



wwPDB EM Validation Summary Report ⓘ

Mar 24, 2026 – 12:29 PM UTC

PDB ID : 9EYS / pdb_00009eys
EMDB ID : EMD-50063
Title : Structure of Far-Red Photosystem I from *C. thermalis* PCC 7203
Authors : Consoli, G.; Tufail, F.; Murray, J.W.; Fantuzzi, A.; Rutherford, A.W.
Deposited on : 2024-04-09
Resolution : 2.01 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.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

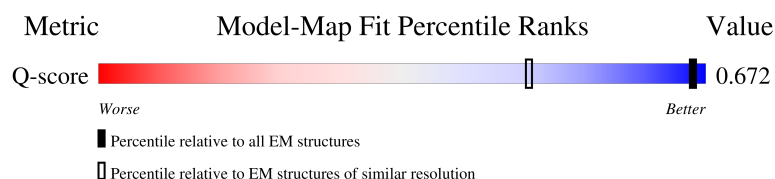
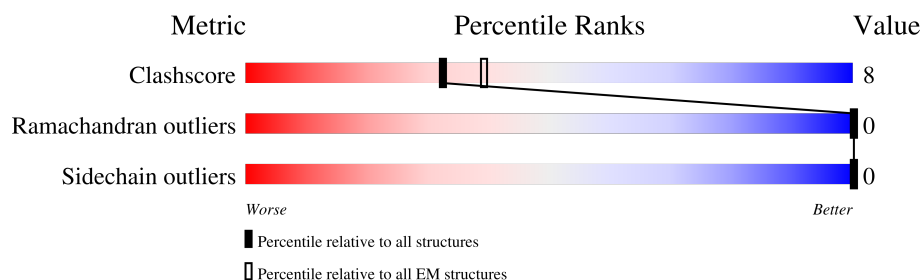
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.01 Å.

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



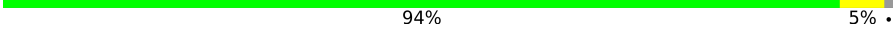
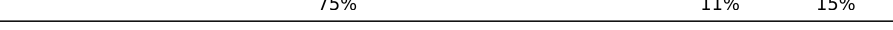
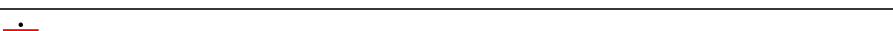
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1691 (1.52 - 2.51)

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	782	 79% 17% .
1	N	782	 81% 15% .
1	a	782	 82% 15% .
2	B	740	 84% 16%

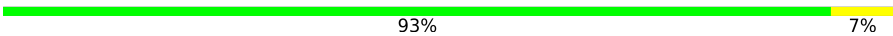
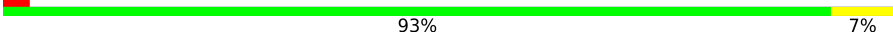
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Mol	Chain	Length	Quality of chain
2	O	740	 87% 13%
2	b	740	 85% 15%
3	C	81	 90% 9% .
3	P	81	 89% 10% .
3	c	81	 94% 5% .
4	D	142	 84% 14% .
4	Q	142	 87% 11% .
4	d	142	 87% 11% .
5	E	66	 92% 6% .
5	R	66	 91% 8% .
5	e	66	 91% 8% .
6	F	161	 71% 14% 15%
6	S	161	 73% 12% 15%
6	f	161	 75% 11% 15%
7	I	51	 49% 33% 18%
7	T	51	 57% 25% 18%
7	g	51	 59% 24% 18%
8	J	46	 80% 20%
8	U	46	 83% 17%
8	h	46	 87% 13%
9	K	80	 85% 9% 6%
9	V	80	 88% 6% 6%
9	i	80	 88% 6% 6%
10	L	183	 84% 10% 6%
10	W	183	 87% 7% 6%

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Mol	Chain	Length	Quality of chain
10	j	183	
11	M	32	
11	Y	32	
11	k	32	
12	X	29	
12	Z	29	
12	l	29	

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	N	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	F6C	A	802	X	-	-	-
14	F6C	A	824	X	-	-	-
14	F6C	A	826	X	-	-	-
14	F6C	A	857	X	-	-	-
14	F6C	B	831	X	-	-	-
14	F6C	B	838	X	-	-	-
14	F6C	L	201	X	-	-	-
14	F6C	L	204	X	-	-	-
14	F6C	N	802	X	-	-	-
14	F6C	N	824	X	-	-	-
14	F6C	N	826	X	-	-	-
14	F6C	N	856	X	-	-	-
14	F6C	O	810	X	-	-	-
14	F6C	O	833	X	-	-	-
14	F6C	O	840	X	-	-	-
14	F6C	W	1503	X	-	-	-
14	F6C	a	802	X	-	-	-
14	F6C	a	824	X	-	-	-
14	F6C	a	826	X	-	-	-
14	F6C	a	856	X	-	-	-
14	F6C	b	810	X	-	-	-
14	F6C	b	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	F6C	b	840	X	-	-	-
14	F6C	j	204	X	-	-	-
15	CLA	A	803	X	-	-	-
15	CLA	A	804	X	-	-	-
15	CLA	A	805	X	-	-	-
15	CLA	A	806	X	-	-	-
15	CLA	A	807	X	-	-	-
15	CLA	A	808	X	-	-	-
15	CLA	A	809	X	-	-	-
15	CLA	A	810	X	-	-	-
15	CLA	A	811	X	-	-	-
15	CLA	A	812	X	-	-	-
15	CLA	A	813	X	-	-	-
15	CLA	A	814	X	-	-	-
15	CLA	A	815	X	-	-	-
15	CLA	A	816	X	-	-	-
15	CLA	A	817	X	-	-	-
15	CLA	A	818	X	-	-	-
15	CLA	A	819	X	-	-	-
15	CLA	A	820	X	-	-	-
15	CLA	A	821	X	-	-	-
15	CLA	A	822	X	-	-	-
15	CLA	A	823	X	-	-	-
15	CLA	A	825	X	-	-	-
15	CLA	A	827	X	-	-	-
15	CLA	A	828	X	-	-	-
15	CLA	A	829	X	-	-	-
15	CLA	A	830	X	-	-	-
15	CLA	A	831	X	-	-	-
15	CLA	A	832	X	-	-	-
15	CLA	A	833	X	-	-	-
15	CLA	A	834	X	-	-	-
15	CLA	A	835	X	-	-	-
15	CLA	A	836	X	-	-	-
15	CLA	A	837	X	-	-	-
15	CLA	A	838	X	-	-	-
15	CLA	A	839	X	-	-	-
15	CLA	A	840	X	-	-	-
15	CLA	A	841	X	-	-	-
15	CLA	A	842	X	-	-	-
15	CLA	A	856	X	-	-	-
15	CLA	B	801	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	B	802	X	-	-	-
15	CLA	B	803	X	-	-	-
15	CLA	B	804	X	-	-	-
15	CLA	B	805	X	-	-	-
15	CLA	B	806	X	-	-	-
15	CLA	B	807	X	-	-	-
15	CLA	B	808	X	-	-	-
15	CLA	B	809	X	-	-	-
15	CLA	B	810	X	-	-	-
15	CLA	B	812	X	-	-	-
15	CLA	B	813	X	-	-	-
15	CLA	B	814	X	-	-	-
15	CLA	B	815	X	-	-	-
15	CLA	B	816	X	-	-	-
15	CLA	B	817	X	-	-	-
15	CLA	B	818	X	-	-	-
15	CLA	B	819	X	-	-	-
15	CLA	B	820	X	-	-	-
15	CLA	B	821	X	-	-	-
15	CLA	B	822	X	-	-	-
15	CLA	B	823	X	-	-	-
15	CLA	B	824	X	-	-	-
15	CLA	B	825	X	-	-	-
15	CLA	B	826	X	-	-	-
15	CLA	B	827	X	-	-	-
15	CLA	B	828	X	-	-	-
15	CLA	B	829	X	-	-	-
15	CLA	B	830	X	-	-	-
15	CLA	B	832	X	-	-	-
15	CLA	B	833	X	-	-	-
15	CLA	B	834	X	-	-	-
15	CLA	B	835	X	-	-	-
15	CLA	B	836	X	-	-	-
15	CLA	B	837	X	-	-	-
15	CLA	B	839	X	-	-	-
15	CLA	F	201	X	-	-	-
15	CLA	K	102	X	-	-	-
15	CLA	K	103	X	-	-	-
15	CLA	L	202	X	-	-	-
15	CLA	L	203	X	-	-	-
15	CLA	N	803	X	-	-	-
15	CLA	N	804	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	N	805	X	-	-	-
15	CLA	N	806	X	-	-	-
15	CLA	N	807	X	-	-	-
15	CLA	N	808	X	-	-	-
15	CLA	N	809	X	-	-	-
15	CLA	N	810	X	-	-	-
15	CLA	N	811	X	-	-	-
15	CLA	N	812	X	-	-	-
15	CLA	N	813	X	-	-	-
15	CLA	N	814	X	-	-	-
15	CLA	N	815	X	-	-	-
15	CLA	N	816	X	-	-	-
15	CLA	N	817	X	-	-	-
15	CLA	N	818	X	-	-	-
15	CLA	N	819	X	-	-	-
15	CLA	N	820	X	-	-	-
15	CLA	N	821	X	-	-	-
15	CLA	N	822	X	-	-	-
15	CLA	N	823	X	-	-	-
15	CLA	N	825	X	-	-	-
15	CLA	N	827	X	-	-	-
15	CLA	N	828	X	-	-	-
15	CLA	N	829	X	-	-	-
15	CLA	N	830	X	-	-	-
15	CLA	N	831	X	-	-	-
15	CLA	N	832	X	-	-	-
15	CLA	N	833	X	-	-	-
15	CLA	N	834	X	-	-	-
15	CLA	N	835	X	-	-	-
15	CLA	N	836	X	-	-	-
15	CLA	N	837	X	-	-	-
15	CLA	N	838	X	-	-	-
15	CLA	N	839	X	-	-	-
15	CLA	N	840	X	-	-	-
15	CLA	N	841	X	-	-	-
15	CLA	N	842	X	-	-	-
15	CLA	O	801	X	-	-	-
15	CLA	O	802	X	-	-	-
15	CLA	O	803	X	-	-	-
15	CLA	O	804	X	-	-	-
15	CLA	O	805	X	-	-	-
15	CLA	O	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	O	807	X	-	-	-
15	CLA	O	808	X	-	-	-
15	CLA	O	809	X	-	-	-
15	CLA	O	811	X	-	-	-
15	CLA	O	812	X	-	-	-
15	CLA	O	814	X	-	-	-
15	CLA	O	815	X	-	-	-
15	CLA	O	816	X	-	-	-
15	CLA	O	817	X	-	-	-
15	CLA	O	818	X	-	-	-
15	CLA	O	819	X	-	-	-
15	CLA	O	820	X	-	-	-
15	CLA	O	821	X	-	-	-
15	CLA	O	822	X	-	-	-
15	CLA	O	823	X	-	-	-
15	CLA	O	824	X	-	-	-
15	CLA	O	825	X	-	-	-
15	CLA	O	826	X	-	-	-
15	CLA	O	827	X	-	-	-
15	CLA	O	828	X	-	-	-
15	CLA	O	829	X	-	-	-
15	CLA	O	830	X	-	-	-
15	CLA	O	831	X	-	-	-
15	CLA	O	832	X	-	-	-
15	CLA	O	834	X	-	-	-
15	CLA	O	835	X	-	-	-
15	CLA	O	836	X	-	-	-
15	CLA	O	837	X	-	-	-
15	CLA	O	838	X	-	-	-
15	CLA	O	839	X	-	-	-
15	CLA	O	841	X	-	-	-
15	CLA	S	201	X	-	-	-
15	CLA	V	102	X	-	-	-
15	CLA	V	103	X	-	-	-
15	CLA	W	1501	X	-	-	-
15	CLA	W	1502	X	-	-	-
15	CLA	X	103	X	-	-	-
15	CLA	Z	103	X	-	-	-
15	CLA	a	803	X	-	-	-
15	CLA	a	804	X	-	-	-
15	CLA	a	805	X	-	-	-
15	CLA	a	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	a	807	X	-	-	-
15	CLA	a	808	X	-	-	-
15	CLA	a	809	X	-	-	-
15	CLA	a	810	X	-	-	-
15	CLA	a	811	X	-	-	-
15	CLA	a	812	X	-	-	-
15	CLA	a	813	X	-	-	-
15	CLA	a	814	X	-	-	-
15	CLA	a	815	X	-	-	-
15	CLA	a	816	X	-	-	-
15	CLA	a	817	X	-	-	-
15	CLA	a	818	X	-	-	-
15	CLA	a	819	X	-	-	-
15	CLA	a	820	X	-	-	-
15	CLA	a	821	X	-	-	-
15	CLA	a	822	X	-	-	-
15	CLA	a	823	X	-	-	-
15	CLA	a	825	X	-	-	-
15	CLA	a	827	X	-	-	-
15	CLA	a	828	X	-	-	-
15	CLA	a	829	X	-	-	-
15	CLA	a	830	X	-	-	-
15	CLA	a	831	X	-	-	-
15	CLA	a	832	X	-	-	-
15	CLA	a	833	X	-	-	-
15	CLA	a	834	X	-	-	-
15	CLA	a	835	X	-	-	-
15	CLA	a	836	X	-	-	-
15	CLA	a	837	X	-	-	-
15	CLA	a	838	X	-	-	-
15	CLA	a	839	X	-	-	-
15	CLA	a	840	X	-	-	-
15	CLA	a	841	X	-	-	-
15	CLA	a	842	X	-	-	-
15	CLA	b	801	X	-	-	-
15	CLA	b	802	X	-	-	-
15	CLA	b	803	X	-	-	-
15	CLA	b	804	X	-	-	-
15	CLA	b	805	X	-	-	-
15	CLA	b	806	X	-	-	-
15	CLA	b	807	X	-	-	-
15	CLA	b	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
15	CLA	b	809	X	-	-	-
15	CLA	b	811	X	-	-	-
15	CLA	b	812	X	-	-	-
15	CLA	b	814	X	-	-	-
15	CLA	b	815	X	-	-	-
15	CLA	b	816	X	-	-	-
15	CLA	b	817	X	-	-	-
15	CLA	b	818	X	-	-	-
15	CLA	b	819	X	-	-	-
15	CLA	b	820	X	-	-	-
15	CLA	b	821	X	-	-	-
15	CLA	b	822	X	-	-	-
15	CLA	b	823	X	-	-	-
15	CLA	b	824	X	-	-	-
15	CLA	b	825	X	-	-	-
15	CLA	b	826	X	-	-	-
15	CLA	b	827	X	-	-	-
15	CLA	b	828	X	-	-	-
15	CLA	b	829	X	-	-	-
15	CLA	b	830	X	-	-	-
15	CLA	b	831	X	-	-	-
15	CLA	b	832	X	-	-	-
15	CLA	b	834	X	-	-	-
15	CLA	b	835	X	-	-	-
15	CLA	b	836	X	-	-	-
15	CLA	b	837	X	-	-	-
15	CLA	b	838	X	-	-	-
15	CLA	b	839	X	-	-	-
15	CLA	b	841	X	-	-	-
15	CLA	f	201	X	-	-	-
15	CLA	i	102	X	-	-	-
15	CLA	i	103	X	-	-	-
15	CLA	j	202	X	-	-	-
15	CLA	j	203	X	-	-	-
15	CLA	l	103	X	-	-	-

2 Entry composition [i](#)

There are 24 unique types of molecules in this entry. The entry contains 75954 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	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	N	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		
1	a	753	Total	C	N	O	S	0	0
			5900	3869	1012	988	31		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	O	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		
2	b	739	Total	C	N	O	S	0	0
			5913	3897	994	1004	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	P	80	Total	C	N	O	S	0	0
			600	368	103	118	11		
3	c	80	Total	C	N	O	S	0	0
			600	368	103	118	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Q	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		
4	d	139	Total	C	N	O	S	0	0
			1090	692	193	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	65	Total	C	N	O		0	0
			530	341	92	97			
5	R	65	Total	C	N	O		0	0
			530	341	92	97			
5	e	65	Total	C	N	O		0	0
			530	341	92	97			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	S	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		
6	f	137	Total	C	N	O	S	0	0
			1075	698	176	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	T	42	Total	C	N	O	S	0	0
			351	247	47	55	2		
7	g	42	Total	C	N	O	S	0	0
			351	247	47	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	46	Total	C	N	O	S	0	0
			373	256	54	59	4		
8	U	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	46	Total	C	N	O	S	0	0
			373	256	54	59	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	V	75	Total	C	N	O	S	0	0
			539	356	88	94	1		
9	i	75	Total	C	N	O	S	0	0
			539	356	88	94	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	12	MET	-	initiating methionine	UNP K9TX25
V	12	MET	-	initiating methionine	UNP K9TX25
i	12	MET	-	initiating methionine	UNP K9TX25

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	W	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		
10	j	172	Total	C	N	O	S	0	0
			1309	839	224	242	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	Y	31	Total	C	N	O	S	0	0
			240	160	37	42	1		
11	k	31	Total	C	N	O	S	0	0
			240	160	37	42	1		

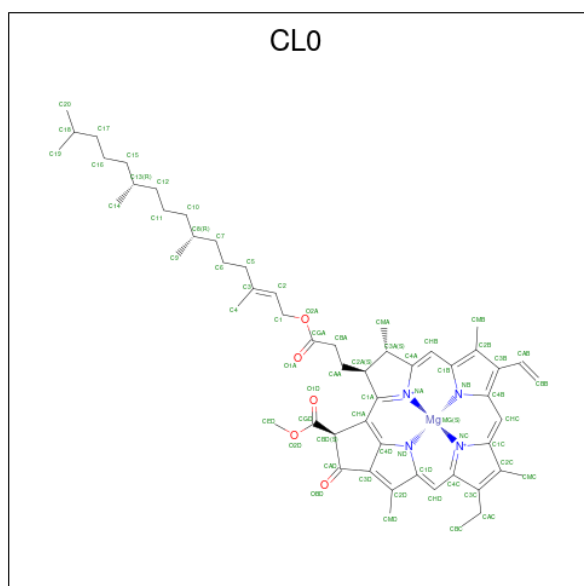
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	0	MET	-	initiating methionine	UNP K9TSY6
Y	0	MET	-	initiating methionine	UNP K9TSY6
k	0	MET	-	initiating methionine	UNP K9TSY6

- Molecule 12 is a protein called Photosystem one Psax.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	29	Total	C	N	O	0	0
			227	157	36	34		
12	Z	29	Total	C	N	O	0	0
			227	157	36	34		
12	l	29	Total	C	N	O	0	0
			227	157	36	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: 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
			65	55	1	4	5
13	N	1	Total	C	Mg	N	O
			65	55	1	4	5
13	a	1	Total	C	Mg	N	O
			65	55	1	4	5

- Molecule 14 is Chlorophyll F (CCD ID: F6C) (formula: $C_{55}H_{68}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).

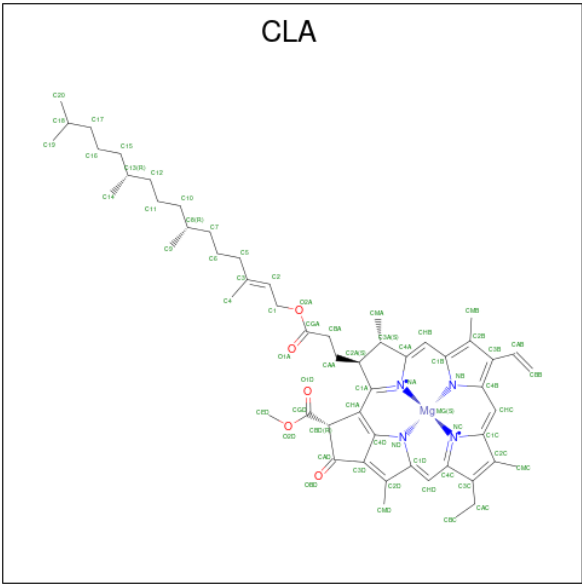


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Mol	Chain	Residues	Atoms					AltConf
14	O	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	W	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	a	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	b	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
14	j	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 15 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 62	C 52	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	K	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	X	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	N	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	N	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	N	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	N	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
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15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	O	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	V	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	W	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	W	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	Z	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
15	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
15	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
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15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
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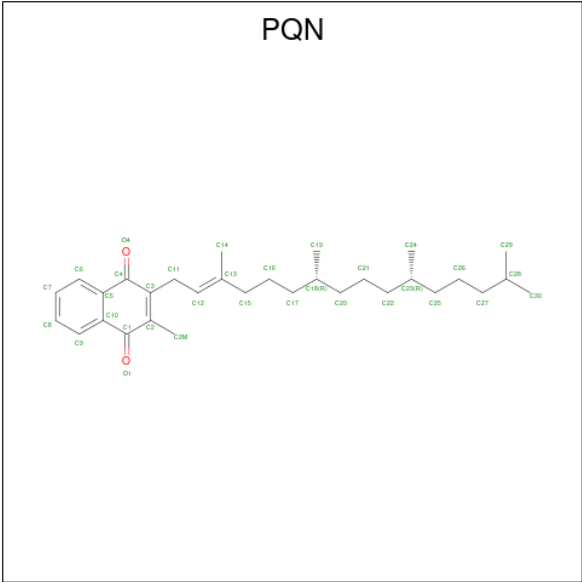
Mol	Chain	Residues	Atoms					AltConf
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15	b	1	Total 56	C 46	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 57	C 47	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 53	C 43	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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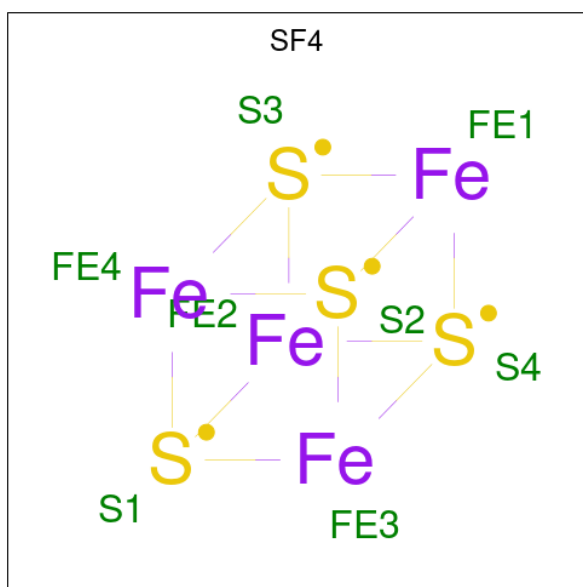
Mol	Chain	Residues	Atoms					AltConf
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	i	1	Total 45	C 35	Mg 1	N 4	O 5	0
15	i	1	Total 50	C 40	Mg 1	N 4	O 5	0
15	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
15	j	1	Total 60	C 50	Mg 1	N 4	O 5	0
15	l	1	Total 55	C 45	Mg 1	N 4	O 5	0

- Molecule 16 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



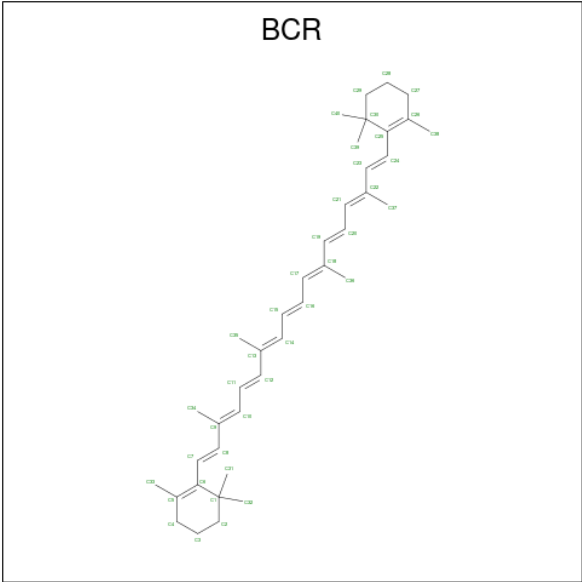
Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	C	O	0
			33	31	2	
16	B	1	Total	C	O	0
			33	31	2	
16	N	1	Total	C	O	0
			33	31	2	
16	O	1	Total	C	O	0
			33	31	2	
16	a	1	Total	C	O	0
			33	31	2	
16	b	1	Total	C	O	0
			33	31	2	

- Molecule 17 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



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

- Molecule 18 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	A	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	B	1	Total	C	0
			40	40	
18	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
18	F	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	I	1	Total C 40 40	0
18	J	1	Total C 40 40	0
18	K	1	Total C 25 25	0
18	L	1	Total C 40 40	0
18	L	1	Total C 40 40	0
18	M	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	N	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0
18	O	1	Total C 40 40	0

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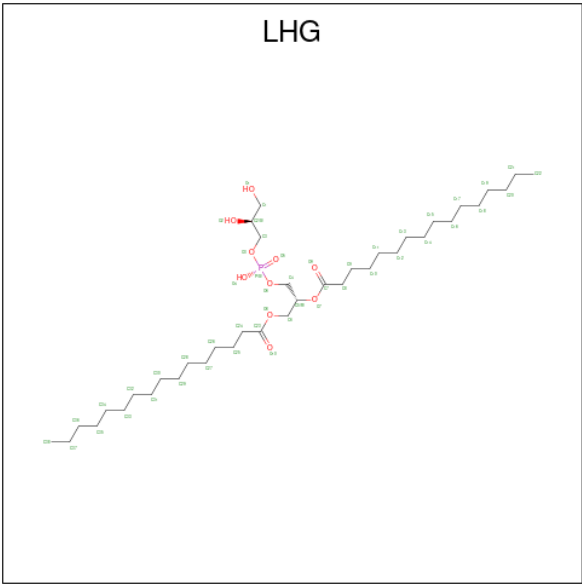
Mol	Chain	Residues	Atoms	AltConf
18	O	1	Total C 40 40	0
18	S	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	T	1	Total C 40 40	0
18	U	1	Total C 40 40	0
18	V	1	Total C 25 25	0
18	W	1	Total C 40 40	0
18	W	1	Total C 40 40	0
18	Y	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	a	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0
18	b	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
18	b	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	f	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	g	1	Total	C	0
			40	40	
18	h	1	Total	C	0
			40	40	
18	i	1	Total	C	0
			25	25	
18	j	1	Total	C	0
			40	40	
18	j	1	Total	C	0
			40	40	
18	k	1	Total	C	0
			40	40	

- Molecule 19 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
19	A	1	Total	C	O	P	0
			42	31	10	1	

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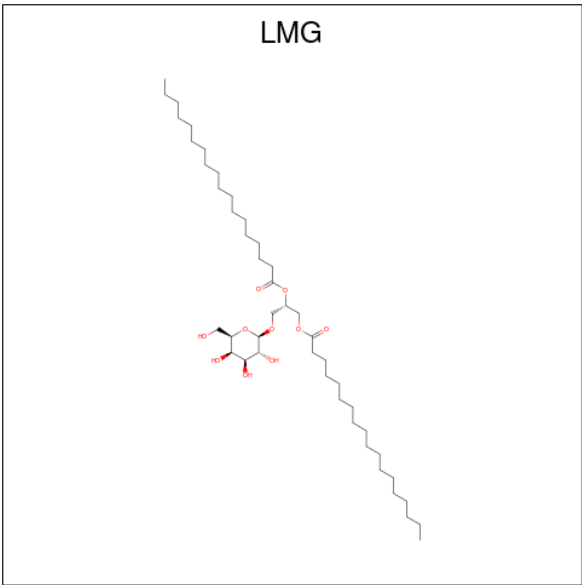
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Mol	Chain	Residues	Atoms				AltConf
19	L	1	Total 49	C 38	O 10	P 1	0
19	M	1	Total 49	C 38	O 10	P 1	0
19	X	1	Total 44	C 33	O 10	P 1	0
19	X	1	Total 49	C 38	O 10	P 1	0
19	N	1	Total 42	C 31	O 10	P 1	0
19	W	1	Total 49	C 38	O 10	P 1	0
19	Y	1	Total 49	C 38	O 10	P 1	0
19	Z	1	Total 44	C 33	O 10	P 1	0
19	Z	1	Total 49	C 38	O 10	P 1	0
19	a	1	Total 42	C 31	O 10	P 1	0
19	j	1	Total 49	C 38	O 10	P 1	0
19	k	1	Total 49	C 38	O 10	P 1	0
19	l	1	Total 44	C 33	O 10	P 1	0
19	l	1	Total 49	C 38	O 10	P 1	0

- Molecule 20 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



- Molecule 21 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



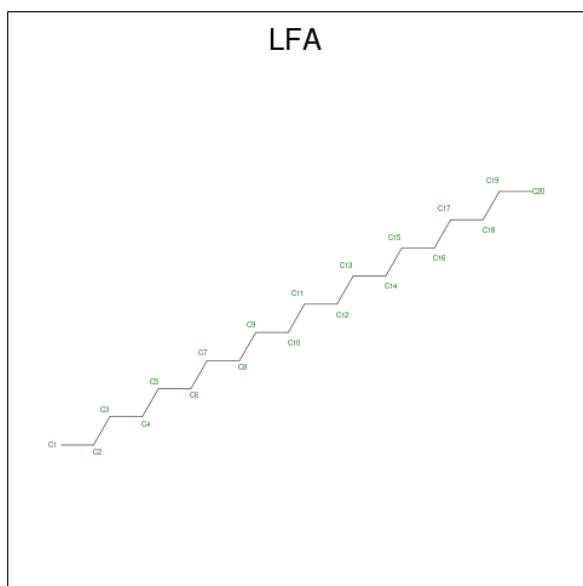
Mol	Chain	Residues	Atoms			AltConf
21	A	1	Total	C	O	0
			44	34	10	
21	B	1	Total	C	O	0
			55	45	10	
21	I	1	Total	C	O	0
			37	27	10	
21	J	1	Total	C	O	0
			55	45	10	
21	L	1	Total	C	O	0
			50	40	10	
21	N	1	Total	C	O	0
			44	34	10	
21	O	1	Total	C	O	0
			55	45	10	
21	T	1	Total	C	O	0
			37	27	10	
21	U	1	Total	C	O	0
			55	45	10	
21	W	1	Total	C	O	0
			50	40	10	
21	a	1	Total	C	O	0
			44	34	10	
21	b	1	Total	C	O	0
			55	45	10	
21	g	1	Total	C	O	0
			37	27	10	
21	h	1	Total	C	O	0
			55	45	10	

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Mol	Chain	Residues	Atoms			AltConf
21	j	1	Total	C	O	0
			50	40	10	

- Molecule 22 is EICOSANE (CCD ID: LFA) (formula: $C_{20}H_{42}$).



Mol	Chain	Residues	Atoms		AltConf
22	B	1	Total	C	0
			16	16	
22	L	1	Total	C	0
			15	15	
22	O	1	Total	C	0
			16	16	
22	W	1	Total	C	0
			15	15	
22	f	1	Total	C	0
			16	16	
22	j	1	Total	C	0
			15	15	

- Molecule 23 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
23	L	1	Total	Ca	0
			1	1	
23	W	1	Total	Ca	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
23	j	1	Total 1	Ca 1	0

- Molecule 24 is water.

Mol	Chain	Residues	Atoms		AltConf
24	A	50	Total 50	O 50	0
24	B	55	Total 55	O 55	0
24	C	3	Total 3	O 3	0
24	D	11	Total 11	O 11	0
24	E	2	Total 2	O 2	0
24	F	2	Total 2	O 2	0
24	I	2	Total 2	O 2	0
24	K	1	Total 1	O 1	0
24	L	8	Total 8	O 8	0
24	N	51	Total 51	O 51	0
24	O	55	Total 55	O 55	0
24	P	2	Total 2	O 2	0
24	Q	11	Total 11	O 11	0
24	R	2	Total 2	O 2	0
24	S	2	Total 2	O 2	0
24	T	2	Total 2	O 2	0
24	V	1	Total 1	O 1	0
24	W	9	Total 9	O 9	0

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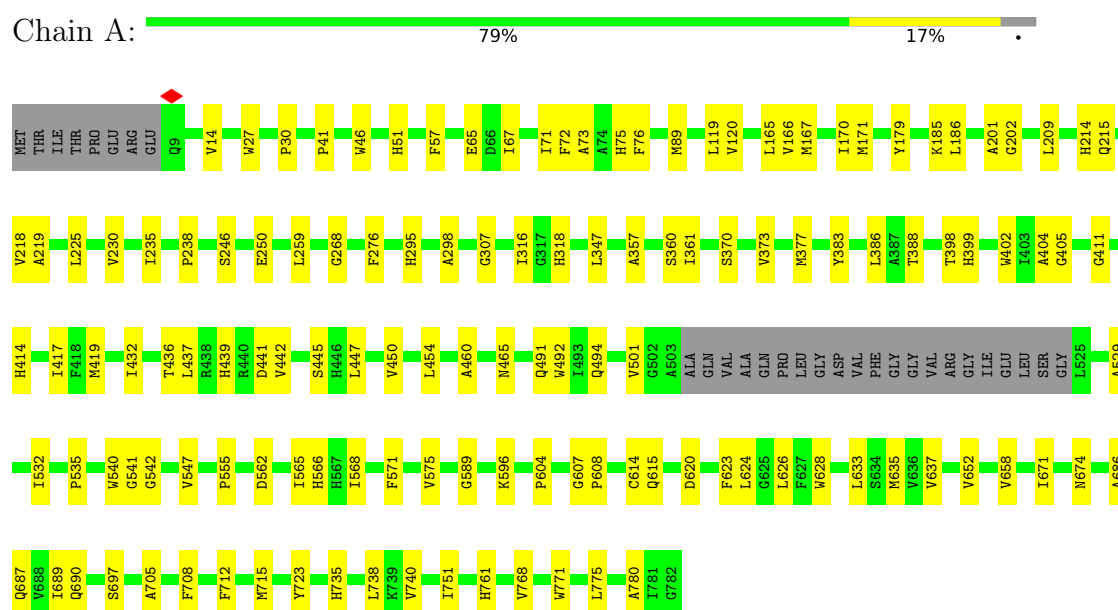
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Mol	Chain	Residues	Atoms		AltConf
24	a	52	Total 52	O 52	0
24	b	55	Total 55	O 55	0
24	c	3	Total 3	O 3	0
24	d	10	Total 10	O 10	0
24	e	2	Total 2	O 2	0
24	f	2	Total 2	O 2	0
24	g	3	Total 3	O 3	0
24	i	1	Total 1	O 1	0
24	j	8	Total 8	O 8	0

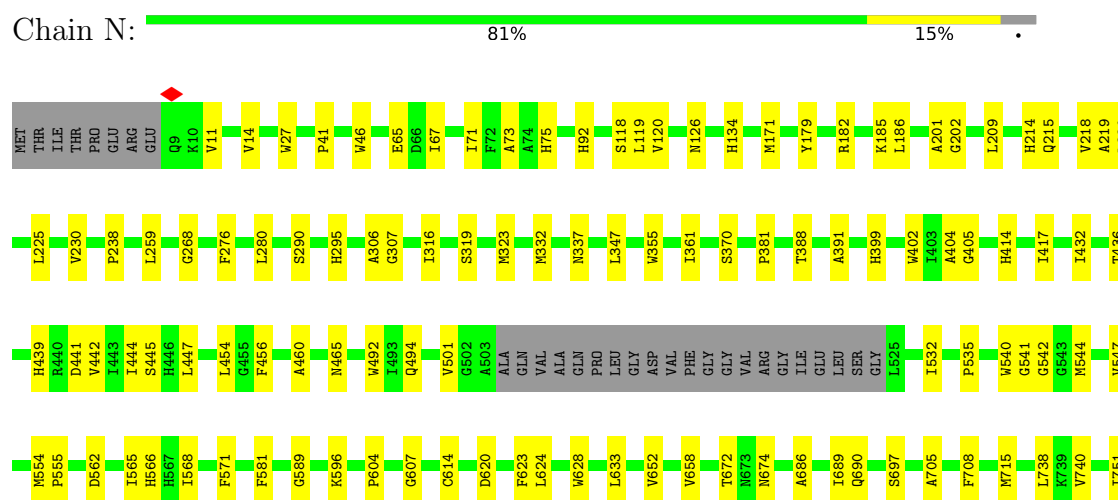
3 Residue-property plots

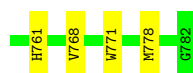
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



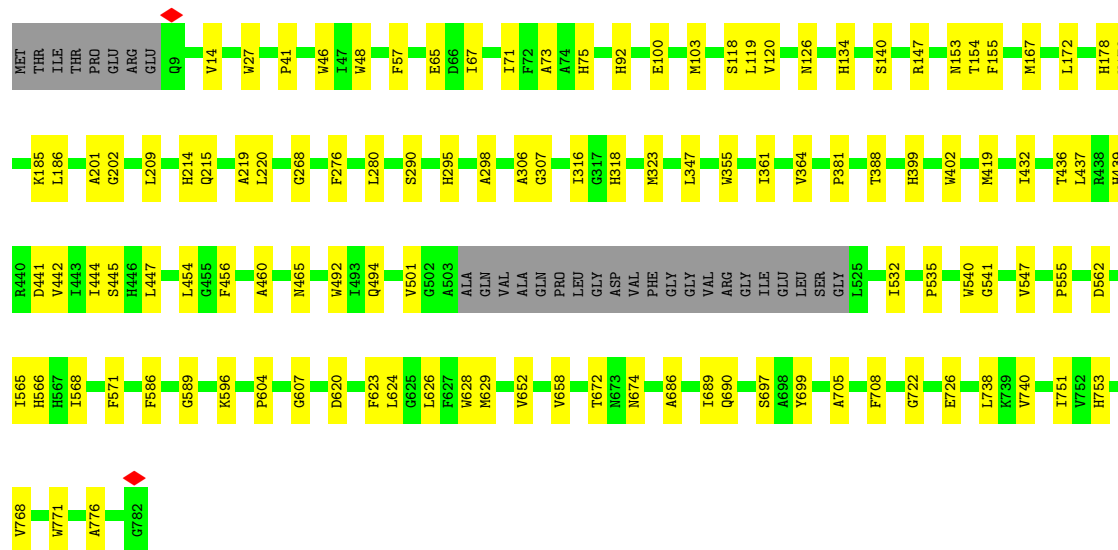
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain a: 82% 15%



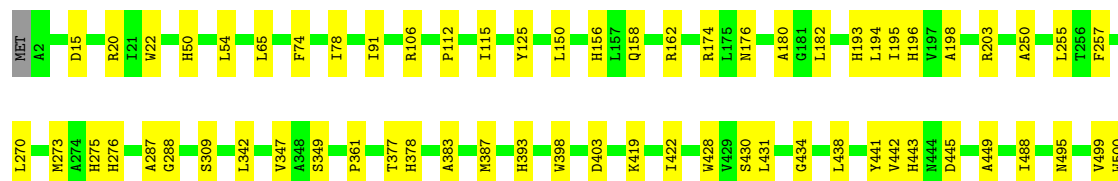
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

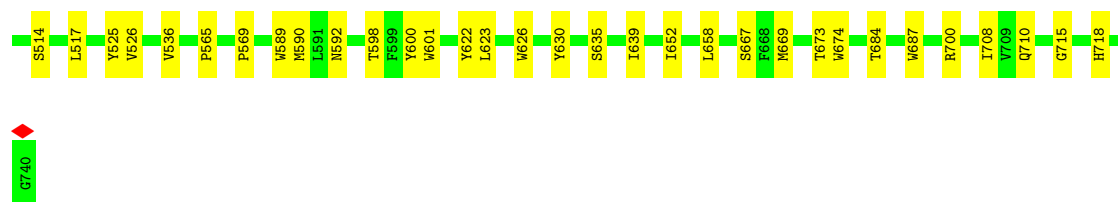
Chain B: 84% 16%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

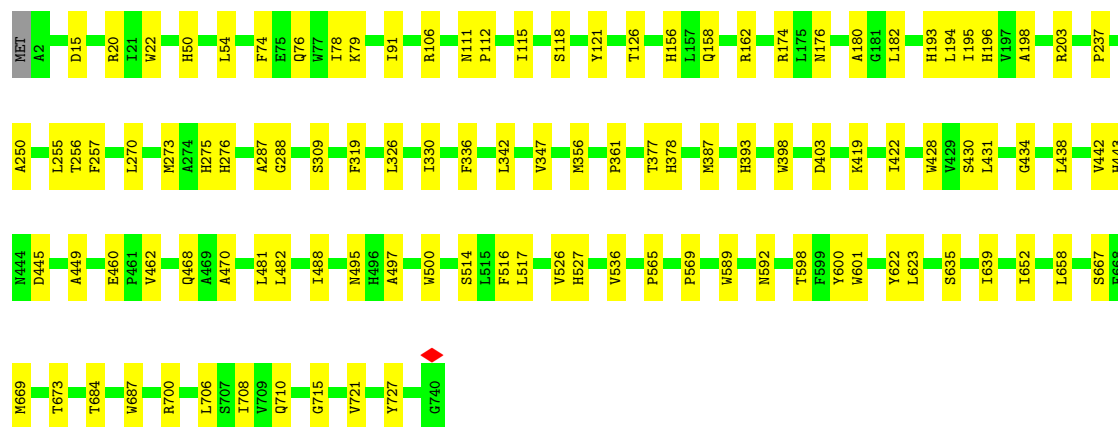
Chain O: 87% 13%





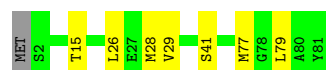
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 85% 15%



- Molecule 3: Photosystem I iron-sulfur center

Chain C: 90% 9%



- Molecule 3: Photosystem I iron-sulfur center

Chain P: 89% 10%



- Molecule 3: Photosystem I iron-sulfur center

Chain c: 94% 5%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 84% 14%



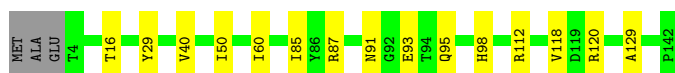
- Molecule 4: Photosystem I reaction center subunit II

Chain Q: 87% 11% .



- Molecule 4: Photosystem I reaction center subunit II

Chain d: 87% 11% .



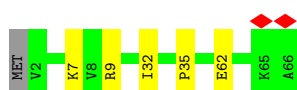
- Molecule 5: Photosystem I reaction center subunit IV

Chain E: 92% 6% .



- Molecule 5: Photosystem I reaction center subunit IV

Chain R: 91% 8% .



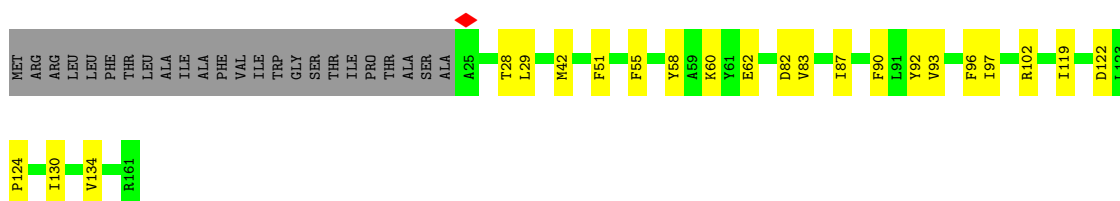
- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 91% 8% .



- Molecule 6: Photosystem I reaction center subunit III

Chain F: 71% 14% 15%



- Molecule 6: Photosystem I reaction center subunit III

Chain S:  73% 12% 15%



- Molecule 6: Photosystem I reaction center subunit III

Chain f:  75% 11% 15%



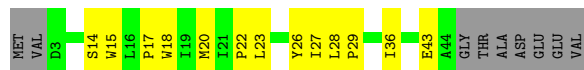
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  49% 33% 18%



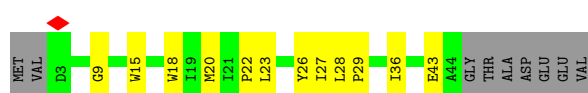
- Molecule 7: Photosystem I reaction center subunit VIII

Chain T:  57% 25% 18%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain g:  59% 24% 18%



- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  80% 20%



- Molecule 8: Photosystem I reaction center subunit IX

Chain U:  83% 17%



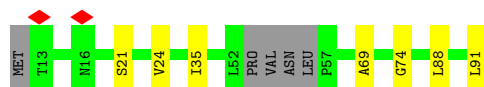
- Molecule 8: Photosystem I reaction center subunit IX

Chain h:  87% 13%



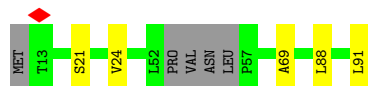
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain K:  85% 9% 6%



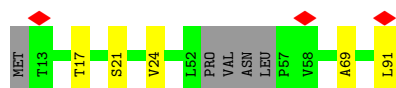
- Molecule 9: Photosystem I reaction center subunit PsaK

Chain V:  88% 6% 6%



- Molecule 9: Photosystem I reaction center subunit PsaK

Chain i:  88% 6% 6%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  84% 10% 6%



- Molecule 10: Photosystem I reaction center subunit XI

Chain W:  87% 7% 6%



- Molecule 10: Photosystem I reaction center subunit XI

Chain j:  85% 9% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  75% 22% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain Y:  88% 9% .



- Molecule 11: Photosystem I reaction center subunit XII

Chain k:  91% 6% .



- Molecule 12: Photosystem one PsaX

Chain X:  93% 7%



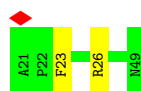
- Molecule 12: Photosystem one PsaX

Chain Z:  86% 14%



- Molecule 12: Photosystem one PsaX

Chain l:  93% 7%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	83138	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.504	Depositor
Minimum map value	-0.162	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.054	Depositor
Map size (Å)	552.6, 552.6, 552.6	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.92099994, 0.92099994, 0.92099994	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: LHG, BCR, SF4, CL0, LMT, CA, PQN, LMG, LFA, CLA, F6C

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	0.13	0/6106	0.29	0/8323
1	N	0.11	0/6106	0.25	0/8323
1	a	0.11	0/6106	0.25	0/8323
2	B	0.13	0/6139	0.29	0/8394
2	O	0.11	0/6139	0.25	0/8394
2	b	0.11	0/6139	0.26	0/8394
3	C	0.12	0/610	0.29	0/827
3	P	0.11	0/610	0.28	0/827
3	c	0.13	0/610	0.29	0/827
4	D	0.11	0/1115	0.31	0/1501
4	Q	0.10	0/1115	0.26	0/1501
4	d	0.10	0/1115	0.26	0/1501
5	E	0.10	0/540	0.26	0/728
5	R	0.09	0/540	0.22	0/728
5	e	0.09	0/540	0.23	0/728
6	F	0.12	0/1104	0.30	0/1501
6	S	0.11	0/1104	0.28	0/1501
6	f	0.10	0/1104	0.27	0/1501
7	I	0.16	0/366	0.43	0/503
7	T	0.15	0/366	0.37	0/503
7	g	0.15	0/366	0.38	0/503
8	J	0.10	0/386	0.25	0/526
8	U	0.09	0/386	0.24	0/526
8	h	0.08	0/386	0.23	0/526
9	K	0.12	0/550	0.32	0/751
9	V	0.10	0/550	0.31	0/751
9	i	0.10	0/550	0.29	0/751
10	L	0.13	0/1340	0.30	0/1821
10	W	0.10	0/1340	0.26	0/1821
10	j	0.10	0/1340	0.26	0/1821
11	M	0.11	0/243	0.21	0/329
11	Y	0.09	0/243	0.18	0/329

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	k	0.08	0/243	0.17	0/329
12	X	0.11	0/233	0.28	0/319
12	Z	0.07	0/233	0.24	0/319
12	l	0.07	0/233	0.23	0/319
All	All	0.11	0/56196	0.27	0/76569

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5900	0	5735	113	0
1	N	5900	0	5735	89	0
1	a	5900	0	5735	93	0
2	B	5913	0	5649	102	0
2	O	5913	0	5649	85	0
2	b	5913	0	5649	93	0
3	C	600	0	579	4	0
3	P	600	0	579	7	0
3	c	600	0	579	3	0
4	D	1090	0	1097	13	0
4	Q	1090	0	1097	11	0
4	d	1090	0	1097	9	0
5	E	530	0	535	2	0
5	R	530	0	535	3	0
5	e	530	0	535	3	0
6	F	1075	0	1081	17	0
6	S	1075	0	1081	15	0
6	f	1075	0	1081	15	0
7	I	351	0	354	15	0
7	T	351	0	354	11	0
7	g	351	0	354	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	J	373	0	390	9	0
8	U	373	0	390	7	0
8	h	373	0	390	6	0
9	K	539	0	578	7	0
9	V	539	0	578	5	0
9	i	539	0	578	4	0
10	L	1309	0	1289	15	0
10	W	1309	0	1289	11	0
10	j	1309	0	1289	12	0
11	M	240	0	261	6	0
11	Y	240	0	261	3	0
11	k	240	0	261	2	0
12	X	227	0	244	2	0
12	Z	227	0	244	5	0
12	l	227	0	244	3	0
13	A	65	0	72	3	0
13	N	65	0	72	2	0
13	a	65	0	72	2	0
14	A	250	0	0	0	0
14	B	132	0	0	1	0
14	L	132	0	0	2	0
14	N	250	0	0	0	0
14	O	198	0	0	3	0
14	W	66	0	0	0	0
14	a	250	0	0	0	0
14	b	198	0	0	3	0
14	j	66	0	0	1	0
15	A	2324	0	2343	115	0
15	B	2238	0	2311	112	0
15	F	65	0	72	1	0
15	K	95	0	72	1	0
15	L	125	0	131	4	0
15	N	2259	0	2271	98	0
15	O	2303	0	2383	124	0
15	S	65	0	72	1	0
15	V	95	0	72	1	0
15	W	125	0	131	3	0
15	X	55	0	49	3	0
15	Z	55	0	49	2	0
15	a	2259	0	2271	98	0
15	b	2303	0	2383	127	0
15	f	65	0	72	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	i	95	0	72	1	0
15	j	125	0	131	4	0
15	l	55	0	49	2	0
16	A	33	0	46	1	0
16	B	33	0	46	1	0
16	N	33	0	46	1	0
16	O	33	0	46	1	0
16	a	33	0	46	1	0
16	b	33	0	46	3	0
17	A	8	0	0	0	0
17	C	16	0	0	0	0
17	N	8	0	0	0	0
17	P	16	0	0	1	0
17	a	8	0	0	0	0
17	c	16	0	0	1	0
18	A	280	0	392	29	0
18	B	240	0	336	16	0
18	F	80	0	112	9	0
18	I	80	0	112	5	0
18	J	40	0	56	1	0
18	K	25	0	33	0	0
18	L	80	0	112	5	0
18	M	40	0	56	4	0
18	N	280	0	392	23	0
18	O	280	0	392	18	0
18	S	40	0	56	5	0
18	T	80	0	112	3	0
18	U	40	0	56	0	0
18	V	25	0	33	0	0
18	W	80	0	112	3	0
18	Y	40	0	56	4	0
18	a	280	0	392	20	0
18	b	240	0	336	15	0
18	f	80	0	112	6	0
18	g	80	0	112	4	0
18	h	40	0	56	1	0
18	i	25	0	33	1	0
18	j	80	0	112	6	0
18	k	40	0	56	3	0
19	A	42	0	54	0	0
19	L	49	0	74	5	0
19	M	49	0	74	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	N	42	0	54	0	0
19	W	49	0	74	5	0
19	X	93	0	135	3	0
19	Y	49	0	74	5	0
19	Z	93	0	135	4	0
19	a	42	0	54	0	0
19	j	49	0	74	5	0
19	k	49	0	74	5	0
19	l	93	0	135	4	0
20	A	94	0	110	3	0
20	N	94	0	110	2	0
20	a	94	0	110	2	0
21	A	44	0	61	1	0
21	B	55	0	86	4	0
21	I	37	0	44	3	0
21	J	55	0	86	1	0
21	L	50	0	70	4	0
21	N	44	0	61	0	0
21	O	55	0	86	5	0
21	T	37	0	44	5	0
21	U	55	0	86	3	0
21	W	50	0	70	4	0
21	a	44	0	61	1	0
21	b	55	0	86	5	0
21	g	37	0	44	3	0
21	h	55	0	86	3	0
21	j	50	0	70	2	0
22	B	16	0	31	1	0
22	L	15	0	29	1	0
22	O	16	0	31	1	0
22	W	15	0	29	1	0
22	f	16	0	31	1	0
22	j	15	0	29	2	0
23	L	1	0	0	0	0
23	W	1	0	0	0	0
23	j	1	0	0	0	0
24	A	50	0	0	0	0
24	B	55	0	0	0	0
24	C	3	0	0	0	0
24	D	11	0	0	0	0
24	E	2	0	0	0	0
24	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	I	2	0	0	0	0
24	K	1	0	0	0	0
24	L	8	0	0	0	0
24	N	51	0	0	0	0
24	O	55	0	0	0	0
24	P	2	0	0	0	0
24	Q	11	0	0	0	0
24	R	2	0	0	0	0
24	S	2	0	0	0	0
24	T	2	0	0	0	0
24	V	1	0	0	0	0
24	W	9	0	0	0	0
24	a	52	0	0	0	0
24	b	55	0	0	1	0
24	c	3	0	0	0	0
24	d	10	0	0	0	0
24	e	2	0	0	0	0
24	f	2	0	0	0	0
24	g	3	0	0	0	0
24	i	1	0	0	0	0
24	j	8	0	0	0	0
All	All	75954	0	74991	1279	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 1279 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:257:PHE:HE2	2:B:500:TRP:HE3	1.32	0.78
18:A:850:BCR:H362	15:A:856:CLA:H42	1.67	0.76
18:a:850:BCR:H362	15:b:802:CLA:H42	1.66	0.76
18:N:850:BCR:H362	15:O:802:CLA:H42	1.69	0.75
2:O:257:PHE:HE2	2:O:500:TRP:HE3	1.34	0.75

There are no symmetry-related clashes.

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	749/782 (96%)	730 (98%)	19 (2%)	0	100	100
1	N	749/782 (96%)	736 (98%)	13 (2%)	0	100	100
1	a	749/782 (96%)	735 (98%)	14 (2%)	0	100	100
2	B	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	O	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
2	b	737/740 (100%)	723 (98%)	14 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	P	78/81 (96%)	77 (99%)	1 (1%)	0	100	100
3	c	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	137/142 (96%)	135 (98%)	2 (2%)	0	100	100
4	Q	137/142 (96%)	134 (98%)	3 (2%)	0	100	100
4	d	137/142 (96%)	136 (99%)	1 (1%)	0	100	100
5	E	63/66 (96%)	63 (100%)	0	0	100	100
5	R	63/66 (96%)	63 (100%)	0	0	100	100
5	e	63/66 (96%)	63 (100%)	0	0	100	100
6	F	135/161 (84%)	132 (98%)	3 (2%)	0	100	100
6	S	135/161 (84%)	131 (97%)	4 (3%)	0	100	100
6	f	135/161 (84%)	131 (97%)	4 (3%)	0	100	100
7	I	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	T	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
7	g	40/51 (78%)	38 (95%)	2 (5%)	0	100	100
8	J	44/46 (96%)	44 (100%)	0	0	100	100
8	U	44/46 (96%)	44 (100%)	0	0	100	100
8	h	44/46 (96%)	44 (100%)	0	0	100	100
9	K	71/80 (89%)	70 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	V	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
9	i	71/80 (89%)	70 (99%)	1 (1%)	0	100	100
10	L	170/183 (93%)	170 (100%)	0	0	100	100
10	W	170/183 (93%)	170 (100%)	0	0	100	100
10	j	170/183 (93%)	170 (100%)	0	0	100	100
11	M	29/32 (91%)	29 (100%)	0	0	100	100
11	Y	29/32 (91%)	29 (100%)	0	0	100	100
11	k	29/32 (91%)	29 (100%)	0	0	100	100
12	X	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
12	Z	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
12	l	27/29 (93%)	25 (93%)	2 (7%)	0	100	100
All	All	6840/7179 (95%)	6715 (98%)	125 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	600/623 (96%)	600 (100%)	0	100	100
1	N	600/623 (96%)	600 (100%)	0	100	100
1	a	600/623 (96%)	600 (100%)	0	100	100
2	B	594/595 (100%)	594 (100%)	0	100	100
2	O	594/595 (100%)	594 (100%)	0	100	100
2	b	594/595 (100%)	594 (100%)	0	100	100
3	C	68/69 (99%)	68 (100%)	0	100	100
3	P	68/69 (99%)	68 (100%)	0	100	100
3	c	68/69 (99%)	68 (100%)	0	100	100
4	D	114/116 (98%)	114 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	114/116 (98%)	114 (100%)	0	100	100
4	d	114/116 (98%)	114 (100%)	0	100	100
5	E	57/58 (98%)	57 (100%)	0	100	100
5	R	57/58 (98%)	57 (100%)	0	100	100
5	e	57/58 (98%)	57 (100%)	0	100	100
6	F	116/135 (86%)	116 (100%)	0	100	100
6	S	116/135 (86%)	116 (100%)	0	100	100
6	f	116/135 (86%)	116 (100%)	0	100	100
7	I	37/44 (84%)	37 (100%)	0	100	100
7	T	37/44 (84%)	37 (100%)	0	100	100
7	g	37/44 (84%)	37 (100%)	0	100	100
8	J	41/41 (100%)	41 (100%)	0	100	100
8	U	41/41 (100%)	41 (100%)	0	100	100
8	h	41/41 (100%)	41 (100%)	0	100	100
9	K	60/65 (92%)	60 (100%)	0	100	100
9	V	60/65 (92%)	60 (100%)	0	100	100
9	i	60/65 (92%)	60 (100%)	0	100	100
10	L	135/146 (92%)	135 (100%)	0	100	100
10	W	135/146 (92%)	135 (100%)	0	100	100
10	j	135/146 (92%)	135 (100%)	0	100	100
11	M	26/27 (96%)	26 (100%)	0	100	100
11	Y	26/27 (96%)	26 (100%)	0	100	100
11	k	26/27 (96%)	26 (100%)	0	100	100
12	X	24/24 (100%)	24 (100%)	0	100	100
12	Z	24/24 (100%)	24 (100%)	0	100	100
12	l	24/24 (100%)	24 (100%)	0	100	100
All	All	5616/5829 (96%)	5616 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
10	W	148	ASN
1	a	665	ASN
6	f	44	ASN
10	W	181	ASN
1	a	239	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 3 are monoatomic - leaving 399 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
15	CLA	B	821	2	59,63,73	1.30	8 (13%)	70,101,113	1.23	6 (8%)
18	BCR	g	101	-	41,41,41	0.32	0	56,56,56	0.70	0
22	LFA	L	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	N	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
15	CLA	N	827	24	59,63,73	1.25	8 (13%)	70,101,113	1.37	8 (11%)
15	CLA	a	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	N	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
15	CLA	b	837	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	F	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	B	816	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	4 (5%)
15	CLA	a	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.35	5 (7%)
15	CLA	j	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	B	829	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	6 (7%)
18	BCR	N	848	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	A	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.45	6 (10%)
15	CLA	b	802	24	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
17	SF4	C	101	3	0,12,12	-	-	-	-	-
22	LFA	f	204	-	15,15,19	0.23	0	14,14,18	0.19	0
15	CLA	A	803	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
15	CLA	N	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
15	CLA	a	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.26	6 (7%)
15	CLA	N	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	5 (7%)
15	CLA	A	813	1	58,62,73	1.27	7 (12%)	68,99,113	1.37	7 (10%)
18	BCR	O	849	-	41,41,41	0.29	0	56,56,56	0.60	0
18	BCR	a	857	-	41,41,41	0.38	0	56,56,56	1.29	8 (14%)
18	BCR	O	844	-	41,41,41	0.31	0	56,56,56	0.68	0
20	LMT	A	854	-	36,36,36	0.55	0	47,47,47	0.63	0
14	F6C	O	810	2	72,74,74	1.60	8 (11%)	83,114,114	1.97	13 (15%)
22	LFA	j	208	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	A	856	24	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	N	822	24	69,73,73	1.19	8 (11%)	82,113,113	1.25	5 (6%)
22	LFA	W	1507	-	14,14,19	0.23	0	13,13,18	0.23	0
15	CLA	N	838	1	59,63,73	1.25	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	O	820	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
15	CLA	a	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.45	6 (10%)
15	CLA	N	805	15,1	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
21	LMG	O	850	-	55,55,55	0.50	0	63,63,63	0.59	0
15	CLA	a	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
21	LMG	a	855	-	44,44,55	0.53	0	52,52,63	0.61	0
15	CLA	N	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.44	4 (6%)
15	CLA	a	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
15	CLA	a	831	1	69,73,73	1.17	9 (13%)	82,113,113	1.26	6 (7%)
15	CLA	a	811	1	61,65,73	1.23	6 (9%)	72,103,113	1.31	6 (8%)
15	CLA	B	804	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	6 (7%)
15	CLA	N	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	A	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
20	LMT	N	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	A	806	1	69,73,73	1.16	7 (10%)	82,113,113	1.26	7 (8%)
18	BCR	F	203	-	41,41,41	0.30	0	56,56,56	0.50	0
15	CLA	b	827	2	66,70,73	1.18	9 (13%)	78,109,113	1.26	5 (6%)
15	CLA	O	817	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	6 (7%)
19	LHG	l	101	-	43,43,48	0.54	0	46,49,54	0.51	0
18	BCR	N	845	-	41,41,41	0.35	0	56,56,56	0.93	0
15	CLA	A	833	1	59,63,73	1.25	8 (13%)	70,101,113	1.34	6 (8%)
18	BCR	T	101	-	41,41,41	0.32	0	56,56,56	0.72	0
18	BCR	N	849	-	41,41,41	0.32	0	56,56,56	0.58	0
15	CLA	O	830	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
18	BCR	a	849	-	41,41,41	0.31	0	56,56,56	0.58	0
21	LMG	W	1505	-	50,50,55	0.50	0	58,58,63	0.59	0
20	LMT	a	852	-	32,32,36	0.57	0	43,43,47	0.69	0
15	CLA	A	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
18	BCR	g	102	-	41,41,41	0.29	0	56,56,56	0.49	0
18	BCR	O	845	-	41,41,41	0.30	0	56,56,56	0.47	0
15	CLA	N	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.34	5 (7%)
15	CLA	N	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	O	828	2	69,73,73	1.15	8 (11%)	82,113,113	1.24	8 (9%)
15	CLA	B	813	2	49,53,73	1.37	6 (12%)	58,89,113	1.45	6 (10%)
17	SF4	N	844	2,1	0,12,12	-	-	-	-	-
15	CLA	N	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.28	6 (7%)
22	LFA	O	851	-	15,15,19	0.23	0	14,14,18	0.19	0
14	F6C	b	833	2	72,74,74	1.59	9 (12%)	83,114,114	2.03	16 (19%)
15	CLA	a	813	1	58,62,73	1.27	7 (12%)	68,99,113	1.37	7 (10%)
19	LHG	L	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	A	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
16	PQN	O	842	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
15	CLA	N	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.35	6 (8%)
18	BCR	a	845	-	41,41,41	0.35	0	56,56,56	0.95	1 (1%)
15	CLA	N	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
18	BCR	Y	102	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
18	BCR	I	101	-	41,41,41	0.33	0	56,56,56	0.73	0
15	CLA	a	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
21	LMG	I	103	-	37,37,55	0.56	0	45,45,63	0.66	0
15	CLA	V	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMG	N	855	-	44,44,55	0.54	0	52,52,63	0.64	0
15	CLA	A	837	1	55,59,73	1.31	8 (14%)	64,96,113	1.37	8 (12%)
16	PQN	a	843	-	34,34,34	0.35	0	43,45,45	0.61	1 (2%)
15	CLA	a	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	b	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	B	815	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	7 (8%)
15	CLA	a	838	1	59,63,73	1.25	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	b	812	2	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
18	BCR	N	850	-	41,41,41	0.31	0	56,56,56	0.87	0
14	F6C	a	802	24	72,74,74	1.59	9 (12%)	83,114,114	1.99	13 (15%)
18	BCR	b	847	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
15	CLA	a	830	1	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
15	CLA	O	824	24	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
18	BCR	B	842	-	41,41,41	0.31	0	56,56,56	0.65	0
18	BCR	W	1508	-	41,41,41	0.30	0	56,56,56	0.65	0
17	SF4	a	844	2,1	0,12,12	-	-	-	-	-
18	BCR	B	845	-	41,41,41	0.32	0	56,56,56	0.87	2 (3%)
15	CLA	A	814	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	O	816	2	61,65,73	1.23	7 (11%)	72,103,113	1.34	8 (11%)
20	LMT	N	852	-	32,32,36	0.56	0	43,43,47	0.68	0
17	SF4	c	102	3	0,12,12	-	-	-	-	-
15	CLA	B	835	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	a	819	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	K	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.40	7 (10%)
15	CLA	W	1502	10	64,68,73	1.20	8 (12%)	76,107,113	1.31	7 (9%)
15	CLA	N	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
15	CLA	S	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	N	837	1	55,59,73	1.30	8 (14%)	64,96,113	1.37	8 (12%)
15	CLA	N	808	1	49,53,73	1.38	8 (16%)	58,89,113	1.46	6 (10%)
18	BCR	A	849	-	41,41,41	0.32	0	56,56,56	0.60	0
18	BCR	j	201	-	41,41,41	0.30	0	56,56,56	0.67	0
18	BCR	O	843	-	41,41,41	0.30	0	56,56,56	0.61	0
15	CLA	a	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
18	BCR	A	845	-	41,41,41	0.35	0	56,56,56	0.97	2 (3%)
15	CLA	N	806	1	69,73,73	1.16	6 (8%)	82,113,113	1.27	7 (8%)
15	CLA	a	805	15,1	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
17	SF4	c	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	B	806	2	69,73,73	1.15	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	O	819	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
14	F6C	a	824	24	58,60,74	1.78	8 (13%)	65,97,114	2.22	14 (21%)
18	BCR	L	205	-	41,41,41	0.33	0	56,56,56	0.66	0
21	LMG	h	102	-	55,55,55	0.49	0	63,63,63	0.61	0
14	F6C	A	824	24	58,60,74	1.78	8 (13%)	65,97,114	2.23	14 (21%)
15	CLA	A	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	835	1	69,73,73	1.16	8 (11%)	82,113,113	1.24	6 (7%)
18	BCR	I	102	-	41,41,41	0.29	0	56,56,56	0.48	0
15	CLA	A	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
15	CLA	O	827	2	66,70,73	1.18	9 (13%)	78,109,113	1.25	5 (6%)
14	F6C	A	826	24	72,74,74	1.60	8 (11%)	83,114,114	2.06	19 (22%)
18	BCR	a	846	-	41,41,41	0.31	0	56,56,56	0.67	1 (1%)
15	CLA	O	836	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
15	CLA	b	822	24	57,61,73	1.28	6 (10%)	67,98,113	1.37	7 (10%)
15	CLA	A	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	816	1	49,53,73	1.39	7 (14%)	58,89,113	1.42	4 (6%)
19	LHG	Z	101	-	43,43,48	0.54	0	46,49,54	0.51	0
15	CLA	A	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	5 (6%)
15	CLA	B	833	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)
18	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.88	1 (1%)
15	CLA	O	815	2	49,53,73	1.38	6 (12%)	58,89,113	1.45	5 (8%)
15	CLA	N	830	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	5 (6%)
18	BCR	S	202	-	41,41,41	0.30	0	56,56,56	0.51	0
15	CLA	A	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	b	835	24	49,53,73	1.39	8 (16%)	58,89,113	1.41	6 (10%)
15	CLA	A	830	1	69,73,73	1.16	7 (10%)	82,113,113	1.24	7 (8%)
18	BCR	O	846	-	41,41,41	0.30	0	56,56,56	0.60	0
15	CLA	B	837	2	69,73,73	1.15	8 (11%)	82,113,113	1.28	9 (10%)
21	LMG	b	849	-	55,55,55	0.49	0	63,63,63	0.59	0
18	BCR	f	203	-	41,41,41	0.30	0	56,56,56	0.48	0
15	CLA	a	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	7 (8%)
15	CLA	N	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.24	6 (7%)
15	CLA	B	808	2	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
18	BCR	i	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.50	0
15	CLA	O	832	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	LMG	j	206	-	50,50,55	0.50	0	58,58,63	0.59	0
20	LMT	a	853	-	29,29,36	0.57	0	40,40,47	1.45	4 (10%)
15	CLA	N	825	1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	W	1501	10	69,73,73	1.16	8 (11%)	82,113,113	1.27	5 (6%)
14	F6C	N	802	24	72,74,74	1.58	9 (12%)	83,114,114	1.99	13 (15%)
15	CLA	a	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.28	7 (9%)
18	BCR	W	1504	-	41,41,41	0.32	0	56,56,56	0.57	0
21	LMG	B	847	-	55,55,55	0.50	0	63,63,63	0.59	0
15	CLA	l	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
19	LHG	W	1506	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	b	823	2	59,63,73	1.30	8 (13%)	70,101,113	1.24	6 (8%)
15	CLA	b	813	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
15	CLA	B	812	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	A	827	24	59,63,73	1.25	7 (11%)	70,101,113	1.38	8 (11%)
15	CLA	O	839	2	69,73,73	1.15	8 (11%)	82,113,113	1.27	8 (9%)
14	F6C	N	826	24	72,74,74	1.62	8 (11%)	83,114,114	2.02	17 (20%)
15	CLA	O	802	24	69,73,73	1.16	7 (10%)	82,113,113	1.21	6 (7%)
15	CLA	b	832	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
15	CLA	a	833	1	59,63,73	1.26	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	a	810	1	61,65,73	1.24	8 (13%)	72,103,113	1.37	8 (11%)
15	CLA	b	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.25	6 (7%)
15	CLA	a	812	15,1	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	b	806	2	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
15	CLA	A	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
15	CLA	A	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
14	F6C	a	826	24	72,74,74	1.60	8 (11%)	83,114,114	2.02	16 (19%)
19	LHG	j	207	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	b	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	b	834	2	59,63,73	1.26	7 (11%)	70,101,113	1.33	6 (8%)
18	BCR	V	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0
16	PQN	N	843	-	34,34,34	0.35	0	43,45,45	0.58	1 (2%)
19	LHG	Z	102	-	48,48,48	0.51	0	51,54,54	0.48	0
18	BCR	N	847	-	41,41,41	0.29	0	56,56,56	0.60	1 (1%)
15	CLA	O	835	24	49,53,73	1.39	8 (16%)	58,89,113	1.42	6 (10%)
15	CLA	B	832	2	59,63,73	1.26	7 (11%)	70,101,113	1.33	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	O	847	-	41,41,41	0.32	0	56,56,56	0.84	3 (5%)
14	F6C	b	840	24	72,74,74	1.57	9 (12%)	83,114,114	2.08	15 (18%)
15	CLA	b	829	2	69,73,73	1.16	8 (11%)	82,113,113	1.30	7 (8%)
14	F6C	W	1503	24	72,74,74	1.58	8 (11%)	83,114,114	2.06	17 (20%)
15	CLA	N	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	A	815	1	59,63,73	1.27	8 (13%)	70,101,113	1.34	6 (8%)
15	CLA	A	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
18	BCR	b	848	-	41,41,41	0.29	0	56,56,56	0.63	0
15	CLA	b	811	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
18	BCR	M	101	-	41,41,41	0.31	0	56,56,56	0.68	1 (1%)
15	CLA	B	834	24	49,53,73	1.40	8 (16%)	58,89,113	1.39	4 (6%)
15	CLA	O	821	2	49,53,73	1.38	8 (16%)	58,89,113	1.44	4 (6%)
15	CLA	N	814	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
20	LMT	a	854	-	36,36,36	0.55	0	47,47,47	0.63	0
15	CLA	N	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
14	F6C	A	802	24	72,74,74	1.59	10 (13%)	83,114,114	1.99	14 (16%)
15	CLA	b	808	2	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
15	CLA	A	819	1	69,73,73	1.18	9 (13%)	82,113,113	1.25	6 (7%)
15	CLA	A	809	1	64,68,73	1.20	8 (12%)	76,107,113	1.29	7 (9%)
15	CLA	O	818	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	4 (5%)
15	CLA	B	817	24	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	a	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
15	CLA	A	807	1	69,73,73	1.16	8 (11%)	82,113,113	1.28	5 (6%)
15	CLA	N	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.37	9 (10%)
16	PQN	B	840	-	34,34,34	0.37	0	43,45,45	0.63	1 (2%)
15	CLA	N	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.26	4 (4%)
16	PQN	A	843	-	34,34,34	0.36	0	43,45,45	0.61	1 (2%)
15	CLA	B	830	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	8 (9%)
18	BCR	A	847	-	41,41,41	0.29	0	56,56,56	0.61	1 (1%)
15	CLA	B	828	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
20	LMT	A	853	-	29,29,36	0.57	0	40,40,47	1.45	4 (10%)
14	F6C	b	810	2	72,74,74	1.60	8 (11%)	83,114,114	1.96	14 (16%)
15	CLA	O	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.21	7 (8%)
22	LFA	B	848	-	15,15,19	0.23	0	14,14,18	0.19	0
18	BCR	A	858	-	41,41,41	0.38	0	56,56,56	1.31	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b	841	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	814	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)
15	CLA	B	819	2	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
19	LHG	Y	101	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	823	2	59,63,73	1.26	9 (15%)	70,101,113	1.37	6 (8%)
15	CLA	B	803	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
14	F6C	j	204	24	72,74,74	1.58	8 (11%)	83,114,114	2.07	17 (20%)
17	SF4	A	844	2,1	0,12,12	-	-	-	-	-
15	CLA	A	810	1	61,65,73	1.24	7 (11%)	72,103,113	1.37	8 (11%)
15	CLA	B	805	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
15	CLA	O	829	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	8 (9%)
15	CLA	B	822	24	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
20	LMT	N	853	-	29,29,36	0.57	0	40,40,47	1.43	4 (10%)
18	BCR	A	846	-	41,41,41	0.31	0	56,56,56	0.65	1 (1%)
15	CLA	O	809	2	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
15	CLA	a	841	1	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
15	CLA	O	831	2	69,73,73	1.16	7 (10%)	82,113,113	1.26	7 (8%)
15	CLA	A	838	1	59,63,73	1.25	9 (15%)	70,101,113	1.32	5 (7%)
15	CLA	A	823	1	60,64,73	1.25	8 (13%)	71,102,113	1.34	6 (8%)
15	CLA	a	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
18	BCR	U	101	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	b	819	24	69,73,73	1.18	8 (11%)	82,113,113	1.25	6 (7%)
14	F6C	O	833	2	72,74,74	1.59	9 (12%)	83,114,114	2.03	15 (18%)
15	CLA	j	203	10	64,68,73	1.20	8 (12%)	76,107,113	1.32	7 (9%)
19	LHG	A	851	-	41,41,48	0.56	0	44,47,54	0.51	0
18	BCR	b	844	-	41,41,41	0.31	0	56,56,56	0.63	0
15	CLA	N	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
15	CLA	a	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	A	832	1	54,58,73	1.31	8 (14%)	64,95,113	1.38	6 (9%)
14	F6C	A	857	24	72,74,74	1.56	8 (11%)	83,114,114	2.10	15 (18%)
14	F6C	a	856	24	72,74,74	1.56	8 (11%)	83,114,114	2.09	15 (18%)
15	CLA	O	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
15	CLA	b	814	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
18	BCR	j	205	-	41,41,41	0.33	0	56,56,56	0.67	0
15	CLA	b	817	2	69,73,73	1.18	8 (11%)	82,113,113	1.26	7 (8%)
15	CLA	a	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.27	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	N	846	-	41,41,41	0.31	0	56,56,56	0.67	1 (1%)
21	LMG	g	103	-	37,37,55	0.56	0	45,45,63	0.66	0
18	BCR	b	843	-	41,41,41	0.30	0	56,56,56	0.61	0
15	CLA	O	834	2	59,63,73	1.26	8 (13%)	70,101,113	1.33	6 (8%)
13	CL0	N	801	1	58,73,73	2.23	10 (17%)	60,113,113	1.63	14 (23%)
15	CLA	b	828	2	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	B	809	2	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
15	CLA	a	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
13	CL0	A	801	1	58,73,73	2.23	9 (15%)	60,113,113	1.62	13 (21%)
15	CLA	a	827	24	59,63,73	1.25	8 (13%)	70,101,113	1.38	7 (10%)
18	BCR	b	845	-	41,41,41	0.29	0	56,56,56	0.47	0
15	CLA	B	818	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	5 (7%)
15	CLA	b	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	7 (8%)
15	CLA	b	825	24	69,73,73	1.16	6 (8%)	82,113,113	1.31	7 (8%)
15	CLA	N	831	1	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
15	CLA	a	836	1	58,62,73	1.27	8 (13%)	68,99,113	1.35	6 (8%)
17	SF4	P	101	3	0,12,12	-	-	-	-	-
15	CLA	b	805	2	69,73,73	1.15	6 (8%)	82,113,113	1.28	6 (7%)
14	F6C	B	831	2	72,74,74	1.58	9 (12%)	83,114,114	2.05	16 (19%)
15	CLA	b	830	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	6 (7%)
15	CLA	b	826	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
15	CLA	B	801	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
15	CLA	O	813	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
21	LMG	U	102	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	B	825	2	66,70,73	1.19	9 (13%)	78,109,113	1.25	5 (6%)
15	CLA	N	840	1	54,58,73	1.30	8 (14%)	64,95,113	1.40	6 (9%)
19	LHG	M	102	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	814	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
17	SF4	C	102	3	0,12,12	-	-	-	-	-
14	F6C	L	204	24	72,74,74	1.58	8 (11%)	83,114,114	2.05	16 (19%)
18	BCR	a	848	-	41,41,41	0.31	0	56,56,56	0.50	0
21	LMG	A	855	-	44,44,55	0.53	0	52,52,63	0.62	0
18	BCR	b	846	-	41,41,41	0.31	0	56,56,56	0.57	0
18	BCR	B	841	-	41,41,41	0.30	0	56,56,56	0.60	0
15	CLA	b	821	2	49,53,73	1.38	7 (14%)	58,89,113	1.44	4 (6%)
19	LHG	a	851	-	41,41,48	0.55	0	44,47,54	0.52	0
15	CLA	N	811	1	61,65,73	1.23	7 (11%)	72,103,113	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	b	816	2	61,65,73	1.24	7 (11%)	72,103,113	1.32	7 (9%)
18	BCR	a	850	-	41,41,41	0.31	0	56,56,56	0.88	1 (1%)
14	F6C	O	840	24	72,74,74	1.57	8 (11%)	83,114,114	2.07	15 (18%)
14	F6C	B	838	24	72,74,74	1.57	8 (11%)	83,114,114	2.08	15 (18%)
15	CLA	A	805	15,1	64,68,73	1.21	7 (10%)	76,107,113	1.29	5 (6%)
15	CLA	B	836	2	69,73,73	1.16	7 (10%)	82,113,113	1.28	8 (9%)
15	CLA	N	839	1	69,73,73	1.16	8 (11%)	82,113,113	1.29	6 (7%)
18	BCR	k	102	-	41,41,41	0.31	0	56,56,56	0.69	1 (1%)
15	CLA	a	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
15	CLA	O	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.29	6 (7%)
18	BCR	B	843	-	41,41,41	0.30	0	56,56,56	0.48	0
18	BCR	h	101	-	41,41,41	0.31	0	56,56,56	0.54	0
15	CLA	N	810	1	61,65,73	1.24	8 (13%)	72,103,113	1.37	8 (11%)
15	CLA	O	841	2	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	6 (7%)
15	CLA	B	810	2	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
15	CLA	a	820	1	69,73,73	1.16	8 (11%)	82,113,113	1.36	9 (10%)
14	F6C	N	856	24	72,74,74	1.56	9 (12%)	83,114,114	2.09	15 (18%)
19	LHG	X	102	-	48,48,48	0.51	0	51,54,54	0.48	0
15	CLA	A	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
15	CLA	X	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
15	CLA	f	201	24	69,73,73	1.17	8 (11%)	82,113,113	1.24	6 (7%)
15	CLA	b	818	2	64,68,73	1.20	8 (12%)	76,107,113	1.24	4 (5%)
15	CLA	b	836	24	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
19	LHG	N	851	-	41,41,48	0.55	0	44,47,54	0.50	0
15	CLA	N	813	1	58,62,73	1.27	8 (13%)	68,99,113	1.36	7 (10%)
15	CLA	B	827	2	69,73,73	1.16	8 (11%)	82,113,113	1.29	8 (9%)
15	CLA	O	805	2	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
15	CLA	O	822	24	57,61,73	1.28	7 (12%)	67,98,113	1.39	8 (11%)
18	BCR	L	209	-	41,41,41	0.30	0	56,56,56	0.65	0
15	CLA	B	826	2	69,73,73	1.15	7 (10%)	82,113,113	1.22	7 (8%)
15	CLA	A	829	1	64,68,73	1.20	7 (10%)	76,107,113	1.26	6 (7%)
15	CLA	B	814	2	61,65,73	1.23	7 (11%)	72,103,113	1.34	8 (11%)
17	SF4	P	102	3	0,12,12	-	-	-	-	-
14	F6C	N	824	24	58,60,74	1.78	7 (12%)	65,97,114	2.20	14 (21%)
15	CLA	A	811	1	61,65,73	1.23	6 (9%)	72,103,113	1.31	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	BCR	T	102	-	41,41,41	0.29	0	56,56,56	0.48	0
15	CLA	b	809	2	69,73,73	1.17	9 (13%)	82,113,113	1.25	6 (7%)
19	LHG	l	102	-	48,48,48	0.52	0	51,54,54	0.48	0
15	CLA	b	815	2	49,53,73	1.38	6 (12%)	58,89,113	1.45	7 (12%)
15	CLA	A	831	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	7 (8%)
15	CLA	B	802	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	6 (7%)
13	CL0	a	801	1	58,73,73	2.23	9 (15%)	60,113,113	1.64	14 (23%)
18	BCR	A	848	-	41,41,41	0.31	0	56,56,56	0.52	0
15	CLA	i	103	24	54,58,73	1.33	8 (14%)	64,95,113	1.39	6 (9%)
19	LHG	X	101	-	43,43,48	0.54	0	46,49,54	0.52	0
15	CLA	b	820	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
18	BCR	a	847	-	41,41,41	0.30	0	56,56,56	0.61	1 (1%)
15	CLA	A	828	1	69,73,73	1.17	9 (13%)	82,113,113	1.25	5 (6%)
15	CLA	A	835	1	69,73,73	1.16	8 (11%)	82,113,113	1.27	7 (8%)
18	BCR	B	846	-	41,41,41	0.29	0	56,56,56	0.61	0
15	CLA	V	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	O	806	2	69,73,73	1.16	7 (10%)	82,113,113	1.30	6 (7%)
15	CLA	b	804	2	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	i	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	K	102	9	49,53,73	1.39	8 (16%)	58,89,113	1.41	4 (6%)
15	CLA	B	811	2	60,64,73	1.26	9 (15%)	71,102,113	1.36	6 (8%)
18	BCR	B	844	-	41,41,41	0.31	0	56,56,56	0.60	0
20	LMT	A	852	-	32,32,36	0.57	0	43,43,47	0.68	0
15	CLA	L	202	10	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
15	CLA	B	820	24	57,61,73	1.27	7 (12%)	67,98,113	1.38	7 (10%)
18	BCR	F	202	-	41,41,41	0.31	0	56,56,56	1.02	4 (7%)
15	CLA	L	203	10	64,68,73	1.20	9 (14%)	76,107,113	1.33	7 (9%)
21	LMG	L	206	-	50,50,55	0.50	0	58,58,63	0.59	0
16	PQN	b	842	-	34,34,34	0.36	0	43,45,45	0.62	1 (2%)
15	CLA	N	807	1	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
15	CLA	B	807	2	69,73,73	1.14	9 (13%)	82,113,113	1.30	8 (9%)
15	CLA	O	811	2	69,73,73	1.17	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	A	842	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
18	BCR	N	857	-	41,41,41	0.38	0	56,56,56	1.32	8 (14%)
15	CLA	Z	103	12	59,63,73	1.27	7 (11%)	70,101,113	1.33	5 (7%)
21	LMG	T	103	-	37,37,55	0.56	0	45,45,63	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	CLA	O	804	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
15	CLA	N	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.29	6 (7%)
18	BCR	O	848	-	41,41,41	0.31	0	56,56,56	1.00	4 (7%)
15	CLA	B	839	2	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
18	BCR	J	101	-	41,41,41	0.31	0	56,56,56	0.54	0
19	LHG	k	101	-	48,48,48	0.51	0	51,54,54	0.50	0
15	CLA	O	812	2	49,53,73	1.38	8 (16%)	58,89,113	1.42	4 (6%)
18	BCR	K	101	-	25,25,41	0.52	1 (4%)	33,33,56	0.51	0
21	LMG	J	102	-	55,55,55	0.49	0	63,63,63	0.60	0
15	CLA	O	807	2	69,73,73	1.16	8 (11%)	82,113,113	1.25	7 (8%)
15	CLA	O	825	24	69,73,73	1.16	8 (11%)	82,113,113	1.30	6 (7%)
15	CLA	O	837	2	69,73,73	1.16	9 (13%)	82,113,113	1.27	7 (8%)
15	CLA	b	824	24	69,73,73	1.17	8 (11%)	82,113,113	1.30	7 (8%)
15	CLA	N	804	1	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	b	838	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	8 (9%)
14	F6C	L	201	2	72,74,74	1.60	8 (11%)	83,114,114	1.97	14 (16%)
15	CLA	a	834	1	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
15	CLA	O	826	2	69,73,73	1.17	9 (13%)	82,113,113	1.30	7 (8%)
15	CLA	b	839	2	69,73,73	1.16	8 (11%)	82,113,113	1.28	9 (10%)
15	CLA	O	808	2	69,73,73	1.14	9 (13%)	82,113,113	1.31	9 (10%)
18	BCR	f	202	-	41,41,41	0.31	0	56,56,56	1.00	4 (7%)
15	CLA	A	817	24	49,53,73	1.40	8 (16%)	58,89,113	1.43	4 (6%)
15	CLA	A	822	24	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
15	CLA	a	837	1	55,59,73	1.30	7 (12%)	64,96,113	1.37	7 (10%)
15	CLA	N	803	-	69,73,73	1.15	9 (13%)	82,113,113	1.28	7 (8%)
15	CLA	B	824	2	69,73,73	1.17	9 (13%)	82,113,113	1.29	7 (8%)
15	CLA	B	823	24	69,73,73	1.16	6 (8%)	82,113,113	1.31	6 (7%)

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
15	CLA	B	821	2	1/1/13/20	11/27/103/115	-
18	BCR	g	101	-	-	7/29/63/63	0/2/2/2
22	LFA	L	208	-	-	0/12/12/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	816	1	1/1/11/20	8/15/91/115	-
15	CLA	N	827	24	1/1/13/20	0/27/103/115	-
15	CLA	a	807	1	1/1/15/20	18/39/115/115	-
15	CLA	N	829	1	1/1/14/20	16/33/109/115	-
15	CLA	b	837	2	1/1/15/20	9/39/115/115	-
15	CLA	F	201	24	1/1/15/20	10/39/115/115	-
15	CLA	B	816	2	1/1/14/20	13/33/109/115	-
15	CLA	a	823	1	1/1/13/20	5/29/105/115	-
15	CLA	j	202	10	1/1/15/20	6/39/115/115	-
15	CLA	B	829	2	1/1/15/20	14/39/115/115	-
18	BCR	N	848	-	-	8/29/63/63	0/2/2/2
15	CLA	A	808	1	1/1/11/20	0/15/91/115	-
15	CLA	b	802	24	1/1/15/20	12/39/115/115	-
17	SF4	C	101	3	-	-	0/6/5/5
22	LFA	f	204	-	-	6/13/13/17	-
15	CLA	A	803	-	1/1/15/20	11/39/115/115	-
15	CLA	N	836	1	1/1/12/20	7/26/102/115	-
15	CLA	a	806	1	1/1/15/20	17/39/115/115	-
15	CLA	N	815	1	1/1/13/20	2/27/103/115	-
15	CLA	A	813	1	1/1/12/20	7/26/102/115	-
18	BCR	O	849	-	-	4/29/63/63	0/2/2/2
18	BCR	a	857	-	-	10/29/63/63	0/2/2/2
18	BCR	O	844	-	-	5/29/63/63	0/2/2/2
20	LMT	A	854	-	-	5/21/61/61	0/2/2/2
14	F6C	O	810	2	1/1/10/16	8/41/97/97	-
22	LFA	j	208	-	-	0/12/12/17	-
15	CLA	A	856	24	1/1/15/20	12/39/115/115	-
15	CLA	N	822	24	1/1/15/20	18/39/115/115	-
22	LFA	W	1507	-	-	0/12/12/17	-
15	CLA	N	838	1	1/1/13/20	10/27/103/115	-
15	CLA	O	820	2	1/1/13/20	13/27/103/115	-
15	CLA	a	808	1	1/1/11/20	0/15/91/115	-
15	CLA	N	805	15,1	1/1/14/20	8/33/109/115	-
21	LMG	O	850	-	-	7/50/70/70	0/1/1/1
15	CLA	a	829	1	1/1/14/20	17/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	LMG	a	855	-	-	8/39/59/70	0/1/1/1
15	CLA	N	817	24	1/1/11/20	5/15/91/115	-
15	CLA	a	832	1	1/1/12/20	3/21/97/115	-
15	CLA	a	831	1	1/1/15/20	14/39/115/115	-
15	CLA	a	811	1	1/1/13/20	11/30/106/115	-
15	CLA	B	804	2	1/1/15/20	14/39/115/115	-
15	CLA	N	812	15,1	1/1/15/20	19/39/115/115	-
15	CLA	A	816	1	1/1/11/20	7/15/91/115	-
20	LMT	N	854	-	-	5/21/61/61	0/2/2/2
15	CLA	A	806	1	1/1/15/20	17/39/115/115	-
18	BCR	F	203	-	-	2/29/63/63	0/2/2/2
15	CLA	b	827	2	1/1/14/20	12/36/112/115	-
15	CLA	O	817	2	1/1/15/20	11/39/115/115	-
19	LHG	l	101	-	-	22/48/48/53	-
18	BCR	N	845	-	-	3/29/63/63	0/2/2/2
15	CLA	A	833	1	1/1/13/20	4/27/103/115	-
18	BCR	T	101	-	-	9/29/63/63	0/2/2/2
18	BCR	N	849	-	-	3/29/63/63	0/2/2/2
15	CLA	O	830	2	1/1/15/20	17/39/115/115	-
18	BCR	a	849	-	-	3/29/63/63	0/2/2/2
21	LMG	W	1505	-	-	11/45/65/70	0/1/1/1
20	LMT	a	852	-	-	0/17/57/61	0/2/2/2
15	CLA	A	840	1	1/1/12/20	0/21/97/115	-
18	BCR	g	102	-	-	4/29/63/63	0/2/2/2
18	BCR	O	845	-	-	4/29/63/63	0/2/2/2
15	CLA	N	823	1	1/1/13/20	6/29/105/115	-
15	CLA	N	842	1	1/1/15/20	12/39/115/115	-
15	CLA	O	828	2	1/1/15/20	6/39/115/115	-
15	CLA	B	813	2	1/1/11/20	7/15/91/115	-
17	SF4	N	844	2,1	-	-	0/6/5/5
15	CLA	N	809	1	1/1/14/20	14/33/109/115	-
22	LFA	O	851	-	-	6/13/13/17	-
14	F6C	b	833	2	1/1/10/16	5/41/97/97	-
15	CLA	a	813	1	1/1/12/20	4/26/102/115	-
19	LHG	L	207	-	-	16/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	841	1	1/1/15/20	14/39/115/115	-
16	PQN	O	842	-	-	0/23/43/43	0/2/2/2
15	CLA	N	833	1	1/1/13/20	3/27/103/115	-
18	BCR	a	845	-	-	3/29/63/63	0/2/2/2
15	CLA	N	834	1	1/1/15/20	8/39/115/115	-
18	BCR	Y	102	-	-	6/29/63/63	0/2/2/2
18	BCR	I	101	-	-	9/29/63/63	0/2/2/2
15	CLA	a	822	24	1/1/15/20	17/39/115/115	-
21	LMG	I	103	-	-	11/32/52/70	0/1/1/1
15	CLA	V	103	24	1/1/12/20	2/21/97/115	-
21	LMG	N	855	-	-	6/39/59/70	0/1/1/1
15	CLA	A	837	1	1/1/12/20	8/23/99/115	-
16	PQN	a	843	-	-	0/23/43/43	0/2/2/2
15	CLA	a	803	-	1/1/15/20	11/39/115/115	-
15	CLA	b	807	2	1/1/15/20	3/39/115/115	-
15	CLA	B	815	2	1/1/15/20	12/39/115/115	-
15	CLA	a	838	1	1/1/13/20	10/27/103/115	-
15	CLA	b	812	2	1/1/11/20	5/15/91/115	-
18	BCR	N	850	-	-	13/29/63/63	0/2/2/2
14	F6C	a	802	24	1/1/10/16	7/41/97/97	-
18	BCR	b	847	-	-	1/29/63/63	0/2/2/2
15	CLA	a	830	1	1/1/15/20	6/39/115/115	-
15	CLA	O	824	24	1/1/15/20	9/39/115/115	-
18	BCR	B	842	-	-	5/29/63/63	0/2/2/2
18	BCR	W	1508	-	-	2/29/63/63	0/2/2/2
17	SF4	a	844	2,1	-	-	0/6/5/5
18	BCR	B	845	-	-	2/29/63/63	0/2/2/2
15	CLA	A	814	1	1/1/15/20	11/39/115/115	-
15	CLA	O	816	2	1/1/13/20	6/30/106/115	-
20	LMT	N	852	-	-	2/17/57/61	0/2/2/2
17	SF4	c	102	3	-	-	0/6/5/5
15	CLA	B	835	2	1/1/15/20	9/39/115/115	-
15	CLA	a	819	1	1/1/15/20	14/39/115/115	-
15	CLA	K	103	24	1/1/12/20	2/21/97/115	-
15	CLA	W	1502	10	1/1/14/20	12/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	841	1	1/1/15/20	15/39/115/115	-
15	CLA	S	201	24	1/1/15/20	10/39/115/115	-
15	CLA	N	837	1	1/1/12/20	8/23/99/115	-
15	CLA	N	808	1	1/1/11/20	2/15/91/115	-
18	BCR	A	849	-	-	3/29/63/63	0/2/2/2
18	BCR	j	201	-	-	4/29/63/63	0/2/2/2
18	BCR	O	843	-	-	3/29/63/63	0/2/2/2
15	CLA	a	825	1	1/1/15/20	10/39/115/115	-
18	BCR	A	845	-	-	3/29/63/63	0/2/2/2
15	CLA	N	806	1	1/1/15/20	17/39/115/115	-
15	CLA	a	805	15,1	1/1/14/20	9/33/109/115	-
17	SF4	c	101	3	-	-	0/6/5/5
15	CLA	B	806	2	1/1/15/20	5/39/115/115	-
15	CLA	O	819	24	1/1/15/20	9/39/115/115	-
14	F6C	a	824	24	1/1/7/16	9/25/81/97	-
18	BCR	L	205	-	-	4/29/63/63	0/2/2/2
21	LMG	h	102	-	-	16/50/70/70	0/1/1/1
14	F6C	A	824	24	1/1/7/16	9/25/81/97	-
15	CLA	A	825	1	1/1/15/20	6/39/115/115	-
15	CLA	a	835	1	1/1/15/20	7/39/115/115	-
18	BCR	I	102	-	-	4/29/63/63	0/2/2/2
15	CLA	A	839	1	1/1/15/20	17/39/115/115	-
15	CLA	O	827	2	1/1/14/20	12/36/112/115	-
14	F6C	A	826	24	1/1/10/16	14/41/97/97	-
18	BCR	a	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	836	24	1/1/11/20	8/15/91/115	-
15	CLA	b	822	24	1/1/12/20	9/25/101/115	-
15	CLA	A	812	15,1	1/1/15/20	19/39/115/115	-
15	CLA	a	816	1	1/1/11/20	7/15/91/115	-
19	LHG	Z	101	-	-	22/48/48/53	-
15	CLA	A	821	1	1/1/14/20	8/33/109/115	-
15	CLA	B	833	24	1/1/11/20	2/15/91/115	-
18	BCR	A	850	-	-	13/29/63/63	0/2/2/2
15	CLA	O	815	2	1/1/11/20	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	N	830	1	1/1/15/20	6/39/115/115	-
18	BCR	S	202	-	-	2/29/63/63	0/2/2/2
15	CLA	A	804	1	1/1/15/20	6/39/115/115	-
15	CLA	b	835	24	1/1/11/20	4/15/91/115	-
15	CLA	A	830	1	1/1/15/20	7/39/115/115	-
18	BCR	O	846	-	-	8/29/63/63	0/2/2/2
15	CLA	B	837	2	1/1/15/20	10/39/115/115	-
21	LMG	b	849	-	-	7/50/70/70	0/1/1/1
18	BCR	f	203	-	-	2/29/63/63	0/2/2/2
15	CLA	a	818	1	1/1/15/20	22/39/115/115	-
15	CLA	N	835	1	1/1/15/20	10/39/115/115	-
15	CLA	B	808	2	1/1/15/20	13/39/115/115	-
18	BCR	i	101	-	-	0/18/35/63	0/1/1/2
15	CLA	O	832	2	1/1/15/20	9/39/115/115	-
21	LMG	j	206	-	-	10/45/65/70	0/1/1/1
20	LMT	a	853	-	-	10/14/54/61	0/2/2/2
15	CLA	N	825	1	1/1/15/20	9/39/115/115	-
15	CLA	a	815	1	1/1/13/20	4/27/103/115	-
15	CLA	W	1501	10	1/1/15/20	7/39/115/115	-
14	F6C	N	802	24	1/1/10/16	7/41/97/97	-
15	CLA	a	809	1	1/1/14/20	10/33/109/115	-
18	BCR	W	1504	-	-	4/29/63/63	0/2/2/2
21	LMG	B	847	-	-	7/50/70/70	0/1/1/1
15	CLA	l	103	12	1/1/13/20	2/27/103/115	-
19	LHG	W	1506	-	-	16/53/53/53	-
15	CLA	b	823	2	1/1/13/20	6/27/103/115	-
15	CLA	b	813	2	-	10/29/105/115	-
15	CLA	B	812	2	1/1/15/20	14/39/115/115	-
15	CLA	A	827	24	1/1/13/20	0/27/103/115	-
15	CLA	O	839	2	1/1/15/20	12/39/115/115	-
14	F6C	N	826	24	1/1/10/16	15/41/97/97	-
15	CLA	O	802	24	1/1/15/20	12/39/115/115	-
15	CLA	b	832	2	1/1/15/20	10/39/115/115	-
15	CLA	a	833	1	1/1/13/20	3/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	810	1	1/1/13/20	7/30/106/115	-
15	CLA	b	831	2	1/1/15/20	11/39/115/115	-
15	CLA	a	812	15,1	1/1/15/20	18/39/115/115	-
15	CLA	b	806	2	1/1/15/20	18/39/115/115	-
15	CLA	A	818	1	1/1/15/20	19/39/115/115	-
15	CLA	A	836	1	1/1/12/20	6/26/102/115	-
14	F6C	a	826	24	1/1/10/16	12/41/97/97	-
19	LHG	j	207	-	-	17/53/53/53	-
15	CLA	b	801	2	1/1/15/20	10/39/115/115	-
15	CLA	b	834	2	1/1/13/20	8/27/103/115	-
18	BCR	V	101	-	-	0/18/35/63	0/1/1/2
16	PQN	N	843	-	-	1/23/43/43	0/2/2/2
19	LHG	Z	102	-	-	23/53/53/53	-
18	BCR	N	847	-	-	6/29/63/63	0/2/2/2
15	CLA	O	835	24	1/1/11/20	2/15/91/115	-
15	CLA	B	832	2	1/1/13/20	8/27/103/115	-
18	BCR	O	847	-	-	1/29/63/63	0/2/2/2
14	F6C	b	840	24	1/1/10/16	13/41/97/97	-
15	CLA	b	829	2	1/1/15/20	11/39/115/115	-
14	F6C	W	1503	24	1/1/10/16	14/41/97/97	-
15	CLA	N	819	1	1/1/15/20	12/39/115/115	-
15	CLA	A	815	1	1/1/13/20	4/27/103/115	-
15	CLA	A	820	1	1/1/15/20	19/39/115/115	-
18	BCR	b	848	-	-	3/29/63/63	0/2/2/2
15	CLA	b	811	2	1/1/15/20	10/39/115/115	-
18	BCR	M	101	-	-	6/29/63/63	0/2/2/2
15	CLA	B	834	24	1/1/11/20	9/15/91/115	-
15	CLA	O	821	2	1/1/11/20	4/15/91/115	-
15	CLA	N	814	1	1/1/15/20	9/39/115/115	-
20	LMT	a	854	-	-	4/21/61/61	0/2/2/2
15	CLA	N	818	1	1/1/15/20	19/39/115/115	-
14	F6C	A	802	24	1/1/10/16	9/41/97/97	-
15	CLA	b	808	2	1/1/15/20	12/39/115/115	-
15	CLA	A	819	1	1/1/15/20	11/39/115/115	-
15	CLA	A	809	1	1/1/14/20	10/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	818	2	1/1/14/20	13/33/109/115	-
15	CLA	B	817	24	1/1/15/20	10/39/115/115	-
15	CLA	a	840	1	1/1/12/20	0/21/97/115	-
15	CLA	A	807	1	1/1/15/20	18/39/115/115	-
15	CLA	N	820	1	1/1/15/20	19/39/115/115	-
16	PQN	B	840	-	-	0/23/43/43	0/2/2/2
15	CLA	N	828	1	1/1/15/20	5/39/115/115	-
16	PQN	A	843	-	-	0/23/43/43	0/2/2/2
15	CLA	B	830	2	1/1/15/20	12/39/115/115	-
18	BCR	A	847	-	-	6/29/63/63	0/2/2/2
15	CLA	B	828	2	1/1/15/20	19/39/115/115	-
20	LMT	A	853	-	-	10/14/54/61	0/2/2/2
14	F6C	b	810	2	1/1/10/16	8/41/97/97	-
15	CLA	O	801	2	1/1/15/20	11/39/115/115	-
22	LFA	B	848	-	-	6/13/13/17	-
18	BCR	A	858	-	-	9/29/63/63	0/2/2/2
15	CLA	b	841	2	1/1/15/20	14/39/115/115	-
15	CLA	a	814	1	1/1/15/20	8/39/115/115	-
15	CLA	B	819	2	1/1/11/20	4/15/91/115	-
19	LHG	Y	101	-	-	17/53/53/53	-
15	CLA	O	823	2	1/1/13/20	10/27/103/115	-
15	CLA	B	803	2	1/1/15/20	8/39/115/115	-
14	F6C	j	204	24	1/1/10/16	13/41/97/97	-
17	SF4	A	844	2,1	-	-	0/6/5/5
15	CLA	A	810	1	1/1/13/20	7/30/106/115	-
15	CLA	B	805	2	1/1/15/20	17/39/115/115	-
15	CLA	O	829	2	1/1/15/20	11/39/115/115	-
15	CLA	B	822	24	1/1/15/20	9/39/115/115	-
20	LMT	N	853	-	-	10/14/54/61	0/2/2/2
18	BCR	A	846	-	-	8/29/63/63	0/2/2/2
15	CLA	O	809	2	1/1/15/20	15/39/115/115	-
15	CLA	a	841	1	1/1/15/20	14/39/115/115	-
15	CLA	O	831	2	1/1/15/20	15/39/115/115	-
15	CLA	A	838	1	1/1/13/20	9/27/103/115	-
15	CLA	A	823	1	1/1/13/20	5/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	839	1	1/1/15/20	16/39/115/115	-
18	BCR	U	101	-	-	7/29/63/63	0/2/2/2
15	CLA	b	819	24	1/1/15/20	9/39/115/115	-
14	F6C	O	833	2	1/1/10/16	5/41/97/97	-
15	CLA	j	203	10	1/1/14/20	13/33/109/115	-
19	LHG	A	851	-	-	11/46/46/53	-
18	BCR	b	844	-	-	5/29/63/63	0/2/2/2
15	CLA	N	832	1	1/1/12/20	3/21/97/115	-
15	CLA	a	817	24	1/1/11/20	5/15/91/115	-
15	CLA	A	832	1	1/1/12/20	3/21/97/115	-
14	F6C	A	857	24	1/1/10/16	18/41/97/97	-
14	F6C	a	856	24	1/1/10/16	18/41/97/97	-
15	CLA	O	838	2	1/1/15/20	10/39/115/115	-
15	CLA	b	814	2	1/1/15/20	14/39/115/115	-
18	BCR	j	205	-	-	4/29/63/63	0/2/2/2
15	CLA	b	817	2	1/1/15/20	11/39/115/115	-
15	CLA	a	828	1	1/1/15/20	7/39/115/115	-
18	BCR	N	846	-	-	8/29/63/63	0/2/2/2
21	LMG	g	103	-	-	14/32/52/70	0/1/1/1
18	BCR	b	843	-	-	3/29/63/63	0/2/2/2
15	CLA	O	834	2	1/1/13/20	8/27/103/115	-
13	CL0	N	801	1	3/3/20/25	11/37/135/135	-
15	CLA	b	828	2	1/1/15/20	10/39/115/115	-
15	CLA	B	809	2	1/1/15/20	10/39/115/115	-
15	CLA	a	821	1	1/1/14/20	7/33/109/115	-
13	CL0	A	801	1	3/3/20/25	9/37/135/135	-
15	CLA	a	827	24	1/1/13/20	1/27/103/115	-
18	BCR	b	845	-	-	4/29/63/63	0/2/2/2
15	CLA	B	818	2	1/1/13/20	11/27/103/115	-
15	CLA	b	803	-	1/1/15/20	7/39/115/115	-
15	CLA	b	825	24	1/1/15/20	14/39/115/115	-
15	CLA	N	831	1	1/1/15/20	13/39/115/115	-
15	CLA	a	836	1	1/1/12/20	6/26/102/115	-
17	SF4	P	101	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	b	805	2	1/1/15/20	11/39/115/115	-
14	F6C	B	831	2	1/1/10/16	7/41/97/97	-
15	CLA	b	830	2	1/1/15/20	17/39/115/115	-
15	CLA	b	826	2	1/1/15/20	5/39/115/115	-
15	CLA	B	801	2	1/1/15/20	10/39/115/115	-
15	CLA	O	813	2	-	9/29/105/115	-
21	LMG	U	102	-	-	19/50/70/70	0/1/1/1
15	CLA	B	825	2	1/1/14/20	13/36/112/115	-
15	CLA	N	840	1	1/1/12/20	0/21/97/115	-
19	LHG	M	102	-	-	17/53/53/53	-
15	CLA	O	814	2	1/1/15/20	14/39/115/115	-
17	SF4	C	102	3	-	-	0/6/5/5
14	F6C	L	204	24	1/1/10/16	11/41/97/97	-
18	BCR	a	848	-	-	6/29/63/63	0/2/2/2
21	LMG	A	855	-	-	10/39/59/70	0/1/1/1
18	BCR	b	846	-	-	5/29/63/63	0/2/2/2
18	BCR	B	841	-	-	3/29/63/63	0/2/2/2
15	CLA	b	821	2	1/1/11/20	5/15/91/115	-
19	LHG	a	851	-	-	12/46/46/53	-
15	CLA	N	811	1	1/1/13/20	11/30/106/115	-
15	CLA	b	816	2	1/1/13/20	7/30/106/115	-
18	BCR	a	850	-	-	13/29/63/63	0/2/2/2
14	F6C	O	840	24	1/1/10/16	13/41/97/97	-
14	F6C	B	838	24	1/1/10/16	13/41/97/97	-
15	CLA	A	805	15,1	1/1/14/20	9/33/109/115	-
15	CLA	B	836	2	1/1/15/20	12/39/115/115	-
15	CLA	N	839	1	1/1/15/20	19/39/115/115	-
18	BCR	k	102	-	-	7/29/63/63	0/2/2/2
15	CLA	a	804	1	1/1/15/20	6/39/115/115	-
15	CLA	O	803	-	1/1/15/20	6/39/115/115	-
18	BCR	B	843	-	-	4/29/63/63	0/2/2/2
18	BCR	h	101	-	-	7/29/63/63	0/2/2/2
15	CLA	N	810	1	1/1/13/20	6/30/106/115	-
15	CLA	O	841	2	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	a	842	1	1/1/15/20	12/39/115/115	-
15	CLA	B	810	2	1/1/11/20	5/15/91/115	-
15	CLA	a	820	1	1/1/15/20	20/39/115/115	-
14	F6C	N	856	24	1/1/10/16	17/41/97/97	-
19	LHG	X	102	-	-	22/53/53/53	-
15	CLA	A	834	1	1/1/15/20	6/39/115/115	-
15	CLA	X	103	12	1/1/13/20	2/27/103/115	-
15	CLA	f	201	24	1/1/15/20	10/39/115/115	-
15	CLA	b	818	2	1/1/14/20	12/33/109/115	-
15	CLA	b	836	24	1/1/11/20	8/15/91/115	-
19	LHG	N	851	-	-	12/46/46/53	-
15	CLA	N	813	1	1/1/12/20	8/26/102/115	-
15	CLA	B	827	2	1/1/15/20	11/39/115/115	-
15	CLA	O	805	2	1/1/15/20	10/39/115/115	-
15	CLA	O	822	24	1/1/12/20	8/25/101/115	-
18	BCR	L	209	-	-	2/29/63/63	0/2/2/2
15	CLA	B	826	2	1/1/15/20	7/39/115/115	-
15	CLA	A	829	1	1/1/14/20	15/33/109/115	-
15	CLA	B	814	2	1/1/13/20	5/30/106/115	-
17	SF4	P	102	3	-	-	0/6/5/5
14	F6C	N	824	24	1/1/7/16	11/25/81/97	-
15	CLA	A	811	1	1/1/13/20	10/30/106/115	-
18	BCR	T	102	-	-	4/29/63/63	0/2/2/2
15	CLA	b	809	2	1/1/15/20	15/39/115/115	-
19	LHG	l	102	-	-	23/53/53/53	-
15	CLA	b	815	2	1/1/11/20	6/15/91/115	-
15	CLA	A	831	1	1/1/15/20	12/39/115/115	-
15	CLA	B	802	-	1/1/15/20	7/39/115/115	-
13	CL0	a	801	1	3/3/20/25	10/37/135/135	-
18	BCR	A	848	-	-	6/29/63/63	0/2/2/2
15	CLA	i	103	24	1/1/12/20	2/21/97/115	-
19	LHG	X	101	-	-	21/48/48/53	-
15	CLA	b	820	2	1/1/13/20	13/27/103/115	-
18	BCR	a	847	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	A	828	1	1/1/15/20	5/39/115/115	-
15	CLA	A	835	1	1/1/15/20	6/39/115/115	-
18	BCR	B	846	-	-	4/29/63/63	0/2/2/2
15	CLA	V	102	9	1/1/11/20	8/15/91/115	-
15	CLA	O	806	2	1/1/15/20	16/39/115/115	-
15	CLA	b	804	2	1/1/15/20	8/39/115/115	-
15	CLA	i	102	9	1/1/11/20	6/15/91/115	-
15	CLA	K	102	9	1/1/11/20	6/15/91/115	-
15	CLA	B	811	2	-	9/29/105/115	-
18	BCR	B	844	-	-	8/29/63/63	0/2/2/2
20	LMT	A	852	-	-	1/17/57/61	0/2/2/2
15	CLA	L	202	10	1/1/15/20	7/39/115/115	-
15	CLA	B	820	24	1/1/12/20	10/25/101/115	-
18	BCR	F	202	-	-	6/29/63/63	0/2/2/2
15	CLA	L	203	10	1/1/14/20	12/33/109/115	-
21	LMG	L	206	-	-	12/45/65/70	0/1/1/1
16	PQN	b	842	-	-	0/23/43/43	0/2/2/2
15	CLA	N	807	1	1/1/15/20	19/39/115/115	-
15	CLA	B	807	2	1/1/15/20	10/39/115/115	-
15	CLA	O	811	2	1/1/15/20	9/39/115/115	-
15	CLA	A	842	1	1/1/15/20	11/39/115/115	-
18	BCR	N	857	-	-	9/29/63/63	0/2/2/2
15	CLA	Z	103	12	1/1/13/20	4/27/103/115	-
21	LMG	T	103	-	-	12/32/52/70	0/1/1/1
15	CLA	O	804	2	1/1/15/20	8/39/115/115	-
15	CLA	N	821	1	1/1/14/20	8/33/109/115	-
18	BCR	O	848	-	-	6/29/63/63	0/2/2/2
15	CLA	B	839	2	1/1/15/20	15/39/115/115	-
18	BCR	J	101	-	-	6/29/63/63	0/2/2/2
19	LHG	k	101	-	-	18/53/53/53	-
15	CLA	O	812	2	1/1/11/20	5/15/91/115	-
18	BCR	K	101	-	-	0/18/35/63	0/1/1/2
21	LMG	J	102	-	-	19/50/70/70	0/1/1/1
15	CLA	O	807	2	1/1/15/20	6/39/115/115	-
15	CLA	O	825	24	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	CLA	O	837	2	1/1/15/20	9/39/115/115	-
15	CLA	b	824	24	1/1/15/20	9/39/115/115	-
15	CLA	N	804	1	1/1/15/20	6/39/115/115	-
15	CLA	b	838	2	1/1/15/20	13/39/115/115	-
14	F6C	L	201	2	1/1/10/16	9/41/97/97	-
15	CLA	a	834	1	1/1/15/20	8/39/115/115	-
15	CLA	O	826	2	1/1/15/20	4/39/115/115	-
15	CLA	b	839	2	1/1/15/20	9/39/115/115	-
15	CLA	O	808	2	1/1/15/20	8/39/115/115	-
18	BCR	f	202	-	-	6/29/63/63	0/2/2/2
15	CLA	A	817	24	1/1/11/20	6/15/91/115	-
15	CLA	A	822	24	1/1/15/20	17/39/115/115	-
15	CLA	a	837	1	1/1/12/20	7/23/99/115	-
15	CLA	N	803	-	1/1/15/20	11/39/115/115	-
15	CLA	B	824	2	1/1/15/20	4/39/115/115	-
15	CLA	B	823	24	1/1/15/20	15/39/115/115	-

The worst 5 of 2175 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	9.00	1.49	1.39
13	N	801	CL0	C1B-C2B	8.99	1.49	1.39
13	a	801	CL0	C1B-C2B	8.99	1.49	1.39
14	N	826	F6C	C2A-C3A	8.63	1.55	1.36
14	L	201	F6C	C2A-C3A	8.59	1.55	1.36

The worst 5 of 1961 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	O	840	F6C	CAA-C2A-C3A	-10.01	109.11	127.87
14	B	838	F6C	CAA-C2A-C3A	-10.00	109.14	127.87
14	b	840	F6C	CAA-C2A-C3A	-9.96	109.21	127.87
14	L	204	F6C	CAA-C2A-C3A	-9.94	109.25	127.87
14	j	204	F6C	CAA-C2A-C3A	-9.90	109.33	127.87

5 of 276 chirality outliers are listed below:

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

5 of 3474 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	F6C	C1B-C2B-CMB-OMB
14	A	802	F6C	C3B-C2B-CMB-OMB
14	A	824	F6C	C1B-C2B-CMB-OMB
14	A	824	F6C	C3B-C2B-CMB-OMB
14	A	826	F6C	CHA-CBD-CGD-O1D

There are no ring outliers.

343 monomers are involved in 870 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	821	CLA	5	0
18	g	101	BCR	3	0
22	L	208	LFA	1	0
15	N	816	CLA	2	0
15	N	827	CLA	2	0
15	a	807	CLA	3	0
15	N	829	CLA	3	0
15	b	837	CLA	4	0
15	F	201	CLA	1	0
15	B	816	CLA	3	0
15	a	823	CLA	5	0
15	j	202	CLA	2	0
15	B	829	CLA	4	0
18	N	848	BCR	2	0
15	b	802	CLA	6	0
22	f	204	LFA	1	0
15	A	803	CLA	7	0
15	a	806	CLA	7	0
15	N	815	CLA	2	0
15	A	813	CLA	2	0
18	O	849	BCR	4	0
18	a	857	BCR	4	0
18	O	844	BCR	2	0
20	A	854	LMT	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	O	810	F6C	2	0
22	j	208	LFA	2	0
15	A	856	CLA	5	0
15	N	822	CLA	3	0
22	W	1507	LFA	1	0
15	N	838	CLA	2	0
15	O	820	CLA	2	0
15	a	808	CLA	1	0
15	N	805	CLA	1	0
21	O	850	LMG	5	0
15	a	829	CLA	5	0
21	a	855	LMG	1	0
15	a	831	CLA	2	0
15	a	811	CLA	3	0
15	B	804	CLA	5	0
15	N	812	CLA	2	0
15	A	816	CLA	3	0
20	N	854	LMT	1	0
15	A	806	CLA	10	0
18	F	203	BCR	6	0
15	b	827	CLA	8	0
15	O	817	CLA	4	0
19	l	101	LHG	2	0
18	N	845	BCR	4	0
15	A	833	CLA	2	0
18	T	101	BCR	2	0
18	N	849	BCR	1	0
15	O	830	CLA	9	0
18	a	849	BCR	1	0
21	W	1505	LMG	4	0
20	a	852	LMT	1	0
15	A	840	CLA	2	0
18	g	102	BCR	1	0
18	O	845	BCR	4	0
15	N	823	CLA	4	0
15	N	842	CLA	1	0
15	O	828	CLA	1	0
15	B	813	CLA	1	0
15	N	809	CLA	1	0
22	O	851	LFA	1	0
14	b	833	F6C	1	0
15	a	813	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	L	207	LHG	5	0
15	A	841	CLA	7	0
16	O	842	PQN	1	0
15	N	833	CLA	2	0
18	a	845	BCR	5	0
15	N	834	CLA	2	0
18	Y	102	BCR	4	0
18	I	101	BCR	3	0
15	a	822	CLA	6	0
21	I	103	LMG	3	0
15	A	837	CLA	2	0
16	a	843	PQN	1	0
15	a	803	CLA	7	0
15	b	807	CLA	3	0
15	B	815	CLA	6	0
15	a	838	CLA	2	0
15	b	812	CLA	1	0
18	N	850	BCR	7	0
18	b	847	BCR	5	0
15	a	830	CLA	3	0
15	O	824	CLA	1	0
18	B	842	BCR	1	0
18	W	1508	BCR	2	0
18	B	845	BCR	5	0
15	A	814	CLA	6	0
15	O	816	CLA	3	0
20	N	852	LMT	1	0
17	c	102	SF4	1	0
15	B	835	CLA	3	0
15	a	819	CLA	7	0
15	W	1502	CLA	2	0
15	N	841	CLA	3	0
15	S	201	CLA	1	0
15	N	837	CLA	2	0
15	N	808	CLA	2	0
18	j	201	BCR	5	0
18	O	843	BCR	3	0
18	A	845	BCR	7	0
15	N	806	CLA	7	0
15	a	805	CLA	1	0
15	B	806	CLA	2	0
15	O	819	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	L	205	BCR	1	0
21	h	102	LMG	3	0
15	A	825	CLA	2	0
15	a	835	CLA	1	0
18	I	102	BCR	2	0
15	A	839	CLA	2	0
15	O	827	CLA	5	0
18	a	846	BCR	1	0
15	O	836	CLA	1	0
15	b	822	CLA	2	0
15	A	812	CLA	3	0
15	a	816	CLA	3	0
19	Z	101	LHG	2	0
15	A	821	CLA	3	0
15	B	833	CLA	3	0
18	A	850	BCR	10	0
15	O	815	CLA	2	0
15	N	830	CLA	2	0
18	S	202	BCR	5	0
15	A	804	CLA	5	0
15	b	835	CLA	4	0
15	A	830	CLA	4	0
15	B	837	CLA	8	0
21	b	849	LMG	5	0
18	f	203	BCR	4	0
15	a	818	CLA	7	0
15	N	835	CLA	1	0
15	B	808	CLA	8	0
18	i	101	BCR	1	0
15	O	832	CLA	6	0
21	j	206	LMG	2	0
15	N	825	CLA	1	0
15	a	815	CLA	2	0
15	W	1501	CLA	1	0
15	a	809	CLA	3	0
18	W	1504	BCR	1	0
21	B	847	LMG	4	0
15	l	103	CLA	2	0
19	W	1506	LHG	5	0
15	b	823	CLA	5	0
15	b	813	CLA	5	0
15	B	812	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	A	827	CLA	1	0
15	O	839	CLA	8	0
15	O	802	CLA	6	0
15	b	832	CLA	6	0
15	a	833	CLA	2	0
15	a	810	CLA	4	0
15	b	831	CLA	4	0
15	a	812	CLA	2	0
15	b	806	CLA	6	0
15	A	818	CLA	7	0
19	j	207	LHG	5	0
15	b	801	CLA	1	0
16	N	843	PQN	1	0
19	Z	102	LHG	2	0
18	N	847	BCR	3	0
15	O	835	CLA	4	0
15	B	832	CLA	1	0
18	O	847	BCR	3	0
15	b	829	CLA	4	0
15	N	819	CLA	6	0
15	A	815	CLA	2	0
15	A	820	CLA	8	0
18	b	848	BCR	4	0
15	b	811	CLA	3	0
18	M	101	BCR	4	0
15	B	834	CLA	1	0
15	O	821	CLA	3	0
15	N	814	CLA	6	0
20	a	854	LMT	1	0
15	N	818	CLA	7	0
15	b	808	CLA	6	0
15	A	819	CLA	7	0
15	A	809	CLA	5	0
15	O	818	CLA	1	0
15	B	817	CLA	4	0
15	a	840	CLA	1	0
15	A	807	CLA	4	0
15	N	820	CLA	7	0
16	B	840	PQN	1	0
15	N	828	CLA	1	0
16	A	843	PQN	1	0
15	B	830	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	A	847	BCR	3	0
15	B	828	CLA	7	0
14	b	810	F6C	2	0
15	O	801	CLA	2	0
22	B	848	LFA	1	0
18	A	858	BCR	4	0
15	b	841	CLA	1	0
15	a	814	CLA	6	0
15	B	819	CLA	2	0
19	Y	101	LHG	5	0
15	O	823	CLA	1	0
15	B	803	CLA	5	0
14	j	204	F6C	1	0
15	A	810	CLA	5	0
15	B	805	CLA	5	0
15	O	829	CLA	4	0
15	B	822	CLA	3	0
18	A	846	BCR	2	0
15	O	809	CLA	8	0
15	a	841	CLA	5	0
15	O	831	CLA	3	0
15	A	838	CLA	1	0
15	A	823	CLA	4	0
15	a	839	CLA	2	0
15	b	819	CLA	3	0
14	O	833	F6C	1	0
15	j	203	CLA	2	0
15	O	838	CLA	6	0
15	b	814	CLA	3	0
18	j	205	BCR	1	0
15	b	817	CLA	4	0
15	a	828	CLA	1	0
21	g	103	LMG	3	0
18	b	843	BCR	3	0
15	O	834	CLA	1	0
13	N	801	CL0	2	0
15	b	828	CLA	2	0
15	B	809	CLA	2	0
15	a	821	CLA	2	0
13	A	801	CL0	3	0
15	a	827	CLA	1	0
18	b	845	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	B	818	CLA	3	0
15	b	803	CLA	6	0
15	b	825	CLA	6	0
15	N	831	CLA	1	0
15	b	805	CLA	4	0
14	B	831	F6C	1	0
15	b	830	CLA	9	0
15	b	826	CLA	2	0
15	B	801	CLA	2	0
15	O	813	CLA	4	0
21	U	102	LMG	3	0
15	B	825	CLA	5	0
15	N	840	CLA	3	0
19	M	102	LHG	5	0
15	O	814	CLA	3	0
18	a	848	BCR	1	0
21	A	855	LMG	1	0
18	b	846	BCR	1	0
18	B	841	BCR	2	0
15	b	821	CLA	3	0
15	N	811	CLA	4	0
15	b	816	CLA	1	0
18	a	850	BCR	7	0
15	A	805	CLA	1	0
15	B	836	CLA	8	0
15	N	839	CLA	2	0
18	k	102	BCR	3	0
15	a	804	CLA	3	0
15	O	803	CLA	9	0
18	B	843	BCR	5	0
18	h	101	BCR	1	0
15	N	810	CLA	5	0
15	O	841	CLA	2	0
15	a	842	CLA	1	0
15	B	810	CLA	1	0
15	a	820	CLA	5	0
15	A	834	CLA	1	0
15	X	103	CLA	3	0
15	f	201	CLA	2	0
15	b	818	CLA	2	0
15	b	836	CLA	1	0
15	N	813	CLA	3	0

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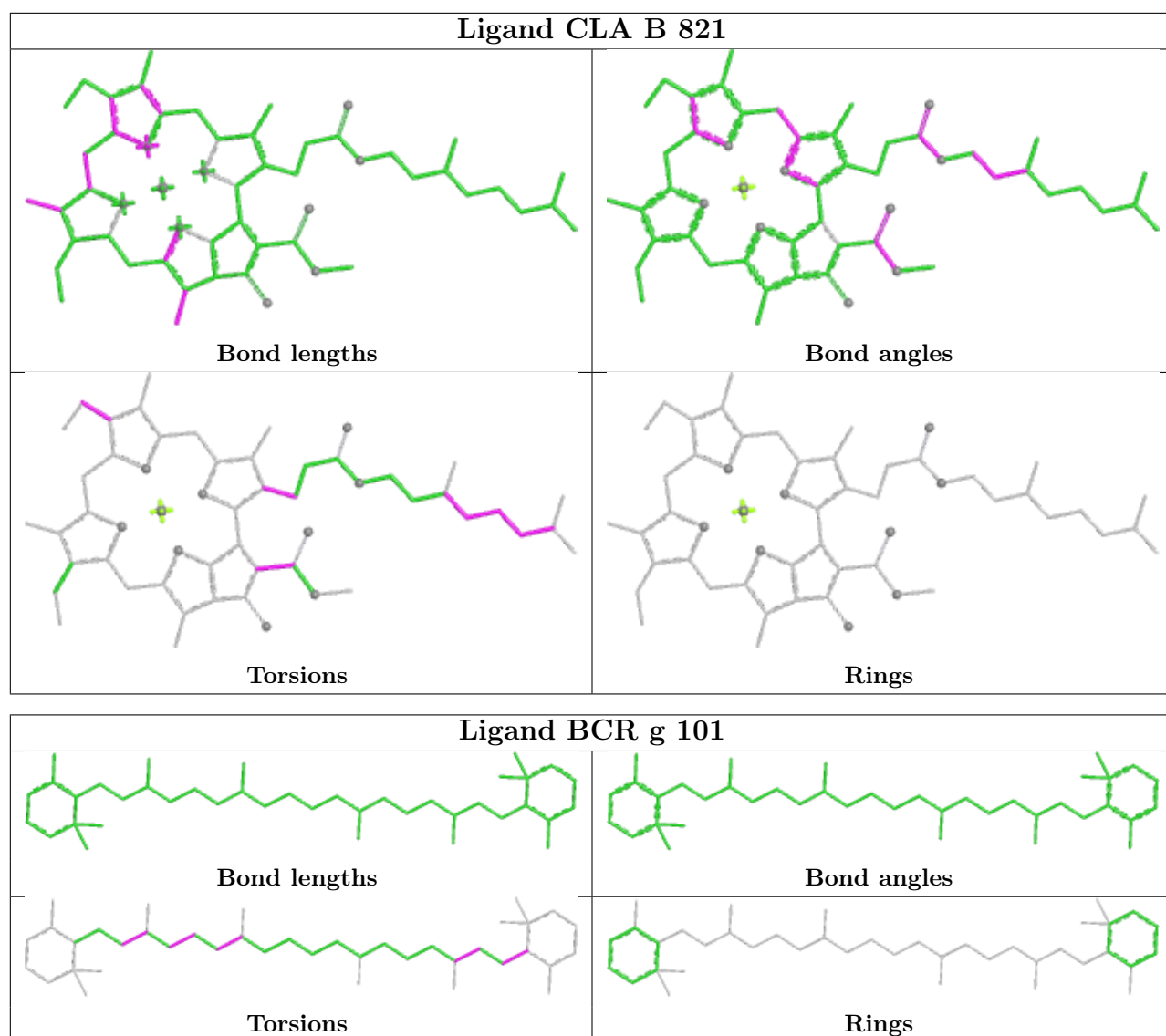
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15	O	805	CLA	3	0
15	O	822	CLA	1	0
18	L	209	BCR	4	0
15	A	829	CLA	4	0
15	B	814	CLA	1	0
17	P	102	SF4	1	0
15	A	811	CLA	2	0
18	T	102	BCR	1	0
15	b	809	CLA	8	0
19	l	102	LHG	2	0
15	b	815	CLA	2	0
15	A	831	CLA	3	0
15	B	802	CLA	6	0
13	a	801	CL0	2	0
18	A	848	BCR	3	0
19	X	101	LHG	3	0
15	b	820	CLA	2	0
18	a	847	BCR	1	0
15	A	828	CLA	2	0
15	A	835	CLA	2	0
18	B	846	BCR	3	0
15	V	102	CLA	1	0
15	O	806	CLA	5	0
15	b	804	CLA	5	0
15	i	102	CLA	1	0
15	K	102	CLA	1	0
15	B	811	CLA	7	0
20	A	852	LMT	2	0
15	L	202	CLA	1	0
15	B	820	CLA	1	0
18	F	202	BCR	3	0
15	L	203	CLA	3	0
21	L	206	LMG	4	0
16	b	842	PQN	3	0
15	N	807	CLA	4	0
15	B	807	CLA	4	0
15	O	811	CLA	1	0
15	A	842	CLA	4	0
18	N	857	BCR	6	0
15	Z	103	CLA	2	0
21	T	103	LMG	5	0

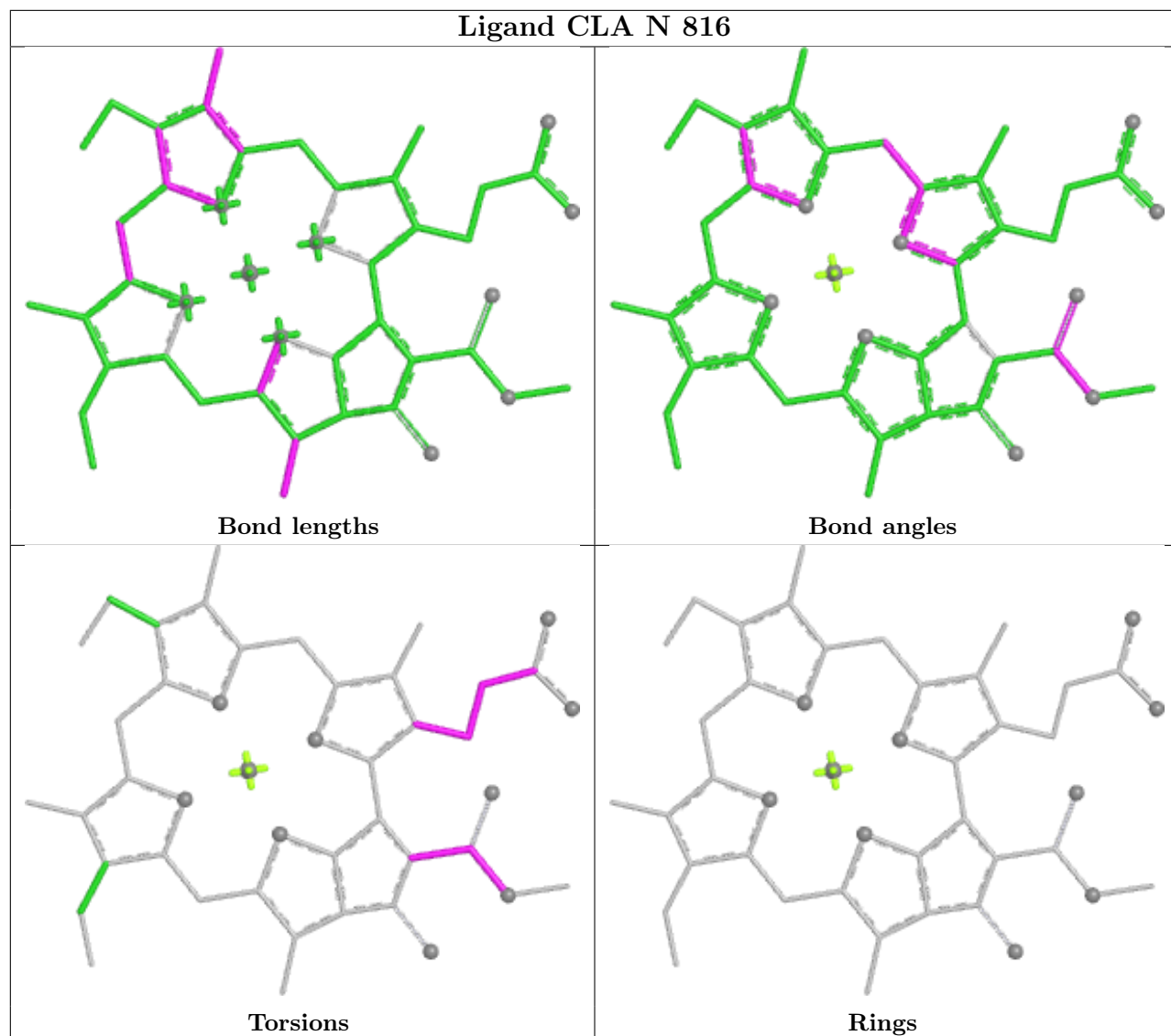
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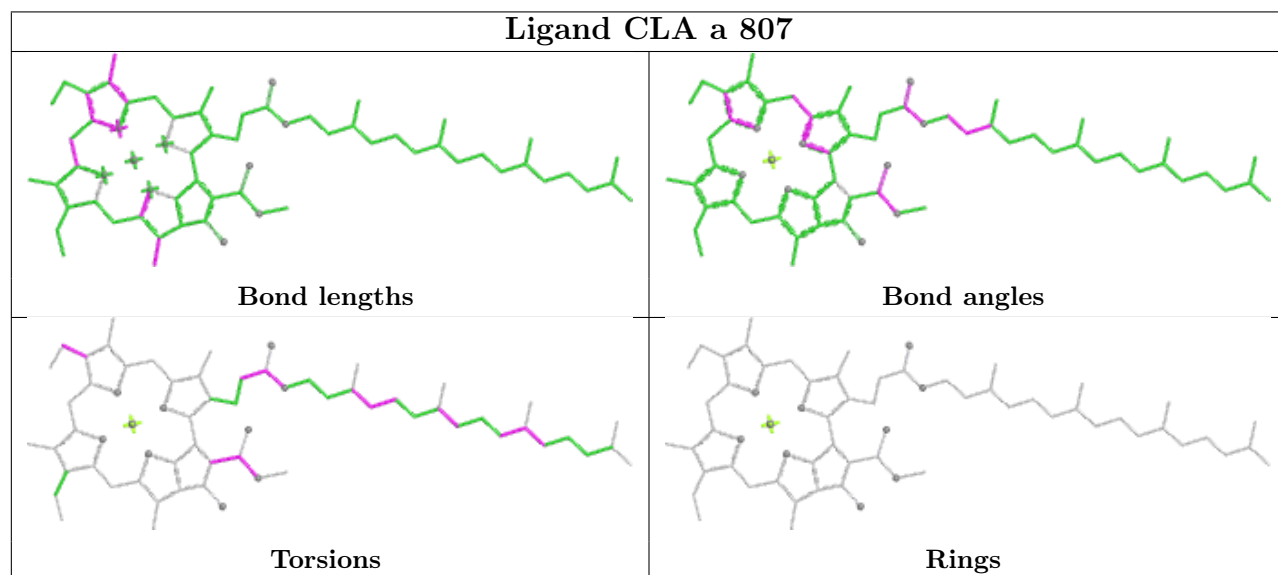
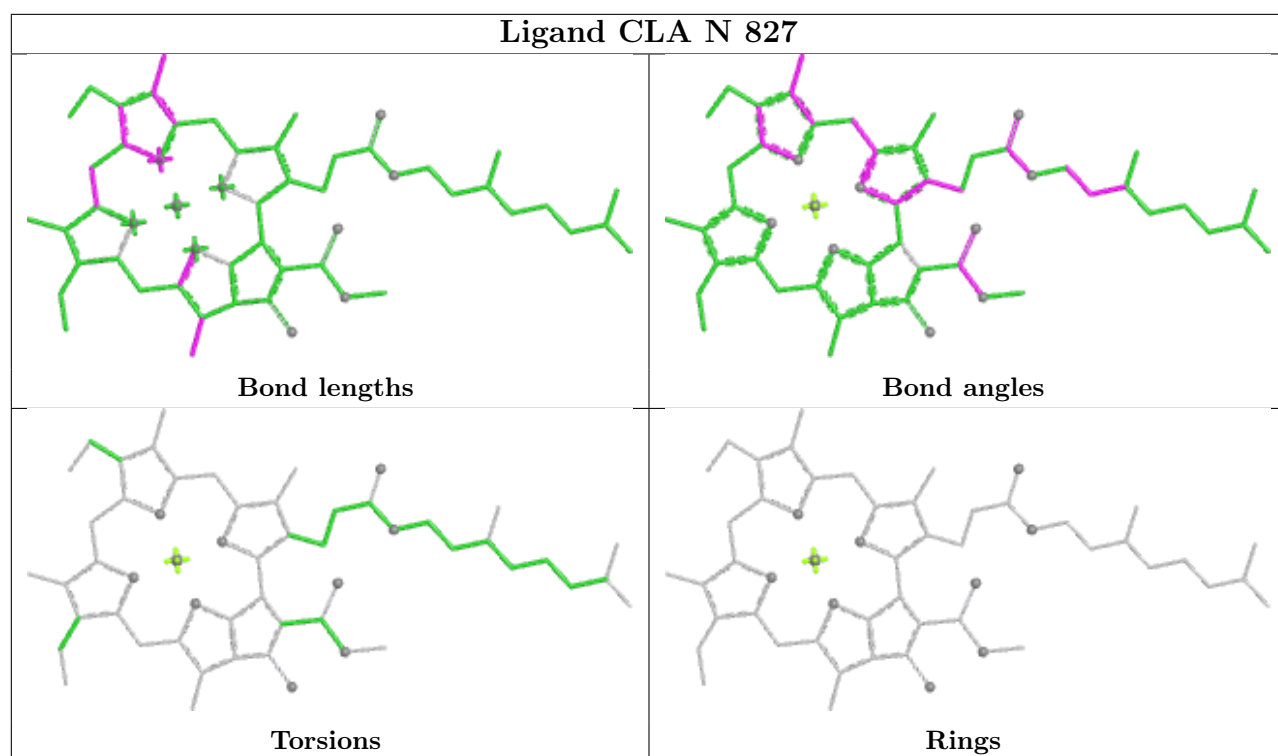
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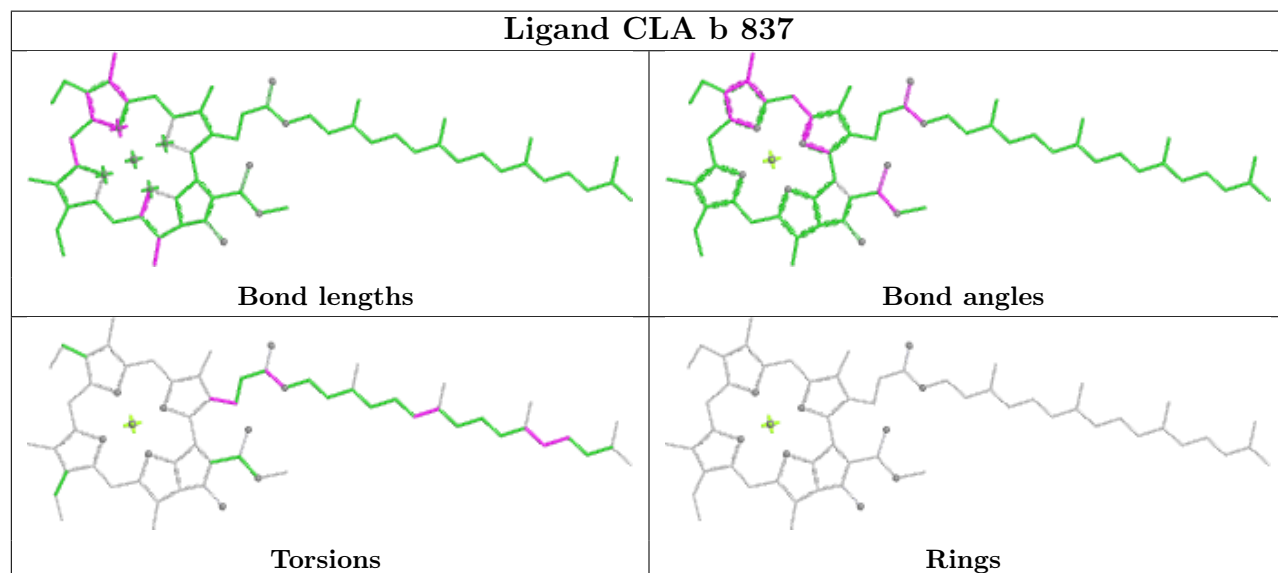
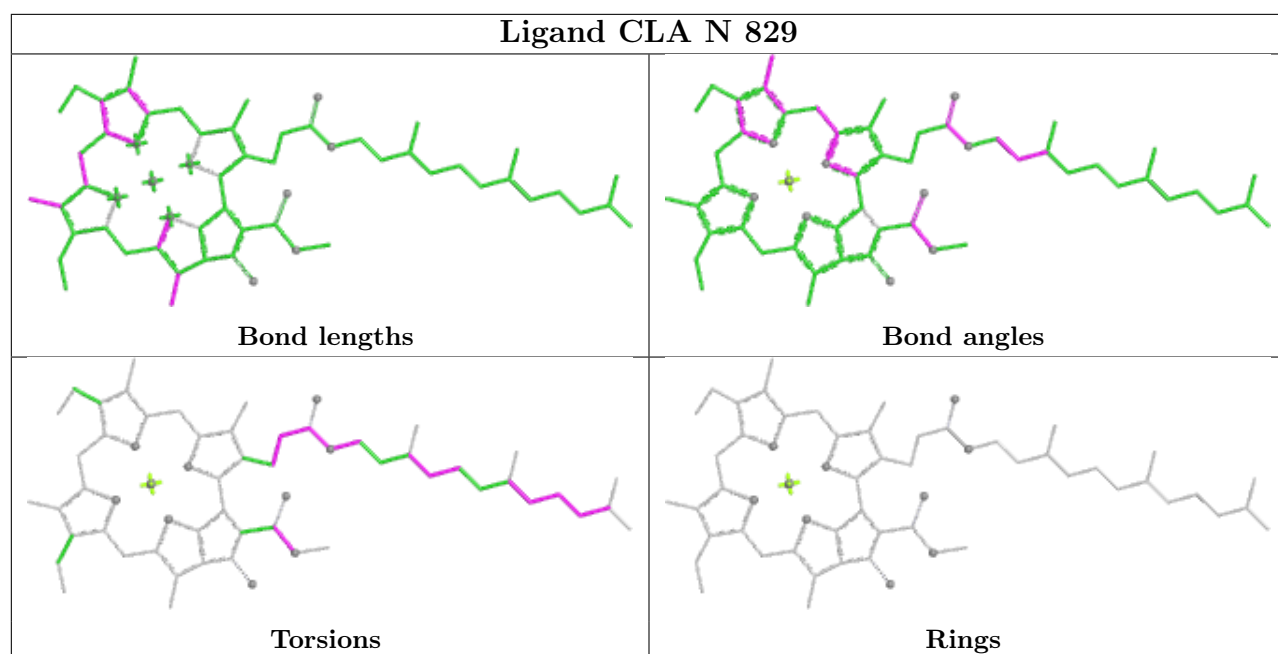
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15	O	804	CLA	5	0
15	N	821	CLA	2	0
18	O	848	BCR	2	0
15	B	839	CLA	2	0
18	J	101	BCR	1	0
19	k	101	LHG	5	0
15	O	812	CLA	1	0
21	J	102	LMG	1	0
15	O	807	CLA	2	0
15	O	825	CLA	7	0
15	O	837	CLA	5	0
15	b	824	CLA	3	0
15	N	804	CLA	4	0
15	b	838	CLA	8	0
14	L	201	F6C	2	0
15	a	834	CLA	3	0
15	O	826	CLA	2	0
15	b	839	CLA	7	0
15	O	808	CLA	7	0
18	f	202	BCR	2	0
15	A	822	CLA	1	0
15	a	837	CLA	1	0
15	N	803	CLA	9	0
15	B	824	CLA	1	0
15	B	823	CLA	5	0

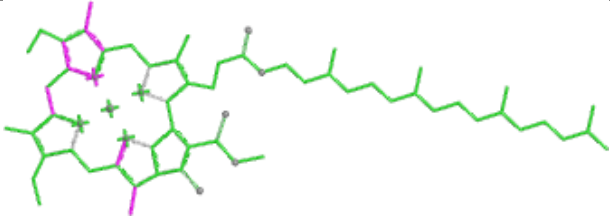
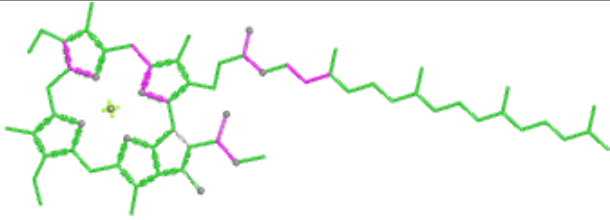
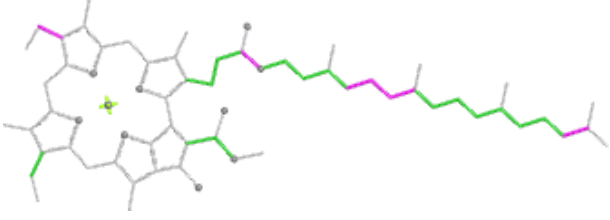
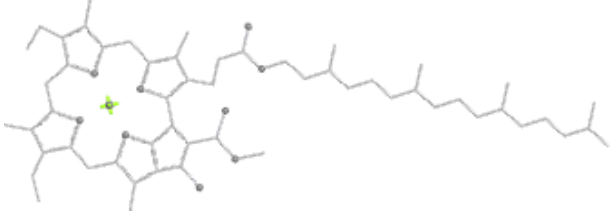
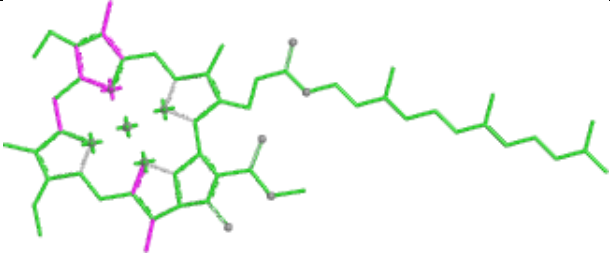
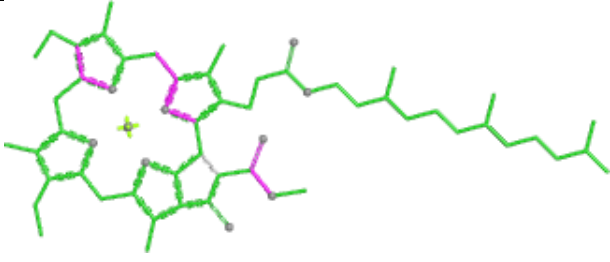
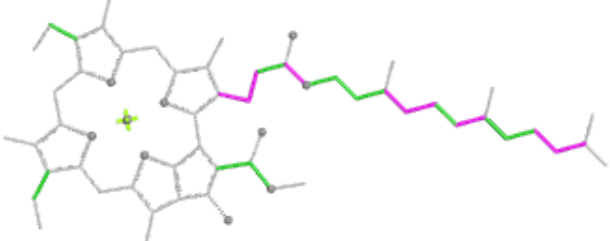
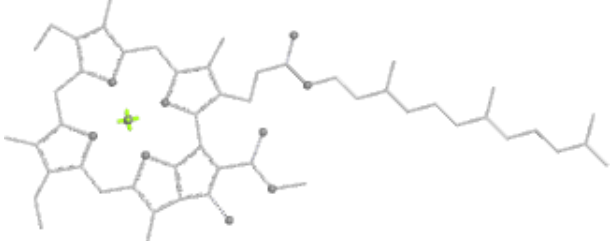
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

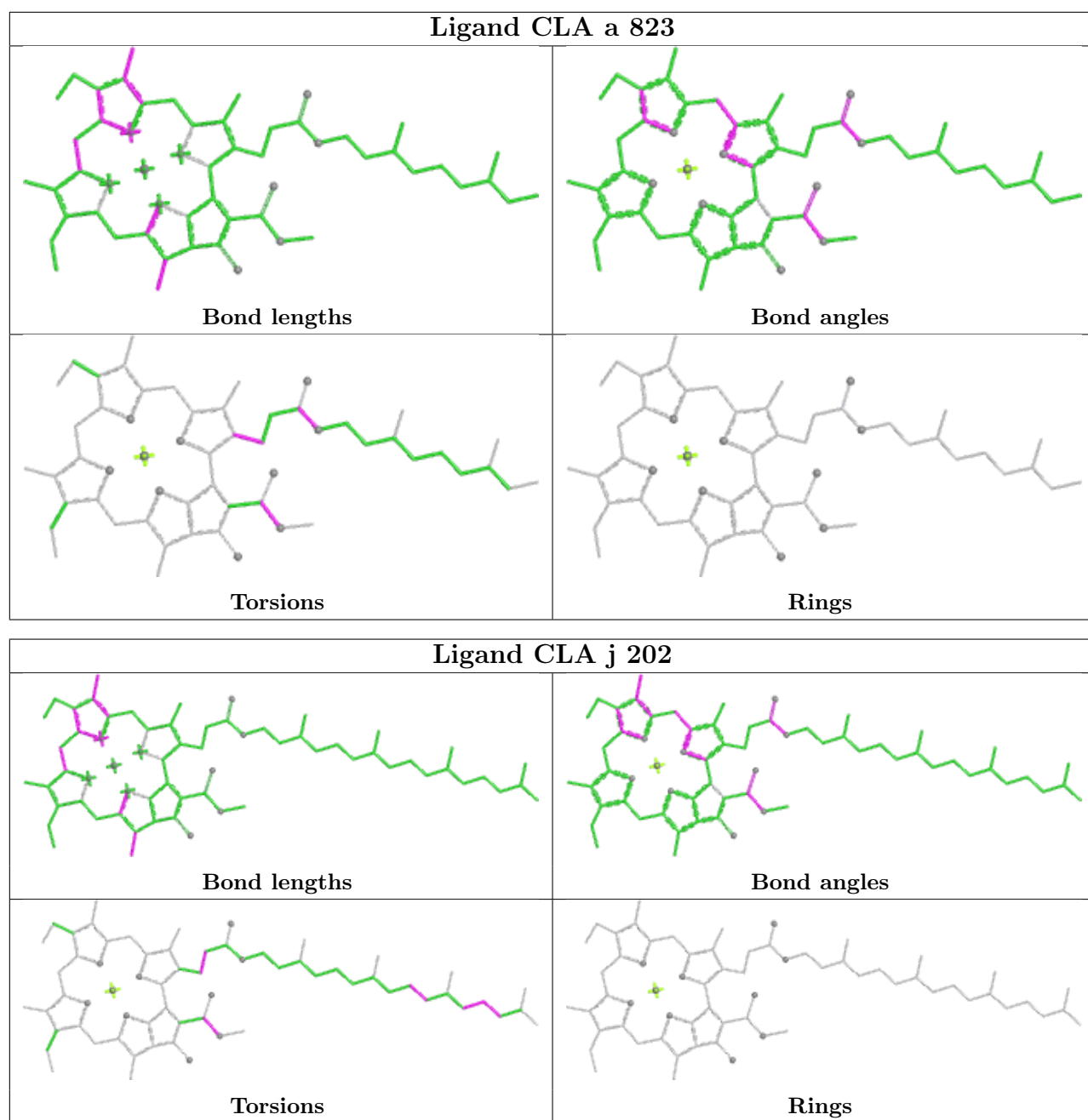


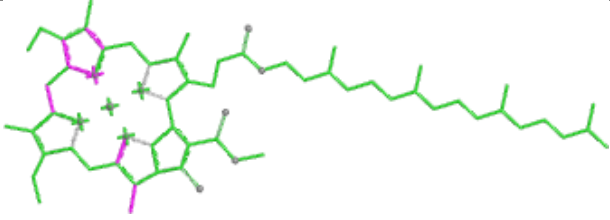
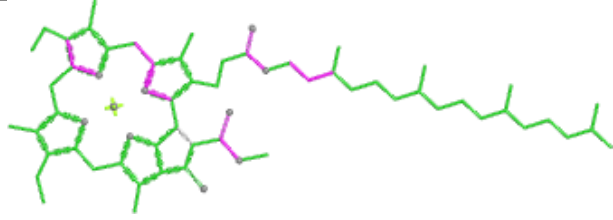
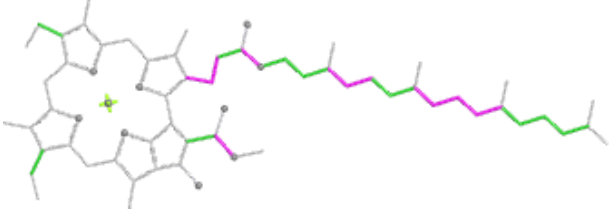
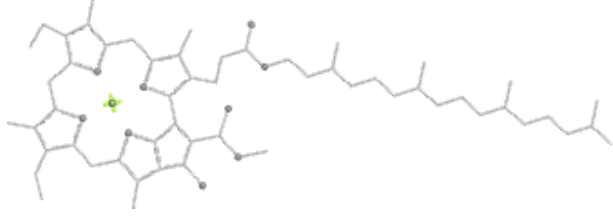
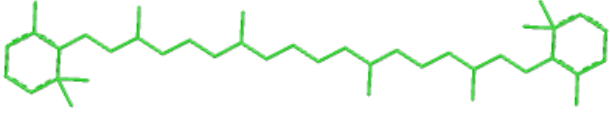
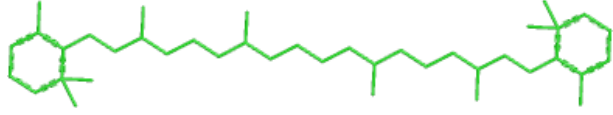
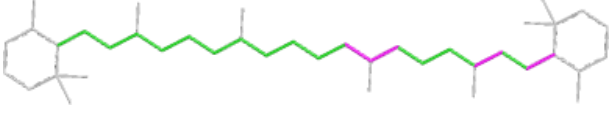
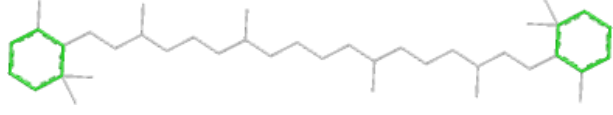


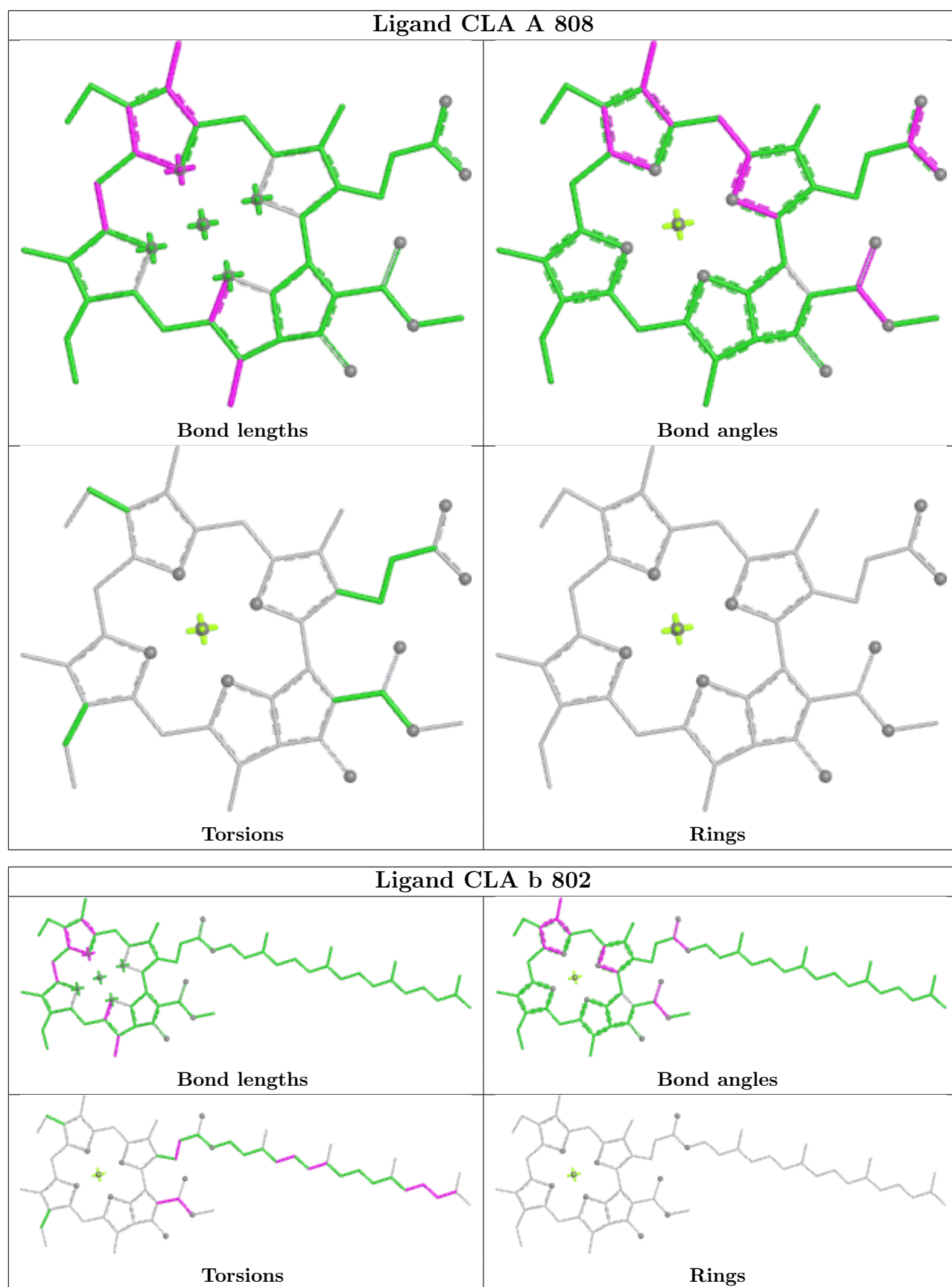


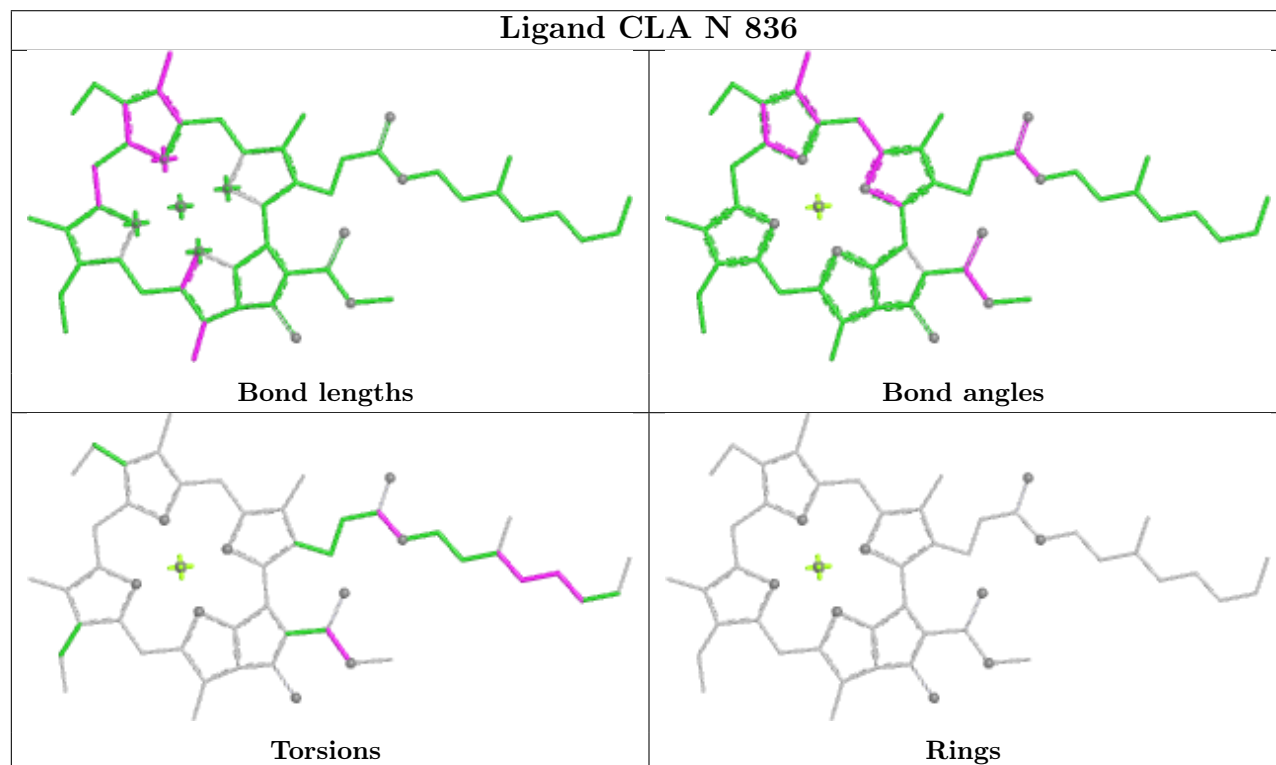
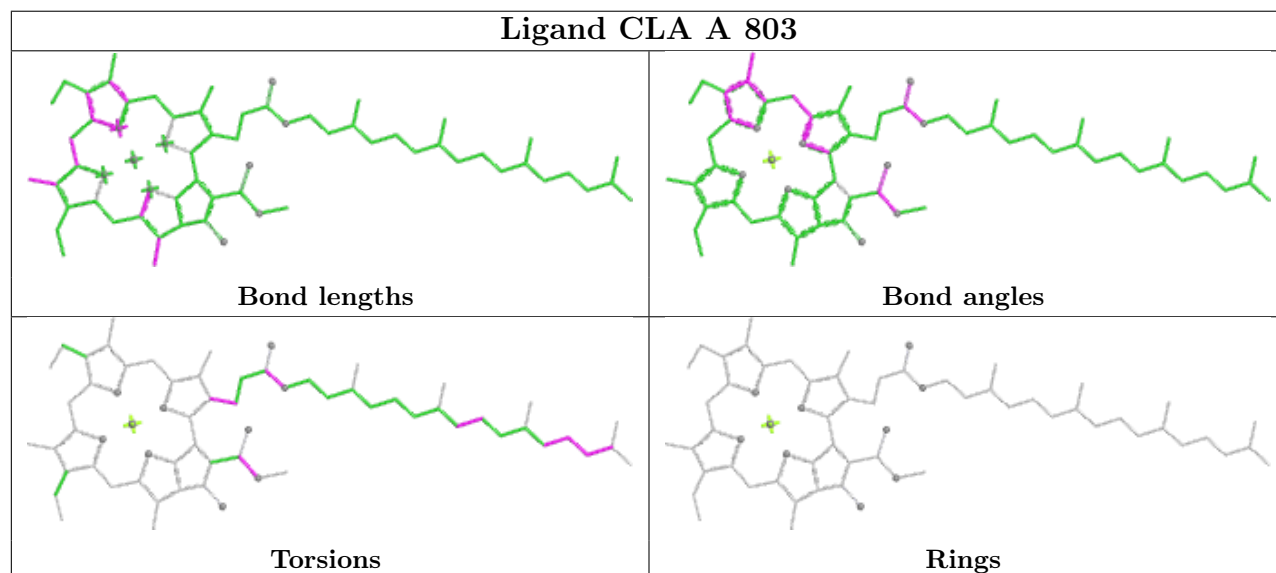
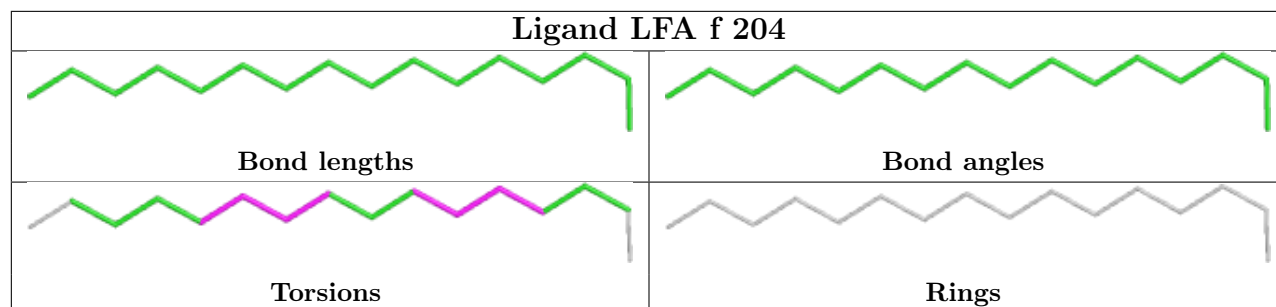


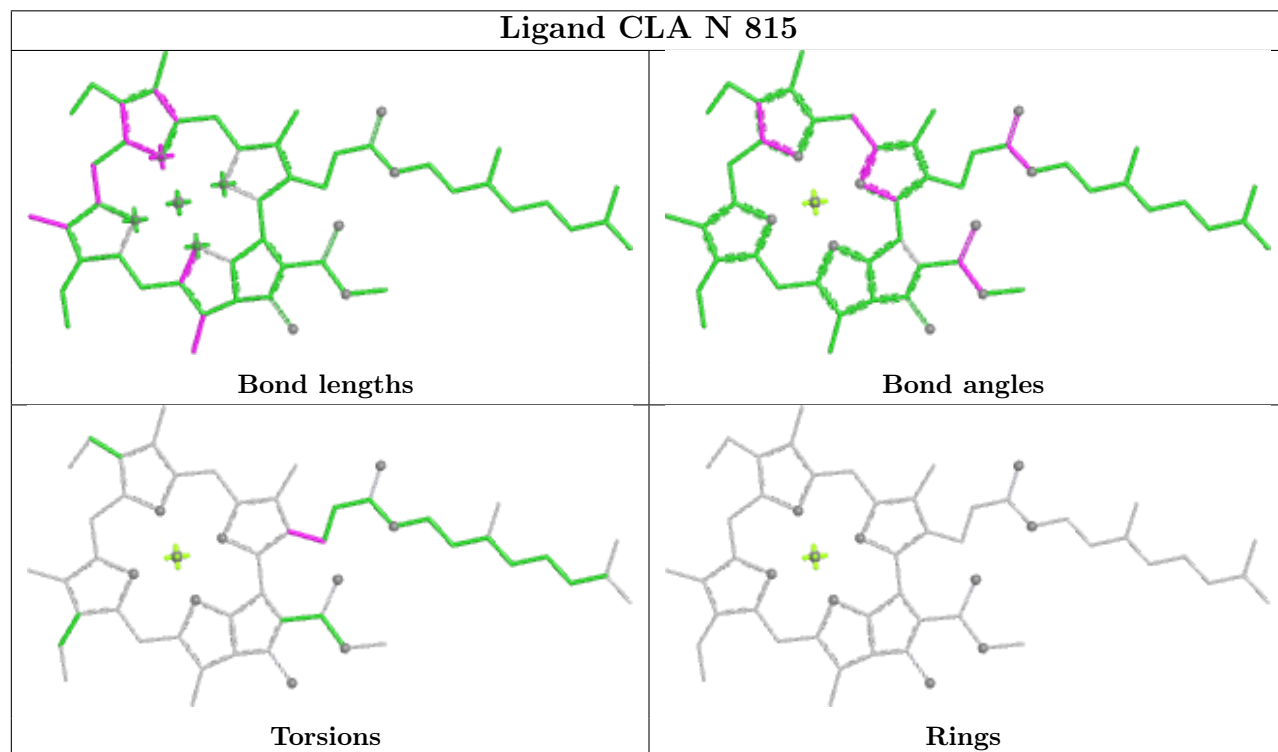
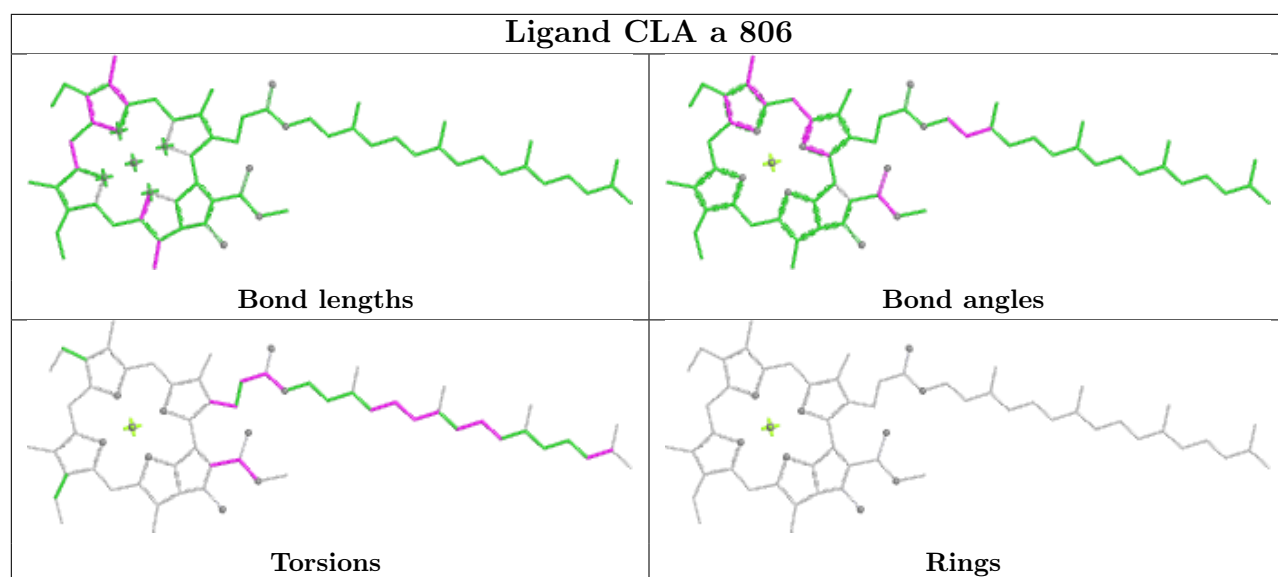
Ligand CLA F 201	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 816	
 Bond lengths	 Bond angles
 Torsions	 Rings

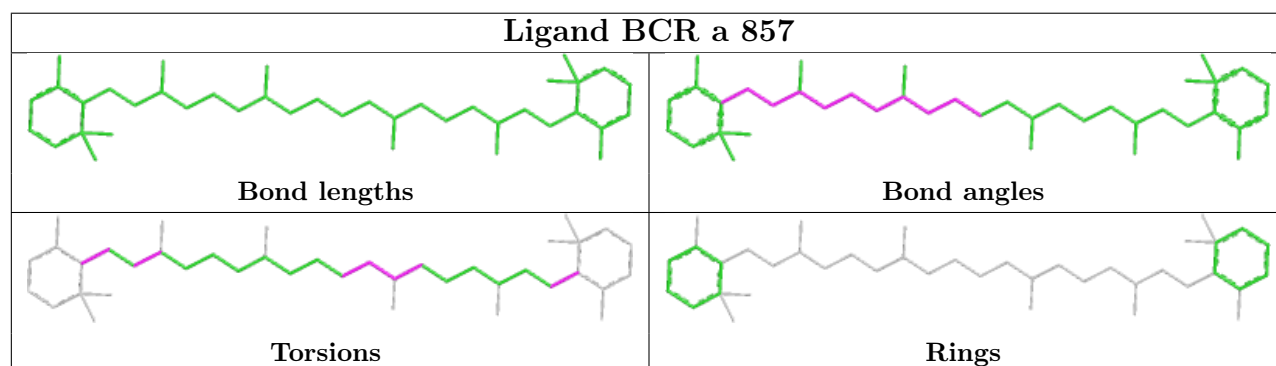
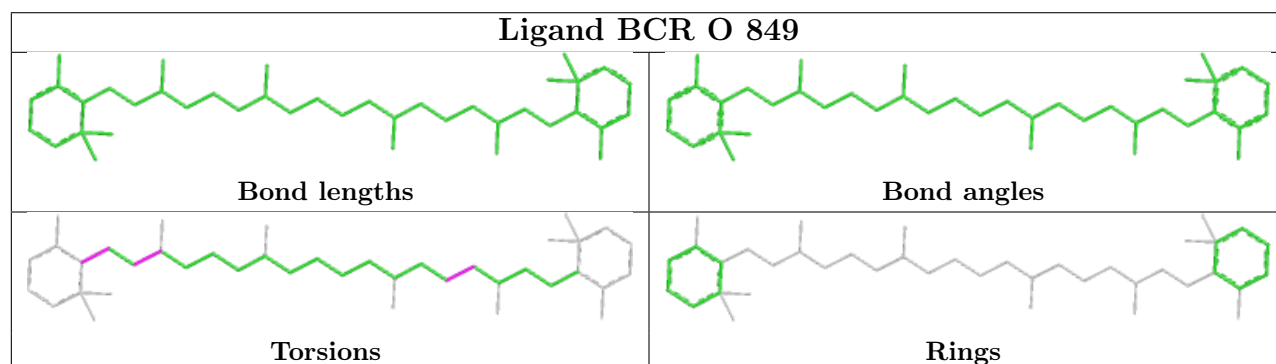
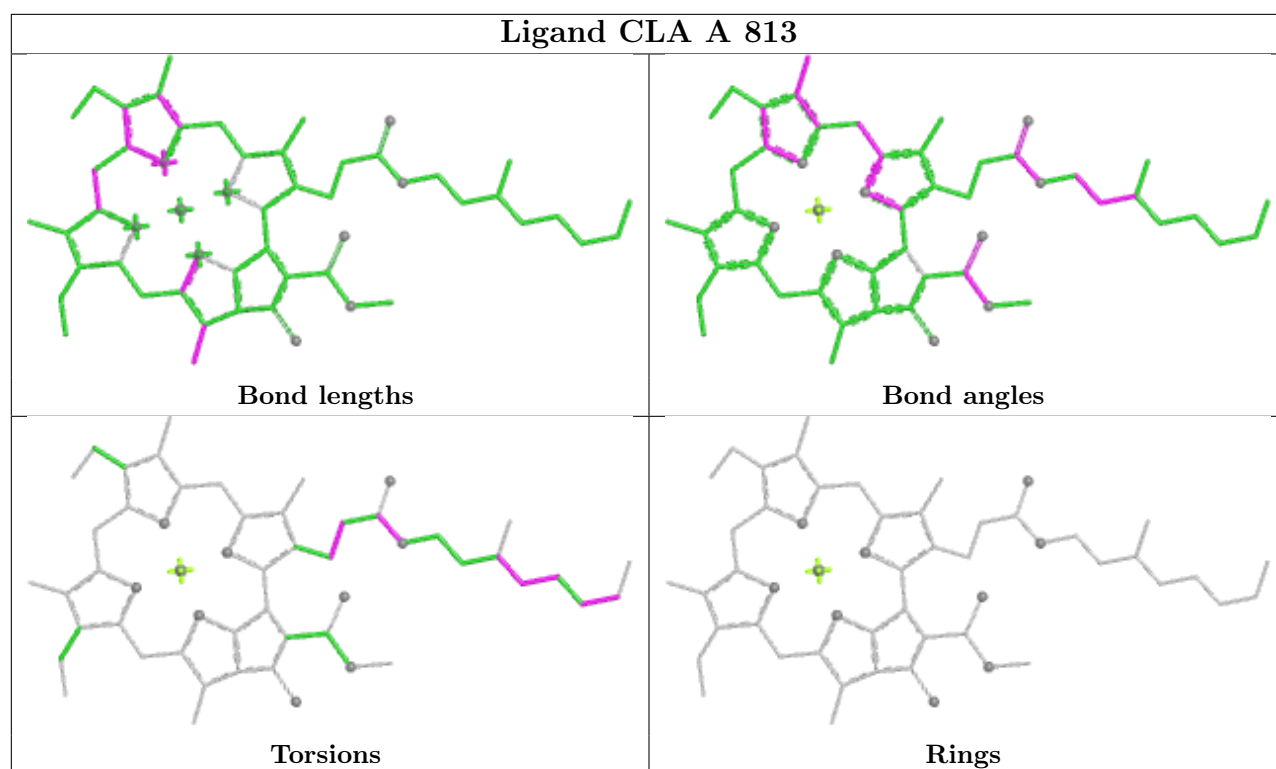


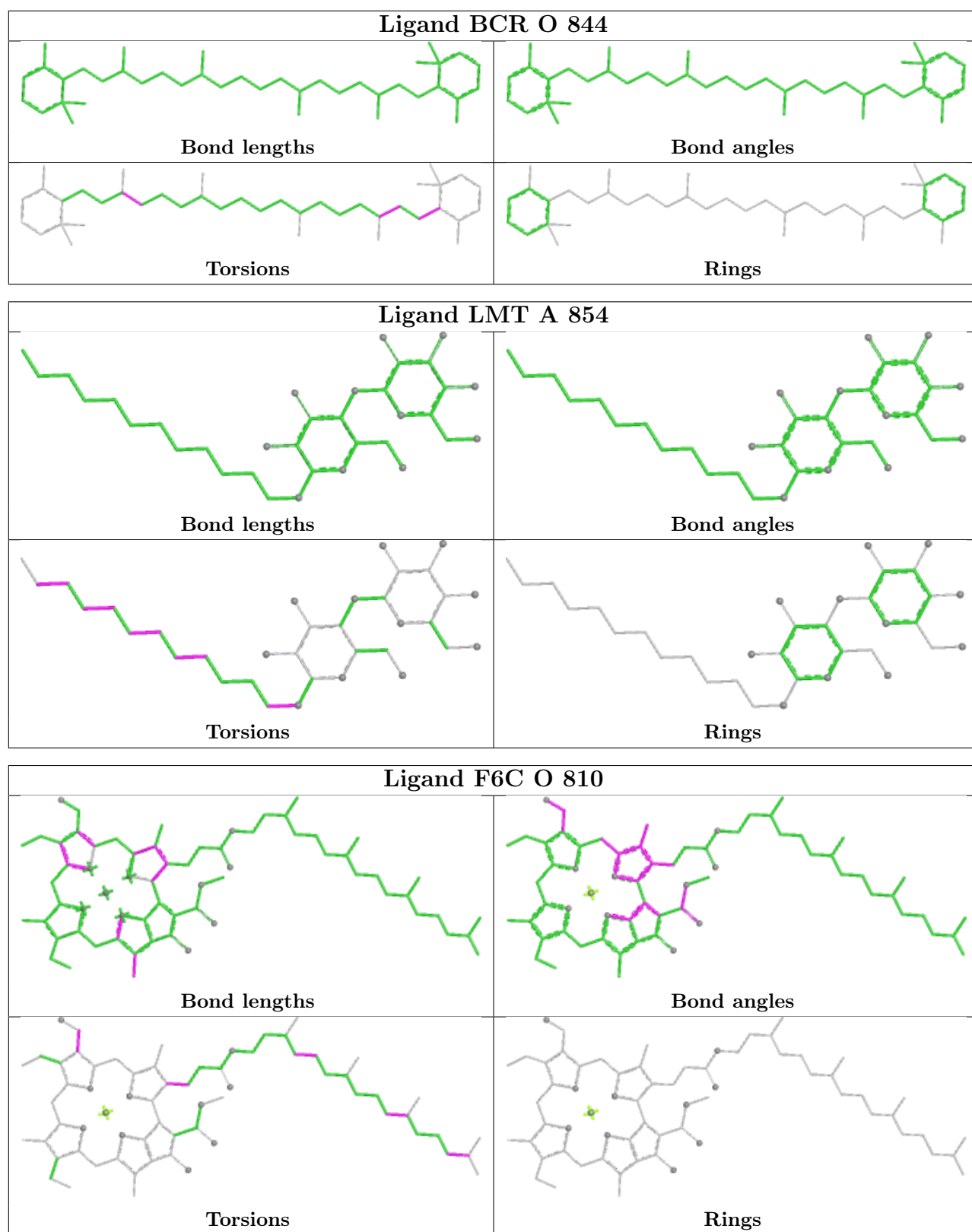
Ligand CLA B 829	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR N 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

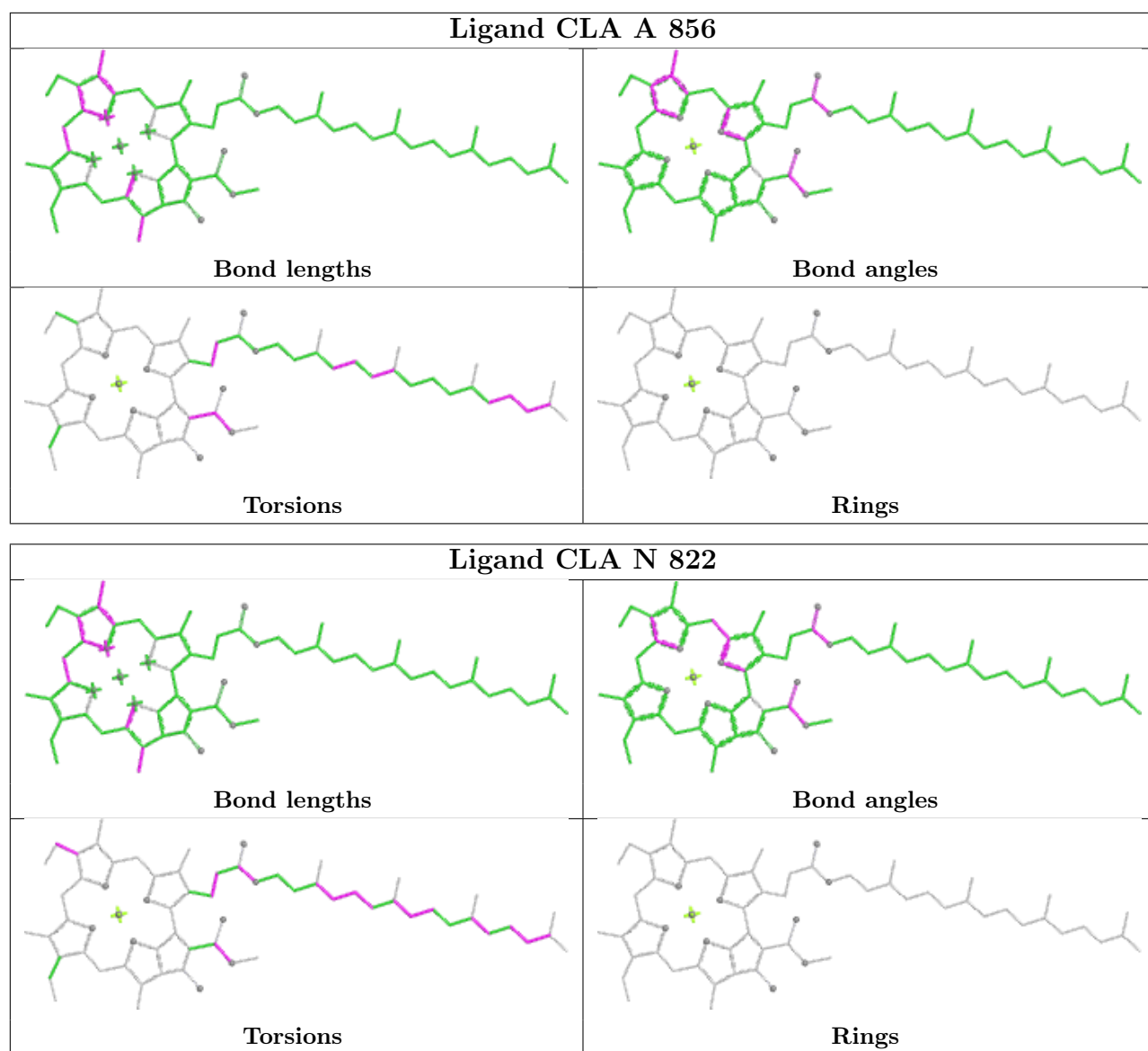




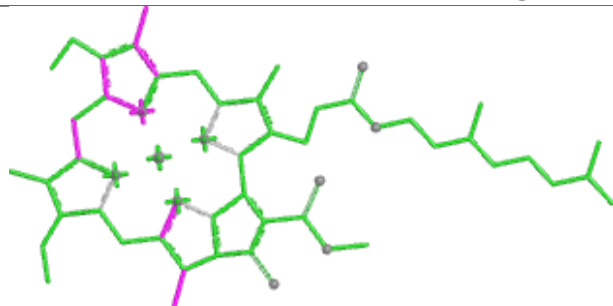




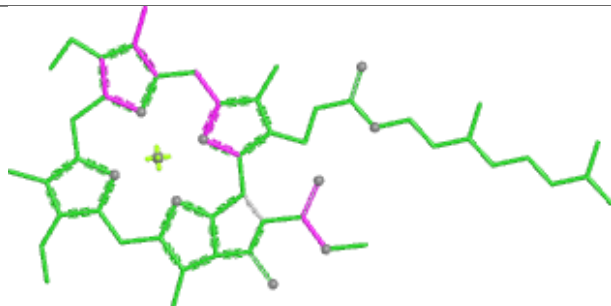




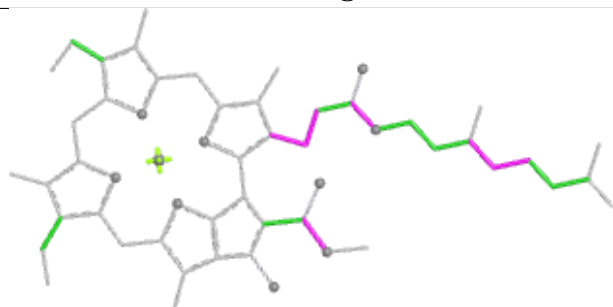
Ligand CLA N 838



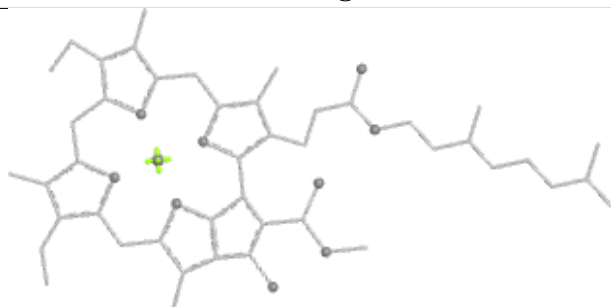
Bond lengths



Bond angles

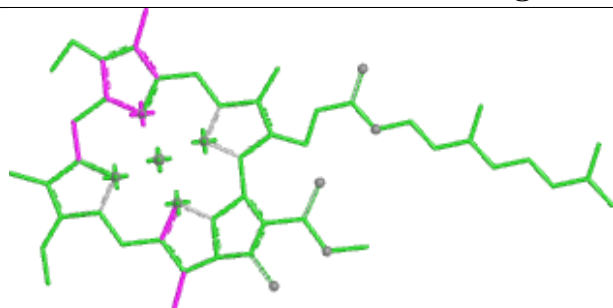


Torsions

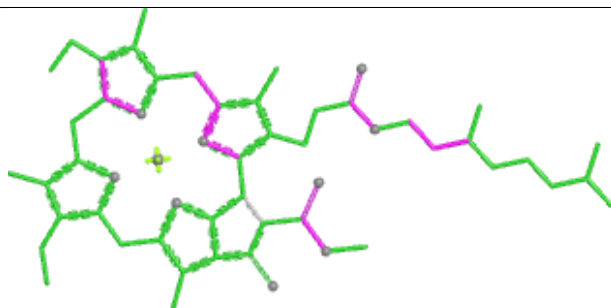


Rings

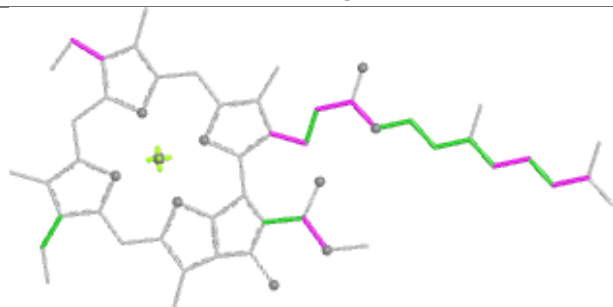
Ligand CLA O 820



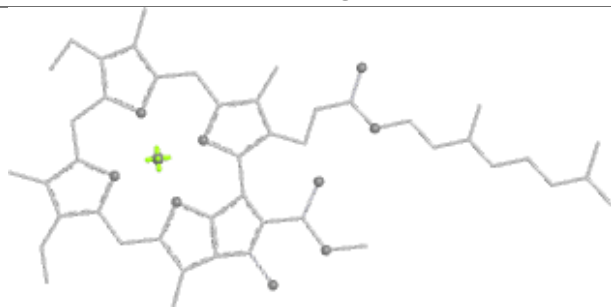
Bond lengths



Bond angles

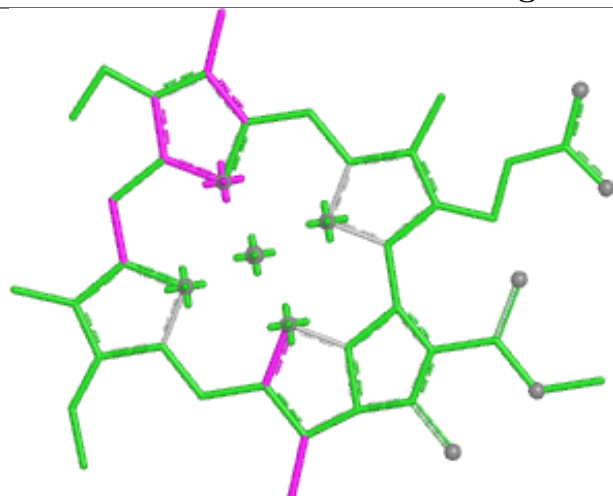


Torsions

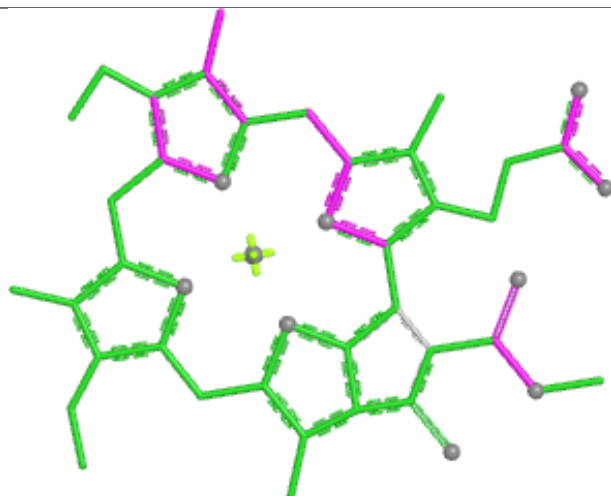


Rings

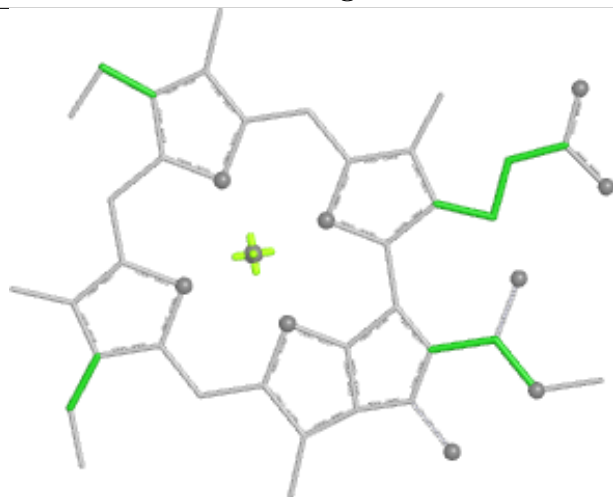
Ligand CLA a 808



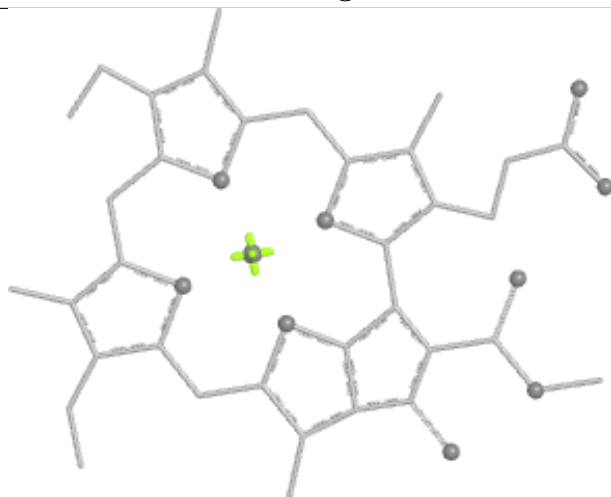
Bond lengths



Bond angles

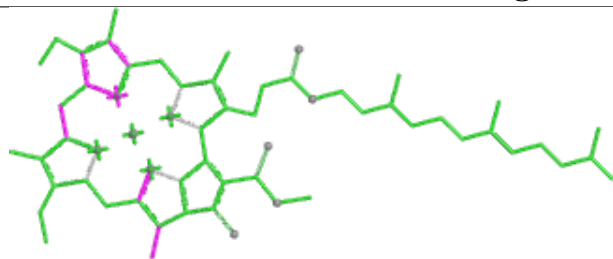


Torsions

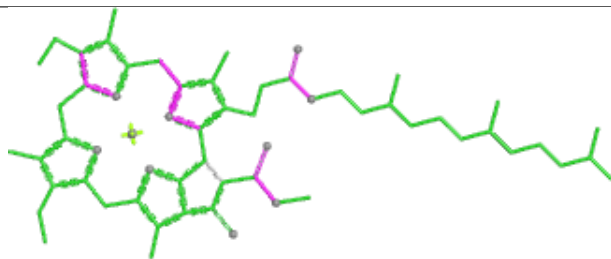


Rings

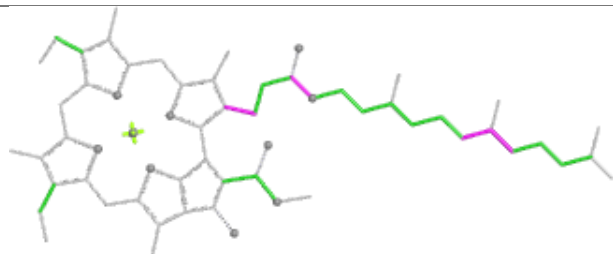
Ligand CLA N 805



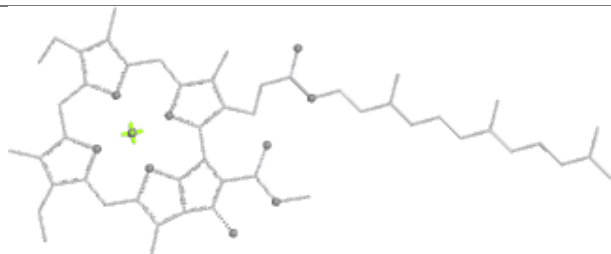
Bond lengths



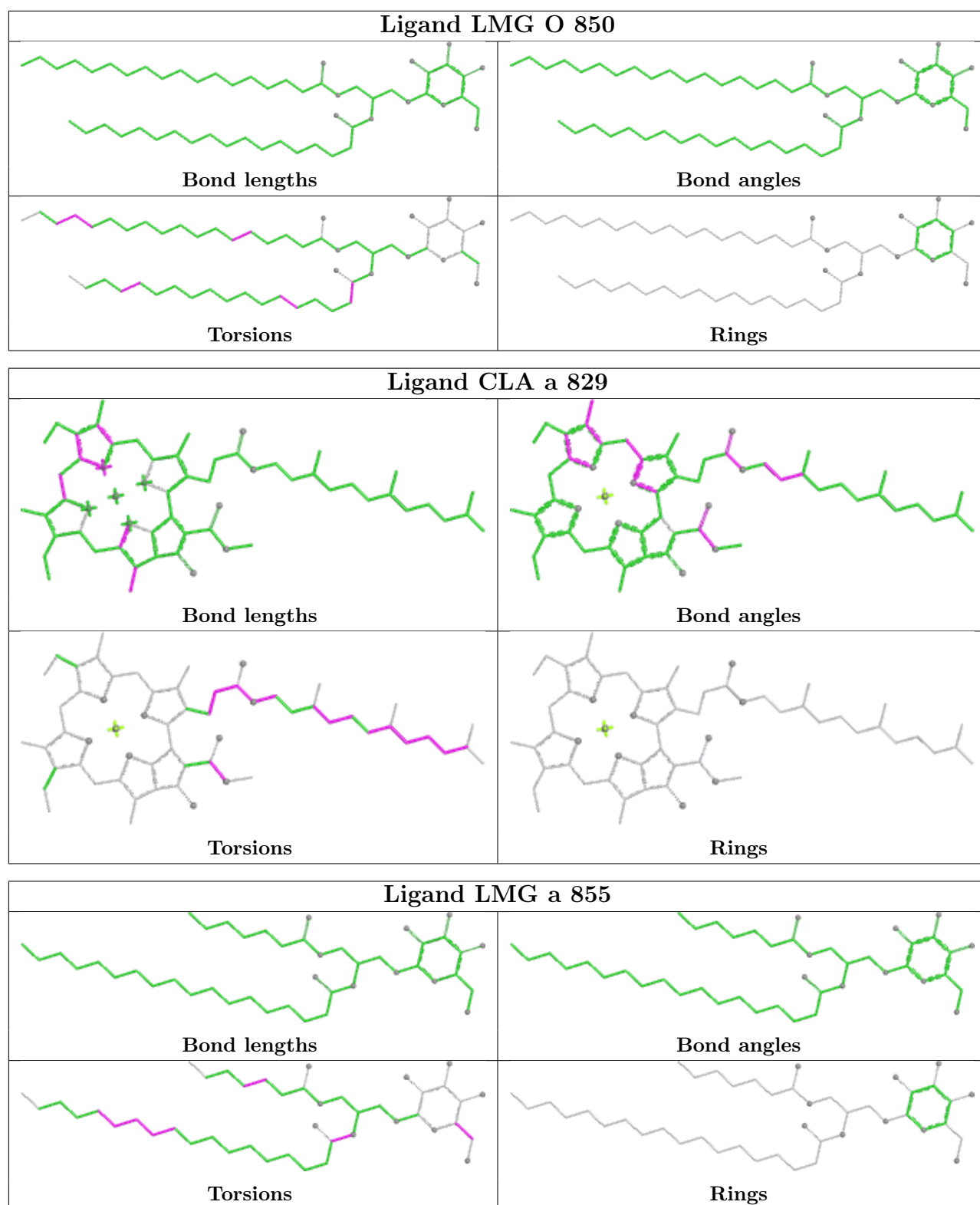
Bond angles

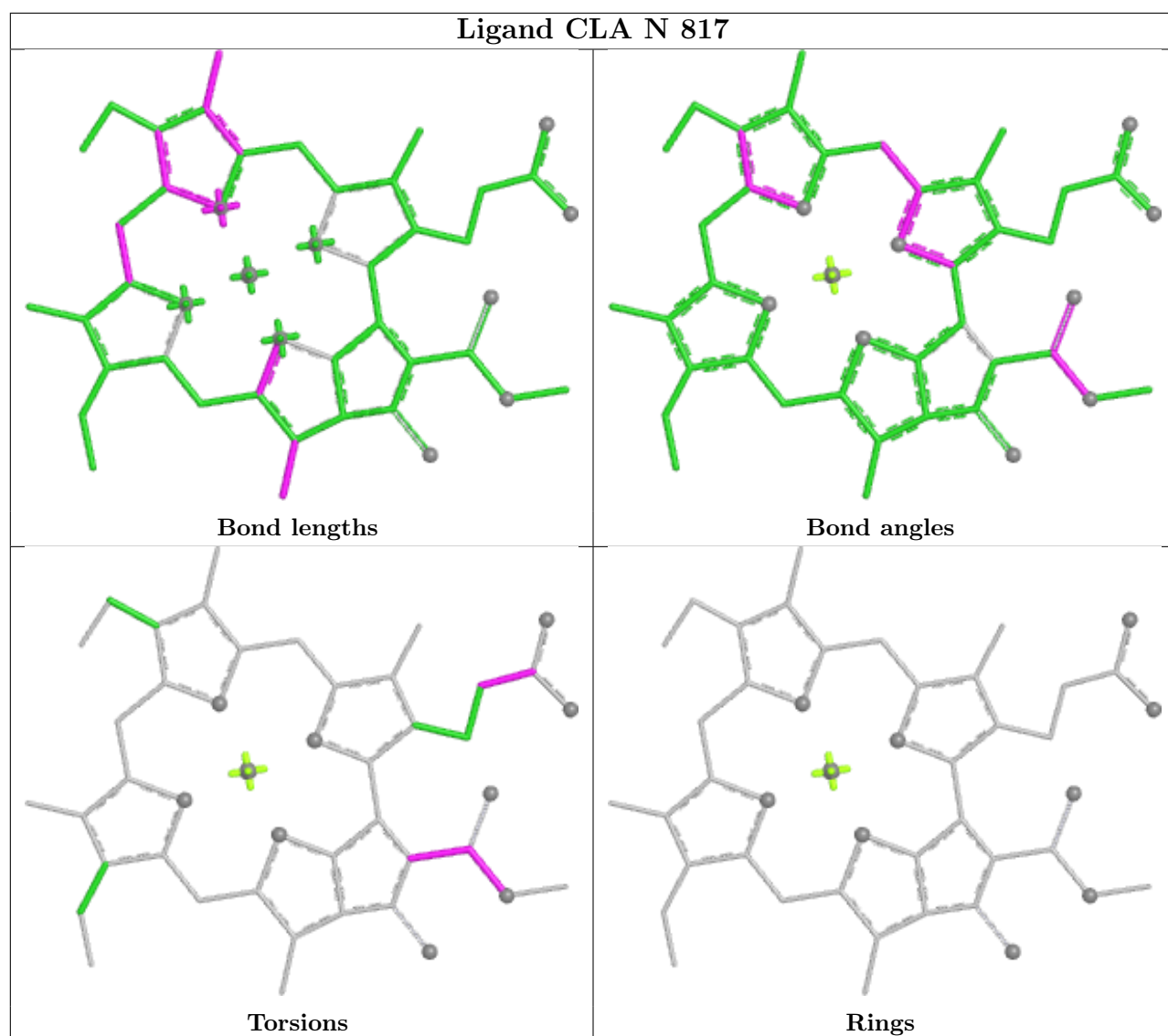


Torsions

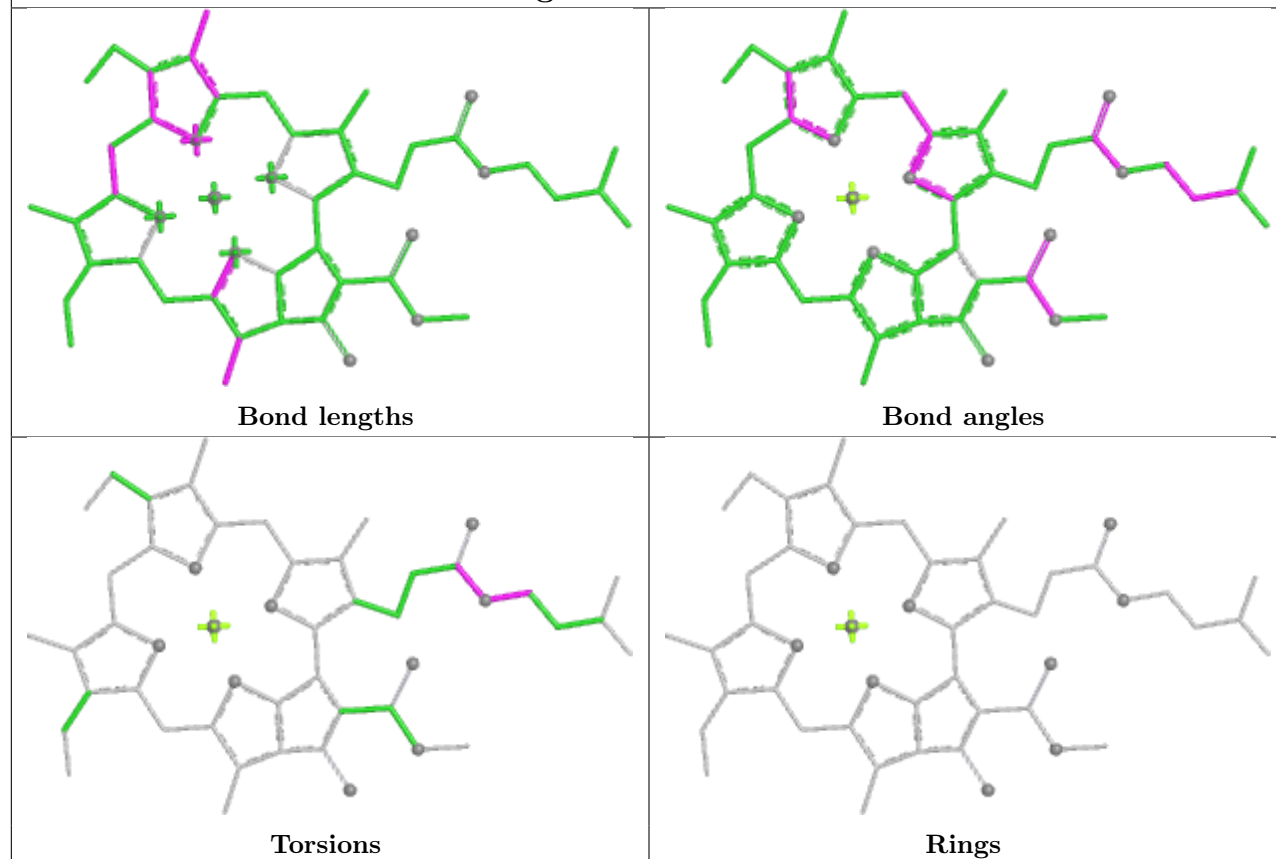


Rings

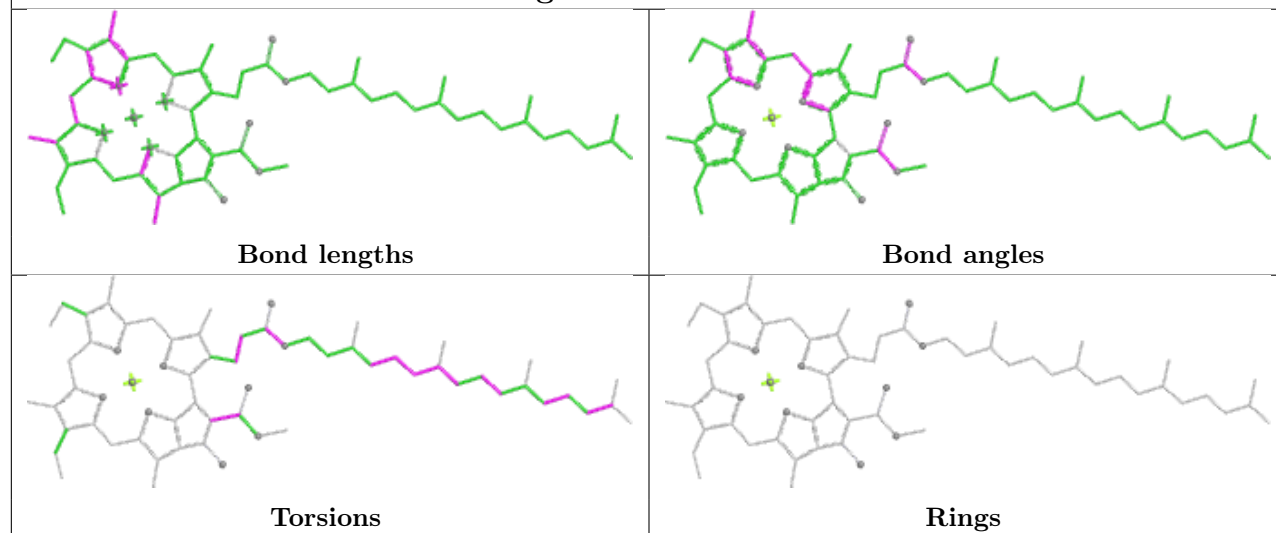




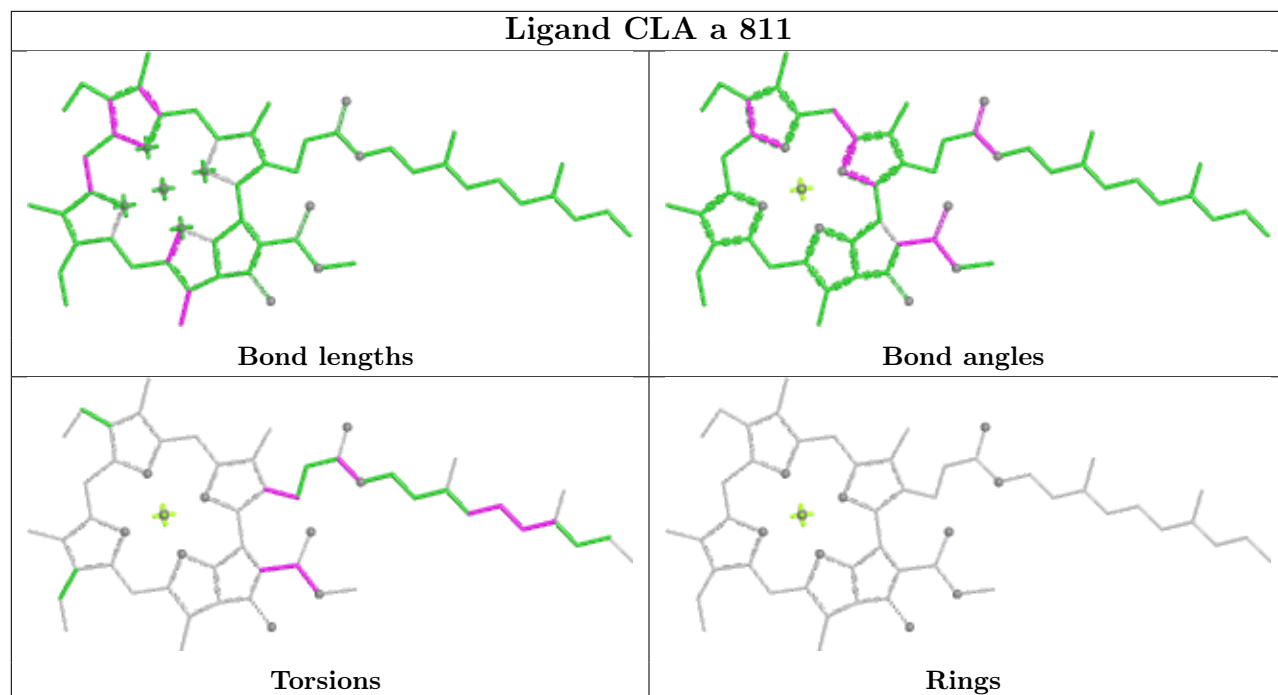
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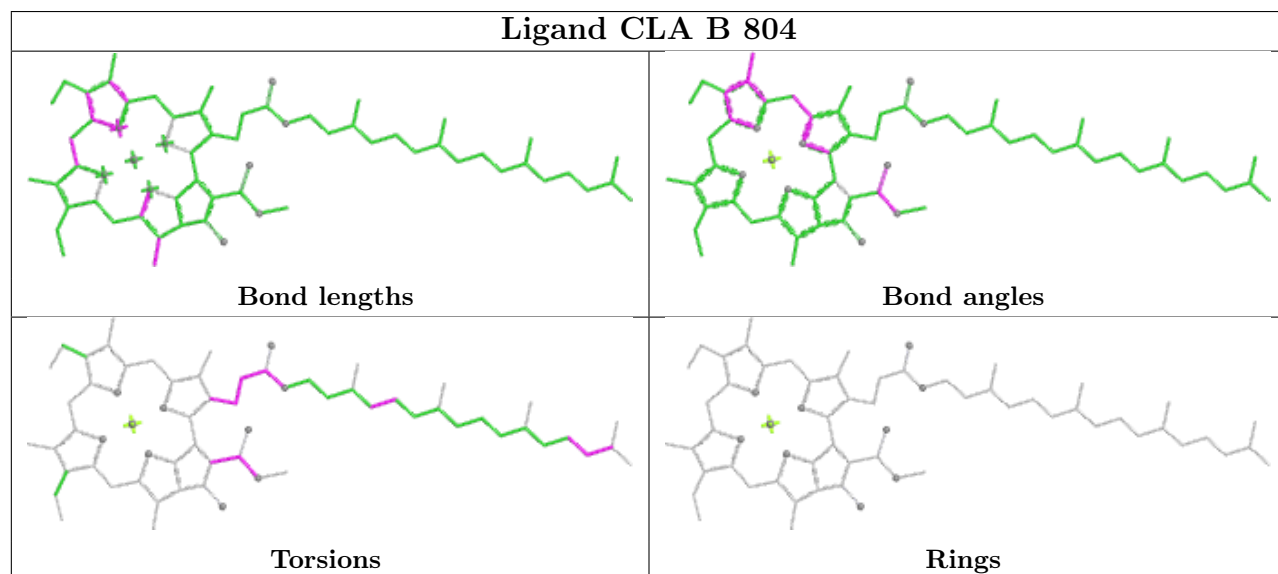
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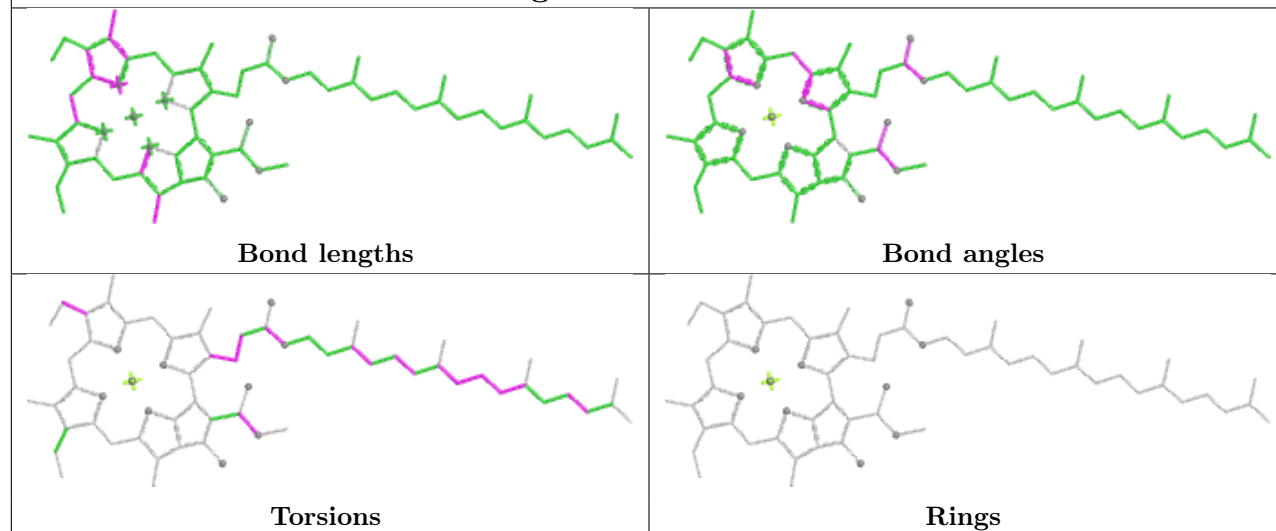
Ligand CLA a 811



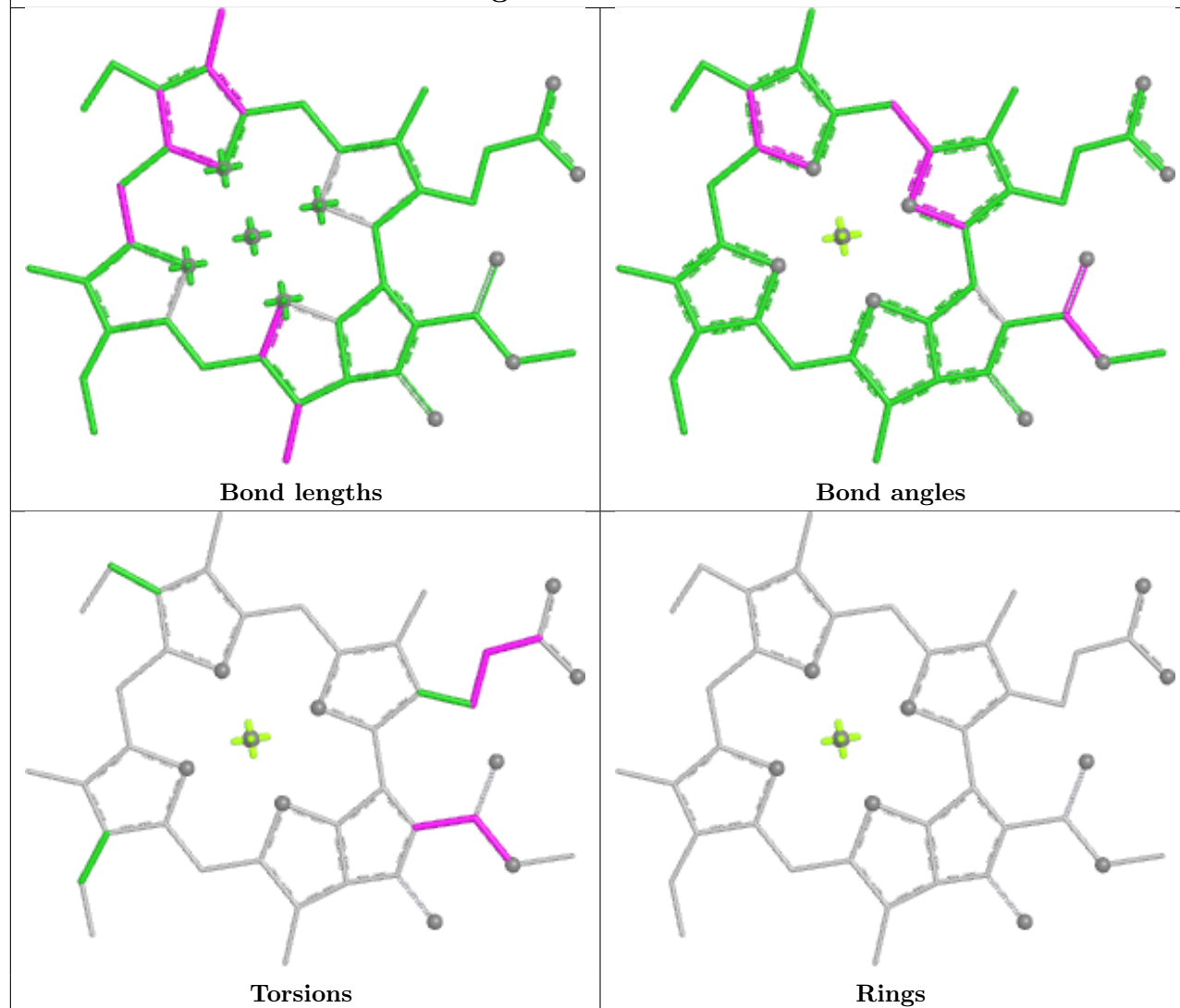
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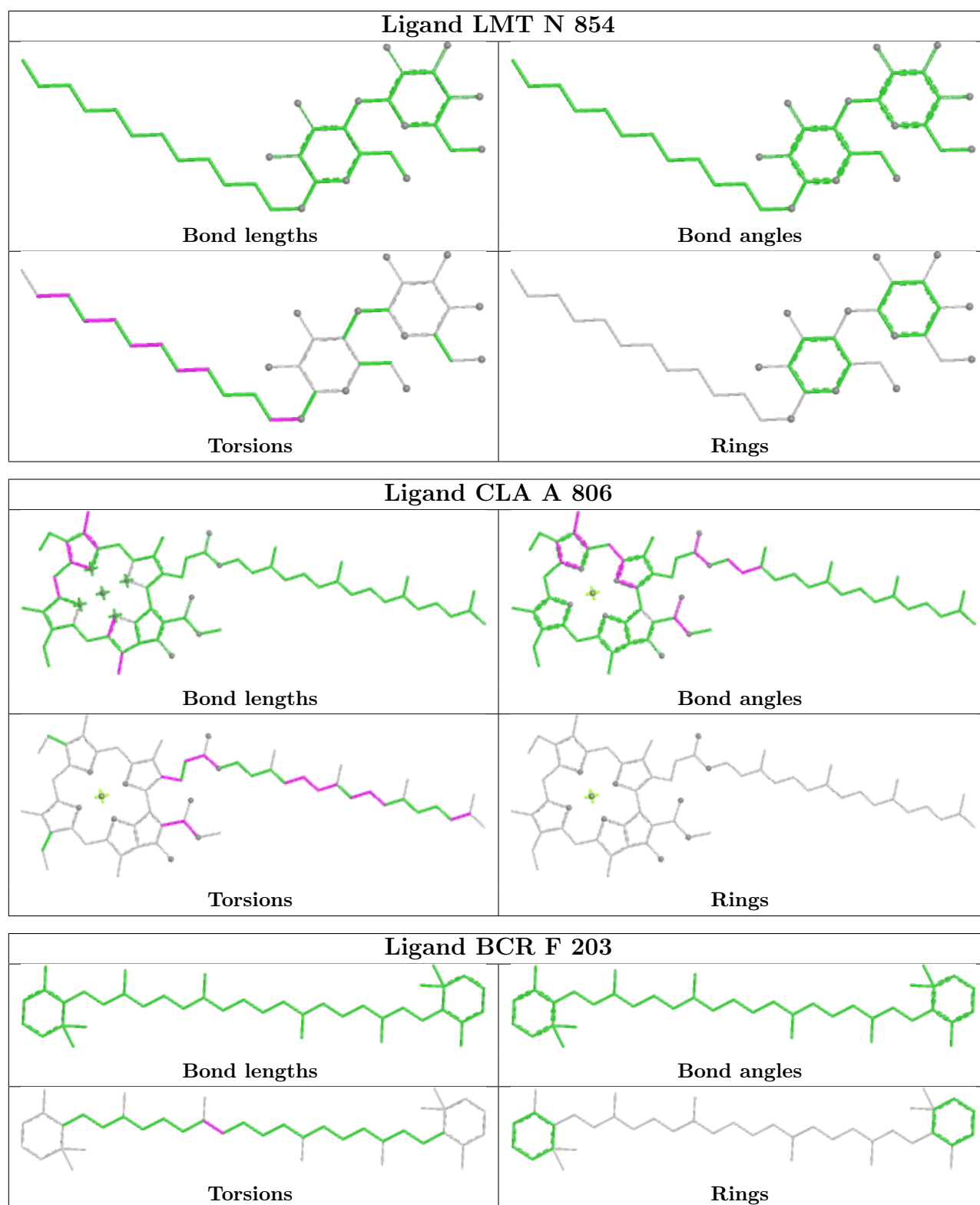


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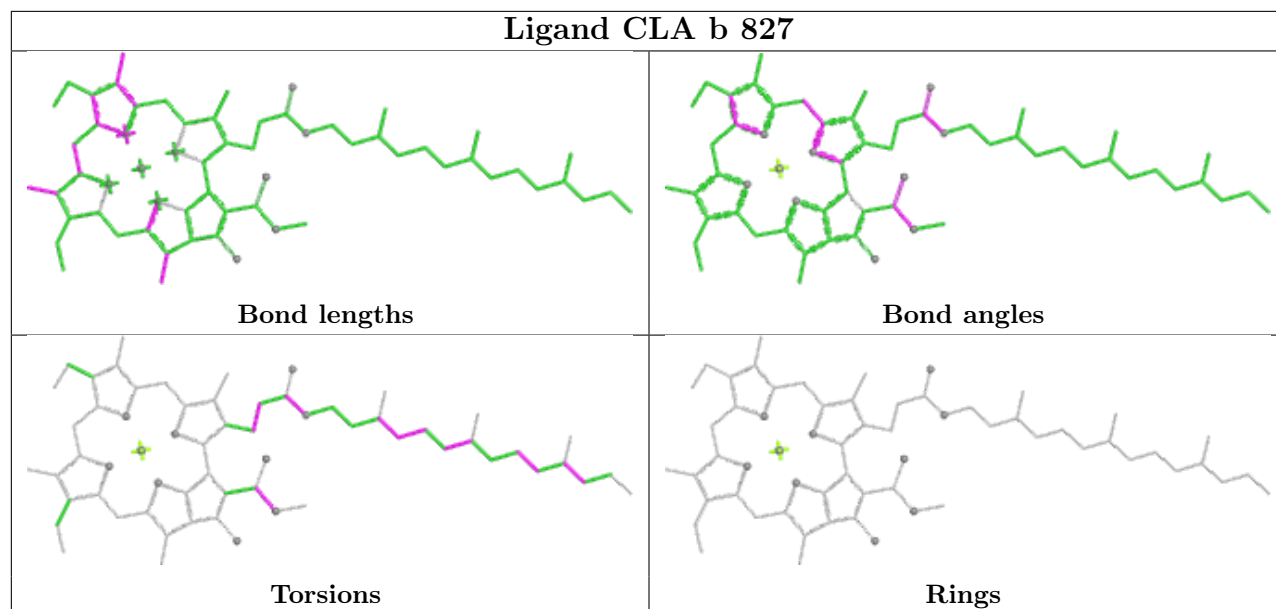


Ligand CLA A 816

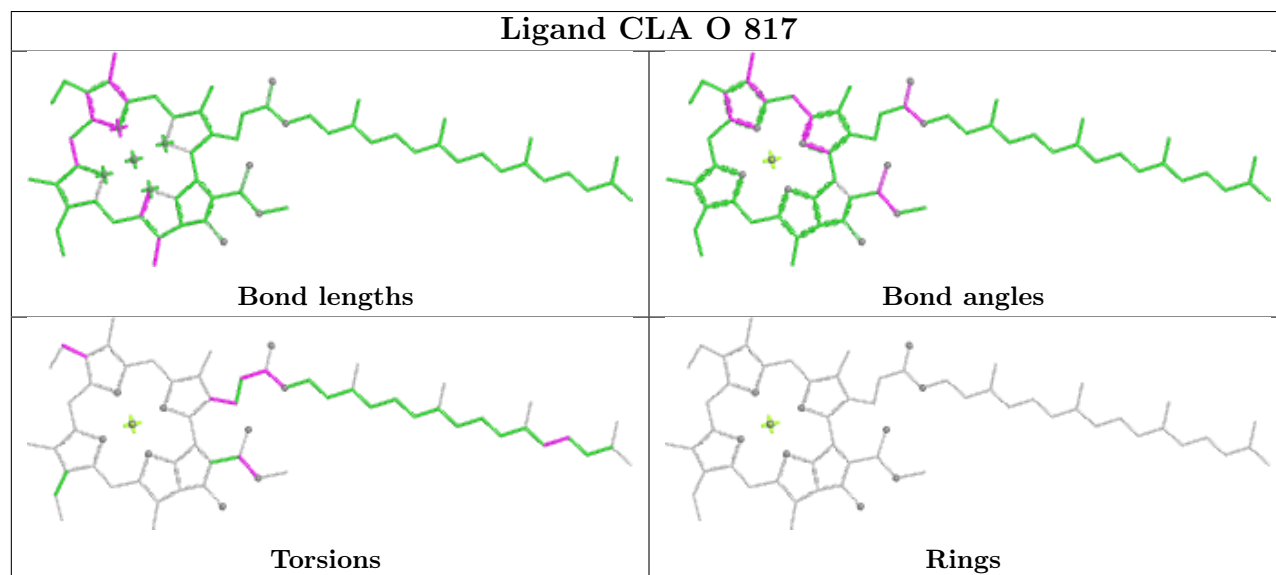


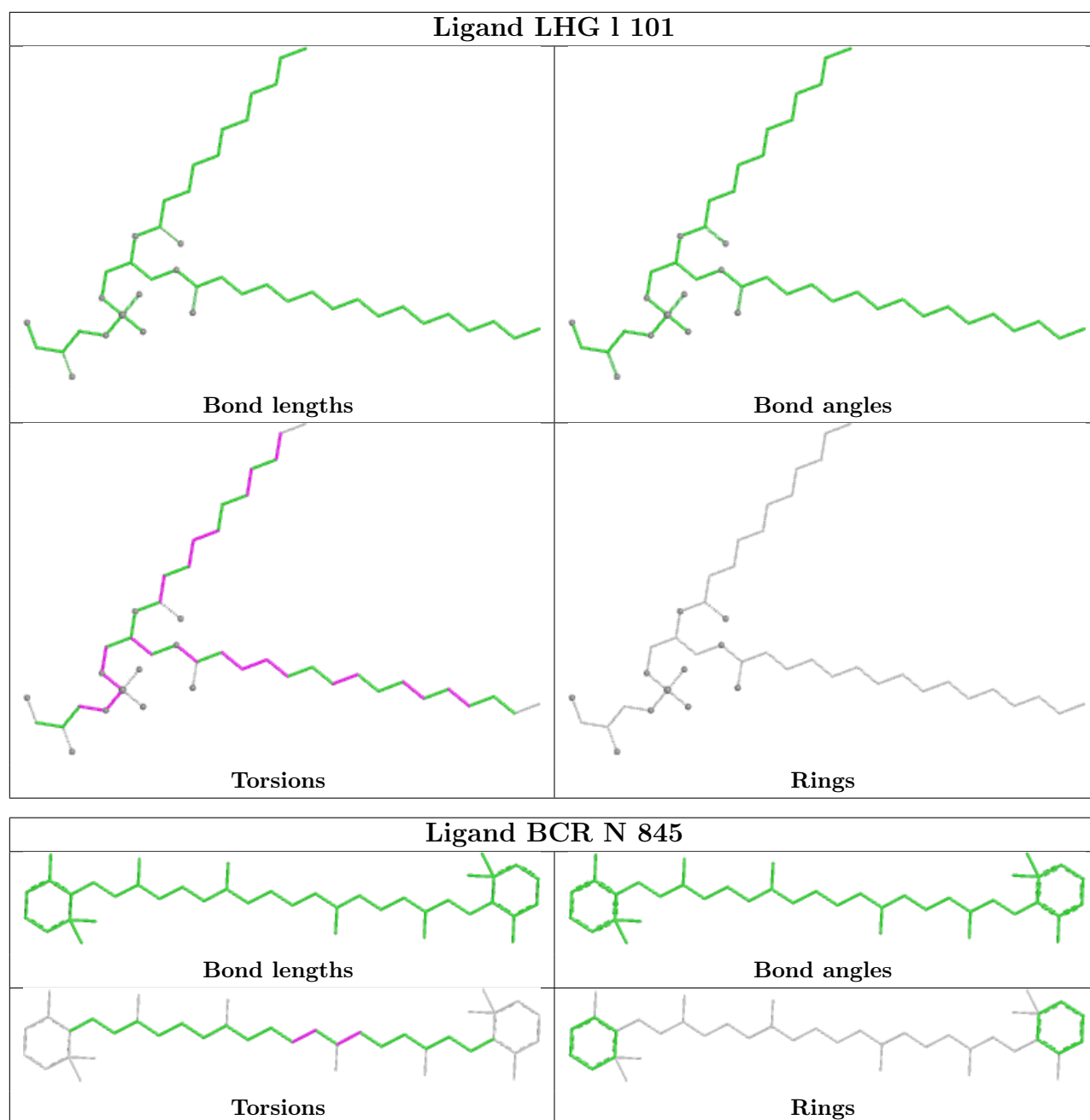


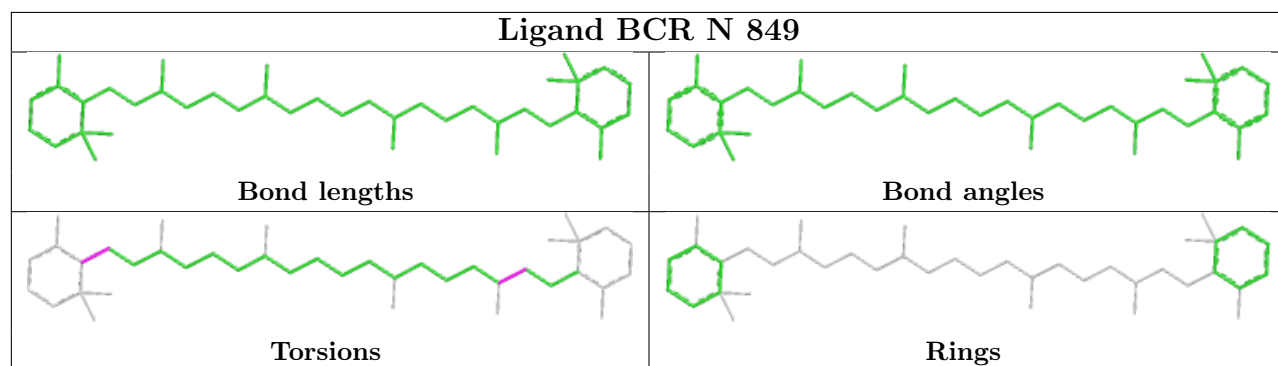
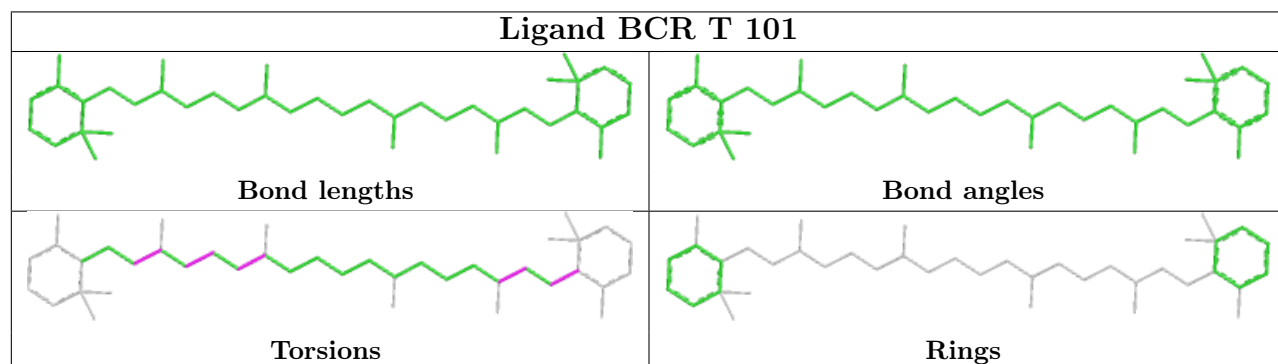
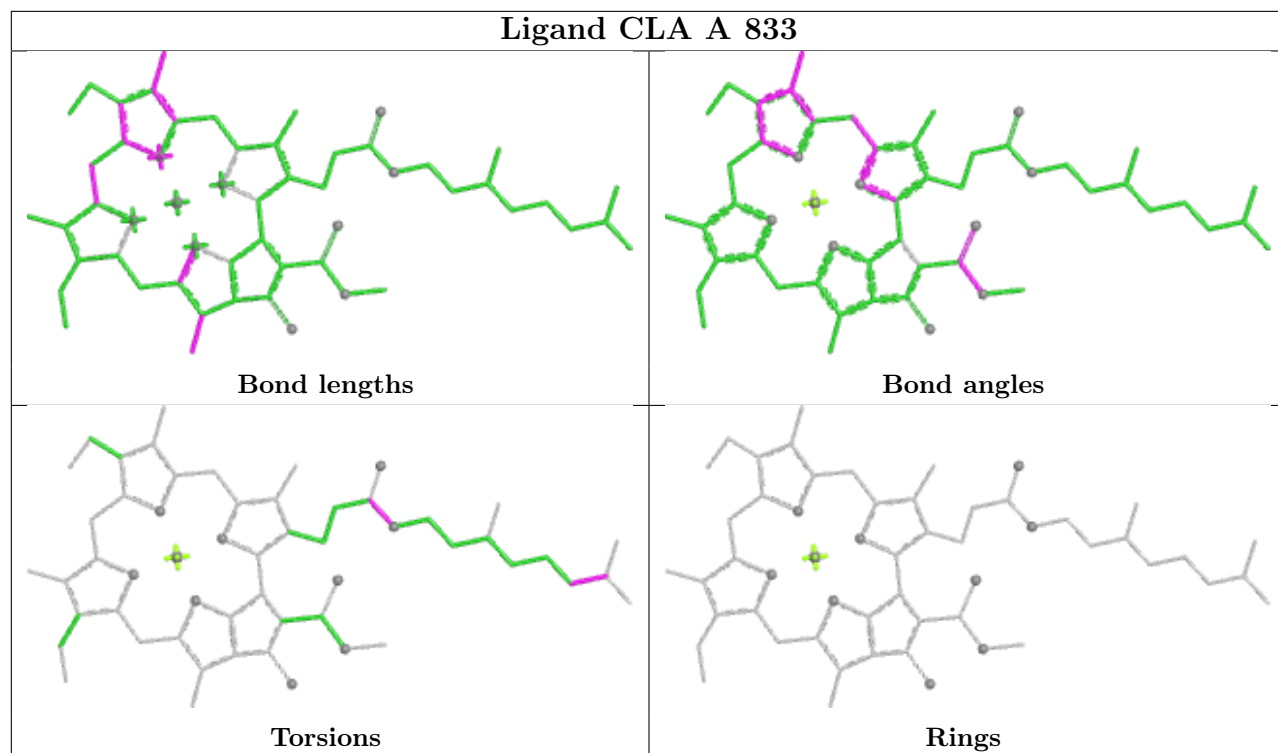
Ligand CLA b 827

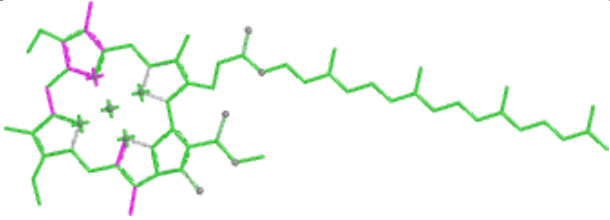
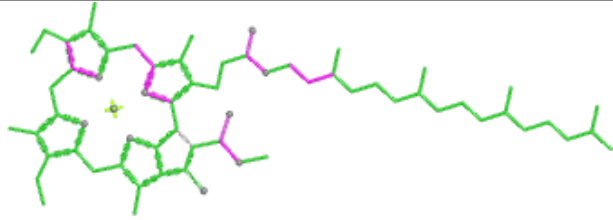
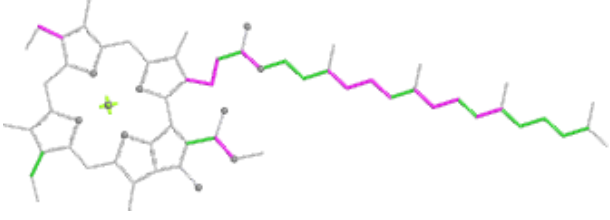
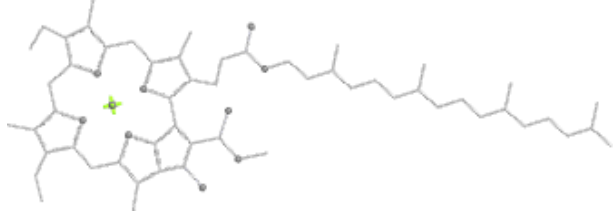
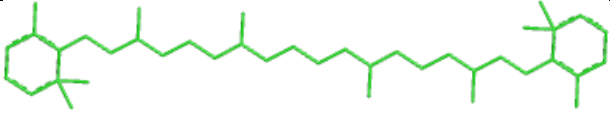
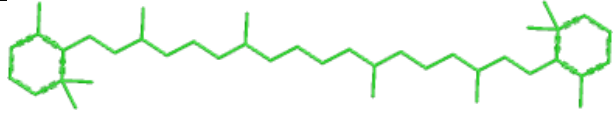
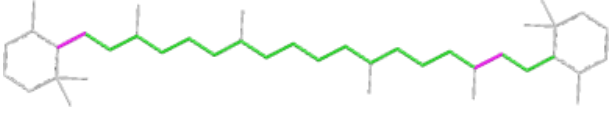
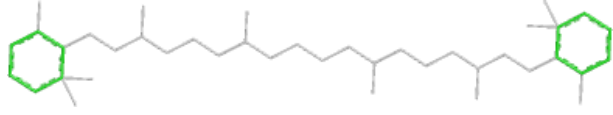
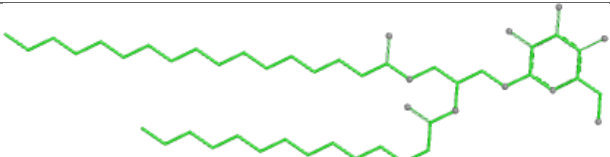
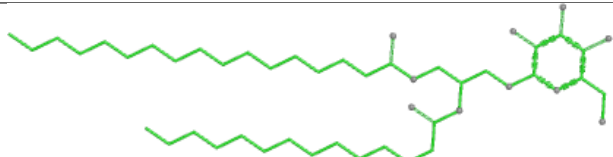
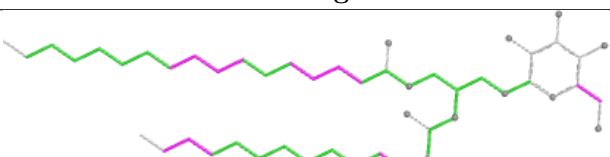
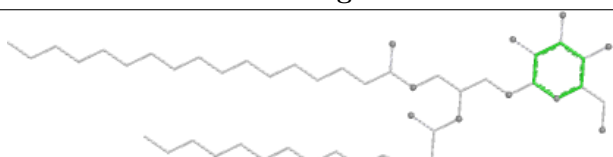


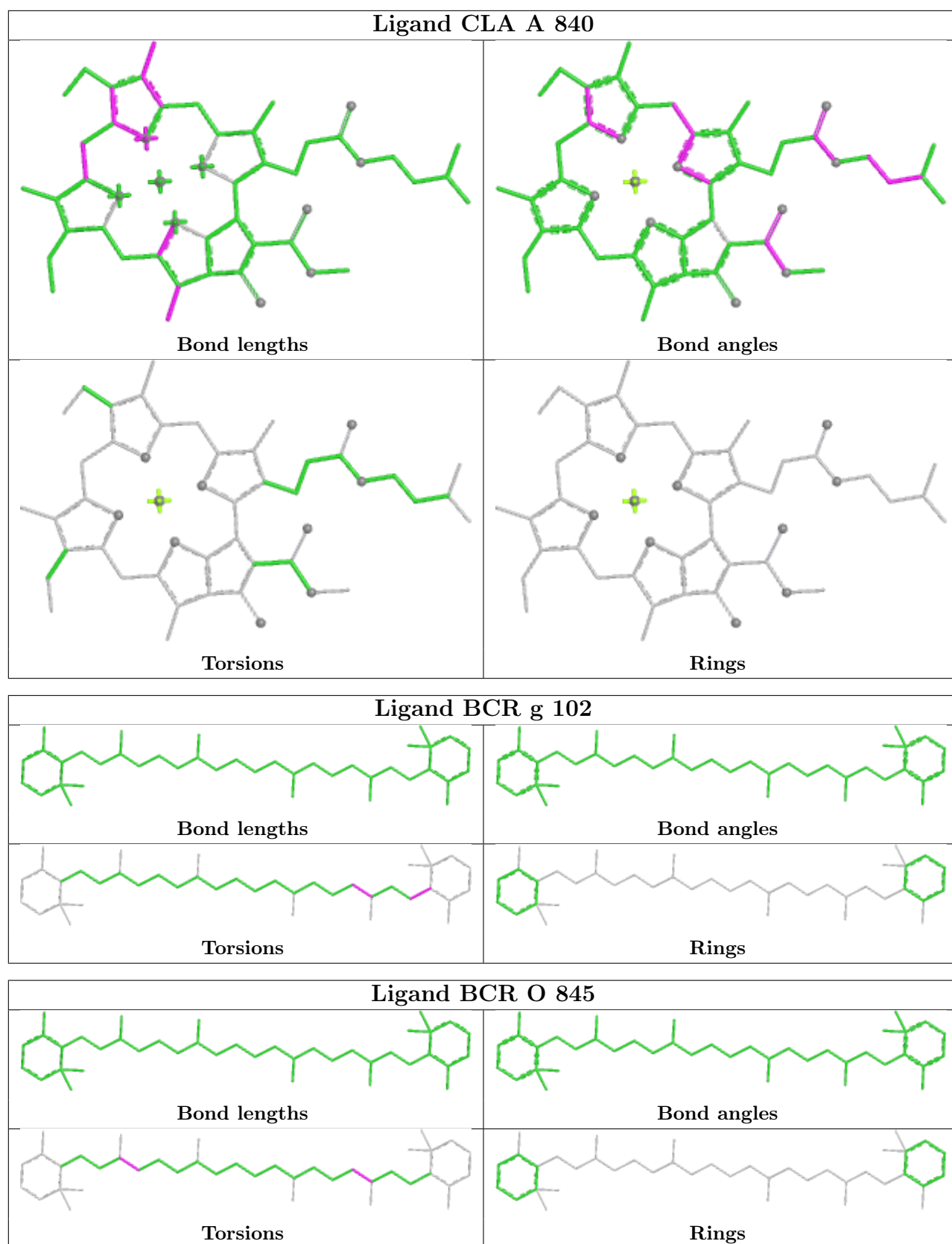
Ligand CLA O 817

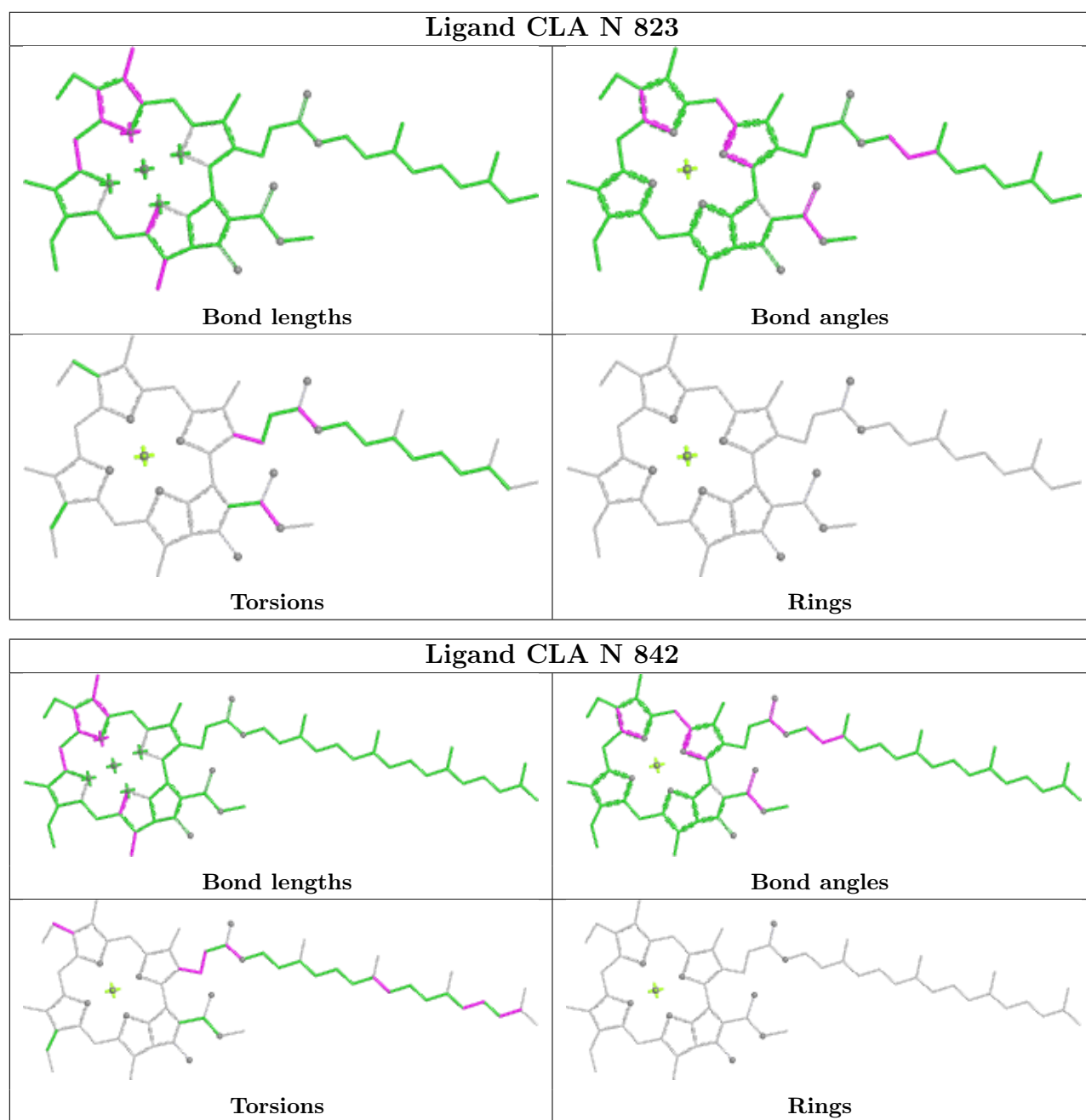




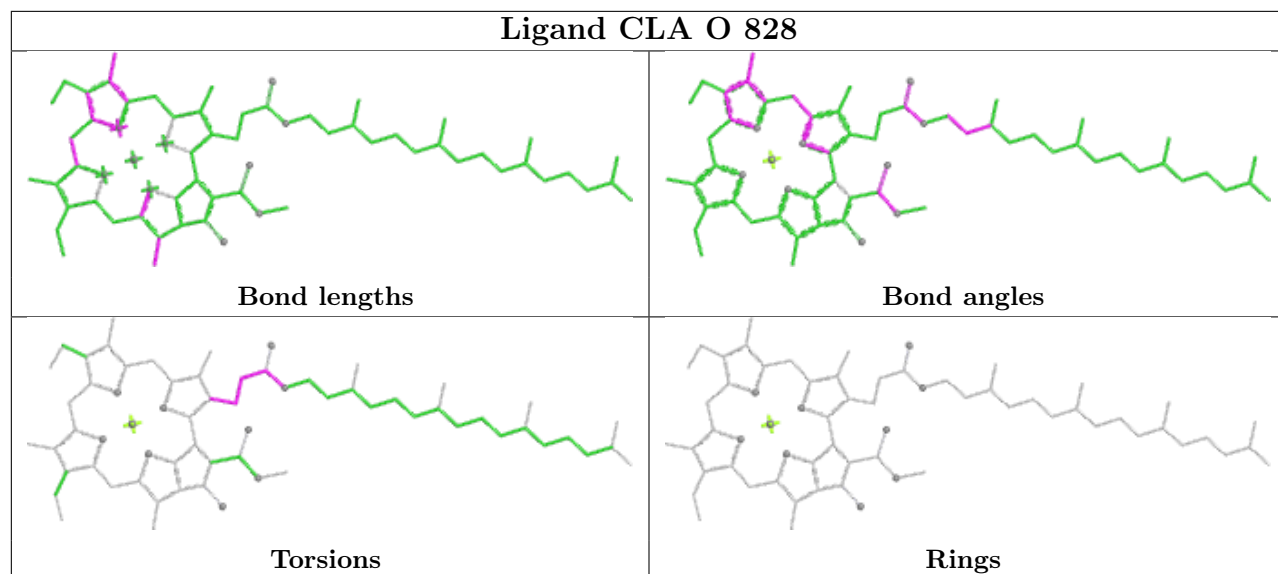


Ligand CLA O 830	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 849	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG W 1505	
 Bond lengths	 Bond angles
 Torsions	 Rings

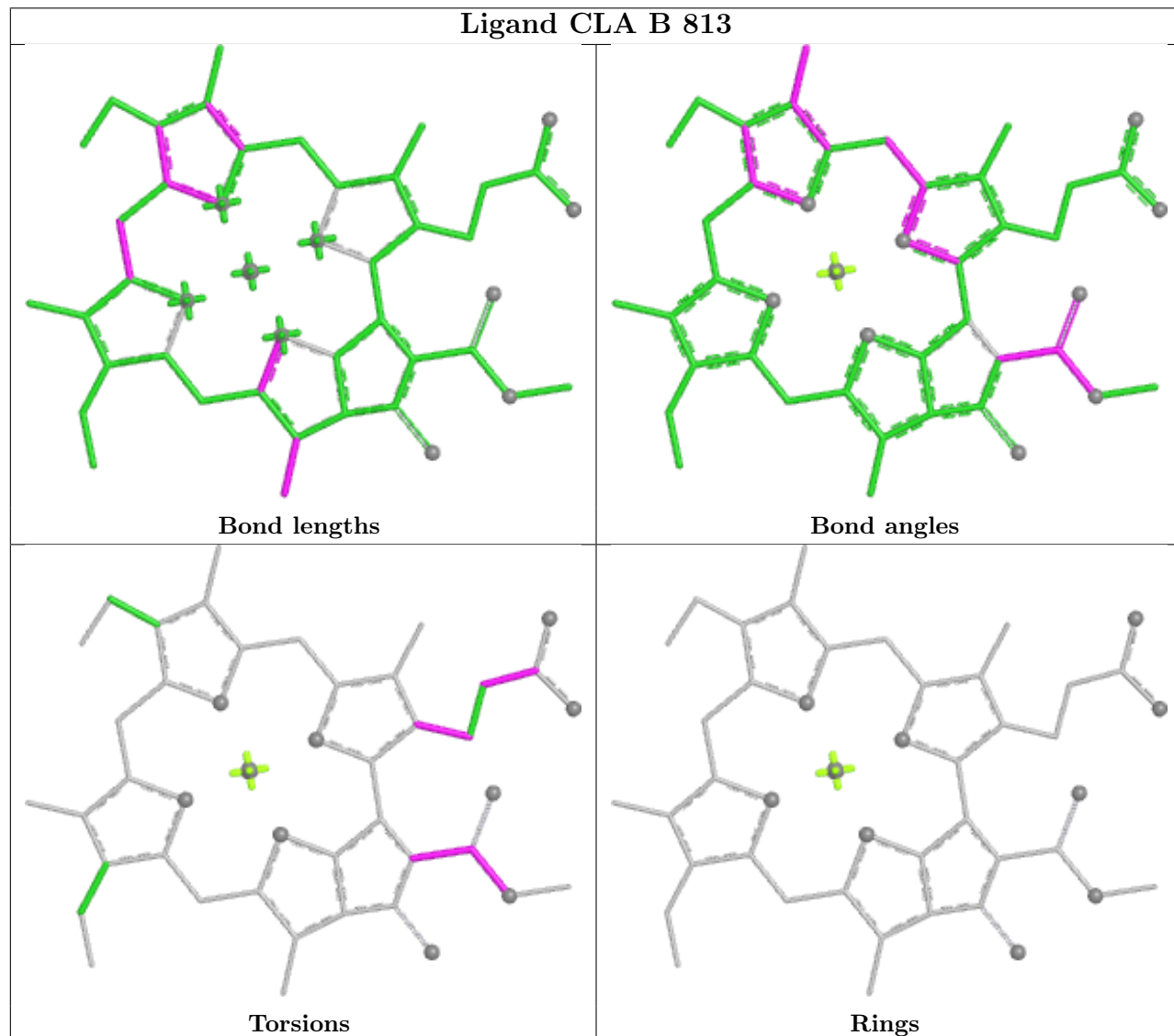


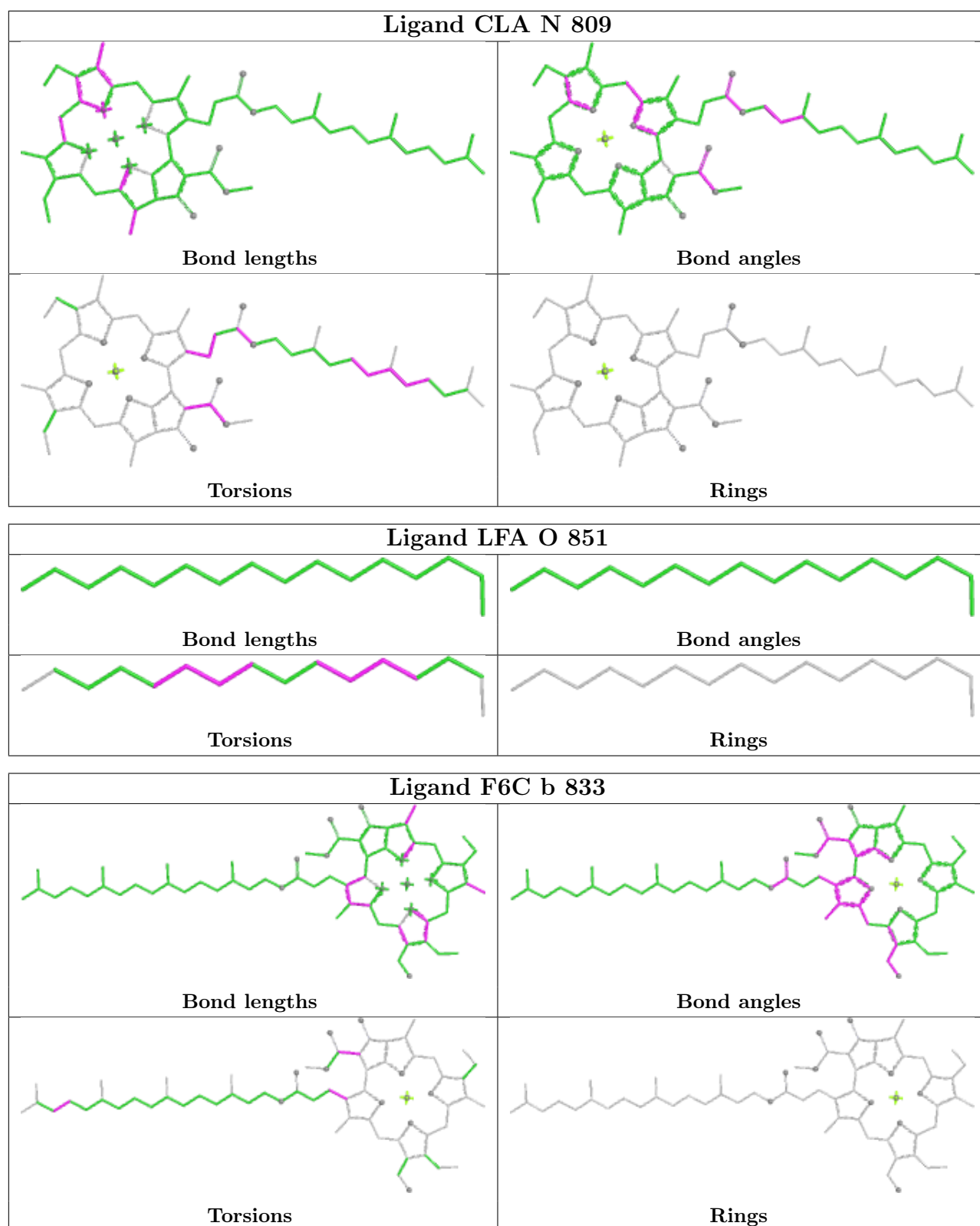


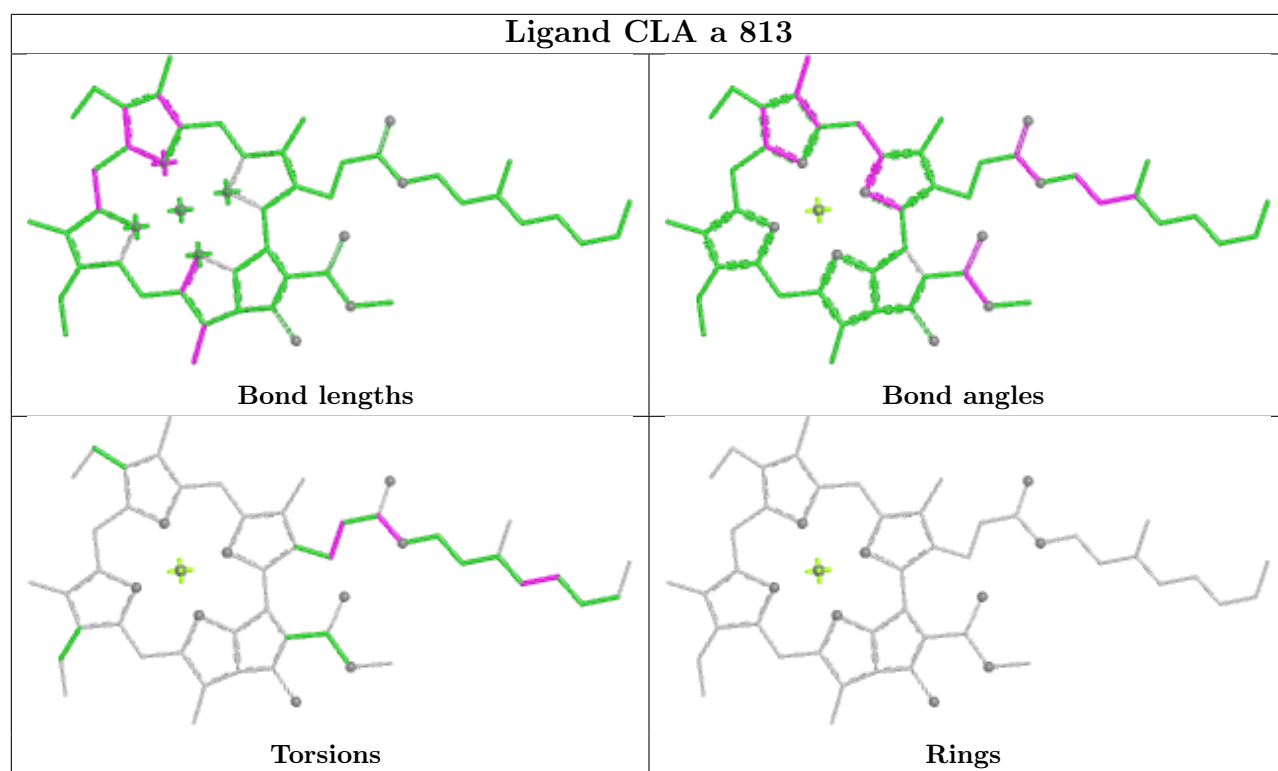
Ligand CLA O 828

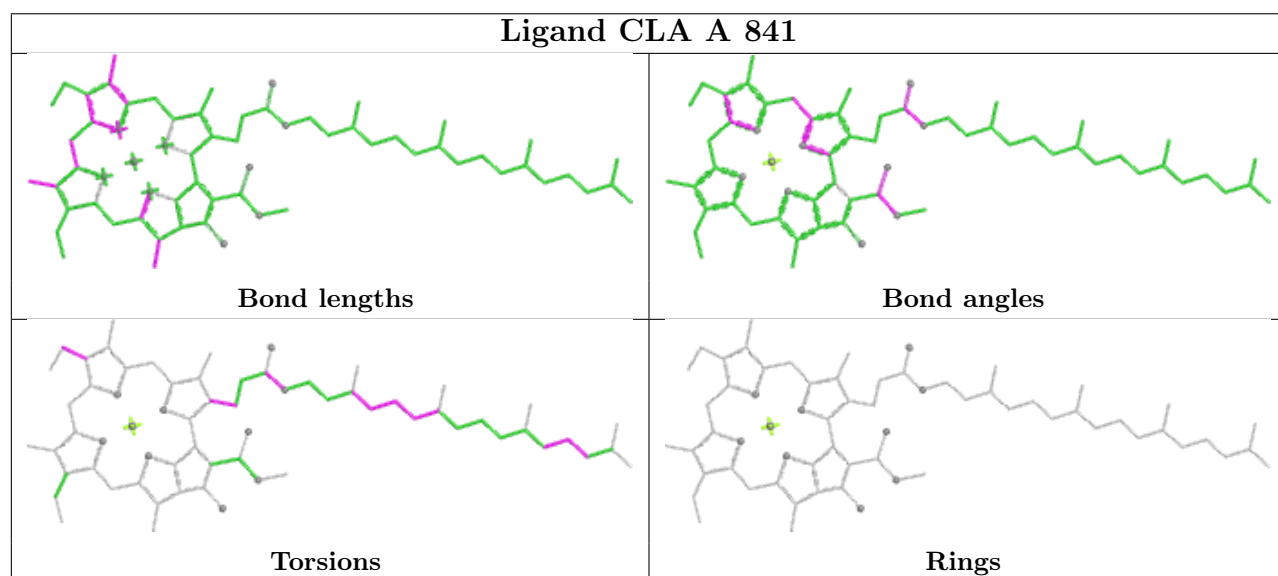
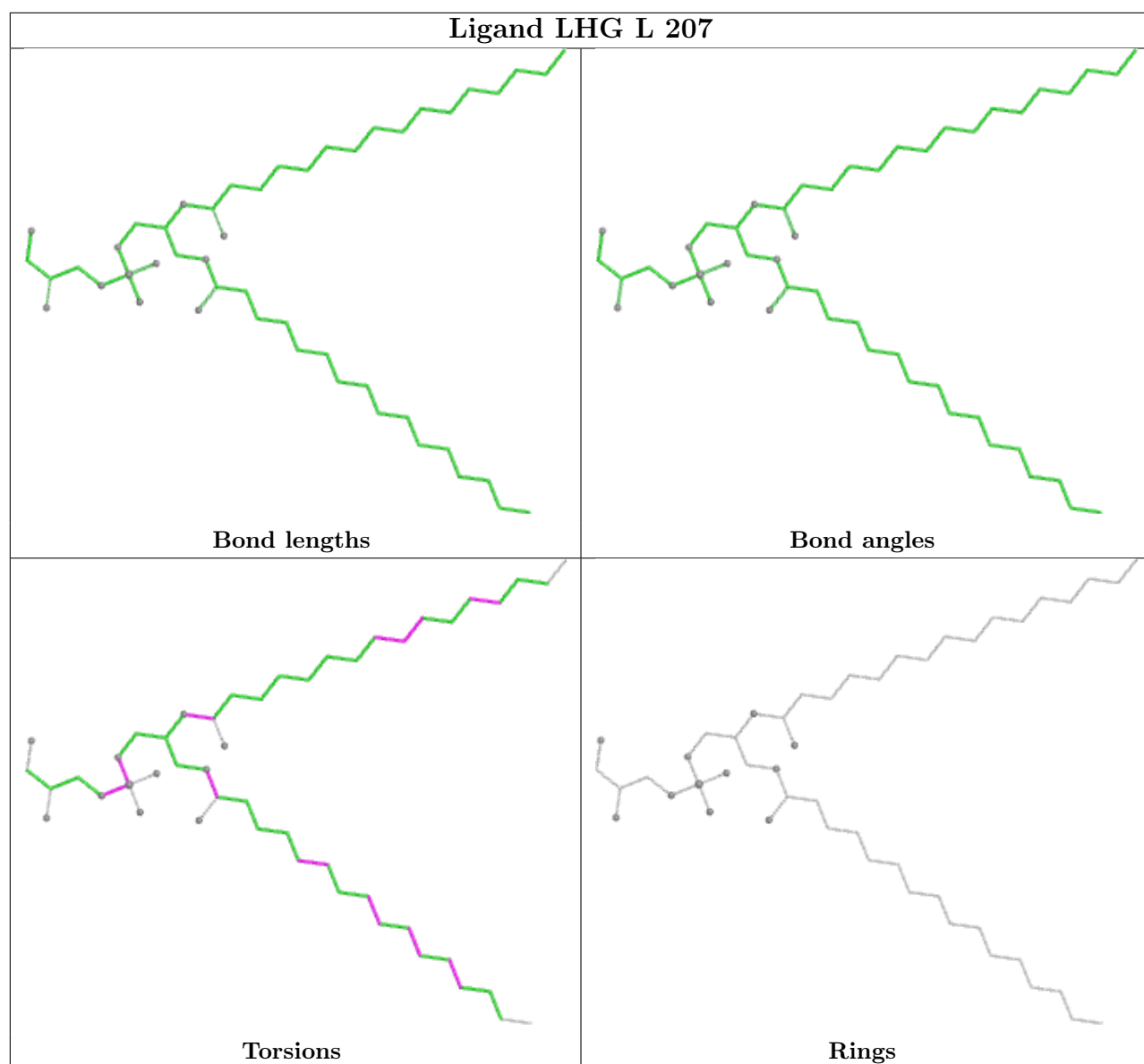


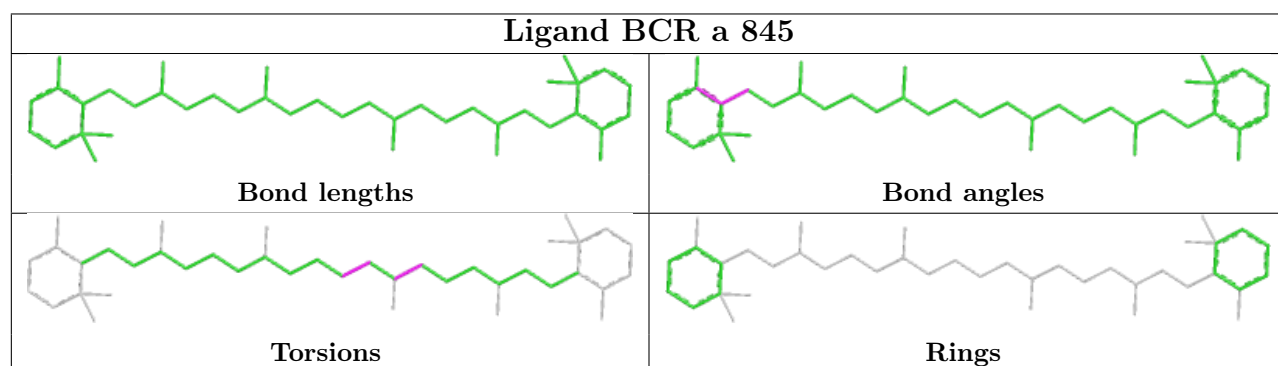
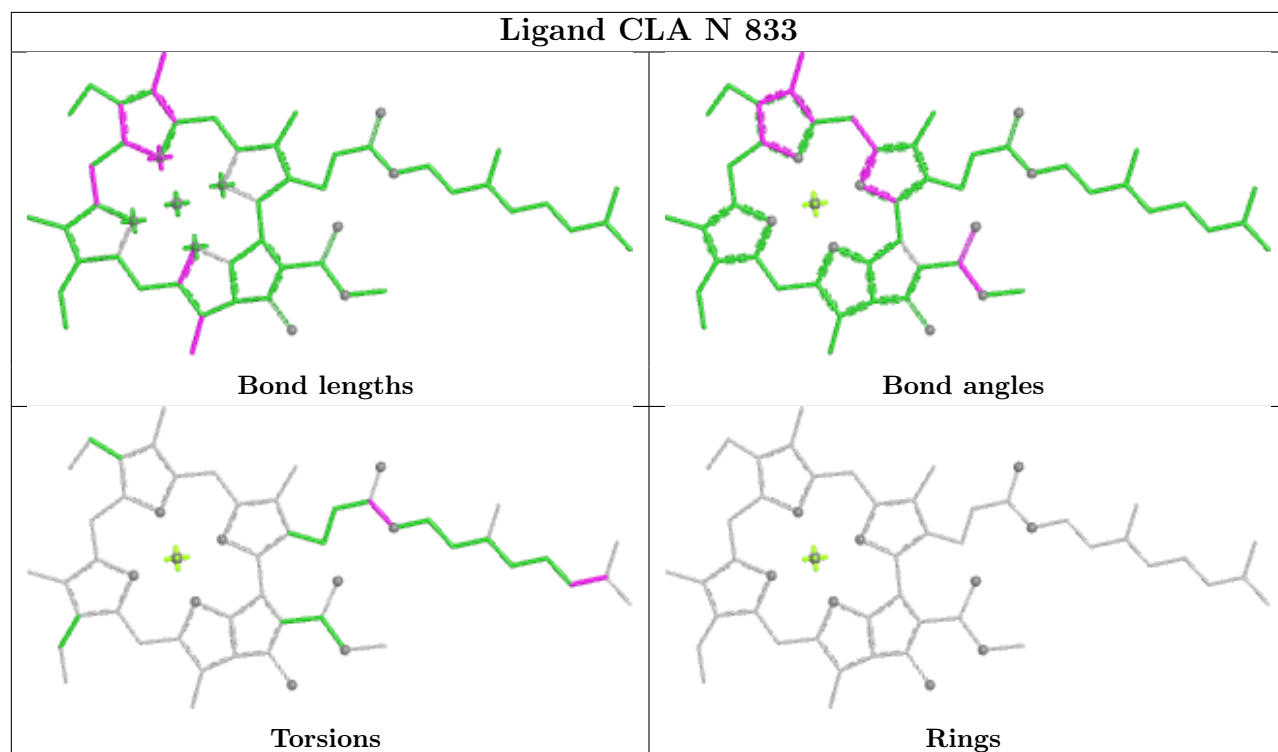
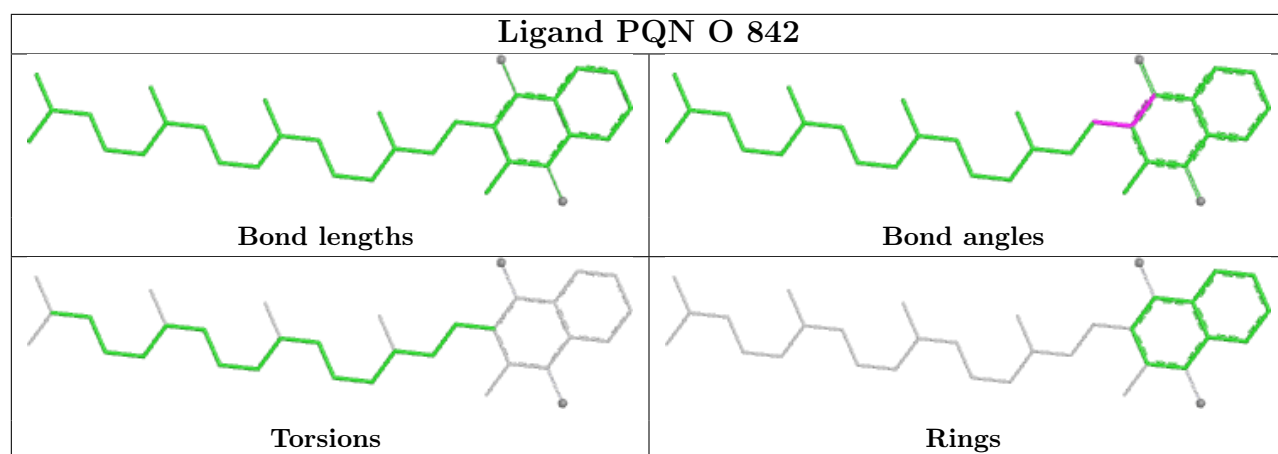
Ligand CLA B 813

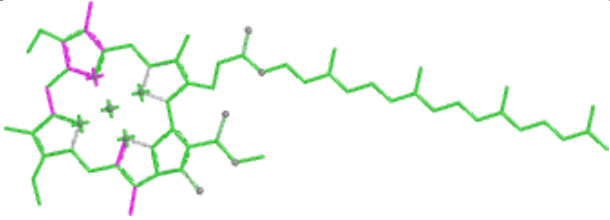
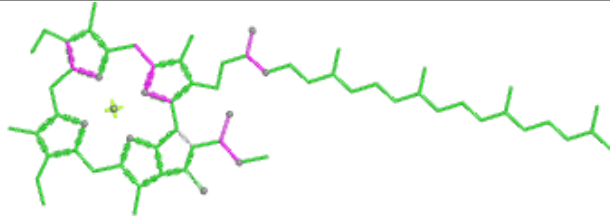
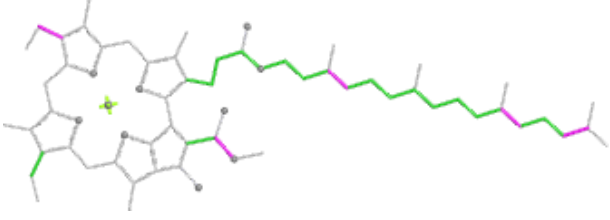
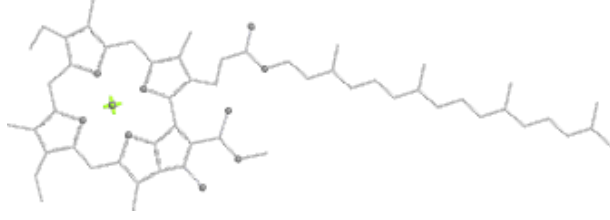
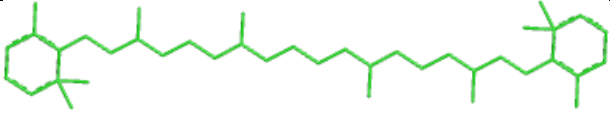
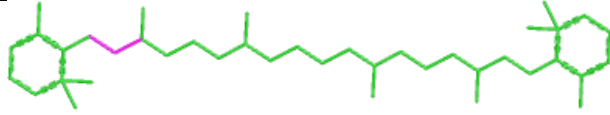
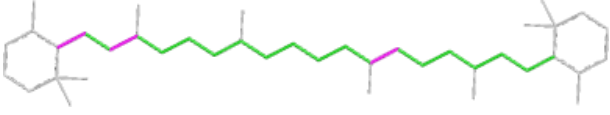
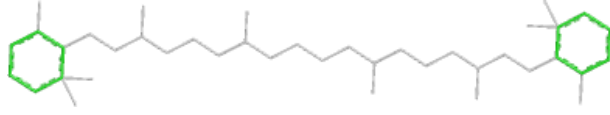
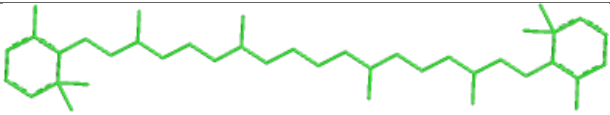
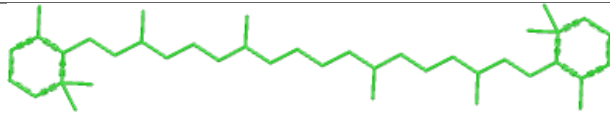
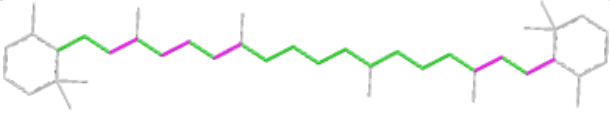
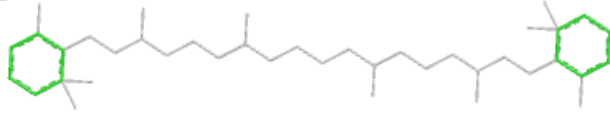


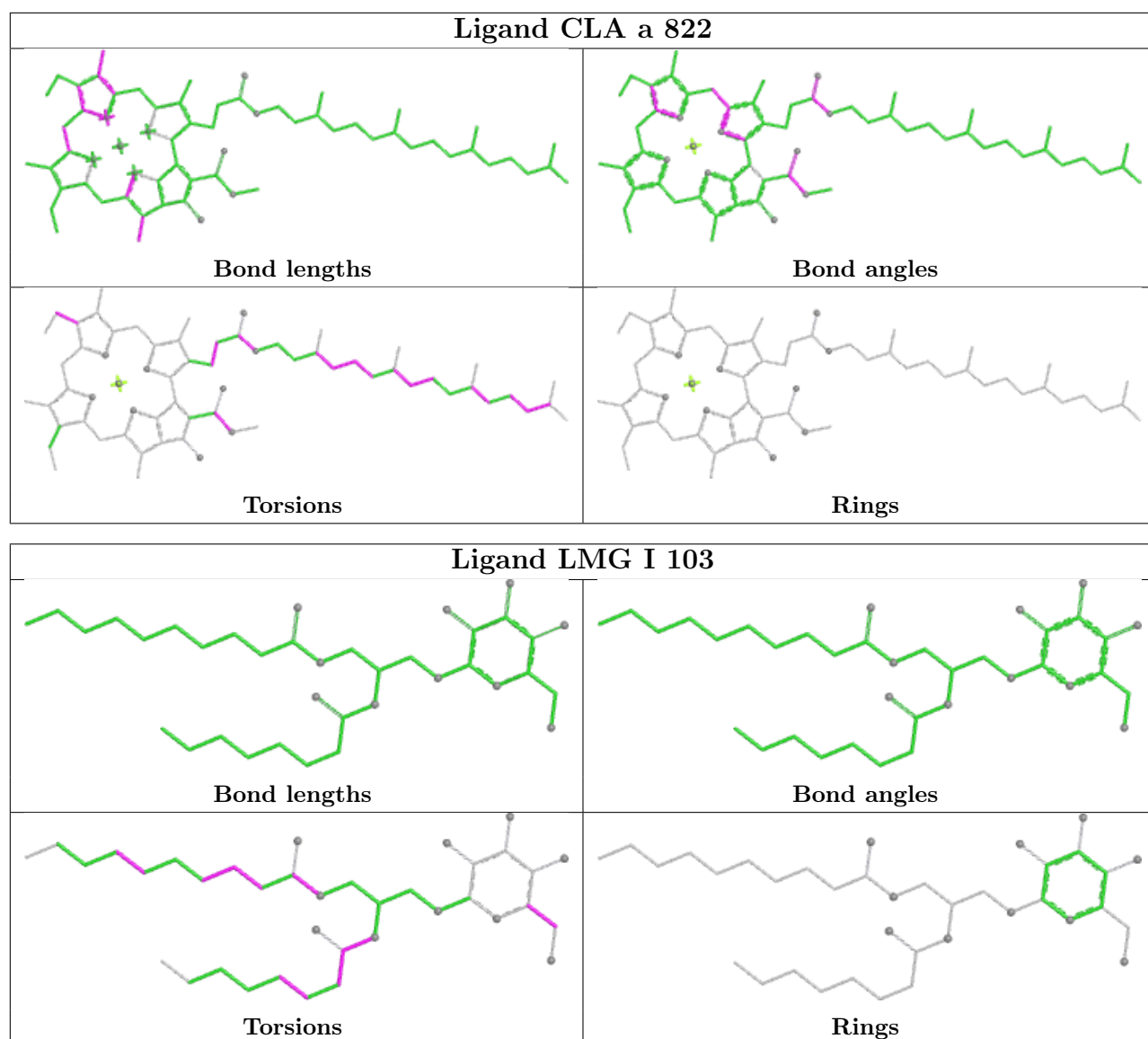




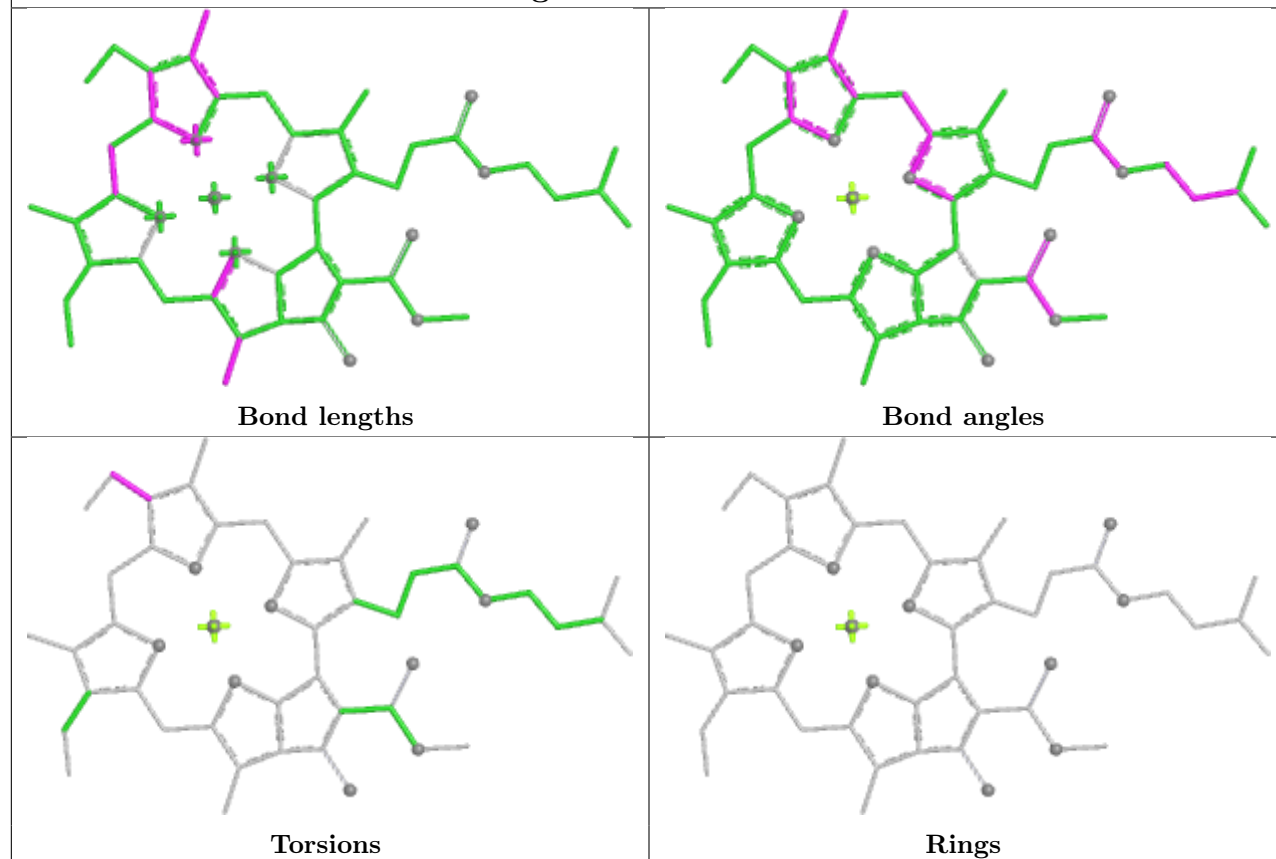




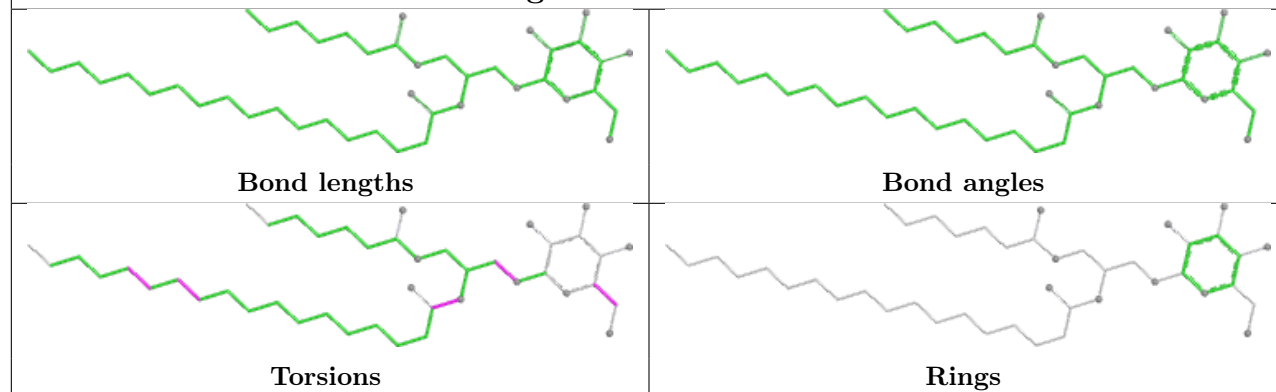
Ligand CLA N 834	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Y 102	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR I 101	
 Bond lengths	 Bond angles
 Torsions	 Rings

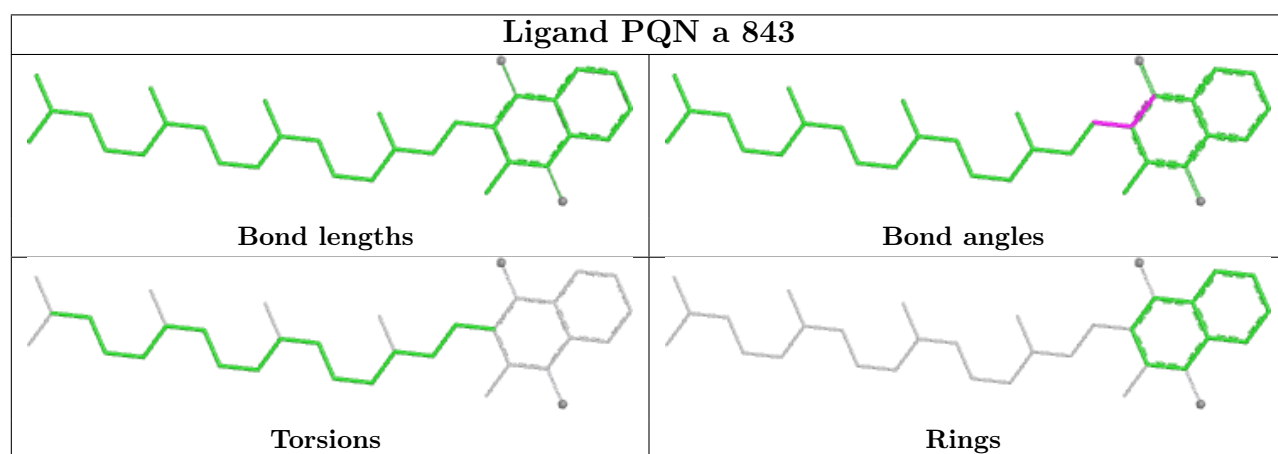
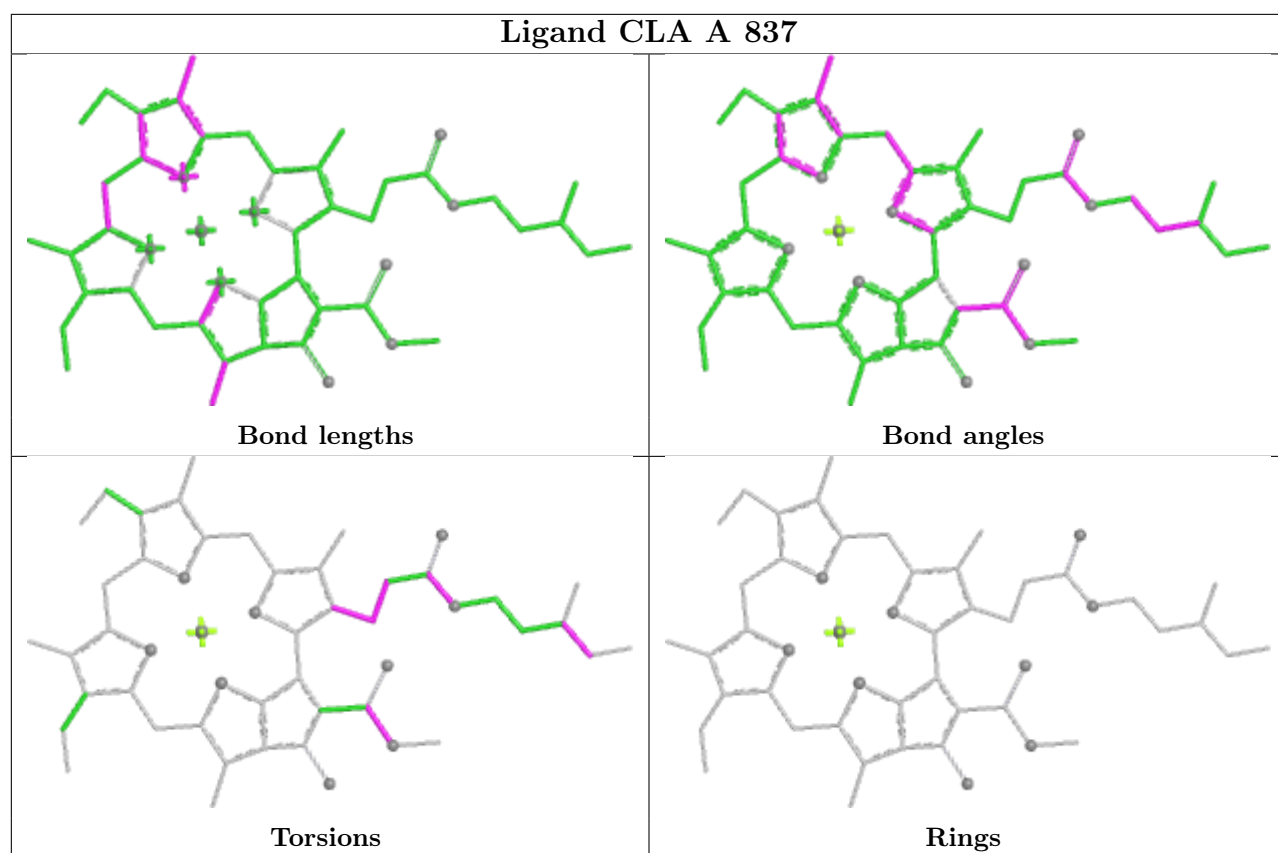


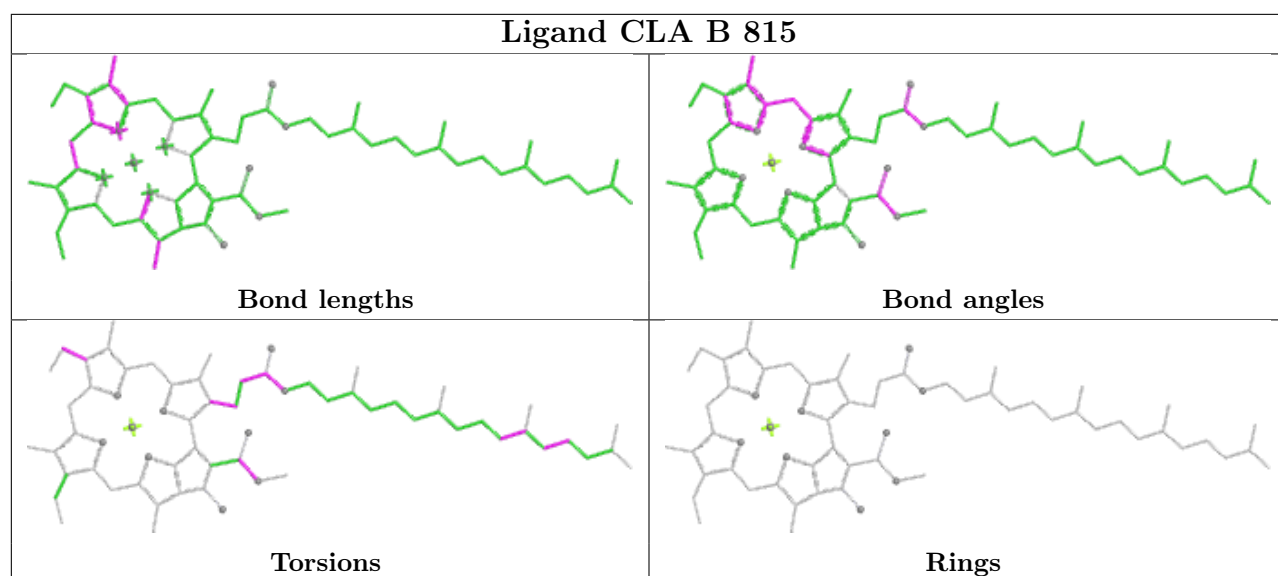
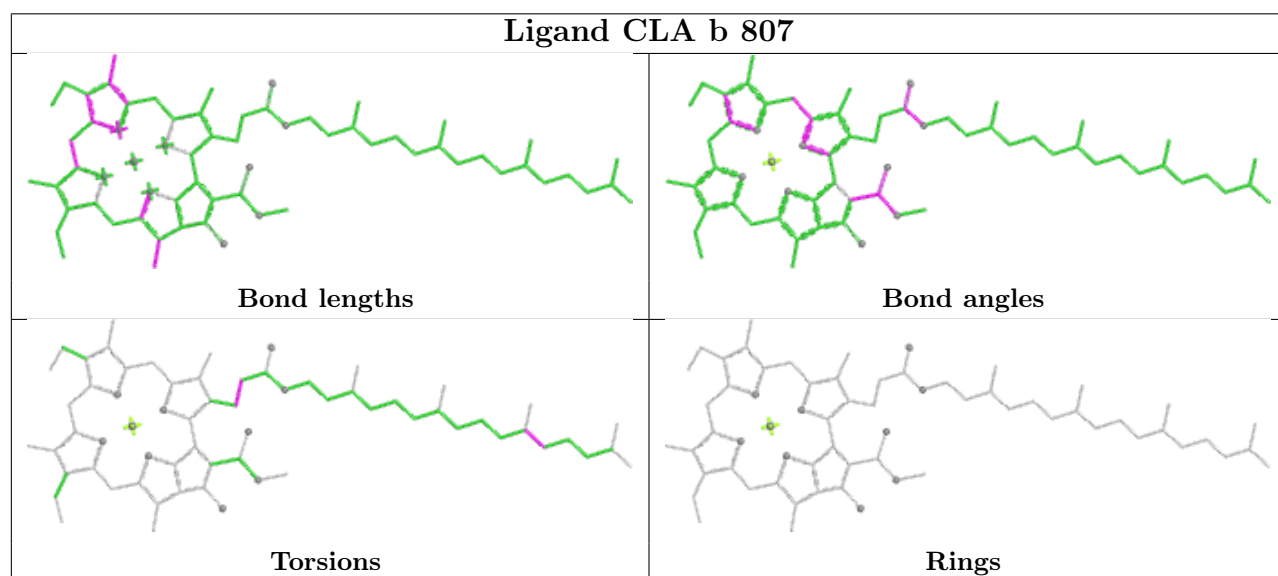
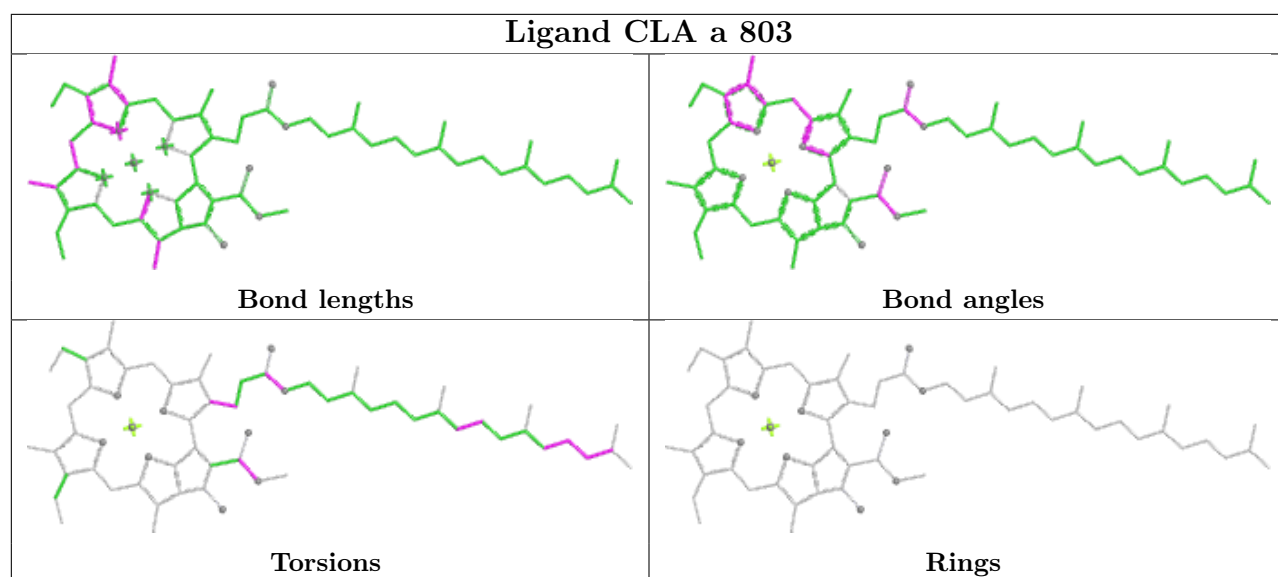
Ligand CLA V 103

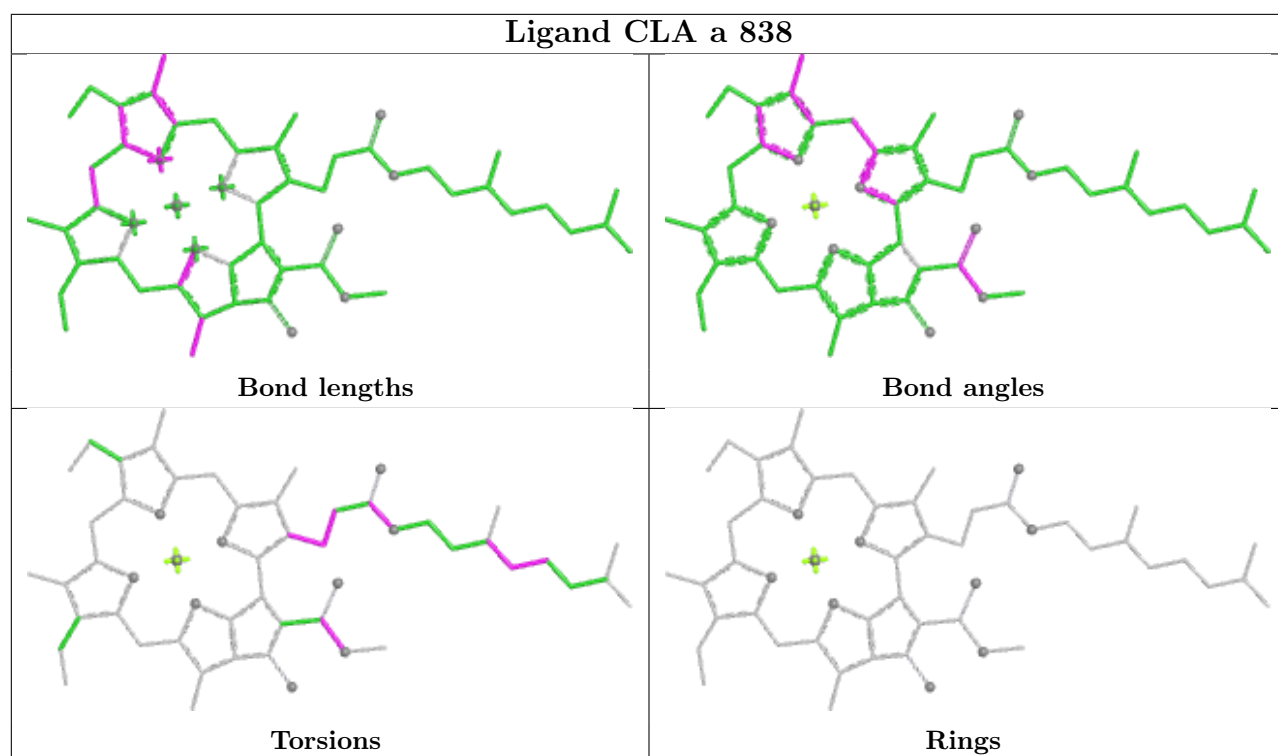


Ligand LMG N 855

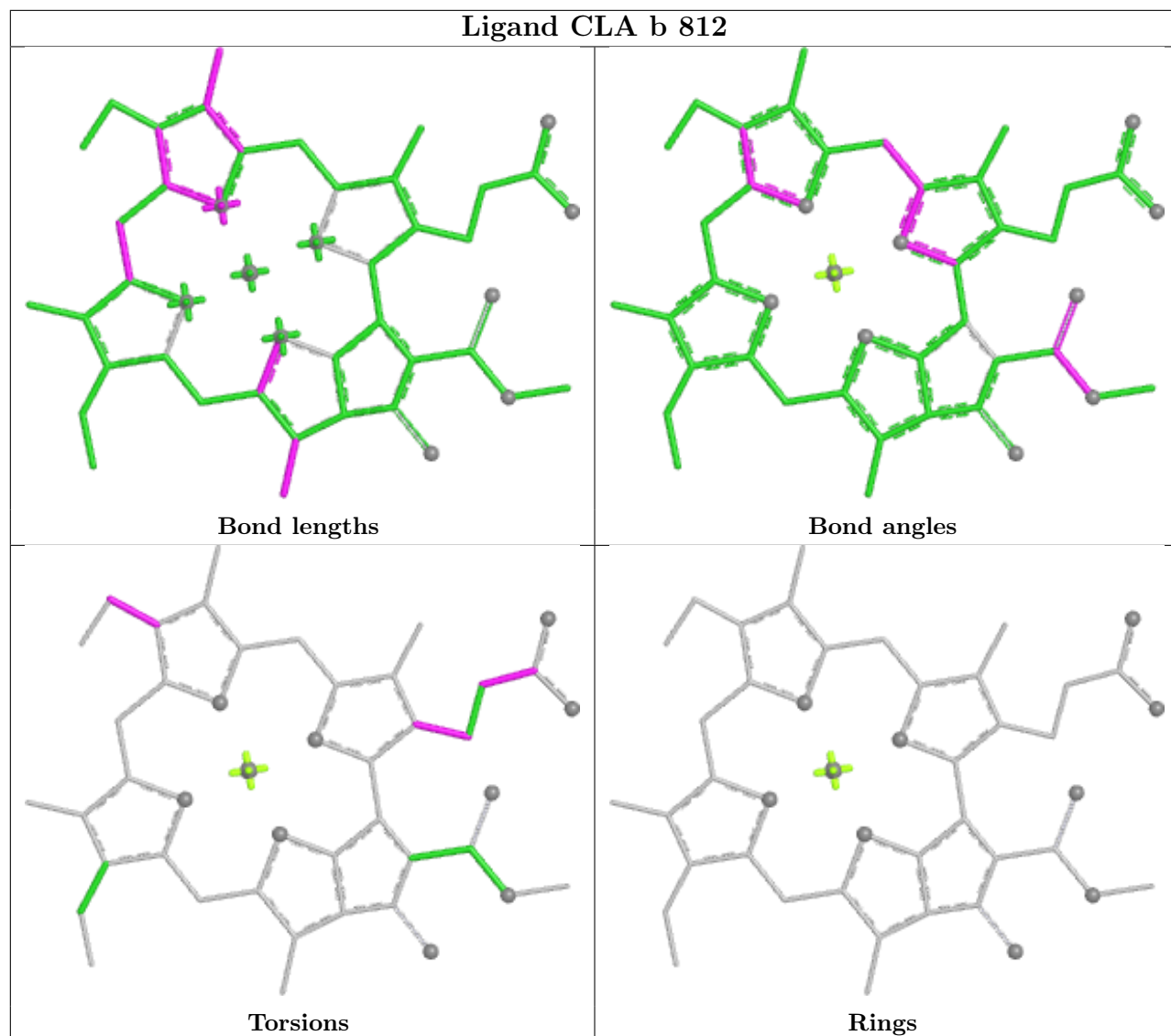




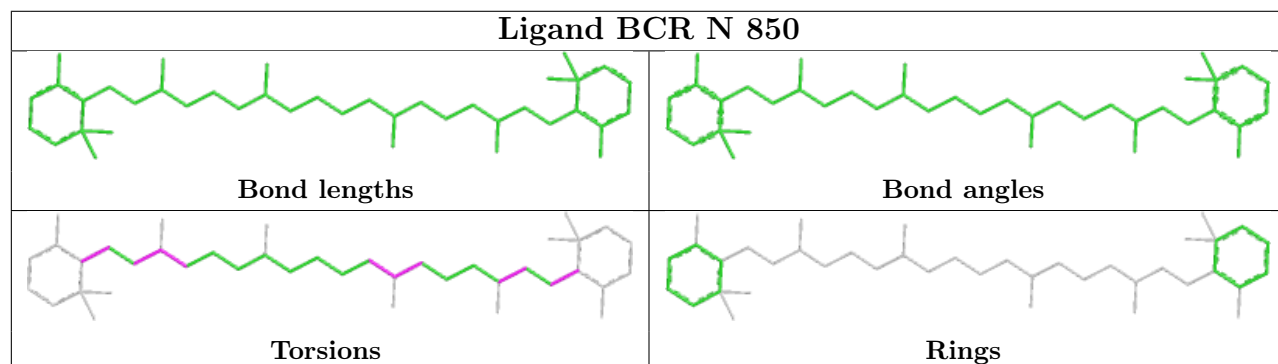


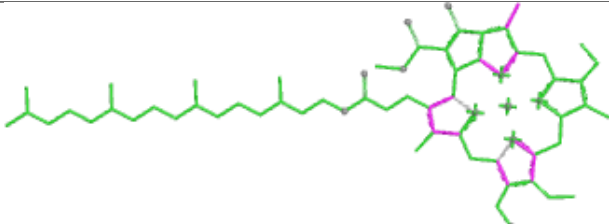
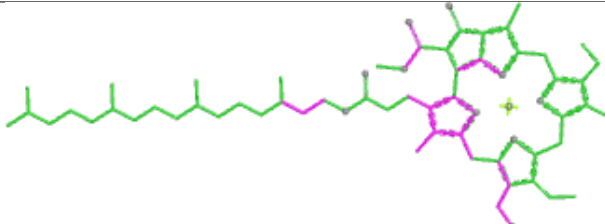
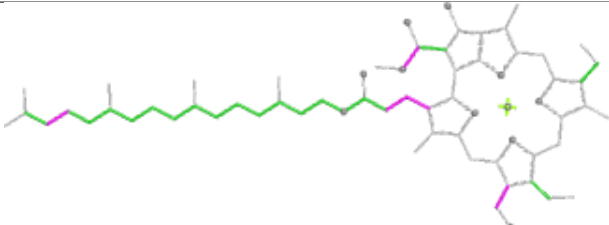
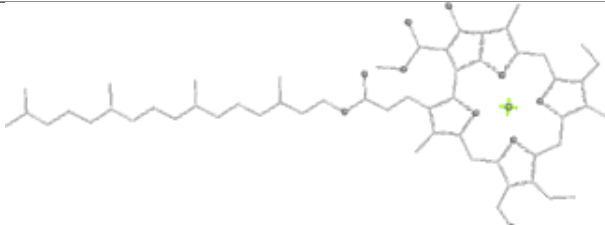


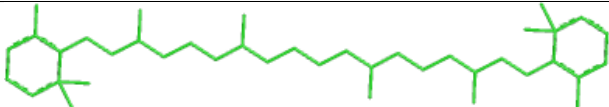
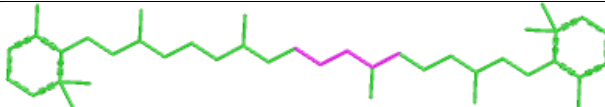
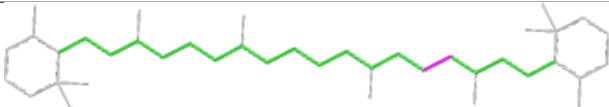
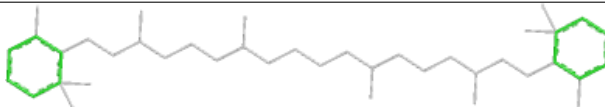
Ligand CLA b 812

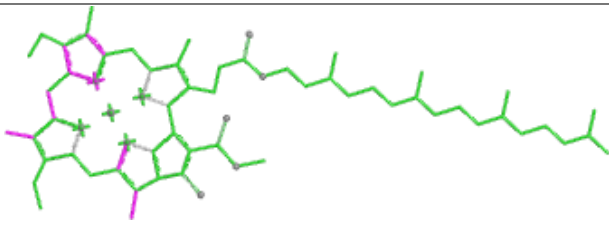
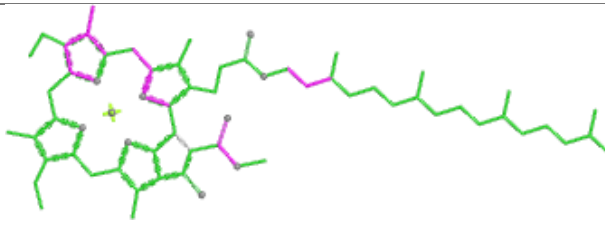
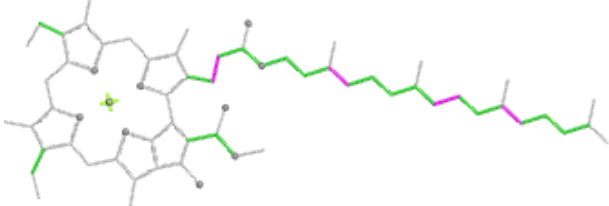
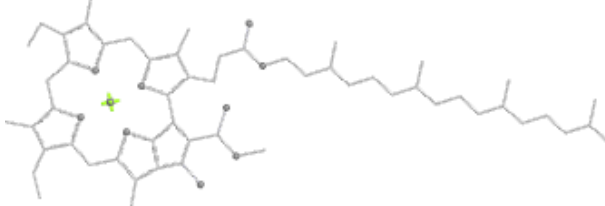


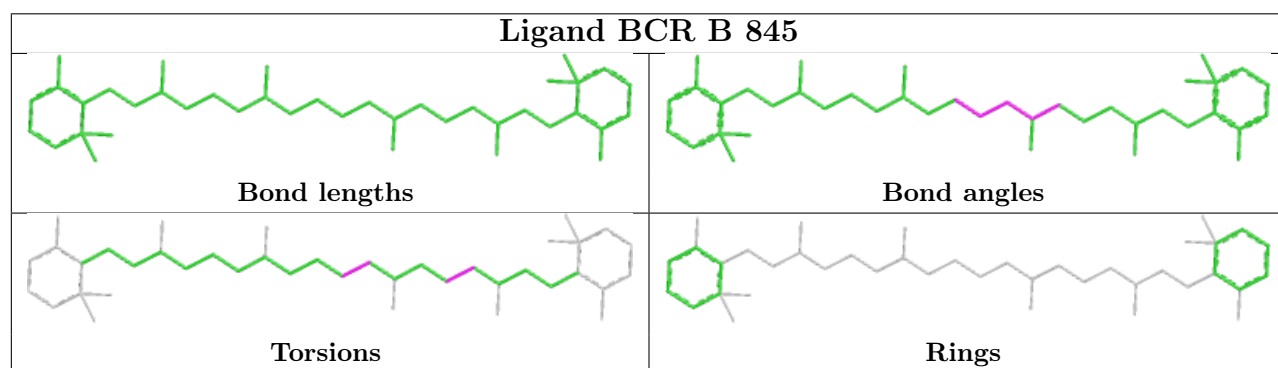
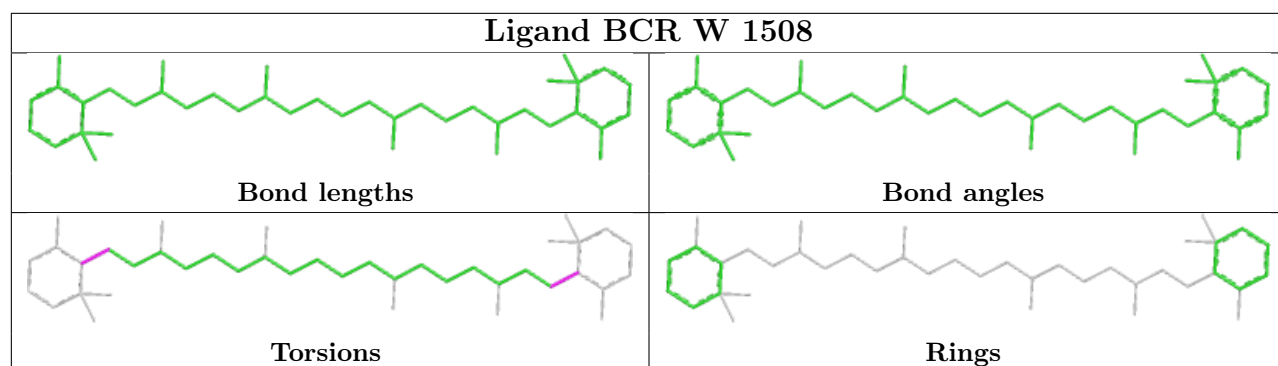
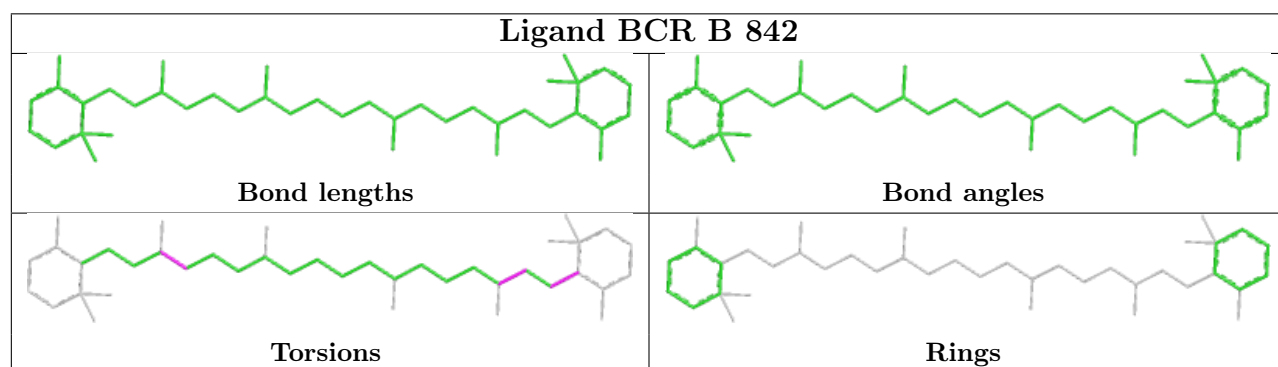
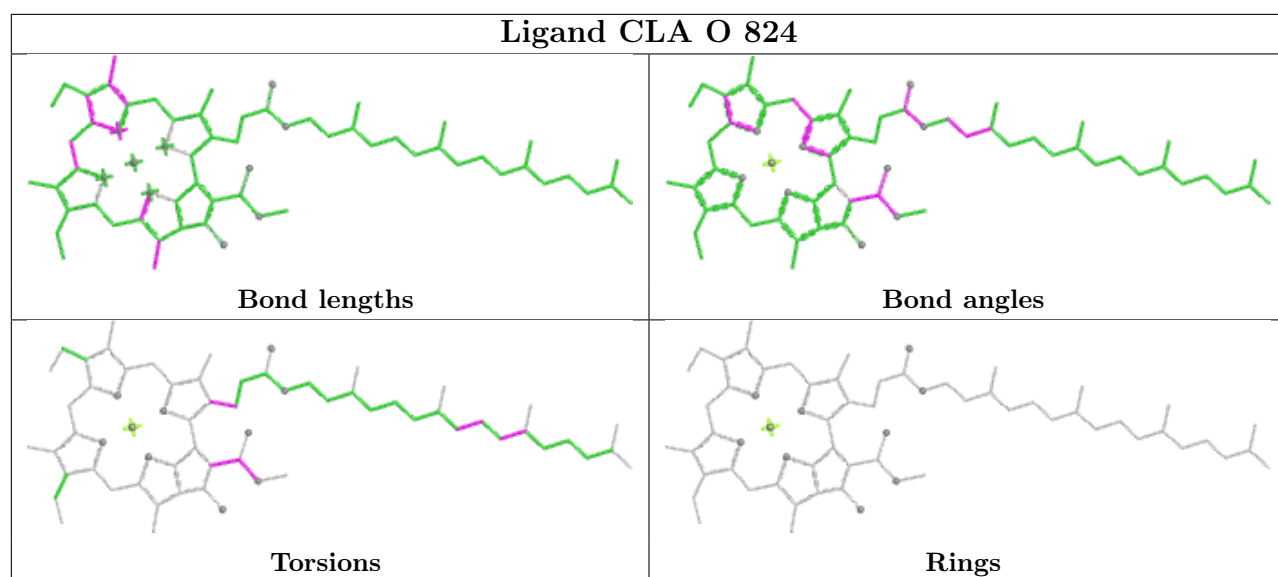
Ligand BCR N 850

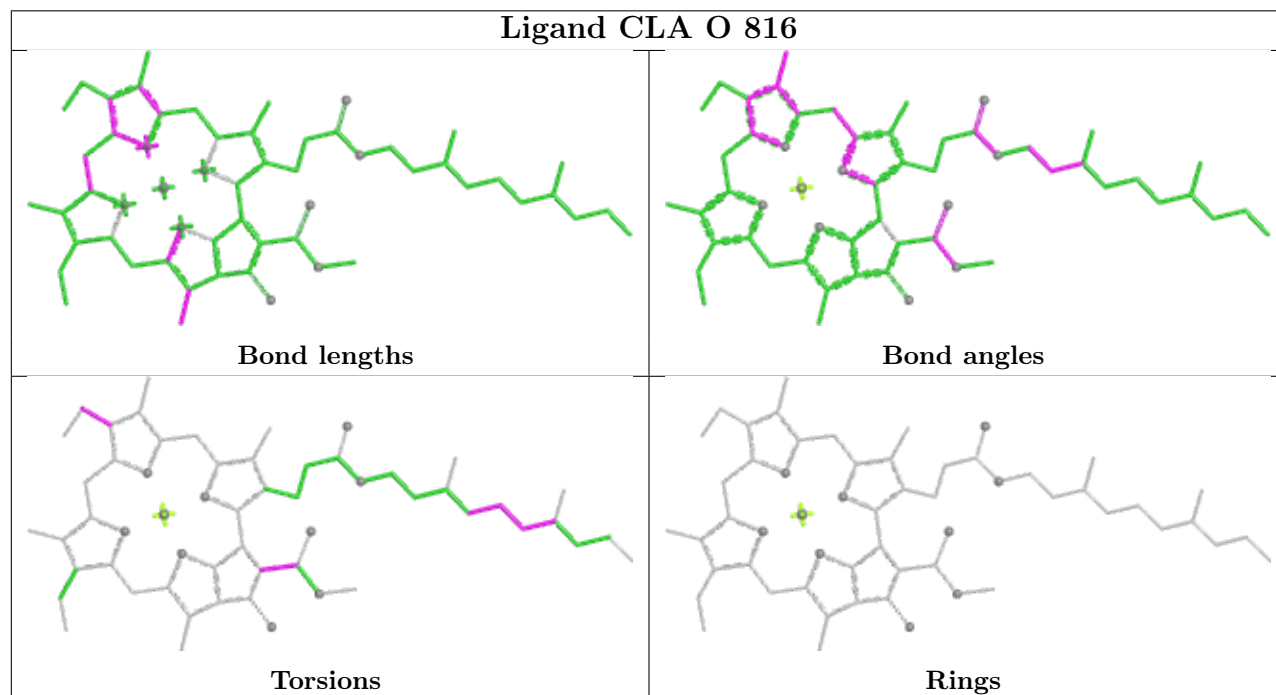
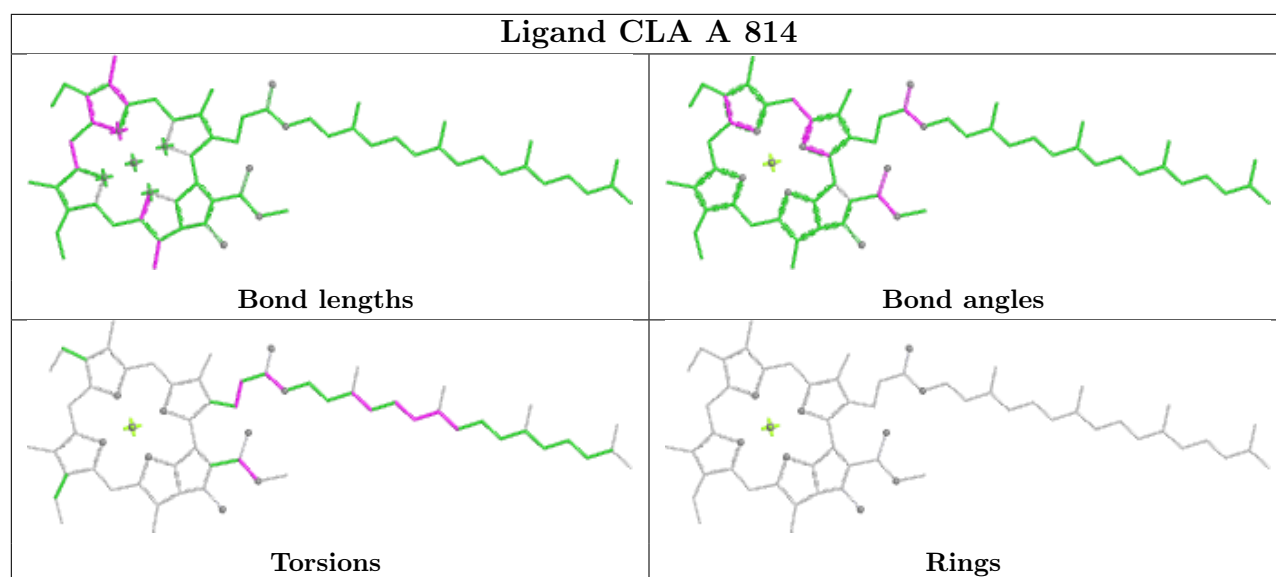


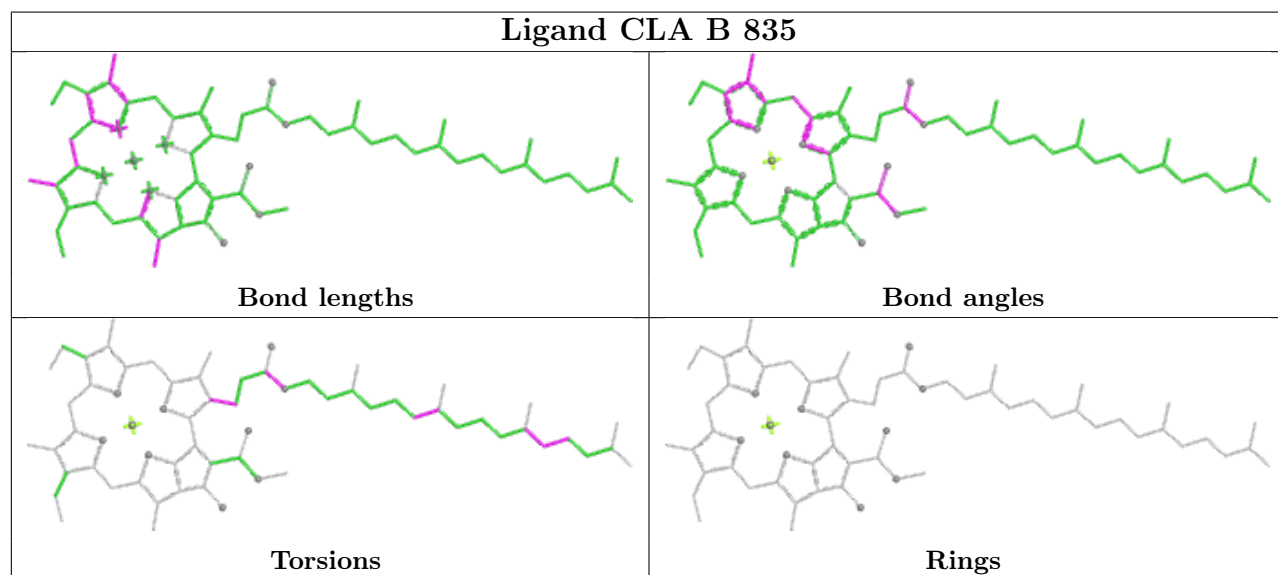
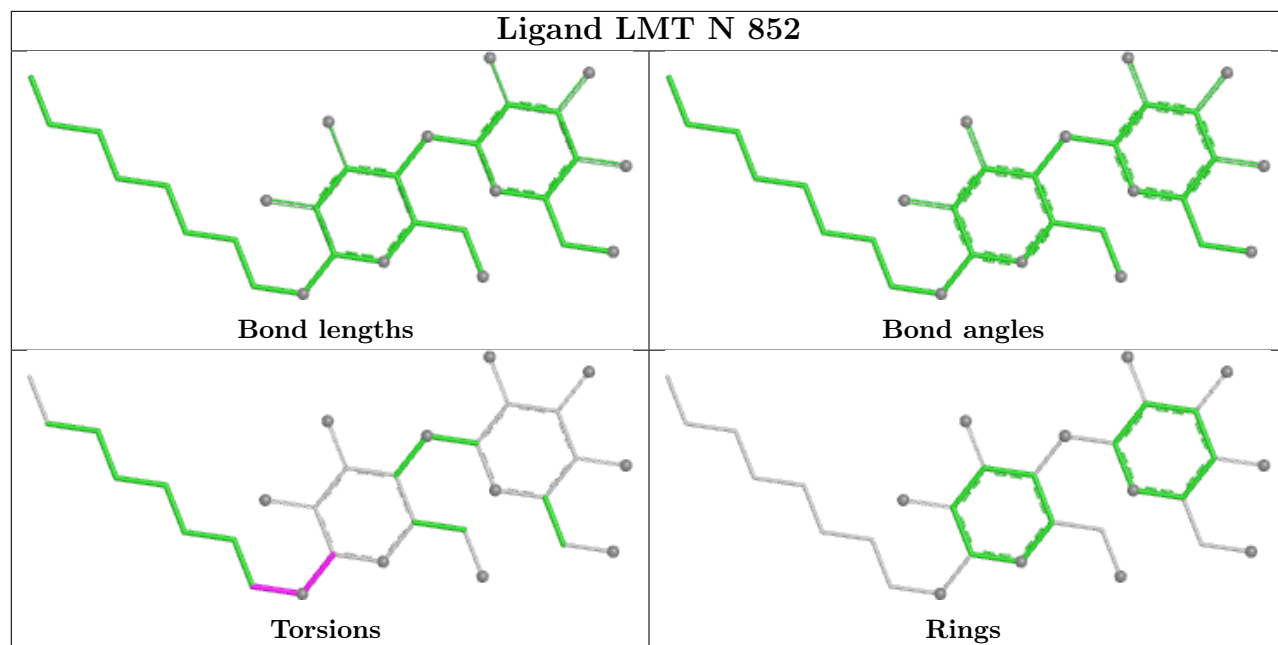
Ligand F6C a 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

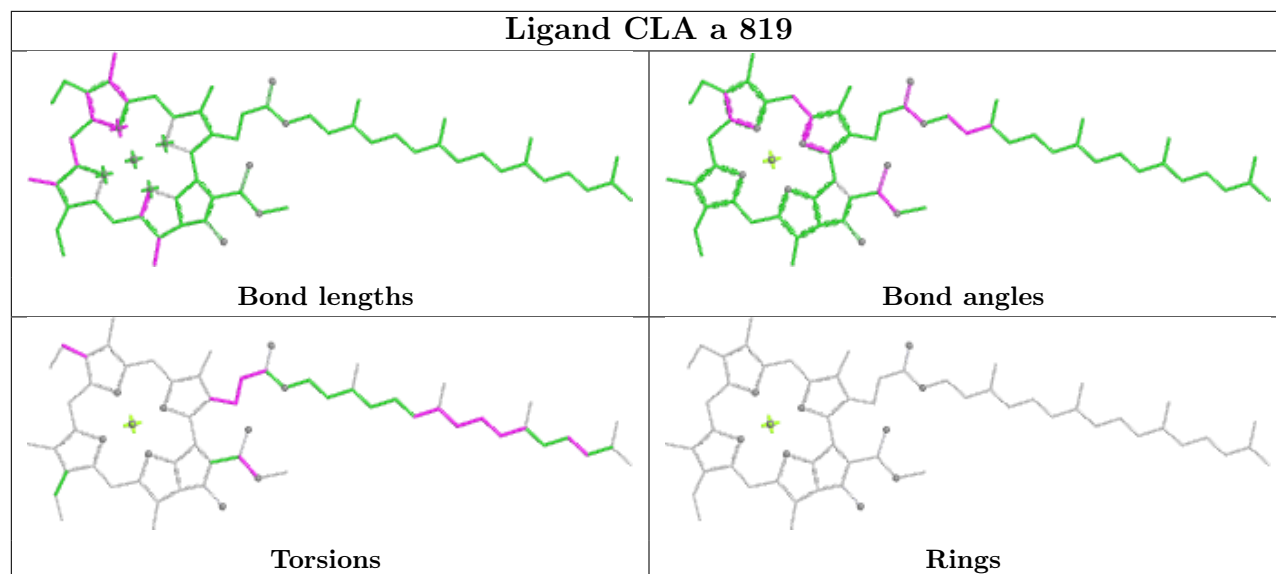
Ligand CLA a 830	
	
Bond lengths	Bond angles
	
Torsions	Rings



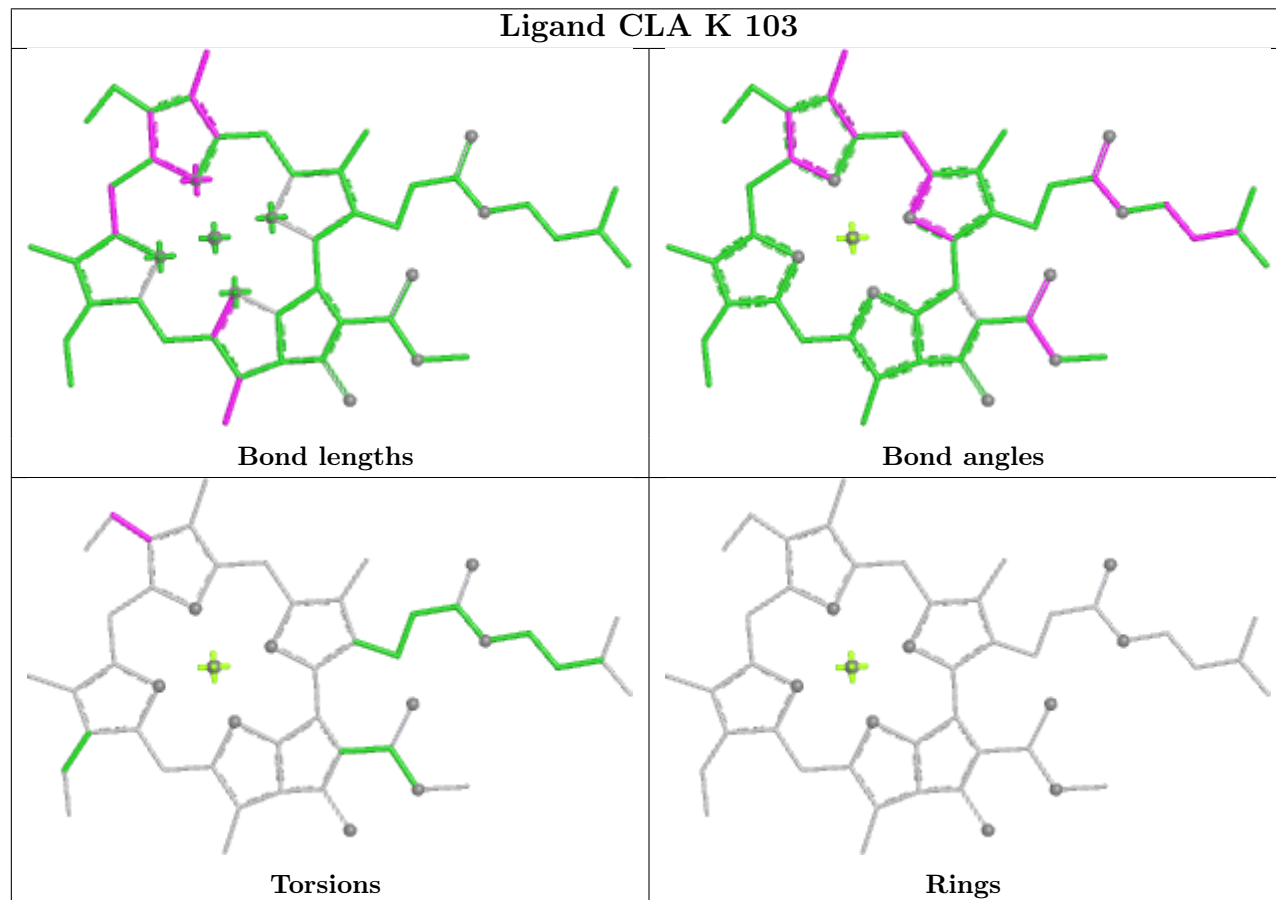




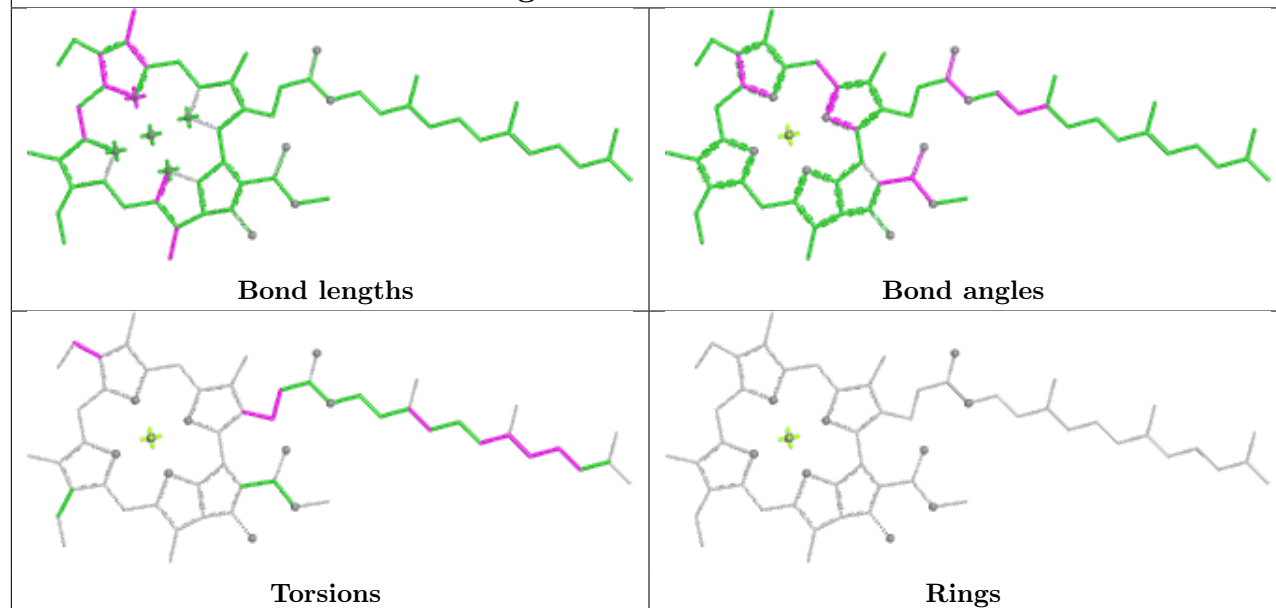
Ligand CLA a 819



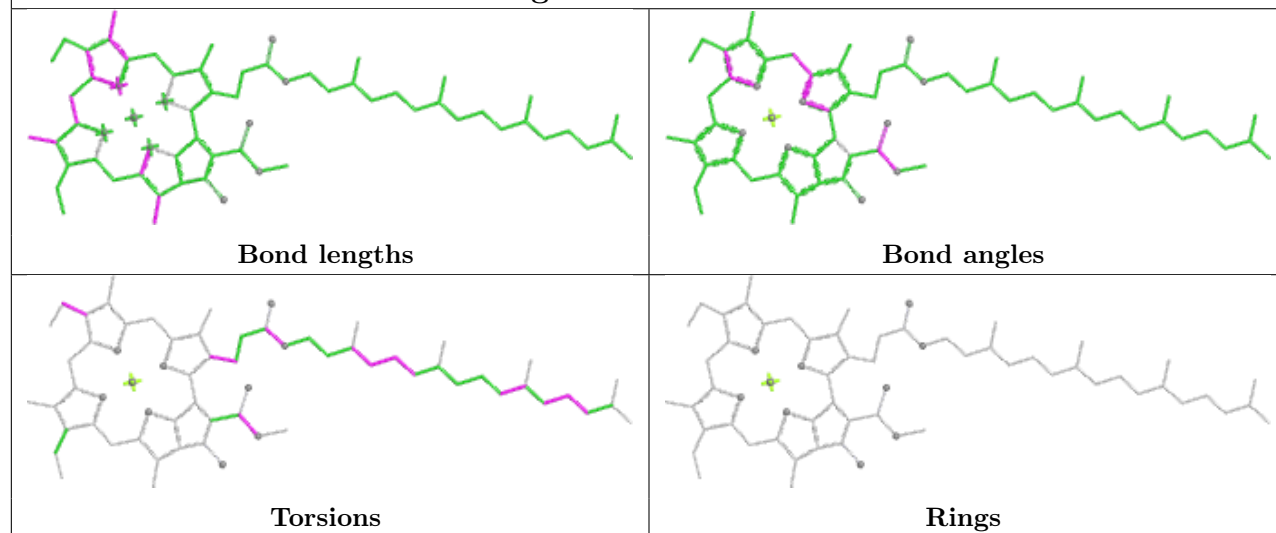
Ligand CLA K 103

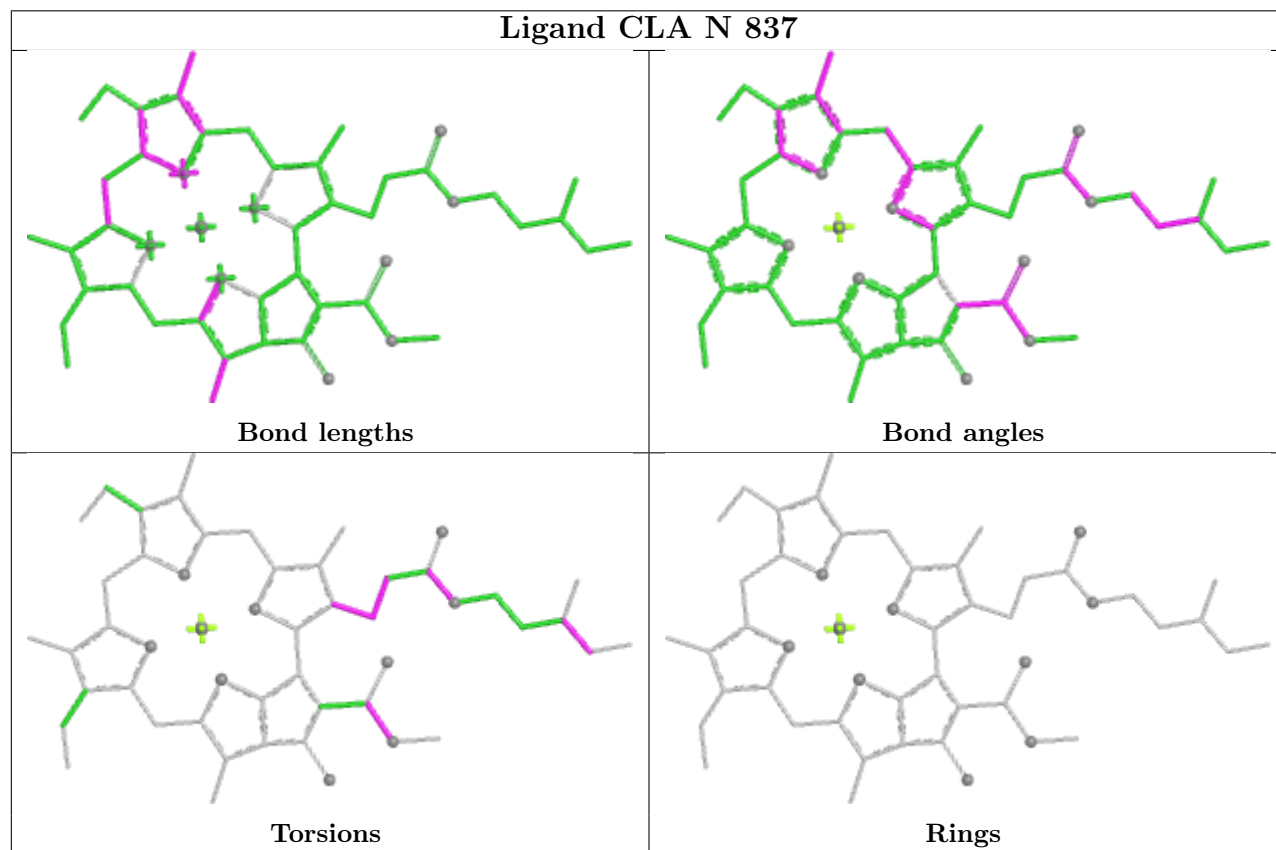
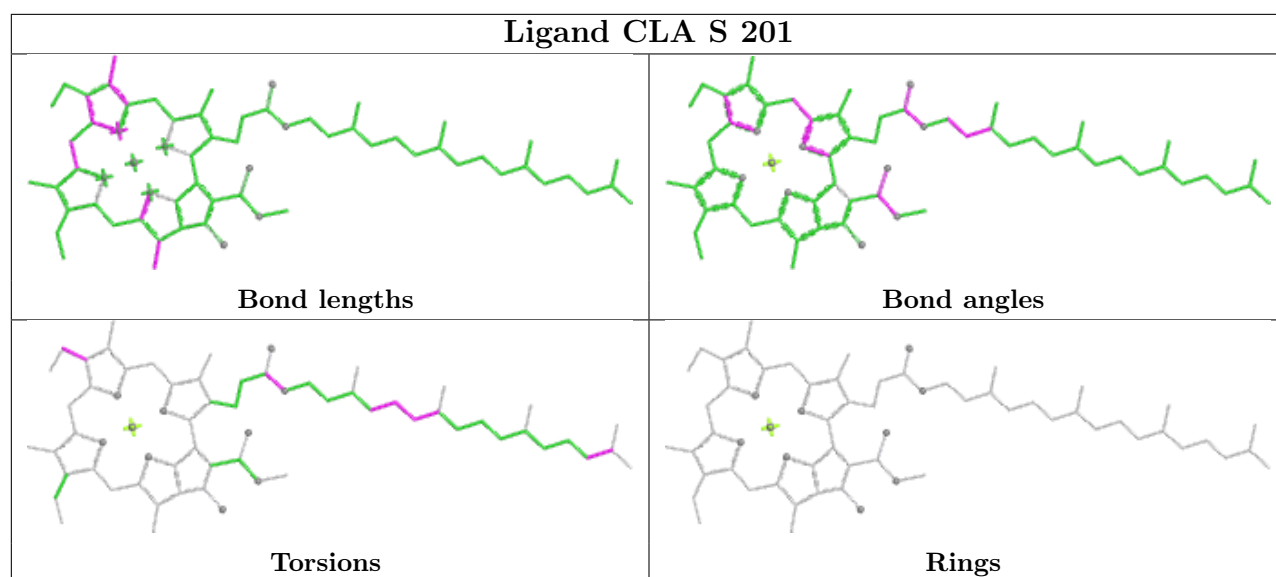


Ligand CLA W 1502

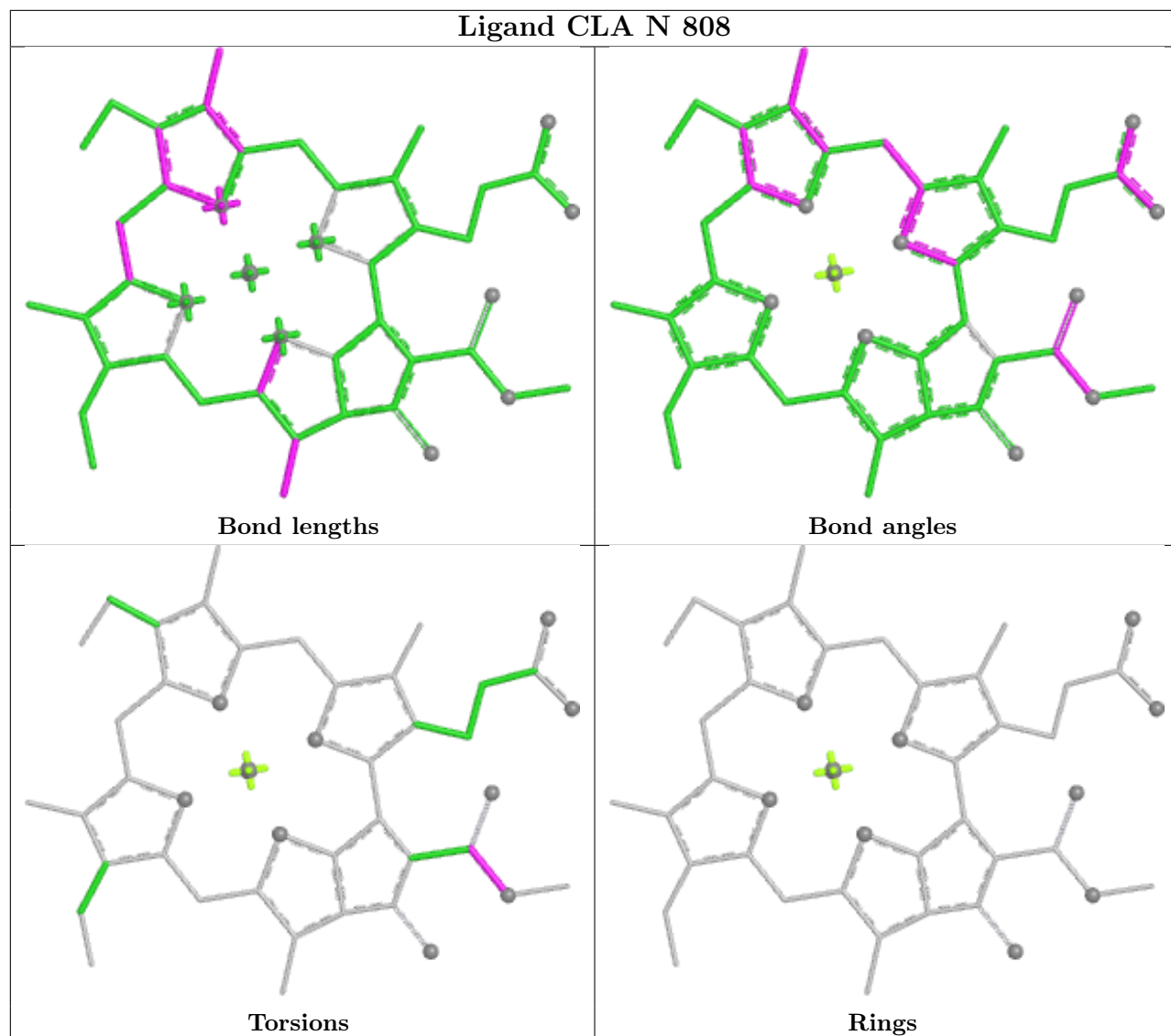


Ligand CLA N 841

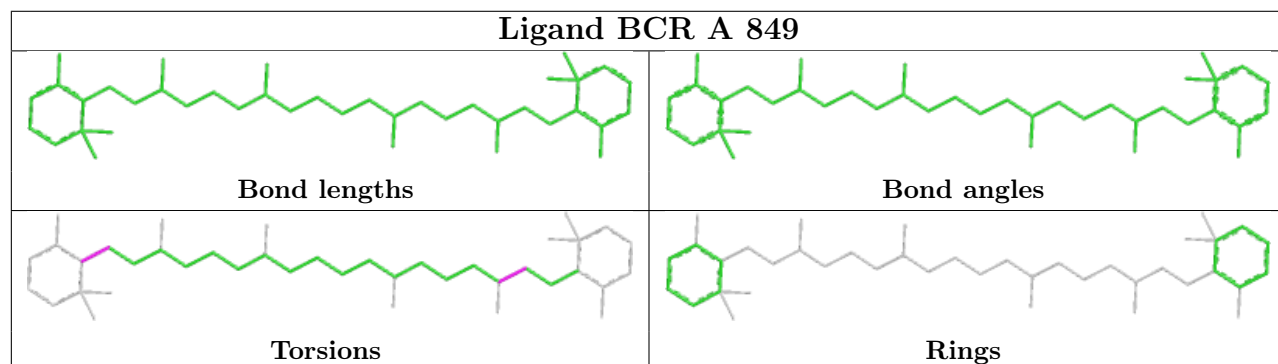


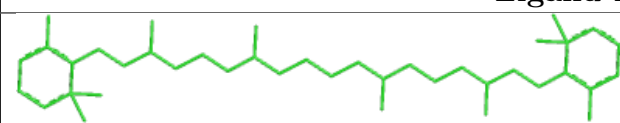
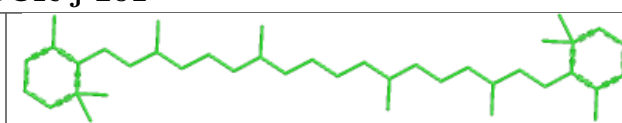
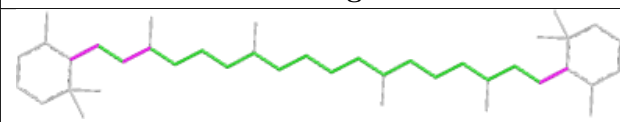
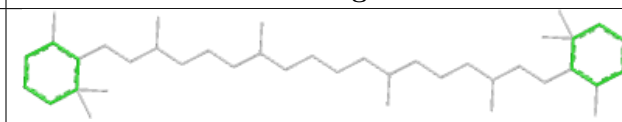


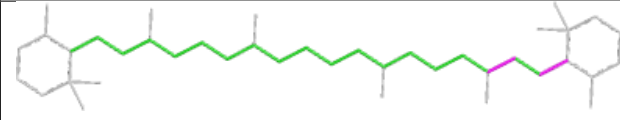
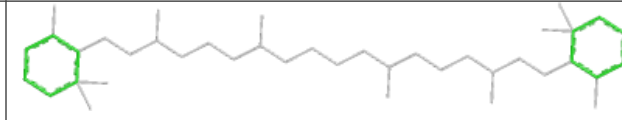
Ligand CLA N 808

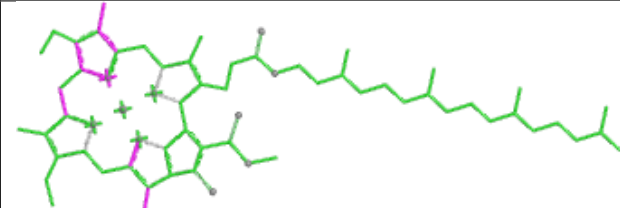
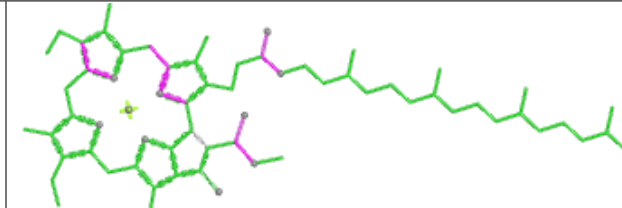
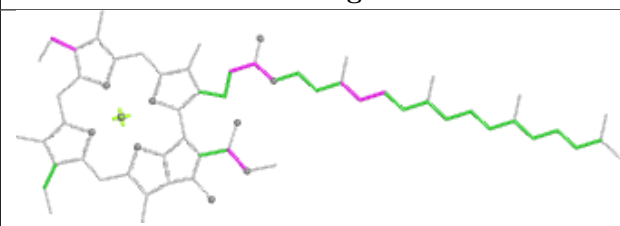
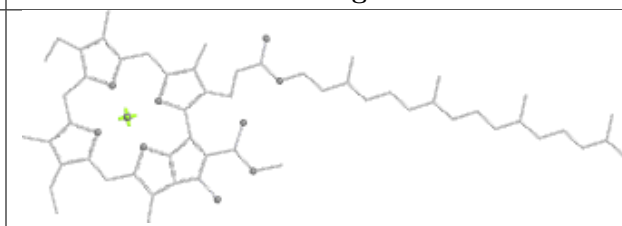


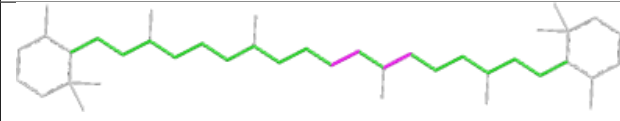
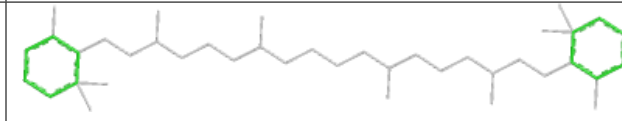
Ligand BCR A 849

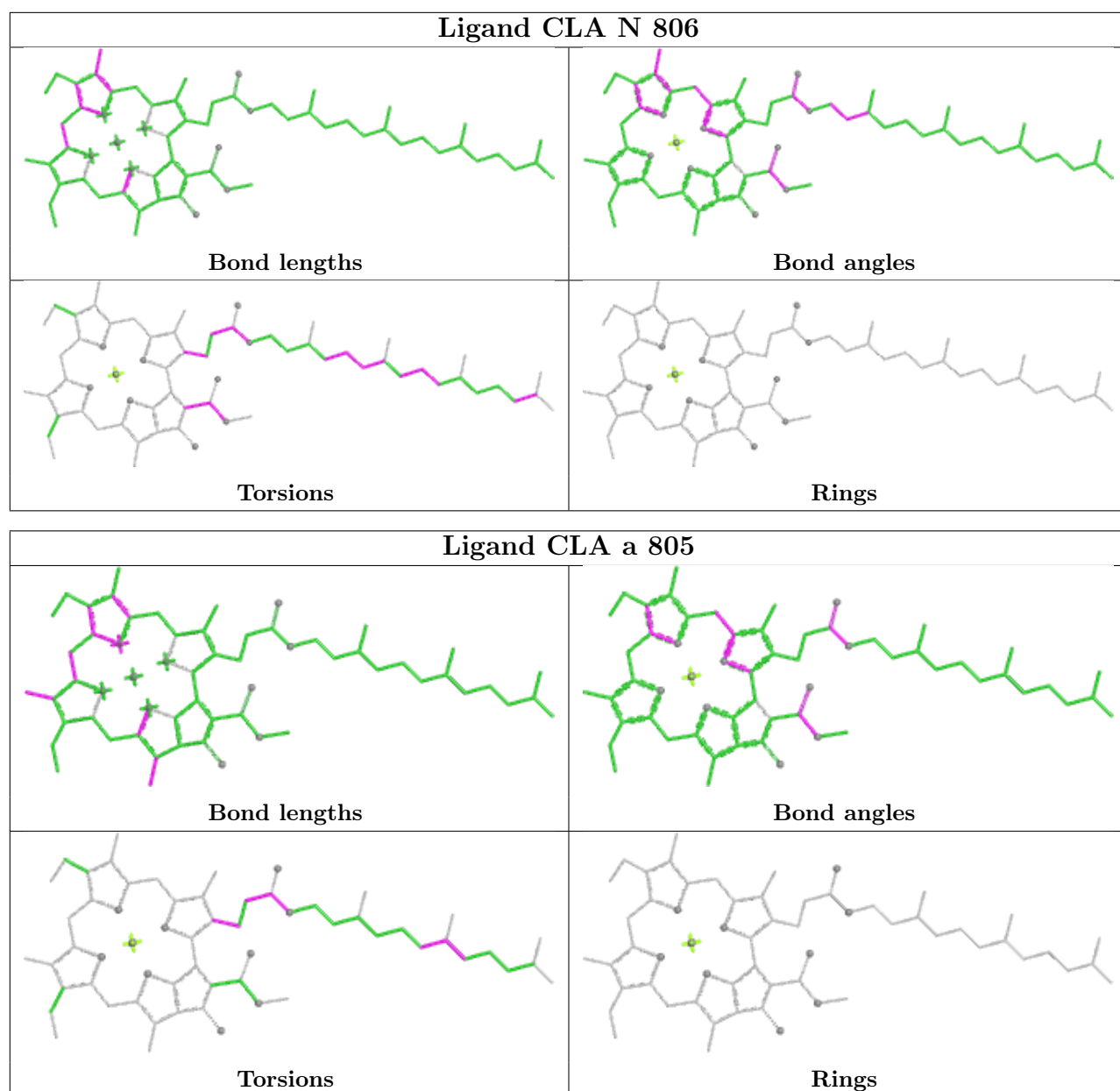


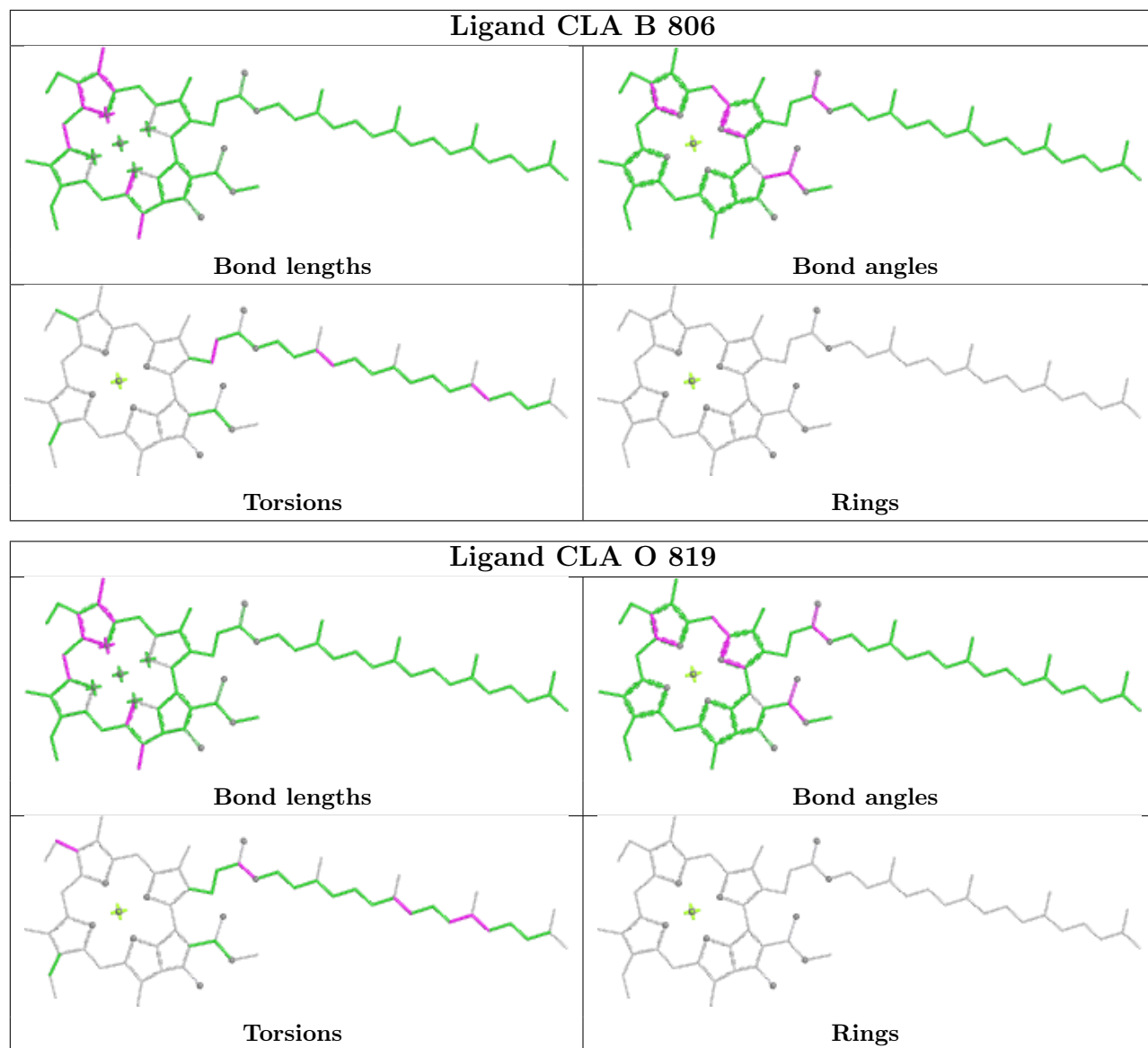
Ligand BCR j 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

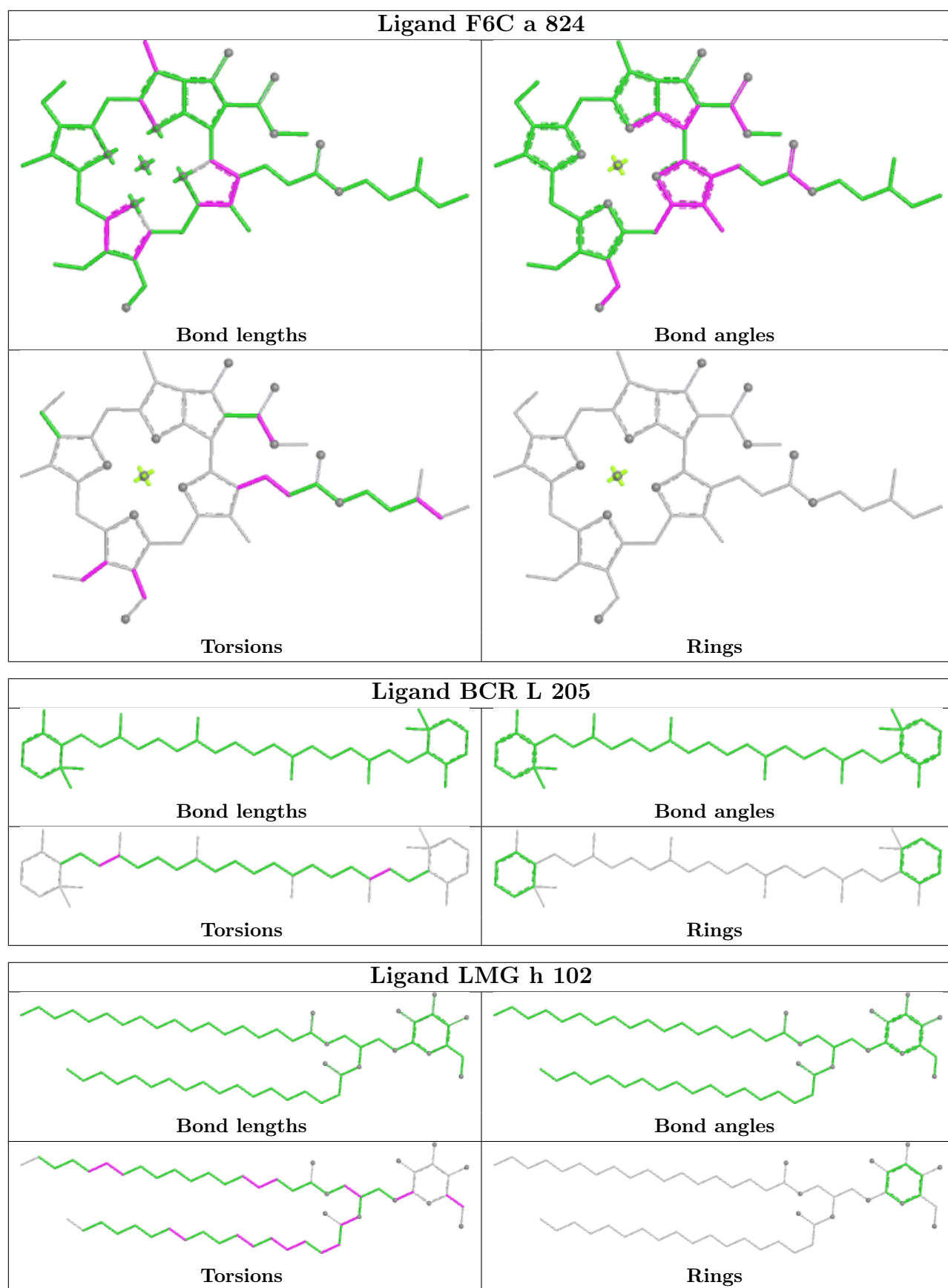
Ligand BCR O 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

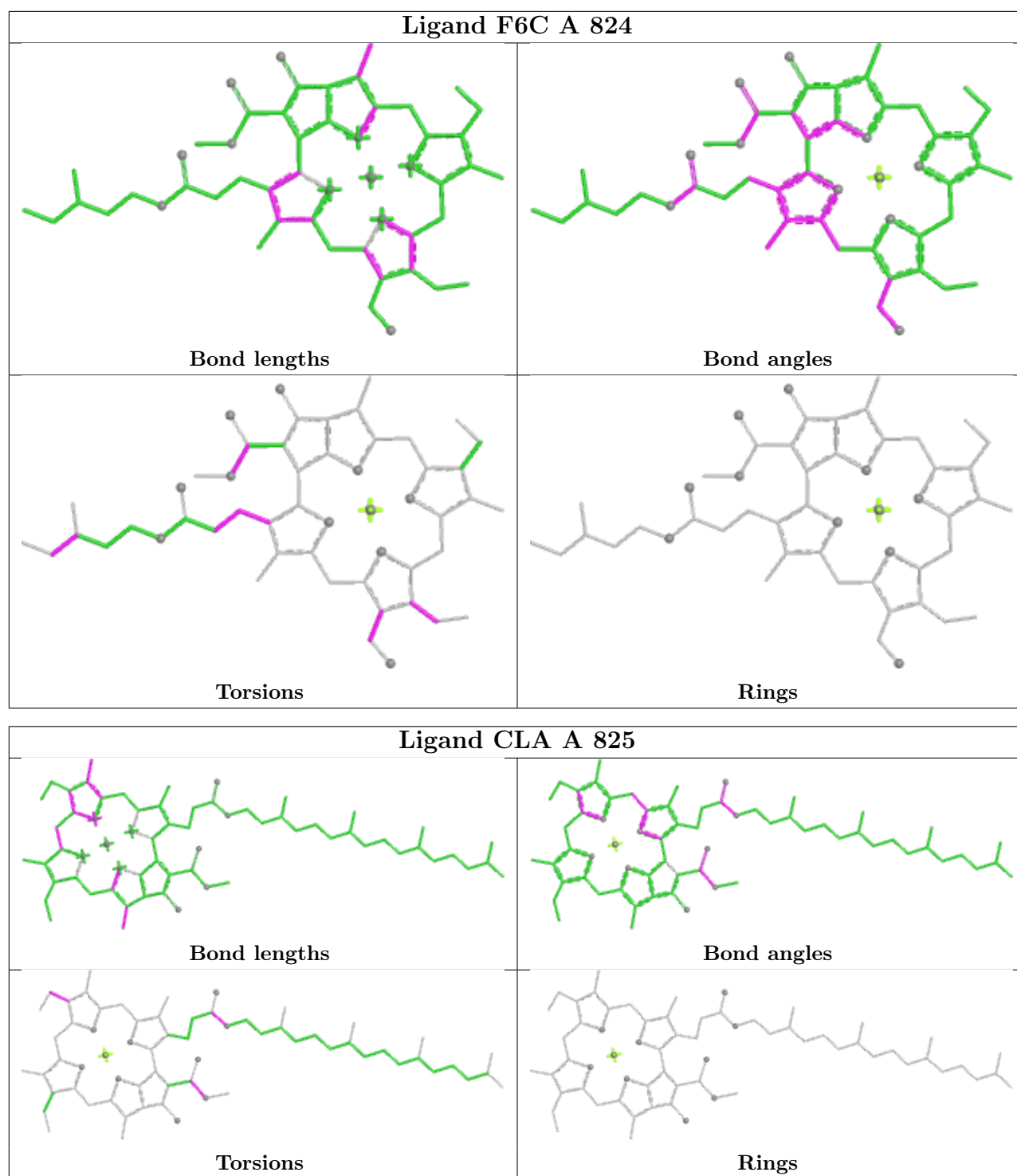
Ligand CLA a 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

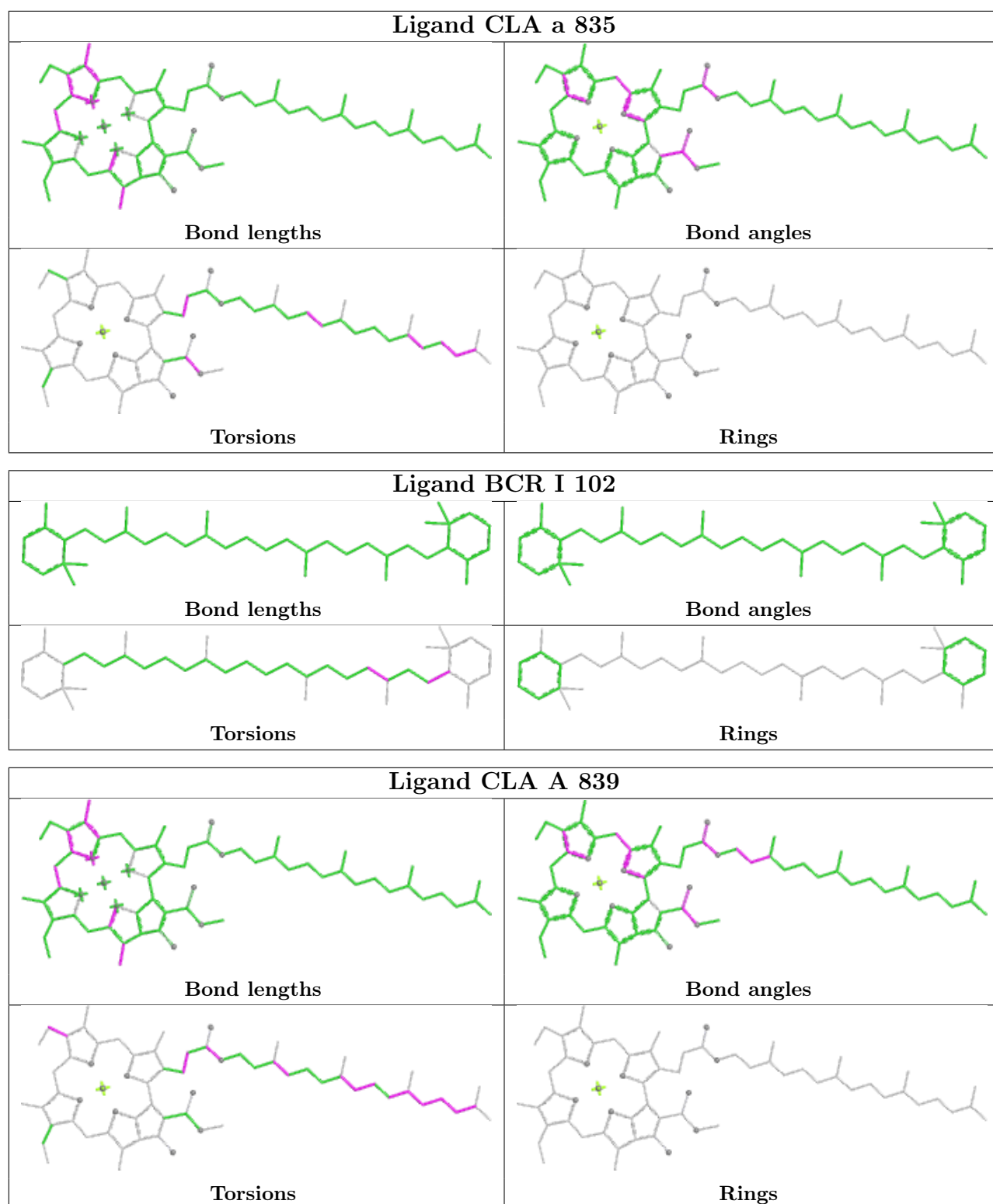
Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

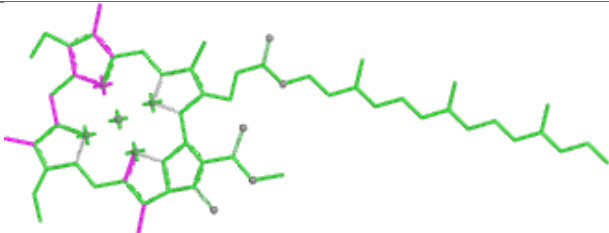
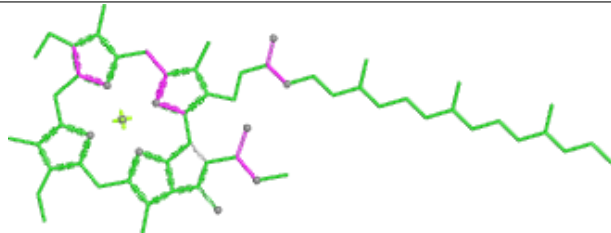
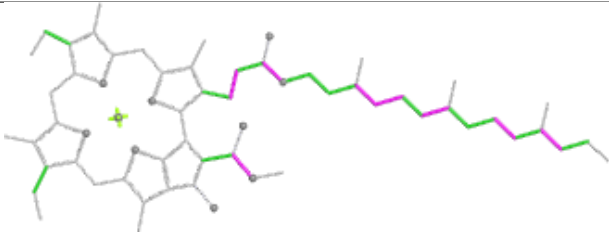
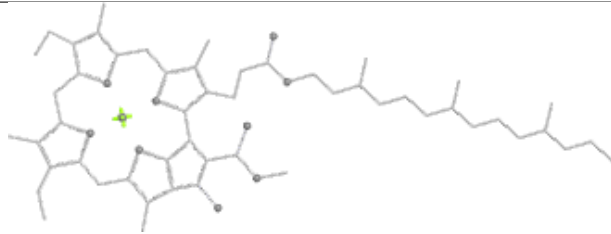


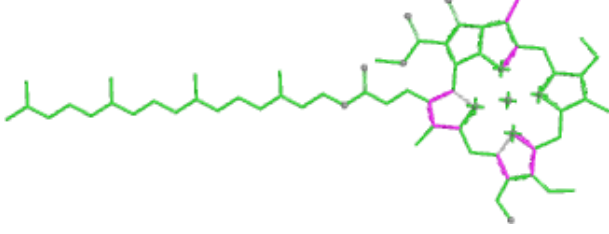
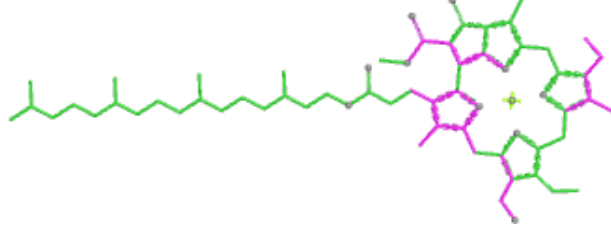
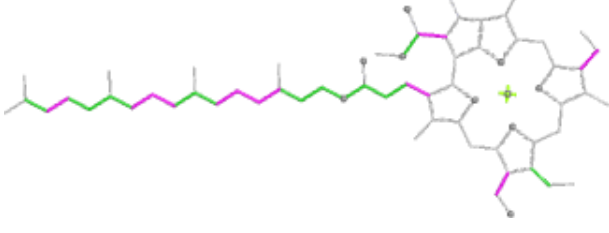
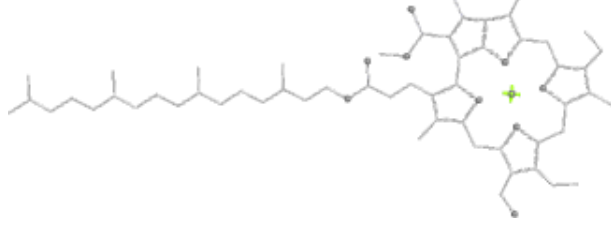


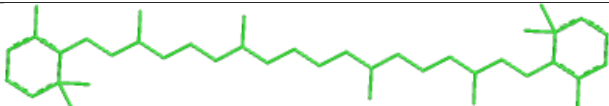
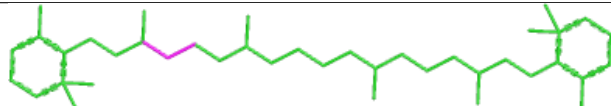
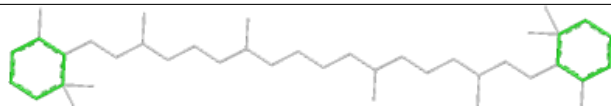




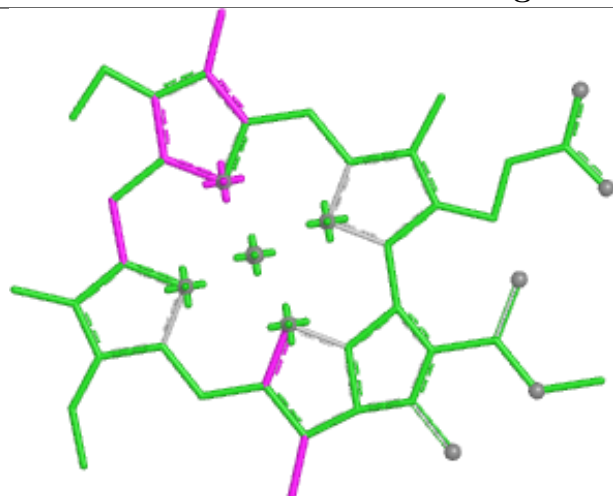


Ligand CLA O 827	
	
Bond lengths	Bond angles
	
Torsions	Rings

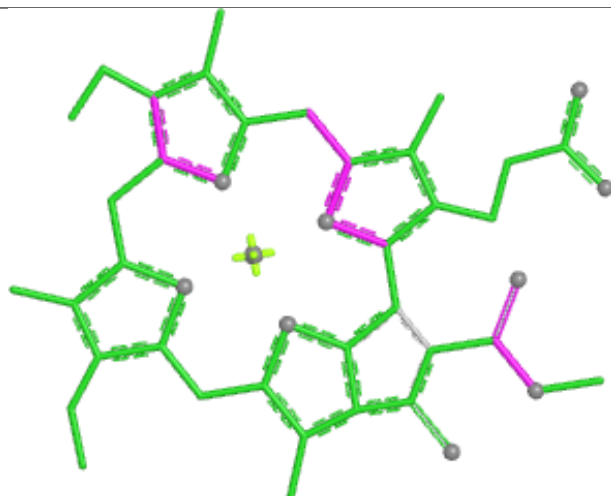
Ligand F6C A 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR a 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

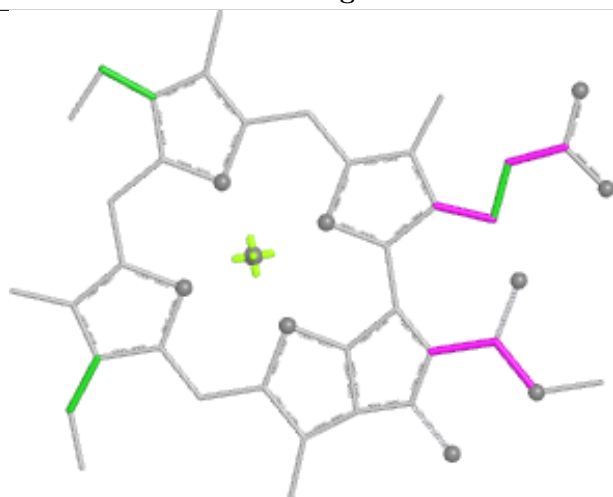
Ligand CLA O 836



Bond lengths



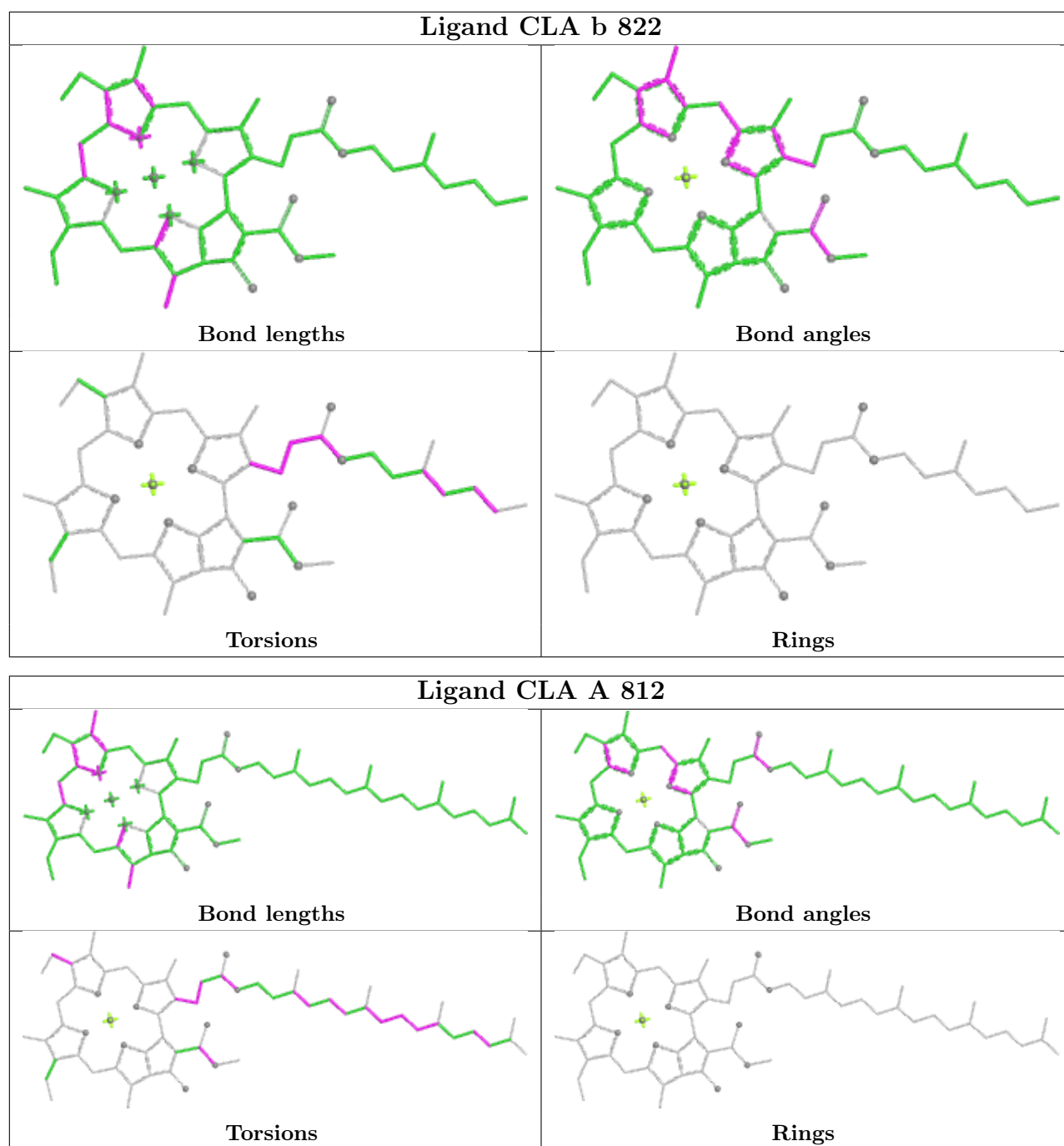
Bond angles



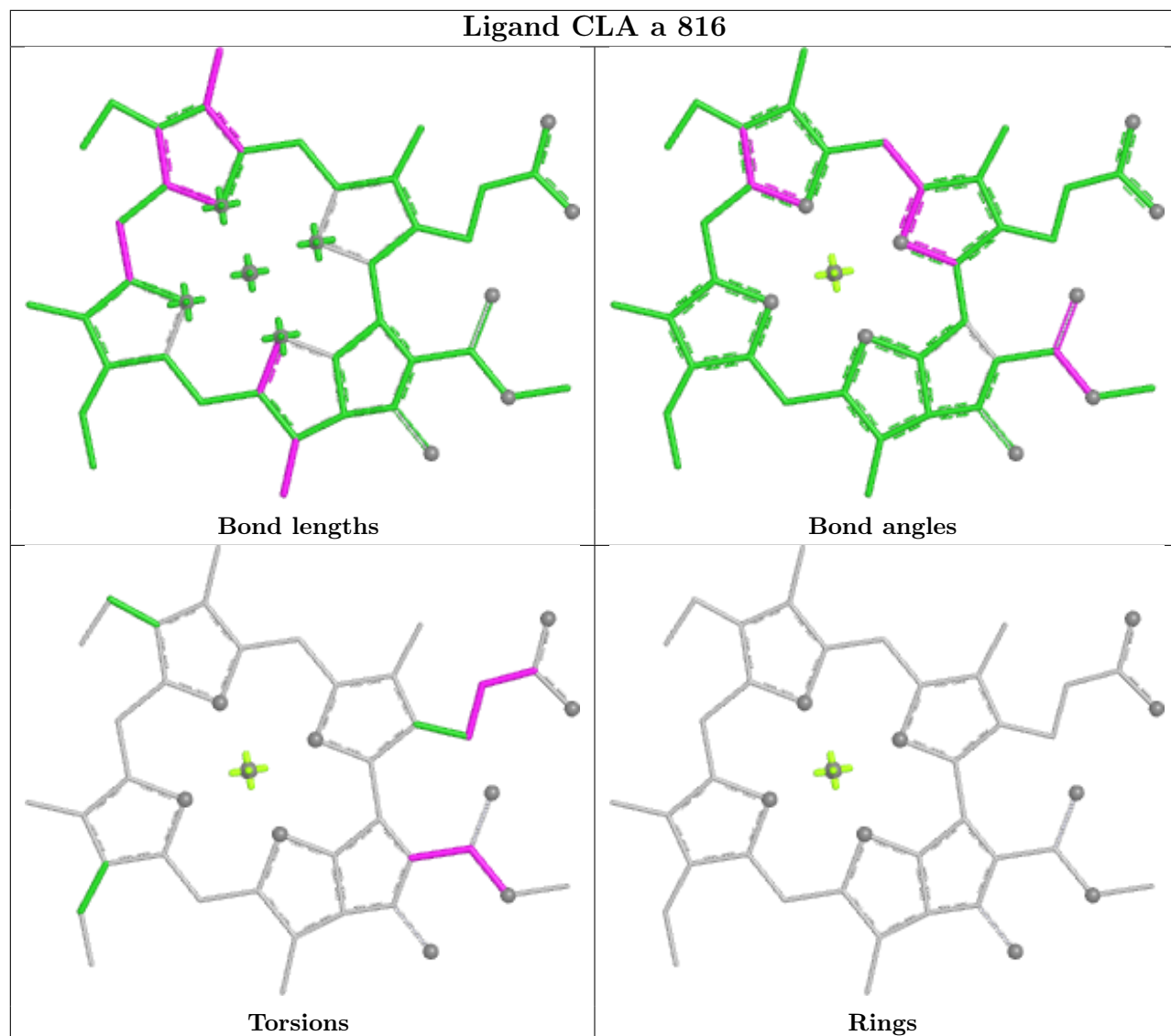
Torsions

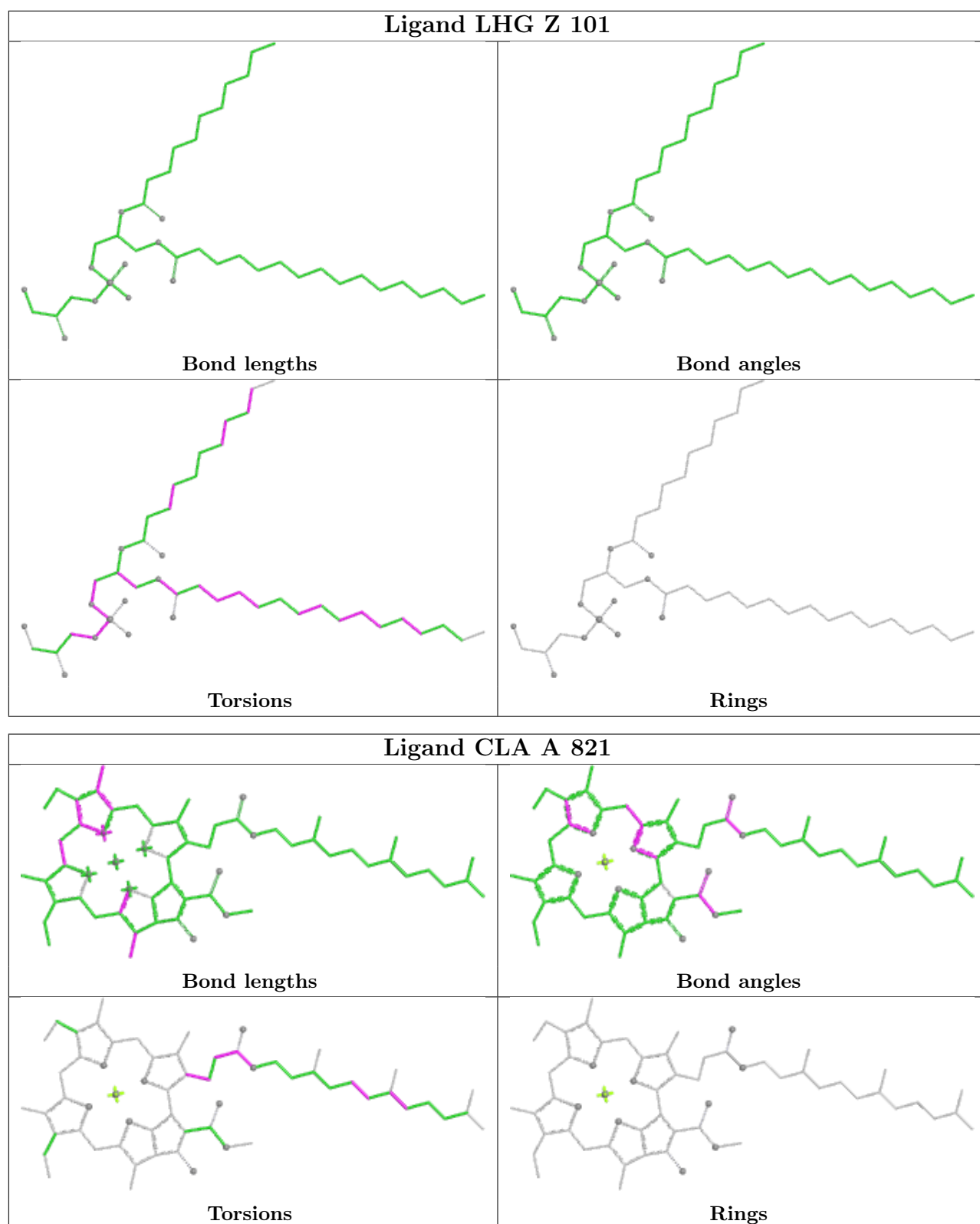


Rings

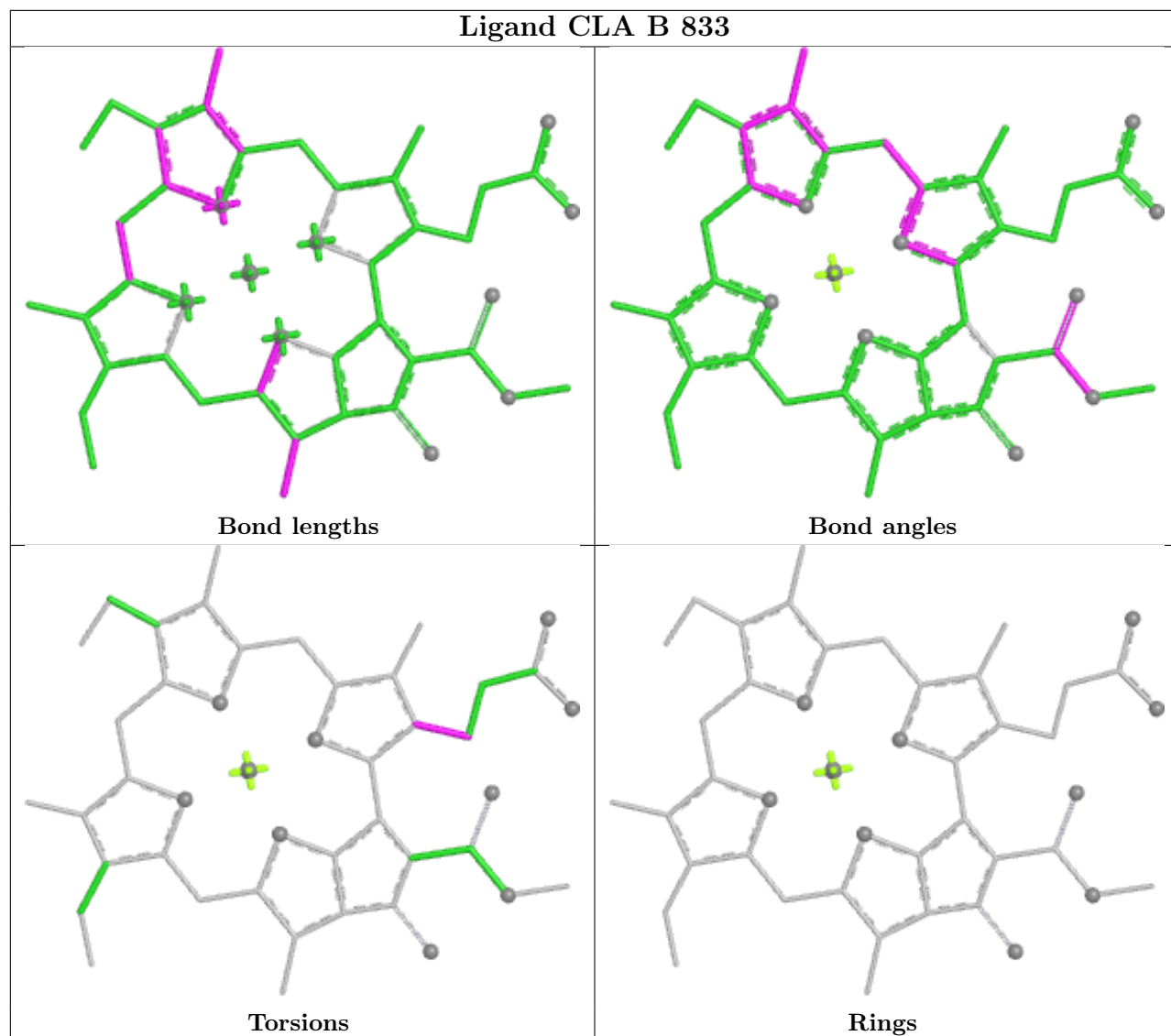


Ligand CLA a 816

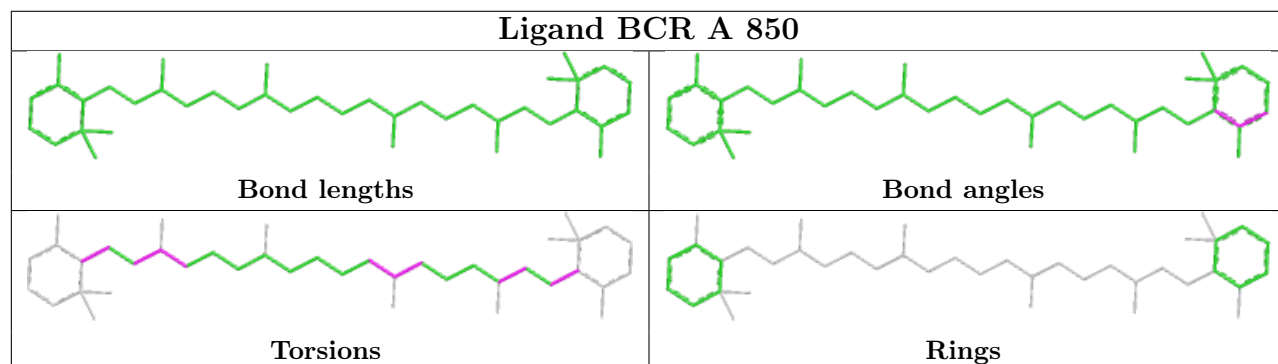




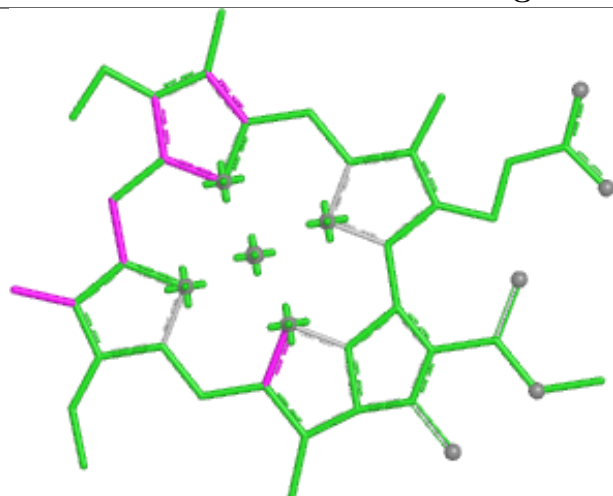
Ligand CLA B 833



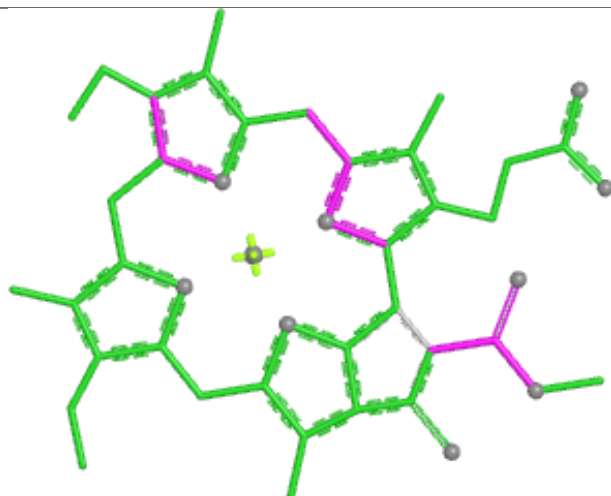
Ligand BCR A 850



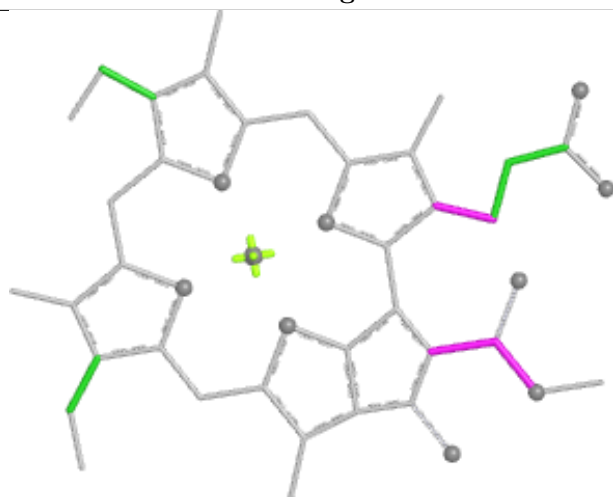
Ligand CLA O 815



Bond lengths



Bond angles

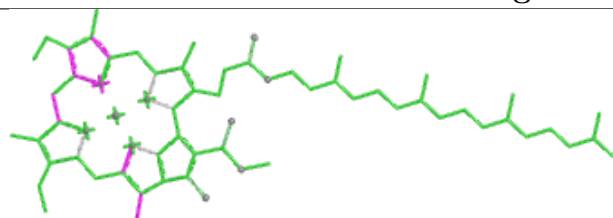


Torsions

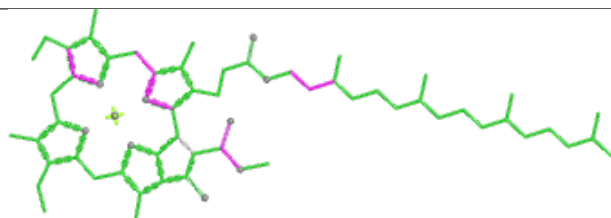


Rings

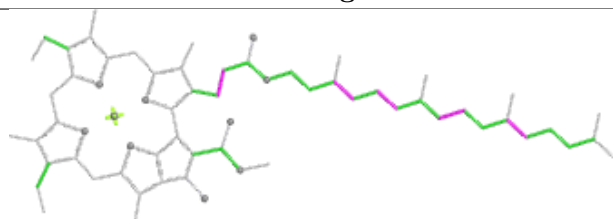
Ligand CLA N 830



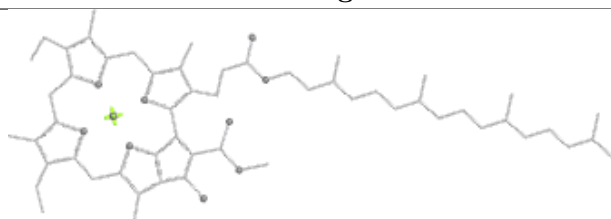
Bond lengths



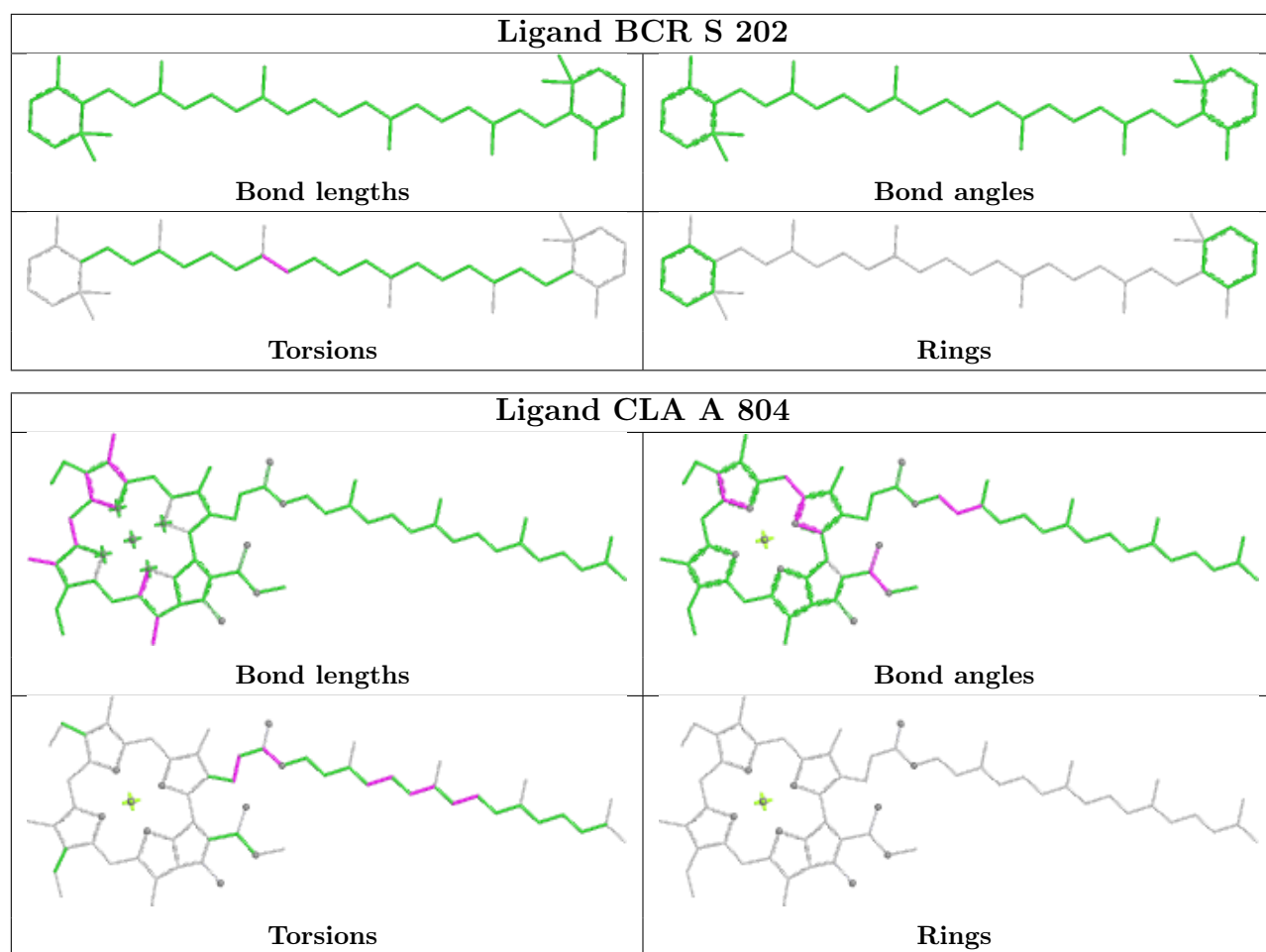
Bond angles



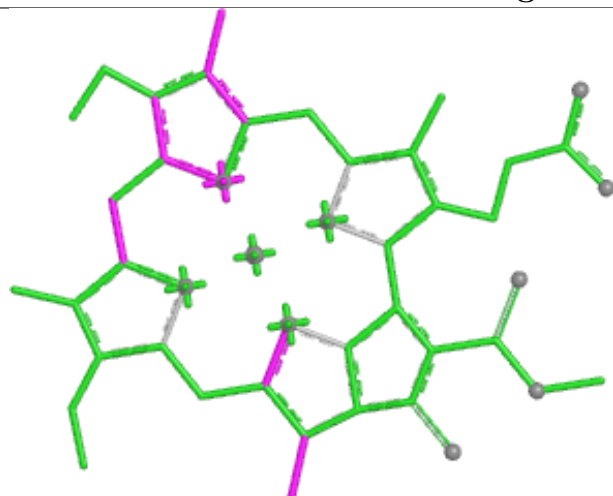
Torsions



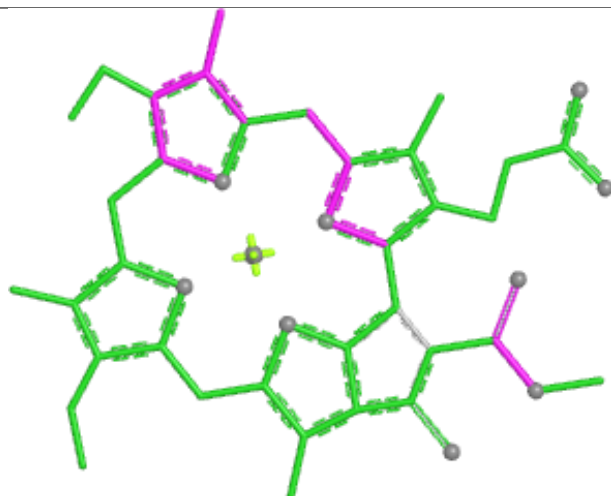
Rings



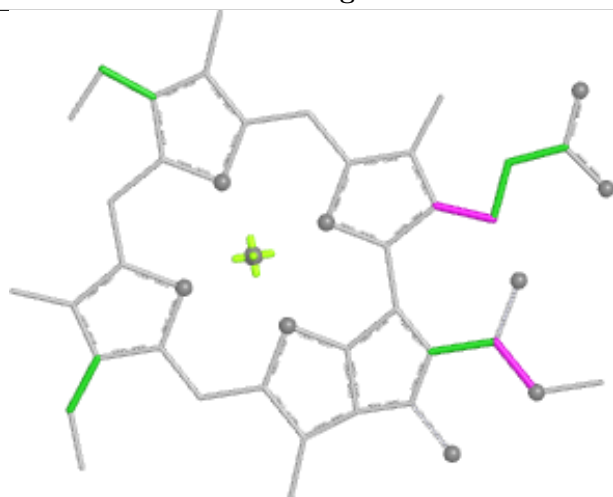
Ligand CLA b 835



Bond lengths



Bond angles

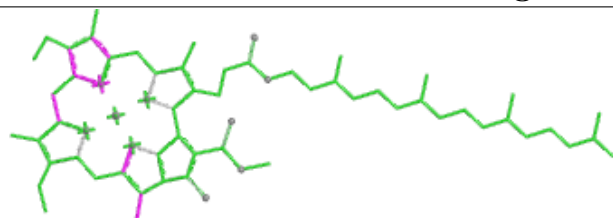


Torsions

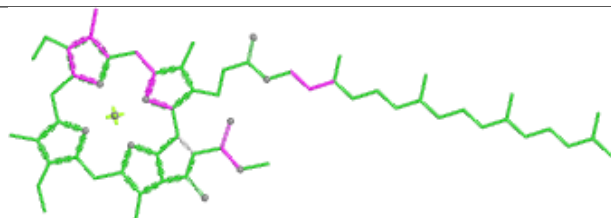


Rings

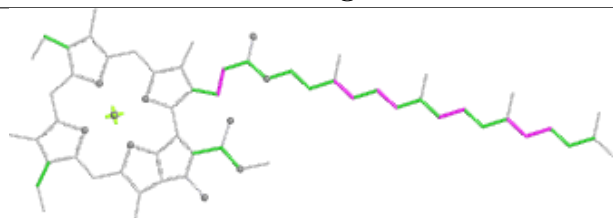
Ligand CLA A 830



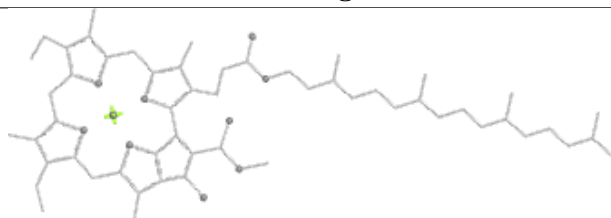
Bond lengths



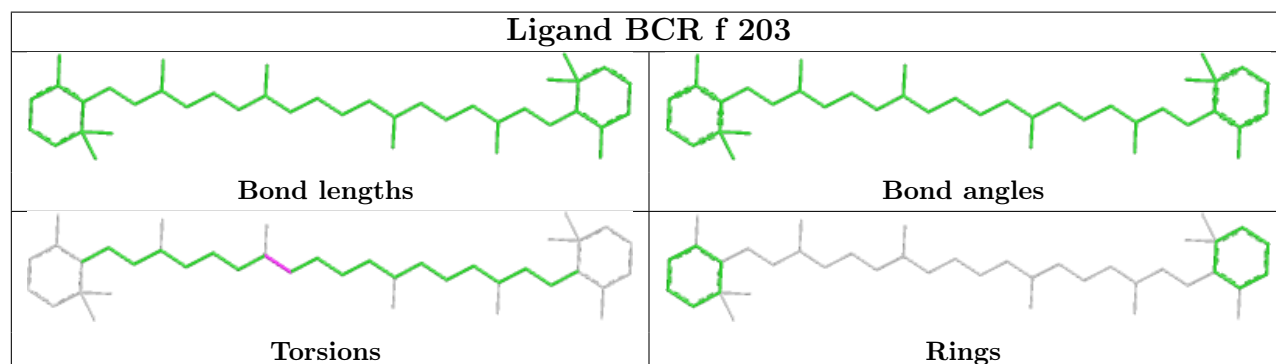
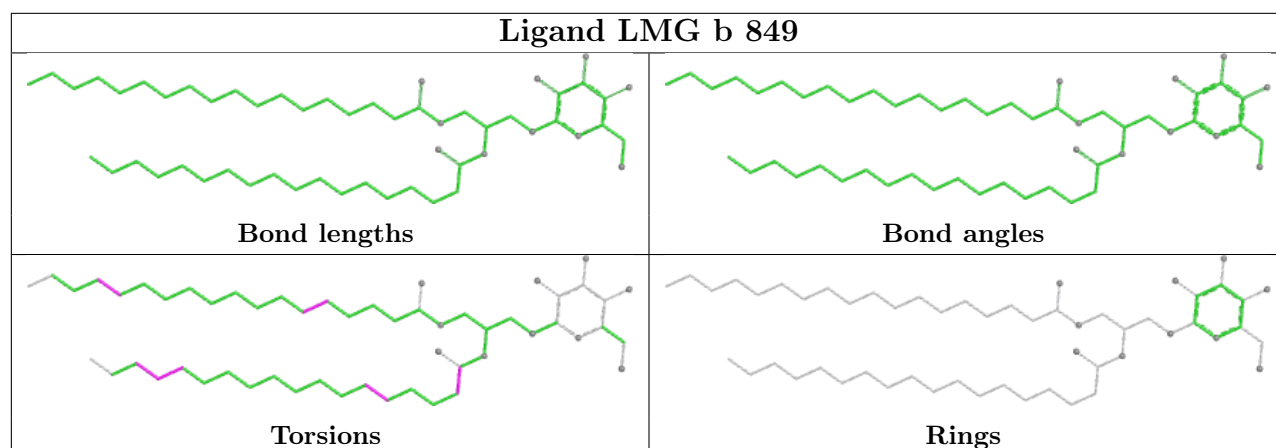
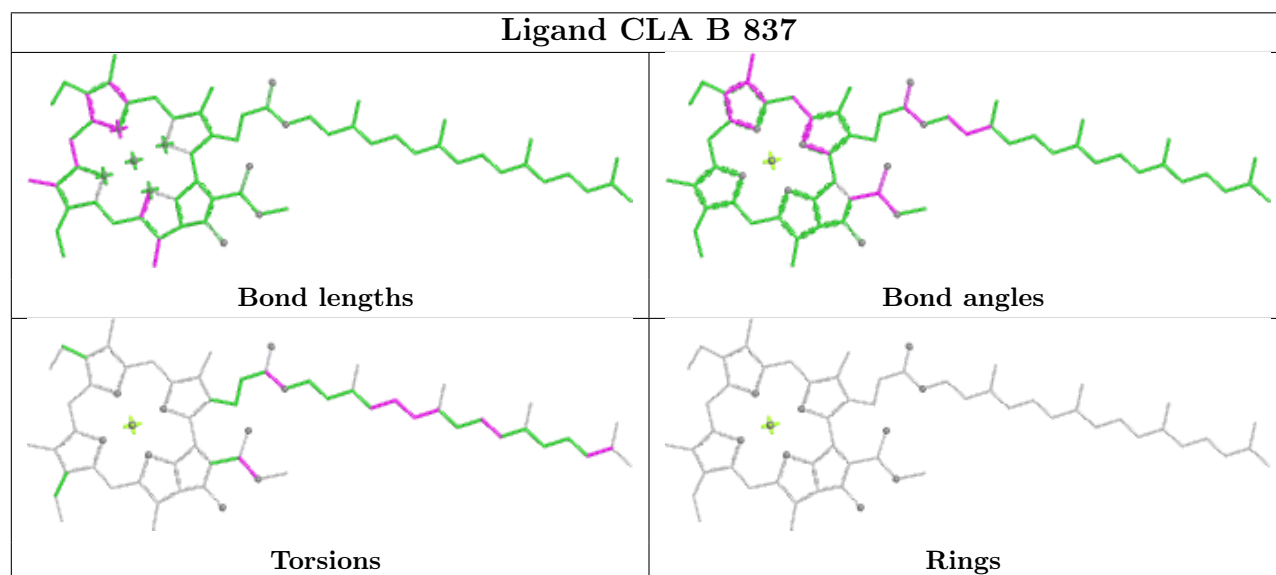
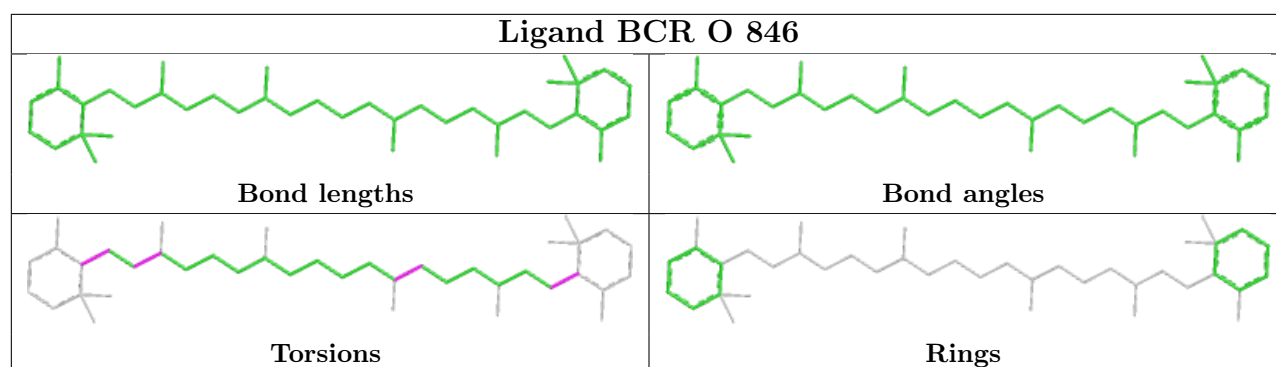
Bond angles

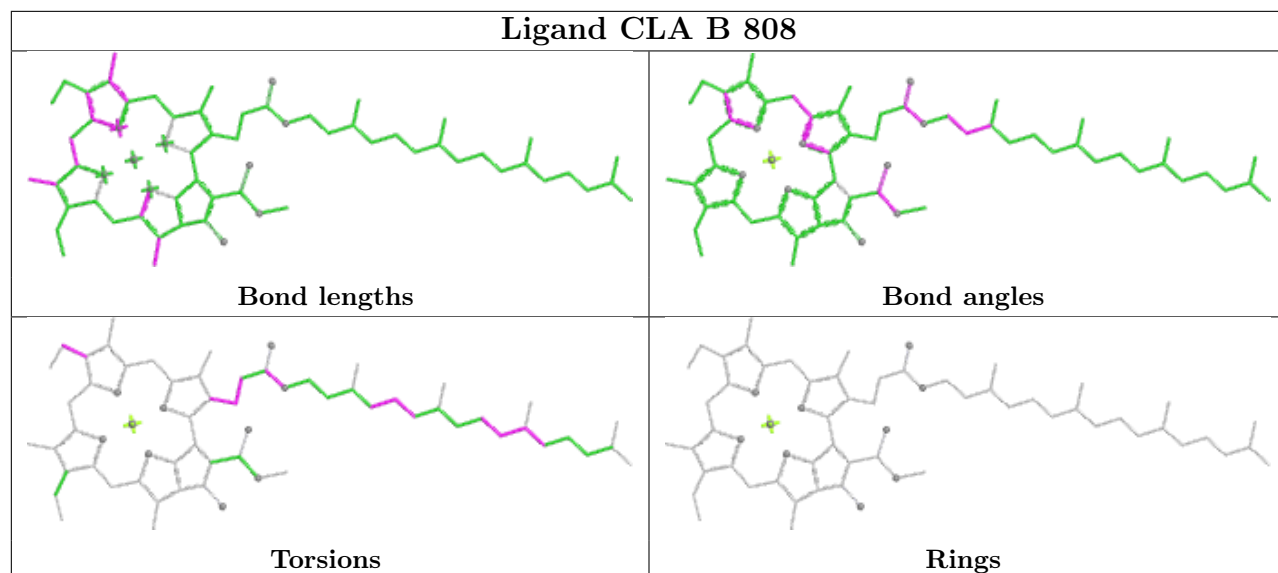
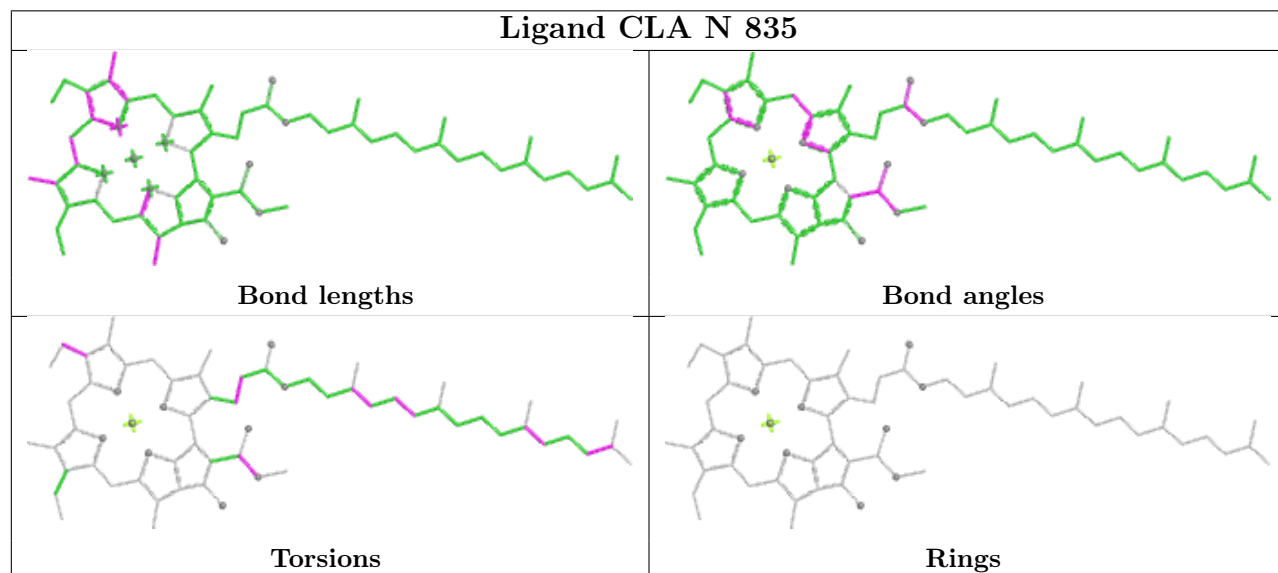
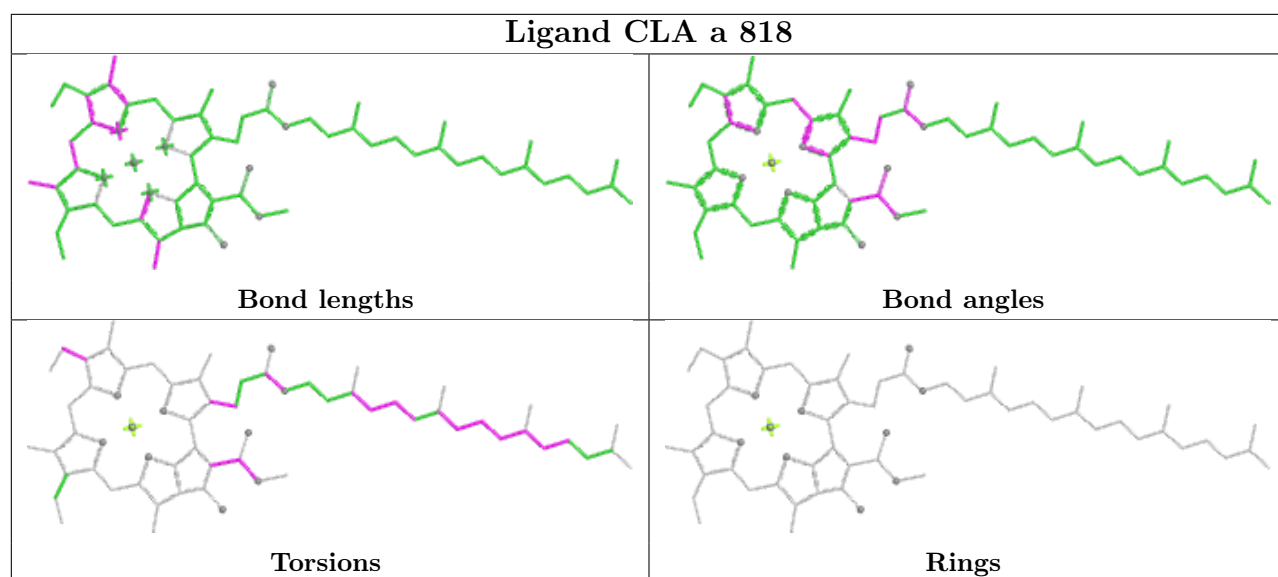


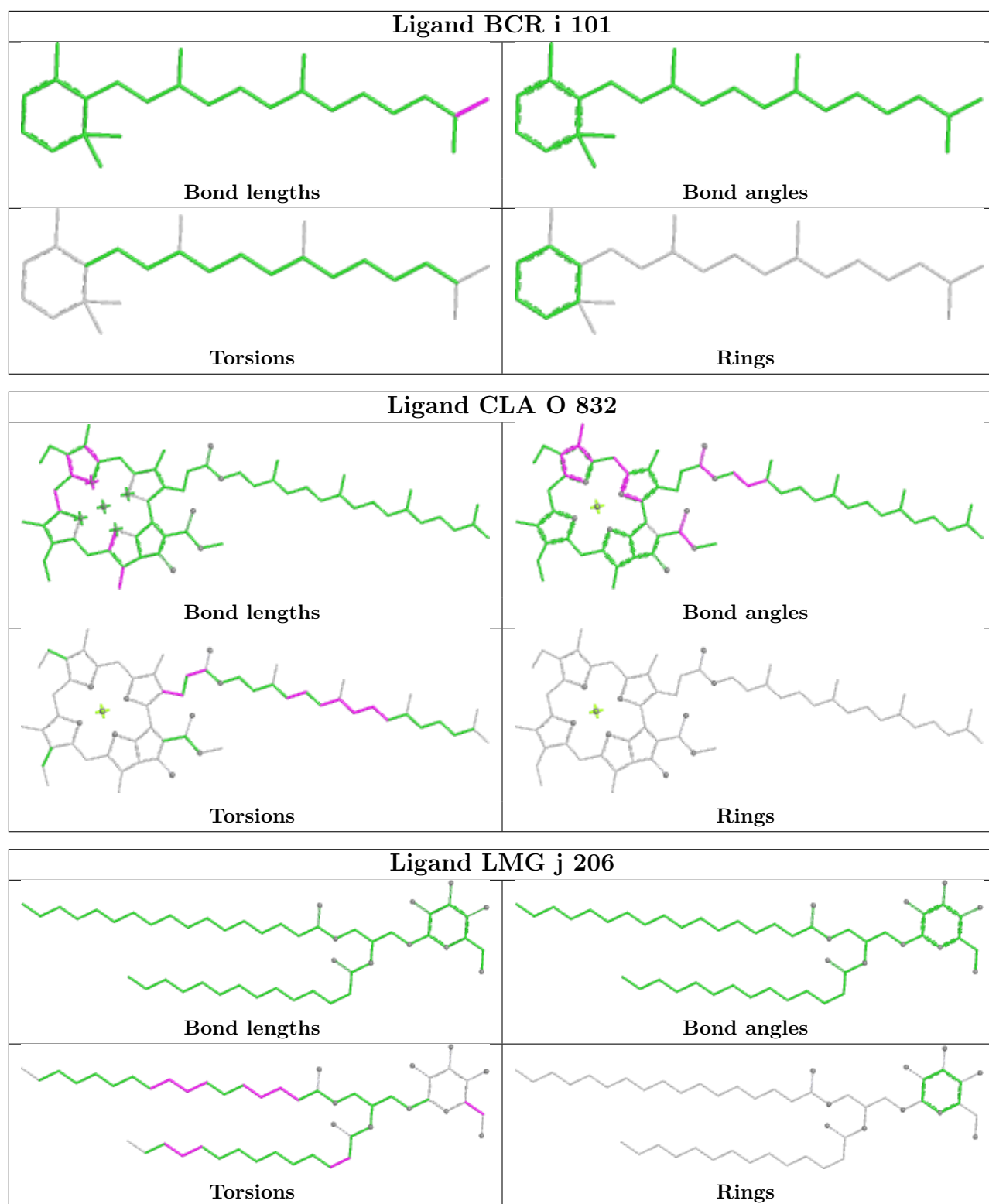
Torsions

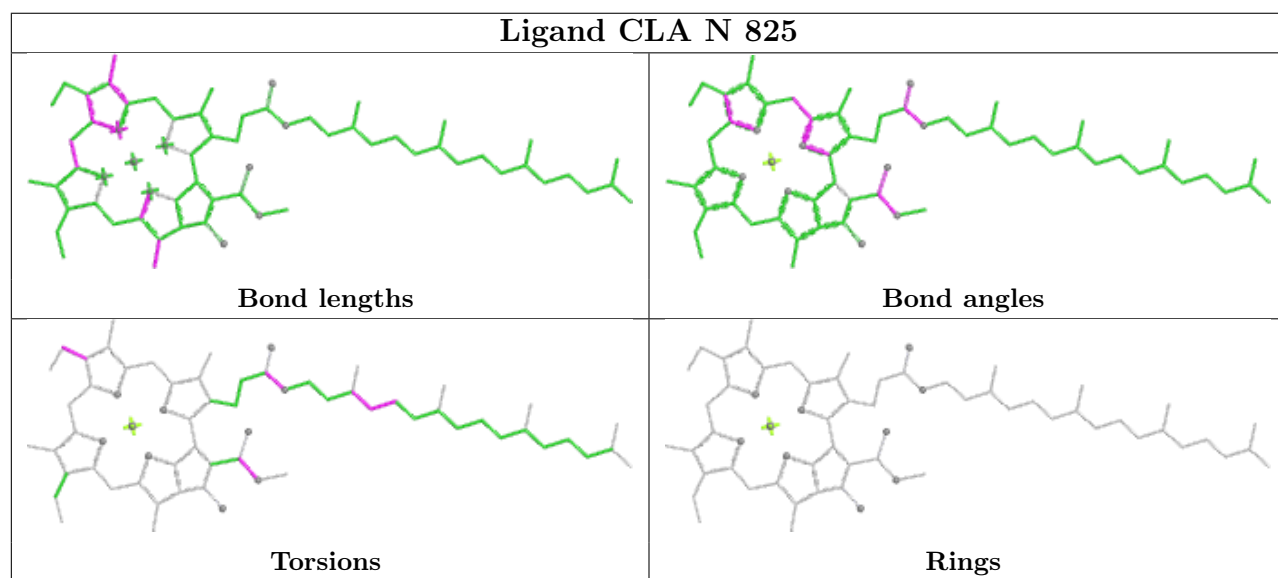
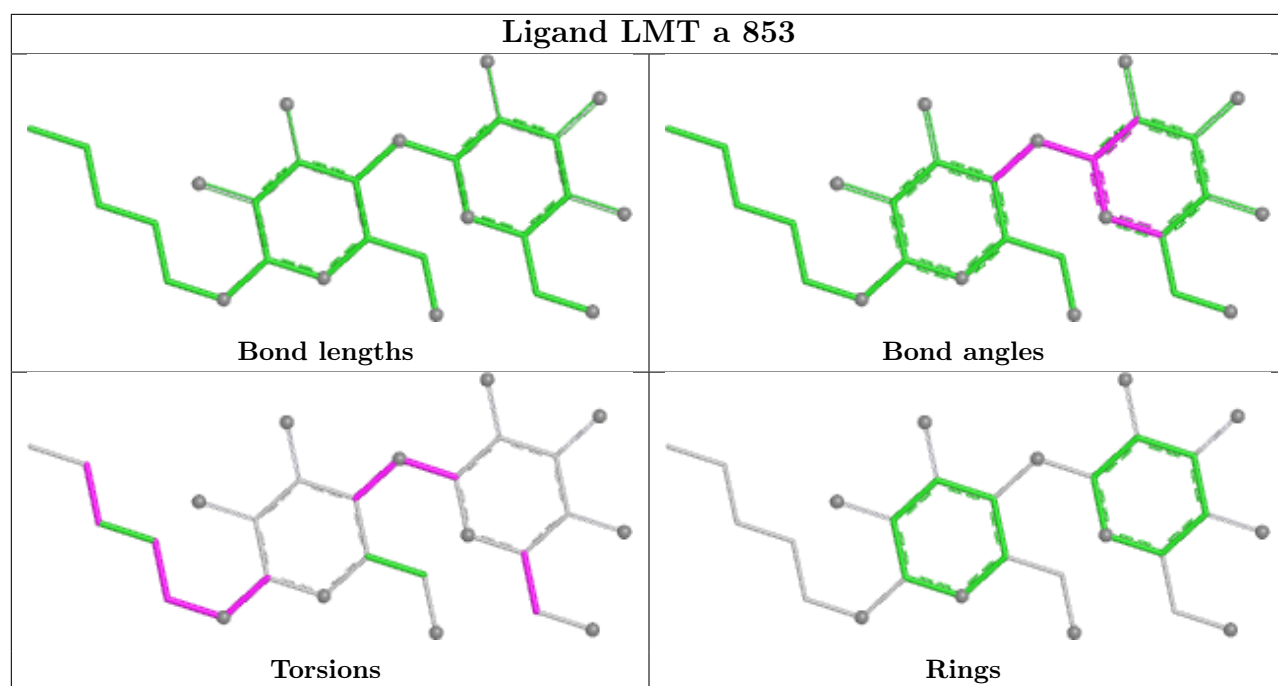


Rings

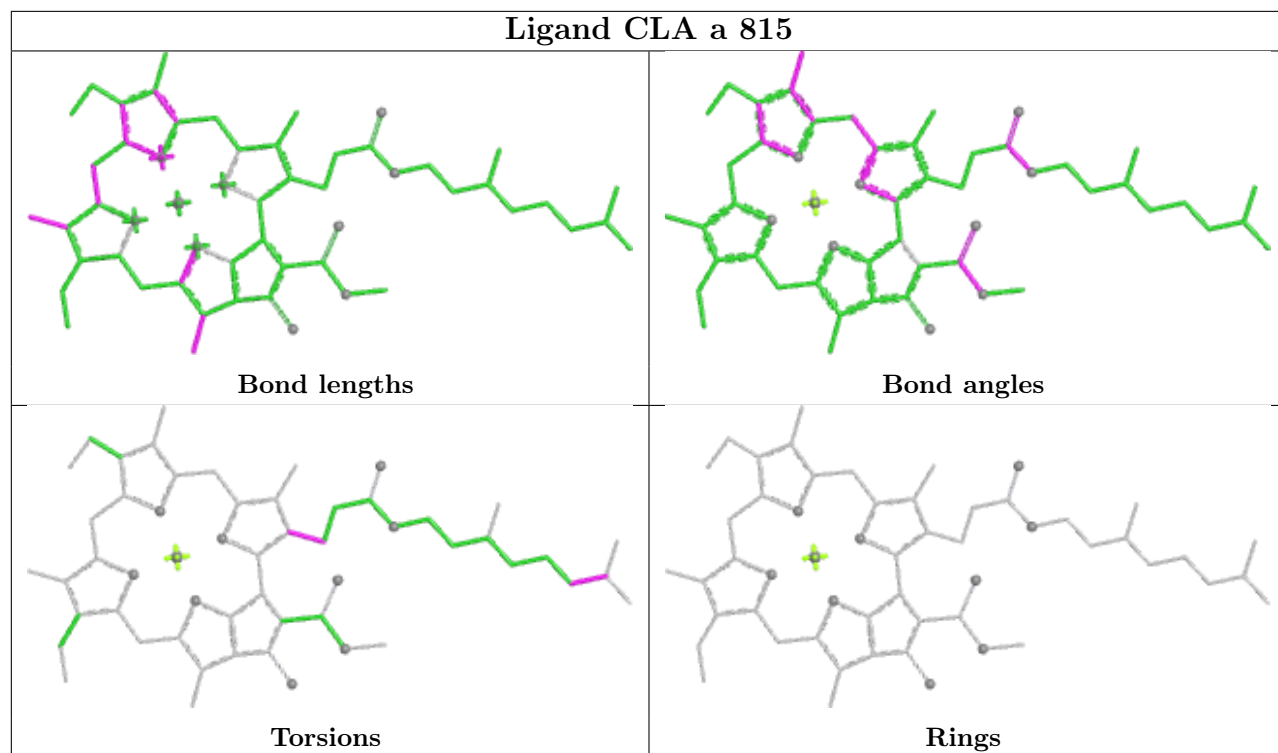




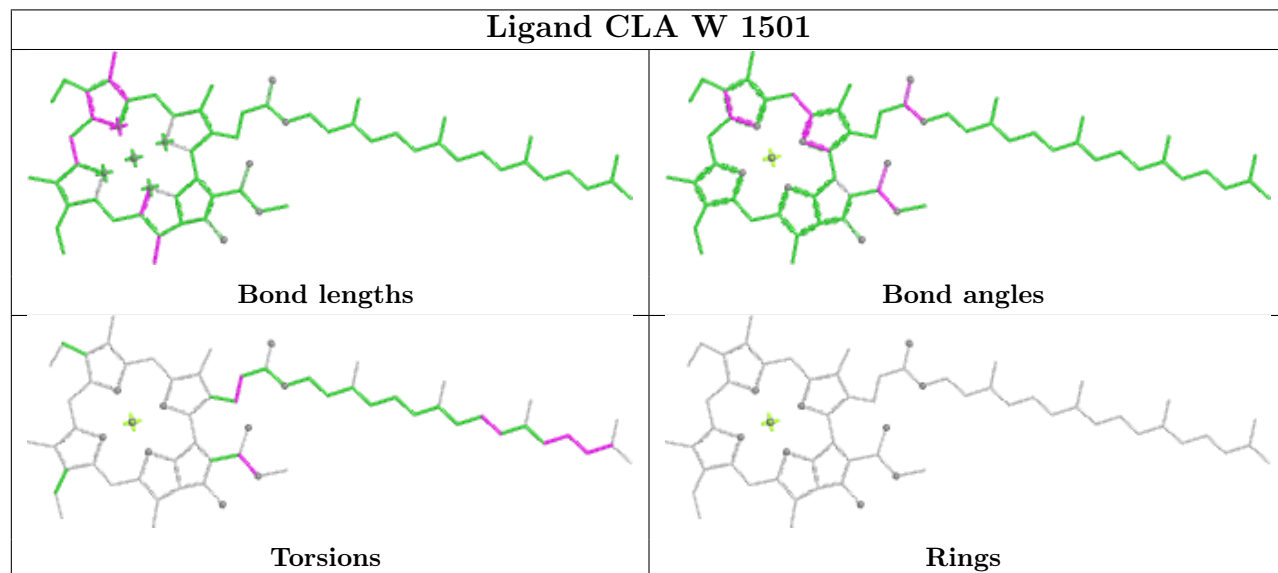


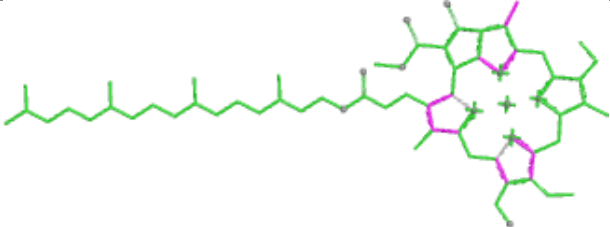
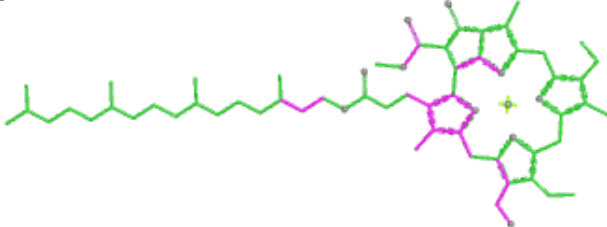
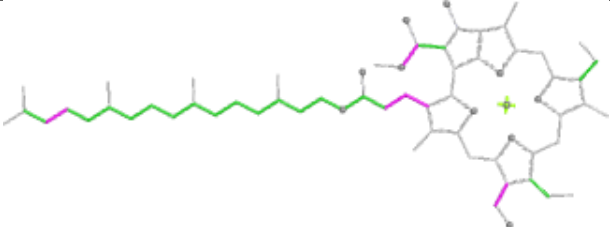
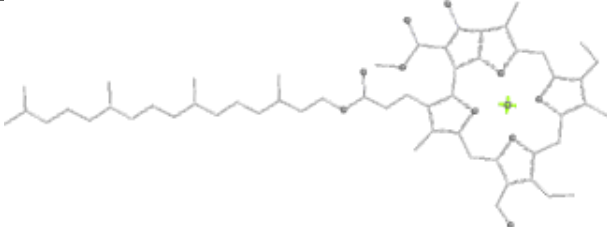
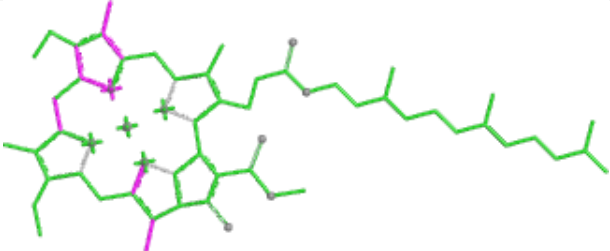
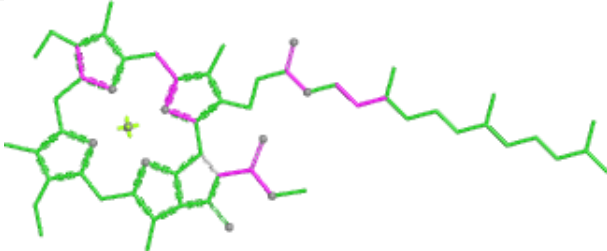
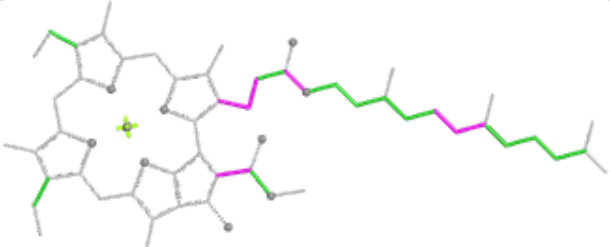
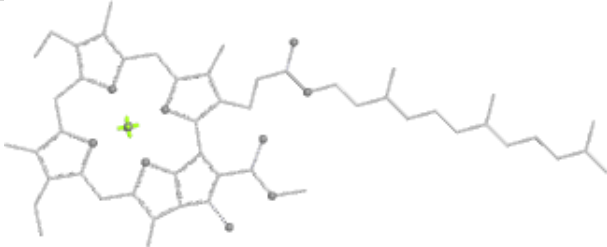
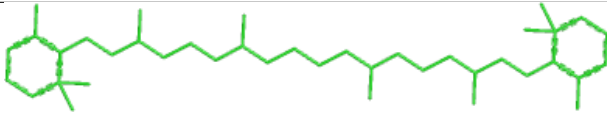
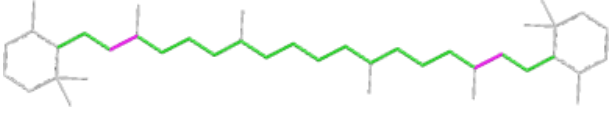
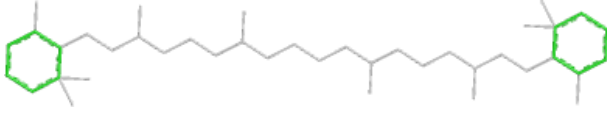


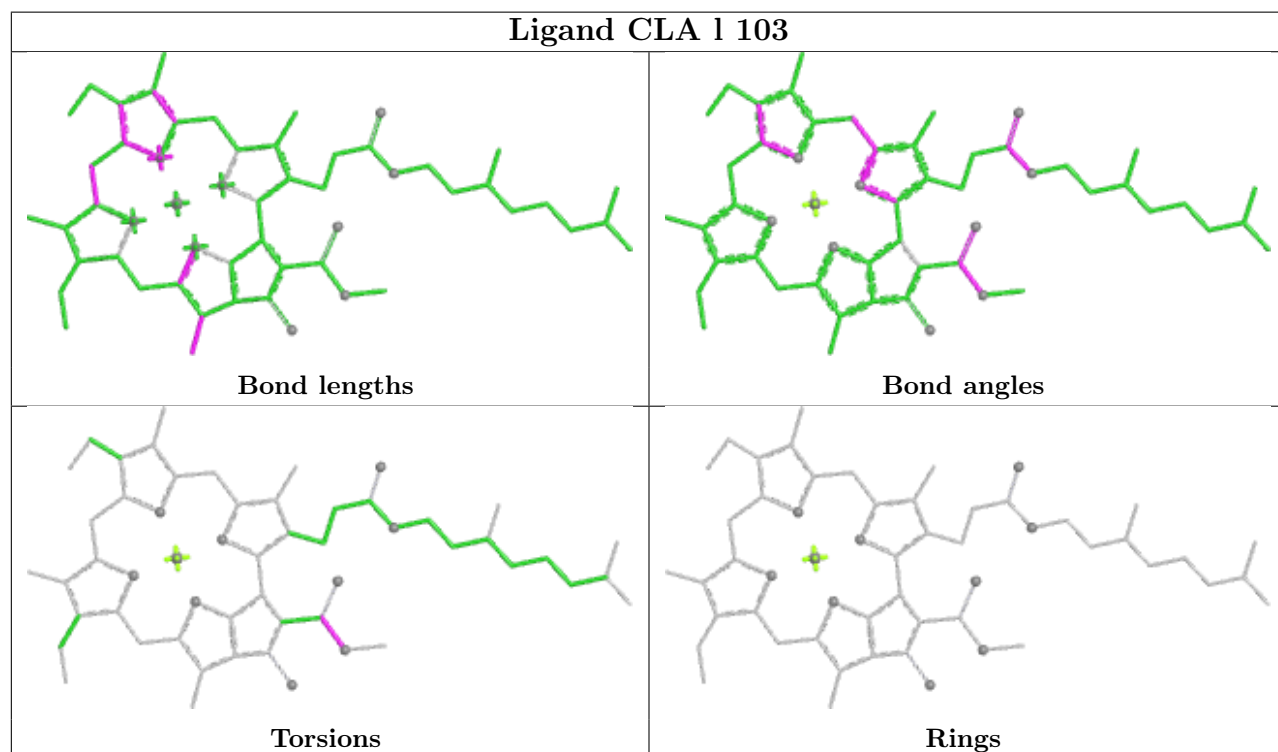
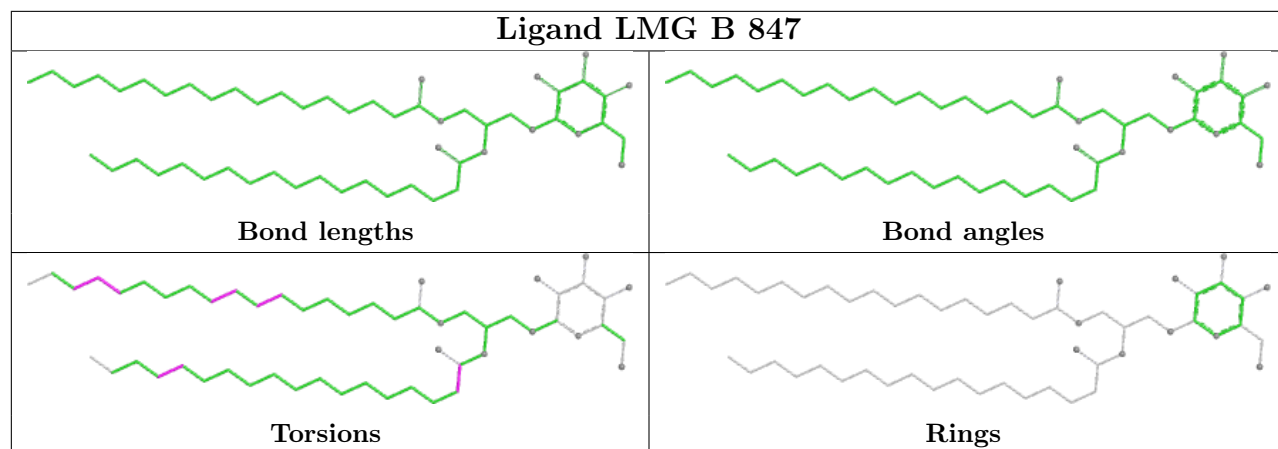
Ligand CLA a 815

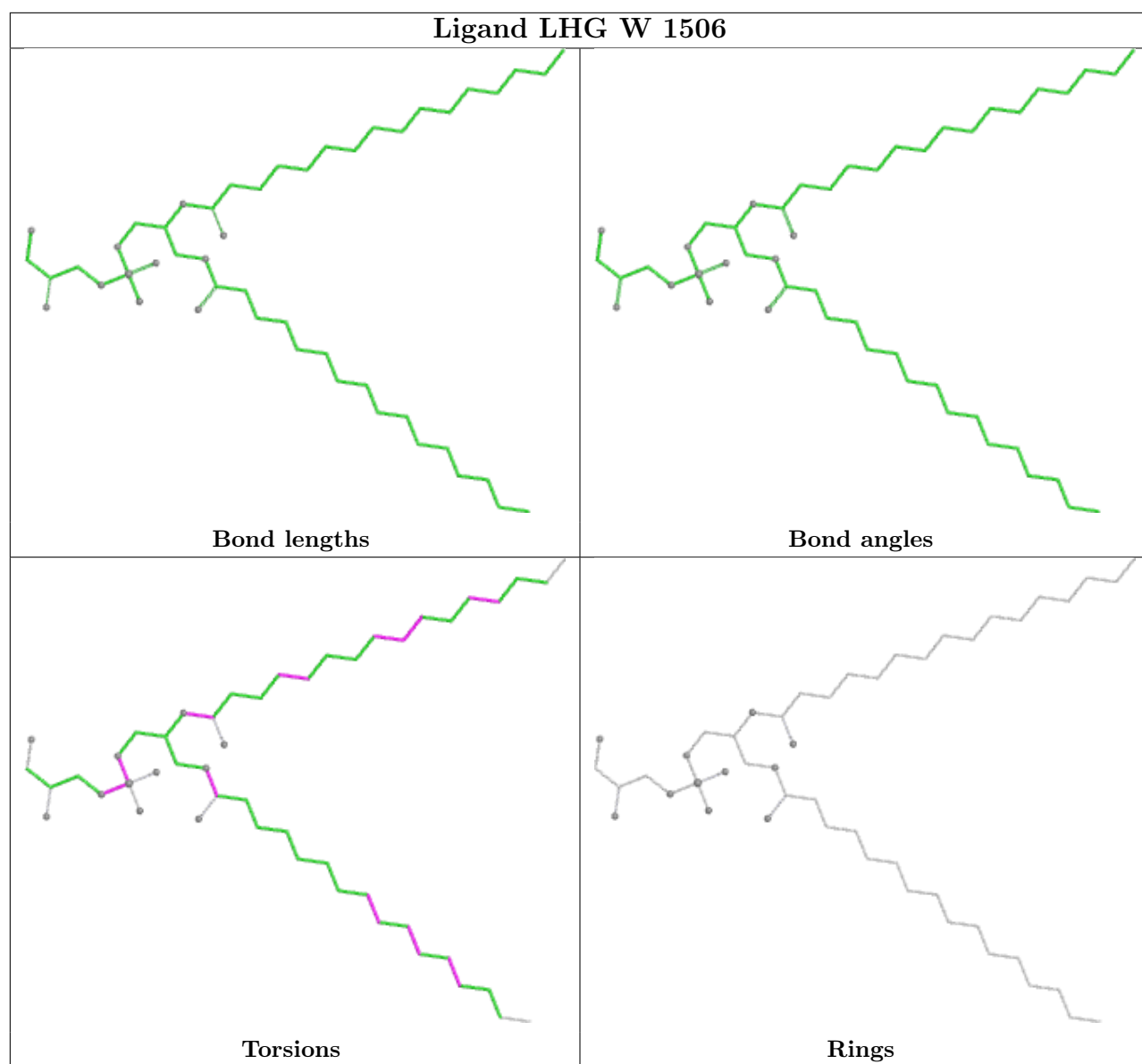


Ligand CLA W 1501

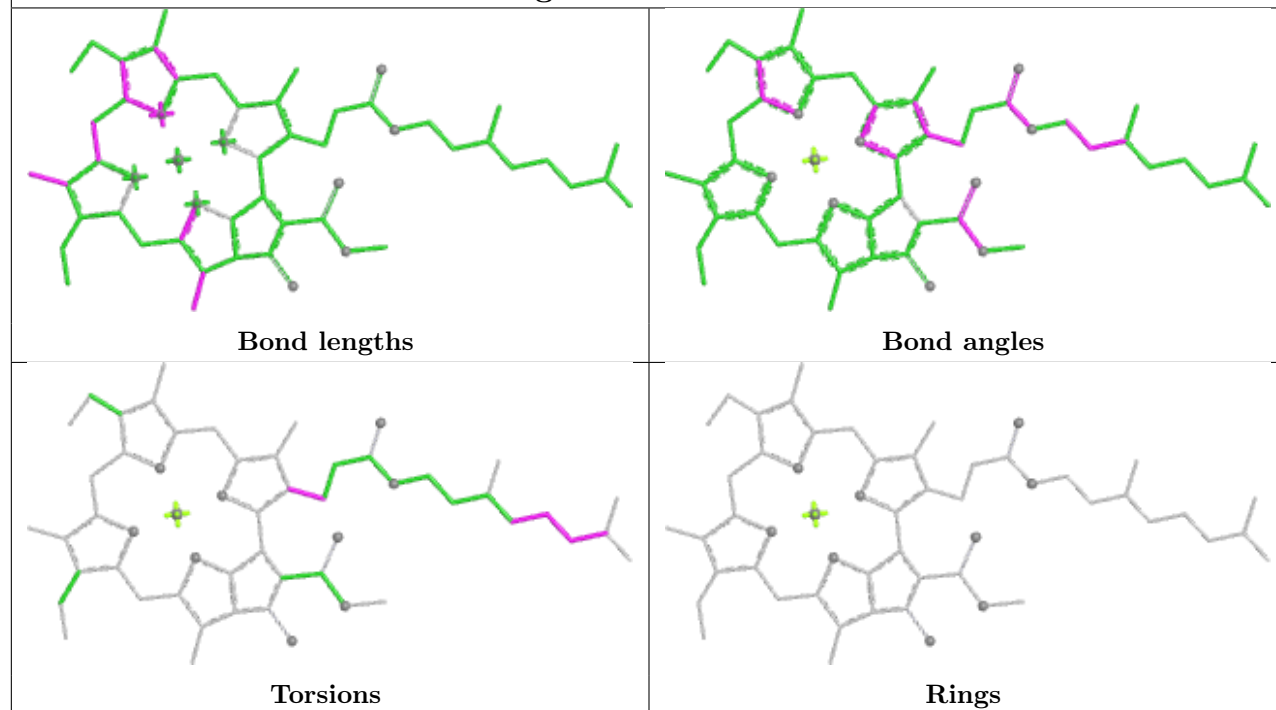


Ligand F6C N 802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 809	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR W 1504	
 Bond lengths	 Bond angles
 Torsions	 Rings

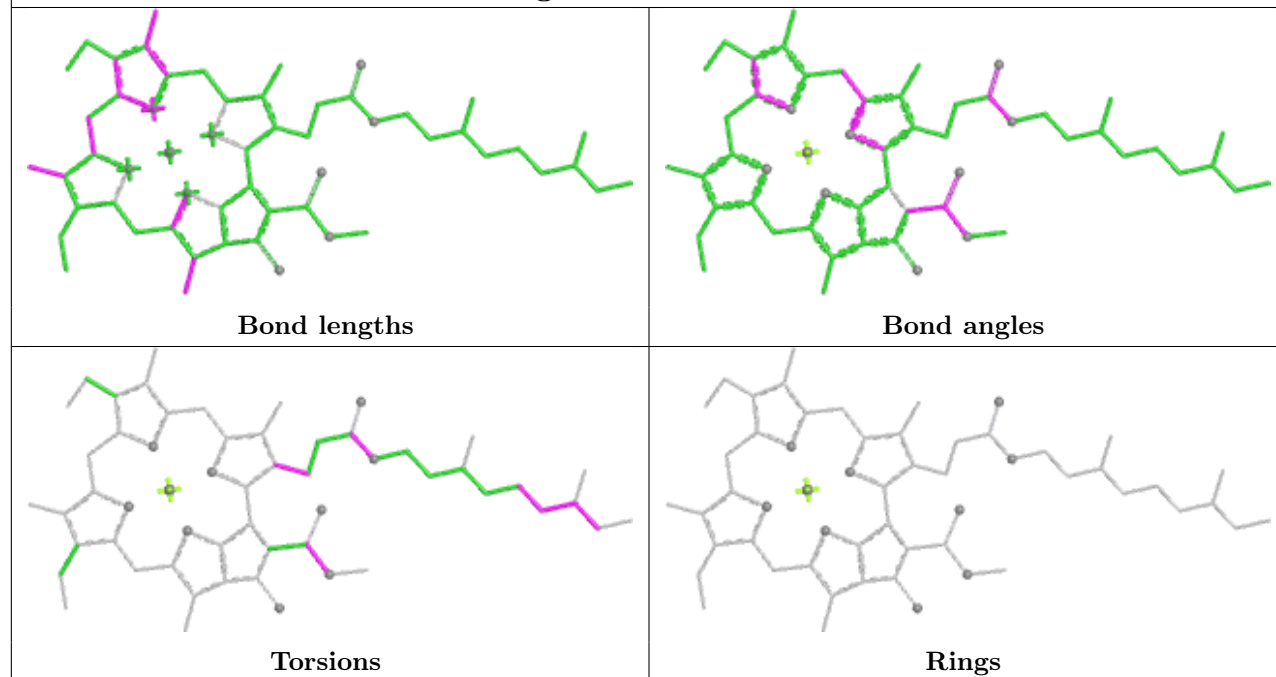


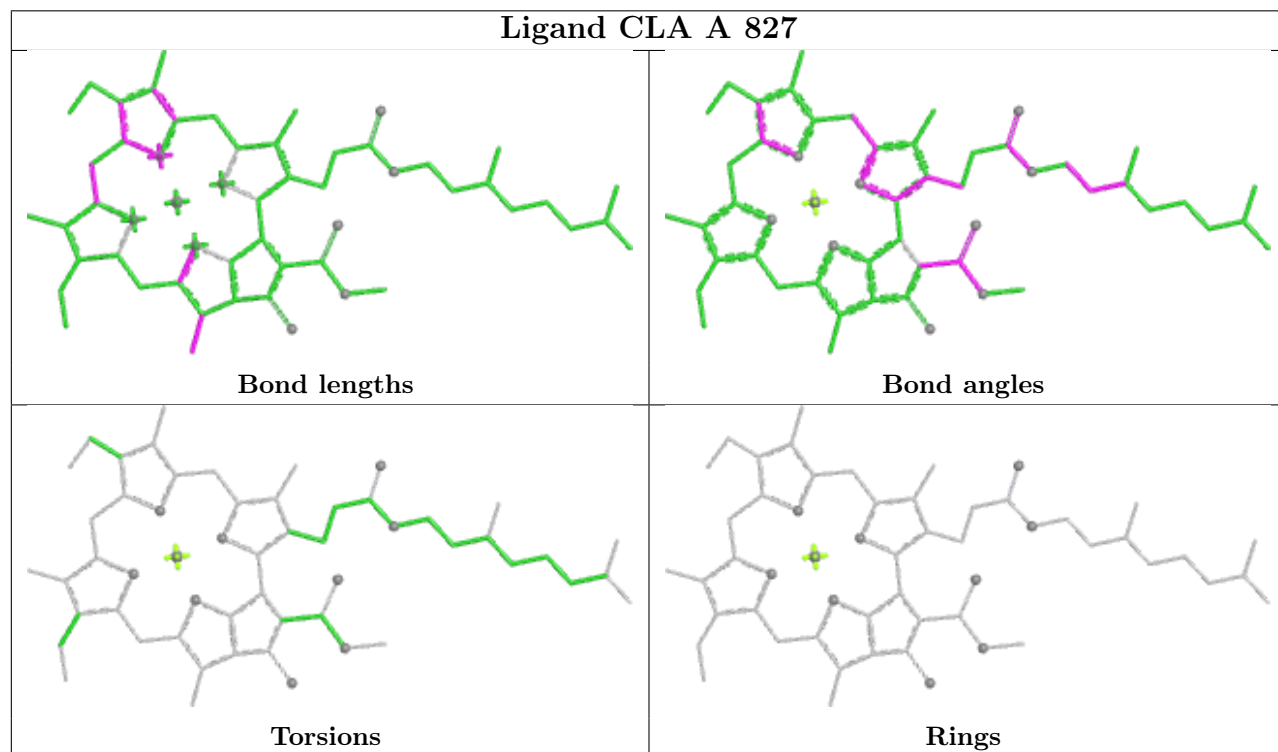
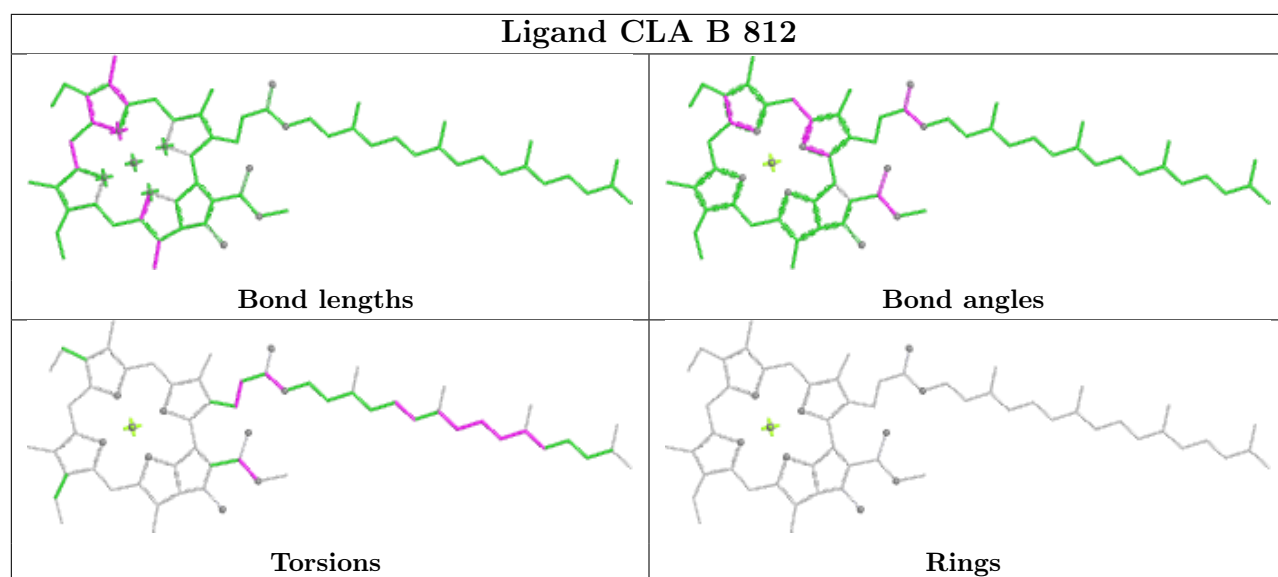


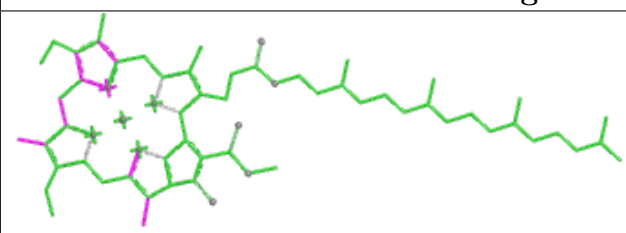
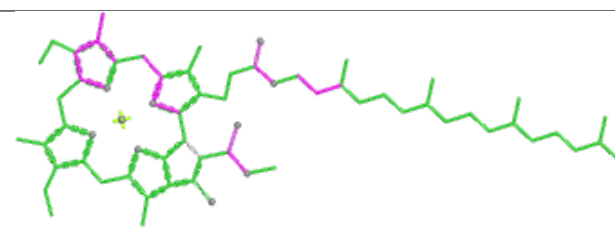
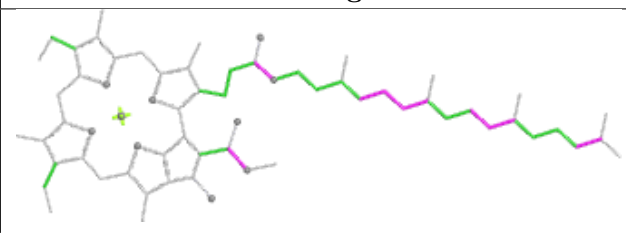
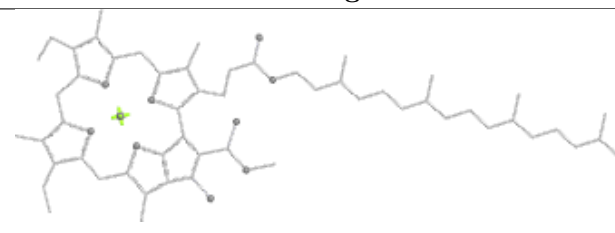
Ligand CLA b 823

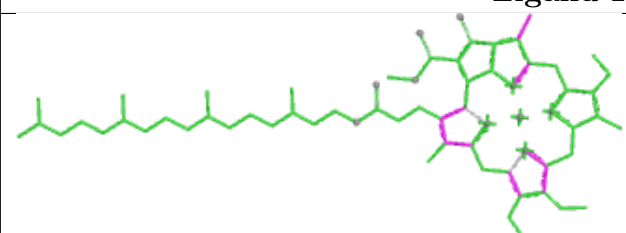
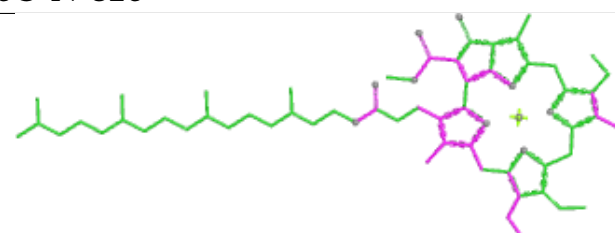
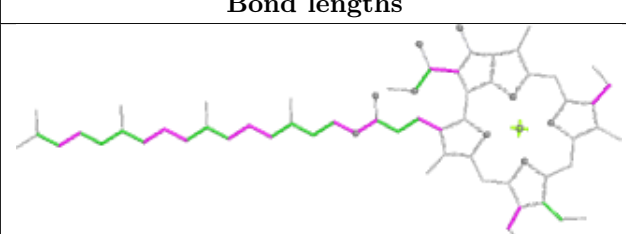
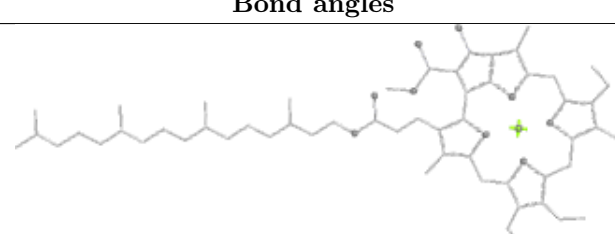


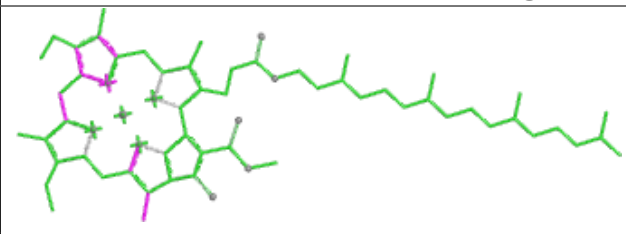
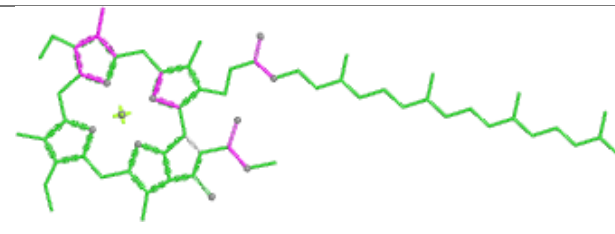
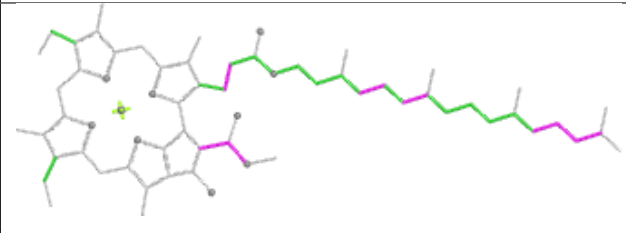
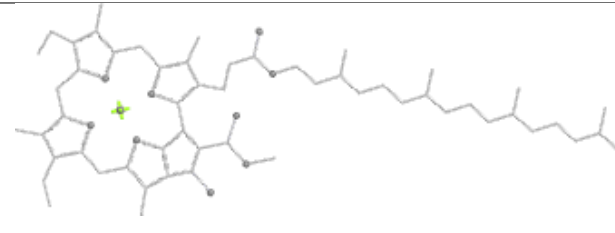
Ligand CLA b 813



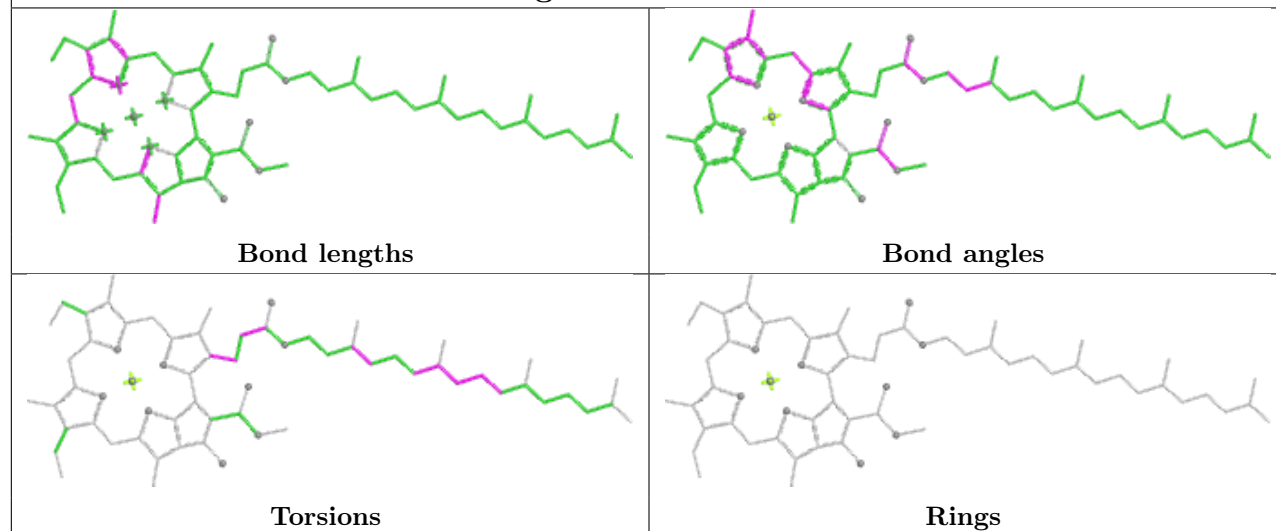


Ligand CLA O 839	
	
Bond lengths	Bond angles
	
Torsions	Rings

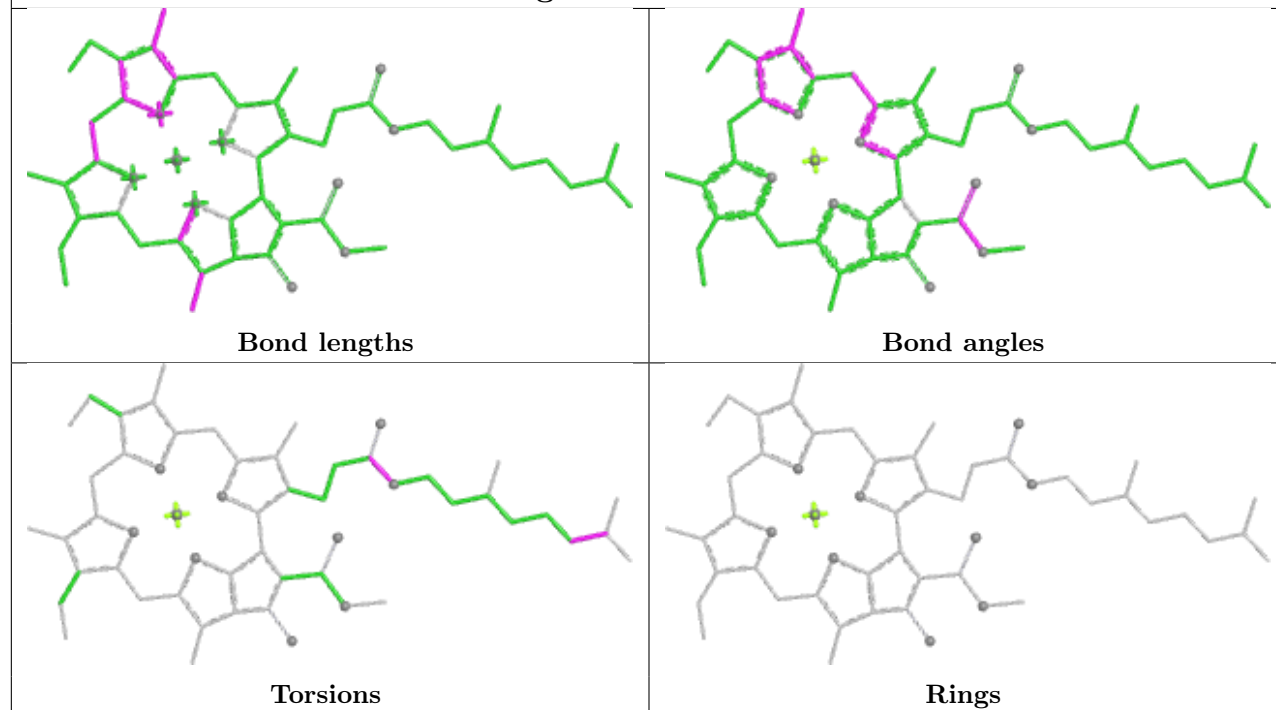
Ligand F6C N 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

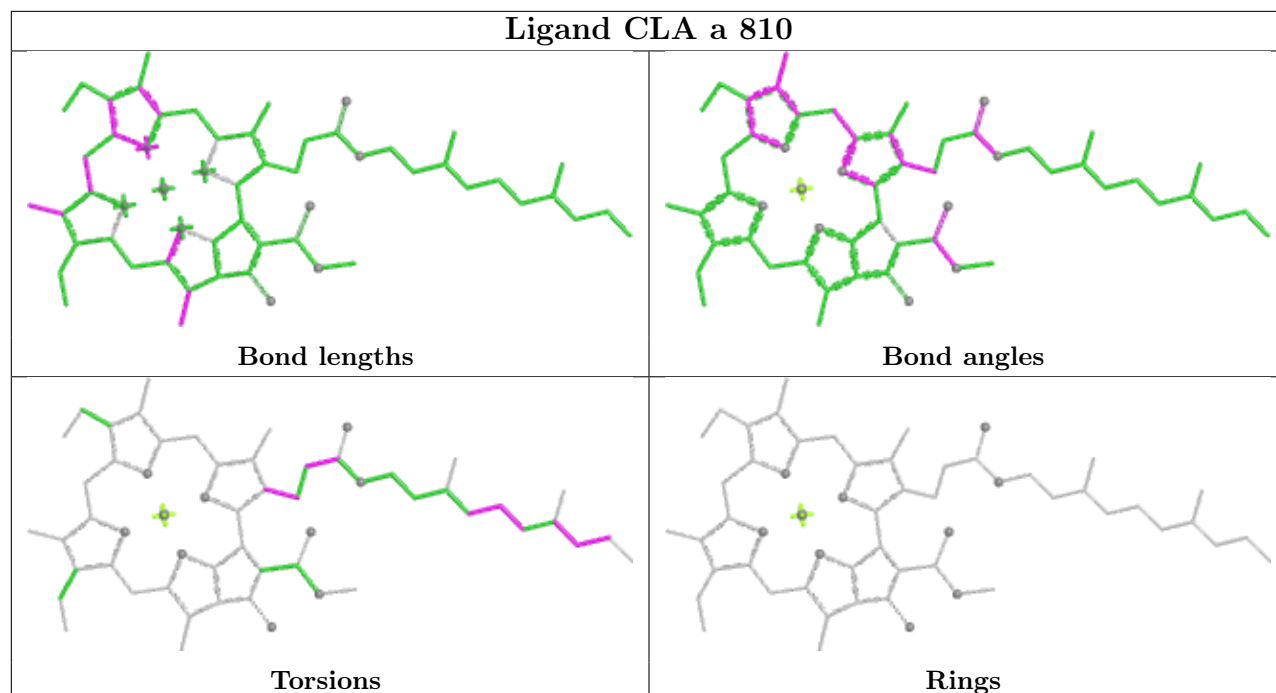
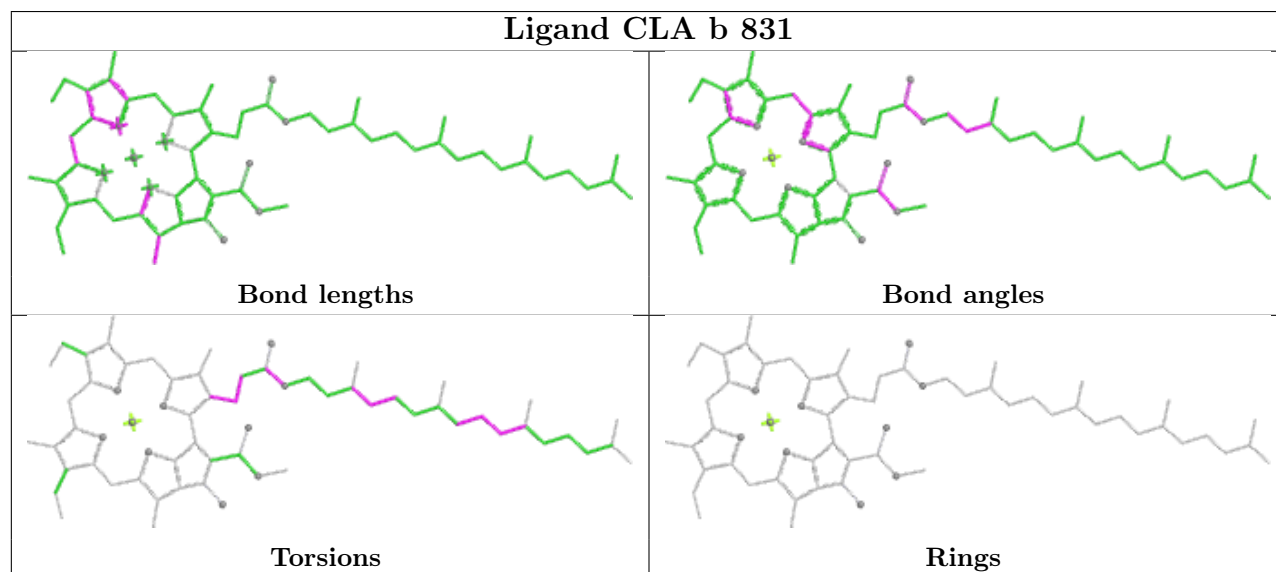
Ligand CLA O 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

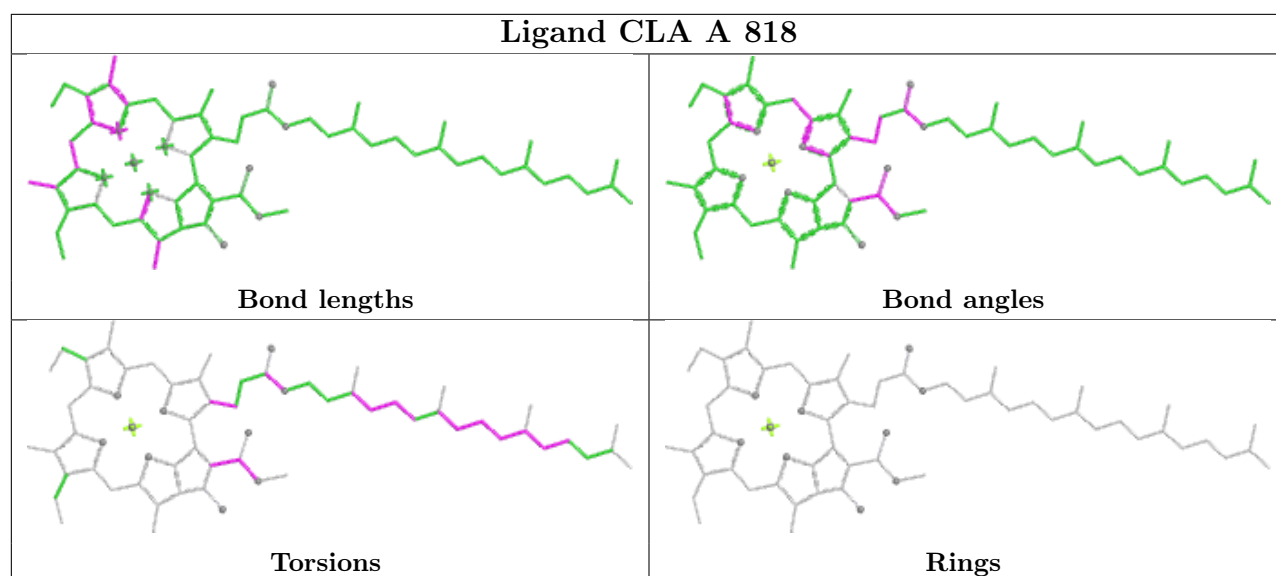
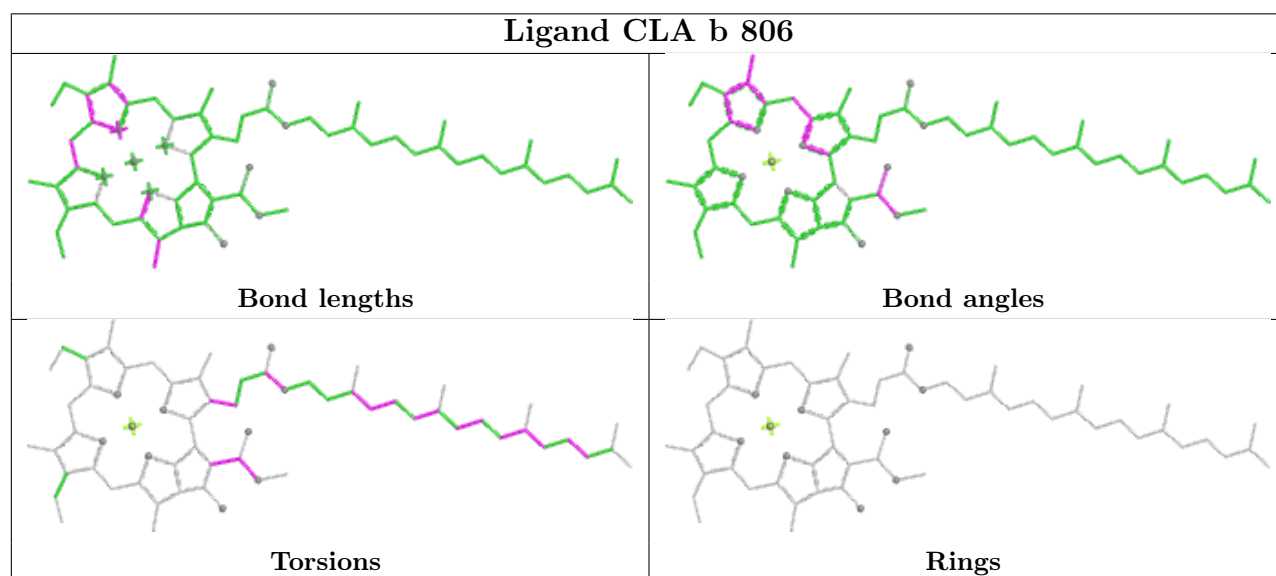
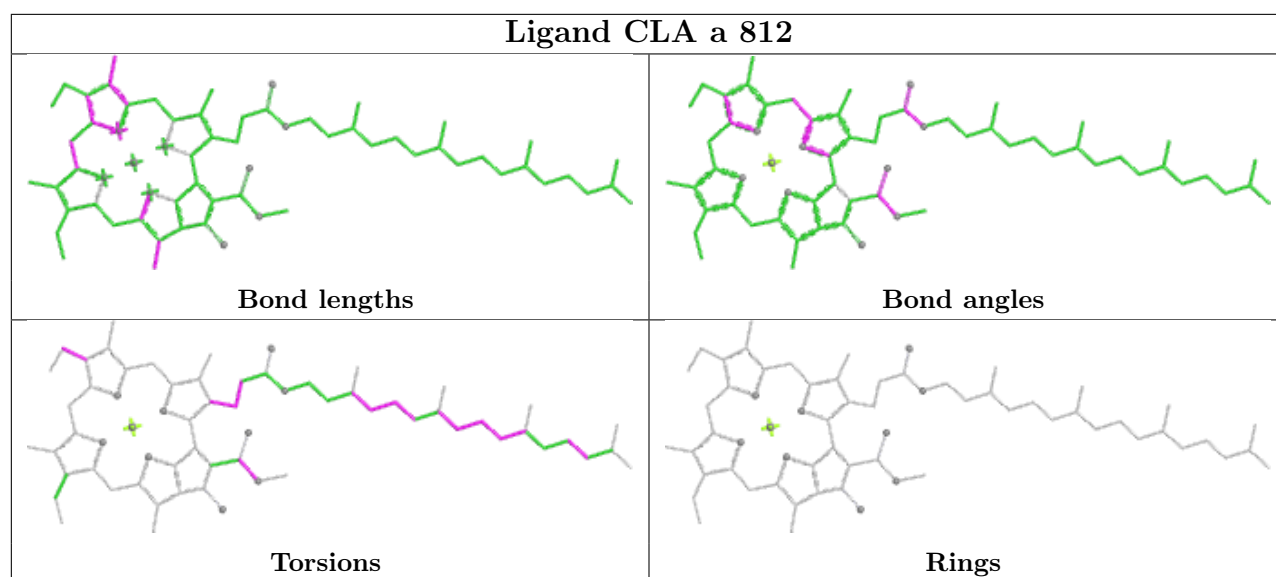
Ligand CLA b 832

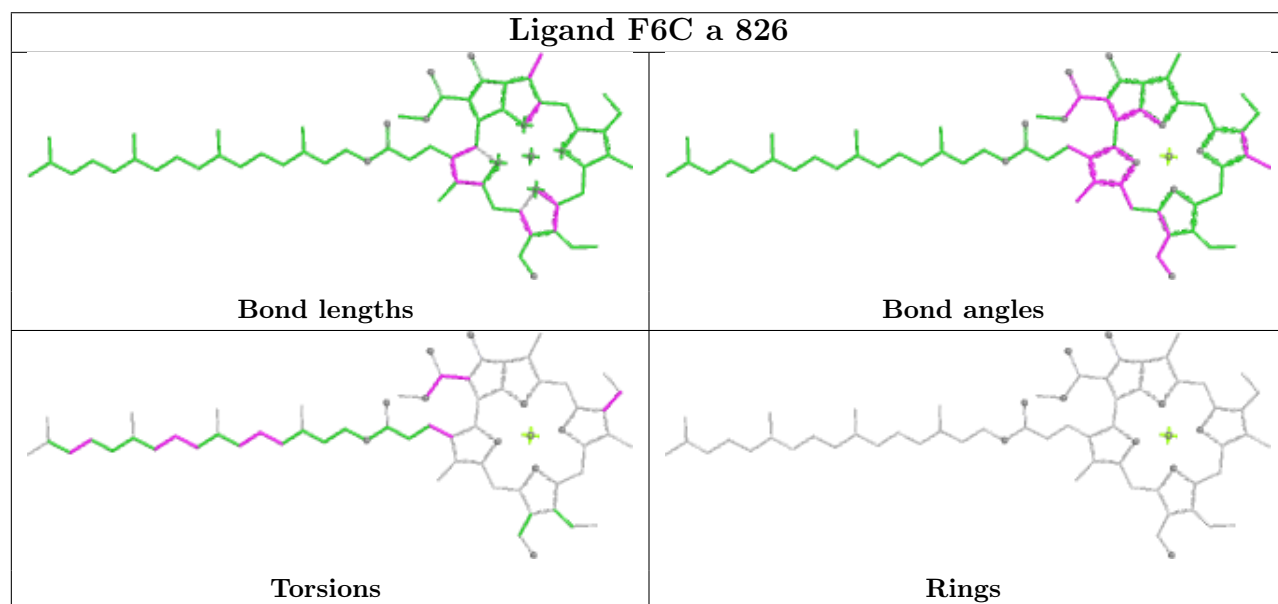
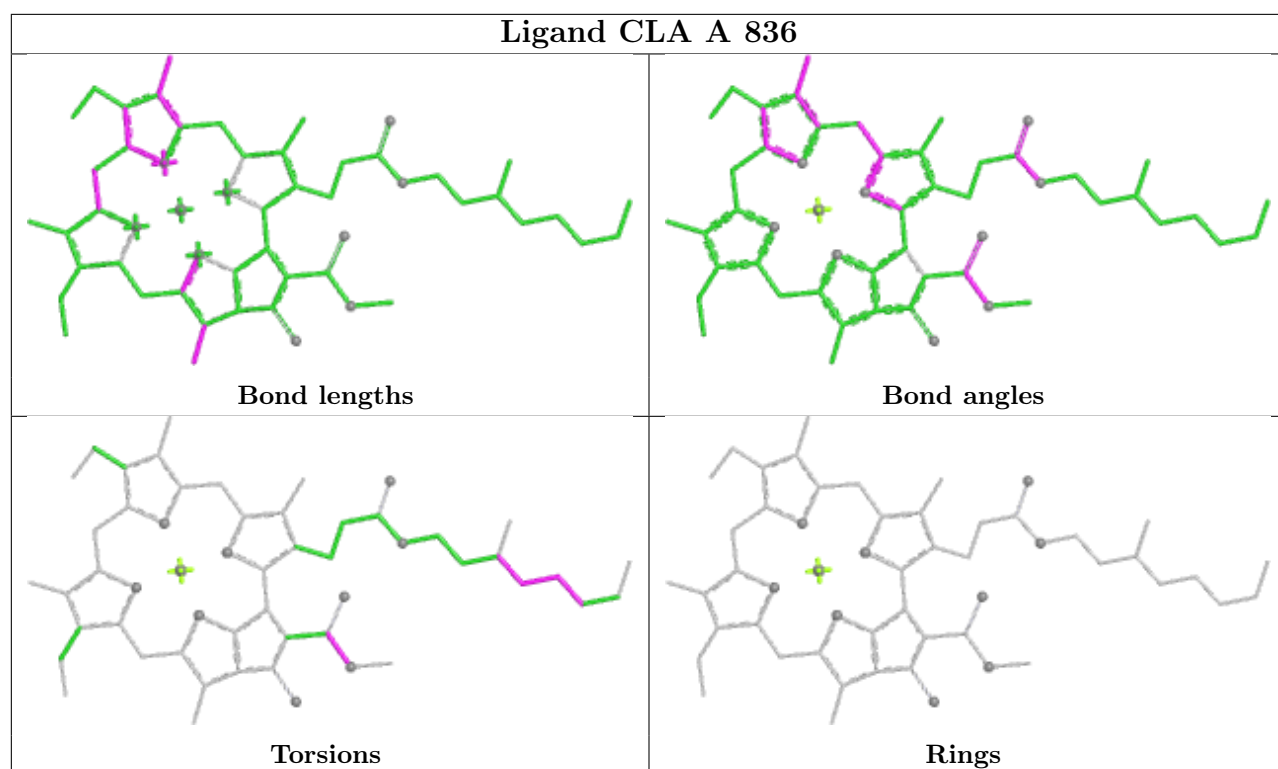


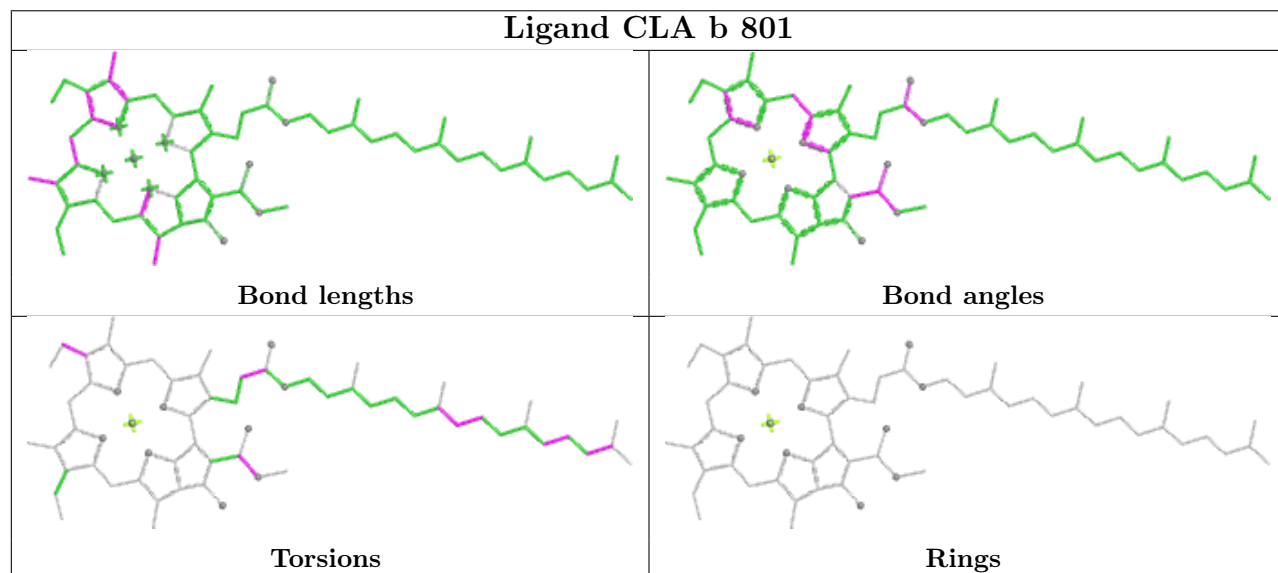
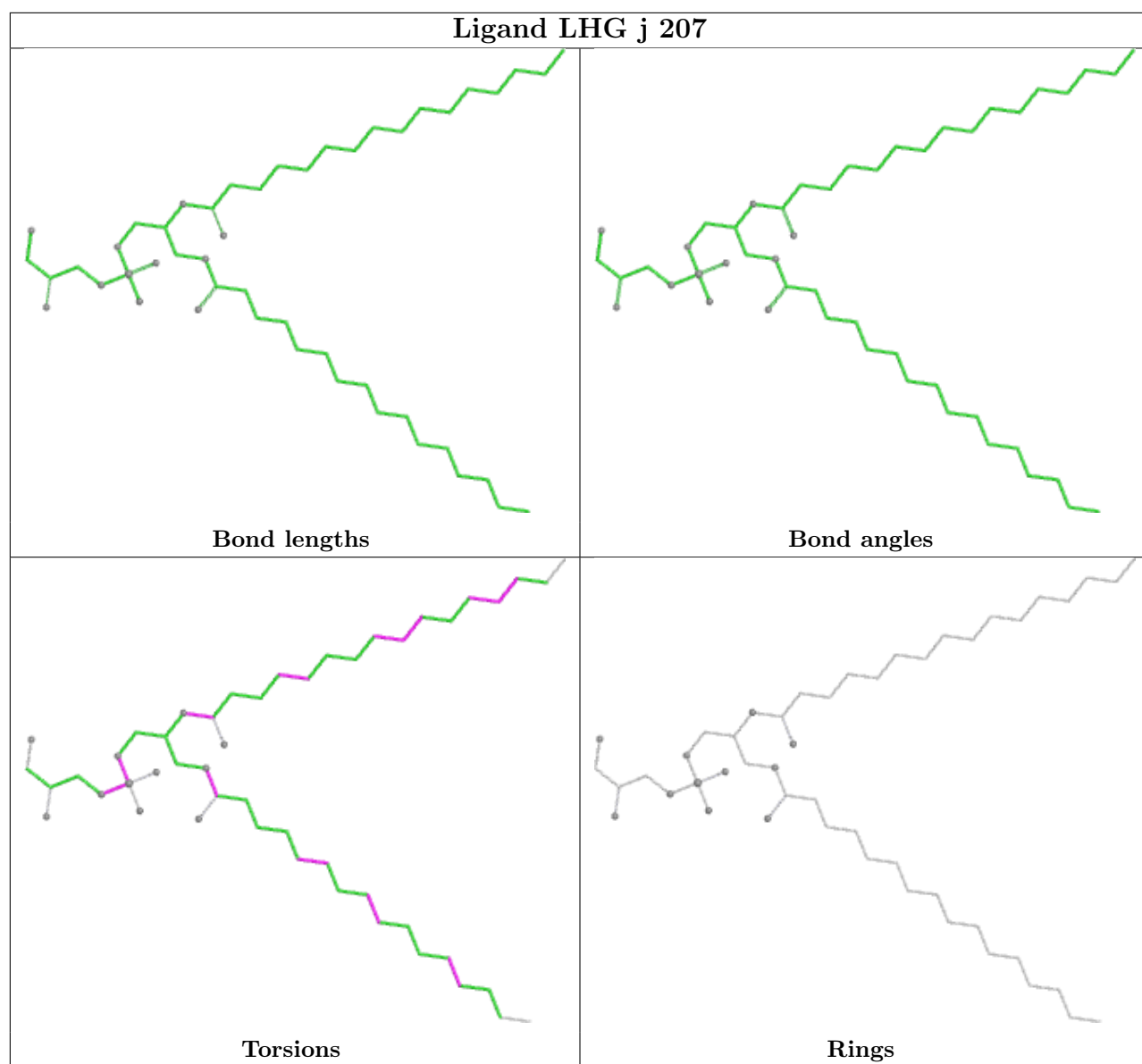
Ligand CLA a 833

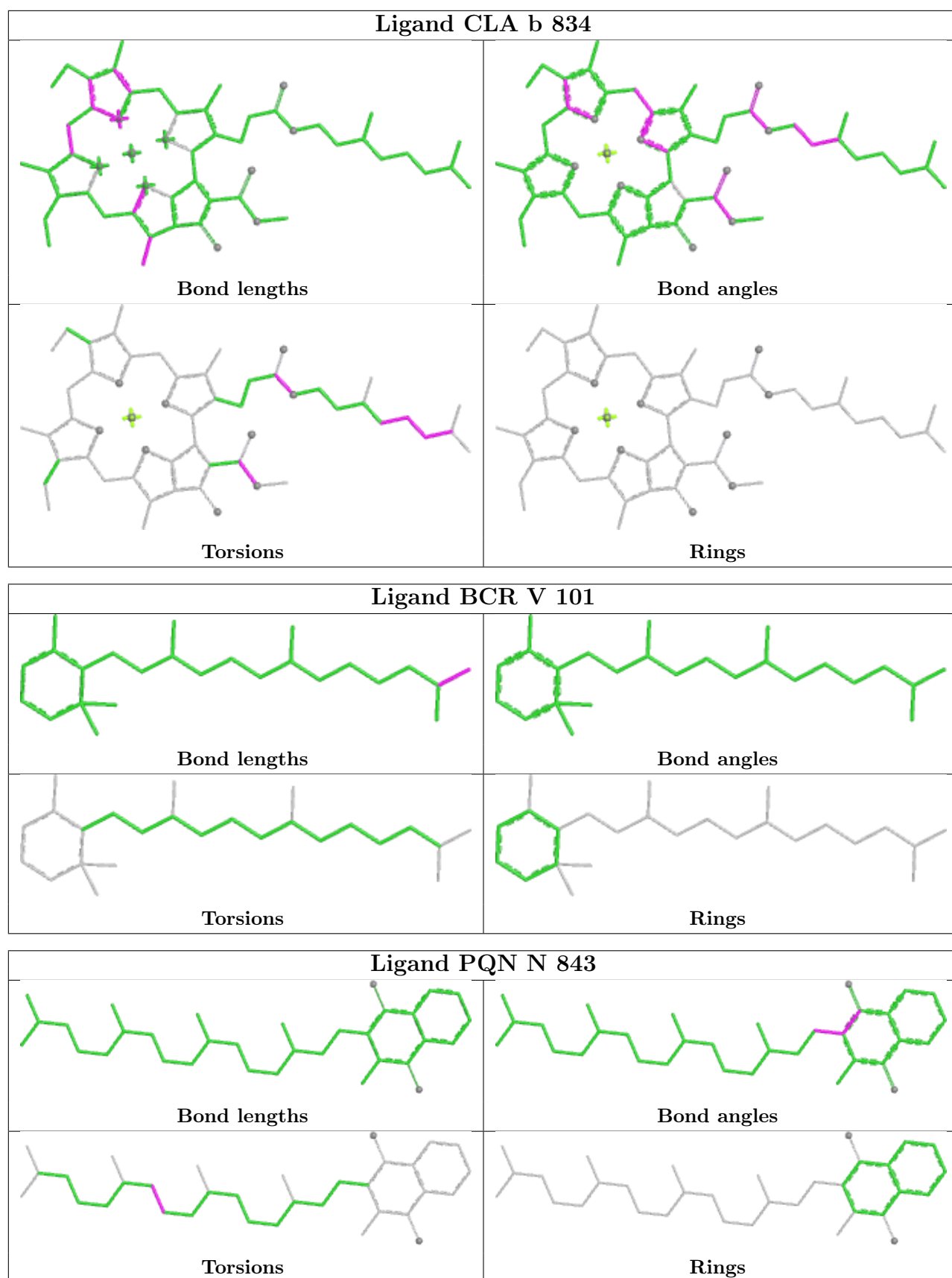


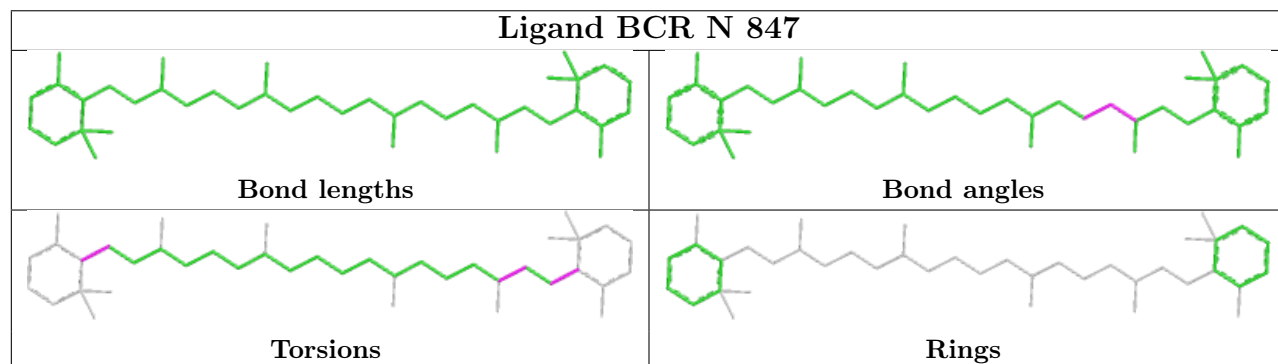
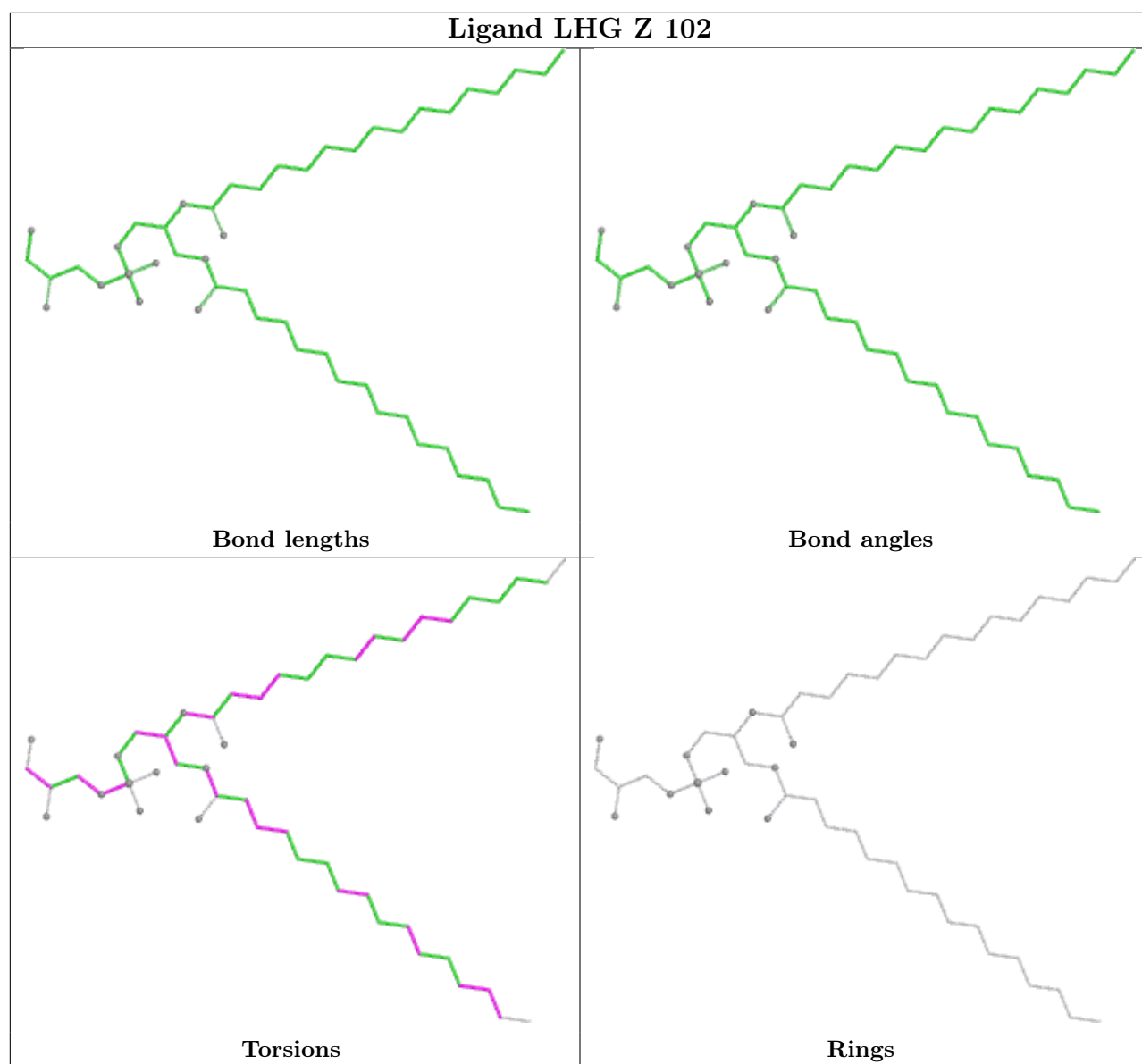
Ligand CLA a 810**Ligand CLA b 831**



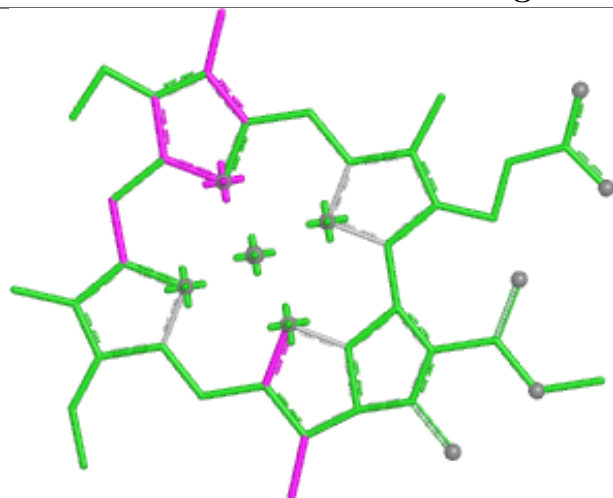




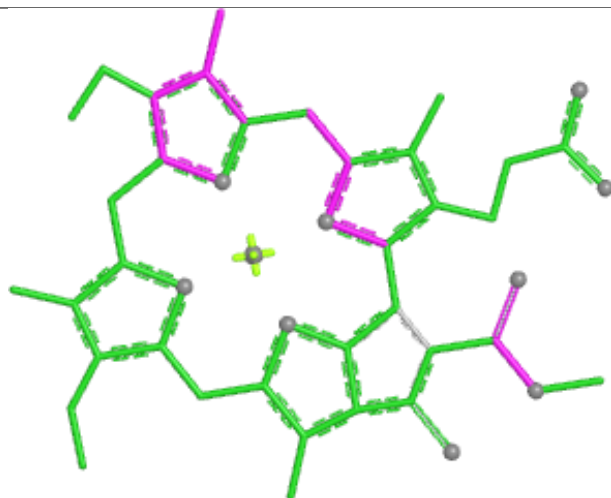




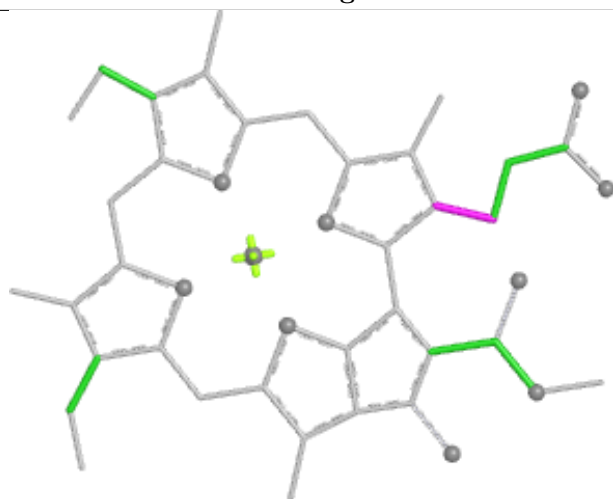
Ligand CLA O 835



Bond lengths



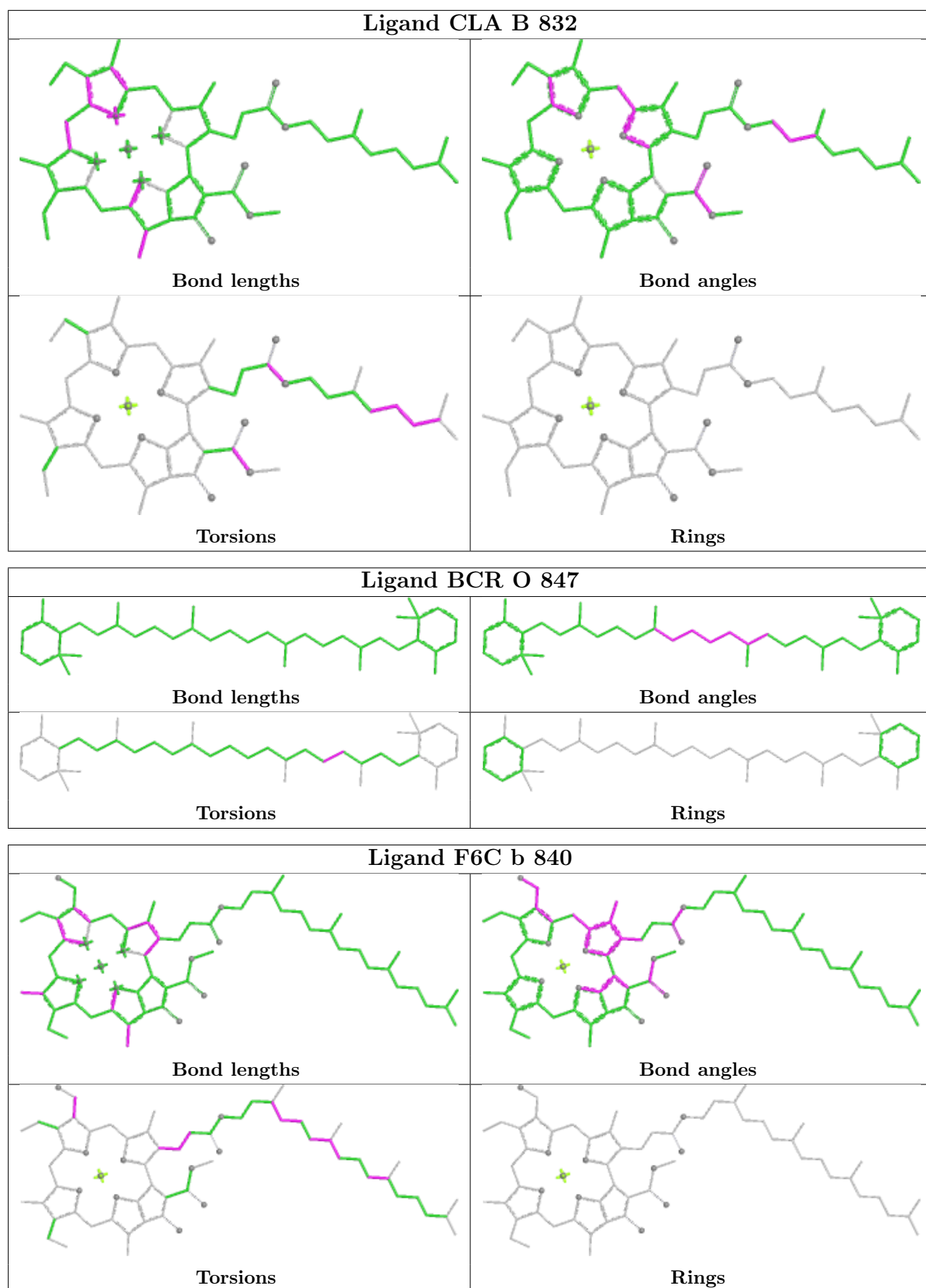
Bond angles

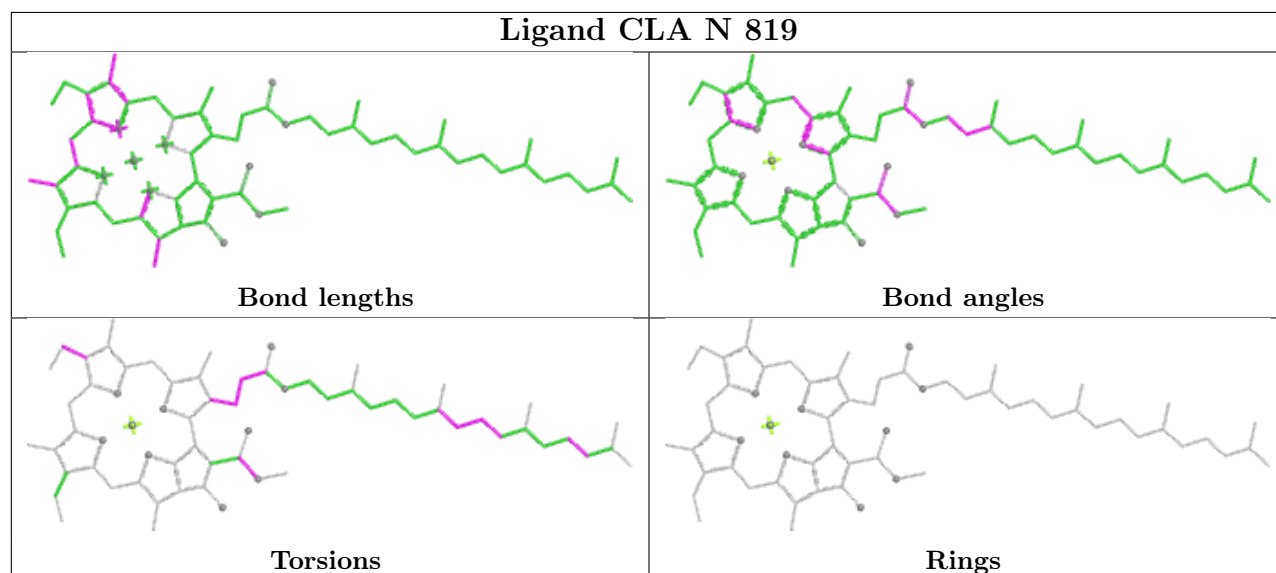
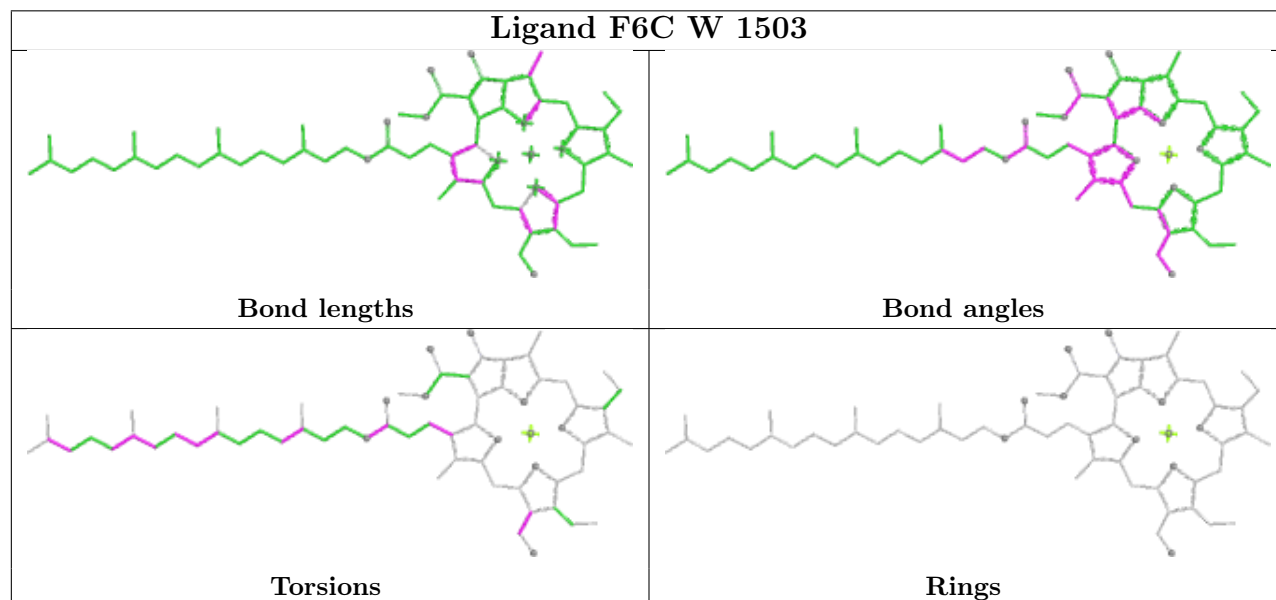
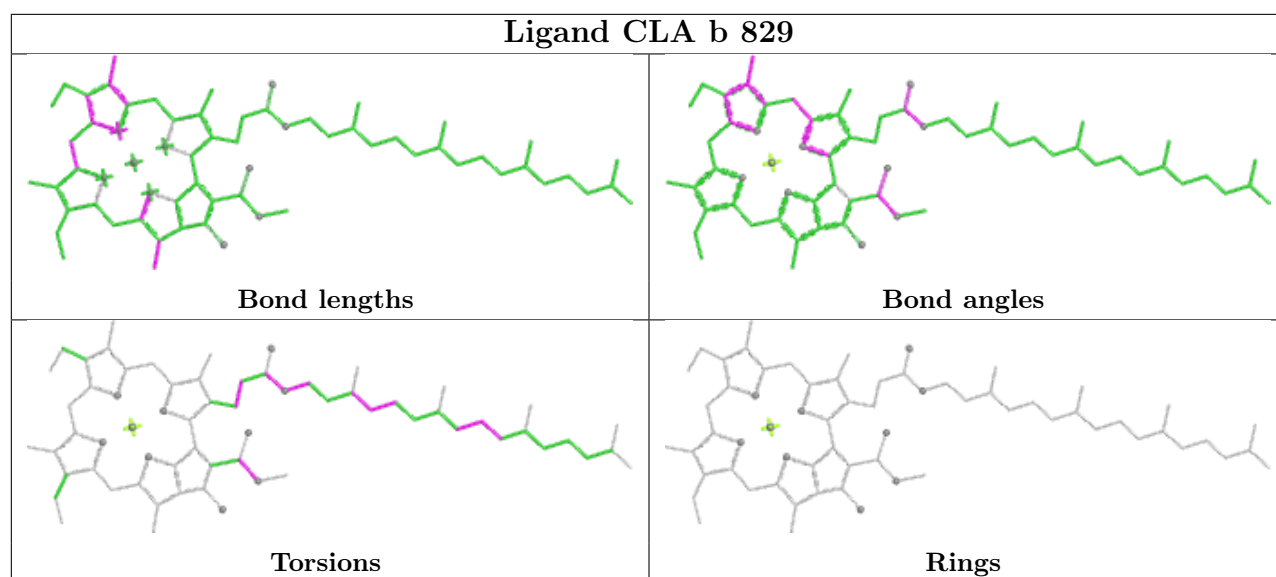


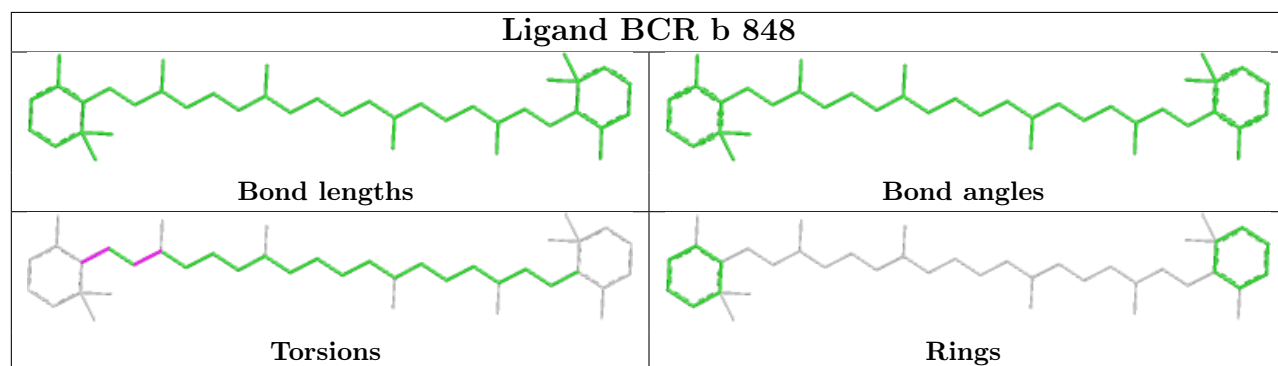
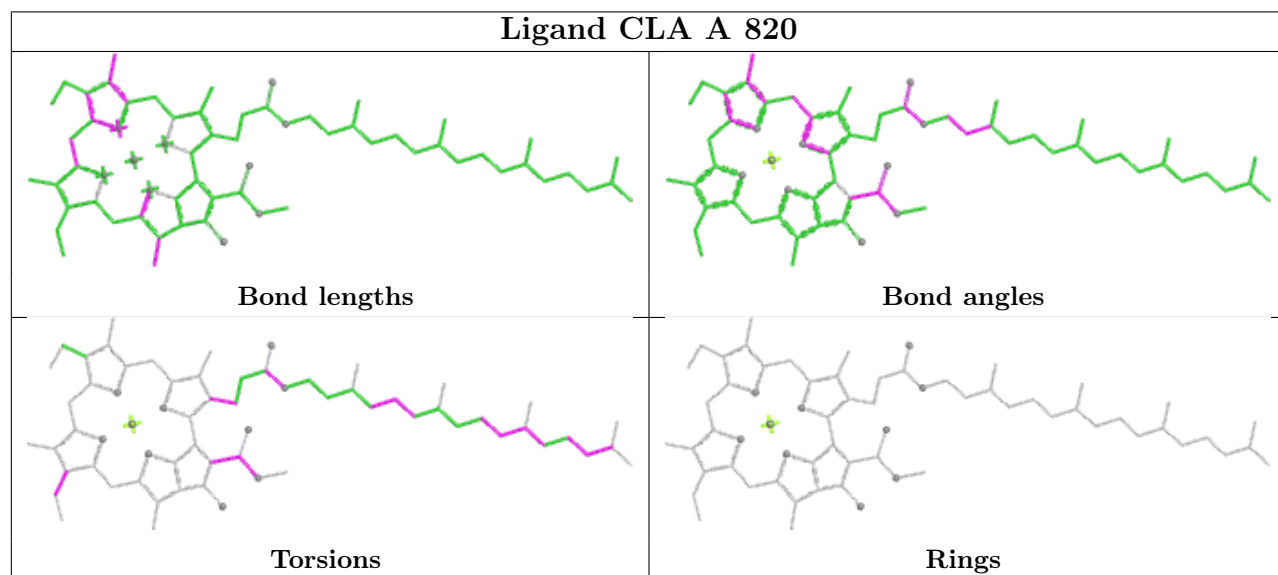
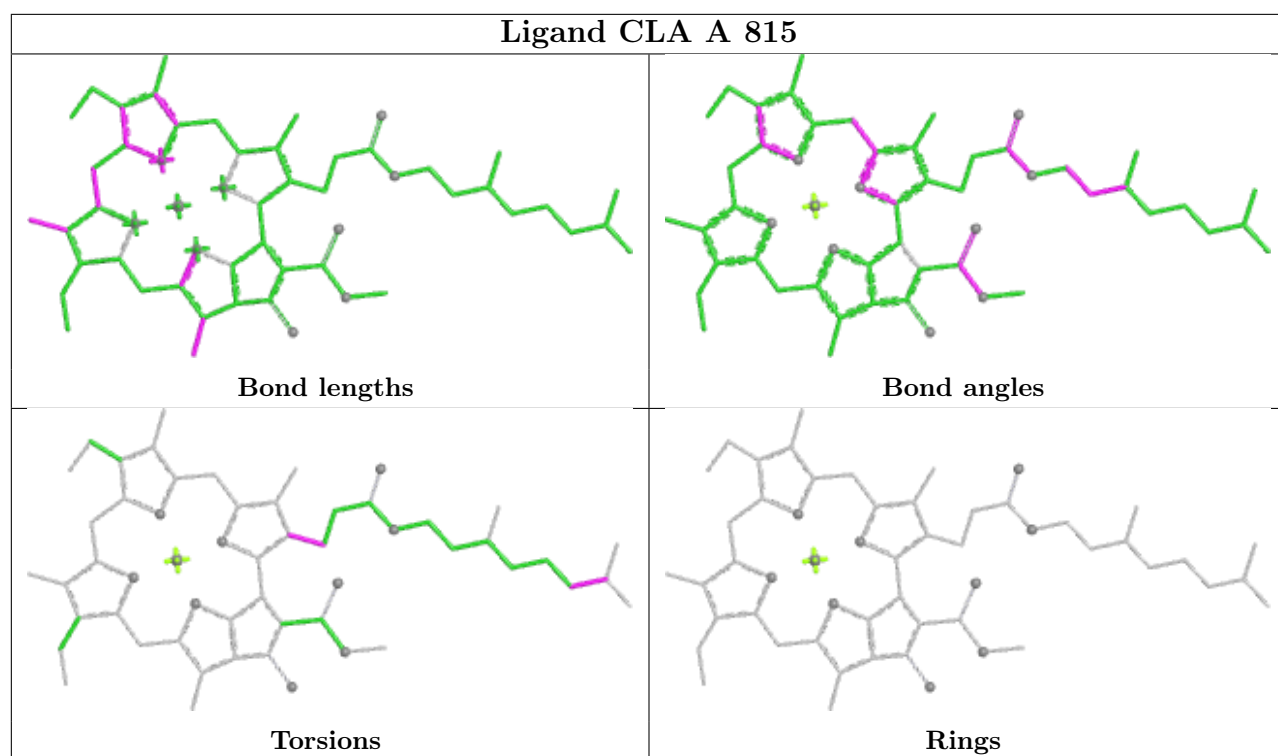
Torsions

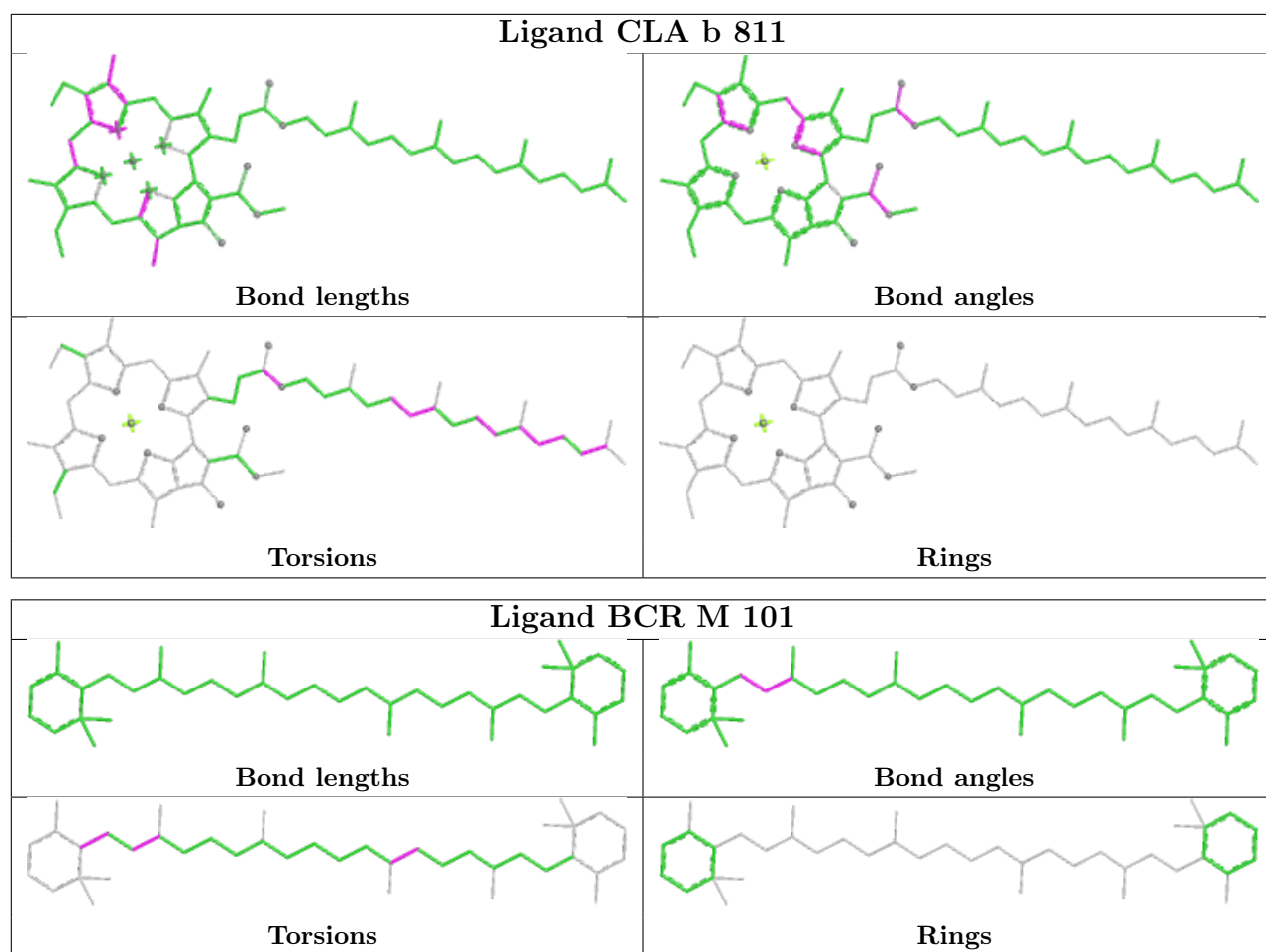


Rings

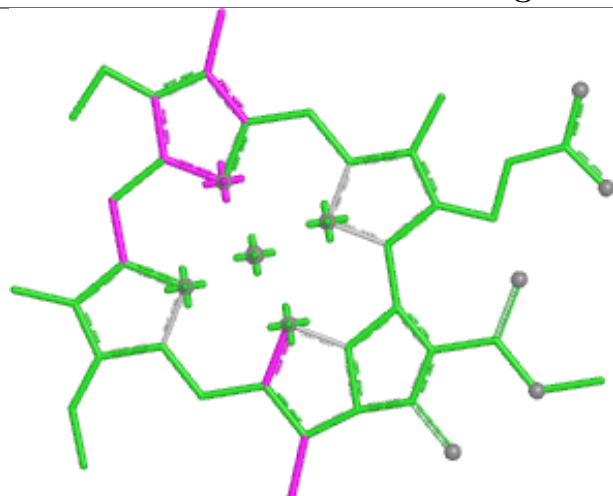




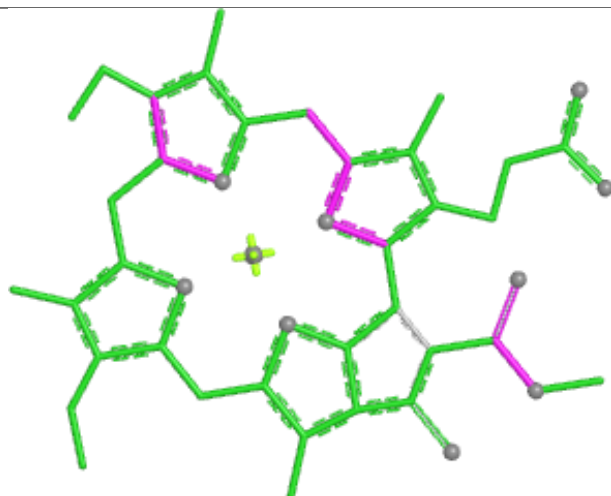




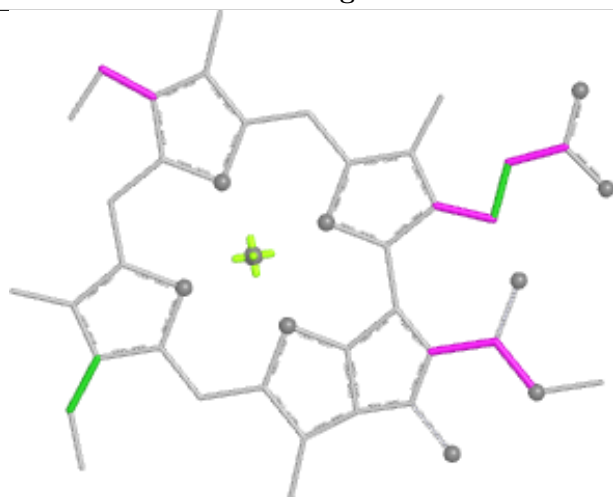
Ligand CLA B 834



Bond lengths



Bond angles

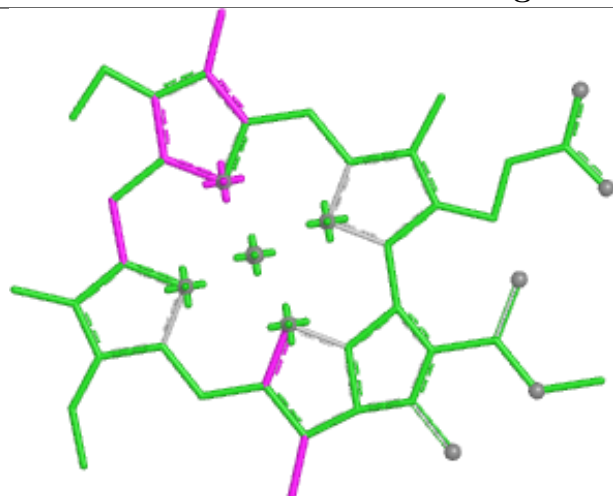


Torsions

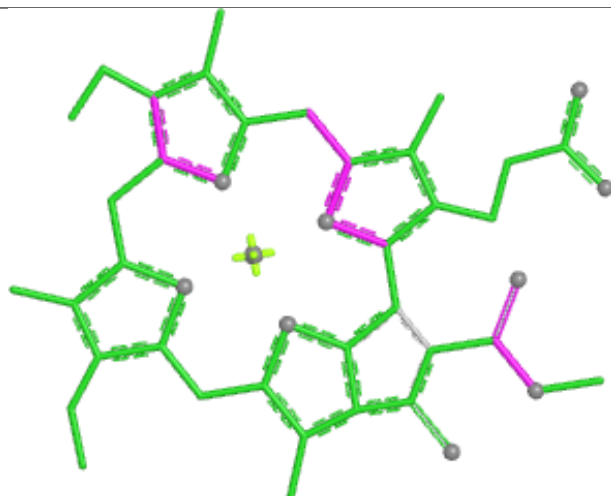


Rings

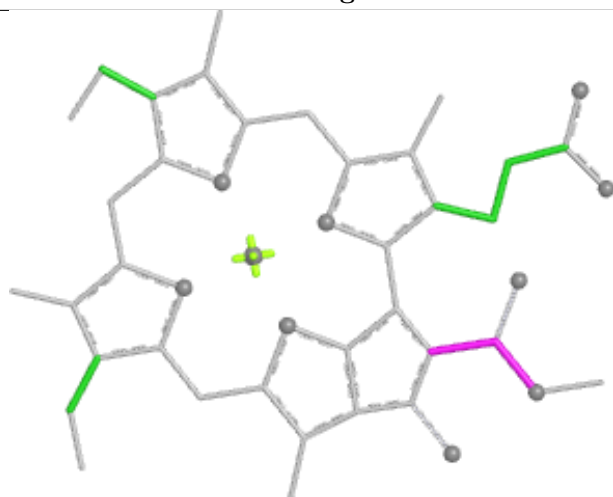
Ligand CLA O 821



Bond lengths



Bond angles

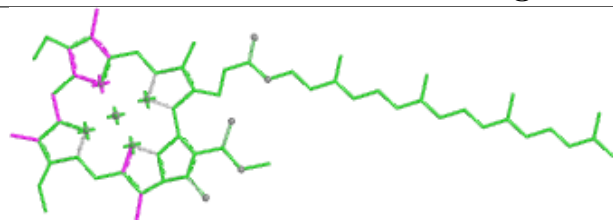


Torsions

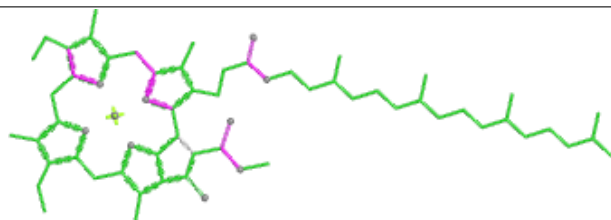


Rings

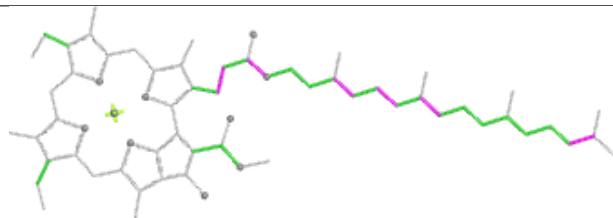
Ligand CLA N 814



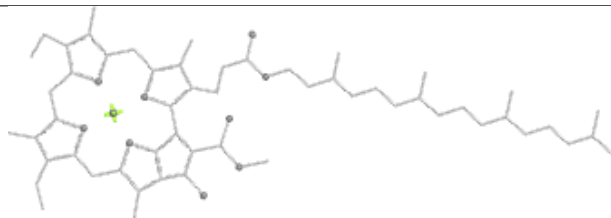
Bond lengths



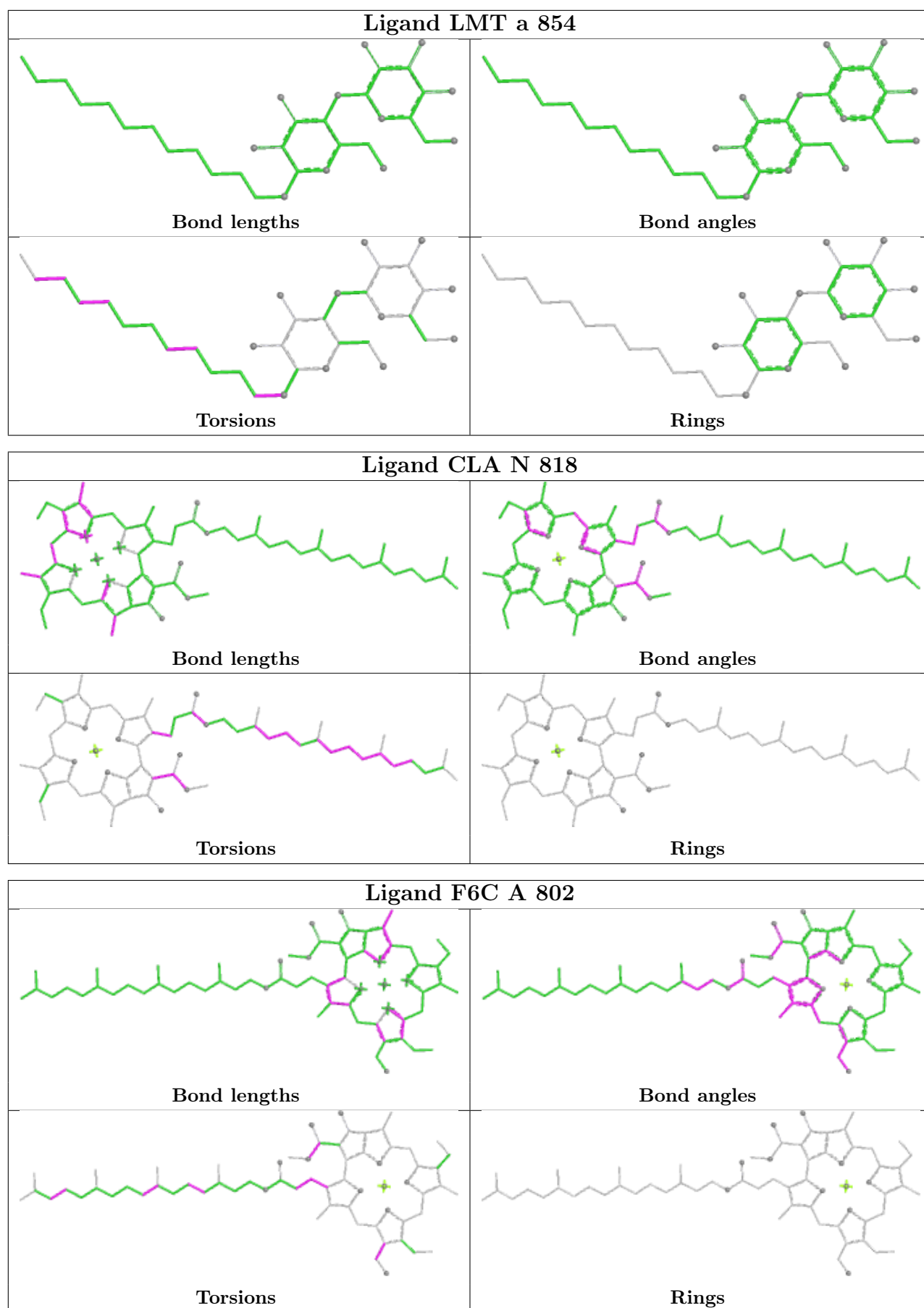
Bond angles

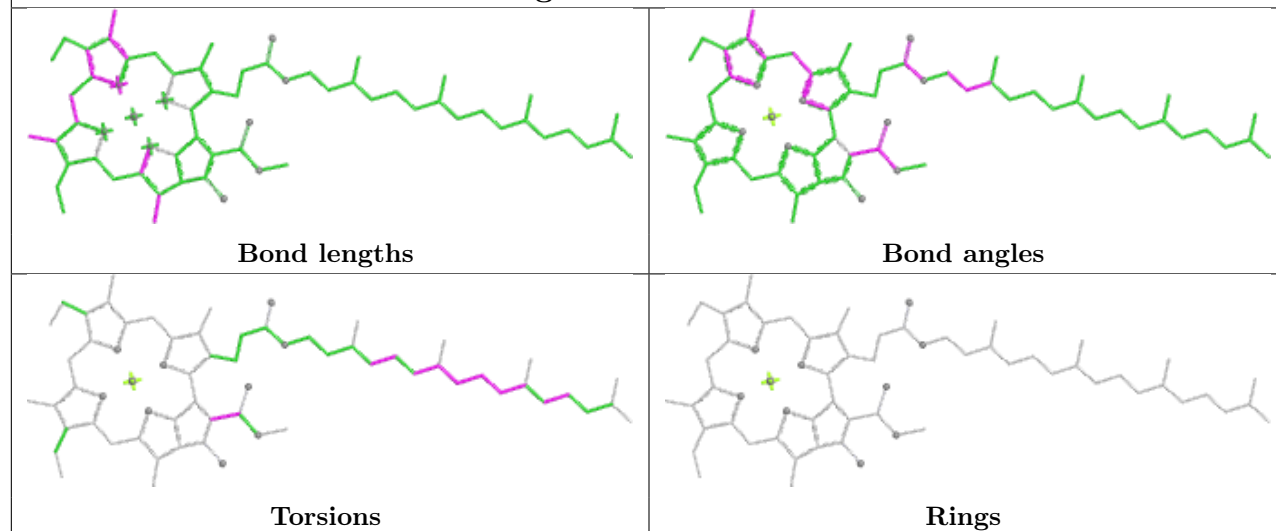
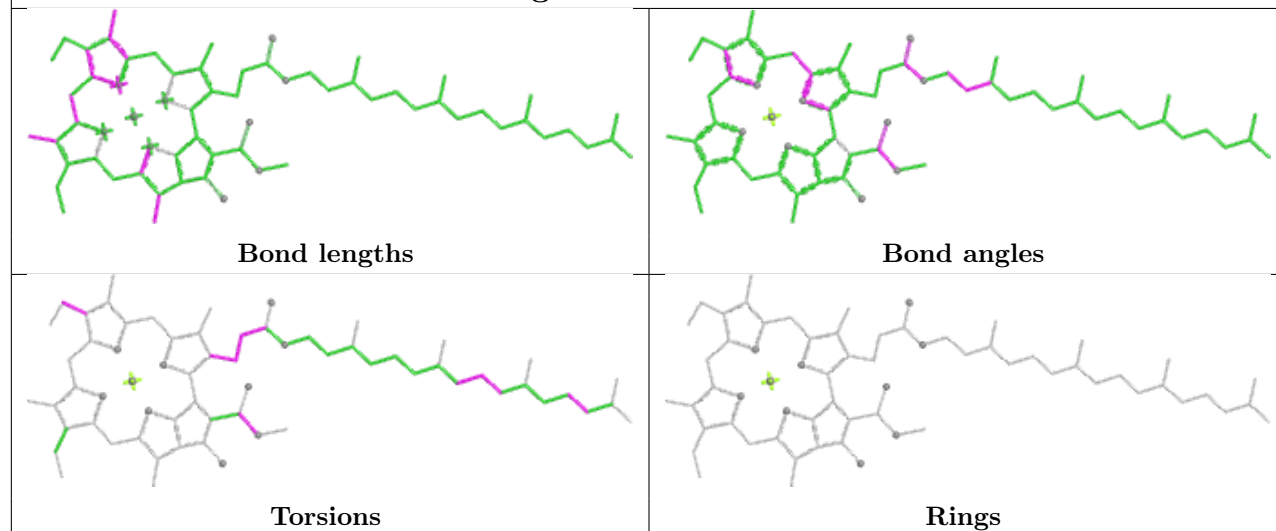


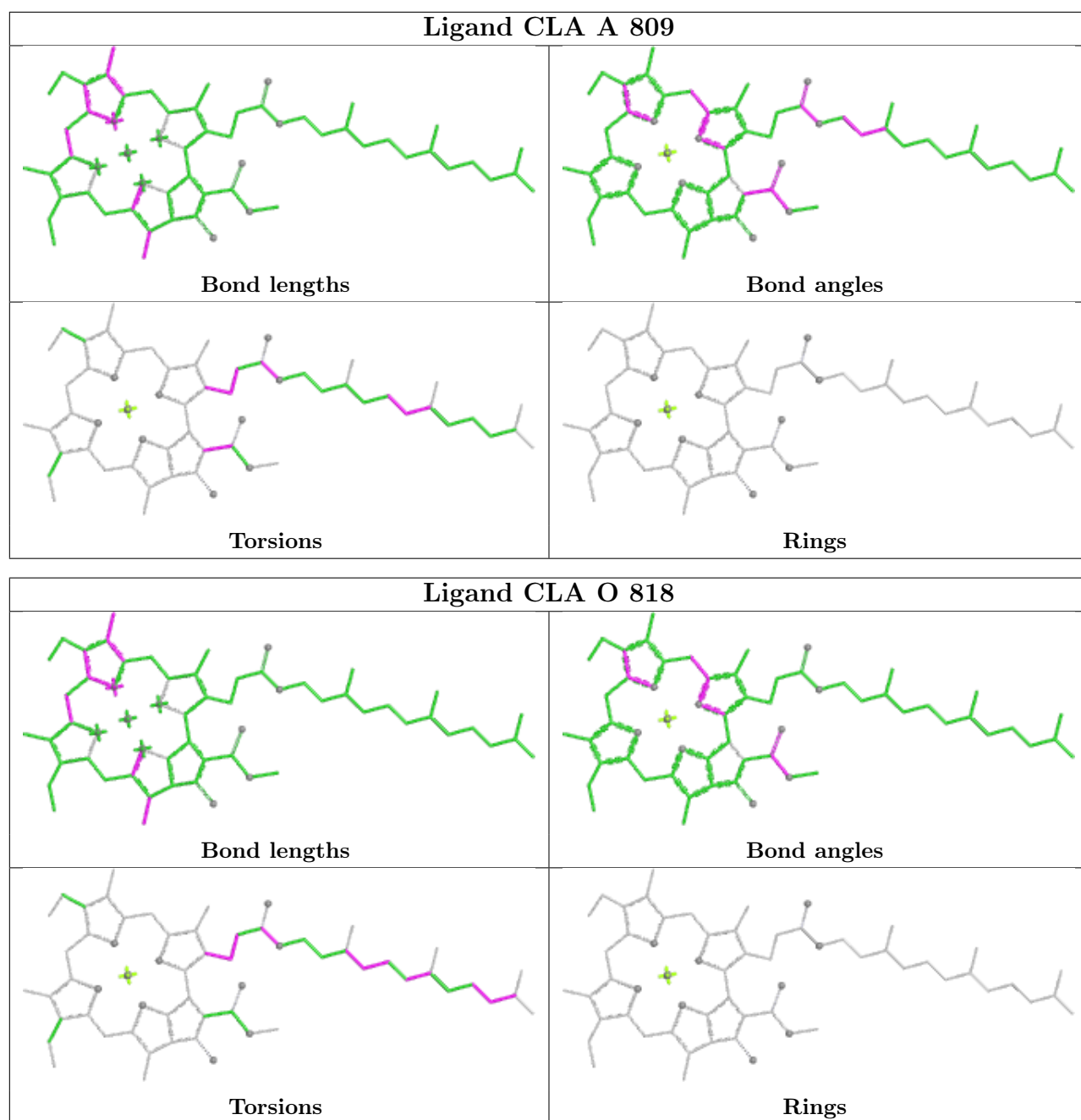
Torsions



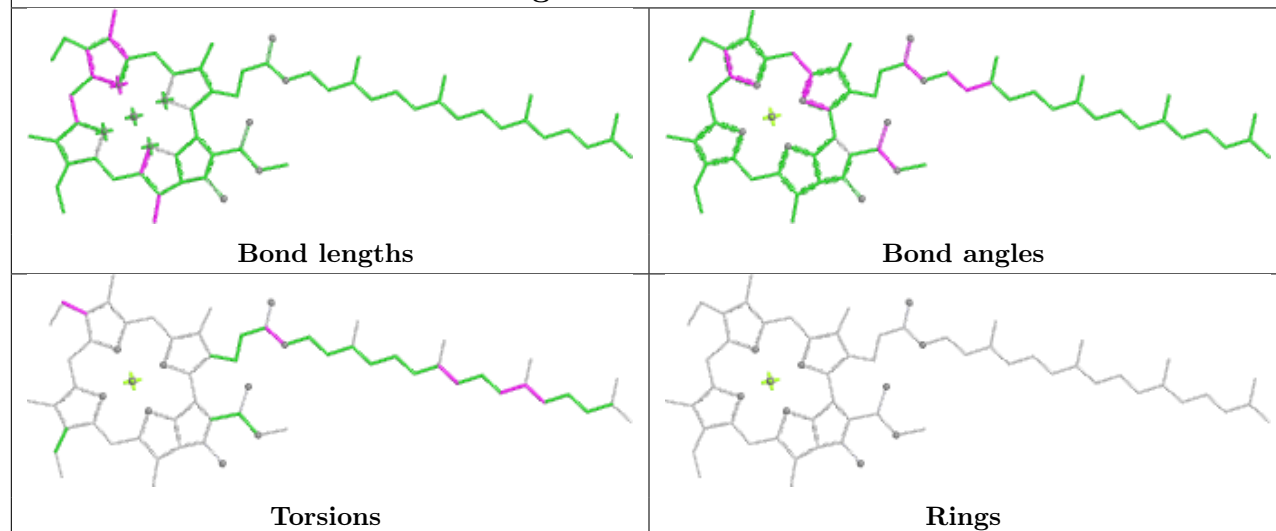
Rings



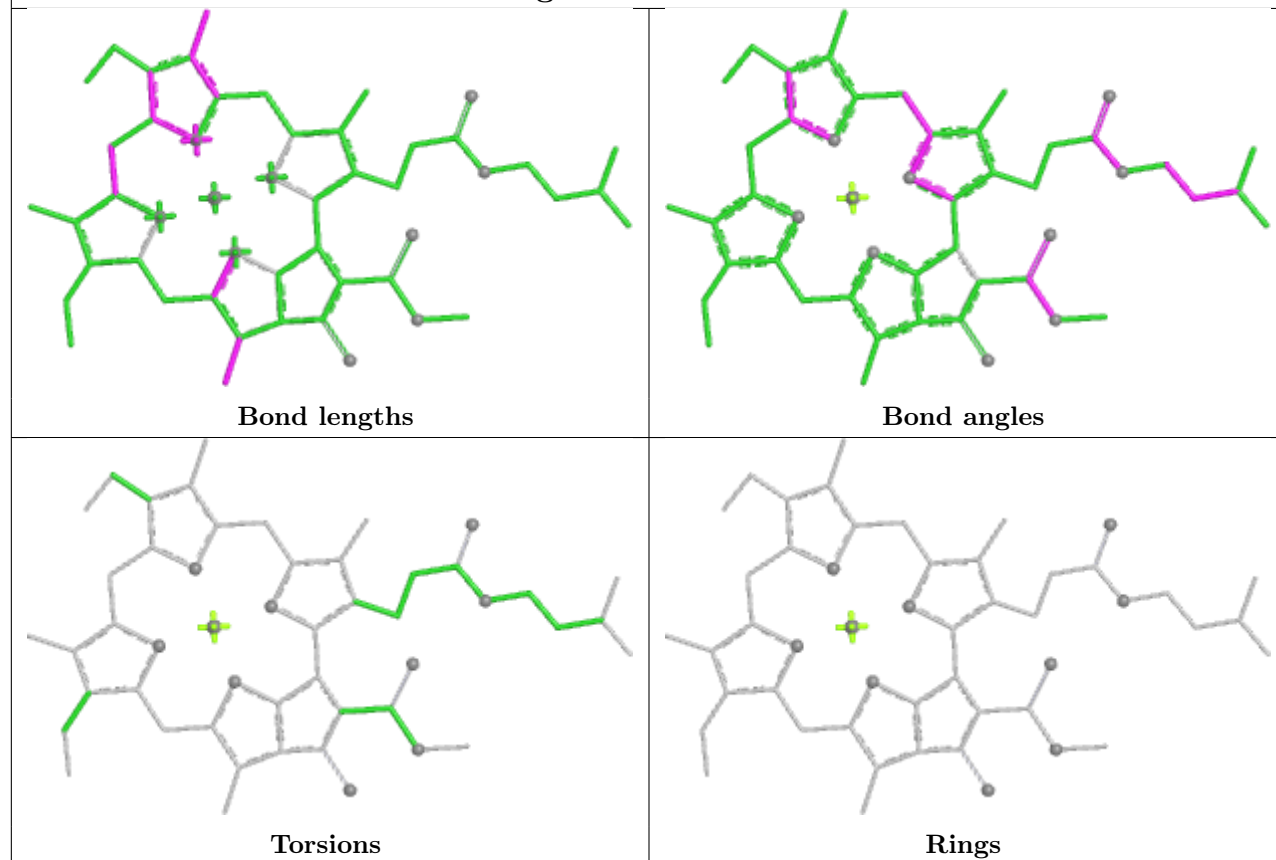
Ligand CLA b 808**Ligand CLA A 819**

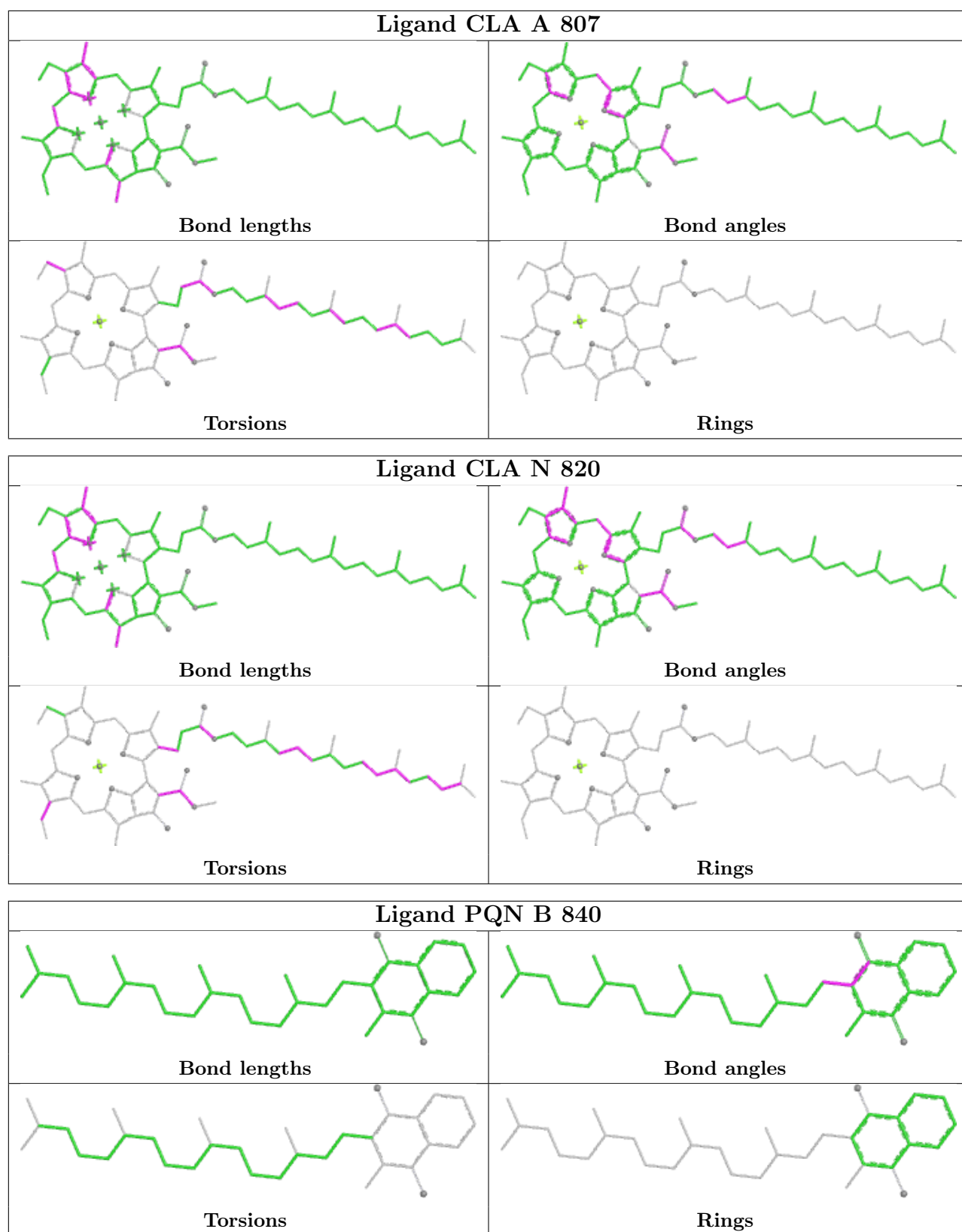


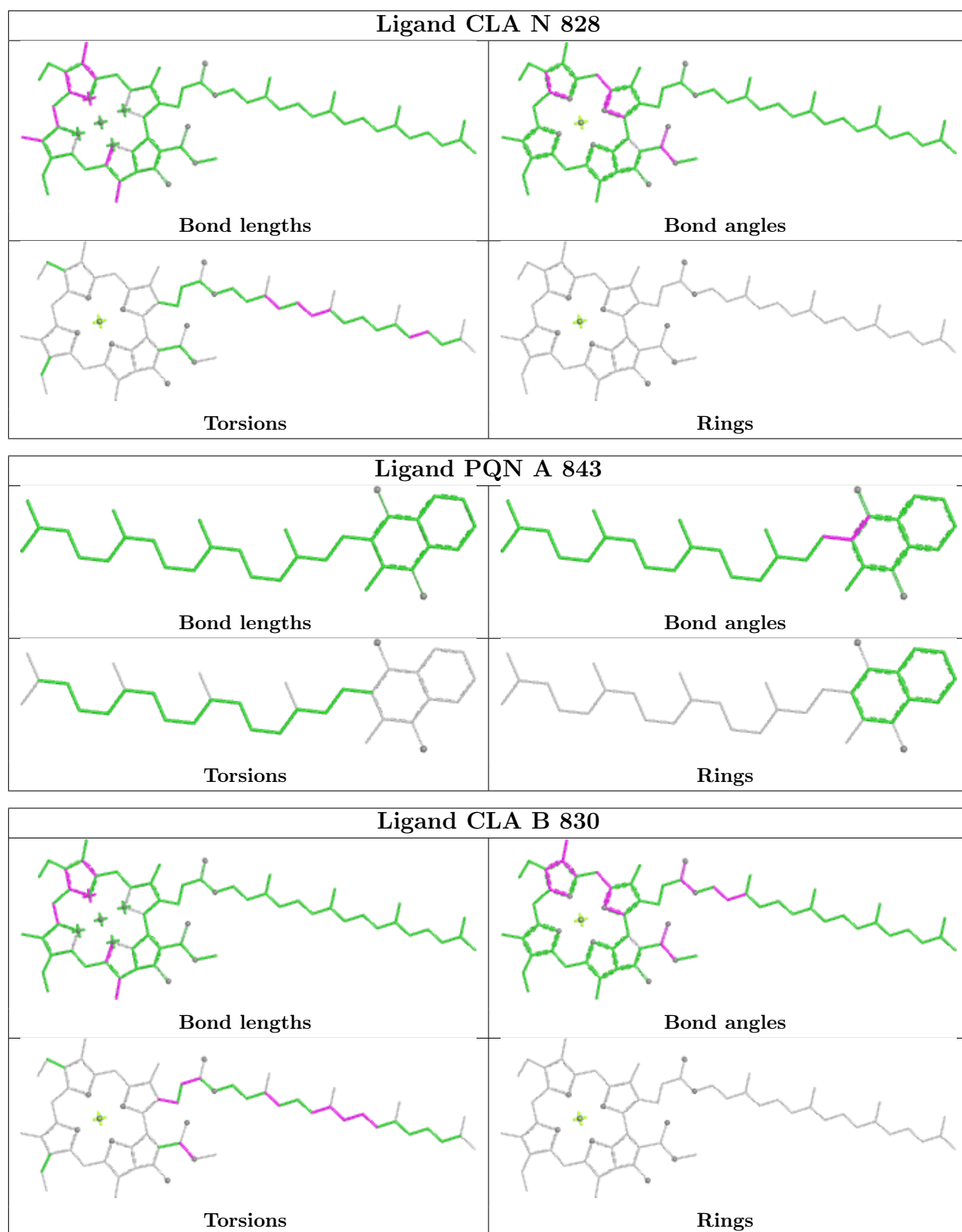
Ligand CLA B 817

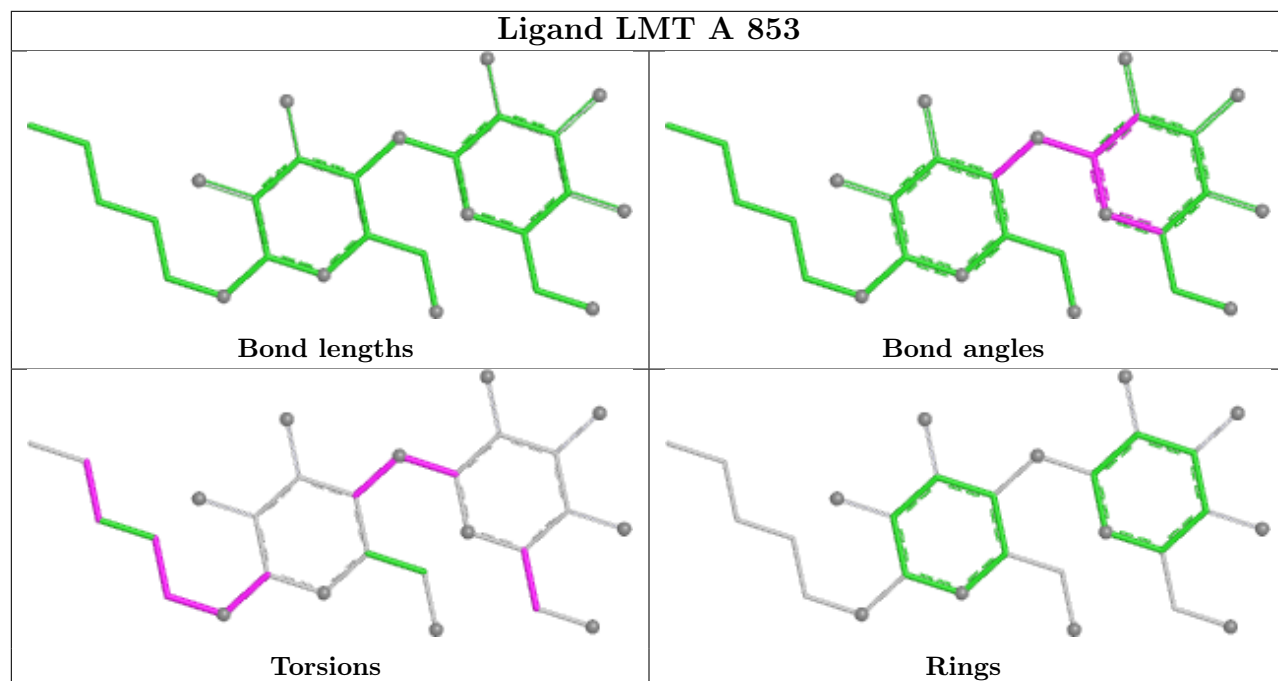
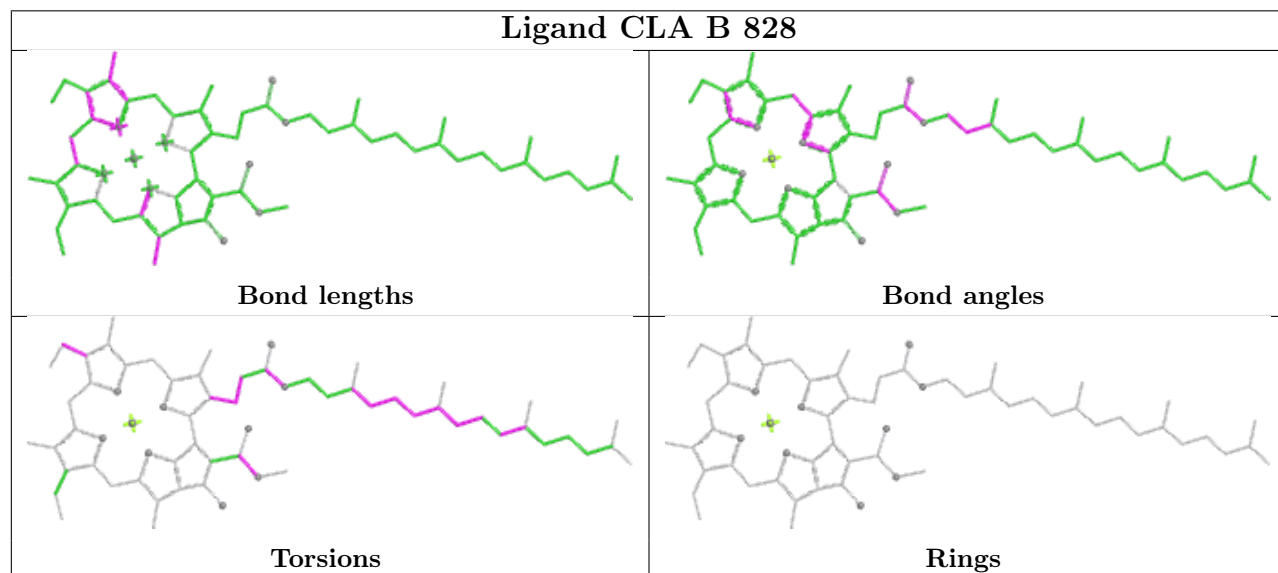
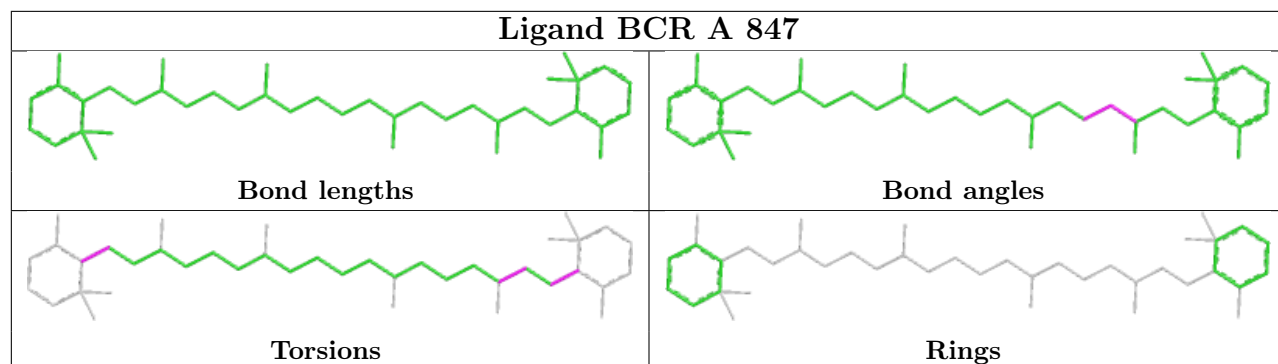


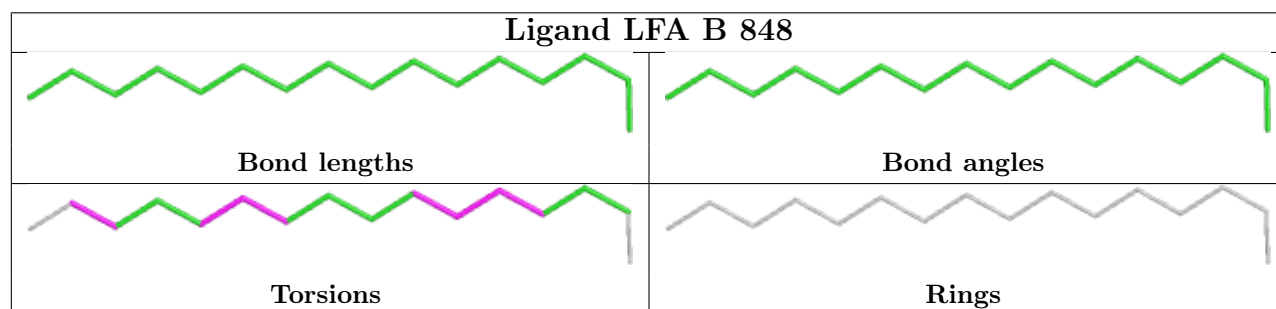
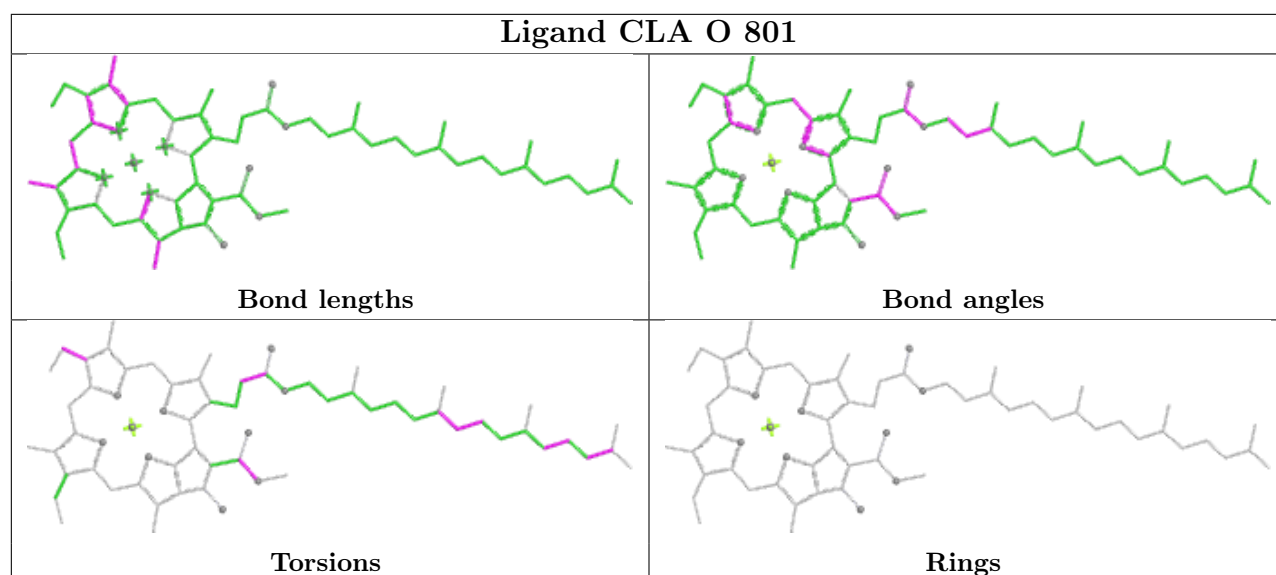
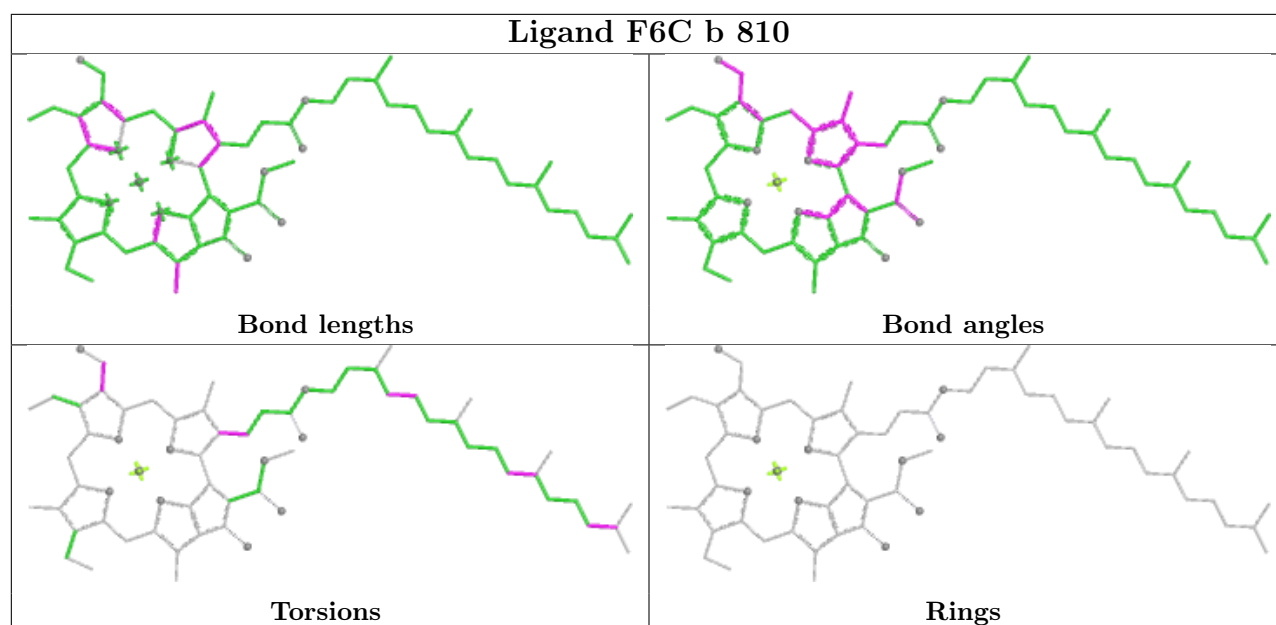
Ligand CLA a 840

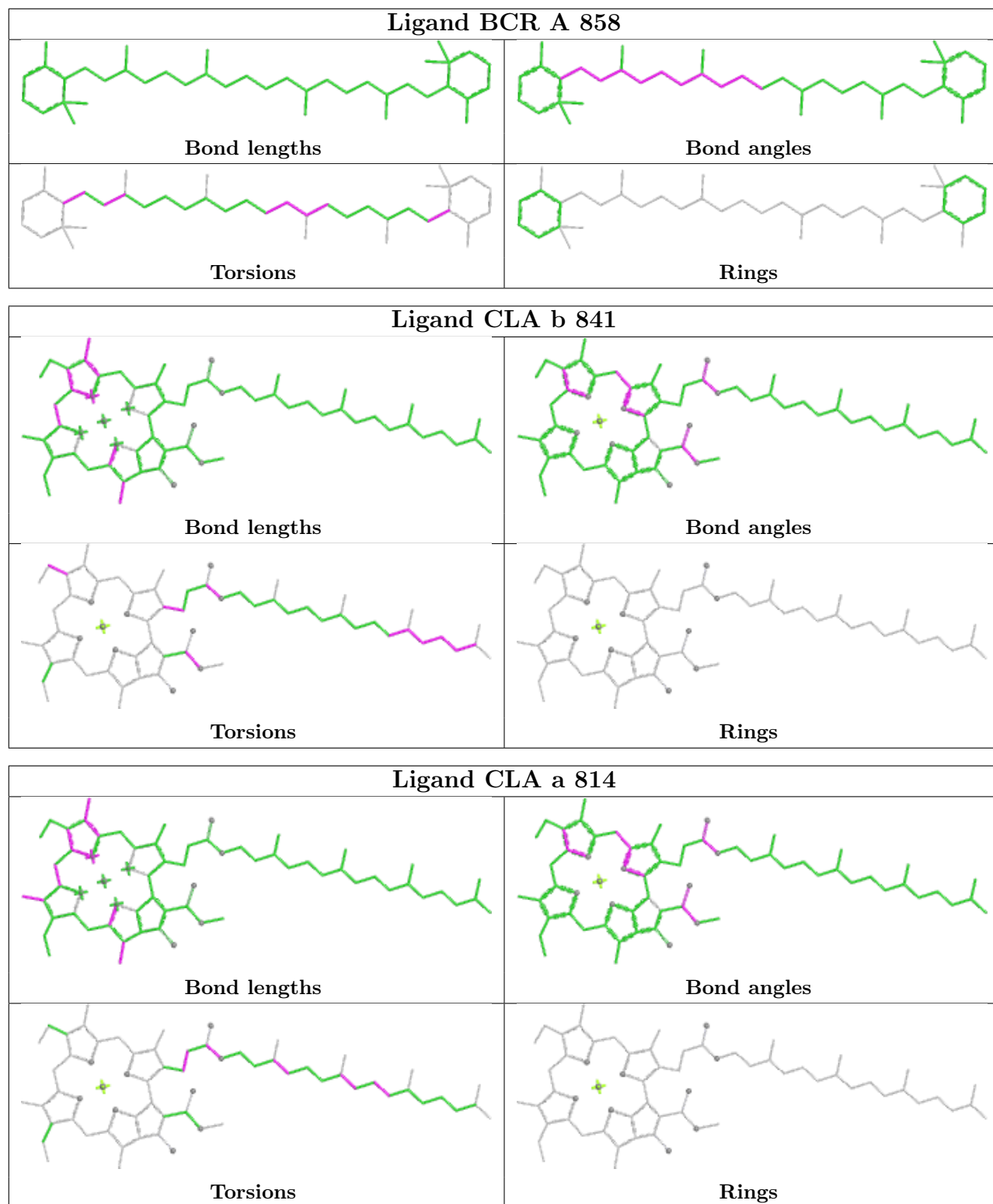




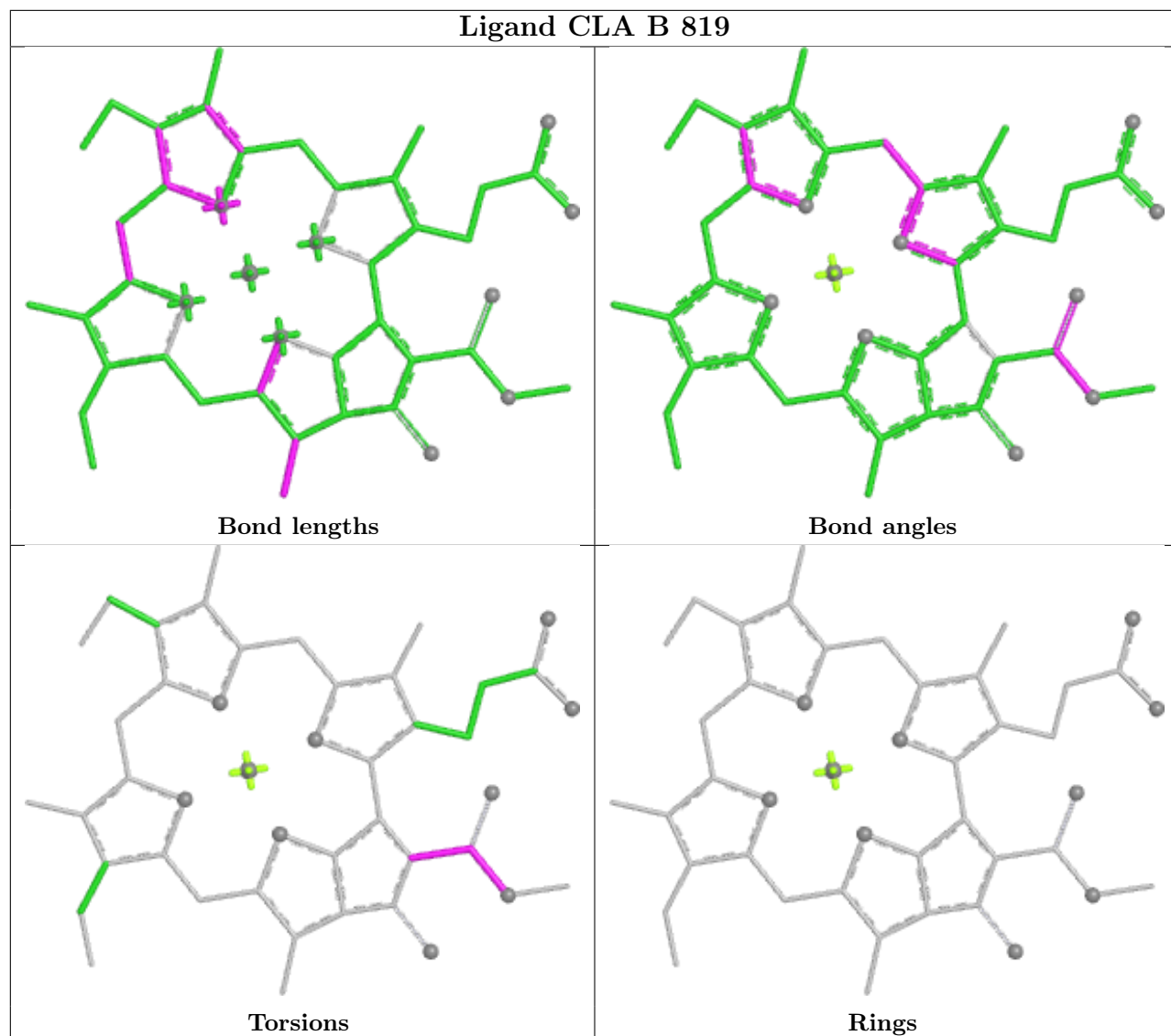


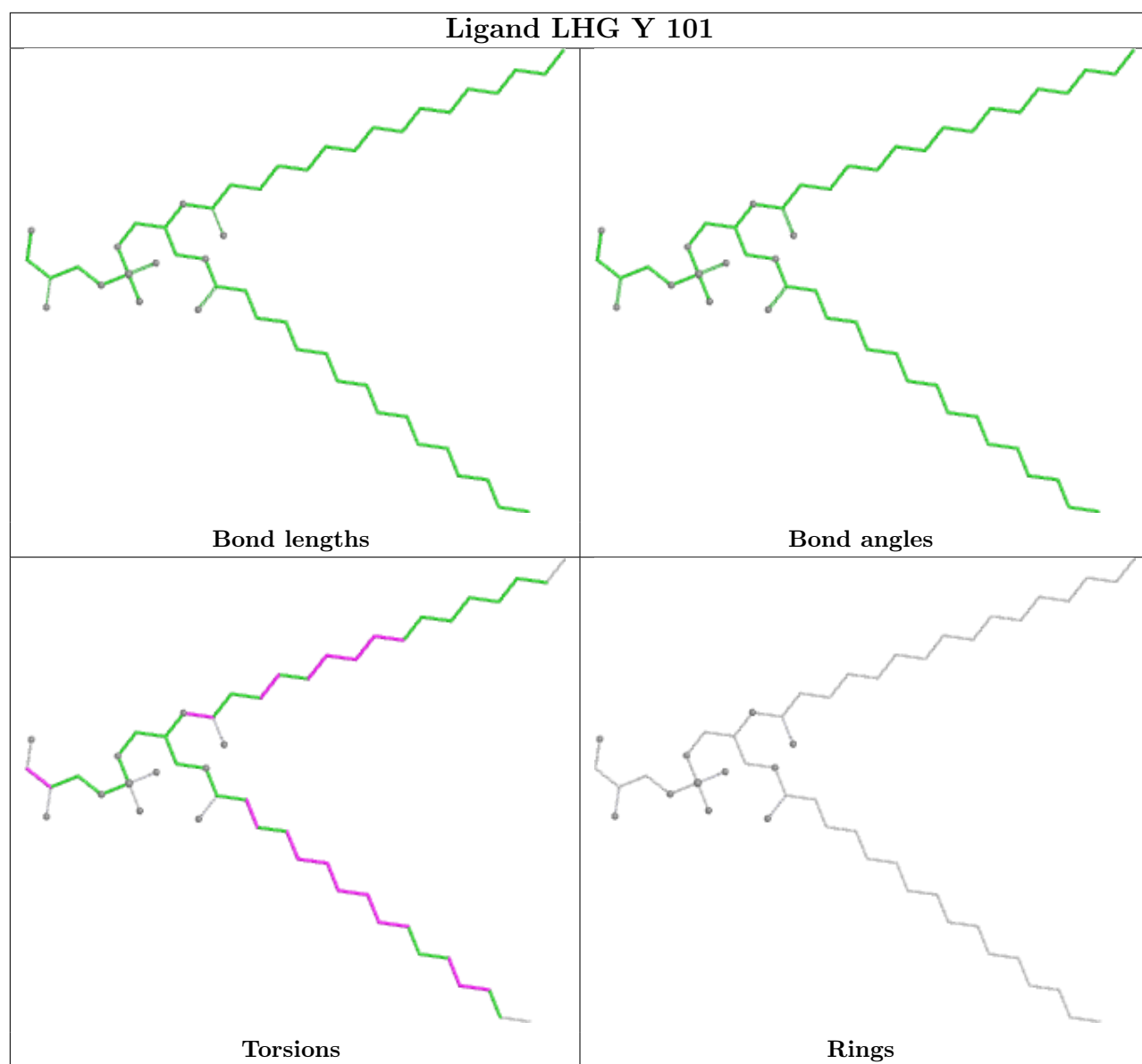


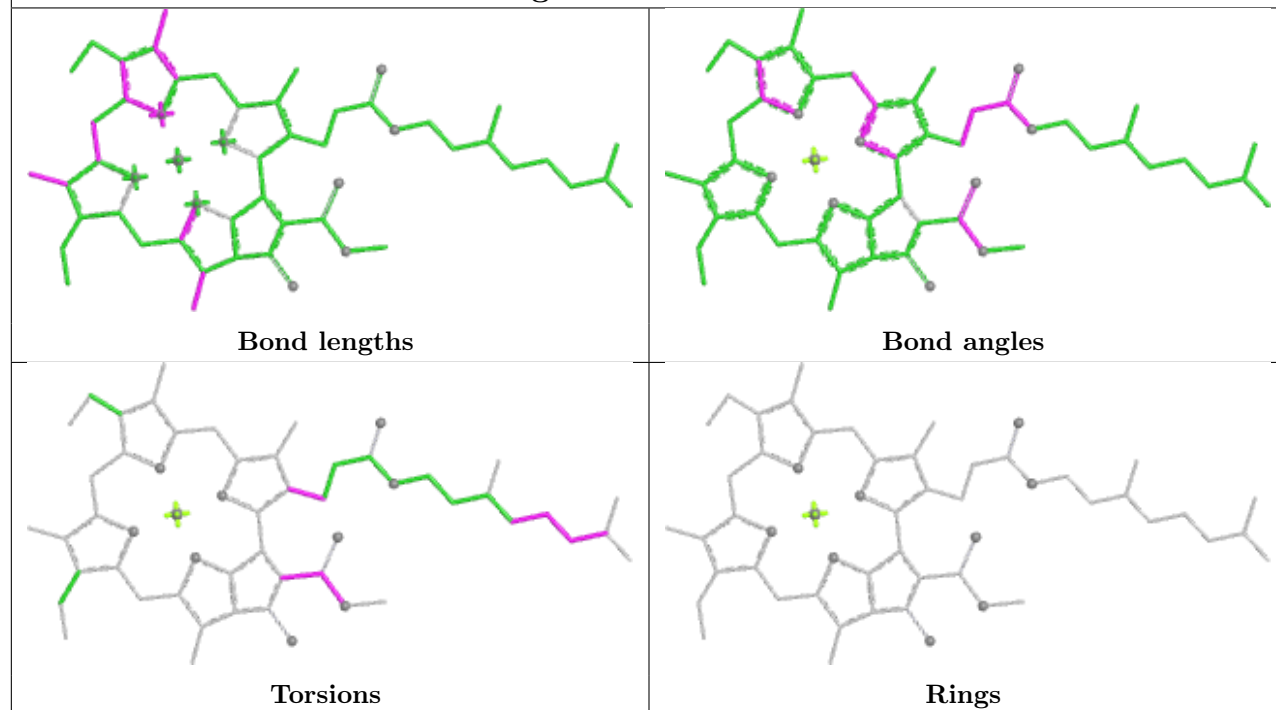
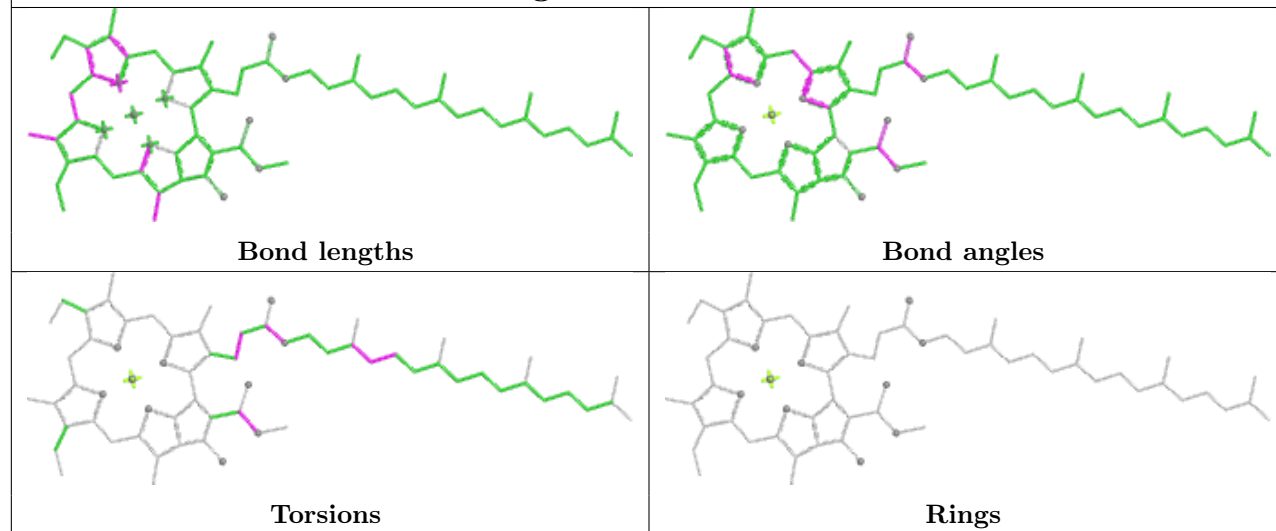


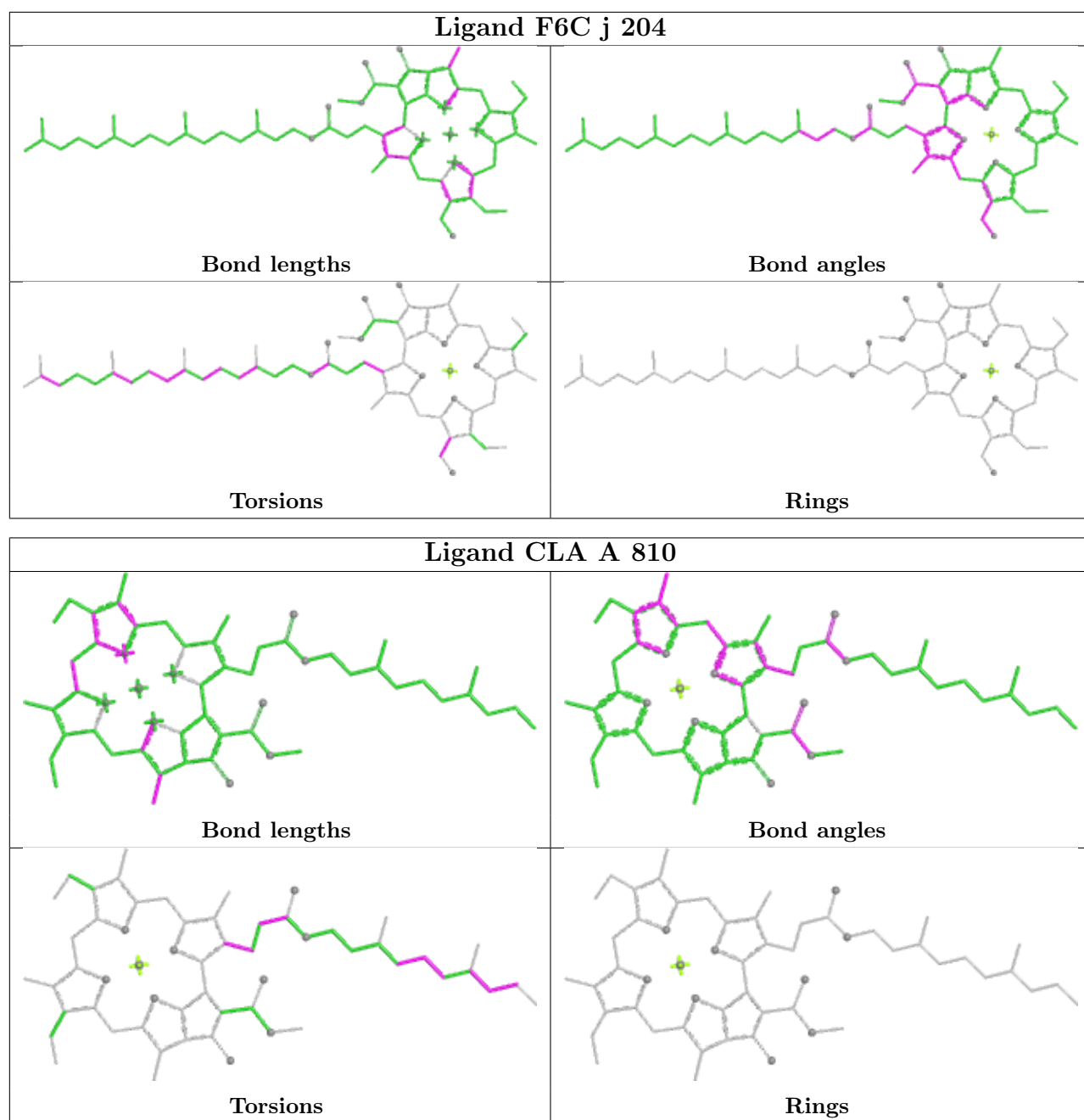


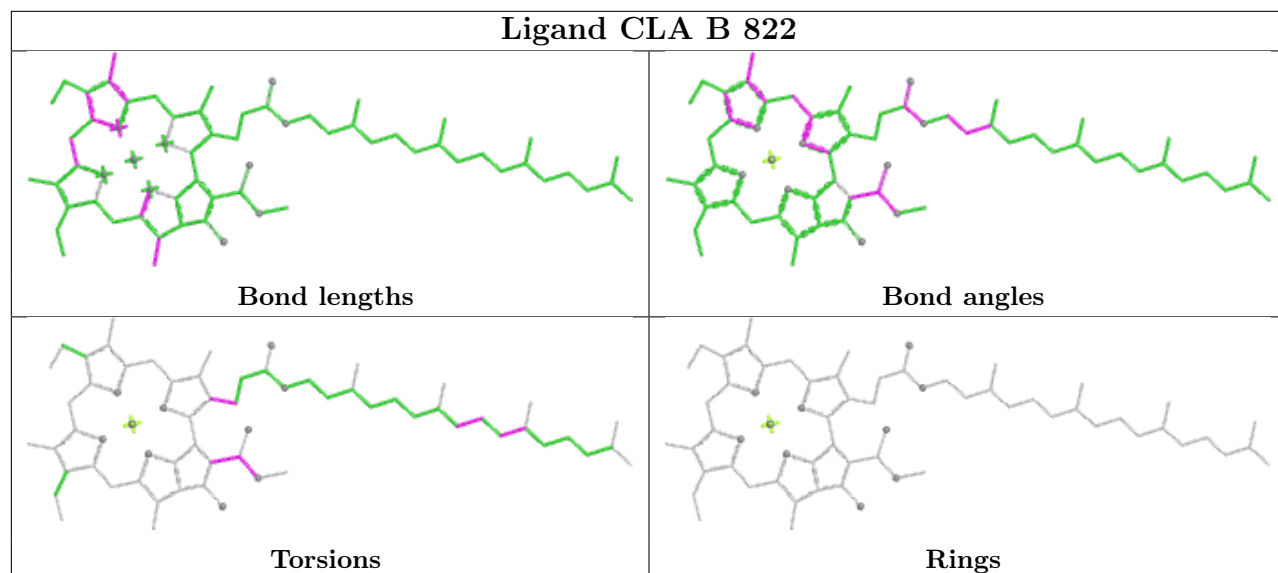
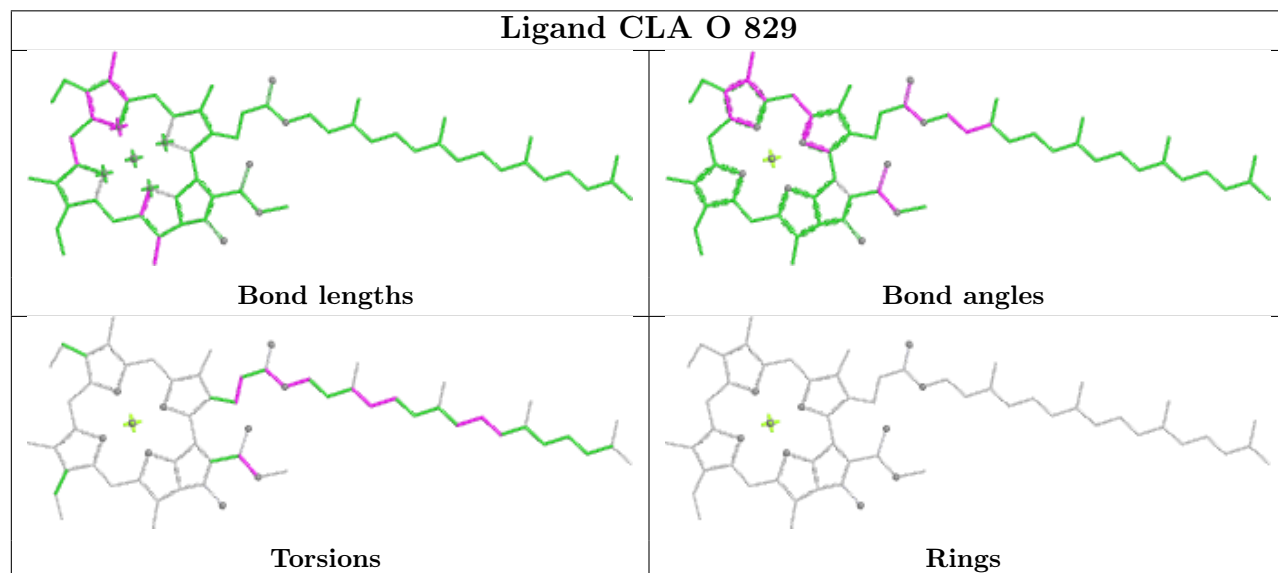
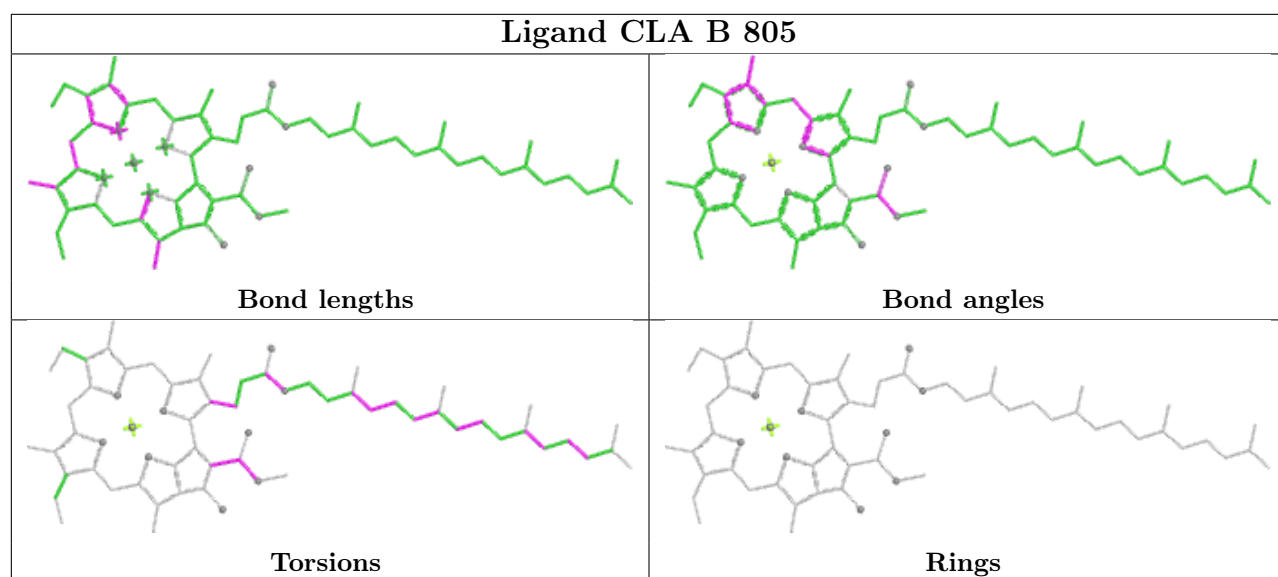
Ligand CLA B 819

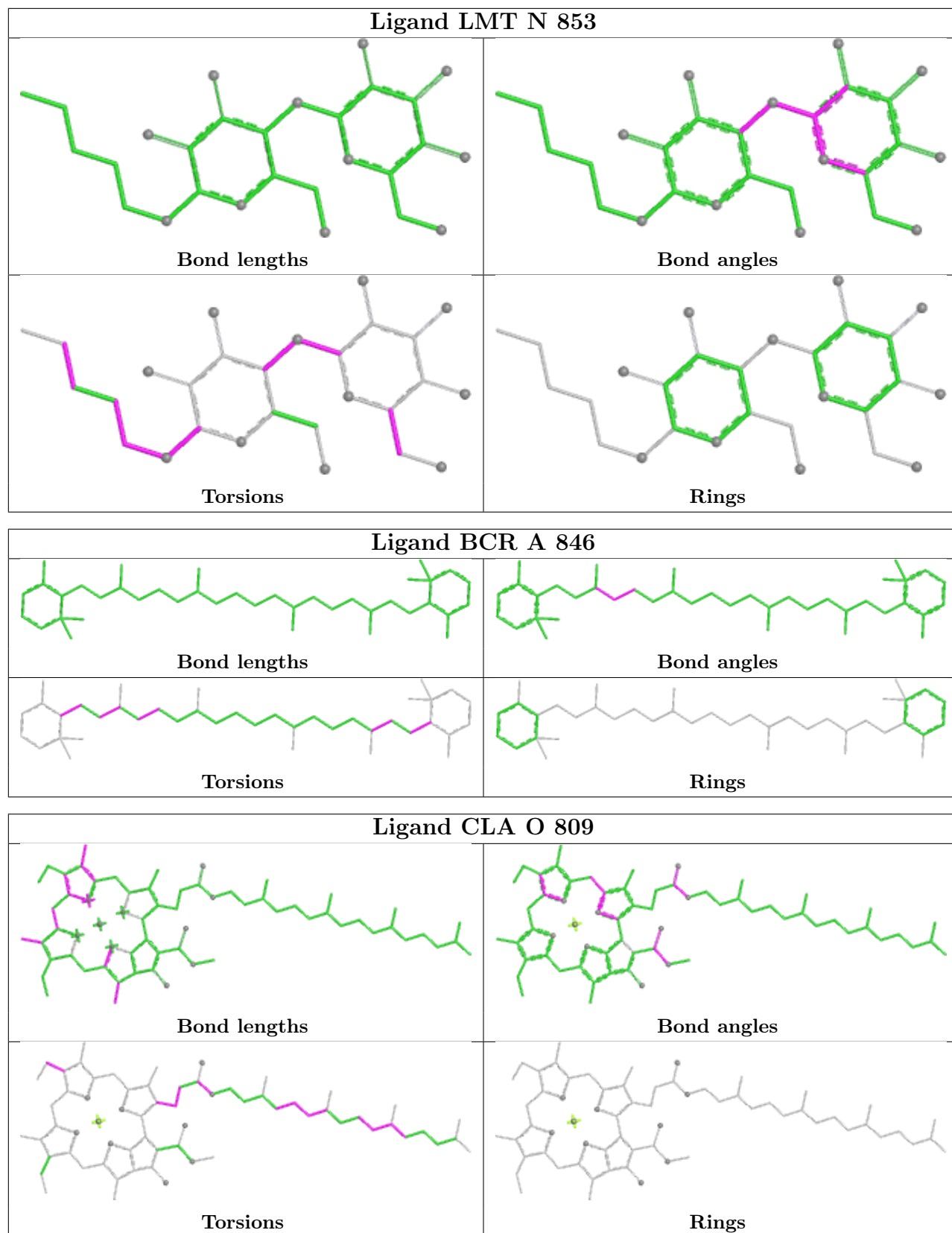


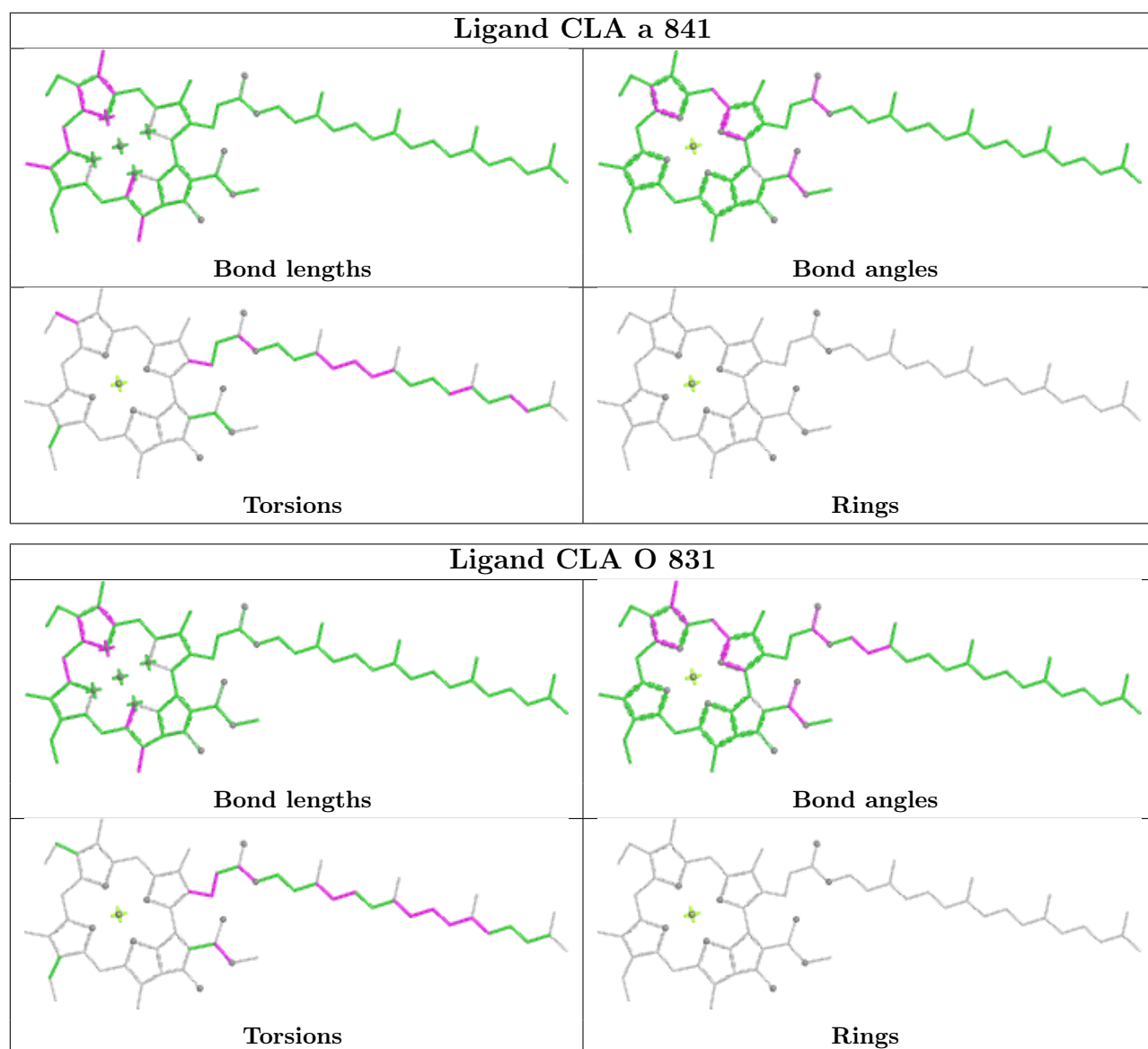


Ligand CLA O 823**Ligand CLA B 803**

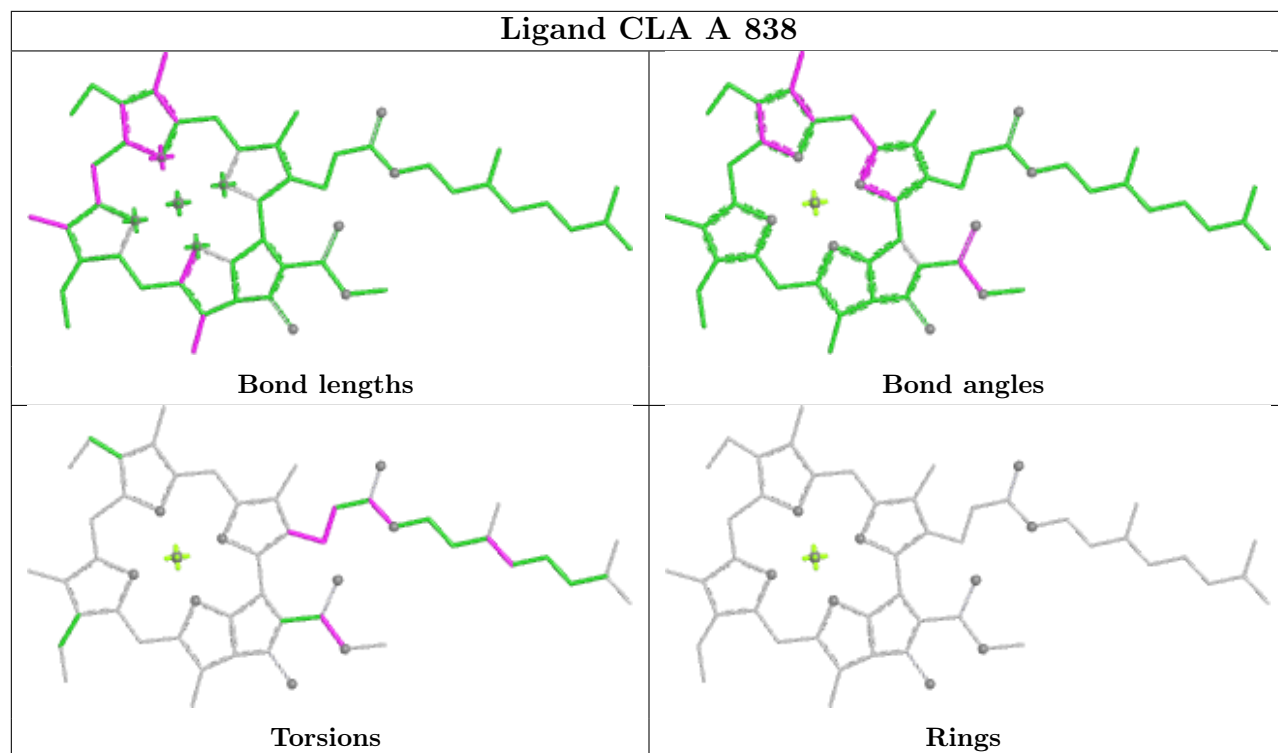




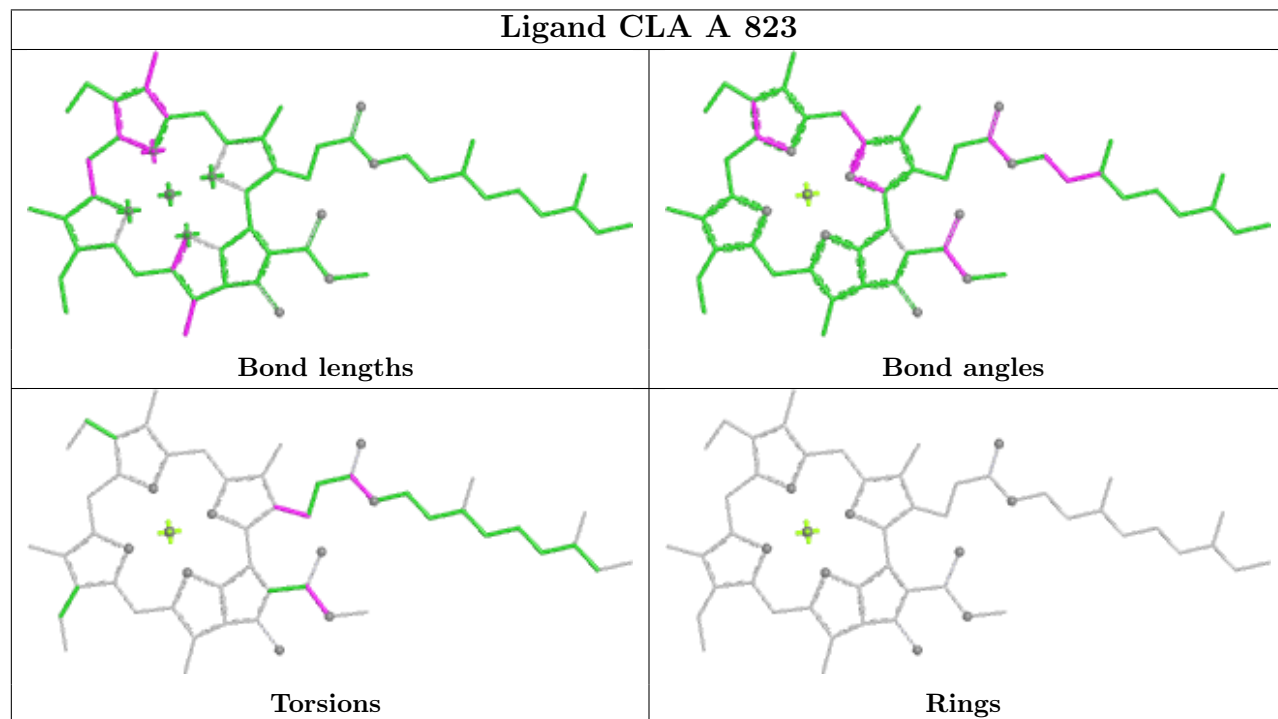


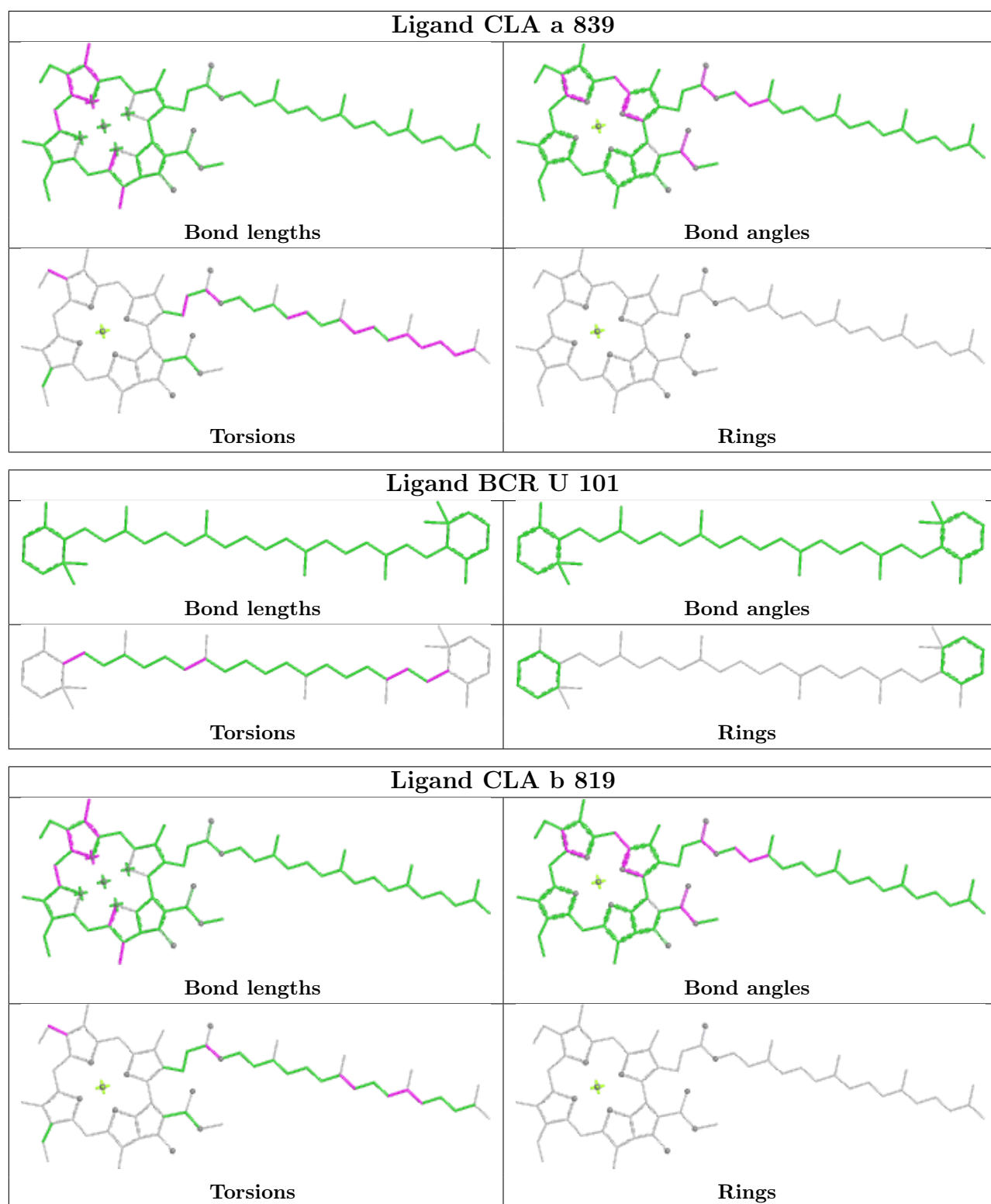


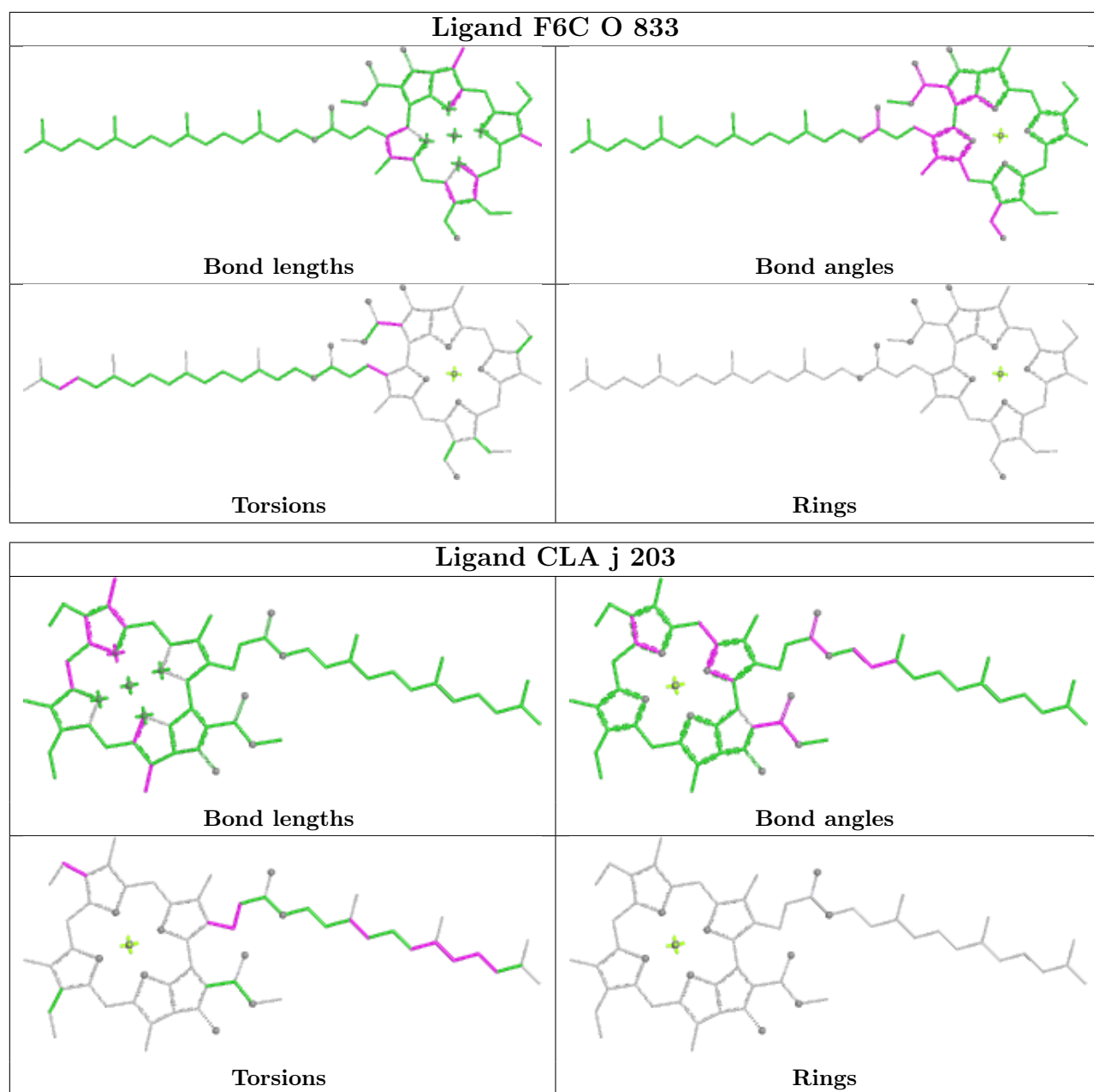
Ligand CLA A 838

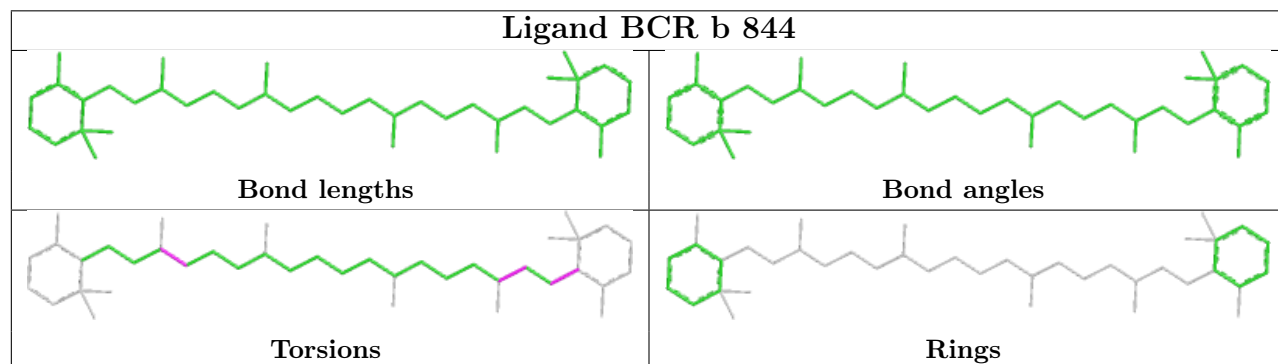
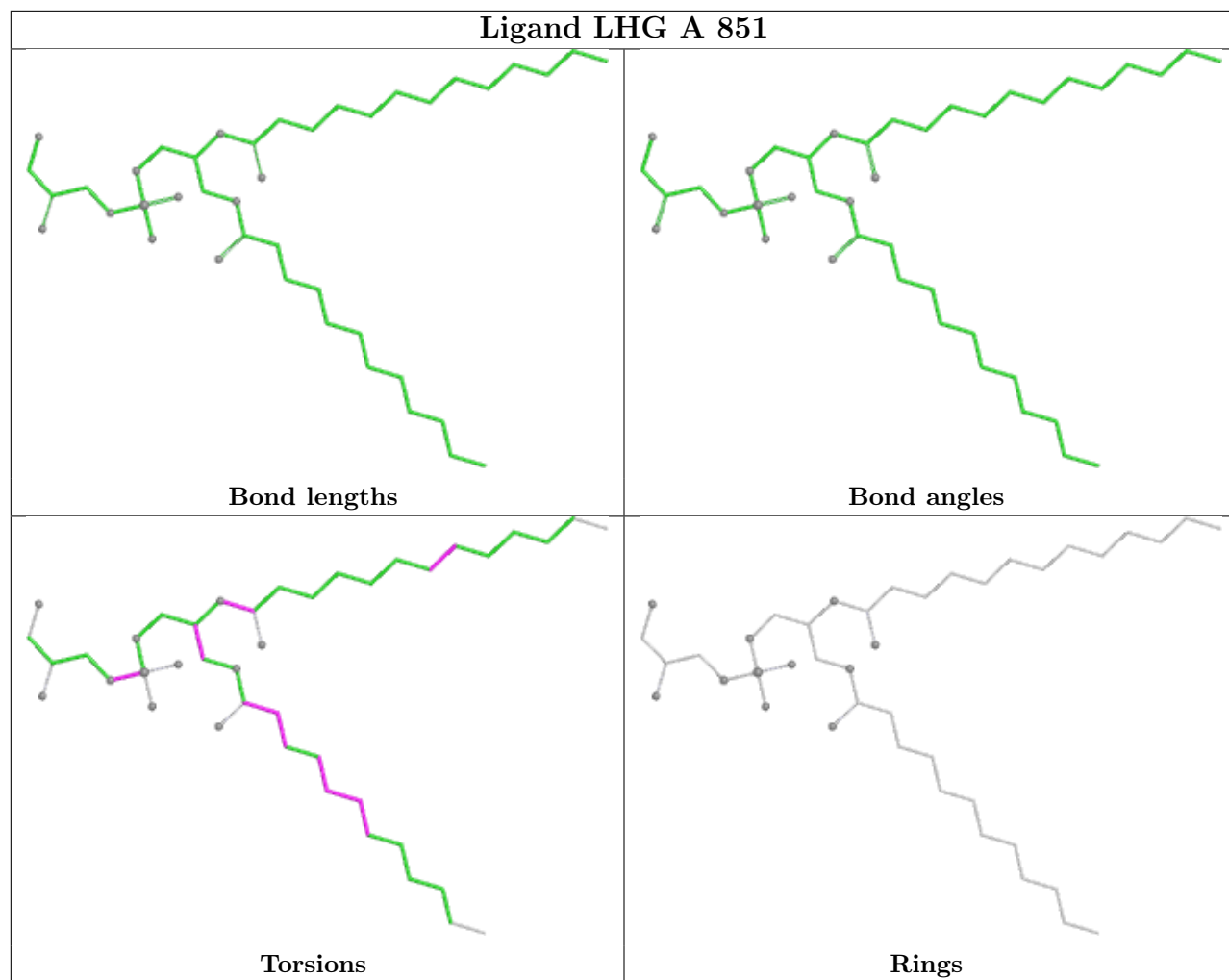


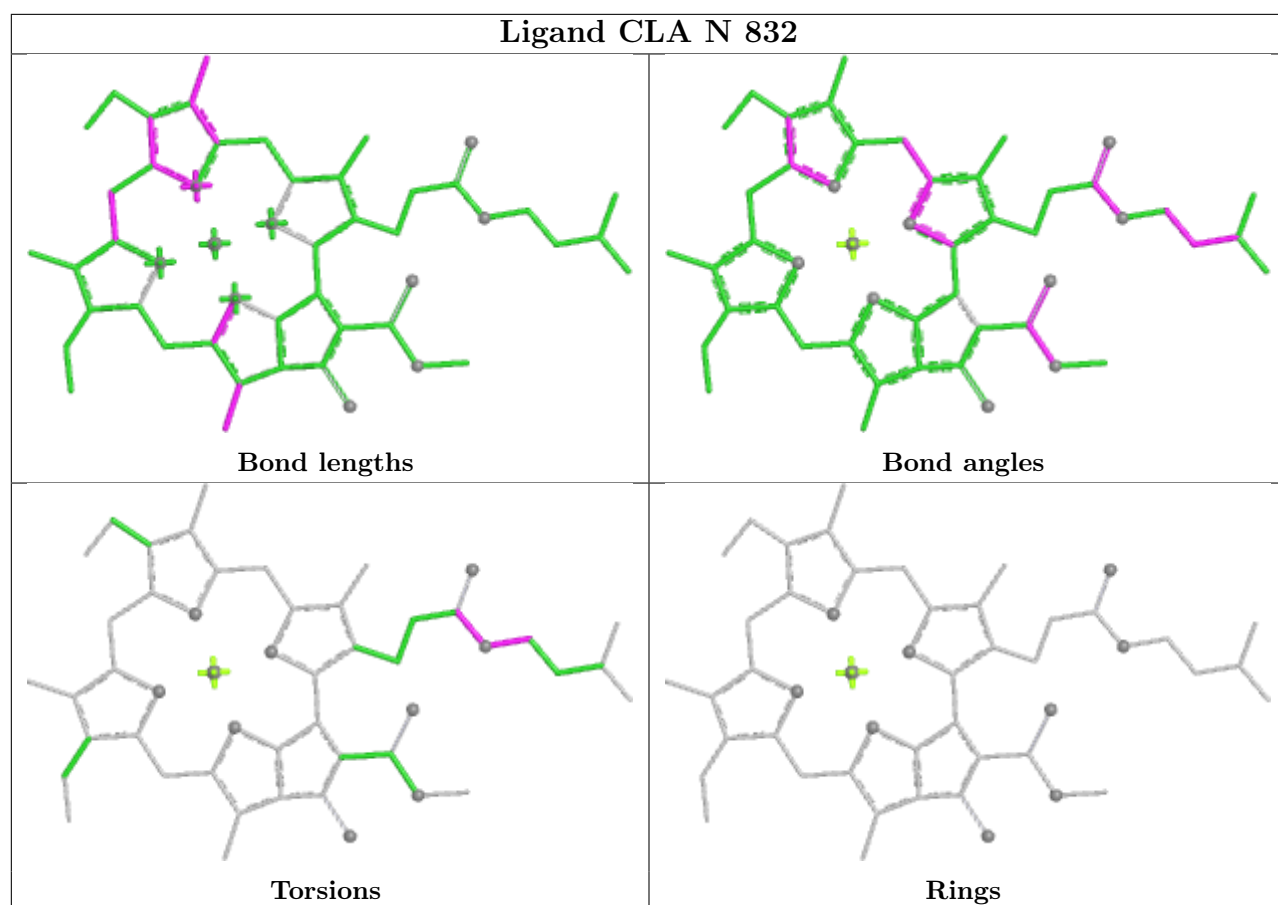
Ligand CLA A 823



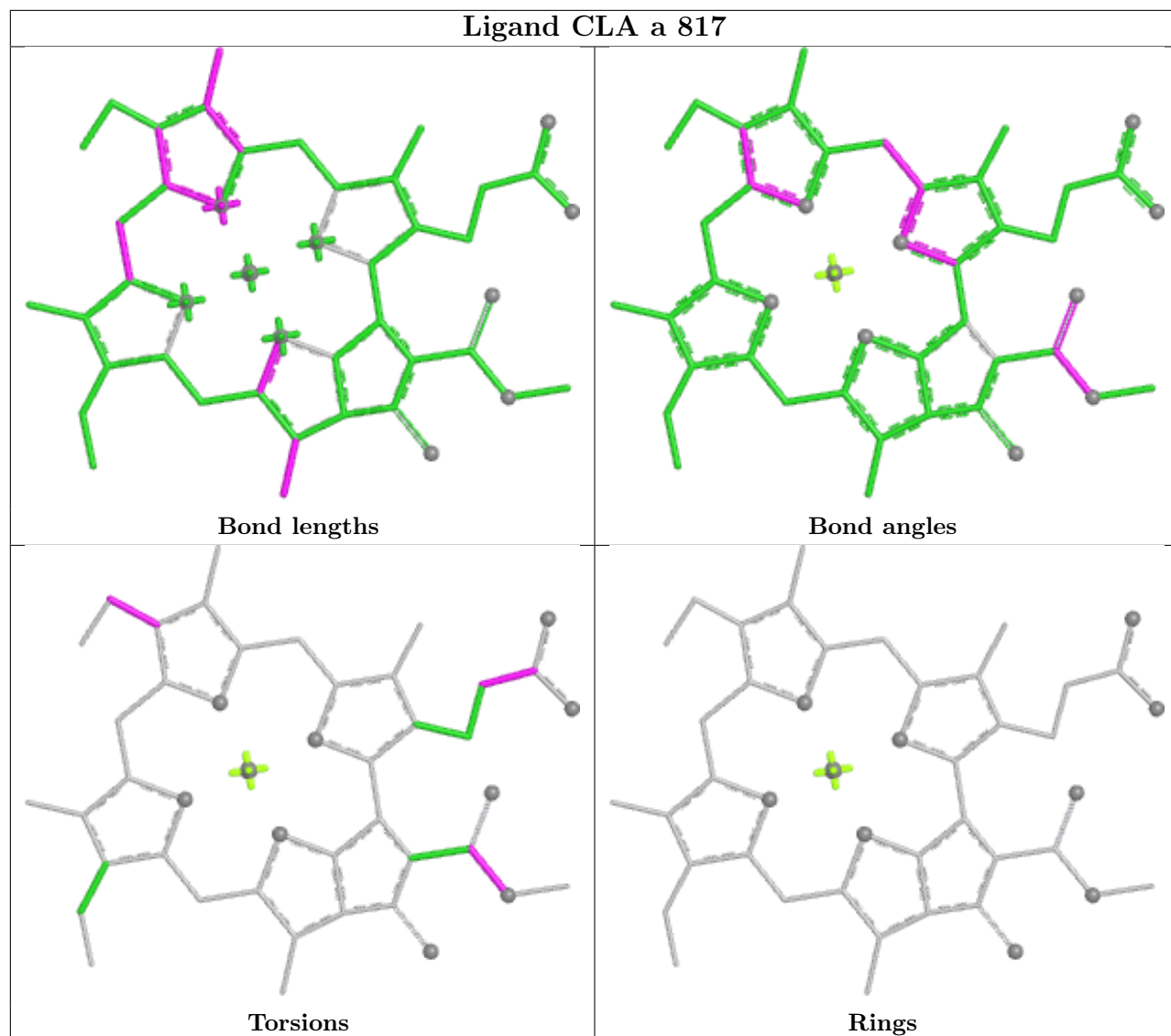




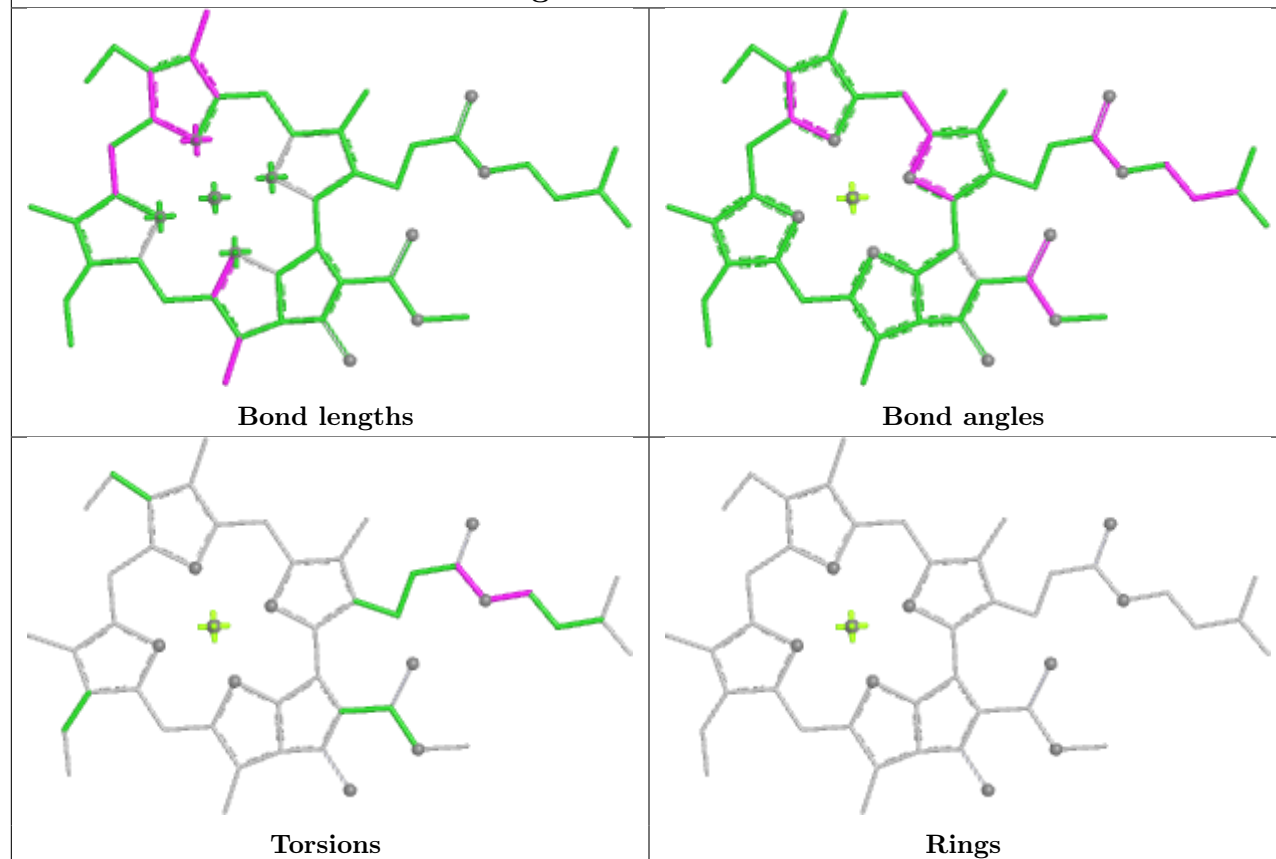




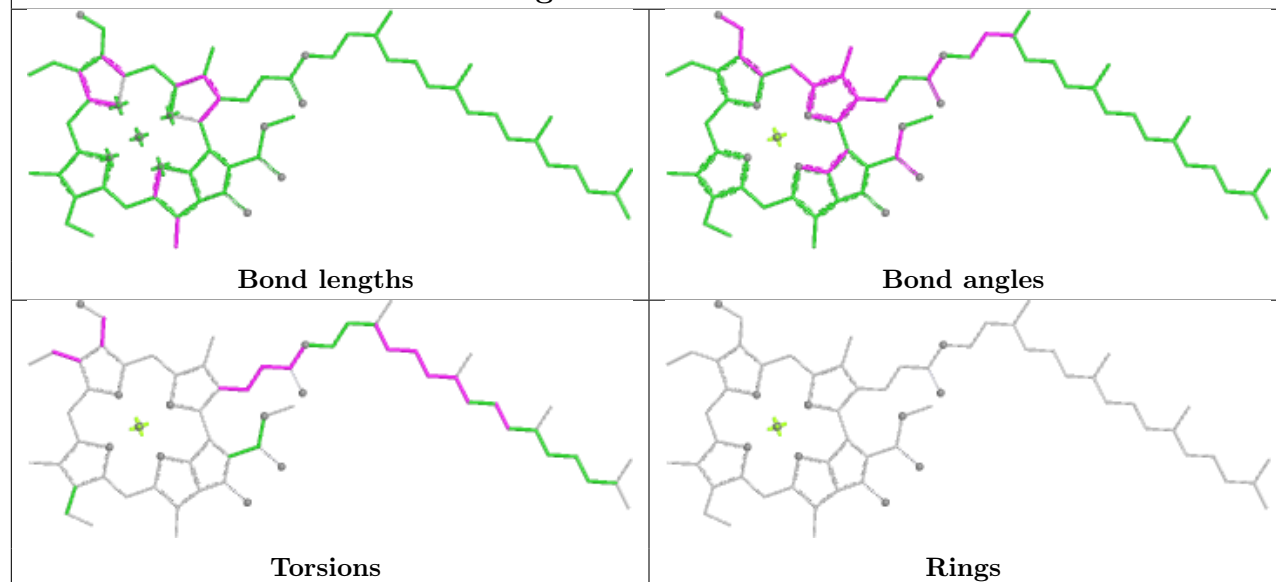
Ligand CLA a 817

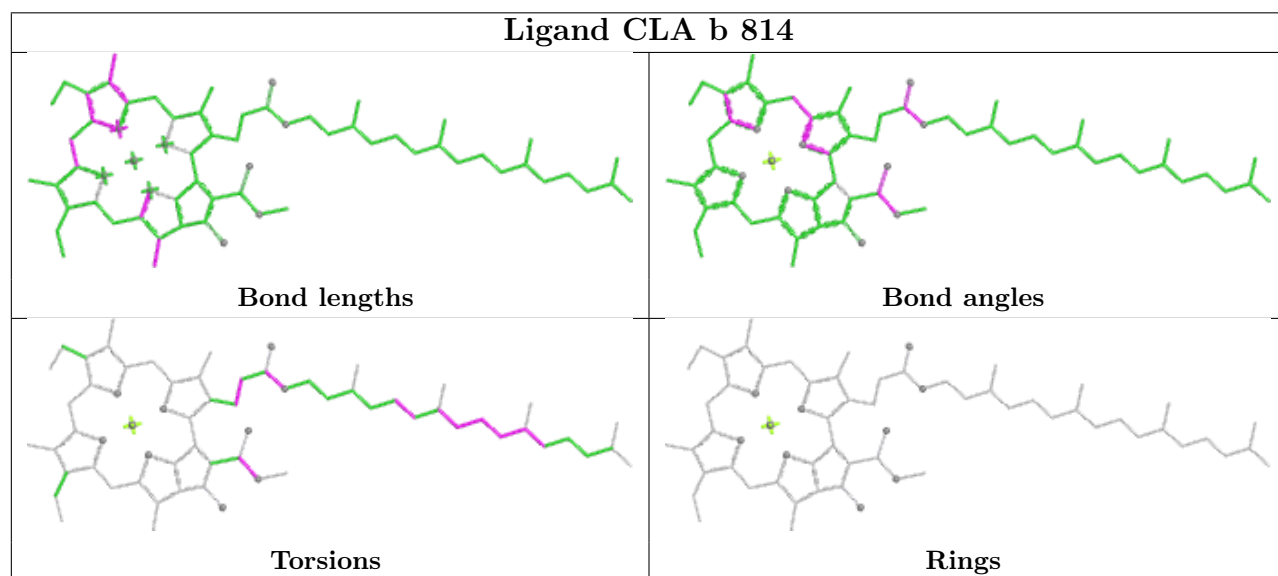
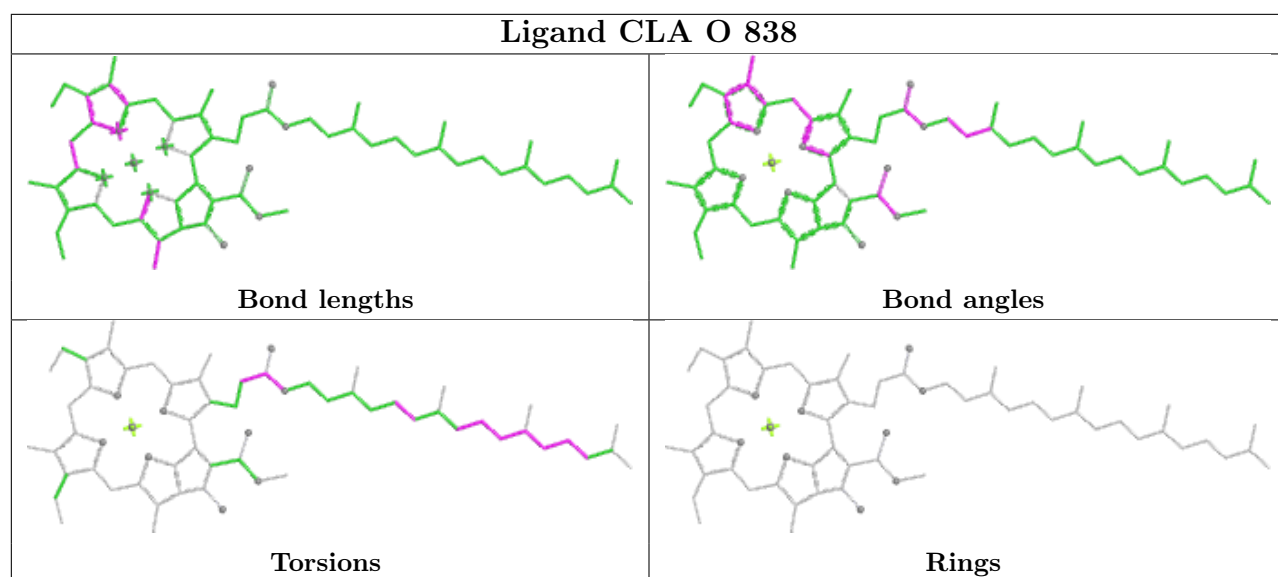
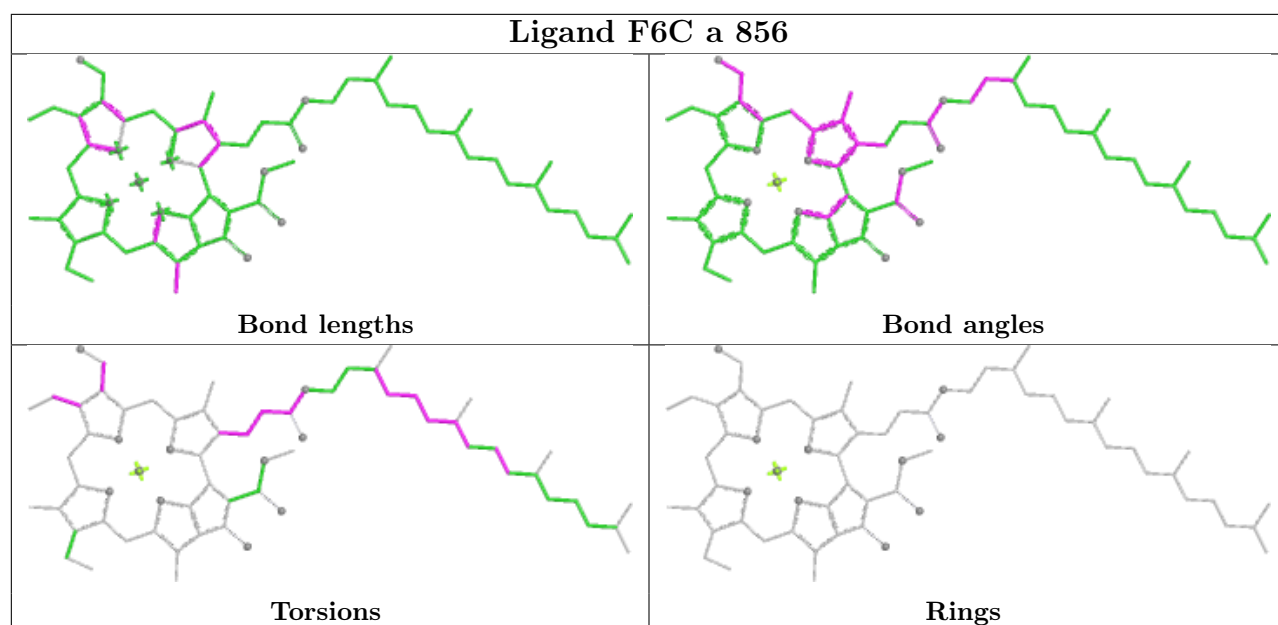


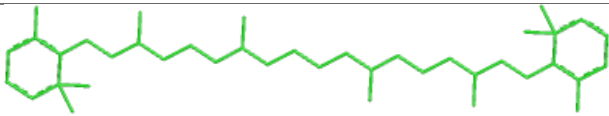
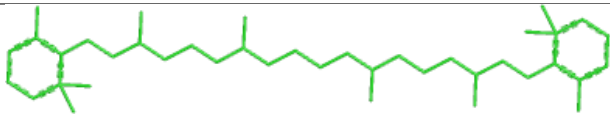
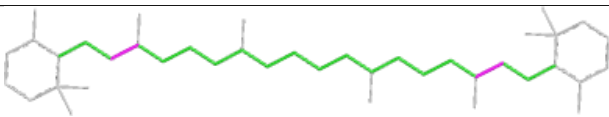
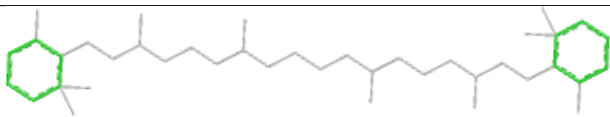
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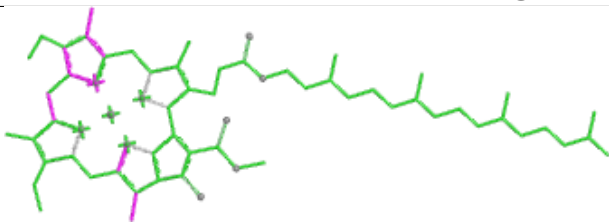
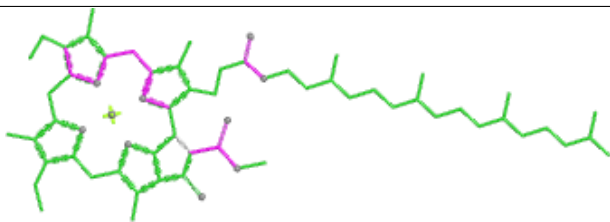
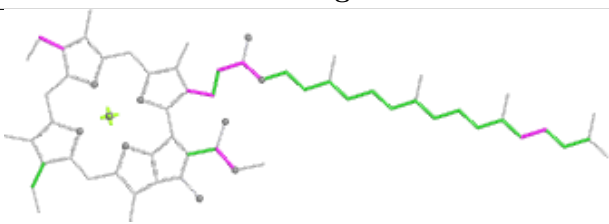
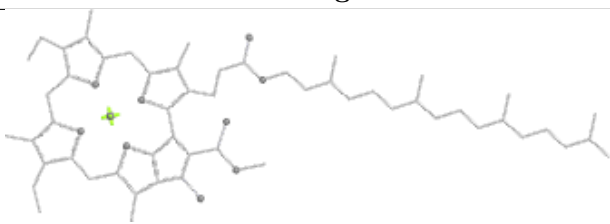


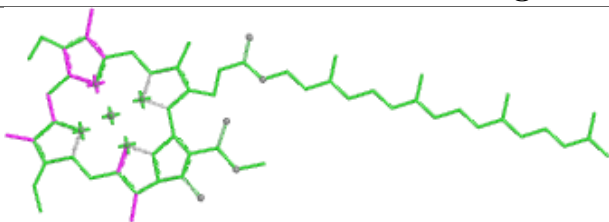
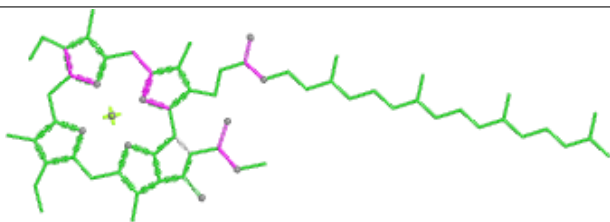
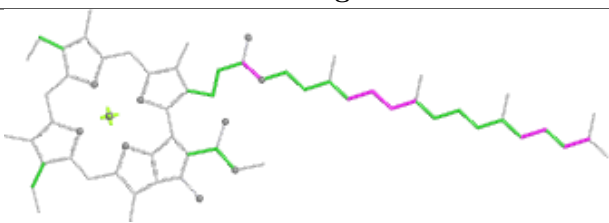
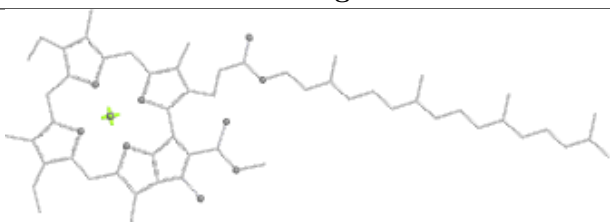
Ligand F6C A 857

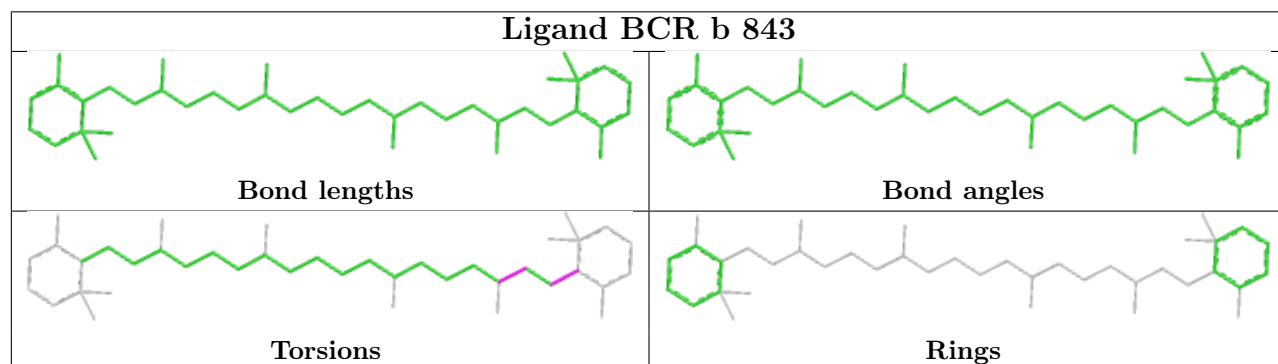
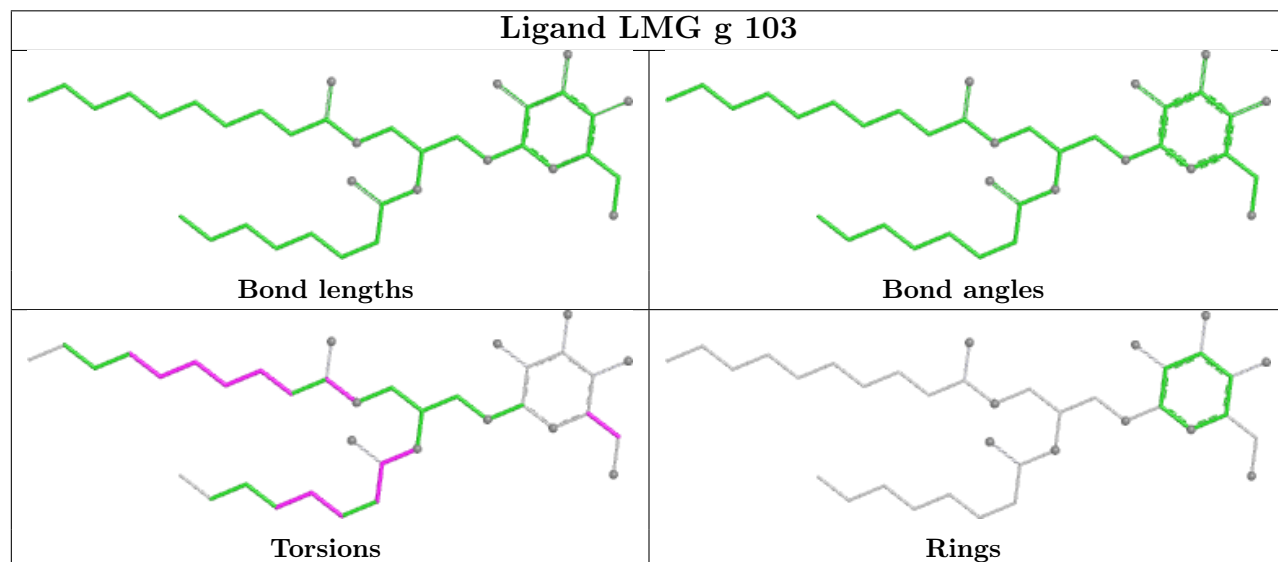
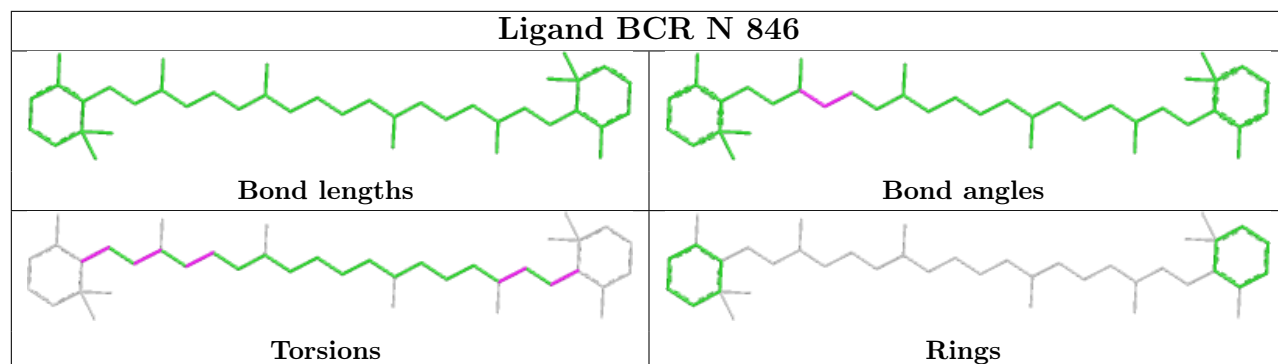




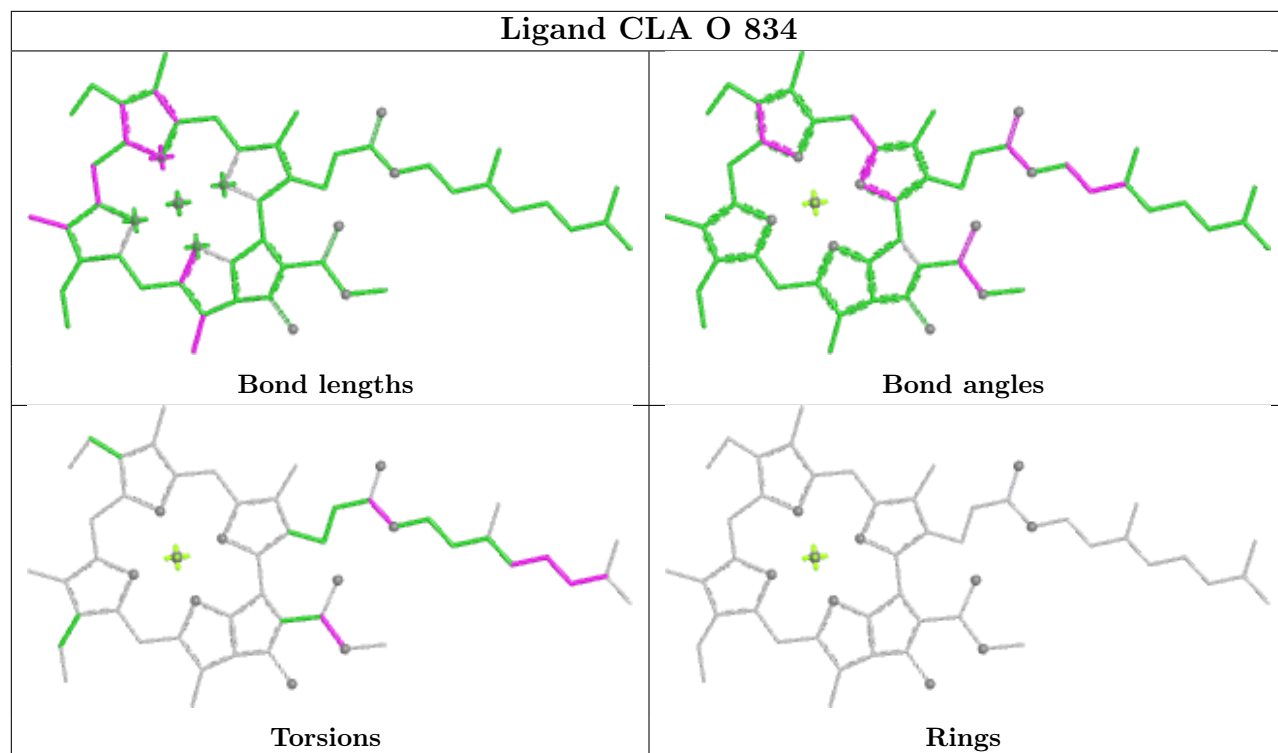
Ligand BCR j 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

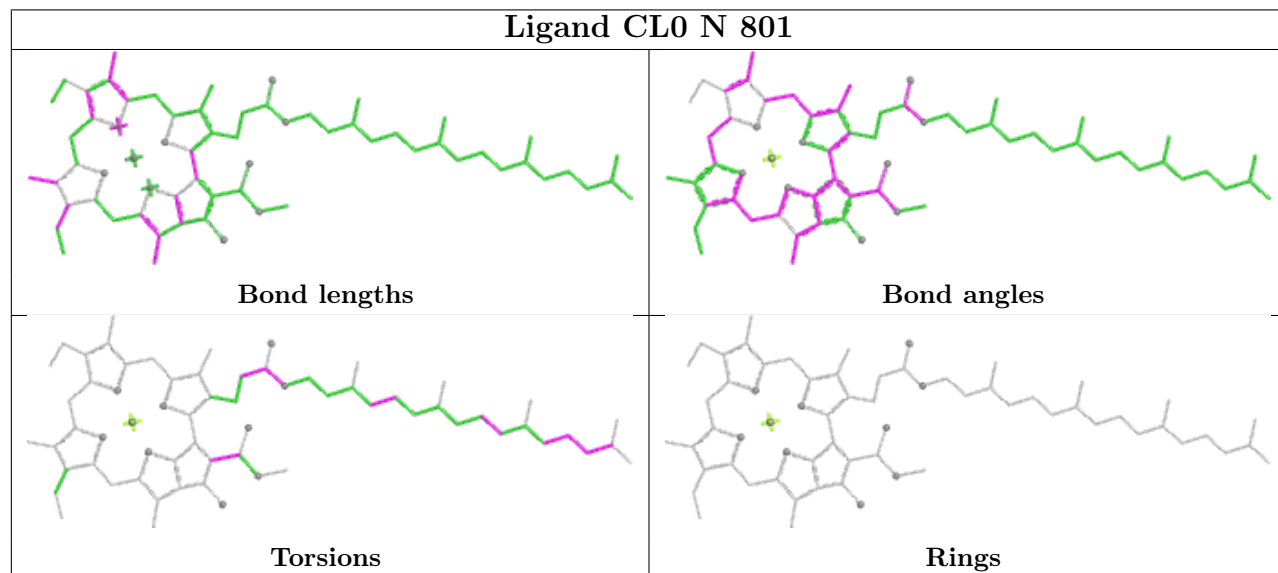
Ligand CLA a 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

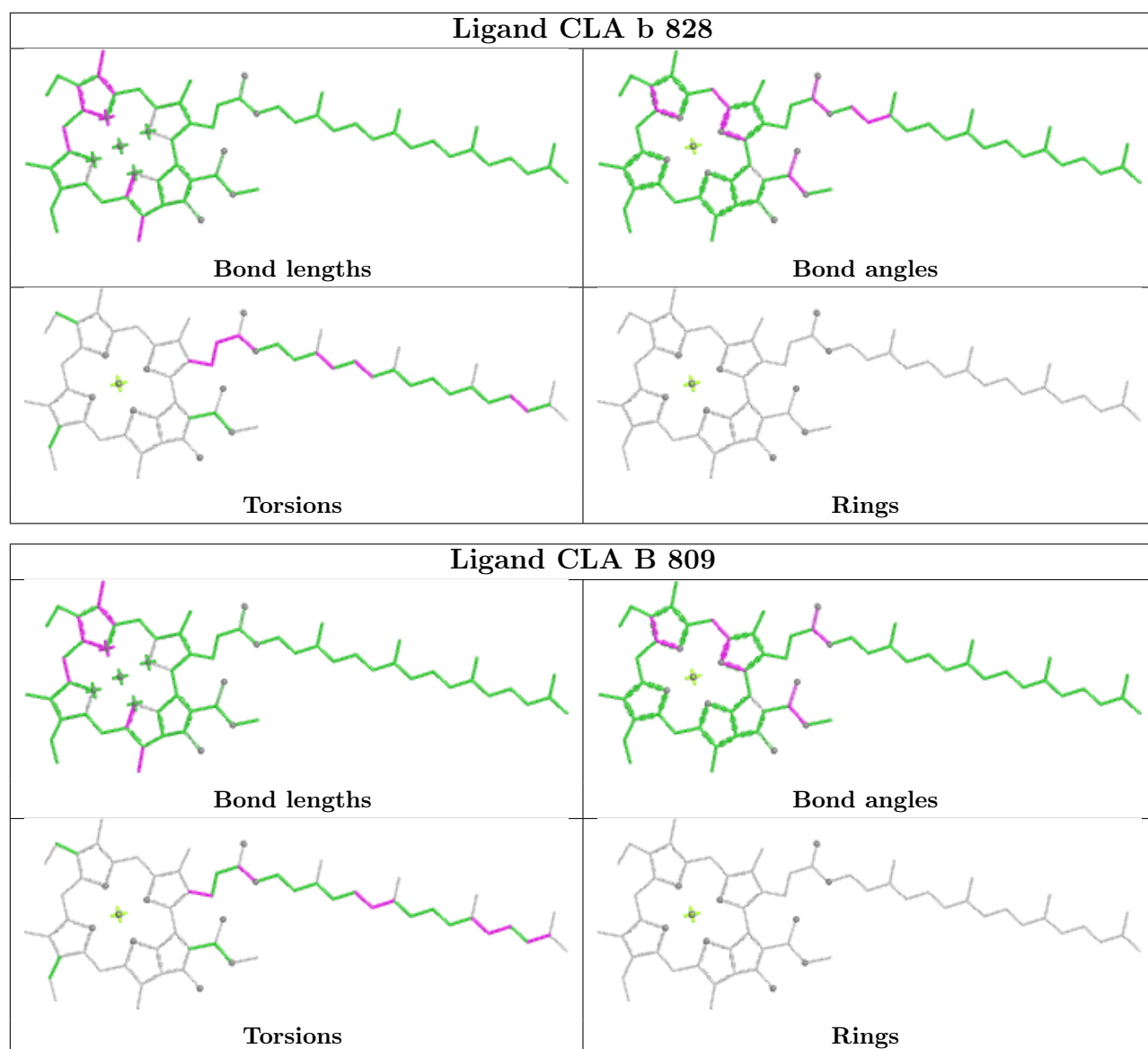


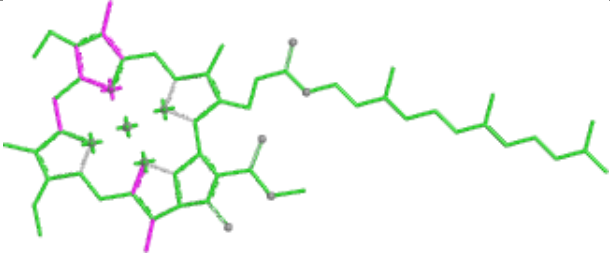
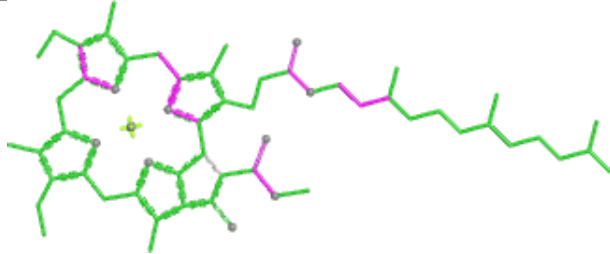
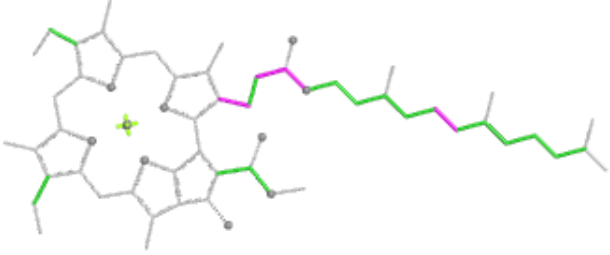
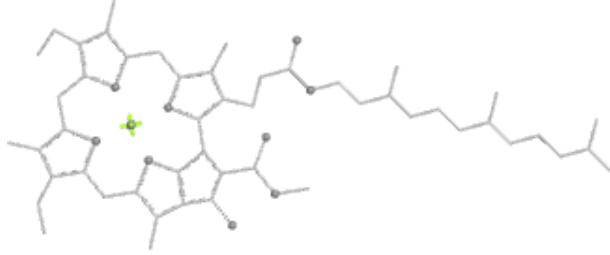
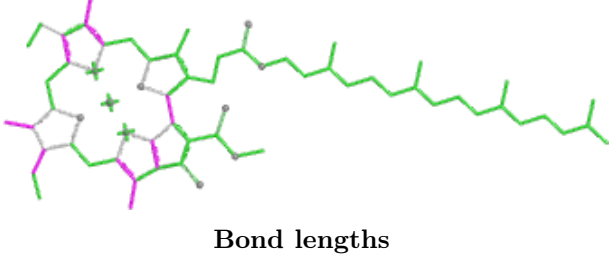
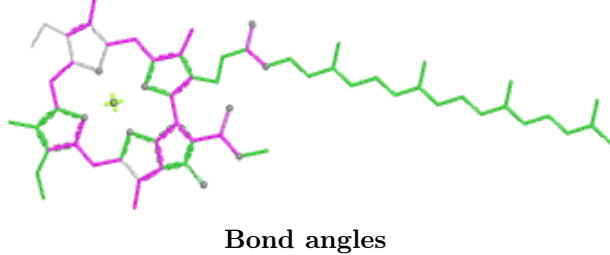
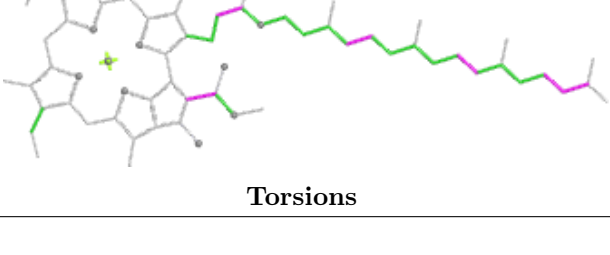
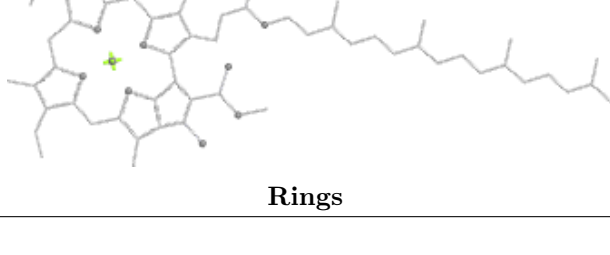
Ligand CLA O 834

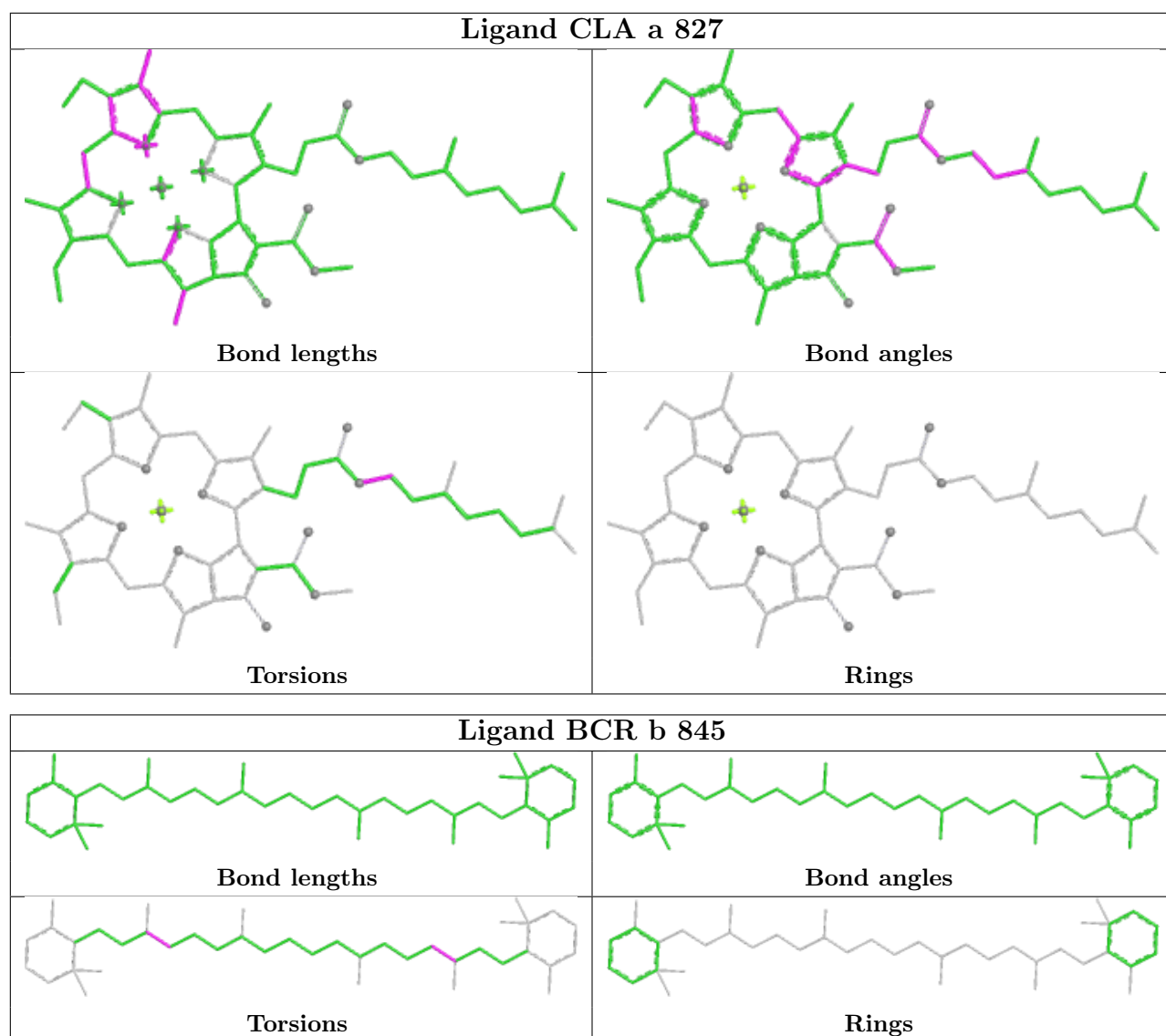


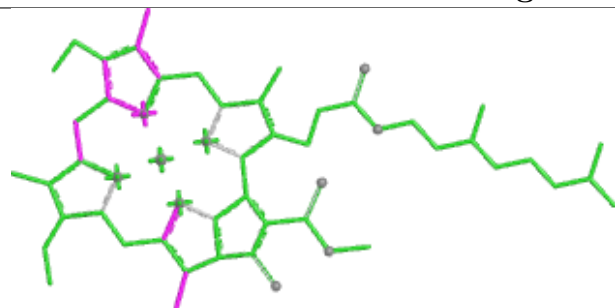
Ligand CL0 N 801



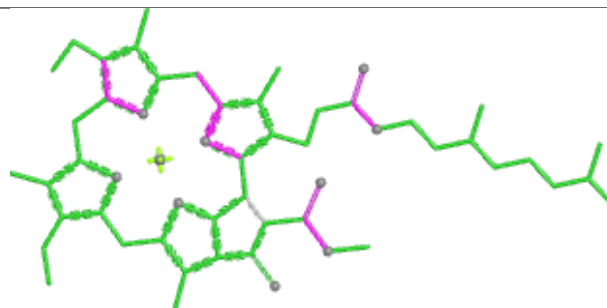


Ligand CLA a 821	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings

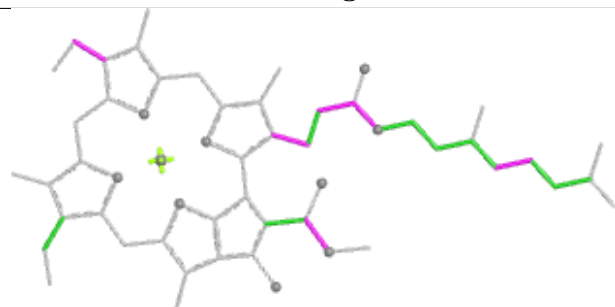


Ligand CLA B 818

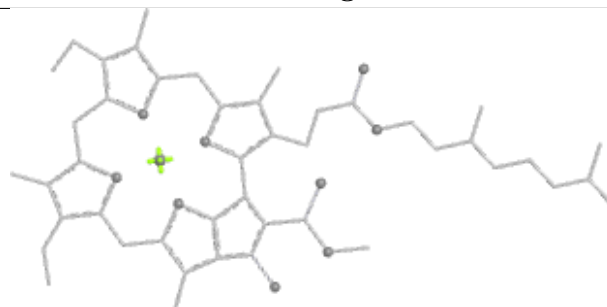
Bond lengths



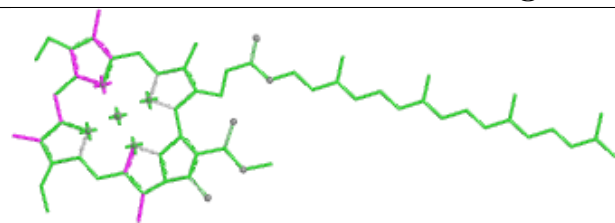
Bond angles



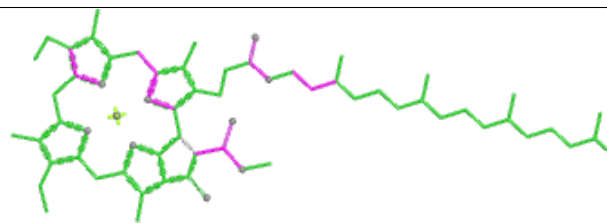
Torsions



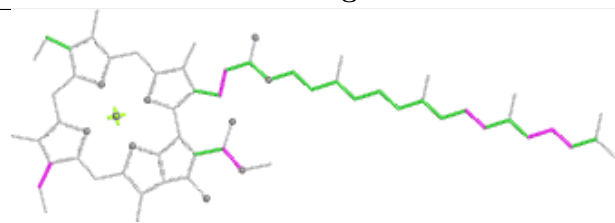
Rings

Ligand CLA b 803

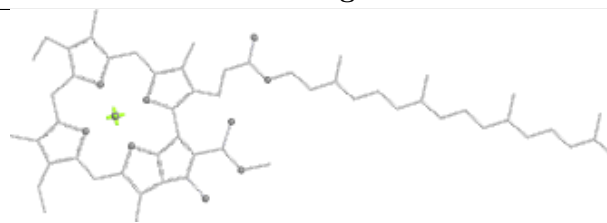
Bond lengths



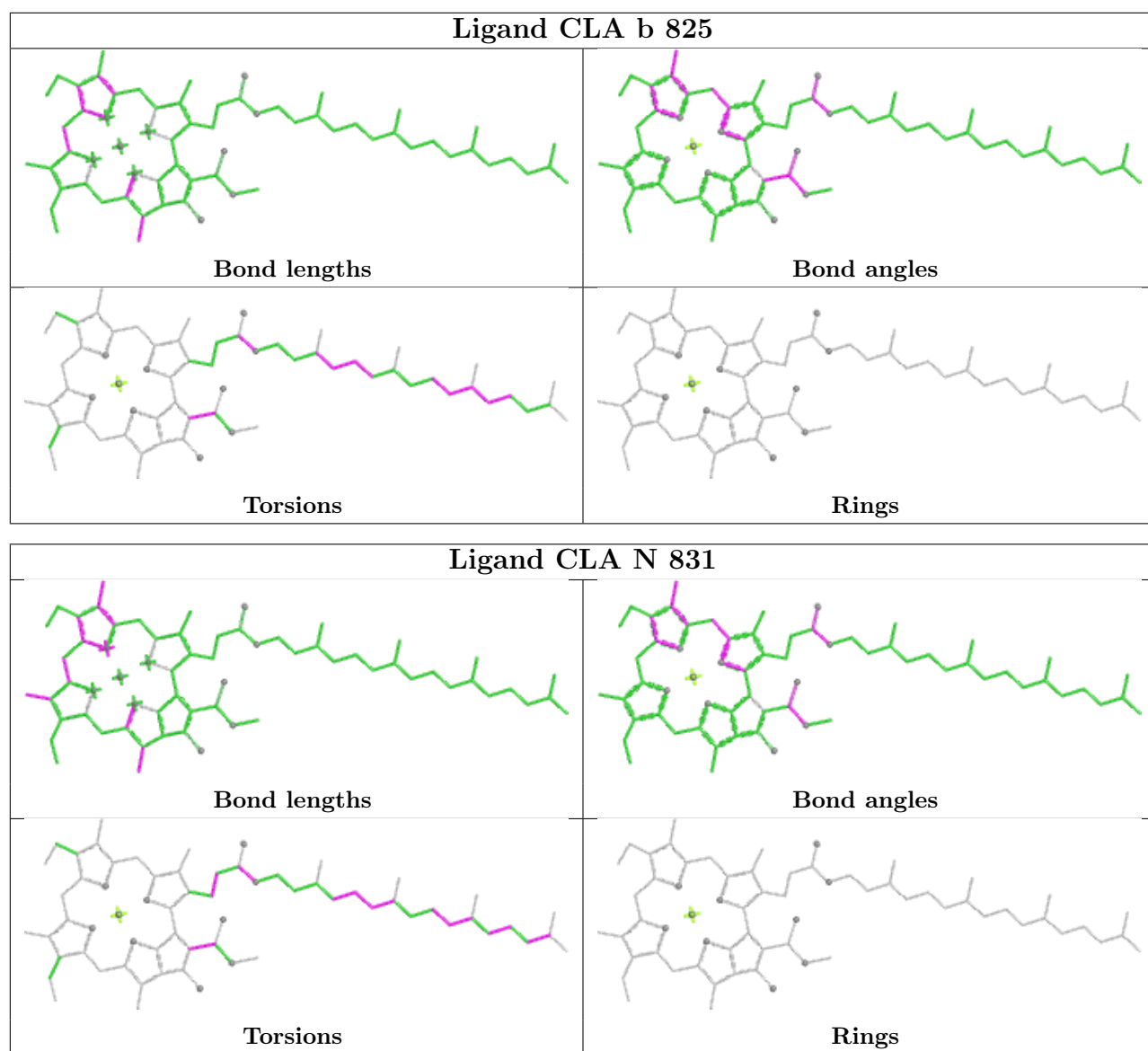
Bond angles

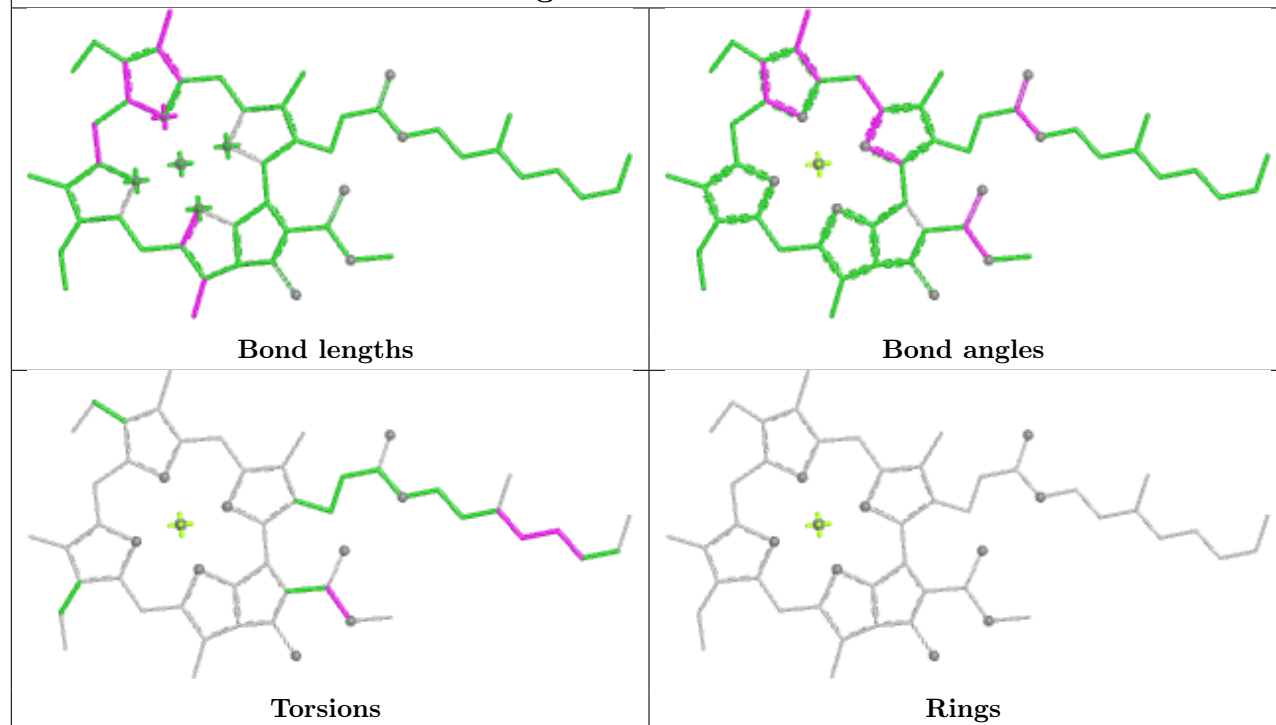
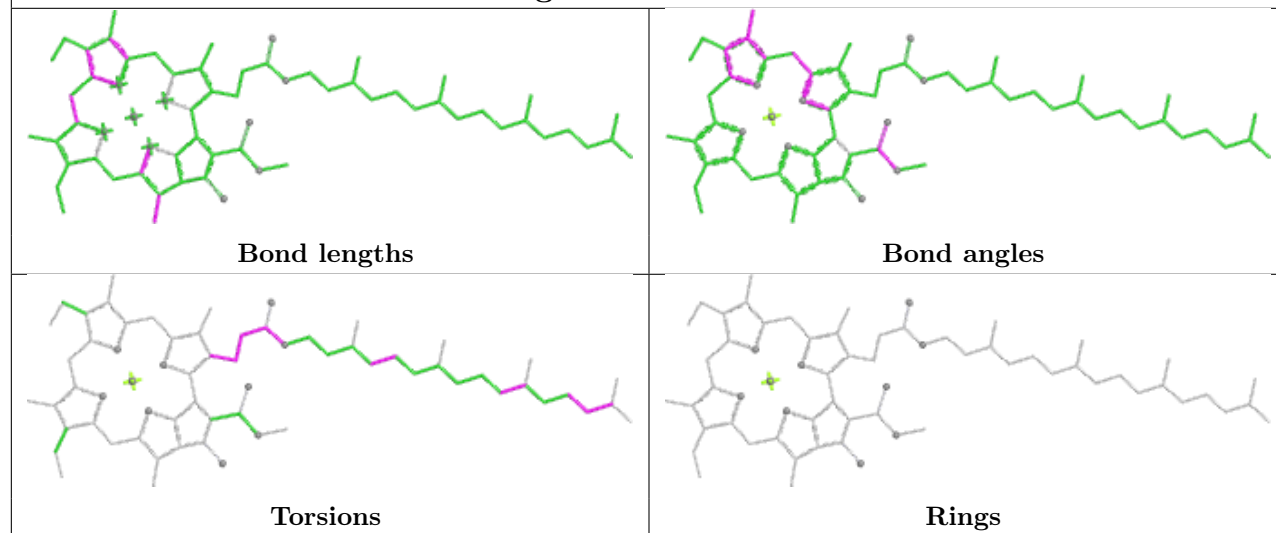


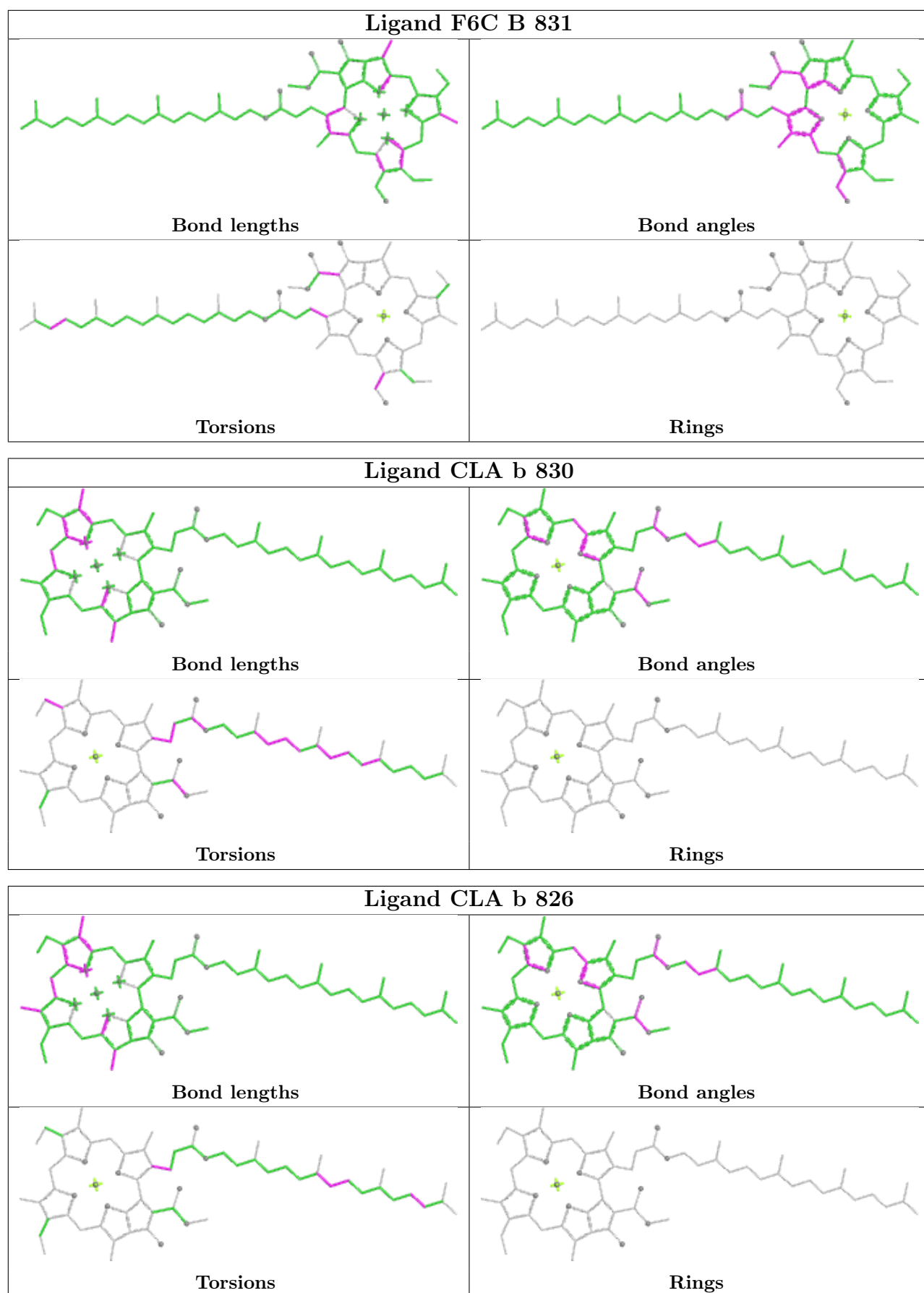
Torsions

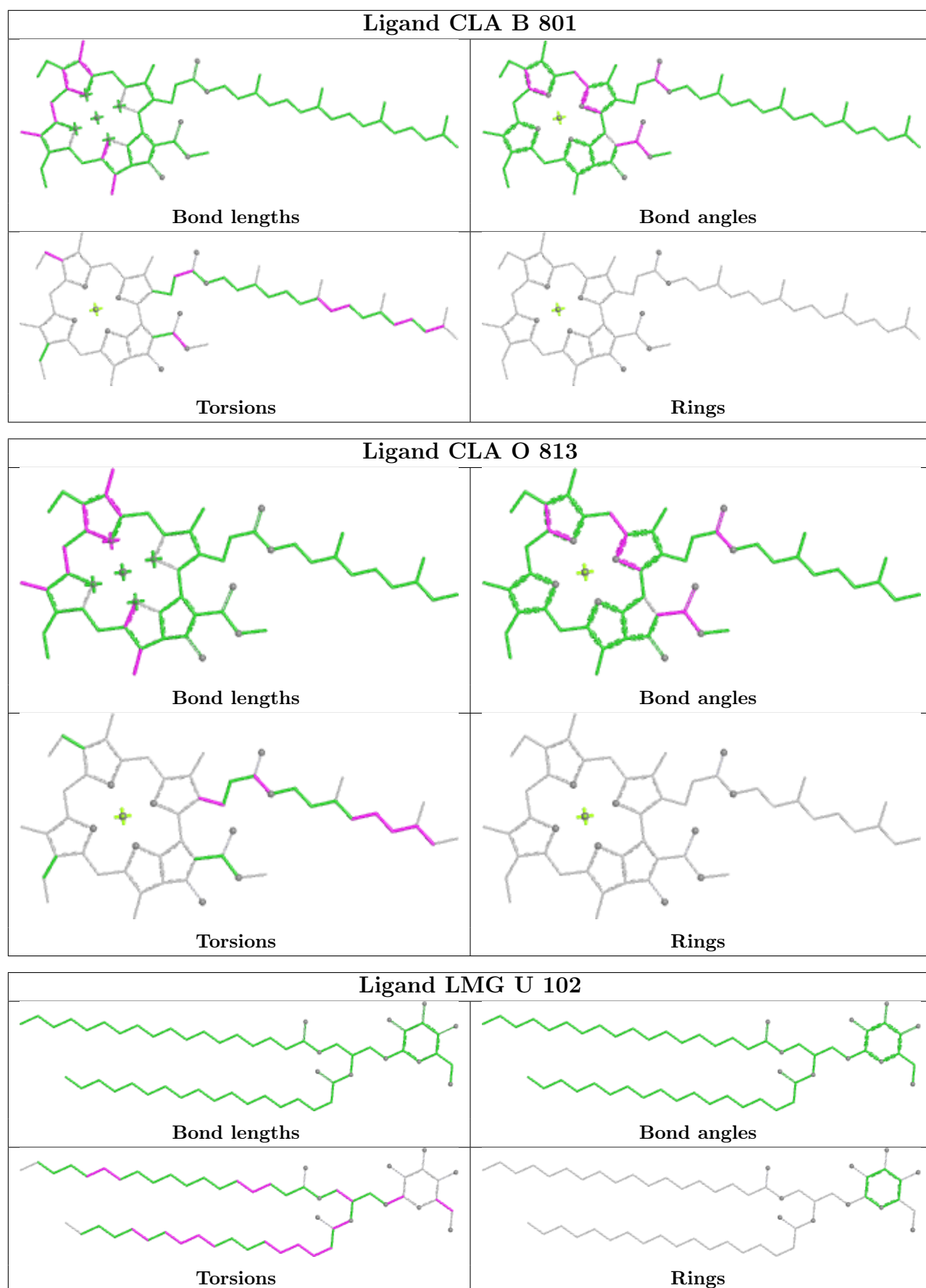


Rings

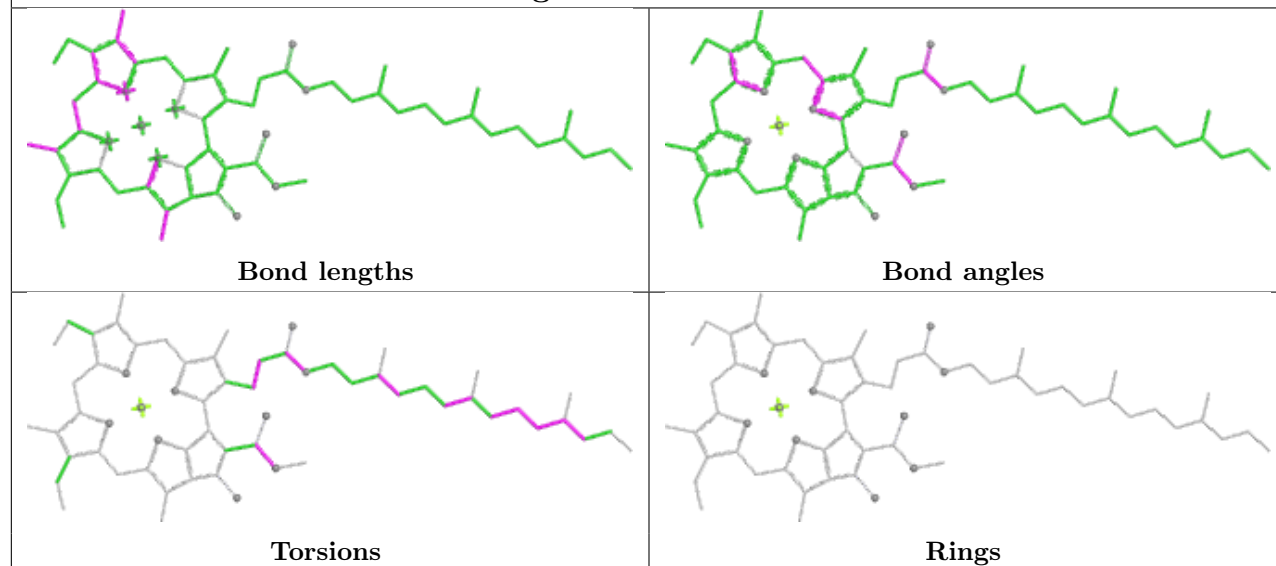


Ligand CLA a 836**Ligand CLA b 805**

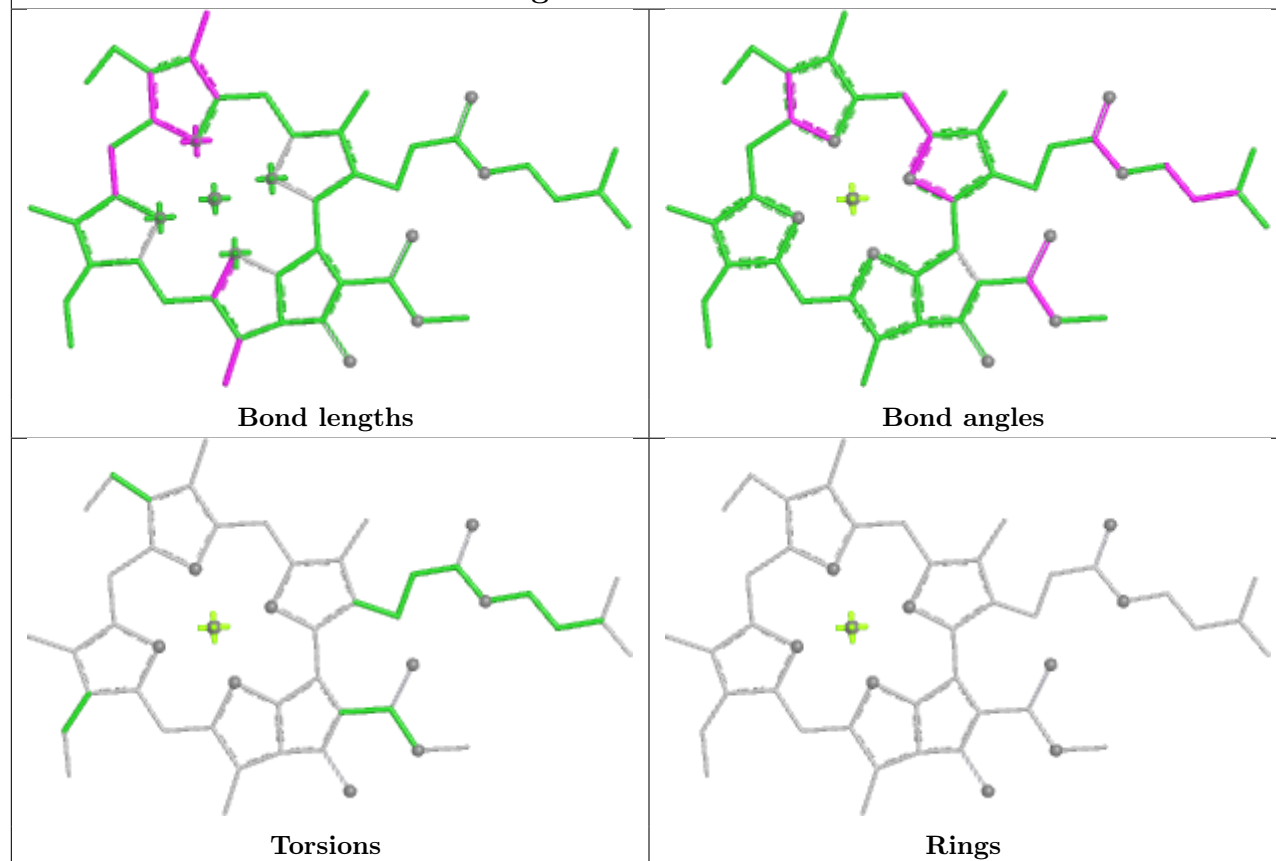


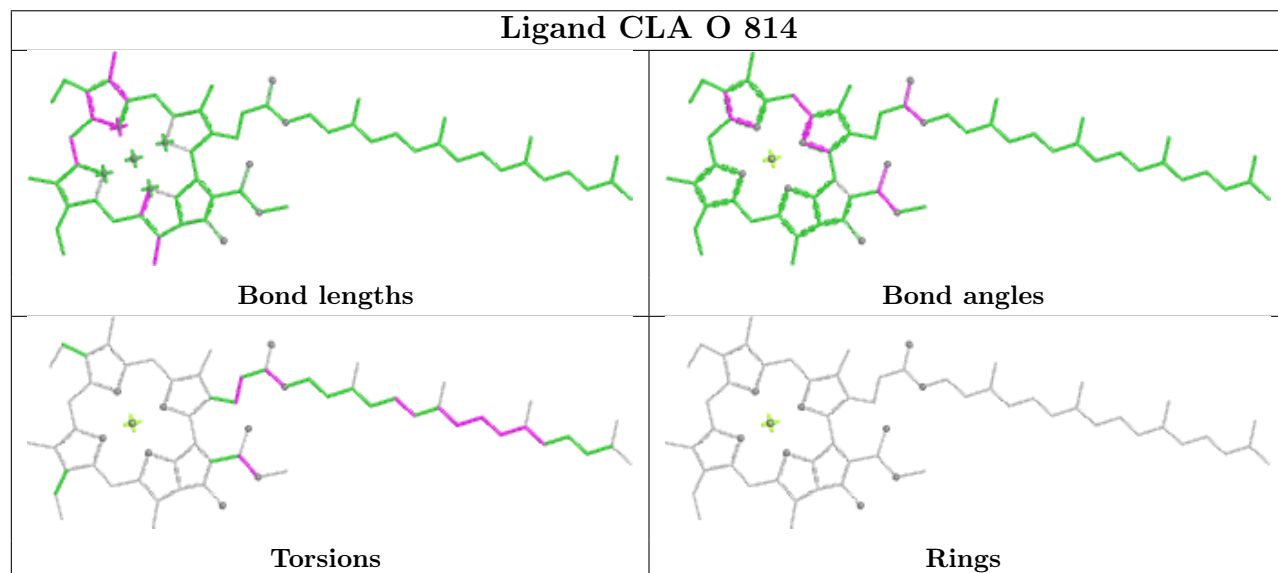
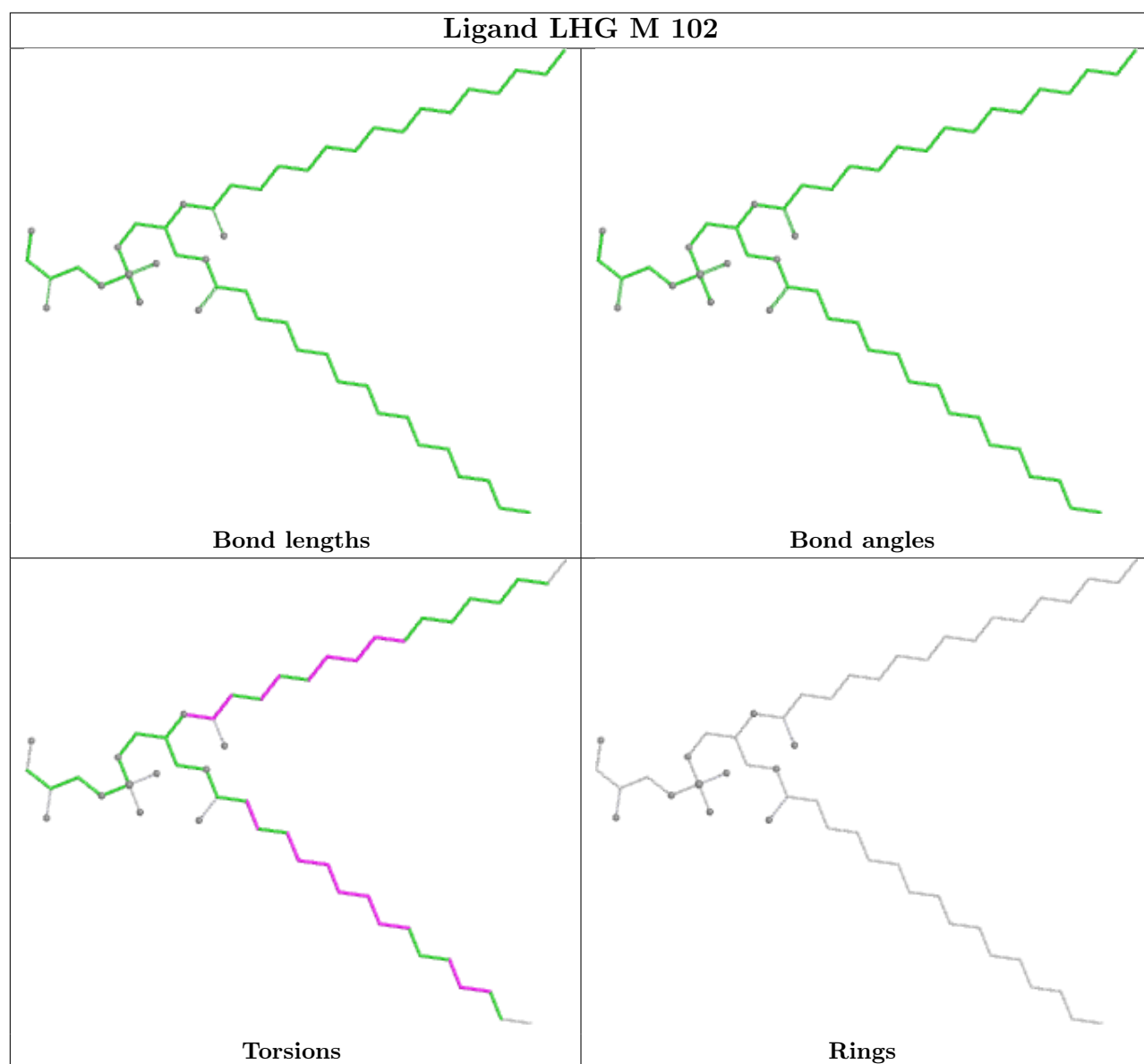


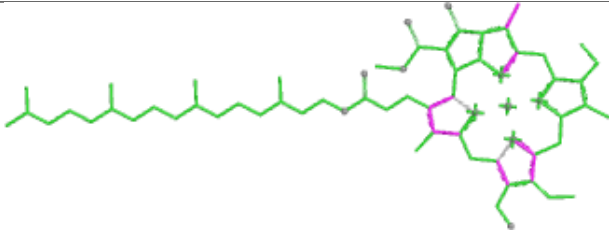
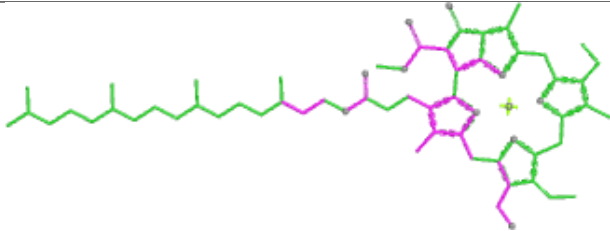
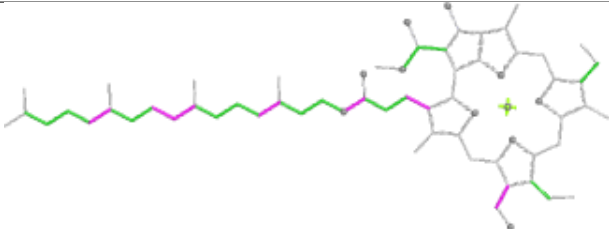
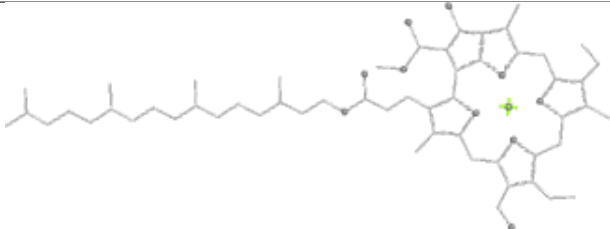
Ligand CLA B 825

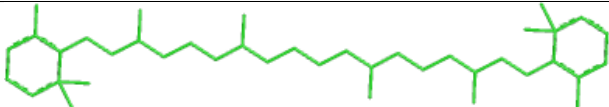
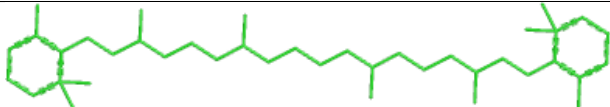
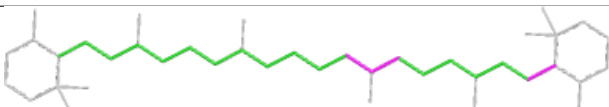
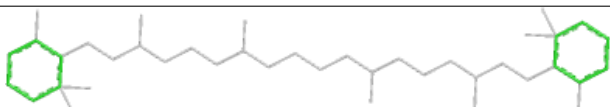


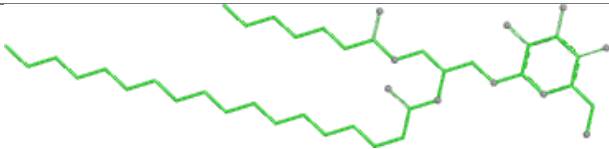
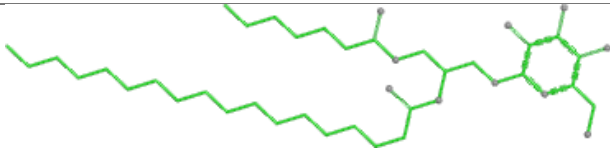
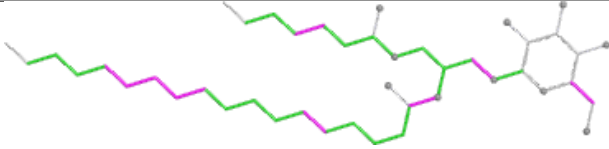
Ligand CLA N 840

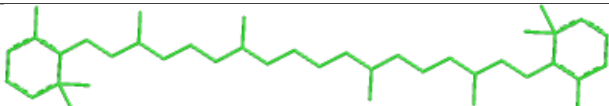
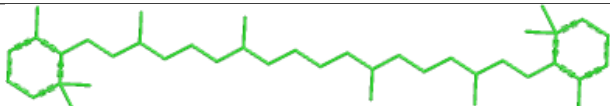
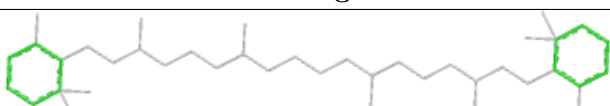


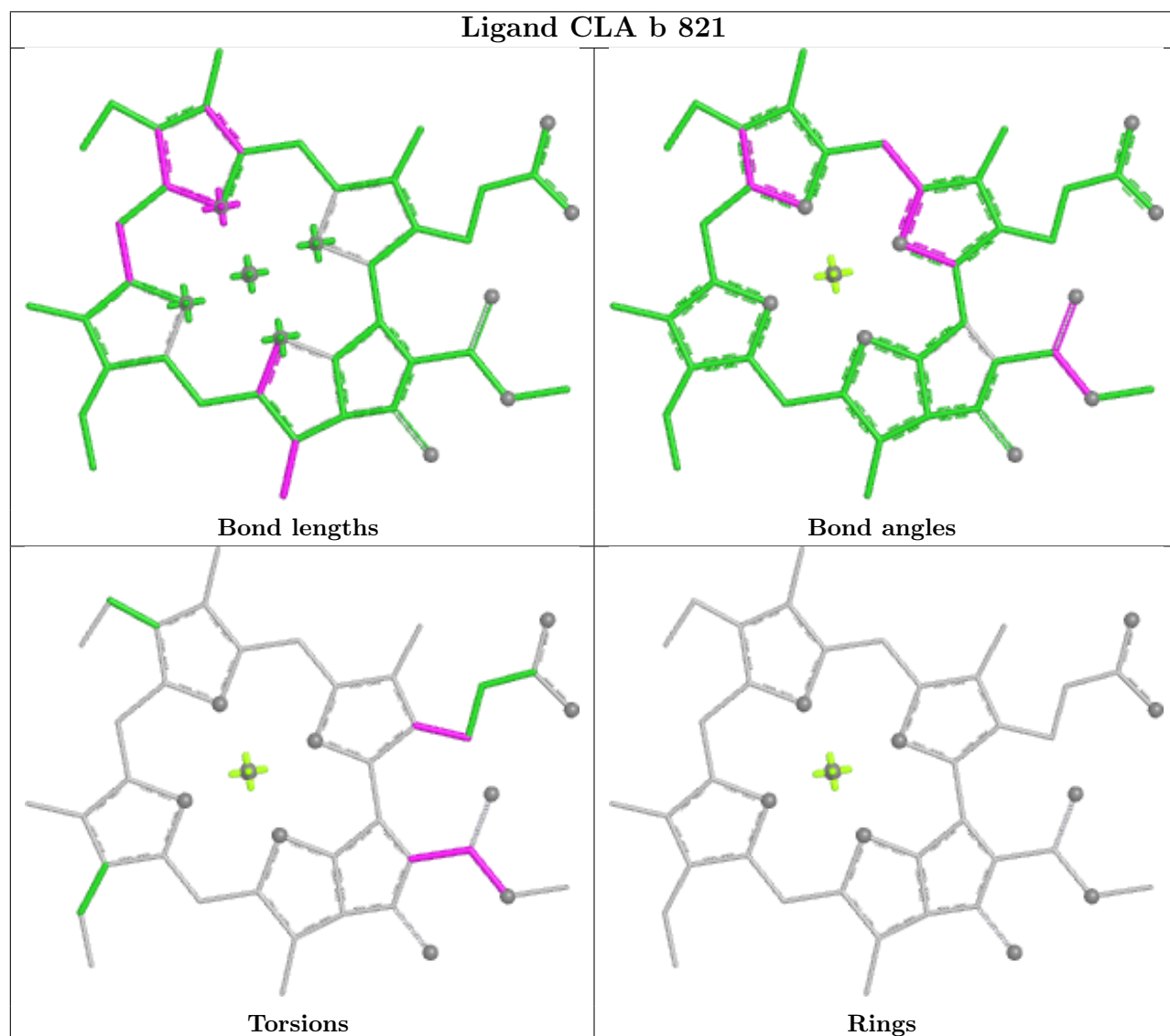
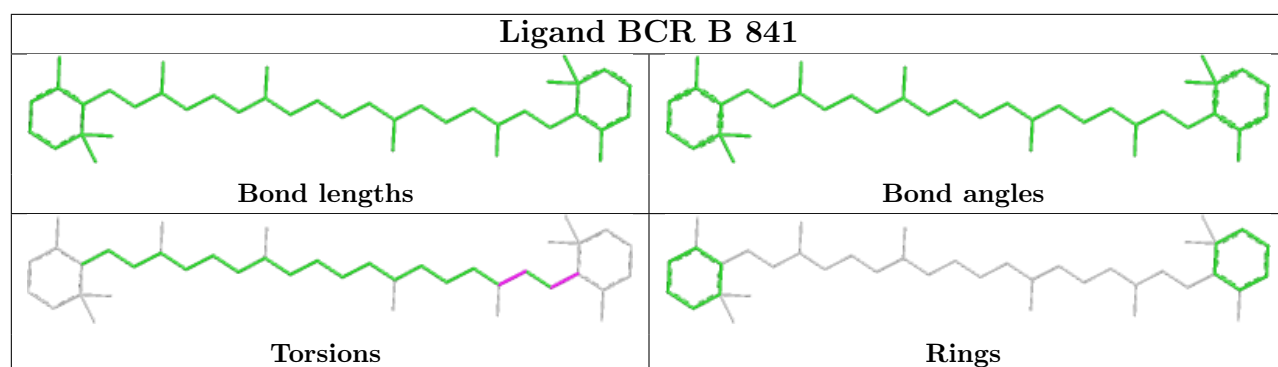


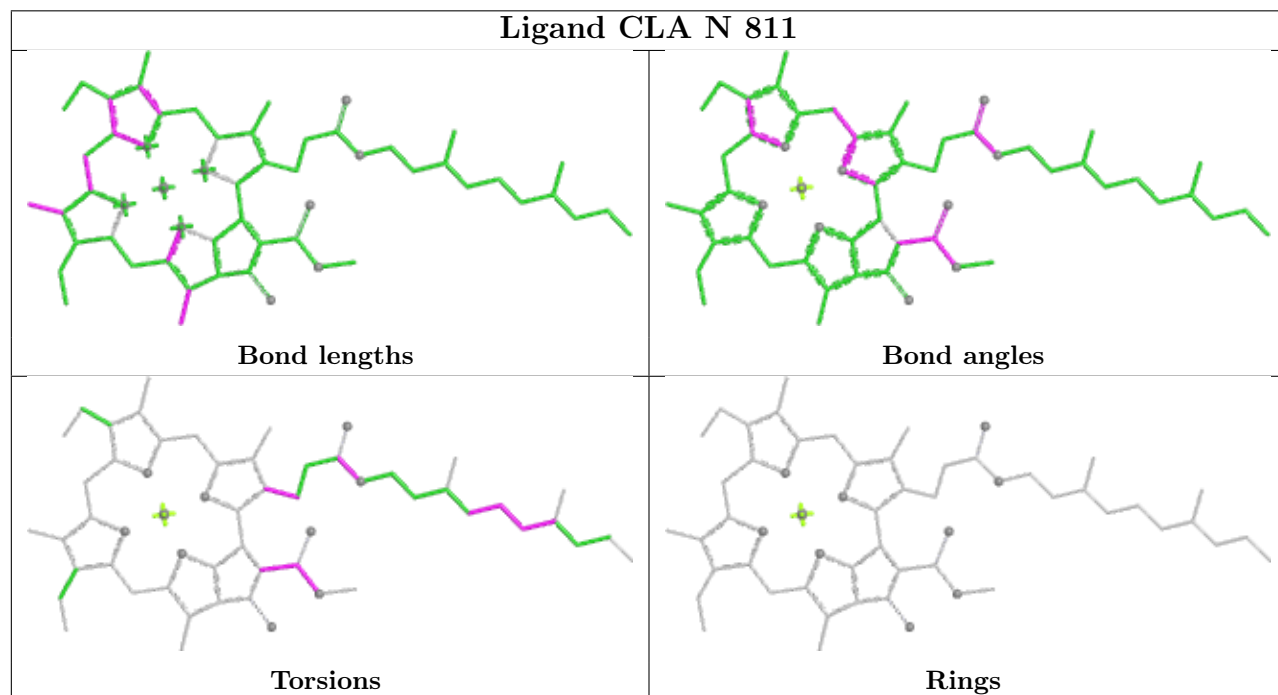
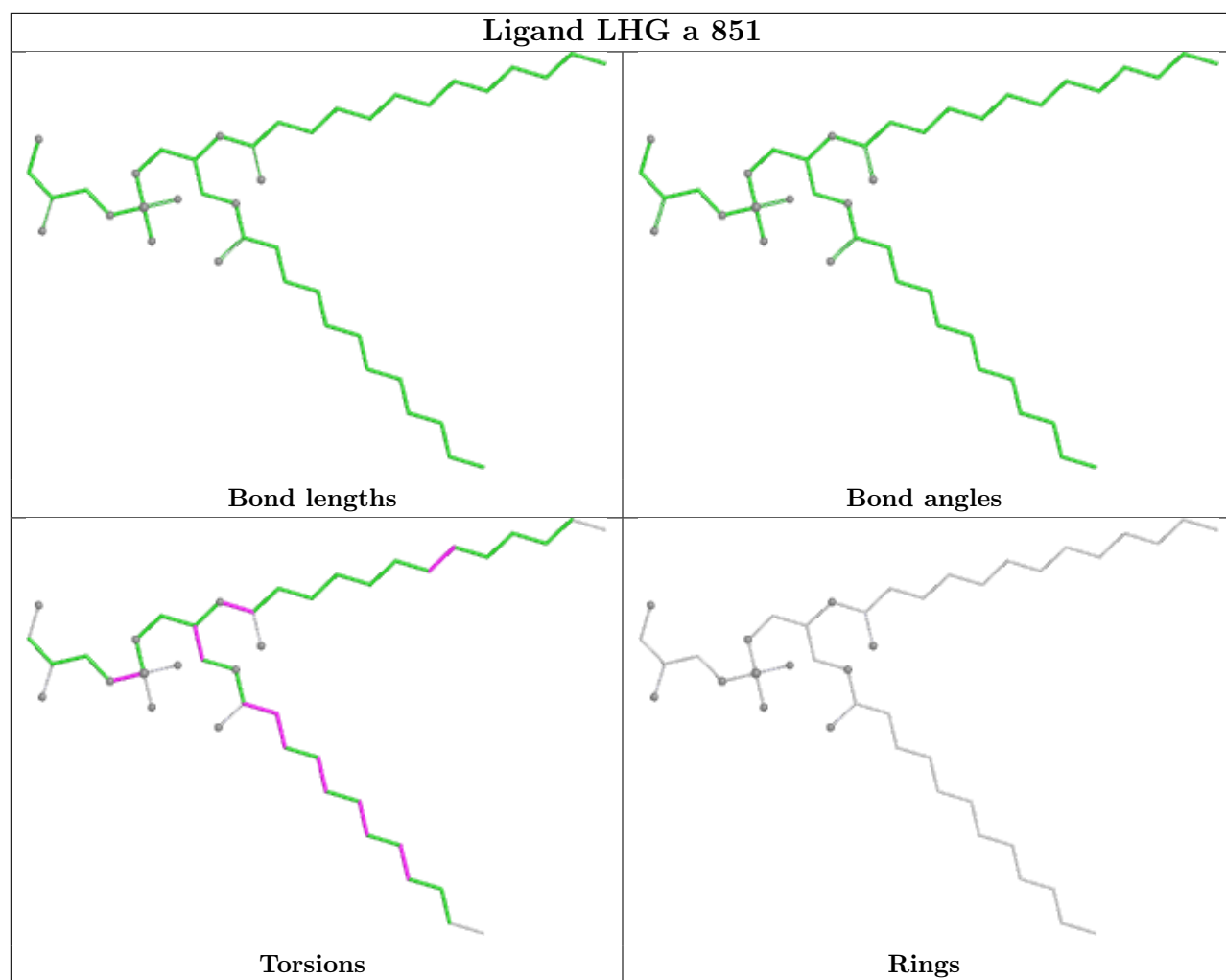
Ligand F6C L 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

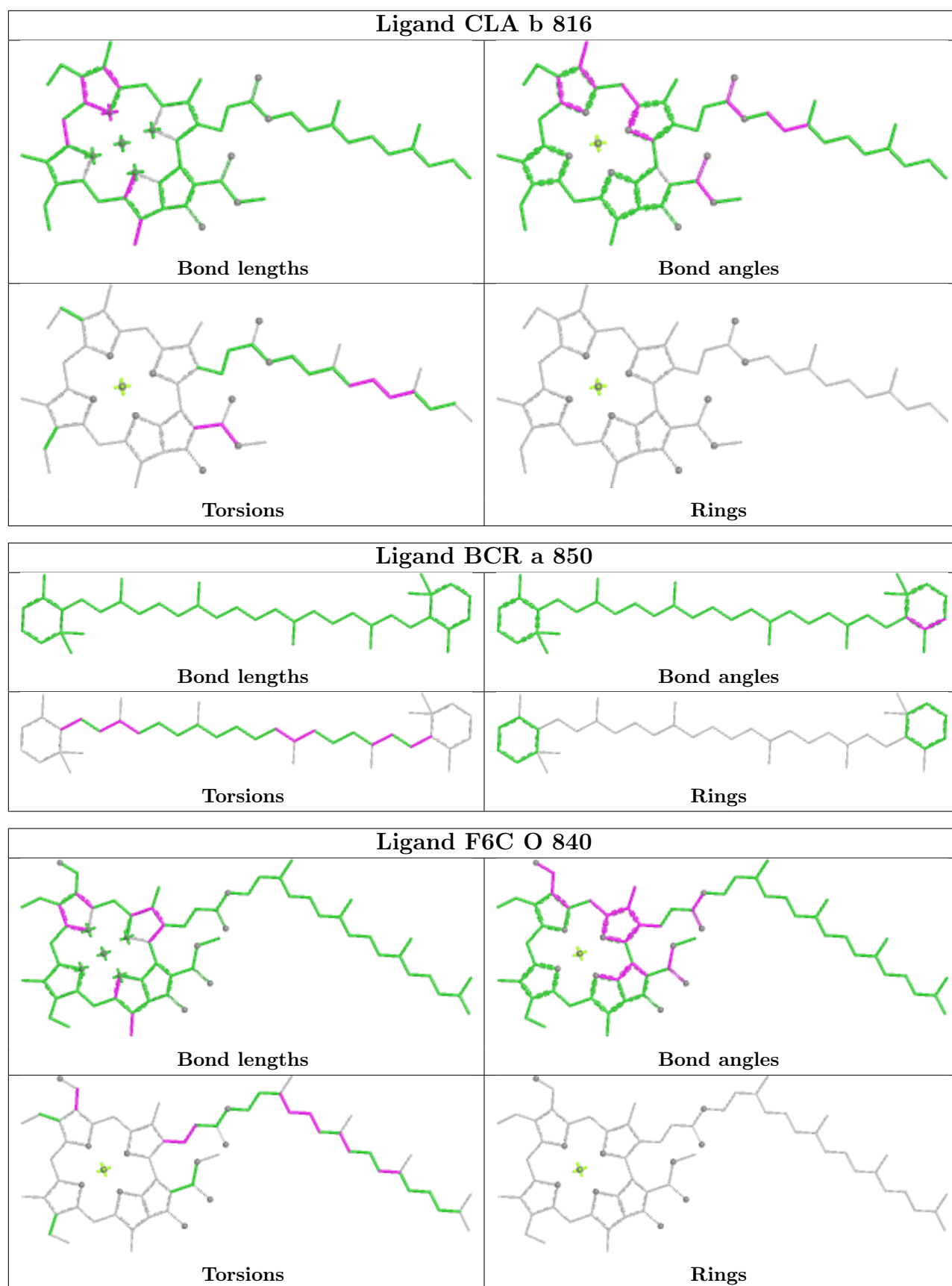
Ligand BCR a 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

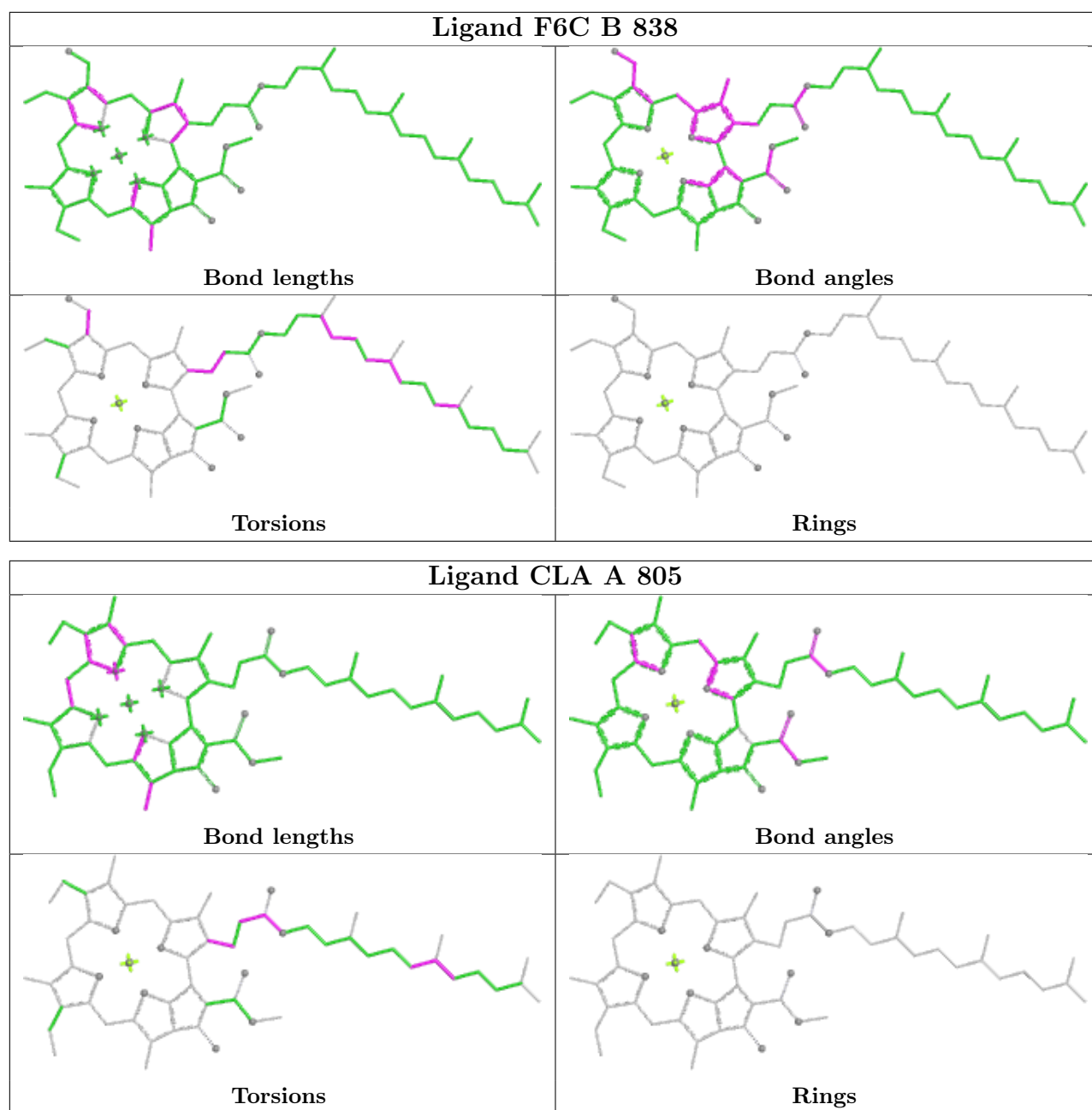
Ligand LMG A 855	
	
Bond lengths	Bond angles
	
Torsions	Rings

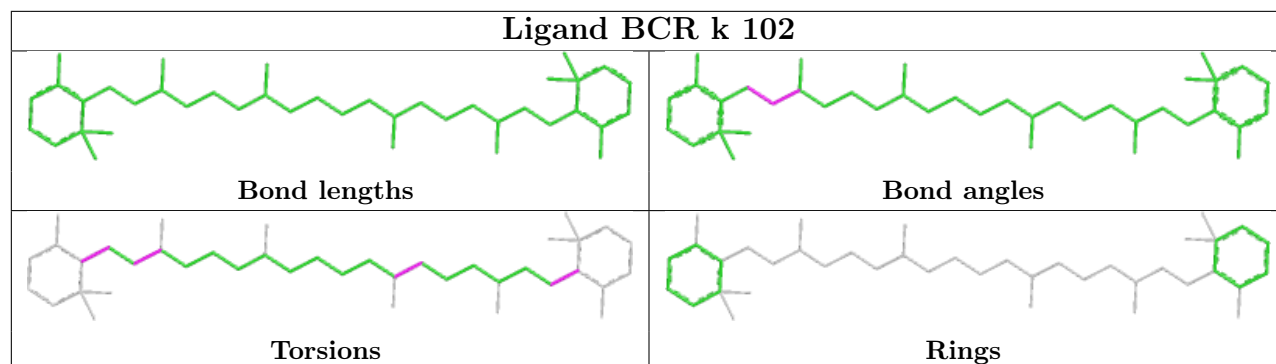
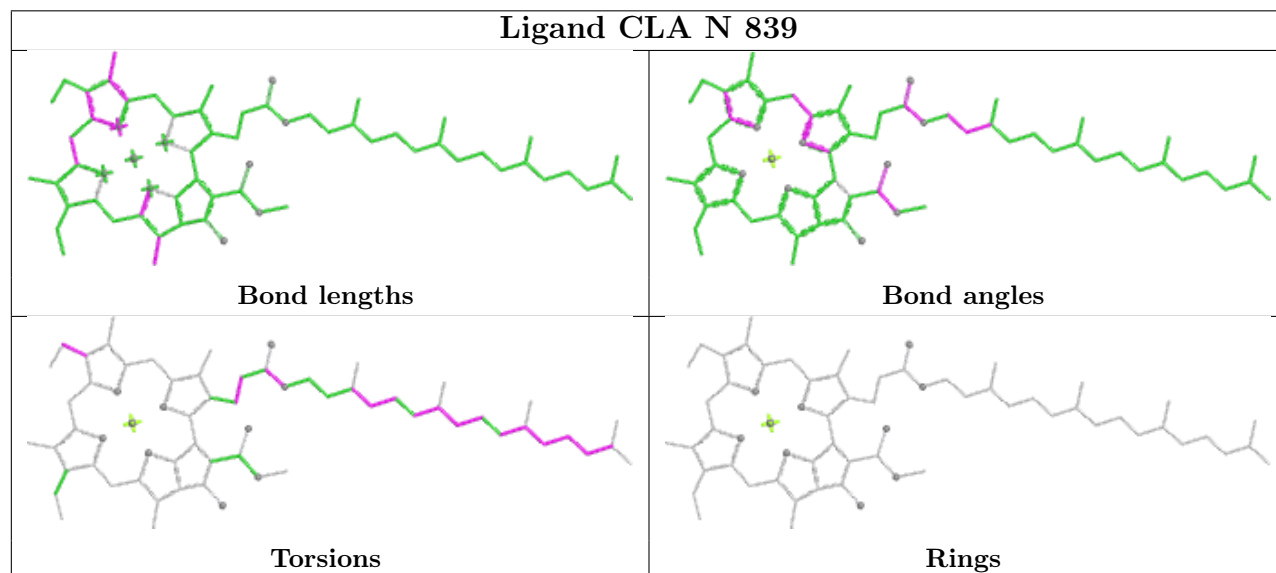
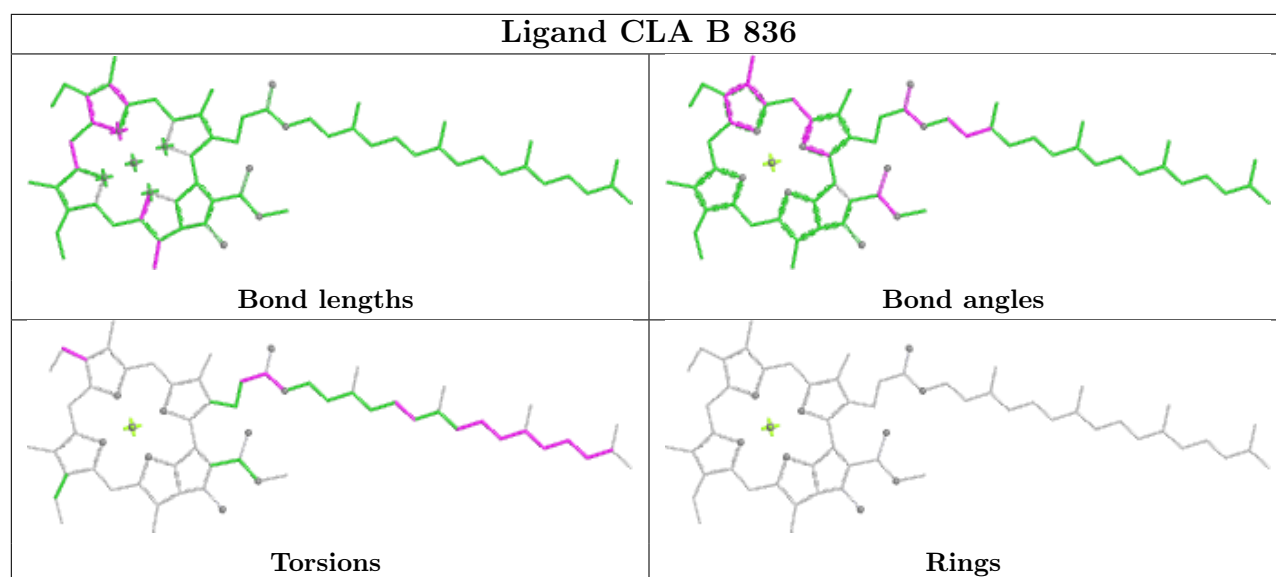
Ligand BCR b 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

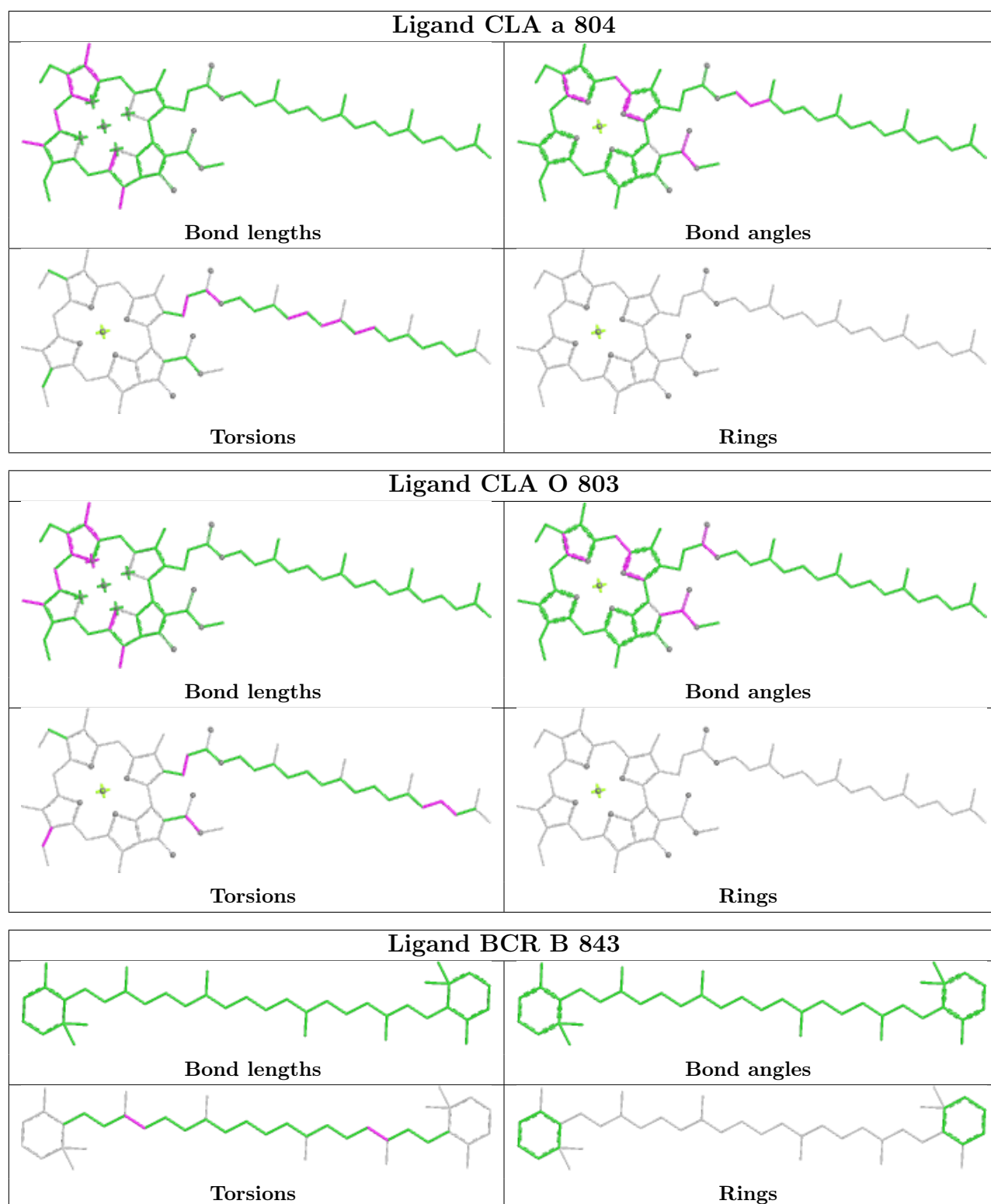


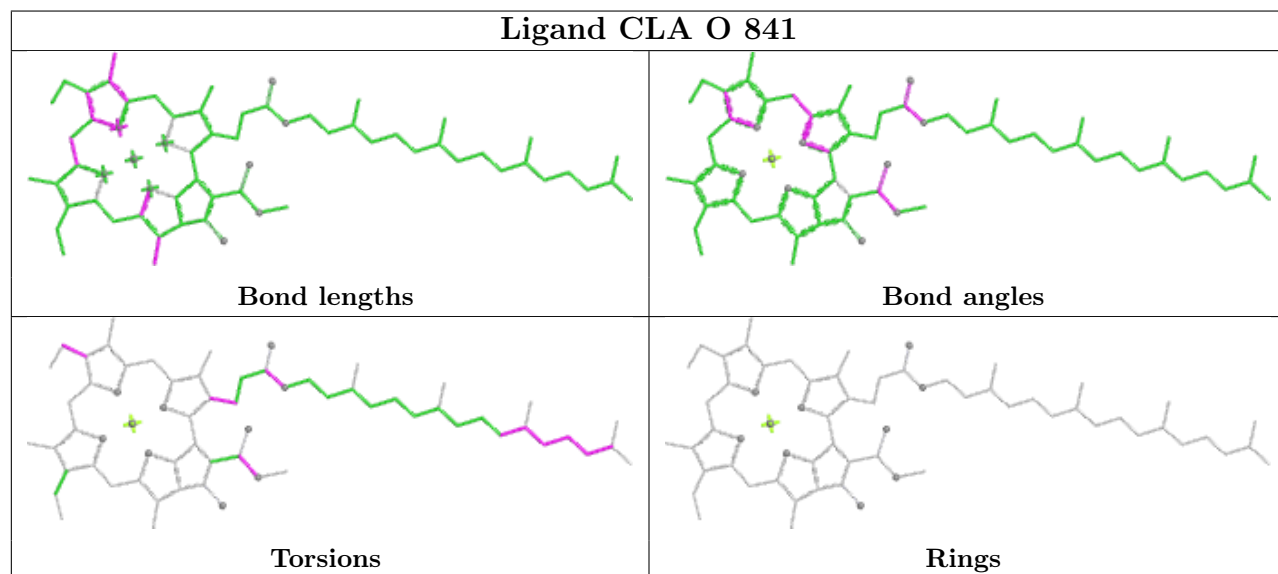
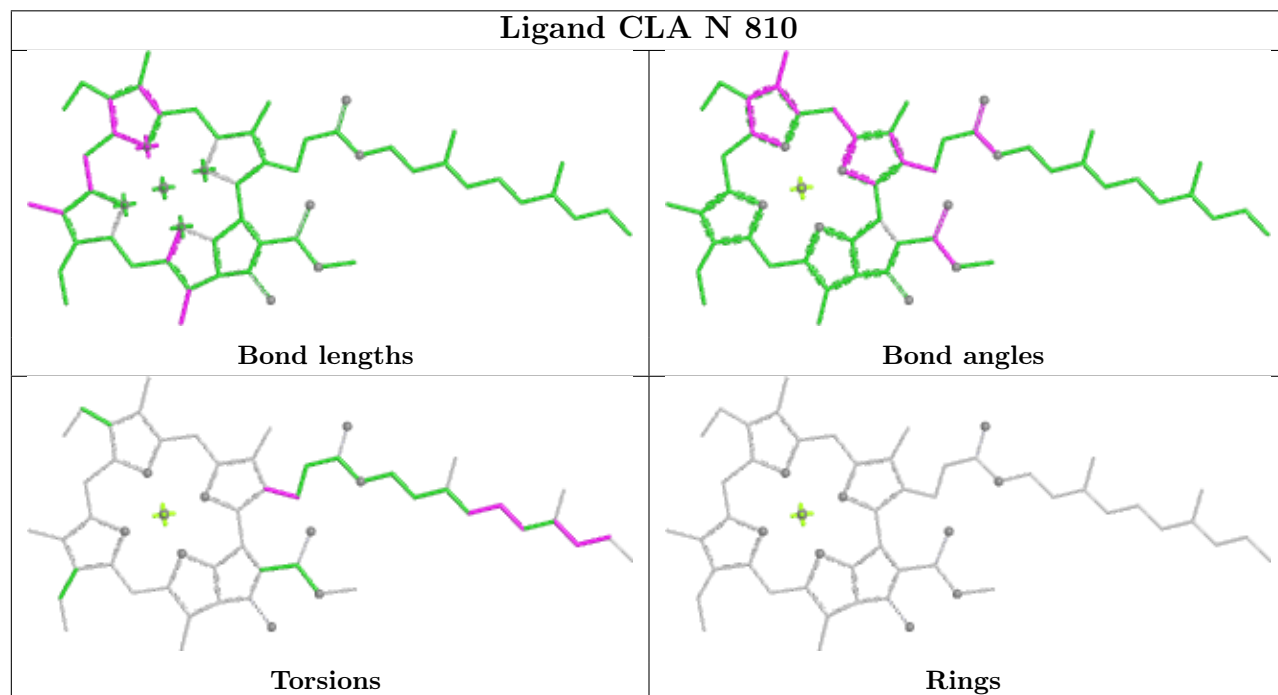
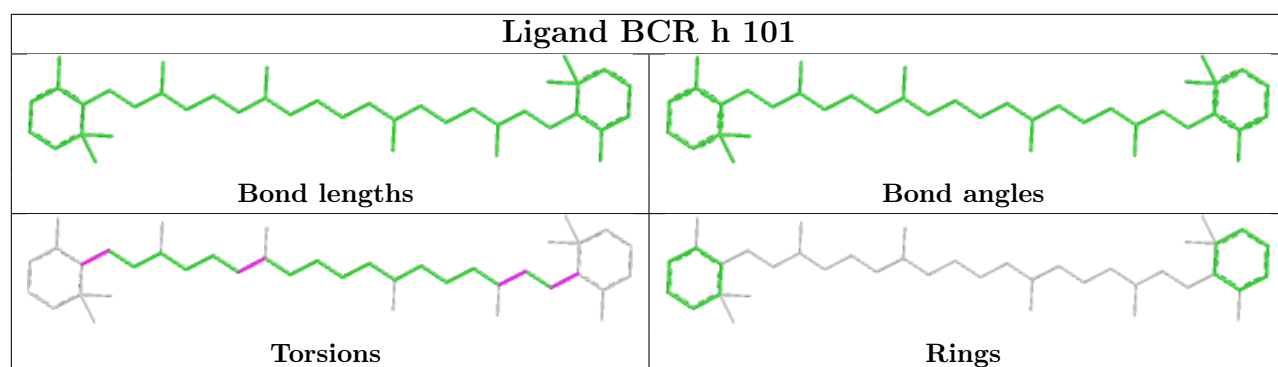




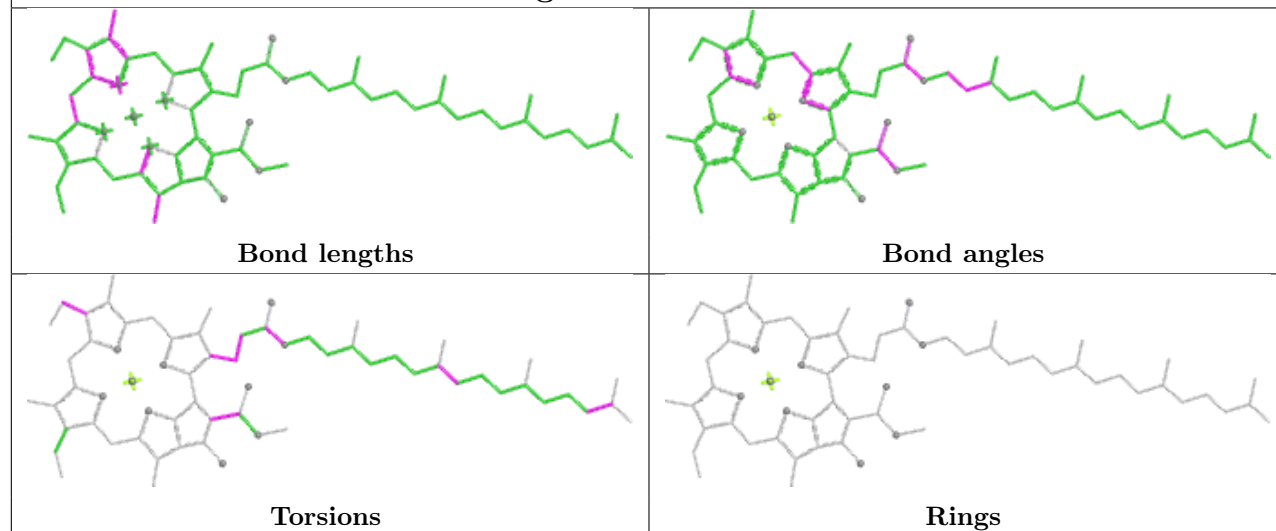




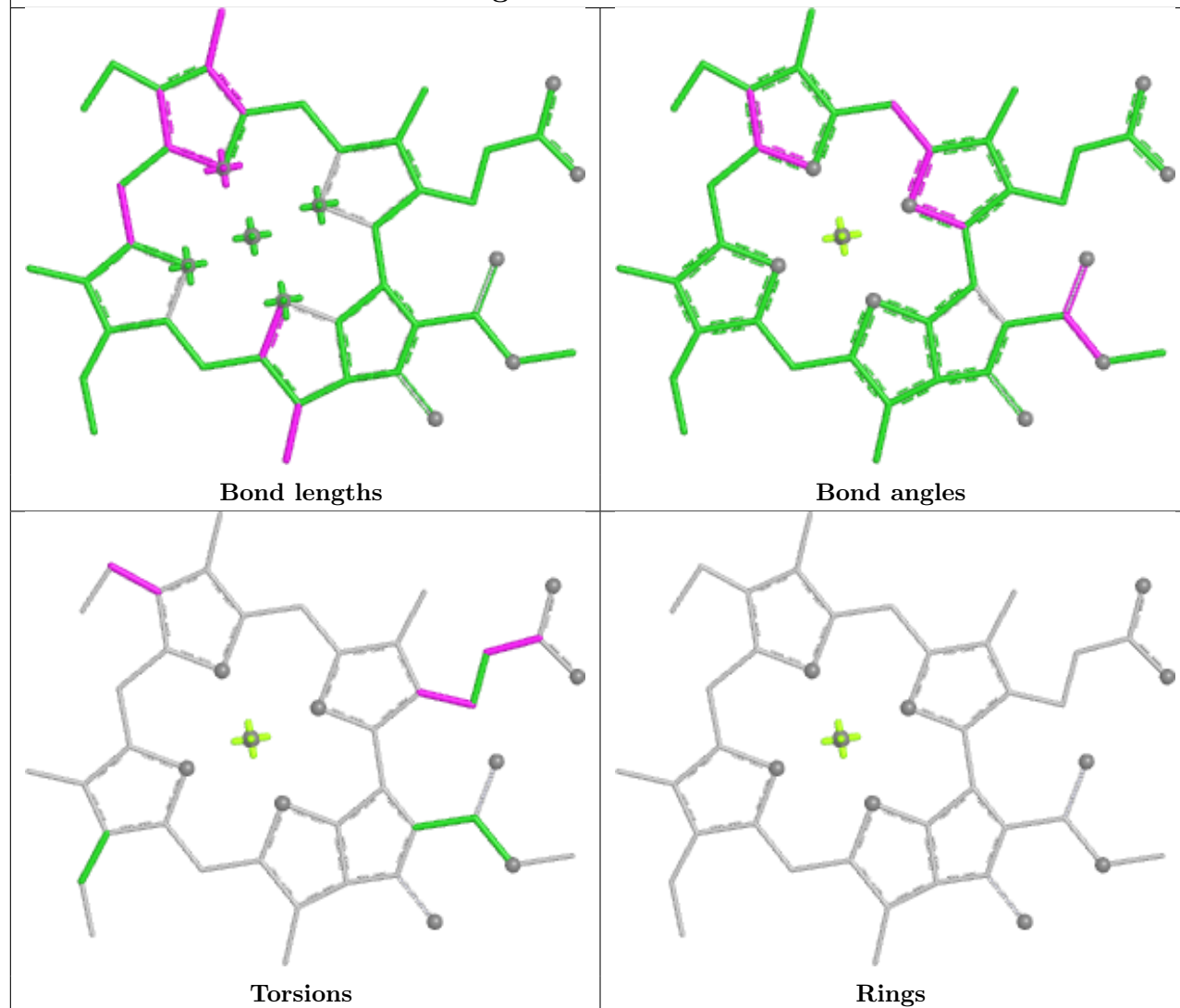


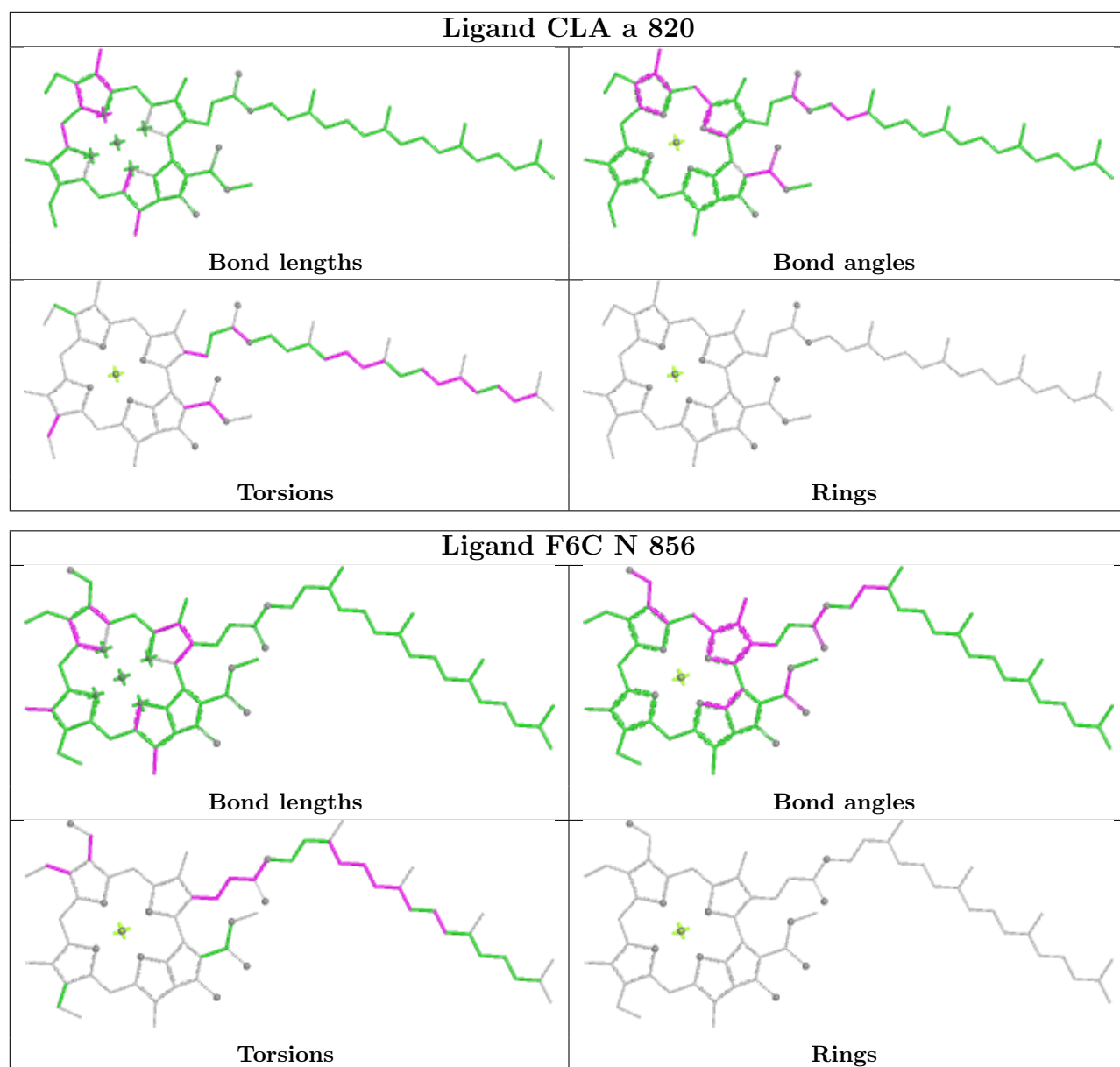


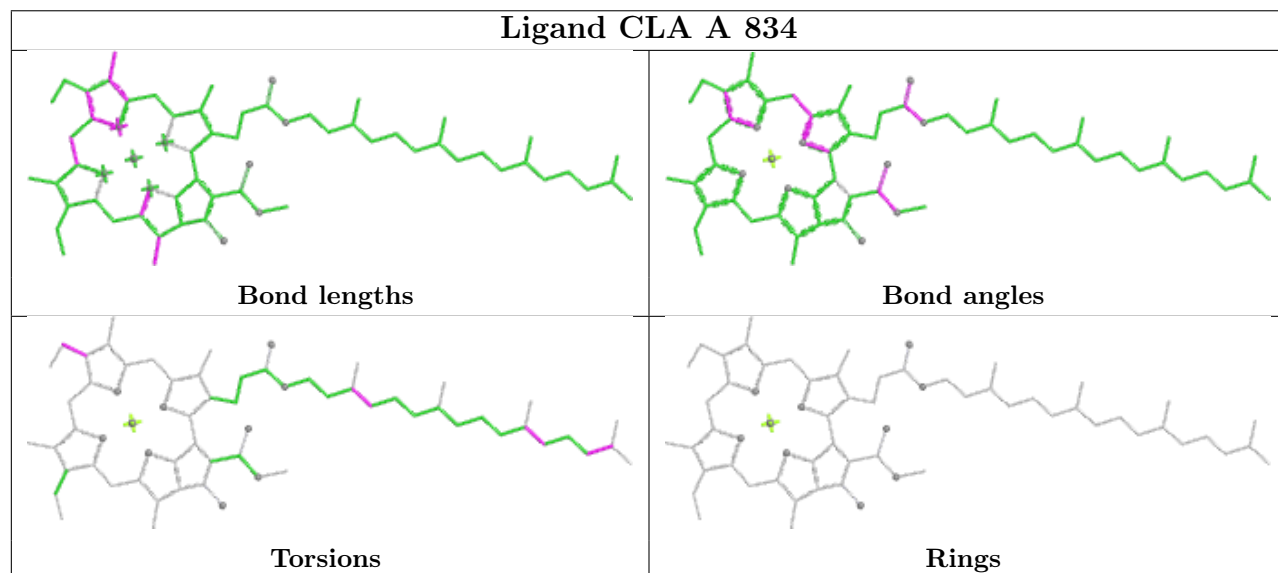
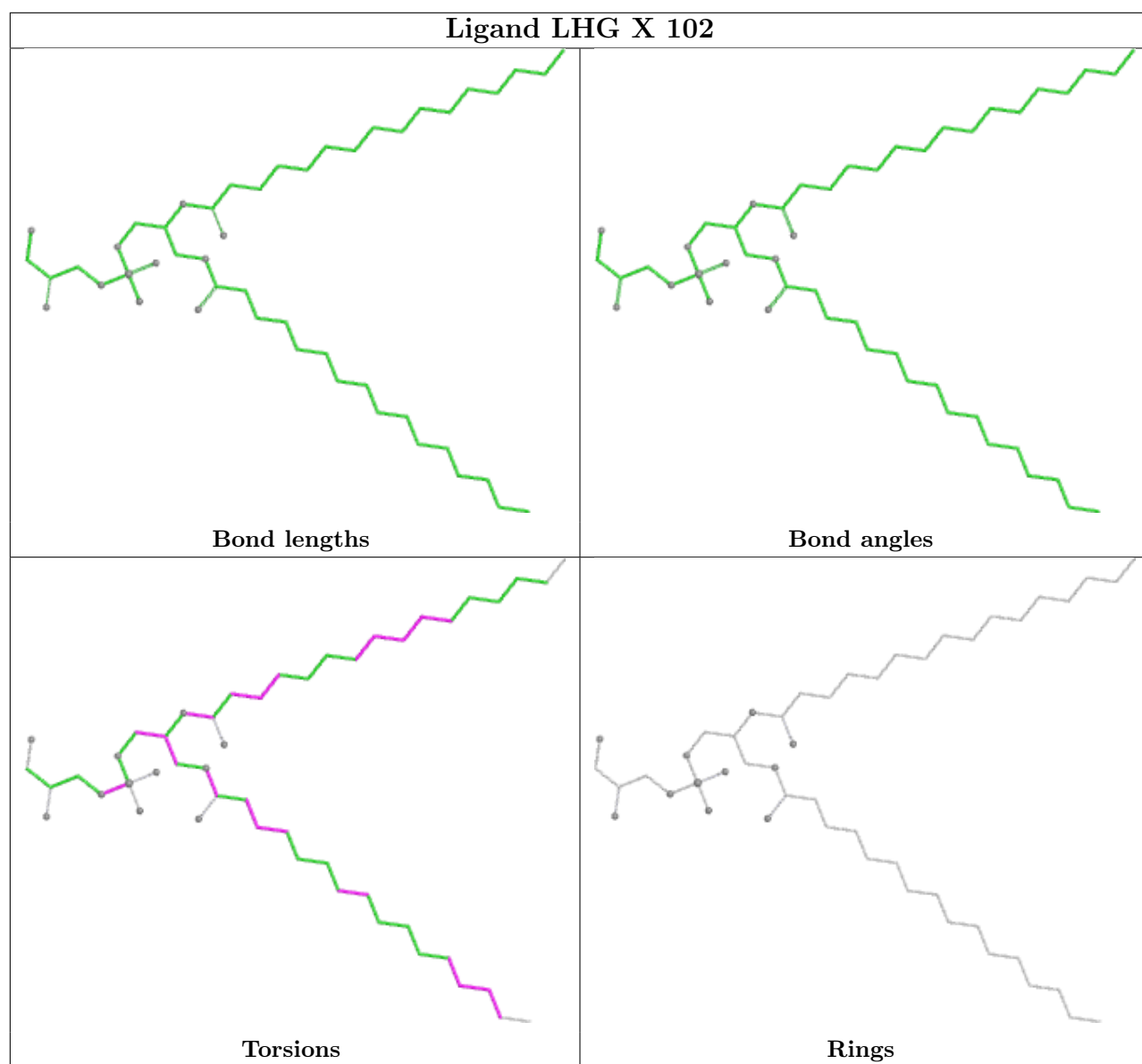
Ligand CLA a 842



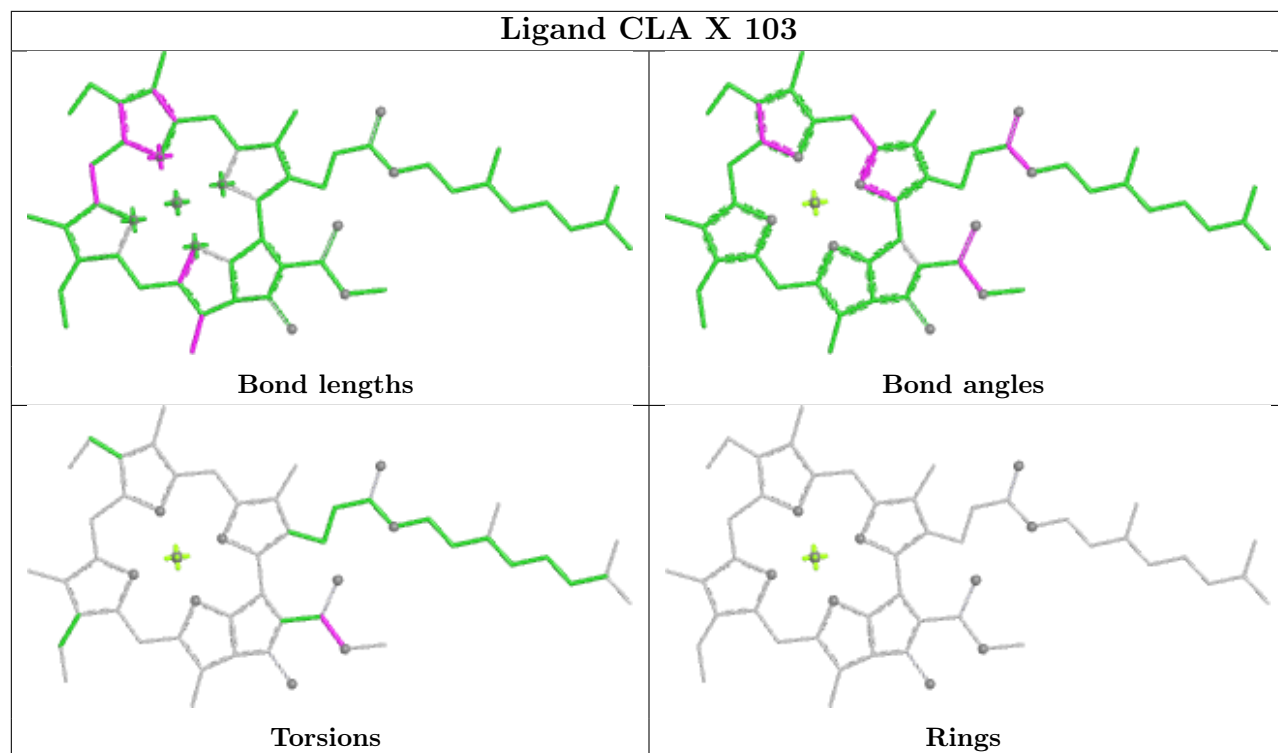
Ligand CLA B 810



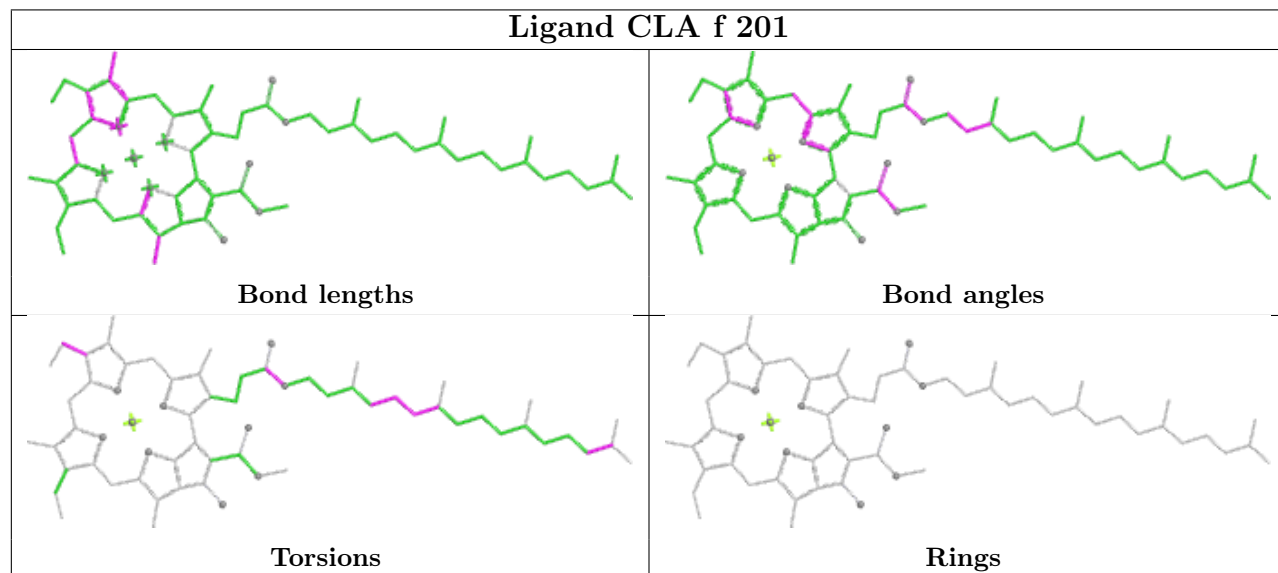




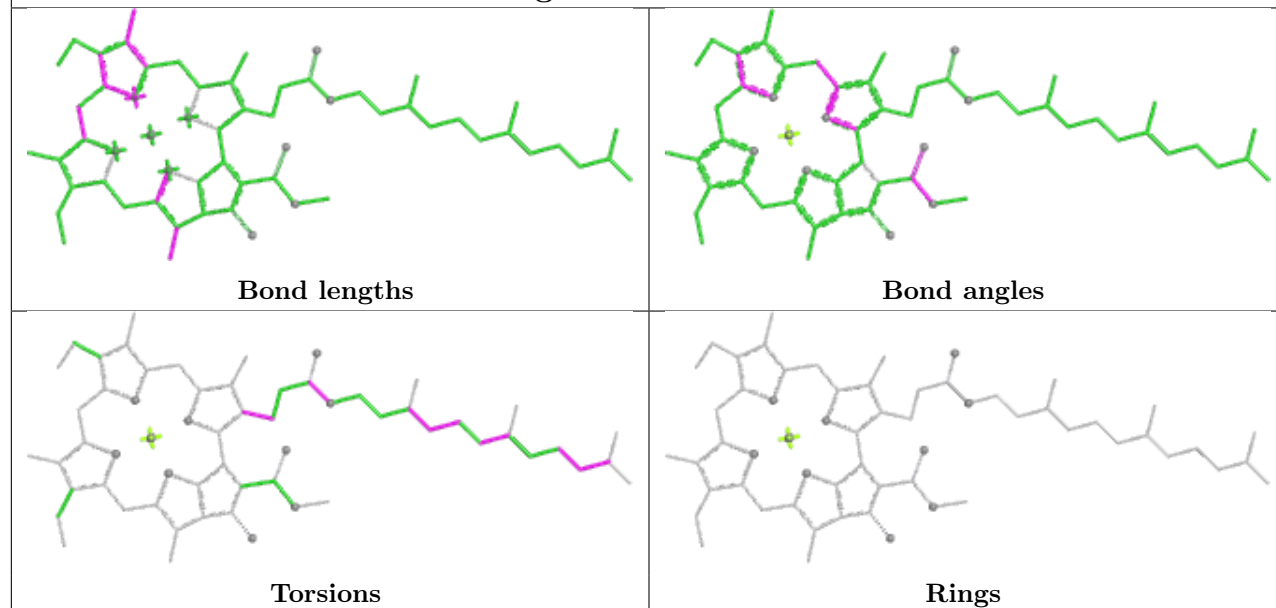
Ligand CLA X 103



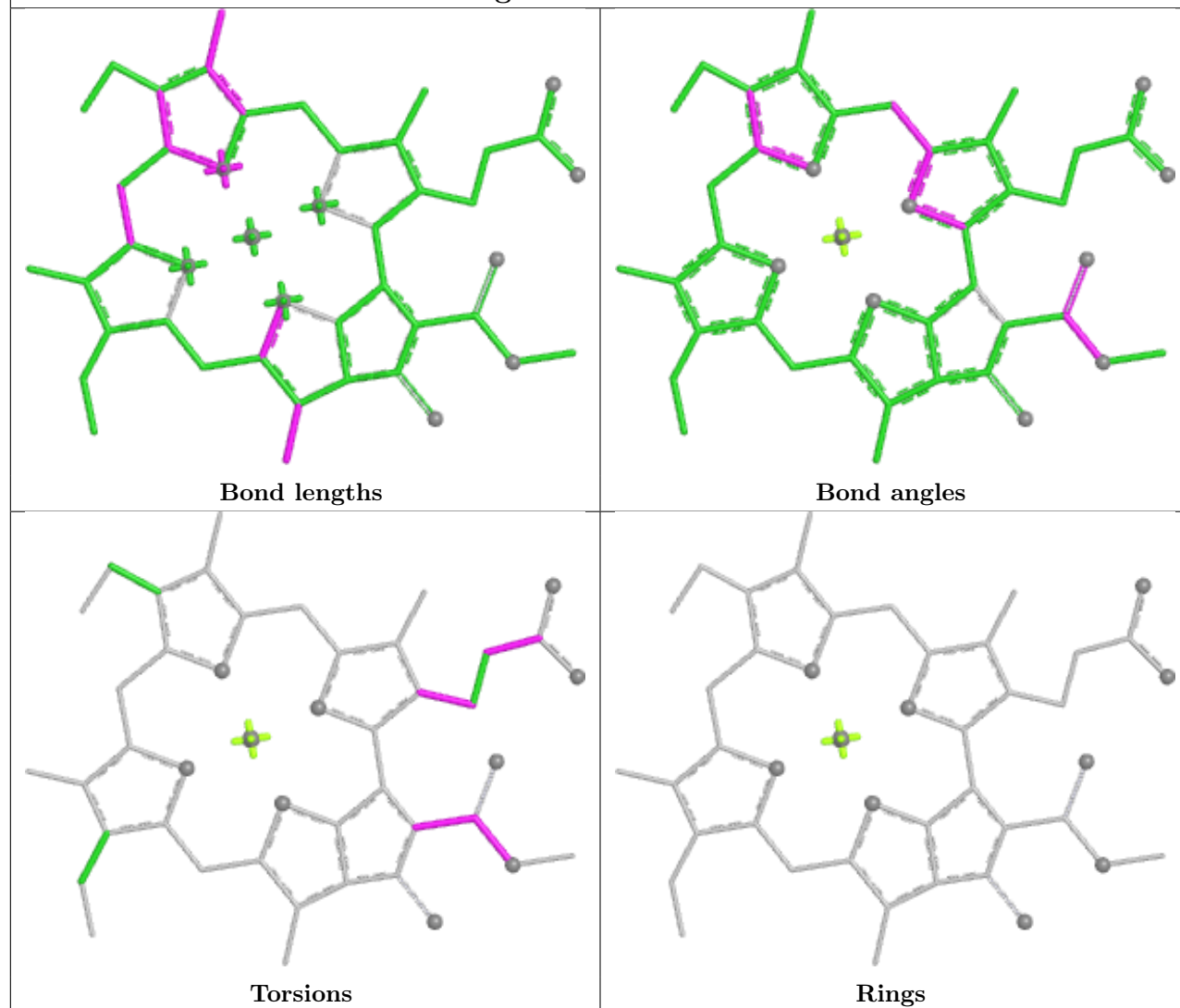
Ligand CLA f 201

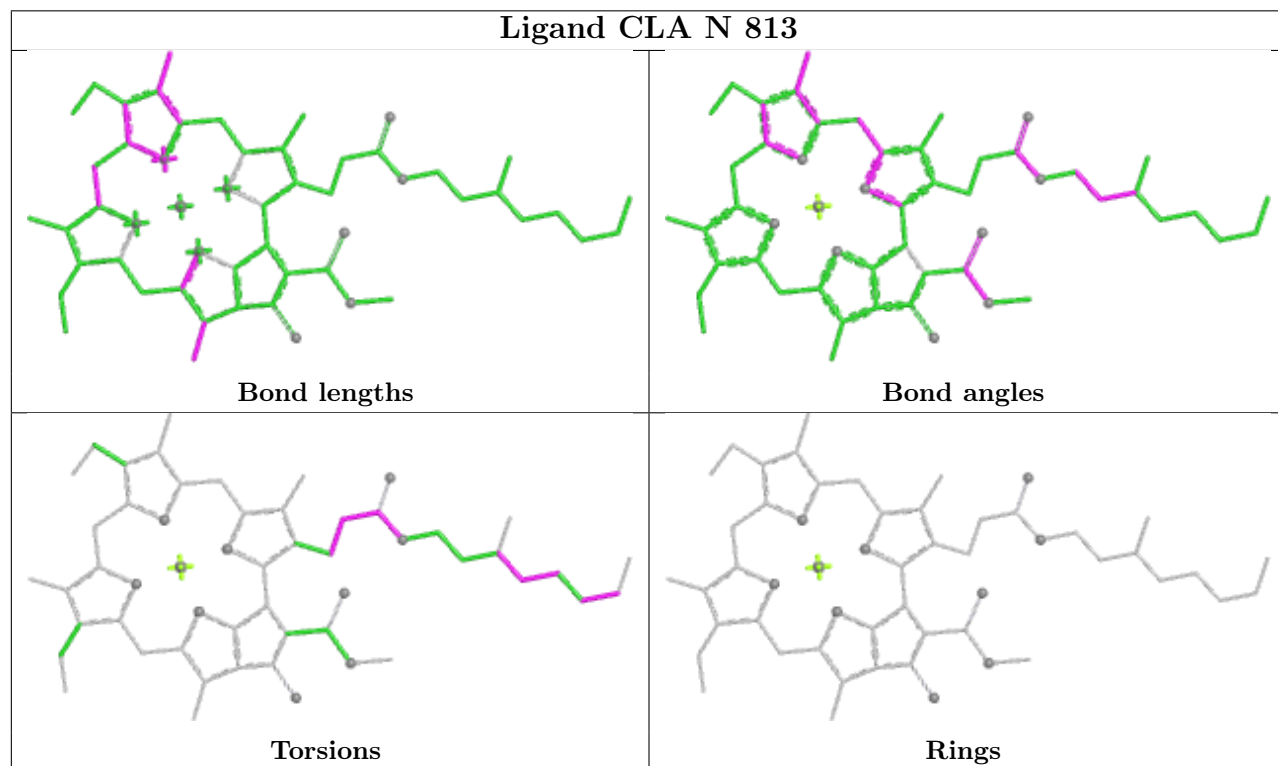
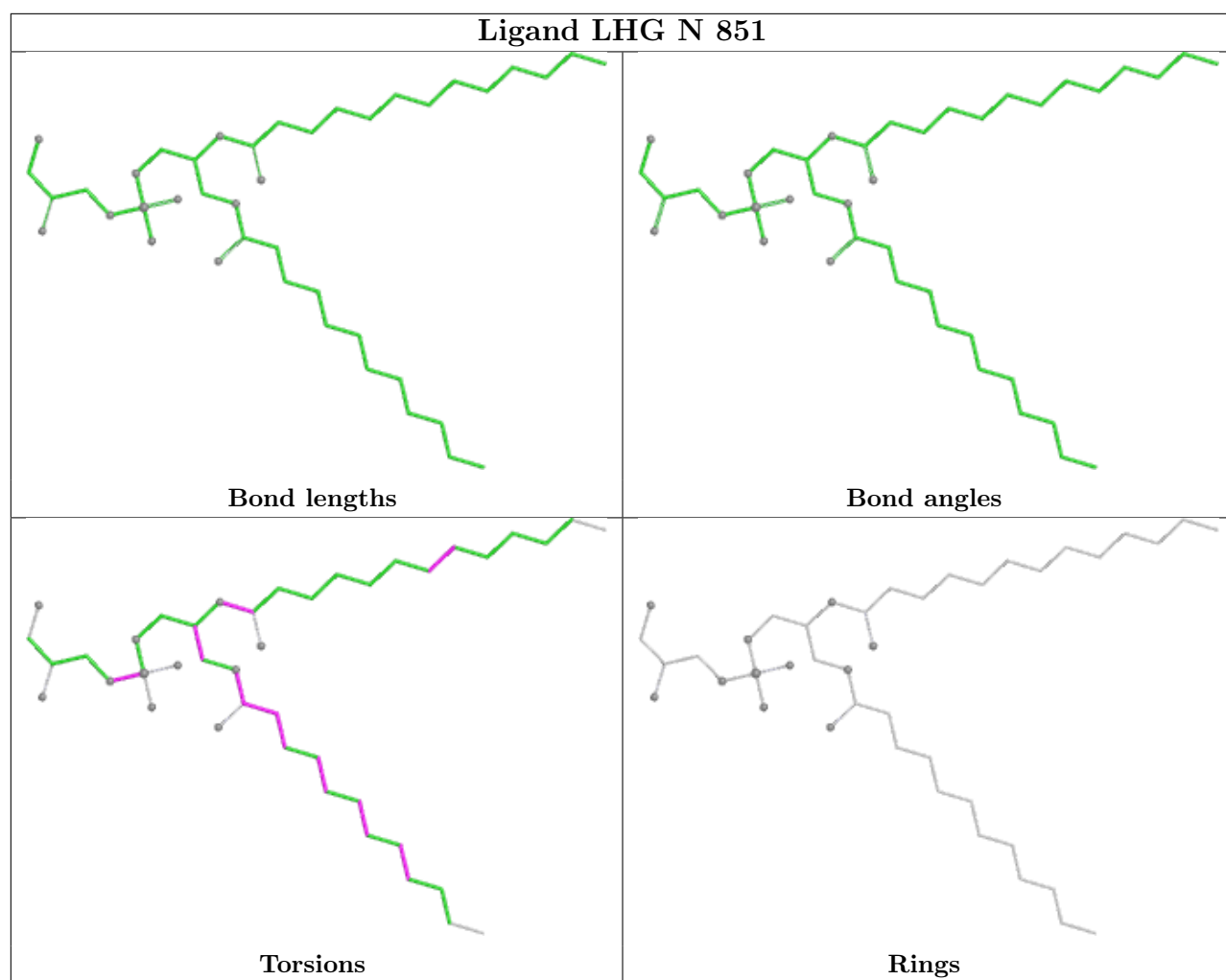


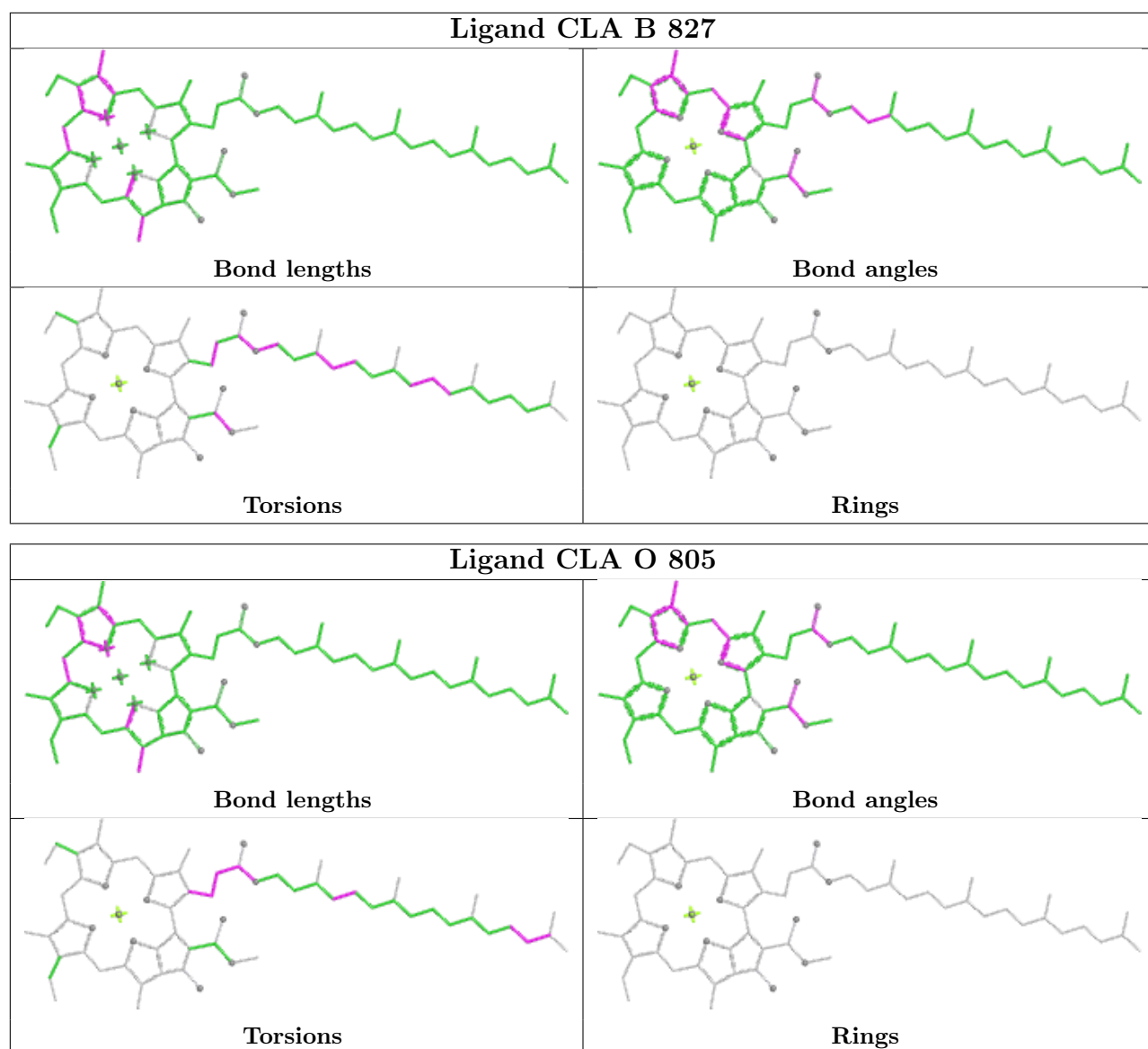
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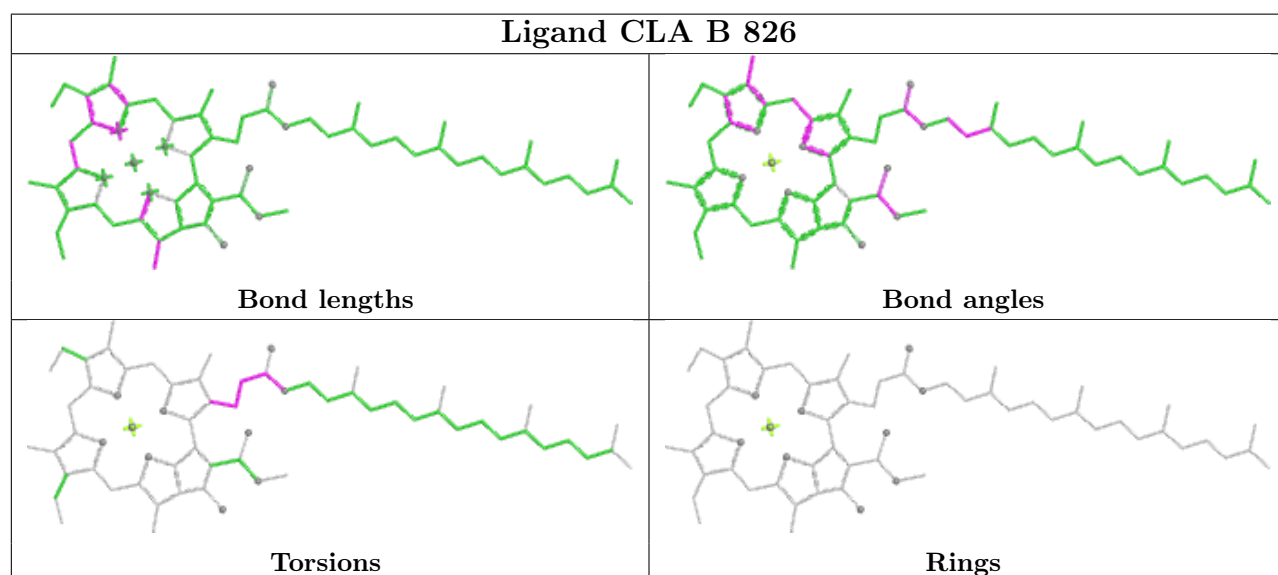
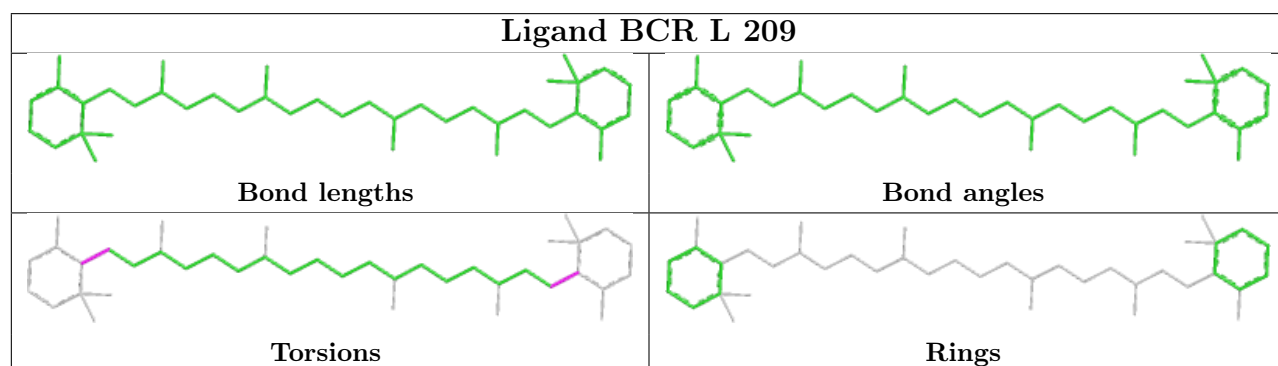
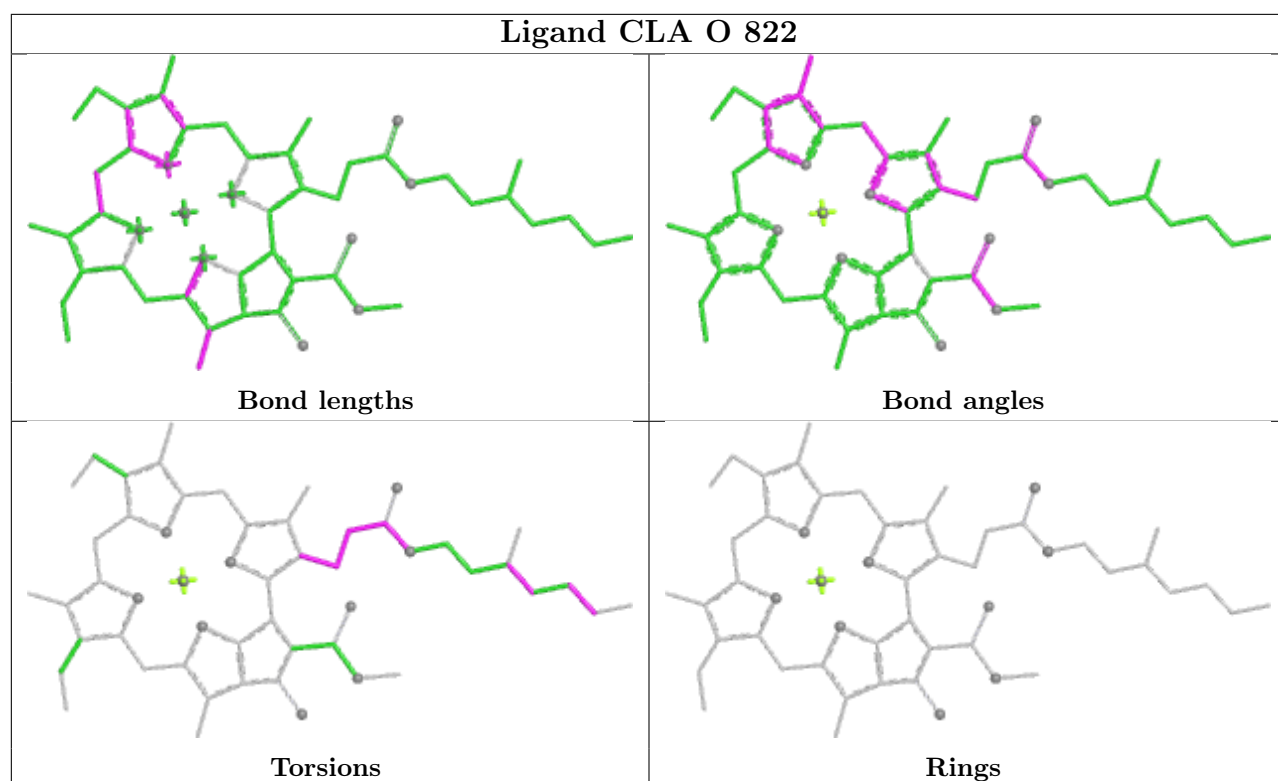


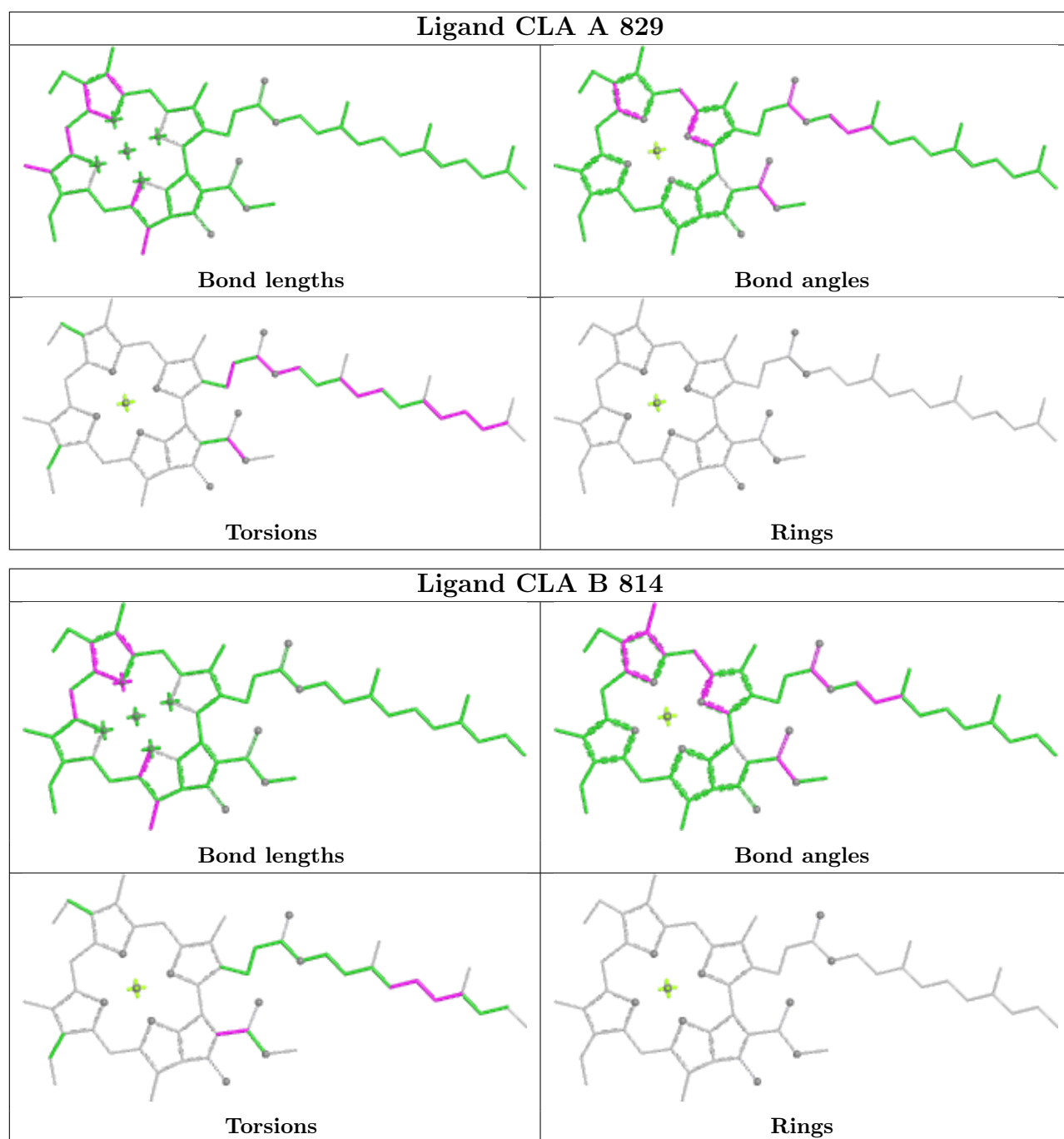
Ligand CLA b 836



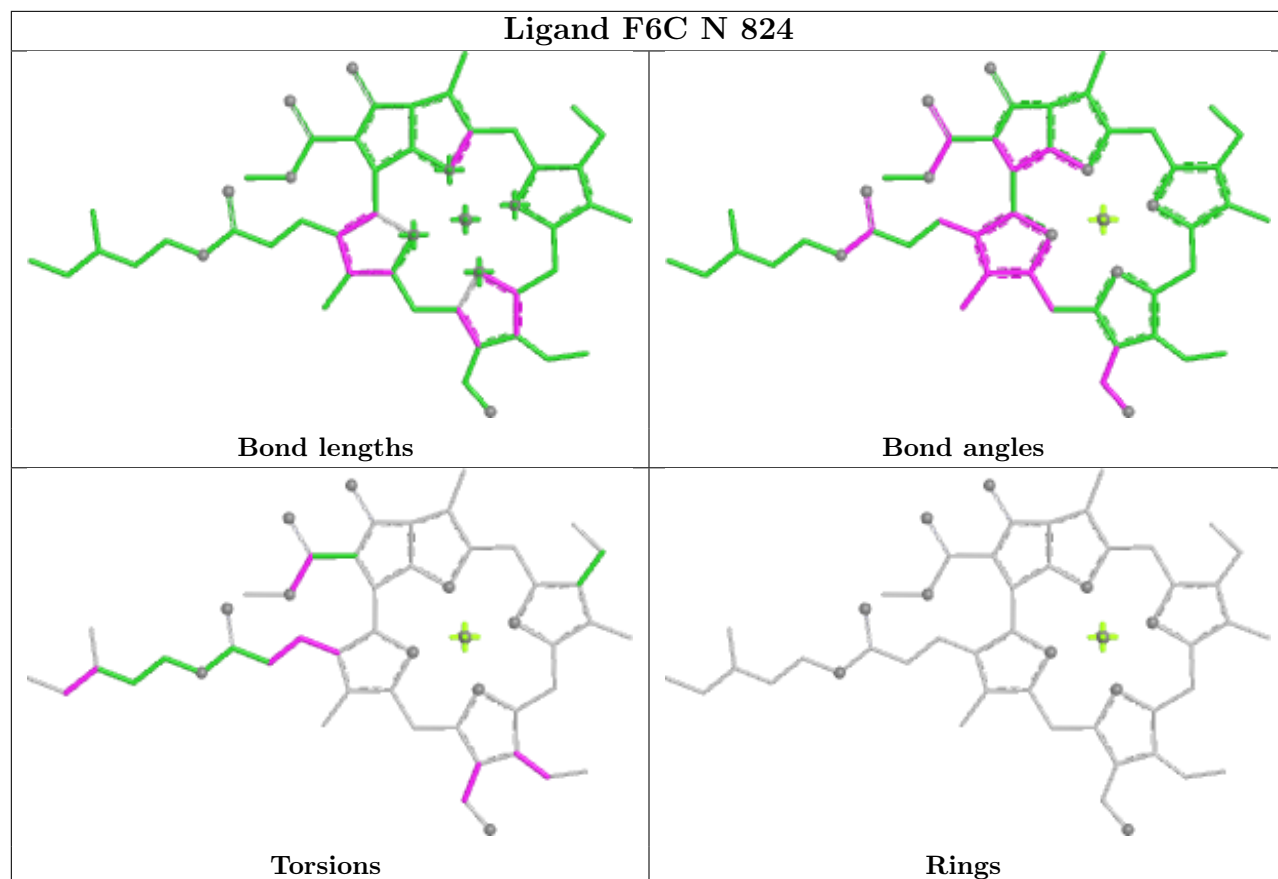




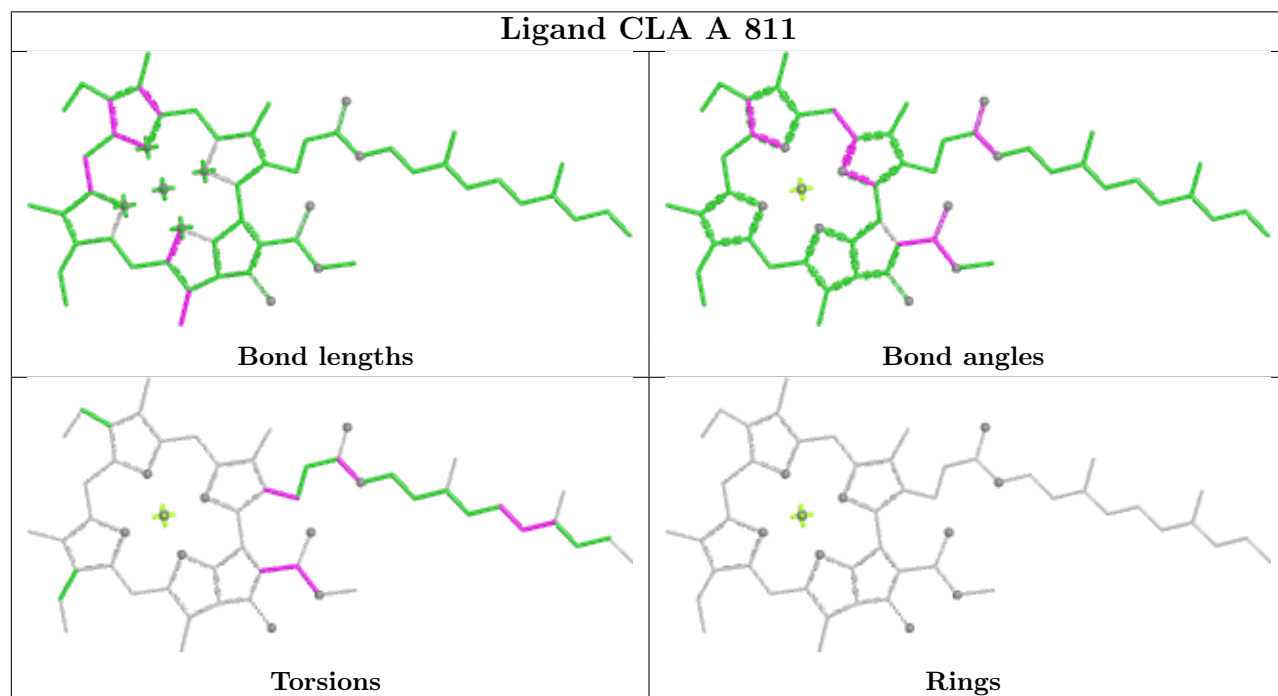


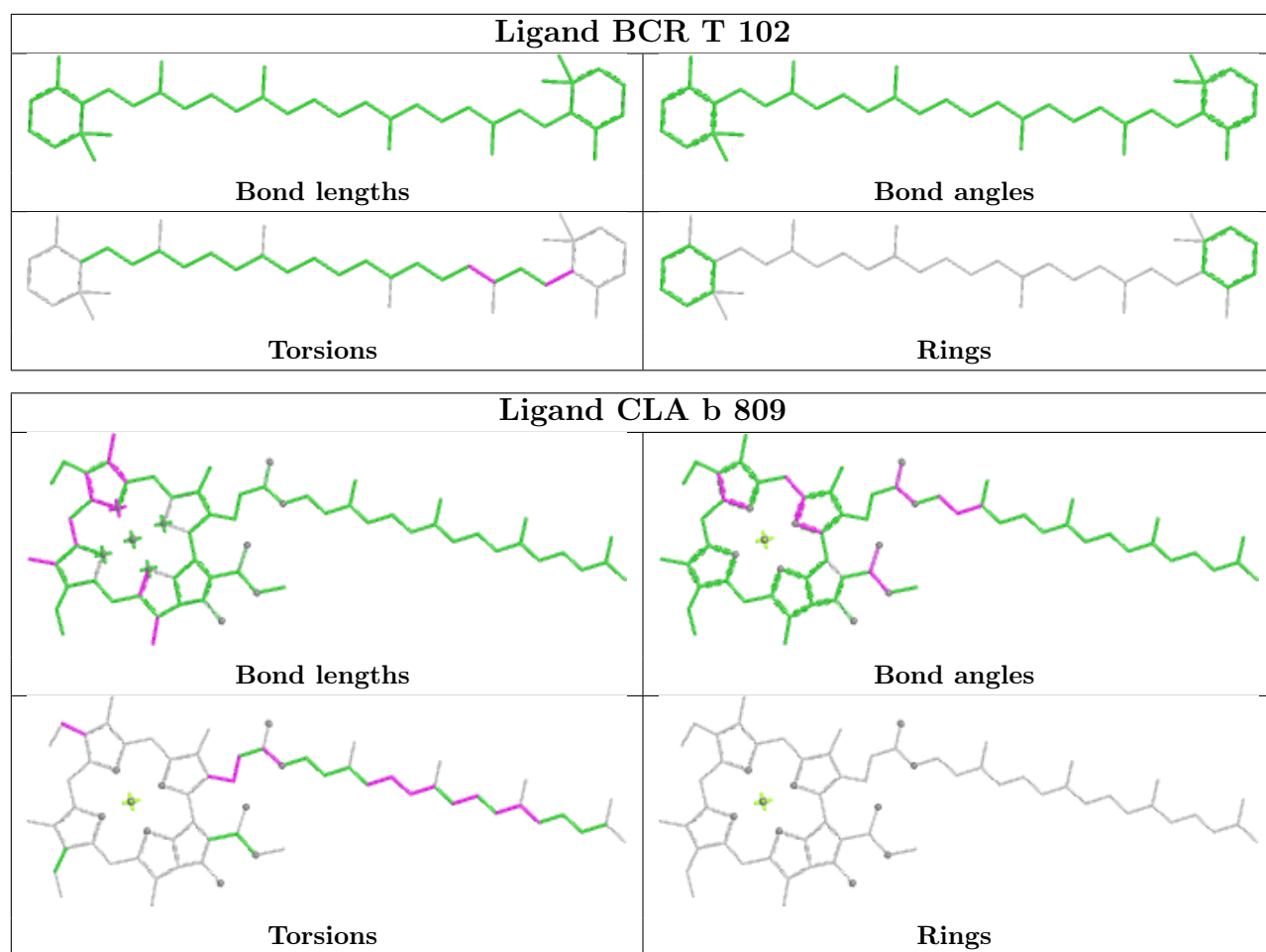


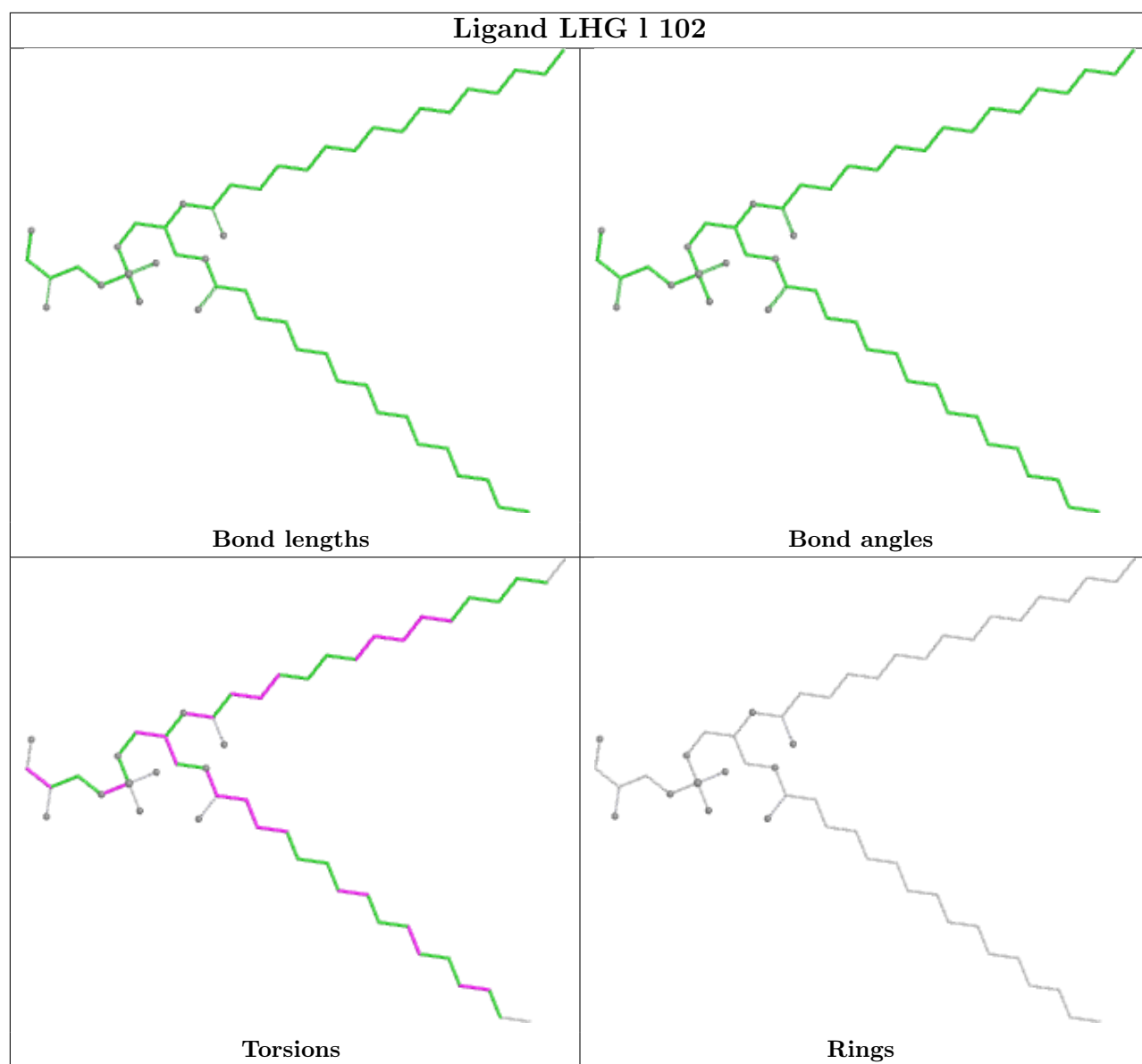
Ligand F6C N 824



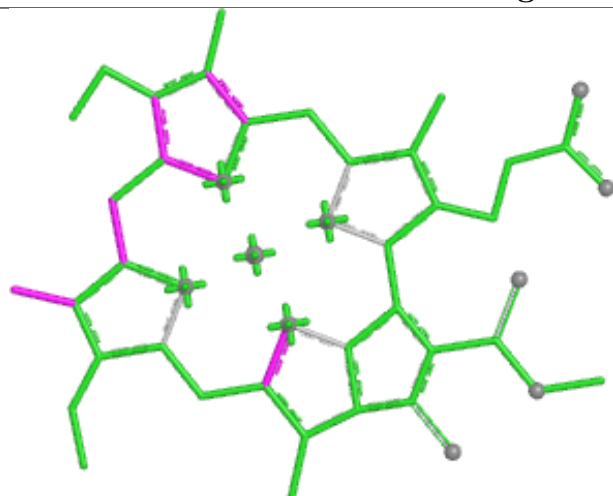
Ligand CLA A 811



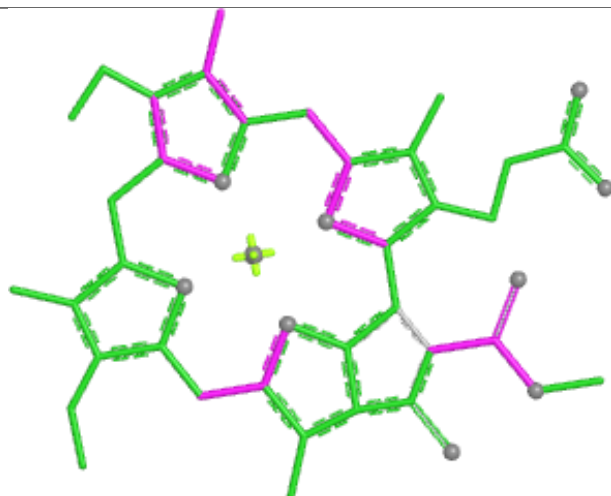




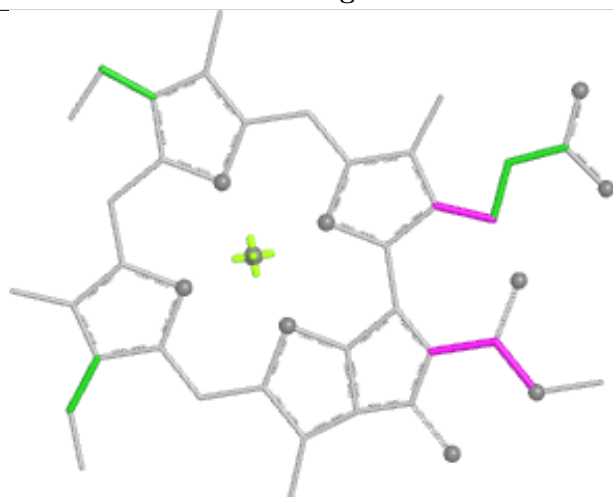
Ligand CLA b 815



Bond lengths



Bond angles

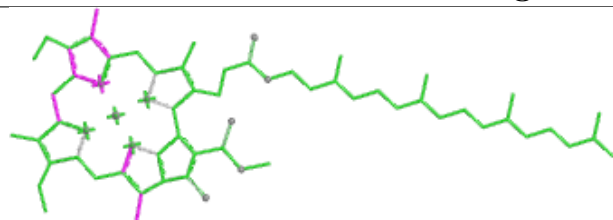


Torsions

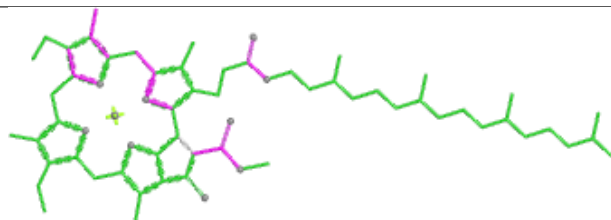


Rings

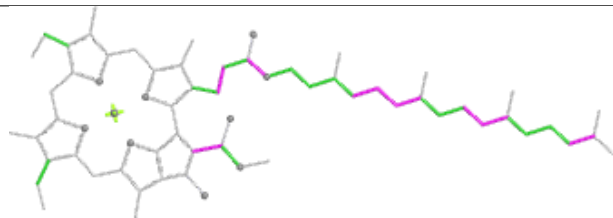
Ligand CLA A 831



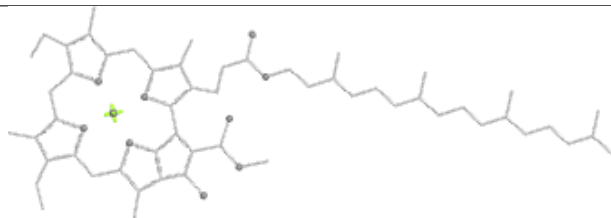
Bond lengths



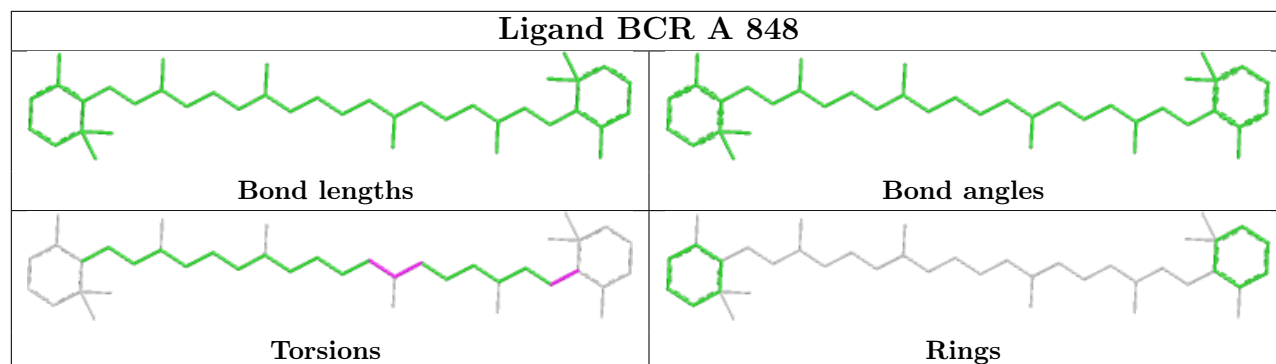
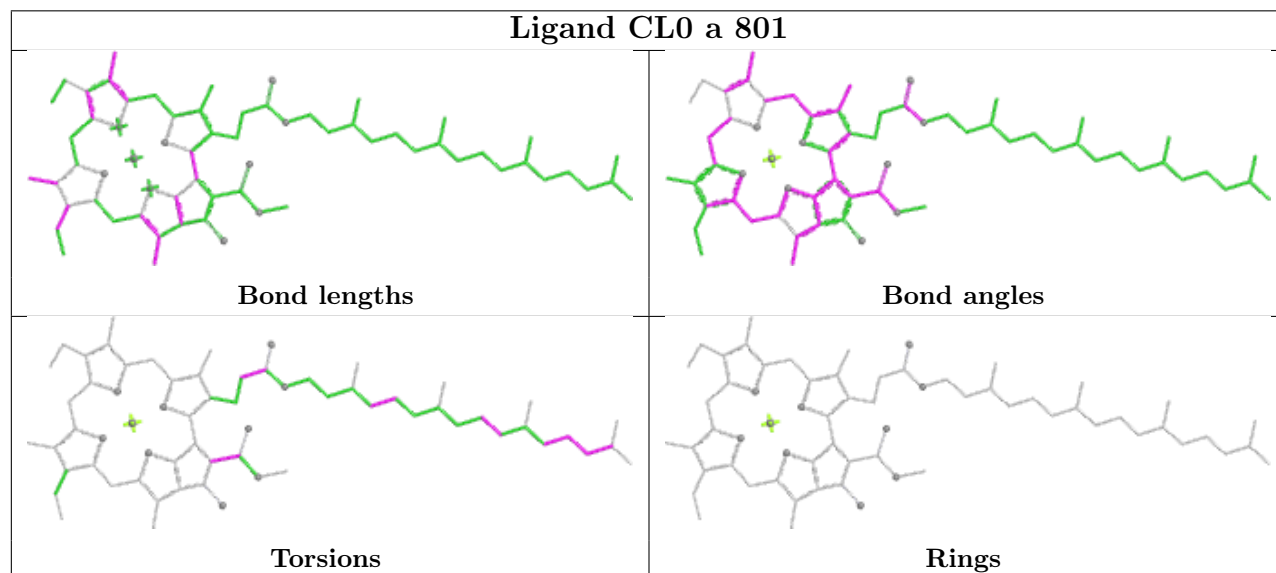
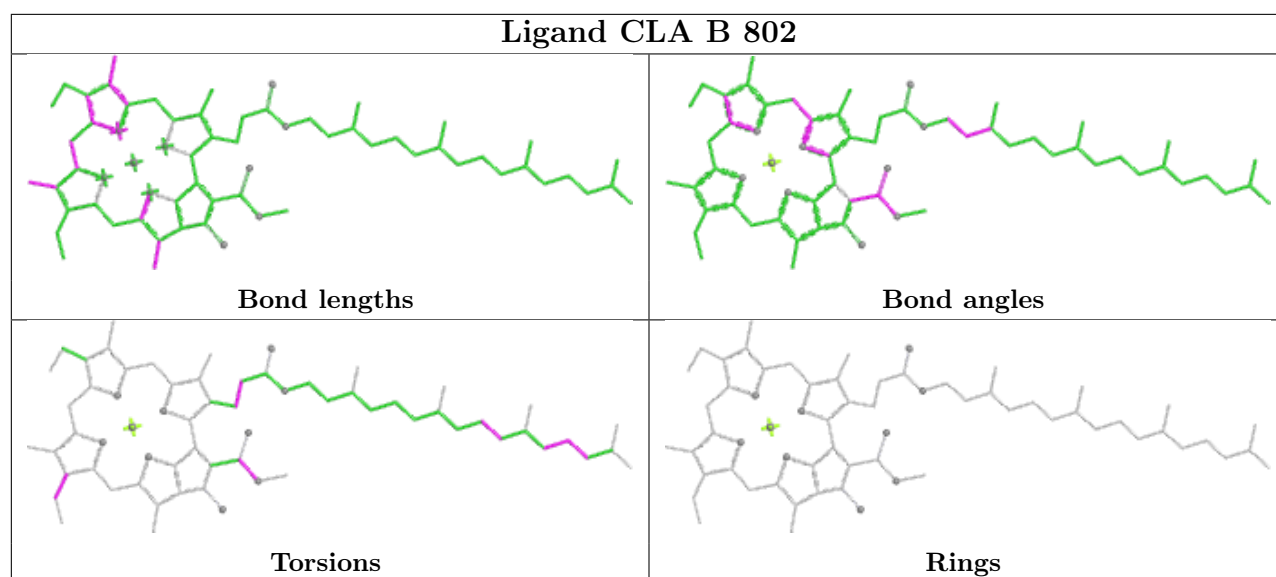
Bond angles



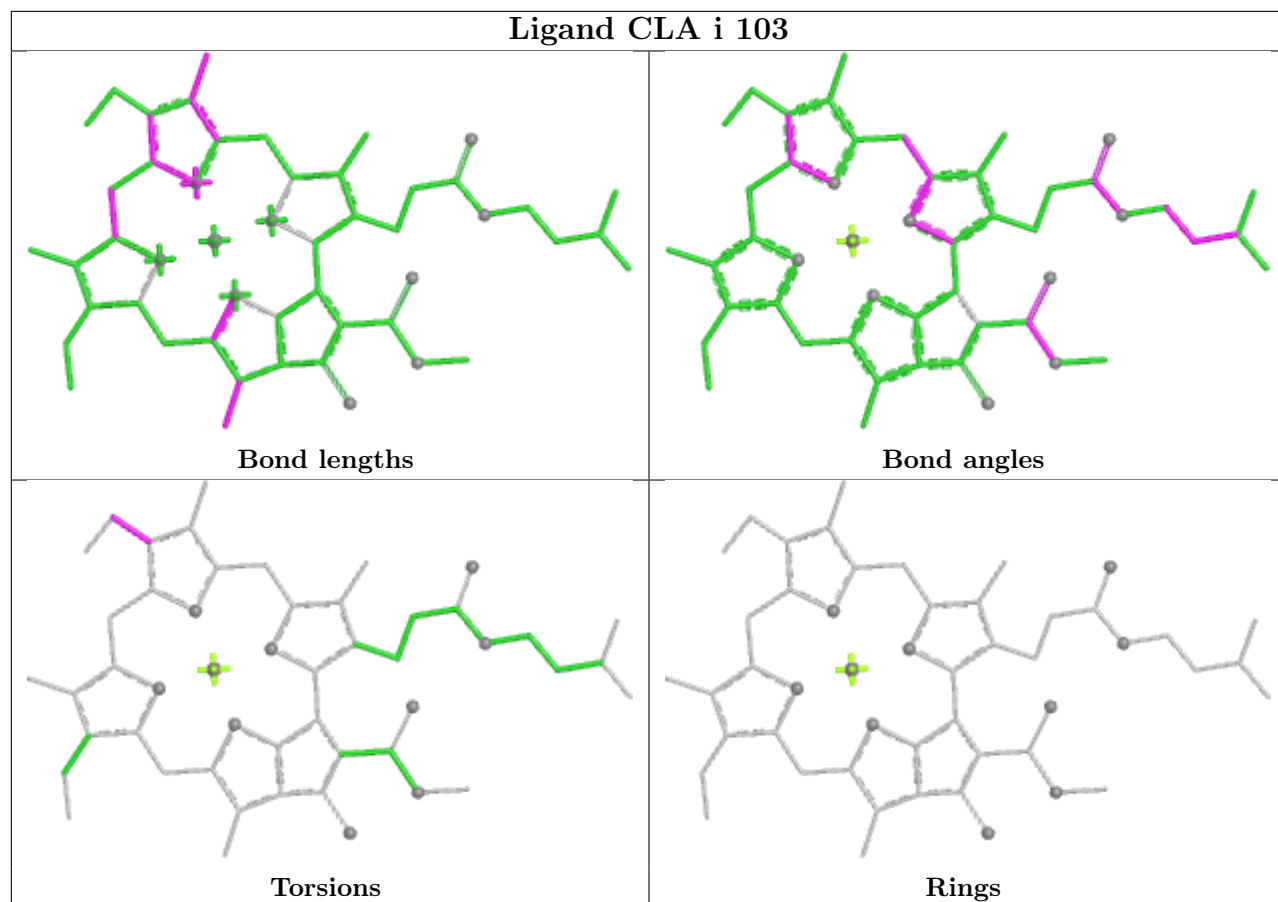
Torsions

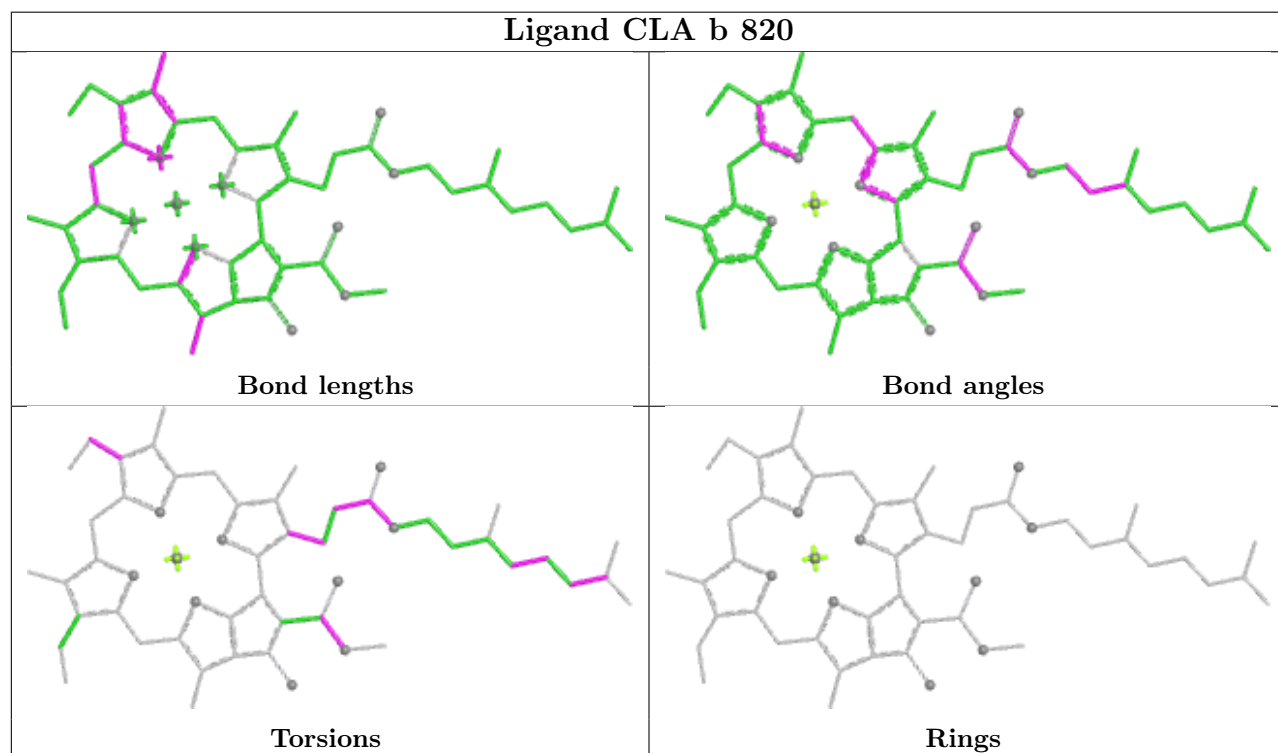
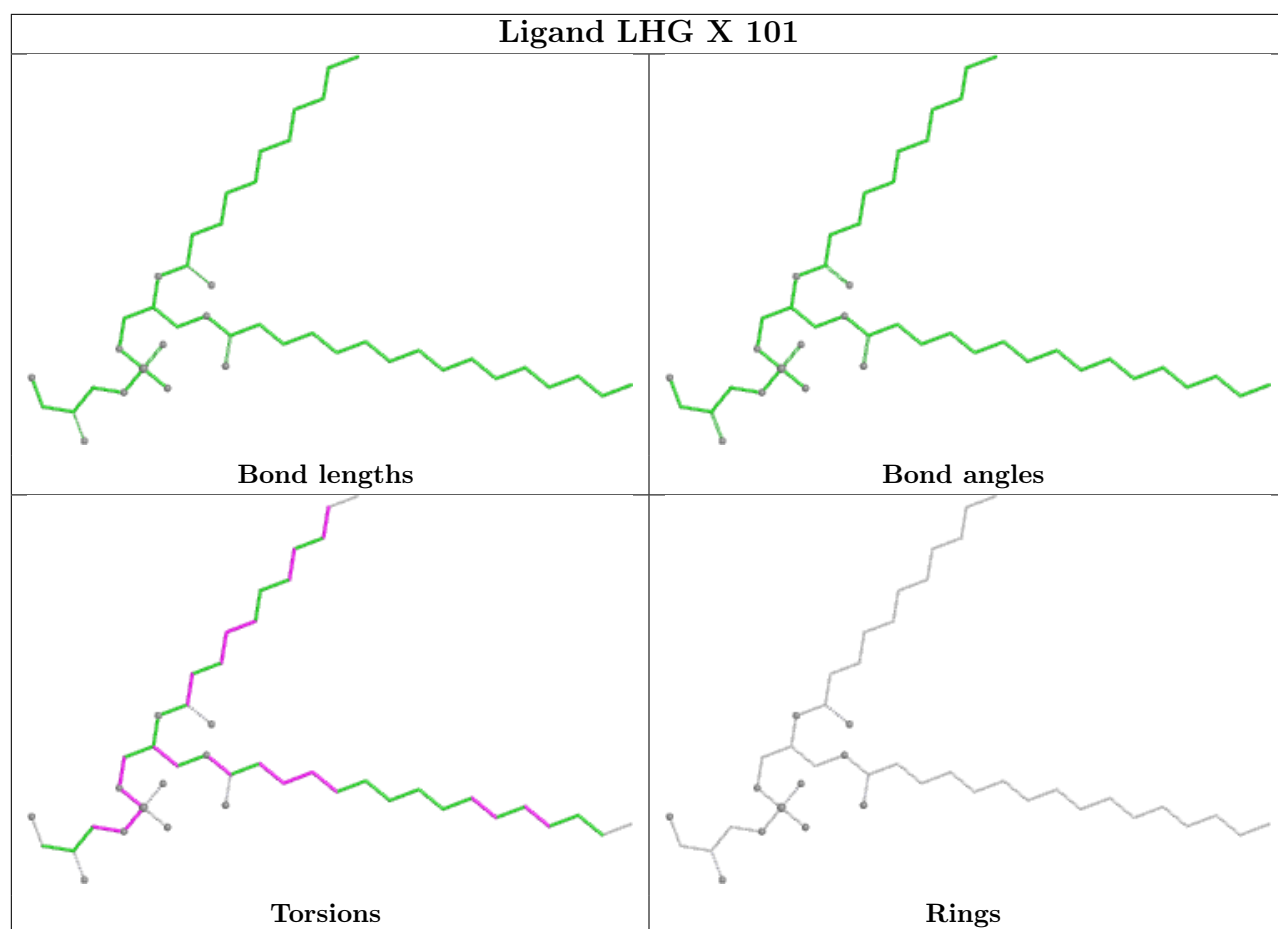


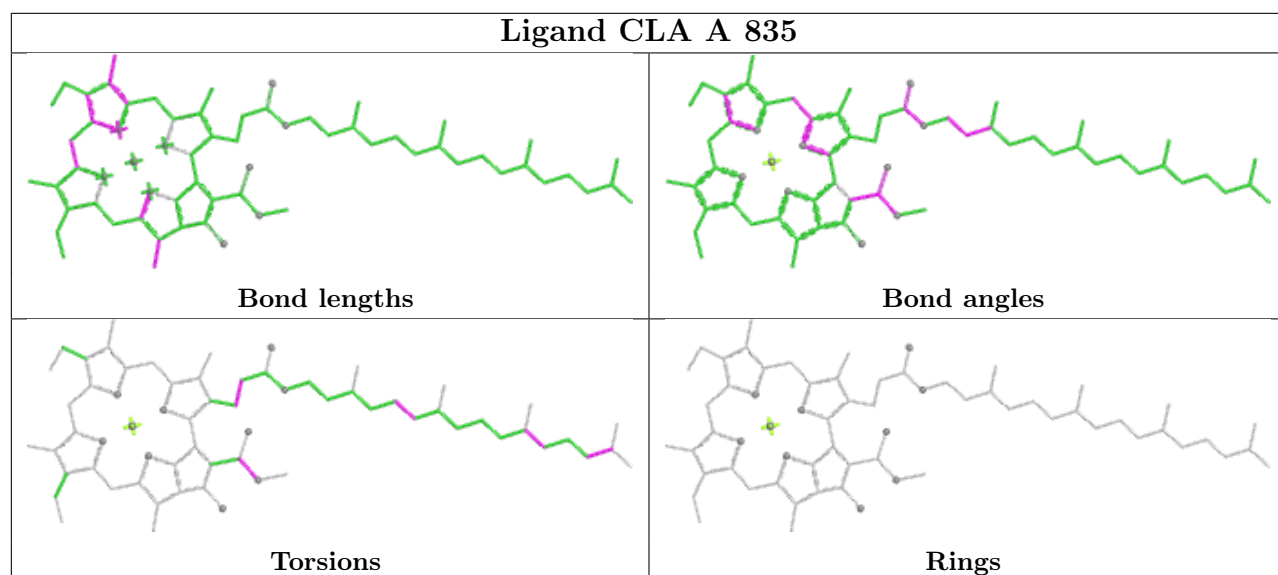
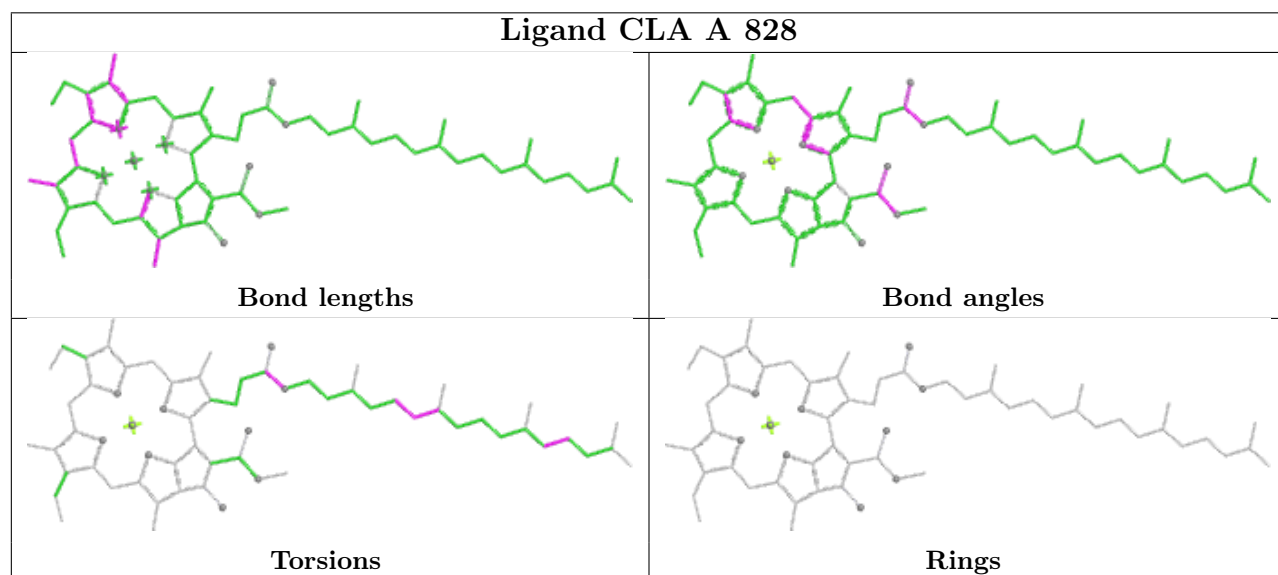
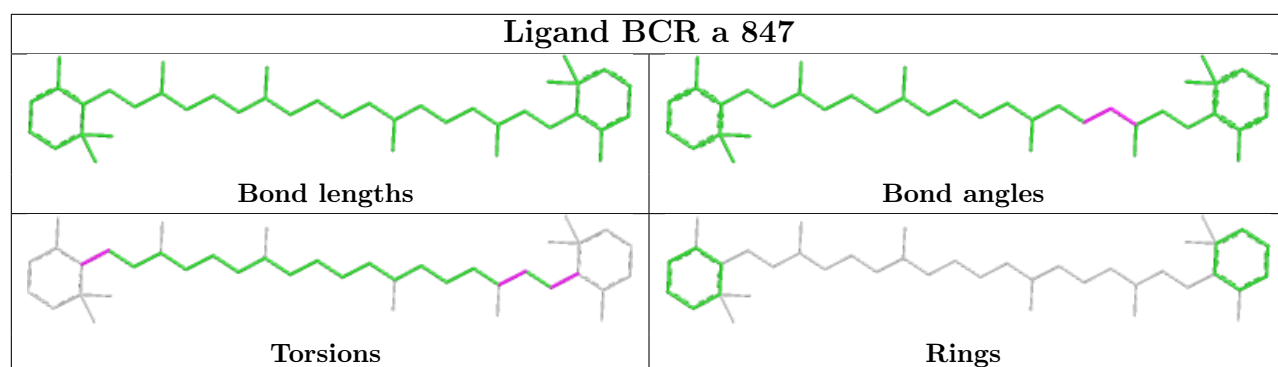
Rings

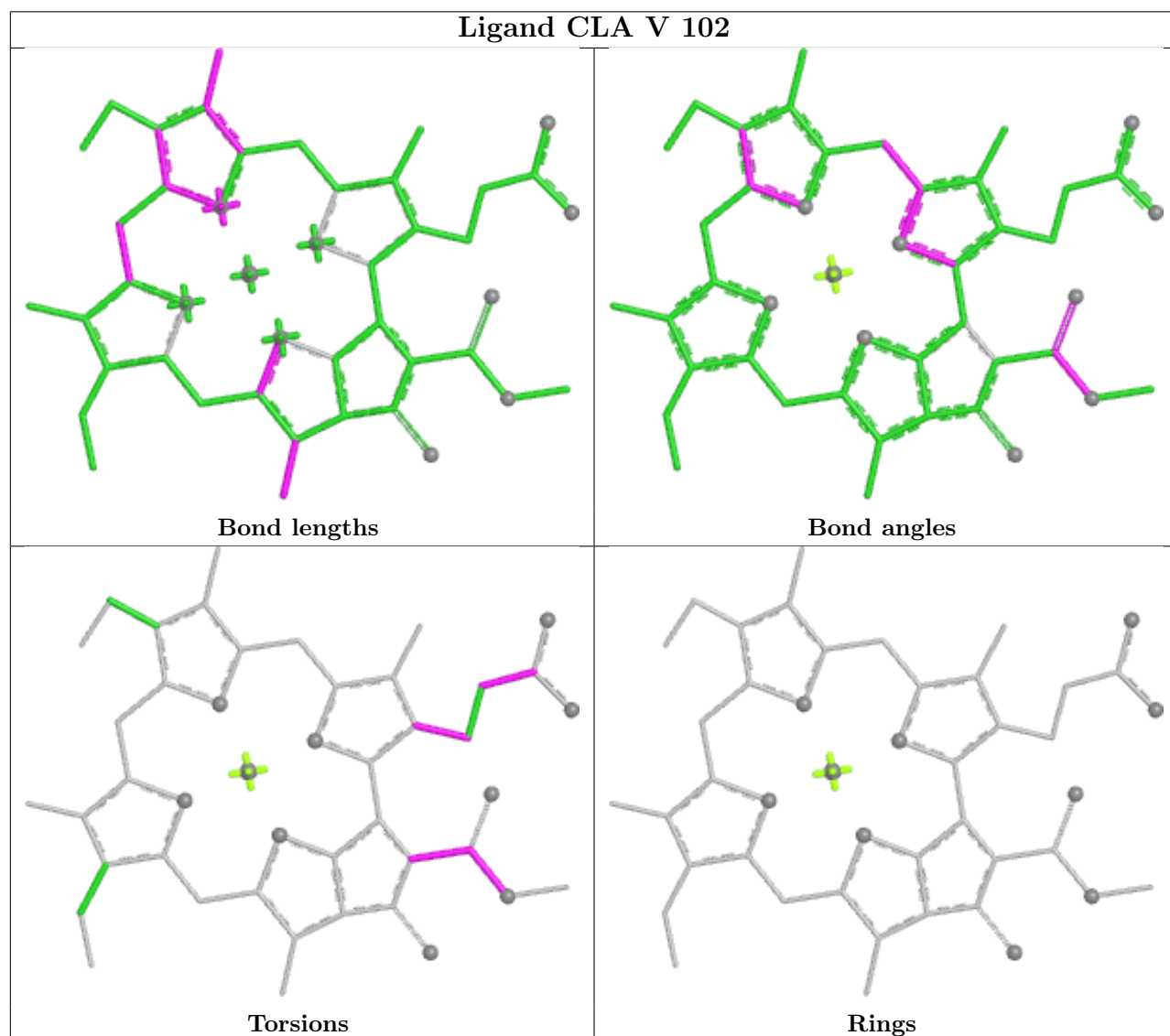
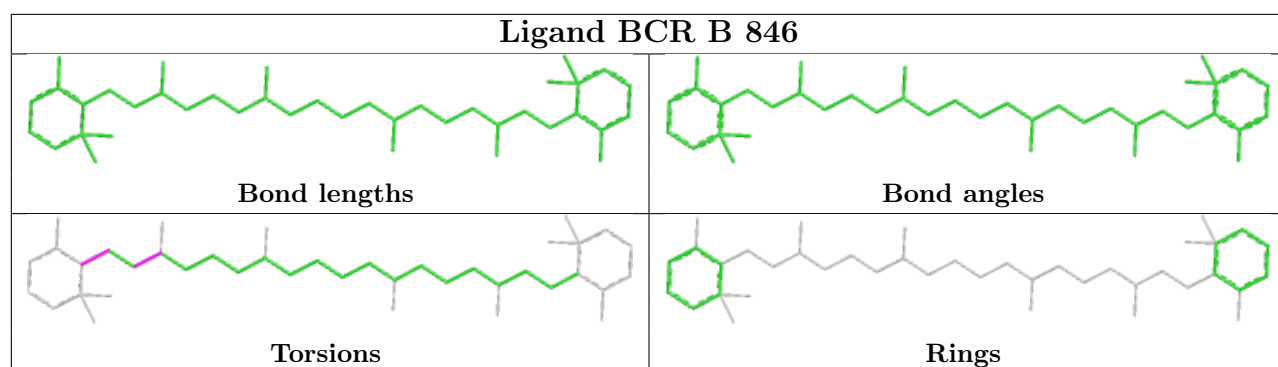


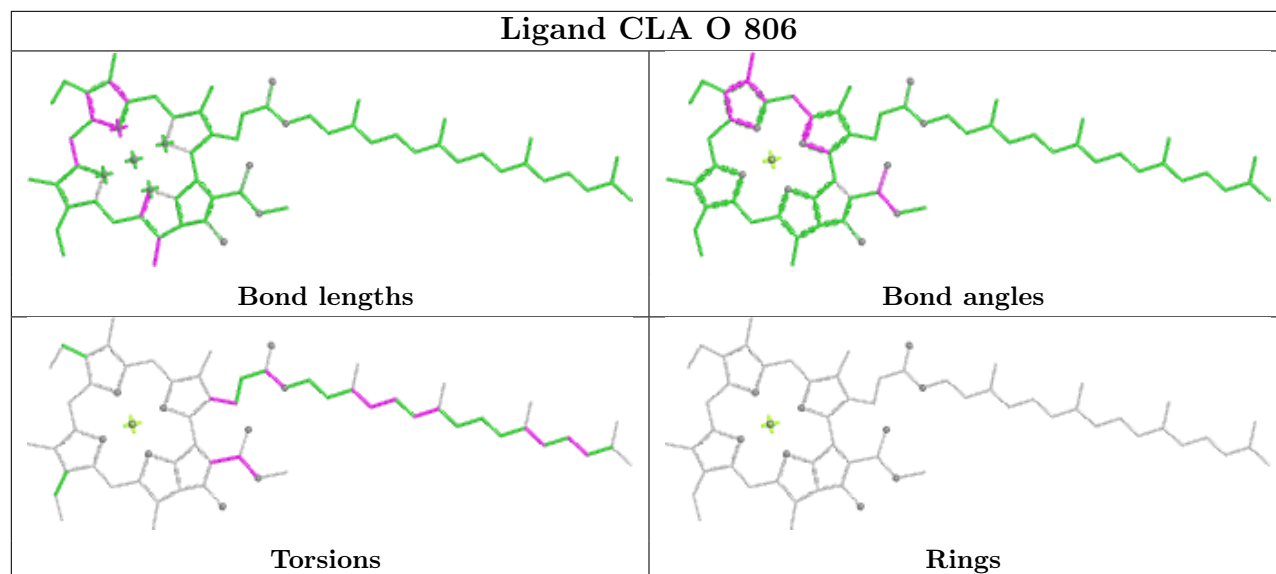
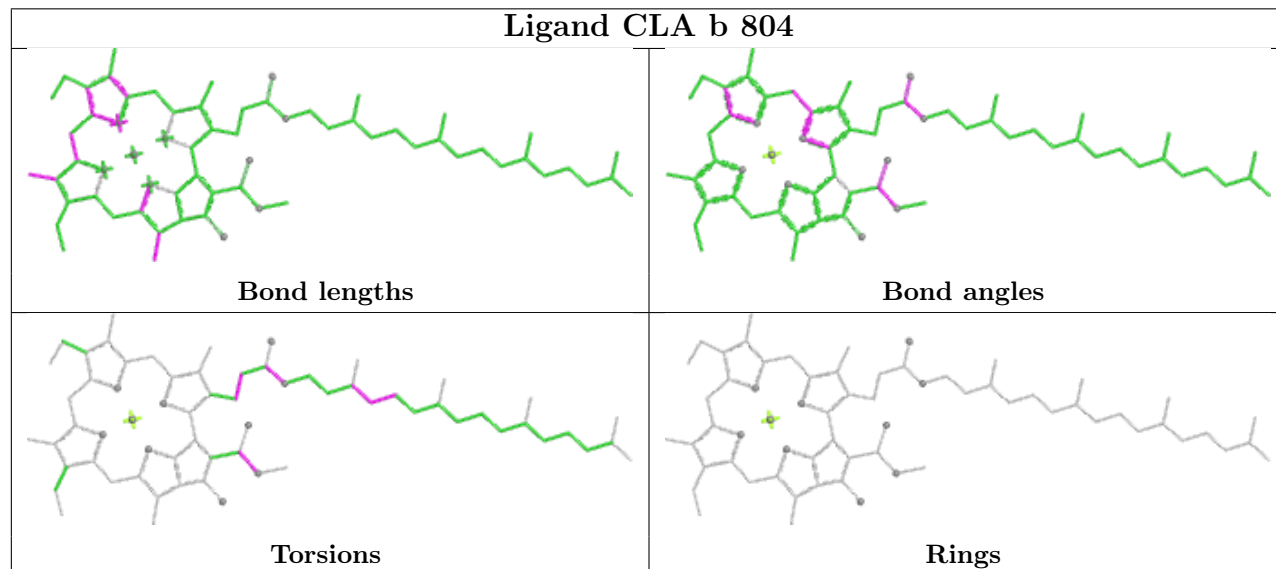
Ligand CLA i 103



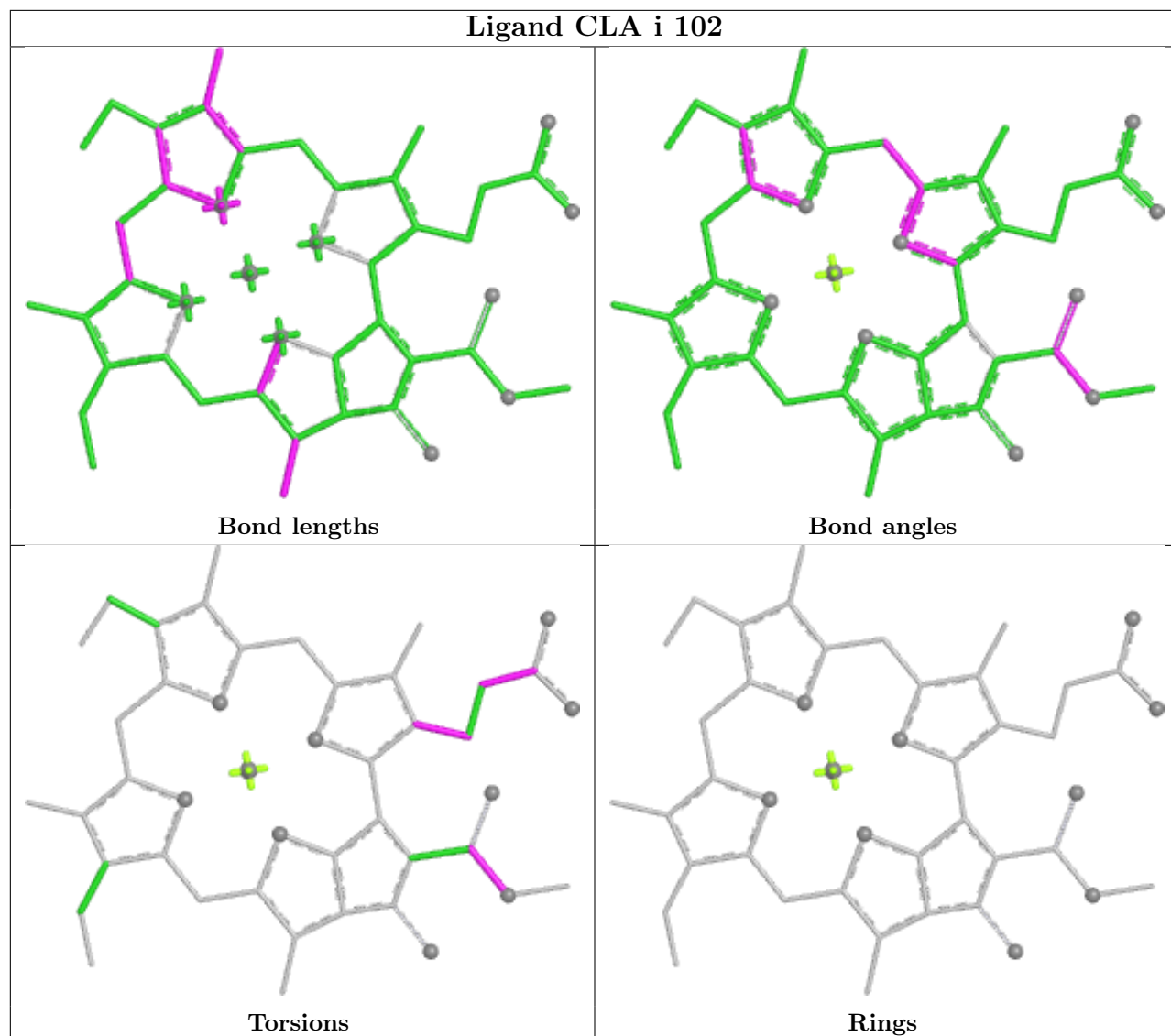




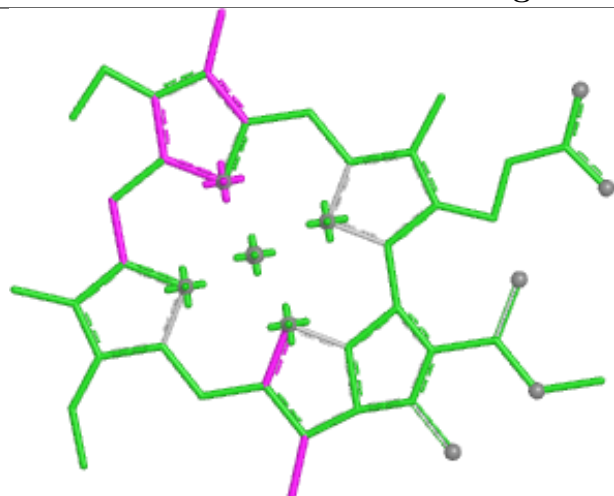


Ligand CLA O 806**Ligand CLA b 804**

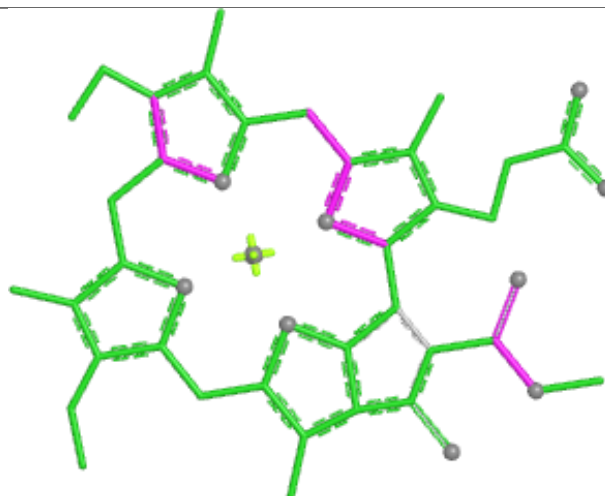
Ligand CLA i 102



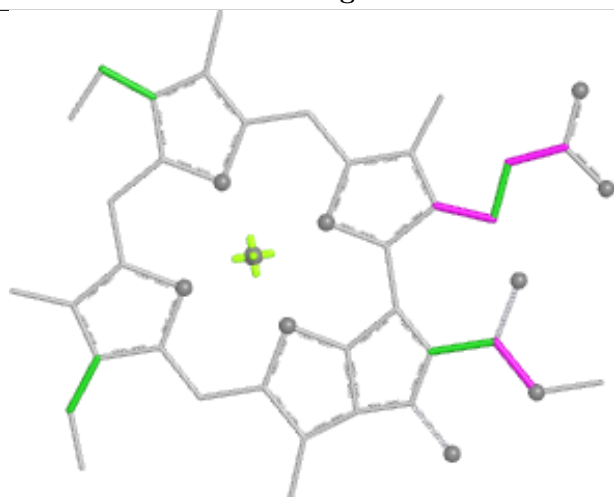
Ligand CLA K 102



Bond lengths



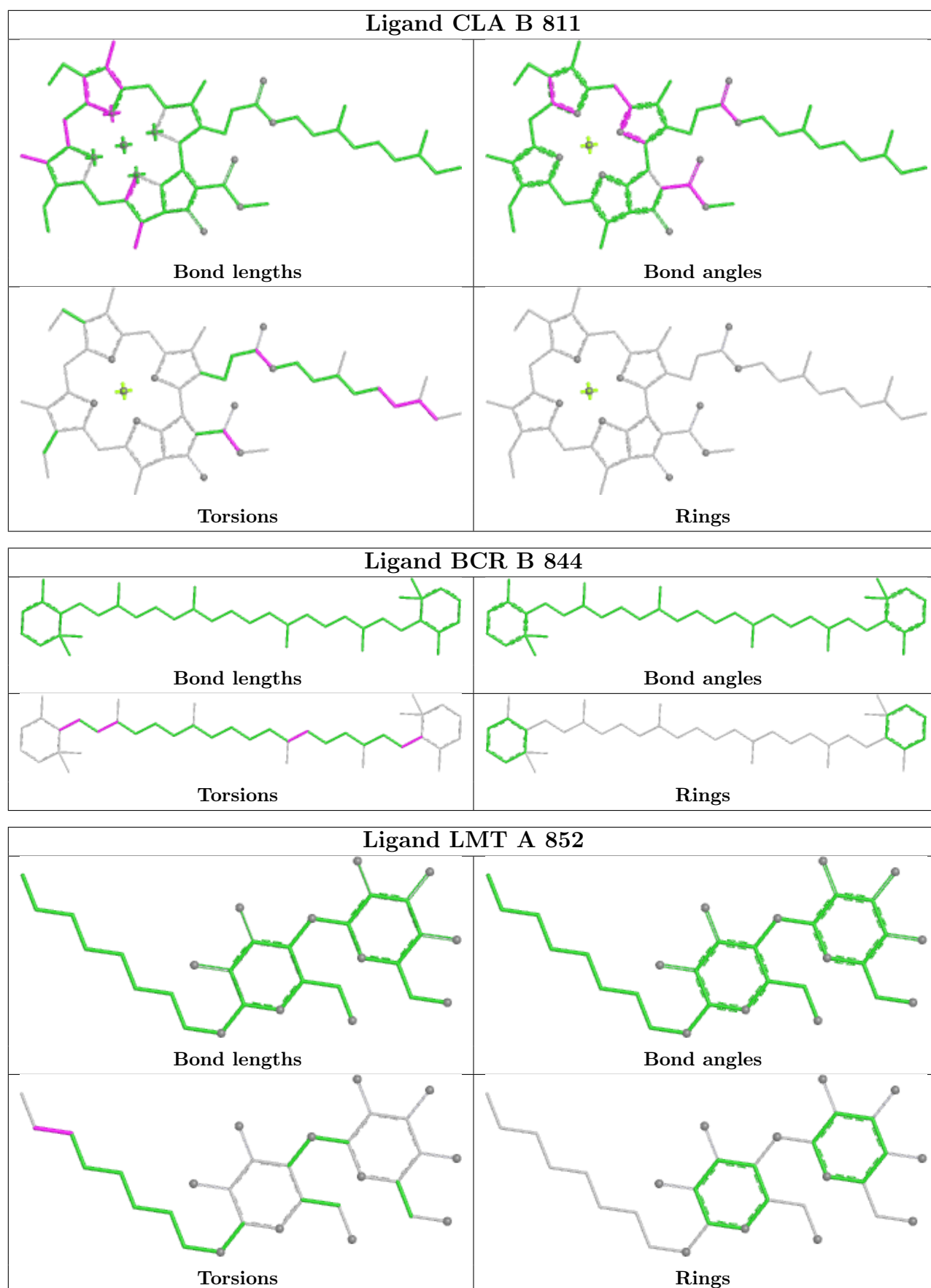
Bond angles



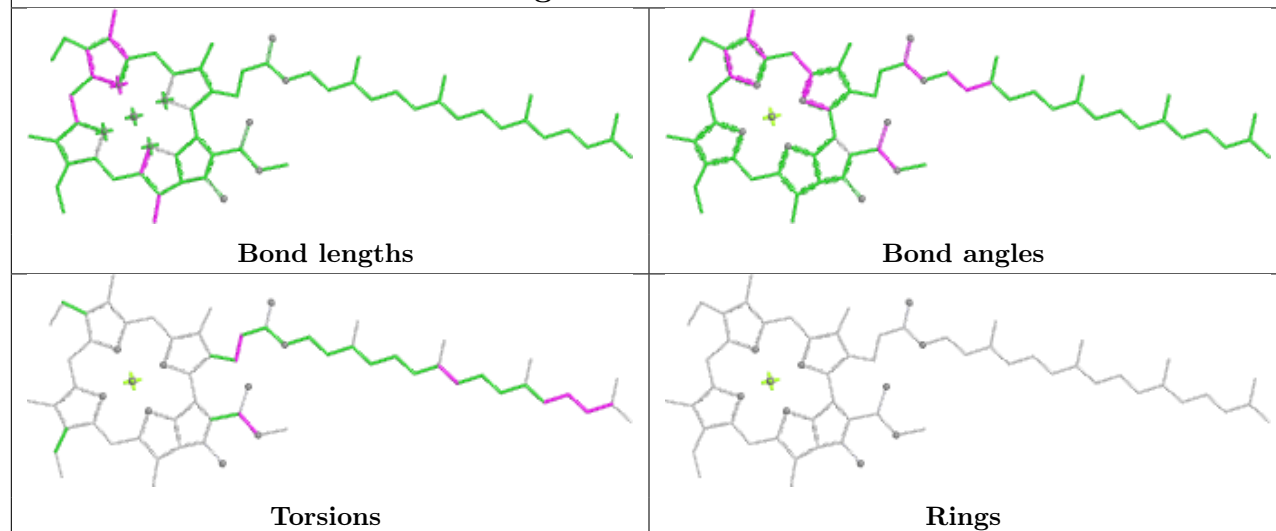
Torsions



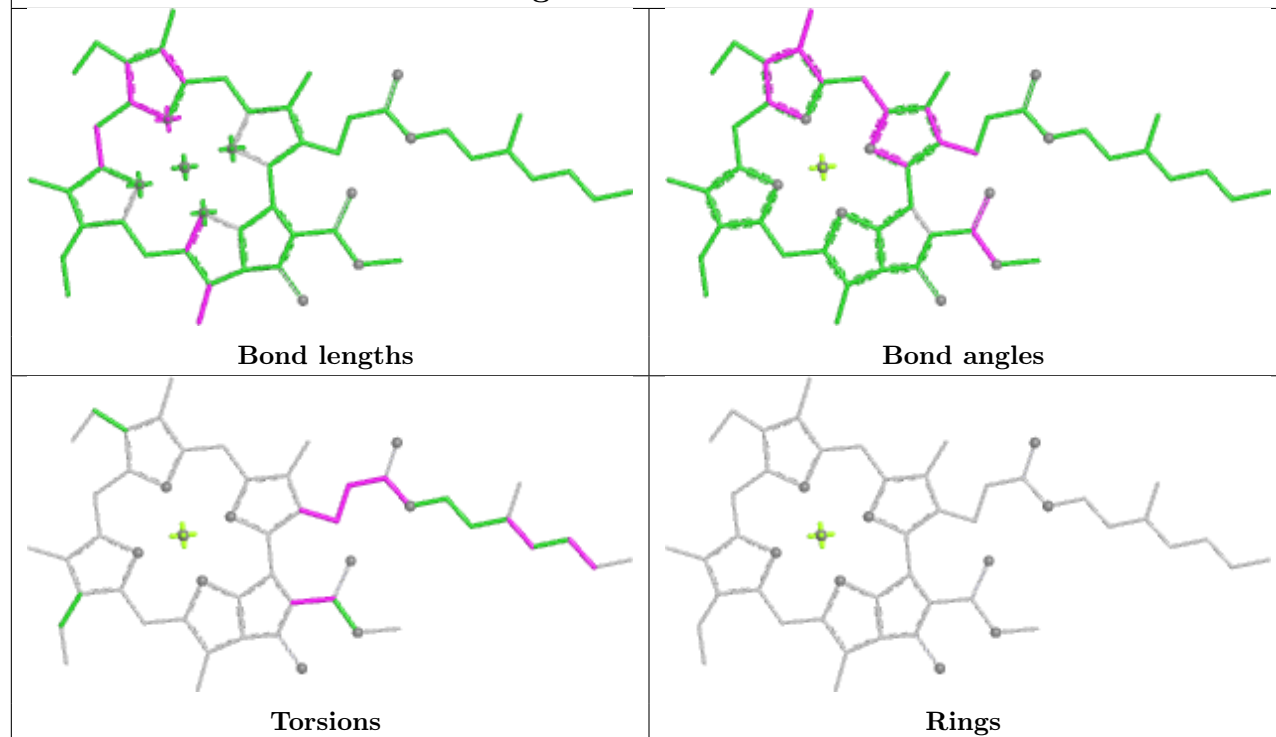
Rings



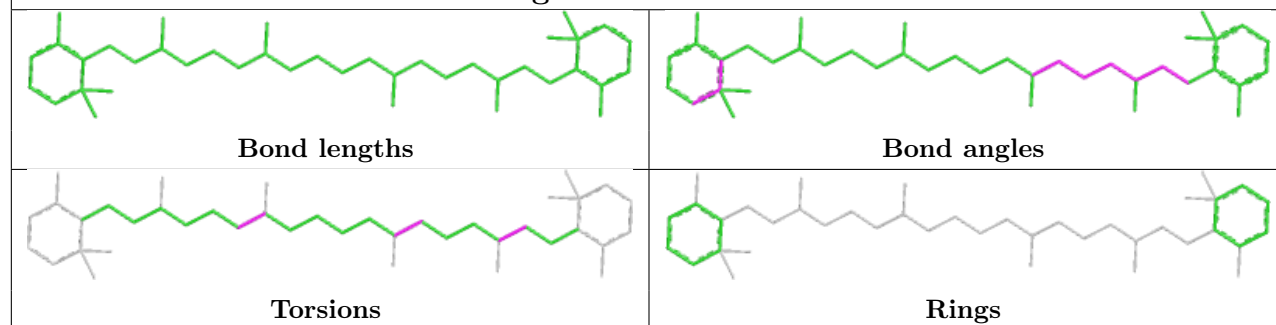
Ligand CLA L 202

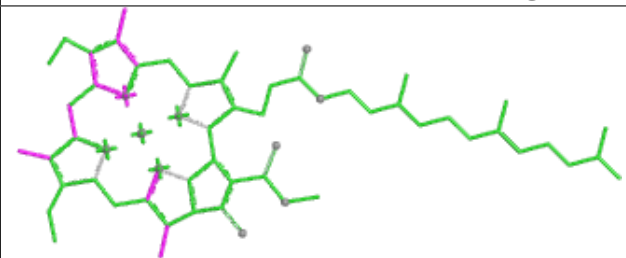
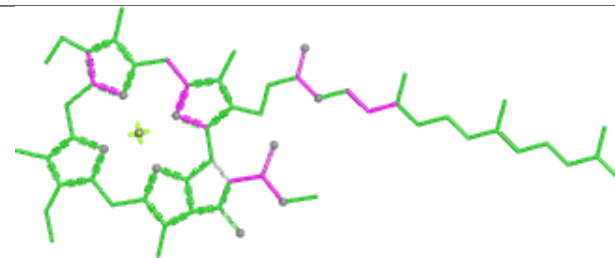
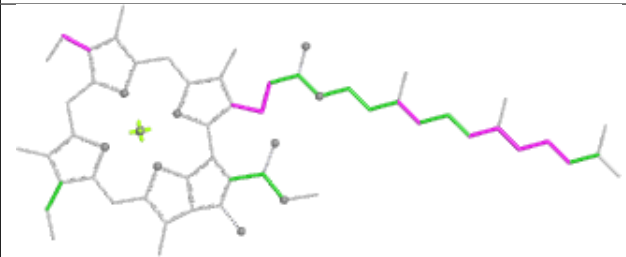
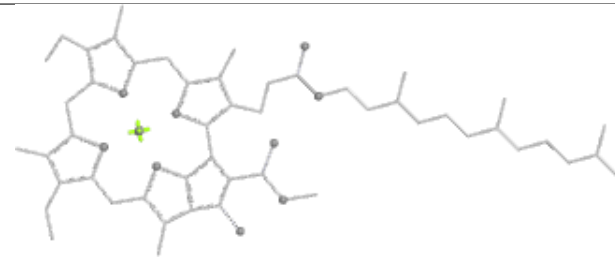


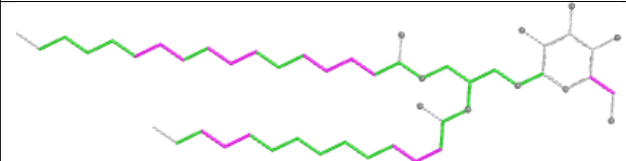
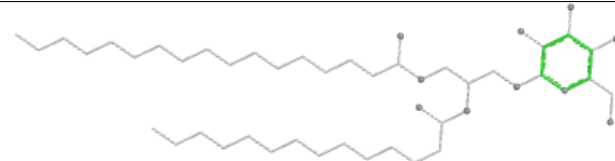
Ligand CLA B 820

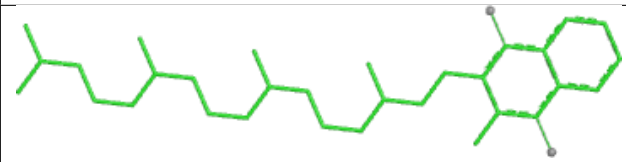
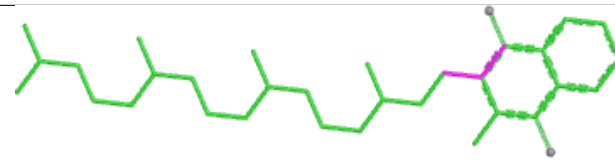
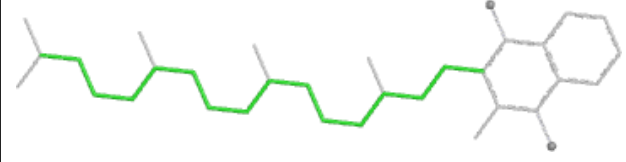
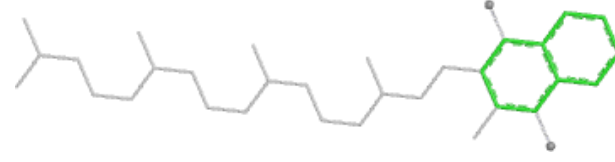


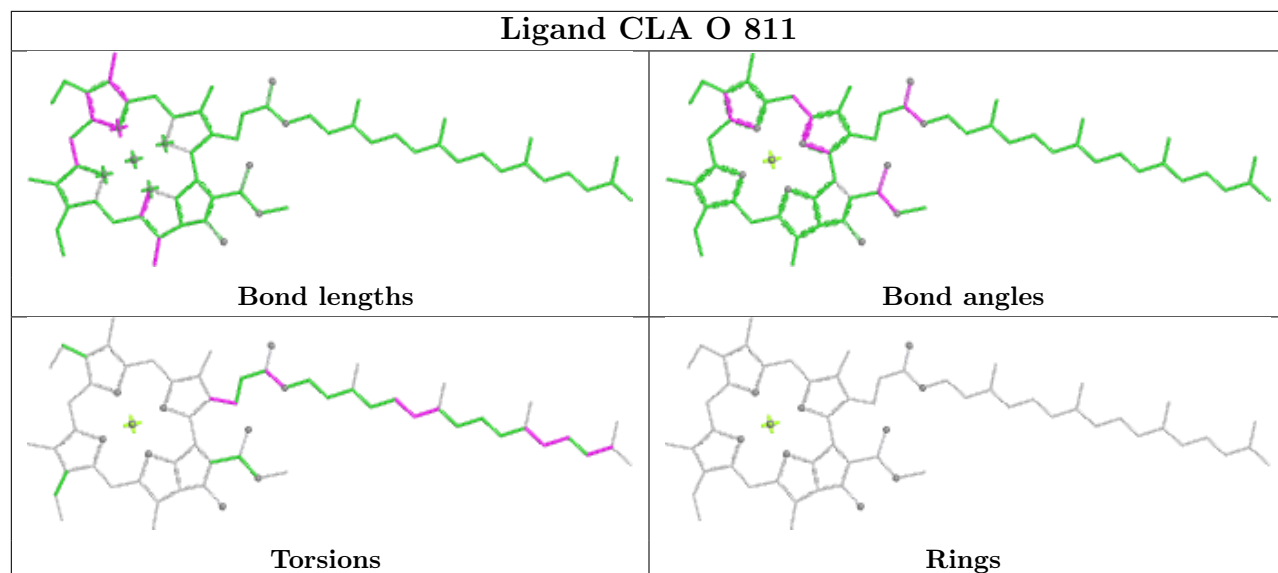
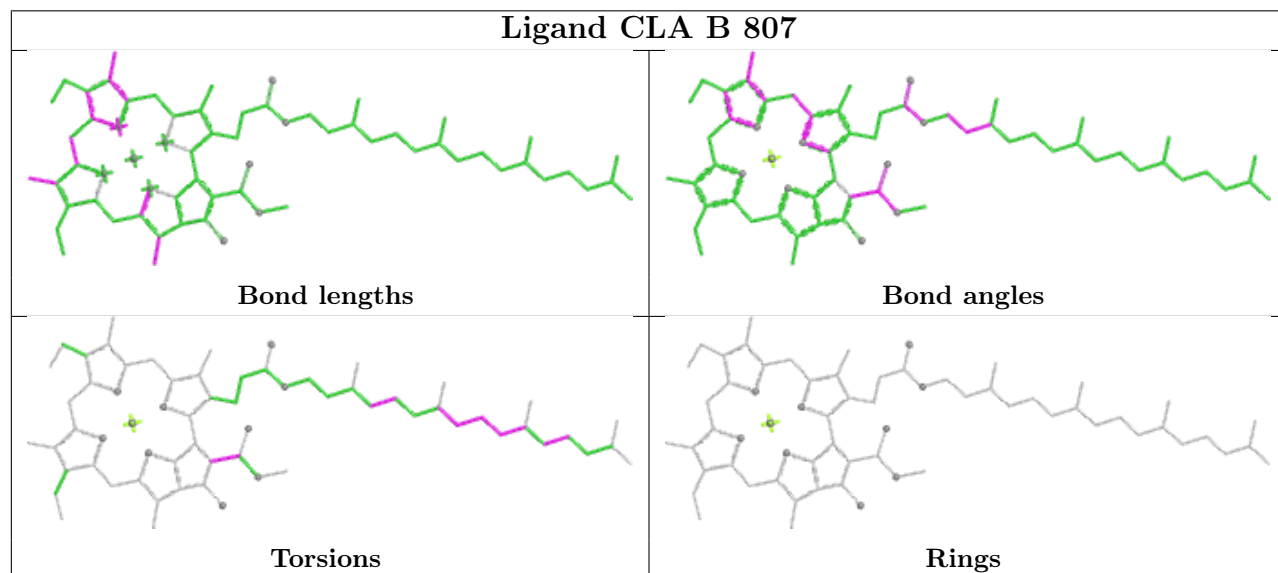
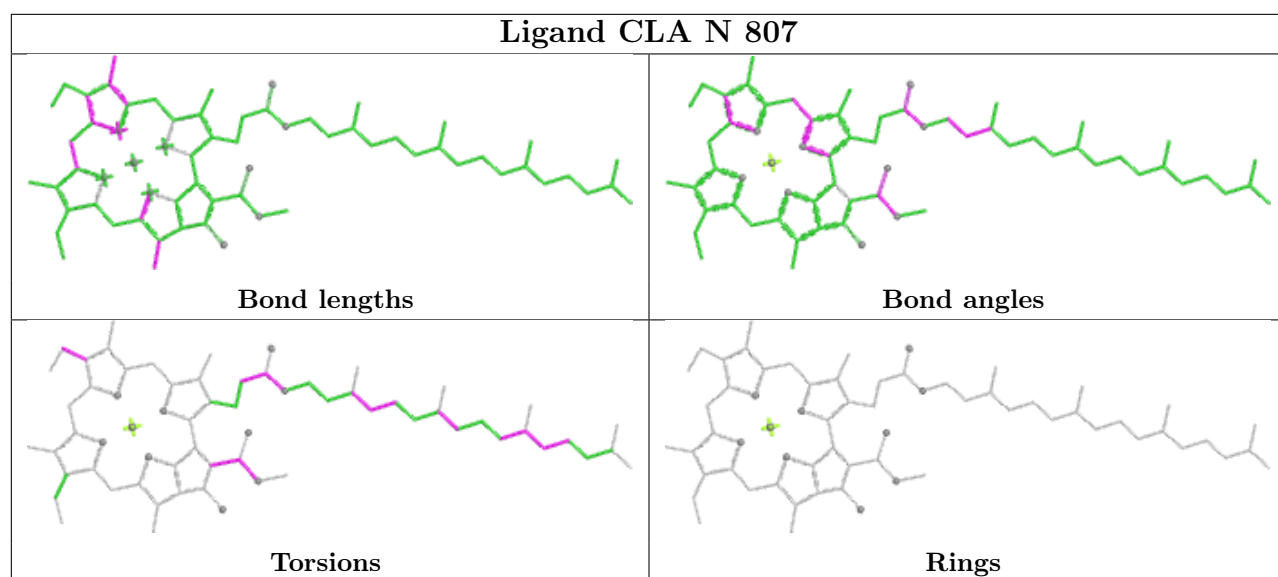
Ligand BCR F 202

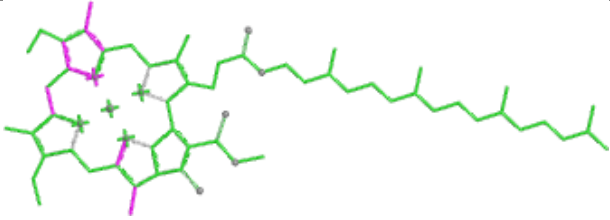
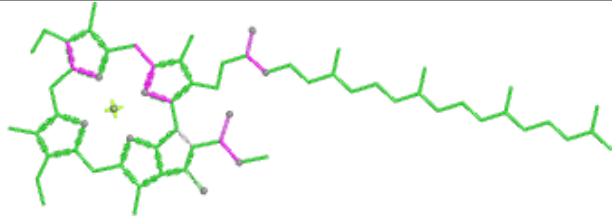
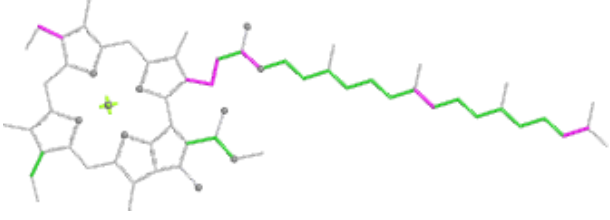
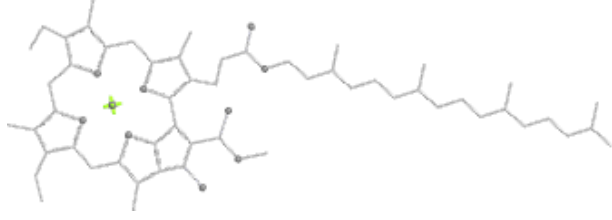
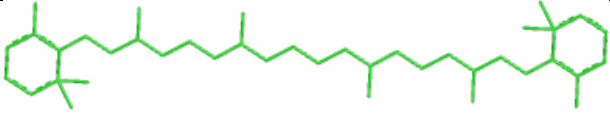
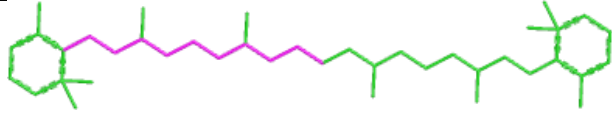
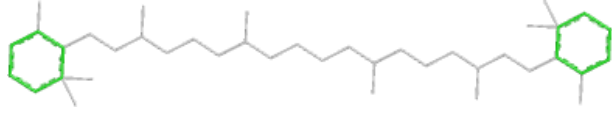
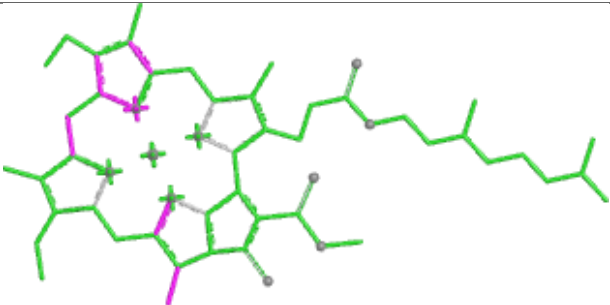
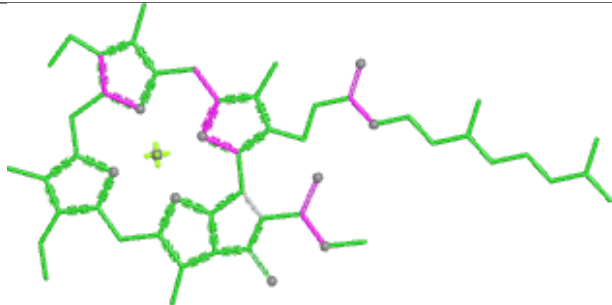
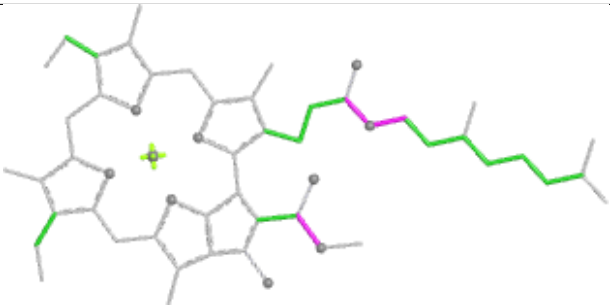
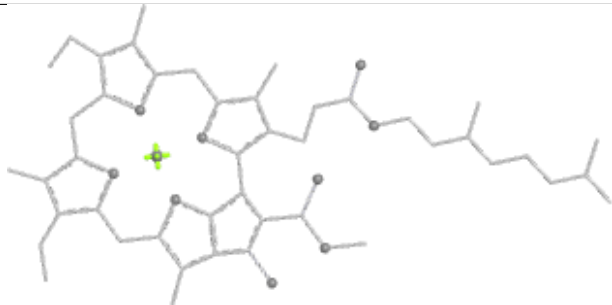


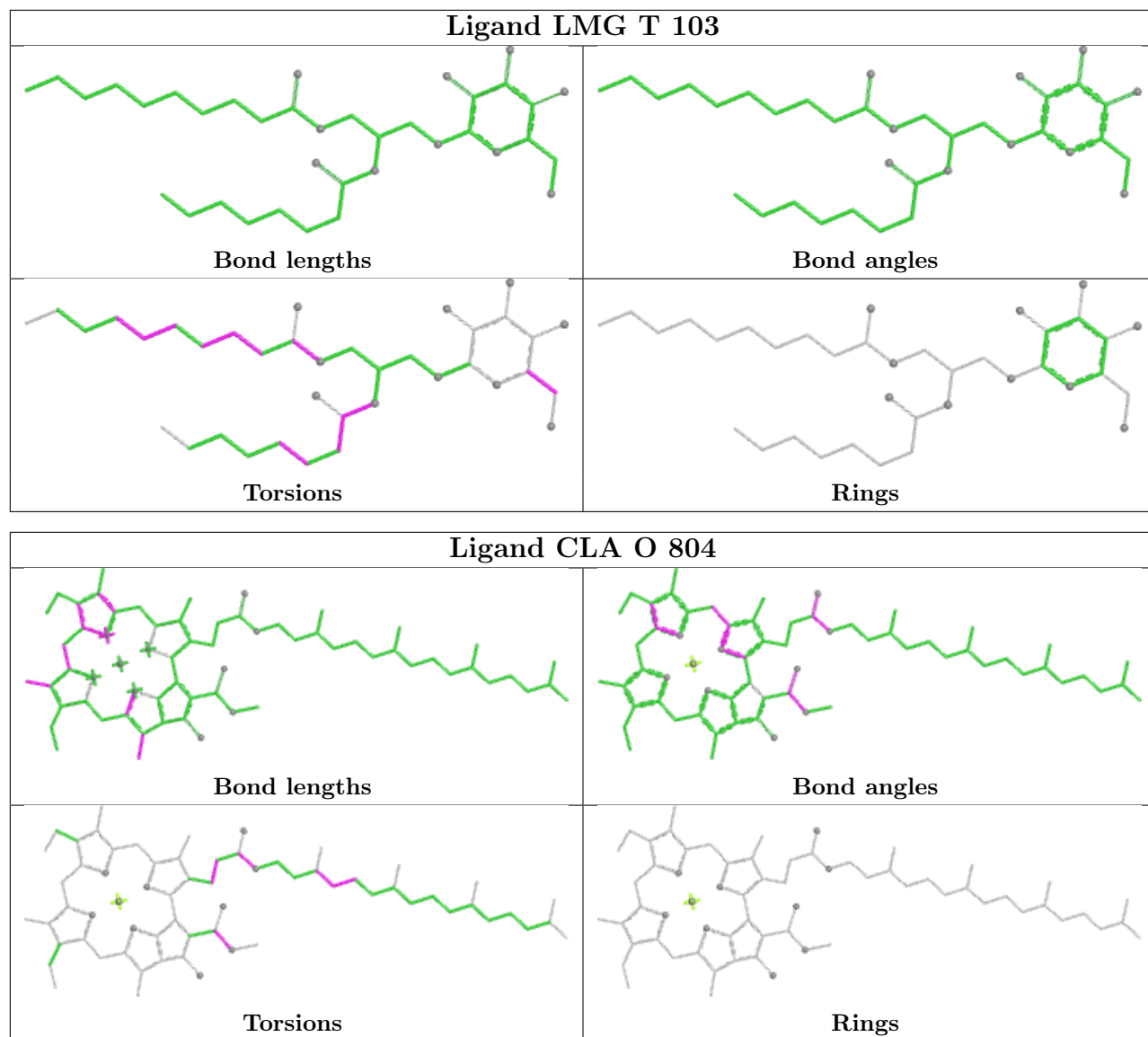
Ligand CLA L 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

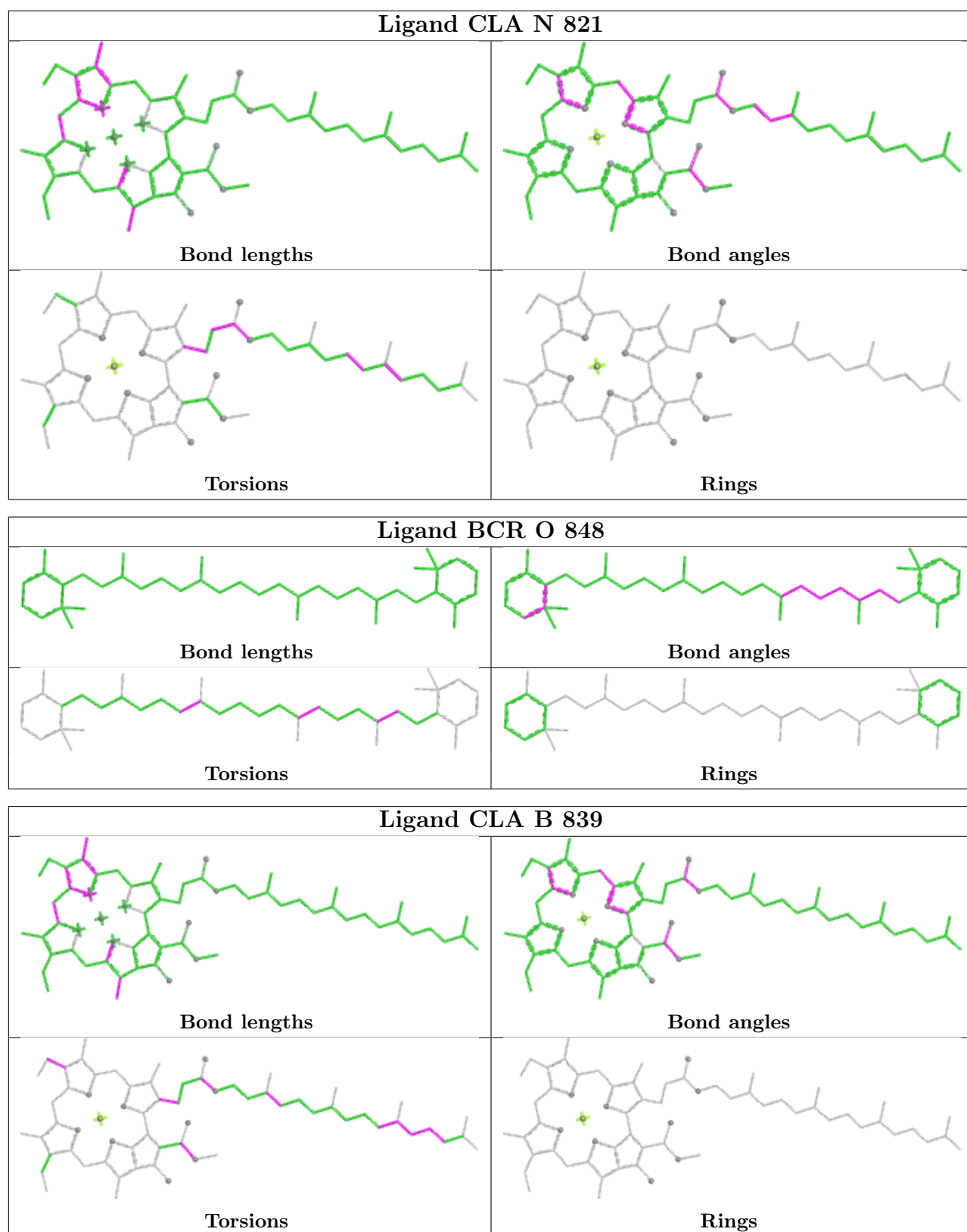
Ligand LMG L 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

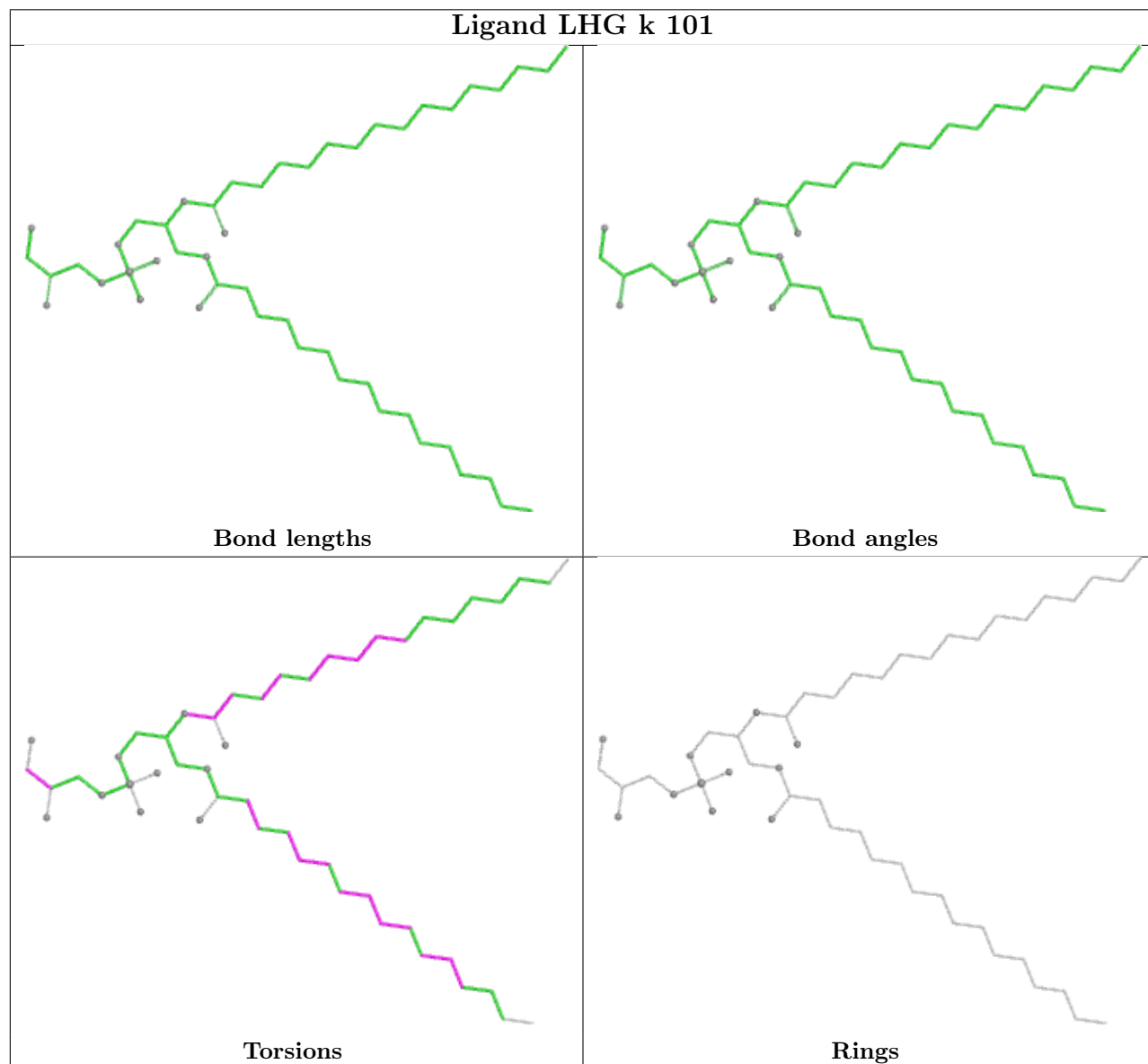
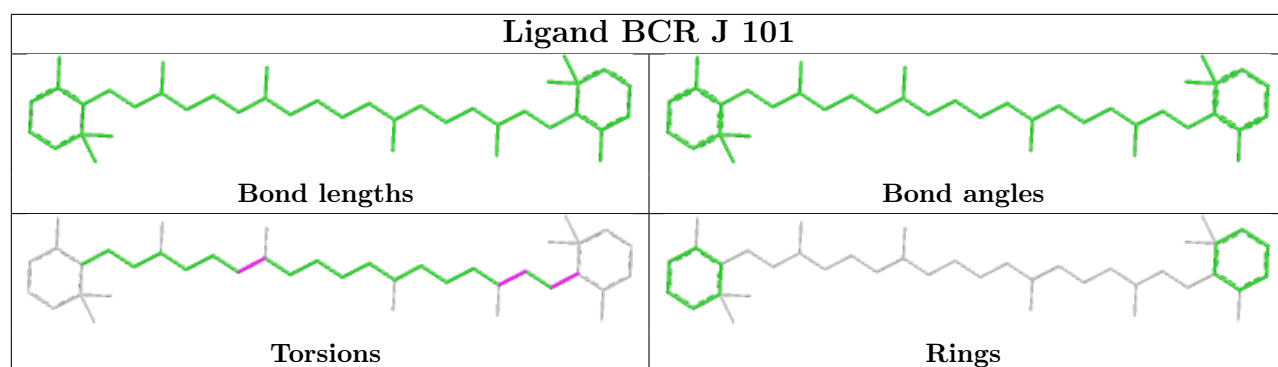
Ligand PQN b 842	
	
Bond lengths	Bond angles
	
Torsions	Rings



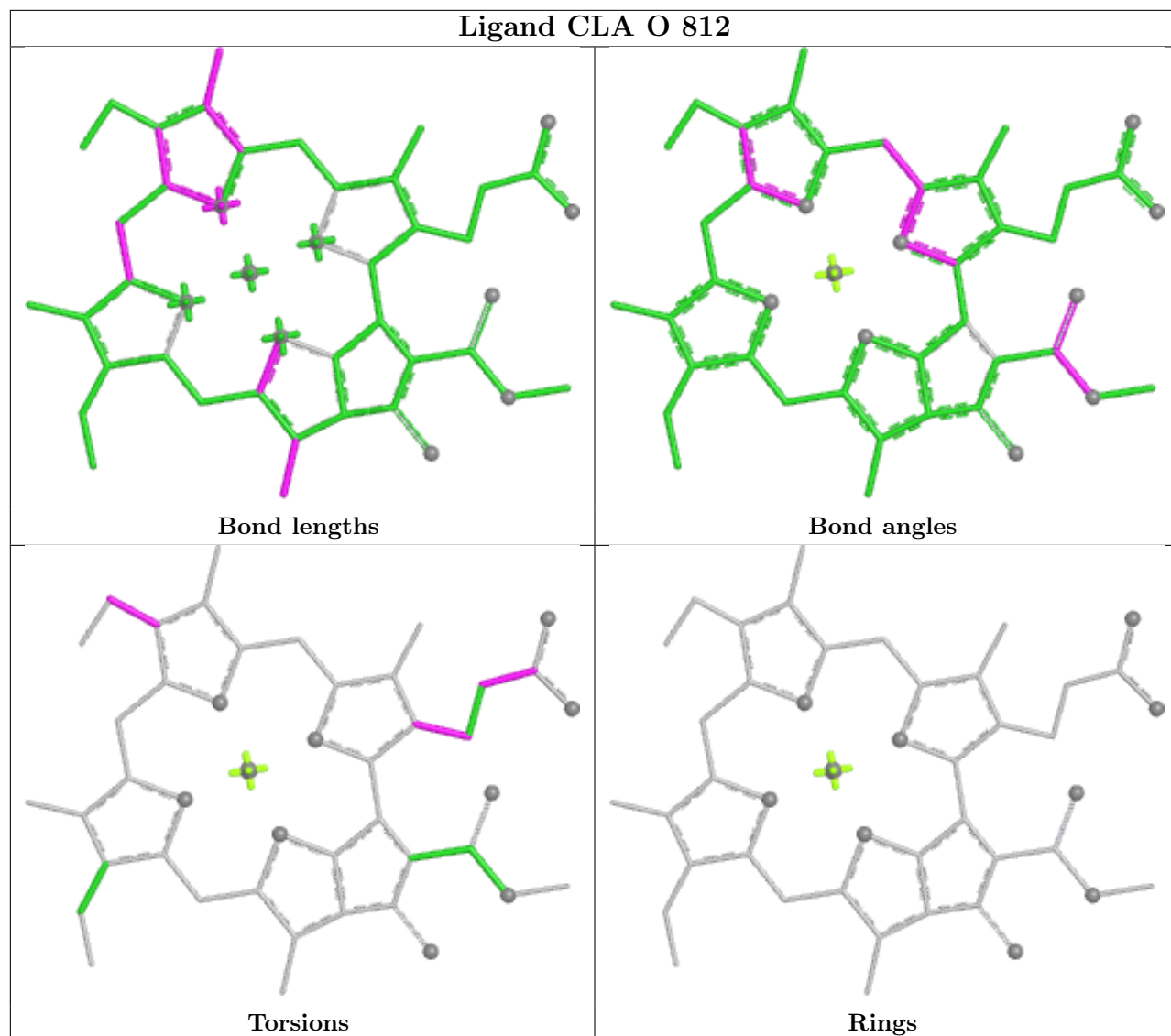
Ligand CLA A 842	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR N 857	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Z 103	
 Bond lengths	 Bond angles
 Torsions	 Rings



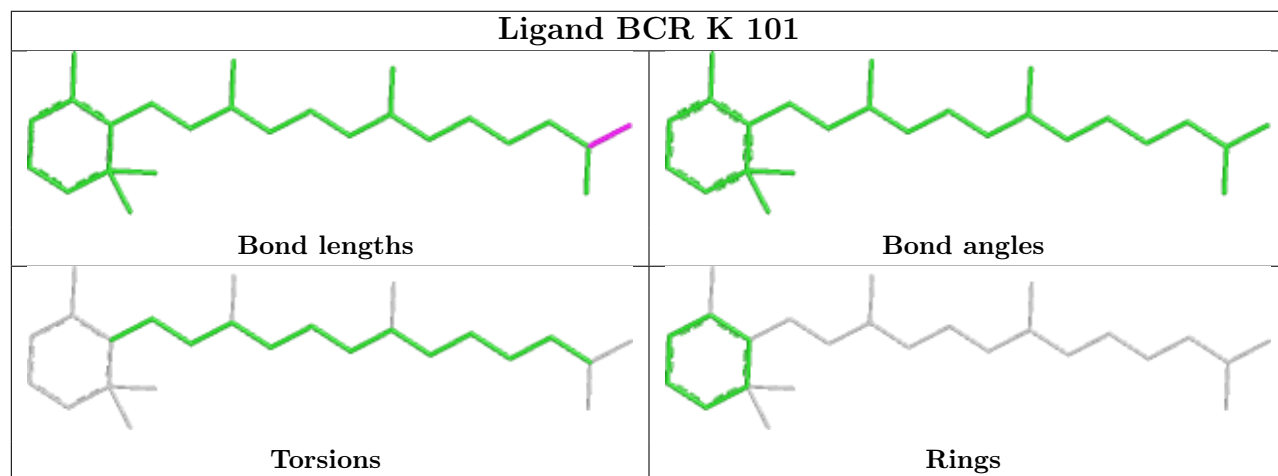


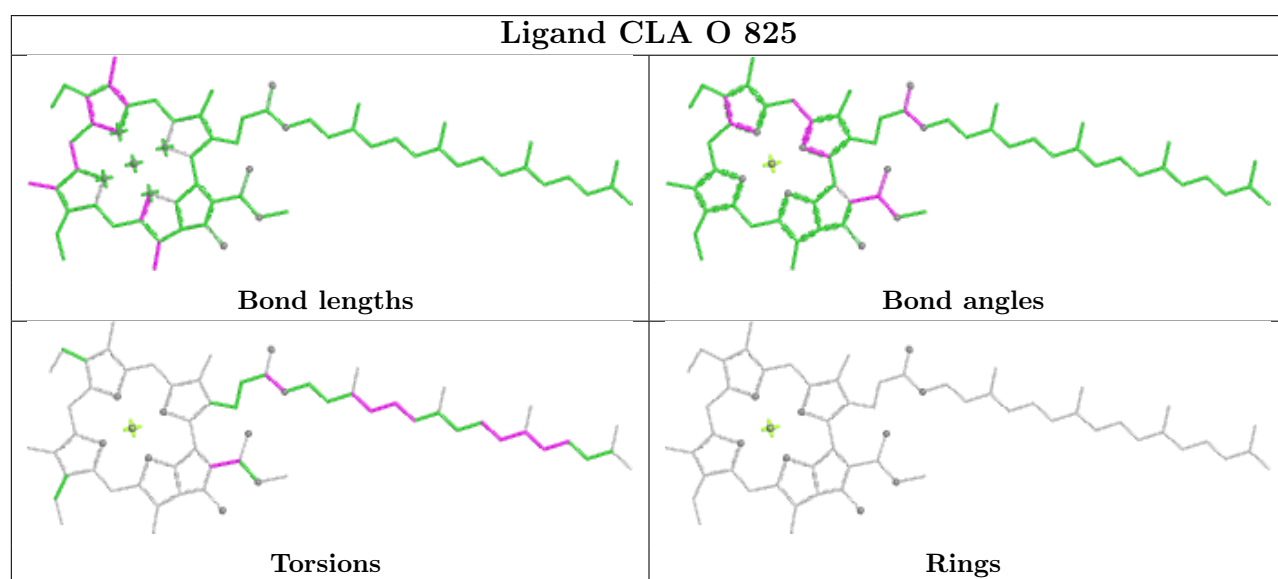
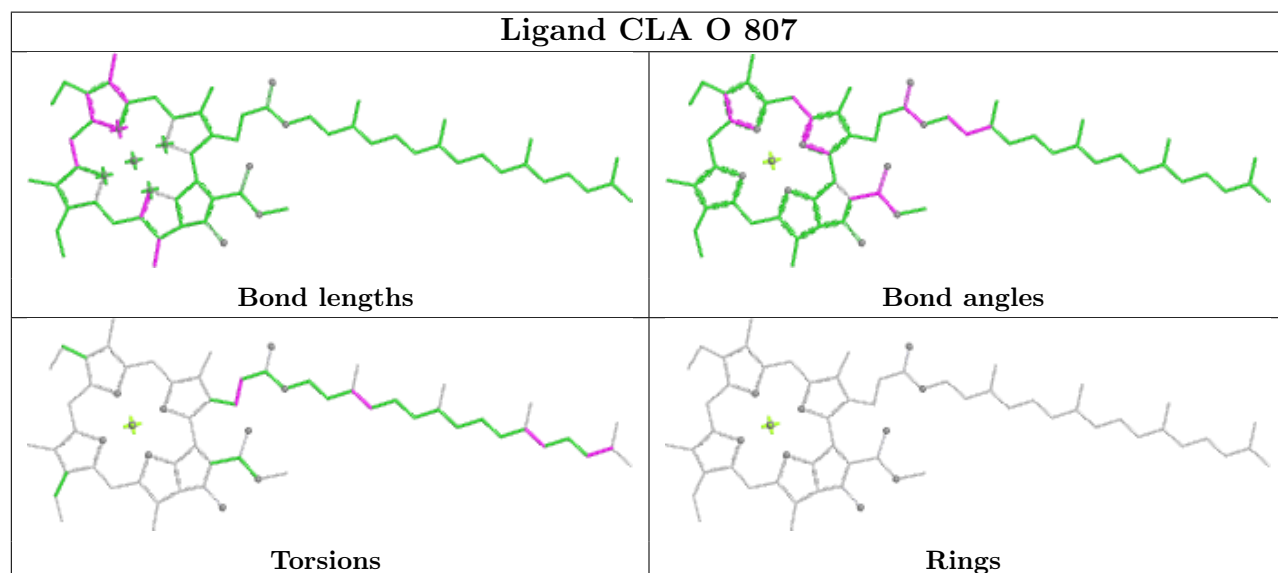
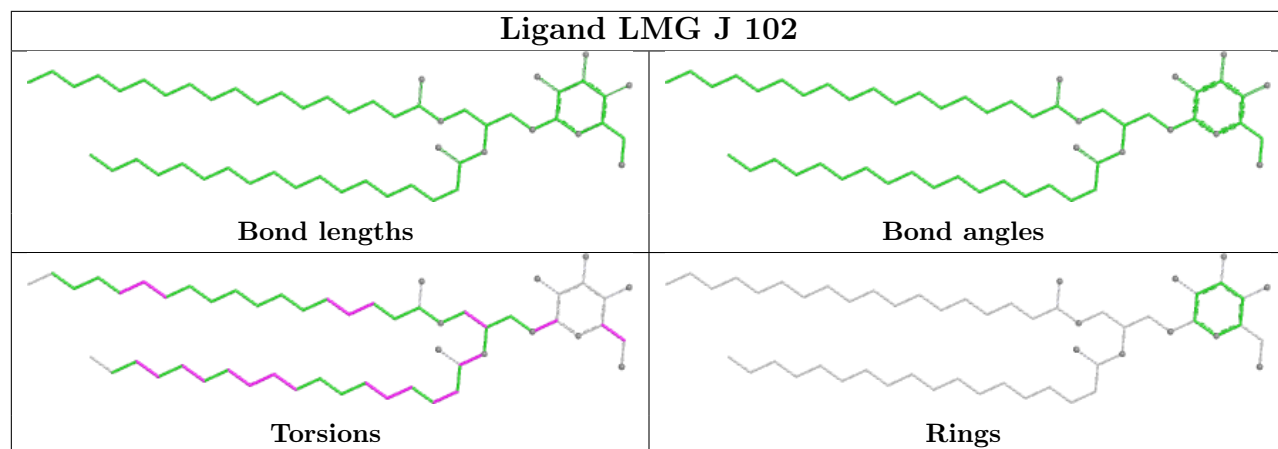


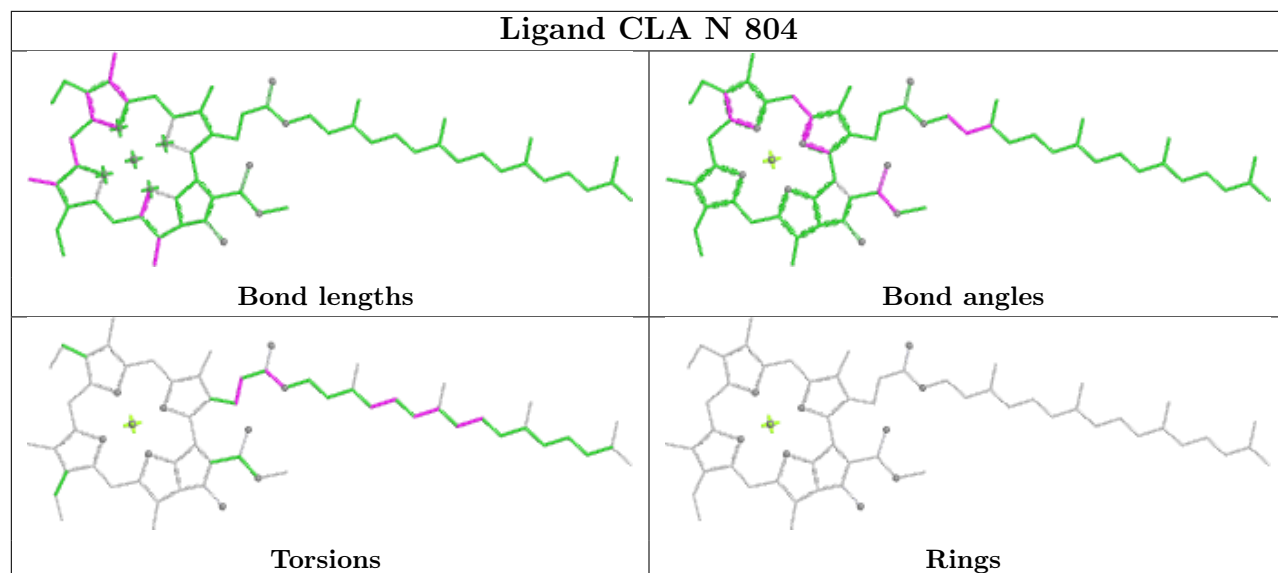
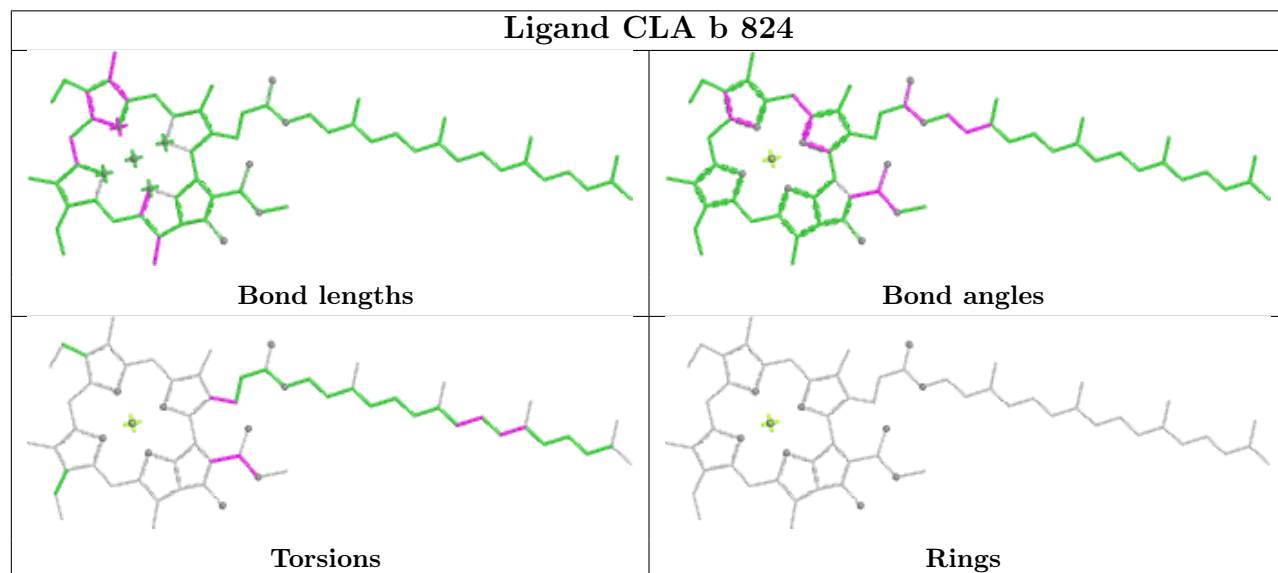
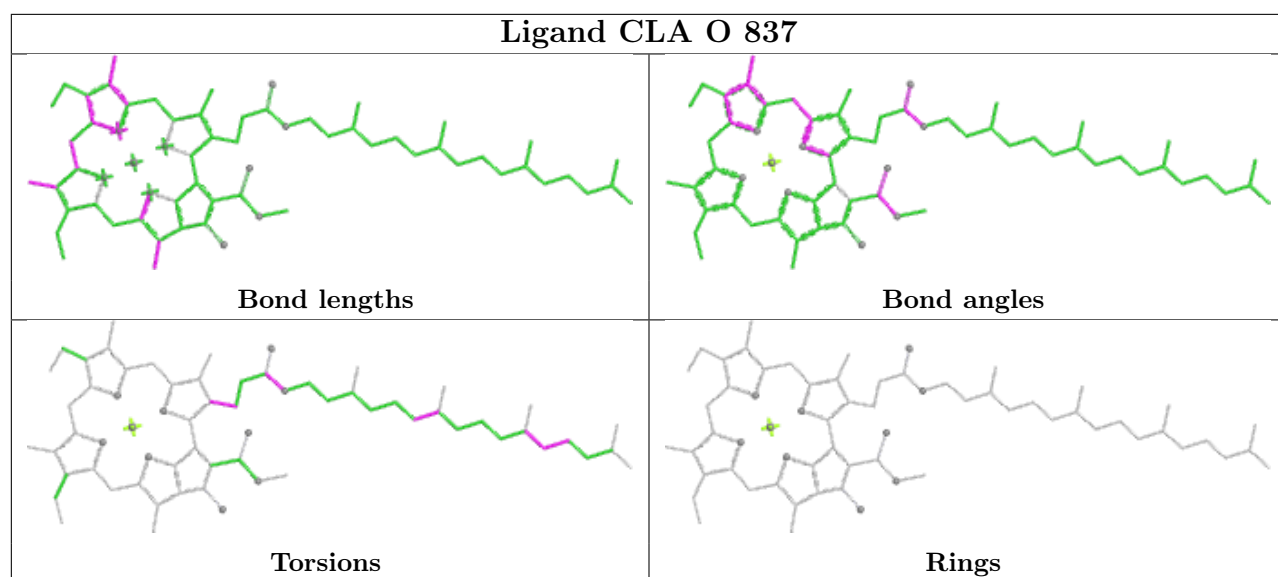
Ligand CLA O 812



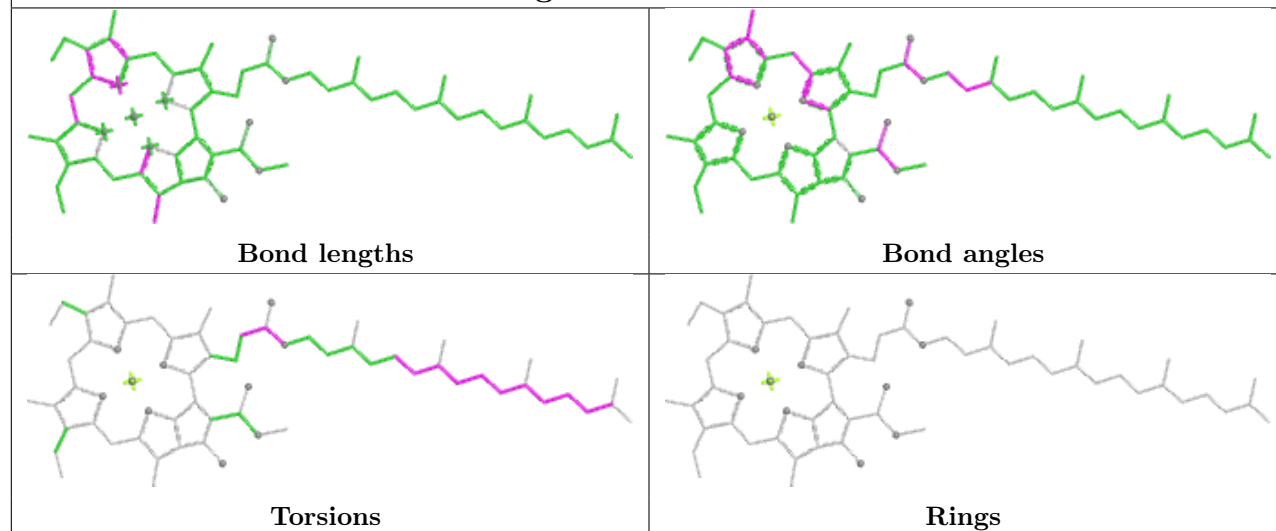
Ligand BCR K 101



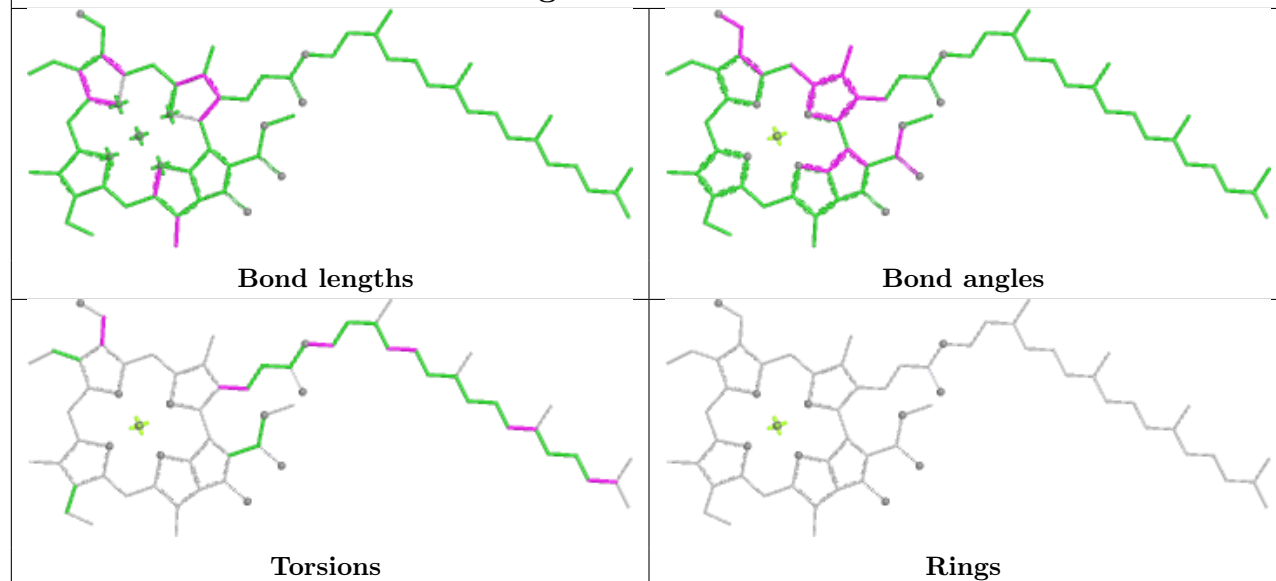




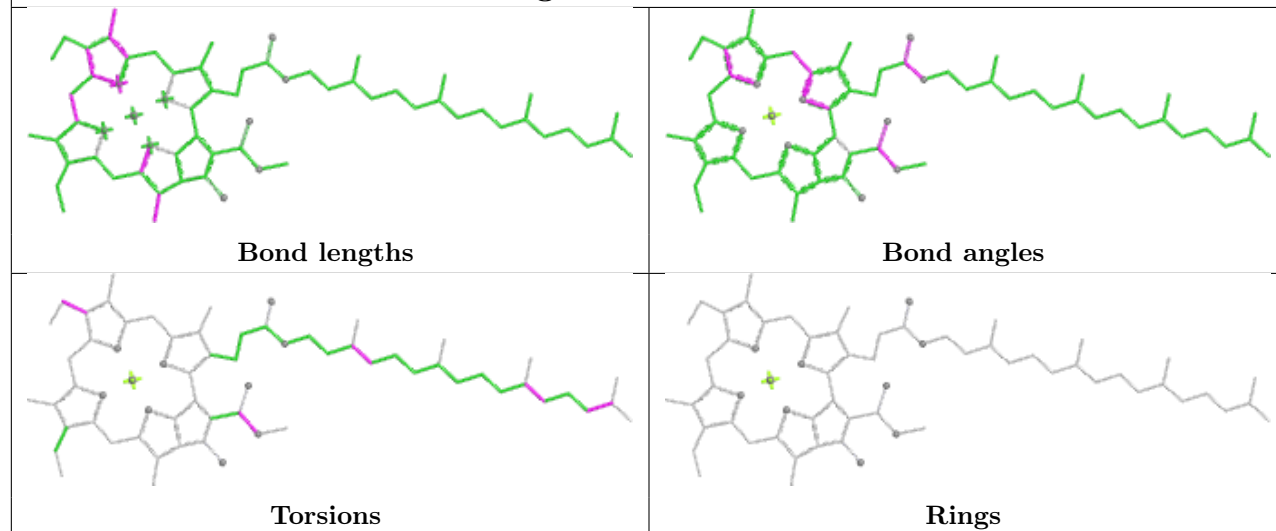
Ligand CLA b 838

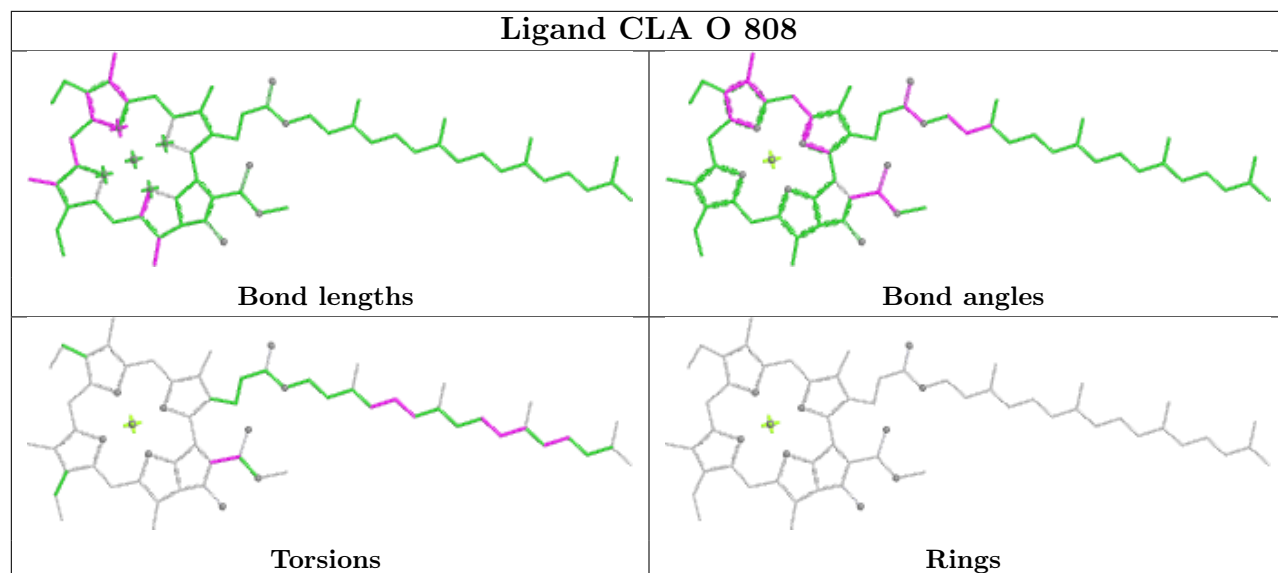
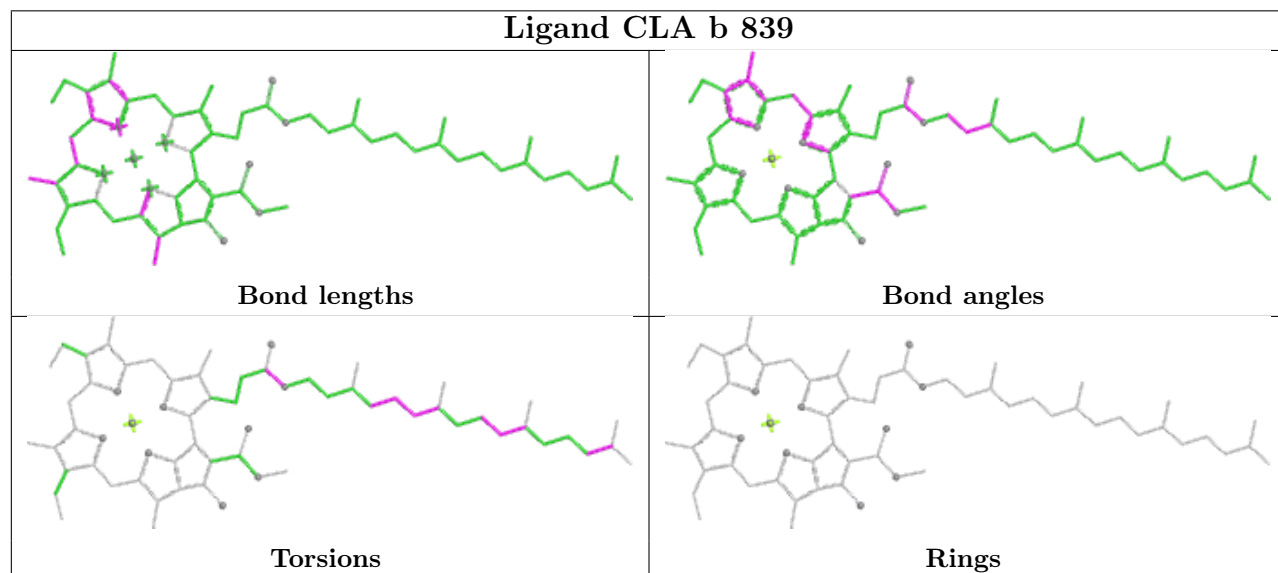
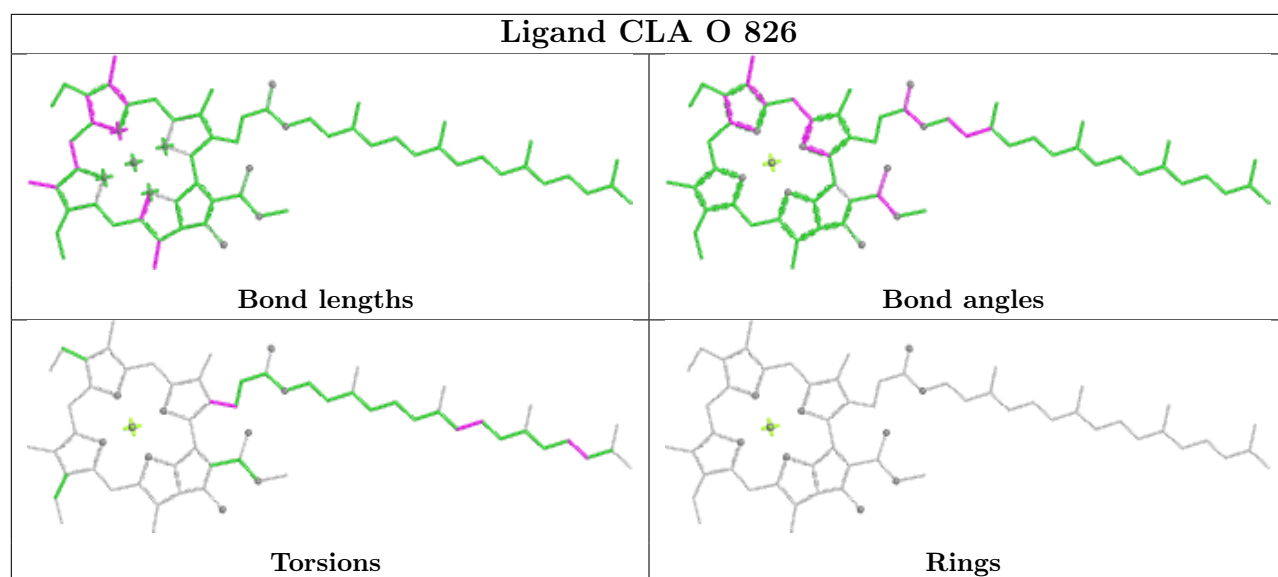


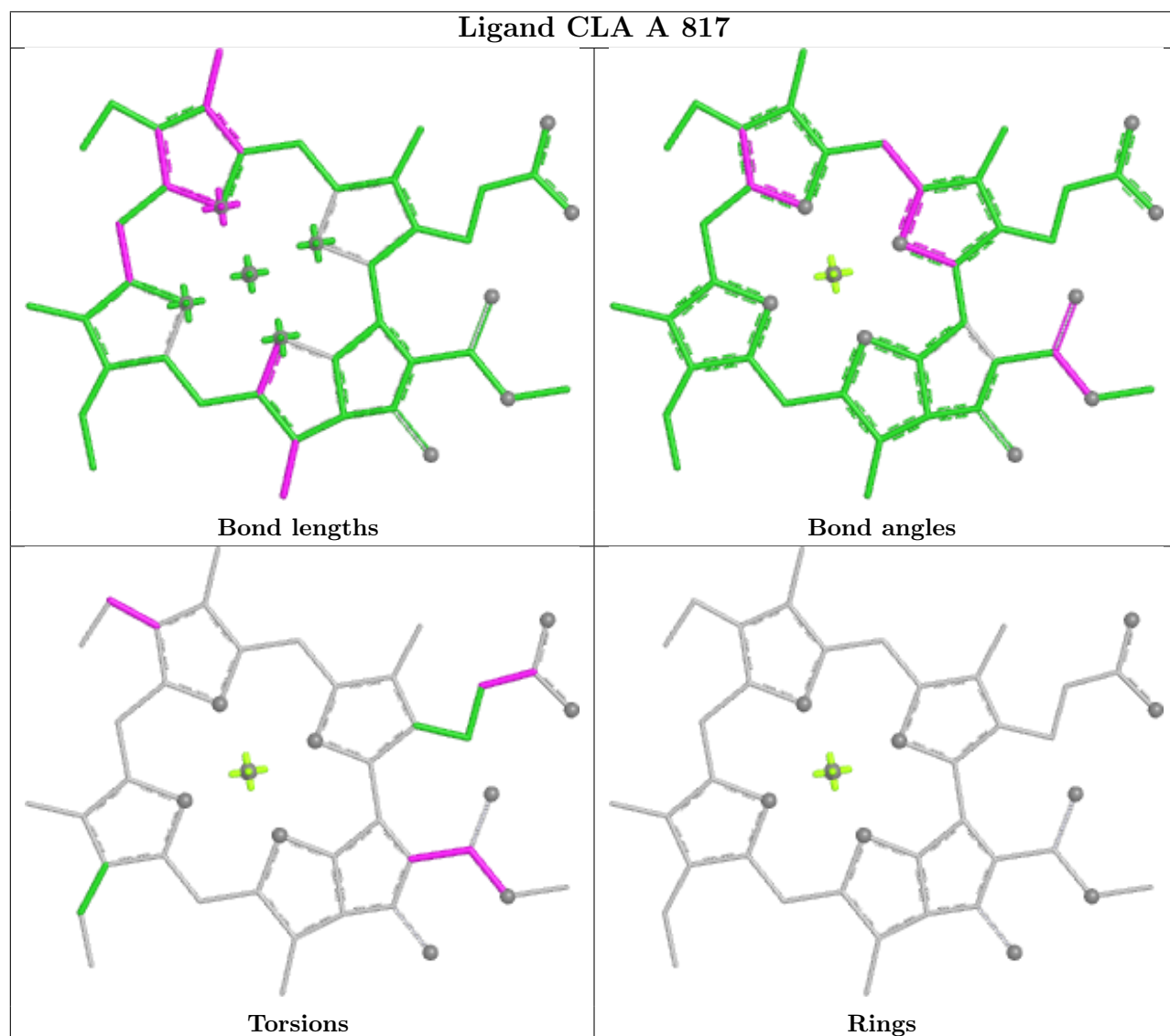
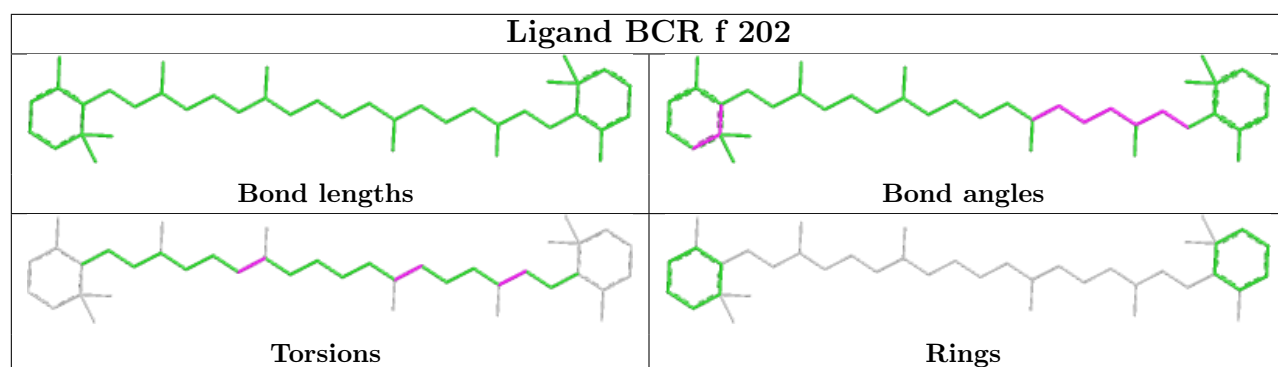
Ligand F6C L 201

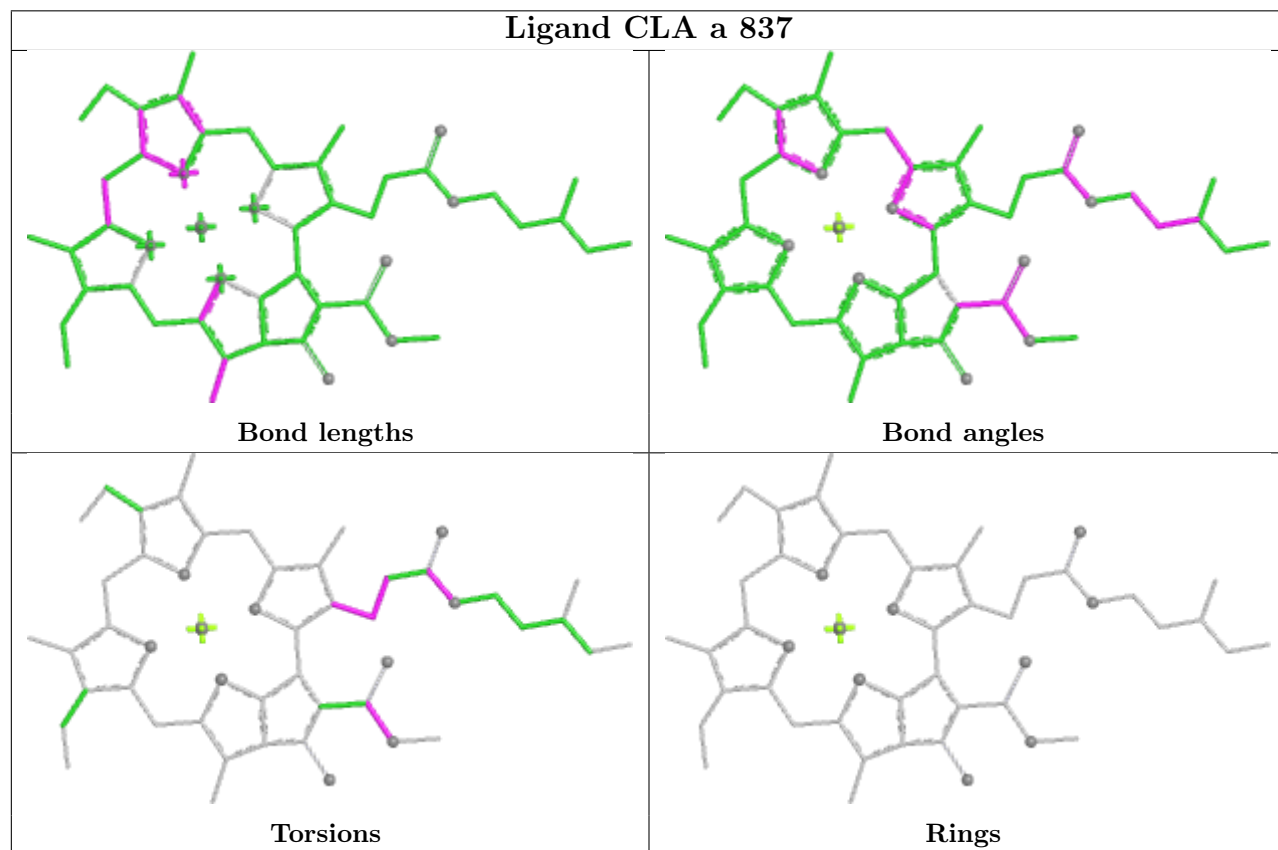
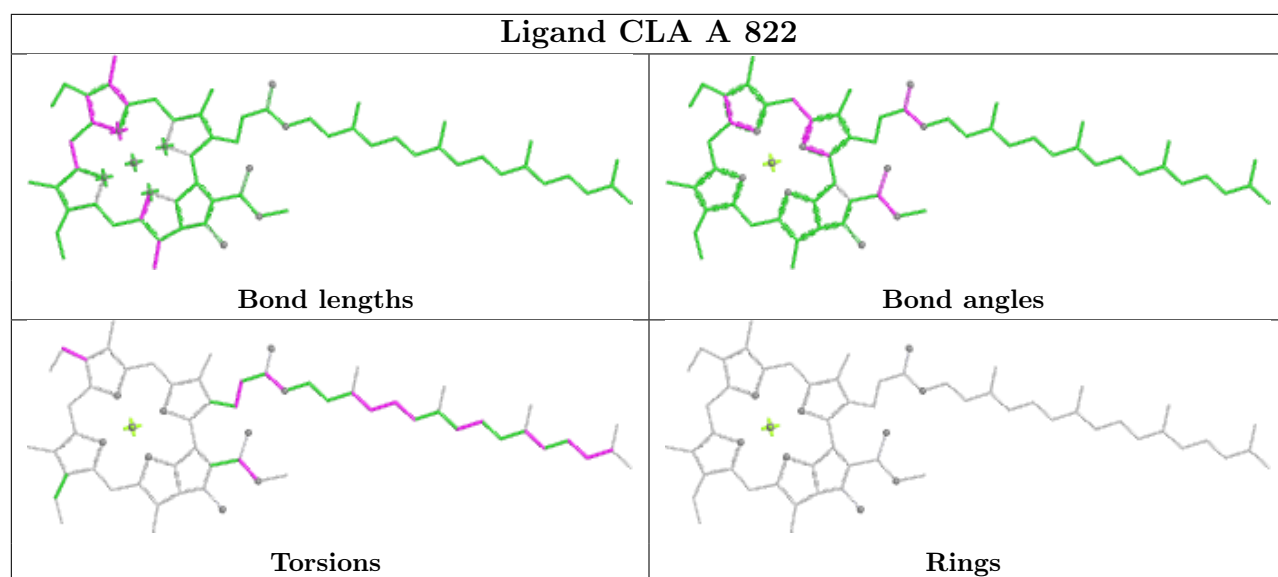


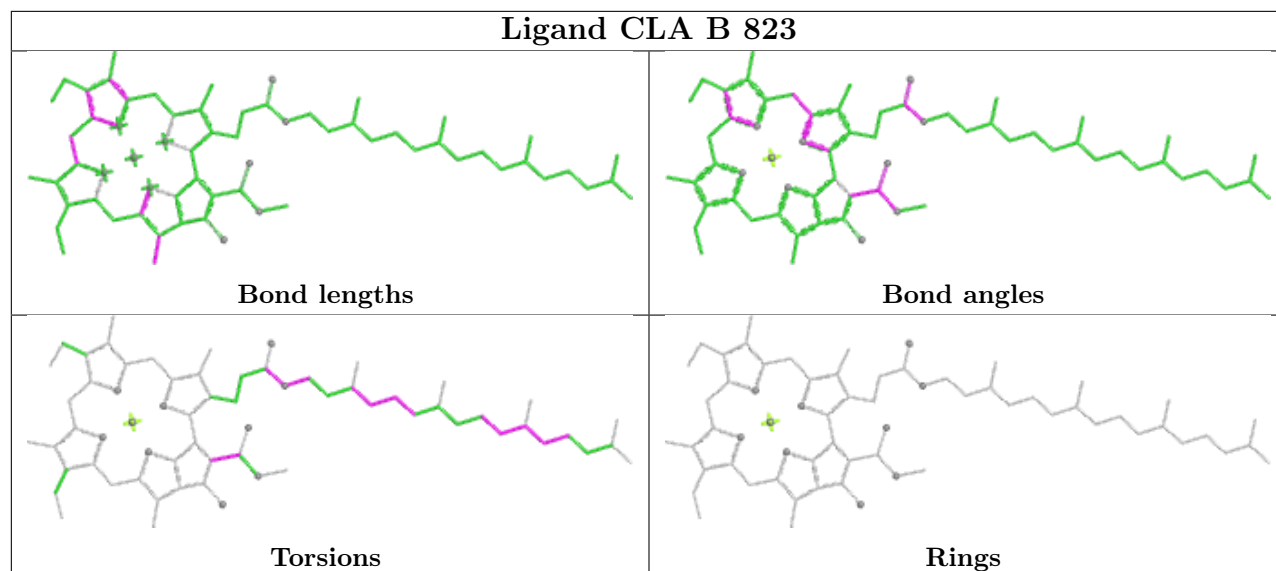
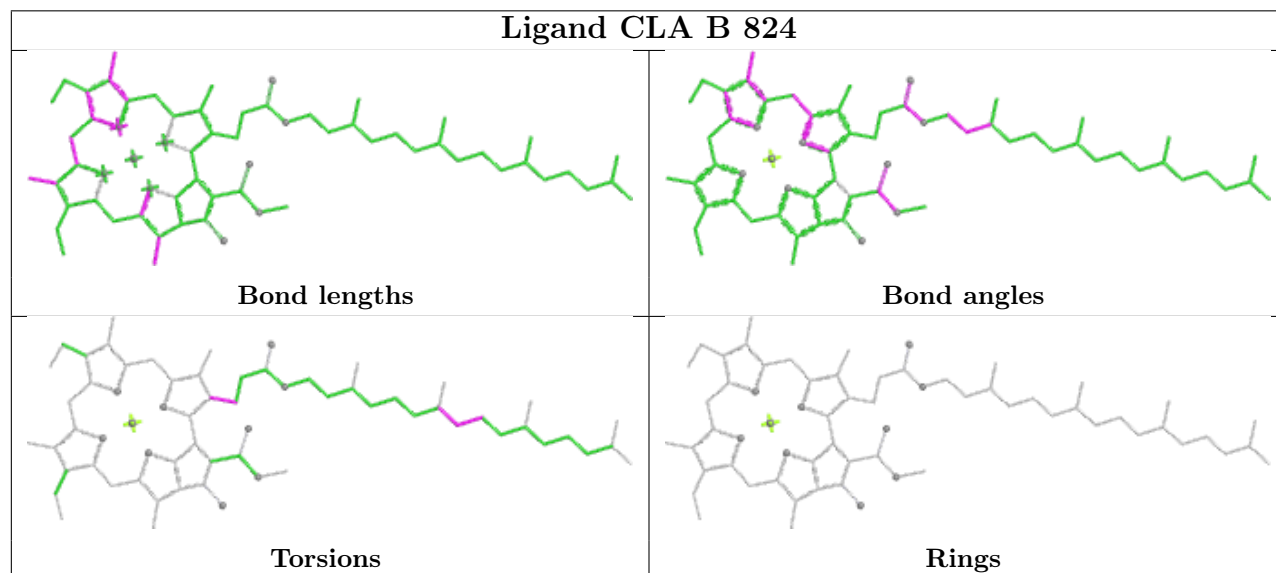
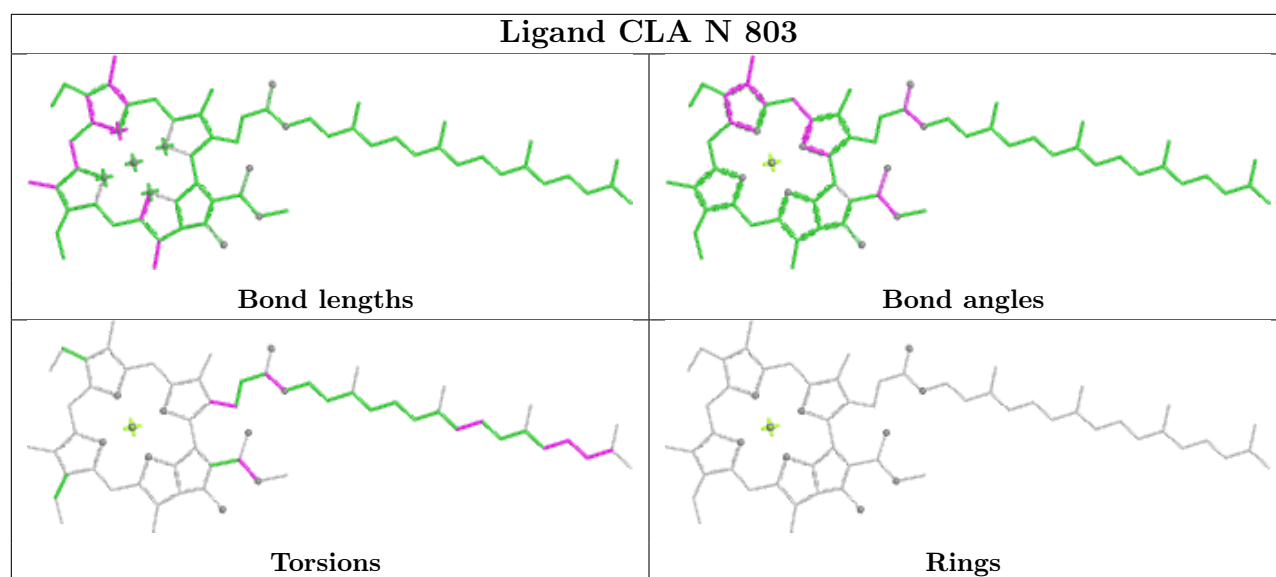
Ligand CLA a 834











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.

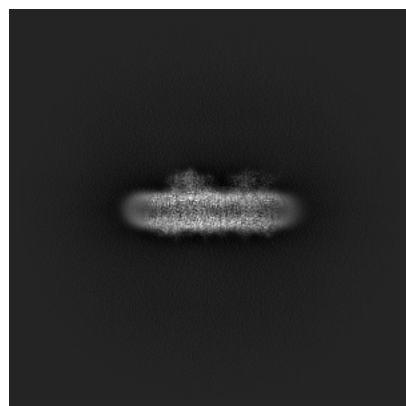
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-50063. These allow visual inspection of the internal detail of the map and identification of artifacts.

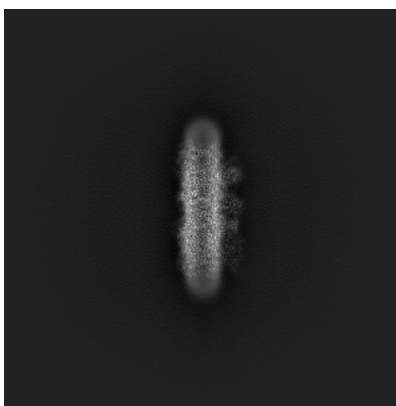
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

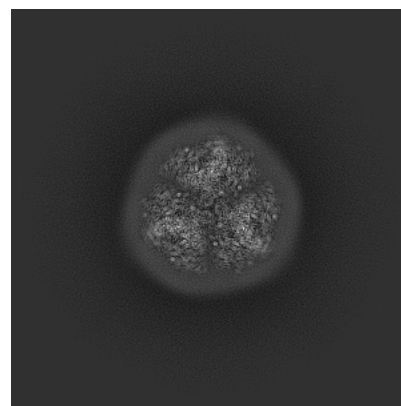
6.1.1 Primary map



X

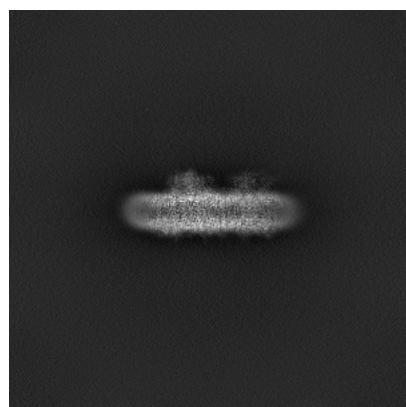


Y

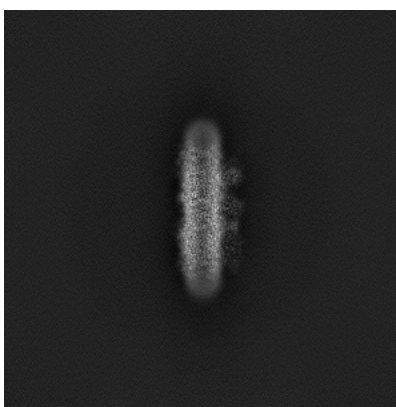


Z

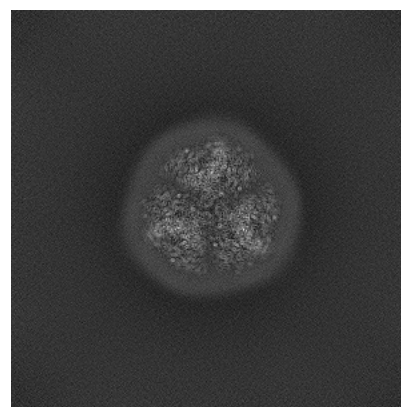
6.1.2 Raw map



X



Y

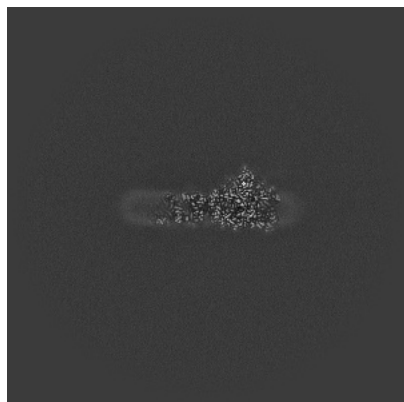


Z

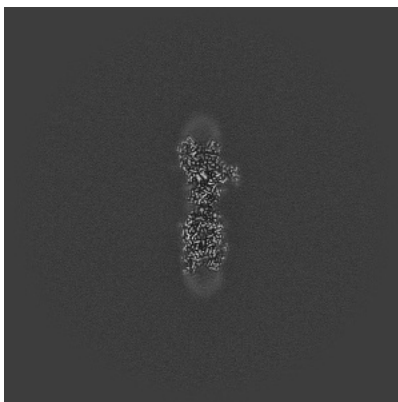
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

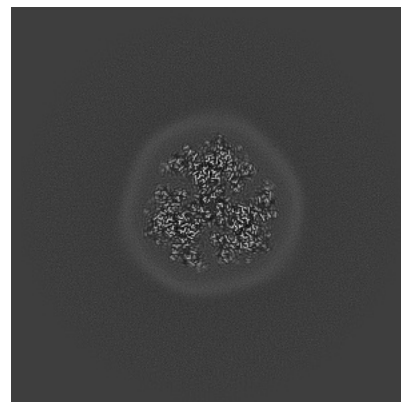
6.2.1 Primary map



X Index: 300

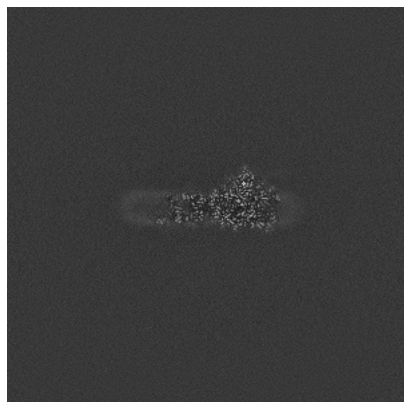


Y Index: 300

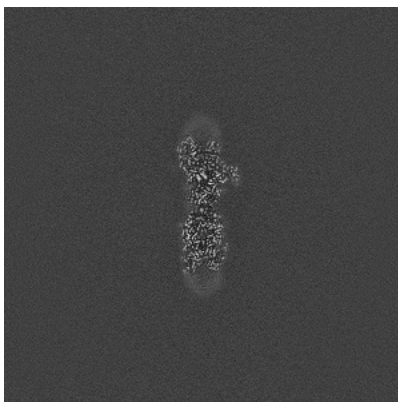


Z Index: 300

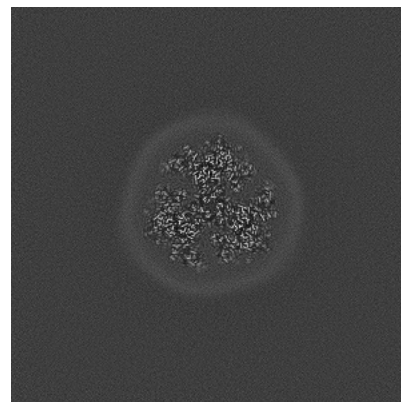
6.2.2 Raw map



X Index: 300



Y Index: 300

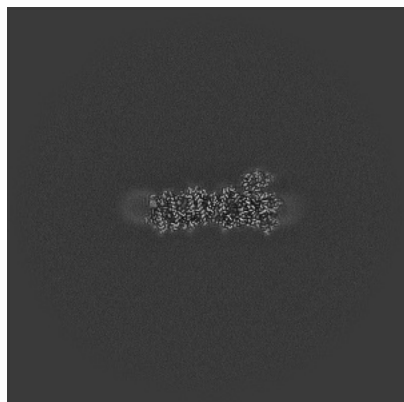


Z Index: 300

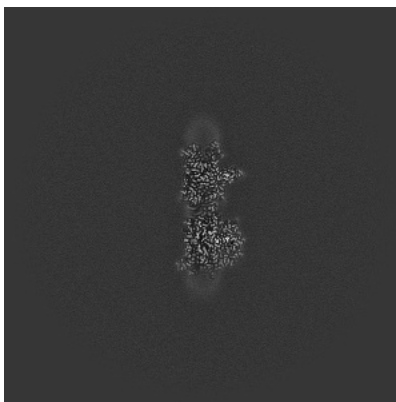
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

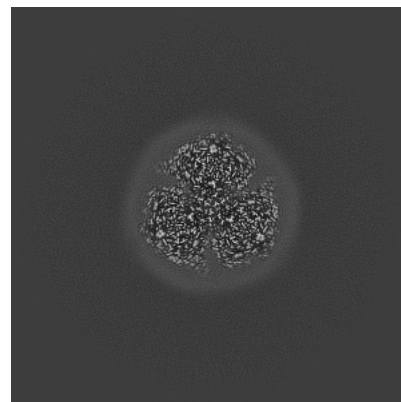
6.3.1 Primary map



X Index: 314

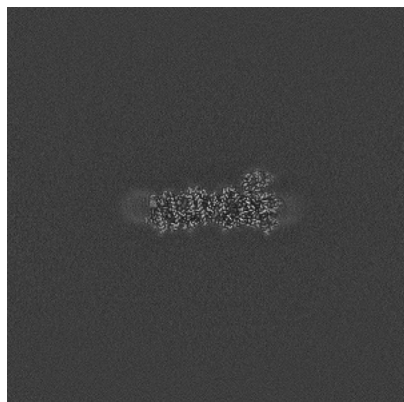


Y Index: 273

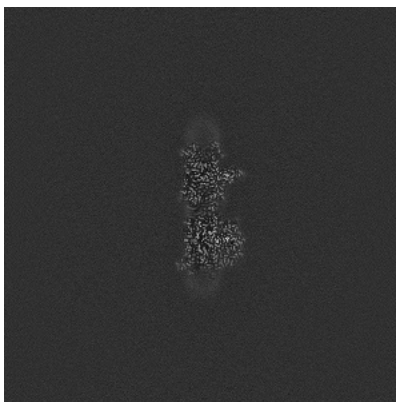


Z Index: 312

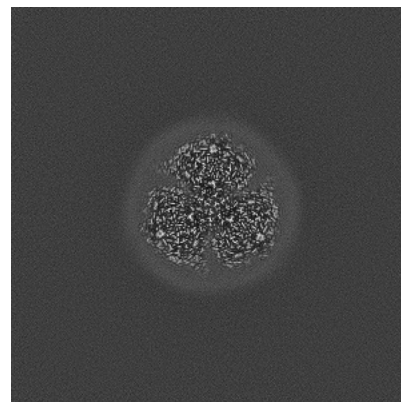
6.3.2 Raw map



X Index: 314



Y Index: 273

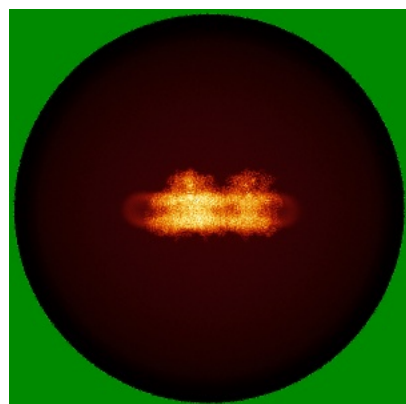


Z Index: 312

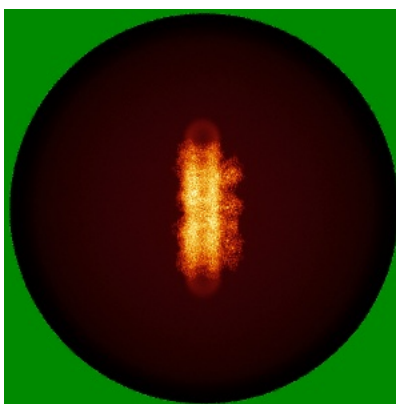
The images above show the largest variance slices of the map in three orthogonal directions.

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

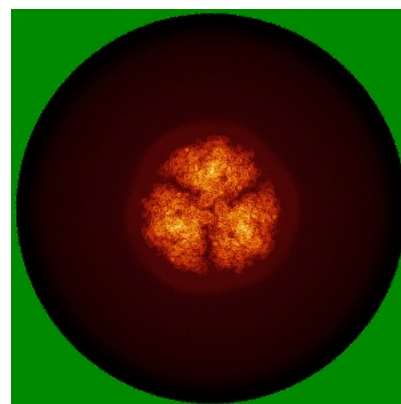
6.4.1 Primary map



X

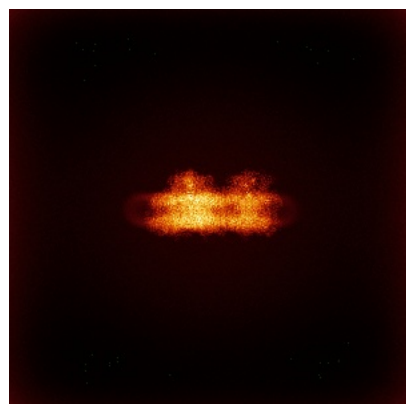


Y

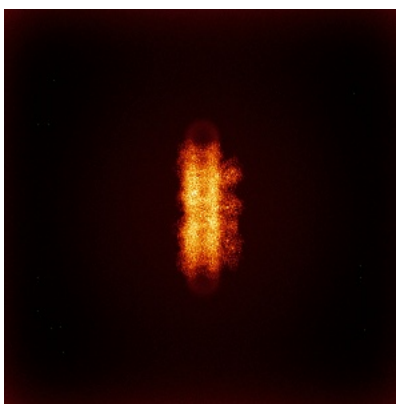


Z

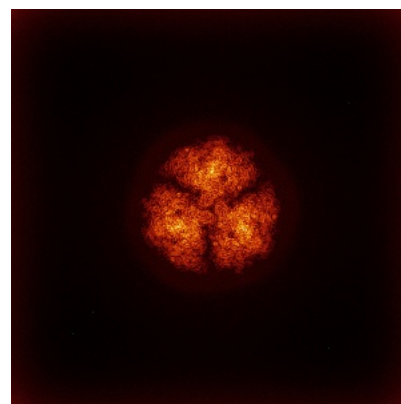
6.4.2 Raw map



X



Y

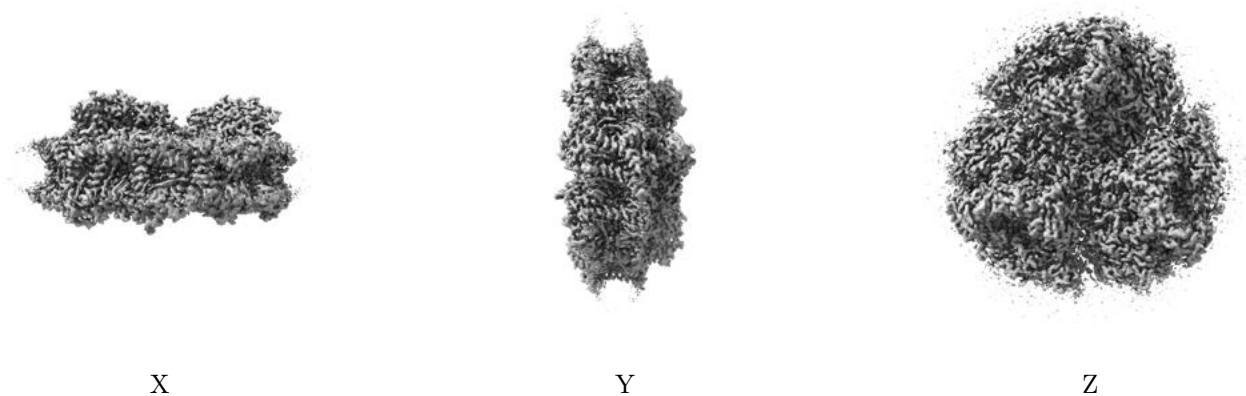


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

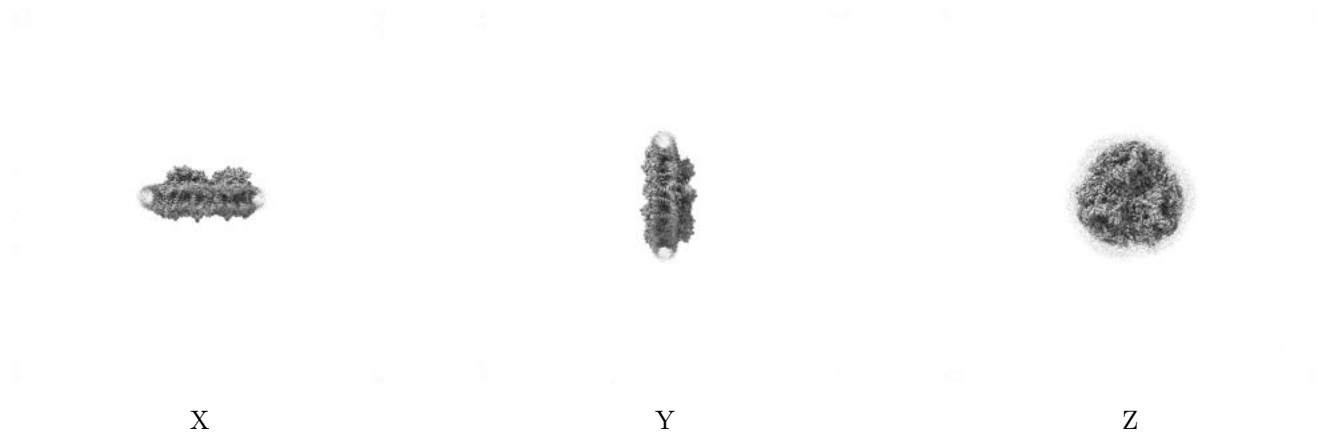
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.054. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

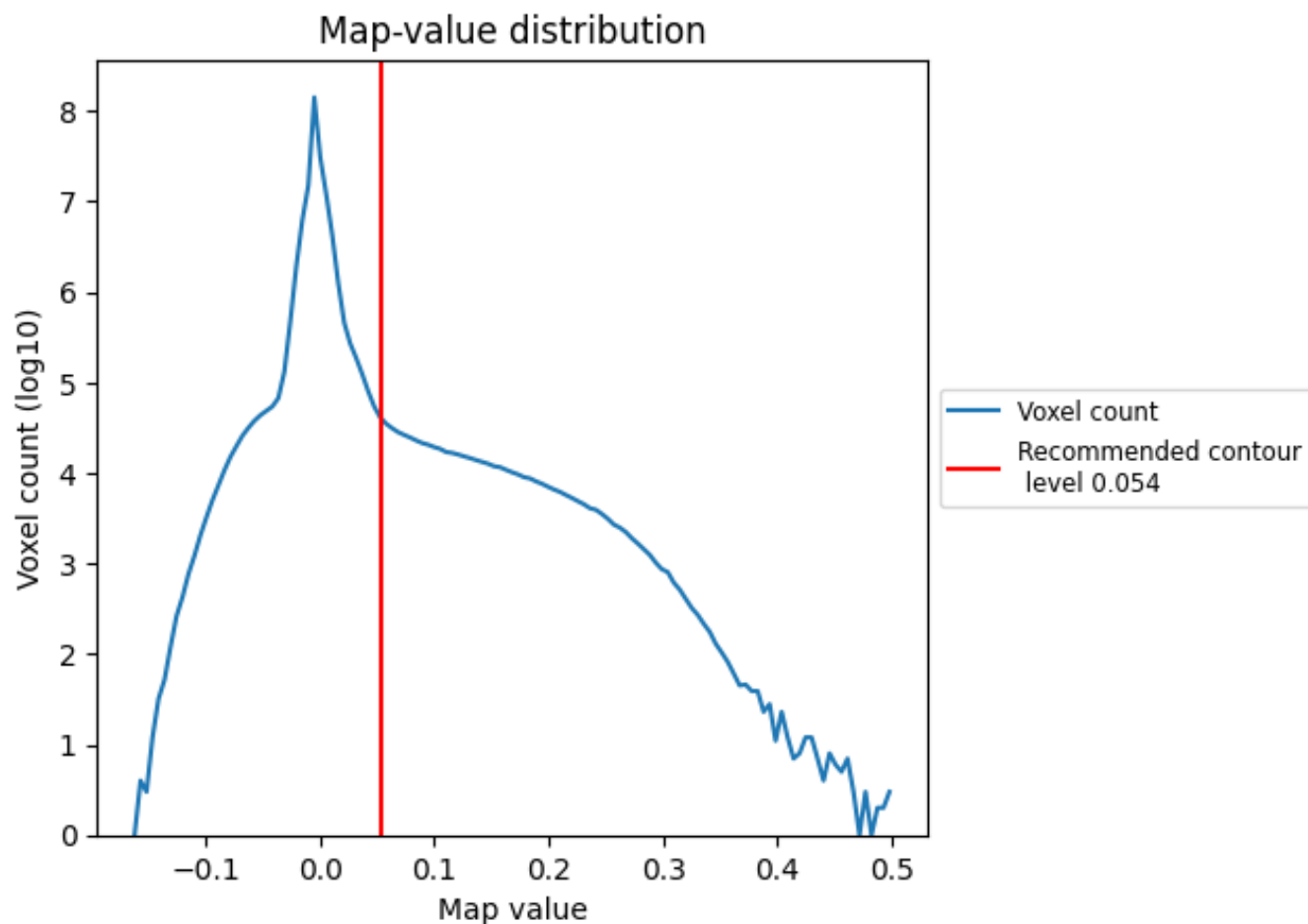
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

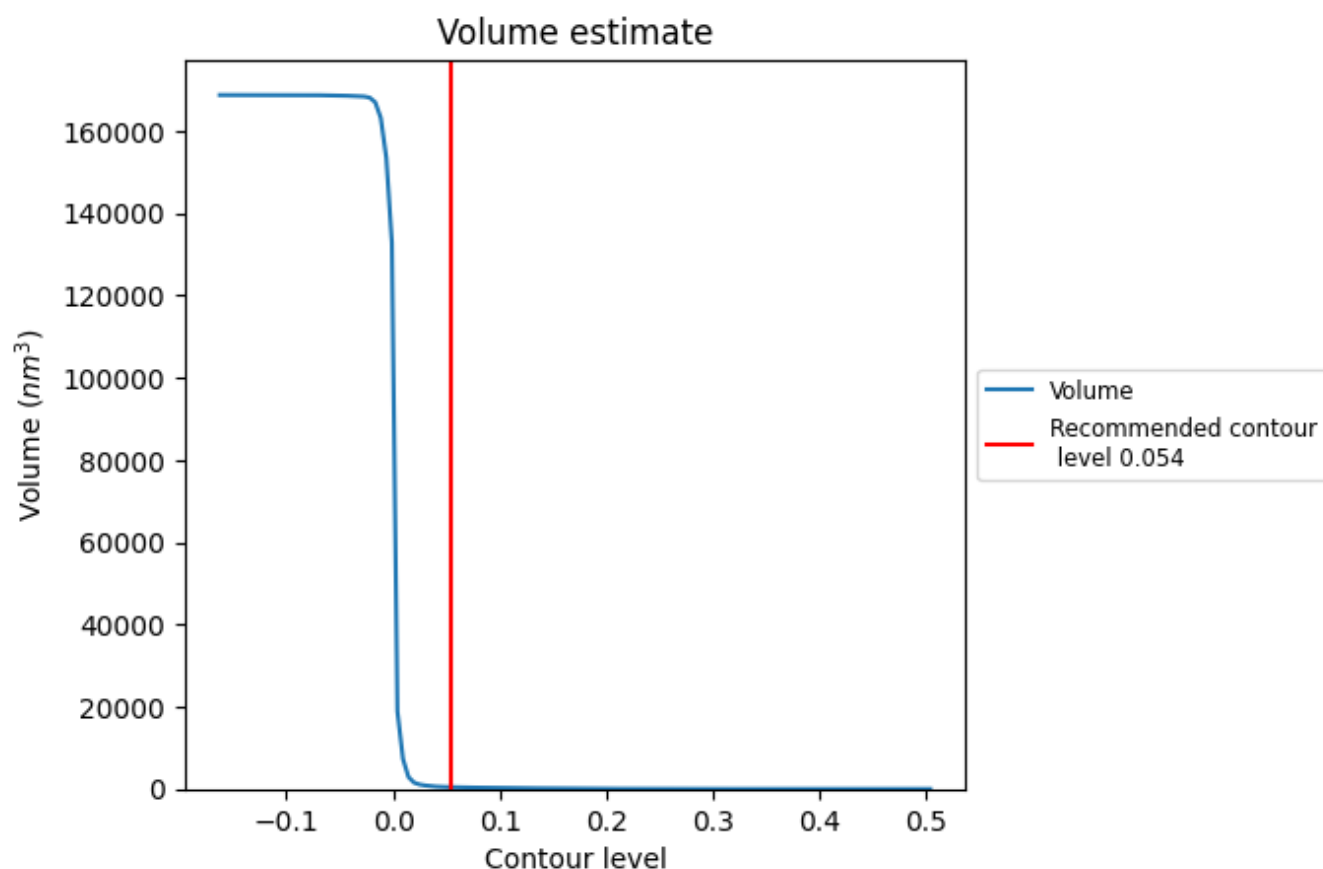
This section contains the results of statistical analysis of the map.

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.

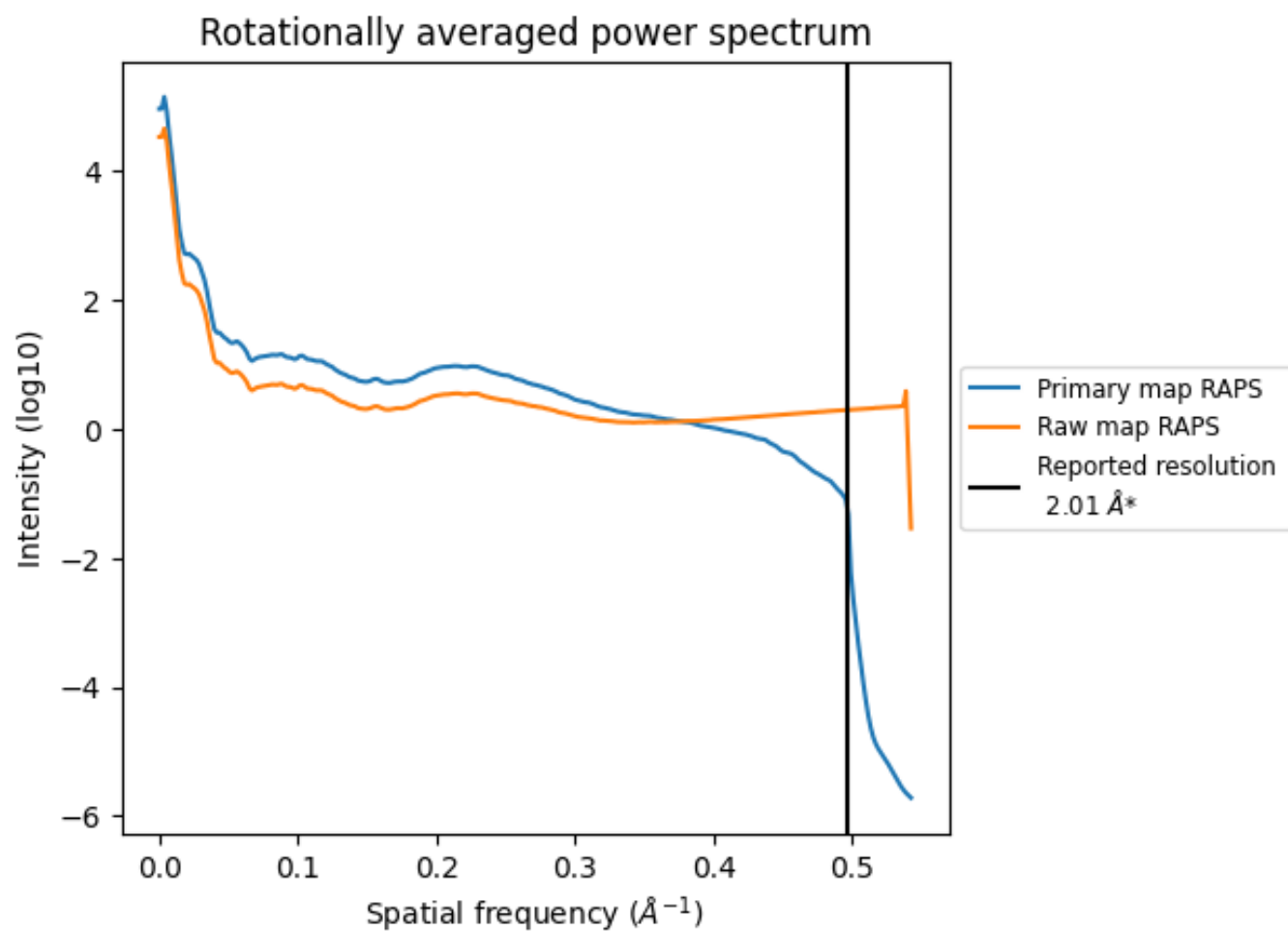
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 439 nm^3 ; this corresponds to an approximate mass of 396 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 ⓘ

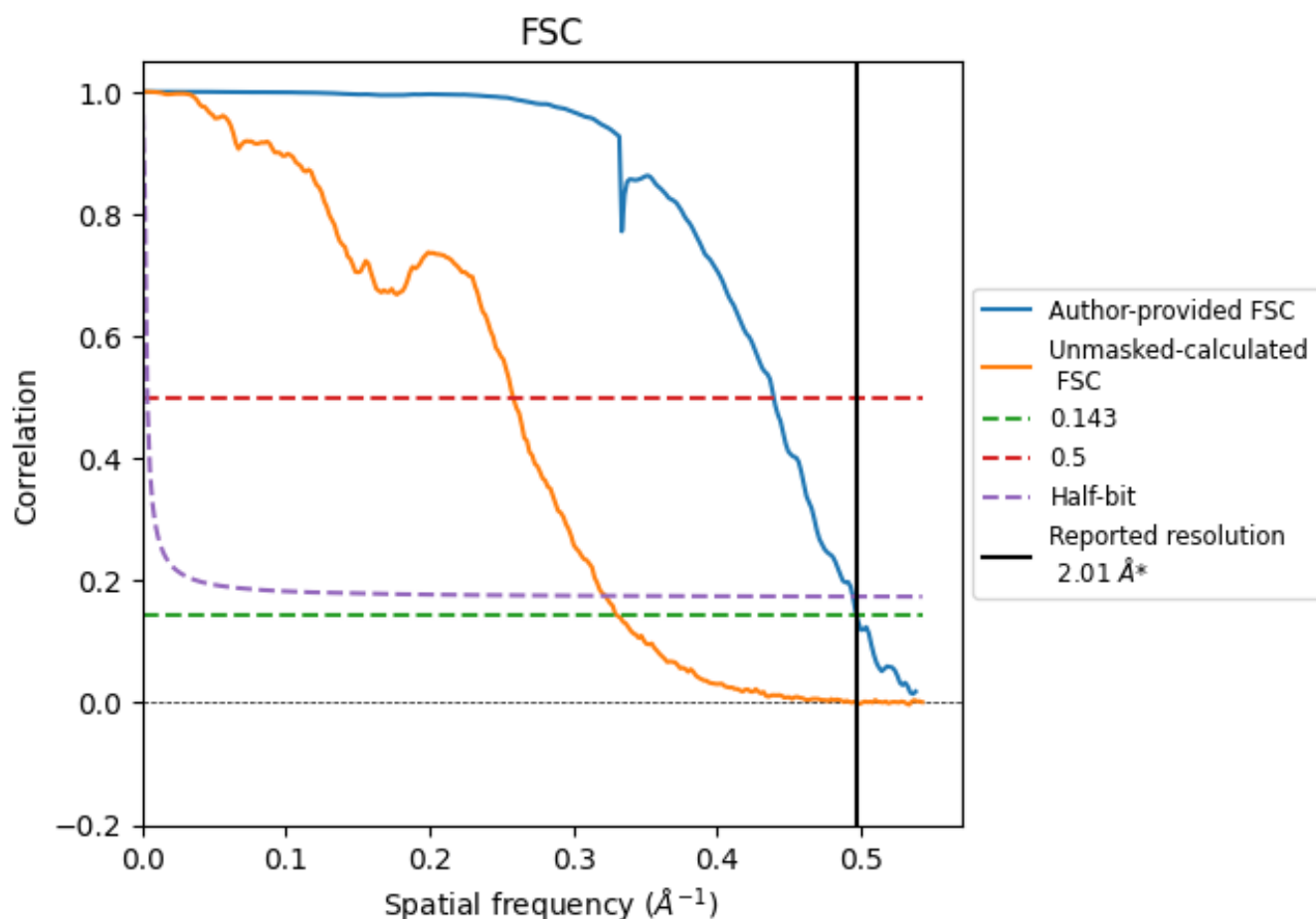


*Reported resolution corresponds to spatial frequency of $0.498 \text{ \AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.498 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

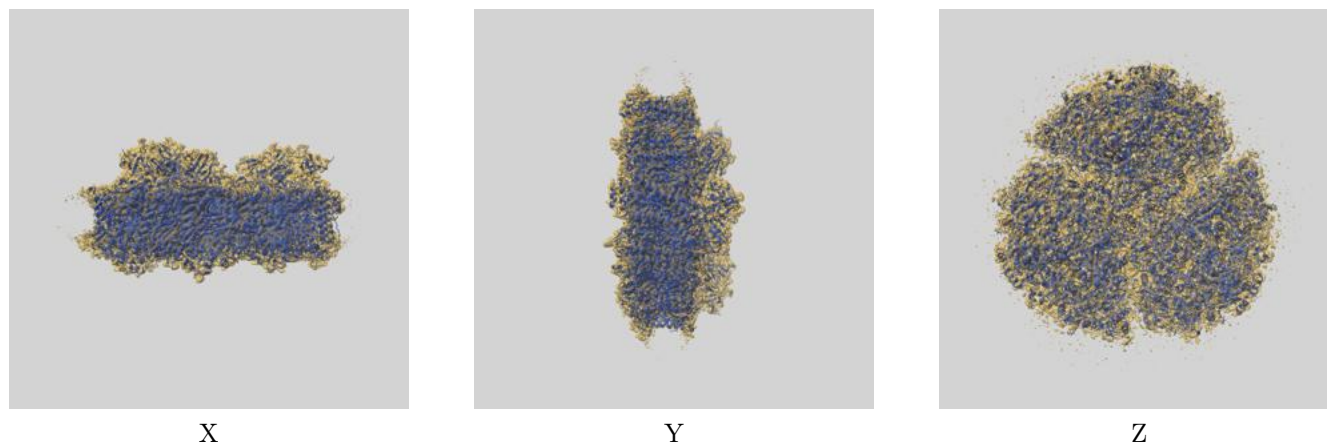
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.01	-	-
Author-provided FSC curve	2.01	2.27	2.02
Unmasked-calculated*	3.03	3.87	3.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.03 differs from the reported value 2.01 by more than 10 %

9 Map-model fit [i](#)

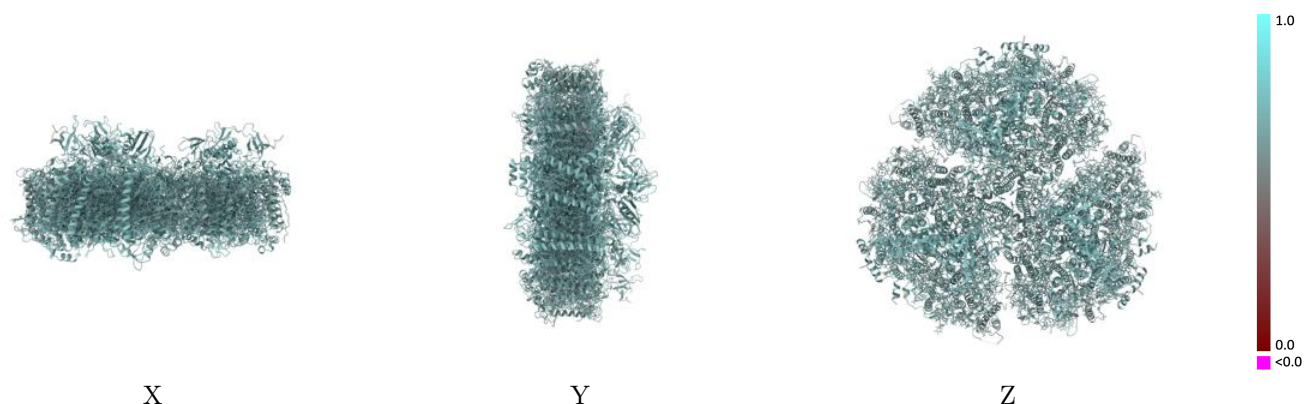
This section contains information regarding the fit between EMDB map EMD-50063 and PDB model 9EYS. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



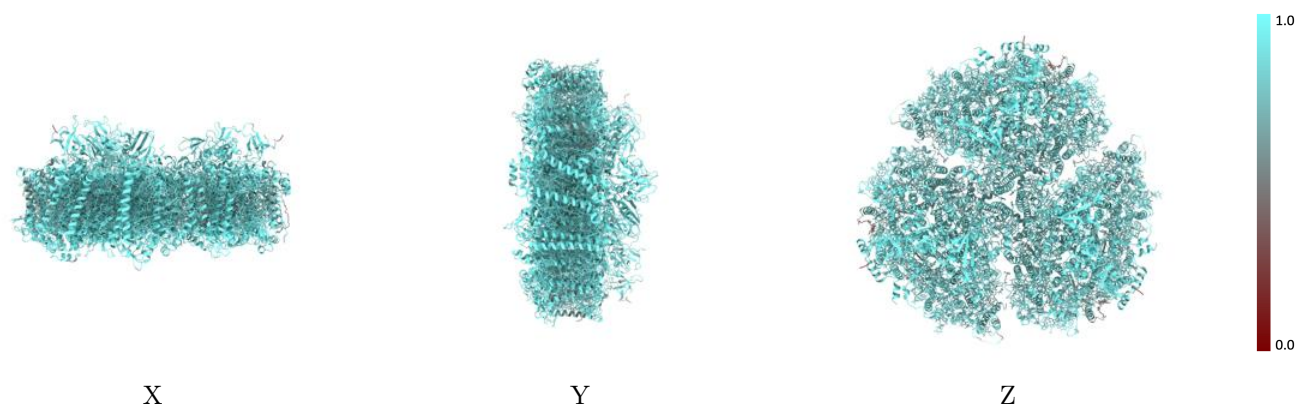
The images above show the 3D surface view of the map at the recommended contour level 0.054 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



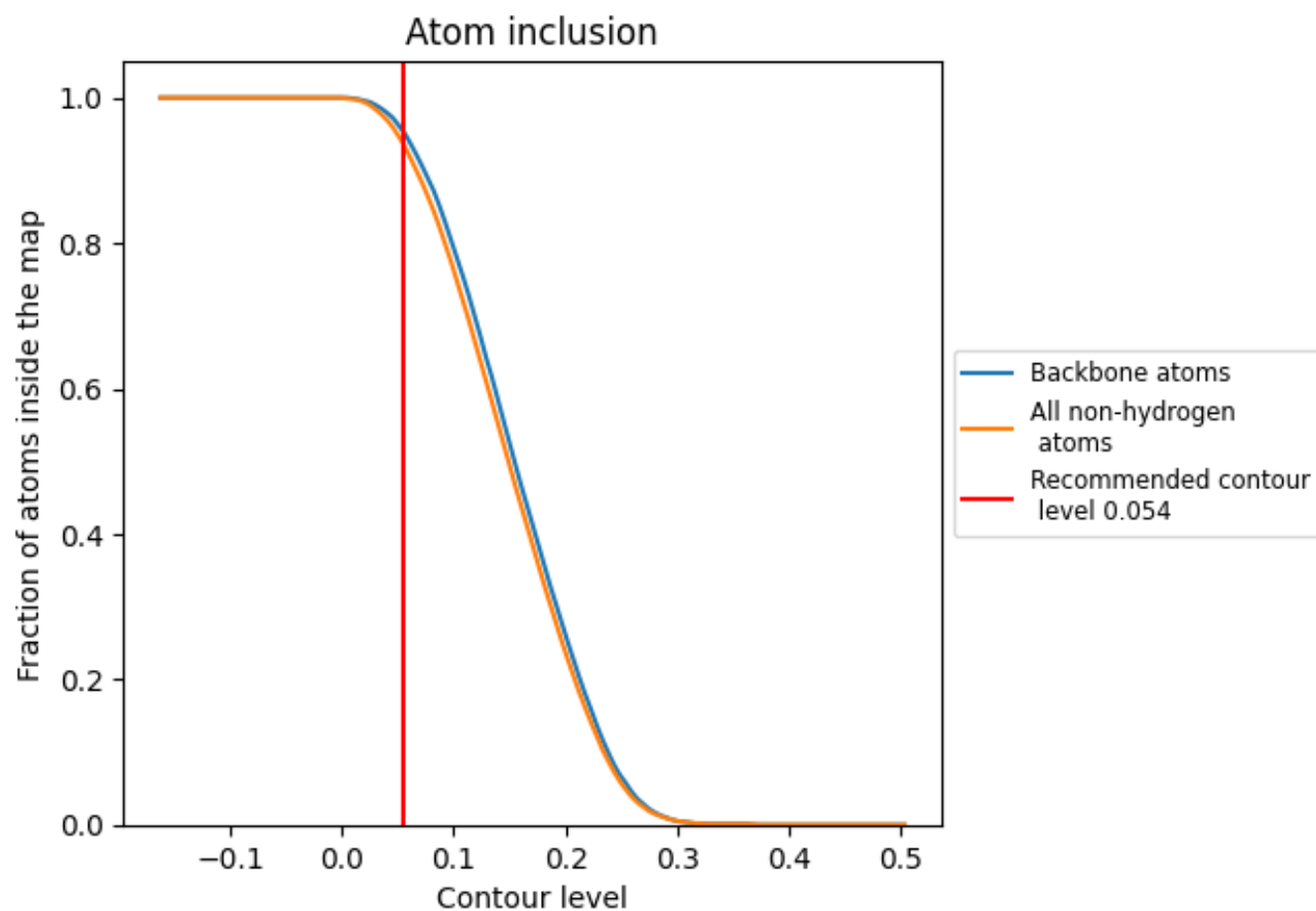
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.054).

9.4 Atom inclusion [i](#)



At the recommended contour level, 96% 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 (0.054) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9390	 0.6720
A	 0.9470	 0.6750
B	 0.9540	 0.6780
C	 0.9900	 0.7050
D	 0.9570	 0.6740
E	 0.8950	 0.6460
F	 0.8920	 0.6430
I	 0.9590	 0.6890
J	 0.8860	 0.6330
K	 0.7630	 0.5740
L	 0.9590	 0.6910
M	 0.9230	 0.6640
N	 0.9460	 0.6760
O	 0.9530	 0.6790
P	 0.9920	 0.7070
Q	 0.9560	 0.6760
R	 0.8950	 0.6430
S	 0.8930	 0.6440
T	 0.9630	 0.6930
U	 0.8900	 0.6370
V	 0.7750	 0.5800
W	 0.9610	 0.6960
X	 0.7170	 0.5900
Y	 0.9230	 0.6650
Z	 0.7280	 0.5910
a	 0.9470	 0.6750
b	 0.9530	 0.6790
c	 0.9930	 0.7030
d	 0.9580	 0.6760
e	 0.8930	 0.6450
f	 0.9010	 0.6470
g	 0.9570	 0.6900
h	 0.8840	 0.6370
i	 0.7740	 0.5870
j	 0.9600	 0.6950



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Chain	Atom inclusion	Q-score
k	 0.9260	 0.6650
l	 0.7090	 0.5940