



## wwPDB EM Validation Summary Report ⓘ

May 6, 2025 – 03:36 PM EDT

PDB ID : 8VU3 / pdb\_00008vu3  
EMDB ID : EMD-43525  
Title : Cryo-EM structure of cyanobacterial PSI with bound platinum nanoparticles  
Authors : Gisriel, C.J.; Malavath, T.; Brudvig, G.W.; Utschig, L.M.  
Deposited on : 2024-01-28  
Resolution : 2.27 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev118  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0rc1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.43.1

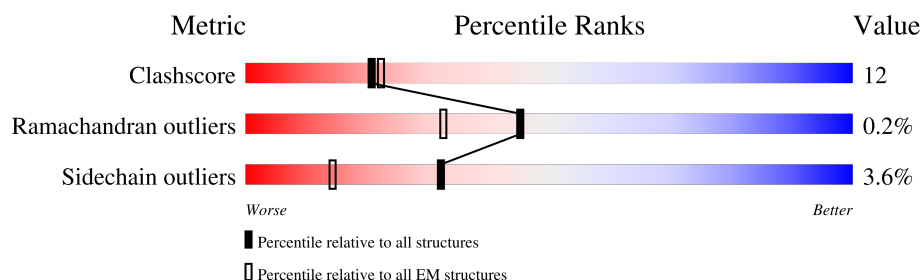
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

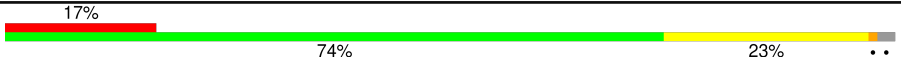



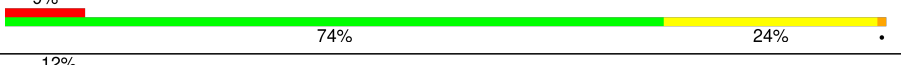

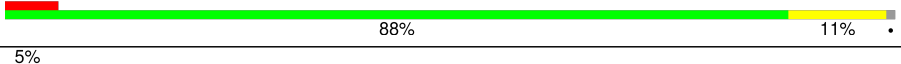

The reported resolution of this entry is 2.27 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	755	
1	G	755	
1	a	755	
2	B	741	
2	H	741	
2	b	741	
3	C	81	
3	N	81	

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Mol	Chain	Length	Quality of chain
3	c	81	
4	D	139	
4	O	139	
4	d	139	
5	E	75	
5	P	75	
5	e	75	
6	F	164	
6	Q	164	
6	f	164	
7	I	40	
7	R	40	
7	i	40	
8	J	43	
8	S	43	
8	j	43	
9	K	83	
9	T	83	
9	k	83	
10	L	155	
10	U	155	
10	l	155	
11	M	31	
11	V	31	
11	m	31	

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Mol	Chain	Length	Quality of chain
12	W	36	<div> <div>61%</div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
12	X	36	<div> <div>64%</div> <div>58%</div> <div>17%</div> <div>25%</div> </div>
12	x	36	<div> <div>64%</div> <div>61%</div> <div>14%</div> <div>25%</div> </div>

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	G	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	845	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	803	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	808	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	820	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	823	X	-	-	-
14	CLA	B	824	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	826	X	-	-	-
14	CLA	B	827	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	F	1301	X	-	-	-
14	CLA	F	1303	X	-	-	-
14	CLA	G	802	X	-	-	-
14	CLA	G	803	X	-	-	-
14	CLA	G	804	X	-	-	-
14	CLA	G	805	X	-	-	-
14	CLA	G	806	X	-	-	-
14	CLA	G	807	X	-	-	-
14	CLA	G	808	X	-	-	-
14	CLA	G	809	X	-	-	-
14	CLA	G	810	X	-	-	-
14	CLA	G	811	X	-	-	-
14	CLA	G	812	X	-	-	-
14	CLA	G	813	X	-	-	-
14	CLA	G	814	X	-	-	-
14	CLA	G	815	X	-	-	-
14	CLA	G	816	X	-	-	-
14	CLA	G	817	X	-	-	-
14	CLA	G	818	X	-	-	-
14	CLA	G	819	X	-	-	-
14	CLA	G	820	X	-	-	-
14	CLA	G	821	X	-	-	-
14	CLA	G	822	X	-	-	-
14	CLA	G	823	X	-	-	-
14	CLA	G	824	X	-	-	-
14	CLA	G	825	X	-	-	-
14	CLA	G	826	X	-	-	-
14	CLA	G	827	X	-	-	-
14	CLA	G	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	G	829	X	-	-	-
14	CLA	G	830	X	-	-	-
14	CLA	G	831	X	-	-	-
14	CLA	G	832	X	-	-	-
14	CLA	G	833	X	-	-	-
14	CLA	G	834	X	-	-	-
14	CLA	G	835	X	-	-	-
14	CLA	G	836	X	-	-	-
14	CLA	G	837	X	-	-	-
14	CLA	G	838	X	-	-	-
14	CLA	G	839	X	-	-	-
14	CLA	G	840	X	-	-	-
14	CLA	G	841	X	-	-	-
14	CLA	G	842	X	-	-	-
14	CLA	G	843	X	-	-	-
14	CLA	G	844	X	-	-	-
14	CLA	G	845	X	-	-	-
14	CLA	H	801	X	-	-	-
14	CLA	H	802	X	-	-	-
14	CLA	H	803	X	-	-	-
14	CLA	H	804	X	-	-	-
14	CLA	H	805	X	-	-	-
14	CLA	H	806	X	-	-	-
14	CLA	H	807	X	-	-	-
14	CLA	H	808	X	-	-	-
14	CLA	H	809	X	-	-	-
14	CLA	H	810	X	-	-	-
14	CLA	H	811	X	-	-	-
14	CLA	H	812	X	-	-	-
14	CLA	H	813	X	-	-	-
14	CLA	H	814	X	-	-	-
14	CLA	H	815	X	-	-	-
14	CLA	H	816	X	-	-	-
14	CLA	H	817	X	-	-	-
14	CLA	H	818	X	-	-	-
14	CLA	H	819	X	-	-	-
14	CLA	H	820	X	-	-	-
14	CLA	H	821	X	-	-	-
14	CLA	H	822	X	-	-	-
14	CLA	H	823	X	-	-	-
14	CLA	H	824	X	-	-	-
14	CLA	H	825	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	H	826	X	-	-	-
14	CLA	H	827	X	-	-	-
14	CLA	H	828	X	-	-	-
14	CLA	H	829	X	-	-	-
14	CLA	H	830	X	-	-	-
14	CLA	H	831	X	-	-	-
14	CLA	H	832	X	-	-	-
14	CLA	H	833	X	-	-	-
14	CLA	H	834	X	-	-	-
14	CLA	H	835	X	-	-	-
14	CLA	H	836	X	-	-	-
14	CLA	H	837	X	-	-	-
14	CLA	H	838	X	-	-	-
14	CLA	H	839	X	-	-	-
14	CLA	H	840	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	L	206	X	-	-	-
14	CLA	M	1601	X	-	-	-
14	CLA	Q	201	X	-	-	-
14	CLA	Q	203	X	-	-	-
14	CLA	S	101	X	-	-	-
14	CLA	S	102	X	-	-	-
14	CLA	T	1401	X	-	-	-
14	CLA	U	201	X	-	-	-
14	CLA	U	204	X	-	-	-
14	CLA	U	205	X	-	-	-
14	CLA	U	206	X	-	-	-
14	CLA	V	1601	X	-	-	-
14	CLA	W	1701	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	842	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	a	844	X	-	-	-
14	CLA	a	855	X	-	-	-
14	CLA	b	801	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	803	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	806	X	-	-	-
14	CLA	b	807	X	-	-	-
14	CLA	b	808	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	816	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	819	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	822	X	-	-	-
14	CLA	b	823	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	825	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	827	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	f	202	X	-	-	-
14	CLA	i	101	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	k	1401	X	-	-	-
14	CLA	l	202	X	-	-	-
14	CLA	l	205	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	l	206	X	-	-	-
14	CLA	l	207	X	-	-	-
14	CLA	m	1601	X	-	-	-
14	CLA	x	1701	X	-	-	-

## 2 Entry composition [i](#)

There are 20 unique types of molecules in this entry. The entry contains 71694 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	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		
1	G	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		
1	a	740	Total	C	N	O	S	0	0
			5777	3791	987	976	23		

- 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
			5892	3876	988	1008	20		
2	H	739	Total	C	N	O	S	0	0
			5892	3876	988	1008	20		
2	b	739	Total	C	N	O	S	0	0
			5892	3876	988	1008	20		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		
4	d	138	Total	C	N	O	S	0	0
			1076	683	187	203	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	69	Total	C	N	O		0	0
			534	337	92	105			
5	P	69	Total	C	N	O		0	0
			534	337	92	105			
5	e	69	Total	C	N	O		0	0
			534	337	92	105			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	53	GLY	SER	conflict	UNP A0A2D2Q1I4
P	53	GLY	SER	conflict	UNP A0A2D2Q1I4
e	53	GLY	SER	conflict	UNP A0A2D2Q1I4

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		
6	Q	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1064	679	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	S	0	0
			308	213	42	48	5		
7	R	39	Total	C	N	O	S	0	0
			308	213	42	48	5		
7	i	39	Total	C	N	O	S	0	0
			308	213	42	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	43	Total	C	N	O	S	0	0
			351	237	54	58	2		
8	S	43	Total	C	N	O	S	0	0
			351	237	54	58	2		
8	j	43	Total	C	N	O	S	0	0
			351	237	54	58	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
9	K	63	Total	C	N	O	0	0
			307	181	63	63		
9	T	63	Total	C	N	O	0	0
			307	181	63	63		
9	k	63	Total	C	N	O	0	0
			307	181	63	63		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1125	737	181	203	4		
10	U	152	Total	C	N	O	S	0	0
			1125	737	181	203	4		
10	l	152	Total	C	N	O	S	0	0
			1125	737	181	203	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	161	36	42	1		
11	V	31	Total	C	N	O	S	0	0
			240	161	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			240	161	36	42	1		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	27	ALA	THR	conflict	UNP A0A3B7MIX8

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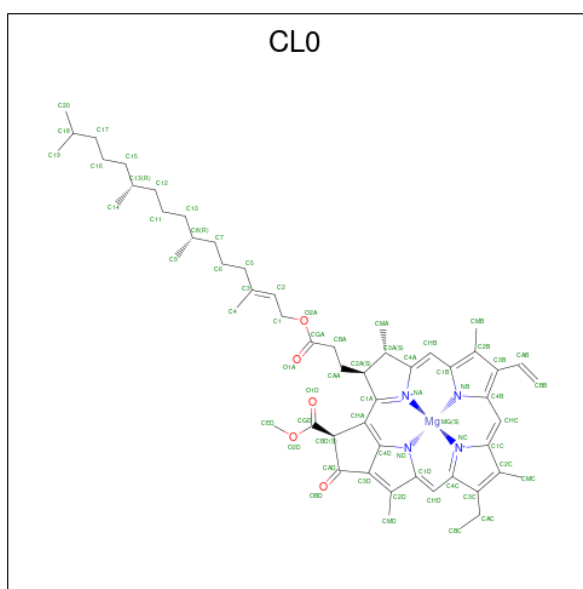
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Chain	Residue	Modelled	Actual	Comment	Reference
V	27	ALA	THR	conflict	UNP A0A3B7MIX8
m	27	ALA	THR	conflict	UNP A0A3B7MIX8

- Molecule 12 is a protein called Phosphorylase.

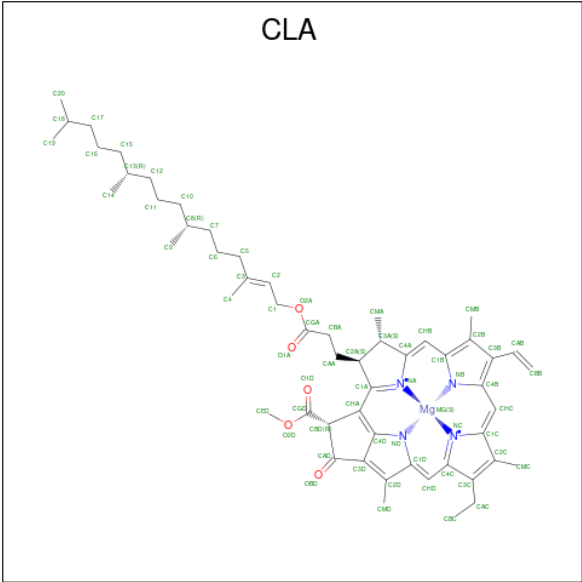
Mol	Chain	Residues	Atoms				AltConf	Trace
12	W	27	Total	C	N	O	0	0
			228	162	32	34		
12	X	27	Total	C	N	O	0	0
			228	162	32	34		
12	x	27	Total	C	N	O	0	0
			228	162	32	34		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
13	A	1	Total	C	Mg	N	O
			65	55	1	4	5
13	G	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 A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	G	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	G	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	H	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	M	1	Total 45	C 35	Mg 1	N 4	O 5	0
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14	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	S	1	Total 37	C 31	Mg 1	N 4	O 1	0

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Mol	Chain	Residues	Atoms					AltConf
14	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	U	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	V	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	W	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 41	C 33	Mg 1	N 4	O 3	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

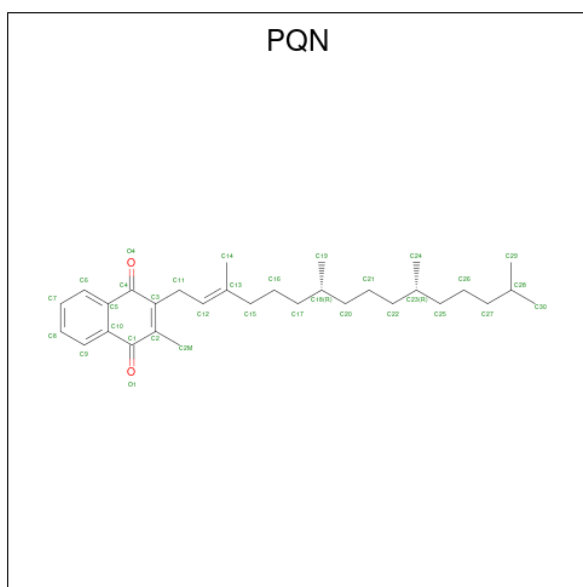
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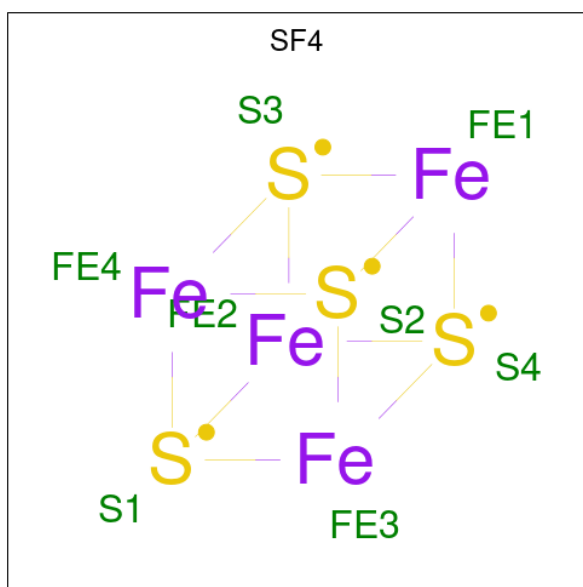
Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	m	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	x	1	Total 45	C 35	Mg 1	N 4	O 5	0

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula: C<sub>31</sub>H<sub>46</sub>O<sub>2</sub>).



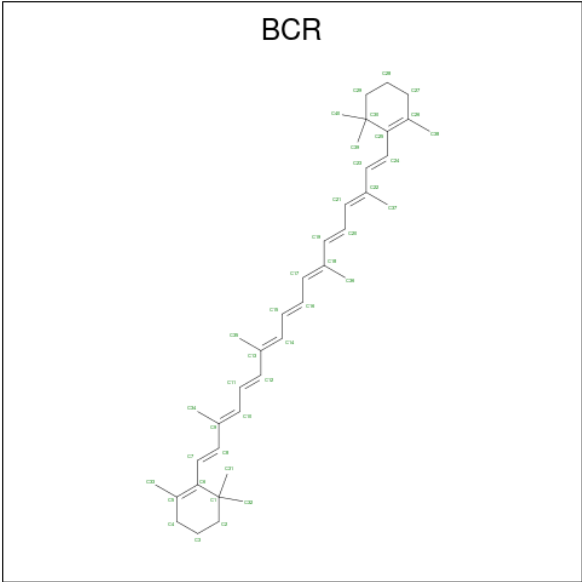
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	G	1	Total	C	O	0
			33	31	2	
15	H	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).



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

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



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

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Mol	Chain	Residues	Atoms	AltConf
17	F	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	G	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 25 25	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	H	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0

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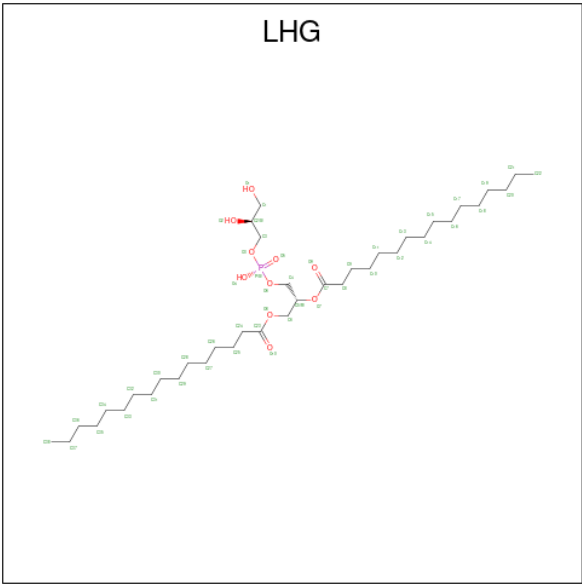
Mol	Chain	Residues	Atoms	AltConf
17	Q	1	Total C 40 40	0
17	Q	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	R	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	S	1	Total C 40 40	0
17	U	1	Total C 40 40	0
17	V	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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

- Molecule 18 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



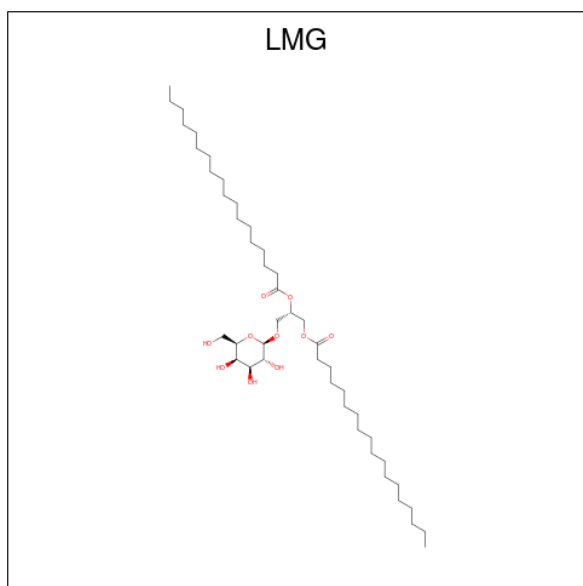
Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
18	A	1	Total	C	O	P	0
			27	16	10	1	
18	G	1	Total	C	O	P	0
			49	38	10	1	
18	G	1	Total	C	O	P	0
			27	16	10	1	
18	a	1	Total	C	O	P	0
			49	38	10	1	
18	a	1	Total	C	O	P	0
			27	16	10	1	

- Molecule 19 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



Mol	Chain	Residues	Atoms			AltConf
19	B	1	Total	C	O	0
			49	39	10	
19	H	1	Total	C	O	0
			49	39	10	
19	b	1	Total	C	O	0
			49	39	10	

- Molecule 20 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
20	L	1	Total	Ca	0
			1	1	

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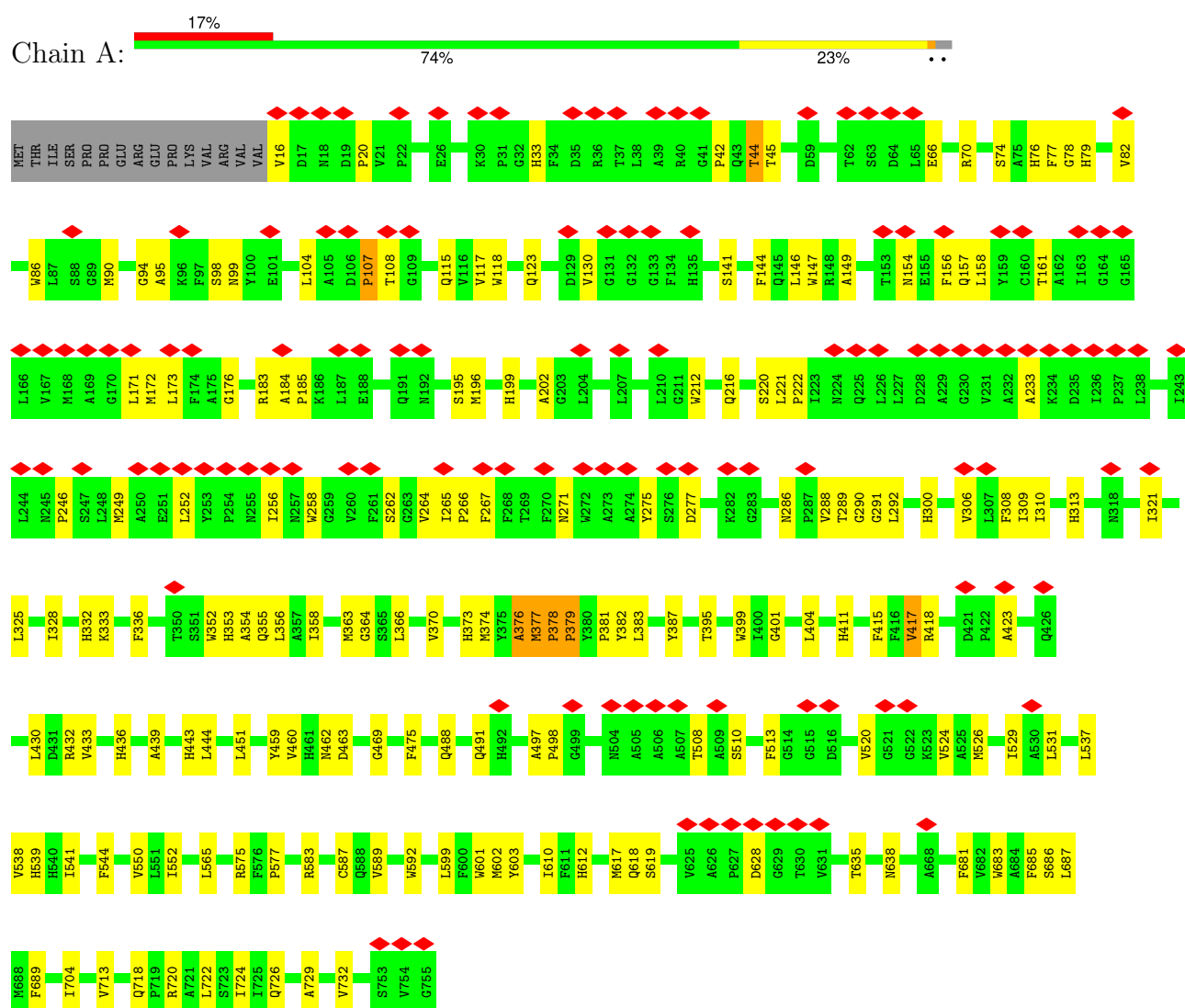
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Mol	Chain	Residues	Atoms		AltConf
20	U	1	Total 1	Ca 1	0
20	1	1	Total 1	Ca 1	0

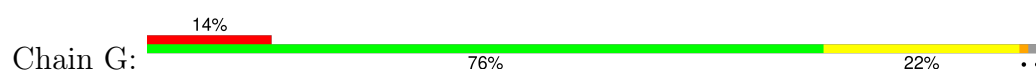
### 3 Residue-property plots

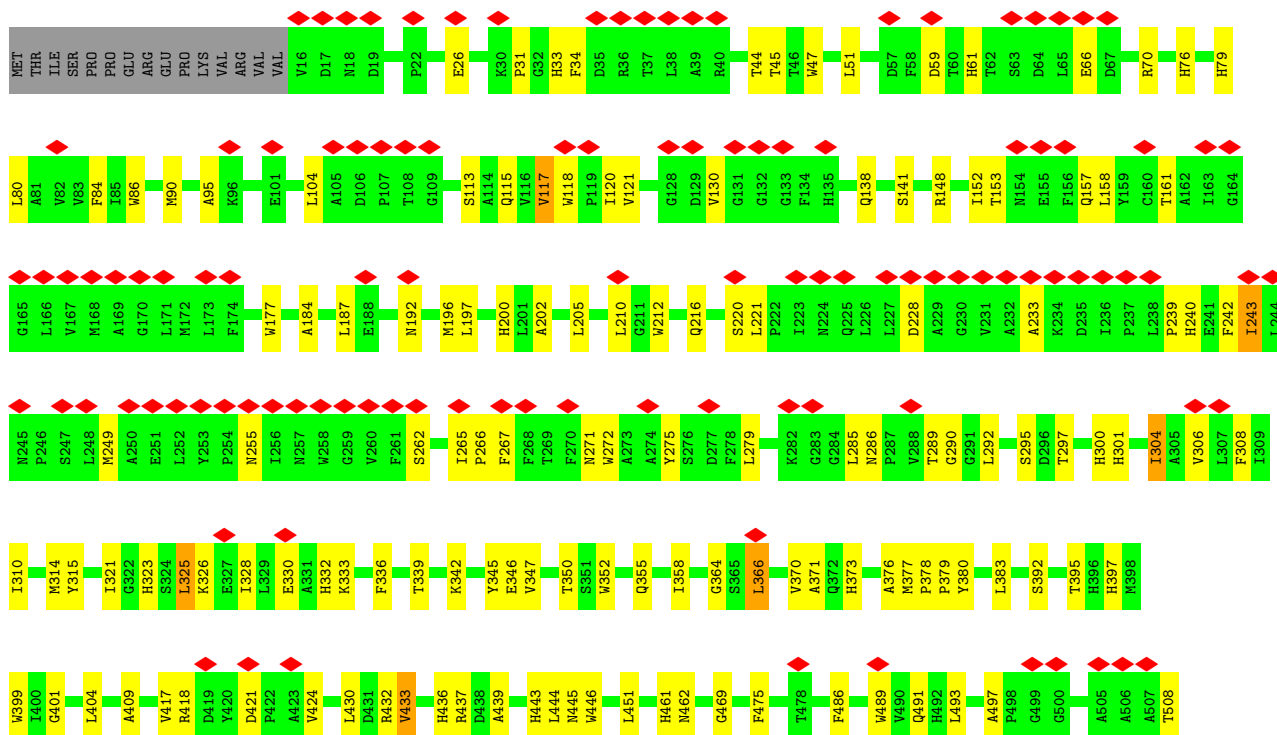
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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.

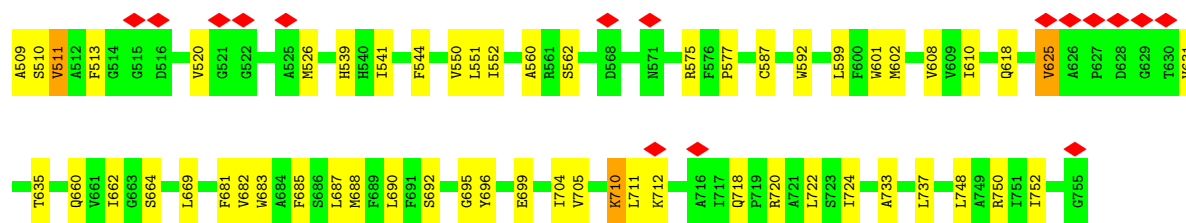
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



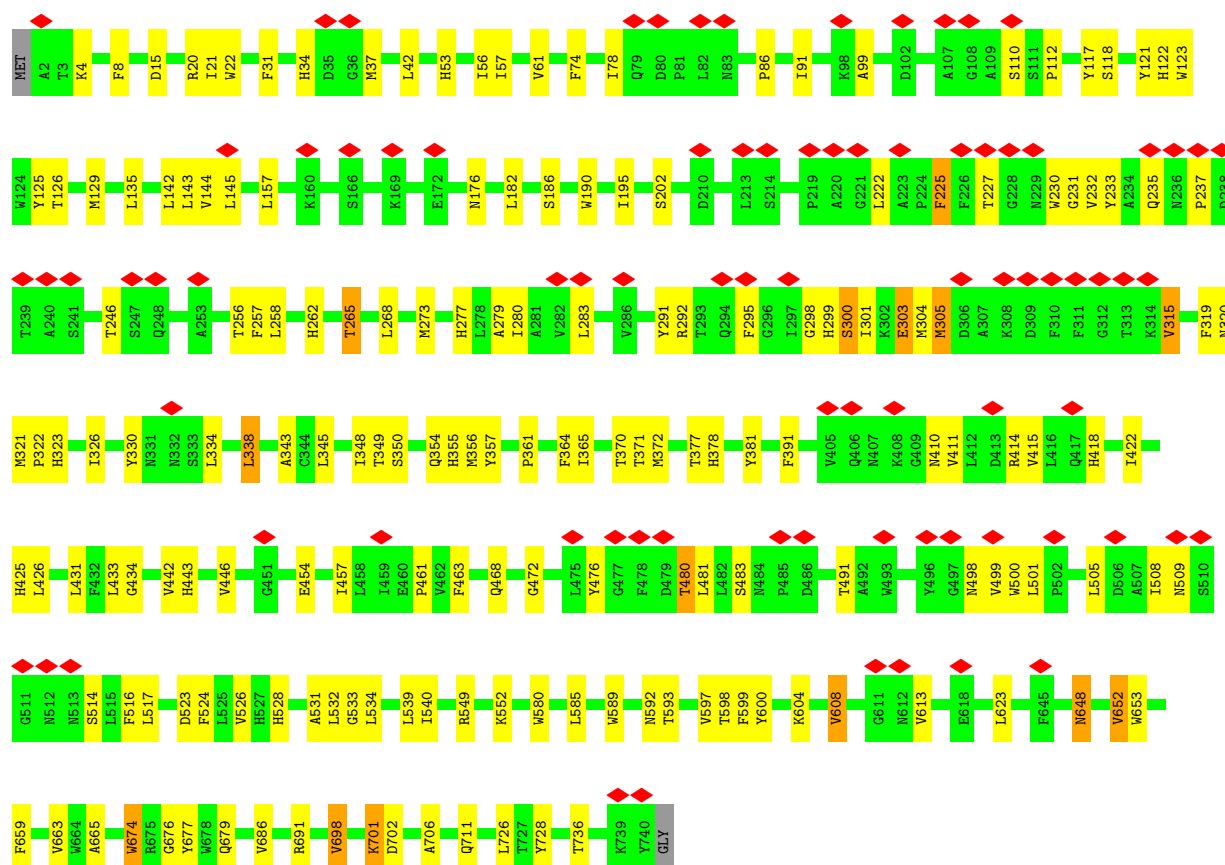
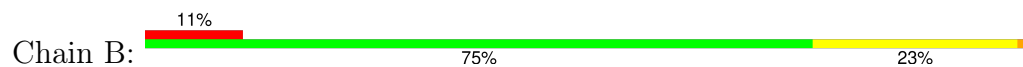
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



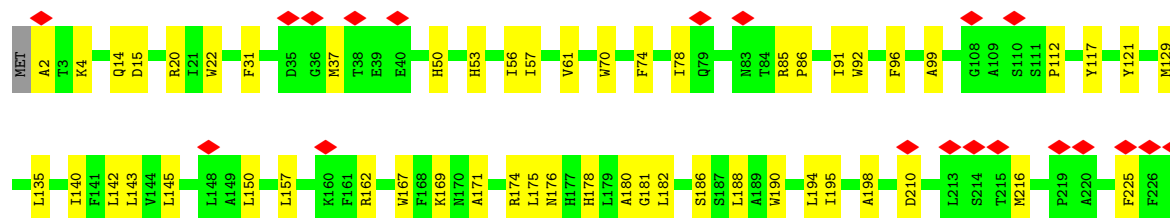


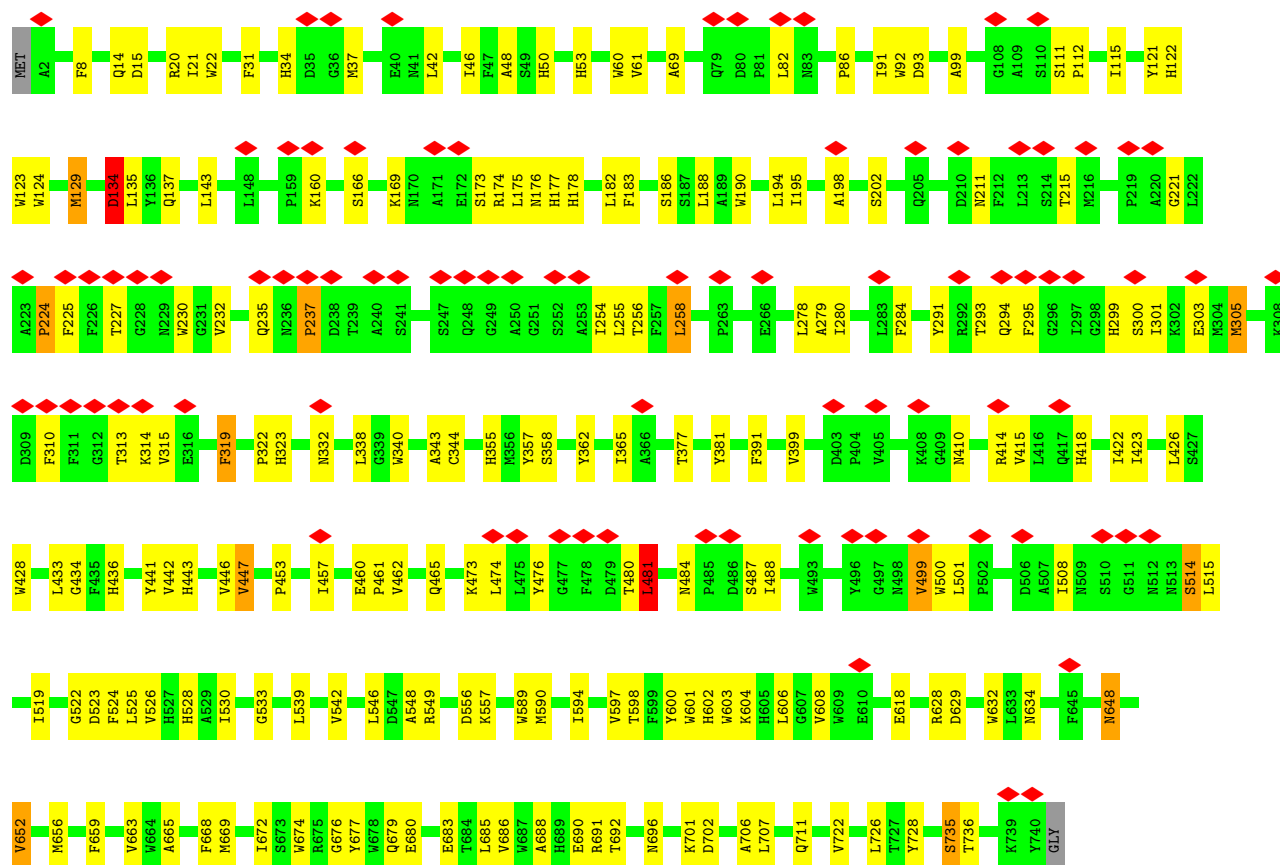


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

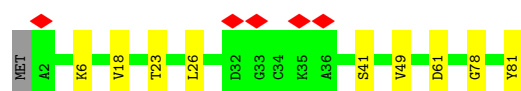
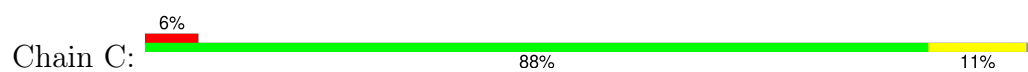


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

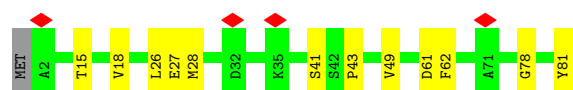
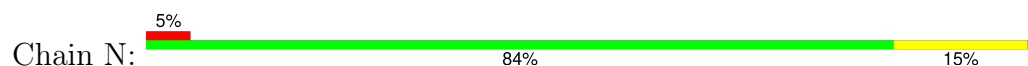




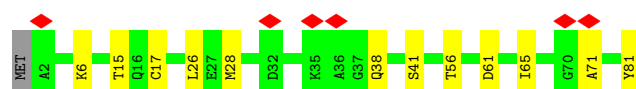
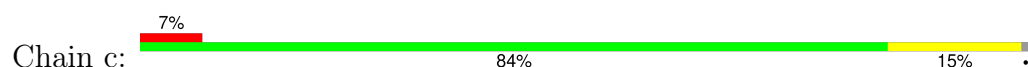
- Molecule 3: Photosystem I iron-sulfur center



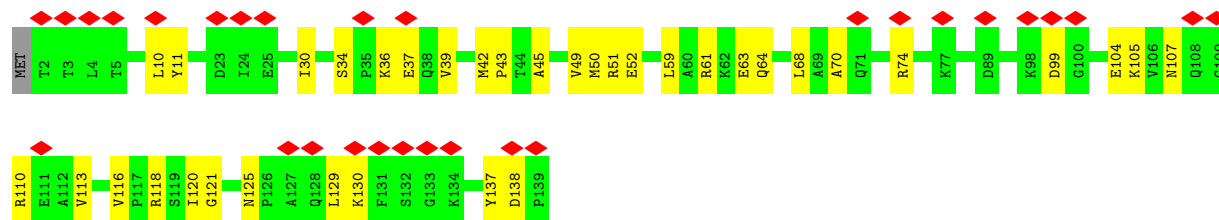
- Molecule 3: Photosystem I iron-sulfur center



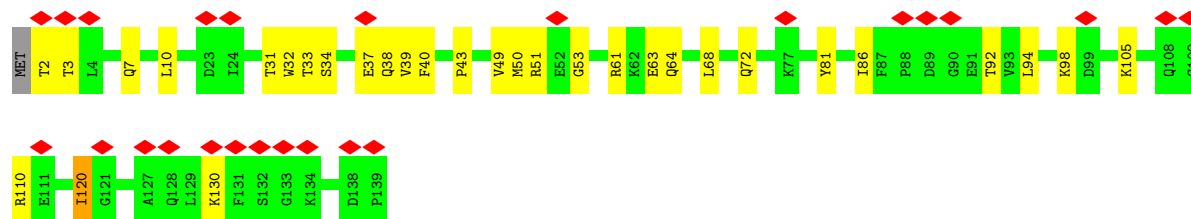
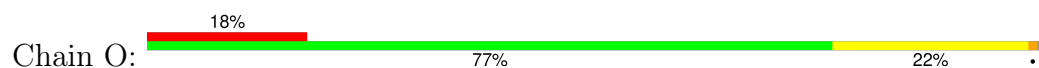
- Molecule 3: Photosystem I iron-sulfur center



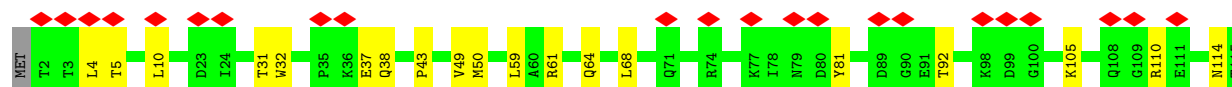
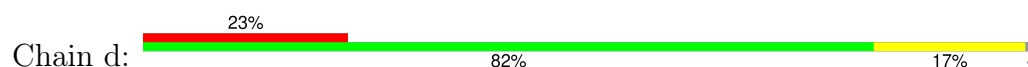
- Molecule 4: Photosystem I reaction center subunit II

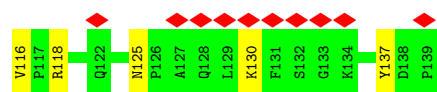


- Molecule 4: Photosystem I reaction center subunit II

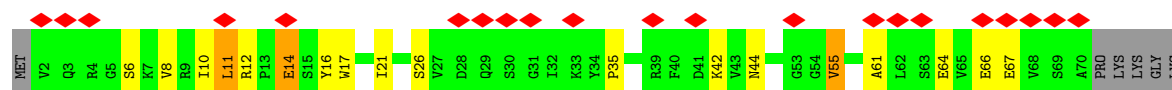


- Molecule 4: Photosystem I reaction center subunit II

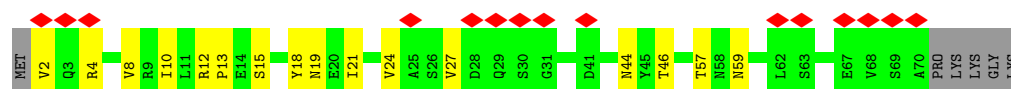




• Molecule 5: Photosystem I reaction center subunit IV



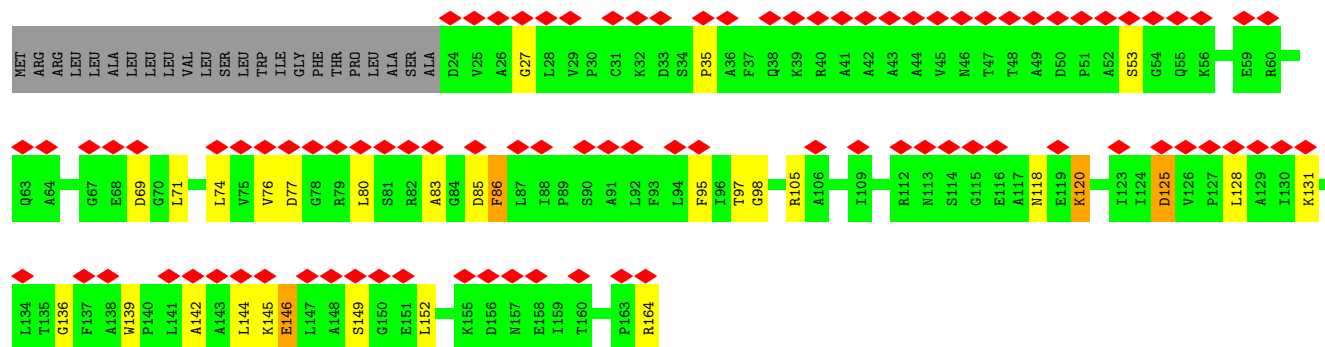
• Molecule 5: Photosystem I reaction center subunit IV



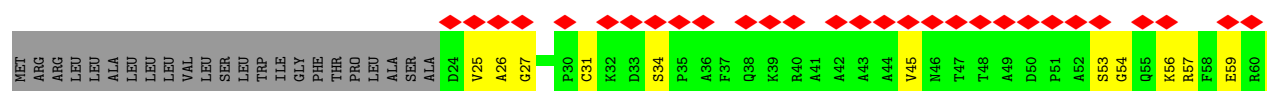
• Molecule 5: Photosystem I reaction center subunit IV

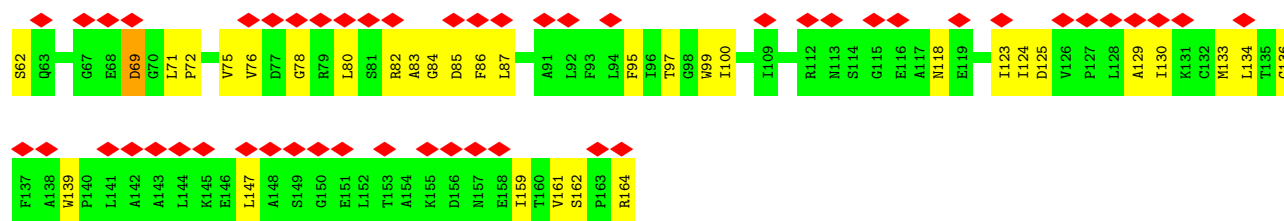


• Molecule 6: Photosystem I reaction center subunit III

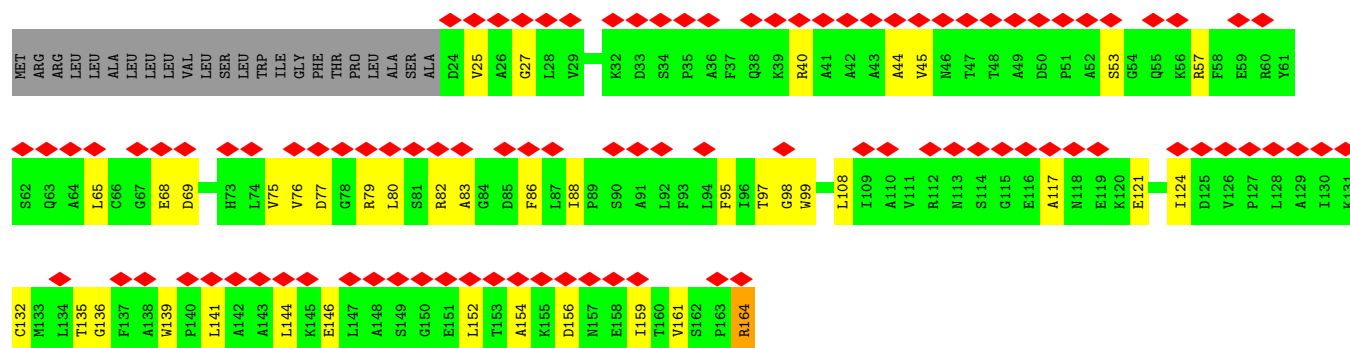


• Molecule 6: Photosystem I reaction center subunit III





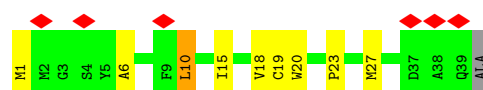
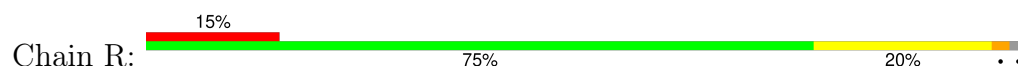
• Molecule 6: Photosystem I reaction center subunit III



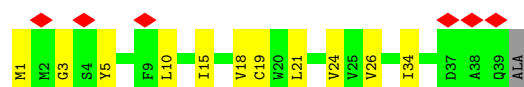
• Molecule 7: Photosystem I reaction center subunit VIII



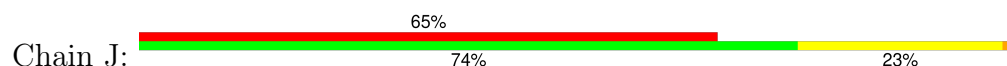
• Molecule 7: Photosystem I reaction center subunit VIII



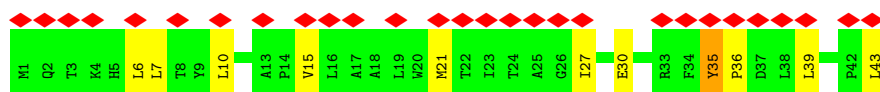
• Molecule 7: Photosystem I reaction center subunit VIII



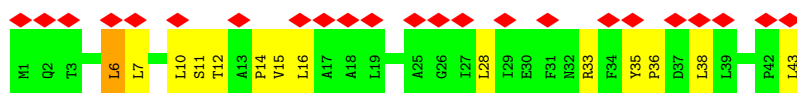
• Molecule 8: Photosystem I reaction center subunit IX



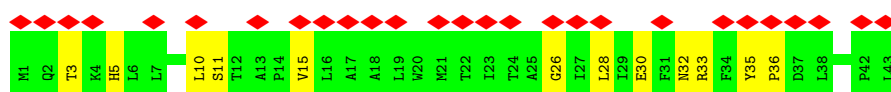
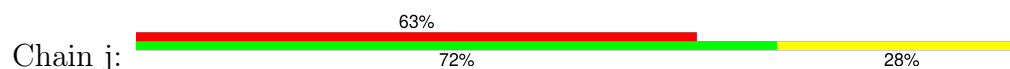




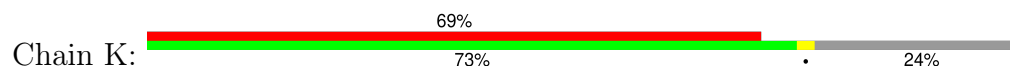
• Molecule 8: Photosystem I reaction center subunit IX



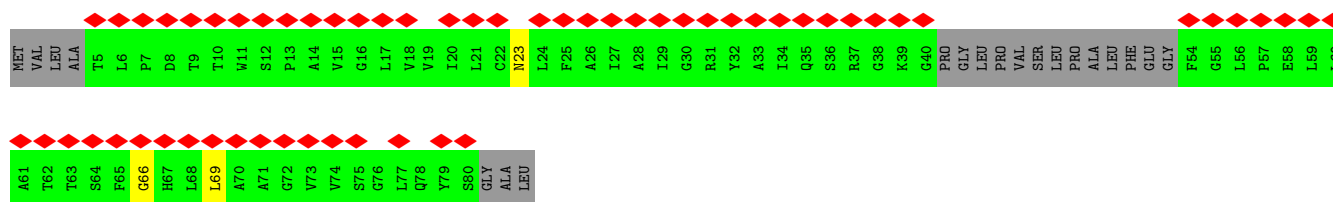
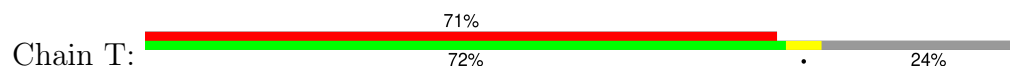
• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 9: Photosystem I reaction center subunit Psak

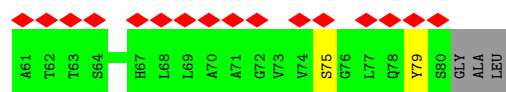


• Molecule 9: Photosystem I reaction center subunit Psak

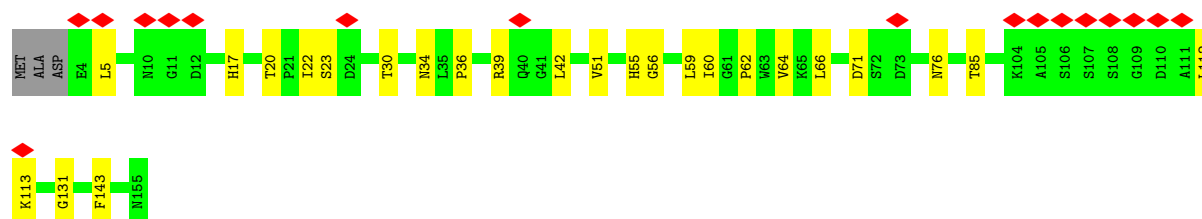
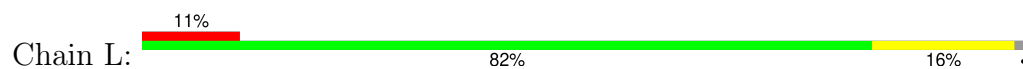


• Molecule 9: Photosystem I reaction center subunit Psak

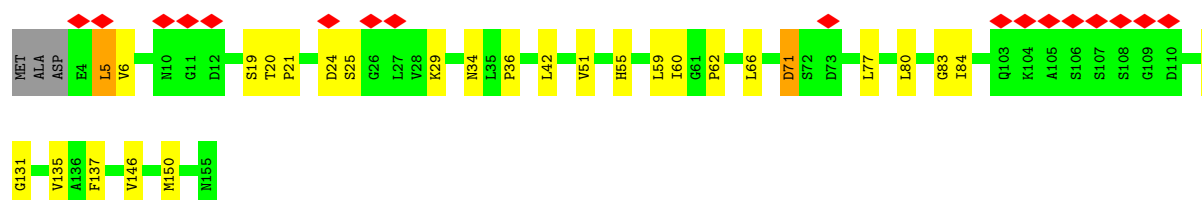
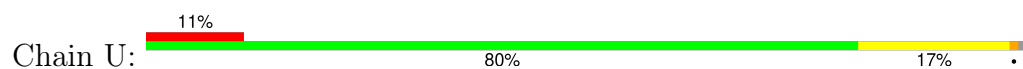




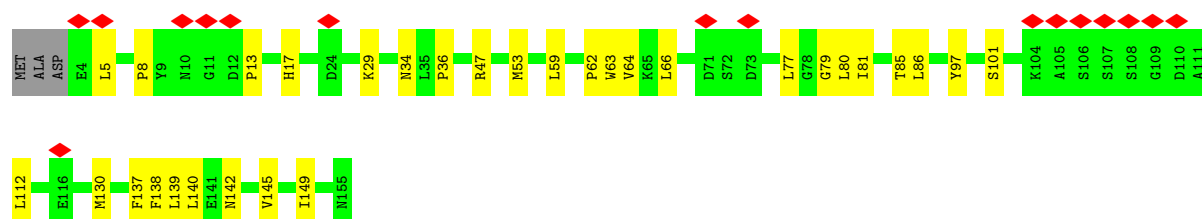
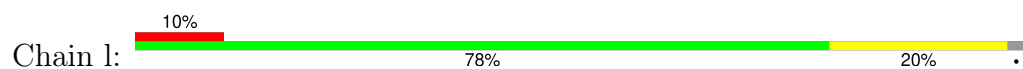
• Molecule 10: Photosystem I reaction center subunit XI



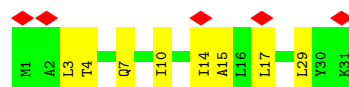
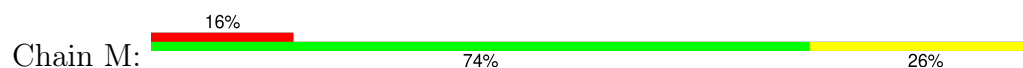
• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI

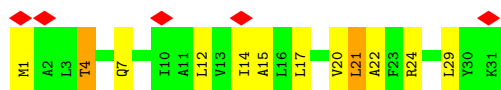


• Molecule 11: Photosystem I reaction center subunit XII

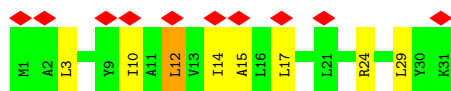
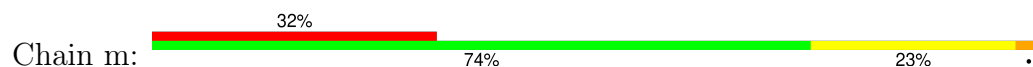


• Molecule 11: Photosystem I reaction center subunit XII





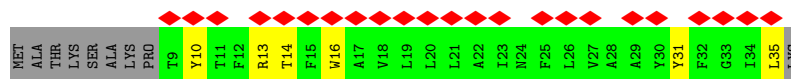
- Molecule 11: Photosystem I reaction center subunit XII



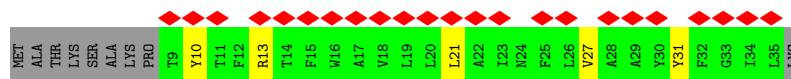
- Molecule 12: Phosphorylase



- Molecule 12: Phosphorylase



- Molecule 12: Phosphorylase



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	189655	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.050	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.00404	Depositor
Map size (Å)	297.0, 297.0, 297.0	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.825, 0.825, 0.825	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, CA, BCR, CL0, PQN, SF4, LMG, CLA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	4/5978 (0.1%)	0.83	11/8158 (0.1%)
1	G	0.30	0/5978	0.63	6/8158 (0.1%)
1	a	0.31	0/5978	0.64	2/8158 (0.0%)
2	B	0.31	0/6110	0.65	2/8350 (0.0%)
2	H	0.40	2/6110 (0.0%)	0.70	9/8350 (0.1%)
2	b	0.49	6/6110 (0.1%)	0.83	20/8350 (0.2%)
3	C	0.24	0/608	0.51	0/824
3	N	0.23	0/608	0.54	0/824
3	c	0.21	0/608	0.54	0/824
4	D	0.27	0/1101	0.64	0/1492
4	O	0.29	0/1101	0.64	0/1492
4	d	0.27	0/1101	0.64	0/1492
5	E	0.22	0/544	0.63	0/737
5	P	0.28	0/544	0.61	0/737
5	e	0.69	2/544 (0.4%)	1.50	3/737 (0.4%)
6	F	0.30	0/1086	0.84	4/1474 (0.3%)
6	Q	0.32	0/1086	0.79	2/1474 (0.1%)
6	f	0.29	0/1086	0.73	0/1474
7	I	0.31	0/319	0.74	0/436
7	R	0.30	0/319	0.67	0/436
7	i	0.31	0/319	0.69	0/436
8	J	0.40	0/362	0.85	0/494
8	S	0.31	0/362	0.79	0/494
8	j	0.33	0/362	0.81	0/494
9	K	0.23	0/305	0.83	0/419
9	T	0.22	0/305	0.84	0/419
9	k	0.22	0/305	0.82	0/419
10	L	0.29	0/1153	0.55	0/1562
10	U	0.29	0/1153	0.56	0/1562
10	l	0.27	0/1153	0.53	0/1562
11	M	0.32	0/243	0.53	0/330
11	V	0.34	0/243	0.52	0/330

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	m	0.36	0/243	0.54	0/330
12	W	0.24	0/236	0.55	0/323
12	X	0.23	0/236	0.61	0/323
12	x	0.23	0/236	0.59	0/323
All	All	0.37	14/54135 (0.0%)	0.71	59/73797 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
2	B	0	1
4	D	0	1
4	O	0	1
4	d	0	1
6	F	0	1
All	All	0	6

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	224	PRO	CG-CD	-22.05	0.75	1.50
1	A	379	PRO	CB-CG	19.23	2.45	1.49
1	A	379	PRO	CG-CD	-18.55	0.87	1.50
2	H	502	PRO	CG-CD	-16.15	0.95	1.50
5	e	13	PRO	N-CA	9.72	1.59	1.47

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	PRO	CB-CG-CD	-33.15	0.01	106.10
2	b	224	PRO	N-CD-CG	-23.99	67.21	103.20
5	e	13	PRO	N-CD-CG	-23.22	68.37	103.20
5	e	13	PRO	CB-CG-CD	23.05	179.88	106.10
5	e	13	PRO	CA-CB-CG	-18.14	70.04	104.50

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	376	ALA	Peptide
2	B	674	TRP	Peptide
4	D	130	LYS	Peptide
6	F	86	PHE	Peptide
4	O	130	LYS	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5777	0	5627	151	0
1	G	5777	0	5627	130	0
1	a	5777	0	5627	156	0
2	B	5892	0	5646	143	0
2	H	5892	0	5646	145	0
2	b	5892	0	5646	156	0
3	C	598	0	577	9	0
3	N	598	0	577	11	0
3	c	598	0	577	11	0
4	D	1076	0	1083	23	0
4	O	1076	0	1083	19	0
4	d	1076	0	1083	13	0
5	E	534	0	519	12	0
5	P	534	0	519	9	0
5	e	534	0	519	11	0
6	F	1064	0	1072	19	0
6	Q	1064	0	1072	29	0
6	f	1064	0	1072	28	0
7	I	308	0	314	7	0
7	R	308	0	314	10	0
7	i	308	0	314	8	0
8	J	351	0	364	6	0
8	S	351	0	364	10	0
8	j	351	0	364	8	0
9	K	307	0	150	1	0
9	T	307	0	150	2	0
9	k	307	0	150	3	0
10	L	1125	0	1129	18	0
10	U	1125	0	1129	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	l	1125	0	1129	25	0
11	M	240	0	264	5	0
11	V	240	0	264	8	0
11	m	240	0	264	5	0
12	W	228	0	230	3	0
12	X	228	0	230	3	0
12	x	228	0	230	5	0
13	A	65	0	72	3	0
13	G	65	0	72	6	0
13	a	65	0	72	5	0
14	A	2455	0	2328	126	0
14	B	2239	0	2141	133	0
14	F	82	0	57	1	0
14	G	2451	0	2327	109	0
14	H	2239	0	2137	127	0
14	J	45	0	32	1	0
14	K	86	0	61	0	0
14	L	255	0	274	17	0
14	M	45	0	32	1	0
14	Q	90	0	65	3	0
14	S	82	0	56	0	0
14	T	45	0	32	1	0
14	U	255	0	273	17	0
14	V	45	0	32	1	0
14	W	45	0	32	1	0
14	X	45	0	32	1	0
14	a	2431	0	2281	125	0
14	b	2239	0	2137	142	0
14	f	45	0	32	2	0
14	i	65	0	72	7	0
14	j	82	0	56	2	0
14	k	45	0	32	0	0
14	l	255	0	274	17	0
14	m	45	0	32	3	0
14	x	45	0	32	1	0
15	A	33	0	46	7	0
15	B	33	0	46	4	0
15	G	33	0	46	6	0
15	H	33	0	46	3	0
15	a	33	0	46	4	0
15	b	33	0	46	4	0
16	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	C	16	0	0	0	0
16	G	8	0	0	1	0
16	N	16	0	0	0	0
16	a	8	0	0	0	0
16	c	16	0	0	1	0
17	A	240	0	293	20	0
17	B	305	0	372	28	0
17	F	40	0	49	3	0
17	G	240	0	294	15	0
17	H	265	0	322	25	0
17	I	80	0	98	9	0
17	J	80	0	97	7	0
17	L	80	0	98	6	0
17	M	40	0	49	2	0
17	Q	80	0	98	7	0
17	R	120	0	147	10	0
17	S	80	0	97	12	0
17	U	40	0	49	3	0
17	V	40	0	49	3	0
17	a	240	0	293	22	0
17	b	265	0	323	26	0
17	f	80	0	98	10	0
17	i	40	0	49	6	0
17	j	80	0	98	11	0
17	l	120	0	147	6	0
17	m	40	0	49	4	0
18	A	76	0	98	6	0
18	G	76	0	98	6	0
18	a	76	0	98	1	0
19	B	49	0	71	3	0
19	H	49	0	71	2	0
19	b	49	0	71	2	0
20	L	1	0	0	0	0
20	U	1	0	0	0	0
20	l	1	0	0	0	0
All	All	71694	0	69952	1676	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 12.

The worst 5 of 1676 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:PRO:CG	1:A:379:PRO:N	1.92	1.32
1:A:379:PRO:CD	1:A:379:PRO:HG2	1.65	1.14
1:A:379:PRO:CD	1:A:379:PRO:HG3	1.65	1.13
1:A:379:PRO:CG	1:A:379:PRO:HD2	1.53	1.00
1:A:379:PRO:CG	1:A:379:PRO:HD3	1.53	1.00

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	738/755 (98%)	707 (96%)	29 (4%)	2 (0%)	37	45
1	G	738/755 (98%)	708 (96%)	28 (4%)	2 (0%)	37	45
1	a	738/755 (98%)	704 (95%)	32 (4%)	2 (0%)	37	45
2	B	737/741 (100%)	701 (95%)	34 (5%)	2 (0%)	37	45
2	H	737/741 (100%)	699 (95%)	36 (5%)	2 (0%)	37	45
2	b	737/741 (100%)	698 (95%)	37 (5%)	2 (0%)	37	45
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	N	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	136/139 (98%)	123 (90%)	13 (10%)	0	100	100
4	O	136/139 (98%)	123 (90%)	13 (10%)	0	100	100
4	d	136/139 (98%)	124 (91%)	12 (9%)	0	100	100
5	E	67/75 (89%)	65 (97%)	2 (3%)	0	100	100
5	P	67/75 (89%)	64 (96%)	3 (4%)	0	100	100
5	e	67/75 (89%)	63 (94%)	4 (6%)	0	100	100
6	F	139/164 (85%)	126 (91%)	12 (9%)	1 (1%)	19	22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Q	139/164 (85%)	125 (90%)	13 (9%)	1 (1%)	19	22
6	f	139/164 (85%)	124 (89%)	14 (10%)	1 (1%)	19	22
7	I	37/40 (92%)	33 (89%)	4 (11%)	0	100	100
7	R	37/40 (92%)	35 (95%)	2 (5%)	0	100	100
7	i	37/40 (92%)	37 (100%)	0	0	100	100
8	J	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
8	S	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
8	j	41/43 (95%)	35 (85%)	6 (15%)	0	100	100
9	K	59/83 (71%)	54 (92%)	5 (8%)	0	100	100
9	T	59/83 (71%)	55 (93%)	4 (7%)	0	100	100
9	k	59/83 (71%)	54 (92%)	5 (8%)	0	100	100
10	L	150/155 (97%)	146 (97%)	4 (3%)	0	100	100
10	U	150/155 (97%)	144 (96%)	6 (4%)	0	100	100
10	l	150/155 (97%)	145 (97%)	5 (3%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
12	W	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
12	X	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
12	x	25/36 (69%)	24 (96%)	1 (4%)	0	100	100
All	All	6708/7029 (95%)	6344 (95%)	349 (5%)	15 (0%)	45	53

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	497	ALA
2	B	315	VAL
1	G	233	ALA
1	G	497	ALA
2	H	315	VAL

### 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	588/603 (98%)	573 (97%)	15 (3%)	41	56
1	G	588/603 (98%)	570 (97%)	18 (3%)	35	49
1	a	588/603 (98%)	569 (97%)	19 (3%)	34	47
2	B	599/600 (100%)	572 (96%)	27 (4%)	23	32
2	H	599/600 (100%)	580 (97%)	19 (3%)	34	47
2	b	599/600 (100%)	570 (95%)	29 (5%)	21	29
3	C	67/68 (98%)	67 (100%)	0	100	100
3	N	67/68 (98%)	67 (100%)	0	100	100
3	c	67/68 (98%)	66 (98%)	1 (2%)	60	74
4	D	115/116 (99%)	114 (99%)	1 (1%)	75	86
4	O	115/116 (99%)	113 (98%)	2 (2%)	56	70
4	d	115/116 (99%)	111 (96%)	4 (4%)	31	43
5	E	58/63 (92%)	53 (91%)	5 (9%)	8	10
5	P	58/63 (92%)	55 (95%)	3 (5%)	19	26
5	e	58/63 (92%)	56 (97%)	2 (3%)	32	45
6	F	109/128 (85%)	106 (97%)	3 (3%)	38	52
6	Q	109/128 (85%)	102 (94%)	7 (6%)	14	18
6	f	109/128 (85%)	105 (96%)	4 (4%)	29	41
7	I	33/33 (100%)	32 (97%)	1 (3%)	36	50
7	R	33/33 (100%)	32 (97%)	1 (3%)	36	50
7	i	33/33 (100%)	32 (97%)	1 (3%)	36	50
8	J	38/38 (100%)	34 (90%)	4 (10%)	5	5
8	S	38/38 (100%)	36 (95%)	2 (5%)	19	25
8	j	38/38 (100%)	37 (97%)	1 (3%)	41	56
10	L	115/117 (98%)	111 (96%)	4 (4%)	31	43
10	U	115/117 (98%)	111 (96%)	4 (4%)	31	43
10	l	115/117 (98%)	114 (99%)	1 (1%)	75	86
11	M	25/25 (100%)	23 (92%)	2 (8%)	10	11
11	V	25/25 (100%)	20 (80%)	5 (20%)	1	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	m	25/25 (100%)	22 (88%)	3 (12%)	4	4
12	W	22/29 (76%)	19 (86%)	3 (14%)	3	2
12	X	22/29 (76%)	20 (91%)	2 (9%)	7	8
12	x	22/29 (76%)	22 (100%)	0	100	100
All	All	5307/5460 (97%)	5114 (96%)	193 (4%)	32	42

5 of 193 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	U	19	SER
1	a	511	VAL
11	V	4	THR
1	a	117	VAL
2	b	160	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 124 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	262	HIS
2	b	407	ASN
4	O	72	GLN
2	b	354	GLN
5	e	19	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 381 ligands modelled in this entry, 3 are monoatomic - leaving 378 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
17	BCR	S	104	-	41,41,41	2.72	6 (14%)	56,56,56	6.88	20 (35%)
14	CLA	a	812	-	48,58,73	2.65	21 (43%)	56,95,113	2.77	22 (39%)
14	CLA	b	810	-	43,53,73	2.72	19 (44%)	50,89,113	2.83	21 (42%)
14	CLA	U	204	10	58,68,73	2.39	20 (34%)	68,107,113	2.61	21 (30%)
14	CLA	B	823	2	48,58,73	2.62	18 (37%)	56,95,113	2.72	22 (39%)
14	CLA	b	804	-	63,73,73	2.24	20 (31%)	74,113,113	2.49	26 (35%)
17	BCR	b	847	-	41,41,41	2.67	6 (14%)	56,56,56	6.78	18 (32%)
14	CLA	j	101	-	43,53,73	2.67	20 (46%)	50,89,113	2.95	24 (48%)
14	CLA	a	822	-	43,53,73	2.66	18 (41%)	50,89,113	2.85	20 (40%)
14	CLA	H	817	-	58,68,73	2.37	21 (36%)	68,107,113	2.57	25 (36%)
17	BCR	B	842	-	41,41,41	2.67	6 (14%)	56,56,56	6.60	18 (32%)
14	CLA	b	821	-	53,63,73	2.51	21 (39%)	62,101,113	2.66	27 (43%)
14	CLA	A	820	-	63,73,73	2.30	21 (33%)	74,113,113	2.44	28 (37%)
14	CLA	A	807	-	63,73,73	2.26	19 (30%)	74,113,113	2.50	24 (32%)
17	BCR	b	846	-	41,41,41	2.69	6 (14%)	56,56,56	6.59	23 (41%)
19	LMG	H	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.05	3 (5%)
14	CLA	X	1701	12	43,53,73	2.65	20 (46%)	50,89,113	2.83	20 (40%)
14	CLA	G	844	-	39,49,73	2.62	17 (43%)	46,83,113	2.86	22 (47%)
14	CLA	G	820	-	63,73,73	2.32	21 (33%)	74,113,113	2.57	27 (36%)
14	CLA	H	840	-	63,73,73	2.22	20 (31%)	74,113,113	2.59	25 (33%)
14	CLA	U	201	2	63,73,73	2.26	21 (33%)	74,113,113	2.62	28 (37%)
15	PQN	B	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.15	5 (11%)
14	CLA	b	817	-	58,68,73	2.36	20 (34%)	68,107,113	2.57	23 (33%)
17	BCR	B	846	-	41,41,41	2.73	6 (14%)	56,56,56	6.59	24 (42%)
14	CLA	H	832	-	53,63,73	2.53	22 (41%)	62,101,113	2.77	24 (38%)
14	CLA	H	828	-	63,73,73	2.32	20 (31%)	74,113,113	2.53	26 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	H	830	-	43,53,73	2.67	20 (46%)	50,89,113	2.80	22 (44%)
14	CLA	Q	203	-	43,53,73	2.66	18 (41%)	50,89,113	2.60	19 (38%)
18	LHG	A	855	14	26,26,48	1.26	2 (7%)	29,32,54	1.19	2 (6%)
14	CLA	b	818	-	63,73,73	2.33	20 (31%)	74,113,113	2.49	25 (33%)
14	CLA	a	825	-	63,73,73	2.35	20 (31%)	74,113,113	2.31	27 (36%)
14	CLA	m	1601	-	43,53,73	2.66	20 (46%)	50,89,113	2.92	23 (46%)
14	CLA	b	807	-	63,73,73	2.27	19 (30%)	74,113,113	2.50	23 (31%)
14	CLA	a	827	-	63,73,73	2.23	19 (30%)	74,113,113	2.71	27 (36%)
14	CLA	H	808	-	63,73,73	2.26	18 (28%)	74,113,113	2.49	24 (32%)
14	CLA	B	839	-	63,73,73	2.27	20 (31%)	74,113,113	2.40	24 (32%)
14	CLA	A	837	1	43,53,73	2.67	19 (44%)	50,89,113	2.78	21 (42%)
17	BCR	R	102	-	41,41,41	2.75	6 (14%)	56,56,56	6.53	25 (44%)
14	CLA	b	824	-	43,53,73	2.69	19 (44%)	50,89,113	2.74	19 (38%)
14	CLA	G	810	1	63,73,73	2.29	19 (30%)	74,113,113	2.48	25 (33%)
14	CLA	H	818	-	63,73,73	2.27	21 (33%)	74,113,113	2.50	24 (32%)
14	CLA	a	802	-	63,73,73	2.26	18 (28%)	74,113,113	2.35	24 (32%)
14	CLA	G	813	-	48,58,73	2.63	20 (41%)	56,95,113	2.76	24 (42%)
14	CLA	b	806	-	63,73,73	2.30	20 (31%)	74,113,113	2.56	28 (37%)
14	CLA	j	102	-	35,45,73	2.80	18 (51%)	42,78,113	2.85	19 (45%)
14	CLA	B	806	-	63,73,73	2.24	19 (30%)	74,113,113	2.54	24 (32%)
14	CLA	G	837	1	43,53,73	2.66	20 (46%)	50,89,113	2.87	21 (42%)
14	CLA	b	836	-	58,68,73	2.43	20 (34%)	68,107,113	2.50	24 (35%)
14	CLA	A	804	-	53,63,73	2.49	20 (37%)	62,101,113	2.71	25 (40%)
14	CLA	b	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.97	24 (48%)
14	CLA	a	833	-	63,73,73	2.29	20 (31%)	74,113,113	2.43	22 (29%)
15	PQN	A	846	-	34,34,34	1.63	2 (5%)	43,45,45	1.27	5 (11%)
14	CLA	a	834	-	63,73,73	2.27	19 (30%)	74,113,113	2.44	22 (29%)
14	CLA	L	205	-	63,73,73	2.28	19 (30%)	74,113,113	2.54	25 (33%)
14	CLA	F	1303	-	35,45,73	2.77	18 (51%)	42,78,113	2.84	18 (42%)
14	CLA	H	833	-	43,53,73	2.66	19 (44%)	50,89,113	2.76	21 (42%)
14	CLA	G	804	-	53,63,73	2.50	20 (37%)	62,101,113	2.72	26 (41%)
18	LHG	a	853	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	3 (5%)
14	CLA	G	841	-	63,73,73	2.29	21 (33%)	74,113,113	2.49	25 (33%)
14	CLA	B	834	-	43,53,73	2.64	19 (44%)	50,89,113	2.78	20 (40%)
17	BCR	M	1602	-	41,41,41	2.57	6 (14%)	56,56,56	6.73	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	a	849	-	41,41,41	2.70	6 (14%)	56,56,56	6.56	23 (41%)
14	CLA	G	827	-	58,68,73	2.39	20 (34%)	68,107,113	2.58	26 (38%)
17	BCR	b	844	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	22 (39%)
14	CLA	B	815	-	43,53,73	2.68	18 (41%)	50,89,113	2.88	21 (42%)
14	CLA	G	821	-	48,58,73	2.61	19 (39%)	56,95,113	2.94	26 (46%)
14	CLA	A	805	14	53,63,73	2.50	21 (39%)	62,101,113	2.81	26 (41%)
14	CLA	b	815	-	43,53,73	2.63	19 (44%)	50,89,113	2.84	21 (42%)
14	CLA	a	809	-	63,73,73	2.29	18 (28%)	74,113,113	2.47	26 (35%)
14	CLA	B	831	-	63,73,73	2.31	20 (31%)	74,113,113	2.51	25 (33%)
14	CLA	G	809	1	63,73,73	2.27	20 (31%)	74,113,113	2.57	27 (36%)
14	CLA	G	843	-	63,73,73	2.26	19 (30%)	74,113,113	2.37	24 (32%)
14	CLA	b	805	-	52,62,73	2.55	21 (40%)	60,99,113	2.80	24 (40%)
14	CLA	a	855	-	63,73,73	2.30	19 (30%)	74,113,113	2.40	25 (33%)
14	CLA	a	838	-	63,73,73	2.28	20 (31%)	74,113,113	2.49	27 (36%)
14	CLA	a	824	-	53,63,73	2.50	20 (37%)	62,101,113	2.68	24 (38%)
14	CLA	A	839	-	63,73,73	2.25	21 (33%)	74,113,113	2.51	28 (37%)
17	BCR	B	847	-	41,41,41	2.69	6 (14%)	56,56,56	6.65	24 (42%)
17	BCR	V	1602	-	41,41,41	2.58	6 (14%)	56,56,56	6.72	20 (35%)
14	CLA	B	804	-	52,62,73	2.54	21 (40%)	60,99,113	2.81	24 (40%)
14	CLA	H	822	-	43,53,73	2.61	17 (39%)	50,89,113	2.83	21 (42%)
19	LMG	b	848	-	49,49,55	1.40	6 (12%)	57,57,63	1.06	4 (7%)
14	CLA	A	810	1	63,73,73	2.28	19 (30%)	74,113,113	2.48	25 (33%)
14	CLA	G	822	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	26 (35%)
14	CLA	a	810	-	43,53,73	2.69	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	816	-	43,53,73	2.68	20 (46%)	50,89,113	2.84	21 (42%)
14	CLA	a	826	-	58,68,73	2.33	19 (32%)	68,107,113	2.70	25 (36%)
14	CLA	S	101	8	43,53,73	2.67	20 (46%)	50,89,113	2.82	22 (44%)
17	BCR	G	851	-	41,41,41	2.73	6 (14%)	56,56,56	6.71	22 (39%)
14	CLA	G	803	-	63,73,73	2.25	17 (26%)	74,113,113	2.35	25 (33%)
17	BCR	a	851	-	41,41,41	2.67	6 (14%)	56,56,56	6.61	22 (39%)
14	CLA	a	807	-	43,53,73	2.66	19 (44%)	50,89,113	2.81	21 (42%)
14	CLA	A	823	-	43,53,73	2.67	19 (44%)	50,89,113	2.91	20 (40%)
14	CLA	A	825	-	53,63,73	2.48	20 (37%)	62,101,113	2.71	24 (38%)
14	CLA	A	841	-	63,73,73	2.33	20 (31%)	74,113,113	2.51	23 (31%)
14	CLA	H	823	2	48,58,73	2.62	18 (37%)	56,95,113	2.68	23 (41%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	H	825	-	63,73,73	2.27	19 (30%)	74,113,113	2.53	26 (35%)
14	CLA	b	839	-	63,73,73	2.26	20 (31%)	74,113,113	2.48	26 (35%)
14	CLA	a	811	14	63,73,73	2.26	21 (33%)	74,113,113	2.54	22 (29%)
14	CLA	G	840	-	43,53,73	2.62	19 (44%)	50,89,113	2.78	19 (38%)
14	CLA	B	818	-	63,73,73	2.28	21 (33%)	74,113,113	2.49	24 (32%)
14	CLA	B	835	-	43,53,73	2.66	19 (44%)	50,89,113	2.83	21 (42%)
14	CLA	G	807	-	63,73,73	2.27	19 (30%)	74,113,113	2.53	23 (31%)
16	SF4	a	846	2,1	0,12,12	-	-	-	-	-
14	CLA	a	823	-	43,53,73	2.65	19 (44%)	50,89,113	2.89	21 (42%)
17	BCR	G	853	-	41,41,41	2.69	6 (14%)	56,56,56	6.81	25 (44%)
14	CLA	A	815	-	43,53,73	2.65	20 (46%)	50,89,113	2.90	22 (44%)
14	CLA	T	1401	-	43,53,73	2.69	20 (46%)	50,89,113	2.74	23 (46%)
14	CLA	G	811	-	43,53,73	2.66	20 (46%)	50,89,113	2.98	22 (44%)
15	PQN	a	845	-	34,34,34	1.61	2 (5%)	43,45,45	1.26	5 (11%)
14	CLA	A	835	-	63,73,73	2.24	18 (28%)	74,113,113	2.42	21 (28%)
14	CLA	M	1601	-	43,53,73	2.64	19 (44%)	50,89,113	2.91	20 (40%)
14	CLA	H	805	-	63,73,73	2.29	18 (28%)	74,113,113	2.51	25 (33%)
15	PQN	G	846	-	34,34,34	1.59	2 (5%)	43,45,45	1.19	4 (9%)
14	CLA	H	804	-	52,62,73	2.56	21 (40%)	60,99,113	2.76	25 (41%)
14	CLA	a	816	-	43,53,73	2.65	20 (46%)	50,89,113	2.78	21 (42%)
17	BCR	a	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.63	19 (33%)
14	CLA	G	802	-	63,73,73	2.23	18 (28%)	74,113,113	2.52	23 (31%)
15	PQN	H	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.11	3 (6%)
14	CLA	B	830	-	43,53,73	2.68	19 (44%)	50,89,113	2.82	24 (48%)
14	CLA	a	832	-	53,63,73	2.55	20 (37%)	62,101,113	2.68	25 (40%)
17	BCR	R	103	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	20 (35%)
14	CLA	A	824	-	43,53,73	2.68	19 (44%)	50,89,113	2.87	21 (42%)
14	CLA	F	1301	-	43,53,73	2.67	18 (41%)	50,89,113	2.66	21 (42%)
14	CLA	H	802	-	63,73,73	2.26	18 (28%)	74,113,113	2.44	25 (33%)
14	CLA	B	816	-	53,63,73	2.50	20 (37%)	62,101,113	2.68	27 (43%)
14	CLA	b	823	2	48,58,73	2.59	18 (37%)	56,95,113	2.66	23 (41%)
14	CLA	B	813	-	53,63,73	2.50	19 (35%)	62,101,113	2.71	22 (35%)
14	CLA	l	202	2	63,73,73	2.25	19 (30%)	74,113,113	2.69	31 (41%)
14	CLA	A	812	14	63,73,73	2.26	21 (33%)	74,113,113	2.52	24 (32%)
17	BCR	L	207	-	41,41,41	2.73	6 (14%)	56,56,56	6.38	22 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	B	844	-	41,41,41	2.64	6 (14%)	56,56,56	6.53	22 (39%)
14	CLA	a	839	-	43,53,73	2.63	19 (44%)	50,89,113	2.78	22 (44%)
14	CLA	A	829	-	63,73,73	2.28	18 (28%)	74,113,113	2.40	24 (32%)
17	BCR	G	850	-	41,41,41	2.79	6 (14%)	56,56,56	6.63	26 (46%)
14	CLA	B	828	-	63,73,73	2.28	19 (30%)	74,113,113	2.49	25 (33%)
14	CLA	H	835	-	43,53,73	2.65	19 (44%)	50,89,113	3.17	24 (48%)
14	CLA	U	206	-	63,73,73	2.30	20 (31%)	74,113,113	2.44	23 (31%)
14	CLA	G	839	-	63,73,73	2.28	20 (31%)	74,113,113	2.43	27 (36%)
14	CLA	b	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.92	21 (42%)
14	CLA	G	829	-	63,73,73	2.30	19 (30%)	74,113,113	2.45	25 (33%)
14	CLA	B	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.97	23 (46%)
14	CLA	A	834	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	23 (31%)
17	BCR	A	851	-	41,41,41	2.76	6 (14%)	56,56,56	6.72	26 (46%)
17	BCR	l	208	-	41,41,41	2.65	6 (14%)	56,56,56	6.63	20 (35%)
14	CLA	G	838	-	48,58,73	2.63	20 (41%)	56,95,113	2.82	25 (44%)
17	BCR	b	849	-	41,41,41	2.61	6 (14%)	56,56,56	6.61	18 (32%)
14	CLA	H	836	-	58,68,73	2.41	20 (34%)	68,107,113	2.59	24 (35%)
17	BCR	H	842	-	41,41,41	2.66	6 (14%)	56,56,56	6.57	18 (32%)
14	CLA	G	825	-	53,63,73	2.52	21 (39%)	62,101,113	2.60	23 (37%)
14	CLA	B	821	-	53,63,73	2.50	22 (41%)	62,101,113	2.58	24 (38%)
14	CLA	H	806	-	63,73,73	2.25	19 (30%)	74,113,113	2.52	25 (33%)
14	CLA	l	205	10	58,68,73	2.39	20 (34%)	68,107,113	2.55	24 (35%)
14	CLA	a	814	-	43,53,73	2.68	20 (46%)	50,89,113	2.96	22 (44%)
14	CLA	G	836	-	43,53,73	2.62	19 (44%)	50,89,113	2.70	20 (40%)
14	CLA	A	813	-	48,58,73	2.63	19 (39%)	56,95,113	2.68	22 (39%)
14	CLA	H	827	-	63,73,73	2.30	19 (30%)	74,113,113	2.28	22 (29%)
14	CLA	H	813	-	53,63,73	2.53	19 (35%)	62,101,113	2.63	25 (40%)
14	CLA	b	820	-	43,53,73	2.59	19 (44%)	50,89,113	2.91	20 (40%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	H	810	-	43,53,73	2.73	20 (46%)	50,89,113	2.86	22 (44%)
14	CLA	b	835	-	43,53,73	2.67	20 (46%)	50,89,113	2.76	21 (42%)
14	CLA	A	811	-	43,53,73	2.67	18 (41%)	50,89,113	2.96	22 (44%)
14	CLA	G	826	-	63,73,73	2.29	20 (31%)	74,113,113	2.42	28 (37%)
14	CLA	H	811	-	43,53,73	2.68	19 (44%)	50,89,113	2.71	18 (36%)
17	BCR	J	103	-	41,41,41	2.62	6 (14%)	56,56,56	6.99	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	G	828	-	63,73,73	2.26	20 (31%)	74,113,113	2.52	23 (31%)
14	CLA	A	838	-	48,58,73	2.64	21 (43%)	56,95,113	2.82	23 (41%)
14	CLA	a	842	-	63,73,73	2.30	20 (31%)	74,113,113	2.54	23 (31%)
17	BCR	b	843	-	41,41,41	2.66	7 (17%)	56,56,56	6.72	22 (39%)
16	SF4	A	847	2,1	0,12,12	-	-	-	-	-
14	CLA	b	813	-	53,63,73	2.50	19 (35%)	62,101,113	2.68	24 (38%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	a	815	-	43,53,73	2.69	20 (46%)	50,89,113	2.83	20 (40%)
14	CLA	B	802	-	63,73,73	2.25	18 (28%)	74,113,113	2.50	25 (33%)
14	CLA	a	821	-	63,73,73	2.32	20 (31%)	74,113,113	2.33	24 (32%)
14	CLA	H	829	-	43,53,73	2.57	18 (41%)	50,89,113	2.81	22 (44%)
14	CLA	W	1701	12	43,53,73	2.65	20 (46%)	50,89,113	2.83	21 (42%)
17	BCR	G	848	-	41,41,41	2.66	6 (14%)	56,56,56	6.58	20 (35%)
14	CLA	B	840	-	63,73,73	2.24	19 (30%)	74,113,113	2.60	24 (32%)
14	CLA	A	803	-	63,73,73	2.26	17 (26%)	74,113,113	2.36	24 (32%)
14	CLA	B	825	-	63,73,73	2.29	19 (30%)	74,113,113	2.50	25 (33%)
14	CLA	A	826	-	63,73,73	2.31	20 (31%)	74,113,113	2.48	28 (37%)
14	CLA	b	831	-	63,73,73	2.33	21 (33%)	74,113,113	2.49	26 (35%)
14	CLA	G	815	-	43,53,73	2.67	19 (44%)	50,89,113	2.89	21 (42%)
17	BCR	f	203	-	41,41,41	2.64	6 (14%)	56,56,56	6.28	23 (41%)
15	PQN	b	841	-	34,34,34	1.59	2 (5%)	43,45,45	1.13	5 (11%)
17	BCR	A	850	-	41,41,41	2.67	6 (14%)	56,56,56	6.52	23 (41%)
17	BCR	B	843	-	41,41,41	2.68	7 (17%)	56,56,56	6.66	23 (41%)
17	BCR	j	103	-	41,41,41	2.66	6 (14%)	56,56,56	6.63	23 (41%)
14	CLA	a	844	18	43,53,73	2.68	19 (44%)	50,89,113	3.08	24 (48%)
17	BCR	H	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.82	17 (30%)
14	CLA	a	837	-	48,58,73	2.66	19 (39%)	56,95,113	2.83	26 (46%)
14	CLA	G	833	-	53,63,73	2.54	20 (37%)	62,101,113	2.67	24 (38%)
14	CLA	a	835	-	43,53,73	2.62	18 (41%)	50,89,113	2.67	19 (38%)
17	BCR	I	101	-	41,41,41	2.71	7 (17%)	56,56,56	6.73	19 (33%)
14	CLA	b	834	-	43,53,73	2.65	19 (44%)	50,89,113	3.05	20 (40%)
14	CLA	B	820	-	43,53,73	2.67	19 (44%)	50,89,113	2.94	19 (38%)
14	CLA	a	804	14	53,63,73	2.52	20 (37%)	62,101,113	2.78	25 (40%)
14	CLA	a	806	-	63,73,73	2.25	19 (30%)	74,113,113	2.53	23 (31%)
17	BCR	F	1302	-	41,41,41	2.59	6 (14%)	56,56,56	6.17	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	H	820	-	43,53,73	2.65	19 (44%)	50,89,113	2.88	19 (38%)
14	CLA	H	839	-	63,73,73	2.27	19 (30%)	74,113,113	2.42	23 (31%)
14	CLA	G	814	-	58,68,73	2.41	21 (36%)	68,107,113	2.51	27 (39%)
14	CLA	A	832	-	48,58,73	2.61	18 (37%)	56,95,113	2.70	23 (41%)
14	CLA	a	828	-	63,73,73	2.29	19 (30%)	74,113,113	2.40	25 (33%)
17	BCR	l	203	-	41,41,41	2.76	6 (14%)	56,56,56	6.44	22 (39%)
14	CLA	b	826	-	63,73,73	2.31	20 (31%)	74,113,113	2.41	21 (28%)
14	CLA	A	827	-	58,68,73	2.34	18 (31%)	68,107,113	2.63	25 (36%)
17	BCR	a	850	-	41,41,41	2.76	6 (14%)	56,56,56	6.79	22 (39%)
14	CLA	V	1601	-	43,53,73	2.66	19 (44%)	50,89,113	2.91	23 (46%)
14	CLA	G	806	-	43,53,73	2.61	18 (41%)	50,89,113	2.85	20 (40%)
14	CLA	G	845	18	43,53,73	2.61	19 (44%)	50,89,113	3.14	25 (50%)
17	BCR	B	850	-	41,41,41	2.60	6 (14%)	56,56,56	6.57	17 (30%)
14	CLA	G	832	-	48,58,73	2.60	19 (39%)	56,95,113	2.70	24 (42%)
14	CLA	b	833	-	43,53,73	2.66	19 (44%)	50,89,113	2.82	20 (40%)
14	CLA	A	809	1	63,73,73	2.21	20 (31%)	74,113,113	2.64	27 (36%)
14	CLA	a	817	-	43,53,73	2.63	18 (41%)	50,89,113	2.74	21 (42%)
14	CLA	B	832	-	53,63,73	2.47	21 (39%)	62,101,113	2.66	24 (38%)
14	CLA	H	834	-	43,53,73	2.63	19 (44%)	50,89,113	2.79	19 (38%)
14	CLA	b	814	-	43,53,73	2.67	19 (44%)	50,89,113	2.96	22 (44%)
14	CLA	A	843	-	63,73,73	2.29	18 (28%)	74,113,113	2.41	23 (31%)
14	CLA	a	843	-	39,49,73	2.63	17 (43%)	46,83,113	2.86	22 (47%)
14	CLA	A	828	-	63,73,73	2.21	20 (31%)	74,113,113	2.58	27 (36%)
14	CLA	G	818	-	43,53,73	2.65	18 (41%)	50,89,113	2.84	20 (40%)
14	CLA	K	102	-	43,53,73	2.67	19 (44%)	50,89,113	2.79	21 (42%)
14	CLA	B	826	-	63,73,73	2.29	18 (28%)	74,113,113	2.46	25 (33%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
17	BCR	S	103	-	41,41,41	2.72	6 (14%)	56,56,56	6.53	23 (41%)
17	BCR	H	843	-	41,41,41	2.66	6 (14%)	56,56,56	6.65	21 (37%)
14	CLA	S	102	-	35,45,73	2.82	19 (54%)	42,78,113	2.85	17 (40%)
14	CLA	K	101	-	39,49,73	2.62	17 (43%)	46,83,113	2.78	22 (47%)
14	CLA	A	817	-	43,53,73	2.65	20 (46%)	50,89,113	2.76	20 (40%)
14	CLA	f	202	-	43,53,73	2.69	20 (46%)	50,89,113	2.73	23 (46%)
18	LHG	G	855	14	26,26,48	1.26	2 (7%)	29,32,54	1.26	2 (6%)
17	BCR	A	848	-	41,41,41	2.61	6 (14%)	56,56,56	6.68	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	844	-	63,73,73	2.25	19 (30%)	74,113,113	2.42	25 (33%)
14	CLA	b	816	-	53,63,73	2.52	20 (37%)	62,101,113	2.68	26 (41%)
14	CLA	b	809	2	63,73,73	2.24	18 (28%)	74,113,113	2.50	26 (35%)
14	CLA	B	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.83	20 (40%)
14	CLA	H	815	-	43,53,73	2.64	18 (41%)	50,89,113	2.83	20 (40%)
14	CLA	G	819	-	48,58,73	2.63	21 (43%)	56,95,113	2.81	25 (44%)
14	CLA	L	204	10	58,68,73	2.37	20 (34%)	68,107,113	2.60	25 (36%)
14	CLA	b	803	-	63,73,73	2.27	18 (28%)	74,113,113	2.45	25 (33%)
17	BCR	L	202	-	41,41,41	2.73	6 (14%)	56,56,56	6.49	19 (33%)
14	CLA	i	101	-	63,73,73	2.28	20 (31%)	74,113,113	2.48	24 (32%)
17	BCR	G	849	-	41,41,41	2.69	6 (14%)	56,56,56	6.81	25 (44%)
14	CLA	a	836	1	43,53,73	2.65	19 (44%)	50,89,113	2.76	20 (40%)
14	CLA	b	840	-	63,73,73	2.25	20 (31%)	74,113,113	2.60	26 (35%)
14	CLA	a	829	-	63,73,73	2.32	20 (31%)	74,113,113	2.39	26 (35%)
17	BCR	l	201	-	41,41,41	2.75	6 (14%)	56,56,56	6.32	22 (39%)
17	BCR	A	852	-	41,41,41	2.68	6 (14%)	56,56,56	6.67	20 (35%)
14	CLA	A	821	-	48,58,73	2.62	20 (41%)	56,95,113	2.84	24 (42%)
17	BCR	a	852	-	41,41,41	2.67	6 (14%)	56,56,56	6.67	21 (37%)
17	BCR	B	848	-	41,41,41	2.67	6 (14%)	56,56,56	6.83	22 (39%)
14	CLA	H	838	-	43,53,73	2.60	19 (44%)	50,89,113	2.90	23 (46%)
14	CLA	b	825	-	63,73,73	2.32	20 (31%)	74,113,113	2.51	25 (33%)
14	CLA	B	836	-	58,68,73	2.40	19 (32%)	68,107,113	2.54	22 (32%)
14	CLA	G	805	14	53,63,73	2.50	20 (37%)	62,101,113	2.79	26 (41%)
14	CLA	l	206	-	63,73,73	2.25	18 (28%)	74,113,113	2.57	23 (31%)
14	CLA	H	809	2	63,73,73	2.27	19 (30%)	74,113,113	2.42	28 (37%)
14	CLA	G	824	-	43,53,73	2.64	19 (44%)	50,89,113	2.83	20 (40%)
14	CLA	B	810	-	43,53,73	2.73	19 (44%)	50,89,113	2.80	21 (42%)
14	CLA	H	824	-	43,53,73	2.67	19 (44%)	50,89,113	2.78	21 (42%)
14	CLA	b	828	-	63,73,73	2.29	19 (30%)	74,113,113	2.50	24 (32%)
14	CLA	B	811	-	43,53,73	2.65	19 (44%)	50,89,113	2.80	21 (42%)
14	CLA	b	830	-	43,53,73	2.66	20 (46%)	50,89,113	2.86	21 (42%)
18	LHG	a	854	14	26,26,48	1.27	2 (7%)	29,32,54	1.38	5 (17%)
14	CLA	A	806	-	43,53,73	2.66	18 (41%)	50,89,113	2.86	22 (44%)
17	BCR	A	853	-	41,41,41	2.67	6 (14%)	56,56,56	6.92	20 (35%)
14	CLA	A	822	-	63,73,73	2.29	20 (31%)	74,113,113	2.41	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	b	837	-	58,68,73	2.37	19 (32%)	68,107,113	2.59	24 (35%)
14	CLA	B	833	-	43,53,73	2.65	19 (44%)	50,89,113	2.74	20 (40%)
14	CLA	A	818	-	43,53,73	2.60	18 (41%)	50,89,113	2.75	20 (40%)
14	CLA	H	826	-	63,73,73	2.27	19 (30%)	74,113,113	2.46	22 (29%)
18	LHG	G	854	-	48,48,48	0.91	2 (4%)	51,54,54	1.03	3 (5%)
14	CLA	G	808	-	43,53,73	2.66	19 (44%)	50,89,113	2.82	21 (42%)
14	CLA	a	803	-	53,63,73	2.50	18 (33%)	62,101,113	2.72	23 (37%)
13	CL0	A	801	-	63,73,73	2.28	19 (30%)	74,113,113	2.39	23 (31%)
14	CLA	A	840	-	43,53,73	2.64	19 (44%)	50,89,113	2.75	22 (44%)
16	SF4	N	102	3	0,12,12	-	-	-	-	-
17	BCR	Q	202	-	41,41,41	2.69	6 (14%)	56,56,56	6.64	19 (33%)
17	BCR	R	101	-	41,41,41	2.70	6 (14%)	56,56,56	6.74	18 (32%)
13	CL0	a	801	-	63,73,73	2.27	18 (28%)	74,113,113	2.41	25 (33%)
14	CLA	B	809	2	63,73,73	2.25	19 (30%)	74,113,113	2.47	26 (35%)
16	SF4	N	101	3	0,12,12	-	-	-	-	-
17	BCR	j	104	-	41,41,41	2.63	7 (17%)	56,56,56	6.73	21 (37%)
17	BCR	J	102	-	41,41,41	2.74	6 (14%)	56,56,56	6.53	22 (39%)
14	CLA	J	101	-	43,53,73	2.67	20 (46%)	50,89,113	2.89	26 (52%)
14	CLA	a	819	-	63,73,73	2.30	20 (31%)	74,113,113	2.52	26 (35%)
14	CLA	A	808	-	43,53,73	2.66	19 (44%)	50,89,113	2.83	23 (46%)
14	CLA	A	831	-	63,73,73	2.27	19 (30%)	74,113,113	2.39	22 (29%)
14	CLA	a	831	-	48,58,73	2.62	19 (39%)	56,95,113	2.70	23 (41%)
14	CLA	G	812	14	63,73,73	2.27	20 (31%)	74,113,113	2.60	25 (33%)
14	CLA	H	812	-	63,73,73	2.26	20 (31%)	74,113,113	2.54	28 (37%)
19	LMG	B	849	-	49,49,55	1.38	6 (12%)	57,57,63	1.08	4 (7%)
14	CLA	G	816	-	43,53,73	2.67	20 (46%)	50,89,113	2.84	23 (46%)
14	CLA	Q	201	-	43,53,73	2.62	17 (39%)	50,89,113	2.78	19 (38%)
14	CLA	H	807	-	63,73,73	2.25	20 (31%)	74,113,113	2.49	24 (32%)
17	BCR	b	842	-	41,41,41	2.63	6 (14%)	56,56,56	6.56	18 (32%)
14	CLA	B	822	-	43,53,73	2.62	17 (39%)	50,89,113	2.72	20 (40%)
17	BCR	H	844	-	41,41,41	2.63	6 (14%)	56,56,56	6.47	21 (37%)
14	CLA	G	823	-	43,53,73	2.67	18 (41%)	50,89,113	2.87	20 (40%)
14	CLA	a	820	-	48,58,73	2.60	20 (41%)	56,95,113	2.91	27 (48%)
14	CLA	U	205	-	63,73,73	2.29	19 (30%)	74,113,113	2.54	24 (32%)
14	CLA	b	819	-	43,53,73	2.64	19 (44%)	50,89,113	2.88	20 (40%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	841	-	43,53,73	2.61	17 (39%)	50,89,113	2.79	20 (40%)
14	CLA	b	832	-	53,63,73	2.48	21 (39%)	62,101,113	2.73	24 (38%)
17	BCR	m	1602	-	41,41,41	2.60	6 (14%)	56,56,56	6.73	20 (35%)
14	CLA	H	801	-	63,73,73	2.27	19 (30%)	74,113,113	2.47	28 (37%)
14	CLA	b	808	-	63,73,73	2.24	18 (28%)	74,113,113	2.55	24 (32%)
14	CLA	L	206	-	63,73,73	2.31	20 (31%)	74,113,113	2.48	25 (33%)
17	BCR	a	848	-	41,41,41	2.68	6 (14%)	56,56,56	6.74	26 (46%)
14	CLA	G	830	-	63,73,73	2.26	19 (30%)	74,113,113	2.45	23 (31%)
18	LHG	A	854	-	48,48,48	0.93	2 (4%)	51,54,54	1.16	4 (7%)
14	CLA	b	811	-	43,53,73	2.67	20 (46%)	50,89,113	2.85	21 (42%)
17	BCR	b	845	-	25,25,41	2.15	2 (8%)	33,33,56	7.38	15 (45%)
17	BCR	G	852	-	41,41,41	2.71	6 (14%)	56,56,56	6.77	21 (37%)
17	BCR	i	102	-	41,41,41	2.70	6 (14%)	56,56,56	6.73	21 (37%)
14	CLA	b	801	-	63,73,73	2.24	18 (28%)	74,113,113	2.50	27 (36%)
14	CLA	B	808	-	63,73,73	2.30	19 (30%)	74,113,113	2.39	25 (33%)
14	CLA	A	814	-	58,68,73	2.40	20 (34%)	68,107,113	2.56	26 (38%)
14	CLA	B	837	-	58,68,73	2.33	19 (32%)	68,107,113	2.69	25 (36%)
17	BCR	B	845	-	25,25,41	2.14	2 (8%)	33,33,56	7.43	16 (48%)
14	CLA	A	830	-	63,73,73	2.29	19 (30%)	74,113,113	2.42	24 (32%)
14	CLA	x	1701	12	43,53,73	2.66	19 (44%)	50,89,113	2.77	21 (42%)
14	CLA	A	819	-	48,58,73	2.63	21 (43%)	56,95,113	2.85	22 (39%)
14	CLA	a	830	-	63,73,73	2.27	19 (30%)	74,113,113	2.44	25 (33%)
14	CLA	H	819	-	43,53,73	2.68	21 (48%)	50,89,113	2.84	20 (40%)
17	BCR	U	202	-	41,41,41	2.75	6 (14%)	56,56,56	6.58	24 (42%)
14	CLA	B	801	-	63,73,73	2.26	20 (31%)	74,113,113	2.46	26 (35%)
17	BCR	H	849	-	41,41,41	2.60	6 (14%)	56,56,56	6.41	19 (33%)
14	CLA	G	831	-	63,73,73	2.28	19 (30%)	74,113,113	2.42	24 (32%)
14	CLA	A	802	-	63,73,73	2.27	18 (28%)	74,113,113	2.47	27 (36%)
14	CLA	H	816	-	53,63,73	2.52	19 (35%)	62,101,113	2.71	26 (41%)
14	CLA	G	817	-	43,53,73	2.63	20 (46%)	50,89,113	2.76	20 (40%)
17	BCR	I	102	-	41,41,41	2.59	6 (14%)	56,56,56	6.64	20 (35%)
14	CLA	H	803	-	63,73,73	2.23	20 (31%)	74,113,113	2.56	25 (33%)
14	CLA	a	818	-	48,58,73	2.61	20 (41%)	56,95,113	2.81	23 (41%)
14	CLA	A	842	-	43,53,73	2.61	18 (41%)	50,89,113	2.71	19 (38%)
16	SF4	c	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	805	-	63,73,73	2.31	20 (31%)	74,113,113	2.49	27 (36%)
14	CLA	G	842	-	63,73,73	2.30	20 (31%)	74,113,113	2.52	26 (35%)
14	CLA	b	812	-	63,73,73	2.28	21 (33%)	74,113,113	2.54	29 (39%)
14	CLA	l	207	-	63,73,73	2.29	20 (31%)	74,113,113	2.45	27 (36%)
13	CL0	G	801	-	63,73,73	2.30	19 (30%)	74,113,113	2.45	25 (33%)
14	CLA	a	840	-	63,73,73	2.32	20 (31%)	74,113,113	2.47	29 (39%)
17	BCR	H	845	-	25,25,41	2.18	2 (8%)	33,33,56	7.45	20 (60%)
14	CLA	B	803	-	63,73,73	2.24	20 (31%)	74,113,113	2.47	24 (32%)
14	CLA	G	834	-	63,73,73	2.31	20 (31%)	74,113,113	2.43	22 (29%)
16	SF4	G	847	2,1	0,12,12	-	-	-	-	-
14	CLA	H	814	-	43,53,73	2.60	19 (44%)	50,89,113	2.98	21 (42%)
14	CLA	A	836	-	43,53,73	2.60	18 (41%)	50,89,113	2.73	18 (36%)
14	CLA	b	822	-	43,53,73	2.68	20 (46%)	50,89,113	2.73	20 (40%)
14	CLA	A	833	-	53,63,73	2.57	20 (37%)	62,101,113	2.66	25 (40%)
17	BCR	A	849	-	41,41,41	2.68	6 (14%)	56,56,56	6.87	27 (48%)
14	CLA	B	817	-	58,68,73	2.36	20 (34%)	68,107,113	2.58	24 (35%)
14	CLA	L	201	2	63,73,73	2.25	19 (30%)	74,113,113	2.65	27 (36%)
14	CLA	B	824	-	43,53,73	2.68	18 (41%)	50,89,113	2.73	19 (38%)
14	CLA	a	805	-	43,53,73	2.62	18 (41%)	50,89,113	2.84	20 (40%)
14	CLA	b	802	-	63,73,73	2.24	19 (30%)	74,113,113	2.42	22 (29%)
14	CLA	H	831	-	63,73,73	2.34	21 (33%)	74,113,113	2.57	27 (36%)
17	BCR	f	201	-	41,41,41	2.77	6 (14%)	56,56,56	6.57	20 (35%)
14	CLA	a	808	1	63,73,73	2.24	20 (31%)	74,113,113	2.58	26 (35%)
14	CLA	H	837	-	58,68,73	2.40	20 (34%)	68,107,113	2.60	23 (33%)
14	CLA	B	814	-	43,53,73	2.62	18 (41%)	50,89,113	2.89	21 (42%)
14	CLA	B	819	-	43,53,73	2.65	19 (44%)	50,89,113	2.78	20 (40%)
14	CLA	A	845	18	43,53,73	2.65	19 (44%)	50,89,113	3.05	24 (48%)
14	CLA	a	813	-	58,68,73	2.36	20 (34%)	68,107,113	2.56	24 (35%)
14	CLA	k	1401	-	43,53,73	2.68	19 (44%)	50,89,113	2.76	20 (40%)
14	CLA	G	835	-	63,73,73	2.27	19 (30%)	74,113,113	2.50	22 (29%)
14	CLA	b	827	-	63,73,73	2.28	19 (30%)	74,113,113	2.37	22 (29%)
14	CLA	H	821	-	53,63,73	2.52	20 (37%)	62,101,113	2.63	23 (37%)
14	CLA	B	812	-	63,73,73	2.29	19 (30%)	74,113,113	2.55	26 (35%)
14	CLA	B	827	-	63,73,73	2.32	19 (30%)	74,113,113	2.23	24 (32%)
17	BCR	H	846	-	41,41,41	2.73	7 (17%)	56,56,56	6.61	25 (44%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	BCR	Q	204	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	22 (39%)
14	CLA	B	807	-	63,73,73	2.27	20 (31%)	74,113,113	2.48	24 (32%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	S	104	-	-	12/29/63/63	0/2/2/2
14	CLA	a	812	-	1/1/12/20	3/19/97/115	-
14	CLA	b	810	-	1/1/11/20	3/13/91/115	-
14	CLA	U	204	10	1/1/14/20	13/31/109/115	-
14	CLA	B	823	2	1/1/12/20	8/19/97/115	-
14	CLA	b	804	-	1/1/15/20	16/37/115/115	-
17	BCR	b	847	-	-	9/29/63/63	0/2/2/2
14	CLA	j	101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	822	-	1/1/11/20	6/13/91/115	-
14	CLA	H	817	-	1/1/14/20	13/31/109/115	-
17	BCR	B	842	-	-	11/29/63/63	0/2/2/2
14	CLA	b	821	-	1/1/13/20	10/25/103/115	-
14	CLA	A	820	-	1/1/15/20	13/37/115/115	-
14	CLA	A	807	-	1/1/15/20	18/37/115/115	-
17	BCR	b	846	-	-	6/29/63/63	0/2/2/2
19	LMG	H	848	-	-	9/44/64/70	0/1/1/1
14	CLA	X	1701	12	1/1/11/20	6/13/91/115	-
14	CLA	G	844	-	1/1/9/20	3/7/81/115	-
14	CLA	G	820	-	1/1/15/20	17/37/115/115	-
14	CLA	H	840	-	1/1/15/20	11/37/115/115	-
14	CLA	U	201	2	1/1/15/20	10/37/115/115	-
15	PQN	B	841	-	-	4/23/43/43	0/2/2/2
14	CLA	b	817	-	1/1/14/20	14/31/109/115	-
17	BCR	B	846	-	-	9/29/63/63	0/2/2/2
14	CLA	H	832	-	1/1/13/20	10/25/103/115	-
14	CLA	H	828	-	1/1/15/20	9/37/115/115	-
14	CLA	H	830	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	Q	203	-	1/1/11/20	4/13/91/115	-
18	LHG	A	855	14	-	16/31/31/53	-
14	CLA	b	818	-	1/1/15/20	13/37/115/115	-
14	CLA	a	825	-	1/1/15/20	17/37/115/115	-
14	CLA	m	1601	-	1/1/11/20	7/13/91/115	-
14	CLA	b	807	-	1/1/15/20	18/37/115/115	-
14	CLA	a	827	-	1/1/15/20	17/37/115/115	-
14	CLA	H	808	-	1/1/15/20	15/37/115/115	-
14	CLA	B	839	-	1/1/15/20	14/37/115/115	-
14	CLA	A	837	1	1/1/11/20	5/13/91/115	-
17	BCR	R	102	-	-	10/29/63/63	0/2/2/2
14	CLA	b	824	-	1/1/11/20	4/13/91/115	-
14	CLA	G	810	1	1/1/15/20	11/37/115/115	-
14	CLA	H	818	-	1/1/15/20	11/37/115/115	-
14	CLA	a	802	-	1/1/15/20	14/37/115/115	-
14	CLA	G	813	-	1/1/12/20	4/19/97/115	-
14	CLA	b	806	-	1/1/15/20	14/37/115/115	-
14	CLA	j	102	-	1/1/8/20	0/2/76/115	-
14	CLA	B	806	-	1/1/15/20	20/37/115/115	-
14	CLA	G	837	1	1/1/11/20	5/13/91/115	-
14	CLA	b	836	-	1/1/14/20	12/31/109/115	-
14	CLA	A	804	-	1/1/13/20	12/25/103/115	-
14	CLA	b	829	-	1/1/11/20	6/13/91/115	-
14	CLA	a	833	-	1/1/15/20	7/37/115/115	-
15	PQN	A	846	-	-	9/23/43/43	0/2/2/2
14	CLA	a	834	-	1/1/15/20	11/37/115/115	-
14	CLA	L	205	-	1/1/15/20	12/37/115/115	-
14	CLA	F	1303	-	1/1/8/20	0/2/76/115	-
14	CLA	H	833	-	1/1/11/20	4/13/91/115	-
14	CLA	G	804	-	1/1/13/20	11/25/103/115	-
18	LHG	a	853	-	-	26/53/53/53	-
14	CLA	G	841	-	1/1/15/20	11/37/115/115	-
14	CLA	B	834	-	1/1/11/20	7/13/91/115	-
17	BCR	M	1602	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	a	849	-	-	11/29/63/63	0/2/2/2
14	CLA	G	827	-	1/1/14/20	7/31/109/115	-
17	BCR	b	844	-	-	10/29/63/63	0/2/2/2
14	CLA	B	815	-	1/1/11/20	4/13/91/115	-
14	CLA	G	821	-	1/1/12/20	9/19/97/115	-
14	CLA	A	805	14	1/1/13/20	12/25/103/115	-
14	CLA	b	815	-	1/1/11/20	3/13/91/115	-
14	CLA	a	809	-	1/1/15/20	14/37/115/115	-
14	CLA	B	831	-	1/1/15/20	18/37/115/115	-
14	CLA	G	809	1	1/1/15/20	17/37/115/115	-
14	CLA	G	843	-	1/1/15/20	15/37/115/115	-
14	CLA	b	805	-	1/1/12/20	8/24/102/115	-
14	CLA	a	855	-	1/1/15/20	15/37/115/115	-
14	CLA	a	838	-	1/1/15/20	9/37/115/115	-
14	CLA	a	824	-	1/1/13/20	8/25/103/115	-
14	CLA	A	839	-	1/1/15/20	10/37/115/115	-
17	BCR	B	847	-	-	9/29/63/63	0/2/2/2
17	BCR	V	1602	-	-	11/29/63/63	0/2/2/2
14	CLA	B	804	-	1/1/12/20	7/24/102/115	-
14	CLA	H	822	-	1/1/11/20	2/13/91/115	-
19	LMG	b	848	-	-	13/44/64/70	0/1/1/1
14	CLA	A	810	1	1/1/15/20	12/37/115/115	-
14	CLA	G	822	-	1/1/15/20	13/37/115/115	-
14	CLA	a	810	-	1/1/11/20	5/13/91/115	-
14	CLA	A	816	-	1/1/11/20	5/13/91/115	-
14	CLA	a	826	-	1/1/14/20	9/31/109/115	-
14	CLA	S	101	8	1/1/11/20	6/13/91/115	-
17	BCR	G	851	-	-	9/29/63/63	0/2/2/2
14	CLA	G	803	-	1/1/15/20	14/37/115/115	-
17	BCR	a	851	-	-	6/29/63/63	0/2/2/2
14	CLA	a	807	-	1/1/11/20	5/13/91/115	-
14	CLA	A	823	-	1/1/11/20	6/13/91/115	-
14	CLA	A	825	-	1/1/13/20	6/25/103/115	-
14	CLA	A	841	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	823	2	1/1/12/20	6/19/97/115	-
14	CLA	H	825	-	1/1/15/20	10/37/115/115	-
14	CLA	b	839	-	1/1/15/20	15/37/115/115	-
14	CLA	a	811	14	1/1/15/20	13/37/115/115	-
14	CLA	G	840	-	1/1/11/20	3/13/91/115	-
14	CLA	B	818	-	1/1/15/20	8/37/115/115	-
14	CLA	B	835	-	1/1/11/20	6/13/91/115	-
14	CLA	G	807	-	1/1/15/20	18/37/115/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5
14	CLA	a	823	-	1/1/11/20	4/13/91/115	-
17	BCR	G	853	-	-	13/29/63/63	0/2/2/2
14	CLA	A	815	-	1/1/11/20	4/13/91/115	-
14	CLA	T	1401	-	1/1/11/20	6/13/91/115	-
14	CLA	G	811	-	1/1/11/20	6/13/91/115	-
15	PQN	a	845	-	-	8/23/43/43	0/2/2/2
14	CLA	A	835	-	1/1/15/20	12/37/115/115	-
14	CLA	M	1601	-	1/1/11/20	9/13/91/115	-
14	CLA	H	805	-	1/1/15/20	17/37/115/115	-
15	PQN	G	846	-	-	9/23/43/43	0/2/2/2
14	CLA	H	804	-	1/1/12/20	8/24/102/115	-
14	CLA	a	816	-	1/1/11/20	3/13/91/115	-
17	BCR	a	847	-	-	10/29/63/63	0/2/2/2
14	CLA	G	802	-	1/1/15/20	12/37/115/115	-
15	PQN	H	841	-	-	5/23/43/43	0/2/2/2
14	CLA	B	830	-	1/1/11/20	7/13/91/115	-
14	CLA	a	832	-	1/1/13/20	11/25/103/115	-
17	BCR	R	103	-	-	8/29/63/63	0/2/2/2
14	CLA	A	824	-	1/1/11/20	4/13/91/115	-
14	CLA	F	1301	-	1/1/11/20	4/13/91/115	-
14	CLA	H	802	-	1/1/15/20	15/37/115/115	-
14	CLA	B	816	-	1/1/13/20	8/25/103/115	-
14	CLA	b	823	2	1/1/12/20	7/19/97/115	-
14	CLA	B	813	-	1/1/13/20	8/25/103/115	-
14	CLA	l	202	2	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	812	14	1/1/15/20	14/37/115/115	-
17	BCR	L	207	-	-	5/29/63/63	0/2/2/2
17	BCR	B	844	-	-	9/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/11/20	3/13/91/115	-
14	CLA	A	829	-	1/1/15/20	17/37/115/115	-
17	BCR	G	850	-	-	13/29/63/63	0/2/2/2
14	CLA	B	828	-	1/1/15/20	8/37/115/115	-
14	CLA	H	835	-	1/1/11/20	6/13/91/115	-
14	CLA	U	206	-	1/1/15/20	16/37/115/115	-
14	CLA	G	839	-	1/1/15/20	12/37/115/115	-
14	CLA	b	838	-	1/1/11/20	5/13/91/115	-
14	CLA	G	829	-	1/1/15/20	17/37/115/115	-
14	CLA	B	829	-	1/1/11/20	7/13/91/115	-
14	CLA	A	834	-	1/1/15/20	15/37/115/115	-
17	BCR	A	851	-	-	11/29/63/63	0/2/2/2
17	BCR	l	208	-	-	8/29/63/63	0/2/2/2
14	CLA	G	838	-	1/1/12/20	5/19/97/115	-
17	BCR	b	849	-	-	9/29/63/63	0/2/2/2
14	CLA	H	836	-	1/1/14/20	16/31/109/115	-
17	BCR	H	842	-	-	12/29/63/63	0/2/2/2
14	CLA	G	825	-	1/1/13/20	6/25/103/115	-
14	CLA	B	821	-	1/1/13/20	9/25/103/115	-
14	CLA	H	806	-	1/1/15/20	19/37/115/115	-
14	CLA	l	205	10	1/1/14/20	10/31/109/115	-
14	CLA	a	814	-	1/1/11/20	5/13/91/115	-
14	CLA	G	836	-	1/1/11/20	5/13/91/115	-
14	CLA	A	813	-	1/1/12/20	4/19/97/115	-
14	CLA	H	827	-	1/1/15/20	12/37/115/115	-
14	CLA	H	813	-	1/1/13/20	9/25/103/115	-
14	CLA	b	820	-	1/1/11/20	4/13/91/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	H	810	-	1/1/11/20	3/13/91/115	-
14	CLA	b	835	-	1/1/11/20	6/13/91/115	-
14	CLA	A	811	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	G	826	-	1/1/15/20	16/37/115/115	-
14	CLA	H	811	-	1/1/11/20	4/13/91/115	-
17	BCR	J	103	-	-	12/29/63/63	0/2/2/2
14	CLA	G	828	-	1/1/15/20	17/37/115/115	-
14	CLA	A	838	-	1/1/12/20	6/19/97/115	-
14	CLA	a	842	-	1/1/15/20	16/37/115/115	-
17	BCR	b	843	-	-	6/29/63/63	0/2/2/2
16	SF4	A	847	2,1	-	-	0/6/5/5
14	CLA	b	813	-	1/1/13/20	8/25/103/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	a	815	-	1/1/11/20	7/13/91/115	-
14	CLA	B	802	-	1/1/15/20	11/37/115/115	-
14	CLA	a	821	-	1/1/15/20	12/37/115/115	-
14	CLA	H	829	-	1/1/11/20	7/13/91/115	-
14	CLA	W	1701	12	1/1/11/20	5/13/91/115	-
17	BCR	G	848	-	-	11/29/63/63	0/2/2/2
14	CLA	B	840	-	1/1/15/20	11/37/115/115	-
14	CLA	A	803	-	1/1/15/20	15/37/115/115	-
14	CLA	B	825	-	1/1/15/20	12/37/115/115	-
14	CLA	A	826	-	1/1/15/20	18/37/115/115	-
14	CLA	b	831	-	1/1/15/20	20/37/115/115	-
14	CLA	G	815	-	1/1/11/20	2/13/91/115	-
17	BCR	f	203	-	-	8/29/63/63	0/2/2/2
15	PQN	b	841	-	-	9/23/43/43	0/2/2/2
17	BCR	A	850	-	-	11/29/63/63	0/2/2/2
17	BCR	B	843	-	-	6/29/63/63	0/2/2/2
17	BCR	j	103	-	-	9/29/63/63	0/2/2/2
14	CLA	a	844	18	1/1/11/20	8/13/91/115	-
17	BCR	H	847	-	-	11/29/63/63	0/2/2/2
14	CLA	a	837	-	1/1/12/20	6/19/97/115	-
14	CLA	G	833	-	1/1/13/20	11/25/103/115	-
14	CLA	a	835	-	1/1/11/20	5/13/91/115	-
17	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	b	834	-	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	820	-	1/1/11/20	6/13/91/115	-
14	CLA	a	804	14	1/1/13/20	12/25/103/115	-
14	CLA	a	806	-	1/1/15/20	17/37/115/115	-
17	BCR	F	1302	-	-	10/29/63/63	0/2/2/2
14	CLA	H	820	-	1/1/11/20	6/13/91/115	-
14	CLA	H	839	-	1/1/15/20	18/37/115/115	-
14	CLA	G	814	-	1/1/14/20	16/31/109/115	-
14	CLA	A	832	-	1/1/12/20	5/19/97/115	-
14	CLA	a	828	-	1/1/15/20	18/37/115/115	-
17	BCR	l	203	-	-	13/29/63/63	0/2/2/2
14	CLA	b	826	-	1/1/15/20	17/37/115/115	-
14	CLA	A	827	-	1/1/14/20	10/31/109/115	-
17	BCR	a	850	-	-	13/29/63/63	0/2/2/2
14	CLA	V	1601	-	1/1/11/20	9/13/91/115	-
14	CLA	G	806	-	1/1/11/20	6/13/91/115	-
14	CLA	G	845	18	1/1/11/20	8/13/91/115	-
17	BCR	B	850	-	-	11/29/63/63	0/2/2/2
14	CLA	G	832	-	1/1/12/20	5/19/97/115	-
14	CLA	b	833	-	1/1/11/20	6/13/91/115	-
14	CLA	A	809	1	1/1/15/20	18/37/115/115	-
14	CLA	a	817	-	1/1/11/20	3/13/91/115	-
14	CLA	B	832	-	1/1/13/20	9/25/103/115	-
14	CLA	H	834	-	1/1/11/20	6/13/91/115	-
14	CLA	b	814	-	1/1/11/20	9/13/91/115	-
14	CLA	A	843	-	1/1/15/20	19/37/115/115	-
14	CLA	a	843	-	1/1/9/20	3/7/81/115	-
14	CLA	A	828	-	1/1/15/20	13/37/115/115	-
14	CLA	G	818	-	1/1/11/20	4/13/91/115	-
14	CLA	K	102	-	1/1/11/20	7/13/91/115	-
14	CLA	B	826	-	1/1/15/20	18/37/115/115	-
16	SF4	c	102	3	-	-	0/6/5/5
17	BCR	S	103	-	-	14/29/63/63	0/2/2/2
17	BCR	H	843	-	-	6/29/63/63	0/2/2/2
14	CLA	S	102	-	1/1/8/20	0/2/76/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	K	101	-	1/1/9/20	4/7/81/115	-
14	CLA	A	817	-	1/1/11/20	4/13/91/115	-
14	CLA	f	202	-	1/1/11/20	2/13/91/115	-
18	LHG	G	855	14	-	14/31/31/53	-
17	BCR	A	848	-	-	13/29/63/63	0/2/2/2
14	CLA	A	844	-	1/1/15/20	19/37/115/115	-
14	CLA	b	816	-	1/1/13/20	7/25/103/115	-
14	CLA	b	809	2	1/1/15/20	18/37/115/115	-
14	CLA	B	838	-	1/1/11/20	5/13/91/115	-
14	CLA	H	815	-	1/1/11/20	5/13/91/115	-
14	CLA	G	819	-	1/1/12/20	8/19/97/115	-
14	CLA	L	204	10	1/1/14/20	13/31/109/115	-
14	CLA	b	803	-	1/1/15/20	13/37/115/115	-
17	BCR	L	202	-	-	10/29/63/63	0/2/2/2
14	CLA	i	101	-	1/1/15/20	5/37/115/115	-
17	BCR	G	849	-	-	11/29/63/63	0/2/2/2
14	CLA	a	836	1	1/1/11/20	4/13/91/115	-
14	CLA	b	840	-	1/1/15/20	17/37/115/115	-
14	CLA	a	829	-	1/1/15/20	16/37/115/115	-
17	BCR	l	201	-	-	4/29/63/63	0/2/2/2
17	BCR	A	852	-	-	7/29/63/63	0/2/2/2
14	CLA	A	821	-	1/1/12/20	7/19/97/115	-
17	BCR	a	852	-	-	11/29/63/63	0/2/2/2
17	BCR	B	848	-	-	11/29/63/63	0/2/2/2
14	CLA	H	838	-	1/1/11/20	5/13/91/115	-
14	CLA	b	825	-	1/1/15/20	9/37/115/115	-
14	CLA	B	836	-	1/1/14/20	12/31/109/115	-
14	CLA	G	805	14	1/1/13/20	8/25/103/115	-
14	CLA	l	206	-	1/1/15/20	10/37/115/115	-
14	CLA	H	809	2	1/1/15/20	11/37/115/115	-
14	CLA	G	824	-	1/1/11/20	5/13/91/115	-
14	CLA	B	810	-	1/1/11/20	3/13/91/115	-
14	CLA	H	824	-	1/1/11/20	4/13/91/115	-
14	CLA	b	828	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	811	-	1/1/11/20	4/13/91/115	-
14	CLA	b	830	-	1/1/11/20	7/13/91/115	-
18	LHG	a	854	14	-	19/31/31/53	-
14	CLA	A	806	-	1/1/11/20	6/13/91/115	-
17	BCR	A	853	-	-	16/29/63/63	0/2/2/2
14	CLA	A	822	-	1/1/15/20	8/37/115/115	-
14	CLA	b	837	-	1/1/14/20	9/31/109/115	-
14	CLA	B	833	-	1/1/11/20	5/13/91/115	-
14	CLA	A	818	-	1/1/11/20	4/13/91/115	-
14	CLA	H	826	-	1/1/15/20	13/37/115/115	-
18	LHG	G	854	-	-	28/53/53/53	-
14	CLA	G	808	-	1/1/11/20	4/13/91/115	-
14	CLA	a	803	-	1/1/13/20	11/25/103/115	-
13	CL0	A	801	-	3/3/20/25	9/37/135/135	-
14	CLA	A	840	-	1/1/11/20	3/13/91/115	-
17	BCR	Q	202	-	-	9/29/63/63	0/2/2/2
16	SF4	N	102	3	-	-	0/6/5/5
17	BCR	R	101	-	-	6/29/63/63	0/2/2/2
13	CL0	a	801	-	3/3/20/25	4/37/135/135	-
14	CLA	B	809	2	1/1/15/20	11/37/115/115	-
16	SF4	N	101	3	-	-	0/6/5/5
17	BCR	j	104	-	-	9/29/63/63	0/2/2/2
17	BCR	J	102	-	-	13/29/63/63	0/2/2/2
14	CLA	J	101	-	1/1/11/20	4/13/91/115	-
14	CLA	a	819	-	1/1/15/20	15/37/115/115	-
14	CLA	A	808	-	1/1/11/20	4/13/91/115	-
14	CLA	A	831	-	1/1/15/20	13/37/115/115	-
14	CLA	a	831	-	1/1/12/20	3/19/97/115	-
14	CLA	G	812	14	1/1/15/20	13/37/115/115	-
14	CLA	H	812	-	1/1/15/20	17/37/115/115	-
19	LMG	B	849	-	-	13/44/64/70	0/1/1/1
14	CLA	G	816	-	1/1/11/20	5/13/91/115	-
14	CLA	Q	201	-	1/1/11/20	6/13/91/115	-
14	CLA	H	807	-	1/1/15/20	7/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	842	-	-	12/29/63/63	0/2/2/2
14	CLA	B	822	-	1/1/11/20	4/13/91/115	-
17	BCR	H	844	-	-	10/29/63/63	0/2/2/2
14	CLA	G	823	-	1/1/11/20	5/13/91/115	-
14	CLA	a	820	-	1/1/12/20	9/19/97/115	-
14	CLA	U	205	-	1/1/15/20	11/37/115/115	-
14	CLA	b	819	-	1/1/11/20	7/13/91/115	-
14	CLA	a	841	-	1/1/11/20	6/13/91/115	-
14	CLA	b	832	-	1/1/13/20	12/25/103/115	-
17	BCR	m	1602	-	-	13/29/63/63	0/2/2/2
14	CLA	H	801	-	1/1/15/20	20/37/115/115	-
14	CLA	b	808	-	1/1/15/20	11/37/115/115	-
14	CLA	L	206	-	1/1/15/20	13/37/115/115	-
17	BCR	a	848	-	-	14/29/63/63	0/2/2/2
14	CLA	G	830	-	1/1/15/20	18/37/115/115	-
18	LHG	A	854	-	-	32/53/53/53	-
14	CLA	b	811	-	1/1/11/20	1/13/91/115	-
17	BCR	b	845	-	-	1/18/35/63	0/1/1/2
17	BCR	G	852	-	-	7/29/63/63	0/2/2/2
17	BCR	i	102	-	-	6/29/63/63	0/2/2/2
14	CLA	b	801	-	1/1/15/20	13/37/115/115	-
14	CLA	B	808	-	1/1/15/20	13/37/115/115	-
14	CLA	A	814	-	1/1/14/20	17/31/109/115	-
14	CLA	B	837	-	1/1/14/20	9/31/109/115	-
17	BCR	B	845	-	-	0/18/35/63	0/1/1/2
14	CLA	A	830	-	1/1/15/20	15/37/115/115	-
14	CLA	x	1701	12	1/1/11/20	5/13/91/115	-
14	CLA	A	819	-	1/1/12/20	8/19/97/115	-
14	CLA	a	830	-	1/1/15/20	13/37/115/115	-
14	CLA	H	819	-	1/1/11/20	6/13/91/115	-
17	BCR	U	202	-	-	8/29/63/63	0/2/2/2
14	CLA	B	801	-	1/1/15/20	14/37/115/115	-
17	BCR	H	849	-	-	12/29/63/63	0/2/2/2
14	CLA	G	831	-	1/1/15/20	13/37/115/115	-
14	CLA	A	802	-	1/1/15/20	17/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	H	816	-	1/1/13/20	10/25/103/115	-
14	CLA	G	817	-	1/1/11/20	3/13/91/115	-
17	BCR	I	102	-	-	8/29/63/63	0/2/2/2
14	CLA	H	803	-	1/1/15/20	11/37/115/115	-
14	CLA	a	818	-	1/1/12/20	9/19/97/115	-
14	CLA	A	842	-	1/1/11/20	4/13/91/115	-
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	B	805	-	1/1/15/20	14/37/115/115	-
14	CLA	G	842	-	1/1/15/20	18/37/115/115	-
14	CLA	b	812	-	1/1/15/20	22/37/115/115	-
14	CLA	l	207	-	1/1/15/20	15/37/115/115	-
13	CL0	G	801	-	3/3/20/25	6/37/135/135	-
14	CLA	a	840	-	1/1/15/20	8/37/115/115	-
17	BCR	H	845	-	-	0/18/35/63	0/1/1/2
14	CLA	B	803	-	1/1/15/20	11/37/115/115	-
14	CLA	G	834	-	1/1/15/20	13/37/115/115	-
16	SF4	G	847	2,1	-	-	0/6/5/5
14	CLA	H	814	-	1/1/11/20	9/13/91/115	-
14	CLA	A	836	-	1/1/11/20	5/13/91/115	-
14	CLA	b	822	-	1/1/11/20	4/13/91/115	-
14	CLA	A	833	-	1/1/13/20	11/25/103/115	-
17	BCR	A	849	-	-	14/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/14/20	16/31/109/115	-
14	CLA	L	201	2	1/1/15/20	13/37/115/115	-
14	CLA	B	824	-	1/1/11/20	4/13/91/115	-
14	CLA	a	805	-	1/1/11/20	6/13/91/115	-
14	CLA	b	802	-	1/1/15/20	19/37/115/115	-
14	CLA	H	831	-	1/1/15/20	15/37/115/115	-
17	BCR	f	201	-	-	7/29/63/63	0/2/2/2
14	CLA	a	808	1	1/1/15/20	17/37/115/115	-
14	CLA	H	837	-	1/1/14/20	12/31/109/115	-
14	CLA	B	814	-	1/1/11/20	7/13/91/115	-
14	CLA	B	819	-	1/1/11/20	6/13/91/115	-
14	CLA	A	845	18	1/1/11/20	6/13/91/115	-
14	CLA	a	813	-	1/1/14/20	10/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	k	1401	-	1/1/11/20	7/13/91/115	-
14	CLA	G	835	-	1/1/15/20	14/37/115/115	-
14	CLA	b	827	-	1/1/15/20	13/37/115/115	-
14	CLA	H	821	-	1/1/13/20	10/25/103/115	-
14	CLA	B	812	-	1/1/15/20	22/37/115/115	-
14	CLA	B	827	-	1/1/15/20	12/37/115/115	-
17	BCR	H	846	-	-	7/29/63/63	0/2/2/2
17	BCR	Q	204	-	-	5/29/63/63	0/2/2/2
14	CLA	B	807	-	1/1/15/20	6/37/115/115	-

The worst 5 of 5995 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	G	850	BCR	C8-C9	-9.07	1.26	1.46
17	I	203	BCR	C8-C9	-8.85	1.27	1.46
17	U	202	BCR	C8-C9	-8.81	1.27	1.46
17	a	850	BCR	C8-C9	-8.74	1.27	1.46
17	R	102	BCR	C8-C9	-8.69	1.27	1.46

The worst 5 of 8181 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	G	849	BCR	C20-C21-C22	25.63	163.23	127.28
17	J	103	BCR	C16-C17-C18	25.34	162.82	127.28
17	A	849	BCR	C20-C21-C22	25.16	162.56	127.28
17	A	853	BCR	C20-C21-C22	24.52	161.67	127.28
17	H	847	BCR	C20-C21-C22	24.46	161.58	127.28

5 of 294 chirality outliers are listed below:

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

5 of 3575 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	A	802	CLA	CBA-CGA-O2A-C1
14	A	802	CLA	O1A-CGA-O2A-C1
14	A	804	CLA	C2-C1-O2A-CGA
14	A	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

344 monomers are involved in 973 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	S	104	BCR	7	0
14	a	812	CLA	1	0
14	U	204	CLA	3	0
14	B	823	CLA	3	0
14	b	804	CLA	7	0
17	b	847	BCR	9	0
14	j	101	CLA	1	0
14	a	822	CLA	1	0
14	H	817	CLA	5	0
17	B	842	BCR	1	0
14	b	821	CLA	3	0
14	A	820	CLA	10	0
14	A	807	CLA	3	0
17	b	846	BCR	3	0
19	H	848	LMG	2	0
14	X	1701	CLA	1	0
14	G	820	CLA	6	0
14	H	840	CLA	3	0
14	U	201	CLA	6	0
15	B	841	PQN	4	0
14	b	817	CLA	4	0
17	B	846	BCR	2	0
14	H	832	CLA	4	0
14	H	828	CLA	3	0
14	H	830	CLA	2	0
14	Q	203	CLA	3	0
18	A	855	LHG	1	0
14	b	818	CLA	2	0
14	a	825	CLA	5	0
14	m	1601	CLA	3	0
14	b	807	CLA	4	0
14	a	827	CLA	6	0
14	H	808	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	839	CLA	6	0
14	A	837	CLA	2	0
17	R	102	BCR	3	0
14	b	824	CLA	4	0
14	G	810	CLA	2	0
14	a	802	CLA	3	0
14	G	813	CLA	1	0
14	b	806	CLA	8	0
14	j	102	CLA	1	0
14	B	806	CLA	4	0
14	b	836	CLA	3	0
14	A	804	CLA	2	0
14	b	829	CLA	5	0
14	a	833	CLA	7	0
15	A	846	PQN	7	0
14	a	834	CLA	2	0
14	L	205	CLA	6	0
14	H	833	CLA	3	0
14	G	804	CLA	1	0
18	a	853	LHG	1	0
14	G	841	CLA	5	0
14	B	834	CLA	3	0
17	M	1602	BCR	2	0
17	a	849	BCR	3	0
14	G	827	CLA	2	0
17	b	844	BCR	2	0
14	B	815	CLA	4	0
14	G	821	CLA	1	0
14	A	805	CLA	1	0
14	b	815	CLA	2	0
14	a	809	CLA	3	0
14	B	831	CLA	4	0
14	G	809	CLA	4	0
14	G	843	CLA	6	0
14	b	805	CLA	1	0
14	a	855	CLA	7	0
14	a	838	CLA	4	0
14	a	824	CLA	3	0
14	A	839	CLA	2	0
17	B	847	BCR	7	0
17	V	1602	BCR	3	0
14	B	804	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	822	CLA	2	0
19	b	848	LMG	2	0
14	A	810	CLA	7	0
14	G	822	CLA	6	0
14	a	810	CLA	1	0
14	a	826	CLA	4	0
17	G	851	BCR	2	0
14	G	803	CLA	2	0
17	a	851	BCR	4	0
14	a	807	CLA	1	0
14	A	823	CLA	1	0
14	A	825	CLA	6	0
14	A	841	CLA	4	0
14	H	823	CLA	5	0
14	H	825	CLA	3	0
14	b	839	CLA	5	0
14	a	811	CLA	5	0
14	B	818	CLA	2	0
14	B	835	CLA	2	0
14	G	807	CLA	3	0
17	G	853	BCR	4	0
14	A	815	CLA	4	0
14	T	1401	CLA	1	0
14	G	811	CLA	1	0
15	a	845	PQN	4	0
14	A	835	CLA	2	0
14	M	1601	CLA	1	0
14	H	805	CLA	6	0
15	G	846	PQN	6	0
14	H	804	CLA	1	0
14	a	816	CLA	1	0
14	G	802	CLA	6	0
15	H	841	PQN	3	0
14	B	830	CLA	3	0
14	a	832	CLA	2	0
17	R	103	BCR	2	0
14	F	1301	CLA	1	0
14	H	802	CLA	3	0
14	B	816	CLA	3	0
14	b	823	CLA	7	0
14	B	813	CLA	4	0
14	l	202	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	812	CLA	4	0
17	L	207	BCR	5	0
17	B	844	BCR	4	0
14	a	839	CLA	2	0
14	A	829	CLA	10	0
17	G	850	BCR	2	0
14	B	828	CLA	7	0
14	H	835	CLA	2	0
14	U	206	CLA	6	0
14	G	839	CLA	1	0
14	b	838	CLA	5	0
14	G	829	CLA	11	0
14	B	829	CLA	6	0
14	A	834	CLA	2	0
17	A	851	BCR	5	0
17	l	208	BCR	3	0
14	G	838	CLA	4	0
17	b	849	BCR	3	0
14	H	836	CLA	2	0
17	H	842	BCR	3	0
14	G	825	CLA	4	0
14	B	821	CLA	4	0
14	H	806	CLA	5	0
14	l	205	CLA	4	0
14	a	814	CLA	3	0
14	G	836	CLA	4	0
14	A	813	CLA	1	0
14	H	827	CLA	9	0
14	H	813	CLA	1	0
14	b	835	CLA	2	0
14	A	811	CLA	1	0
14	G	826	CLA	4	0
14	H	811	CLA	2	0
17	J	103	BCR	3	0
14	G	828	CLA	5	0
14	A	838	CLA	1	0
14	a	842	CLA	10	0
17	b	843	BCR	2	0
14	b	813	CLA	1	0
14	a	815	CLA	1	0
14	B	802	CLA	5	0
14	a	821	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	829	CLA	10	0
14	W	1701	CLA	1	0
17	G	848	BCR	2	0
14	B	840	CLA	5	0
14	A	803	CLA	4	0
14	B	825	CLA	1	0
14	A	826	CLA	7	0
14	b	831	CLA	11	0
14	G	815	CLA	1	0
17	f	203	BCR	5	0
15	b	841	PQN	4	0
17	A	850	BCR	3	0
17	j	103	BCR	5	0
14	a	844	CLA	3	0
17	H	847	BCR	7	0
14	a	837	CLA	2	0
14	G	833	CLA	1	0
14	a	835	CLA	3	0
17	I	101	BCR	7	0
14	b	834	CLA	5	0
14	B	820	CLA	1	0
14	a	804	CLA	1	0
14	a	806	CLA	2	0
17	F	1302	BCR	3	0
14	H	820	CLA	2	0
14	H	839	CLA	6	0
14	G	814	CLA	4	0
14	A	832	CLA	3	0
14	a	828	CLA	12	0
17	l	203	BCR	2	0
14	b	826	CLA	6	0
14	A	827	CLA	6	0
17	a	850	BCR	6	0
14	V	1601	CLA	1	0
14	G	806	CLA	2	0
14	G	845	CLA	3	0
17	B	850	BCR	4	0
14	G	832	CLA	3	0
14	b	833	CLA	1	0
14	A	809	CLA	4	0
14	a	817	CLA	1	0
14	B	832	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	H	834	CLA	5	0
14	b	814	CLA	2	0
14	A	843	CLA	10	0
14	A	828	CLA	4	0
14	B	826	CLA	8	0
16	c	102	SF4	1	0
17	S	103	BCR	5	0
17	H	843	BCR	3	0
14	A	817	CLA	1	0
14	f	202	CLA	2	0
18	G	855	LHG	2	0
17	A	848	BCR	2	0
14	A	844	CLA	4	0
14	b	816	CLA	4	0
14	b	809	CLA	7	0
14	B	838	CLA	5	0
14	H	815	CLA	3	0
14	G	819	CLA	5	0
14	L	204	CLA	3	0
14	b	803	CLA	4	0
17	L	202	BCR	1	0
14	i	101	CLA	7	0
17	G	849	BCR	2	0
14	a	836	CLA	2	0
14	b	840	CLA	4	0
14	a	829	CLA	3	0
17	l	201	BCR	1	0
17	A	852	BCR	4	0
14	A	821	CLA	1	0
17	a	852	BCR	6	0
17	B	848	BCR	8	0
14	H	838	CLA	4	0
14	b	825	CLA	3	0
14	B	836	CLA	5	0
14	G	805	CLA	4	0
14	l	206	CLA	7	0
14	H	809	CLA	2	0
14	G	824	CLA	1	0
14	H	824	CLA	2	0
14	b	828	CLA	1	0
14	B	811	CLA	1	0
14	b	830	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	806	CLA	3	0
17	A	853	BCR	4	0
14	A	822	CLA	5	0
14	b	837	CLA	3	0
14	H	826	CLA	6	0
18	G	854	LHG	4	0
14	G	808	CLA	1	0
14	a	803	CLA	2	0
13	A	801	CL0	3	0
14	A	840	CLA	2	0
17	Q	202	BCR	3	0
17	R	101	BCR	5	0
13	a	801	CL0	5	0
14	B	809	CLA	3	0
17	j	104	BCR	6	0
17	J	102	BCR	4	0
14	J	101	CLA	1	0
14	a	819	CLA	4	0
14	A	808	CLA	1	0
14	A	831	CLA	7	0
14	a	831	CLA	2	0
14	G	812	CLA	4	0
14	H	812	CLA	6	0
19	B	849	LMG	3	0
14	G	816	CLA	3	0
14	H	807	CLA	5	0
17	b	842	BCR	2	0
14	B	822	CLA	4	0
17	H	844	BCR	3	0
14	a	820	CLA	2	0
14	U	205	CLA	2	0
14	b	819	CLA	2	0
14	b	832	CLA	5	0
17	m	1602	BCR	4	0
14	H	801	CLA	7	0
14	b	808	CLA	6	0
14	L	206	CLA	6	0
17	a	848	BCR	3	0
14	G	830	CLA	2	0
18	A	854	LHG	5	0
14	b	811	CLA	3	0
17	b	845	BCR	5	0

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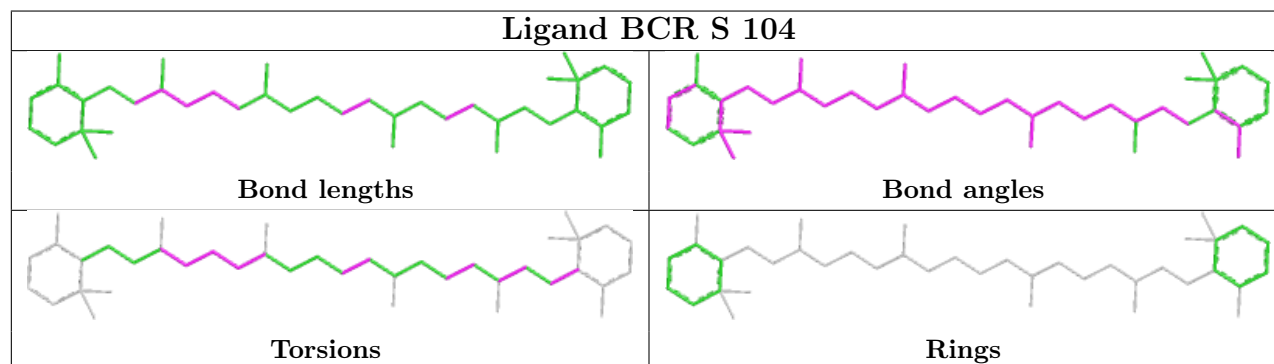
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17	G	852	BCR	3	0
17	i	102	BCR	6	0
14	b	801	CLA	6	0
14	B	808	CLA	2	0
14	A	814	CLA	4	0
14	B	837	CLA	3	0
17	B	845	BCR	3	0
14	A	830	CLA	4	0
14	x	1701	CLA	1	0
14	A	819	CLA	3	0
14	a	830	CLA	4	0
14	H	819	CLA	2	0
17	U	202	BCR	3	0
14	B	801	CLA	7	0
17	H	849	BCR	3	0
14	G	831	CLA	7	0
14	A	802	CLA	7	0
14	H	816	CLA	7	0
14	G	817	CLA	1	0
17	I	102	BCR	2	0
14	H	803	CLA	9	0
14	a	818	CLA	2	0
14	A	842	CLA	1	0
14	B	805	CLA	5	0
14	G	842	CLA	9	0
14	b	812	CLA	6	0
14	l	207	CLA	4	0
13	G	801	CL0	6	0
14	a	840	CLA	7	0
17	H	845	BCR	2	0
14	B	803	CLA	7	0
14	G	834	CLA	1	0
16	G	847	SF4	1	0
14	H	814	CLA	1	0
14	A	836	CLA	2	0
14	b	822	CLA	5	0
14	A	833	CLA	1	0
17	A	849	BCR	3	0
14	B	817	CLA	5	0
14	L	201	CLA	4	0
14	B	824	CLA	3	0
14	a	805	CLA	2	0

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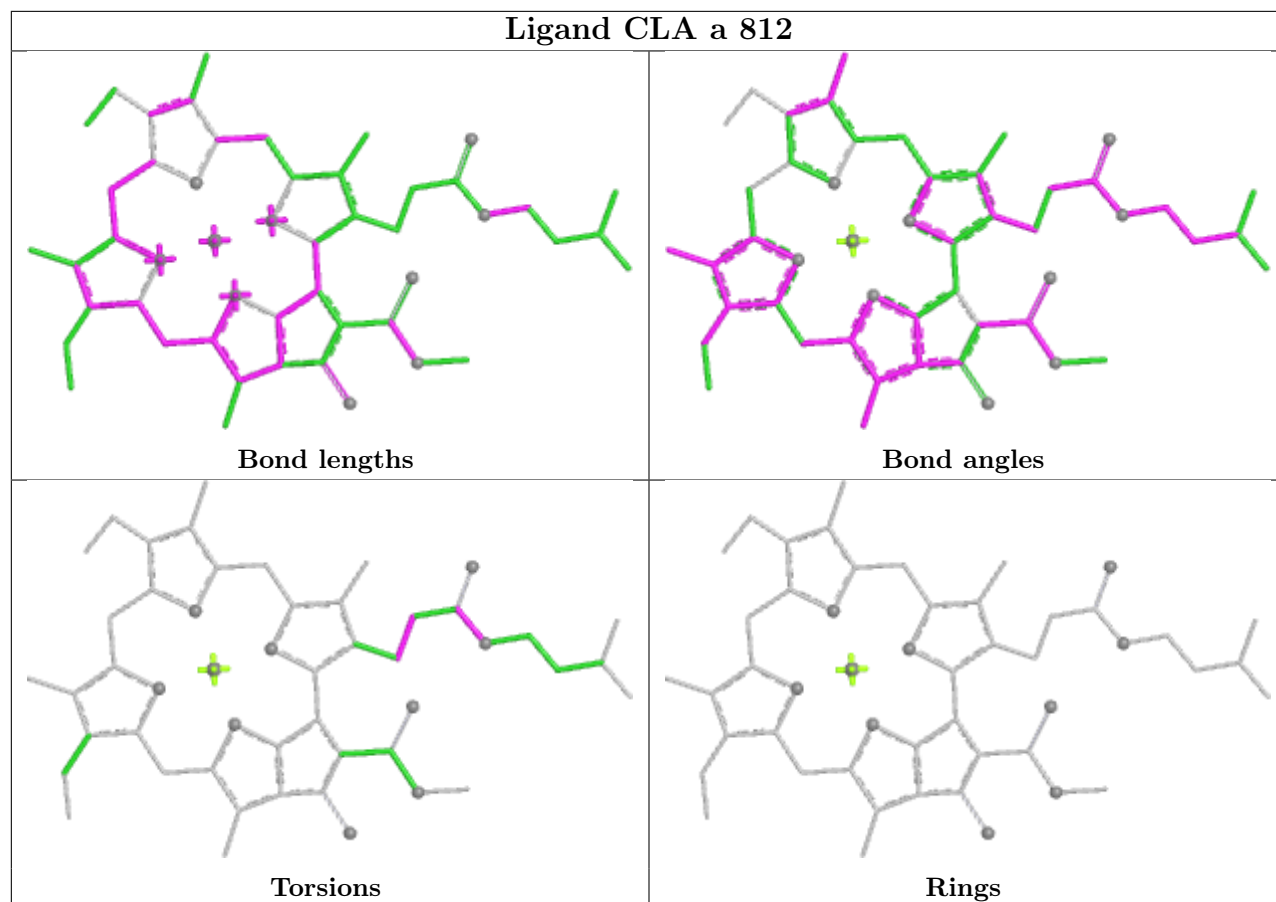
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	802	CLA	5	0
14	H	831	CLA	1	0
17	f	201	BCR	5	0
14	a	808	CLA	5	0
14	H	837	CLA	3	0
14	B	814	CLA	1	0
14	B	819	CLA	2	0
14	A	845	CLA	4	0
14	a	813	CLA	8	0
14	G	835	CLA	1	0
14	b	827	CLA	5	0
14	H	821	CLA	3	0
14	B	812	CLA	5	0
14	B	827	CLA	8	0
17	H	846	BCR	4	0
17	Q	204	BCR	4	0
14	B	807	CLA	2	0

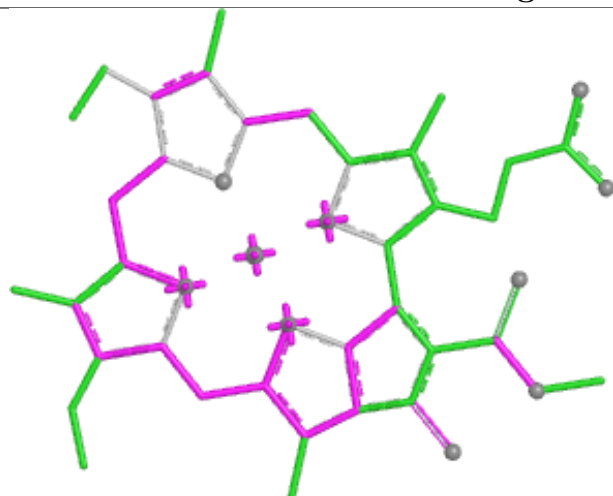
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



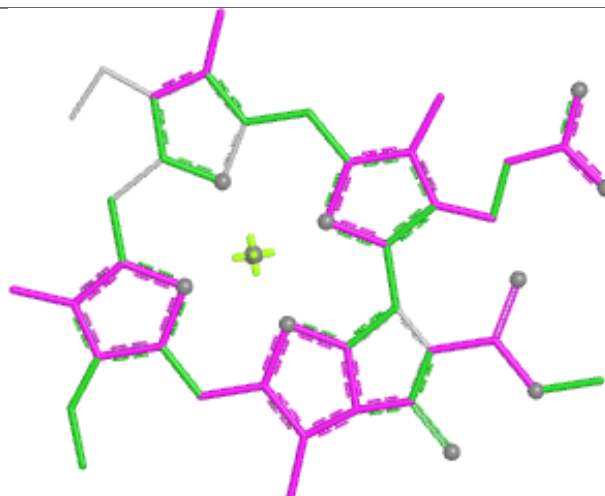
## Ligand CLA a 812



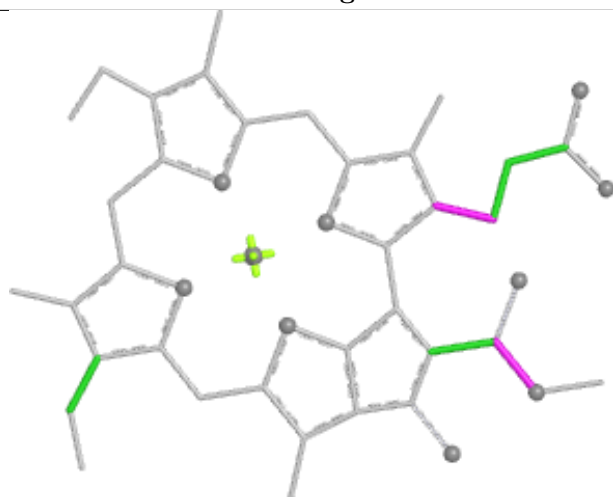
## Ligand CLA b 810



Bond lengths



Bond angles

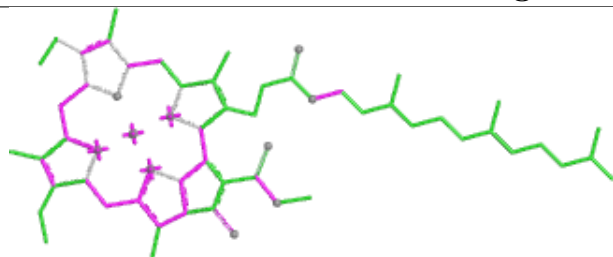


Torsions

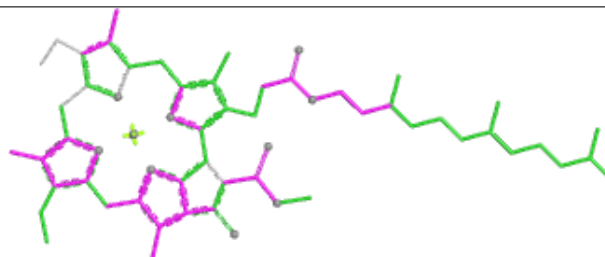


Rings

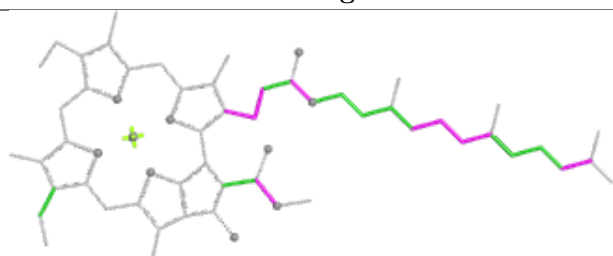
## Ligand CLA U 204



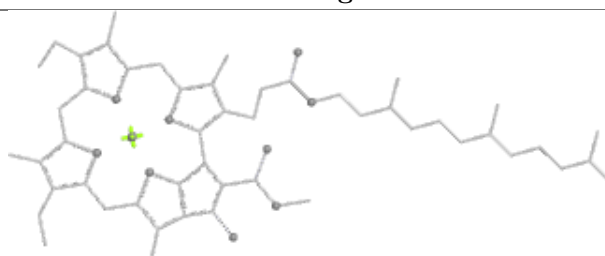
Bond lengths



Bond angles

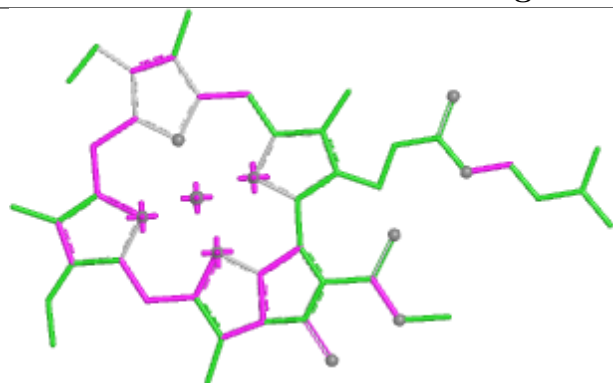


Torsions

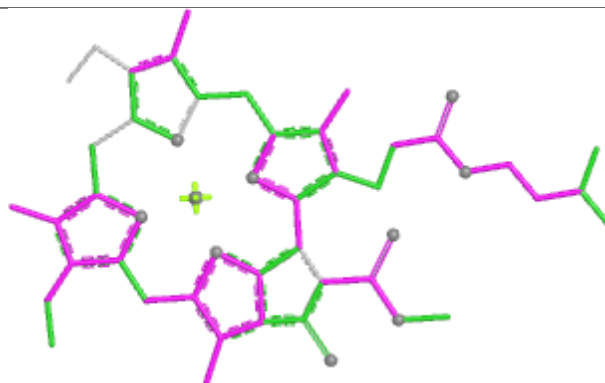


Rings

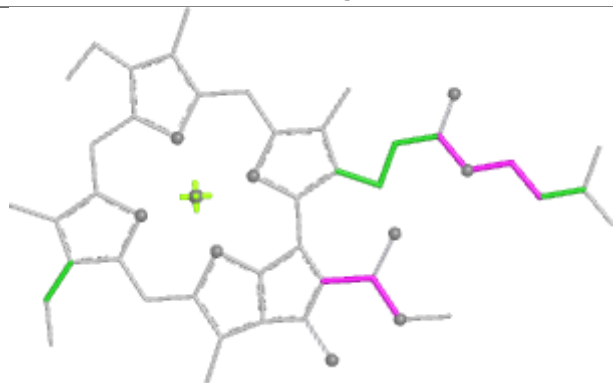
## Ligand CLA B 823



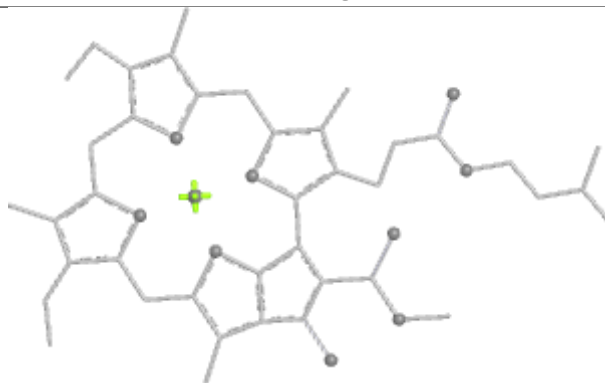
Bond lengths



Bond angles

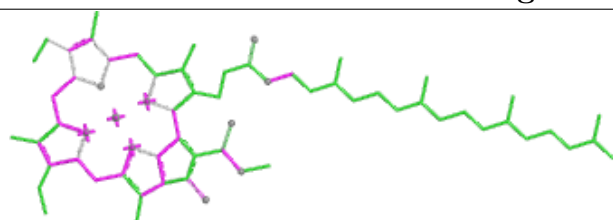


Torsions

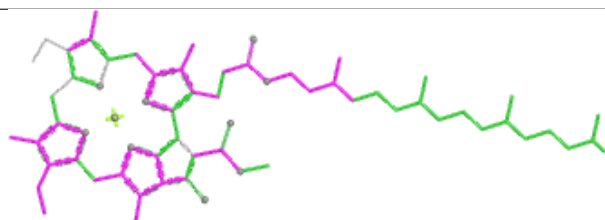


Rings

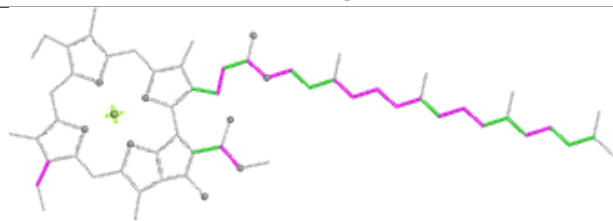
## Ligand CLA b 804



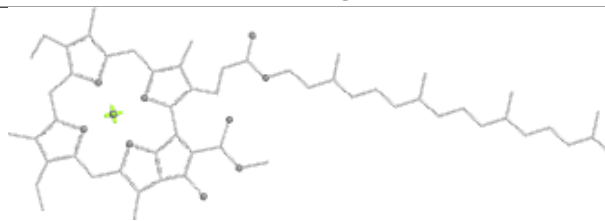
Bond lengths



Bond angles

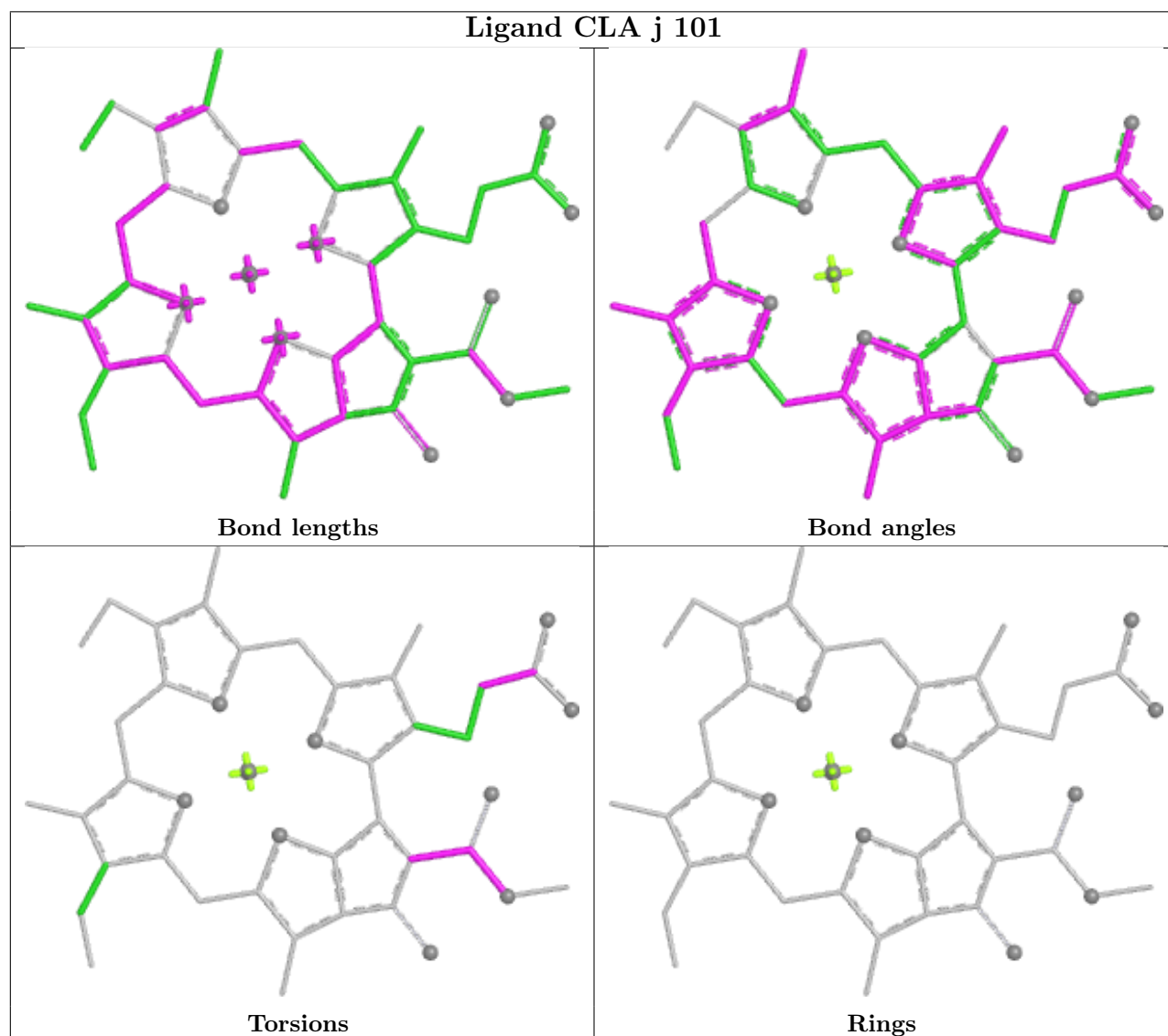
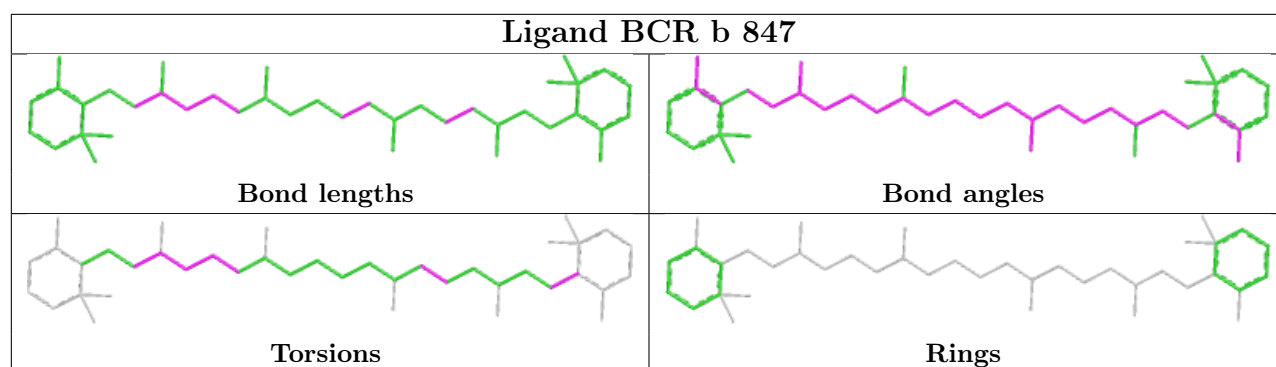


Torsions

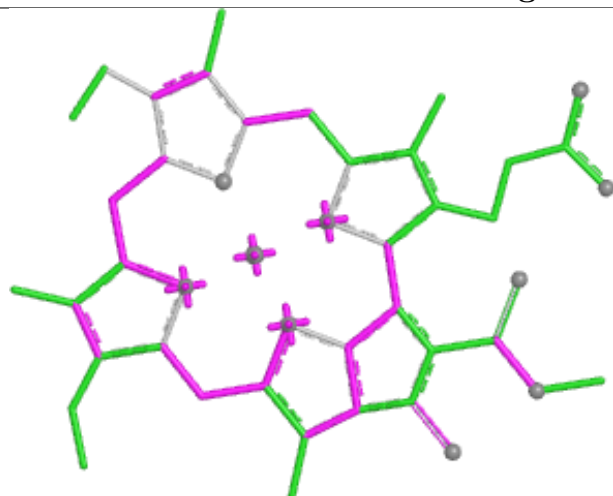


Rings

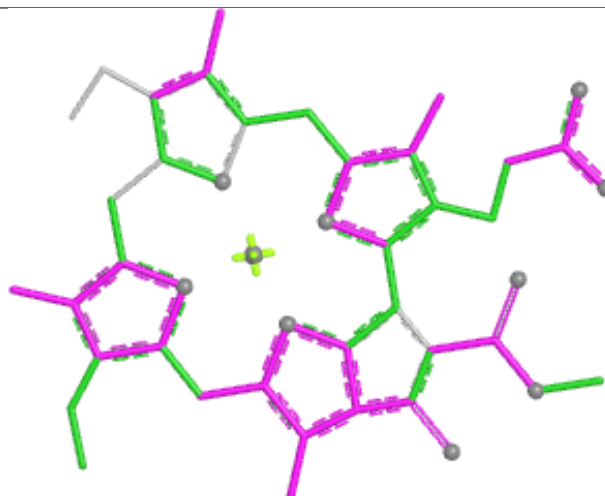




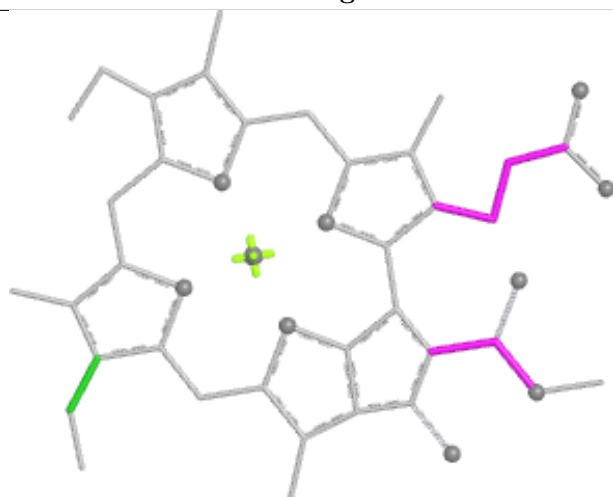
## Ligand CLA a 822



Bond lengths



Bond angles

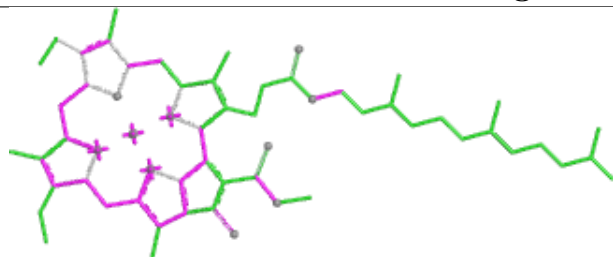


Torsions

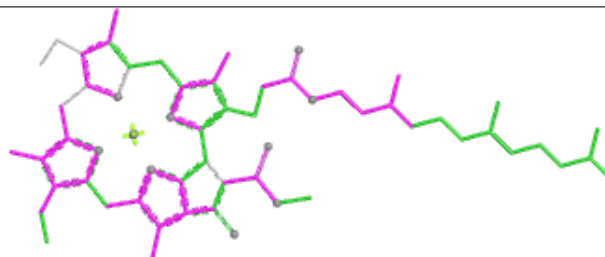


Rings

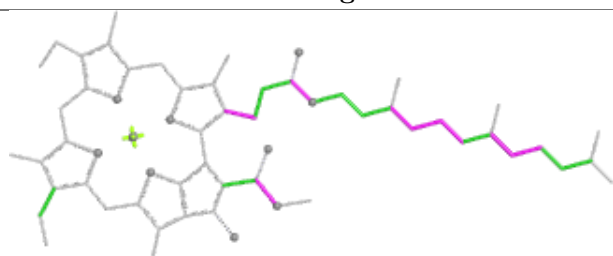
## Ligand CLA H 817



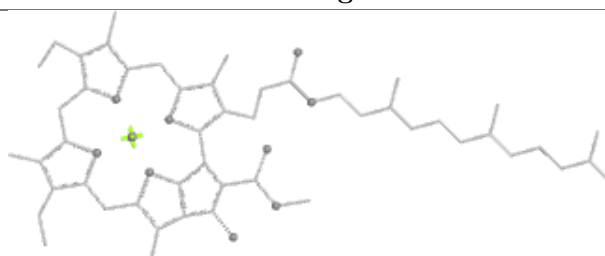
Bond lengths



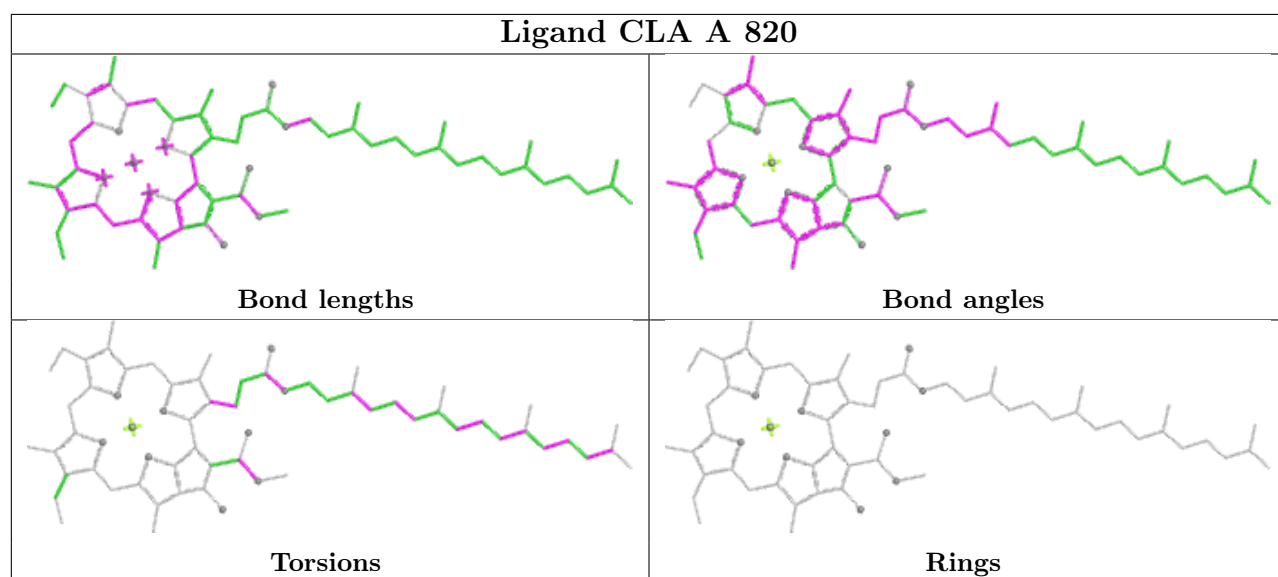
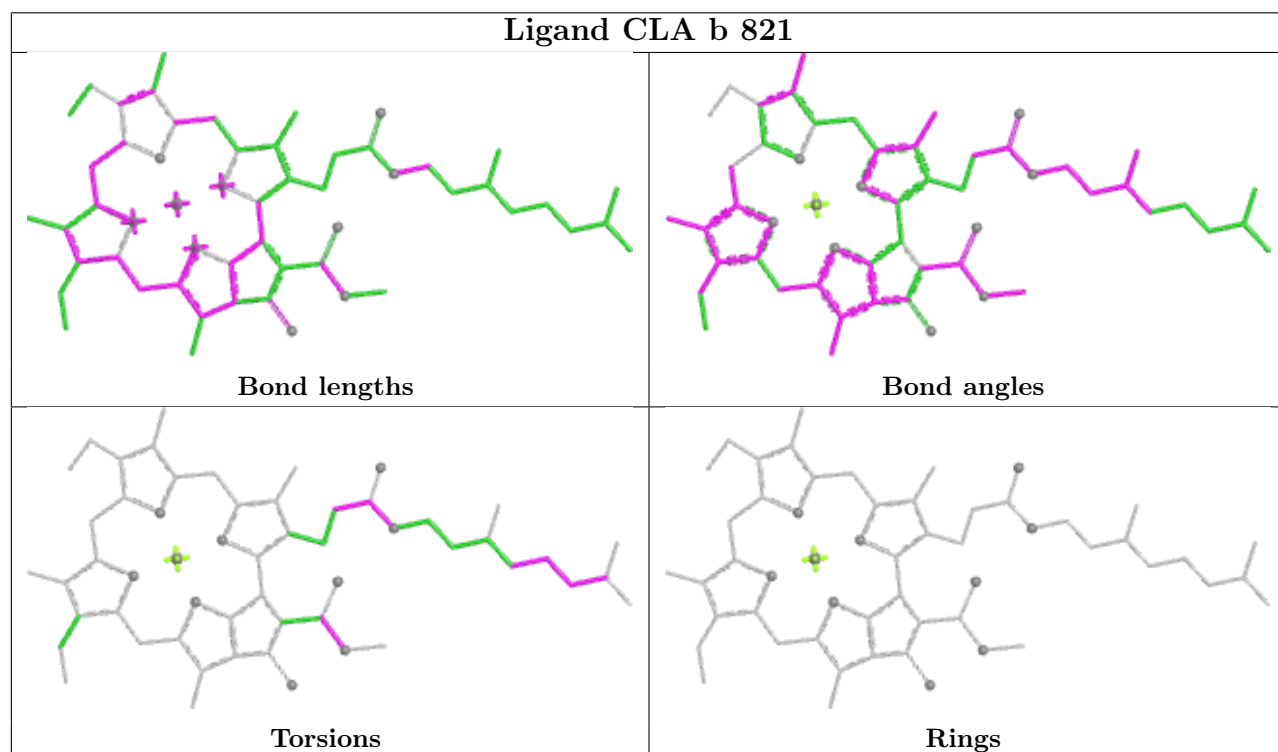
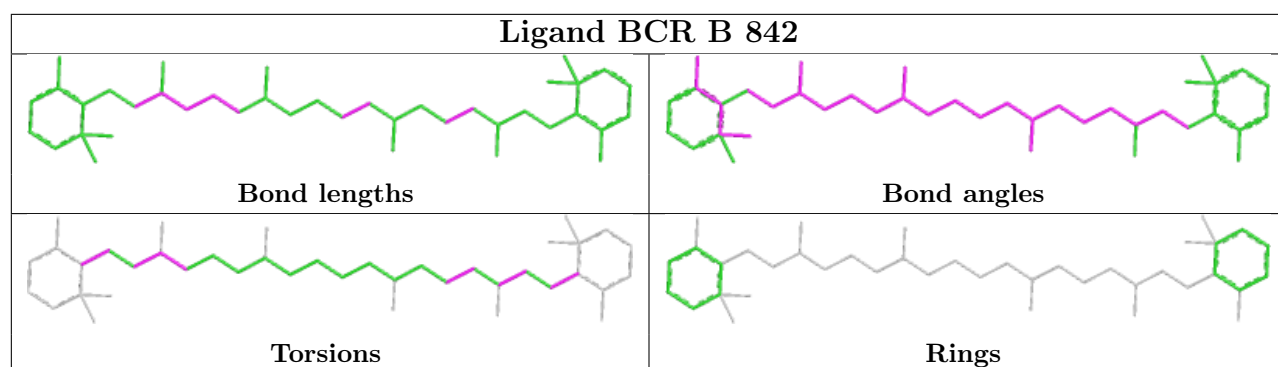
Bond angles

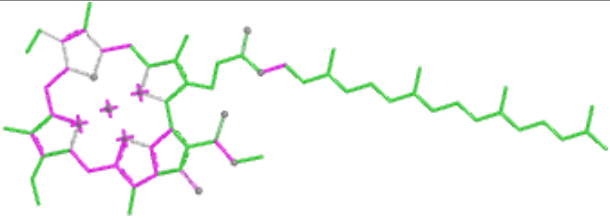
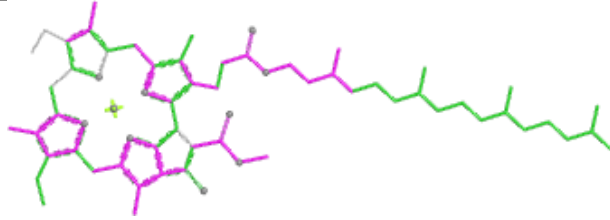
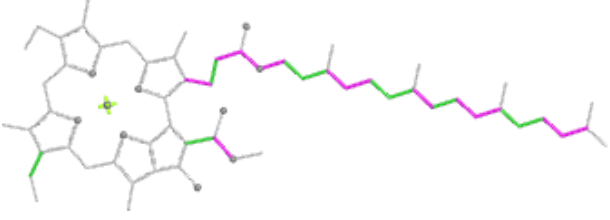
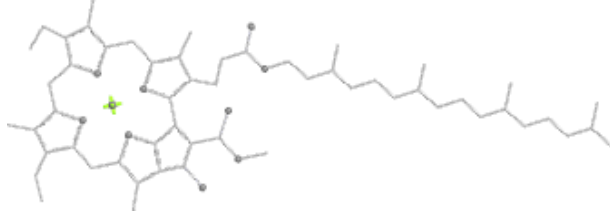
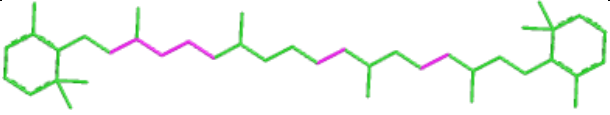
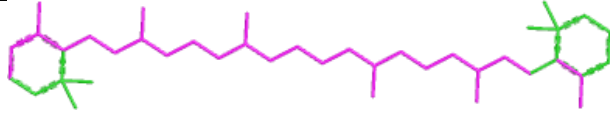
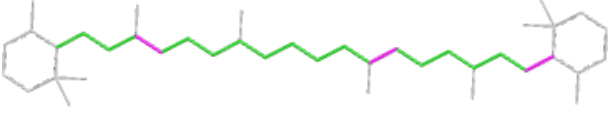
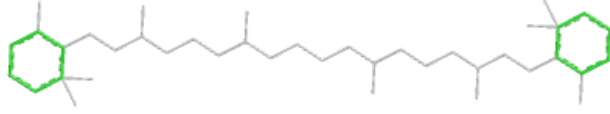
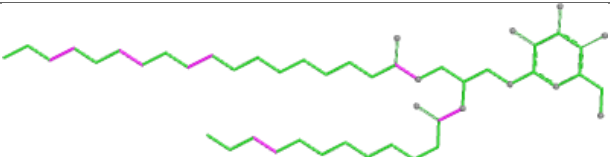
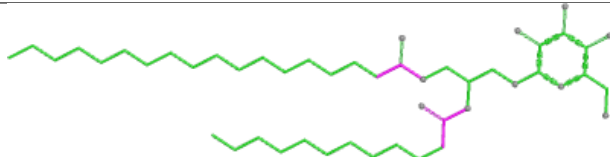
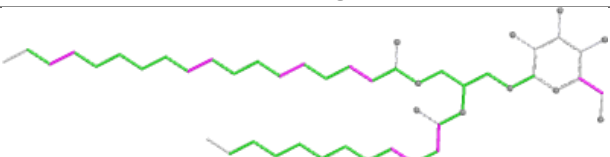
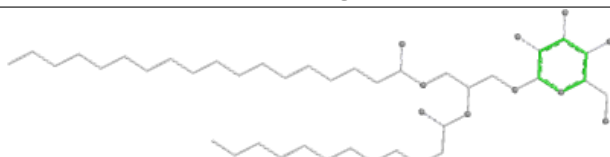


Torsions

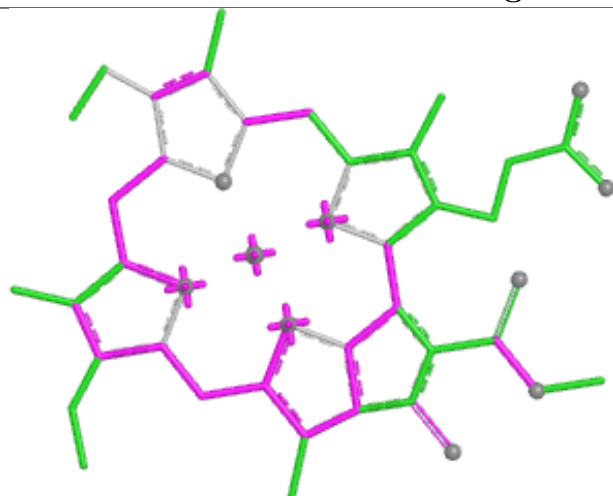


Rings

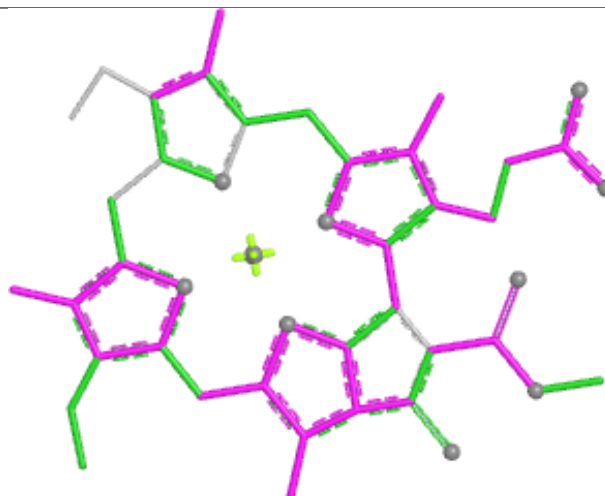


Ligand CLA A 807	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 846	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LMG H 848	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

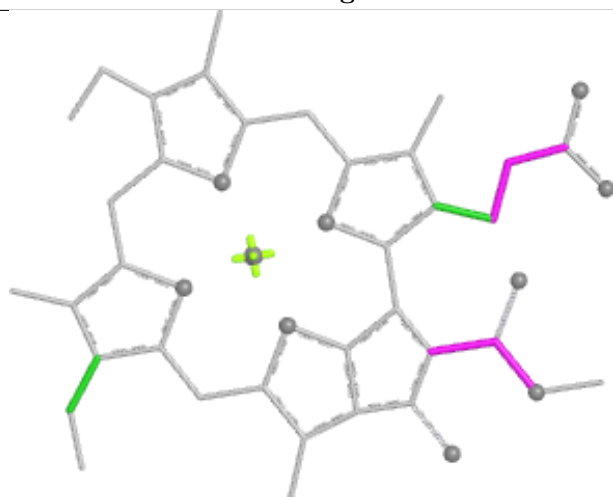
## Ligand CLA X 1701



Bond lengths



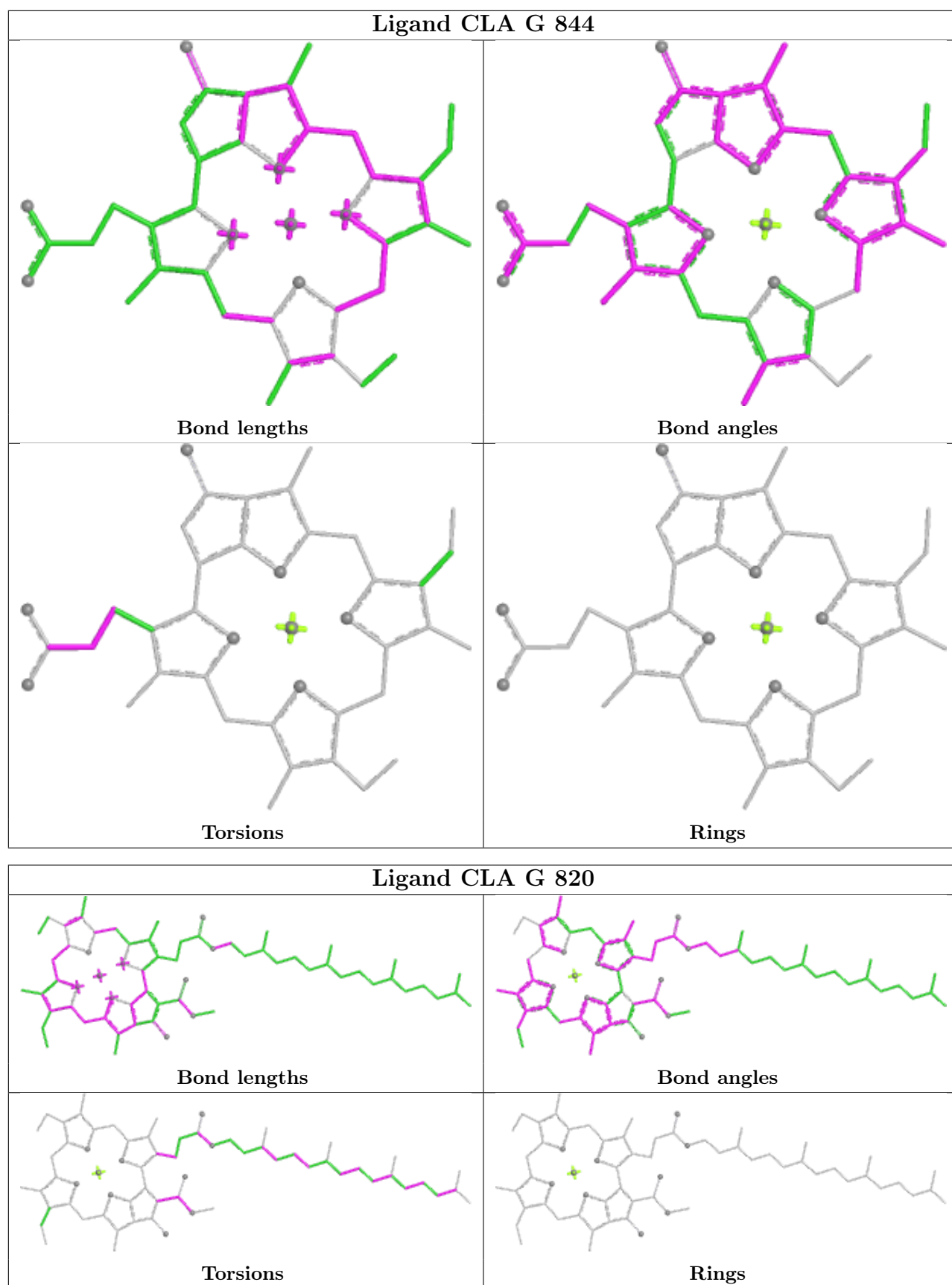
Bond angles

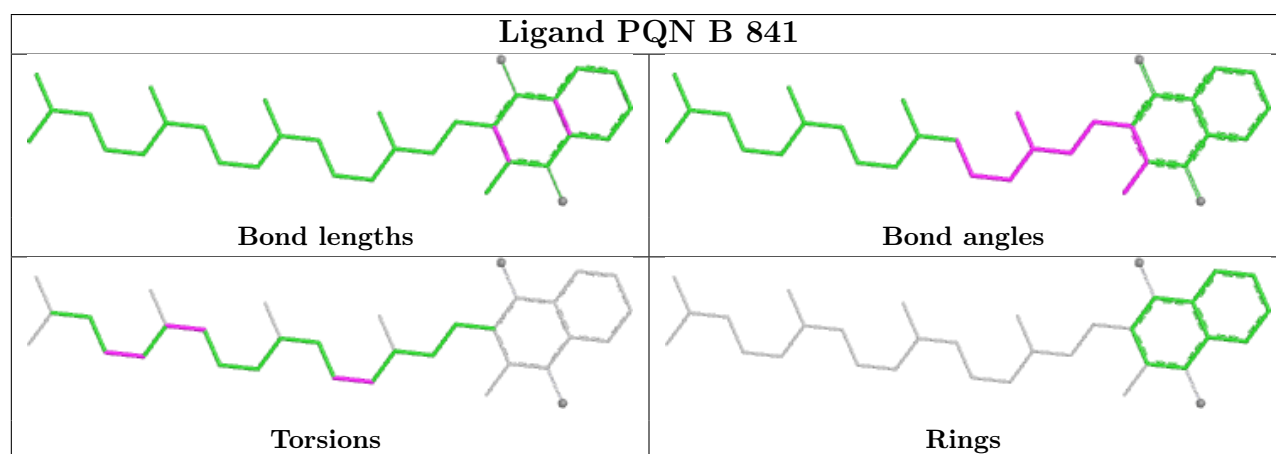
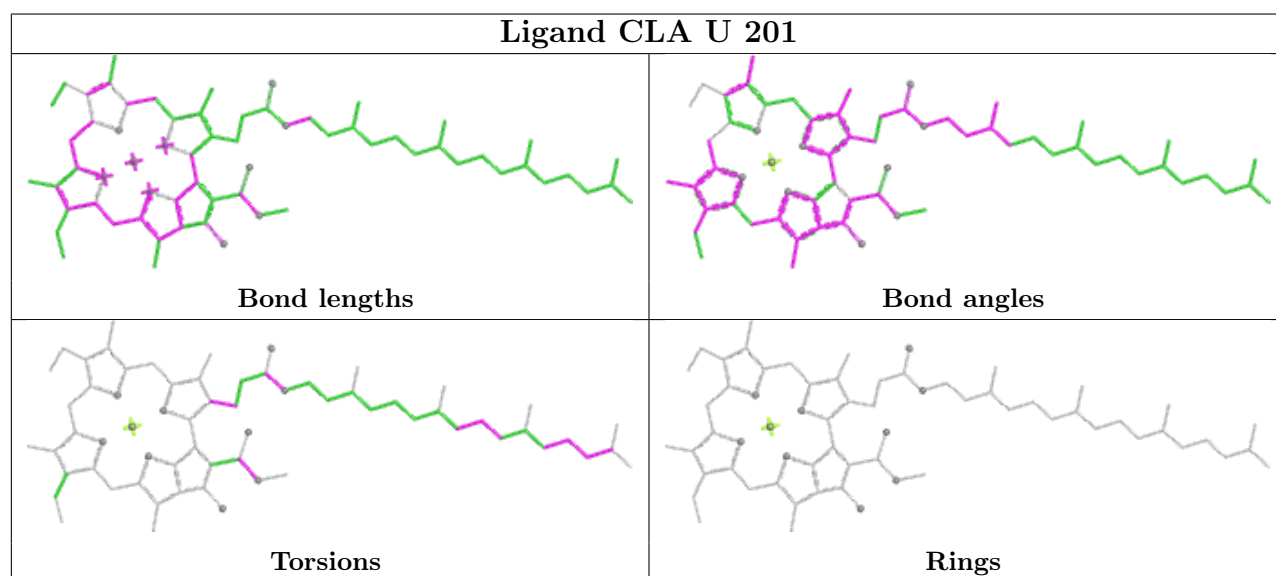
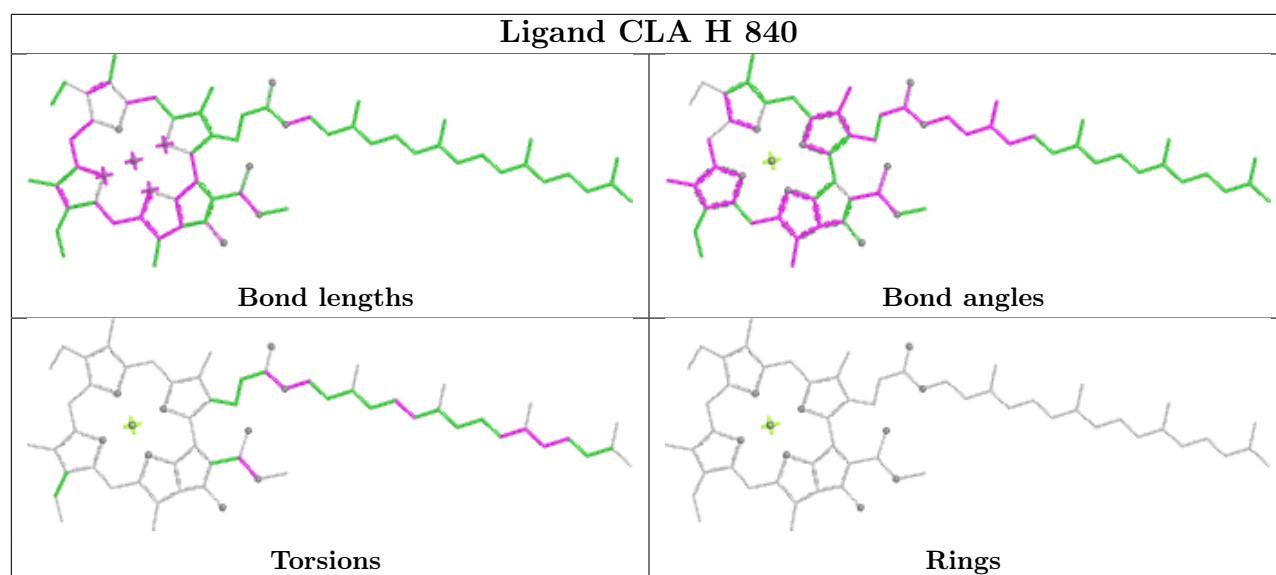


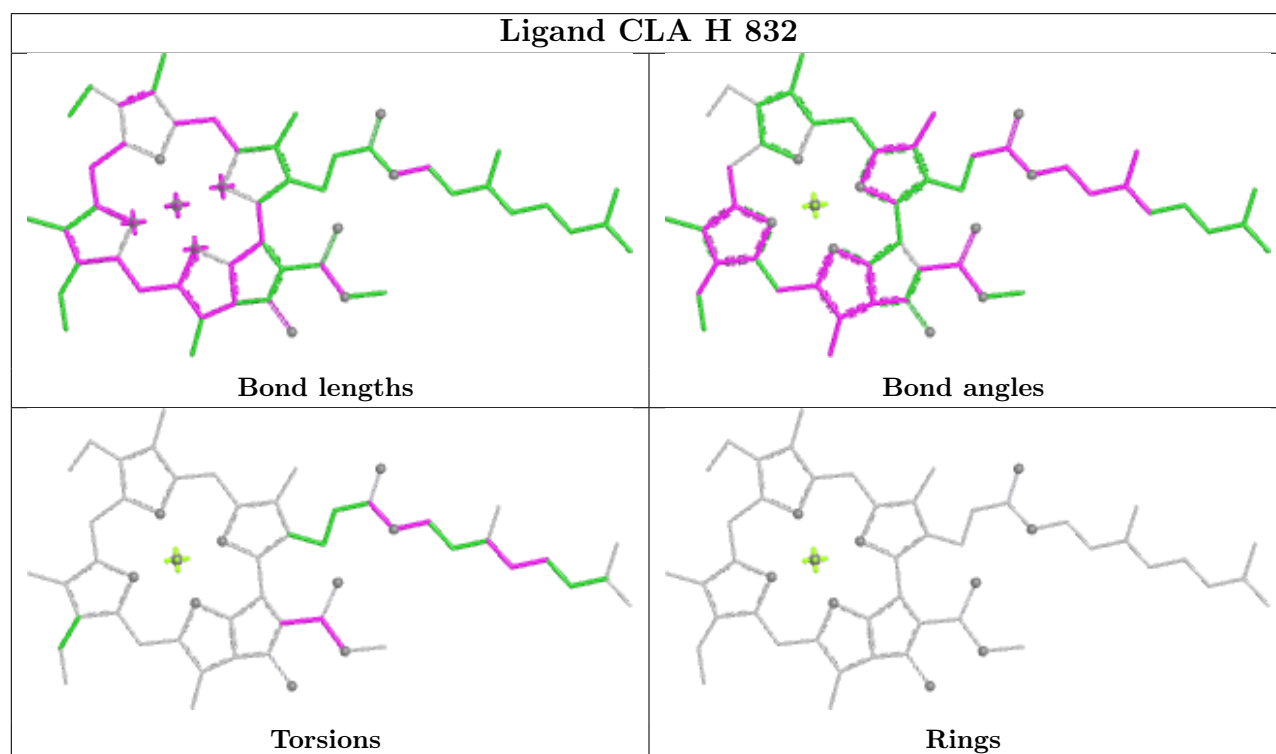
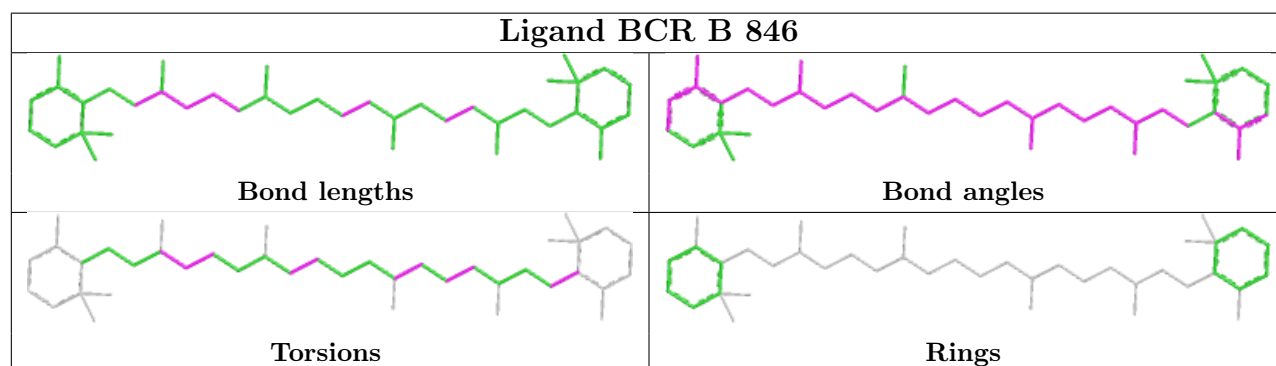
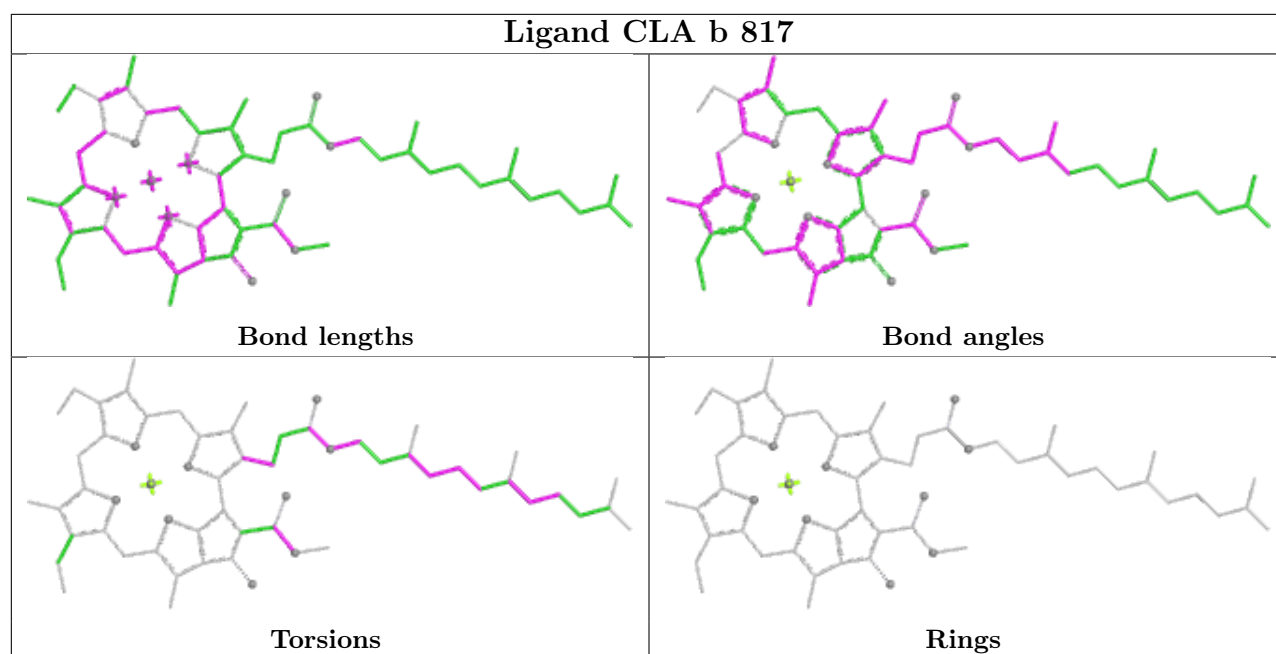
Torsions



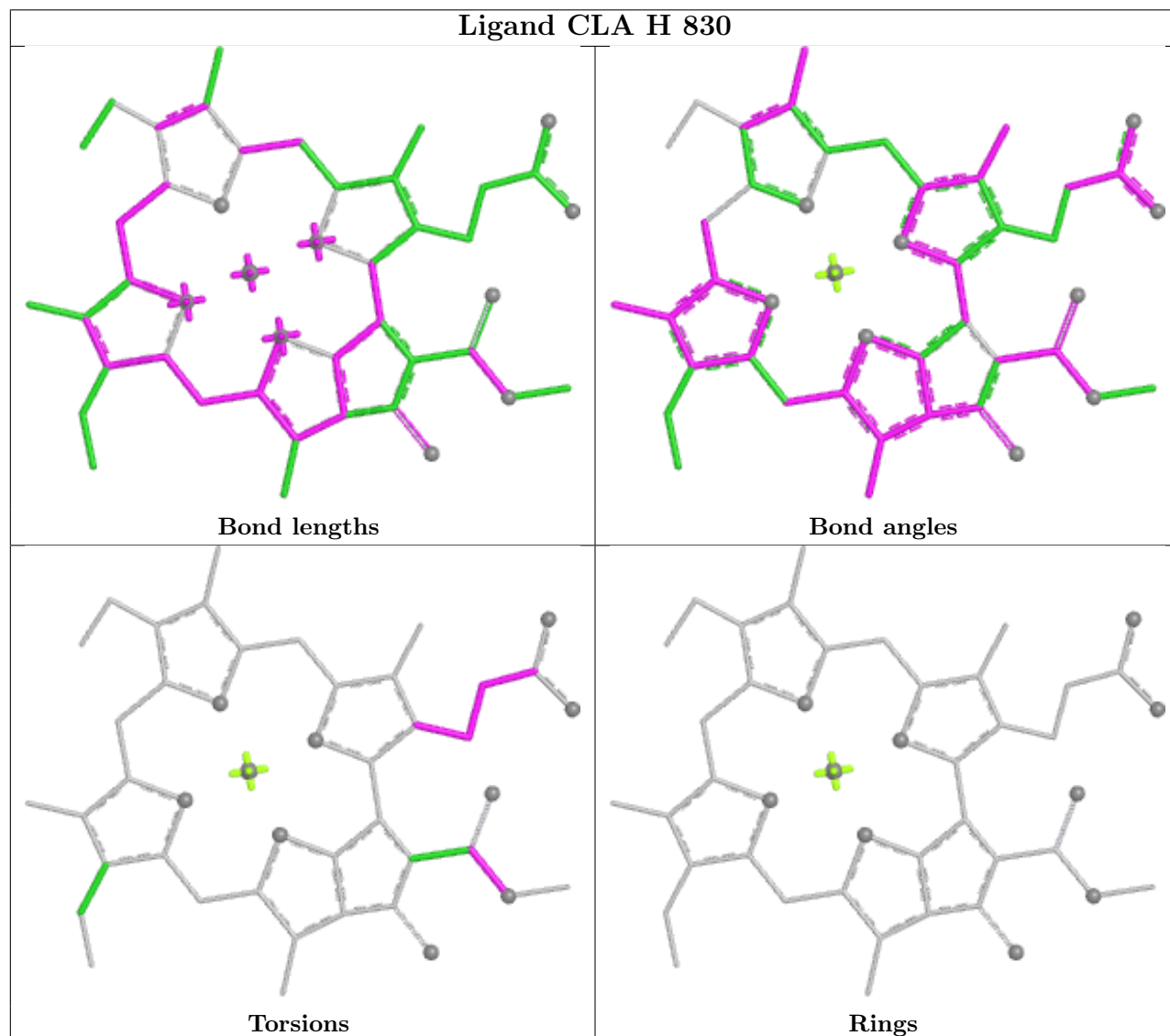
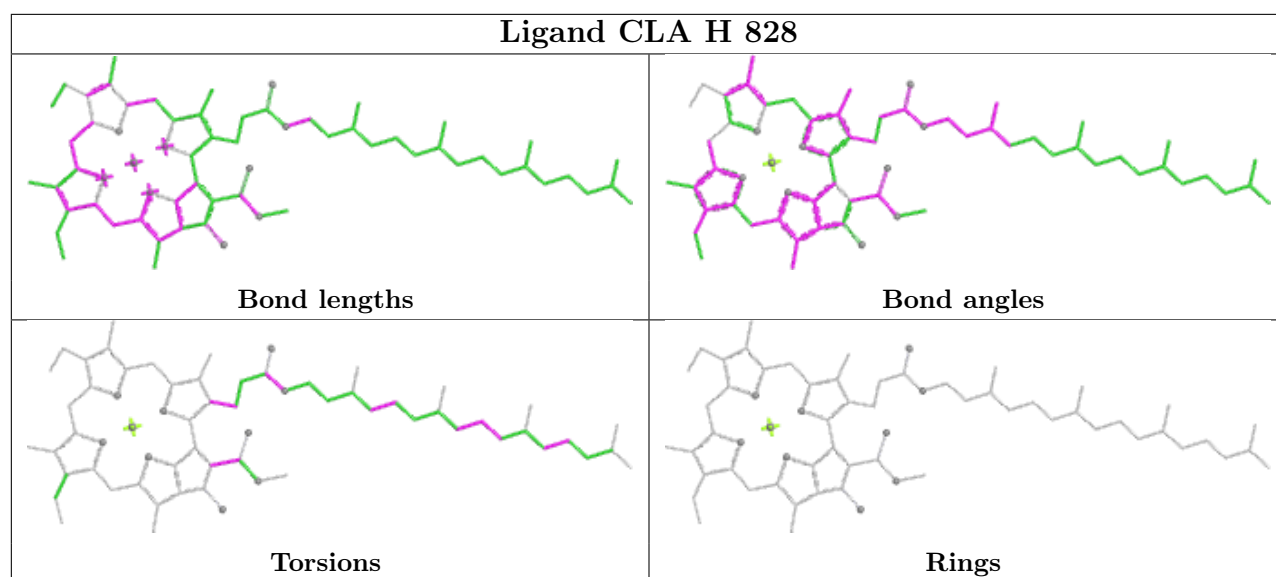
Rings



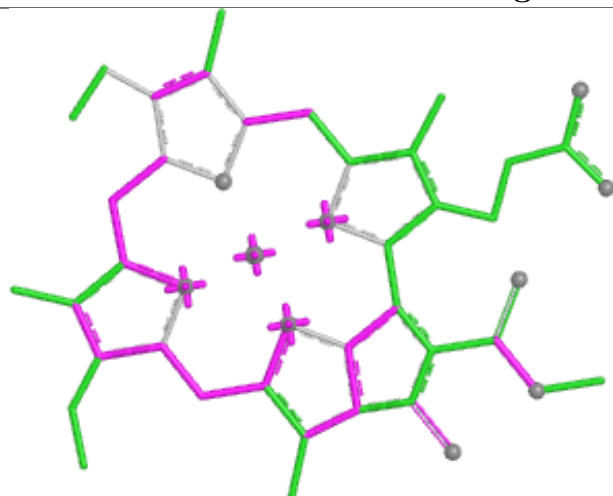




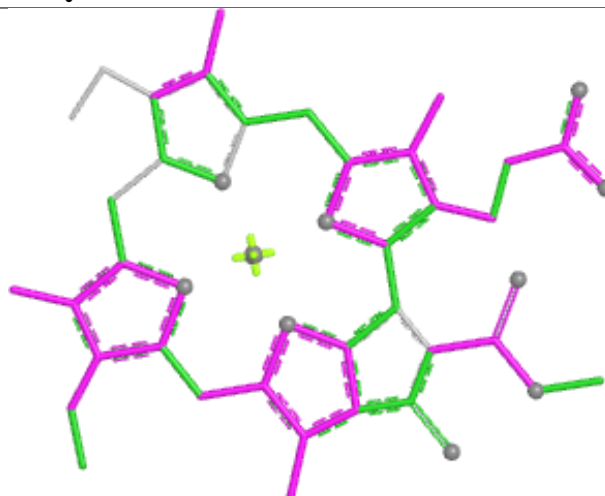




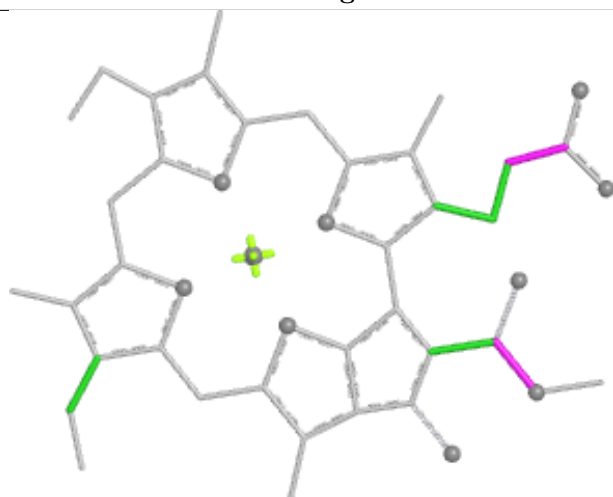
## Ligand CLA Q 203



Bond lengths



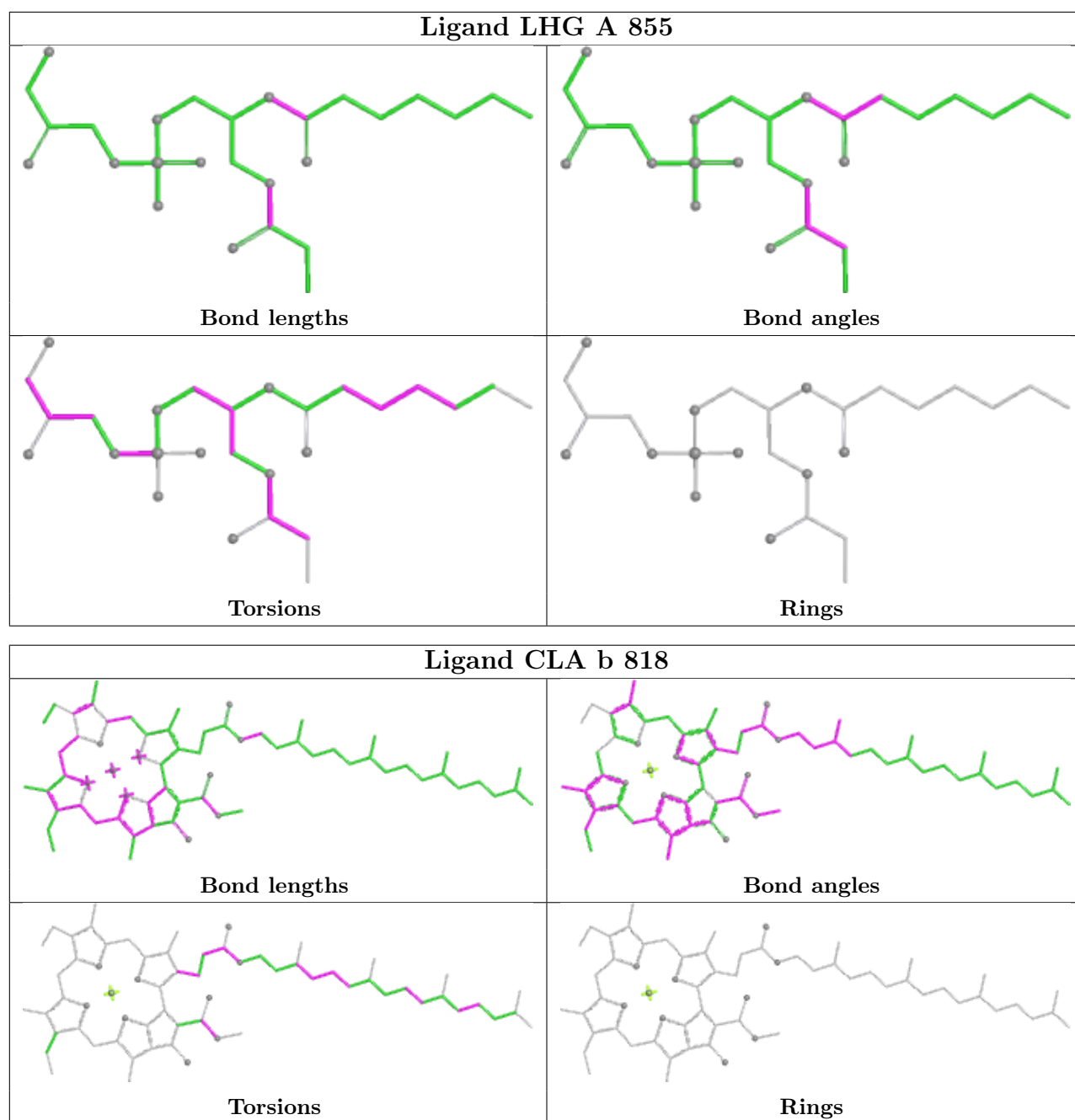
Bond angles

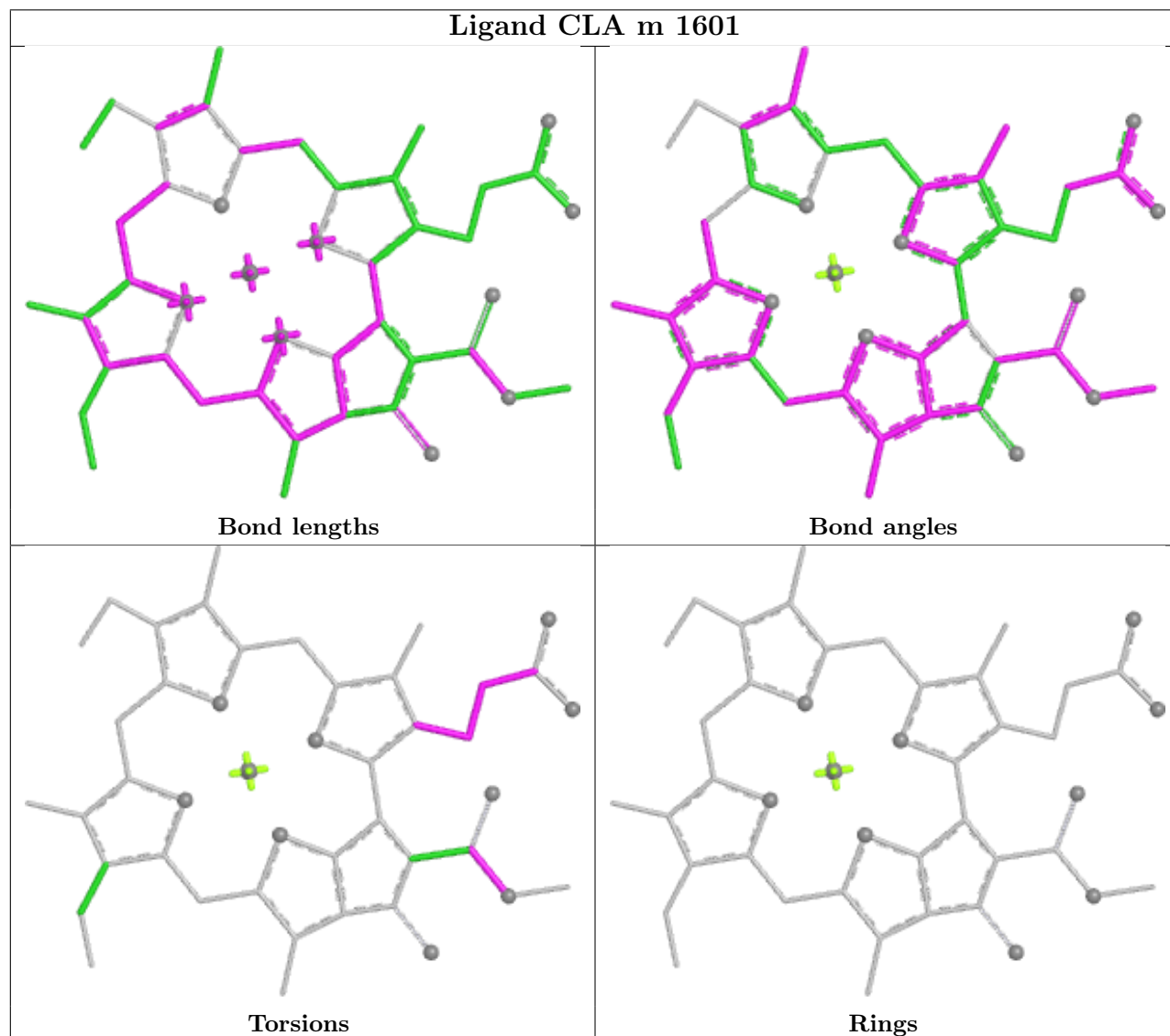
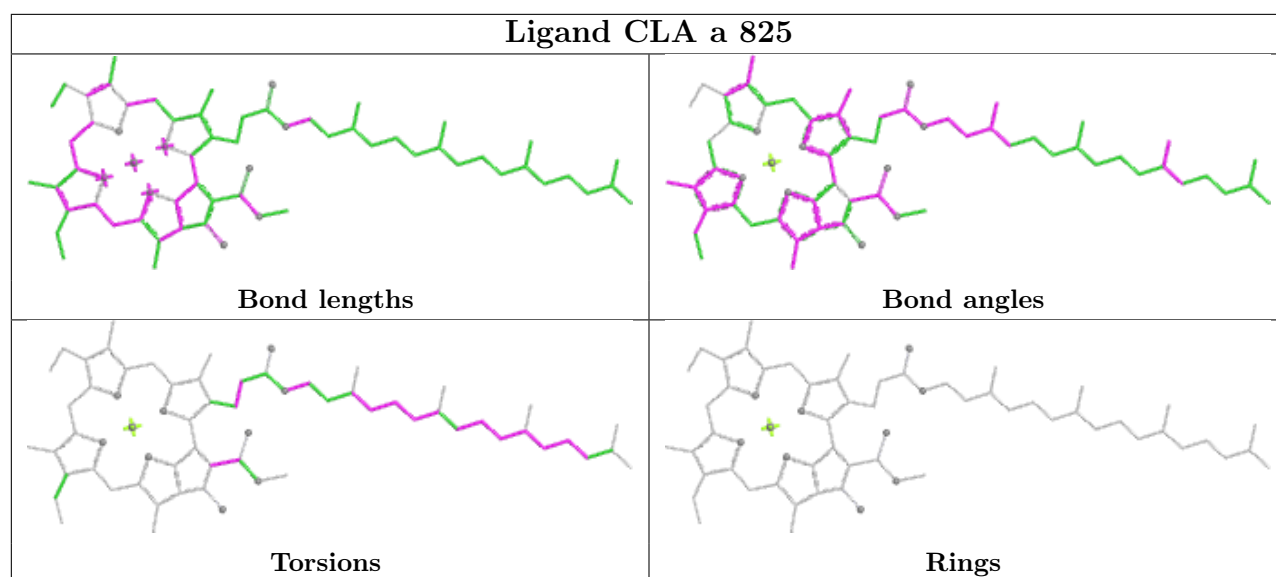


Torsions

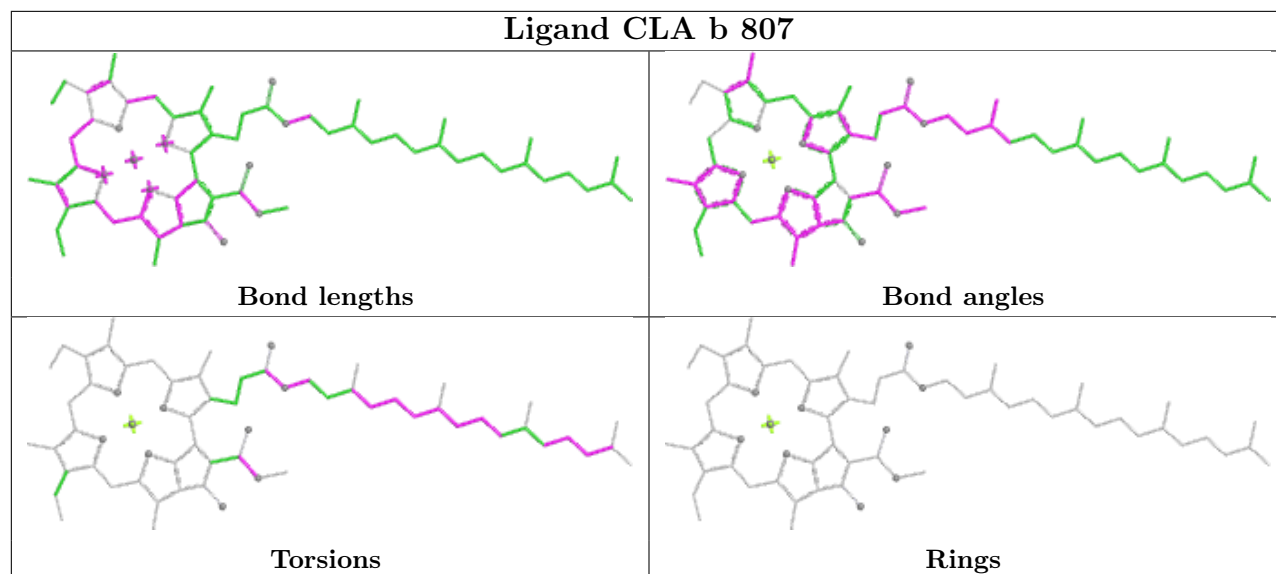


Rings

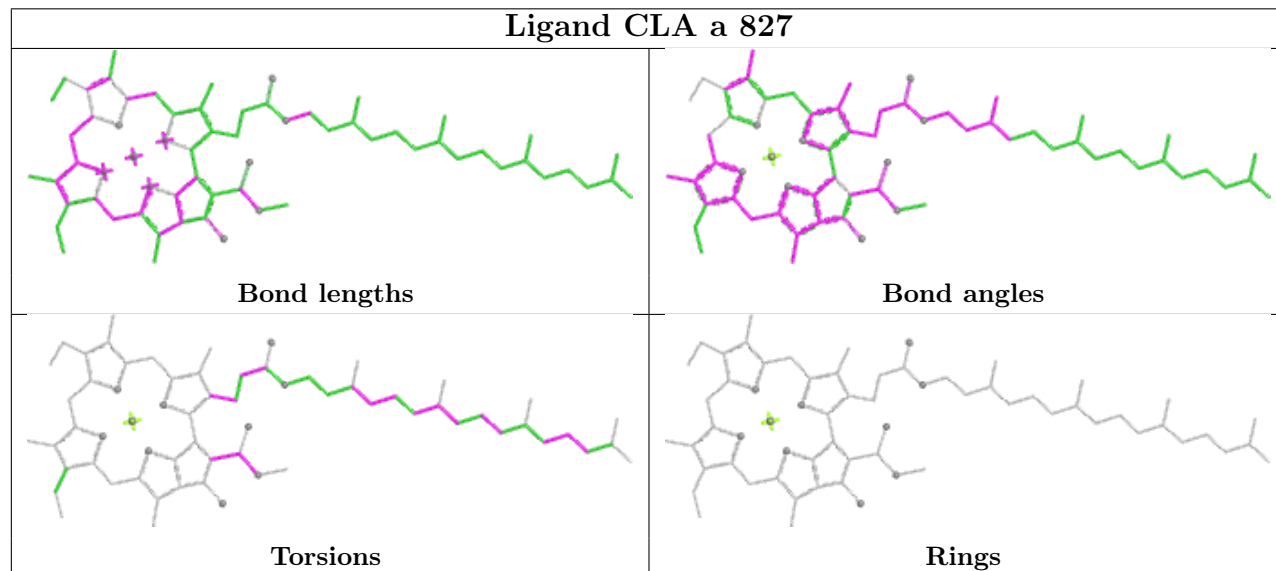




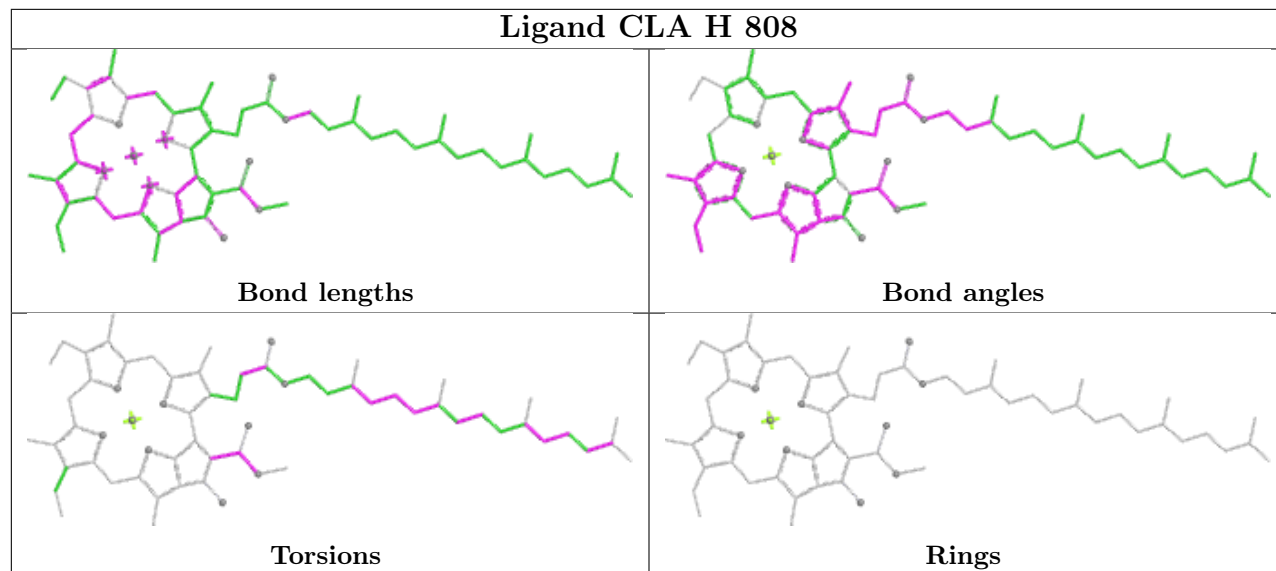
## Ligand CLA b 807



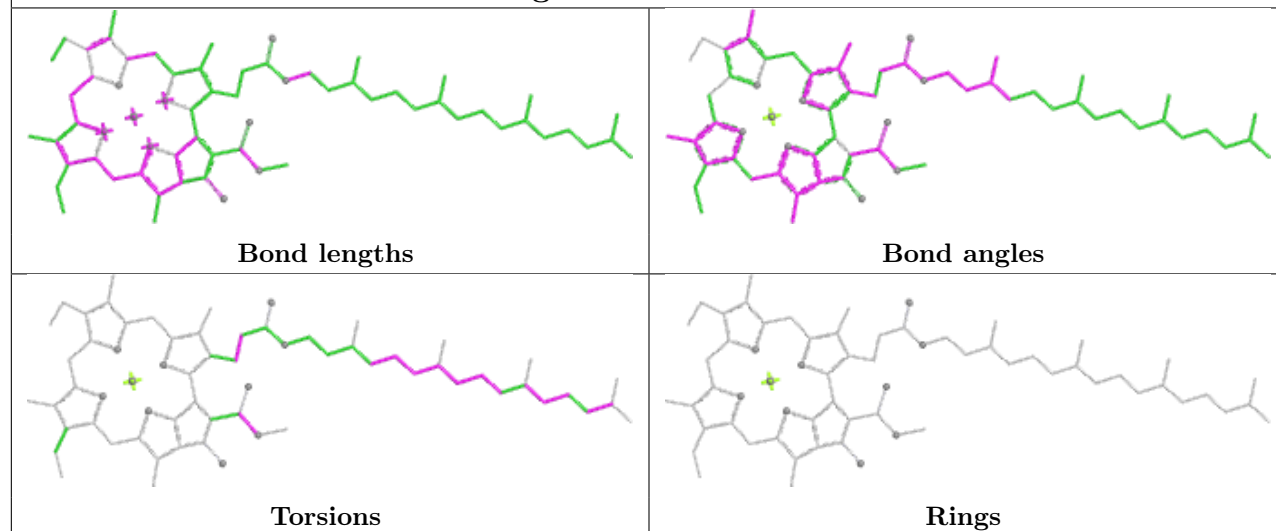
## Ligand CLA a 827



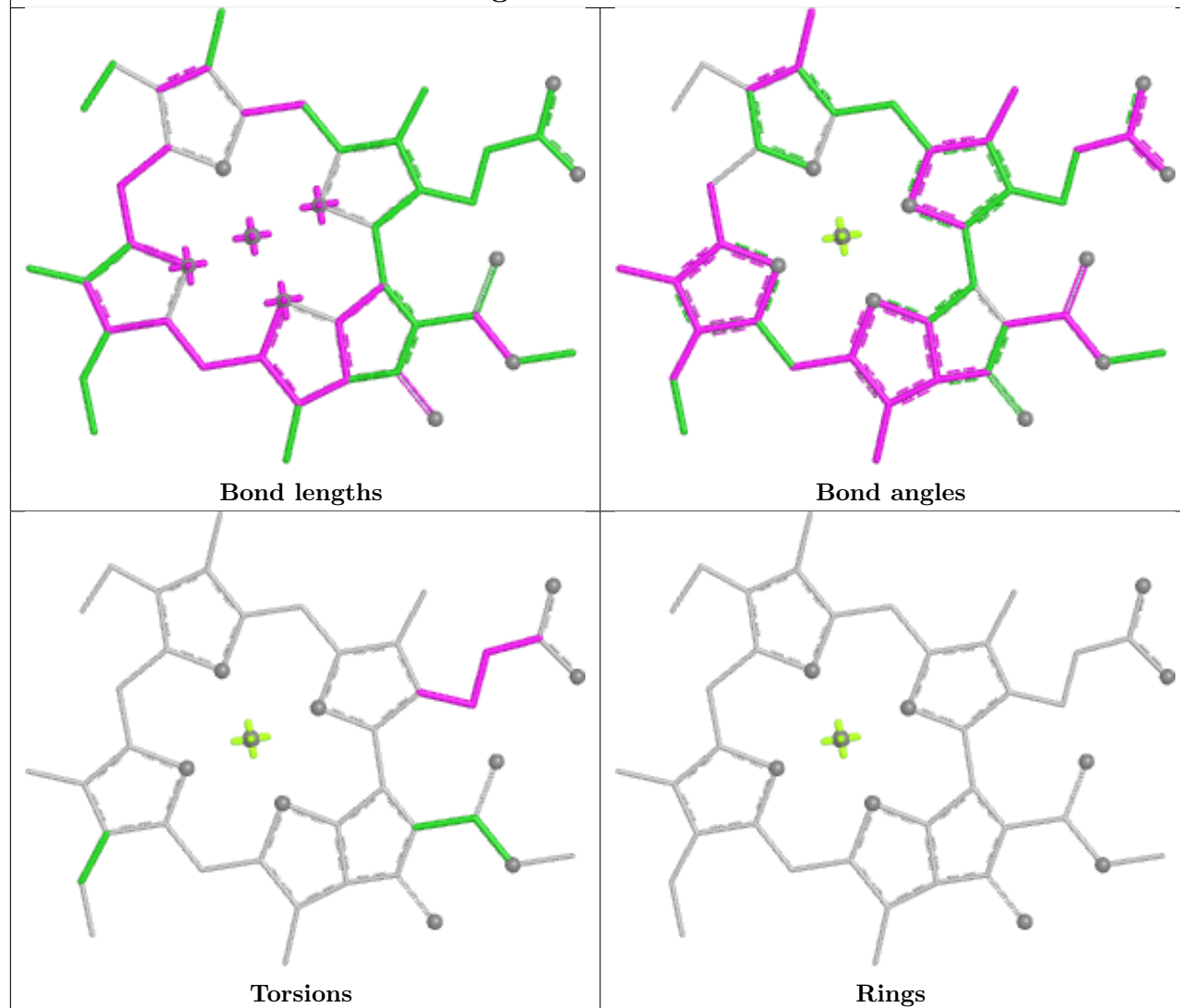
## Ligand CLA H 808

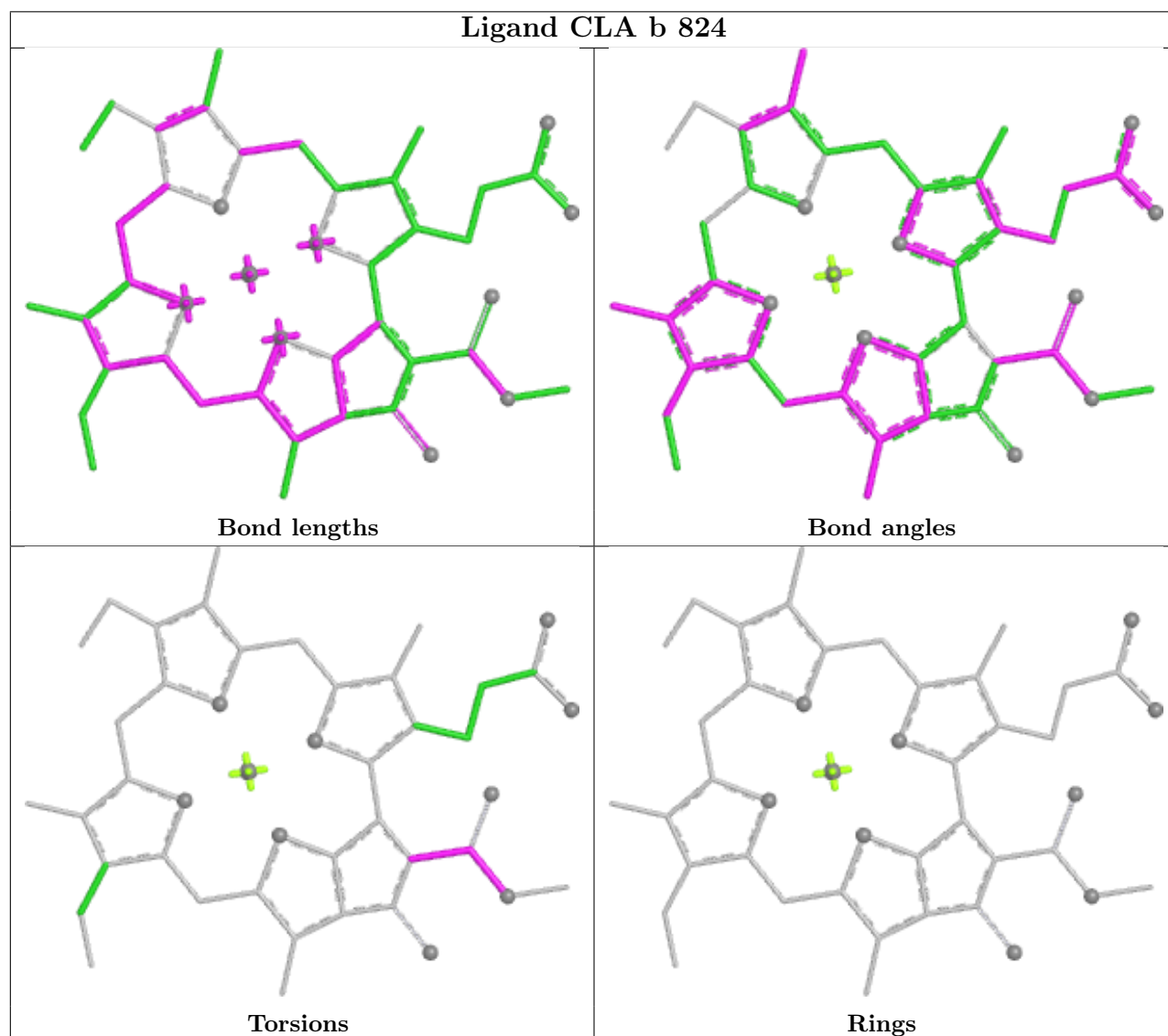
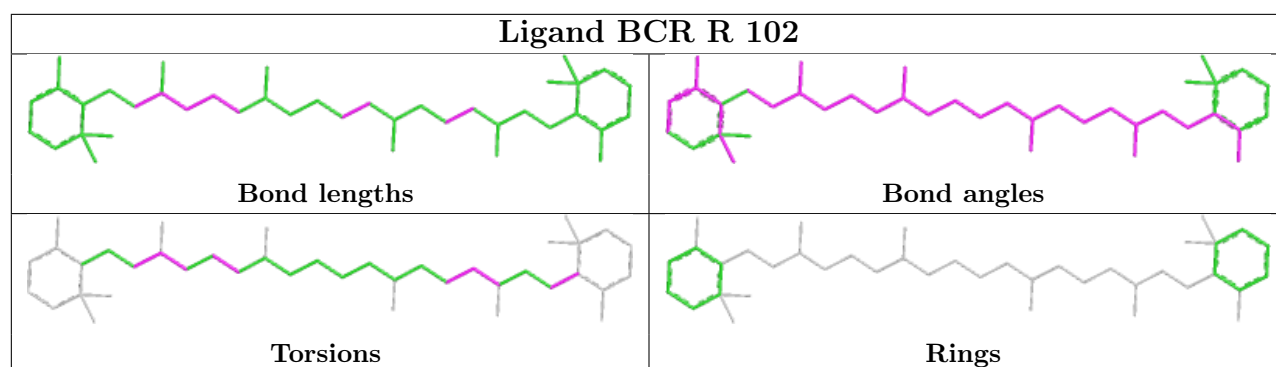


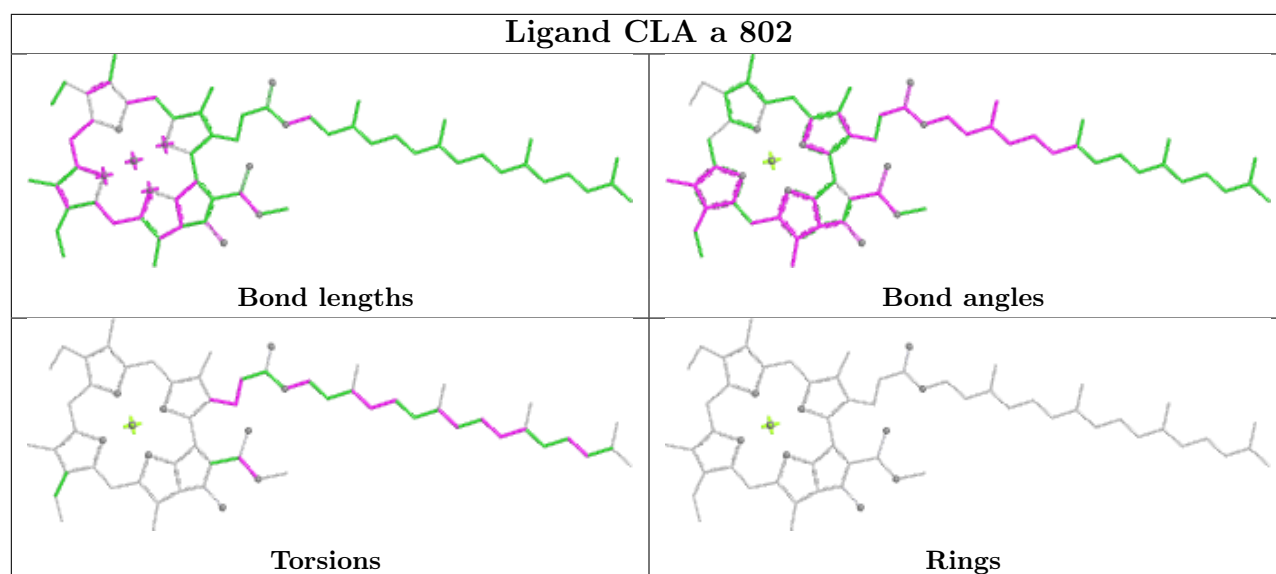
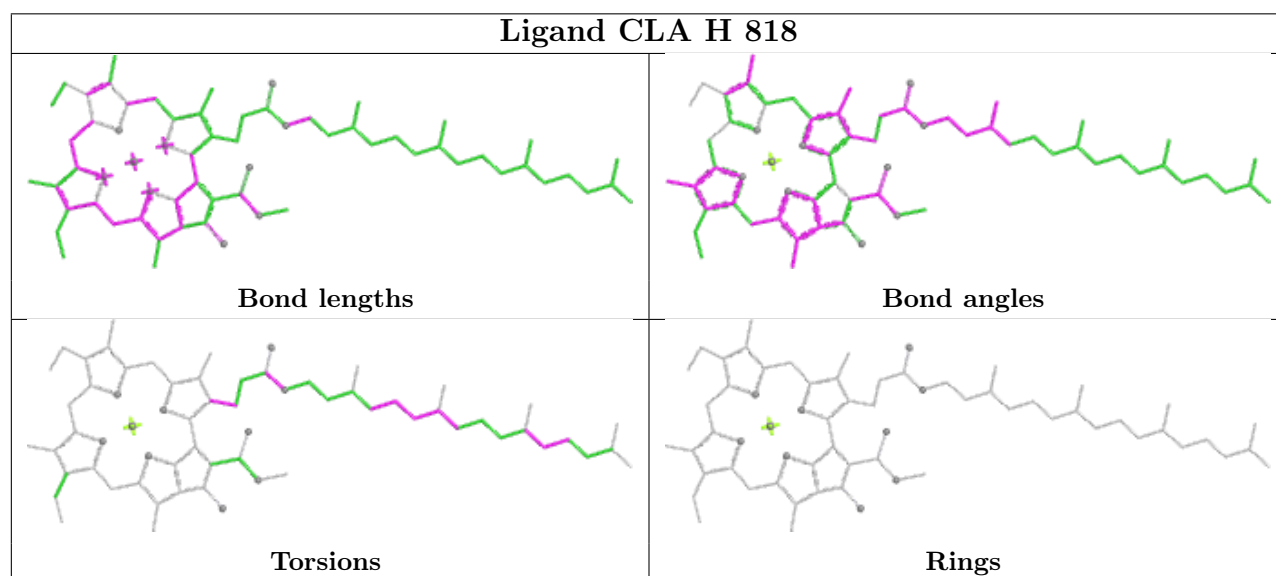
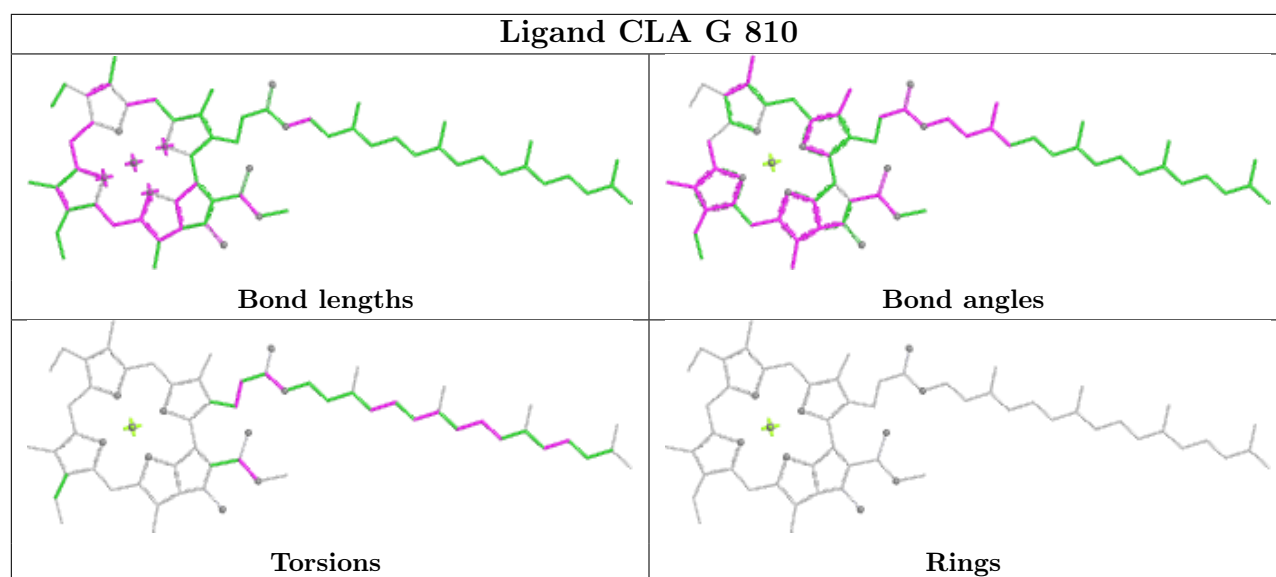
## Ligand CLA B 839



## Ligand CLA A 837

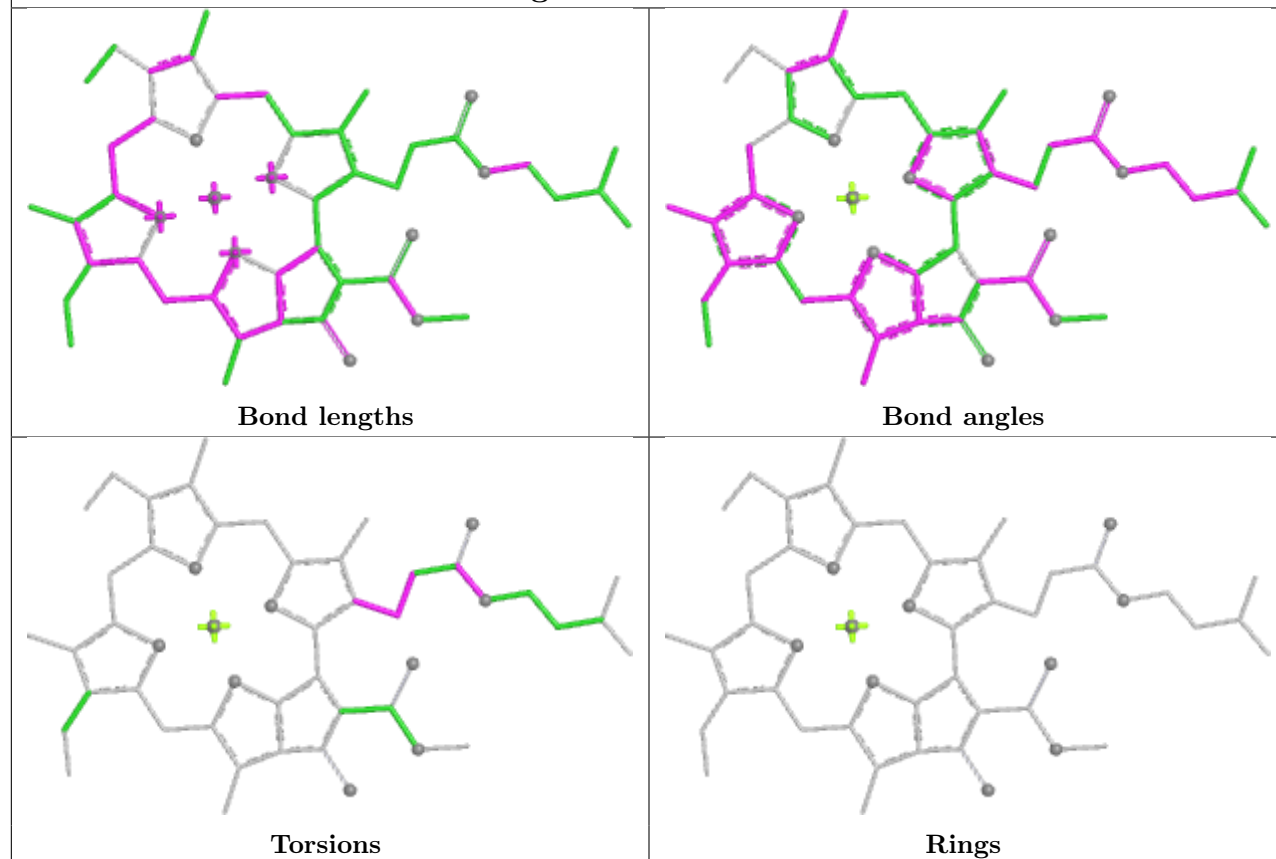




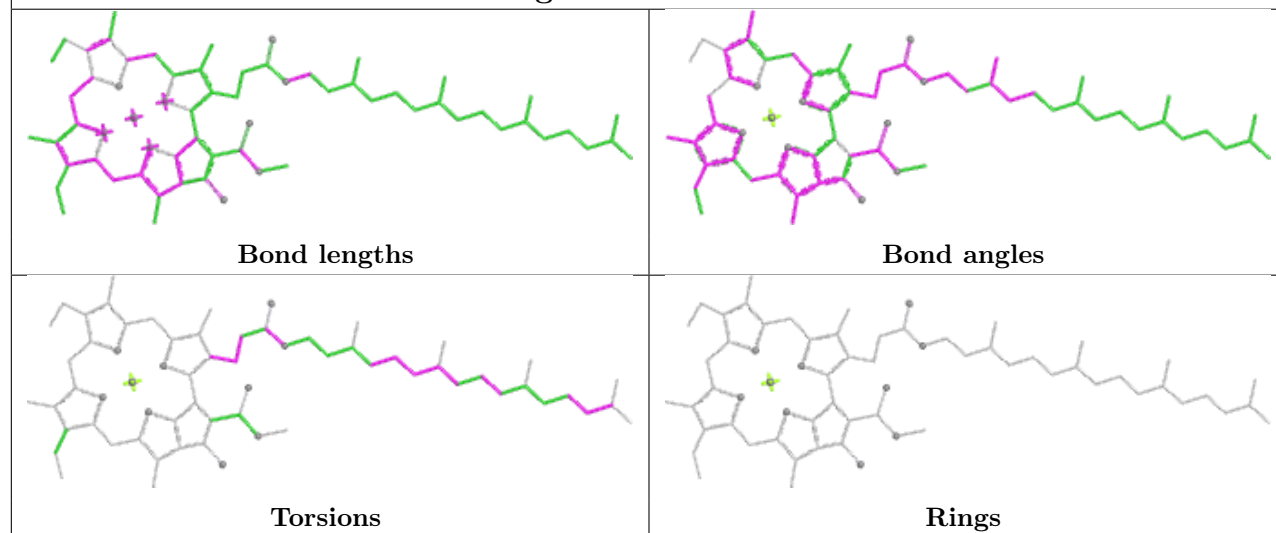




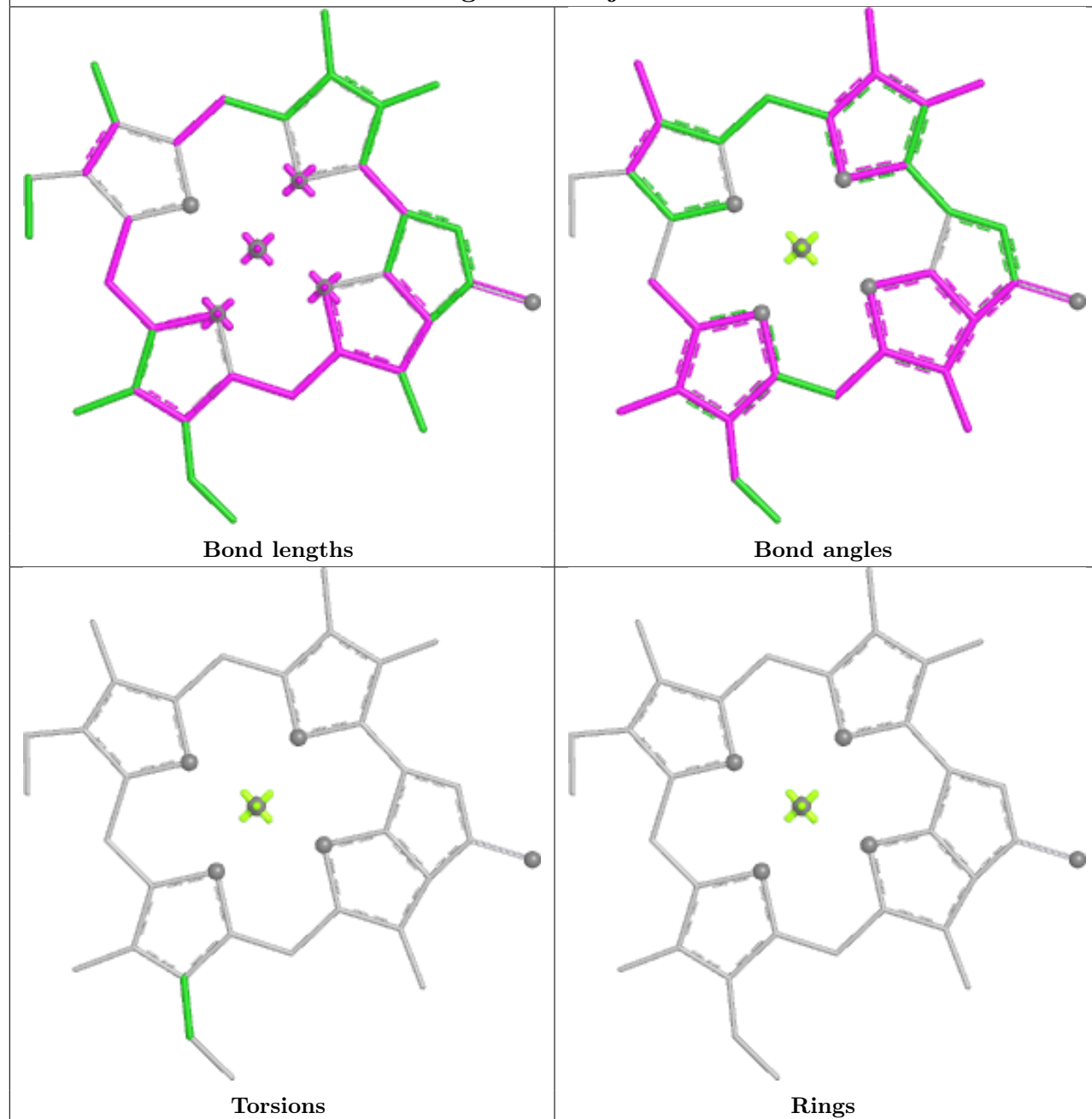
## Ligand CLA G 813



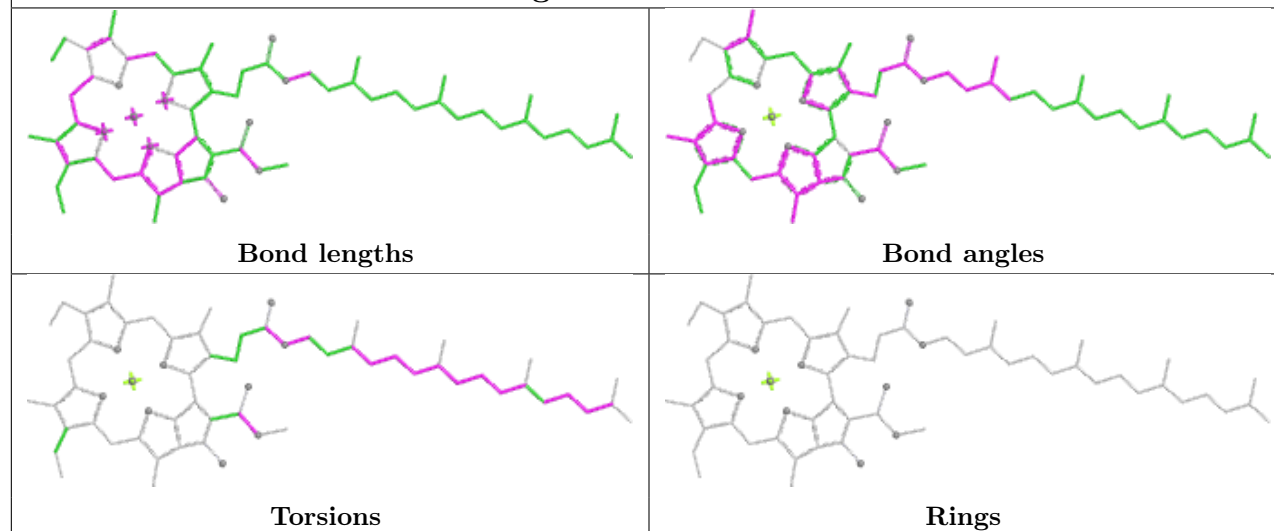
## Ligand CLA b 806



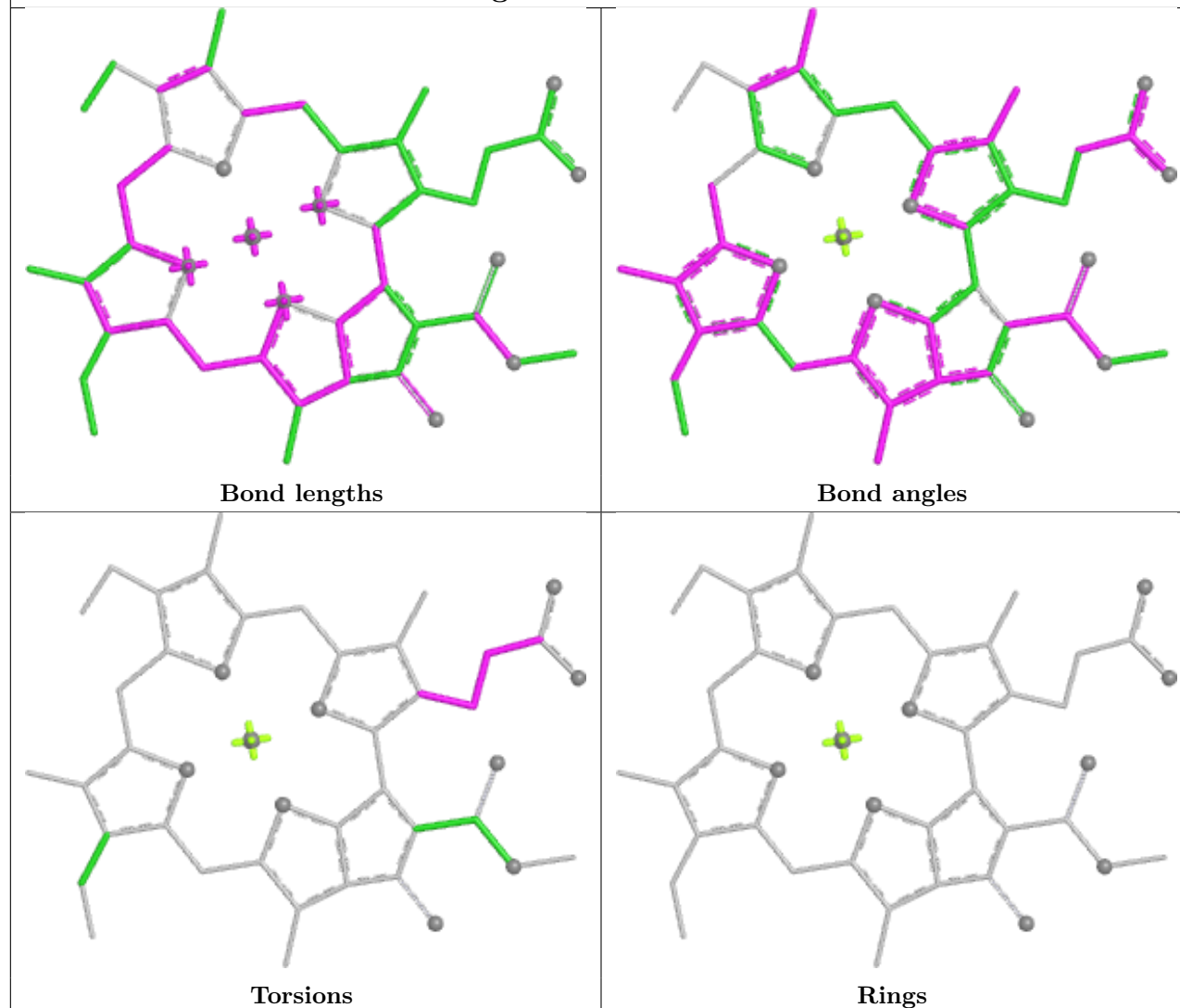
## Ligand CLA j 102



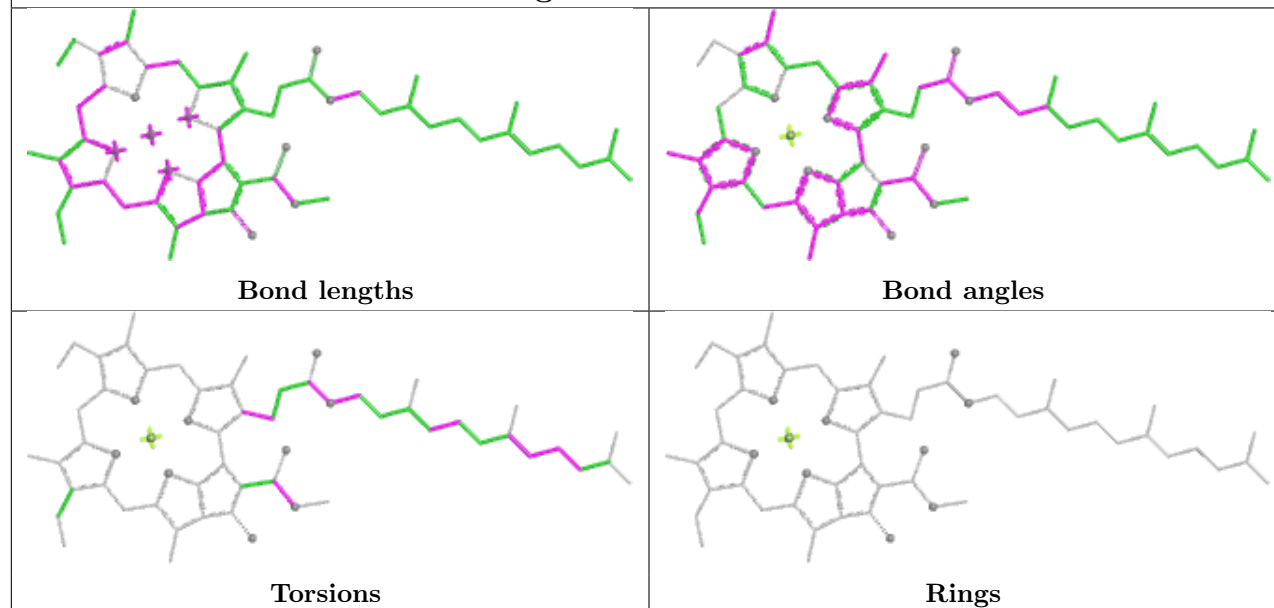
## Ligand CLA B 806



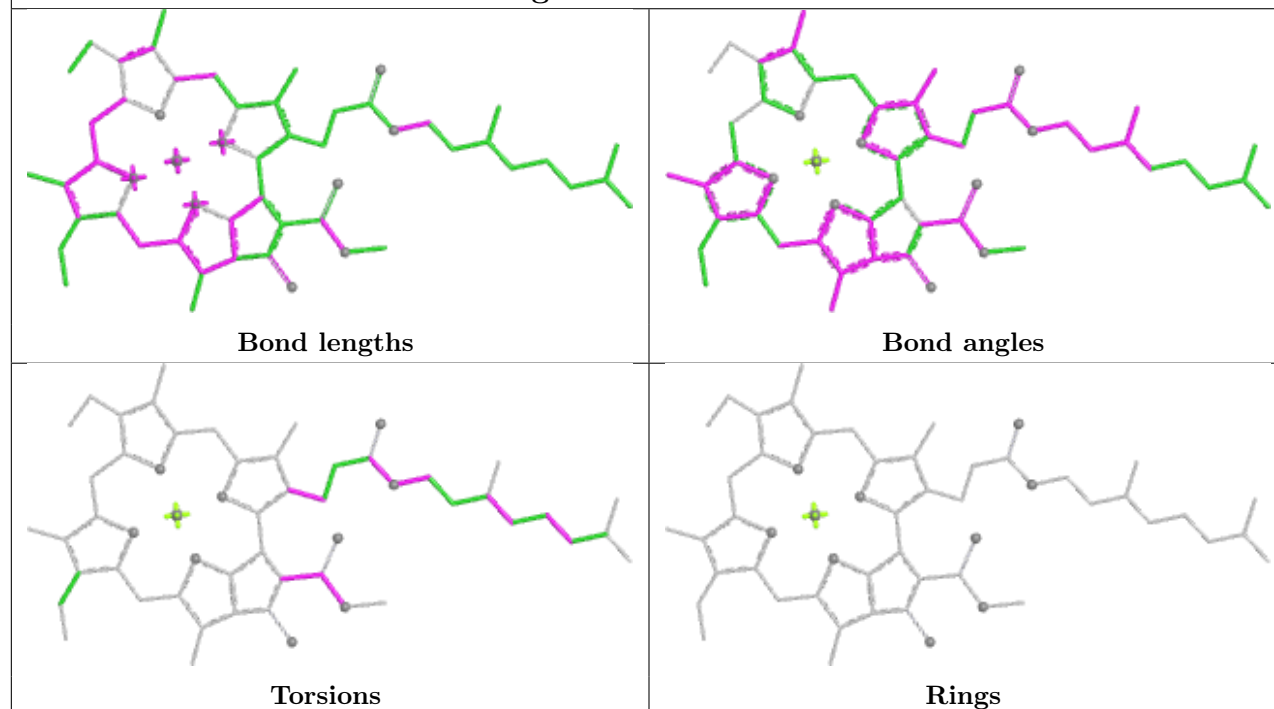
## Ligand CLA G 837



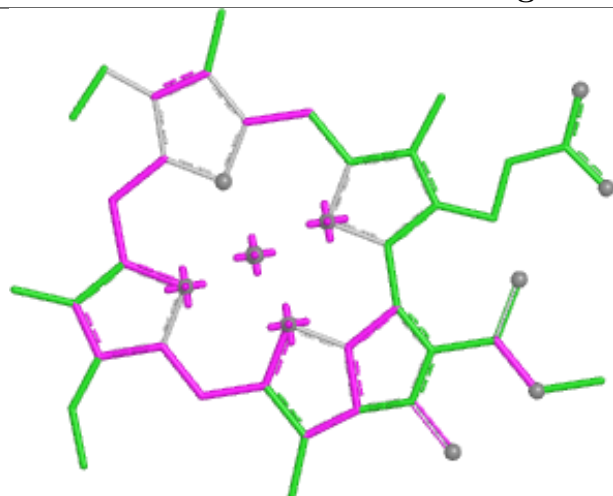
## Ligand CLA b 836



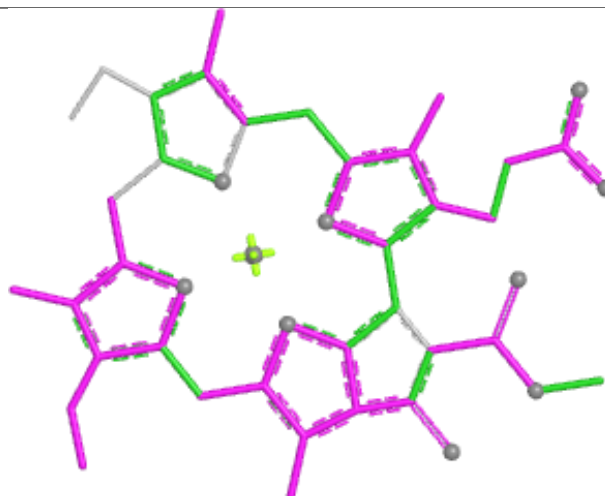
## Ligand CLA A 804



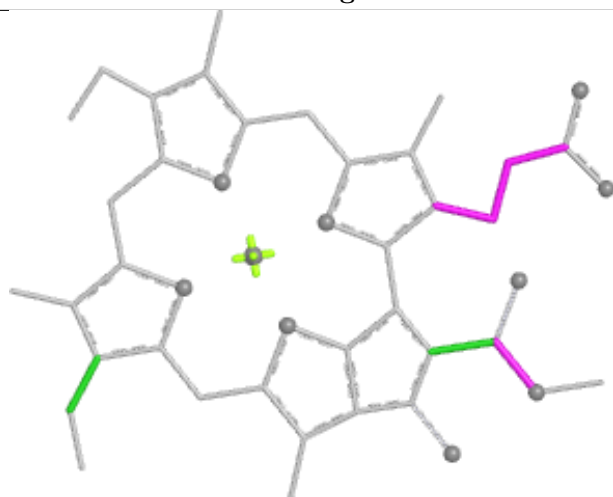
## Ligand CLA b 829



Bond lengths



Bond angles

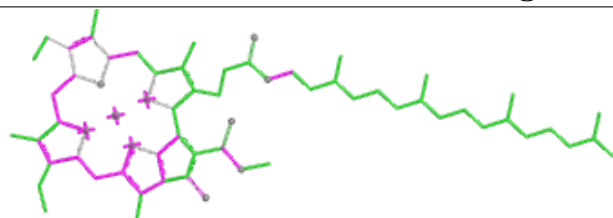


Torsions

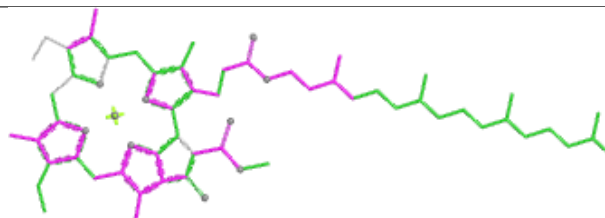


Rings

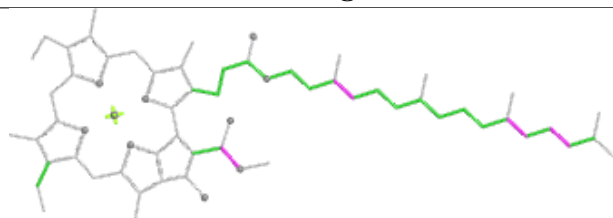
## Ligand CLA a 833



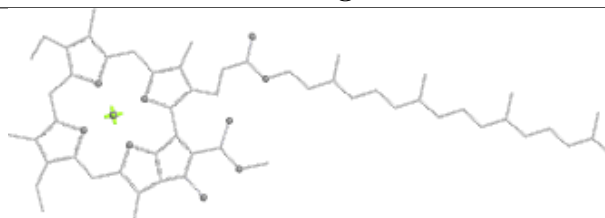
Bond lengths



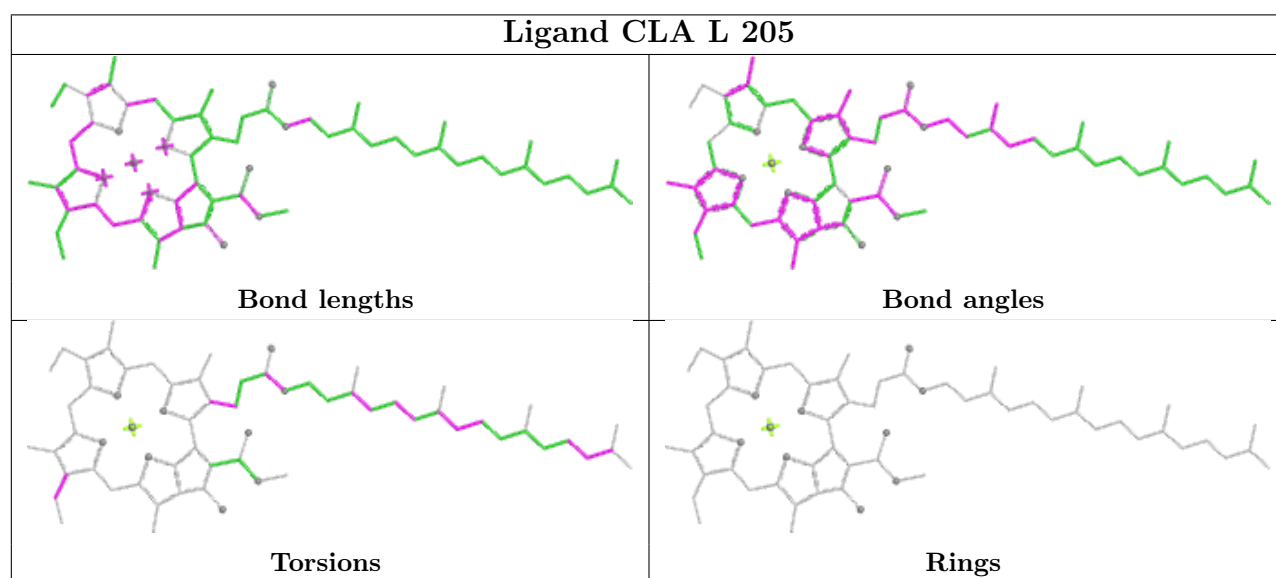
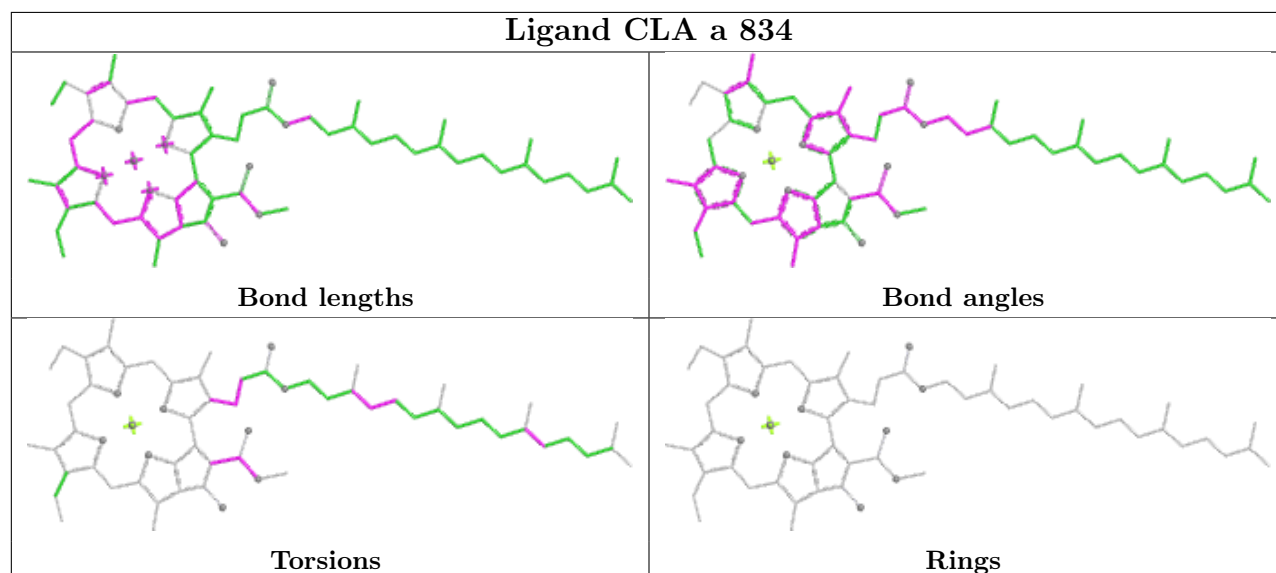
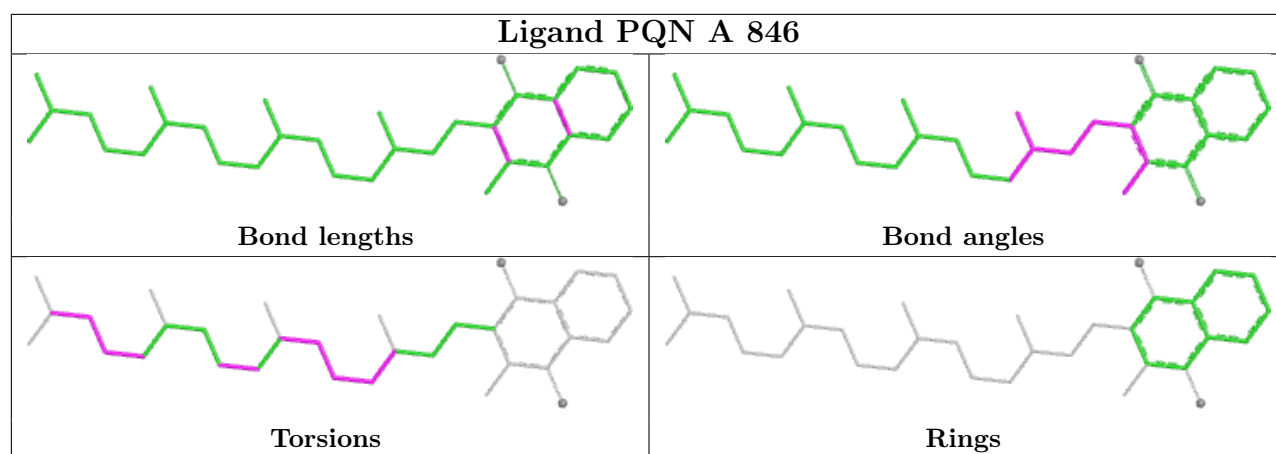
Bond angles

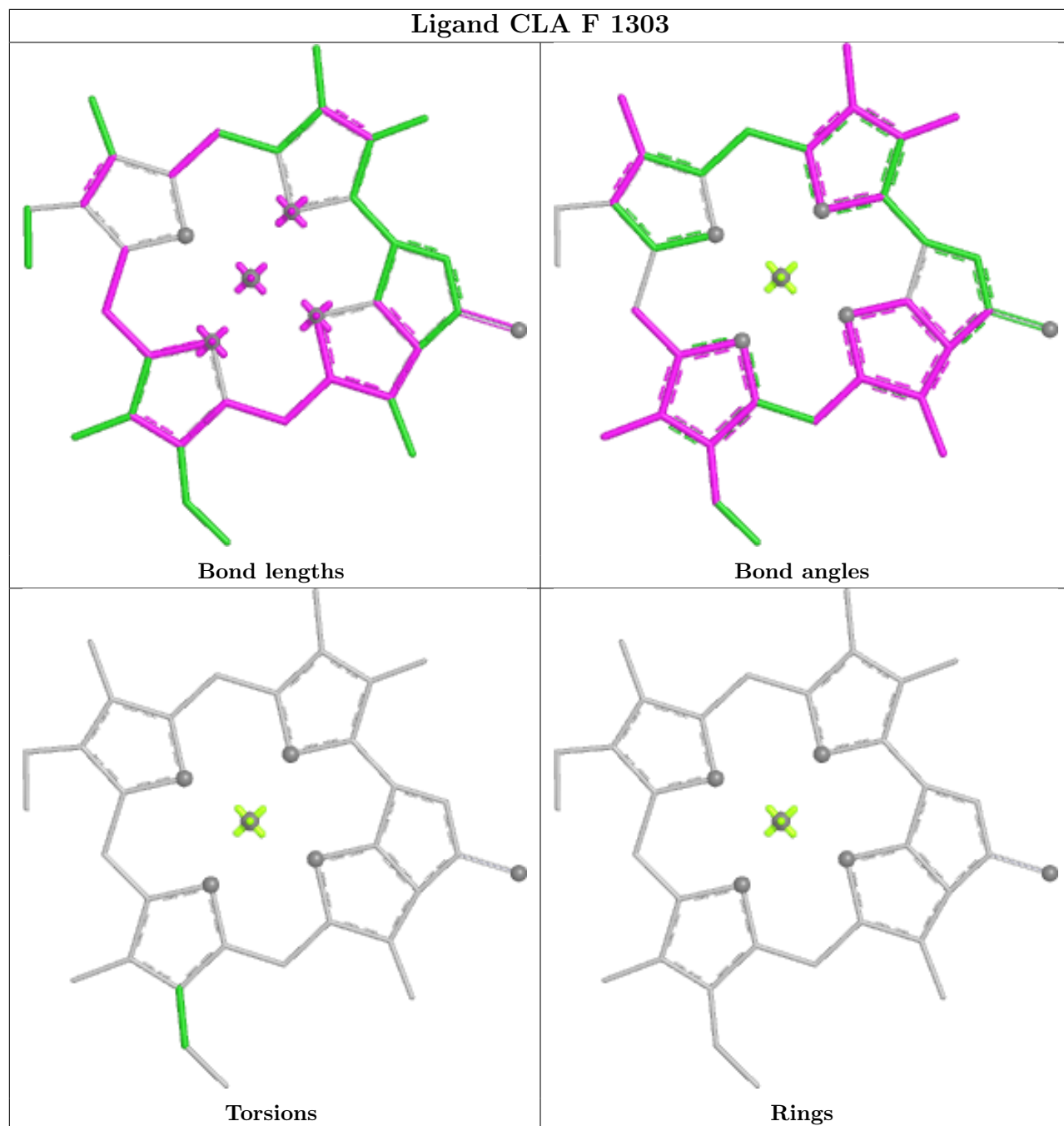


Torsions

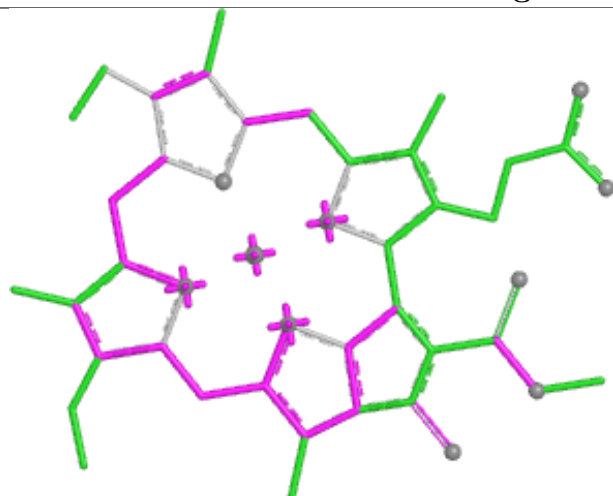


Rings

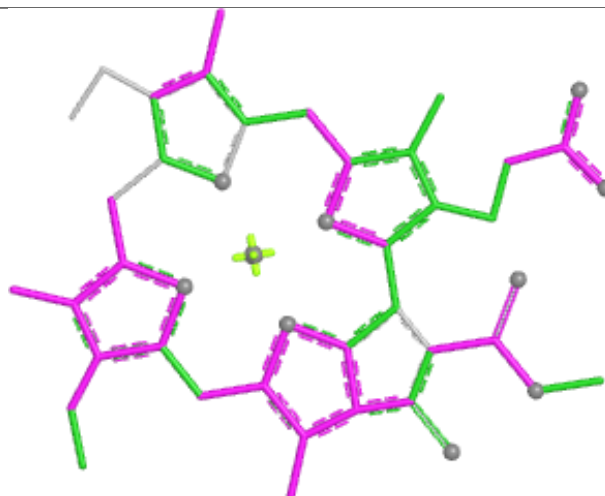




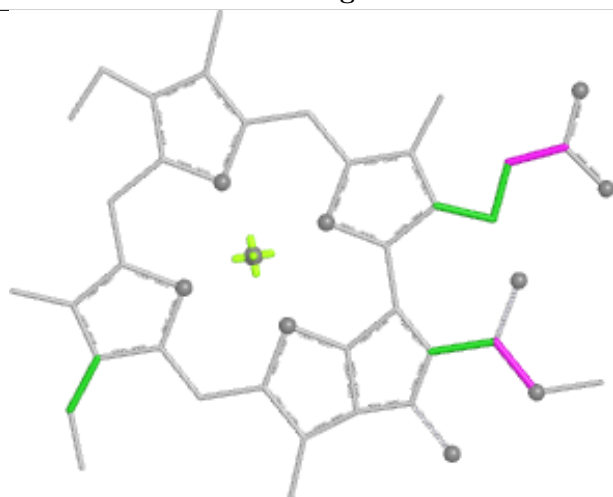
## Ligand CLA H 833



Bond lengths



Bond angles

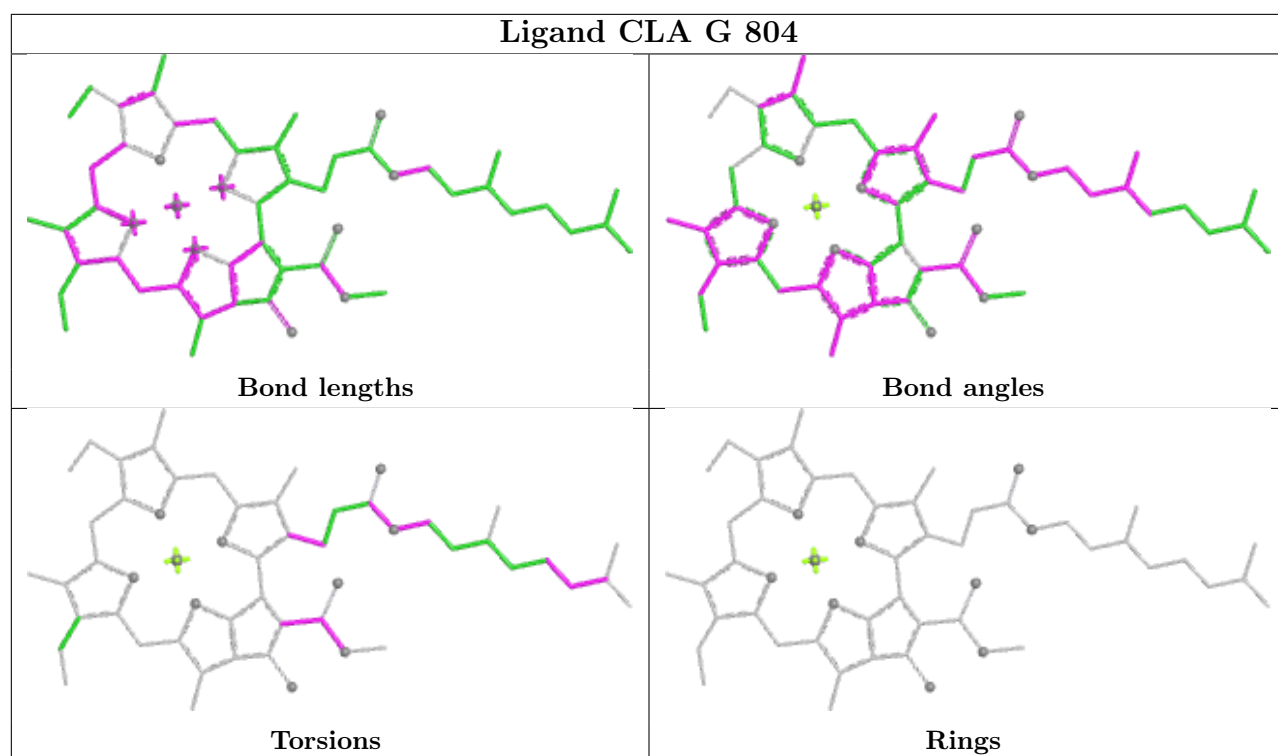


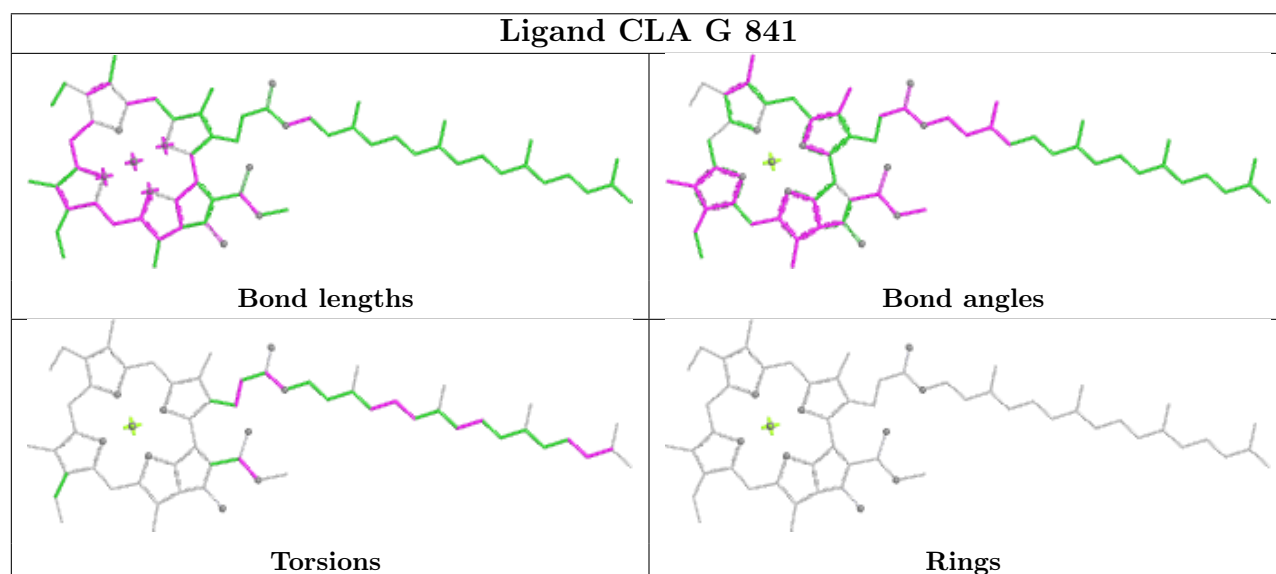
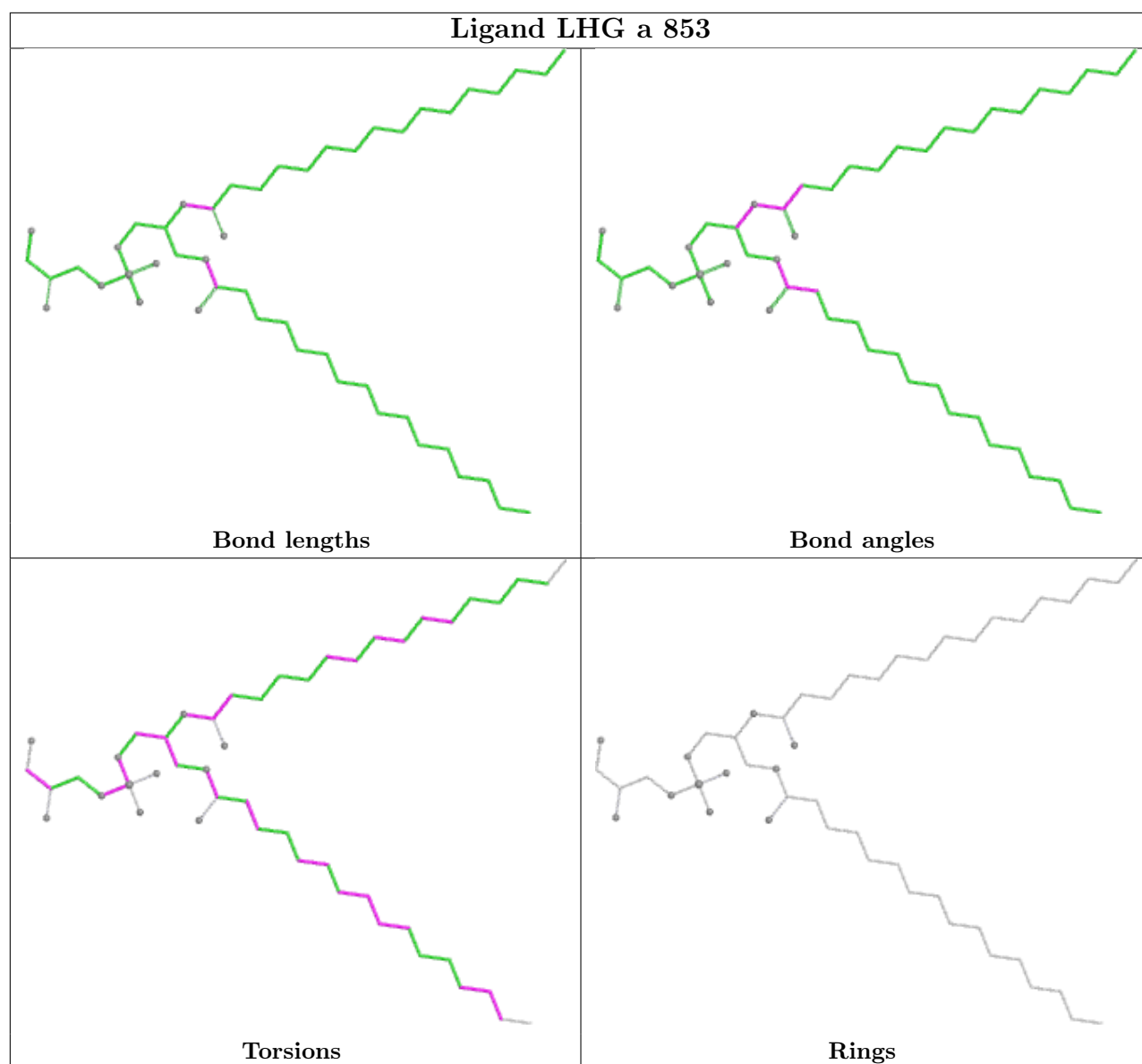
Torsions



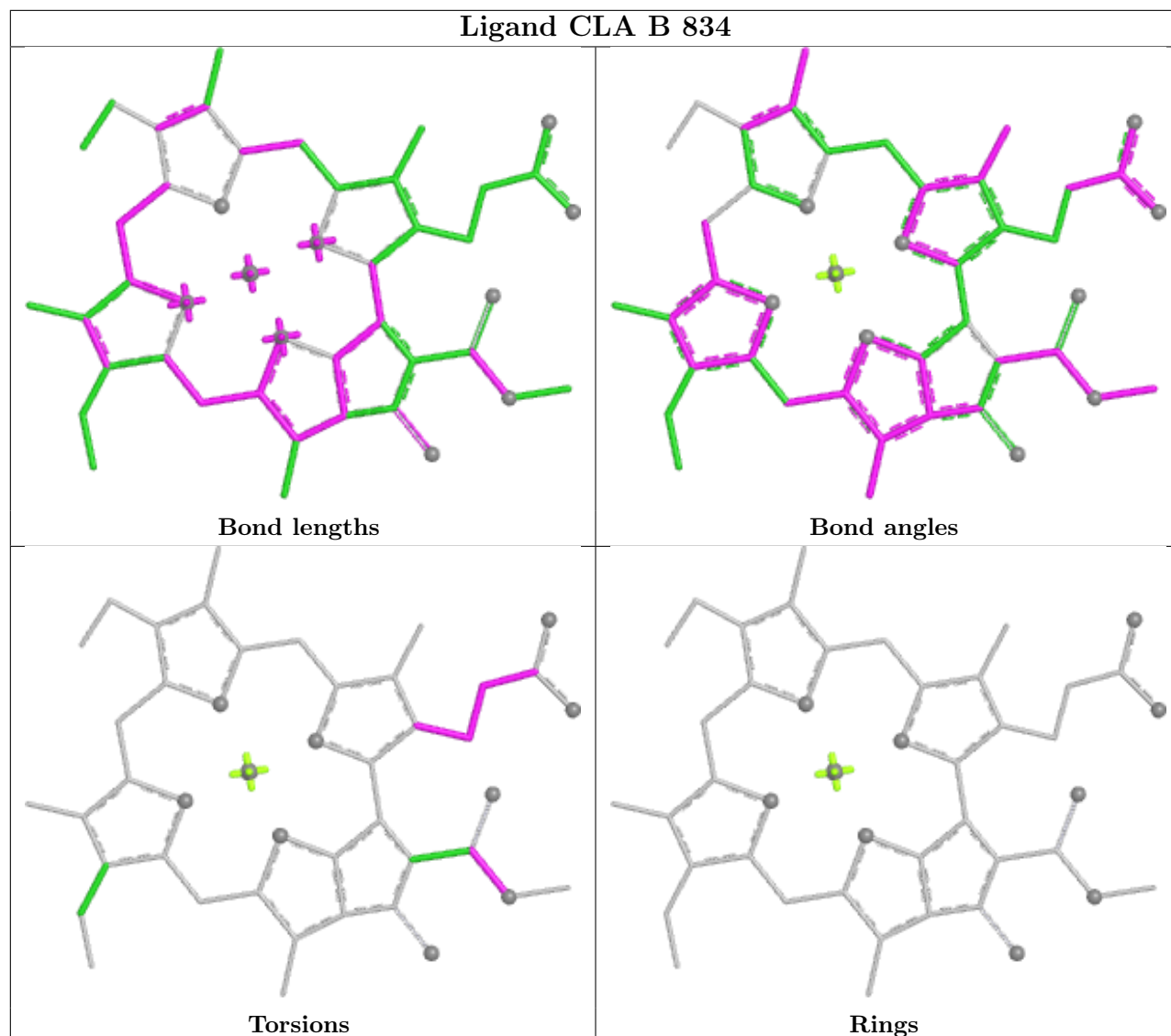
Rings



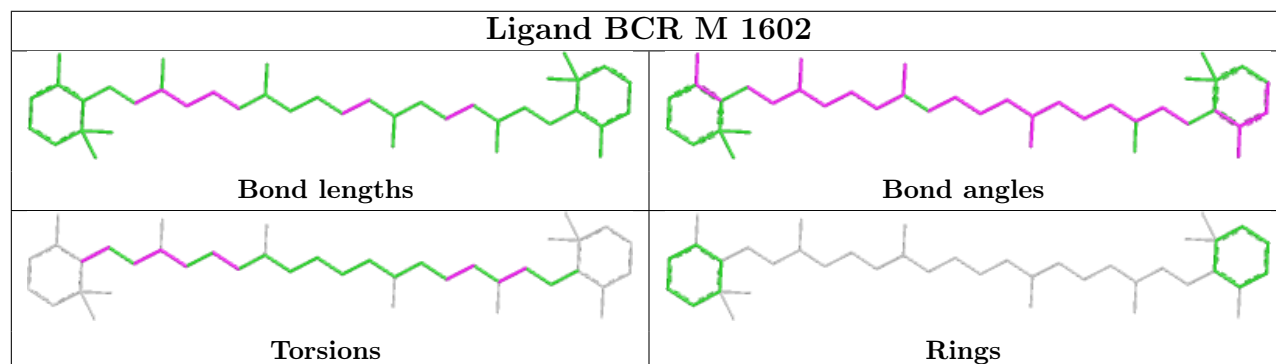


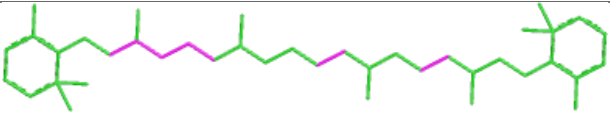
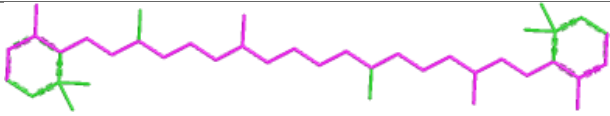
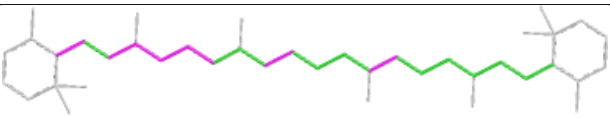
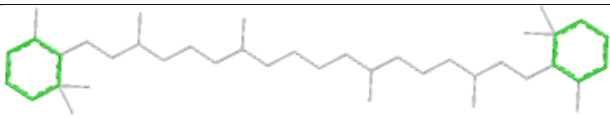
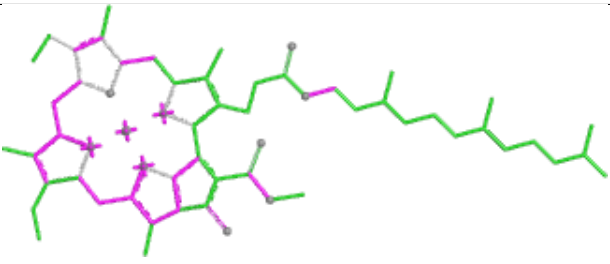
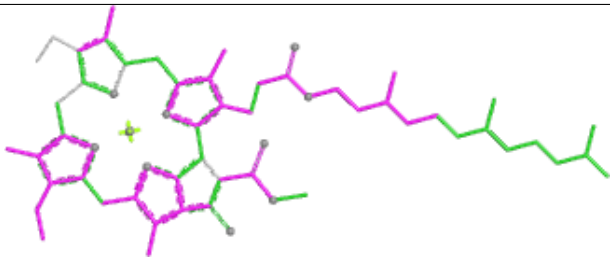
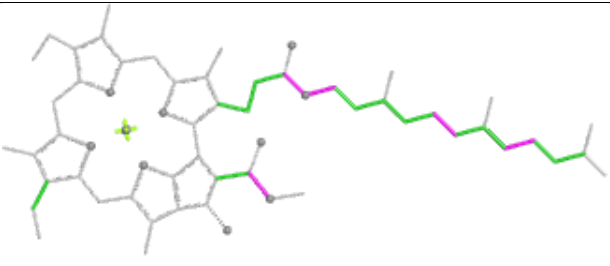
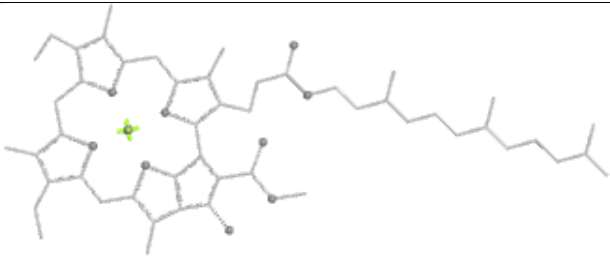
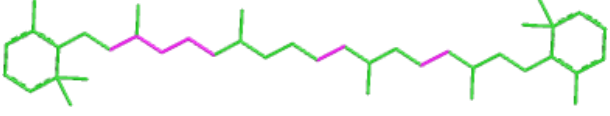
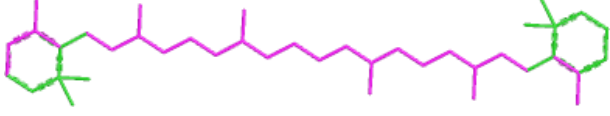
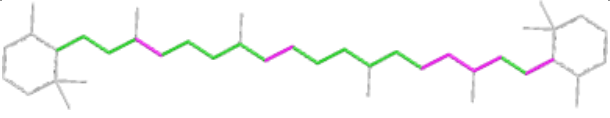
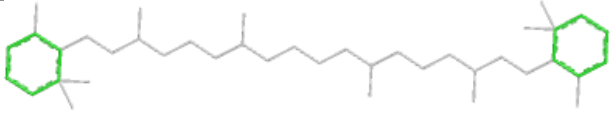


## Ligand CLA B 834

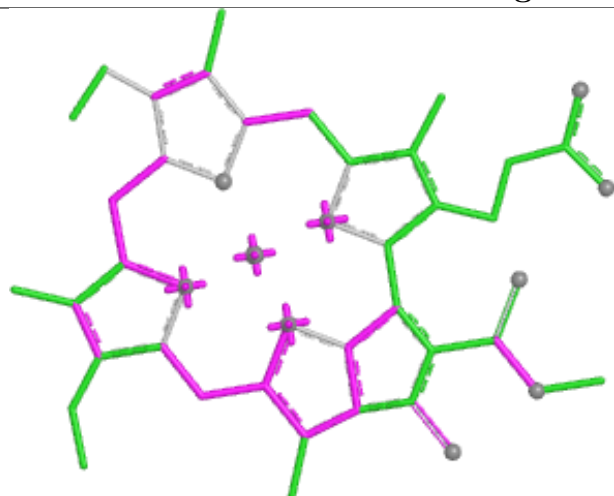


## Ligand BCR M 1602

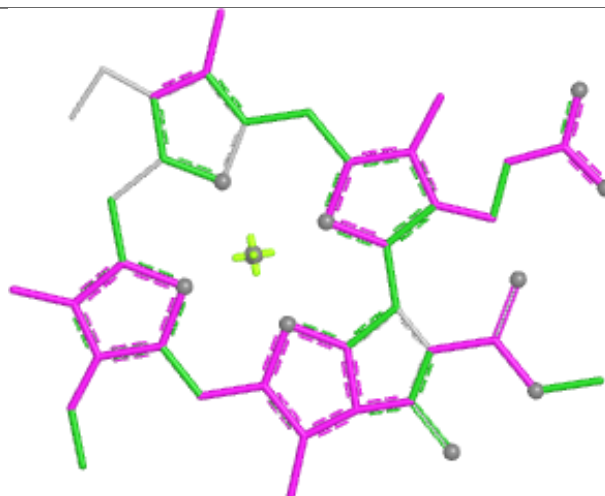


Ligand BCR a 849	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA G 827	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR b 844	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

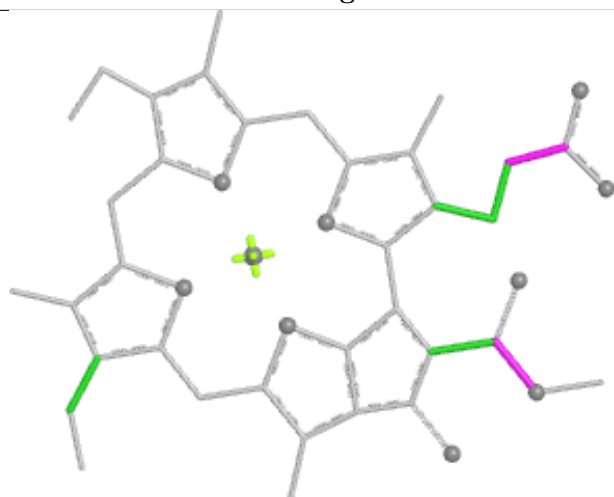
## Ligand CLA B 815



Bond lengths



Bond angles

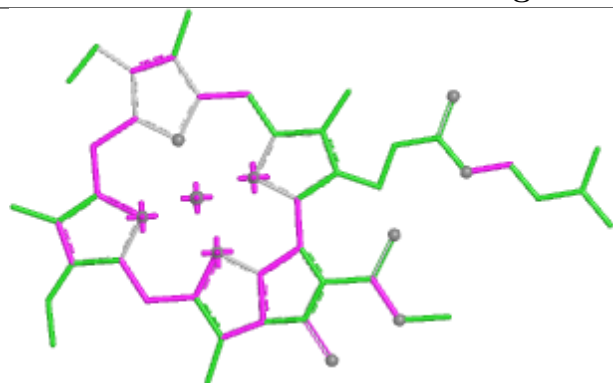


Torsions

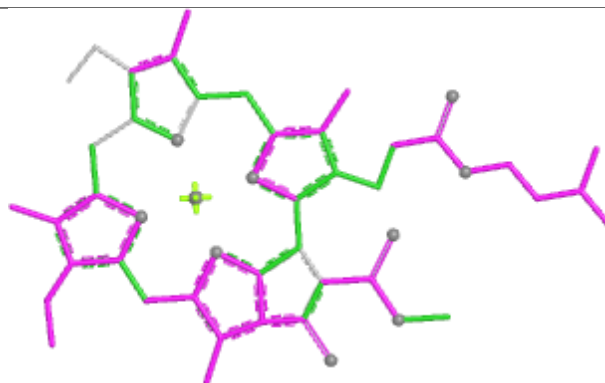


Rings

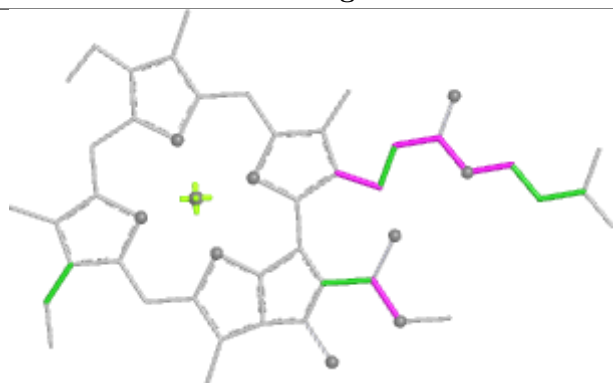
## Ligand CLA G 821



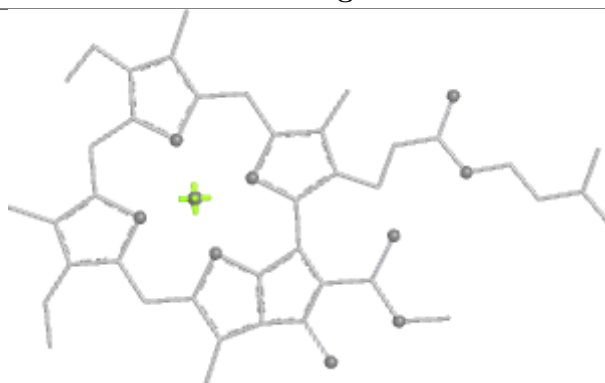
Bond lengths



Bond angles

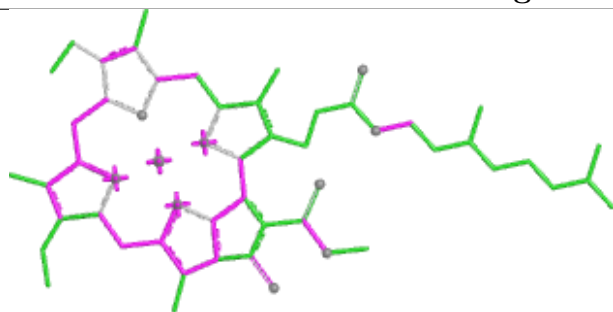


Torsions

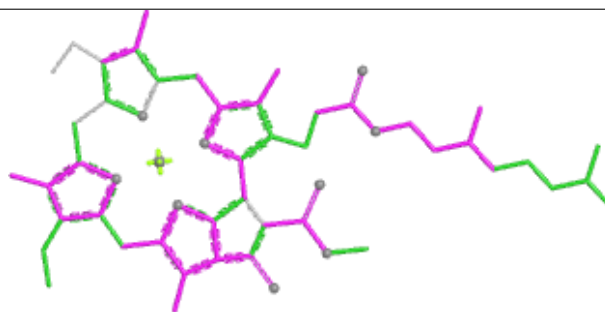


Rings

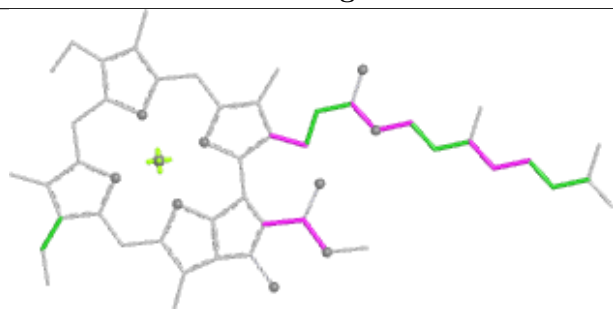
## Ligand CLA A 805



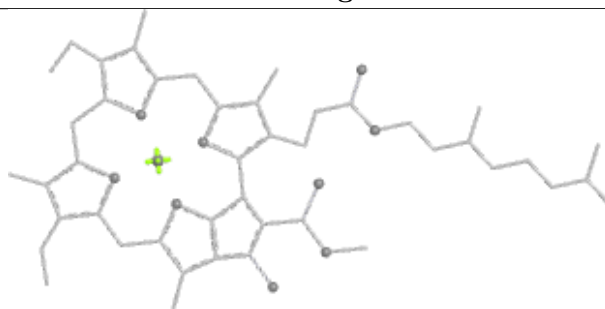
Bond lengths



Bond angles

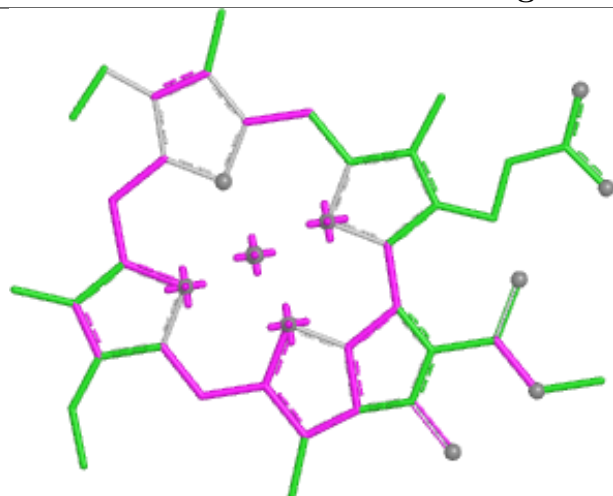


Torsions

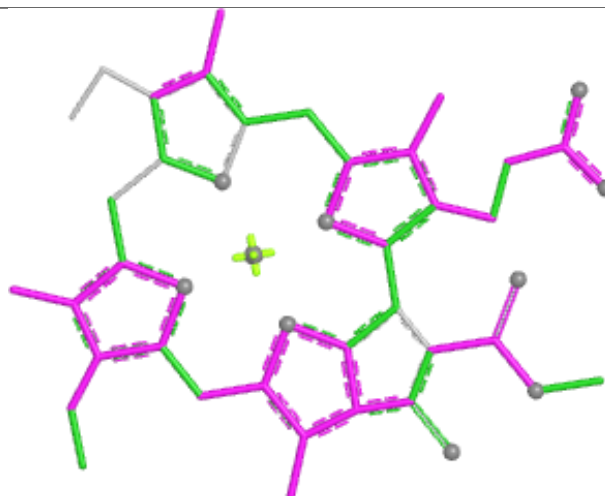


Rings

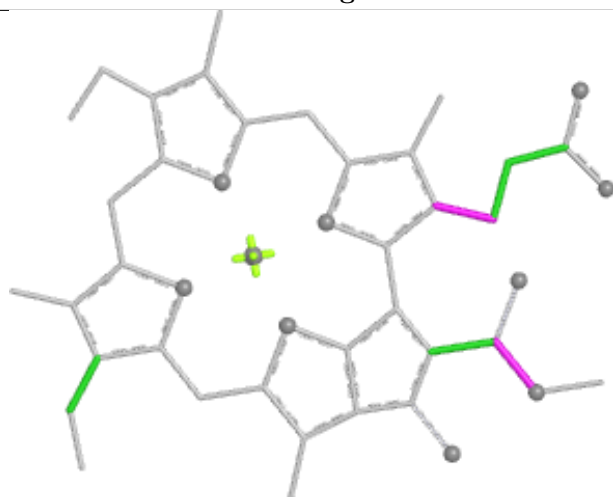
## Ligand CLA b 815



Bond lengths



Bond angles

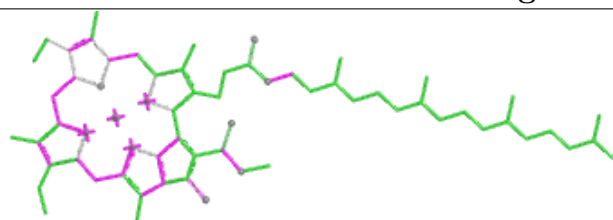


Torsions

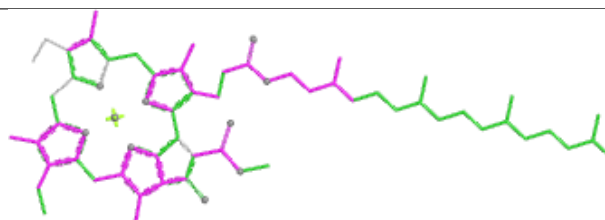


Rings

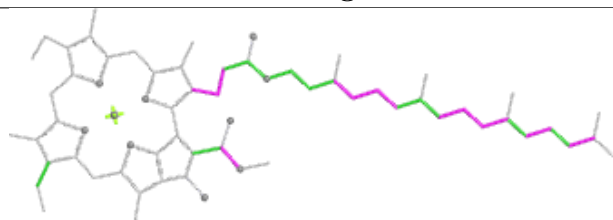
## Ligand CLA a 809



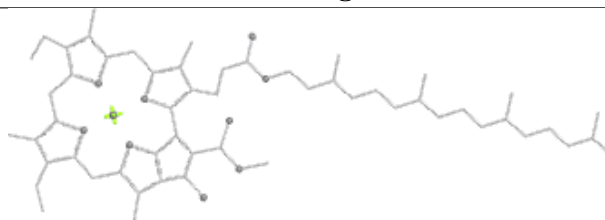
Bond lengths



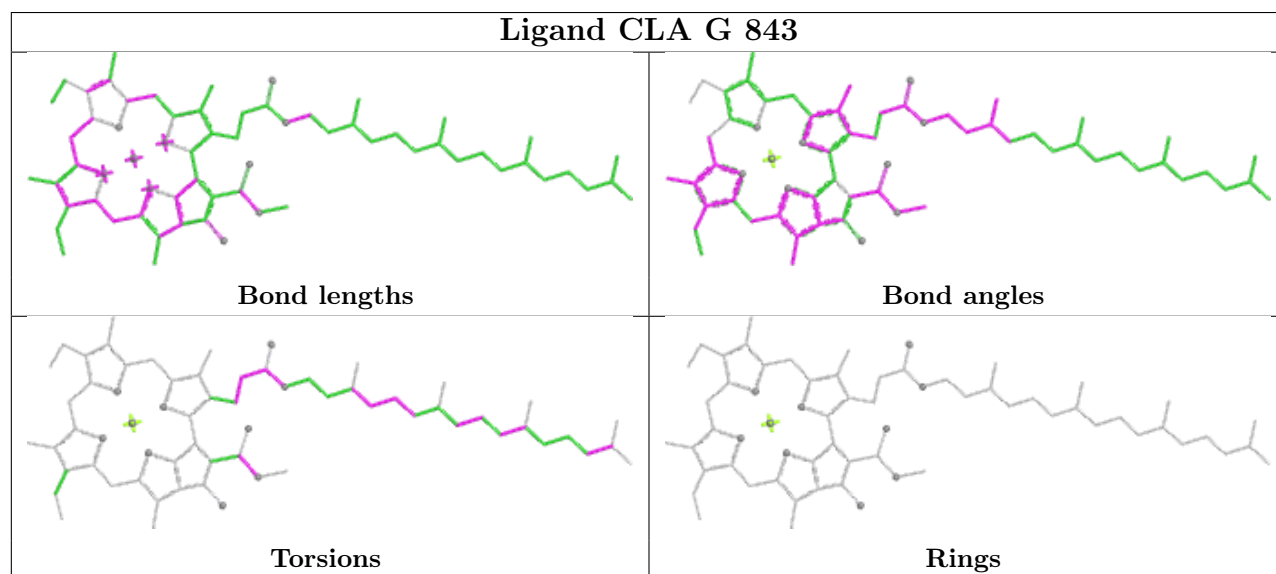
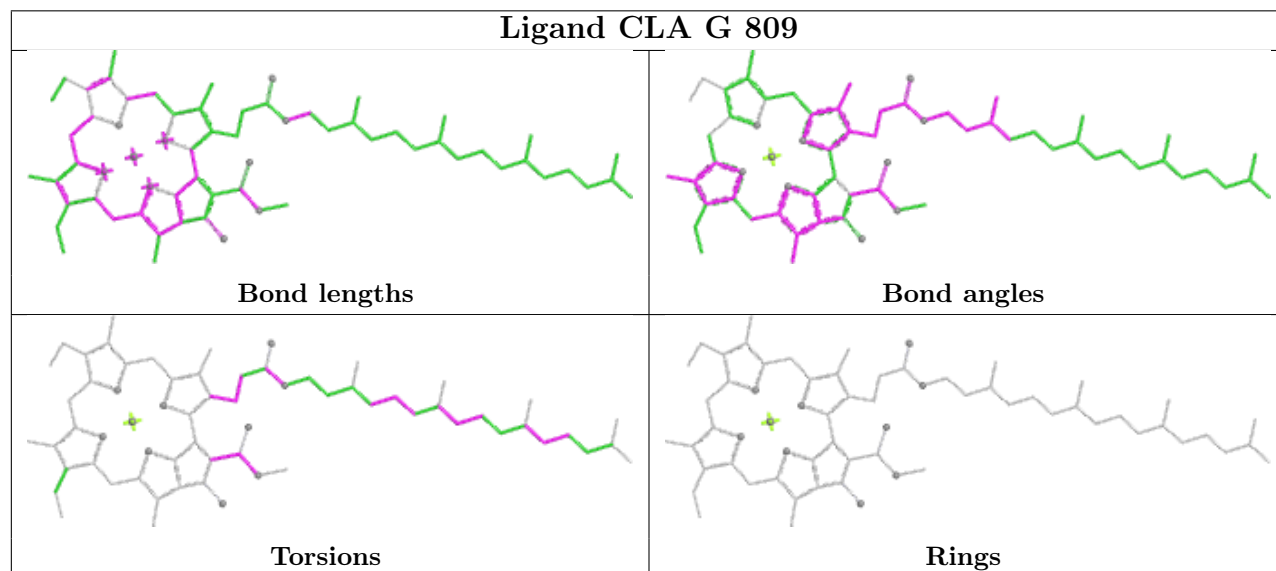
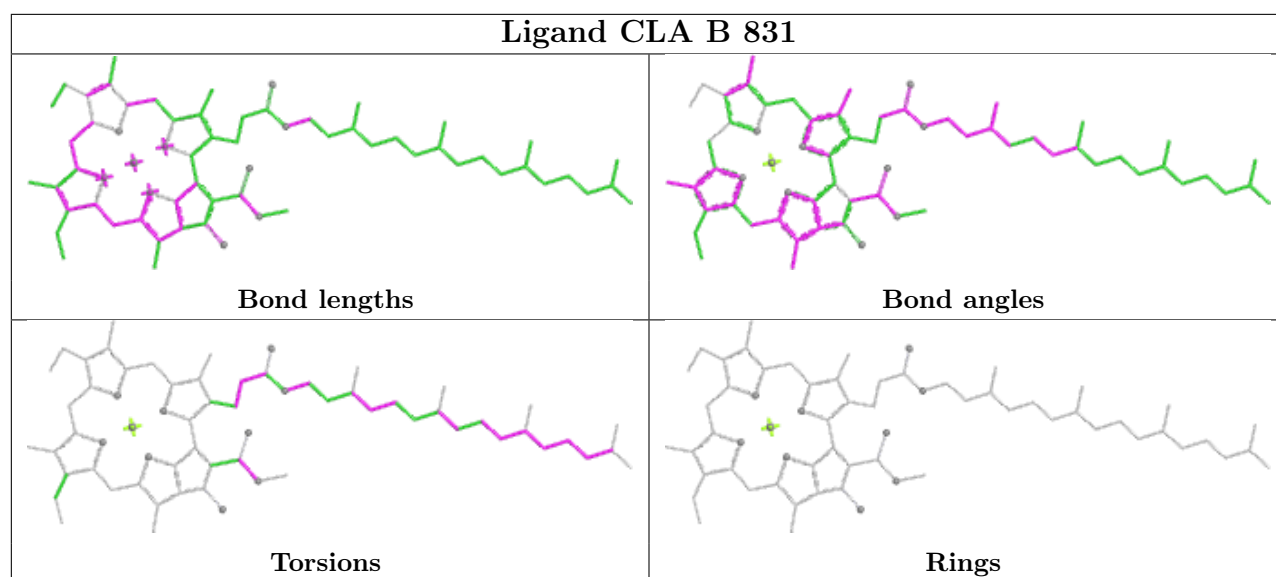
Bond angles



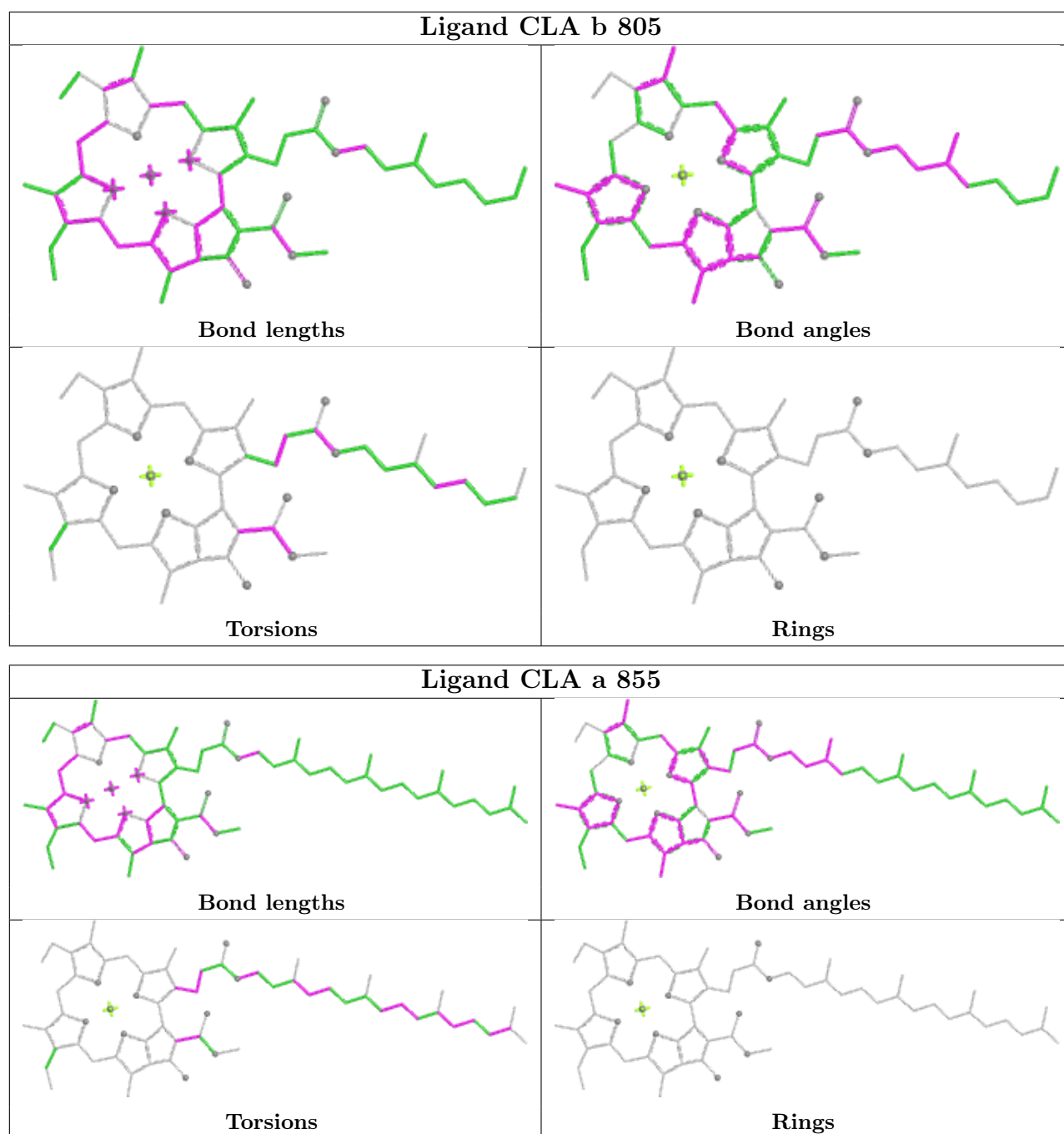
Torsions

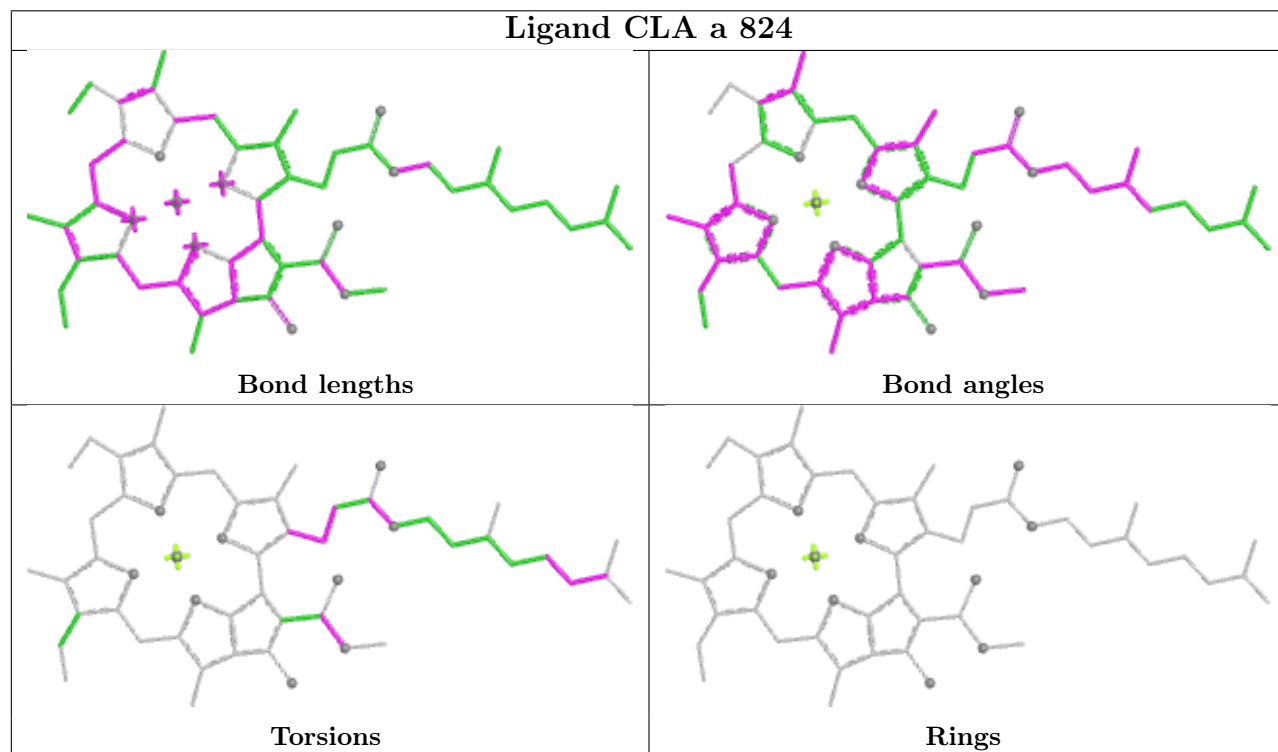
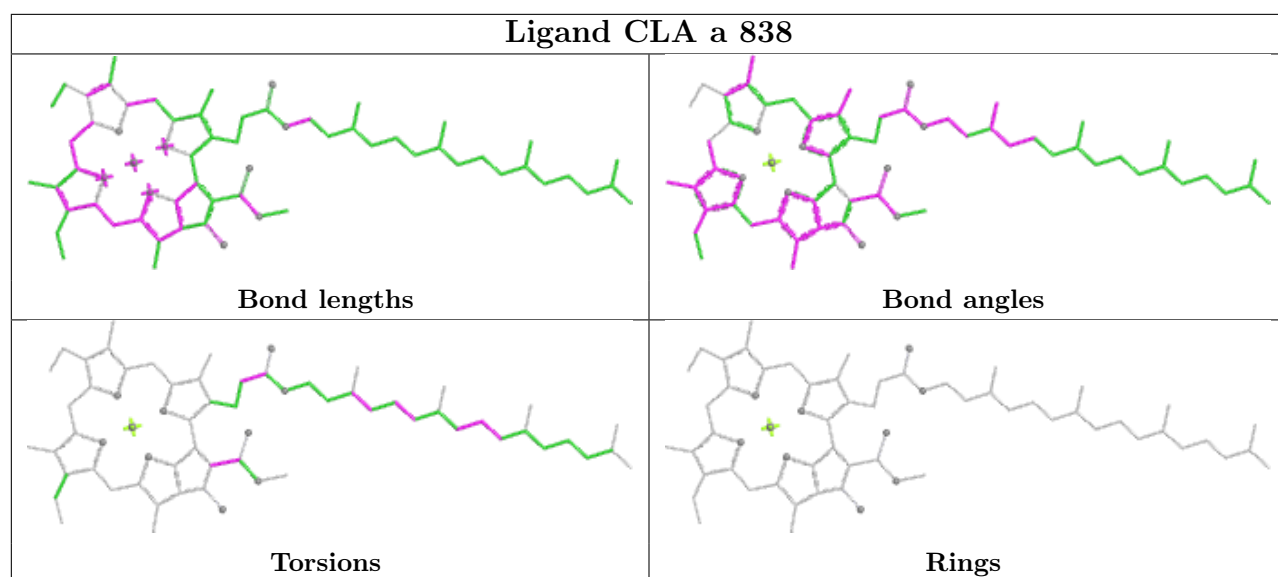


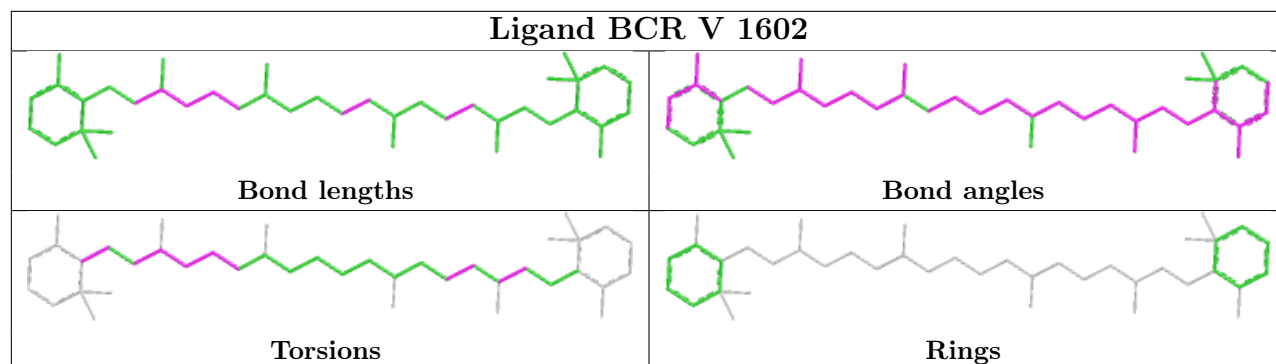
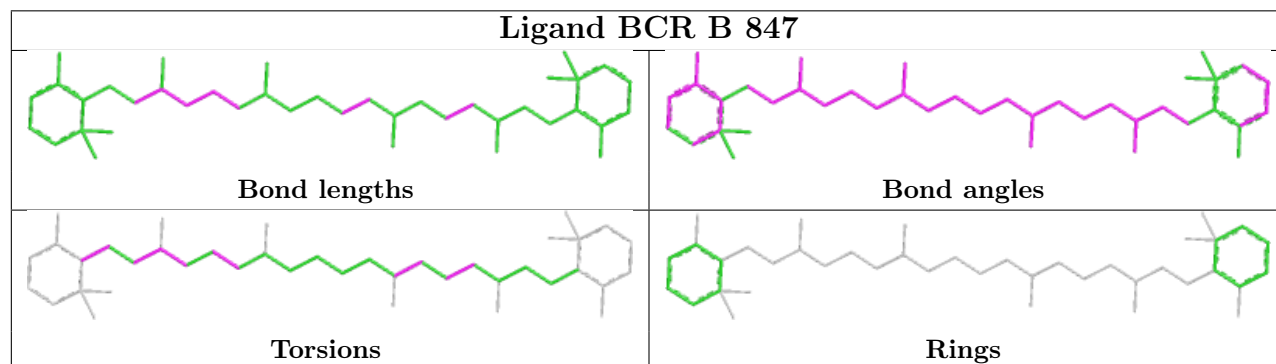
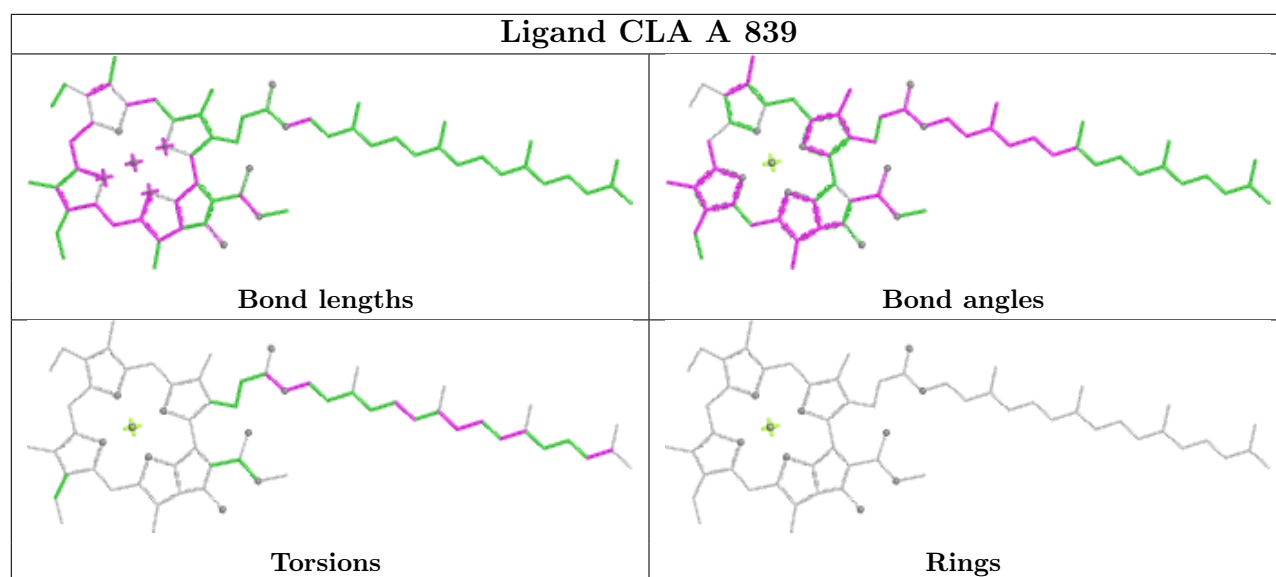
Rings

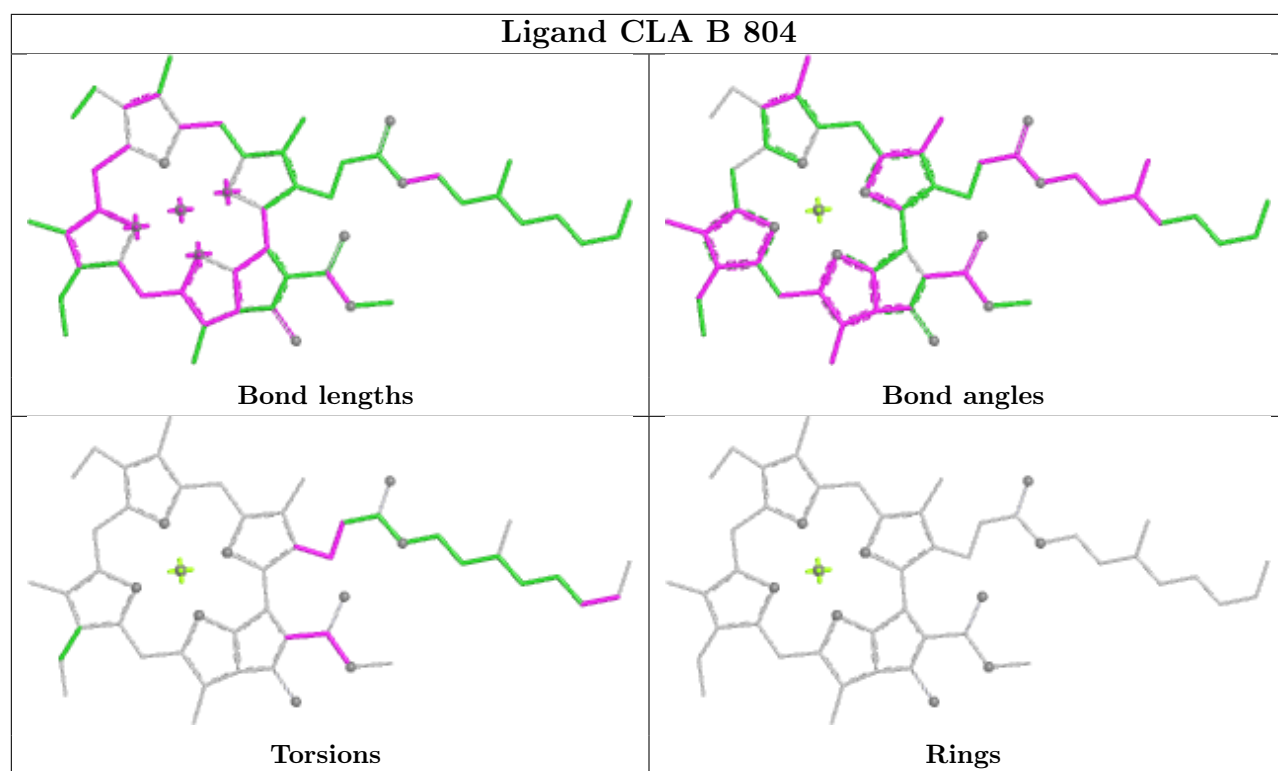


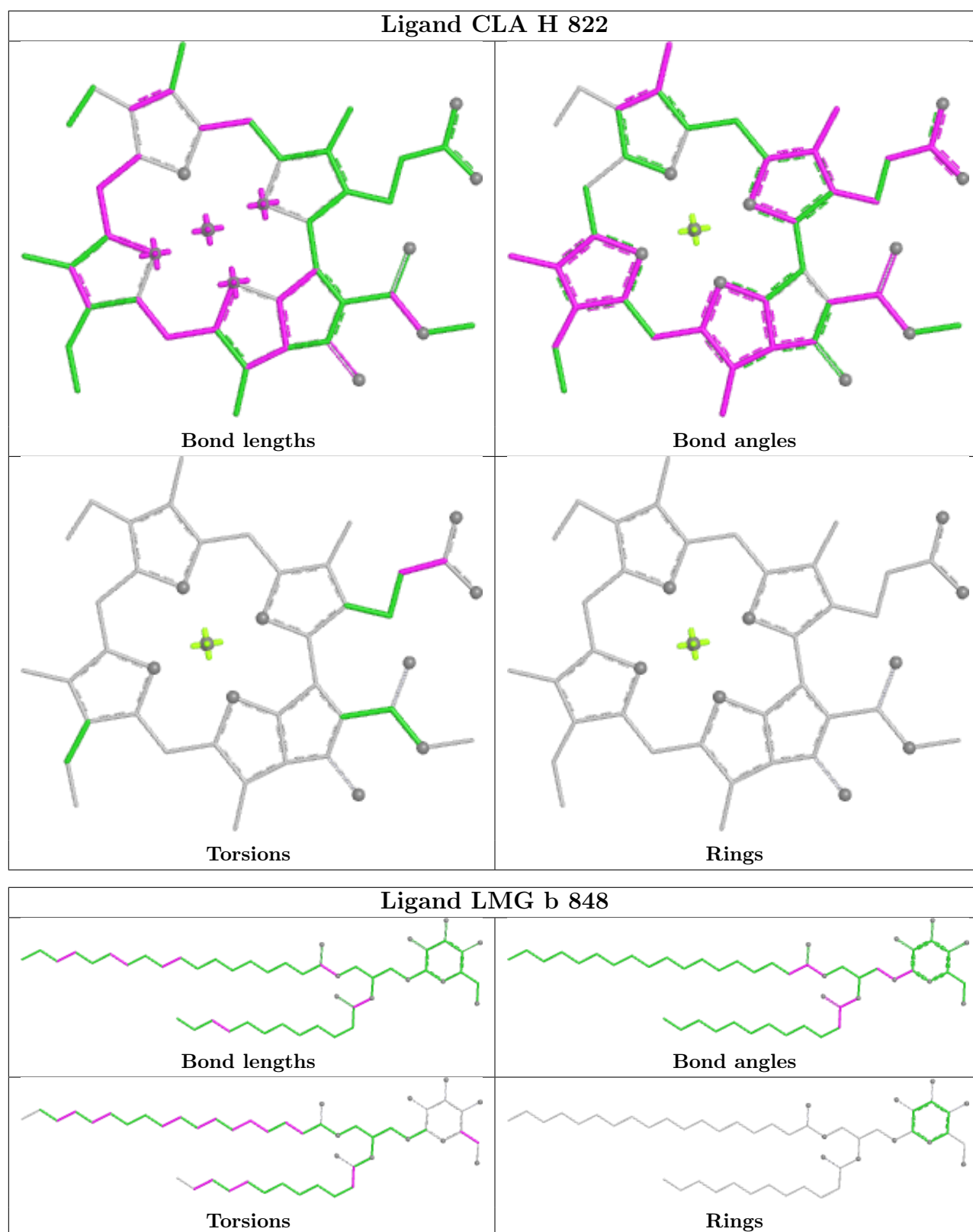


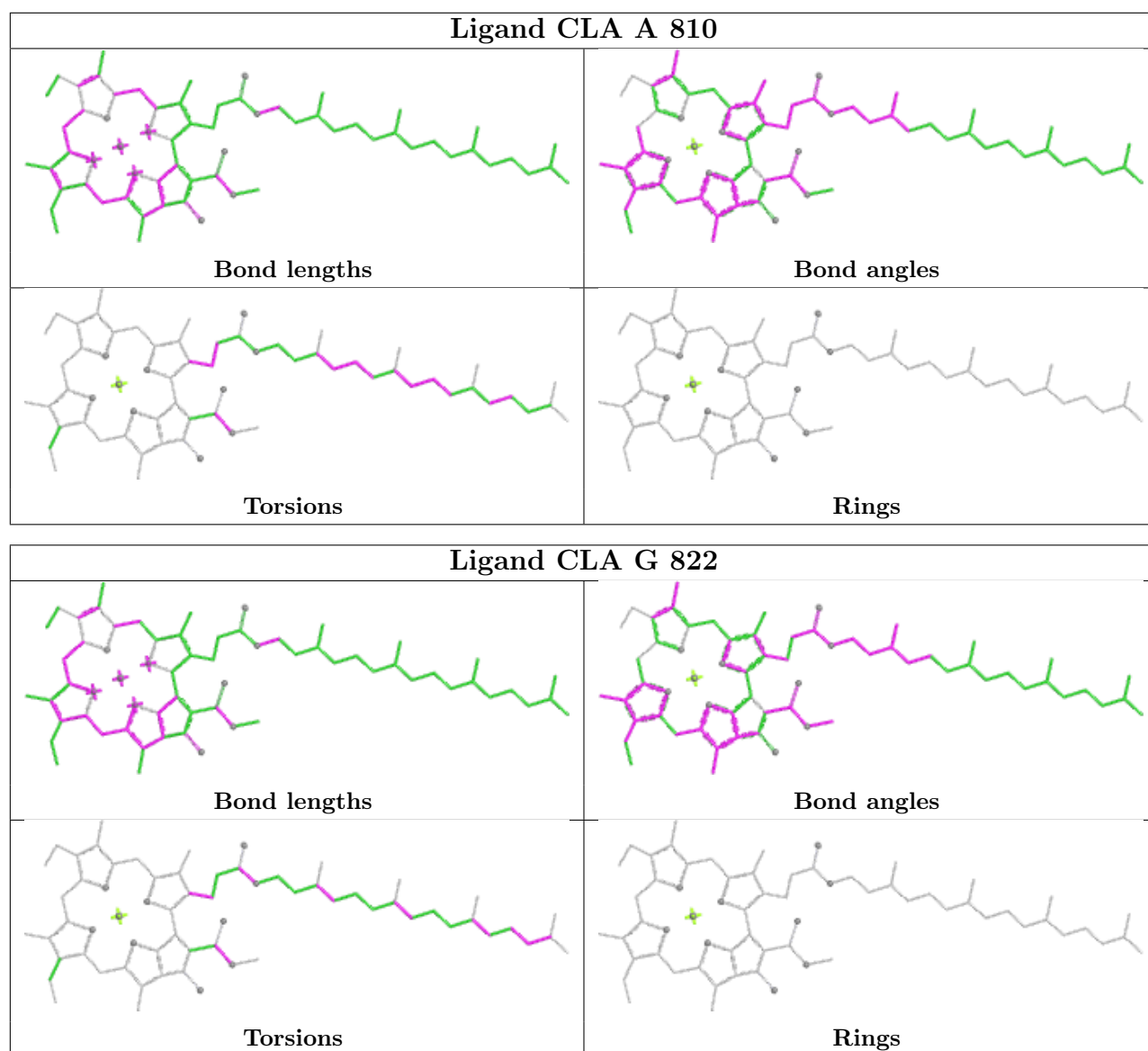




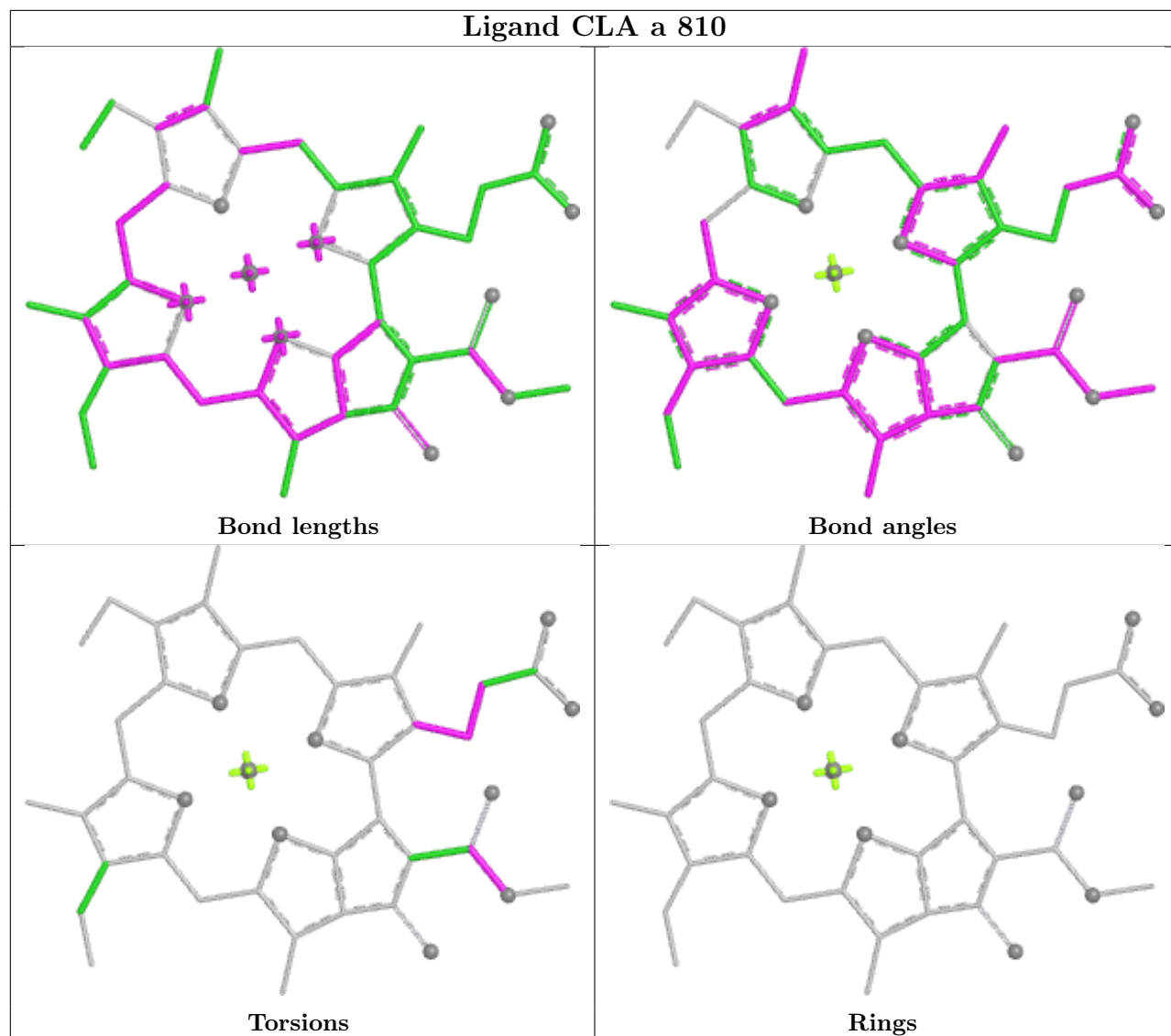




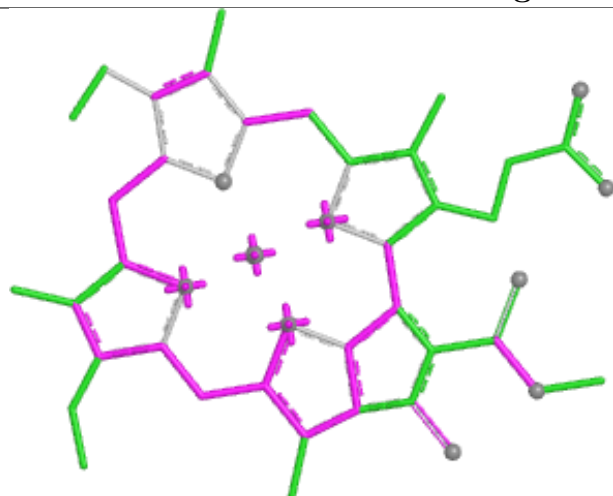




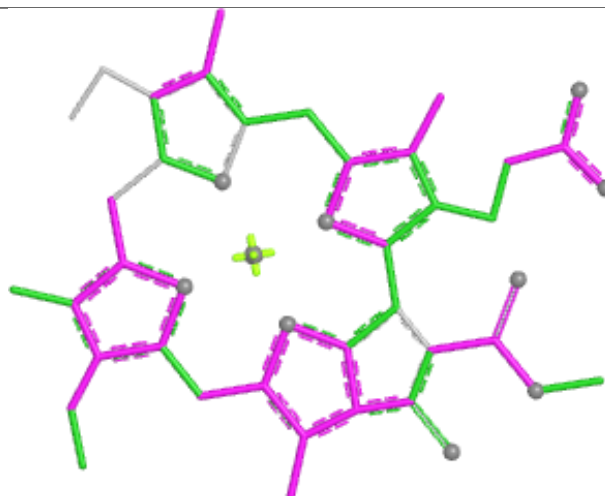
## Ligand CLA a 810



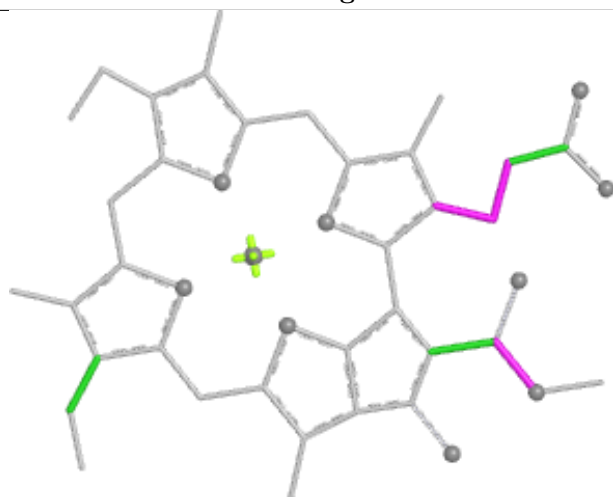
## Ligand CLA A 816



Bond lengths



Bond angles

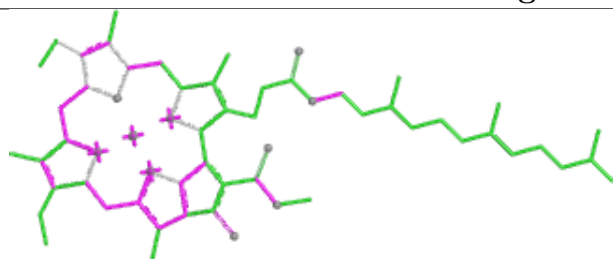


Torsions

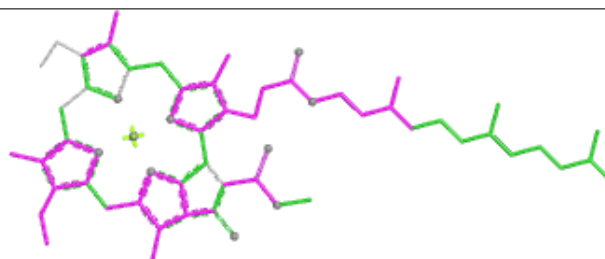


Rings

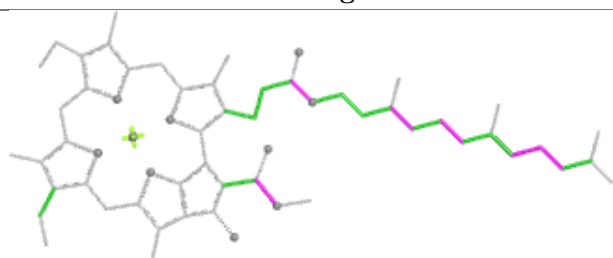
## Ligand CLA a 826



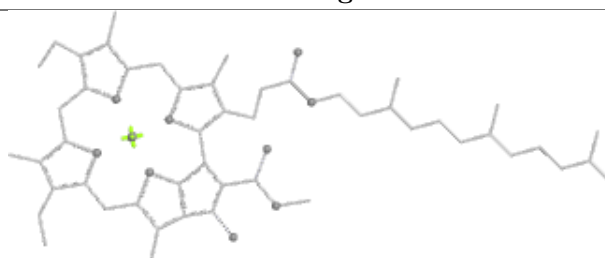
Bond lengths



Bond angles



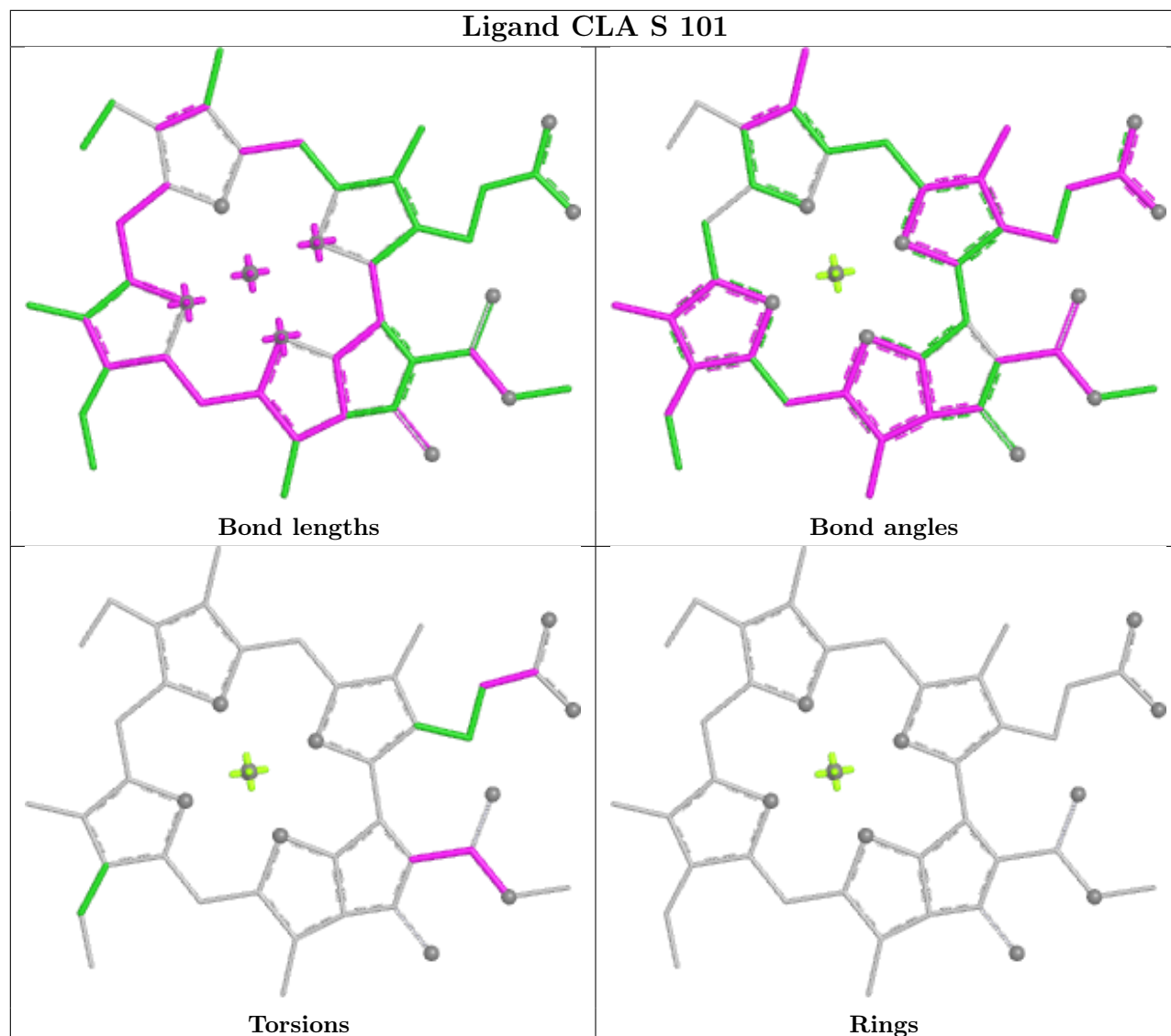
Torsions



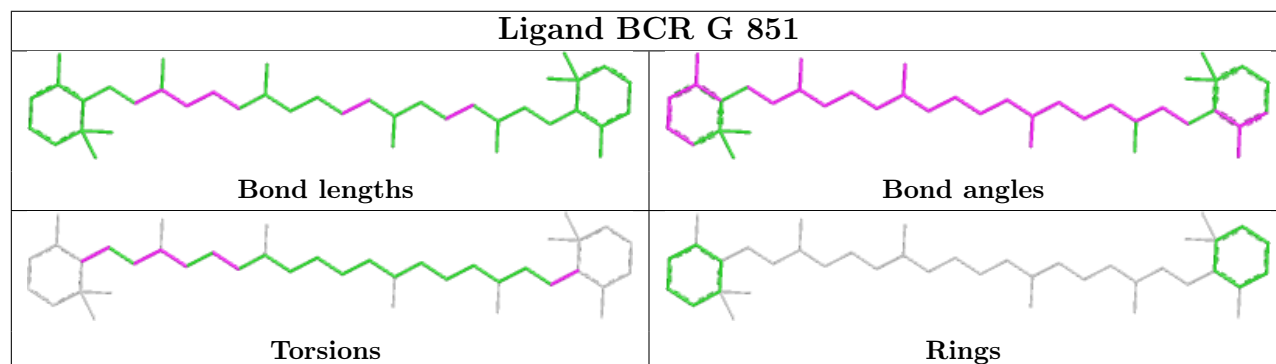
Rings

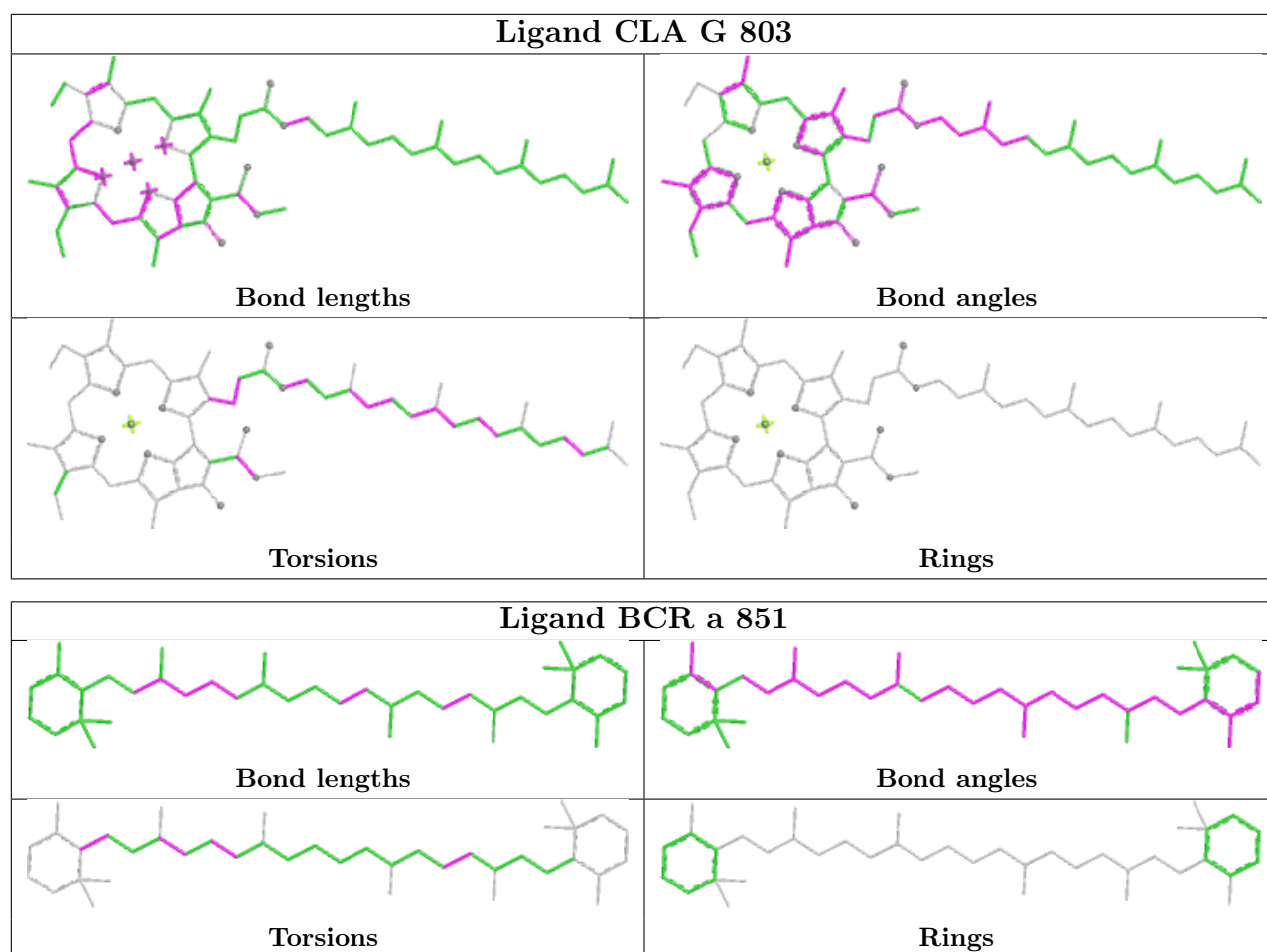


## Ligand CLA S 101

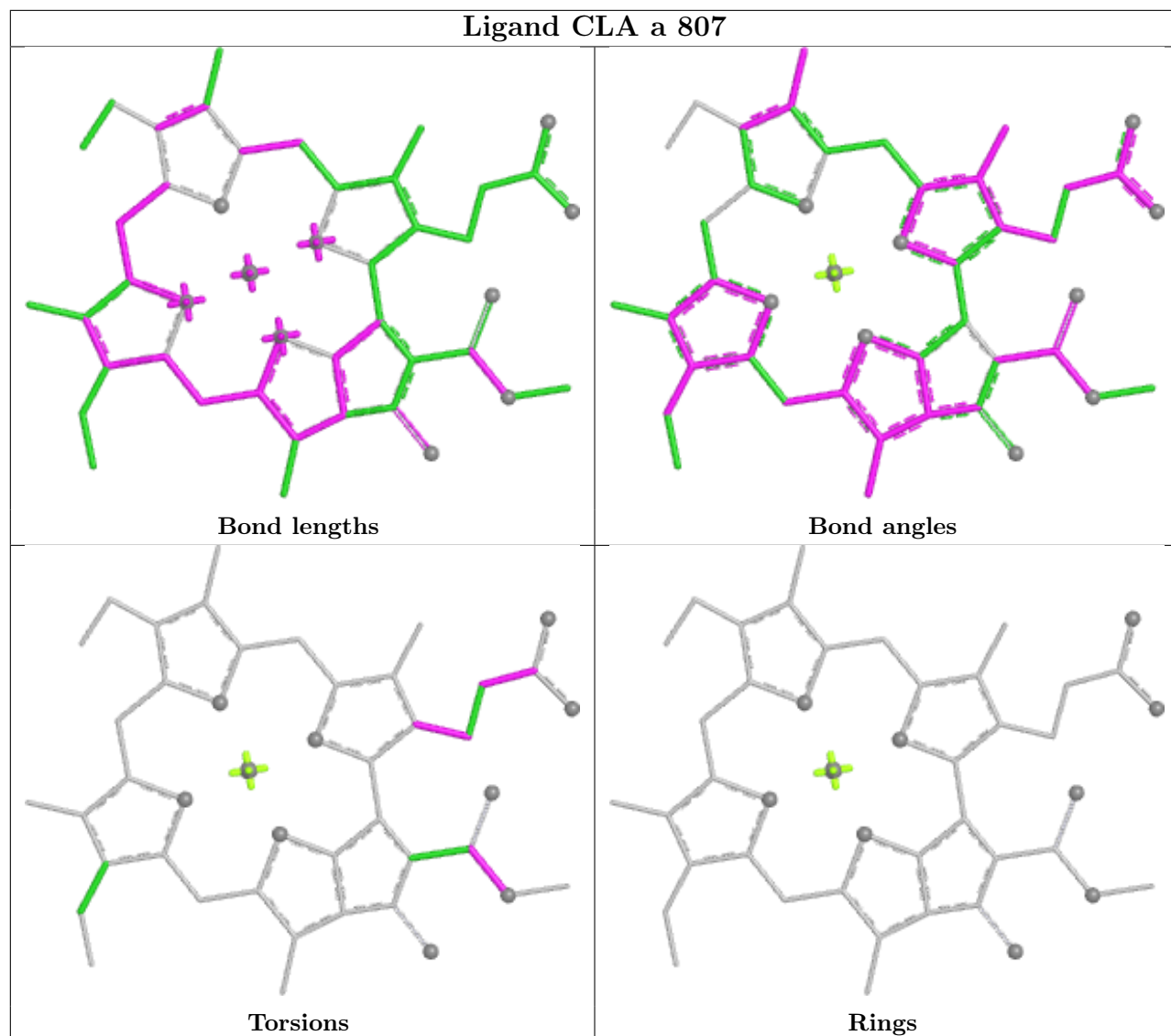


## Ligand BCR G 851

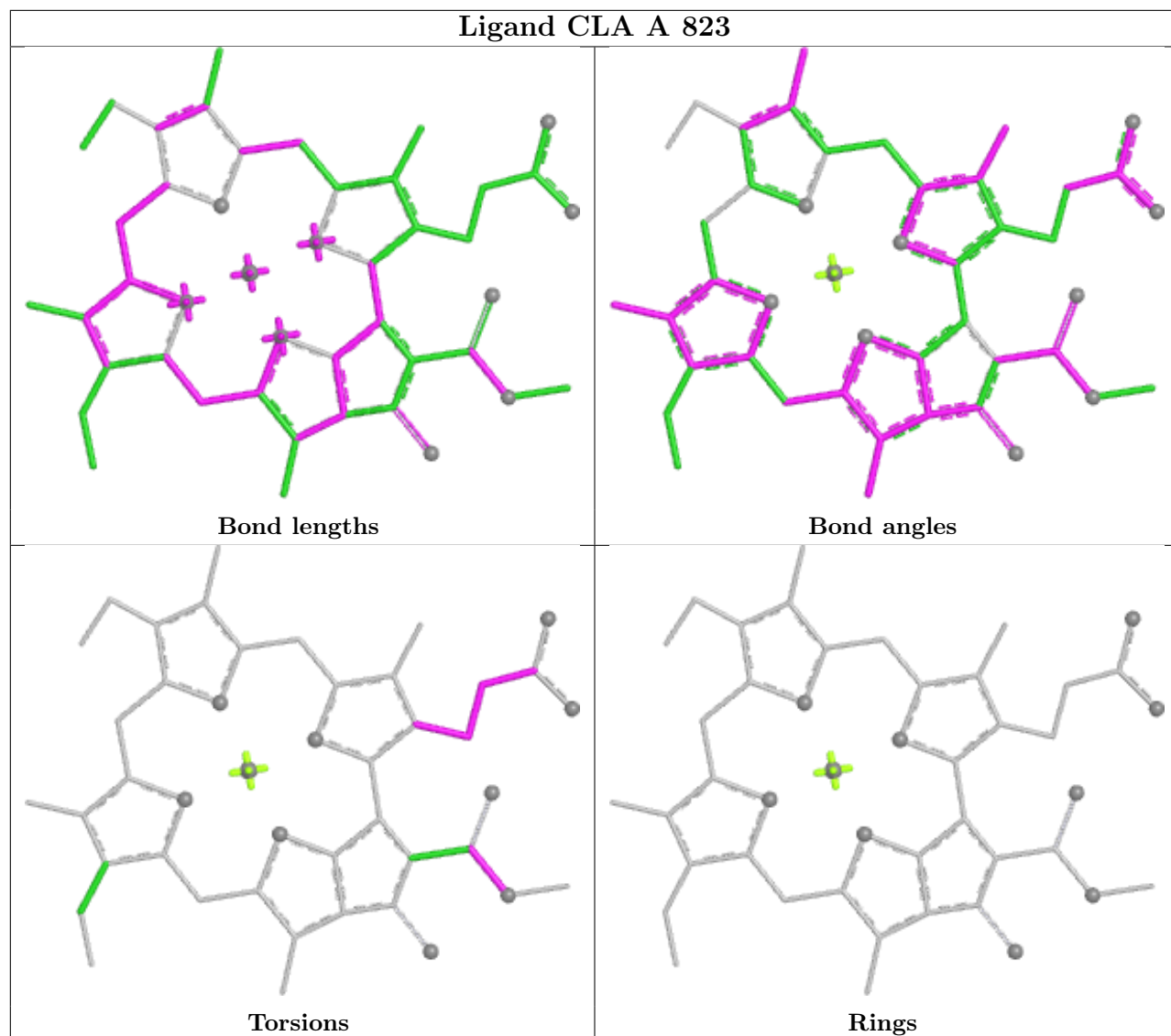




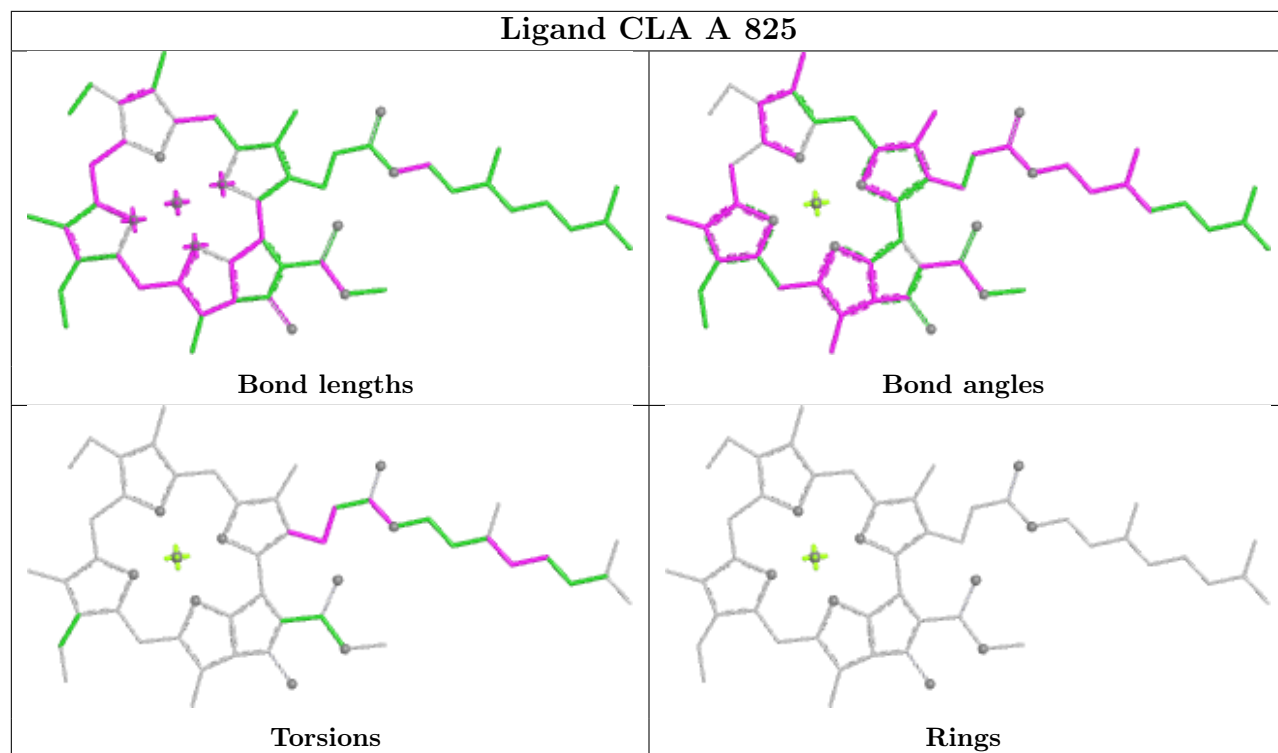
## Ligand CLA a 807



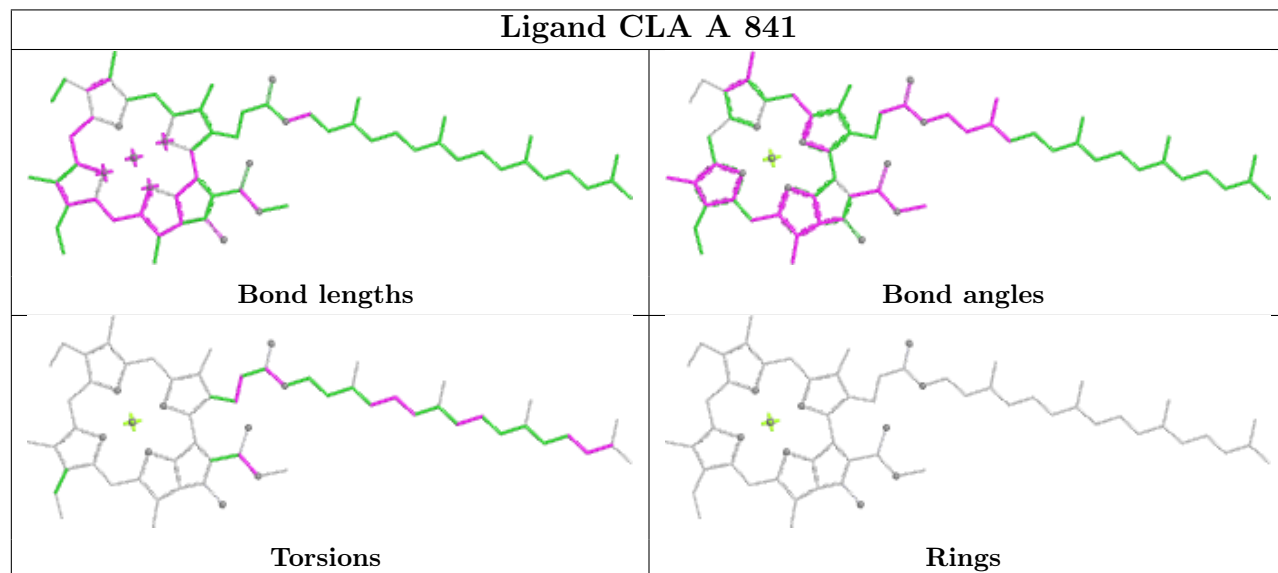
## Ligand CLA A 823



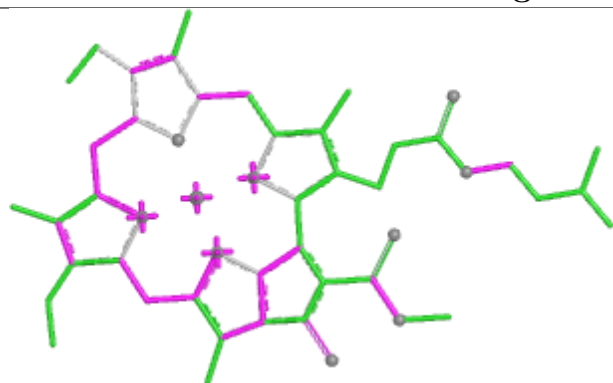
## Ligand CLA A 825



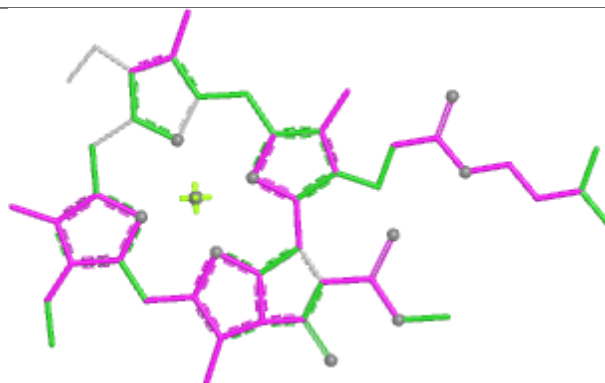
## Ligand CLA A 841



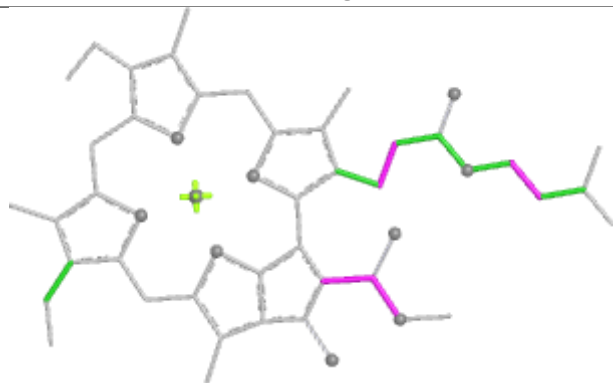
## Ligand CLA H 823



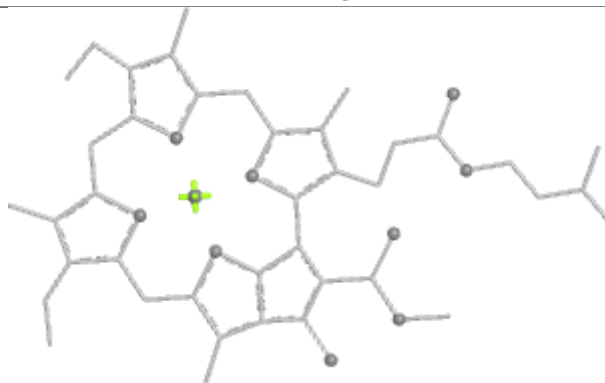
Bond lengths



Bond angles

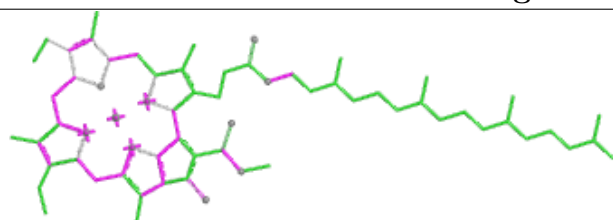


Torsions

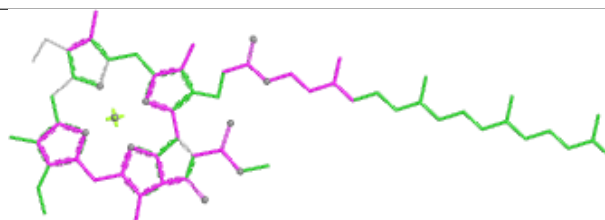


Rings

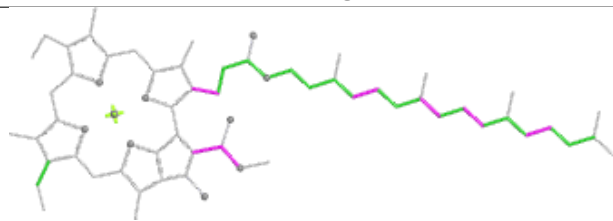
## Ligand CLA H 825



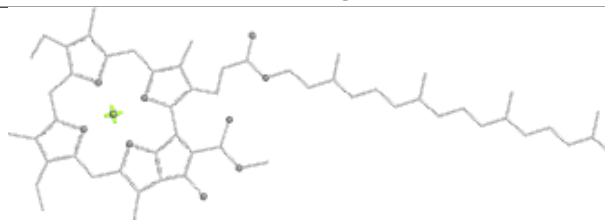
Bond lengths



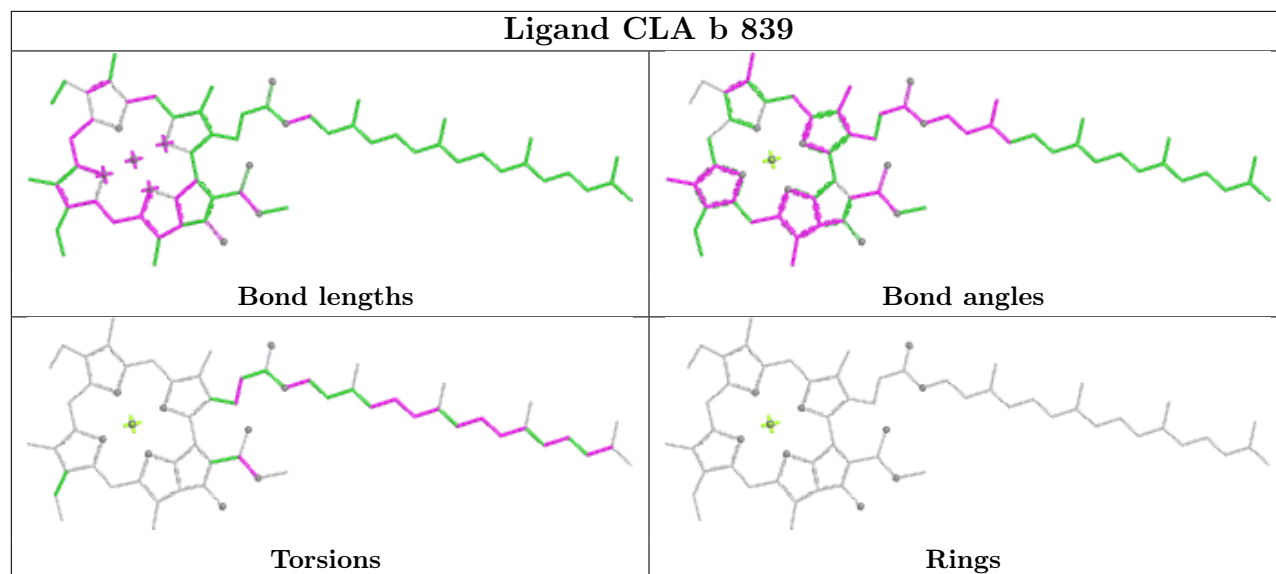
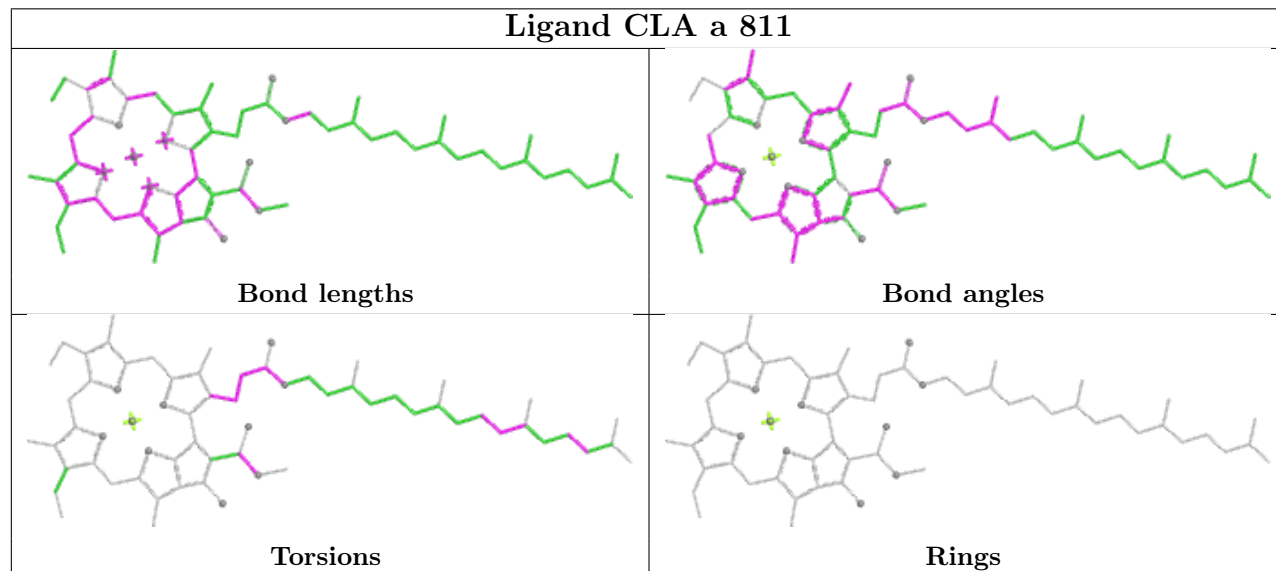
Bond angles

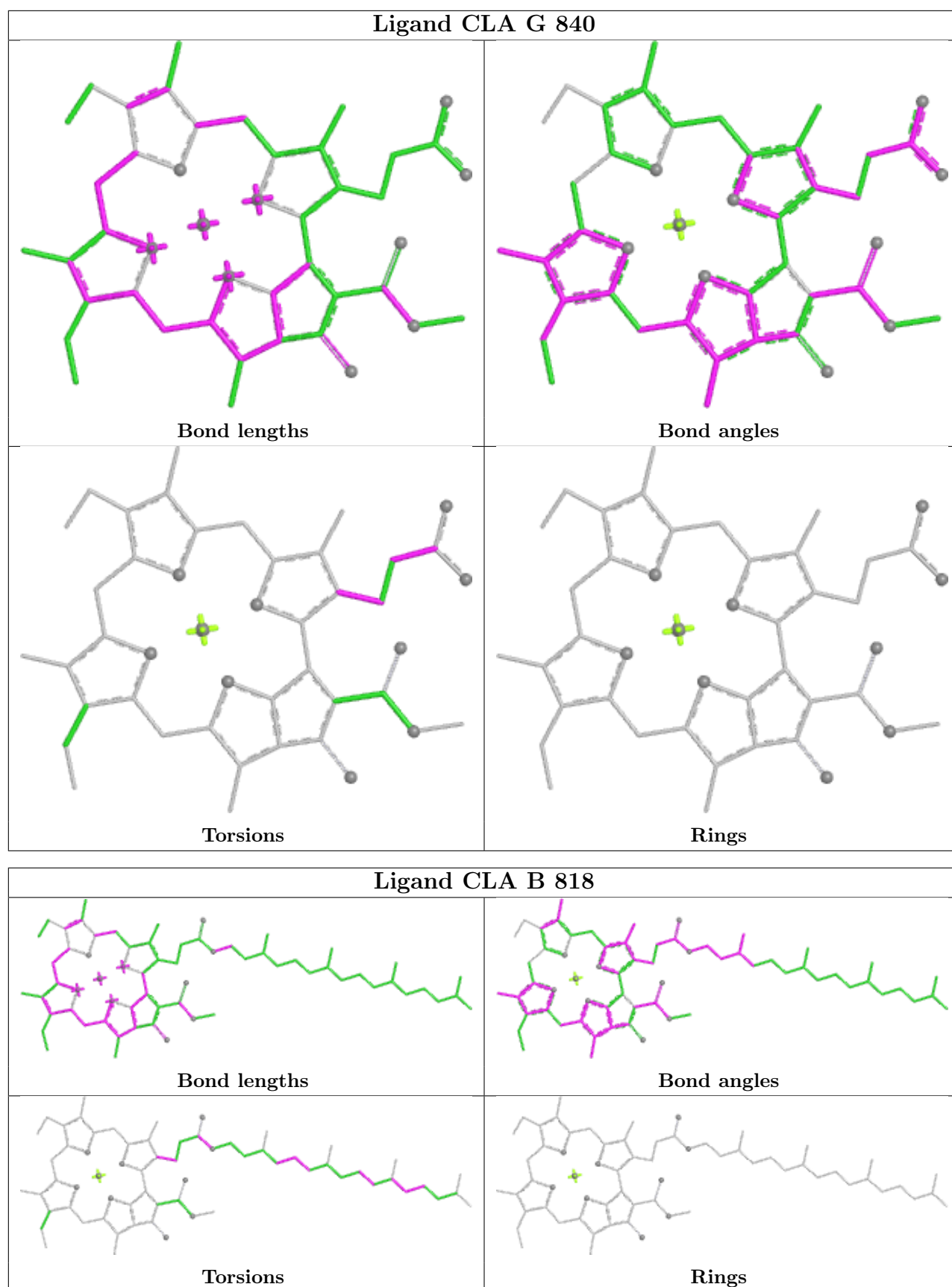


Torsions



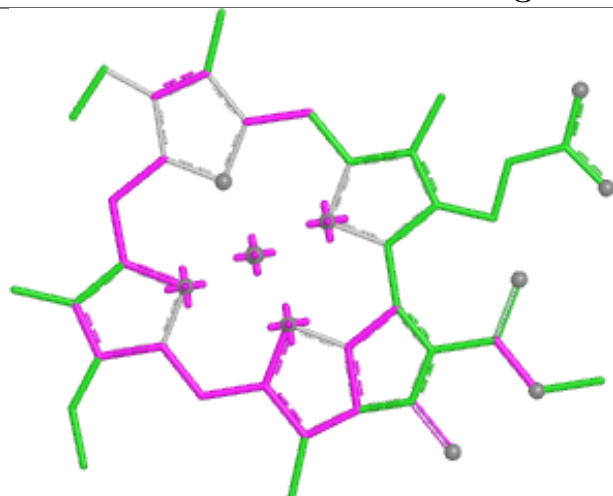
Rings

**Ligand CLA b 839****Ligand CLA a 811**

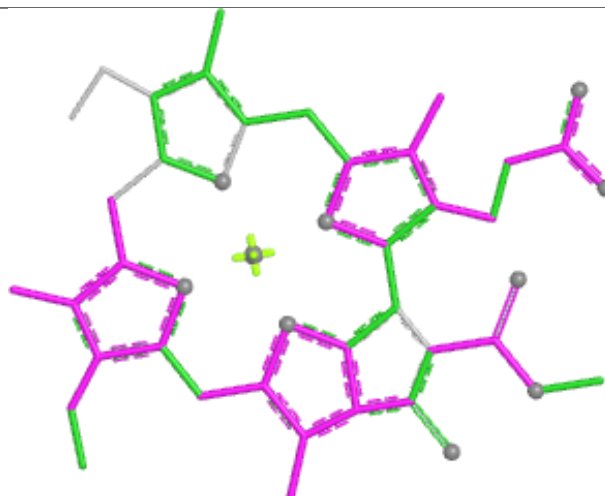




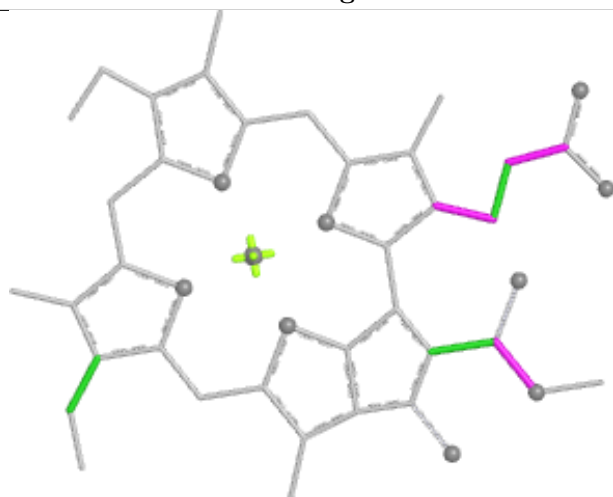
## Ligand CLA B 835



Bond lengths



Bond angles

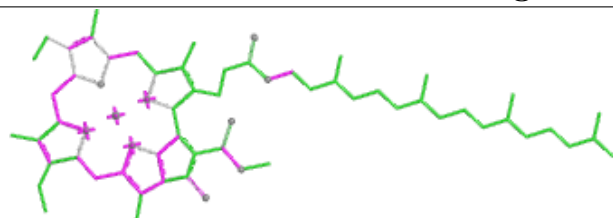


Torsions

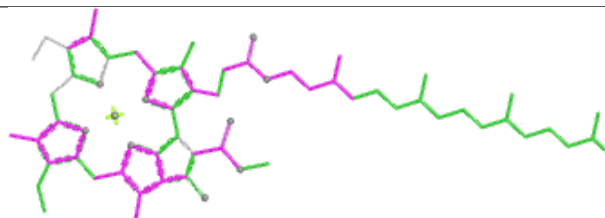


Rings

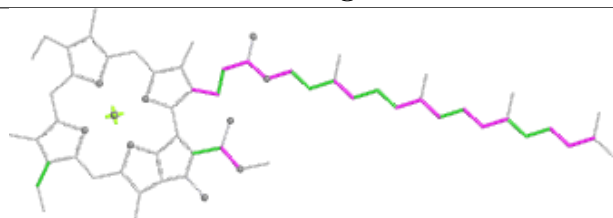
## Ligand CLA G 807



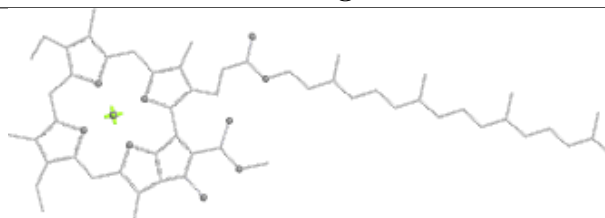
Bond lengths



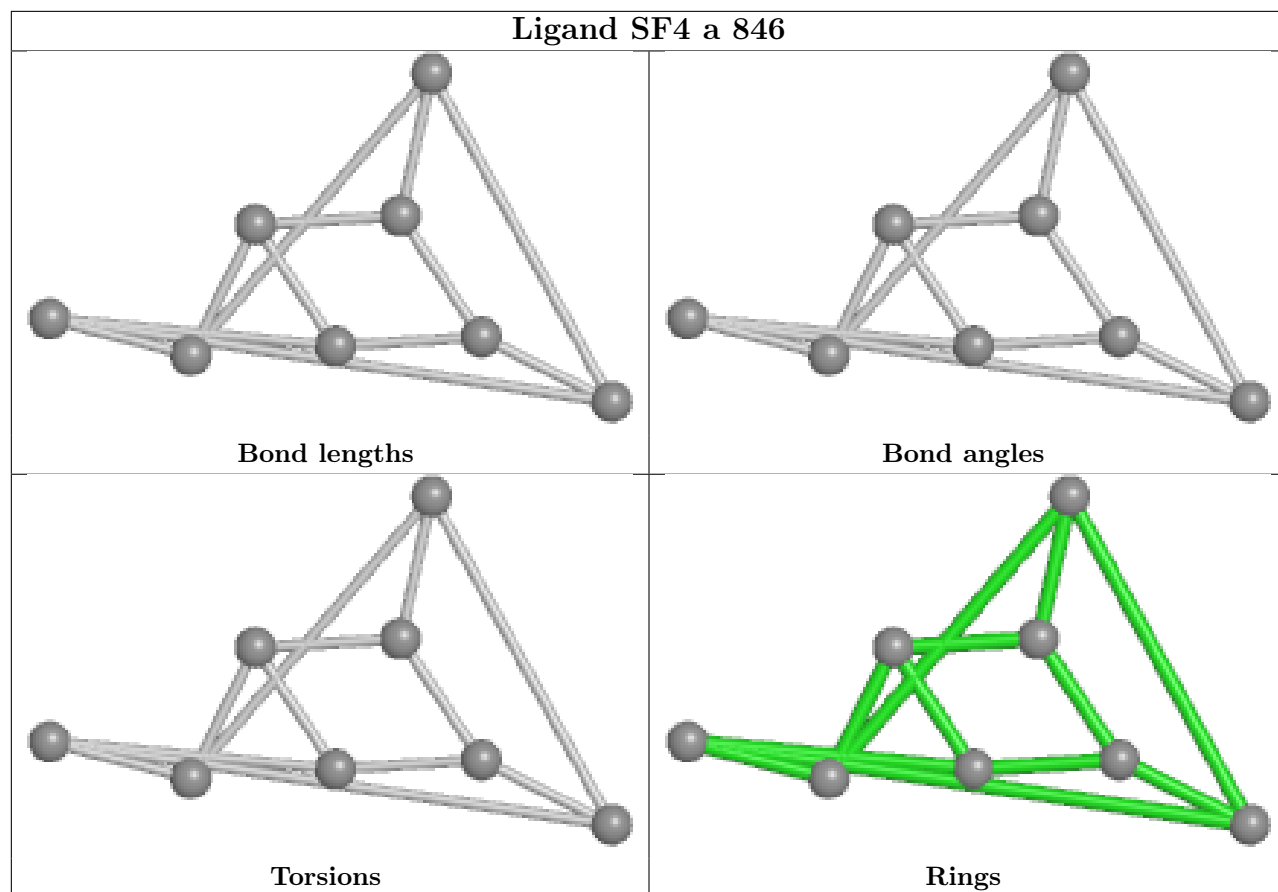
Bond angles



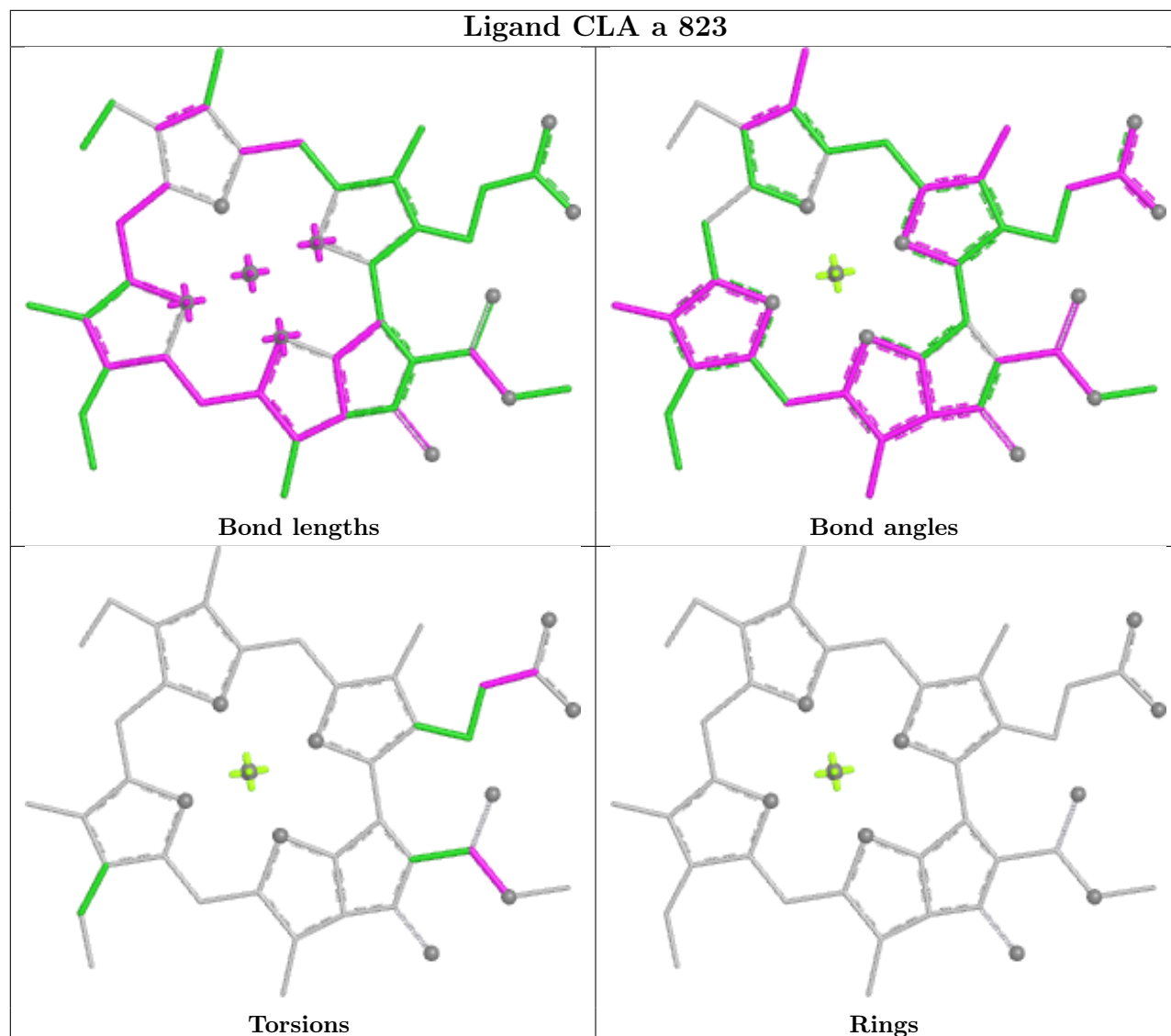
Torsions



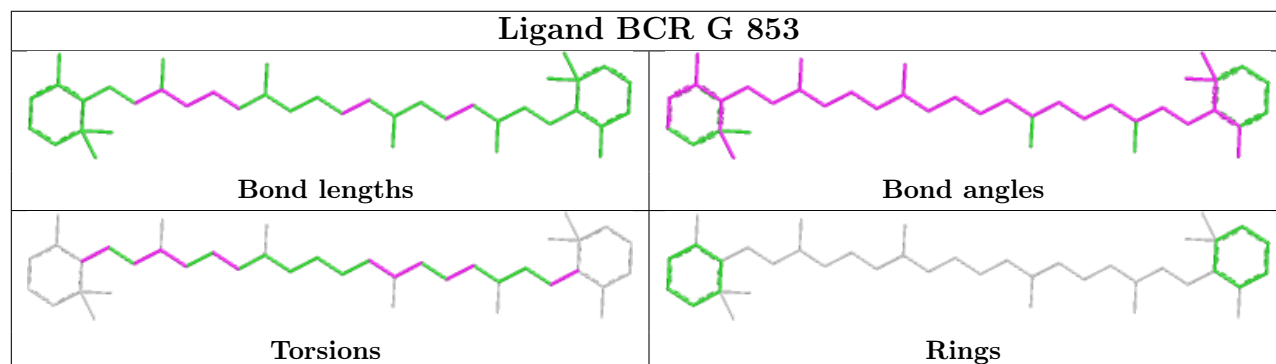
Rings

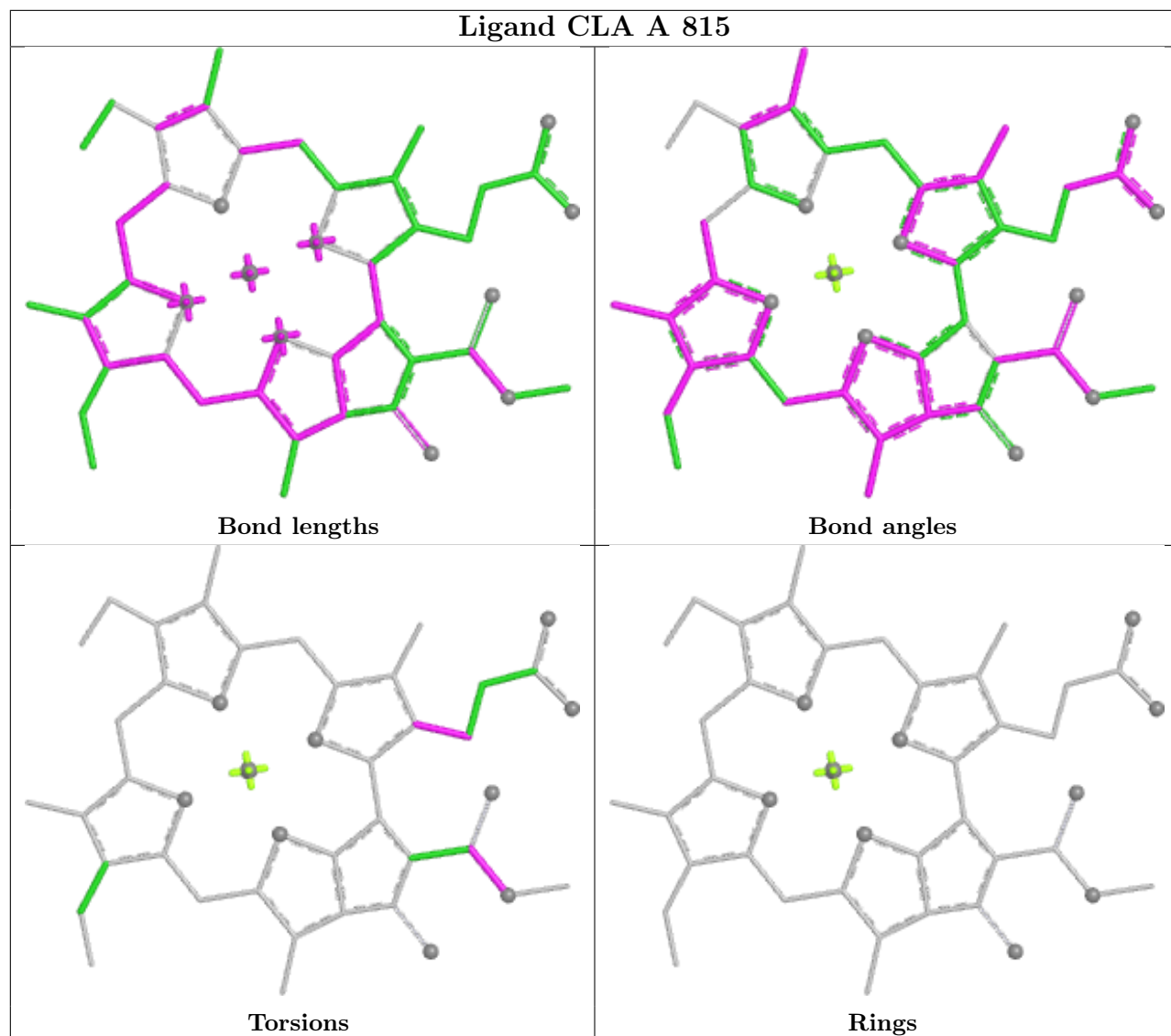


## Ligand CLA a 823

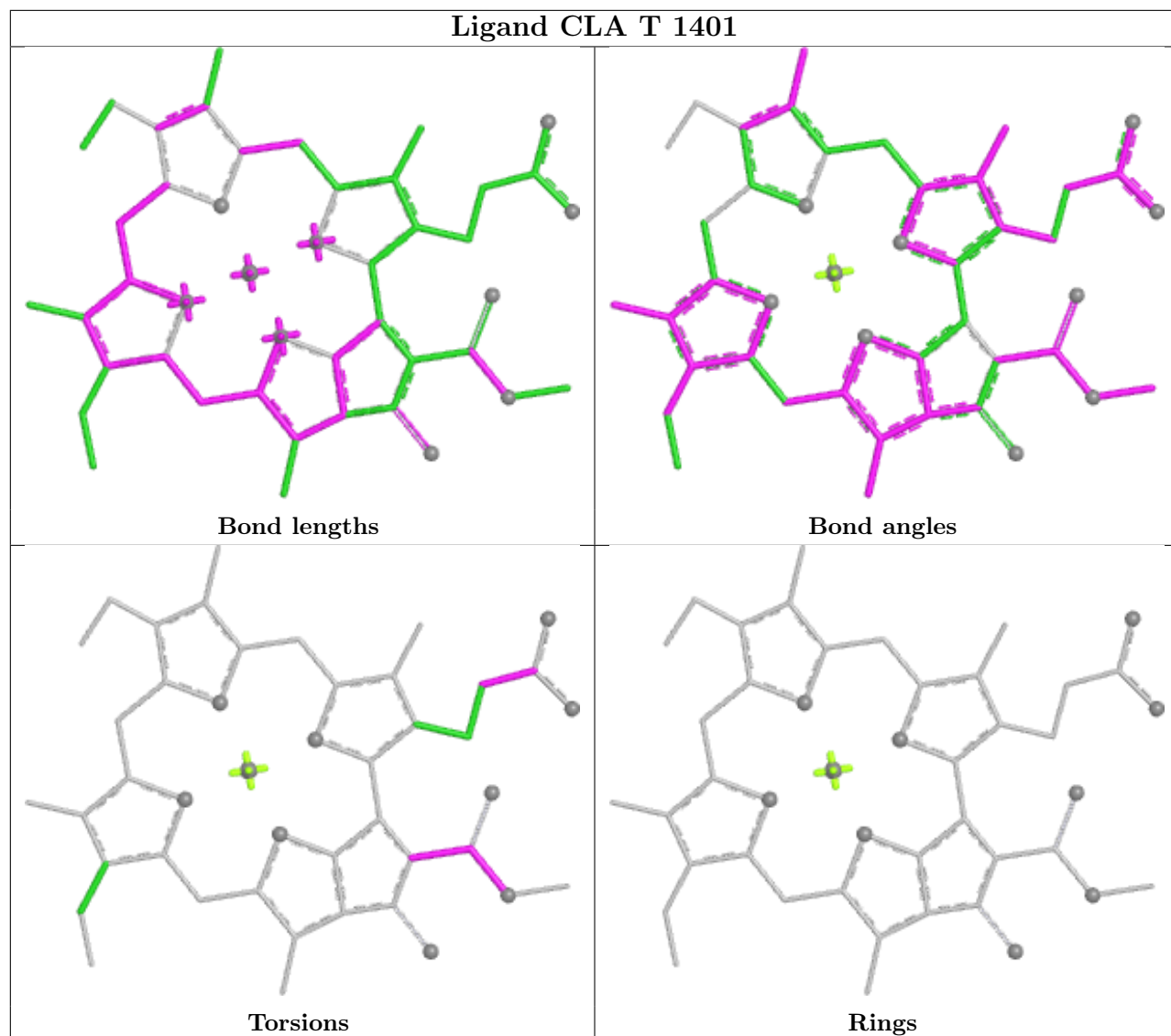


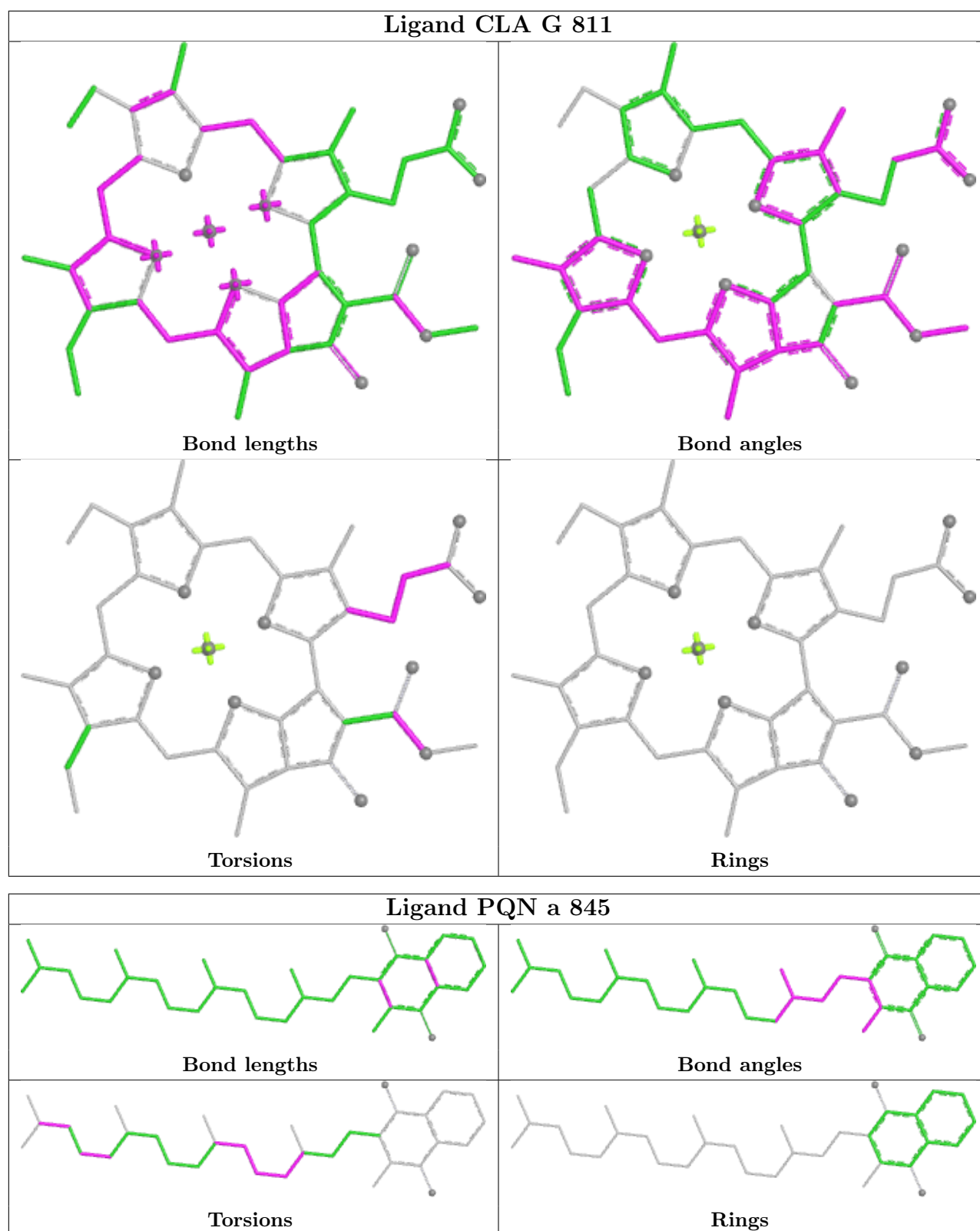
## Ligand BCR G 853

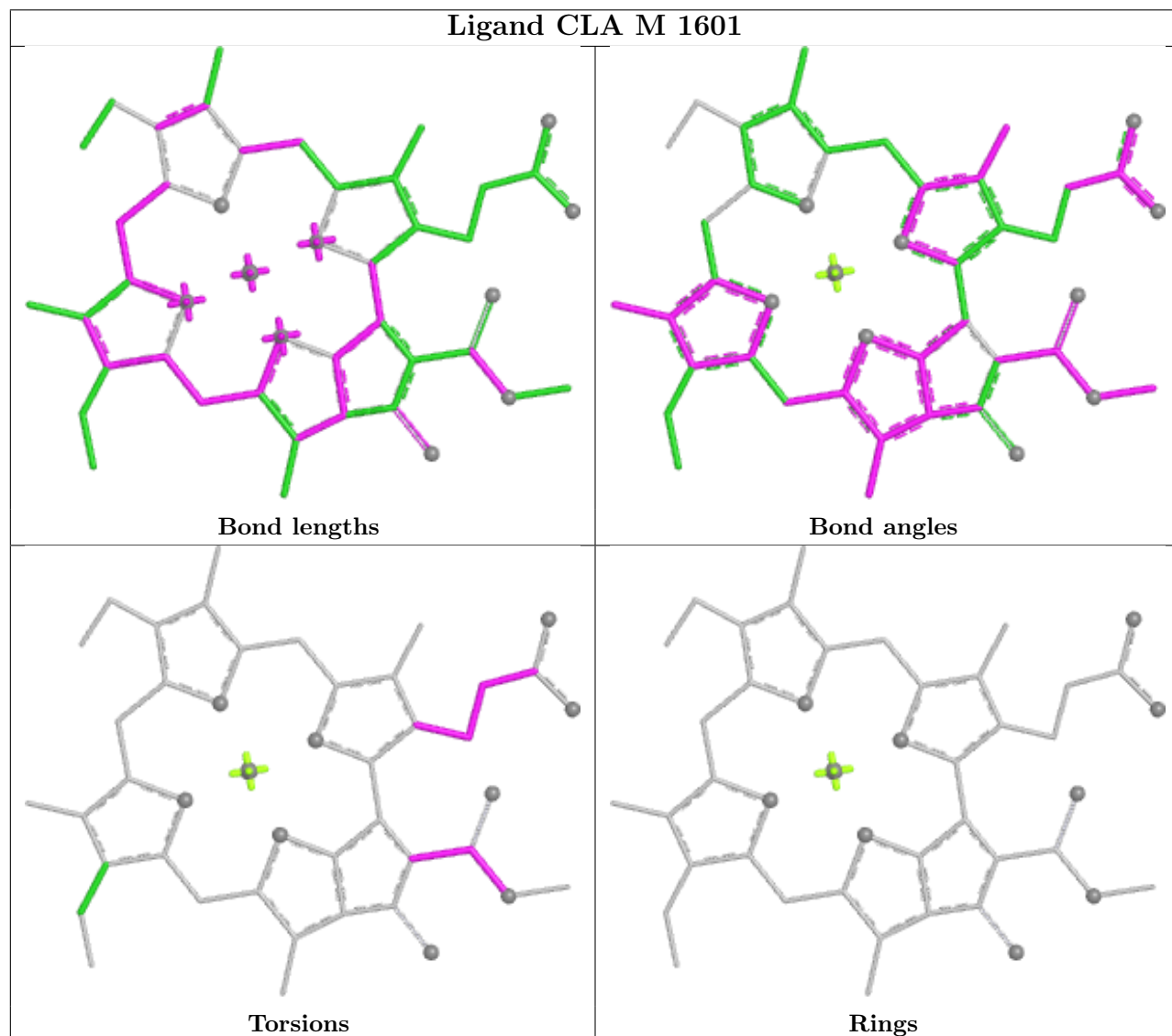
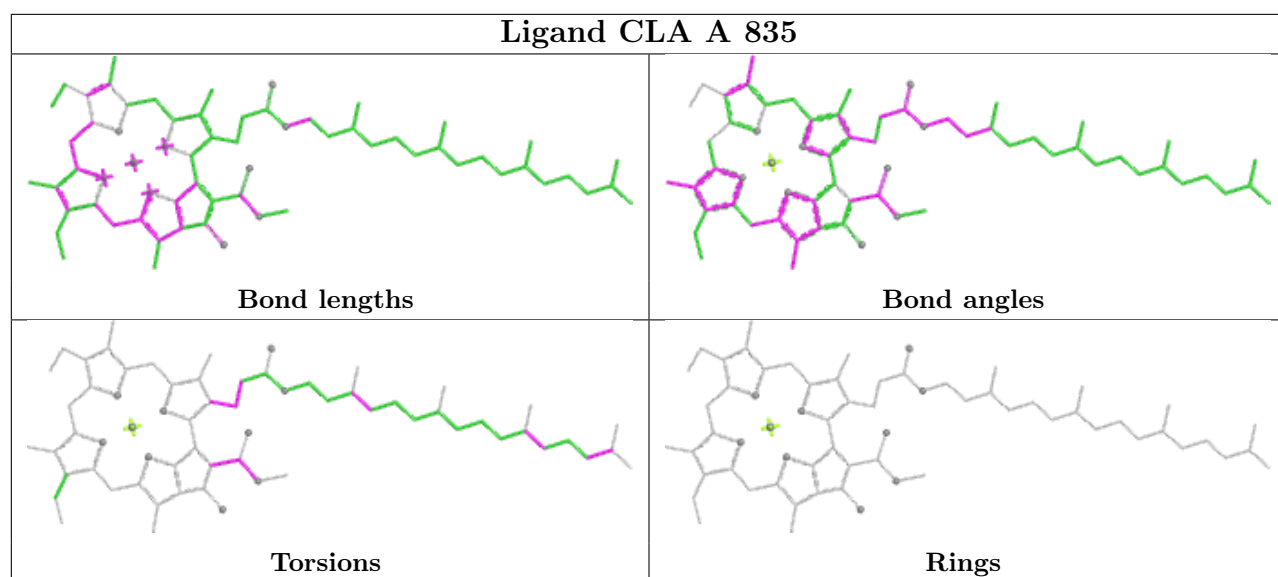


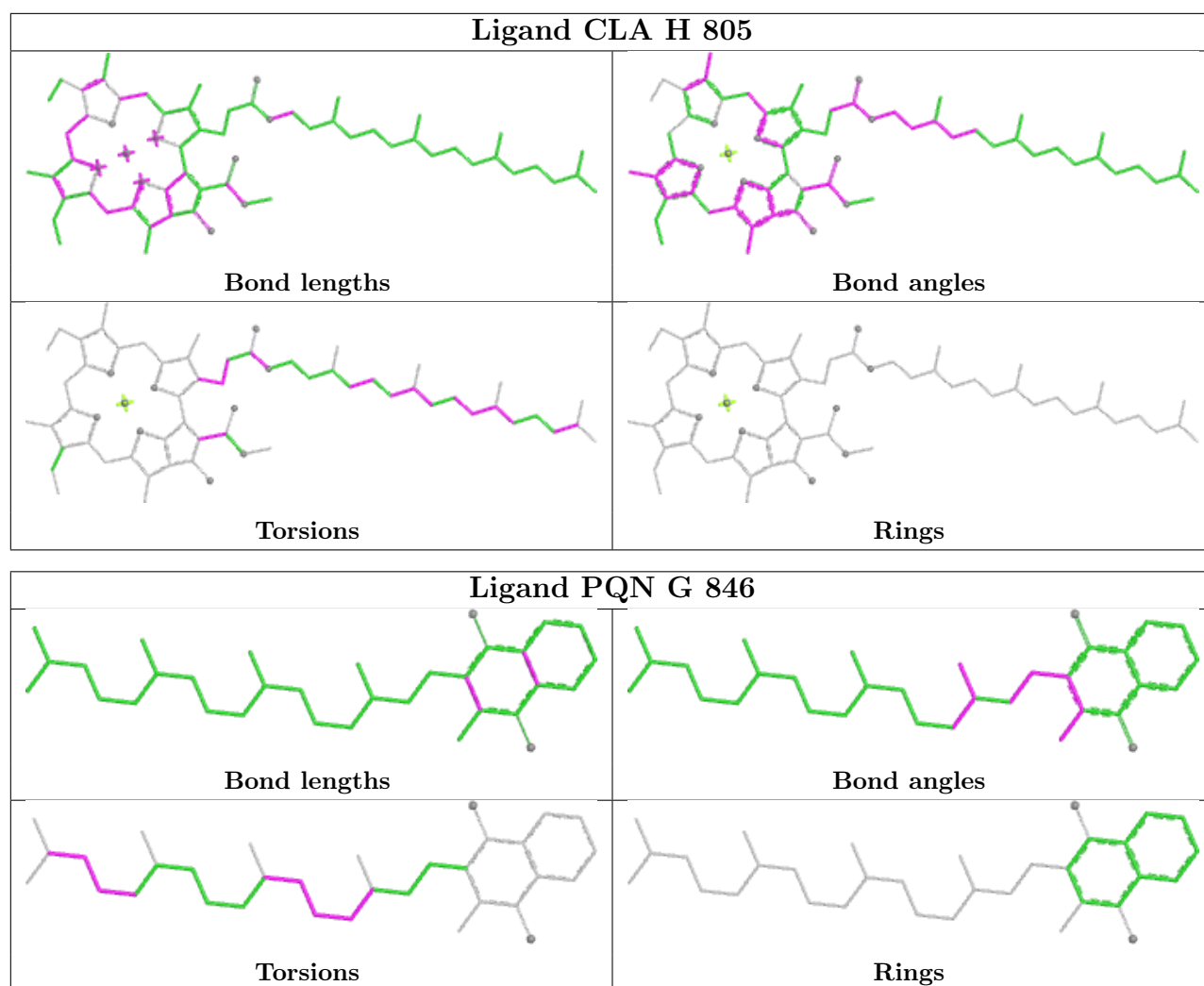


## Ligand CLA T 1401

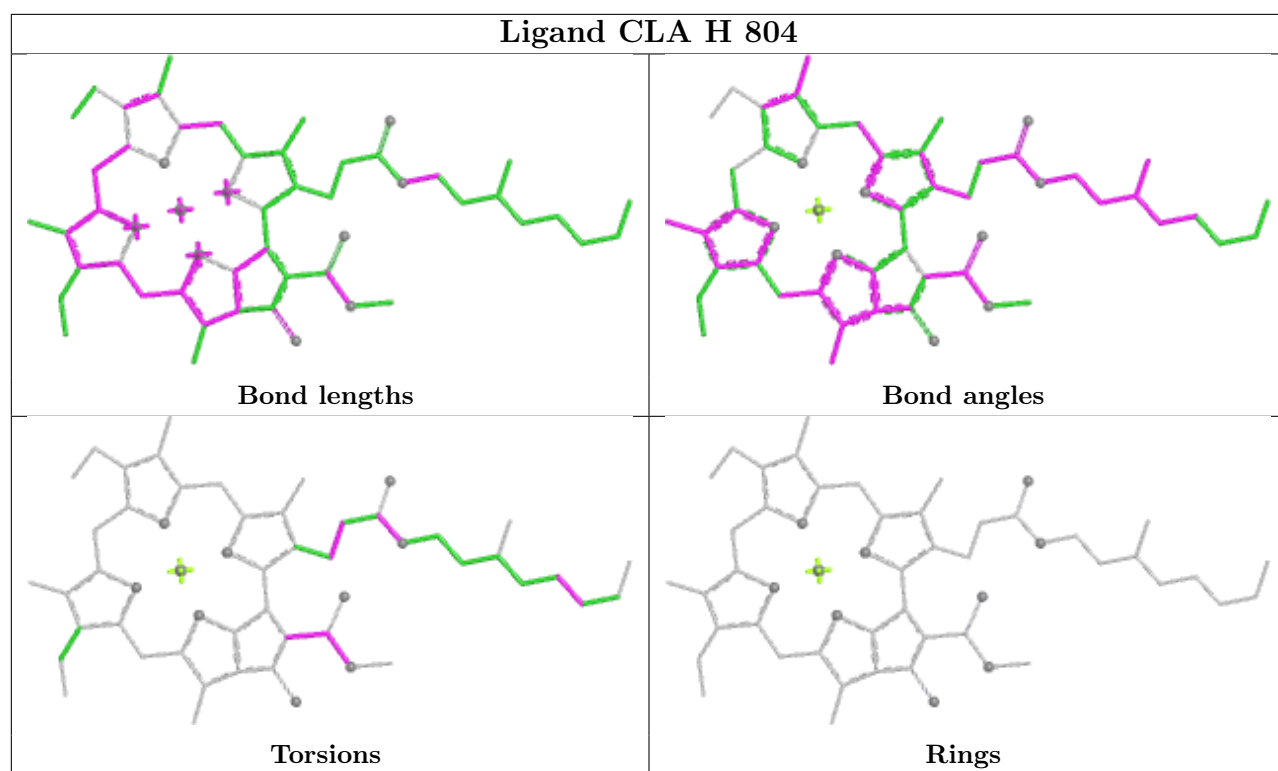




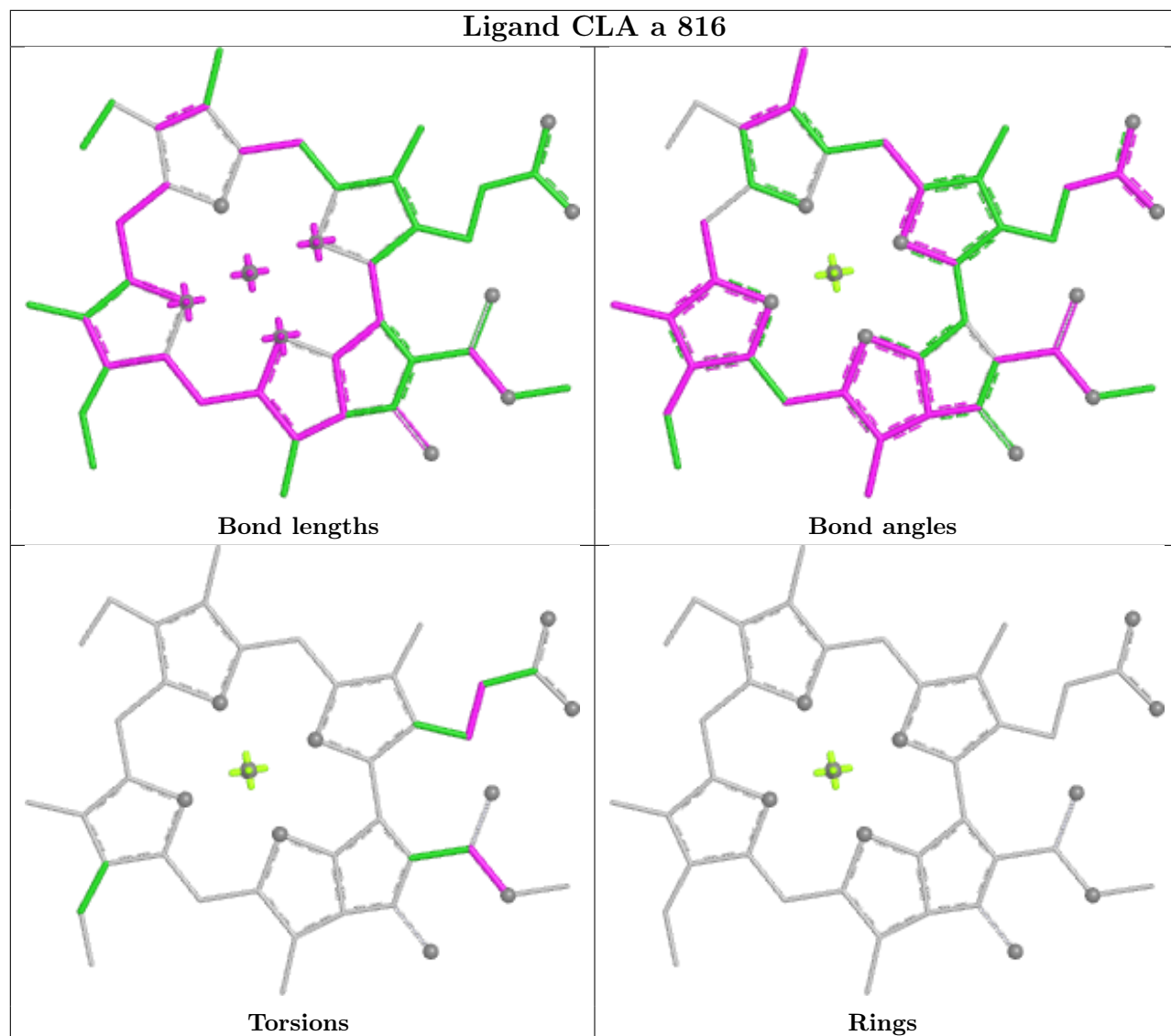




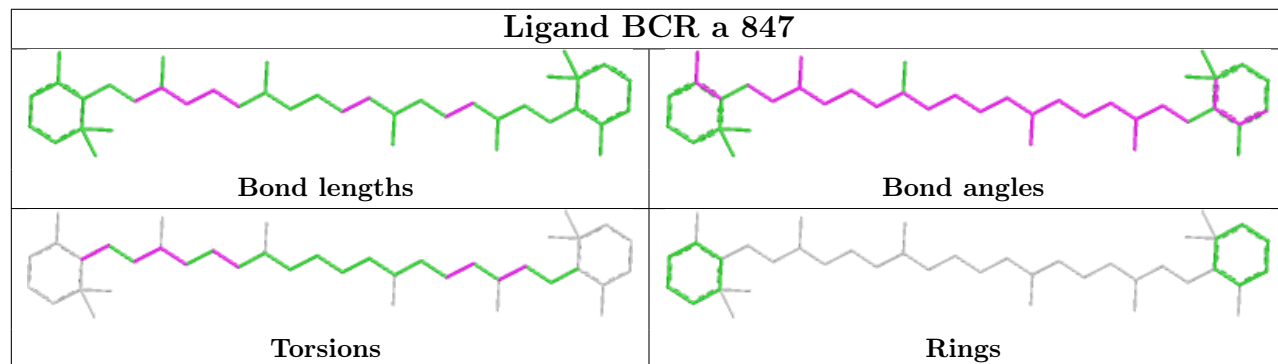


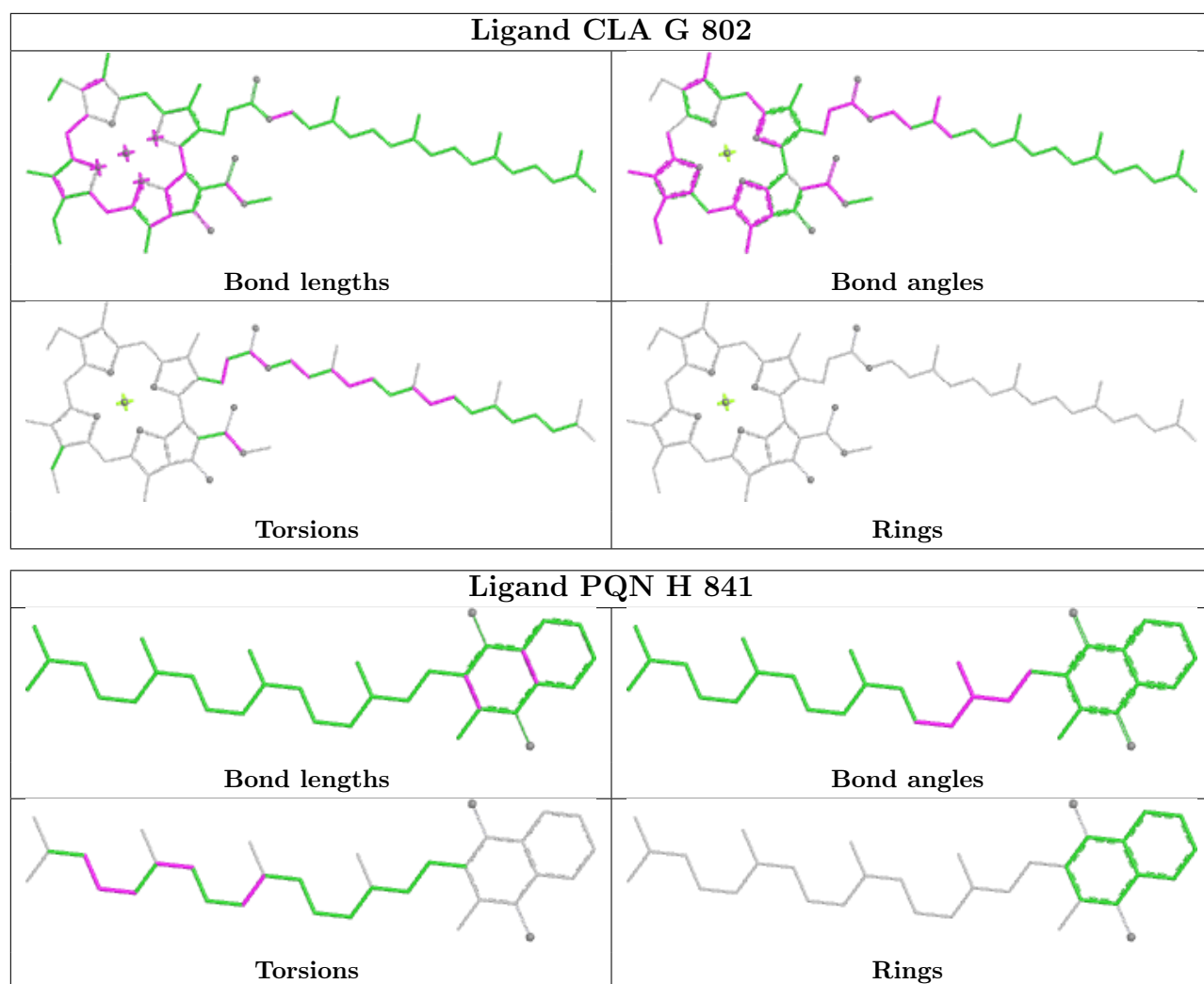


## Ligand CLA a 816

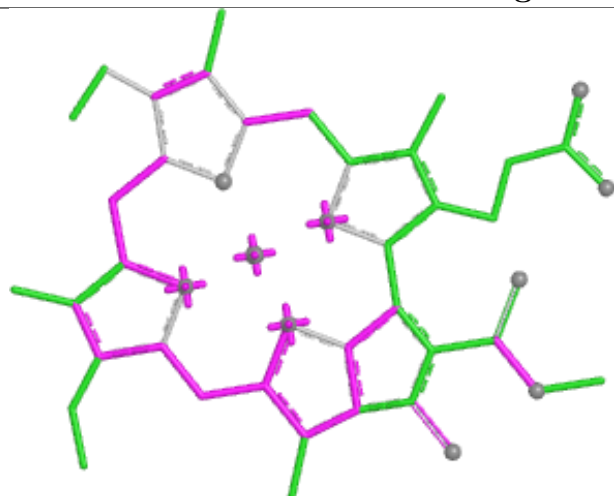


## Ligand BCR a 847

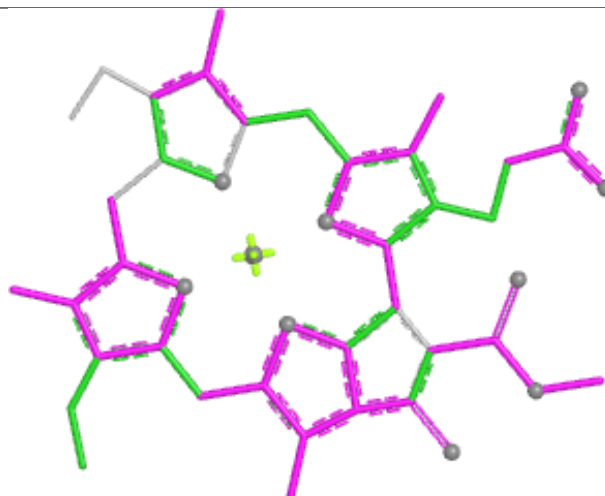




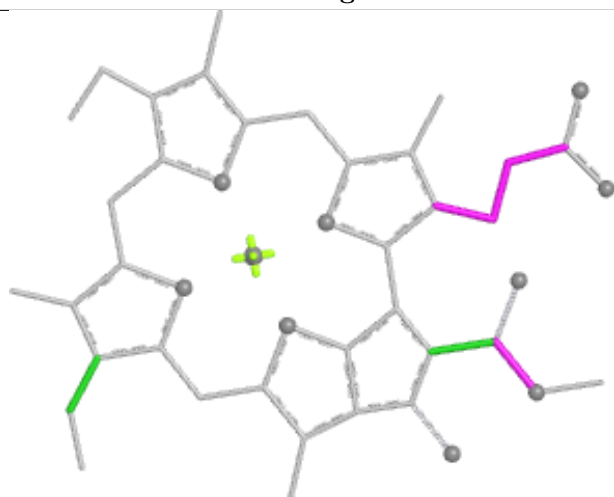
## Ligand CLA B 830



Bond lengths



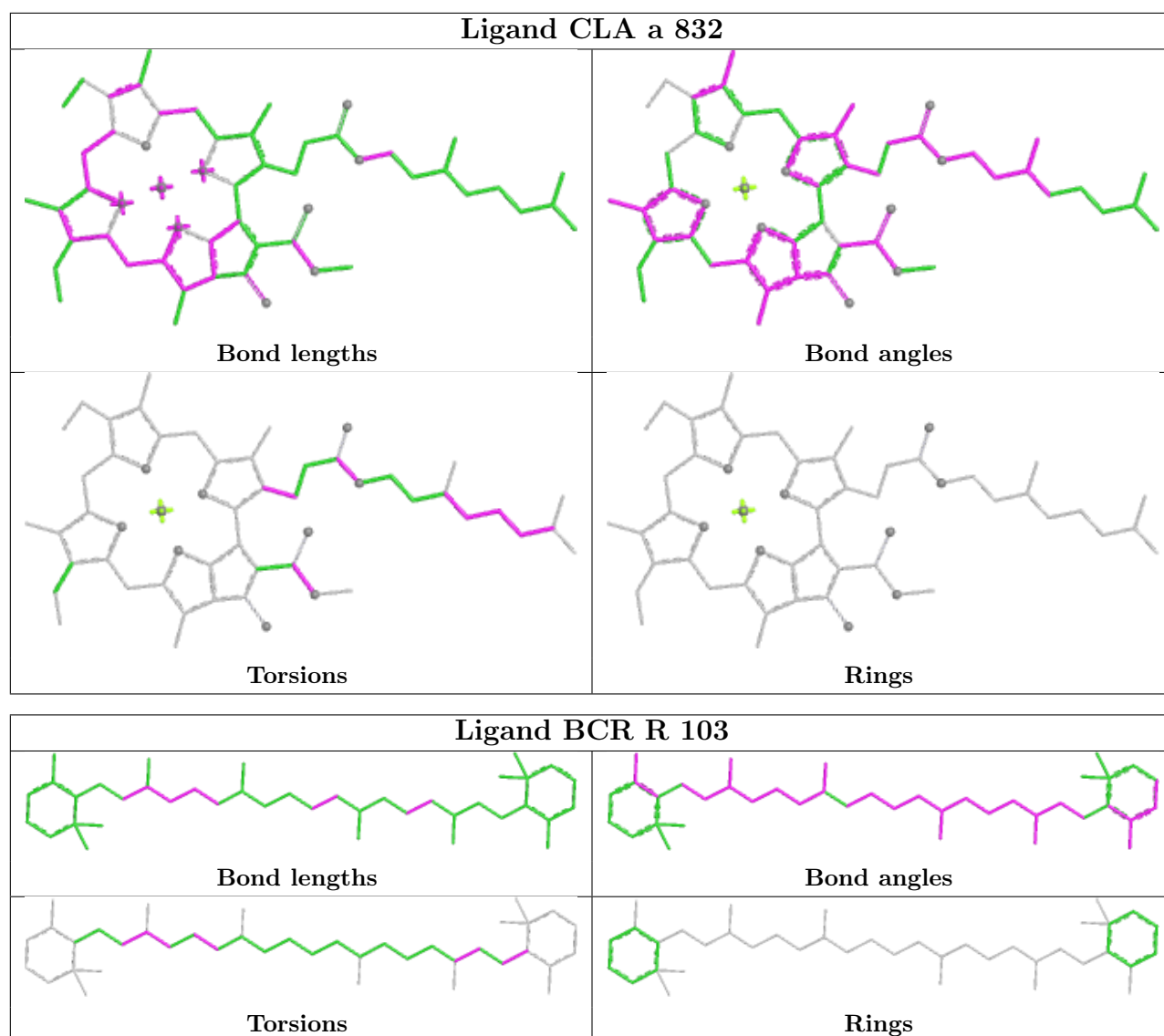
Bond angles



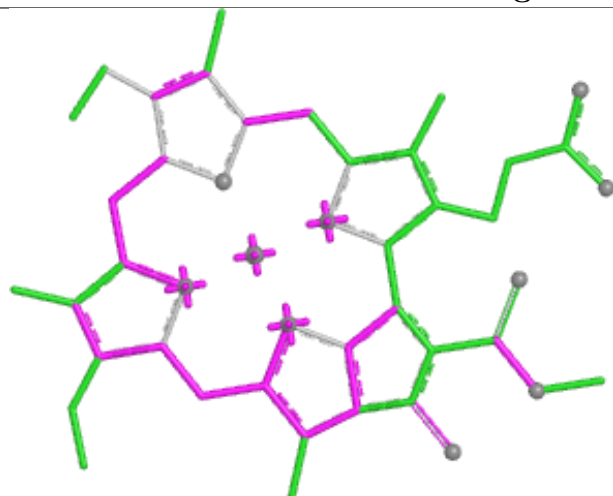
Torsions



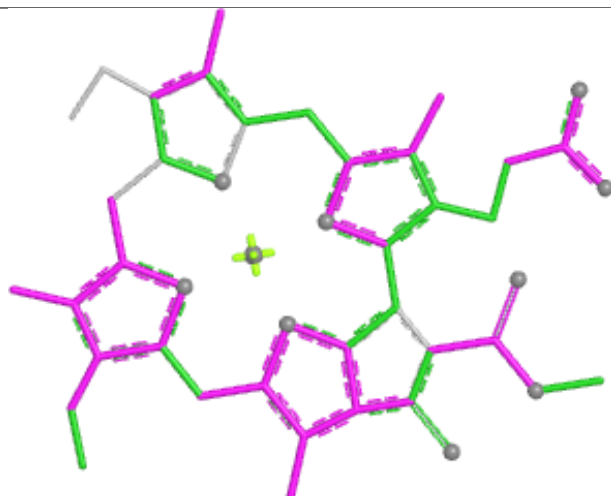
Rings



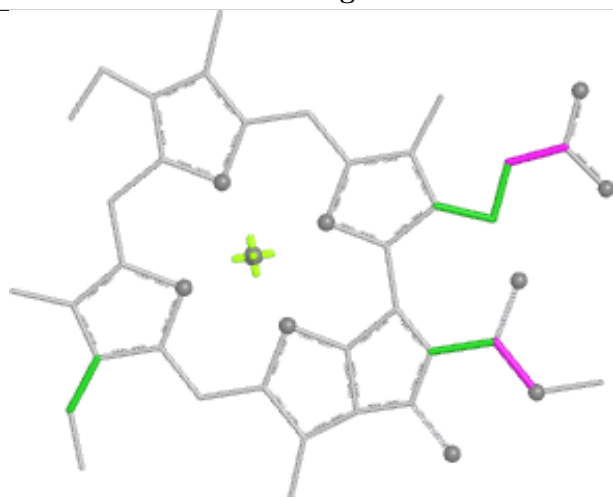
## Ligand CLA A 824



Bond lengths



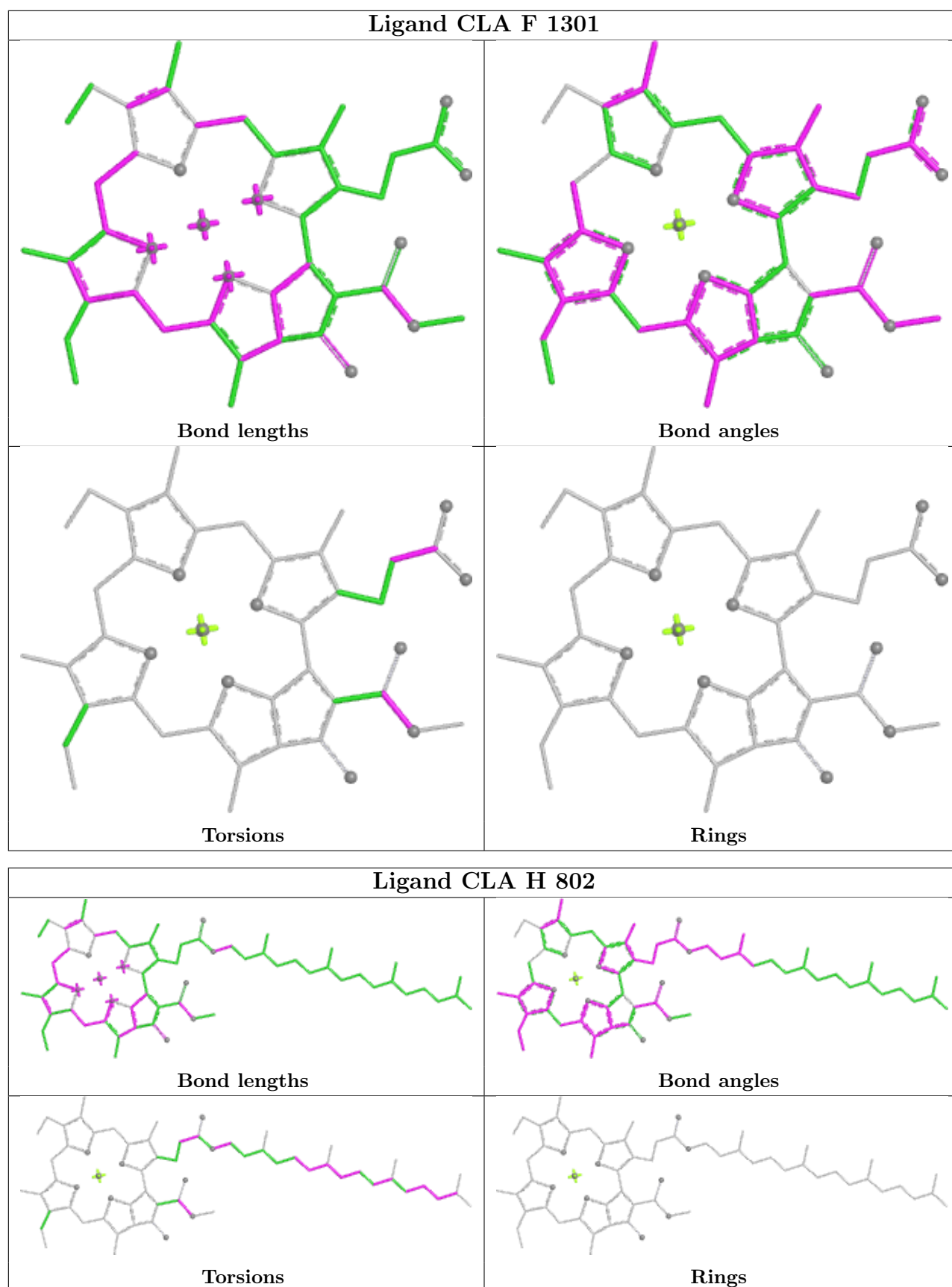
Bond angles



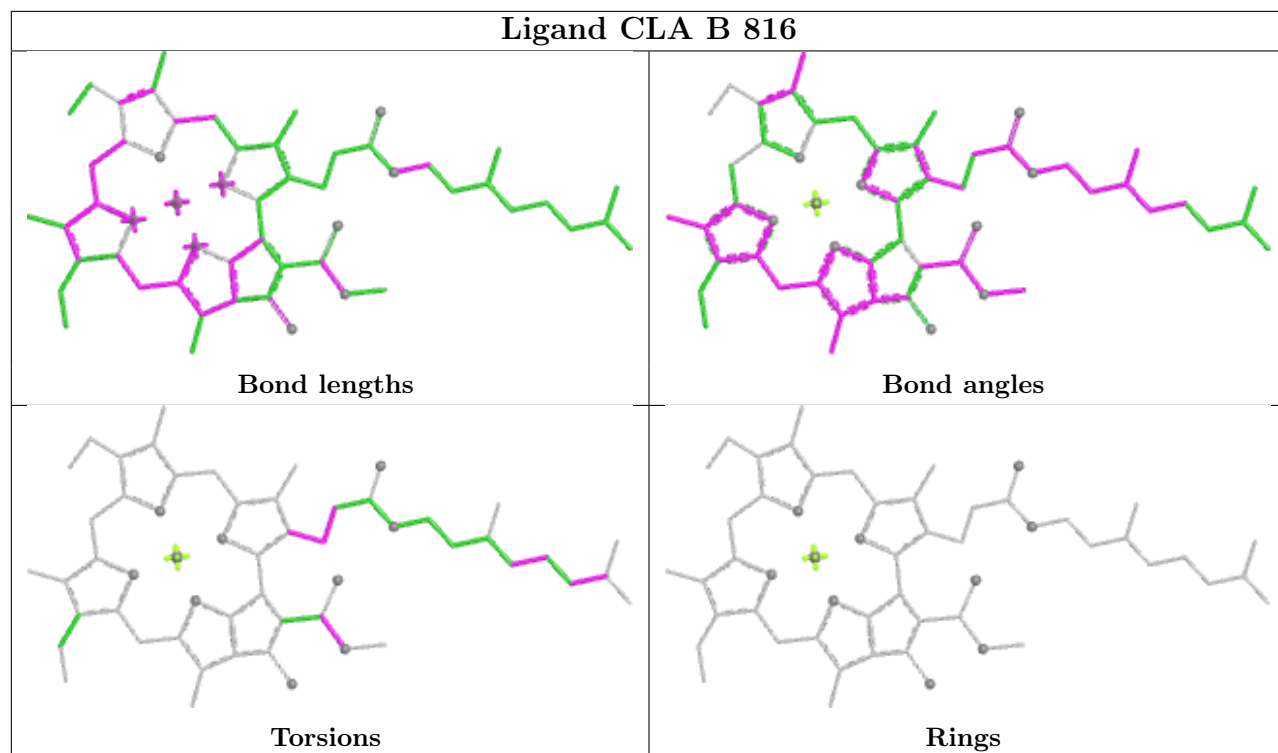
Torsions



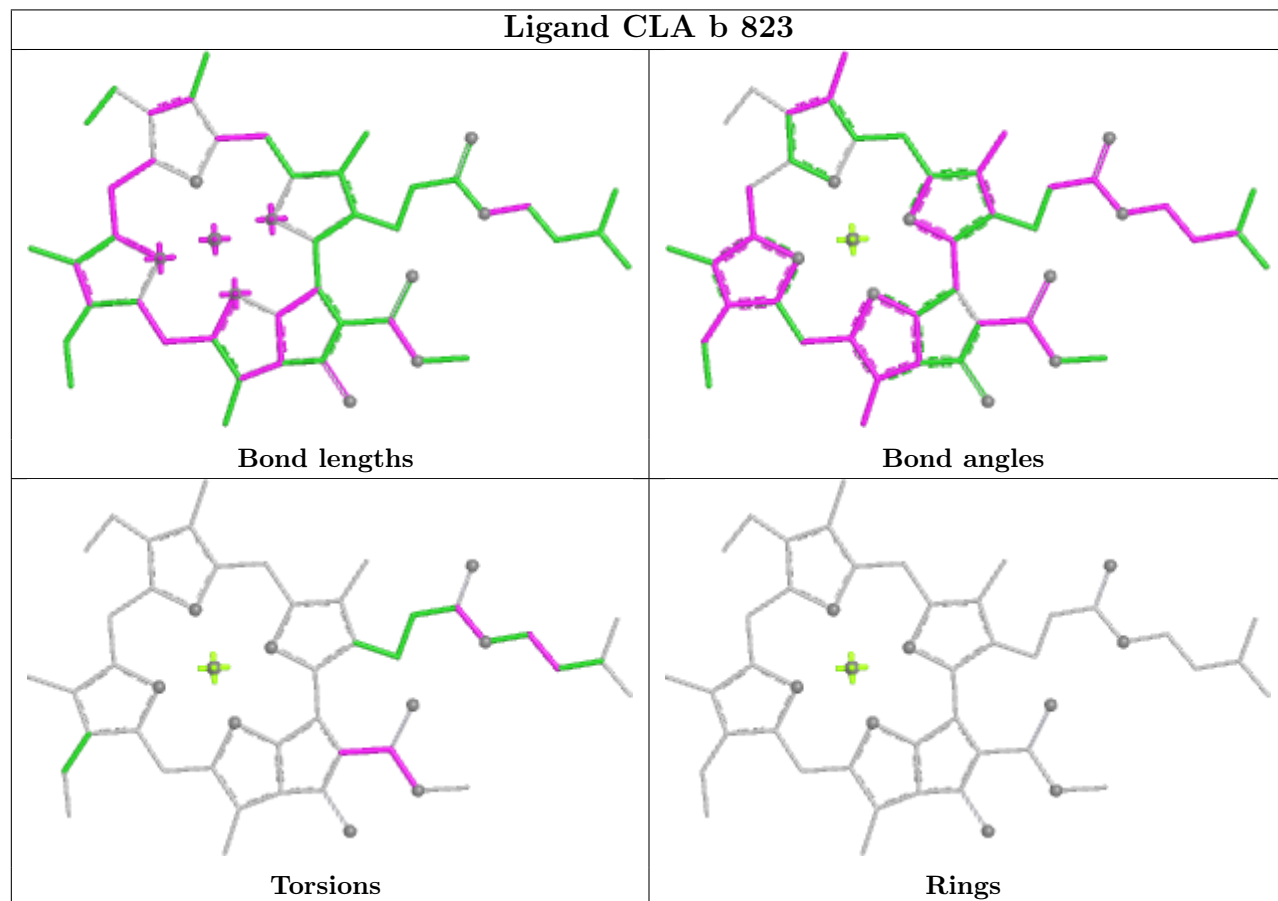
Rings



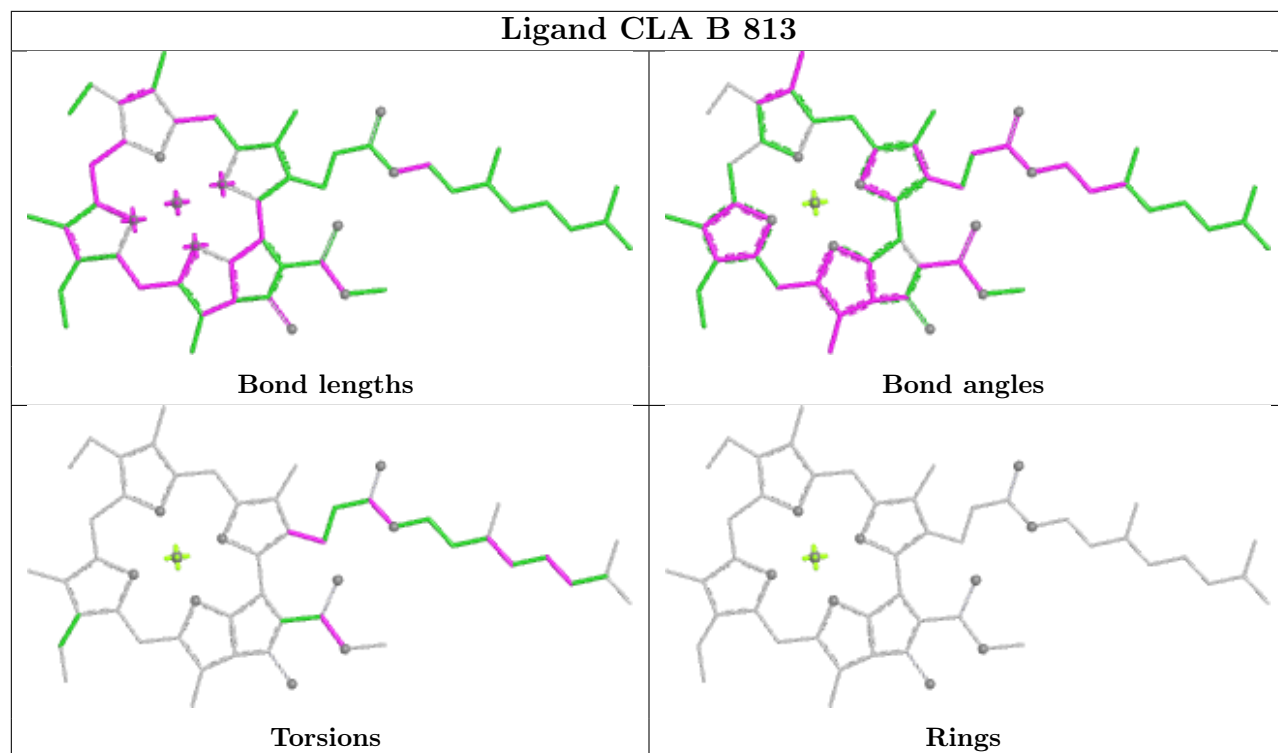
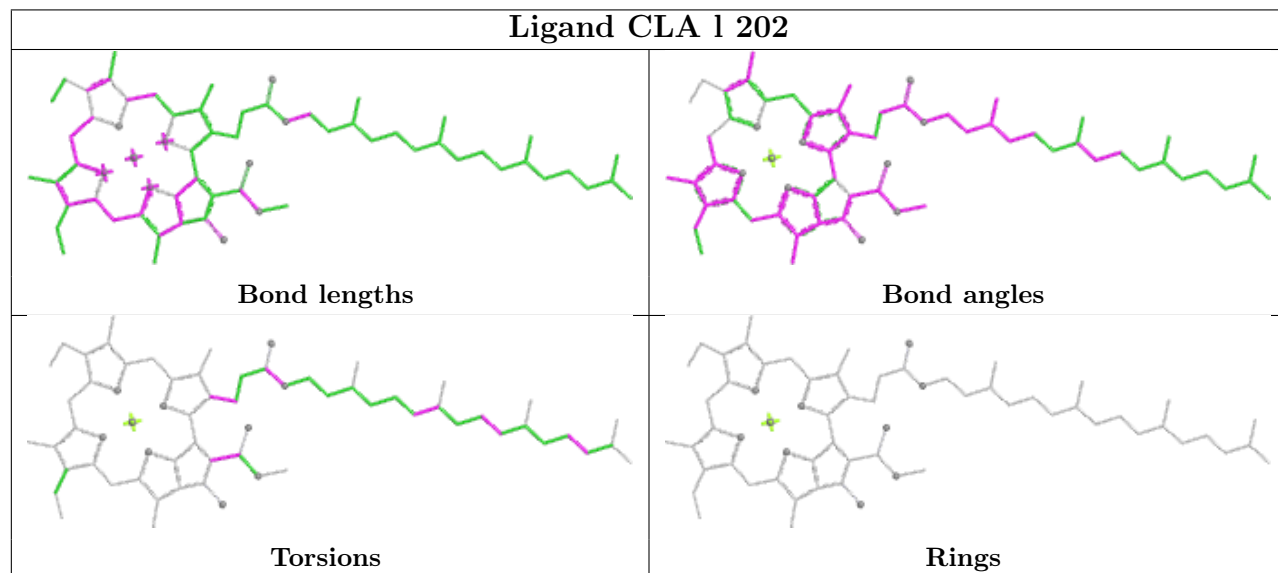
## Ligand CLA B 816

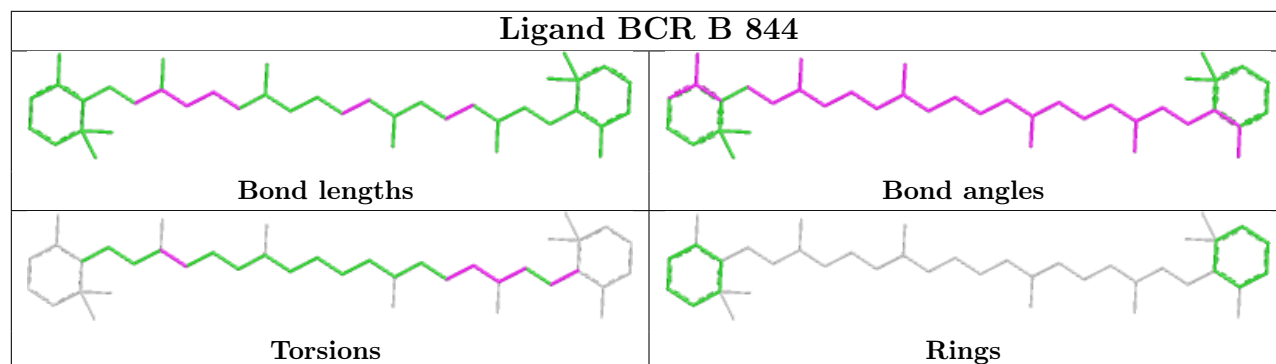
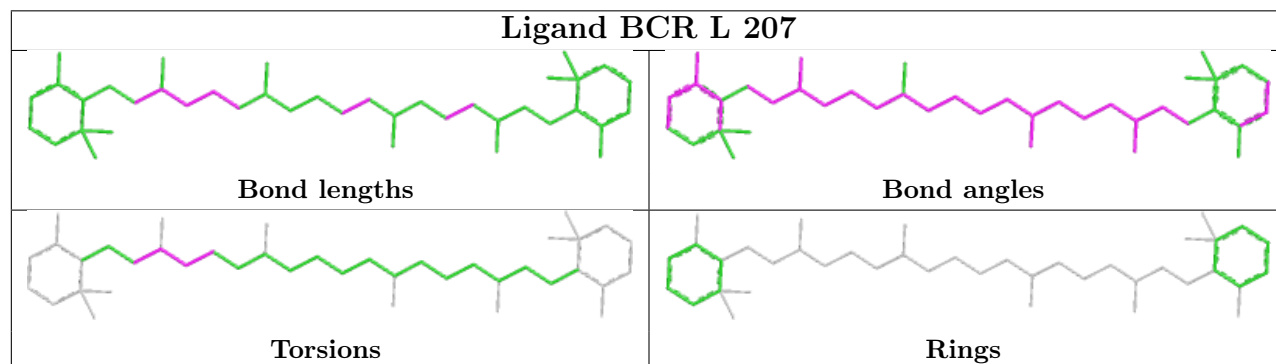
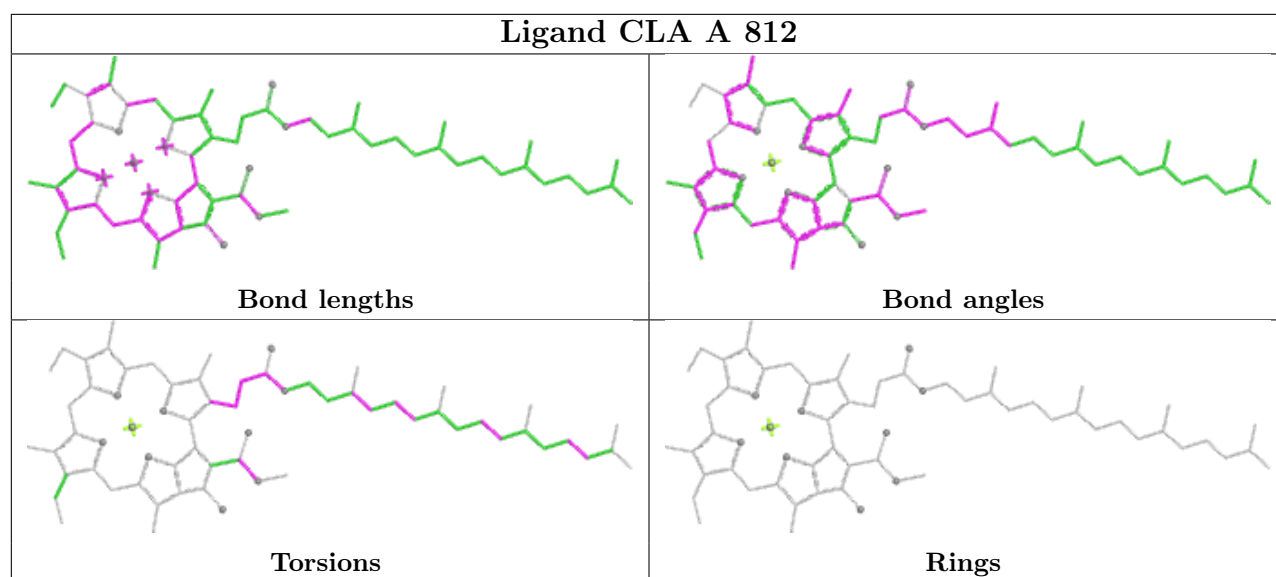


## Ligand CLA b 823

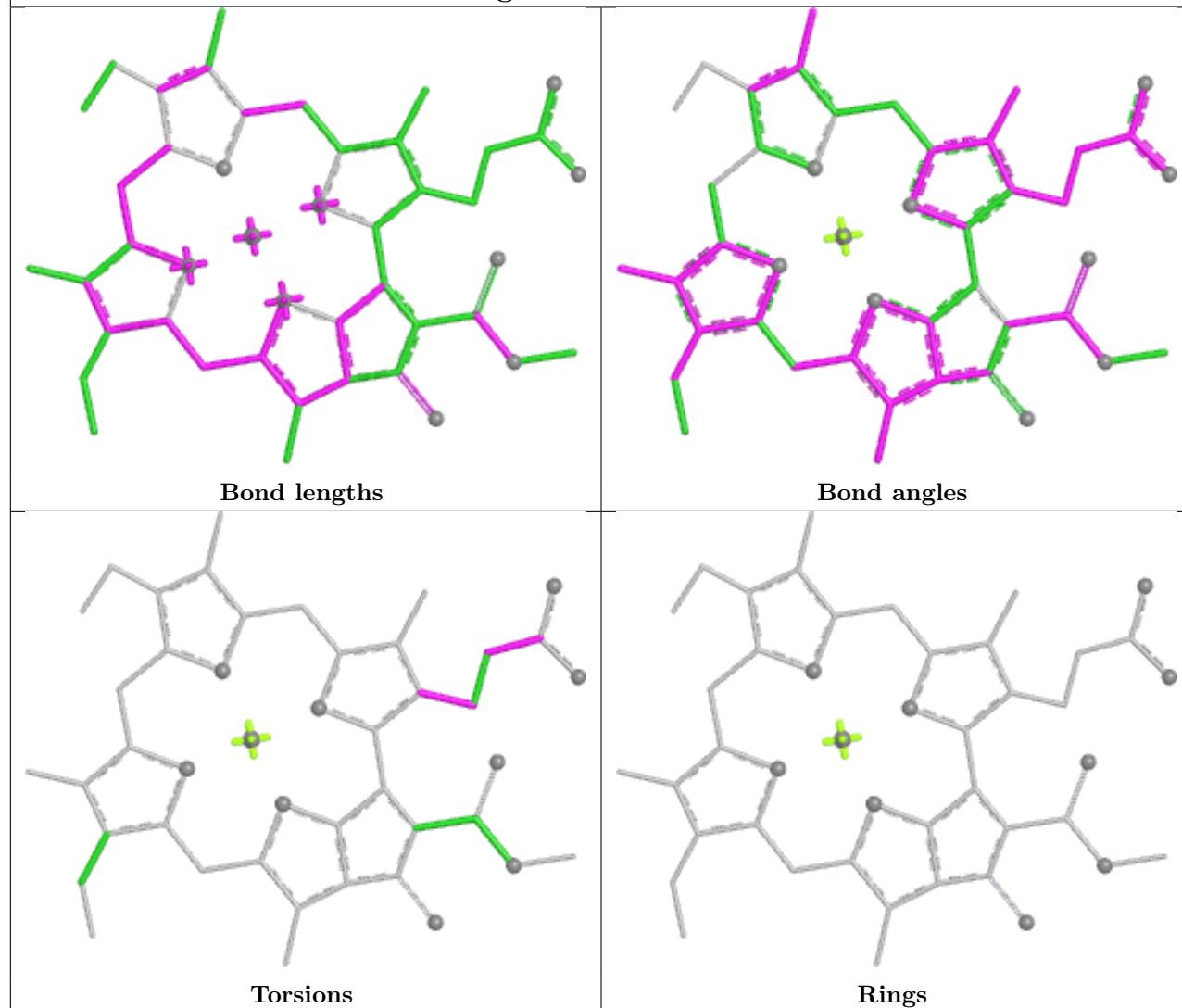




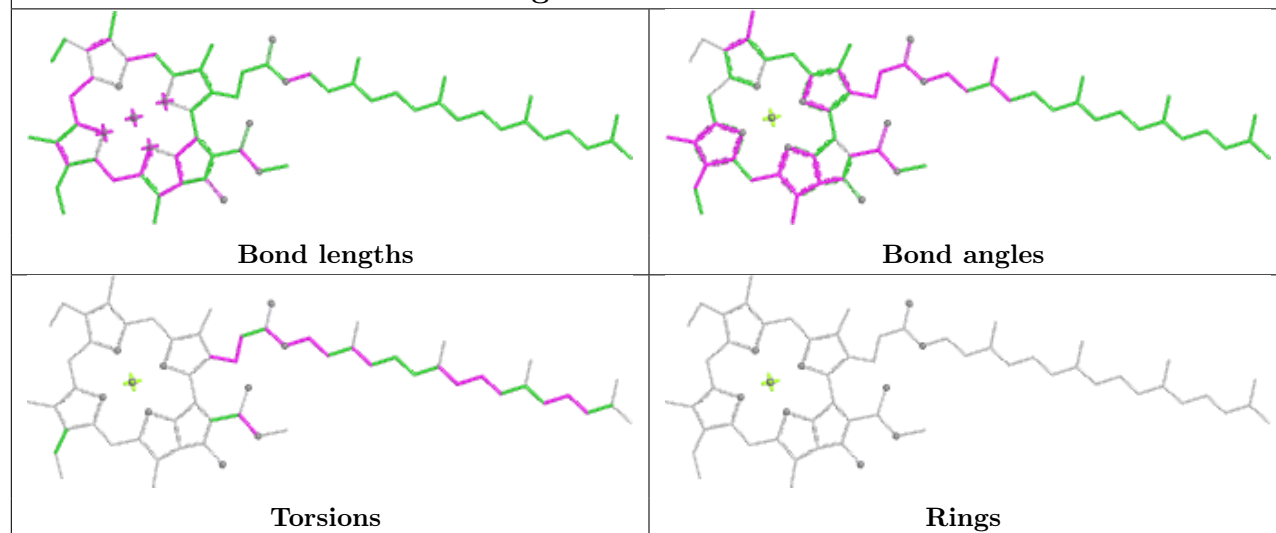
**Ligand CLA B 813****Ligand CLA I 202**

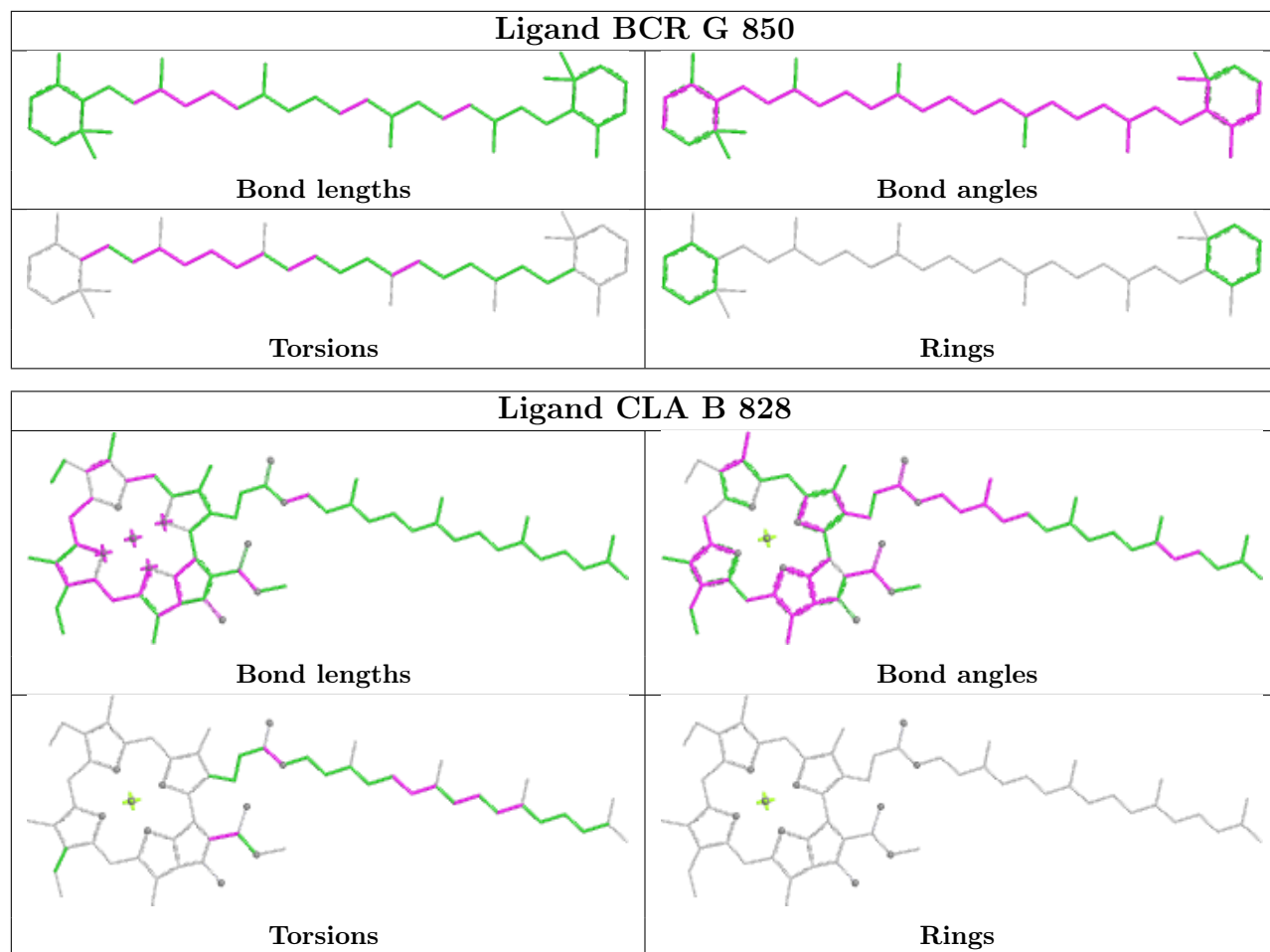


## Ligand CLA a 839

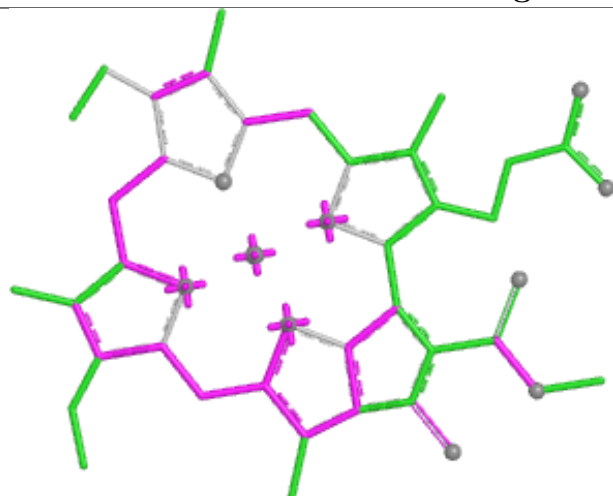


## Ligand CLA A 829

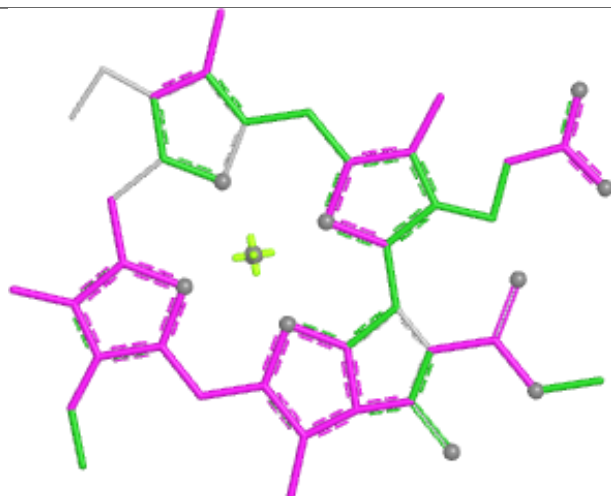




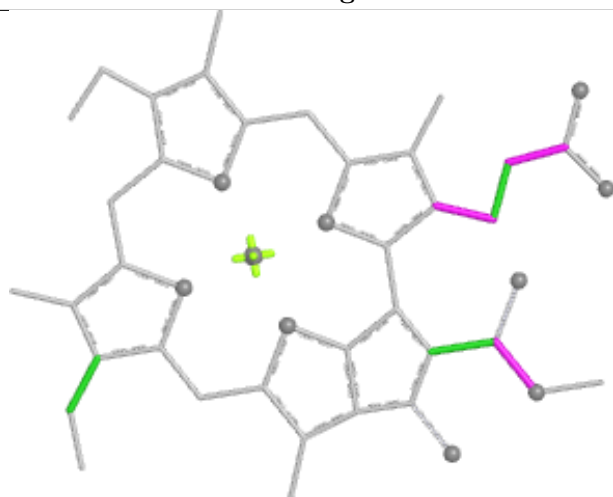
## Ligand CLA H 835



Bond lengths



Bond angles

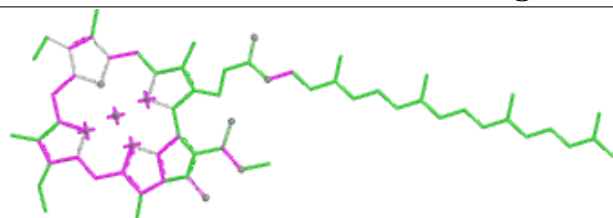


Torsions

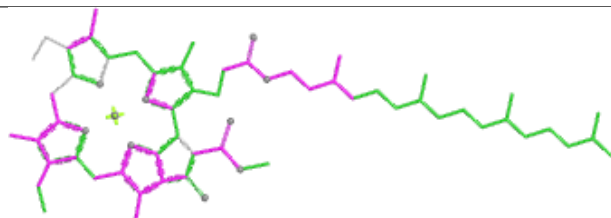


Rings

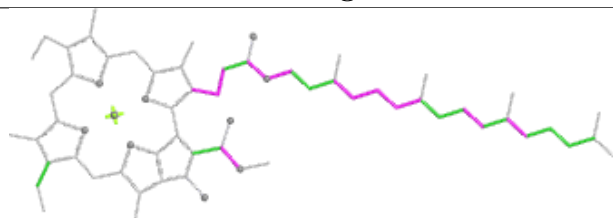
## Ligand CLA U 206



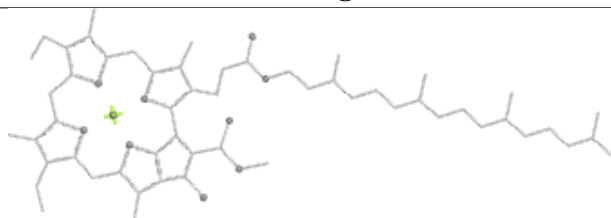
Bond lengths



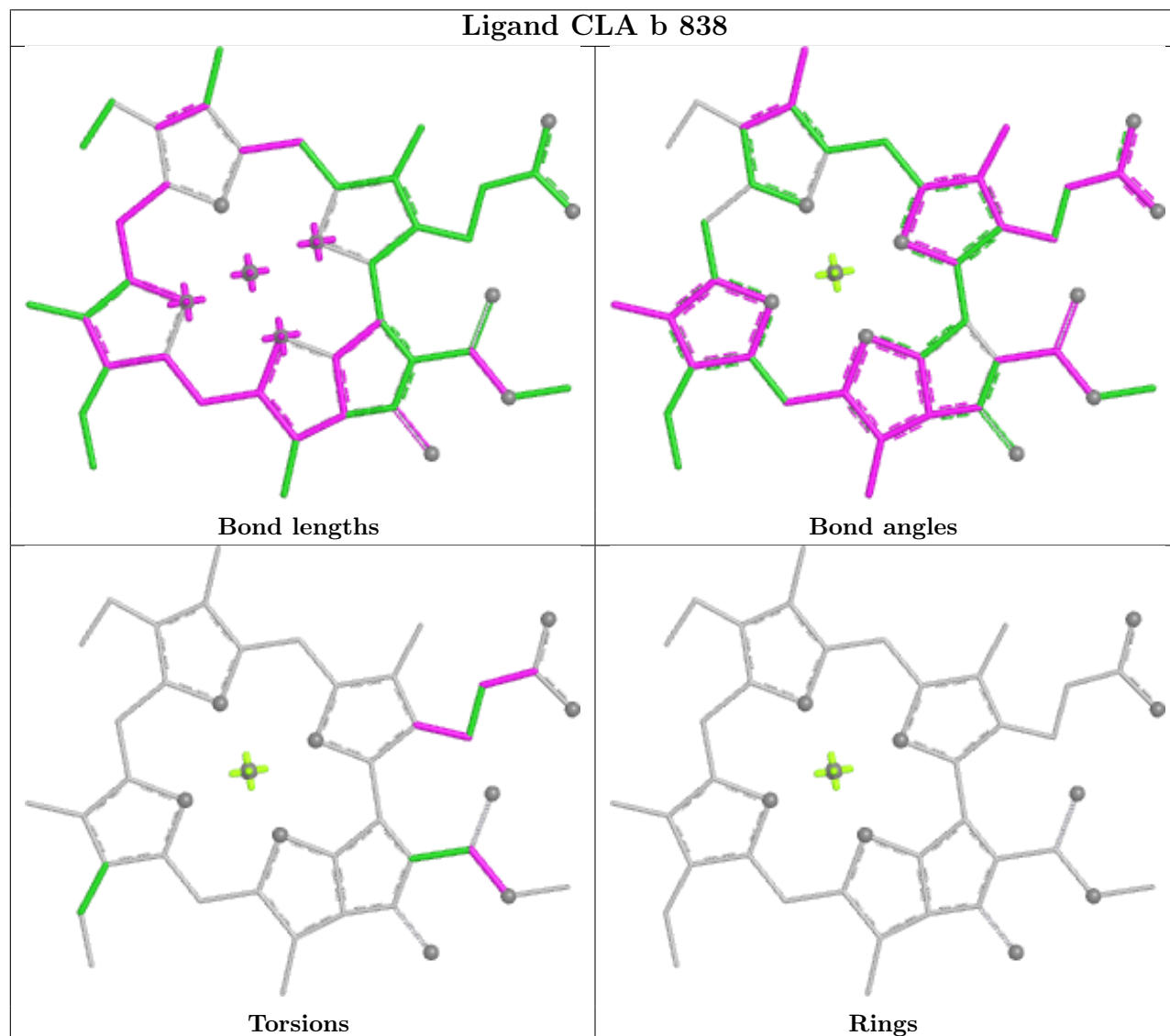
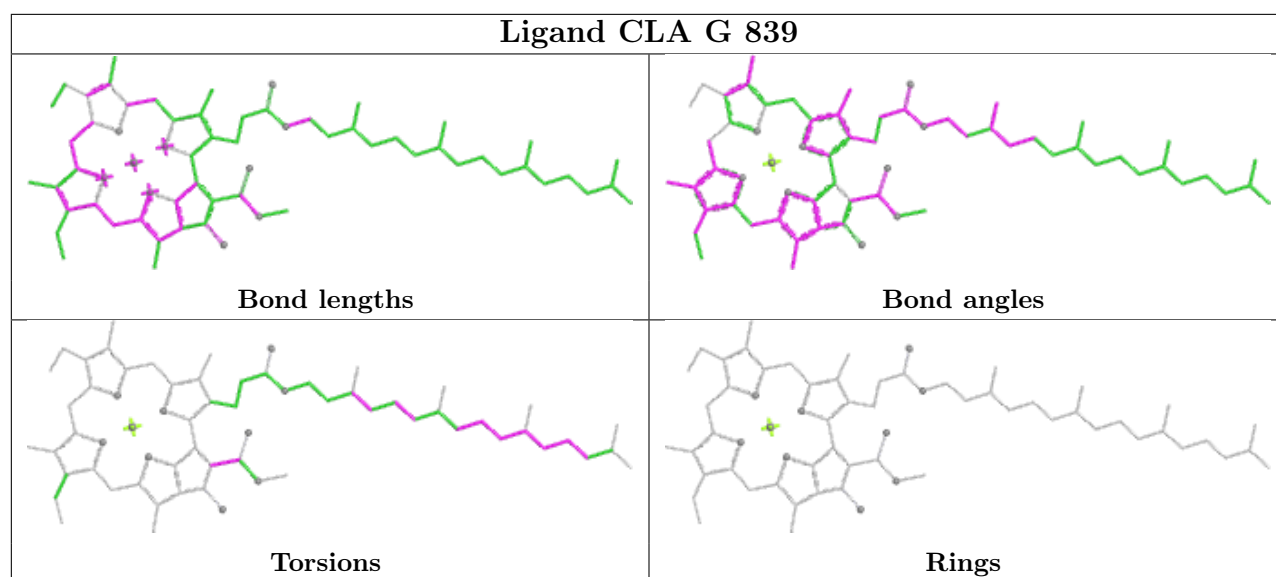
Bond angles



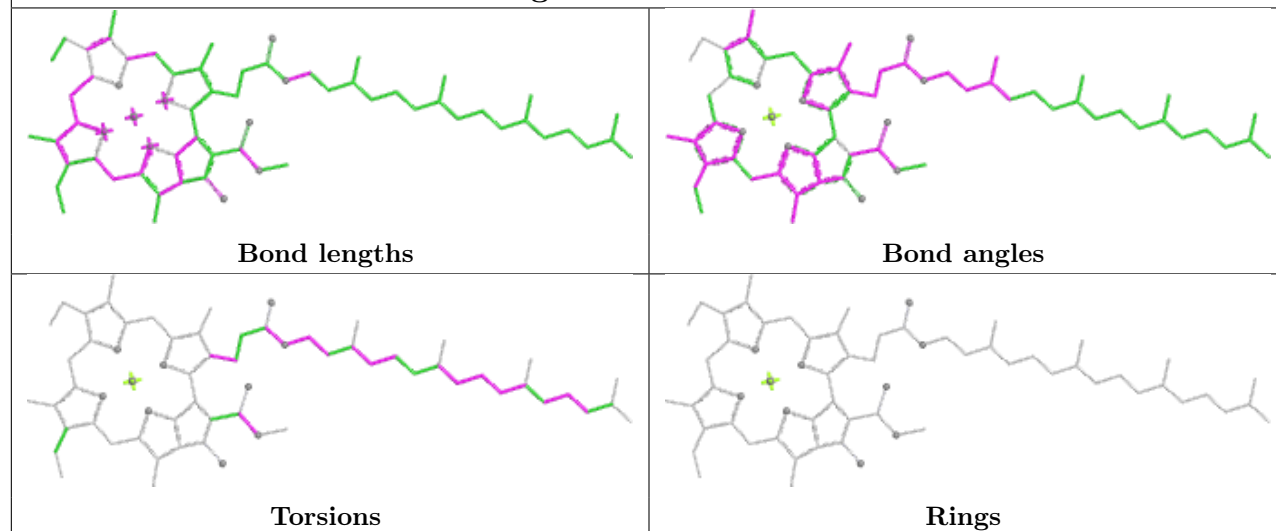
Torsions



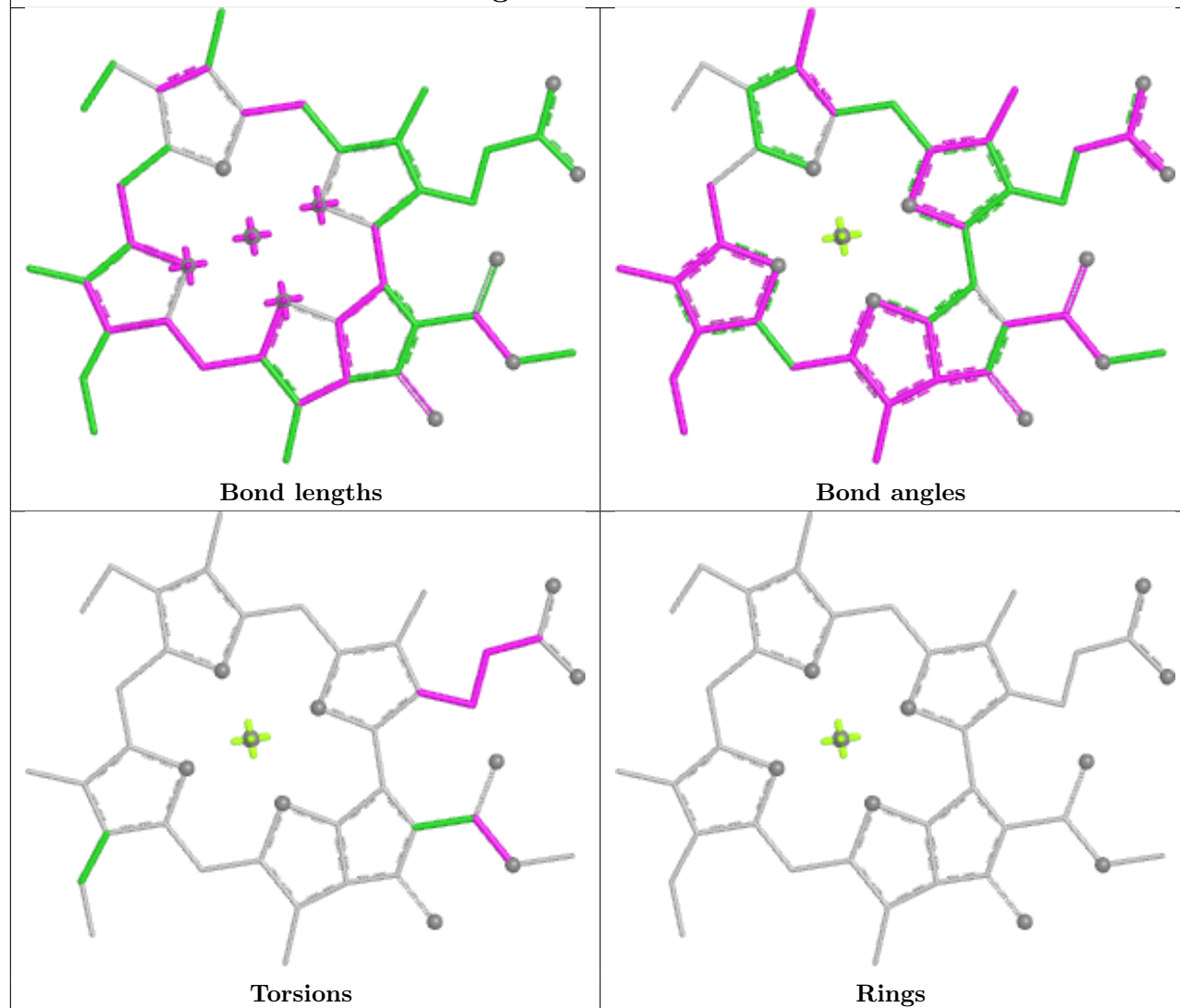
Rings

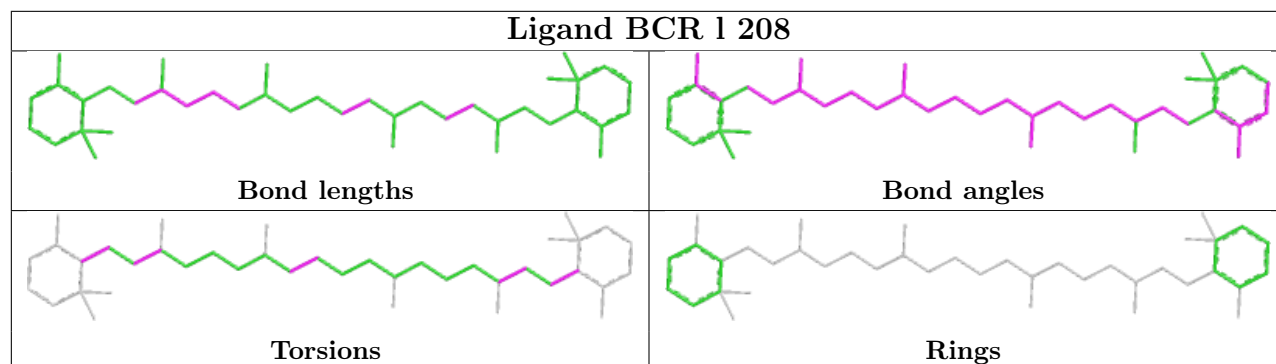
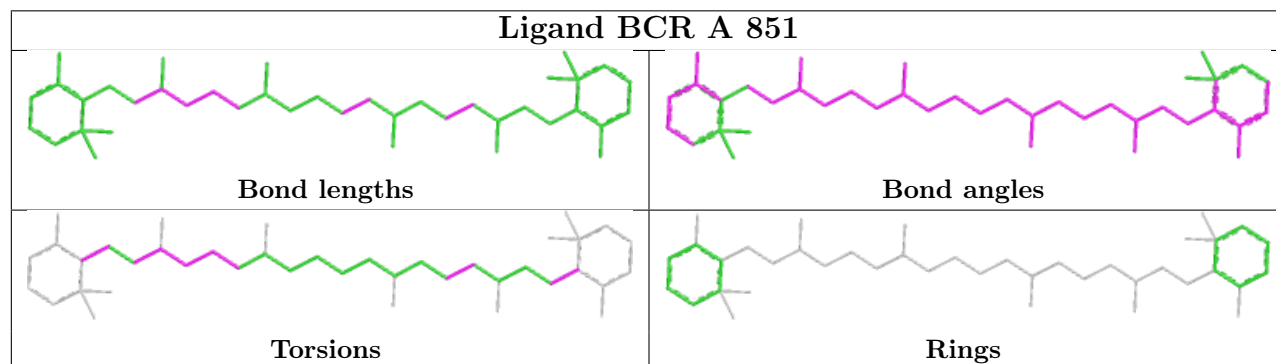
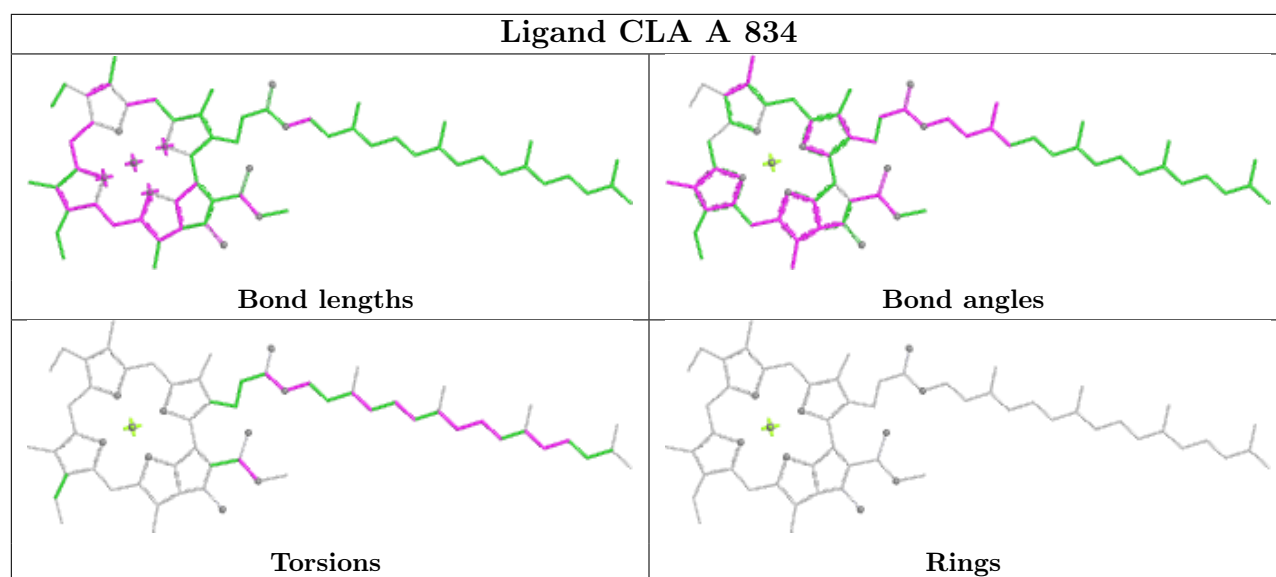


## Ligand CLA G 829

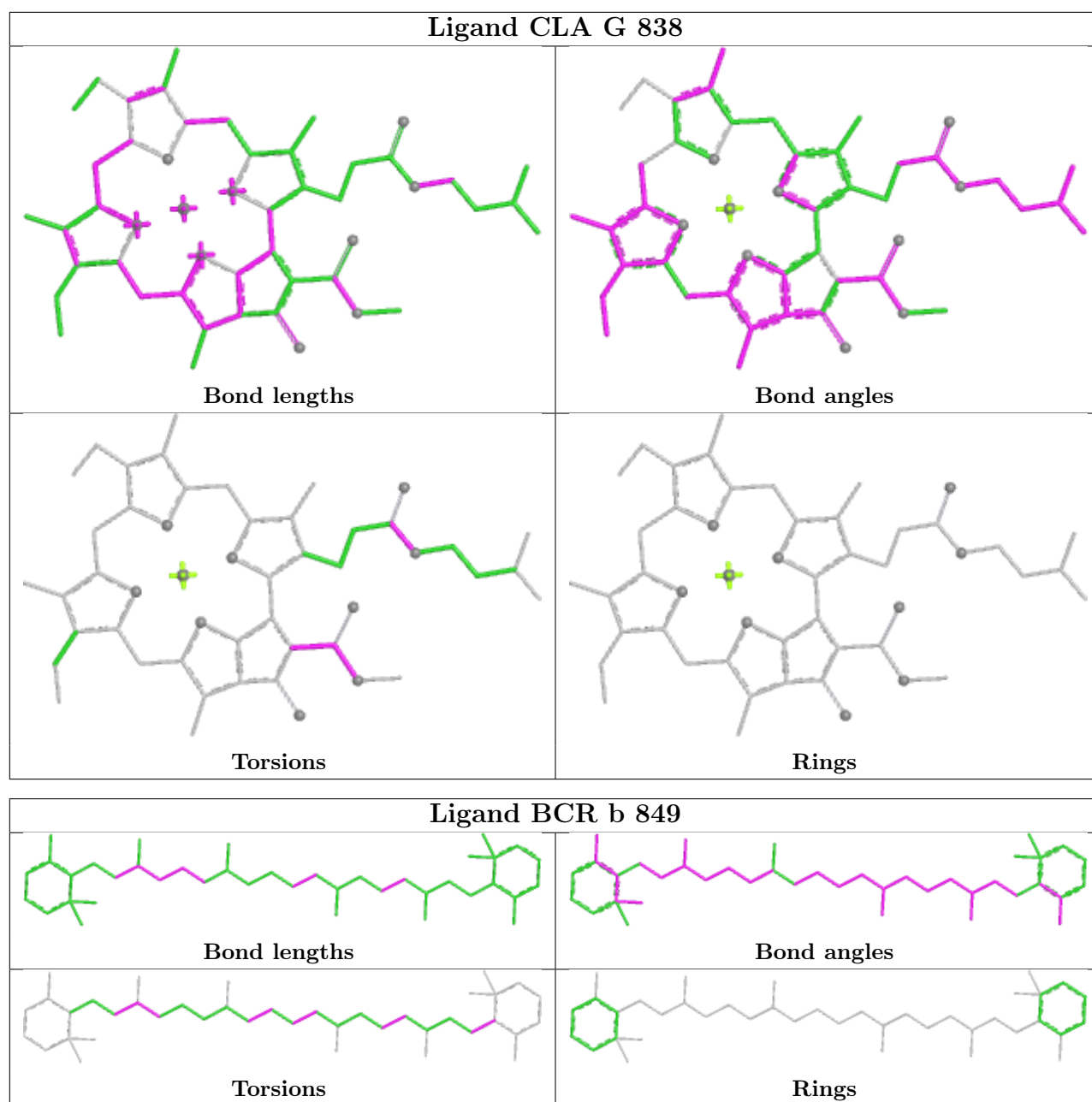


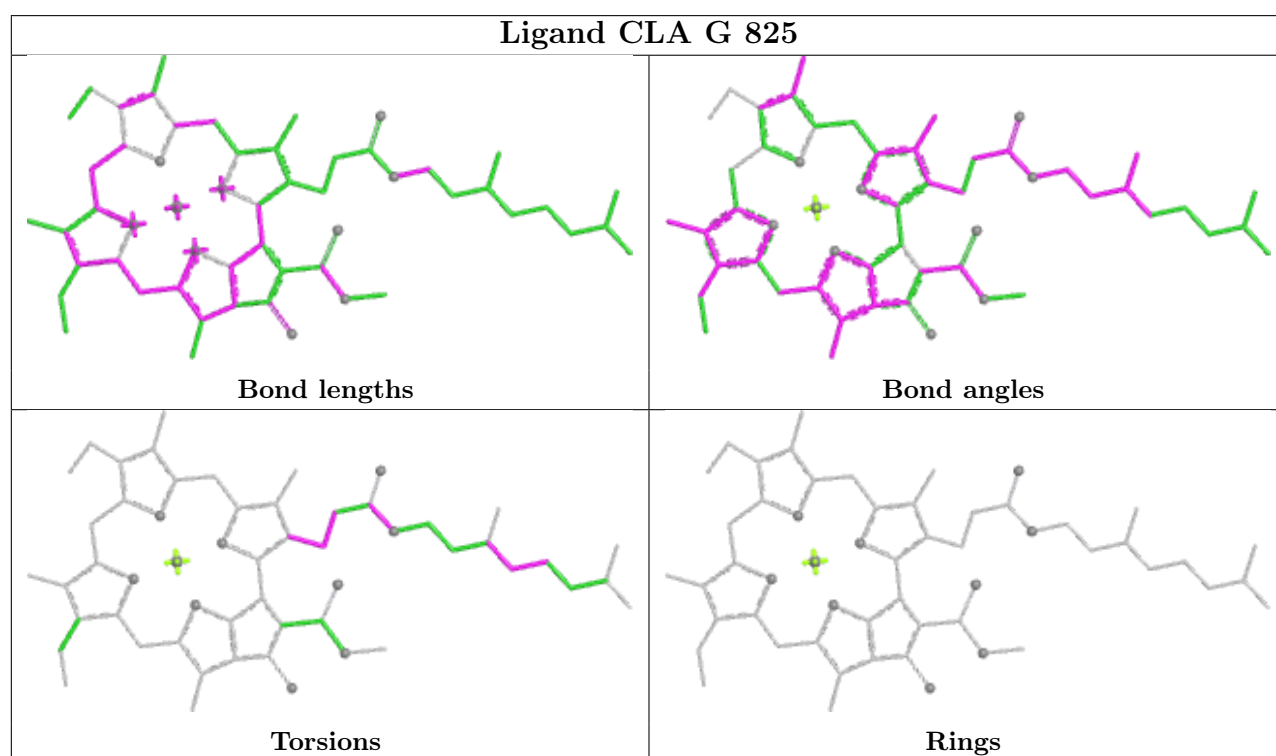
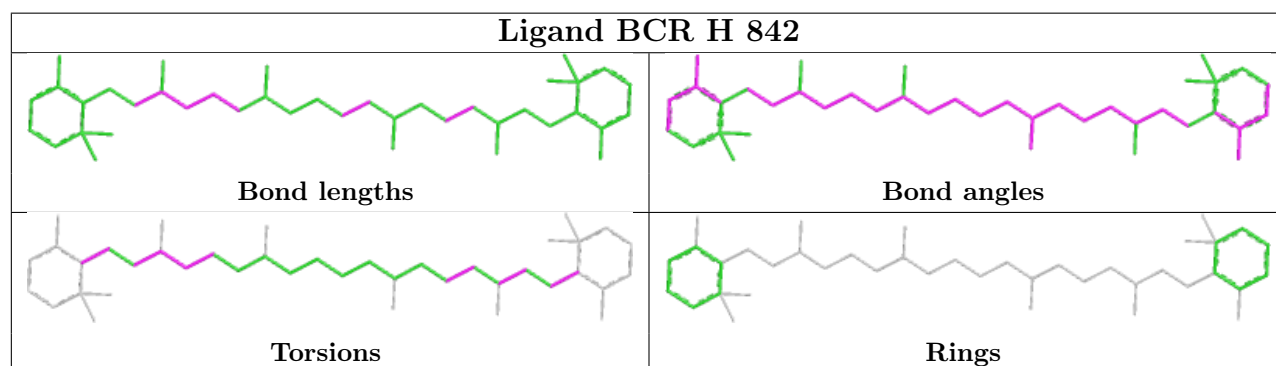
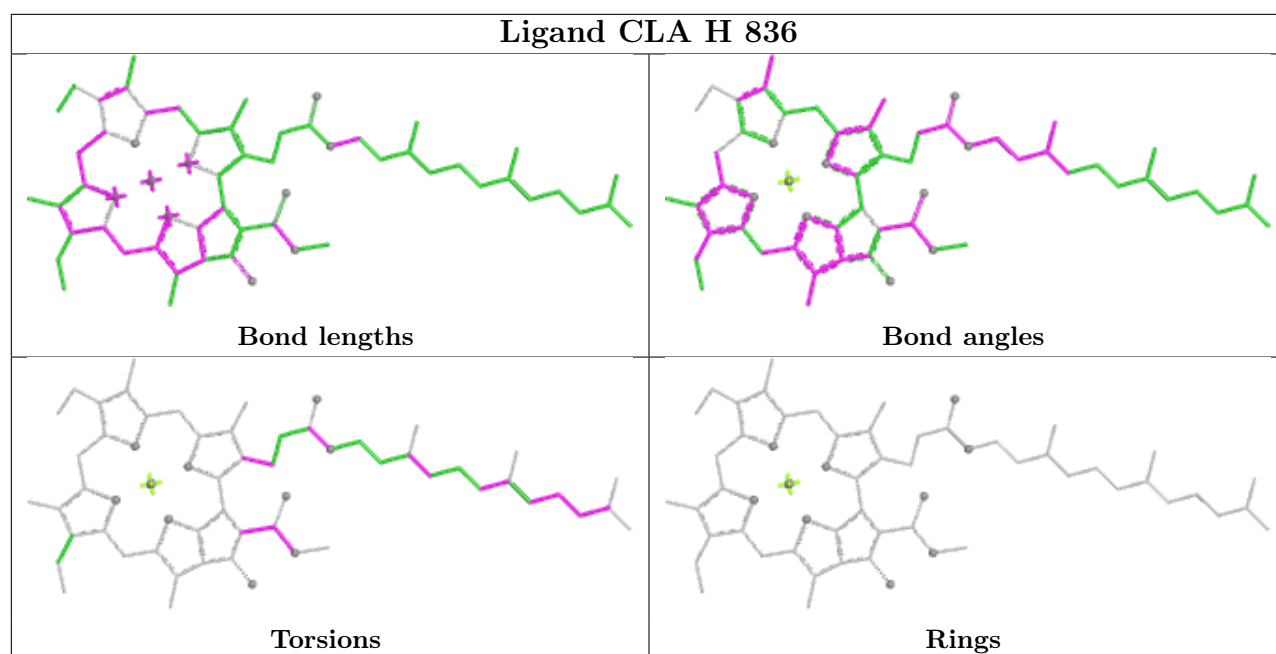
## Ligand CLA B 829



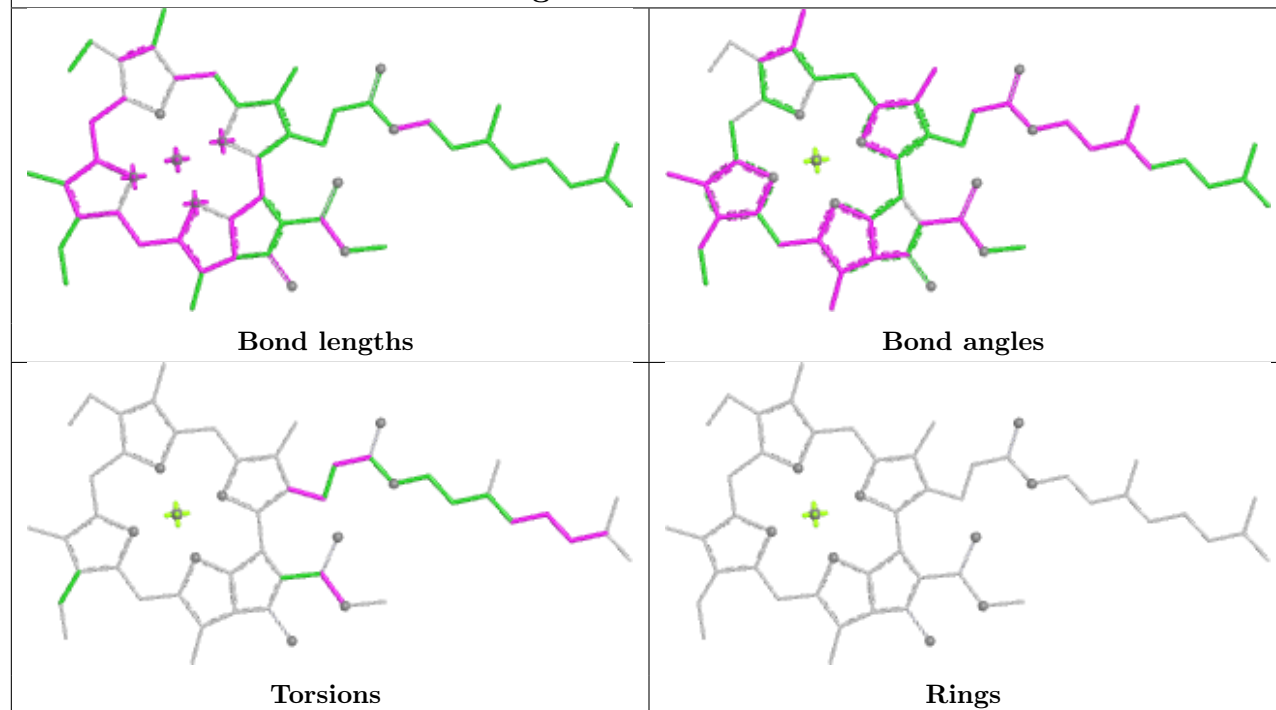




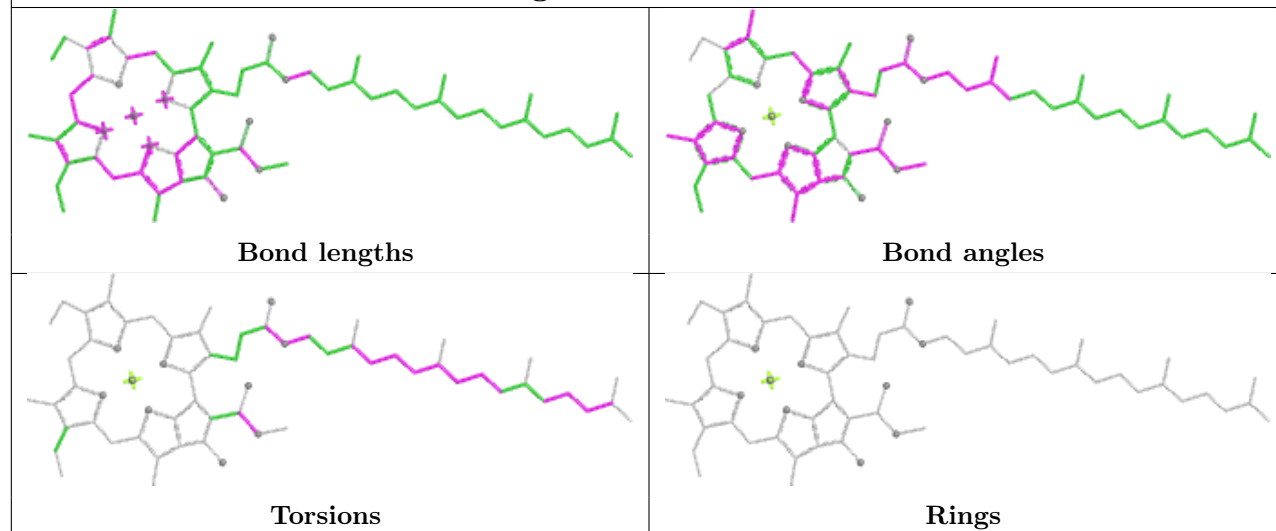




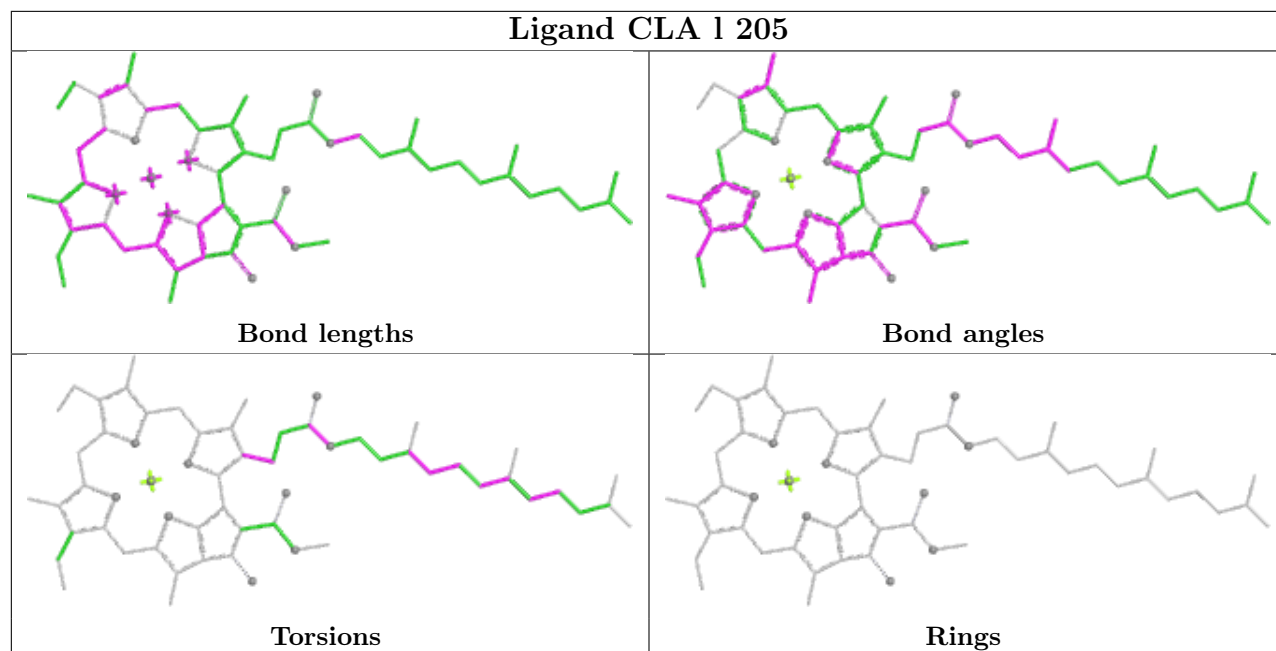
## Ligand CLA B 821



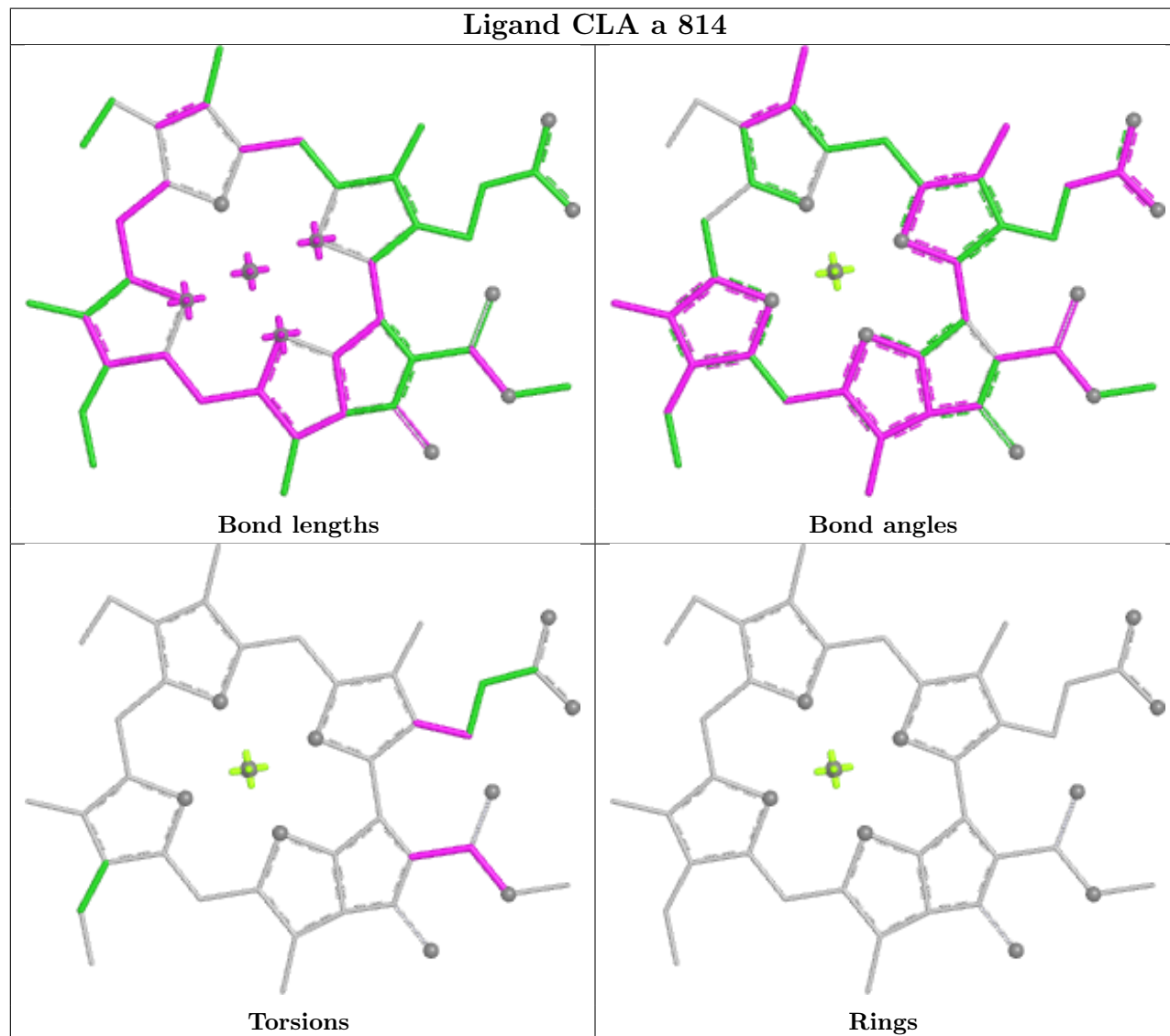
## Ligand CLA H 806



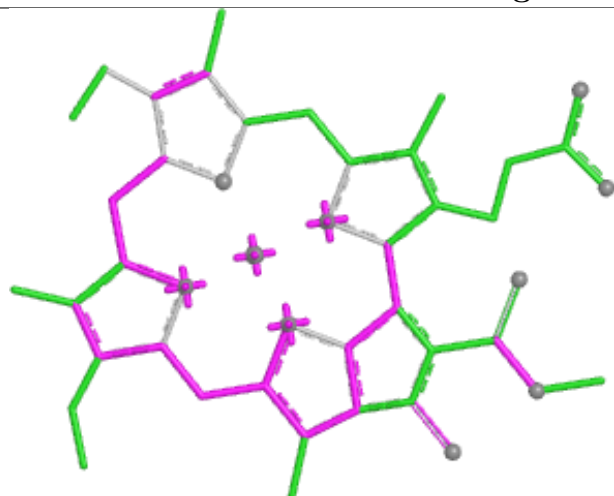
## Ligand CLA 1 205



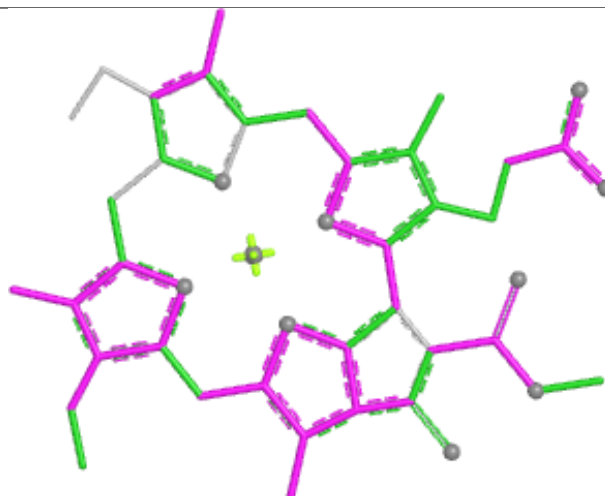
## Ligand CLA a 814



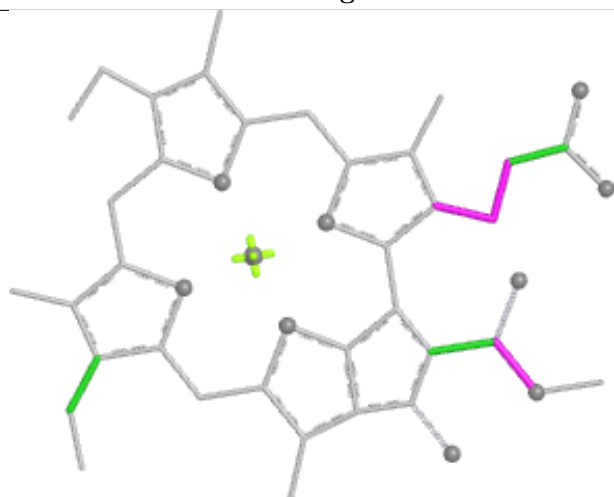
## Ligand CLA G 836



Bond lengths



Bond angles

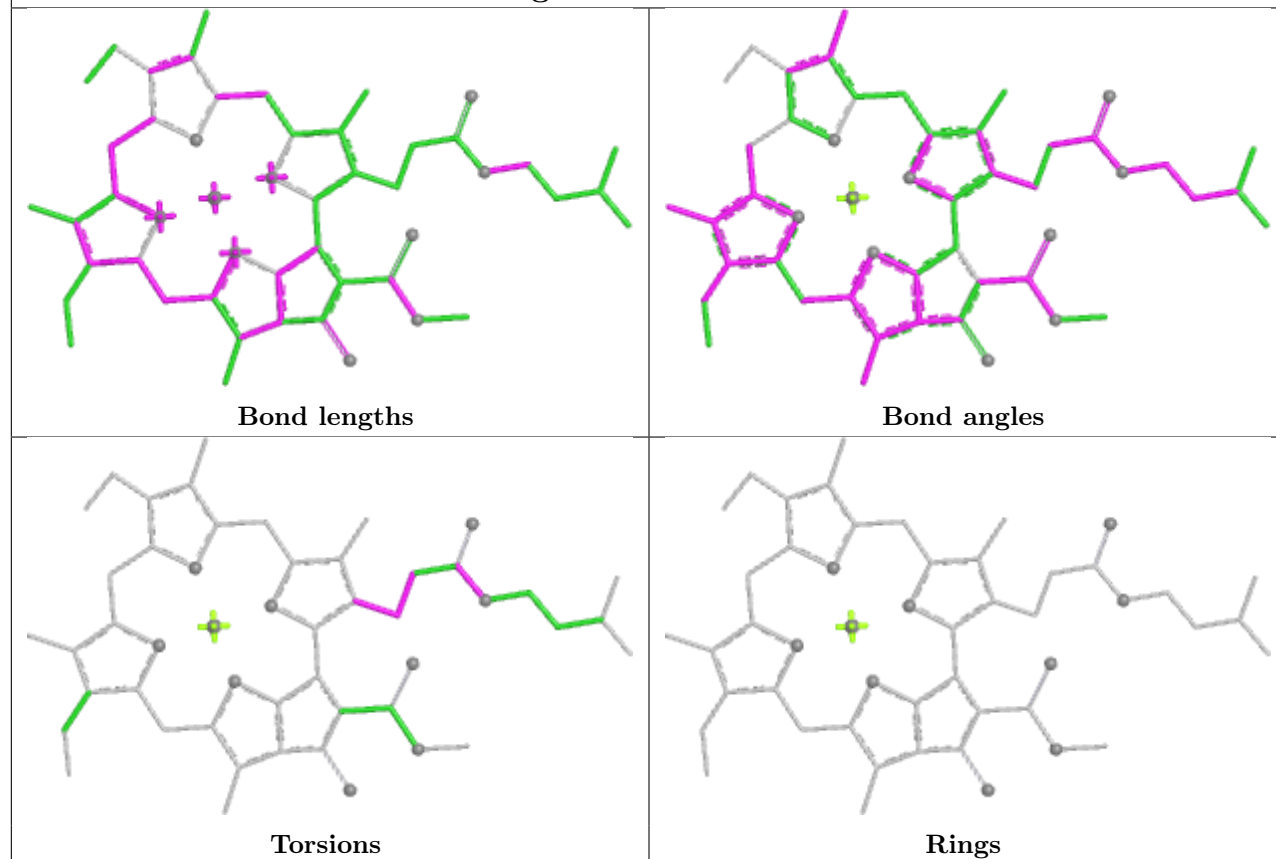


Torsions

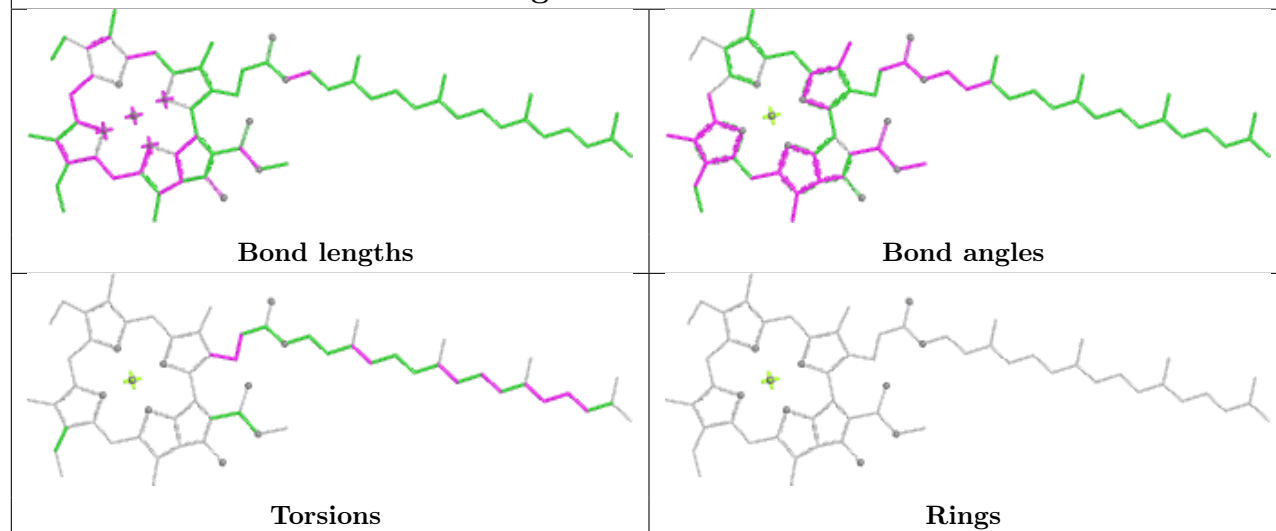


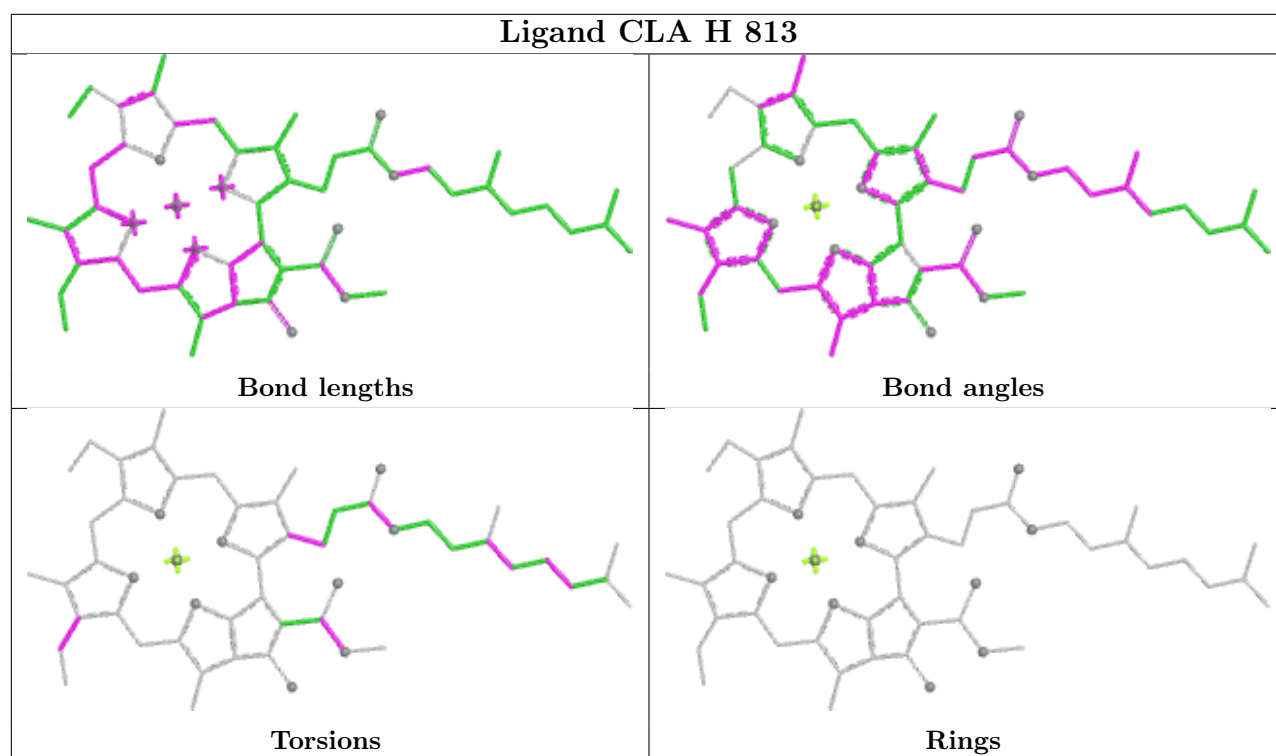
Rings

## Ligand CLA A 813

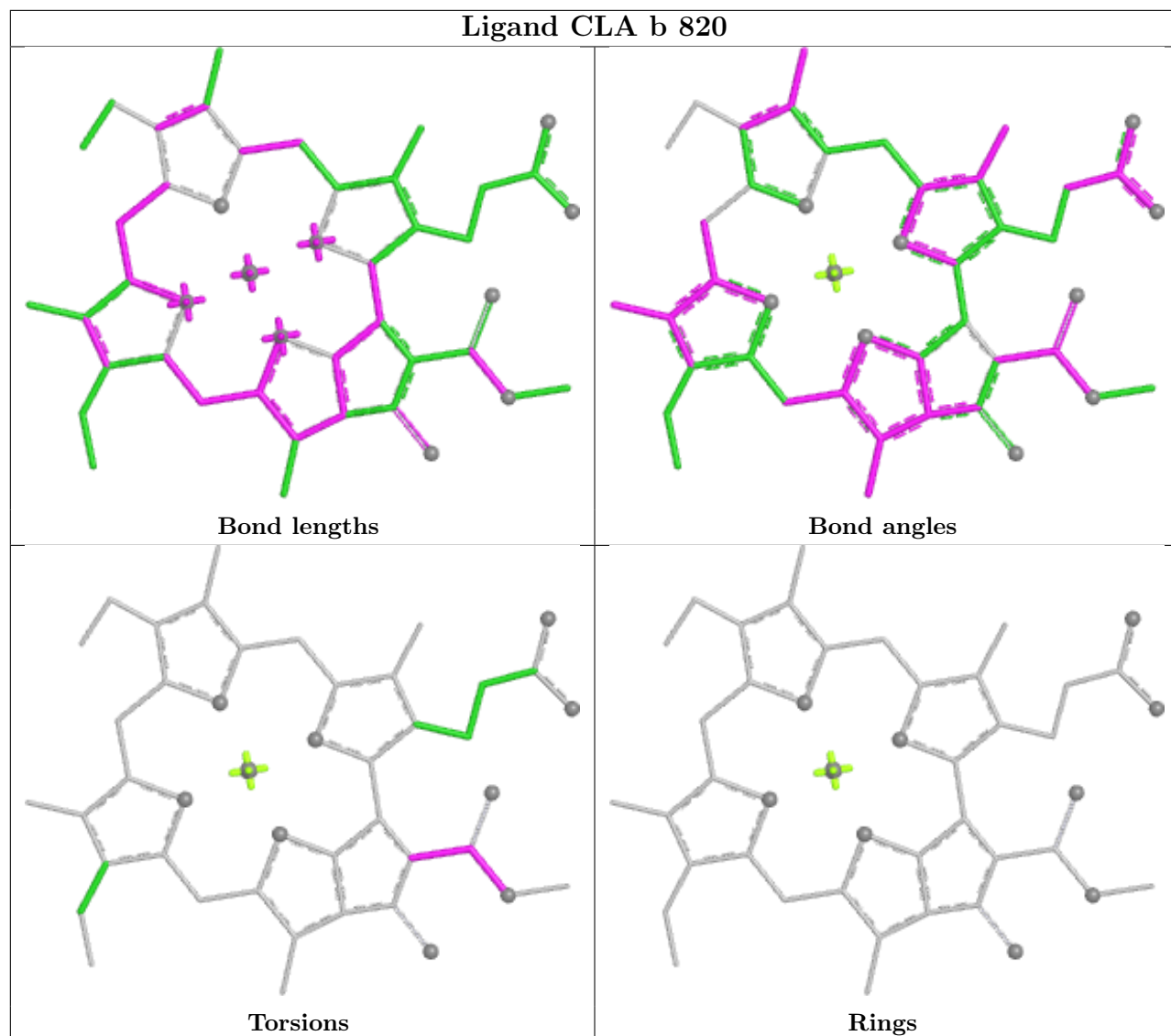


## Ligand CLA H 827

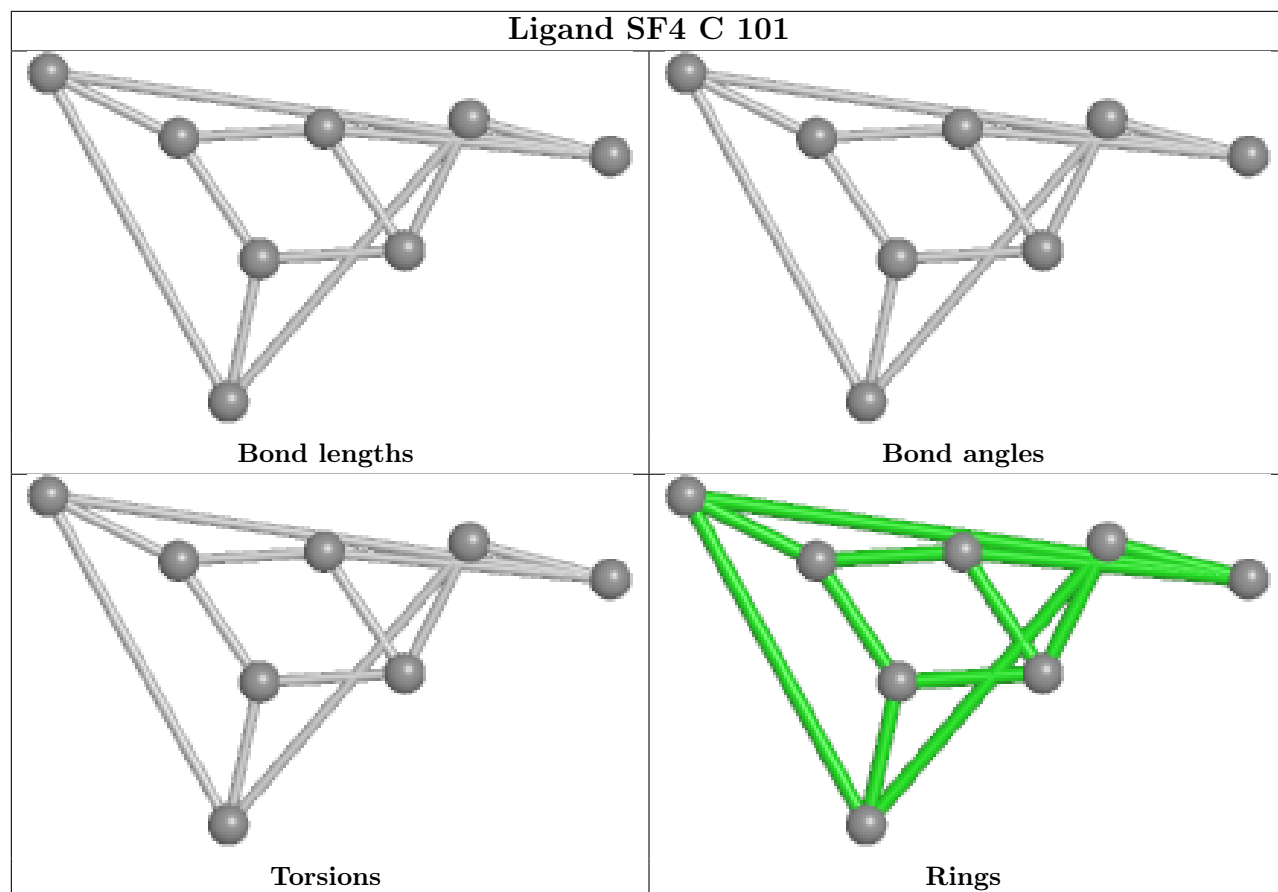




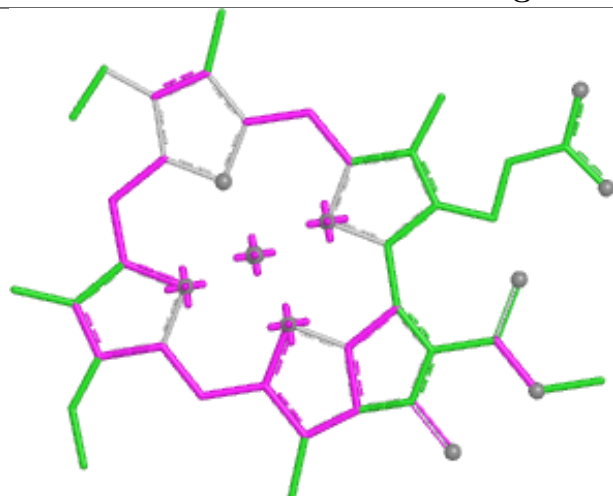
## Ligand CLA b 820



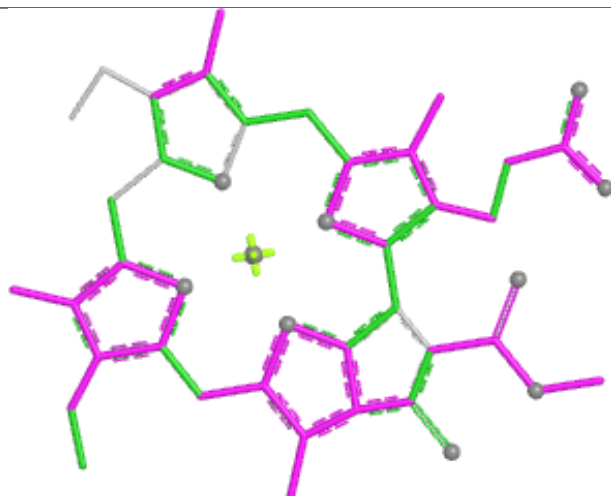




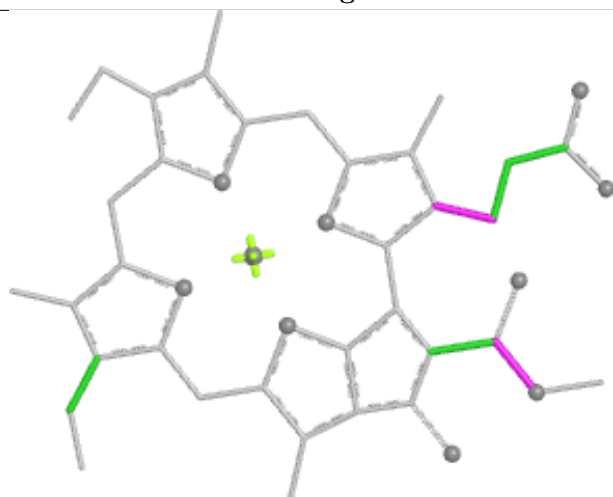
## Ligand CLA H 810



Bond lengths



Bond angles

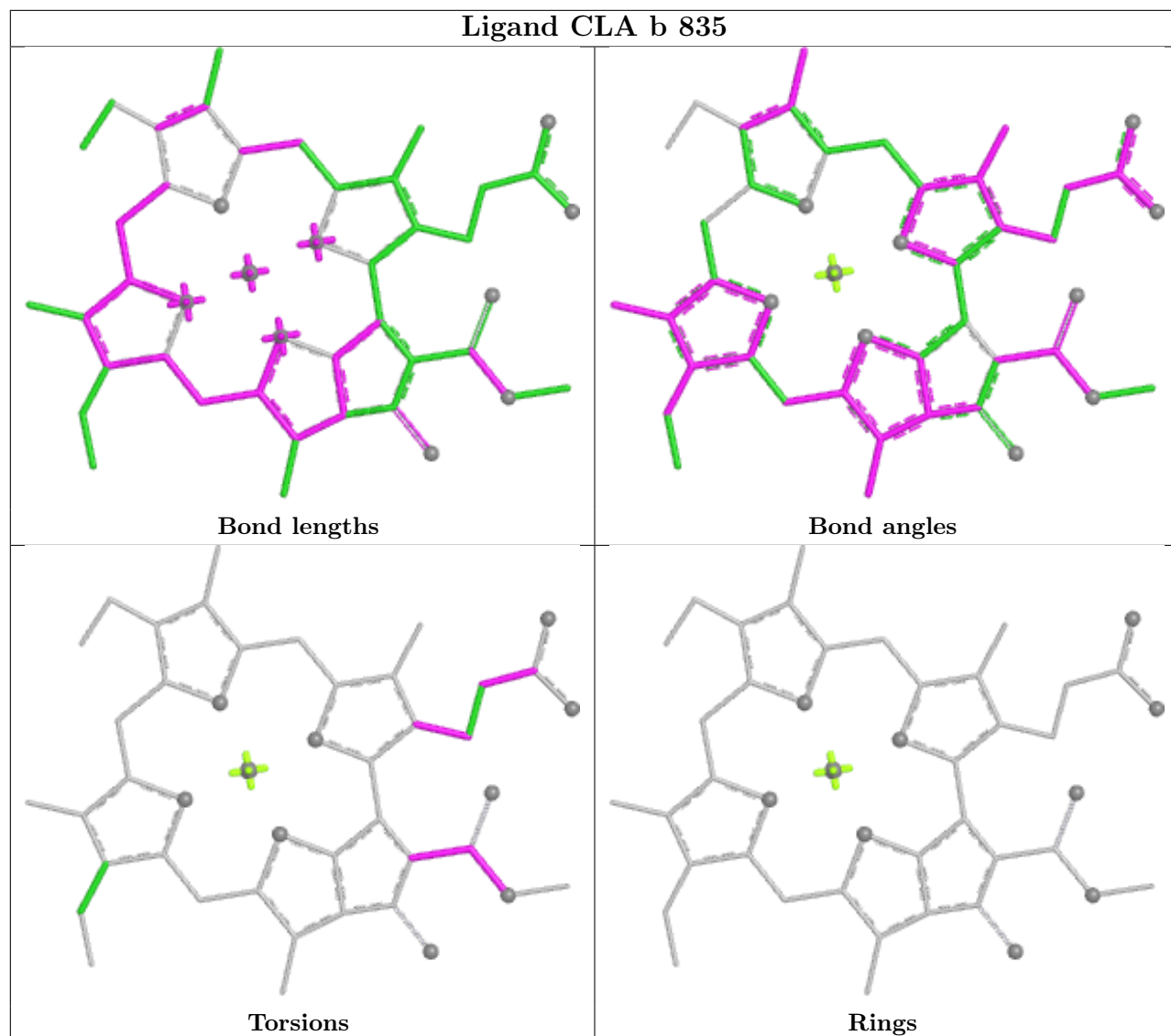


Torsions

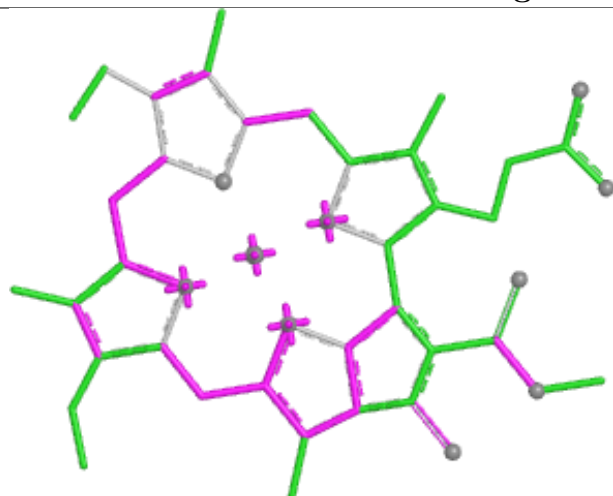


Rings

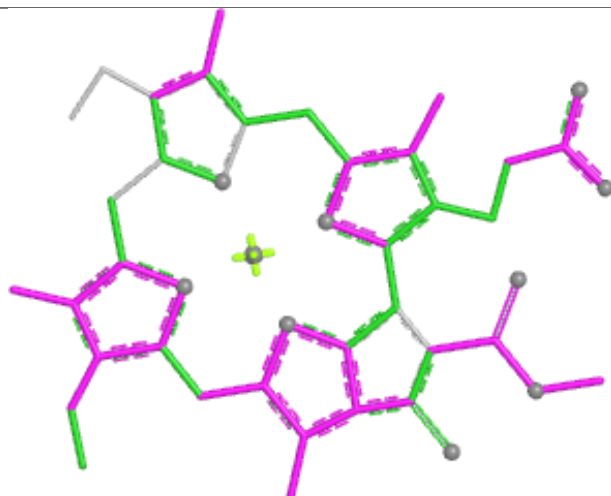
## Ligand CLA b 835



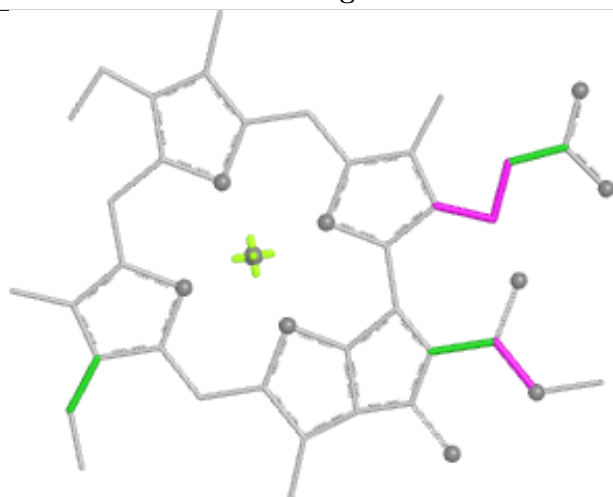
## Ligand CLA A 811



Bond lengths



Bond angles

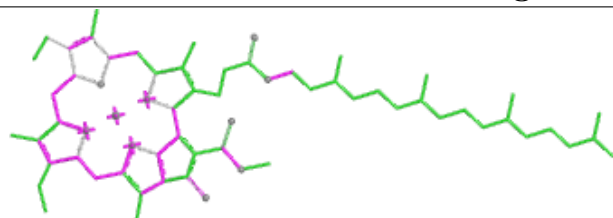


Torsions

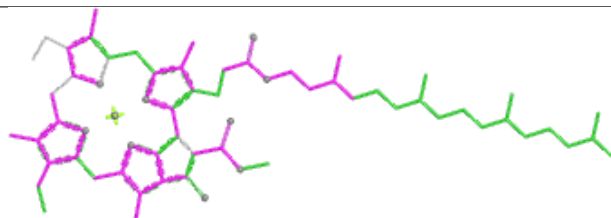


Rings

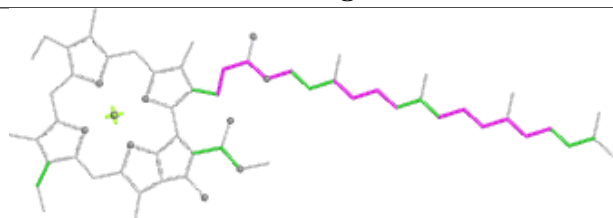
## Ligand CLA G 826



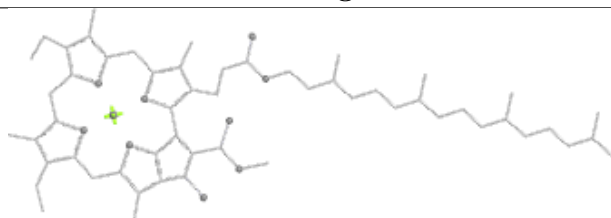
Bond lengths



Bond angles

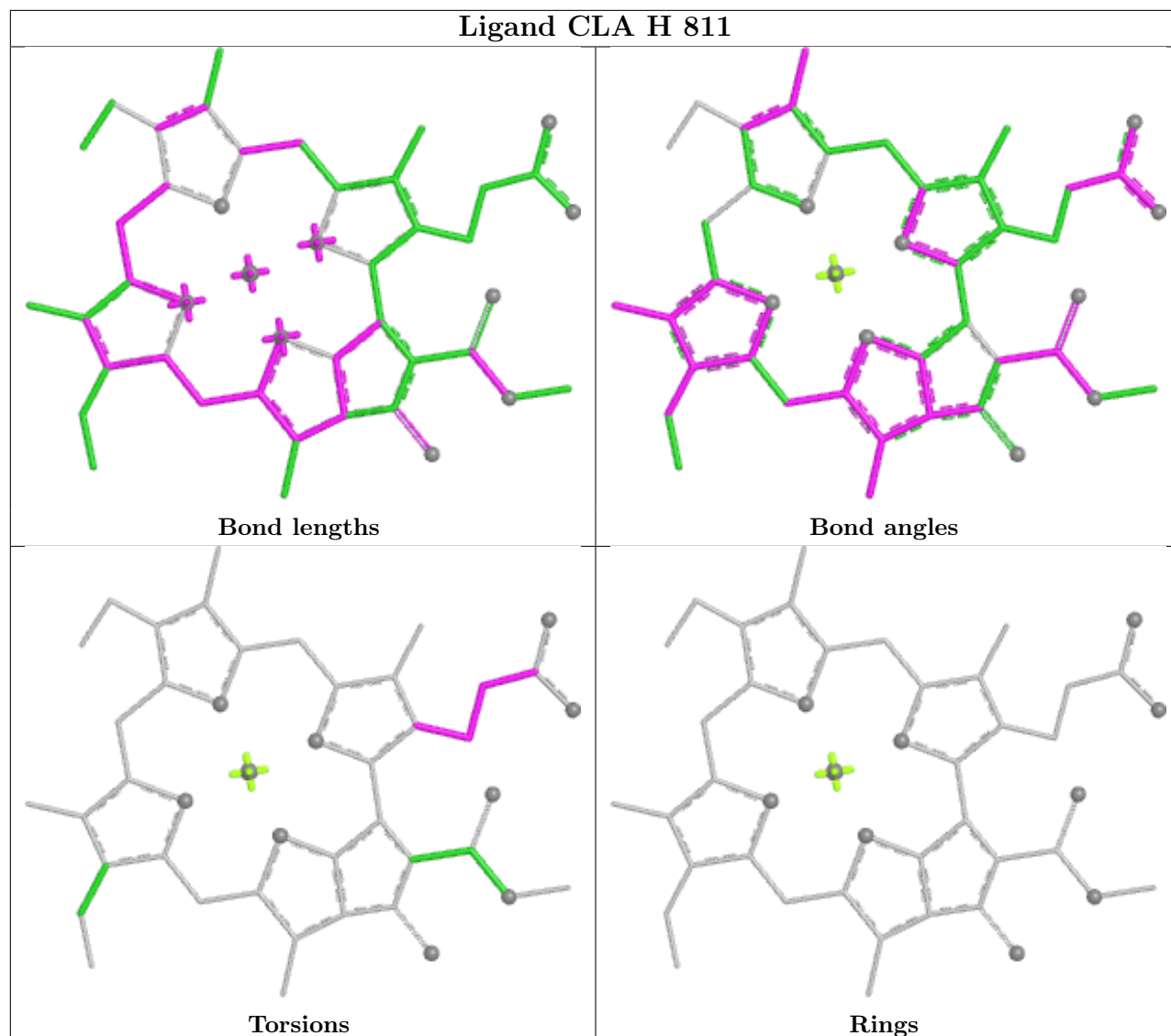


Torsions

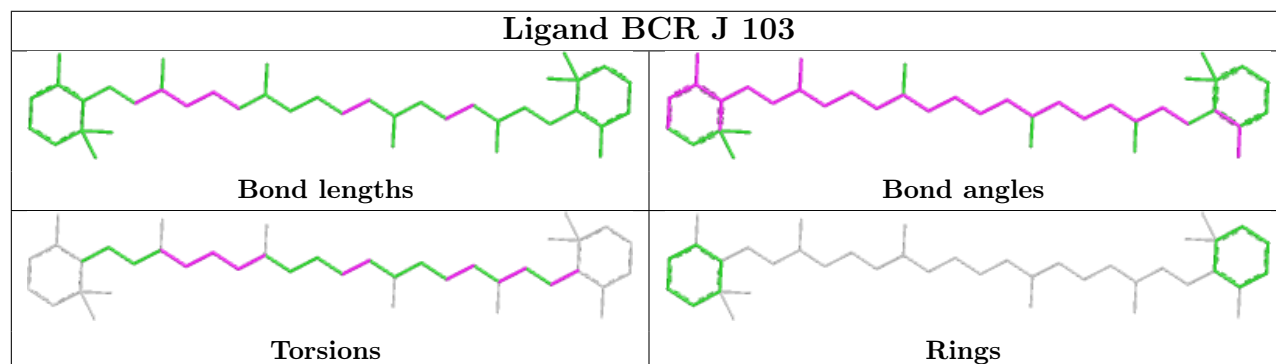


Rings

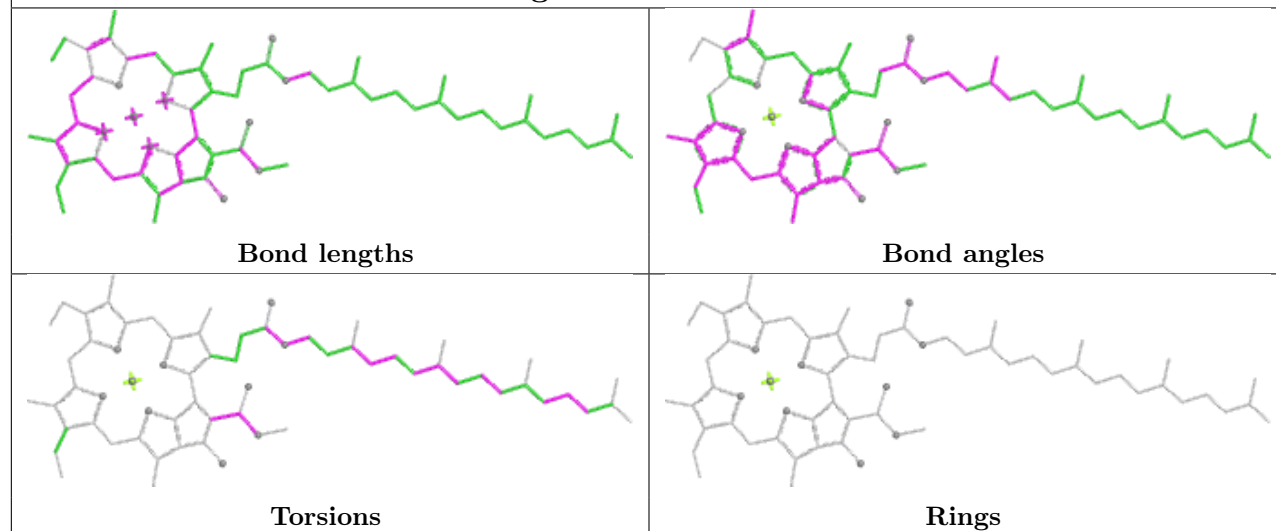
## Ligand CLA H 811



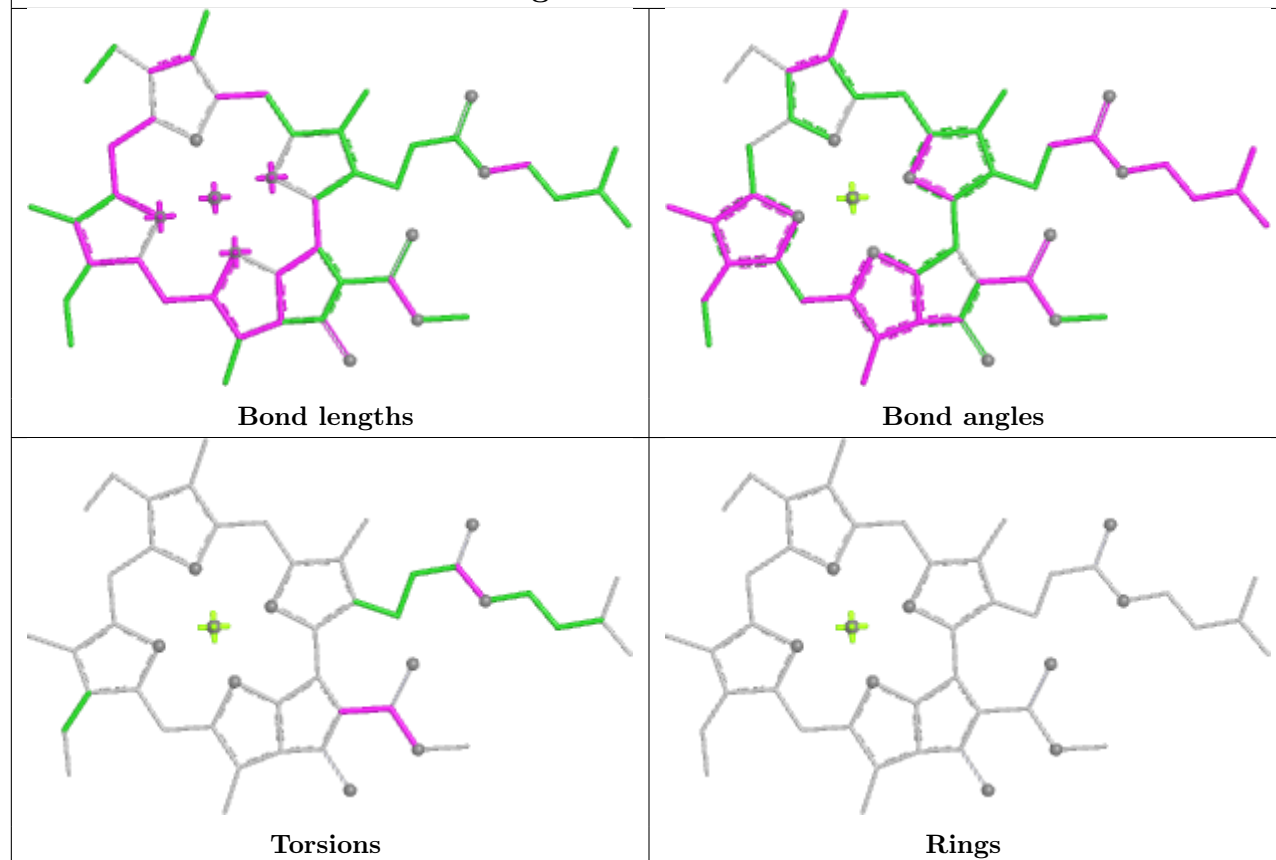
## Ligand BCR J 103

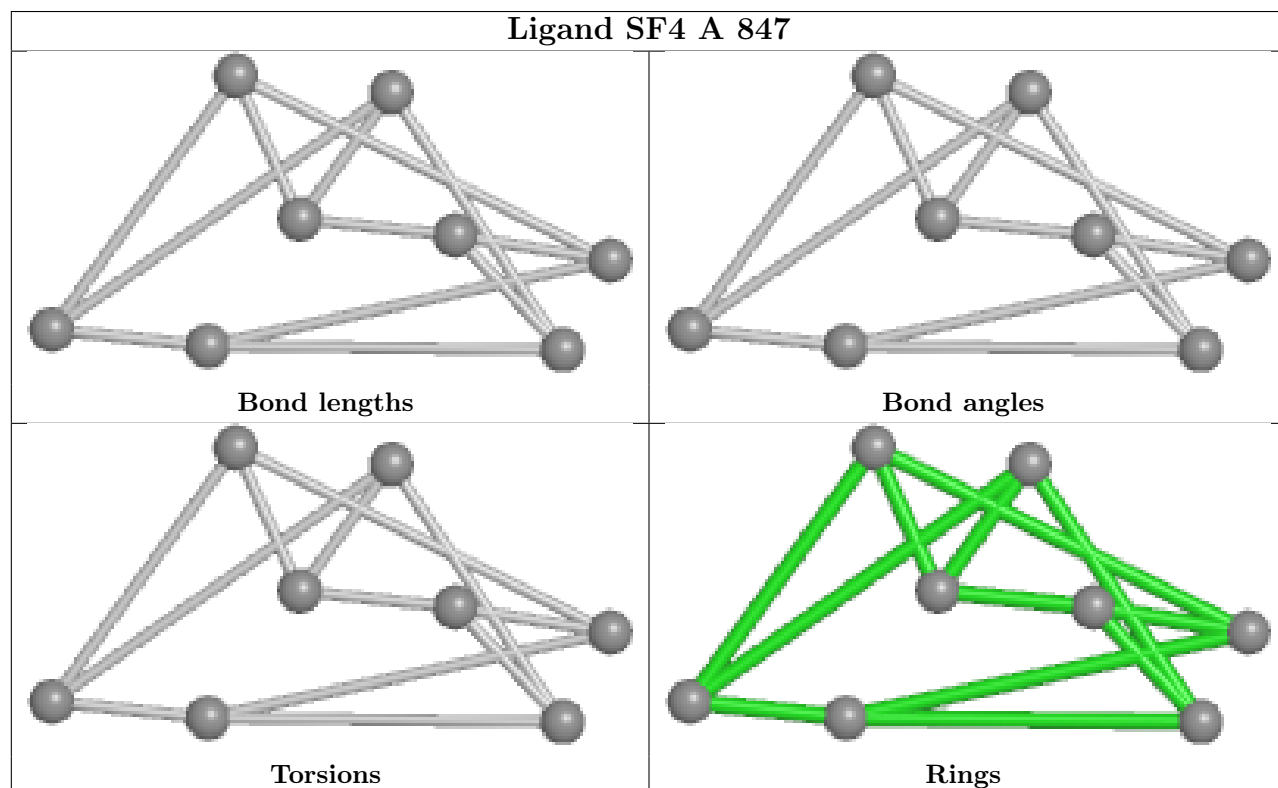
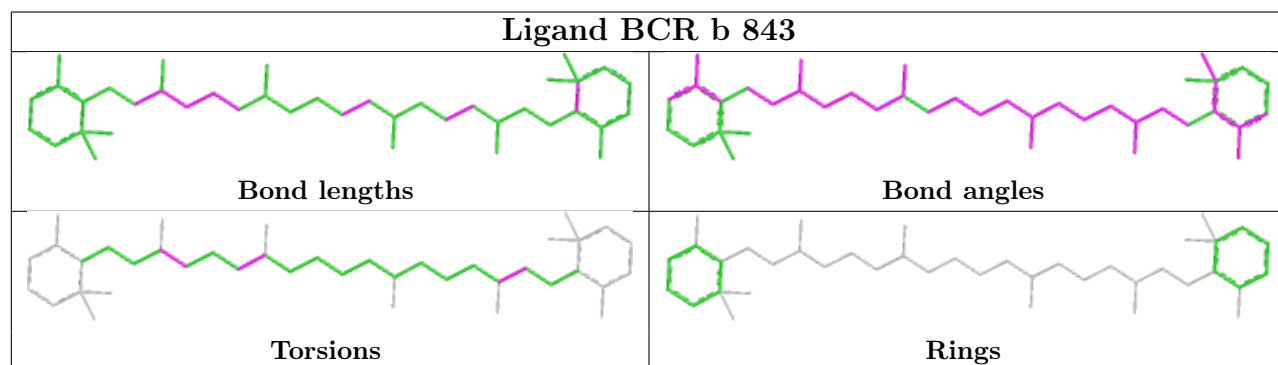
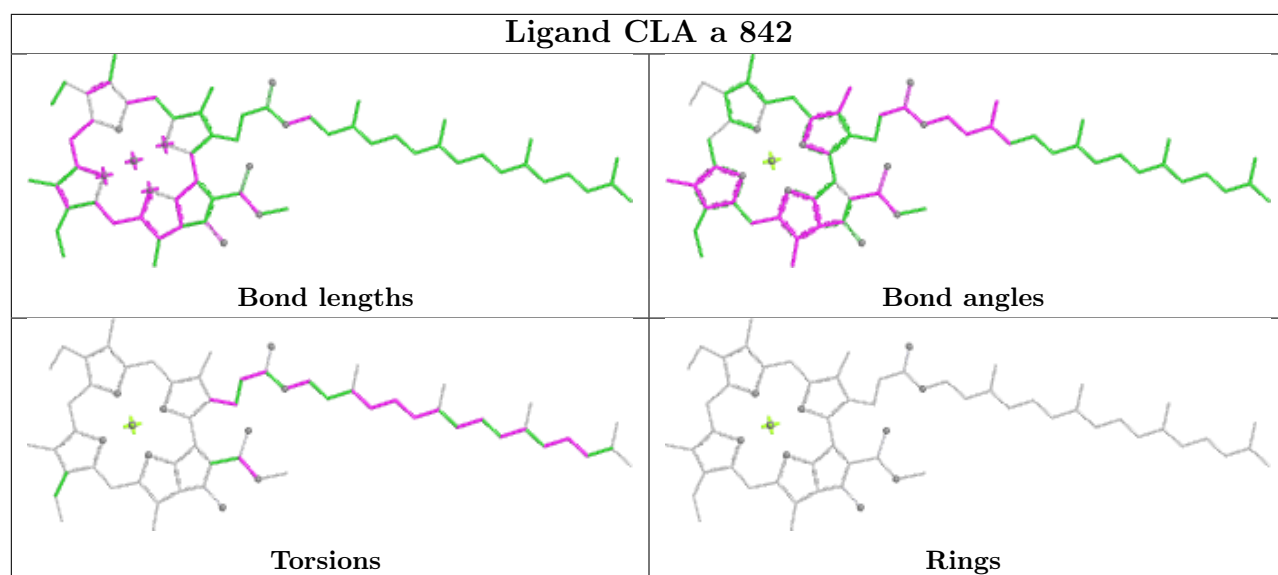


## Ligand CLA G 828

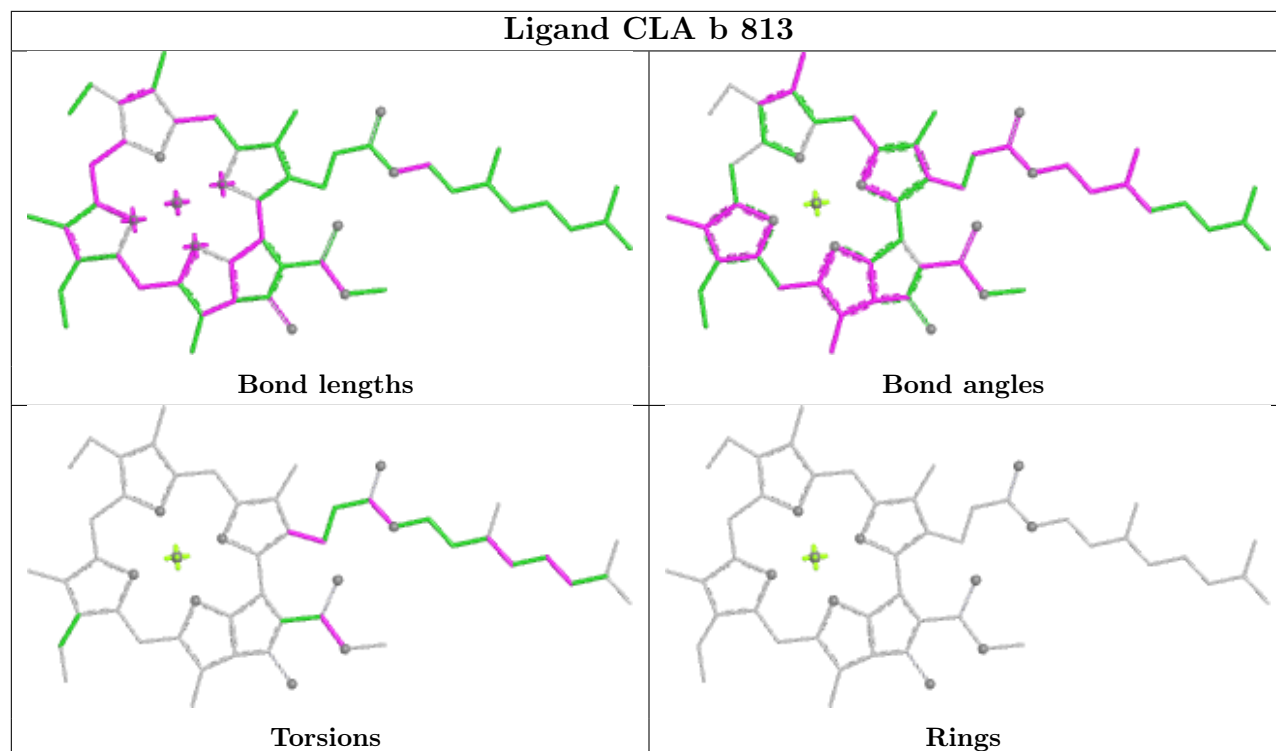


## Ligand CLA A 838

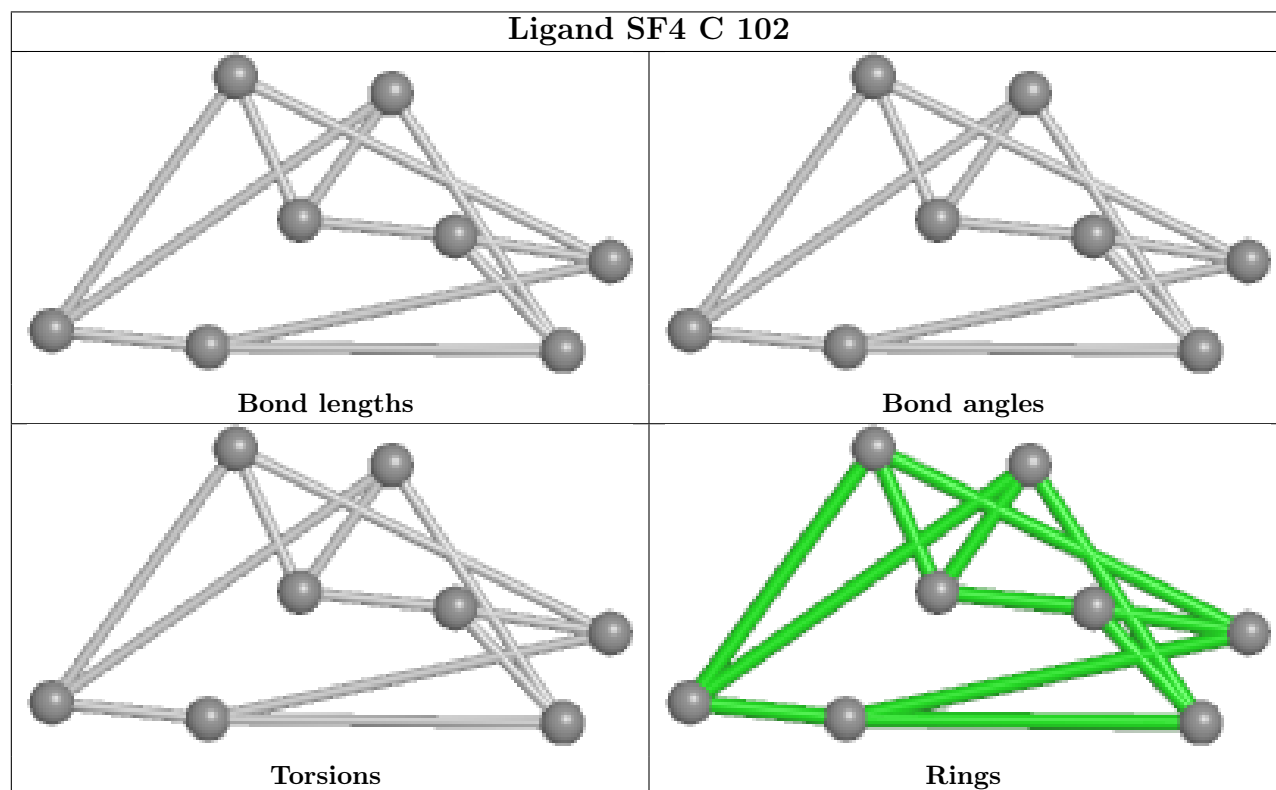




## Ligand CLA b 813

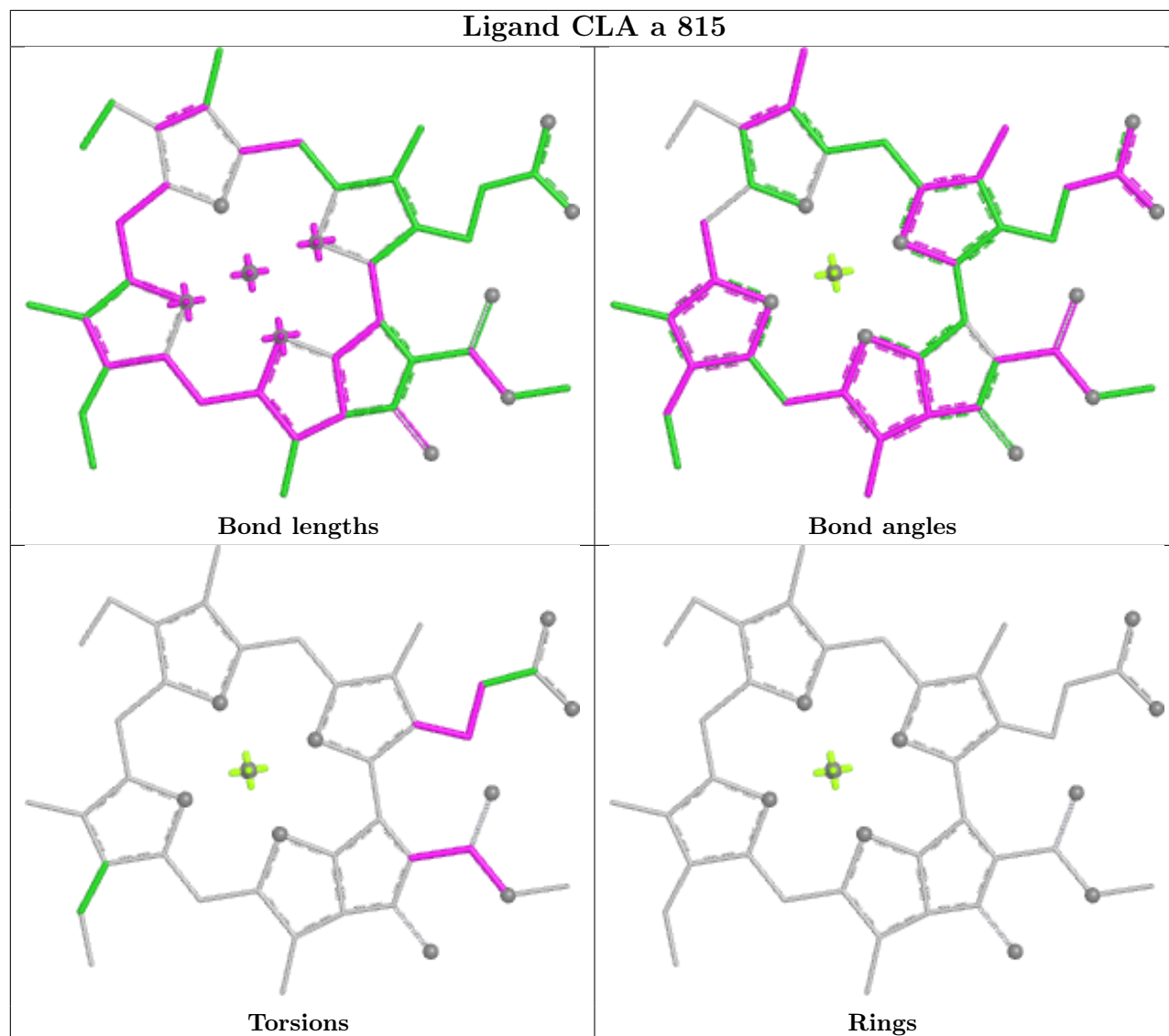


## Ligand SF4 C 102

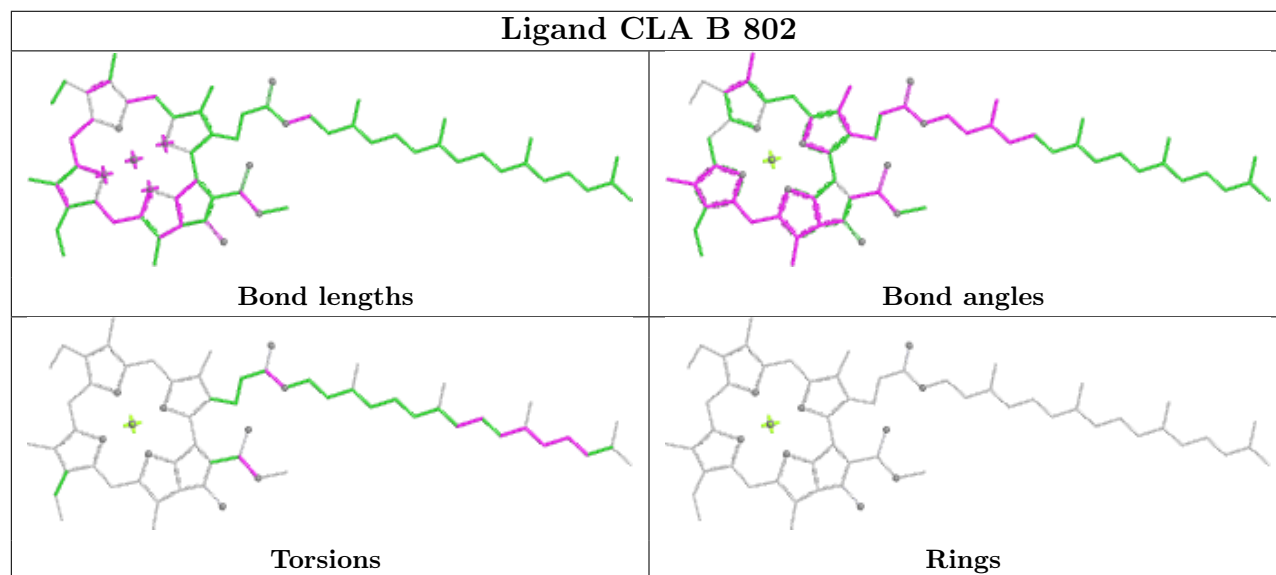




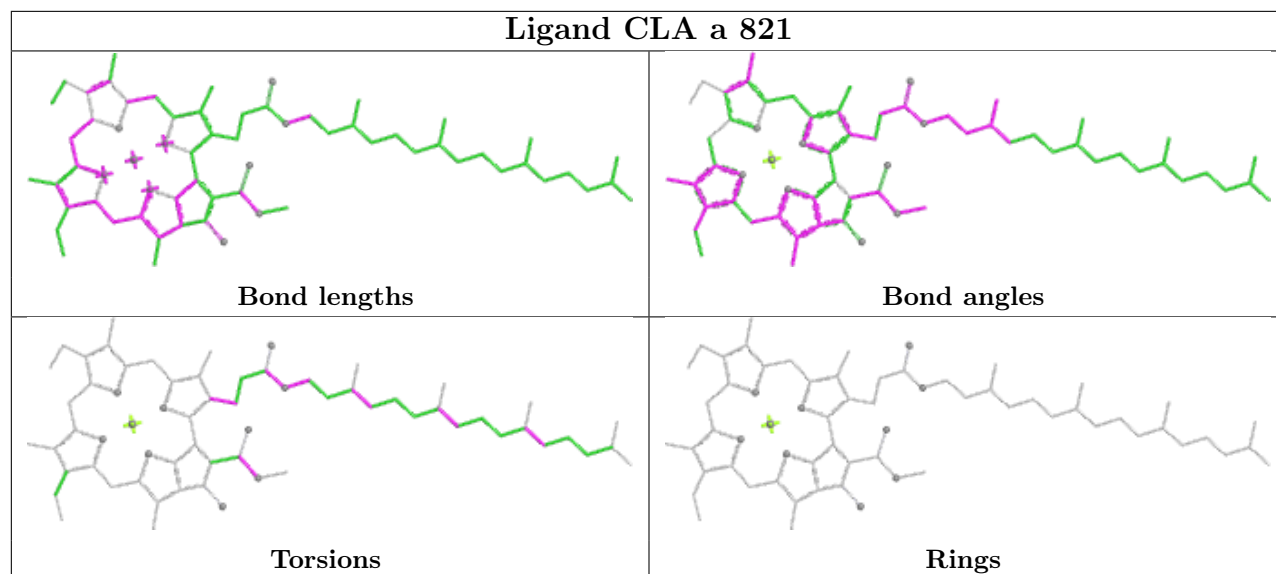
## Ligand CLA a 815



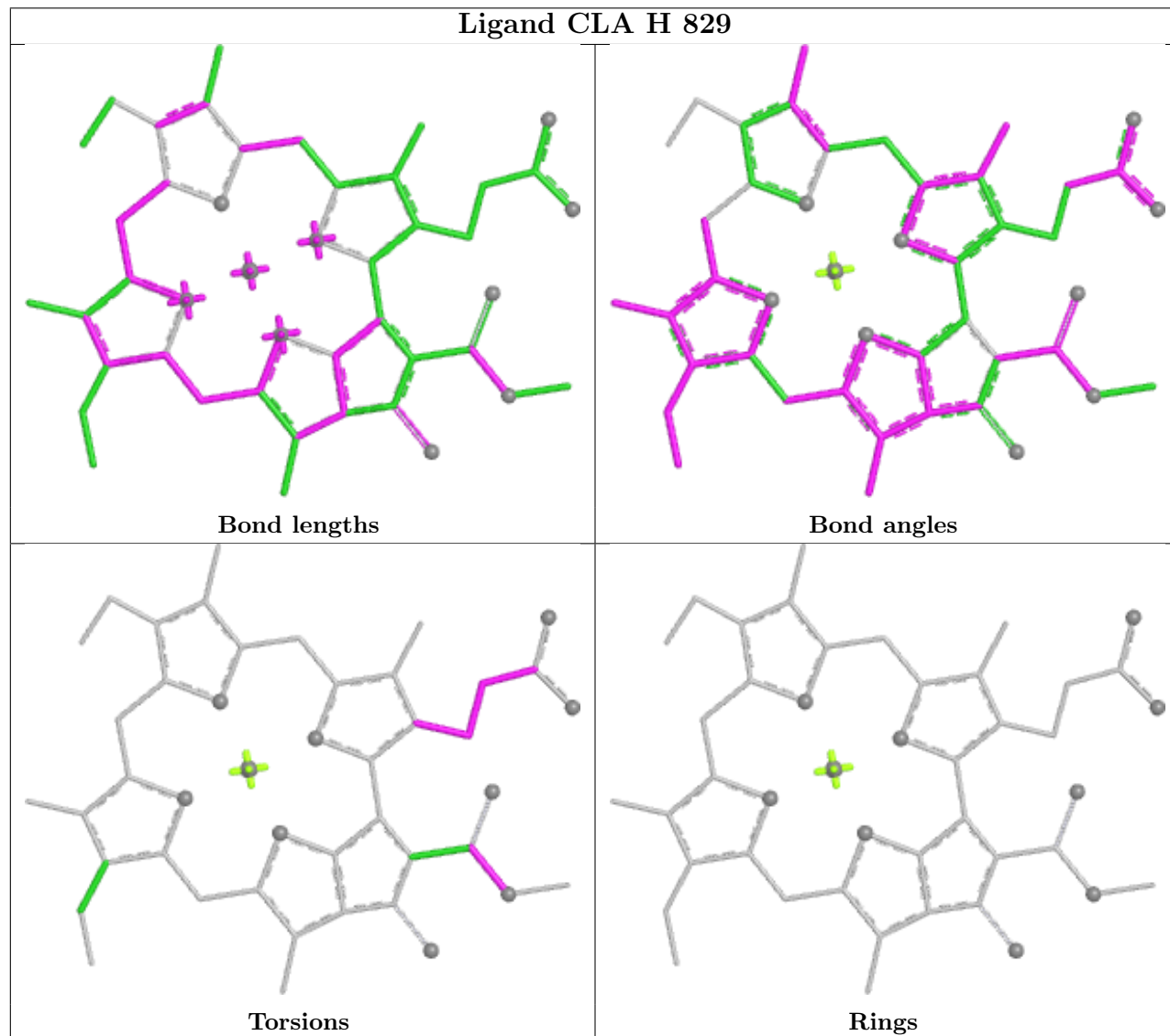
## Ligand CLA B 802



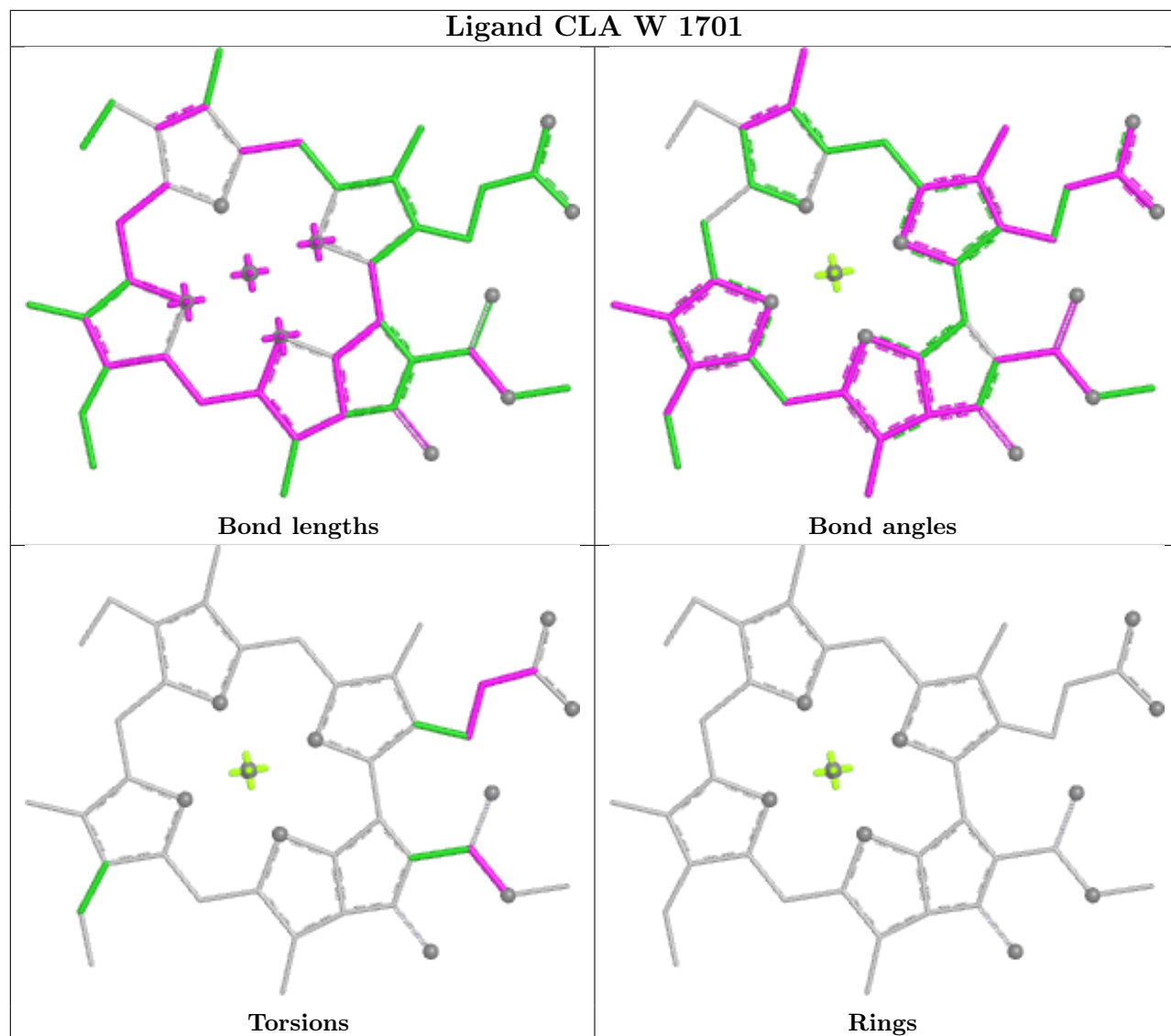
## Ligand CLA a 821



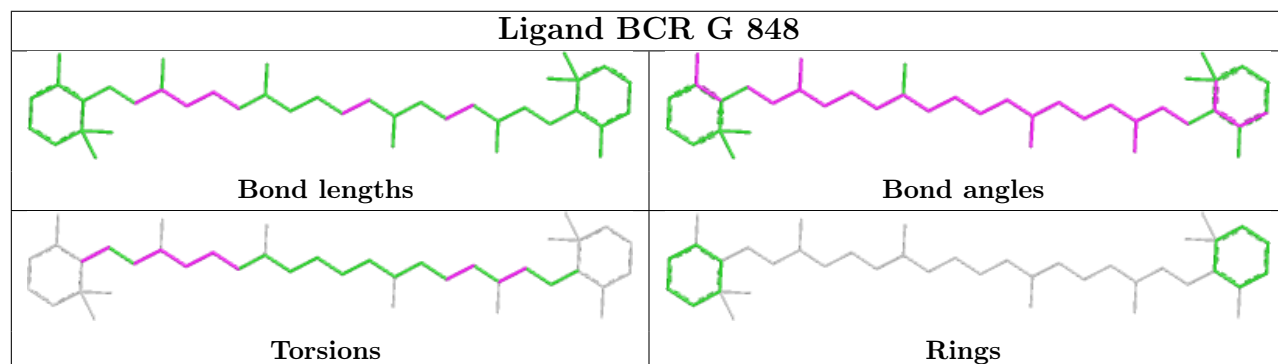
## Ligand CLA H 829

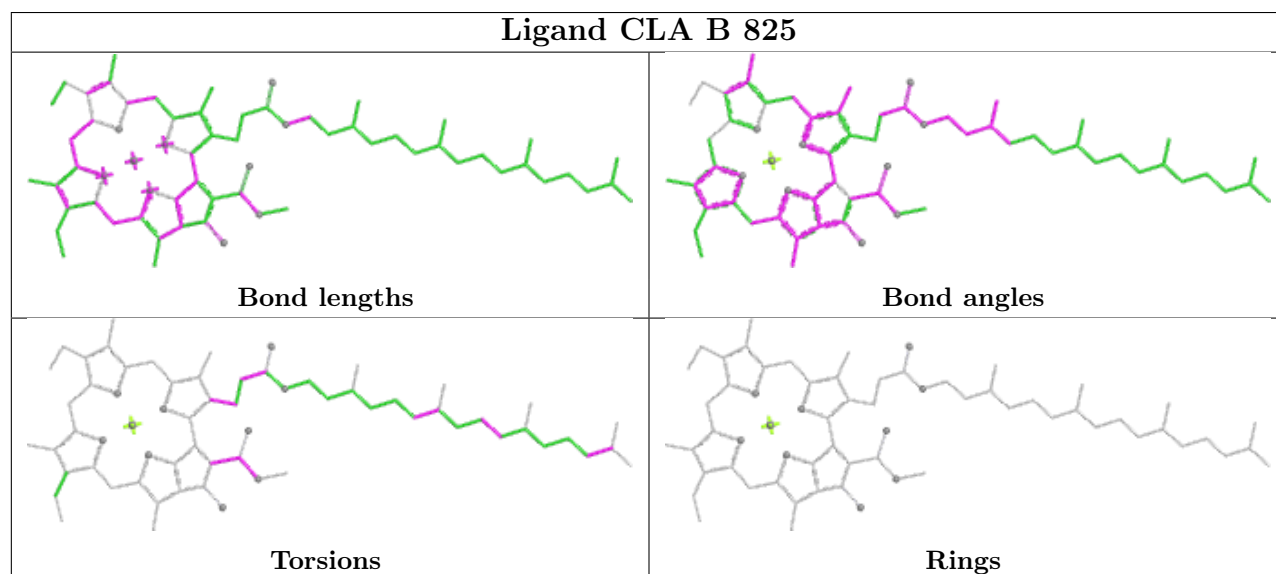
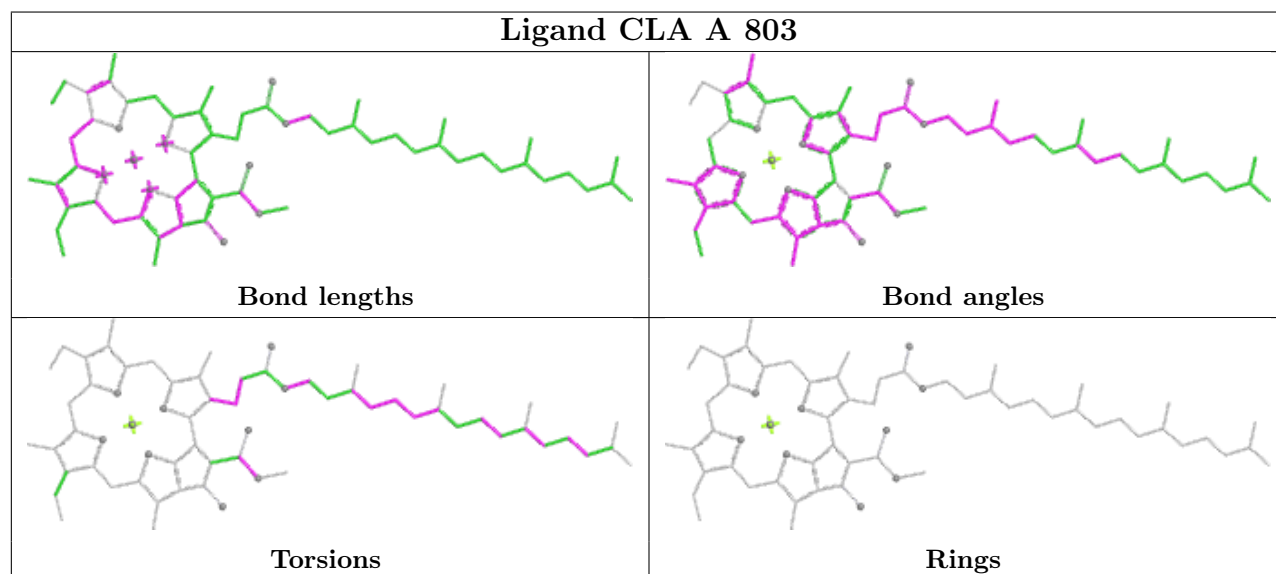
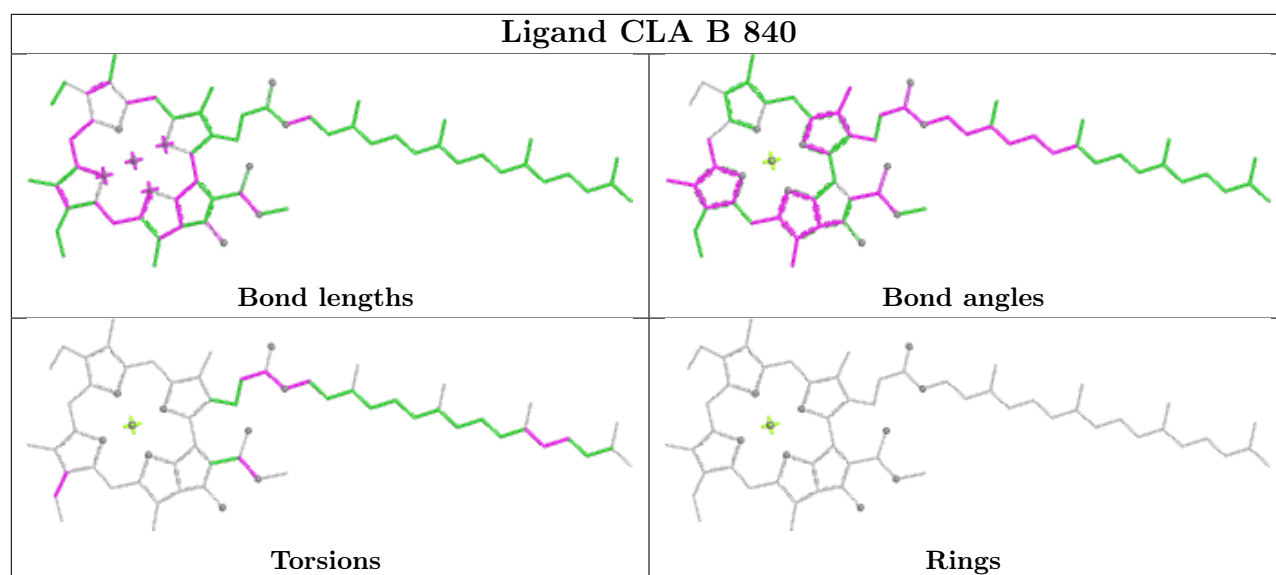


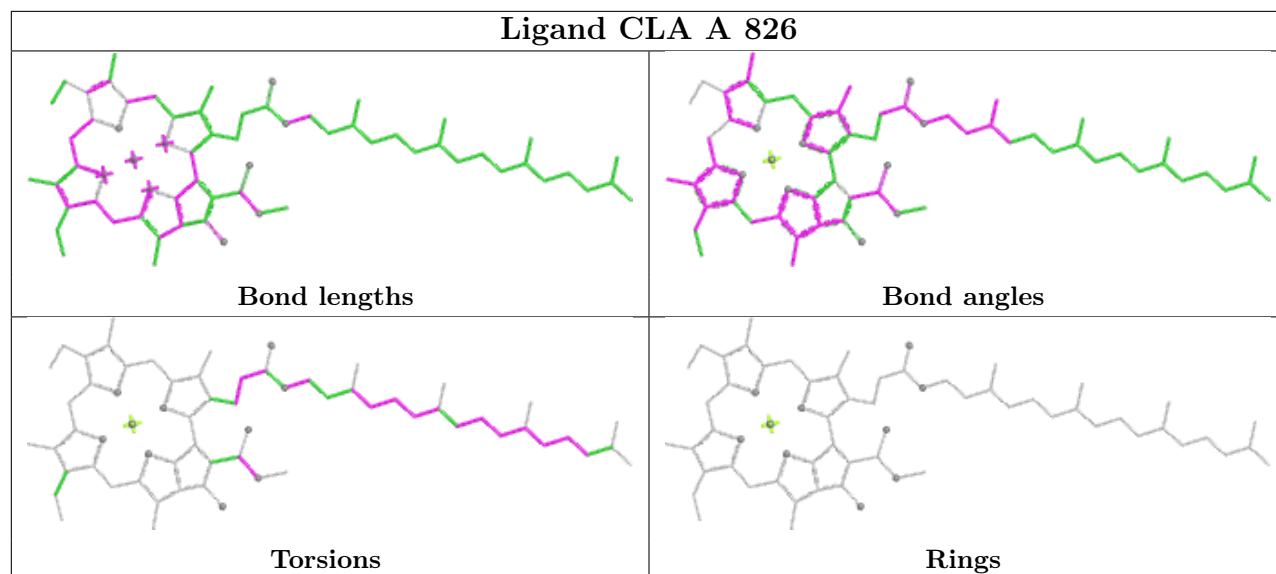
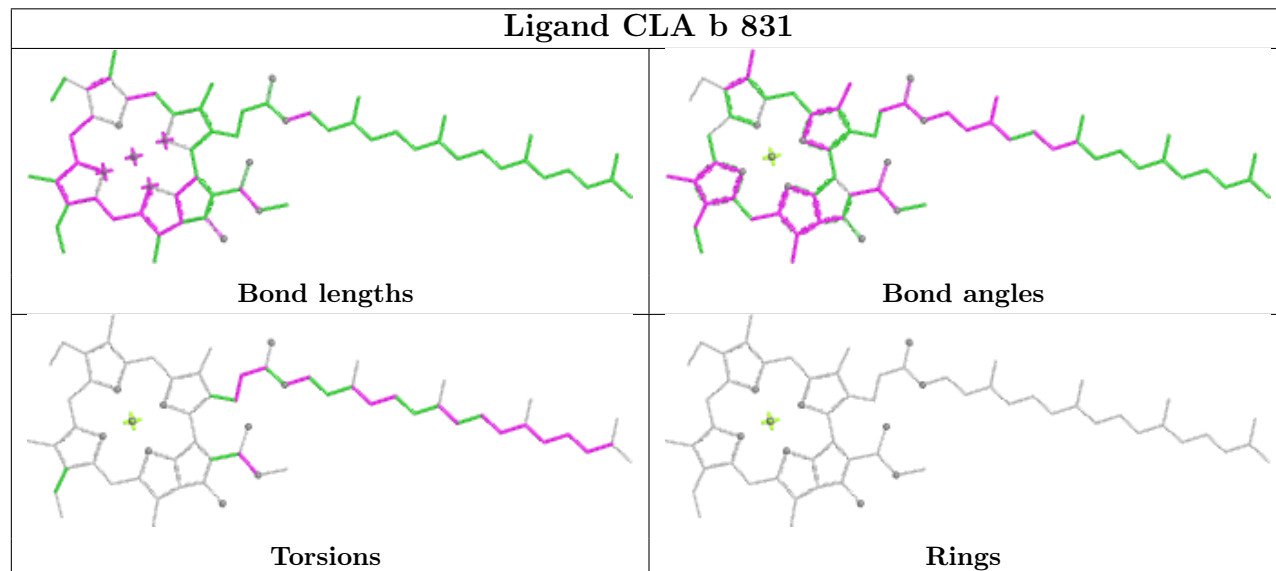
## Ligand CLA W 1701

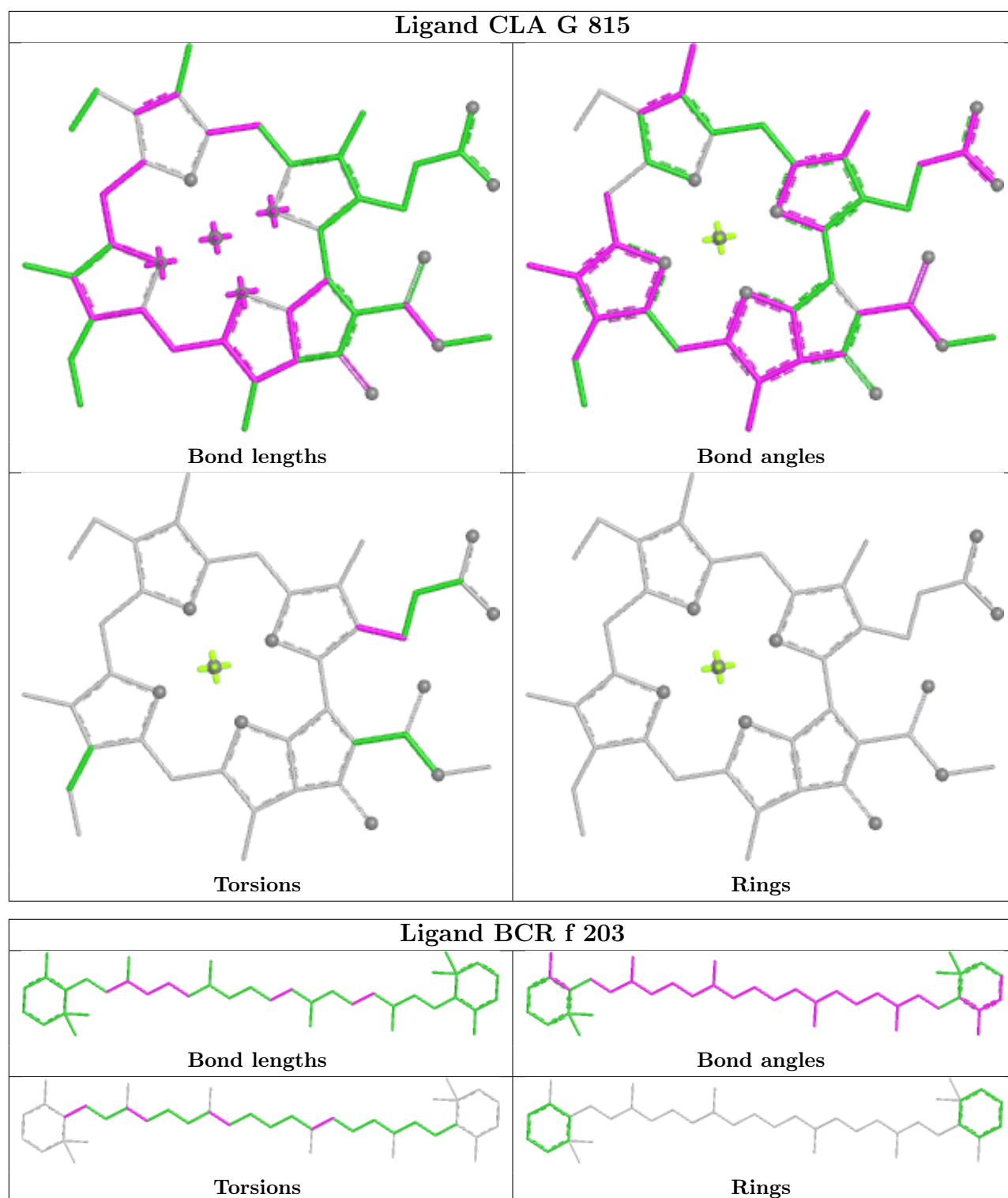


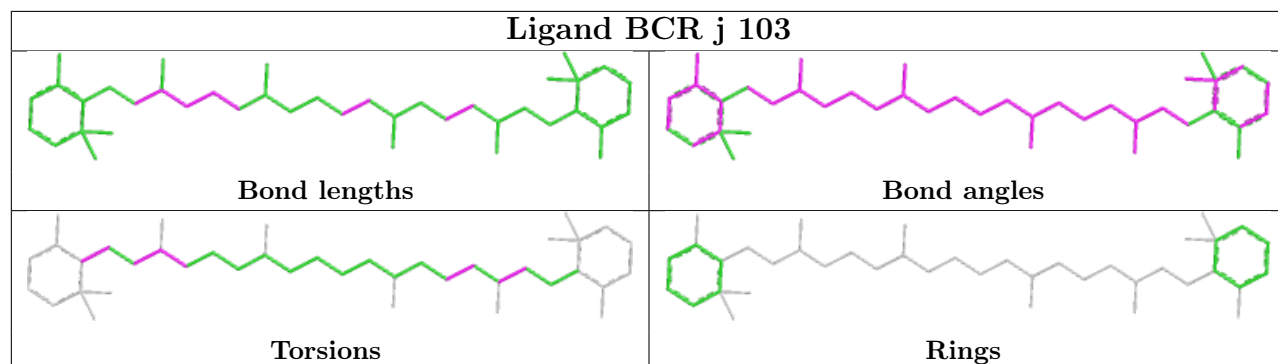
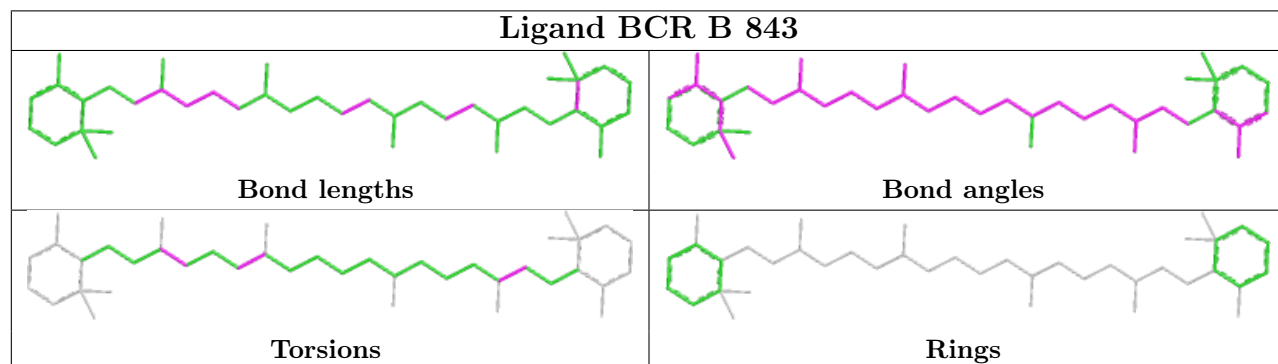
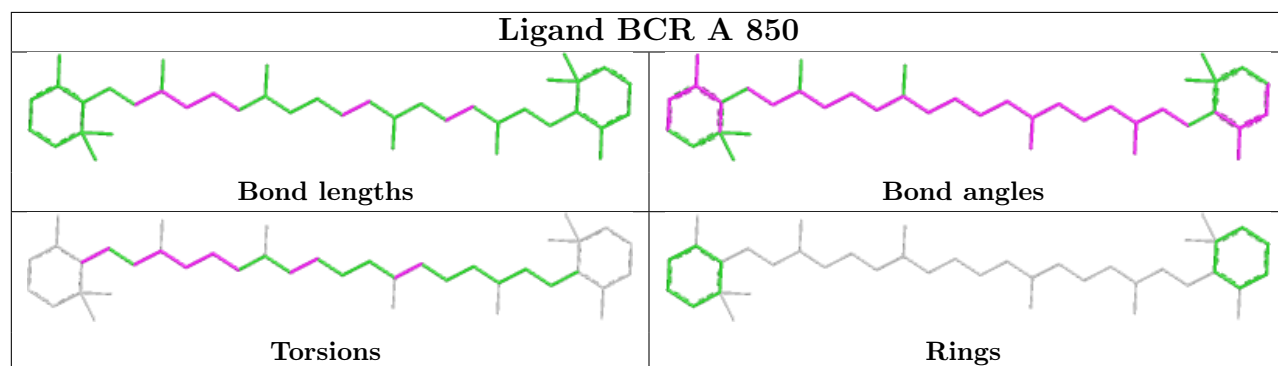
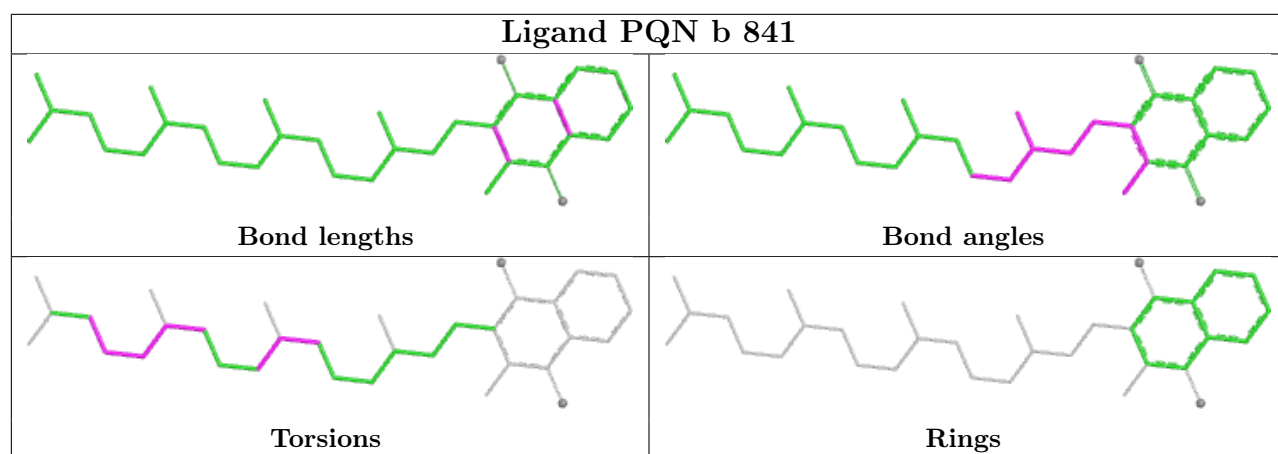
## Ligand BCR G 848



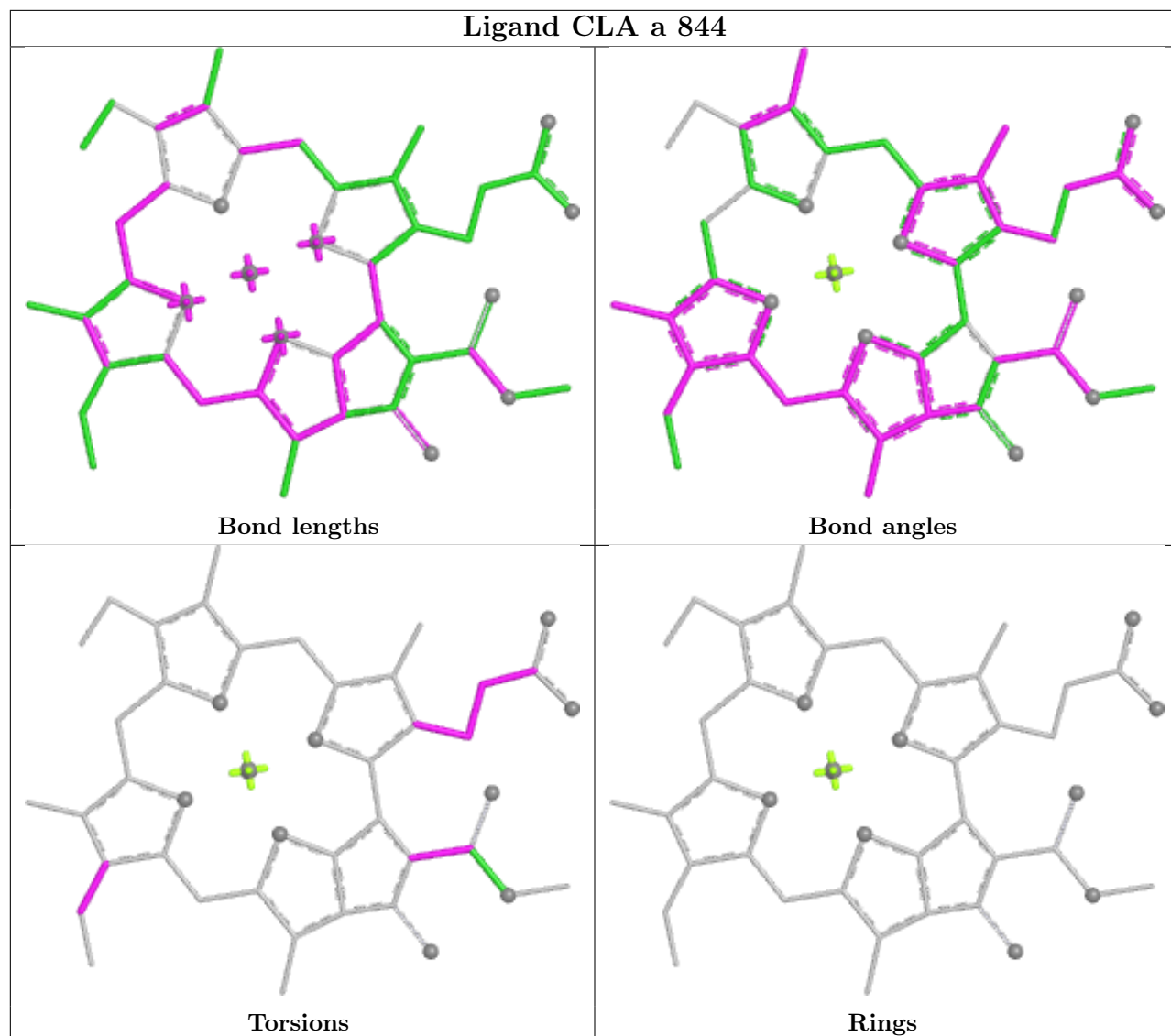


**Ligand CLA A 826****Ligand CLA b 831**

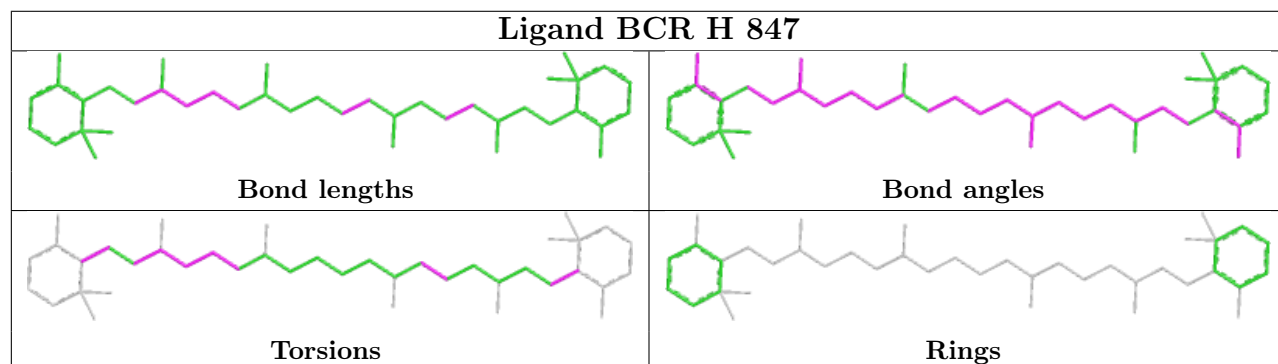




## Ligand CLA a 844

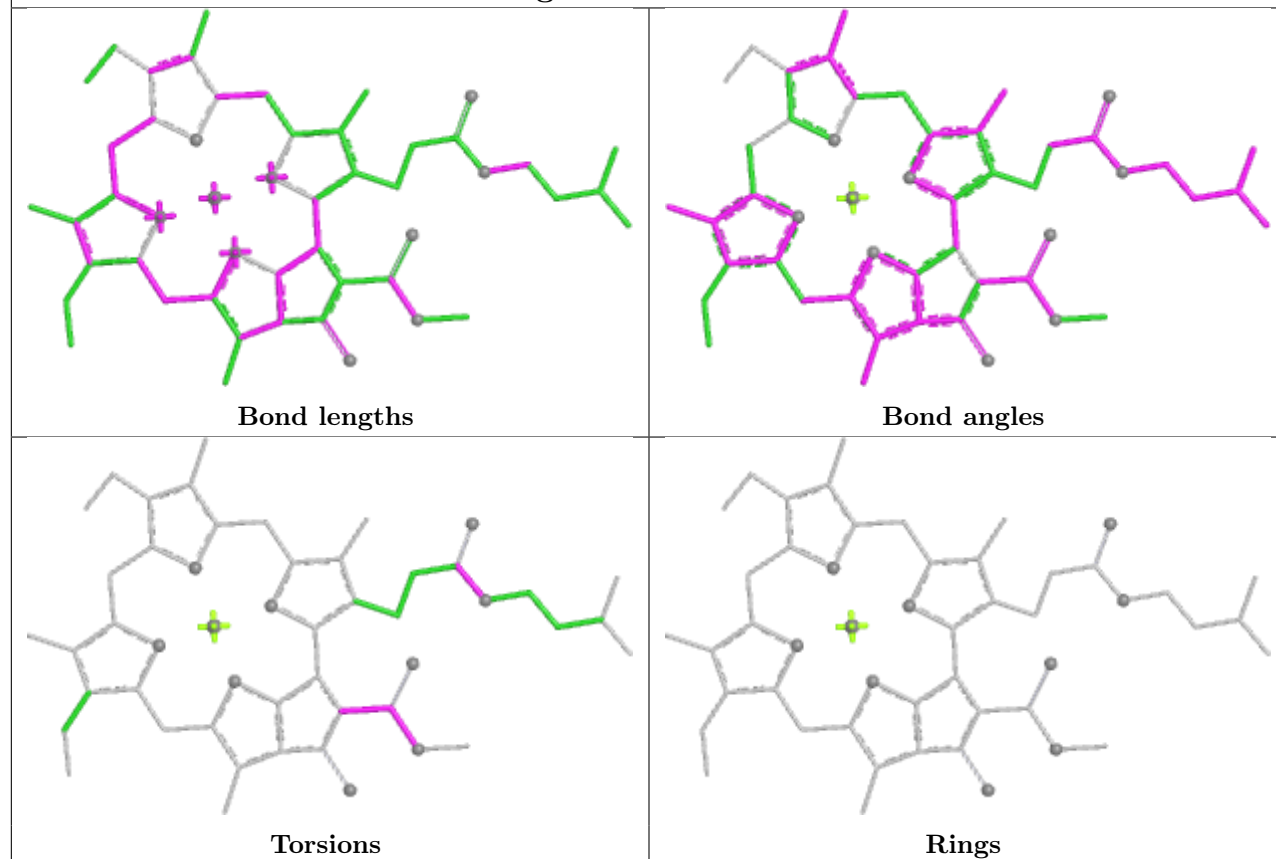


## Ligand BCR H 847

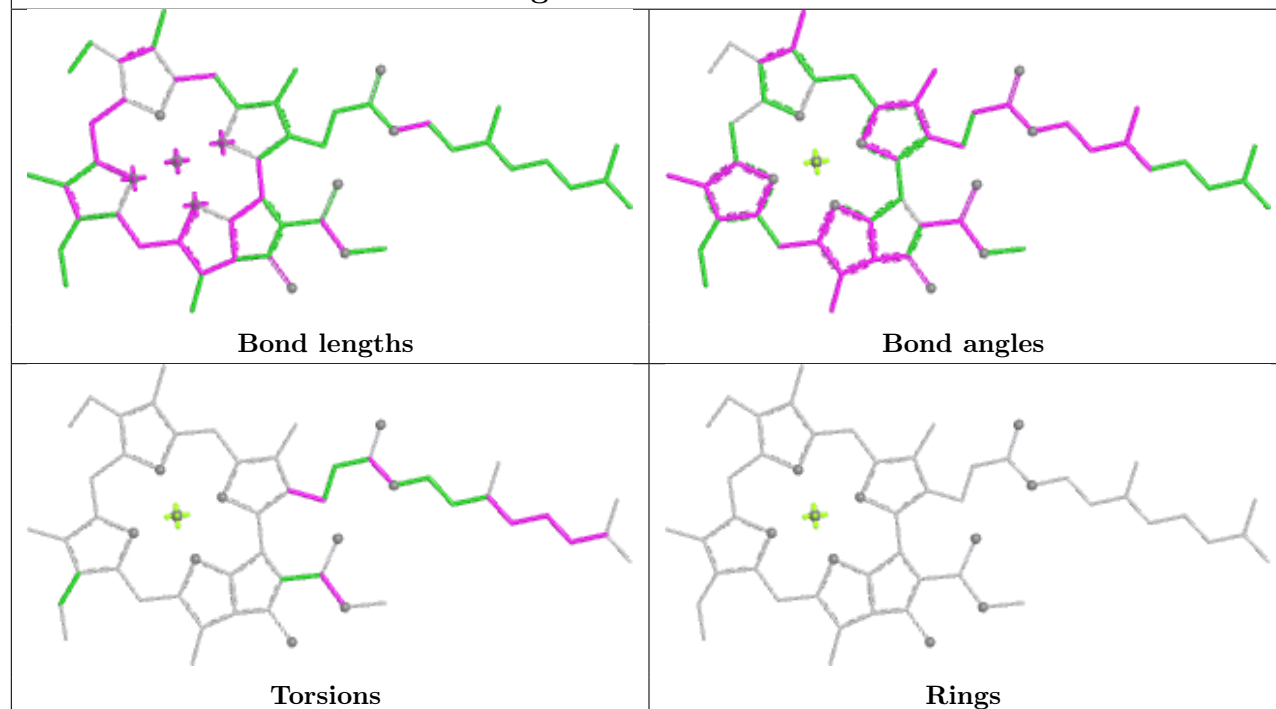


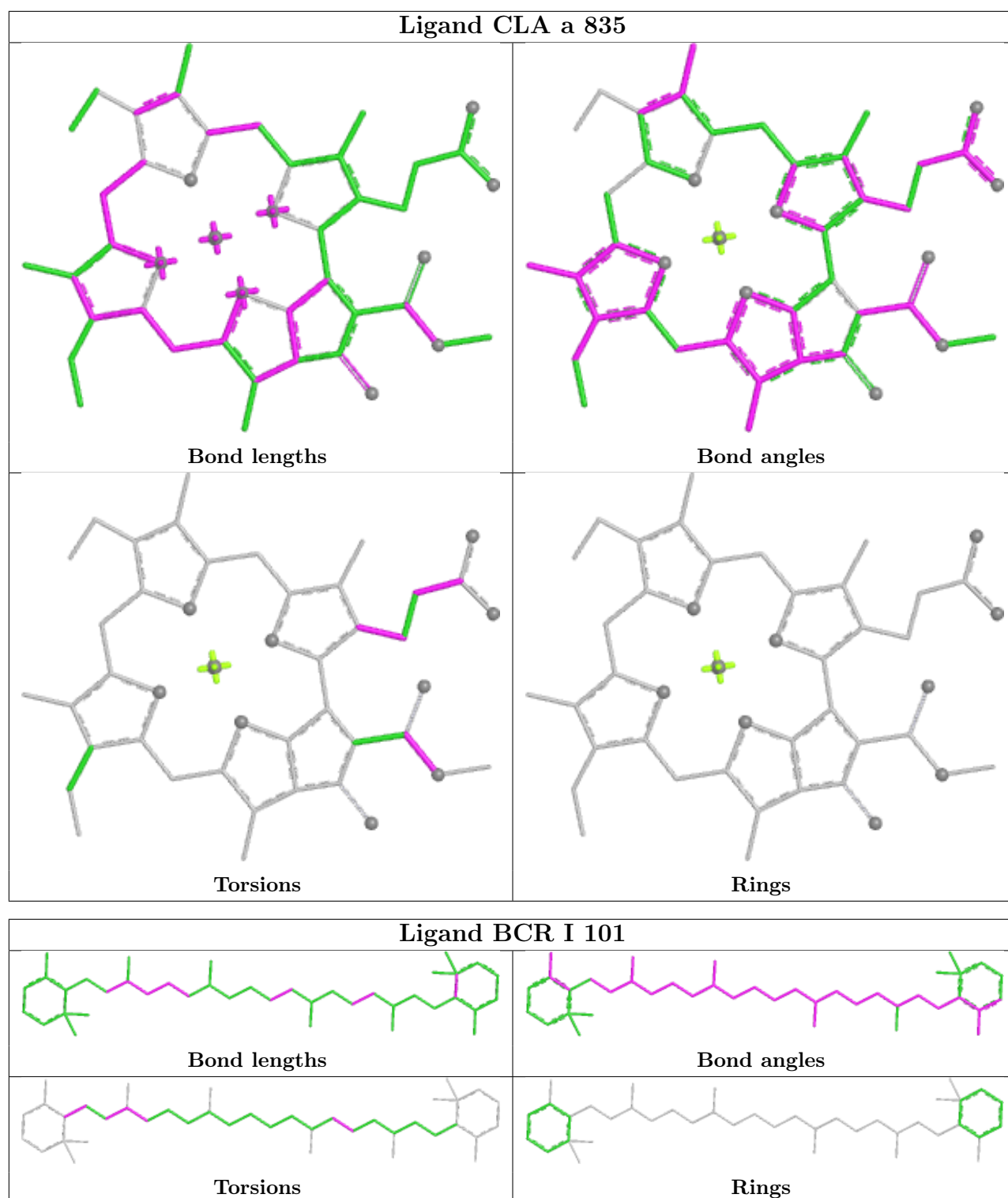


## Ligand CLA a 837

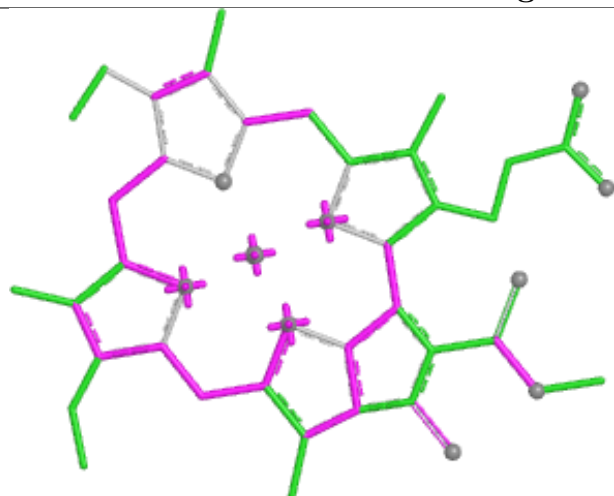


## Ligand CLA G 833

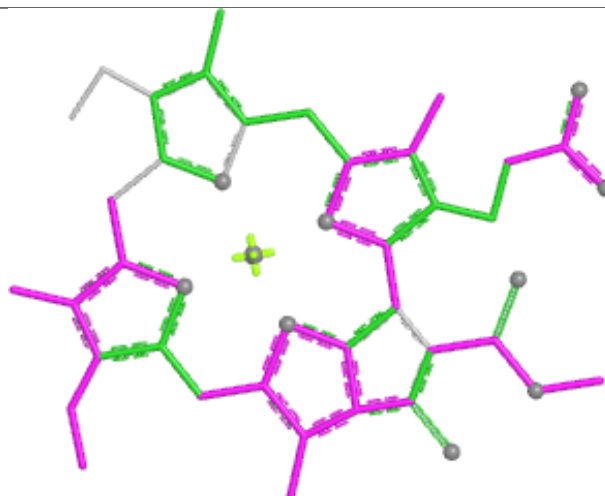




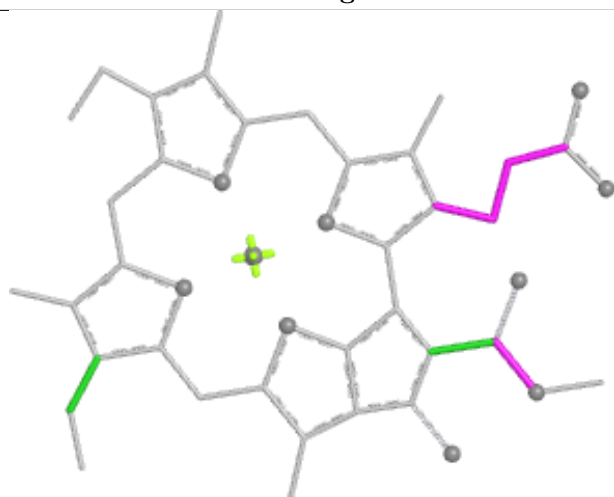
## Ligand CLA b 834



Bond lengths



Bond angles

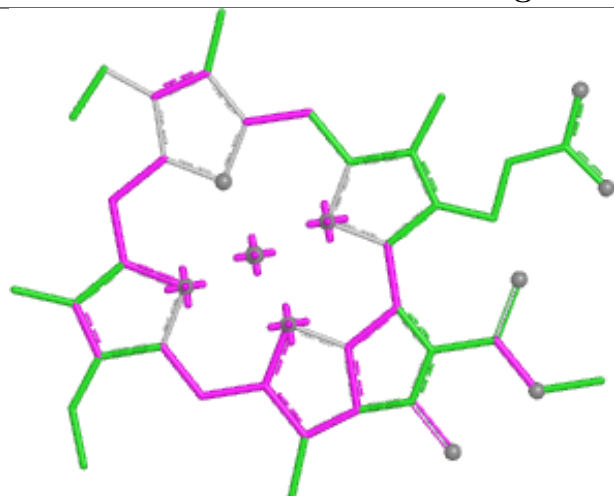


Torsions

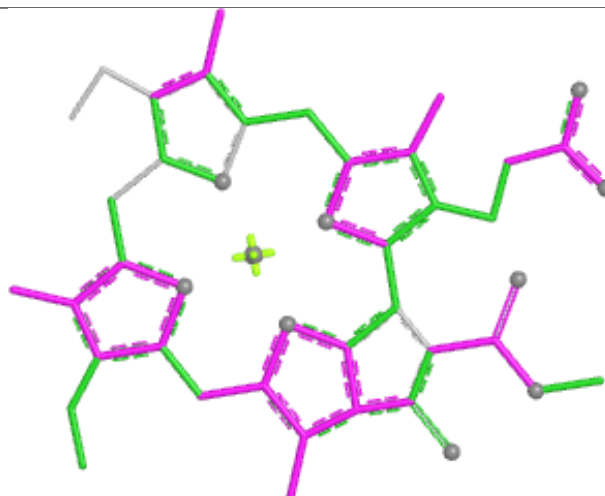


Rings

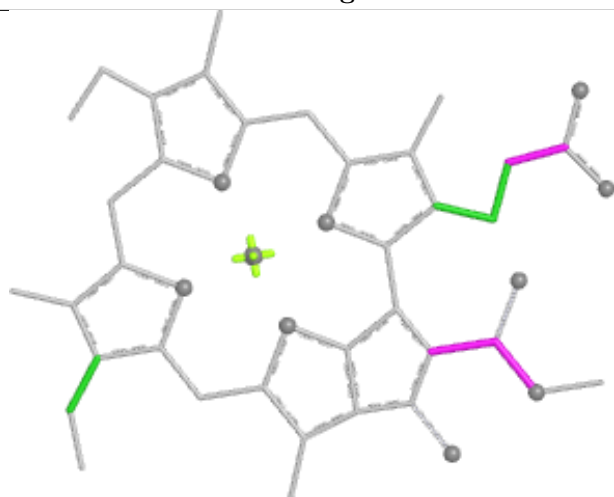
## Ligand CLA B 820



Bond lengths



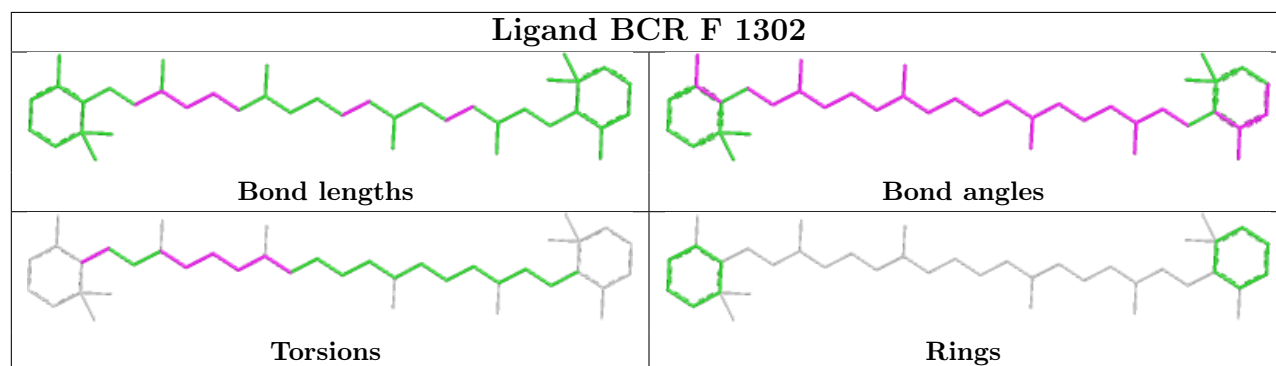
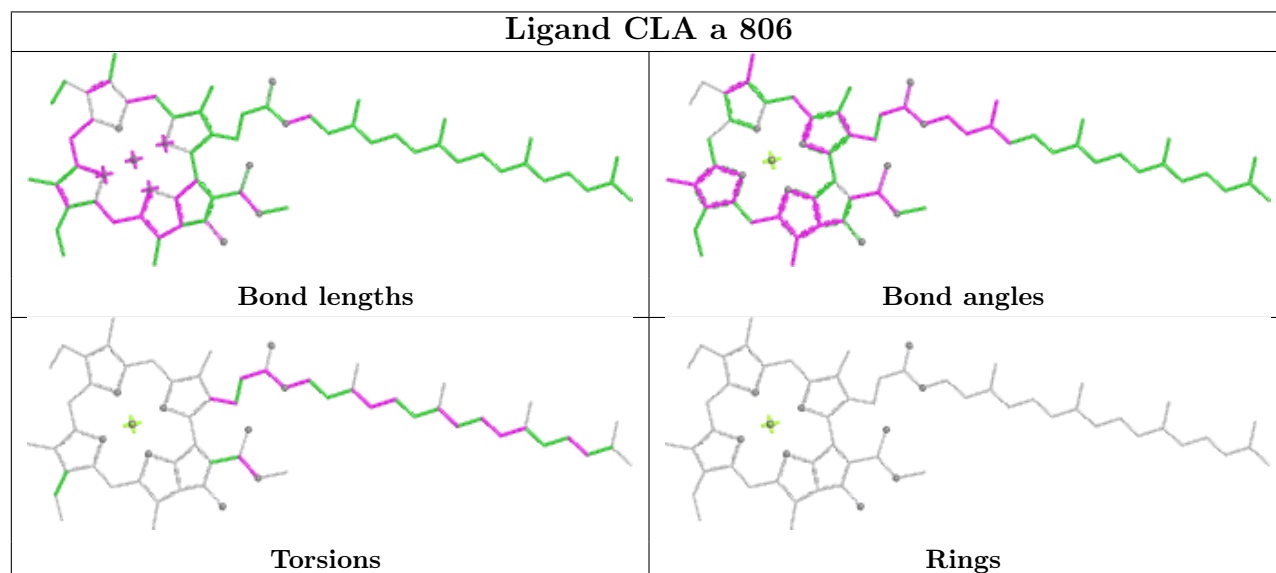
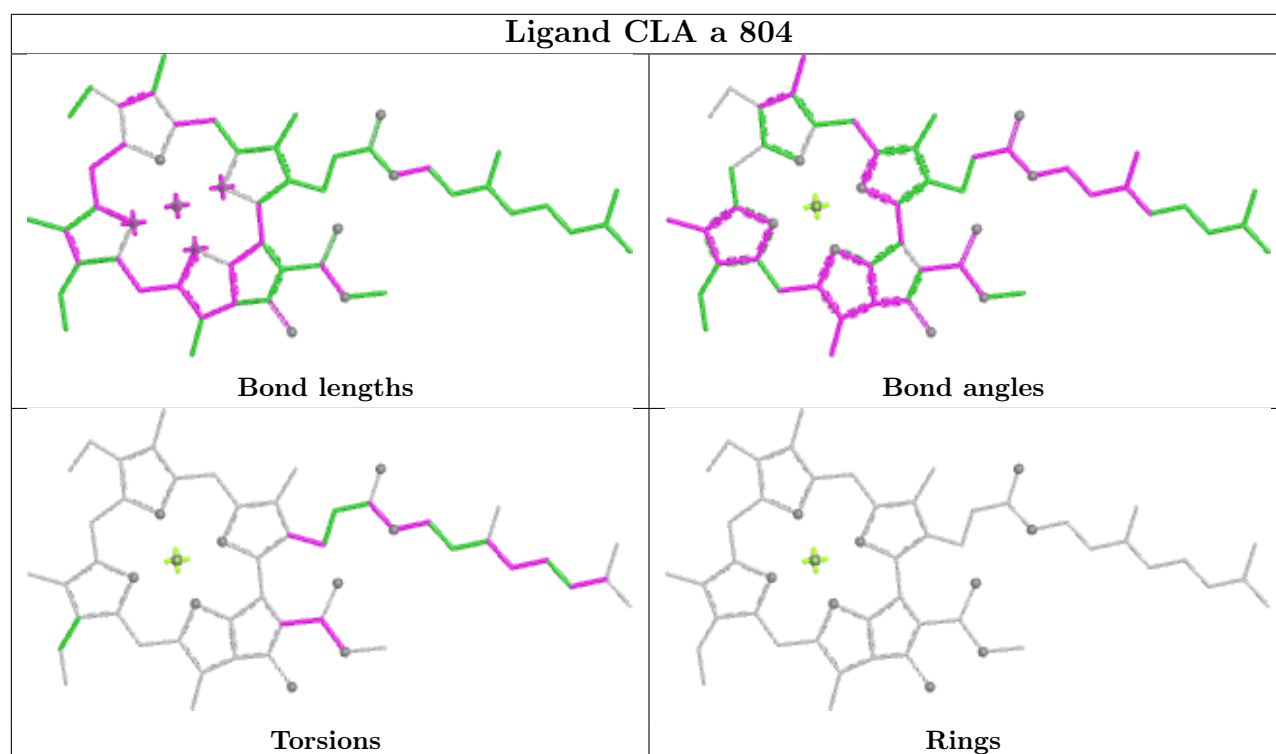
Bond angles

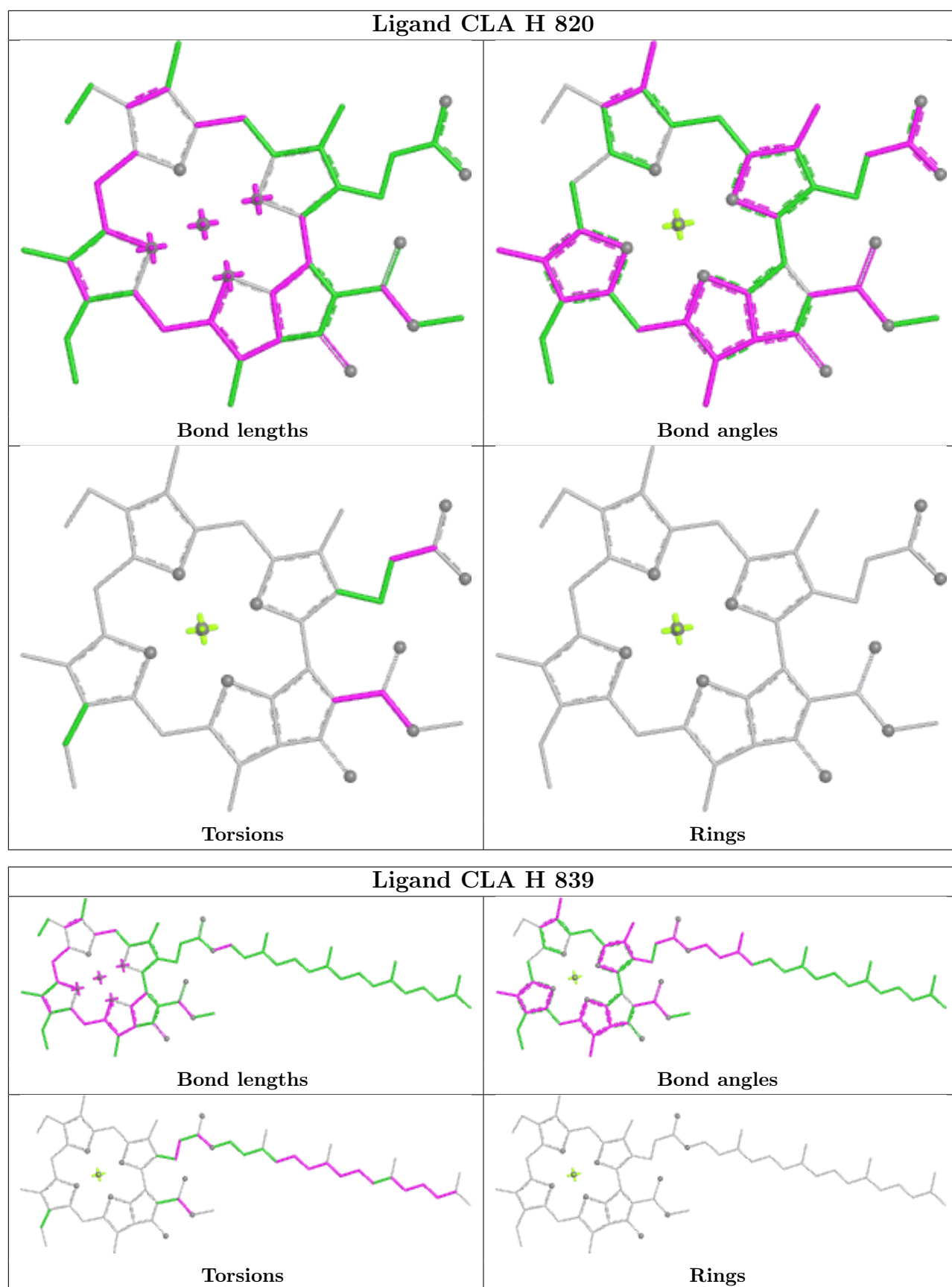


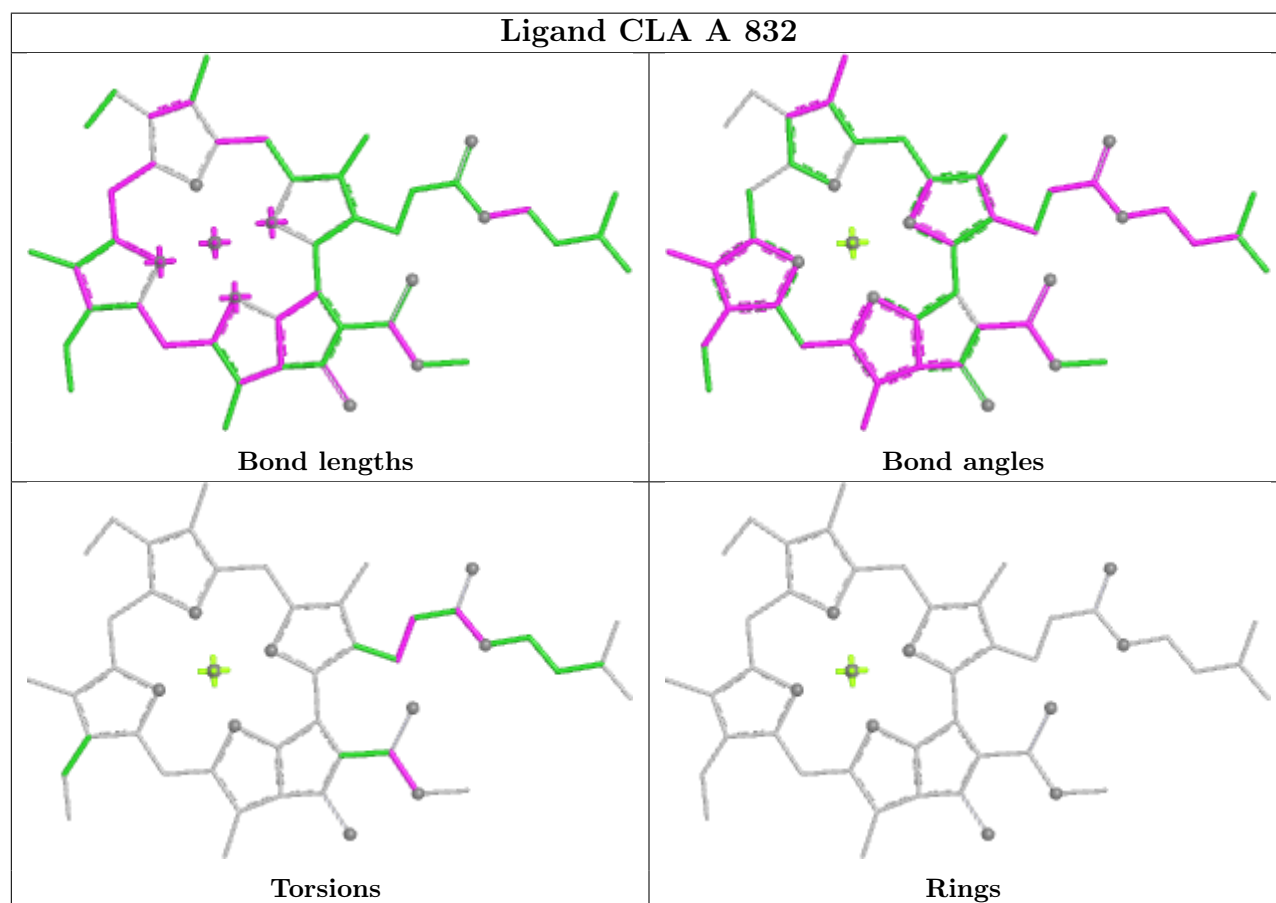
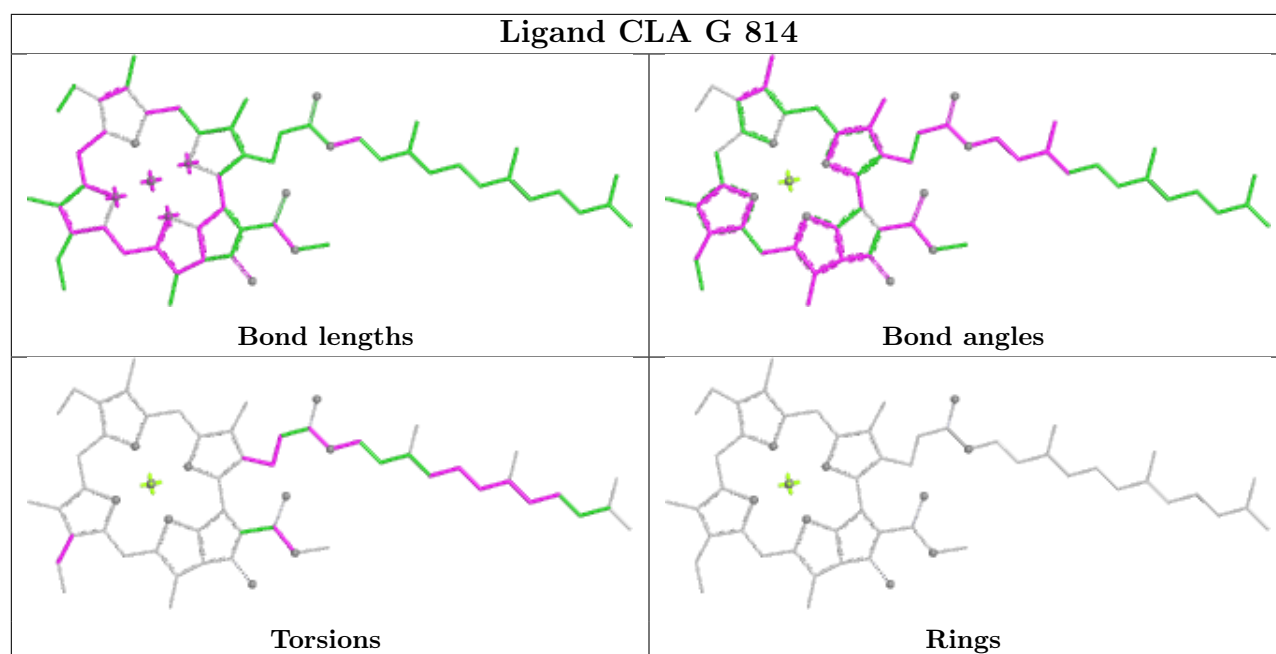
Torsions

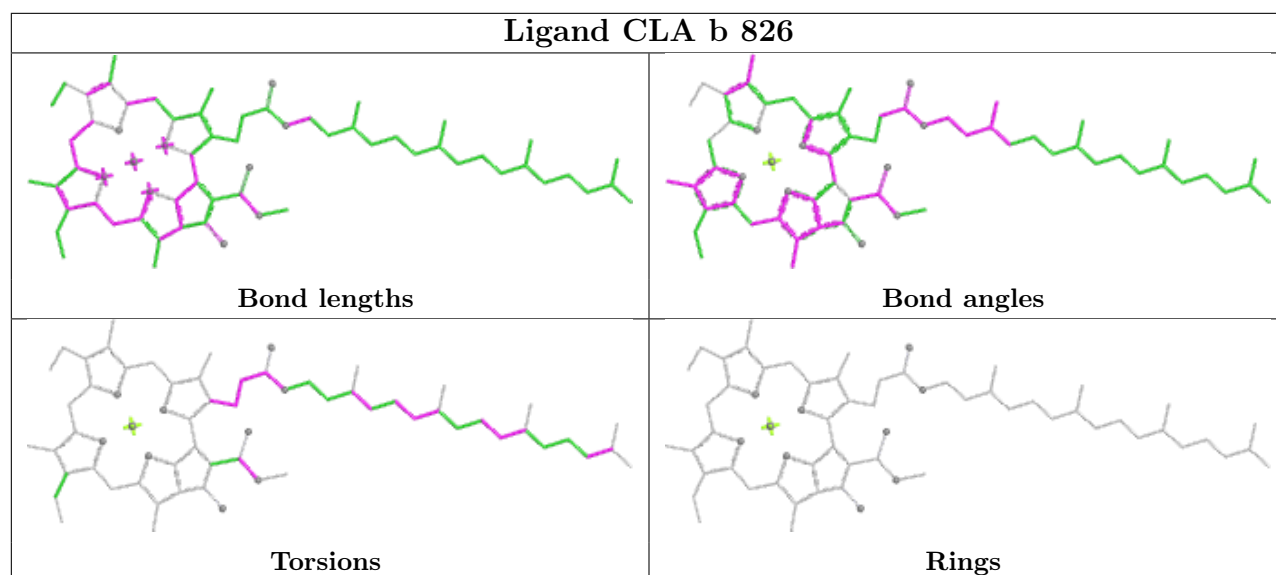
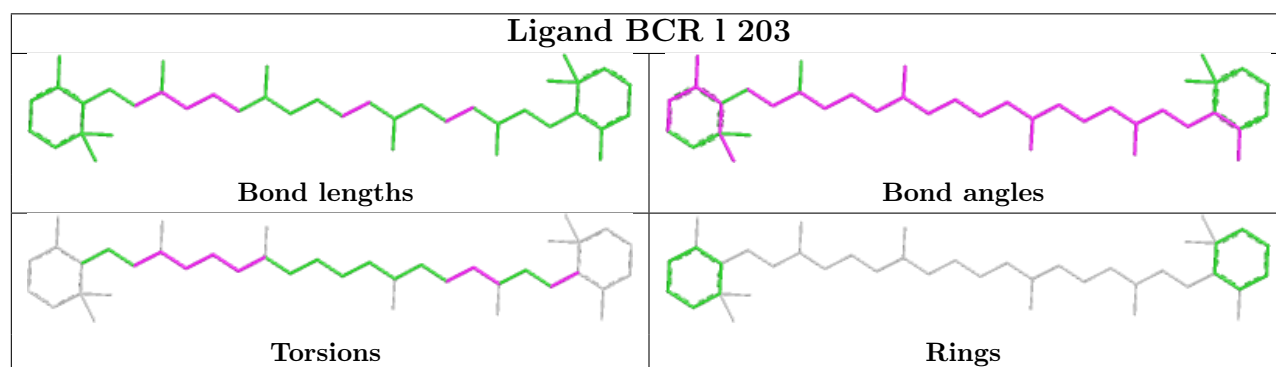
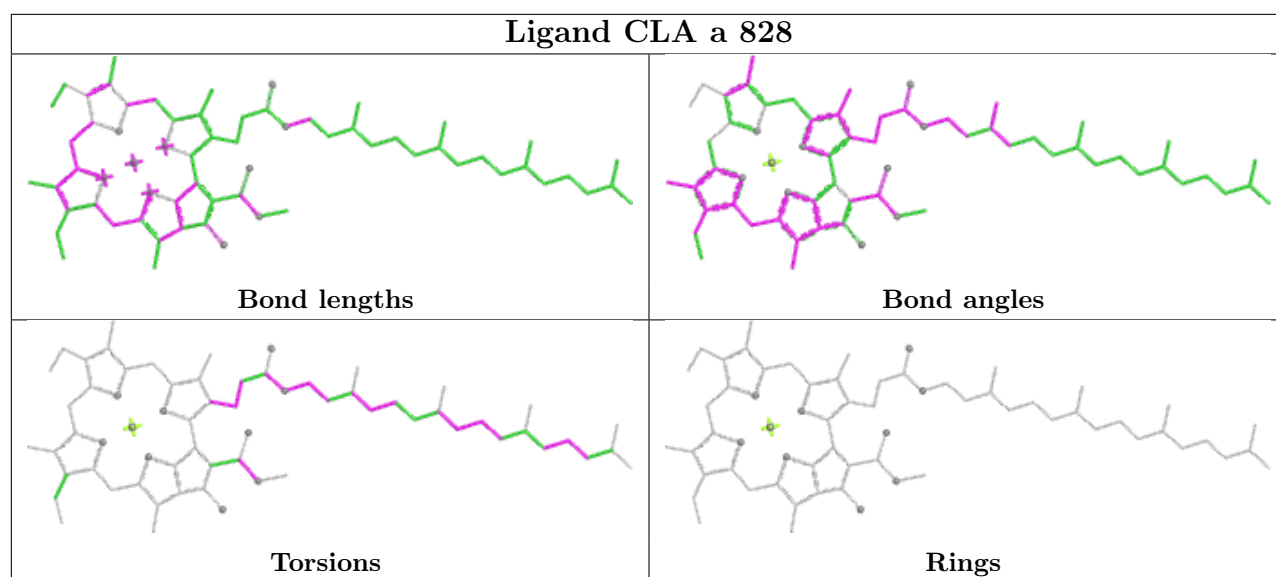


Rings

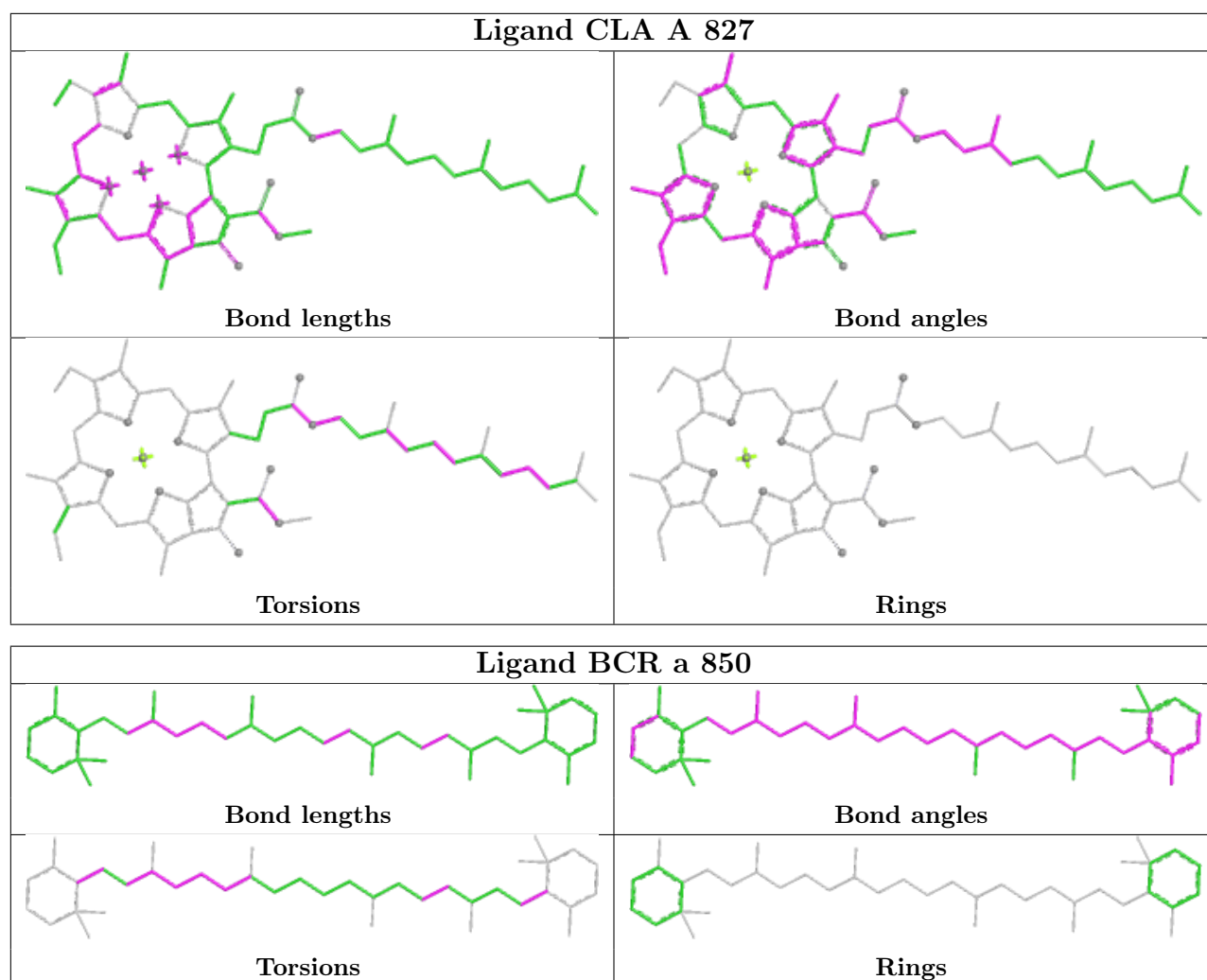




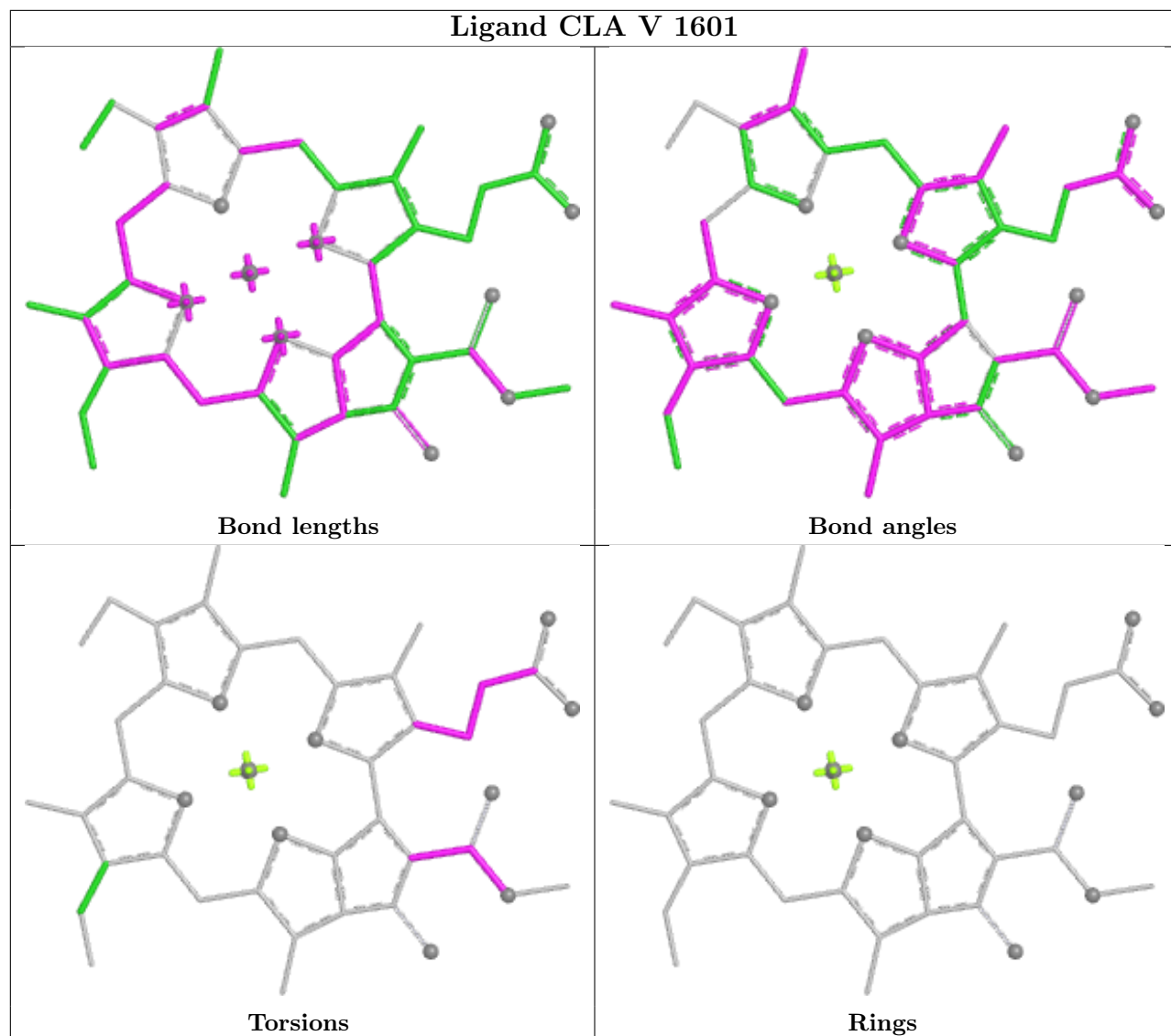




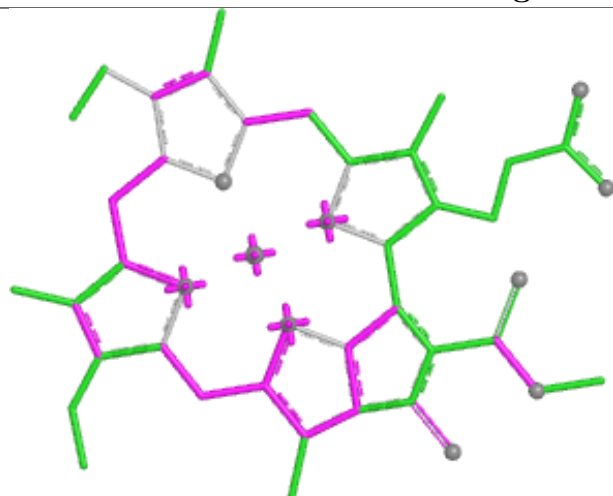




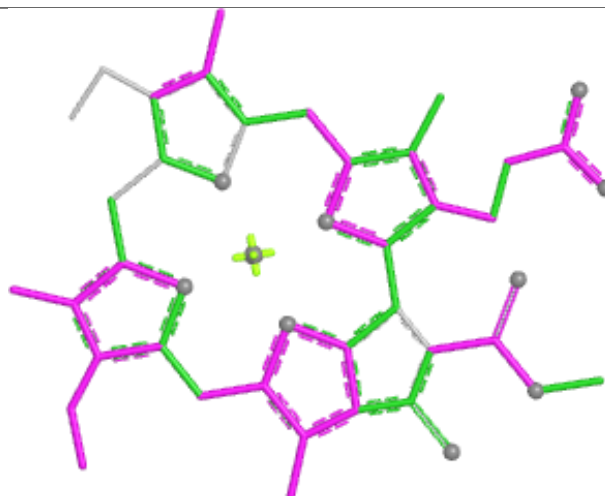
## Ligand CLA V 1601



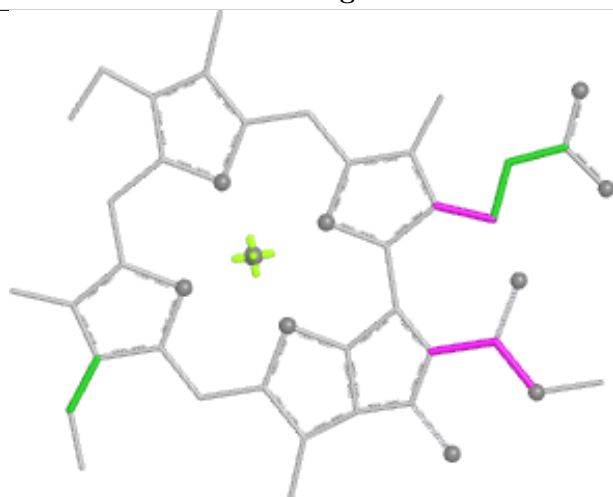
## Ligand CLA G 806



Bond lengths



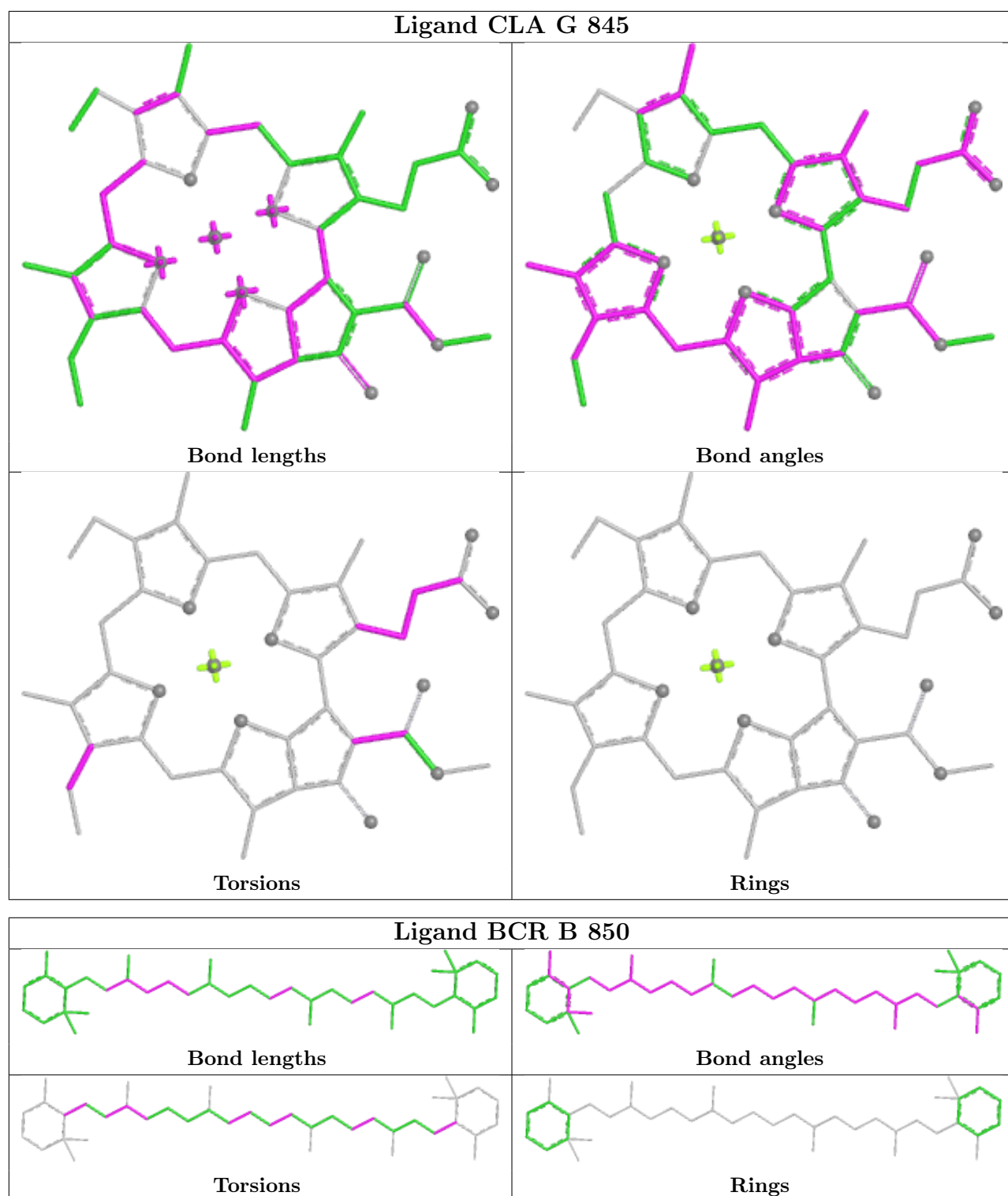
Bond angles

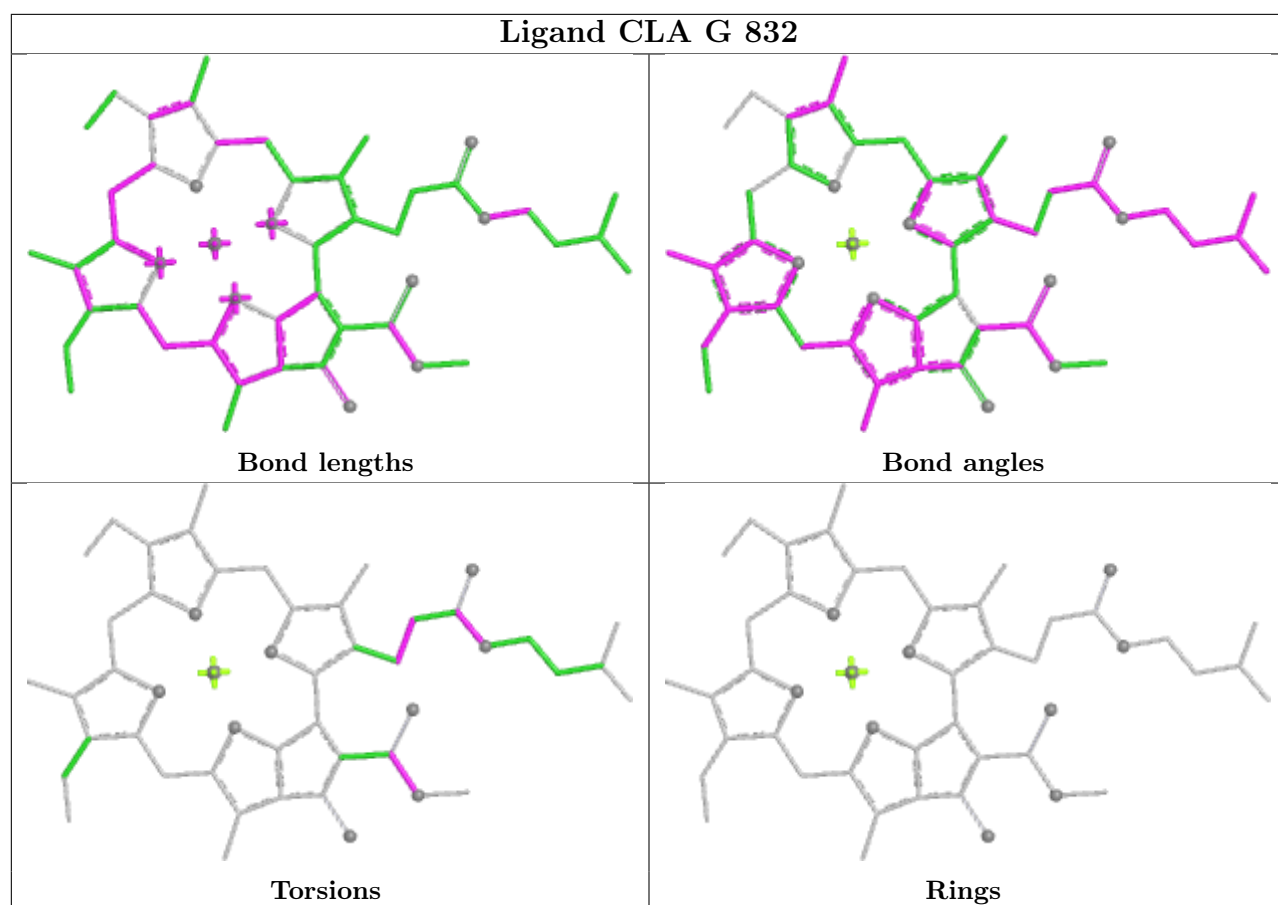


Torsions

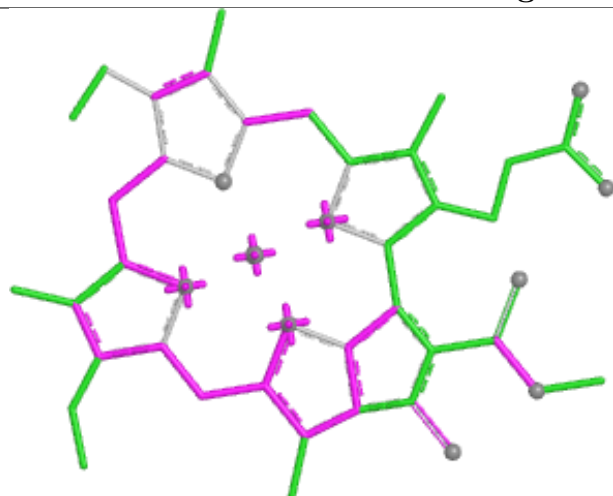


Rings

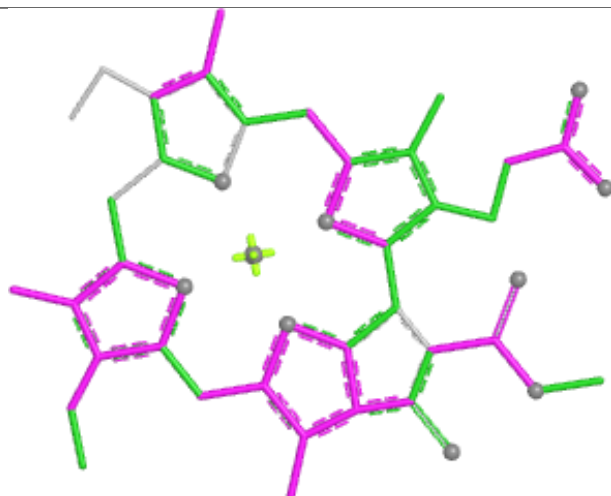




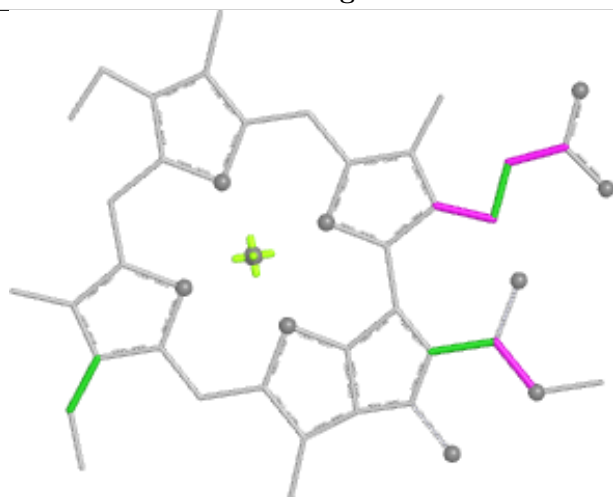
## Ligand CLA b 833



Bond lengths



Bond angles

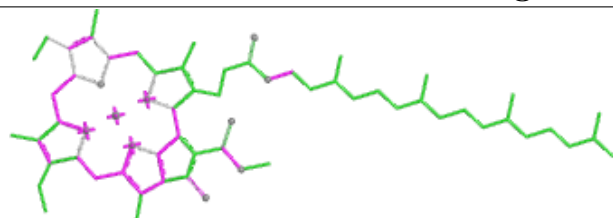


Torsions

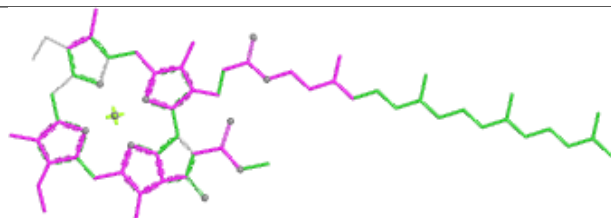


Rings

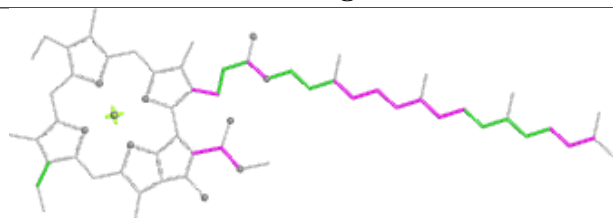
## Ligand CLA A 809



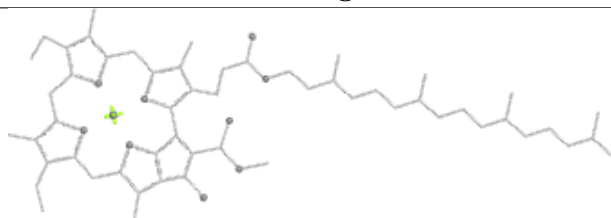
Bond lengths



Bond angles

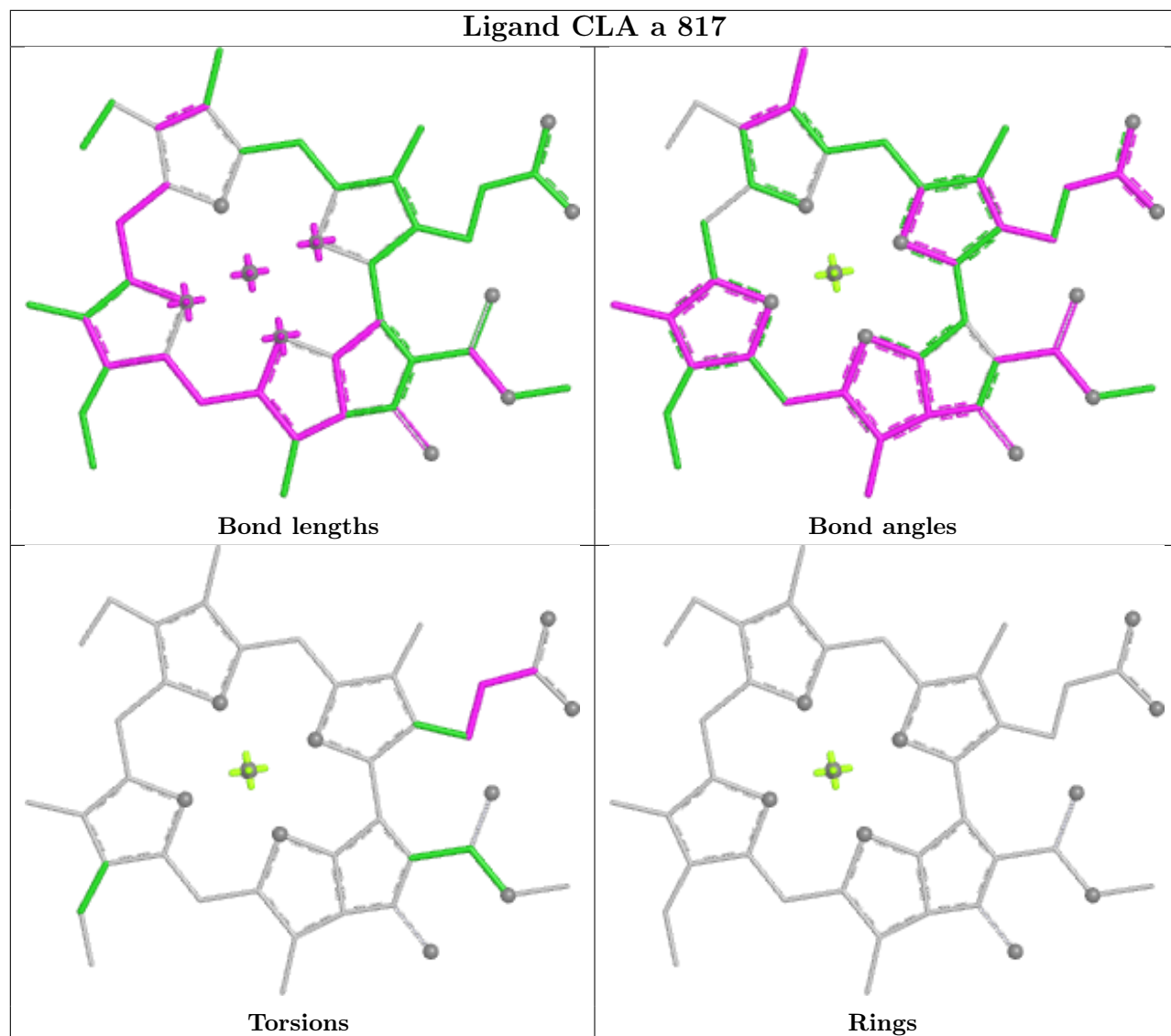


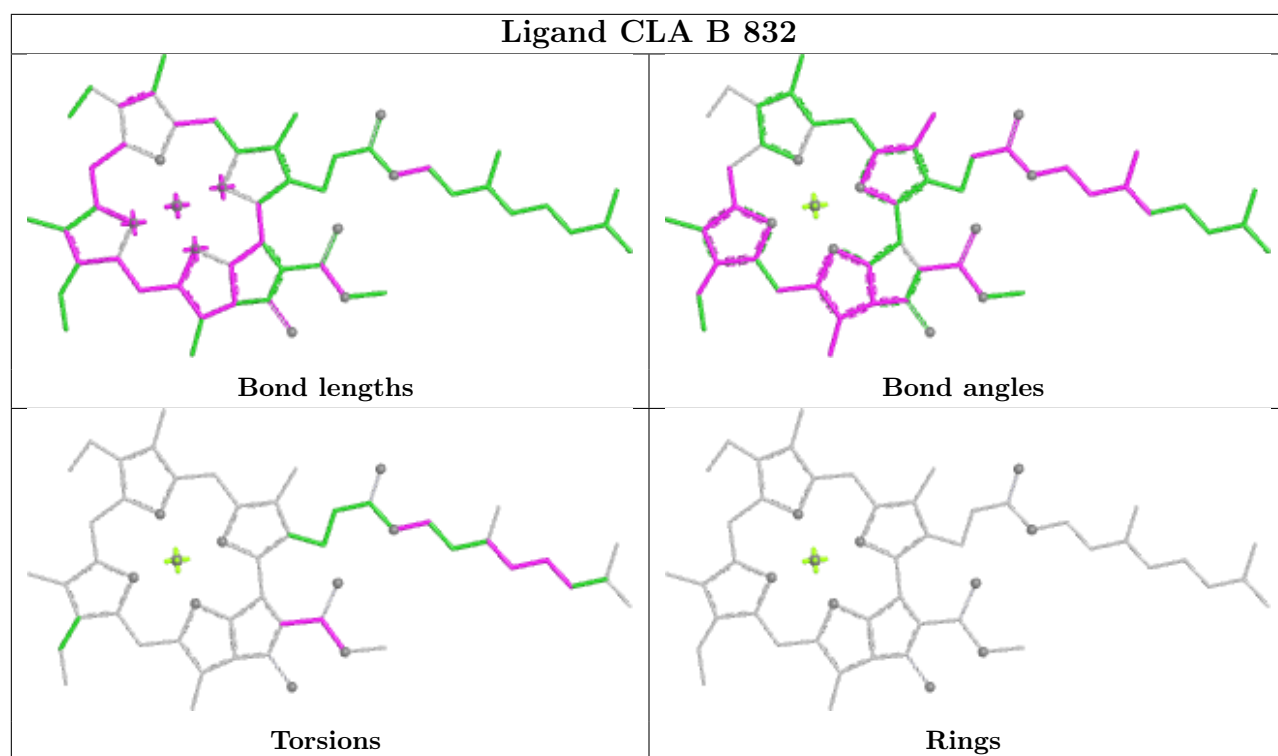
Torsions



Rings

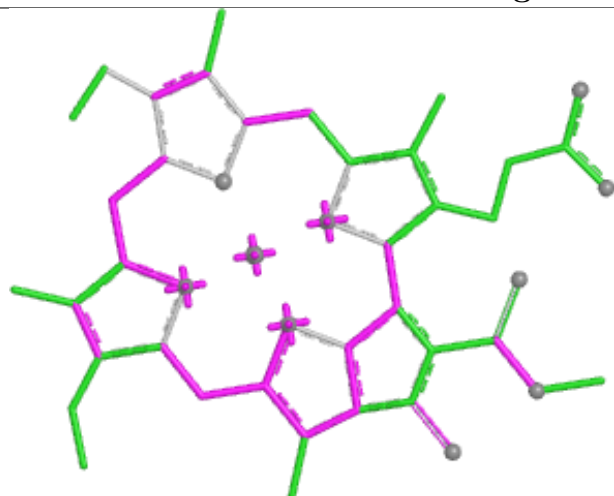
## Ligand CLA a 817



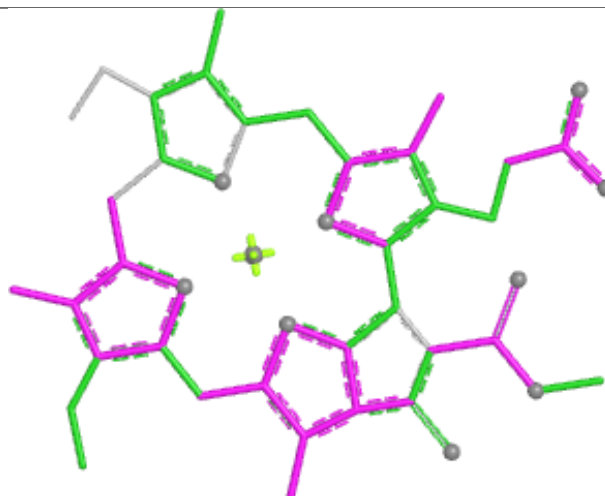




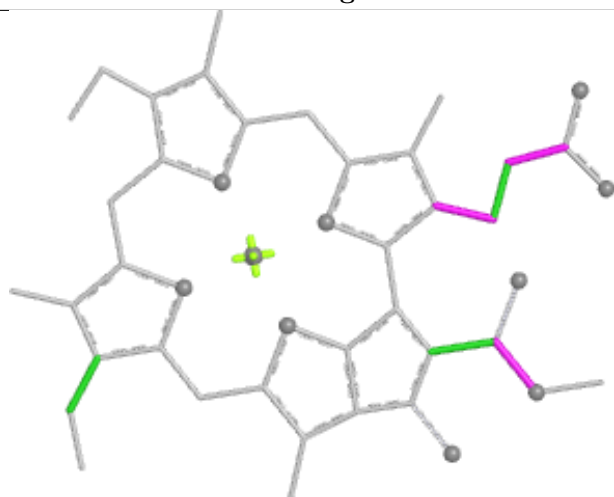
## Ligand CLA H 834



Bond lengths



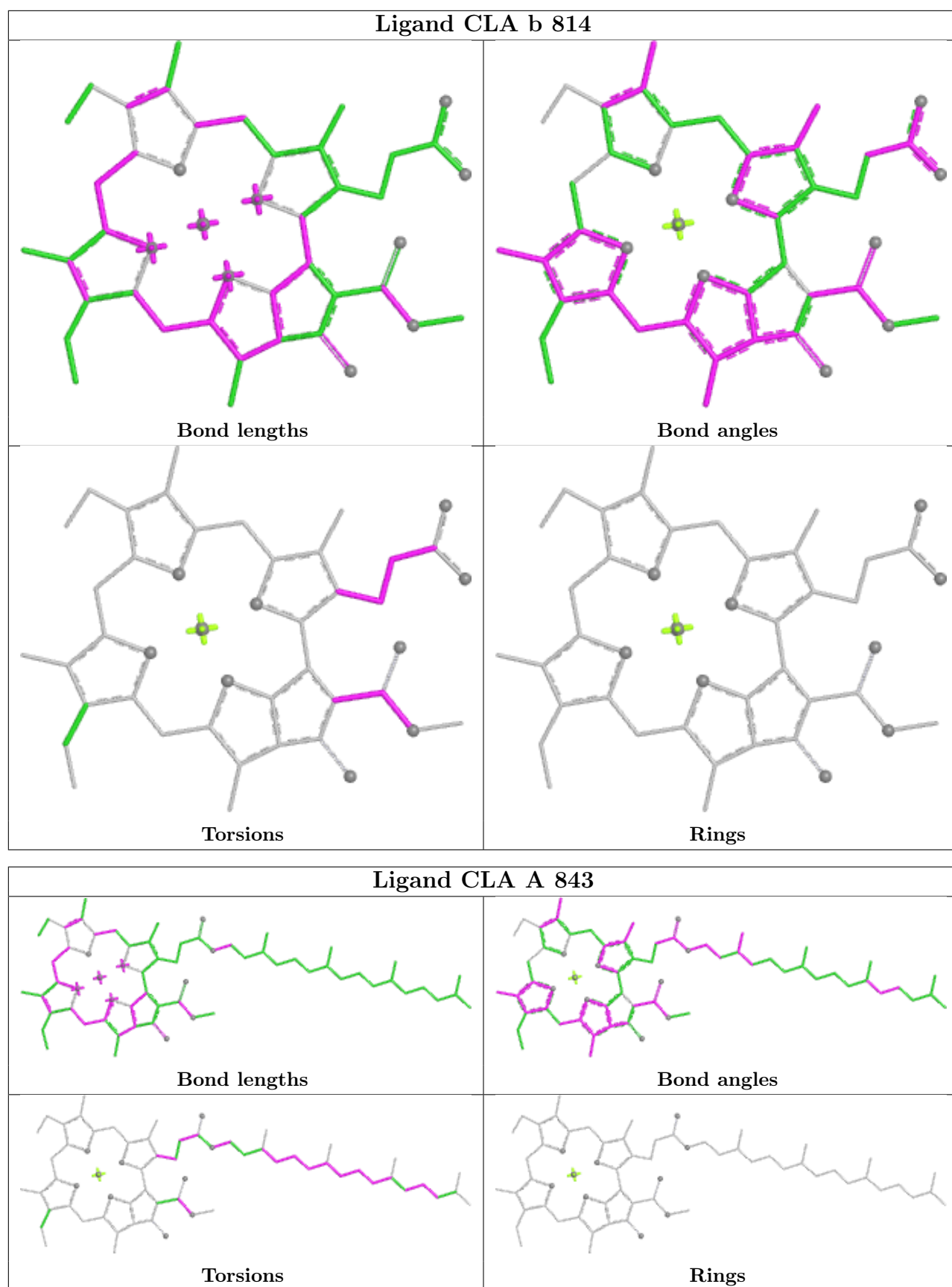
Bond angles

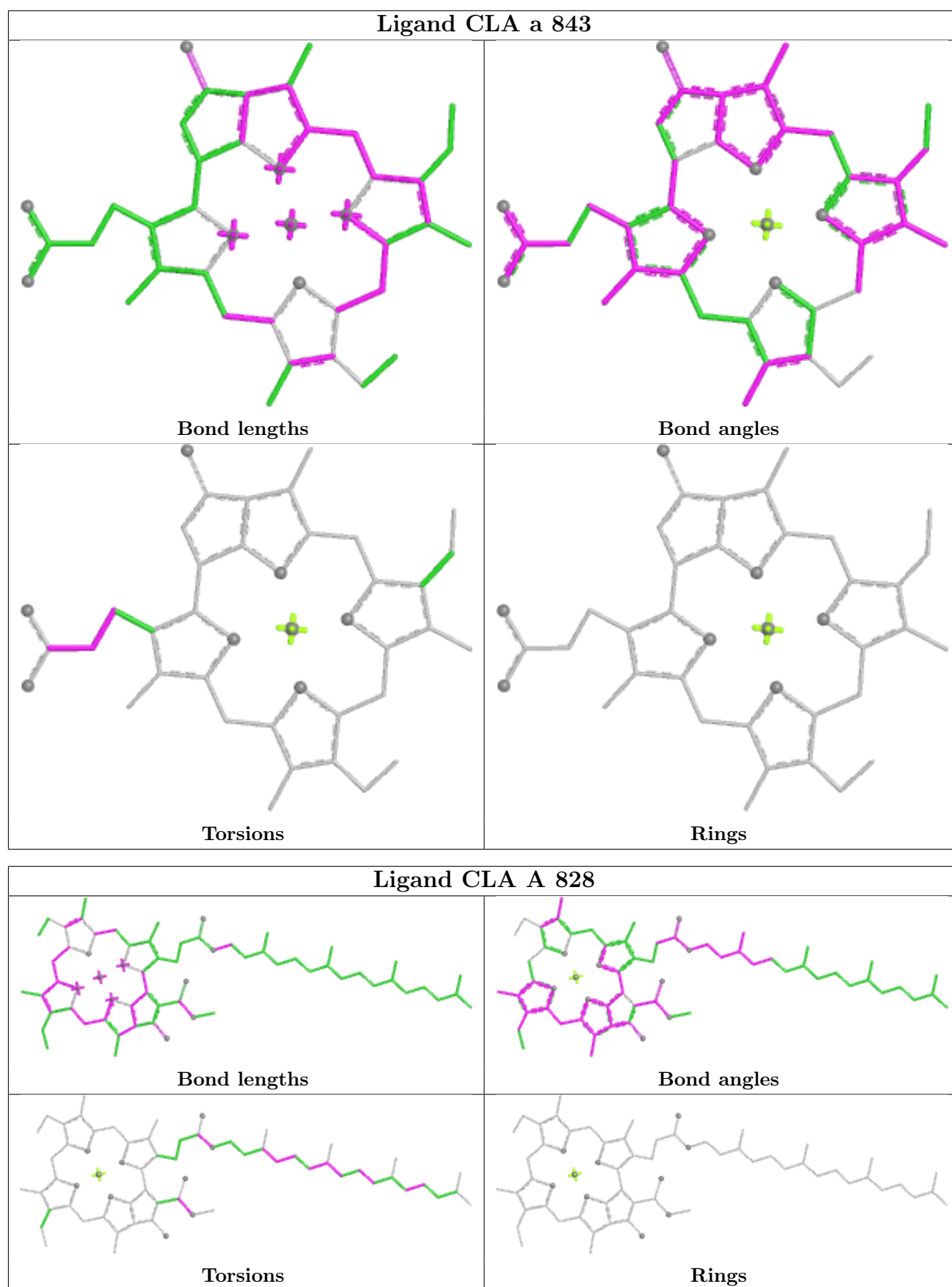


Torsions

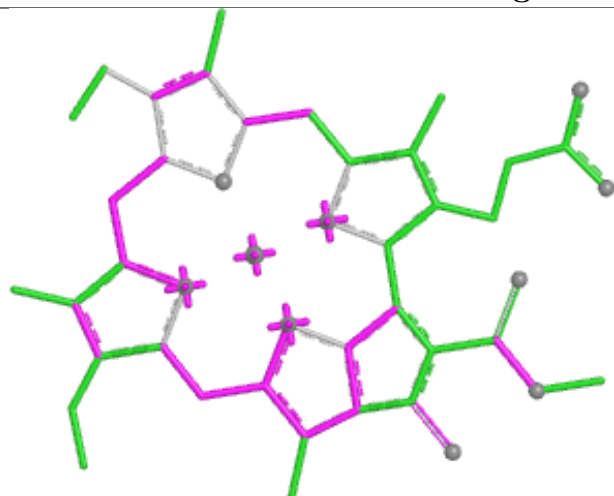


Rings

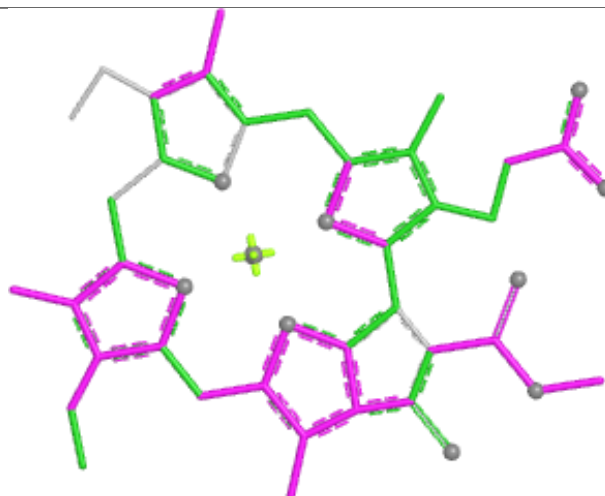




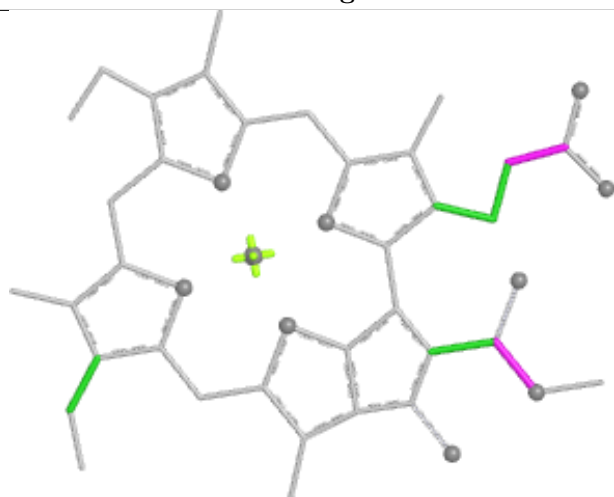
## Ligand CLA G 818



Bond lengths



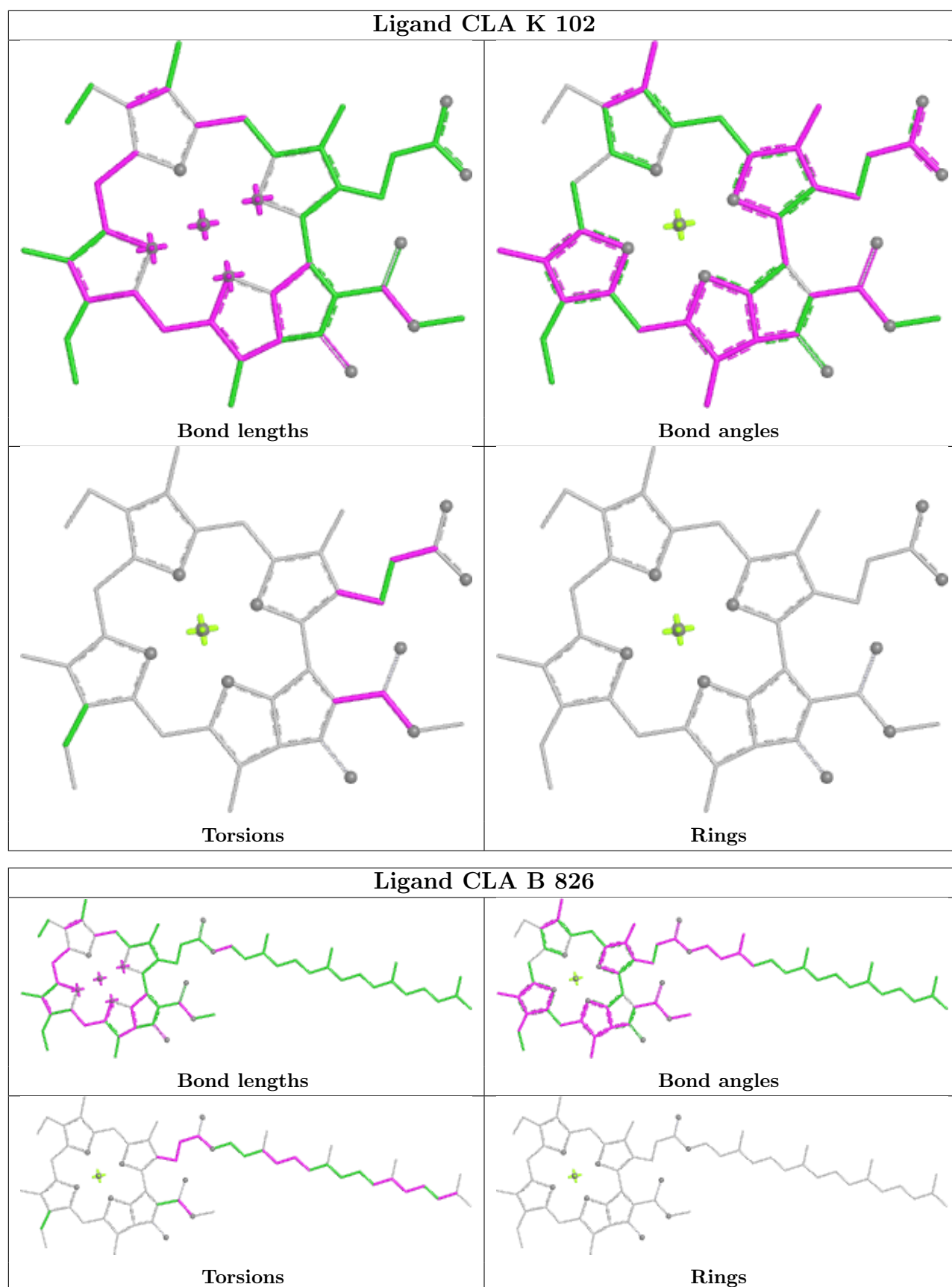
Bond angles

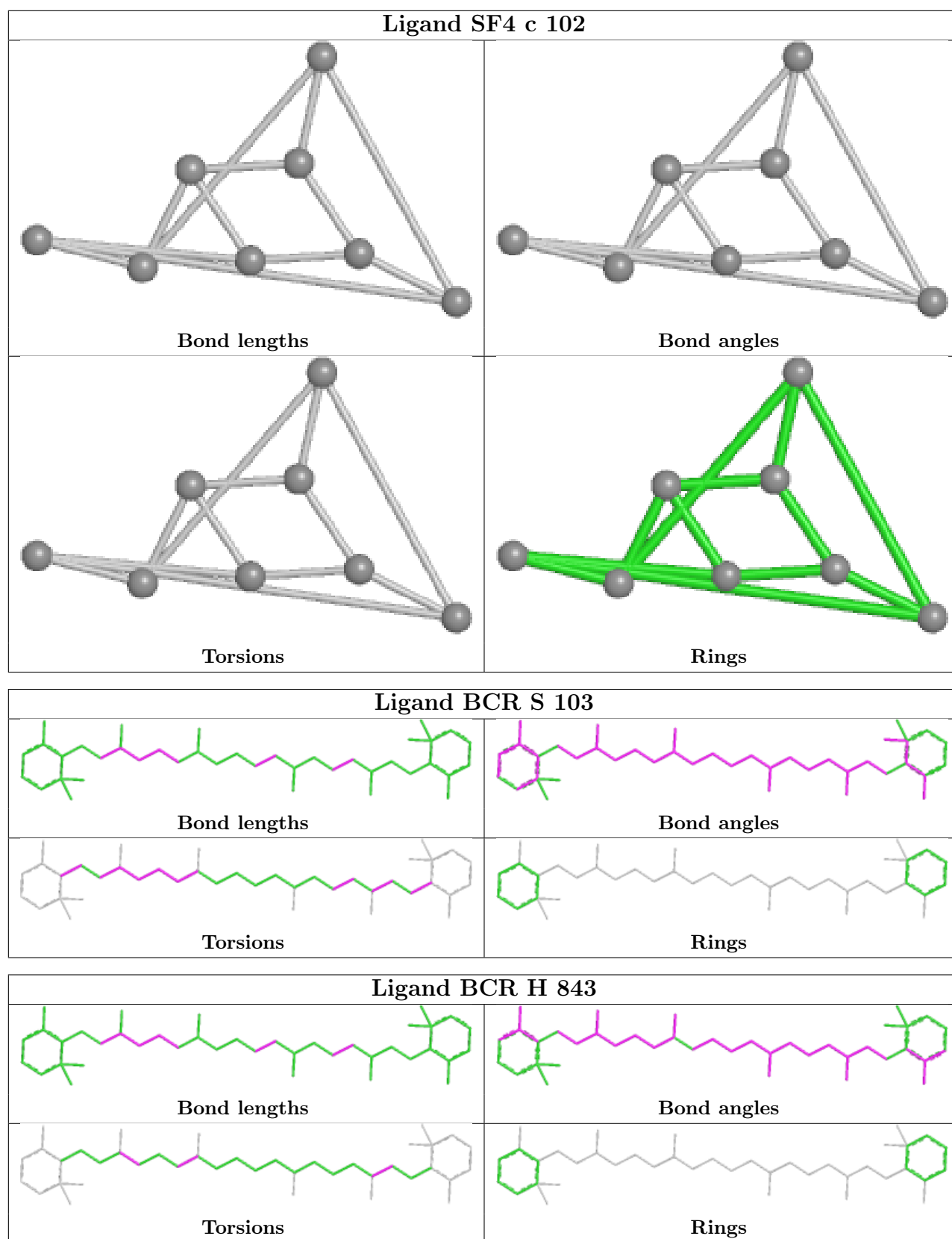


Torsions

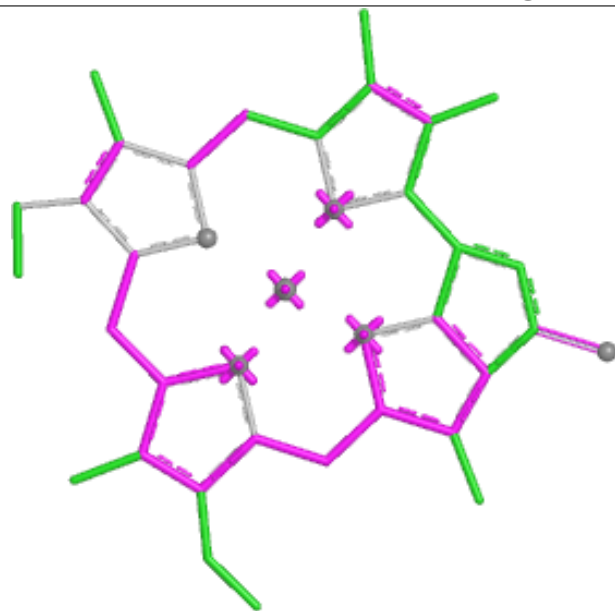


Rings

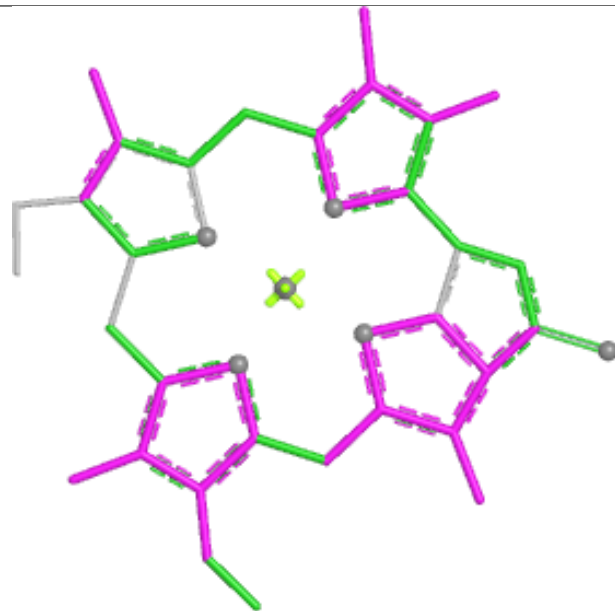




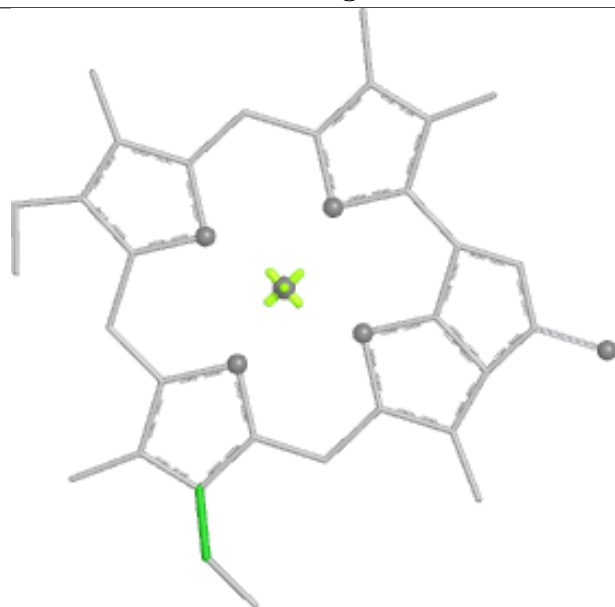
## Ligand CLA S 102



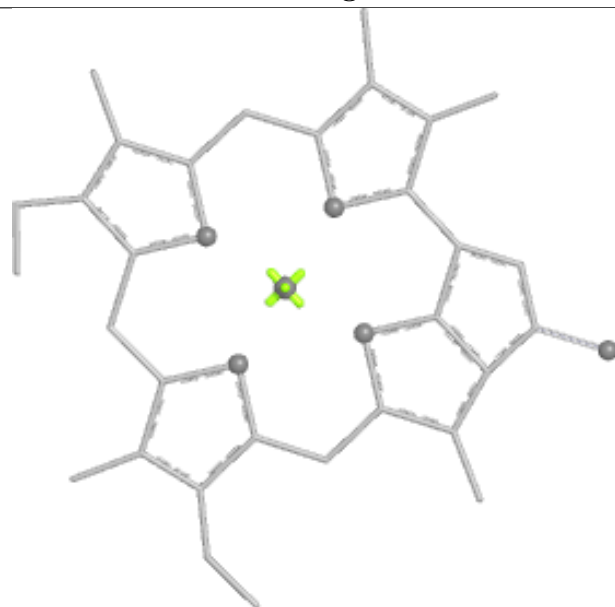
Bond lengths



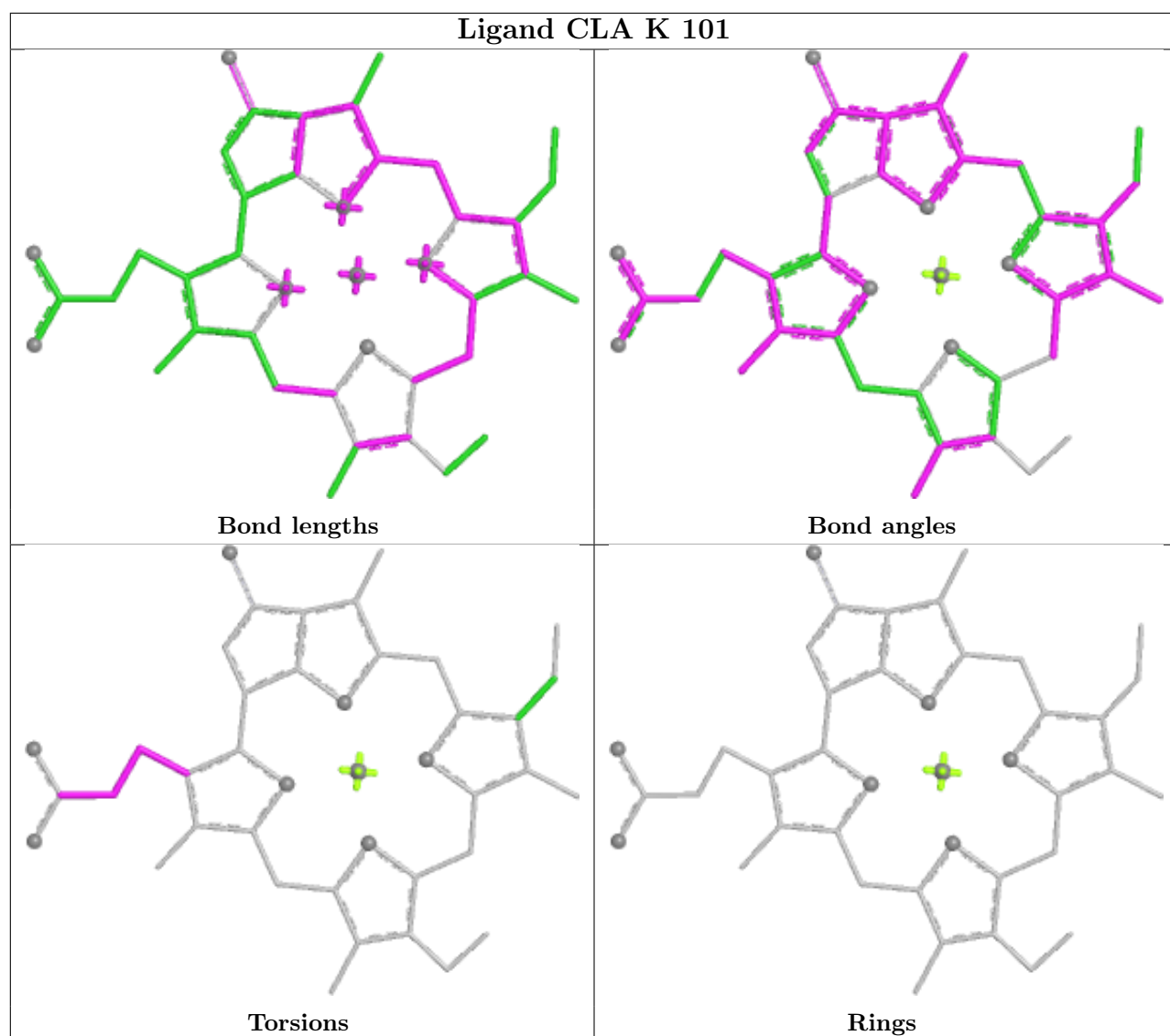
Bond angles



Torsions

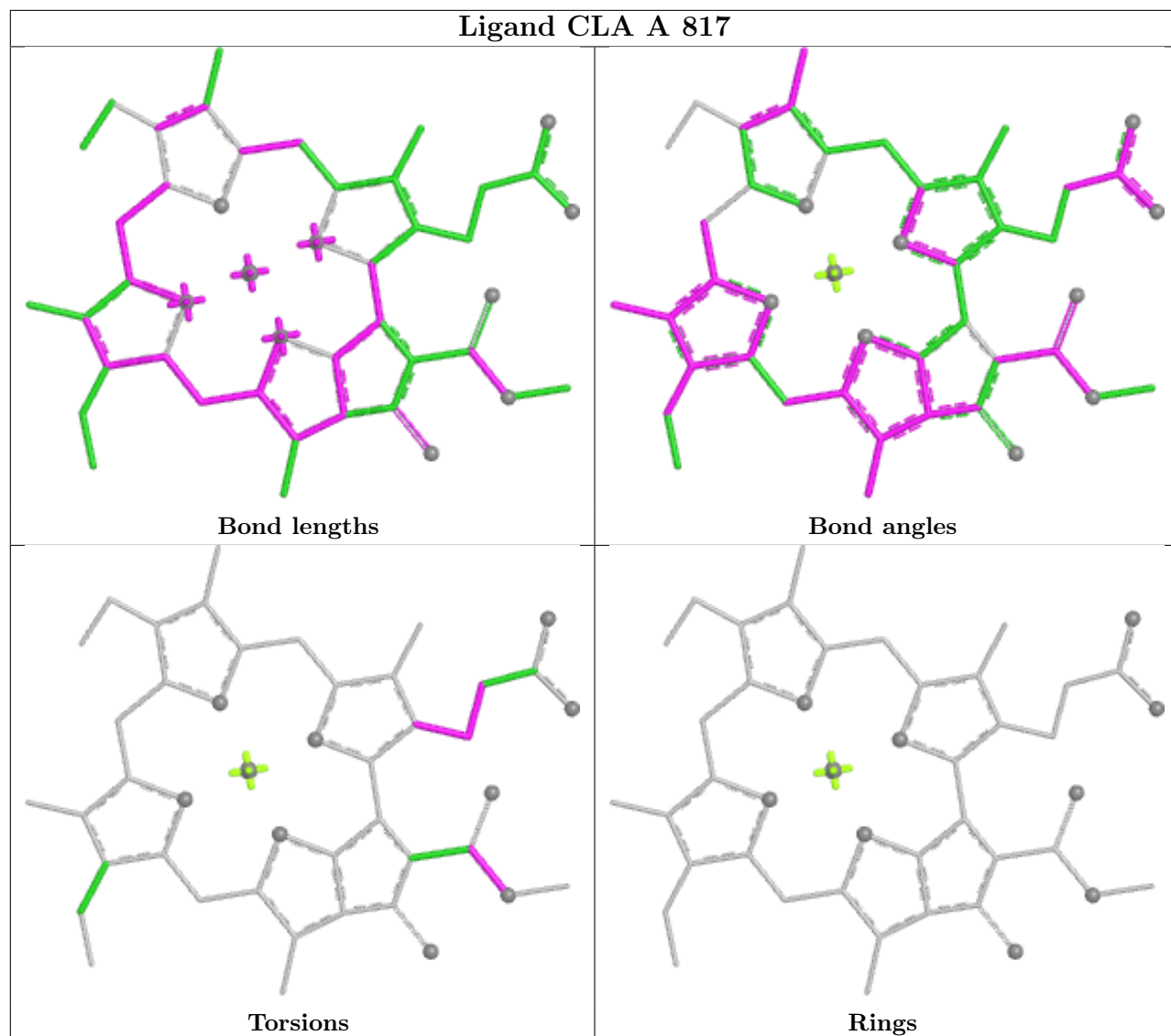


Rings

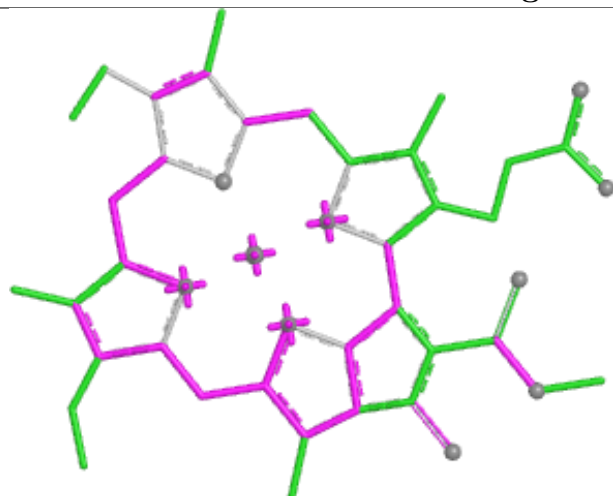




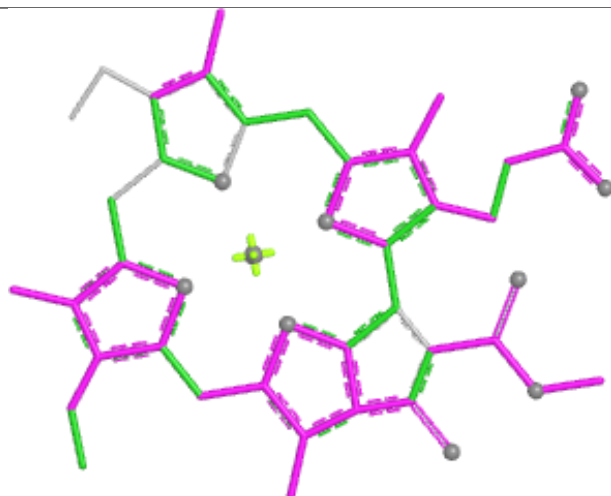
## Ligand CLA A 817



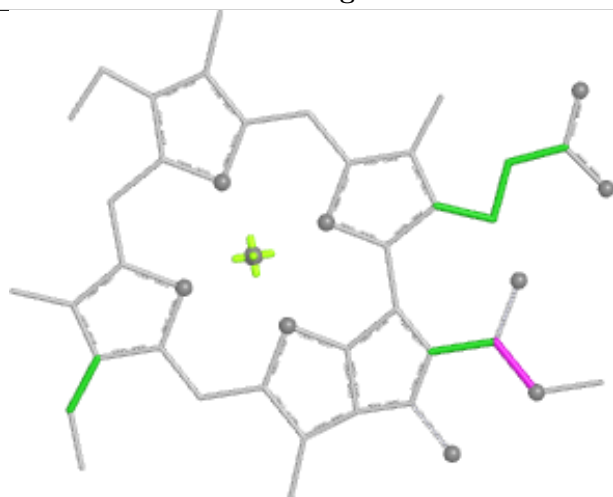
## Ligand CLA f 202



Bond lengths



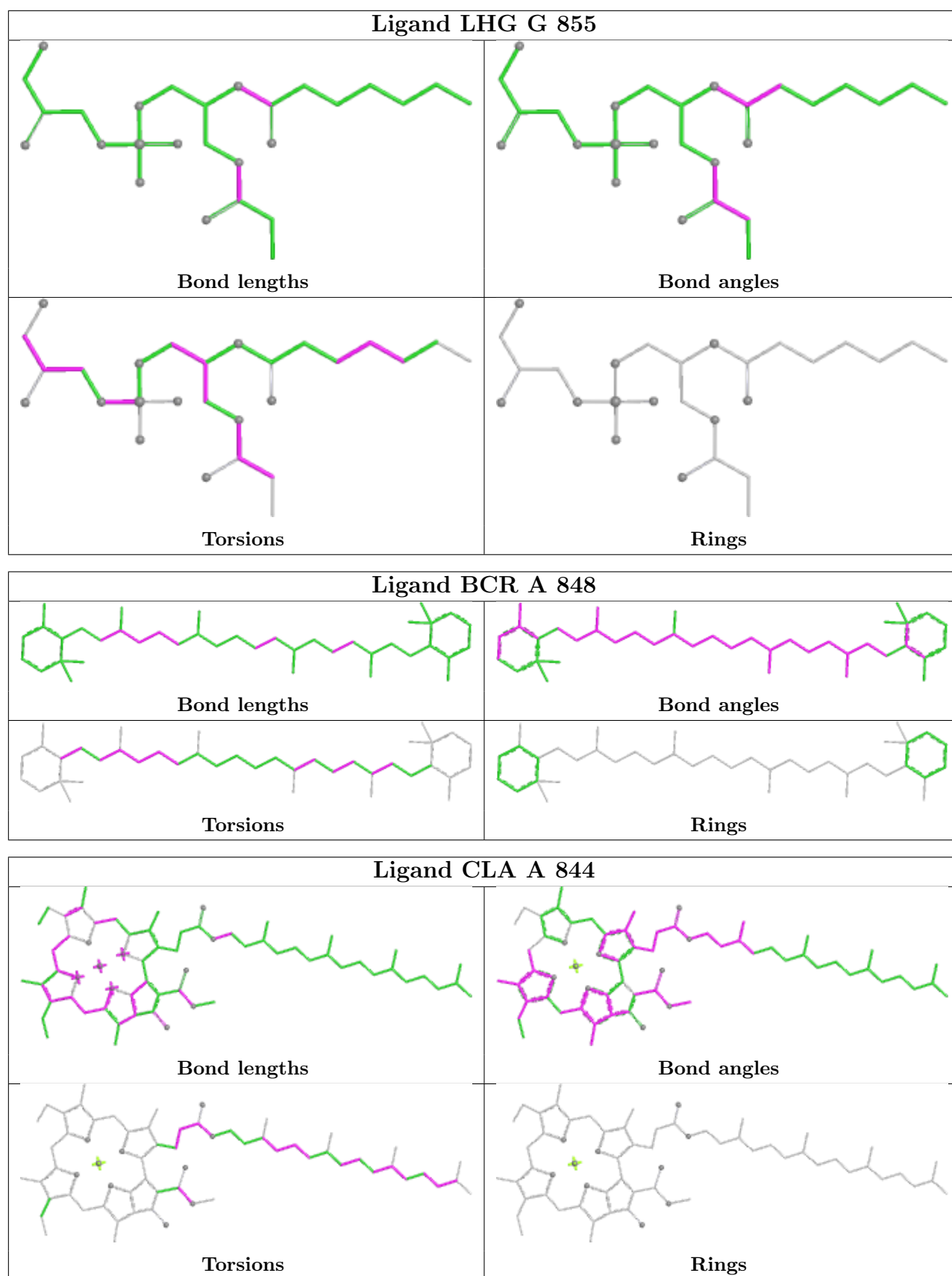
Bond angles



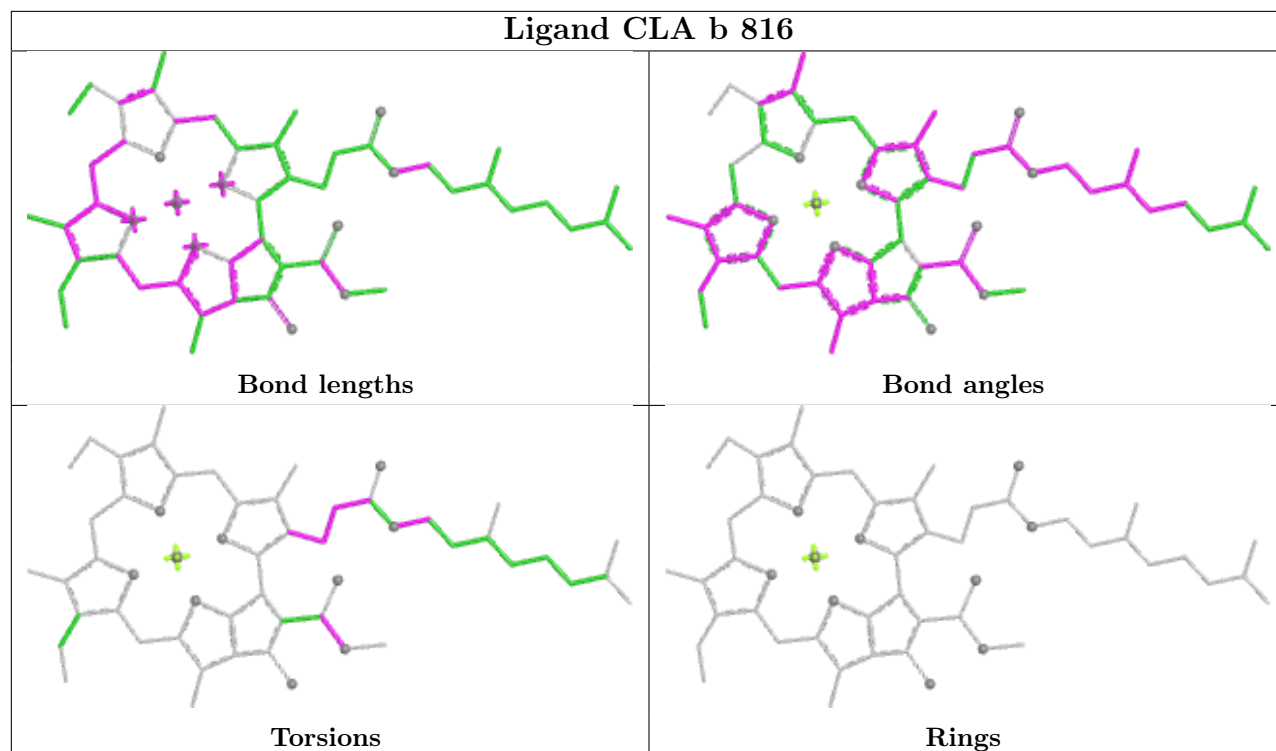
Torsions



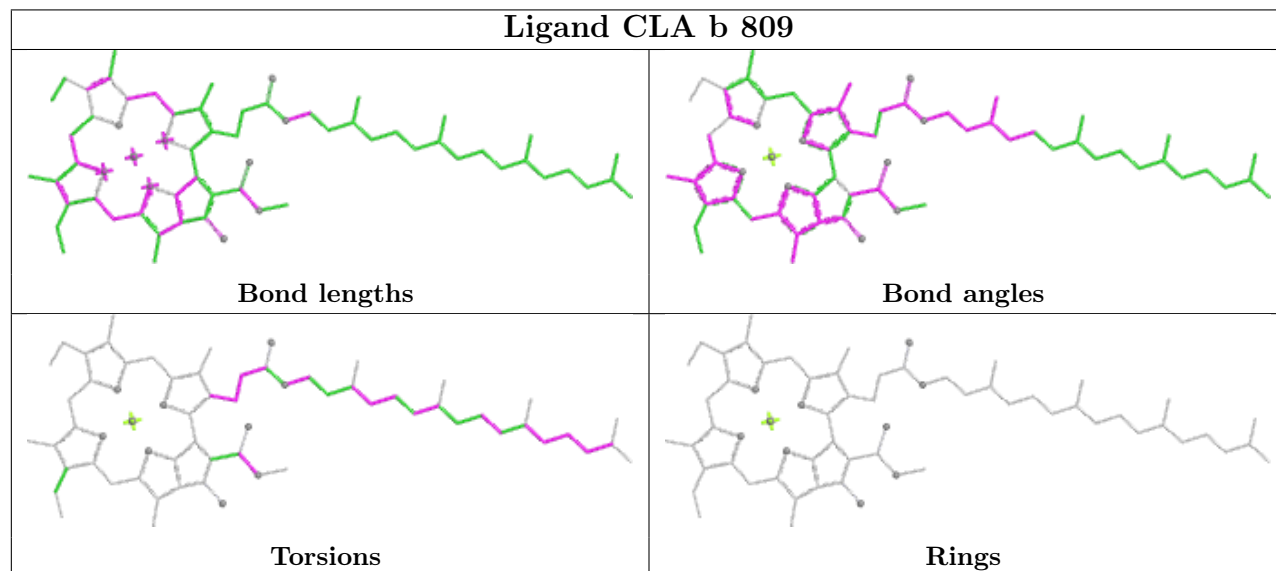
Rings



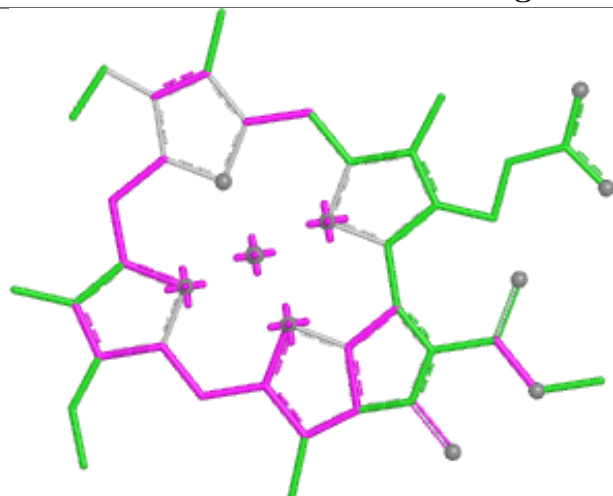
## Ligand CLA b 816



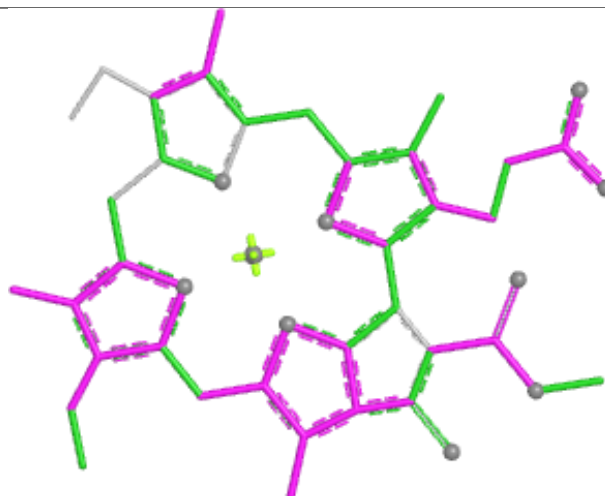
## Ligand CLA b 809



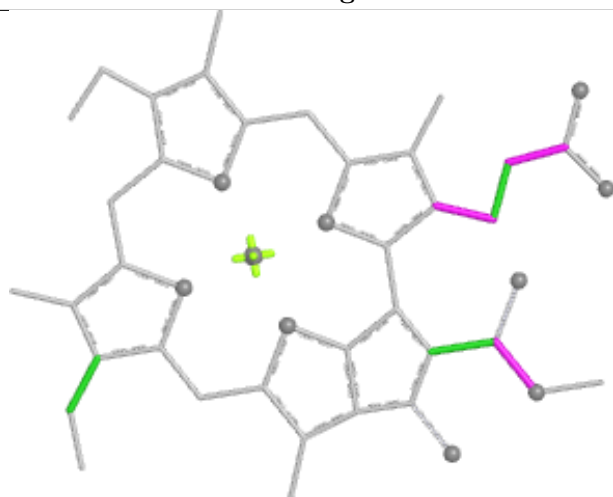
## Ligand CLA B 838



Bond lengths



Bond angles

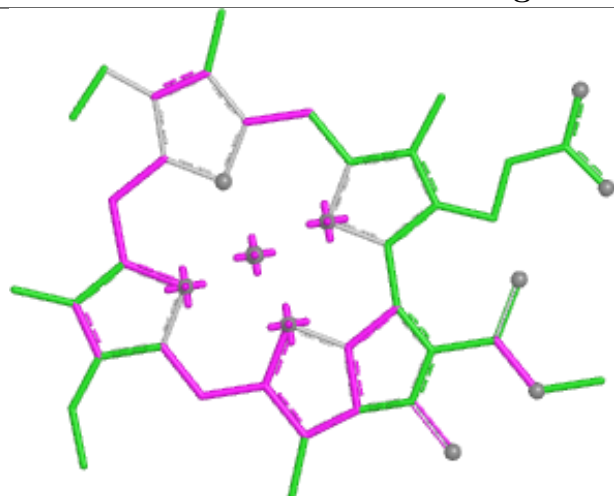


Torsions

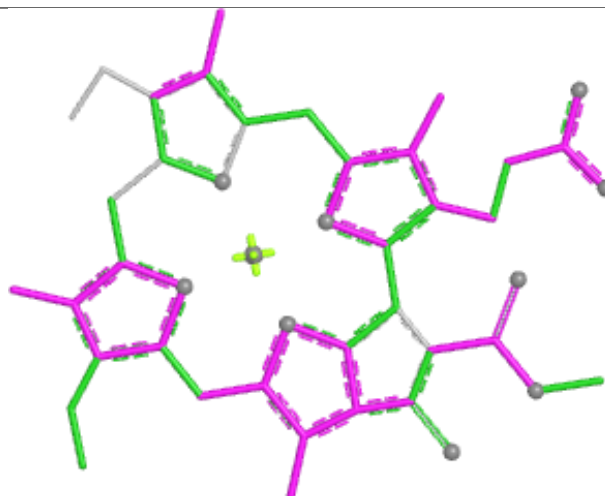


Rings

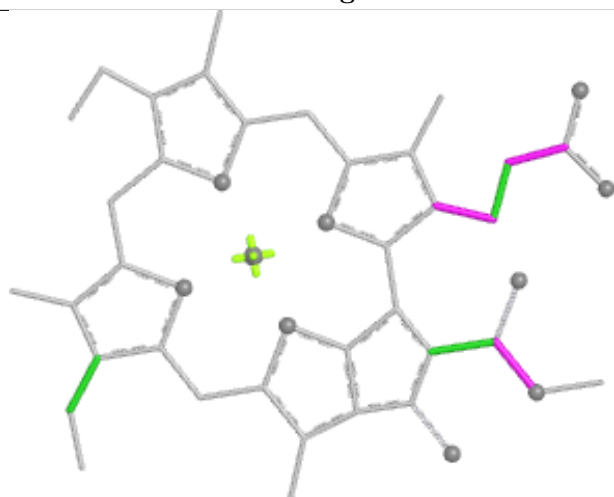
## Ligand CLA H 815



Bond lengths



Bond angles

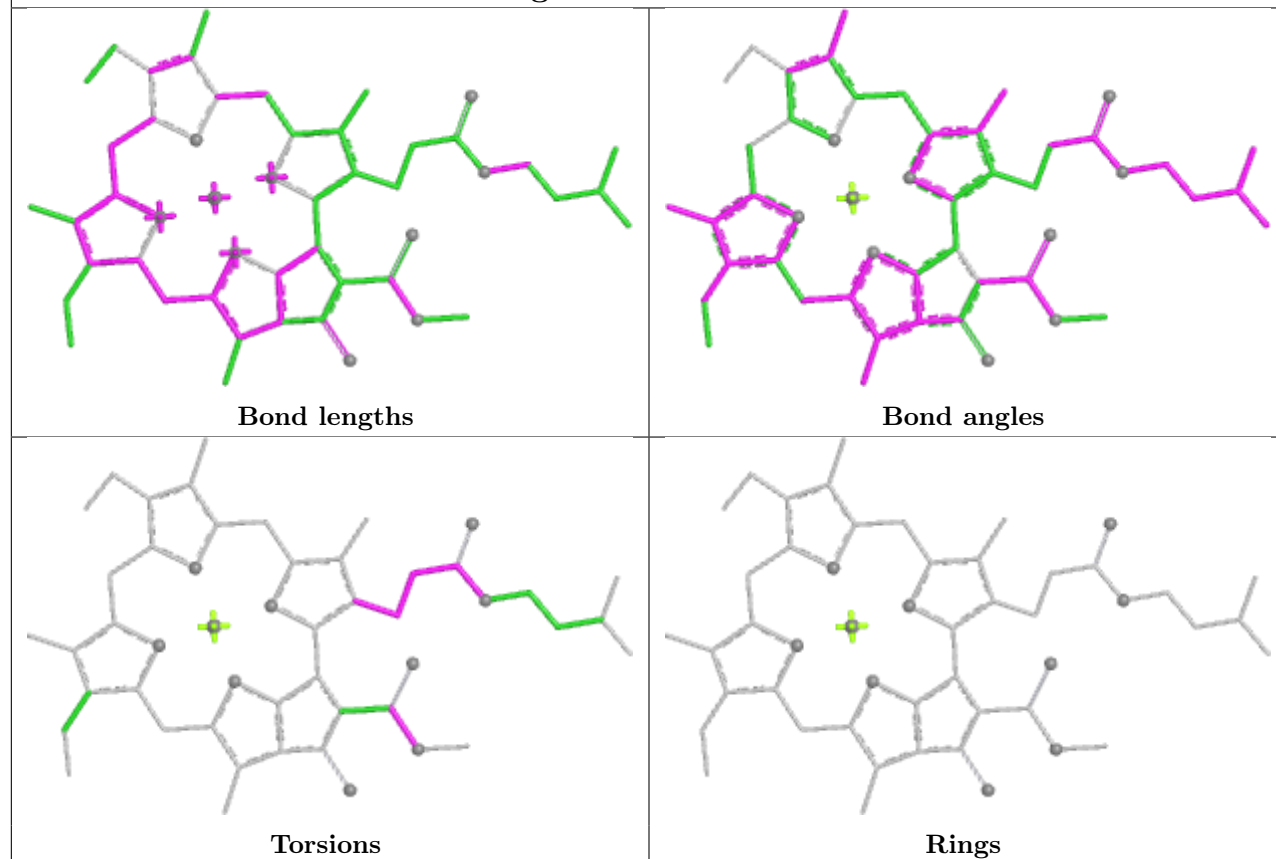


Torsions

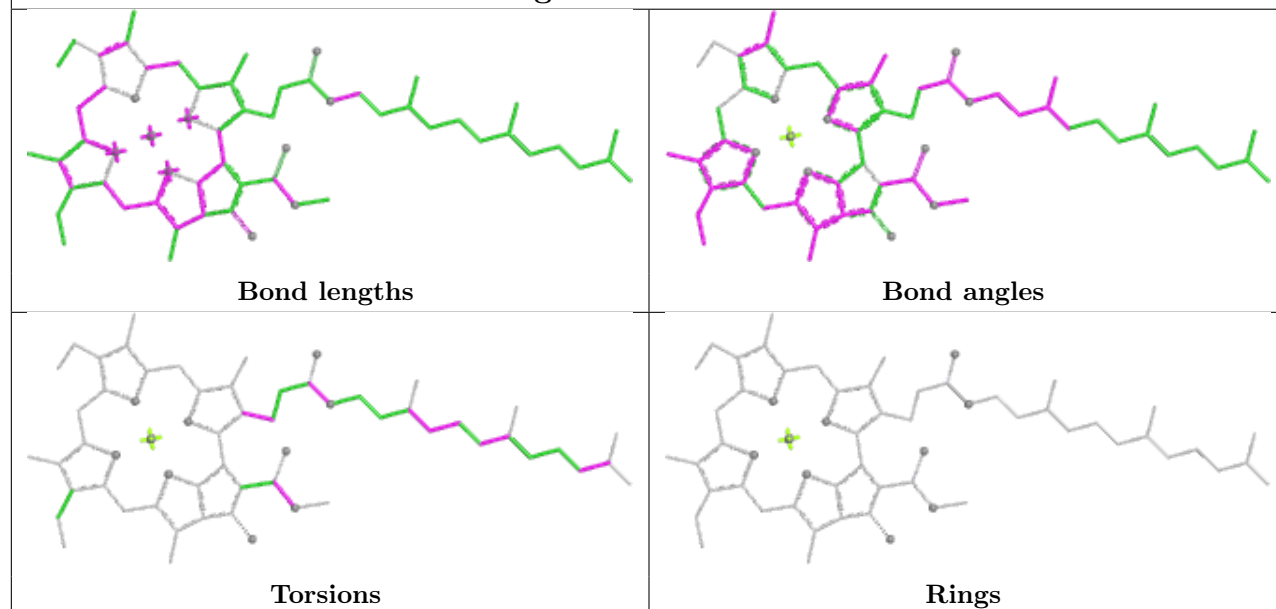


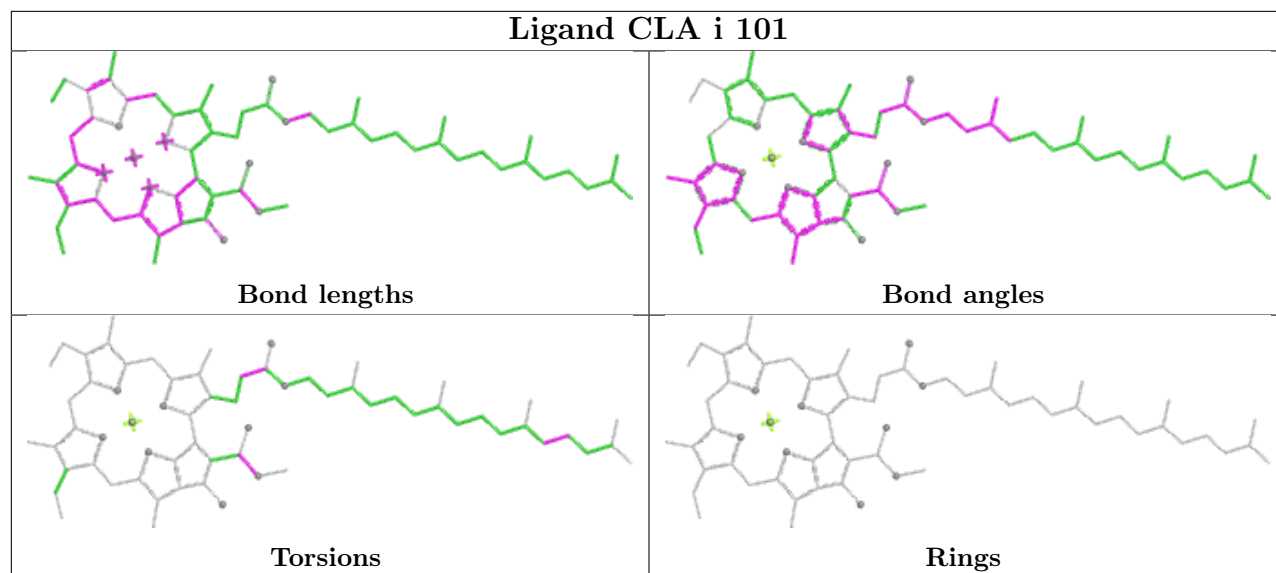
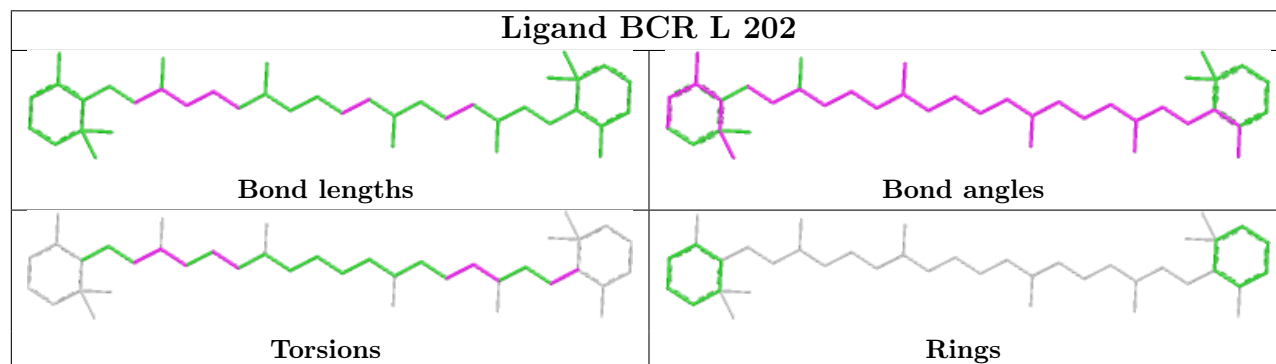
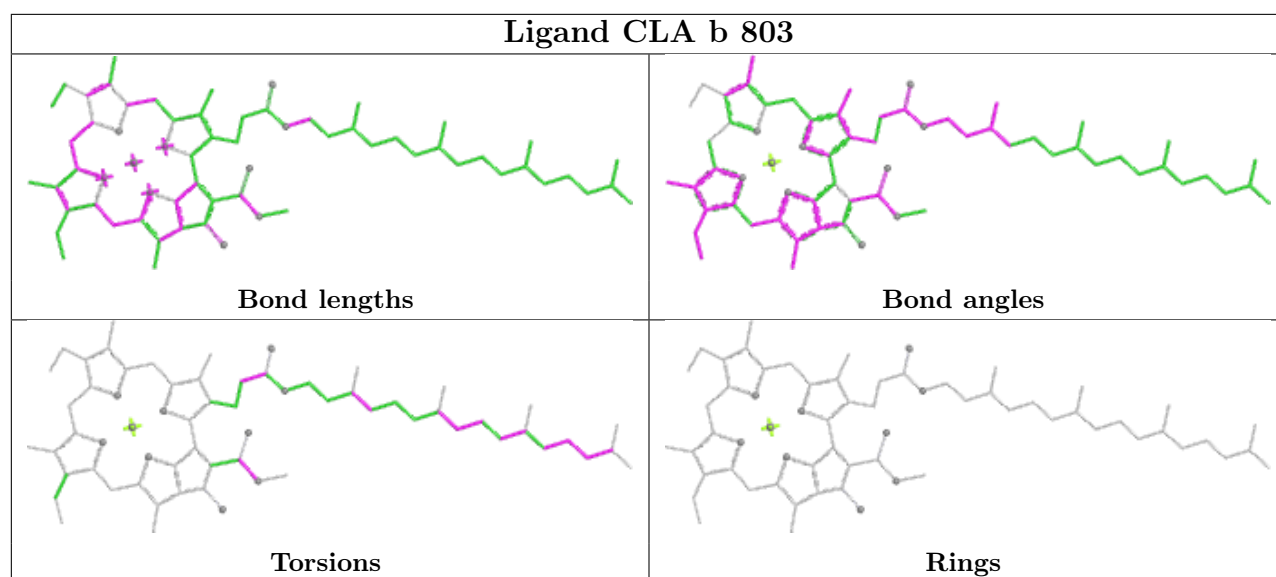
Rings

## Ligand CLA G 819

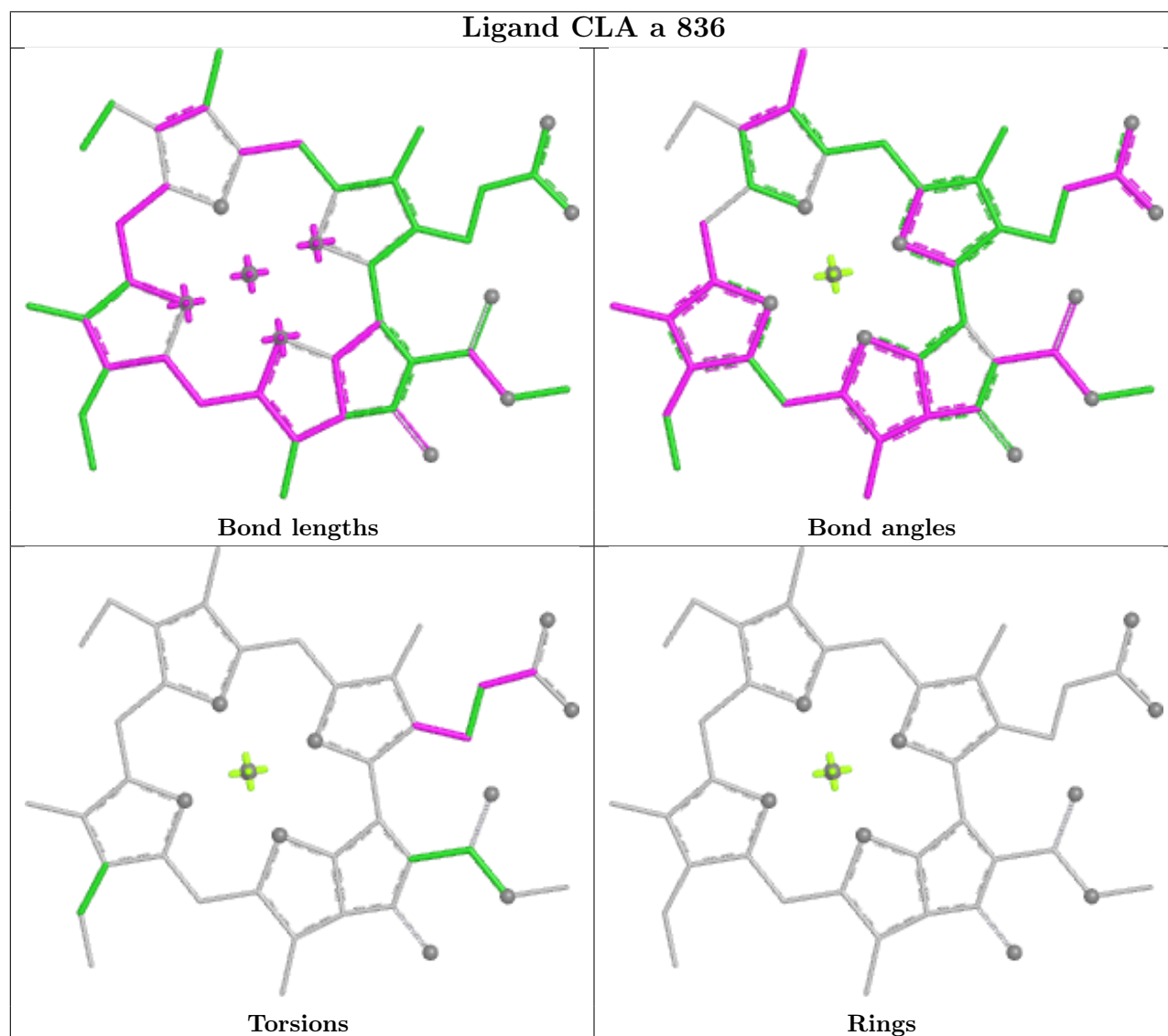
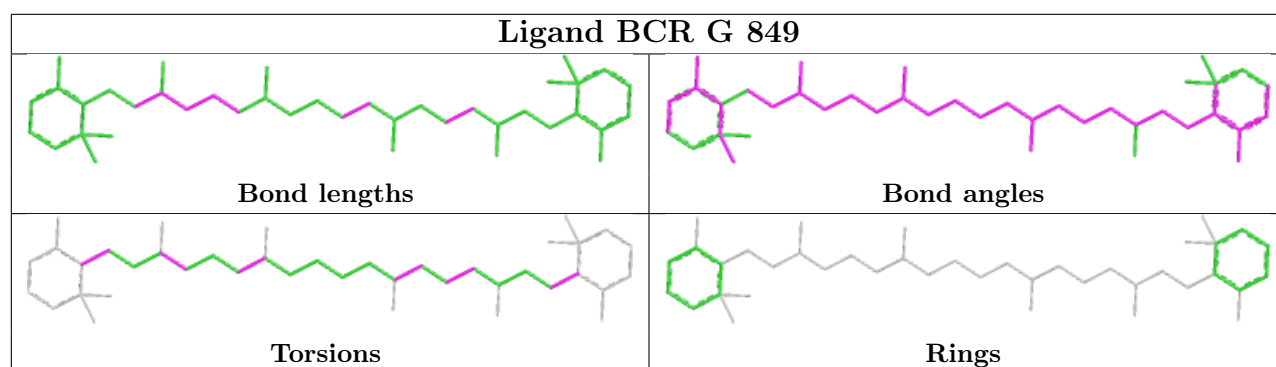


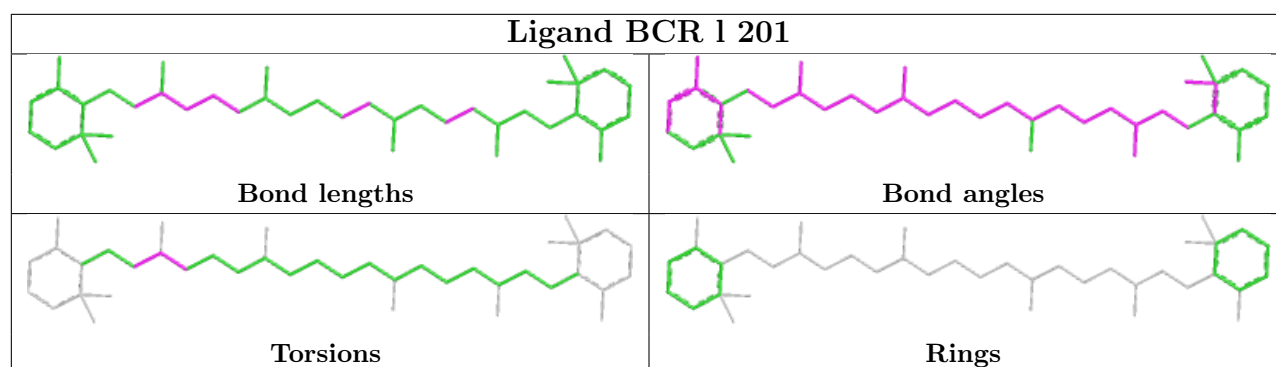
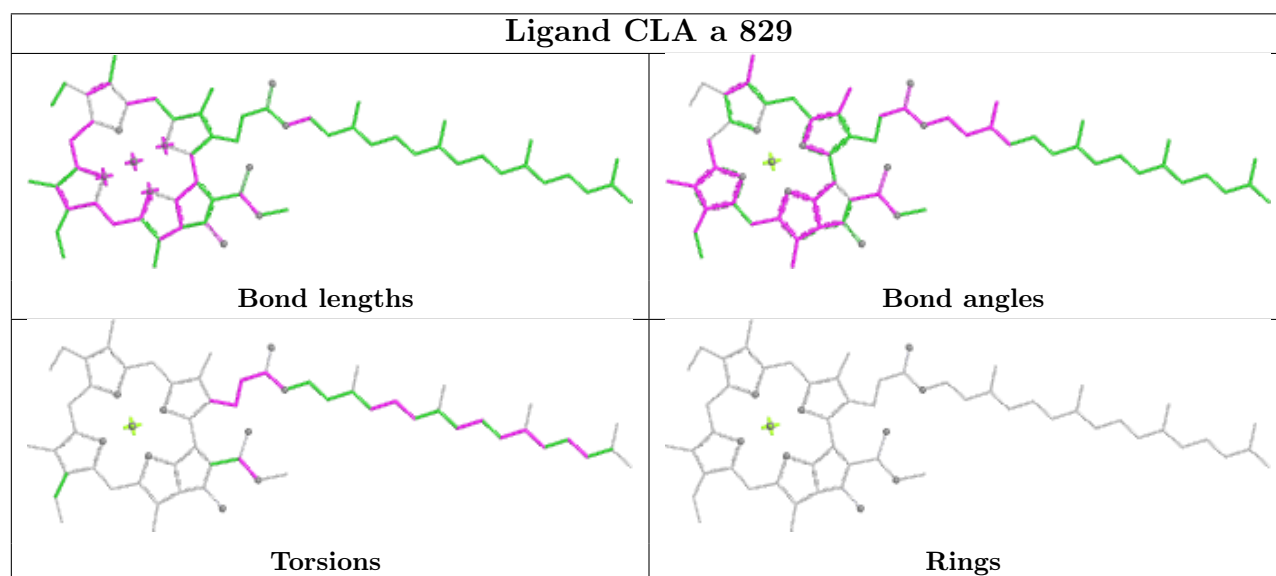
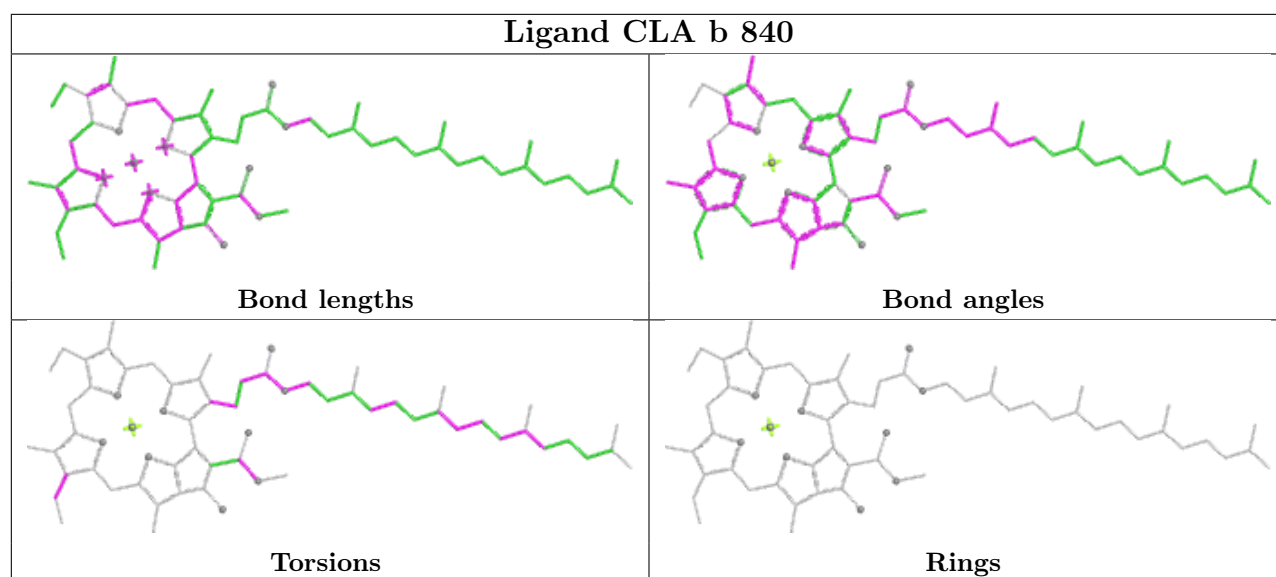
## Ligand CLA L 204

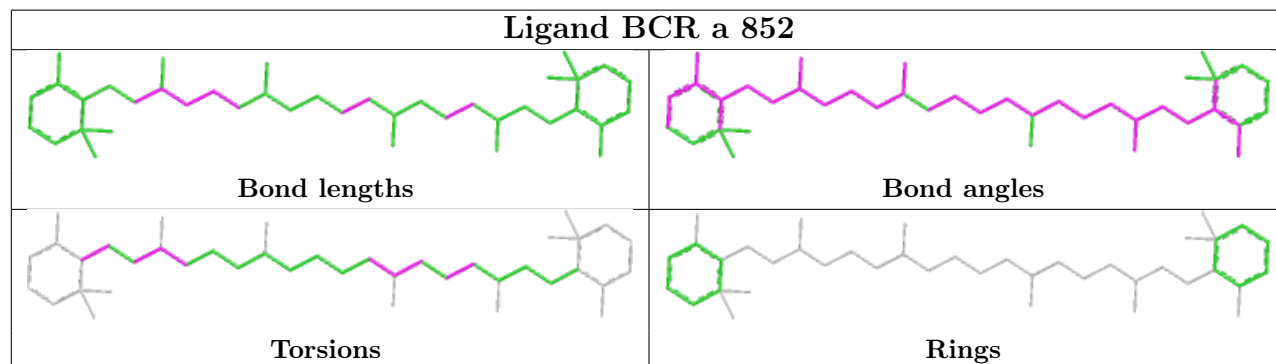
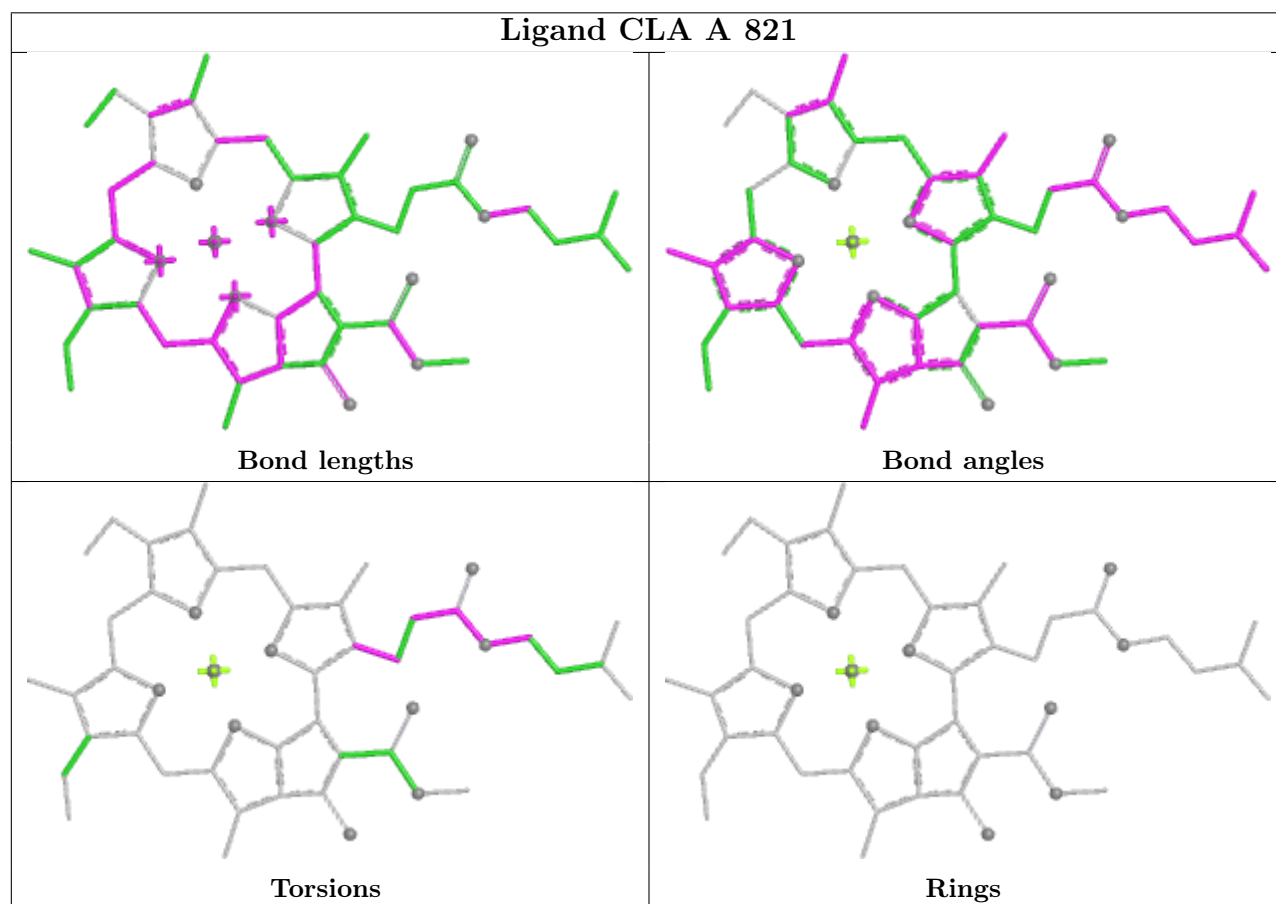
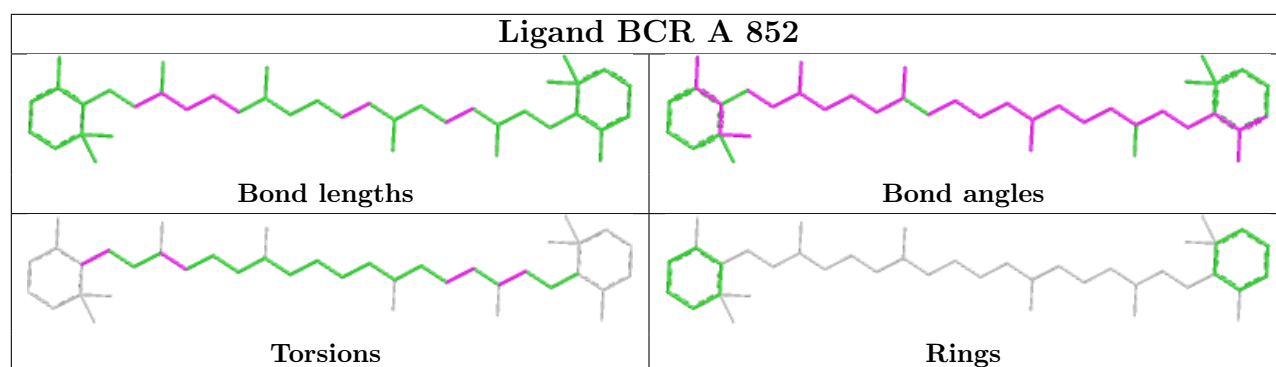


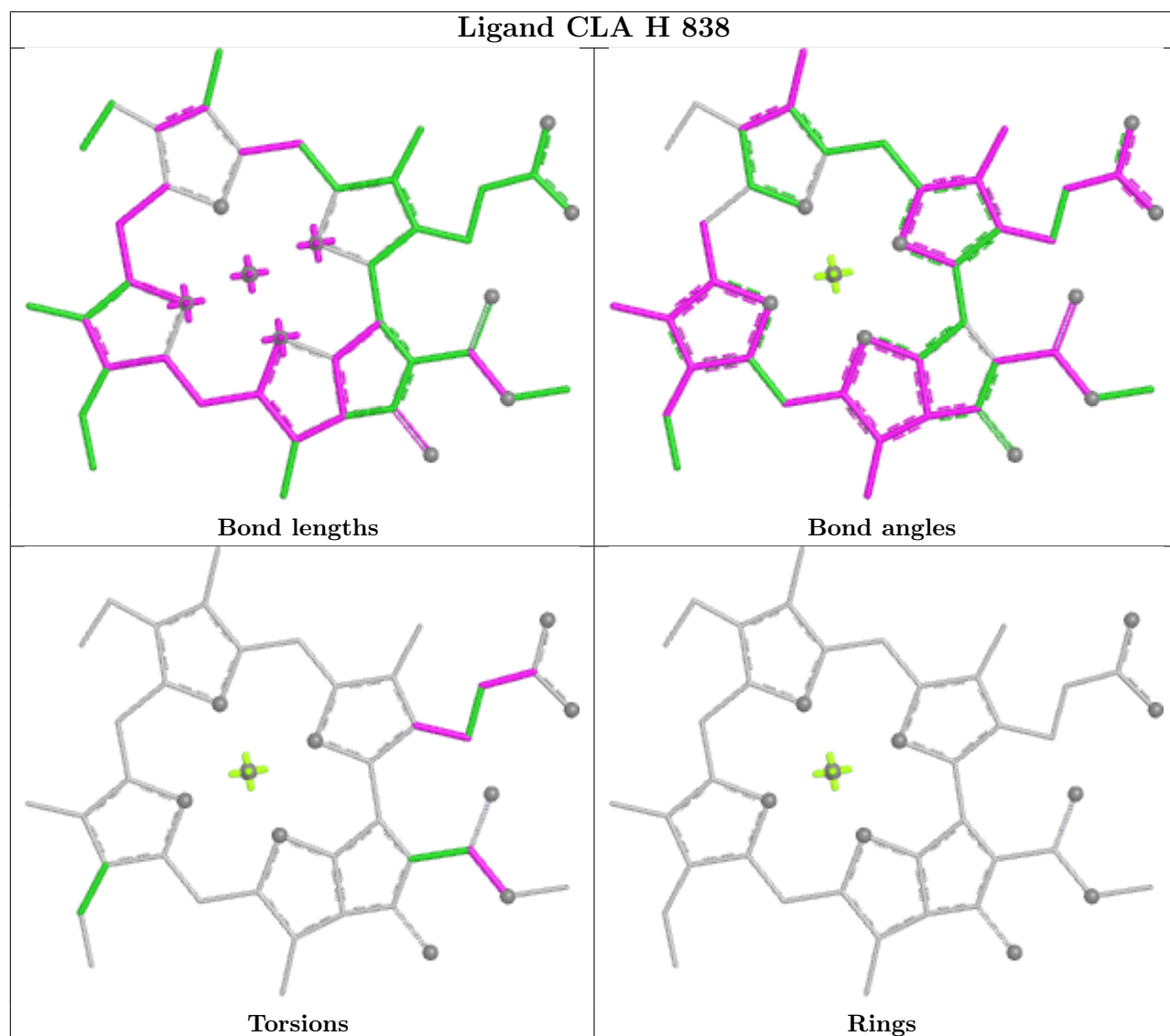
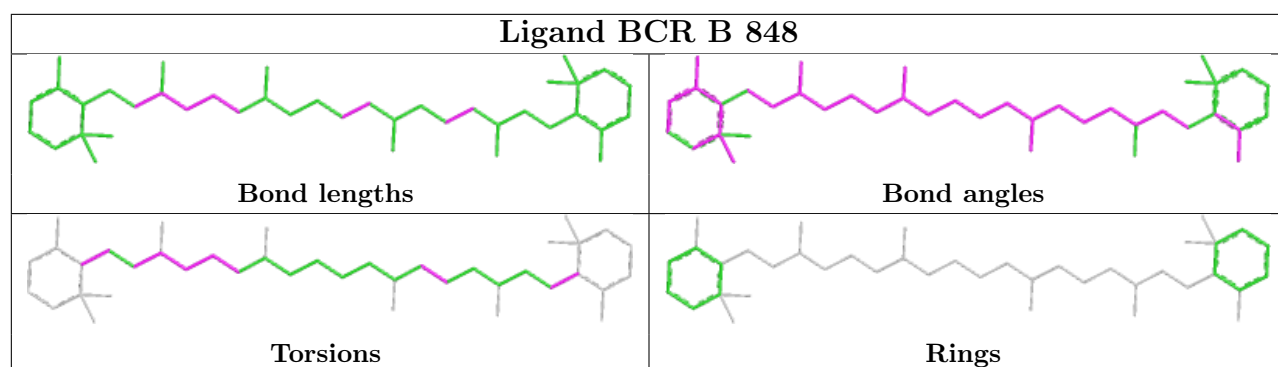


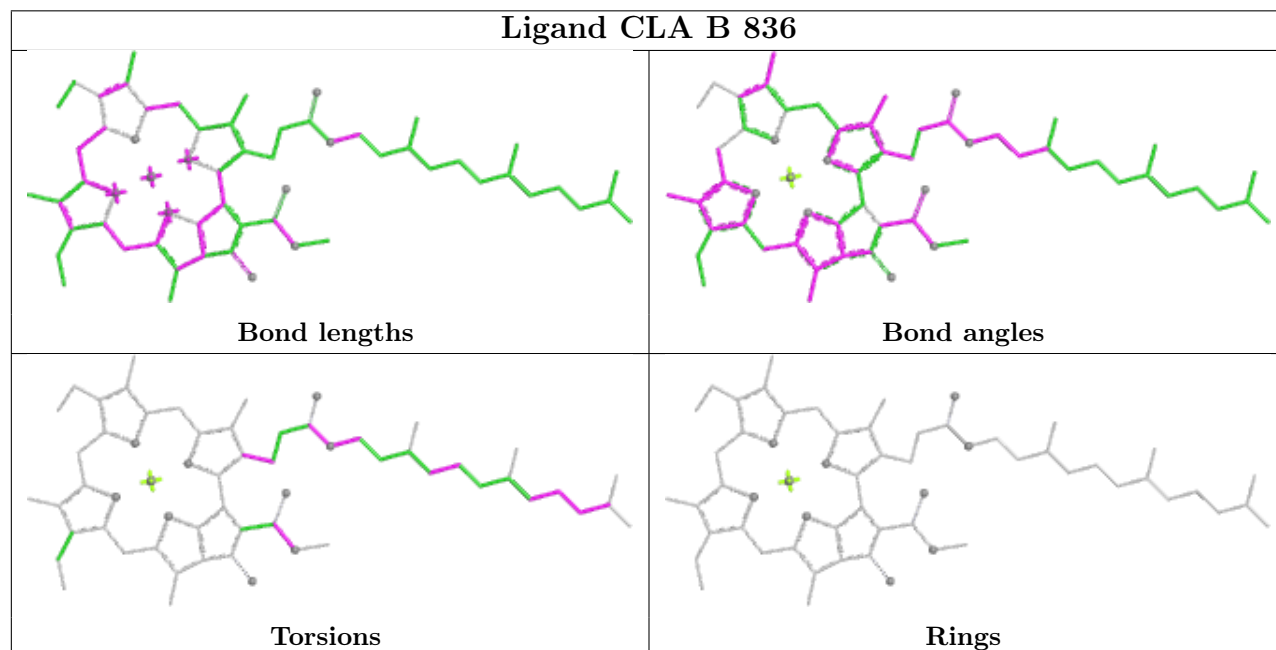
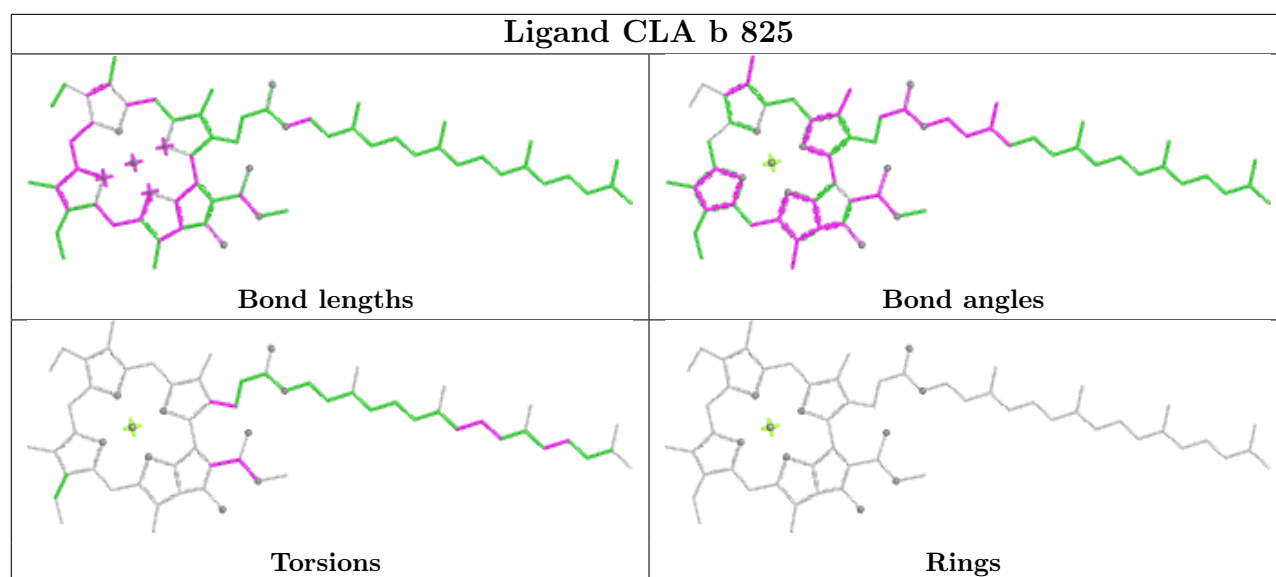




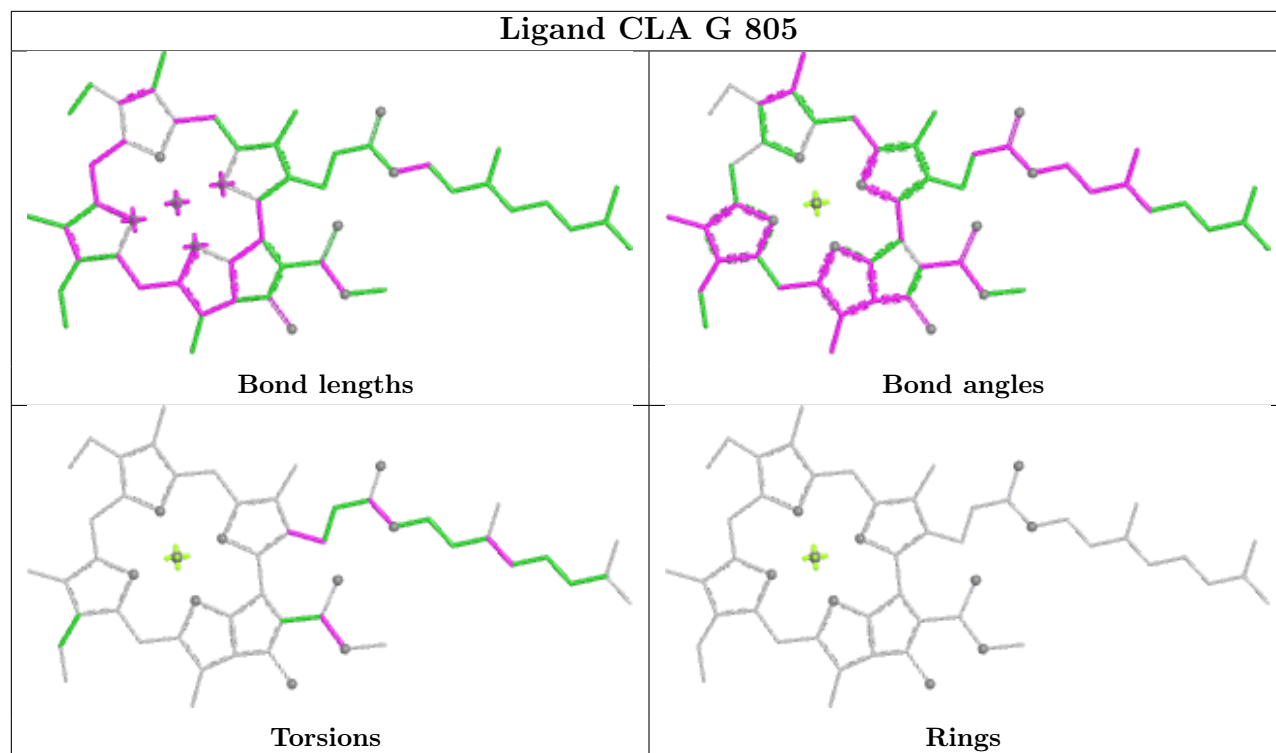




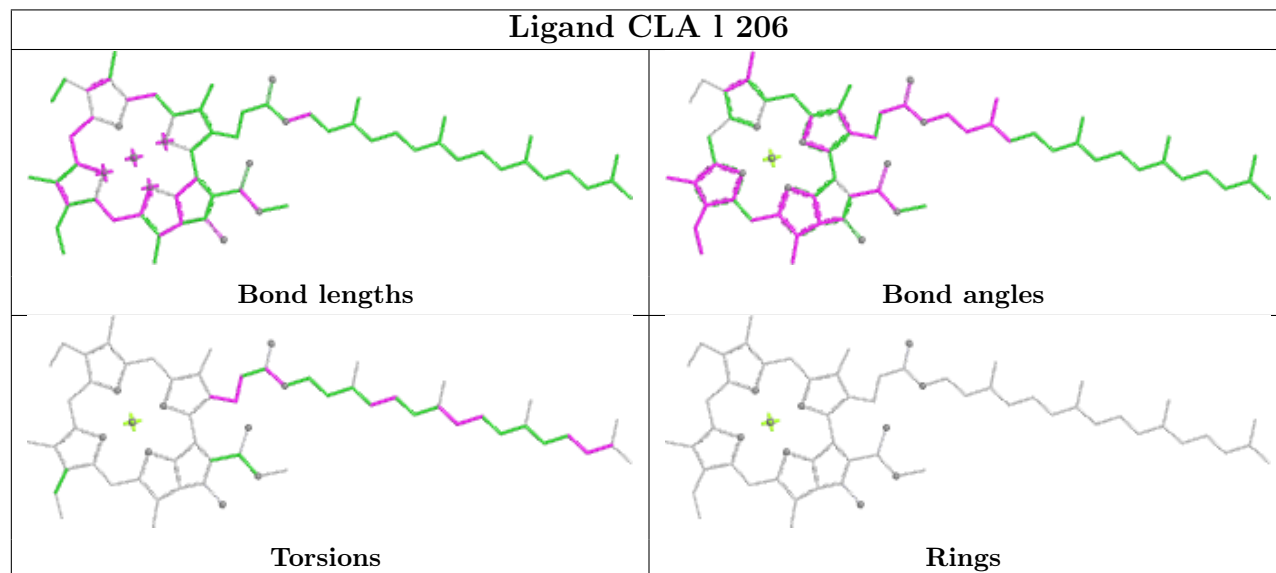


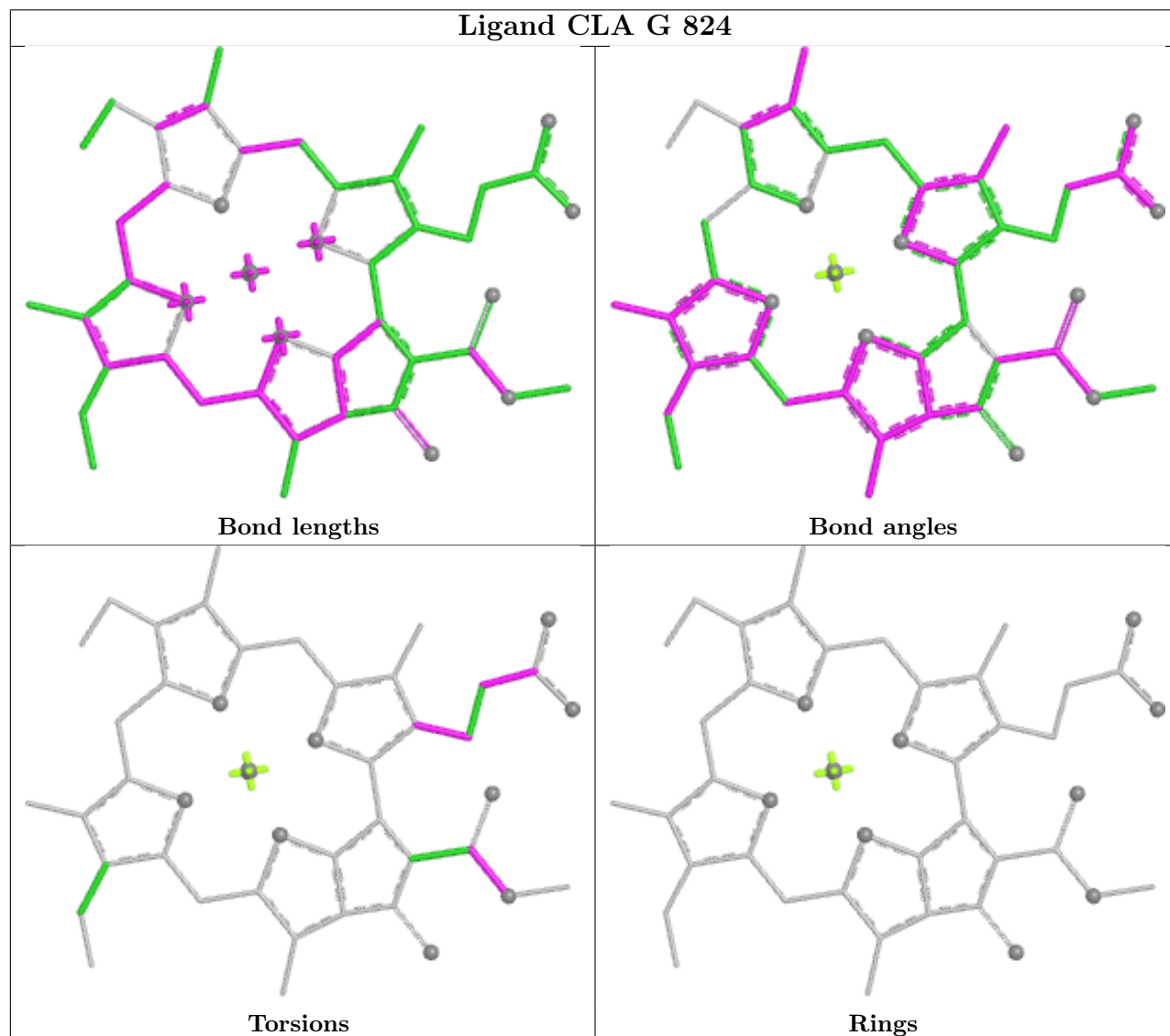
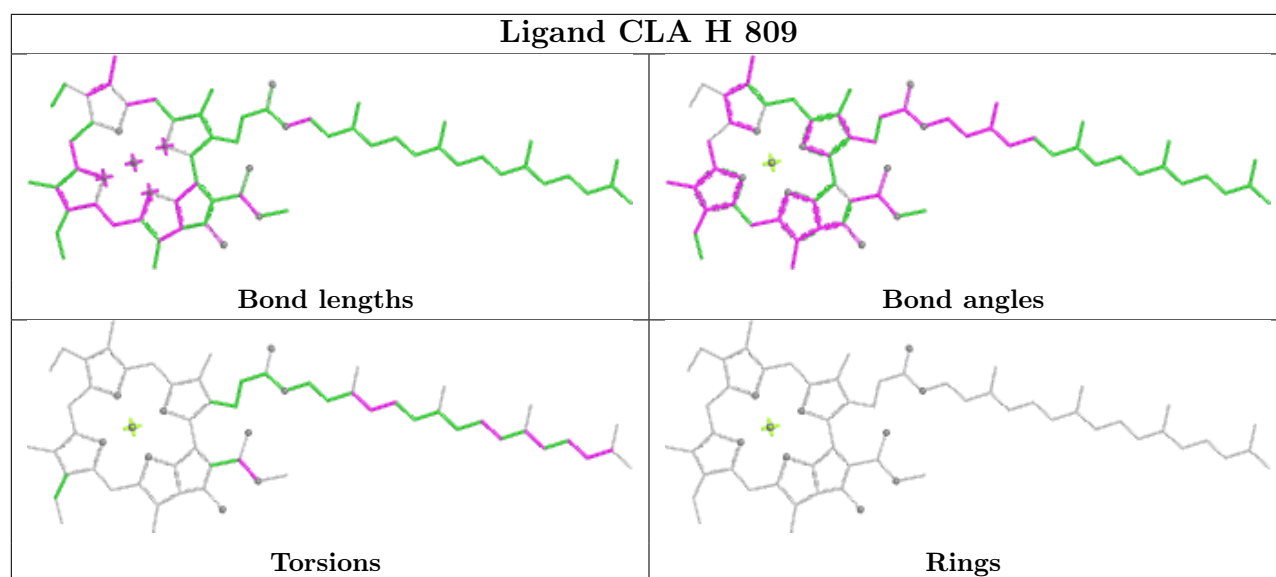


## Ligand CLA G 805

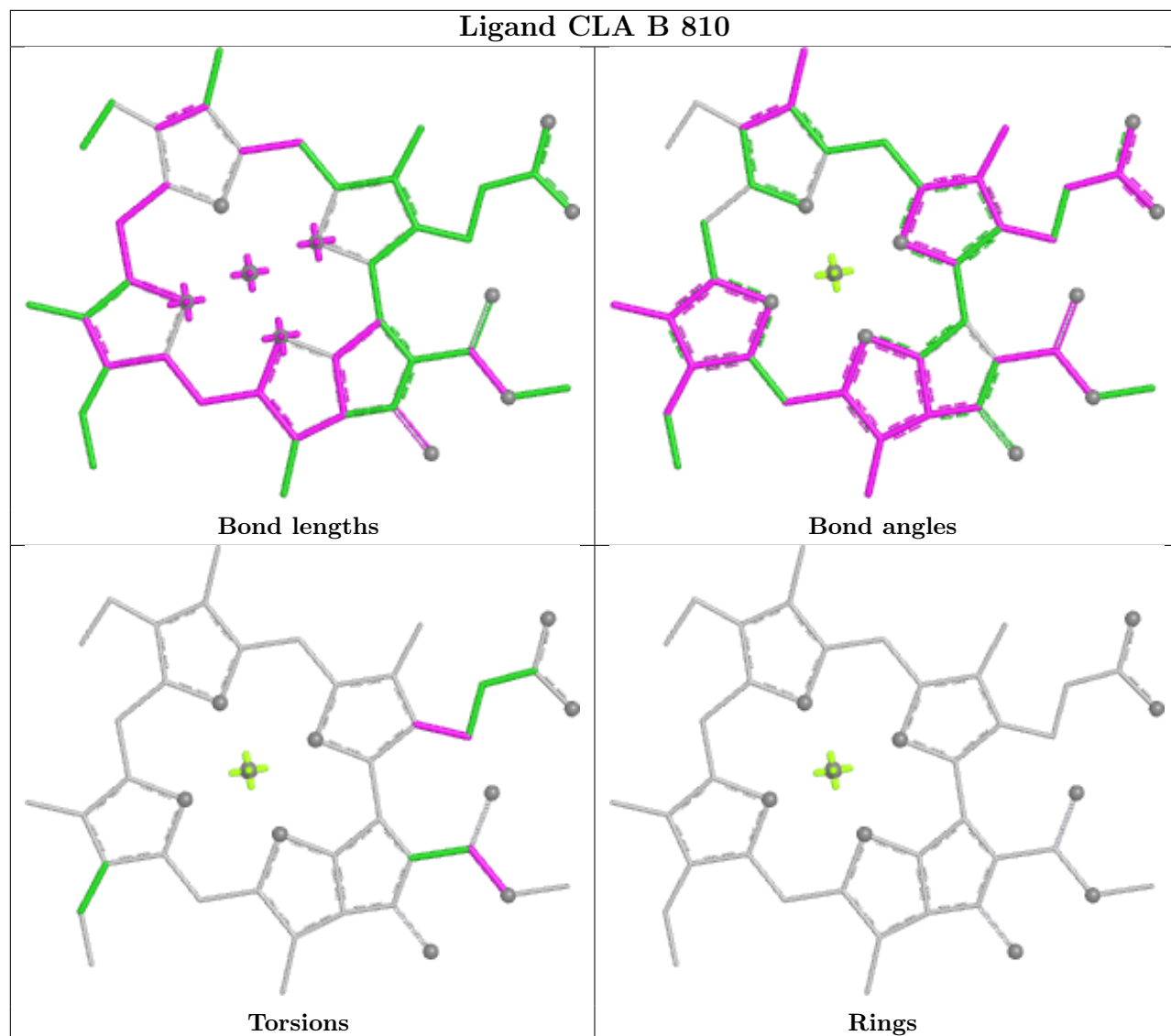


## Ligand CLA I 206

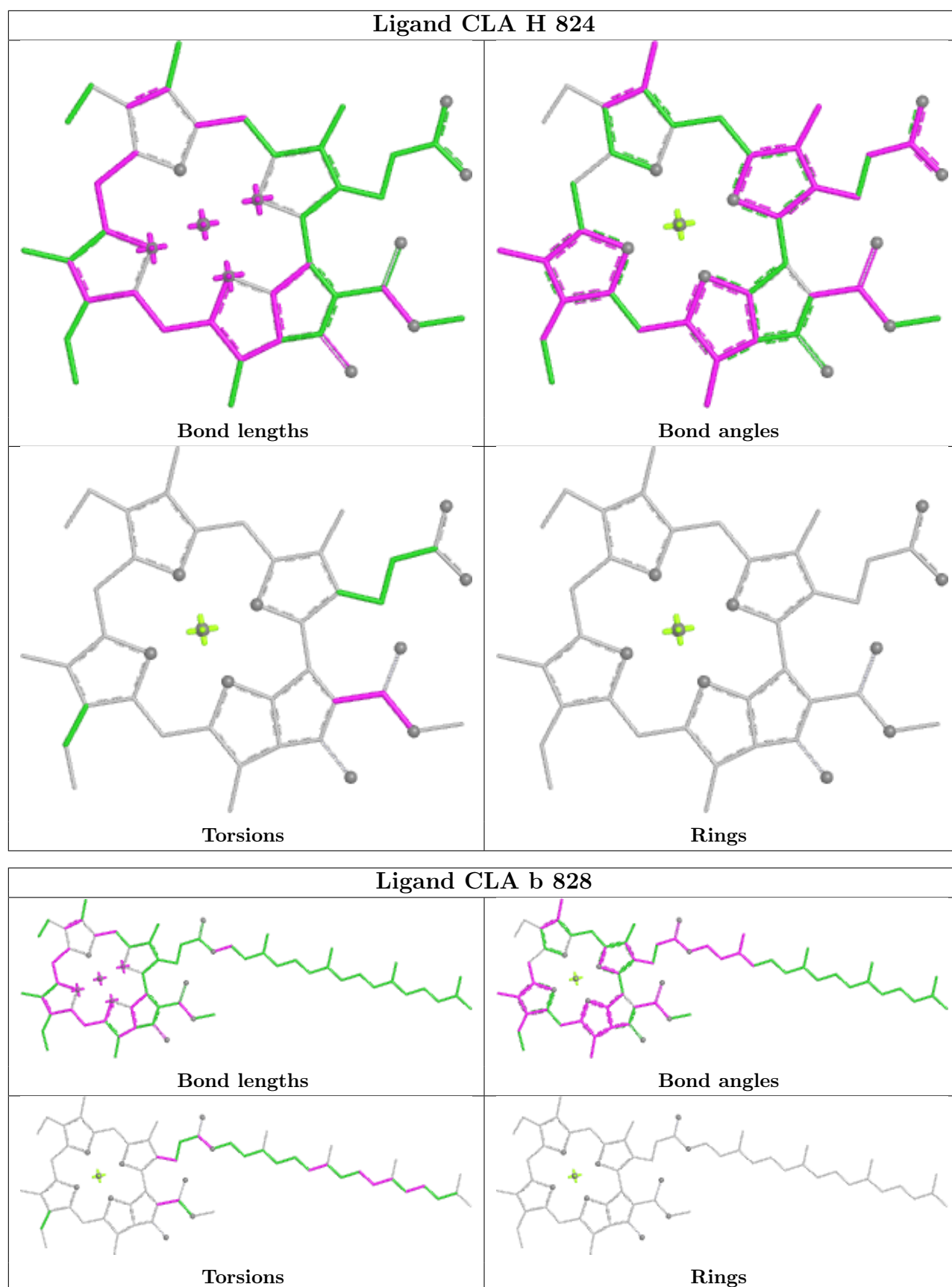




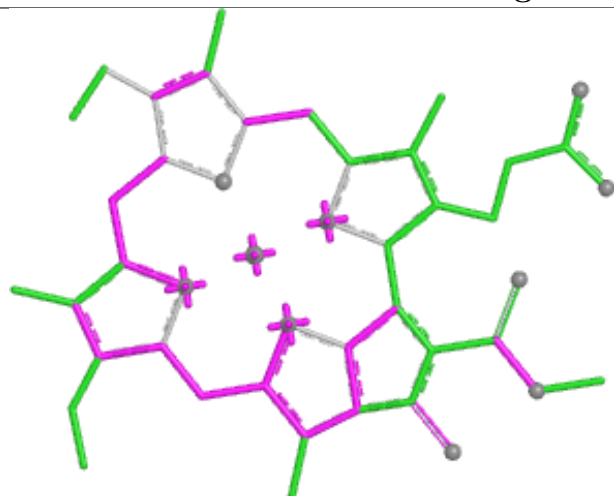
## Ligand CLA B 810



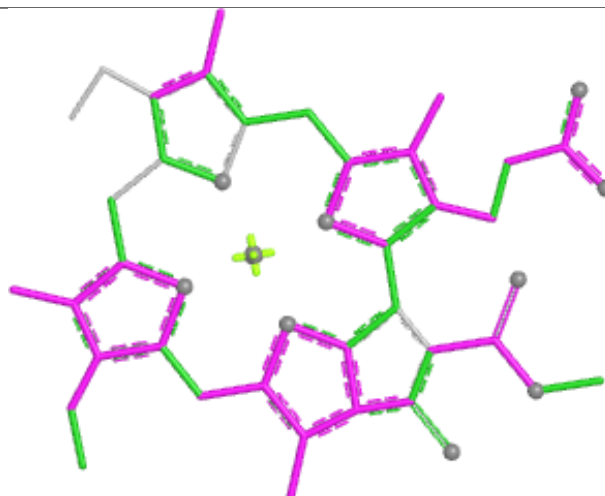




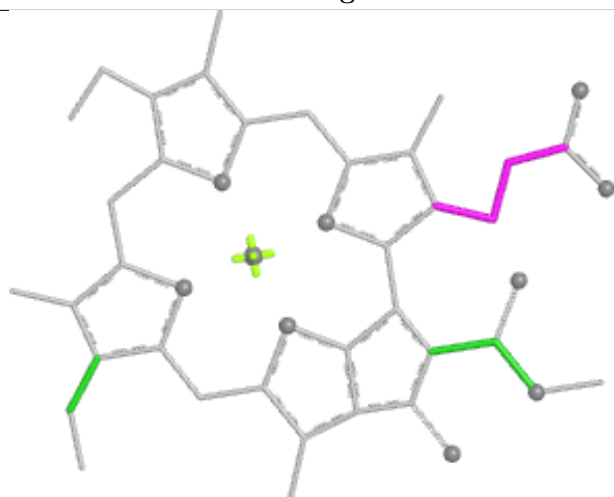
## Ligand CLA B 811



Bond lengths



Bond angles

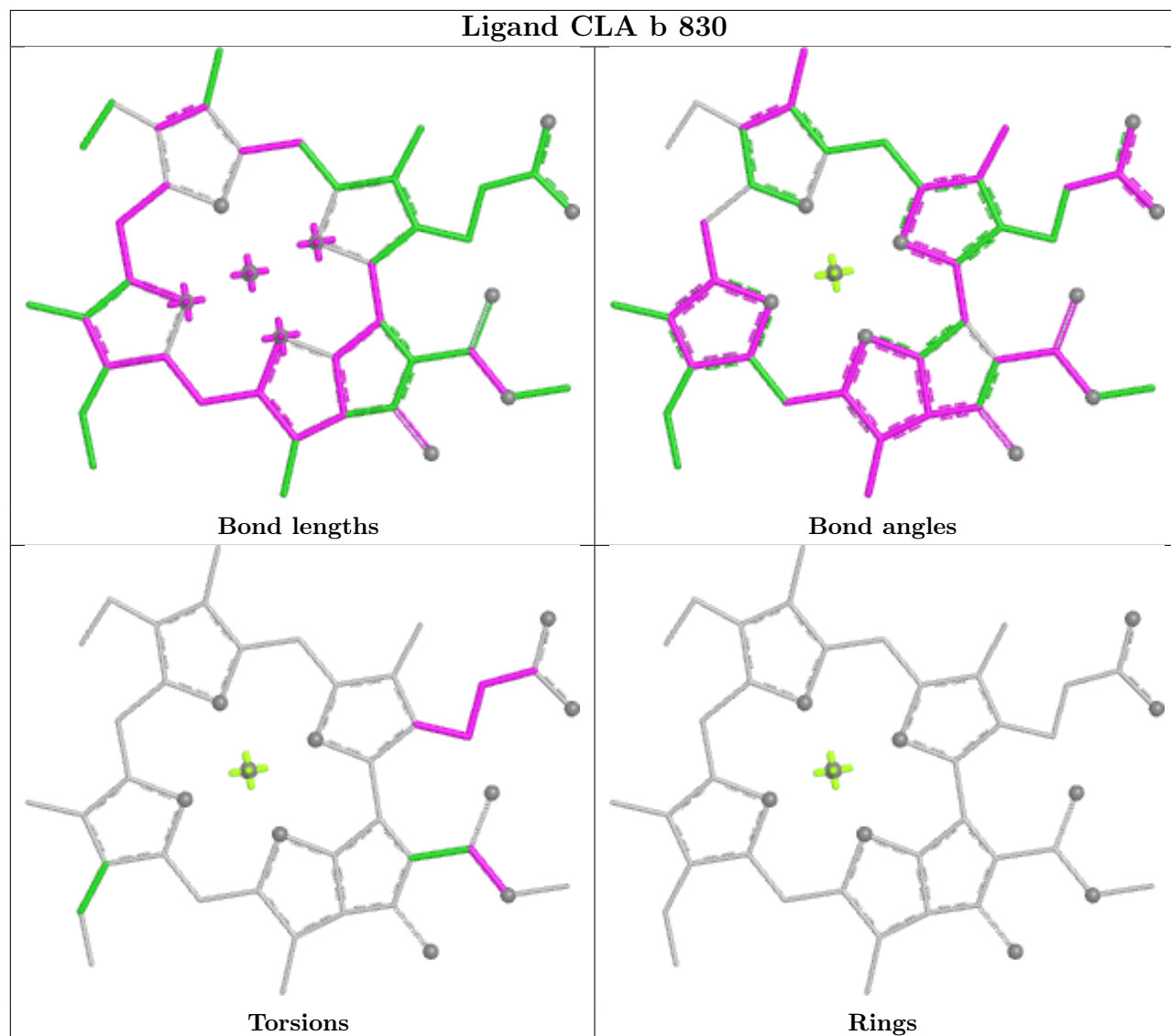


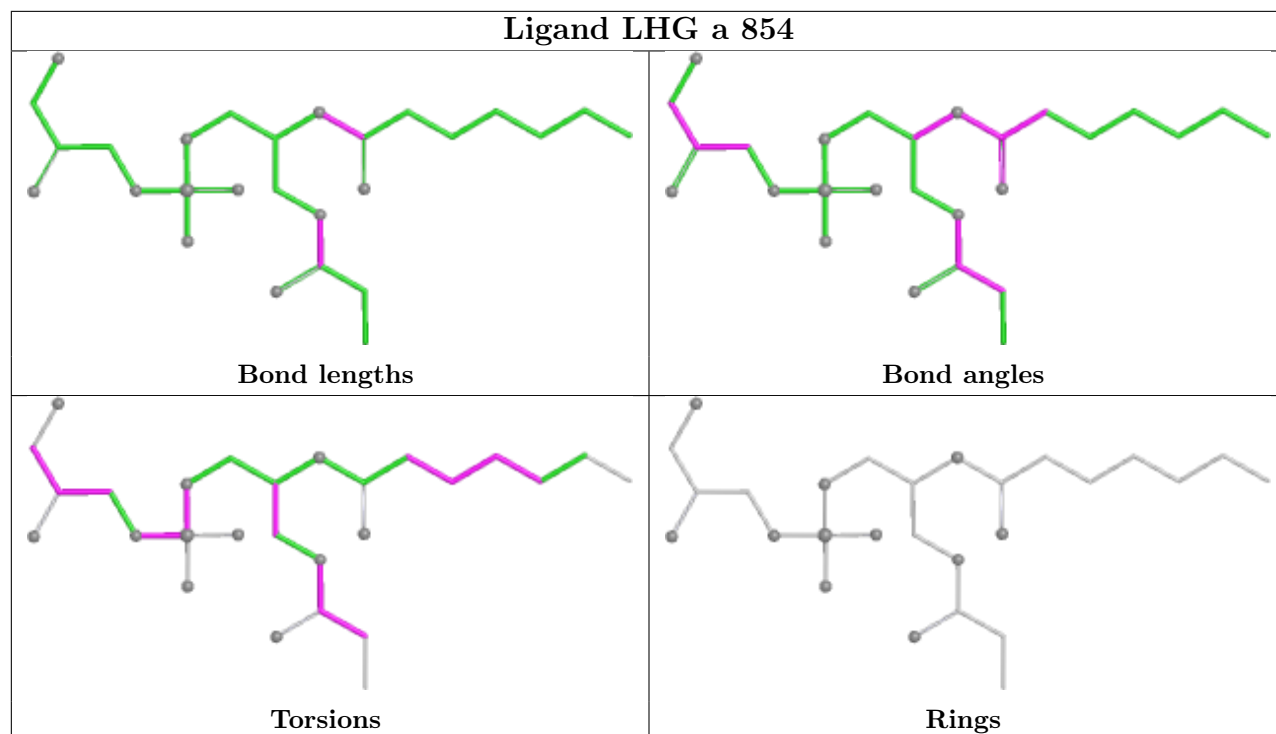
Torsions



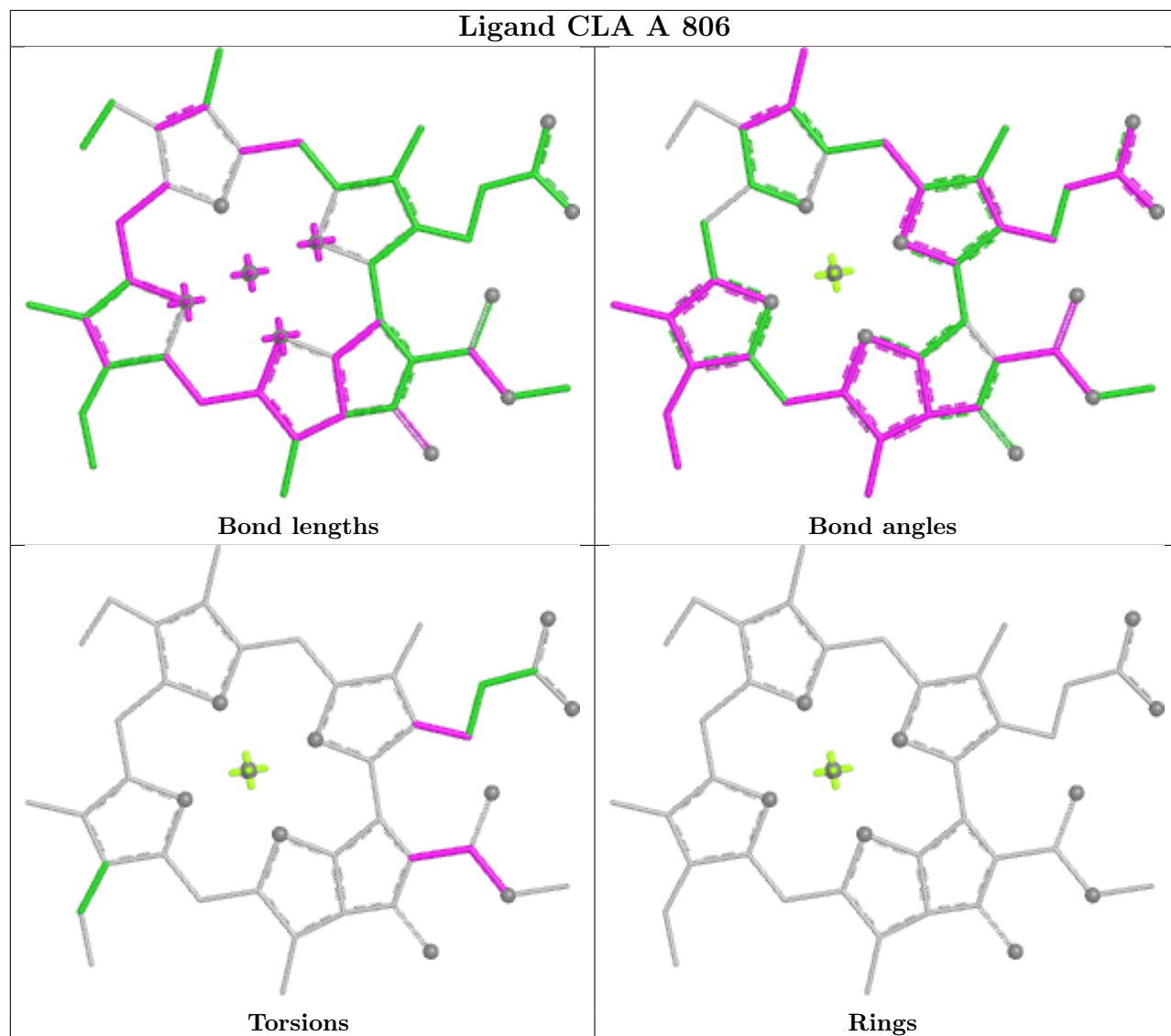
Rings

## Ligand CLA b 830

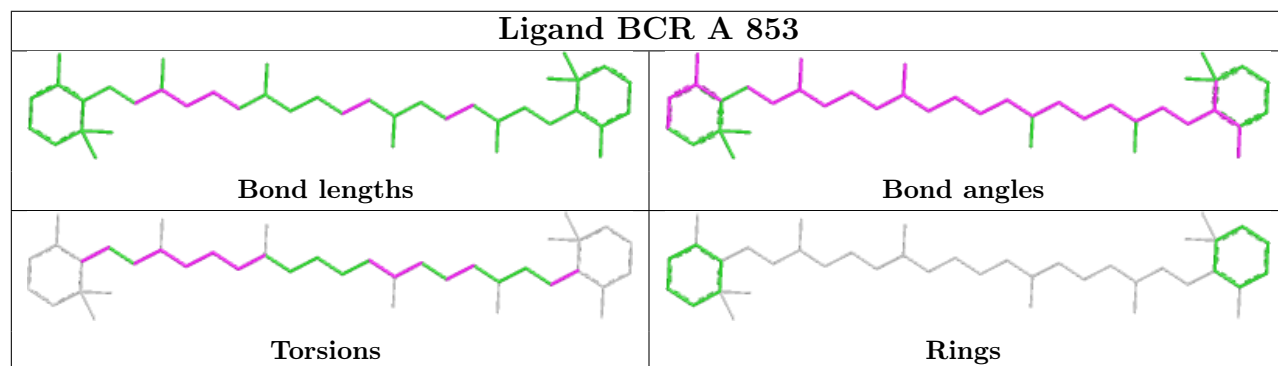


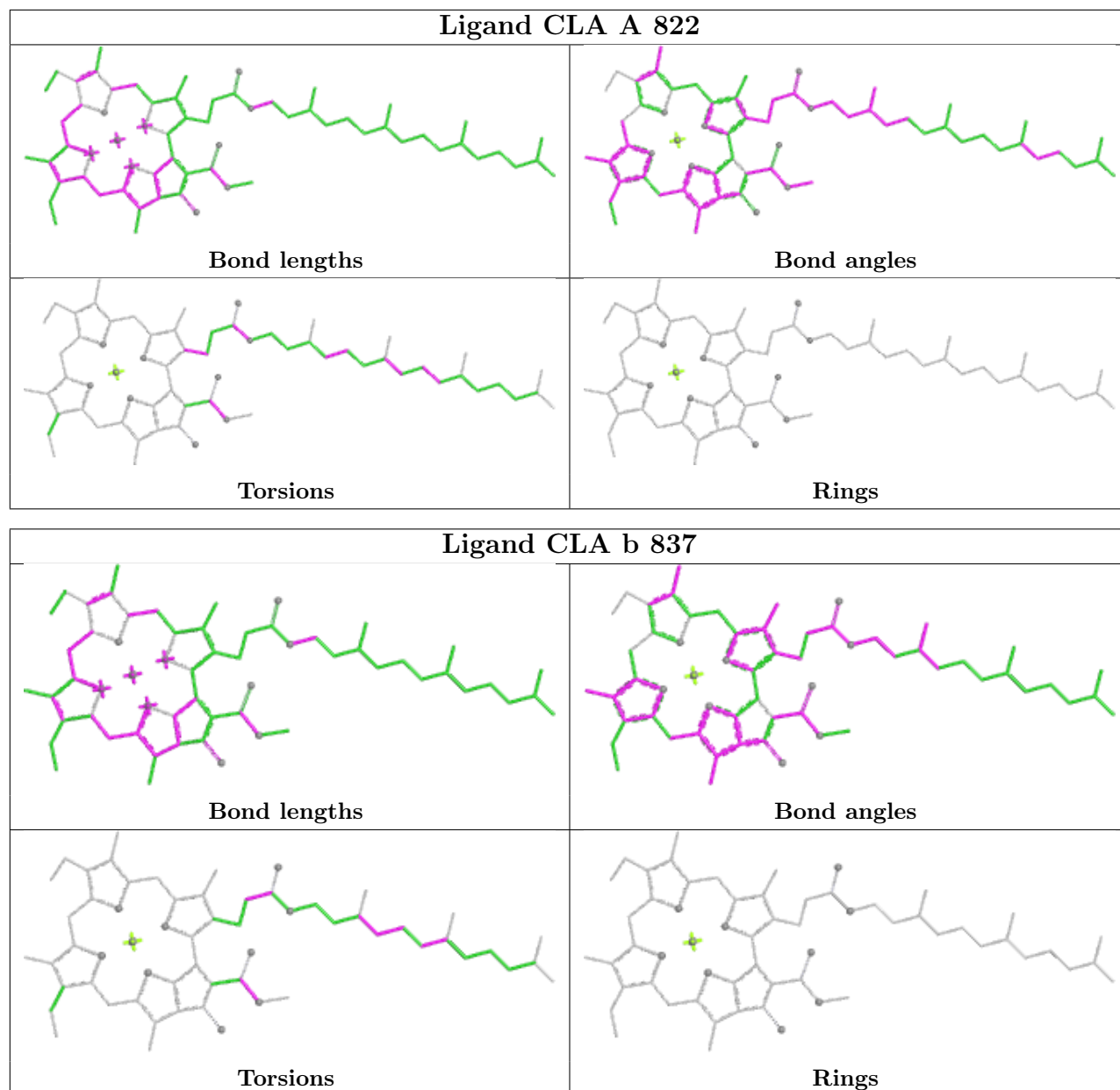


## Ligand CLA A 806

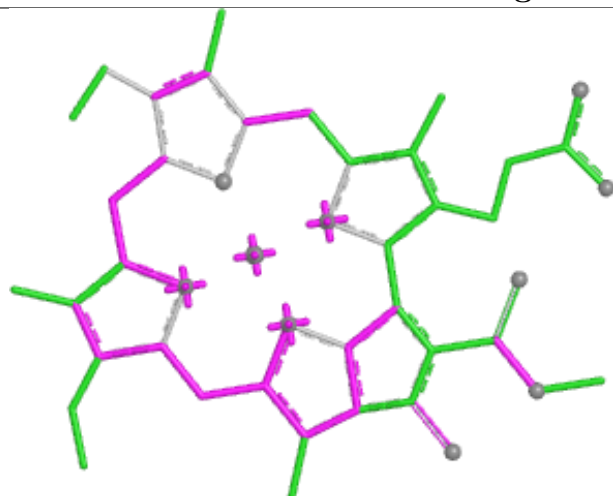


## Ligand BCR A 853

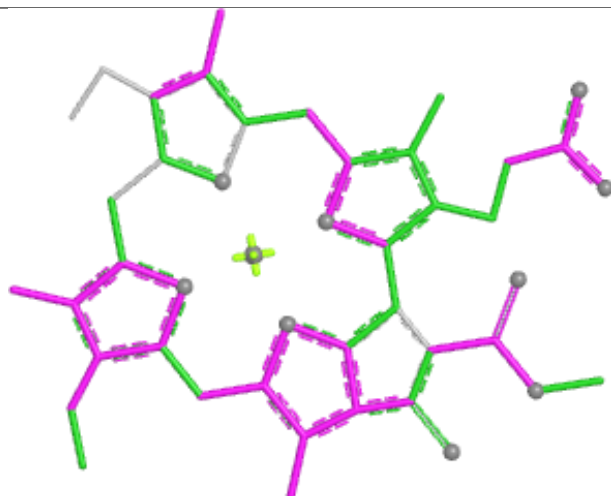




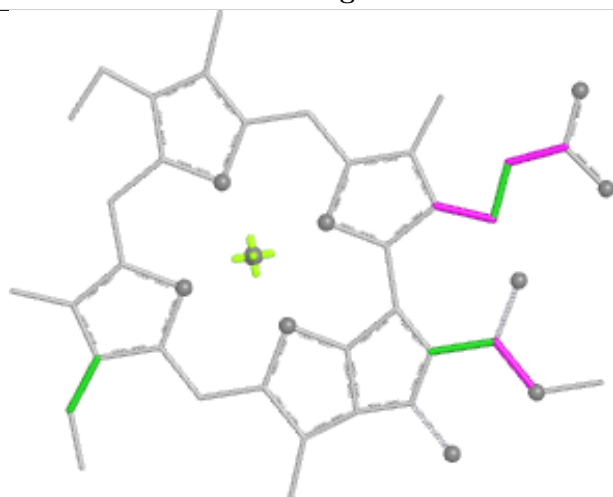
## Ligand CLA B 833



Bond lengths



Bond angles

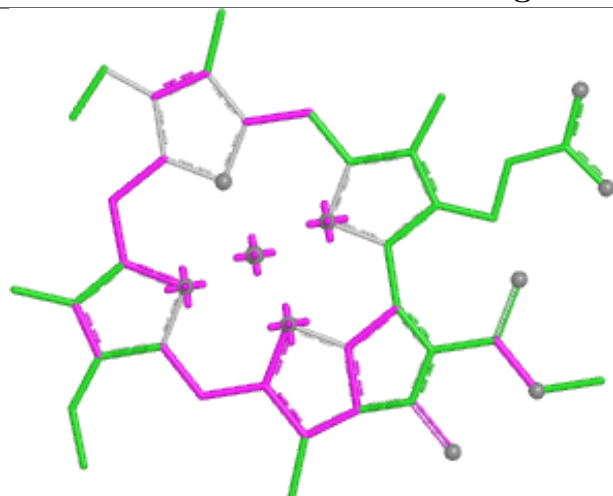


Torsions

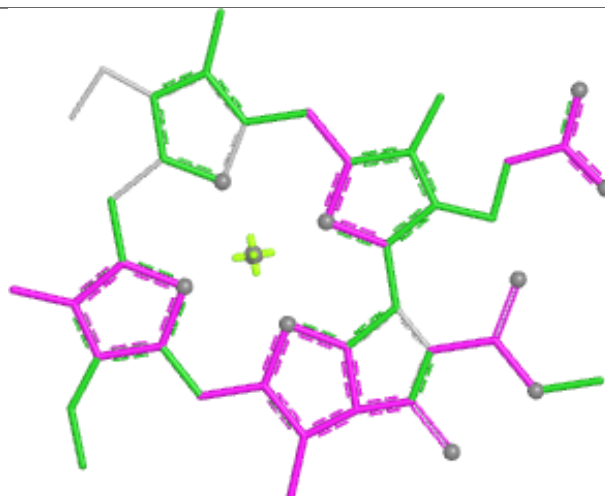


Rings

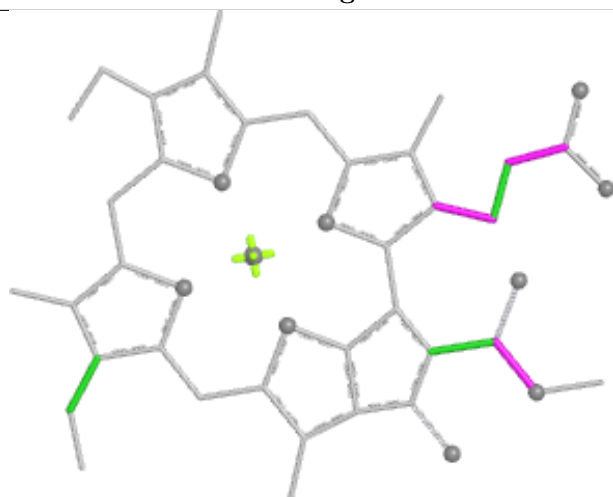
## Ligand CLA A 818



Bond lengths



Bond angles

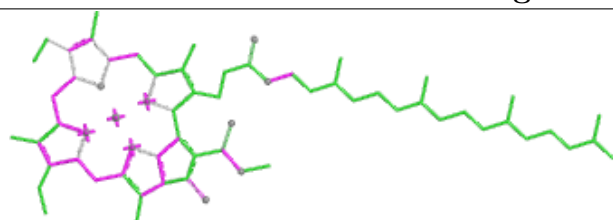


Torsions

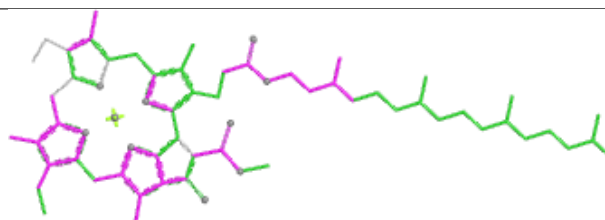


Rings

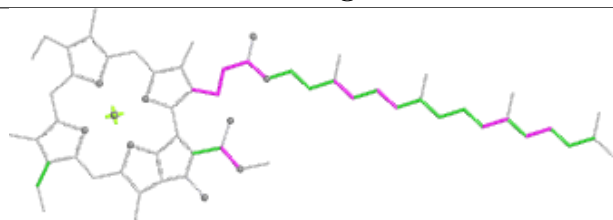
## Ligand CLA H 826



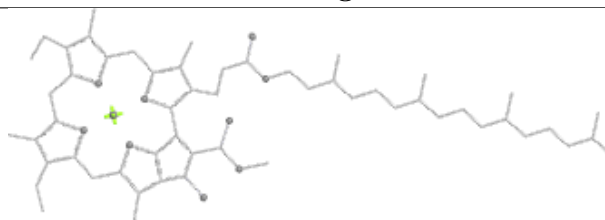
Bond lengths



Bond angles

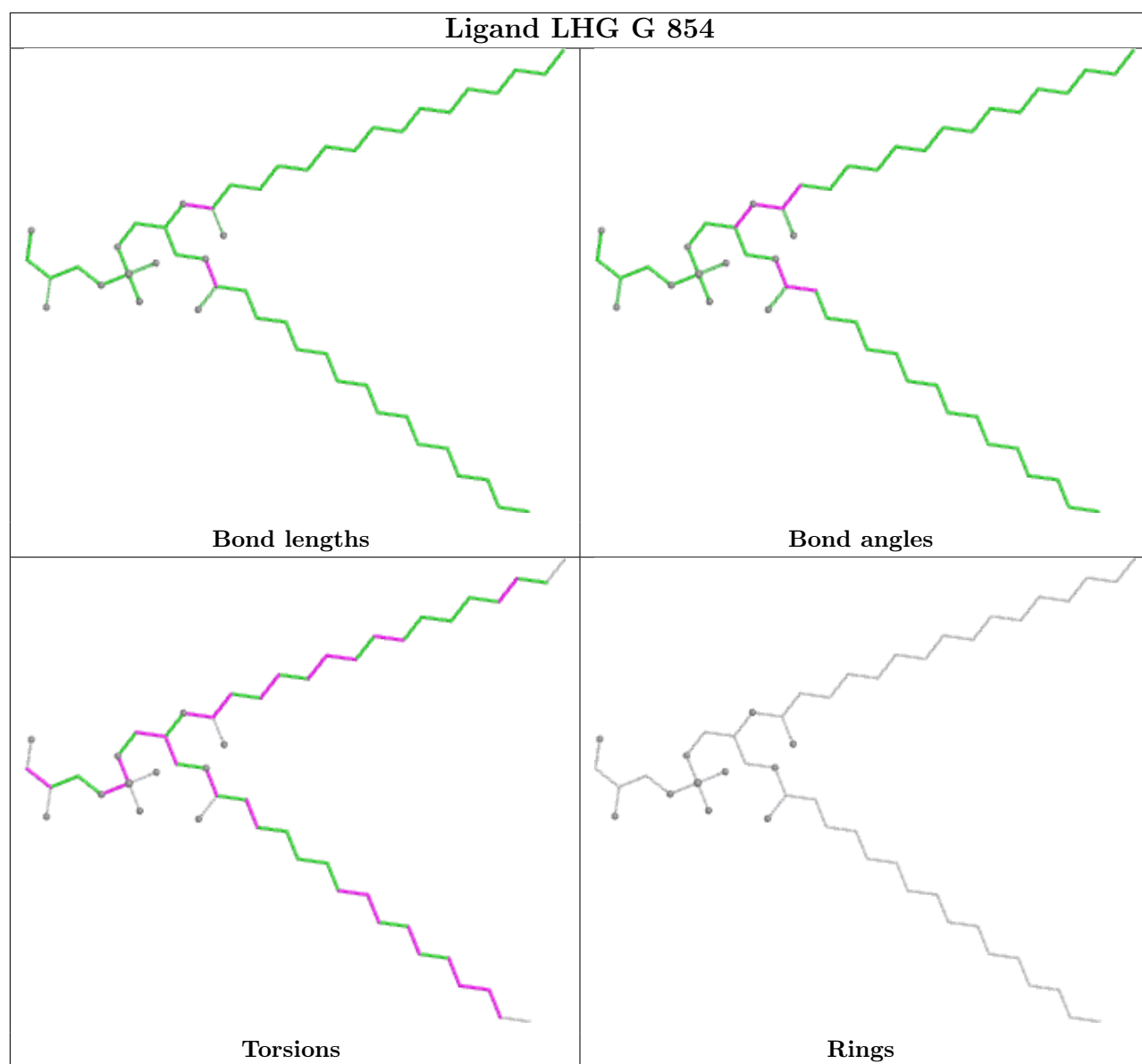


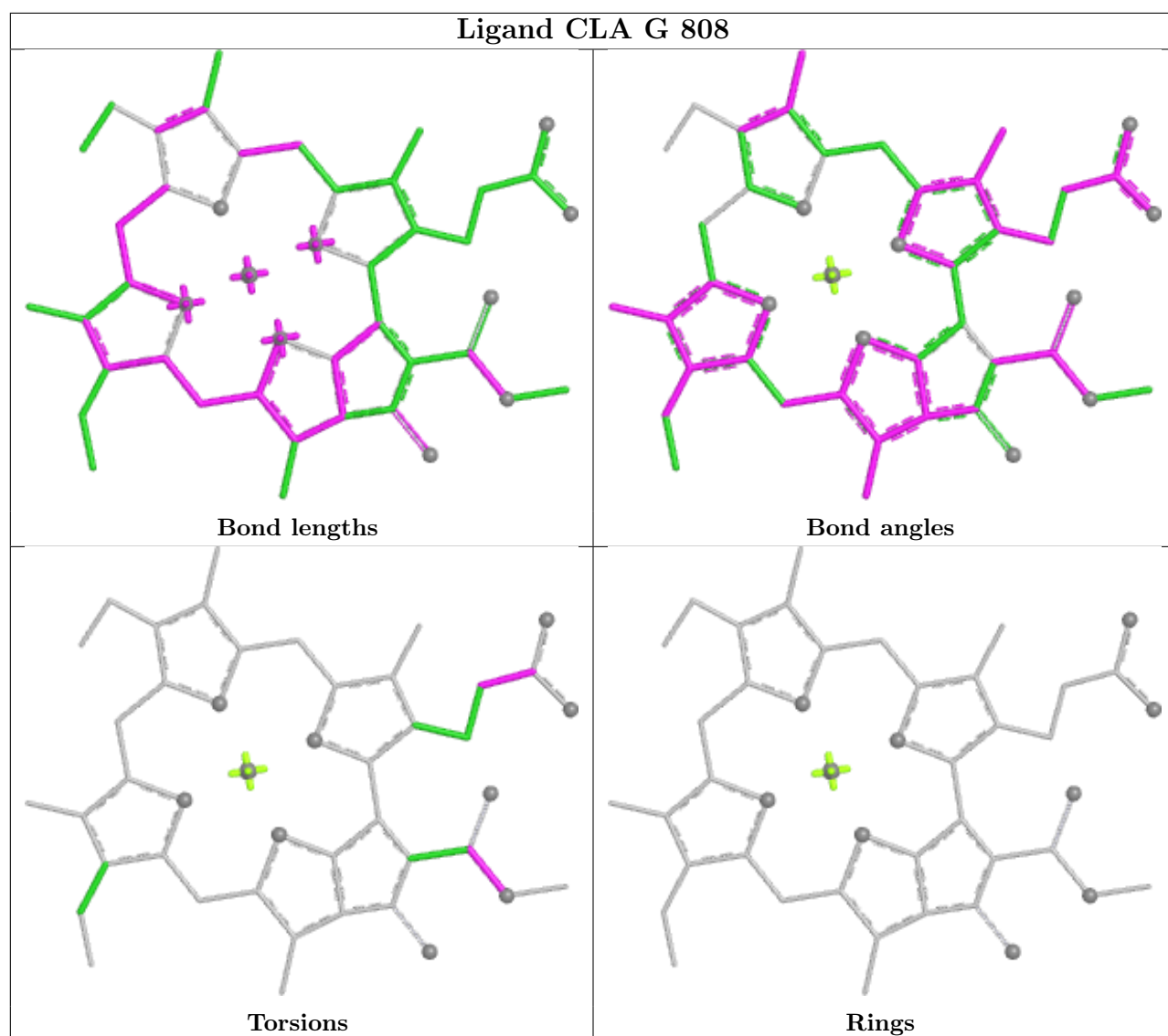
Torsions

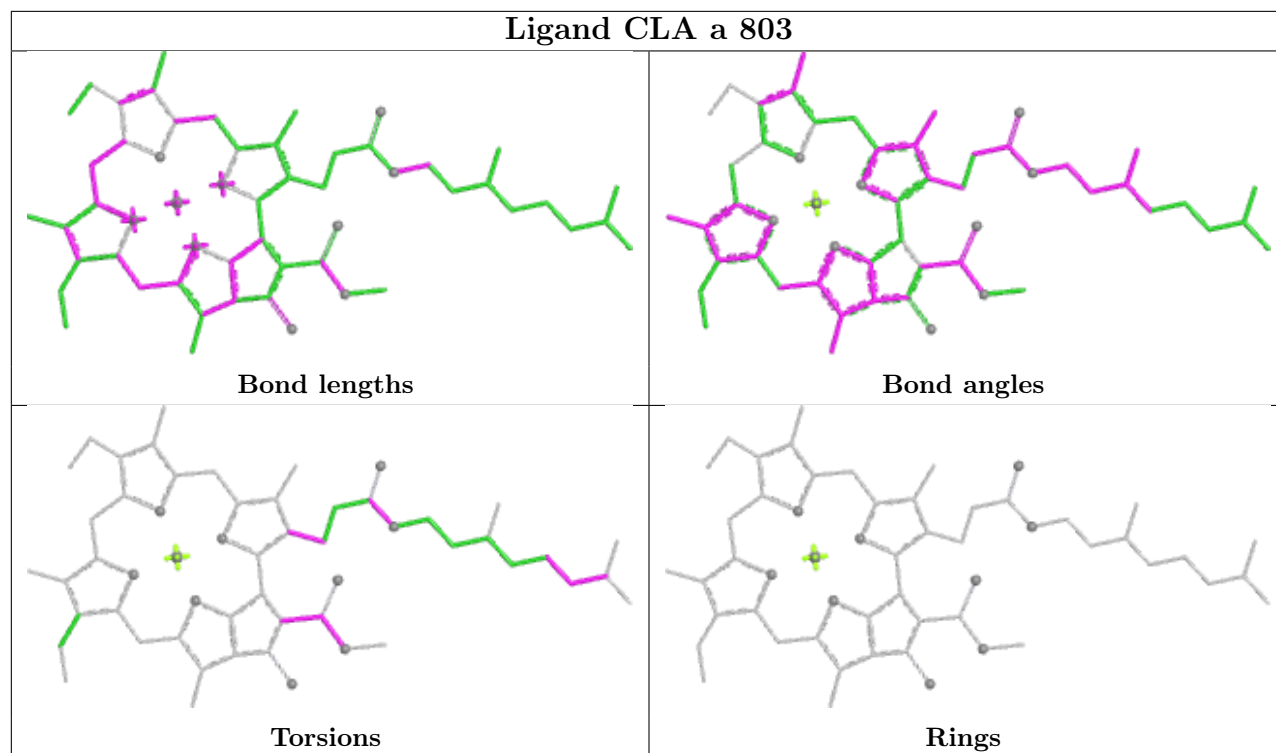
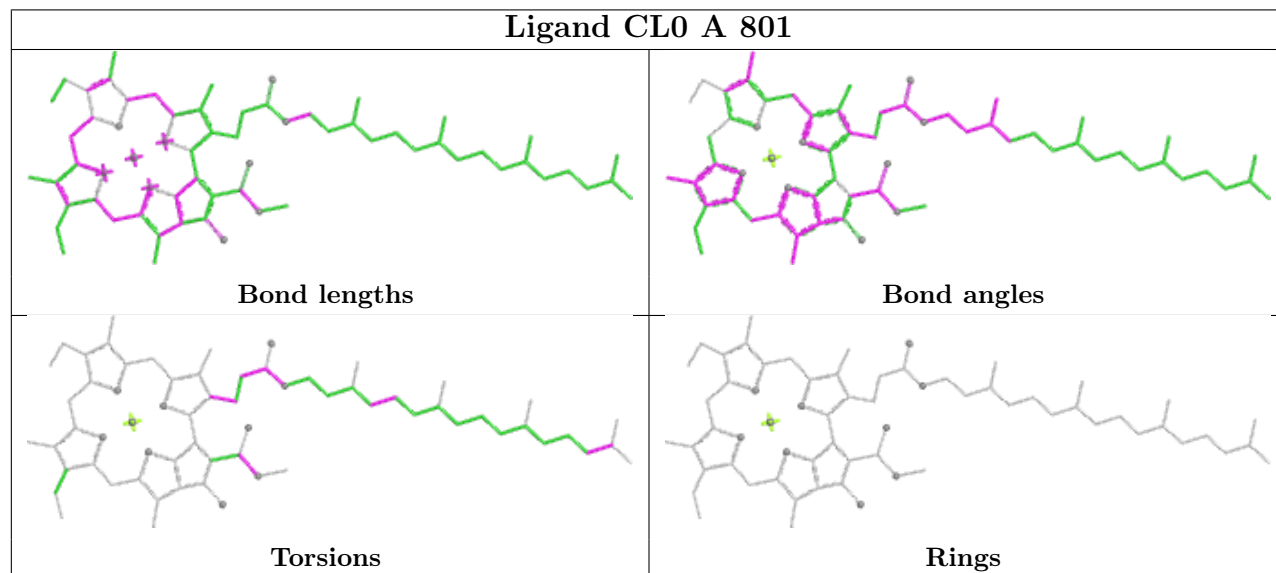


Rings

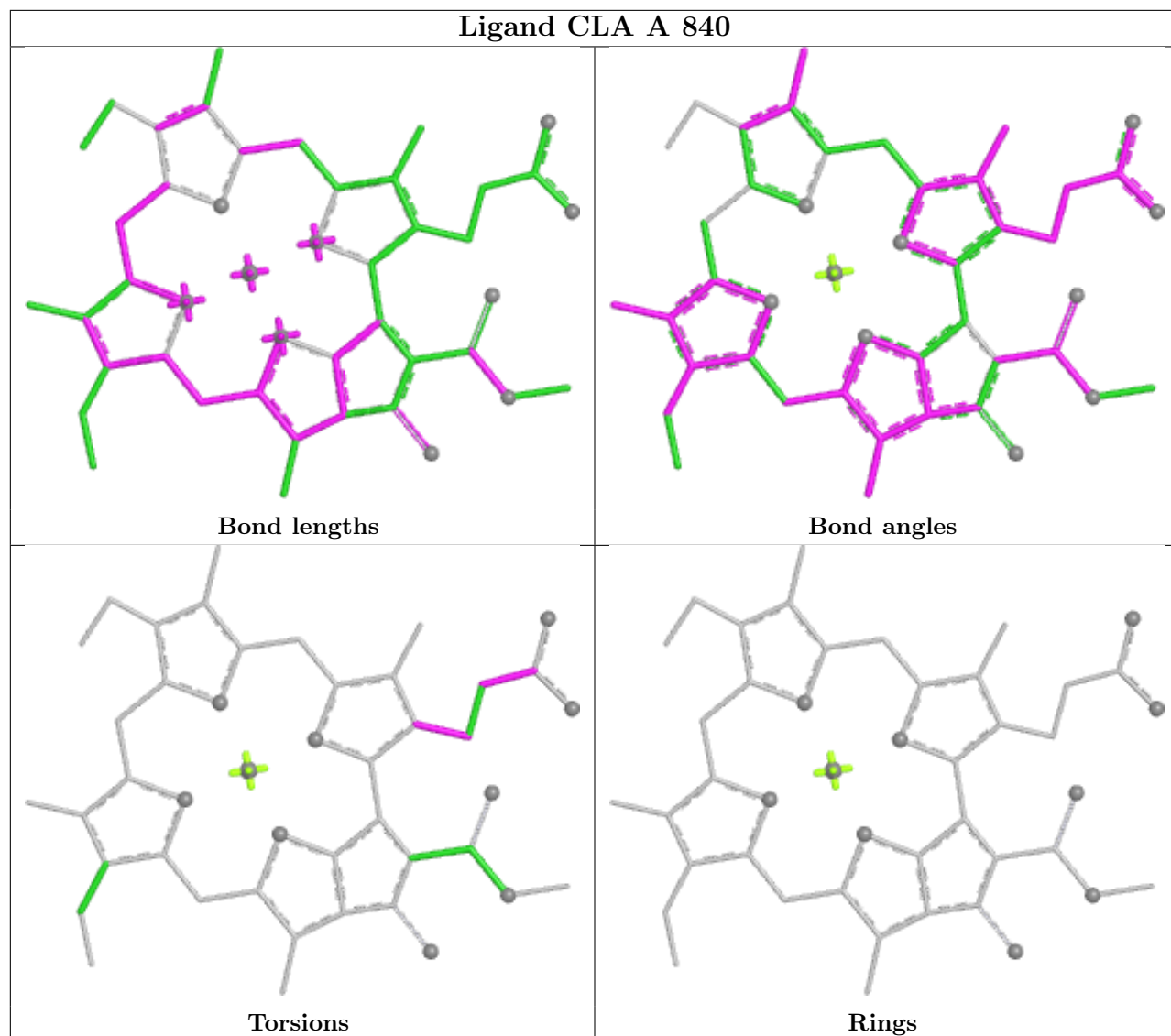


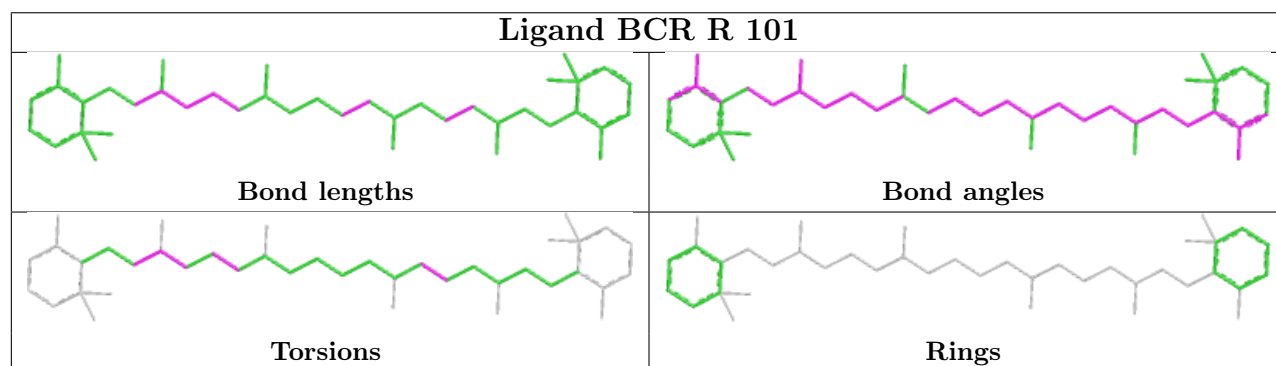
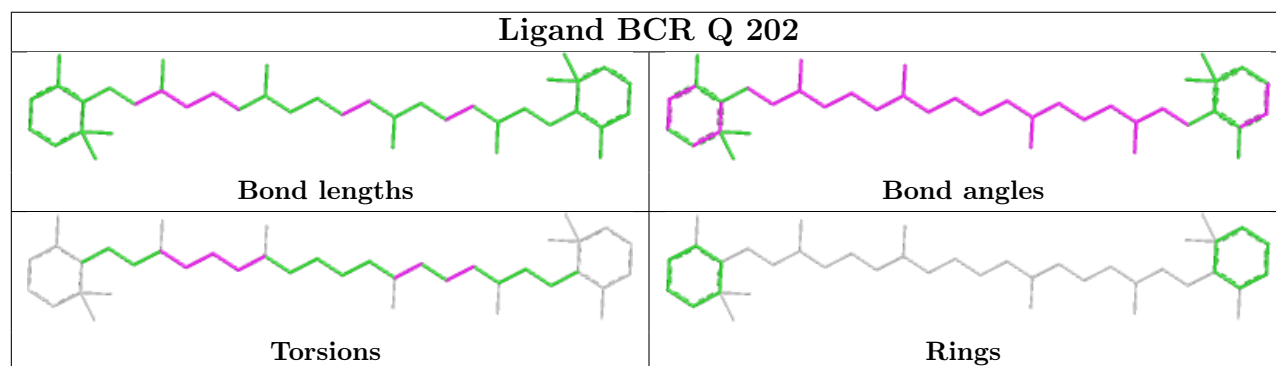
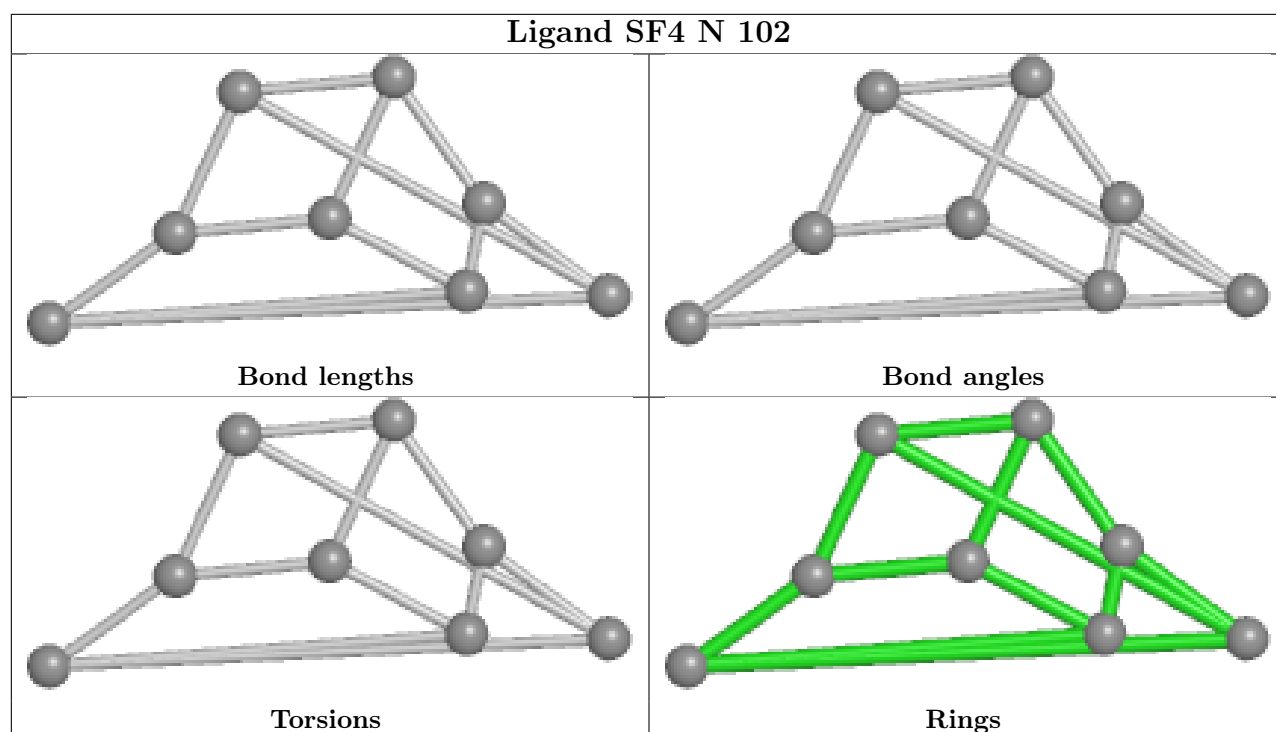


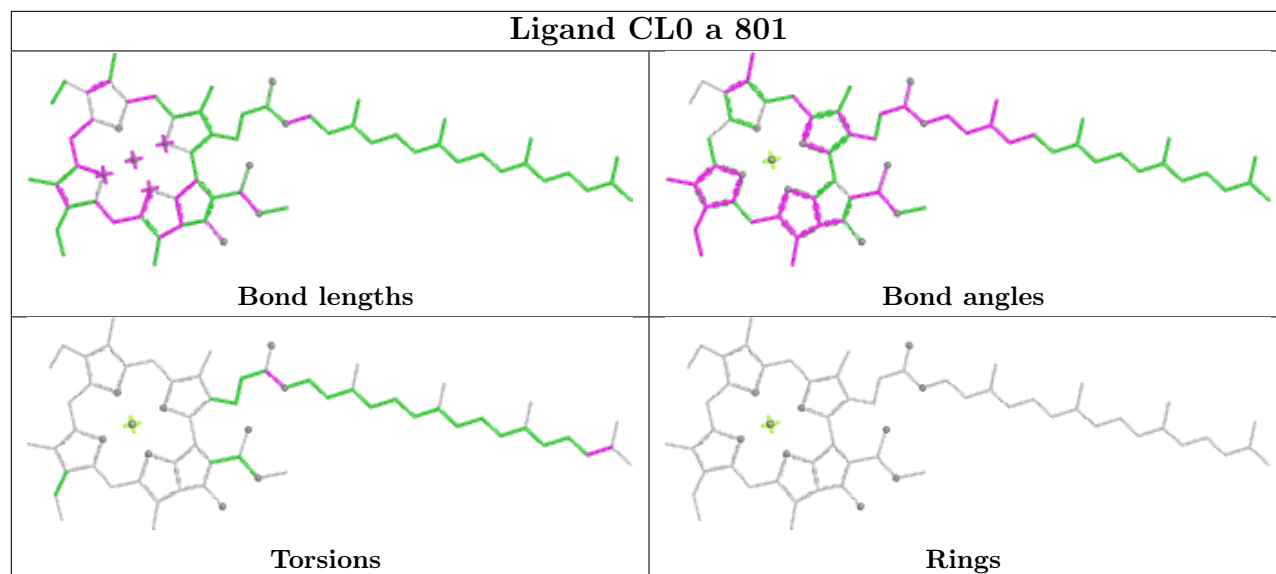
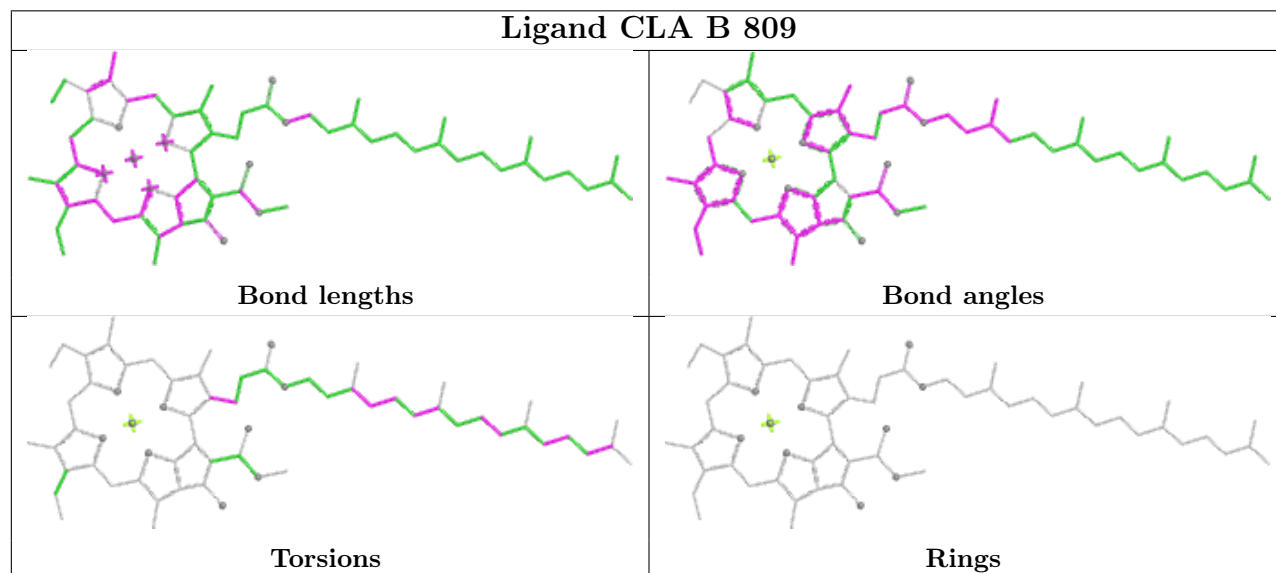


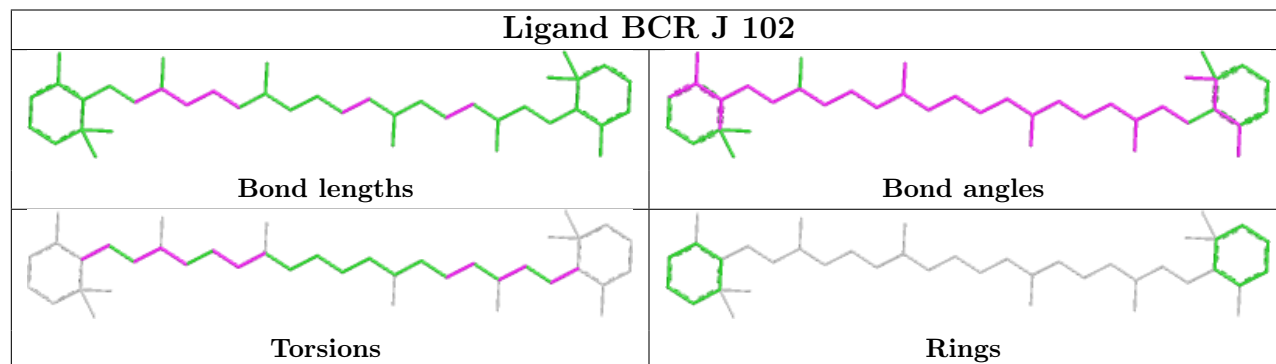
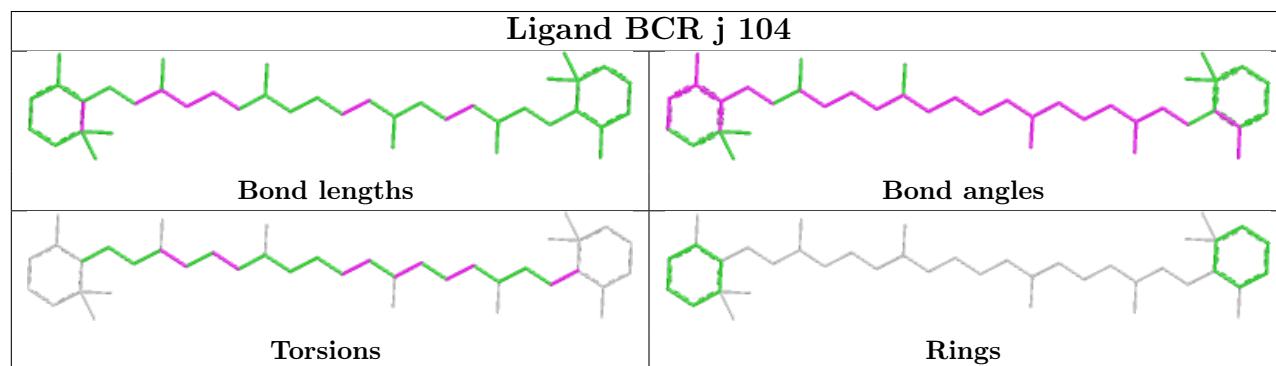
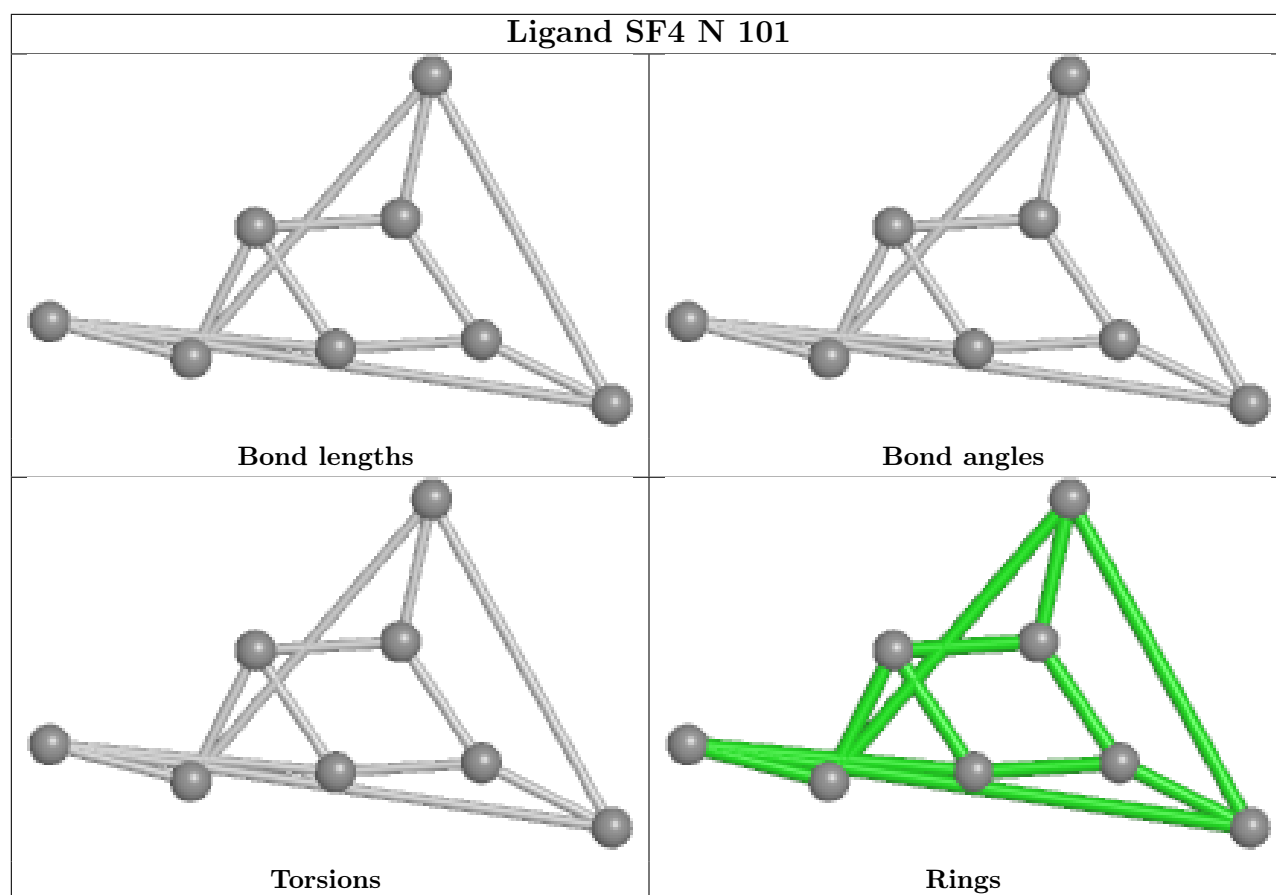
**Ligand CLA a 803****Ligand CL0 A 801**

## Ligand CLA A 840

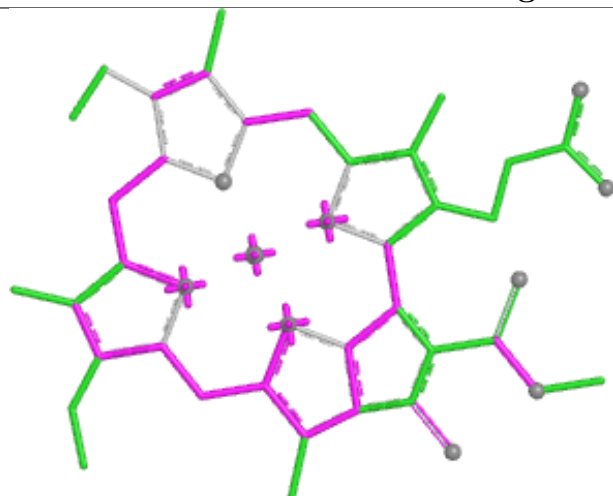




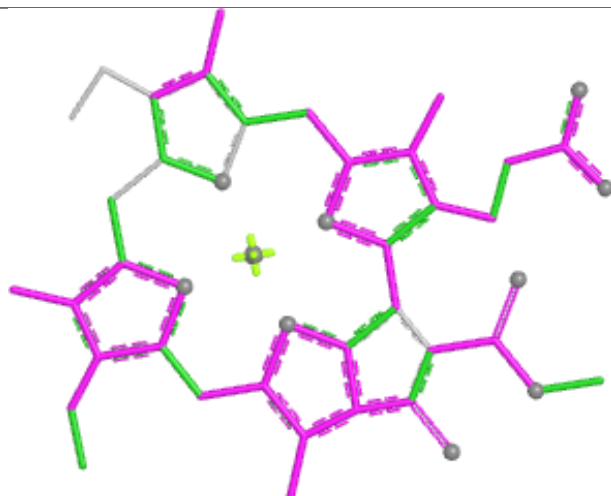
**Ligand CL0 a 801****Ligand CLA B 809**



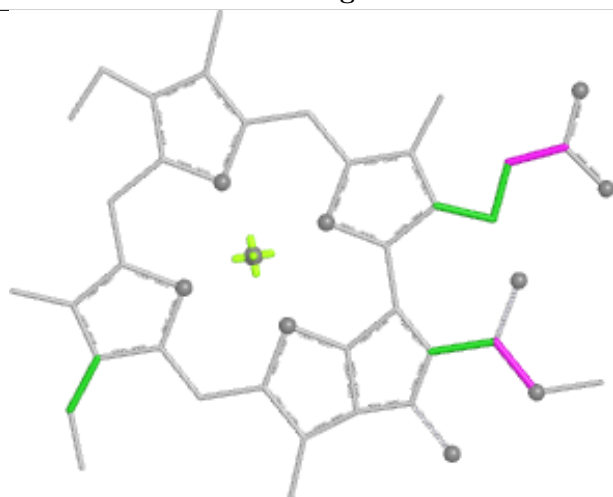
## Ligand CLA J 101



Bond lengths



Bond angles

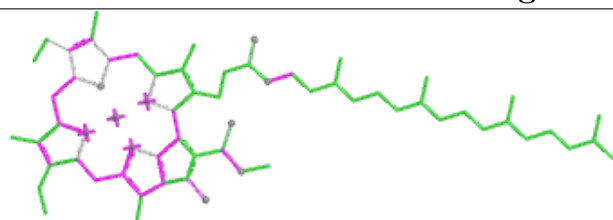


Torsions

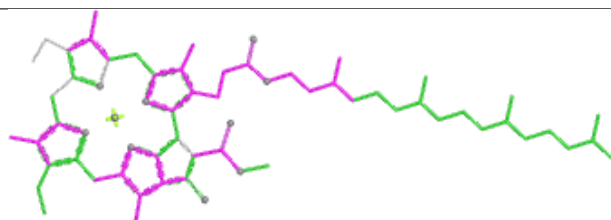


Rings

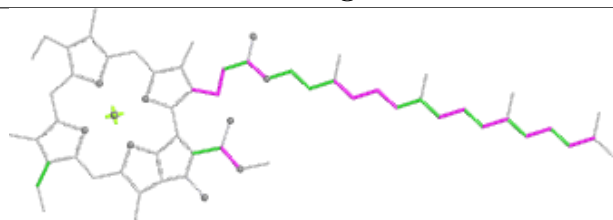
## Ligand CLA a 819



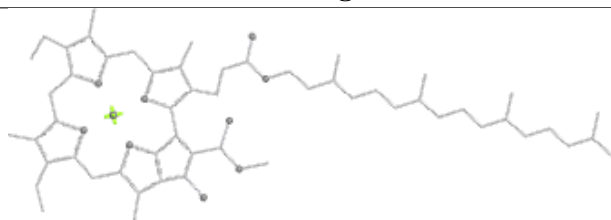
Bond lengths



Bond angles



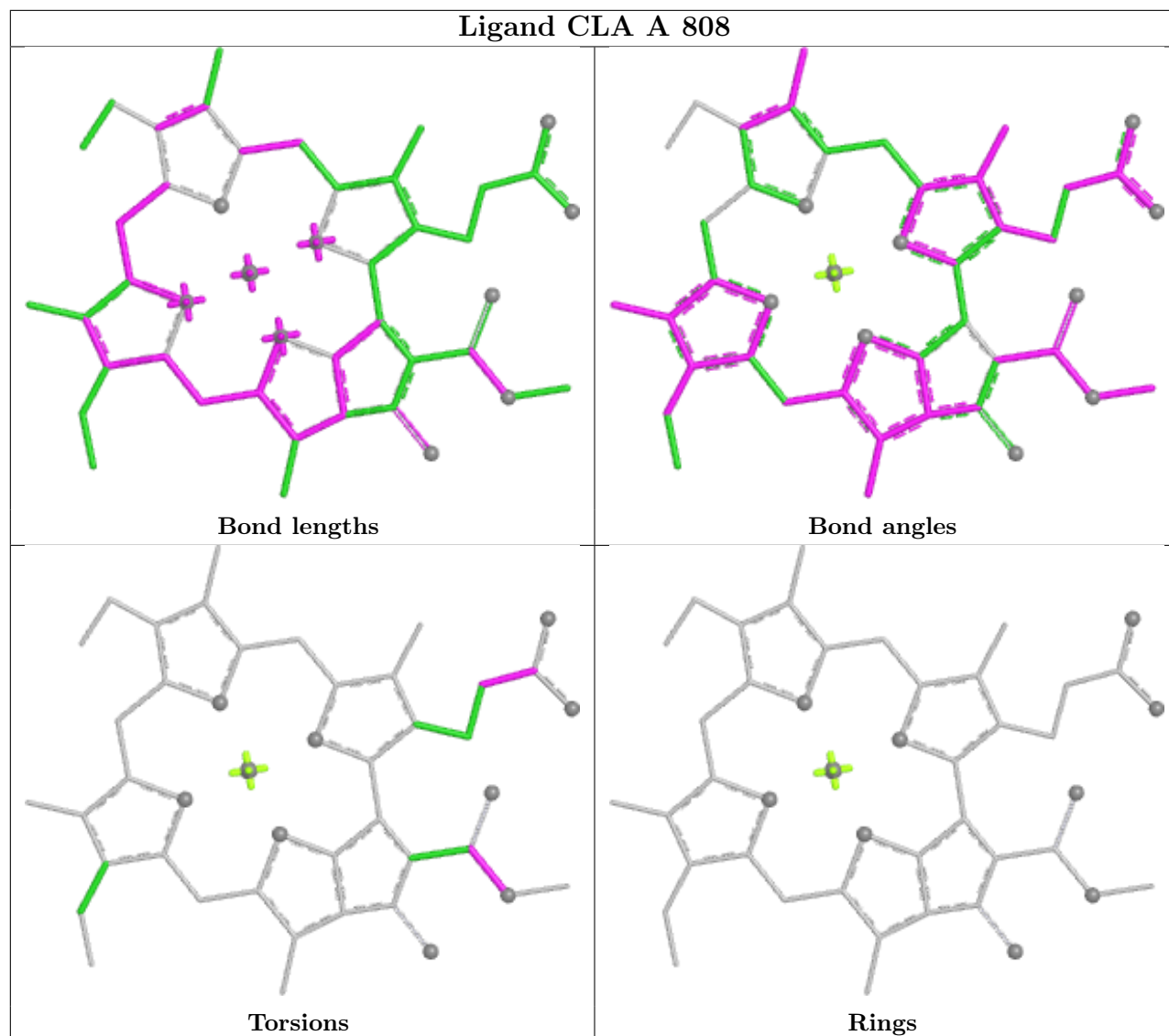
Torsions



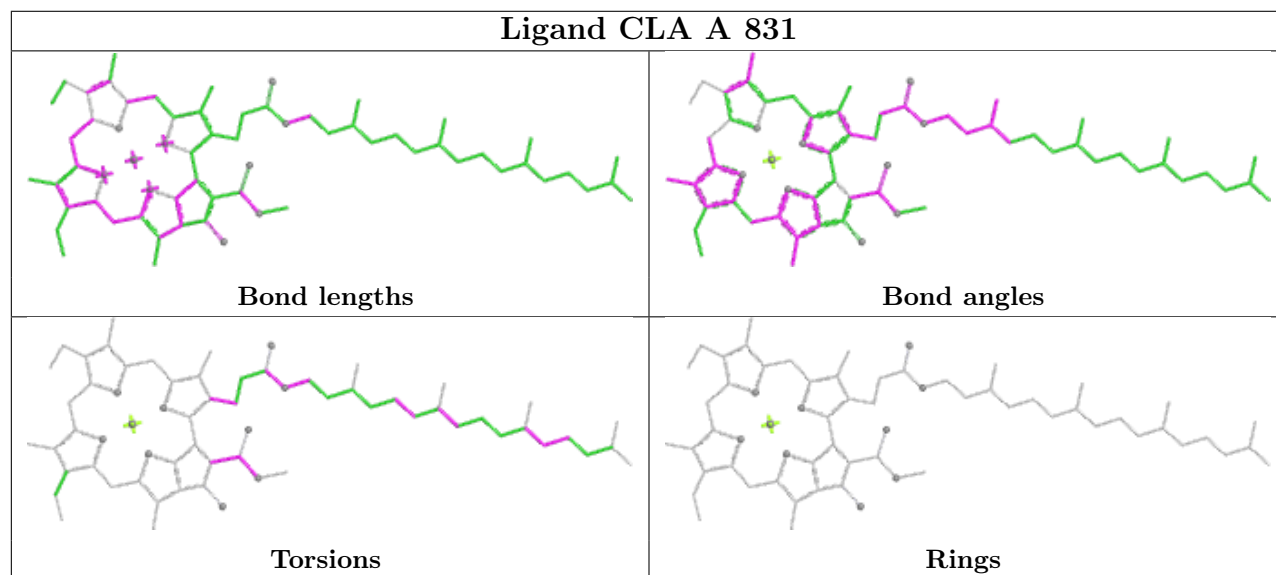
Rings



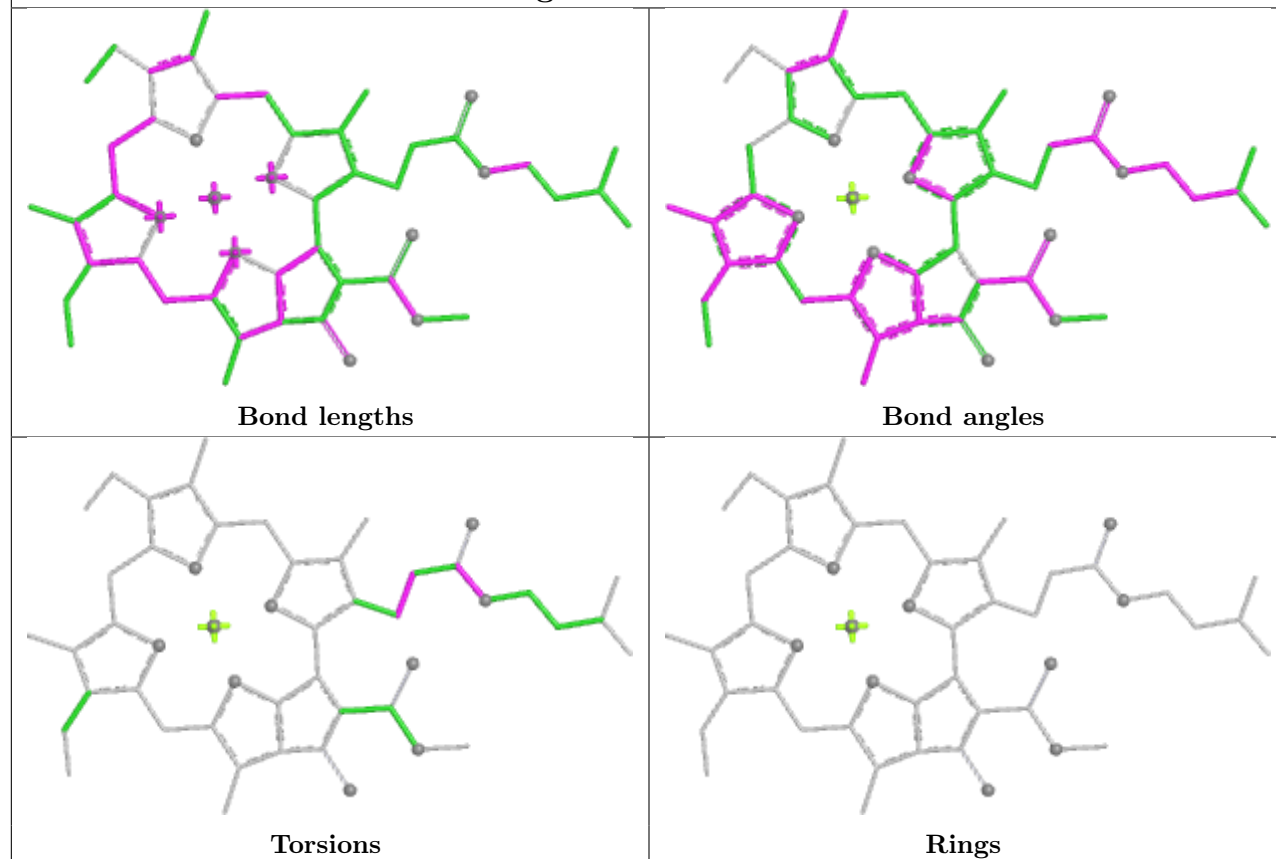
## Ligand CLA A 808



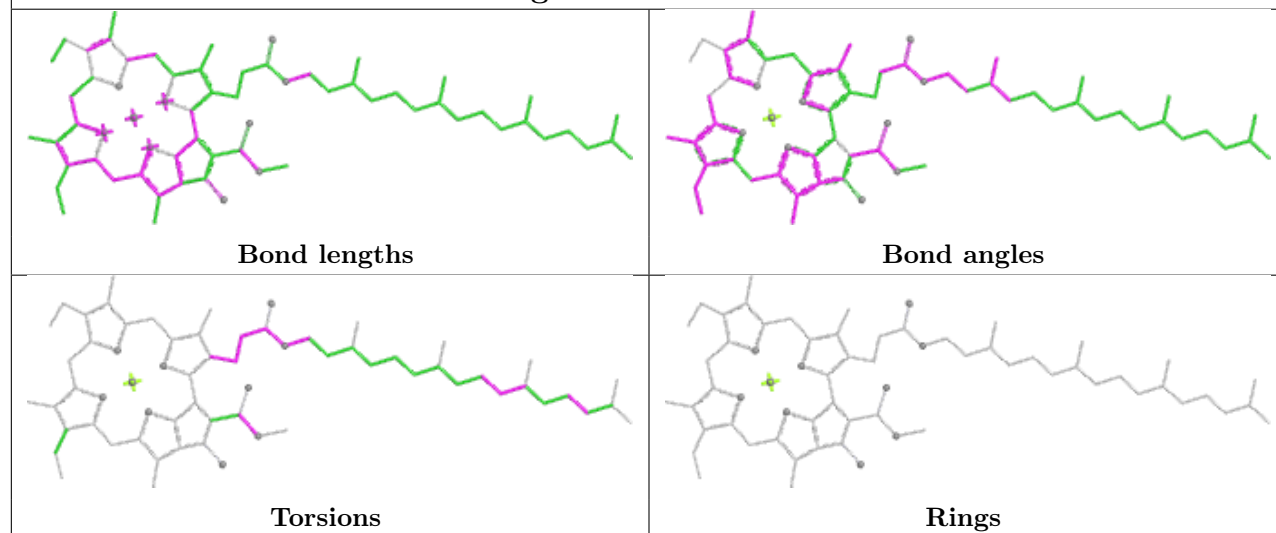
## Ligand CLA A 831

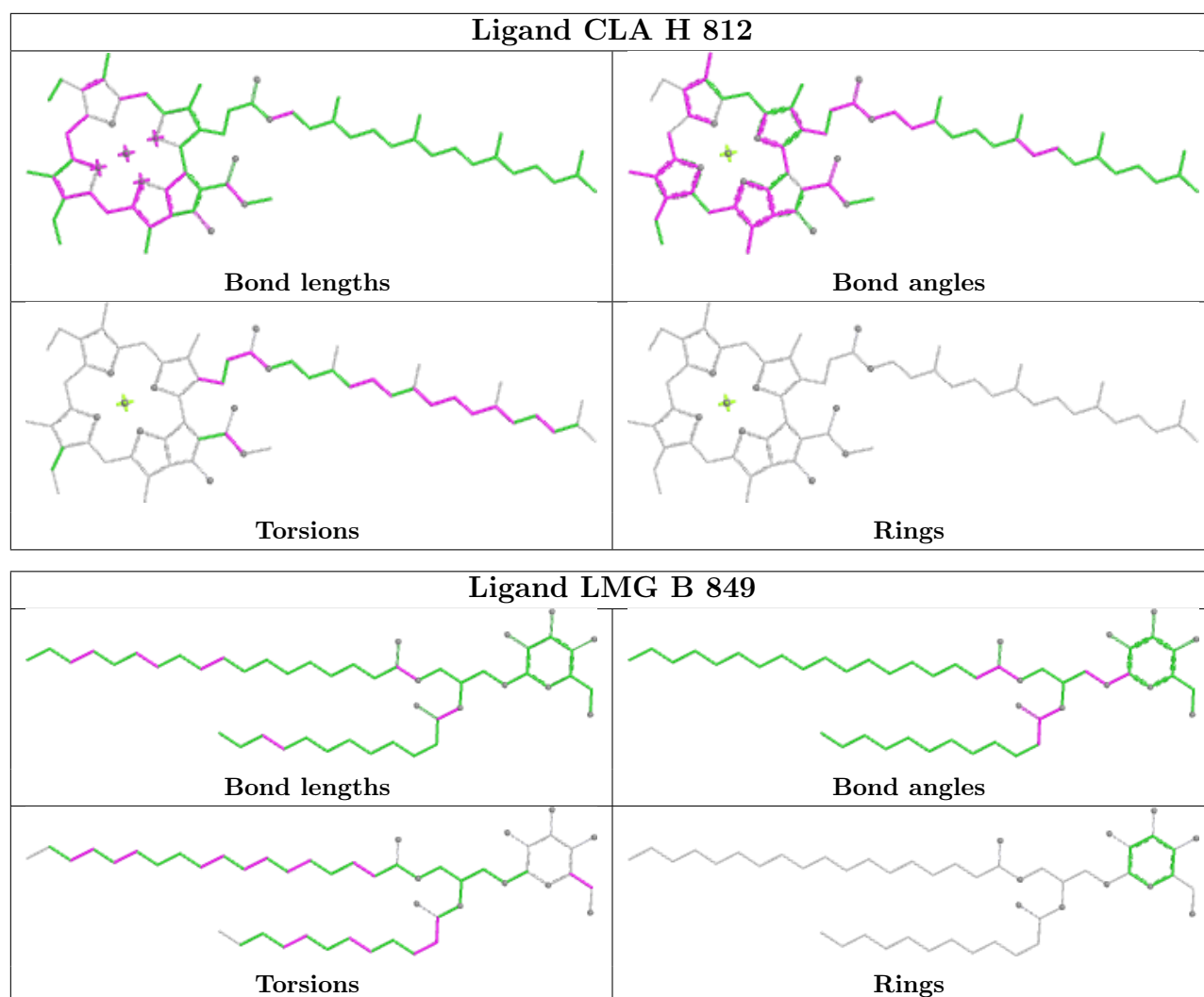


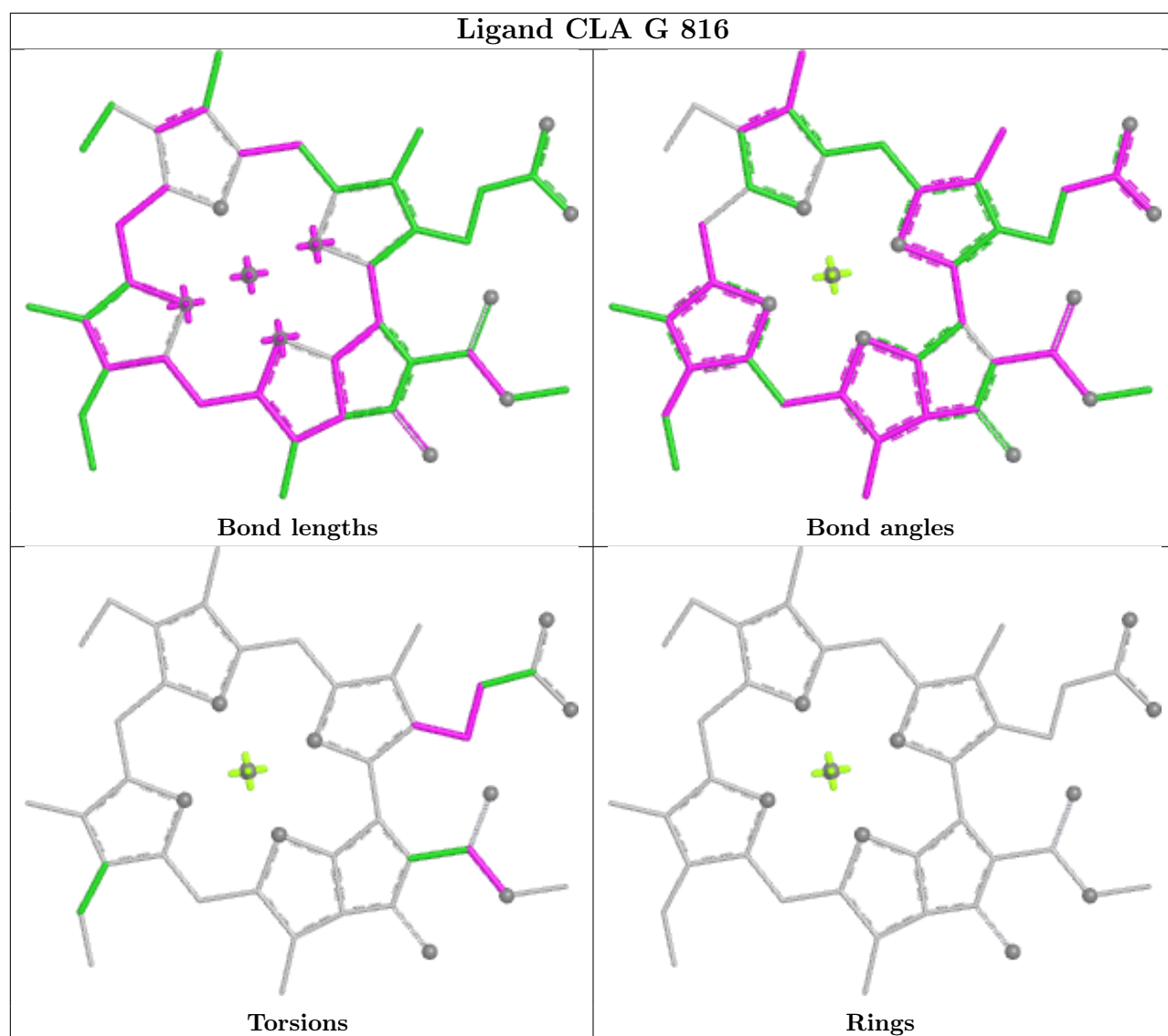
## Ligand CLA a 831



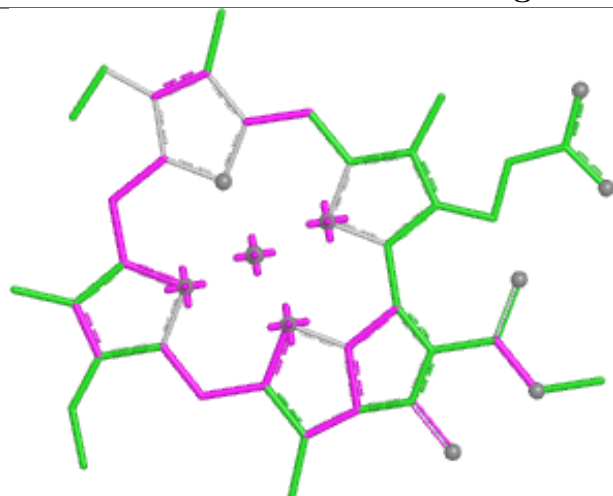
## Ligand CLA G 812



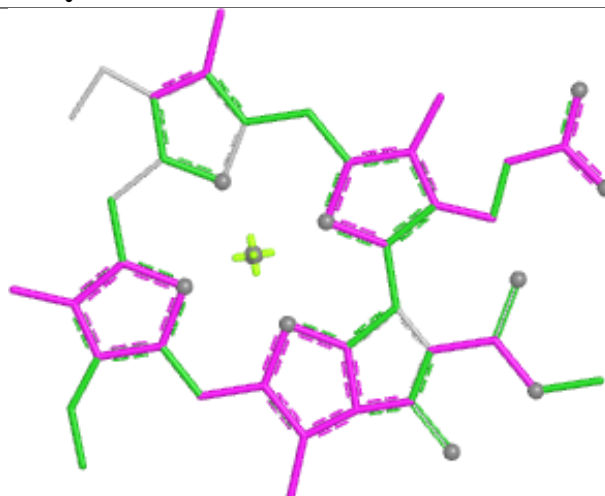




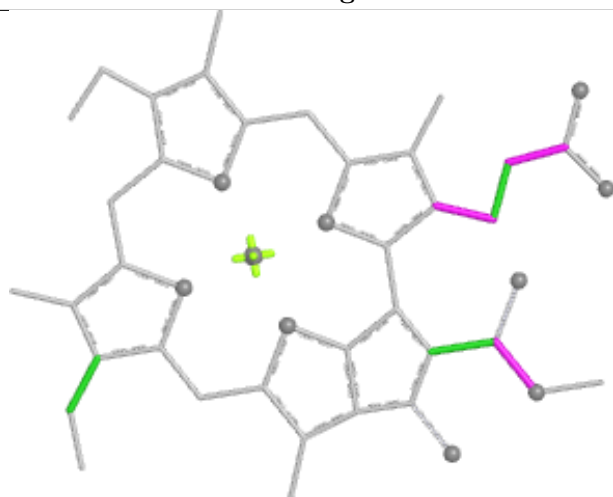
## Ligand CLA Q 201



Bond lengths



Bond angles

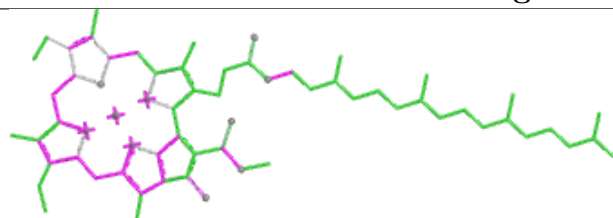


Torsions

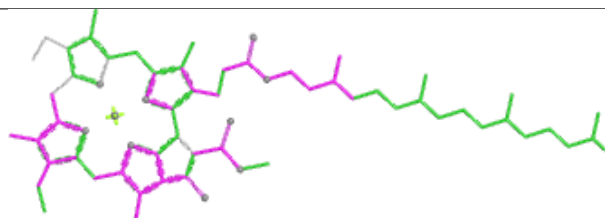


Rings

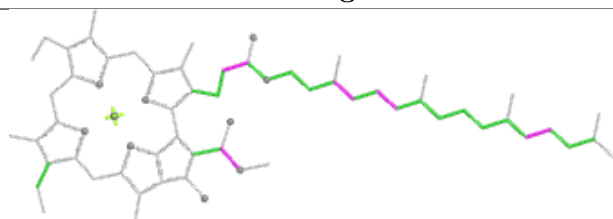
## Ligand CLA H 807



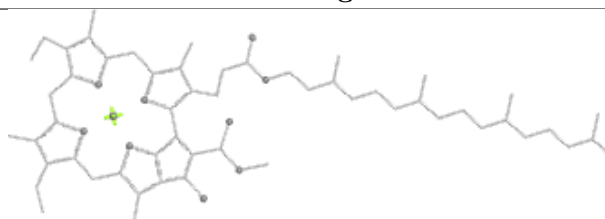
Bond lengths



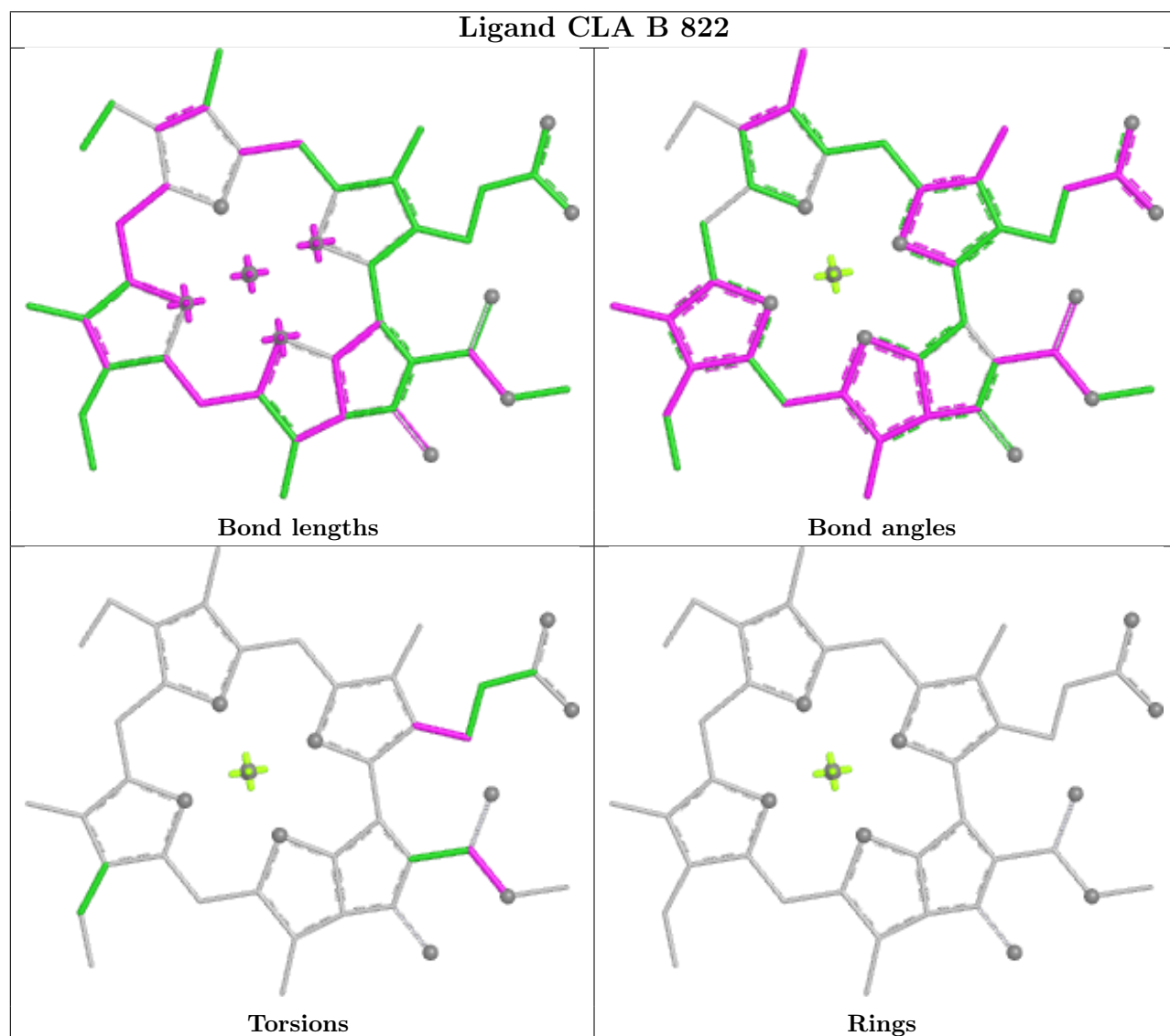
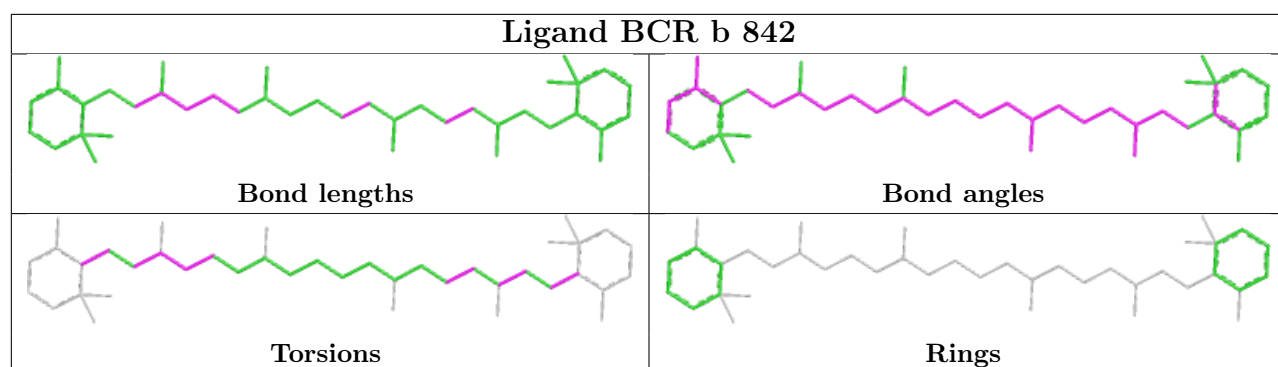
Bond angles

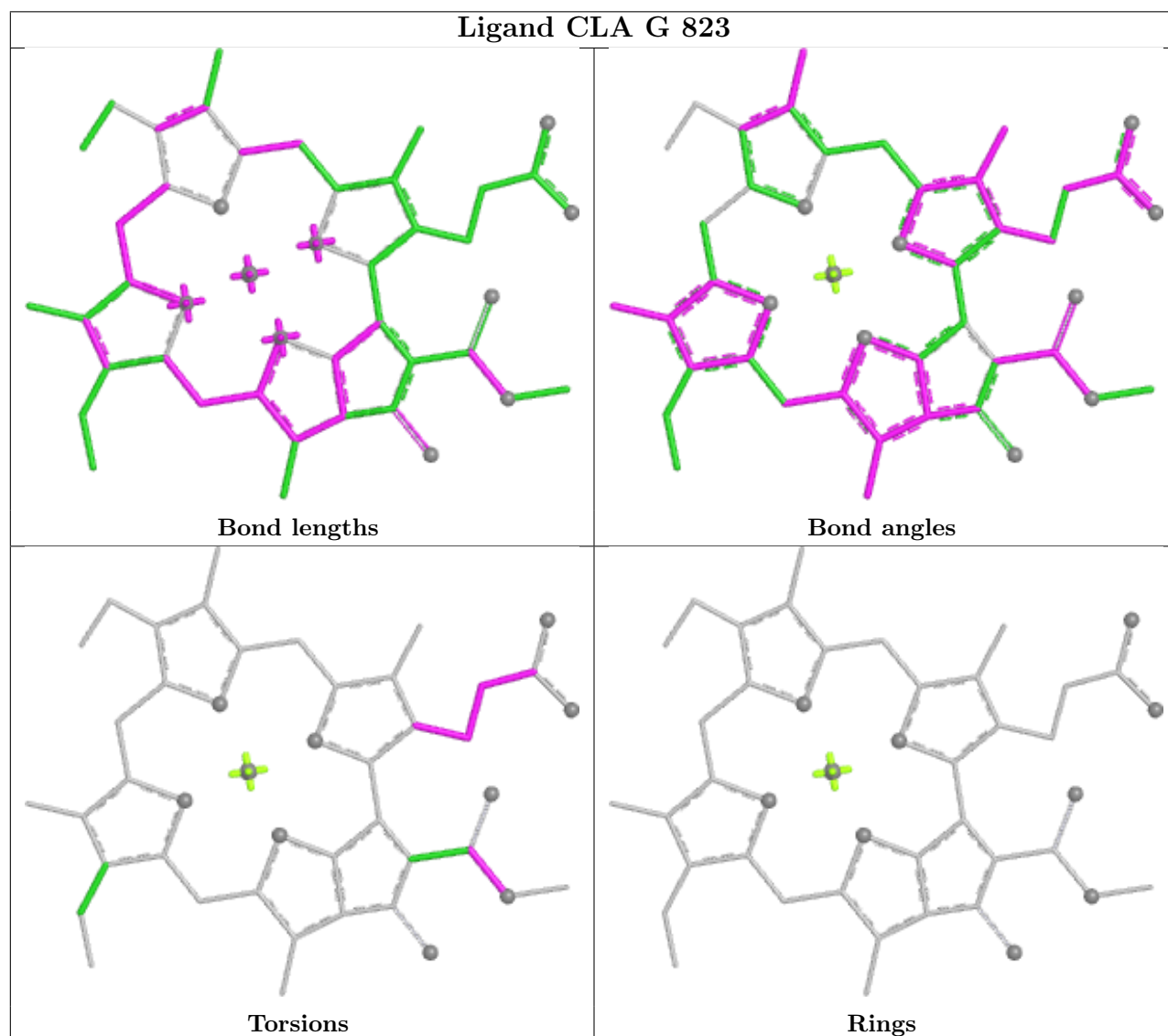
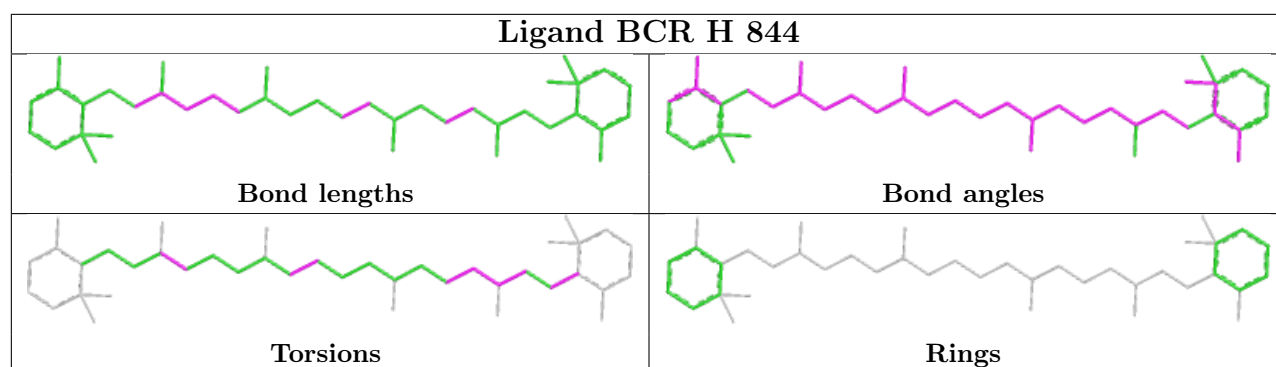


Torsions

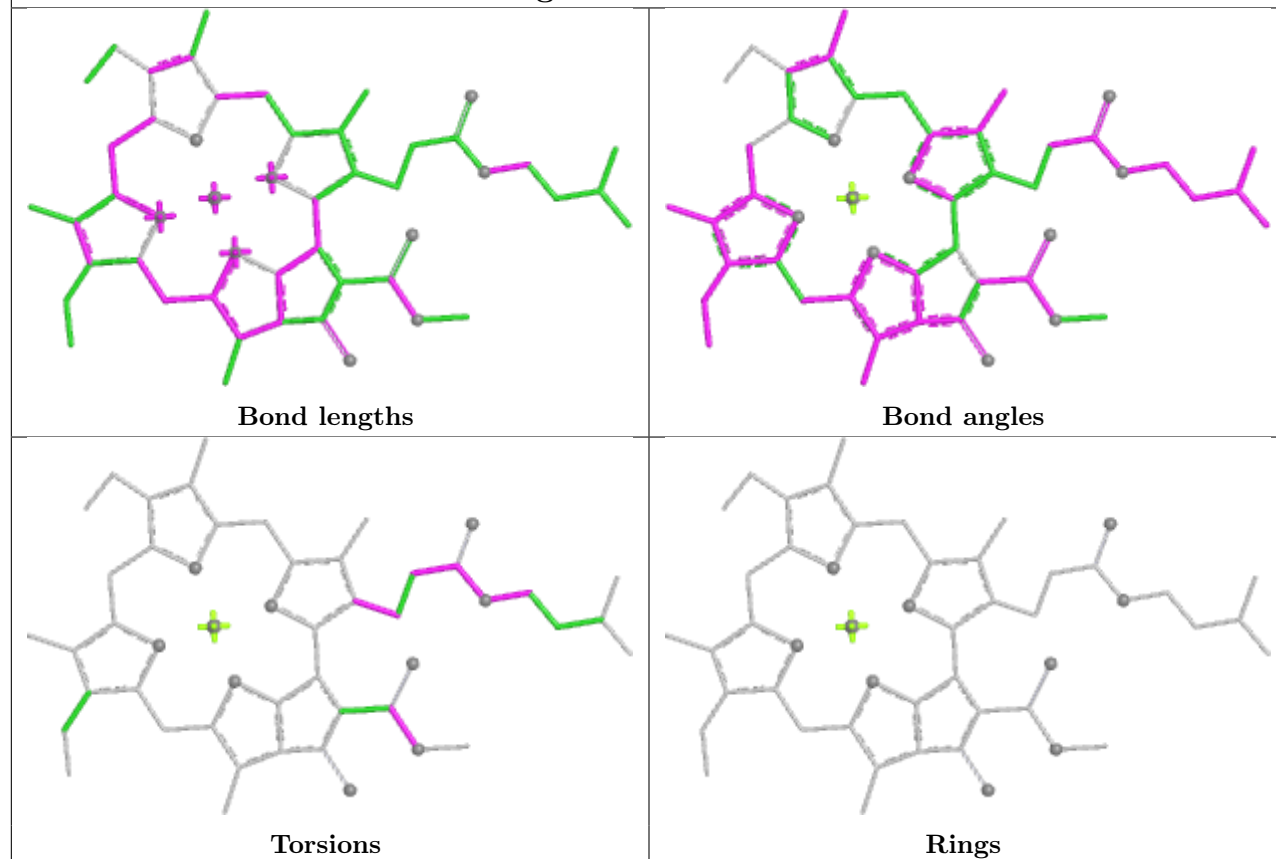


Rings

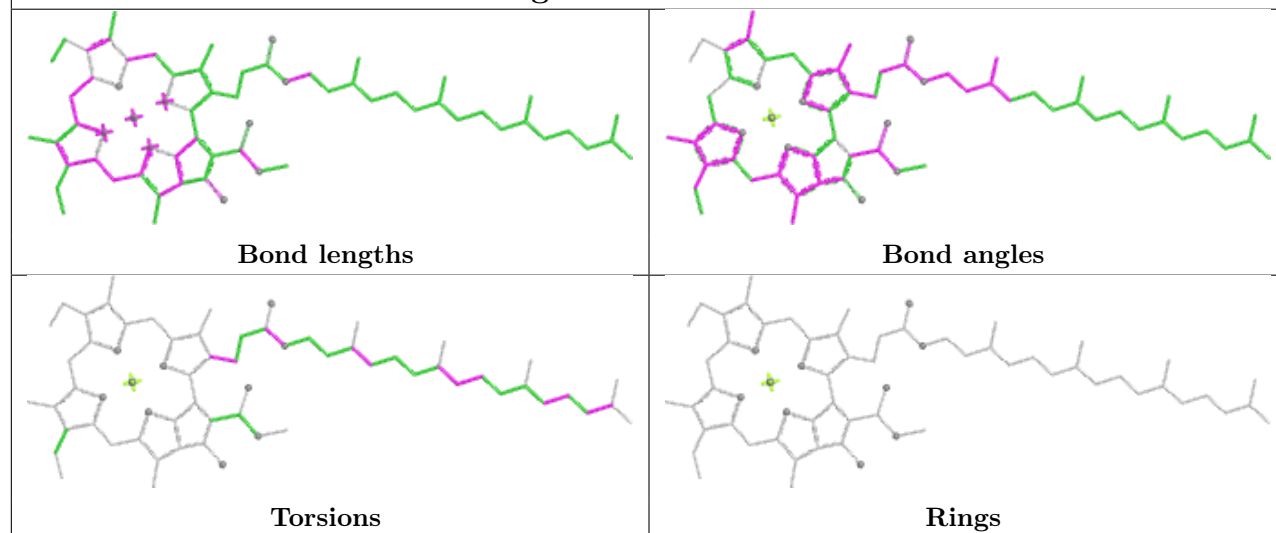




## Ligand CLA a 820

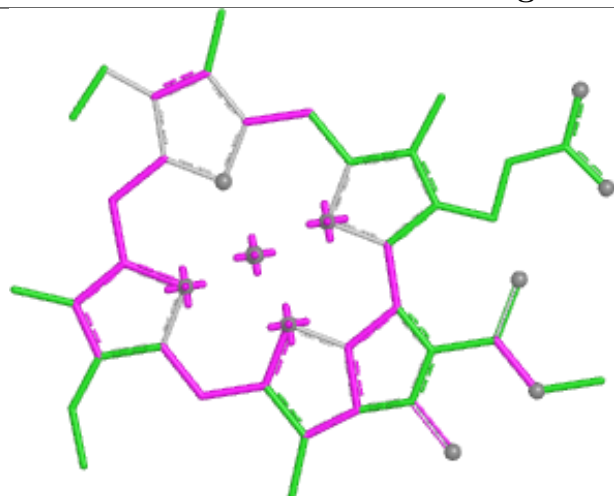


## Ligand CLA U 205

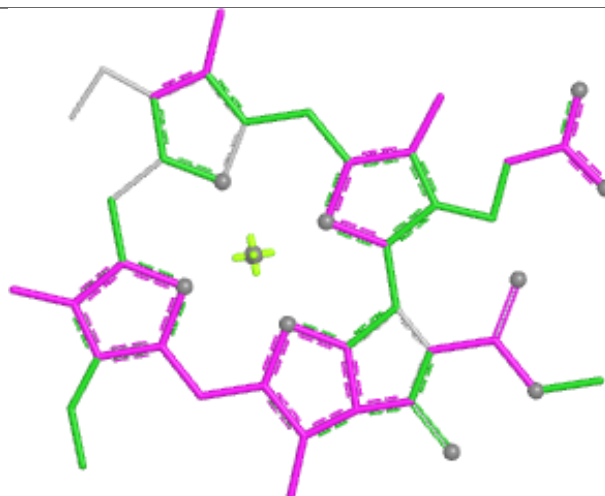




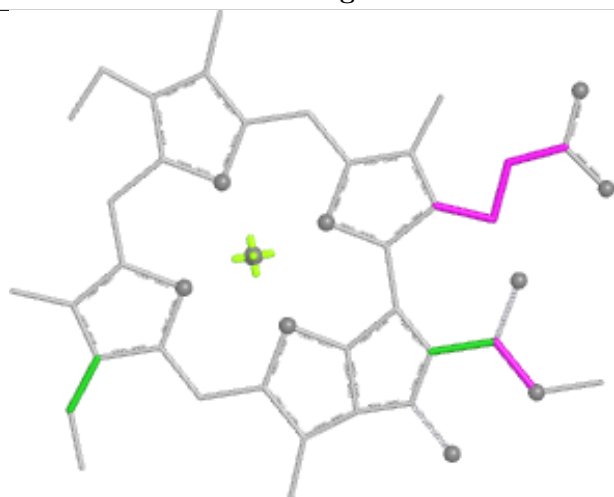
## Ligand CLA b 819



Bond lengths



Bond angles

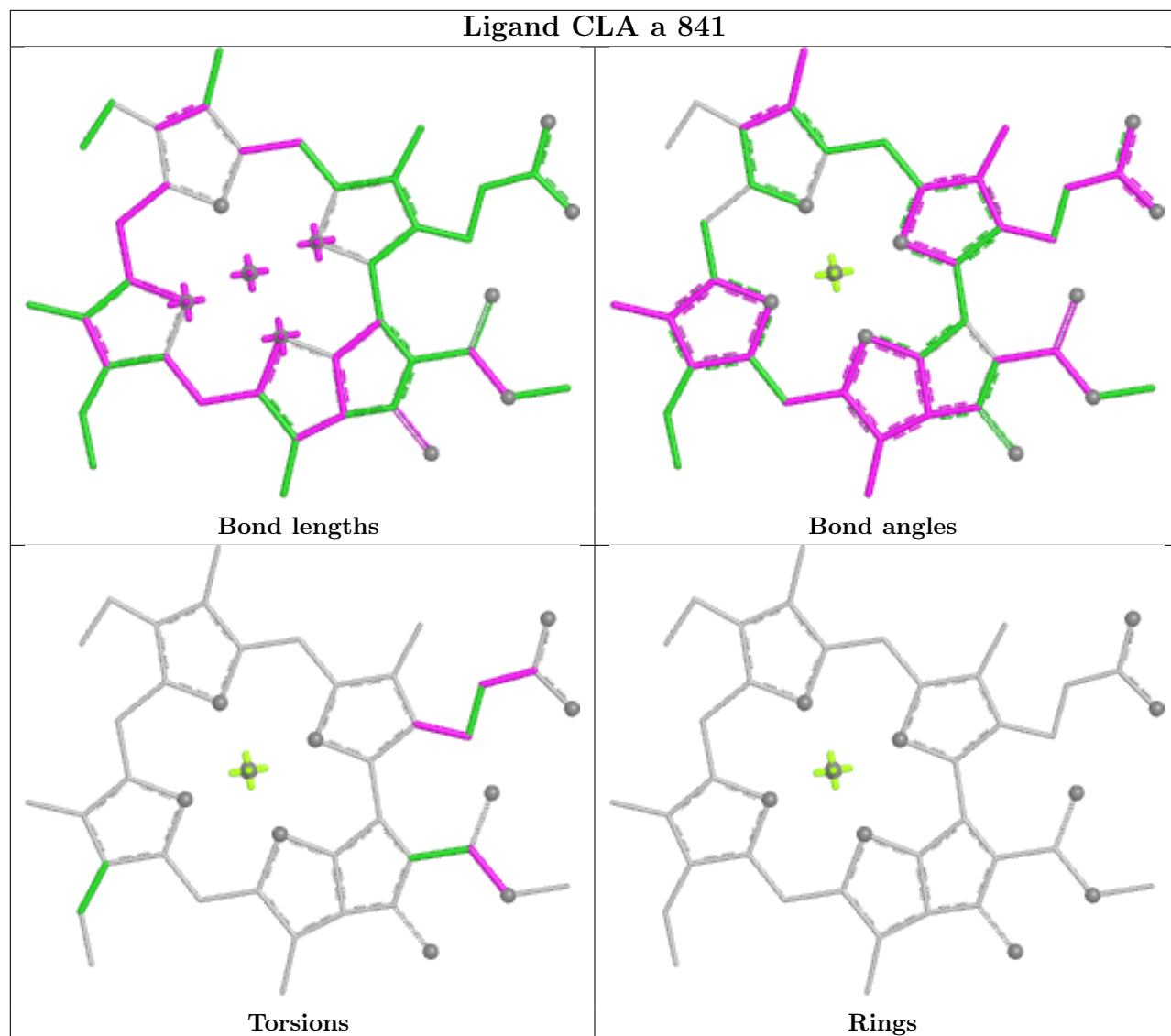


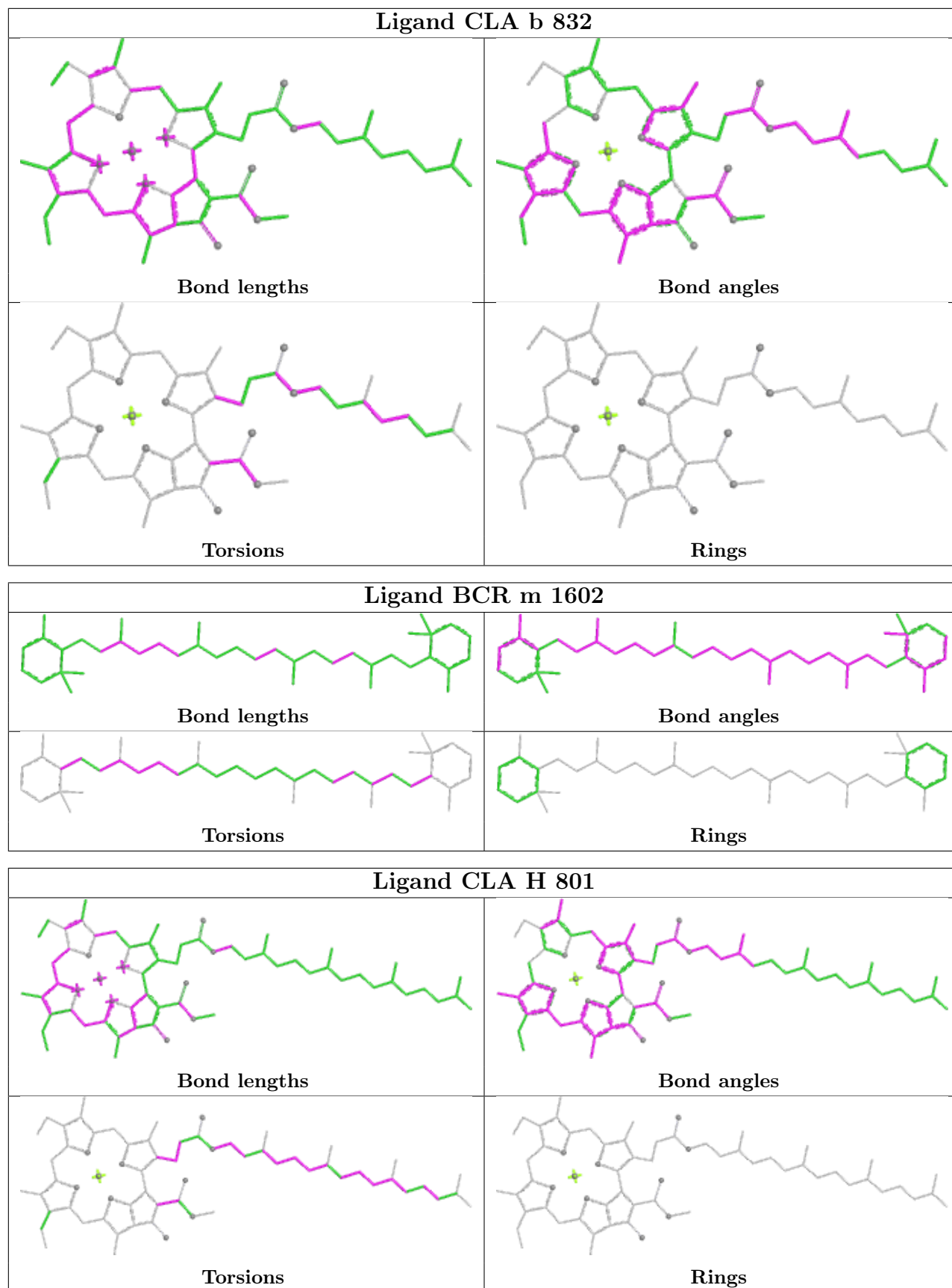
Torsions

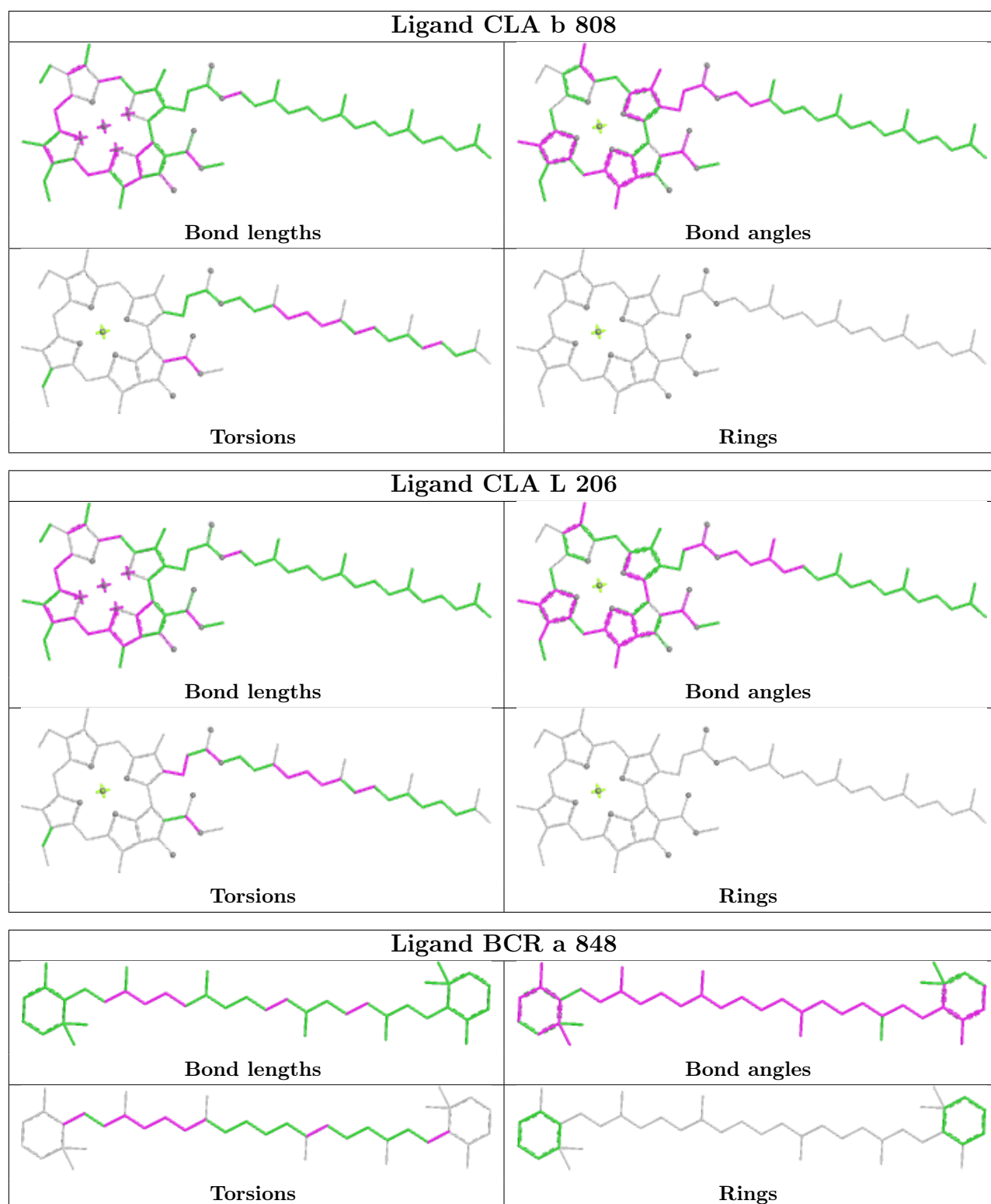


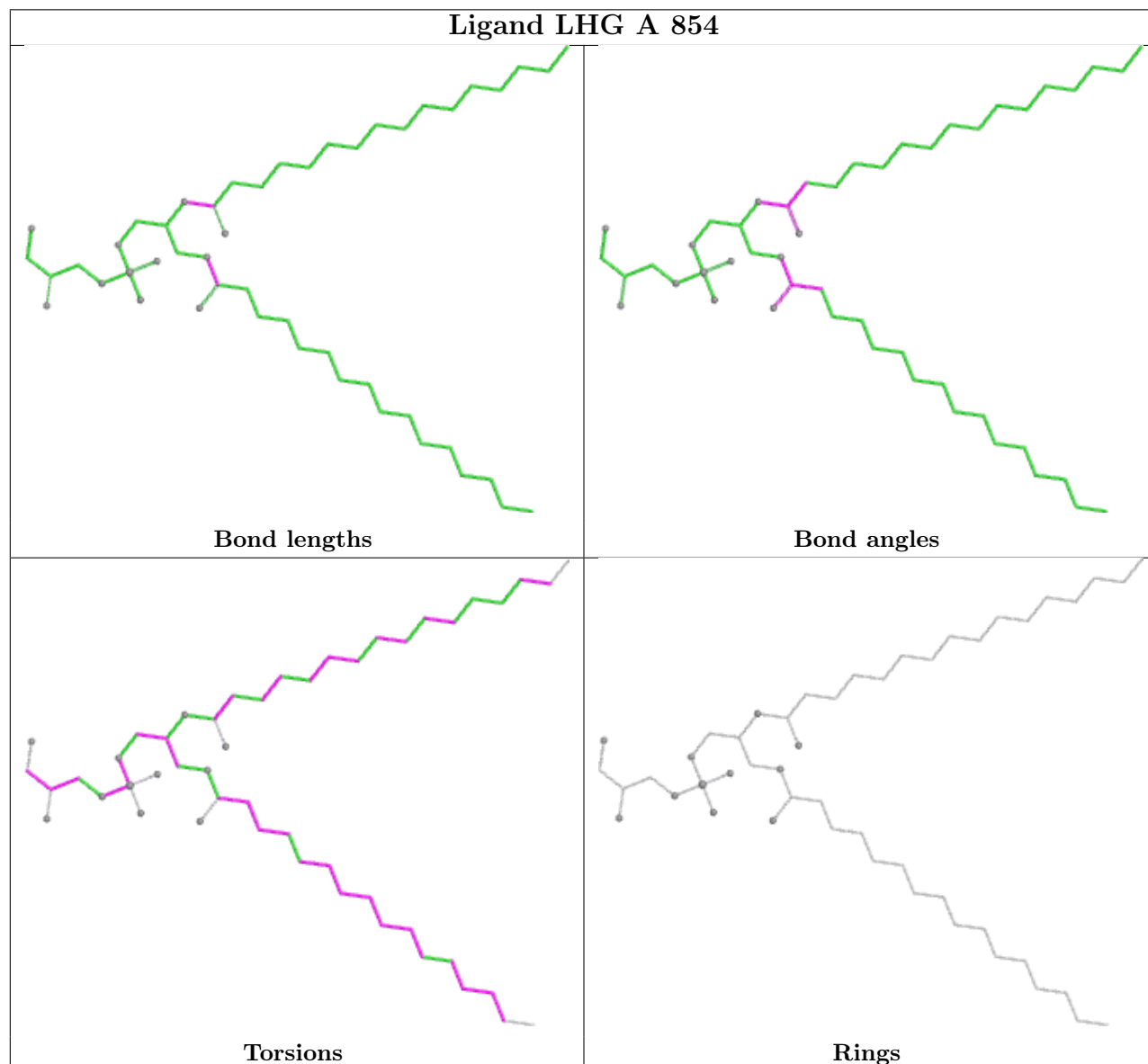
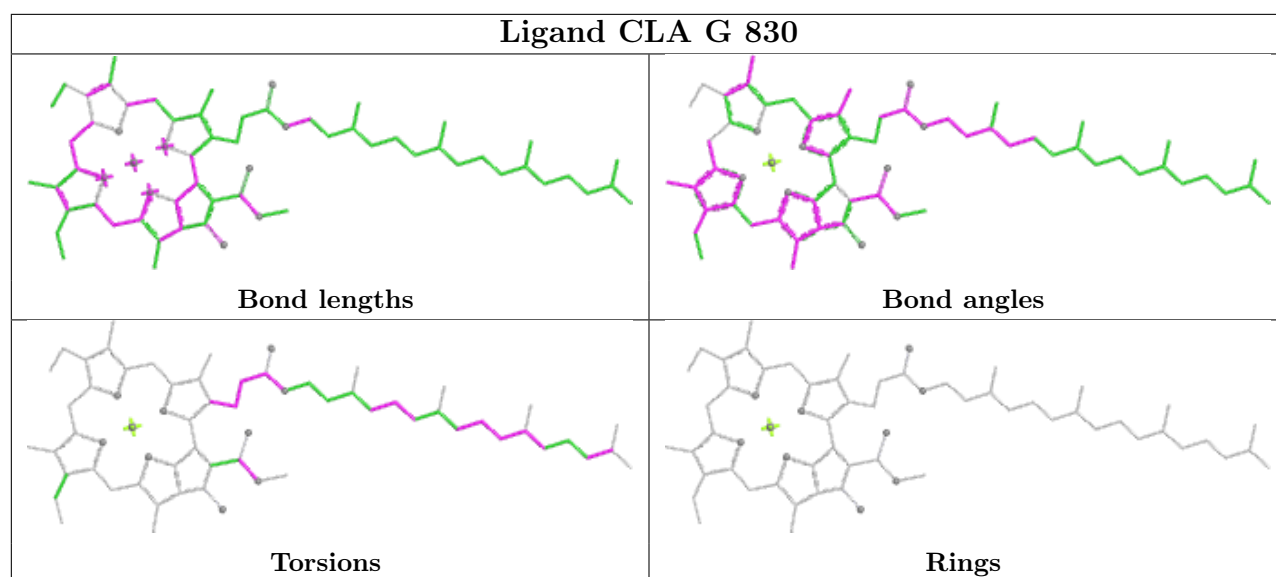
Rings

## Ligand CLA a 841

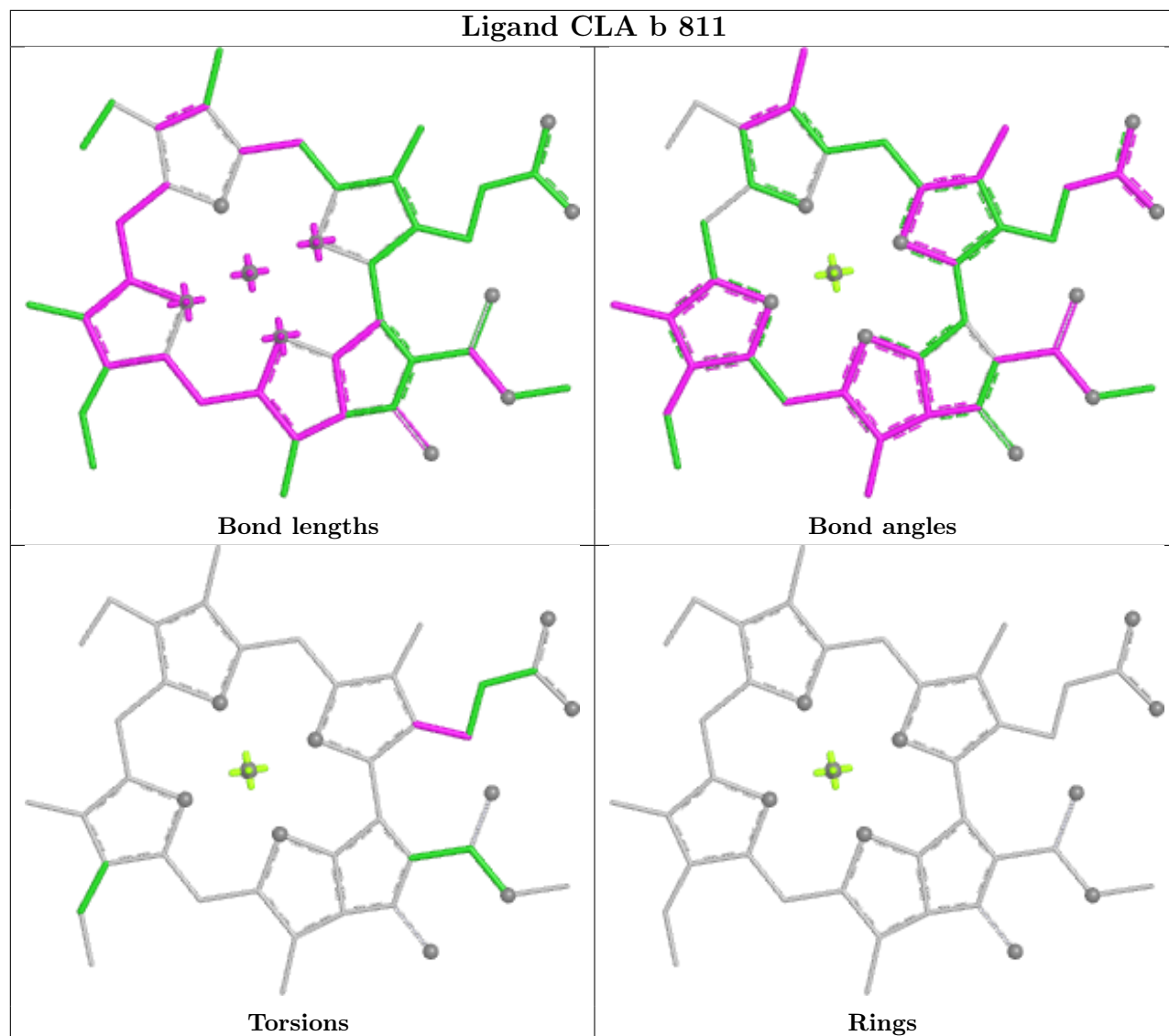




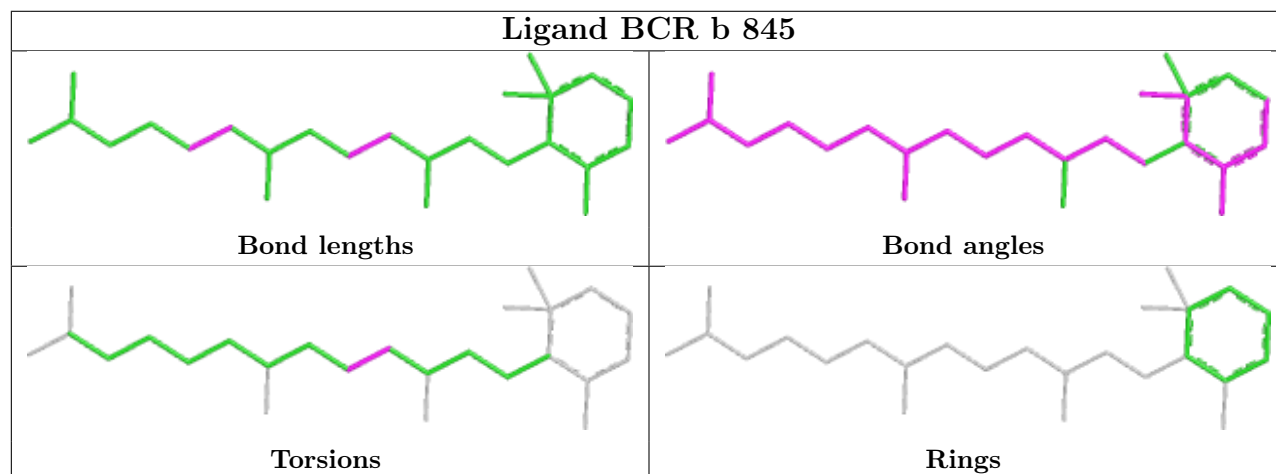


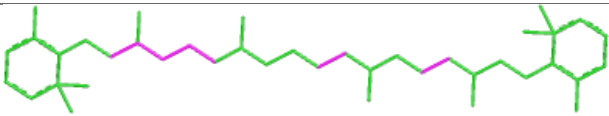
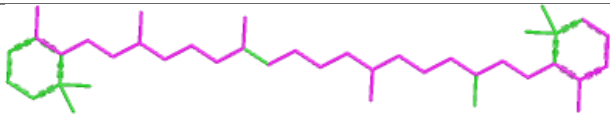
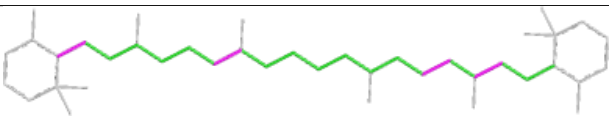
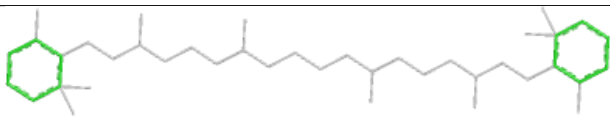



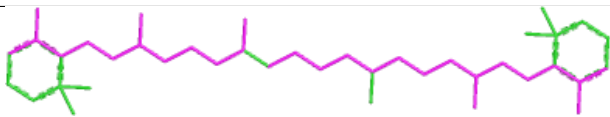
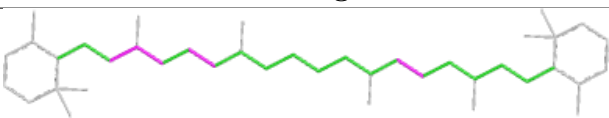
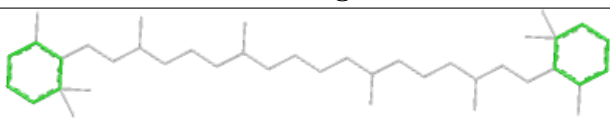
## Ligand CLA b 811

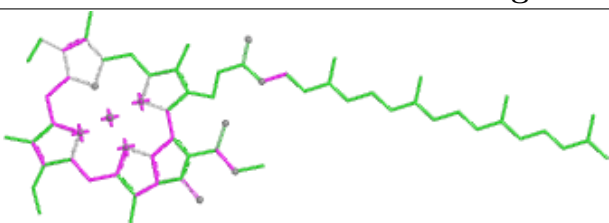
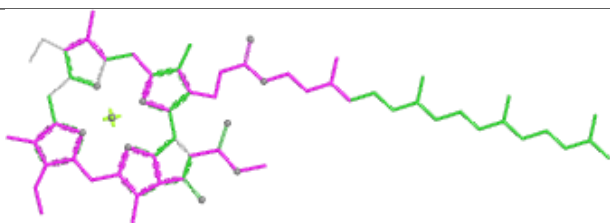
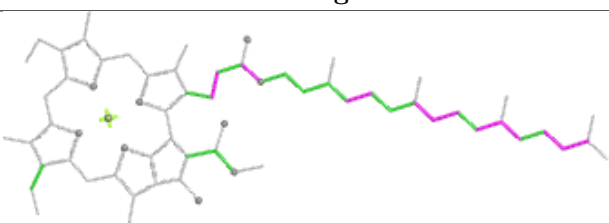
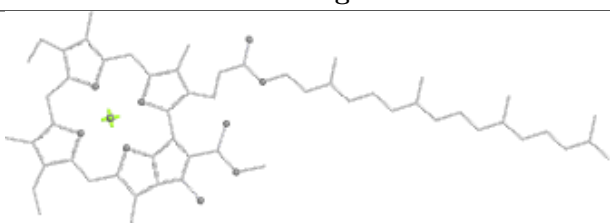


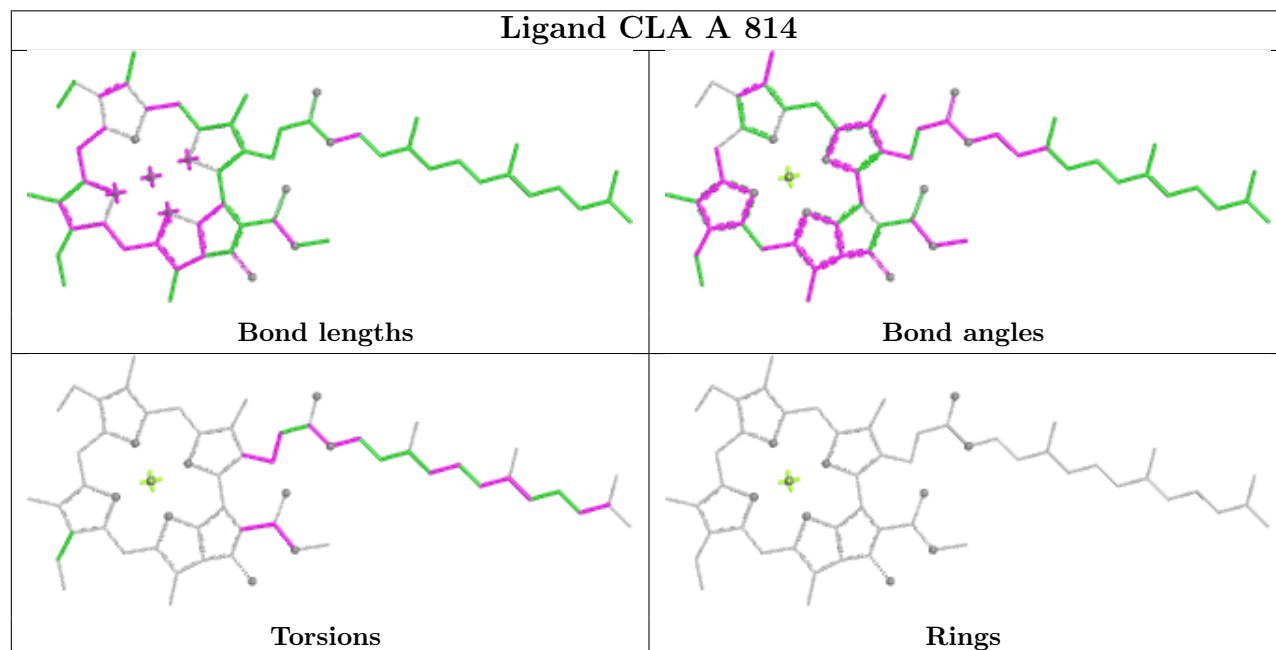
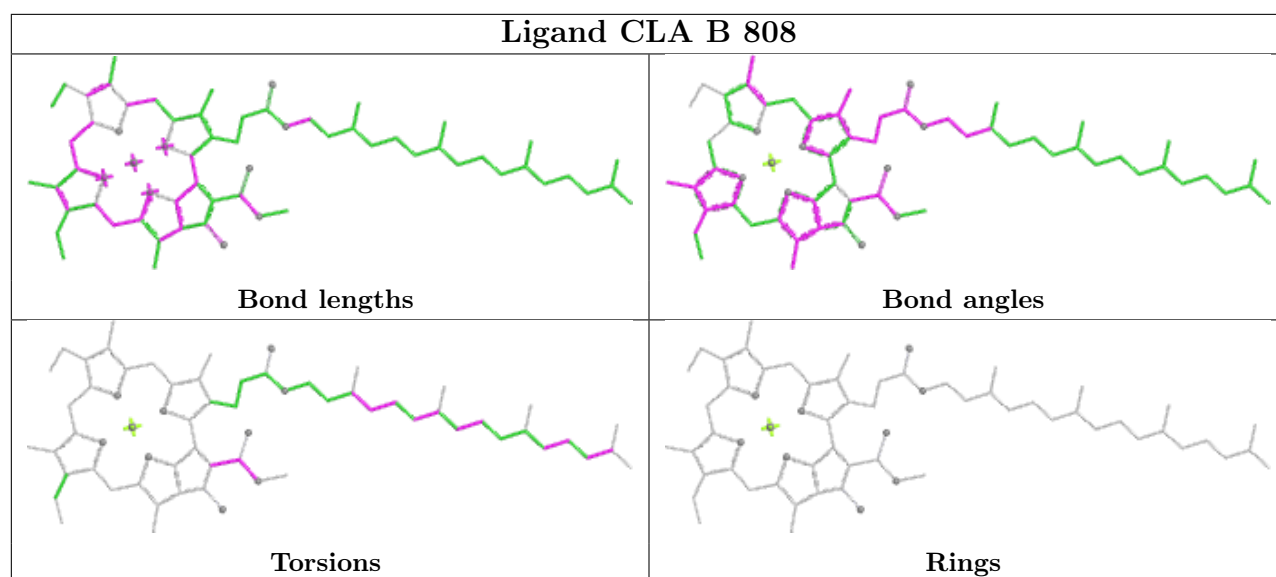
## Ligand BCR b 845



Ligand BCR G 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

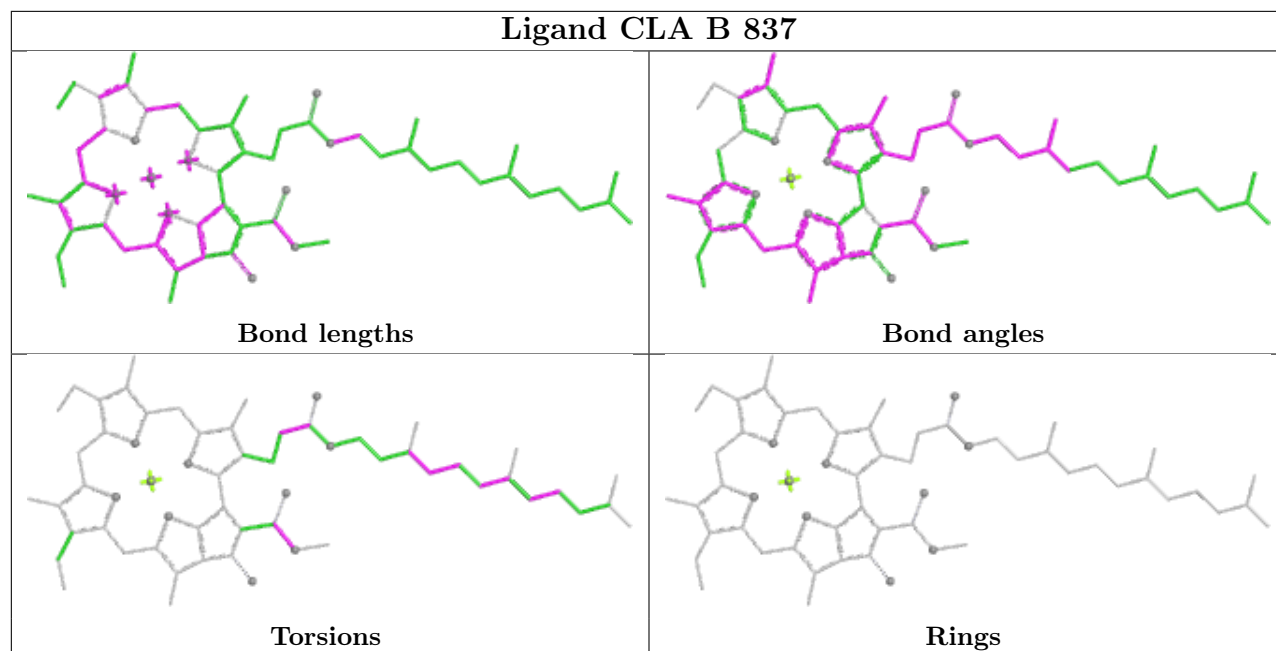
Ligand BCR i 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

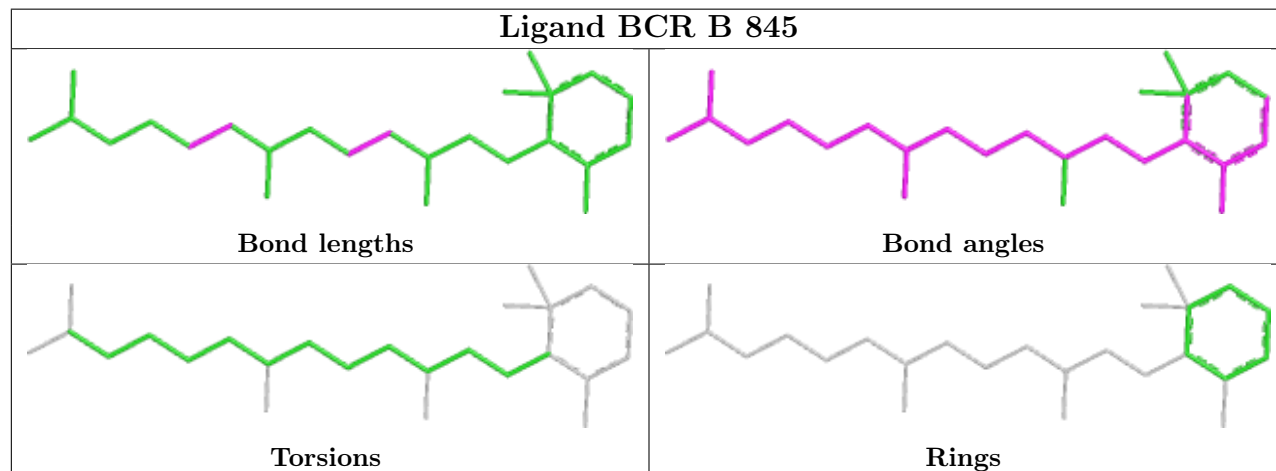




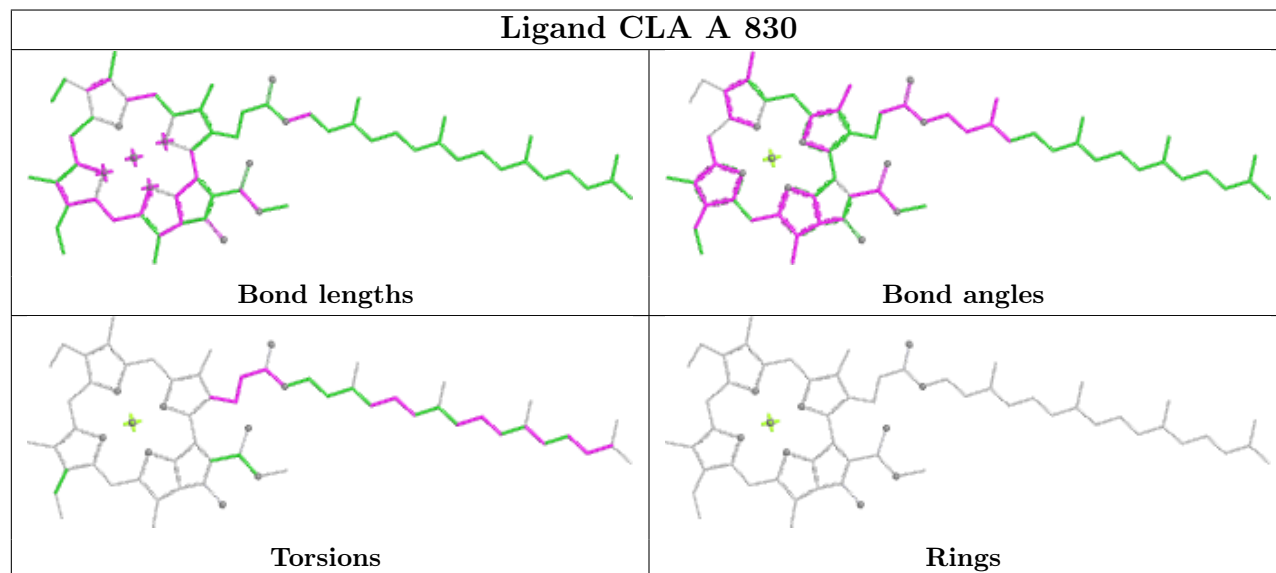
## Ligand CLA B 837

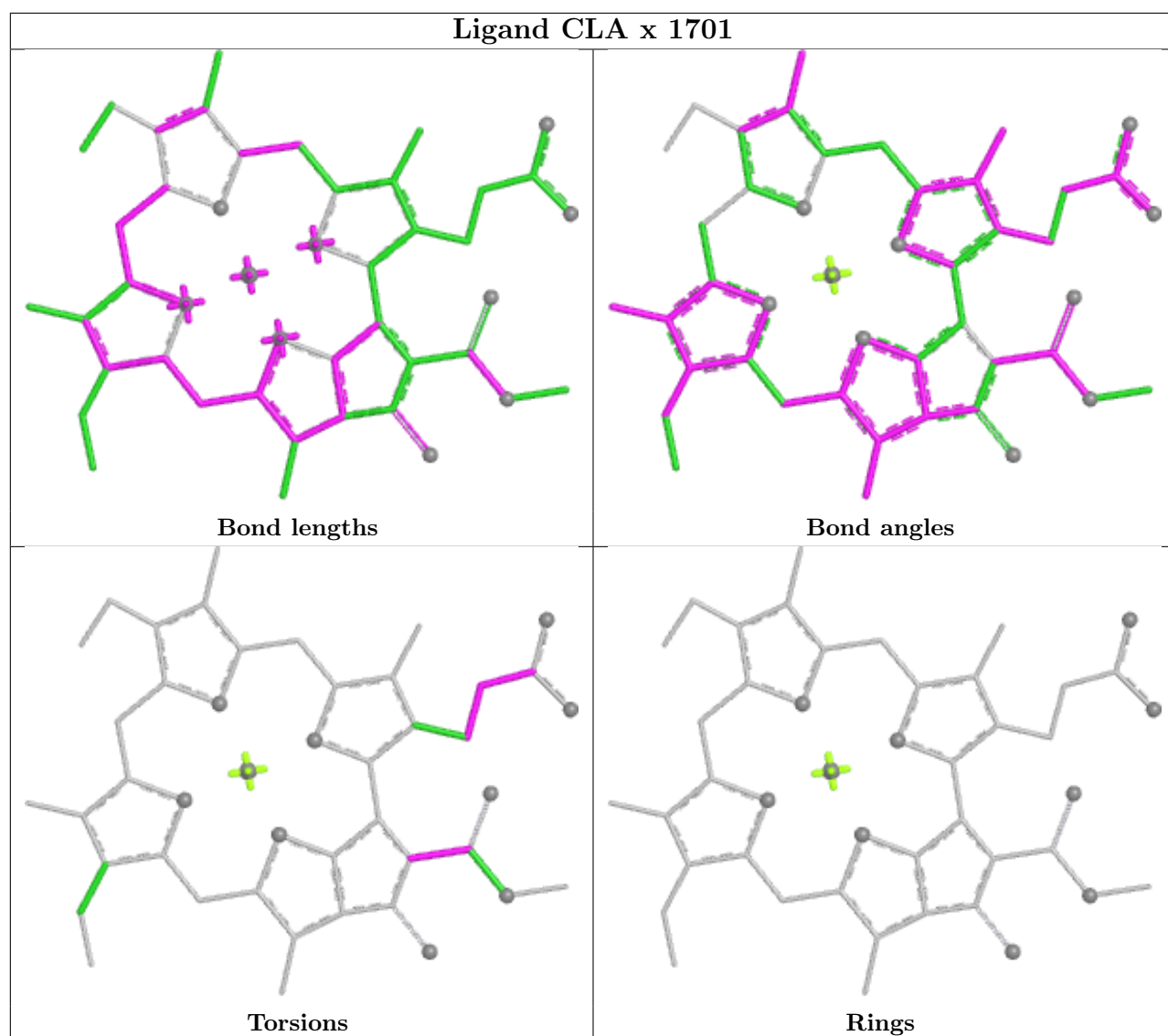


## Ligand BCR B 845

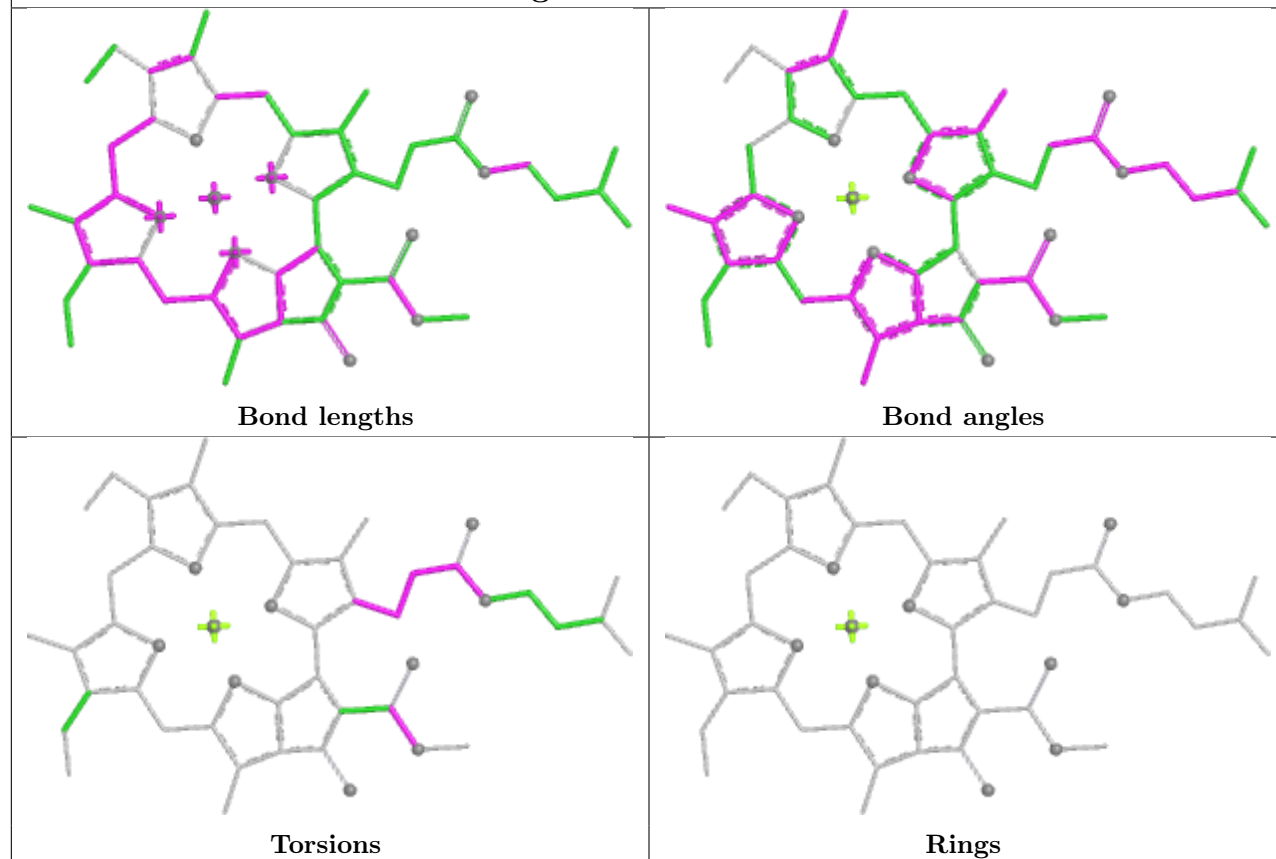


## Ligand CLA A 830

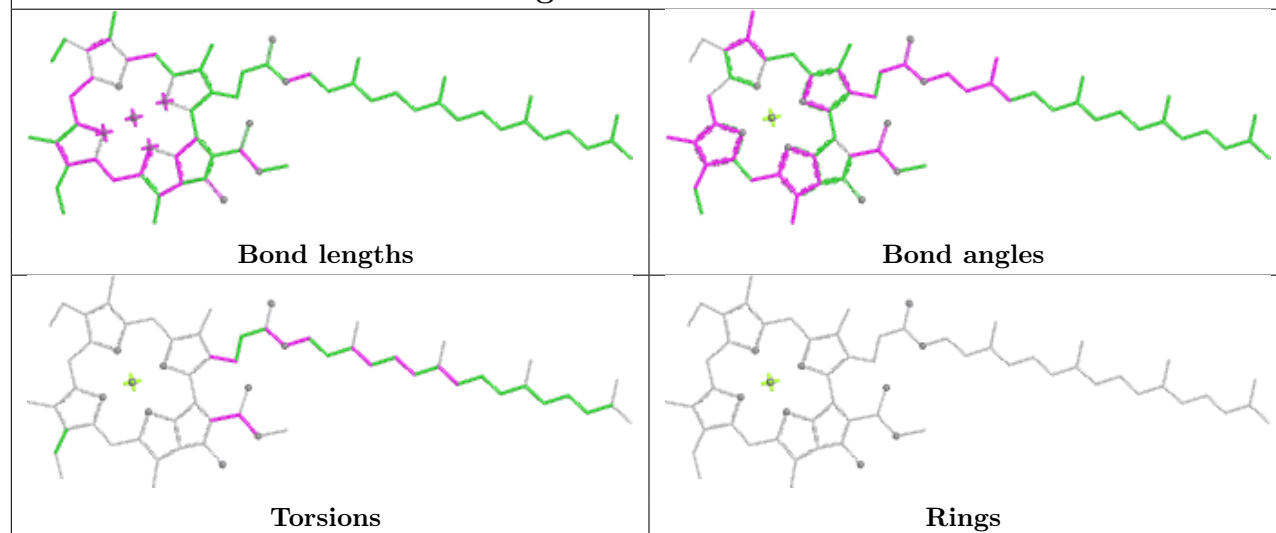


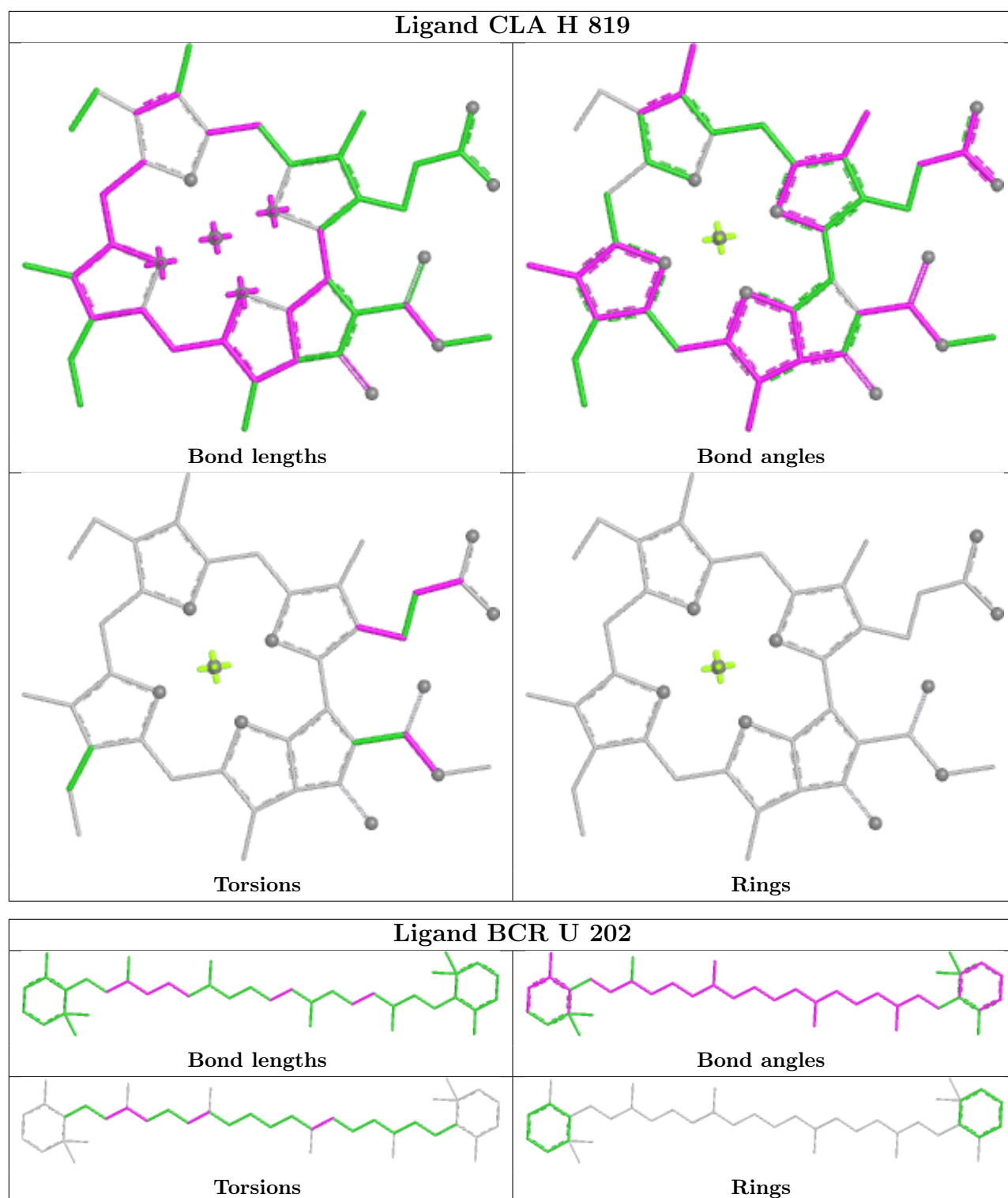


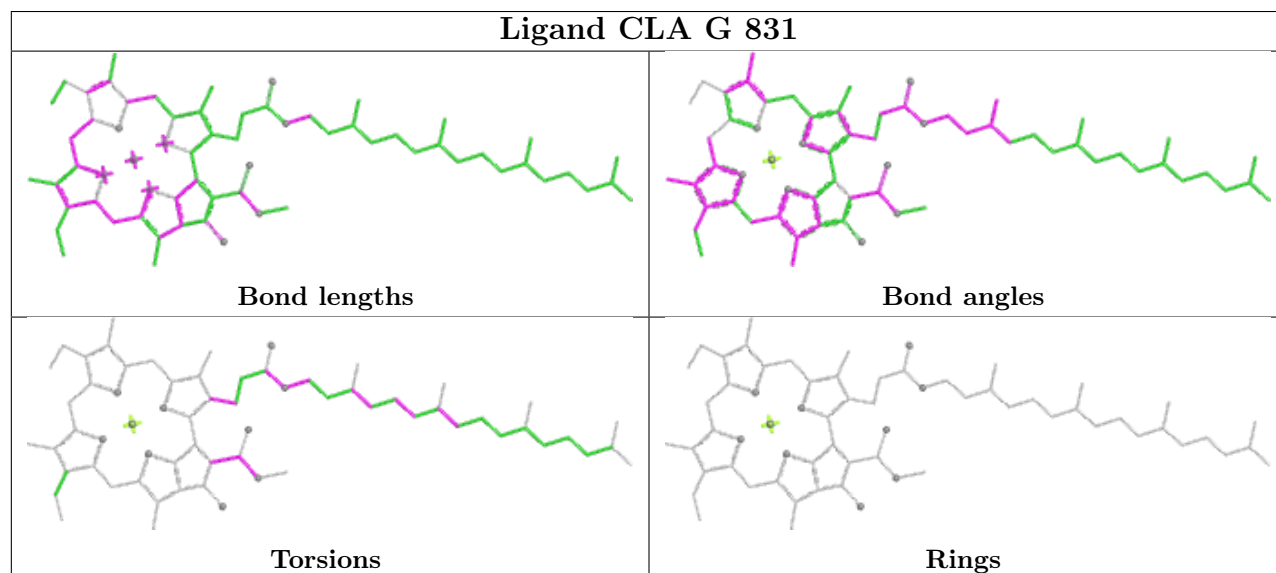
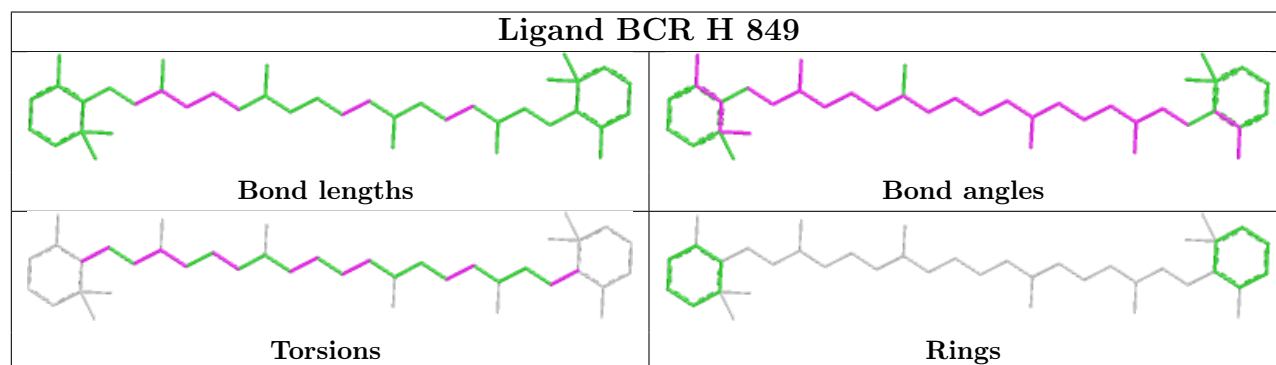
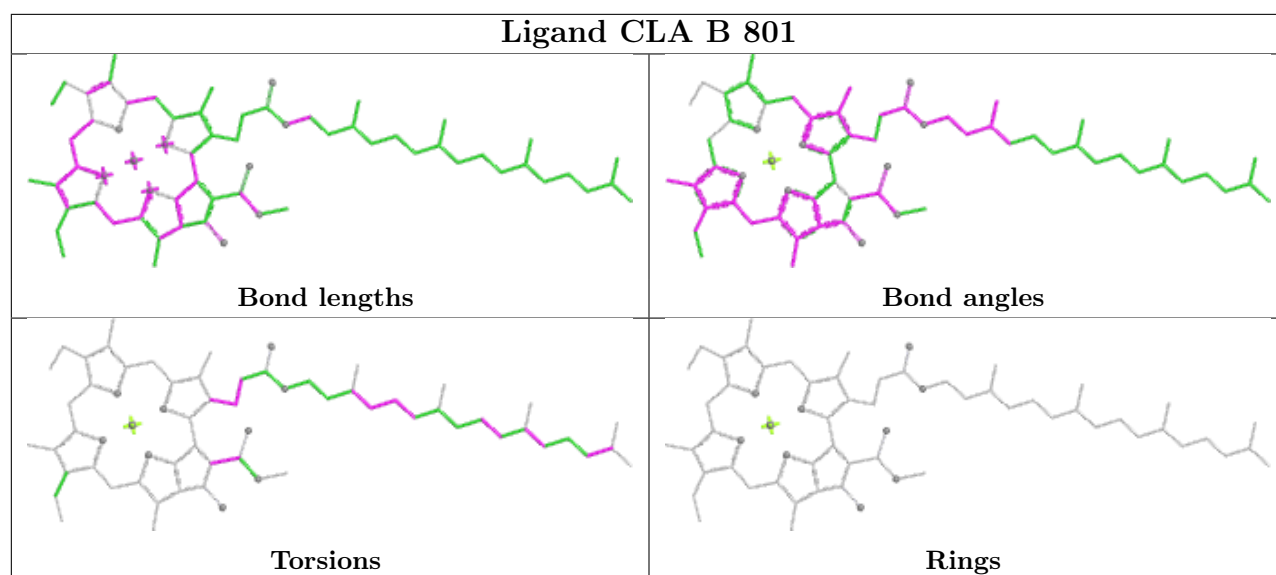
## Ligand CLA A 819

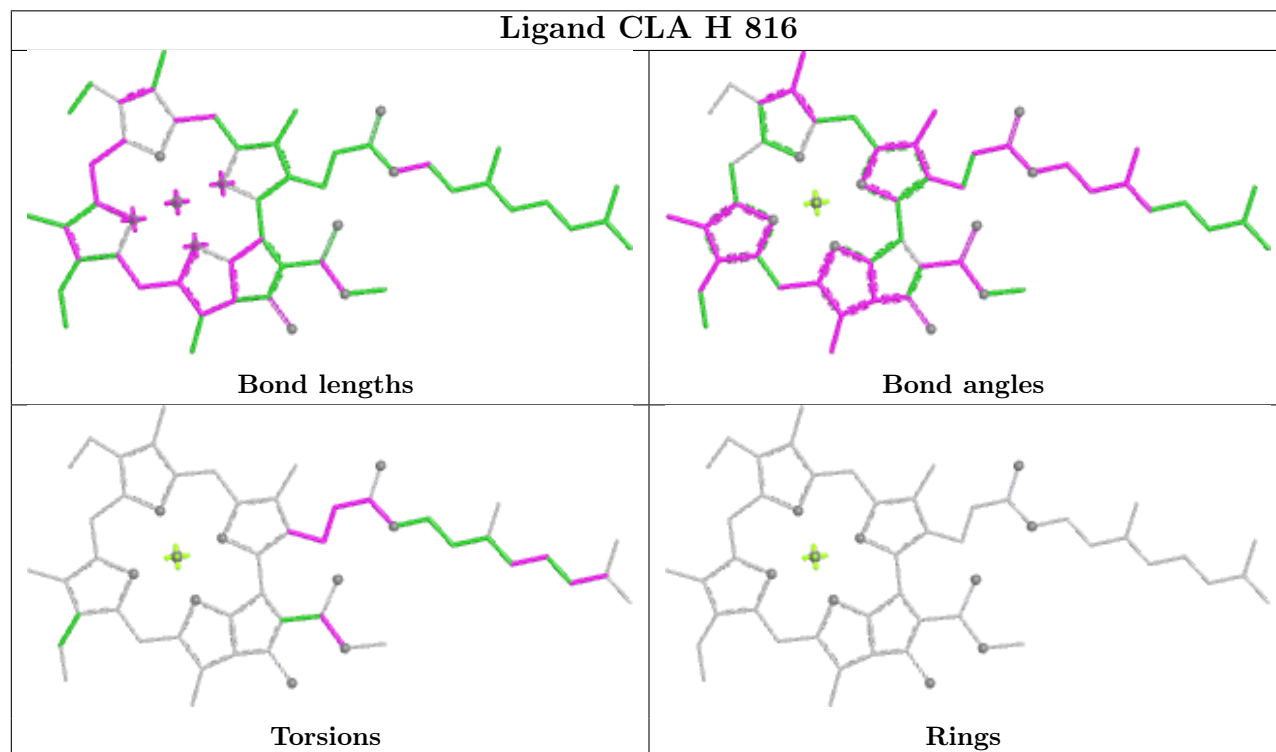
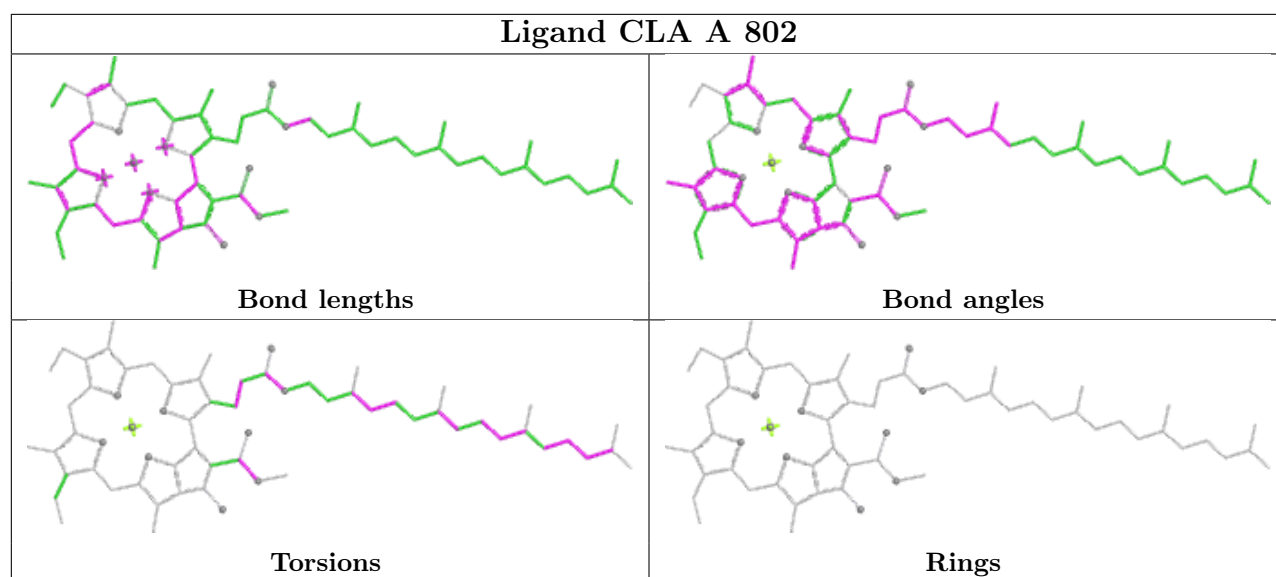


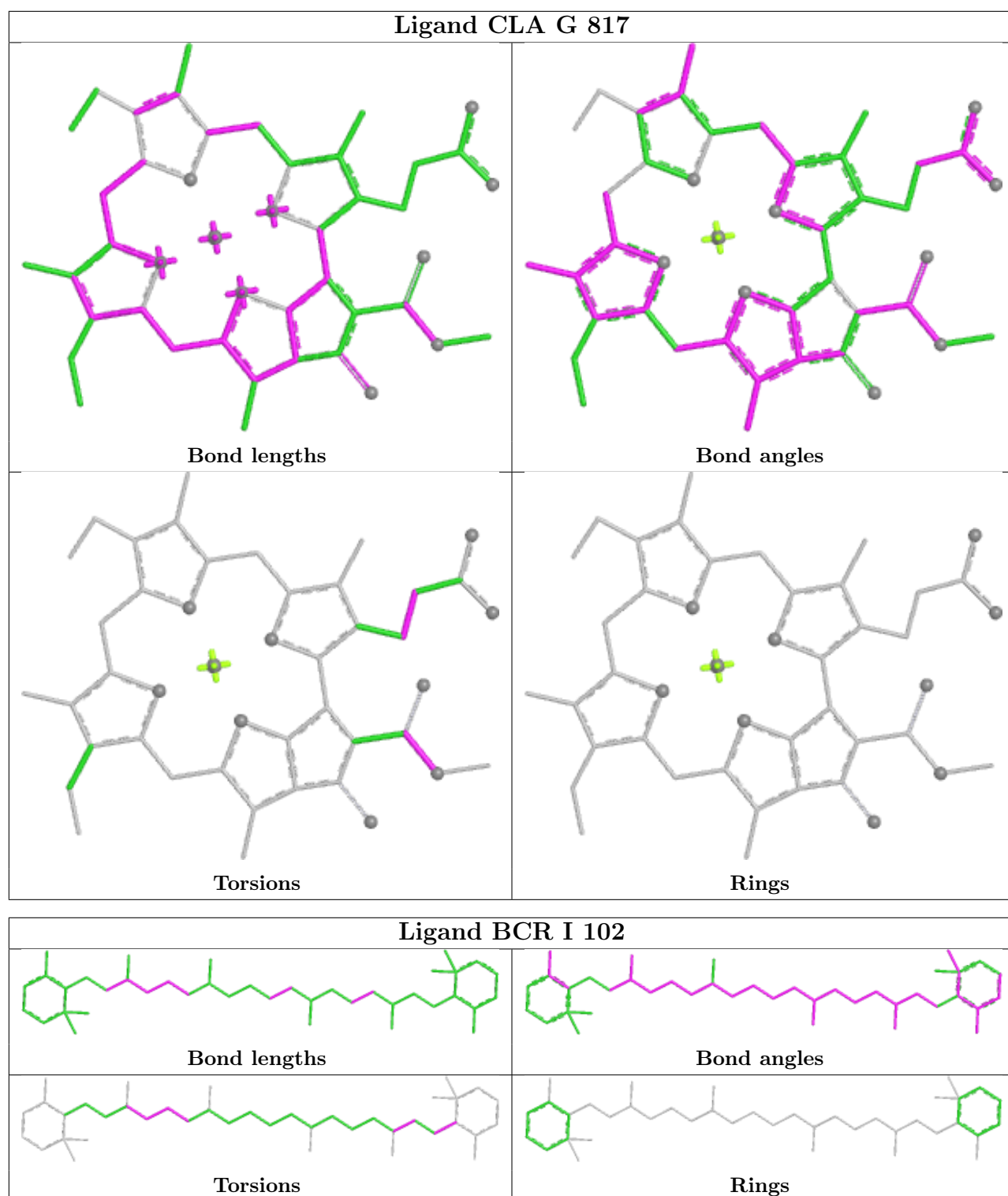
## Ligand CLA a 830



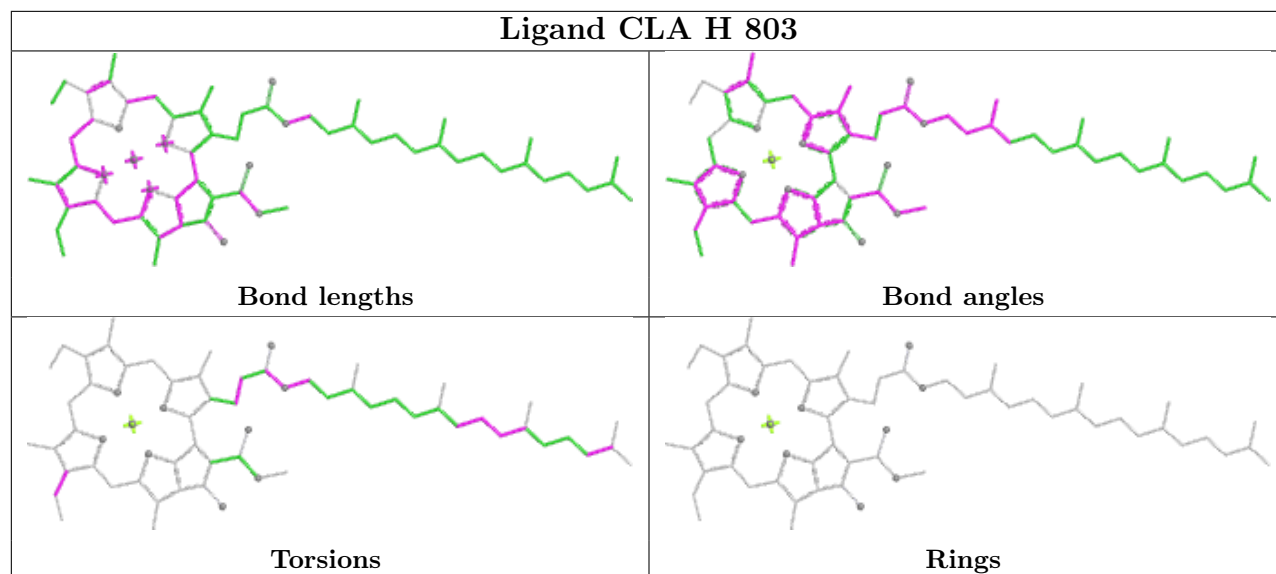




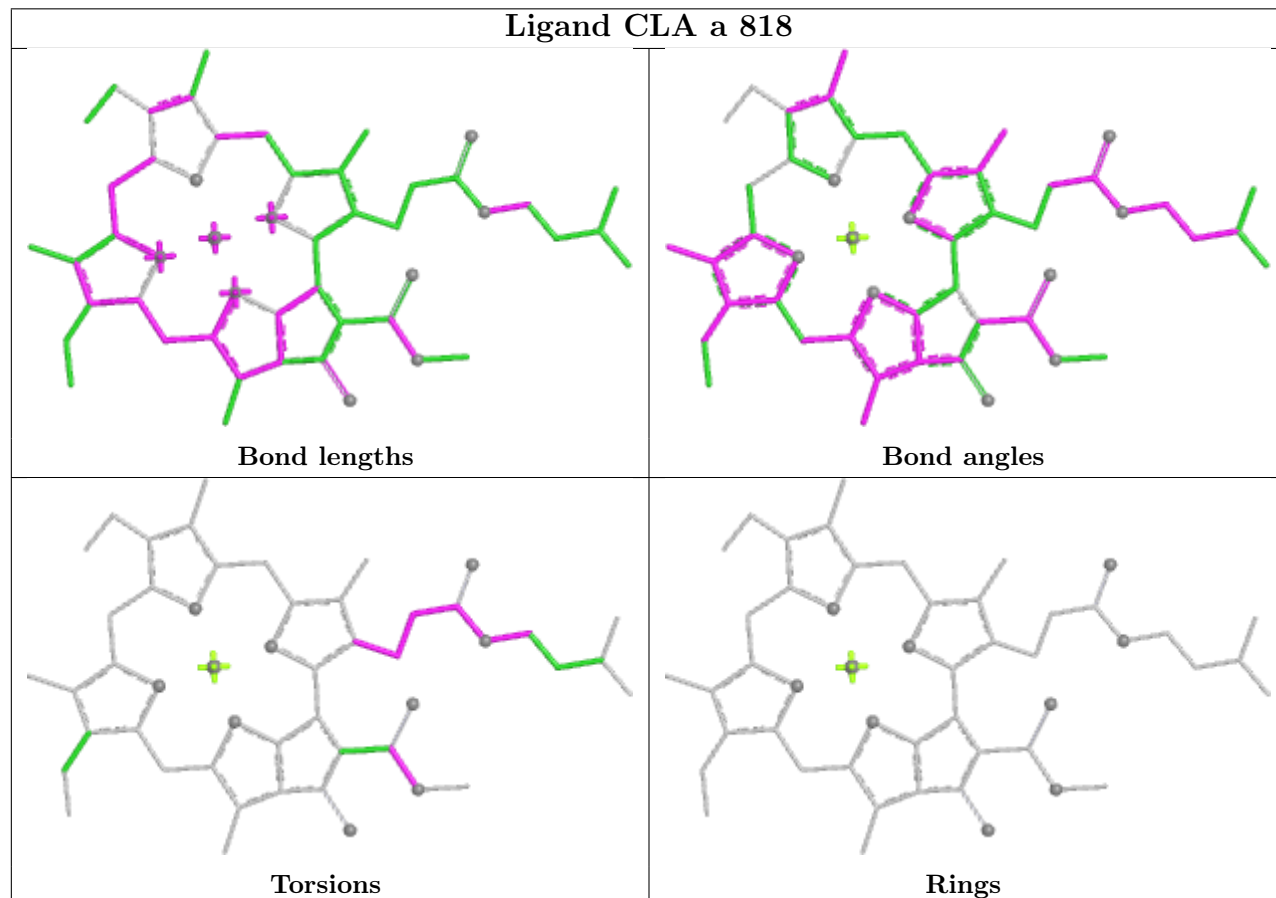




## Ligand CLA H 803

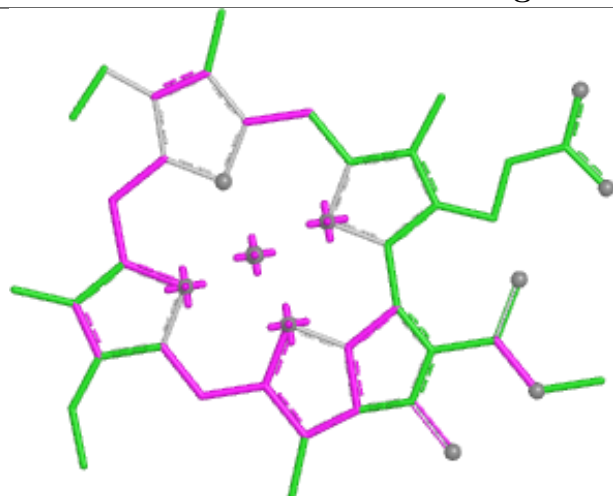


## Ligand CLA a 818

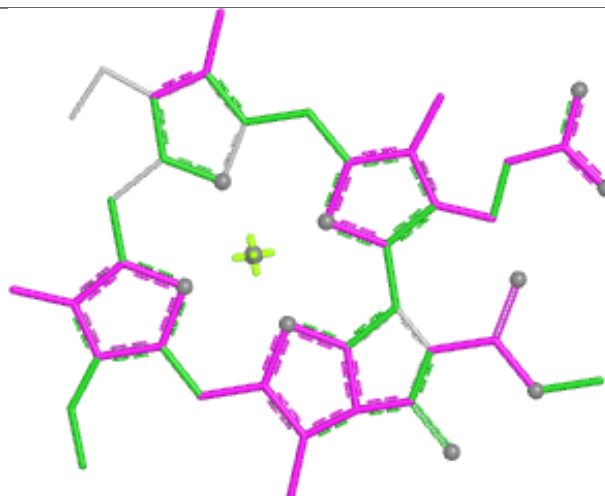




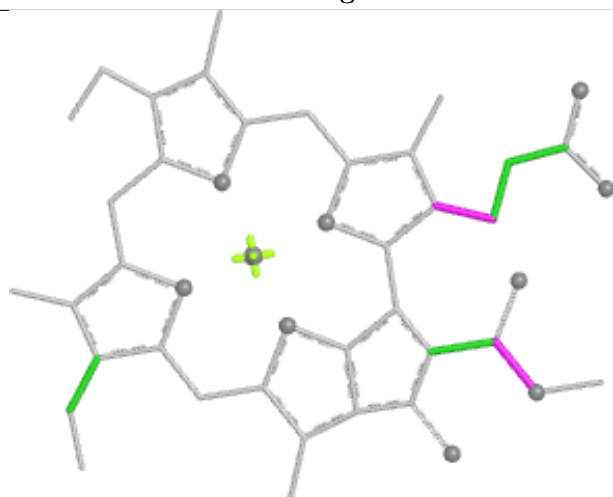
## Ligand CLA A 842



Bond lengths



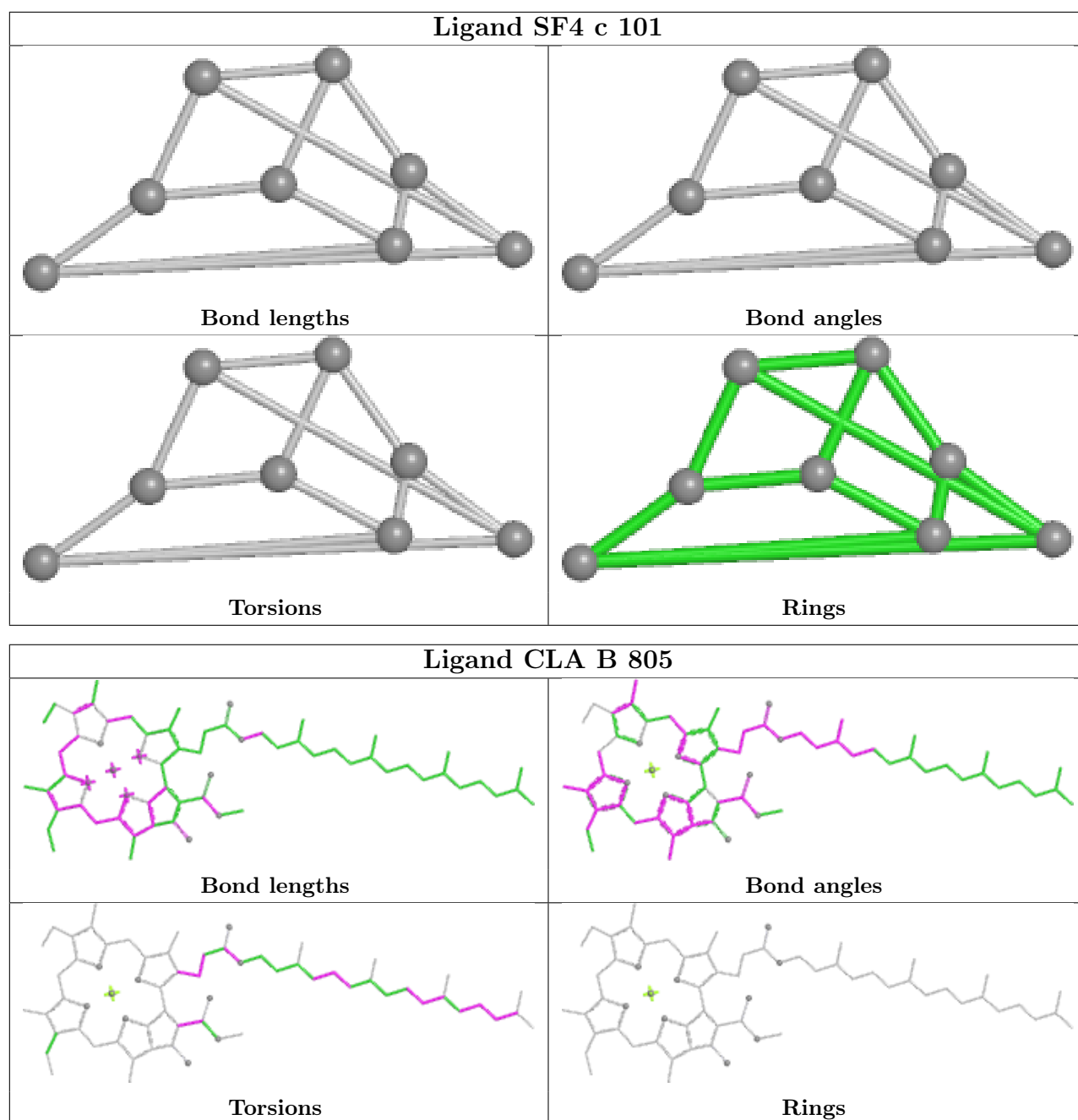
Bond angles

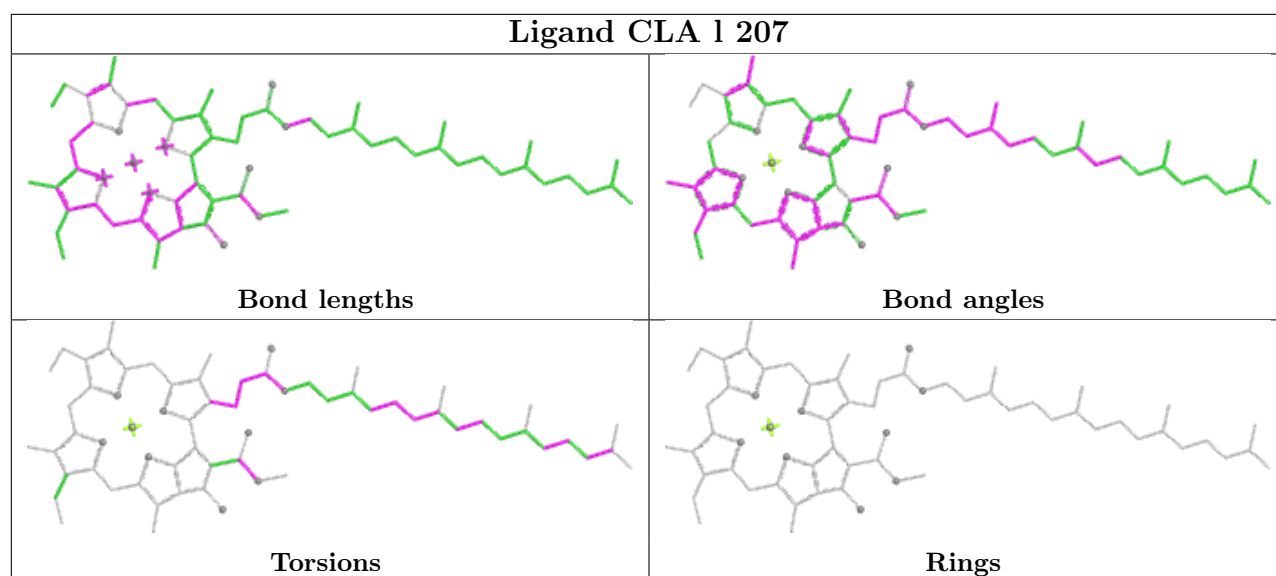
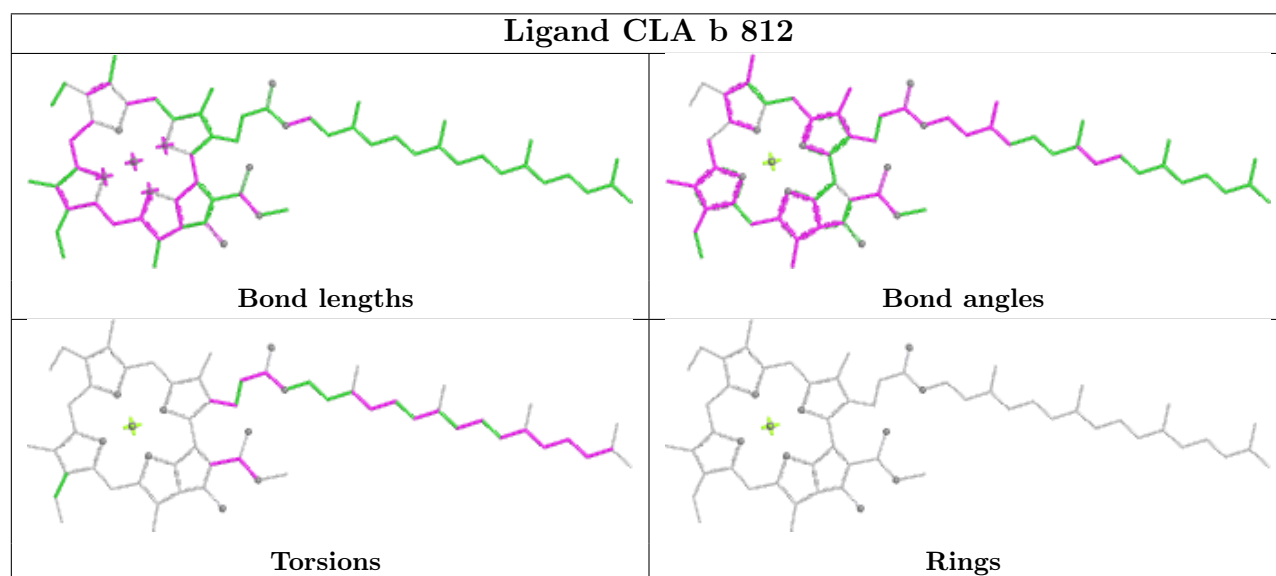
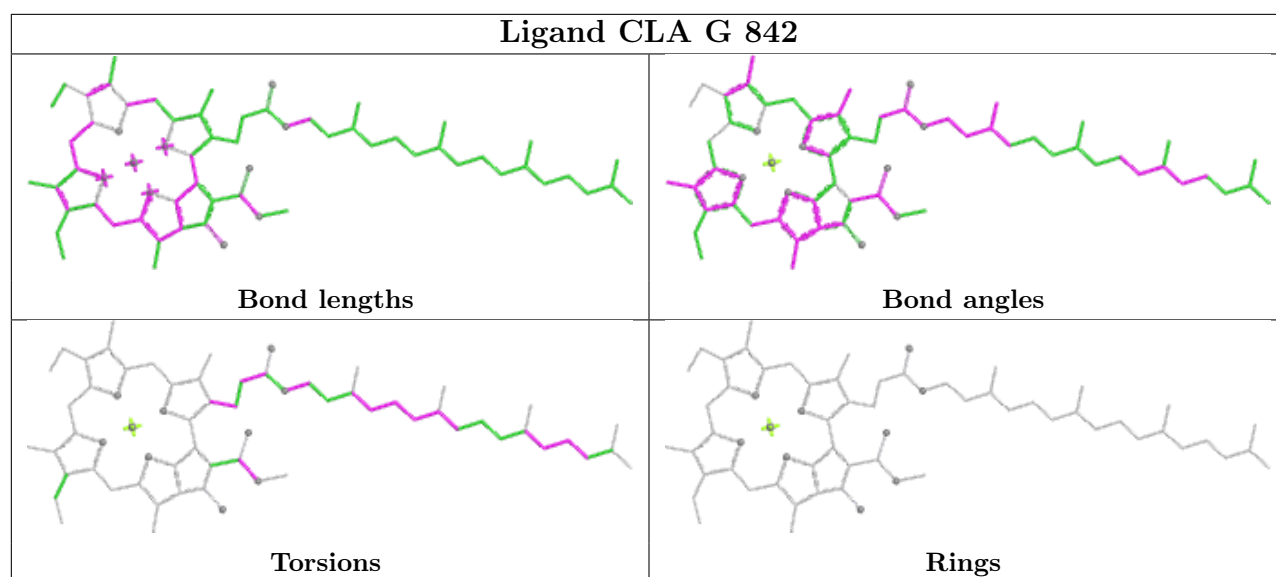


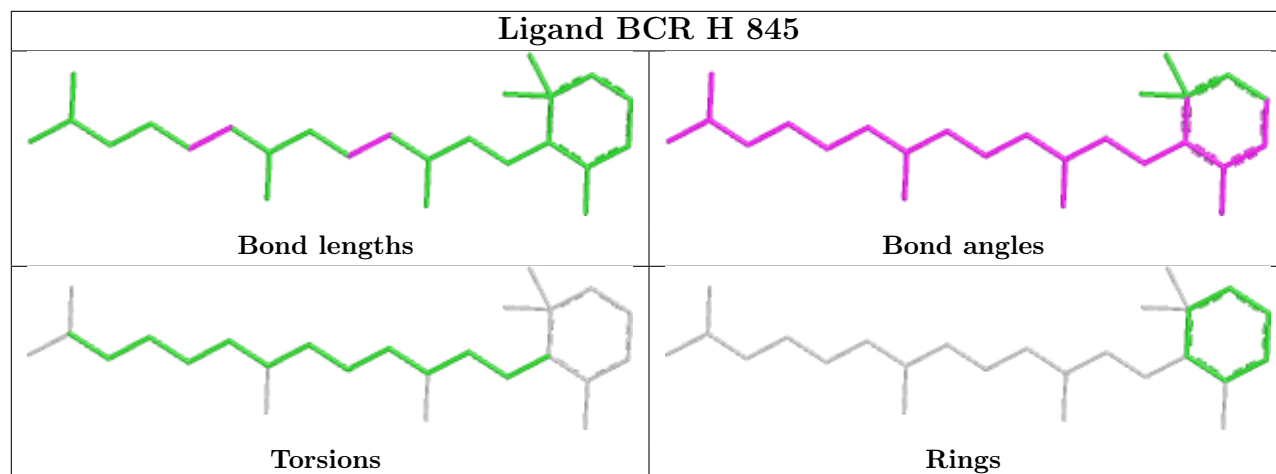
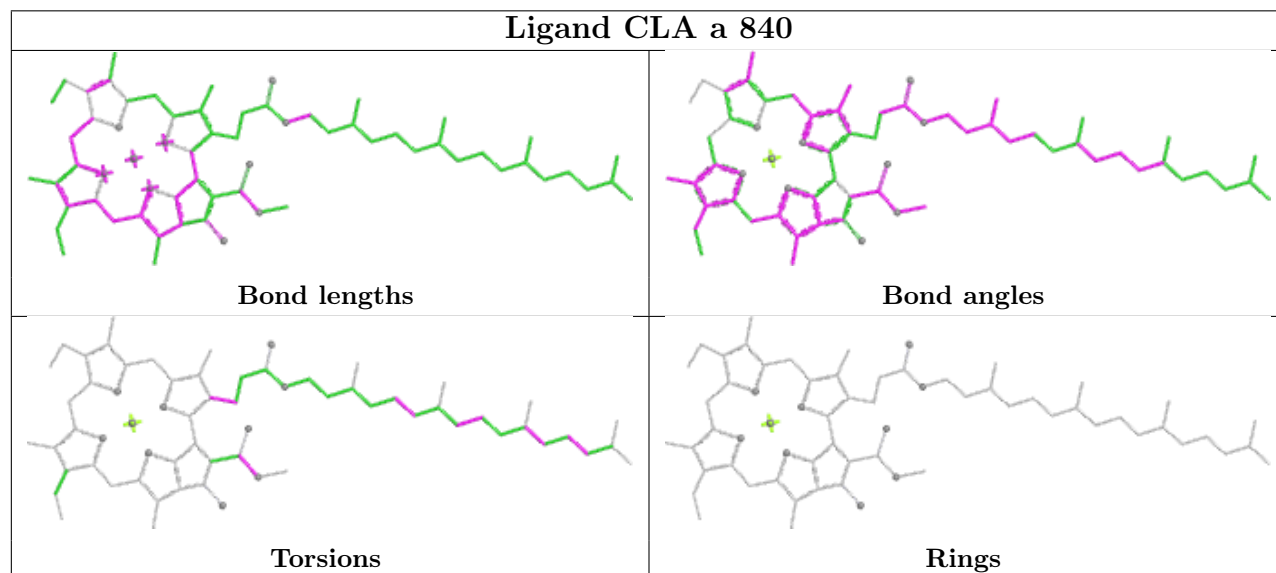
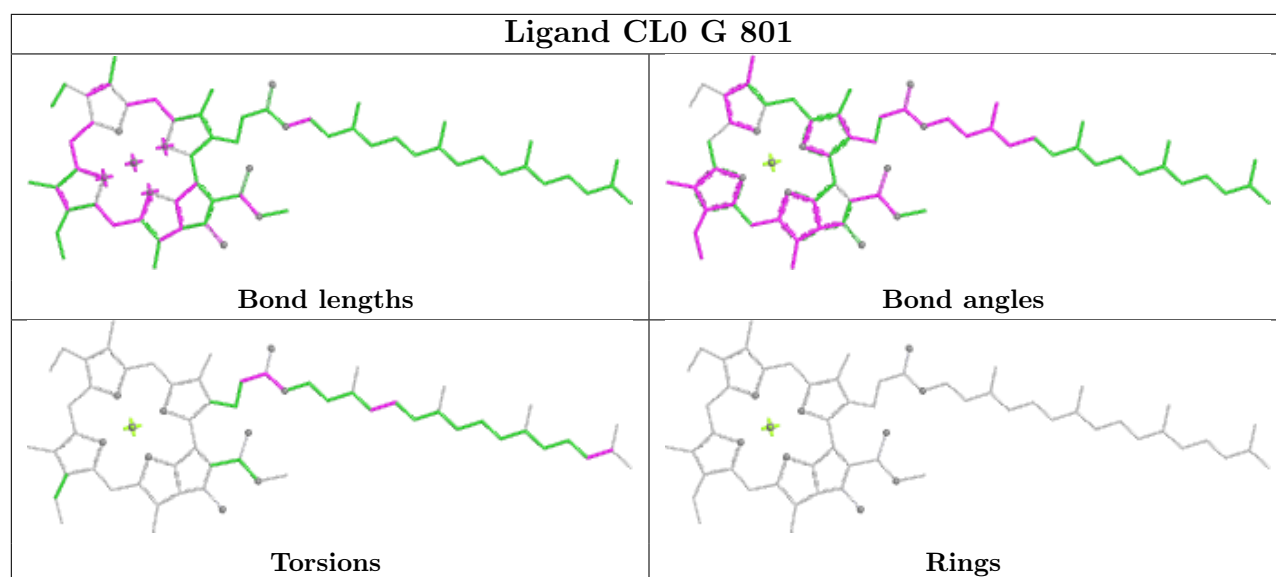
Torsions

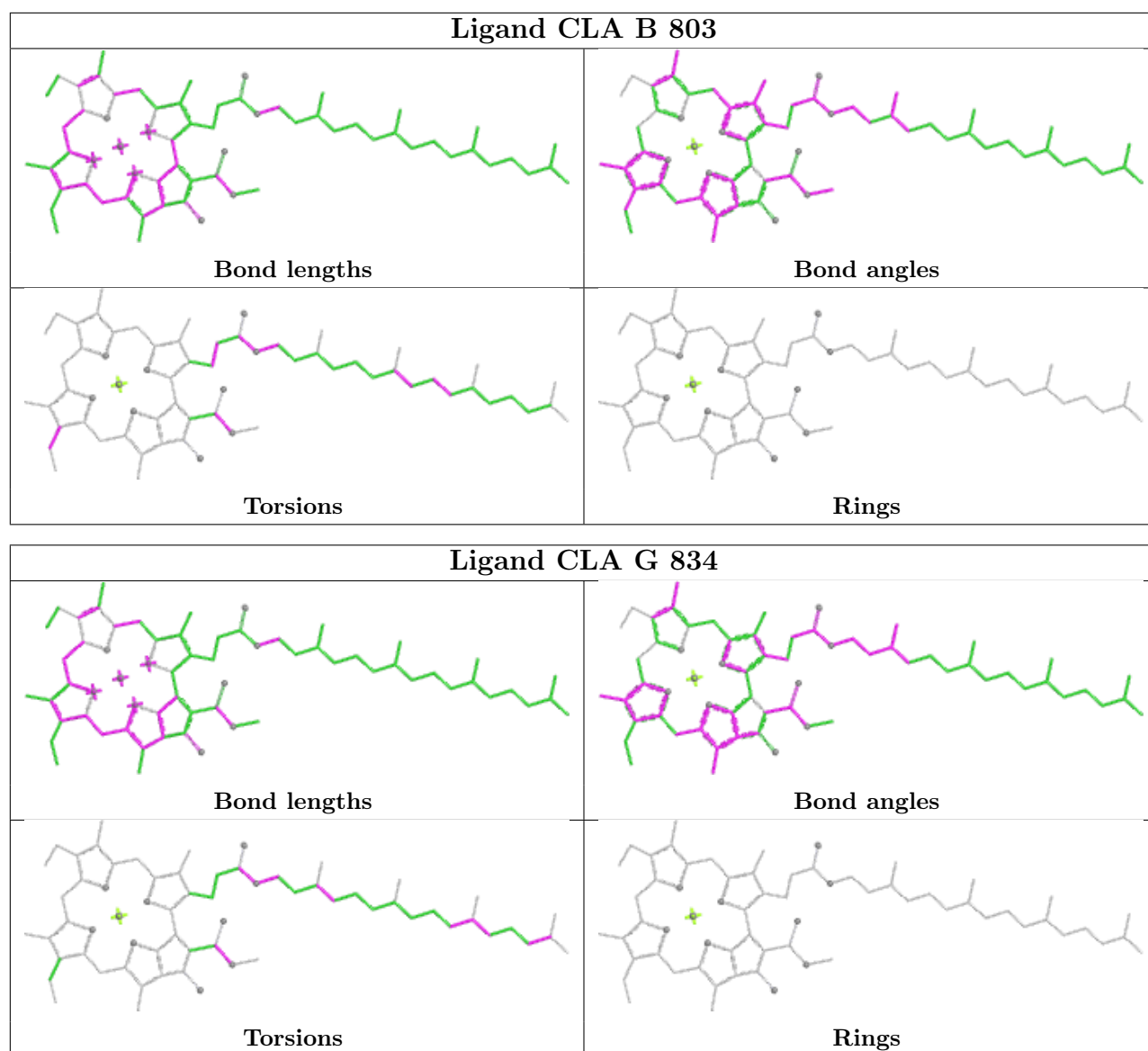


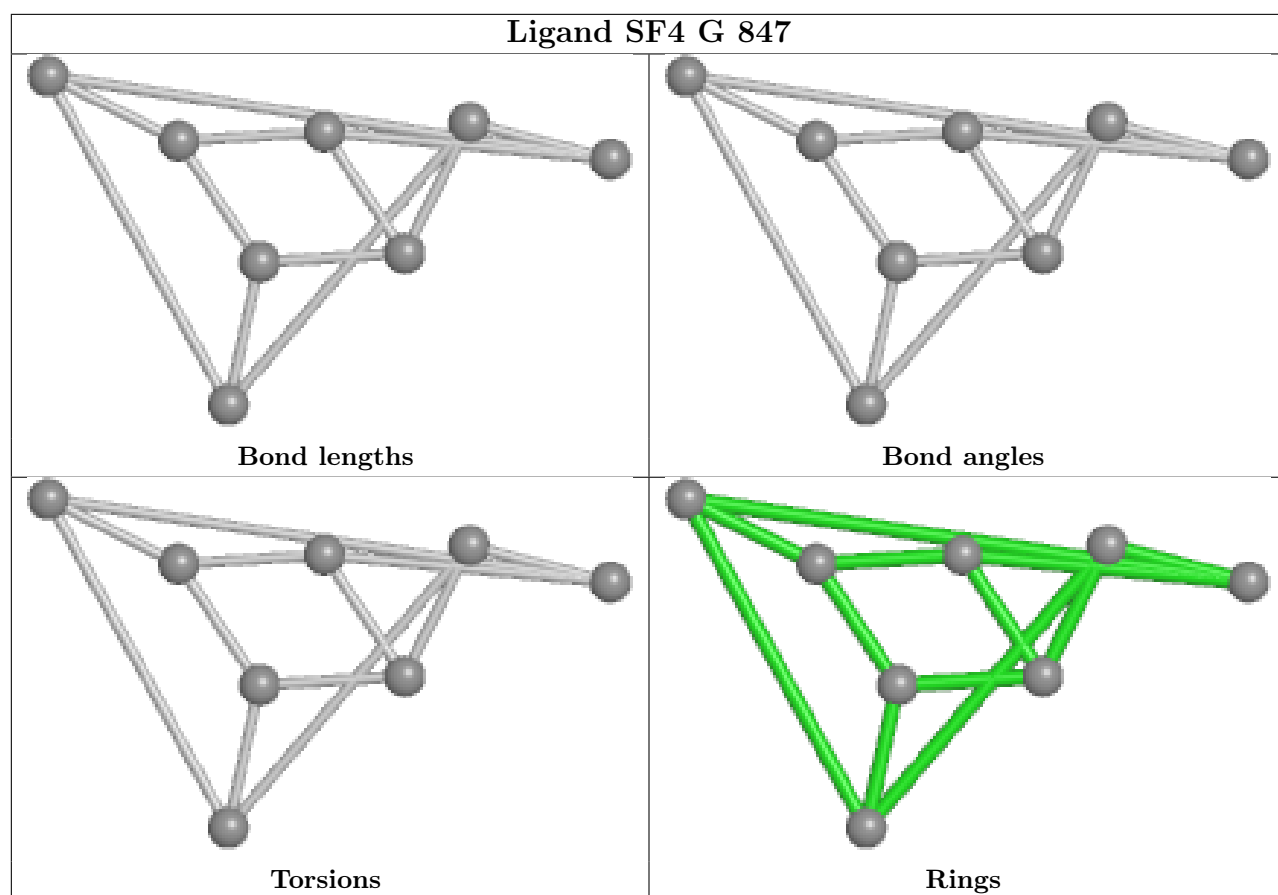
Rings

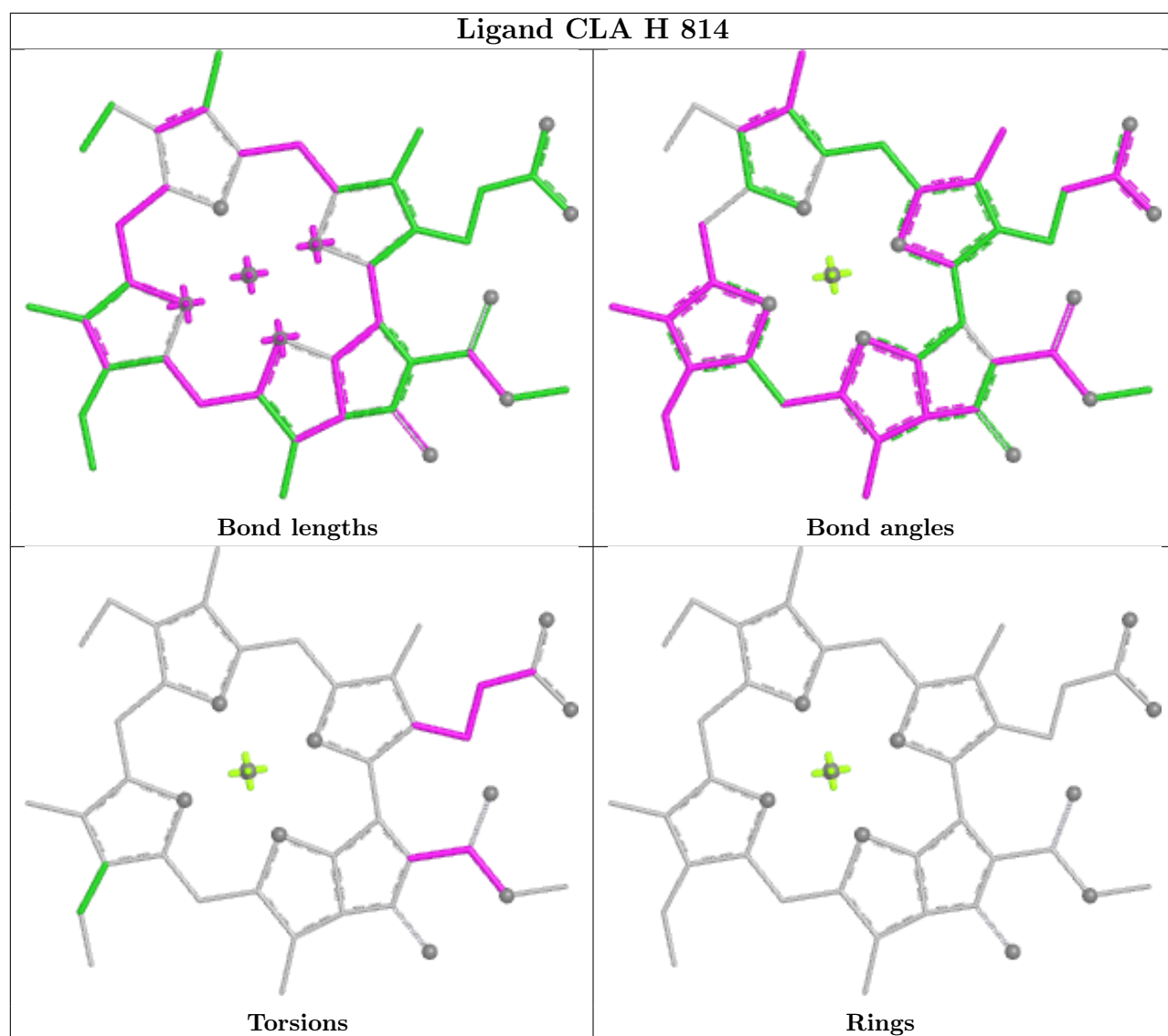




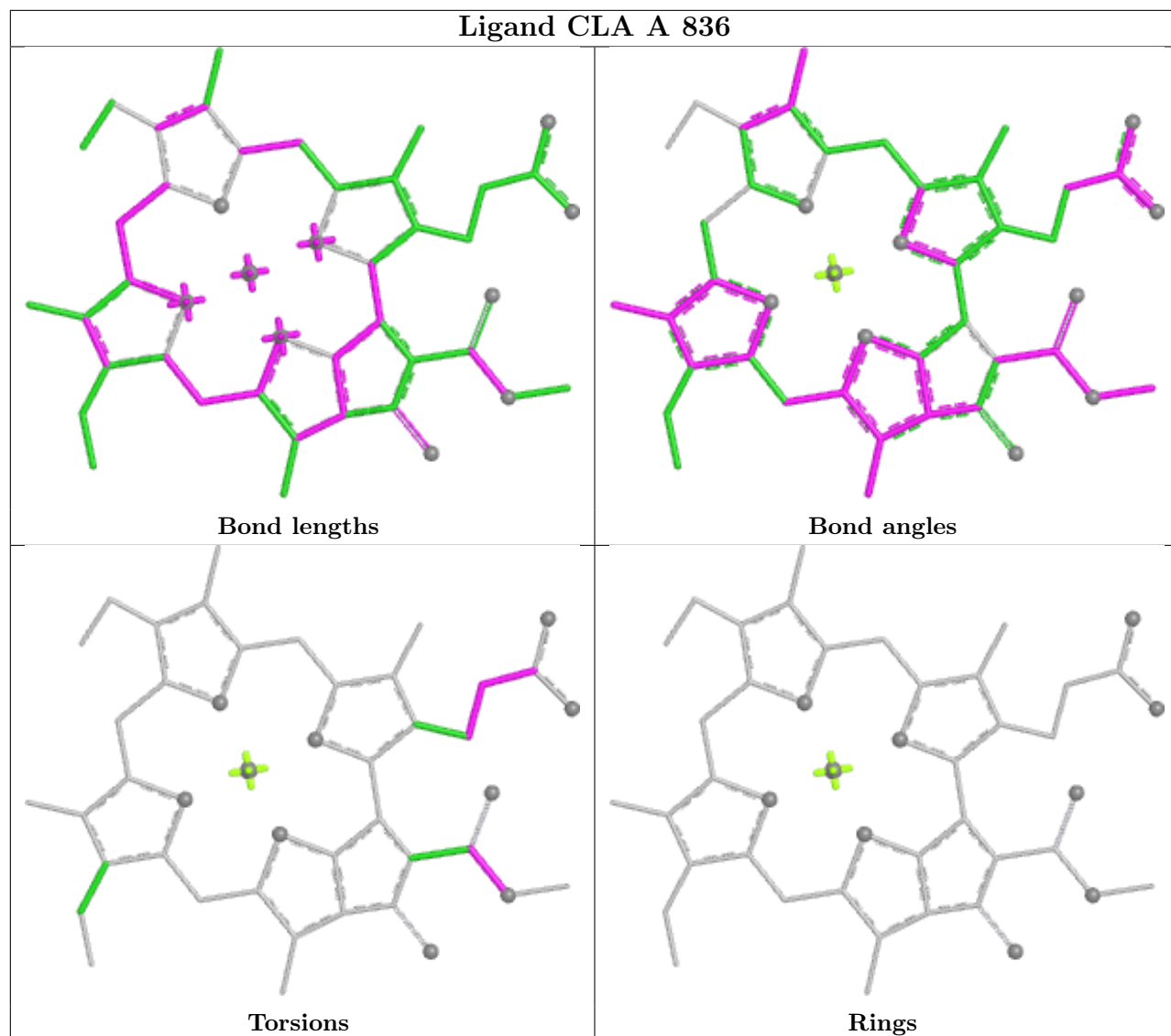






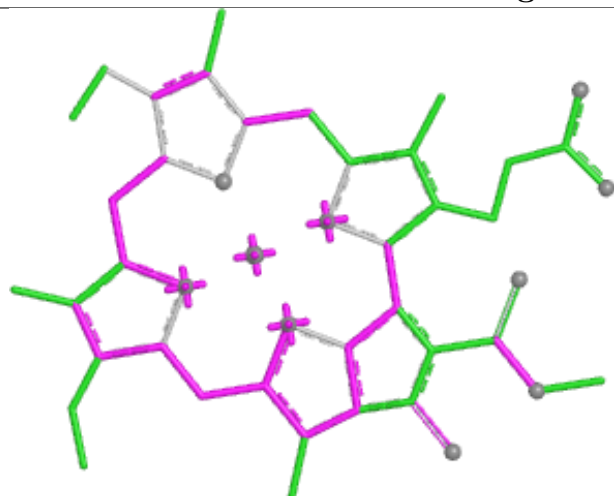


## Ligand CLA A 836

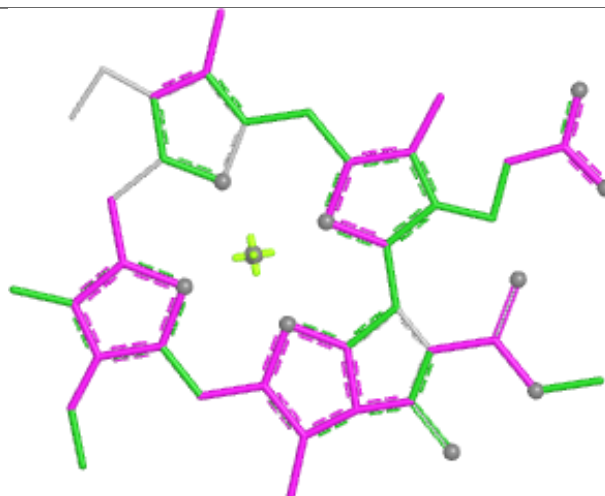




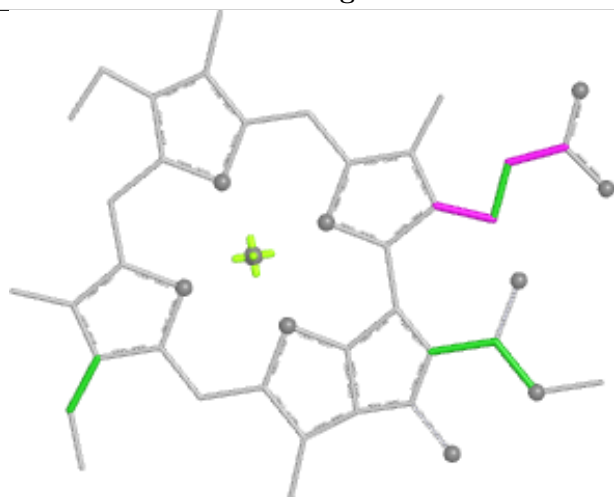
## Ligand CLA b 822



Bond lengths



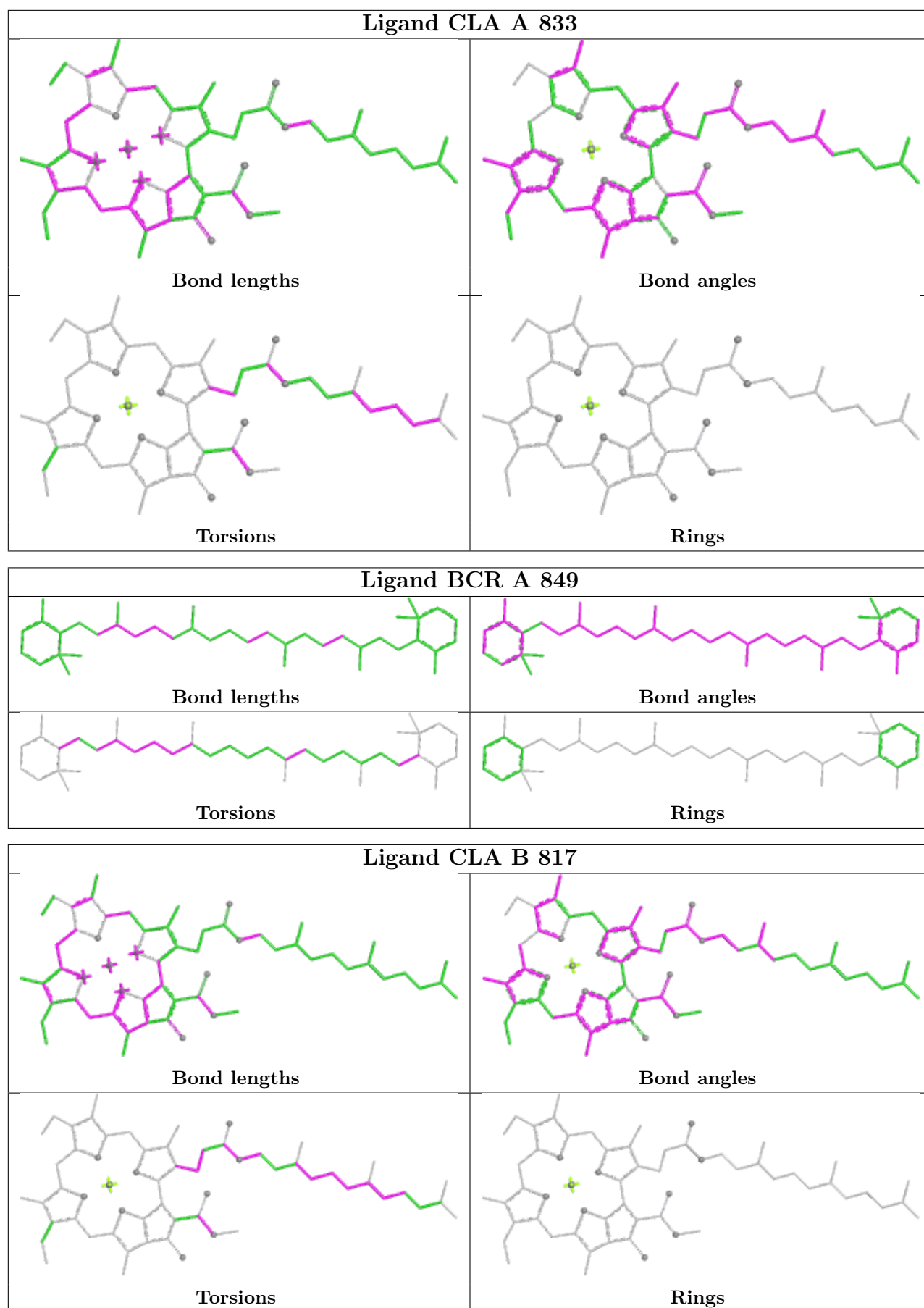
Bond angles



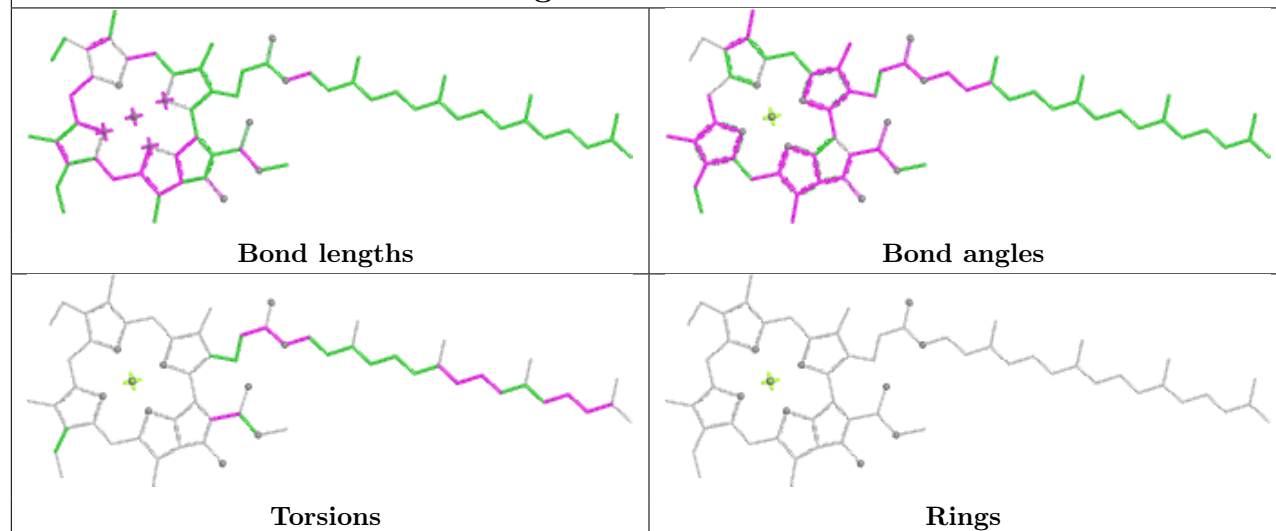
Torsions



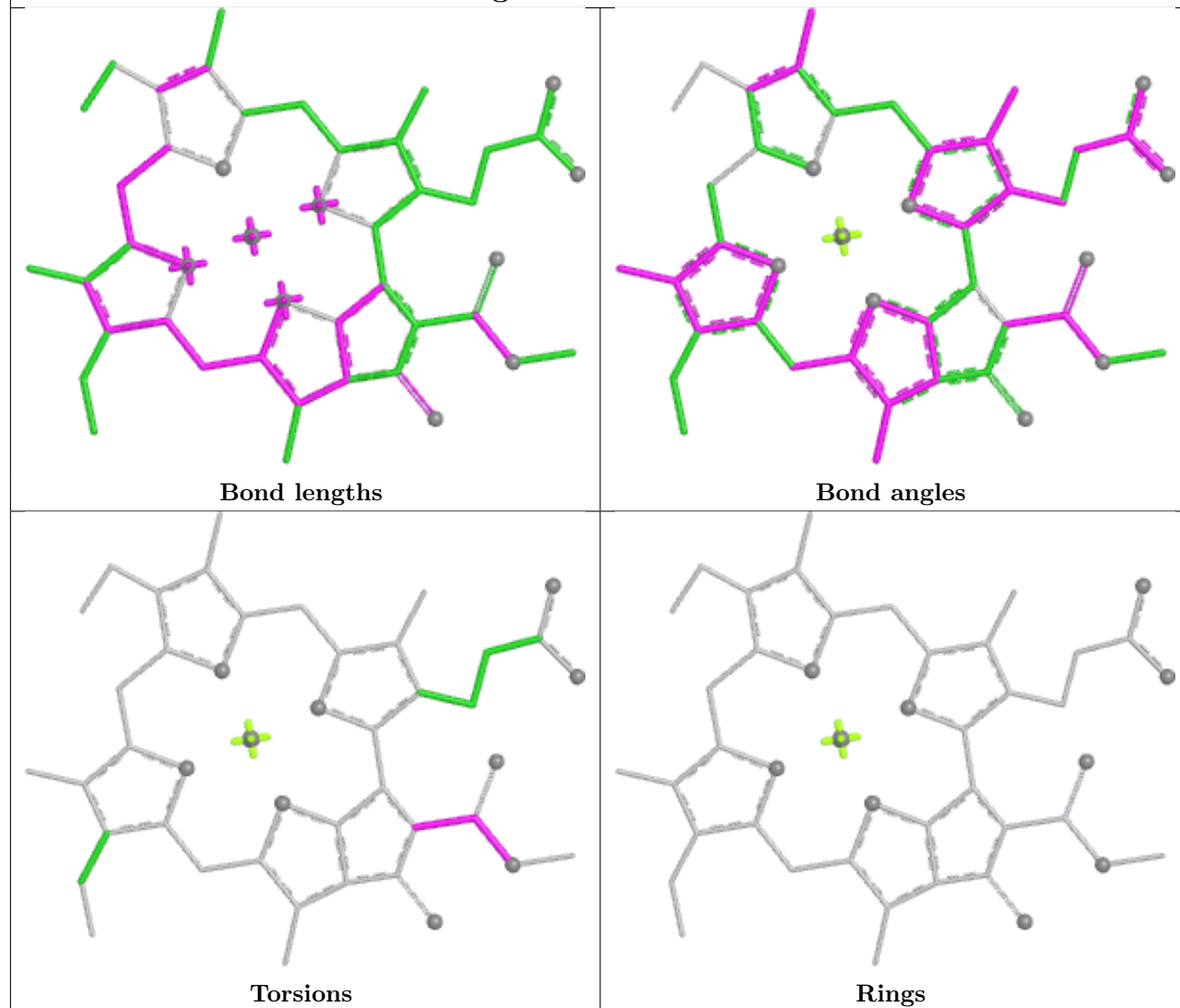
Rings



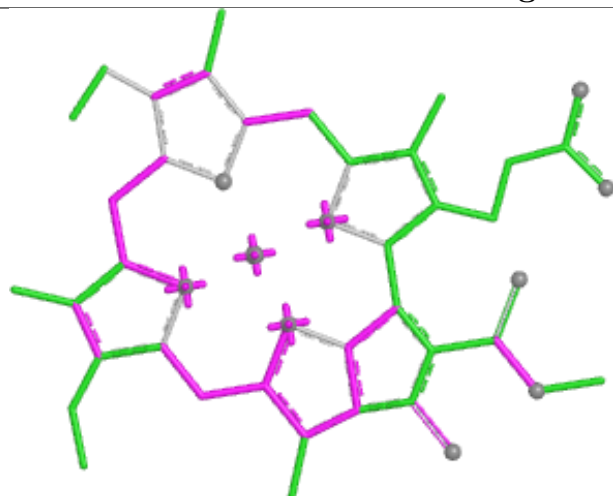
## Ligand CLA L 201



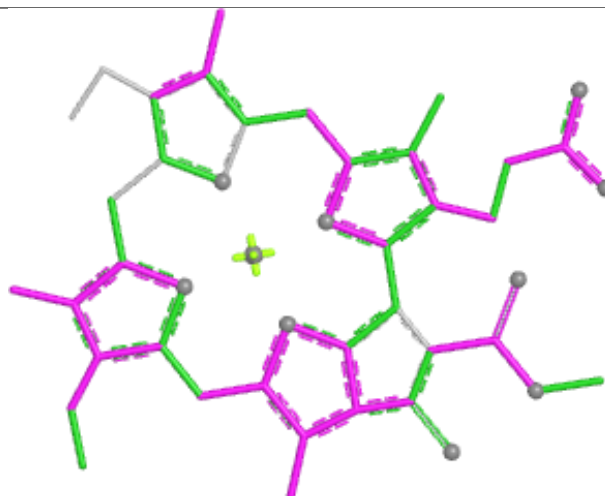
## Ligand CLA B 824



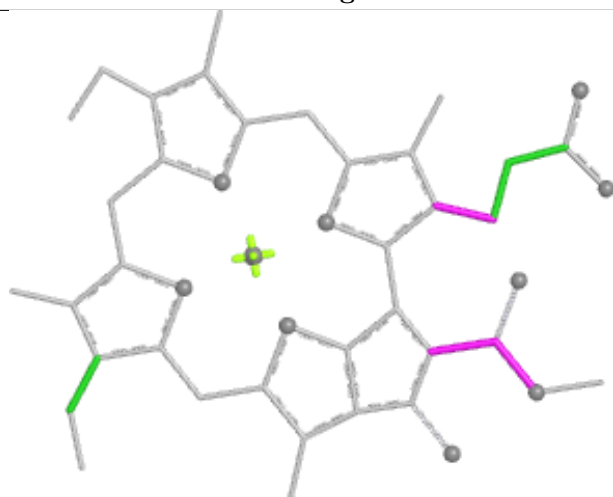
## Ligand CLA a 805



Bond lengths



Bond angles

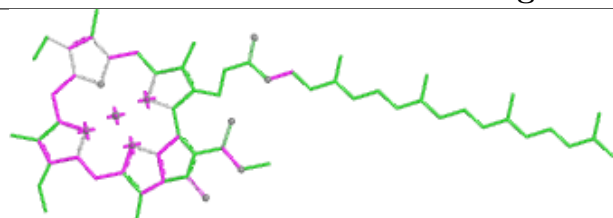


Torsions

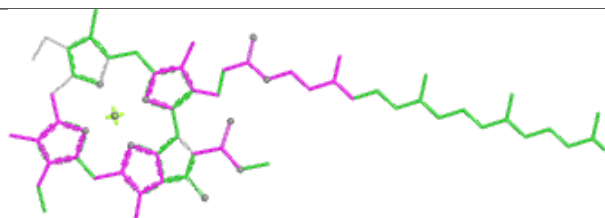


Rings

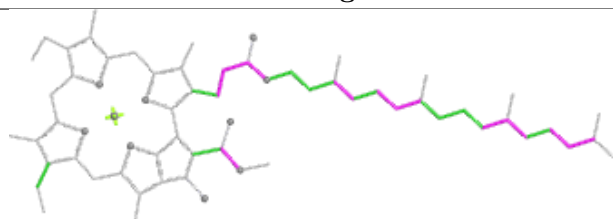
## Ligand CLA b 802



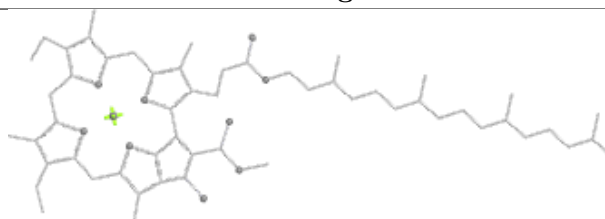
Bond lengths



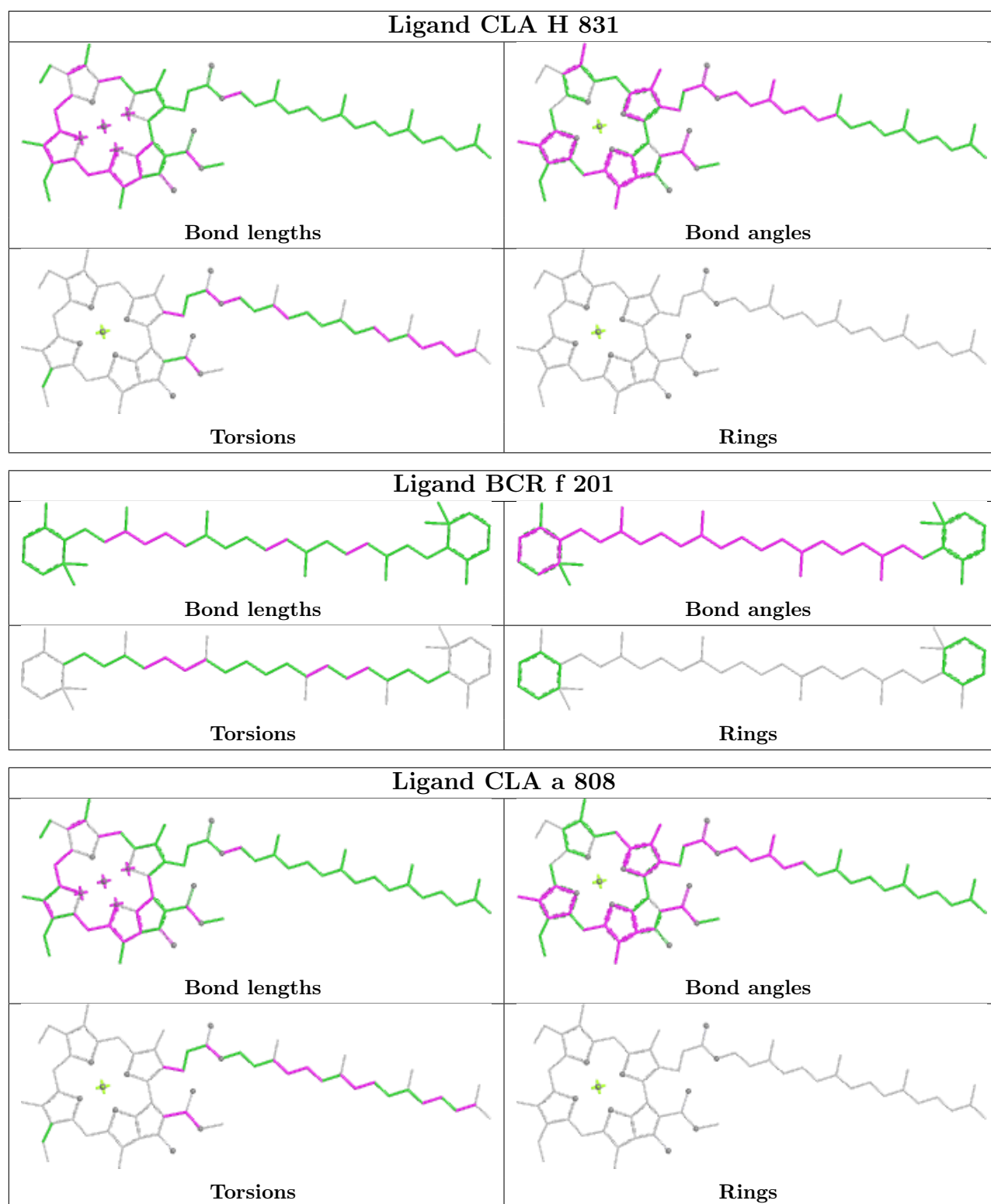
Bond angles



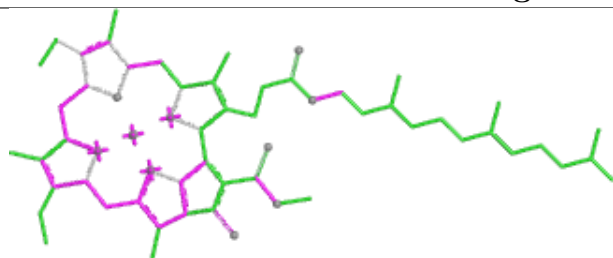
Torsions



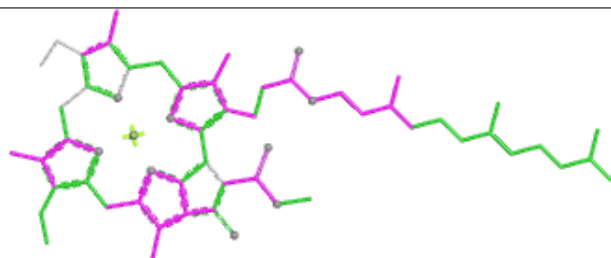
Rings



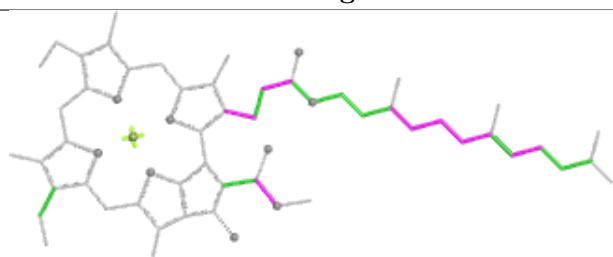
## Ligand CLA H 837



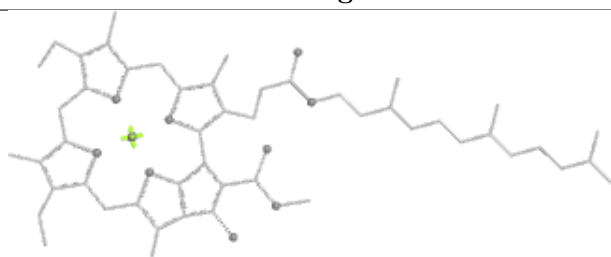
Bond lengths



Bond angles

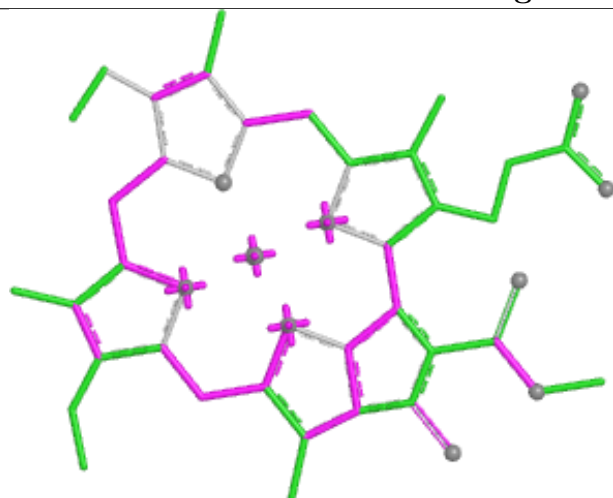


Torsions

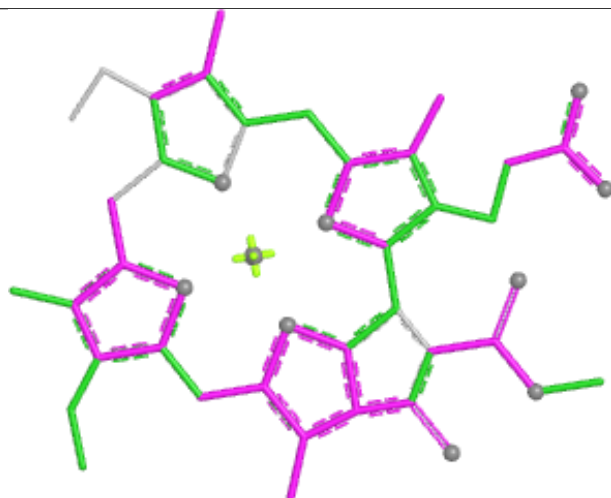


Rings

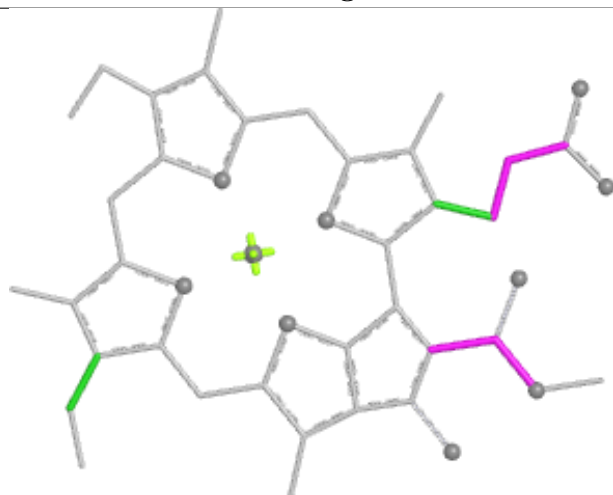
## Ligand CLA B 814



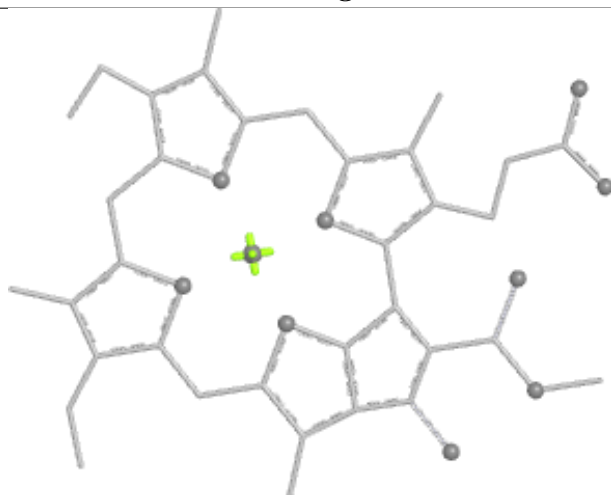
Bond lengths



Bond angles

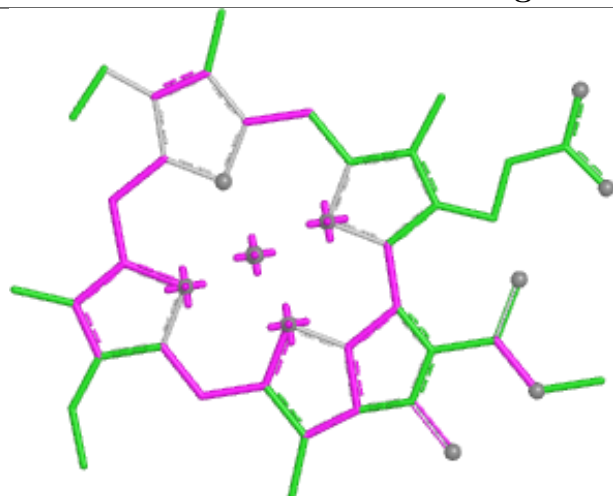


Torsions

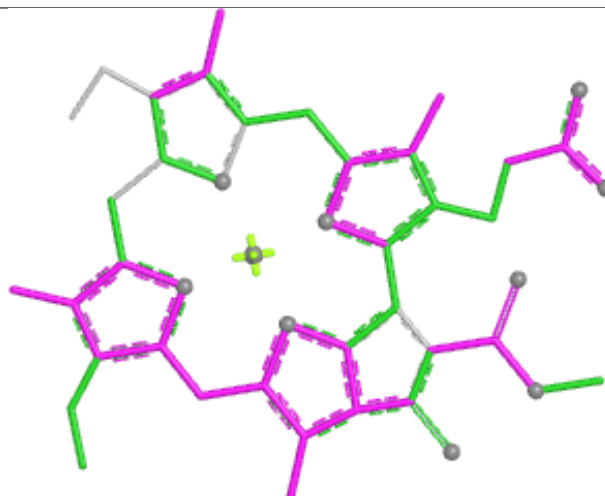


Rings

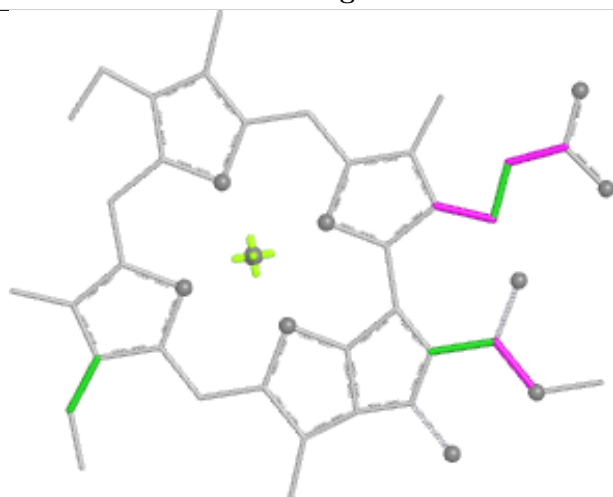
## Ligand CLA B 819



Bond lengths



Bond angles

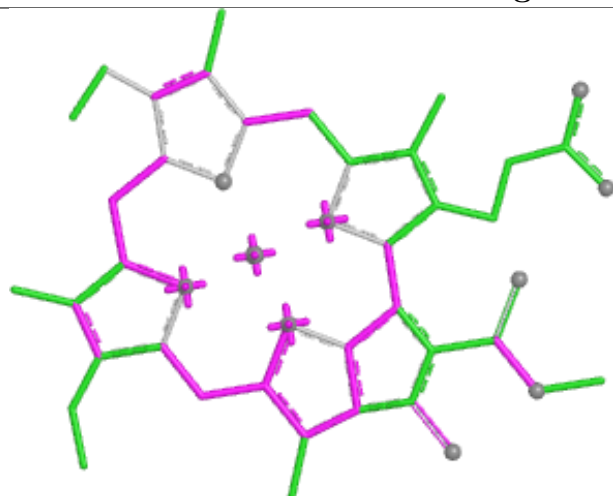


Torsions

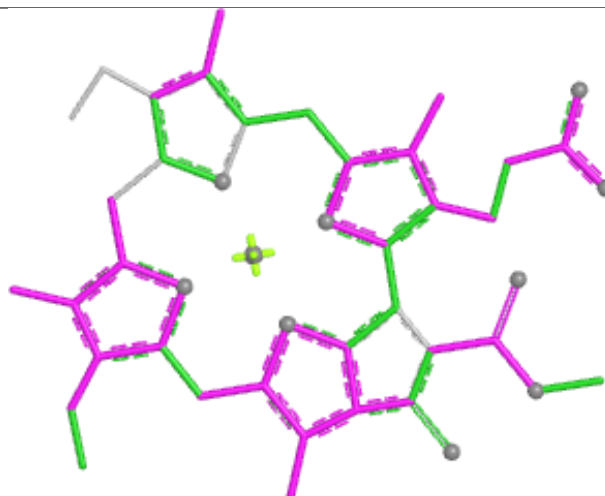


Rings

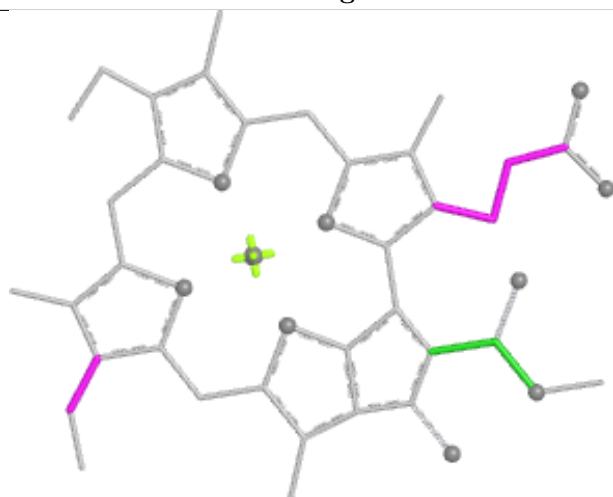
## Ligand CLA A 845



Bond lengths



Bond angles

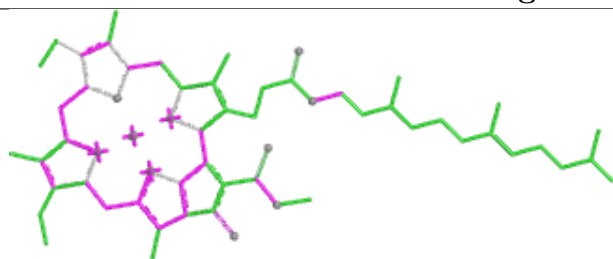


Torsions

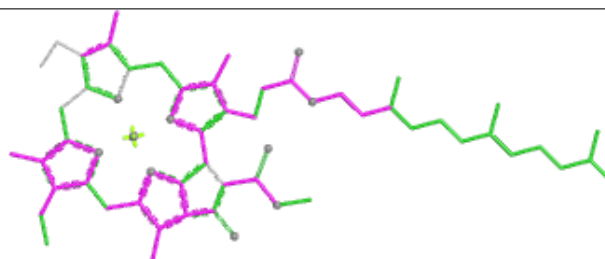


Rings

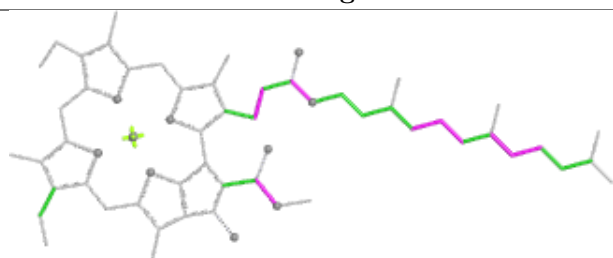
## Ligand CLA a 813



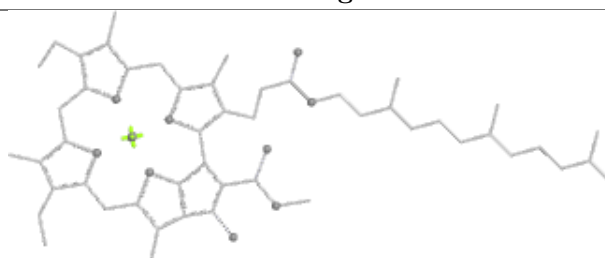
Bond lengths



Bond angles

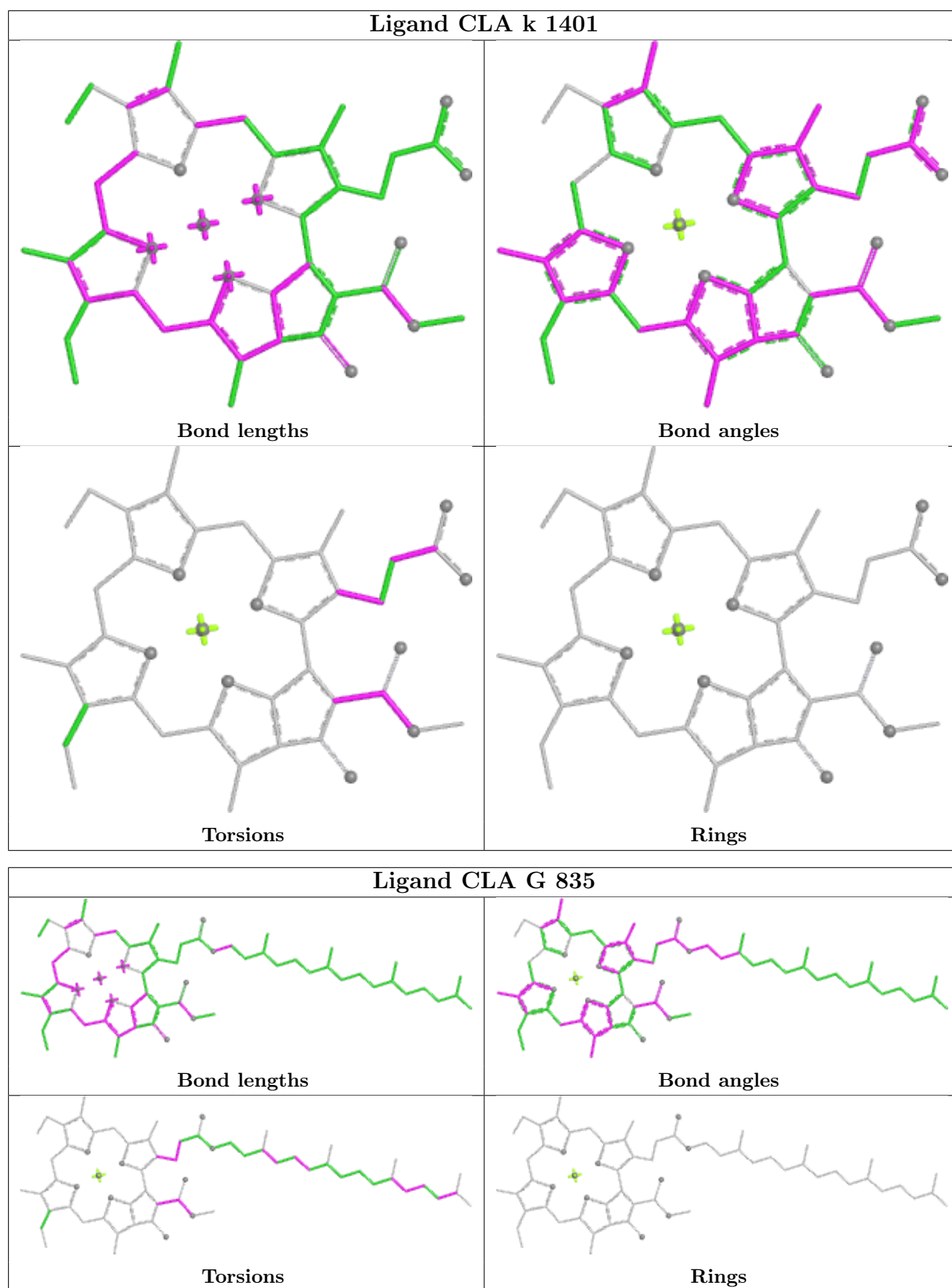


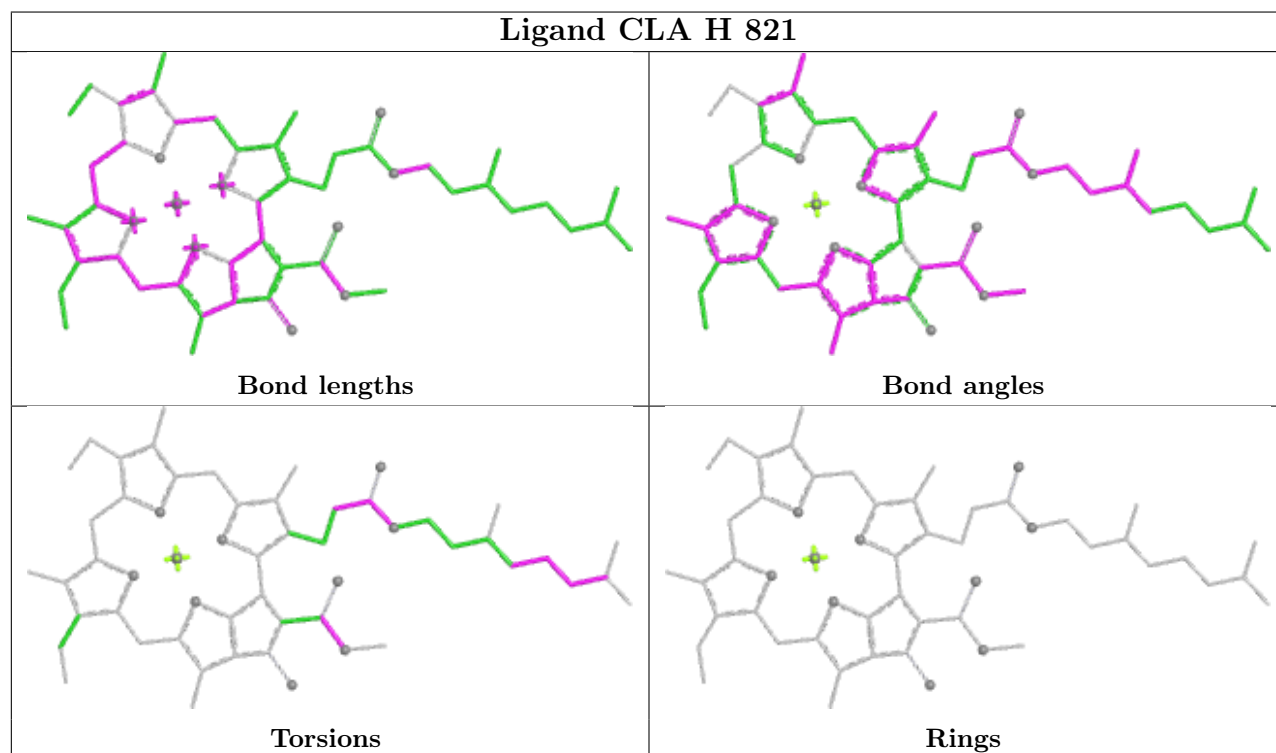
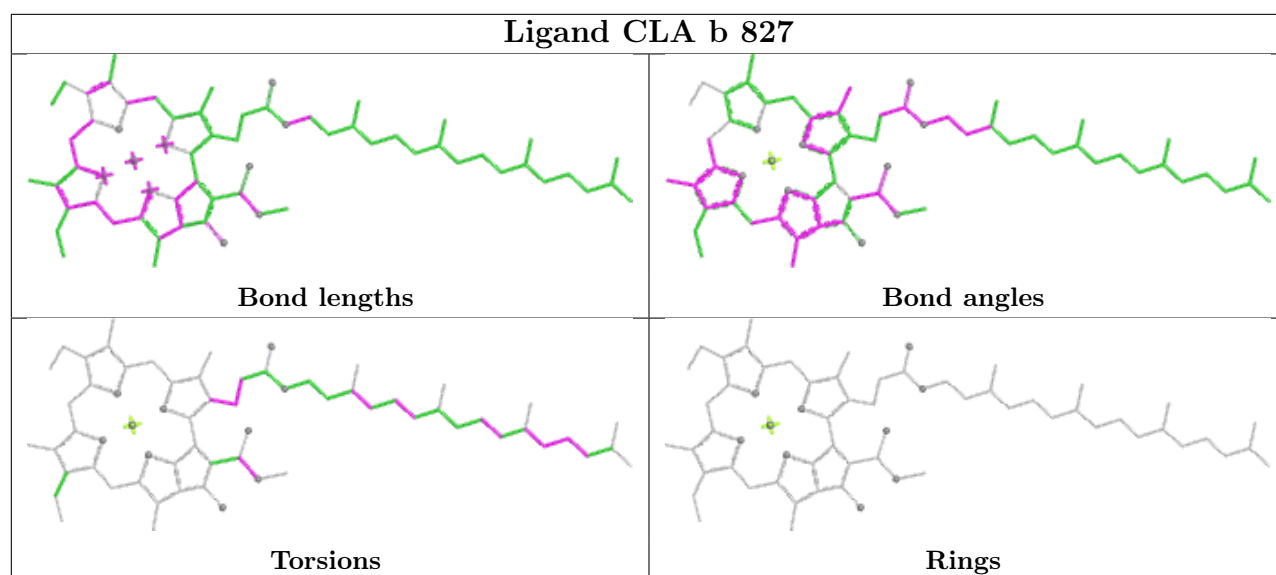
Torsions

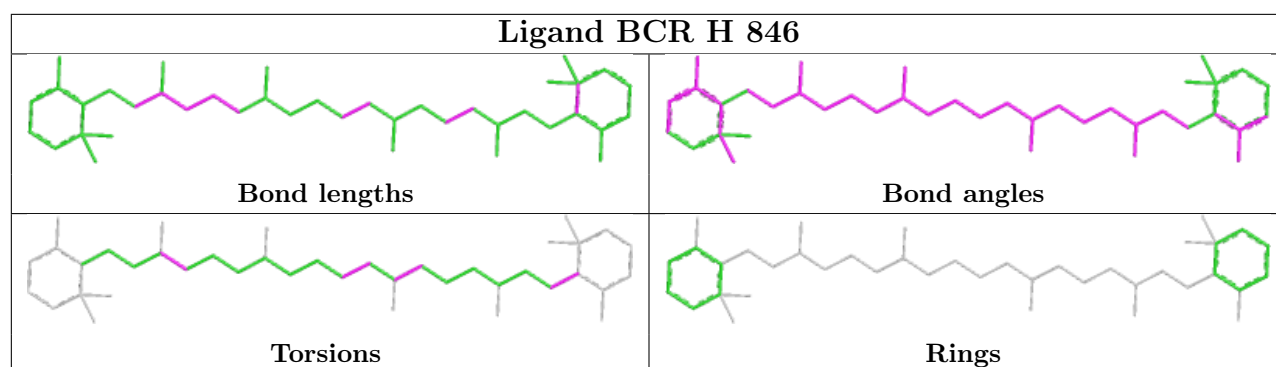
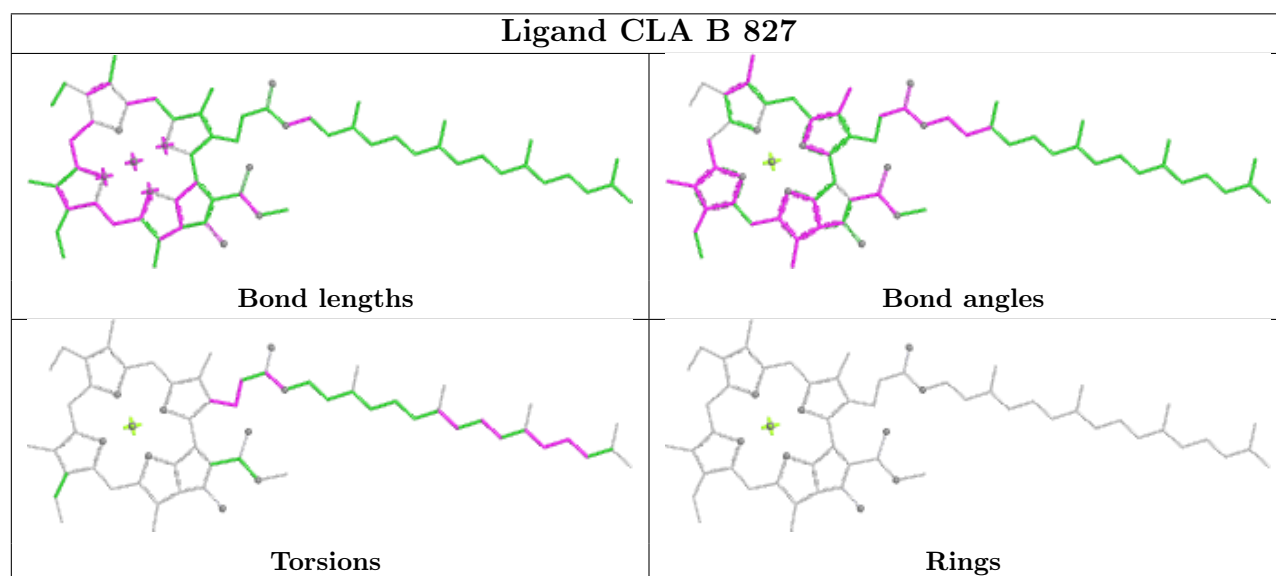
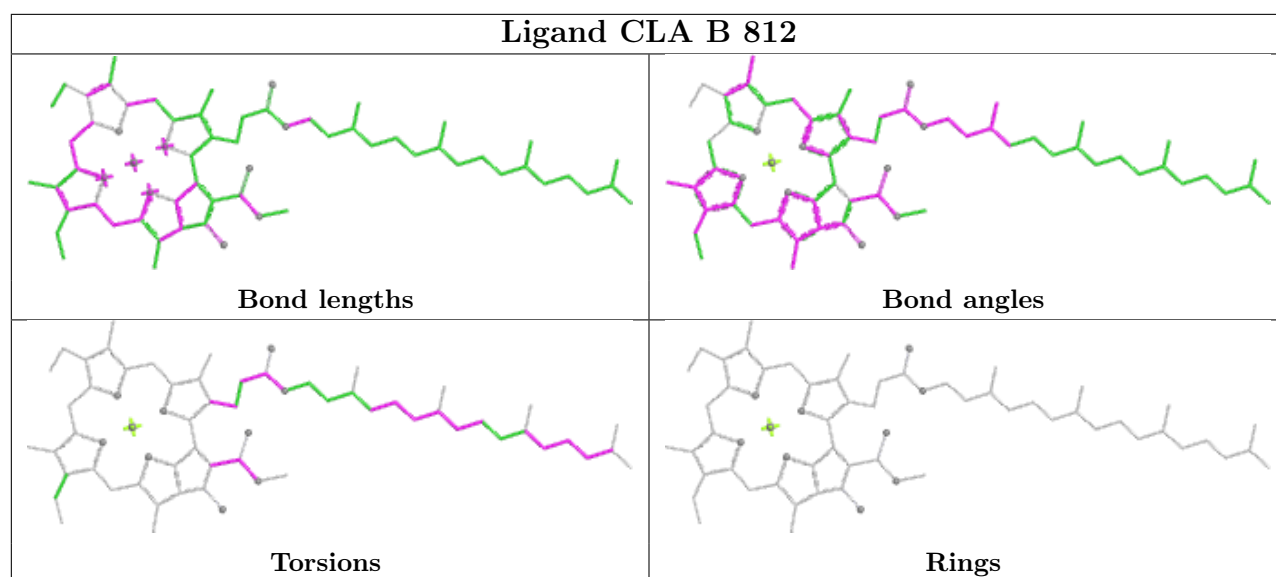


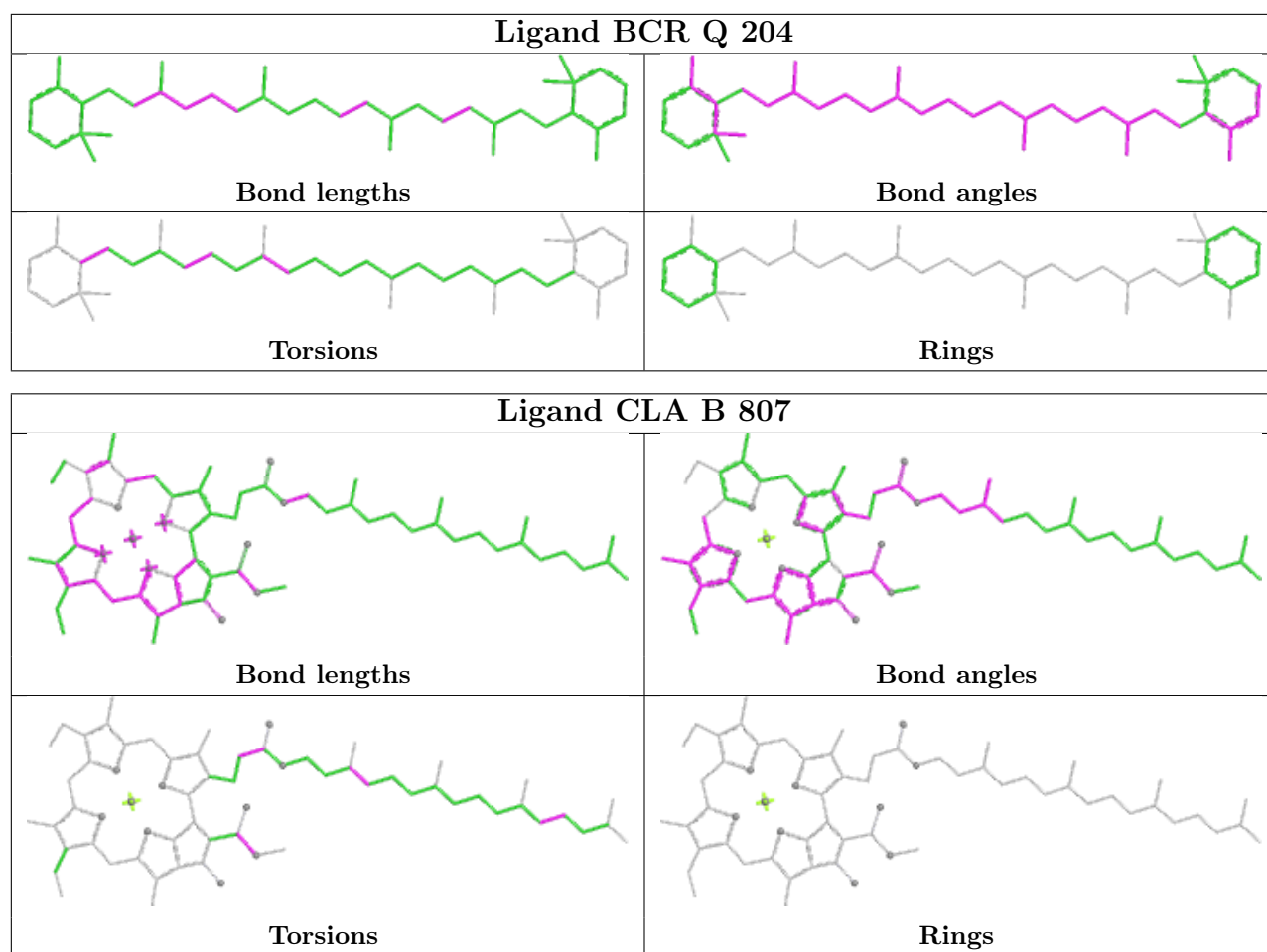
Rings











## 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.

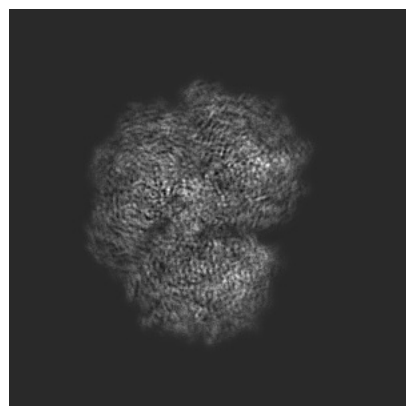
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43525. These allow visual inspection of the internal detail of the map and identification of artifacts.

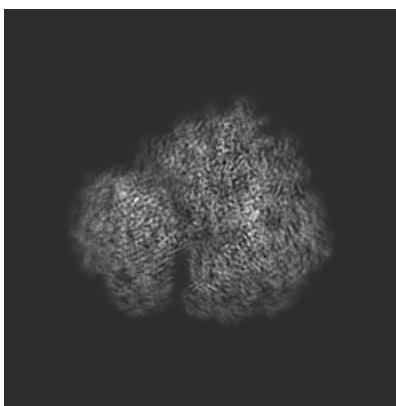
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

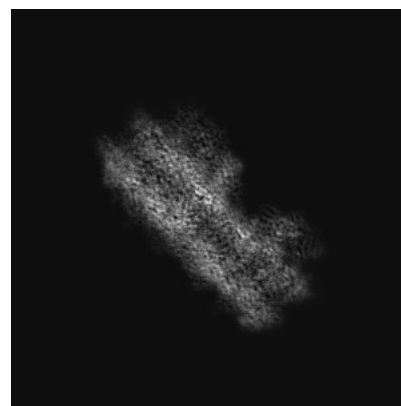
#### 6.1.1 Primary map



X

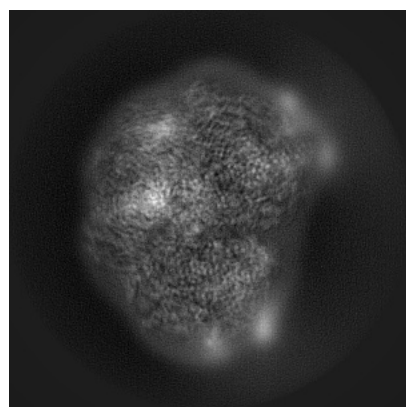


Y

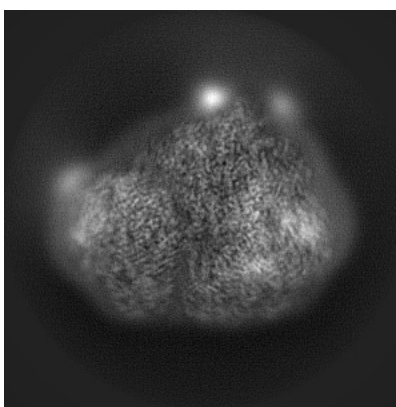


Z

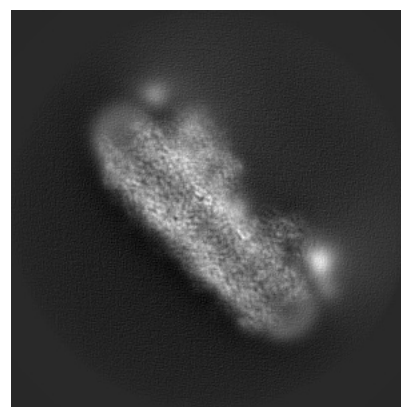
#### 6.1.2 Raw map



X



Y

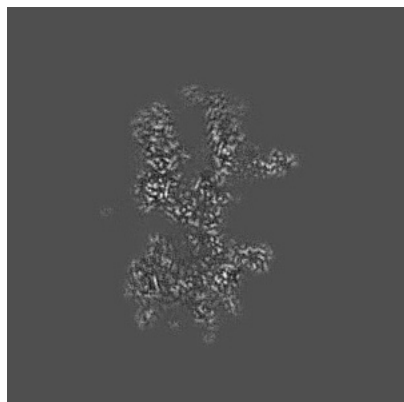


Z

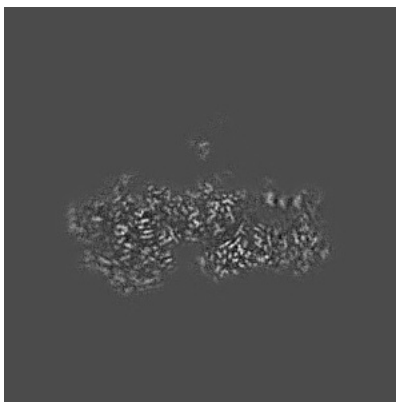
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

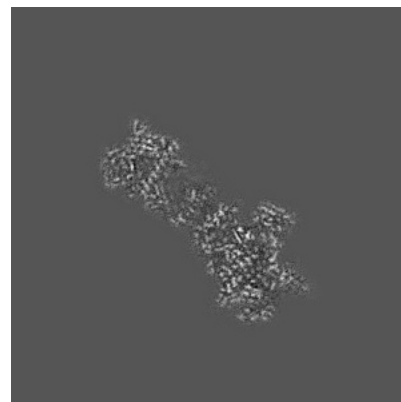
### 6.2.1 Primary map



X Index: 180

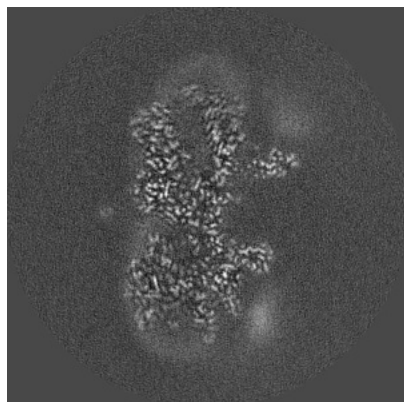


Y Index: 180

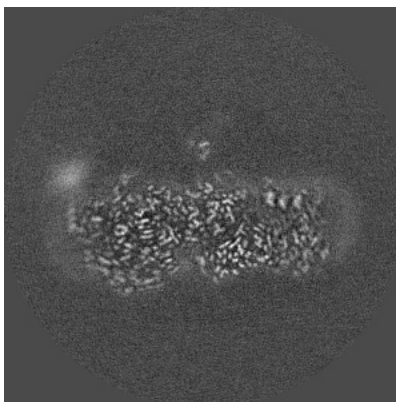


Z Index: 180

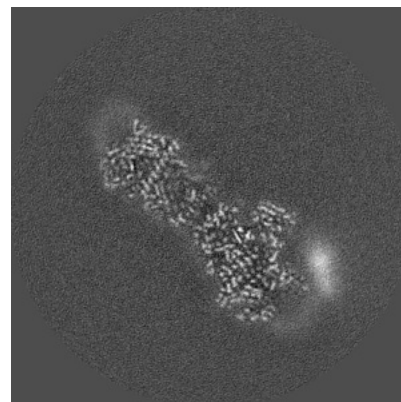
### 6.2.2 Raw map



X Index: 180



Y Index: 180

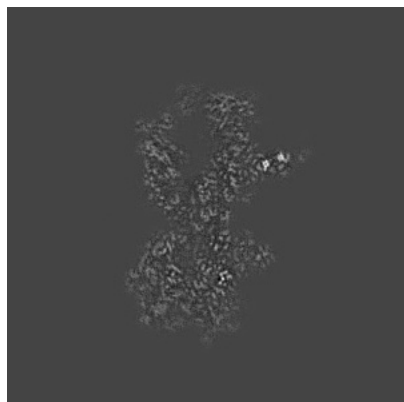


Z Index: 180

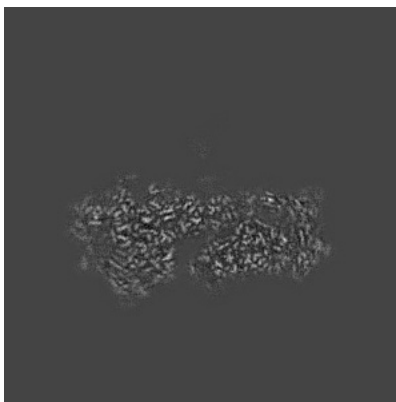
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

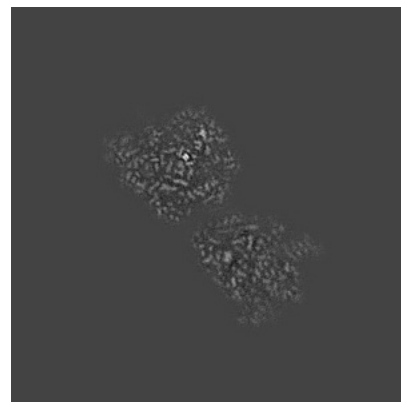
### 6.3.1 Primary map



X Index: 172

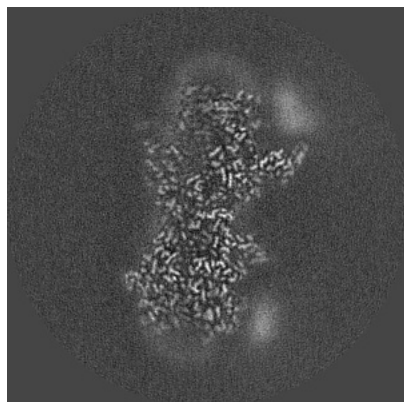


Y Index: 185

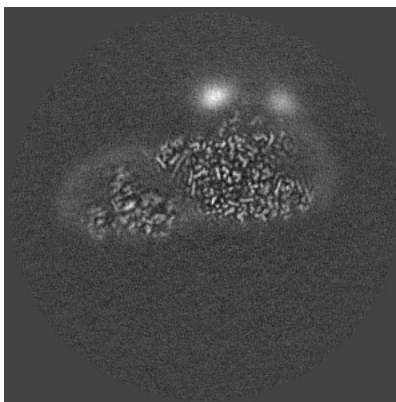


Z Index: 223

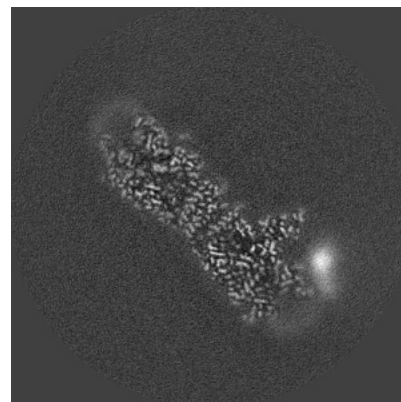
### 6.3.2 Raw map



X Index: 167



Y Index: 133



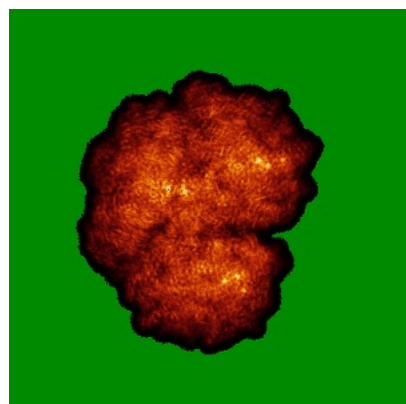
Z Index: 191

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

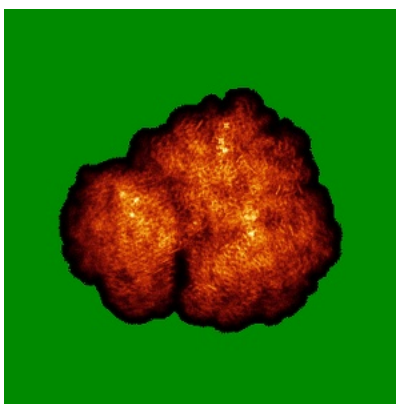


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

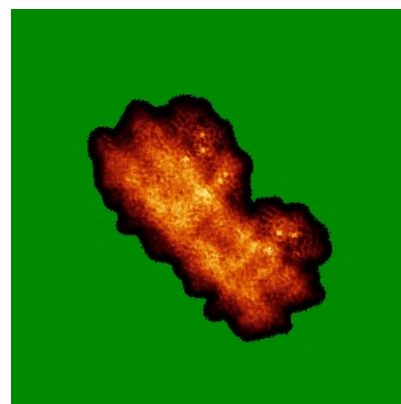
### 6.4.1 Primary map



X

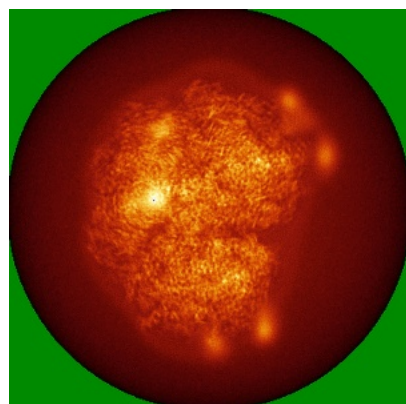


Y

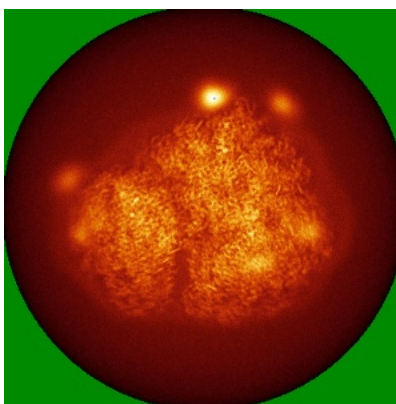


Z

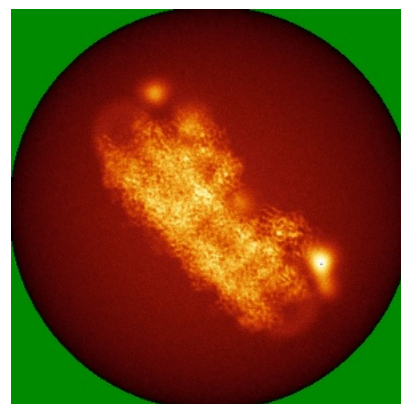
### 6.4.2 Raw map



X



Y



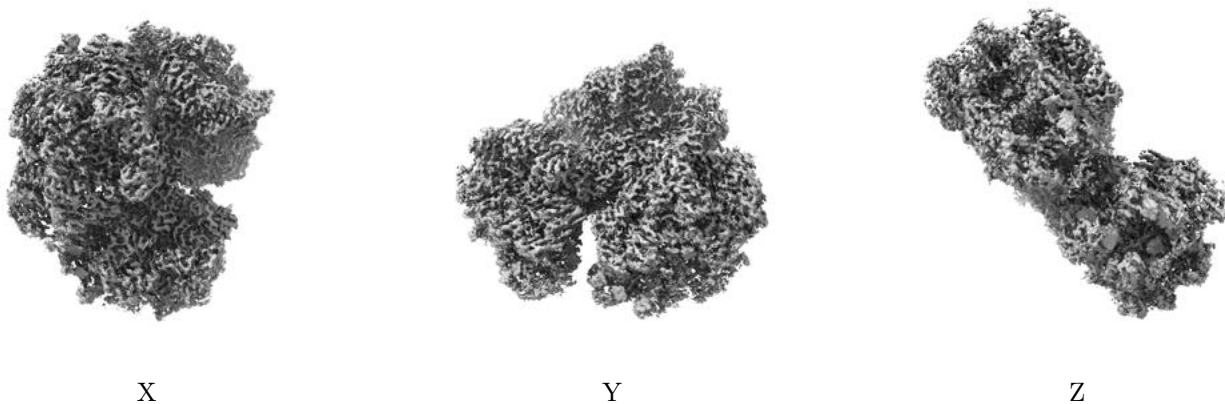
Z

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.



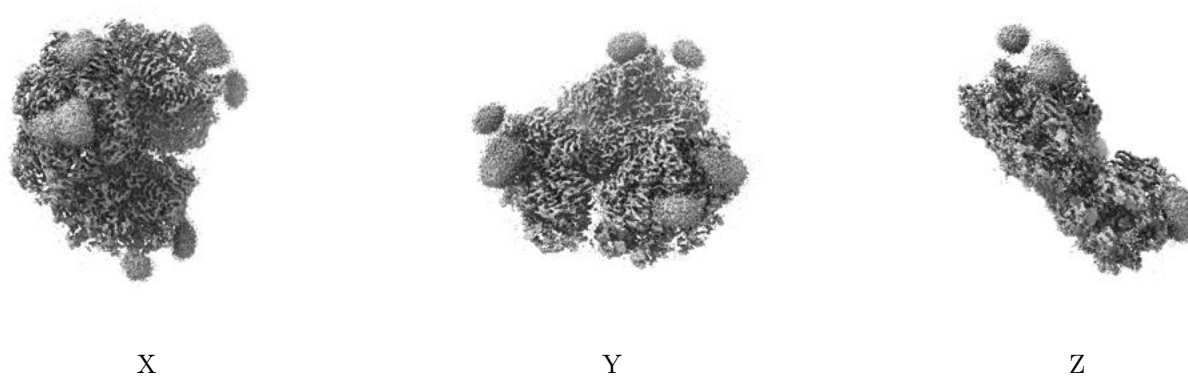
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00404. 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.

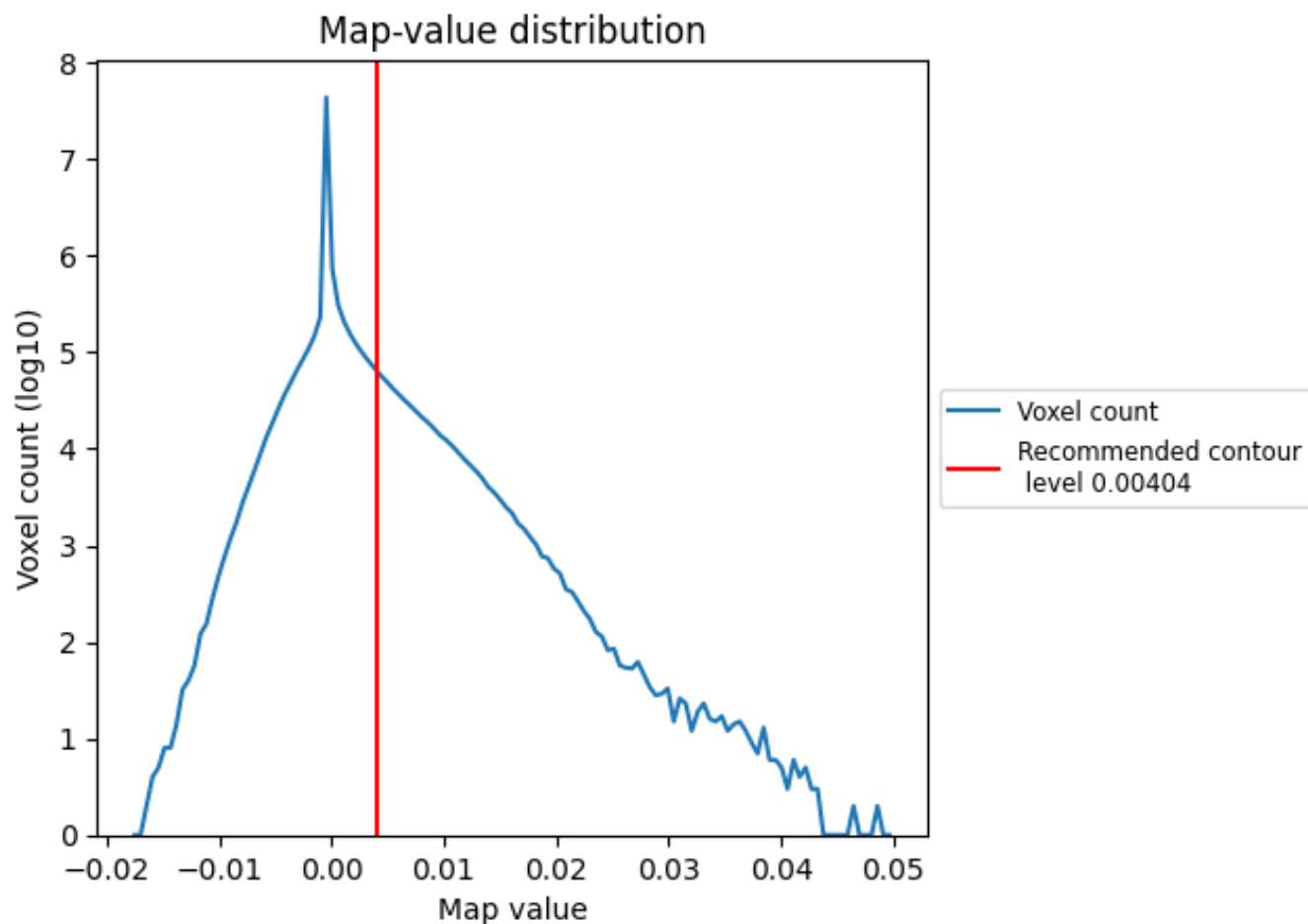
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

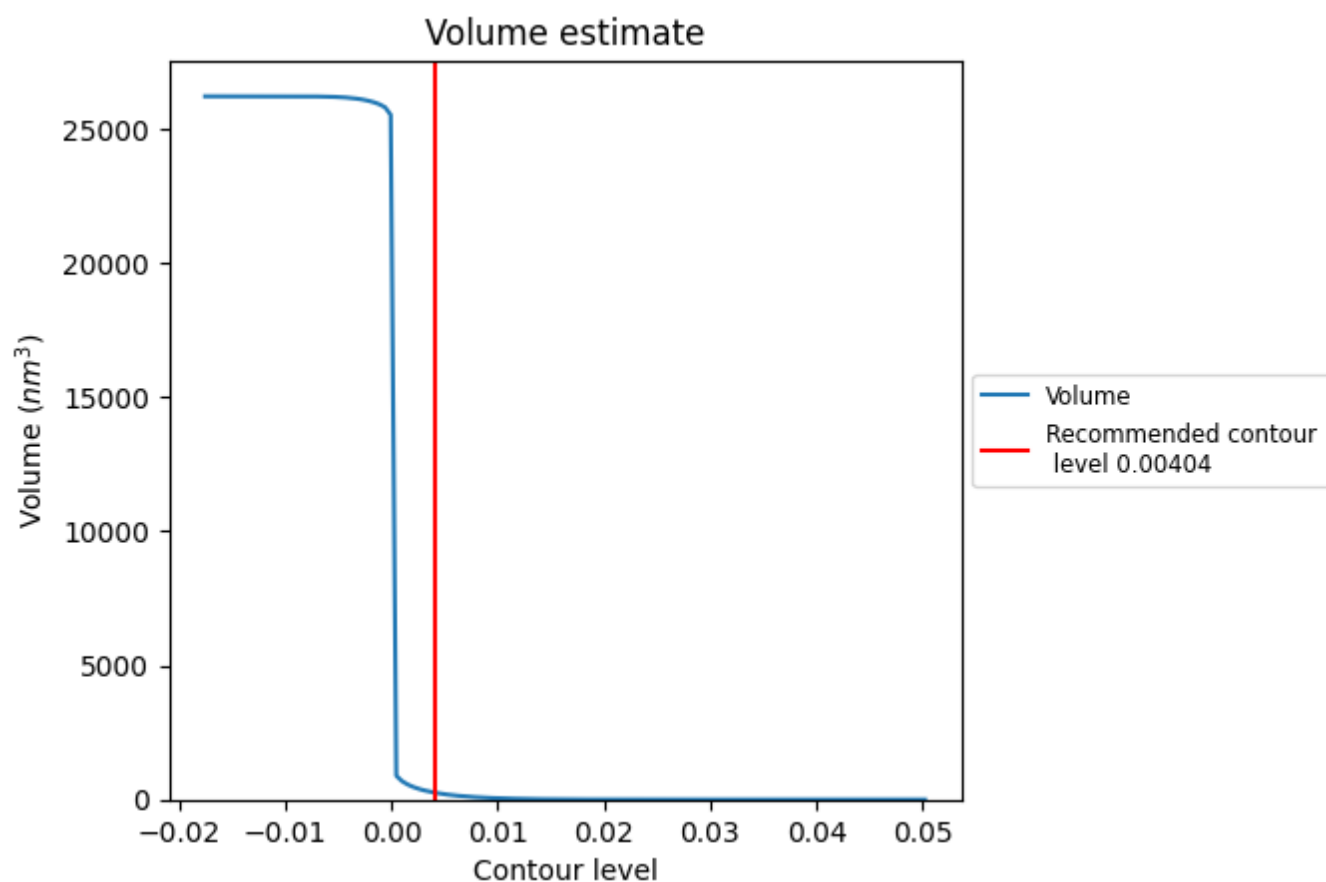
This section contains the results of statistical analysis of the map.

### 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.

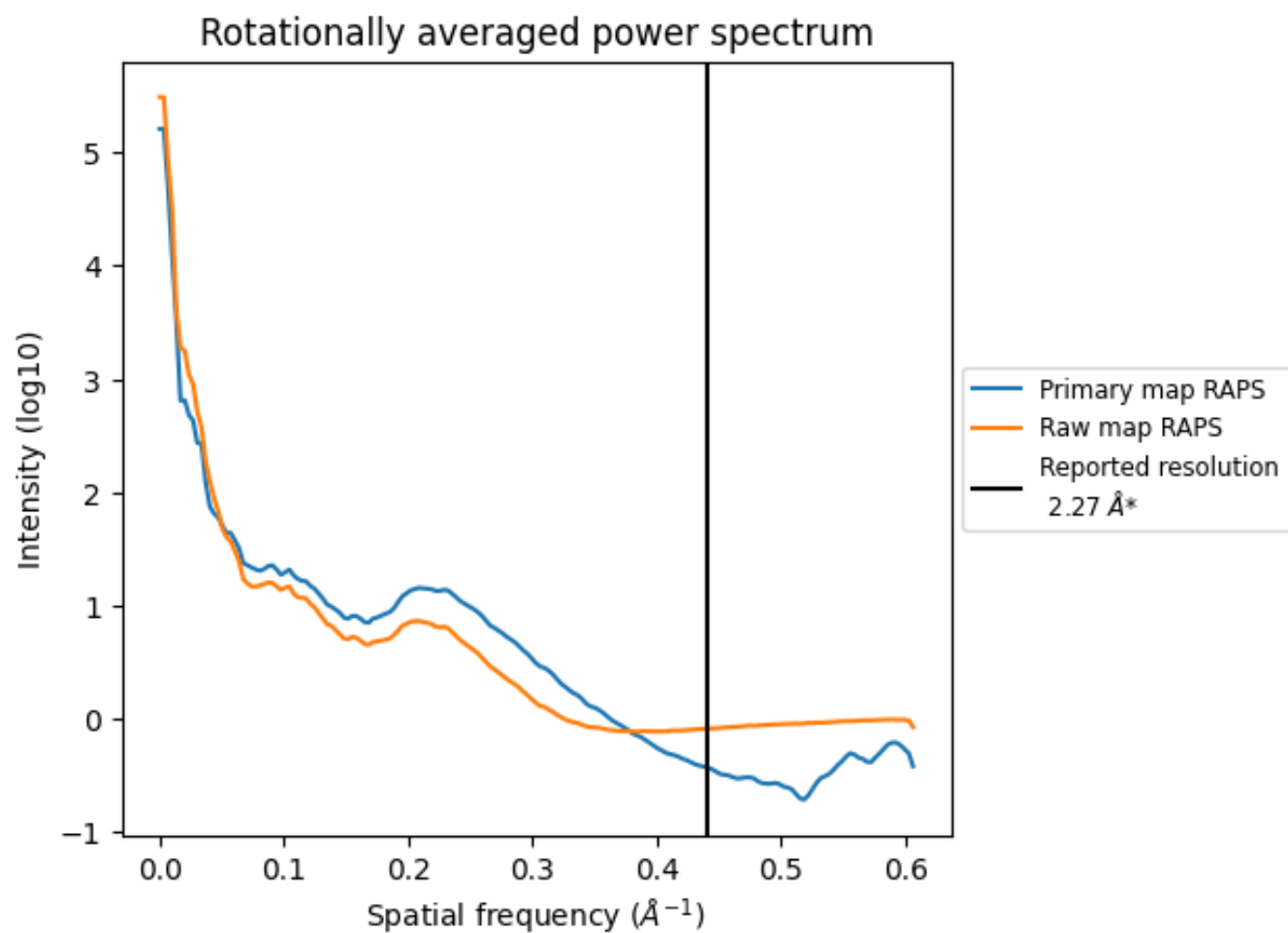
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 261  $\text{nm}^3$ ; this corresponds to an approximate mass of 235 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 ⓘ

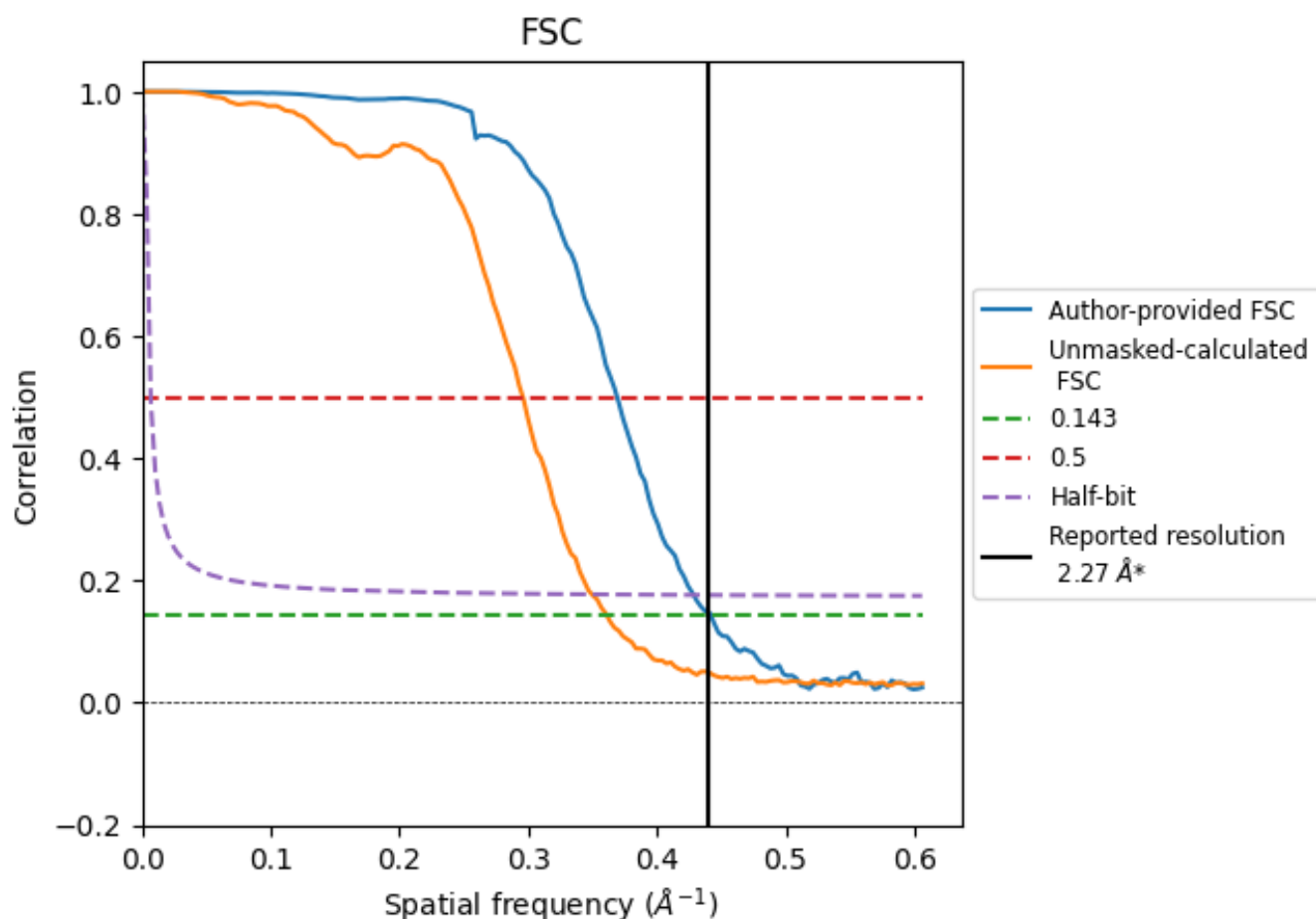


\*Reported resolution corresponds to spatial frequency of 0.441 Å<sup>-1</sup>

## 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 0.441 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

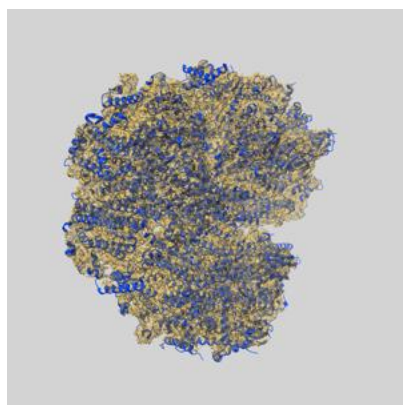
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.27	-	-
Author-provided FSC curve	2.26	2.71	2.33
Unmasked-calculated*	2.77	3.38	2.86

\*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 2.77 differs from the reported value 2.27 by more than 10 %

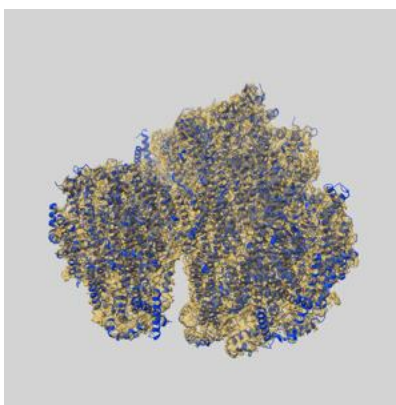
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43525 and PDB model 8VU3. Per-residue inclusion information can be found in [section 3](#) on [page 38](#).

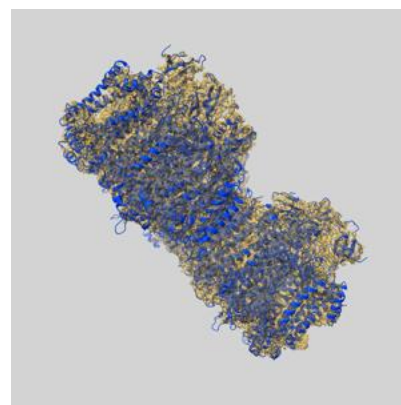
### 9.1 Map-model overlay [i](#)



X



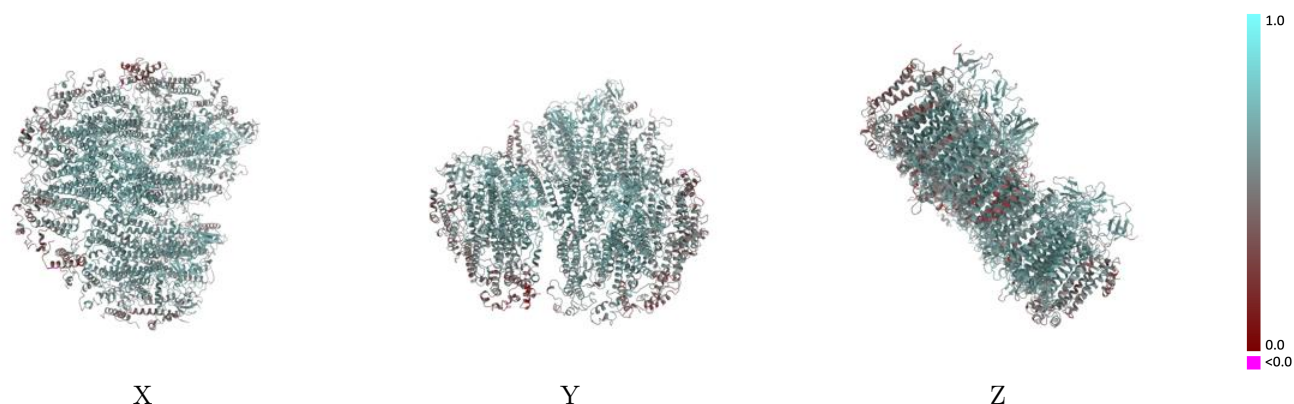
Y



Z

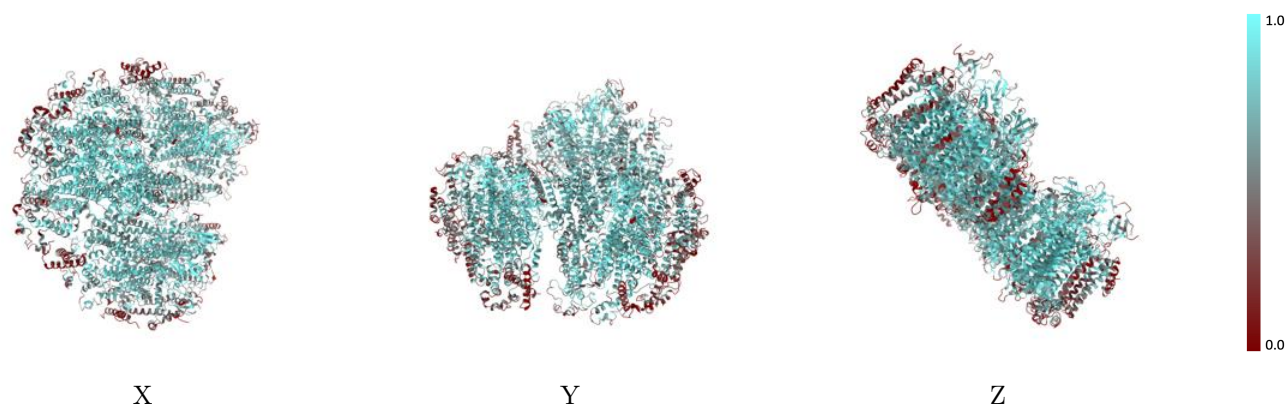
The images above show the 3D surface view of the map at the recommended contour level 0.00404 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



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

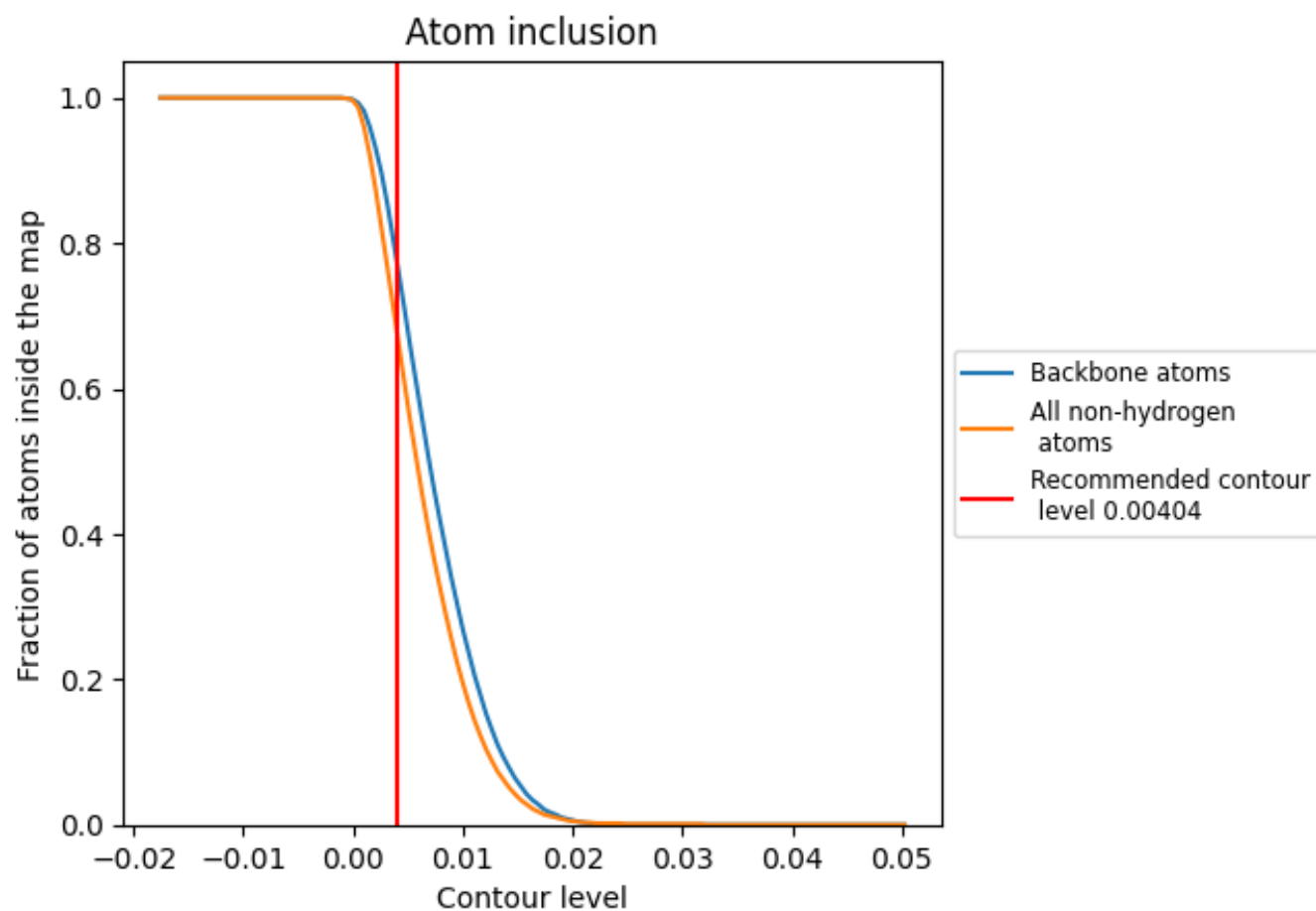
## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00404).









































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 77% of all backbone atoms, 67% 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 (0.00404) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6720	 0.5780
A	 0.6840	 0.5640
B	 0.7340	 0.6050
C	 0.8770	 0.6690
D	 0.6810	 0.6160
E	 0.5850	 0.5720
F	 0.3030	 0.4580
G	 0.7180	 0.5850
H	 0.7490	 0.6090
I	 0.7110	 0.6300
J	 0.3040	 0.4590
K	 0.1450	 0.3370
L	 0.7520	 0.6490
M	 0.4350	 0.5210
N	 0.9020	 0.6730
O	 0.7010	 0.6180
P	 0.6410	 0.5910
Q	 0.4090	 0.4840
R	 0.7590	 0.6360
S	 0.3500	 0.4650
T	 0.1470	 0.3150
U	 0.7410	 0.6430
V	 0.4640	 0.5230
W	 0.2430	 0.4390
X	 0.2020	 0.4370
a	 0.6820	 0.5690
b	 0.7270	 0.5930
c	 0.8880	 0.6710
d	 0.6740	 0.6020
e	 0.5640	 0.5570
f	 0.3000	 0.4390
i	 0.7160	 0.6300
j	 0.2980	 0.4320
k	 0.1380	 0.3200
l	 0.7440	 0.6410



*Continued on next page...*

*Continued from previous page...*

Chain	Atom inclusion	Q-score
m	 0.4040	 0.5130
x	 0.1900	 0.4080