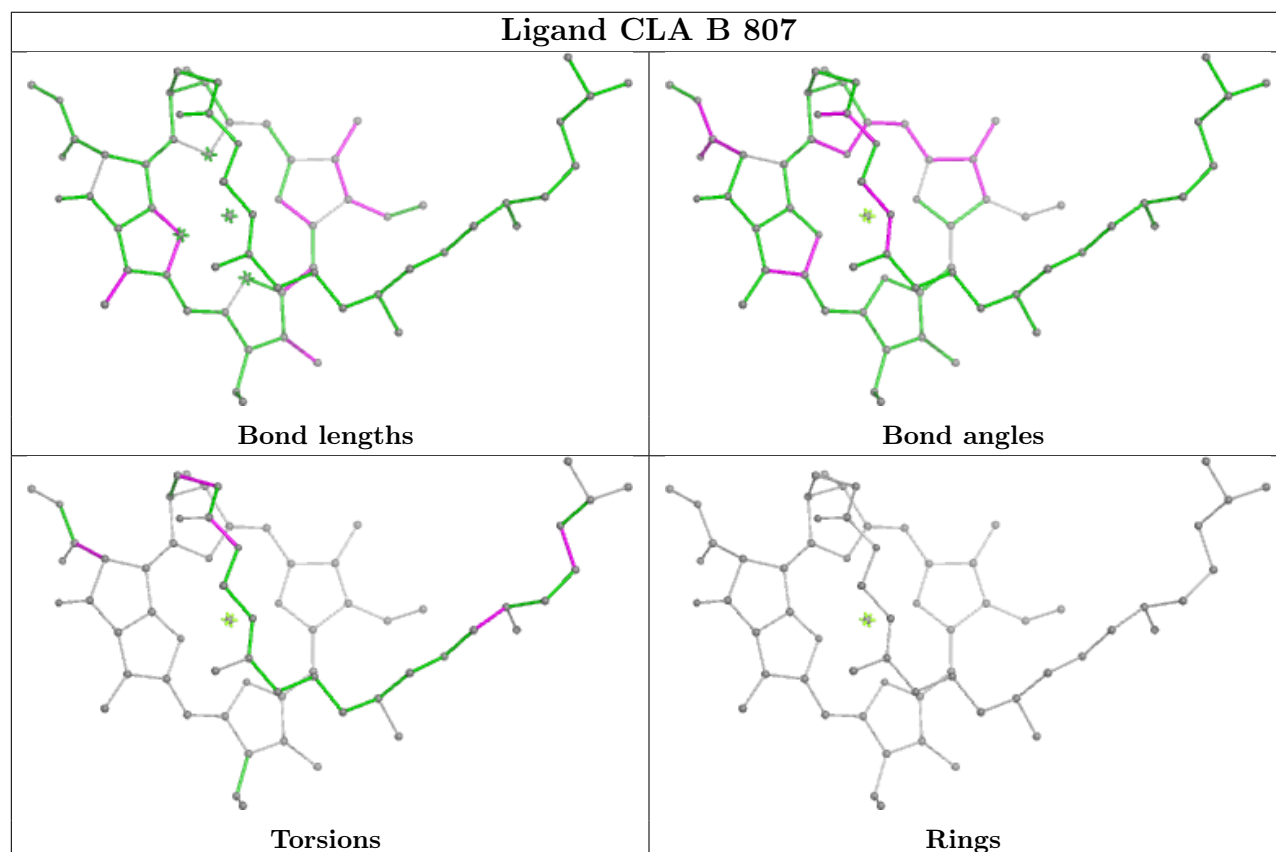
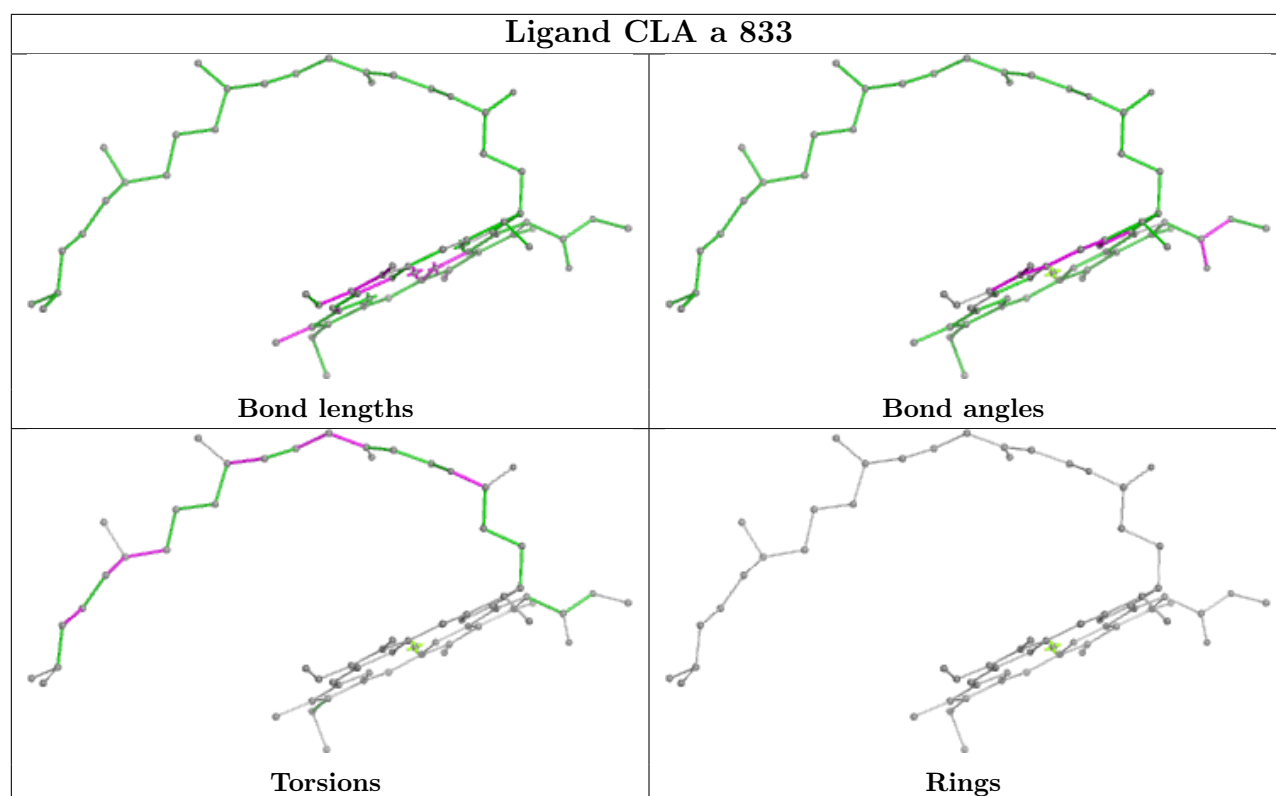


Ligand CLA B 822

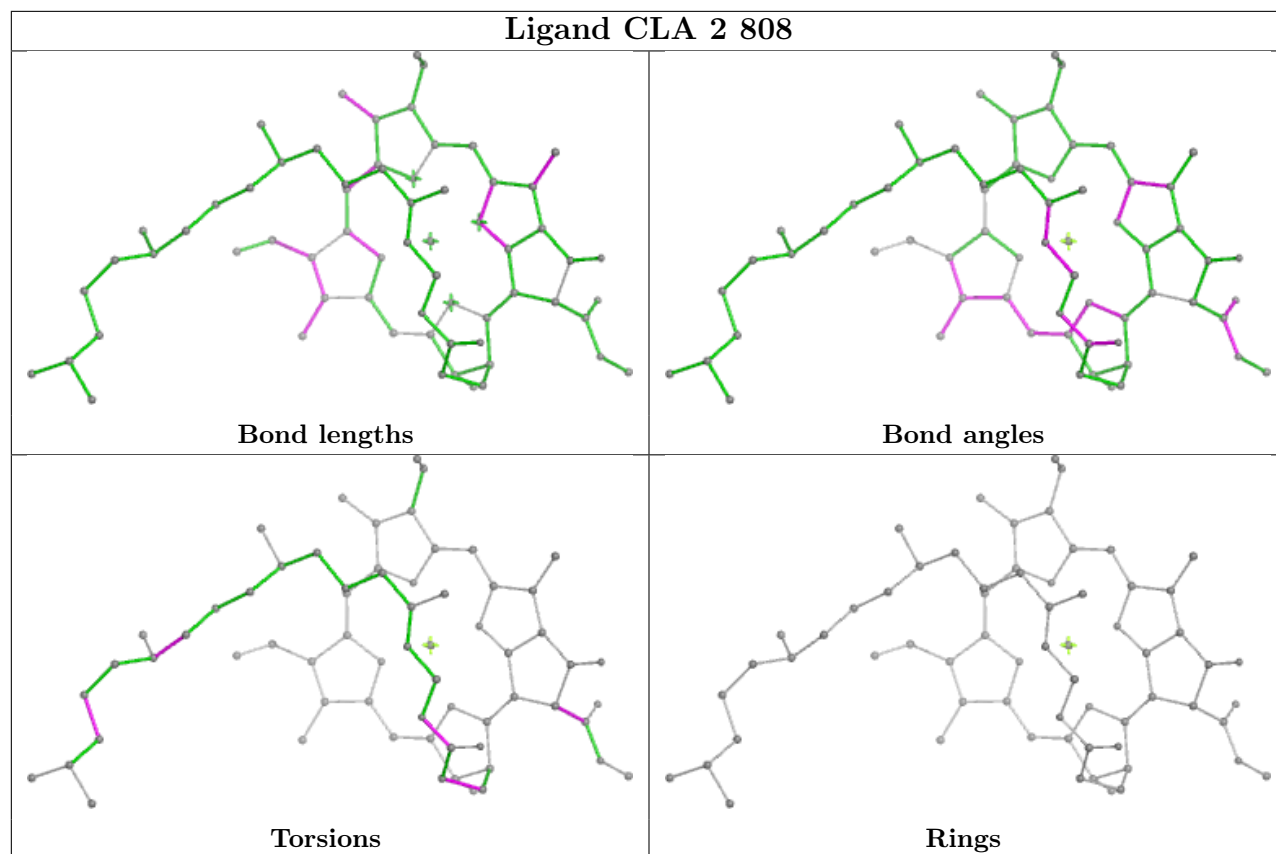


Ligand BCR a 847

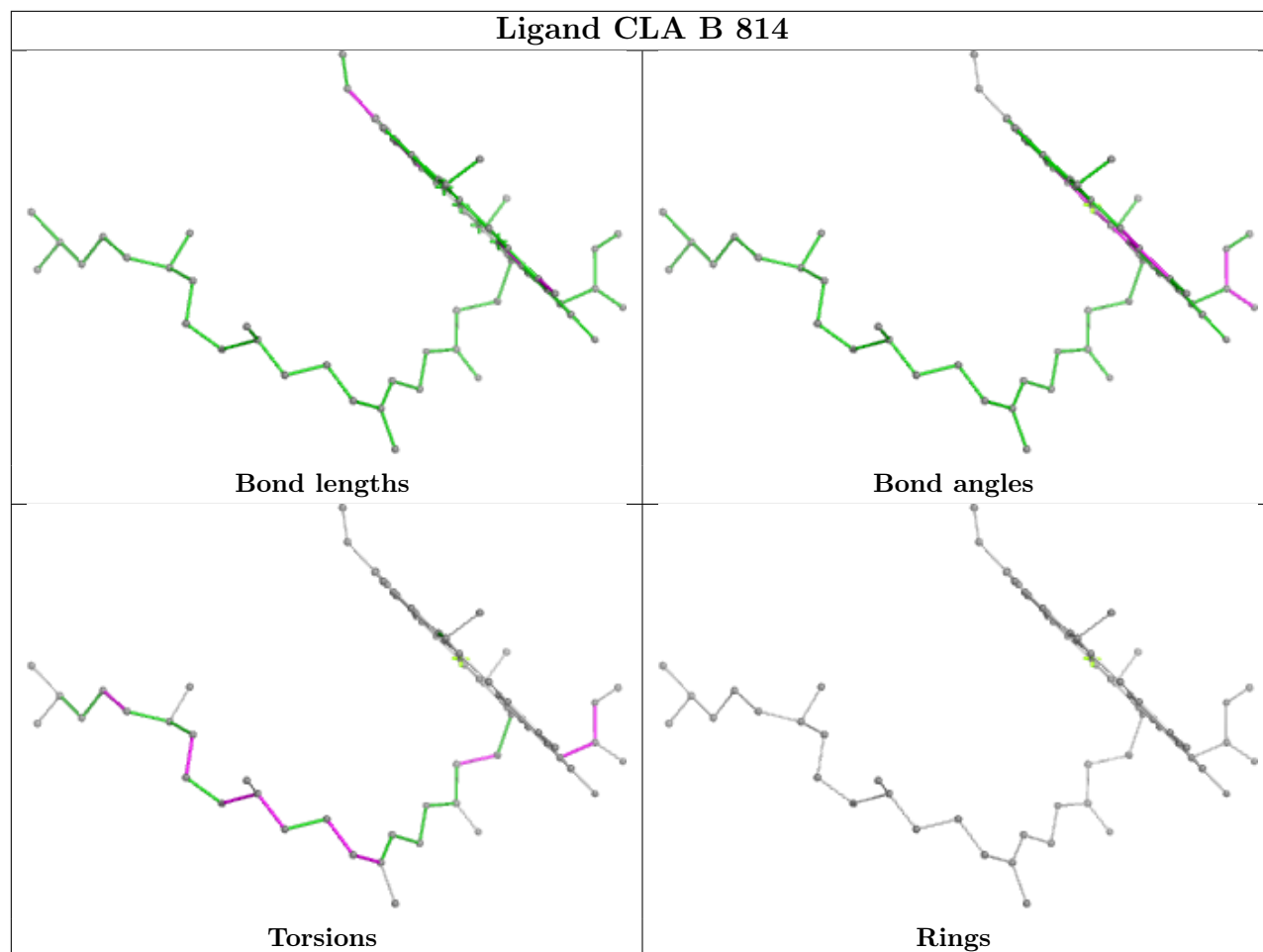




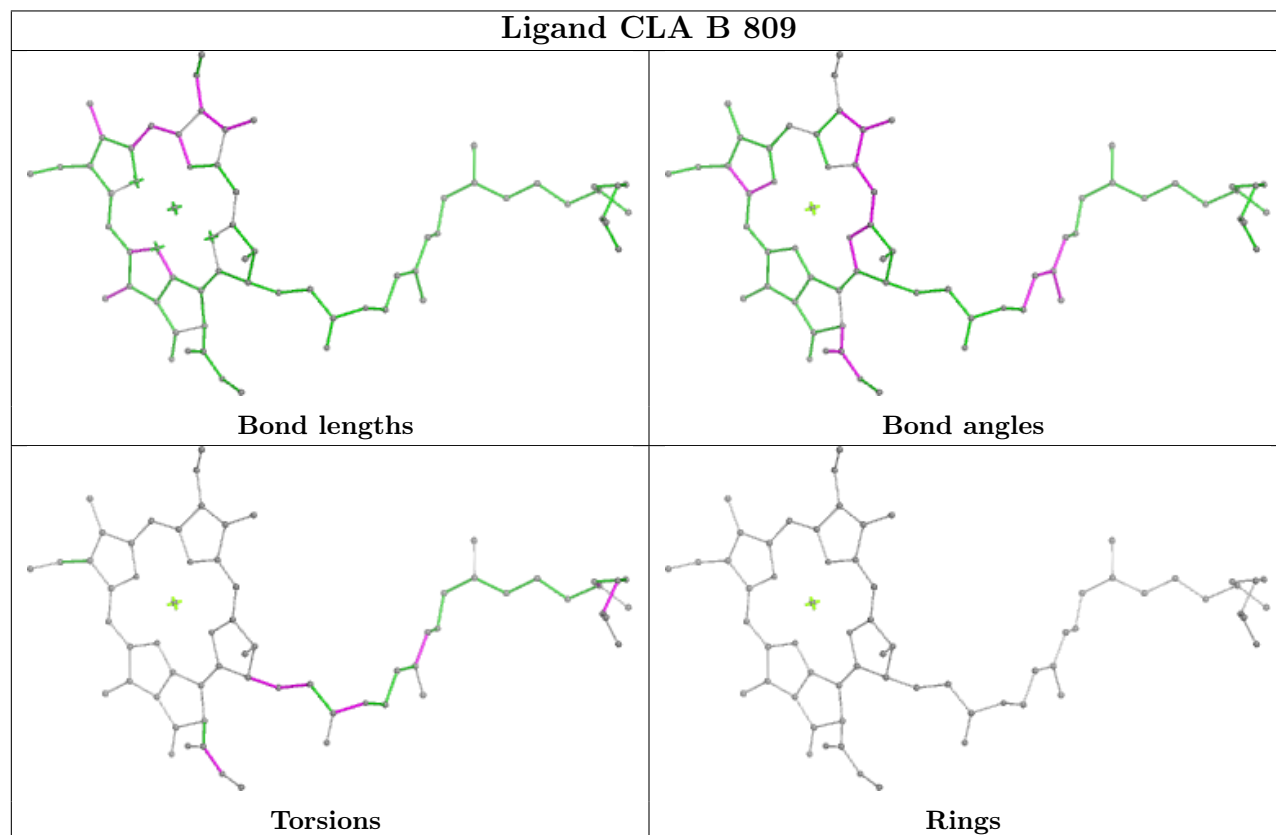
Ligand CLA 2 808

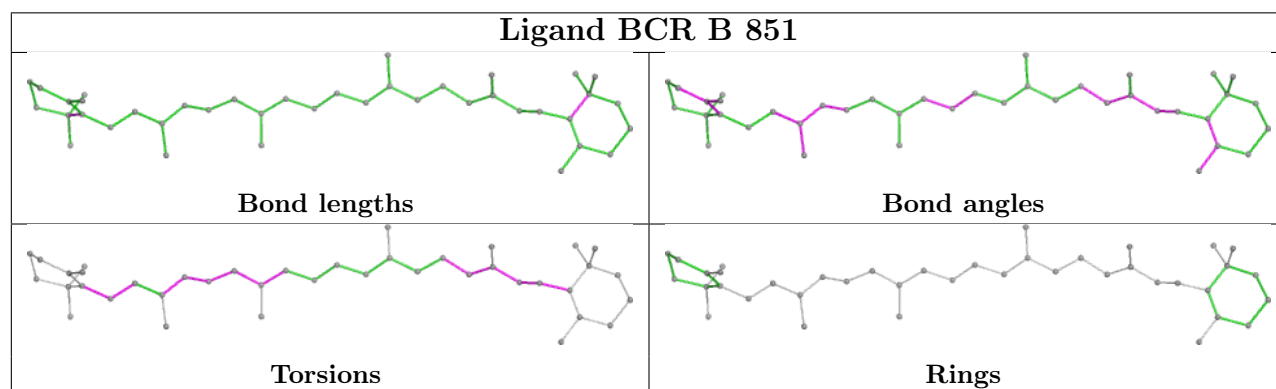
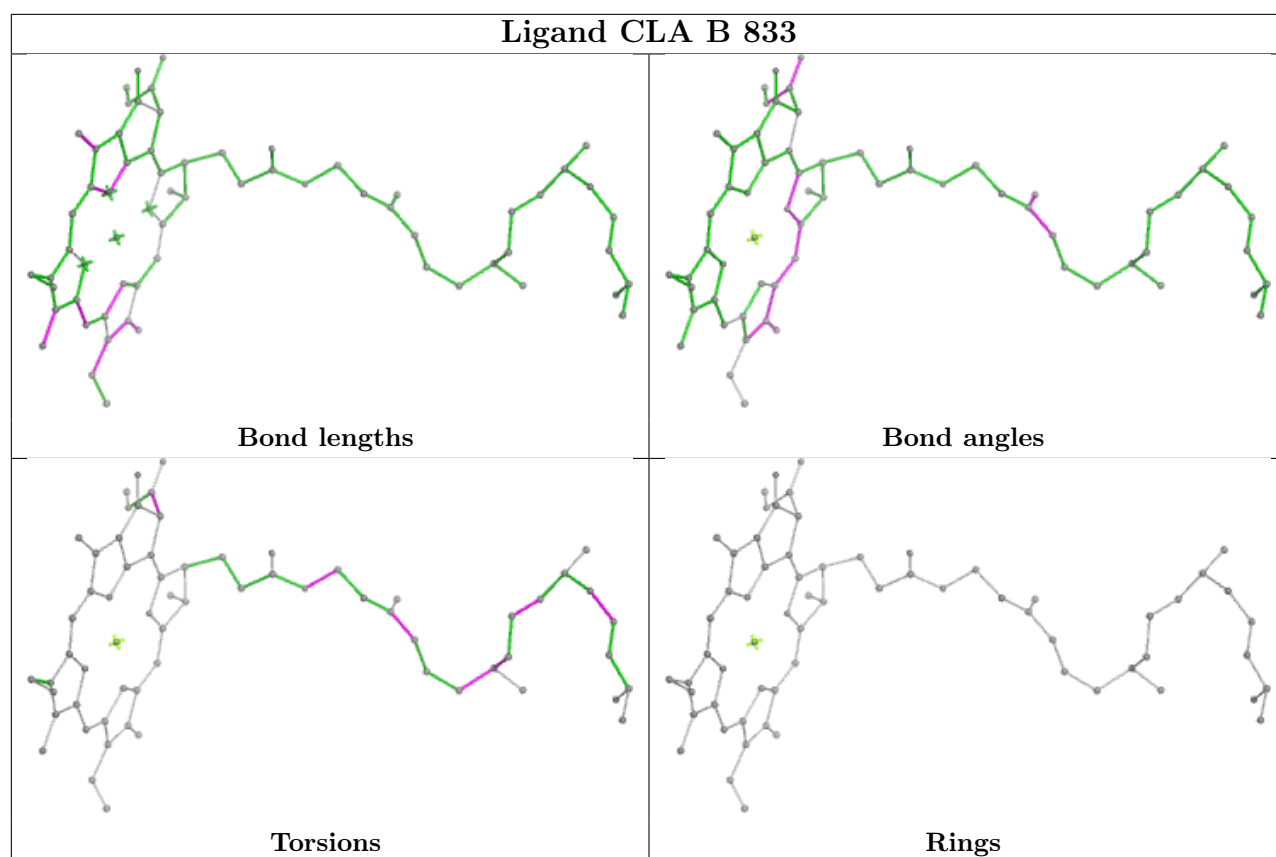


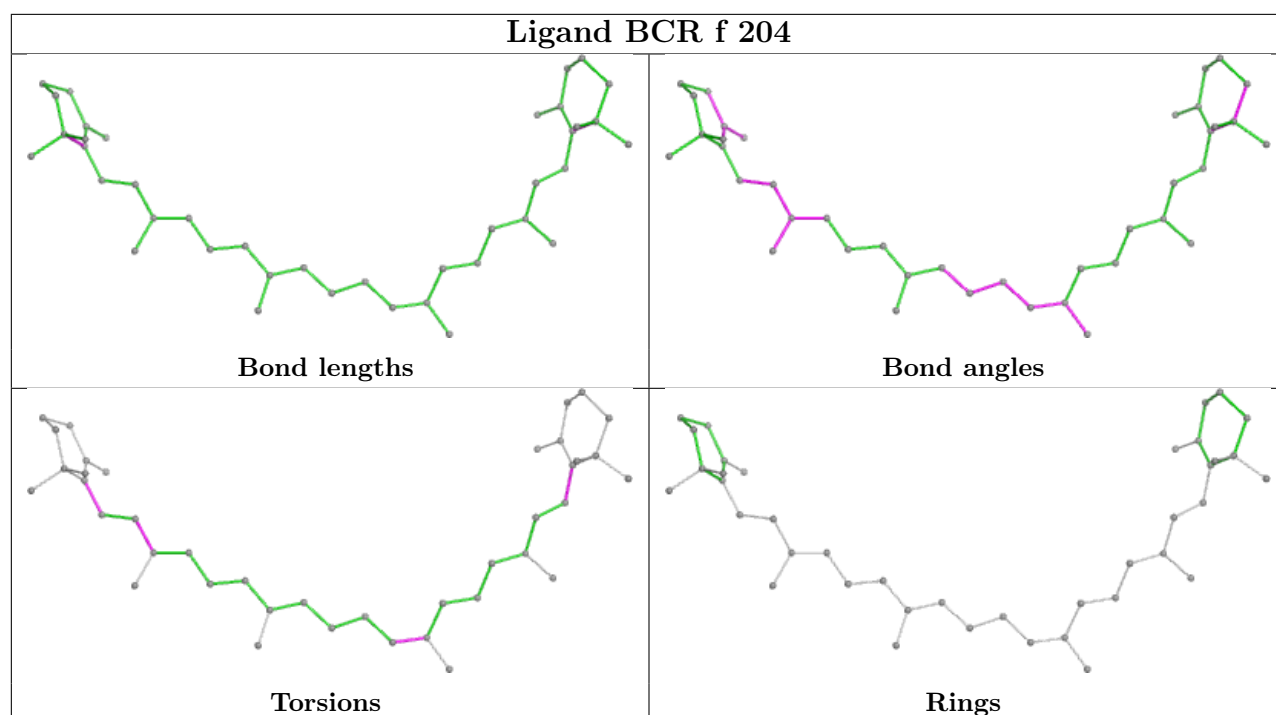
Ligand CLA B 814



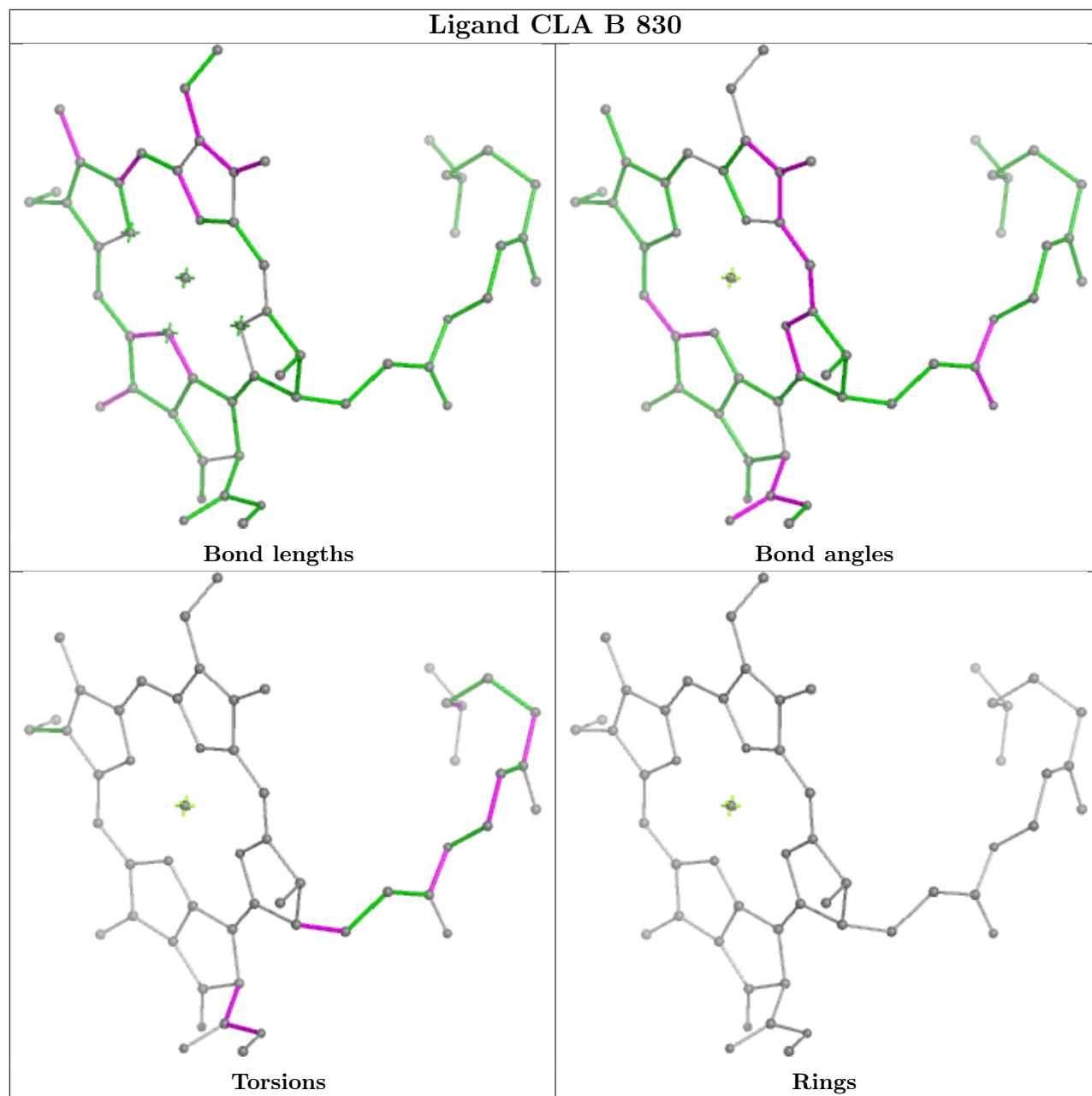
Ligand CLA B 809



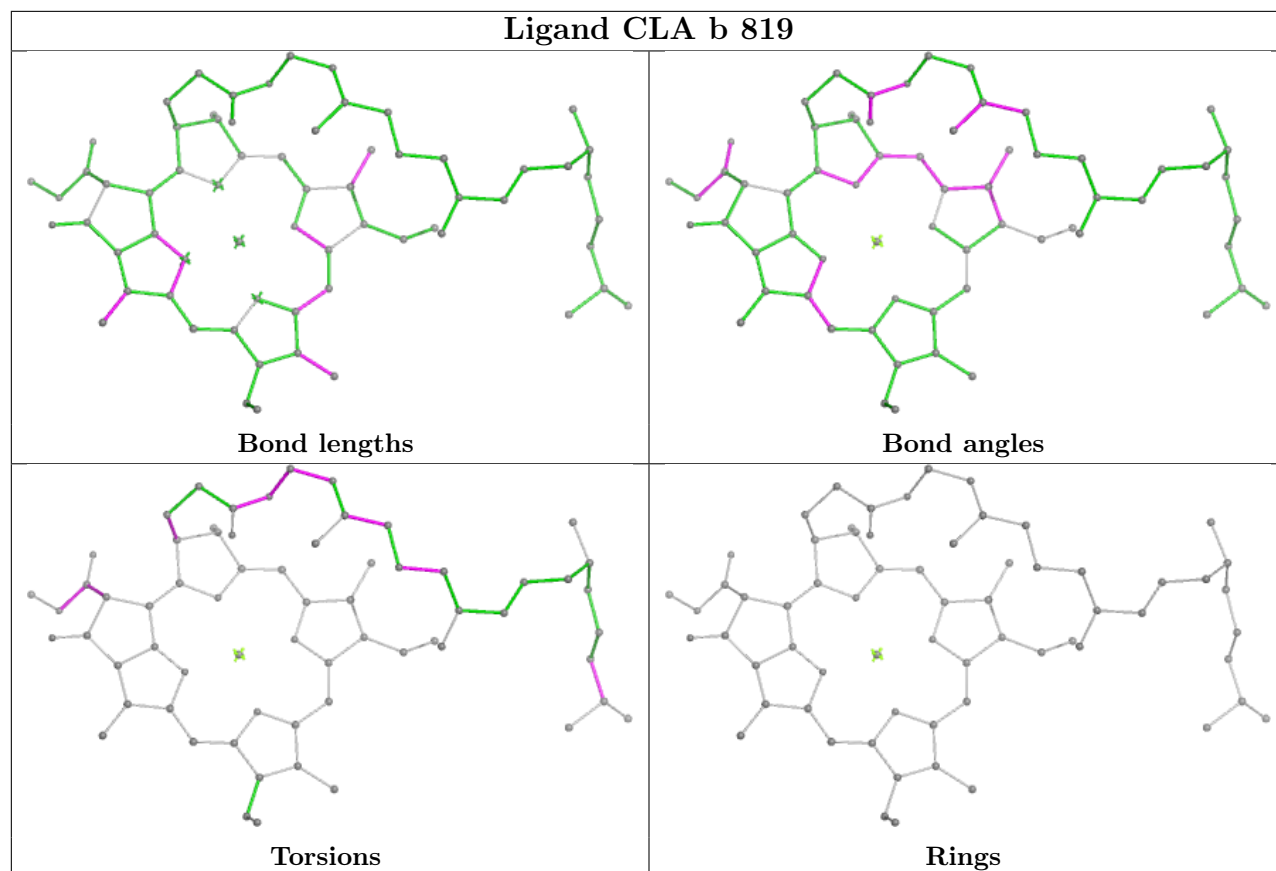




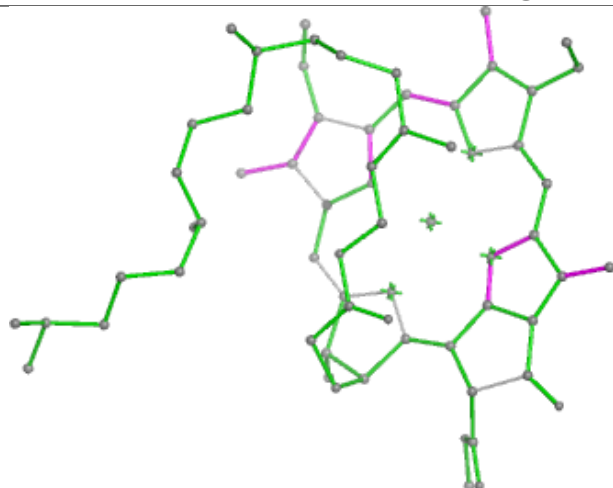
Ligand CLA B 830



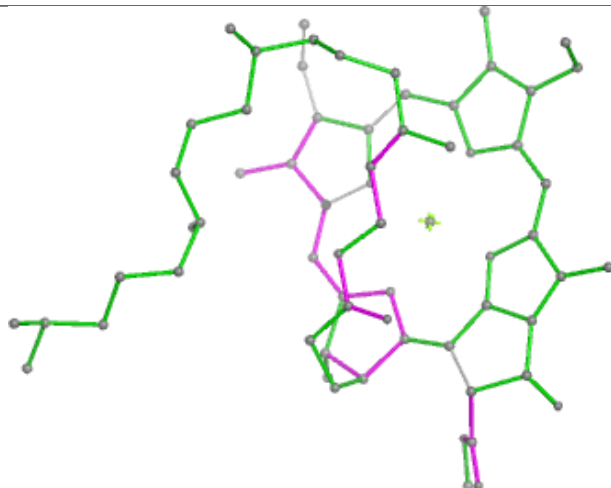
Ligand CLA b 819



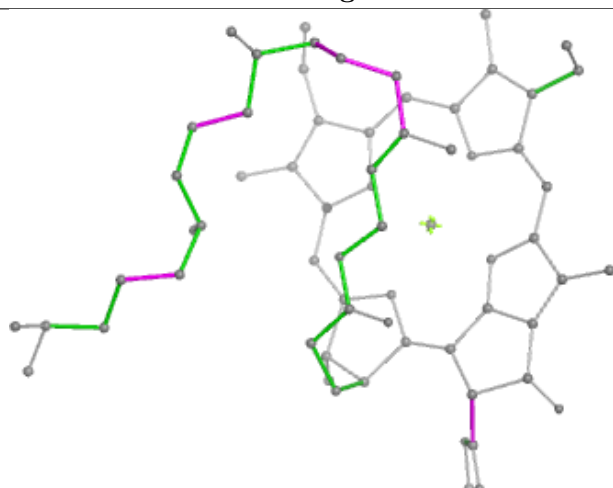
Ligand CLA b 809



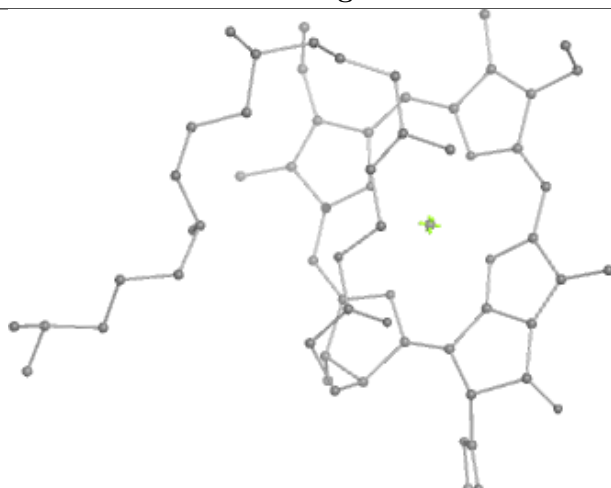
Bond lengths



Bond angles

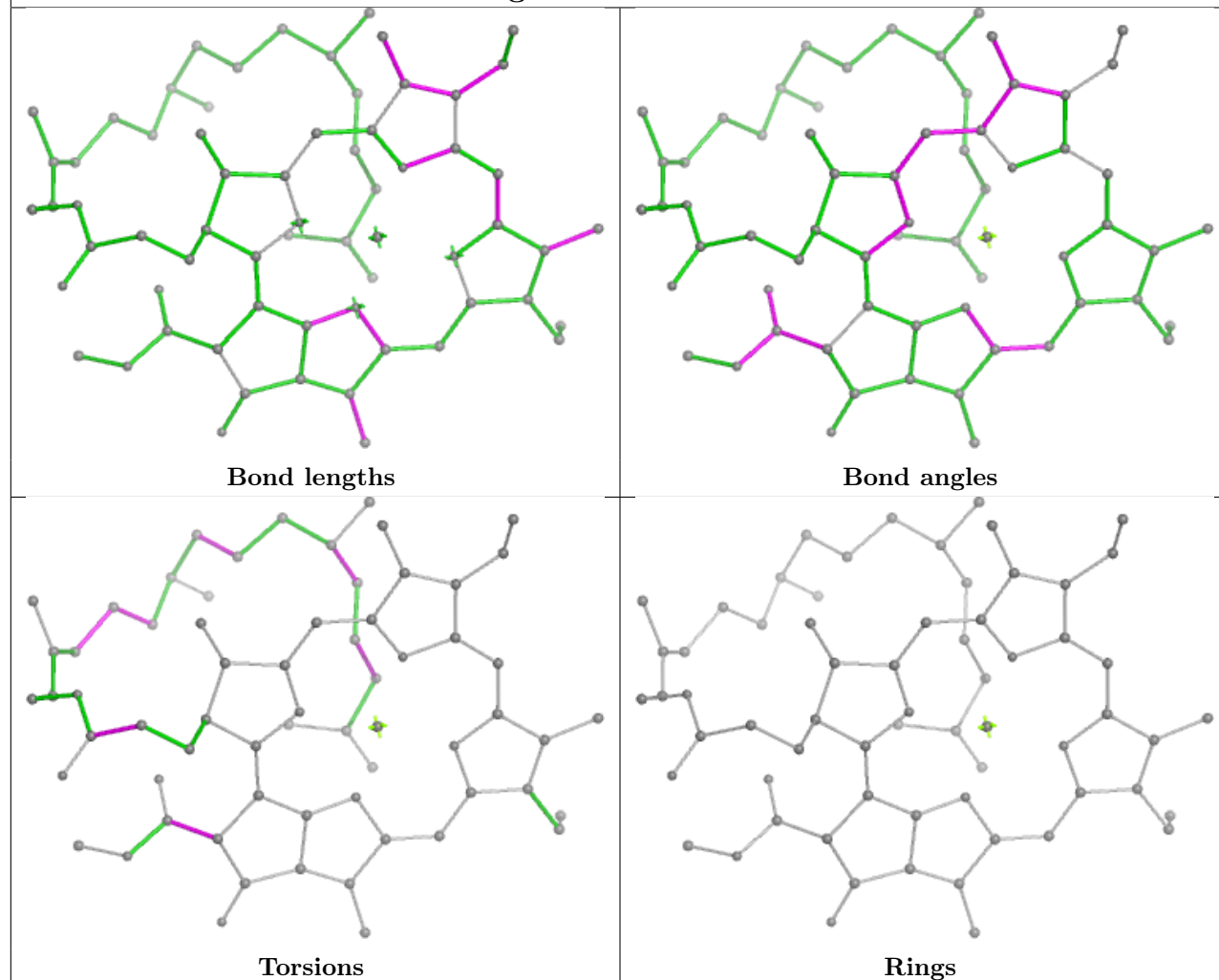


Torsions

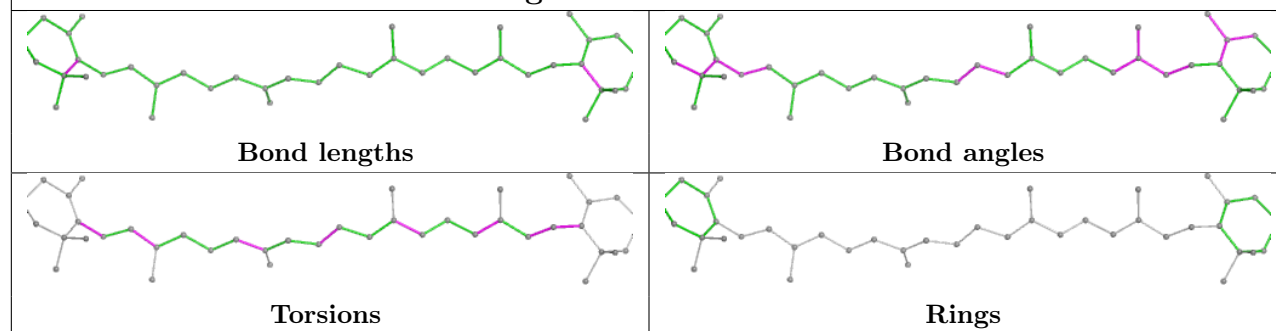


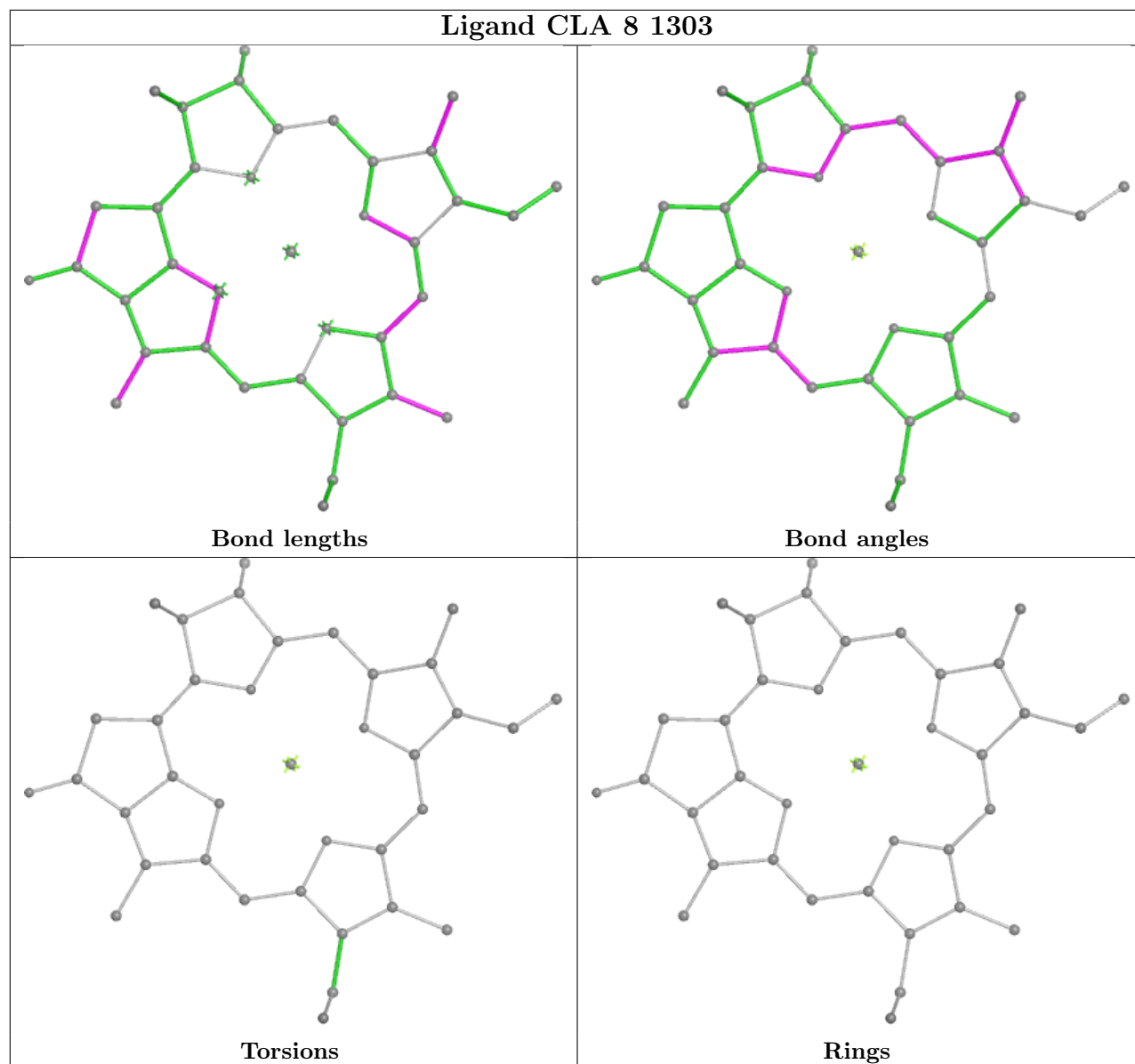
Rings

Ligand CLA B 806

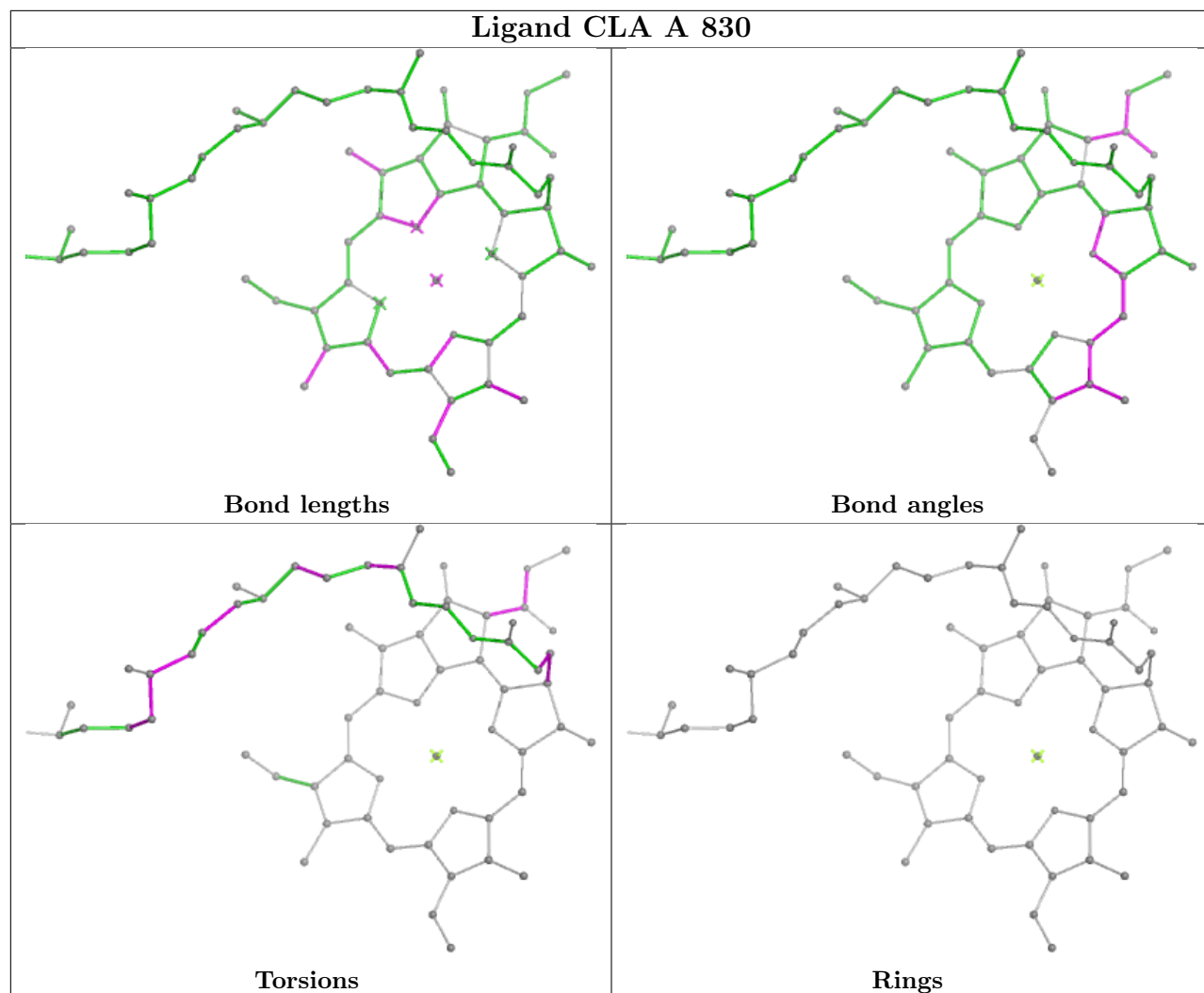


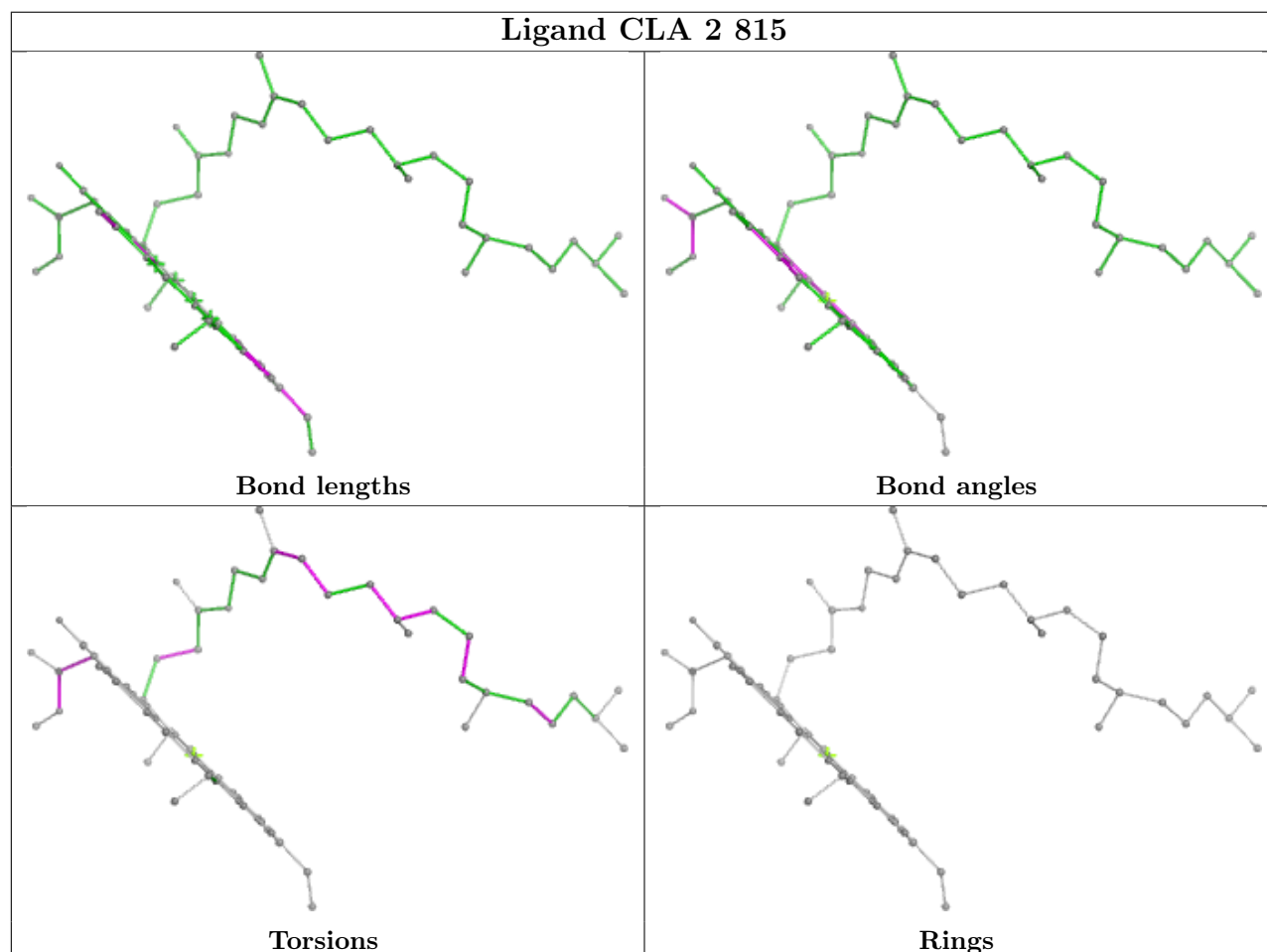
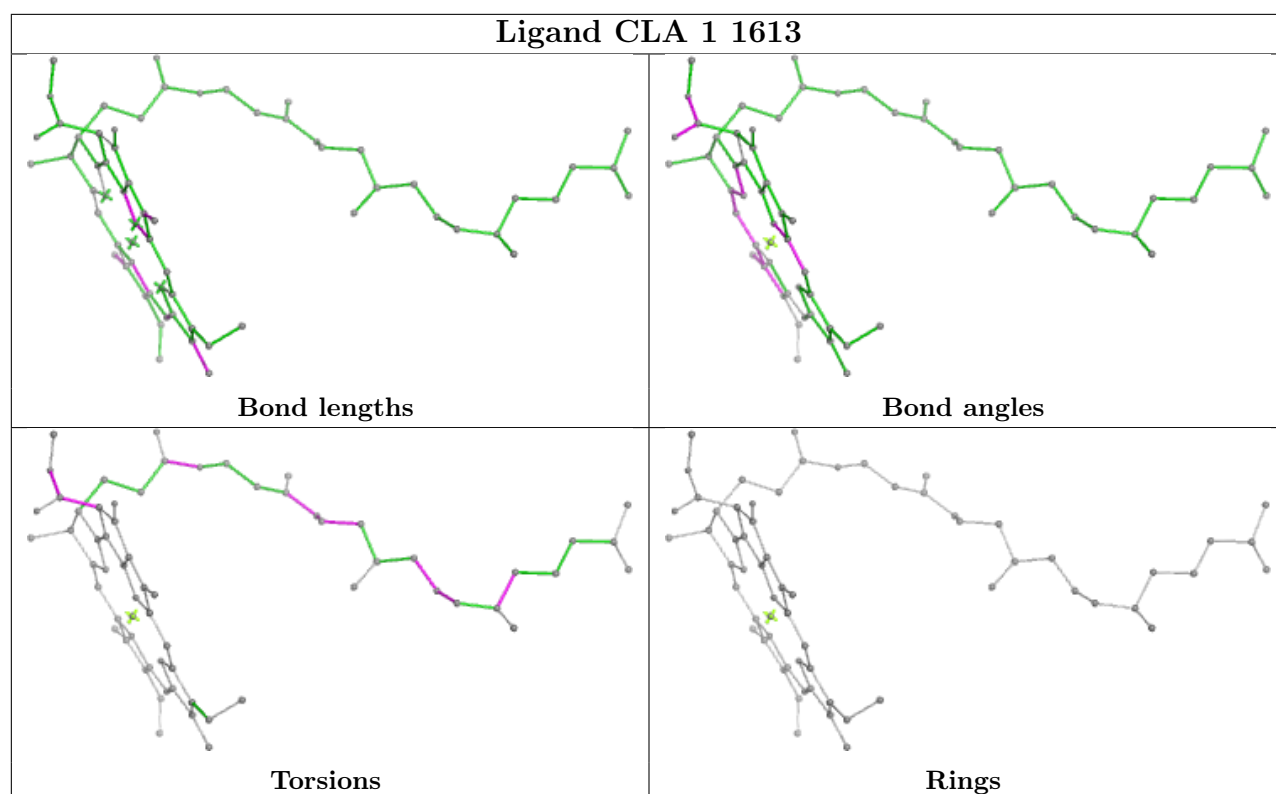
Ligand BCR 1 1648

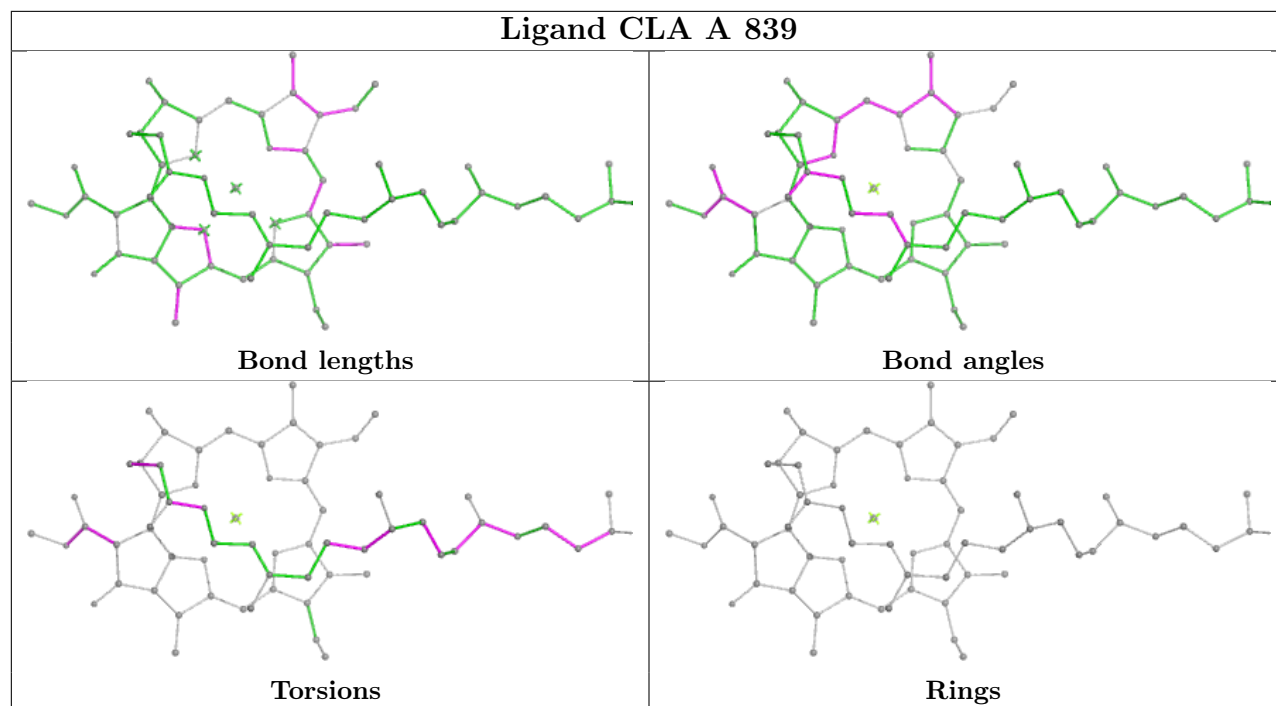


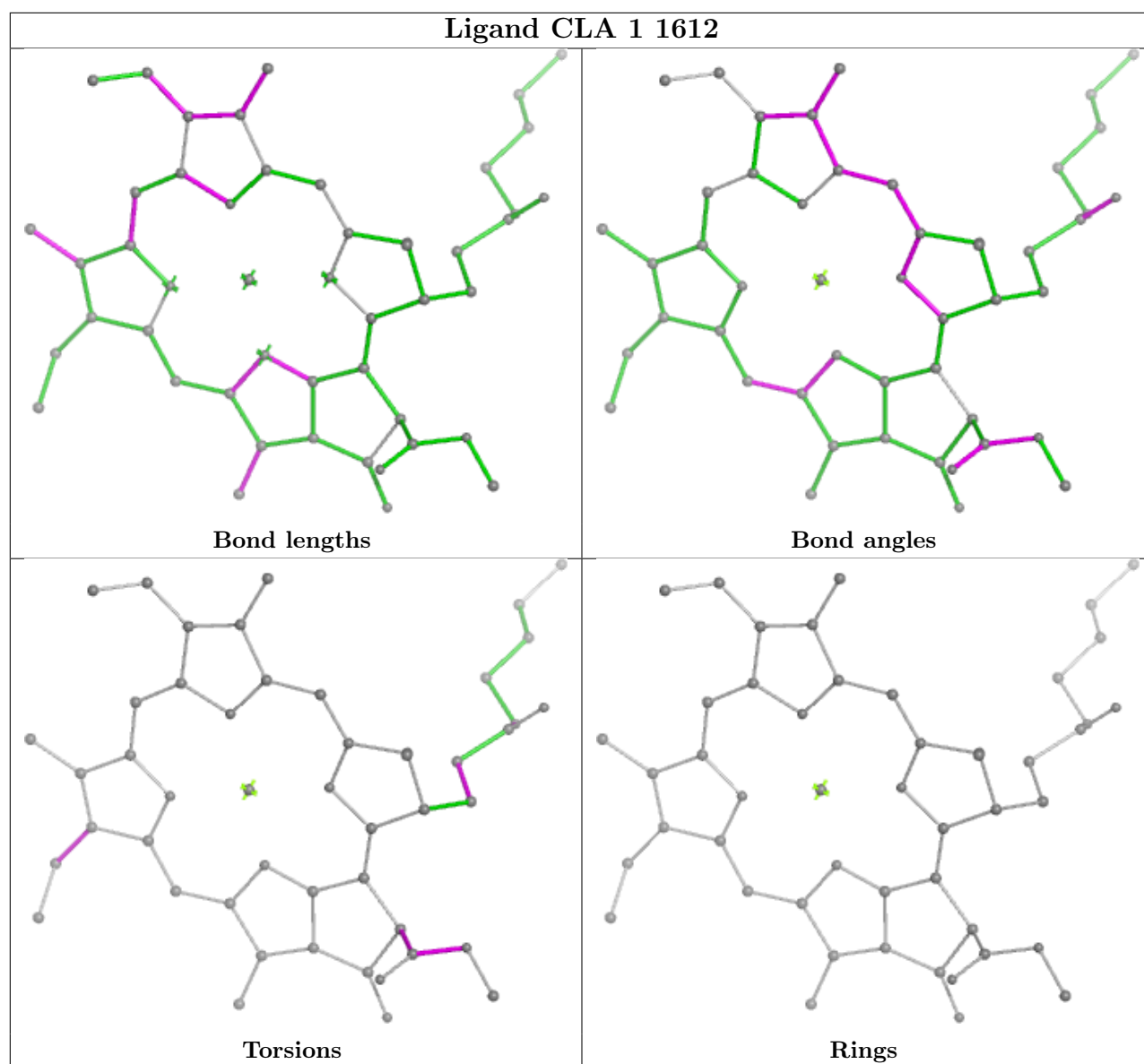


Ligand CLA A 830

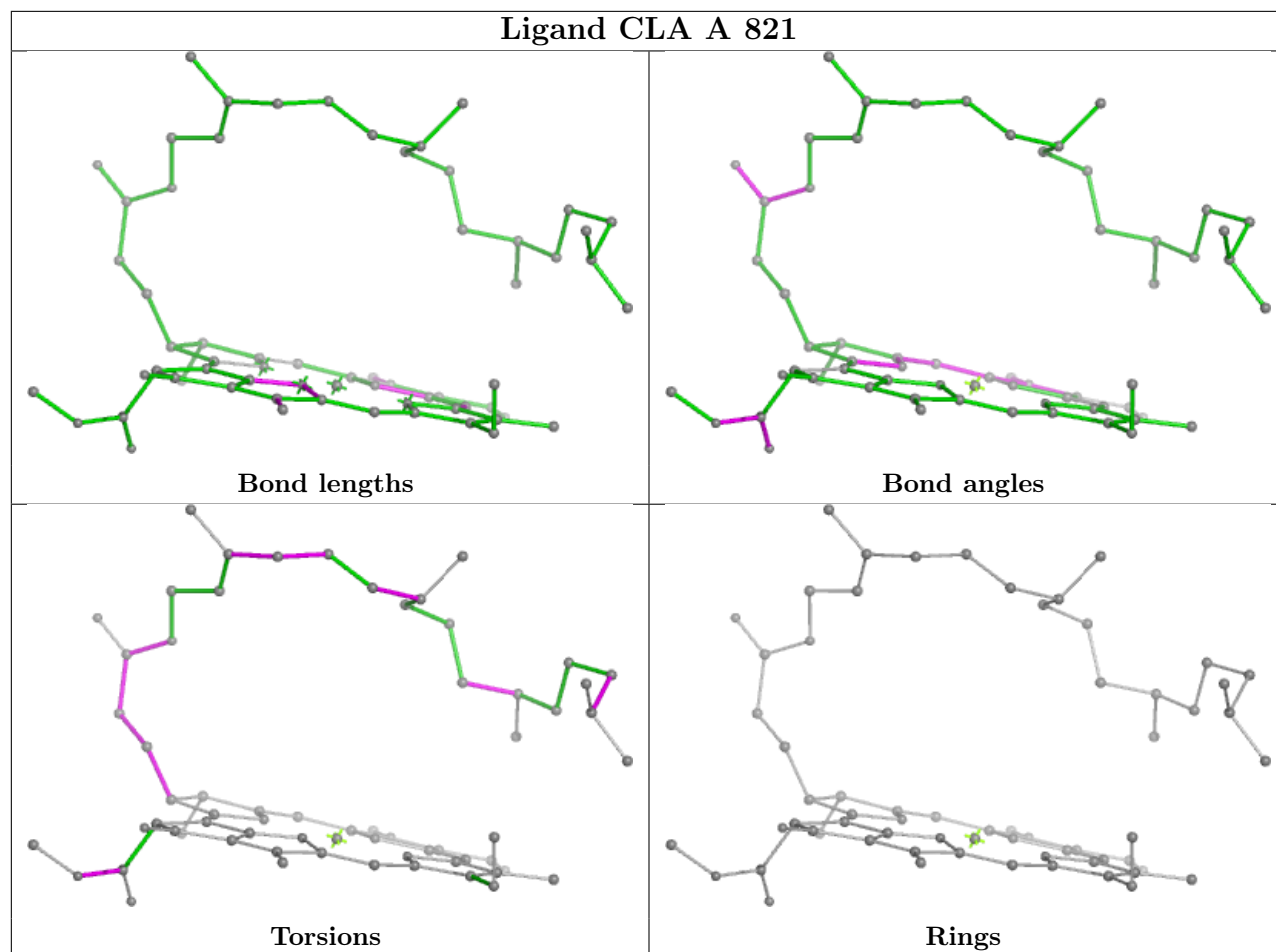




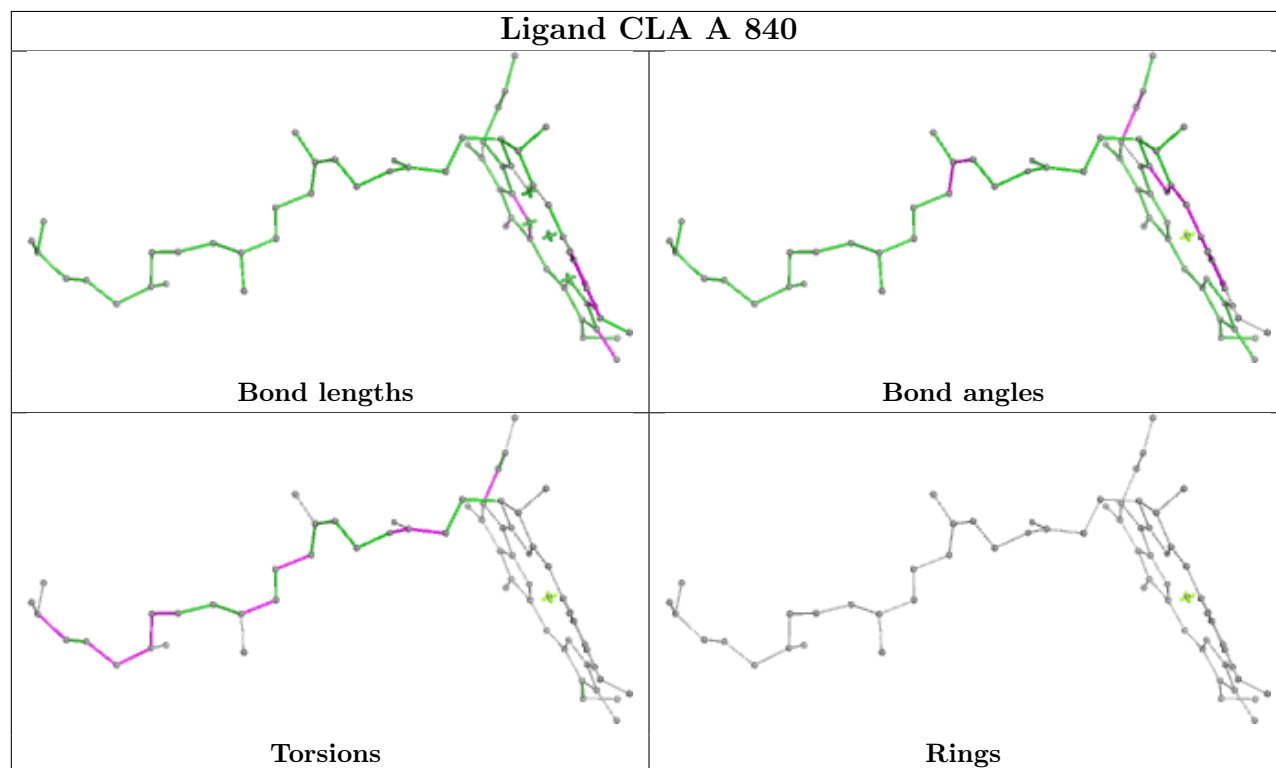


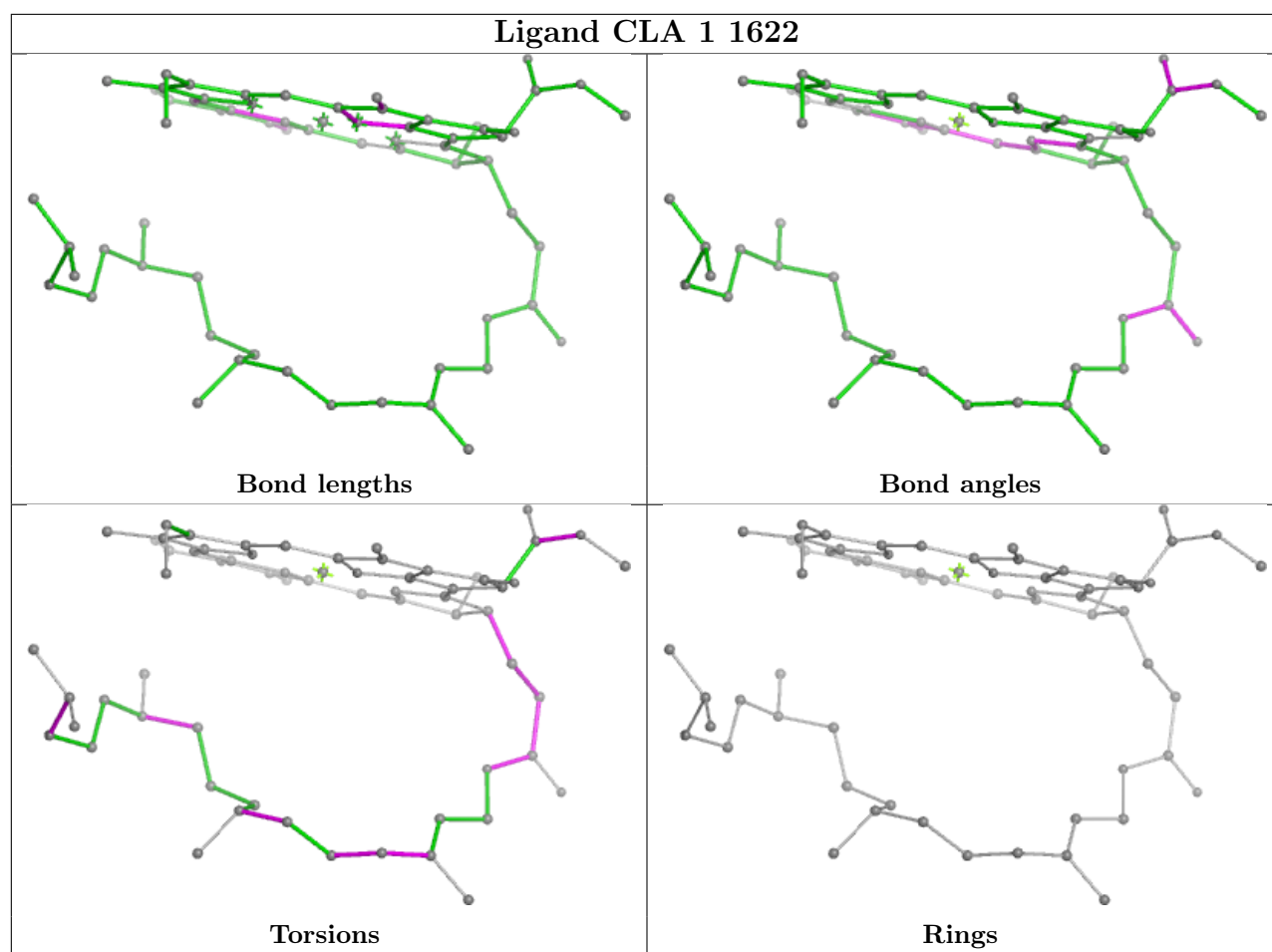


Ligand CLA A 821

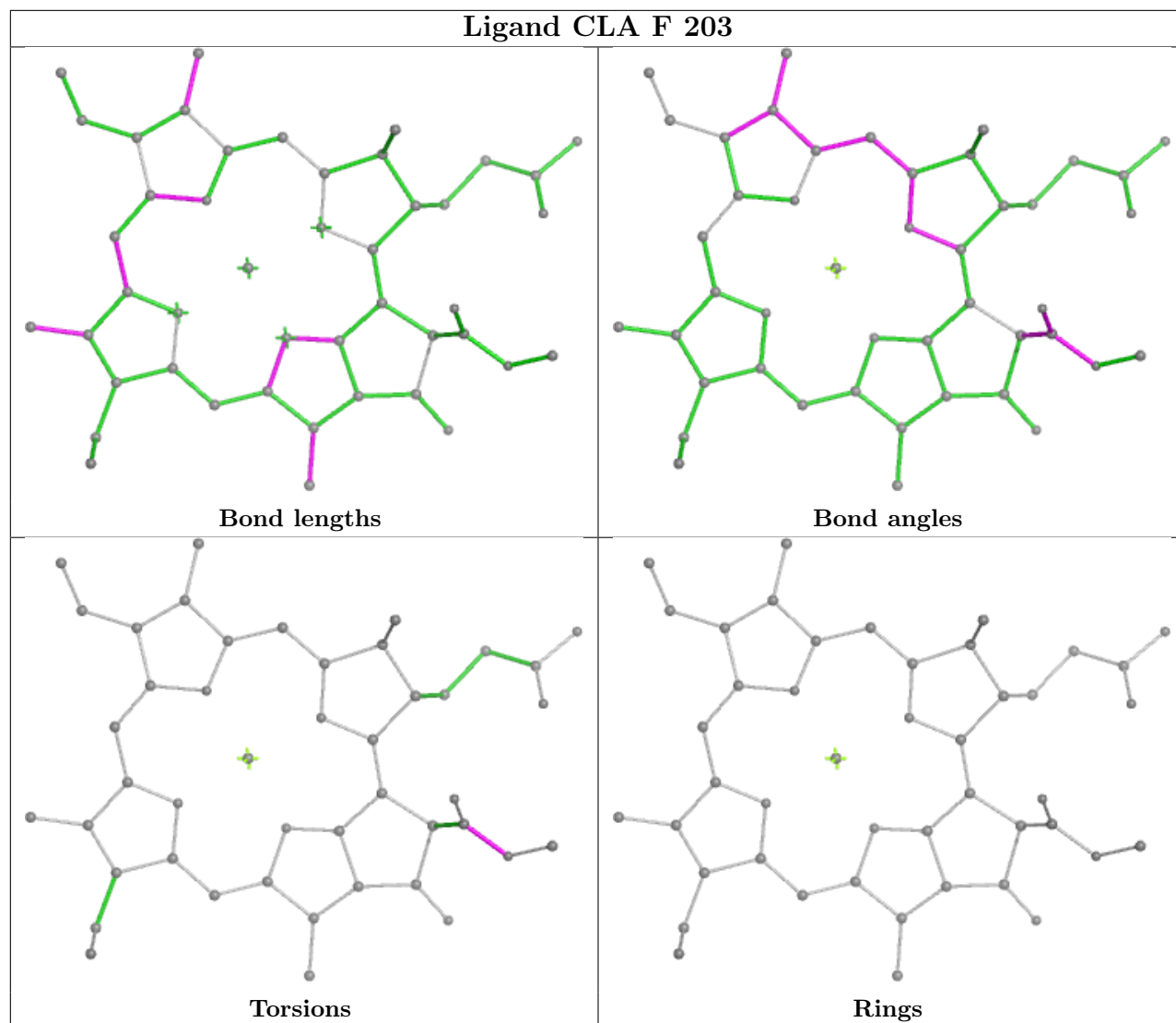


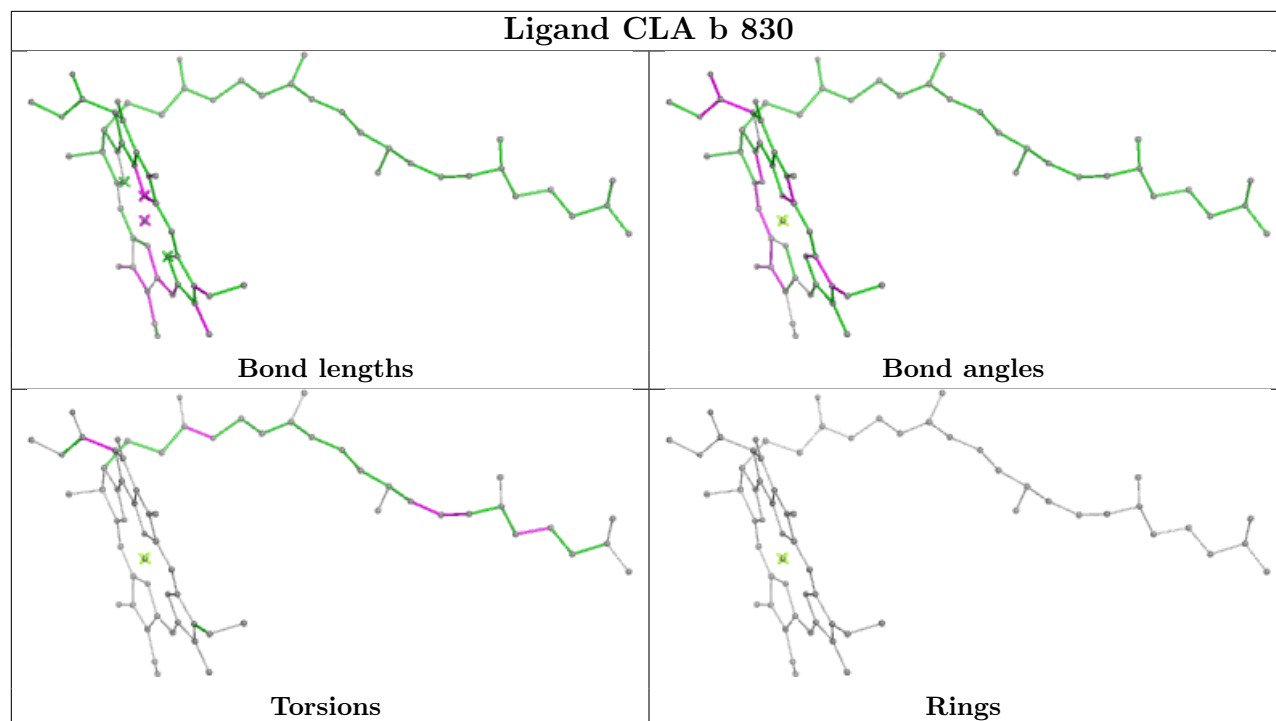
Ligand CLA A 840



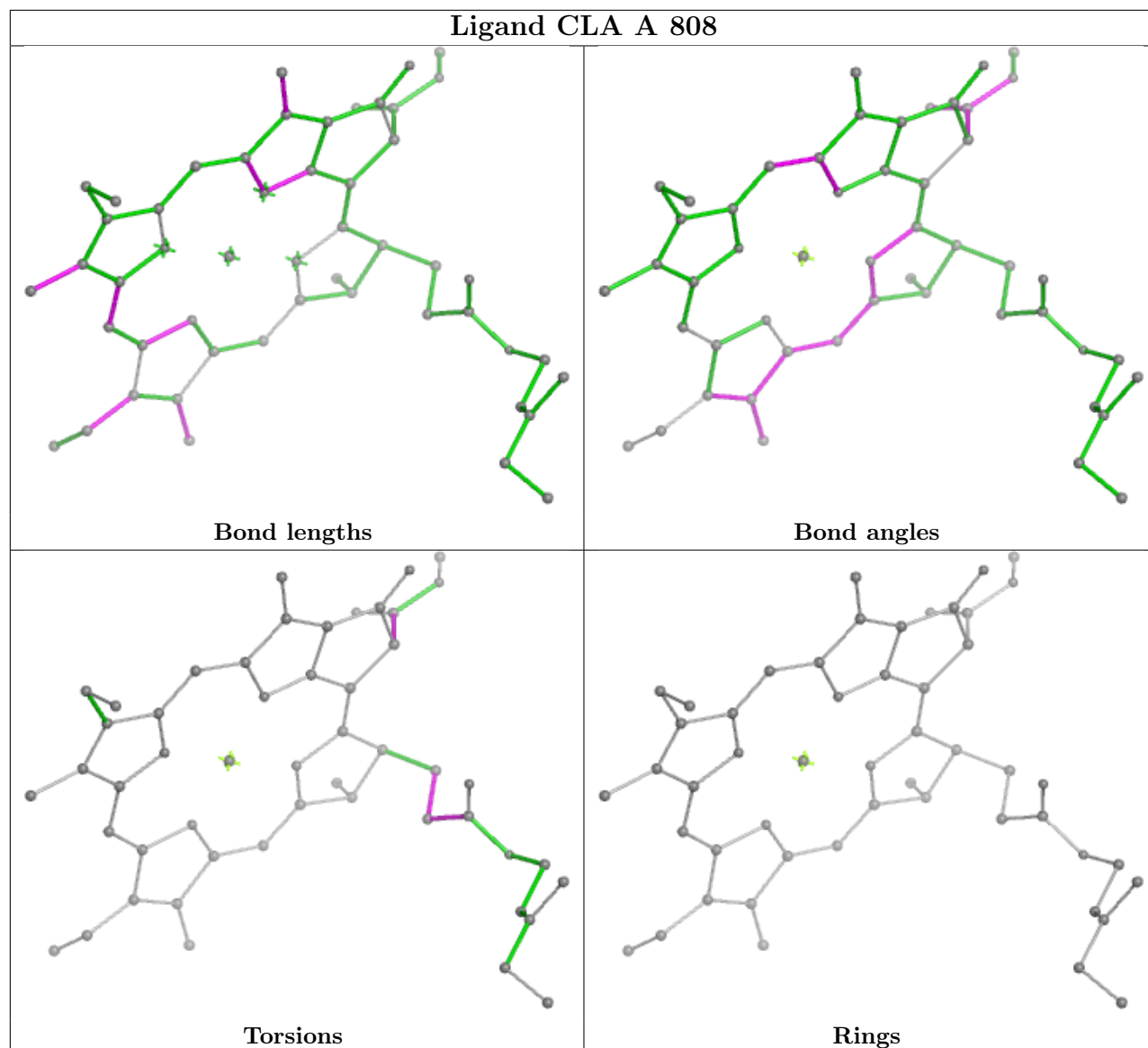


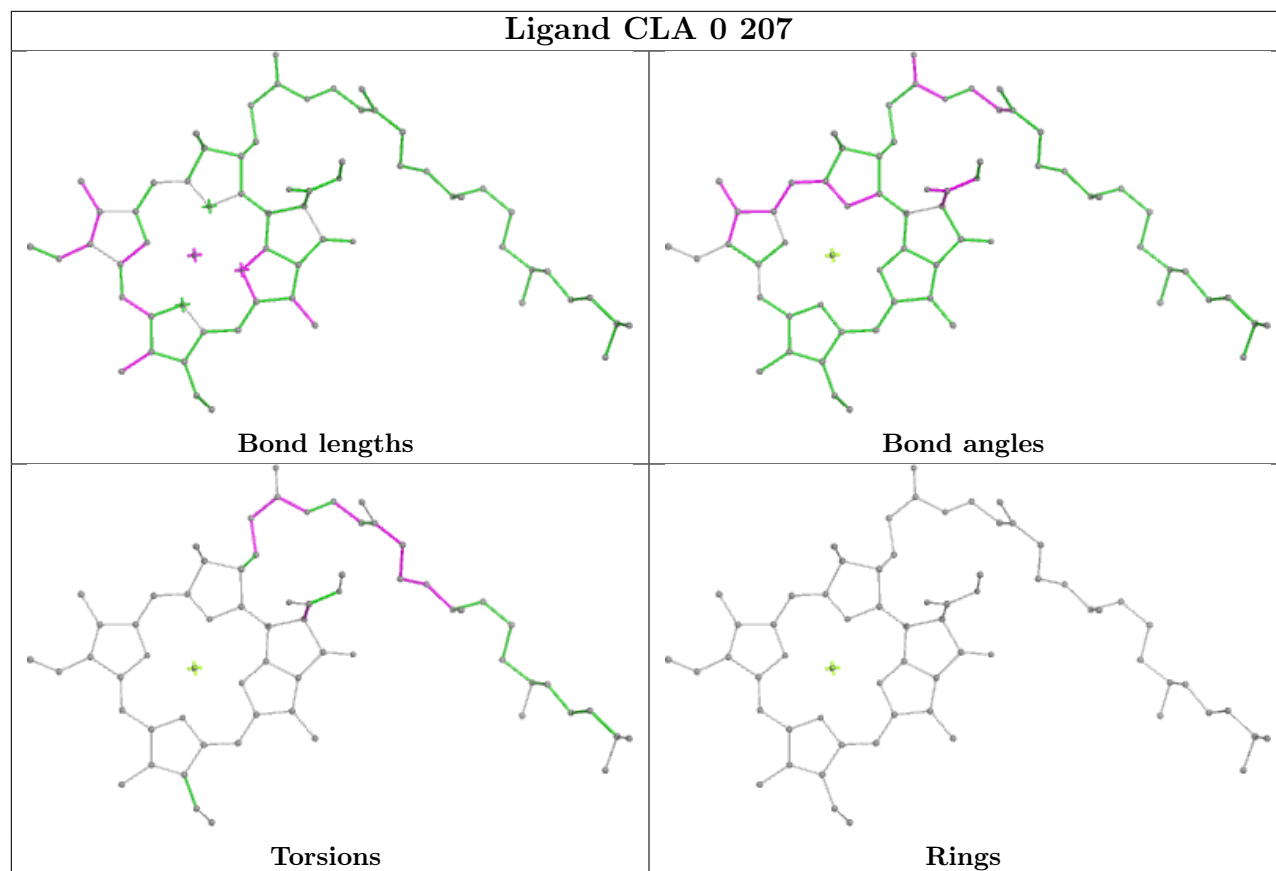
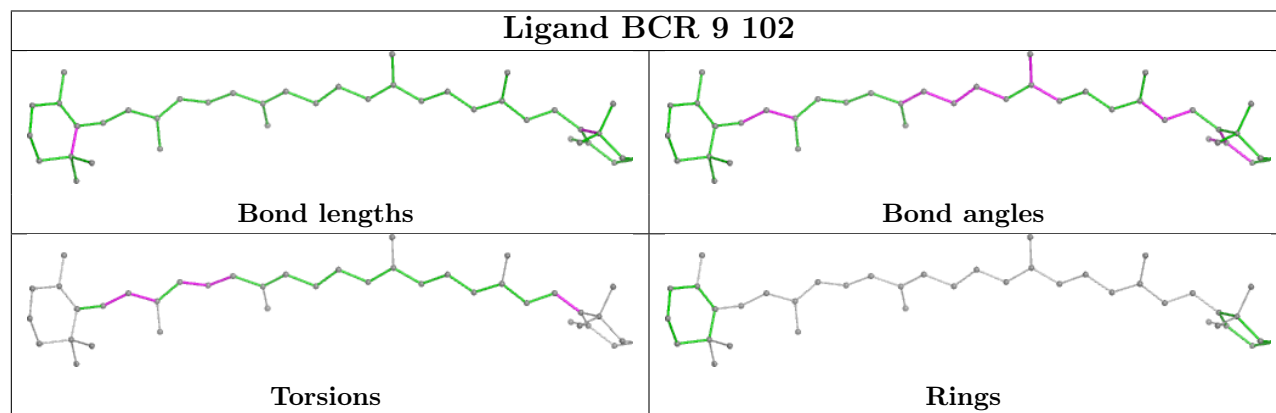
Ligand CLA F 203



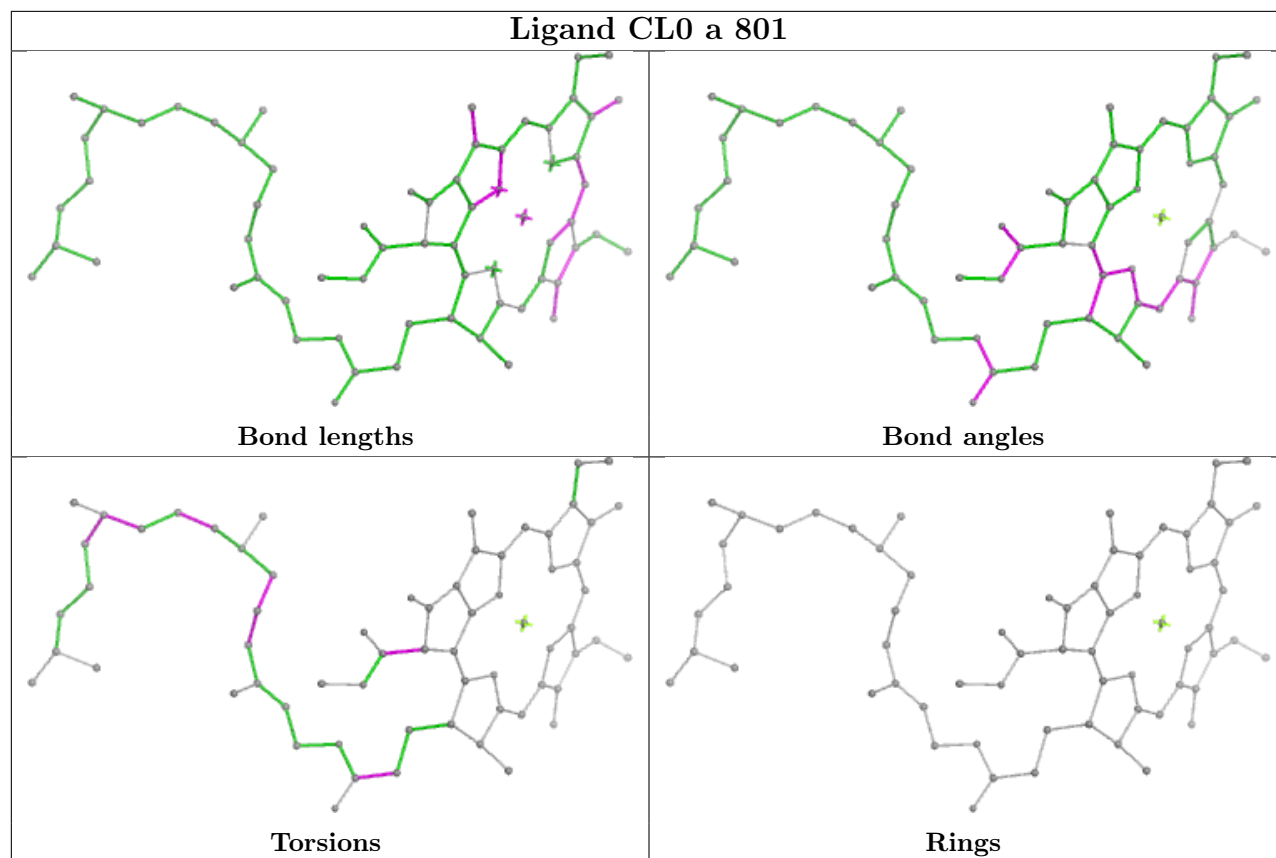


Ligand CLA A 808

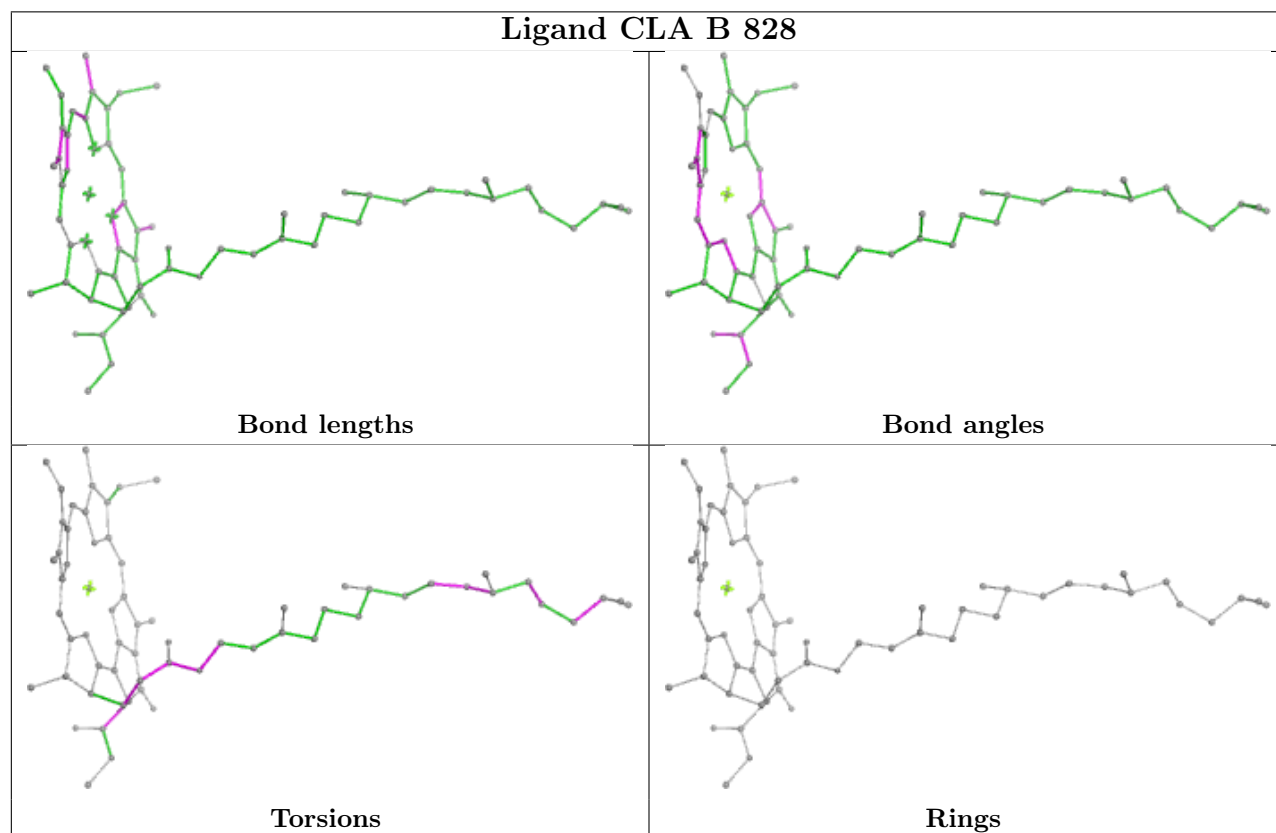


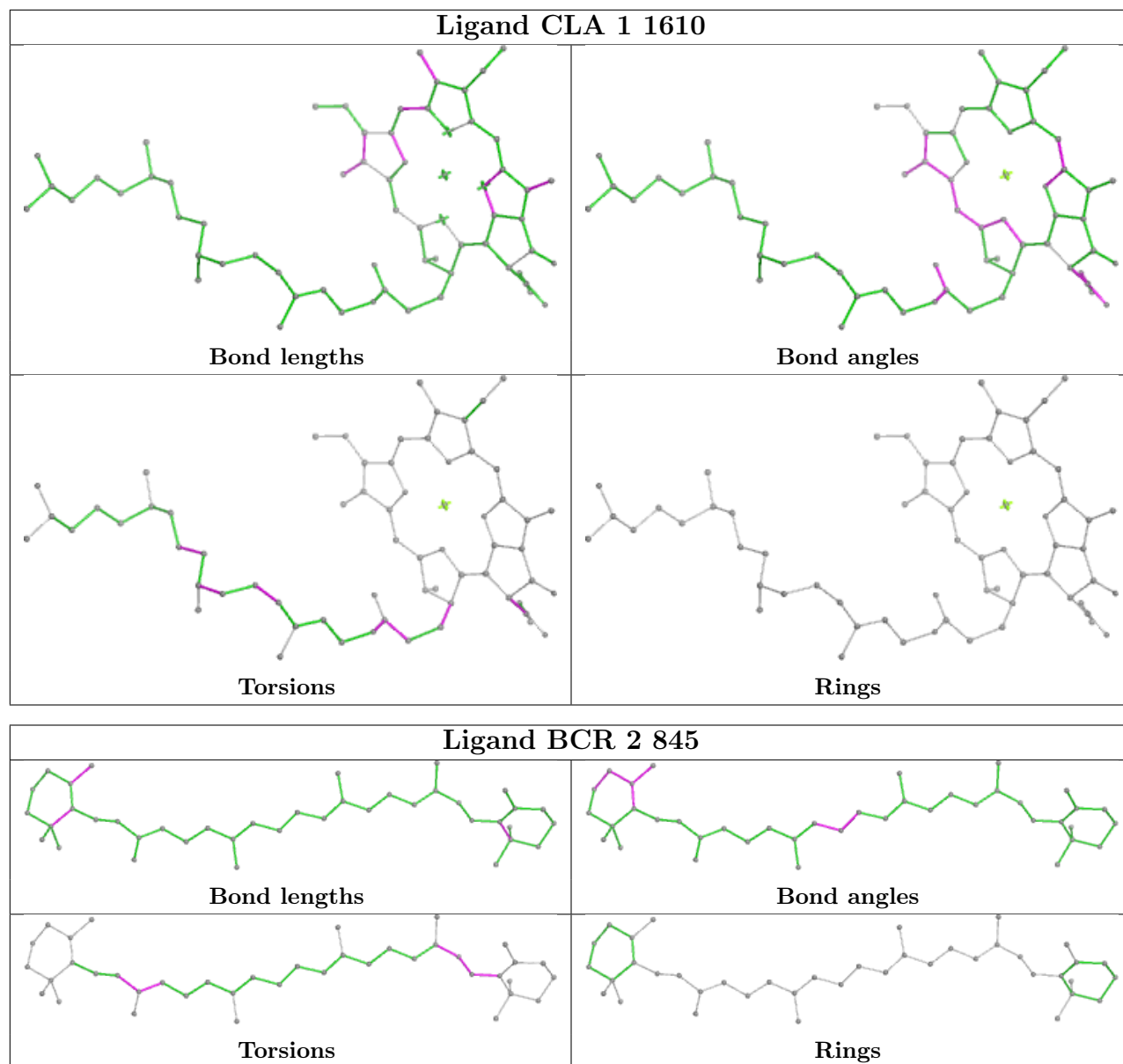
Ligand CLA 0 207**Ligand BCR 9 102**

Ligand CL0 a 801

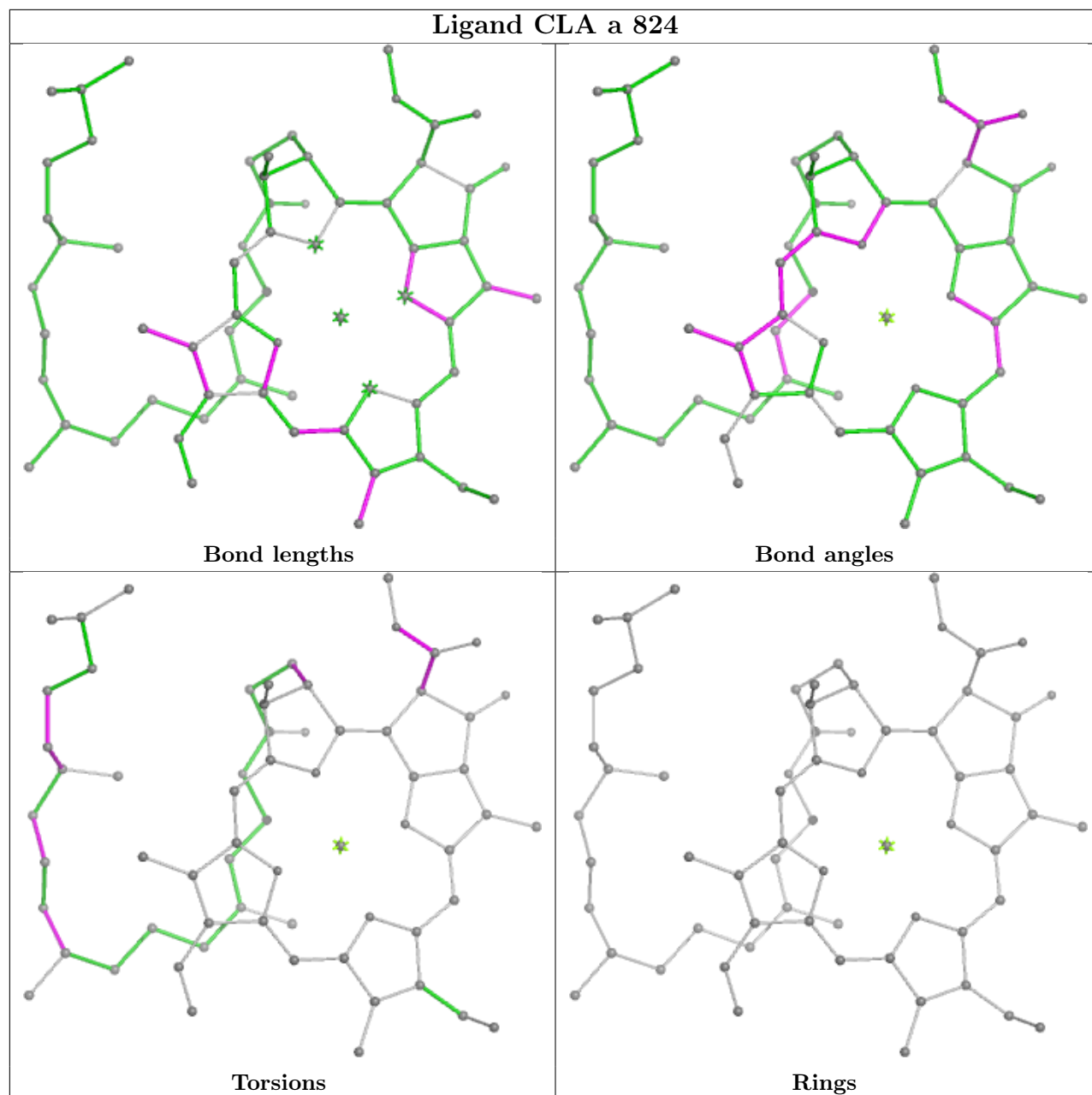


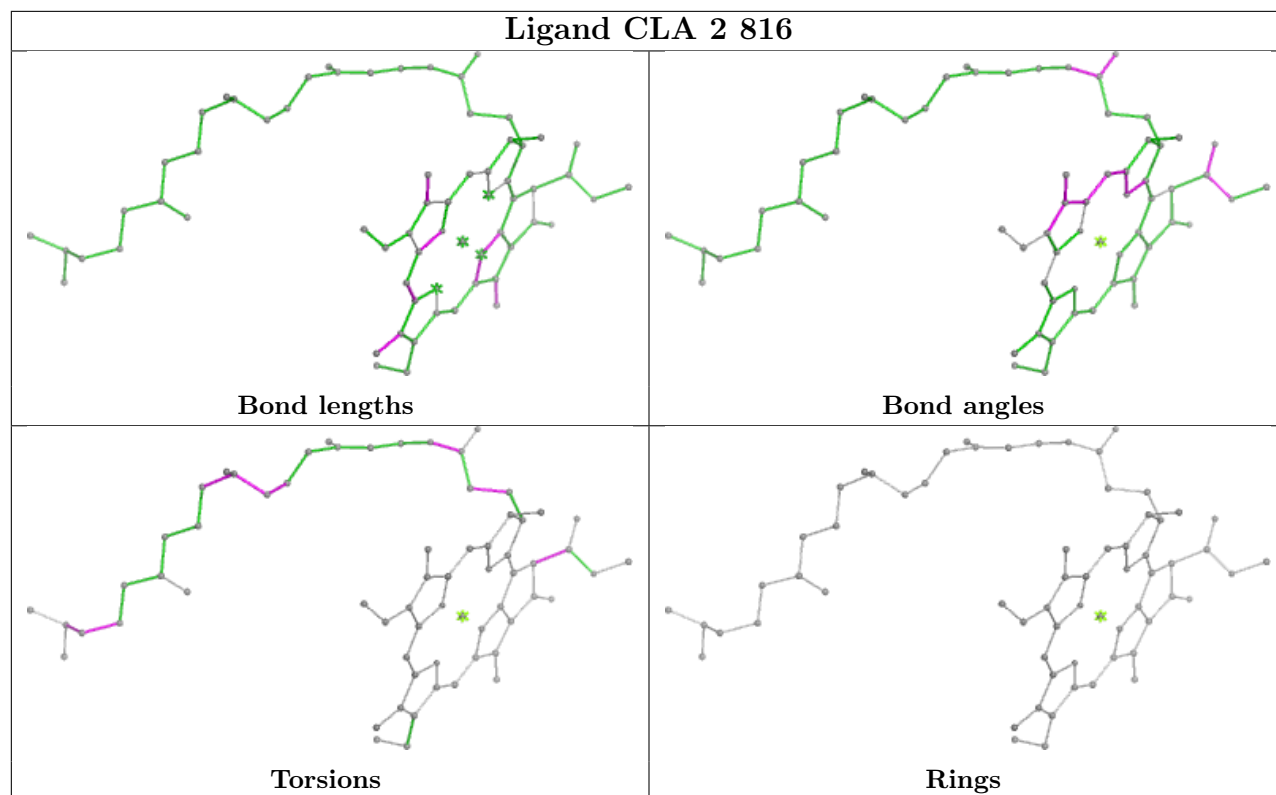
Ligand CLA B 828



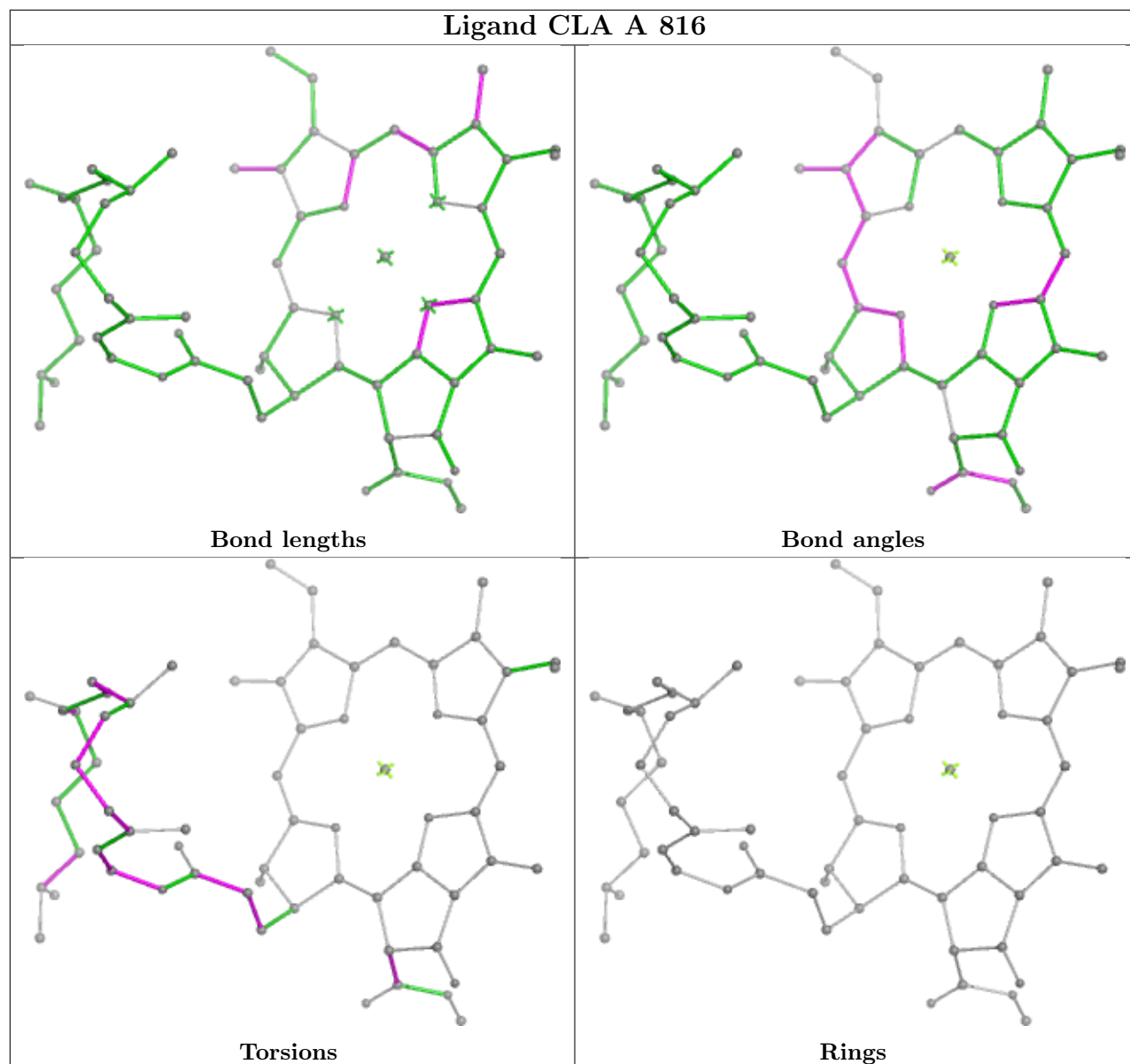


Ligand CLA a 824

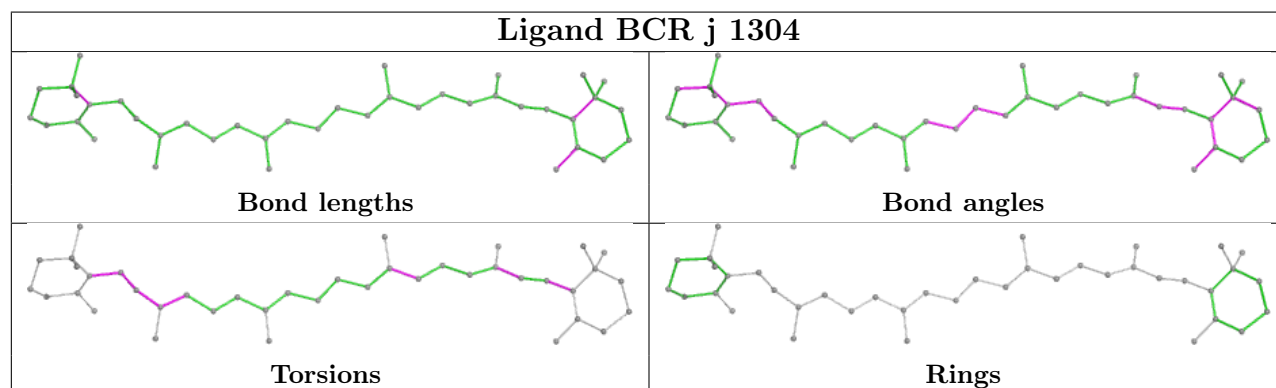


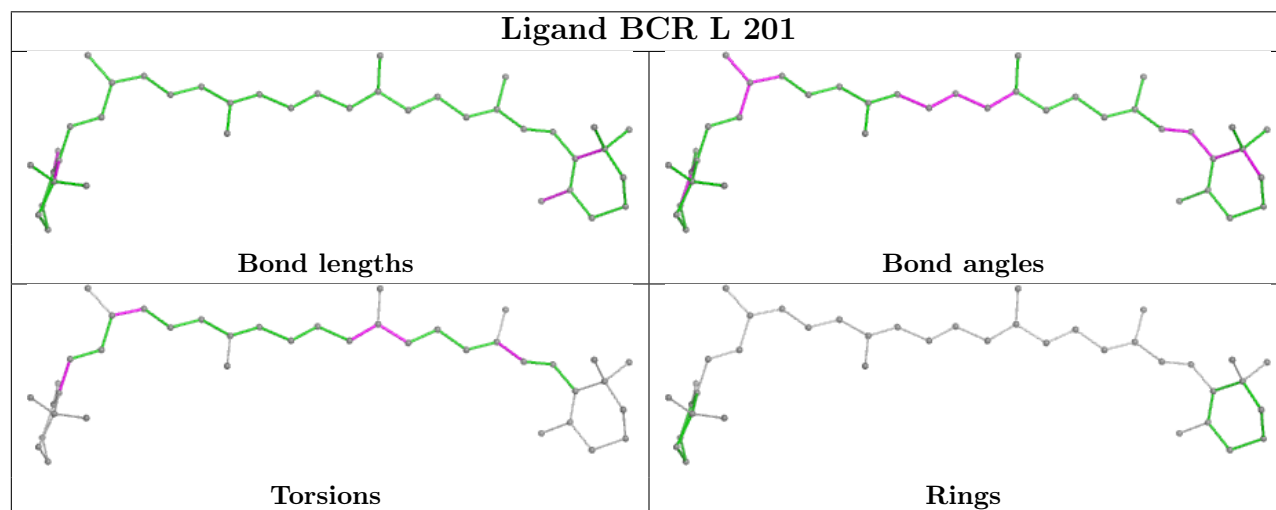
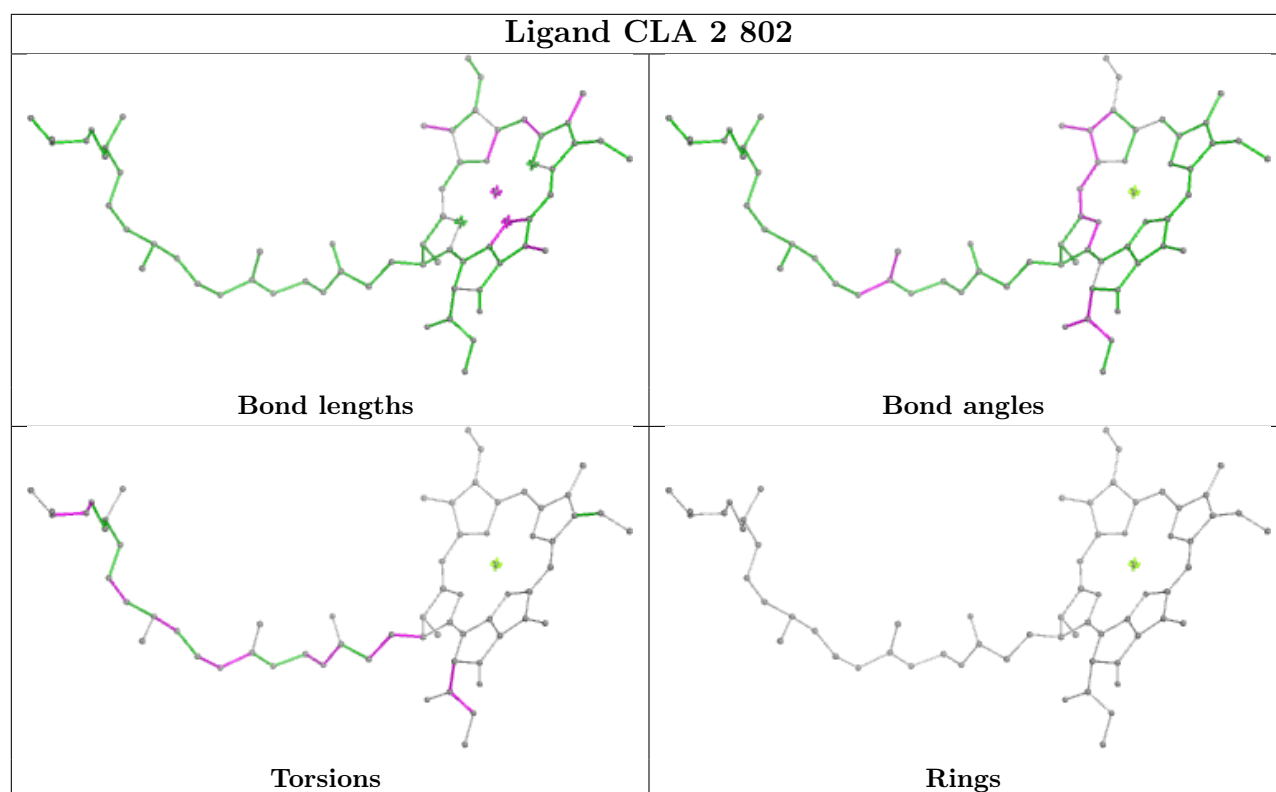


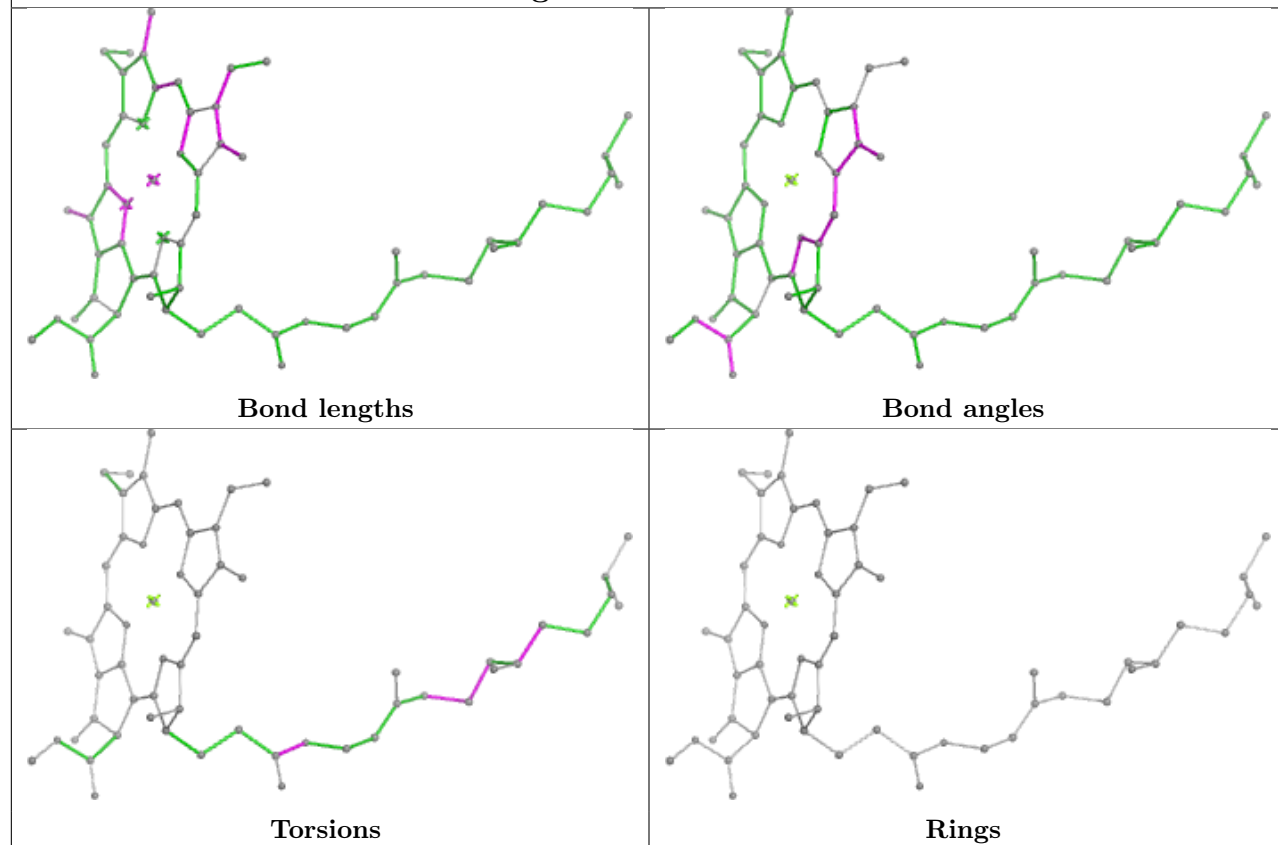
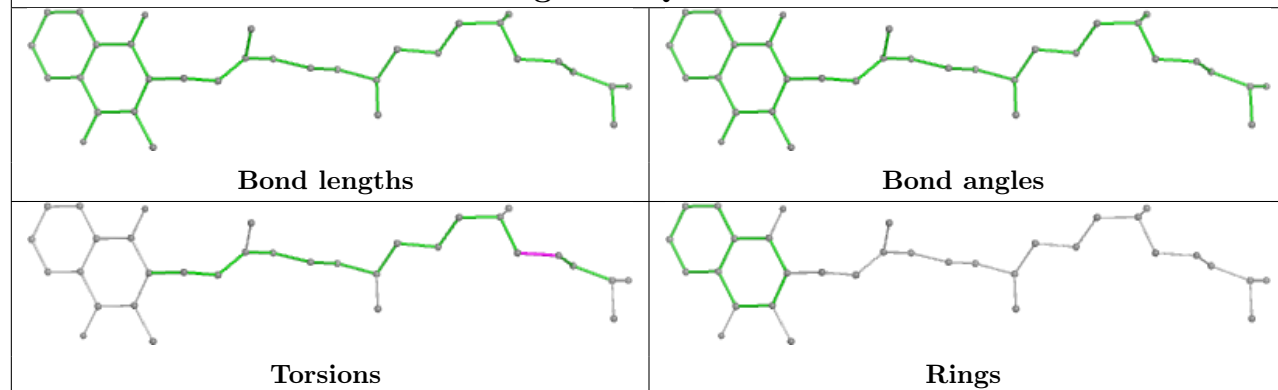
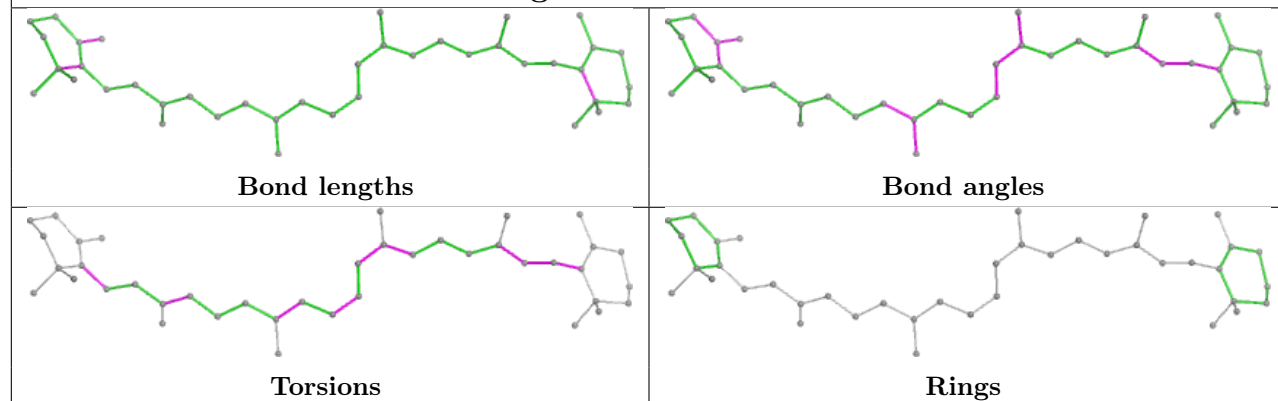
Ligand CLA A 816

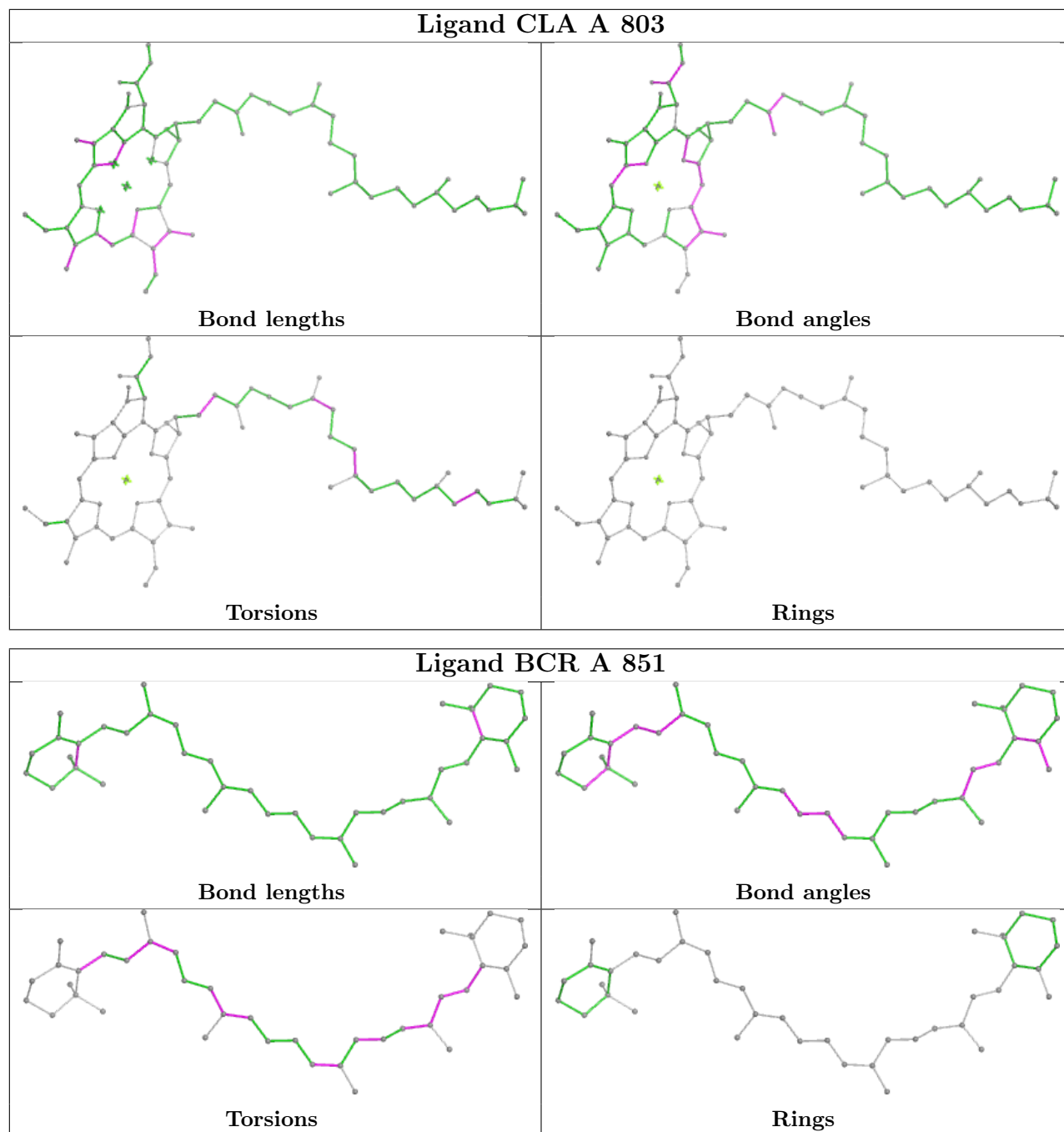


Ligand BCR j 1304

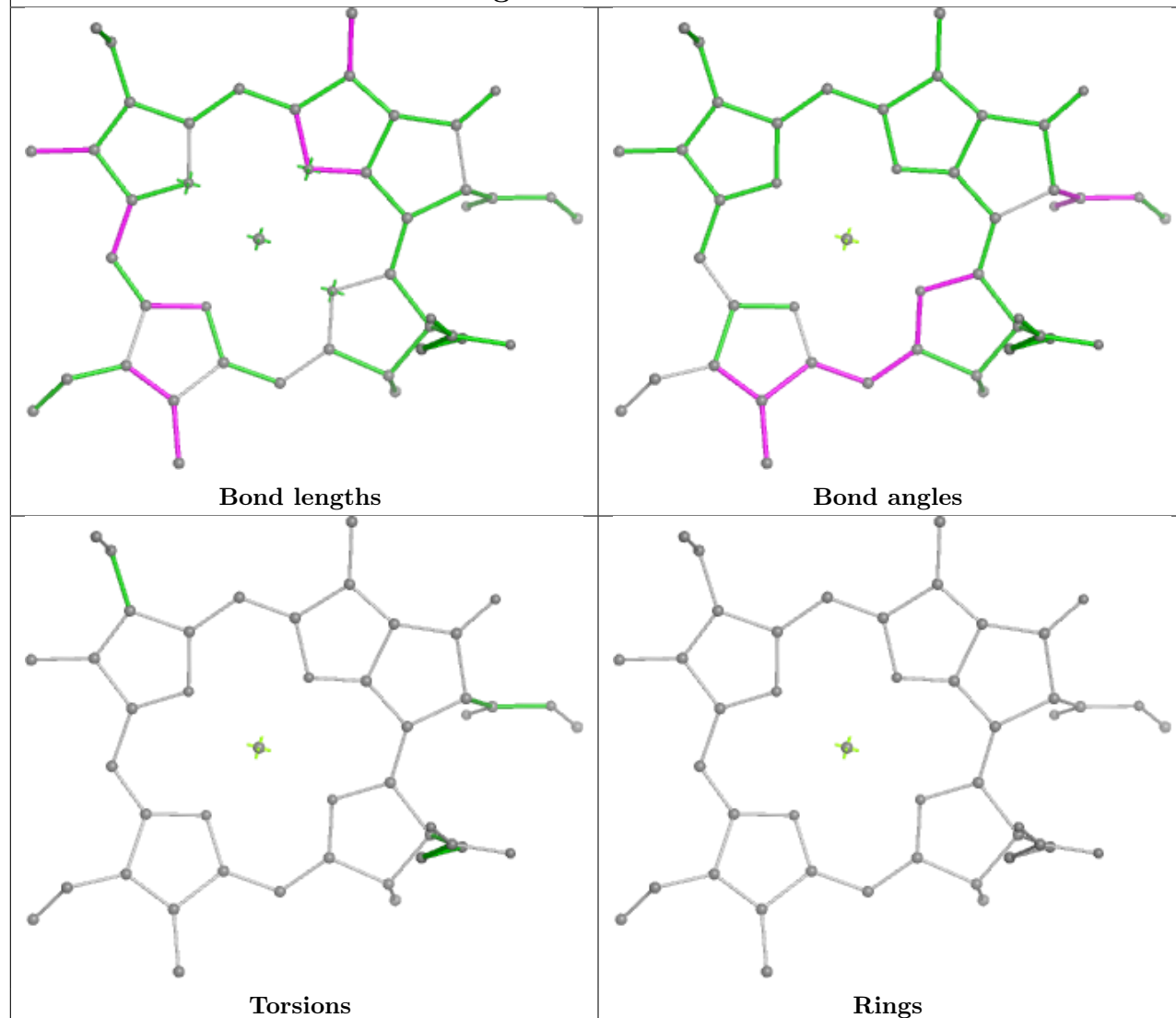




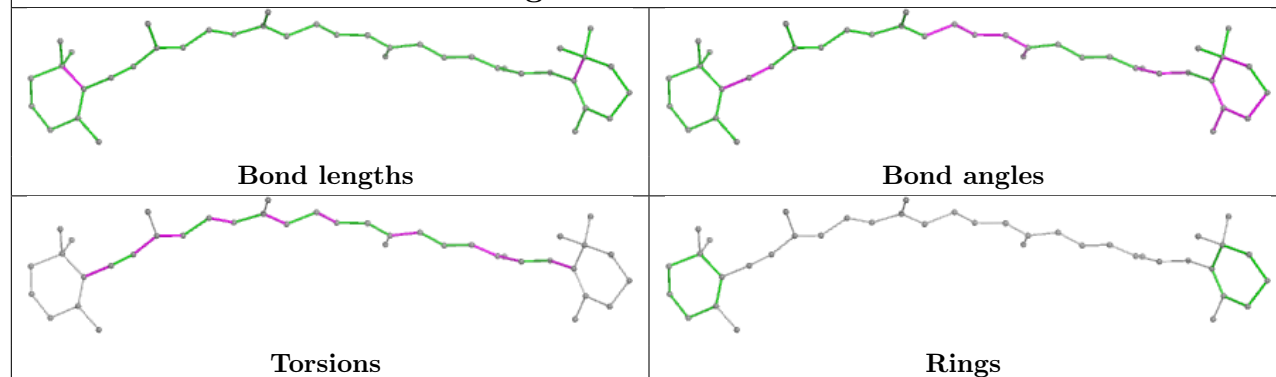
Ligand CLA A 832**Ligand PQN a 845****Ligand BCR B 846**

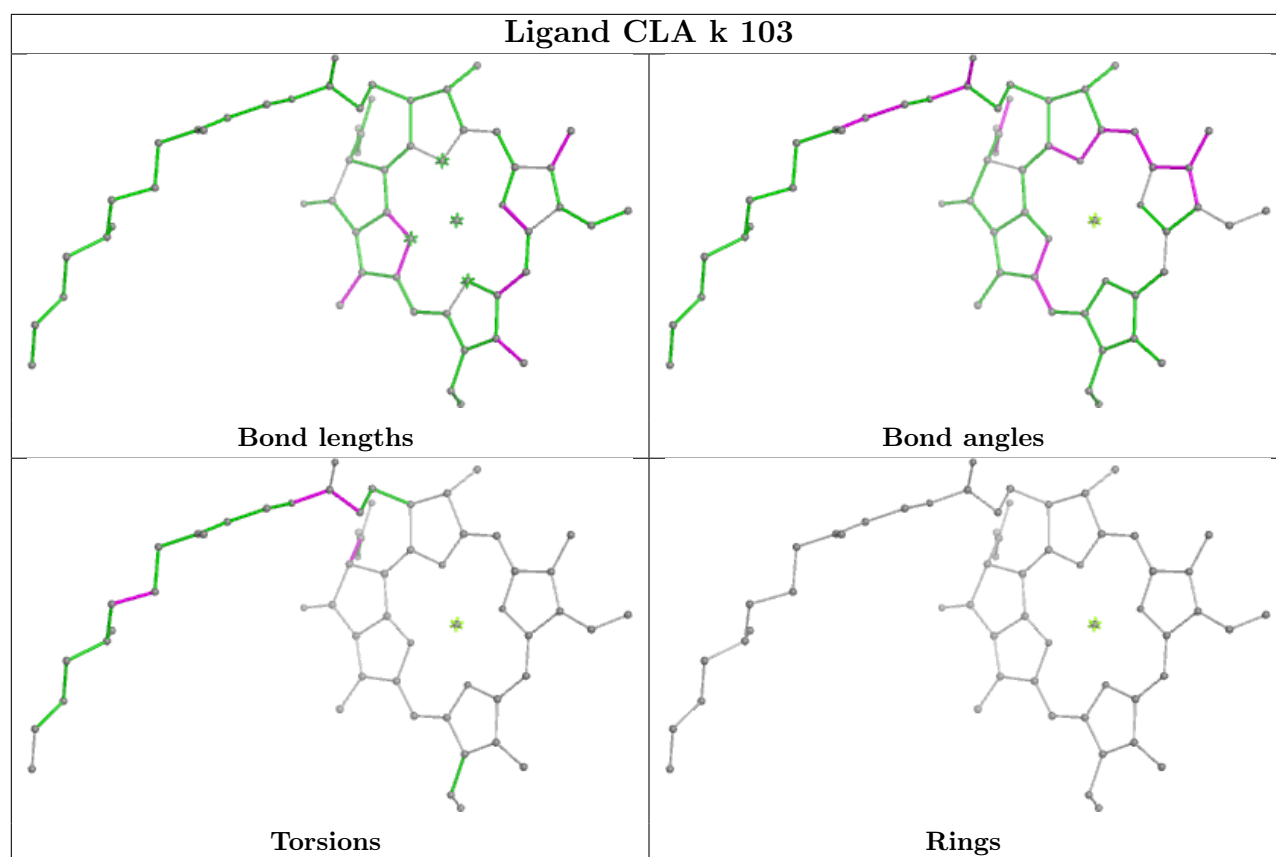


Ligand CLA b 813

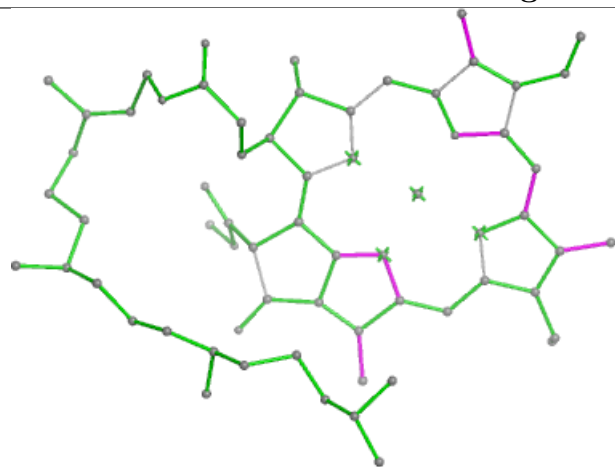


Ligand BCR 8 1305

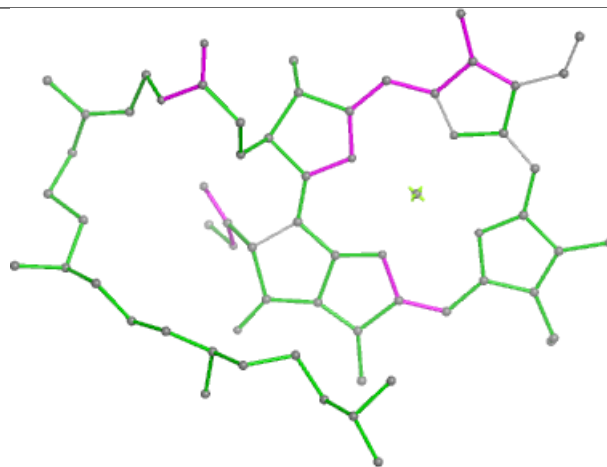




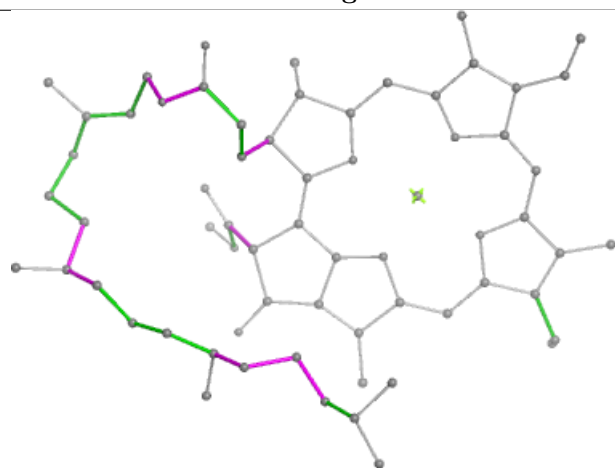
Ligand CLA 2 806



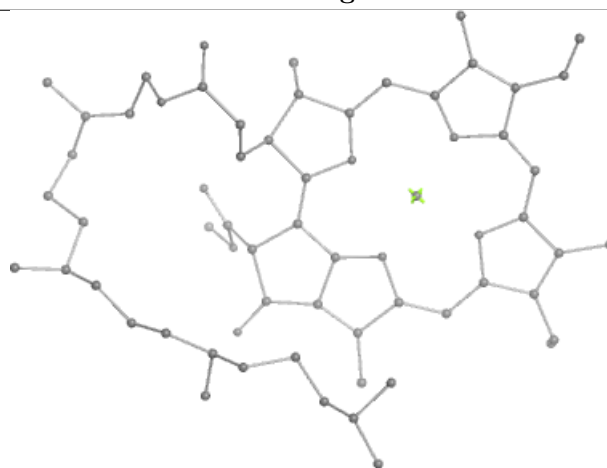
Bond lengths



Bond angles

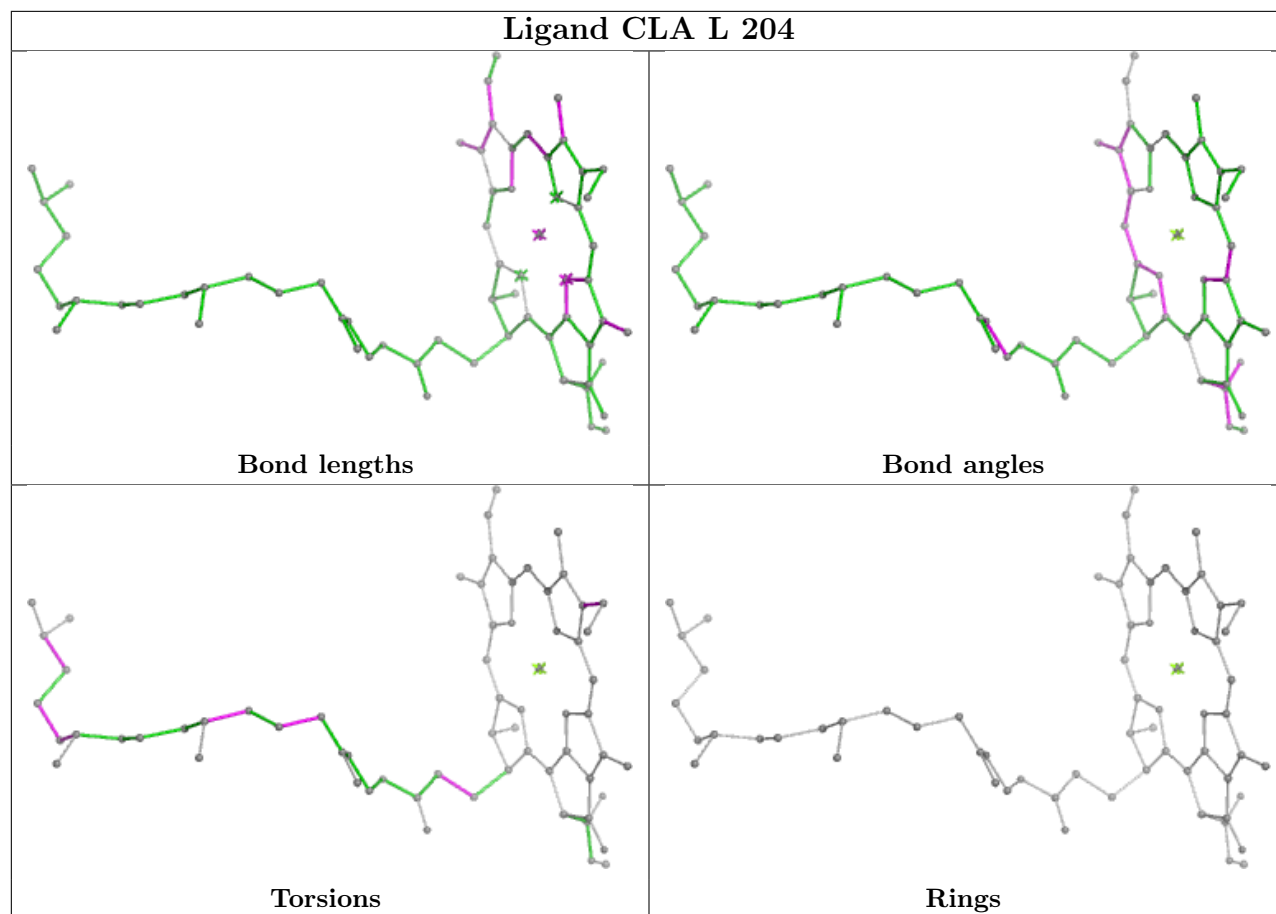


Torsions

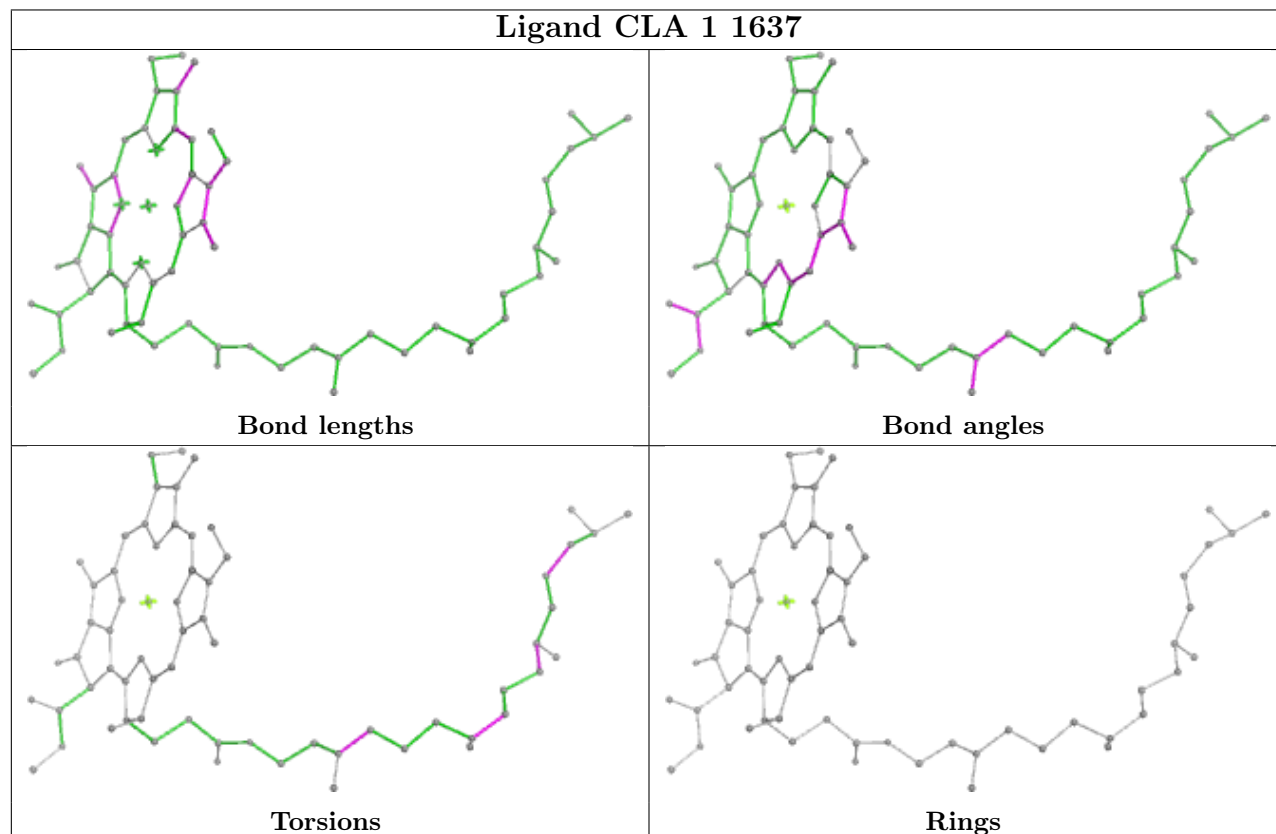


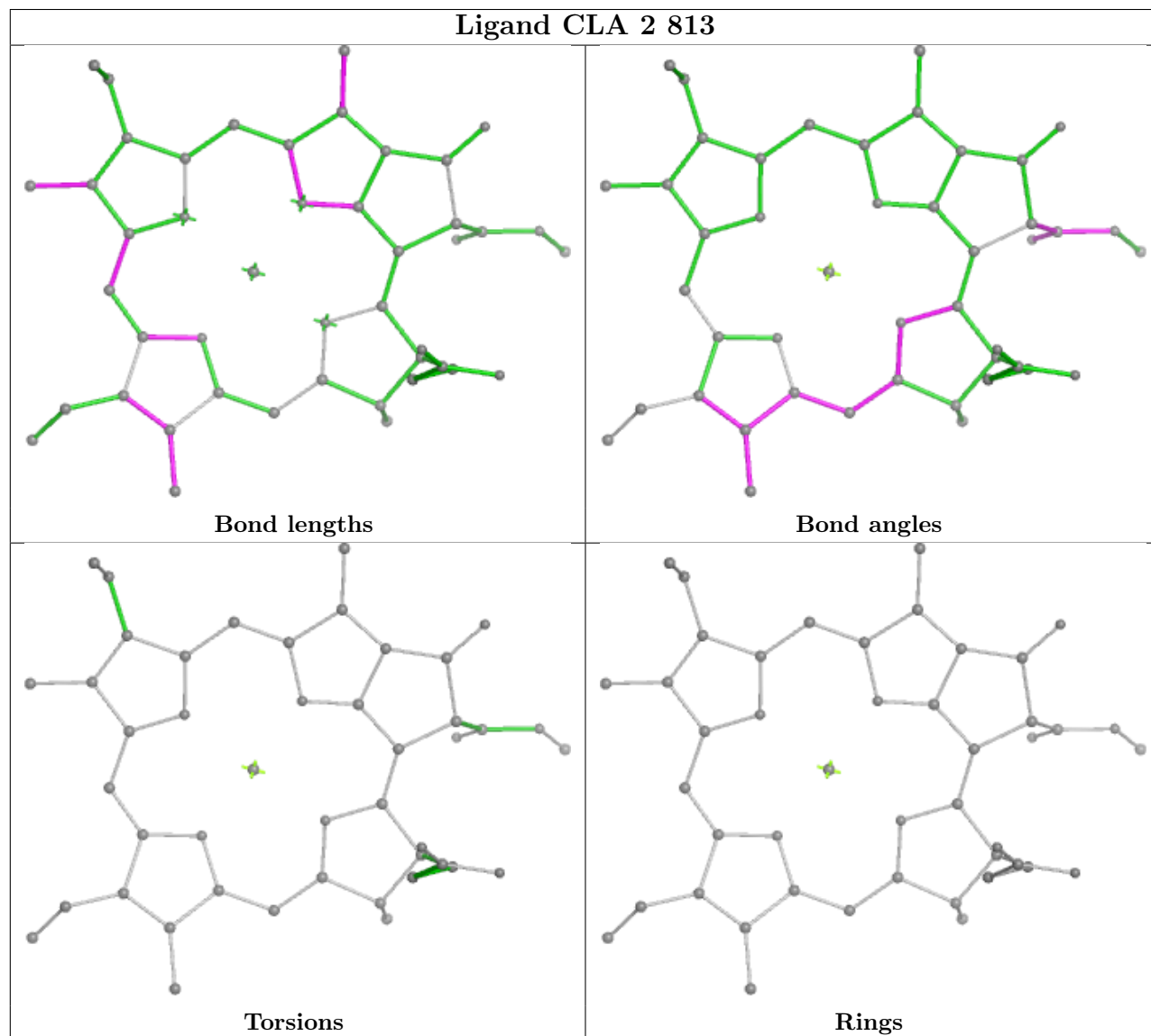
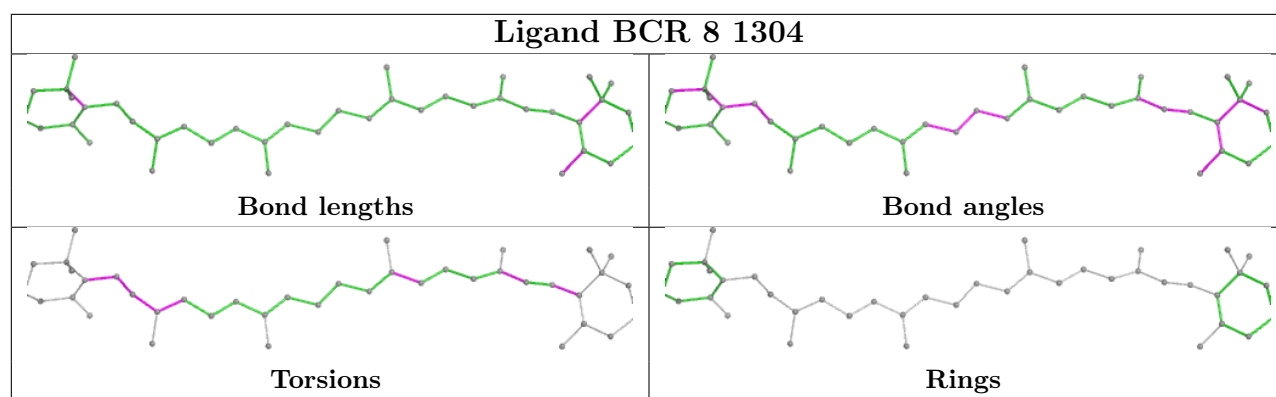
Rings

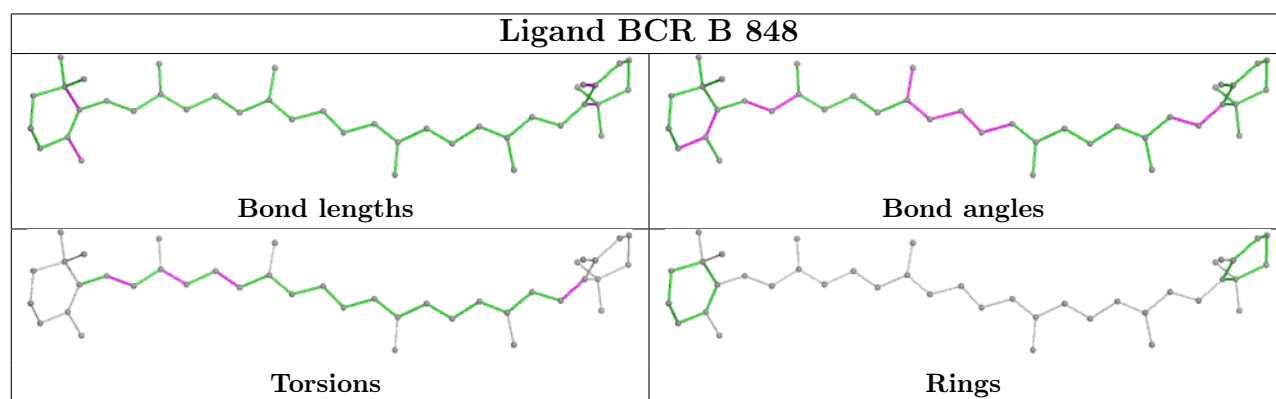
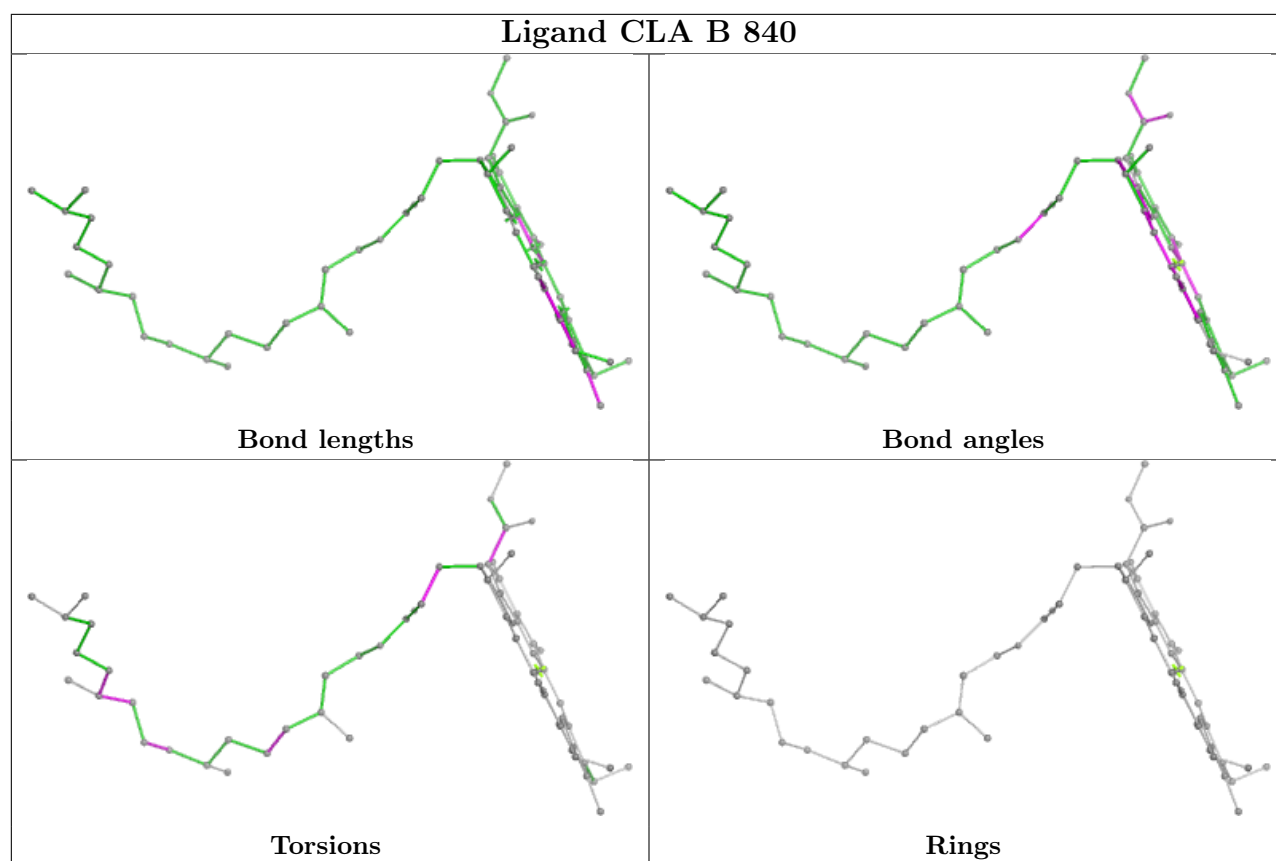
Ligand CLA L 204



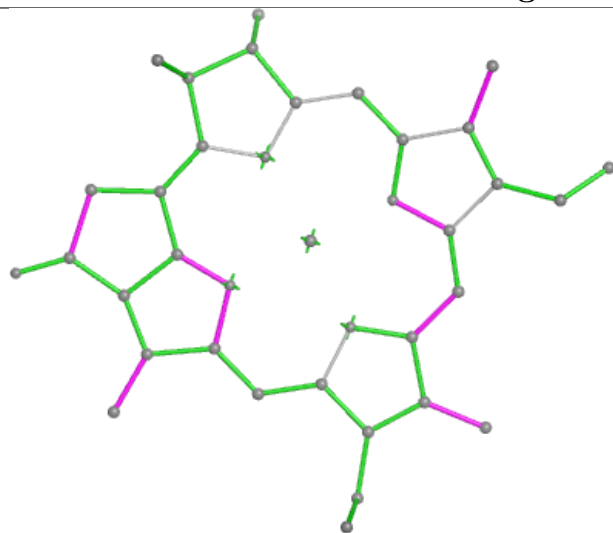
Ligand CLA 1 1637



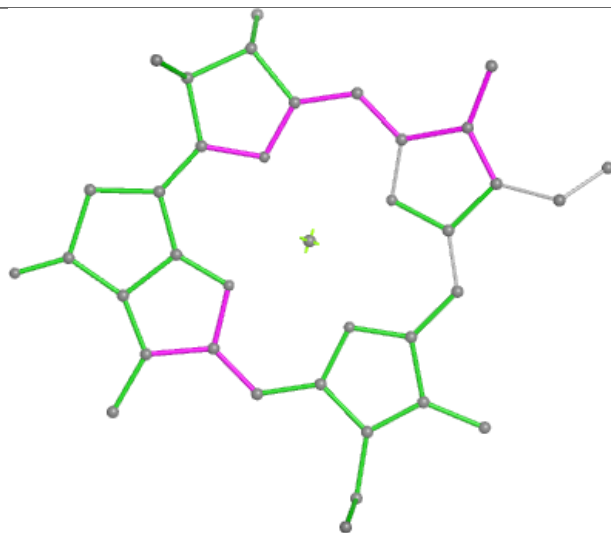




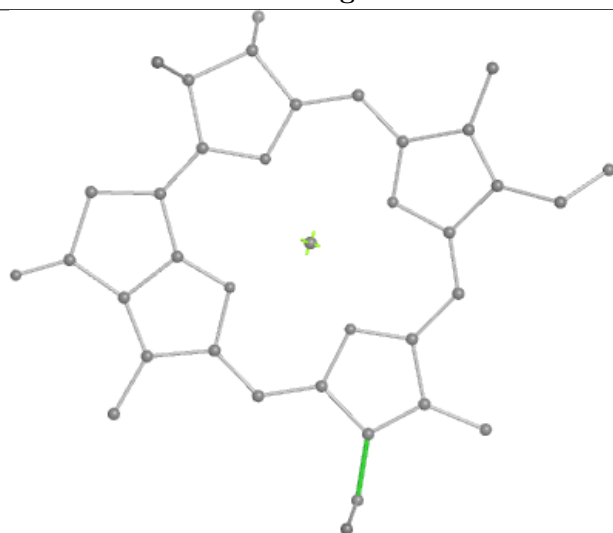
Ligand CLA J 102



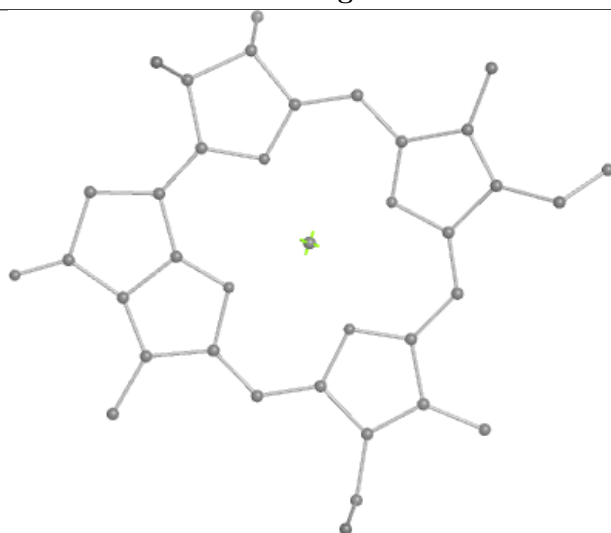
Bond lengths



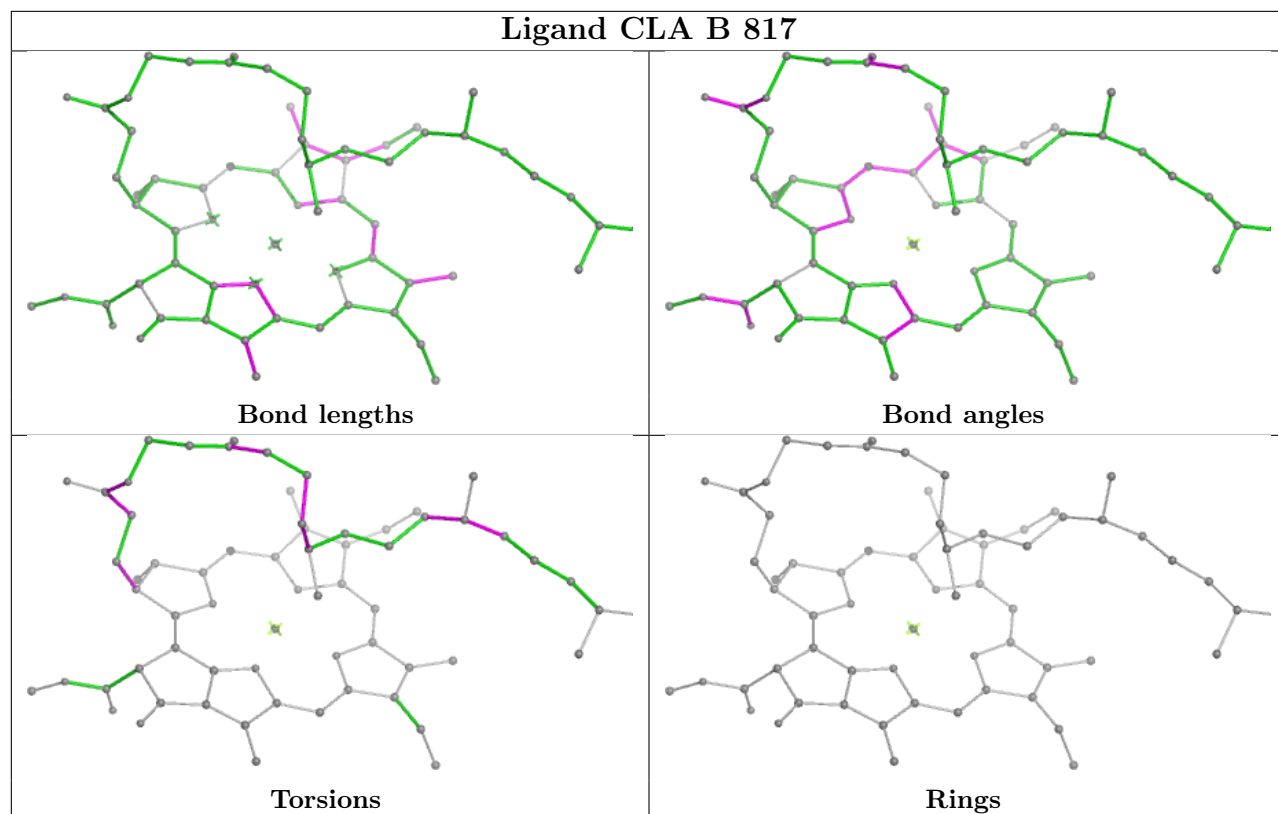
Bond angles

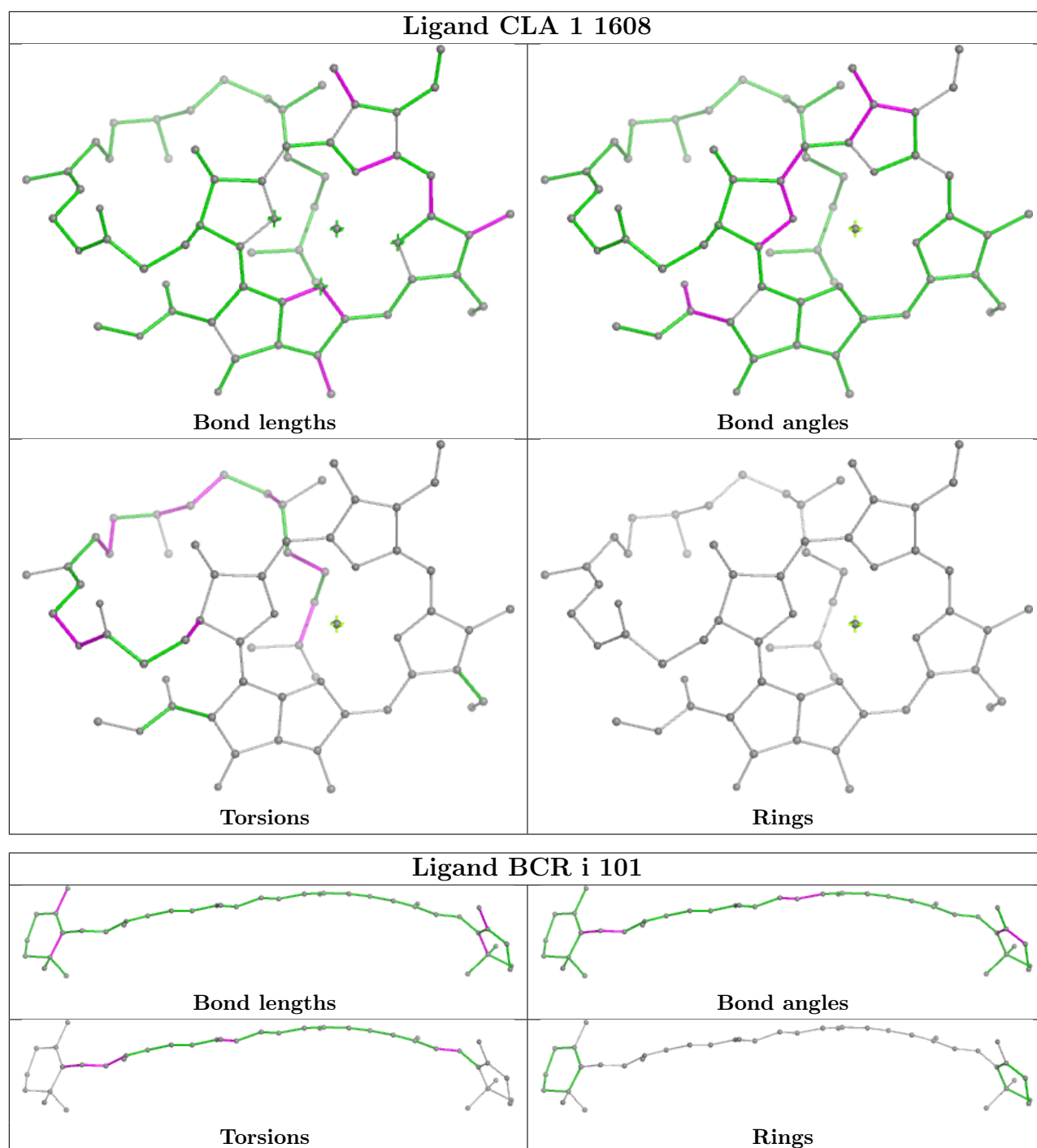


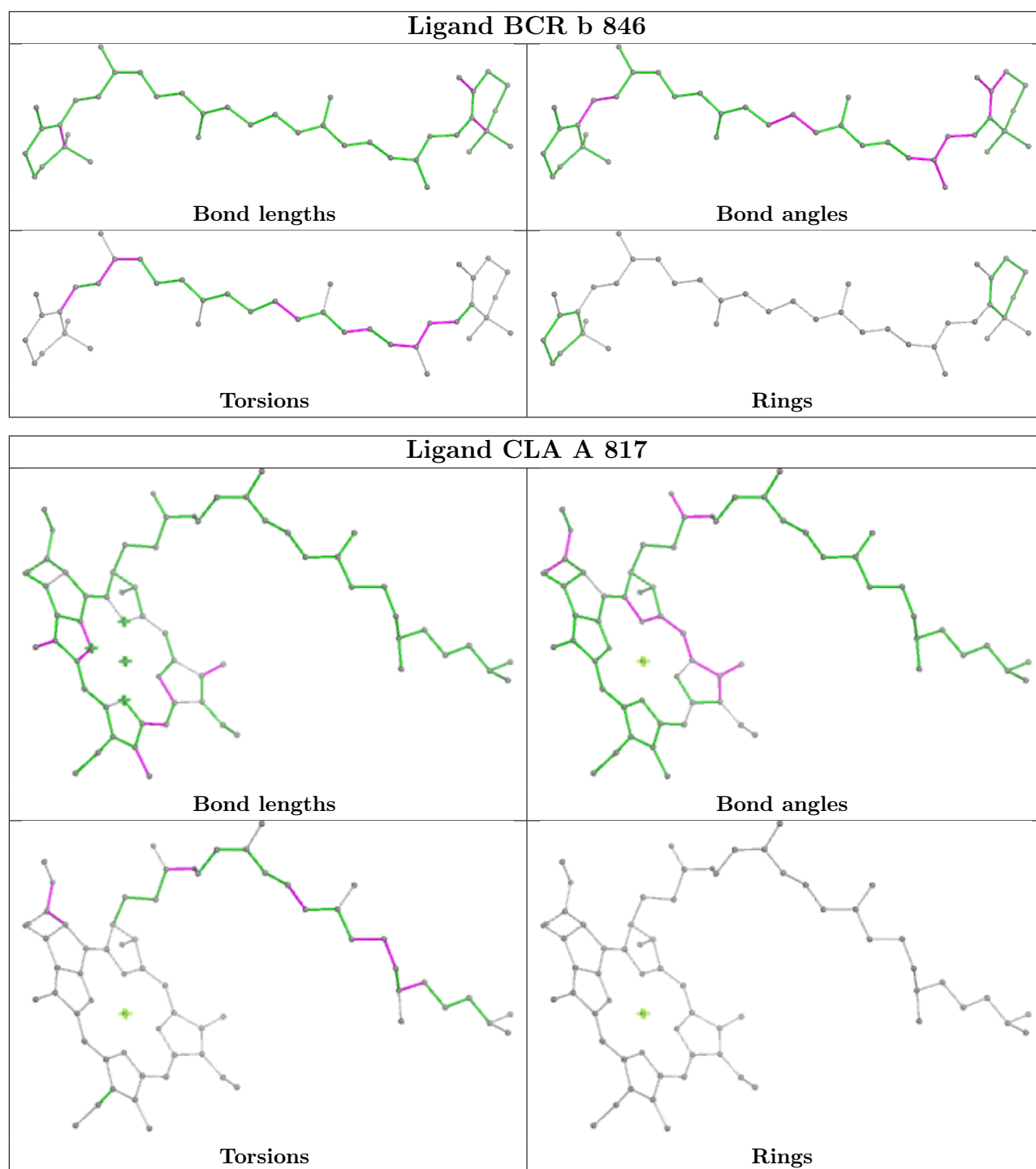
Torsions

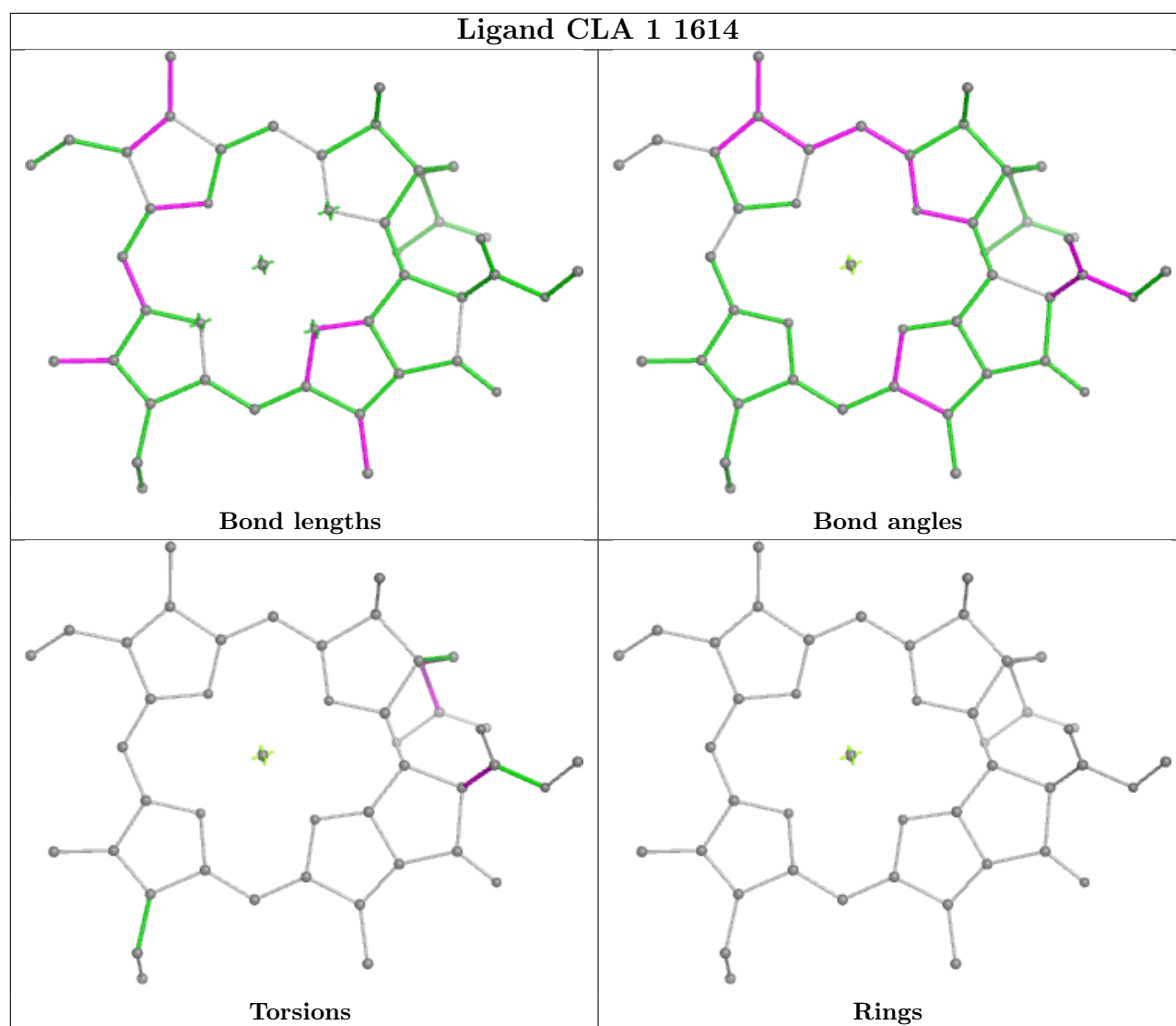


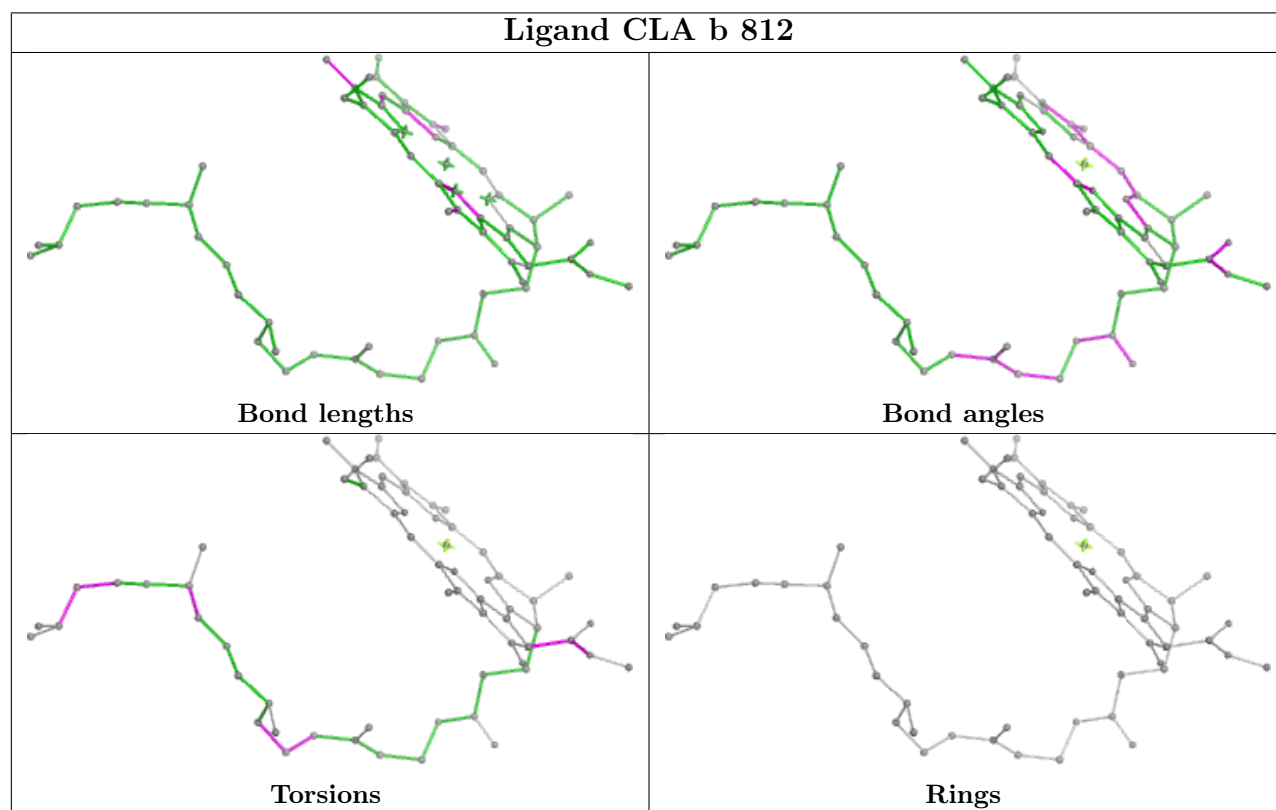
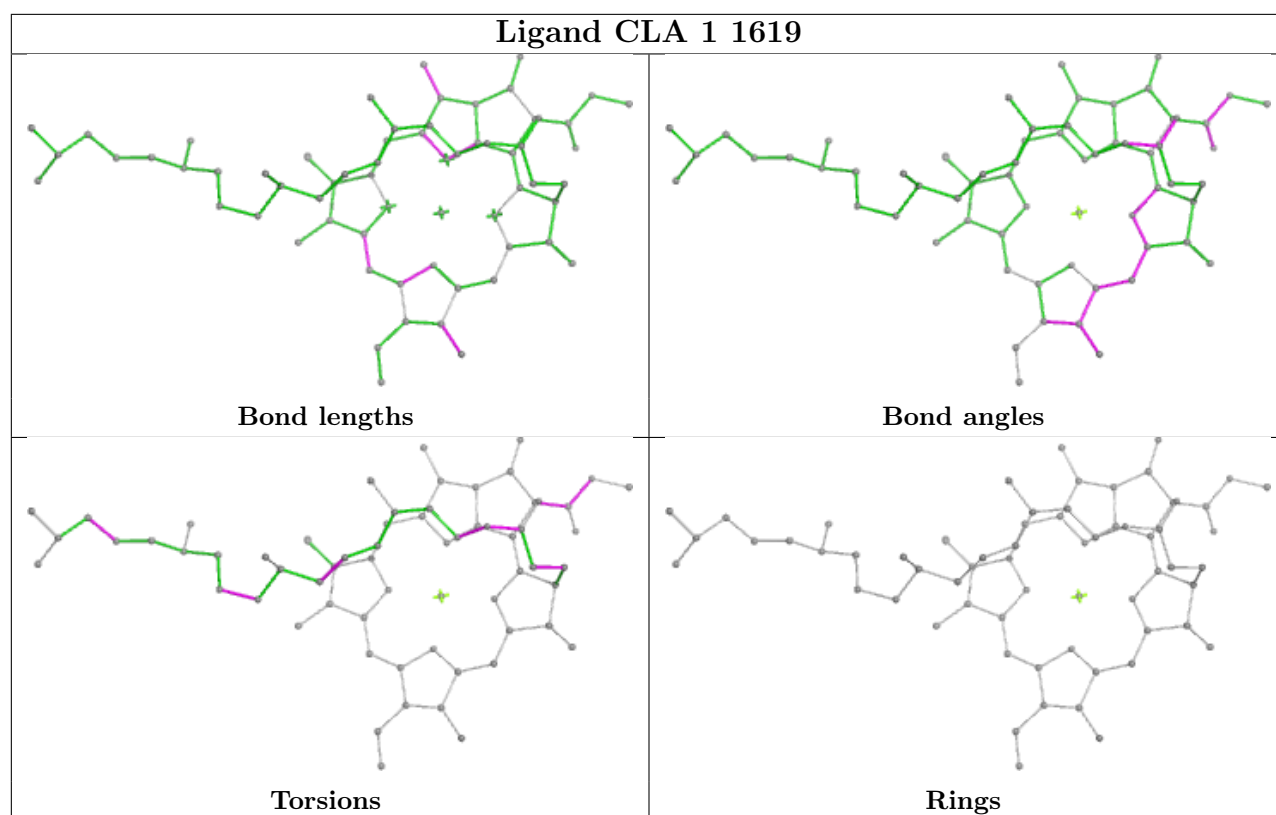
Rings



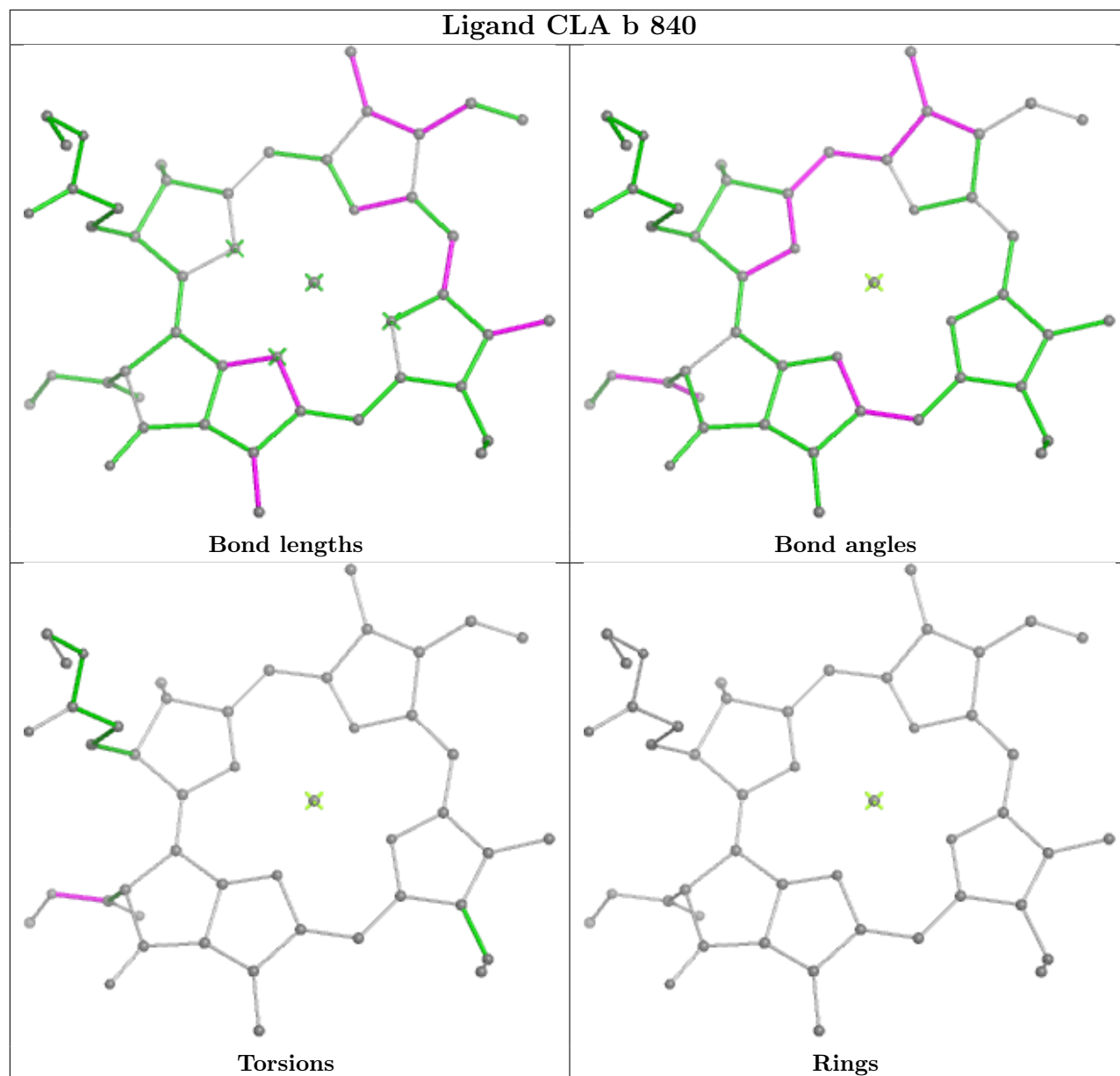


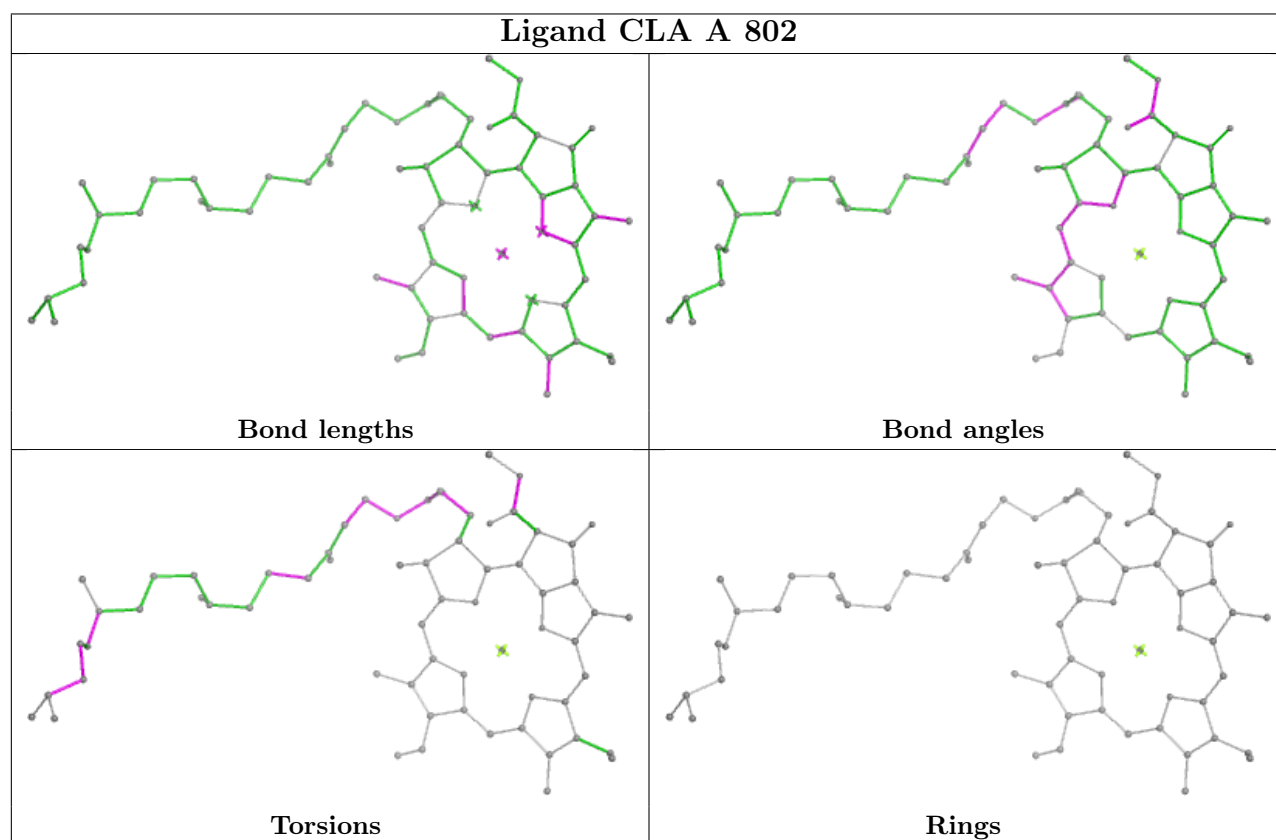
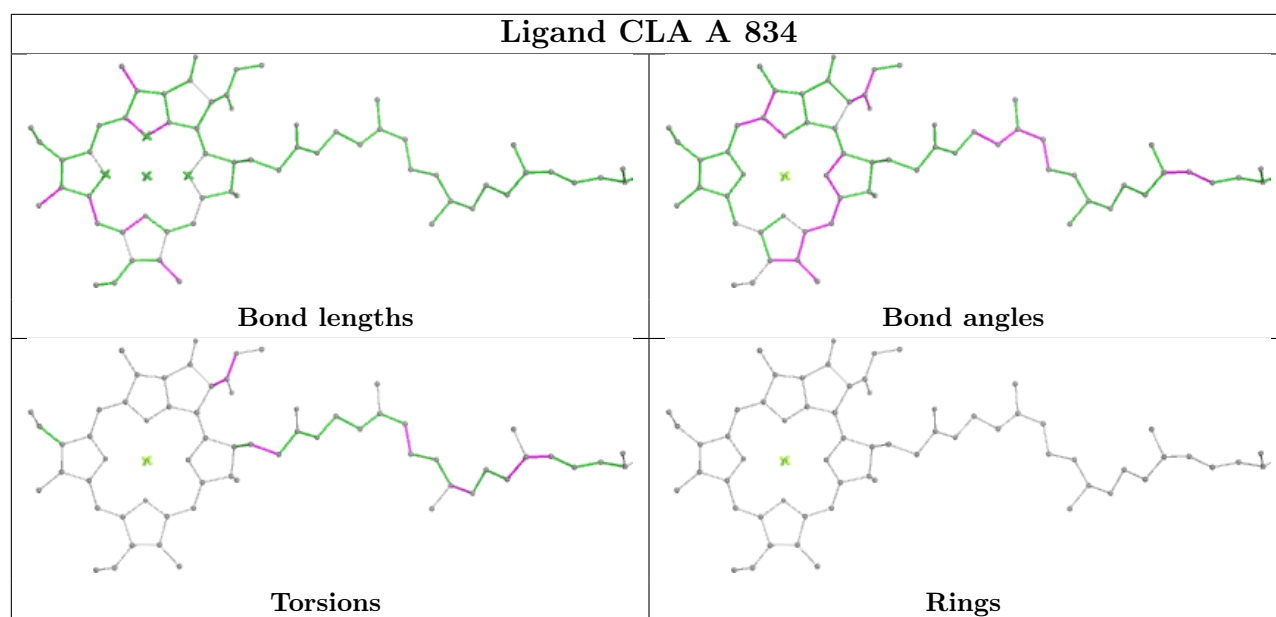


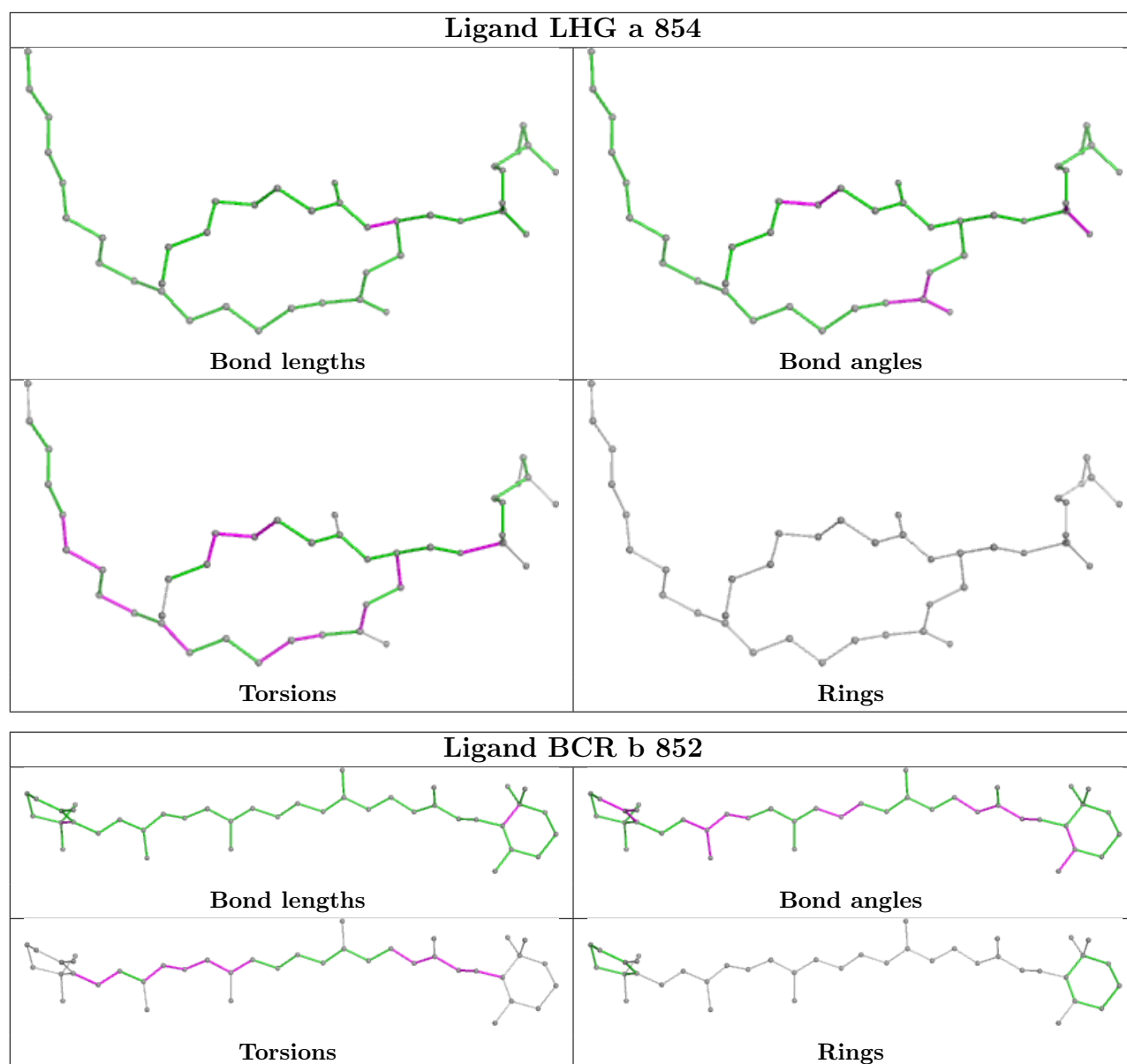


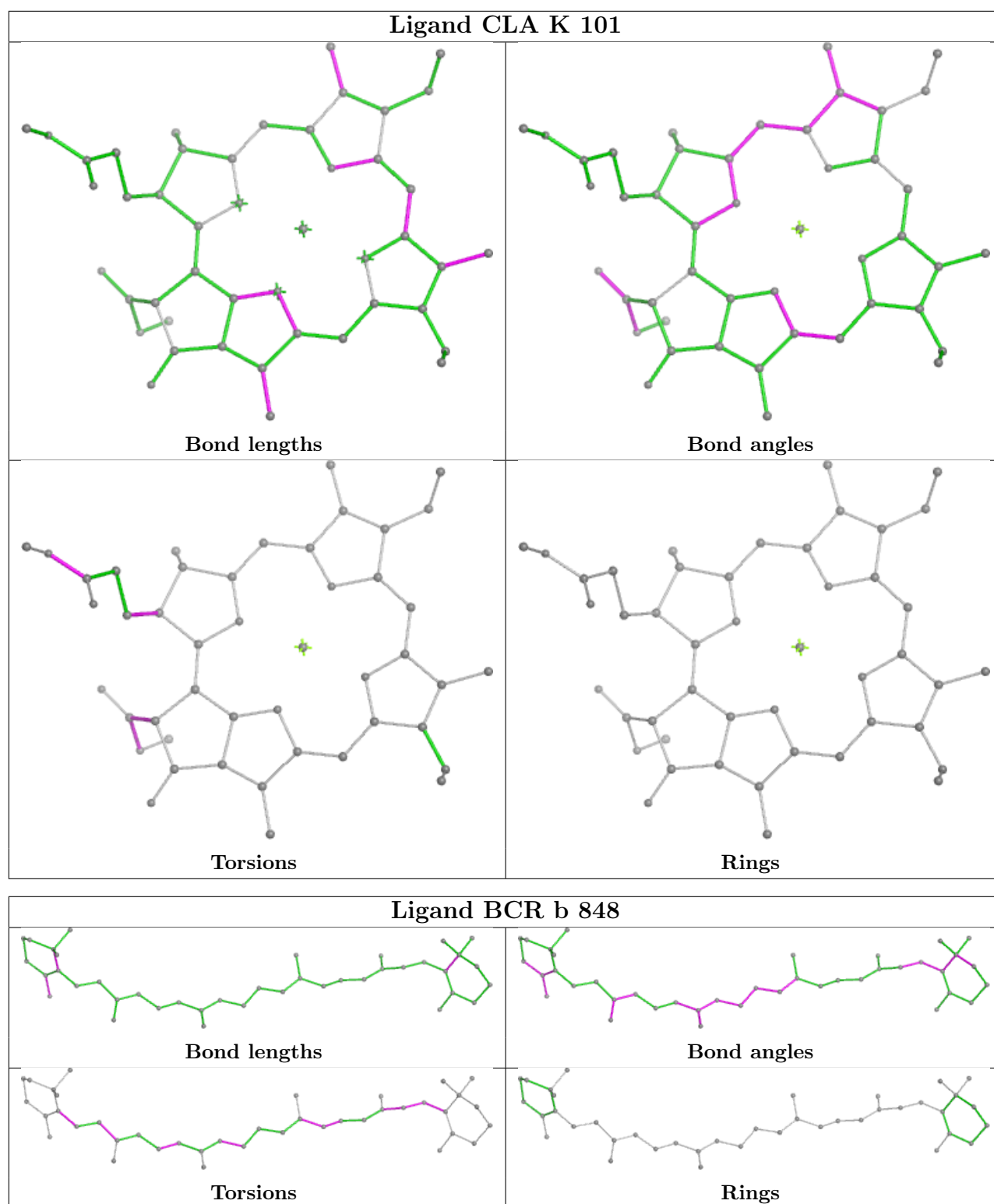


Ligand CLA b 840

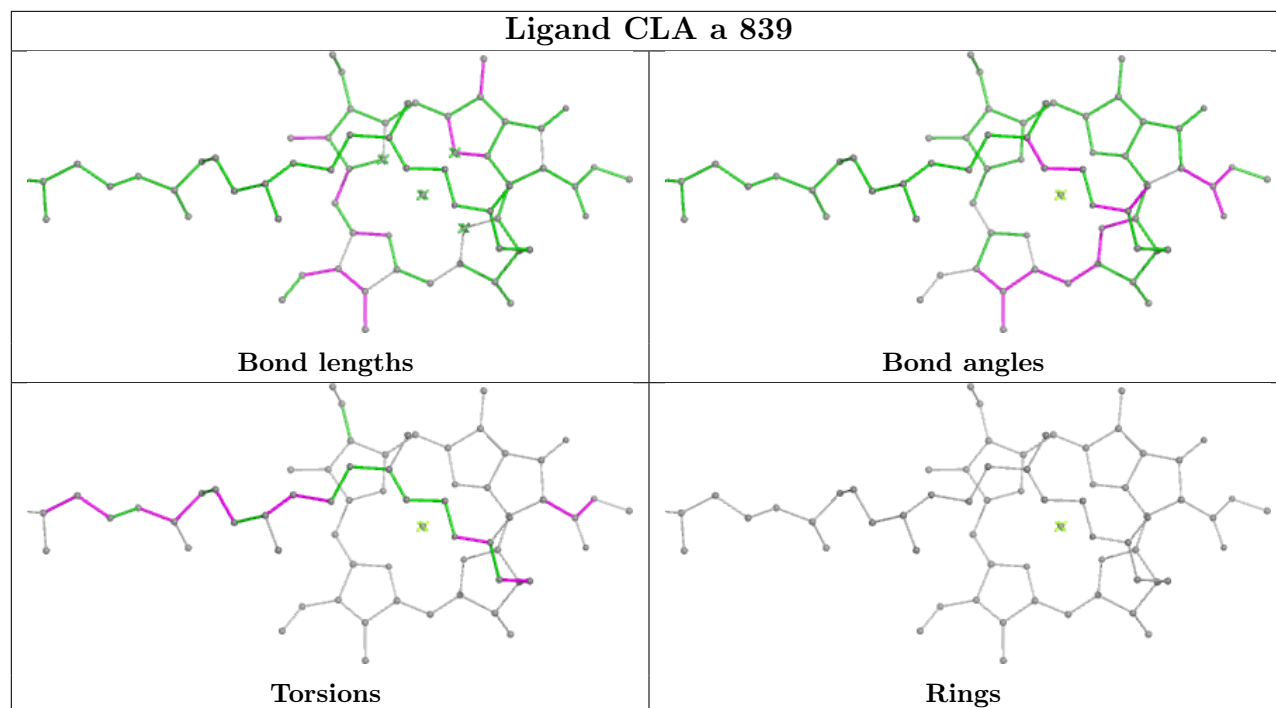




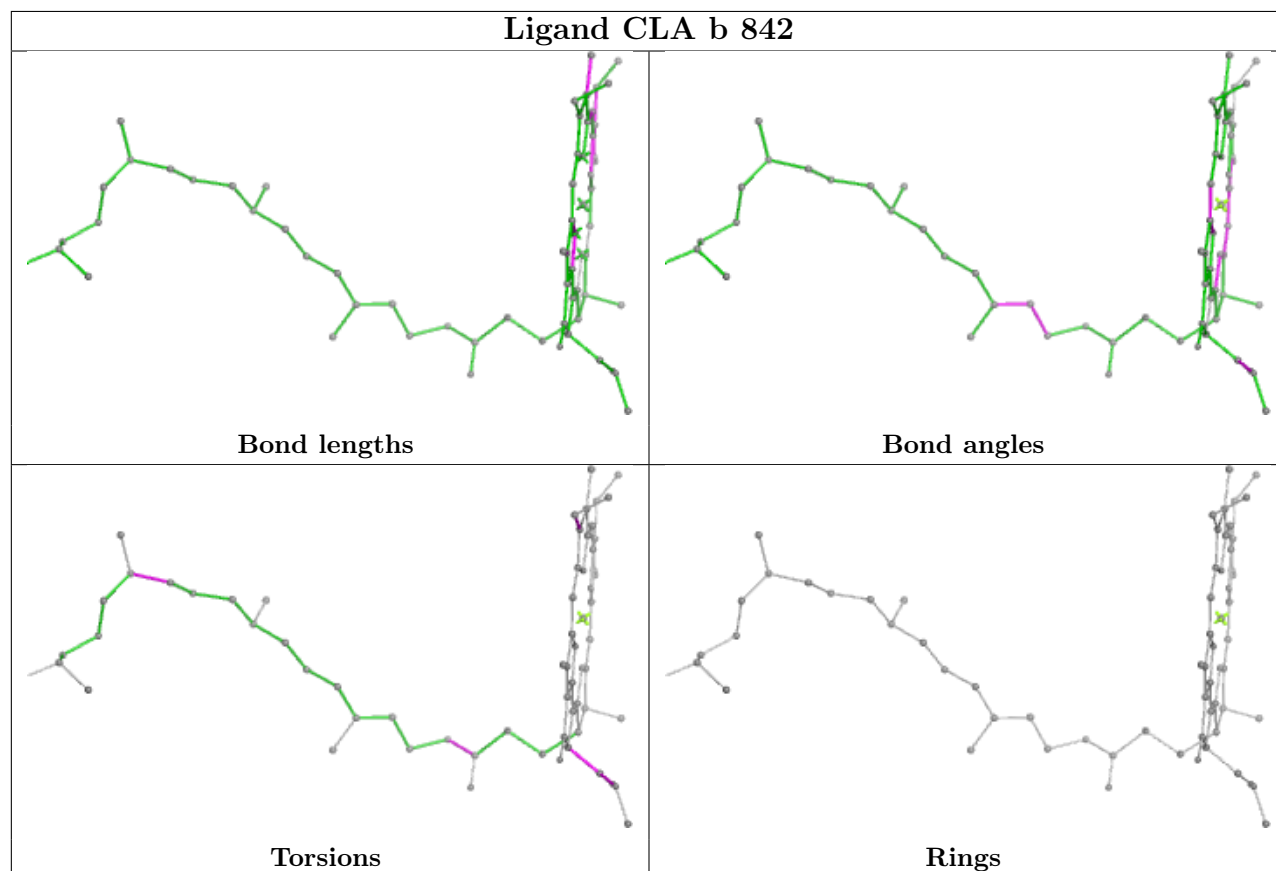


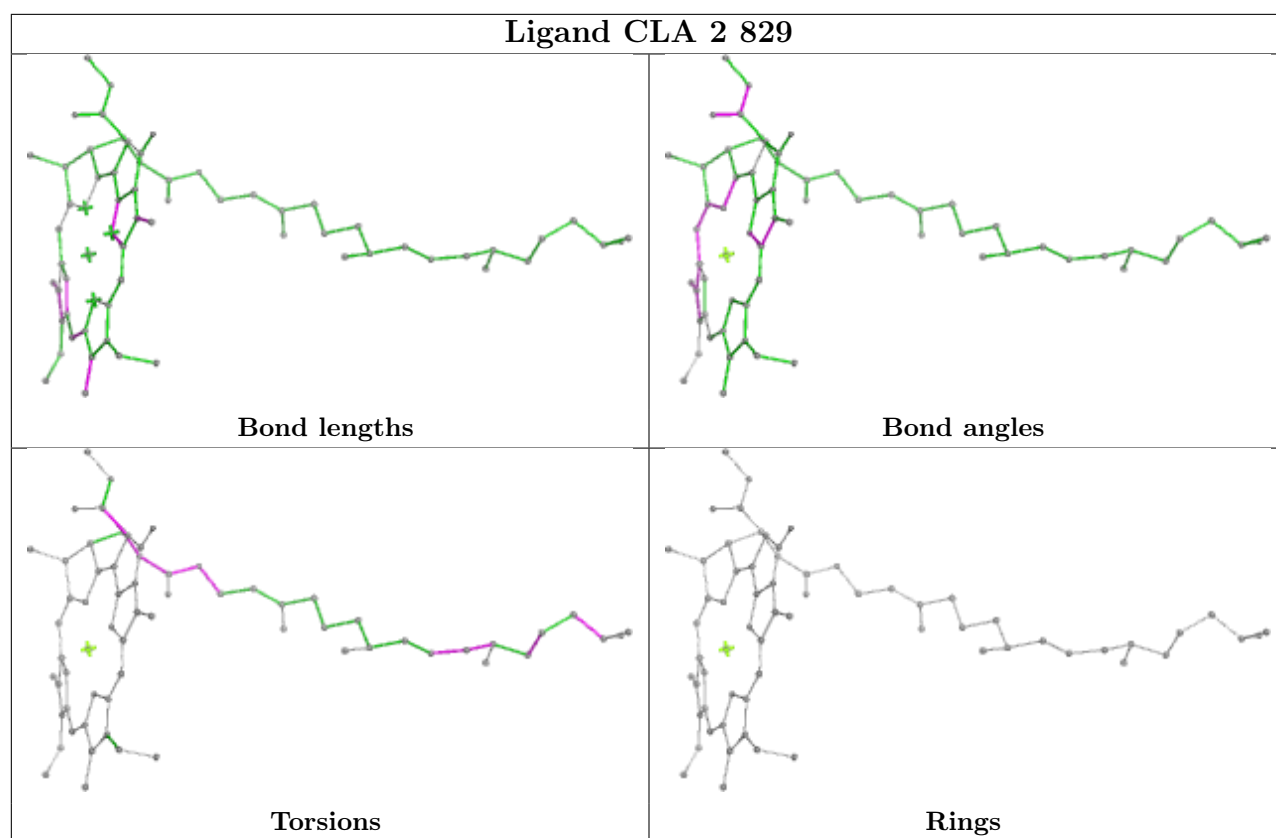


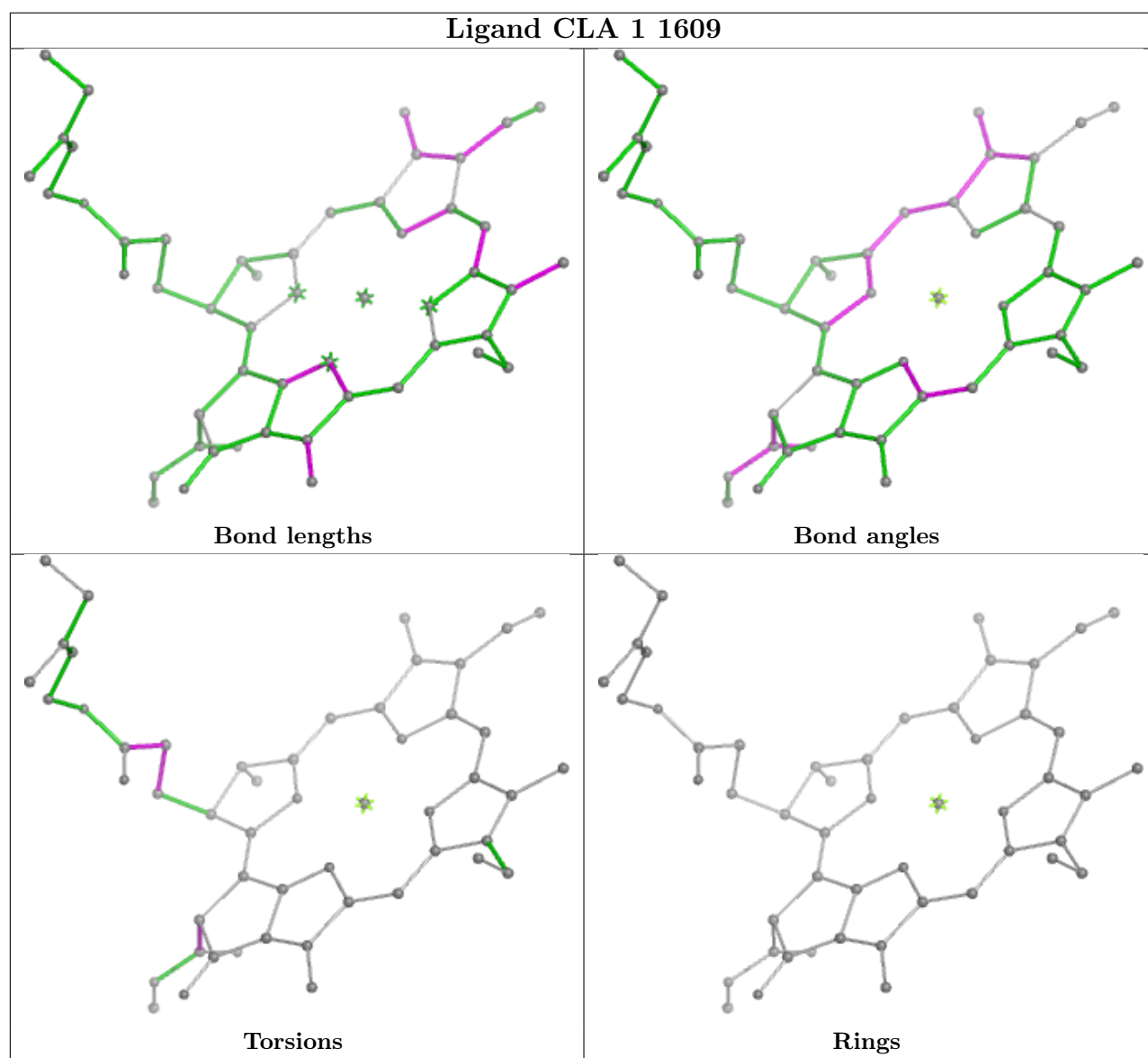
Ligand CLA a 839

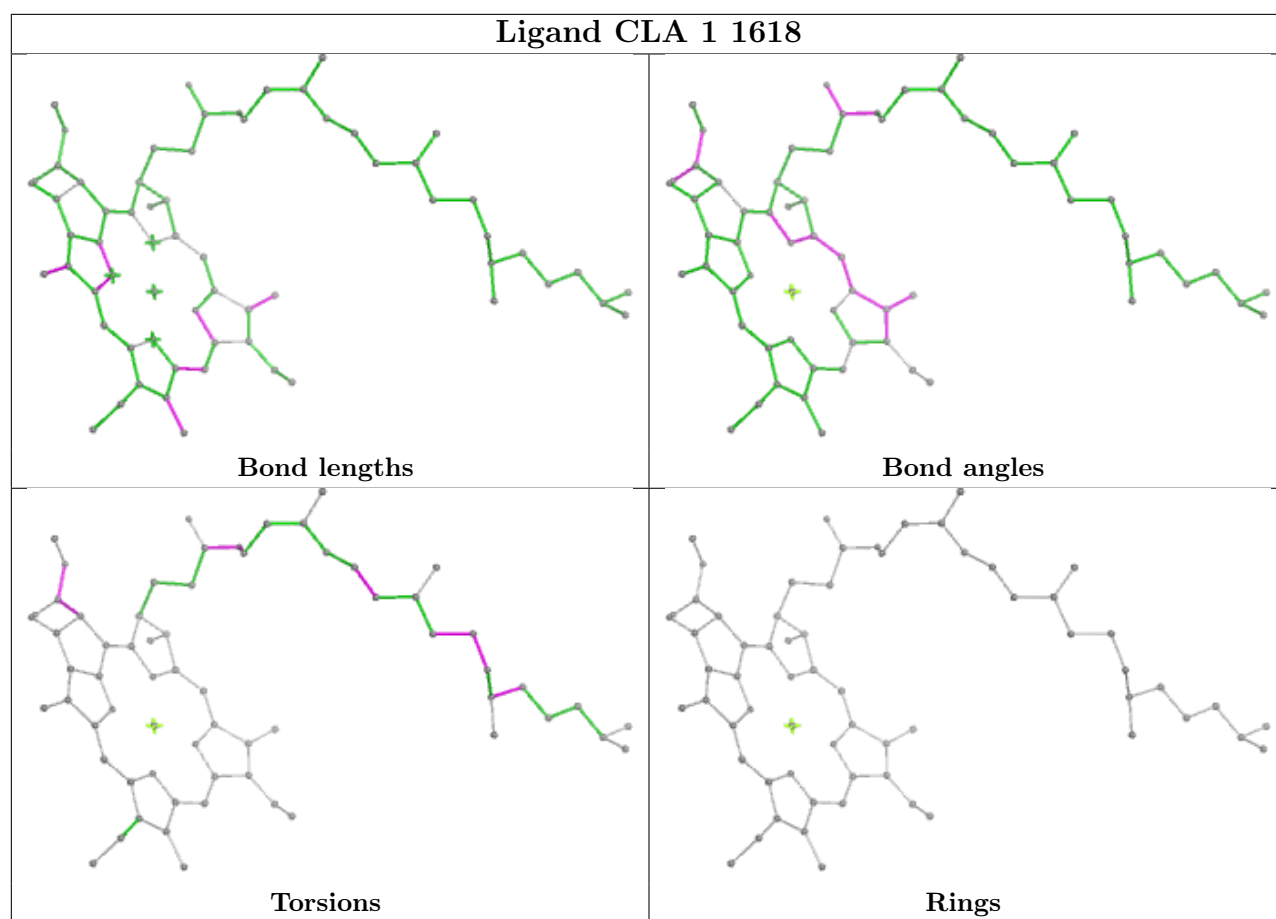


Ligand CLA b 842

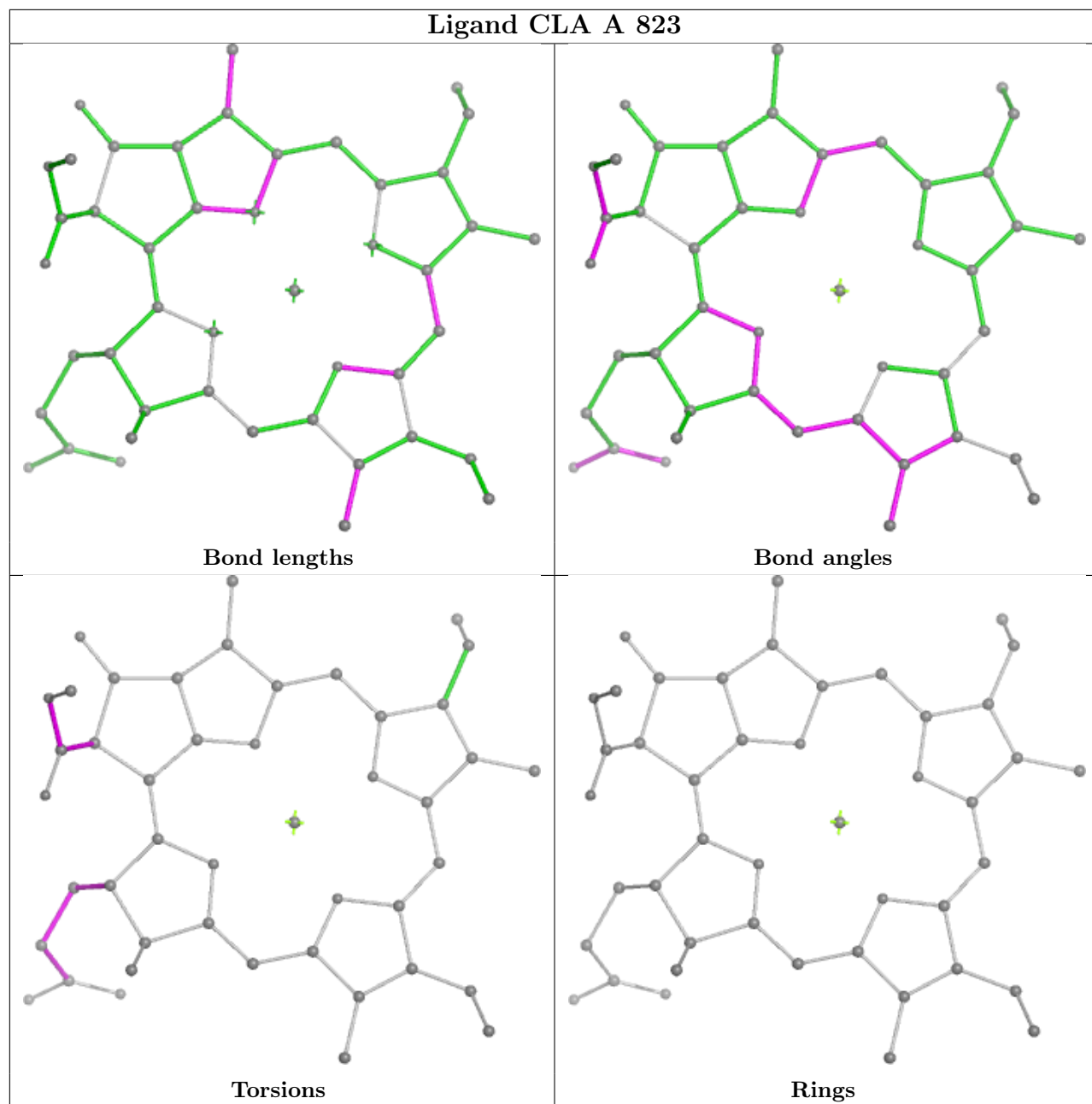


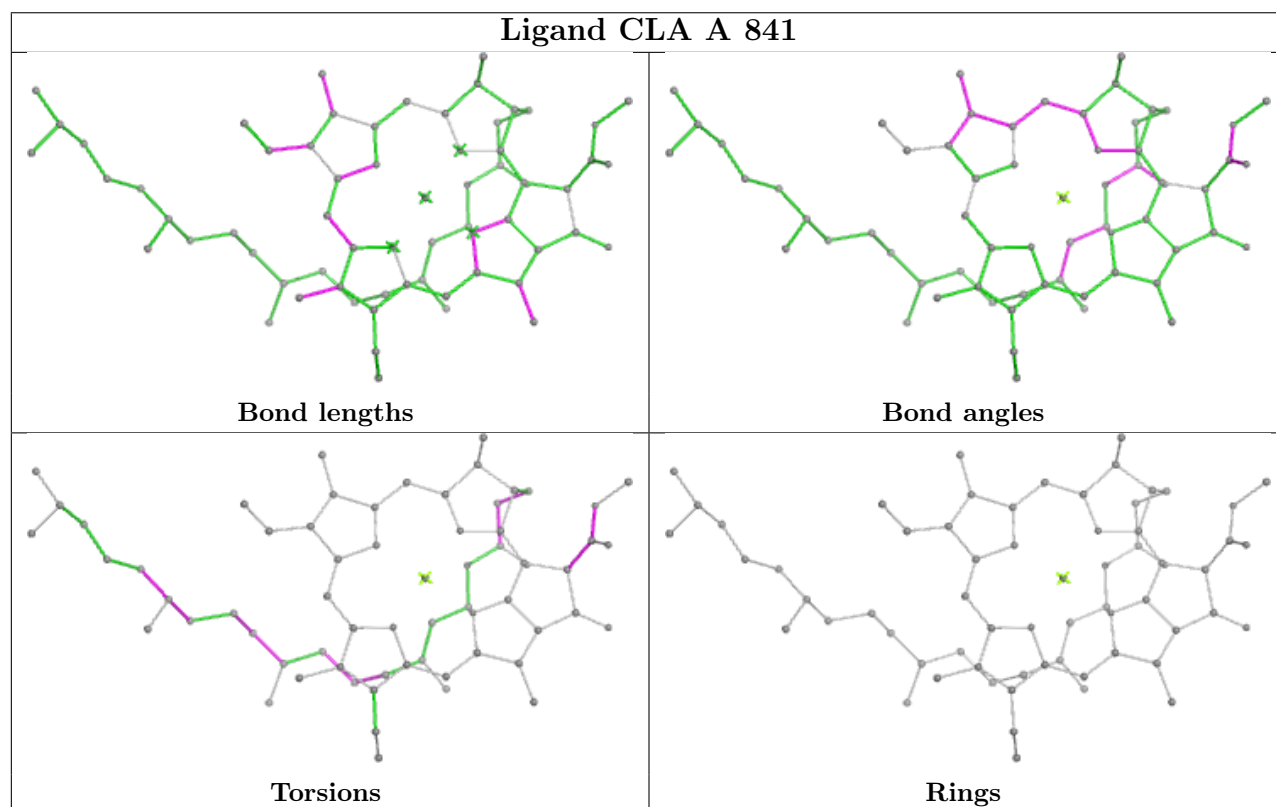
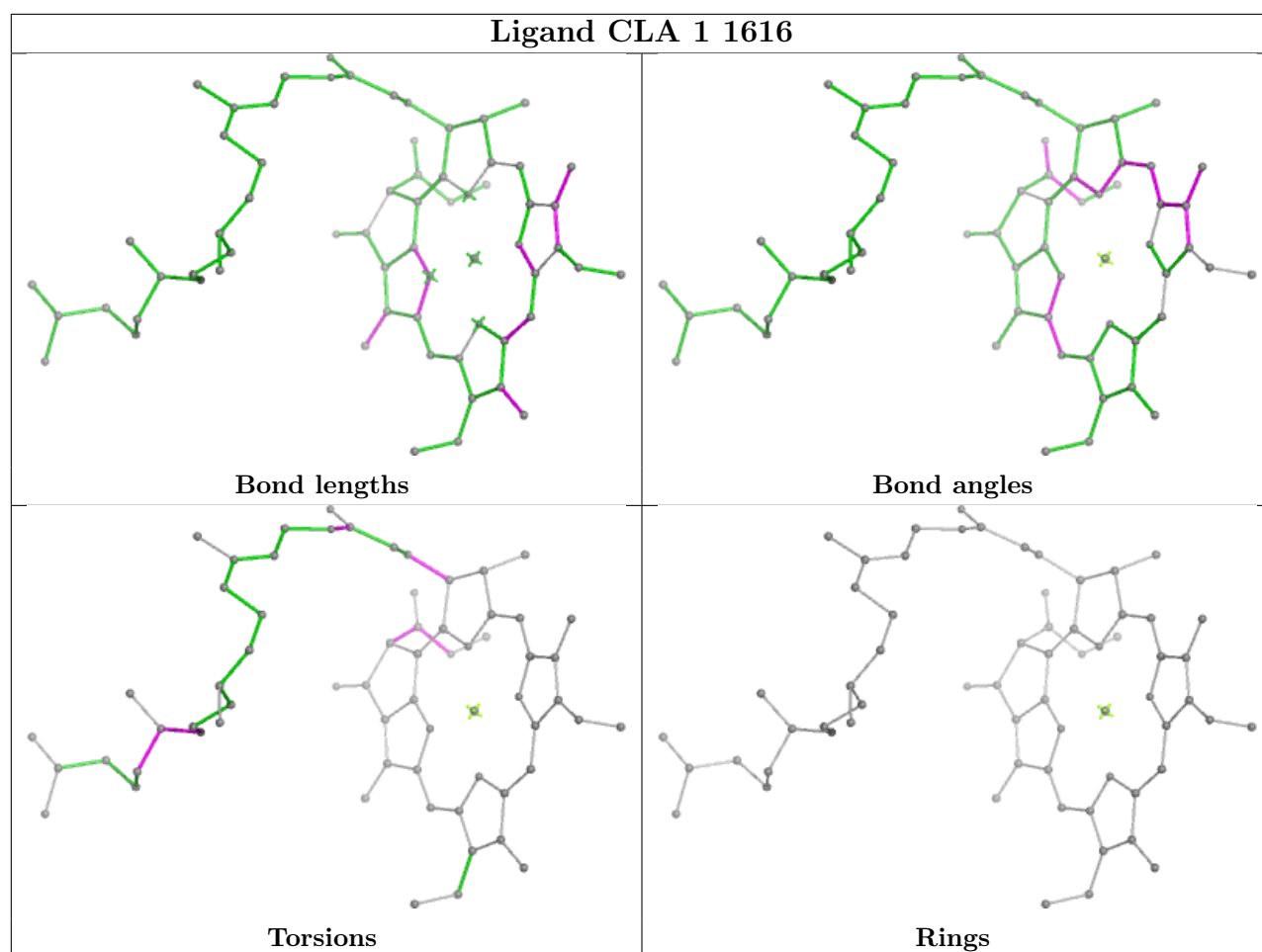


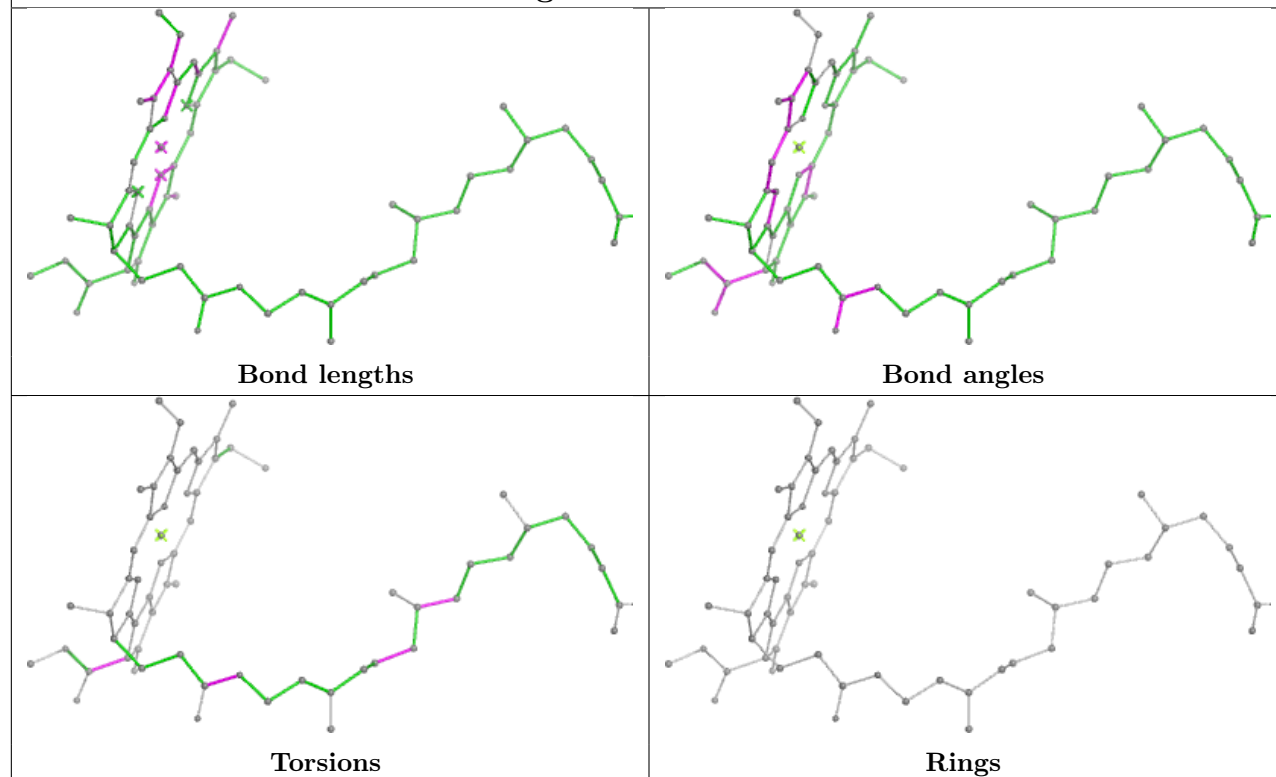
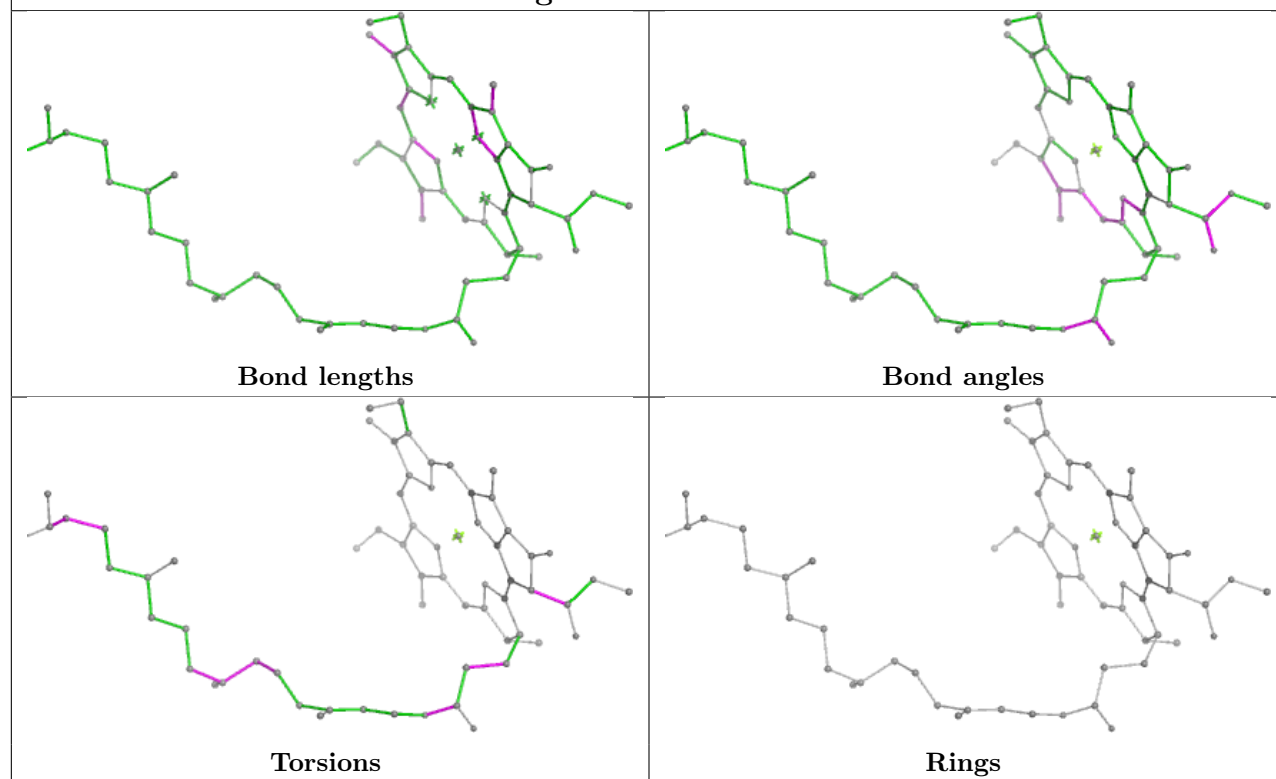




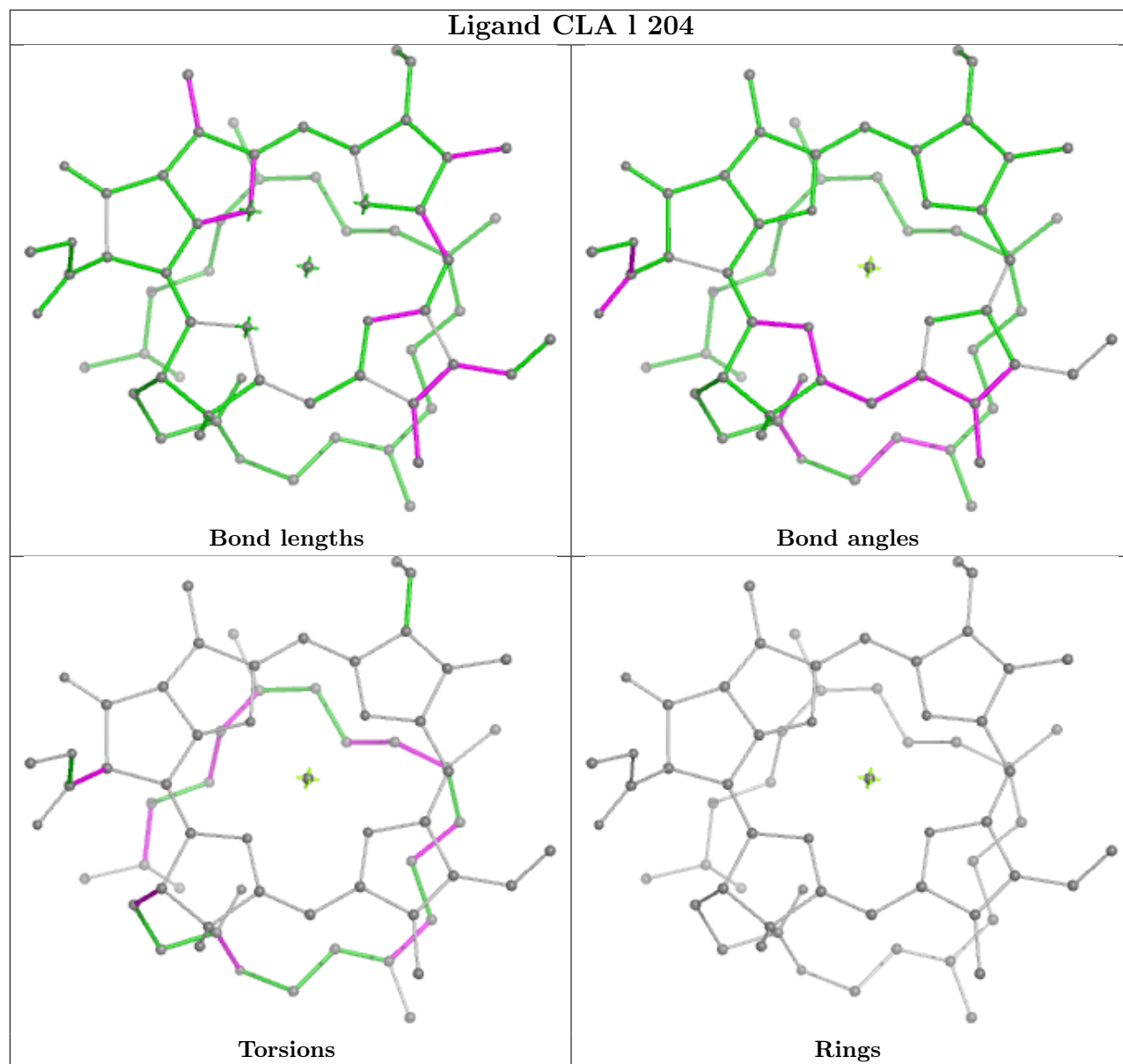
Ligand CLA A 823

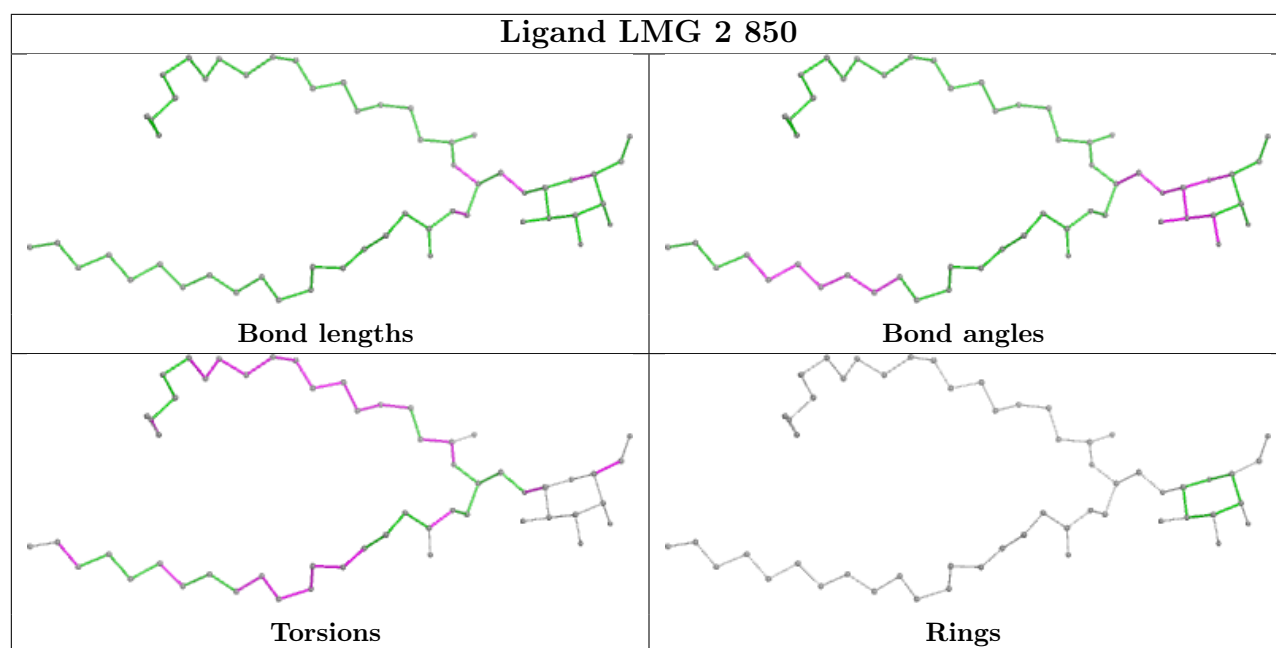


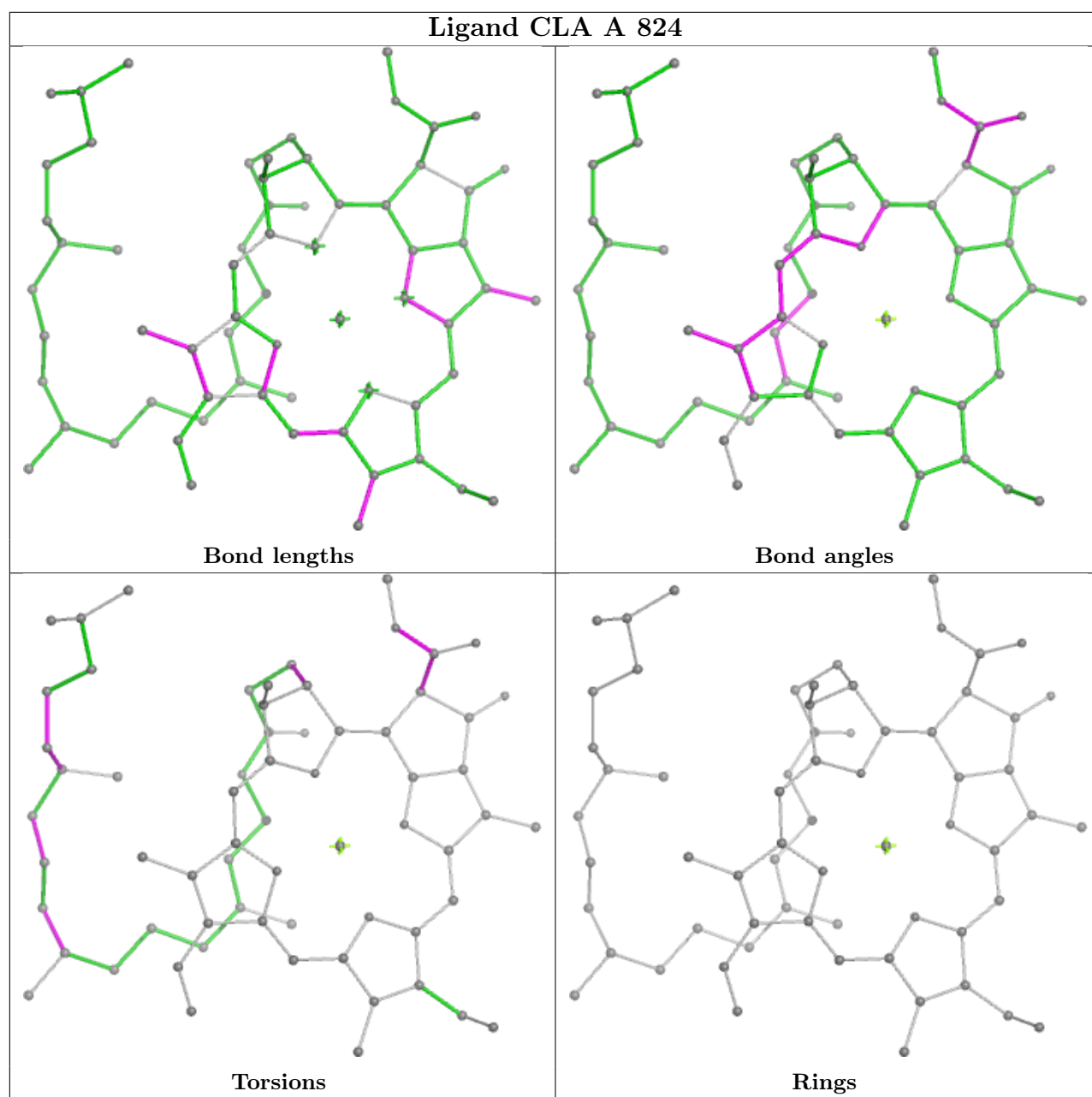


Ligand CLA a 831**Ligand CLA b 816**

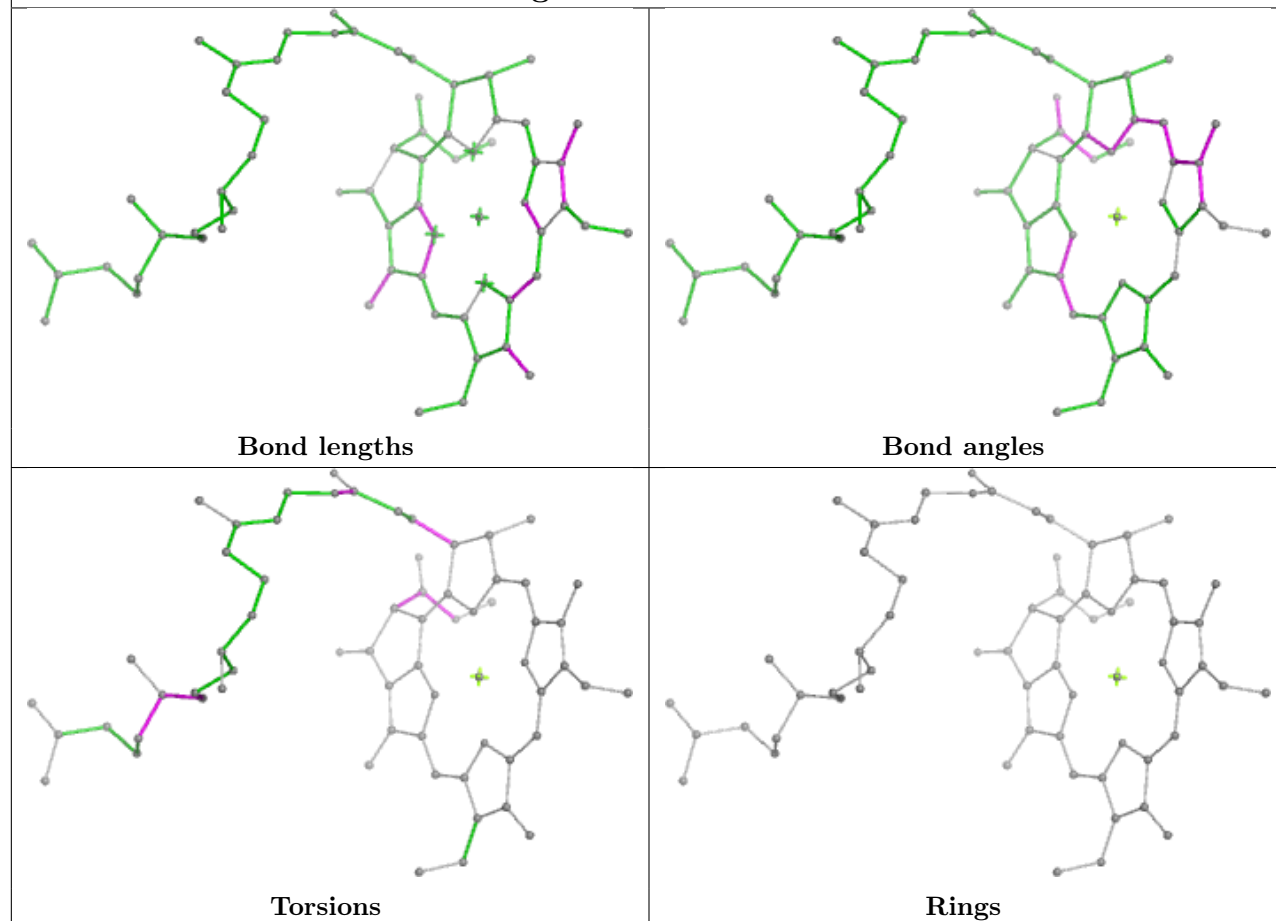
Ligand CLA 1 204



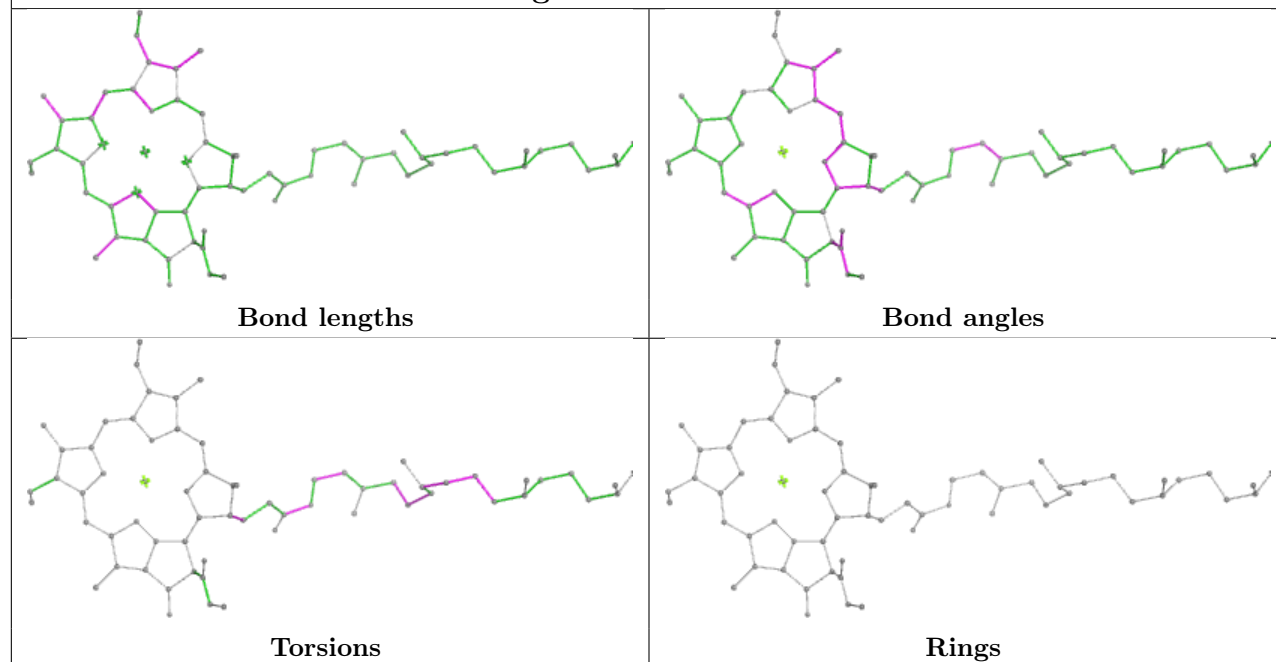


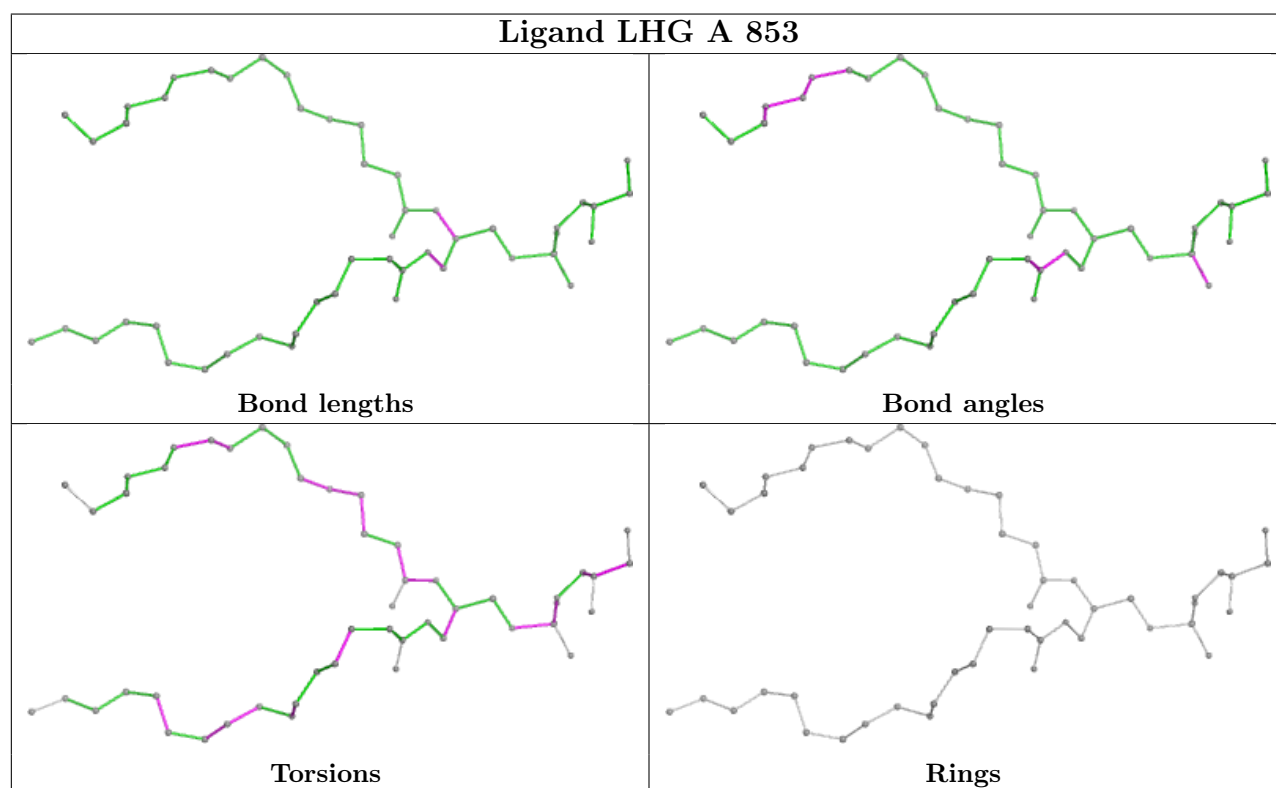
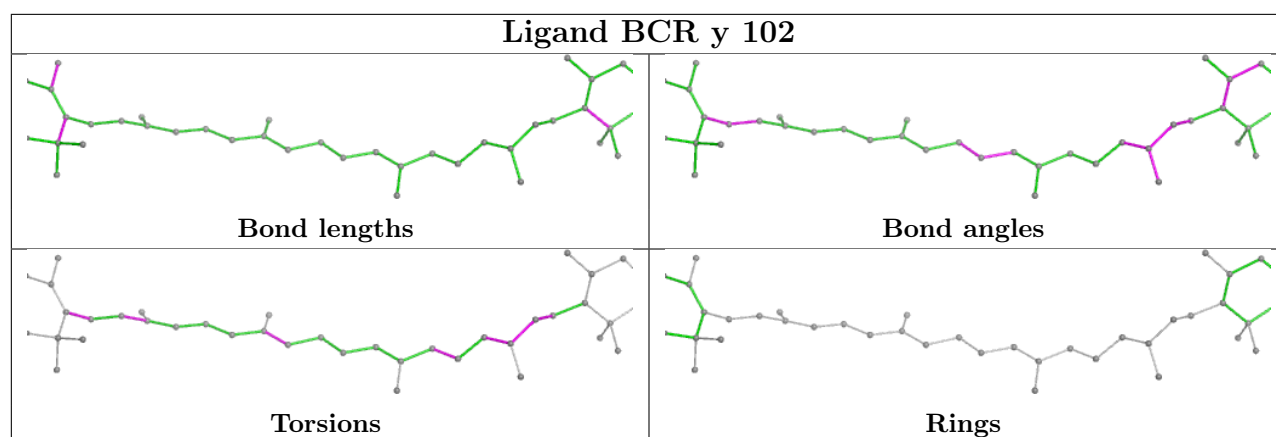


Ligand CLA A 815

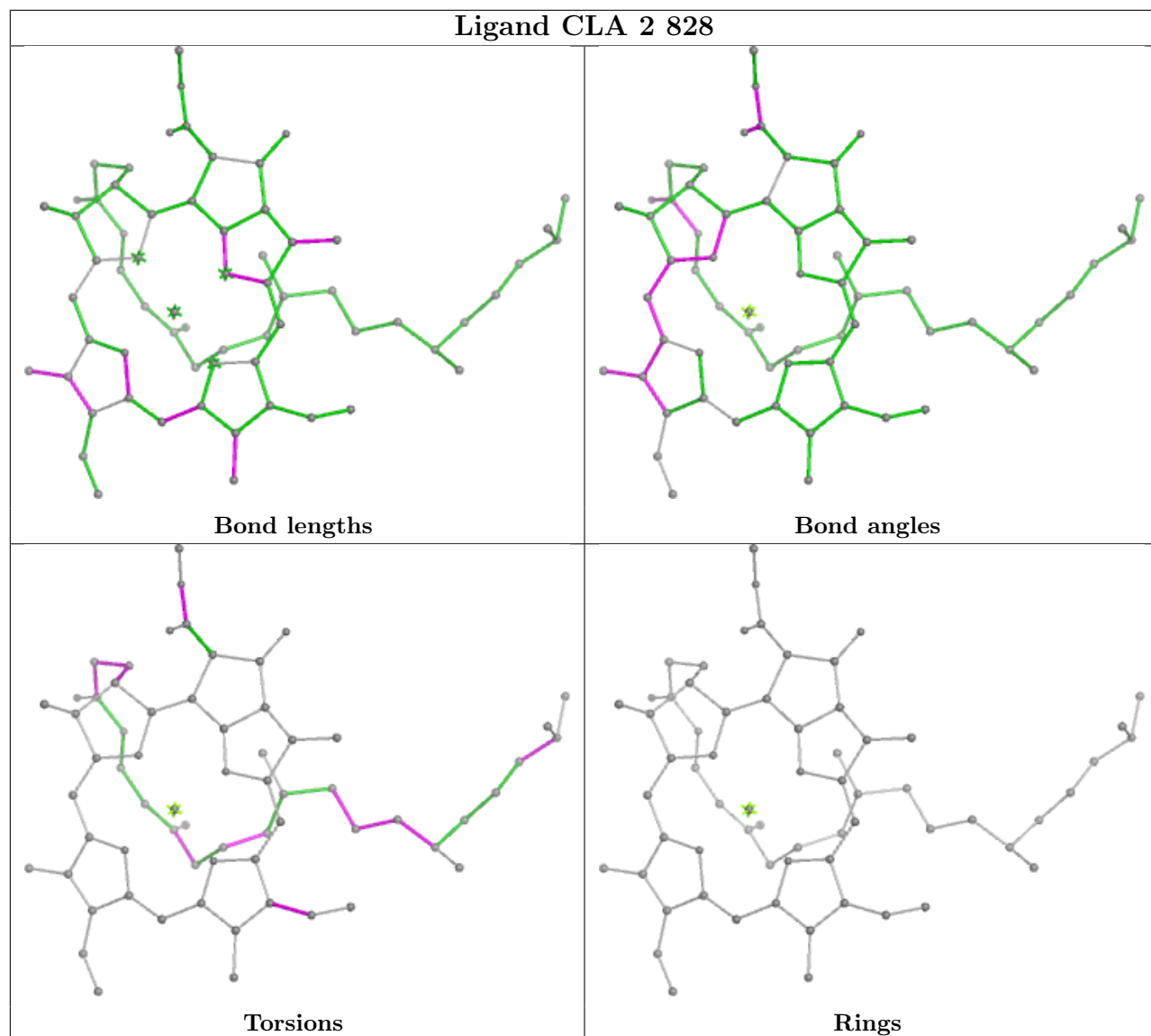


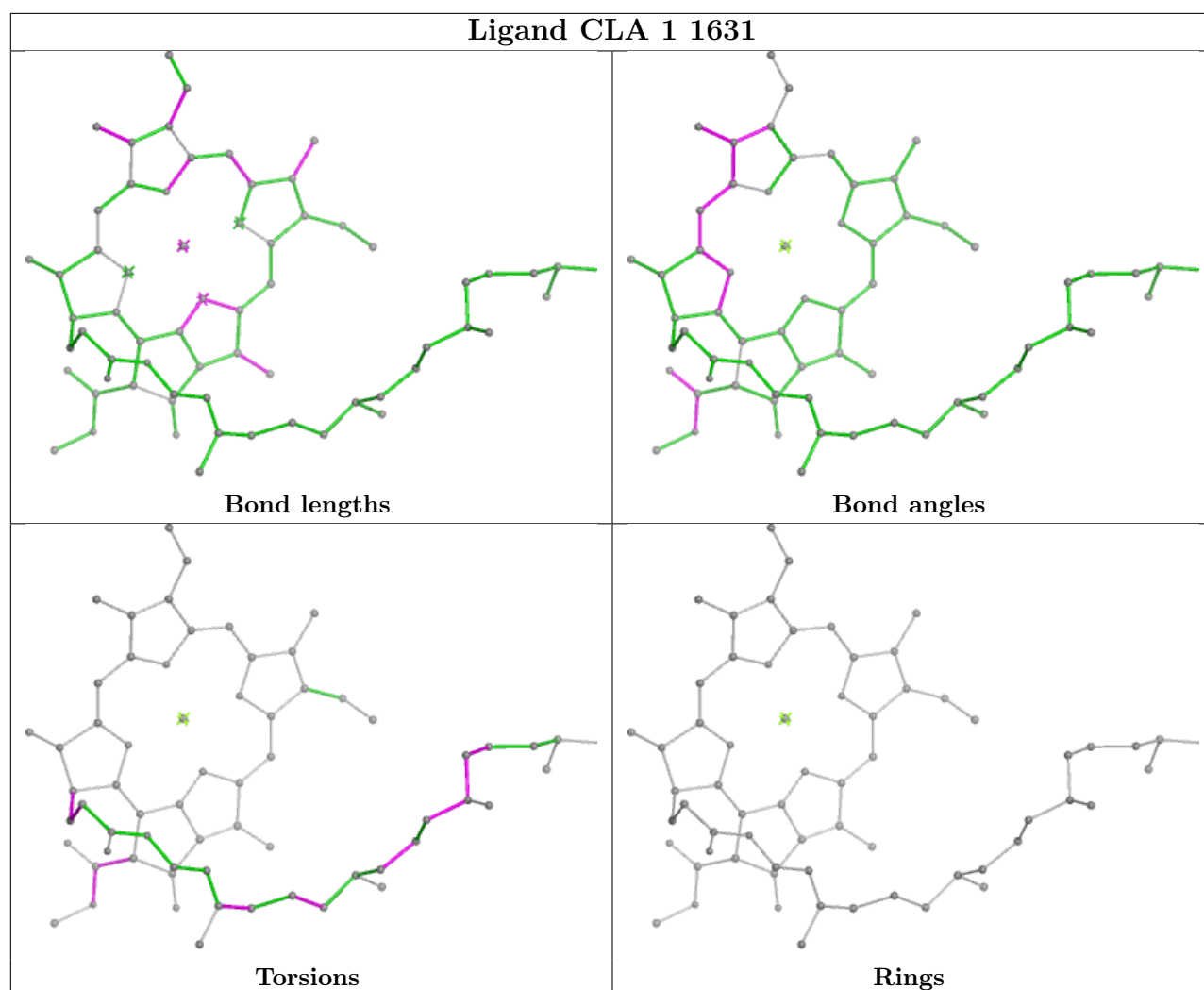
Ligand CLA B 825

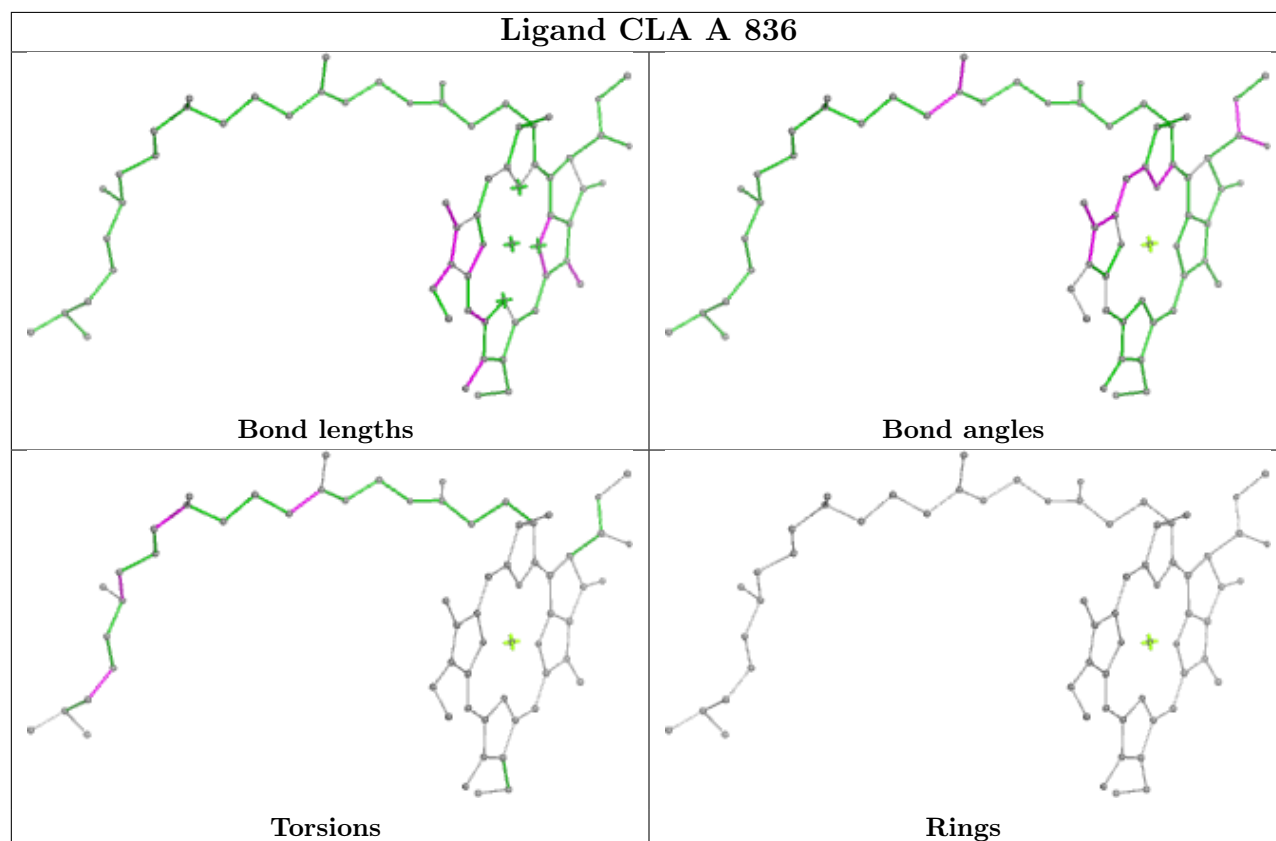
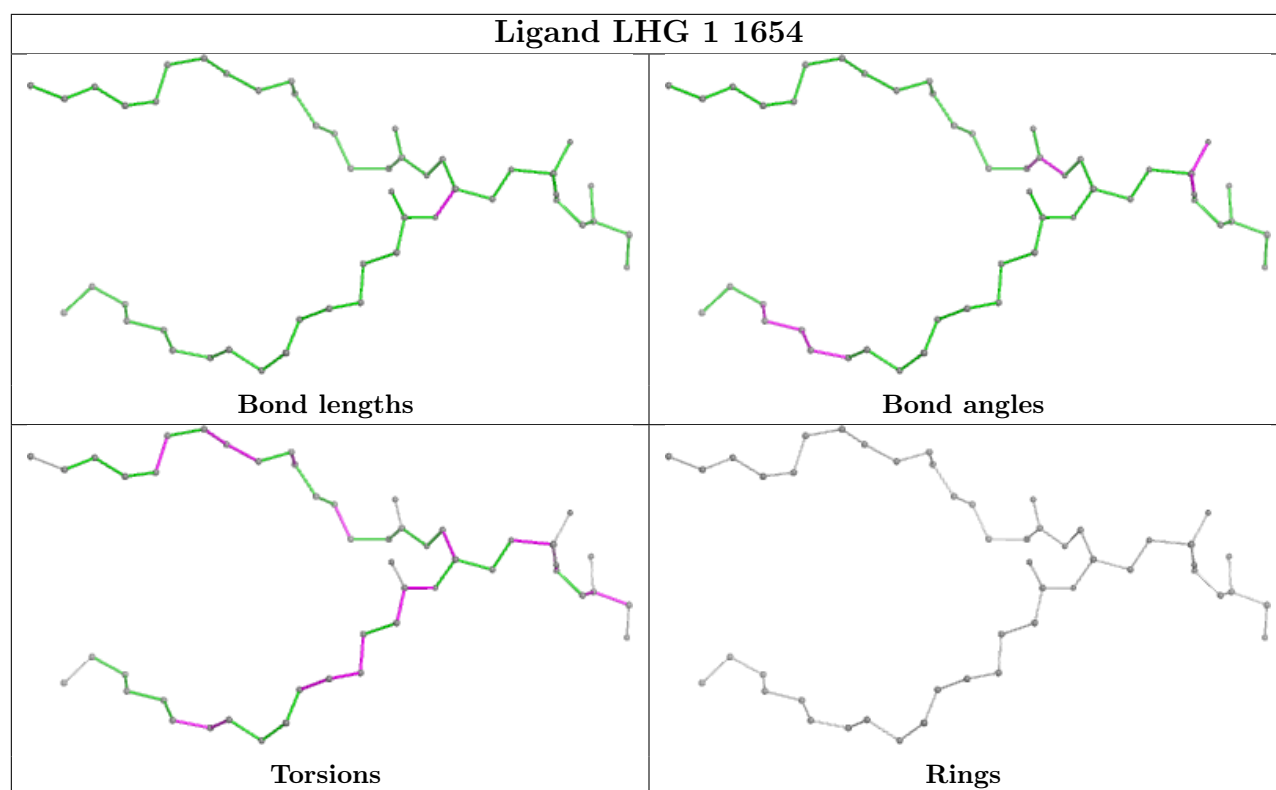




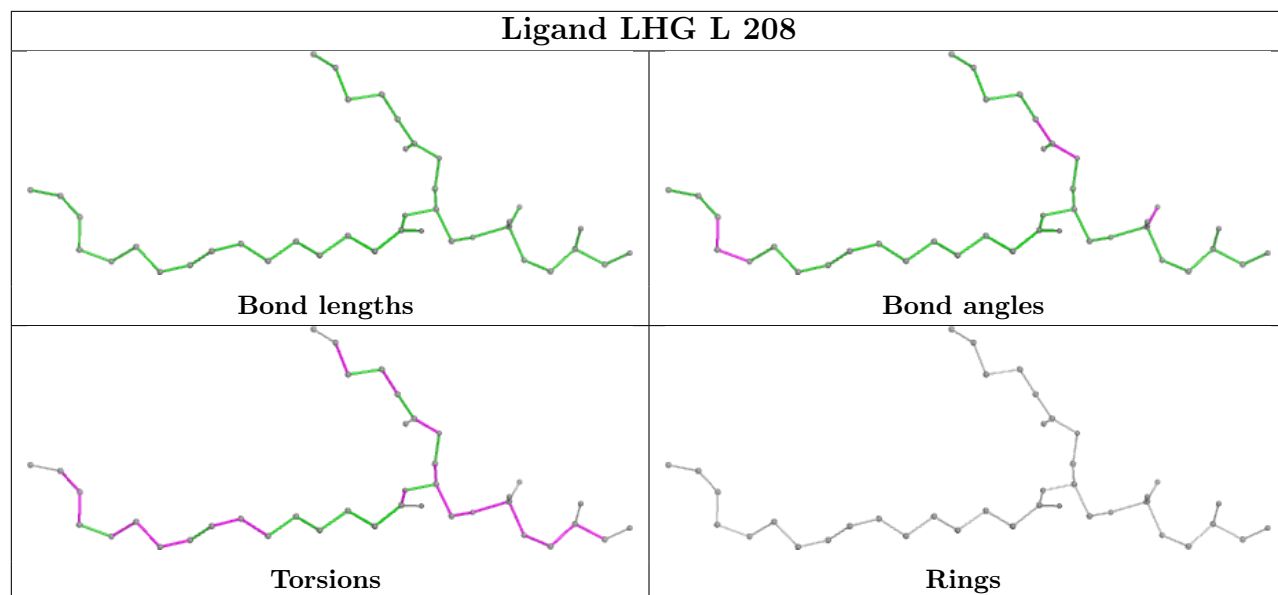
Ligand CLA 2 828



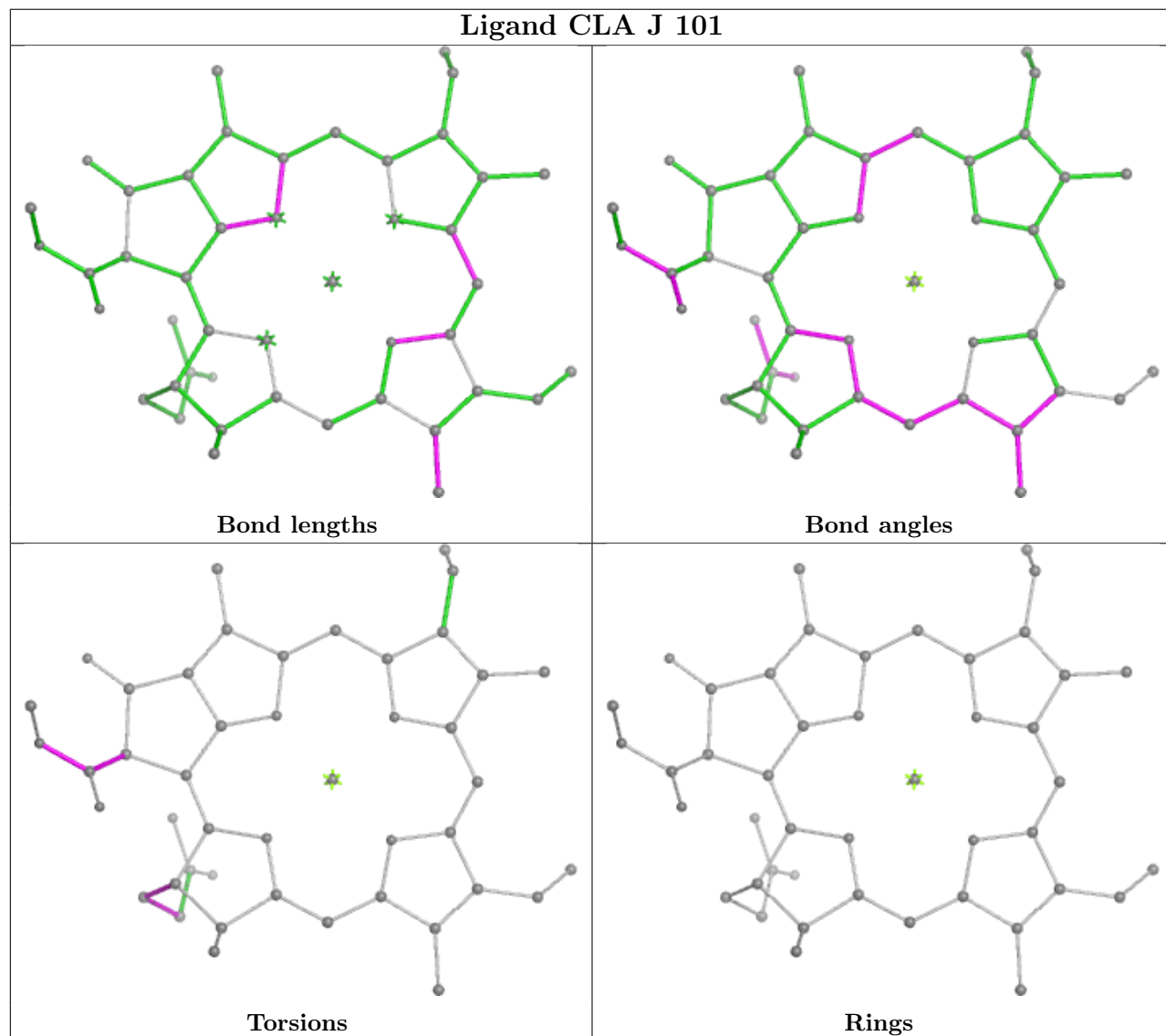




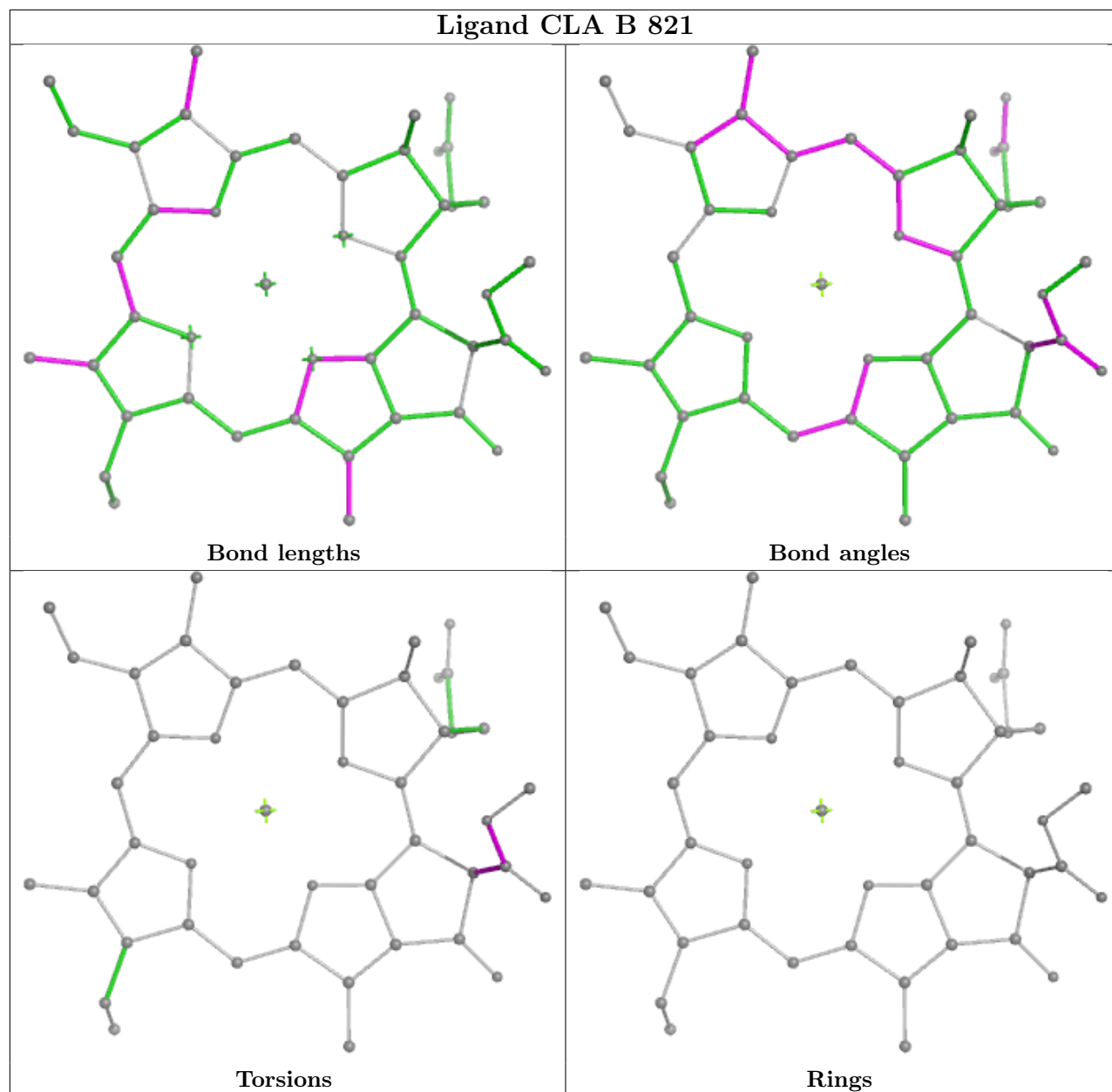
Ligand LHG L 208

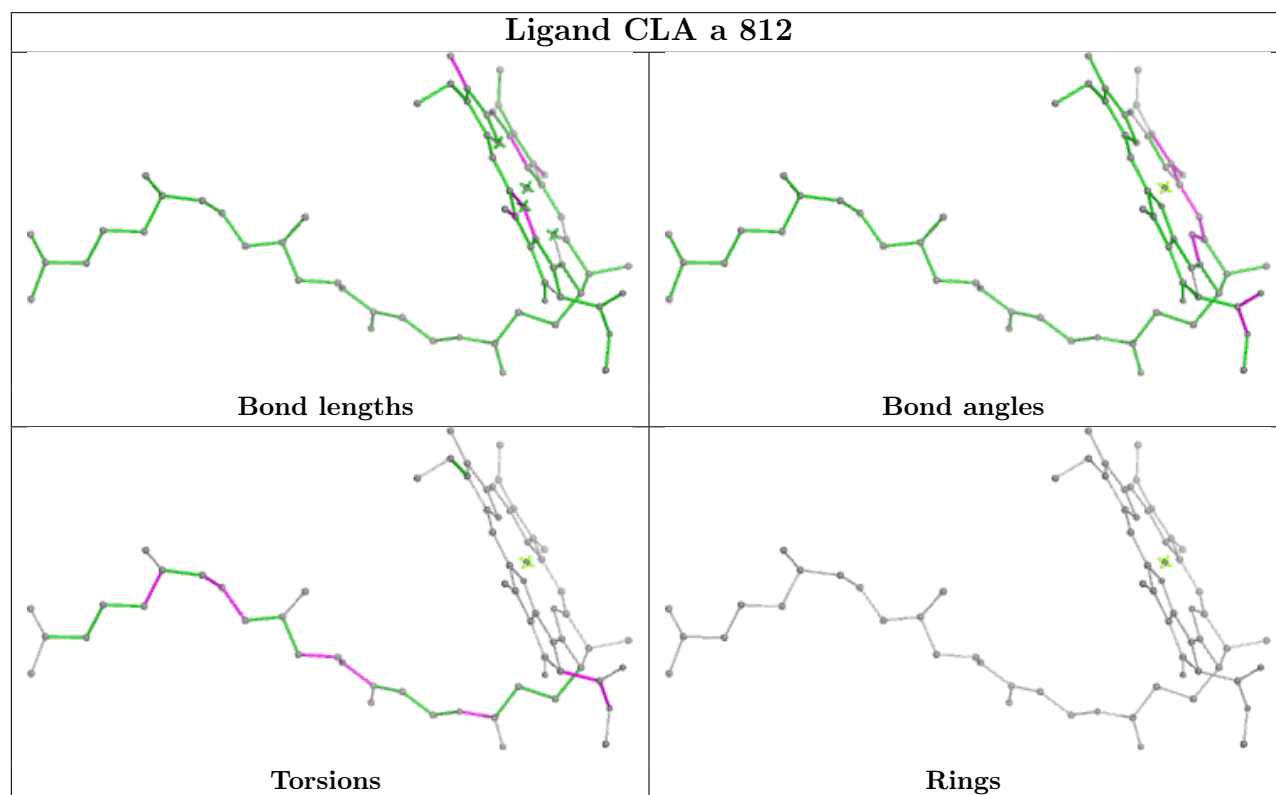
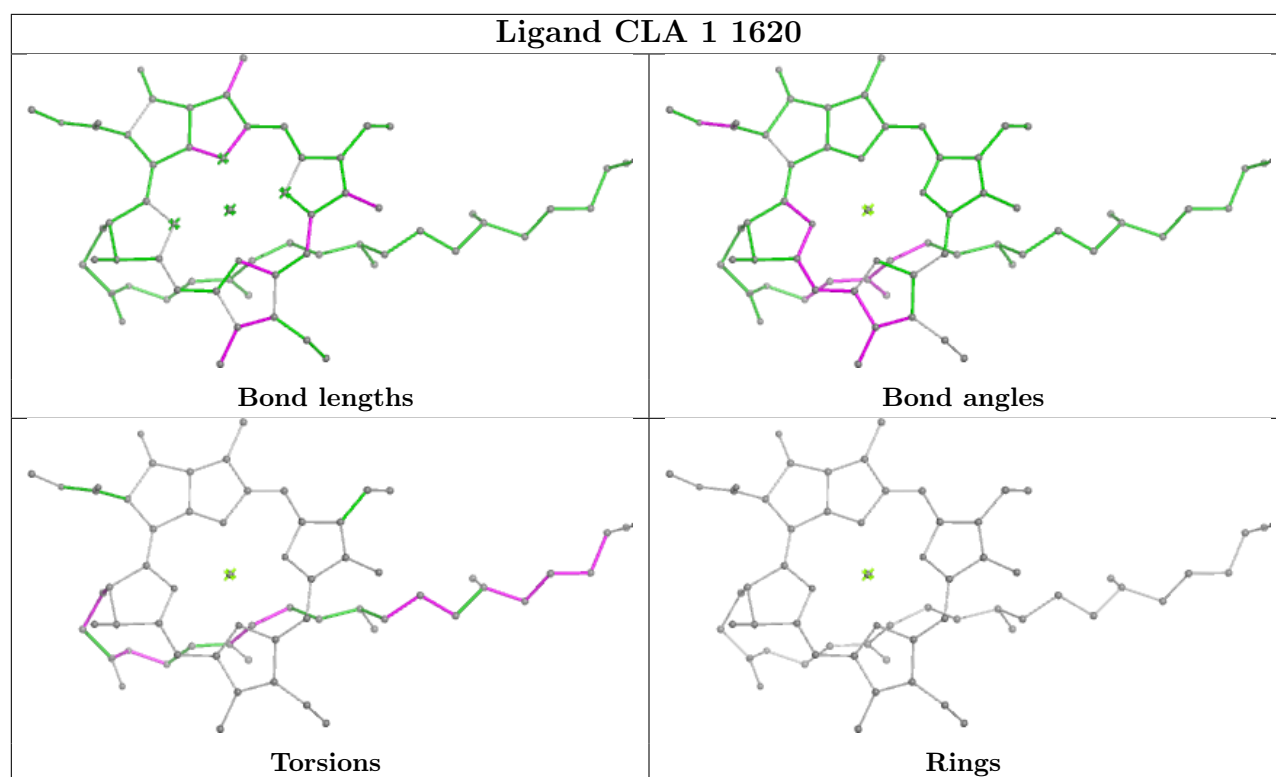


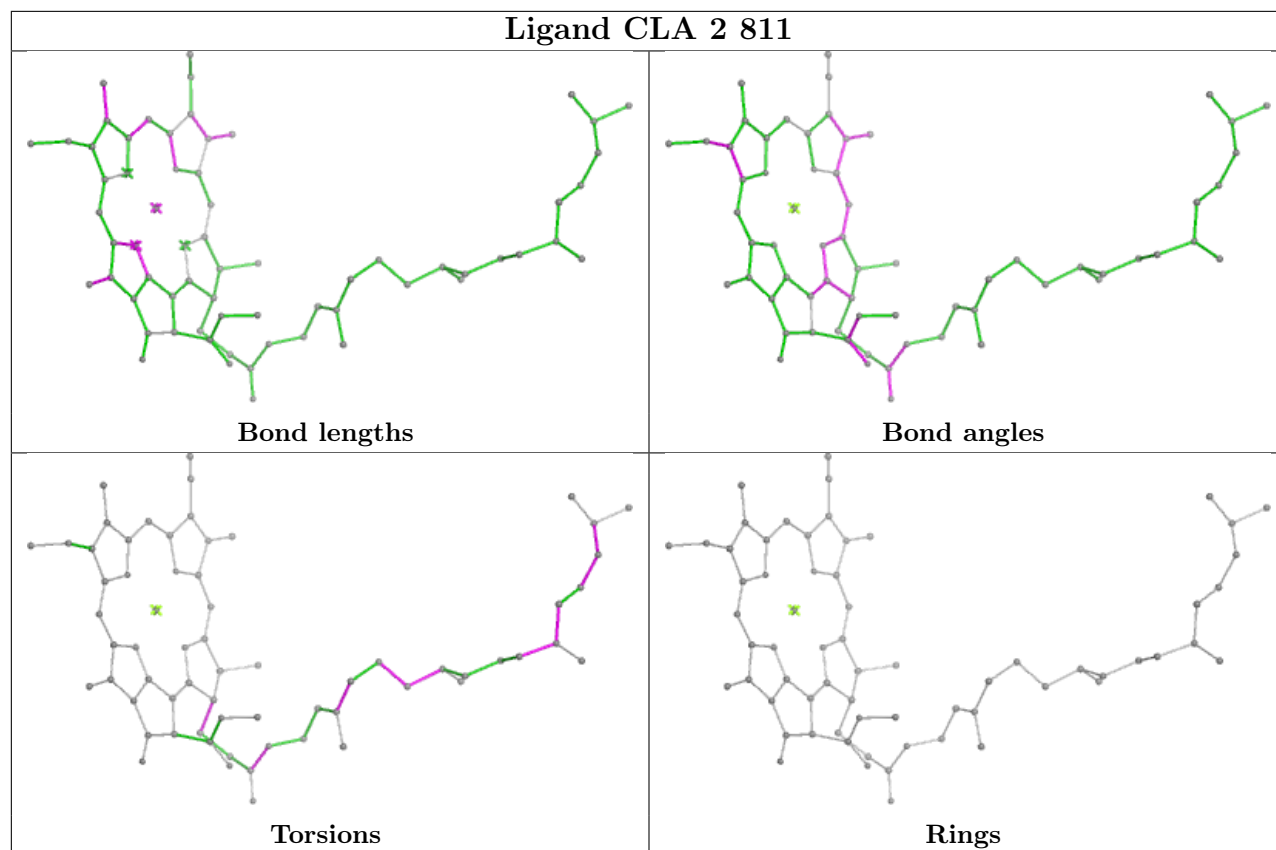
Ligand CLA J 101



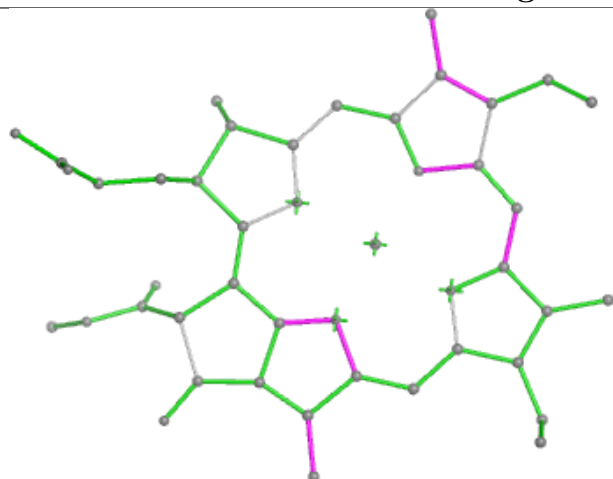
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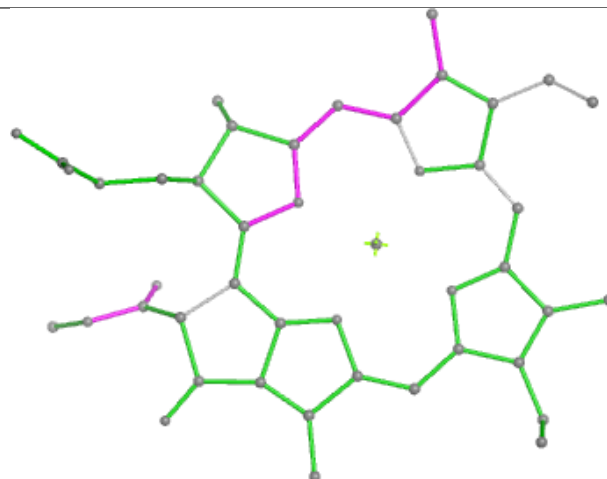




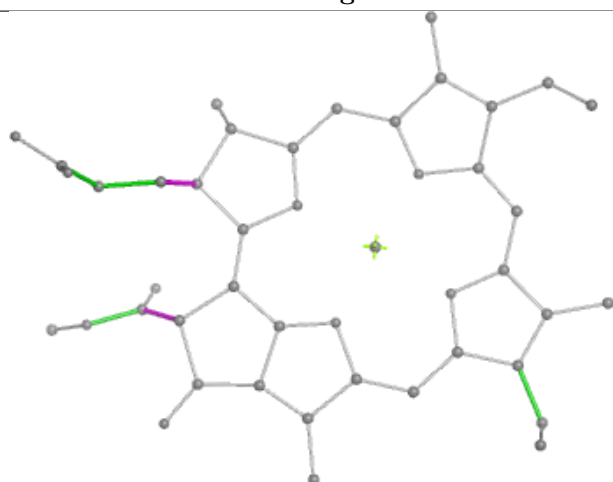
Ligand CLA b 837



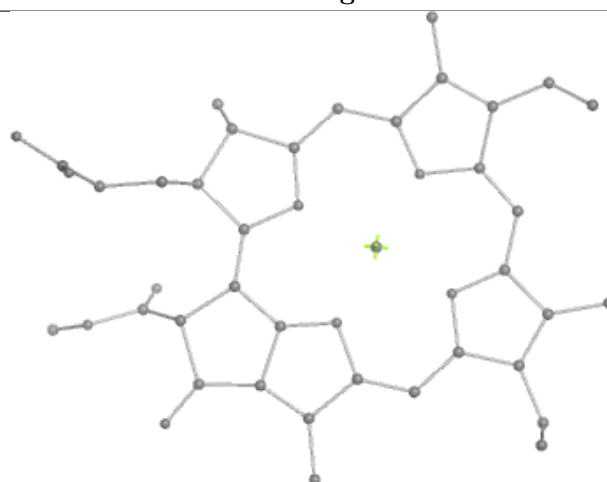
Bond lengths



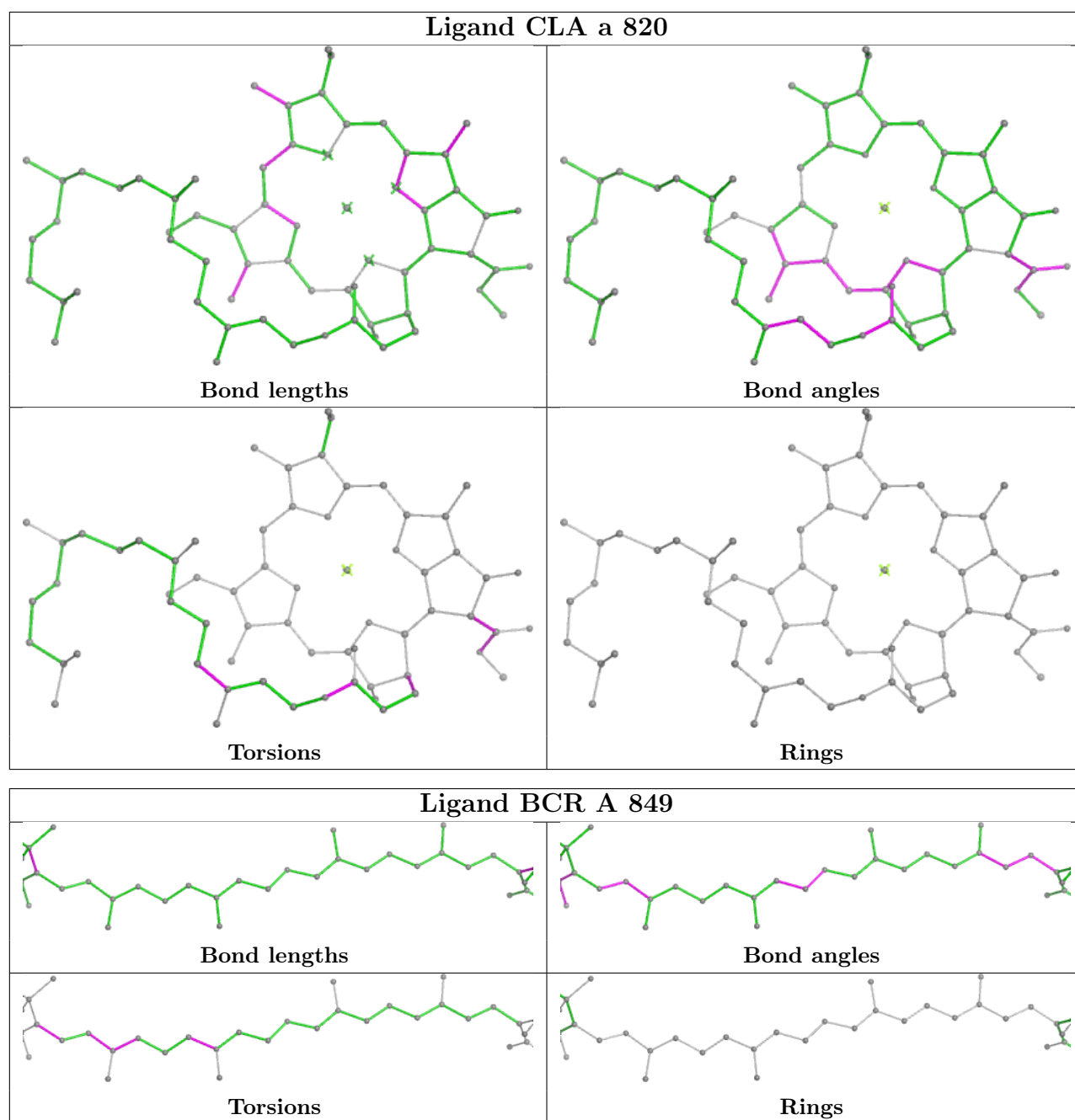
Bond angles



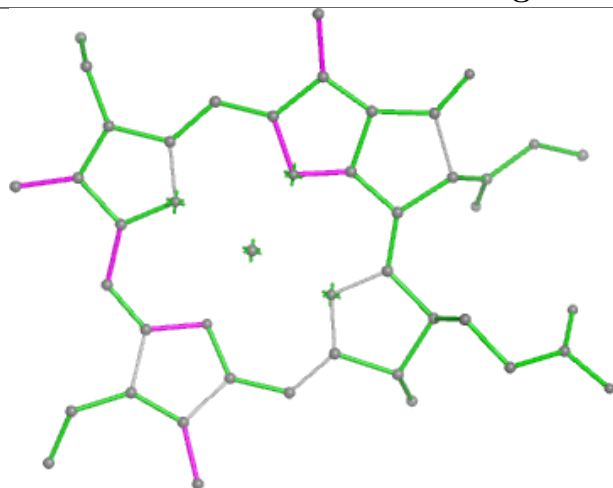
Torsions



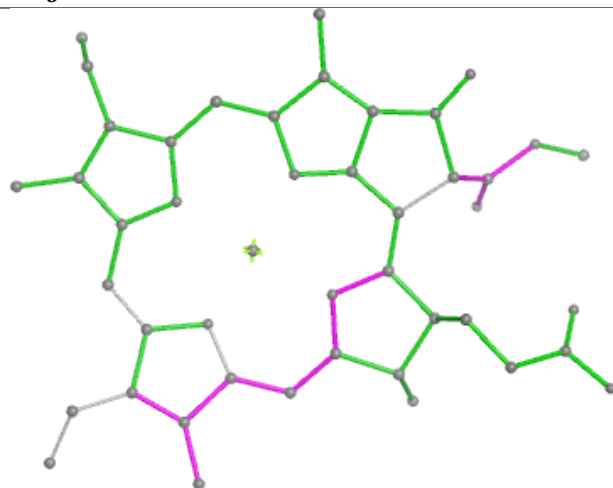
Rings



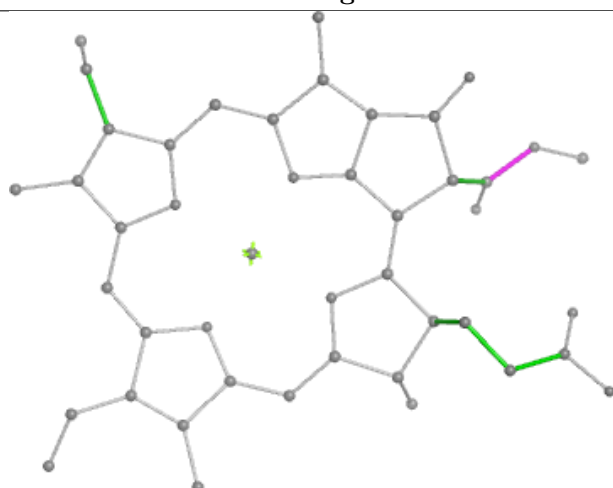
Ligand CLA j 1301



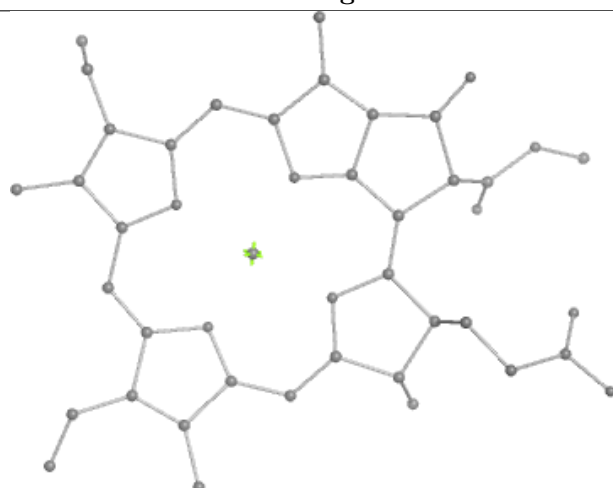
Bond lengths



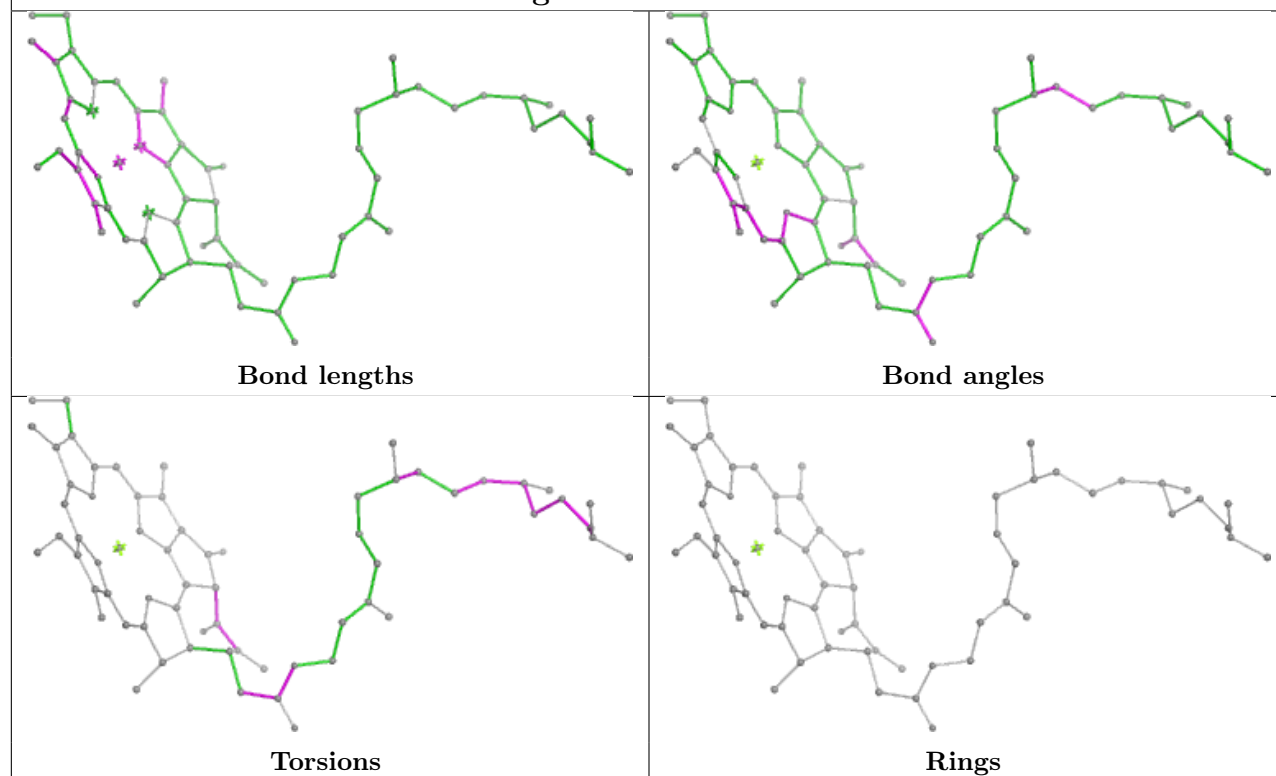
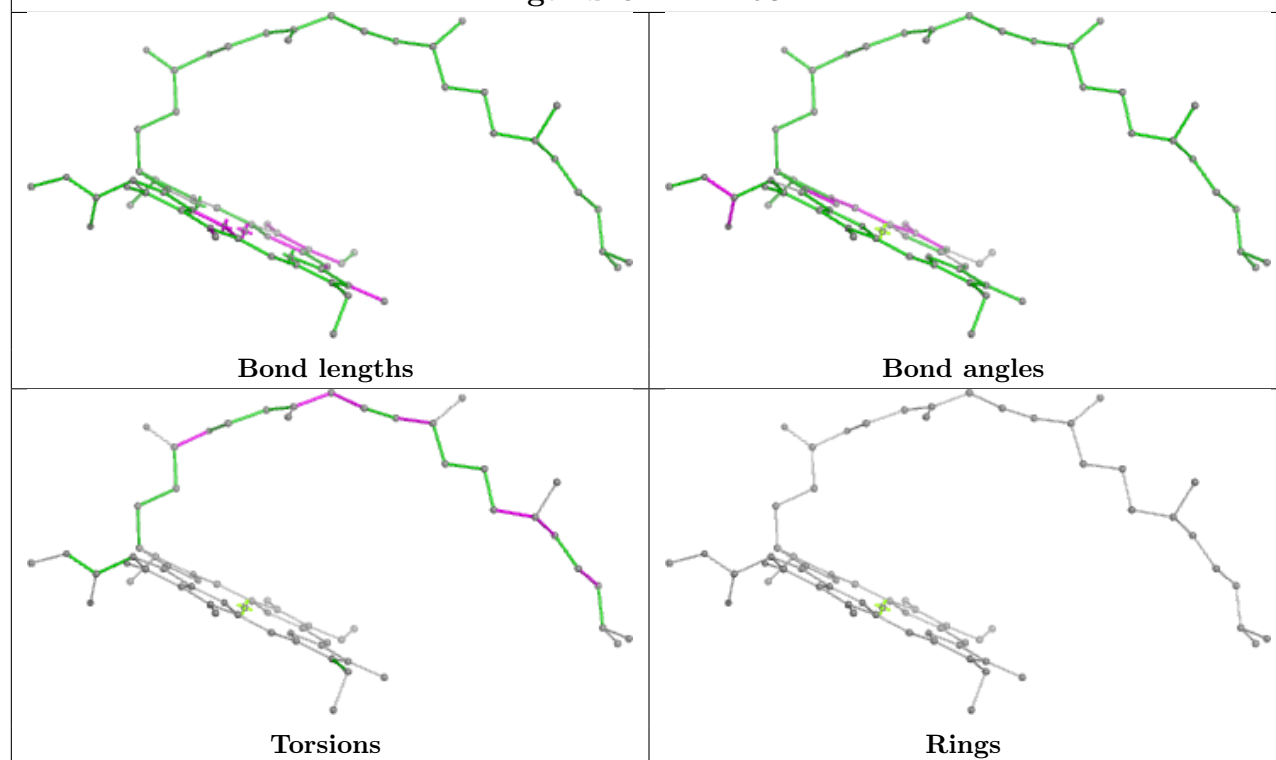
Bond angles

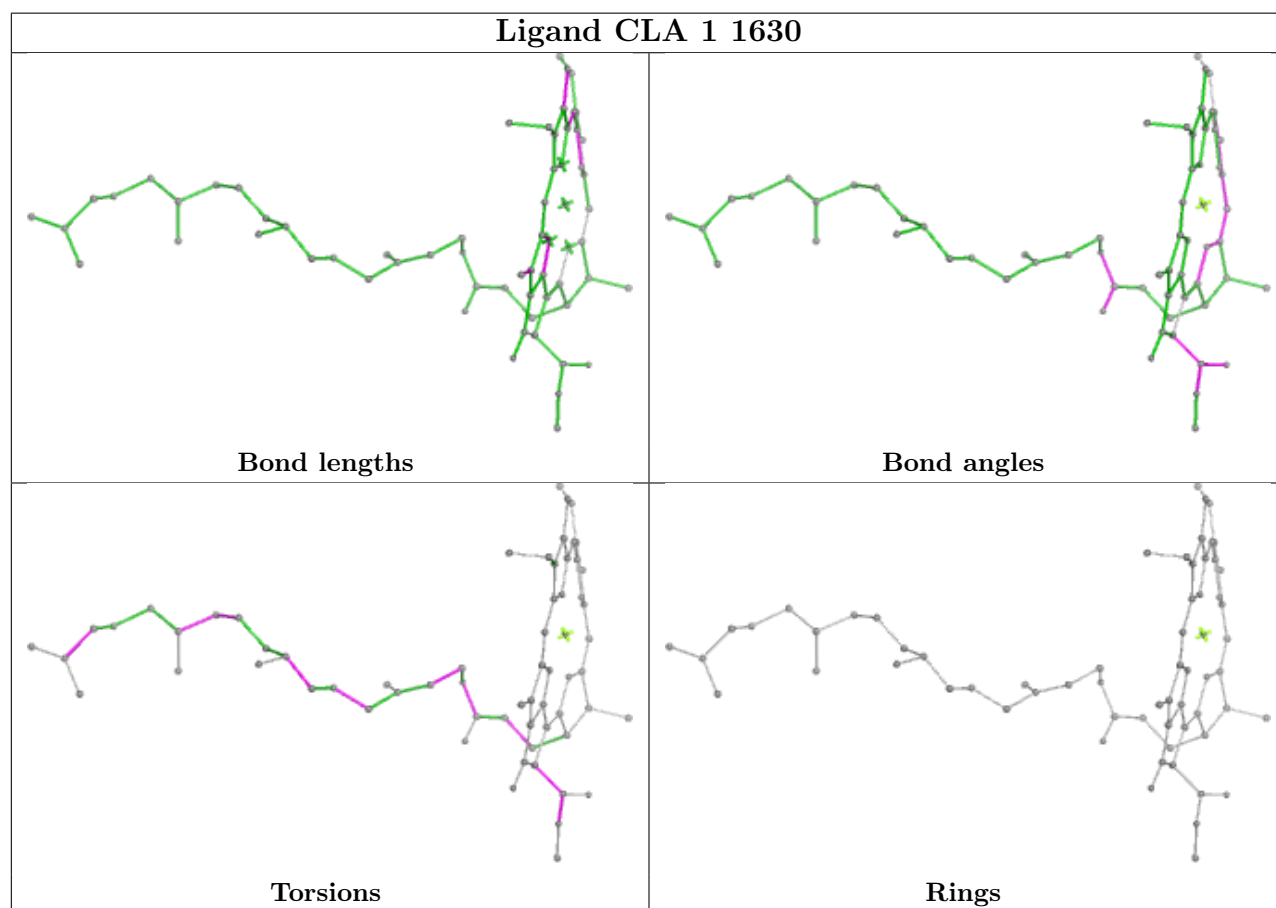
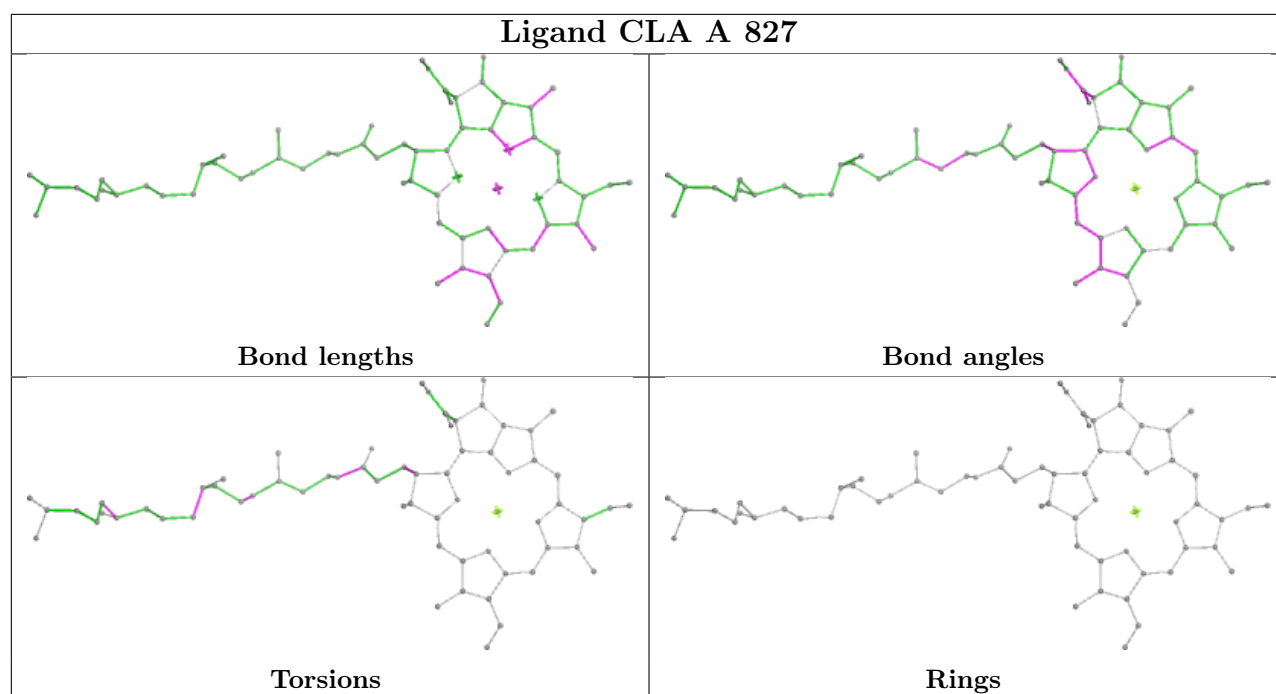


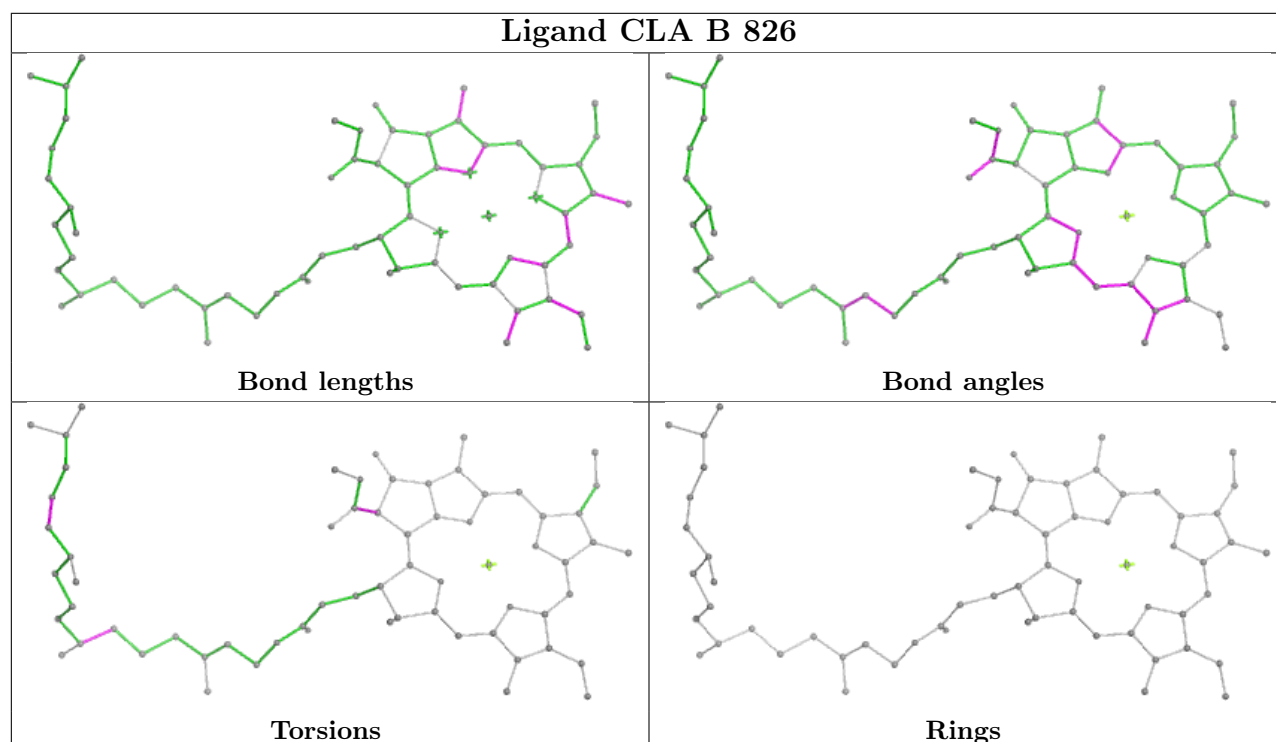
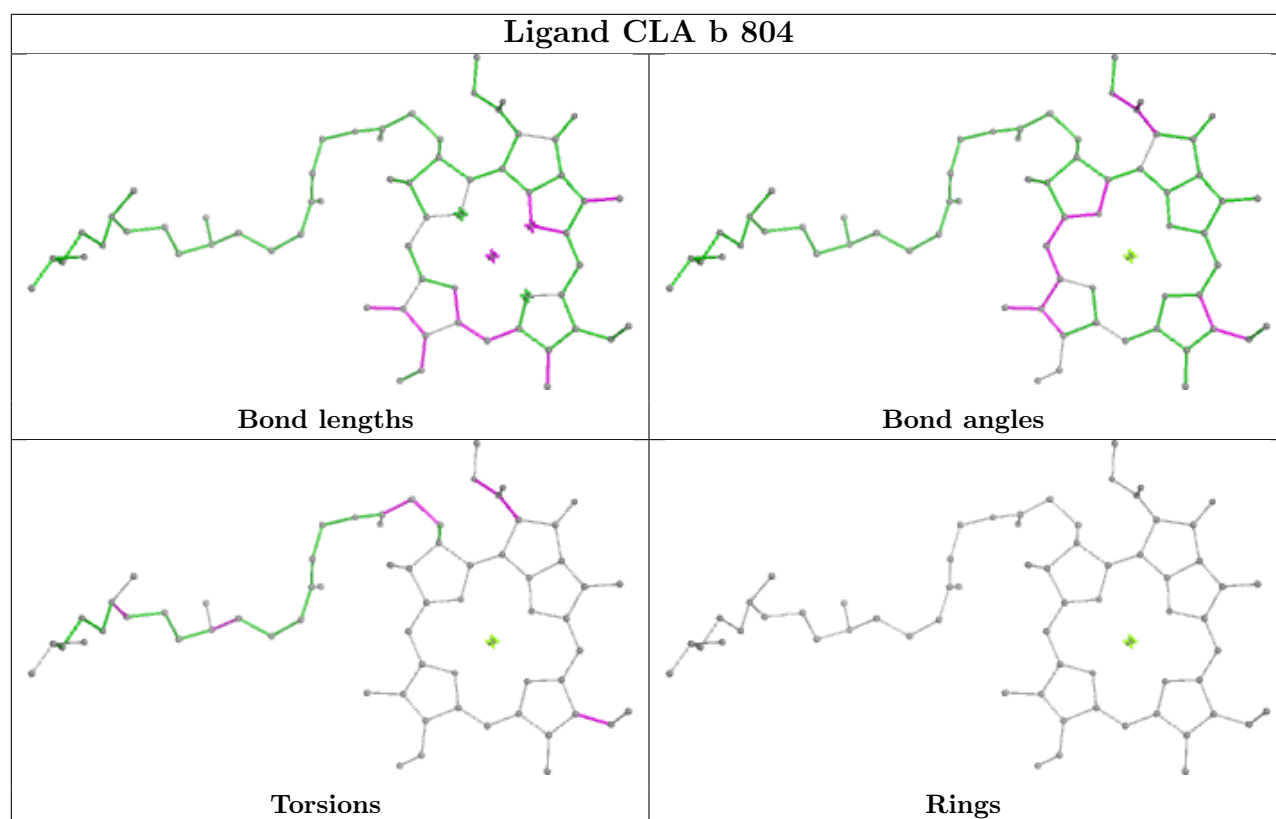
Torsions



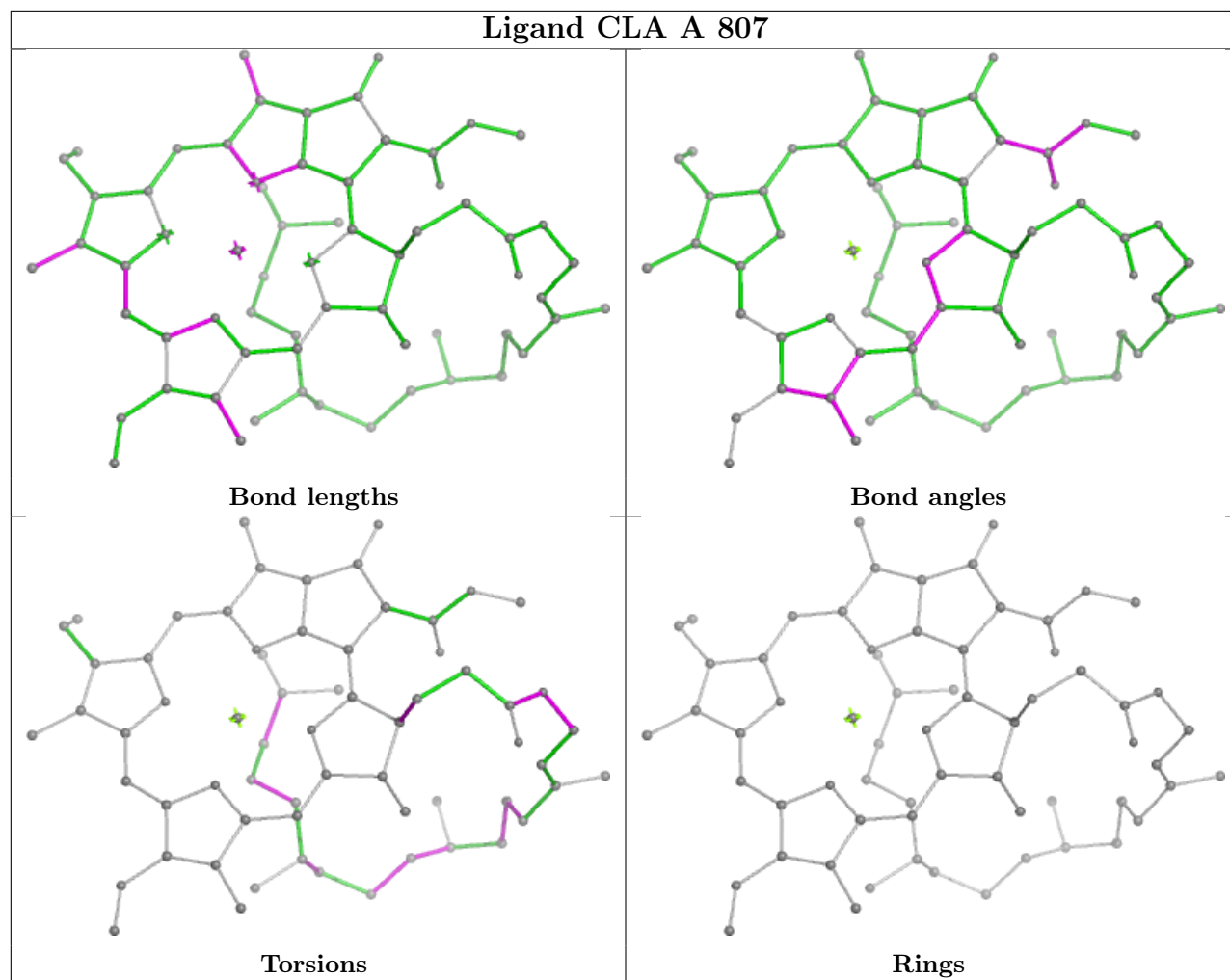
Rings

Ligand CLA B 802**Ligand CLA 1 1634**

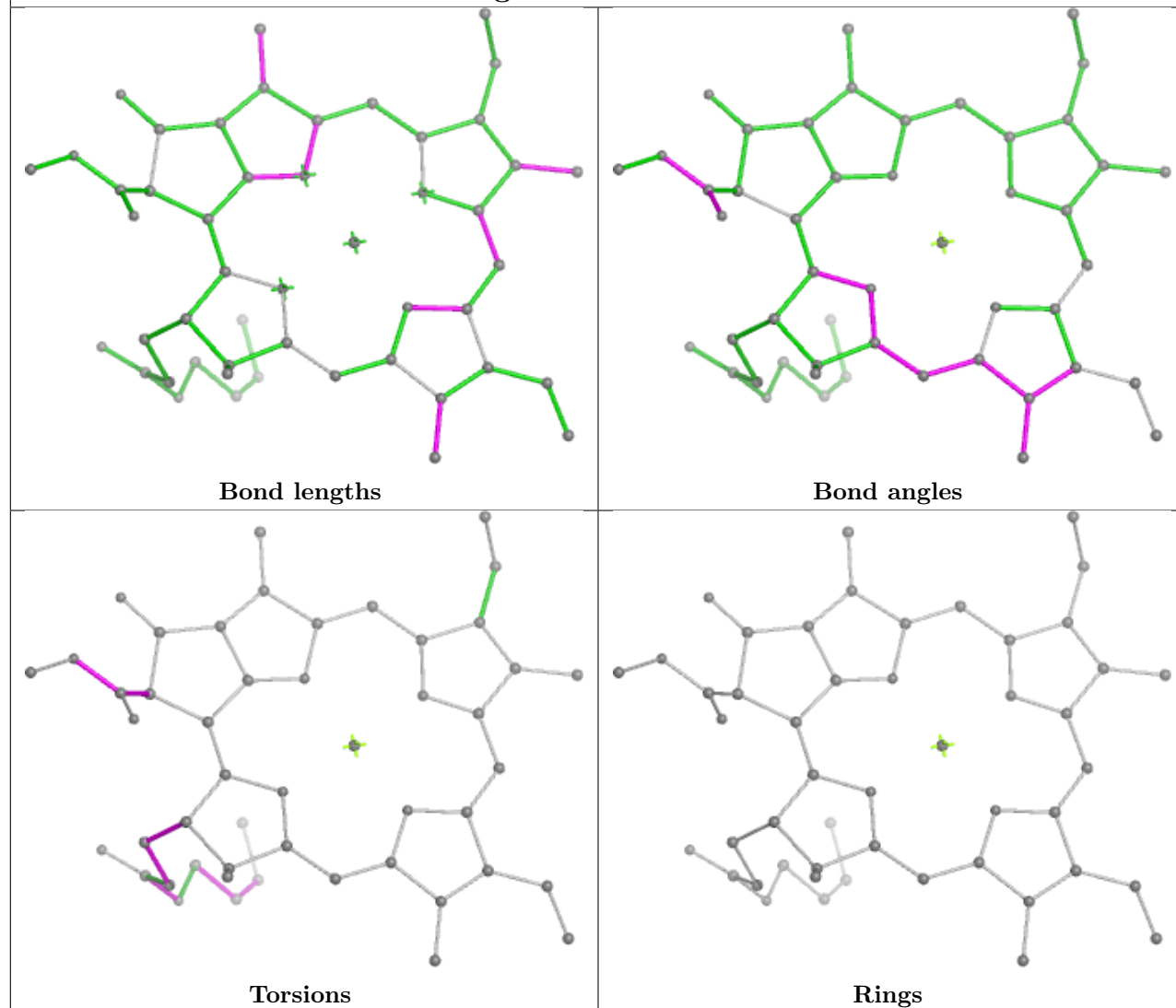




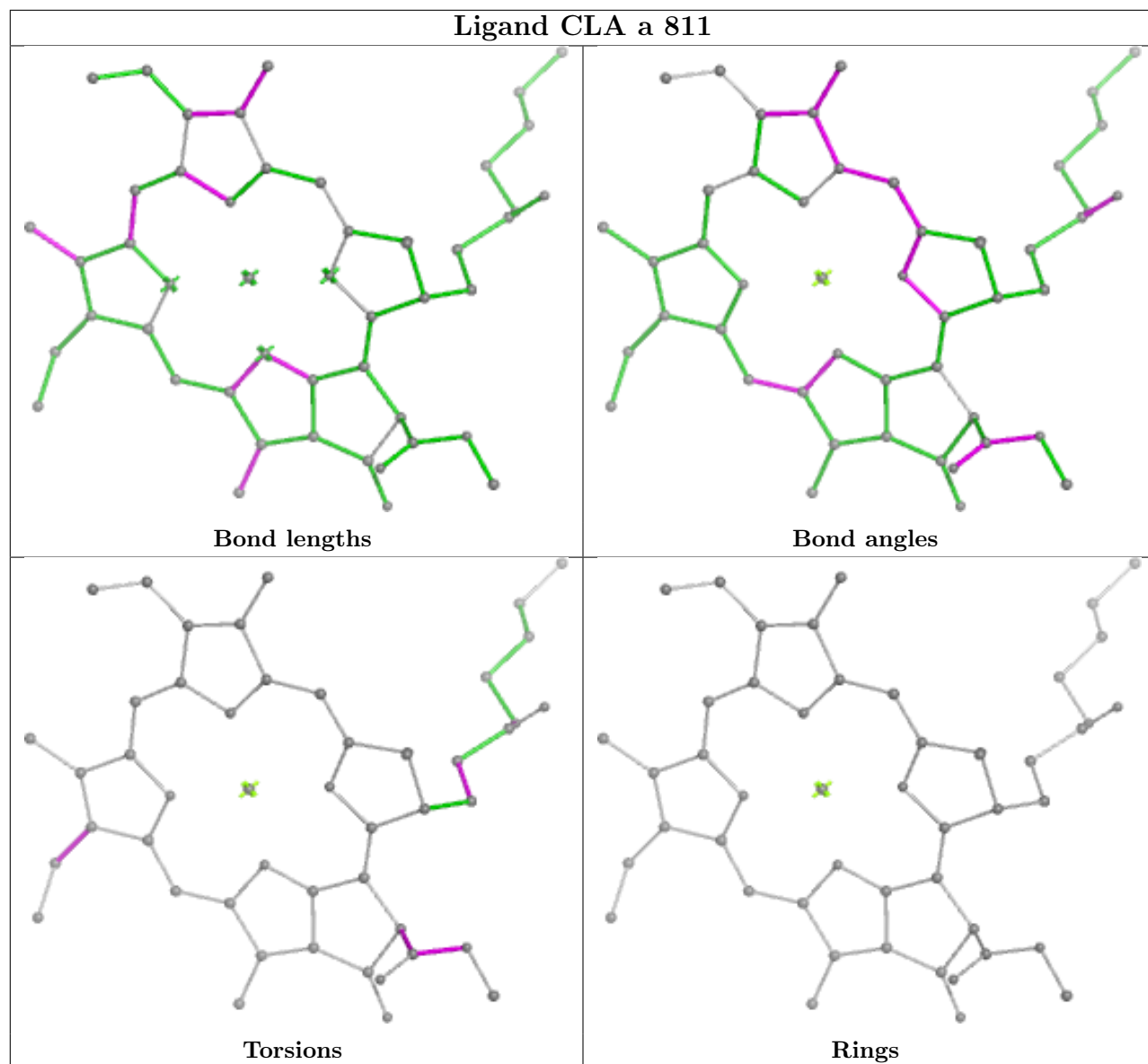
Ligand CLA A 807

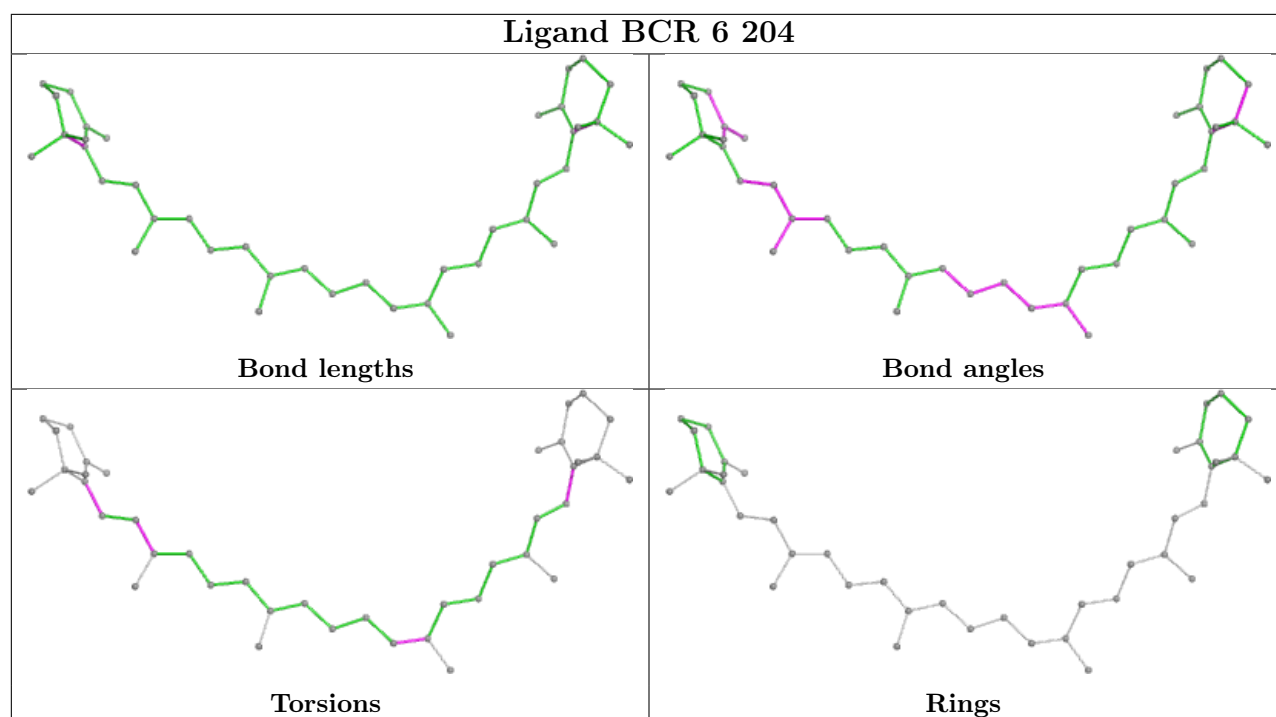


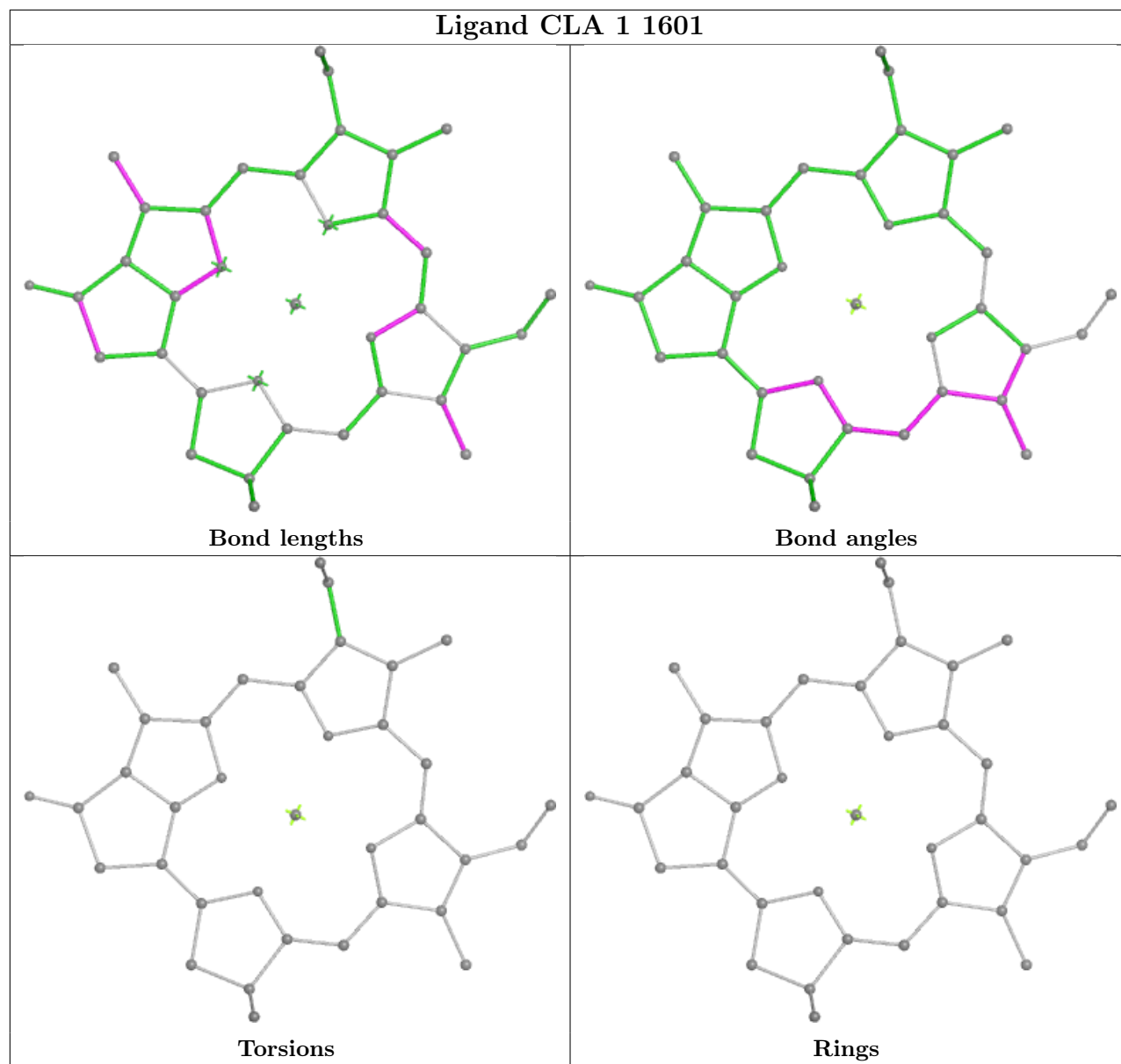
Ligand CLA 2 832

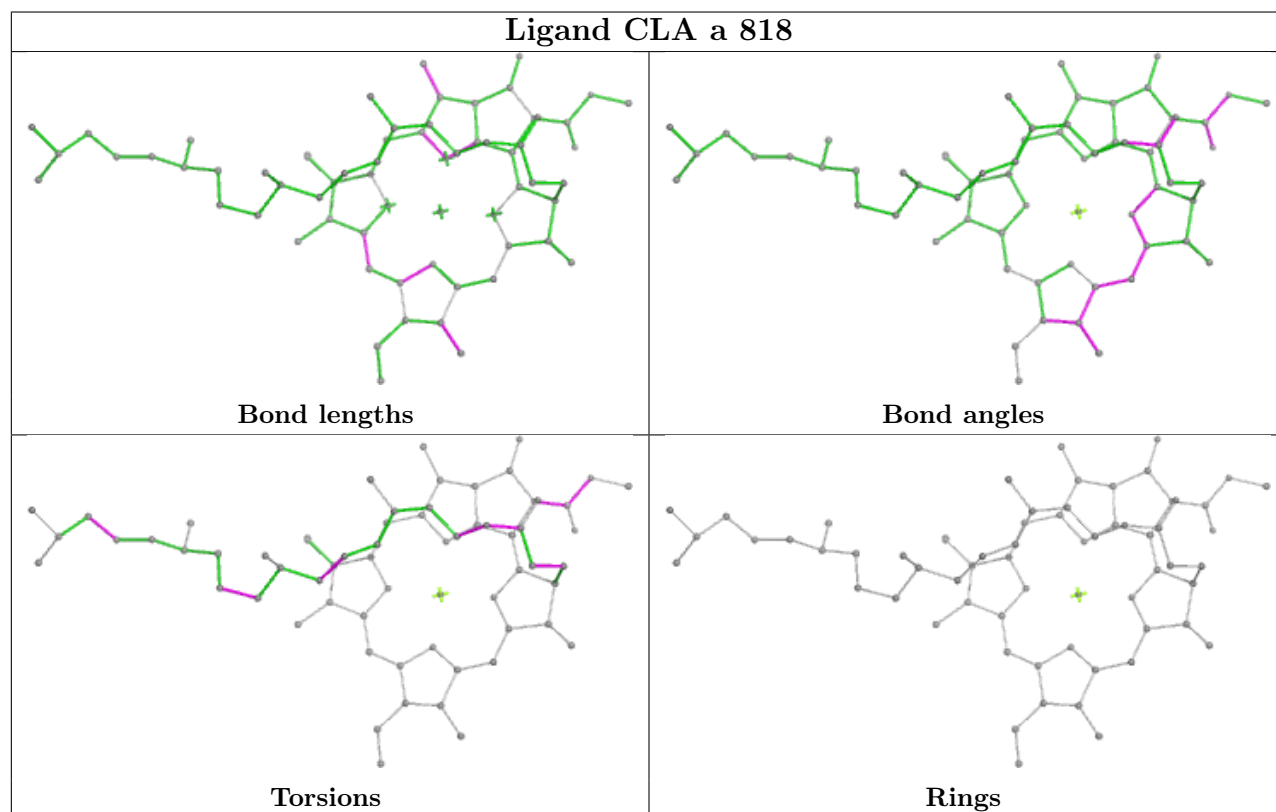
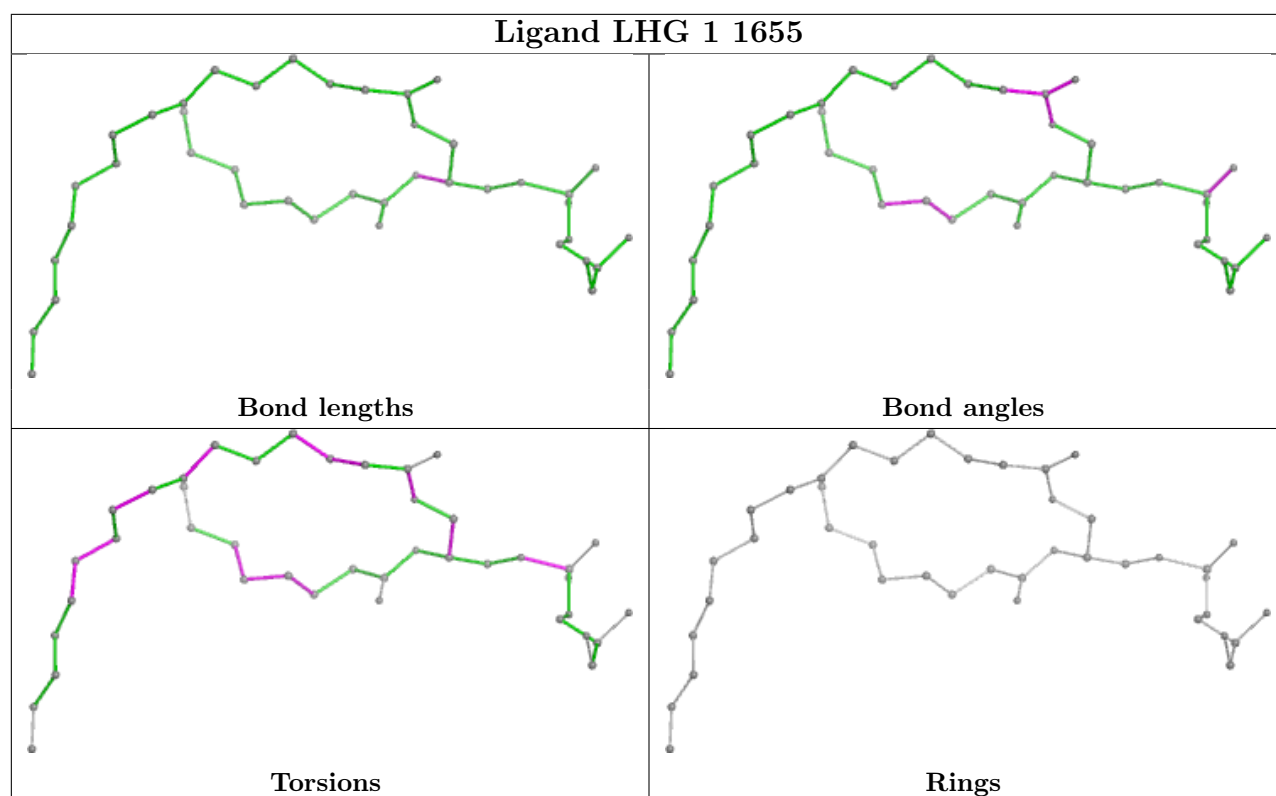


Ligand CLA a 811

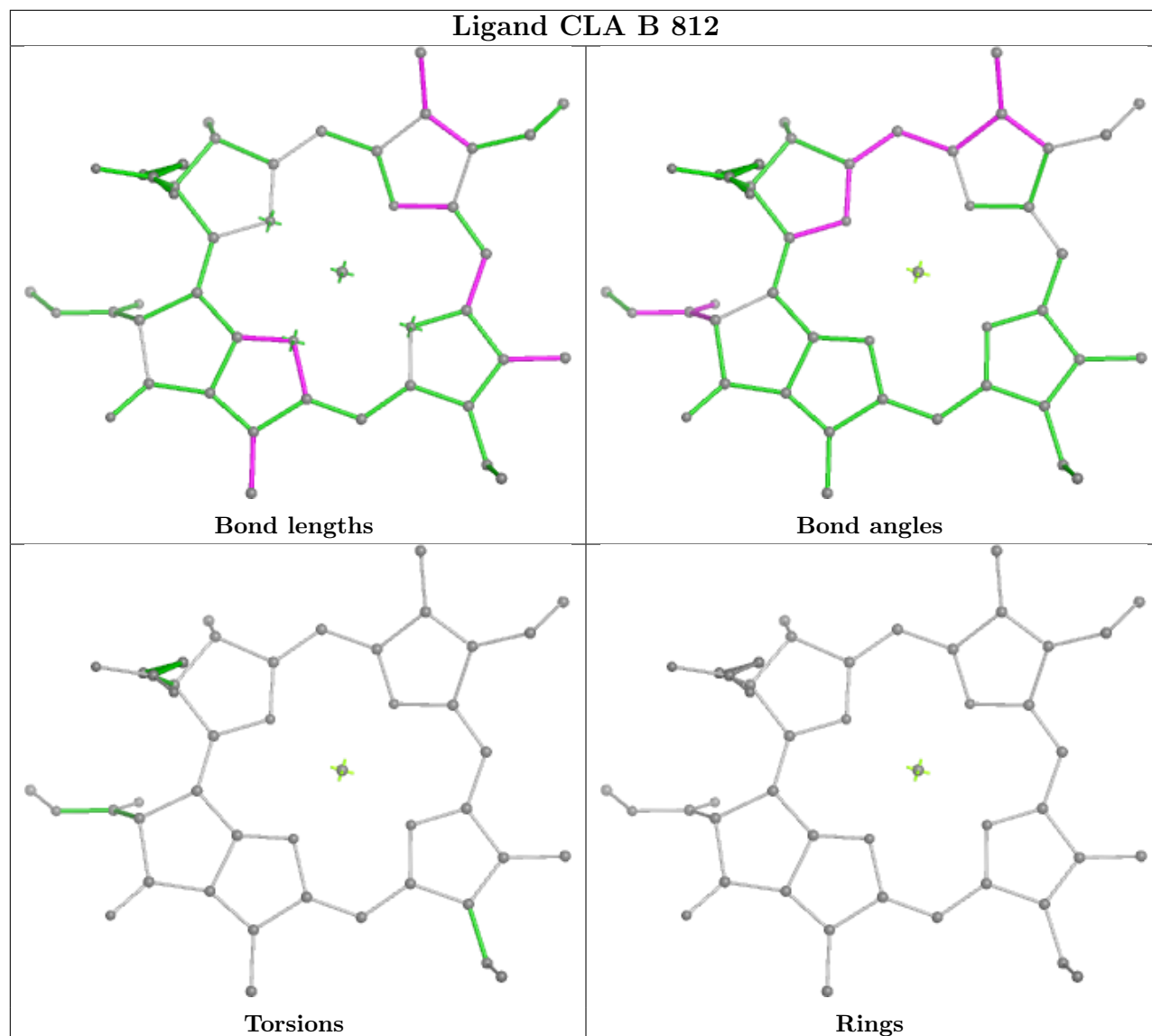




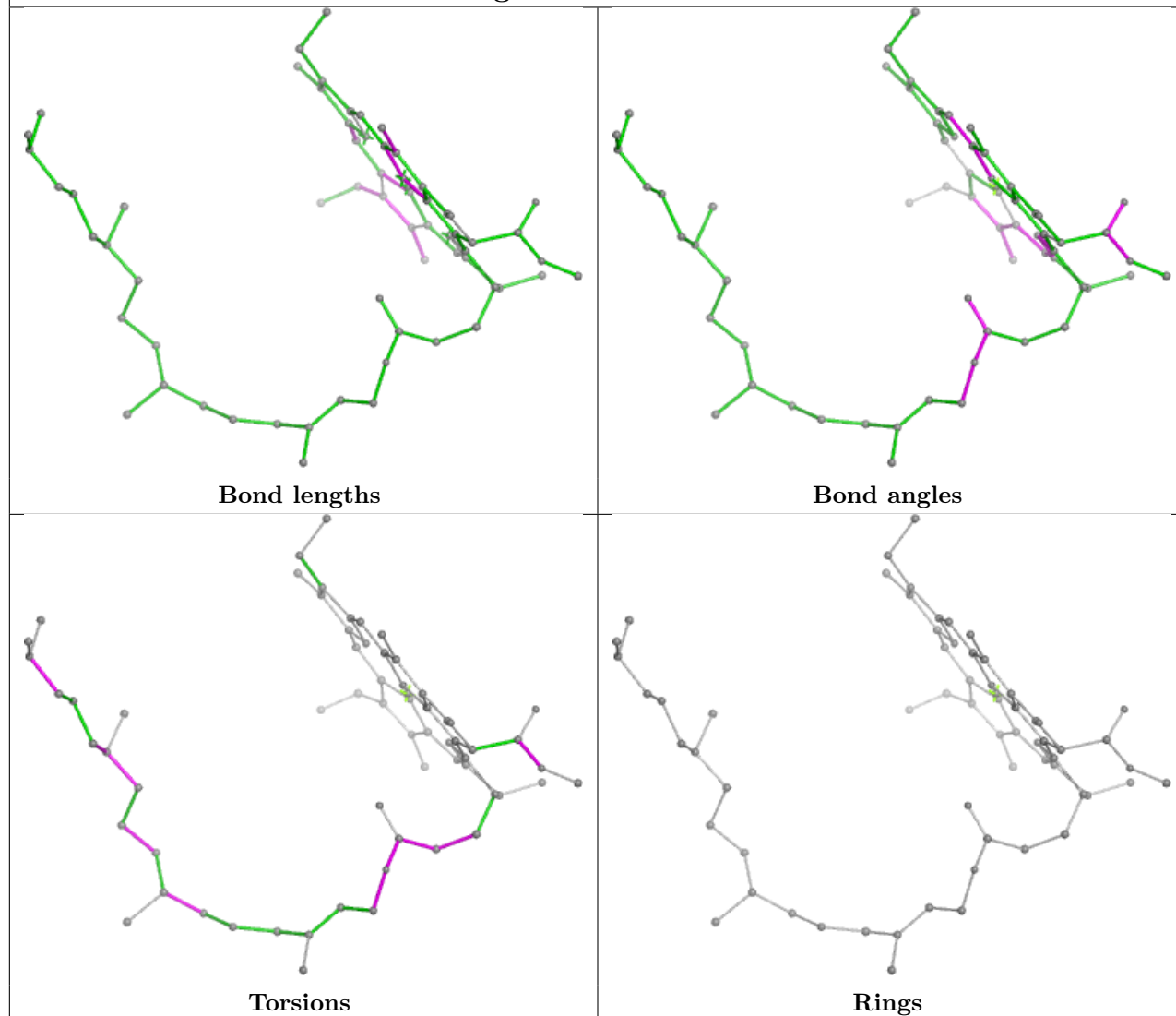




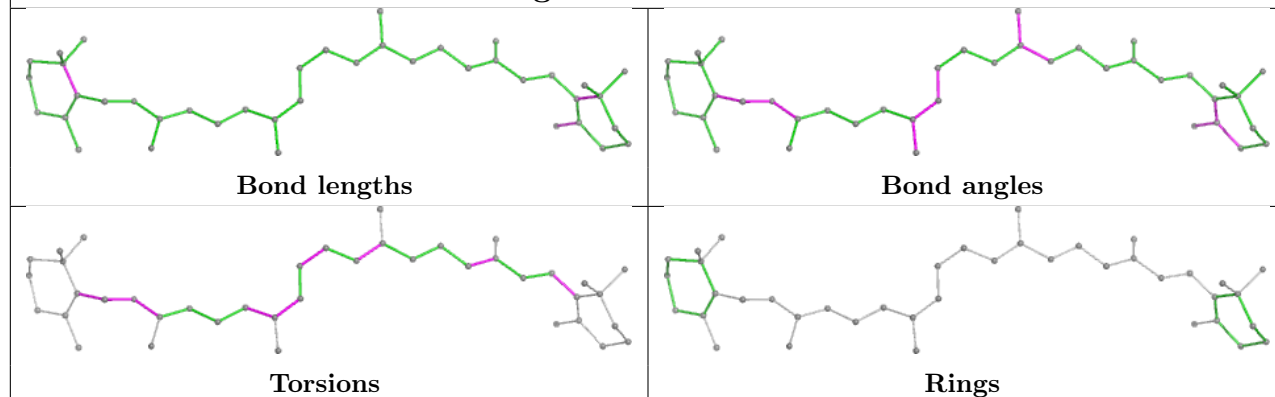
Ligand CLA B 812

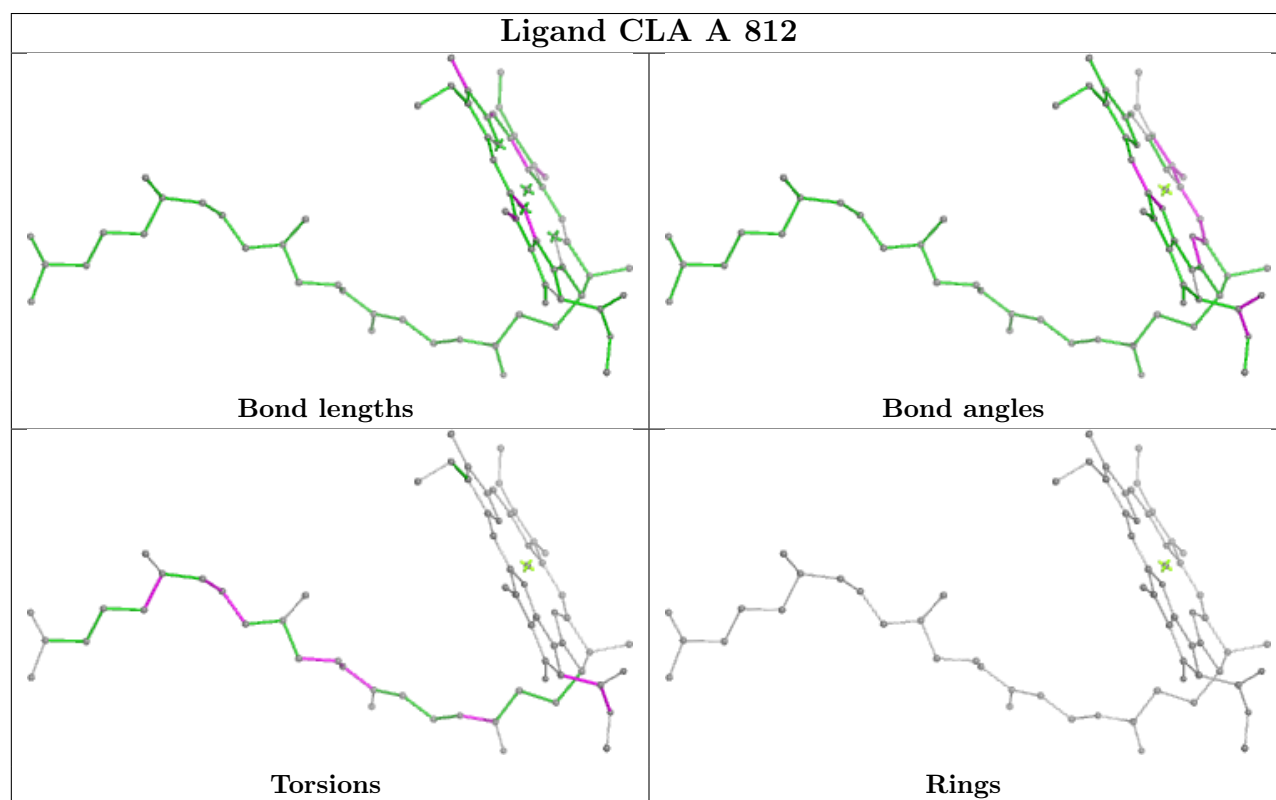
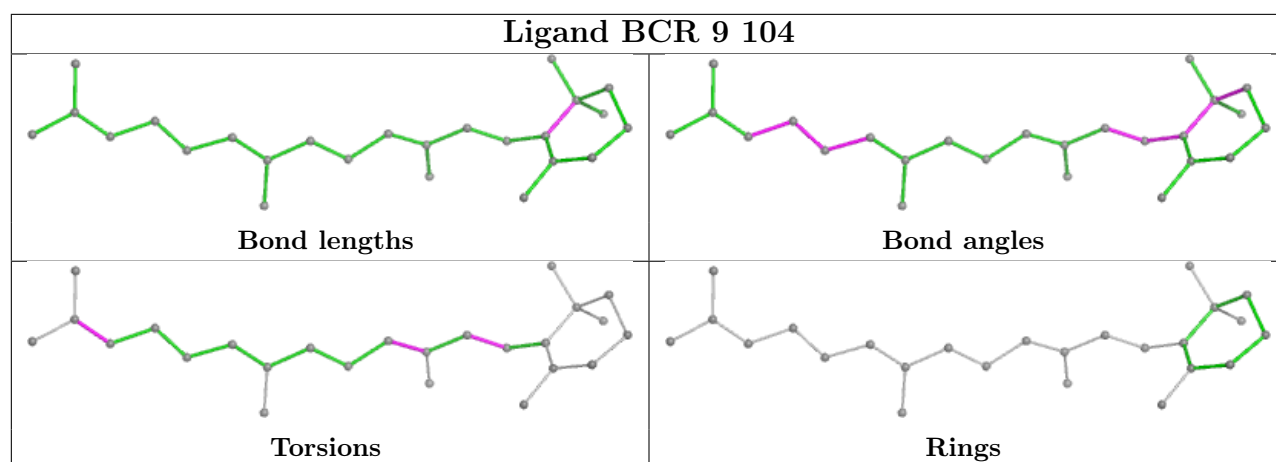


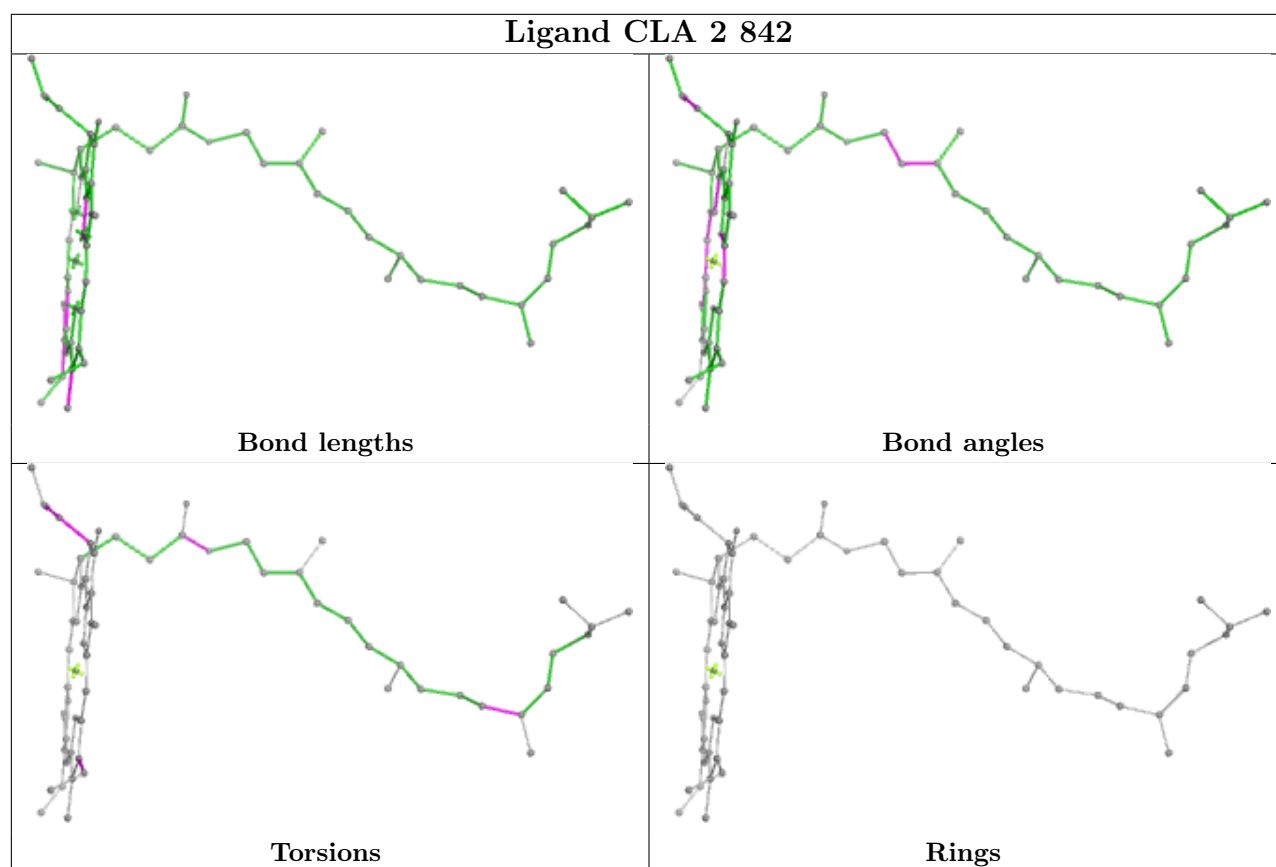
Ligand CLA 2 820



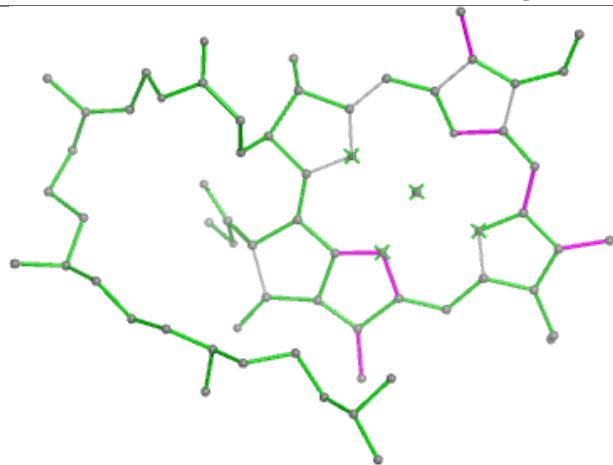
Ligand BCR 2 847



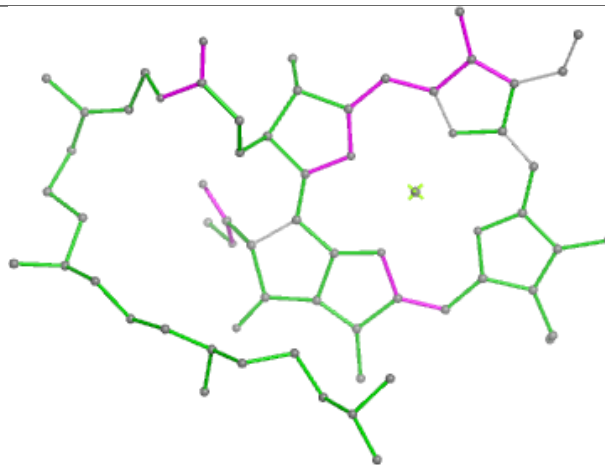




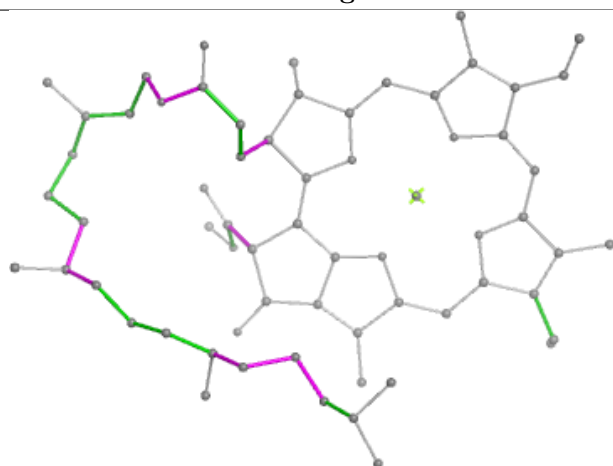
Ligand CLA b 806



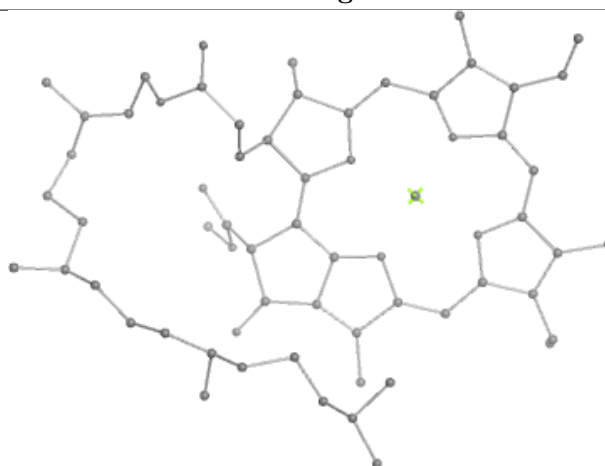
Bond lengths



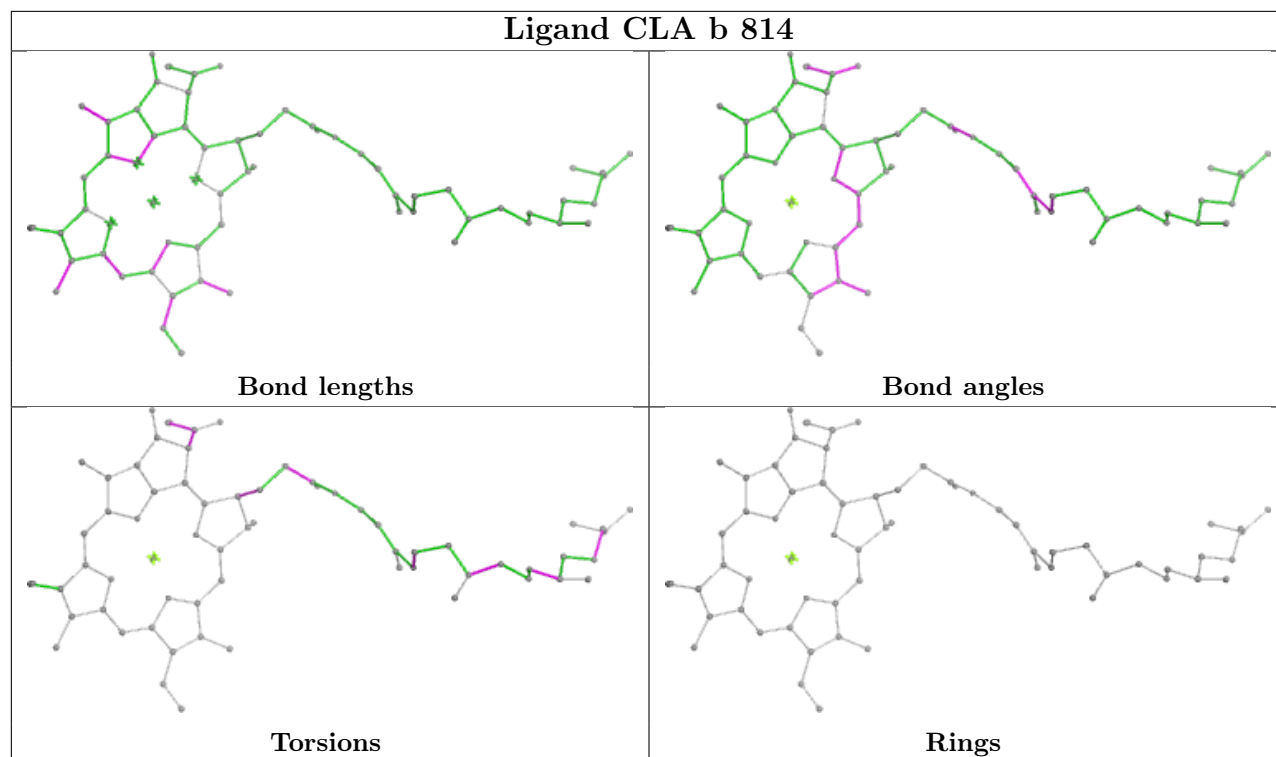
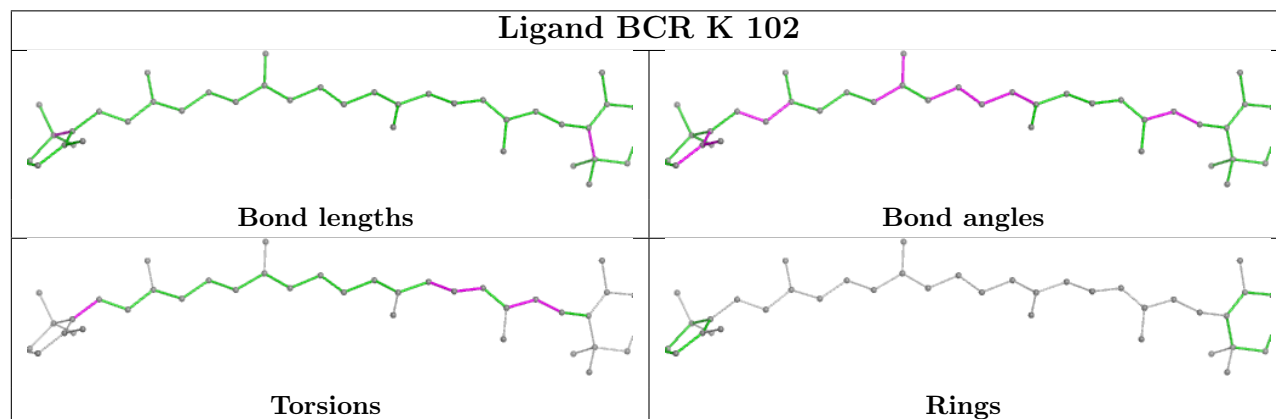
Bond angles

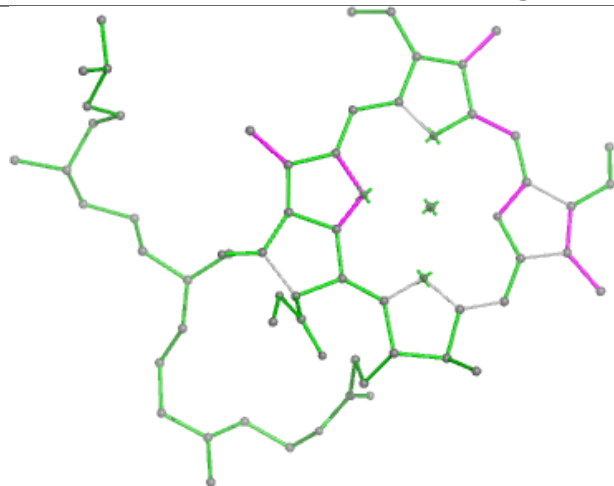


Torsions

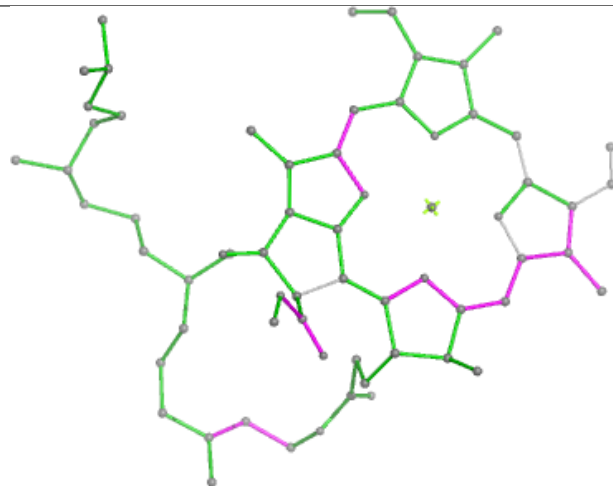


Rings

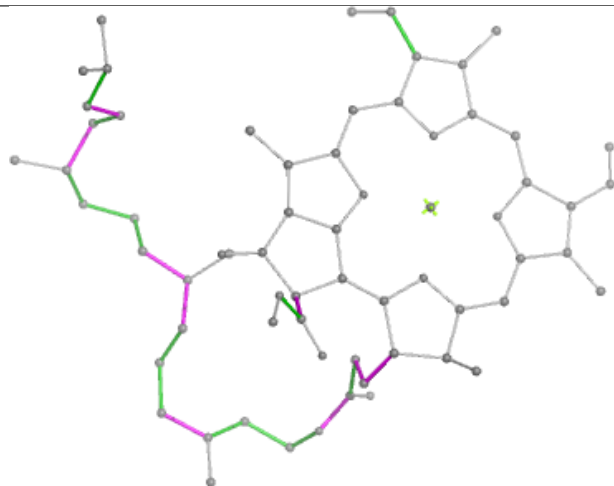
Ligand CLA b 814**Ligand BCR K 102**

Ligand CLA B 832

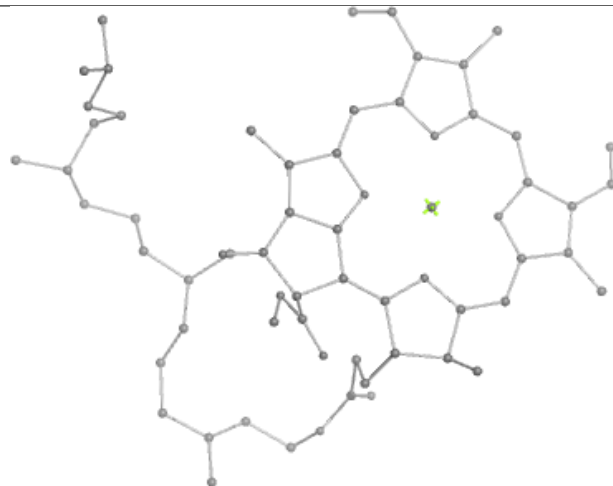
Bond lengths



Bond angles

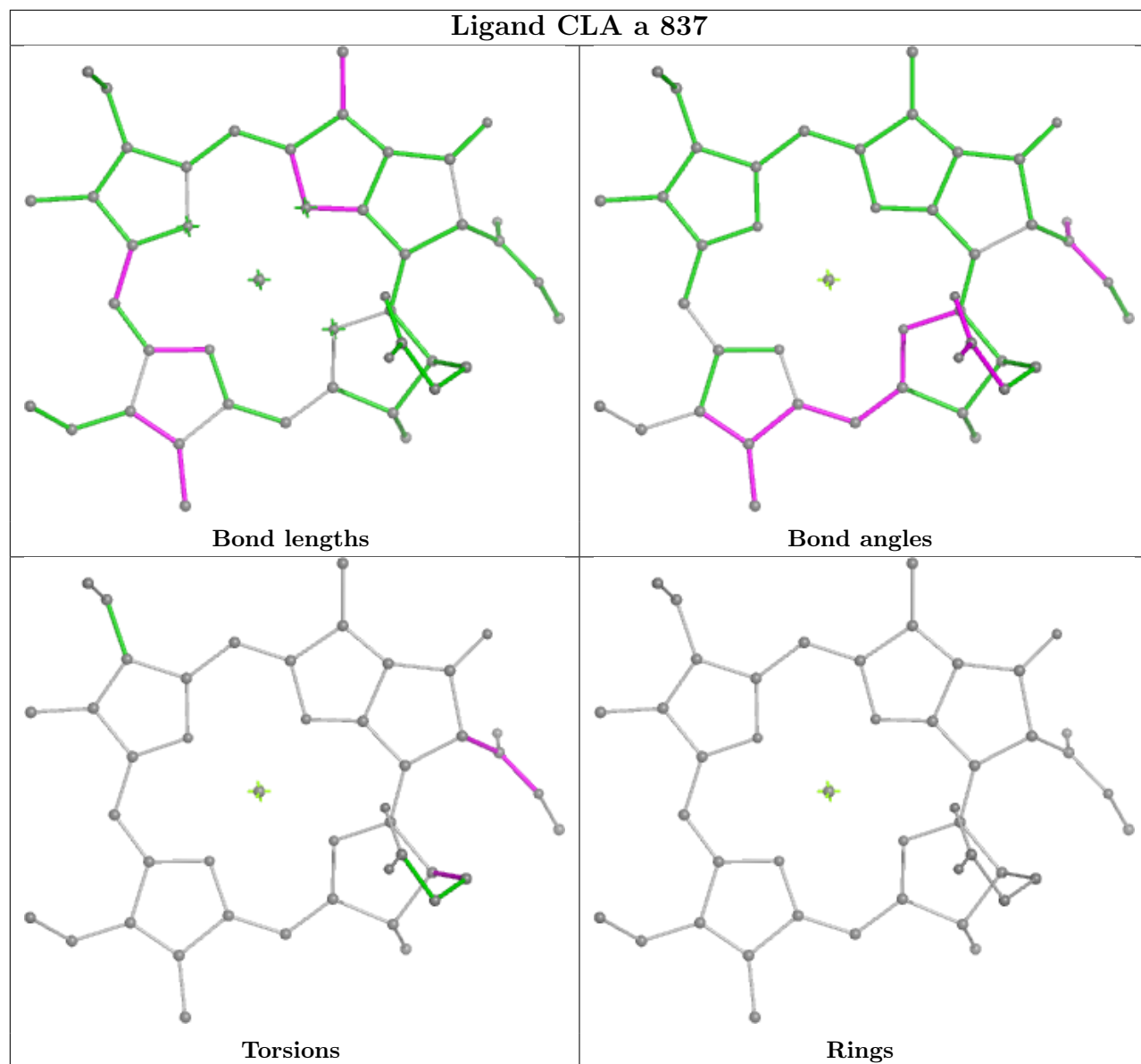


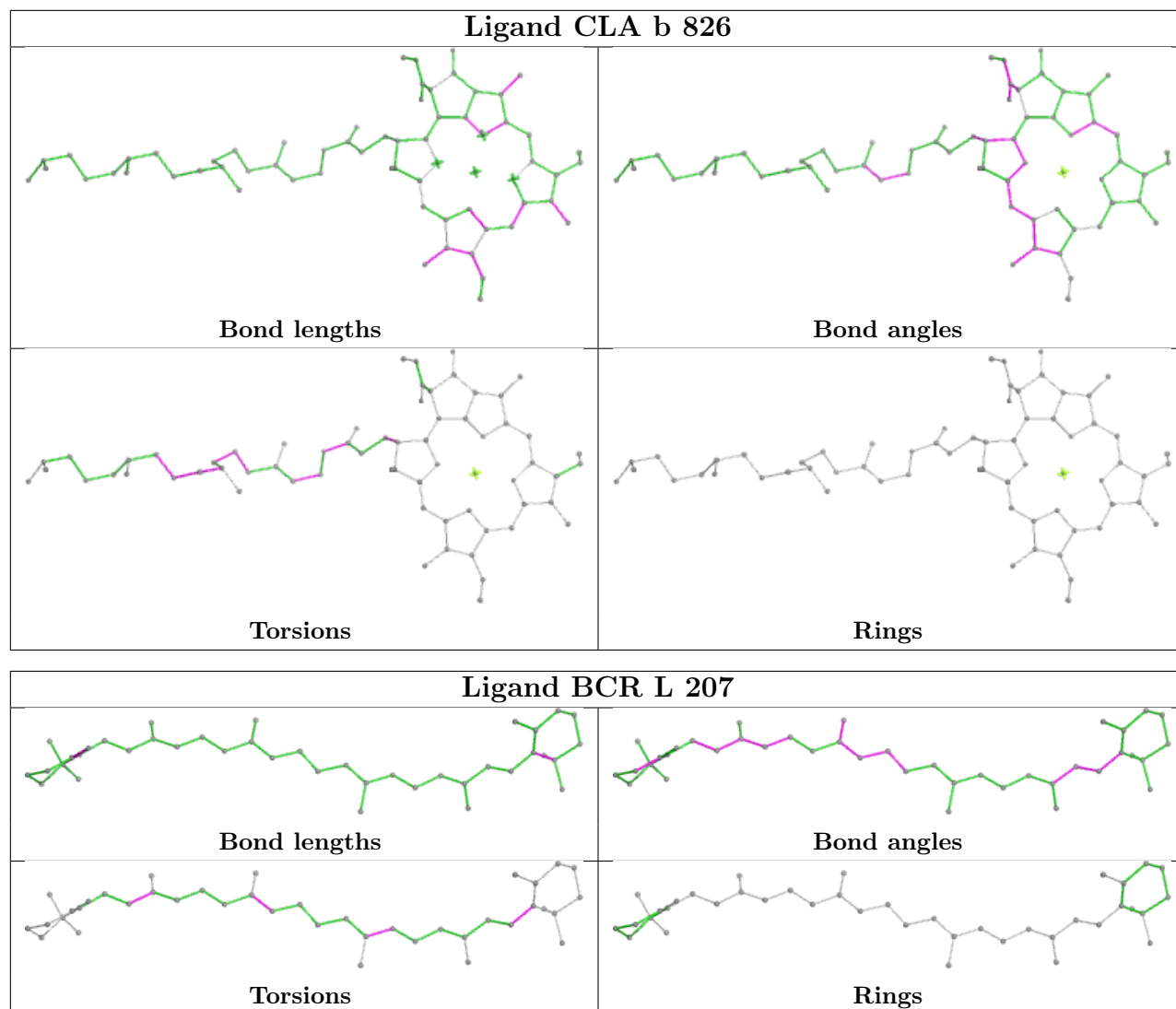
Torsions



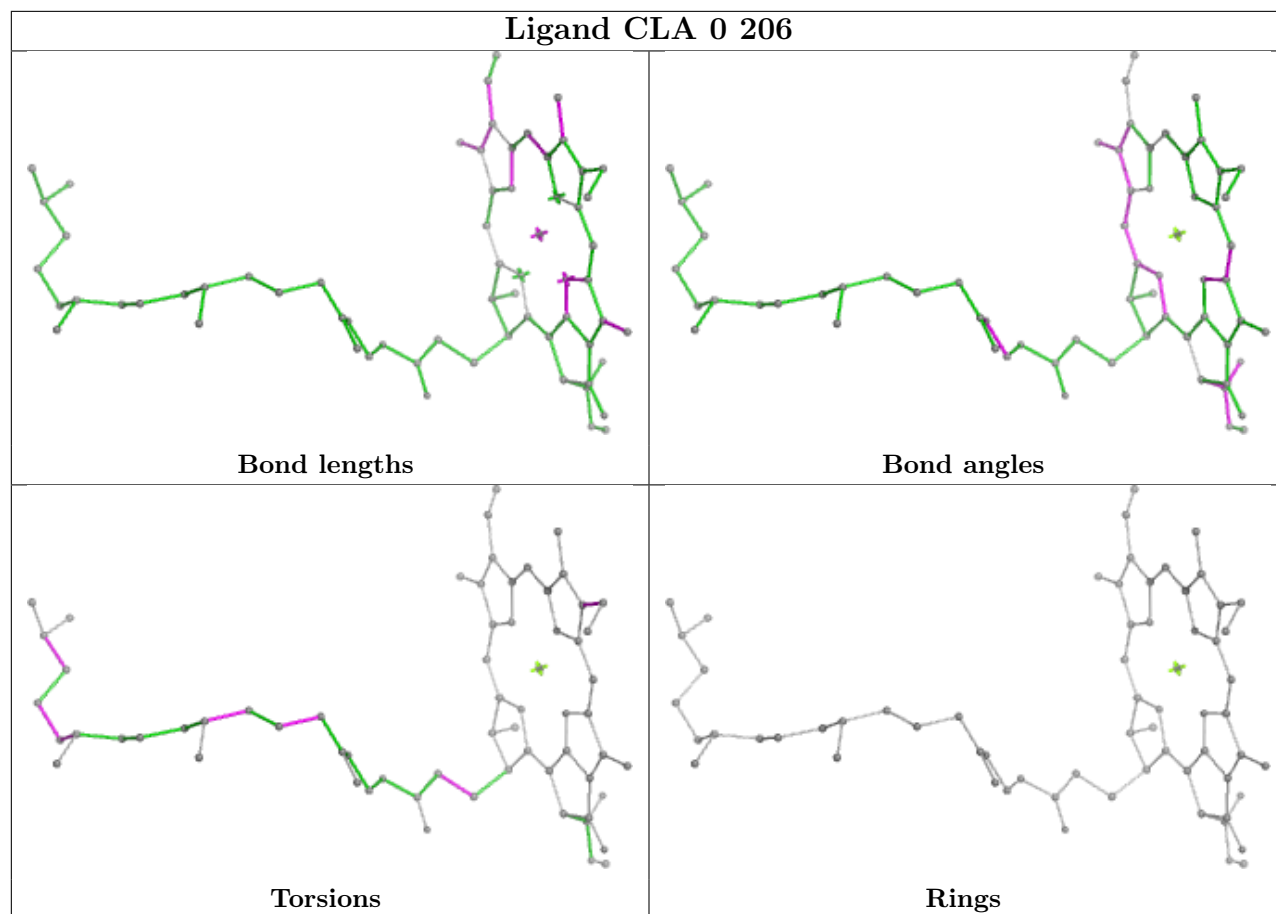
Rings

Ligand CLA a 837

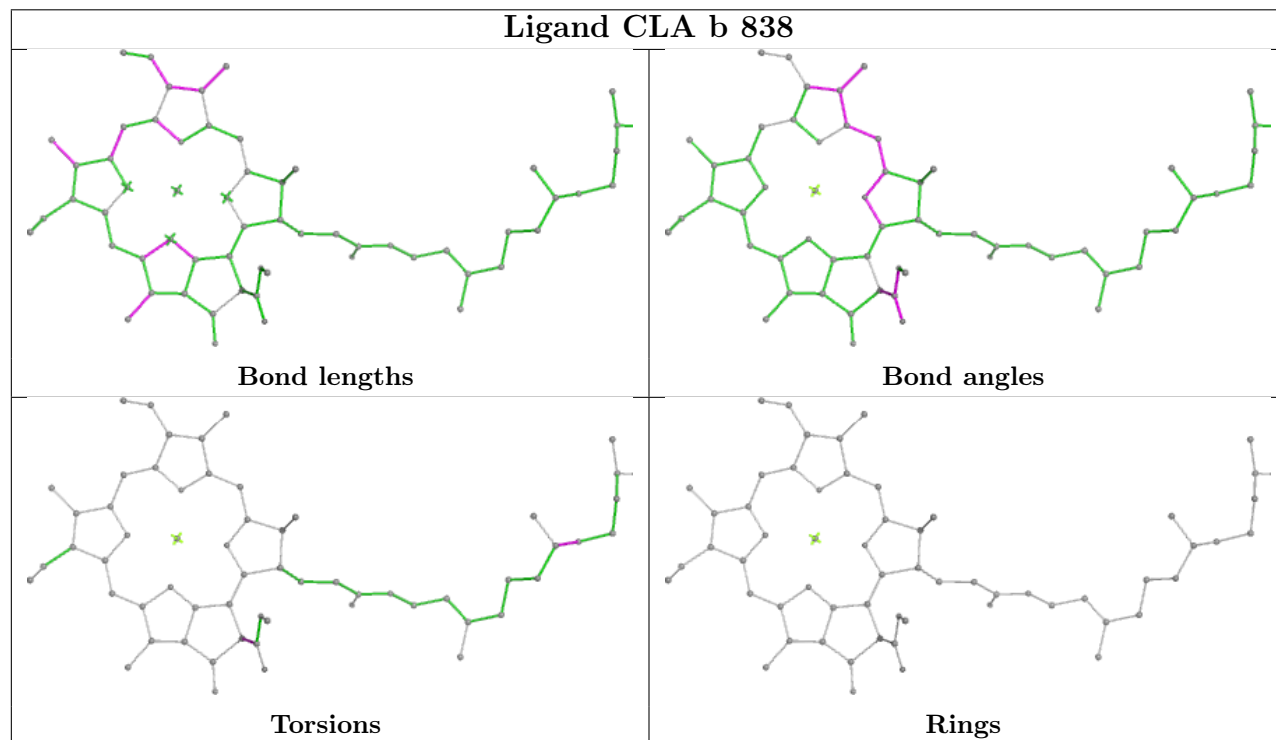




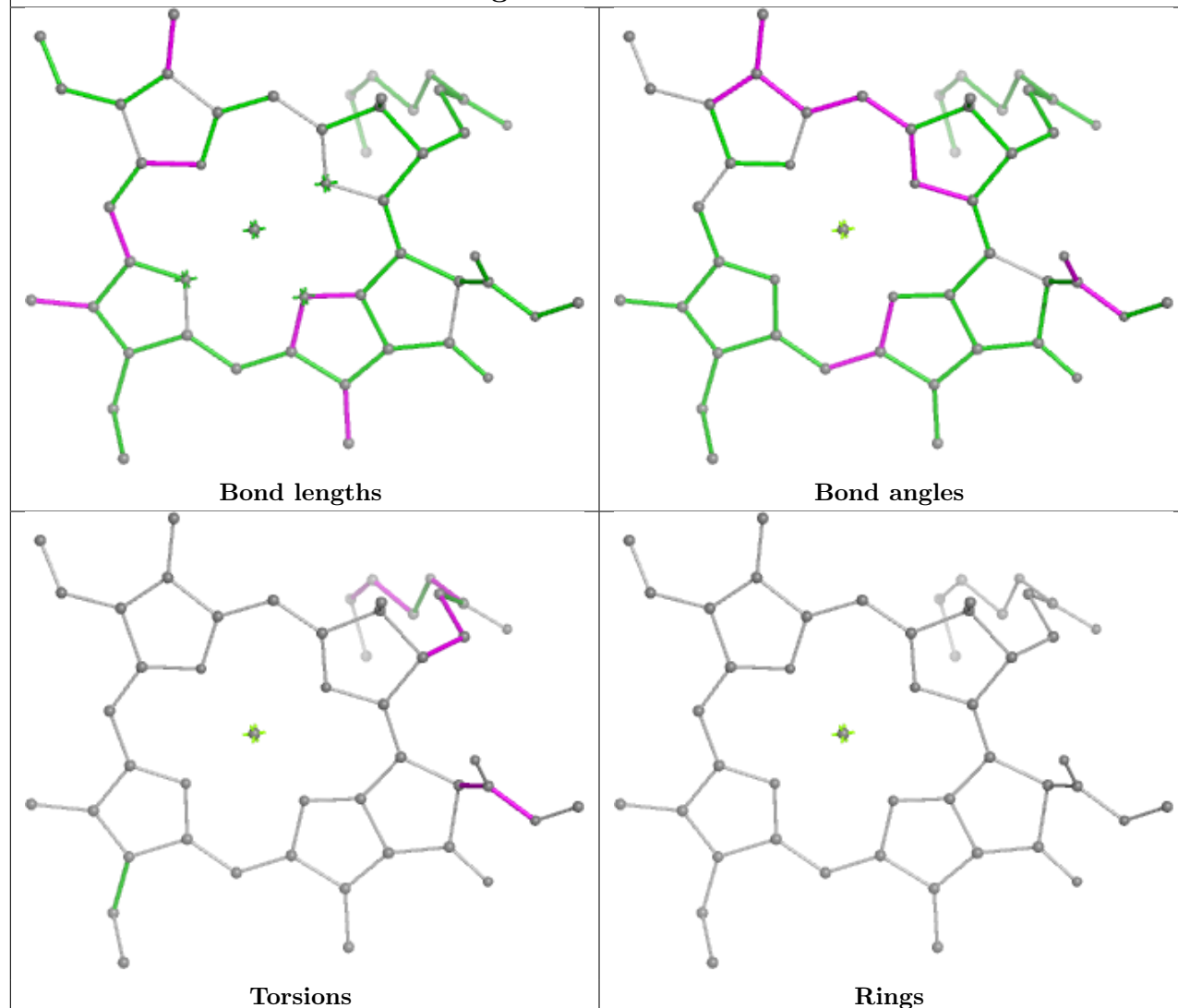
Ligand CLA 0 206



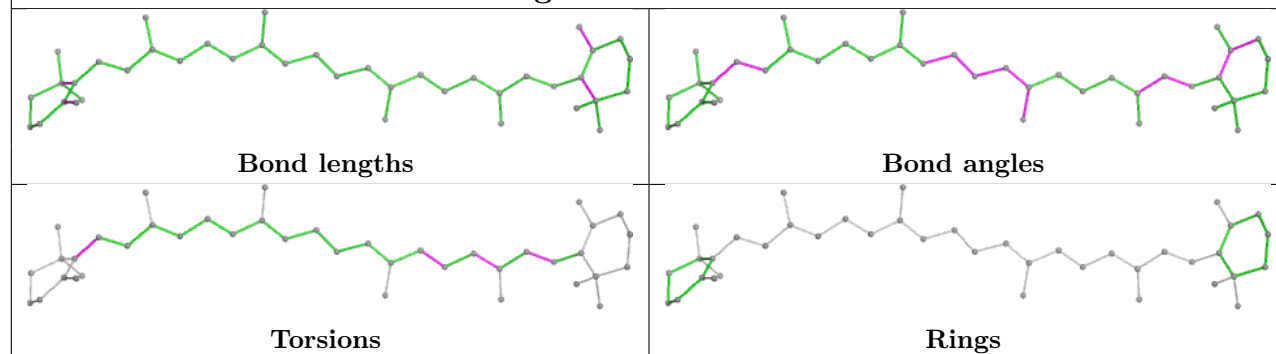
Ligand CLA b 838

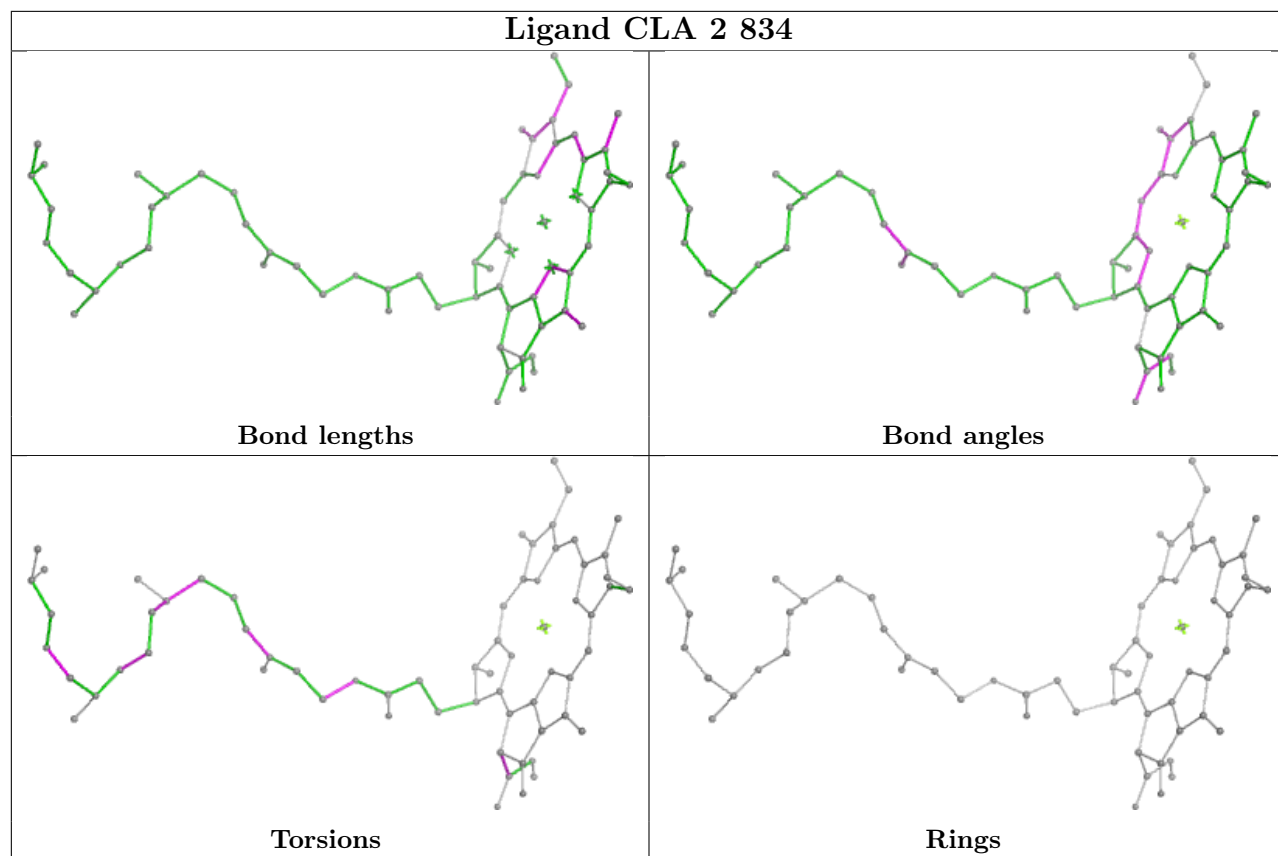


Ligand CLA B 831

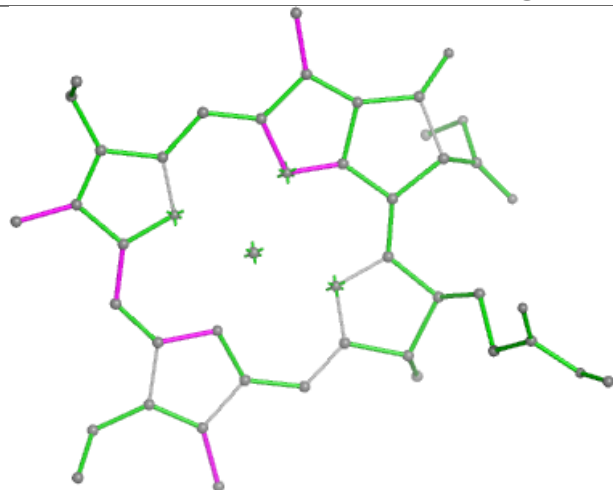


Ligand BCR 2 849

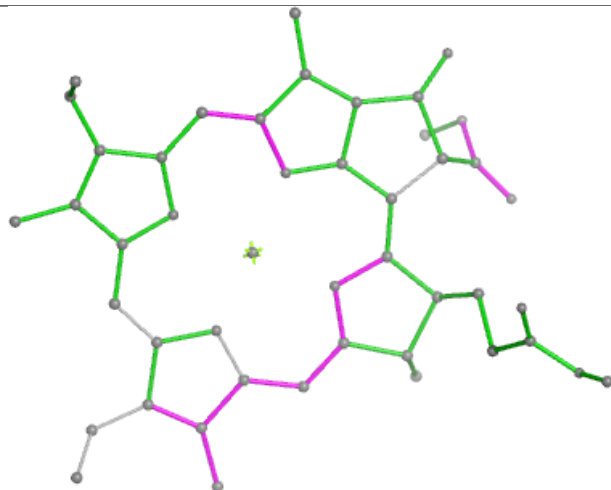




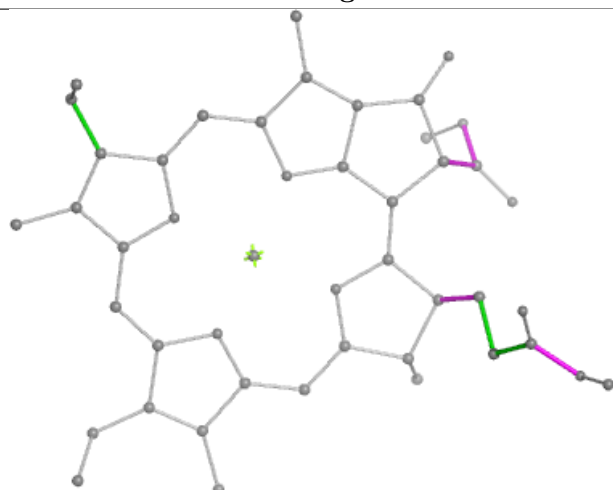
Ligand CLA 9 101



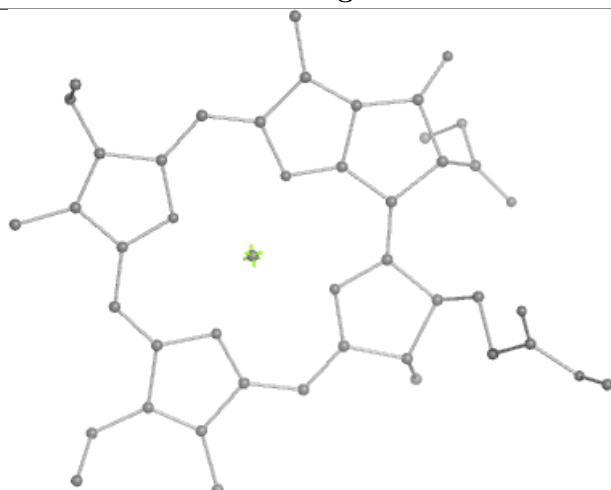
Bond lengths



Bond angles

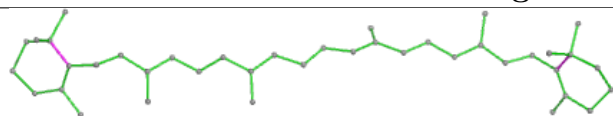


Torsions

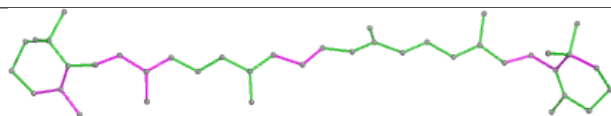


Rings

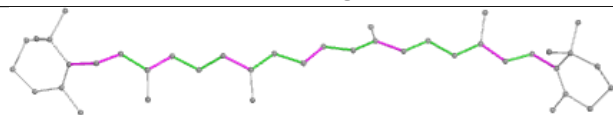
Ligand BCR A 847



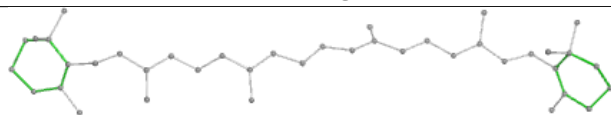
Bond lengths



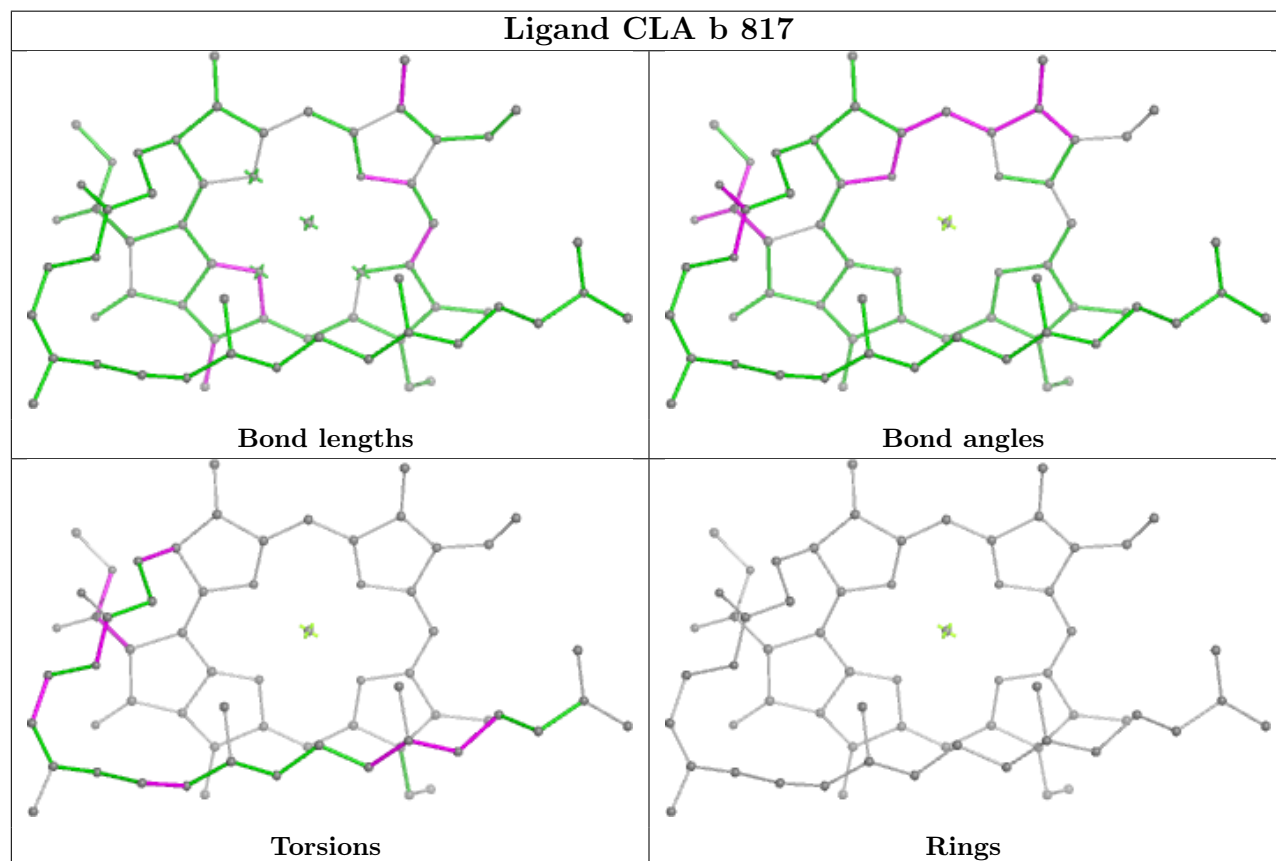
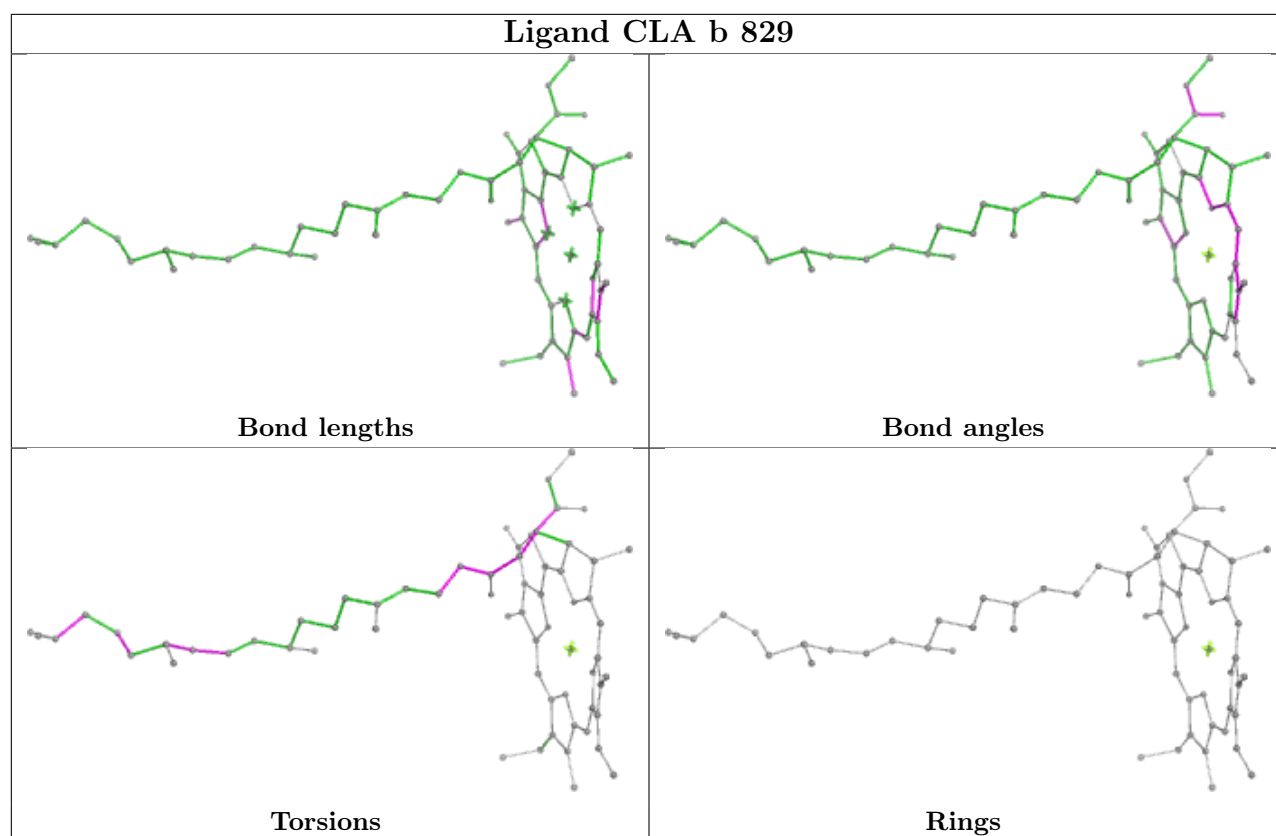
Bond angles

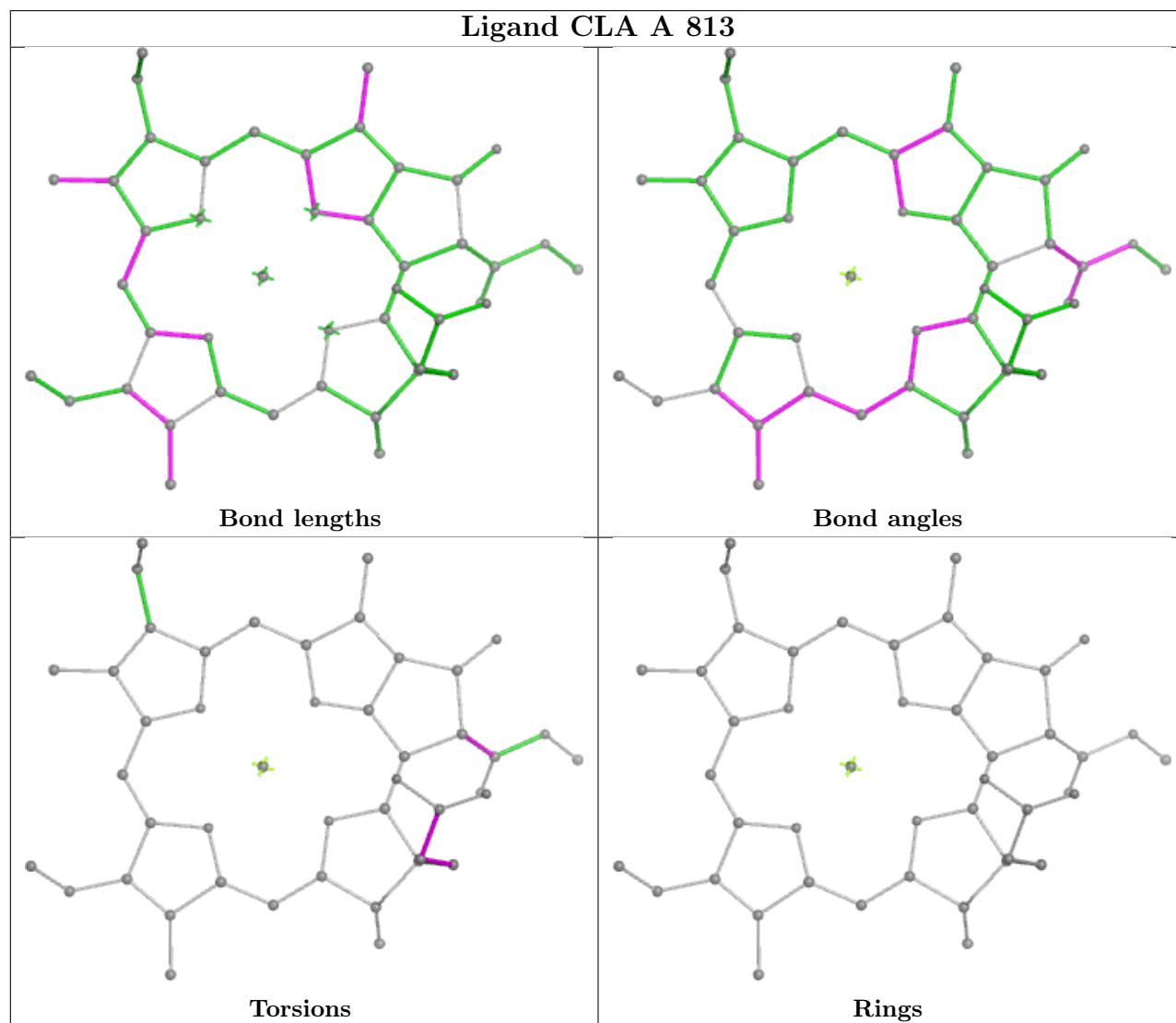
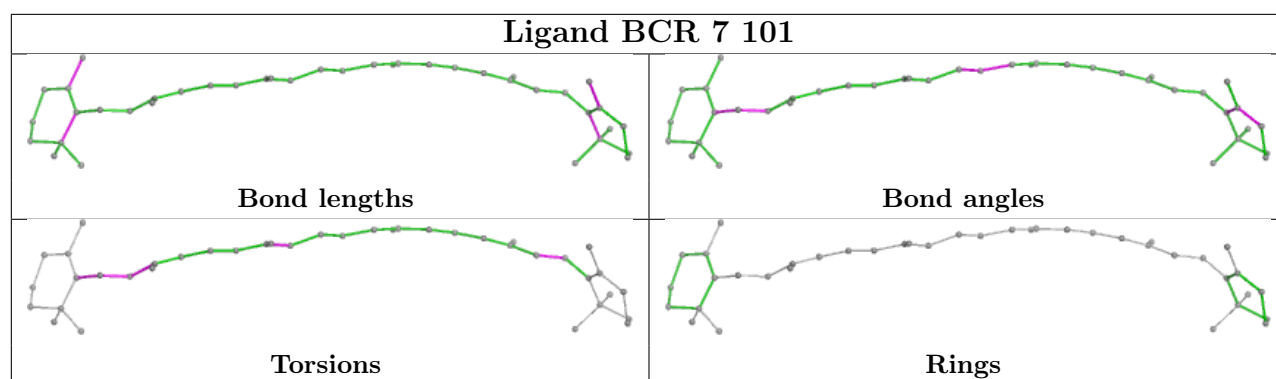


Torsions

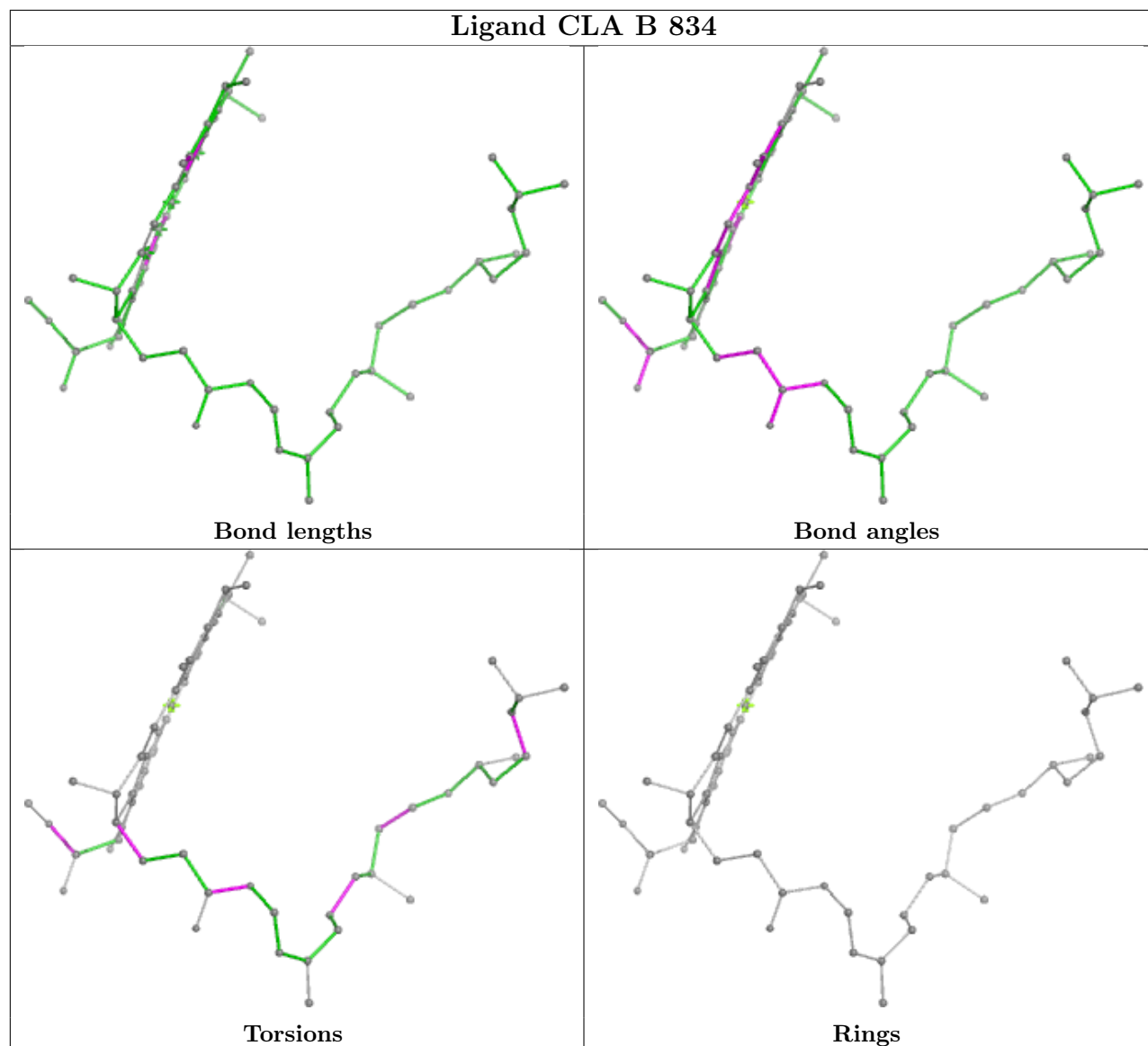


Rings

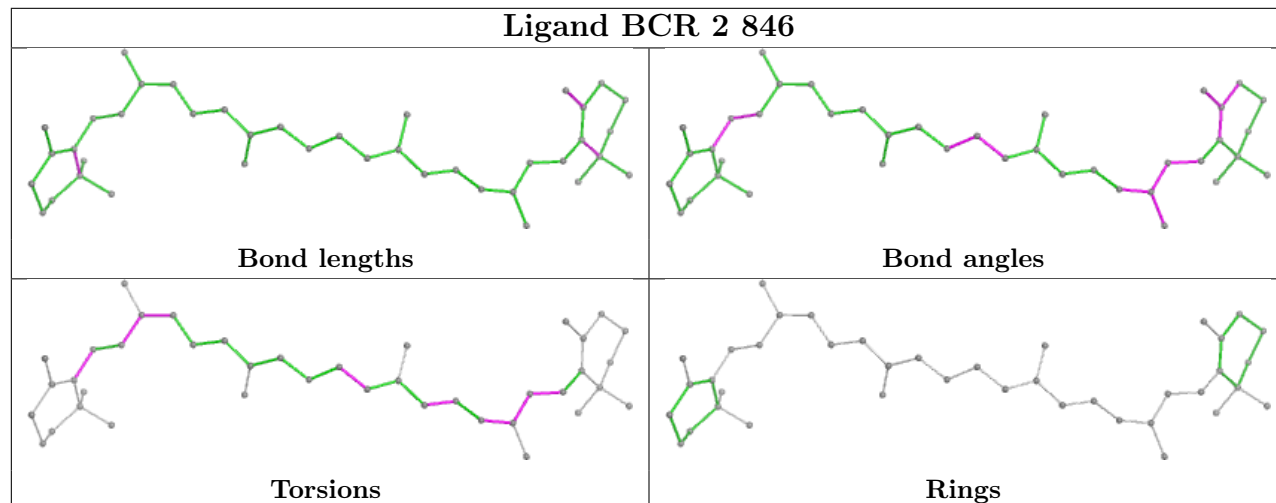


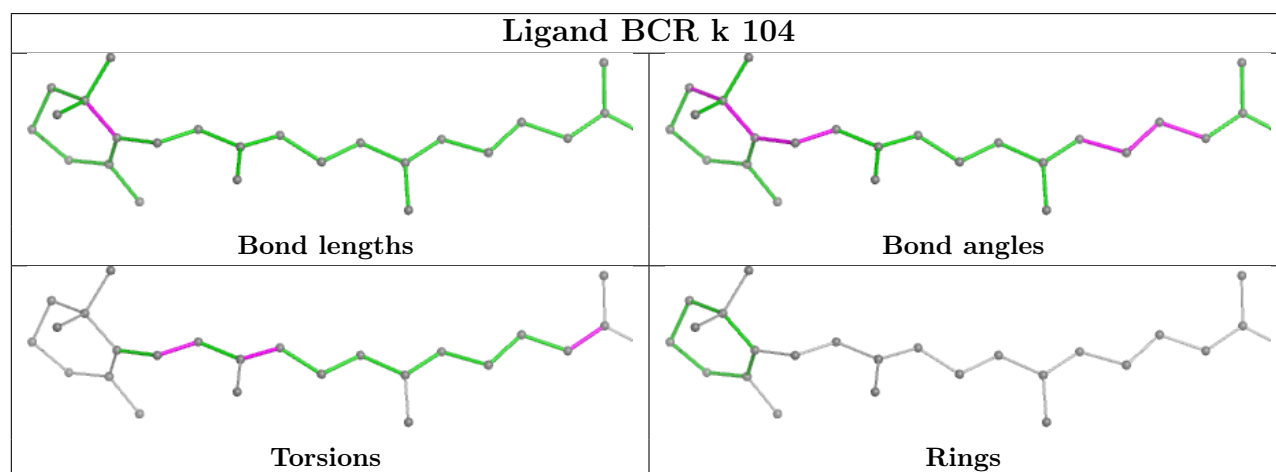
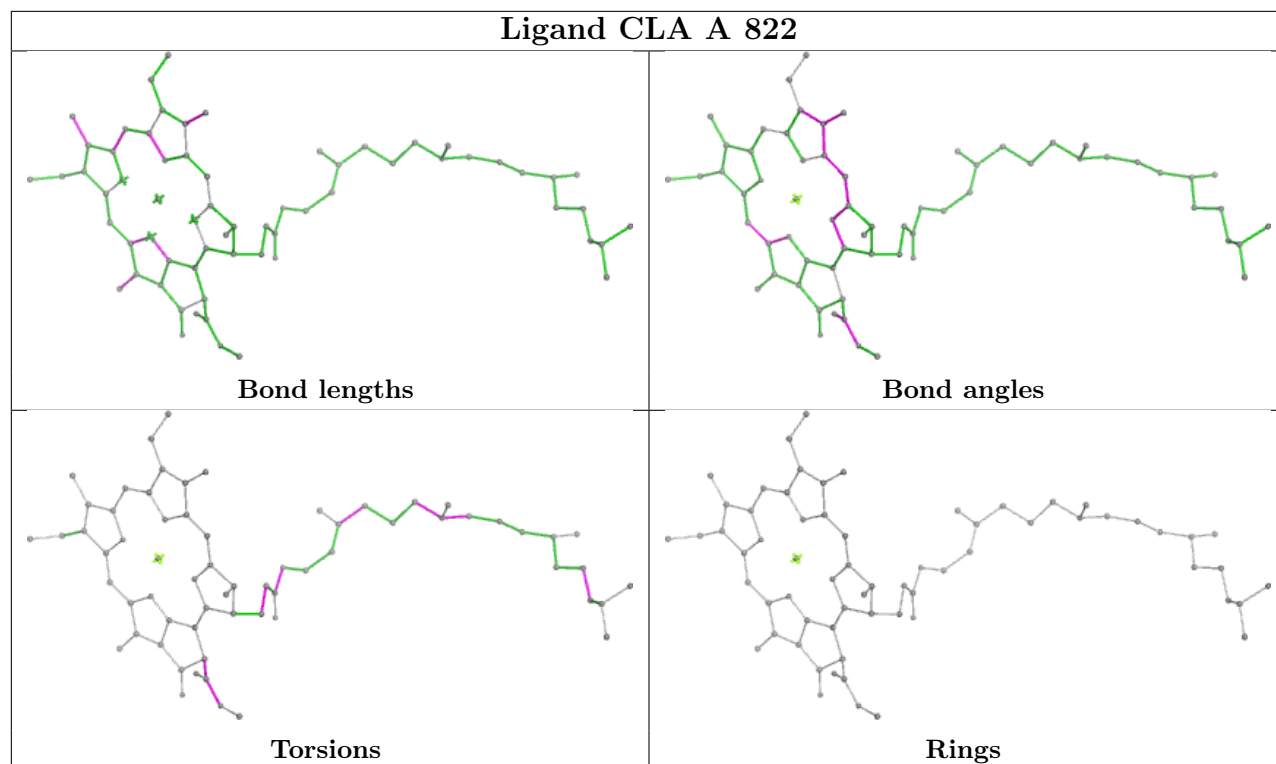


Ligand CLA B 834

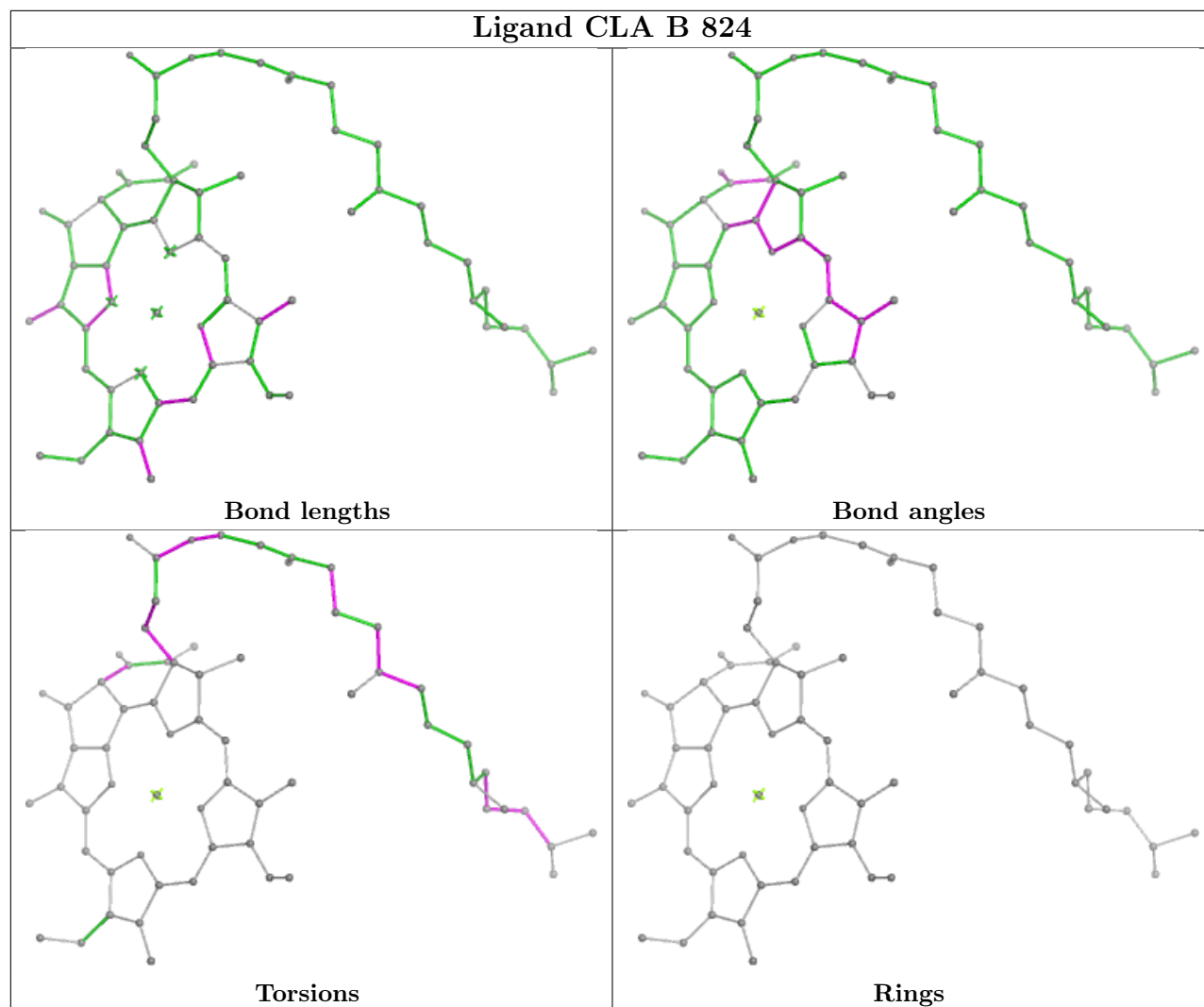


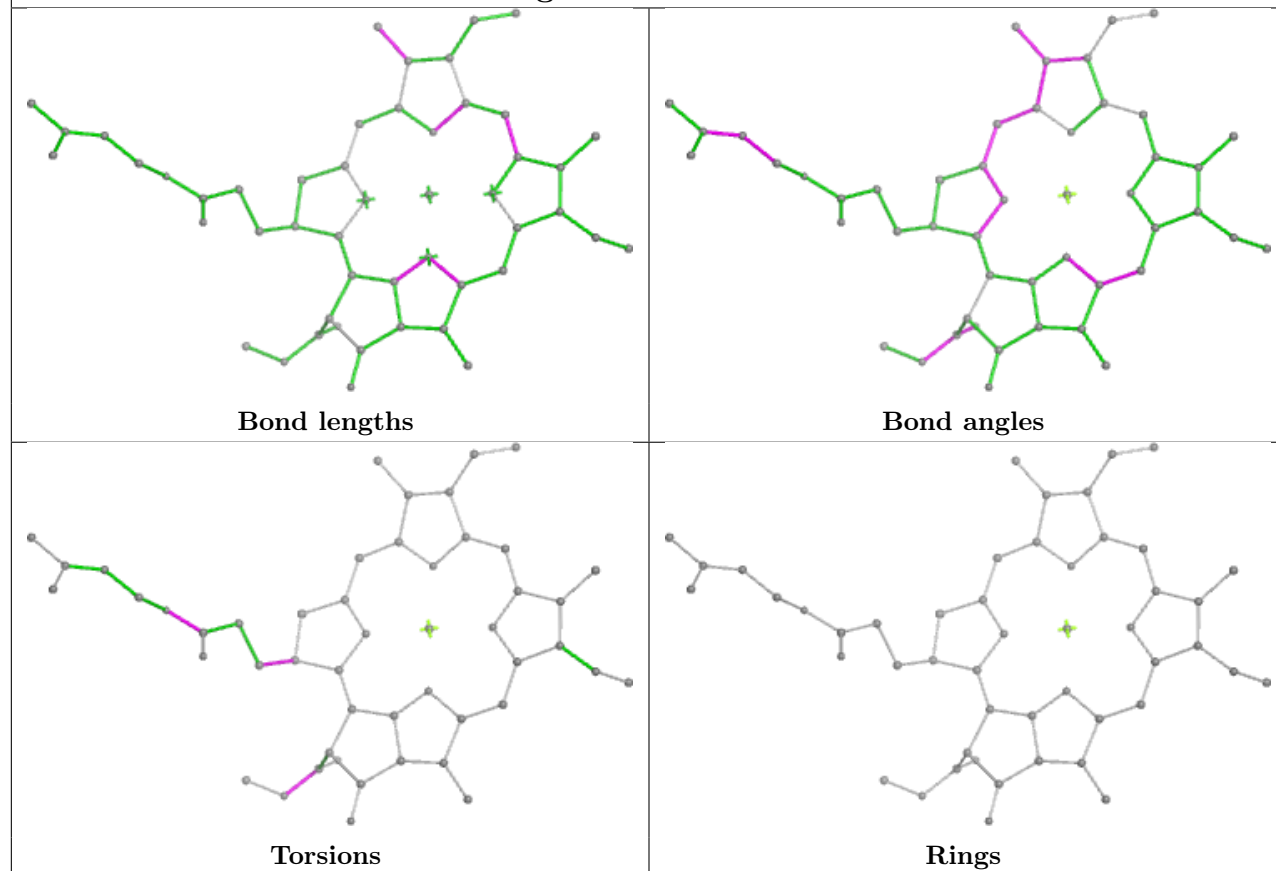
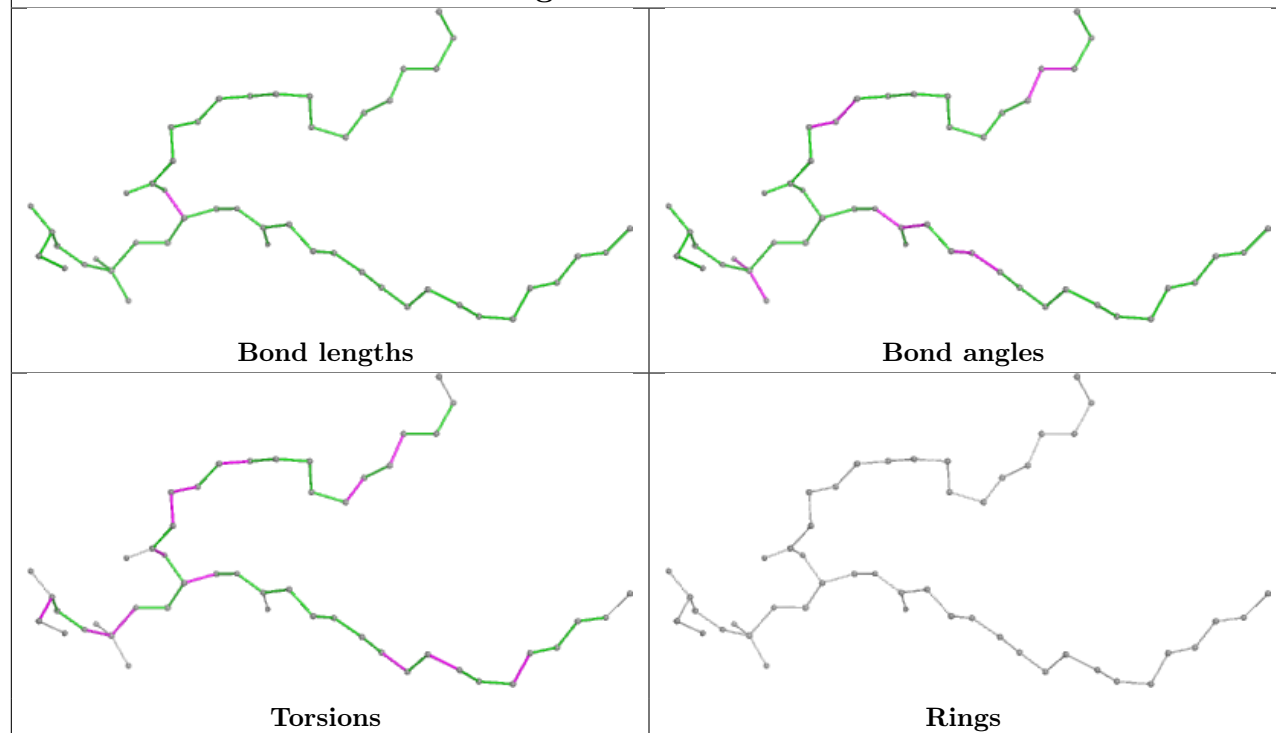
Ligand BCR 2 846

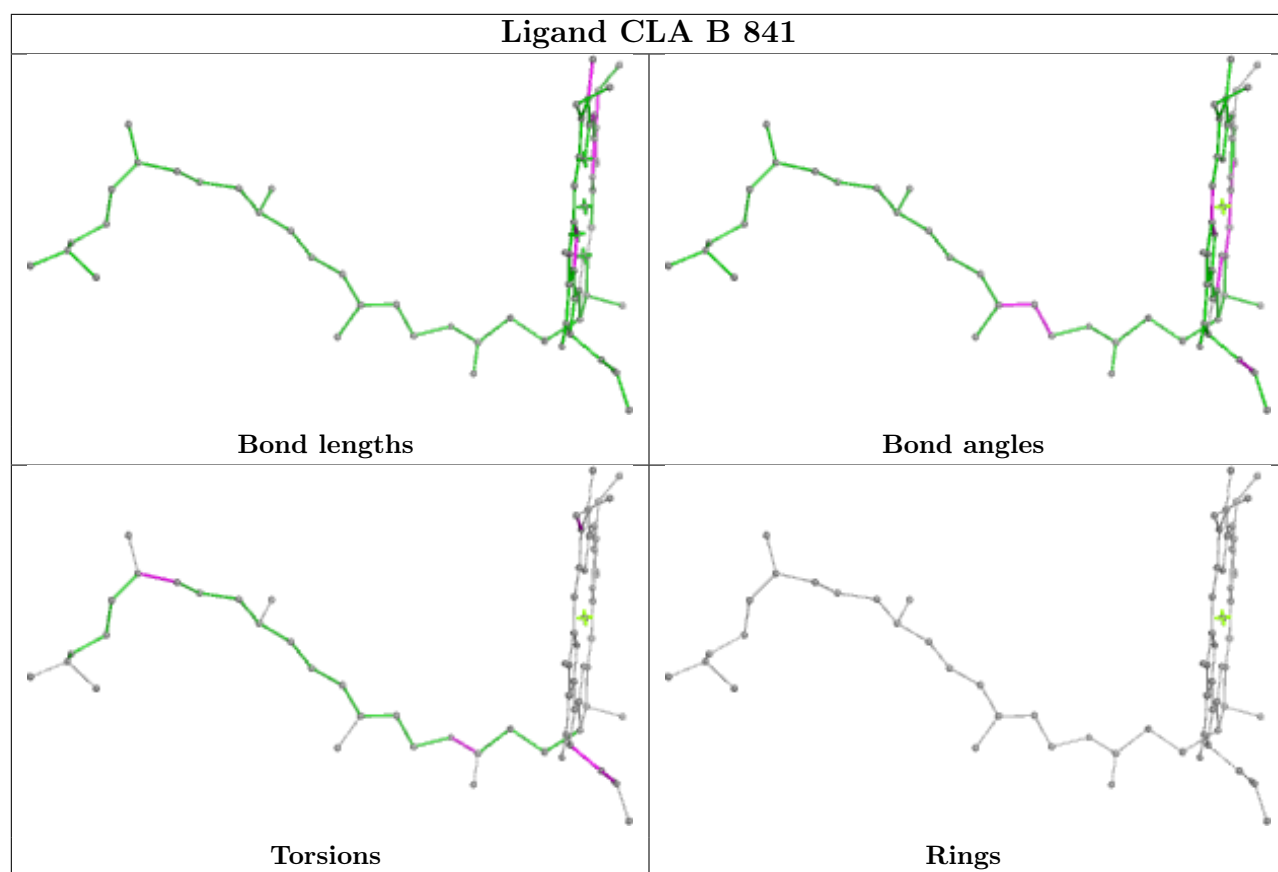




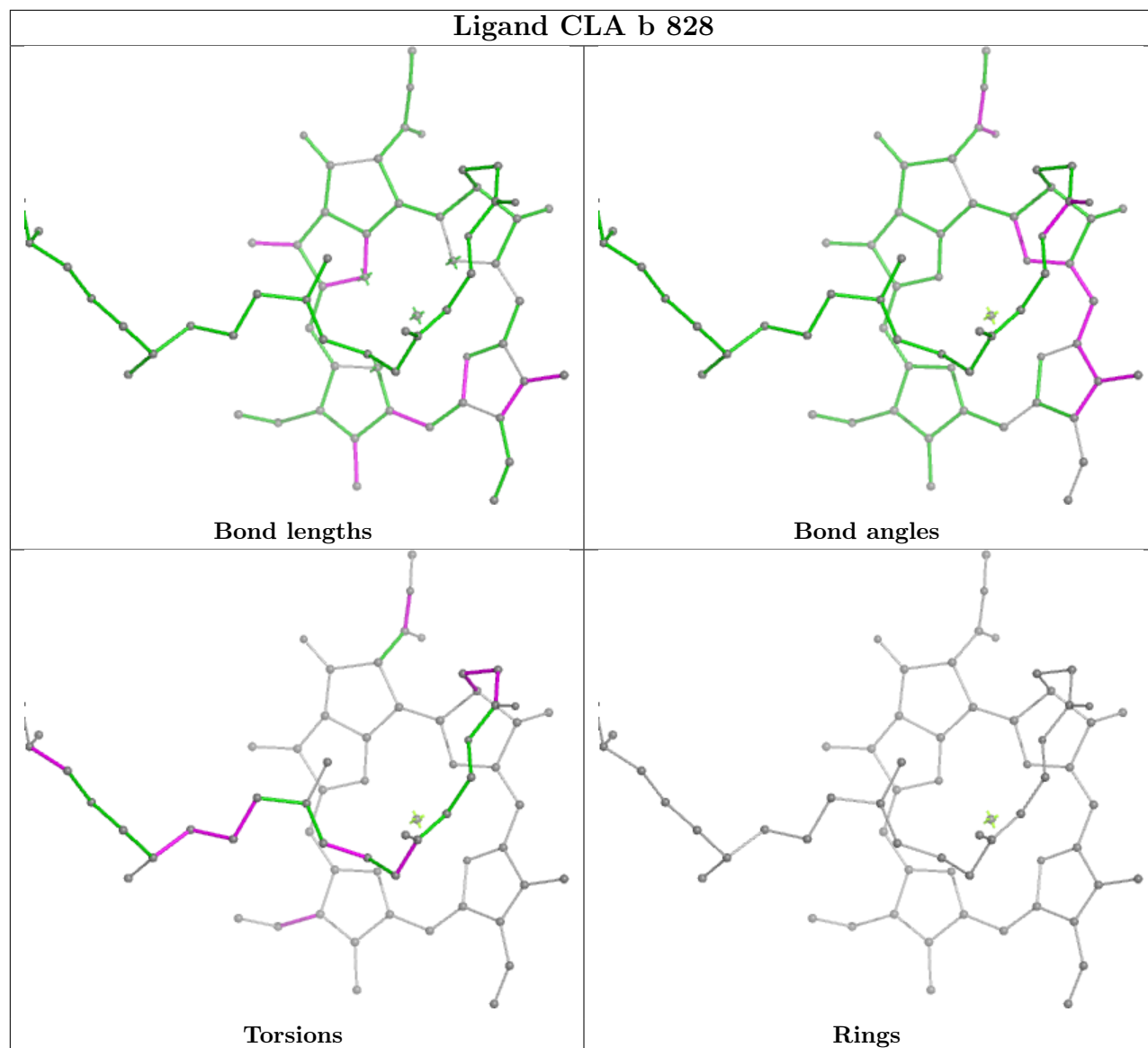
Ligand CLA B 824

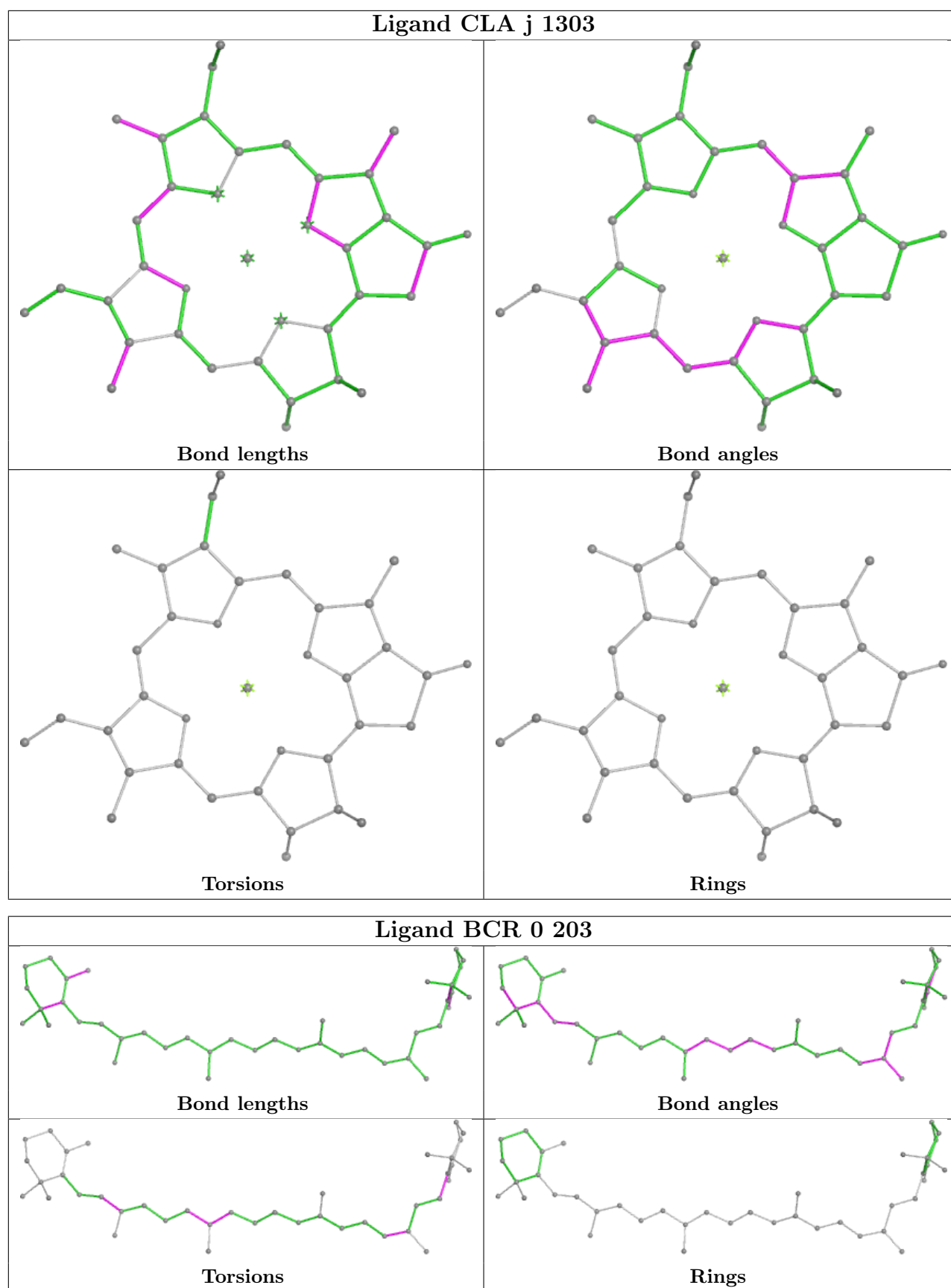


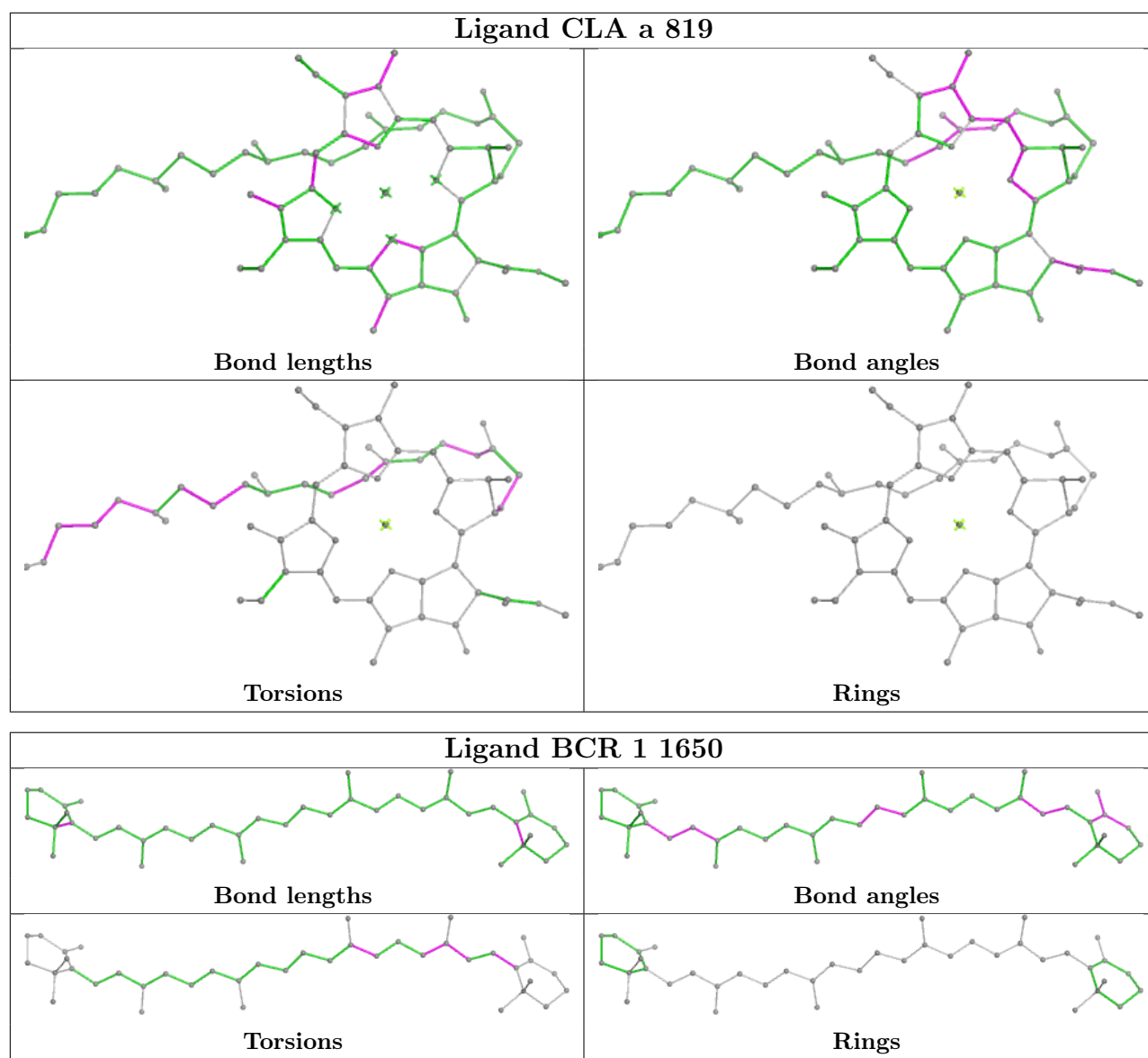
Ligand CLA 6 203**Ligand LHG z 101**



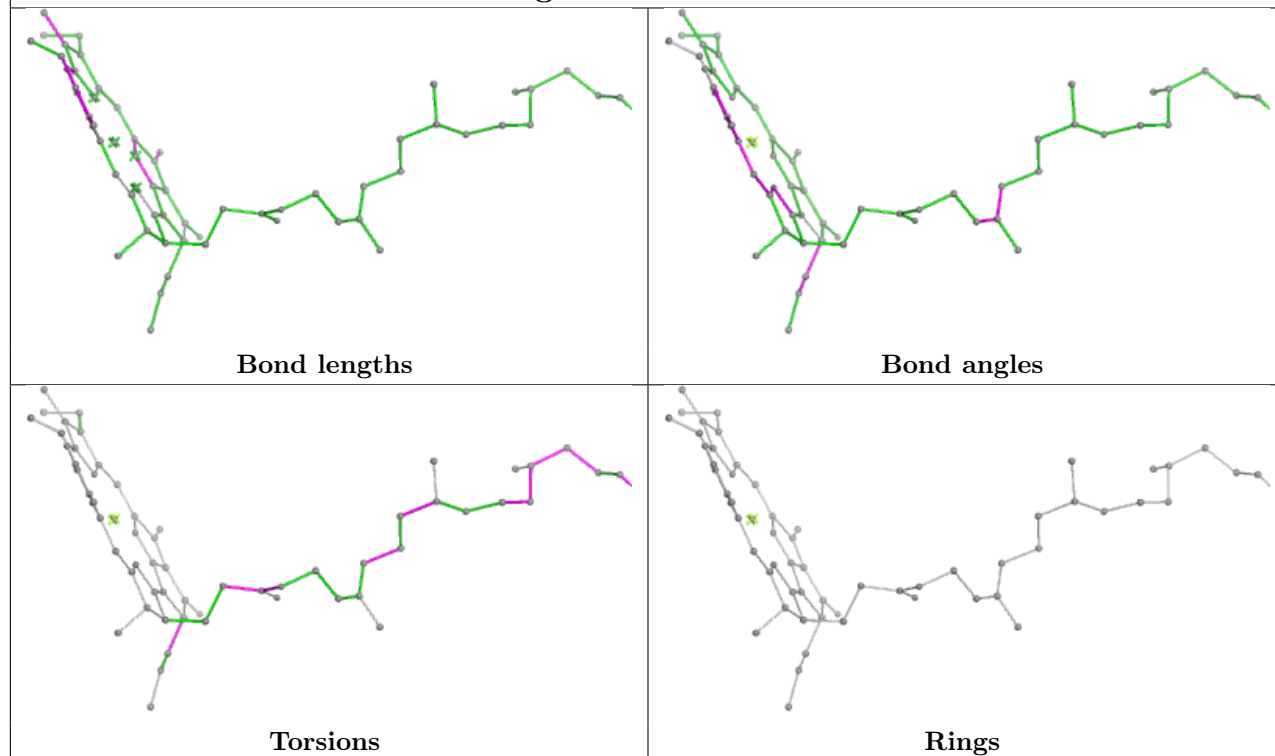
Ligand CLA b 828



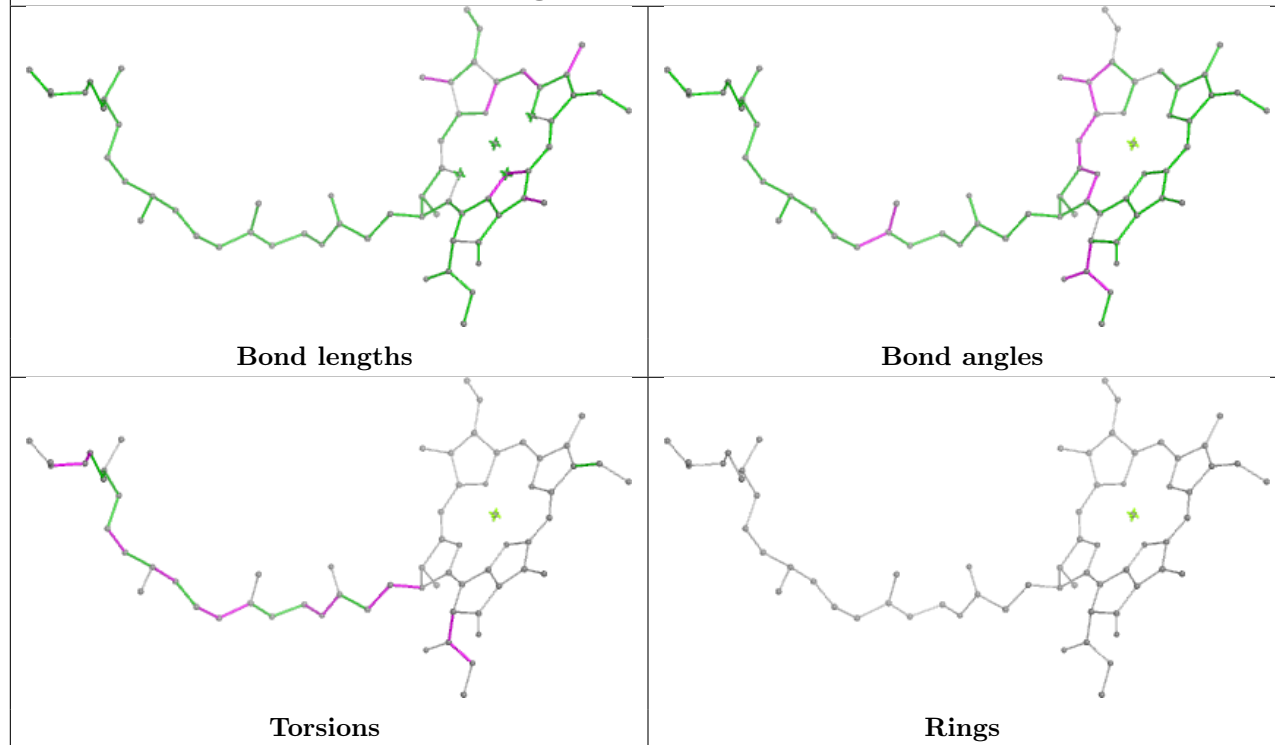


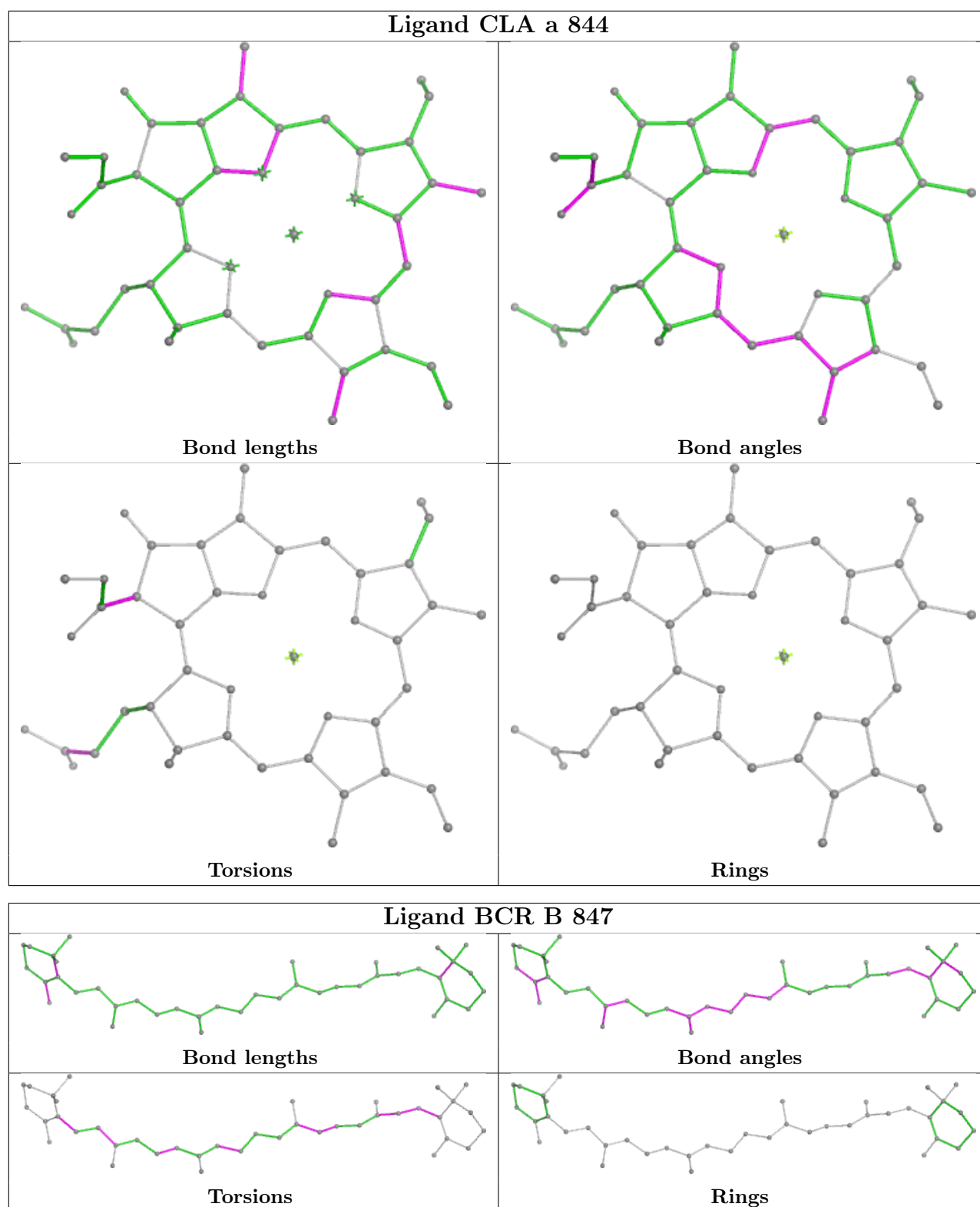


Ligand CLA a 840



Ligand CLA A 855





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10559. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

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

7 Map analysis ⓘ

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

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.