



wwPDB EM Validation Summary Report ⓘ

Nov 15, 2022 – 03:46 AM JST

PDB ID : 6K61
EMDB ID : EMD-9918
Title : Cryo-EM structure of the tetrameric photosystem I from a heterocyst-forming cyanobacterium *Anabaena* sp. PCC7120
Authors : Zheng, L.; Li, Y.; Li, X.; Zhong, Q.; Li, N.; Zhang, K.; Zhang, Y.; Chu, H.; Ma, C.; Li, G.; Zhao, J.; Gao, N.
Deposited on : 2019-05-31
Resolution : 2.37 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

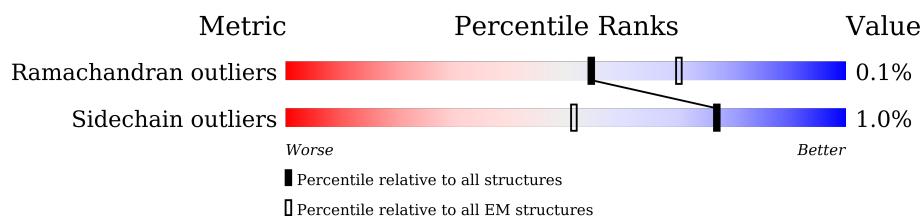
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

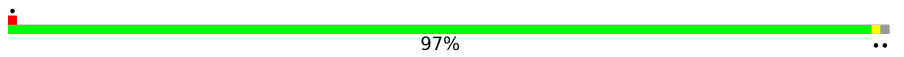
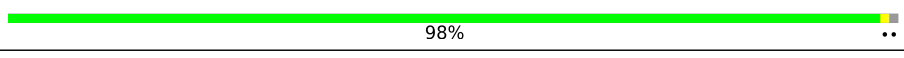


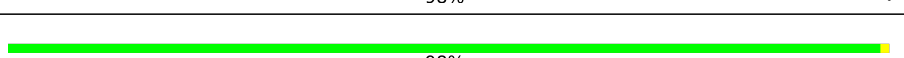
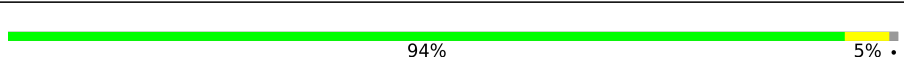
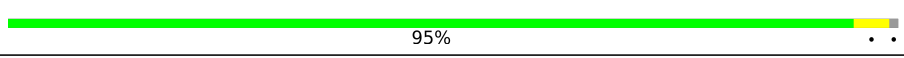
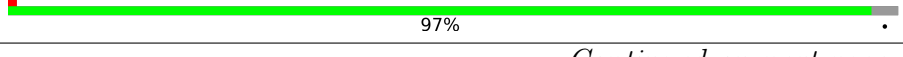

The reported resolution of this entry is 2.37 Å.

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	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	752	
1	a	752	
2	X	44	
2	x	44	
3	B	741	
3	b	741	
4	C	81	
4	c	81	
5	D	139	

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Mol	Chain	Length	Quality of chain
5	d	139	
6	E	70	
6	e	70	
7	F	164	
7	f	164	
8	J	49	
8	j	49	
9	K	86	
9	k	86	
10	I	46	
10	i	46	
11	L	172	
11	l	172	
12	M	32	
12	m	32	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	A	801	X	-	-	-
13	CL0	a	801	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	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	B	843	X	-	-	-
14	CLA	F	202	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	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	b	802	X	-	-	-
14	CLA	b	803	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-
14	CLA	b	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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	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	840	X	-	-	-
14	CLA	b	841	X	-	-	-
14	CLA	b	842	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	j	103	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	102	X	-	-	-
14	CLA	l	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	l	205	X	-	-	-
14	CLA	m	1201	X	-	-	-
14	CLA	x	1701	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 49283 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	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		
1	a	742	Total	C	N	O	S	0	0
			5823	3820	1003	979	21		

- Molecule 2 is a protein called Photosystem I 4.8 kDa protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	X	31	Total	C	N	O	0	0
			257	179	40	38		
2	x	31	Total	C	N	O	0	0
			257	179	40	38		

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		
3	b	740	Total	C	N	O	S	0	0
			5918	3905	991	1004	18		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	135	Total	C	N	O	S	0	0
			1040	666	179	194	1		
5	d	136	Total	C	N	O	S	0	0
			1047	670	180	196	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	61	Total	C	N	O	S	0	0
			490	313	84	93			
6	e	61	Total	C	N	O	S	0	0
			490	313	84	93			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		
7	f	141	Total	C	N	O	S	0	0
			1080	690	184	204	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	45	Total	C	N	O	S	0	0
			359	244	54	61			
8	j	45	Total	C	N	O	S	0	0
			359	244	54	61			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	73	Total	C	N	O	S	0	0
			537	357	89	90	1		
9	k	78	Total	C	N	O	S	0	0
			568	376	94	97	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	34	Total	C	N	O	S	0	0
			275	189	38	48			

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Mol	Chain	Residues	Atoms				AltConf	Trace
10	i	34	Total	C	N	O	0	0
			275	189	38	48		

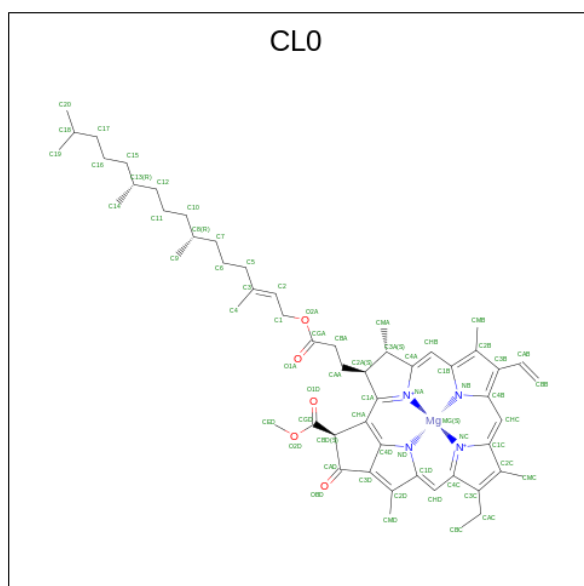
- Molecule 11 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total	C	N	O	S	0	0
			1163	763	197	202	1		
11	l	155	Total	C	N	O	S	0	0
			1163	763	197	202	1		

- Molecule 12 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	M	31	Total	C	N	O	0	0
			241	160	37	44		
12	m	31	Total	C	N	O	0	0
			241	160	37	44		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



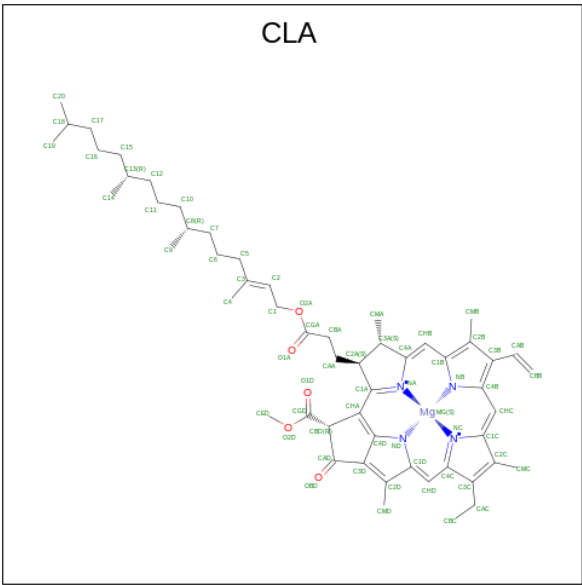
Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	A	1	Total 2466	C 2046	Mg 42	N 168	O 210	0
14	X	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	B	1	Total 2495	C 2075	Mg 42	N 168	O 210	0
14	F	1	Total 110	C 90	Mg 2	N 8	O 10	0
14	F	1	Total 110	C 90	Mg 2	N 8	O 10	0
14	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
14	J	1	Total 82	C 66	Mg 2	N 8	O 6	0
14	K	1	Total 90	C 72	Mg 2	N 8	O 8	0
14	K	1	Total 90	C 72	Mg 2	N 8	O 8	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0
14	L	1	Total 156	C 126	Mg 3	N 12	O 15	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	a	1	Total 2342	C 1942	Mg 40	N 160	O 200	0
14	x	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0
14	b	1	Total 2512	C 2092	Mg 42	N 168	O 210	0

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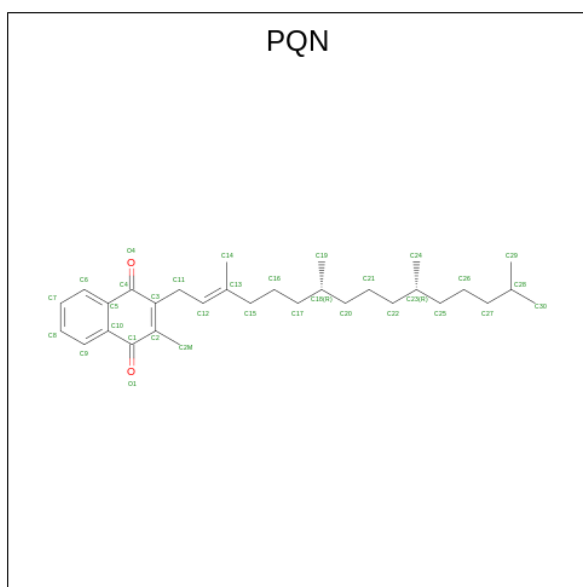
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	b	1	Total	C	Mg	N	O	0
			2512	2092	42	168	210	
14	f	1	Total	C	Mg	N	O	0
			104	84	2	8	10	

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Mol	Chain	Residues	Atoms					AltConf
14	f	1	Total	C	Mg	N	O	0
			104	84	2	8	10	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	j	1	Total	C	Mg	N	O	0
			140	114	3	12	11	
14	k	1	Total	C	Mg	N	O	0
			90	72	2	8	8	
14	k	1	Total	C	Mg	N	O	0
			90	72	2	8	8	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	l	1	Total	C	Mg	N	O	0
			150	120	3	12	15	
14	m	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$) (labeled as "Ligand of Interest" by depositor).



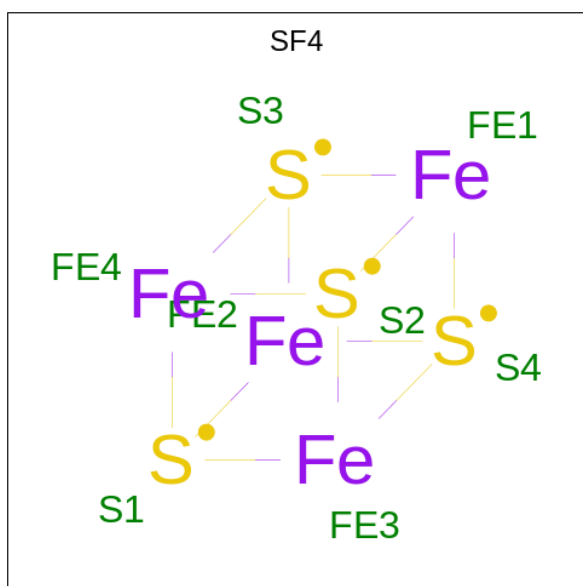
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	

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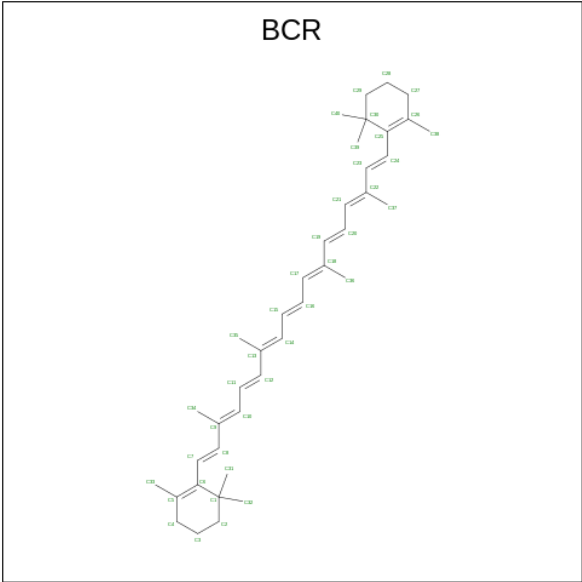
Mol	Chain	Residues	Atoms			AltConf
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: $\text{C}_{40}\text{H}_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	A	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	B	1	Total	C	0
			240	240	
17	F	1	Total	C	0
			80	80	
17	F	1	Total	C	0
			80	80	

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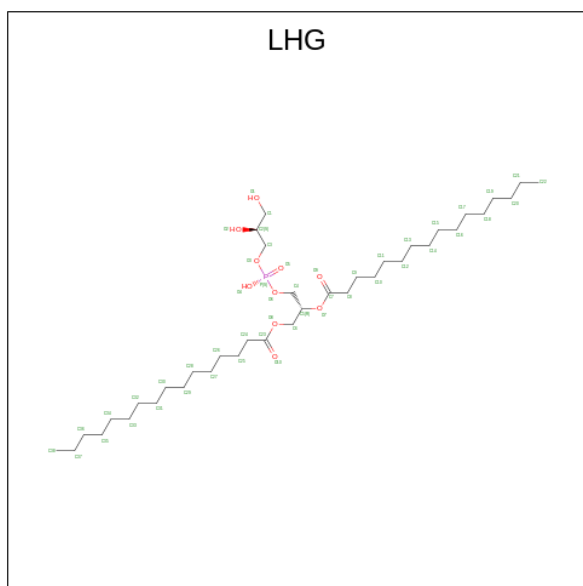
Mol	Chain	Residues	Atoms		AltConf
17	J	1	Total 120	C 120	0
17	J	1	Total 120	C 120	0
17	J	1	Total 120	C 120	0
17	K	1	Total 40	C 40	0
17	I	1	Total 80	C 80	0
17	I	1	Total 80	C 80	0
17	L	1	Total 40	C 40	0
17	M	1	Total 40	C 40	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	a	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	b	1	Total 240	C 240	0
17	f	1	Total 80	C 80	0

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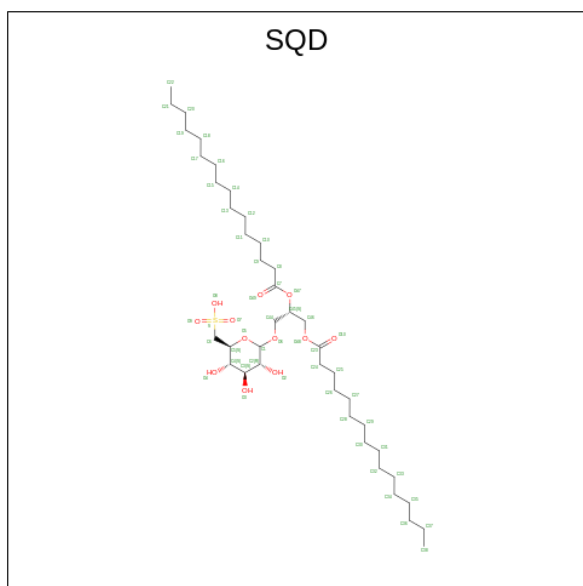
Mol	Chain	Residues	Atoms		AltConf
17	f	1	Total	C	0
			80	80	
17	j	1	Total	C	0
			120	120	
17	j	1	Total	C	0
			120	120	
17	j	1	Total	C	0
			120	120	
17	k	1	Total	C	0
			40	40	
17	i	1	Total	C	0
			80	80	
17	i	1	Total	C	0
			80	80	
17	l	1	Total	C	0
			120	120	
17	l	1	Total	C	0
			120	120	
17	l	1	Total	C	0
			120	120	
17	m	1	Total	C	0
			40	40	

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			98	76	20	2	
18	A	1	Total	C	O	P	0
			98	76	20	2	
18	F	1	Total	C	O	P	0
			43	32	10	1	
18	a	1	Total	C	O	P	0
			98	76	20	2	
18	a	1	Total	C	O	P	0
			98	76	20	2	
18	i	1	Total	C	O	P	0
			43	32	10	1	

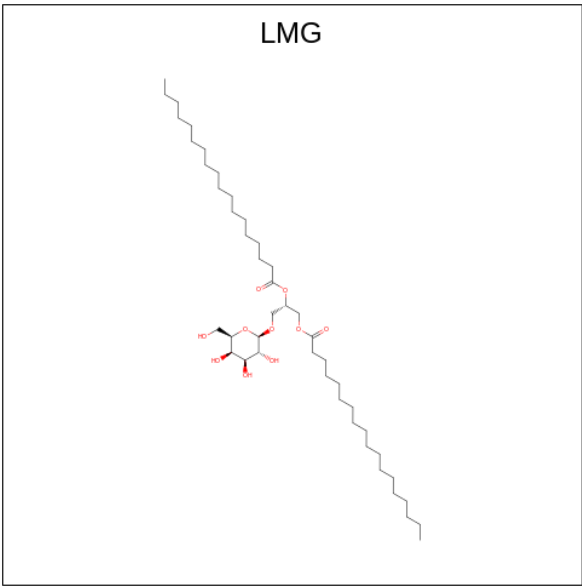
- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
19	X	1	Total	C	O	S	0
			54	41	12	1	
19	x	1	Total	C	O	S	0
			54	41	12	1	
19	b	1	Total	C	O	S	0
			54	41	12	1	
19	l	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter

code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).

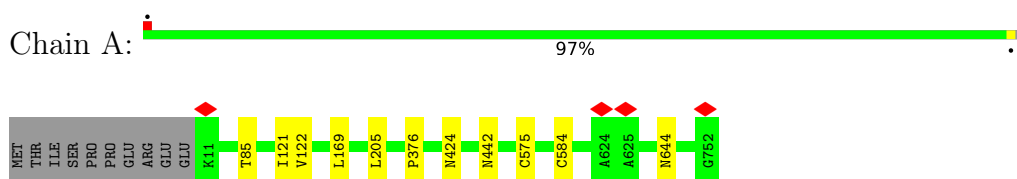


Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			90	70	20	
20	B	1	Total	C	O	0
			90	70	20	
20	b	1	Total	C	O	0
			55	45	10	

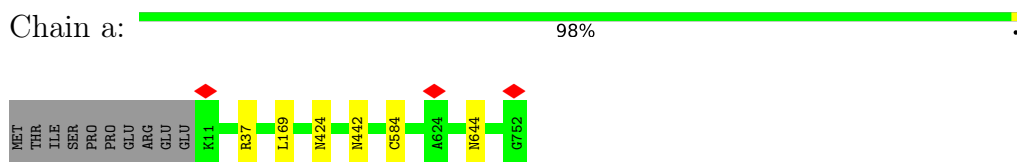
3 Residue-property plots [i](#)

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

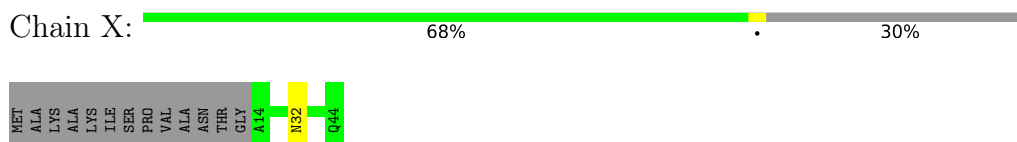
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



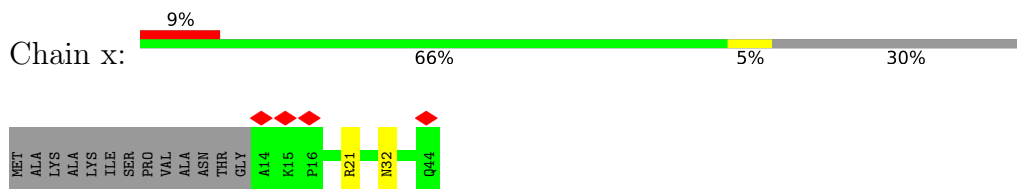
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



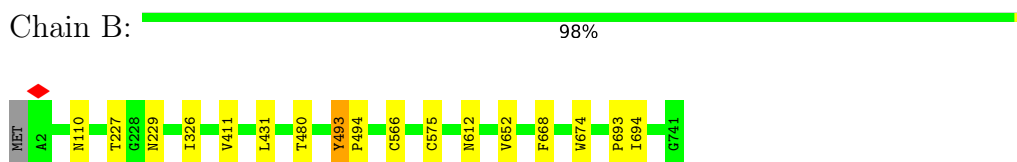
- Molecule 2: Photosystem I 4.8 kDa protein



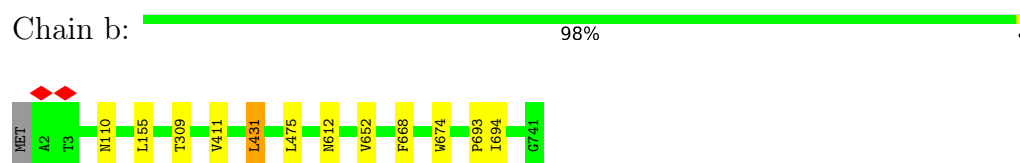
- Molecule 2: Photosystem I 4.8 kDa protein



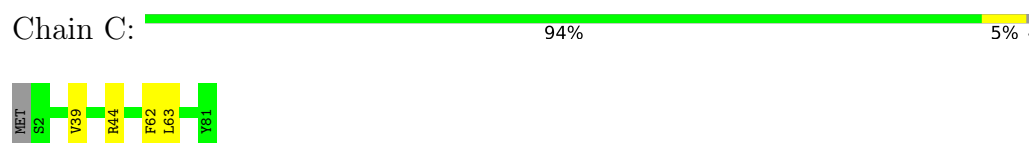
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1



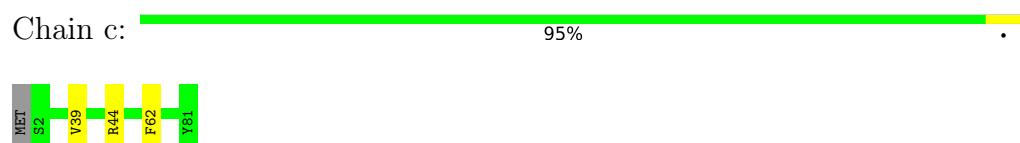
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2 1



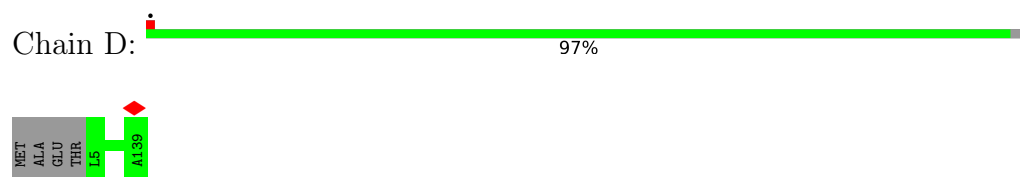
- Molecule 4: Photosystem I iron-sulfur center



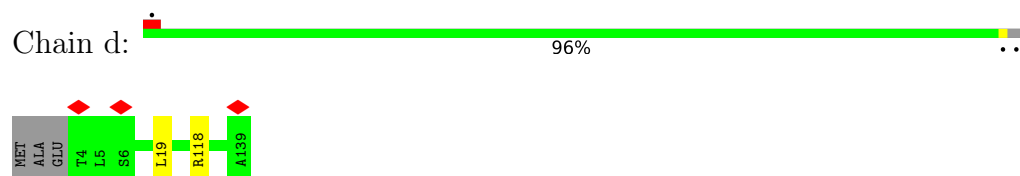
- Molecule 4: Photosystem I iron-sulfur center



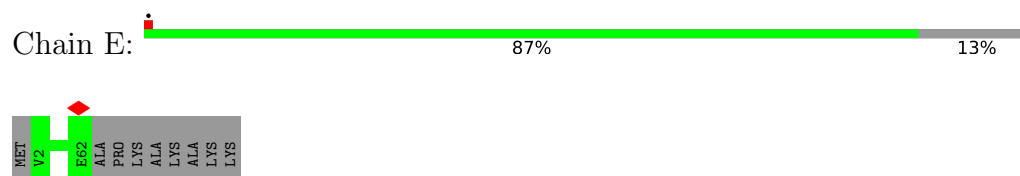
- Molecule 5: Photosystem I reaction center subunit II



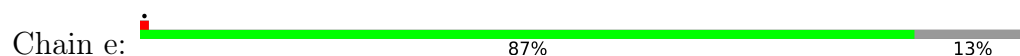
- Molecule 5: Photosystem I reaction center subunit II

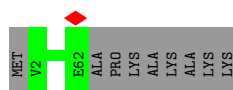


- Molecule 6: Photosystem I reaction center subunit IV



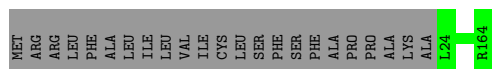
- Molecule 6: Photosystem I reaction center subunit IV





- Molecule 7: Photosystem I reaction center subunit III

Chain F: 86% 14%



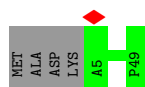
- Molecule 7: Photosystem I reaction center subunit III

Chain f: 85% 14%



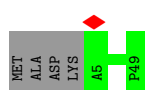
- Molecule 8: Photosystem I reaction center subunit IX

Chain J: 92% 8%



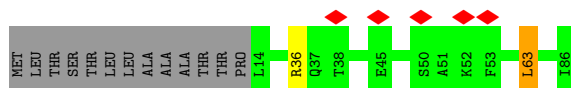
- Molecule 8: Photosystem I reaction center subunit IX

Chain j: 92% 8%



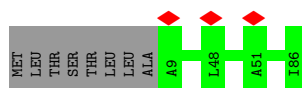
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K: 6% 83% 15%




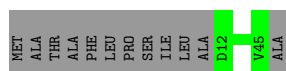
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain k: 91% 9%



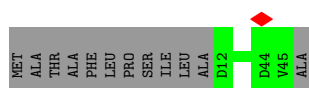
- Molecule 10: Photosystem I reaction center subunit VIII

Chain I:  74% 26%




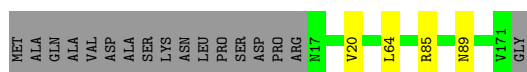
- Molecule 10: Photosystem I reaction center subunit VIII

Chain i:  74% 26%



- Molecule 11: Photosystem I reaction center subunit XI

Chain L:  88% 10%



- Molecule 11: Photosystem I reaction center subunit XI

Chain l:  89% 10%



- Molecule 12: Photosystem I reaction center subunit XII

Chain M:  97%



- Molecule 12: Photosystem I reaction center subunit XII

Chain m:  97%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	71600	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	58	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.173	Depositor
Minimum map value	-0.073	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	420.80002, 420.80002, 420.80002	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.052, 1.052, 1.052	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.49	1/6022 (0.0%)	0.59	3/8214 (0.0%)
1	a	0.50	0/6022	0.58	1/8214 (0.0%)
2	X	0.41	0/267	0.54	0/366
2	x	0.34	0/267	0.48	0/366
3	B	0.54	2/6142 (0.0%)	0.71	5/8396 (0.1%)
3	b	0.54	2/6142 (0.0%)	0.62	4/8396 (0.0%)
4	C	0.52	0/608	0.68	0/825
4	c	0.55	0/608	0.65	0/825
5	D	0.45	0/1064	0.62	0/1436
5	d	0.45	0/1071	0.62	1/1446 (0.1%)
6	E	0.43	0/499	0.48	0/677
6	e	0.41	0/499	0.46	0/677
7	F	0.38	0/1104	0.57	0/1500
7	f	0.40	0/1104	0.54	0/1500
8	J	0.38	0/371	0.52	0/509
8	j	0.36	0/371	0.51	0/509
9	K	0.35	0/551	0.67	1/750 (0.1%)
9	k	0.41	0/583	0.58	0/796
10	I	0.43	0/284	0.54	0/388
10	i	0.53	0/284	0.59	0/388
11	L	0.48	0/1198	0.64	1/1642 (0.1%)
11	l	0.50	0/1198	0.60	0/1642
12	M	0.44	0/245	0.57	0/334
12	m	0.46	0/245	0.59	0/334
All	All	0.49	5/36749 (0.0%)	0.61	16/50130 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	B	0	4
3	b	0	2
4	c	0	1
All	All	0	8

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	VAL	CB-CG1	-8.36	1.35	1.52
3	B	652	VAL	CB-CG2	-6.76	1.38	1.52
3	b	411	VAL	CB-CG1	-6.03	1.40	1.52
3	b	652	VAL	CB-CG2	-5.68	1.41	1.52
1	A	376	PRO	C-N	-5.04	1.22	1.34

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	493	TYR	C-N-CD	-20.83	74.77	120.60
3	B	493	TYR	C-N-CA	13.79	179.94	122.00
3	b	431	LEU	CA-CB-CG	7.55	132.66	115.30
5	d	19	LEU	CA-CB-CG	7.06	131.54	115.30
3	b	155	LEU	CA-CB-CG	6.75	130.83	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	121	ILE	Peptide
3	B	480	THR	Peptide
3	B	493	TYR	Peptide
3	B	674	TRP	Peptide
3	B	693	PRO	Peptide

5.2 Too-close contacts

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	A	740/752 (98%)	709 (96%)	30 (4%)	1 (0%)	51	67
1	a	740/752 (98%)	710 (96%)	30 (4%)	0	100	100
2	X	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
2	x	29/44 (66%)	28 (97%)	1 (3%)	0	100	100
3	B	738/741 (100%)	715 (97%)	21 (3%)	2 (0%)	41	53
3	b	738/741 (100%)	721 (98%)	16 (2%)	1 (0%)	51	67
4	C	78/81 (96%)	73 (94%)	3 (4%)	2 (3%)	5	4
4	c	78/81 (96%)	72 (92%)	6 (8%)	0	100	100
5	D	133/139 (96%)	130 (98%)	3 (2%)	0	100	100
5	d	134/139 (96%)	131 (98%)	3 (2%)	0	100	100
6	E	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
6	e	59/70 (84%)	57 (97%)	2 (3%)	0	100	100
7	F	139/164 (85%)	131 (94%)	8 (6%)	0	100	100
7	f	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
8	J	43/49 (88%)	43 (100%)	0	0	100	100
8	j	43/49 (88%)	43 (100%)	0	0	100	100
9	K	71/86 (83%)	69 (97%)	2 (3%)	0	100	100
9	k	76/86 (88%)	74 (97%)	2 (3%)	0	100	100
10	I	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
10	i	32/46 (70%)	31 (97%)	1 (3%)	0	100	100
11	L	153/172 (89%)	152 (99%)	1 (1%)	0	100	100
11	l	153/172 (89%)	151 (99%)	2 (1%)	0	100	100
12	M	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
12	m	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
All	All	4494/4752 (95%)	4347 (97%)	141 (3%)	6 (0%)	54	67

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	VAL
3	B	494	PRO
3	B	694	ILE
3	b	694	ILE
4	C	63	LEU

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	595/605 (98%)	590 (99%)	5 (1%)	81	91
1	a	595/605 (98%)	590 (99%)	5 (1%)	81	91
2	X	25/34 (74%)	24 (96%)	1 (4%)	31	47
2	x	25/34 (74%)	23 (92%)	2 (8%)	12	17
3	B	600/602 (100%)	594 (99%)	6 (1%)	76	87
3	b	600/602 (100%)	596 (99%)	4 (1%)	84	92
4	C	67/69 (97%)	65 (97%)	2 (3%)	41	59
4	c	67/69 (97%)	65 (97%)	2 (3%)	41	59
5	D	107/110 (97%)	107 (100%)	0	100	100
5	d	108/110 (98%)	107 (99%)	1 (1%)	78	89
6	E	54/60 (90%)	54 (100%)	0	100	100
6	e	54/60 (90%)	54 (100%)	0	100	100
7	F	110/129 (85%)	110 (100%)	0	100	100
7	f	110/129 (85%)	109 (99%)	1 (1%)	78	89
8	J	39/42 (93%)	39 (100%)	0	100	100
8	j	39/42 (93%)	39 (100%)	0	100	100
9	K	54/64 (84%)	52 (96%)	2 (4%)	34	50
9	k	57/64 (89%)	57 (100%)	0	100	100
10	I	31/39 (80%)	31 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	i	31/39 (80%)	31 (100%)	0	100	100
11	L	118/131 (90%)	115 (98%)	3 (2%)	47	65
11	l	118/131 (90%)	116 (98%)	2 (2%)	60	76
12	M	26/27 (96%)	26 (100%)	0	100	100
12	m	26/27 (96%)	26 (100%)	0	100	100
All	All	3656/3824 (96%)	3620 (99%)	36 (1%)	77	87

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	b	431	LEU
11	l	141	ASN
3	b	612	ASN
5	d	118	ARG
4	C	39	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
3	b	612	ASN
3	b	640	ASN
7	f	46	ASN
3	B	689	HIS
3	B	679	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

259 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	a	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.81	13 (17%)
14	CLA	J	101	-	45,53,73	1.73	8 (17%)	52,89,113	1.71	8 (15%)
17	BCR	A	851	-	41,41,41	1.19	3 (7%)	56,56,56	1.22	4 (7%)
17	BCR	M	101	-	41,41,41	1.08	2 (4%)	56,56,56	1.32	9 (16%)
14	CLA	B	830	3	65,73,73	1.46	8 (12%)	76,113,113	1.54	11 (14%)
20	LMG	B	851	-	55,55,55	0.91	2 (3%)	63,63,63	1.44	8 (12%)
14	CLA	A	804	-	54,62,73	1.55	8 (14%)	62,99,113	1.70	7 (11%)
14	CLA	A	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.53	12 (17%)
14	CLA	a	830	1	54,62,73	1.53	9 (16%)	62,99,113	1.43	9 (14%)
14	CLA	A	828	-	65,73,73	1.34	7 (10%)	76,113,113	1.64	11 (14%)
14	CLA	A	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.66	12 (15%)
14	CLA	A	806	1	65,73,73	1.42	9 (13%)	76,113,113	1.58	10 (13%)
14	CLA	B	819	-	45,53,73	1.70	8 (17%)	52,89,113	1.62	9 (17%)
14	CLA	B	835	-	58,66,73	1.52	9 (15%)	67,104,113	1.51	7 (10%)
14	CLA	a	831	1	65,73,73	1.42	9 (13%)	76,113,113	1.57	11 (14%)
14	CLA	a	818	-	65,73,73	1.36	7 (10%)	76,113,113	1.73	13 (17%)
17	BCR	A	847	-	41,41,41	1.09	3 (7%)	56,56,56	1.28	6 (10%)
17	BCR	B	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
17	BCR	l	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.44	7 (12%)
19	SQD	b	801	-	53,54,54	0.97	6 (11%)	62,65,65	1.73	11 (17%)
14	CLA	B	814	3	54,62,73	1.48	7 (12%)	62,99,113	1.81	11 (17%)
14	CLA	B	841	3	47,55,73	1.73	8 (17%)	54,91,113	1.57	8 (14%)
14	CLA	f	203	-	45,53,73	1.72	8 (17%)	52,89,113	1.69	6 (11%)
14	CLA	B	815	3	54,62,73	1.58	7 (12%)	62,99,113	1.57	9 (14%)
14	CLA	A	830	1	65,73,73	1.57	9 (13%)	76,113,113	1.72	10 (13%)
14	CLA	A	820	-	54,62,73	1.58	8 (14%)	62,99,113	1.61	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	821	-	65,73,73	1.56	7 (10%)	76,113,113	1.35	10 (13%)
17	BCR	m	1202	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	10 (17%)
14	CLA	a	817	-	60,68,73	1.56	10 (16%)	70,107,113	1.52	10 (14%)
18	LHG	A	853	14	48,48,48	0.77	2 (4%)	51,54,54	1.21	6 (11%)
14	CLA	A	808	1	65,73,73	1.38	7 (10%)	76,113,113	1.57	10 (13%)
17	BCR	b	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.45	5 (8%)
16	SF4	C	101	-	0,12,12	-	-	-	-	-
14	CLA	B	811	3	65,73,73	1.47	10 (15%)	76,113,113	1.86	14 (18%)
14	CLA	b	833	-	54,62,73	1.61	10 (18%)	62,99,113	1.53	7 (11%)
14	CLA	J	102	-	38,45,73	1.87	7 (18%)	43,78,113	1.71	7 (16%)
14	CLA	A	814	1	54,62,73	1.55	7 (12%)	62,99,113	1.80	9 (14%)
14	CLA	B	804	-	65,73,73	1.39	7 (10%)	76,113,113	1.53	12 (15%)
14	CLA	b	829	-	65,73,73	1.42	8 (12%)	76,113,113	1.61	9 (11%)
14	CLA	A	840	-	59,67,73	1.50	9 (15%)	68,105,113	1.35	7 (10%)
14	CLA	a	832	1	65,73,73	1.36	7 (10%)	76,113,113	1.54	11 (14%)
14	CLA	b	827	3	65,73,73	1.36	8 (12%)	76,113,113	1.55	12 (15%)
14	CLA	B	806	-	65,73,73	1.46	8 (12%)	76,113,113	2.08	13 (17%)
14	CLA	B	809	3	65,73,73	1.40	9 (13%)	76,113,113	1.59	10 (13%)
14	CLA	b	828	-	65,73,73	1.40	5 (7%)	76,113,113	1.74	14 (18%)
14	CLA	a	811	-	59,67,73	1.53	7 (11%)	68,105,113	1.50	8 (11%)
14	CLA	A	835	1	54,62,73	1.61	8 (14%)	62,99,113	1.54	8 (12%)
14	CLA	F	204	-	45,53,73	1.74	7 (15%)	52,89,113	1.64	10 (19%)
14	CLA	b	806	3	65,73,73	1.39	9 (13%)	76,113,113	1.54	8 (10%)
14	CLA	b	809	3	65,73,73	1.37	8 (12%)	76,113,113	1.54	9 (11%)
14	CLA	B	818	3	49,57,73	1.52	7 (14%)	55,93,113	1.69	9 (16%)
14	CLA	A	823	1	54,62,73	1.52	7 (12%)	62,99,113	1.72	10 (16%)
14	CLA	j	103	-	38,45,73	1.86	9 (23%)	43,78,113	1.69	7 (16%)
17	BCR	b	847	-	41,41,41	1.17	3 (7%)	56,56,56	1.41	10 (17%)
14	CLA	a	819	-	54,62,73	1.58	7 (12%)	62,99,113	1.66	8 (12%)
14	CLA	b	818	-	49,57,73	1.62	9 (18%)	55,93,113	1.71	8 (14%)
17	BCR	b	849	-	41,41,41	1.21	4 (9%)	56,56,56	1.42	8 (14%)
18	LHG	F	201	-	42,42,48	0.73	1 (2%)	45,48,54	1.18	4 (8%)
14	CLA	b	831	-	65,73,73	1.31	9 (13%)	76,113,113	1.48	5 (6%)
14	CLA	B	838	-	45,53,73	1.83	8 (17%)	52,89,113	1.57	9 (17%)
14	CLA	b	821	3	65,73,73	1.35	9 (13%)	76,113,113	1.56	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	m	1201	3	55,63,73	1.53	9 (16%)	64,101,113	1.60	9 (14%)
15	PQN	b	844	-	34,34,34	1.41	2 (5%)	42,45,45	1.38	7 (16%)
14	CLA	L	1503	-	45,53,73	1.65	6 (13%)	52,89,113	1.88	9 (17%)
14	CLA	a	815	-	45,53,73	1.73	7 (15%)	52,89,113	1.75	6 (11%)
14	CLA	B	837	-	45,53,73	1.68	7 (15%)	52,89,113	1.96	11 (21%)
14	CLA	a	824	-	65,73,73	1.39	6 (9%)	76,113,113	1.65	10 (13%)
17	BCR	j	105	-	41,41,41	1.17	2 (4%)	56,56,56	1.32	7 (12%)
14	CLA	x	1701	2	49,57,73	1.66	8 (16%)	55,93,113	1.54	6 (10%)
14	CLA	a	810	-	65,73,73	1.45	9 (13%)	76,113,113	1.59	9 (11%)
14	CLA	a	835	1	45,53,73	1.69	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	b	803	-	65,73,73	1.44	10 (15%)	76,113,113	1.58	13 (17%)
19	SQD	l	202	-	53,54,54	0.97	6 (11%)	62,65,65	2.03	14 (22%)
14	CLA	A	819	-	65,73,73	1.44	7 (10%)	76,113,113	1.65	10 (13%)
14	CLA	a	837	1	65,73,73	1.38	10 (15%)	76,113,113	1.69	11 (14%)
17	BCR	B	850	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	3 (5%)
14	CLA	b	843	3	65,73,73	1.47	9 (13%)	76,113,113	1.94	15 (19%)
14	CLA	A	809	1	65,73,73	1.42	6 (9%)	76,113,113	1.58	10 (13%)
14	CLA	b	807	-	65,73,73	1.42	10 (15%)	76,113,113	1.91	12 (15%)
17	BCR	I	101	-	41,41,41	1.07	1 (2%)	56,56,56	1.30	8 (14%)
20	LMG	B	803	-	35,35,55	0.94	1 (2%)	43,43,63	1.24	4 (9%)
17	BCR	J	104	-	41,41,41	1.18	3 (7%)	56,56,56	1.39	9 (16%)
14	CLA	b	841	3	47,55,73	1.65	9 (19%)	54,91,113	1.59	9 (16%)
16	SF4	c	101	-	0,12,12	-	-	-	-	-
14	CLA	A	812	-	59,67,73	1.53	7 (11%)	68,105,113	1.47	7 (10%)
14	CLA	A	827	1	65,73,73	1.42	6 (9%)	76,113,113	1.52	7 (9%)
17	BCR	j	106	-	41,41,41	1.15	2 (4%)	56,56,56	1.37	6 (10%)
14	CLA	B	836	3	54,62,73	1.43	7 (12%)	62,99,113	1.83	12 (19%)
14	CLA	a	813	-	54,62,73	1.55	7 (12%)	62,99,113	1.65	7 (11%)
14	CLA	A	831	1	54,62,73	1.54	8 (14%)	62,99,113	1.62	10 (16%)
14	CLA	b	805	-	65,73,73	1.43	7 (10%)	76,113,113	1.57	11 (14%)
14	CLA	b	830	-	65,73,73	1.39	8 (12%)	76,113,113	1.49	10 (13%)
14	CLA	a	833	1	65,73,73	1.44	7 (10%)	76,113,113	1.83	17 (22%)
14	CLA	b	822	-	65,73,73	1.49	7 (10%)	76,113,113	1.64	9 (11%)
17	BCR	K	103	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	b	836	3	54,62,73	1.54	8 (14%)	62,99,113	1.78	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	816	-	65,73,73	1.45	8 (12%)	76,113,113	1.50	10 (13%)
17	BCR	A	848	-	41,41,41	1.13	1 (2%)	56,56,56	1.46	9 (16%)
17	BCR	b	846	-	41,41,41	1.08	2 (4%)	56,56,56	1.26	7 (12%)
14	CLA	B	832	3	65,73,73	1.57	10 (15%)	76,113,113	1.76	11 (14%)
14	CLA	b	838	-	45,53,73	1.74	7 (15%)	52,89,113	1.60	6 (11%)
20	LMG	b	851	-	55,55,55	0.92	2 (3%)	63,63,63	1.49	11 (17%)
17	BCR	A	850	-	41,41,41	1.15	3 (7%)	56,56,56	1.25	7 (12%)
19	SQD	X	1702	-	53,54,54	0.98	5 (9%)	62,65,65	1.74	12 (19%)
14	CLA	B	813	-	60,68,73	1.52	9 (15%)	70,107,113	1.41	9 (12%)
14	CLA	a	836	-	51,59,73	1.54	9 (17%)	59,96,113	1.71	11 (18%)
14	CLA	B	840	3	65,73,73	1.40	8 (12%)	76,113,113	1.60	12 (15%)
14	CLA	B	842	-	65,73,73	1.38	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	a	808	1	65,73,73	1.41	8 (12%)	76,113,113	1.59	10 (13%)
14	CLA	b	814	-	54,62,73	1.54	7 (12%)	62,99,113	1.66	9 (14%)
14	CLA	b	840	3	65,73,73	1.34	7 (10%)	76,113,113	1.61	10 (13%)
17	BCR	a	848	-	41,41,41	1.16	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	X	1701	2	49,57,73	1.63	8 (16%)	55,93,113	1.73	10 (18%)
14	CLA	L	1502	11	60,68,73	1.45	8 (13%)	70,107,113	1.67	10 (14%)
14	CLA	A	807	-	60,68,73	1.51	8 (13%)	70,107,113	5.15	11 (15%)
14	CLA	A	826	-	54,62,73	1.51	7 (12%)	62,99,113	1.68	12 (19%)
17	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.28	3 (5%)
17	BCR	a	849	-	41,41,41	1.21	3 (7%)	56,56,56	1.29	4 (7%)
14	CLA	A	841	1	65,73,73	1.44	9 (13%)	76,113,113	1.48	10 (13%)
14	CLA	b	835	3	65,73,73	1.48	8 (12%)	76,113,113	1.37	11 (14%)
14	CLA	B	828	-	65,73,73	1.37	5 (7%)	76,113,113	1.74	19 (25%)
17	BCR	I	102	-	41,41,41	1.20	4 (9%)	56,56,56	1.46	8 (14%)
14	CLA	l	203	11	45,53,73	1.68	7 (15%)	52,89,113	1.93	11 (21%)
14	CLA	a	814	-	45,53,73	1.69	7 (15%)	52,89,113	1.86	7 (13%)
14	CLA	a	821	1	45,53,73	1.73	8 (17%)	52,89,113	1.80	11 (21%)
14	CLA	A	805	1	65,73,73	1.36	7 (10%)	76,113,113	1.76	15 (19%)
14	CLA	a	803	-	54,62,73	1.56	6 (11%)	62,99,113	1.65	6 (9%)
14	CLA	a	840	1	65,73,73	1.47	9 (13%)	76,113,113	1.52	8 (10%)
14	CLA	A	836	1	45,53,73	1.68	7 (15%)	52,89,113	1.84	8 (15%)
14	CLA	B	831	-	65,73,73	1.37	8 (12%)	76,113,113	1.48	6 (7%)
17	BCR	A	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.27	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	839	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	11 (15%)
17	BCR	a	847	-	41,41,41	1.12	2 (4%)	56,56,56	1.26	6 (10%)
14	CLA	l	204	11	60,68,73	1.46	8 (13%)	70,107,113	1.64	9 (12%)
17	BCR	F	205	-	41,41,41	1.12	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	a	838	-	65,73,73	1.43	8 (12%)	76,113,113	1.40	7 (9%)
14	CLA	B	833	3	54,62,73	1.57	8 (14%)	62,99,113	1.51	7 (11%)
14	CLA	a	827	-	65,73,73	1.36	6 (9%)	76,113,113	1.63	11 (14%)
14	CLA	a	807	-	65,73,73	1.45	9 (13%)	76,113,113	1.54	10 (13%)
14	CLA	l	205	-	45,53,73	1.68	7 (15%)	52,89,113	1.92	9 (17%)
14	CLA	K	101	-	42,49,73	1.77	7 (16%)	48,83,113	1.55	7 (14%)
14	CLA	b	804	-	65,73,73	1.47	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	B	805	-	65,73,73	1.36	8 (12%)	76,113,113	1.47	6 (7%)
14	CLA	B	829	3	65,73,73	1.50	7 (10%)	76,113,113	1.69	10 (13%)
14	CLA	B	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.74	8 (15%)
14	CLA	A	816	-	45,53,73	1.73	7 (15%)	52,89,113	1.72	8 (15%)
14	CLA	A	842	-	65,73,73	1.46	9 (13%)	76,113,113	1.66	10 (13%)
14	CLA	b	819	-	45,53,73	1.67	7 (15%)	52,89,113	1.80	8 (15%)
14	CLA	b	824	3	45,53,73	1.69	7 (15%)	52,89,113	1.68	7 (13%)
14	CLA	j	101	-	58,66,73	1.55	9 (15%)	67,104,113	1.59	10 (14%)
14	CLA	b	825	-	55,63,73	1.54	7 (12%)	64,101,113	1.57	7 (10%)
14	CLA	a	834	1	54,62,73	1.59	9 (16%)	62,99,113	1.58	6 (9%)
14	CLA	a	812	-	60,68,73	1.54	9 (15%)	70,107,113	1.41	7 (10%)
18	LHG	i	103	-	42,42,48	0.64	0	45,48,54	1.26	6 (13%)
14	CLA	A	802	-	65,73,73	1.47	9 (13%)	76,113,113	1.52	11 (14%)
14	CLA	A	834	-	65,73,73	1.37	7 (10%)	76,113,113	1.69	14 (18%)
16	SF4	a	843	-	0,12,12	-	-	-	-	-
18	LHG	a	850	-	48,48,48	0.76	1 (2%)	51,54,54	1.33	6 (11%)
14	CLA	B	834	-	60,68,73	1.43	7 (11%)	70,107,113	1.61	6 (8%)
17	BCR	B	849	-	41,41,41	1.21	6 (14%)	56,56,56	1.46	7 (12%)
17	BCR	k	103	-	41,41,41	1.06	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	A	829	-	65,73,73	1.36	8 (12%)	76,113,113	1.61	13 (17%)
14	CLA	a	828	-	65,73,73	1.39	8 (12%)	76,113,113	1.53	8 (10%)
18	LHG	a	851	14	48,48,48	0.93	5 (10%)	51,54,54	0.98	2 (3%)
14	CLA	b	834	-	60,68,73	1.48	8 (13%)	70,107,113	1.54	8 (11%)
14	CLA	B	821	3	65,73,73	1.44	8 (12%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	808	-	65,73,73	1.36	10 (15%)	76,113,113	1.76	11 (14%)
15	PQN	B	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.26	4 (9%)
17	BCR	b	850	-	41,41,41	1.10	3 (7%)	56,56,56	1.10	3 (5%)
14	CLA	B	817	-	50,58,73	1.57	7 (14%)	58,95,113	1.62	9 (15%)
14	CLA	B	826	-	65,73,73	1.37	6 (9%)	76,113,113	1.60	10 (13%)
17	BCR	B	845	-	41,41,41	1.12	3 (7%)	56,56,56	1.25	6 (10%)
14	CLA	B	823	3	45,53,73	1.68	9 (20%)	52,89,113	1.99	14 (26%)
14	CLA	b	817	3	50,58,73	1.65	8 (16%)	58,95,113	1.69	8 (13%)
14	CLA	a	820	-	65,73,73	1.45	7 (10%)	76,113,113	1.64	10 (13%)
14	CLA	a	816	-	59,67,73	1.49	10 (16%)	68,105,113	1.57	11 (16%)
14	CLA	b	823	3	45,53,73	1.72	9 (20%)	52,89,113	1.64	7 (13%)
17	BCR	b	845	-	41,41,41	1.12	2 (4%)	56,56,56	1.17	3 (5%)
17	BCR	a	844	-	41,41,41	1.18	4 (9%)	56,56,56	1.32	8 (14%)
14	CLA	b	815	-	54,62,73	1.61	7 (12%)	62,99,113	1.70	10 (16%)
17	BCR	f	202	-	41,41,41	1.20	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	A	839	-	65,73,73	1.41	8 (12%)	76,113,113	1.51	10 (13%)
14	CLA	A	824	1	45,53,73	1.69	8 (17%)	52,89,113	1.70	8 (15%)
17	BCR	i	101	-	41,41,41	1.08	1 (2%)	56,56,56	1.43	9 (16%)
13	CL0	a	801	1	65,73,73	2.36	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	a	823	1	45,53,73	1.64	6 (13%)	52,89,113	1.83	9 (17%)
16	SF4	C	102	-	0,12,12	-	-	-	-	-
14	CLA	B	843	3	65,73,73	1.39	9 (13%)	76,113,113	1.63	14 (18%)
14	CLA	b	832	3	65,73,73	1.51	9 (13%)	76,113,113	1.71	15 (19%)
14	CLA	A	837	-	51,59,73	1.49	7 (13%)	59,96,113	1.89	10 (16%)
15	PQN	A	844	-	34,34,34	1.50	2 (5%)	42,45,45	1.08	4 (9%)
17	BCR	l	206	-	41,41,41	1.09	1 (2%)	56,56,56	1.56	12 (21%)
14	CLA	B	802	1	65,73,73	1.40	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	b	802	-	65,73,73	1.28	7 (10%)	76,113,113	1.67	7 (9%)
17	BCR	A	849	-	41,41,41	1.17	3 (7%)	56,56,56	1.44	8 (14%)
14	CLA	B	827	3	65,73,73	1.40	8 (12%)	76,113,113	1.72	13 (17%)
14	CLA	a	826	-	65,73,73	1.39	9 (13%)	76,113,113	1.59	8 (10%)
17	BCR	B	848	-	41,41,41	1.09	3 (7%)	56,56,56	1.30	5 (8%)
17	BCR	L	1504	-	41,41,41	1.07	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	B	801	-	65,73,73	1.38	7 (10%)	76,113,113	1.71	11 (14%)
14	CLA	B	816	-	65,73,73	1.42	9 (13%)	76,113,113	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	841	18	45,53,73	1.61	7 (15%)	52,89,113	4.16	9 (17%)
14	CLA	A	803	-	65,73,73	1.39	7 (10%)	76,113,113	1.62	8 (10%)
17	BCR	B	846	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	9 (16%)
14	CLA	A	817	-	59,67,73	1.56	8 (13%)	68,105,113	1.57	9 (13%)
14	CLA	a	822	1	54,62,73	1.61	8 (14%)	62,99,113	1.47	12 (19%)
17	BCR	i	102	-	41,41,41	1.20	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	a	805	1	65,73,73	1.40	8 (12%)	76,113,113	1.53	8 (10%)
14	CLA	B	812	-	65,73,73	1.39	8 (12%)	76,113,113	1.69	13 (17%)
14	CLA	b	811	-	65,73,73	1.42	11 (16%)	76,113,113	1.71	10 (13%)
17	BCR	J	103	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	6 (10%)
17	BCR	a	846	-	41,41,41	1.13	2 (4%)	56,56,56	1.45	9 (16%)
14	CLA	A	838	1	65,73,73	1.35	7 (10%)	76,113,113	1.62	10 (13%)
14	CLA	b	812	3	65,73,73	1.51	9 (13%)	76,113,113	1.65	10 (13%)
14	CLA	B	810	3	65,73,73	1.31	7 (10%)	76,113,113	1.46	7 (9%)
14	CLA	b	842	-	65,73,73	1.44	6 (9%)	76,113,113	1.47	8 (10%)
14	CLA	k	101	-	42,49,73	1.78	7 (16%)	48,83,113	1.62	5 (10%)
16	SF4	A	845	-	0,12,12	-	-	-	-	-
14	CLA	A	832	1	65,73,73	1.38	8 (12%)	76,113,113	1.62	7 (9%)
14	CLA	A	843	18	45,53,73	1.73	8 (17%)	52,89,113	1.73	9 (17%)
17	BCR	l	201	-	41,41,41	1.07	2 (4%)	56,56,56	1.30	8 (14%)
14	CLA	b	810	3	65,73,73	1.34	7 (10%)	76,113,113	1.57	9 (11%)
14	CLA	B	808	-	65,73,73	1.51	10 (15%)	76,113,113	2.02	20 (26%)
16	SF4	c	102	-	0,12,12	-	-	-	-	-
19	SQD	x	1702	-	53,54,54	0.97	5 (9%)	62,65,65	1.76	9 (14%)
14	CLA	B	807	3	55,63,73	1.50	7 (12%)	64,101,113	1.61	8 (12%)
14	CLA	B	825	-	55,63,73	1.54	6 (10%)	64,101,113	1.64	7 (10%)
18	LHG	A	852	-	48,48,48	0.83	3 (6%)	51,54,54	1.33	7 (13%)
14	CLA	b	837	-	45,53,73	1.70	7 (15%)	52,89,113	1.79	10 (19%)
14	CLA	j	102	-	45,53,73	1.72	7 (15%)	52,89,113	1.67	7 (13%)
15	PQN	a	842	-	34,34,34	1.47	2 (5%)	42,45,45	1.27	5 (11%)
13	CL0	A	801	-	65,73,73	2.35	18 (27%)	76,113,113	2.61	22 (28%)
14	CLA	A	815	-	45,53,73	1.66	7 (15%)	52,89,113	1.92	6 (11%)
14	CLA	A	822	-	45,53,73	1.68	7 (15%)	52,89,113	1.69	8 (15%)
14	CLA	a	825	-	54,62,73	1.54	7 (12%)	62,99,113	1.60	9 (14%)
14	CLA	B	839	3	60,68,73	1.53	10 (16%)	70,107,113	1.45	11 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	K	102	-	49,57,73	1.65	6 (12%)	55,93,113	1.69	8 (14%)
14	CLA	b	813	-	60,68,73	1.58	9 (15%)	70,107,113	1.49	13 (18%)
14	CLA	k	102	-	49,57,73	1.67	8 (16%)	55,93,113	1.74	10 (18%)
17	BCR	F	203	-	41,41,41	1.17	2 (4%)	56,56,56	1.35	8 (14%)
14	CLA	A	825	-	65,73,73	1.38	8 (12%)	76,113,113	1.55	9 (11%)
17	BCR	J	105	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
14	CLA	a	804	1	65,73,73	1.37	7 (10%)	76,113,113	1.67	14 (18%)
17	BCR	f	204	-	41,41,41	1.11	2 (4%)	56,56,56	1.31	8 (14%)
14	CLA	a	839	1	65,73,73	1.40	9 (13%)	76,113,113	1.49	8 (10%)
14	CLA	B	820	3	65,73,73	1.43	9 (13%)	76,113,113	1.54	7 (9%)
14	CLA	F	202	3	65,73,73	1.46	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	A	818	1	60,68,73	1.54	10 (16%)	70,107,113	1.46	7 (10%)
14	CLA	a	806	-	60,68,73	1.50	10 (16%)	70,107,113	1.49	9 (12%)
14	CLA	A	810	1	45,53,73	1.70	7 (15%)	52,89,113	1.73	7 (13%)
14	CLA	B	822	-	65,73,73	1.43	7 (10%)	76,113,113	1.55	8 (10%)
14	CLA	a	809	1	45,53,73	1.68	7 (15%)	52,89,113	1.80	5 (9%)
14	CLA	f	201	-	59,67,73	1.55	8 (13%)	68,105,113	1.35	7 (10%)
14	CLA	a	802	1	65,73,73	1.42	7 (10%)	76,113,113	1.53	8 (10%)
14	CLA	L	1501	11	51,59,73	1.76	9 (17%)	59,96,113	1.60	10 (16%)
17	BCR	j	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.33	7 (12%)
14	CLA	b	820	-	65,73,73	1.44	10 (15%)	76,113,113	1.43	8 (10%)
14	CLA	b	826	-	65,73,73	1.35	6 (9%)	76,113,113	1.56	10 (13%)
14	CLA	A	833	1	65,73,73	1.45	8 (12%)	76,113,113	1.46	9 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	829	-	1/1/15/20	11/37/115/115	-
14	CLA	J	101	-	1/1/11/20	8/13/91/115	-
17	BCR	A	851	-	-	16/29/63/63	0/2/2/2
17	BCR	M	101	-	-	12/29/63/63	0/2/2/2
14	CLA	B	830	3	1/1/15/20	12/37/115/115	-
20	LMG	B	851	-	-	28/50/70/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	804	-	1/1/12/20	4/24/102/115	-
14	CLA	A	813	-	1/1/14/20	14/31/109/115	-
14	CLA	a	830	1	1/1/12/20	7/24/102/115	-
14	CLA	A	828	-	1/1/15/20	16/37/115/115	-
14	CLA	A	811	-	1/1/15/20	10/37/115/115	-
14	CLA	A	806	1	1/1/15/20	14/37/115/115	-
14	CLA	B	819	-	1/1/11/20	1/13/91/115	-
14	CLA	B	835	-	1/1/13/20	12/29/107/115	-
14	CLA	a	831	1	1/1/15/20	15/37/115/115	-
14	CLA	a	818	-	1/1/15/20	13/37/115/115	-
17	BCR	A	847	-	-	10/29/63/63	0/2/2/2
17	BCR	B	847	-	-	13/29/63/63	0/2/2/2
17	BCR	l	207	-	-	6/29/63/63	0/2/2/2
19	SQD	b	801	-	-	22/49/69/69	0/1/1/1
14	CLA	B	814	3	1/1/12/20	9/24/102/115	-
14	CLA	B	841	3	1/1/11/20	3/16/94/115	-
14	CLA	f	203	-	1/1/11/20	5/13/91/115	-
14	CLA	B	815	3	1/1/12/20	5/24/102/115	-
14	CLA	A	830	1	1/1/15/20	9/37/115/115	-
14	CLA	A	820	-	1/1/12/20	9/24/102/115	-
14	CLA	A	821	-	1/1/15/20	12/37/115/115	-
17	BCR	m	1202	-	-	11/29/63/63	0/2/2/2
14	CLA	a	817	-	1/1/14/20	13/31/109/115	-
18	LHG	A	853	14	-	21/53/53/53	-
14	CLA	A	808	1	1/1/15/20	21/37/115/115	-
17	BCR	b	848	-	-	15/29/63/63	0/2/2/2
16	SF4	C	101	-	-	-	0/6/5/5
14	CLA	B	811	3	1/1/15/20	7/37/115/115	-
14	CLA	b	833	-	1/1/12/20	7/24/102/115	-
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	A	814	1	1/1/12/20	5/24/102/115	-
14	CLA	B	804	-	1/1/15/20	15/37/115/115	-
14	CLA	b	829	-	1/1/15/20	10/37/115/115	-
14	CLA	A	840	-	1/1/13/20	7/30/108/115	-
14	CLA	a	832	1	1/1/15/20	8/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	827	3	-	13/37/115/115	-
14	CLA	B	806	-	1/1/15/20	12/37/115/115	-
14	CLA	B	809	3	1/1/15/20	16/37/115/115	-
14	CLA	b	828	-	1/1/15/20	15/37/115/115	-
14	CLA	a	811	-	1/1/13/20	11/30/108/115	-
14	CLA	A	835	1	1/1/12/20	8/24/102/115	-
14	CLA	F	204	-	1/1/11/20	1/13/91/115	-
14	CLA	b	806	3	1/1/15/20	9/37/115/115	-
14	CLA	b	809	3	1/1/15/20	20/37/115/115	-
14	CLA	B	818	3	1/1/11/20	5/18/96/115	-
14	CLA	A	823	1	1/1/12/20	9/24/102/115	-
14	CLA	j	103	-	1/1/8/20	0/2/76/115	-
17	BCR	b	847	-	-	10/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/12/20	9/24/102/115	-
14	CLA	b	818	-	1/1/11/20	5/18/96/115	-
17	BCR	b	849	-	-	8/29/63/63	0/2/2/2
18	LHG	F	201	-	-	27/47/47/53	-
14	CLA	b	831	-	1/1/15/20	12/37/115/115	-
14	CLA	B	838	-	1/1/11/20	6/13/91/115	-
14	CLA	b	821	3	1/1/15/20	9/37/115/115	-
14	CLA	m	1201	3	1/1/13/20	9/25/103/115	-
15	PQN	b	844	-	-	5/23/43/43	0/2/2/2
14	CLA	L	1503	-	1/1/11/20	6/13/91/115	-
14	CLA	a	815	-	1/1/11/20	0/13/91/115	-
14	CLA	B	837	-	1/1/11/20	2/13/91/115	-
14	CLA	a	824	-	1/1/15/20	13/37/115/115	-
17	BCR	j	105	-	-	11/29/63/63	0/2/2/2
14	CLA	x	1701	2	1/1/11/20	7/18/96/115	-
14	CLA	a	810	-	1/1/15/20	7/37/115/115	-
14	CLA	a	835	1	1/1/11/20	7/13/91/115	-
14	CLA	b	803	-	1/1/15/20	9/37/115/115	-
19	SQD	l	202	-	-	25/49/69/69	0/1/1/1
14	CLA	A	819	-	1/1/15/20	12/37/115/115	-
14	CLA	a	837	1	1/1/15/20	16/37/115/115	-
17	BCR	B	850	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	843	3	-	12/37/115/115	-
14	CLA	A	809	1	1/1/15/20	12/37/115/115	-
14	CLA	b	807	-	1/1/15/20	12/37/115/115	-
17	BCR	I	101	-	-	11/29/63/63	0/2/2/2
20	LMG	B	803	-	-	12/30/50/70	0/1/1/1
17	BCR	J	104	-	-	13/29/63/63	0/2/2/2
14	CLA	b	841	3	1/1/11/20	7/16/94/115	-
16	SF4	c	101	-	-	-	0/6/5/5
14	CLA	A	812	-	1/1/13/20	7/30/108/115	-
14	CLA	A	827	1	1/1/15/20	14/37/115/115	-
17	BCR	j	106	-	-	15/29/63/63	0/2/2/2
14	CLA	B	836	3	1/1/12/20	11/24/102/115	-
14	CLA	a	813	-	1/1/12/20	2/24/102/115	-
14	CLA	A	831	1	1/1/12/20	6/24/102/115	-
14	CLA	b	805	-	1/1/15/20	18/37/115/115	-
14	CLA	b	830	-	1/1/15/20	16/37/115/115	-
14	CLA	a	833	1	1/1/15/20	16/37/115/115	-
14	CLA	b	822	-	1/1/15/20	9/37/115/115	-
17	BCR	K	103	-	-	12/29/63/63	0/2/2/2
14	CLA	b	836	3	1/1/12/20	8/24/102/115	-
14	CLA	b	816	-	-	16/37/115/115	-
17	BCR	A	848	-	-	12/29/63/63	0/2/2/2
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	B	832	3	1/1/15/20	9/37/115/115	-
14	CLA	b	838	-	1/1/11/20	5/13/91/115	-
20	LMG	b	851	-	-	23/50/70/70	0/1/1/1
17	BCR	A	850	-	-	13/29/63/63	0/2/2/2
19	SQD	X	1702	-	-	17/49/69/69	0/1/1/1
14	CLA	B	813	-	1/1/14/20	13/31/109/115	-
14	CLA	a	836	-	1/1/12/20	8/21/99/115	-
14	CLA	B	840	3	1/1/15/20	9/37/115/115	-
14	CLA	B	842	-	1/1/15/20	5/37/115/115	-
14	CLA	a	808	1	1/1/15/20	13/37/115/115	-
14	CLA	b	814	-	1/1/12/20	11/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	840	3	1/1/15/20	9/37/115/115	-
17	BCR	a	848	-	-	9/29/63/63	0/2/2/2
14	CLA	X	1701	2	1/1/11/20	9/18/96/115	-
14	CLA	L	1502	11	-	8/31/109/115	-
14	CLA	A	807	-	1/1/14/20	17/31/109/115	-
14	CLA	A	826	-	1/1/12/20	6/24/102/115	-
17	BCR	a	845	-	-	7/29/63/63	0/2/2/2
17	BCR	a	849	-	-	15/29/63/63	0/2/2/2
14	CLA	A	841	1	1/1/15/20	21/37/115/115	-
14	CLA	b	835	3	1/1/15/20	15/37/115/115	-
14	CLA	B	828	-	1/1/15/20	12/37/115/115	-
17	BCR	I	102	-	-	11/29/63/63	0/2/2/2
14	CLA	l	203	11	1/1/11/20	8/13/91/115	-
14	CLA	a	814	-	1/1/11/20	6/13/91/115	-
14	CLA	a	821	1	1/1/11/20	4/13/91/115	-
14	CLA	A	805	1	1/1/15/20	16/37/115/115	-
14	CLA	a	803	-	1/1/12/20	5/24/102/115	-
14	CLA	a	840	1	1/1/15/20	6/37/115/115	-
14	CLA	A	836	1	1/1/11/20	3/13/91/115	-
14	CLA	B	831	-	1/1/15/20	11/37/115/115	-
17	BCR	A	846	-	-	10/29/63/63	0/2/2/2
14	CLA	b	839	-	1/1/14/20	8/31/109/115	-
17	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	l	204	11	-	9/31/109/115	-
17	BCR	F	205	-	-	10/29/63/63	0/2/2/2
14	CLA	a	838	-	1/1/15/20	11/37/115/115	-
14	CLA	B	833	3	1/1/12/20	6/24/102/115	-
14	CLA	a	827	-	1/1/15/20	9/37/115/115	-
14	CLA	a	807	-	1/1/15/20	20/37/115/115	-
14	CLA	l	205	-	1/1/11/20	4/13/91/115	-
14	CLA	K	101	-	1/1/9/20	5/7/81/115	-
14	CLA	b	804	-	1/1/15/20	21/37/115/115	-
14	CLA	B	805	-	1/1/15/20	12/37/115/115	-
14	CLA	B	829	3	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	824	3	1/1/11/20	2/13/91/115	-
14	CLA	A	816	-	1/1/11/20	0/13/91/115	-
14	CLA	A	842	-	1/1/15/20	20/37/115/115	-
14	CLA	b	819	-	1/1/11/20	2/13/91/115	-
14	CLA	b	824	3	1/1/11/20	2/13/91/115	-
14	CLA	j	101	-	1/1/13/20	10/29/107/115	-
14	CLA	b	825	-	1/1/13/20	13/25/103/115	-
14	CLA	a	834	1	1/1/12/20	4/24/102/115	-
14	CLA	a	812	-	1/1/14/20	15/31/109/115	-
18	LHG	i	103	-	-	28/47/47/53	-
14	CLA	A	802	-	1/1/15/20	8/37/115/115	-
14	CLA	A	834	-	1/1/15/20	13/37/115/115	-
18	LHG	a	850	-	-	17/53/53/53	-
16	SF4	a	843	-	-	-	0/6/5/5
14	CLA	B	834	-	1/1/14/20	16/31/109/115	-
17	BCR	B	849	-	-	12/29/63/63	0/2/2/2
17	BCR	k	103	-	-	7/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	10/37/115/115	-
14	CLA	a	828	-	1/1/15/20	15/37/115/115	-
18	LHG	a	851	14	-	24/53/53/53	-
14	CLA	b	834	-	1/1/14/20	16/31/109/115	-
14	CLA	B	821	3	1/1/15/20	11/37/115/115	-
14	CLA	b	808	-	1/1/15/20	13/37/115/115	-
15	PQN	B	844	-	-	4/23/43/43	0/2/2/2
17	BCR	b	850	-	-	10/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/12/20	2/19/97/115	-
14	CLA	B	826	-	1/1/15/20	9/37/115/115	-
17	BCR	B	845	-	-	12/29/63/63	0/2/2/2
14	CLA	B	823	3	1/1/11/20	7/13/91/115	-
14	CLA	b	817	3	1/1/12/20	3/19/97/115	-
14	CLA	a	820	-	1/1/15/20	16/37/115/115	-
14	CLA	a	816	-	1/1/13/20	9/30/108/115	-
14	CLA	b	823	3	1/1/11/20	6/13/91/115	-
17	BCR	b	845	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	844	-	-	11/29/63/63	0/2/2/2
14	CLA	b	815	-	1/1/12/20	9/24/102/115	-
17	BCR	f	202	-	-	16/29/63/63	0/2/2/2
14	CLA	A	839	-	-	16/37/115/115	-
14	CLA	A	824	1	1/1/11/20	2/13/91/115	-
17	BCR	i	101	-	-	14/29/63/63	0/2/2/2
13	CL0	a	801	1	3/3/20/25	4/37/135/135	-
14	CLA	a	823	1	1/1/11/20	4/13/91/115	-
16	SF4	C	102	-	-	-	0/6/5/5
14	CLA	B	843	3	1/1/15/20	15/37/115/115	-
14	CLA	b	832	3	1/1/15/20	11/37/115/115	-
14	CLA	A	837	-	1/1/12/20	11/21/99/115	-
15	PQN	A	844	-	-	5/23/43/43	0/2/2/2
17	BCR	l	206	-	-	10/29/63/63	0/2/2/2
14	CLA	B	802	1	1/1/15/20	12/37/115/115	-
14	CLA	b	802	-	1/1/15/20	10/37/115/115	-
17	BCR	A	849	-	-	15/29/63/63	0/2/2/2
14	CLA	B	827	3	1/1/15/20	7/37/115/115	-
14	CLA	a	826	-	-	7/37/115/115	-
17	BCR	B	848	-	-	12/29/63/63	0/2/2/2
17	BCR	L	1504	-	-	13/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	10/37/115/115	-
14	CLA	B	816	-	1/1/15/20	13/37/115/115	-
14	CLA	a	841	18	1/1/11/20	8/13/91/115	-
14	CLA	A	803	-	1/1/15/20	9/37/115/115	-
17	BCR	B	846	-	-	9/29/63/63	0/2/2/2
14	CLA	A	817	-	1/1/13/20	6/30/108/115	-
14	CLA	a	822	1	1/1/12/20	9/24/102/115	-
17	BCR	i	102	-	-	12/29/63/63	0/2/2/2
14	CLA	a	805	1	1/1/15/20	16/37/115/115	-
14	CLA	B	812	-	1/1/15/20	13/37/115/115	-
14	CLA	b	811	-	1/1/15/20	7/37/115/115	-
17	BCR	J	103	-	-	12/29/63/63	0/2/2/2
17	BCR	a	846	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	838	1	1/1/15/20	13/37/115/115	-
14	CLA	b	812	3	1/1/15/20	19/37/115/115	-
14	CLA	B	810	3	1/1/15/20	9/37/115/115	-
14	CLA	b	842	-	1/1/15/20	6/37/115/115	-
14	CLA	k	101	-	1/1/9/20	2/7/81/115	-
16	SF4	A	845	-	-	-	0/6/5/5
14	CLA	A	832	1	1/1/15/20	18/37/115/115	-
14	CLA	A	843	18	1/1/11/20	7/13/91/115	-
17	BCR	l	201	-	-	9/29/63/63	0/2/2/2
14	CLA	b	810	3	1/1/15/20	7/37/115/115	-
14	CLA	B	808	-	1/1/15/20	17/37/115/115	-
19	SQD	x	1702	-	-	14/49/69/69	0/1/1/1
16	SF4	c	102	-	-	-	0/6/5/5
14	CLA	B	807	3	1/1/13/20	6/25/103/115	-
14	CLA	B	825	-	1/1/13/20	11/25/103/115	-
18	LHG	A	852	-	-	21/53/53/53	-
14	CLA	b	837	-	1/1/11/20	2/13/91/115	-
14	CLA	j	102	-	1/1/11/20	9/13/91/115	-
15	PQN	a	842	-	-	5/23/43/43	0/2/2/2
13	CL0	A	801	-	3/3/20/25	4/37/135/135	-
14	CLA	A	815	-	1/1/11/20	3/13/91/115	-
14	CLA	A	822	-	1/1/11/20	6/13/91/115	-
14	CLA	a	825	-	1/1/12/20	6/24/102/115	-
14	CLA	B	839	3	1/1/14/20	7/31/109/115	-
14	CLA	K	102	-	1/1/11/20	2/18/96/115	-
14	CLA	b	813	-	1/1/14/20	16/31/109/115	-
14	CLA	k	102	-	1/1/11/20	4/18/96/115	-
17	BCR	F	203	-	-	14/29/63/63	0/2/2/2
14	CLA	A	825	-	1/1/15/20	16/37/115/115	-
17	BCR	J	105	-	-	9/29/63/63	0/2/2/2
14	CLA	a	804	1	1/1/15/20	17/37/115/115	-
17	BCR	f	204	-	-	15/29/63/63	0/2/2/2
14	CLA	a	839	1	1/1/15/20	5/37/115/115	-
14	CLA	B	820	3	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	F	202	3	1/1/15/20	17/37/115/115	-
14	CLA	A	818	1	1/1/14/20	8/31/109/115	-
14	CLA	a	806	-	1/1/14/20	8/31/109/115	-
14	CLA	A	810	1	1/1/11/20	3/13/91/115	-
14	CLA	B	822	-	1/1/15/20	10/37/115/115	-
14	CLA	a	809	1	1/1/11/20	7/13/91/115	-
14	CLA	f	201	-	1/1/13/20	7/30/108/115	-
14	CLA	a	802	1	1/1/15/20	10/37/115/115	-
14	CLA	L	1501	11	1/1/12/20	5/21/99/115	-
17	BCR	j	104	-	-	14/29/63/63	0/2/2/2
14	CLA	b	820	-	1/1/15/20	5/37/115/115	-
14	CLA	b	826	-	1/1/15/20	8/37/115/115	-
14	CLA	A	833	1	1/1/15/20	10/37/115/115	-

The worst 5 of 1676 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	801	CL0	MG-NA	9.30	2.28	2.06
13	A	801	CL0	MG-NA	9.30	2.28	2.06
14	A	821	CLA	C4B-NB	7.66	1.42	1.35
14	B	838	CLA	C4B-NB	7.58	1.42	1.35
14	A	811	CLA	C4B-NB	7.57	1.42	1.35

The worst 5 of 2279 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	807	CLA	O2D-CGD-CBD	25.81	157.13	111.27
14	A	807	CLA	O2D-CGD-O1D	-24.58	75.78	123.84
14	A	807	CLA	O1D-CGD-CBD	-21.05	81.42	124.48
14	a	841	CLA	O2A-CGA-O1A	-20.37	72.52	123.30
14	a	841	CLA	O2A-CGA-CBA	13.87	158.58	114.03

5 of 187 chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
13	a	801	CL0	ND

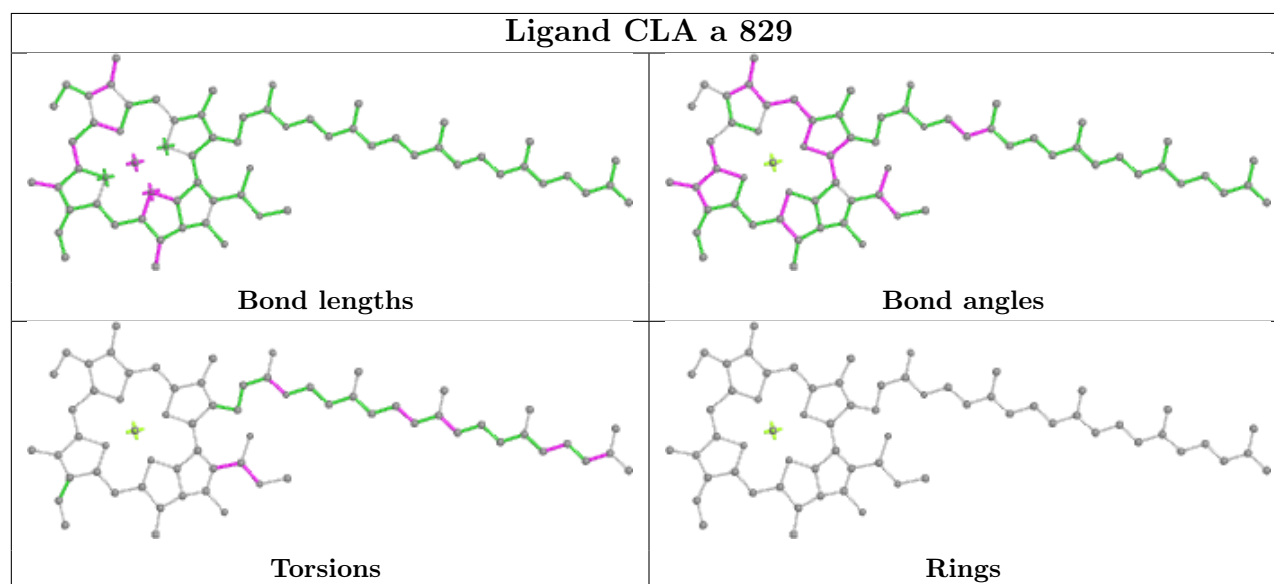
5 of 2625 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	CBA-CGA-O2A-C1
14	A	805	CLA	O1A-CGA-O2A-C1
14	A	805	CLA	CHA-CBD-CGD-O1D

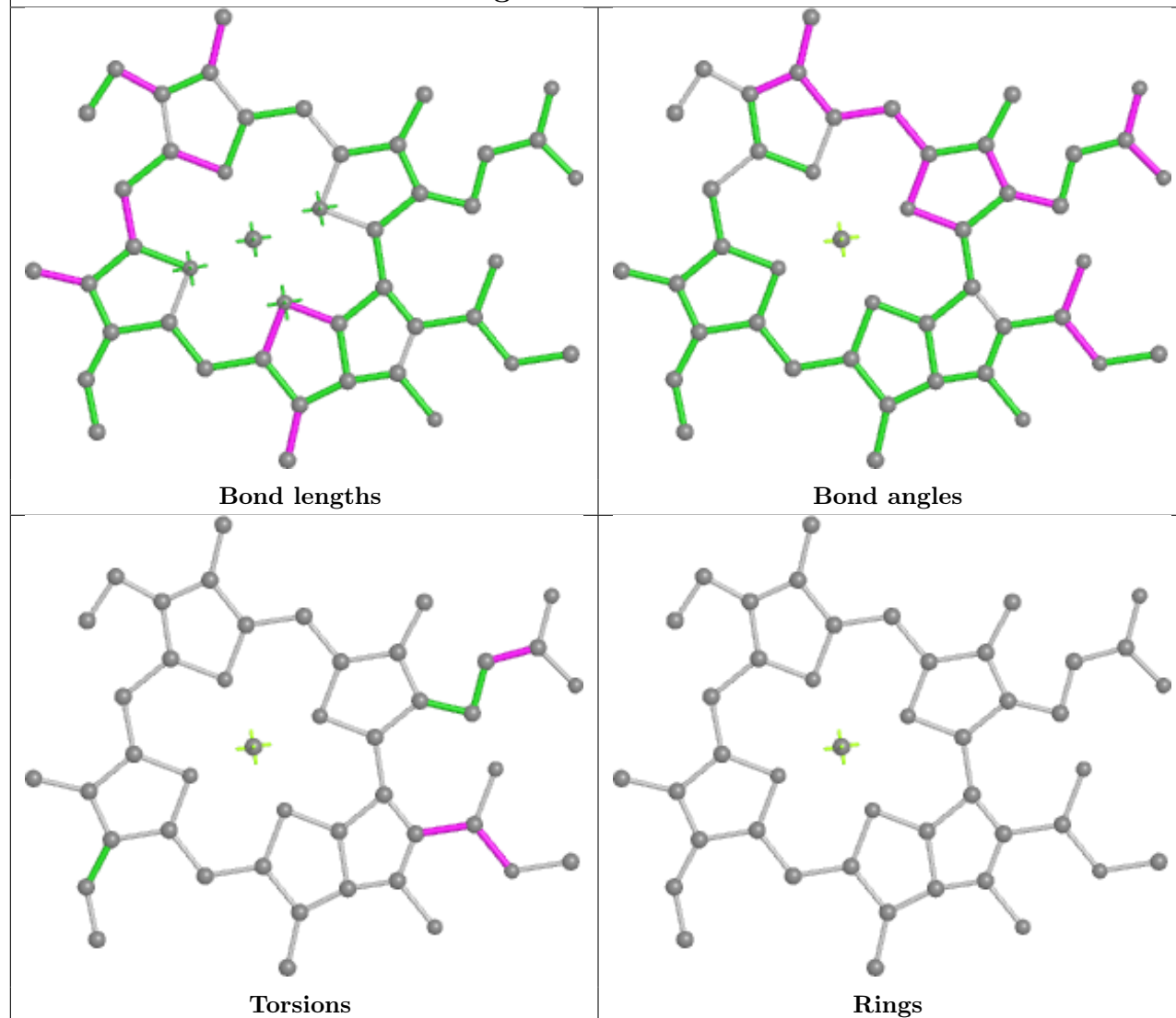
There are no ring outliers.

No monomer is involved in short contacts.

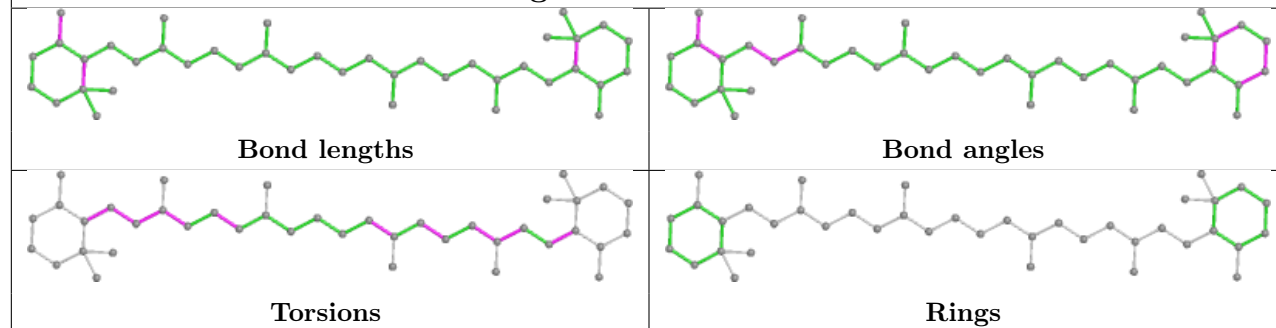
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

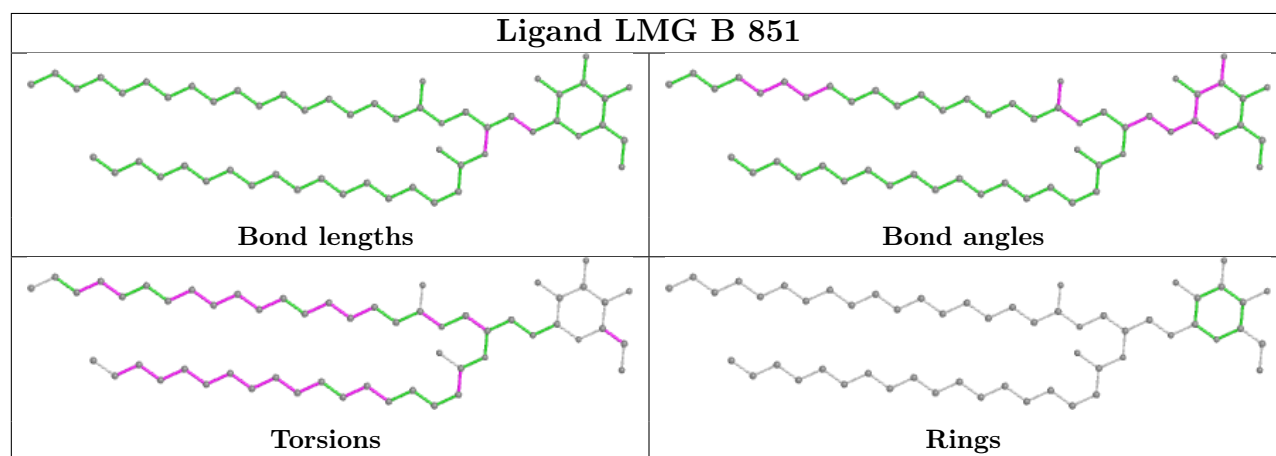
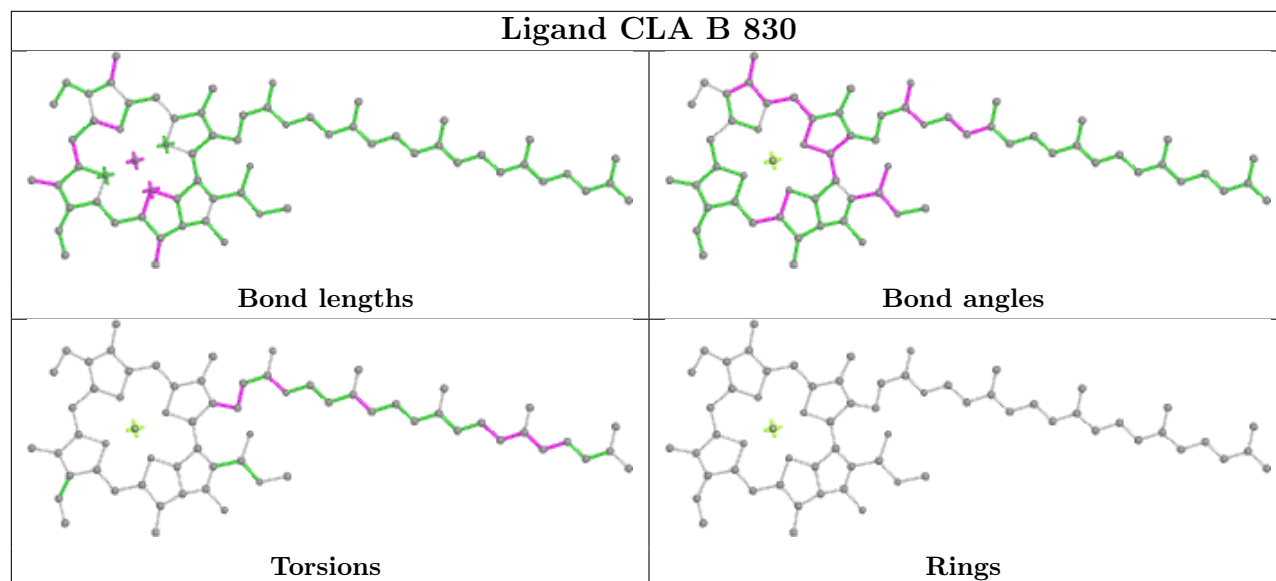
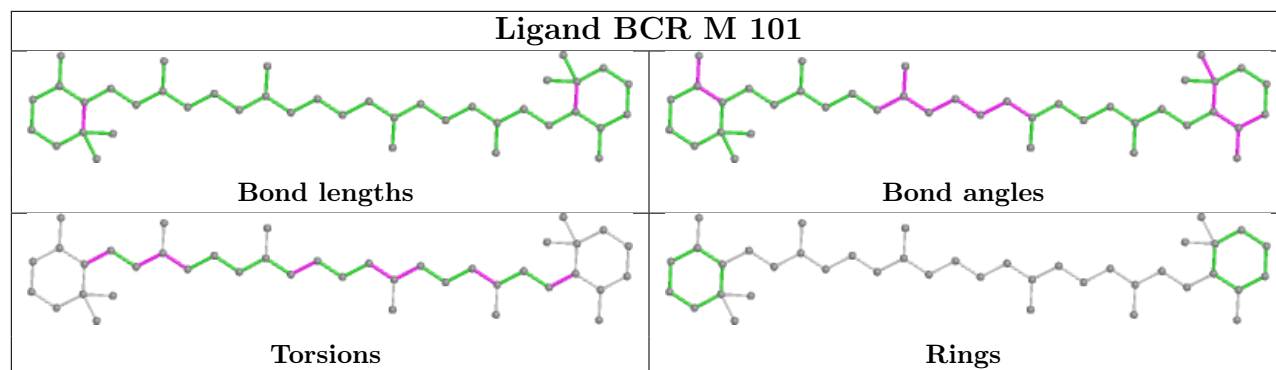


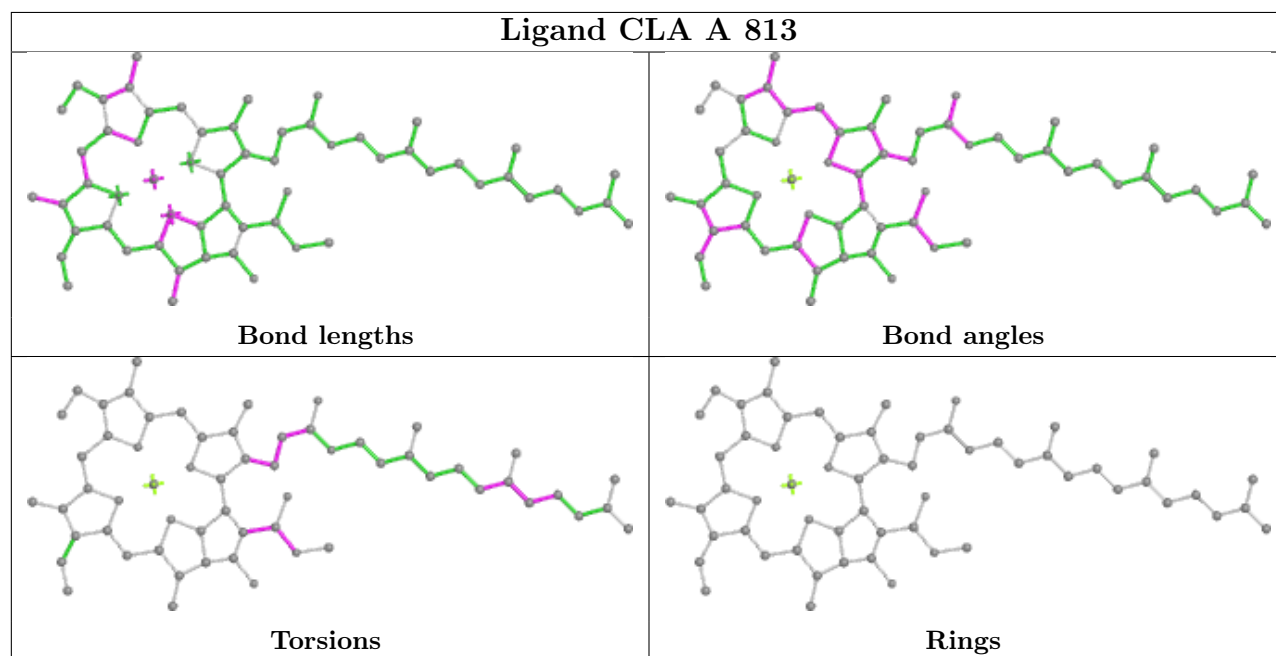
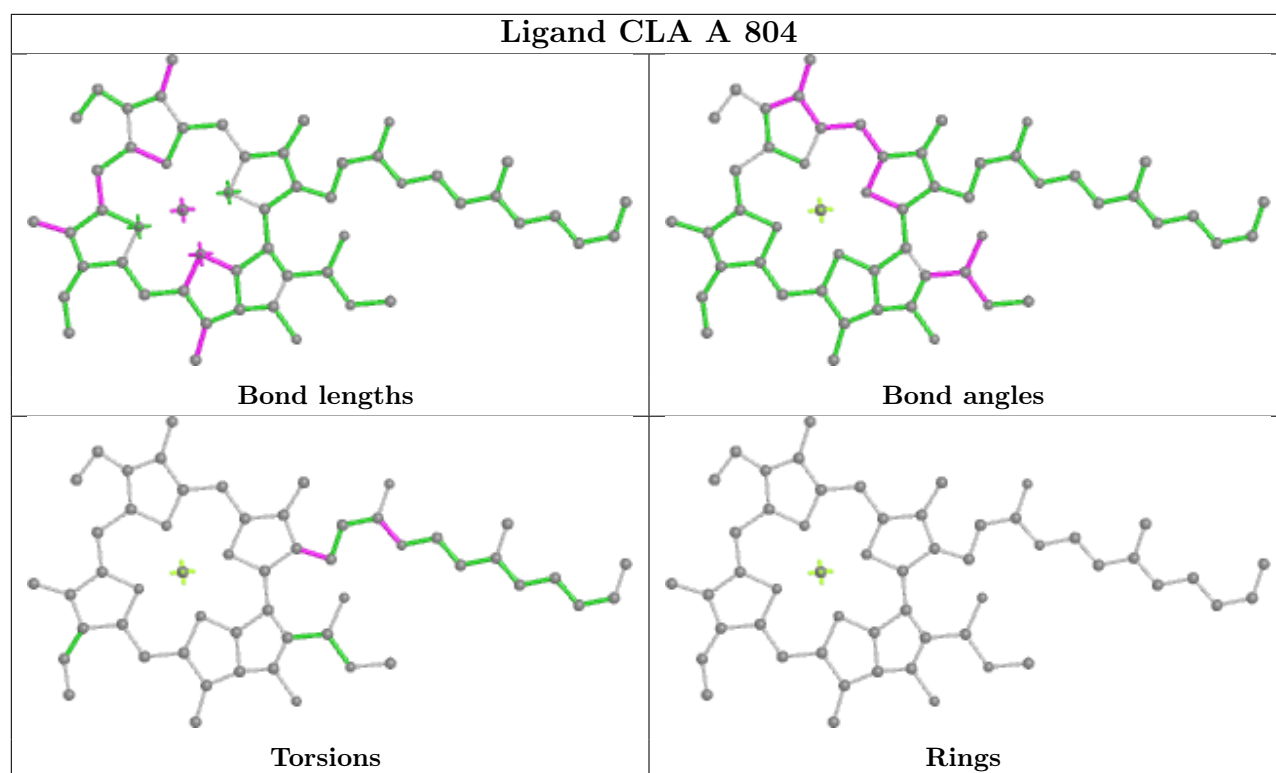
Ligand CLA J 101

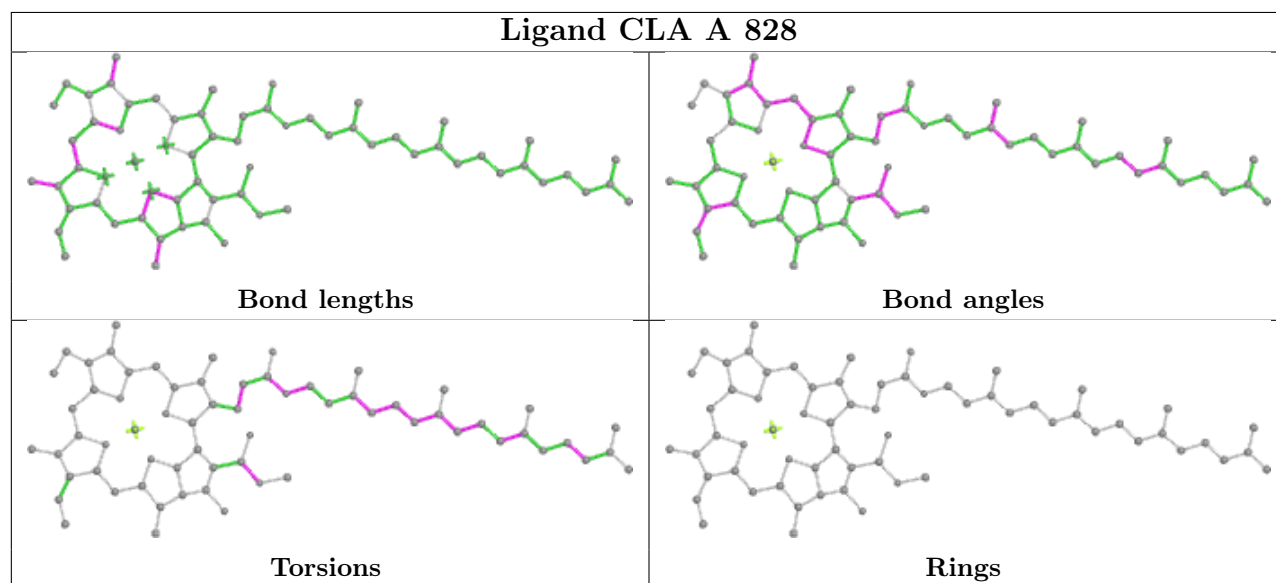
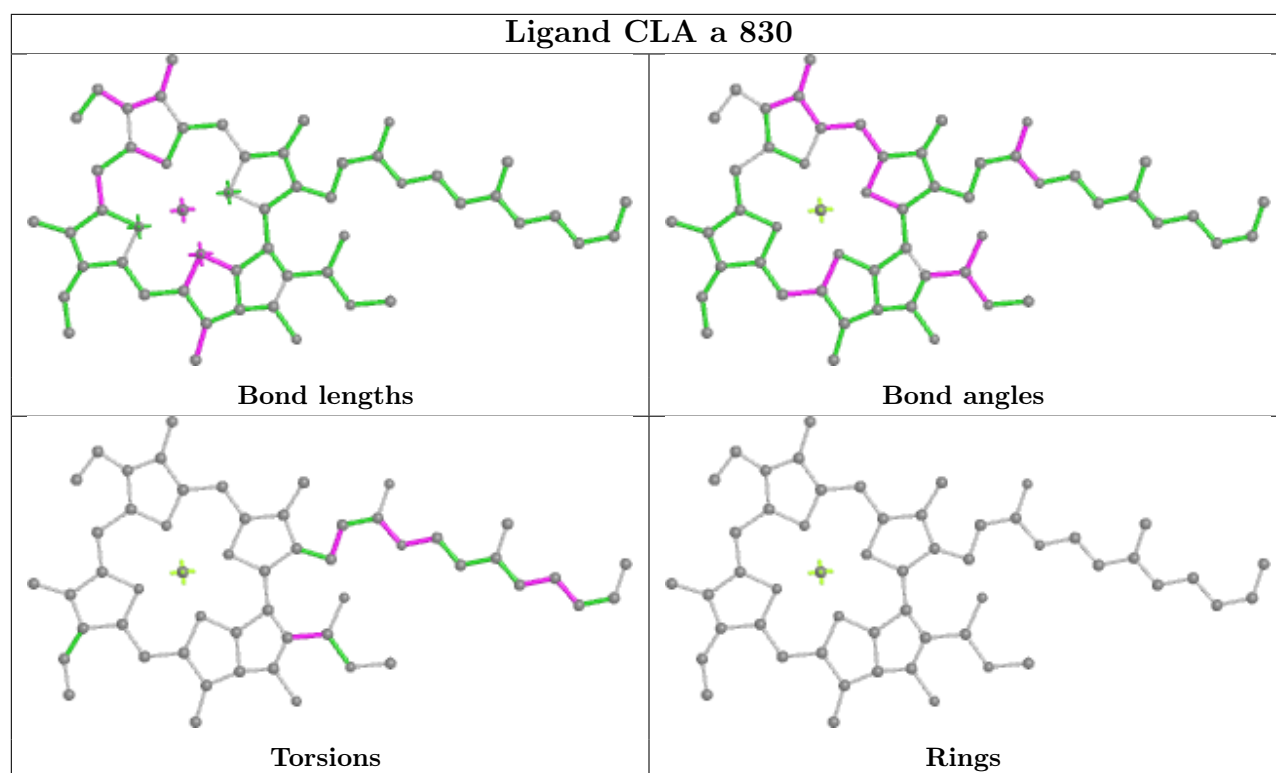


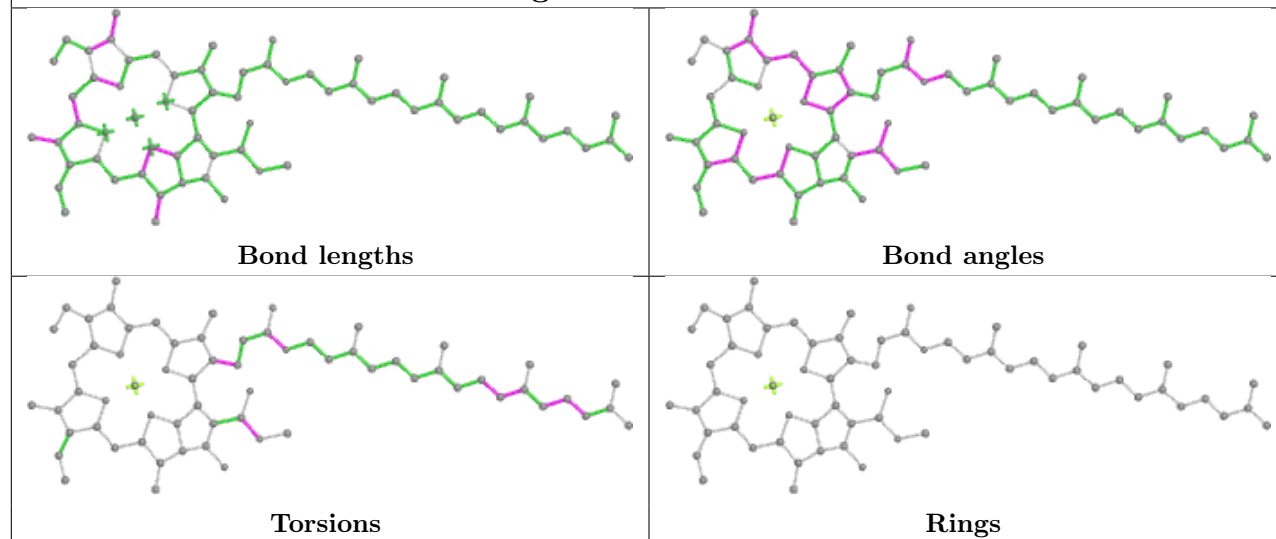
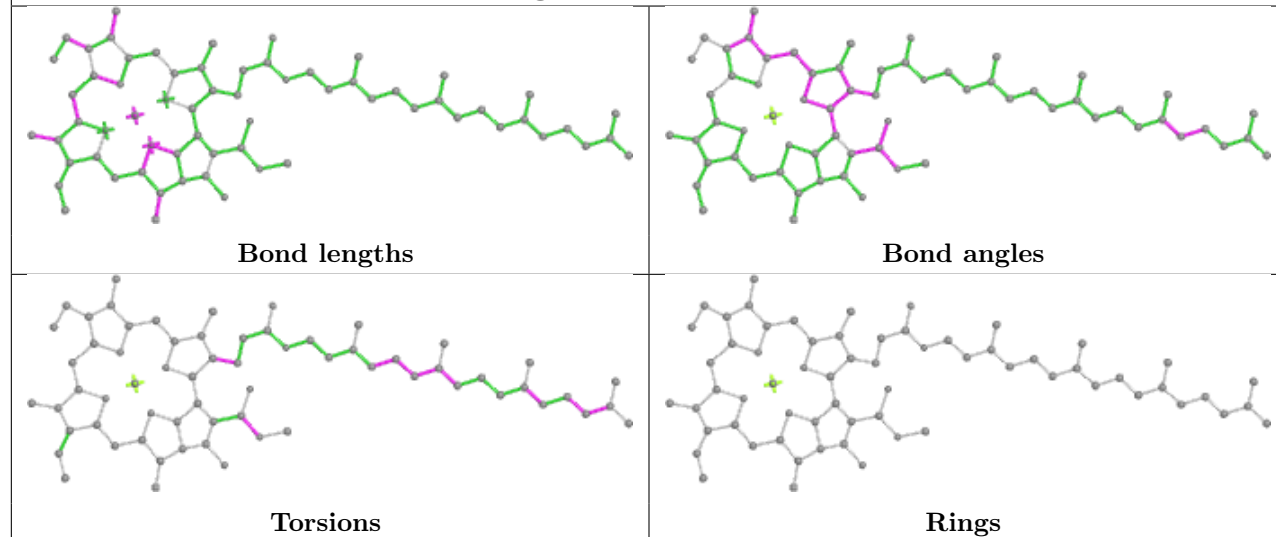
Ligand BCR A 851



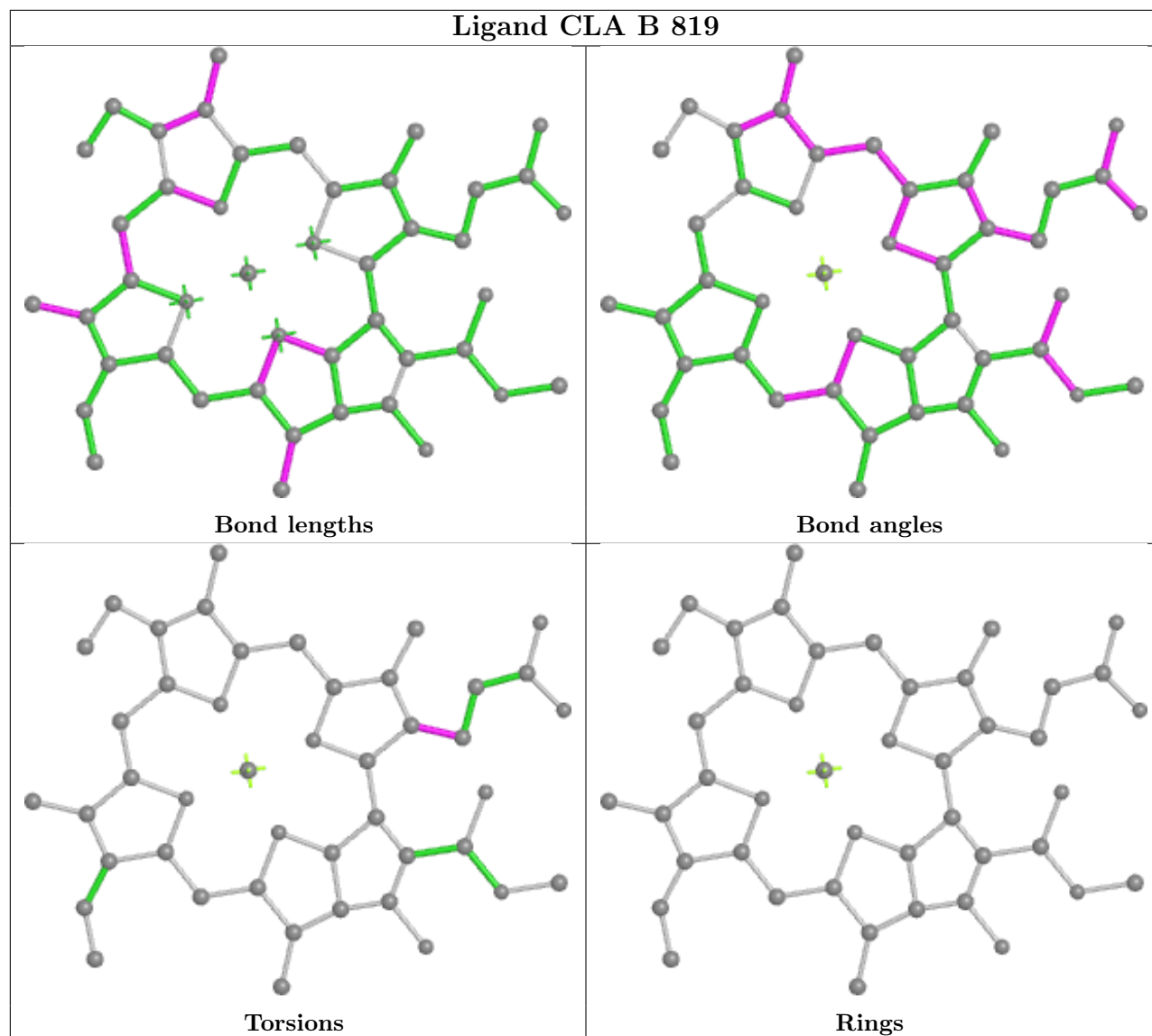


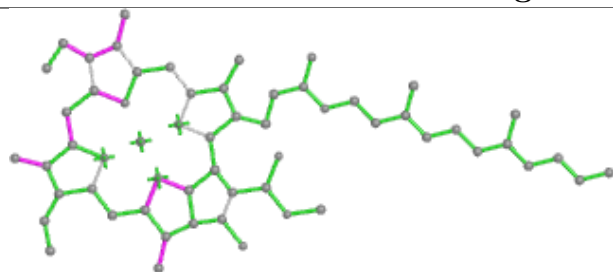
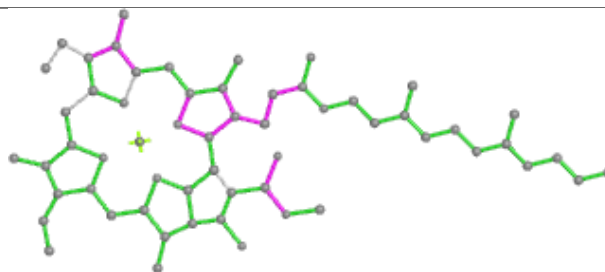
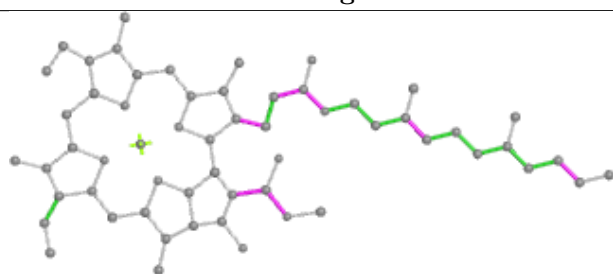
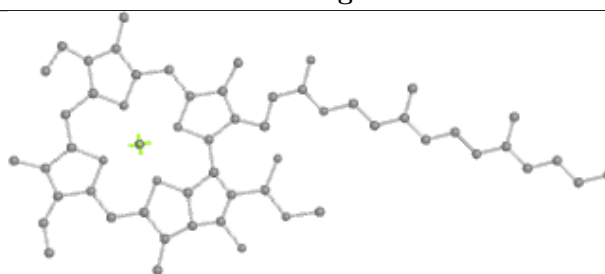
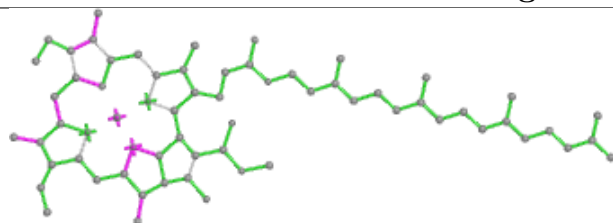
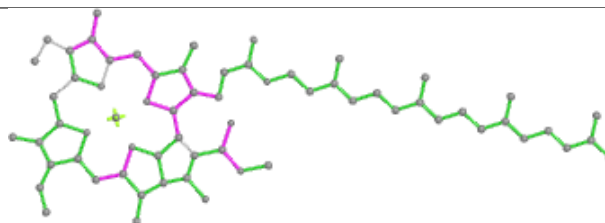
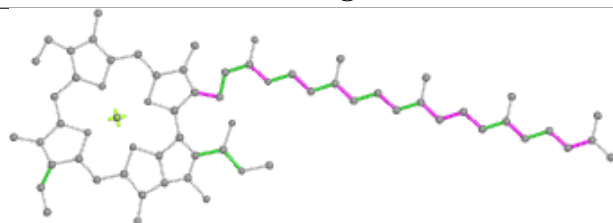
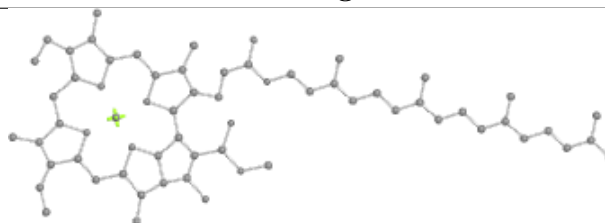


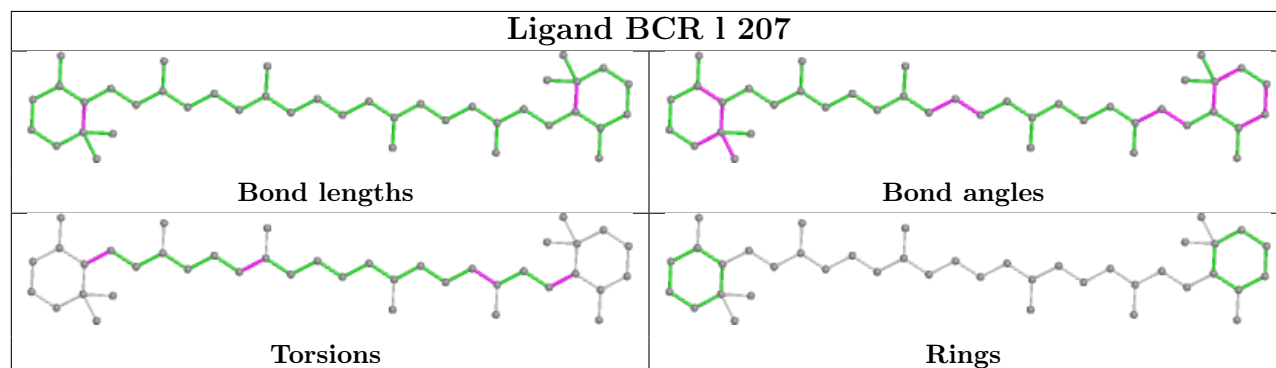
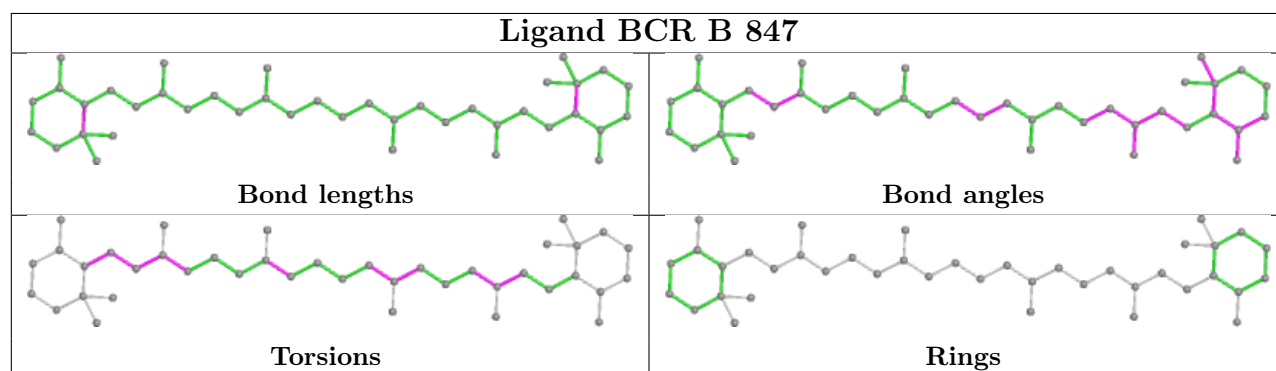
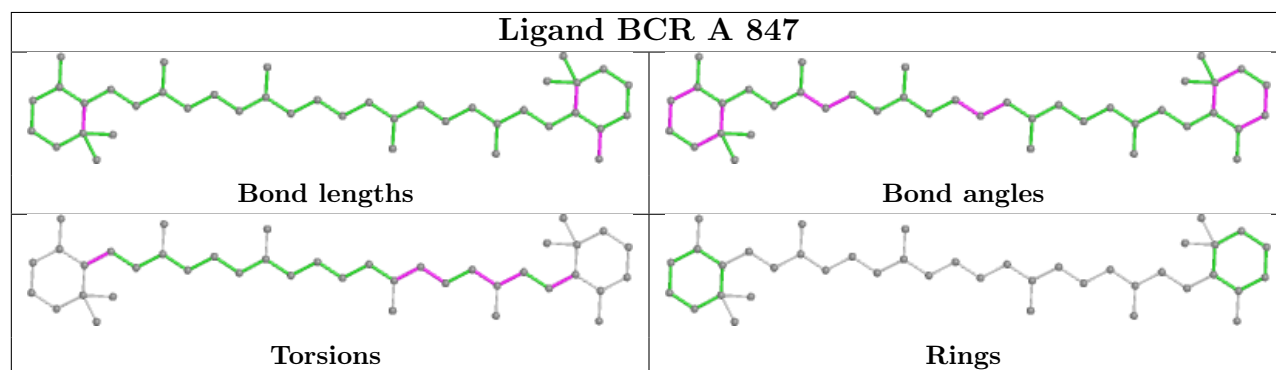
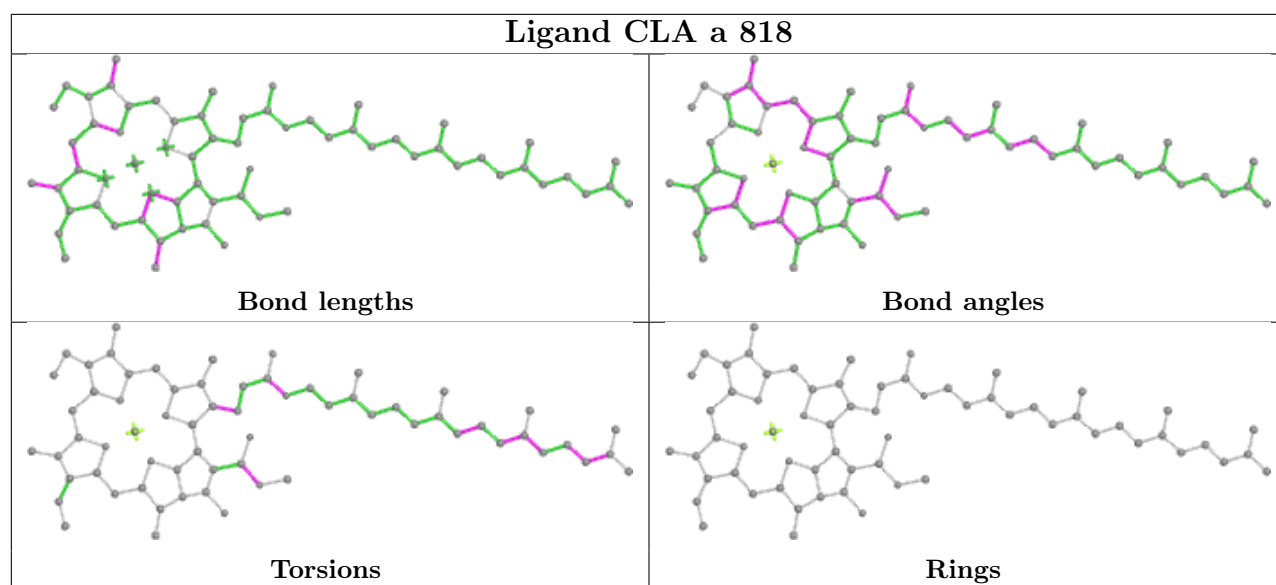


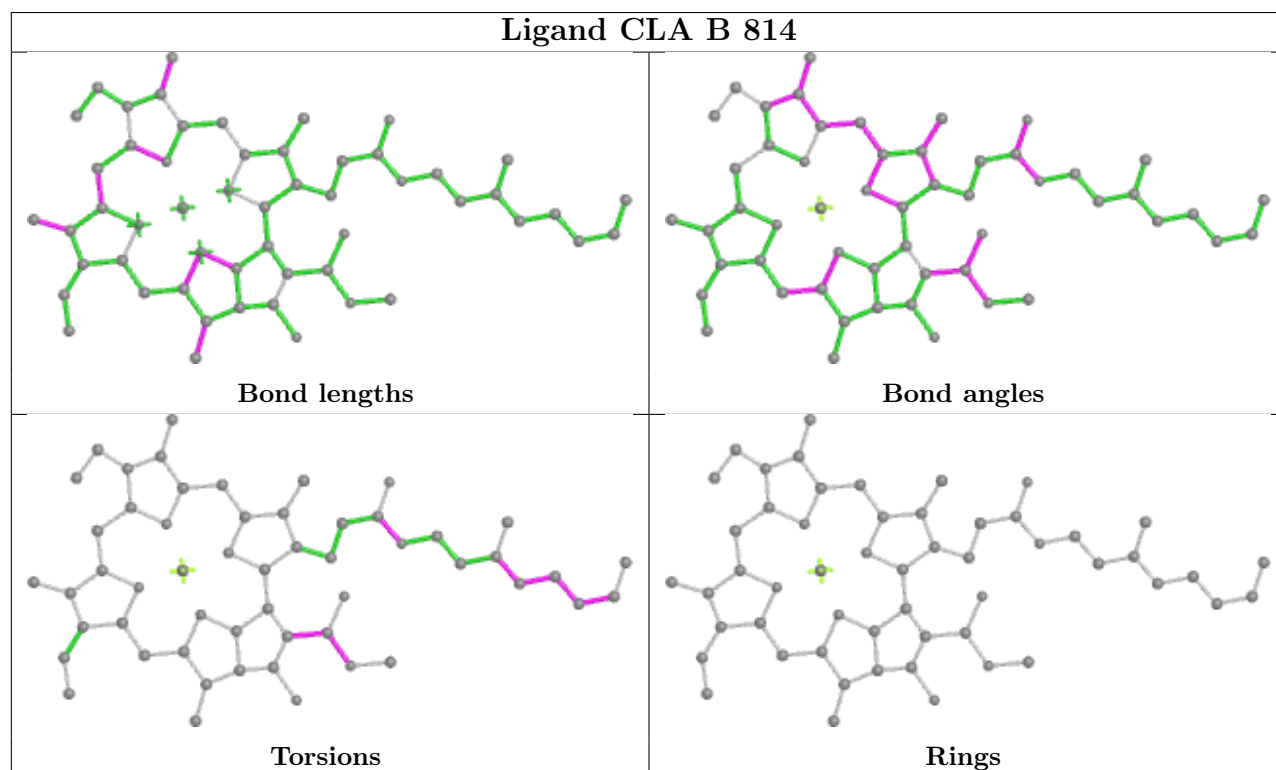
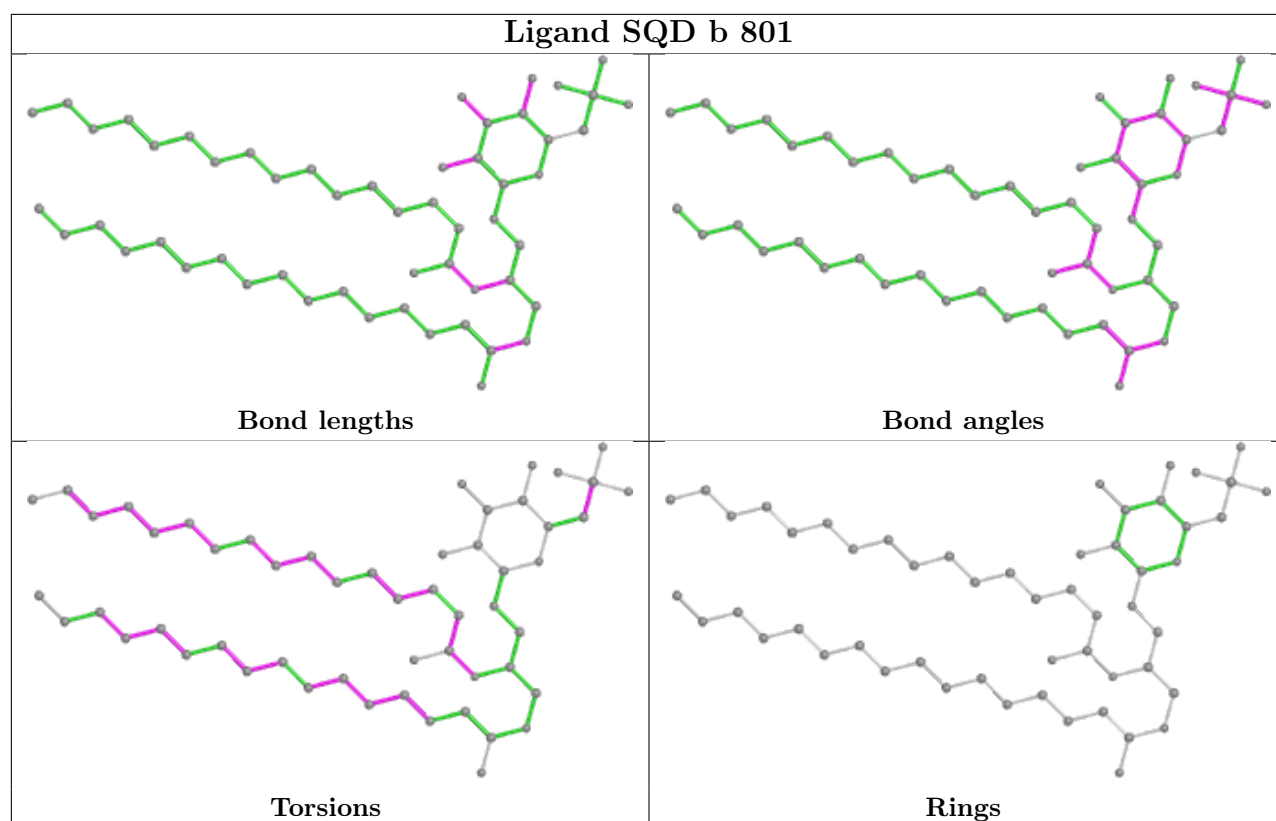
Ligand CLA A 811**Ligand CLA A 806**

Ligand CLA B 819

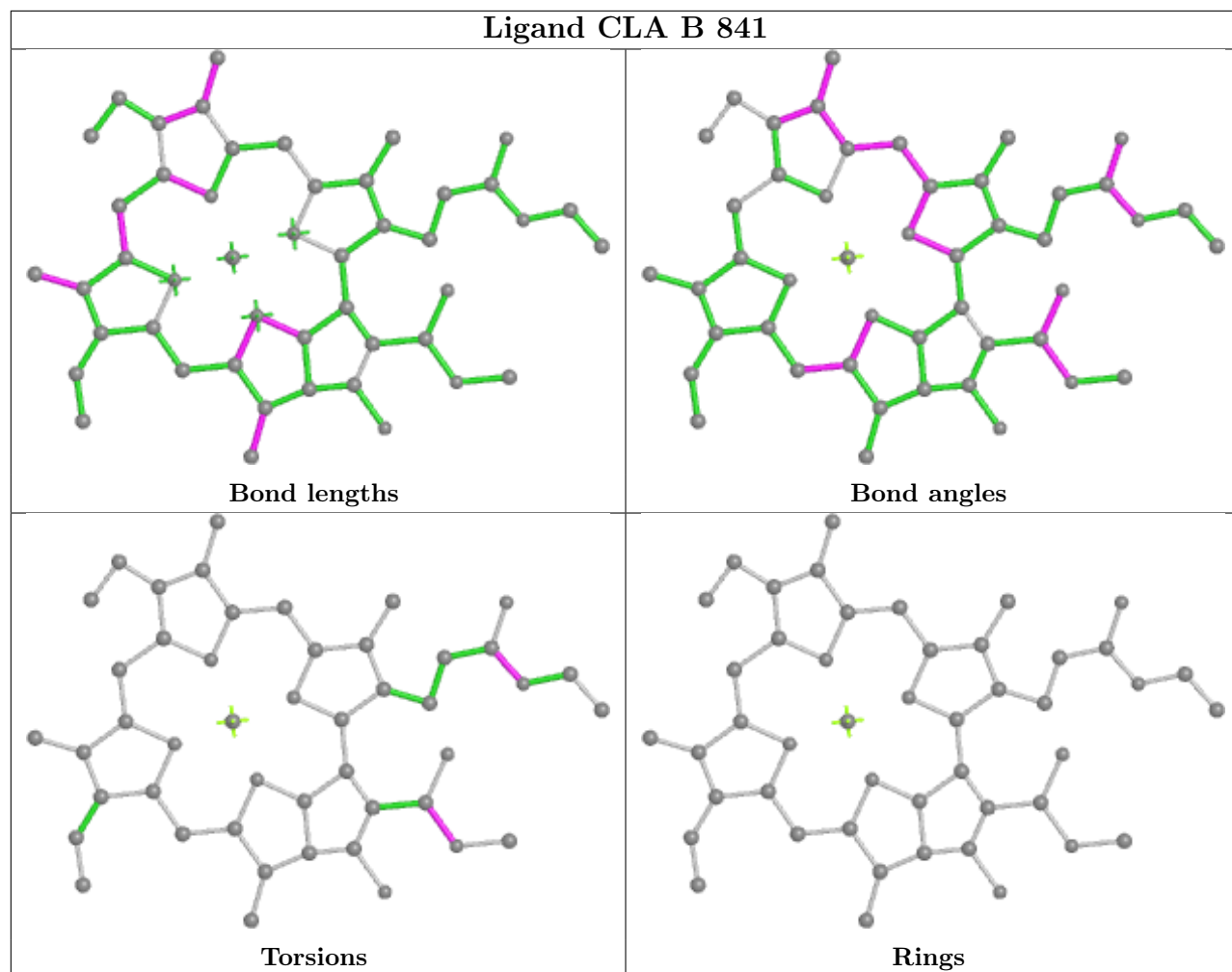


Ligand CLA B 835**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA a 831****Bond lengths****Bond angles****Torsions****Rings**

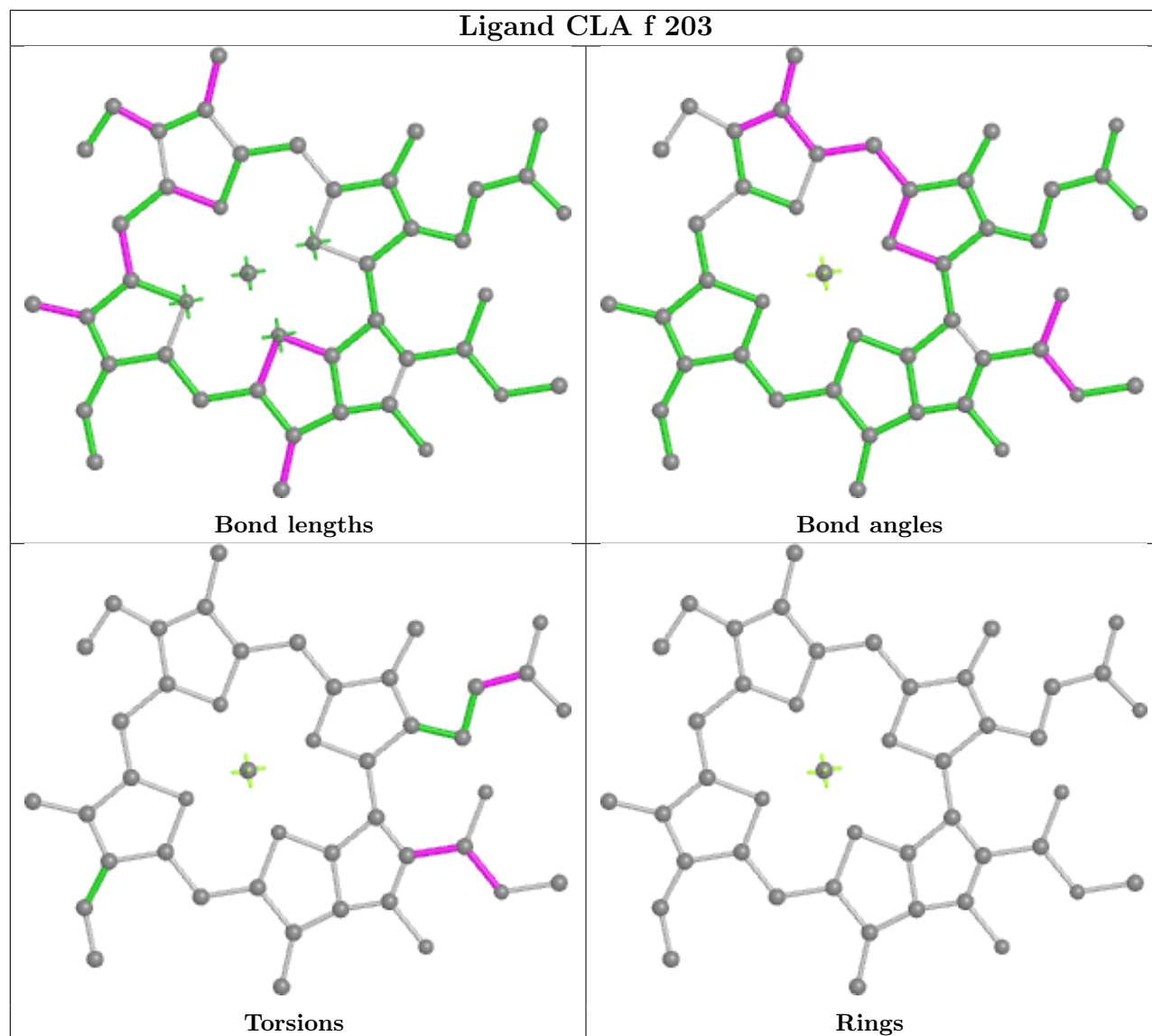


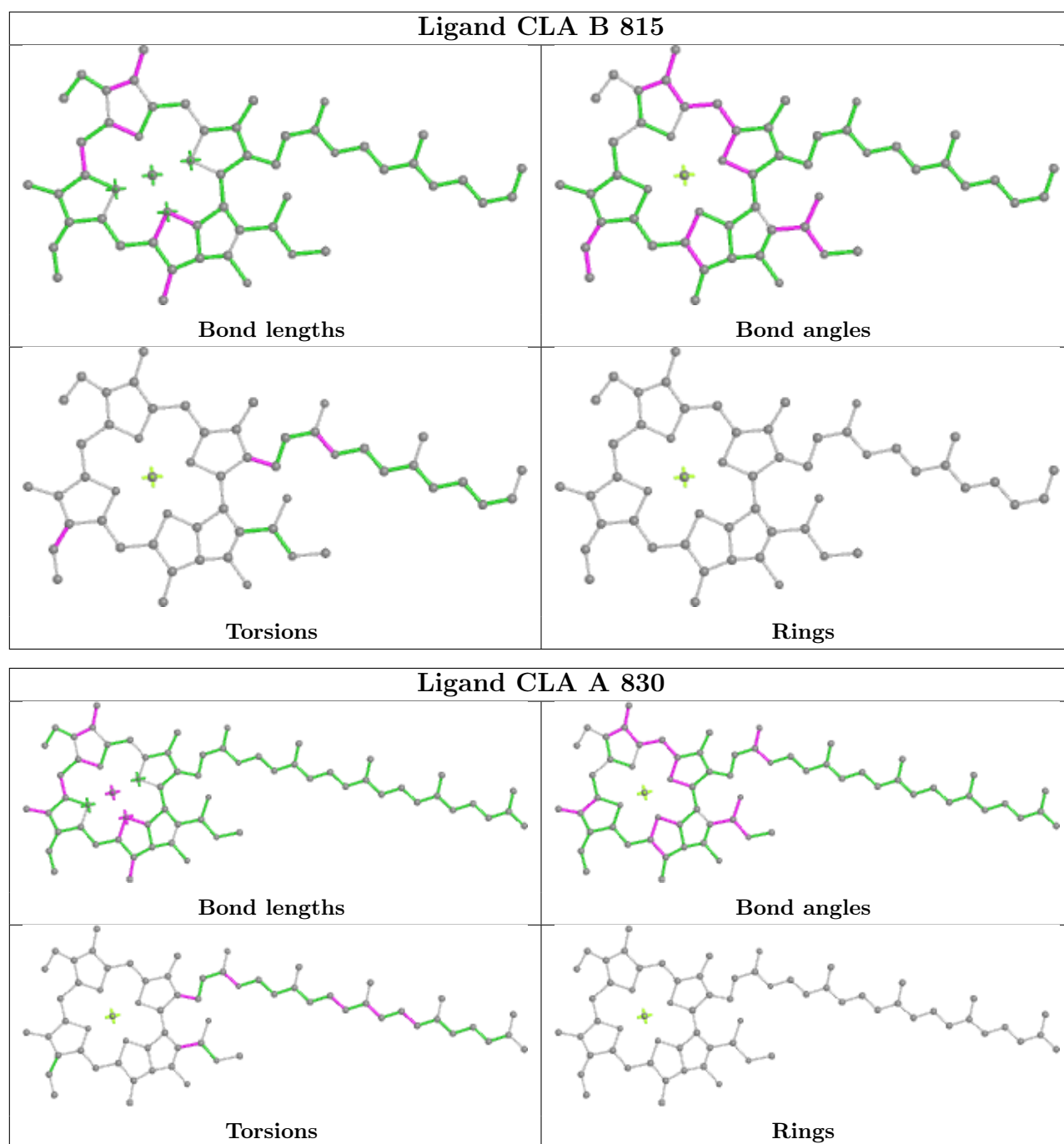


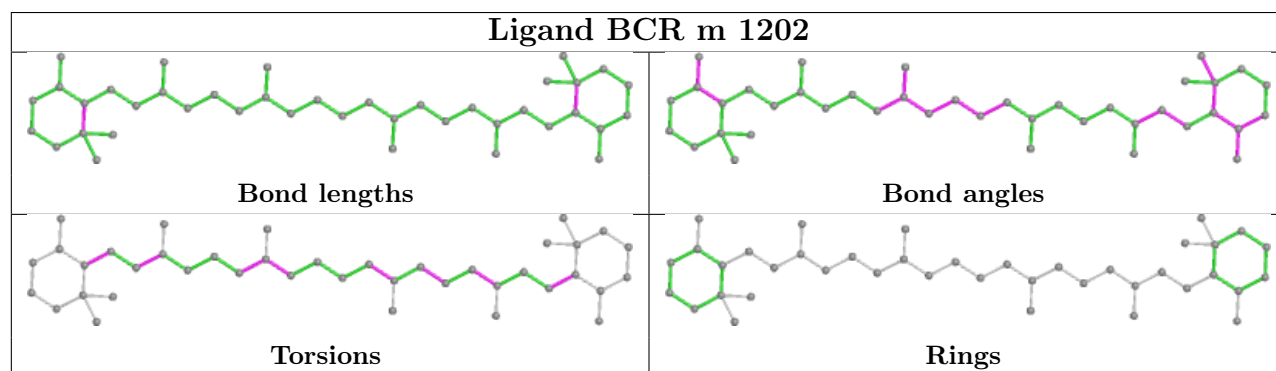
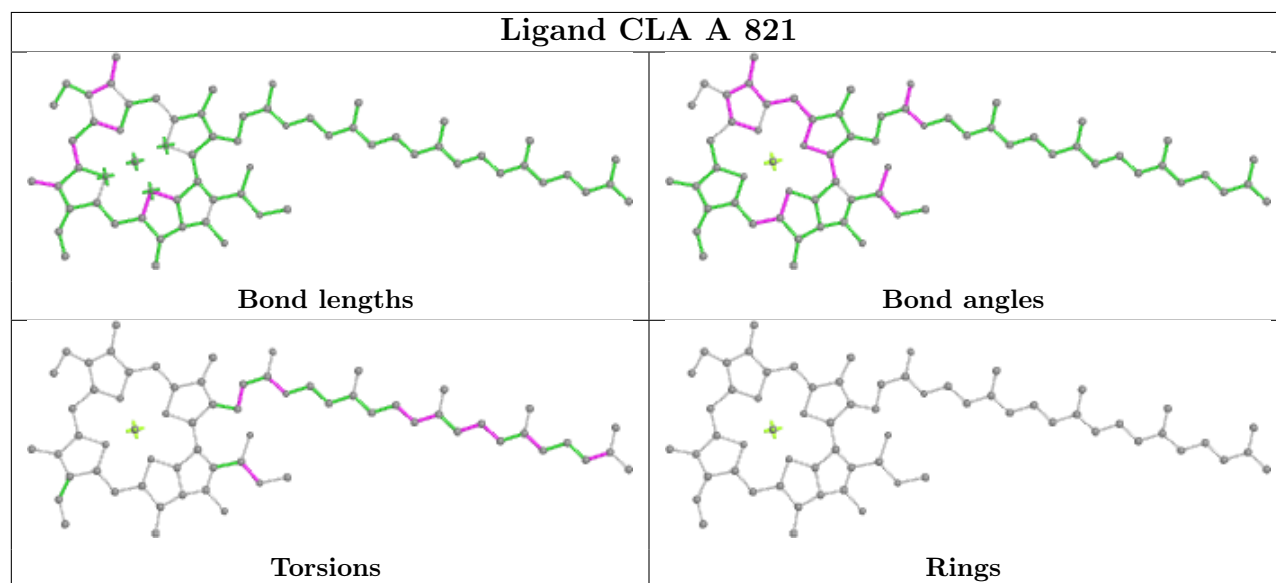
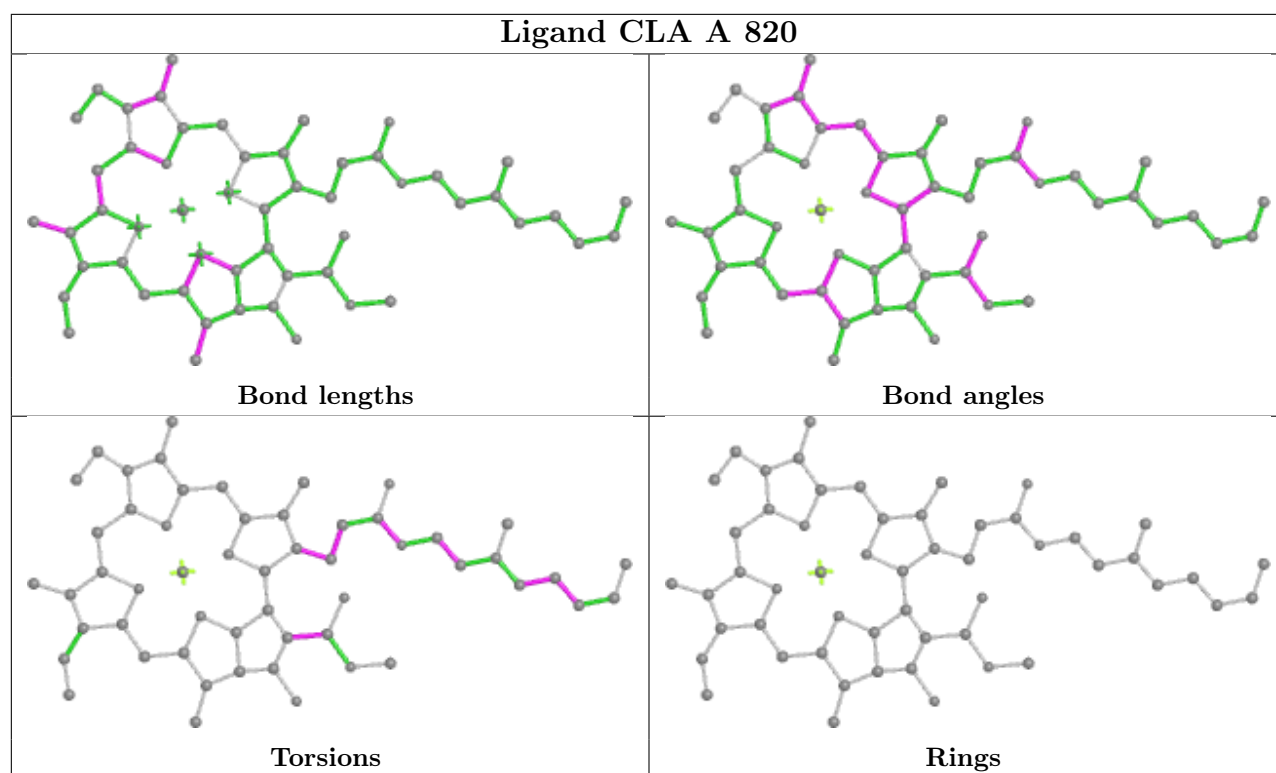
Ligand CLA B 841

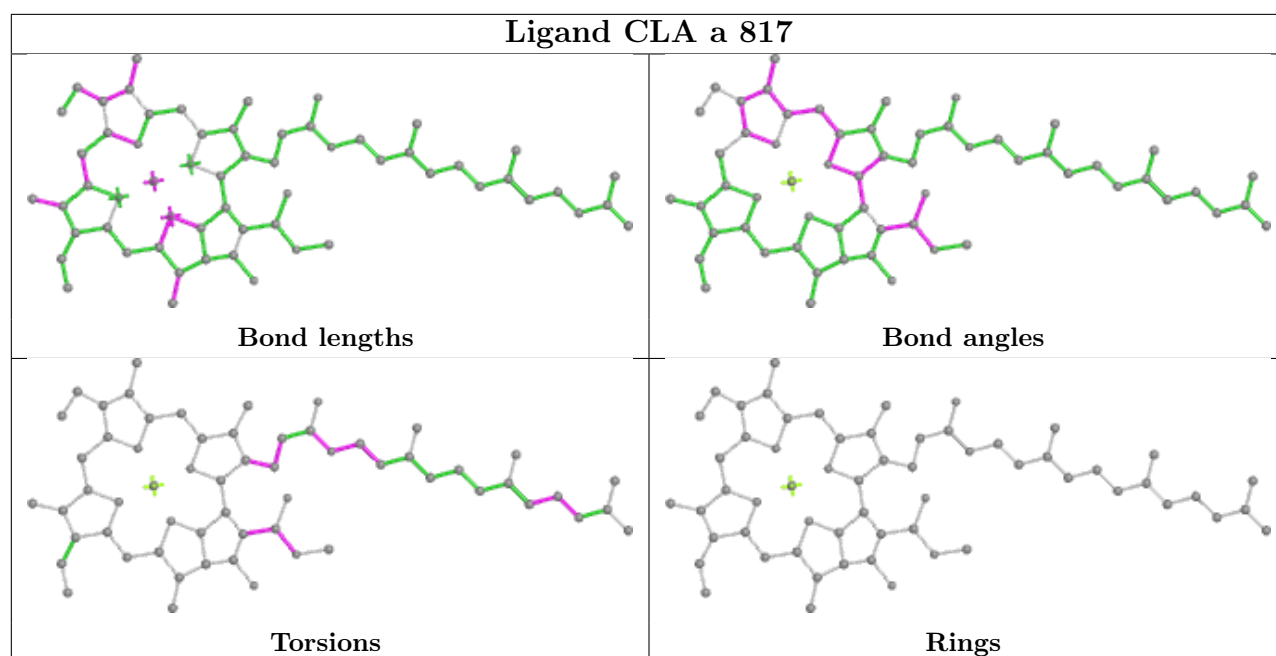


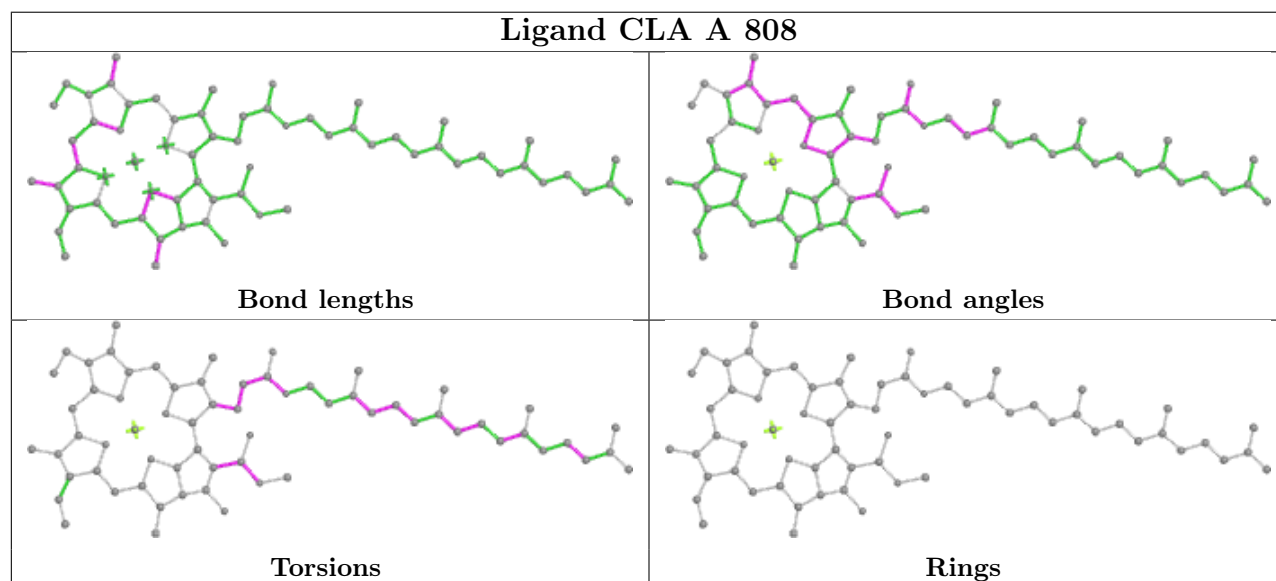
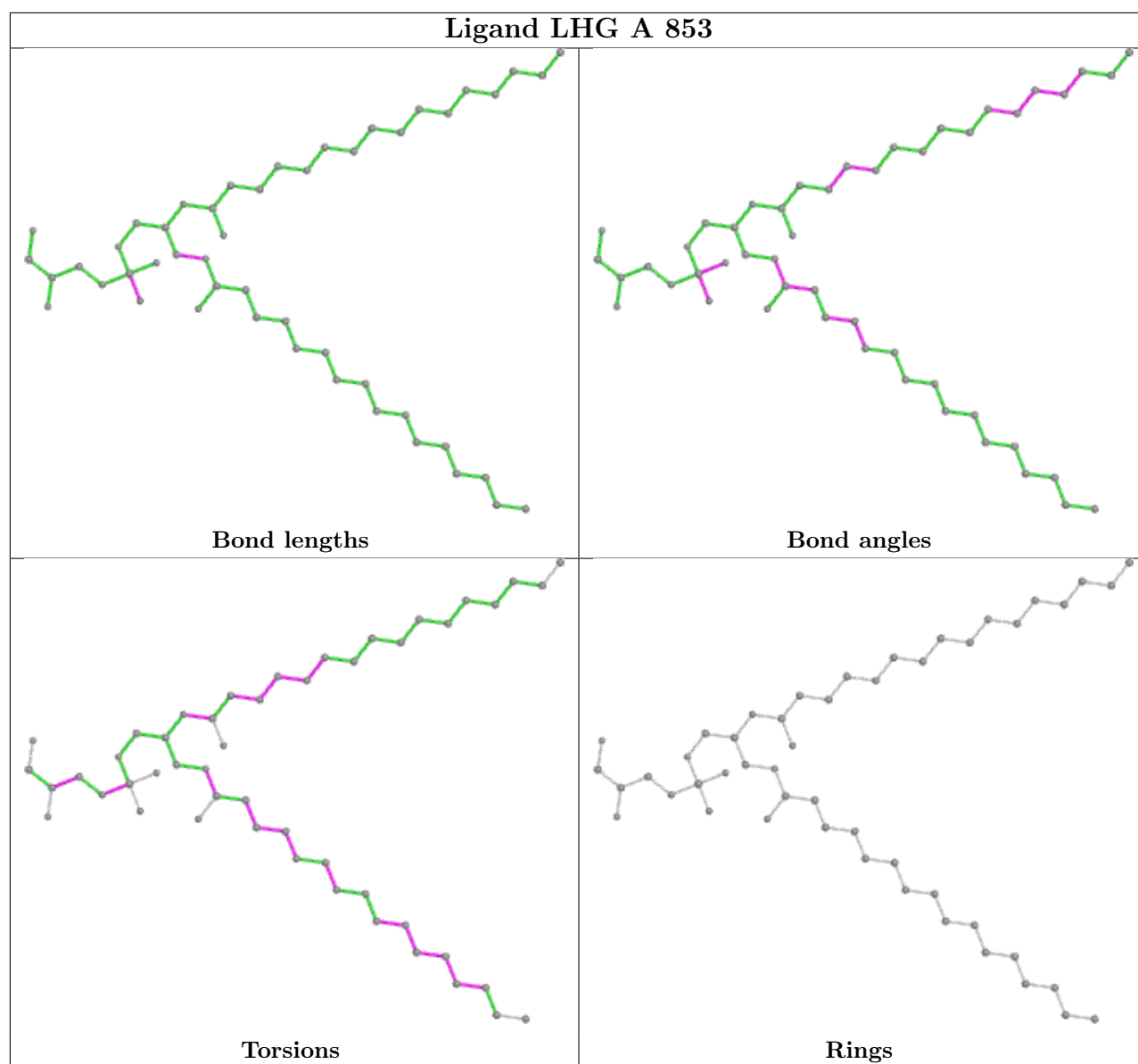
Ligand CLA f 203

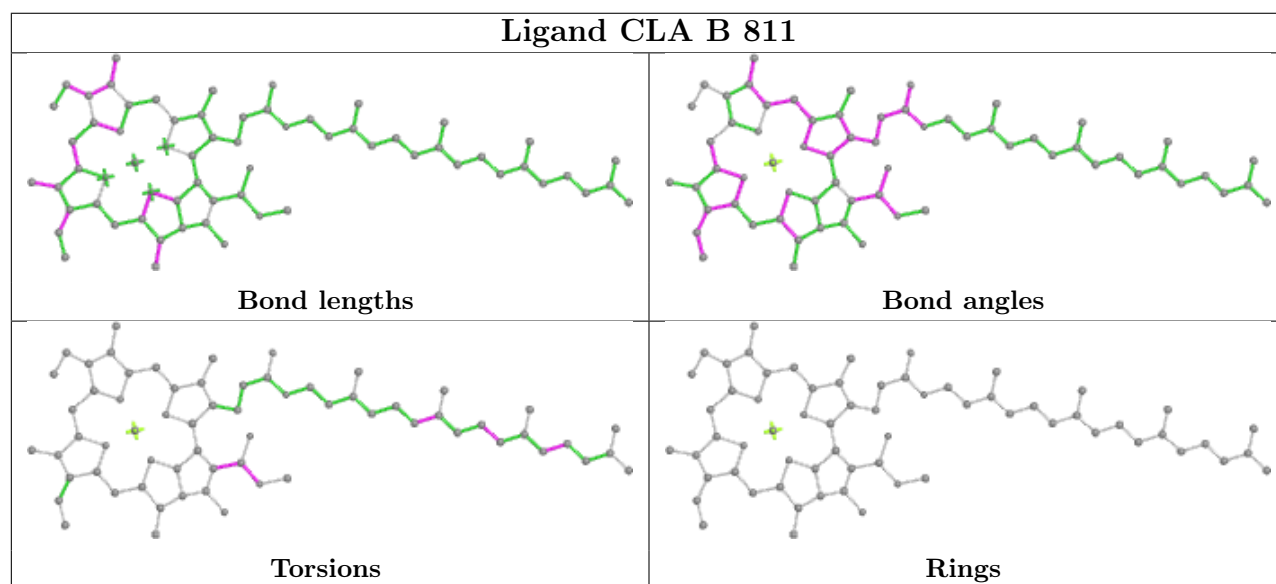
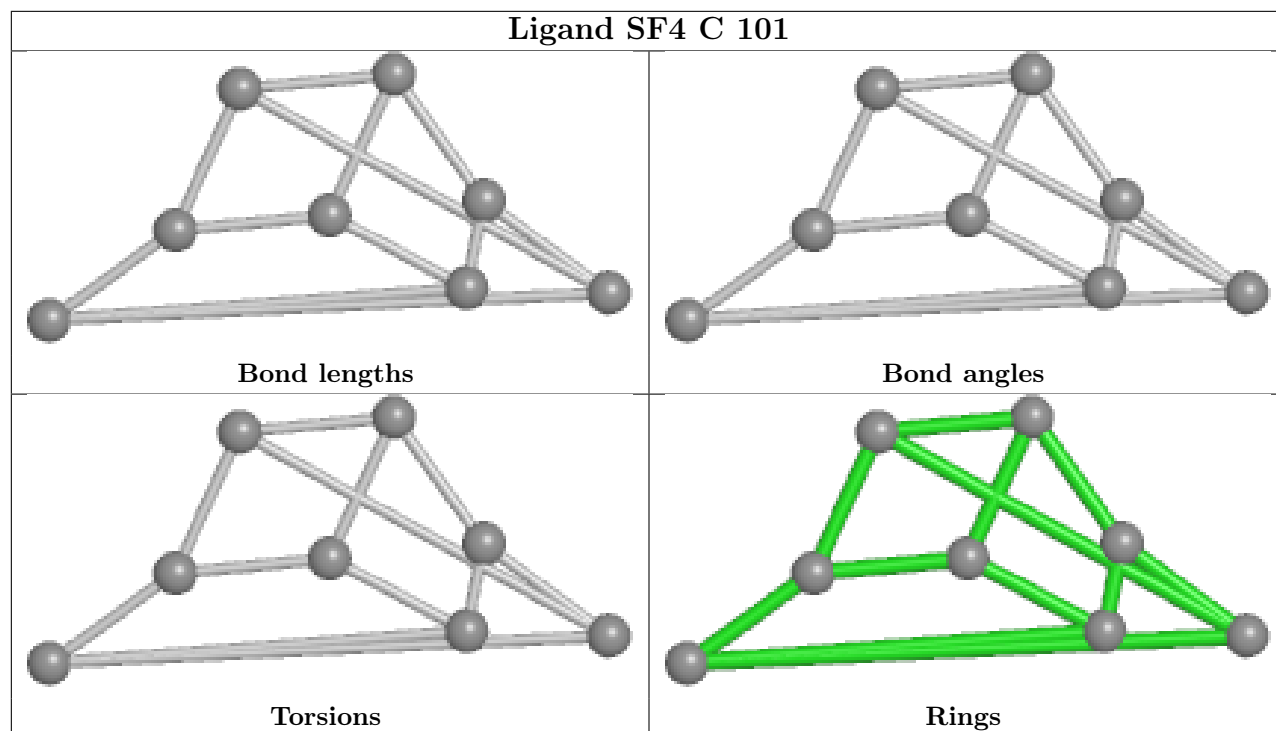
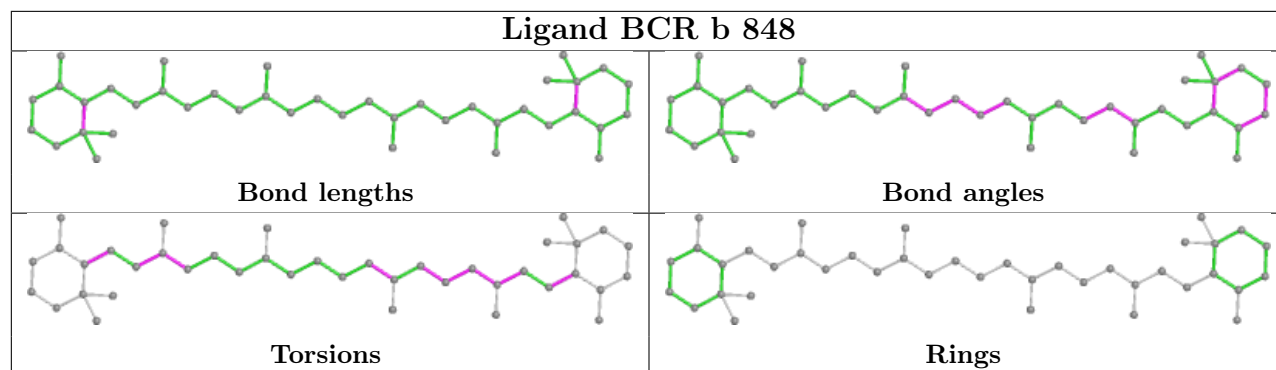


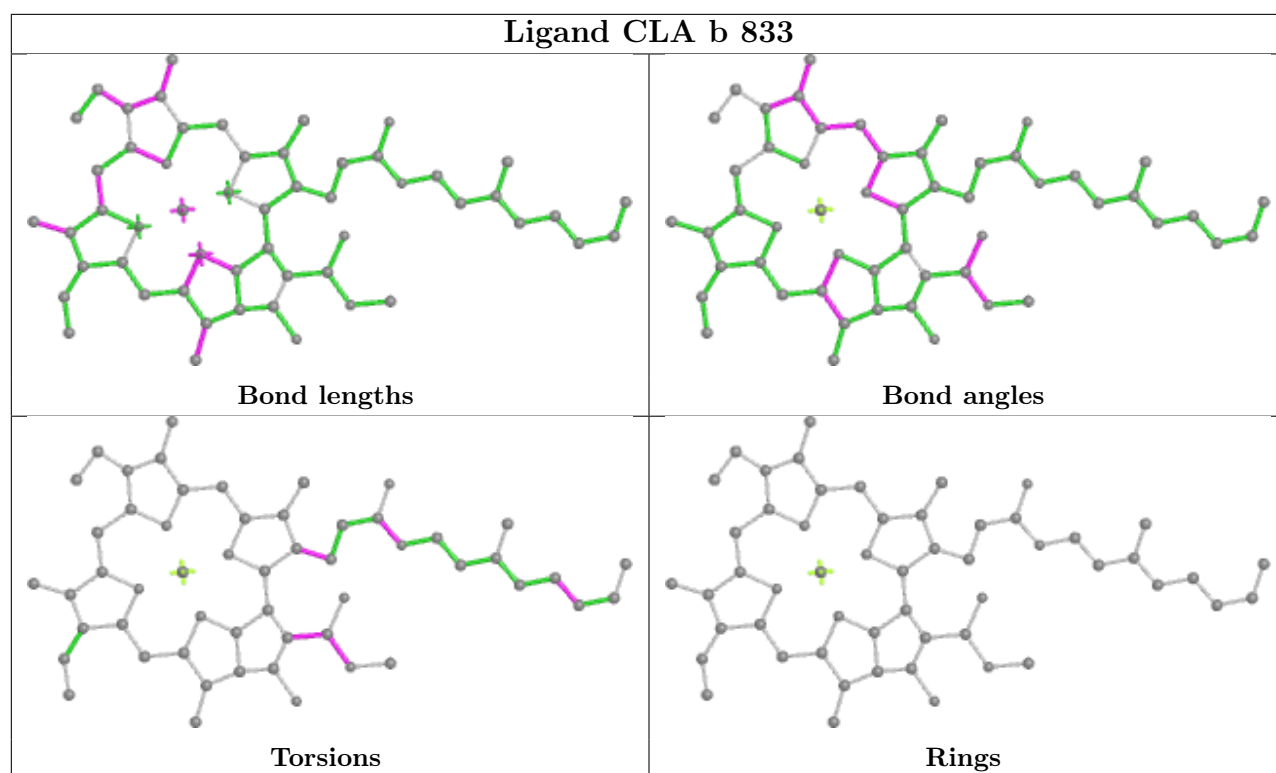




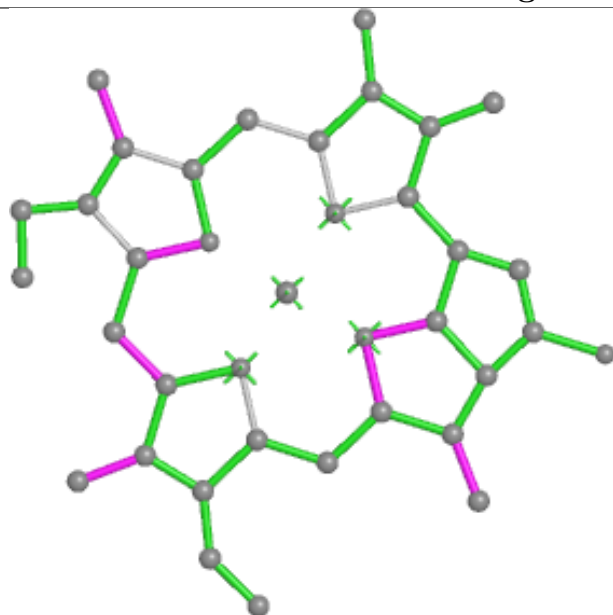




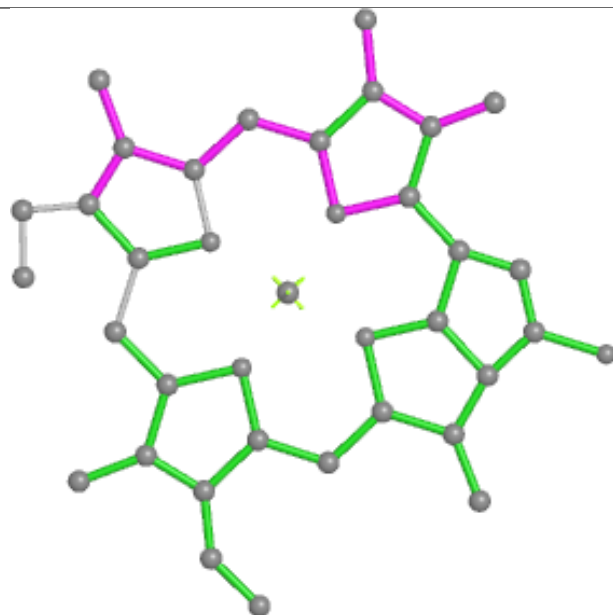




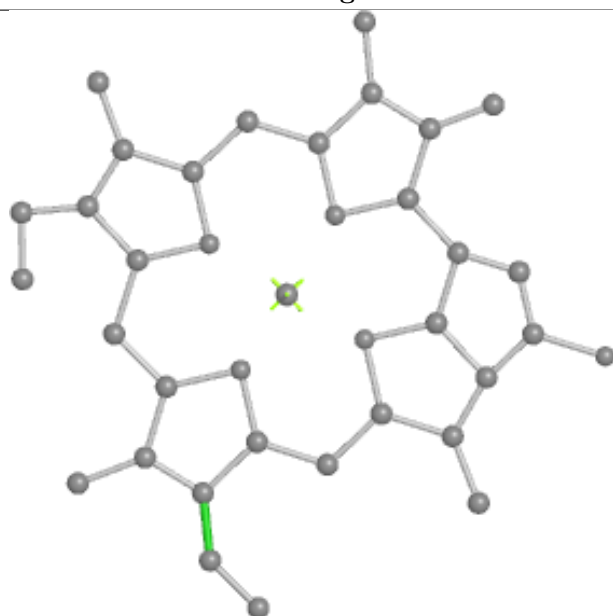
Ligand CLA J 102



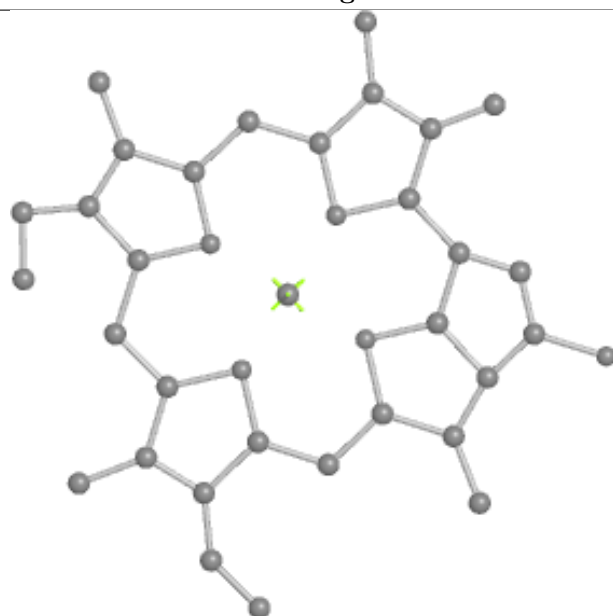
Bond lengths



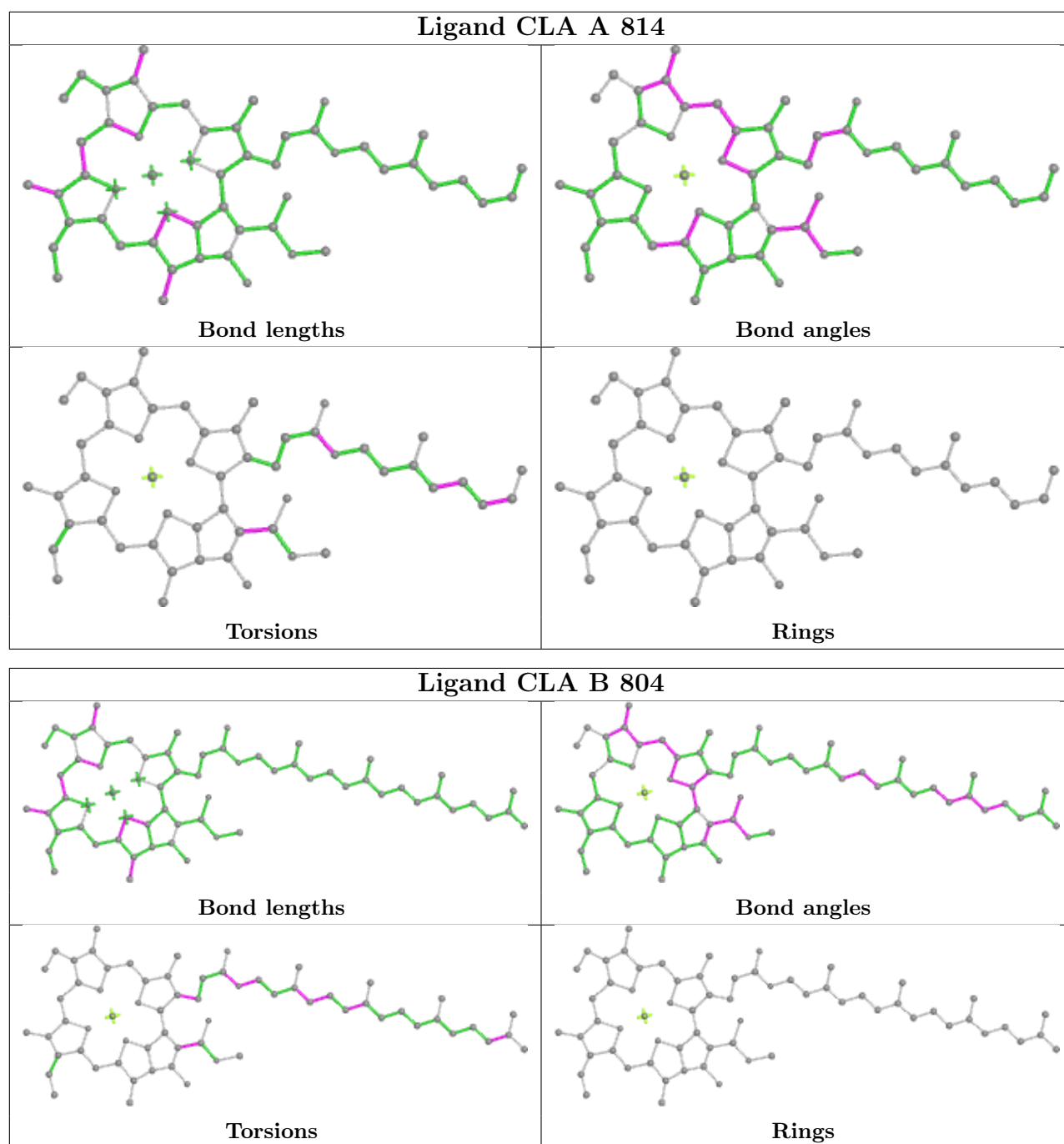
Bond angles

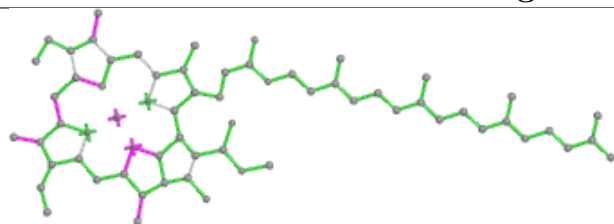
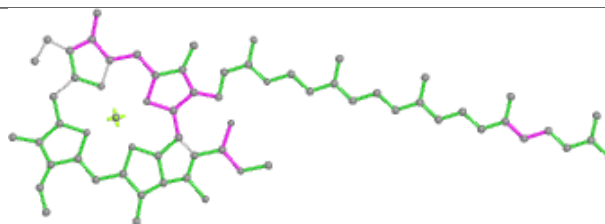
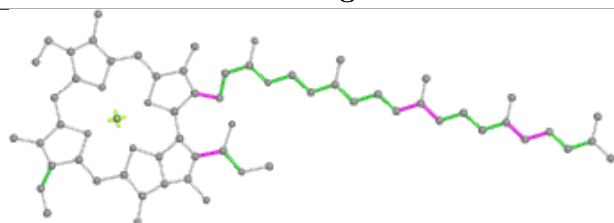
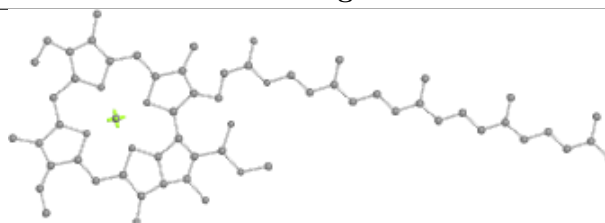
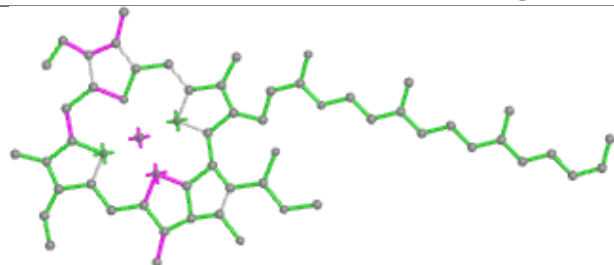
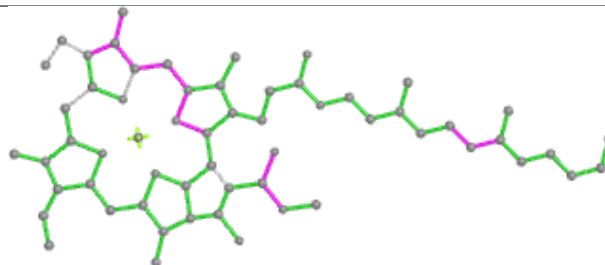
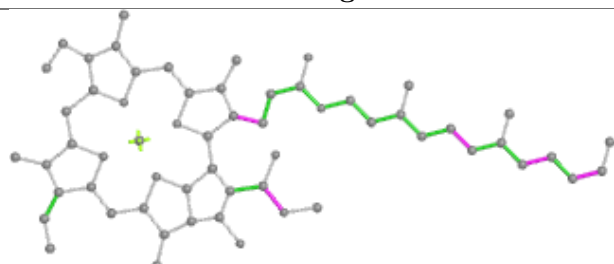
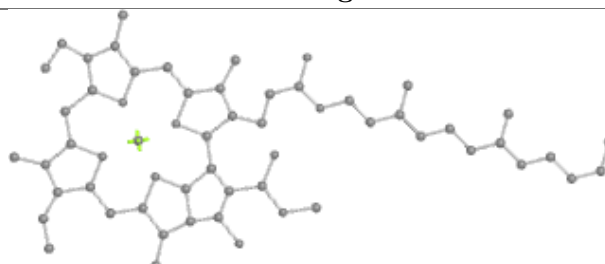


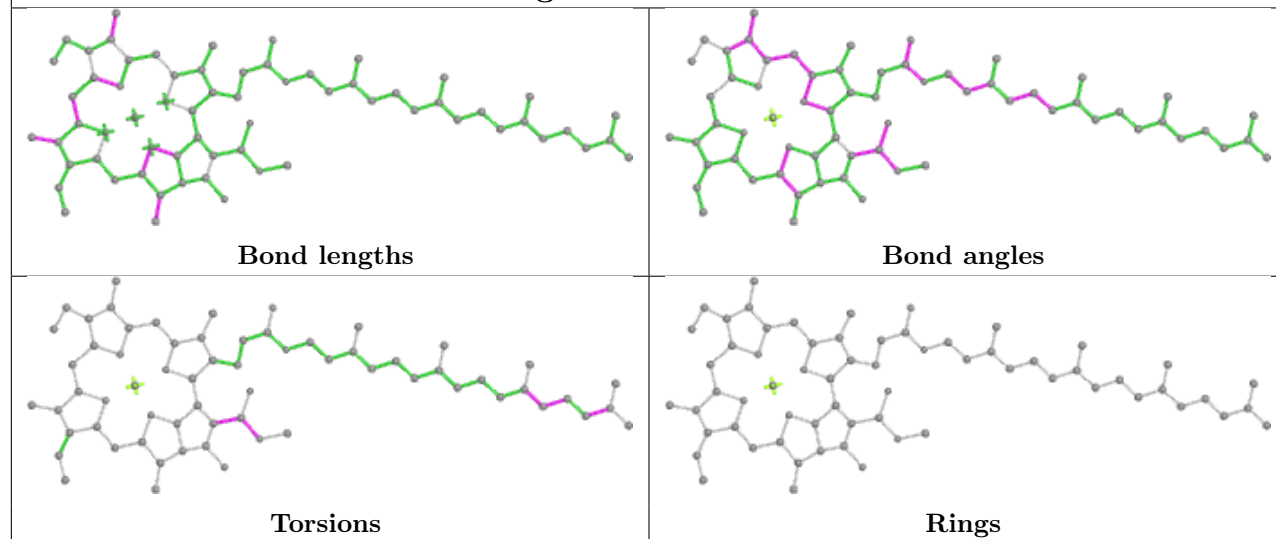
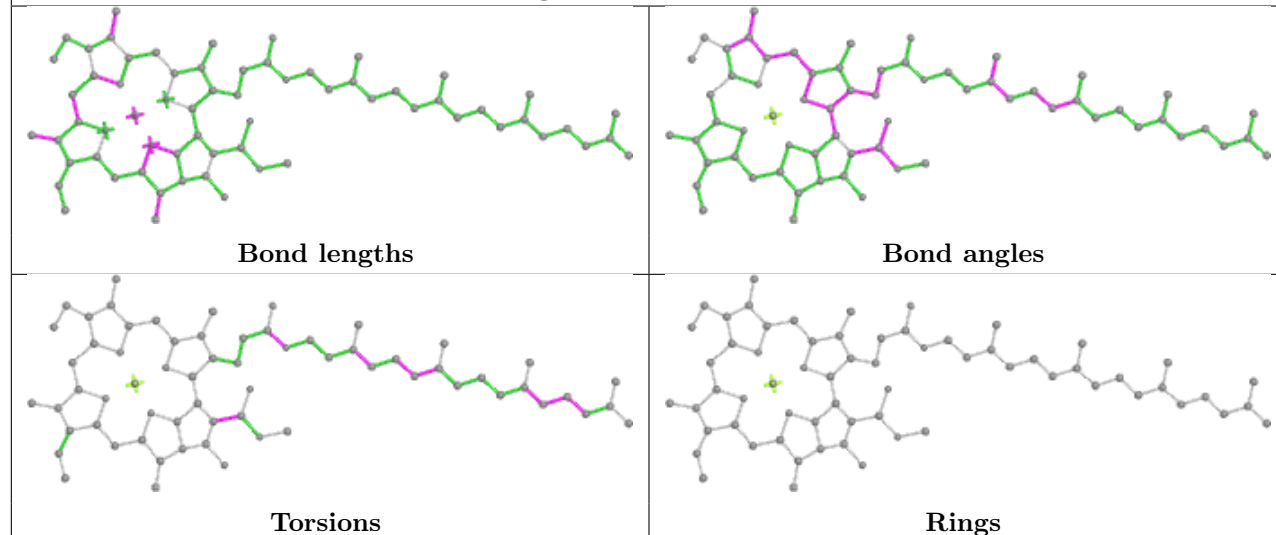
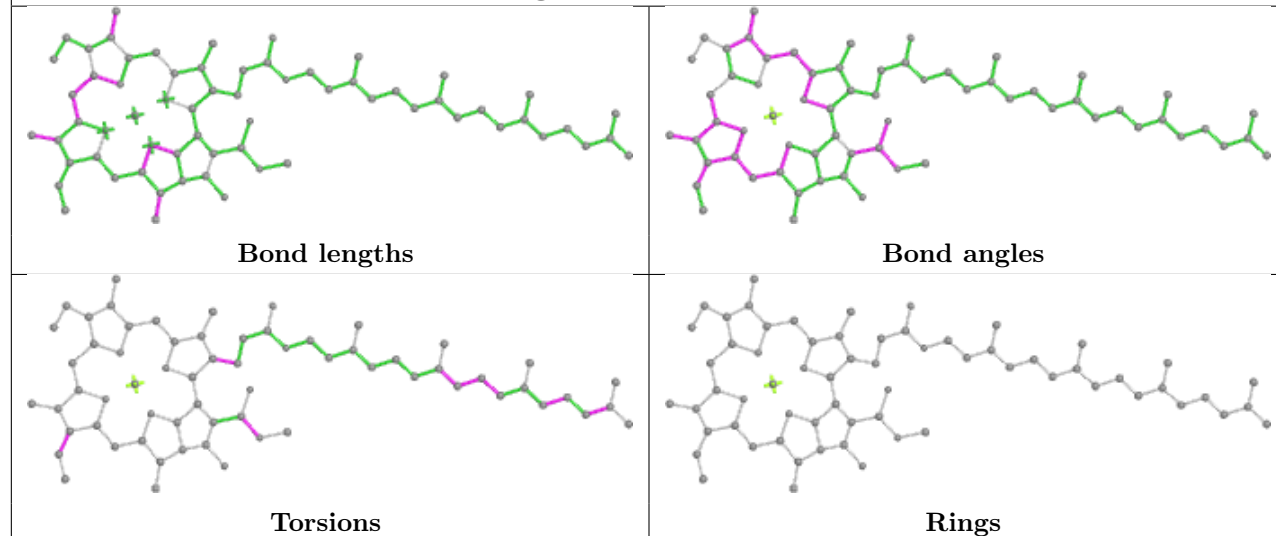
Torsions

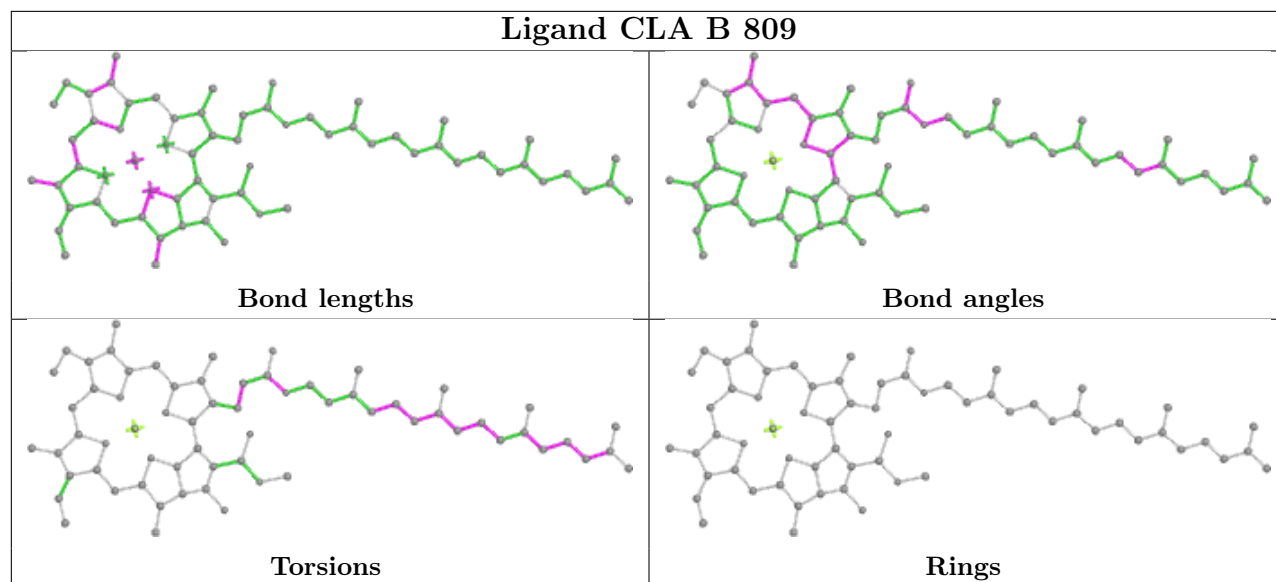
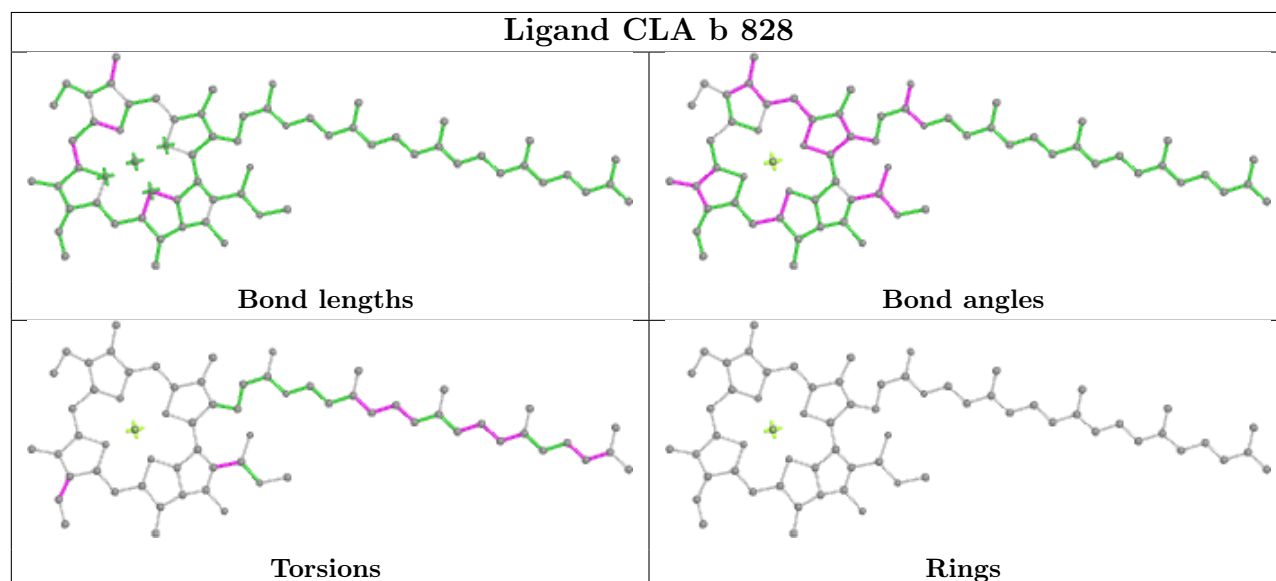


Rings

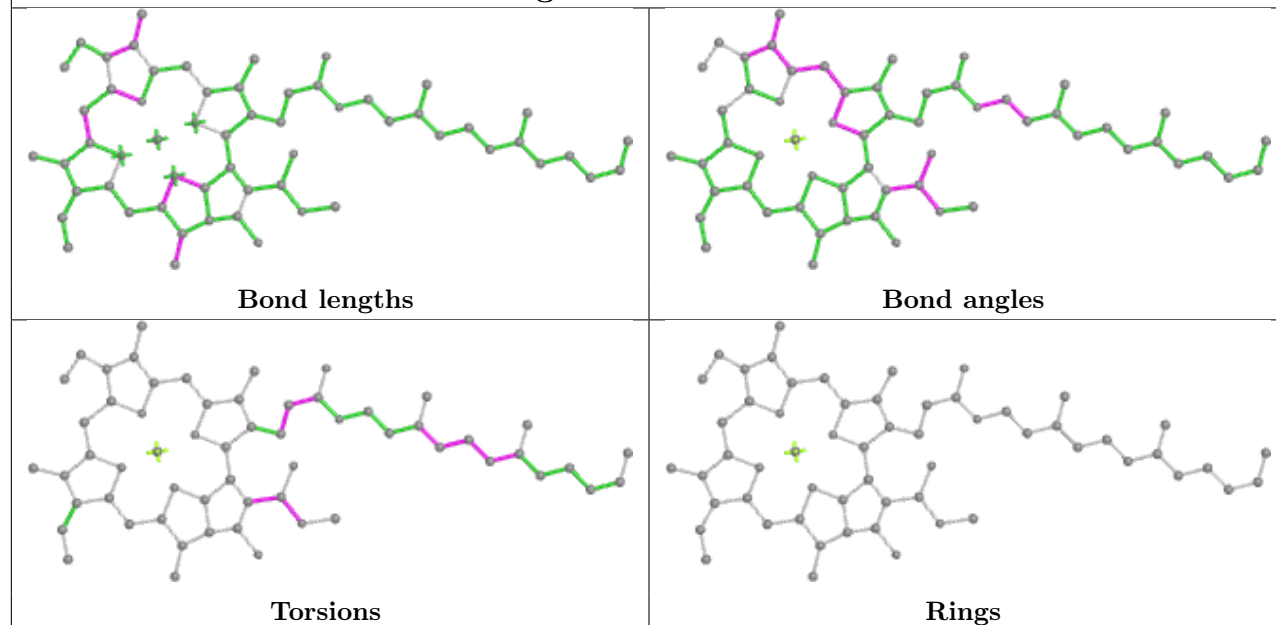


Ligand CLA b 829**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 840****Bond lengths****Bond angles****Torsions****Rings**

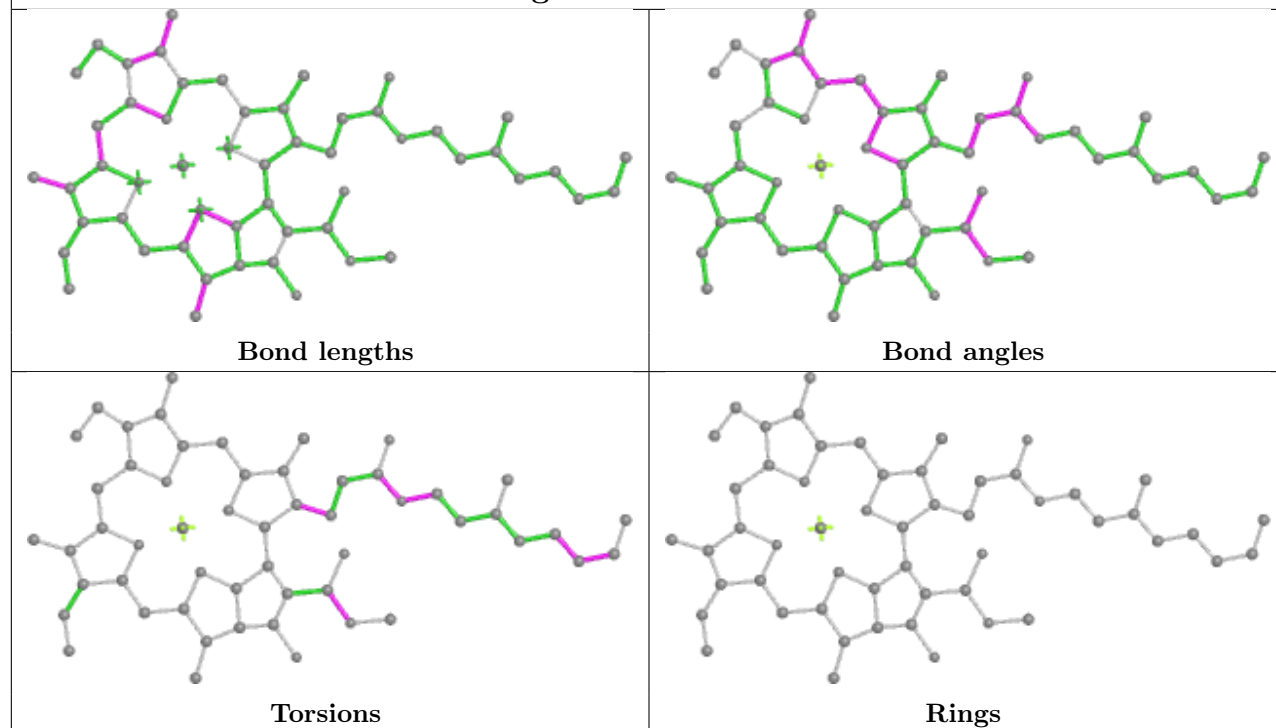
Ligand CLA a 832**Ligand CLA b 827****Ligand CLA B 806**

Ligand CLA B 809**Ligand CLA b 828**

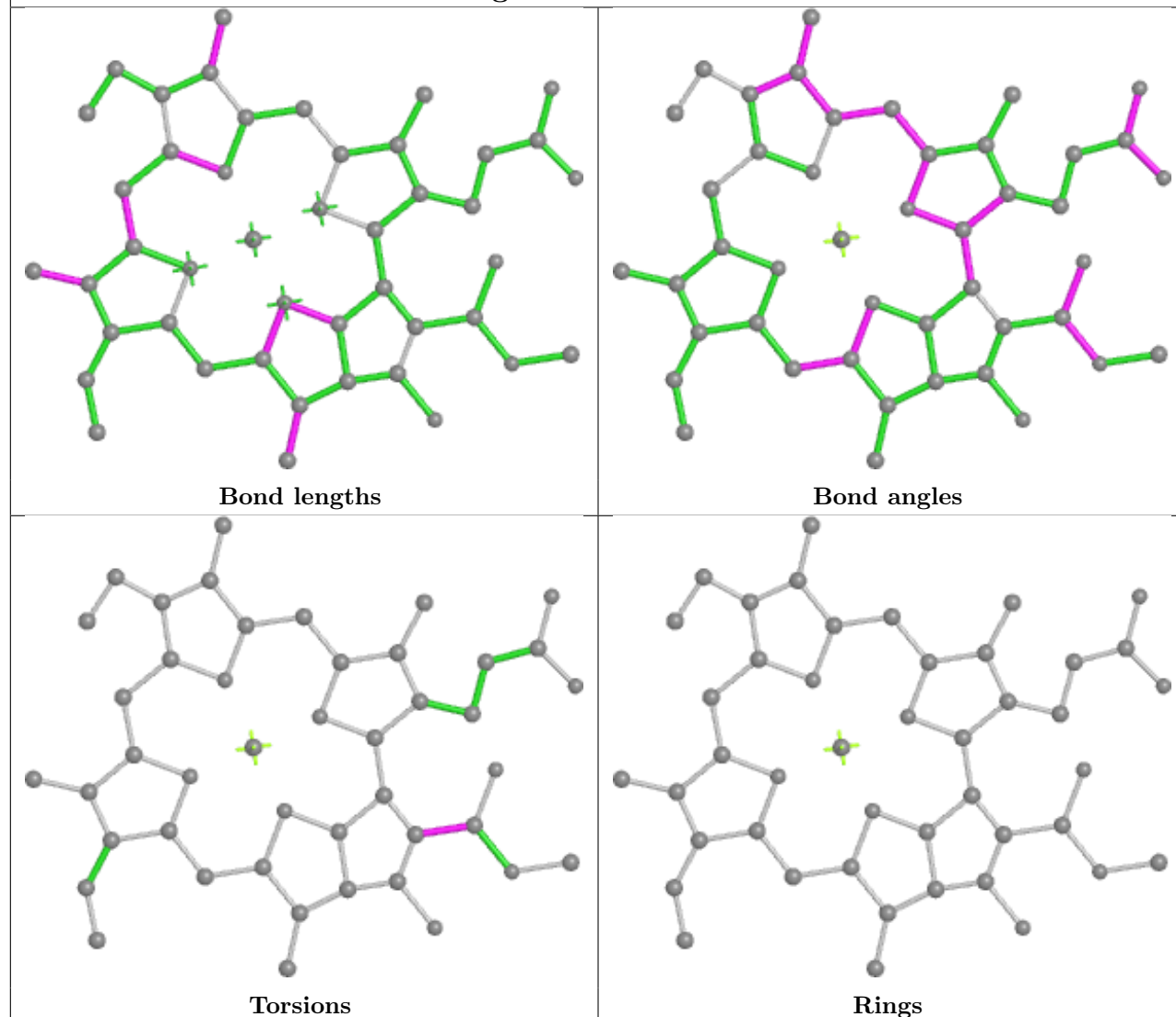
Ligand CLA a 811



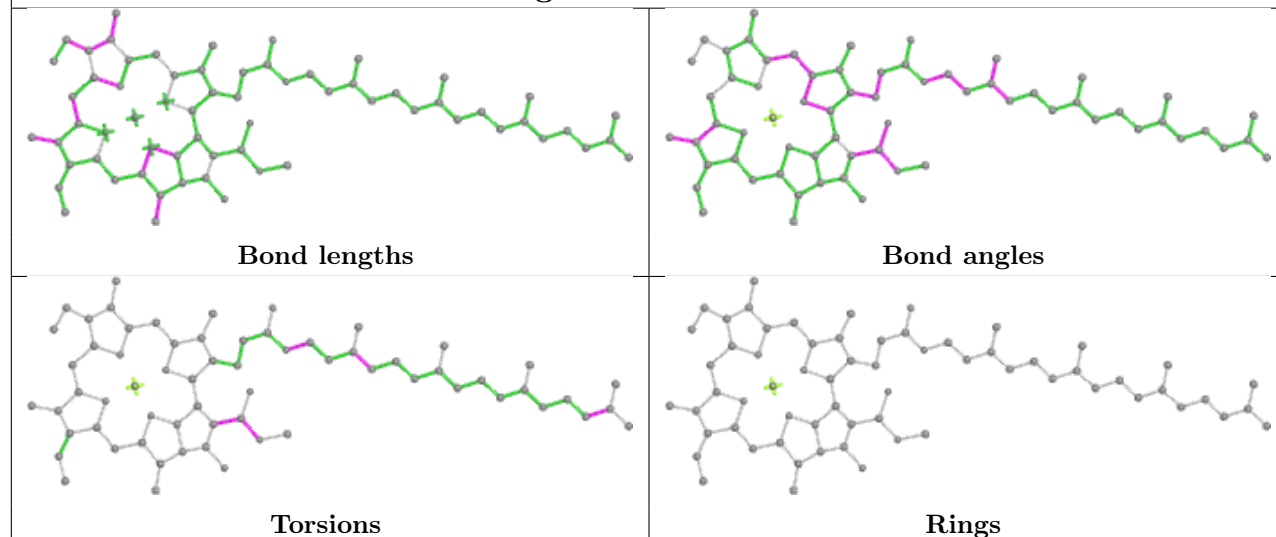
Ligand CLA A 835



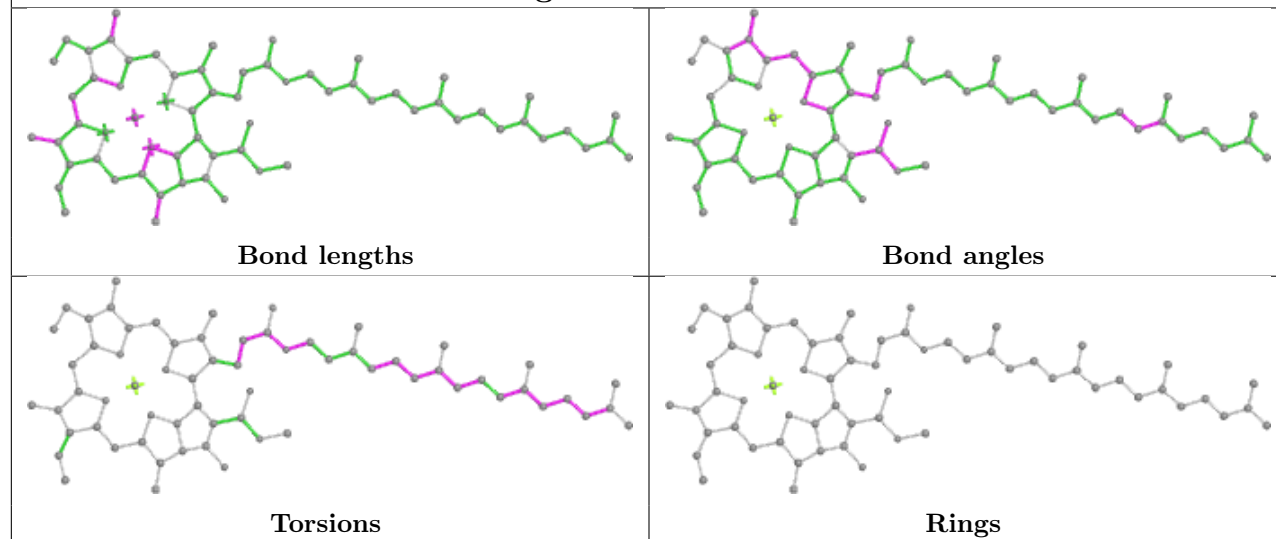
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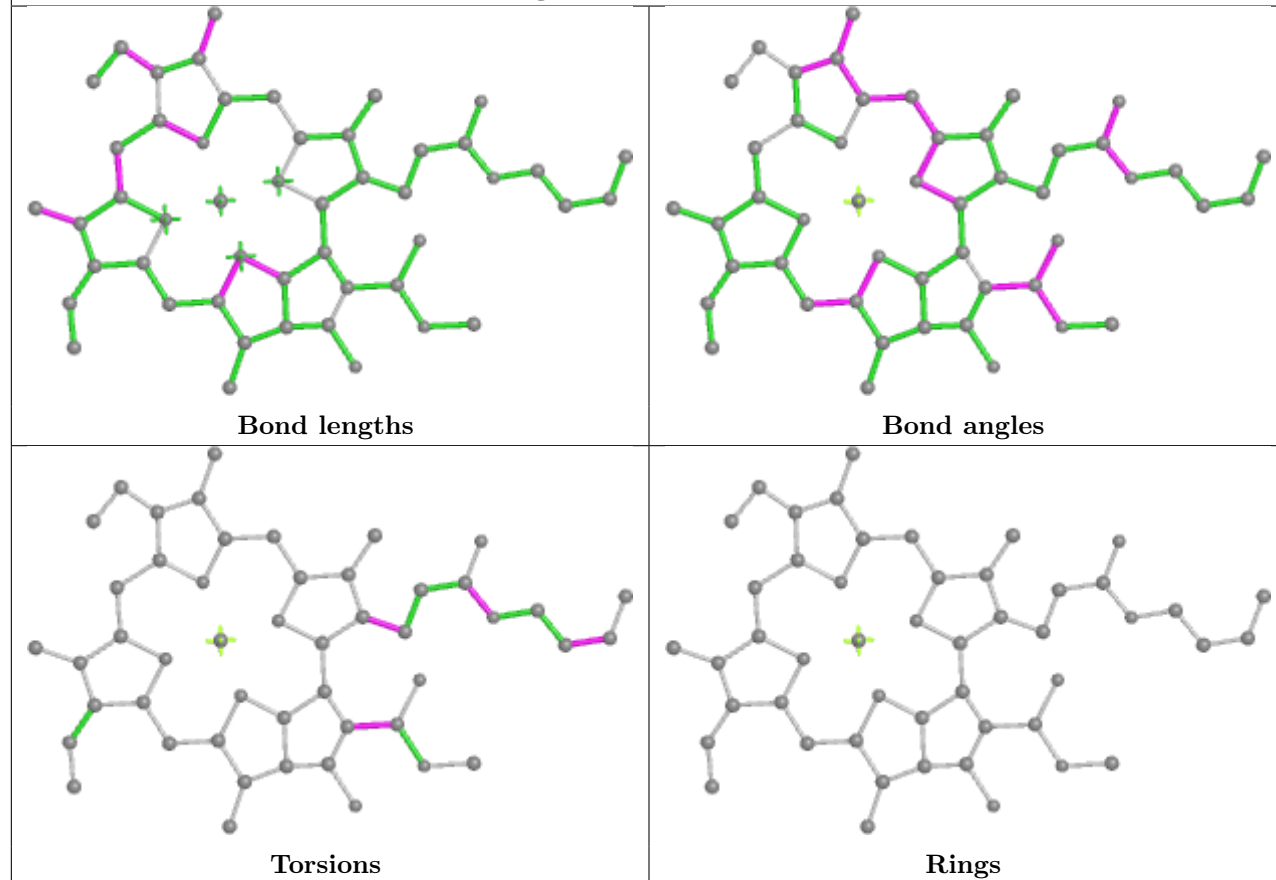
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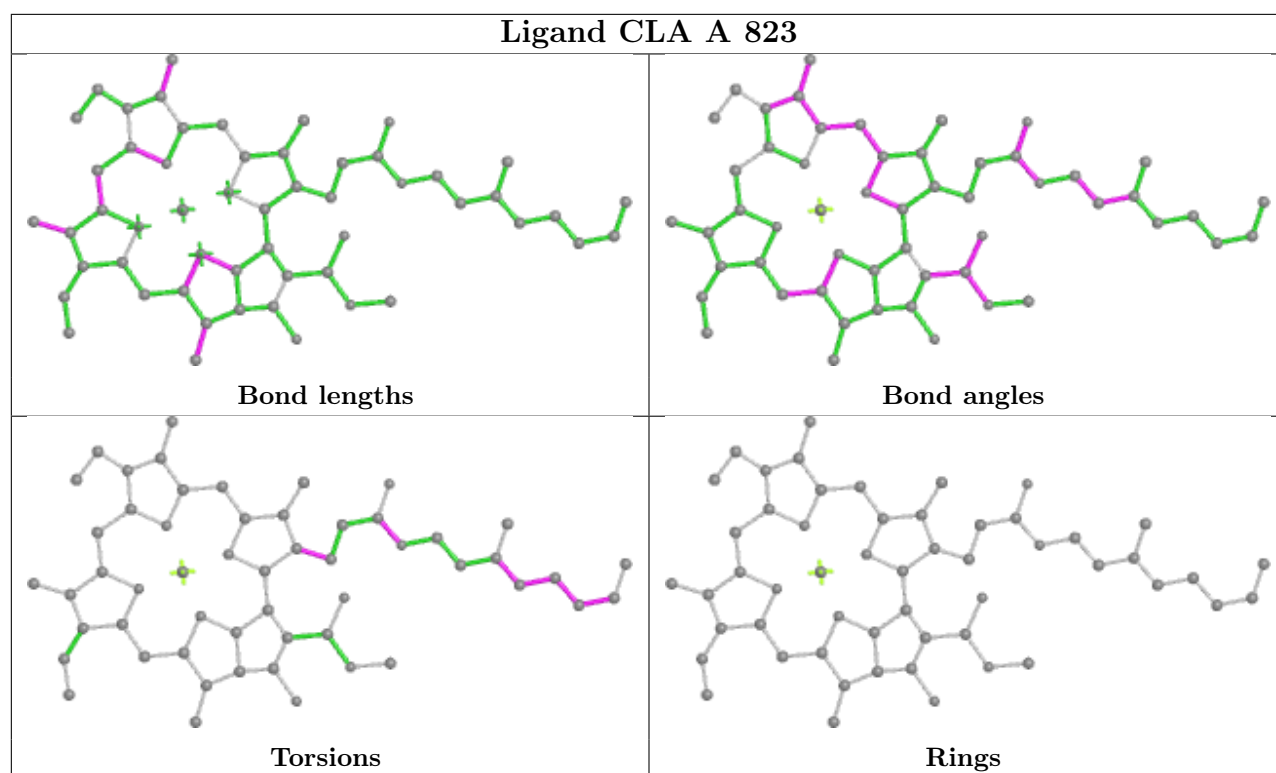


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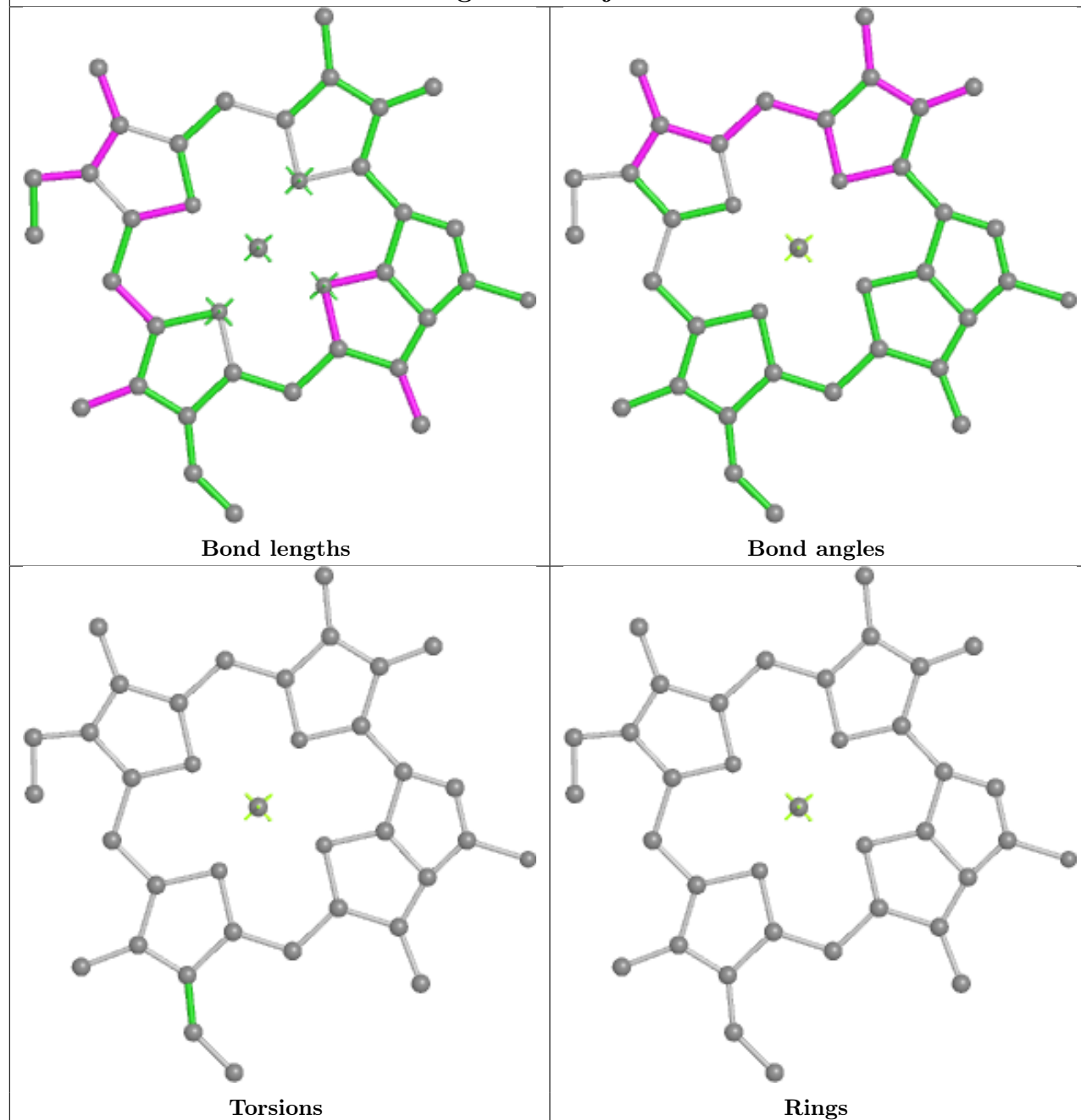


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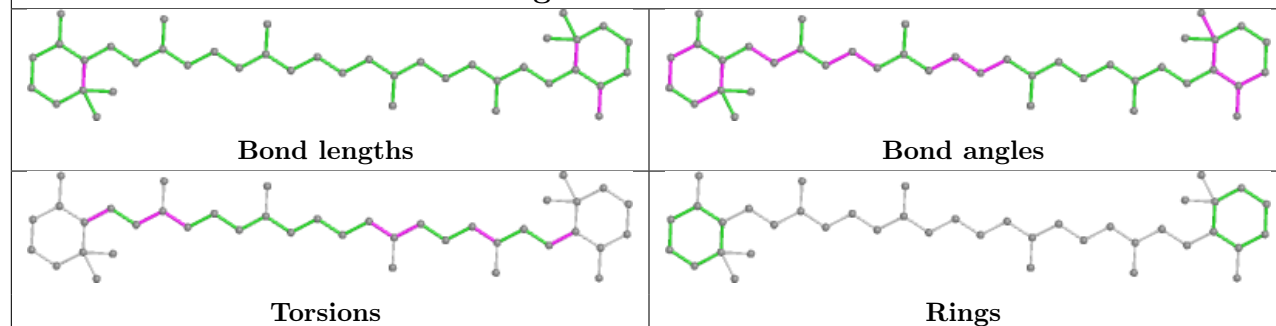




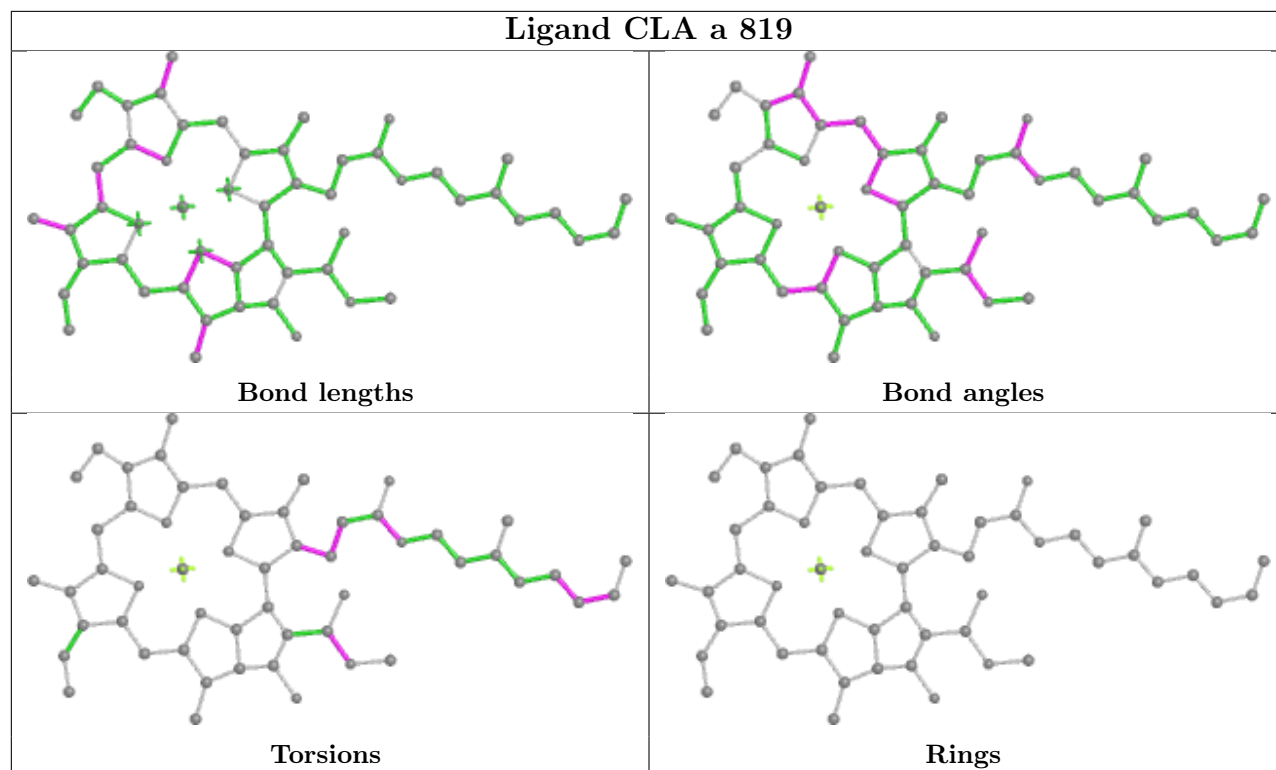
Ligand CLA j 103



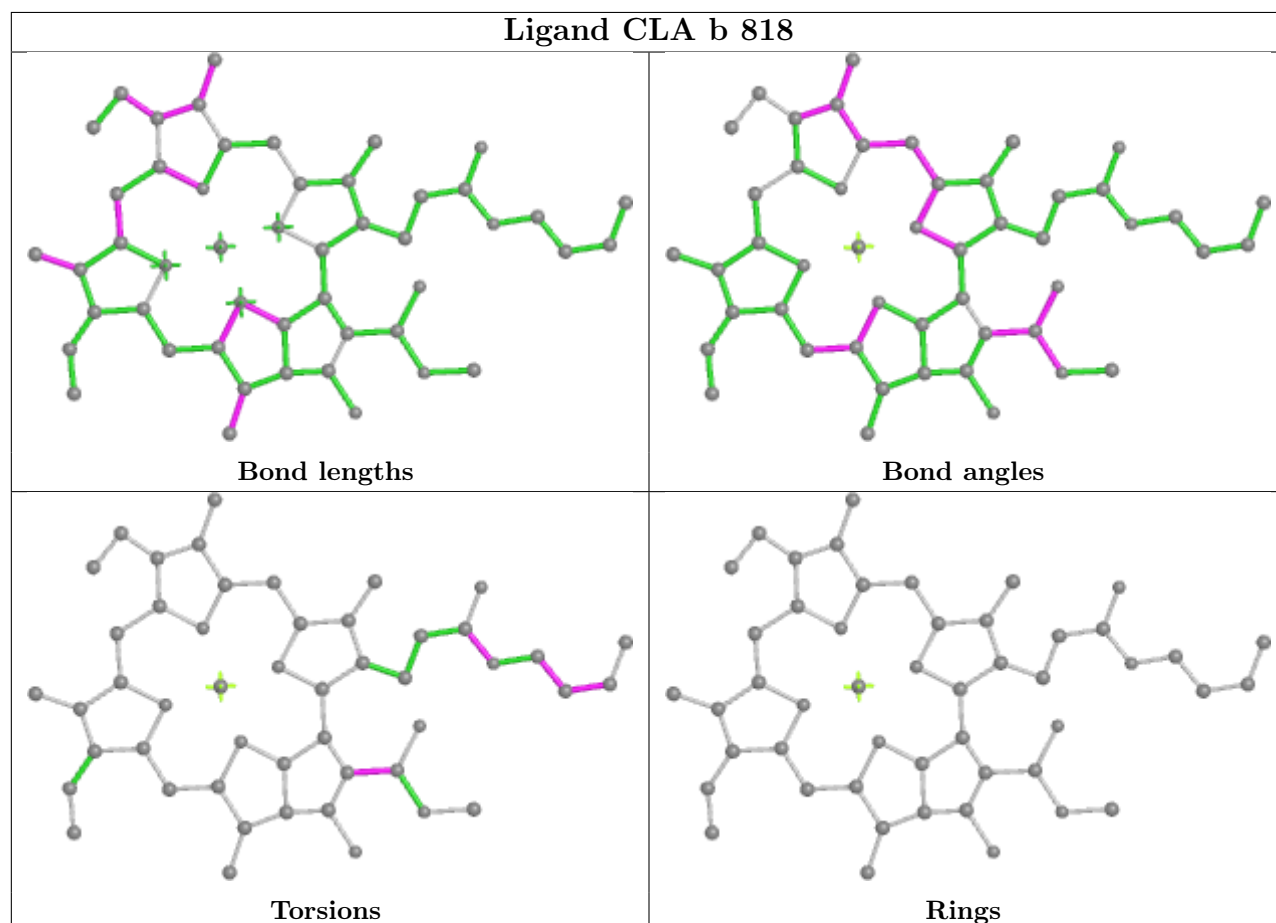
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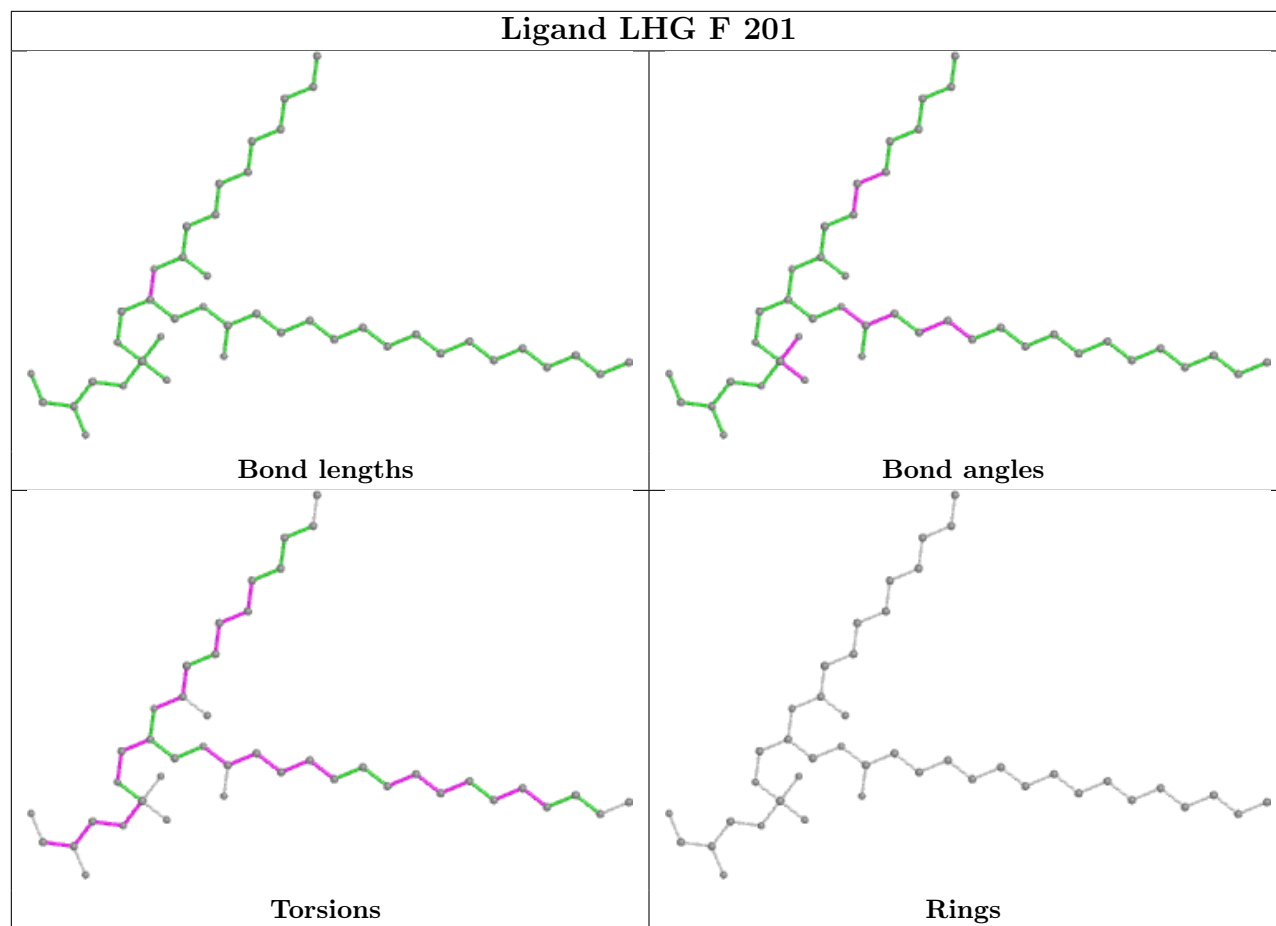
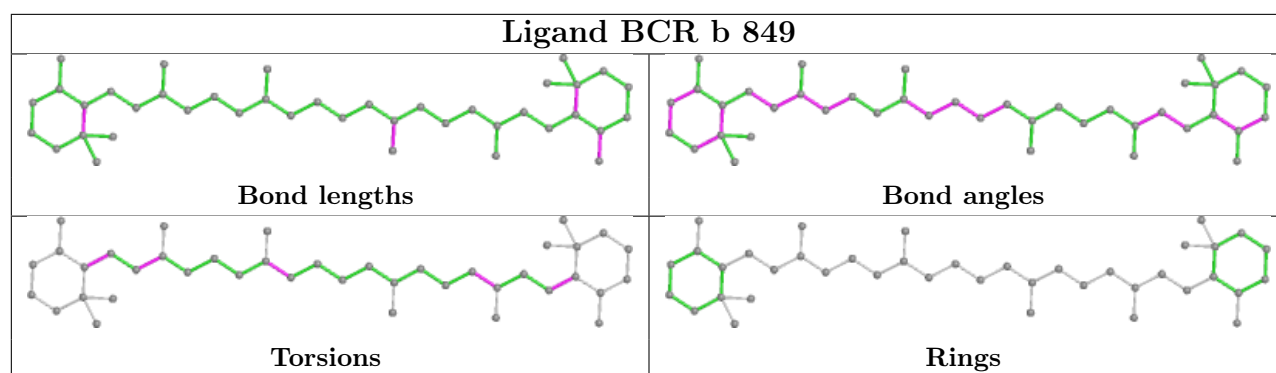


Ligand CLA a 819

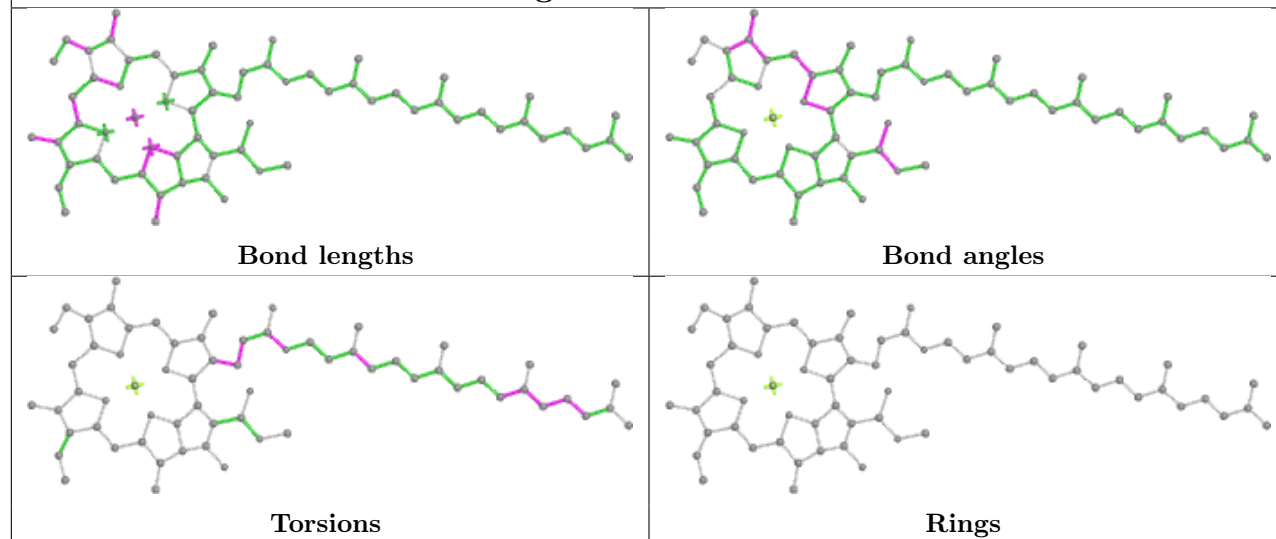


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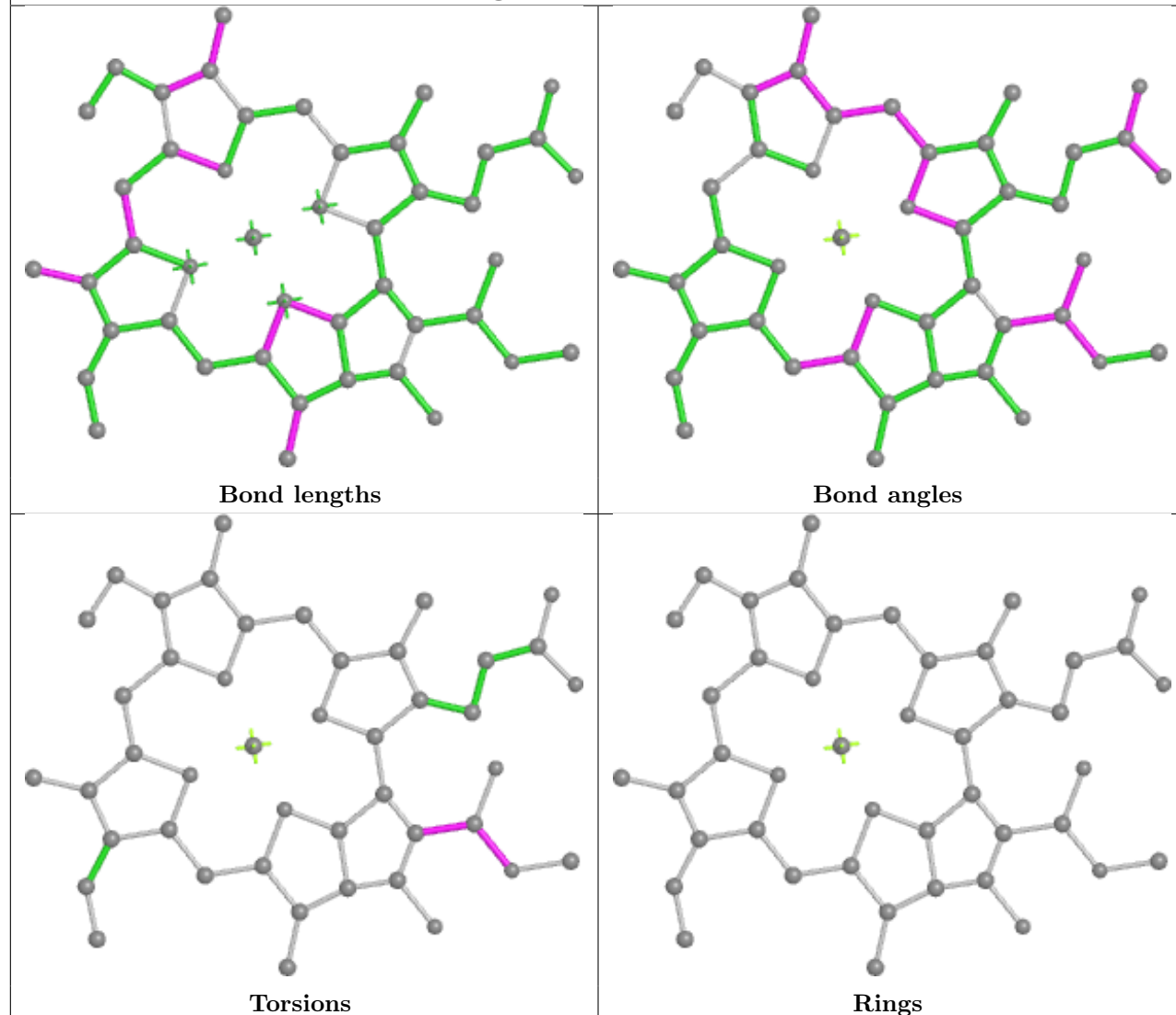


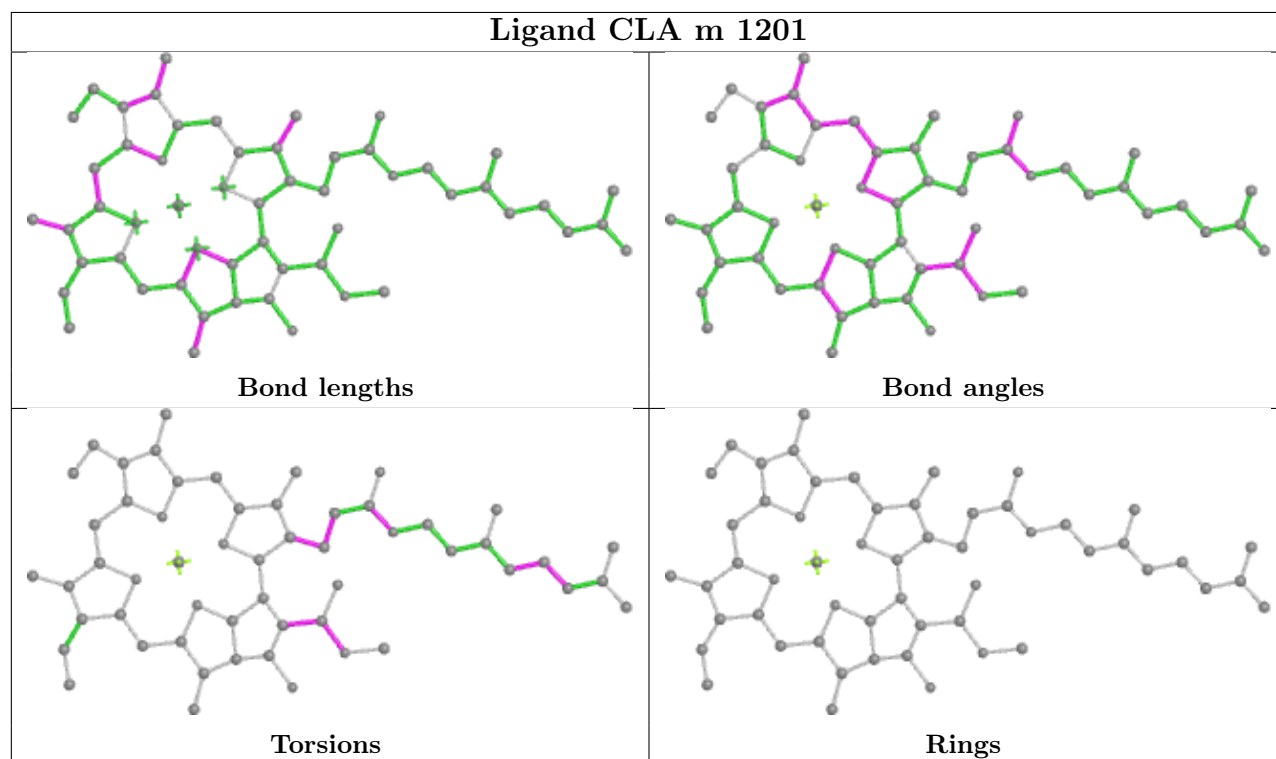
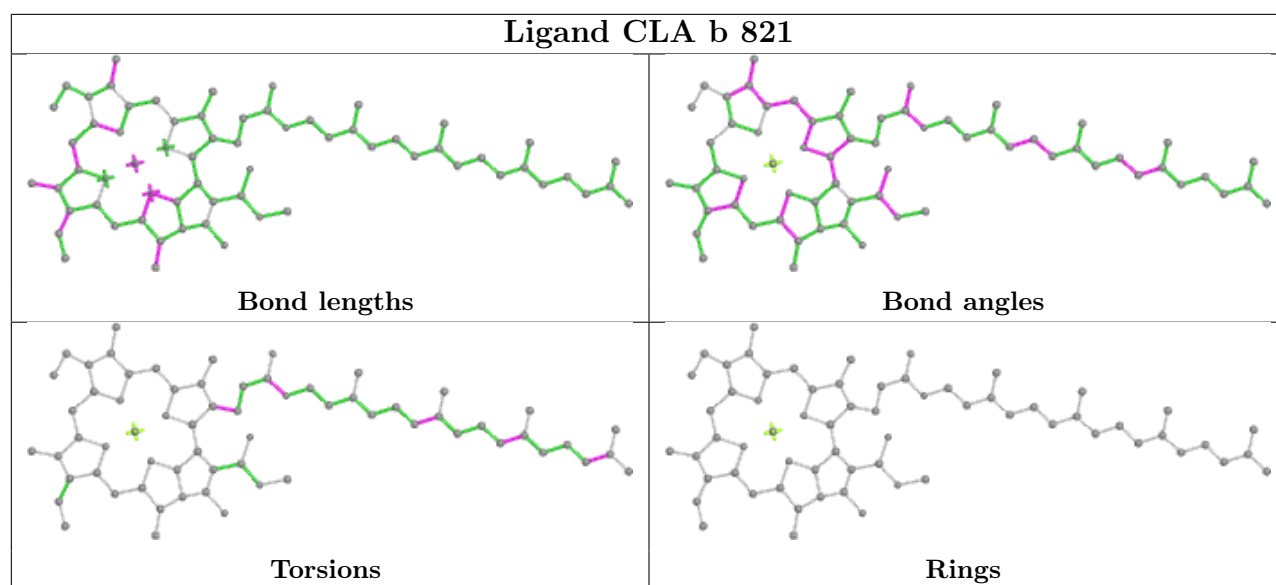


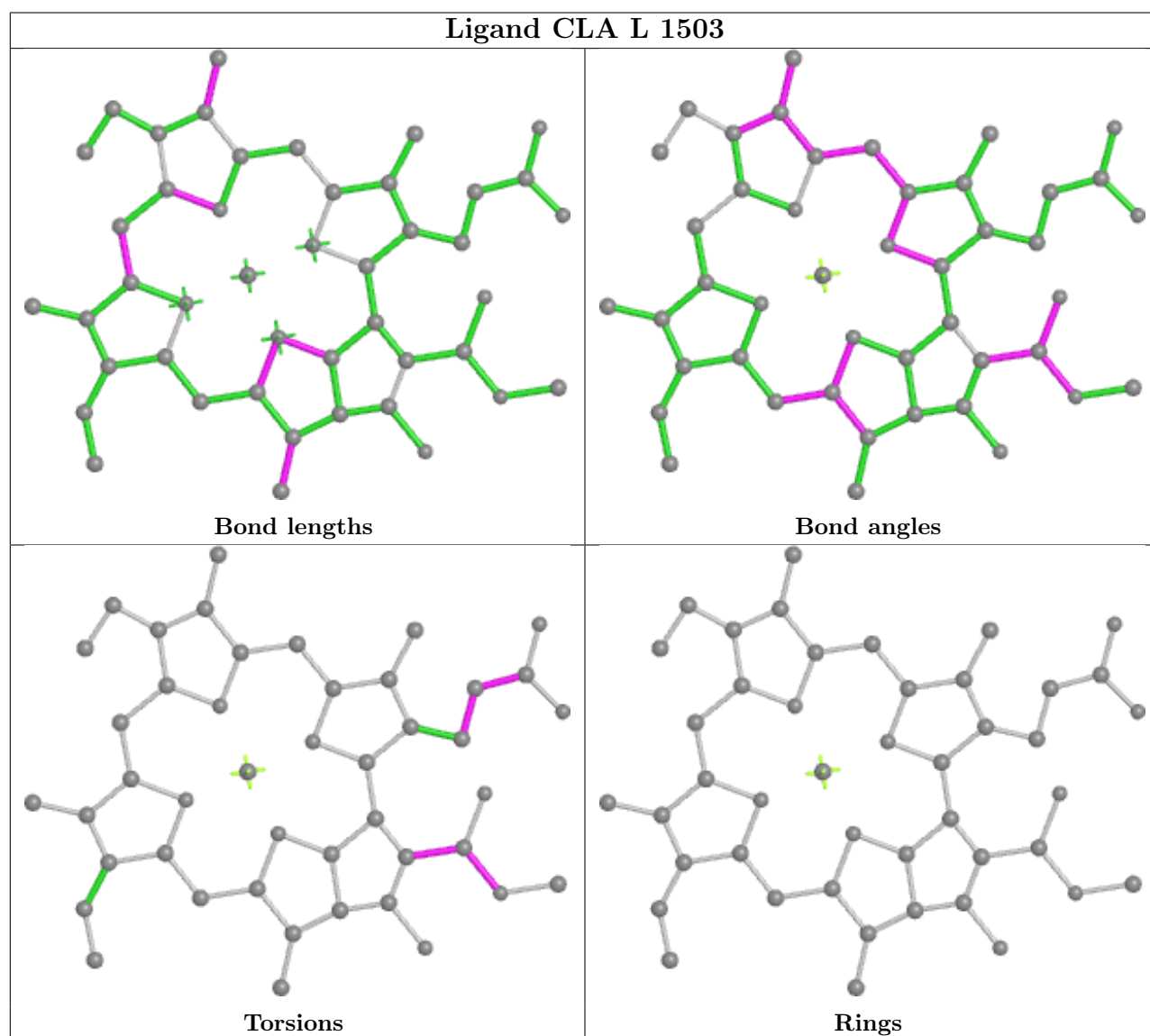
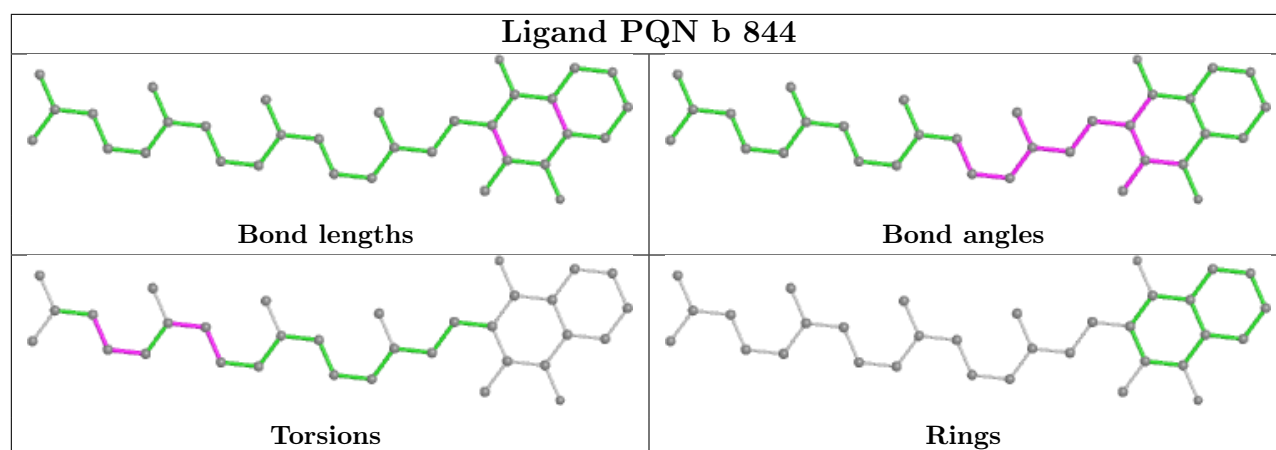
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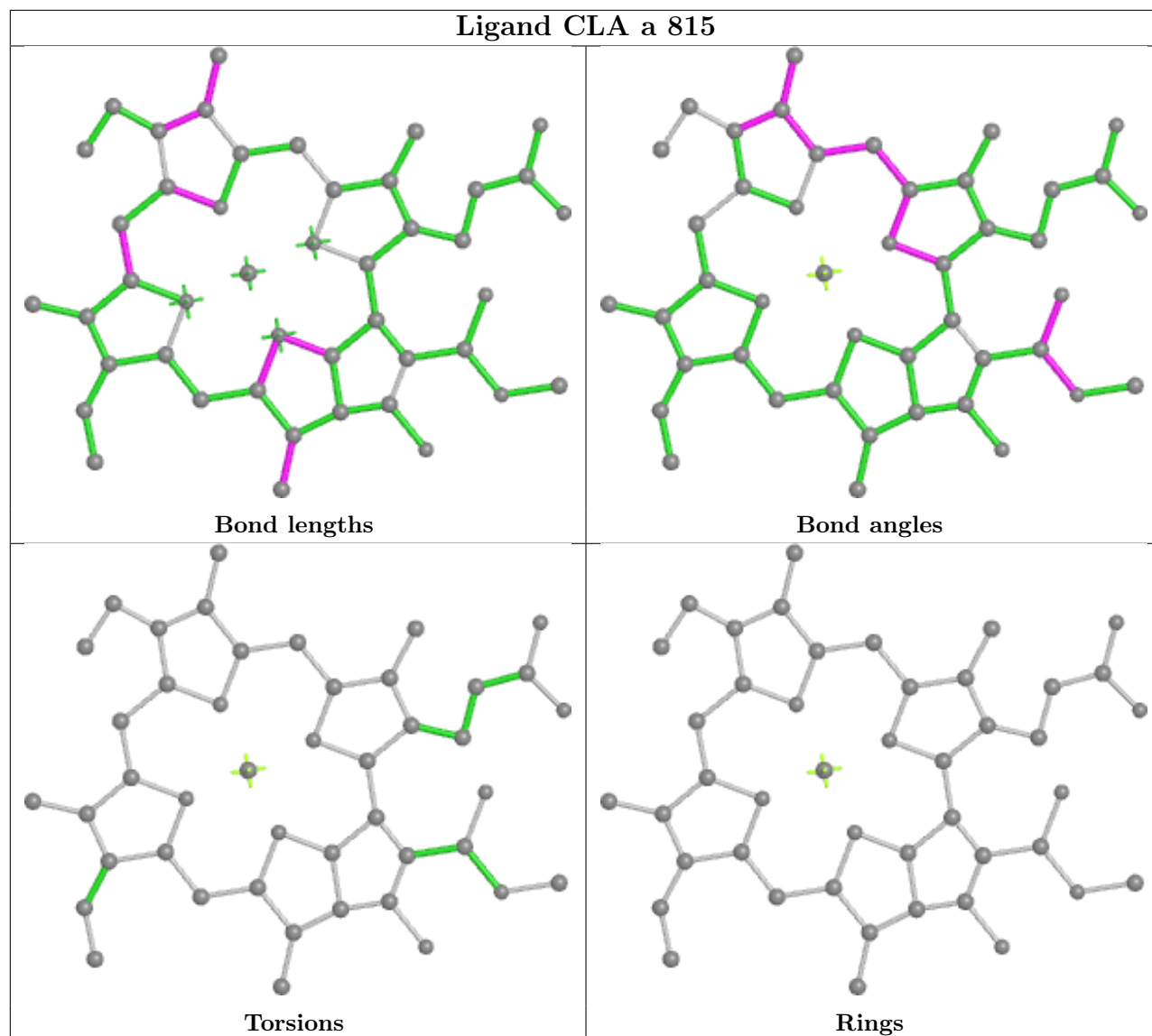
Ligand CLA B 838



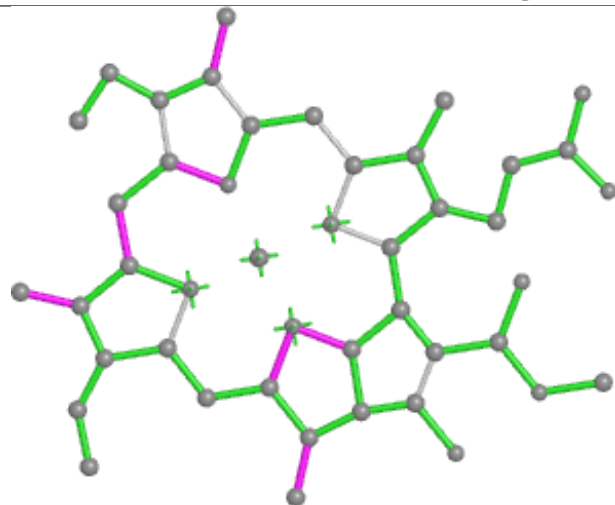




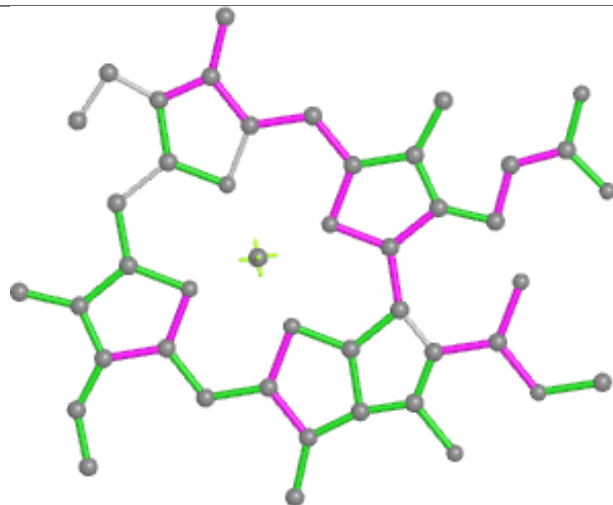
Ligand CLA a 815



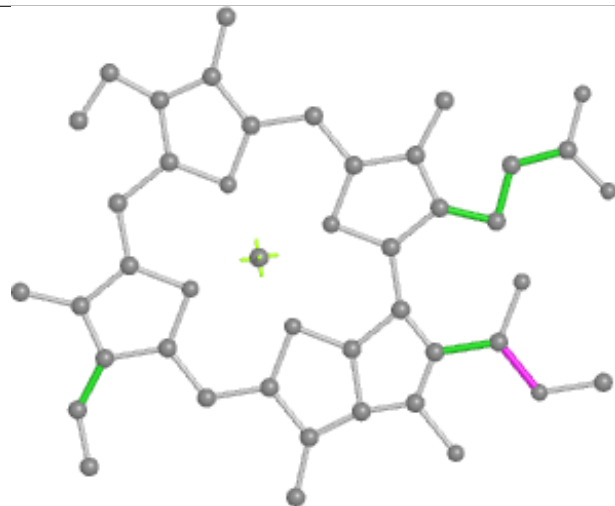
Ligand CLA B 837



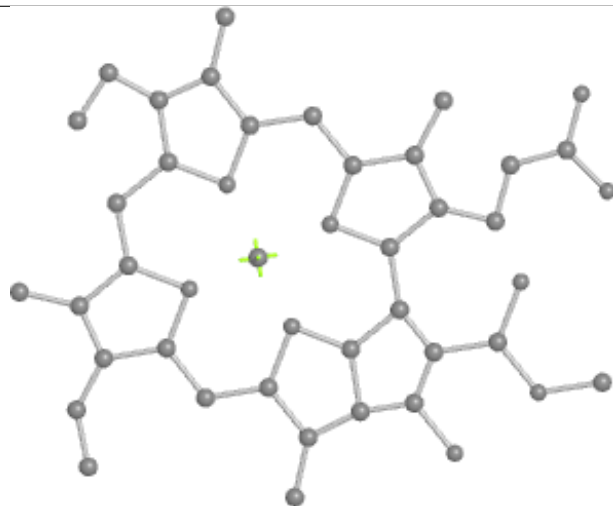
Bond lengths



Bond angles

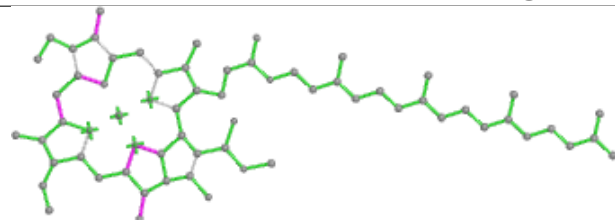


Torsions

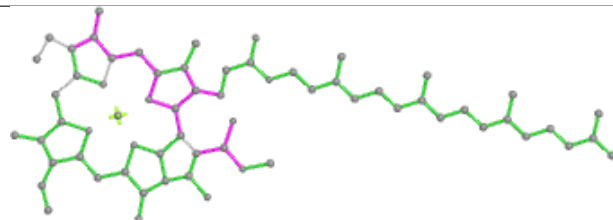


Rings

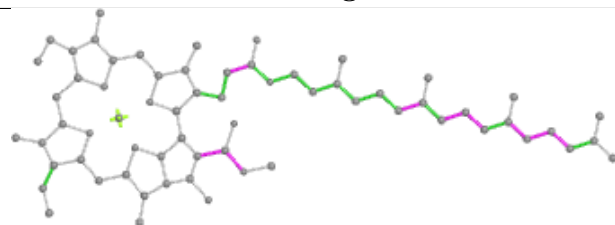
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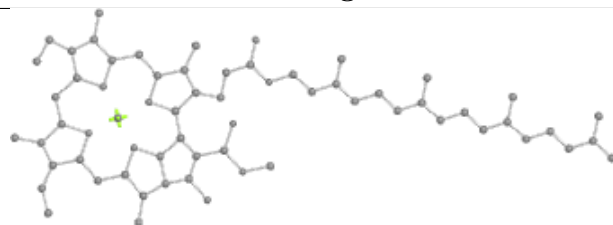
Bond lengths



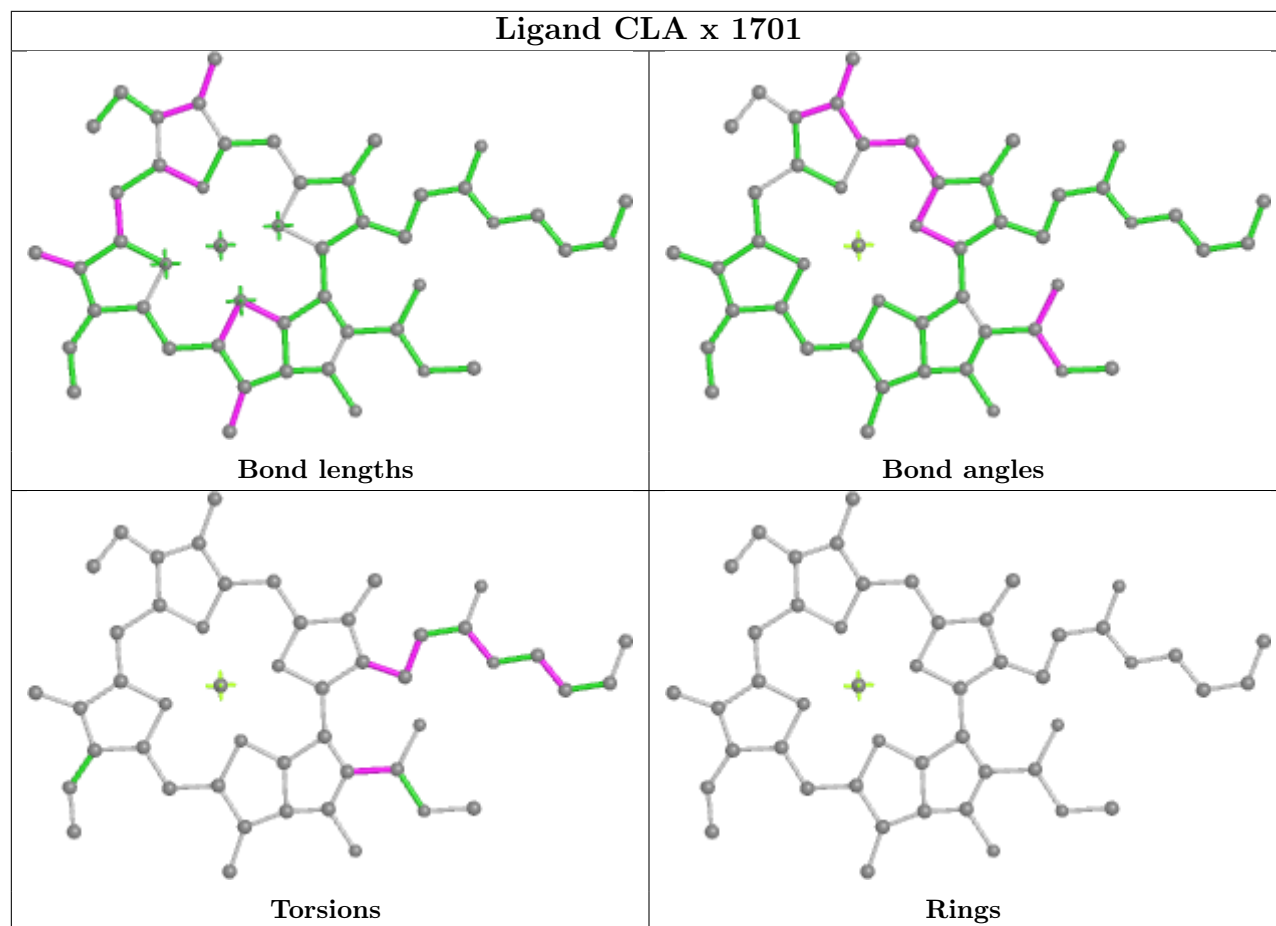
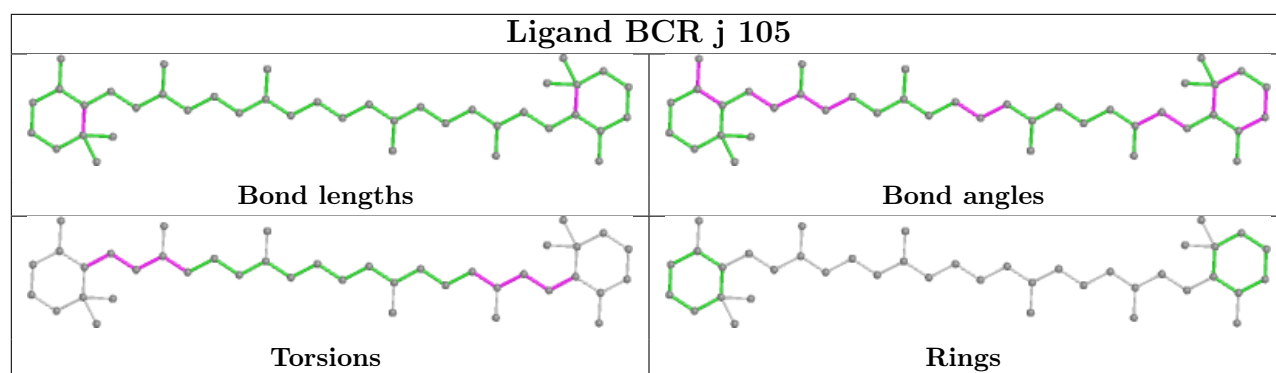
Bond angles



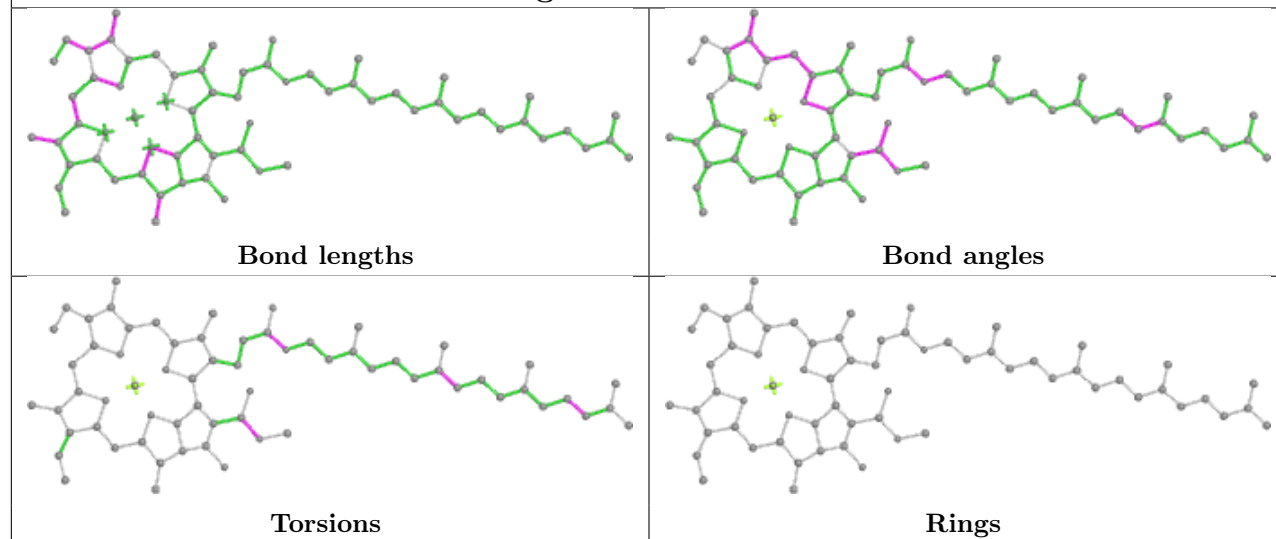
Torsions



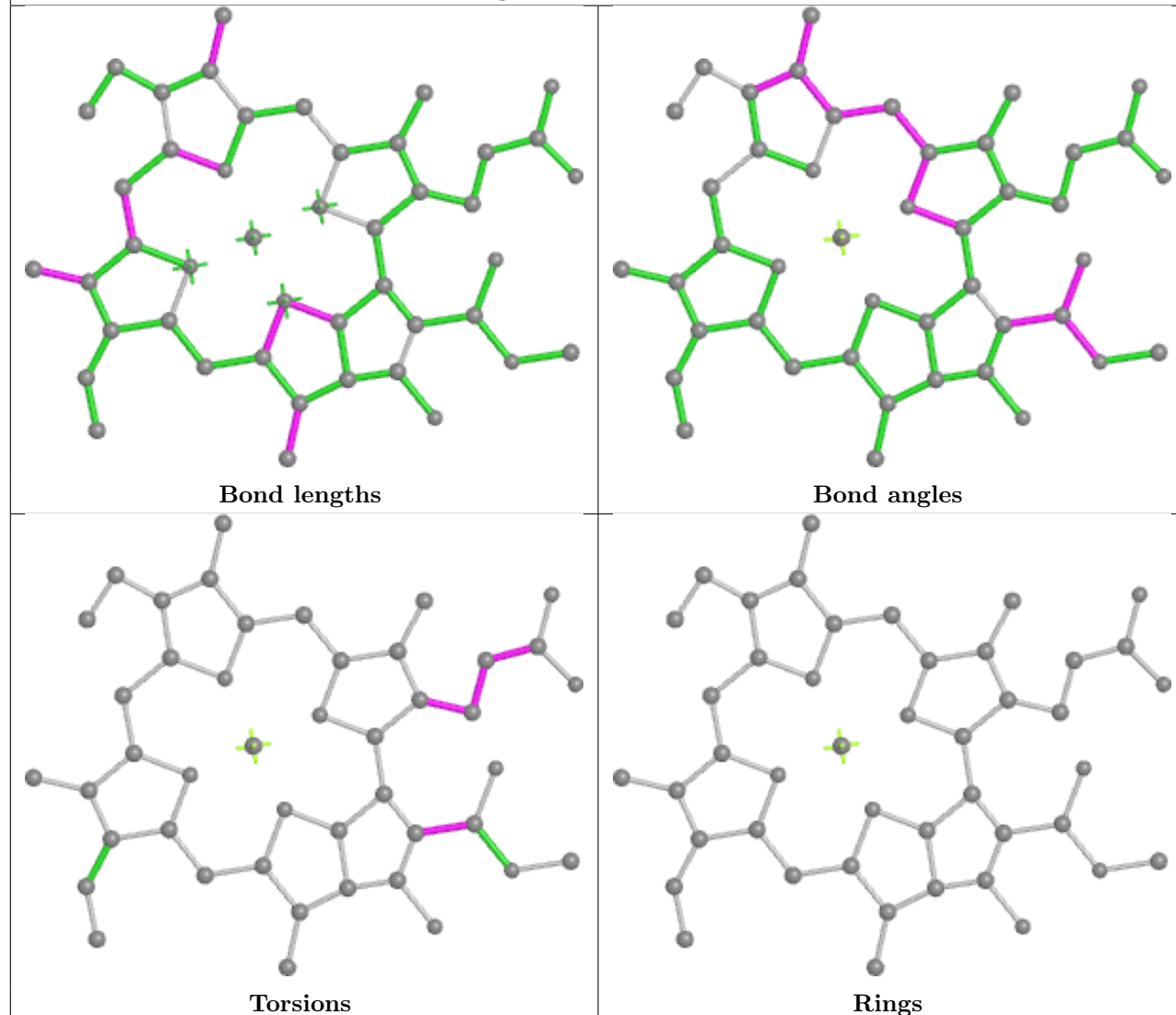
Rings

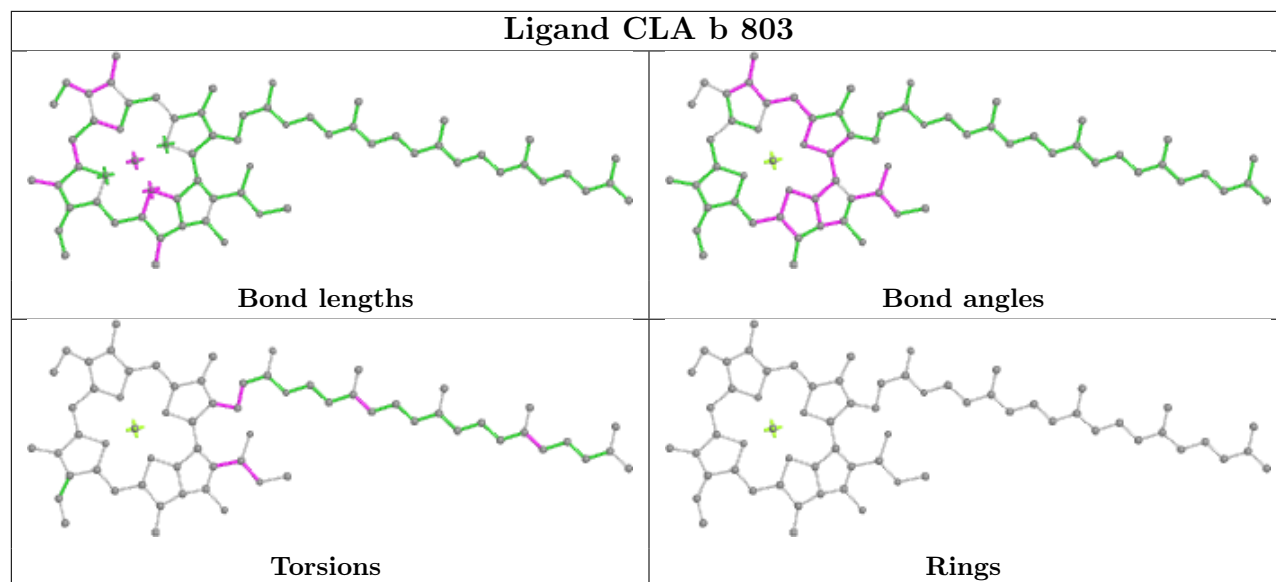
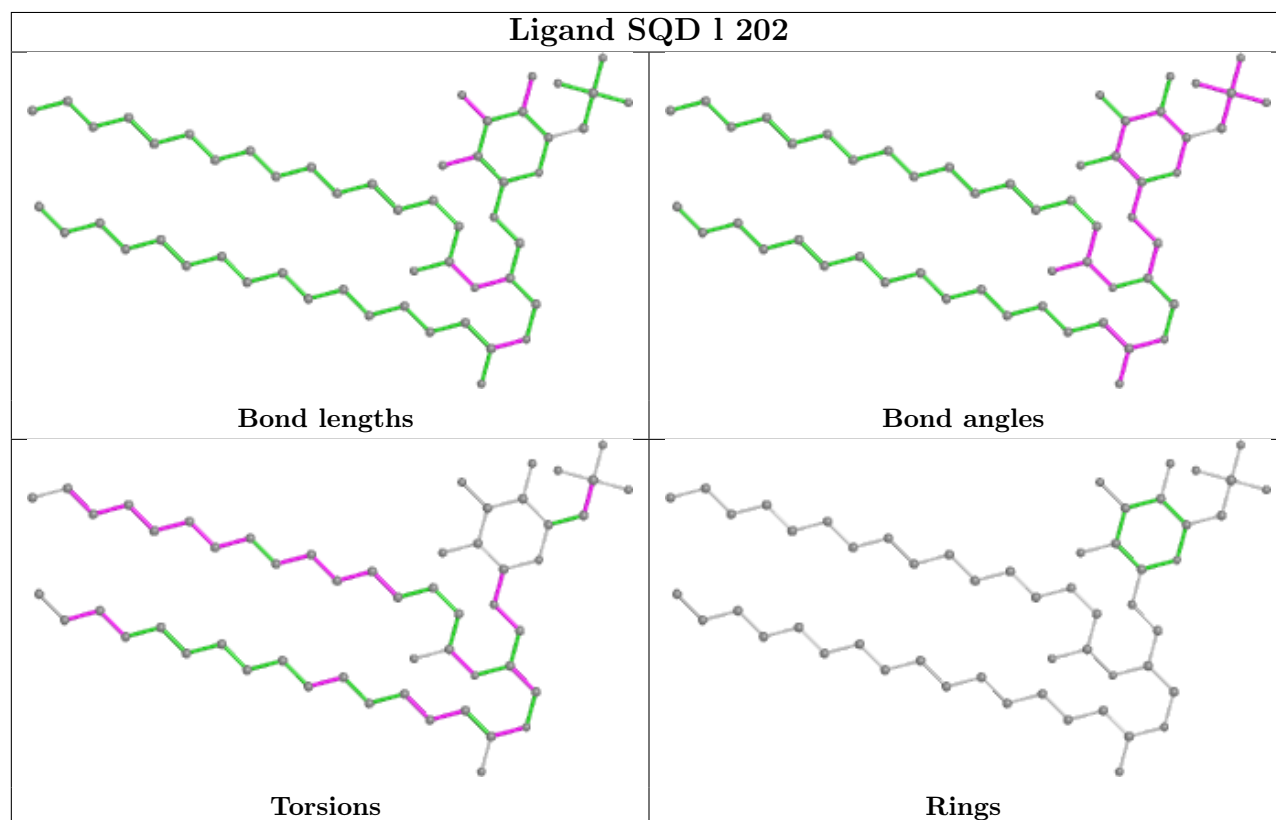


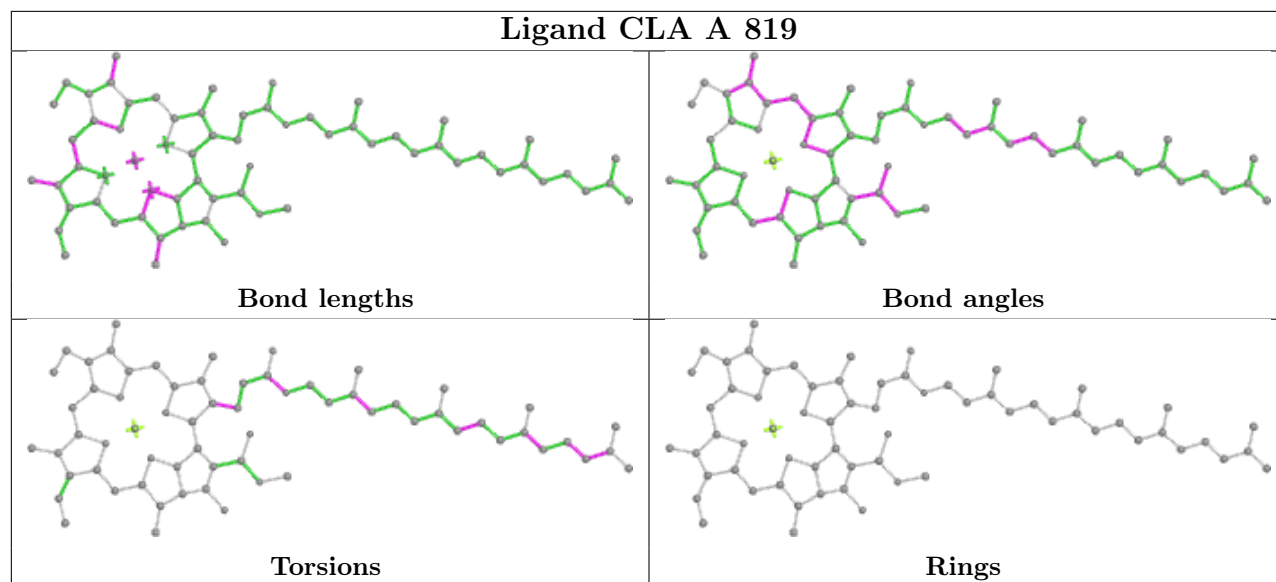
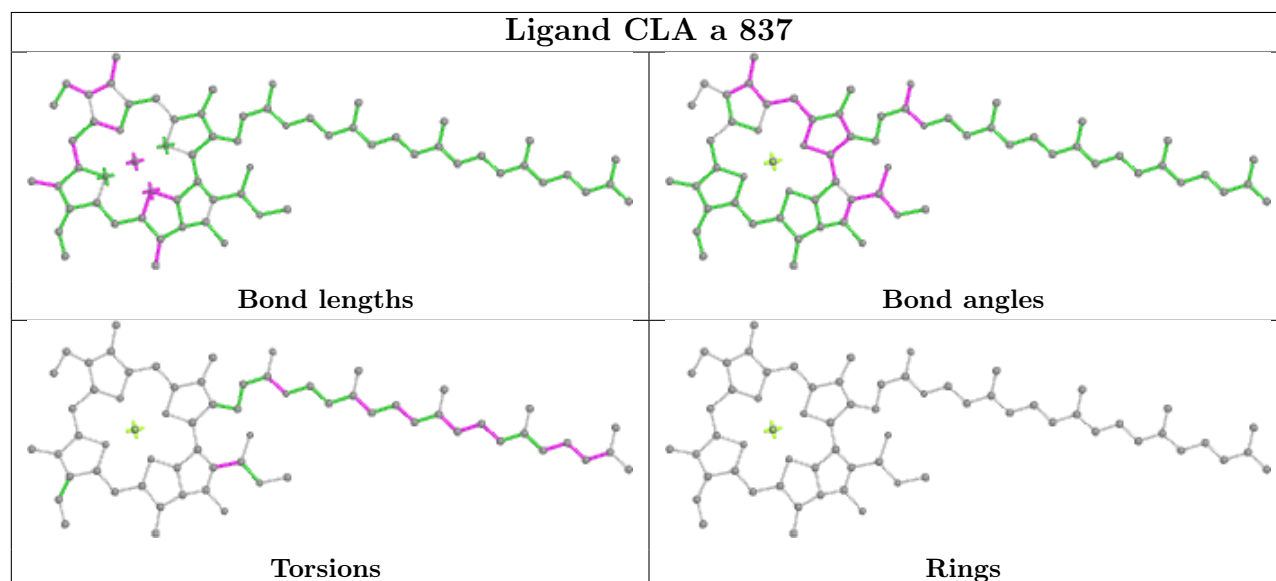
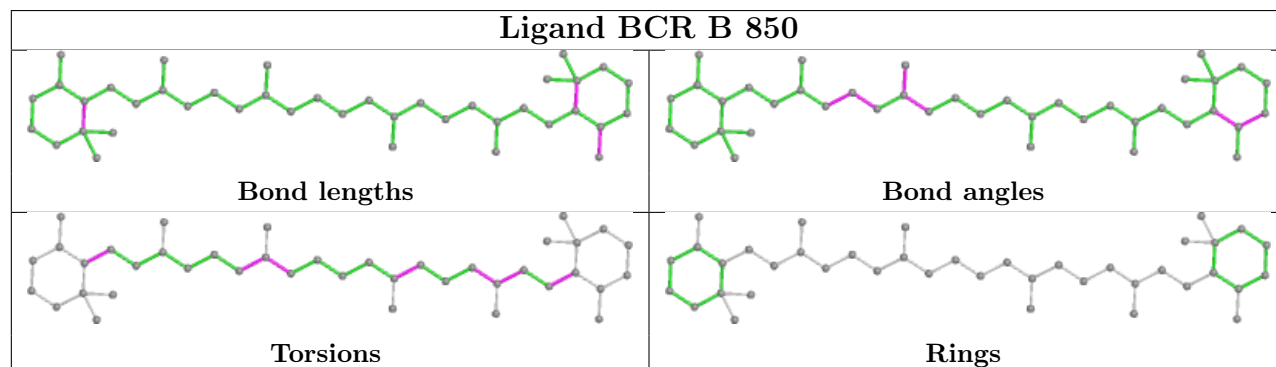
Ligand CLA a 810

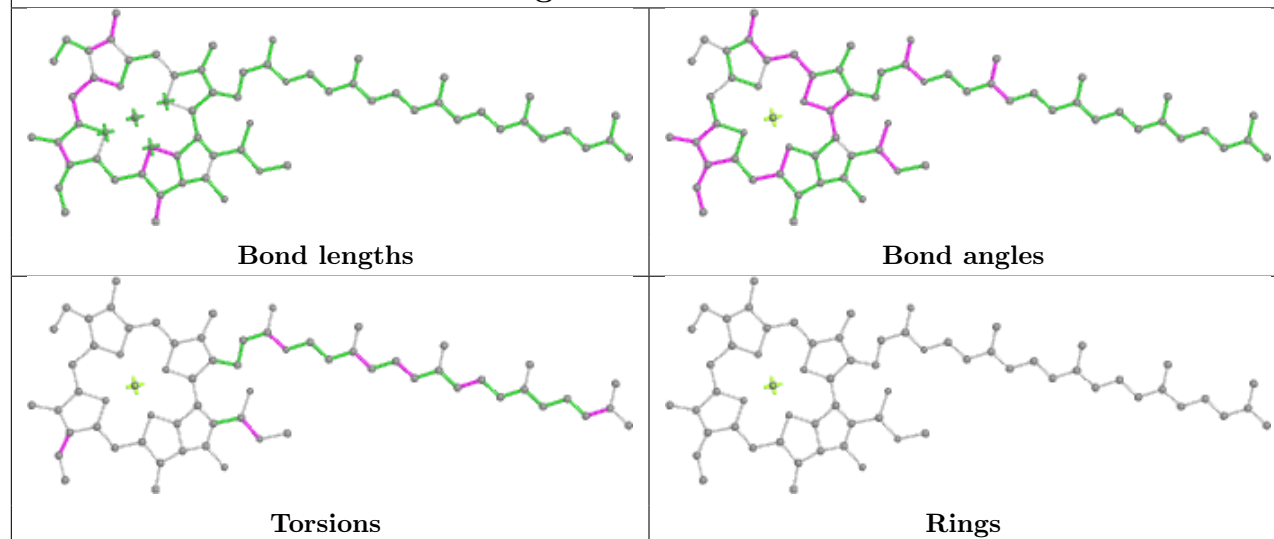
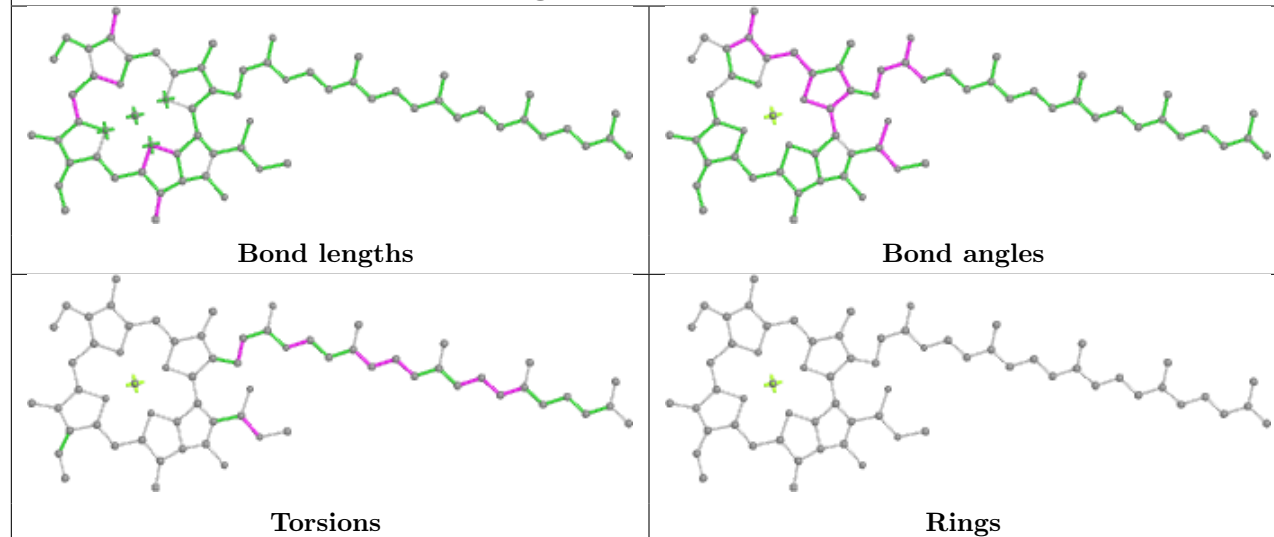
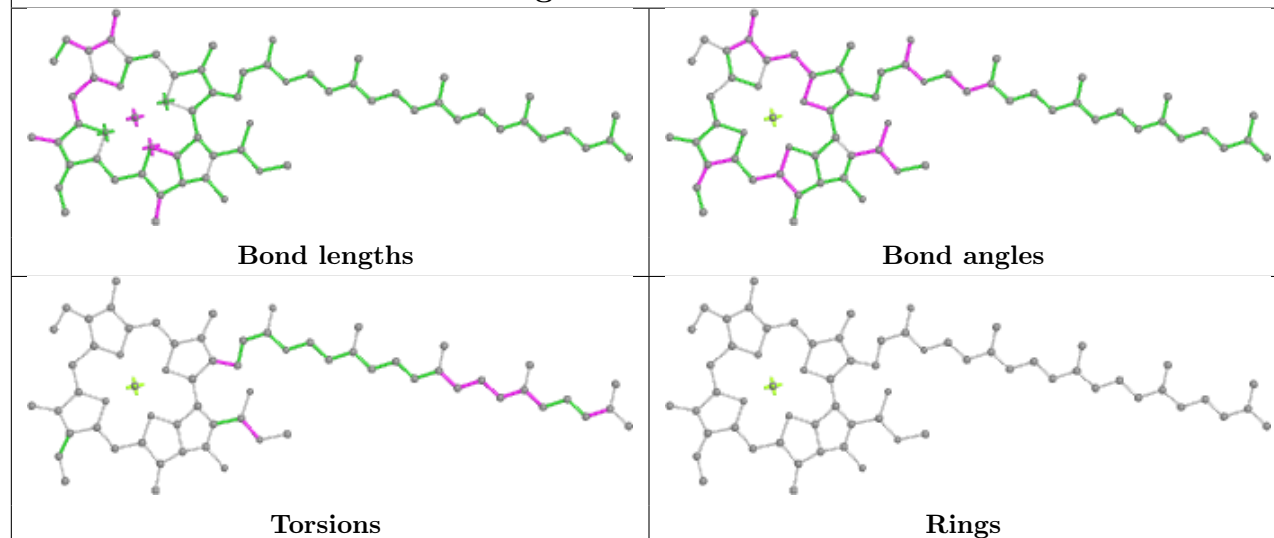


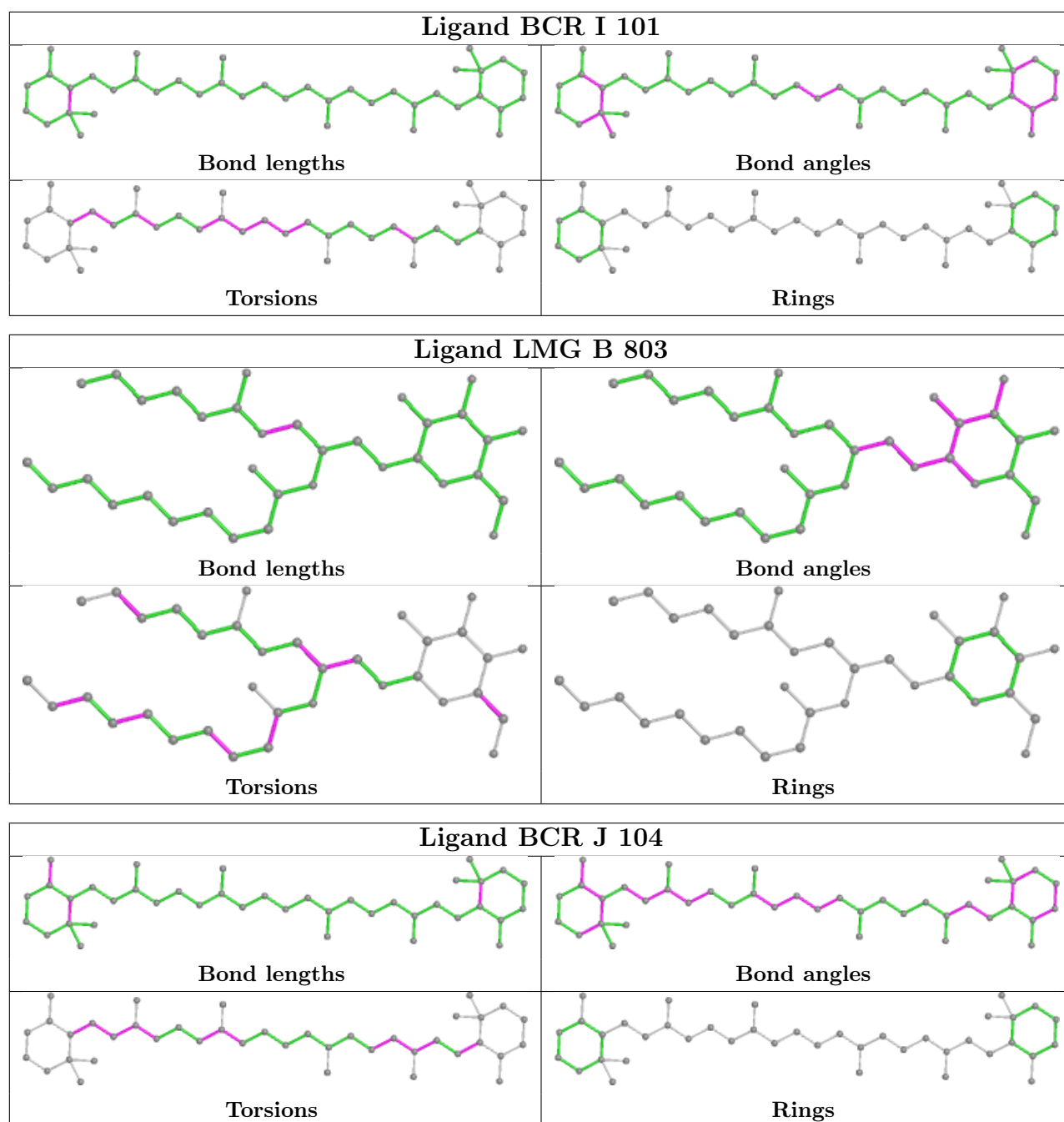
Ligand CLA a 835



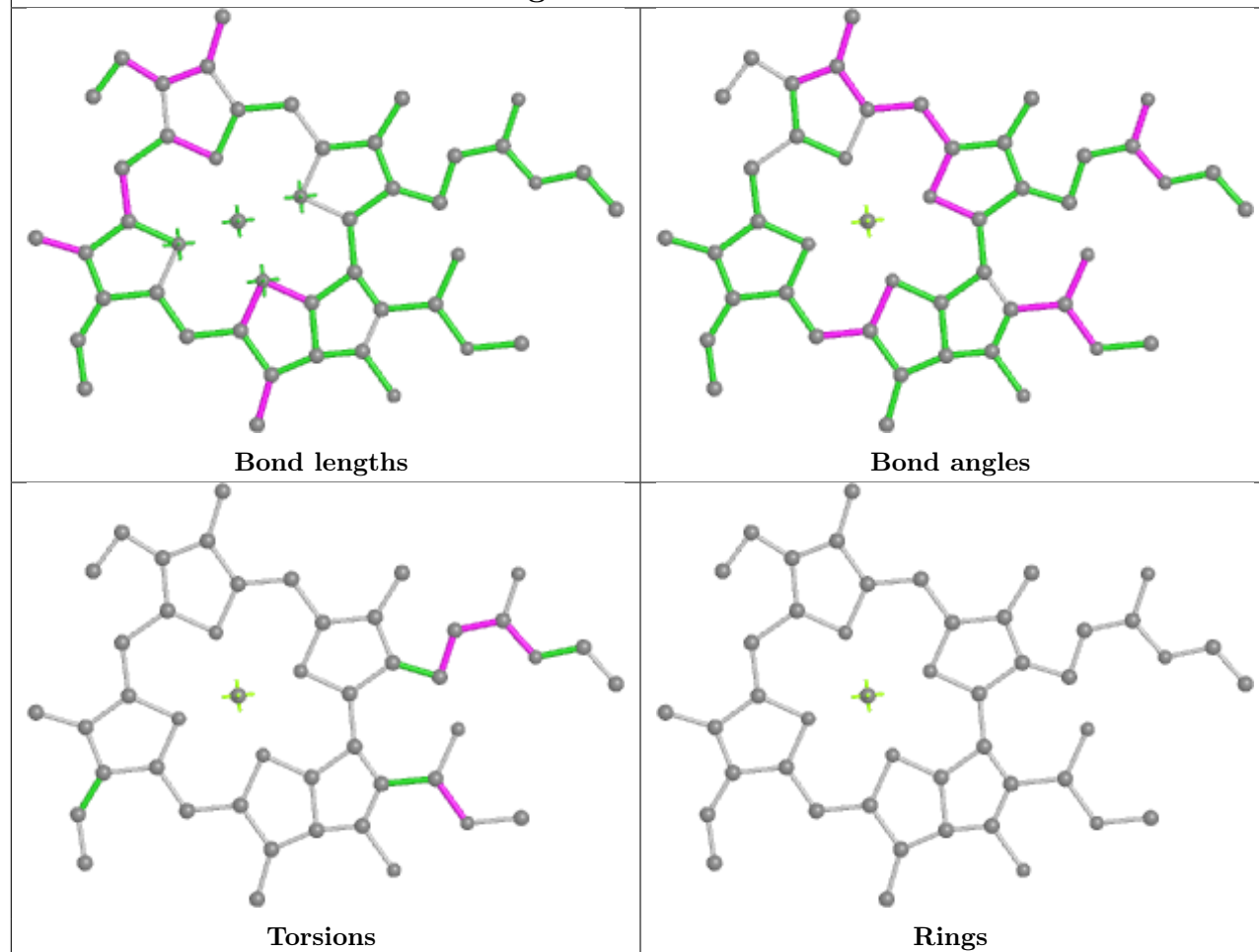
Ligand CLA b 803**Ligand SQD 1 202**

Ligand CLA A 819**Ligand CLA a 837****Ligand BCR B 850**

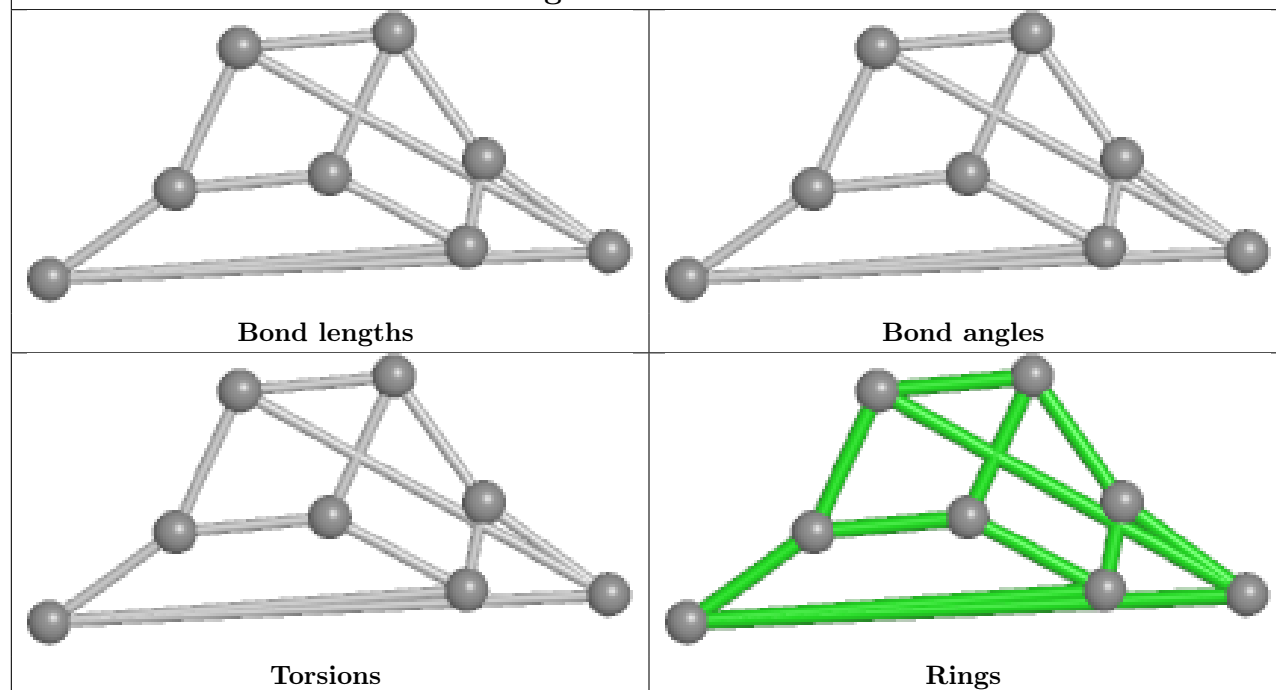
Ligand CLA b 843**Ligand CLA A 809****Ligand CLA b 807**

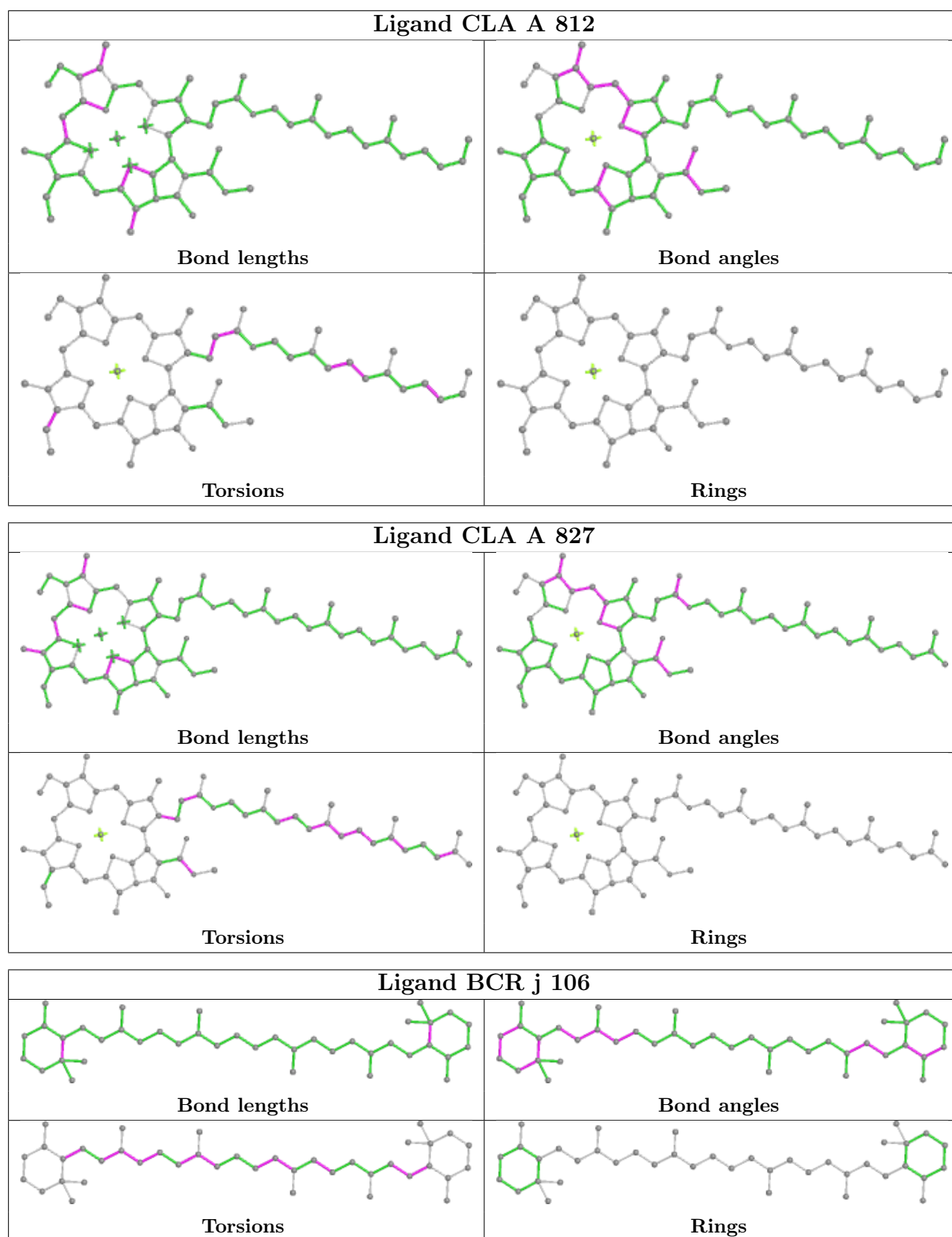


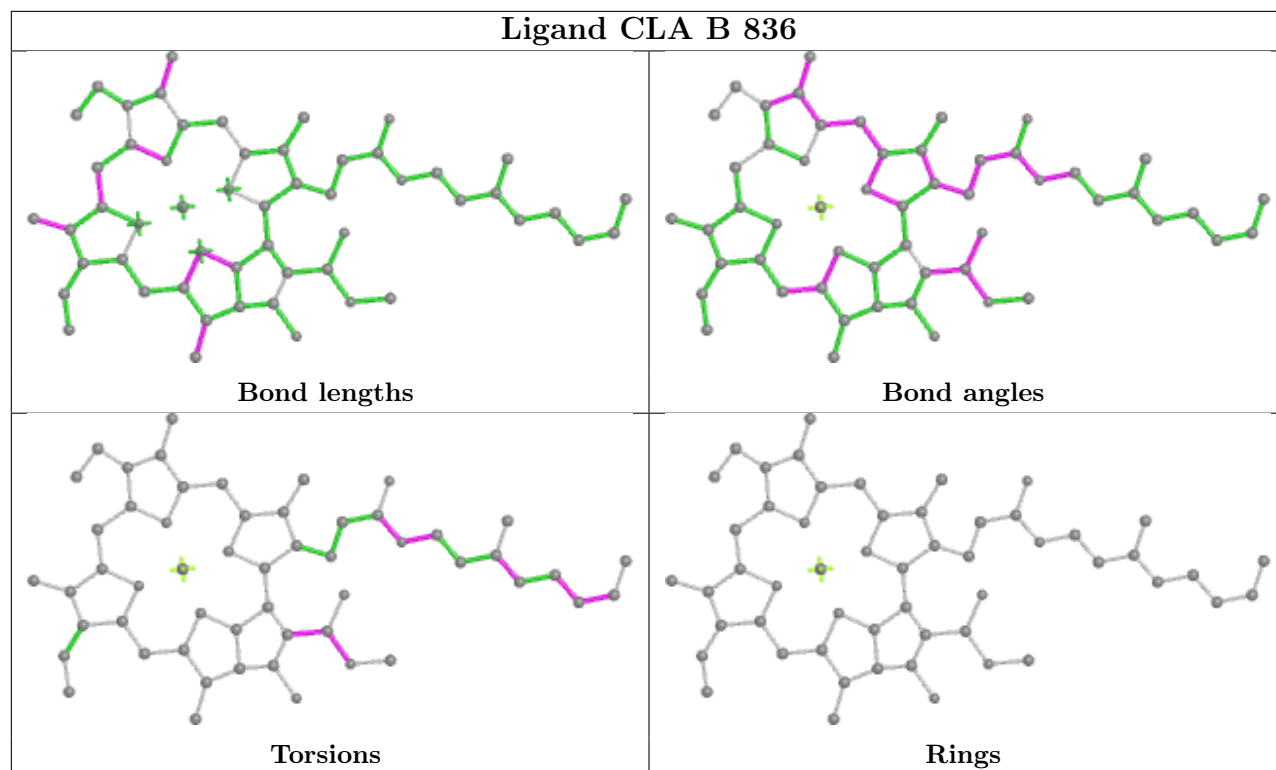
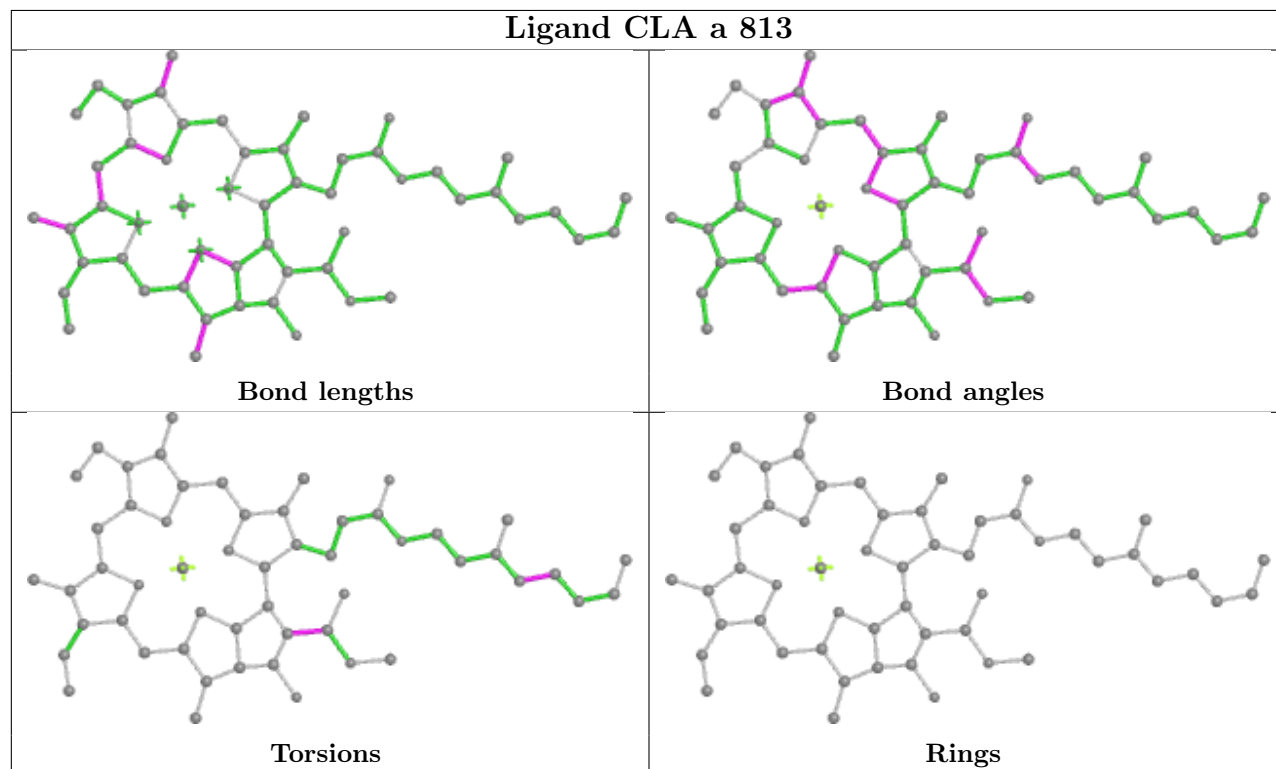
Ligand CLA b 841



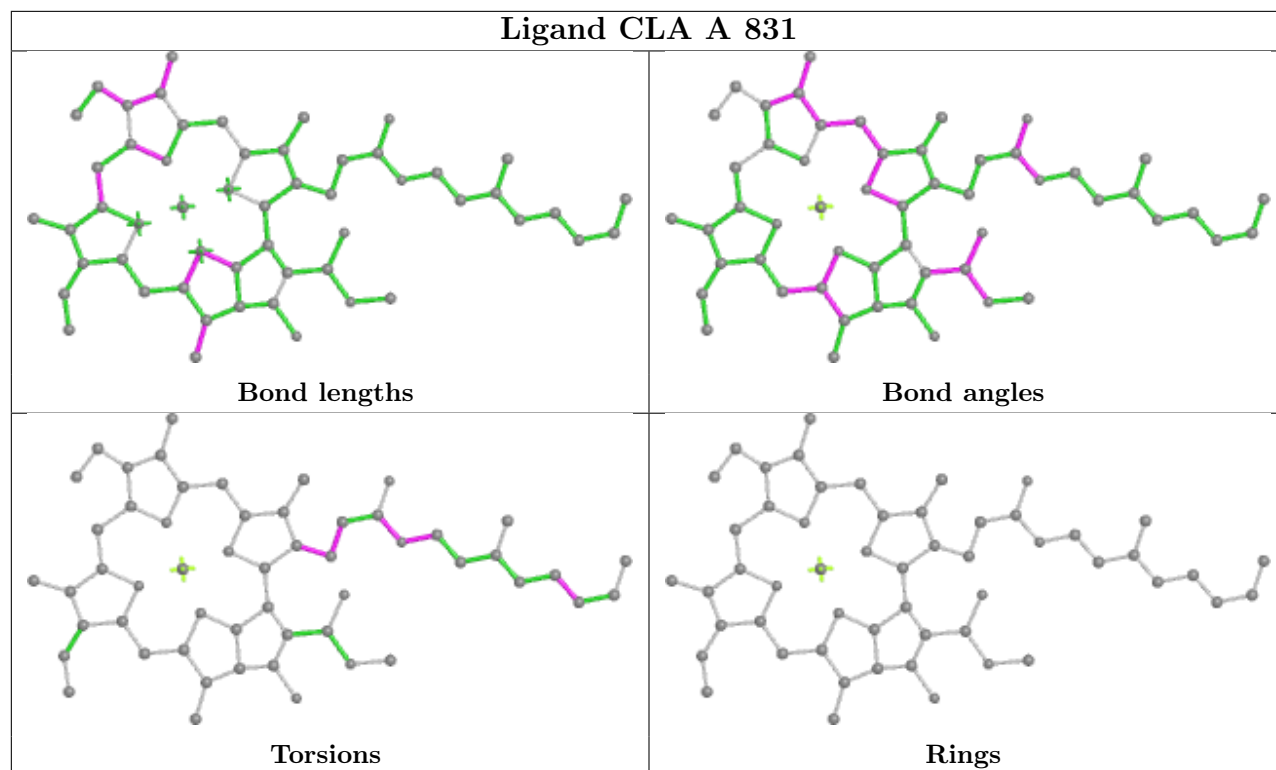
Ligand SF4 c 101



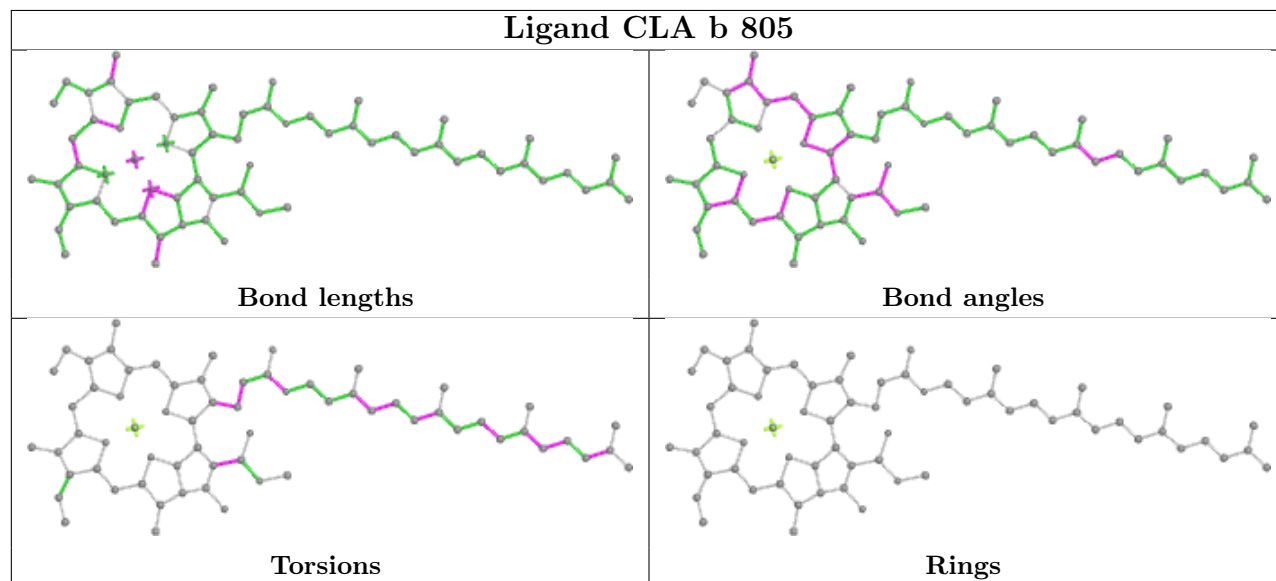


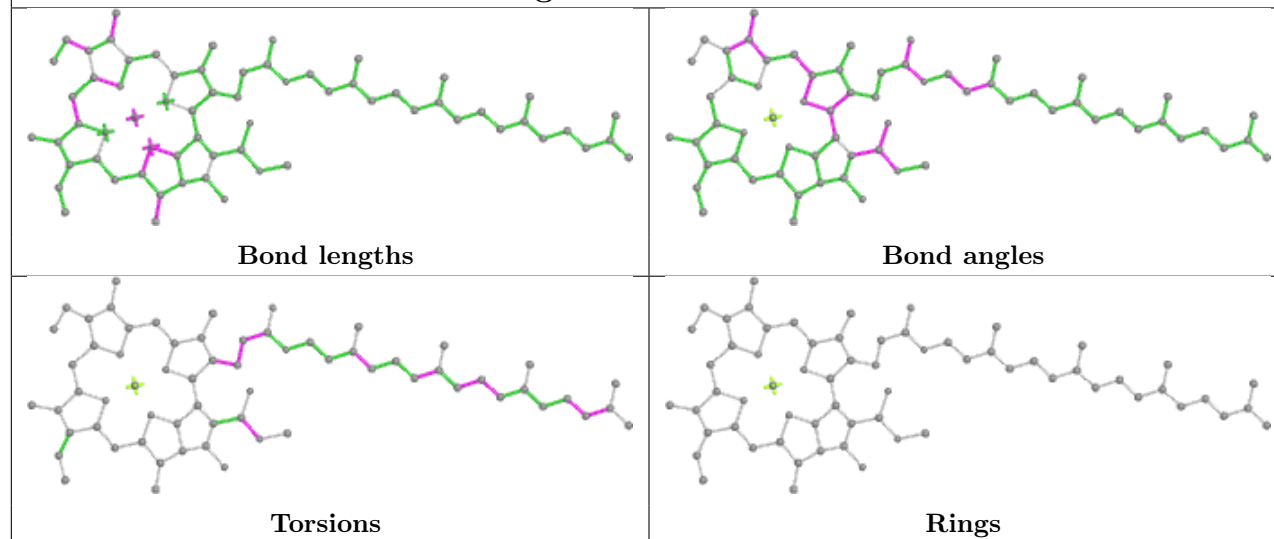
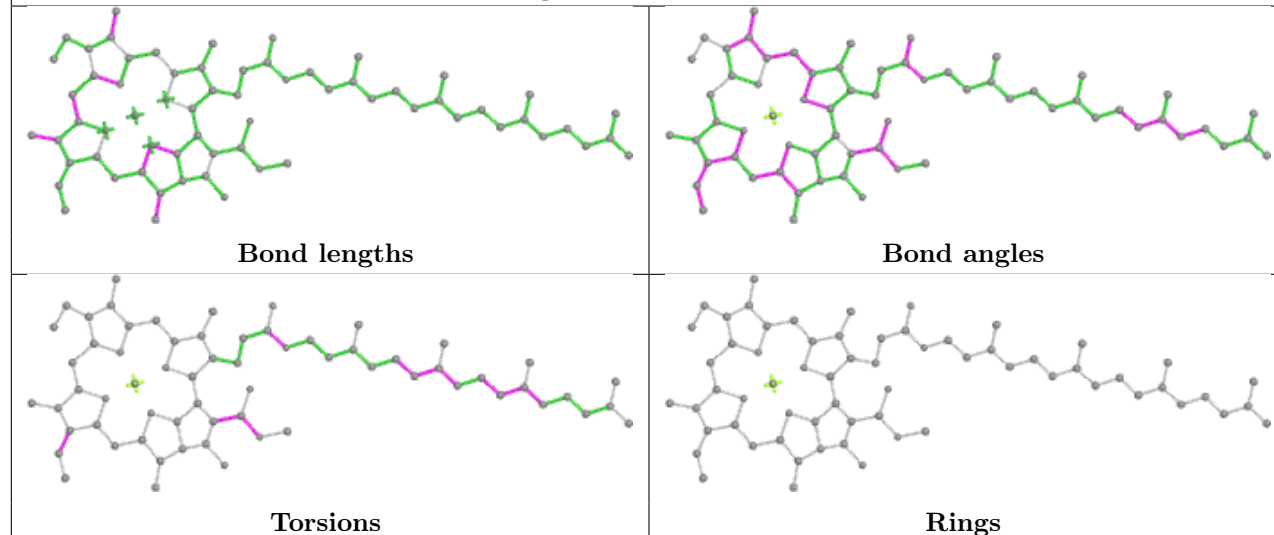
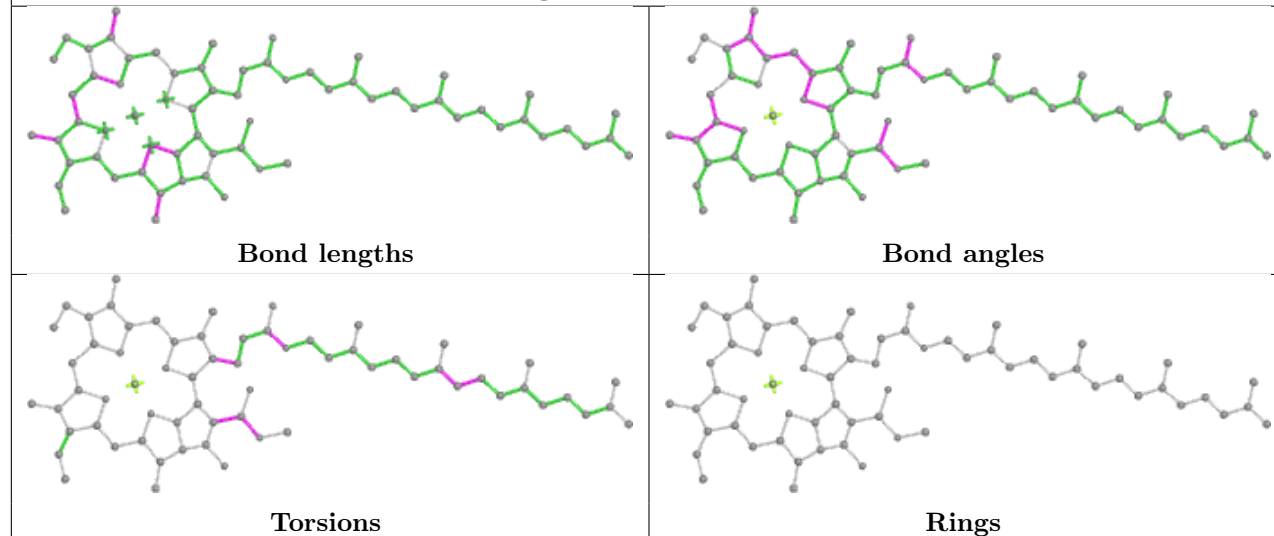
Ligand CLA B 836**Ligand CLA a 813**

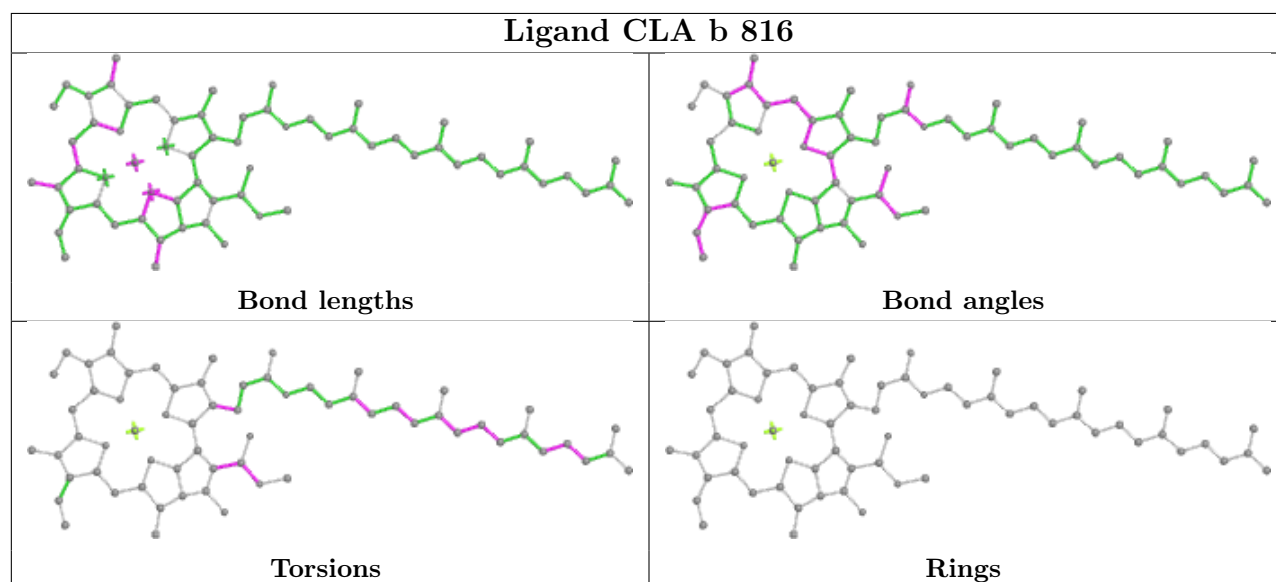
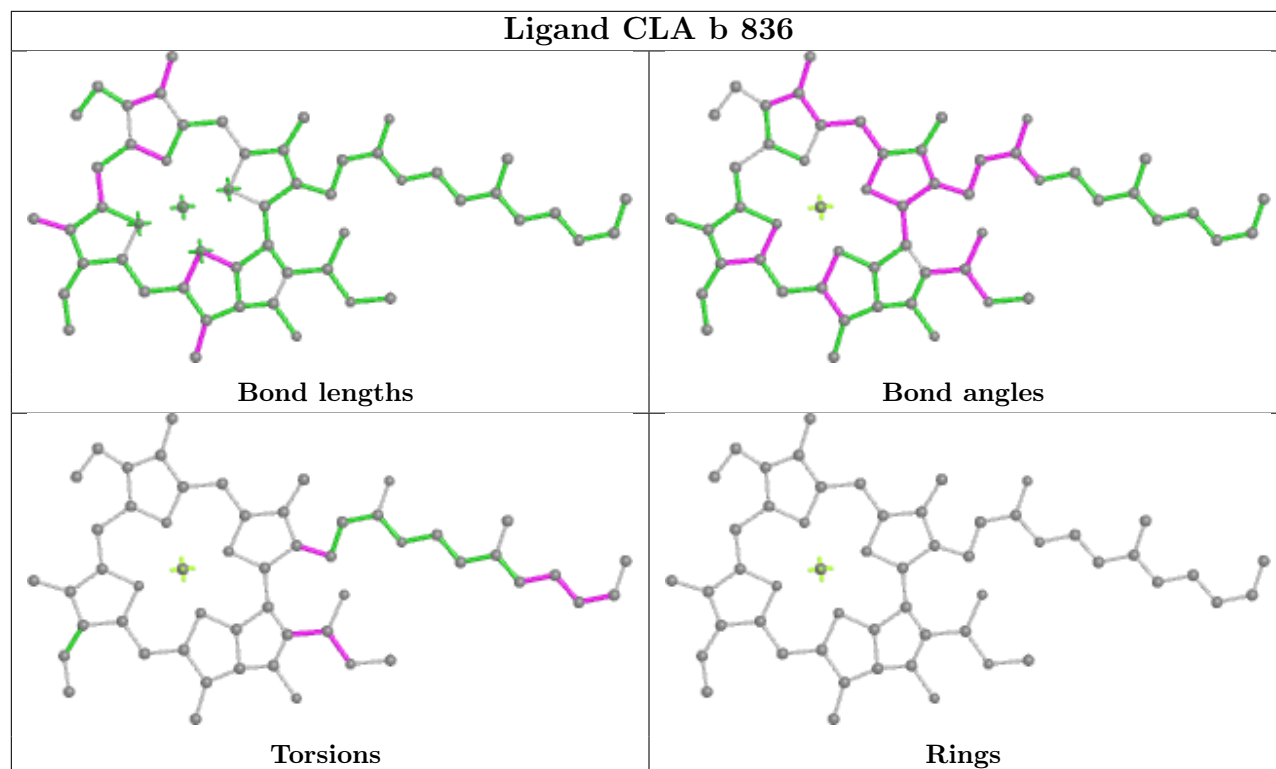
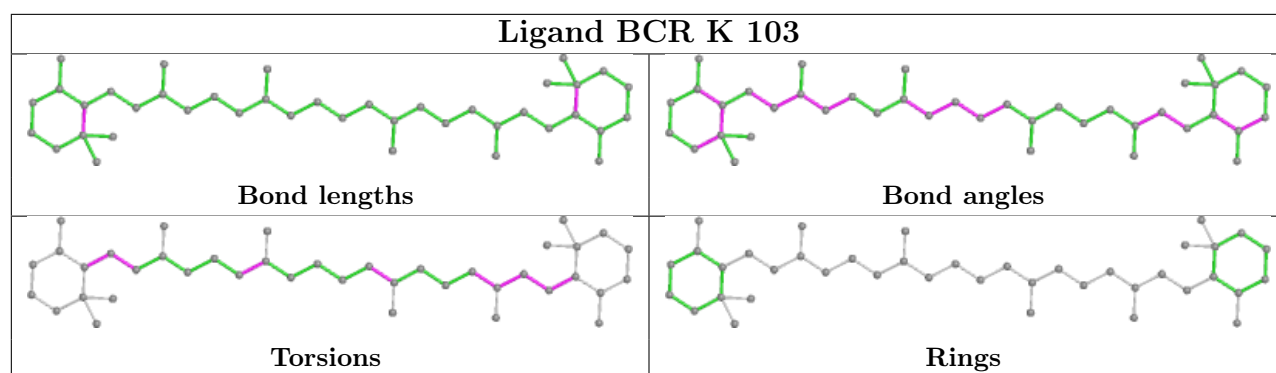
Ligand CLA A 831

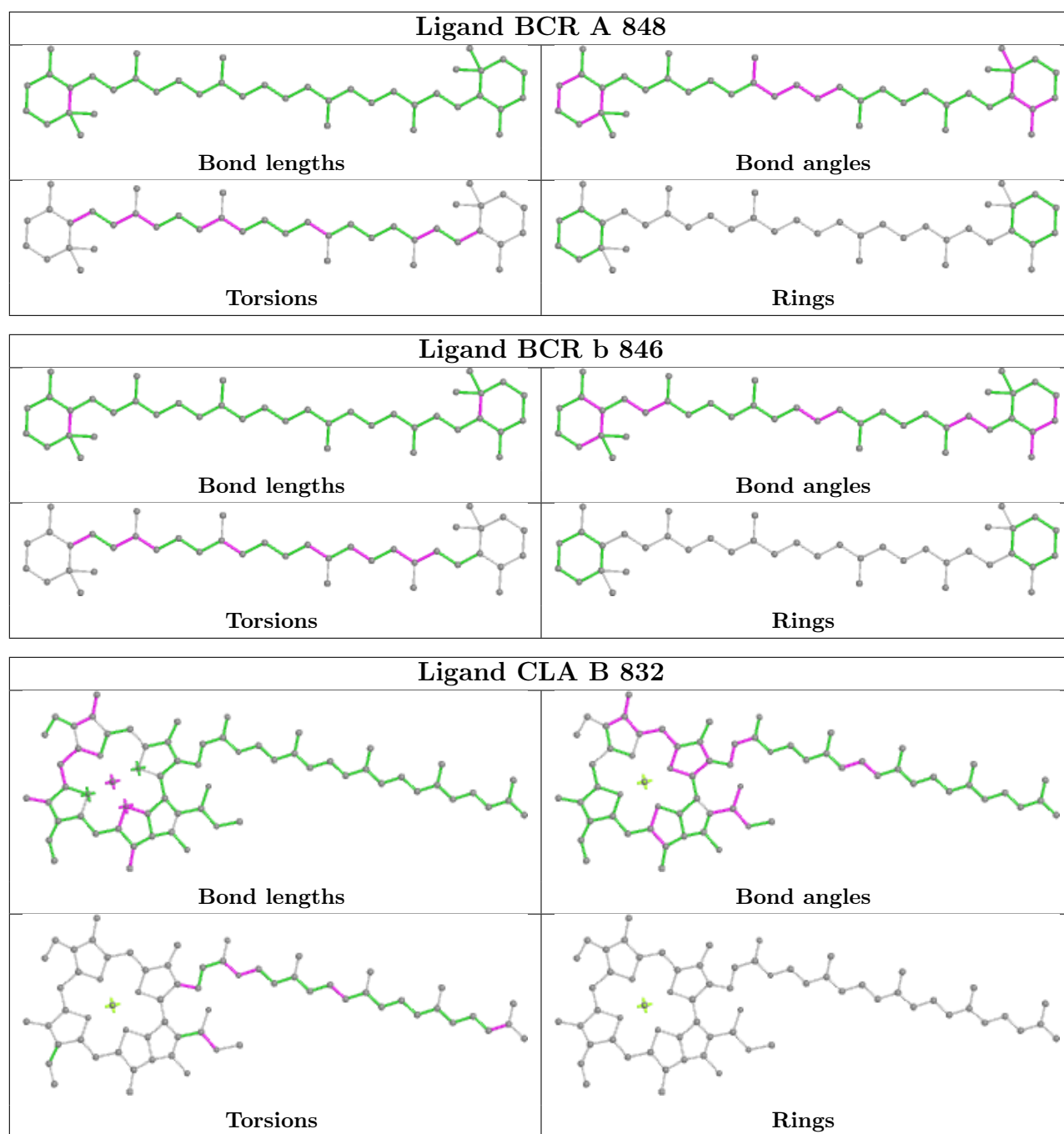


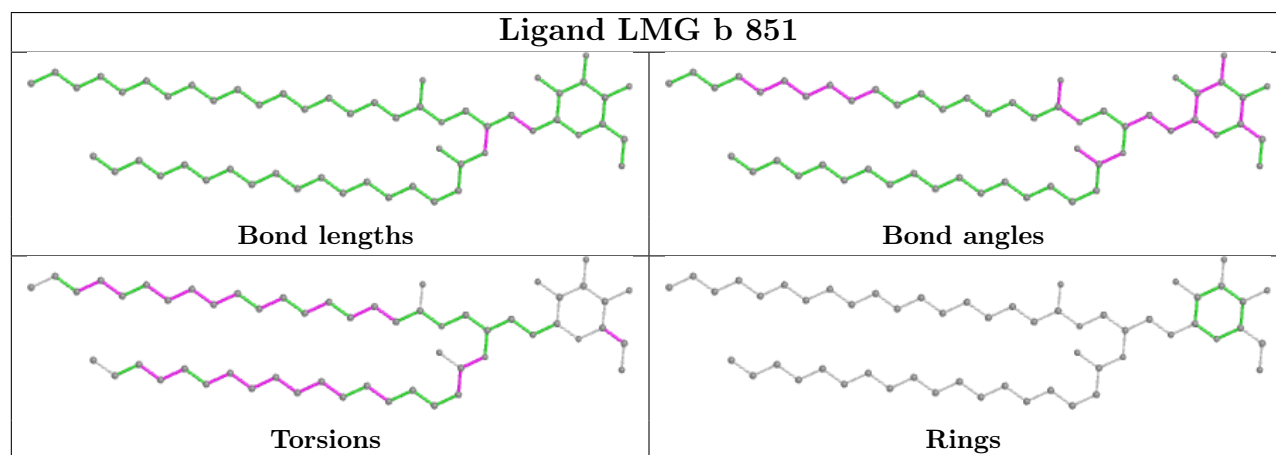
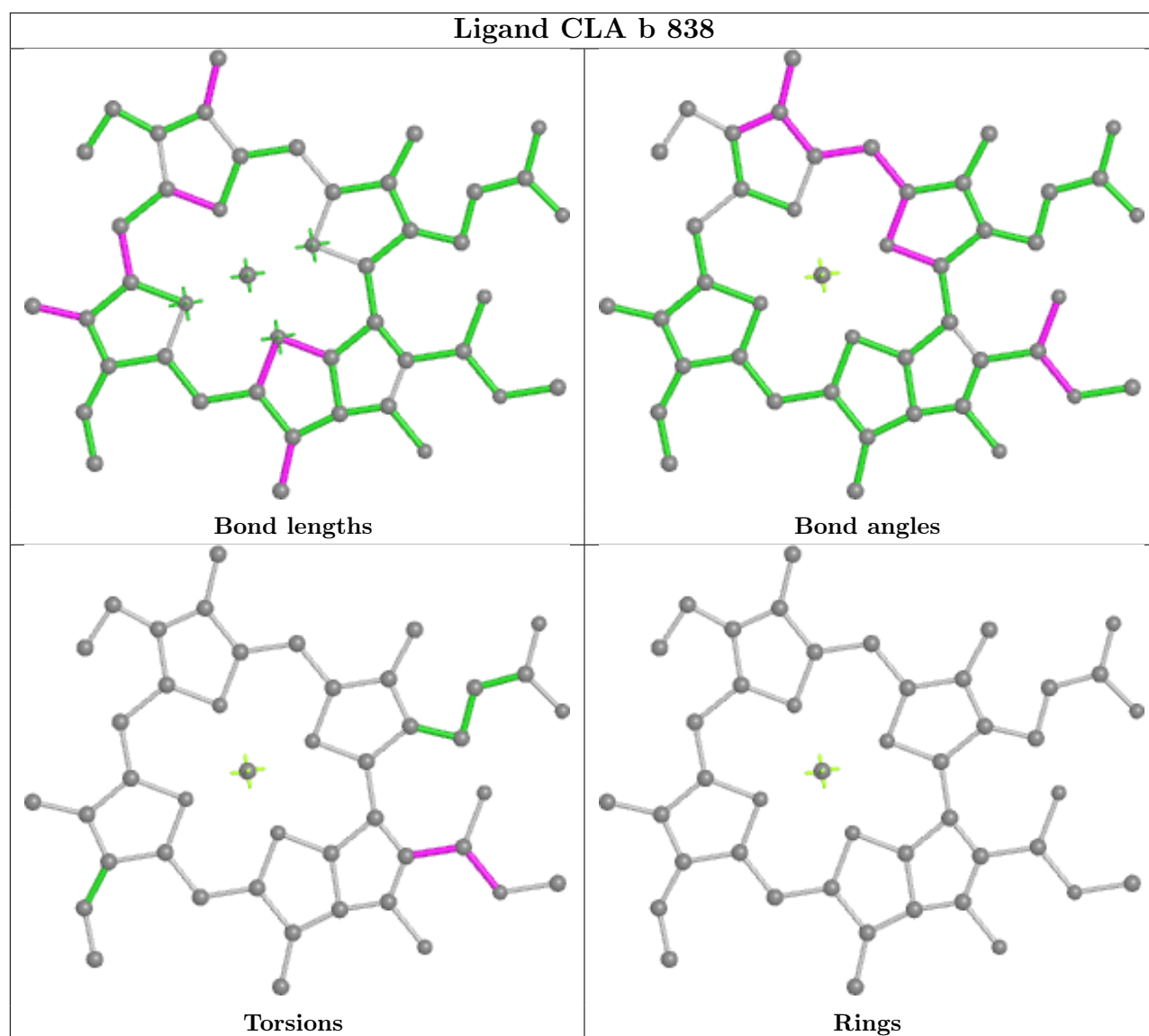
Ligand CLA b 805

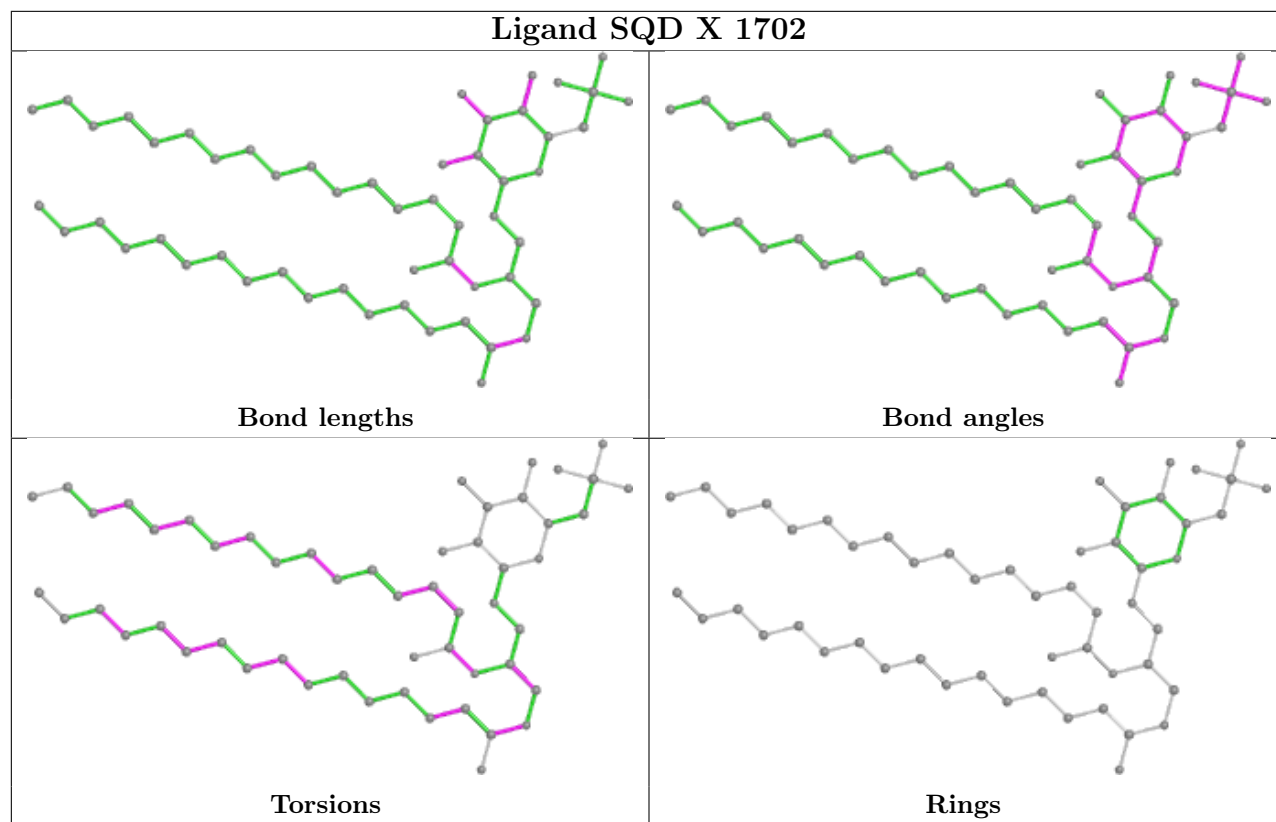
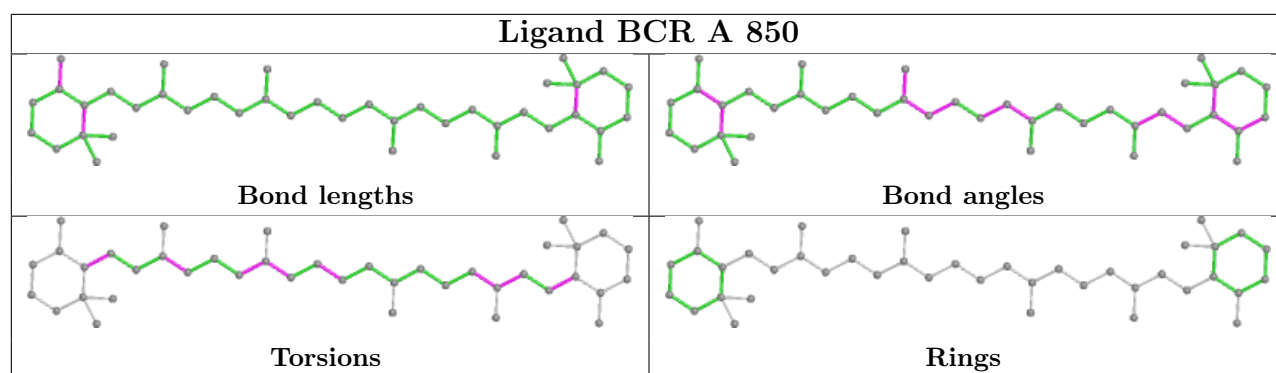


Ligand CLA b 830**Ligand CLA a 833****Ligand CLA b 822**

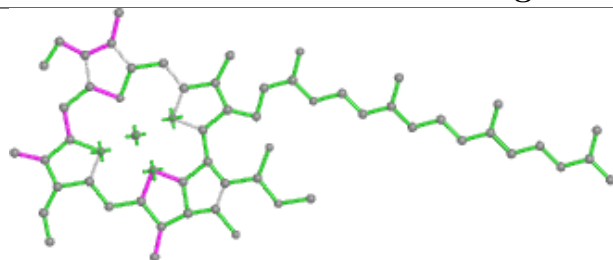




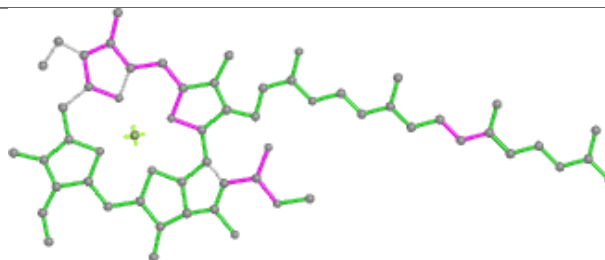




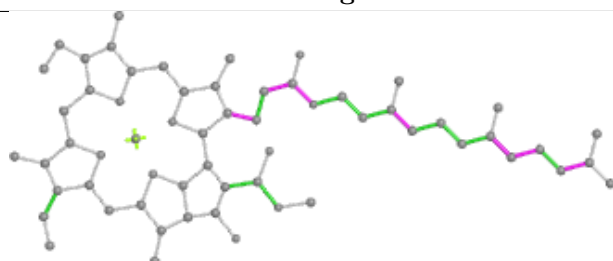
Ligand CLA B 813



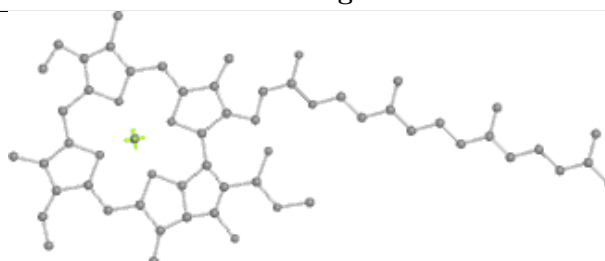
Bond lengths



Bond angles

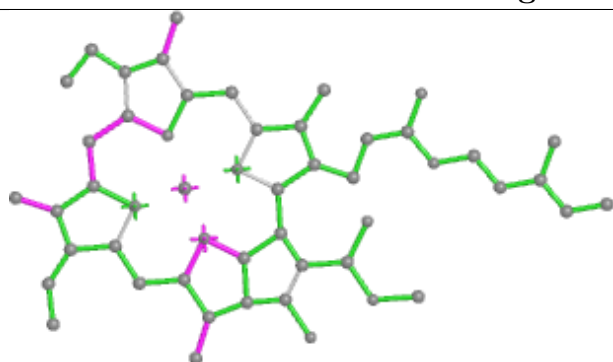


Torsions

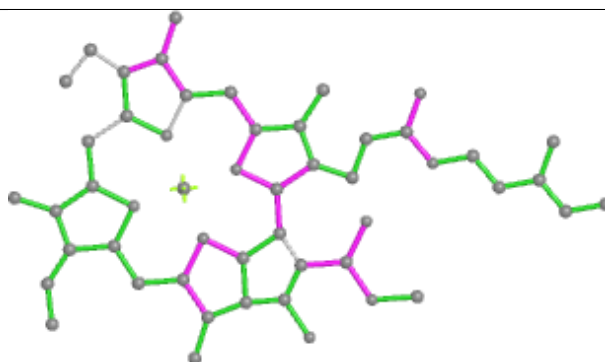


Rings

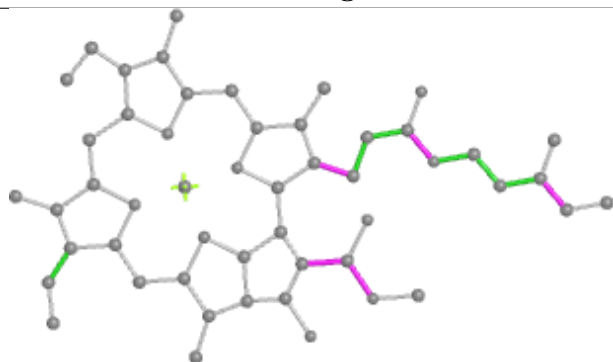
Ligand CLA a 836



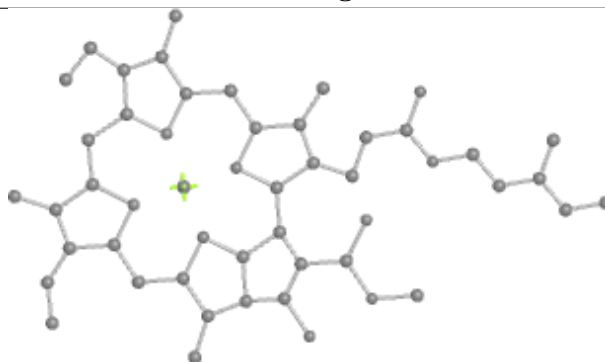
Bond lengths



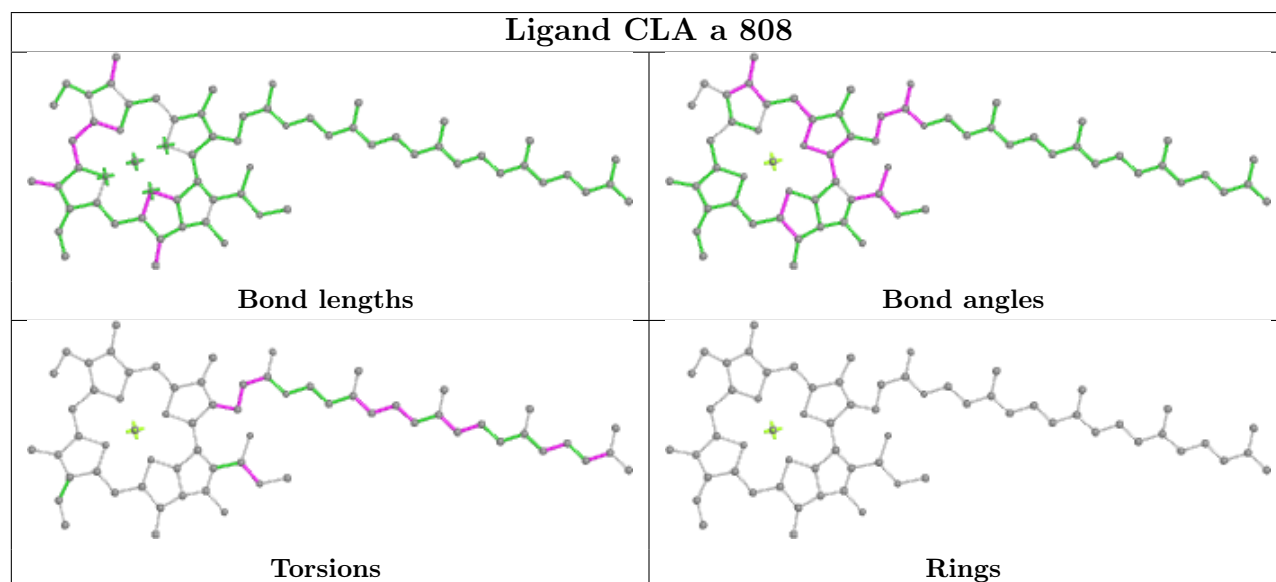
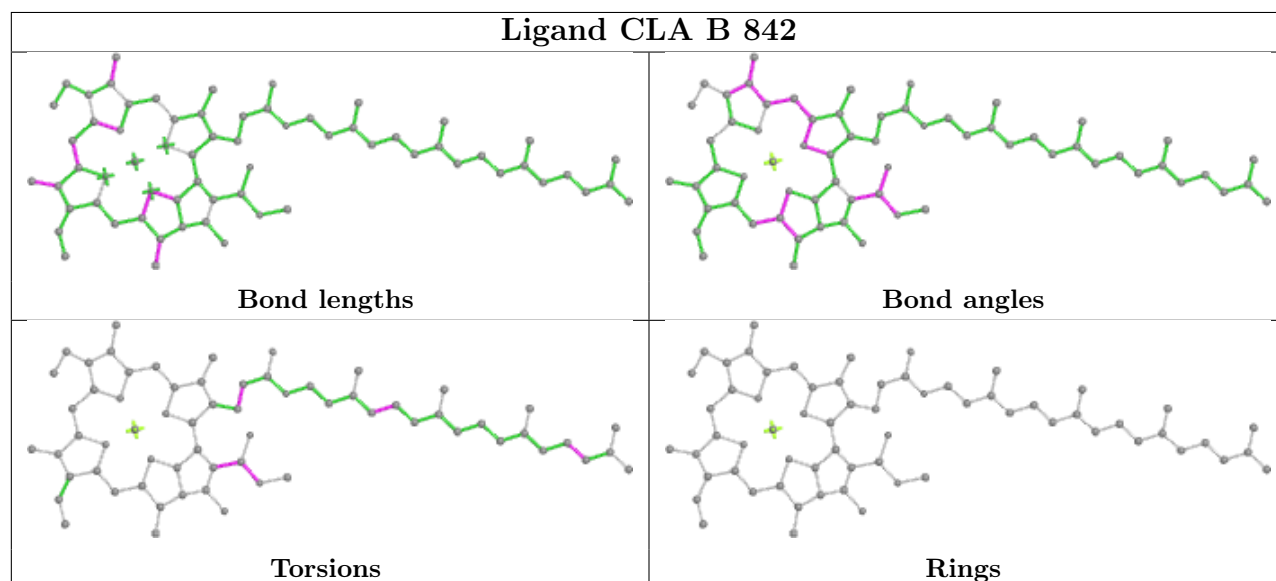
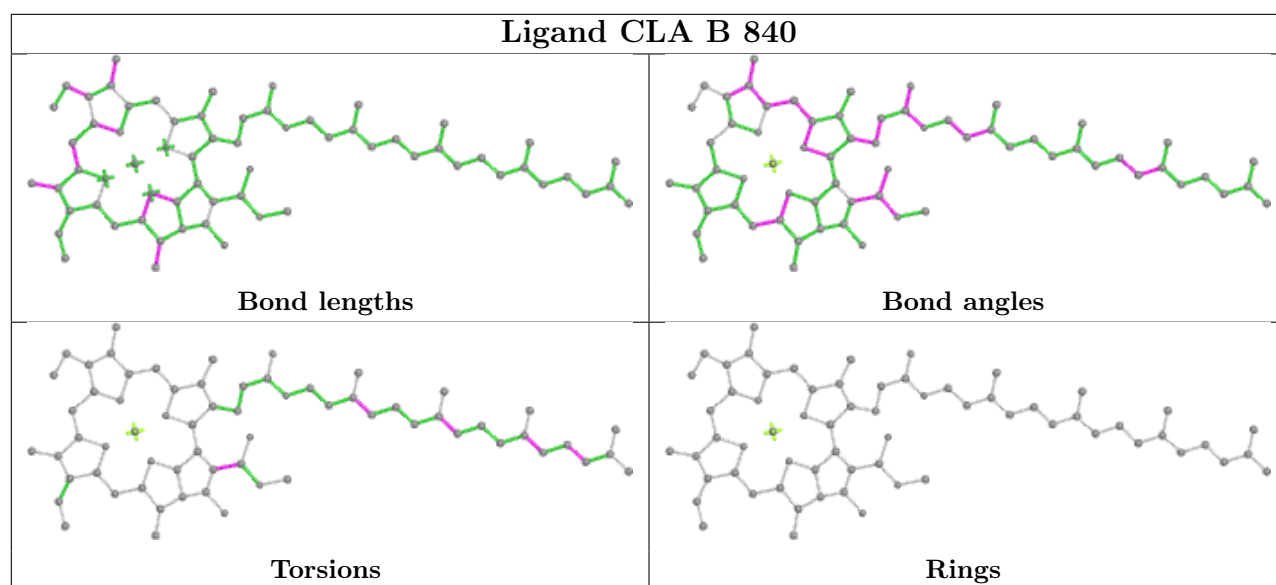
Bond angles

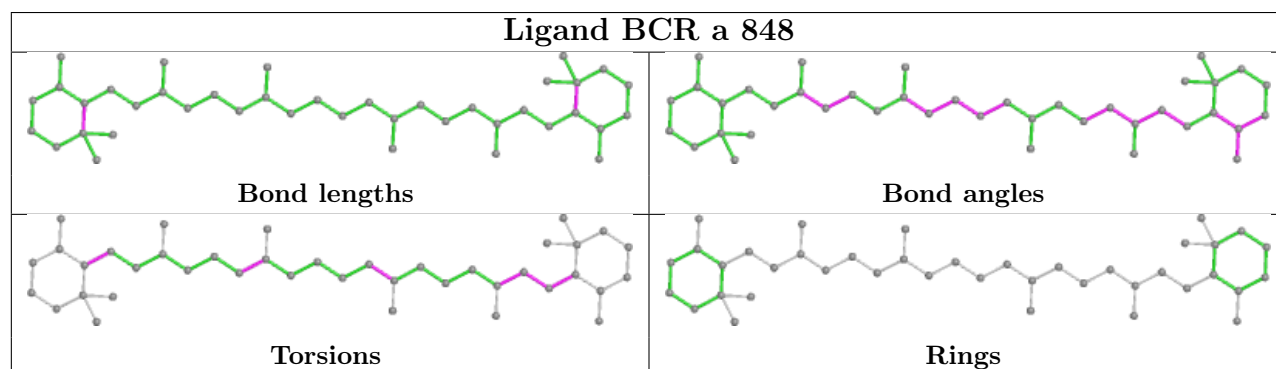
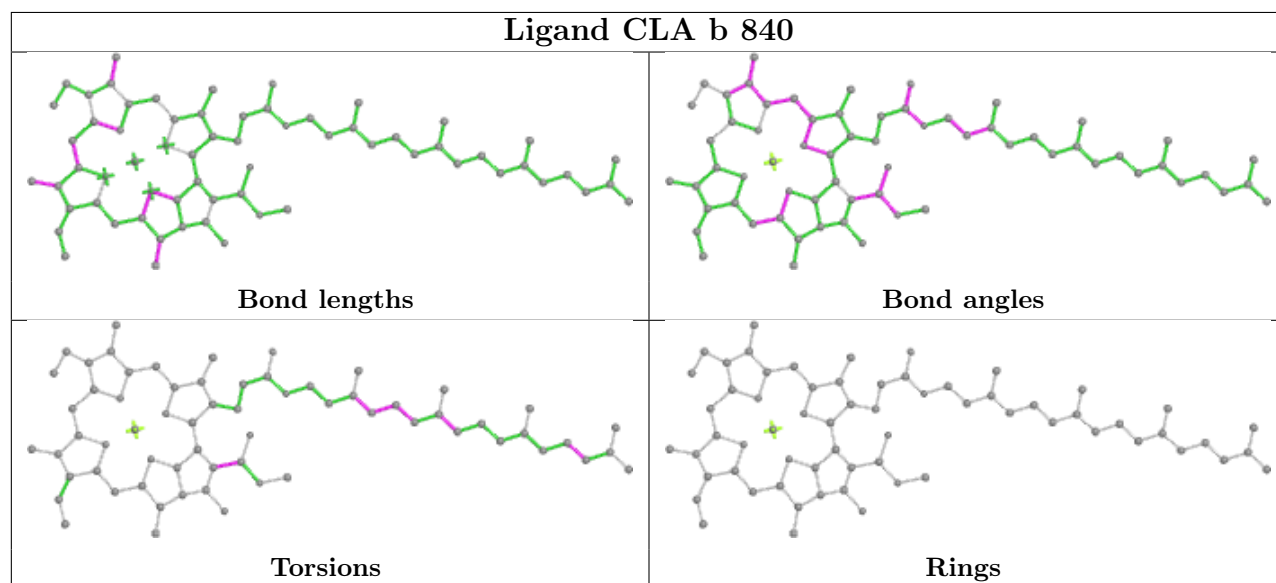
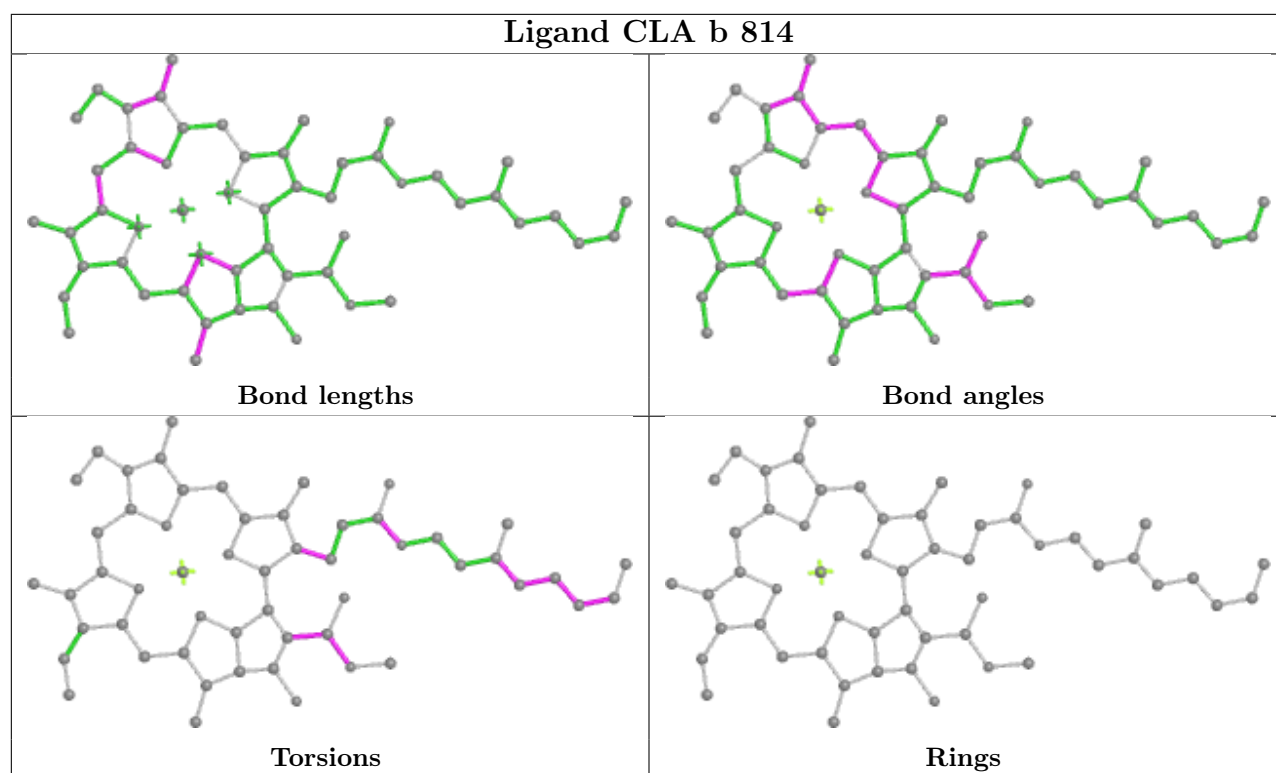


Torsions

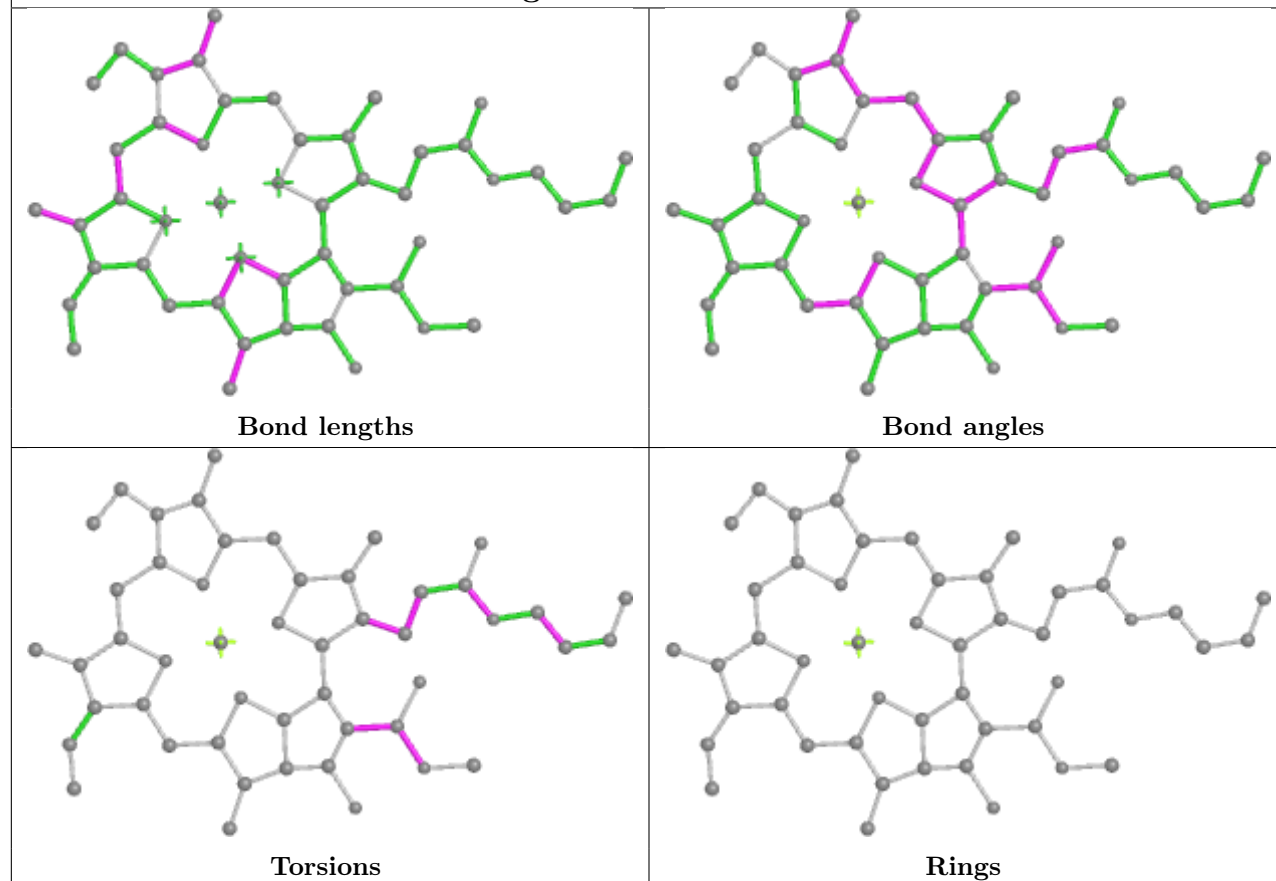


Rings

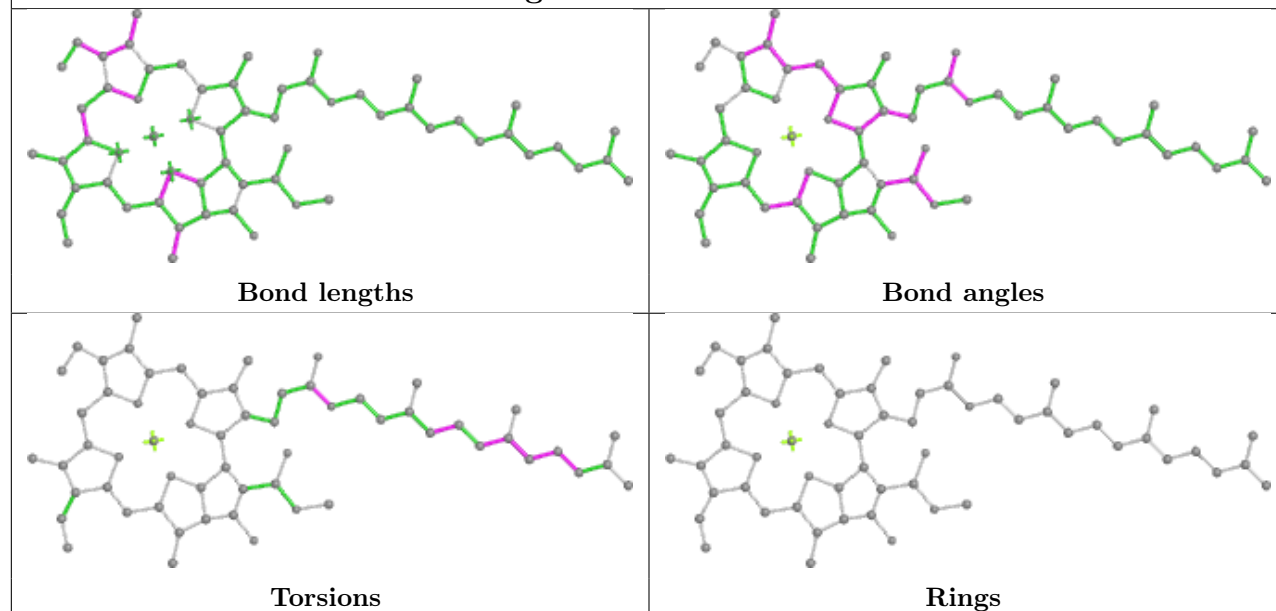




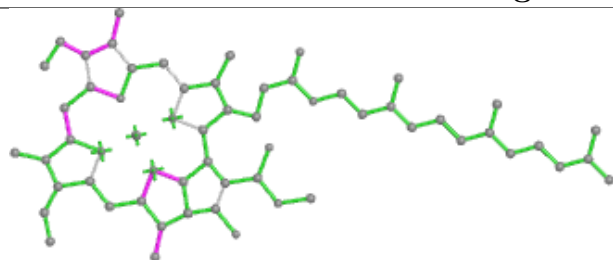
Ligand CLA X 1701



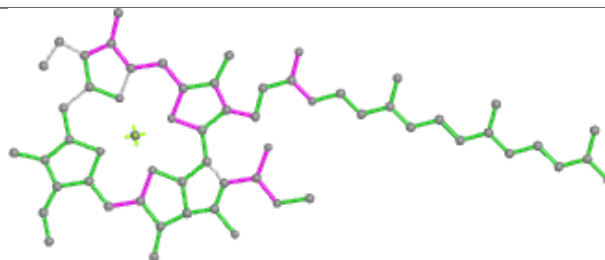
Ligand CLA L 1502



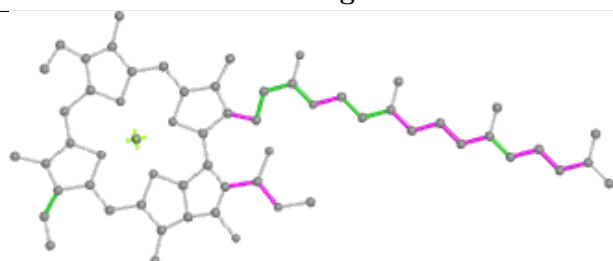
Ligand CLA A 807



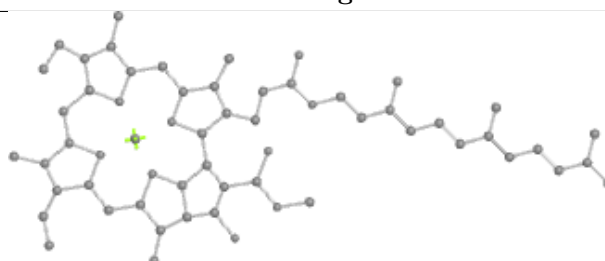
Bond lengths



Bond angles

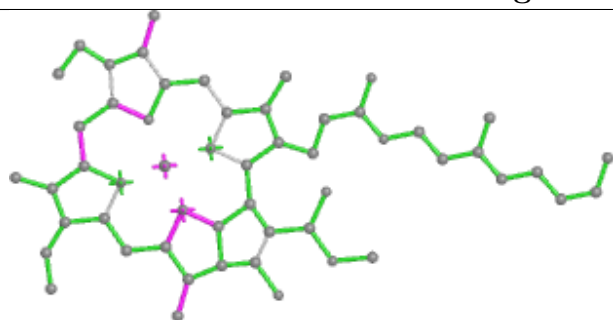


Torsions

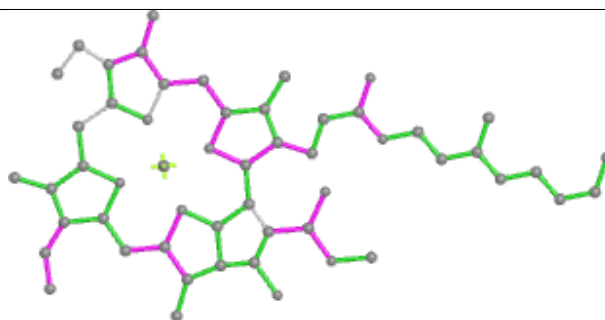


Rings

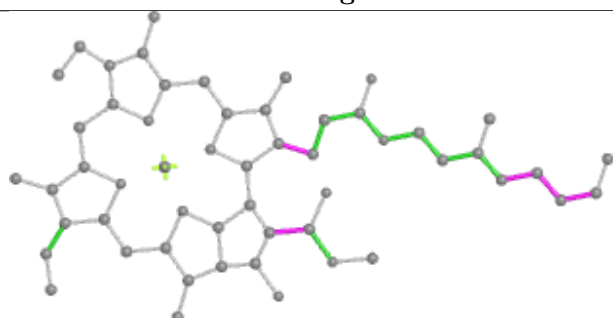
Ligand CLA A 826



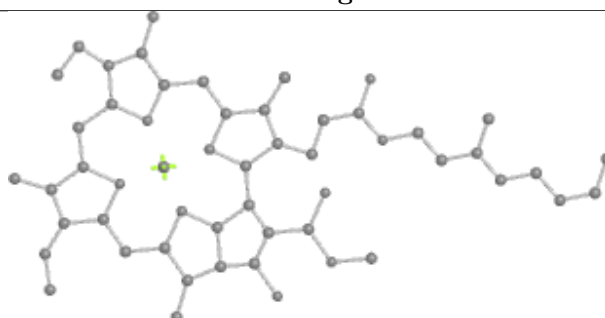
Bond lengths



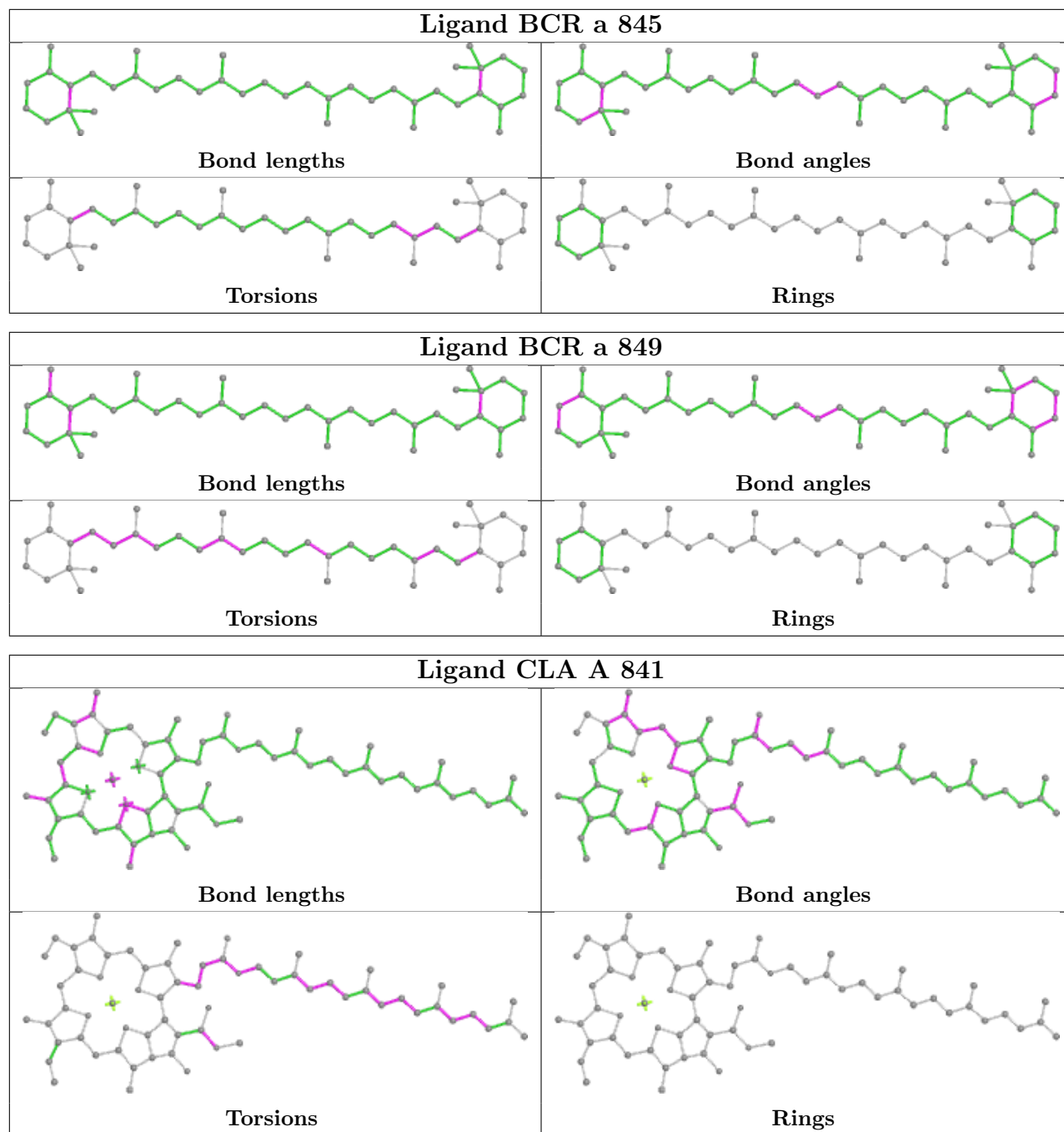
Bond angles

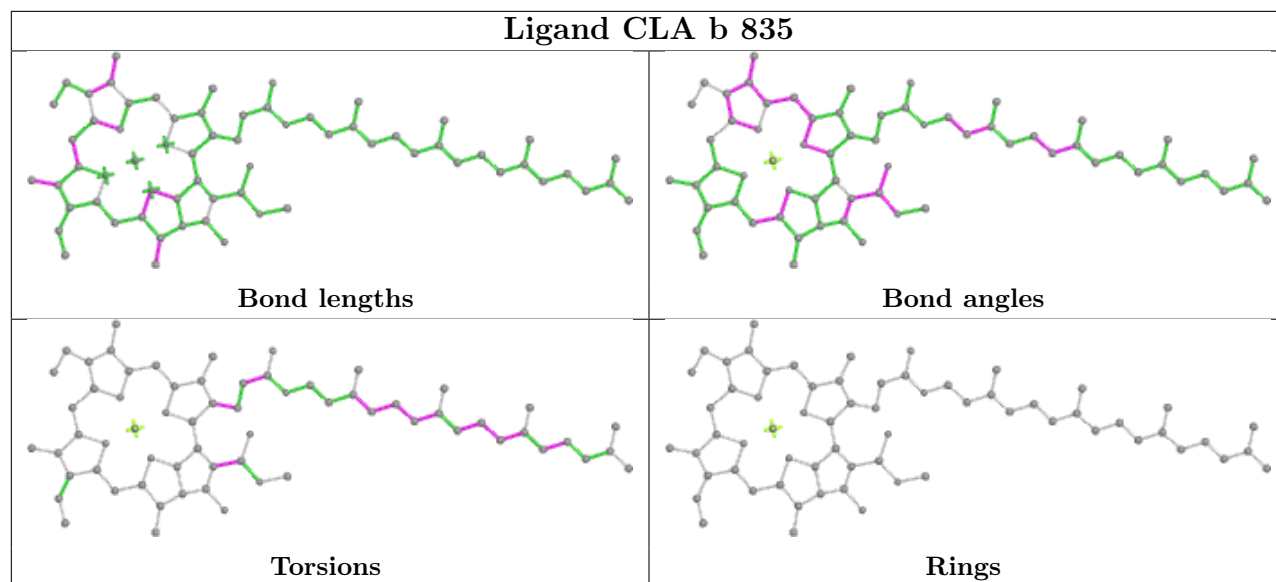
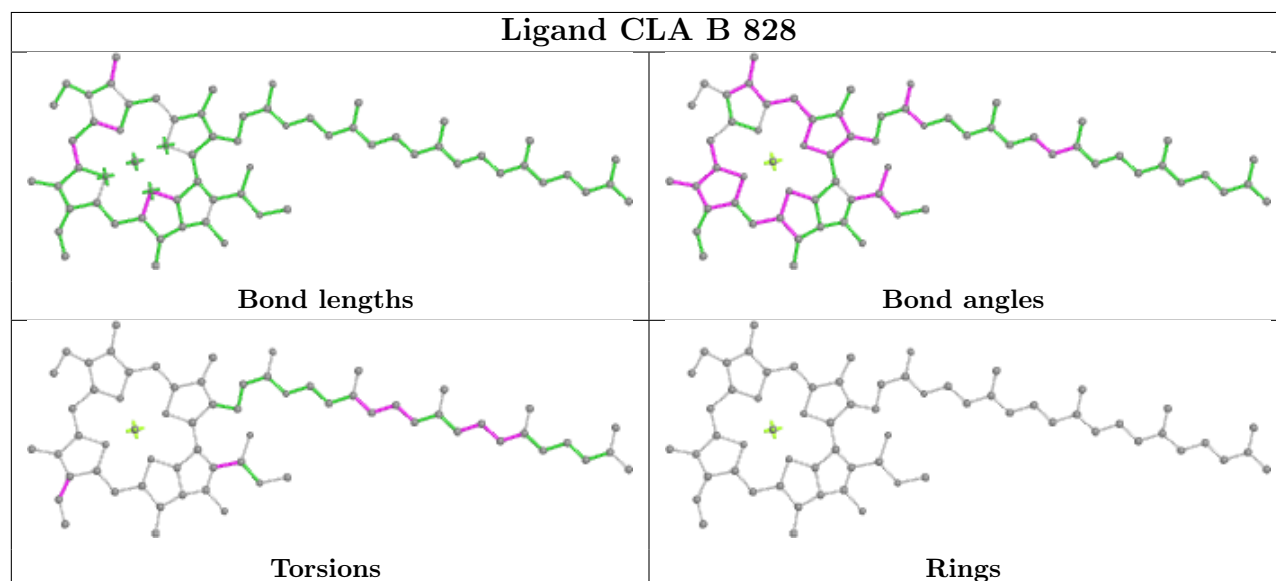
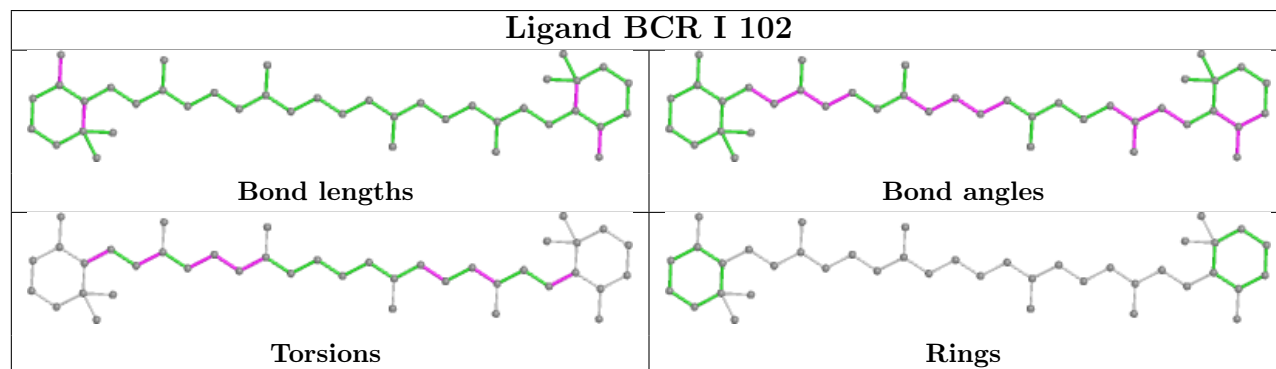


Torsions

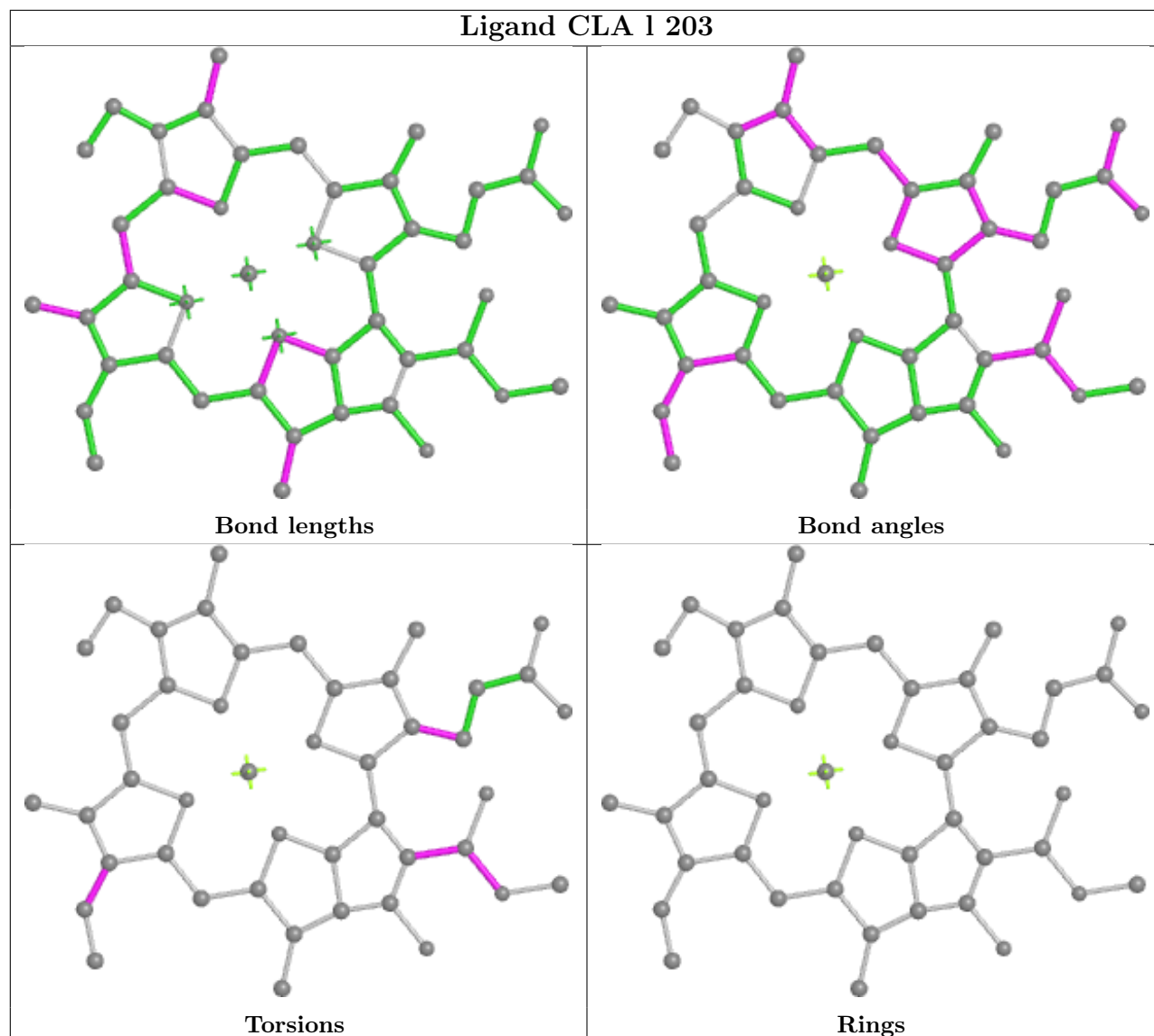


Rings

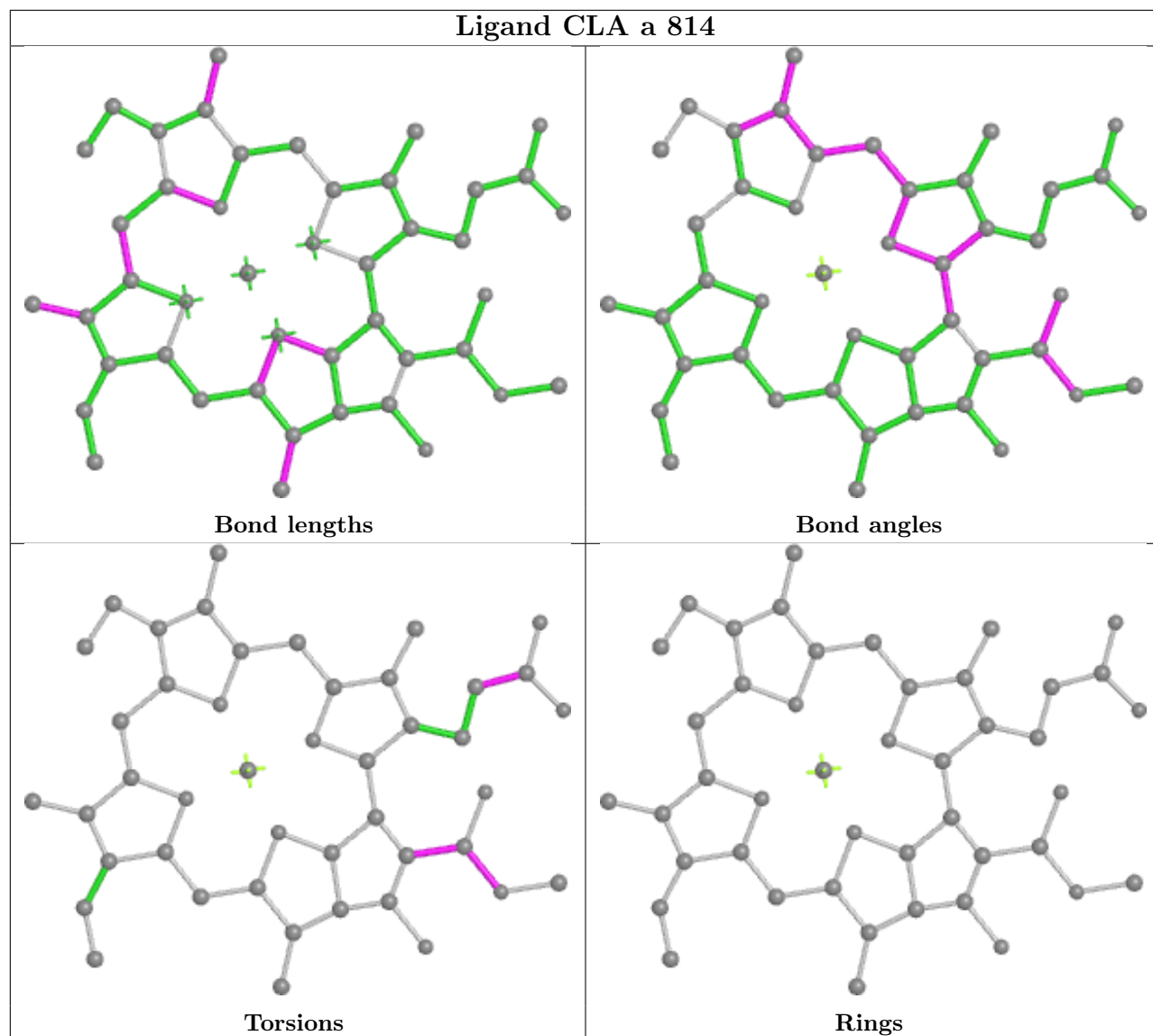


Ligand CLA b 835**Ligand CLA B 828****Ligand BCR I 102**

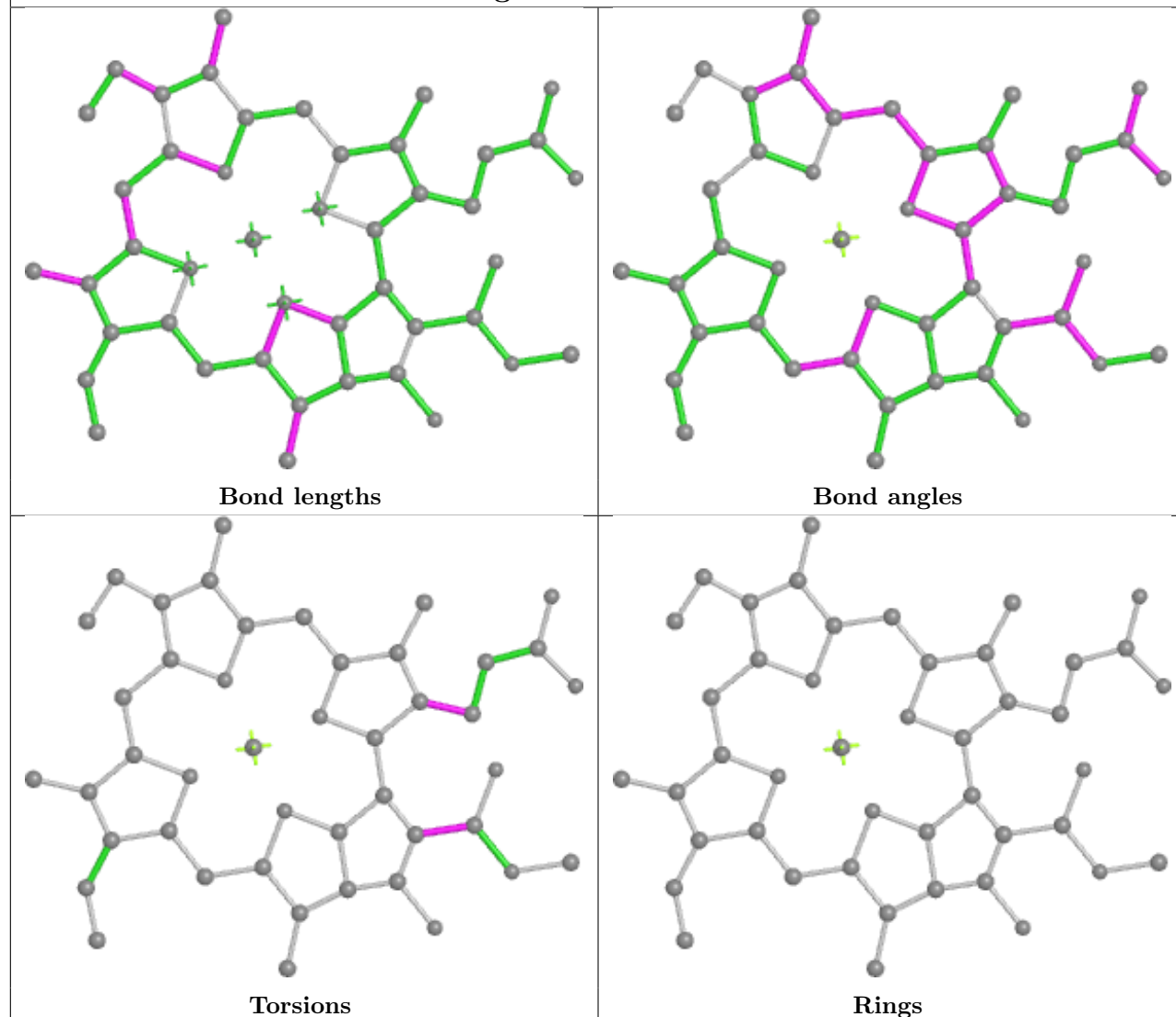
Ligand CLA 1 203



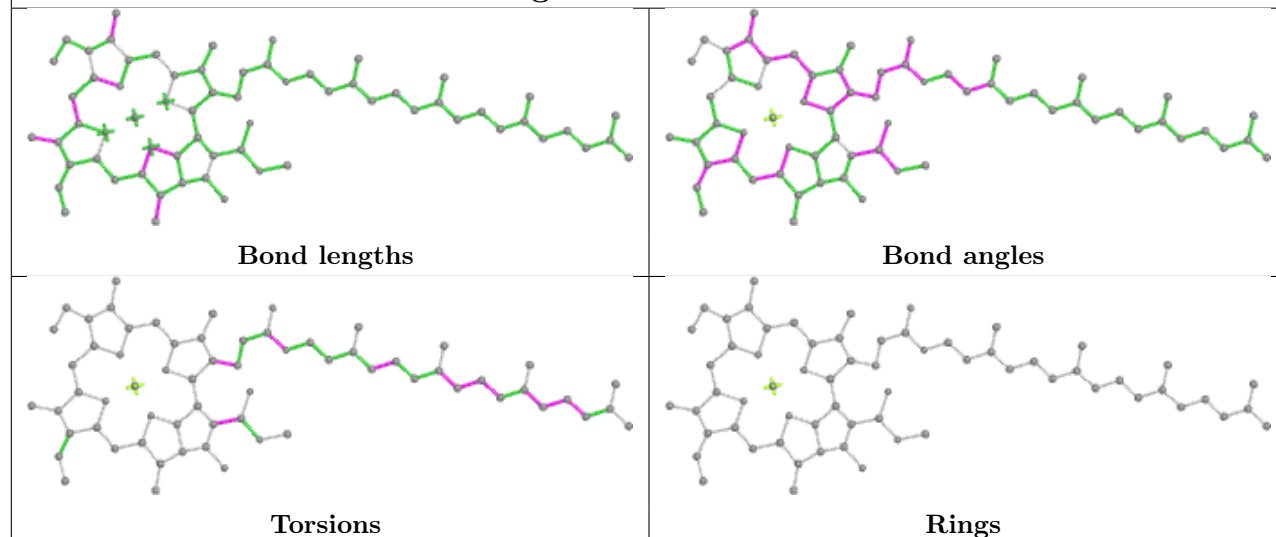
Ligand CLA a 814

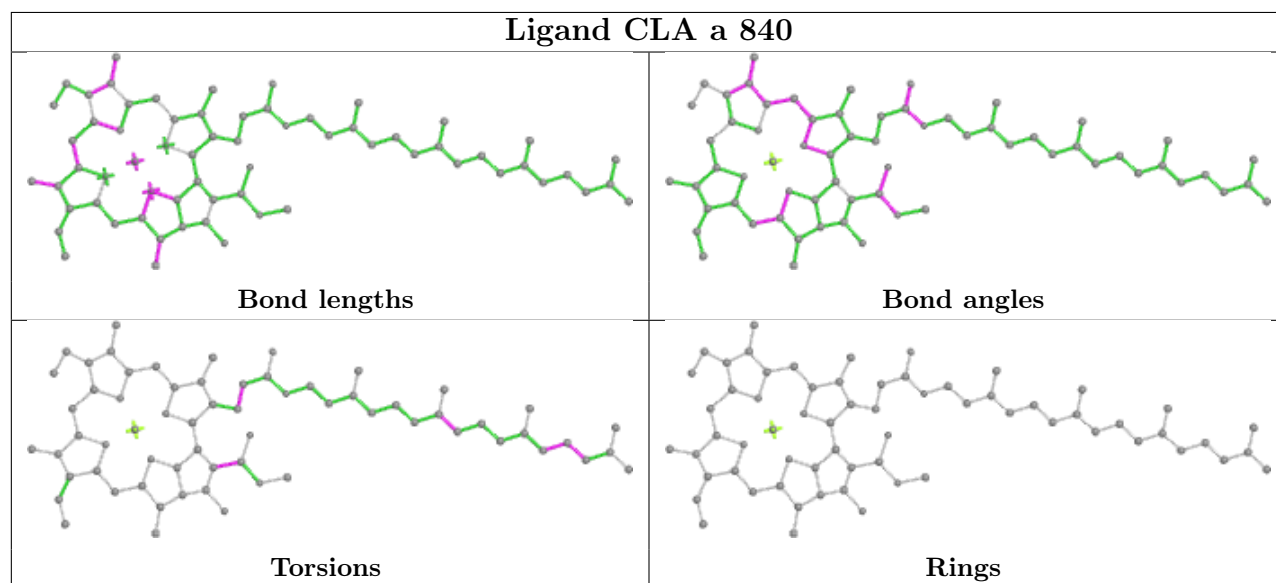
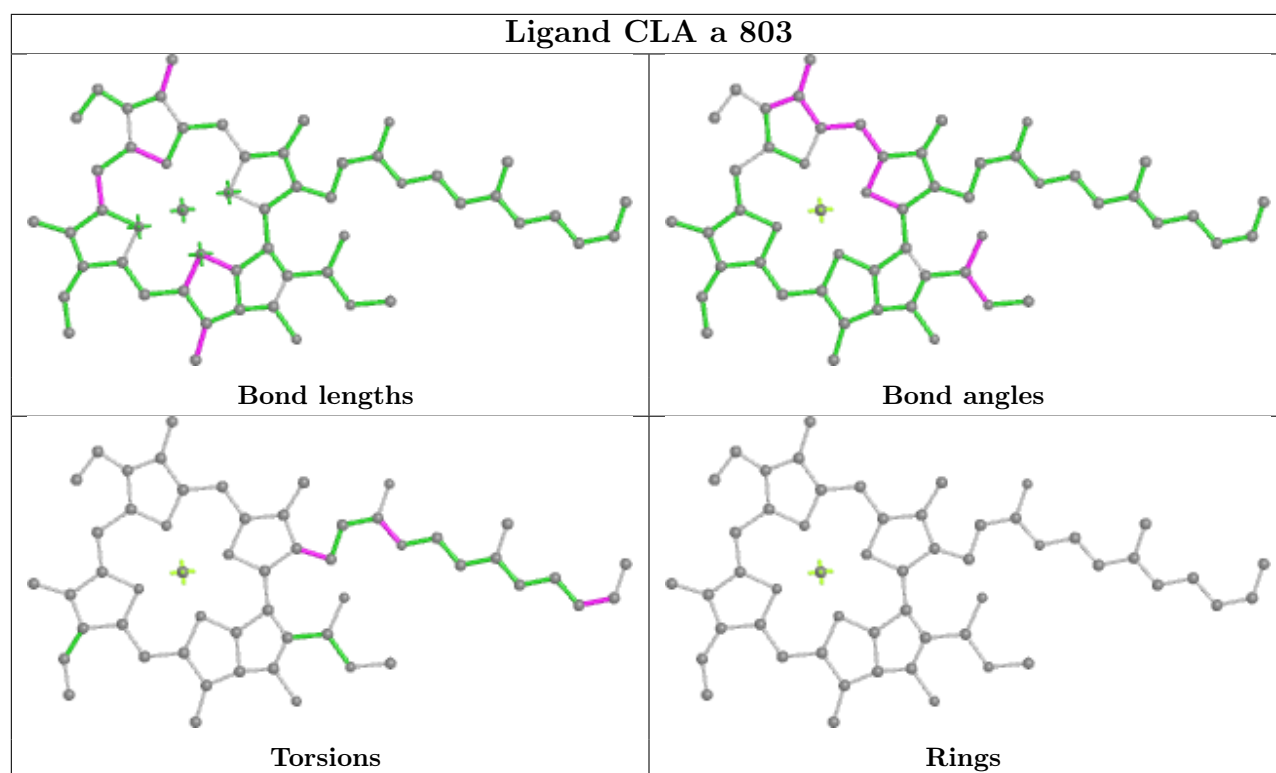


Ligand CLA a 821

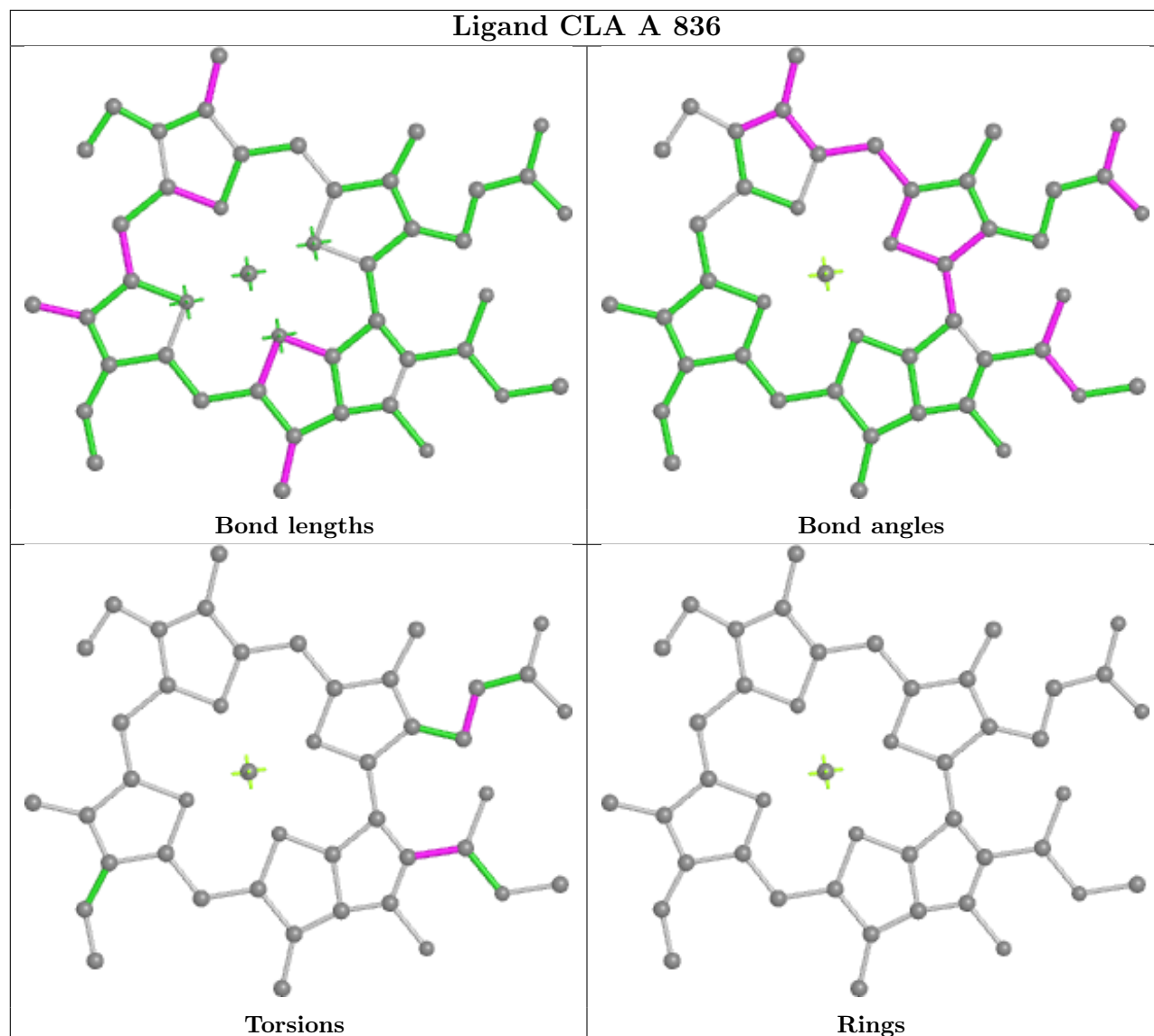


Ligand CLA A 805

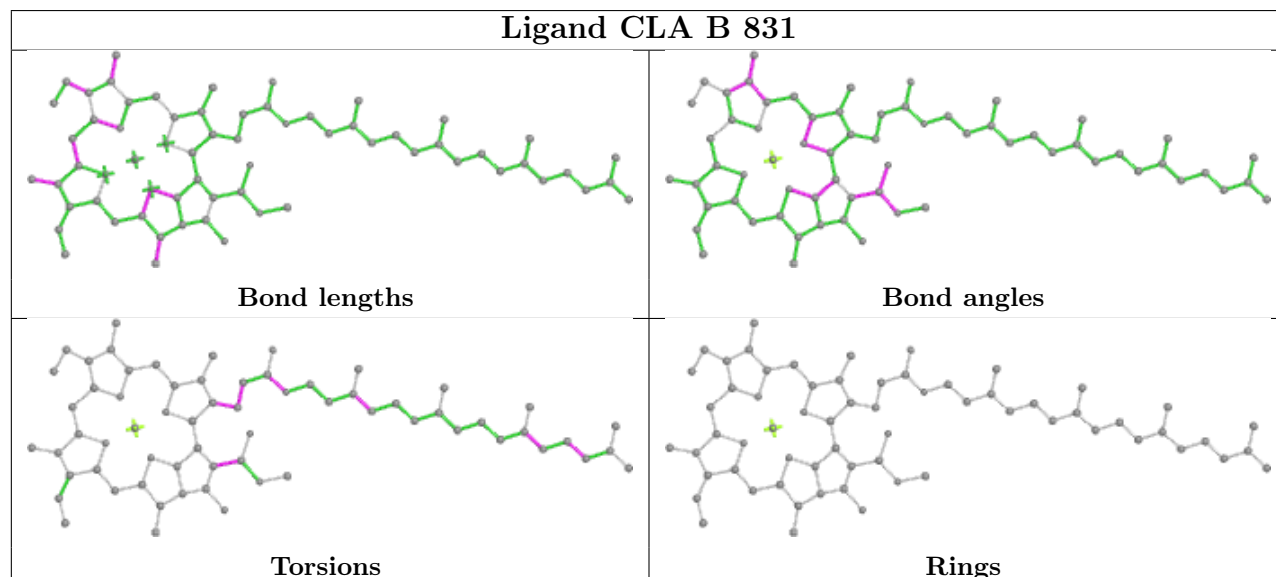


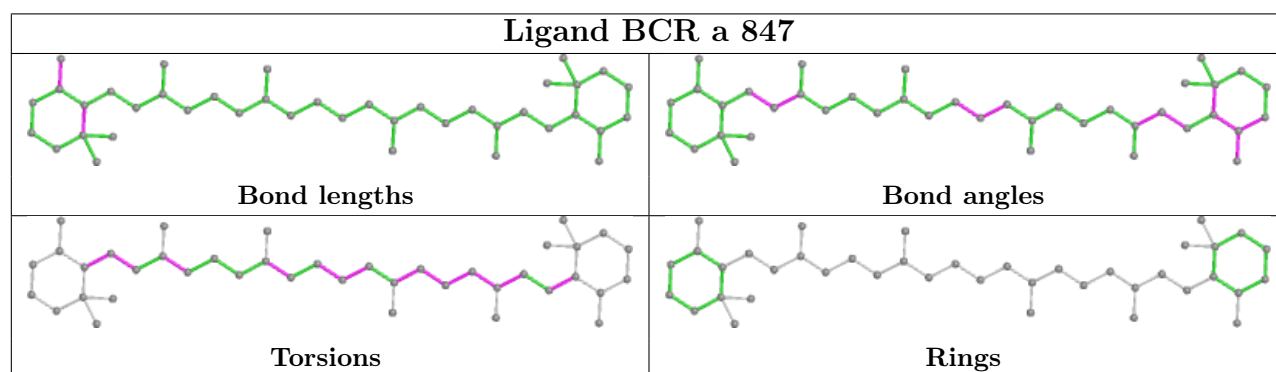
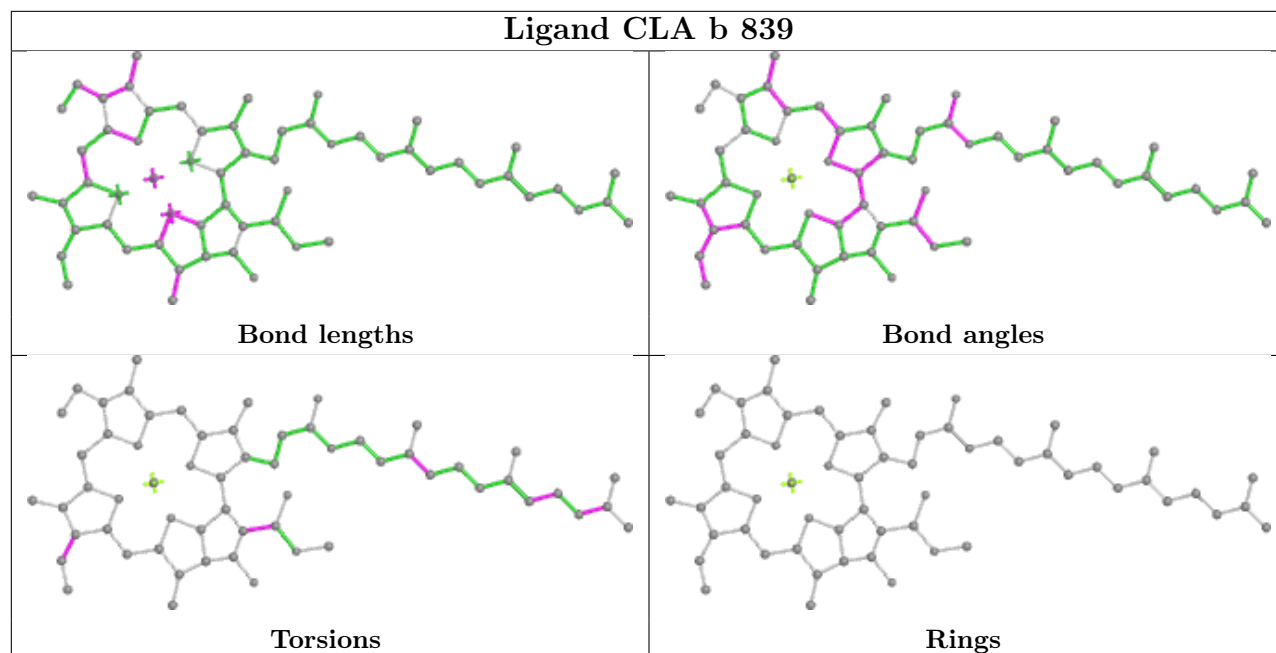
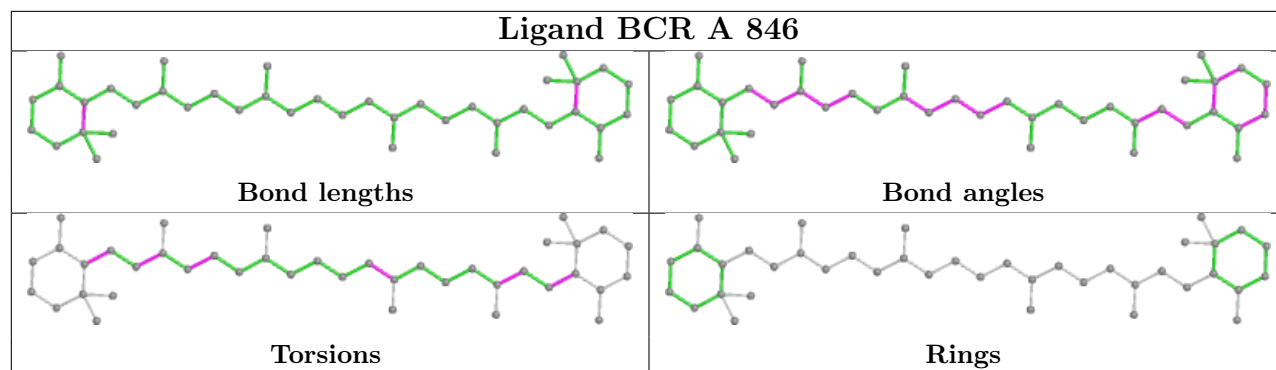


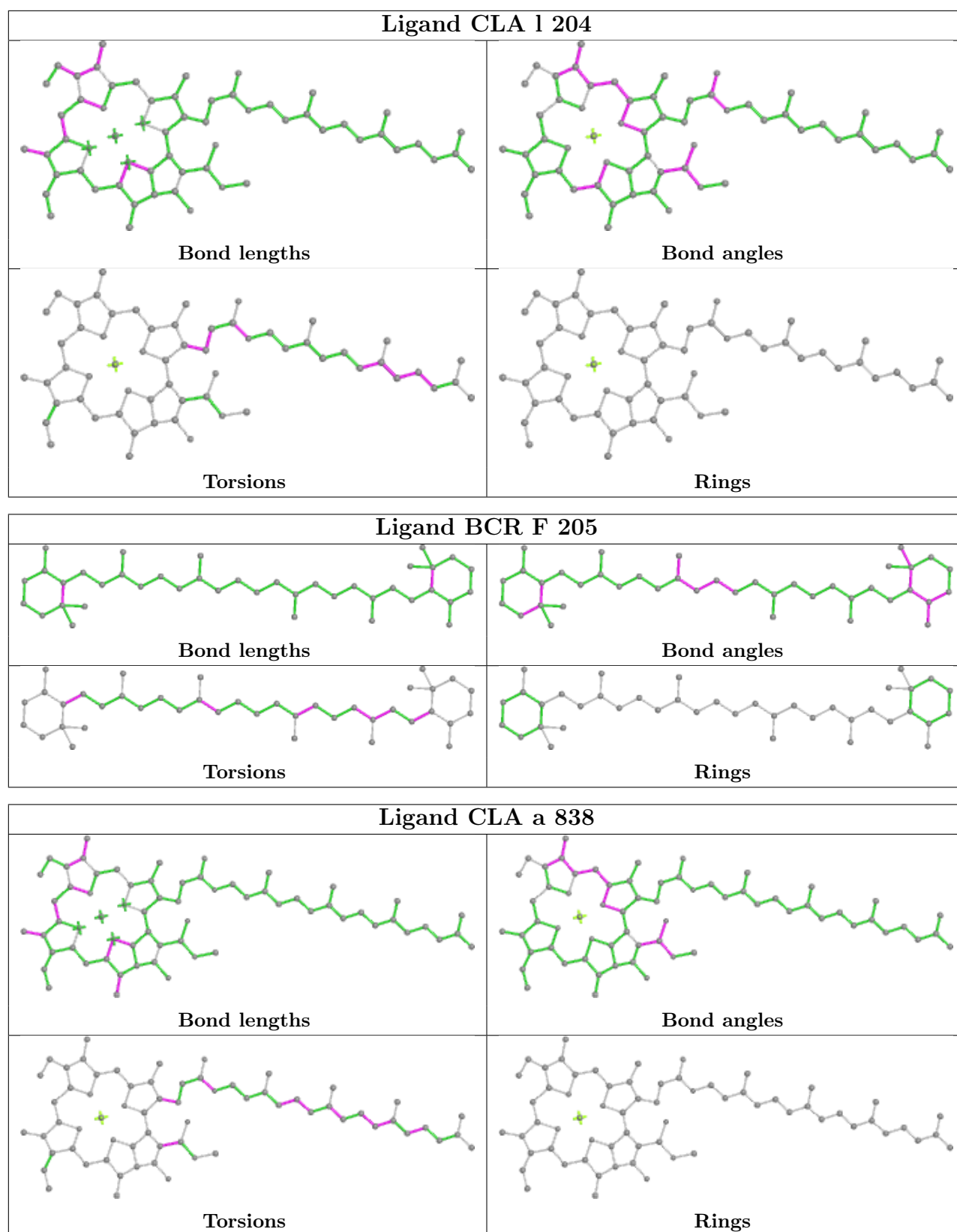
Ligand CLA A 836

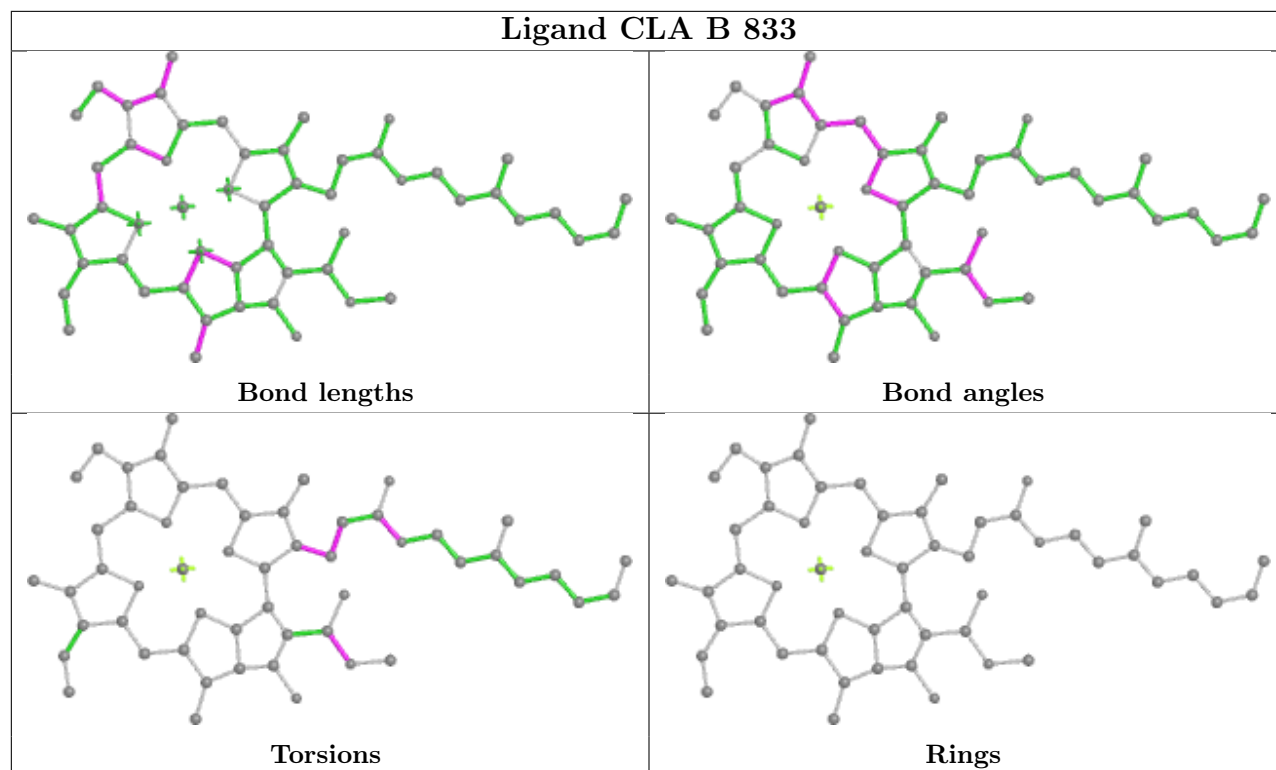
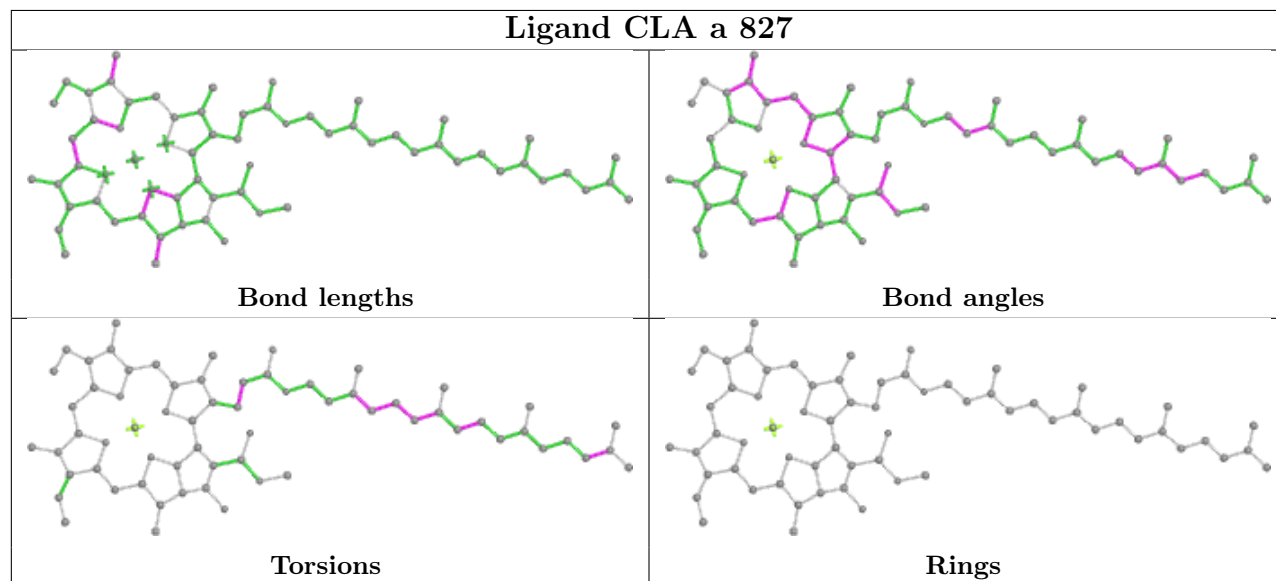


Ligand CLA B 831

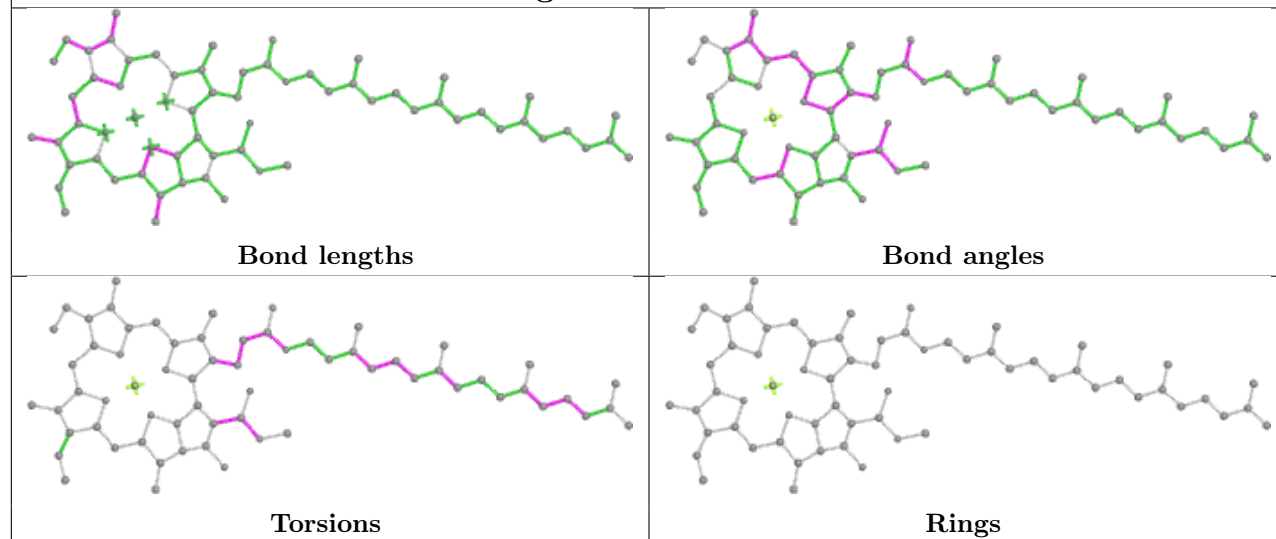




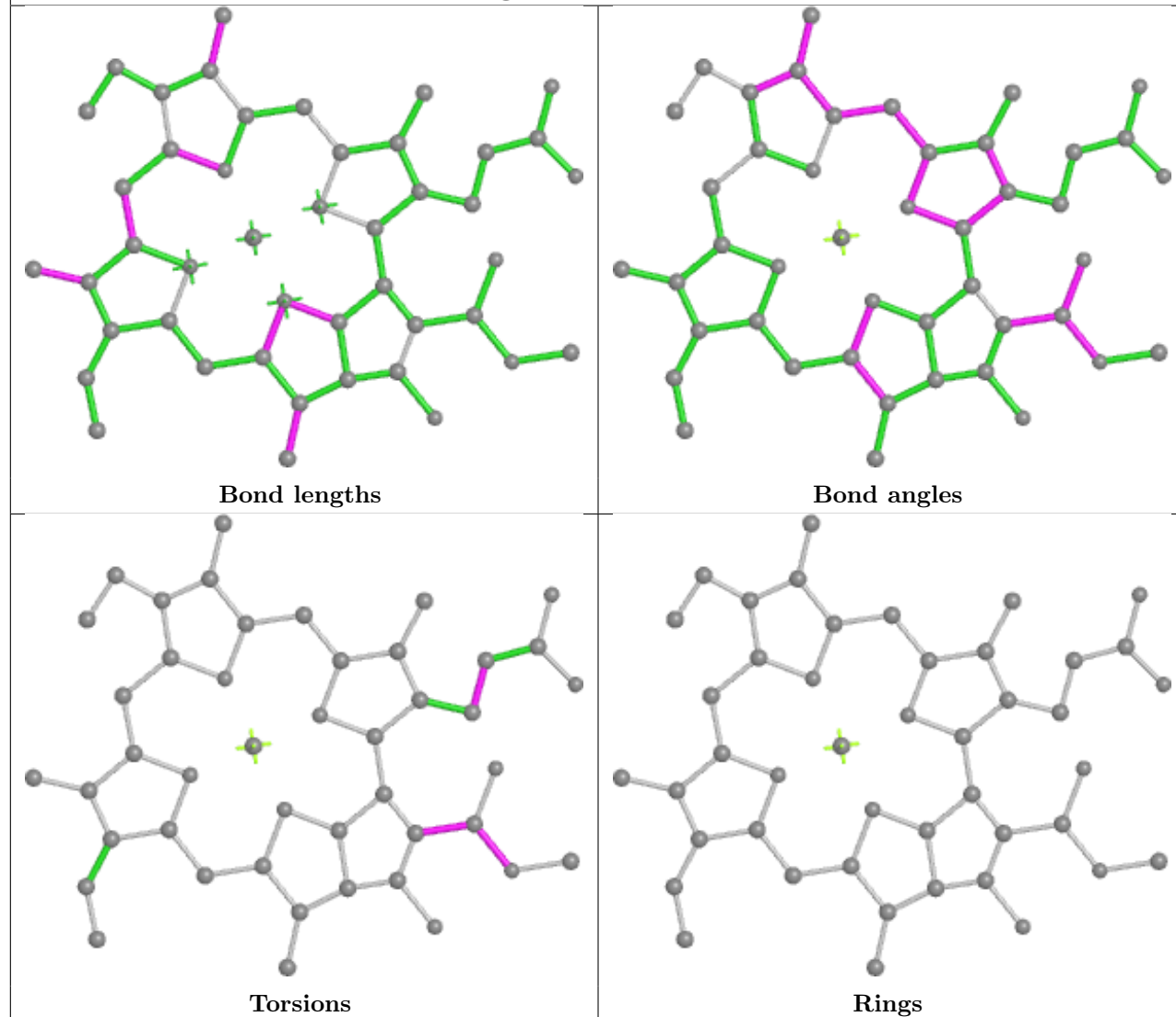


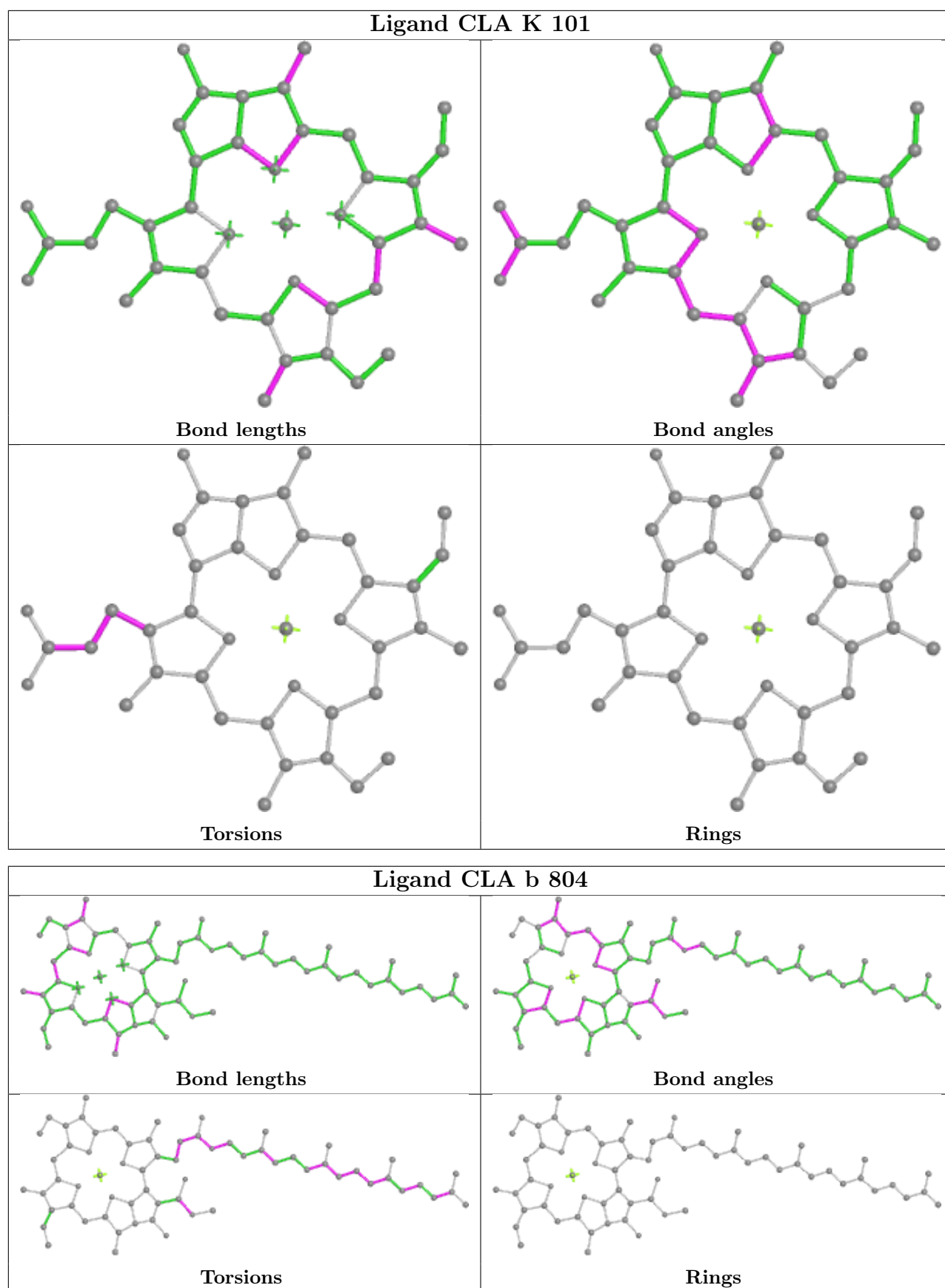
Ligand CLA B 833**Ligand CLA a 827**

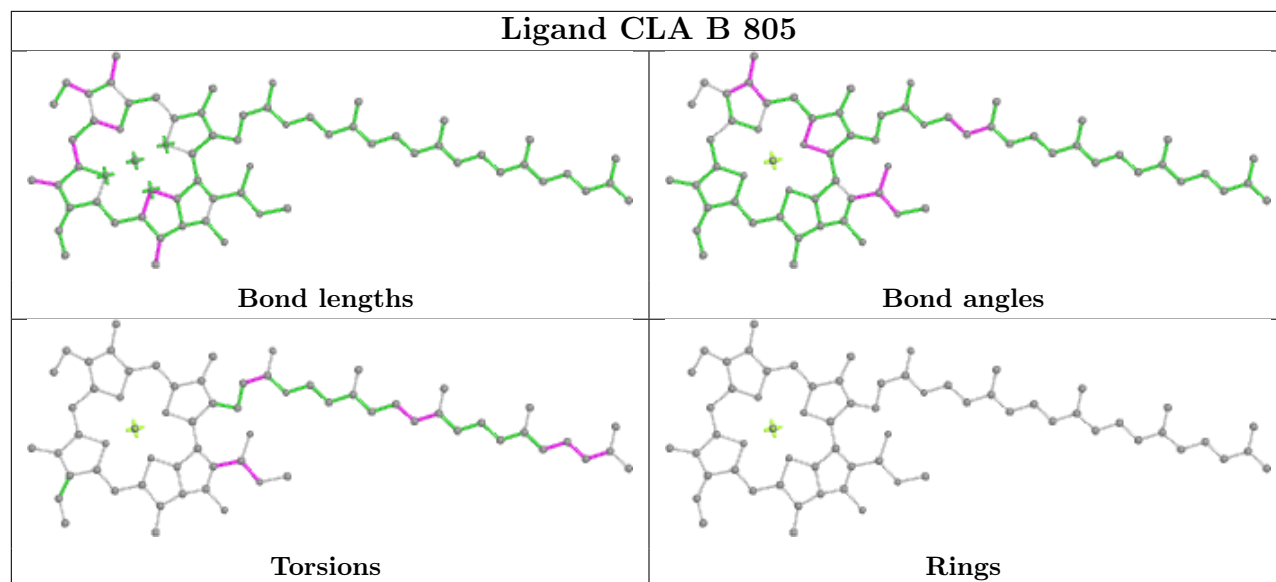
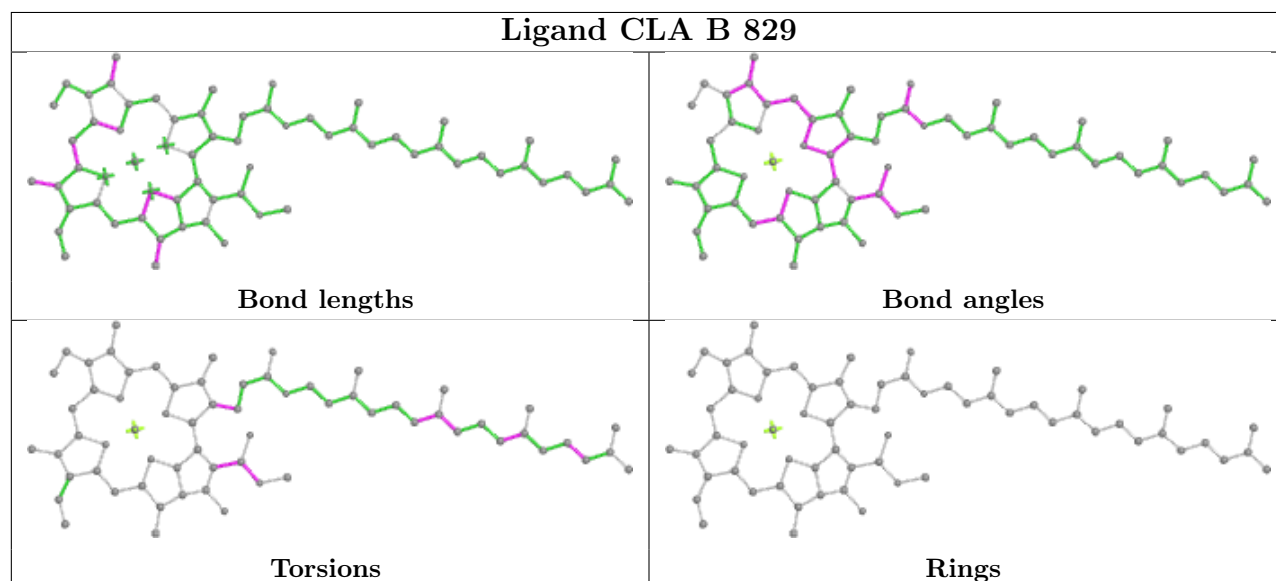
Ligand CLA a 807



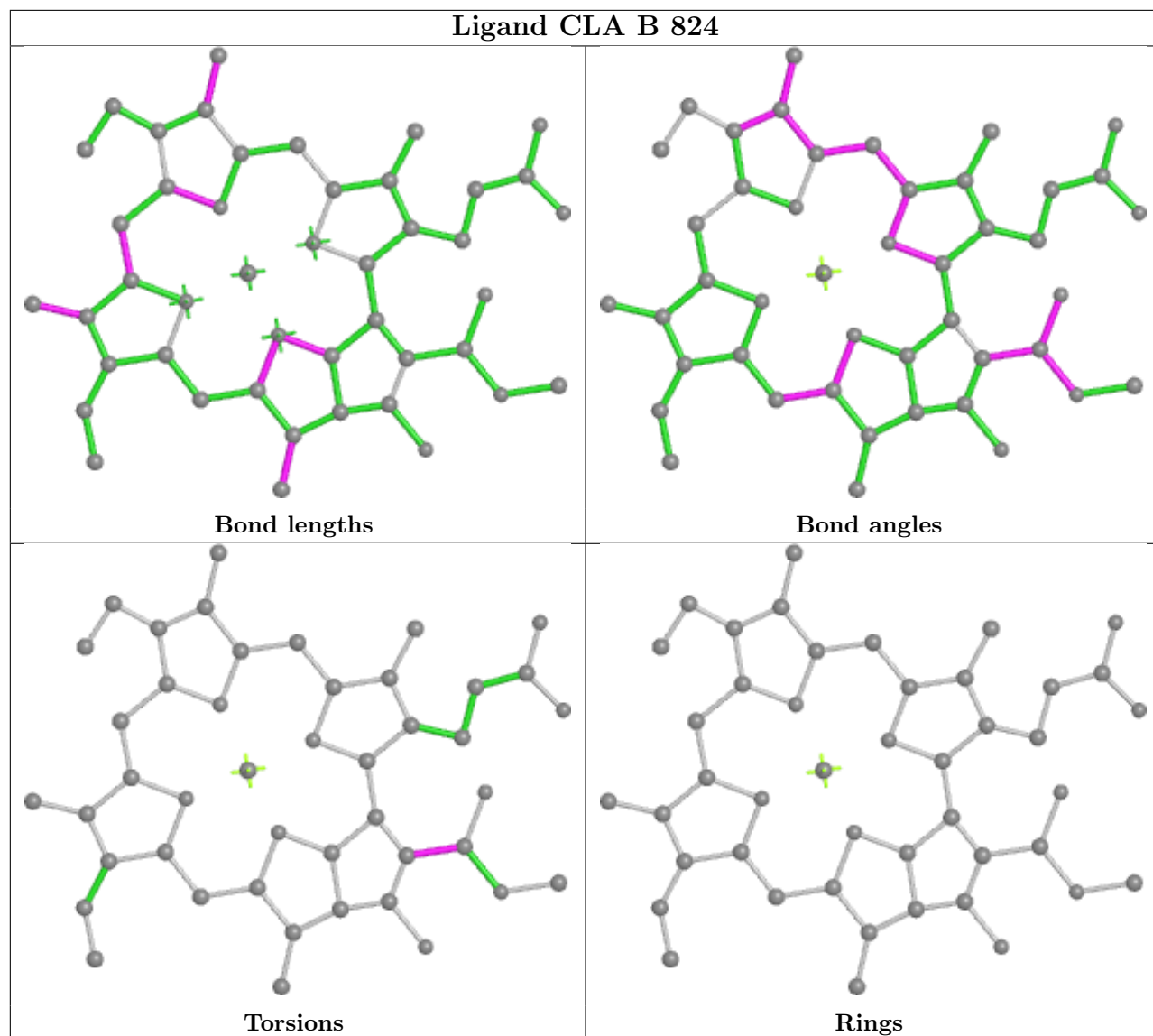
Ligand CLA l 205



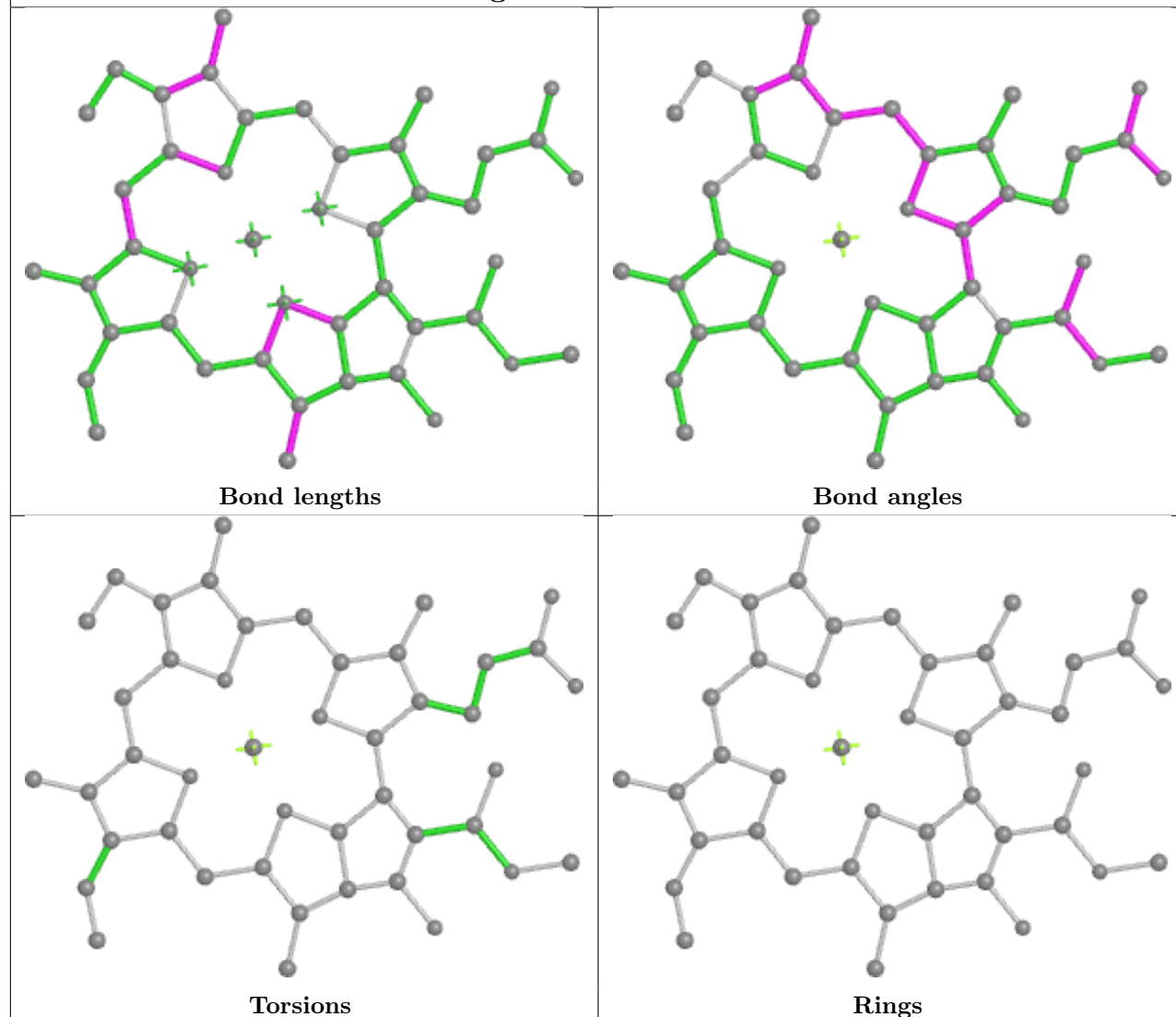


Ligand CLA B 805**Ligand CLA B 829**

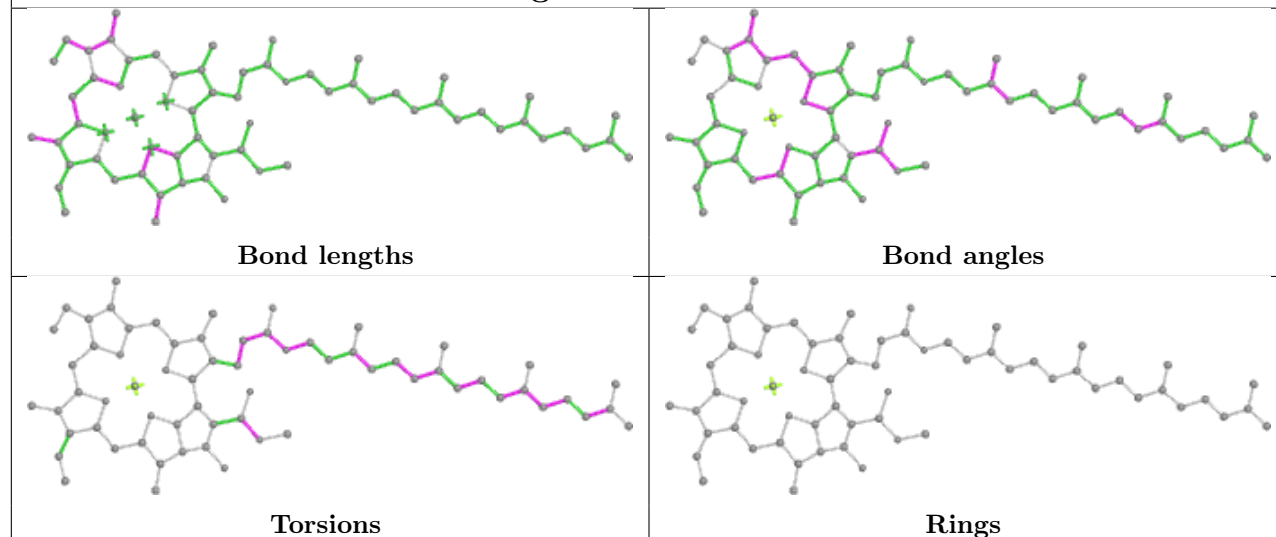
Ligand CLA B 824



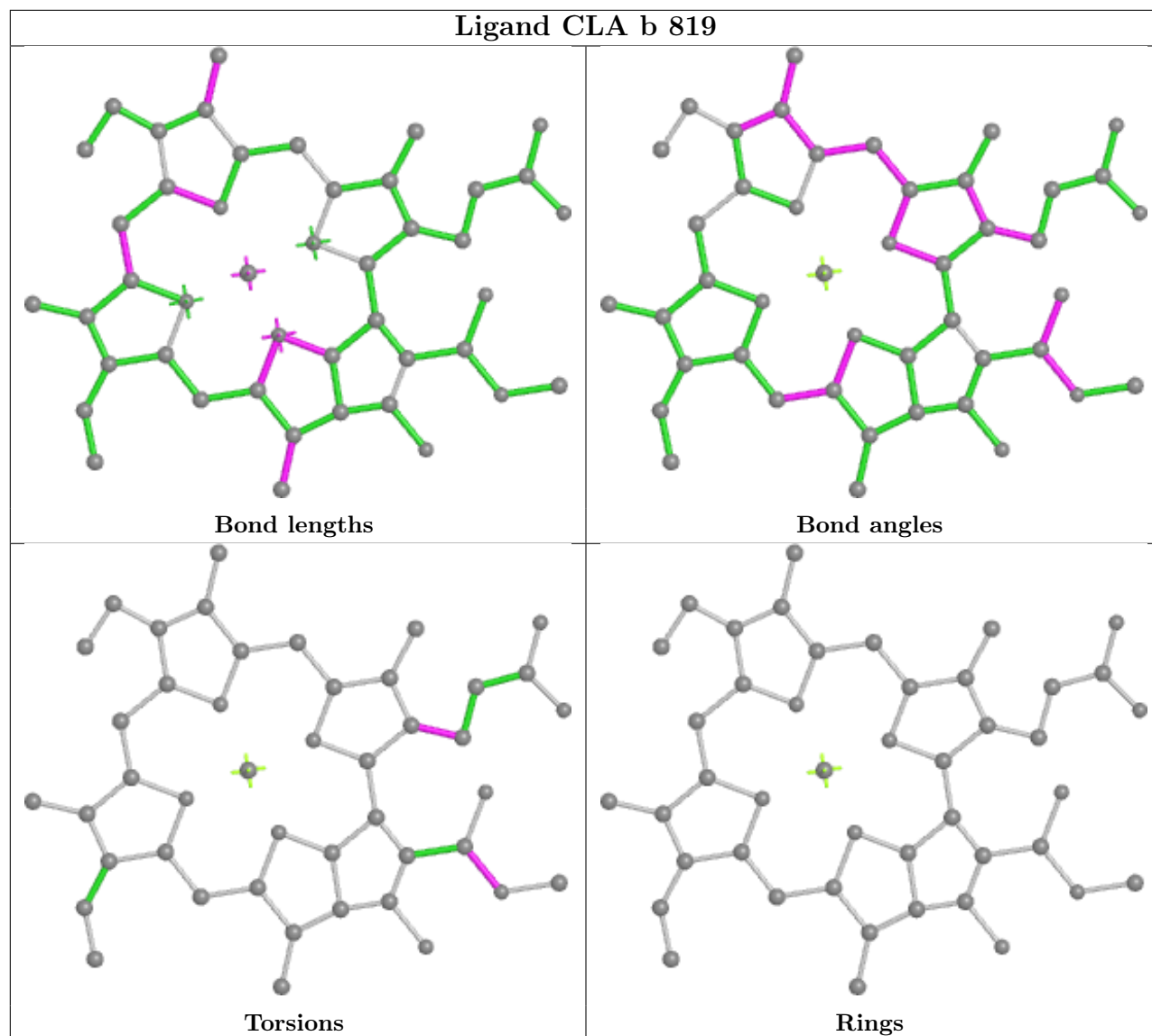
Ligand CLA A 816



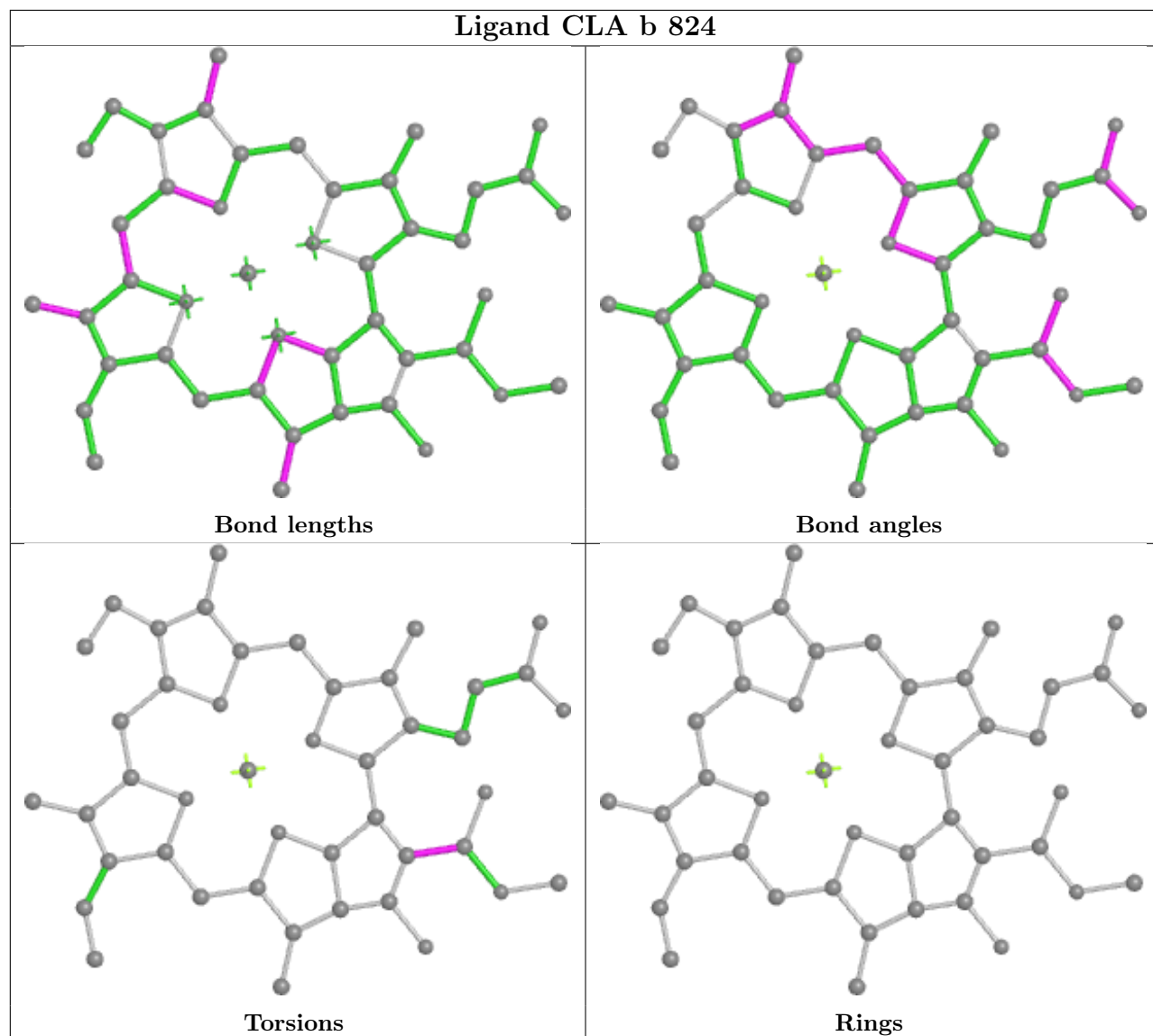
Ligand CLA A 842



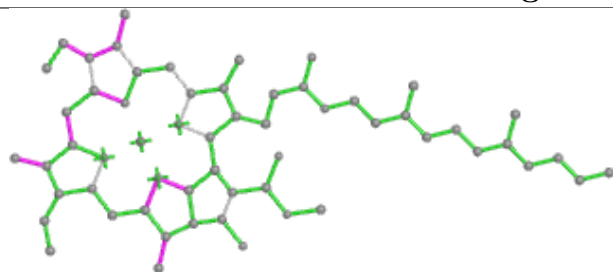
Ligand CLA b 819



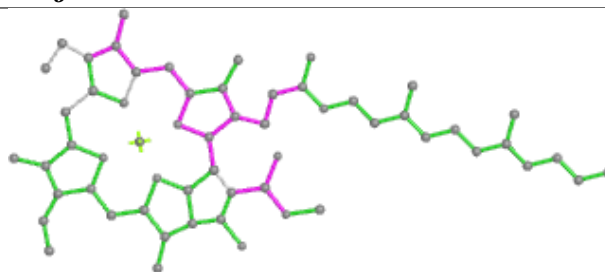
Ligand CLA b 824



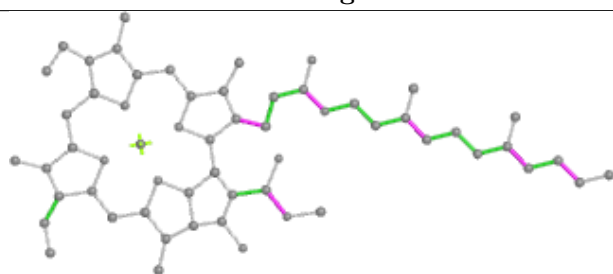
Ligand CLA j 101



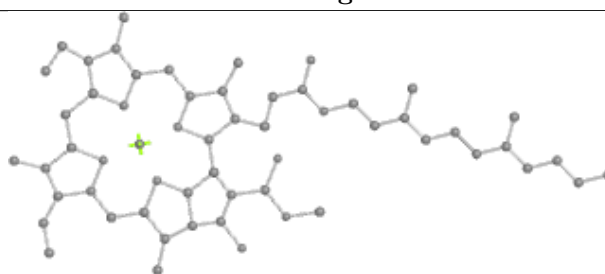
Bond lengths



Bond angles

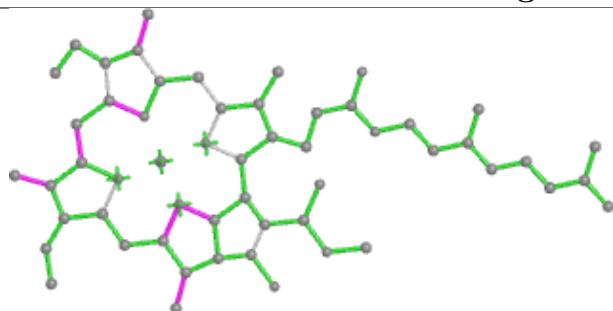


Torsions

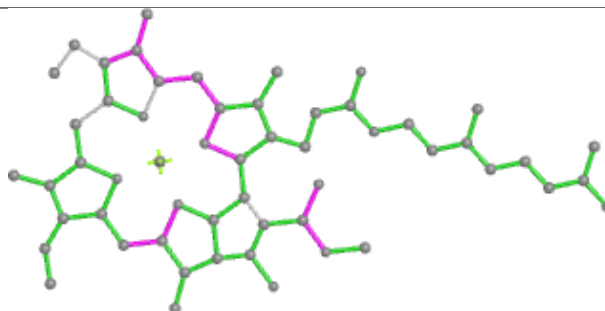


Rings

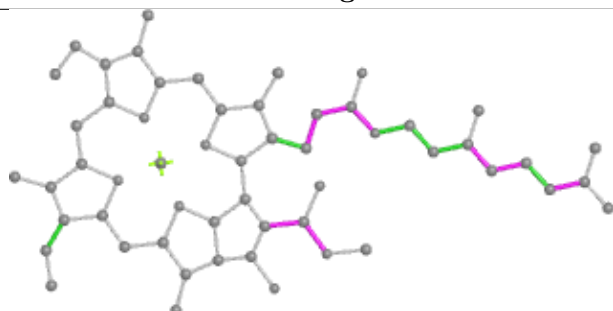
Ligand CLA b 825



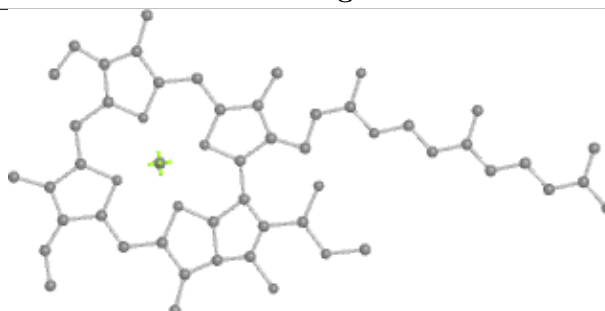
Bond lengths



Bond angles

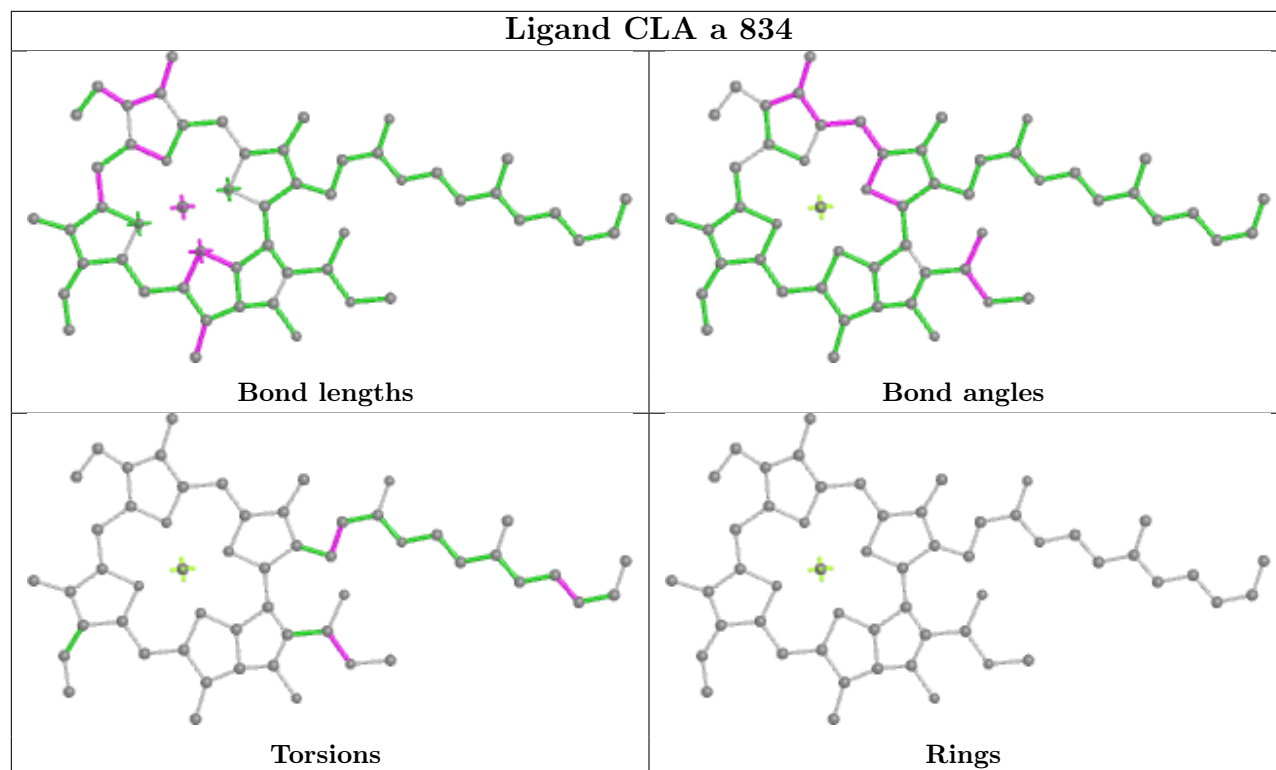


Torsions

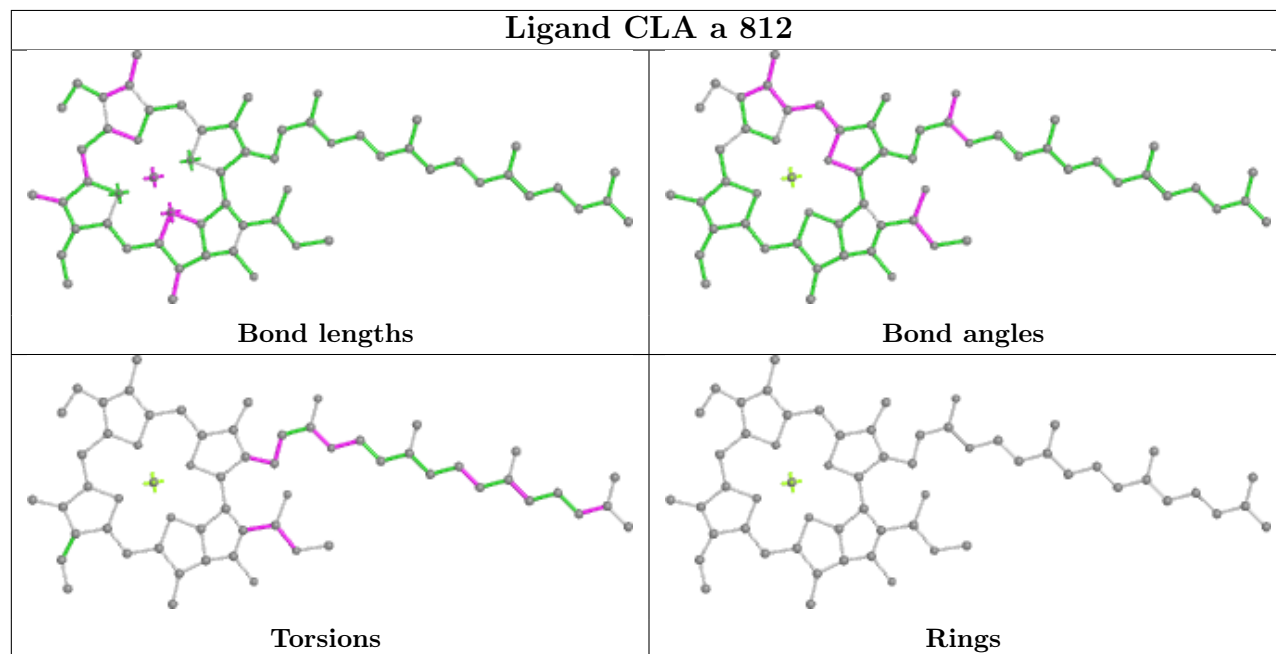


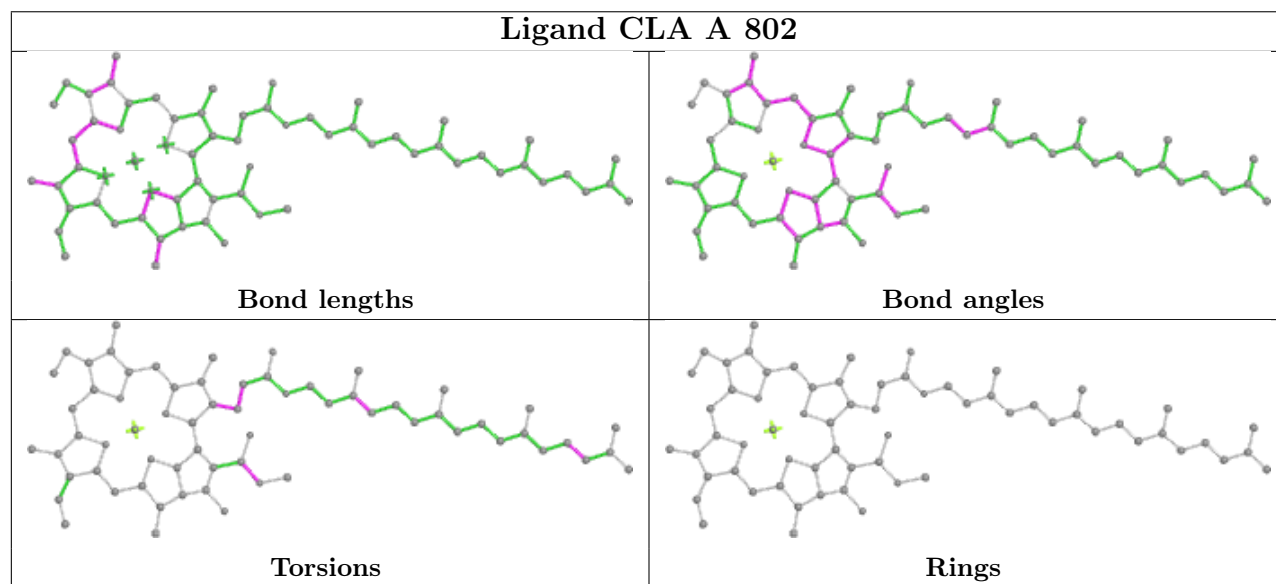
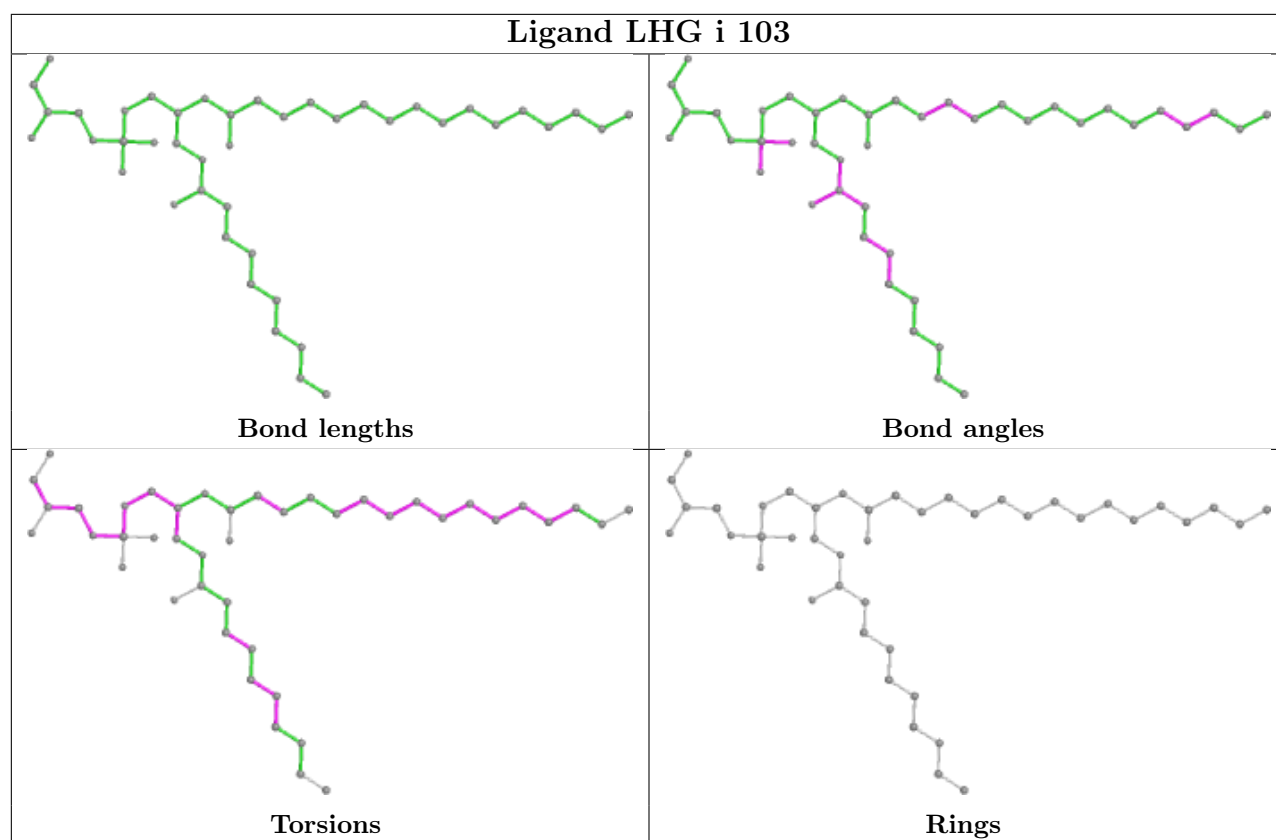
Rings

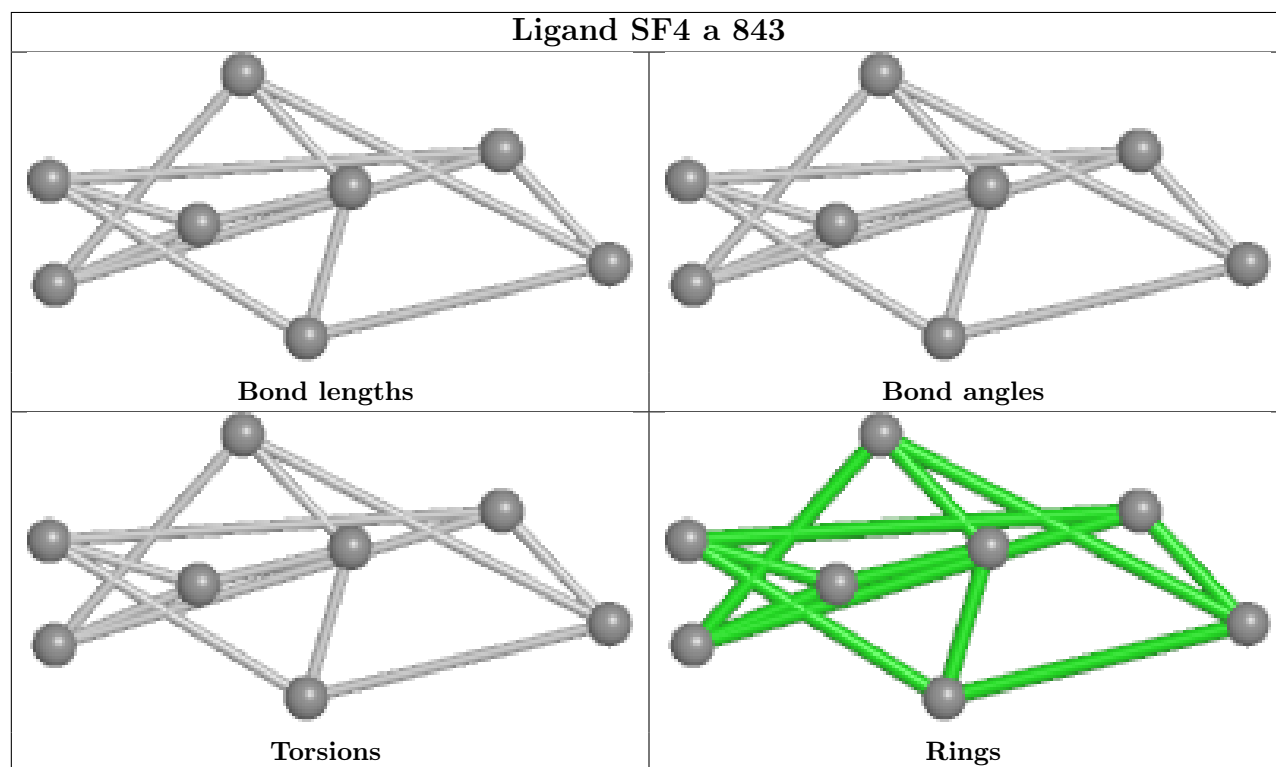
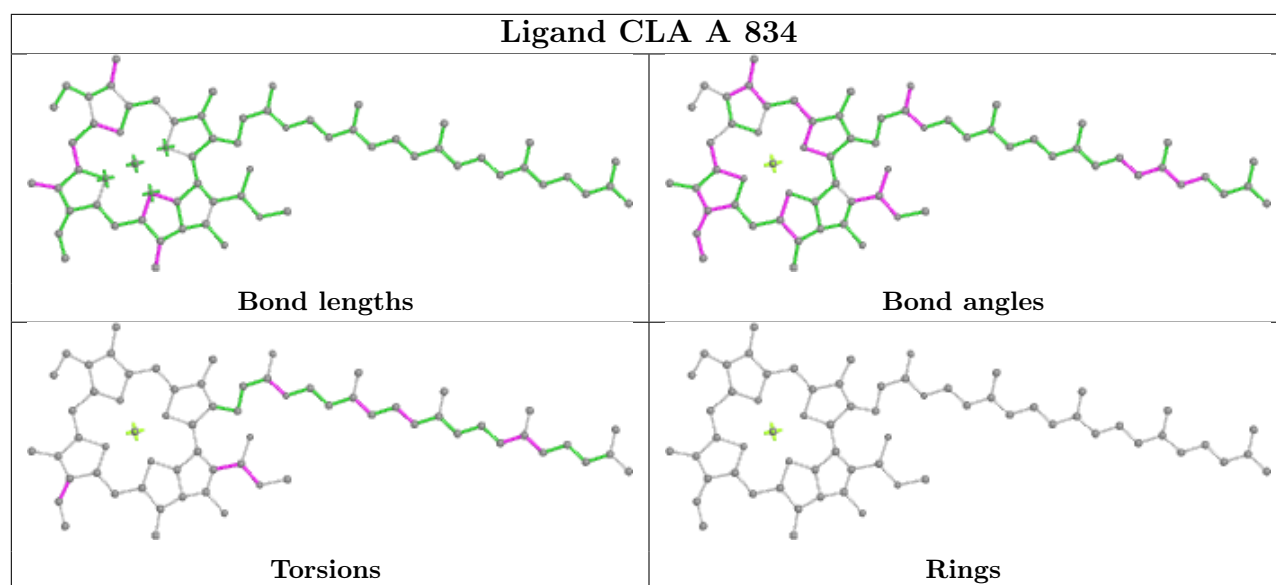
Ligand CLA a 834

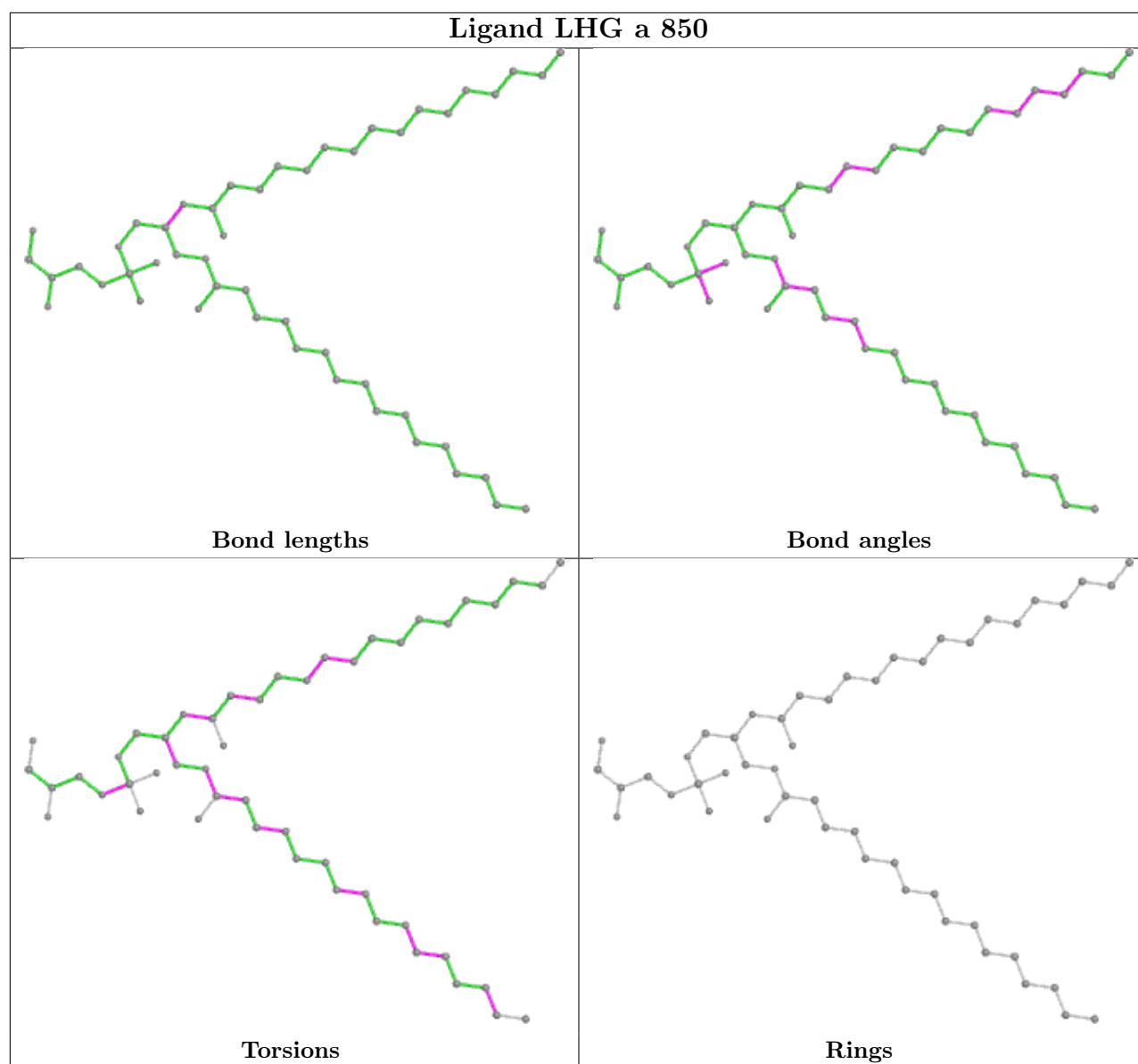


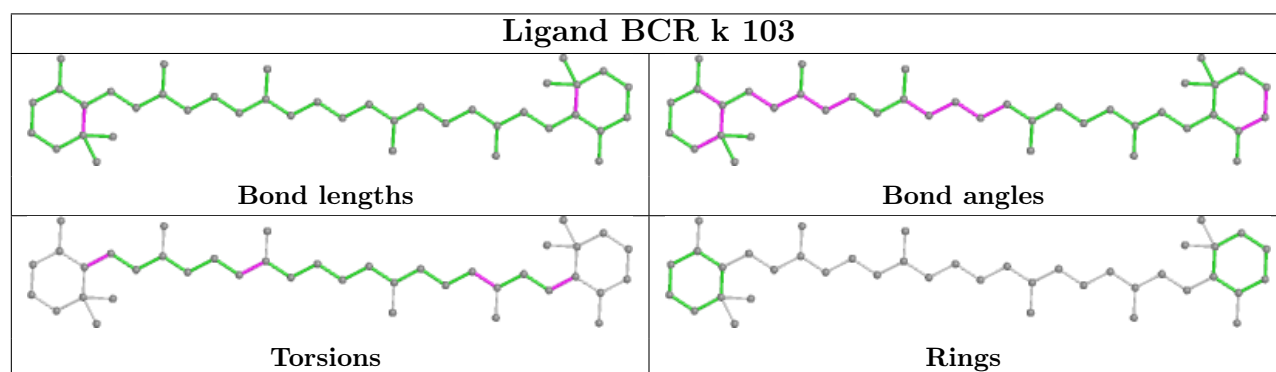
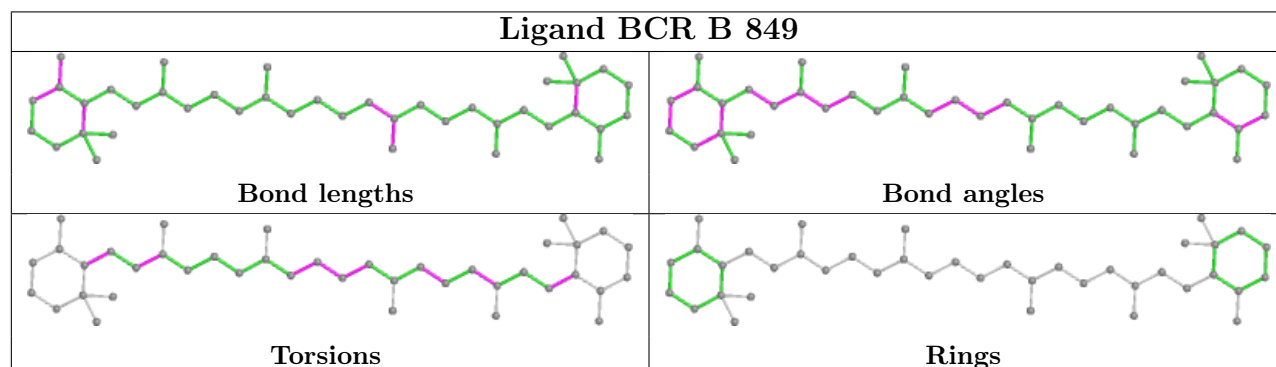
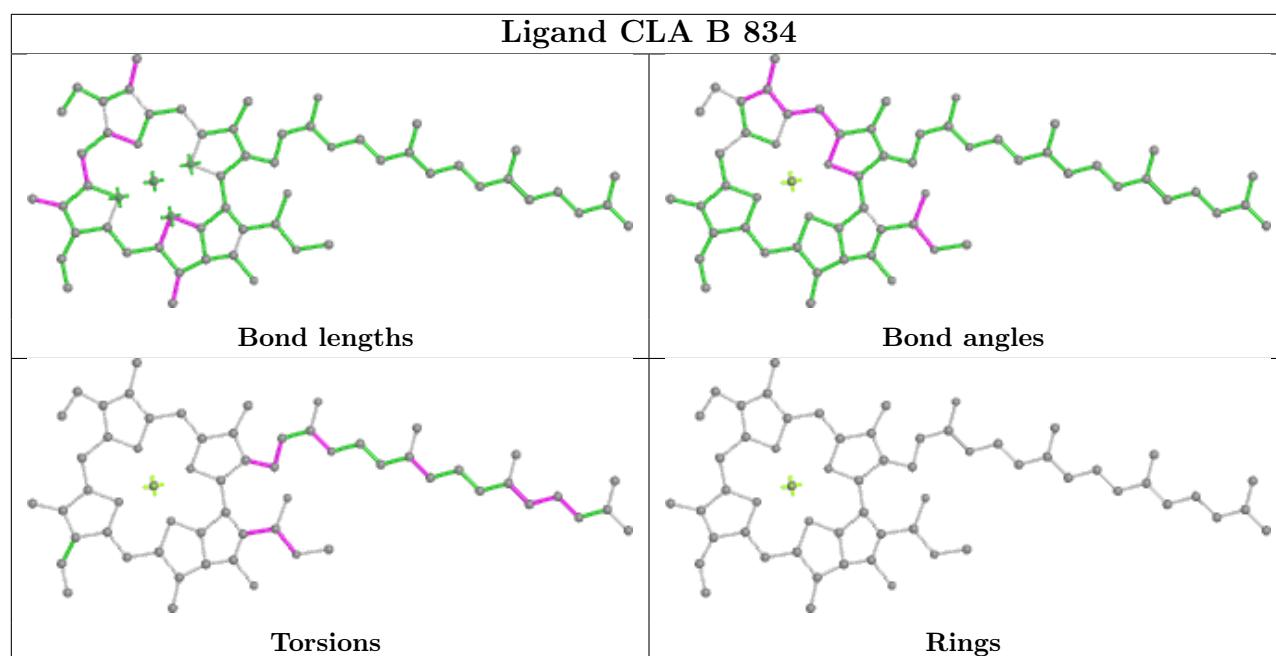
Ligand CLA a 812

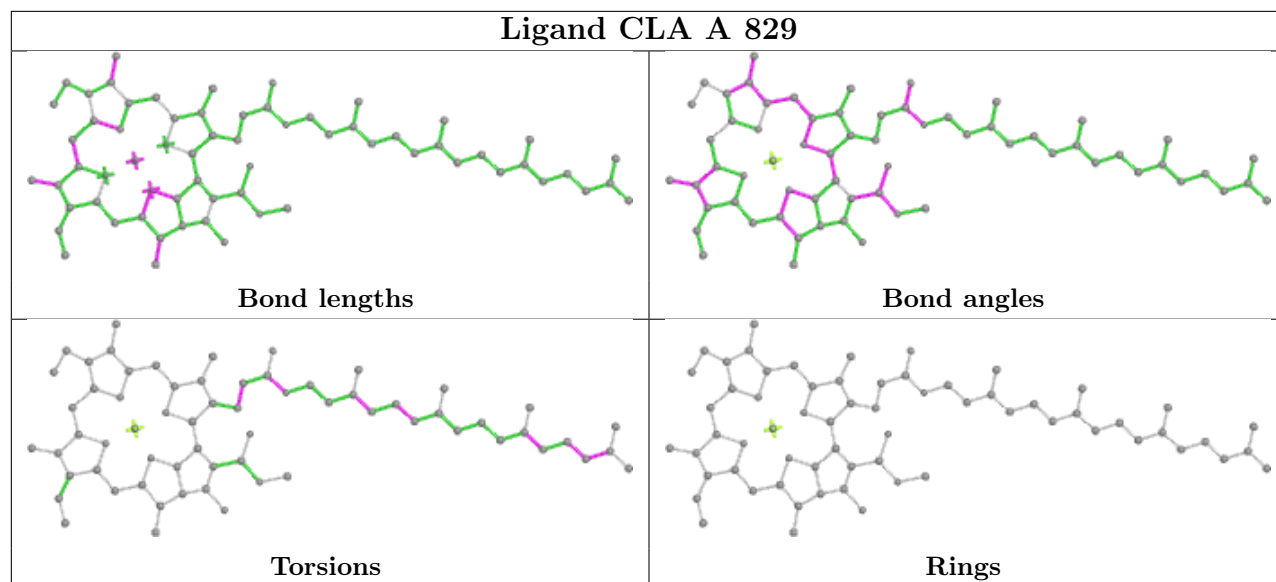
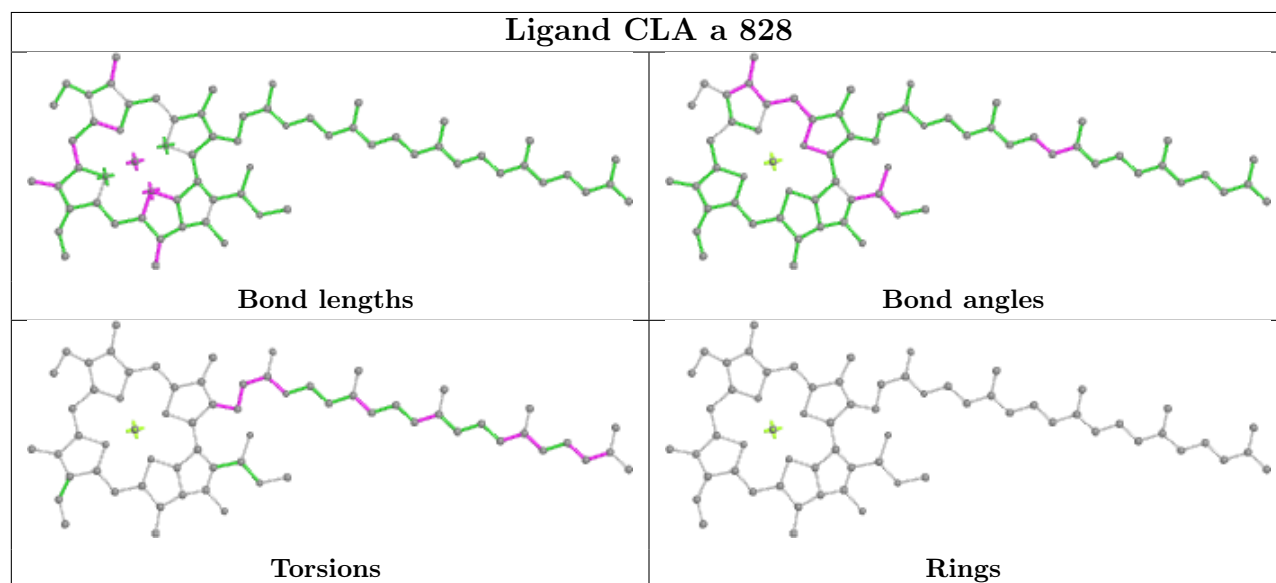


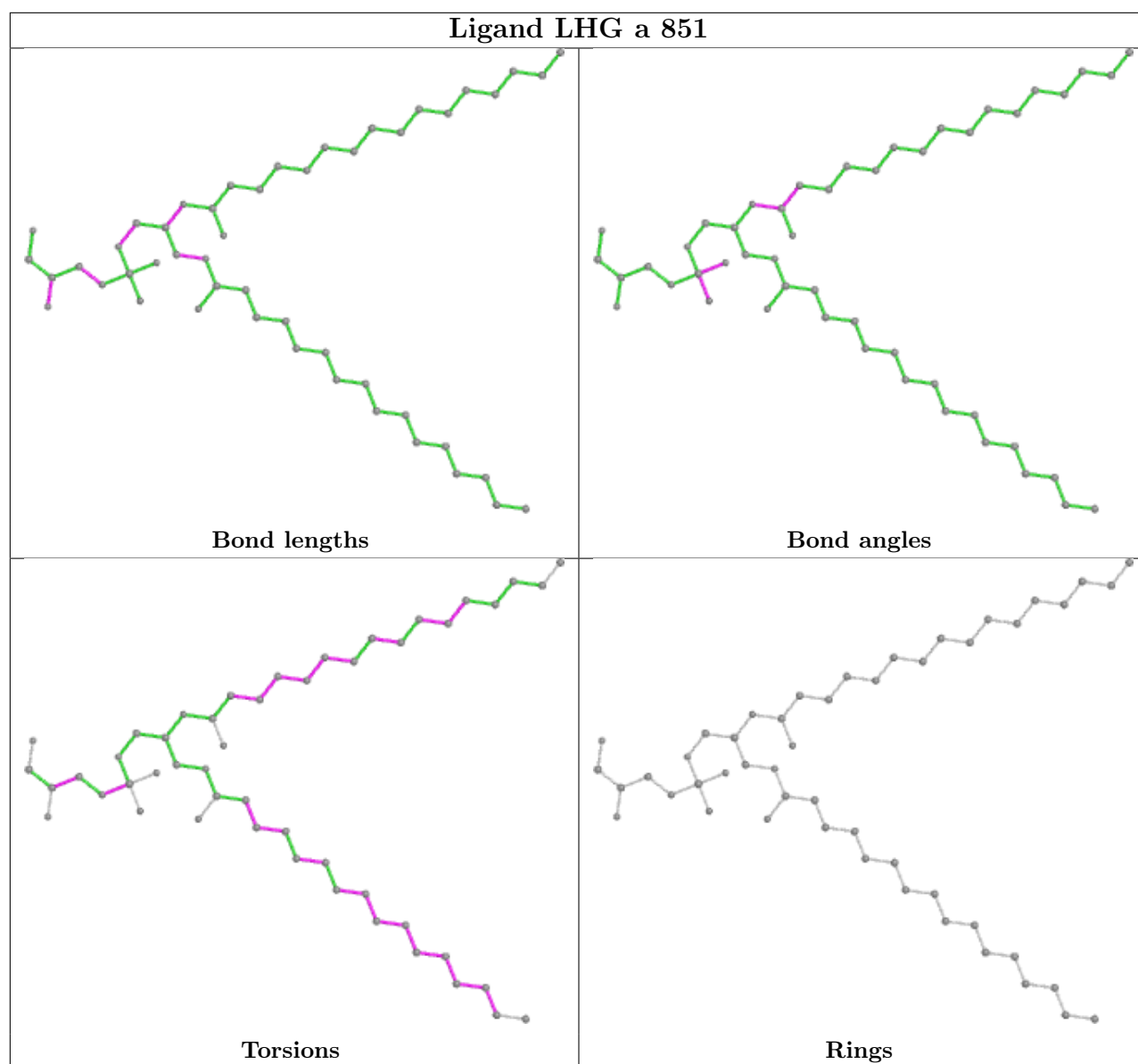


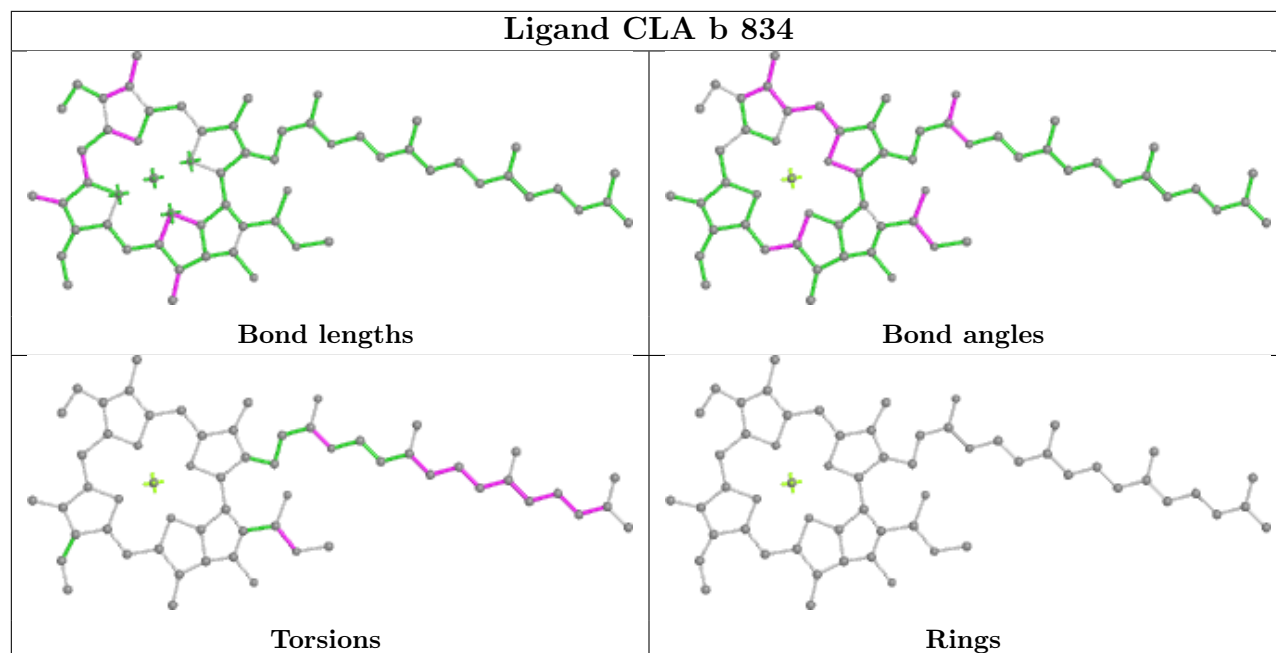
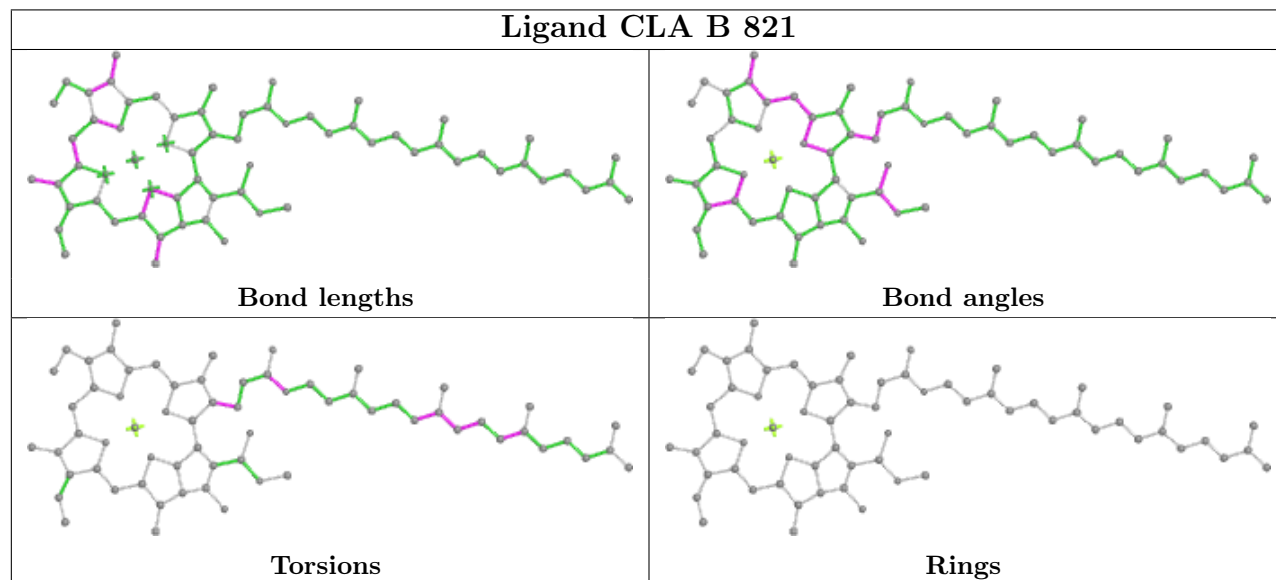




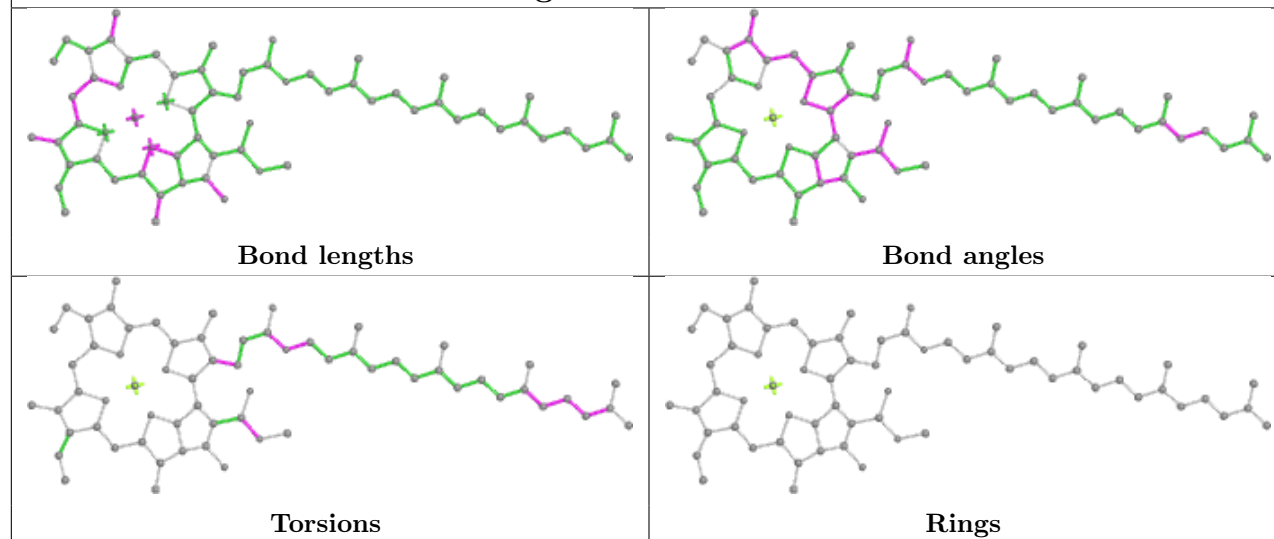


Ligand CLA A 829**Ligand CLA a 828**

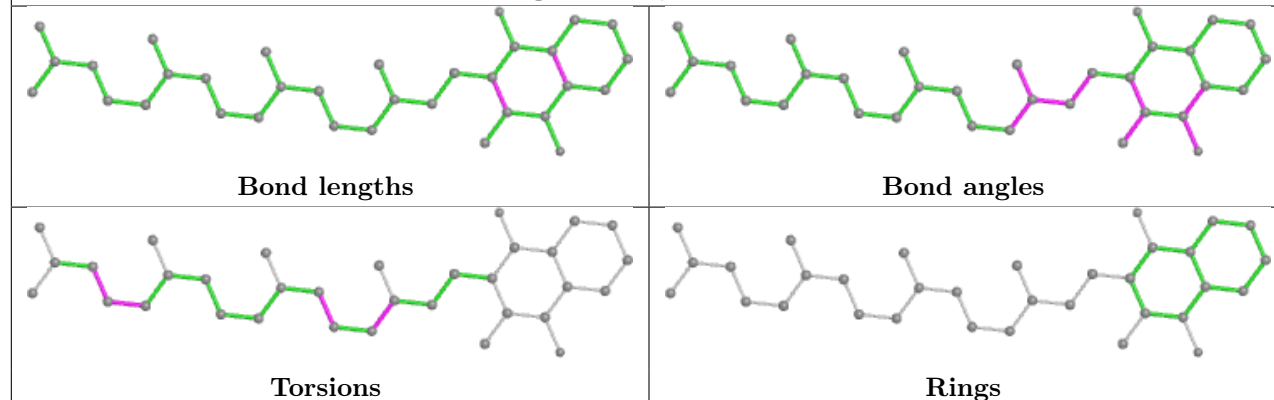


Ligand CLA b 834**Ligand CLA B 821**

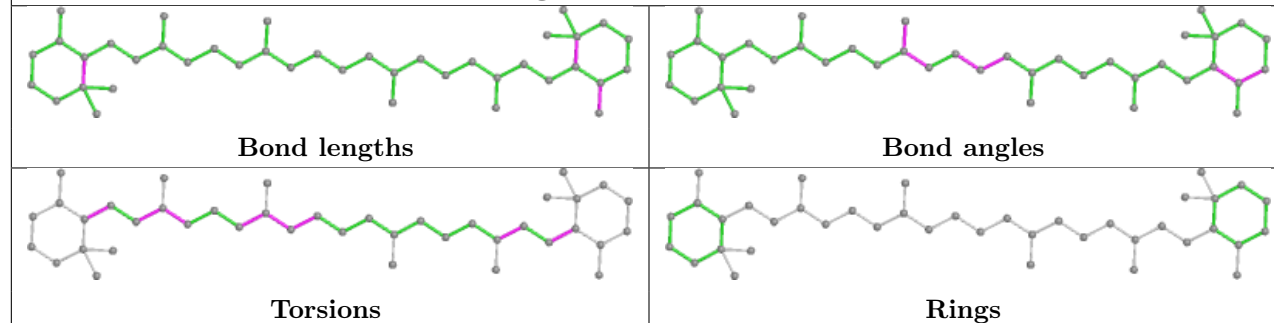
Ligand CLA b 808



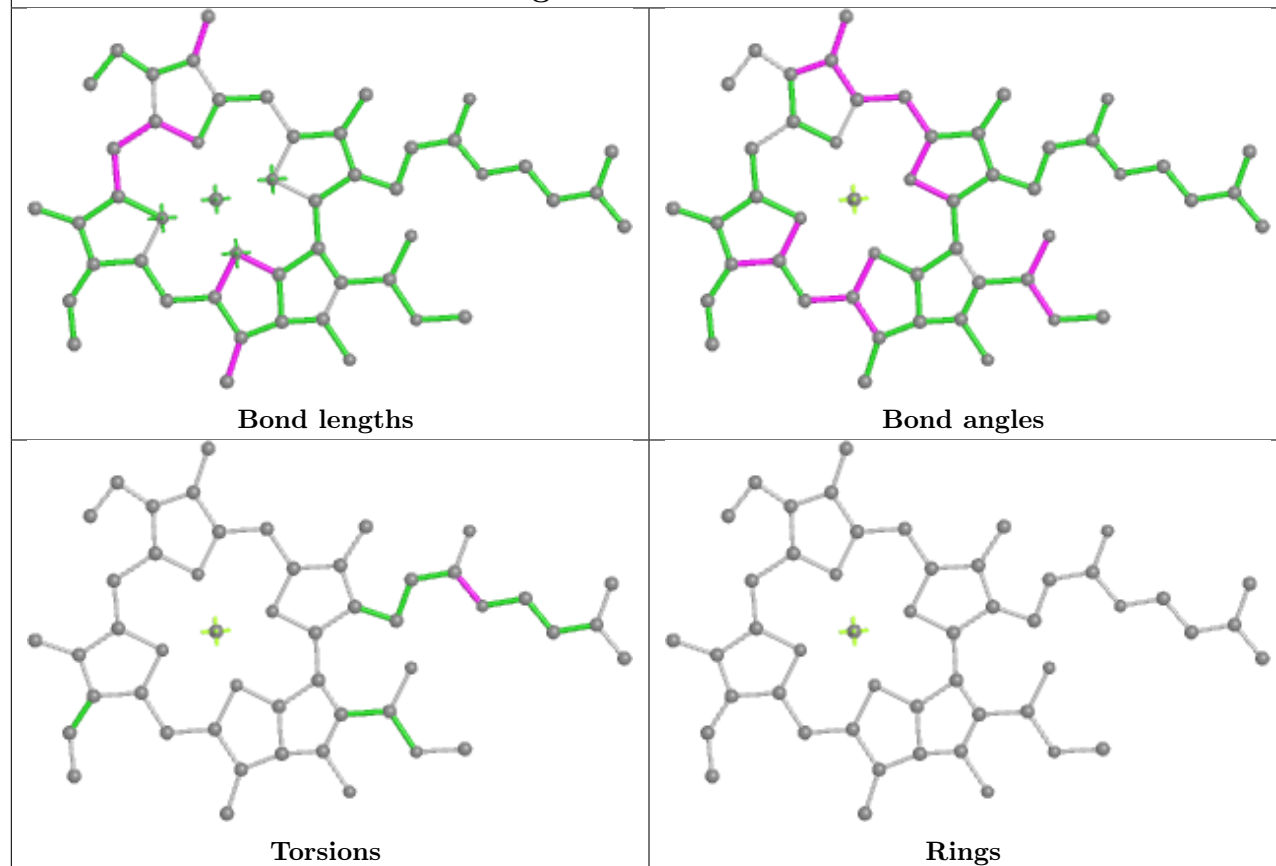
Ligand PQN B 844



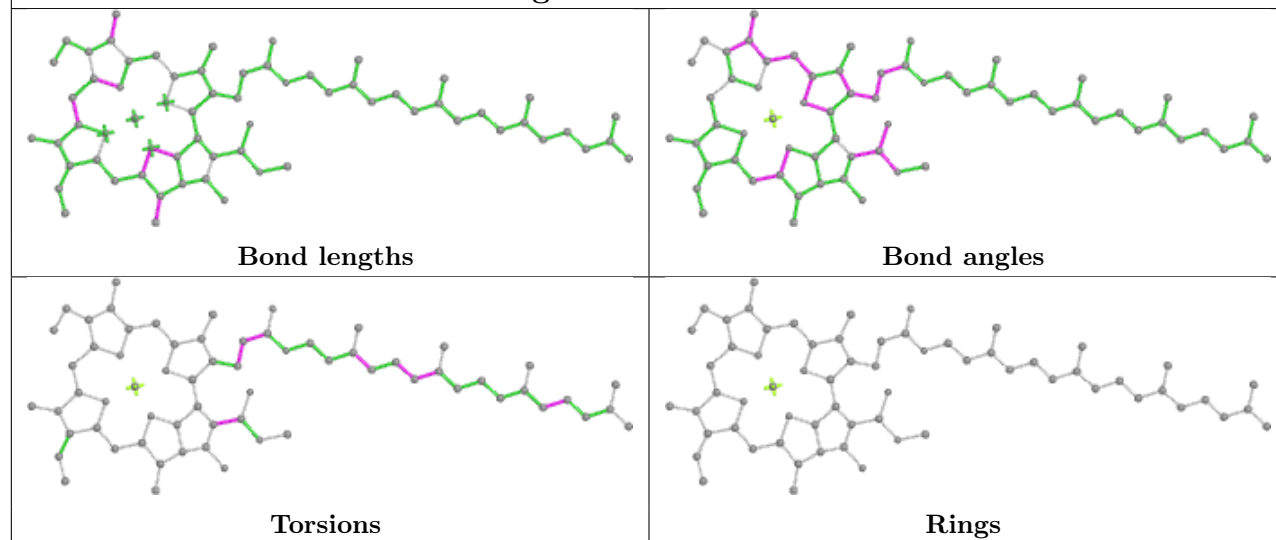
Ligand BCR b 850

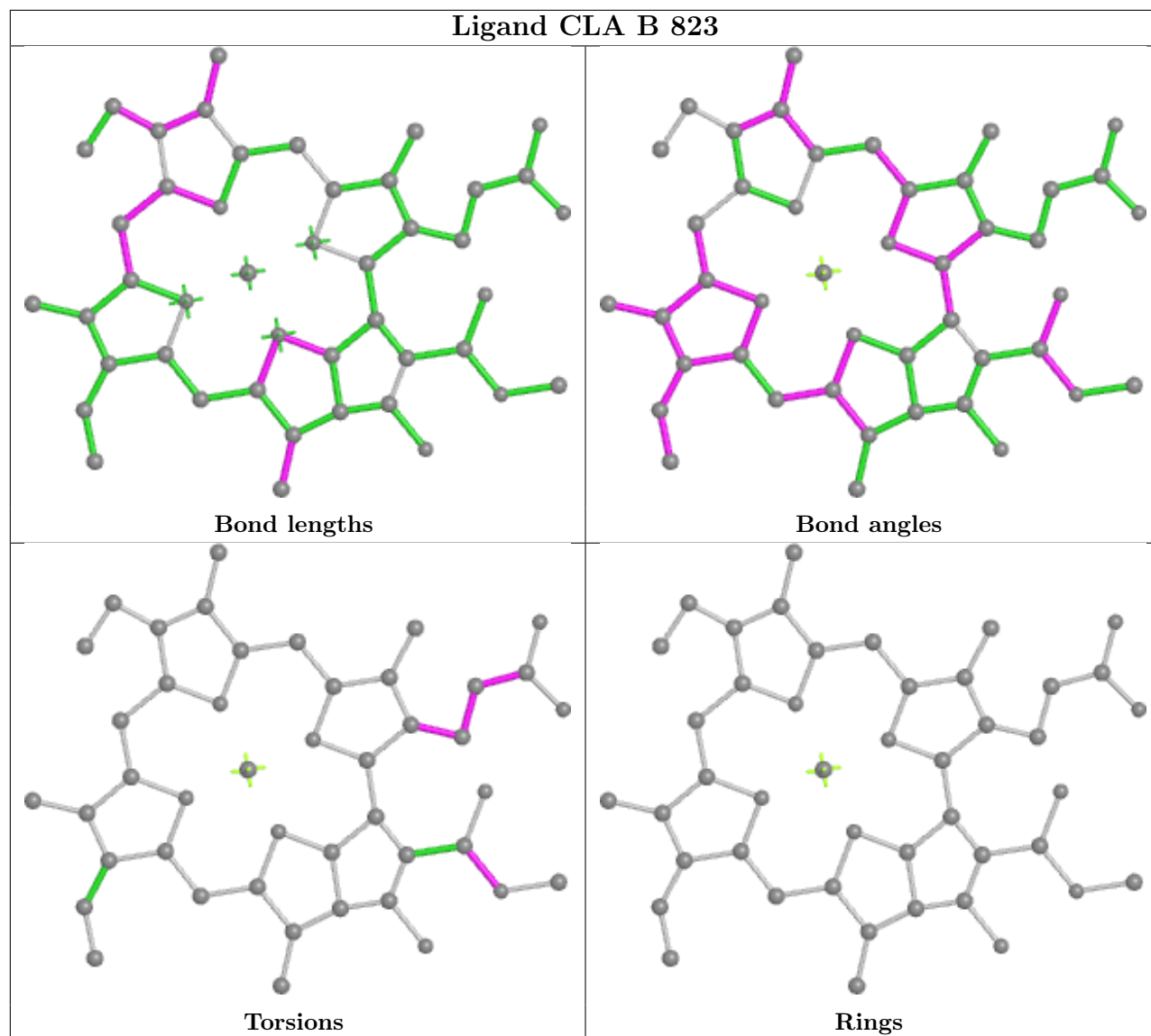
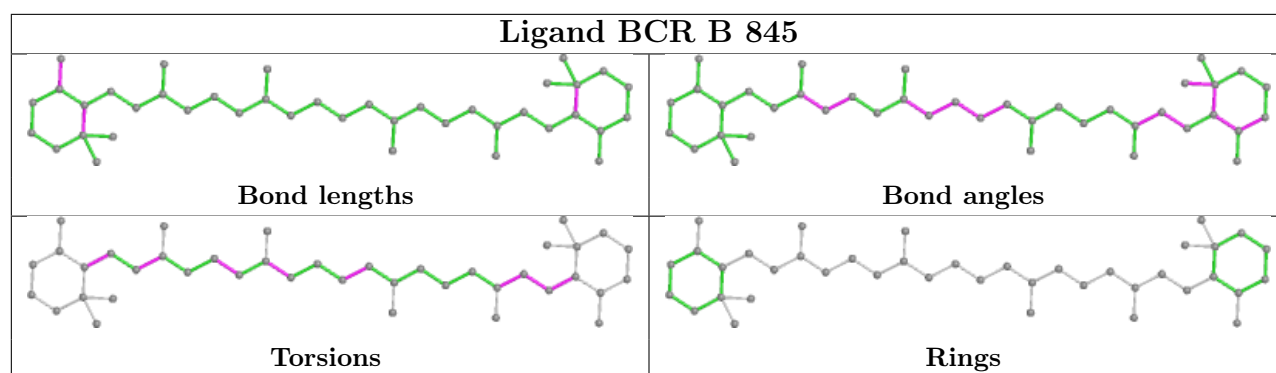


Ligand CLA B 817

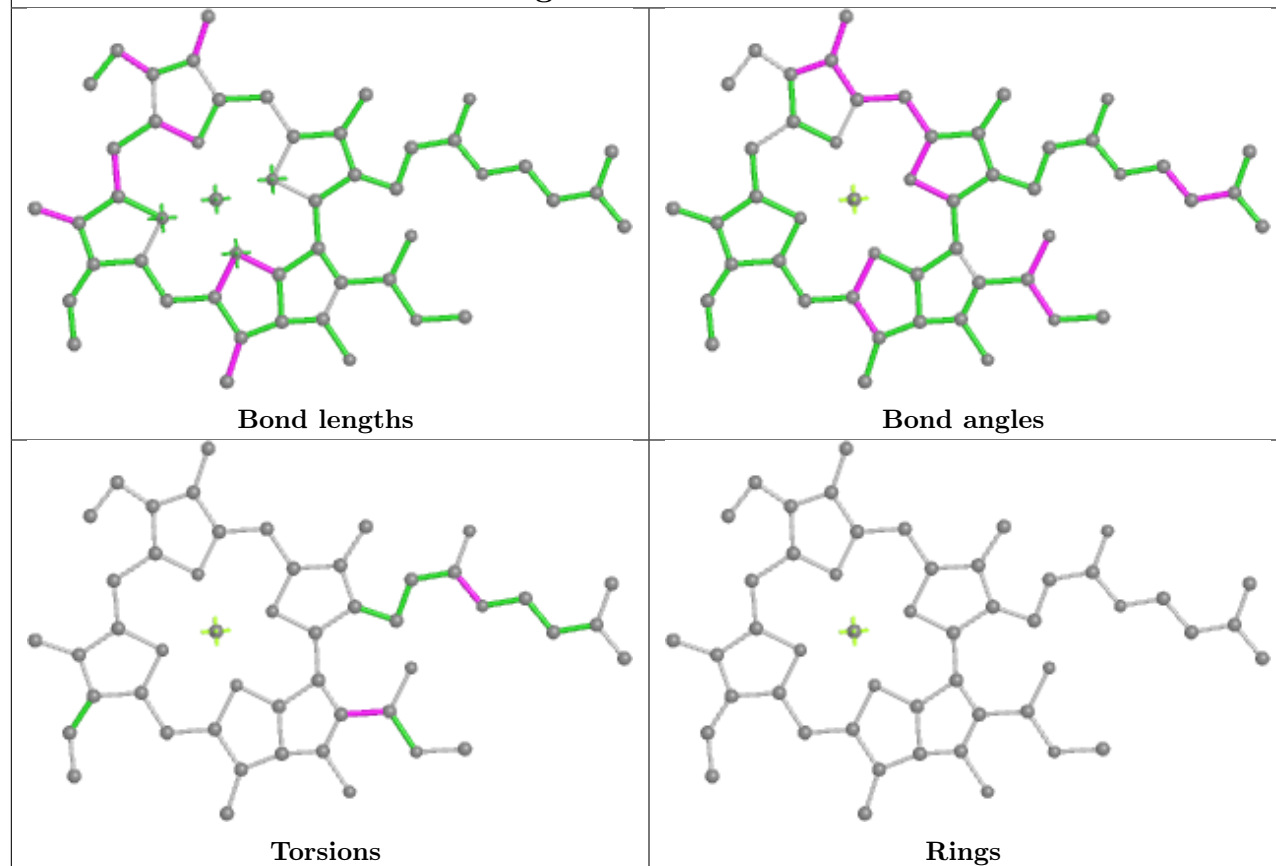


Ligand CLA B 826

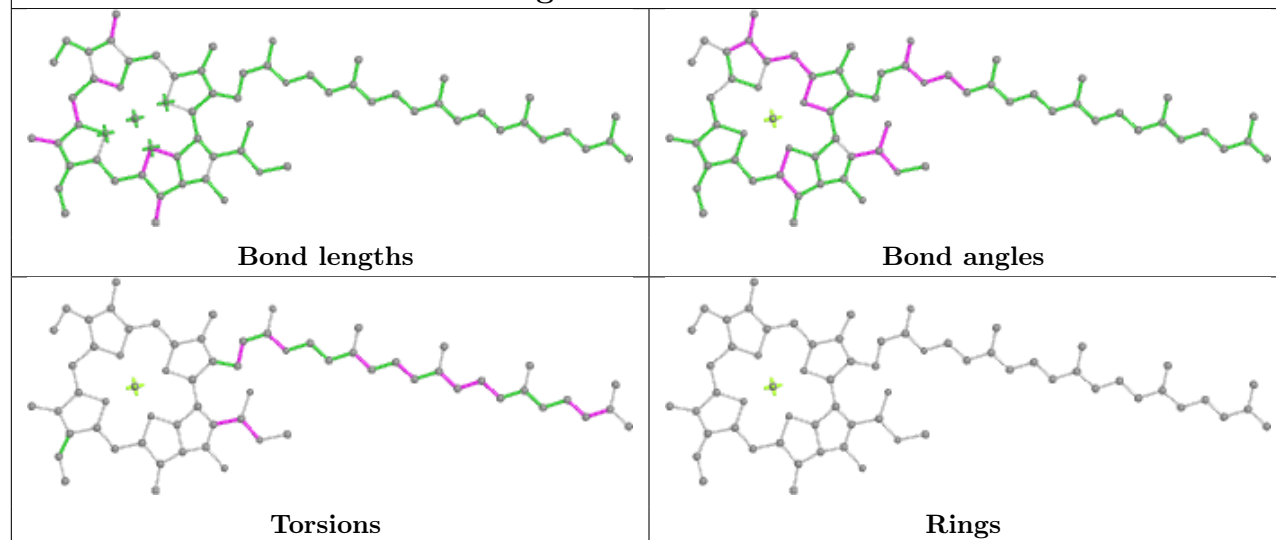


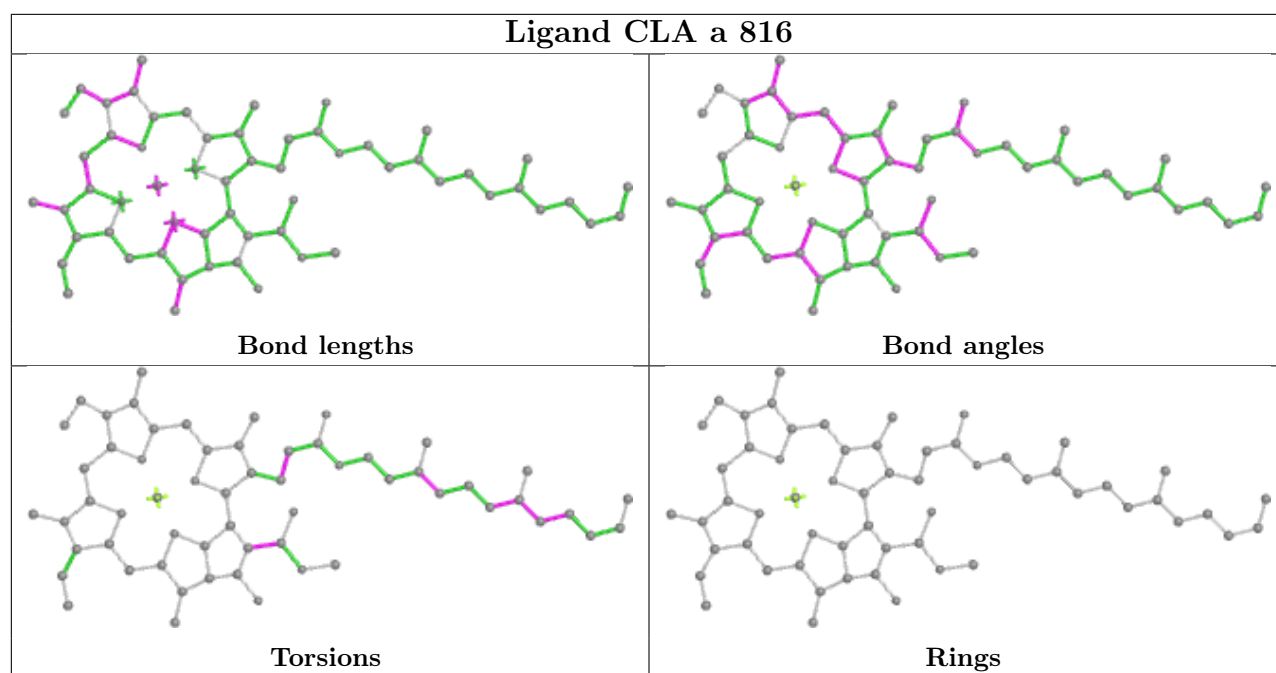


Ligand CLA b 817

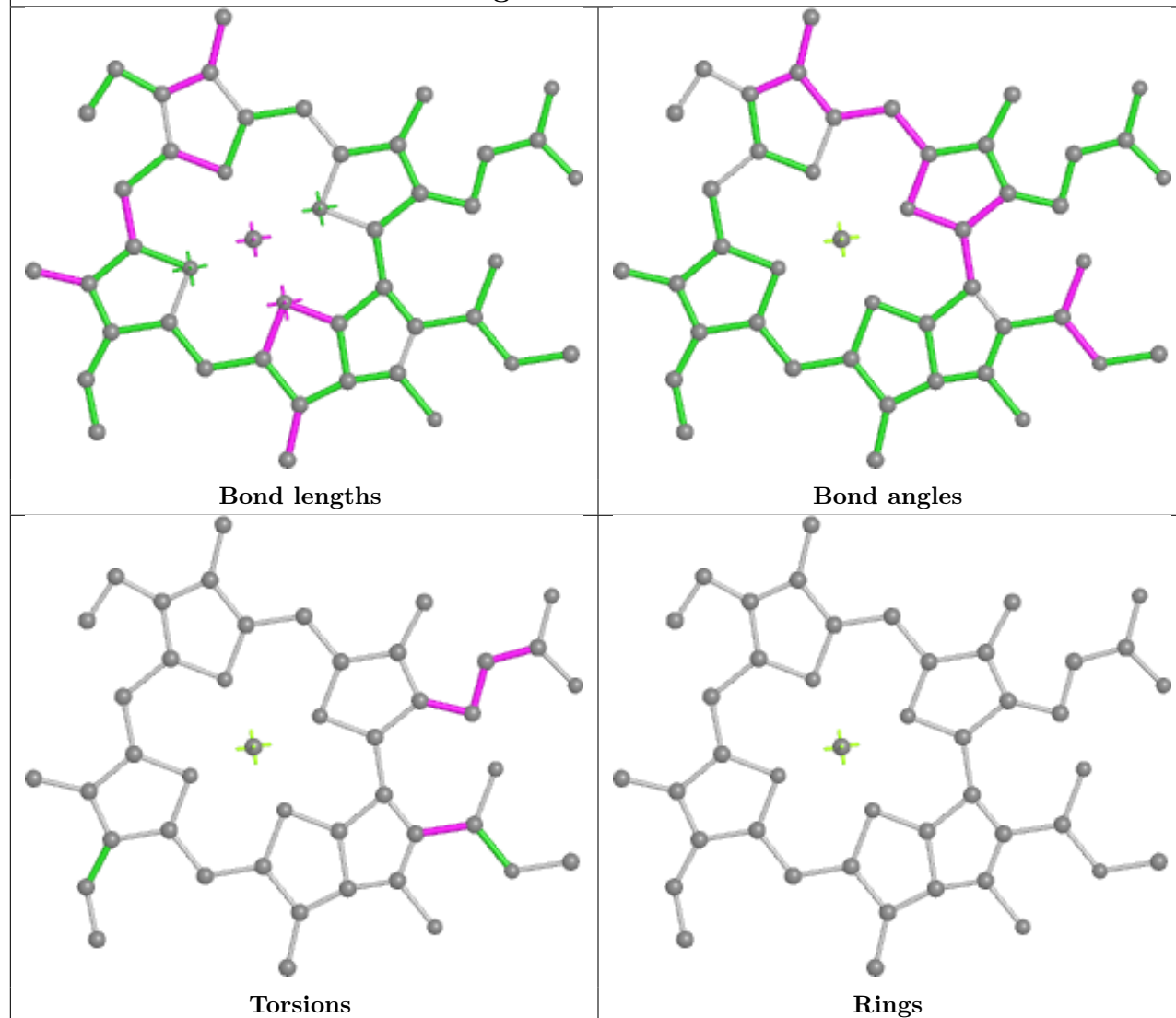


Ligand CLA a 820

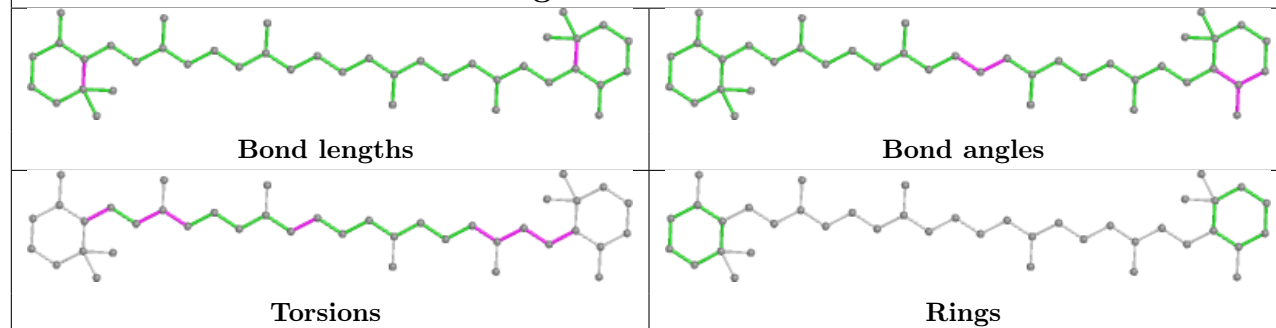


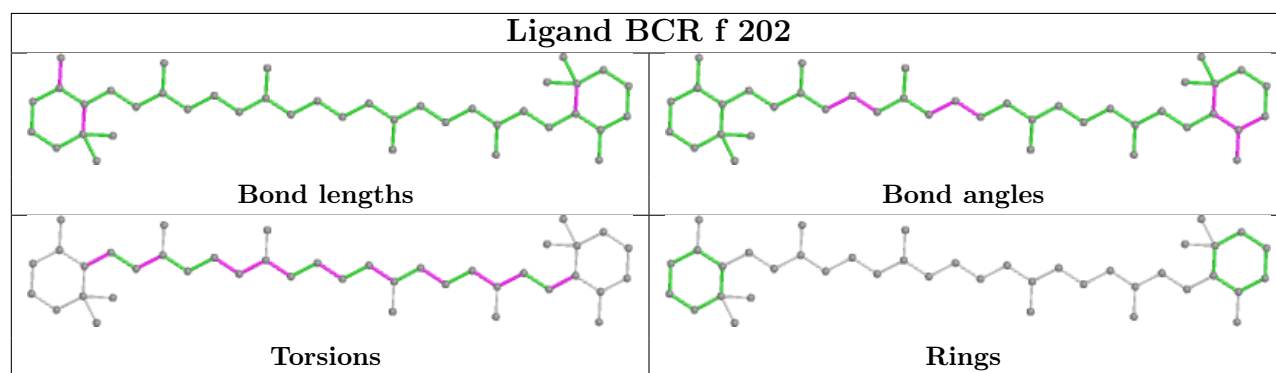
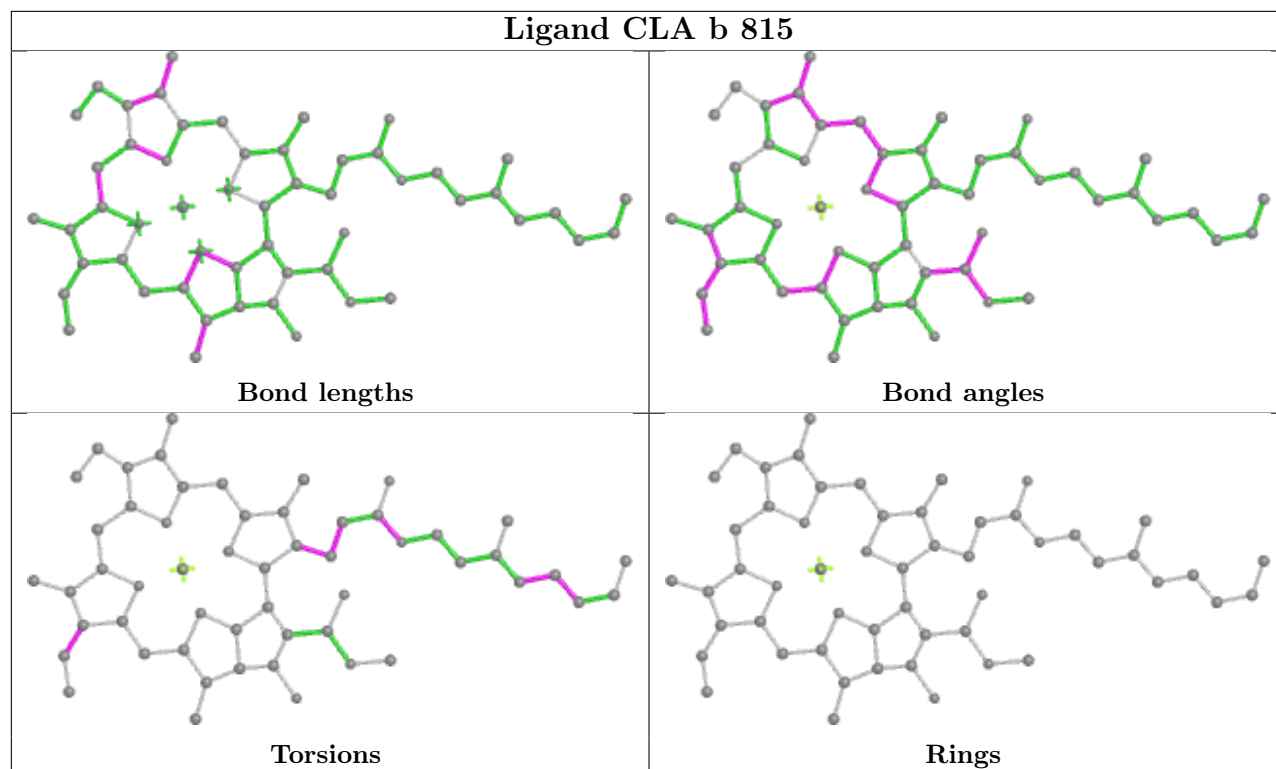
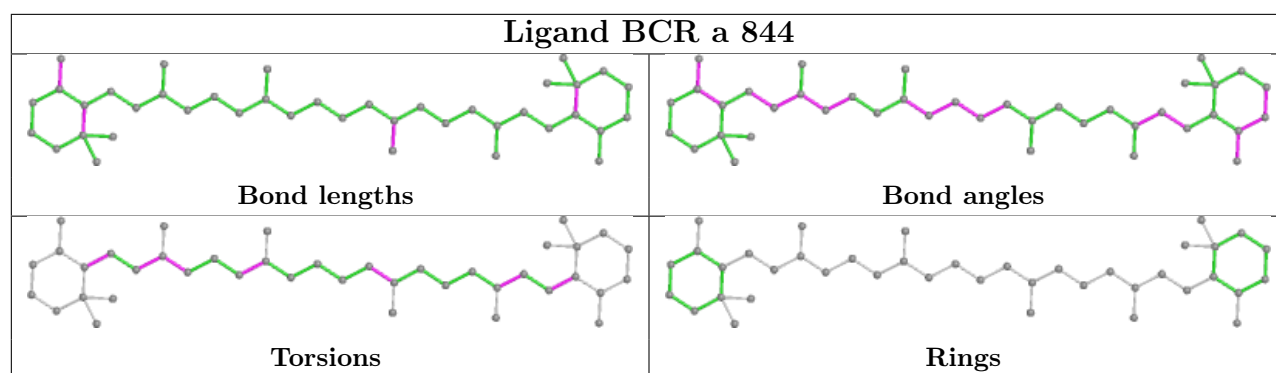


Ligand CLA b 823

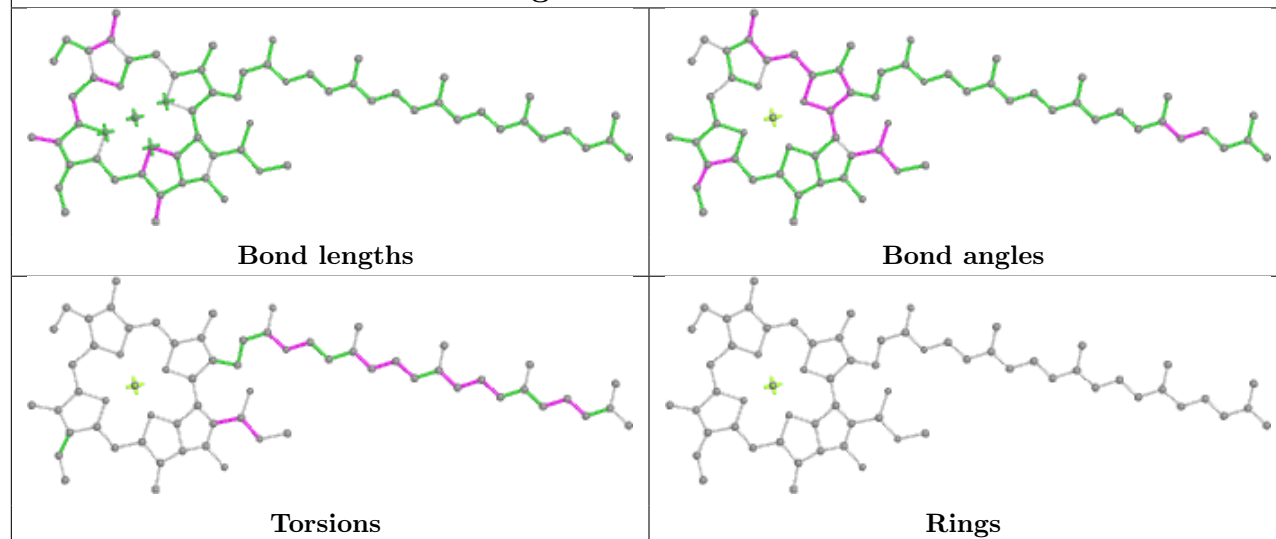


Ligand BCR b 845

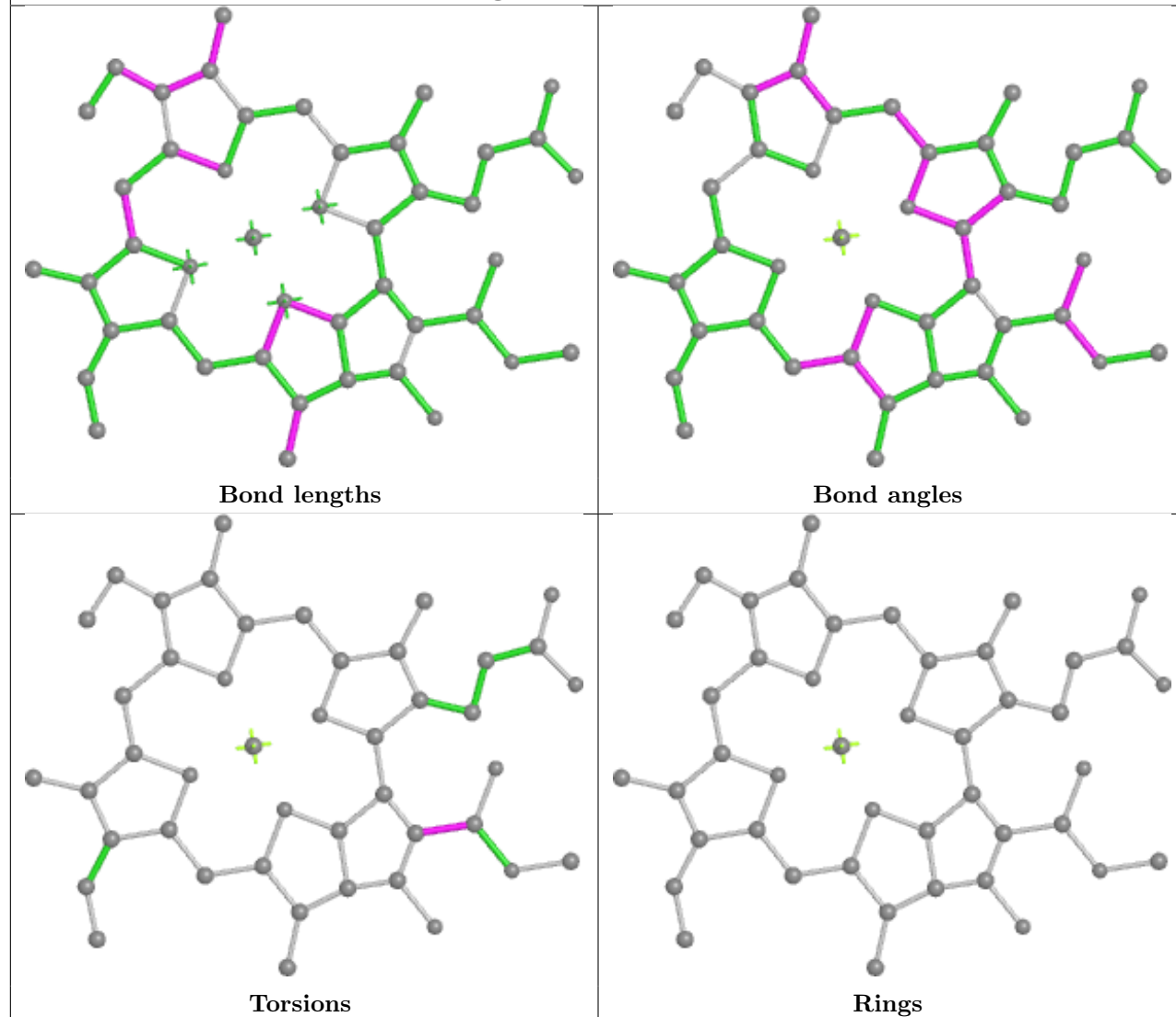


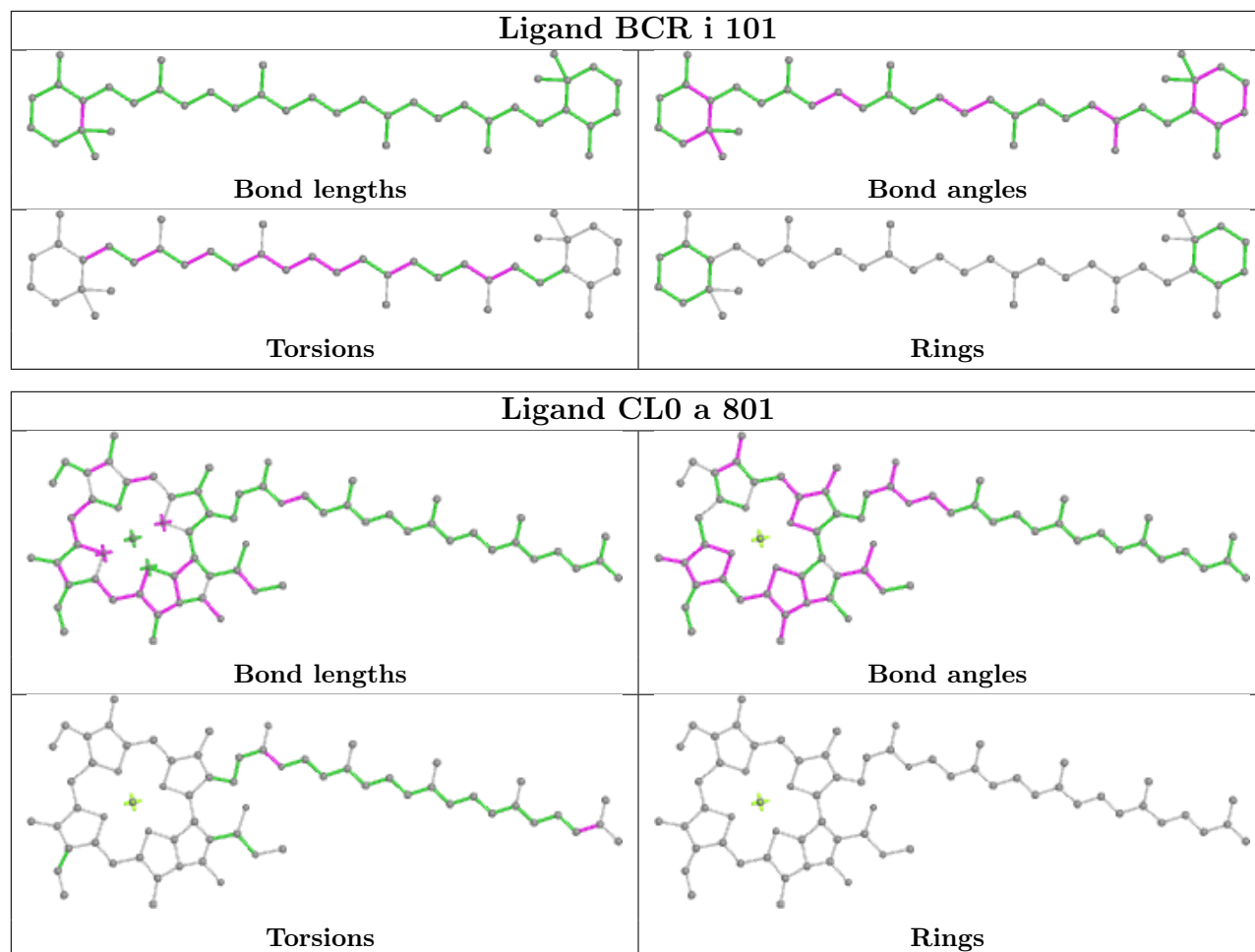


Ligand CLA A 839

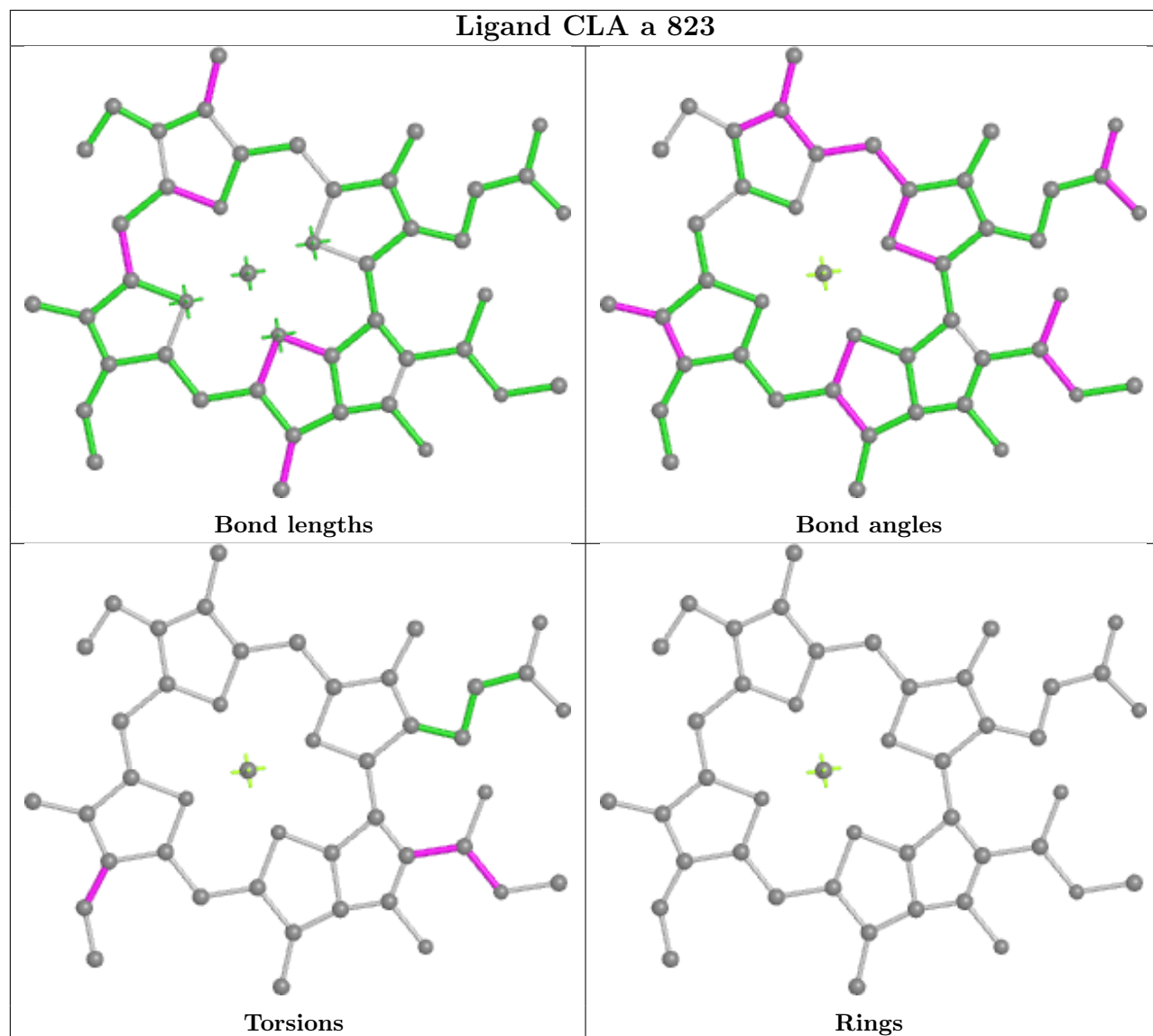


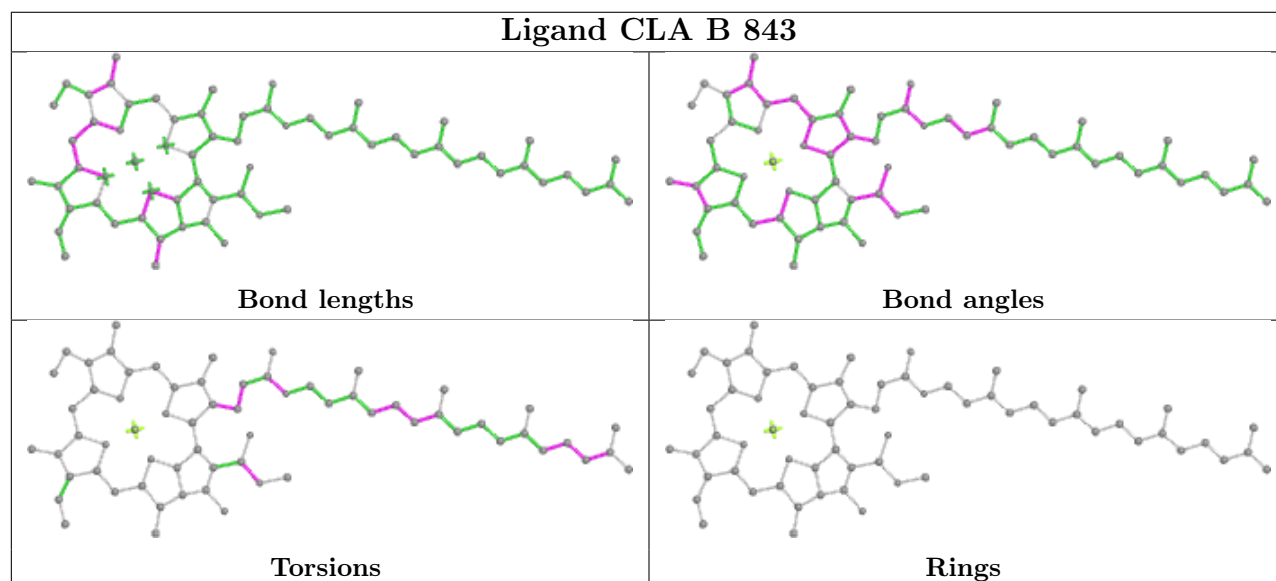
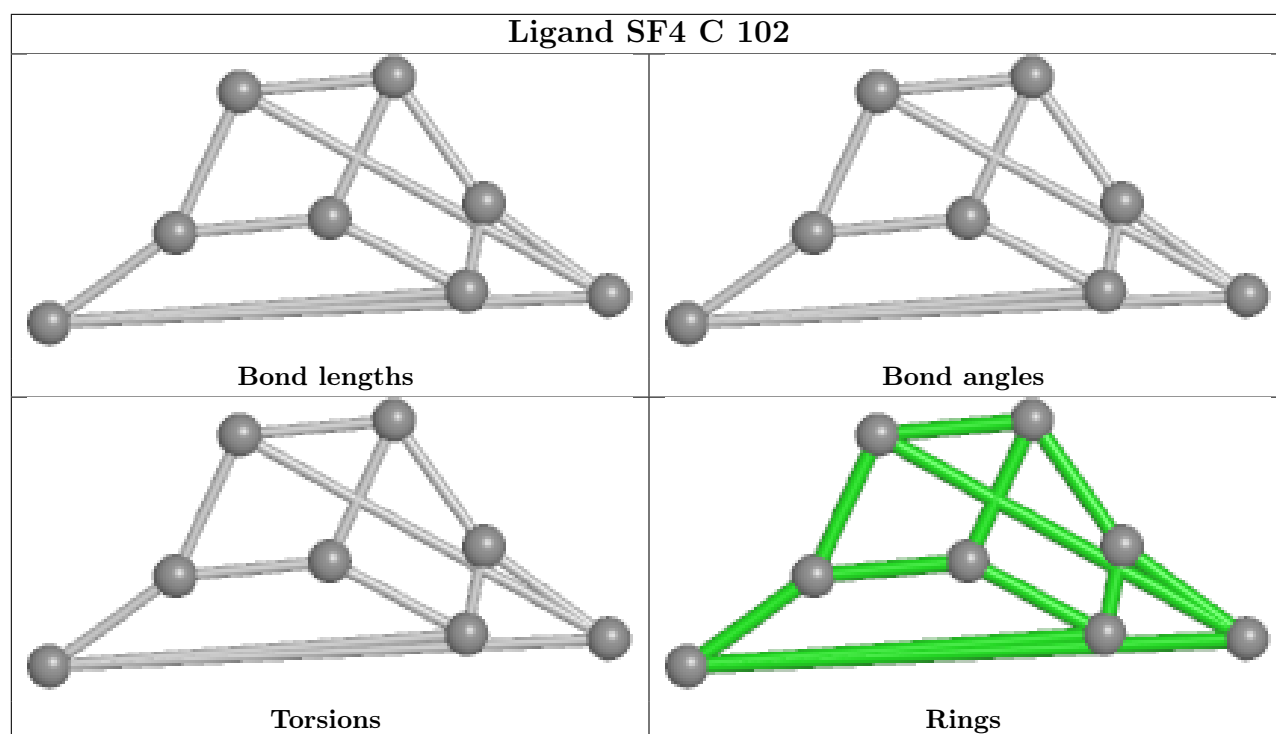
Ligand CLA A 824



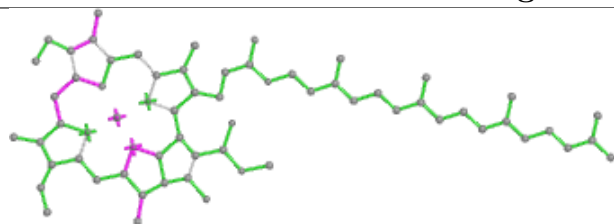


Ligand CLA a 823

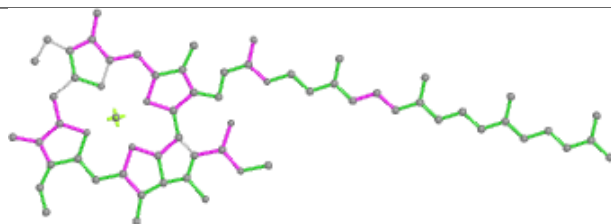




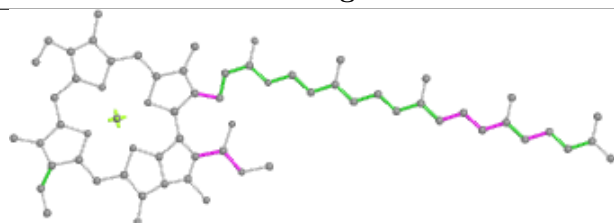
Ligand CLA b 832



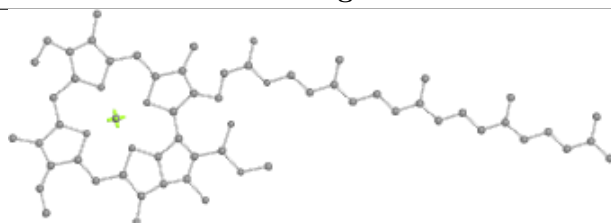
Bond lengths



Bond angles

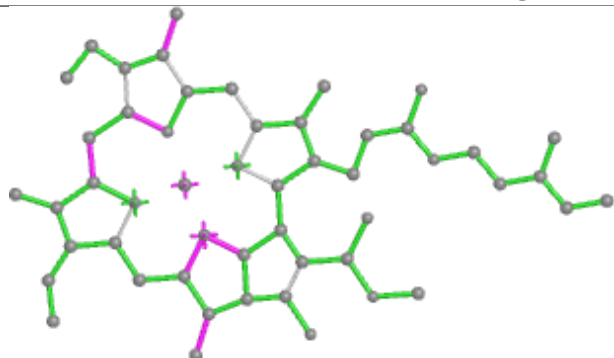


Torsions

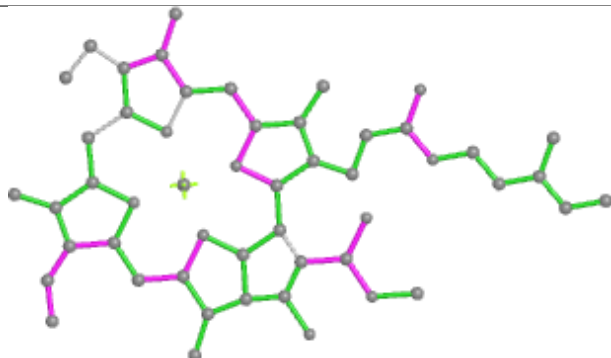


Rings

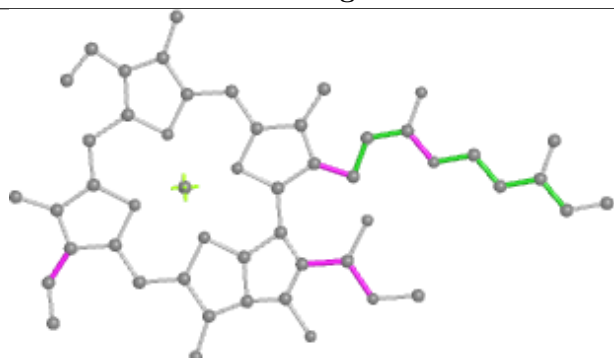
Ligand CLA A 837



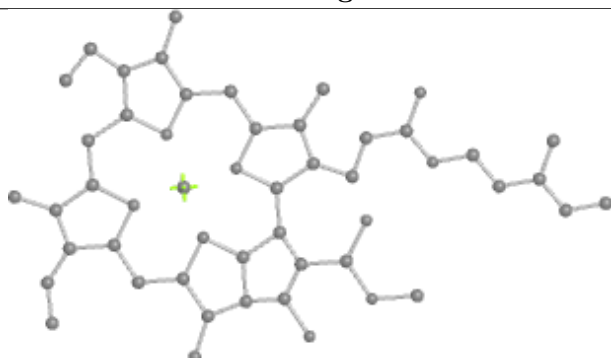
Bond lengths



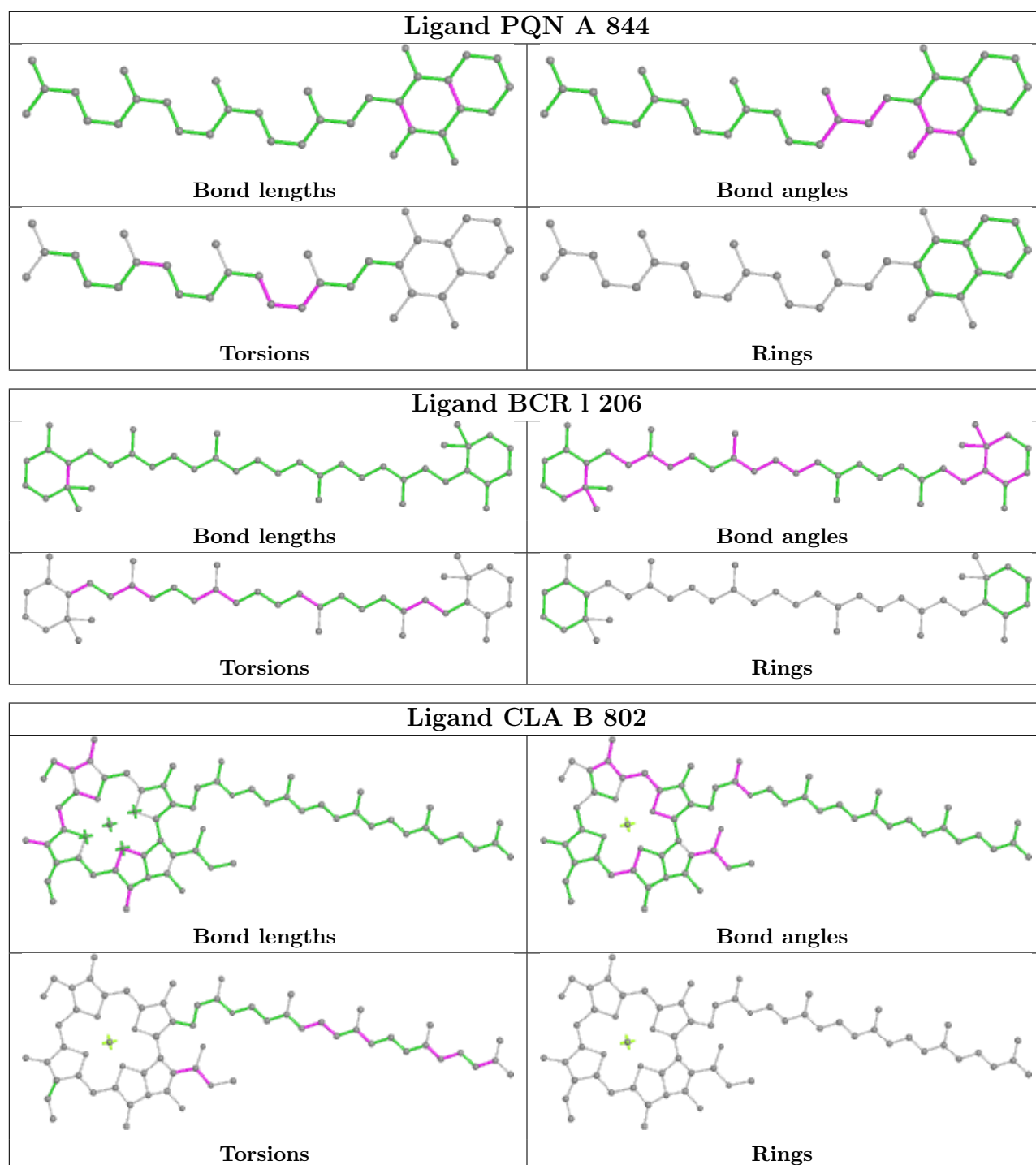
Bond angles

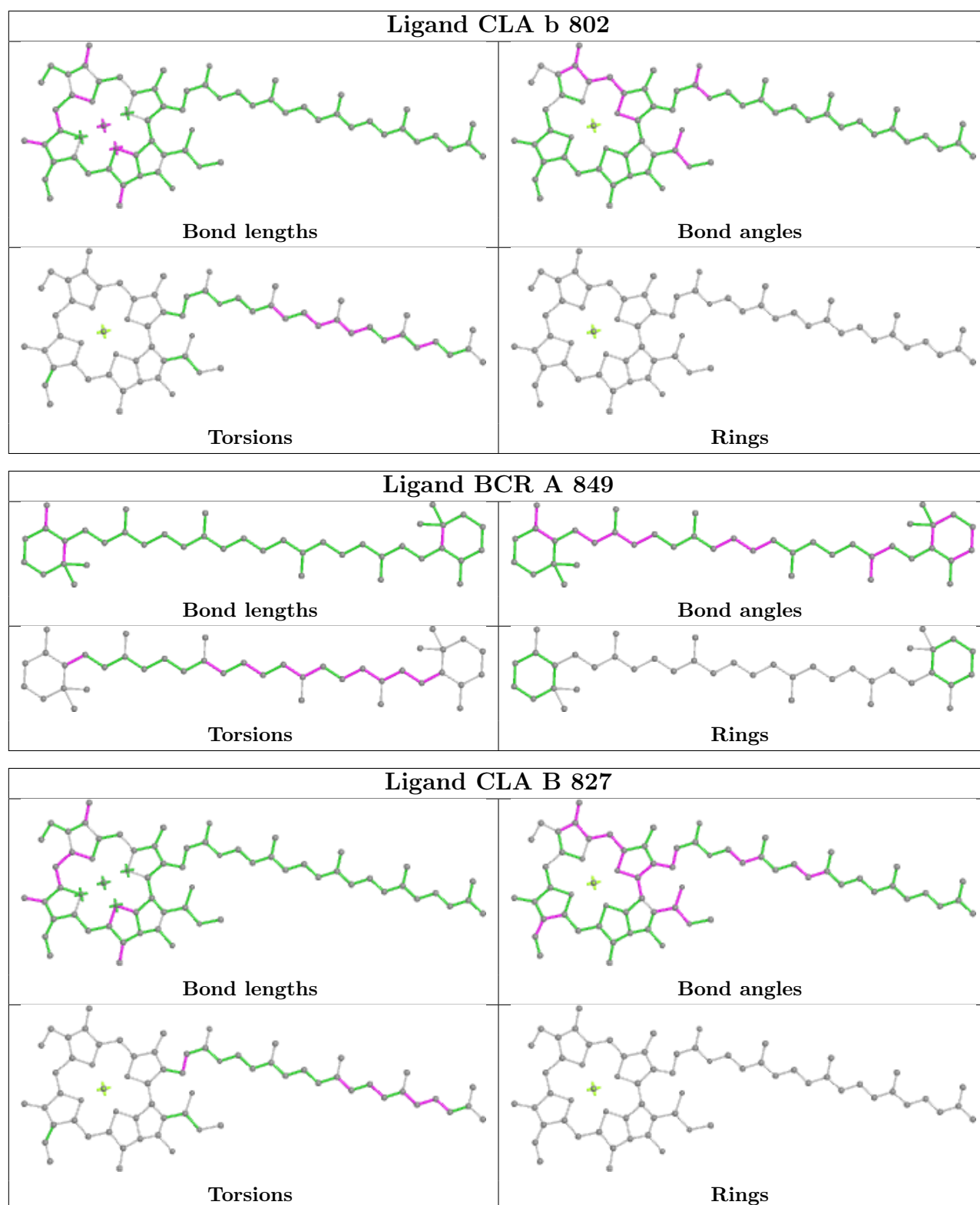


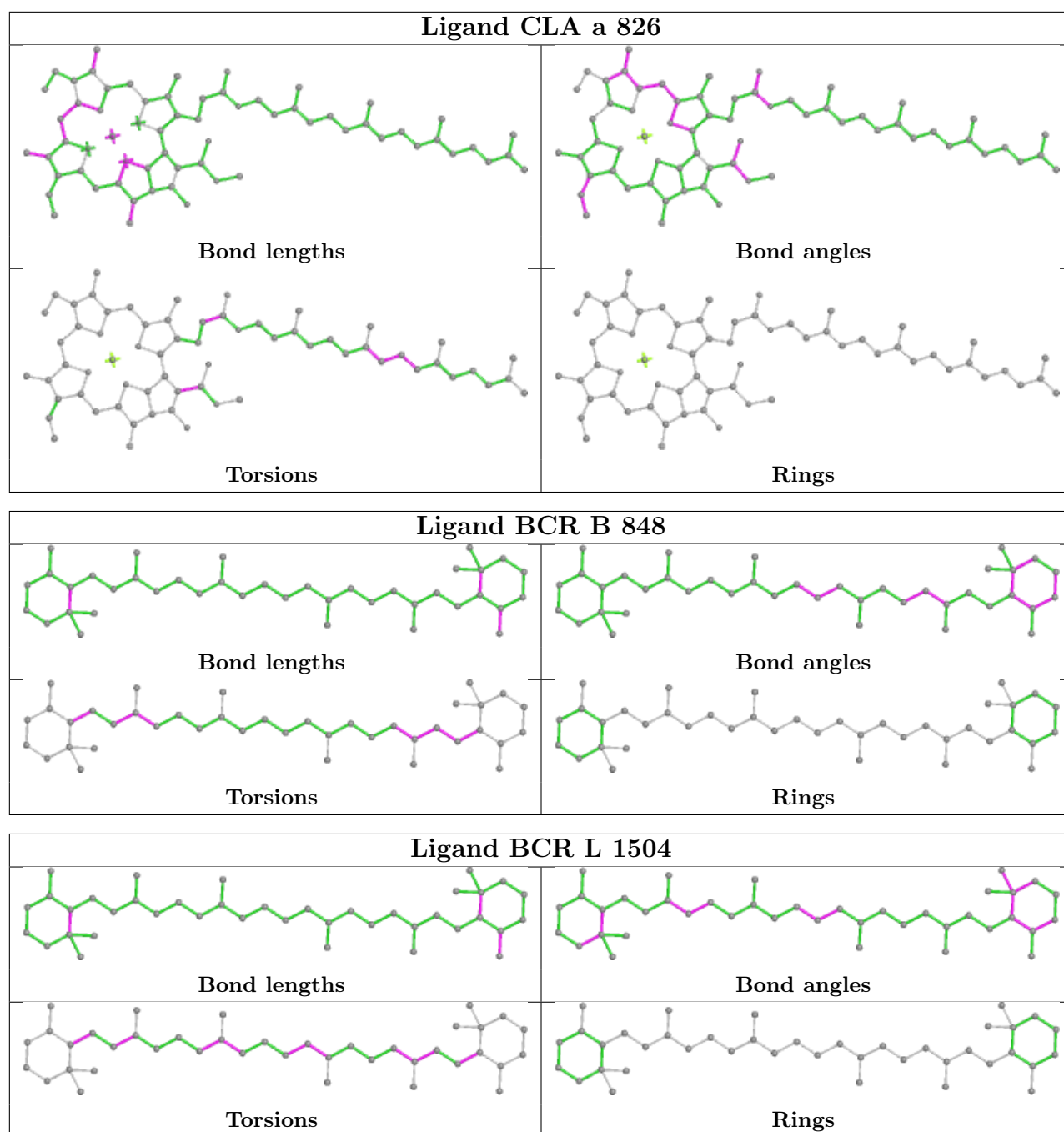
Torsions

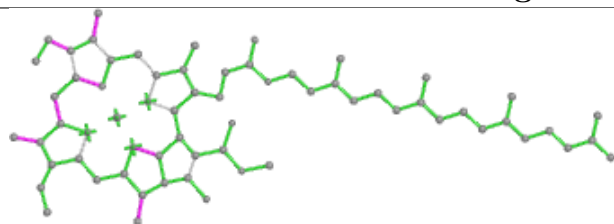
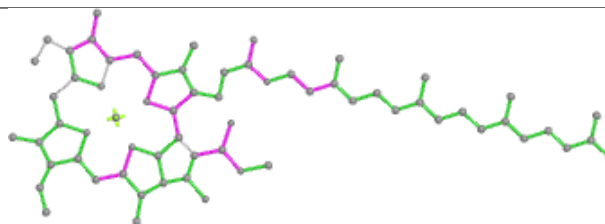
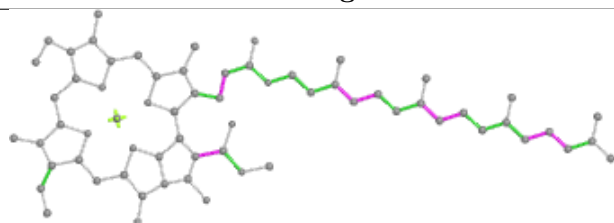
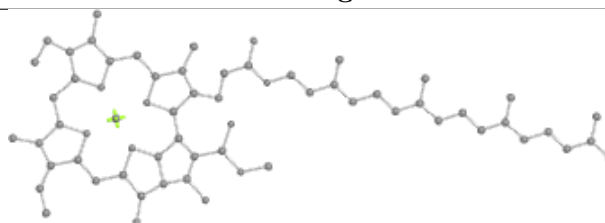
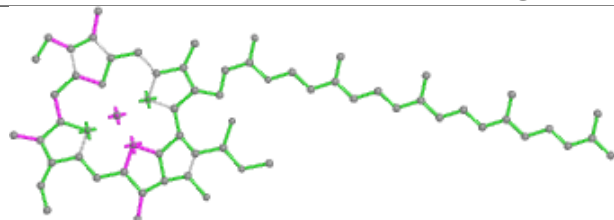
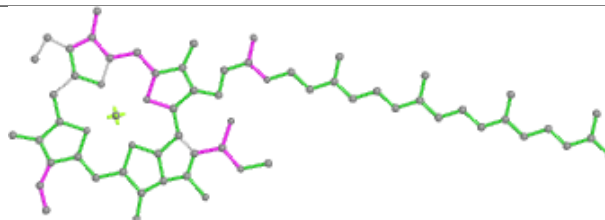
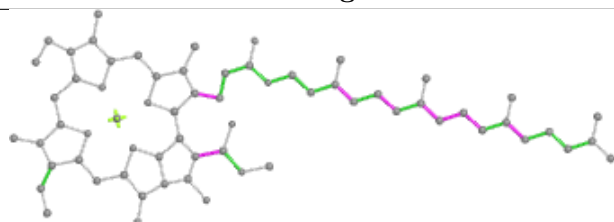
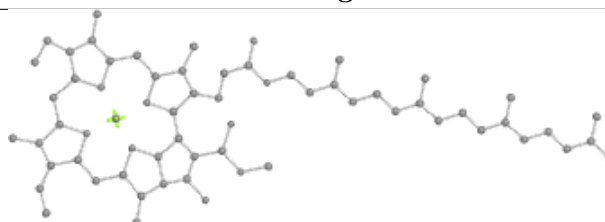


Rings

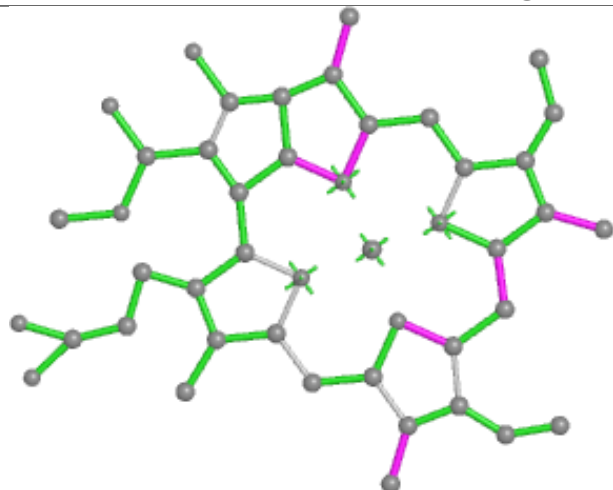




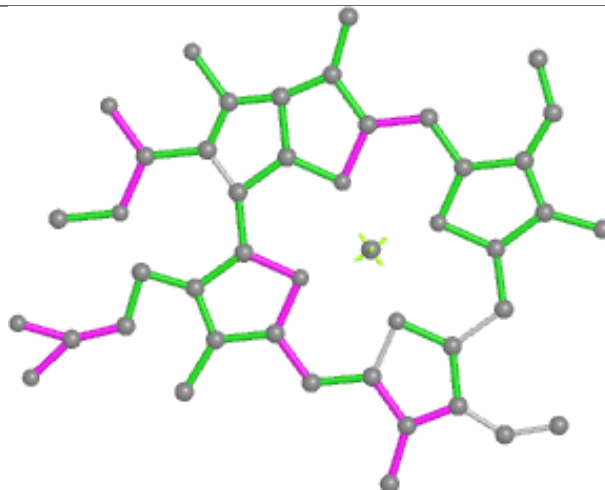


Ligand CLA B 801**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 816****Bond lengths****Bond angles****Torsions****Rings**

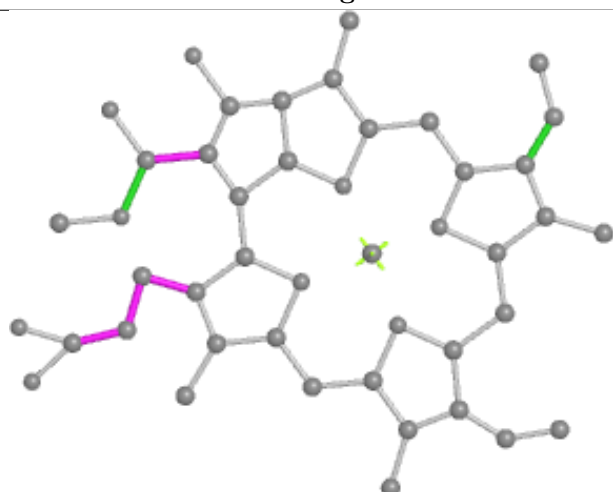
Ligand CLA a 841



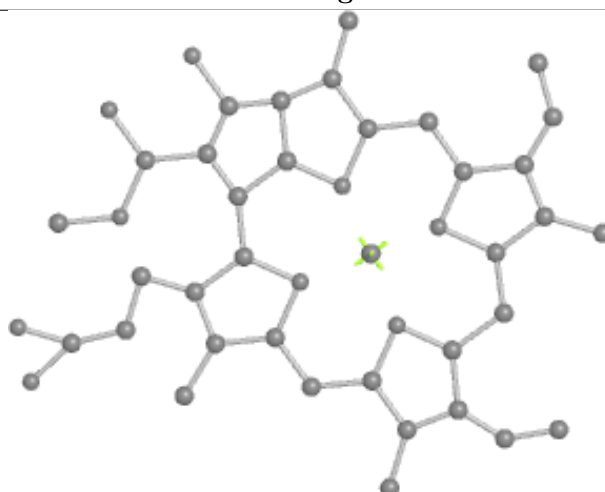
Bond lengths



Bond angles

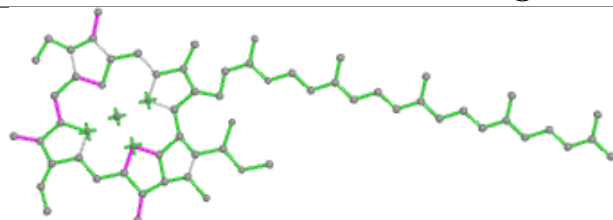


Torsions

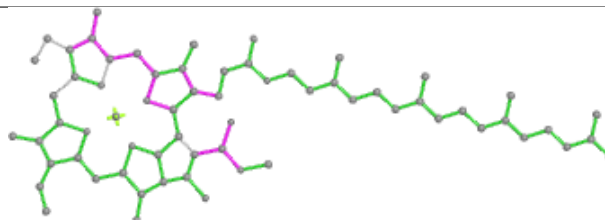


Rings

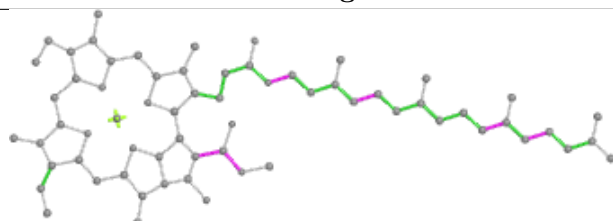
Ligand CLA A 803



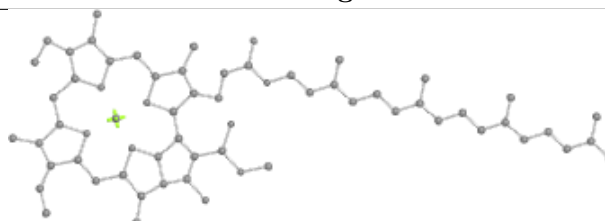
Bond lengths



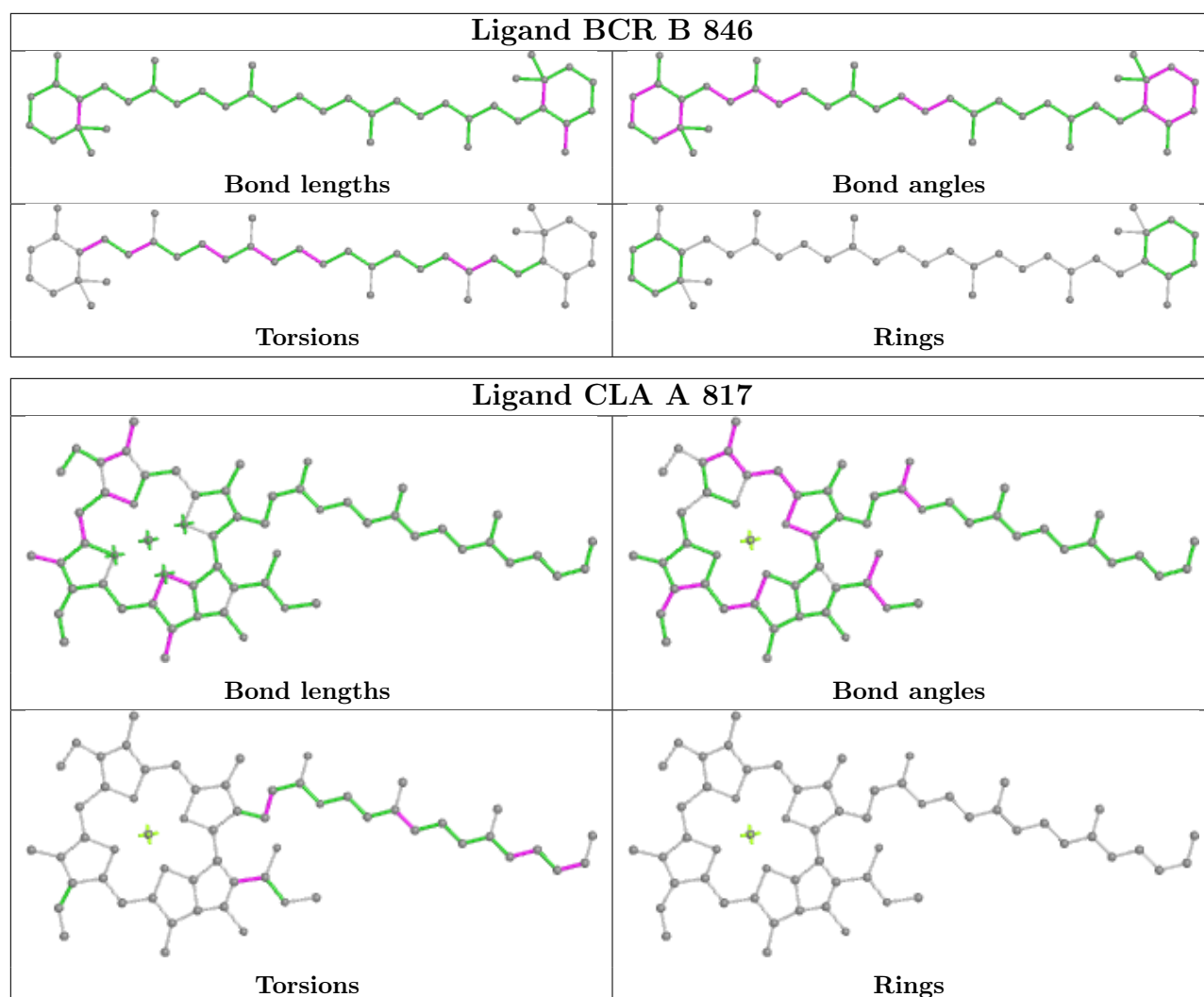
Bond angles

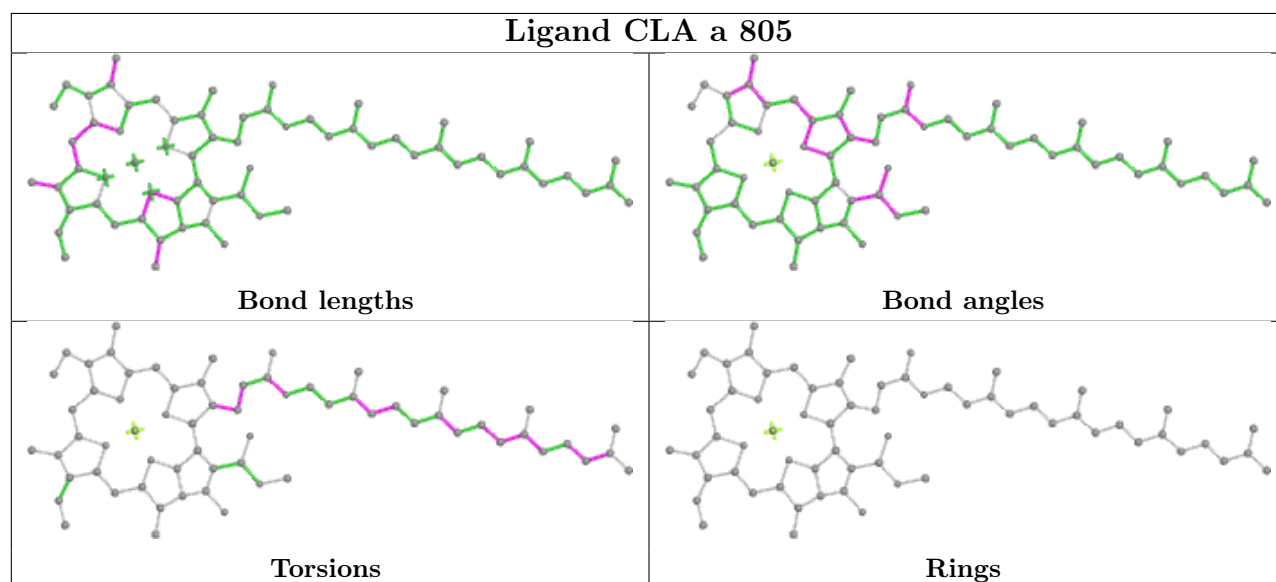
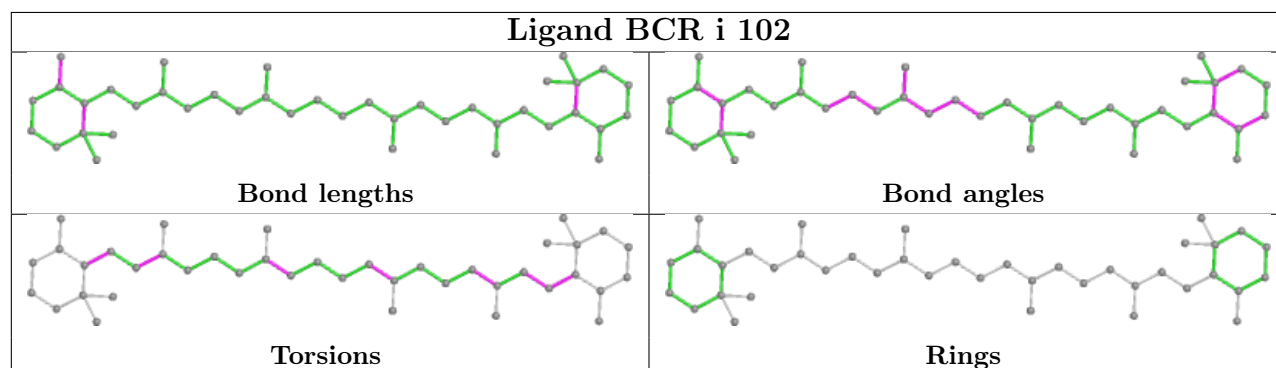
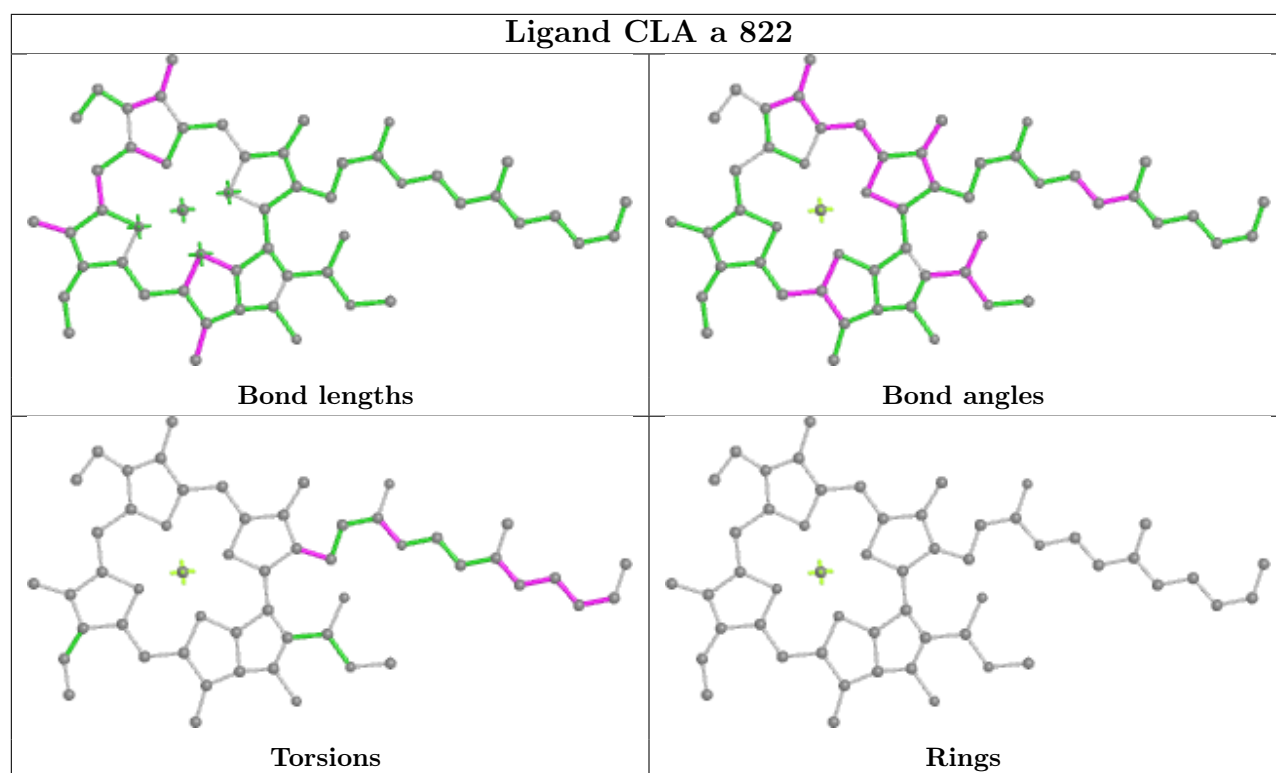


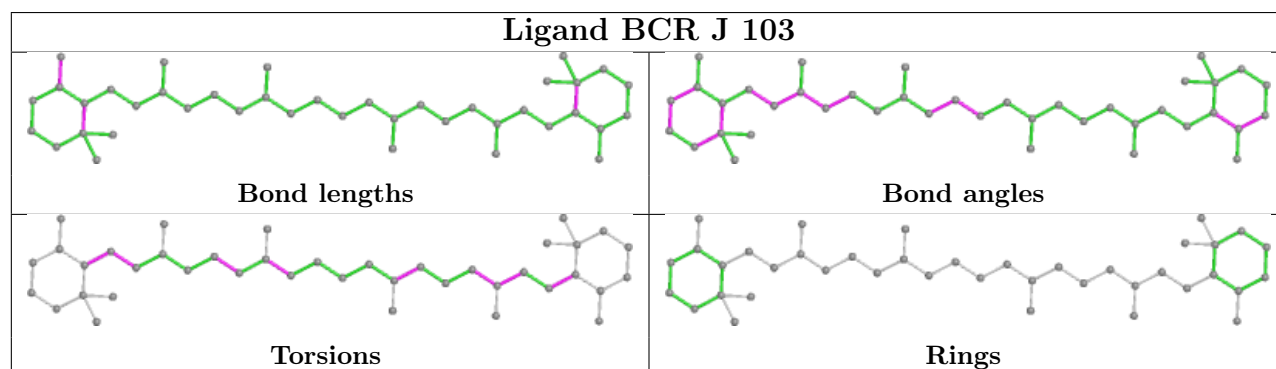
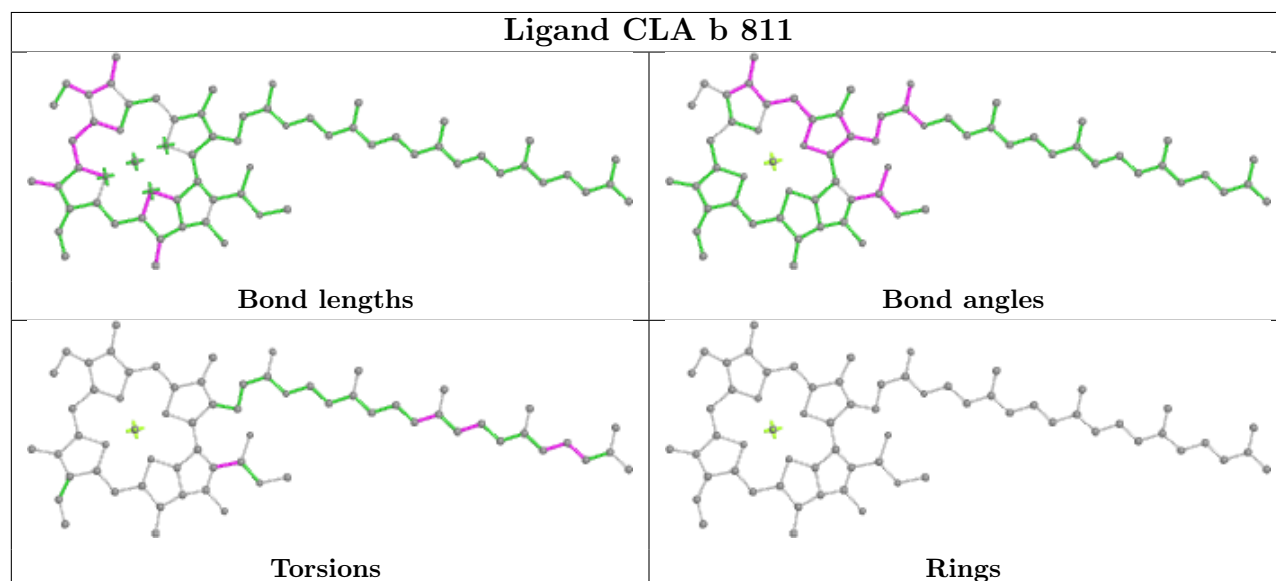
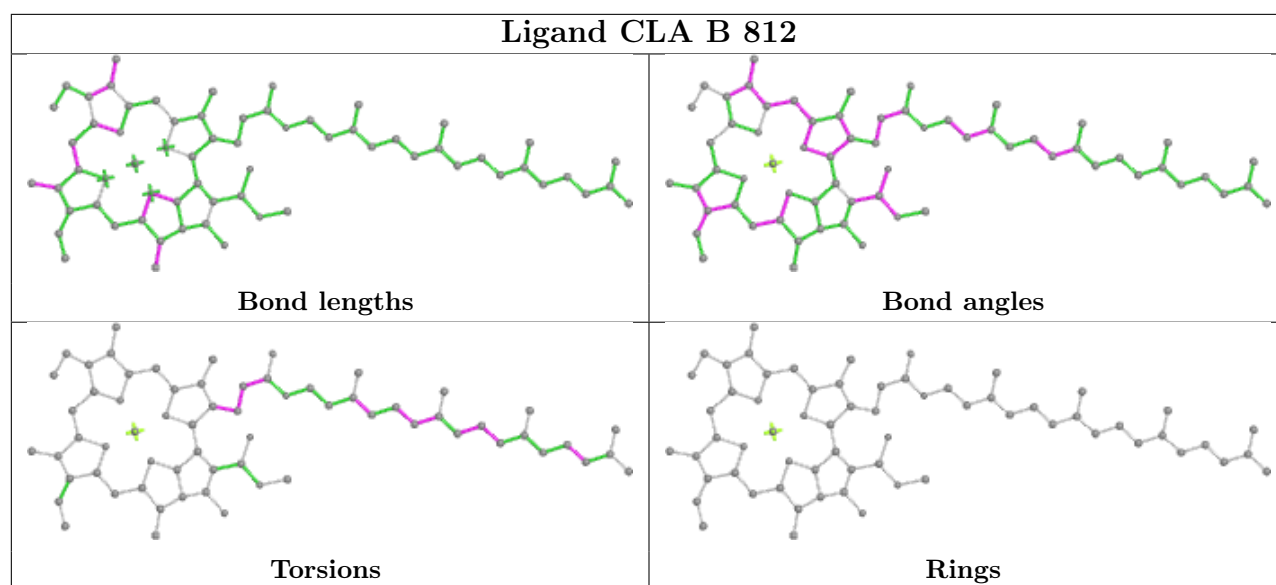
Torsions

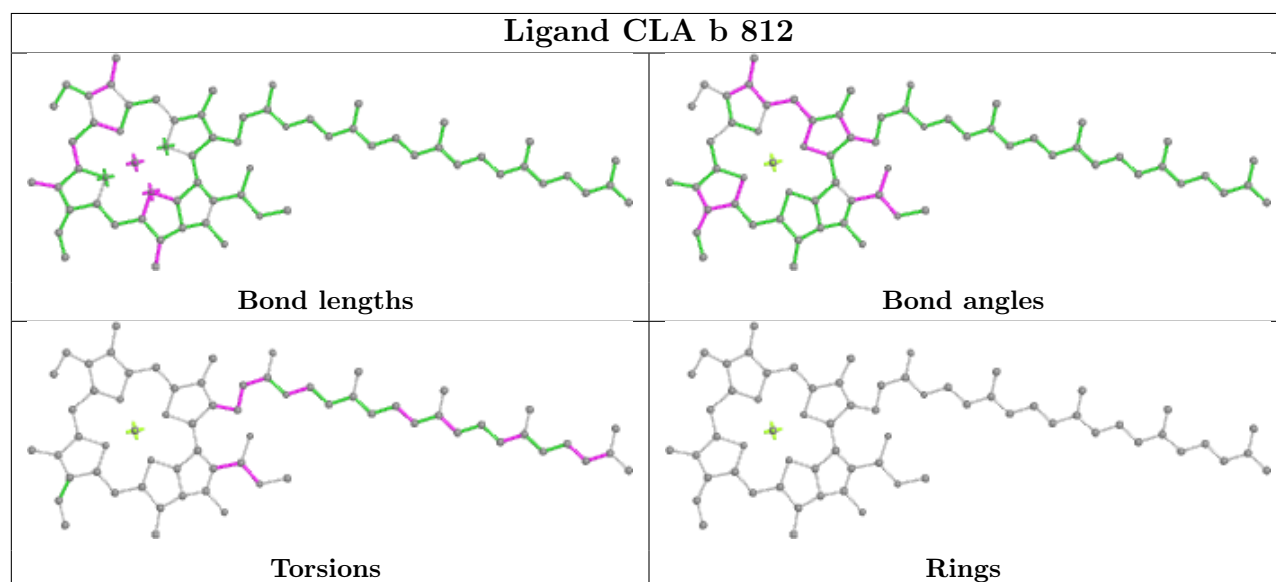
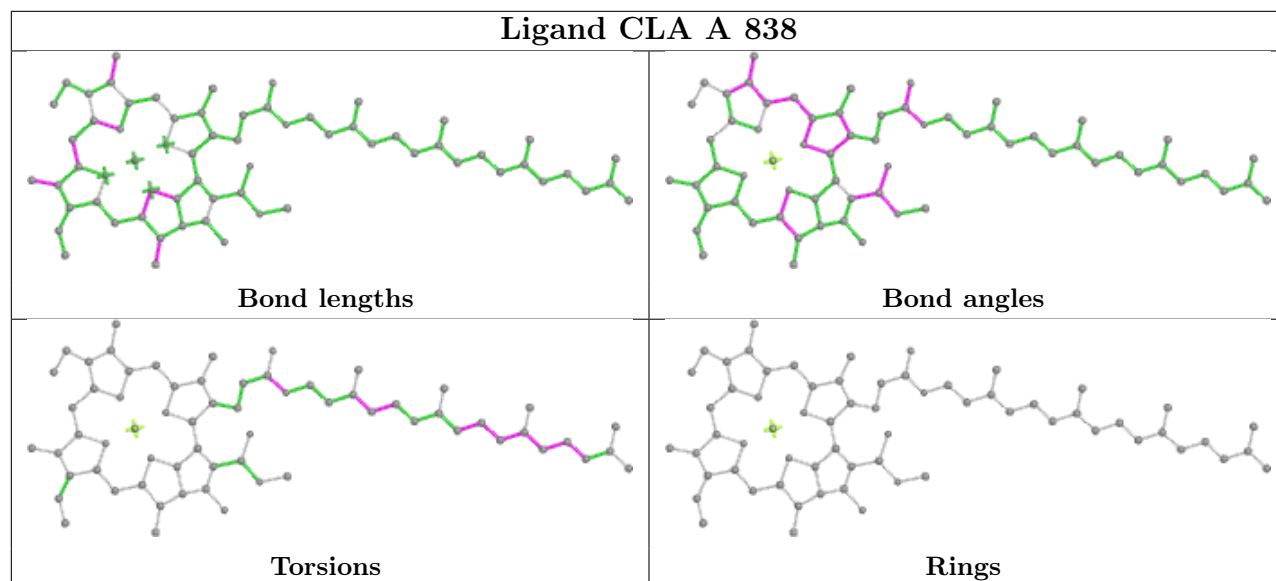
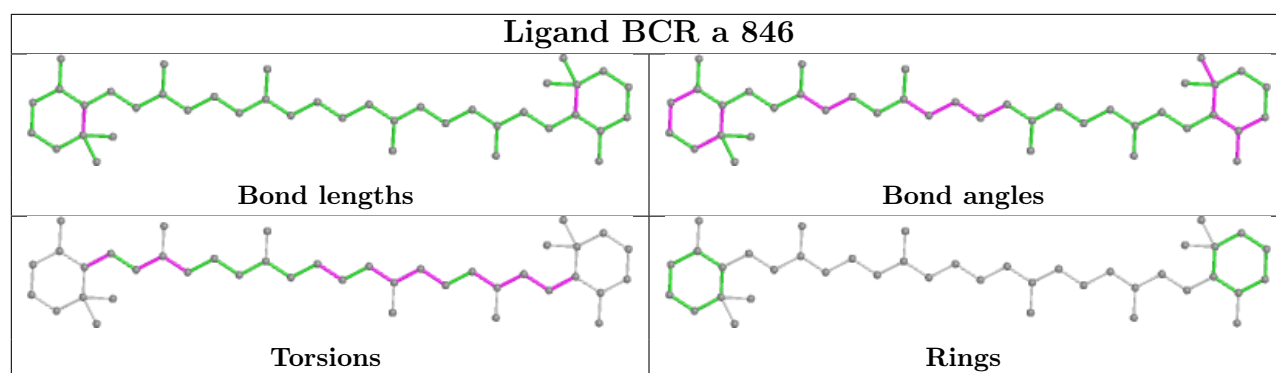


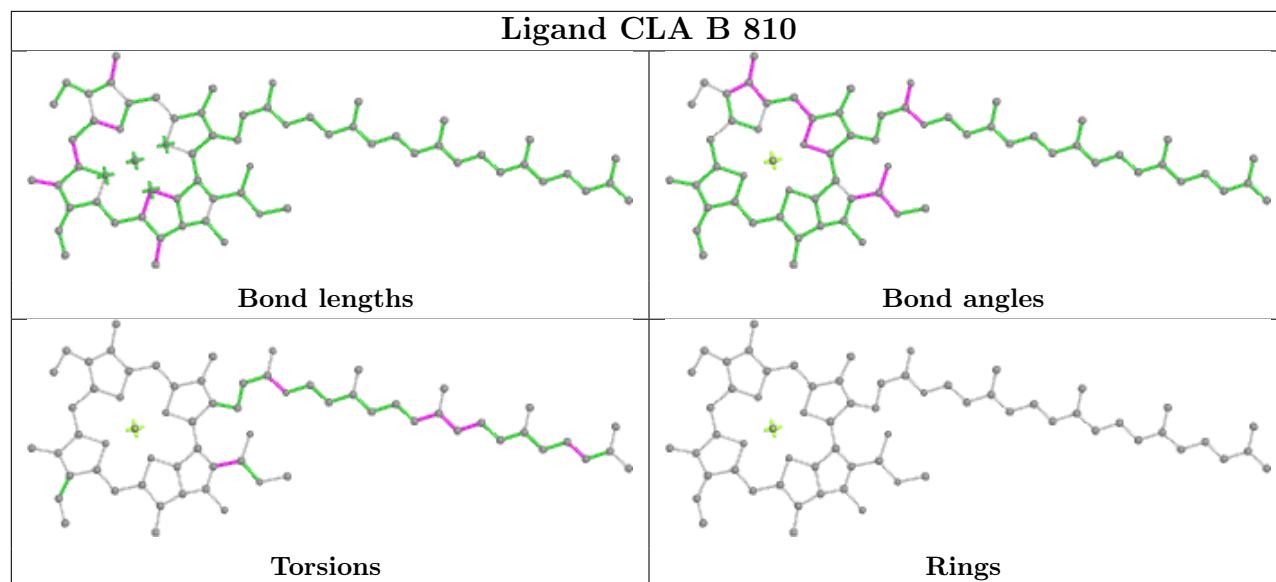
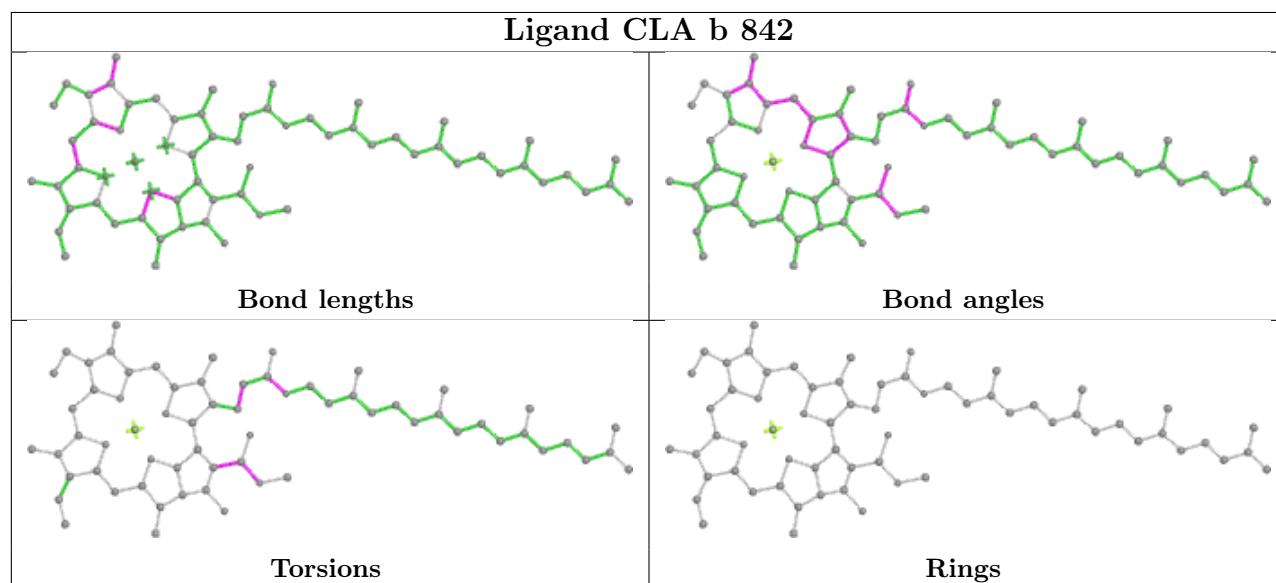
Rings

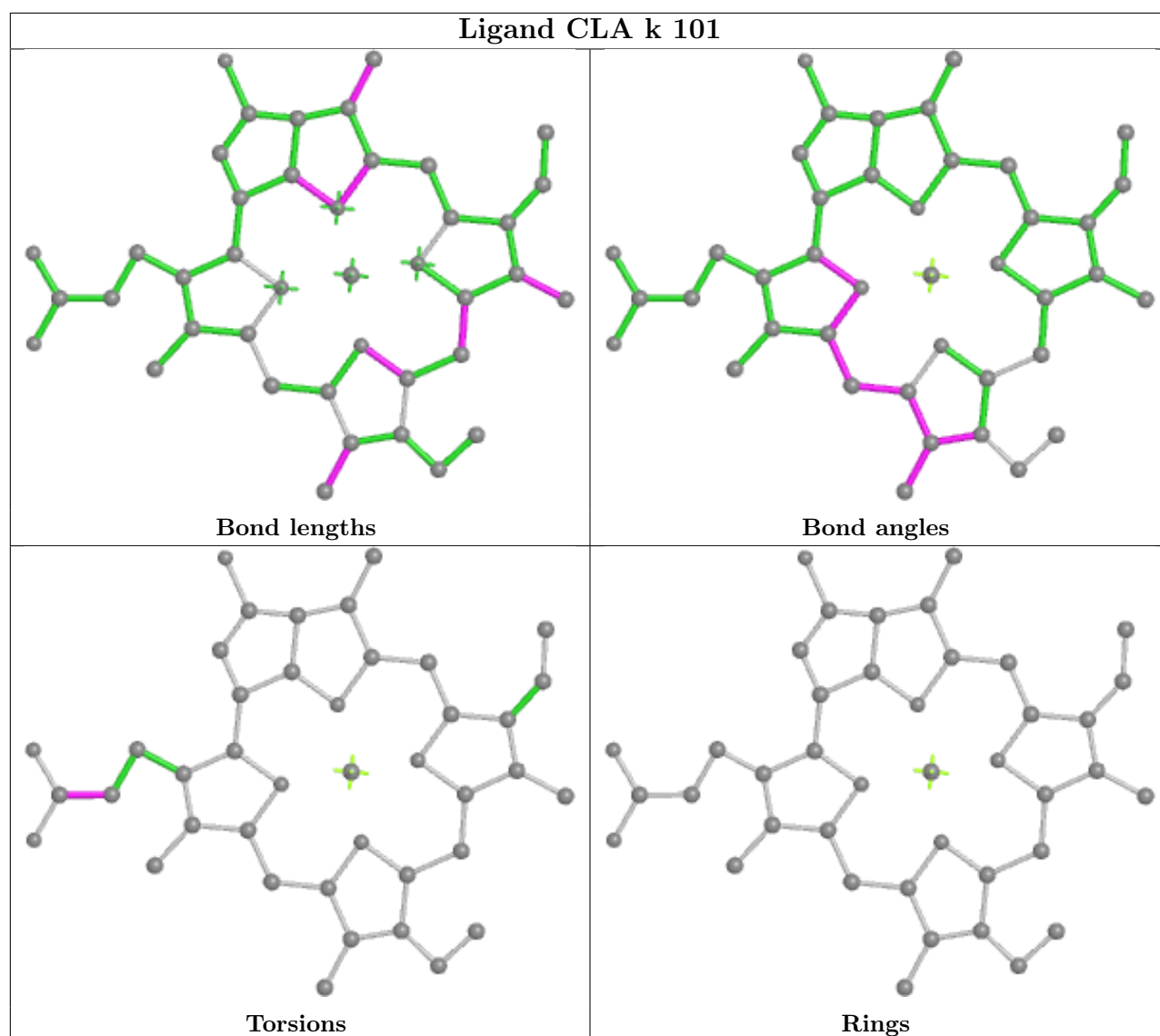


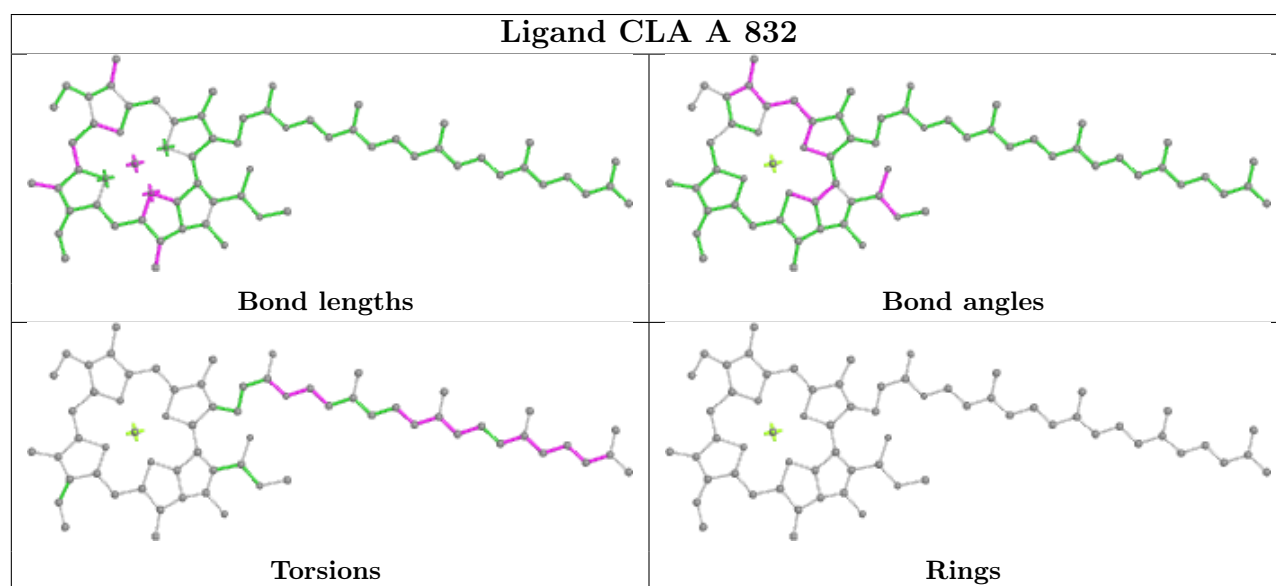
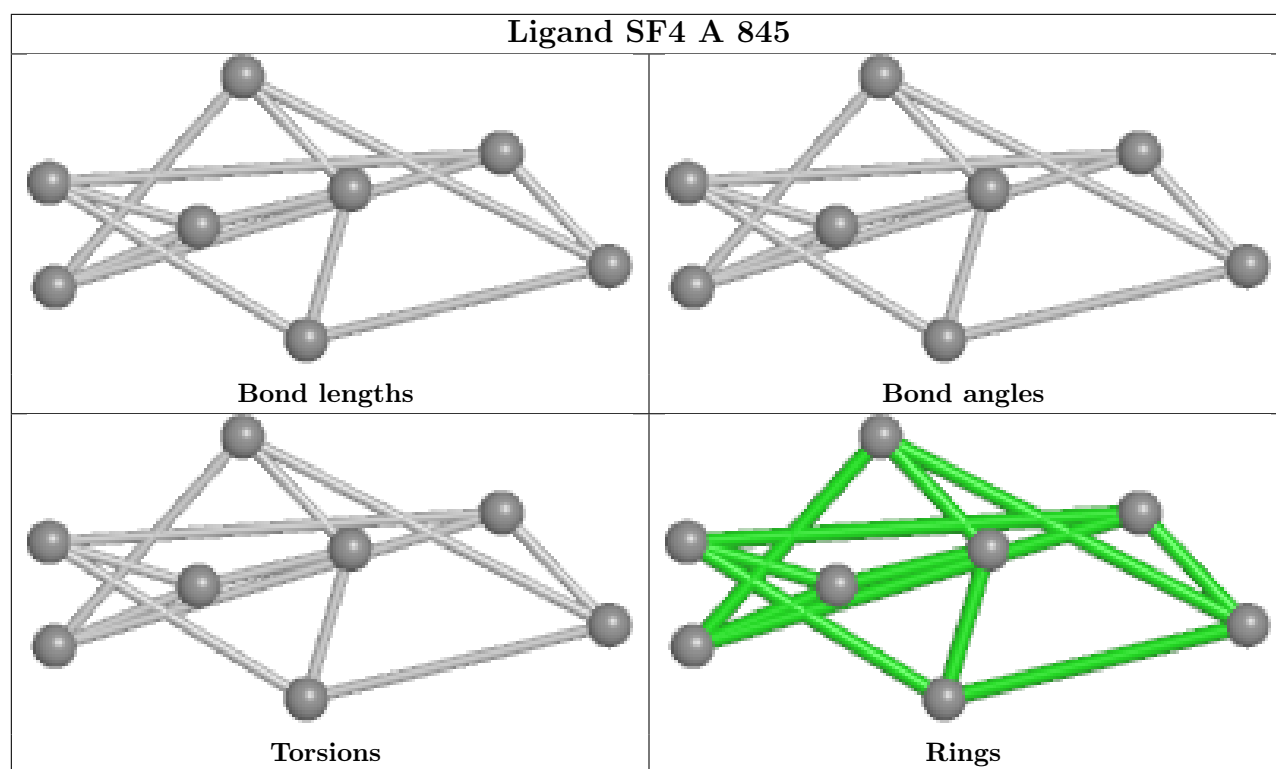




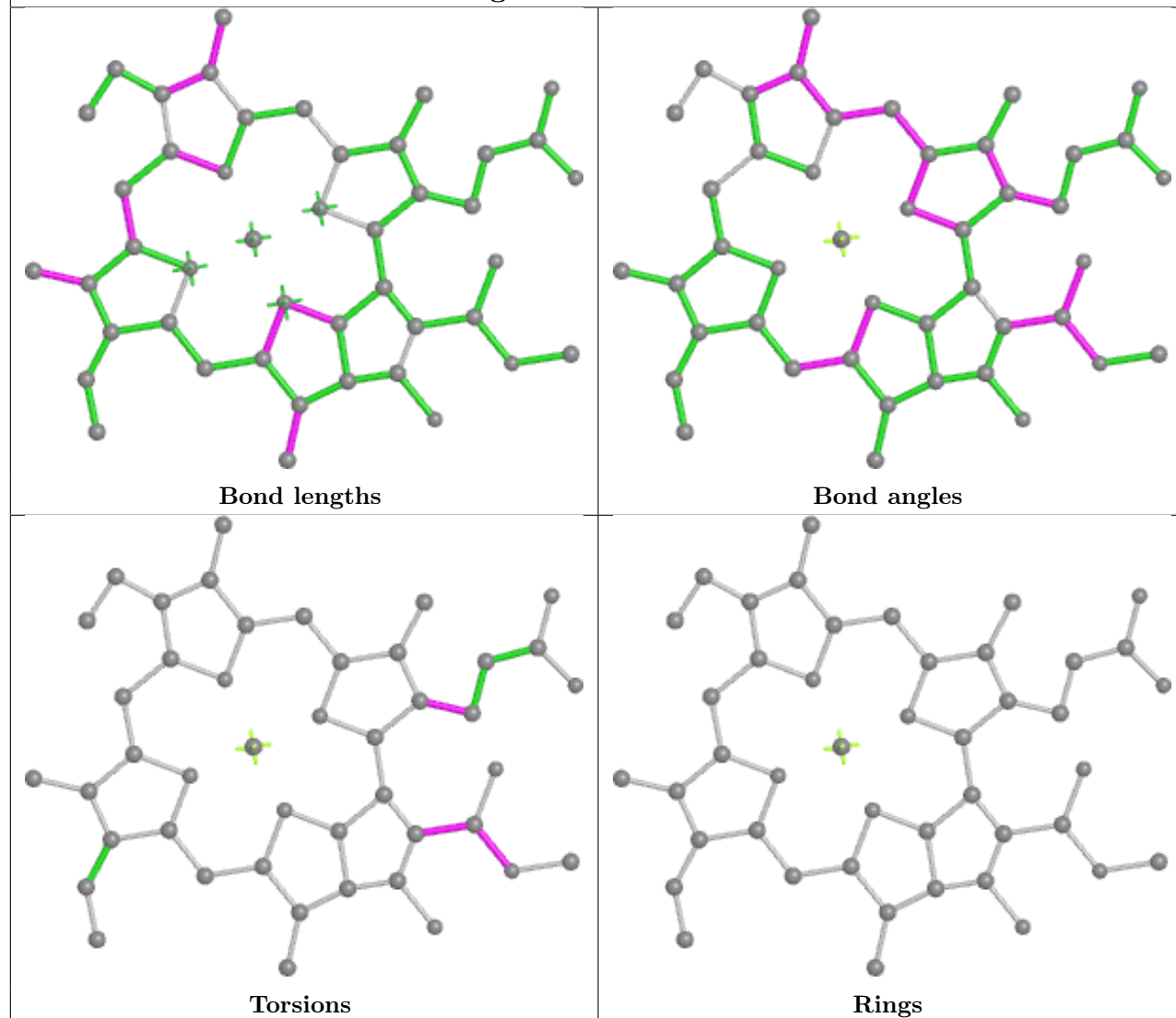


Ligand CLA B 810**Ligand CLA b 842**

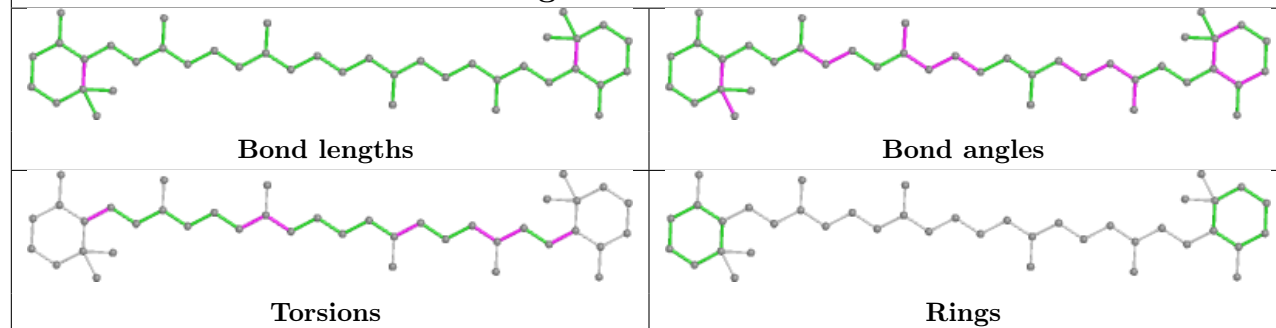


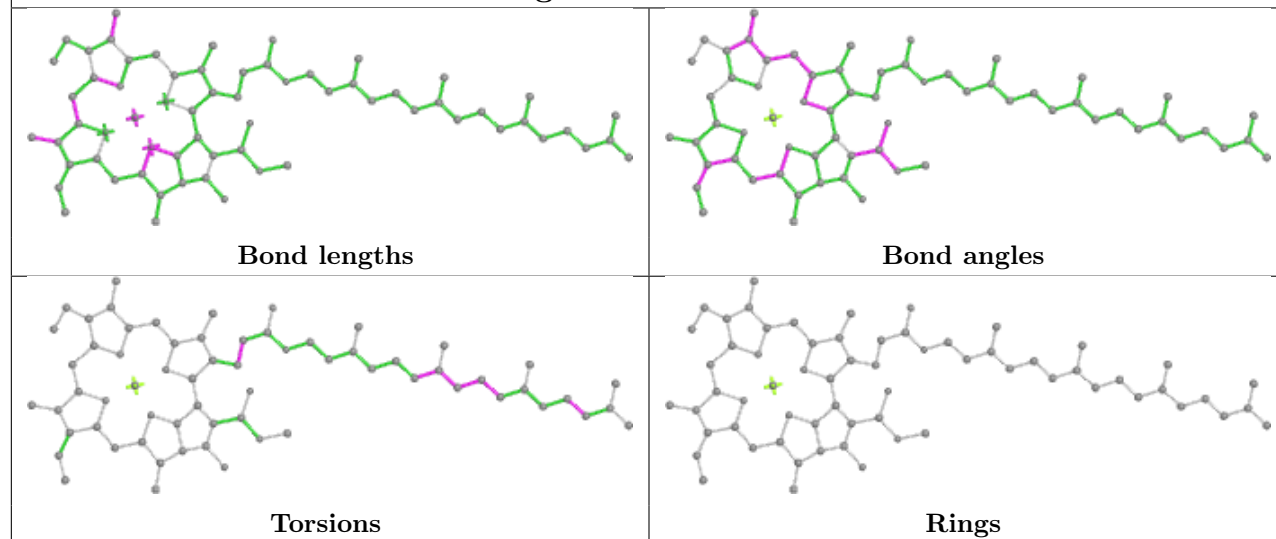
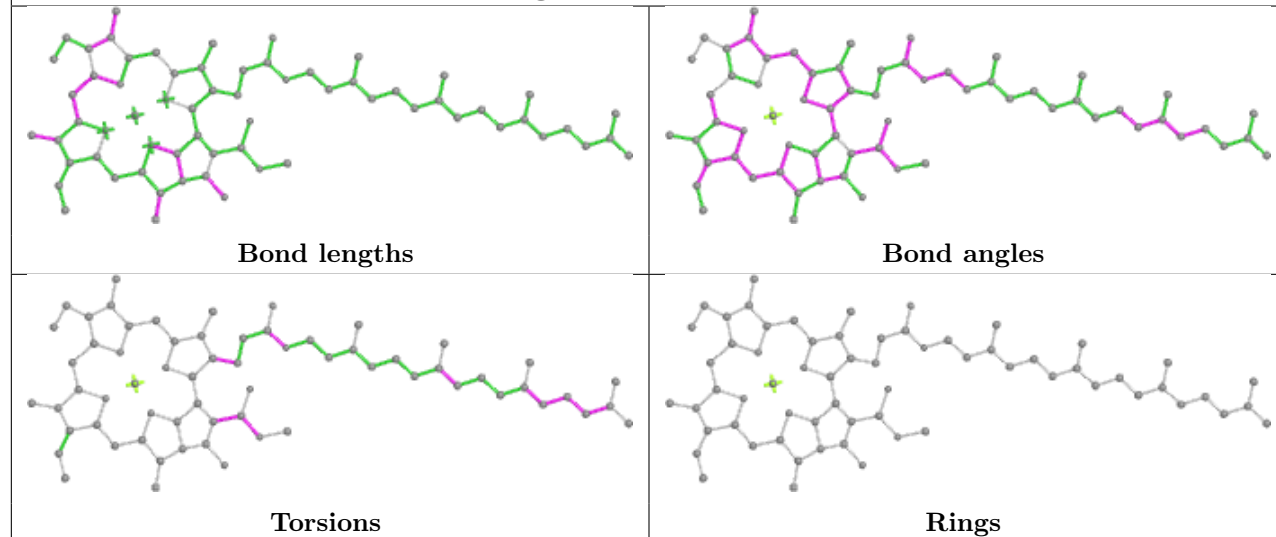


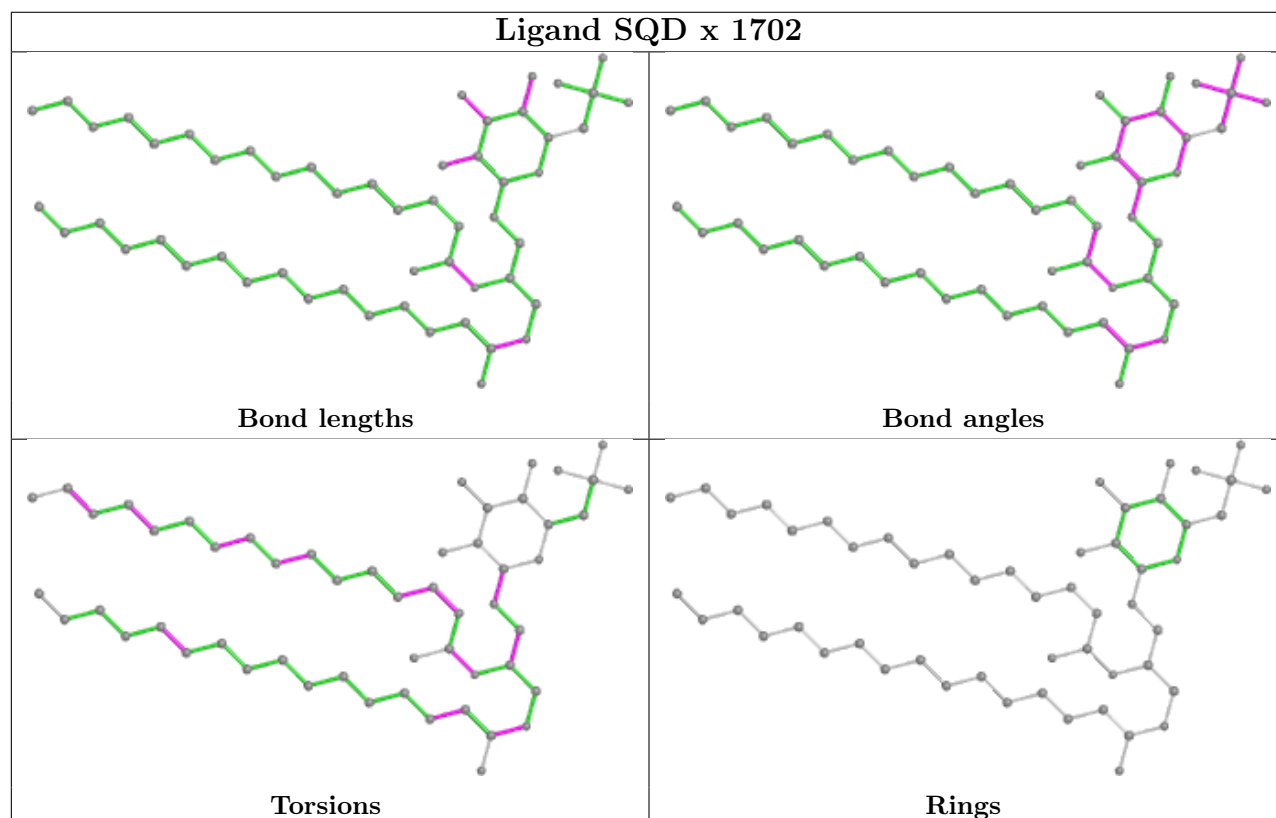
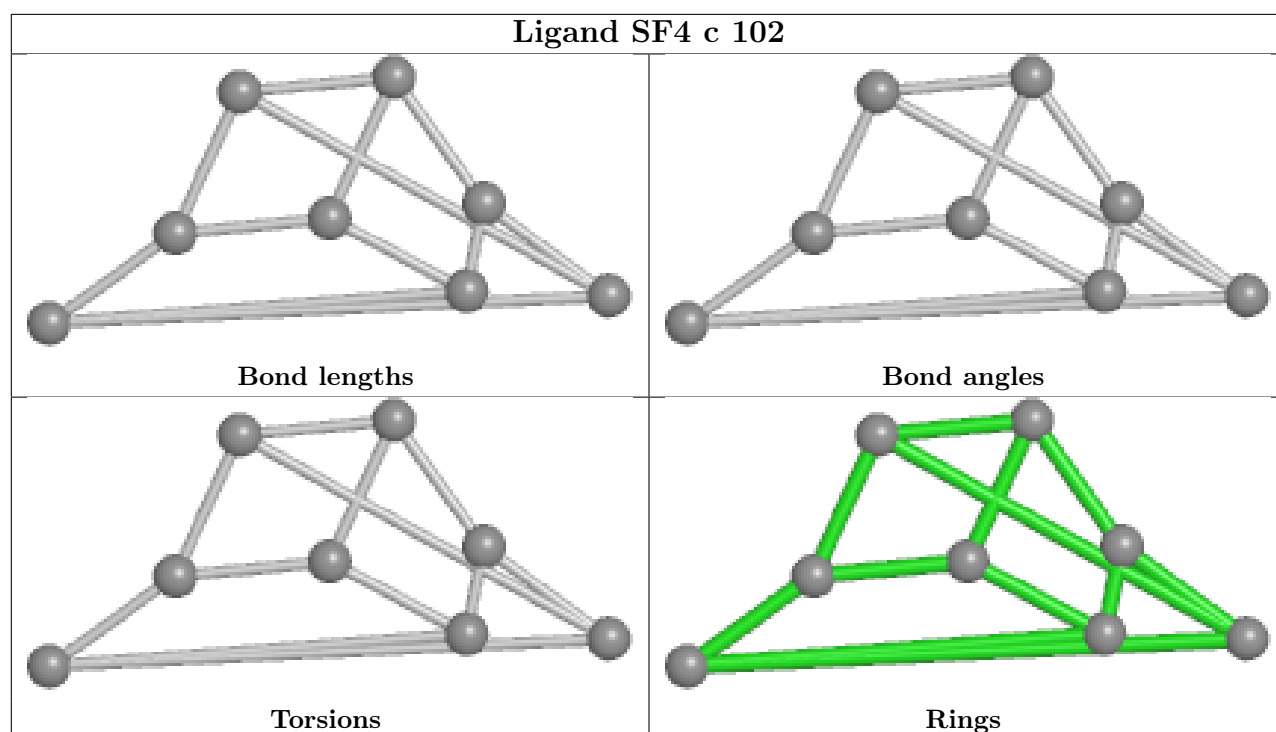
Ligand CLA A 843



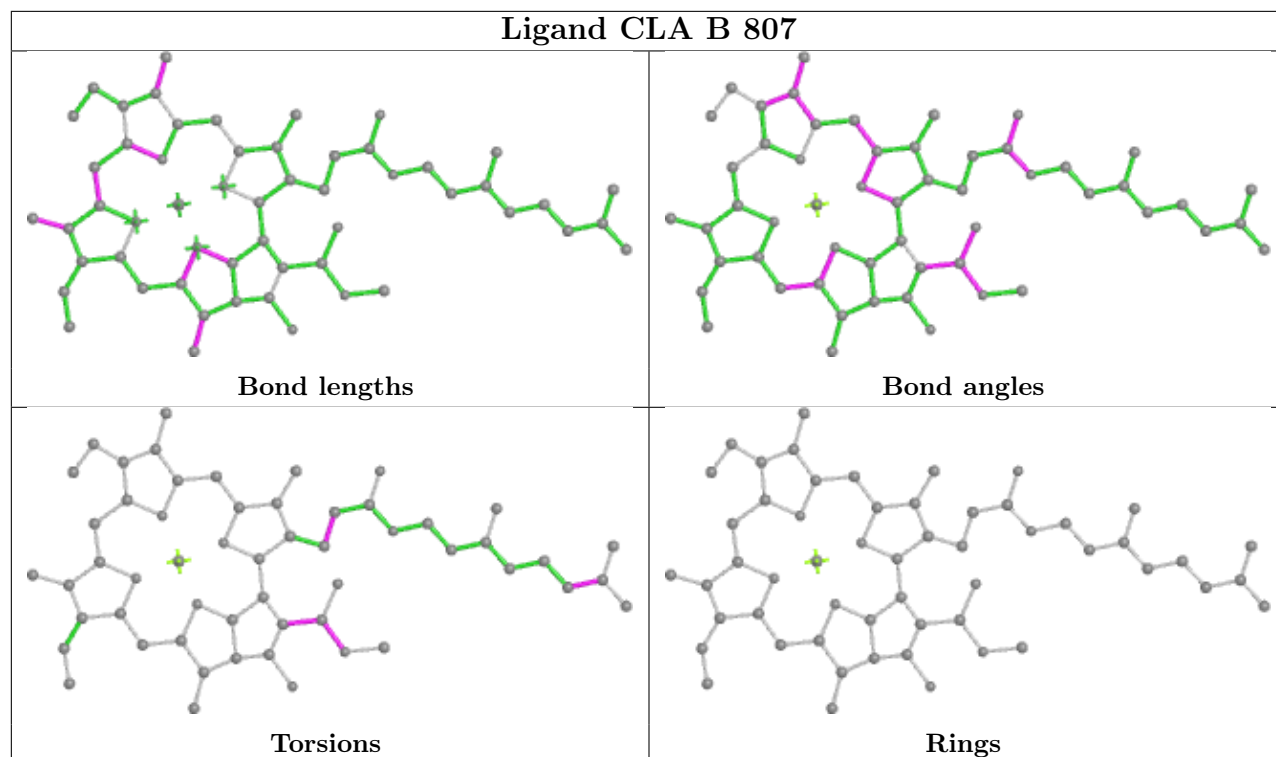
Ligand BCR 1 201



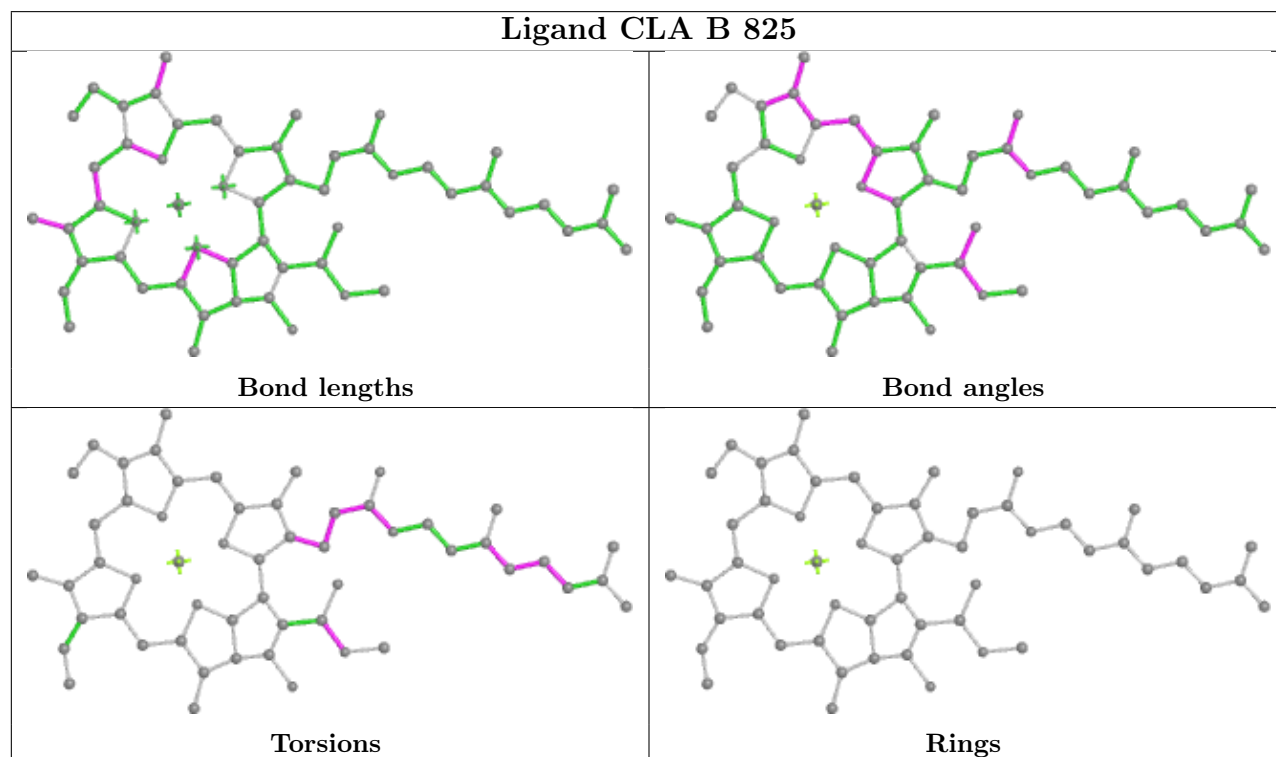
Ligand CLA b 810**Ligand CLA B 808**

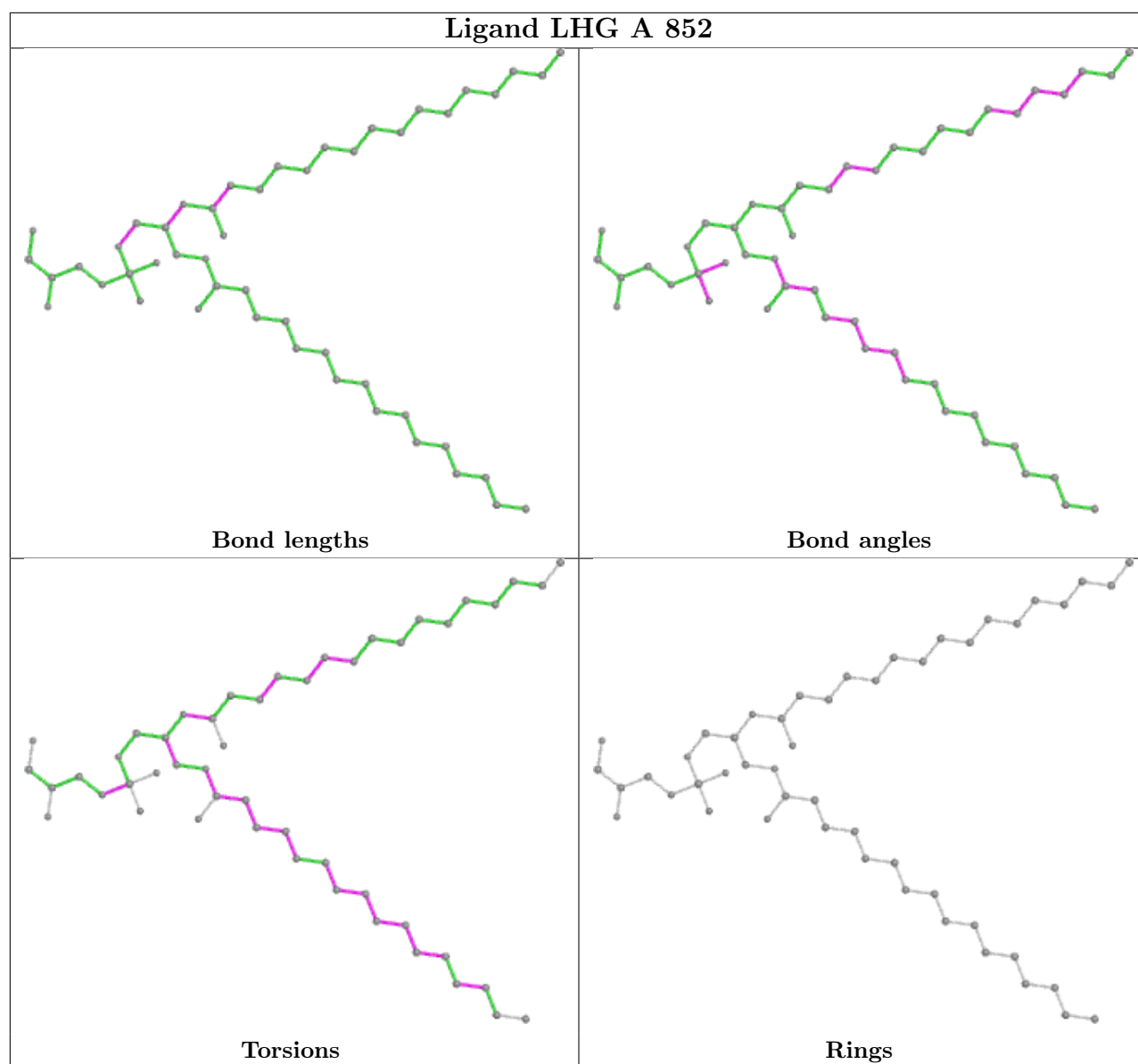


Ligand CLA B 807

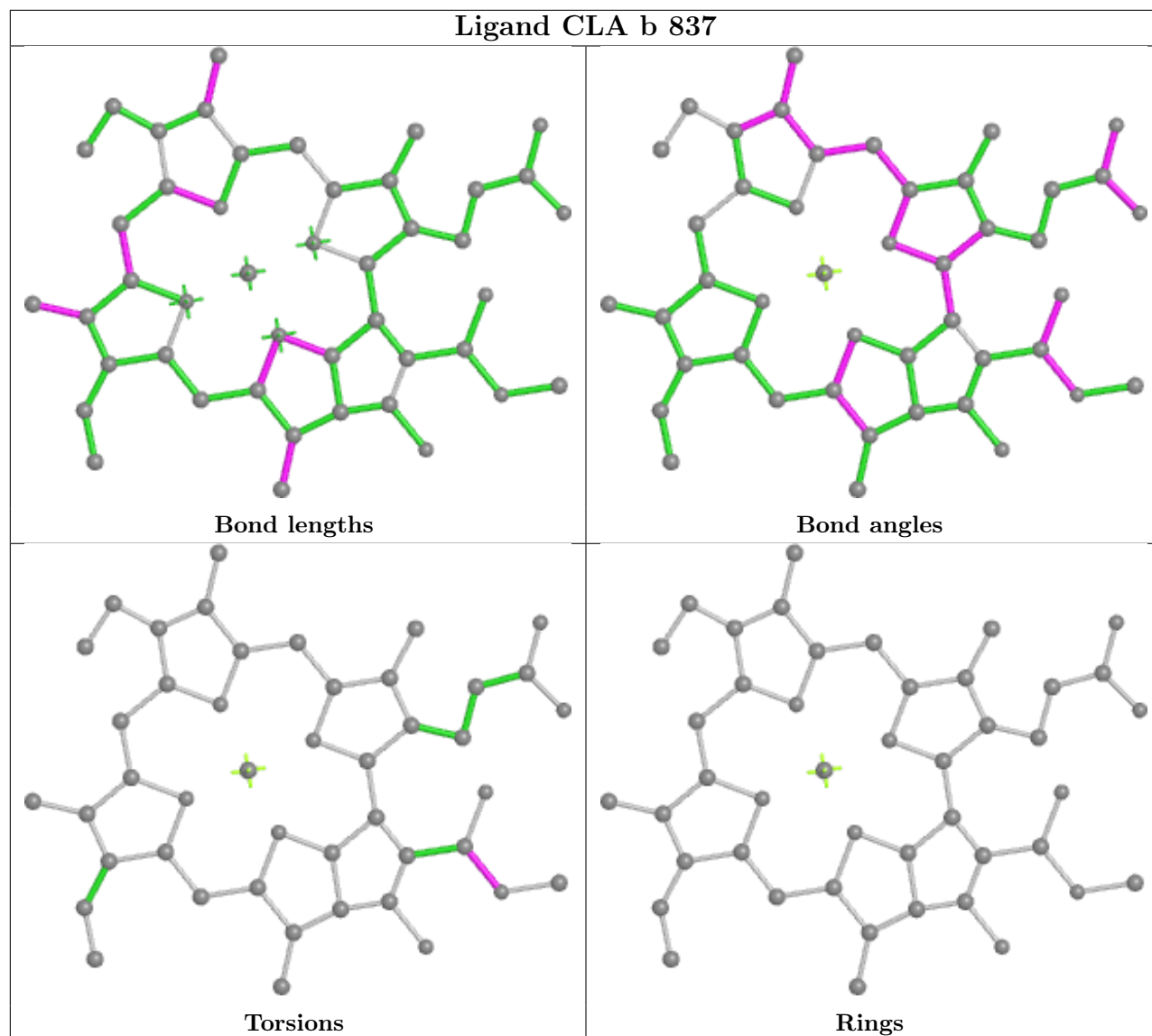


Ligand CLA B 825

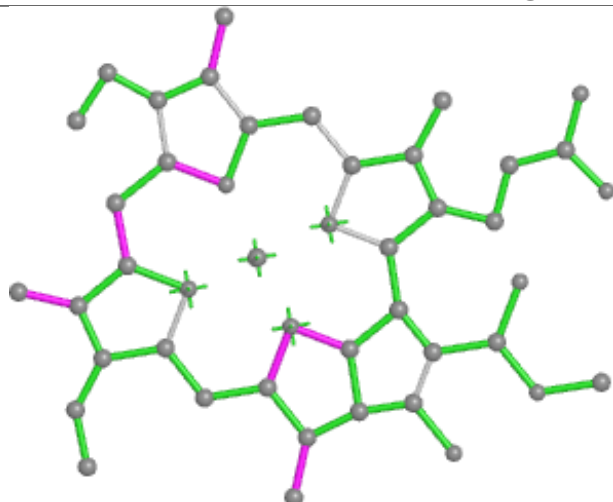




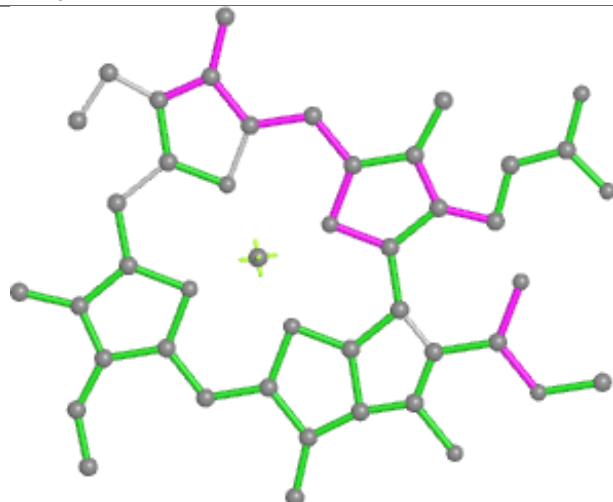
Ligand CLA b 837



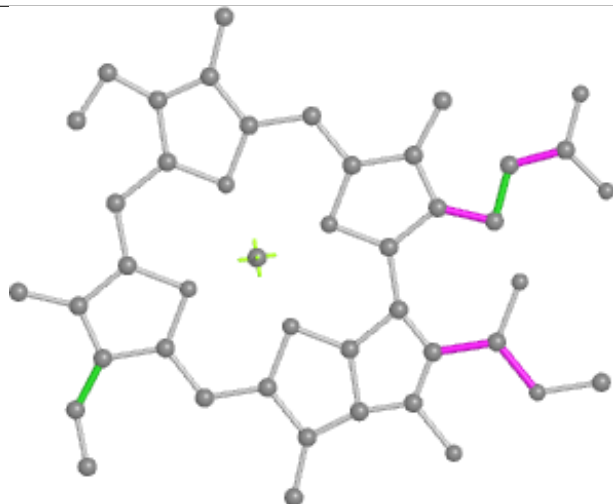
Ligand CLA j 102



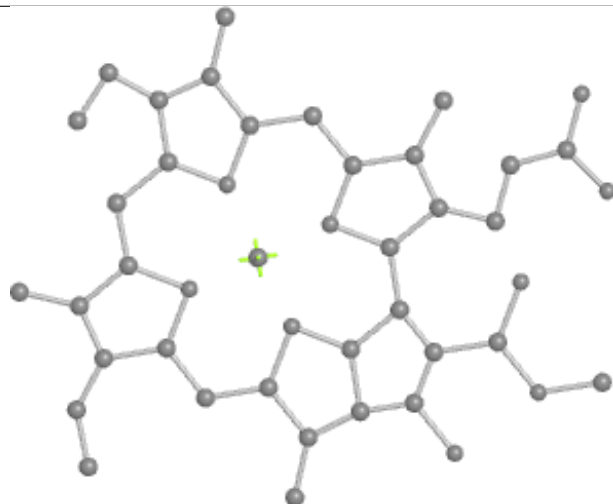
Bond lengths



Bond angles

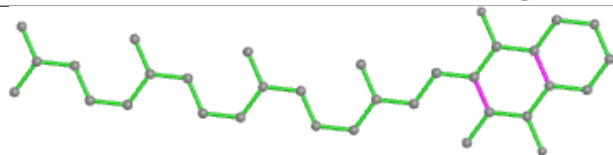


Torsions

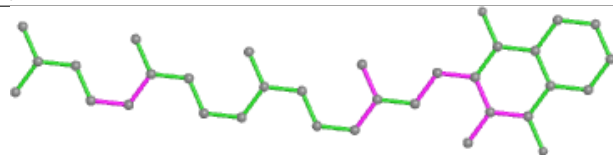


Rings

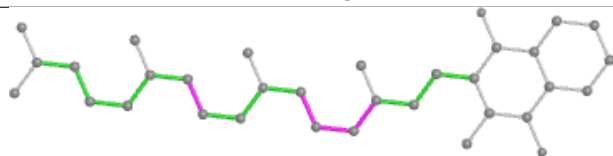
Ligand PQN a 842



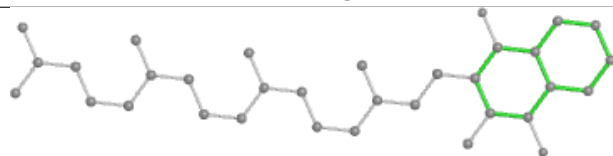
Bond lengths



Bond angles

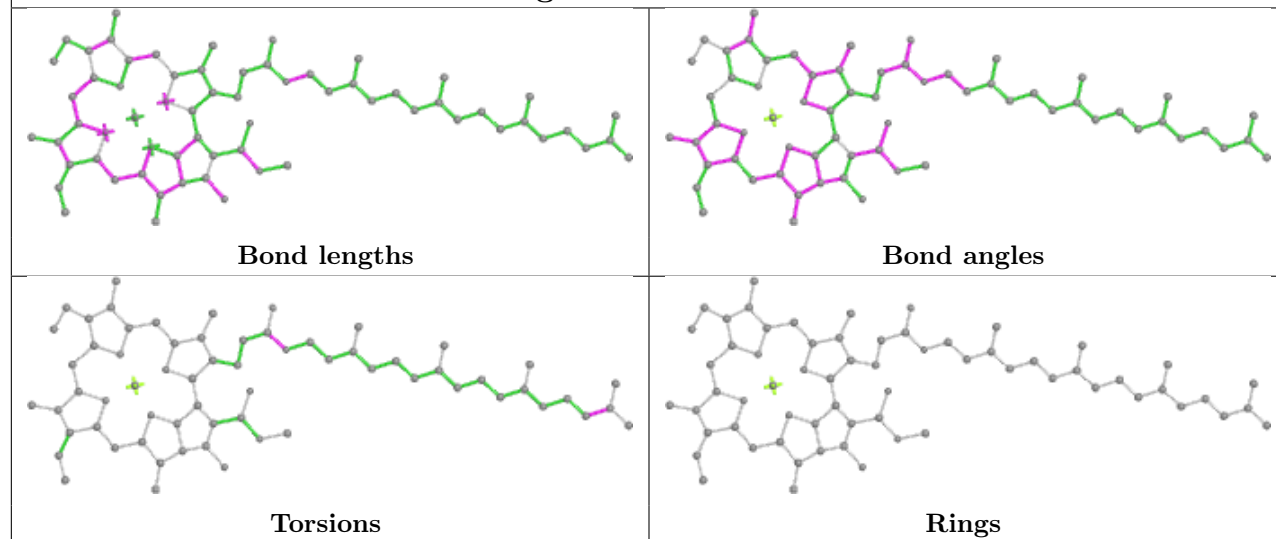


Torsions

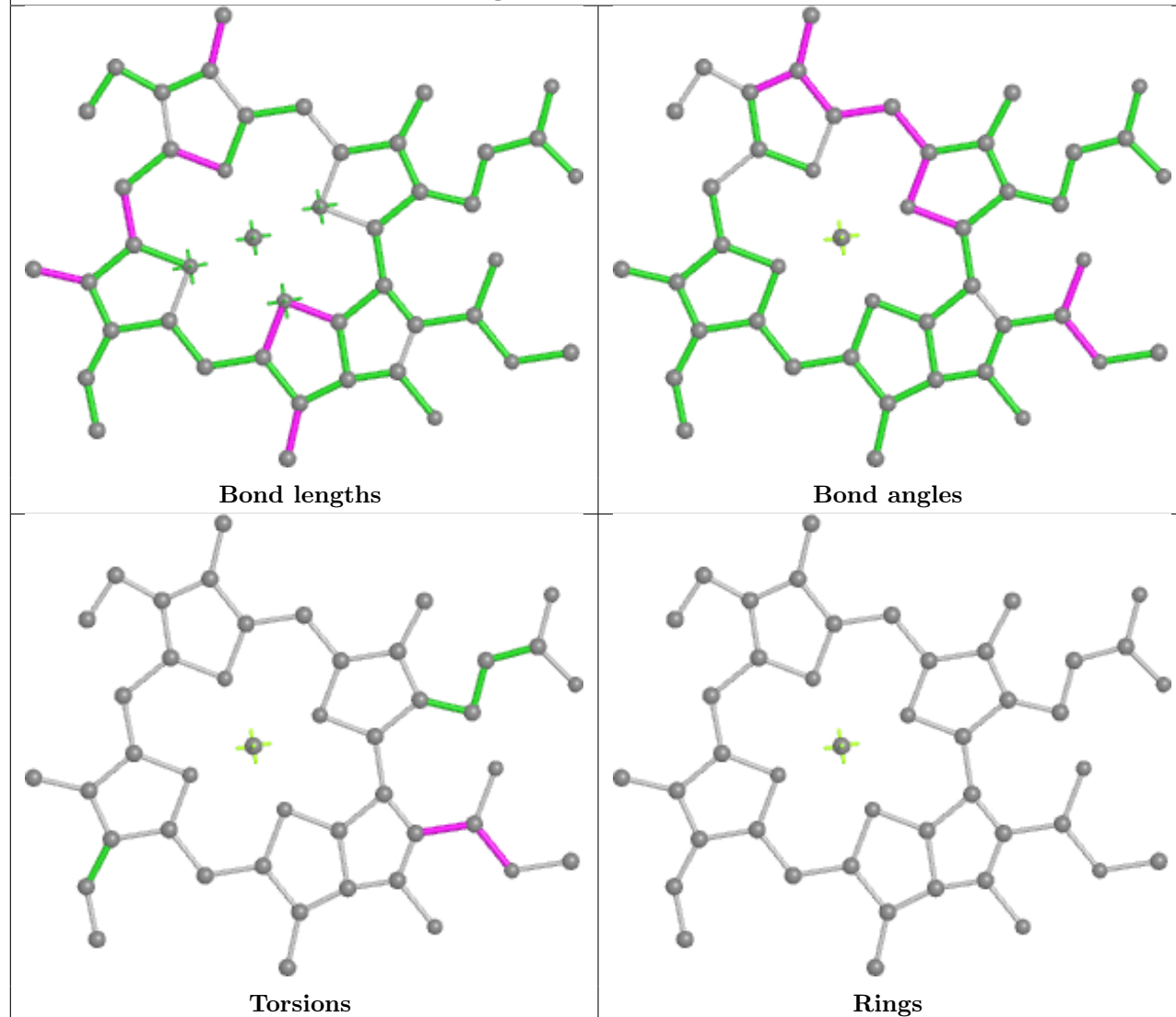


Rings

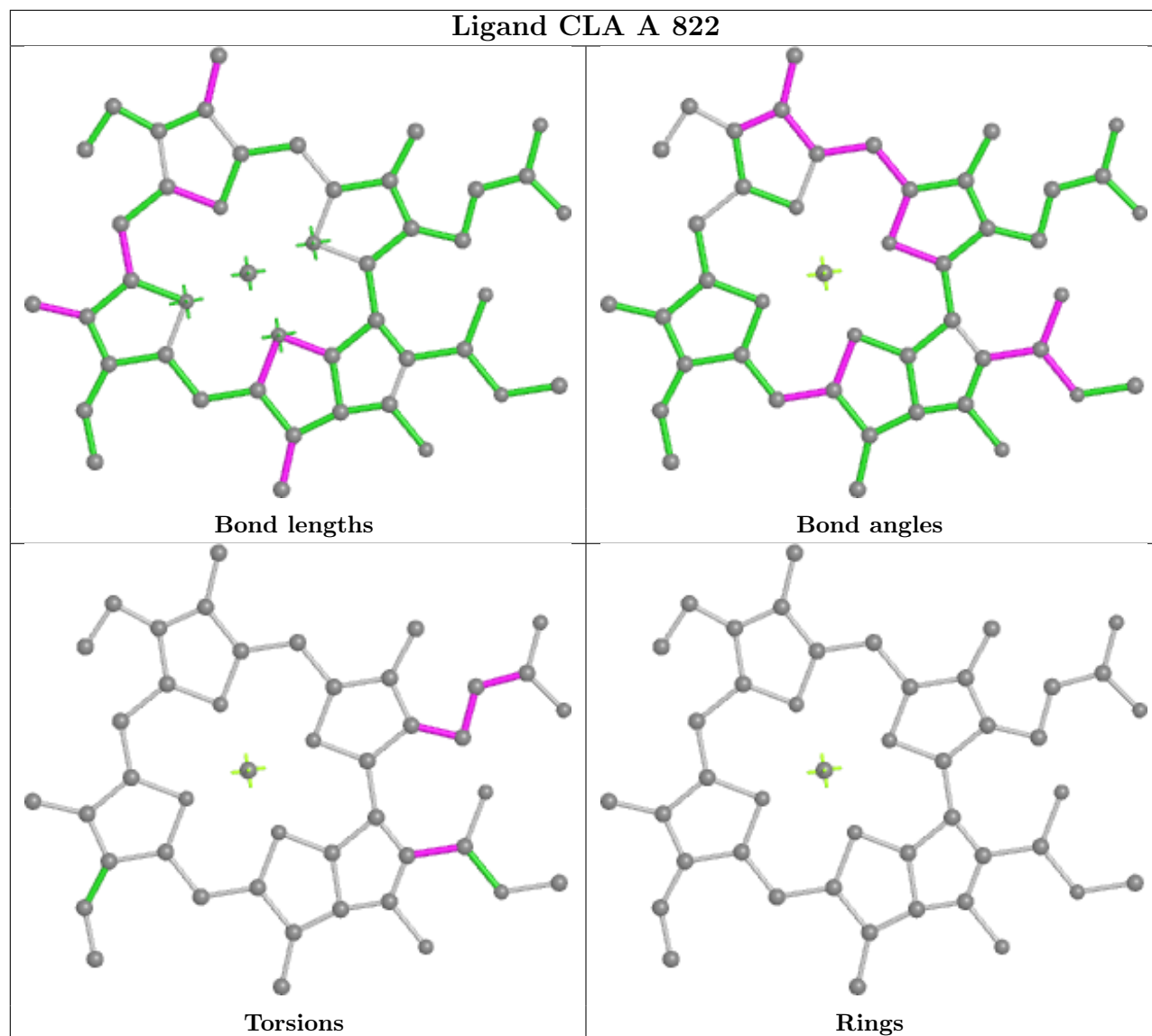
Ligand CL0 A 801



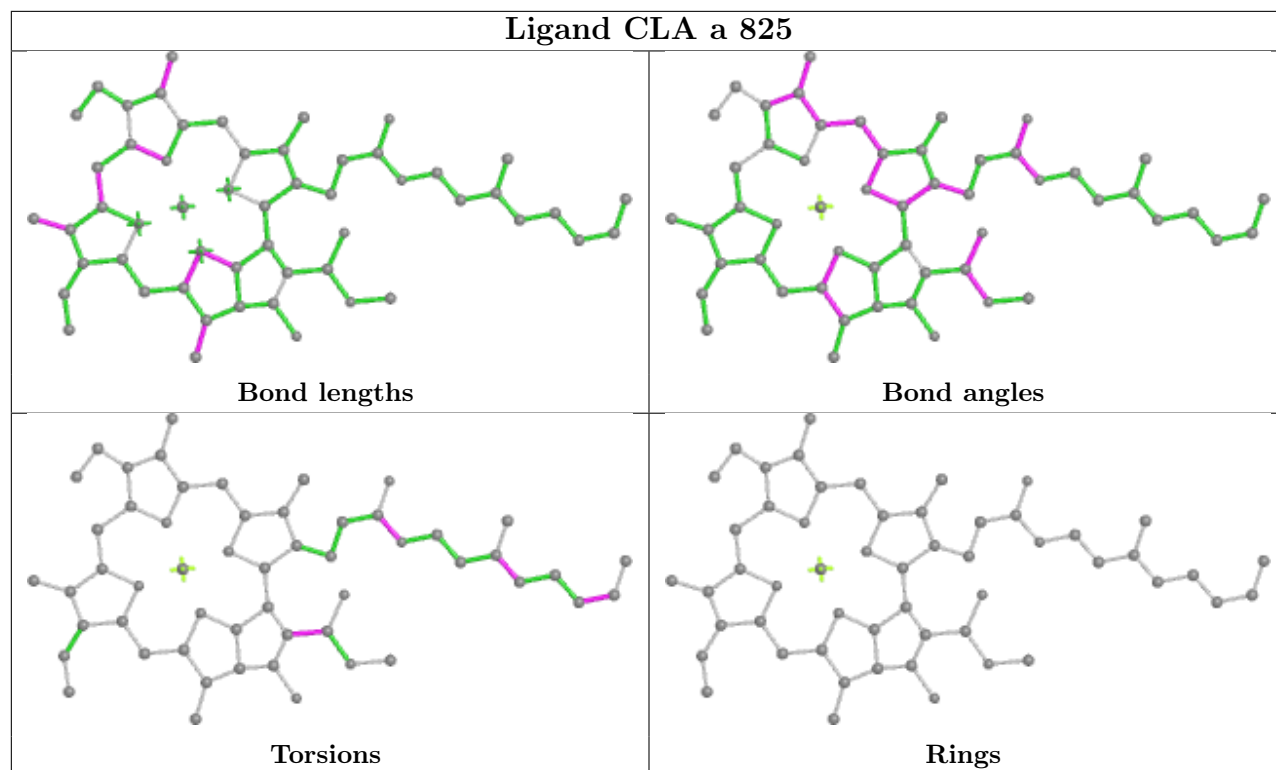
Ligand CLA A 815



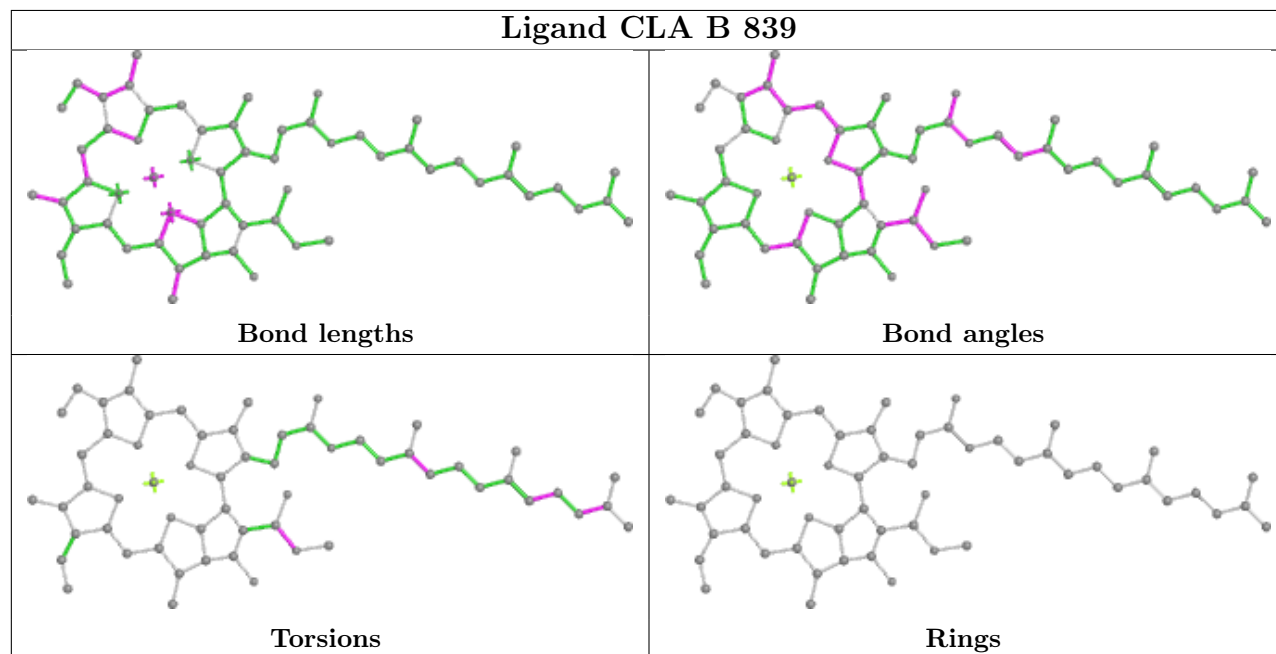
Ligand CLA A 822



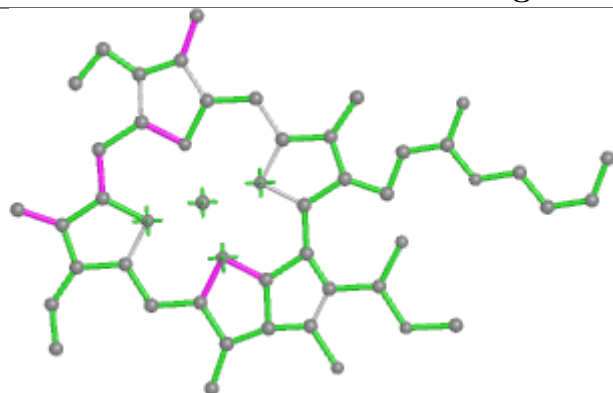
Ligand CLA a 825



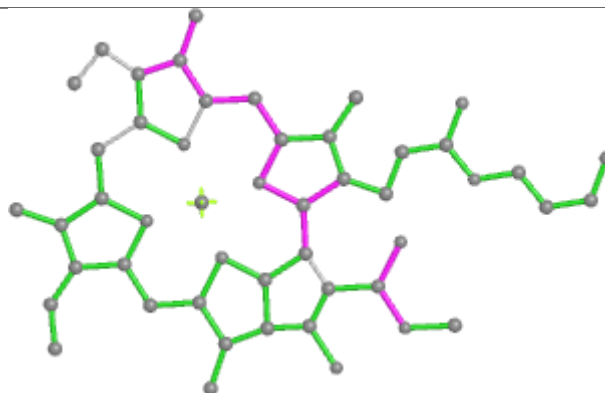
Ligand CLA B 839



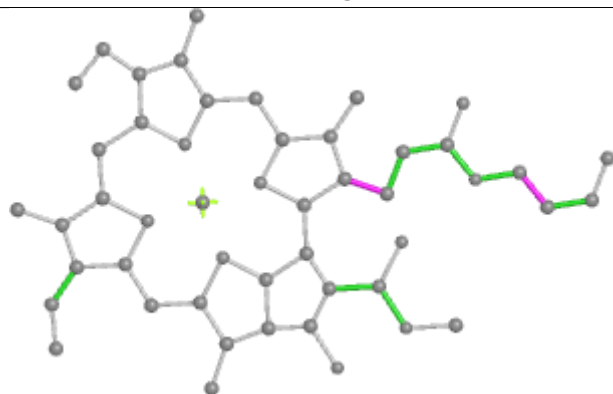
Ligand CLA K 102



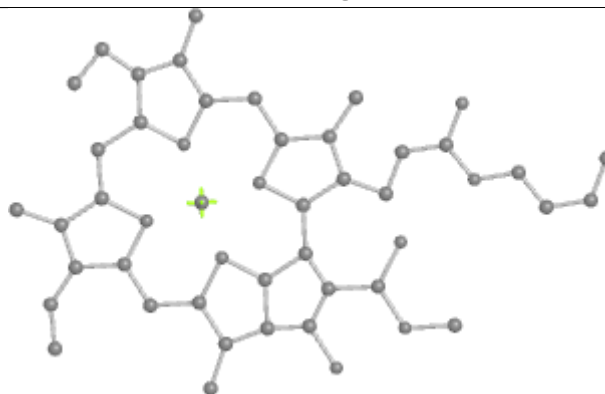
Bond lengths



Bond angles

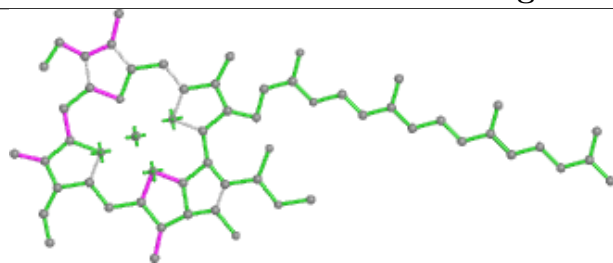


Torsions

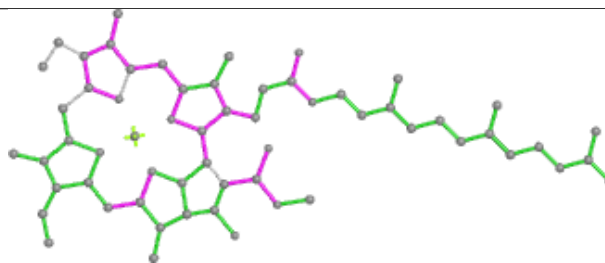


Rings

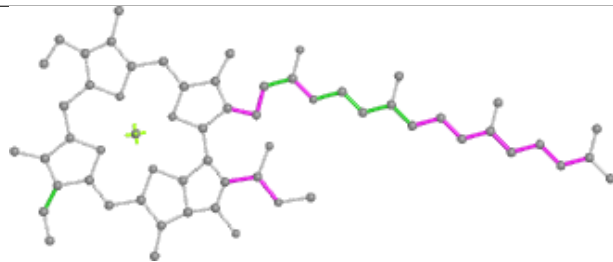
Ligand CLA b 813



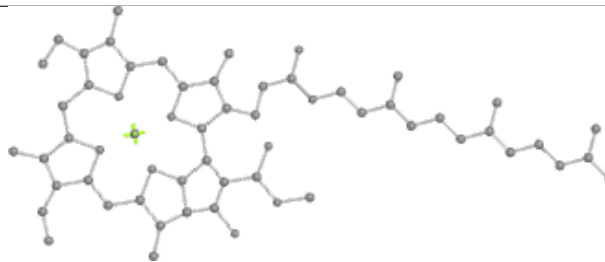
Bond lengths



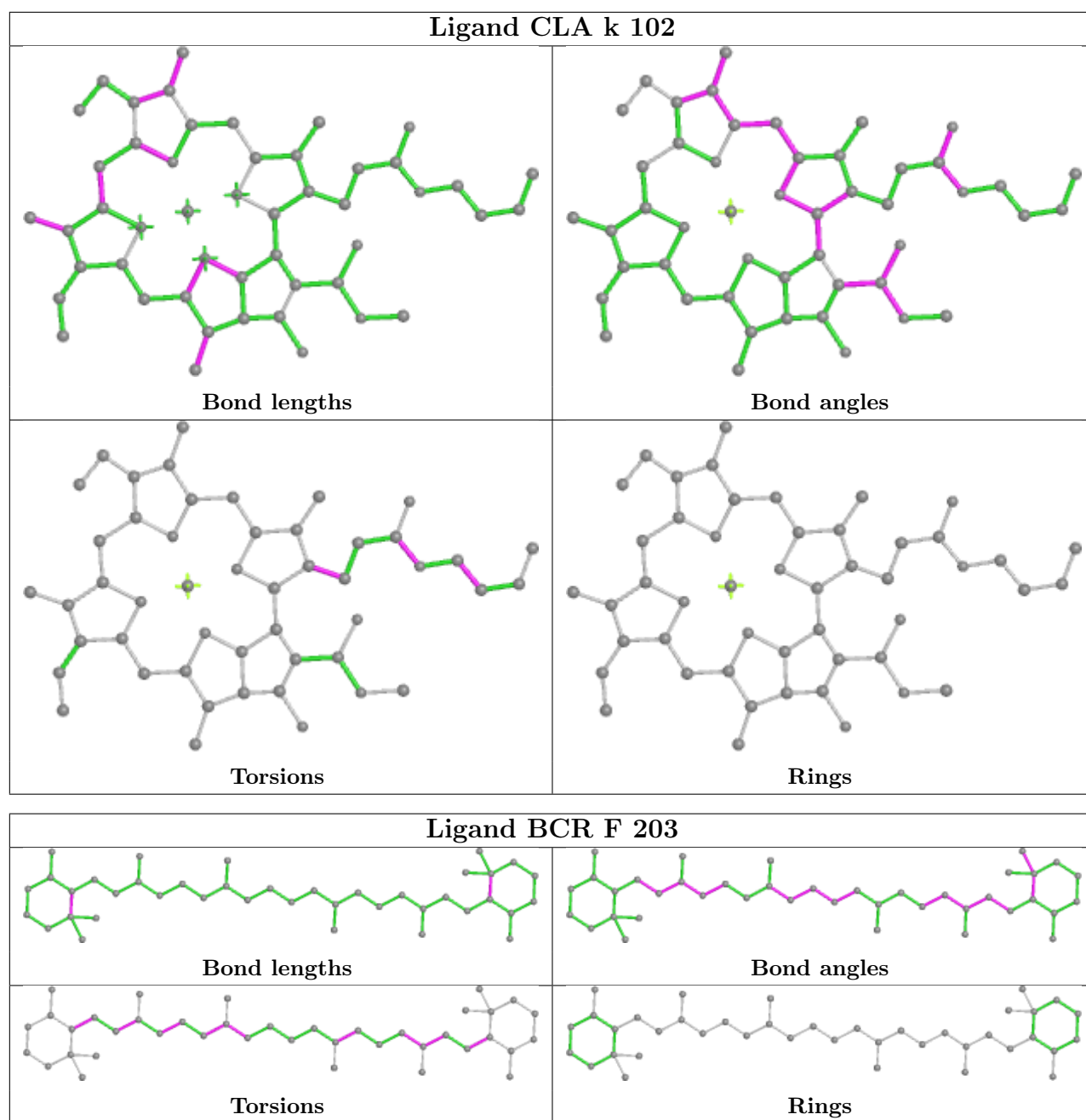
Bond angles

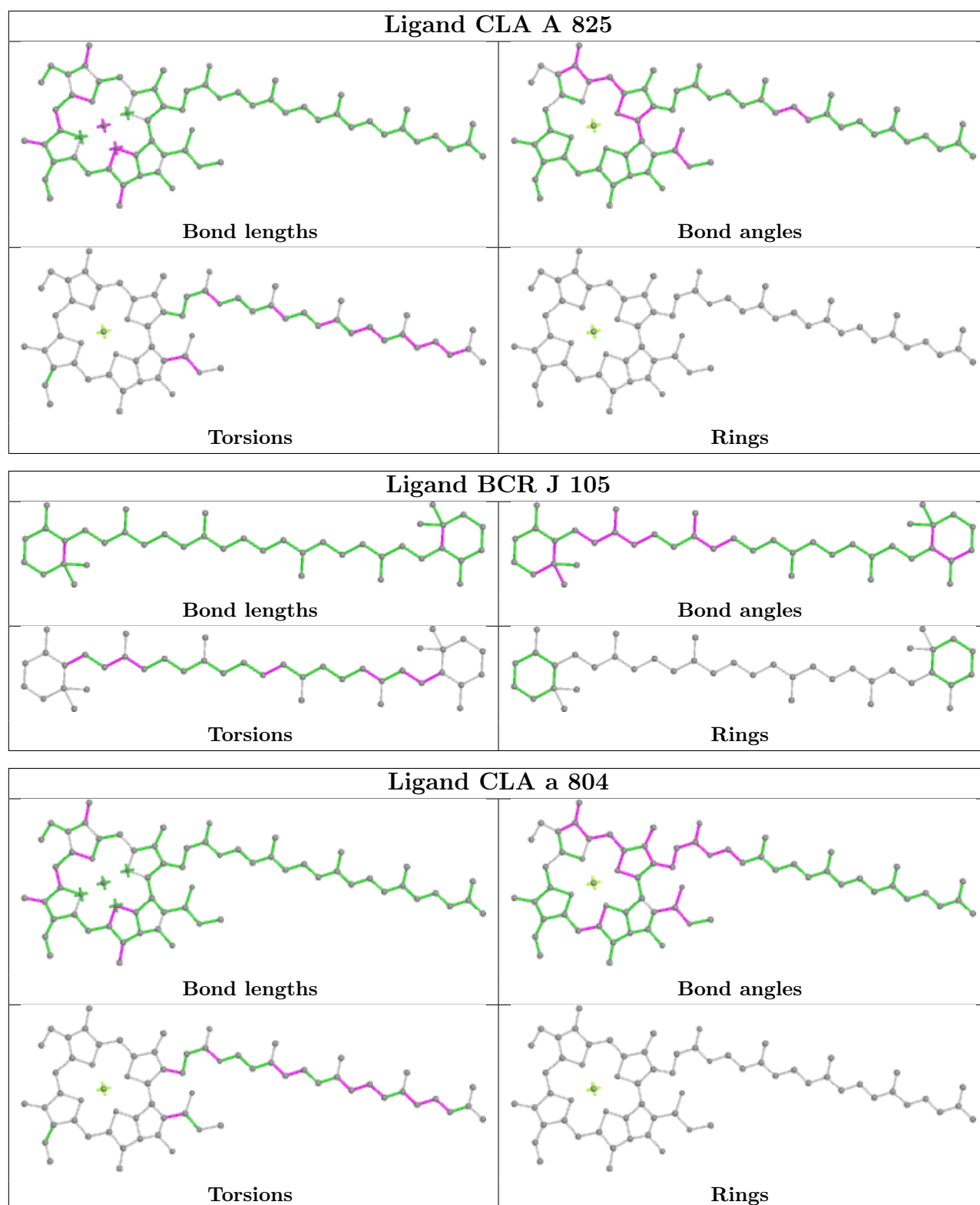


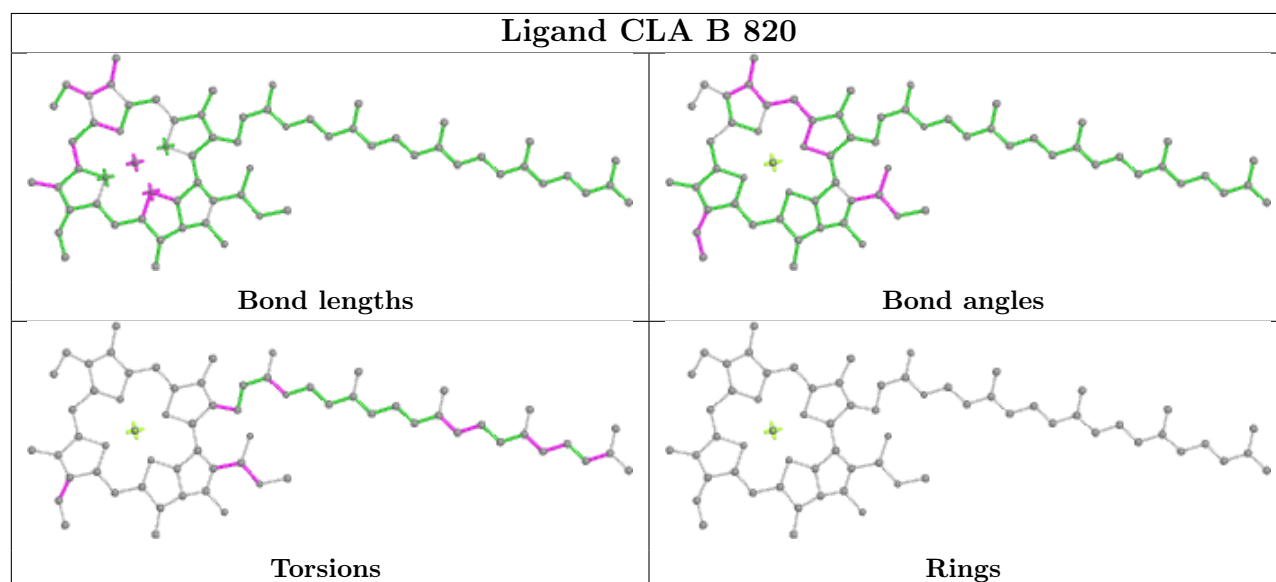
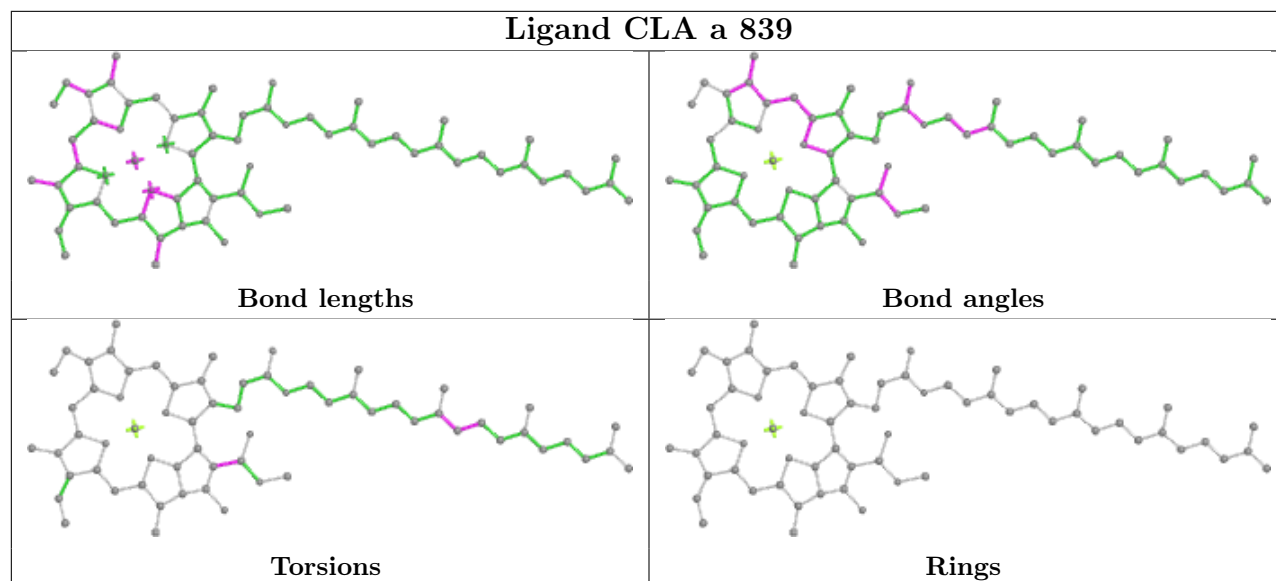
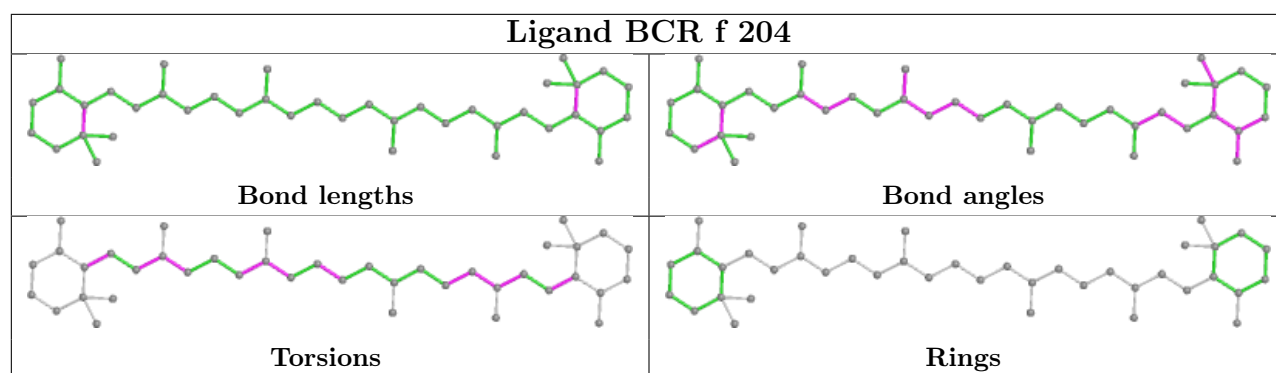
Torsions



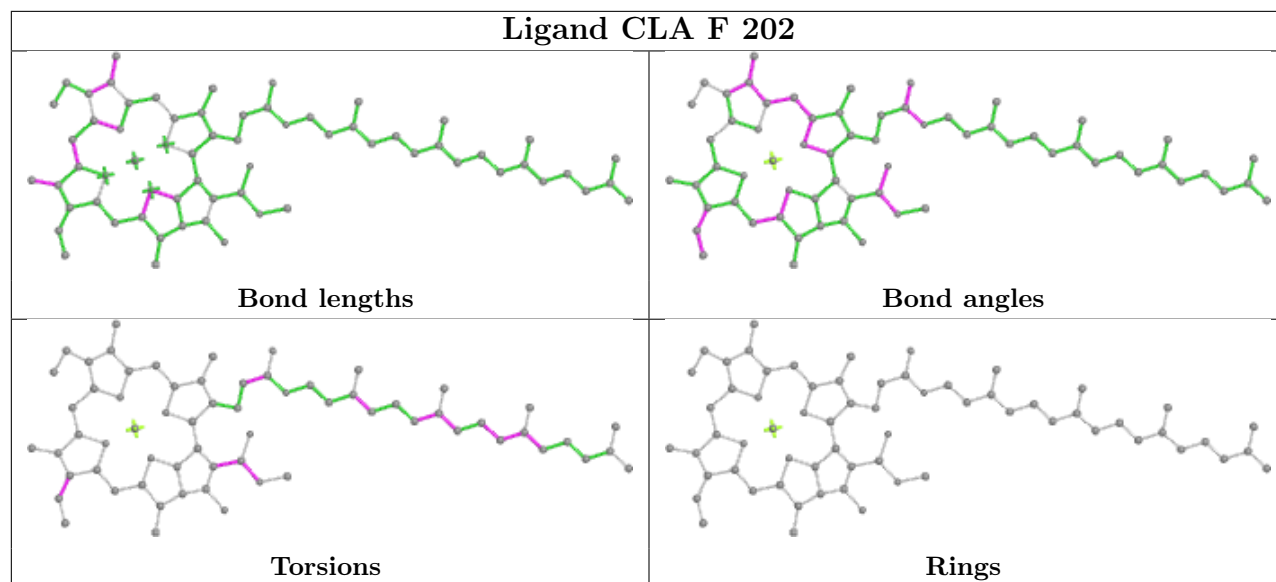
Rings



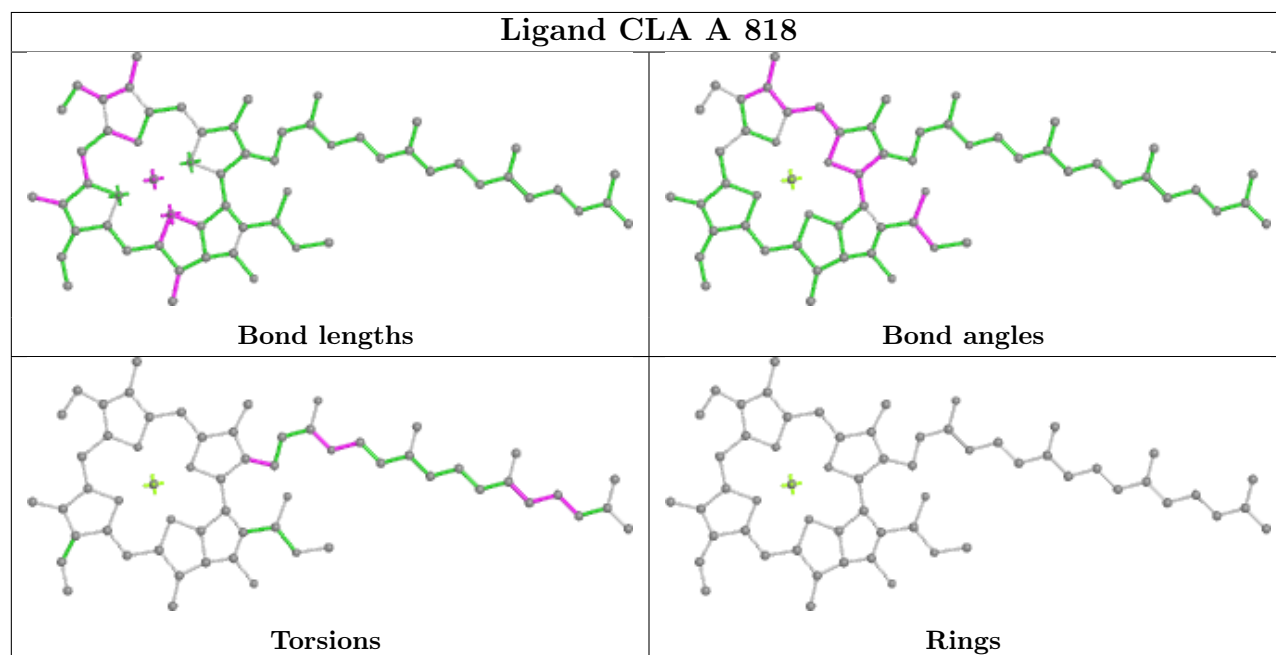


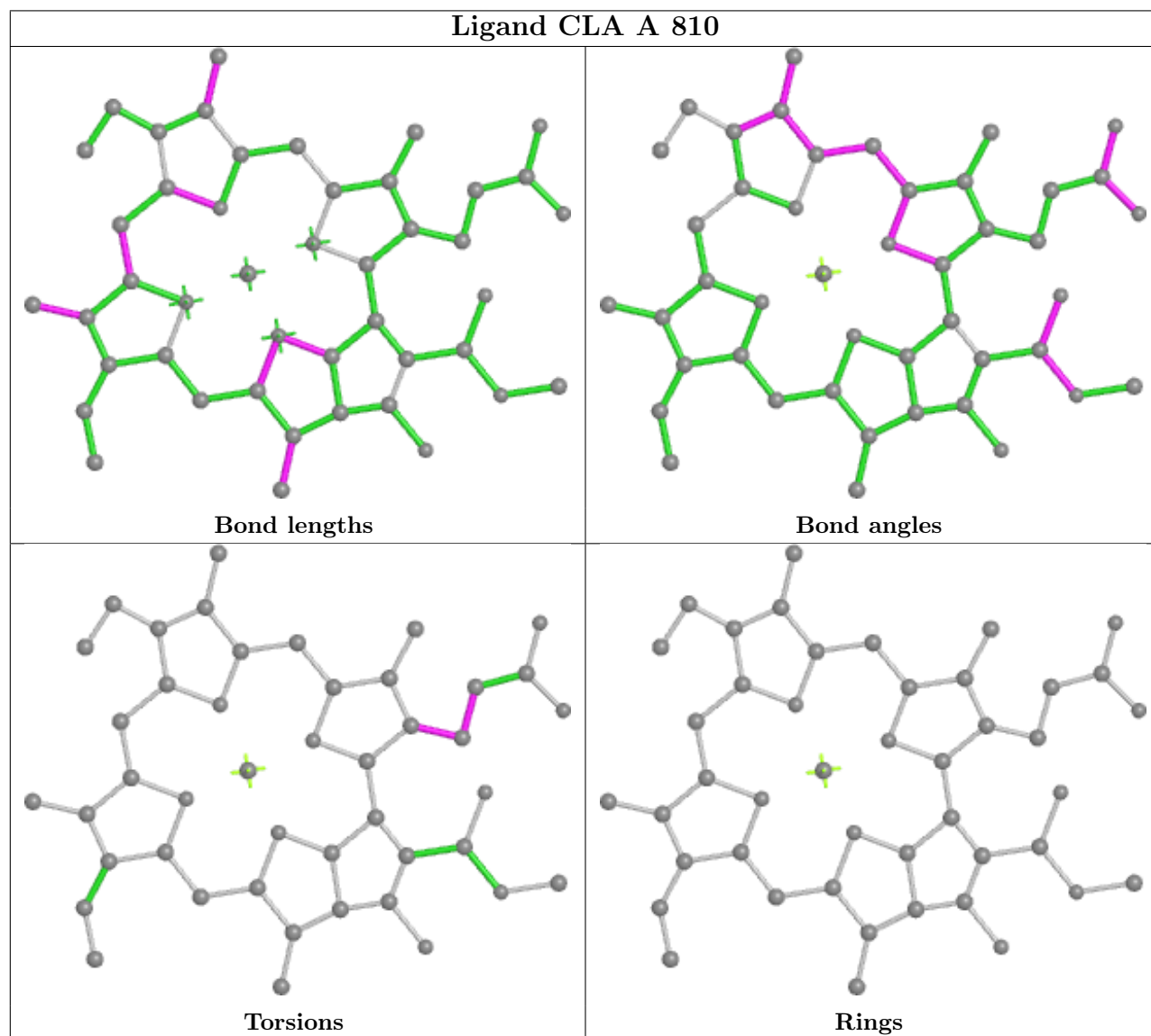
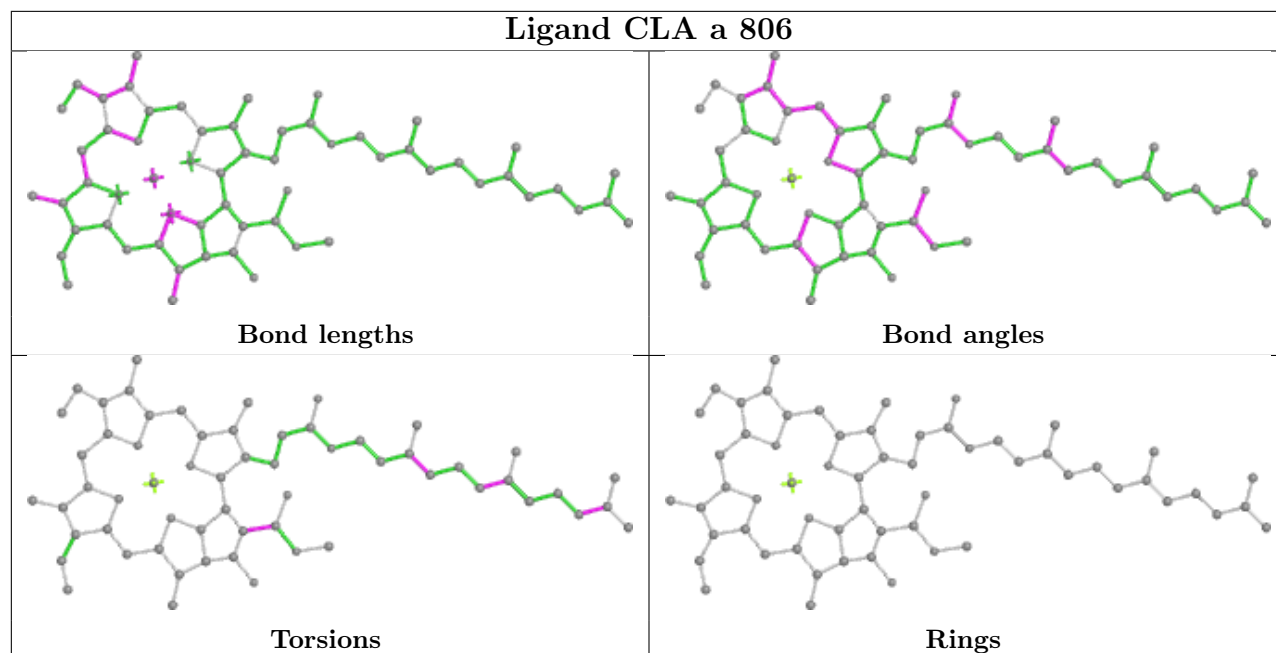


Ligand CLA F 202

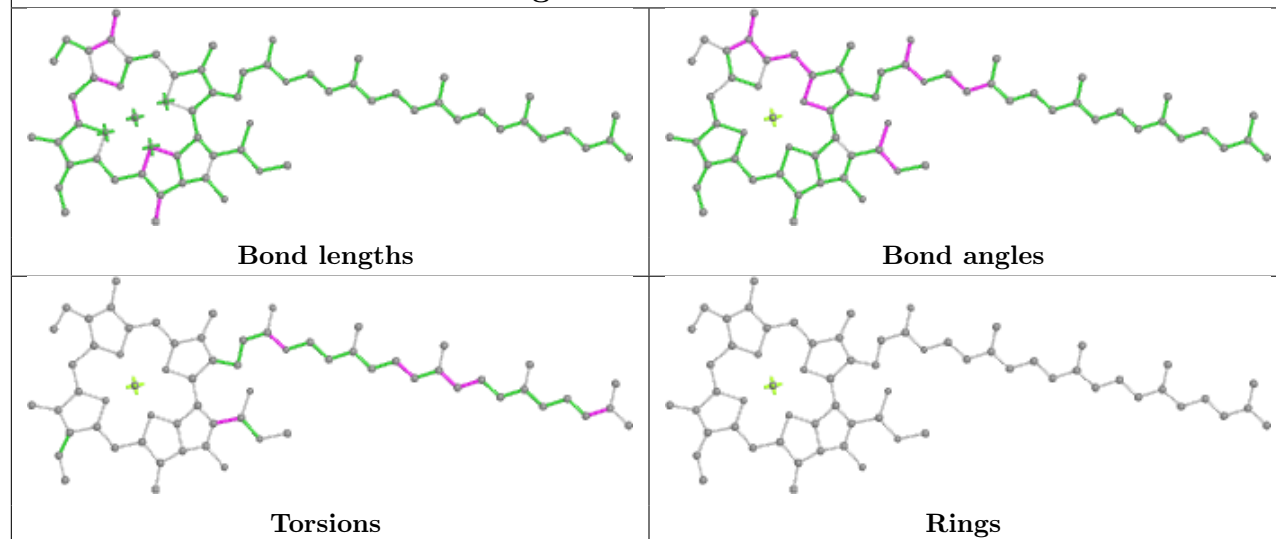


Ligand CLA A 818

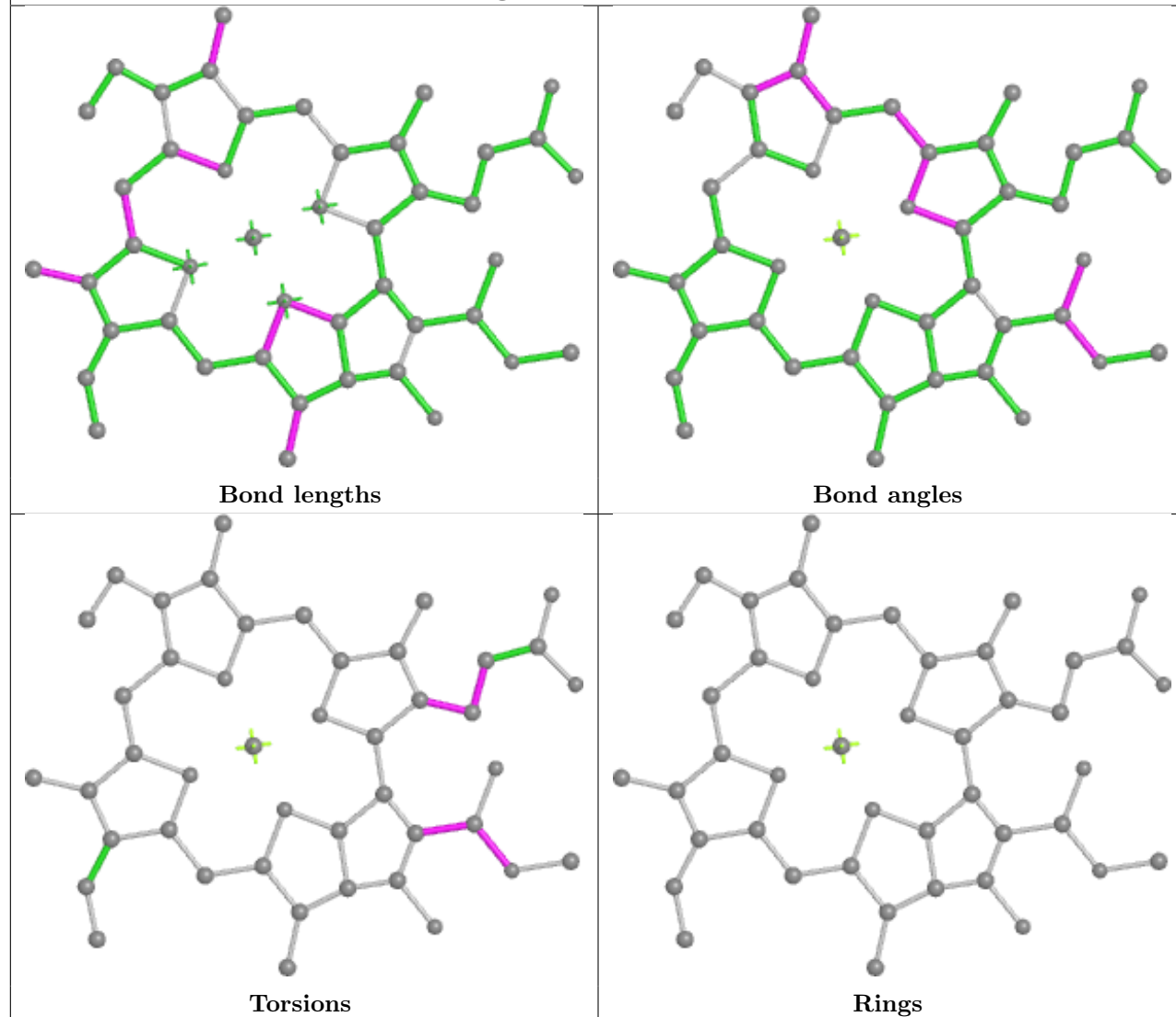




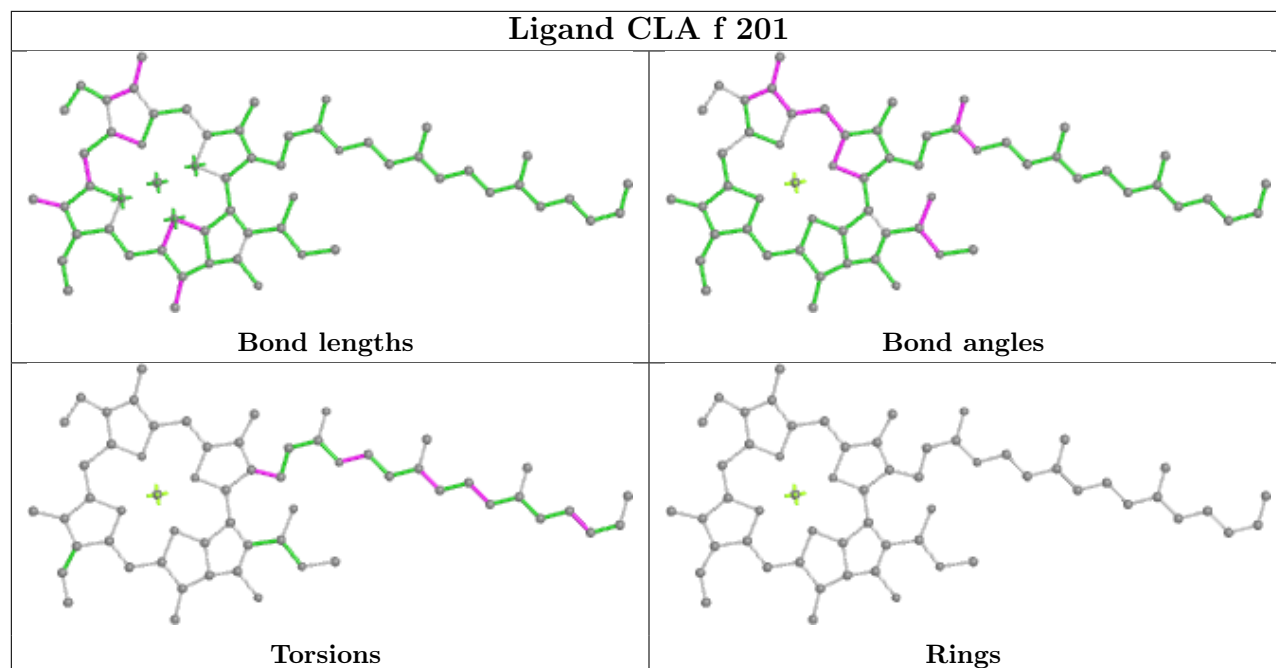
Ligand CLA B 822



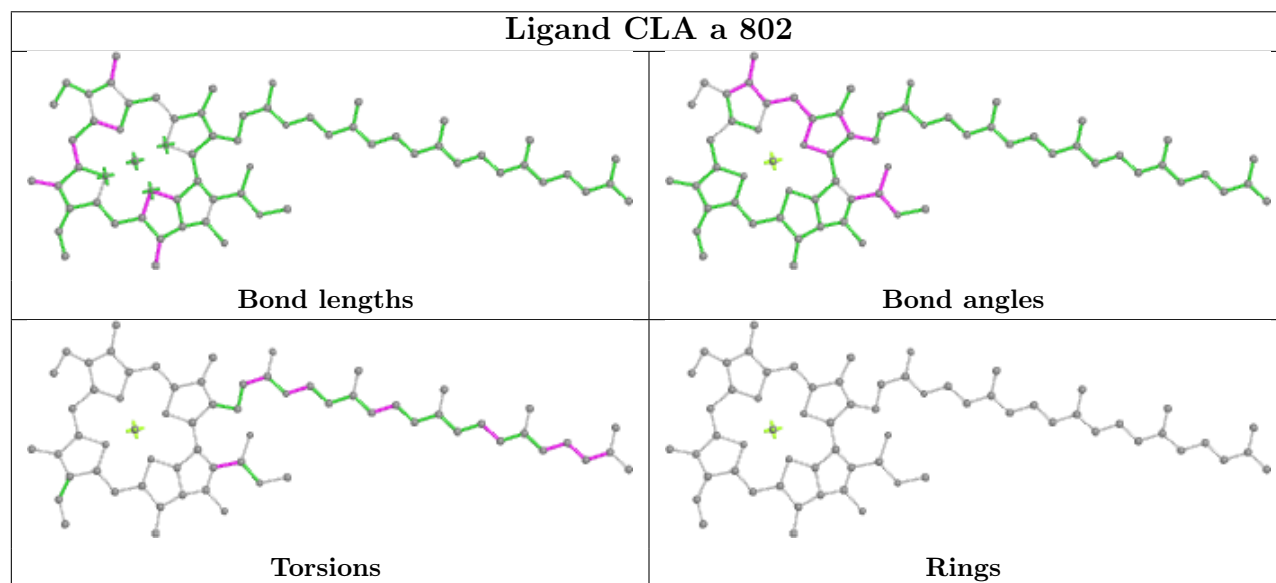
Ligand CLA a 809

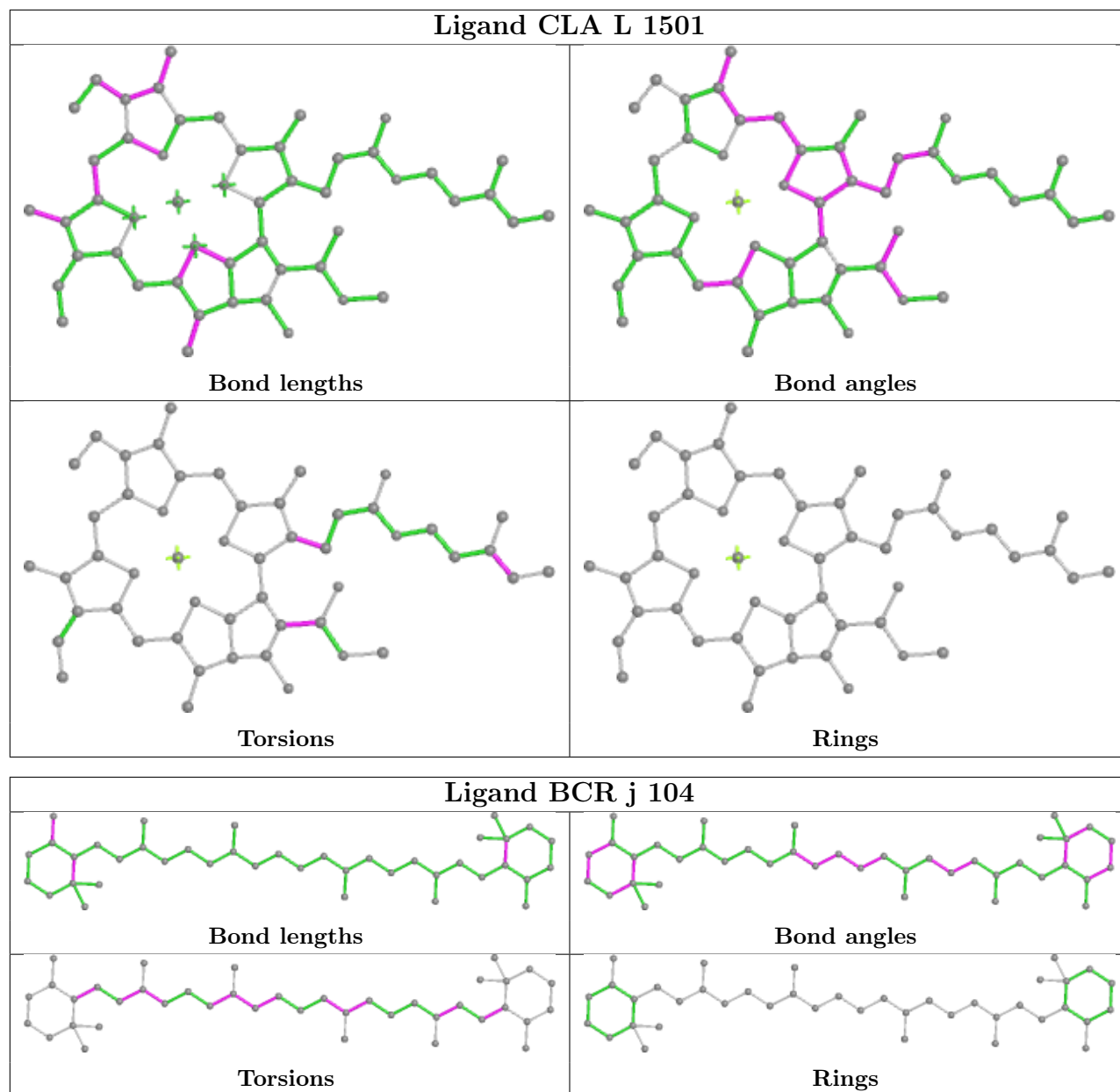


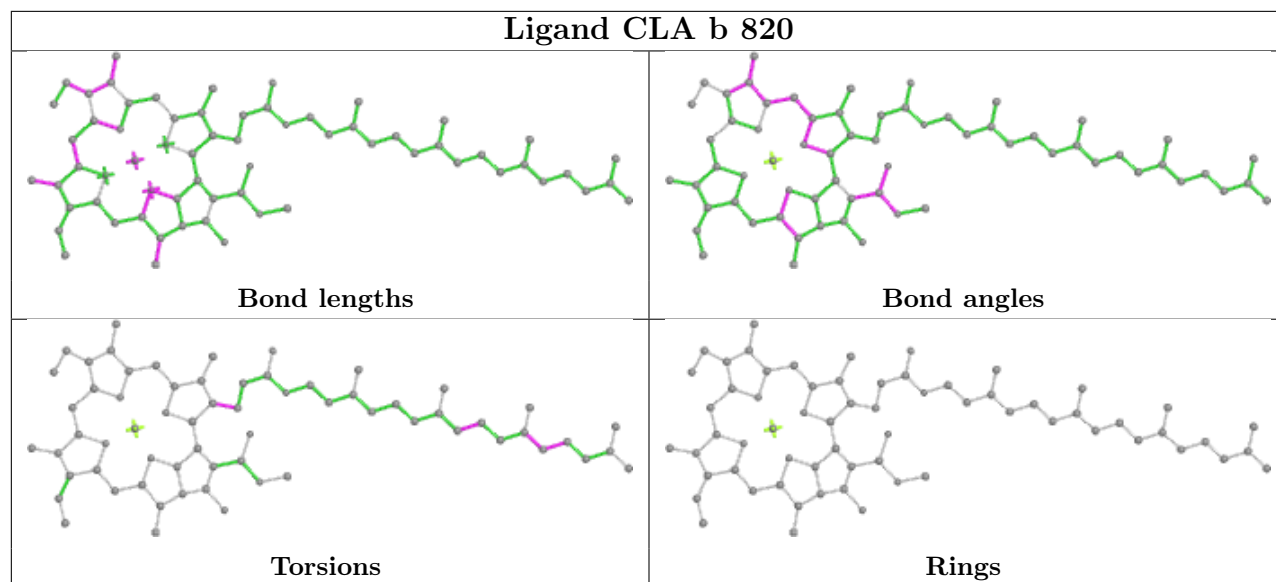
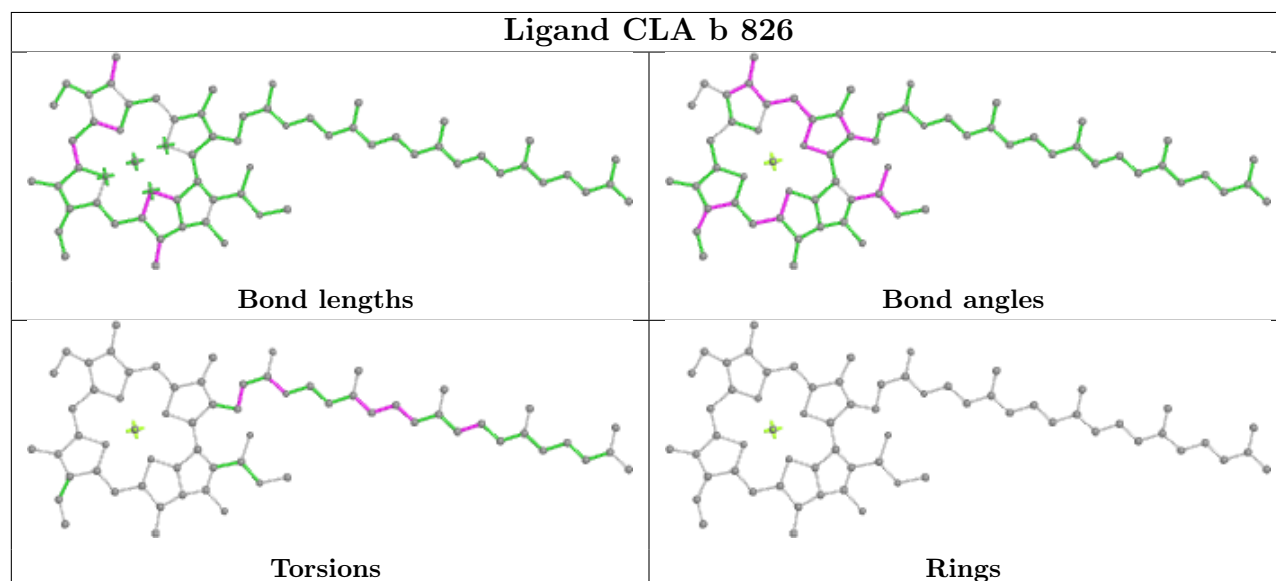
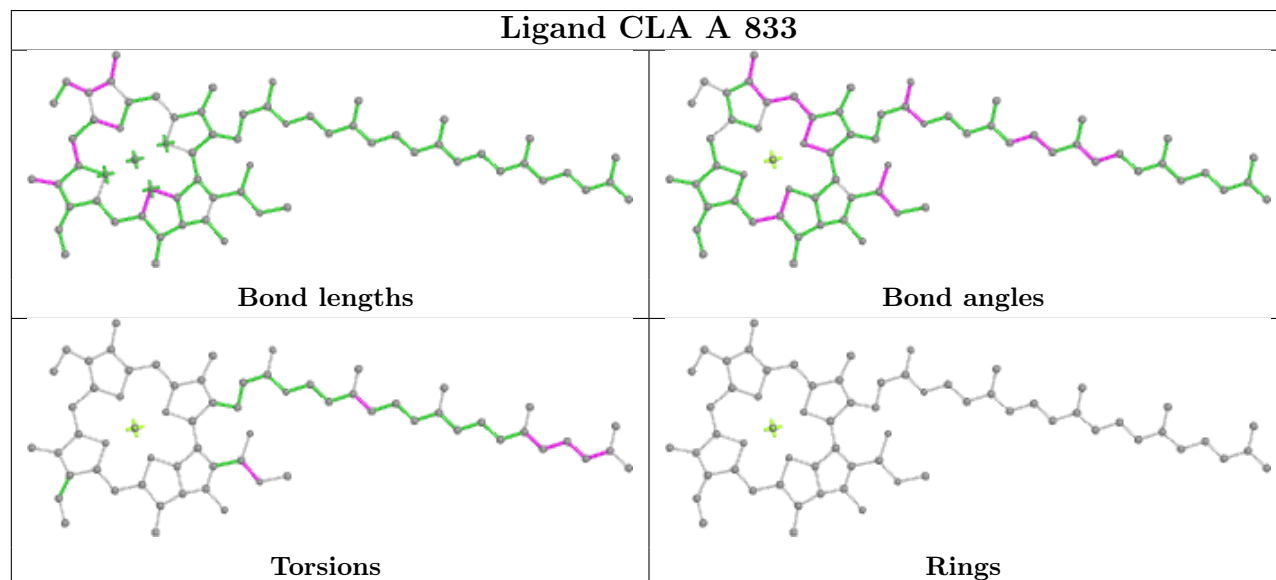
Ligand CLA f 201



Ligand CLA a 802





Ligand CLA b 820**Ligand CLA b 826****Ligand CLA A 833**

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

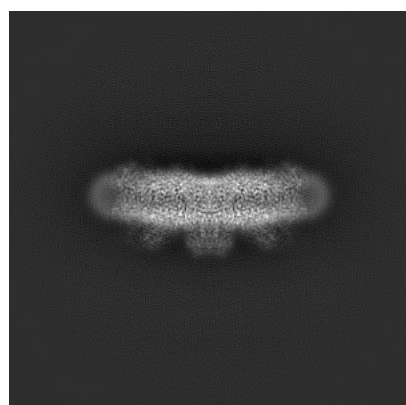
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9918. These allow visual inspection of the internal detail of the map and identification of artifacts.

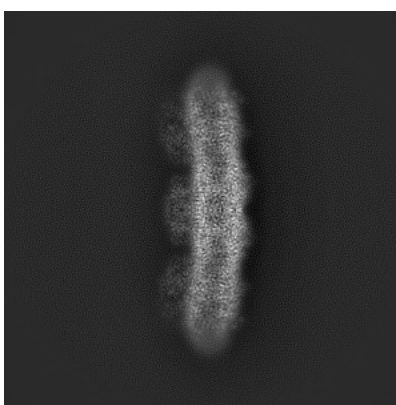
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

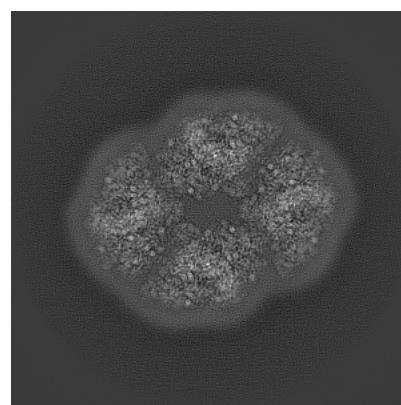
6.1.1 Primary map



X



Y

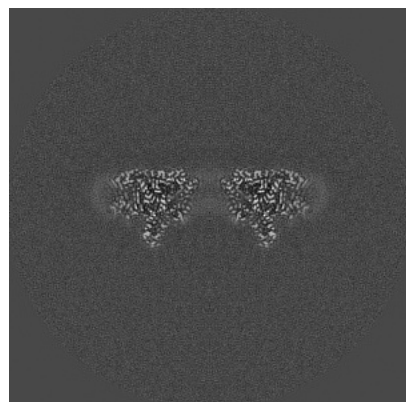


Z

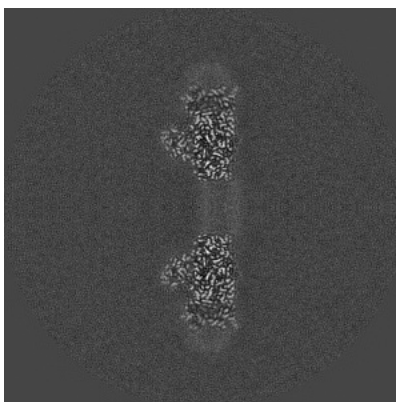
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

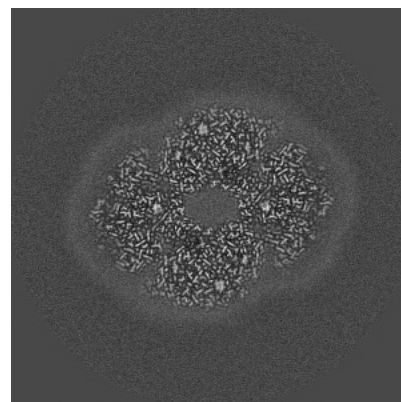
6.2.1 Primary map



X Index: 200



Y Index: 200

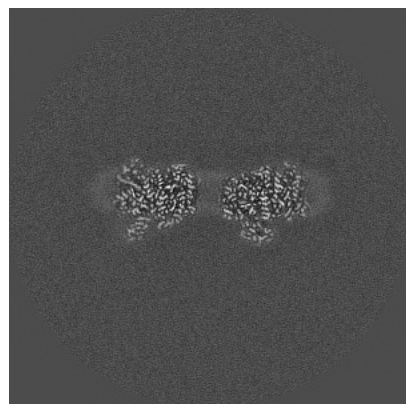


Z Index: 200

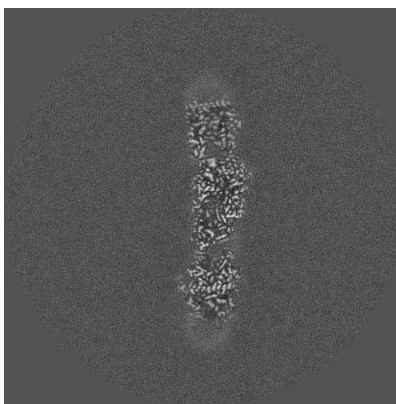
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

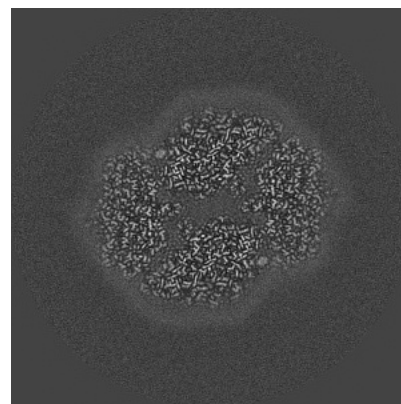
6.3.1 Primary map



X Index: 219



Y Index: 171

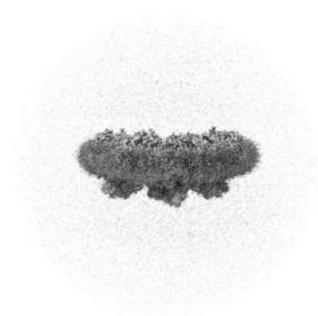


Z Index: 223

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

6.4 Orthogonal surface views [i](#)

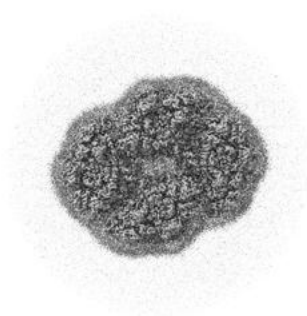
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

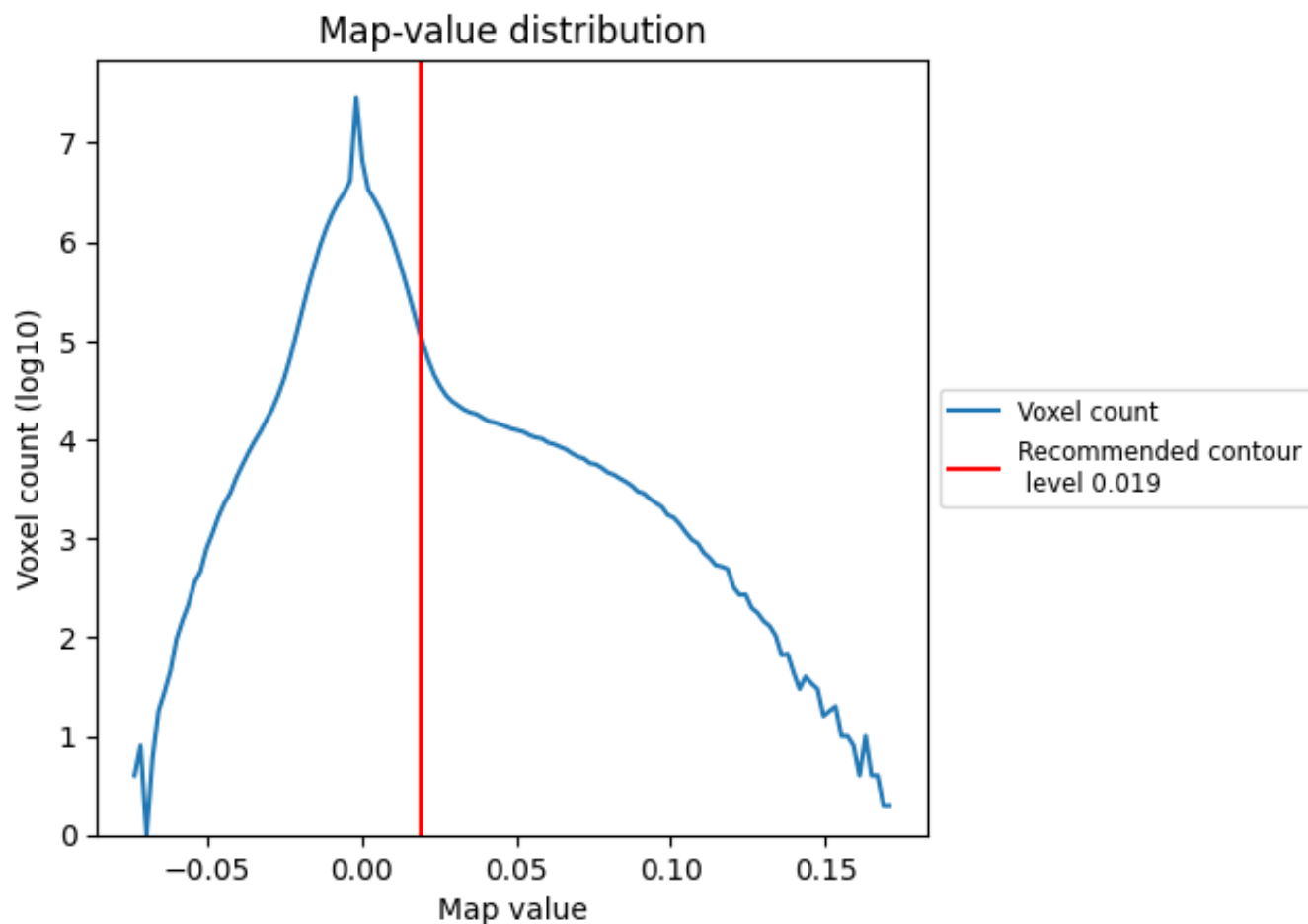
6.5 Mask visualisation

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

7 Map analysis [i](#)

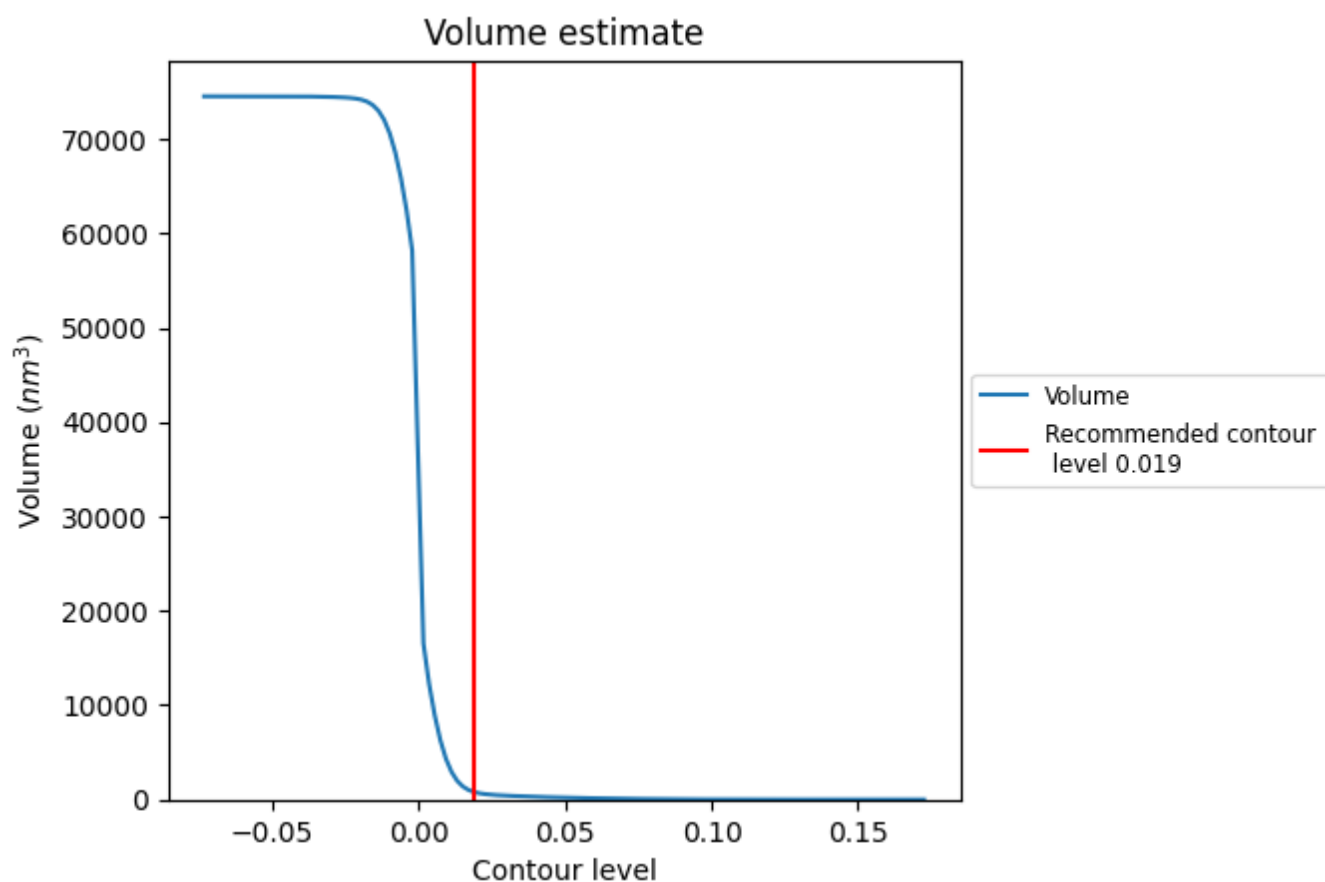
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

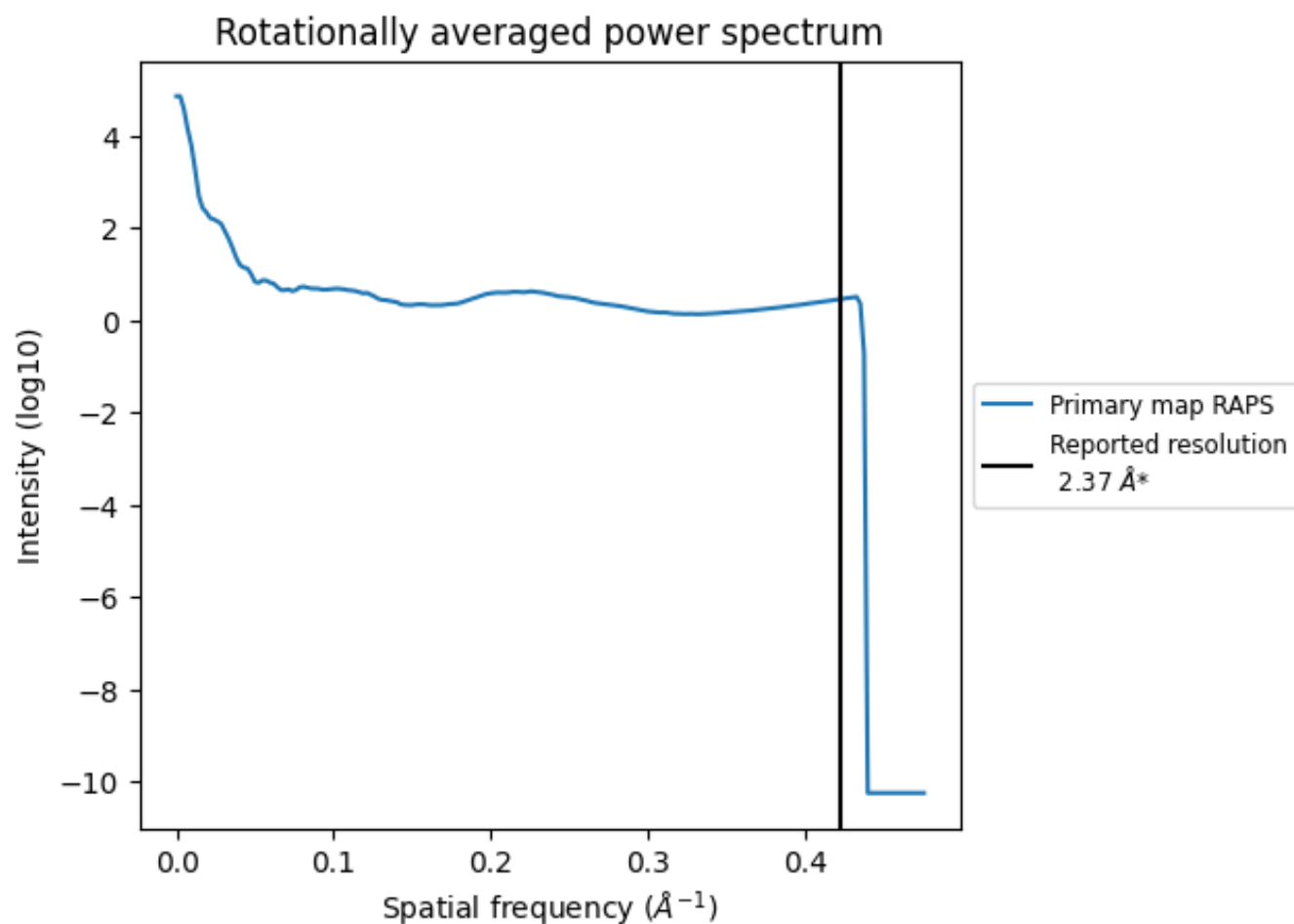
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 790 nm³; this corresponds to an approximate mass of 714 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.422 Å⁻¹

8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

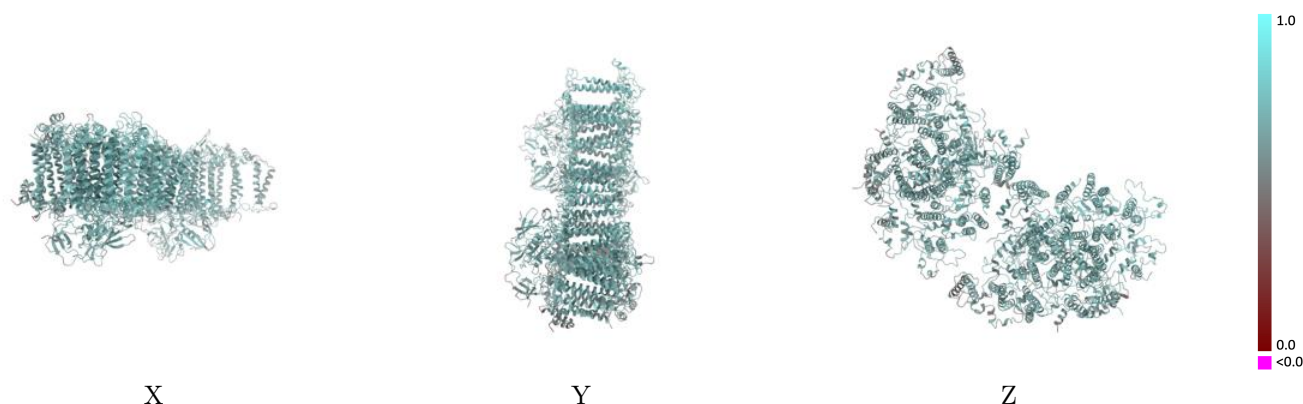
This section contains information regarding the fit between EMDB map EMD-9918 and PDB model 6K61. Per-residue inclusion information can be found in section [3](#) on page [28](#).

9.1 Map-model overlay [i](#)



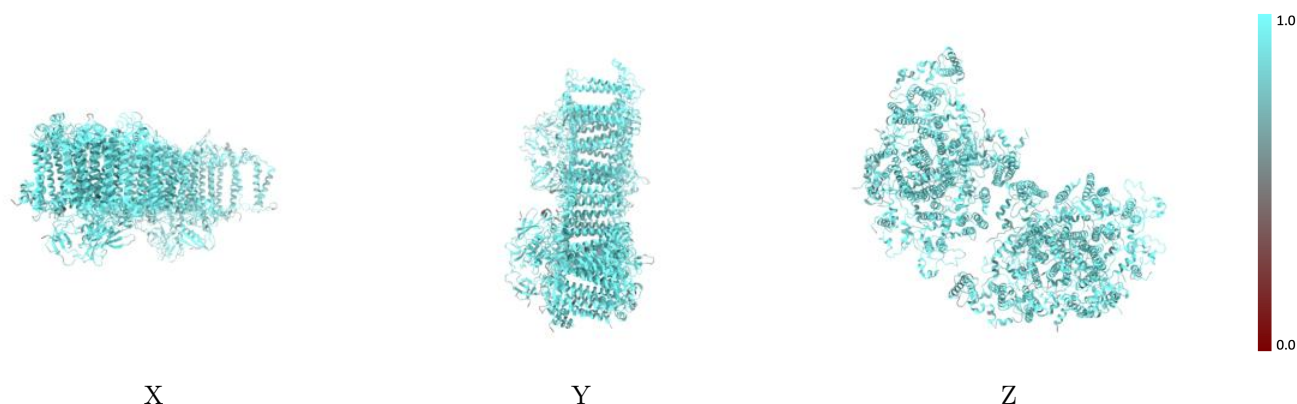
The images above show the 3D surface view of the map at the recommended contour level 0.019 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



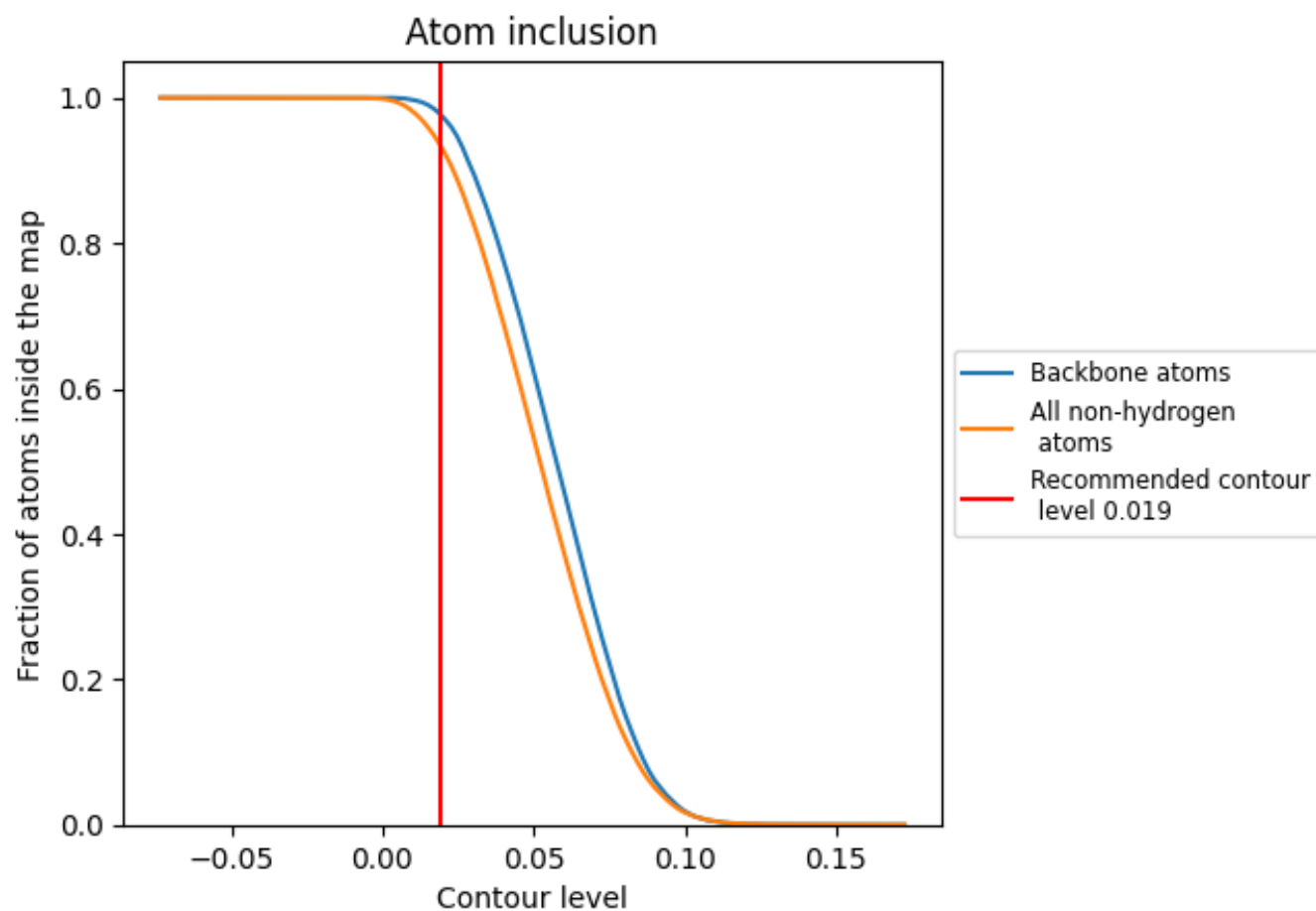
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.019).



















































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 94% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9353	 0.6500
A	 0.9498	 0.6610
B	 0.9671	 0.6840
C	 0.9600	 0.6560
D	 0.9187	 0.6340
E	 0.8787	 0.5980
F	 0.8910	 0.6090
I	 0.9601	 0.6630
J	 0.9217	 0.6240
K	 0.7810	 0.5180
L	 0.9473	 0.6660
M	 0.9384	 0.6720
X	 0.8743	 0.6140
a	 0.9412	 0.6510
b	 0.9495	 0.6590
c	 0.9633	 0.6480
d	 0.9066	 0.6180
e	 0.8473	 0.5610
f	 0.8470	 0.5680
i	 0.9137	 0.6670
j	 0.8706	 0.5820
k	 0.7880	 0.5380
l	 0.9299	 0.6700
m	 0.9480	 0.6580
x	 0.7686	 0.5330

