



wwPDB EM Validation Summary Report ⓘ

Mar 21, 2026 – 05:15 PM UTC

PDB ID : 9E0J / pdb_00009e0j
EMDB ID : EMD-47359
Title : Structure and evolution of Photosystem I in the early-branching cyanobacterium *Anthocerotibacter panamensis*
Authors : Gisriel, C.J.; Ho, M.
Deposited on : 2024-10-18
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

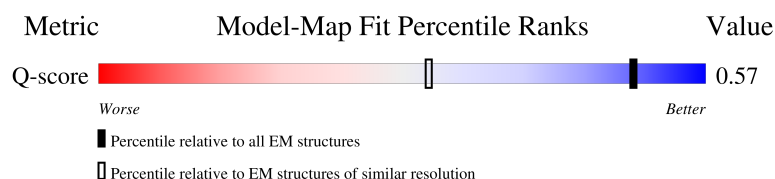
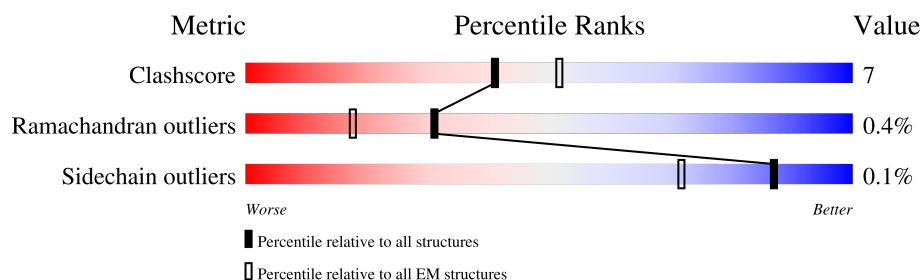
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 2.40 Å.

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



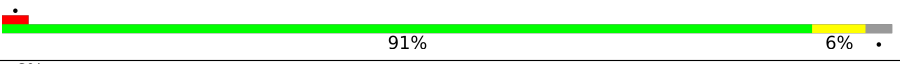


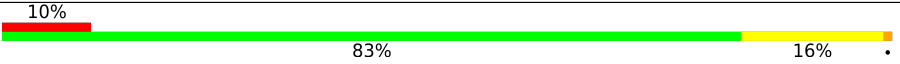
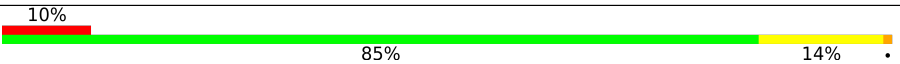
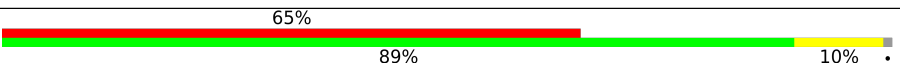
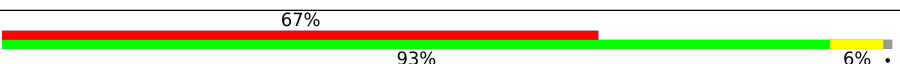
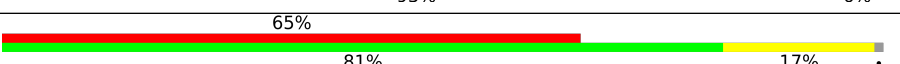
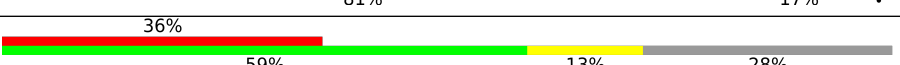
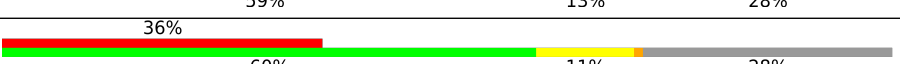
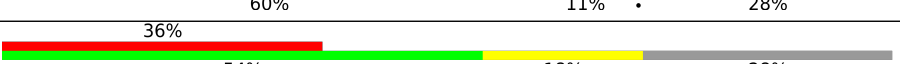
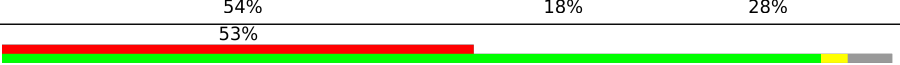
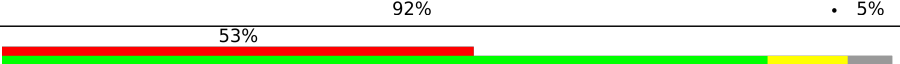




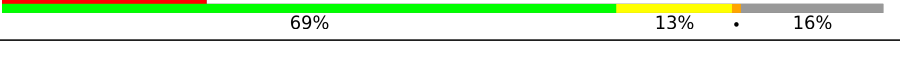

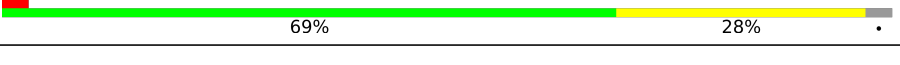
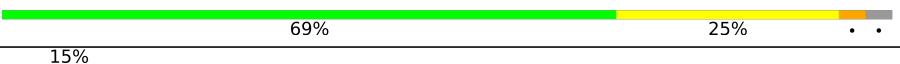


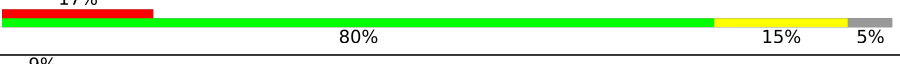

Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5628 (1.90 - 2.90)

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

Mol	Chain	Length	Quality of chain
1	A	785	<div> <div>7%</div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	G	785	<div> <div>7%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
1	a	785	<div> <div>7%</div> <div>82%</div> <div>16%</div> <div>..</div> </div>
2	M	32	<div> <div>88%</div> <div>9%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
2	T	32	
2	m	32	
3	B	749	
3	H	749	
3	b	749	
4	C	81	
4	K	81	
4	c	81	
5	D	143	
5	N	143	
5	d	143	
6	E	64	
6	O	64	
6	e	64	
7	F	177	
7	P	177	
7	f	177	
8	I	32	
8	Q	32	
8	i	32	
9	J	41	
9	R	41	
9	j	41	
10	L	160	
10	S	160	

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Mol	Chain	Length	Quality of chain
10	1	160	

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
11	CL0	A	801	X	-	-	-
11	CL0	G	801	X	-	-	-
11	CL0	a	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	812	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	815	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	817	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-
12	CLA	A	821	X	-	-	-
12	CLA	A	822	X	-	-	-
12	CLA	A	823	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	830	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	834	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	839	X	-	-	-
12	CLA	A	840	X	-	-	-
12	CLA	A	841	X	-	-	-
12	CLA	A	854	X	-	-	-
12	CLA	A	855	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	804	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	810	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	812	X	-	-	-
12	CLA	B	813	X	-	-	-
12	CLA	B	814	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	816	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	818	X	-	-	-
12	CLA	B	819	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-
12	CLA	B	823	X	-	-	-
12	CLA	B	824	X	-	-	-
12	CLA	B	825	X	-	-	-
12	CLA	B	826	X	-	-	-
12	CLA	B	827	X	-	-	-
12	CLA	B	828	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	831	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	B	833	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	834	X	-	-	-
12	CLA	B	835	X	-	-	-
12	CLA	B	836	X	-	-	-
12	CLA	B	837	X	-	-	-
12	CLA	B	838	X	-	-	-
12	CLA	F	201	X	-	-	-
12	CLA	F	203	X	-	-	-
12	CLA	G	802	X	-	-	-
12	CLA	G	803	X	-	-	-
12	CLA	G	804	X	-	-	-
12	CLA	G	805	X	-	-	-
12	CLA	G	806	X	-	-	-
12	CLA	G	807	X	-	-	-
12	CLA	G	808	X	-	-	-
12	CLA	G	809	X	-	-	-
12	CLA	G	810	X	-	-	-
12	CLA	G	811	X	-	-	-
12	CLA	G	812	X	-	-	-
12	CLA	G	813	X	-	-	-
12	CLA	G	814	X	-	-	-
12	CLA	G	815	X	-	-	-
12	CLA	G	816	X	-	-	-
12	CLA	G	817	X	-	-	-
12	CLA	G	818	X	-	-	-
12	CLA	G	819	X	-	-	-
12	CLA	G	820	X	-	-	-
12	CLA	G	821	X	-	-	-
12	CLA	G	822	X	-	-	-
12	CLA	G	823	X	-	-	-
12	CLA	G	824	X	-	-	-
12	CLA	G	825	X	-	-	-
12	CLA	G	826	X	-	-	-
12	CLA	G	827	X	-	-	-
12	CLA	G	828	X	-	-	-
12	CLA	G	829	X	-	-	-
12	CLA	G	830	X	-	-	-
12	CLA	G	831	X	-	-	-
12	CLA	G	832	X	-	-	-
12	CLA	G	833	X	-	-	-
12	CLA	G	834	X	-	-	-
12	CLA	G	835	X	-	-	-
12	CLA	G	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	G	837	X	-	-	-
12	CLA	G	838	X	-	-	-
12	CLA	G	839	X	-	-	-
12	CLA	G	840	X	-	-	-
12	CLA	G	841	X	-	-	-
12	CLA	G	842	X	-	-	-
12	CLA	G	855	X	-	-	-
12	CLA	G	856	X	-	-	-
12	CLA	H	801	X	-	-	-
12	CLA	H	802	X	-	-	-
12	CLA	H	803	X	-	-	-
12	CLA	H	804	X	-	-	-
12	CLA	H	805	X	-	-	-
12	CLA	H	806	X	-	-	-
12	CLA	H	807	X	-	-	-
12	CLA	H	808	X	-	-	-
12	CLA	H	809	X	-	-	-
12	CLA	H	810	X	-	-	-
12	CLA	H	811	X	-	-	-
12	CLA	H	812	X	-	-	-
12	CLA	H	813	X	-	-	-
12	CLA	H	814	X	-	-	-
12	CLA	H	815	X	-	-	-
12	CLA	H	816	X	-	-	-
12	CLA	H	817	X	-	-	-
12	CLA	H	818	X	-	-	-
12	CLA	H	819	X	-	-	-
12	CLA	H	820	X	-	-	-
12	CLA	H	821	X	-	-	-
12	CLA	H	822	X	-	-	-
12	CLA	H	823	X	-	-	-
12	CLA	H	824	X	-	-	-
12	CLA	H	825	X	-	-	-
12	CLA	H	826	X	-	-	-
12	CLA	H	827	X	-	-	-
12	CLA	H	828	X	-	-	-
12	CLA	H	829	X	-	-	-
12	CLA	H	830	X	-	-	-
12	CLA	H	831	X	-	-	-
12	CLA	H	832	X	-	-	-
12	CLA	H	833	X	-	-	-
12	CLA	H	834	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	H	835	X	-	-	-
12	CLA	H	836	X	-	-	-
12	CLA	H	837	X	-	-	-
12	CLA	H	838	X	-	-	-
12	CLA	H	839	X	-	-	-
12	CLA	H	850	X	-	-	-
12	CLA	J	103	X	-	-	-
12	CLA	L	202	X	-	-	-
12	CLA	L	204	X	-	-	-
12	CLA	L	205	X	-	-	-
12	CLA	L	206	X	-	-	-
12	CLA	P	201	X	-	-	-
12	CLA	P	203	X	-	-	-
12	CLA	R	103	X	-	-	-
12	CLA	S	202	X	-	-	-
12	CLA	S	203	X	-	-	-
12	CLA	S	204	X	-	-	-
12	CLA	a	802	X	-	-	-
12	CLA	a	803	X	-	-	-
12	CLA	a	804	X	-	-	-
12	CLA	a	805	X	-	-	-
12	CLA	a	806	X	-	-	-
12	CLA	a	807	X	-	-	-
12	CLA	a	808	X	-	-	-
12	CLA	a	809	X	-	-	-
12	CLA	a	810	X	-	-	-
12	CLA	a	811	X	-	-	-
12	CLA	a	812	X	-	-	-
12	CLA	a	813	X	-	-	-
12	CLA	a	814	X	-	-	-
12	CLA	a	815	X	-	-	-
12	CLA	a	816	X	-	-	-
12	CLA	a	817	X	-	-	-
12	CLA	a	818	X	-	-	-
12	CLA	a	819	X	-	-	-
12	CLA	a	820	X	-	-	-
12	CLA	a	821	X	-	-	-
12	CLA	a	822	X	-	-	-
12	CLA	a	823	X	-	-	-
12	CLA	a	824	X	-	-	-
12	CLA	a	825	X	-	-	-
12	CLA	a	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	a	827	X	-	-	-
12	CLA	a	828	X	-	-	-
12	CLA	a	829	X	-	-	-
12	CLA	a	831	X	-	-	-
12	CLA	a	832	X	-	-	-
12	CLA	a	833	X	-	-	-
12	CLA	a	834	X	-	-	-
12	CLA	a	835	X	-	-	-
12	CLA	a	836	X	-	-	-
12	CLA	a	837	X	-	-	-
12	CLA	a	838	X	-	-	-
12	CLA	a	839	X	-	-	-
12	CLA	a	840	X	-	-	-
12	CLA	a	841	X	-	-	-
12	CLA	a	854	X	-	-	-
12	CLA	a	855	X	-	-	-
12	CLA	b	801	X	-	-	-
12	CLA	b	802	X	-	-	-
12	CLA	b	803	X	-	-	-
12	CLA	b	804	X	-	-	-
12	CLA	b	805	X	-	-	-
12	CLA	b	806	X	-	-	-
12	CLA	b	807	X	-	-	-
12	CLA	b	808	X	-	-	-
12	CLA	b	809	X	-	-	-
12	CLA	b	810	X	-	-	-
12	CLA	b	811	X	-	-	-
12	CLA	b	812	X	-	-	-
12	CLA	b	813	X	-	-	-
12	CLA	b	814	X	-	-	-
12	CLA	b	815	X	-	-	-
12	CLA	b	816	X	-	-	-
12	CLA	b	817	X	-	-	-
12	CLA	b	818	X	-	-	-
12	CLA	b	819	X	-	-	-
12	CLA	b	820	X	-	-	-
12	CLA	b	821	X	-	-	-
12	CLA	b	822	X	-	-	-
12	CLA	b	823	X	-	-	-
12	CLA	b	824	X	-	-	-
12	CLA	b	825	X	-	-	-
12	CLA	b	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	b	827	X	-	-	-
12	CLA	b	828	X	-	-	-
12	CLA	b	829	X	-	-	-
12	CLA	b	830	X	-	-	-
12	CLA	b	831	X	-	-	-
12	CLA	b	832	X	-	-	-
12	CLA	b	833	X	-	-	-
12	CLA	b	834	X	-	-	-
12	CLA	b	835	X	-	-	-
12	CLA	b	836	X	-	-	-
12	CLA	b	837	X	-	-	-
12	CLA	b	848	X	-	-	-
12	CLA	f	201	X	-	-	-
12	CLA	f	203	X	-	-	-
12	CLA	j	102	X	-	-	-
12	CLA	j	104	X	-	-	-
12	CLA	l	202	X	-	-	-
12	CLA	l	204	X	-	-	-
12	CLA	l	205	X	-	-	-
12	CLA	l	206	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 69921 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	G	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		
1	a	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		
1	A	773	Total	C	N	O	S	0	0
			5997	3925	1024	1023	25		

- Molecule 2 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	T	31	Total	C	N	O	S	0	0
			226	152	34	38	2		
2	m	31	Total	C	N	O	S	0	0
			226	152	34	38	2		
2	M	31	Total	C	N	O	S	0	0
			226	152	34	38	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	H	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		
3	b	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		
3	B	746	Total	C	N	O	S	0	0
			5866	3864	981	1001	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	K	80	Total	C	N	O	S	0	0
			599	367	105	117	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	c	80	Total	C	N	O	S	0	0
			599	367	105	117	10		
4	C	80	Total	C	N	O	S	0	0
			599	367	105	117	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	103	Total	C	N	O	S	0	0
			784	500	138	143	3		
5	d	103	Total	C	N	O	S	0	0
			784	500	138	143	3		
5	D	103	Total	C	N	O	S	0	0
			784	500	138	143	3		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
6	O	61	Total	C	N	O	0	0
			489	308	84	97		
6	e	61	Total	C	N	O	0	0
			489	308	84	97		
6	E	61	Total	C	N	O	0	0
			489	308	84	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	P	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		
7	f	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		
7	F	148	Total	C	N	O	S	0	0
			1148	738	191	215	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Q	31	Total	C	N	O	S	0	0
			254	175	36	42	1		
8	i	31	Total	C	N	O	S	0	0
			254	175	36	42	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	31	Total	C	N	O	S	0	0
			254	175	36	42	1		

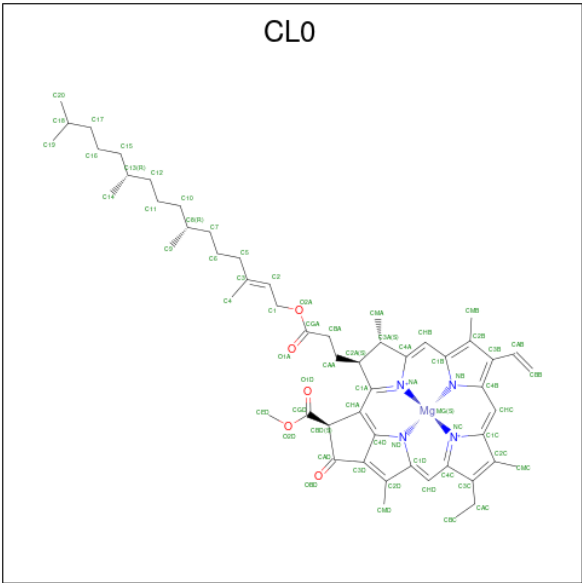
- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	39	Total	C	N	O		0	0
			293	204	44	45			
9	j	39	Total	C	N	O		0	0
			293	204	44	45			
9	J	39	Total	C	N	O		0	0
			293	204	44	45			

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

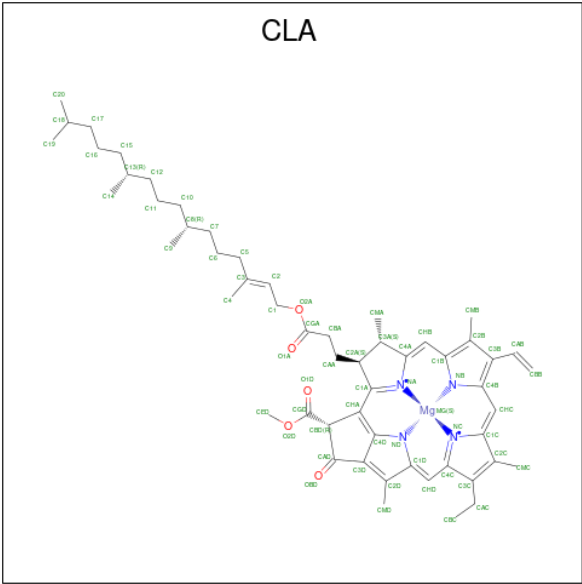
Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	l	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	L	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		

- Molecule 11 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 12 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	H	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	P	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	P	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	S	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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

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

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

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

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

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

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

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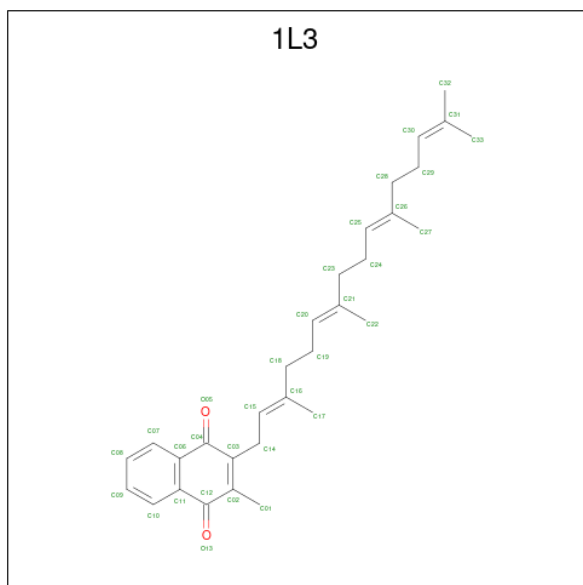
Mol	Chain	Residues	Atoms					AltConf
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12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	L	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	L	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
12	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 13 is Menaquinone-4 (CCD ID: 1L3) (formula: $C_{31}H_{40}O_2$).



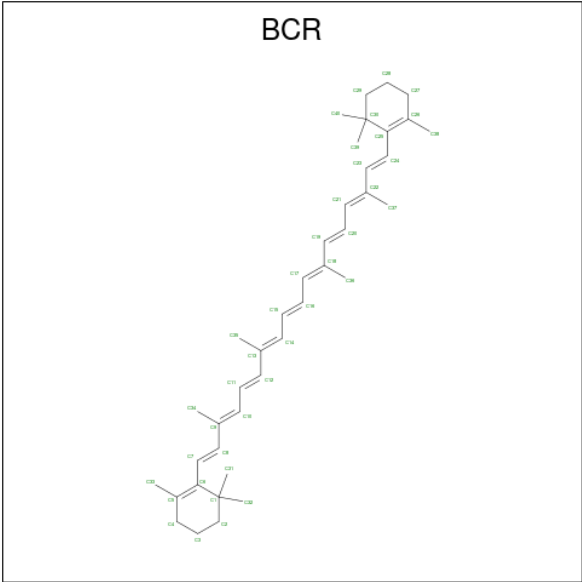
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			33	31	2	
13	H	1	Total	C	O	0
			33	31	2	
13	a	1	Total	C	O	0
			33	31	2	
13	b	1	Total	C	O	0
			33	31	2	
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 15 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
15	G	1	Total	C	0
			40	40	
15	G	1	Total	C	0
			40	40	
15	G	1	Total	C	0
			40	40	
15	G	1	Total	C	0
			40	40	
15	G	1	Total	C	0
			40	40	
15	G	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			25	25	
15	H	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			40	40	
15	H	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
15	P	1	Total C 40 40	0
15	P	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	Q	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	R	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	S	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 25 25	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0

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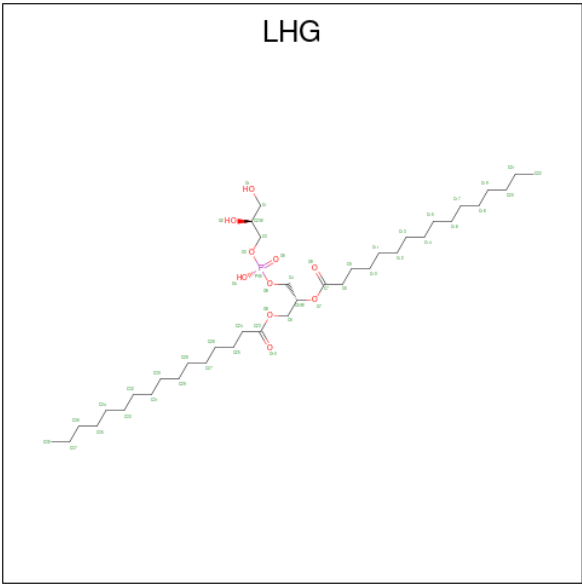
Mol	Chain	Residues	Atoms	AltConf
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 40 40	0
15	B	1	Total C 25 25	0
15	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	F	1	Total	C	0
			40	40	
15	I	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	J	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	

- Molecule 16 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



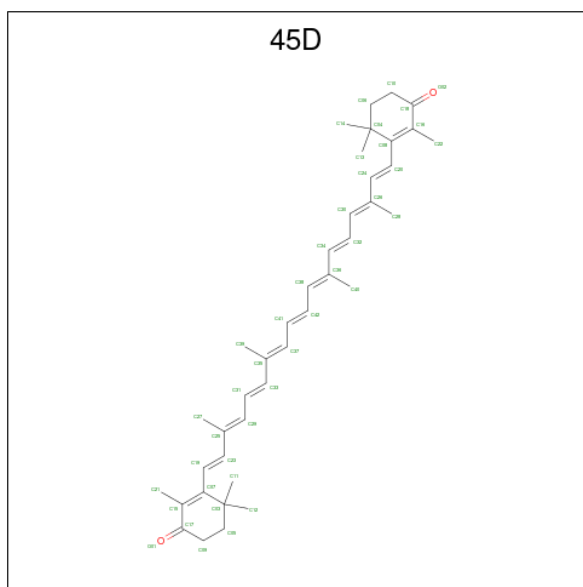
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			49	38	10	1	

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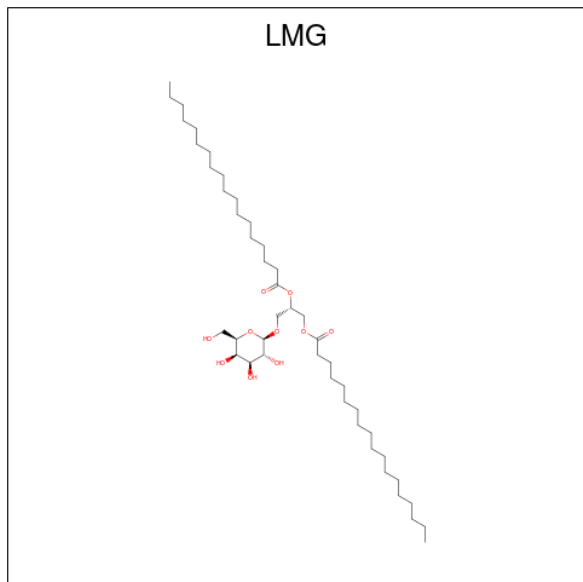
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			27	16	10	1	
16	G	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			27	16	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			27	16	10	1	
16	A	1	Total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

- Molecule 17 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: $C_{40}H_{52}O_2$) (labeled as "Ligand of Interest" by depositor).



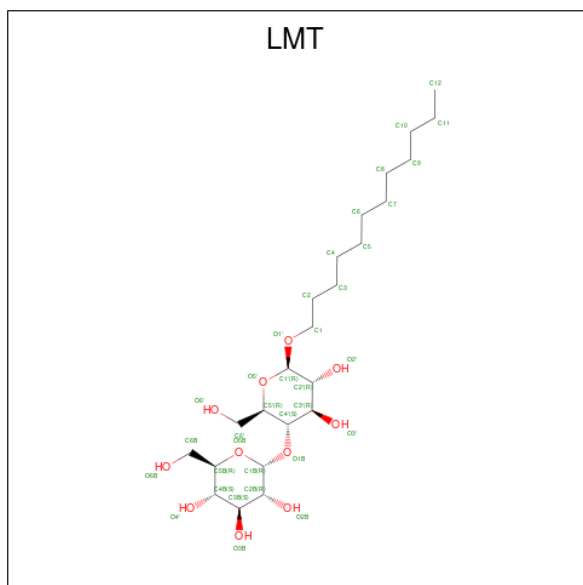
Mol	Chain	Residues	Atoms			AltConf
17	T	1	Total	C	O	0
			42	40	2	
17	m	1	Total	C	O	0
			42	40	2	
17	M	1	Total	C	O	0
			42	40	2	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



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

- Molecule 19 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
19	H	1	Total	C	O	0
			35	24	11	
19	b	1	Total	C	O	0
			35	24	11	
19	B	1	Total	C	O	0
			35	24	11	

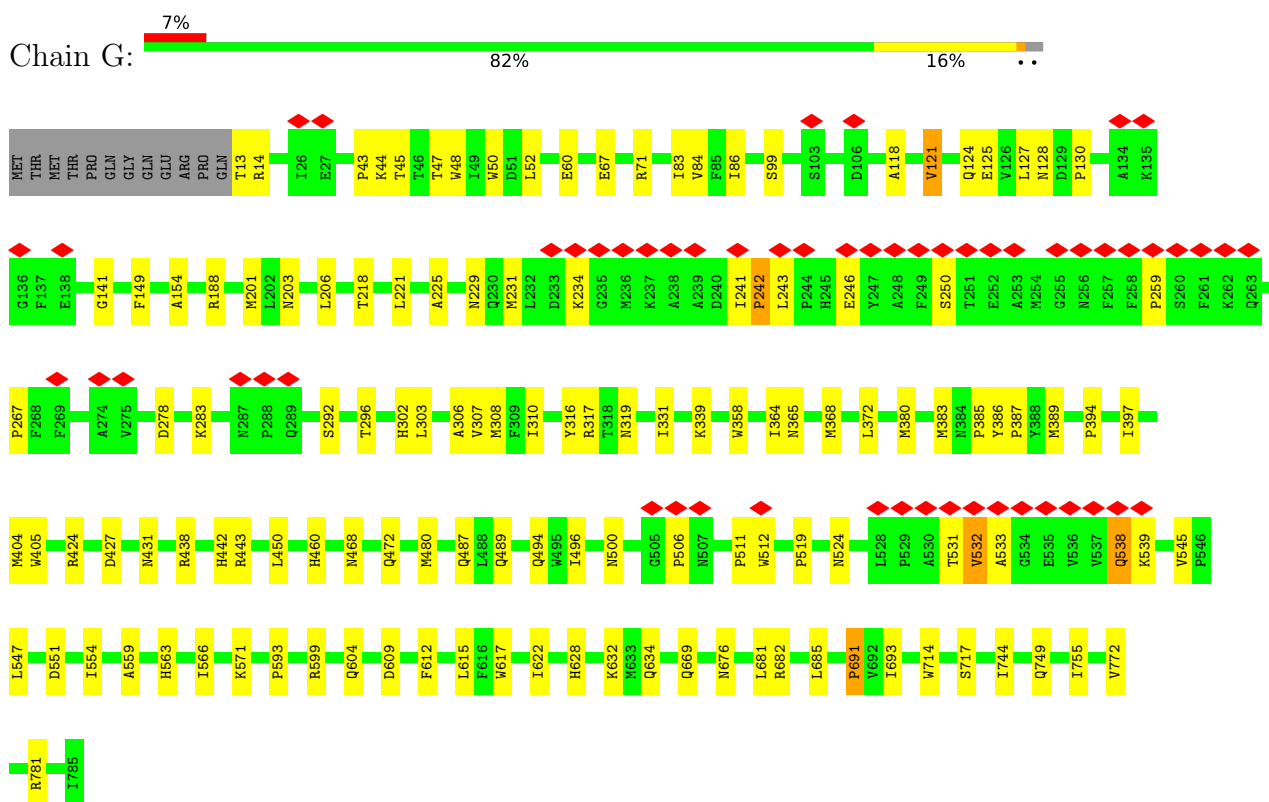
- Molecule 20 is water.

Mol	Chain	Residues	Atoms		AltConf
20	G	58	Total	O	0
			58	58	
20	H	80	Total	O	0
			80	80	
20	K	26	Total	O	0
			26	26	
20	N	15	Total	O	0
			15	15	
20	O	1	Total	O	0
			1	1	
20	S	5	Total	O	0
			5	5	
20	a	57	Total	O	0
			57	57	
20	b	82	Total	O	0
			82	82	
20	c	22	Total	O	0
			22	22	
20	d	17	Total	O	0
			17	17	
20	e	1	Total	O	0
			1	1	
20	l	6	Total	O	0
			6	6	
20	A	56	Total	O	0
			56	56	
20	B	82	Total	O	0
			82	82	
20	C	24	Total	O	0
			24	24	
20	D	16	Total	O	0
			16	16	
20	L	7	Total	O	0
			7	7	

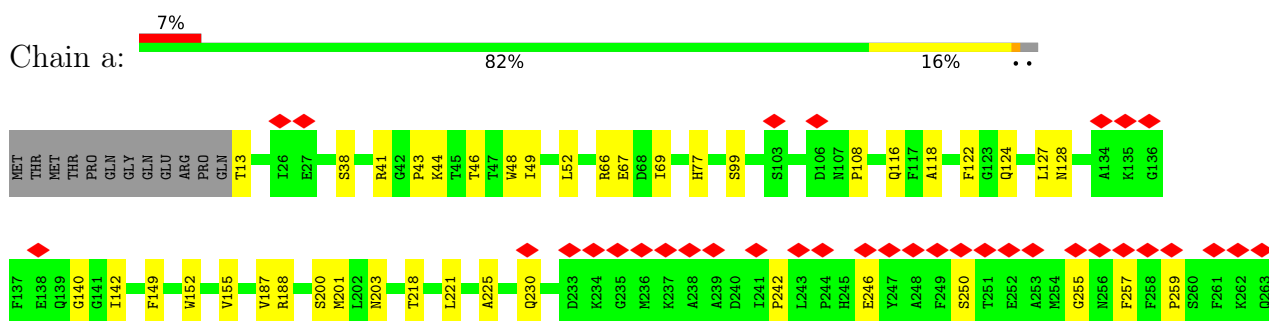
3 Residue-property plots

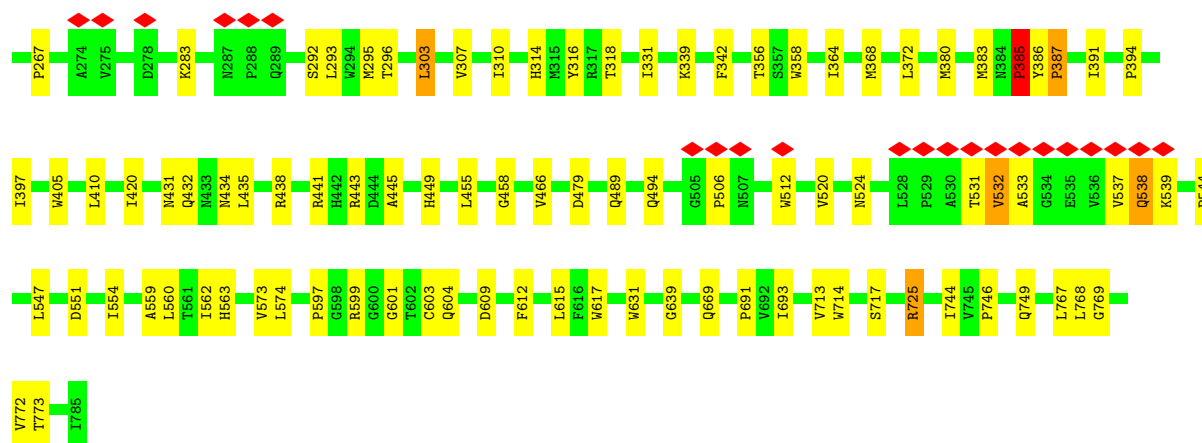
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

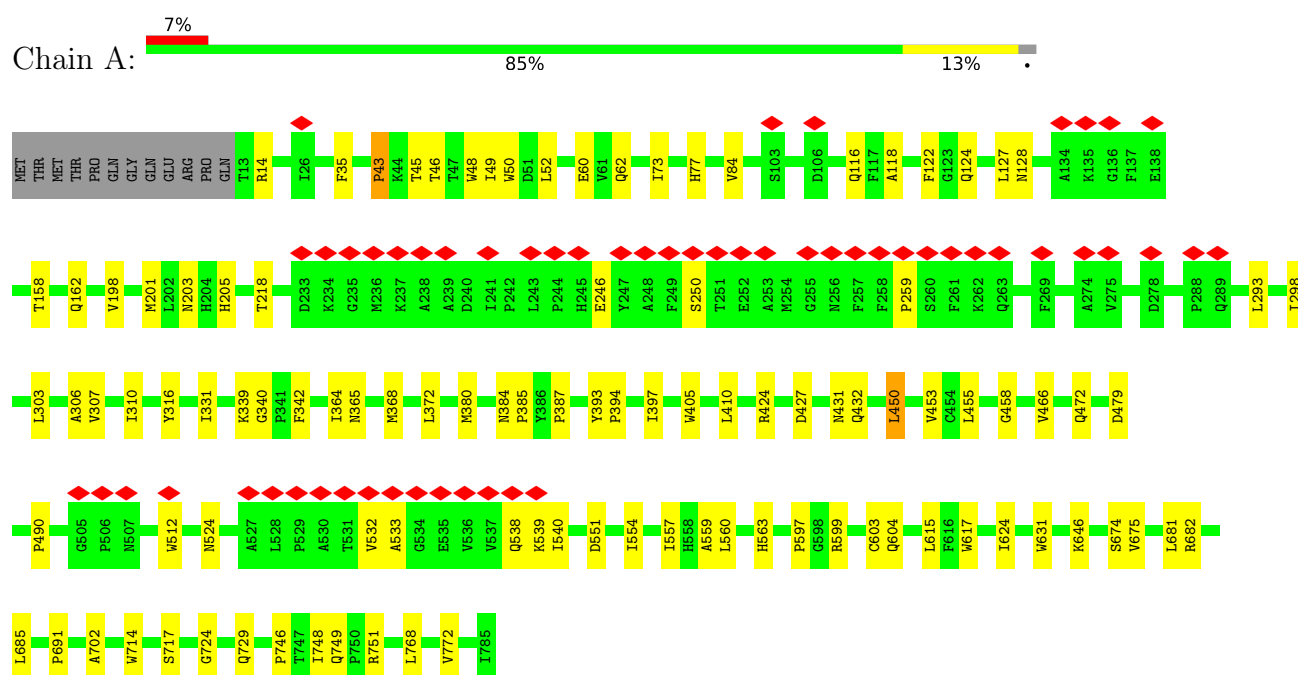


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

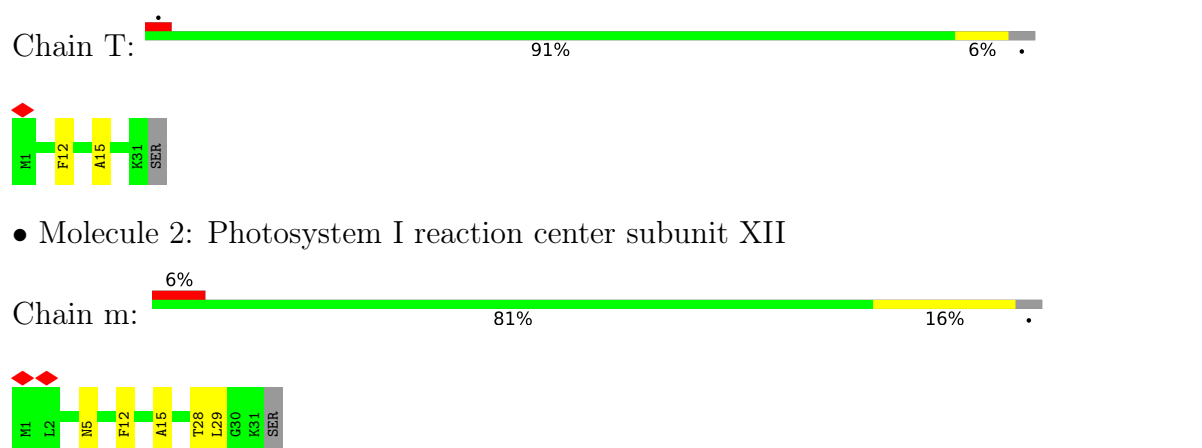




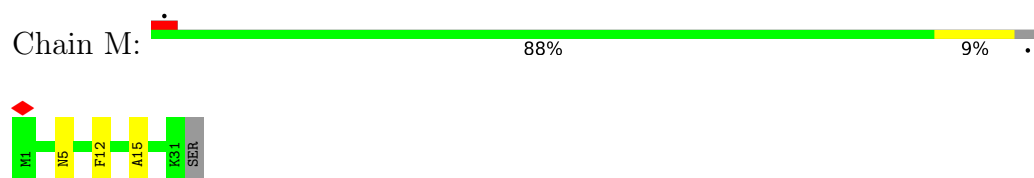
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



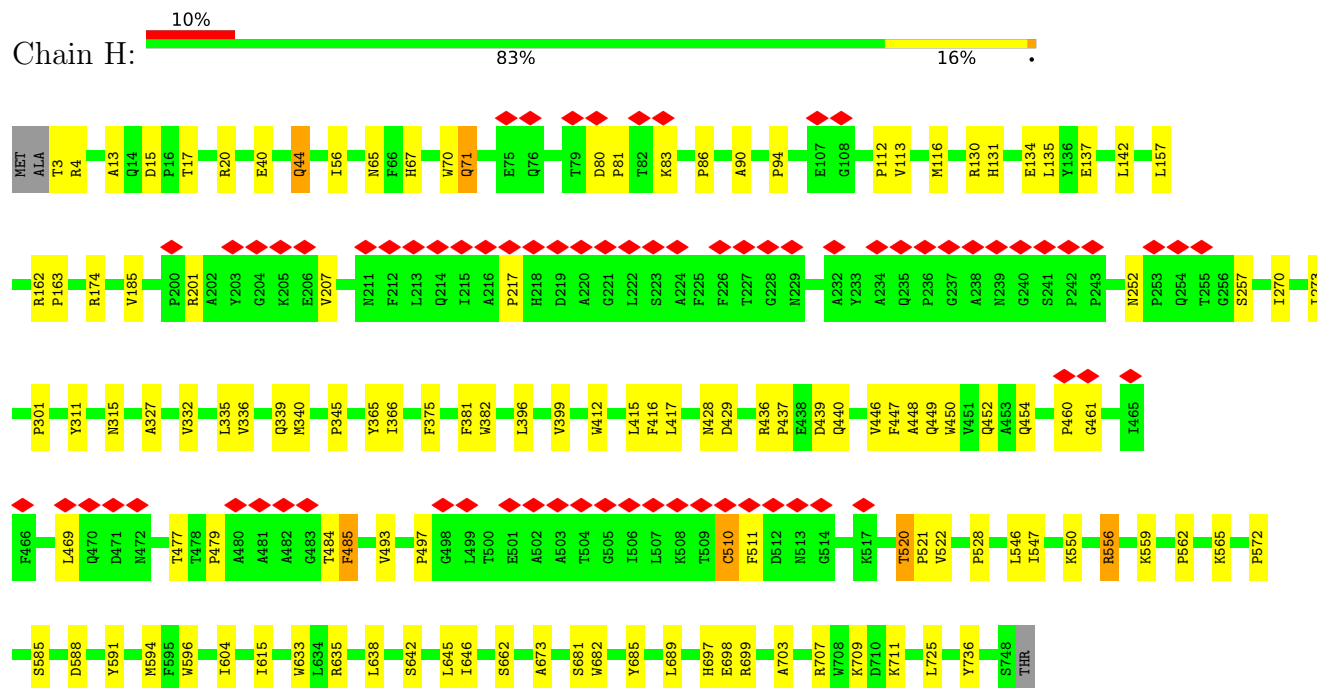
- Molecule 2: Photosystem I reaction center subunit XII



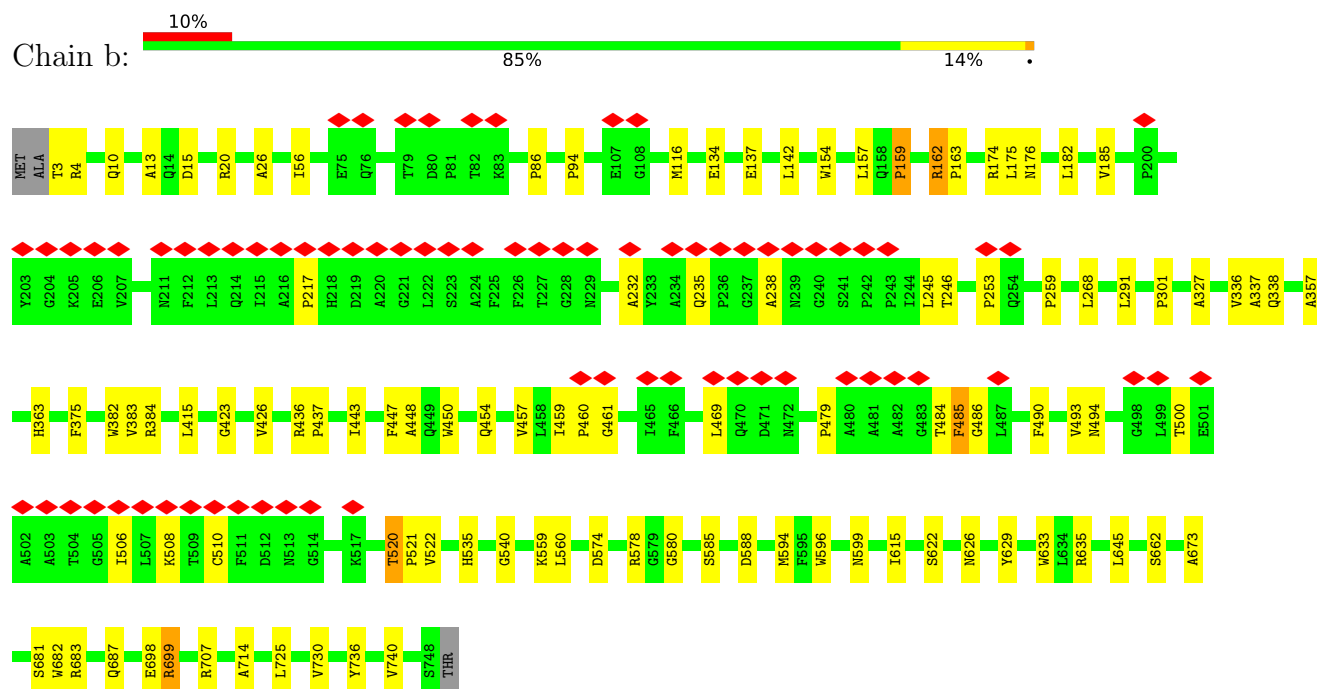
- Molecule 2: Photosystem I reaction center subunit XII



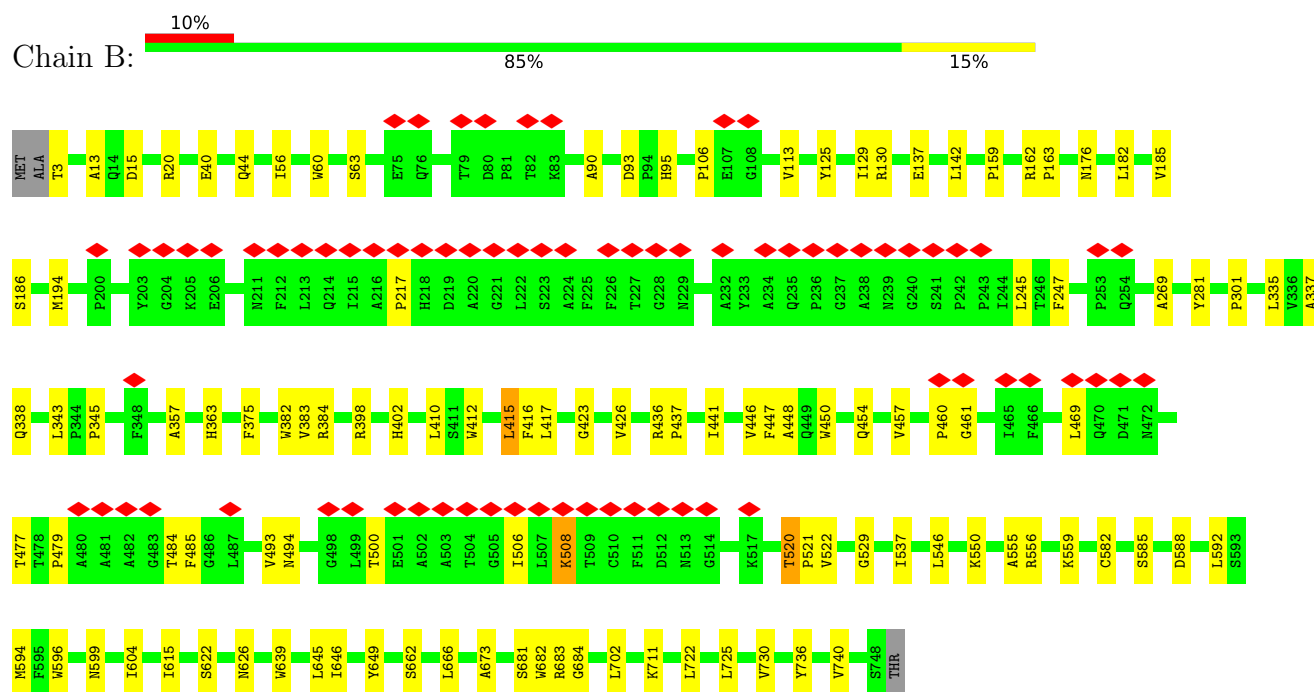
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



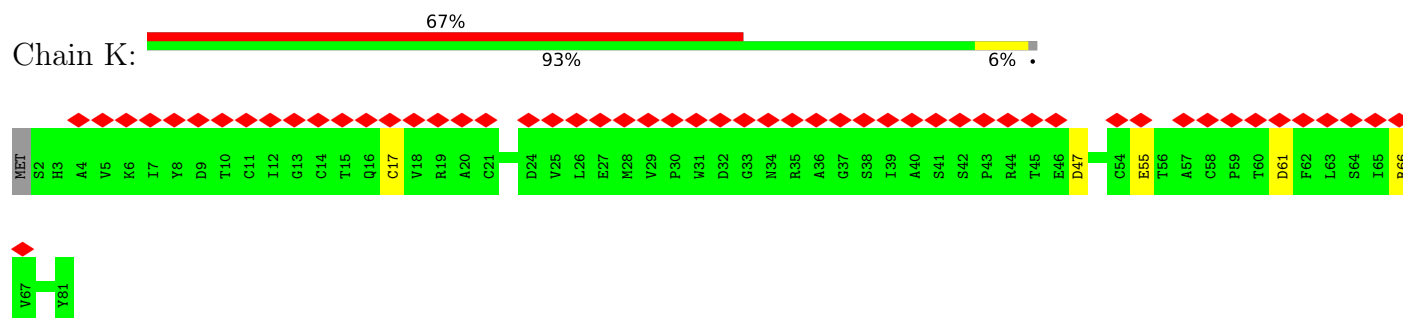
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



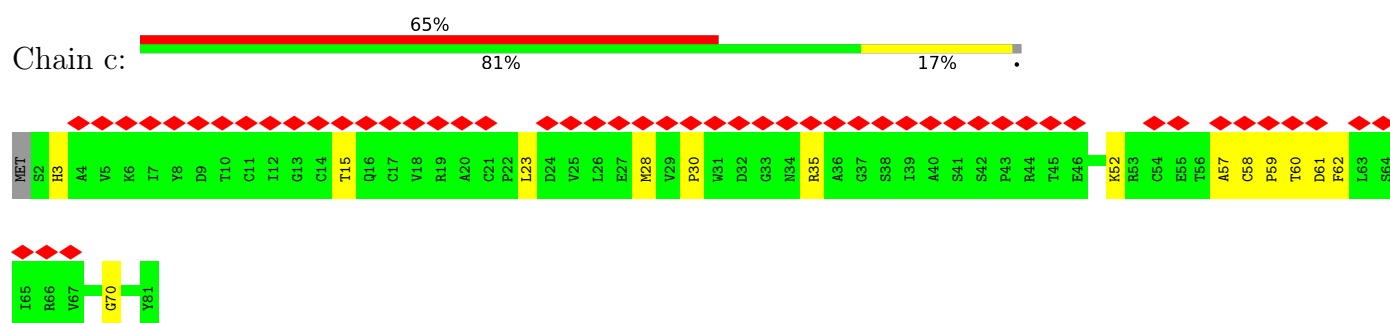
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



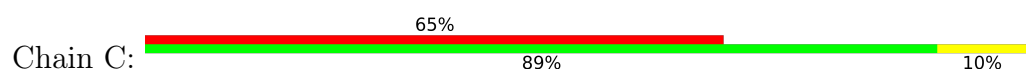
- Molecule 4: Photosystem I iron-sulfur center

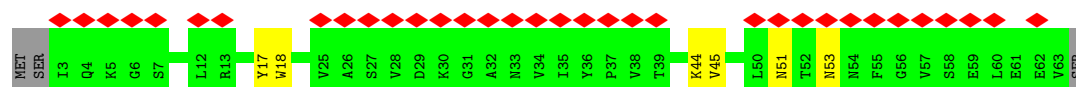


- Molecule 4: Photosystem I iron-sulfur center




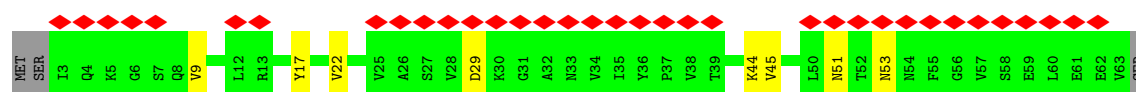
- Molecule 4: Photosystem I iron-sulfur center






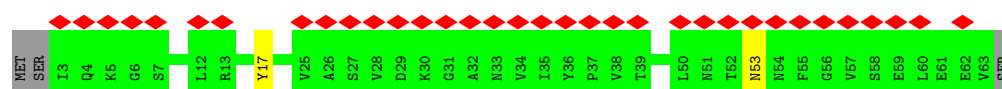
- Molecule 6: Photosystem I reaction center subunit IV

Chain e: 



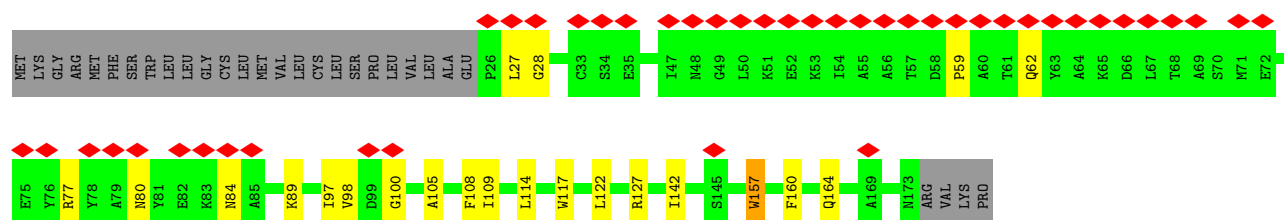
- Molecule 6: Photosystem I reaction center subunit IV

Chain E: 



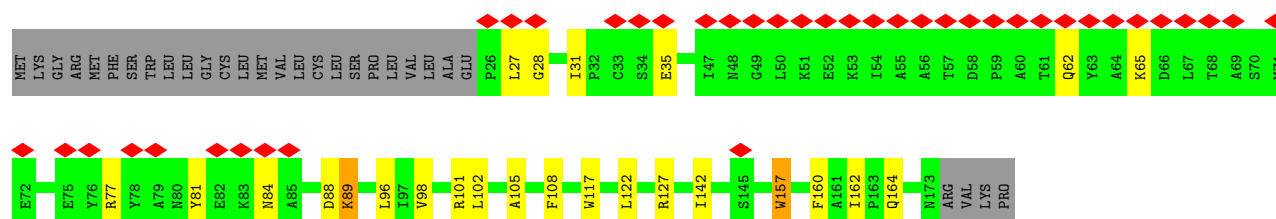
- Molecule 7: Photosystem I reaction center subunit III

Chain P: 




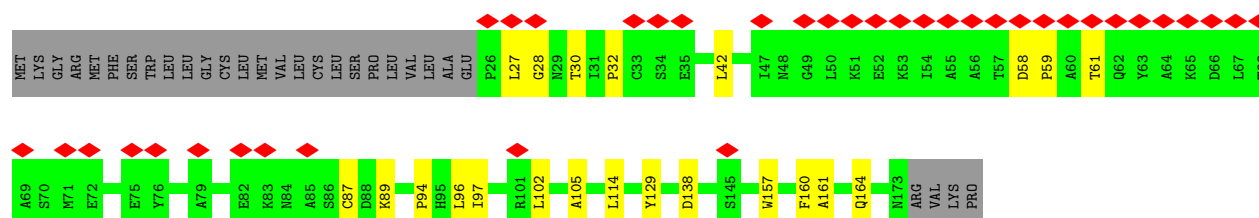
- Molecule 7: Photosystem I reaction center subunit III

Chain f: 



- Molecule 7: Photosystem I reaction center subunit III

Chain F: 



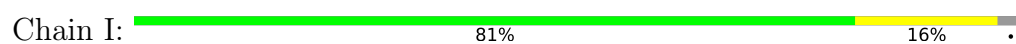
- Molecule 8: Photosystem I reaction center subunit VIII



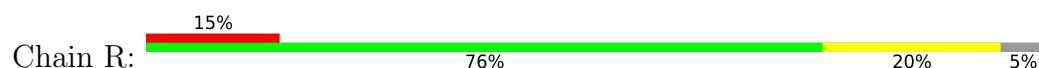
- Molecule 8: Photosystem I reaction center subunit VIII



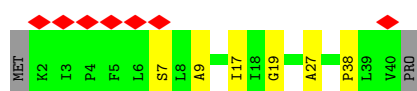
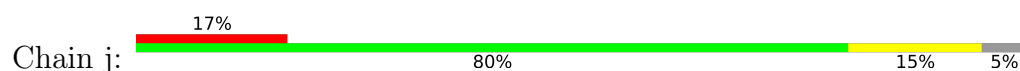
- Molecule 8: Photosystem I reaction center subunit VIII



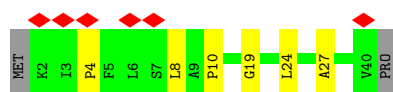
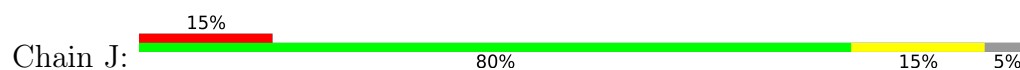
- Molecule 9: Photosystem I reaction center subunit IX



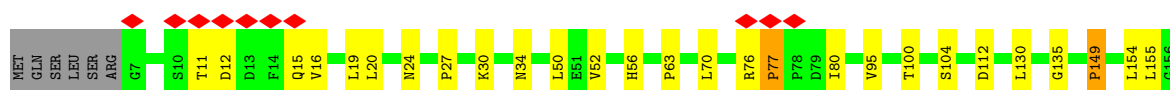
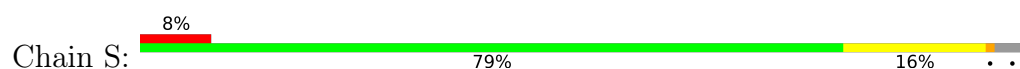
- Molecule 9: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit IX

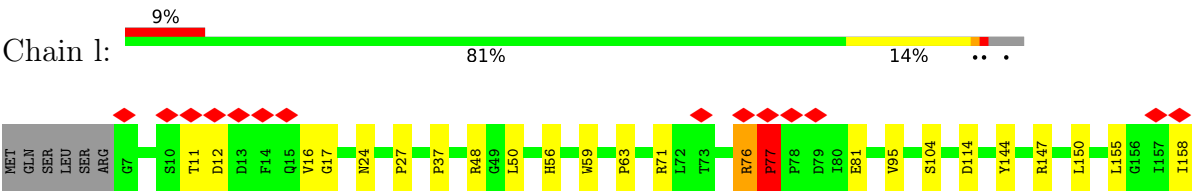


- Molecule 10: Photosystem I reaction center subunit XI

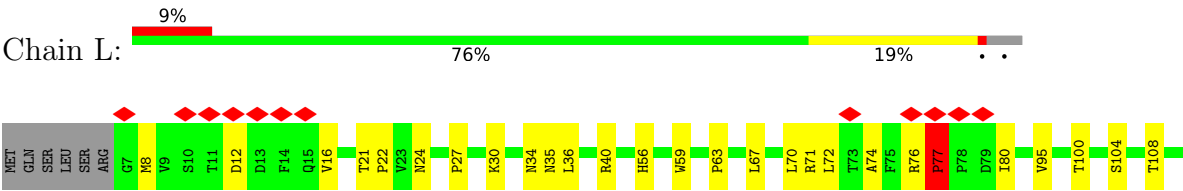




• Molecule 10: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XI



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	403080	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	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	0.066	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.00112	Depositor
Map size (Å)	264.0, 264.0, 264.0	wwPDB
Map dimensions	320, 320, 320	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: LMT, 45D, 1L3, BCR, LMG, CLA, SF4, LHG, CL0

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	0.57	3/6200 (0.0%)	1.03	16/8468 (0.2%)
1	G	0.60	6/6200 (0.1%)	1.07	25/8468 (0.3%)
1	a	0.62	9/6200 (0.1%)	1.14	29/8468 (0.3%)
2	M	0.37	0/229	0.79	0/308
2	T	0.40	0/229	0.69	0/308
2	m	0.42	0/229	0.75	0/308
3	B	0.62	7/6079 (0.1%)	1.16	32/8310 (0.4%)
3	H	0.62	7/6079 (0.1%)	1.13	33/8310 (0.4%)
3	b	0.68	9/6079 (0.1%)	1.17	36/8310 (0.4%)
4	C	0.39	0/609	0.81	3/825 (0.4%)
4	K	0.34	0/609	0.74	0/825
4	c	0.41	0/609	0.95	4/825 (0.5%)
5	D	0.40	0/800	0.72	0/1079
5	N	0.40	1/800 (0.1%)	0.76	3/1079 (0.3%)
5	d	0.40	1/800 (0.1%)	0.76	3/1079 (0.3%)
6	E	0.25	0/497	0.54	0/675
6	O	0.32	0/497	0.70	0/675
6	e	0.29	0/497	0.59	0/675
7	F	0.55	2/1175 (0.2%)	1.11	10/1596 (0.6%)
7	P	0.52	1/1175 (0.1%)	1.06	4/1596 (0.3%)
7	f	0.57	2/1175 (0.2%)	1.03	2/1596 (0.1%)
8	I	0.43	0/261	0.82	0/360
8	Q	0.45	0/261	0.91	0/360
8	i	0.52	0/261	0.95	0/360
9	J	0.56	0/301	1.21	2/413 (0.5%)
9	R	1.38	3/301 (1.0%)	1.89	7/413 (1.7%)
9	j	0.58	1/301 (0.3%)	1.02	0/413
10	L	0.59	2/1193 (0.2%)	1.09	6/1628 (0.4%)
10	S	0.56	1/1193 (0.1%)	1.10	7/1628 (0.4%)
10	l	0.72	2/1193 (0.2%)	1.22	14/1628 (0.9%)
All	All	0.59	57/52032 (0.1%)	1.08	236/70986 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	1
3	B	0	3
3	H	0	5
3	b	0	5
5	D	0	1
8	i	0	1
10	S	0	1
10	l	0	3
All	All	0	20

The worst 5 of 57 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	b	163	PRO	CG-CD	-24.62	0.67	1.50
1	a	387	PRO	CG-CD	-19.52	0.84	1.50
1	A	746	PRO	CG-CD	-17.89	0.90	1.50
9	R	38	PRO	CG-CD	-17.11	0.92	1.50
3	H	528	PRO	CG-CD	-16.43	0.94	1.50

The worst 5 of 236 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	b	163	PRO	N-CD-CG	-28.03	61.15	103.20
1	G	242	PRO	CB-CG-CD	-25.47	24.60	106.10
3	B	163	PRO	N-CD-CG	-25.10	65.55	103.20
1	a	387	PRO	N-CD-CG	-25.02	65.67	103.20
1	A	746	PRO	N-CD-CG	-23.74	67.59	103.20

There are no chirality outliers.

5 of 20 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	H	485	PHE	Peptide
3	H	510	CYS	Peptide
3	H	556	ARG	Sidechain
3	H	682	TRP	Peptide
3	H	70	TRP	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	5997	0	5811	69	0
1	G	5997	0	5811	81	0
1	a	5997	0	5811	87	0
2	M	226	0	240	3	0
2	T	226	0	240	2	0
2	m	226	0	240	5	0
3	B	5866	0	5675	75	0
3	H	5866	0	5675	86	0
3	b	5866	0	5675	73	0
4	C	599	0	577	5	0
4	K	599	0	577	4	0
4	c	599	0	577	8	0
5	D	784	0	798	12	0
5	N	784	0	798	12	0
5	d	784	0	798	16	0
6	E	489	0	474	2	0
6	O	489	0	474	6	0
6	e	489	0	474	7	0
7	F	1148	0	1143	10	0
7	P	1148	0	1143	16	0
7	f	1148	0	1143	15	0
8	I	254	0	269	5	0
8	Q	254	0	269	10	0
8	i	254	0	269	9	0
9	J	293	0	327	5	0
9	R	293	0	327	8	0
9	j	293	0	327	5	0
10	L	1159	0	1179	21	0
10	S	1159	0	1179	16	0
10	l	1159	0	1179	15	0
11	A	65	0	72	4	0
11	G	65	0	72	1	0
11	a	65	0	72	0	0
12	A	2375	0	2267	65	0
12	B	2190	0	2162	57	0
12	F	110	0	104	4	0
12	G	2440	0	2339	67	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	H	2310	0	2282	68	0
12	J	45	0	32	1	0
12	L	250	0	265	11	0
12	P	110	0	104	5	0
12	R	45	0	32	1	0
12	S	185	0	193	7	0
12	a	2375	0	2270	75	0
12	b	2185	0	2148	66	0
12	f	110	0	104	5	0
12	j	110	0	104	2	0
12	l	250	0	265	12	0
13	A	33	0	0	0	0
13	B	33	0	0	0	0
13	G	33	0	0	0	0
13	H	33	0	0	0	0
13	a	33	0	0	0	0
13	b	33	0	0	0	0
14	A	8	0	0	0	0
14	C	16	0	0	0	0
14	G	8	0	0	0	0
14	K	16	0	0	1	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
15	A	280	0	341	15	0
15	B	225	0	273	13	0
15	F	80	0	98	5	0
15	G	280	0	341	14	0
15	H	265	0	322	21	0
15	I	40	0	49	4	0
15	J	120	0	145	6	0
15	L	120	0	147	5	0
15	P	80	0	98	5	0
15	Q	80	0	98	5	0
15	R	80	0	96	5	0
15	S	80	0	98	5	0
15	a	280	0	341	15	0
15	b	265	0	322	21	0
15	f	80	0	98	4	0
15	i	80	0	98	3	0
15	j	80	0	96	5	0
15	l	80	0	98	4	0
16	A	125	0	172	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	G	125	0	172	5	0
16	a	125	0	172	4	0
17	M	42	0	52	3	0
17	T	42	0	52	3	0
17	m	42	0	52	4	0
18	B	55	0	86	4	0
18	H	55	0	86	5	0
18	b	55	0	86	3	0
19	B	35	0	44	2	0
19	H	35	0	45	1	0
19	b	35	0	46	1	0
20	A	56	0	0	1	0
20	B	82	0	0	0	0
20	C	24	0	0	0	0
20	D	16	0	0	0	0
20	G	58	0	0	2	0
20	H	80	0	0	0	0
20	K	26	0	0	0	0
20	L	7	0	0	0	0
20	N	15	0	0	0	0
20	O	1	0	0	0	0
20	S	5	0	0	0	0
20	a	57	0	0	2	0
20	b	82	0	0	0	0
20	c	22	0	0	0	0
20	d	17	0	0	1	0
20	e	1	0	0	0	0
20	l	6	0	0	0	0
All	All	69921	0	68590	949	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 7.

The worst 5 of 949 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)
3:H:67:HIS:O	3:H:71:GLN:HB3	1.71	0.88
5:d:42:GLU:HA	5:d:55:MET:O	1.78	0.83
12:a:839:CLA:HAB	12:a:839:CLA:H111	1.66	0.78
5:N:42:GLU:HA	5:N:55:MET:O	1.84	0.77
12:A:839:CLA:H111	12:A:839:CLA:HAB	1.69	0.74

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	771/785 (98%)	720 (93%)	46 (6%)	5 (1%)	21	32
1	G	771/785 (98%)	725 (94%)	40 (5%)	6 (1%)	16	25
1	a	771/785 (98%)	722 (94%)	45 (6%)	4 (0%)	24	37
2	M	29/32 (91%)	29 (100%)	0	0	100	100
2	T	29/32 (91%)	29 (100%)	0	0	100	100
2	m	29/32 (91%)	29 (100%)	0	0	100	100
3	B	744/749 (99%)	707 (95%)	36 (5%)	1 (0%)	48	64
3	H	744/749 (99%)	702 (94%)	41 (6%)	1 (0%)	48	64
3	b	744/749 (99%)	700 (94%)	43 (6%)	1 (0%)	48	64
4	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	K	78/81 (96%)	73 (94%)	5 (6%)	0	100	100
4	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
5	D	101/143 (71%)	98 (97%)	3 (3%)	0	100	100
5	N	101/143 (71%)	97 (96%)	4 (4%)	0	100	100
5	d	101/143 (71%)	95 (94%)	6 (6%)	0	100	100
6	E	59/64 (92%)	57 (97%)	2 (3%)	0	100	100
6	O	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
6	e	59/64 (92%)	56 (95%)	3 (5%)	0	100	100
7	F	146/177 (82%)	132 (90%)	13 (9%)	1 (1%)	18	28
7	P	146/177 (82%)	134 (92%)	11 (8%)	1 (1%)	18	28
7	f	146/177 (82%)	135 (92%)	10 (7%)	1 (1%)	18	28
8	I	29/32 (91%)	27 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	Q	29/32 (91%)	29 (100%)	0	0	100	100
8	i	29/32 (91%)	28 (97%)	1 (3%)	0	100	100
9	J	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
9	R	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
9	j	37/41 (90%)	35 (95%)	2 (5%)	0	100	100
10	L	152/160 (95%)	143 (94%)	7 (5%)	2 (1%)	9	14
10	S	152/160 (95%)	145 (95%)	5 (3%)	2 (1%)	9	14
10	l	152/160 (95%)	143 (94%)	7 (5%)	2 (1%)	9	14
All	All	6438/6792 (95%)	6065 (94%)	346 (5%)	27 (0%)	31	43

5 of 27 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	259	PRO
7	P	89	LYS
10	S	12	ASP
10	S	77	PRO
7	f	89	LYS

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	603/628 (96%)	603 (100%)	0	100	100
1	G	603/628 (96%)	602 (100%)	1 (0%)	87	94
1	a	603/628 (96%)	601 (100%)	2 (0%)	86	93
2	M	22/23 (96%)	22 (100%)	0	100	100
2	T	22/23 (96%)	22 (100%)	0	100	100
2	m	22/23 (96%)	22 (100%)	0	100	100
3	B	591/593 (100%)	591 (100%)	0	100	100
3	H	591/593 (100%)	591 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	b	591/593 (100%)	591 (100%)	0	100	100
4	C	67/68 (98%)	67 (100%)	0	100	100
4	K	67/68 (98%)	67 (100%)	0	100	100
4	c	67/68 (98%)	67 (100%)	0	100	100
5	D	81/116 (70%)	81 (100%)	0	100	100
5	N	81/116 (70%)	80 (99%)	1 (1%)	63	81
5	d	81/116 (70%)	81 (100%)	0	100	100
6	E	55/58 (95%)	55 (100%)	0	100	100
6	O	55/58 (95%)	55 (100%)	0	100	100
6	e	55/58 (95%)	55 (100%)	0	100	100
7	F	120/146 (82%)	120 (100%)	0	100	100
7	P	120/146 (82%)	120 (100%)	0	100	100
7	f	120/146 (82%)	120 (100%)	0	100	100
8	I	29/30 (97%)	29 (100%)	0	100	100
8	Q	29/30 (97%)	29 (100%)	0	100	100
8	i	29/30 (97%)	29 (100%)	0	100	100
9	J	32/34 (94%)	32 (100%)	0	100	100
9	R	32/34 (94%)	32 (100%)	0	100	100
9	j	32/34 (94%)	32 (100%)	0	100	100
10	L	119/125 (95%)	119 (100%)	0	100	100
10	S	119/125 (95%)	119 (100%)	0	100	100
10	l	119/125 (95%)	119 (100%)	0	100	100
All	All	5157/5463 (94%)	5153 (100%)	4 (0%)	87	95

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	691	PRO
5	N	93	PRO
1	a	385	PRO
1	a	387	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 145 such sidechains are listed below:

Mol	Chain	Res	Type
3	B	158	GLN
10	L	34	ASN
3	B	298	GLN
5	D	5	ASN
1	a	489	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

366 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
15	BCR	j	103	-	41,41,41	2.65	6 (14%)	56,56,56	6.80	16 (28%)
15	BCR	F	202	-	41,41,41	2.79	6 (14%)	56,56,56	6.76	23 (41%)
12	CLA	A	808	1	54,58,73	2.54	23 (42%)	64,95,113	2.88	25 (39%)
15	BCR	R	101	-	41,41,41	2.67	6 (14%)	56,56,56	6.58	23 (41%)
12	CLA	B	817	3	49,53,73	2.53	21 (42%)	58,89,113	2.95	23 (39%)
15	BCR	Q	101	-	41,41,41	2.62	6 (14%)	56,56,56	6.90	22 (39%)
12	CLA	A	806	1	69,73,73	2.17	21 (30%)	82,113,113	2.64	25 (30%)
12	CLA	b	811	-	64,68,73	2.33	23 (35%)	76,107,113	2.59	27 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	f	203	-	49,53,73	2.57	22 (44%)	58,89,113	4.46	25 (43%)
12	CLA	b	822	20	69,73,73	2.24	24 (34%)	82,113,113	2.61	28 (34%)
12	CLA	H	819	-	49,53,73	2.59	23 (46%)	58,89,113	2.83	24 (41%)
12	CLA	H	802	-	69,73,73	2.19	22 (31%)	82,113,113	2.80	34 (41%)
12	CLA	H	832	-	49,53,73	2.52	22 (44%)	58,89,113	2.71	24 (41%)
12	CLA	b	824	3	69,73,73	2.18	23 (33%)	82,113,113	2.53	32 (39%)
12	CLA	b	837	-	69,73,73	2.20	23 (33%)	82,113,113	2.60	30 (36%)
19	LMT	b	846	-	36,36,36	1.17	4 (11%)	47,47,47	1.01	2 (4%)
12	CLA	a	807	-	69,73,73	2.22	22 (31%)	82,113,113	2.61	29 (35%)
12	CLA	G	819	-	69,73,73	2.20	24 (34%)	82,113,113	2.56	30 (36%)
12	CLA	H	825	-	69,73,73	2.18	21 (30%)	82,113,113	2.44	28 (34%)
12	CLA	B	816	-	69,73,73	2.25	24 (34%)	82,113,113	2.35	29 (35%)
12	CLA	b	813	3	59,63,73	2.42	25 (42%)	70,101,113	2.70	26 (37%)
12	CLA	A	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.92	27 (46%)
12	CLA	G	840	1	54,58,73	2.54	22 (40%)	64,95,113	2.70	26 (40%)
15	BCR	L	203	-	41,41,41	2.78	6 (14%)	56,56,56	6.44	21 (37%)
15	BCR	b	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.59	25 (44%)
12	CLA	b	801	-	64,68,73	2.30	22 (34%)	76,107,113	2.58	27 (35%)
15	BCR	H	849	-	41,41,41	2.57	6 (14%)	56,56,56	6.50	20 (35%)
12	CLA	G	814	1	49,53,73	2.52	22 (44%)	58,89,113	3.00	24 (41%)
12	CLA	b	831	3	49,53,73	2.57	22 (44%)	58,89,113	2.85	25 (43%)
15	BCR	I	101	-	41,41,41	2.61	6 (14%)	56,56,56	6.86	21 (37%)
12	CLA	B	827	3	49,53,73	2.58	21 (42%)	58,89,113	2.70	24 (41%)
12	CLA	B	802	-	69,73,73	2.18	22 (31%)	82,113,113	2.71	31 (37%)
12	CLA	a	824	20	69,73,73	2.26	23 (33%)	82,113,113	2.48	32 (39%)
12	CLA	G	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.47	26 (31%)
12	CLA	b	807	-	69,73,73	2.18	22 (31%)	82,113,113	2.52	27 (32%)
15	BCR	a	848	-	41,41,41	2.72	6 (14%)	56,56,56	6.78	21 (37%)
12	CLA	B	825	-	69,73,73	2.27	22 (31%)	82,113,113	2.12	26 (31%)
15	BCR	b	841	-	41,41,41	2.55	6 (14%)	56,56,56	6.66	26 (46%)
15	BCR	i	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	19 (33%)
12	CLA	G	808	1	69,73,73	2.17	22 (31%)	82,113,113	2.60	27 (32%)
12	CLA	b	828	3	49,53,73	2.55	24 (48%)	58,89,113	2.83	26 (44%)
15	BCR	a	846	-	41,41,41	2.68	6 (14%)	56,56,56	6.62	22 (39%)
12	CLA	G	835	1	49,53,73	2.52	23 (46%)	58,89,113	2.84	25 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	819	1	49,53,73	2.55	23 (46%)	58,89,113	2.84	25 (43%)
12	CLA	H	818	-	49,53,73	2.54	22 (44%)	58,89,113	2.84	23 (39%)
14	SF4	c	102	4	0,12,12	-	-	-	-	-
15	BCR	G	850	-	41,41,41	2.65	6 (14%)	56,56,56	6.77	25 (44%)
12	CLA	A	840	1	54,58,73	2.54	21 (38%)	64,95,113	2.66	26 (40%)
15	BCR	b	844	-	41,41,41	2.57	6 (14%)	56,56,56	6.69	22 (39%)
15	BCR	a	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.76	26 (46%)
12	CLA	H	828	3	49,53,73	2.56	21 (42%)	58,89,113	2.87	24 (41%)
12	CLA	H	820	-	49,53,73	2.54	22 (44%)	58,89,113	2.85	25 (43%)
12	CLA	B	821	20	69,73,73	2.19	22 (31%)	82,113,113	2.54	31 (37%)
12	CLA	B	819	-	49,53,73	2.54	22 (44%)	58,89,113	2.84	26 (44%)
12	CLA	B	836	20	69,73,73	2.28	23 (33%)	82,113,113	2.52	29 (35%)
12	CLA	j	104	-	49,53,73	2.60	23 (46%)	58,89,113	2.74	24 (41%)
12	CLA	G	809	1	54,58,73	2.56	23 (42%)	64,95,113	2.87	27 (42%)
12	CLA	G	837	1	69,73,73	2.20	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	A	855	-	69,73,73	2.15	23 (33%)	82,113,113	2.70	30 (36%)
12	CLA	B	808	3	49,53,73	2.56	23 (46%)	58,89,113	2.84	27 (46%)
12	CLA	a	822	-	54,58,73	2.56	23 (42%)	64,95,113	2.77	25 (39%)
12	CLA	a	835	1	49,53,73	2.51	23 (46%)	58,89,113	2.85	24 (41%)
12	CLA	G	829	1	69,73,73	2.28	23 (33%)	82,113,113	2.27	26 (31%)
12	CLA	a	836	1	54,58,73	2.64	24 (44%)	64,95,113	2.95	31 (48%)
12	CLA	A	827	1	64,68,73	2.28	21 (32%)	76,107,113	2.59	29 (38%)
12	CLA	B	838	-	69,73,73	2.22	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	G	842	16	64,68,73	2.29	22 (34%)	76,107,113	2.55	26 (34%)
13	1L3	G	843	-	34,34,34	2.68	15 (44%)	43,45,45	1.48	10 (23%)
12	CLA	H	839	-	69,73,73	2.21	23 (33%)	82,113,113	2.59	31 (37%)
12	CLA	H	830	3	69,73,73	2.22	23 (33%)	82,113,113	2.59	25 (30%)
12	CLA	A	835	-	49,53,73	2.53	21 (42%)	58,89,113	2.85	25 (43%)
15	BCR	a	852	-	41,41,41	2.71	6 (14%)	56,56,56	6.46	20 (35%)
15	BCR	b	842	-	25,25,41	2.19	2 (8%)	33,33,56	7.60	18 (54%)
12	CLA	a	841	20	69,73,73	2.18	21 (30%)	82,113,113	2.42	28 (34%)
15	BCR	P	202	-	41,41,41	2.72	6 (14%)	56,56,56	6.71	23 (41%)
15	BCR	B	842	-	41,41,41	2.58	6 (14%)	56,56,56	6.62	21 (37%)
12	CLA	G	828	-	64,68,73	2.30	21 (32%)	76,107,113	2.59	28 (36%)
16	LHG	G	854	-	48,48,48	0.94	2 (4%)	51,54,54	3.78	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	804	-	69,73,73	2.17	21 (30%)	82,113,113	2.60	26 (31%)
12	CLA	S	204	20	69,73,73	2.23	21 (30%)	82,113,113	2.46	25 (30%)
12	CLA	S	202	10	59,63,73	2.41	21 (35%)	70,101,113	2.63	27 (38%)
15	BCR	G	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.69	22 (39%)
18	LMG	b	845	-	55,55,55	1.49	8 (14%)	63,63,63	1.11	3 (4%)
15	BCR	S	205	-	41,41,41	2.67	6 (14%)	56,56,56	6.46	25 (44%)
12	CLA	l	206	20	69,73,73	2.23	21 (30%)	82,113,113	2.46	24 (29%)
15	BCR	H	846	-	41,41,41	2.59	6 (14%)	56,56,56	6.68	19 (33%)
15	BCR	A	845	-	41,41,41	2.62	6 (14%)	56,56,56	6.64	22 (39%)
12	CLA	B	810	3	69,73,73	2.21	22 (31%)	82,113,113	2.71	29 (35%)
12	CLA	A	829	1	69,73,73	2.19	22 (31%)	82,113,113	2.37	28 (34%)
12	CLA	b	802	-	69,73,73	2.15	21 (30%)	82,113,113	2.85	33 (40%)
15	BCR	A	852	-	41,41,41	2.70	6 (14%)	56,56,56	6.43	20 (35%)
15	BCR	A	849	-	41,41,41	2.63	6 (14%)	56,56,56	6.81	25 (44%)
12	CLA	a	837	1	69,73,73	2.21	23 (33%)	82,113,113	2.61	30 (36%)
12	CLA	A	805	-	69,73,73	2.19	23 (33%)	82,113,113	2.64	28 (34%)
15	BCR	H	845	-	41,41,41	2.64	6 (14%)	56,56,56	6.83	25 (44%)
12	CLA	a	819	1	49,53,73	2.49	22 (44%)	58,89,113	2.86	26 (44%)
12	CLA	H	835	3	69,73,73	2.19	22 (31%)	82,113,113	2.43	26 (31%)
12	CLA	a	803	1	69,73,73	2.25	23 (33%)	82,113,113	2.53	32 (39%)
16	LHG	a	850	-	48,48,48	0.92	2 (4%)	51,54,54	0.93	2 (3%)
12	CLA	H	806	-	69,73,73	2.20	21 (30%)	82,113,113	2.72	28 (34%)
12	CLA	b	803	-	69,73,73	2.27	22 (31%)	82,113,113	2.56	27 (32%)
15	BCR	L	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.55	26 (46%)
15	BCR	G	848	-	41,41,41	2.65	6 (14%)	56,56,56	6.74	25 (44%)
12	CLA	G	813	1	54,58,73	2.51	23 (42%)	64,95,113	2.91	28 (43%)
12	CLA	H	815	3	59,63,73	2.39	21 (35%)	70,101,113	2.69	28 (40%)
12	CLA	b	819	-	49,53,73	2.55	22 (44%)	58,89,113	2.81	23 (39%)
12	CLA	H	809	3	49,53,73	2.55	22 (44%)	58,89,113	2.83	27 (46%)
12	CLA	a	817	-	59,63,73	2.45	25 (42%)	70,101,113	2.75	28 (40%)
12	CLA	b	808	3	49,53,73	2.53	22 (44%)	58,89,113	2.87	28 (48%)
12	CLA	l	202	3	69,73,73	2.26	23 (33%)	82,113,113	2.41	25 (30%)
12	CLA	F	203	-	49,53,73	2.57	23 (46%)	58,89,113	4.48	26 (44%)
12	CLA	H	838	-	69,73,73	2.23	22 (31%)	82,113,113	2.65	32 (39%)
12	CLA	H	811	3	69,73,73	2.19	22 (31%)	82,113,113	2.61	32 (39%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	f	201	20	69,73,73	2.27	22 (31%)	82,113,113	2.29	26 (31%)
12	CLA	b	814	3	59,63,73	2.39	21 (35%)	70,101,113	2.61	26 (37%)
16	LHG	A	850	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
12	CLA	a	814	-	49,53,73	2.53	21 (42%)	58,89,113	2.82	24 (41%)
12	CLA	H	822	20	69,73,73	2.22	21 (30%)	82,113,113	2.41	30 (36%)
15	BCR	G	845	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	21 (37%)
12	CLA	A	812	-	54,58,73	2.53	24 (44%)	64,95,113	2.90	28 (43%)
15	BCR	B	845	-	41,41,41	2.58	6 (14%)	56,56,56	6.68	18 (32%)
12	CLA	H	826	-	69,73,73	2.29	22 (31%)	82,113,113	2.09	26 (31%)
12	CLA	G	824	-	59,63,73	2.39	23 (38%)	70,101,113	2.65	25 (35%)
12	CLA	B	835	3	49,53,73	2.49	21 (42%)	58,89,113	2.93	25 (43%)
12	CLA	a	805	1	69,73,73	2.19	23 (33%)	82,113,113	2.55	27 (32%)
15	BCR	a	844	-	41,41,41	2.61	6 (14%)	56,56,56	6.65	21 (37%)
12	CLA	B	829	3	69,73,73	2.26	25 (36%)	82,113,113	2.54	26 (31%)
12	CLA	b	835	20	69,73,73	2.28	23 (33%)	82,113,113	2.49	29 (35%)
13	1L3	B	839	-	34,34,34	2.67	12 (35%)	43,45,45	1.54	9 (20%)
11	CL0	a	801	1	58,73,73	3.01	21 (36%)	60,113,113	3.02	23 (38%)
12	CLA	H	813	-	49,53,73	2.48	22 (44%)	58,89,113	3.02	26 (44%)
12	CLA	B	834	3	69,73,73	2.19	22 (31%)	82,113,113	2.48	28 (34%)
12	CLA	G	803	20	69,73,73	2.24	20 (28%)	82,113,113	2.23	26 (31%)
12	CLA	A	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.46	29 (35%)
12	CLA	L	205	10	69,73,73	2.20	21 (30%)	82,113,113	2.61	27 (32%)
15	BCR	i	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.97	21 (37%)
12	CLA	G	818	-	59,63,73	2.50	23 (38%)	70,101,113	2.72	33 (47%)
12	CLA	A	813	-	49,53,73	2.60	22 (44%)	58,89,113	2.96	26 (44%)
12	CLA	G	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.90	26 (44%)
12	CLA	a	826	1	69,73,73	2.23	23 (33%)	82,113,113	2.57	28 (34%)
12	CLA	b	832	3	64,68,73	2.31	22 (34%)	76,107,113	2.58	28 (36%)
12	CLA	a	827	-	64,68,73	2.29	21 (32%)	76,107,113	2.61	28 (36%)
13	1L3	H	840	-	34,34,34	2.70	13 (38%)	43,45,45	1.46	8 (18%)
12	CLA	a	834	-	69,73,73	2.23	22 (31%)	82,113,113	2.39	29 (35%)
12	CLA	B	820	3	49,53,73	2.53	22 (44%)	58,89,113	2.79	25 (43%)
12	CLA	b	820	-	49,53,73	2.51	22 (44%)	58,89,113	2.83	23 (39%)
15	BCR	J	102	-	41,41,41	2.65	6 (14%)	56,56,56	6.86	19 (33%)
12	CLA	H	807	3	69,73,73	2.23	22 (31%)	82,113,113	2.45	30 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	808	1	54,58,73	2.56	22 (40%)	64,95,113	2.82	27 (42%)
15	BCR	A	847	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	27 (48%)
12	CLA	A	836	1	54,58,73	2.63	23 (42%)	64,95,113	3.26	32 (50%)
12	CLA	a	833	-	69,73,73	2.21	22 (31%)	82,113,113	2.49	28 (34%)
12	CLA	H	827	3	69,73,73	2.31	22 (31%)	82,113,113	2.74	34 (41%)
12	CLA	H	829	3	49,53,73	2.55	23 (46%)	58,89,113	2.79	26 (44%)
12	CLA	a	831	1	59,63,73	2.44	23 (38%)	70,101,113	2.59	27 (38%)
12	CLA	b	830	-	49,53,73	2.54	21 (42%)	58,89,113	2.71	24 (41%)
12	CLA	A	823	-	59,63,73	2.38	22 (37%)	70,101,113	2.68	25 (35%)
14	SF4	C	102	4	0,12,12	-	-	-	-	-
12	CLA	l	205	10	69,73,73	2.19	21 (30%)	82,113,113	2.63	27 (32%)
12	CLA	A	828	-	69,73,73	2.28	22 (31%)	82,113,113	2.28	27 (32%)
15	BCR	S	201	-	41,41,41	2.80	6 (14%)	56,56,56	6.51	23 (41%)
12	CLA	b	833	3	69,73,73	2.21	23 (33%)	82,113,113	2.48	30 (36%)
12	CLA	a	828	-	69,73,73	2.23	21 (30%)	82,113,113	2.31	30 (36%)
12	CLA	B	806	3	69,73,73	2.19	21 (30%)	82,113,113	2.75	29 (35%)
12	CLA	G	827	-	69,73,73	2.23	23 (33%)	82,113,113	2.54	31 (37%)
12	CLA	b	818	-	49,53,73	2.57	23 (46%)	58,89,113	2.85	24 (41%)
12	CLA	B	813	3	59,63,73	2.43	24 (40%)	70,101,113	2.67	25 (35%)
12	CLA	G	831	1	54,58,73	2.54	22 (40%)	64,95,113	2.70	30 (46%)
12	CLA	H	821	-	49,53,73	2.50	21 (42%)	58,89,113	2.83	26 (44%)
12	CLA	H	810	3	49,53,73	2.57	22 (44%)	58,89,113	2.82	24 (41%)
15	BCR	J	104	-	41,41,41	2.54	6 (14%)	56,56,56	6.56	23 (41%)
11	CL0	A	801	1	58,73,73	3.04	19 (32%)	60,113,113	2.88	21 (35%)
12	CLA	G	825	20	69,73,73	2.28	23 (33%)	82,113,113	2.37	30 (36%)
12	CLA	a	830	1	54,58,73	2.54	22 (40%)	64,95,113	2.77	29 (45%)
12	CLA	a	832	1	69,73,73	2.25	22 (31%)	82,113,113	2.33	26 (31%)
12	CLA	B	812	-	49,53,73	2.55	24 (48%)	58,89,113	2.84	24 (41%)
15	BCR	b	839	-	41,41,41	2.68	6 (14%)	56,56,56	6.58	20 (35%)
12	CLA	b	848	16	64,68,73	2.29	21 (32%)	76,107,113	2.57	25 (32%)
12	CLA	b	829	3	69,73,73	2.26	23 (33%)	82,113,113	2.57	27 (32%)
12	CLA	B	801	-	64,68,73	2.30	21 (32%)	76,107,113	2.60	27 (35%)
12	CLA	A	821	1	49,53,73	2.55	23 (46%)	58,89,113	2.91	23 (39%)
12	CLA	G	816	-	49,53,73	2.55	23 (46%)	58,89,113	2.85	25 (43%)
15	BCR	G	849	-	41,41,41	2.75	6 (14%)	56,56,56	6.76	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	856	-	69,73,73	2.18	23 (33%)	82,113,113	2.55	28 (34%)
12	CLA	b	809	3	49,53,73	2.57	22 (44%)	58,89,113	2.82	25 (43%)
12	CLA	b	806	-	69,73,73	2.19	21 (30%)	82,113,113	2.75	29 (35%)
13	1L3	A	842	-	34,34,34	2.63	14 (41%)	43,45,45	1.50	11 (25%)
14	SF4	a	843	1,3	0,12,12	-	-	-		
12	CLA	A	841	20	69,73,73	2.21	21 (30%)	82,113,113	2.41	27 (32%)
12	CLA	B	826	3	69,73,73	2.33	22 (31%)	82,113,113	2.57	31 (37%)
15	BCR	l	203	-	41,41,41	2.79	6 (14%)	56,56,56	6.50	22 (39%)
12	CLA	b	816	-	69,73,73	2.23	24 (34%)	82,113,113	2.33	28 (34%)
12	CLA	G	817	1	54,58,73	2.51	23 (42%)	64,95,113	2.79	32 (50%)
12	CLA	H	836	3	49,53,73	2.49	22 (44%)	58,89,113	2.95	23 (39%)
12	CLA	B	823	3	69,73,73	2.22	21 (30%)	82,113,113	2.50	32 (39%)
13	1L3	b	838	-	34,34,34	2.67	12 (35%)	43,45,45	1.51	8 (18%)
12	CLA	B	828	3	49,53,73	2.55	23 (46%)	58,89,113	2.81	26 (44%)
15	BCR	B	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.68	20 (35%)
12	CLA	b	815	-	64,68,73	2.25	22 (34%)	76,107,113	2.73	27 (35%)
12	CLA	P	201	20	69,73,73	2.27	21 (30%)	82,113,113	2.34	25 (30%)
18	LMG	H	847	-	55,55,55	1.49	8 (14%)	63,63,63	1.10	4 (6%)
12	CLA	A	817	-	59,63,73	2.52	22 (37%)	70,101,113	2.66	32 (45%)
12	CLA	G	815	-	49,53,73	2.53	22 (44%)	58,89,113	2.85	25 (43%)
12	CLA	H	816	-	64,68,73	2.36	22 (34%)	76,107,113	2.90	28 (36%)
12	CLA	H	812	3	64,68,73	2.33	24 (37%)	76,107,113	2.57	26 (34%)
16	LHG	a	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.09	3 (5%)
12	CLA	G	804	1	69,73,73	2.25	23 (33%)	82,113,113	2.50	29 (35%)
15	BCR	A	848	-	41,41,41	2.71	6 (14%)	56,56,56	6.77	20 (35%)
15	BCR	f	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.44	22 (39%)
12	CLA	G	820	1	49,53,73	2.51	22 (44%)	58,89,113	2.83	26 (44%)
15	BCR	f	202	-	41,41,41	2.80	6 (14%)	56,56,56	6.66	24 (42%)
12	CLA	G	811	1,12	54,58,73	2.49	24 (44%)	64,95,113	2.97	28 (43%)
12	CLA	G	821	-	69,73,73	2.26	23 (33%)	82,113,113	2.41	30 (36%)
12	CLA	b	825	-	69,73,73	2.29	22 (31%)	82,113,113	2.17	25 (30%)
15	BCR	B	841	-	41,41,41	2.61	6 (14%)	56,56,56	6.61	25 (44%)
12	CLA	H	817	-	69,73,73	2.26	24 (34%)	82,113,113	2.33	27 (32%)
12	CLA	A	803	1	69,73,73	2.26	23 (33%)	82,113,113	2.53	30 (36%)
12	CLA	G	826	20	59,63,73	2.41	21 (35%)	70,101,113	2.68	32 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	808	3	69,73,73	2.26	21 (30%)	82,113,113	2.41	27 (32%)
12	CLA	A	820	-	69,73,73	2.23	21 (30%)	82,113,113	2.66	30 (36%)
12	CLA	G	834	-	69,73,73	2.23	22 (31%)	82,113,113	2.45	28 (34%)
14	SF4	K	101	4	0,12,12	-	-	-	-	-
12	CLA	H	814	3	59,63,73	2.42	24 (40%)	70,101,113	2.64	24 (34%)
12	CLA	a	829	1	69,73,73	2.19	22 (31%)	82,113,113	2.38	26 (31%)
12	CLA	B	837	3	69,73,73	2.20	21 (30%)	82,113,113	2.68	31 (37%)
16	LHG	a	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.25	3 (10%)
12	CLA	b	805	3	69,73,73	2.21	22 (31%)	82,113,113	2.57	29 (35%)
12	CLA	A	834	-	69,73,73	2.24	23 (33%)	82,113,113	2.43	27 (32%)
15	BCR	B	844	-	41,41,41	2.64	6 (14%)	56,56,56	6.82	25 (44%)
12	CLA	G	812	-	49,53,73	2.54	22 (44%)	58,89,113	2.75	22 (37%)
12	CLA	a	838	1	49,53,73	2.55	22 (44%)	58,89,113	2.89	27 (46%)
12	CLA	H	803	-	69,73,73	2.26	22 (31%)	82,113,113	2.53	26 (31%)
12	CLA	H	805	3	69,73,73	2.24	24 (34%)	82,113,113	2.59	29 (35%)
12	CLA	A	804	12	59,63,73	2.42	23 (38%)	70,101,113	2.81	30 (42%)
12	CLA	A	810	1,12	54,58,73	2.48	23 (42%)	64,95,113	2.93	27 (42%)
12	CLA	b	826	3	69,73,73	2.36	21 (30%)	82,113,113	2.55	30 (36%)
12	CLA	B	824	-	69,73,73	2.18	21 (30%)	82,113,113	2.41	29 (35%)
12	CLA	b	823	3	69,73,73	2.22	21 (30%)	82,113,113	2.49	30 (36%)
12	CLA	H	834	20	64,68,73	2.30	22 (34%)	76,107,113	2.56	25 (32%)
14	SF4	C	101	4	0,12,12	-	-	-	-	-
15	BCR	L	207	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	18 (32%)
12	CLA	A	832	1	69,73,73	2.25	22 (31%)	82,113,113	2.35	25 (30%)
16	LHG	G	852	12	26,26,48	1.24	2 (7%)	29,32,54	1.25	4 (13%)
12	CLA	B	809	3	49,53,73	2.57	22 (44%)	58,89,113	2.81	25 (43%)
12	CLA	G	806	-	69,73,73	2.17	21 (30%)	82,113,113	2.61	26 (31%)
12	CLA	G	805	1,12	59,63,73	2.40	24 (40%)	70,101,113	2.80	31 (44%)
12	CLA	G	832	1	69,73,73	2.26	24 (34%)	82,113,113	2.33	27 (32%)
15	BCR	G	853	-	41,41,41	2.71	6 (14%)	56,56,56	6.40	20 (35%)
12	CLA	H	831	-	69,73,73	2.22	20 (28%)	82,113,113	2.48	28 (34%)
14	SF4	c	101	4	0,12,12	-	-	-	-	-
12	CLA	l	204	10	59,63,73	2.41	21 (35%)	70,101,113	2.65	25 (35%)
17	45D	M	101	-	43,43,43	3.99	19 (44%)	54,60,60	7.88	31 (57%)
15	BCR	P	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.51	23 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	825	20	59,63,73	2.42	23 (38%)	70,101,113	2.68	28 (40%)
12	CLA	H	801	1	59,63,73	2.43	24 (40%)	70,101,113	2.61	28 (40%)
15	BCR	G	847	-	41,41,41	2.70	6 (14%)	56,56,56	6.50	21 (37%)
12	CLA	b	827	3	49,53,73	2.58	22 (44%)	58,89,113	2.79	24 (41%)
12	CLA	a	813	-	49,53,73	2.52	23 (46%)	58,89,113	2.83	26 (44%)
15	BCR	H	841	-	41,41,41	2.62	6 (14%)	56,56,56	6.61	20 (35%)
12	CLA	A	830	1	54,58,73	2.52	22 (40%)	64,95,113	2.83	30 (46%)
12	CLA	G	823	1	54,58,73	2.56	24 (44%)	64,95,113	2.76	24 (37%)
12	CLA	H	833	-	49,53,73	2.57	22 (44%)	58,89,113	2.82	24 (41%)
12	CLA	A	854	20	69,73,73	2.31	24 (34%)	82,113,113	2.57	33 (40%)
12	CLA	G	822	1	49,53,73	2.56	23 (46%)	58,89,113	2.90	24 (41%)
15	BCR	H	843	-	41,41,41	2.57	6 (14%)	56,56,56	6.64	24 (42%)
12	CLA	A	833	-	69,73,73	2.20	22 (31%)	82,113,113	2.49	28 (34%)
12	CLA	a	821	-	49,53,73	2.55	23 (46%)	58,89,113	2.91	24 (41%)
17	45D	T	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.84	31 (57%)
12	CLA	H	837	20	69,73,73	2.29	23 (33%)	82,113,113	2.54	26 (31%)
12	CLA	A	818	-	69,73,73	2.19	23 (33%)	82,113,113	2.60	27 (32%)
15	BCR	b	847	-	41,41,41	2.63	6 (14%)	56,56,56	6.61	22 (39%)
12	CLA	a	823	-	59,63,73	2.38	22 (37%)	70,101,113	2.70	26 (37%)
12	CLA	A	826	1	69,73,73	2.23	21 (30%)	82,113,113	2.57	29 (35%)
12	CLA	b	836	-	69,73,73	2.23	22 (31%)	82,113,113	2.67	32 (39%)
11	CL0	G	801	1	58,73,73	3.04	19 (32%)	60,113,113	2.87	20 (33%)
12	CLA	B	833	3	64,68,73	2.28	22 (34%)	76,107,113	2.68	26 (34%)
12	CLA	J	103	-	49,53,73	2.58	24 (48%)	58,89,113	2.78	23 (39%)
15	BCR	j	101	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	21 (37%)
12	CLA	G	836	1	54,58,73	2.61	24 (44%)	64,95,113	2.89	27 (42%)
12	CLA	A	814	-	49,53,73	2.54	22 (44%)	58,89,113	2.78	25 (43%)
12	CLA	b	821	20	69,73,73	2.18	22 (31%)	82,113,113	2.53	33 (40%)
15	BCR	J	101	-	41,41,41	2.71	6 (14%)	56,56,56	6.56	22 (39%)
12	CLA	a	854	20	69,73,73	2.26	24 (34%)	82,113,113	2.55	30 (36%)
15	BCR	l	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.52	24 (42%)
12	CLA	a	804	12	59,63,73	2.41	23 (38%)	70,101,113	2.80	30 (42%)
12	CLA	L	206	20	69,73,73	2.23	21 (30%)	82,113,113	2.44	24 (29%)
12	CLA	b	810	3	69,73,73	2.20	21 (30%)	82,113,113	2.71	32 (39%)
15	BCR	A	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	LHG	A	853	-	48,48,48	0.93	2 (4%)	51,54,54	3.77	6 (11%)
15	BCR	A	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.91	19 (33%)
12	CLA	A	811	-	49,53,73	2.56	22 (44%)	58,89,113	2.71	22 (37%)
12	CLA	P	203	-	49,53,73	2.55	22 (44%)	58,89,113	4.47	25 (43%)
12	CLA	a	820	-	69,73,73	2.27	23 (33%)	82,113,113	2.37	26 (31%)
15	BCR	a	849	-	41,41,41	2.64	6 (14%)	56,56,56	6.77	26 (46%)
15	BCR	B	843	-	25,25,41	2.18	2 (8%)	33,33,56	7.57	17 (51%)
12	CLA	H	824	3	69,73,73	2.23	21 (30%)	82,113,113	2.51	32 (39%)
12	CLA	A	822	-	54,58,73	2.57	23 (42%)	64,95,113	2.72	27 (42%)
12	CLA	B	832	3	49,53,73	2.56	22 (44%)	58,89,113	2.82	25 (43%)
12	CLA	b	804	-	69,73,73	2.18	21 (30%)	82,113,113	2.63	26 (31%)
12	CLA	A	831	1	59,63,73	2.42	23 (38%)	70,101,113	2.62	29 (41%)
15	BCR	H	842	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	25 (44%)
12	CLA	A	802	20	69,73,73	2.23	21 (30%)	82,113,113	2.26	26 (31%)
12	CLA	A	815	-	49,53,73	2.52	23 (46%)	58,89,113	2.90	25 (43%)
12	CLA	a	840	1	54,58,73	2.54	22 (40%)	64,95,113	2.72	27 (42%)
12	CLA	H	804	-	69,73,73	2.18	21 (30%)	82,113,113	2.65	25 (30%)
18	LMG	B	846	-	55,55,55	1.48	8 (14%)	63,63,63	1.12	3 (4%)
12	CLA	j	102	-	69,73,73	2.23	22 (31%)	82,113,113	2.34	29 (35%)
13	1L3	a	842	-	34,34,34	2.65	14 (41%)	43,45,45	1.51	11 (25%)
14	SF4	G	844	1,3	0,12,12	-	-	-	-	-
12	CLA	b	834	3	49,53,73	2.50	22 (44%)	58,89,113	2.95	23 (39%)
12	CLA	a	812	-	54,58,73	2.53	23 (42%)	64,95,113	2.87	29 (45%)
12	CLA	H	823	20	69,73,73	2.25	23 (33%)	82,113,113	2.47	27 (32%)
12	CLA	a	818	-	69,73,73	2.22	24 (34%)	82,113,113	2.54	28 (34%)
12	CLA	G	802	-	64,68,73	2.33	22 (34%)	76,107,113	2.64	30 (39%)
12	CLA	B	814	-	59,63,73	2.36	22 (37%)	70,101,113	2.64	25 (35%)
12	CLA	a	816	1	54,58,73	2.52	20 (37%)	64,95,113	2.72	31 (48%)
12	CLA	b	812	-	49,53,73	2.54	21 (42%)	58,89,113	3.01	25 (43%)
12	CLA	B	830	-	69,73,73	2.23	22 (31%)	82,113,113	2.36	27 (32%)
12	CLA	G	807	1	69,73,73	2.16	22 (31%)	82,113,113	2.63	24 (29%)
17	45D	m	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.90	31 (57%)
12	CLA	A	807	1	69,73,73	2.20	21 (30%)	82,113,113	2.63	28 (34%)
12	CLA	b	817	3	49,53,73	2.53	21 (42%)	58,89,113	2.85	24 (41%)
12	CLA	B	811	-	64,68,73	2.32	23 (35%)	76,107,113	2.55	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	824	20	69,73,73	2.26	23 (33%)	82,113,113	2.39	26 (31%)
12	CLA	a	802	20	69,73,73	2.23	20 (28%)	82,113,113	2.26	27 (32%)
12	CLA	a	855	-	69,73,73	2.15	22 (31%)	82,113,113	2.72	29 (35%)
12	CLA	H	850	16	64,68,73	2.30	22 (34%)	76,107,113	2.53	28 (36%)
15	BCR	H	844	-	25,25,41	2.21	2 (8%)	33,33,56	7.59	18 (54%)
12	CLA	a	839	1	69,73,73	2.27	24 (34%)	82,113,113	2.49	24 (29%)
12	CLA	B	818	-	49,53,73	2.57	23 (46%)	58,89,113	2.87	23 (39%)
12	CLA	B	822	20	69,73,73	2.26	23 (33%)	82,113,113	2.44	27 (32%)
12	CLA	a	806	-	69,73,73	2.16	20 (28%)	82,113,113	2.63	27 (32%)
16	LHG	G	851	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
19	LMT	H	848	-	36,36,36	1.18	4 (11%)	47,47,47	0.96	1 (2%)
12	CLA	A	816	1	54,58,73	2.51	22 (40%)	64,95,113	2.78	30 (46%)
12	CLA	A	809	1	49,53,73	2.57	22 (44%)	58,89,113	2.88	25 (43%)
12	CLA	A	837	1	69,73,73	2.21	23 (33%)	82,113,113	2.58	30 (36%)
12	CLA	S	203	10	69,73,73	2.20	21 (30%)	82,113,113	2.60	27 (32%)
12	CLA	L	202	3	69,73,73	2.25	21 (30%)	82,113,113	2.40	27 (32%)
16	LHG	A	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.24	3 (10%)
15	BCR	Q	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	17 (30%)
12	CLA	G	855	20	69,73,73	2.27	23 (33%)	82,113,113	2.57	28 (34%)
12	CLA	G	810	1	49,53,73	2.54	22 (44%)	58,89,113	2.86	25 (43%)
12	CLA	F	201	20	69,73,73	2.27	23 (33%)	82,113,113	2.30	27 (32%)
12	CLA	a	815	-	49,53,73	2.56	22 (44%)	58,89,113	2.82	23 (39%)
15	BCR	b	843	-	41,41,41	2.63	6 (14%)	56,56,56	6.84	24 (42%)
12	CLA	R	103	-	49,53,73	2.58	23 (46%)	58,89,113	2.78	23 (39%)
14	SF4	A	843	1,3	0,12,12	-	-	-	-	-
12	CLA	L	204	10	59,63,73	2.41	21 (35%)	70,101,113	2.68	24 (34%)
15	BCR	R	102	-	41,41,41	2.63	6 (14%)	56,56,56	6.83	17 (30%)
12	CLA	G	841	20	69,73,73	2.20	21 (30%)	82,113,113	2.39	26 (31%)
14	SF4	K	102	4	0,12,12	-	-	-	-	-
12	CLA	B	831	-	49,53,73	2.59	22 (44%)	58,89,113	2.71	24 (41%)
12	CLA	G	830	-	69,73,73	2.23	22 (31%)	82,113,113	2.40	25 (30%)
12	CLA	a	810	1,12	54,58,73	2.49	23 (42%)	64,95,113	2.88	28 (43%)
12	CLA	A	825	20	59,63,73	2.40	23 (38%)	70,101,113	2.68	28 (40%)
15	BCR	F	204	-	41,41,41	2.63	6 (14%)	56,56,56	6.47	22 (39%)
12	CLA	B	815	-	64,68,73	2.30	24 (37%)	76,107,113	2.67	26 (34%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	833	1	69,73,73	2.22	21 (30%)	82,113,113	2.42	27 (32%)
12	CLA	B	807	3	69,73,73	2.19	21 (30%)	82,113,113	2.44	30 (36%)
15	BCR	a	845	-	41,41,41	2.65	6 (14%)	56,56,56	6.65	23 (41%)
19	LMT	B	847	-	36,36,36	1.26	5 (13%)	47,47,47	1.11	3 (6%)
12	CLA	a	811	-	49,53,73	2.56	22 (44%)	58,89,113	2.74	23 (39%)
12	CLA	a	809	1	49,53,73	2.49	21 (42%)	58,89,113	2.89	25 (43%)
12	CLA	B	803	-	69,73,73	2.23	24 (34%)	82,113,113	2.68	28 (34%)
12	CLA	B	805	3	69,73,73	2.22	23 (33%)	82,113,113	2.56	28 (34%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	j	103	-	-	17/29/63/63	0/2/2/2
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	A	808	1	1/1/12/20	7/21/97/115	-
15	BCR	R	101	-	-	11/29/63/63	0/2/2/2
12	CLA	B	817	3	1/1/11/20	10/15/91/115	-
15	BCR	Q	101	-	-	8/29/63/63	0/2/2/2
12	CLA	A	806	1	1/1/15/20	13/39/115/115	-
12	CLA	b	811	-	1/1/14/20	10/33/109/115	-
12	CLA	f	203	-	1/1/11/20	8/15/91/115	-
12	CLA	b	822	20	1/1/15/20	16/39/115/115	-
12	CLA	H	819	-	1/1/11/20	3/15/91/115	-
12	CLA	H	802	-	1/1/15/20	13/39/115/115	-
12	CLA	H	832	-	1/1/11/20	6/15/91/115	-
12	CLA	b	824	3	1/1/15/20	22/39/115/115	-
12	CLA	b	837	-	1/1/15/20	14/39/115/115	-
19	LMT	b	846	-	-	10/21/61/61	0/2/2/2
12	CLA	a	807	-	1/1/15/20	22/39/115/115	-
12	CLA	G	819	-	1/1/15/20	15/39/115/115	-
12	CLA	H	825	-	1/1/15/20	22/39/115/115	-
12	CLA	B	816	-	1/1/15/20	15/39/115/115	-
12	CLA	b	813	3	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	838	1	1/1/11/20	3/15/91/115	-
12	CLA	G	840	1	1/1/12/20	7/21/97/115	-
15	BCR	L	203	-	-	14/29/63/63	0/2/2/2
15	BCR	b	840	-	-	8/29/63/63	0/2/2/2
12	CLA	b	801	-	1/1/14/20	7/33/109/115	-
15	BCR	H	849	-	-	8/29/63/63	0/2/2/2
12	CLA	G	814	1	1/1/11/20	4/15/91/115	-
12	CLA	b	831	3	1/1/11/20	5/15/91/115	-
15	BCR	I	101	-	-	8/29/63/63	0/2/2/2
12	CLA	B	827	3	1/1/11/20	6/15/91/115	-
12	CLA	B	802	-	1/1/15/20	15/39/115/115	-
12	CLA	a	824	20	1/1/15/20	16/39/115/115	-
12	CLA	G	839	1	1/1/15/20	7/39/115/115	-
12	CLA	b	807	-	1/1/15/20	10/39/115/115	-
15	BCR	a	848	-	-	12/29/63/63	0/2/2/2
12	CLA	B	825	-	1/1/15/20	11/39/115/115	-
15	BCR	b	841	-	-	9/29/63/63	0/2/2/2
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
12	CLA	G	808	1	1/1/15/20	21/39/115/115	-
12	CLA	b	828	3	1/1/11/20	4/15/91/115	-
15	BCR	a	846	-	-	8/29/63/63	0/2/2/2
12	CLA	G	835	1	1/1/11/20	9/15/91/115	-
12	CLA	A	819	1	1/1/11/20	9/15/91/115	-
12	CLA	H	818	-	1/1/11/20	10/15/91/115	-
14	SF4	c	102	4	-	-	0/6/5/5
15	BCR	G	850	-	-	12/29/63/63	0/2/2/2
12	CLA	A	840	1	1/1/12/20	9/21/97/115	-
15	BCR	b	844	-	-	6/29/63/63	0/2/2/2
15	BCR	a	847	-	-	4/29/63/63	0/2/2/2
12	CLA	H	828	3	1/1/11/20	5/15/91/115	-
12	CLA	H	820	-	1/1/11/20	7/15/91/115	-
12	CLA	B	821	20	1/1/15/20	17/39/115/115	-
12	CLA	B	819	-	1/1/11/20	7/15/91/115	-
12	CLA	B	836	20	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	j	104	-	1/1/11/20	7/15/91/115	-
12	CLA	G	809	1	1/1/12/20	7/21/97/115	-
12	CLA	G	837	1	1/1/15/20	14/39/115/115	-
12	CLA	A	855	-	1/1/15/20	11/39/115/115	-
12	CLA	B	808	3	1/1/11/20	3/15/91/115	-
12	CLA	a	822	-	1/1/12/20	6/21/97/115	-
12	CLA	a	835	1	1/1/11/20	7/15/91/115	-
12	CLA	G	829	1	1/1/15/20	14/39/115/115	-
12	CLA	a	836	1	1/1/12/20	5/21/97/115	-
12	CLA	A	827	1	1/1/14/20	14/33/109/115	-
12	CLA	B	838	-	1/1/15/20	19/39/115/115	-
12	CLA	G	842	16	1/1/14/20	13/33/109/115	-
13	1L3	G	843	-	-	5/23/43/43	0/2/2/2
12	CLA	H	839	-	1/1/15/20	14/39/115/115	-
12	CLA	H	830	3	1/1/15/20	18/39/115/115	-
12	CLA	A	835	-	1/1/11/20	9/15/91/115	-
15	BCR	a	852	-	-	13/29/63/63	0/2/2/2
15	BCR	b	842	-	-	3/18/35/63	0/1/1/2
12	CLA	a	841	20	1/1/15/20	15/39/115/115	-
15	BCR	P	202	-	-	13/29/63/63	0/2/2/2
15	BCR	B	842	-	-	9/29/63/63	0/2/2/2
12	CLA	G	828	-	1/1/14/20	13/33/109/115	-
16	LHG	G	854	-	-	37/53/53/53	-
12	CLA	B	804	-	1/1/15/20	18/39/115/115	-
12	CLA	S	204	20	1/1/15/20	10/39/115/115	-
12	CLA	S	202	10	1/1/13/20	9/27/103/115	-
15	BCR	G	846	-	-	3/29/63/63	0/2/2/2
18	LMG	b	845	-	-	18/50/70/70	0/1/1/1
15	BCR	S	205	-	-	9/29/63/63	0/2/2/2
12	CLA	l	206	20	1/1/15/20	11/39/115/115	-
15	BCR	H	846	-	-	9/29/63/63	0/2/2/2
15	BCR	A	845	-	-	7/29/63/63	0/2/2/2
12	CLA	B	810	3	1/1/15/20	27/39/115/115	-
12	CLA	A	829	1	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	802	-	1/1/15/20	13/39/115/115	-
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
15	BCR	A	849	-	-	12/29/63/63	0/2/2/2
12	CLA	a	837	1	1/1/15/20	14/39/115/115	-
12	CLA	A	805	-	1/1/15/20	12/39/115/115	-
15	BCR	H	845	-	-	9/29/63/63	0/2/2/2
12	CLA	a	819	1	1/1/11/20	8/15/91/115	-
12	CLA	H	835	3	1/1/15/20	12/39/115/115	-
12	CLA	a	803	1	1/1/15/20	14/39/115/115	-
16	LHG	a	850	-	-	26/53/53/53	-
12	CLA	H	806	-	1/1/15/20	13/39/115/115	-
12	CLA	b	803	-	1/1/15/20	16/39/115/115	-
15	BCR	L	201	-	-	8/29/63/63	0/2/2/2
15	BCR	G	848	-	-	4/29/63/63	0/2/2/2
12	CLA	G	813	1	1/1/12/20	10/21/97/115	-
12	CLA	H	815	3	1/1/13/20	8/27/103/115	-
12	CLA	b	819	-	1/1/11/20	7/15/91/115	-
12	CLA	H	809	3	1/1/11/20	3/15/91/115	-
12	CLA	a	817	-	1/1/13/20	15/27/103/115	-
12	CLA	b	808	3	1/1/11/20	3/15/91/115	-
12	CLA	l	202	3	1/1/15/20	17/39/115/115	-
12	CLA	F	203	-	1/1/11/20	8/15/91/115	-
12	CLA	H	838	-	1/1/15/20	20/39/115/115	-
12	CLA	H	811	3	1/1/15/20	23/39/115/115	-
12	CLA	f	201	20	1/1/15/20	16/39/115/115	-
12	CLA	b	814	3	1/1/13/20	8/27/103/115	-
16	LHG	A	850	-	-	30/53/53/53	-
12	CLA	a	814	-	1/1/11/20	7/15/91/115	-
12	CLA	H	822	20	1/1/15/20	16/39/115/115	-
15	BCR	G	845	-	-	10/29/63/63	0/2/2/2
12	CLA	A	812	-	1/1/12/20	10/21/97/115	-
15	BCR	B	845	-	-	6/29/63/63	0/2/2/2
12	CLA	H	826	-	1/1/15/20	12/39/115/115	-
12	CLA	G	824	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	835	3	1/1/11/20	7/15/91/115	-
12	CLA	a	805	1	1/1/15/20	14/39/115/115	-
15	BCR	a	844	-	-	11/29/63/63	0/2/2/2
12	CLA	B	829	3	1/1/15/20	18/39/115/115	-
12	CLA	b	835	20	1/1/15/20	13/39/115/115	-
13	1L3	B	839	-	-	5/23/43/43	0/2/2/2
11	CL0	a	801	1	3/3/20/25	8/37/135/135	-
12	CLA	H	813	-	1/1/11/20	9/15/91/115	-
12	CLA	B	834	3	1/1/15/20	9/39/115/115	-
12	CLA	G	803	20	1/1/15/20	8/39/115/115	-
12	CLA	A	839	1	1/1/15/20	7/39/115/115	-
12	CLA	L	205	10	1/1/15/20	14/39/115/115	-
15	BCR	i	101	-	-	9/29/63/63	0/2/2/2
12	CLA	G	818	-	1/1/13/20	15/27/103/115	-
12	CLA	A	813	-	1/1/11/20	2/15/91/115	-
12	CLA	G	838	1	1/1/11/20	3/15/91/115	-
12	CLA	a	826	1	1/1/15/20	15/39/115/115	-
12	CLA	b	832	3	1/1/14/20	15/33/109/115	-
12	CLA	a	827	-	1/1/14/20	12/33/109/115	-
13	1L3	H	840	-	-	5/23/43/43	0/2/2/2
12	CLA	a	834	-	1/1/15/20	20/39/115/115	-
12	CLA	B	820	3	1/1/11/20	4/15/91/115	-
12	CLA	b	820	-	1/1/11/20	2/15/91/115	-
15	BCR	J	102	-	-	18/29/63/63	0/2/2/2
12	CLA	H	807	3	1/1/15/20	9/39/115/115	-
12	CLA	a	808	1	1/1/12/20	7/21/97/115	-
15	BCR	A	847	-	-	4/29/63/63	0/2/2/2
12	CLA	A	836	1	-	7/21/97/115	-
12	CLA	a	833	-	1/1/15/20	15/39/115/115	-
12	CLA	H	827	3	1/1/15/20	12/39/115/115	-
12	CLA	H	829	3	1/1/11/20	4/15/91/115	-
12	CLA	a	831	1	1/1/13/20	11/27/103/115	-
12	CLA	b	830	-	1/1/11/20	6/15/91/115	-
12	CLA	A	823	-	1/1/13/20	13/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	C	102	4	-	-	0/6/5/5
12	CLA	l	205	10	1/1/15/20	13/39/115/115	-
12	CLA	A	828	-	1/1/15/20	13/39/115/115	-
15	BCR	S	201	-	-	16/29/63/63	0/2/2/2
12	CLA	b	833	3	1/1/15/20	11/39/115/115	-
12	CLA	a	828	-	1/1/15/20	11/39/115/115	-
12	CLA	B	806	3	1/1/15/20	13/39/115/115	-
12	CLA	G	827	-	1/1/15/20	16/39/115/115	-
12	CLA	b	818	-	1/1/11/20	4/15/91/115	-
12	CLA	B	813	3	1/1/13/20	7/27/103/115	-
12	CLA	G	831	1	1/1/12/20	8/21/97/115	-
12	CLA	H	821	-	1/1/11/20	2/15/91/115	-
12	CLA	H	810	3	1/1/11/20	2/15/91/115	-
15	BCR	J	104	-	-	5/29/63/63	0/2/2/2
11	CL0	A	801	1	3/3/20/25	6/37/135/135	-
12	CLA	G	825	20	1/1/15/20	16/39/115/115	-
12	CLA	a	830	1	-	10/21/97/115	-
12	CLA	a	832	1	1/1/15/20	15/39/115/115	-
12	CLA	B	812	-	1/1/11/20	9/15/91/115	-
15	BCR	b	839	-	-	13/29/63/63	0/2/2/2
12	CLA	b	848	16	1/1/14/20	15/33/109/115	-
12	CLA	b	829	3	1/1/15/20	18/39/115/115	-
12	CLA	B	801	-	1/1/14/20	6/33/109/115	-
12	CLA	A	821	1	1/1/11/20	9/15/91/115	-
12	CLA	G	816	-	1/1/11/20	5/15/91/115	-
15	BCR	G	849	-	-	12/29/63/63	0/2/2/2
12	CLA	G	856	-	1/1/15/20	12/39/115/115	-
12	CLA	b	809	3	1/1/11/20	2/15/91/115	-
12	CLA	b	806	-	1/1/15/20	13/39/115/115	-
13	1L3	A	842	-	-	5/23/43/43	0/2/2/2
14	SF4	a	843	1,3	-	-	0/6/5/5
12	CLA	A	841	20	1/1/15/20	17/39/115/115	-
12	CLA	B	826	3	1/1/15/20	12/39/115/115	-
15	BCR	l	203	-	-	16/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	816	-	1/1/15/20	15/39/115/115	-
12	CLA	G	817	1	1/1/12/20	6/21/97/115	-
12	CLA	H	836	3	1/1/11/20	5/15/91/115	-
12	CLA	B	823	3	1/1/15/20	17/39/115/115	-
13	1L3	b	838	-	-	5/23/43/43	0/2/2/2
12	CLA	B	828	3	1/1/11/20	4/15/91/115	-
15	BCR	B	840	-	-	10/29/63/63	0/2/2/2
12	CLA	b	815	-	1/1/14/20	8/33/109/115	-
12	CLA	P	201	20	1/1/15/20	16/39/115/115	-
18	LMG	H	847	-	-	16/50/70/70	0/1/1/1
12	CLA	A	817	-	1/1/13/20	15/27/103/115	-
12	CLA	G	815	-	1/1/11/20	7/15/91/115	-
12	CLA	H	816	-	1/1/14/20	10/33/109/115	-
12	CLA	H	812	3	1/1/14/20	11/33/109/115	-
16	LHG	a	853	-	-	35/53/53/53	-
12	CLA	G	804	1	1/1/15/20	15/39/115/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
15	BCR	f	204	-	-	7/29/63/63	0/2/2/2
12	CLA	G	820	1	1/1/11/20	8/15/91/115	-
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2
12	CLA	G	811	1,12	1/1/12/20	8/21/97/115	-
12	CLA	G	821	-	1/1/15/20	11/39/115/115	-
12	CLA	b	825	-	1/1/15/20	12/39/115/115	-
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2
12	CLA	H	817	-	1/1/15/20	15/39/115/115	-
12	CLA	A	803	1	1/1/15/20	14/39/115/115	-
12	CLA	G	826	20	1/1/13/20	7/27/103/115	-
12	CLA	H	808	3	1/1/15/20	13/39/115/115	-
12	CLA	A	820	-	1/1/15/20	17/39/115/115	-
12	CLA	G	834	-	1/1/15/20	21/39/115/115	-
14	SF4	K	101	4	-	-	0/6/5/5
12	CLA	H	814	3	1/1/13/20	6/27/103/115	-
12	CLA	a	829	1	1/1/15/20	10/39/115/115	-
12	CLA	B	837	3	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LHG	a	851	12	-	18/31/31/53	-
12	CLA	b	805	3	1/1/15/20	20/39/115/115	-
12	CLA	A	834	-	1/1/15/20	18/39/115/115	-
15	BCR	B	844	-	-	8/29/63/63	0/2/2/2
12	CLA	G	812	-	1/1/11/20	6/15/91/115	-
12	CLA	a	838	1	1/1/11/20	3/15/91/115	-
12	CLA	H	803	-	1/1/15/20	17/39/115/115	-
12	CLA	H	805	3	1/1/15/20	16/39/115/115	-
12	CLA	A	804	12	1/1/13/20	14/27/103/115	-
12	CLA	A	810	1,12	1/1/12/20	7/21/97/115	-
12	CLA	b	826	3	1/1/15/20	10/39/115/115	-
12	CLA	B	824	-	1/1/15/20	24/39/115/115	-
12	CLA	b	823	3	1/1/15/20	16/39/115/115	-
12	CLA	H	834	20	1/1/14/20	15/33/109/115	-
14	SF4	C	101	4	-	-	0/6/5/5
15	BCR	L	207	-	-	10/29/63/63	0/2/2/2
12	CLA	A	832	1	1/1/15/20	15/39/115/115	-
16	LHG	G	852	12	-	16/31/31/53	-
12	CLA	B	809	3	1/1/11/20	5/15/91/115	-
12	CLA	G	806	-	1/1/15/20	10/39/115/115	-
12	CLA	G	805	1,12	1/1/13/20	13/27/103/115	-
12	CLA	G	832	1	1/1/15/20	14/39/115/115	-
15	BCR	G	853	-	-	12/29/63/63	0/2/2/2
12	CLA	H	831	-	1/1/15/20	13/39/115/115	-
14	SF4	c	101	4	-	-	0/6/5/5
12	CLA	l	204	10	1/1/13/20	6/27/103/115	-
17	45D	M	101	-	-	13/29/69/69	0/2/2/2
15	BCR	P	204	-	-	7/29/63/63	0/2/2/2
12	CLA	a	825	20	1/1/13/20	5/27/103/115	-
12	CLA	H	801	1	1/1/13/20	11/27/103/115	-
15	BCR	G	847	-	-	6/29/63/63	0/2/2/2
12	CLA	b	827	3	1/1/11/20	5/15/91/115	-
12	CLA	a	813	-	1/1/11/20	2/15/91/115	-
15	BCR	H	841	-	-	14/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	830	1	1/1/12/20	7/21/97/115	-
12	CLA	G	823	1	1/1/12/20	7/21/97/115	-
12	CLA	H	833	-	1/1/11/20	7/15/91/115	-
12	CLA	A	854	20	1/1/15/20	18/39/115/115	-
12	CLA	G	822	1	1/1/11/20	9/15/91/115	-
15	BCR	H	843	-	-	9/29/63/63	0/2/2/2
12	CLA	A	833	-	1/1/15/20	15/39/115/115	-
12	CLA	a	821	-	1/1/11/20	9/15/91/115	-
17	45D	T	101	-	-	13/29/69/69	0/2/2/2
12	CLA	H	837	20	1/1/15/20	14/39/115/115	-
12	CLA	A	818	-	1/1/15/20	15/39/115/115	-
15	BCR	b	847	-	-	7/29/63/63	0/2/2/2
12	CLA	a	823	-	1/1/13/20	11/27/103/115	-
12	CLA	A	826	1	1/1/15/20	15/39/115/115	-
12	CLA	b	836	-	1/1/15/20	18/39/115/115	-
11	CL0	G	801	1	3/3/20/25	10/37/135/135	-
12	CLA	B	833	3	1/1/14/20	15/33/109/115	-
12	CLA	J	103	-	1/1/11/20	8/15/91/115	-
15	BCR	j	101	-	-	12/29/63/63	0/2/2/2
12	CLA	G	836	1	1/1/12/20	5/21/97/115	-
12	CLA	A	814	-	1/1/11/20	7/15/91/115	-
12	CLA	b	821	20	1/1/15/20	15/39/115/115	-
15	BCR	J	101	-	-	10/29/63/63	0/2/2/2
12	CLA	a	854	20	1/1/15/20	19/39/115/115	-
15	BCR	l	201	-	-	8/29/63/63	0/2/2/2
12	CLA	a	804	12	1/1/13/20	13/27/103/115	-
12	CLA	L	206	20	1/1/15/20	10/39/115/115	-
12	CLA	b	810	3	1/1/15/20	25/39/115/115	-
15	BCR	A	844	-	-	10/29/63/63	0/2/2/2
16	LHG	A	853	-	-	39/53/53/53	-
15	BCR	A	846	-	-	8/29/63/63	0/2/2/2
12	CLA	A	811	-	1/1/11/20	6/15/91/115	-
12	CLA	P	203	-	1/1/11/20	8/15/91/115	-
12	CLA	a	820	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	a	849	-	-	12/29/63/63	0/2/2/2
15	BCR	B	843	-	-	3/18/35/63	0/1/1/2
12	CLA	H	824	3	1/1/15/20	18/39/115/115	-
12	CLA	A	822	-	1/1/12/20	6/21/97/115	-
12	CLA	B	832	3	1/1/11/20	5/15/91/115	-
12	CLA	b	804	-	1/1/15/20	18/39/115/115	-
12	CLA	A	831	1	1/1/13/20	11/27/103/115	-
15	BCR	H	842	-	-	8/29/63/63	0/2/2/2
12	CLA	A	802	20	1/1/15/20	8/39/115/115	-
12	CLA	A	815	-	1/1/11/20	5/15/91/115	-
12	CLA	a	840	1	1/1/12/20	9/21/97/115	-
12	CLA	H	804	-	1/1/15/20	18/39/115/115	-
18	LMG	B	846	-	-	18/50/70/70	0/1/1/1
12	CLA	j	102	-	1/1/15/20	13/39/115/115	-
13	1L3	a	842	-	-	5/23/43/43	0/2/2/2
14	SF4	G	844	1,3	-	-	0/6/5/5
12	CLA	b	834	3	1/1/11/20	7/15/91/115	-
12	CLA	a	812	-	1/1/12/20	10/21/97/115	-
12	CLA	H	823	20	1/1/15/20	19/39/115/115	-
12	CLA	a	818	-	1/1/15/20	17/39/115/115	-
12	CLA	G	802	-	1/1/14/20	7/33/109/115	-
12	CLA	B	814	-	1/1/13/20	9/27/103/115	-
12	CLA	a	816	1	1/1/12/20	9/21/97/115	-
12	CLA	b	812	-	1/1/11/20	9/15/91/115	-
12	CLA	B	830	-	1/1/15/20	13/39/115/115	-
12	CLA	G	807	1	1/1/15/20	13/39/115/115	-
17	45D	m	101	-	-	13/29/69/69	0/2/2/2
12	CLA	A	807	1	1/1/15/20	23/39/115/115	-
12	CLA	b	817	3	1/1/11/20	10/15/91/115	-
12	CLA	B	811	-	1/1/14/20	11/33/109/115	-
12	CLA	A	824	20	1/1/15/20	18/39/115/115	-
12	CLA	a	802	20	1/1/15/20	10/39/115/115	-
12	CLA	a	855	-	1/1/15/20	13/39/115/115	-
12	CLA	H	850	16	1/1/14/20	14/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	H	844	-	-	3/18/35/63	0/1/1/2
12	CLA	a	839	1	1/1/15/20	11/39/115/115	-
12	CLA	B	818	-	1/1/11/20	3/15/91/115	-
12	CLA	B	822	20	1/1/15/20	18/39/115/115	-
12	CLA	a	806	-	1/1/15/20	13/39/115/115	-
16	LHG	G	851	-	-	31/53/53/53	-
19	LMT	H	848	-	-	11/21/61/61	0/2/2/2
12	CLA	A	816	1	1/1/12/20	6/21/97/115	-
12	CLA	A	809	1	1/1/11/20	7/15/91/115	-
12	CLA	A	837	1	1/1/15/20	17/39/115/115	-
12	CLA	S	203	10	1/1/15/20	14/39/115/115	-
12	CLA	L	202	3	1/1/15/20	13/39/115/115	-
16	LHG	A	851	12	-	14/31/31/53	-
15	BCR	Q	102	-	-	11/29/63/63	0/2/2/2
12	CLA	G	855	20	1/1/15/20	18/39/115/115	-
12	CLA	G	810	1	1/1/11/20	7/15/91/115	-
12	CLA	F	201	20	1/1/15/20	13/39/115/115	-
12	CLA	a	815	-	1/1/11/20	5/15/91/115	-
15	BCR	b	843	-	-	9/29/63/63	0/2/2/2
12	CLA	R	103	-	1/1/11/20	7/15/91/115	-
14	SF4	A	843	1,3	-	-	0/6/5/5
12	CLA	L	204	10	1/1/13/20	7/27/103/115	-
15	BCR	R	102	-	-	19/29/63/63	0/2/2/2
12	CLA	G	841	20	1/1/15/20	15/39/115/115	-
14	SF4	K	102	4	-	-	0/6/5/5
12	CLA	B	831	-	1/1/11/20	6/15/91/115	-
12	CLA	G	830	-	1/1/15/20	10/39/115/115	-
12	CLA	a	810	1,12	1/1/12/20	9/21/97/115	-
12	CLA	A	825	20	1/1/13/20	5/27/103/115	-
15	BCR	F	204	-	-	7/29/63/63	0/2/2/2
12	CLA	B	815	-	1/1/14/20	11/33/109/115	-
12	CLA	G	833	1	1/1/15/20	15/39/115/115	-
12	CLA	B	807	3	1/1/15/20	8/39/115/115	-
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	LMT	B	847	-	-	10/21/61/61	0/2/2/2
12	CLA	a	811	-	1/1/11/20	6/15/91/115	-
12	CLA	a	809	1	1/1/11/20	7/15/91/115	-
12	CLA	B	803	-	1/1/15/20	17/39/115/115	-
12	CLA	B	805	3	1/1/15/20	17/39/115/115	-

The worst 5 of 6512 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	101	45D	C07-C15	13.72	1.54	1.35
17	m	101	45D	C07-C15	13.70	1.54	1.35
17	M	101	45D	C07-C15	13.69	1.54	1.35
17	m	101	45D	C08-C16	13.67	1.54	1.35
17	M	101	45D	C08-C16	13.59	1.54	1.35

The worst 5 of 8871 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	i	101	BCR	C16-C17-C18	24.83	162.10	127.28
15	A	846	BCR	C16-C17-C18	24.60	161.77	127.28
15	R	102	BCR	C16-C17-C18	24.51	161.65	127.28
15	j	103	BCR	C16-C17-C18	24.44	161.55	127.28
15	G	849	BCR	C20-C21-C22	24.28	161.33	127.28

5 of 271 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
11	G	801	CL0	ND
11	G	801	CL0	NA
11	G	801	CL0	NC
11	a	801	CL0	ND
11	a	801	CL0	NA

5 of 4013 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	805	CLA	C1A-C2A-CAA-CBA
12	G	805	CLA	C3A-C2A-CAA-CBA
12	G	806	CLA	CAD-CBD-CGD-O1D
12	G	806	CLA	CAD-CBD-CGD-O2D
12	G	807	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

278 monomers are involved in 560 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	j	103	BCR	3	0
15	F	202	BCR	3	0
12	A	808	CLA	1	0
15	R	101	BCR	2	0
15	Q	101	BCR	4	0
12	A	806	CLA	2	0
12	f	203	CLA	2	0
12	b	822	CLA	8	0
12	H	802	CLA	3	0
12	H	832	CLA	2	0
12	b	824	CLA	2	0
12	b	837	CLA	1	0
19	b	846	LMT	1	0
12	a	807	CLA	5	0
12	G	819	CLA	4	0
12	H	825	CLA	5	0
12	b	813	CLA	1	0
12	G	840	CLA	1	0
15	L	203	BCR	2	0
15	b	840	BCR	4	0
12	b	801	CLA	1	0
15	H	849	BCR	3	0
15	I	101	BCR	4	0
12	B	827	CLA	2	0
12	B	802	CLA	2	0
12	a	824	CLA	5	0
12	G	839	CLA	2	0
12	b	807	CLA	2	0
15	a	848	BCR	2	0
12	B	825	CLA	4	0
15	b	841	BCR	1	0
12	G	808	CLA	3	0
12	b	828	CLA	2	0
15	a	846	BCR	4	0
12	G	835	CLA	2	0
15	G	850	BCR	3	0
12	A	840	CLA	4	0
15	b	844	BCR	3	0
15	a	847	BCR	3	0
12	H	828	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	836	CLA	1	0
12	G	837	CLA	1	0
12	A	855	CLA	3	0
12	a	822	CLA	1	0
12	a	835	CLA	2	0
12	G	829	CLA	5	0
12	a	836	CLA	1	0
12	A	827	CLA	3	0
12	G	842	CLA	2	0
12	A	835	CLA	1	0
15	a	852	BCR	1	0
15	b	842	BCR	4	0
12	a	841	CLA	2	0
15	P	202	BCR	4	0
15	B	842	BCR	1	0
12	G	828	CLA	1	0
16	G	854	LHG	1	0
12	B	804	CLA	3	0
12	S	204	CLA	3	0
12	S	202	CLA	1	0
15	G	846	BCR	1	0
18	b	845	LMG	3	0
15	S	205	BCR	3	0
12	l	206	CLA	3	0
15	H	846	BCR	2	0
15	A	845	BCR	3	0
12	B	810	CLA	1	0
12	A	829	CLA	4	0
12	b	802	CLA	3	0
15	A	852	BCR	2	0
15	A	849	BCR	5	0
12	A	805	CLA	2	0
15	H	845	BCR	6	0
12	H	835	CLA	4	0
12	a	803	CLA	1	0
16	a	850	LHG	2	0
12	H	806	CLA	2	0
12	b	803	CLA	1	0
15	L	201	BCR	2	0
15	G	848	BCR	2	0
12	G	813	CLA	1	0
12	H	815	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	817	CLA	3	0
12	l	202	CLA	5	0
12	F	203	CLA	1	0
12	H	838	CLA	4	0
12	H	811	CLA	2	0
12	f	201	CLA	3	0
12	a	814	CLA	1	0
12	H	822	CLA	2	0
15	G	845	BCR	1	0
12	A	812	CLA	1	0
15	B	845	BCR	3	0
12	H	826	CLA	3	0
12	G	824	CLA	4	0
12	B	835	CLA	2	0
12	a	805	CLA	4	0
12	B	829	CLA	1	0
12	b	835	CLA	2	0
12	B	834	CLA	2	0
12	G	803	CLA	2	0
12	A	839	CLA	1	0
12	L	205	CLA	3	0
15	i	101	BCR	3	0
12	G	818	CLA	4	0
12	a	826	CLA	3	0
12	b	832	CLA	5	0
12	a	827	CLA	2	0
12	a	834	CLA	2	0
15	J	102	BCR	2	0
12	H	807	CLA	3	0
15	A	847	BCR	1	0
12	a	833	CLA	4	0
12	H	827	CLA	1	0
12	H	829	CLA	1	0
12	a	831	CLA	2	0
12	b	830	CLA	1	0
12	A	823	CLA	2	0
12	l	205	CLA	4	0
12	A	828	CLA	2	0
15	S	201	BCR	2	0
12	b	833	CLA	2	0
12	a	828	CLA	6	0
12	B	806	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	827	CLA	3	0
15	J	104	BCR	2	0
11	A	801	CL0	4	0
12	G	825	CLA	7	0
12	a	832	CLA	3	0
12	B	812	CLA	1	0
15	b	839	BCR	1	0
12	b	848	CLA	2	0
12	b	829	CLA	1	0
12	B	801	CLA	5	0
12	A	821	CLA	1	0
15	G	849	BCR	3	0
12	G	856	CLA	4	0
12	b	806	CLA	3	0
12	A	841	CLA	1	0
15	l	203	BCR	2	0
12	b	816	CLA	2	0
12	G	817	CLA	1	0
12	H	836	CLA	3	0
12	B	823	CLA	2	0
12	B	828	CLA	2	0
12	b	815	CLA	2	0
12	P	201	CLA	5	0
18	H	847	LMG	5	0
12	A	817	CLA	1	0
12	H	816	CLA	3	0
12	H	812	CLA	1	0
16	a	853	LHG	1	0
12	G	804	CLA	2	0
15	A	848	BCR	2	0
15	f	204	BCR	2	0
15	f	202	BCR	2	0
12	G	821	CLA	3	0
12	b	825	CLA	4	0
15	B	841	BCR	3	0
12	H	817	CLA	2	0
12	A	803	CLA	3	0
12	G	826	CLA	2	0
12	H	808	CLA	4	0
12	A	820	CLA	2	0
12	G	834	CLA	3	0
12	a	829	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	837	CLA	3	0
16	a	851	LHG	1	0
12	b	805	CLA	7	0
12	A	834	CLA	2	0
15	B	844	BCR	4	0
12	H	805	CLA	5	0
12	A	804	CLA	2	0
12	b	826	CLA	2	0
12	B	824	CLA	1	0
12	b	823	CLA	2	0
12	H	834	CLA	4	0
15	L	207	BCR	1	0
12	A	832	CLA	3	0
16	G	852	LHG	1	0
12	G	806	CLA	3	0
12	G	832	CLA	2	0
15	G	853	BCR	1	0
12	H	831	CLA	3	0
12	l	204	CLA	2	0
17	M	101	45D	3	0
15	P	204	BCR	1	0
12	a	825	CLA	1	0
12	H	801	CLA	1	0
15	G	847	BCR	3	0
12	b	827	CLA	3	0
15	H	841	BCR	1	0
12	G	823	CLA	1	0
12	A	854	CLA	4	0
12	G	822	CLA	1	0
15	H	843	BCR	4	0
12	A	833	CLA	3	0
12	a	821	CLA	1	0
17	T	101	45D	3	0
12	H	837	CLA	2	0
12	A	818	CLA	5	0
15	b	847	BCR	4	0
12	a	823	CLA	1	0
12	A	826	CLA	2	0
12	b	836	CLA	5	0
11	G	801	CL0	1	0
12	B	833	CLA	7	0
12	J	103	CLA	1	0

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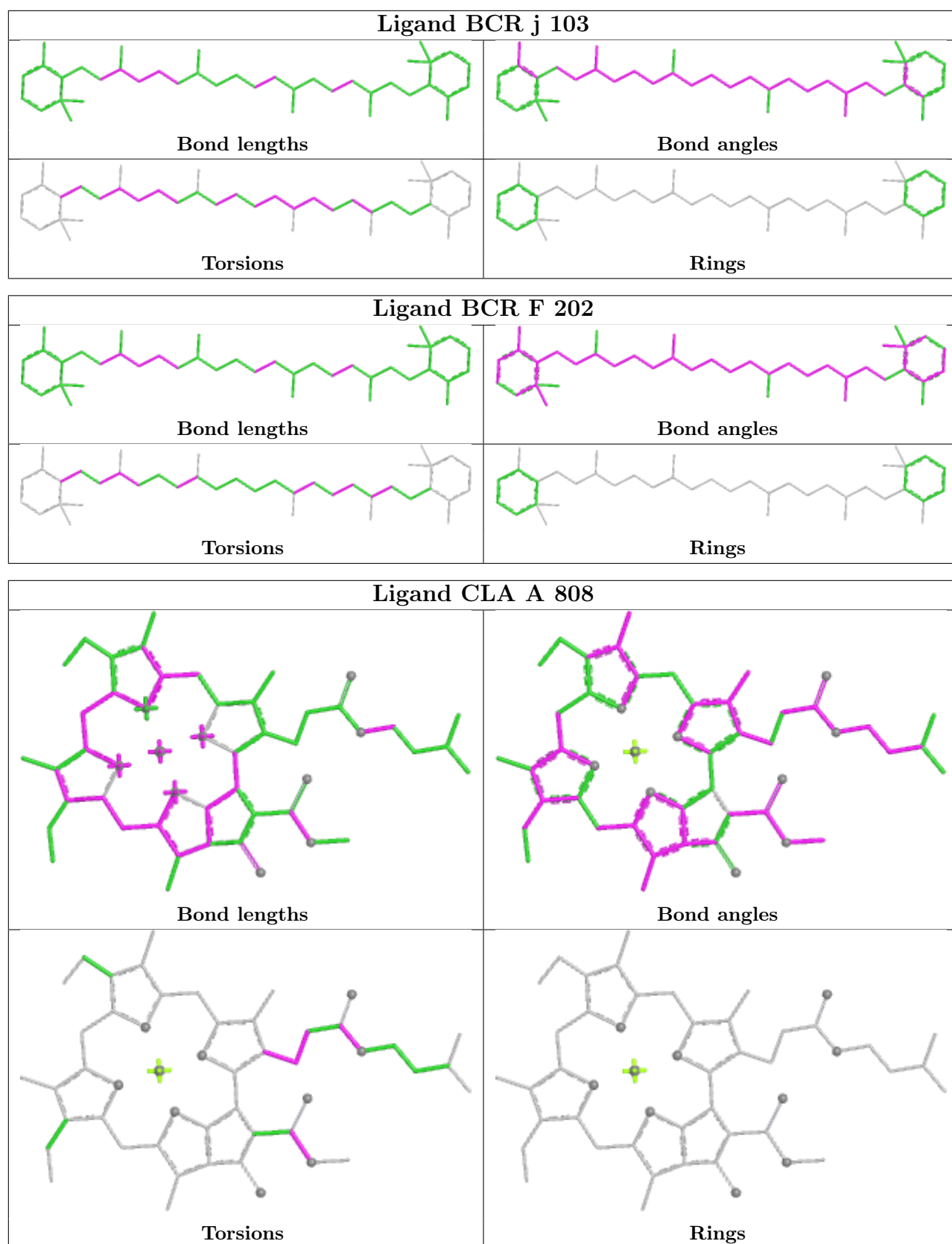
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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12	b	821	CLA	3	0
15	J	101	BCR	2	0
12	a	854	CLA	5	0
15	l	201	BCR	2	0
12	L	206	CLA	4	0
12	b	810	CLA	3	0
15	A	846	BCR	3	0
12	a	820	CLA	1	0
15	a	849	BCR	3	0
15	B	843	BCR	3	0
12	H	824	CLA	3	0
12	b	804	CLA	3	0
12	A	831	CLA	2	0
15	H	842	BCR	2	0
12	A	802	CLA	3	0
12	a	840	CLA	1	0
12	H	804	CLA	3	0
18	B	846	LMG	4	0
12	j	102	CLA	2	0
12	b	834	CLA	2	0
12	a	812	CLA	2	0
12	H	823	CLA	6	0
12	a	818	CLA	5	0
12	G	802	CLA	5	0
12	B	814	CLA	2	0
12	a	816	CLA	1	0
12	b	812	CLA	2	0
12	B	830	CLA	4	0
12	G	807	CLA	2	0
17	m	101	45D	4	0
12	A	807	CLA	3	0
12	b	817	CLA	1	0
12	A	824	CLA	7	0
12	a	802	CLA	3	0
12	a	855	CLA	6	0
12	H	850	CLA	3	0
15	H	844	BCR	4	0
12	a	839	CLA	2	0
12	B	822	CLA	6	0
12	a	806	CLA	3	0
16	G	851	LHG	3	0

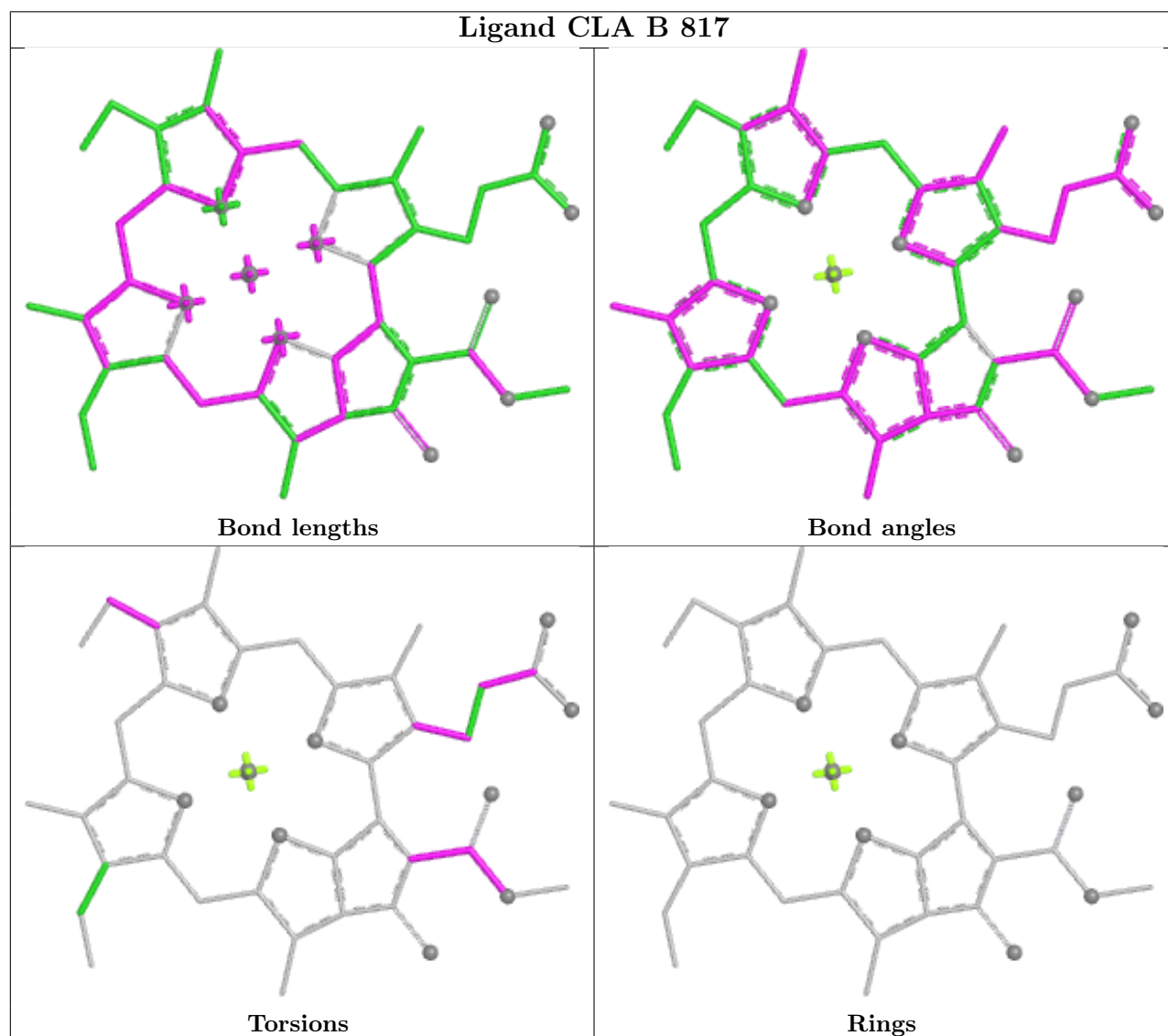
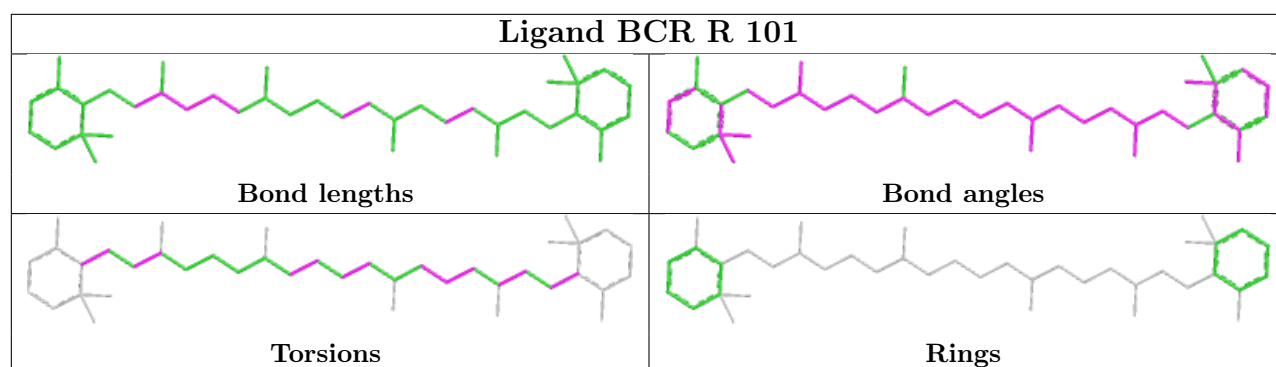
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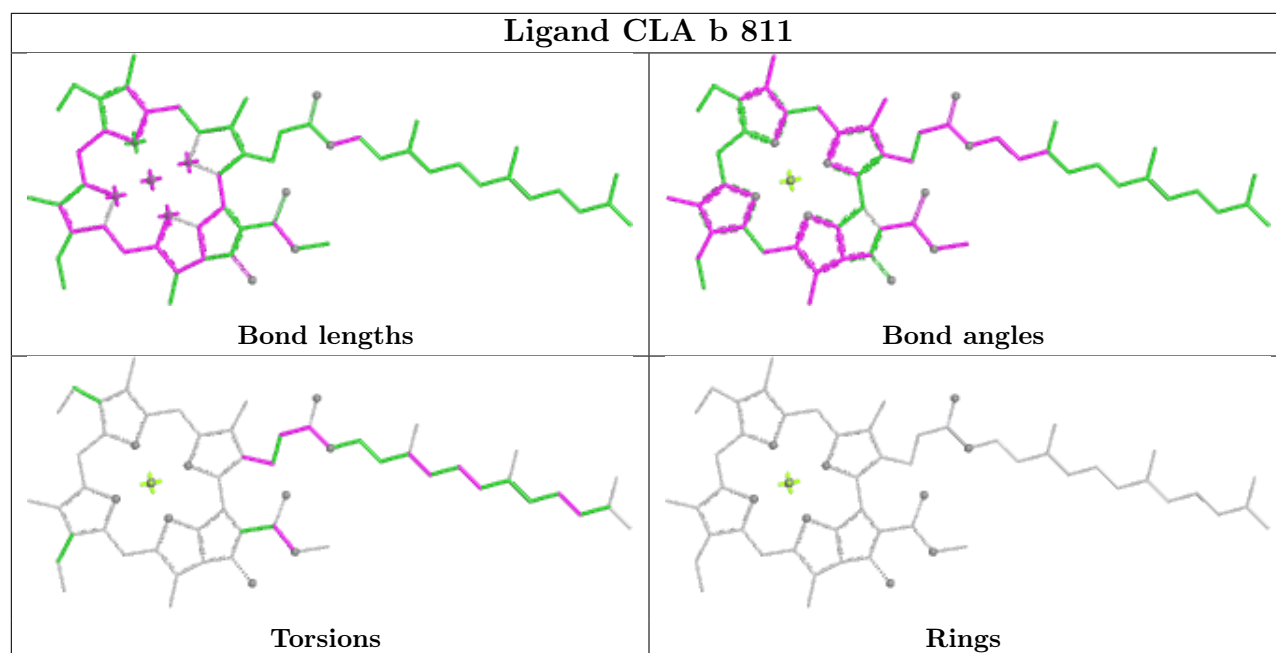
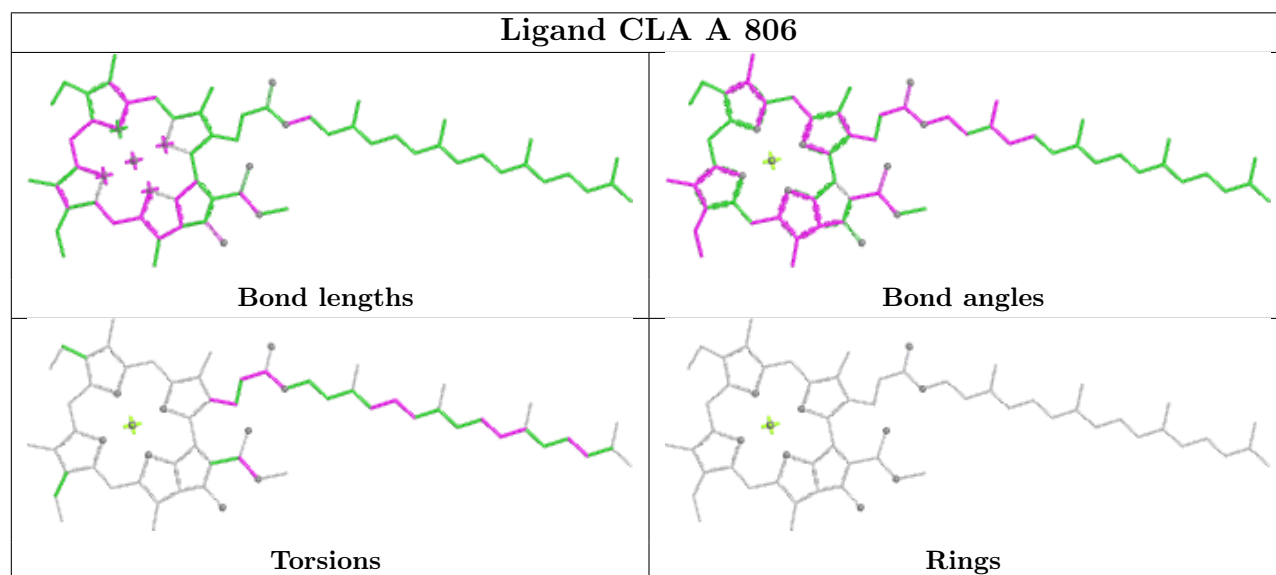
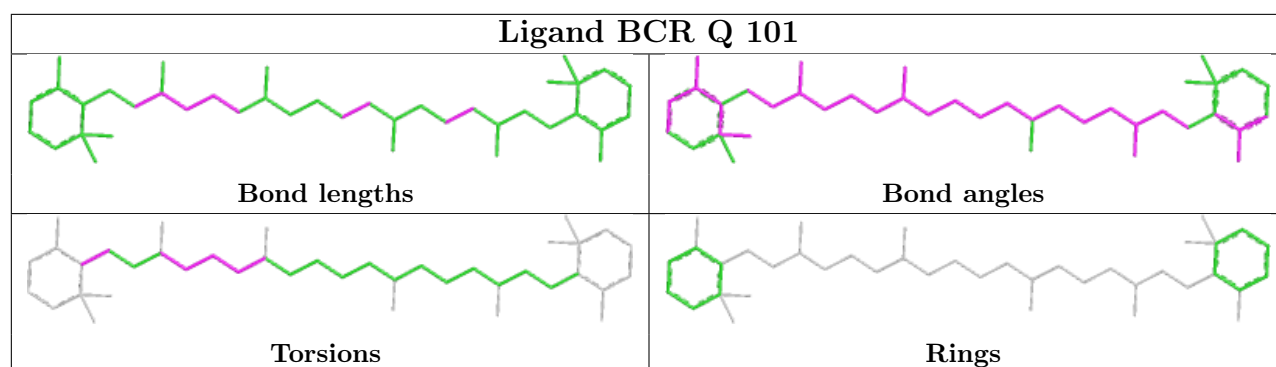
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	H	848	LMT	1	0
12	A	816	CLA	1	0
12	A	837	CLA	1	0
12	S	203	CLA	3	0
12	L	202	CLA	2	0
16	A	851	LHG	3	0
15	Q	102	BCR	1	0
12	G	855	CLA	3	0
12	G	810	CLA	1	0
12	F	201	CLA	3	0
15	b	843	BCR	6	0
12	R	103	CLA	1	0
12	L	204	CLA	2	0
15	R	102	BCR	3	0
12	G	841	CLA	1	0
14	K	102	SF4	1	0
12	B	831	CLA	2	0
12	G	830	CLA	3	0
12	A	825	CLA	2	0
15	F	204	BCR	2	0
12	B	815	CLA	1	0
12	G	833	CLA	2	0
12	B	807	CLA	4	0
15	a	845	BCR	2	0
19	B	847	LMT	2	0
12	a	809	CLA	2	0
12	B	803	CLA	1	0
12	B	805	CLA	6	0

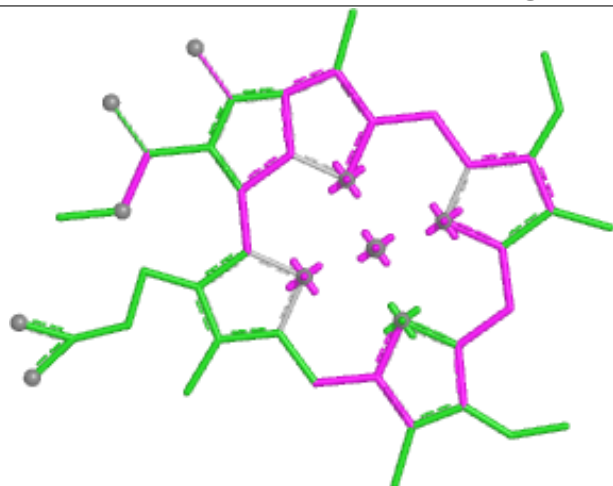
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



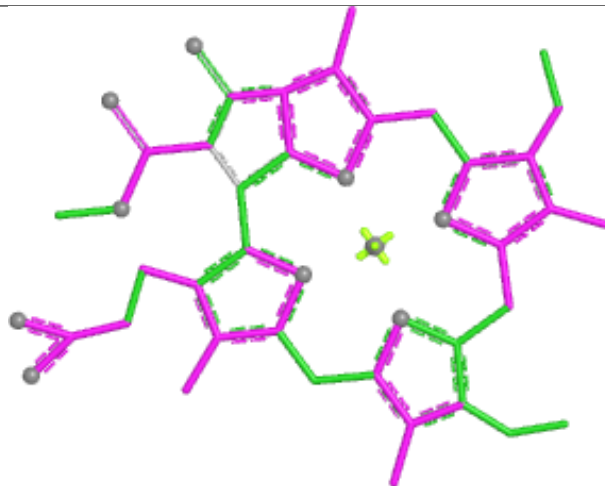




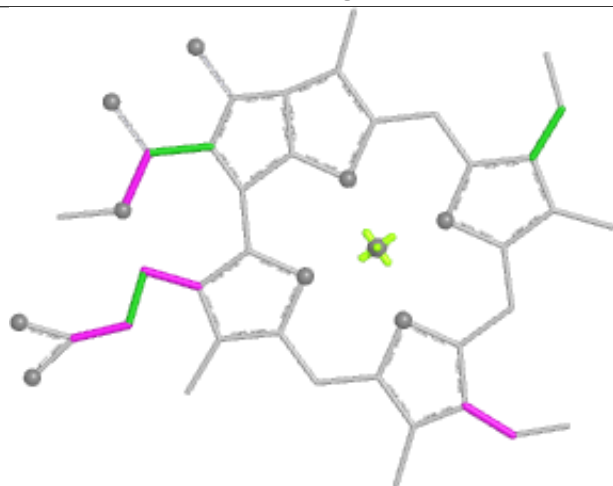
Ligand CLA f 203



Bond lengths



Bond angles

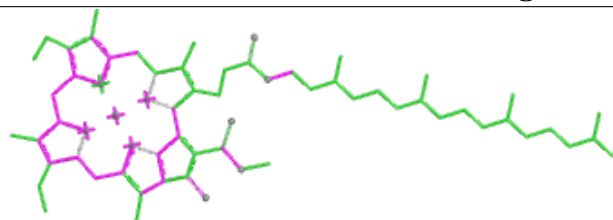


Torsions

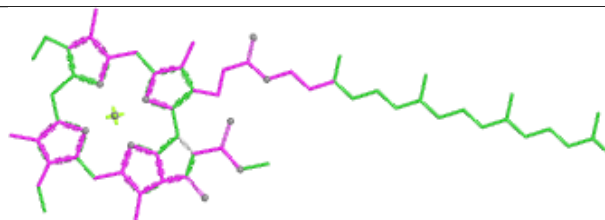


Rings

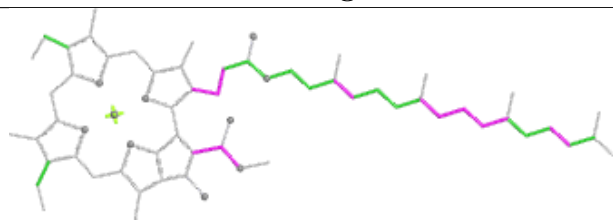
Ligand CLA b 822



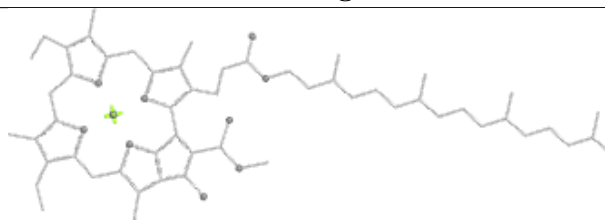
Bond lengths



Bond angles

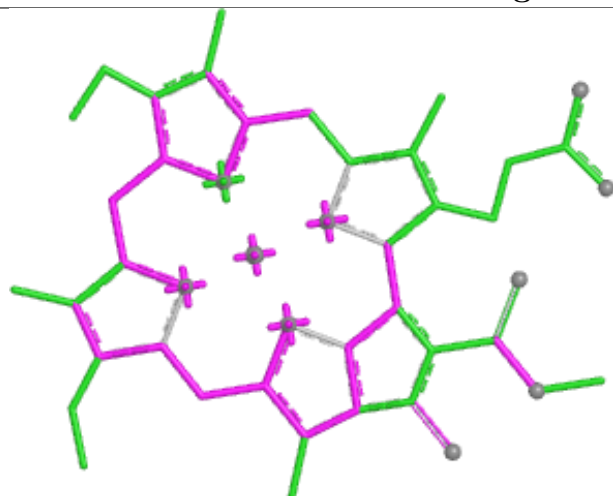


Torsions

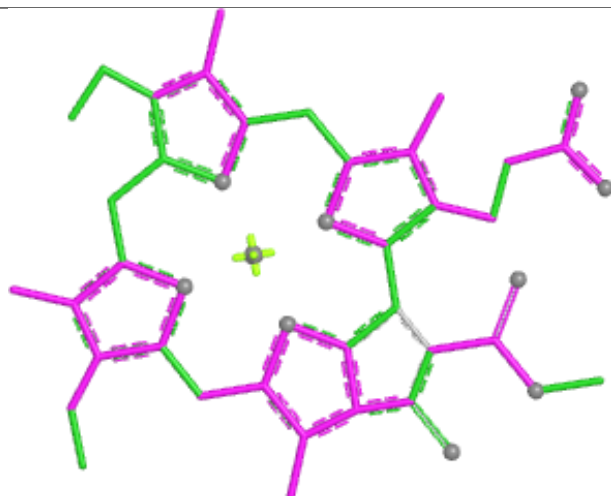


Rings

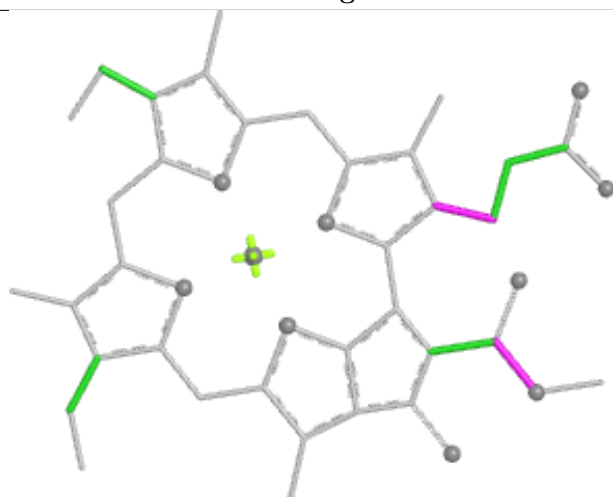
Ligand CLA H 819



Bond lengths



Bond angles

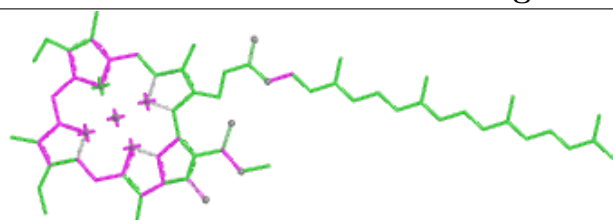


Torsions

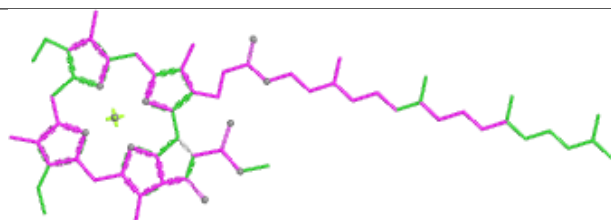


Rings

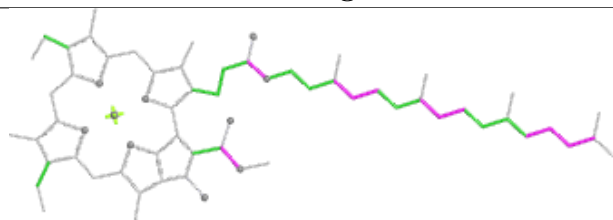
Ligand CLA H 802



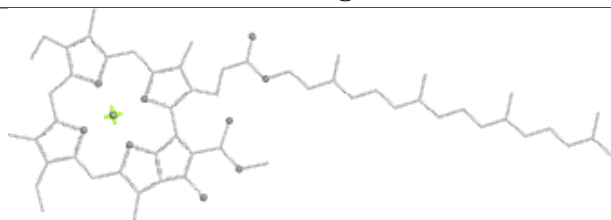
Bond lengths



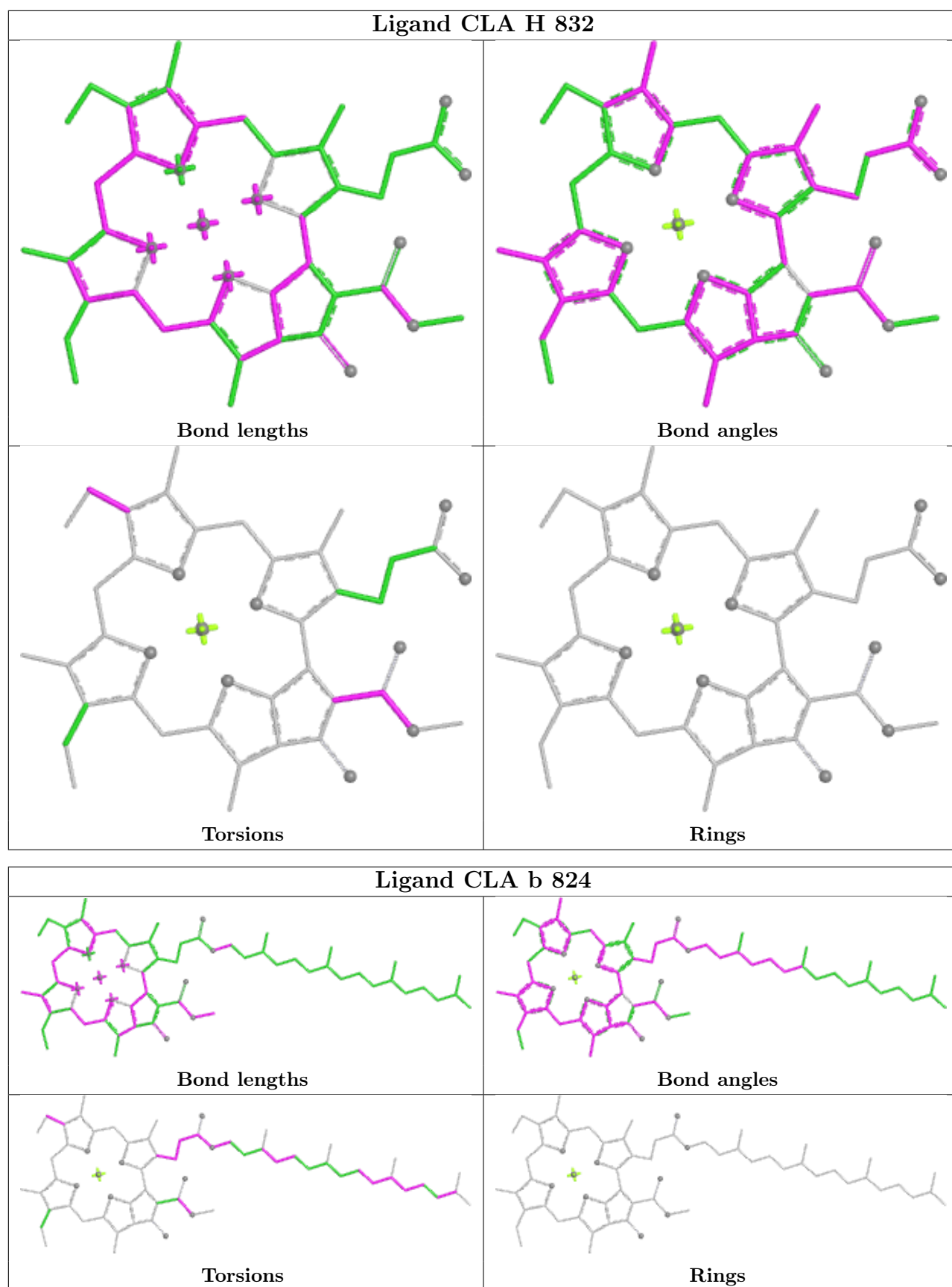
Bond angles

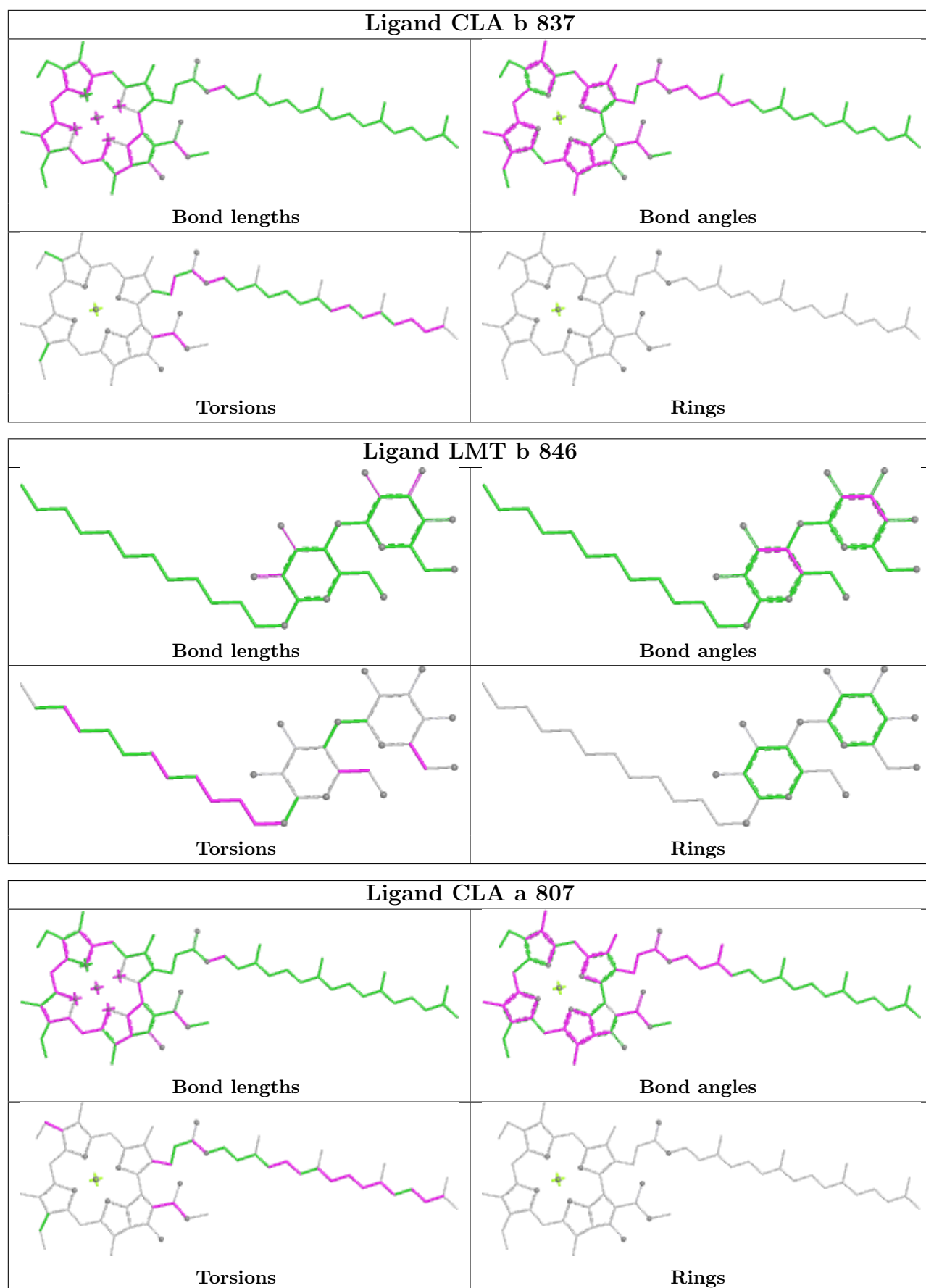


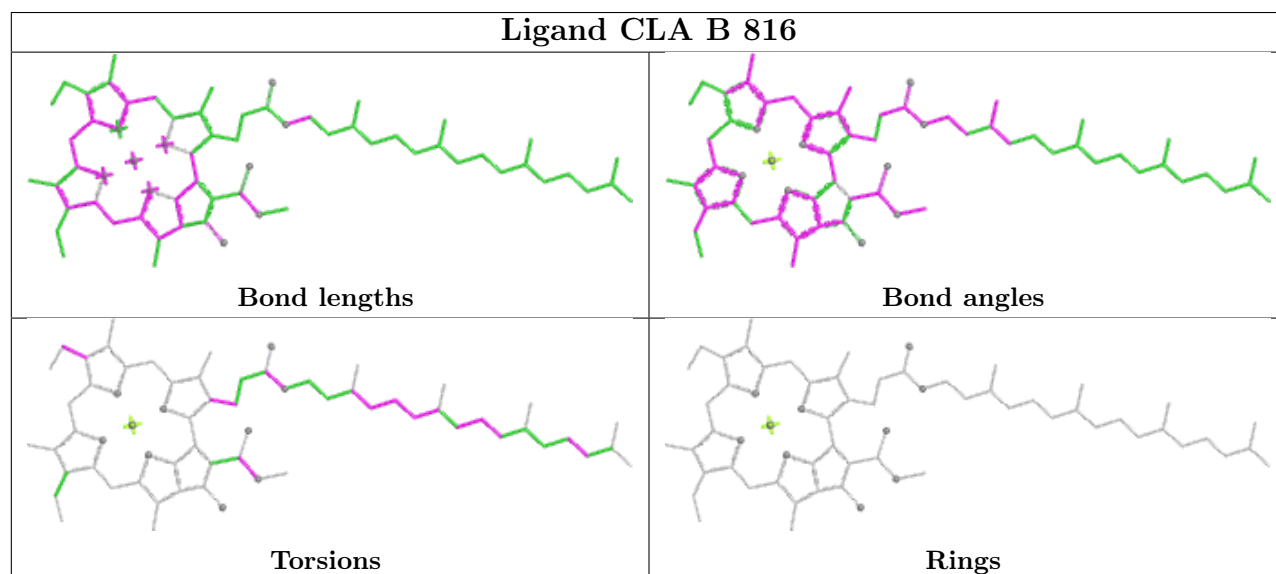
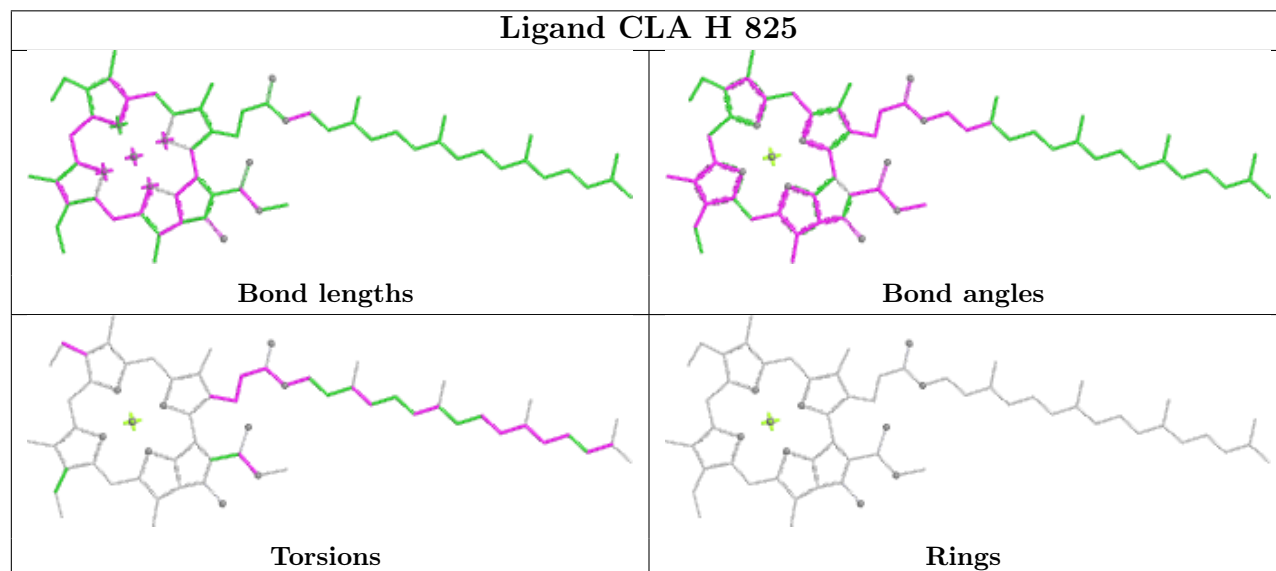
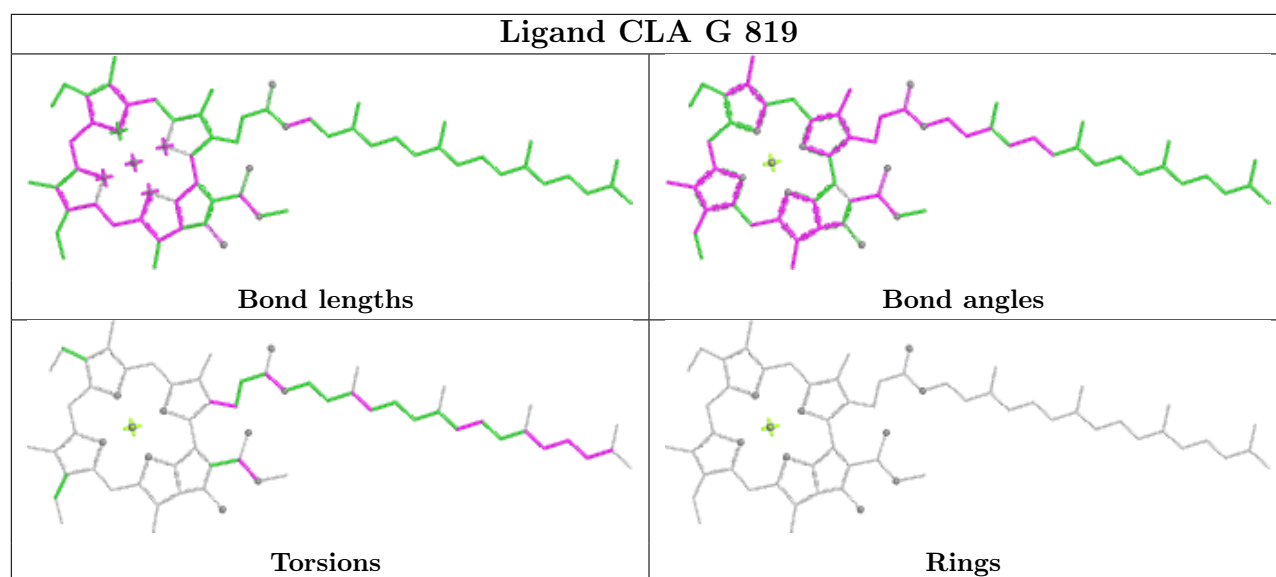
Torsions

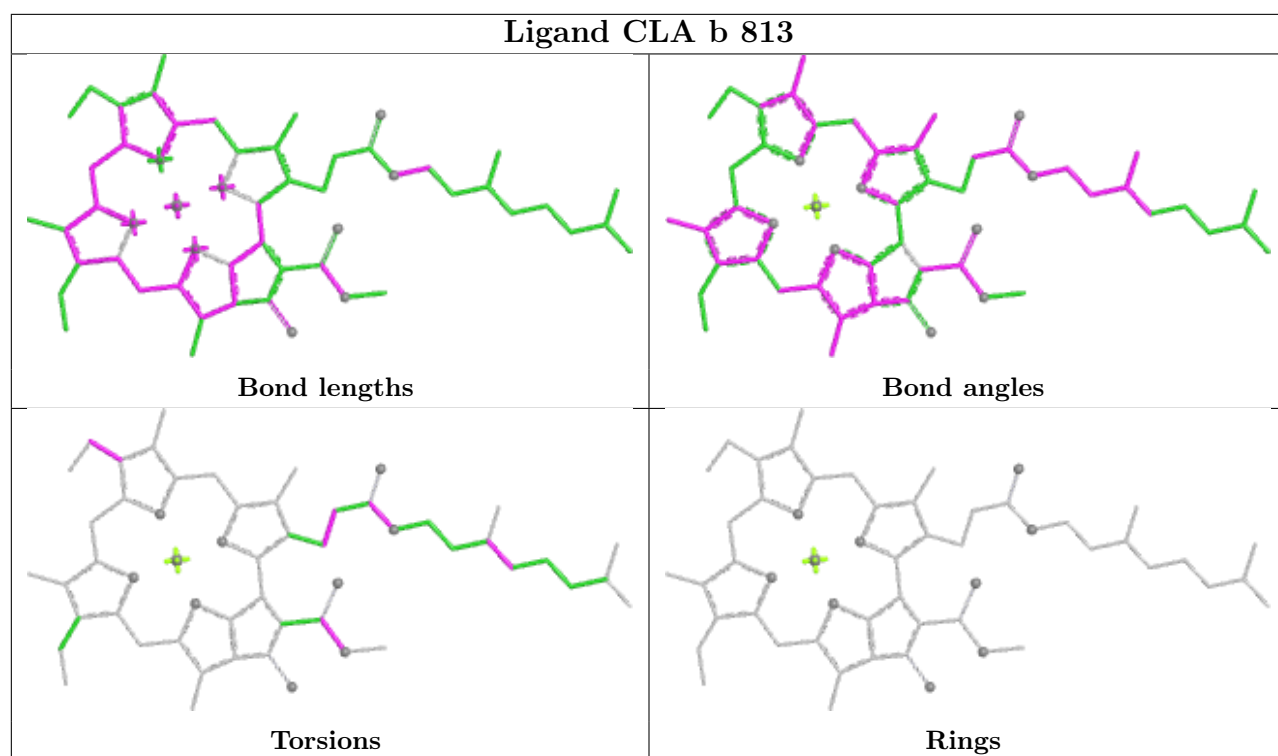


Rings

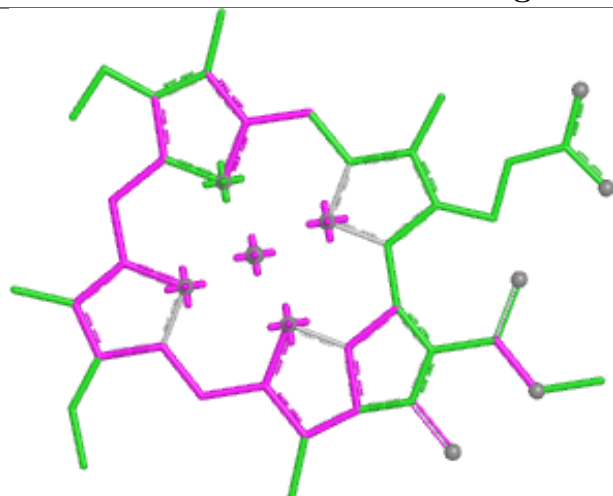




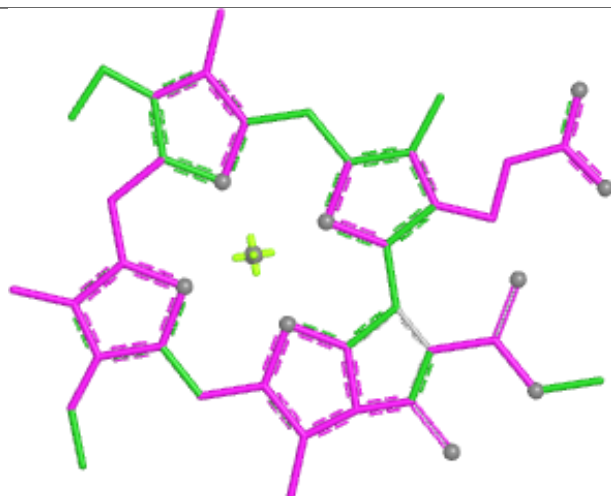




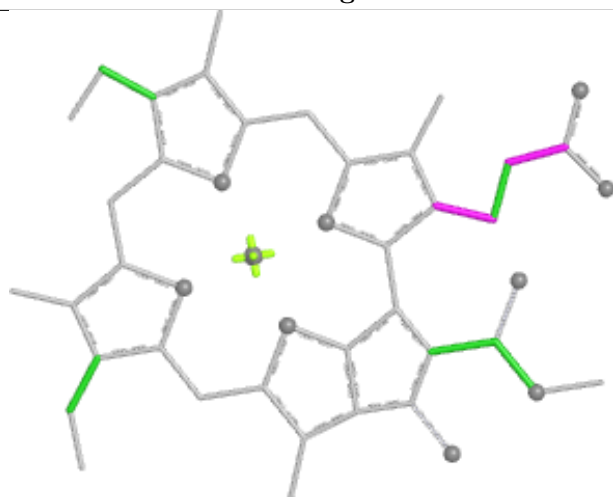
Ligand CLA A 838



Bond lengths



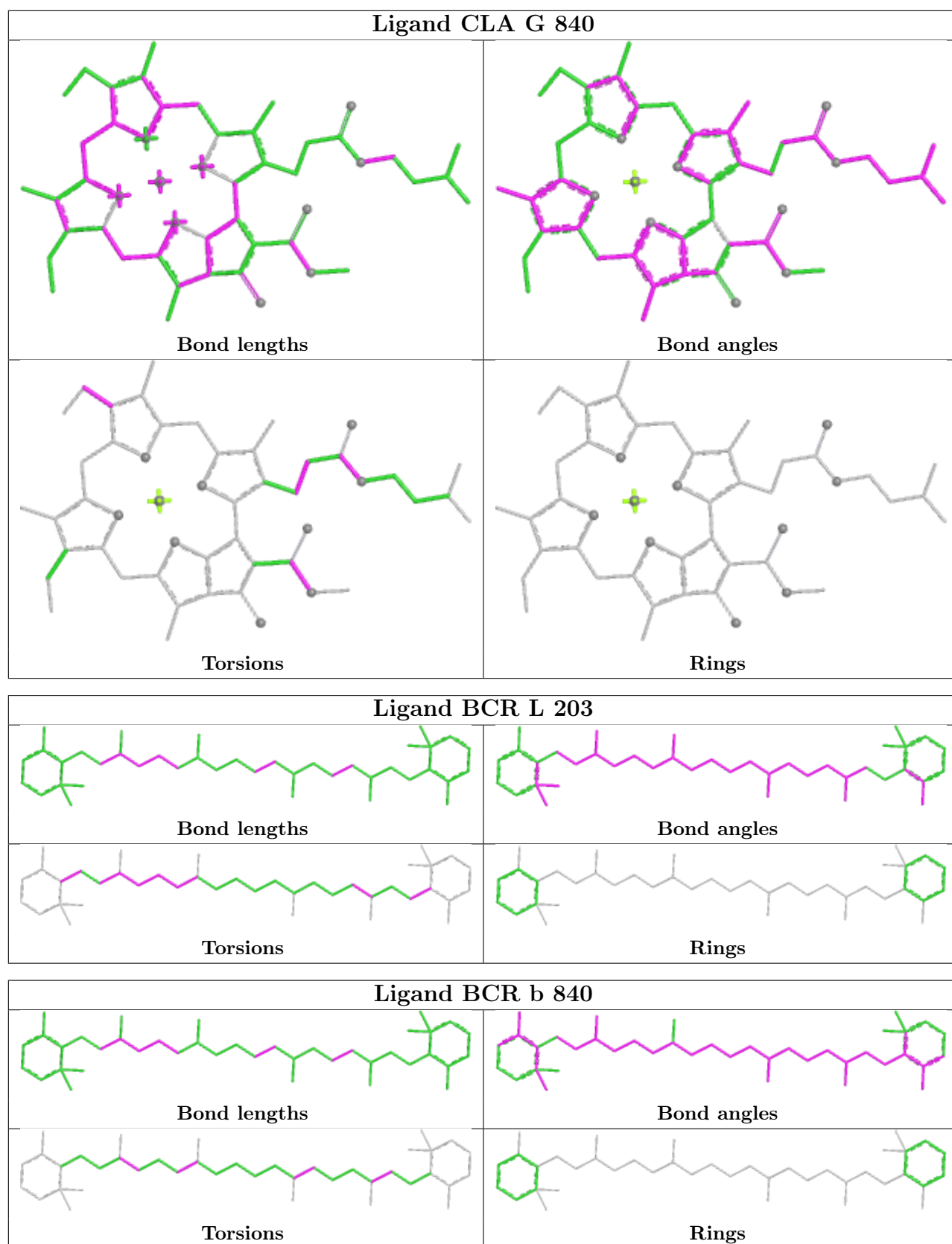
Bond angles

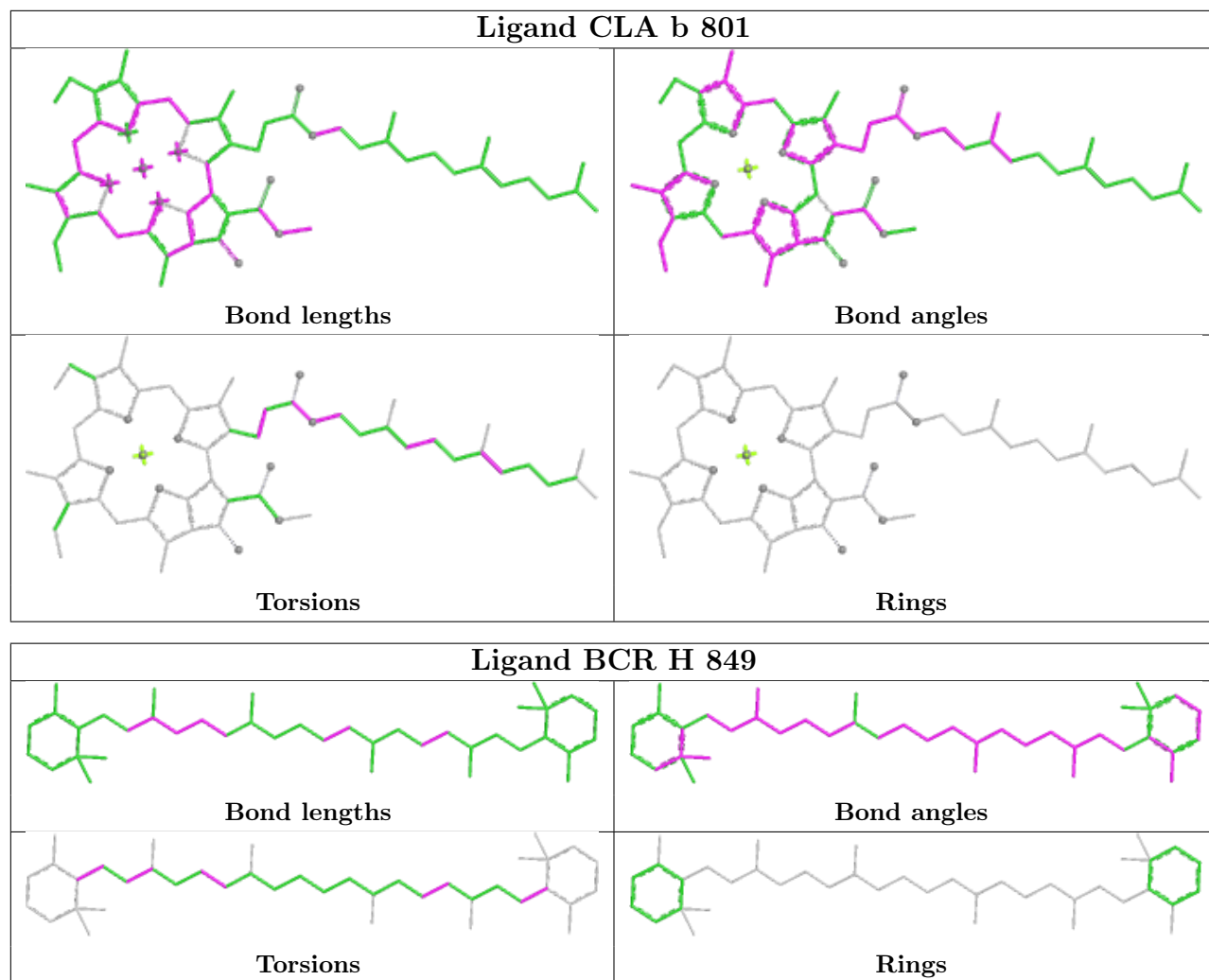


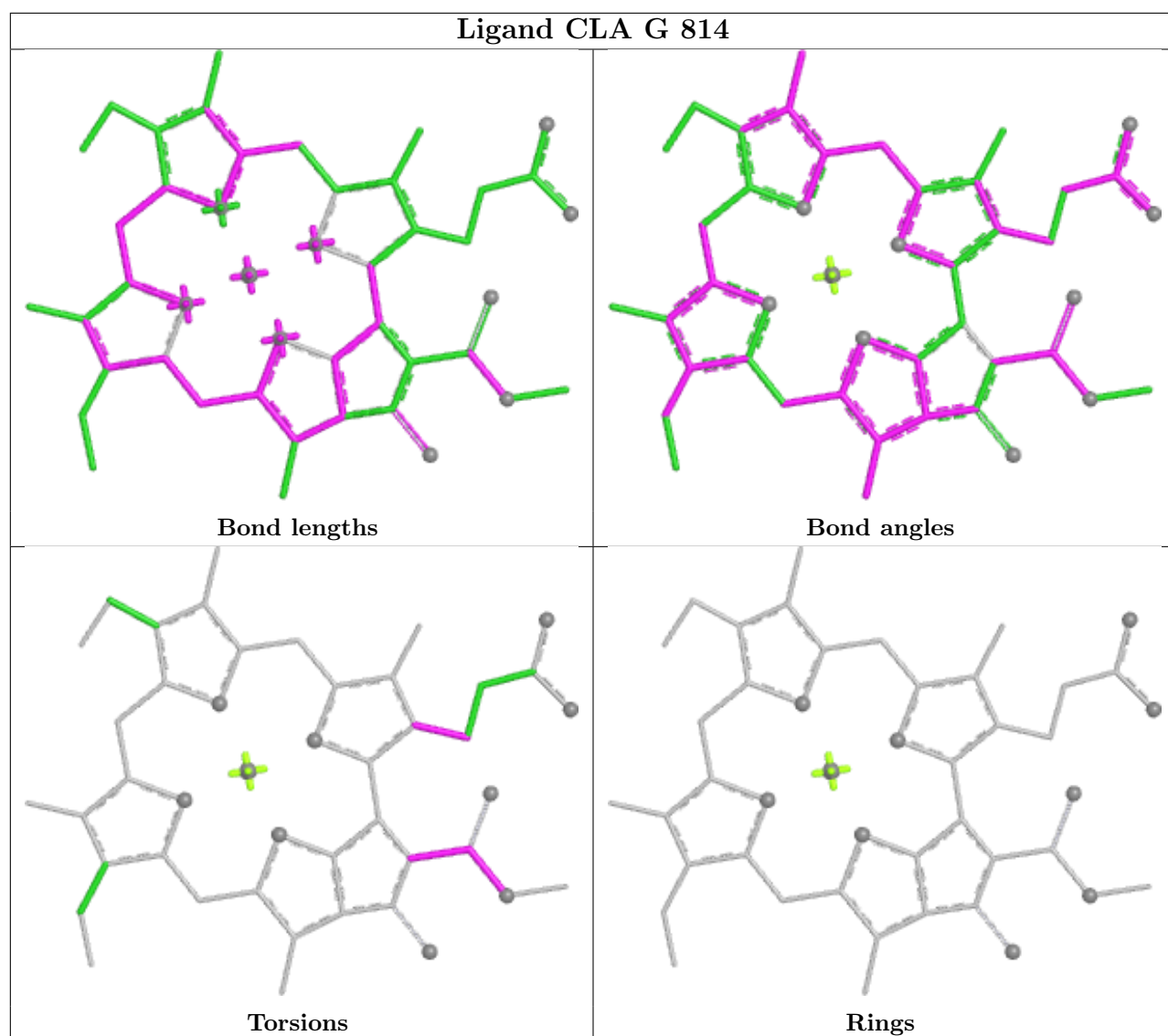
Torsions



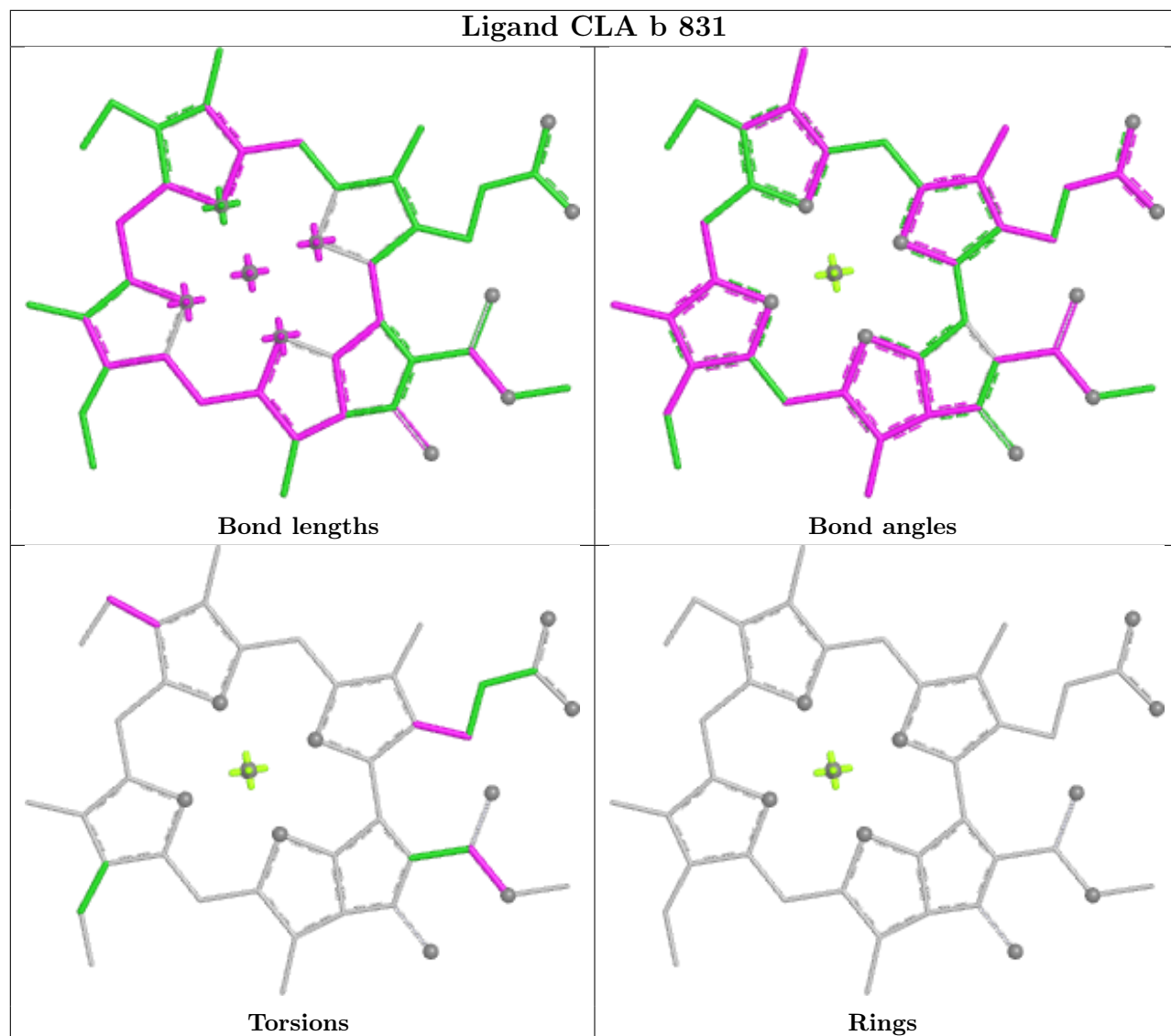
Rings



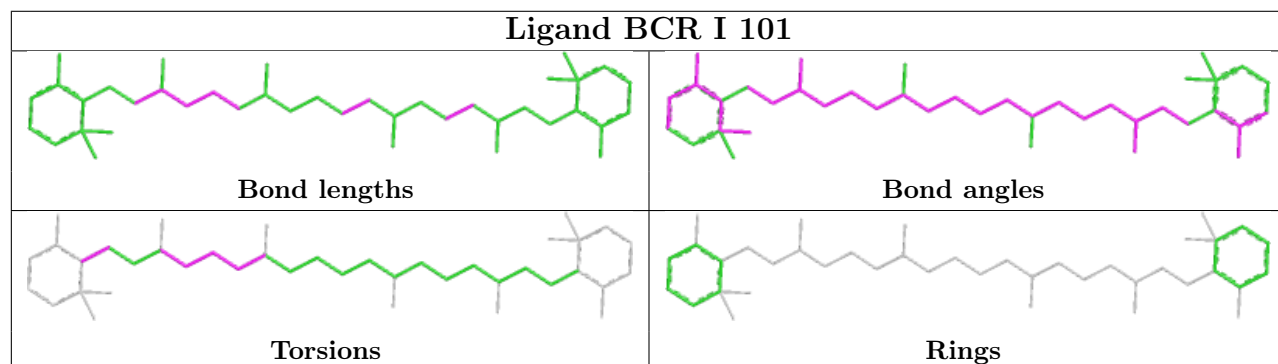




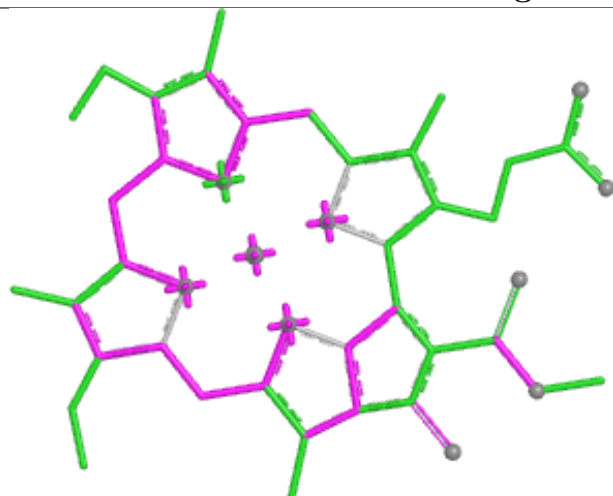
Ligand CLA b 831



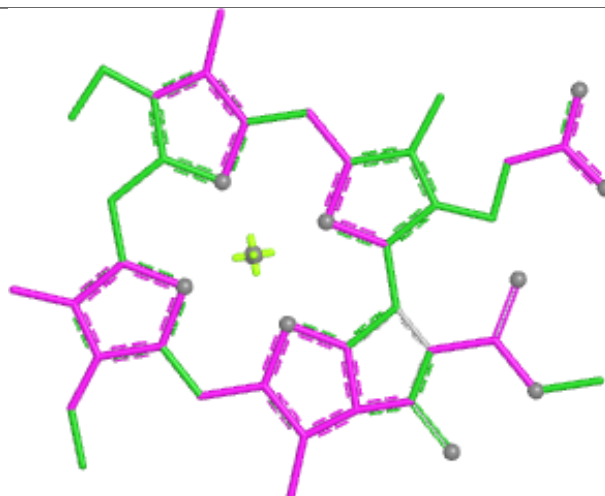
Ligand BCR I 101



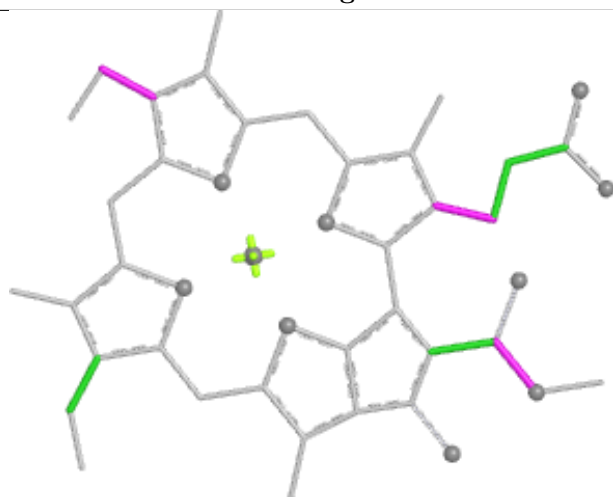
Ligand CLA B 827



Bond lengths



Bond angles

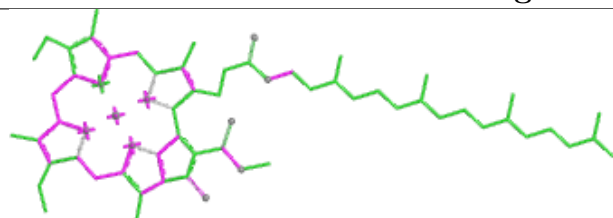


Torsions

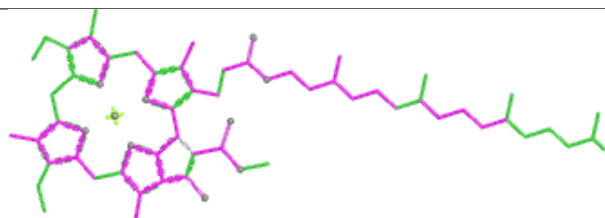


Rings

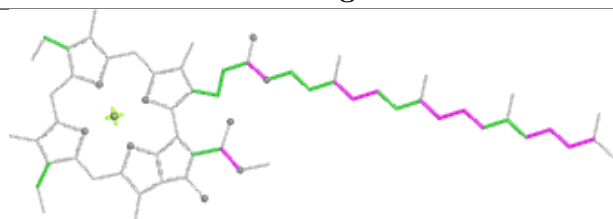
Ligand CLA B 802



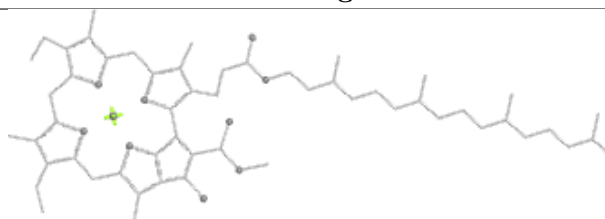
Bond lengths



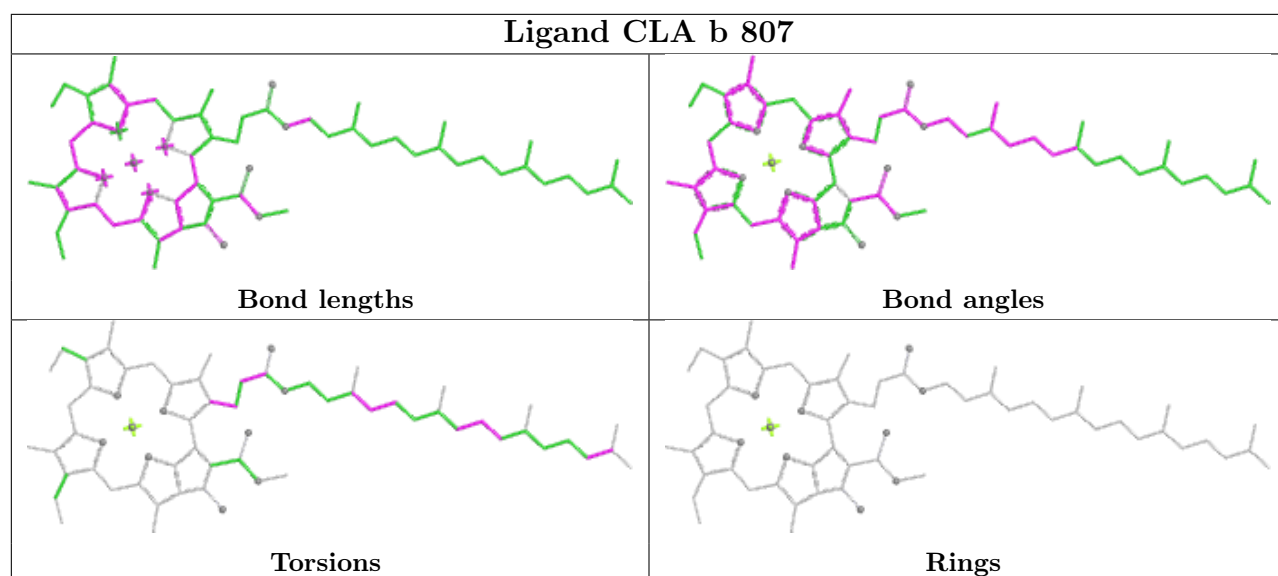
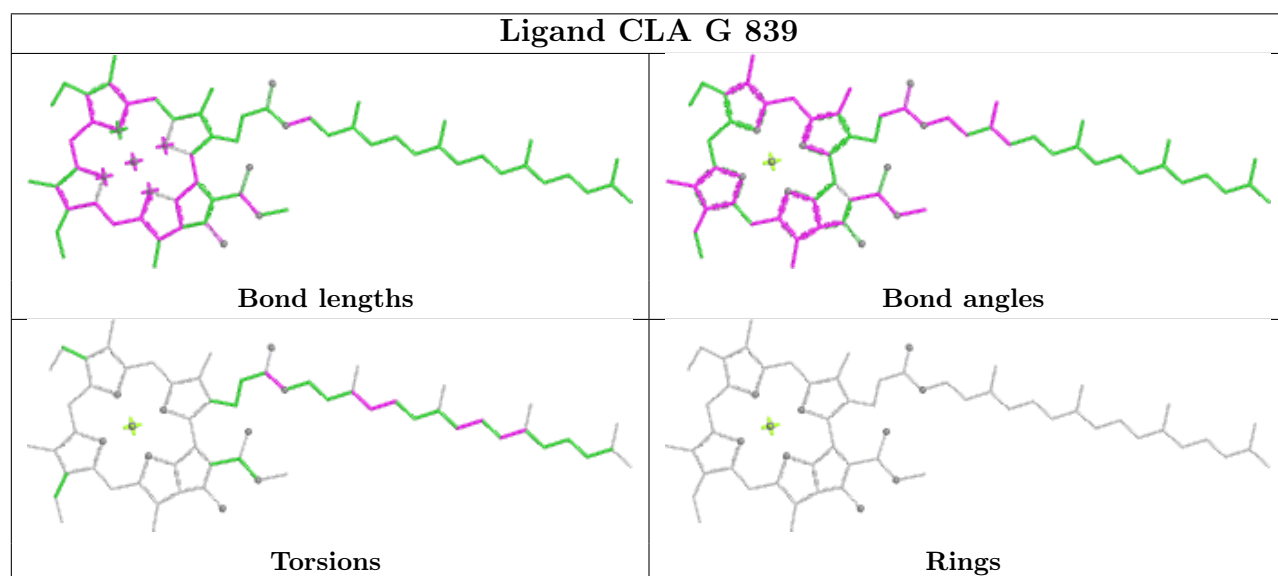
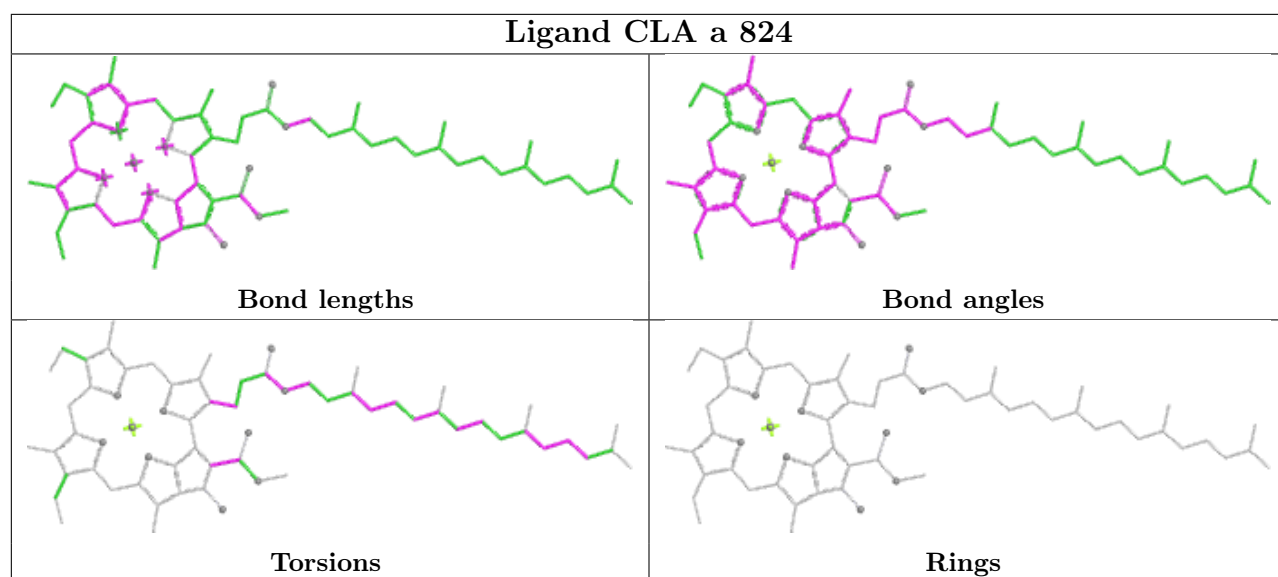
Bond angles

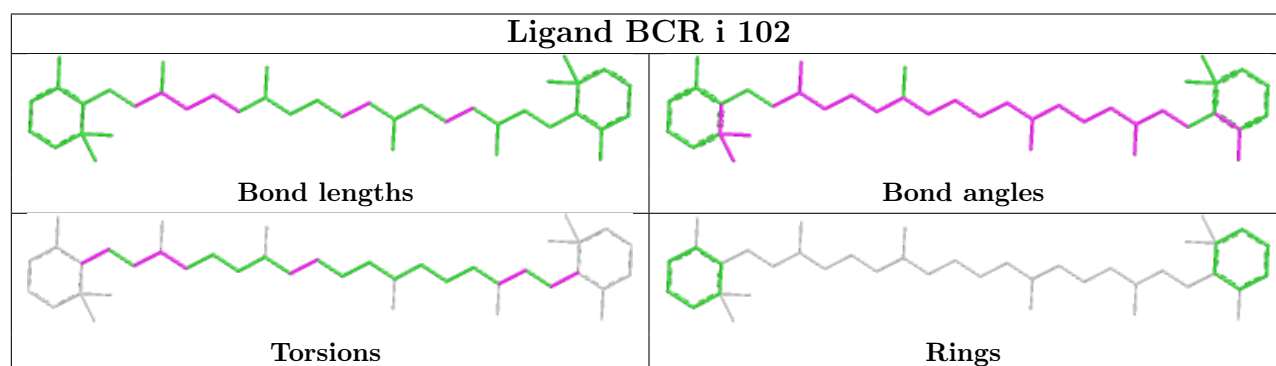
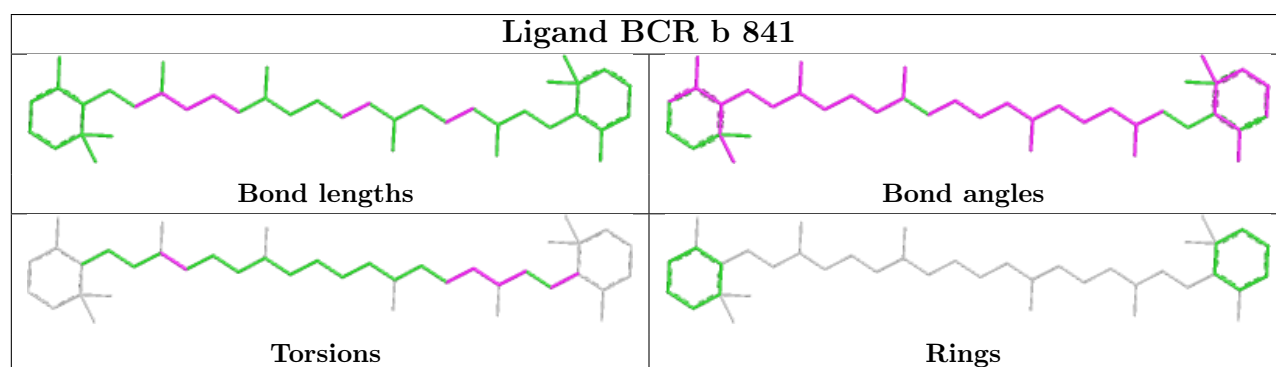
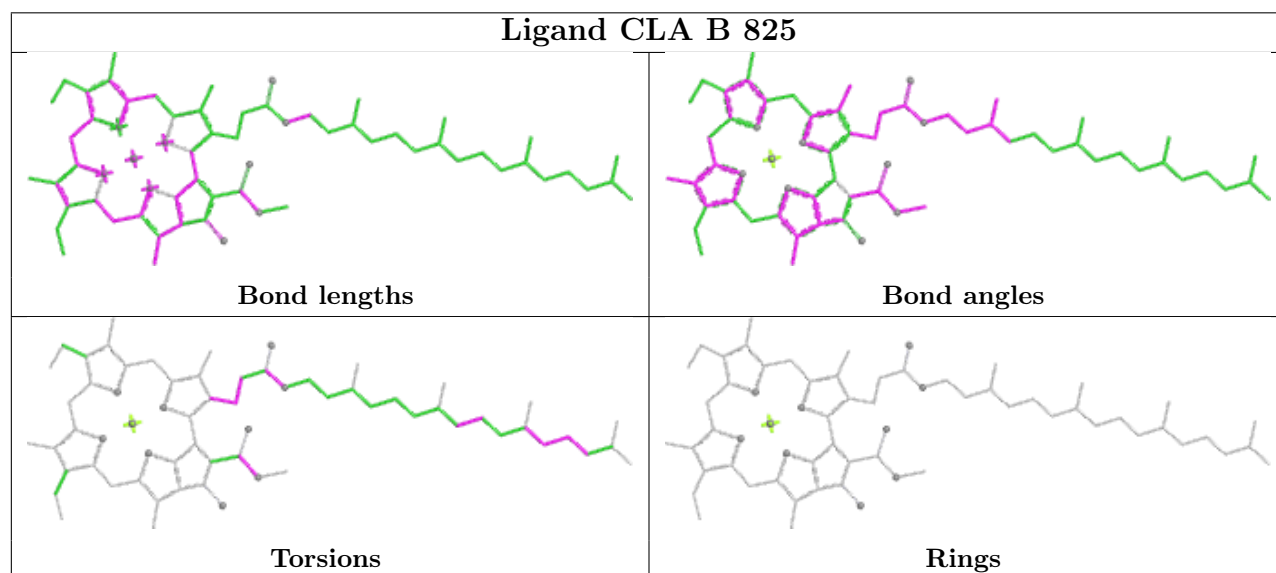
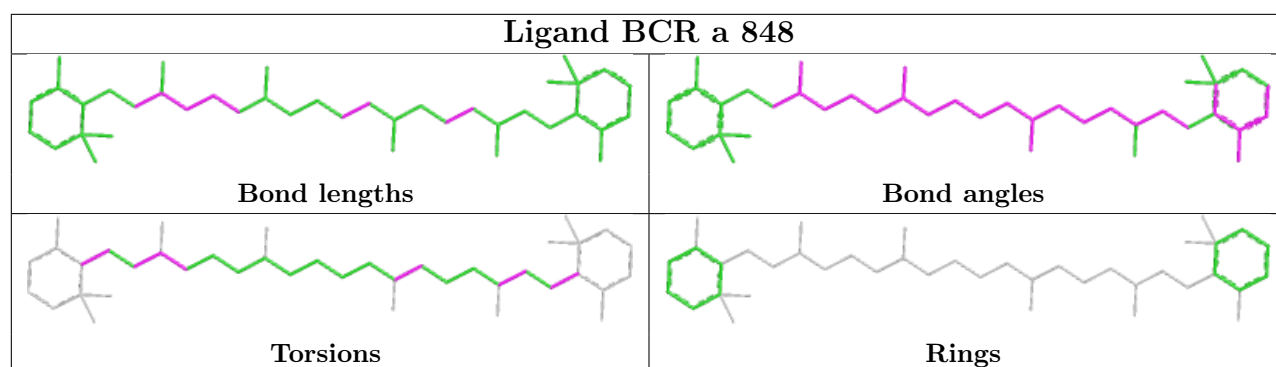


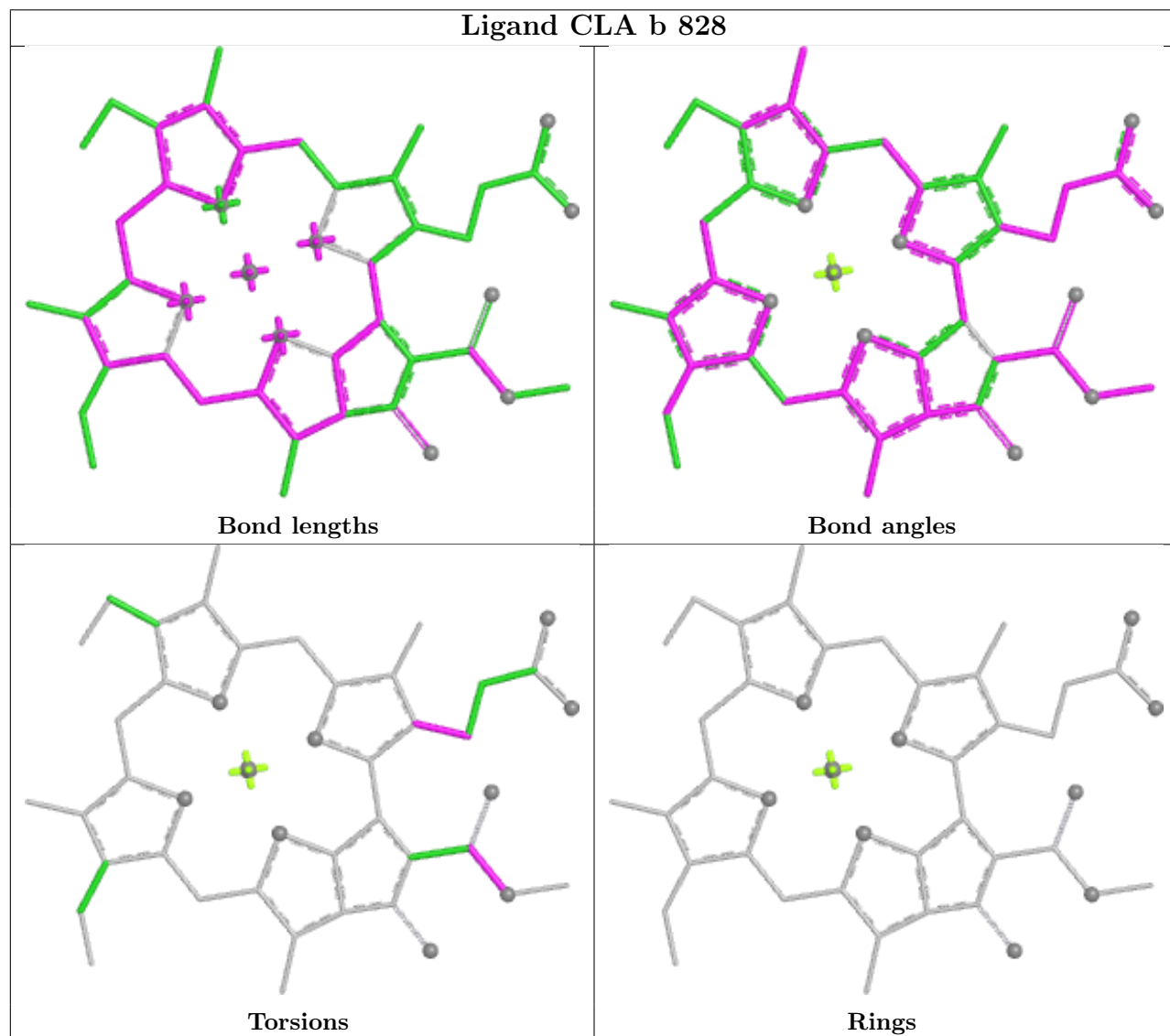
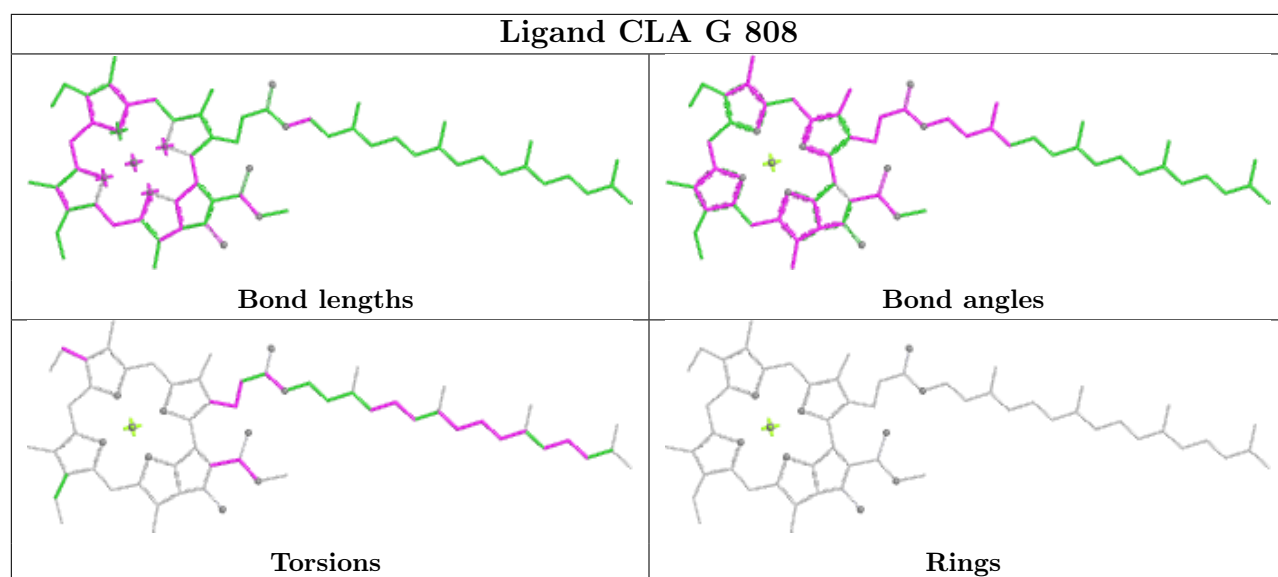
Torsions

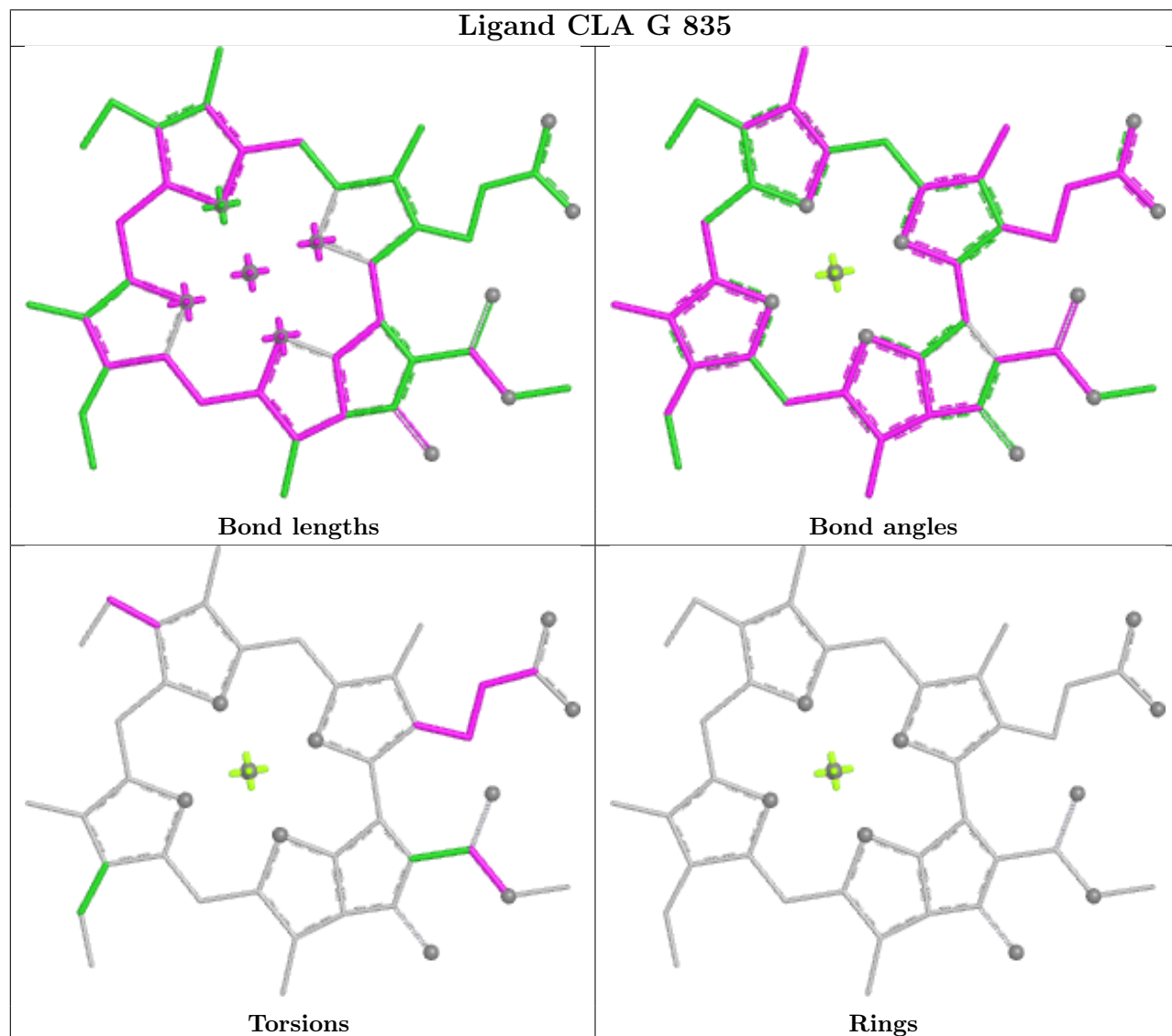
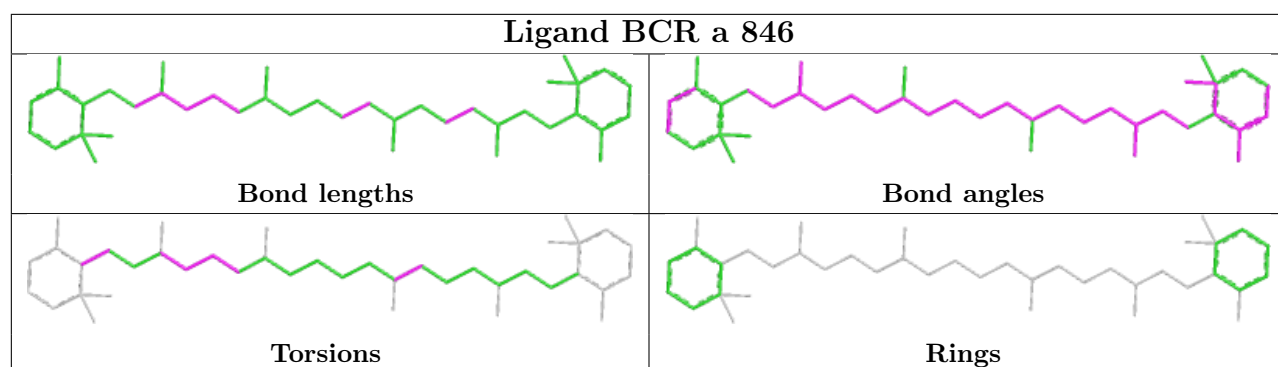


Rings

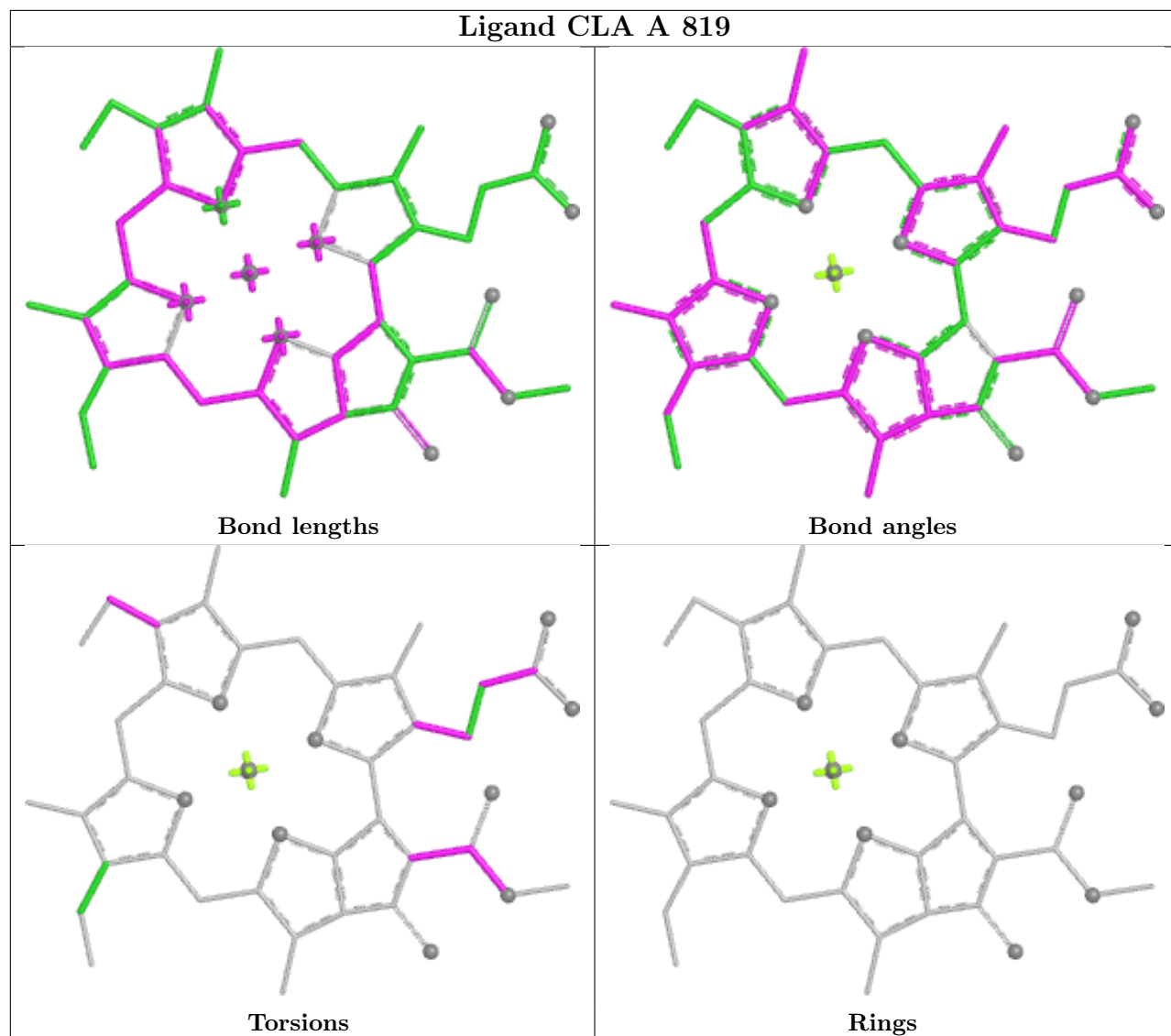


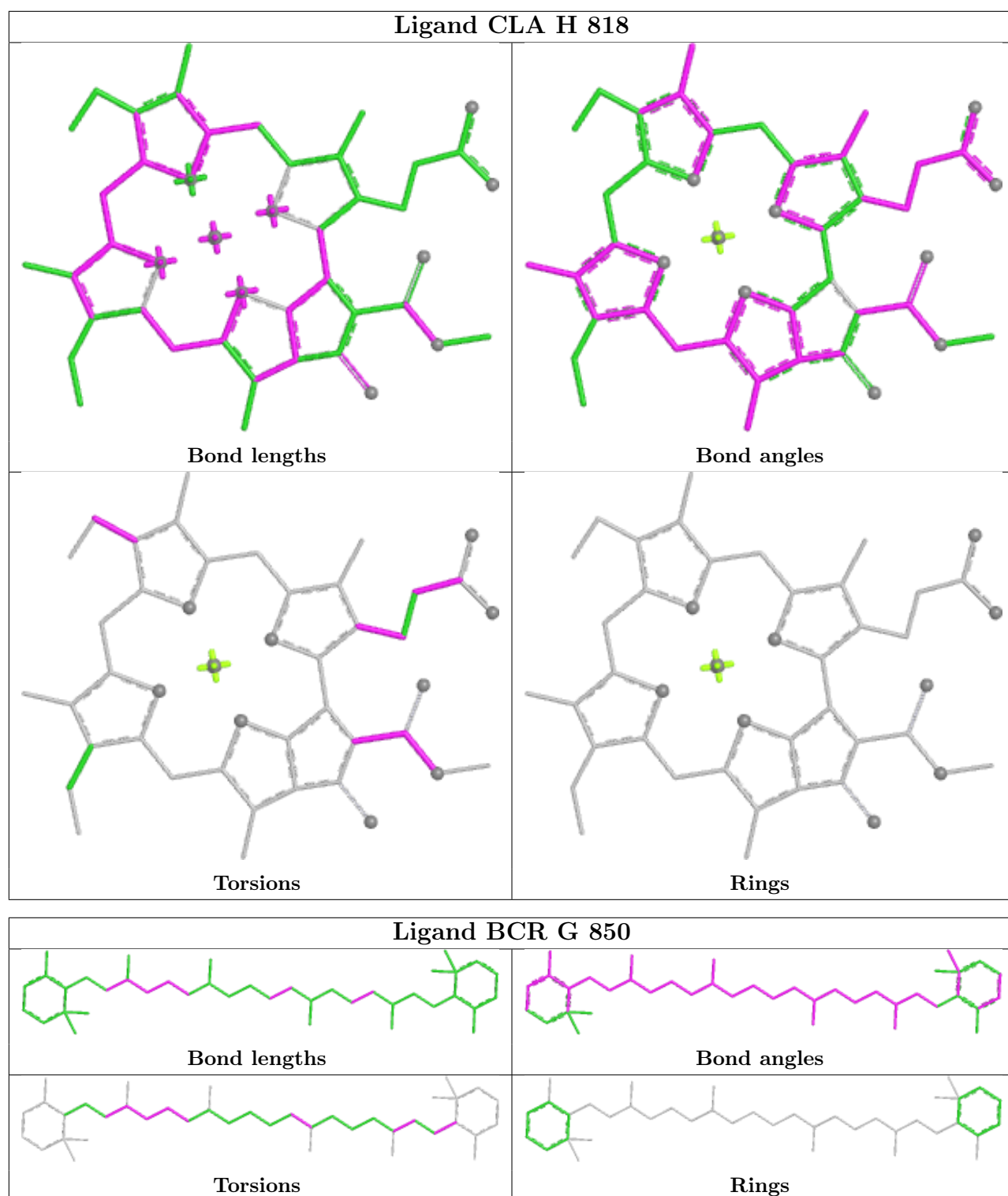


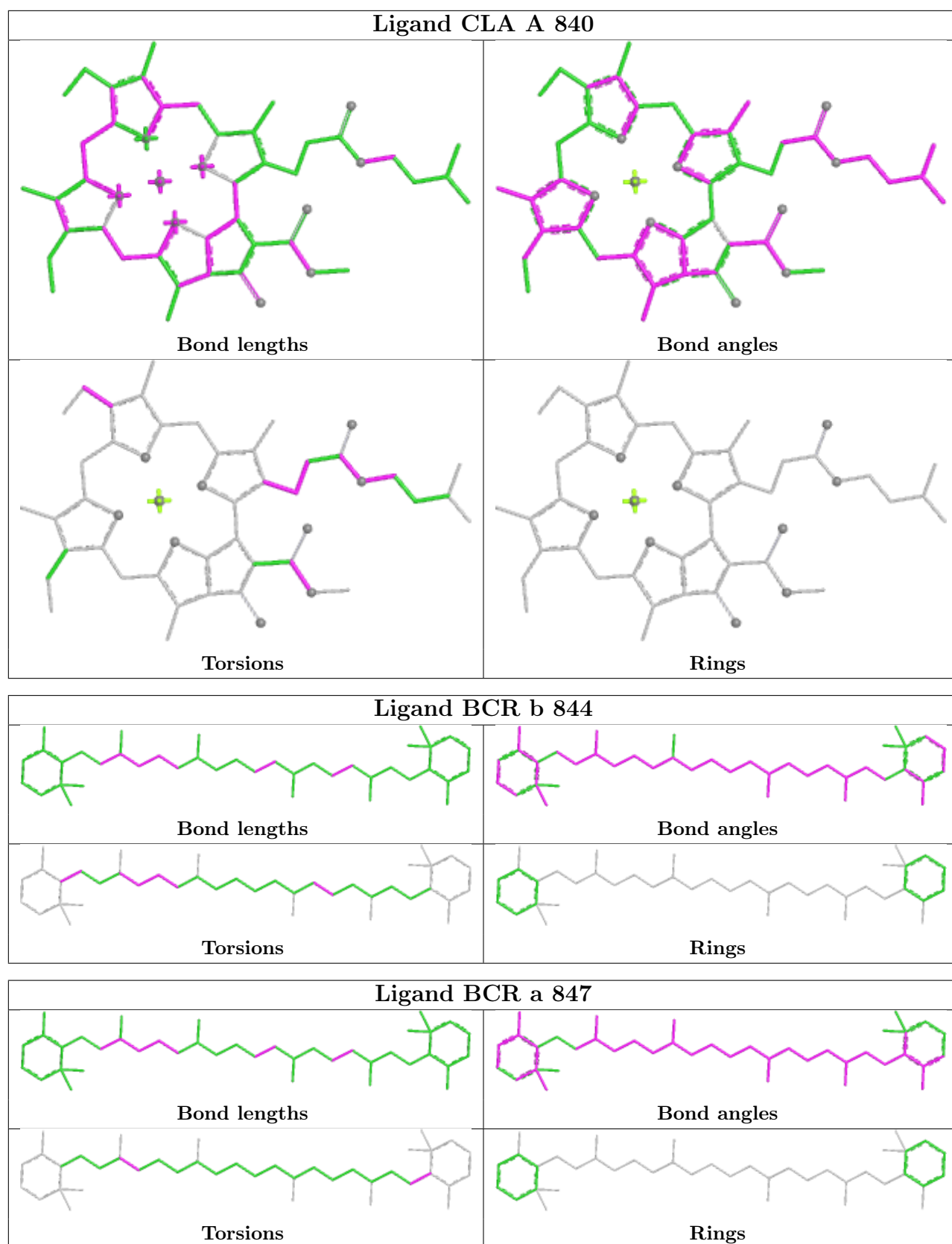


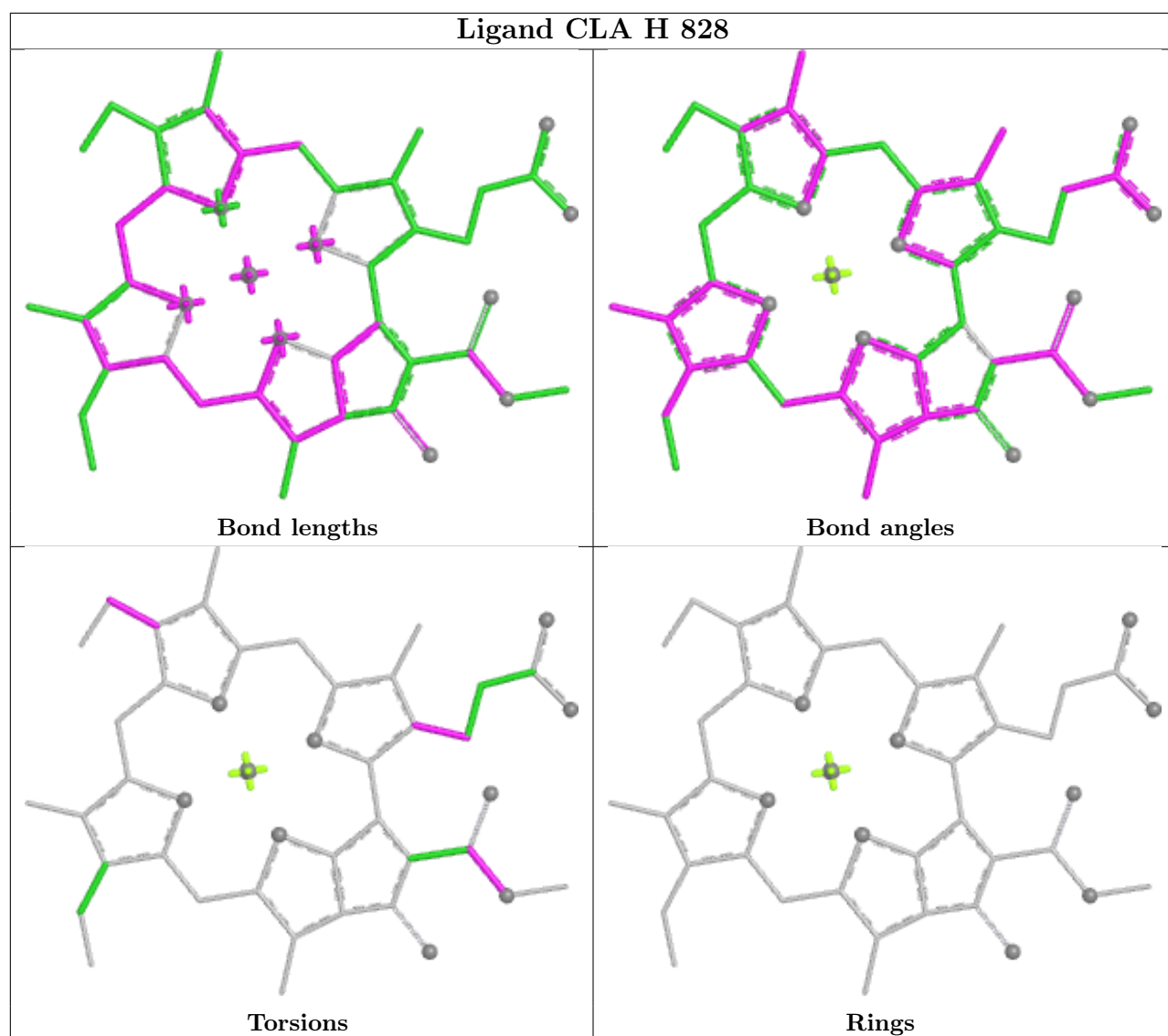


Ligand CLA A 819

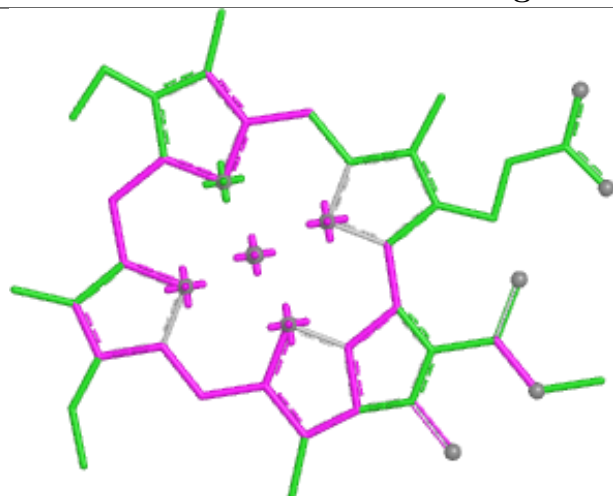




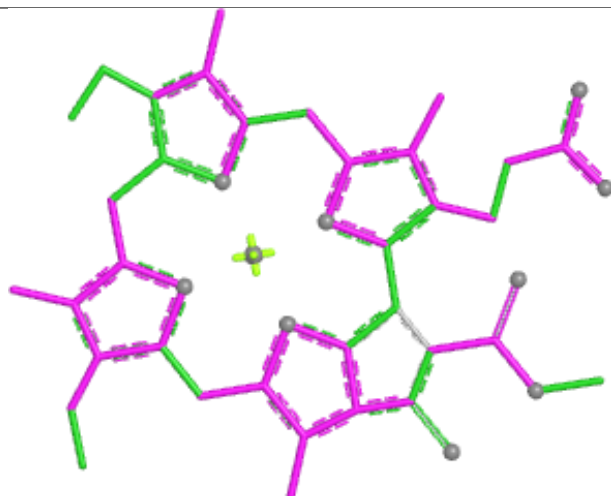




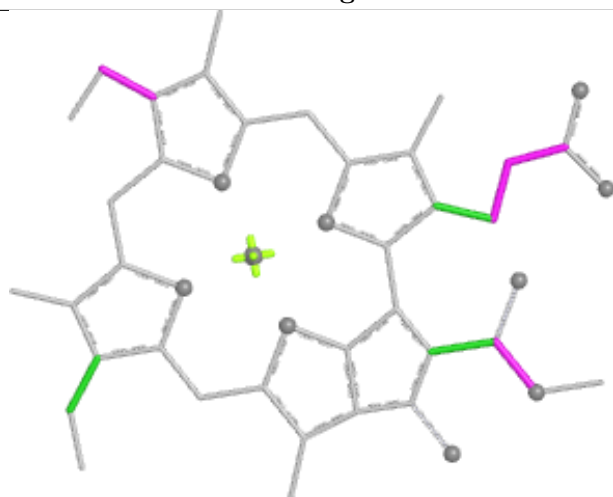
Ligand CLA H 820



Bond lengths



Bond angles

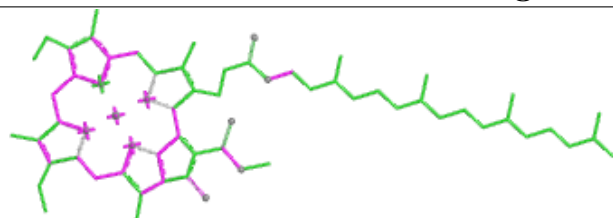


Torsions

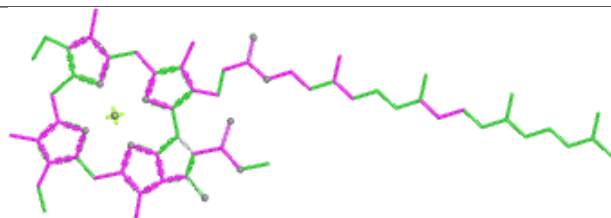


Rings

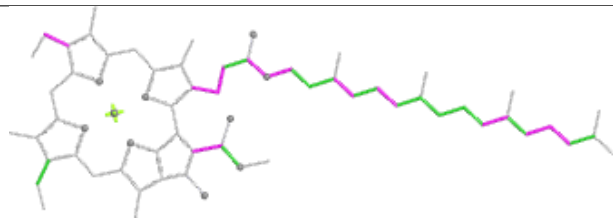
Ligand CLA B 821



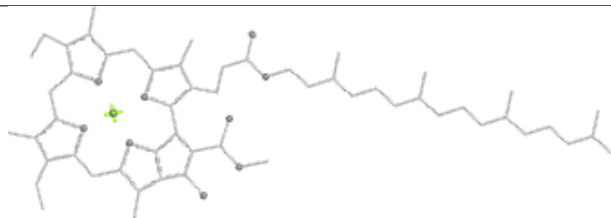
Bond lengths



Bond angles

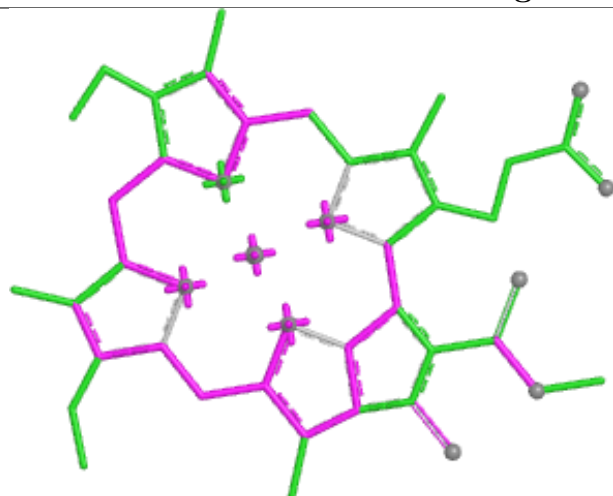


Torsions

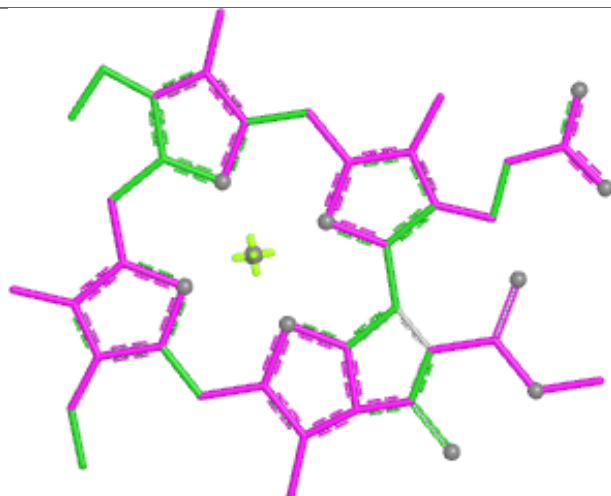


Rings

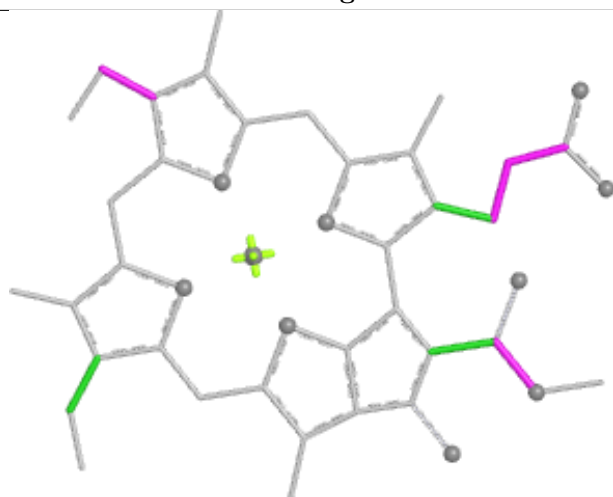
Ligand CLA B 819



Bond lengths



Bond angles

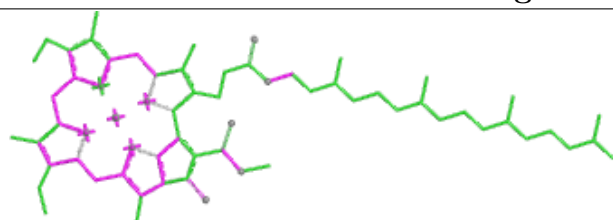


Torsions

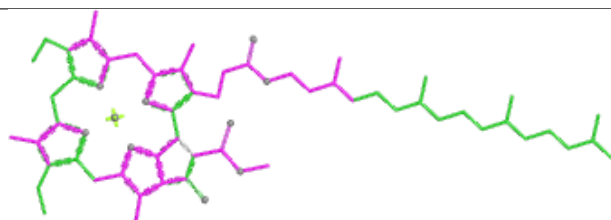


Rings

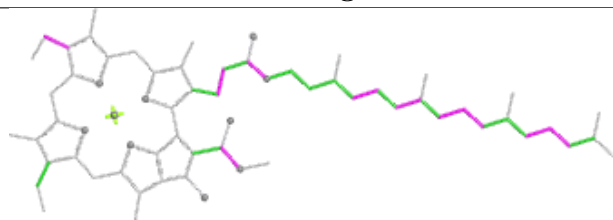
Ligand CLA B 836



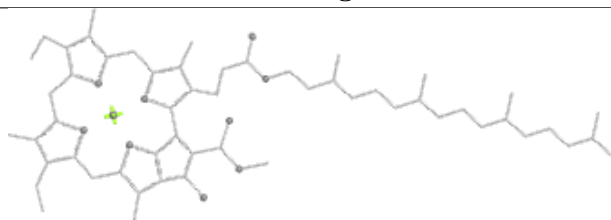
Bond lengths



Bond angles

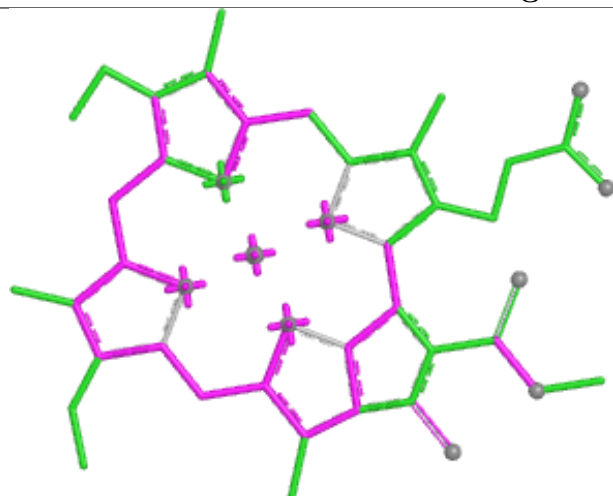


Torsions

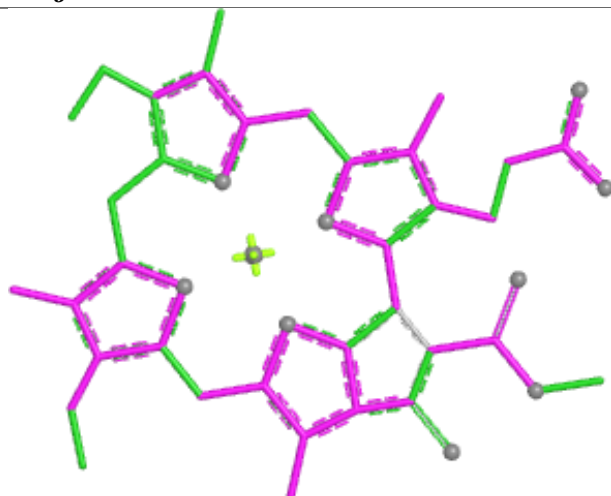


Rings

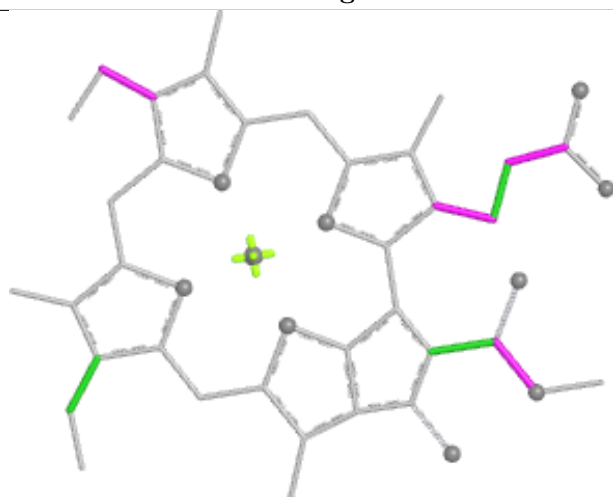
Ligand CLA j 104



Bond lengths



Bond angles

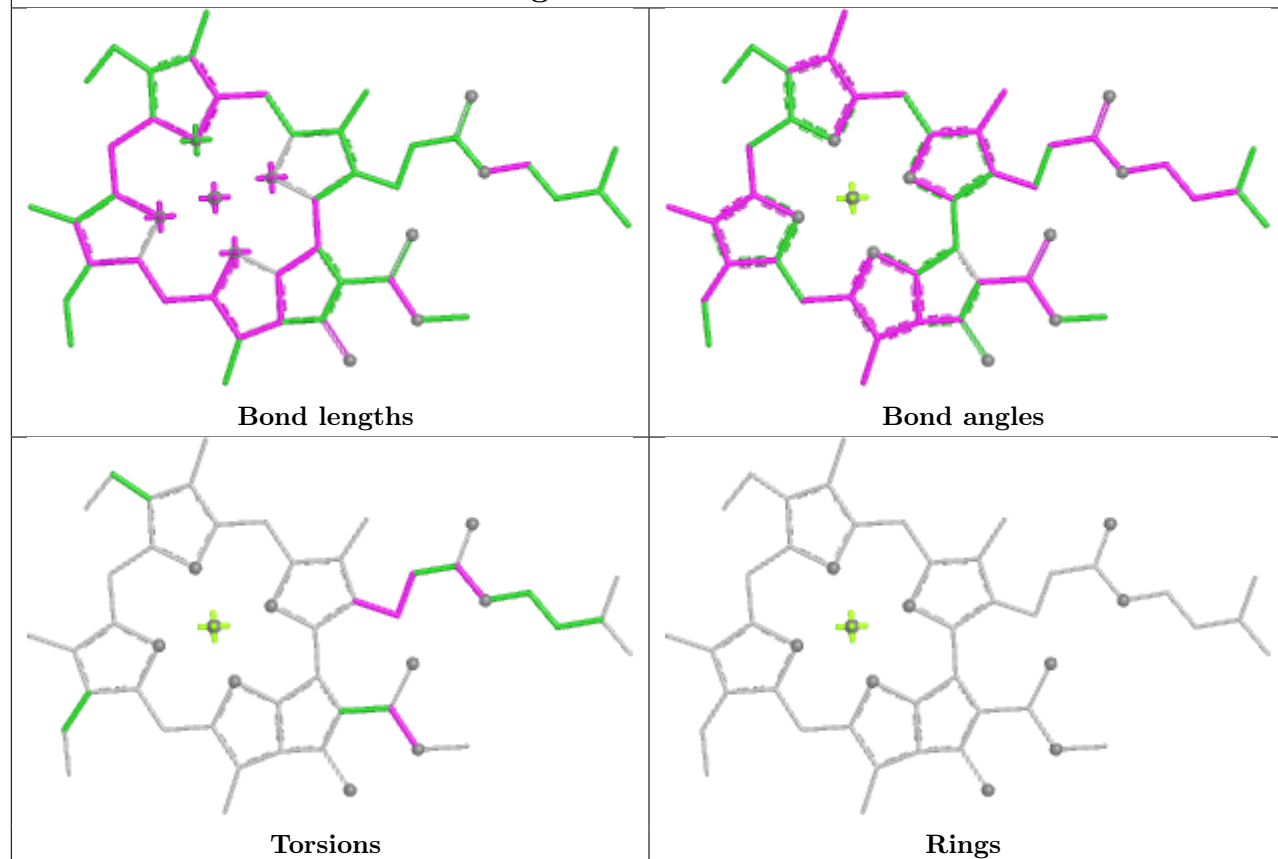


Torsions

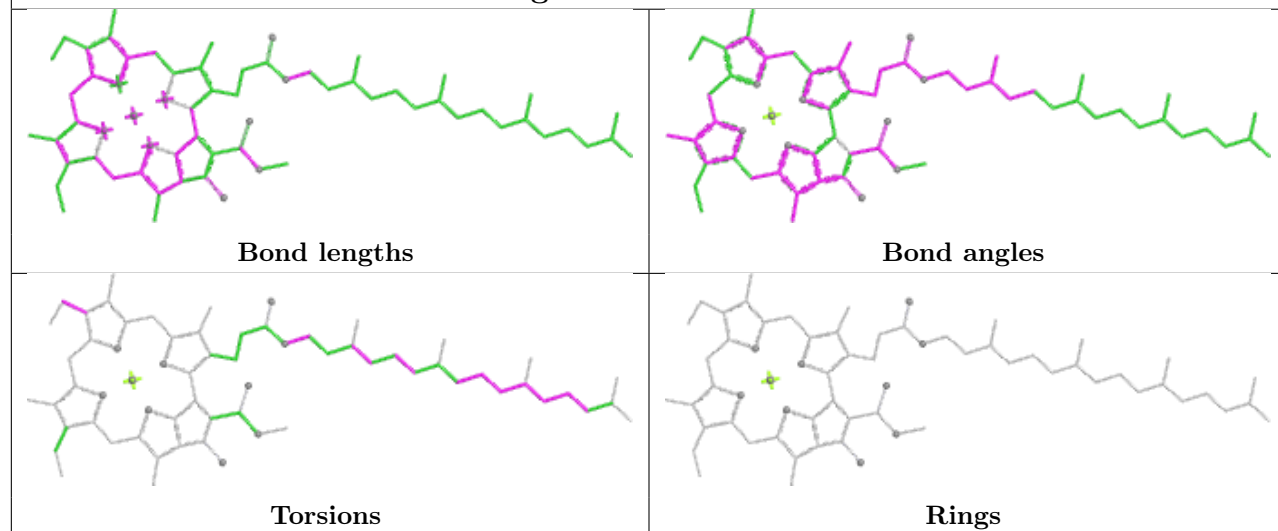


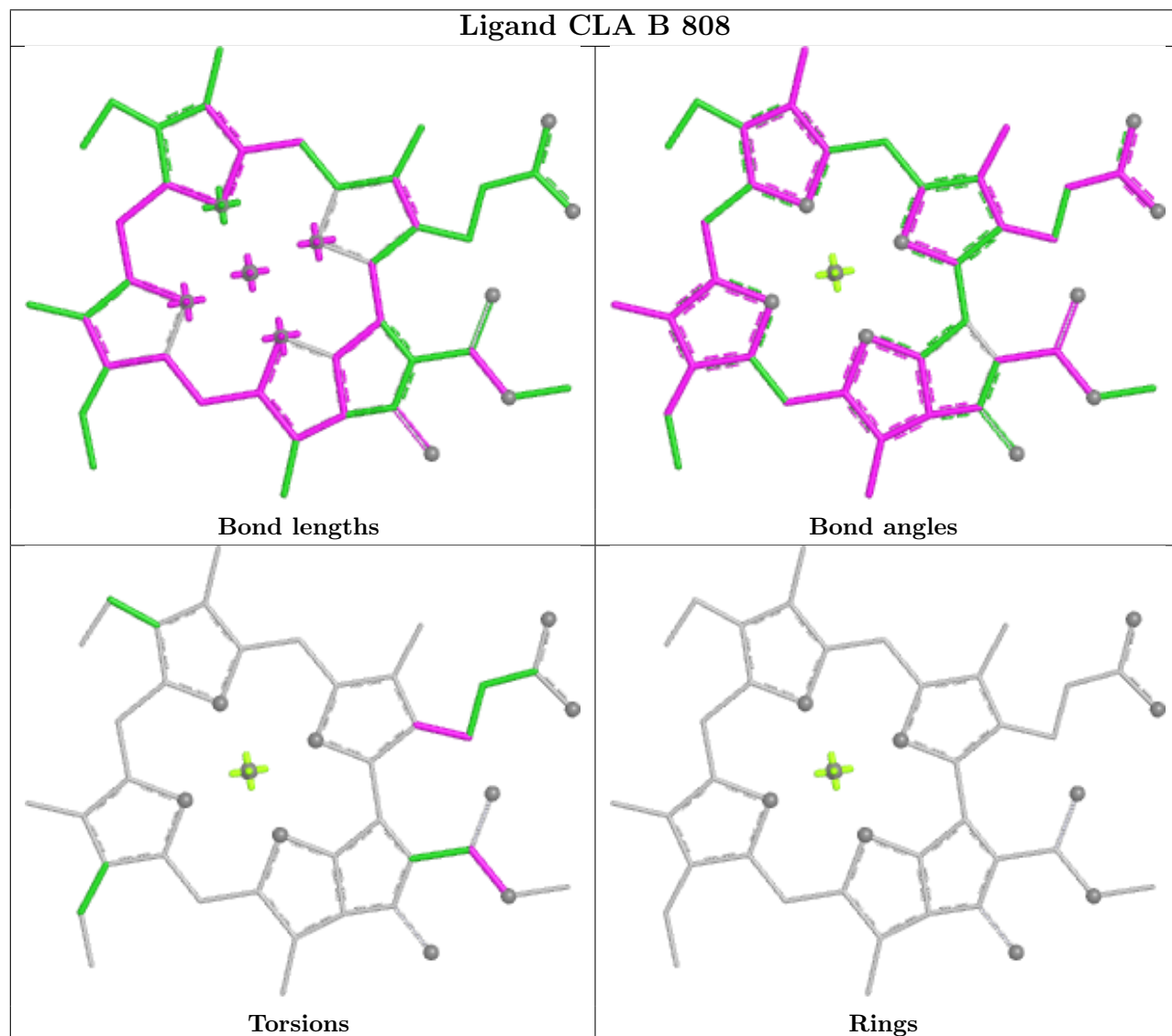
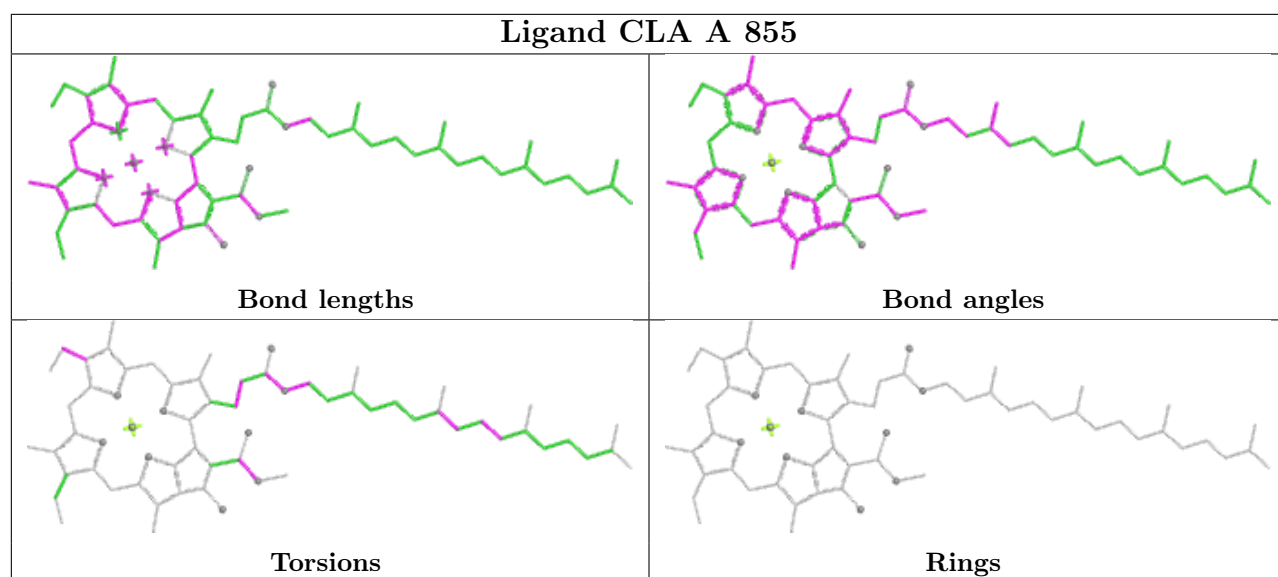
Rings

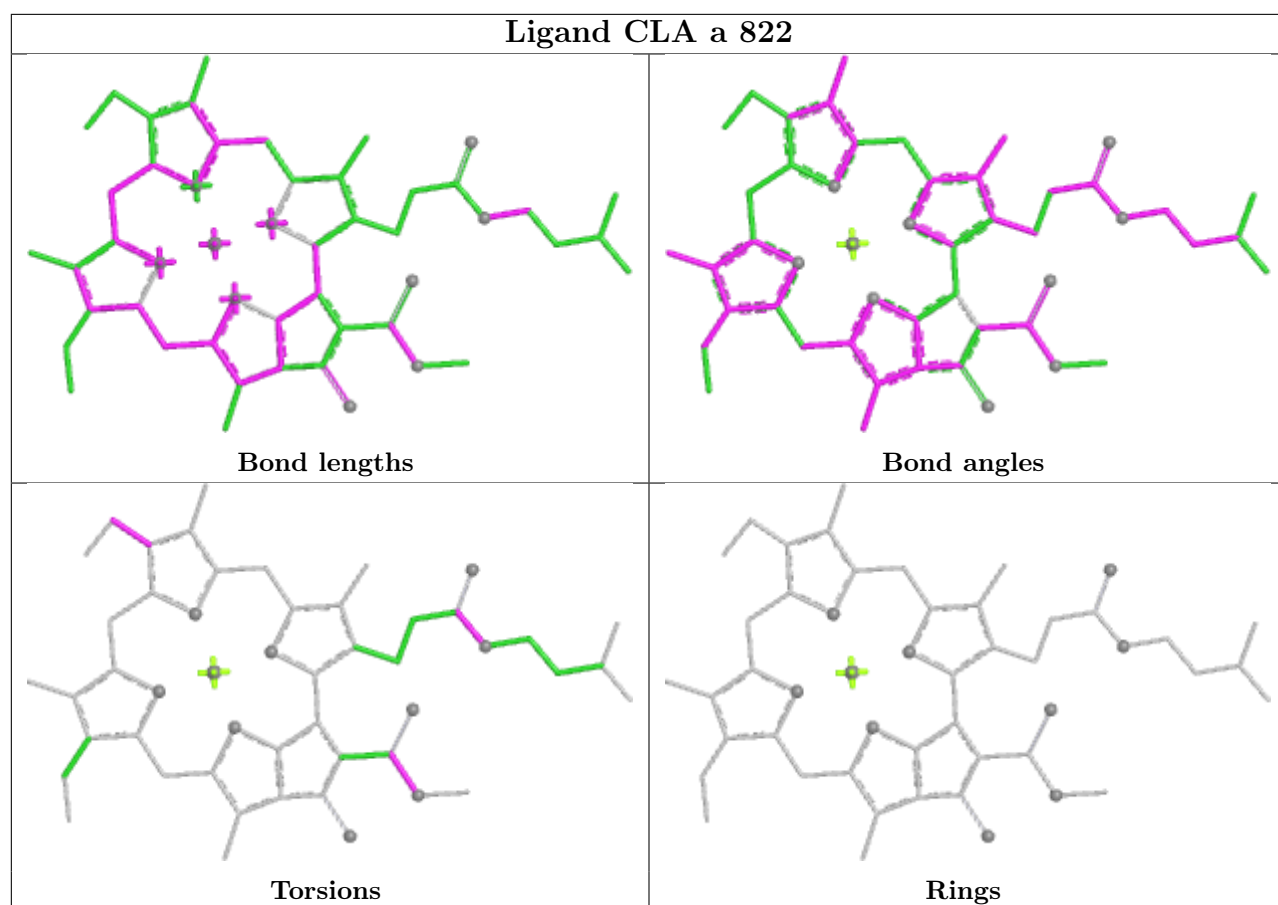
Ligand CLA G 809



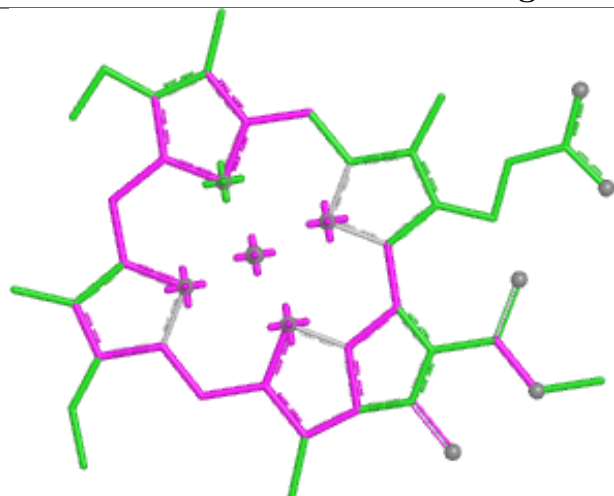
Ligand CLA G 837



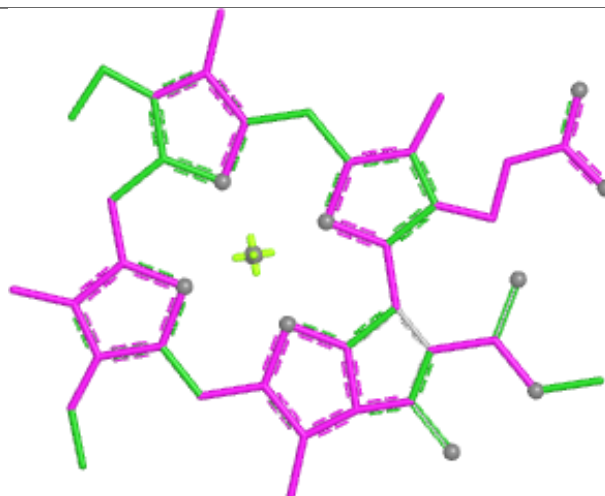




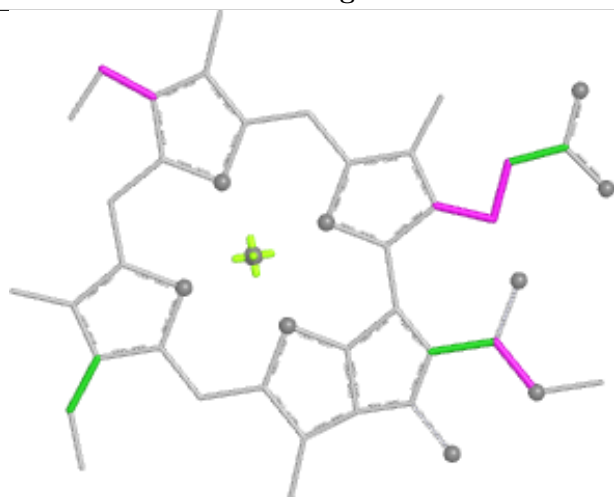
Ligand CLA a 835



Bond lengths



Bond angles

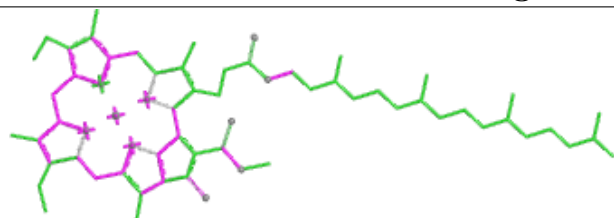


Torsions

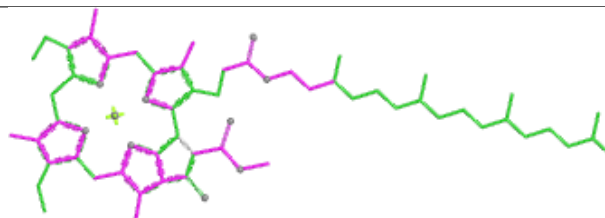


Rings

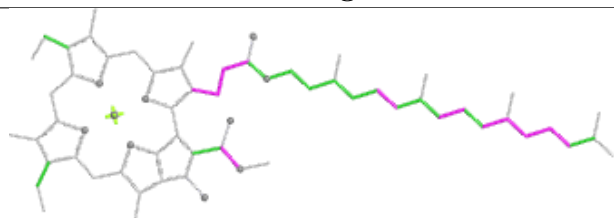
Ligand CLA G 829



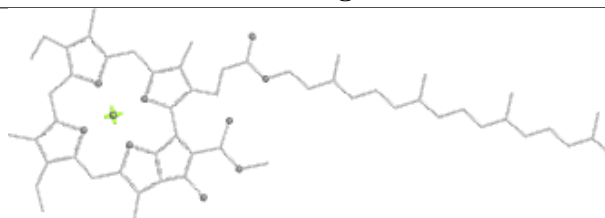
Bond lengths



Bond angles

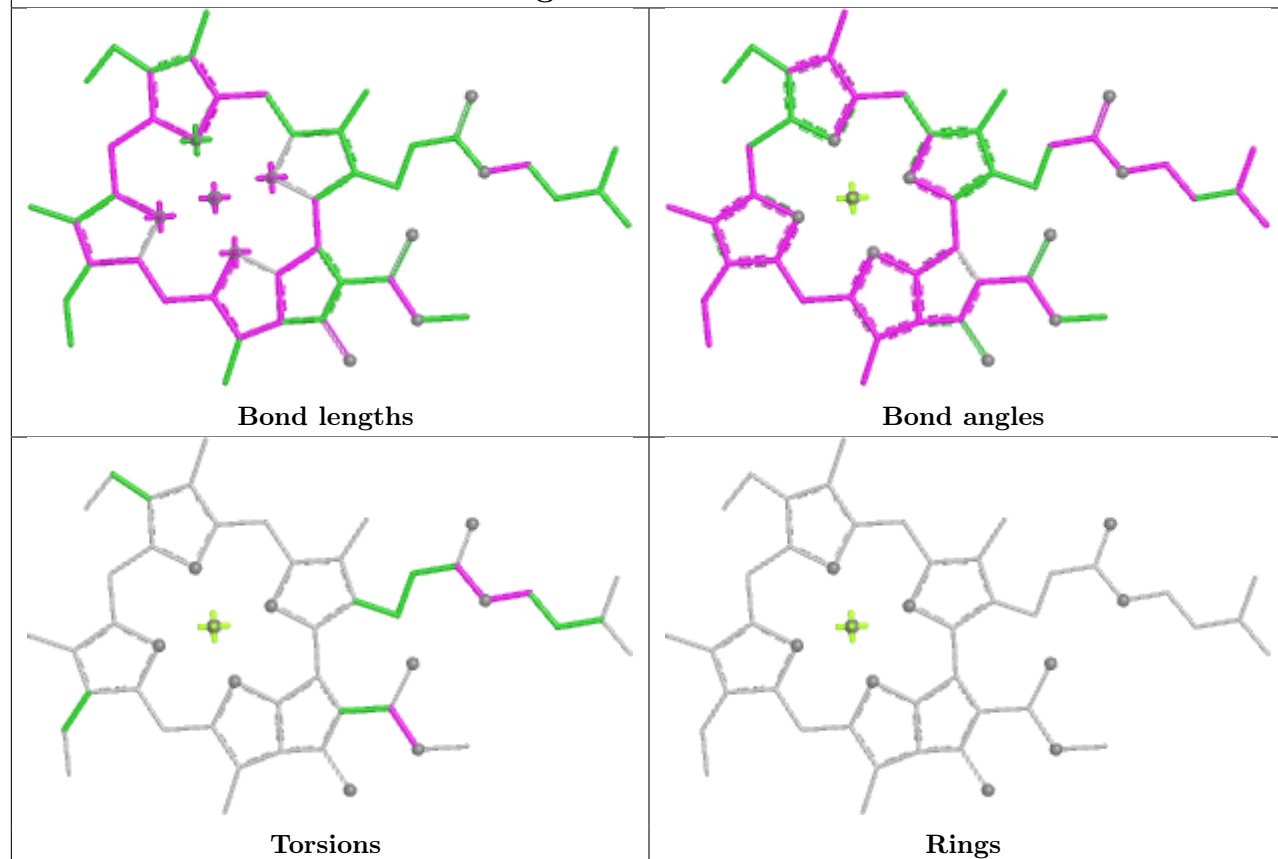


Torsions

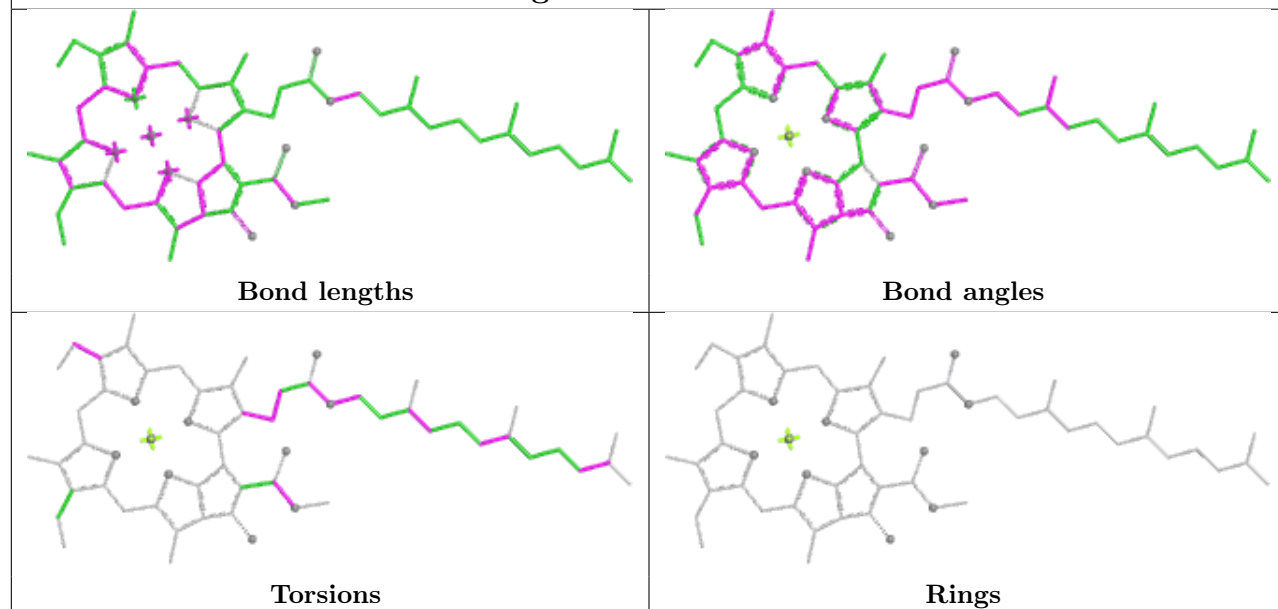


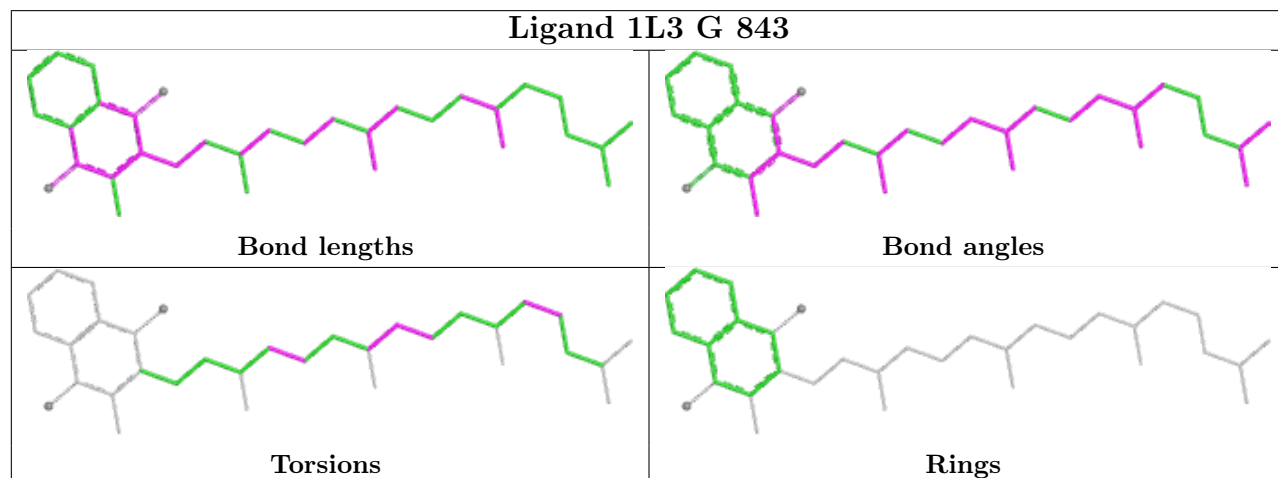
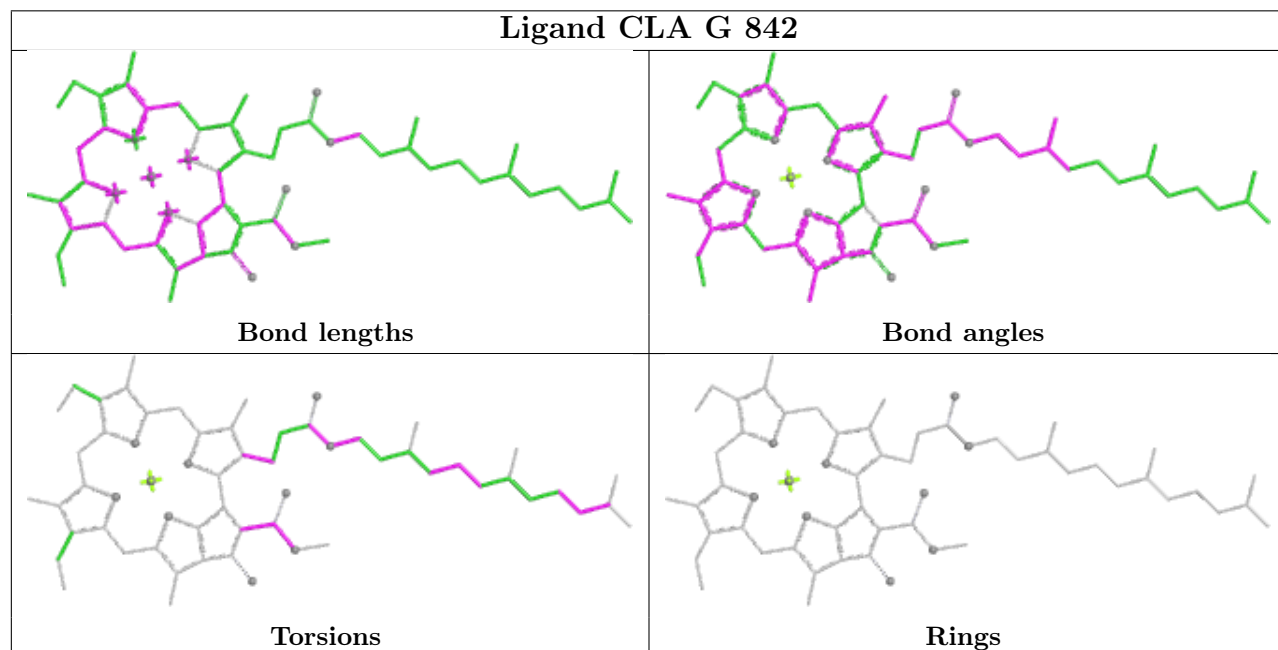
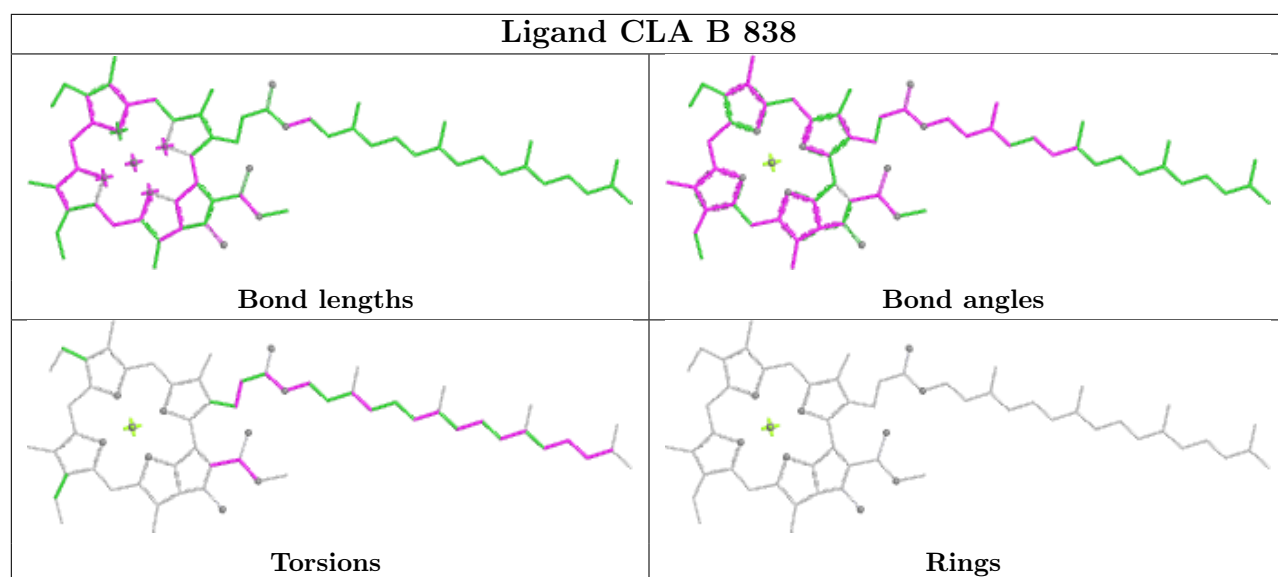
Rings

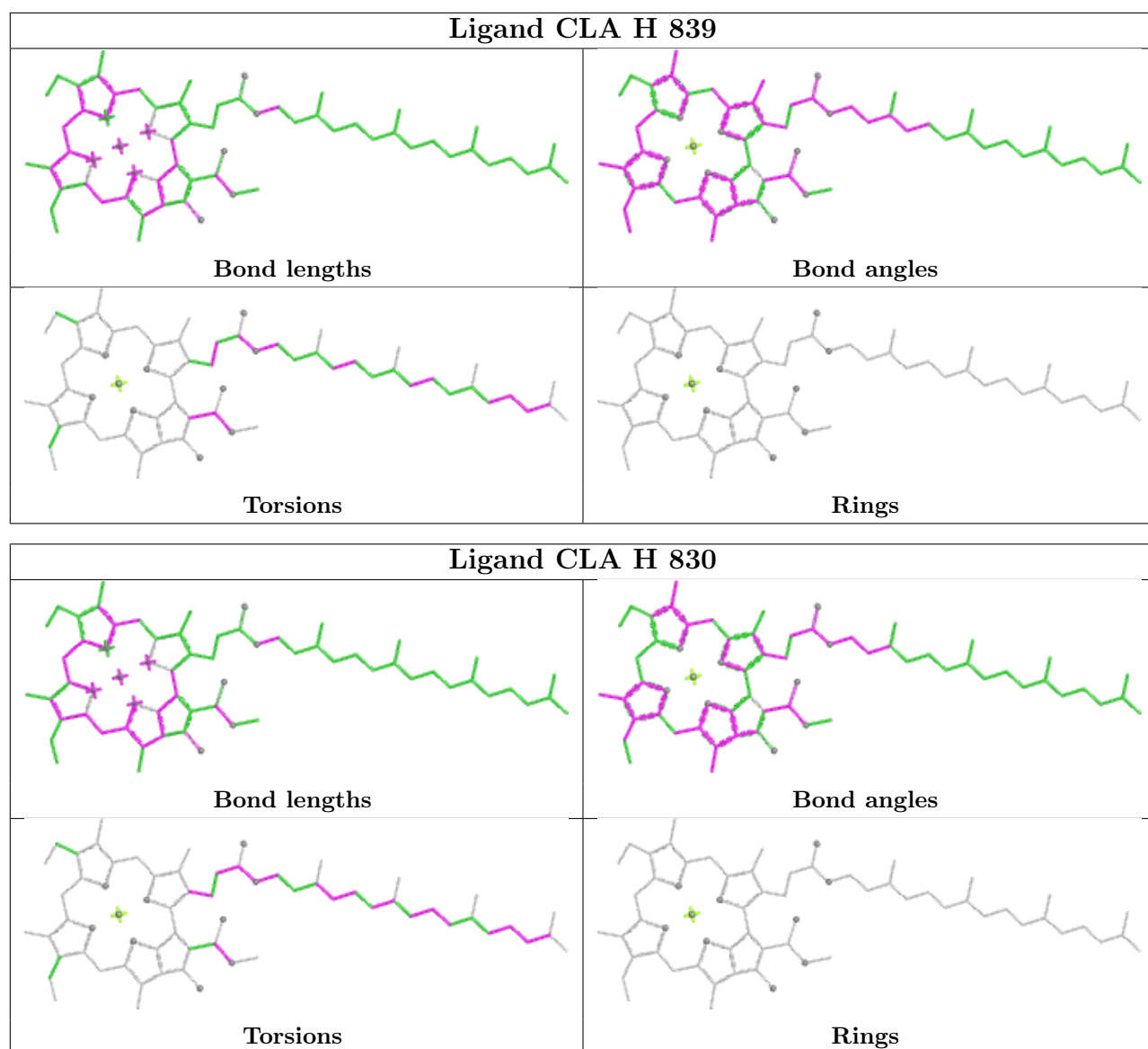
Ligand CLA a 836



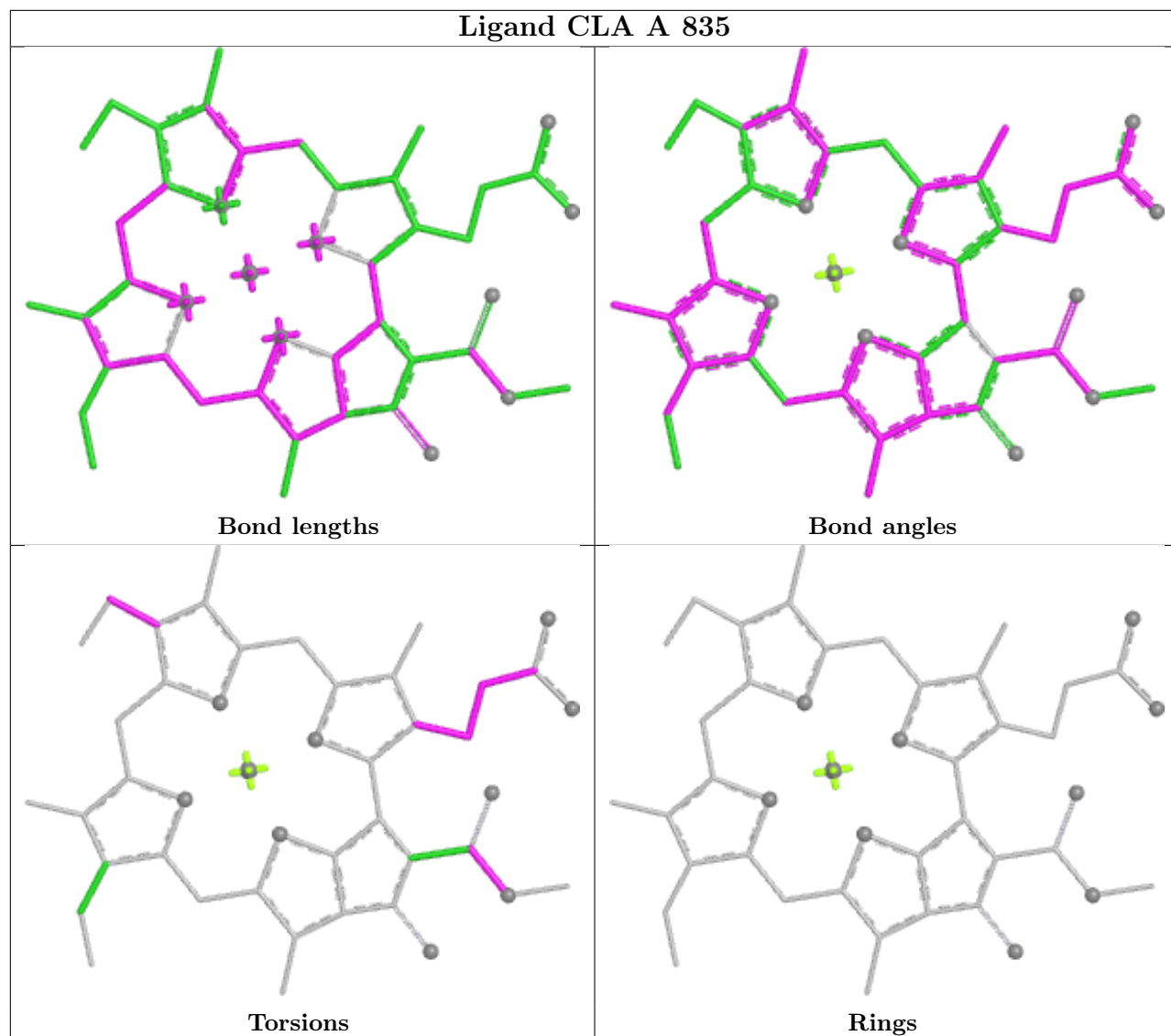
Ligand CLA A 827



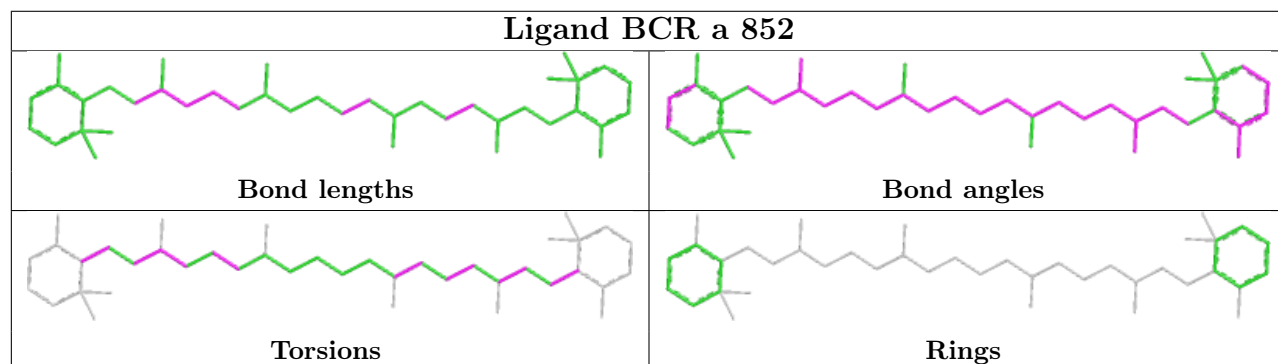


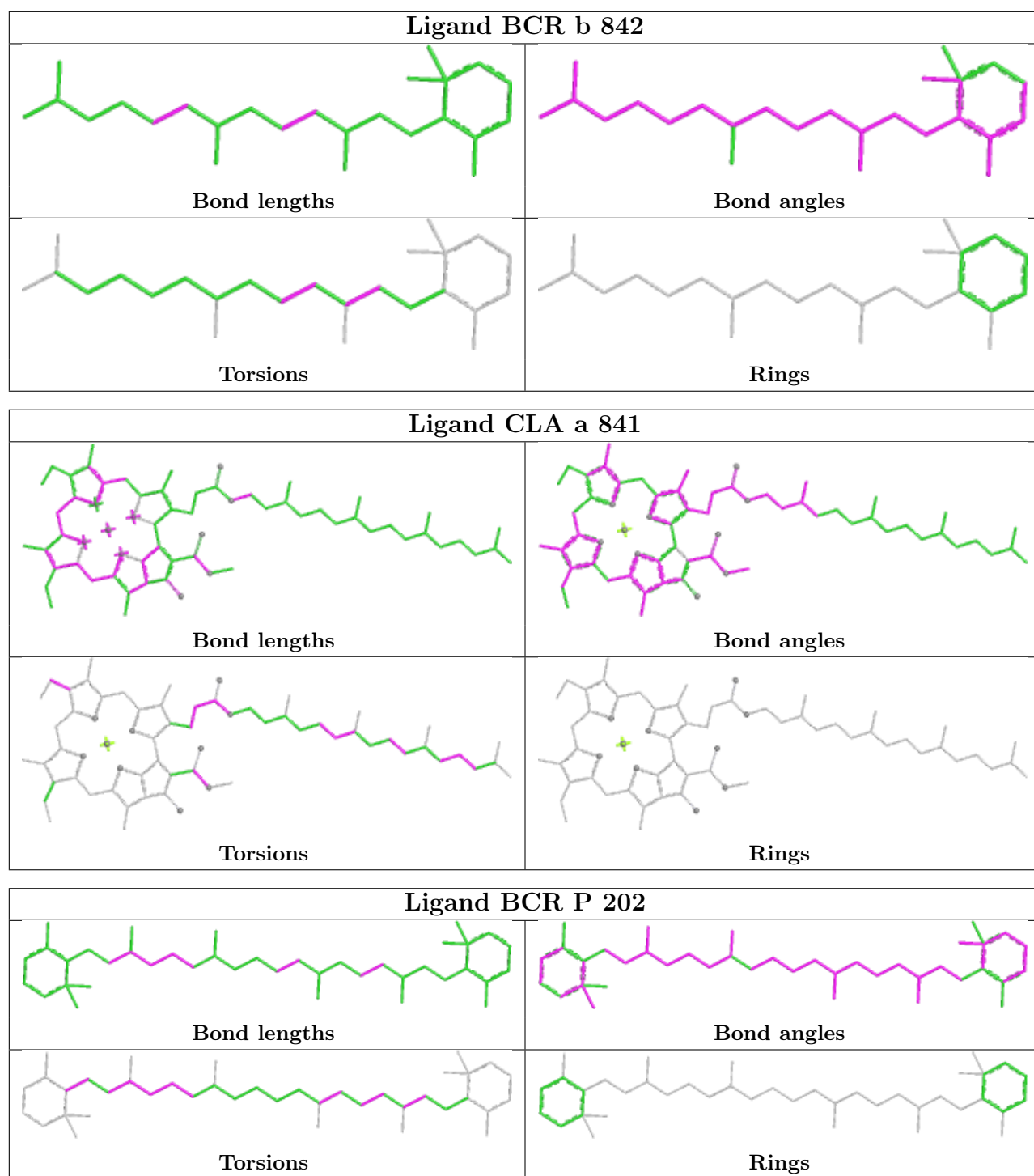


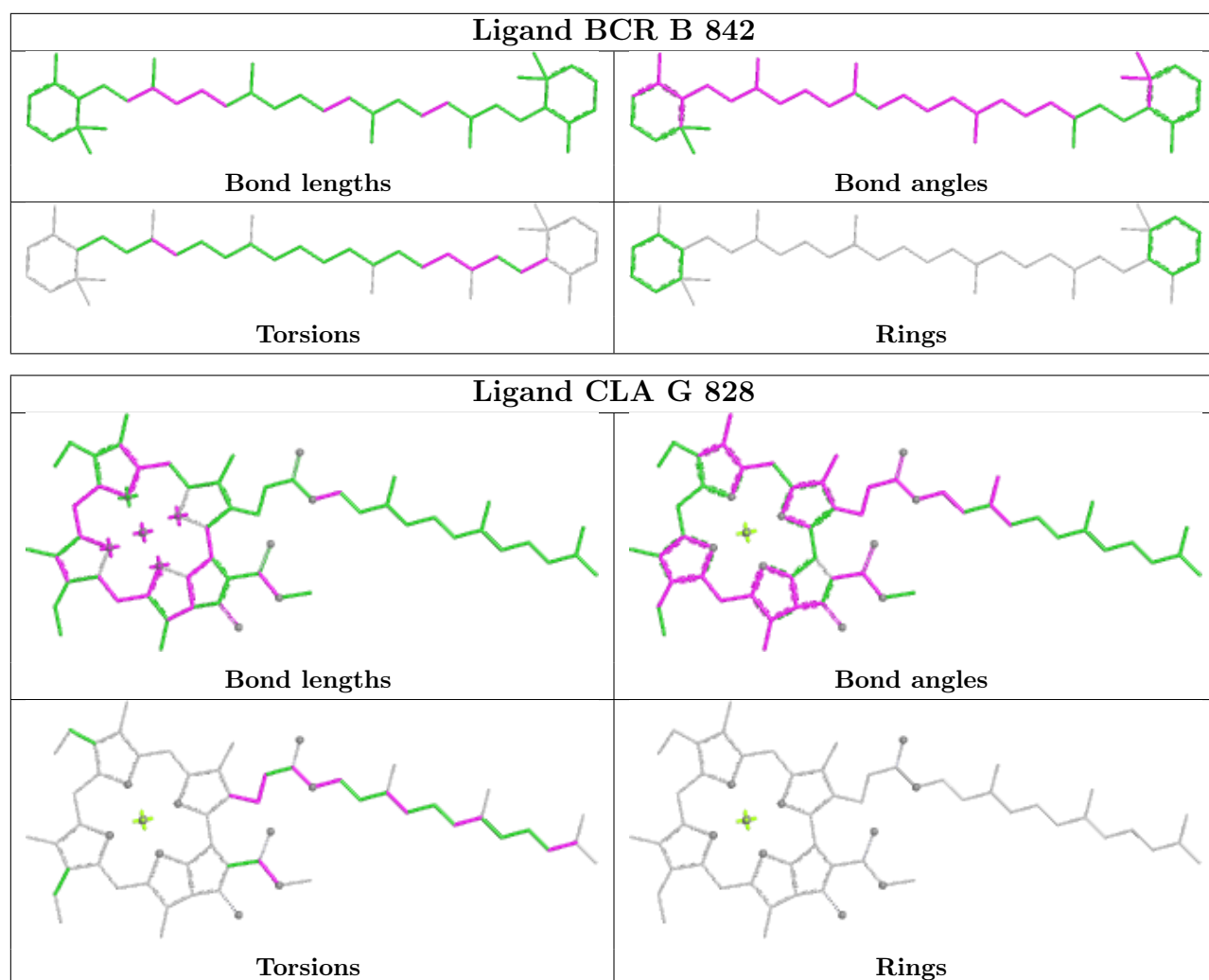
Ligand CLA A 835

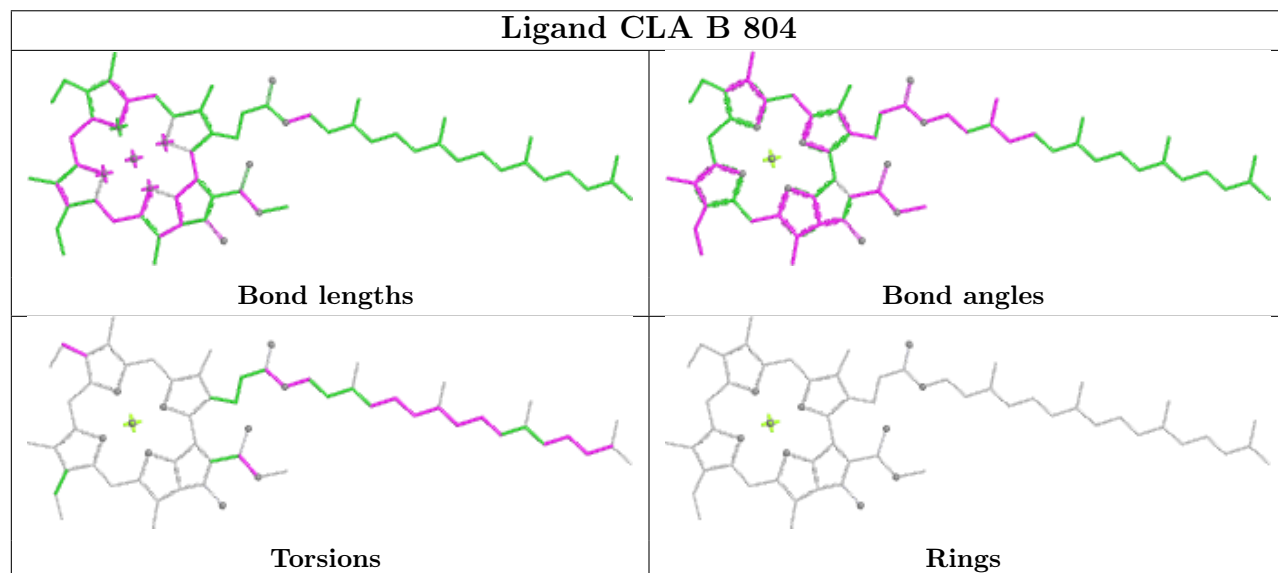
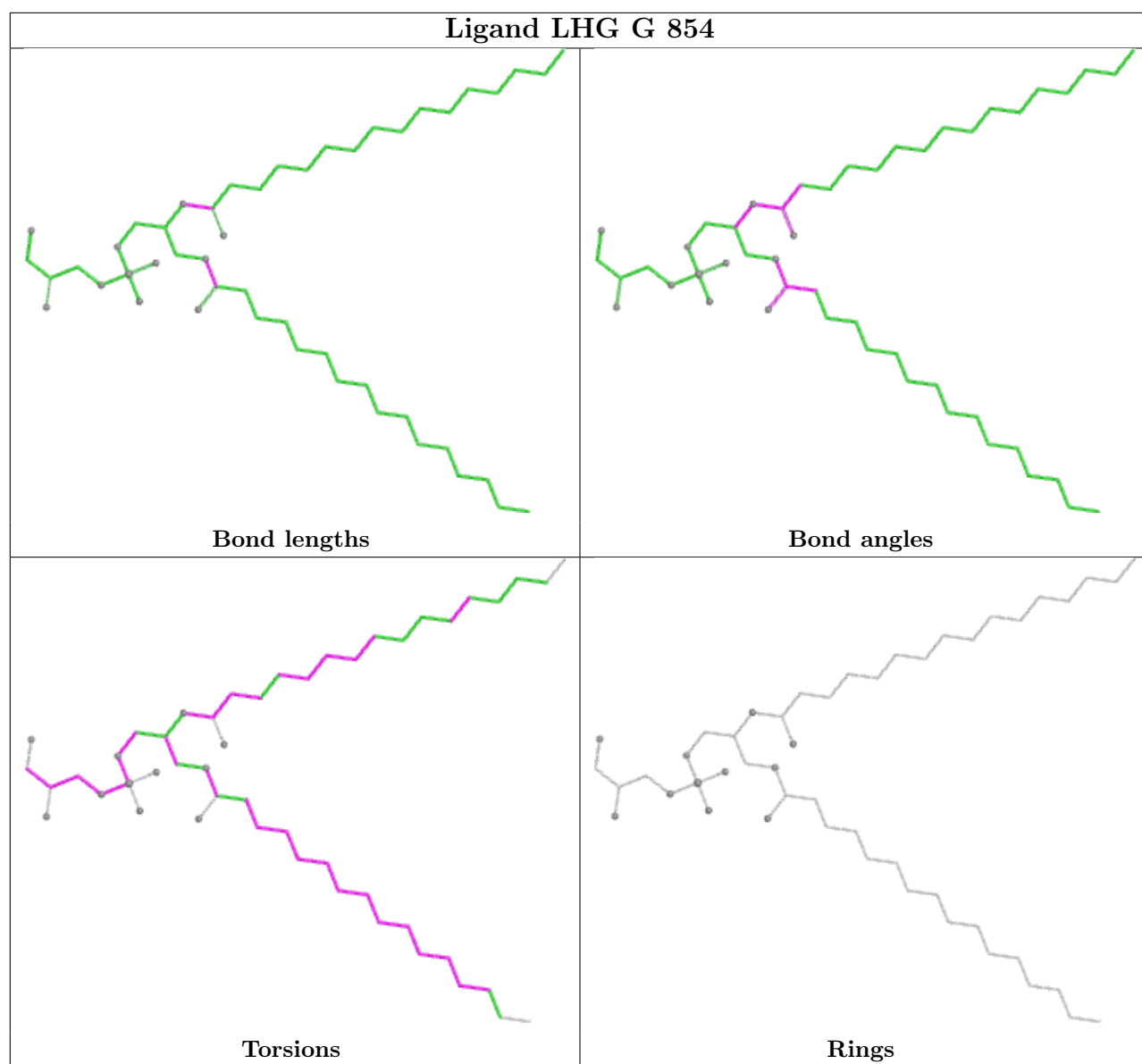


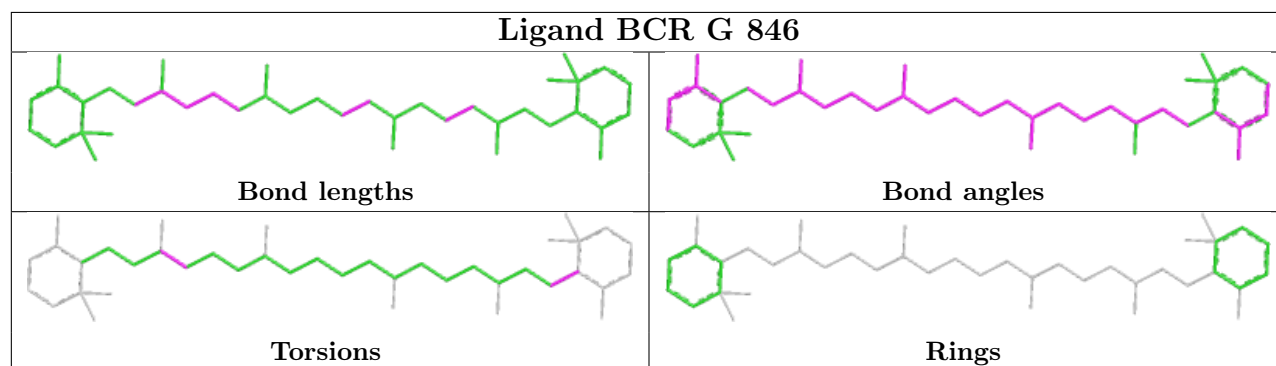
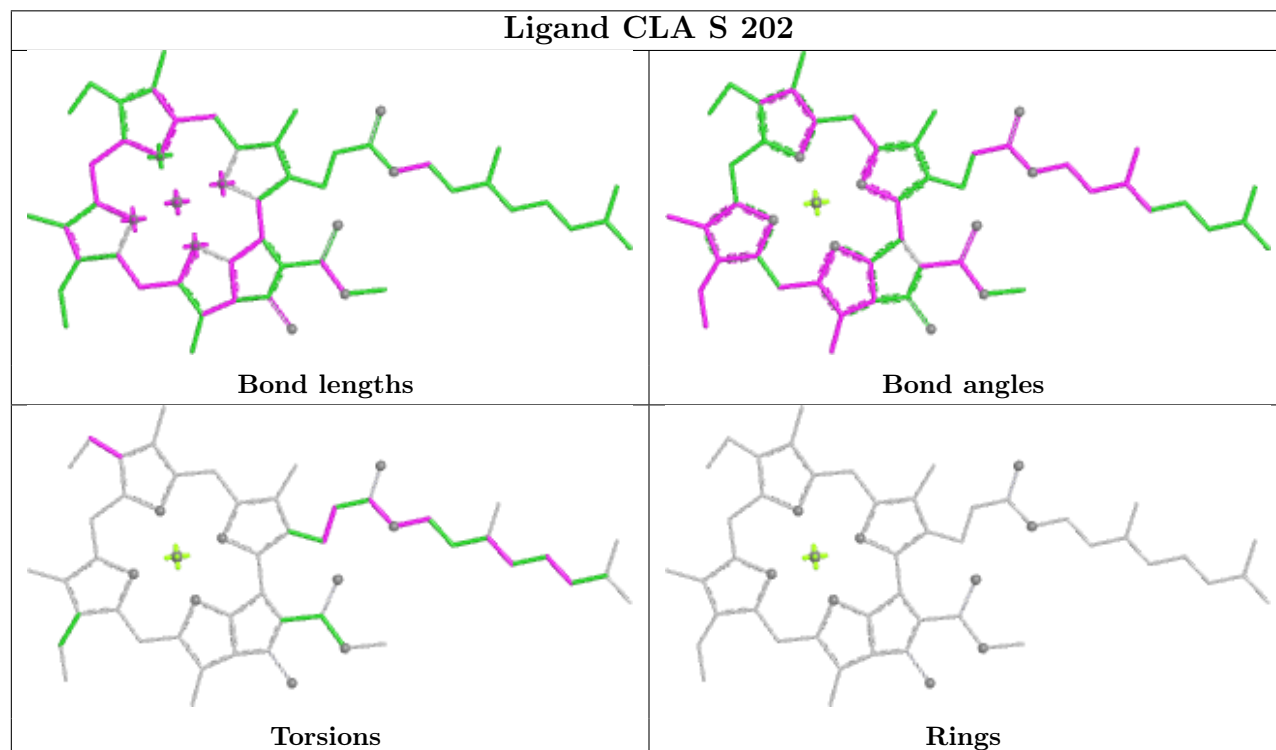
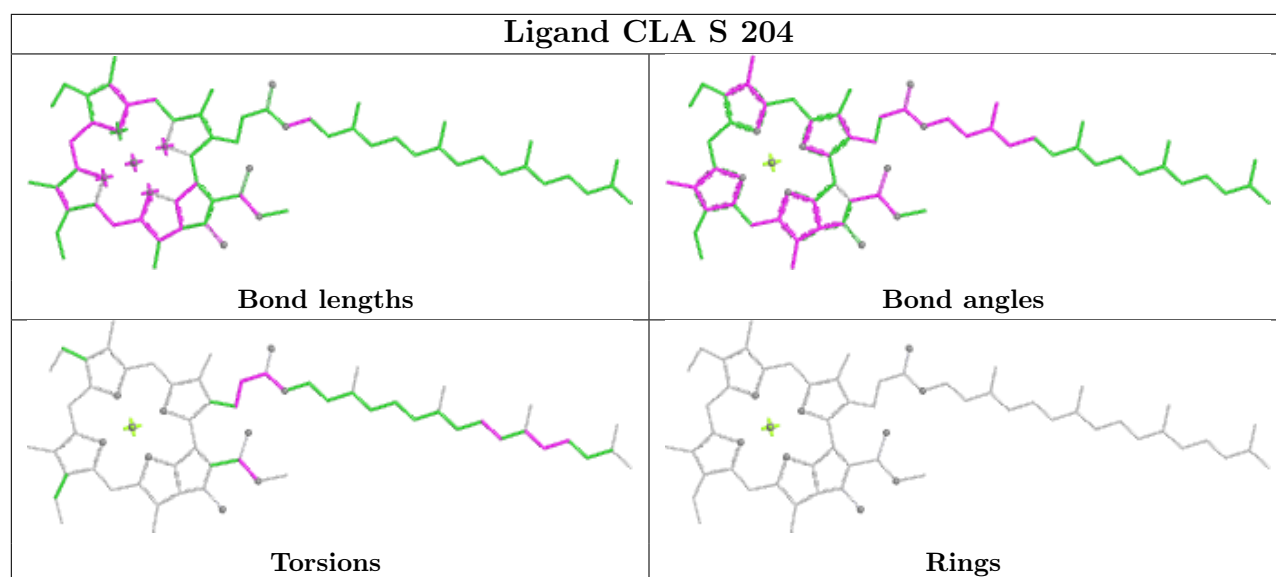
Ligand BCR a 852

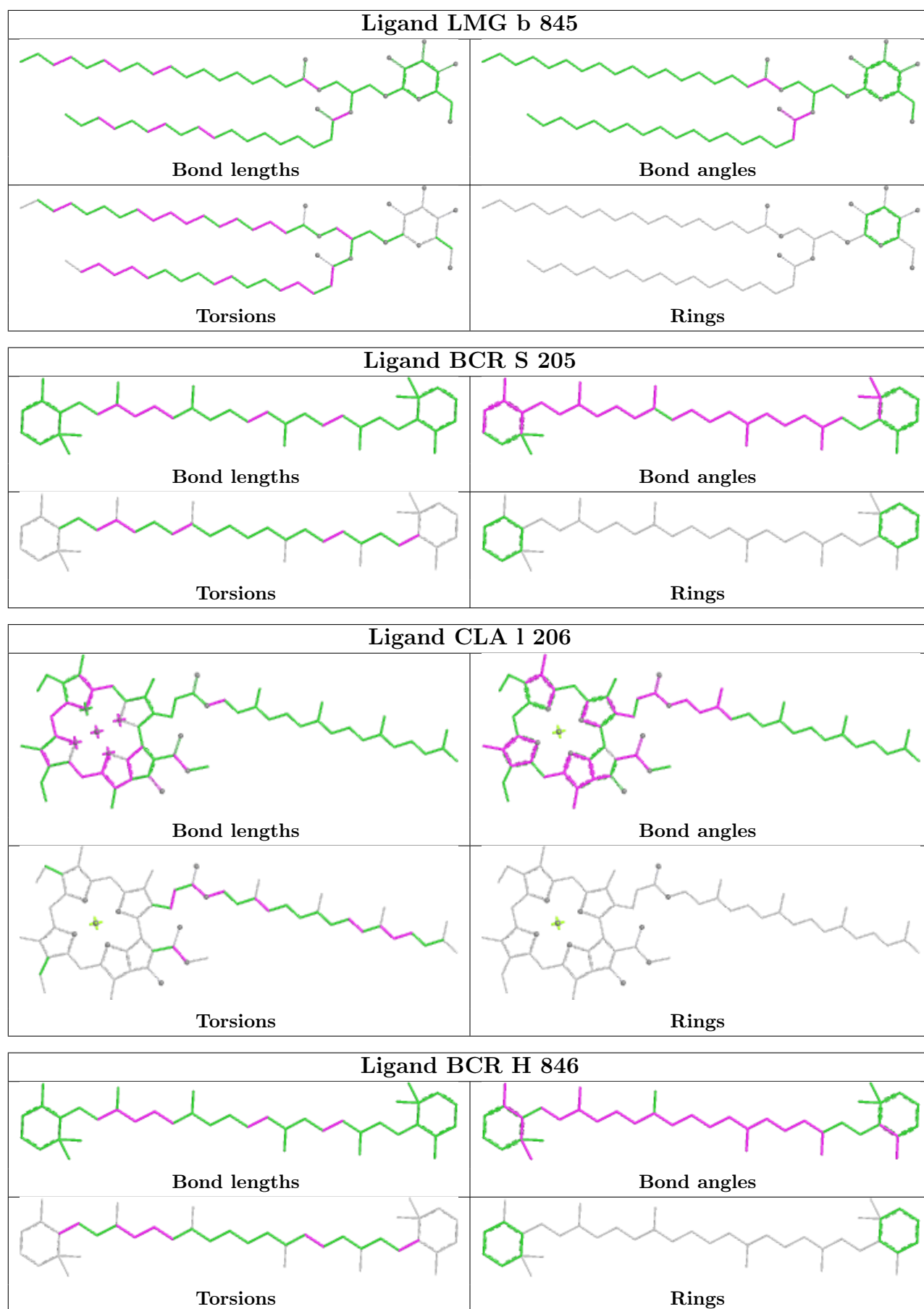


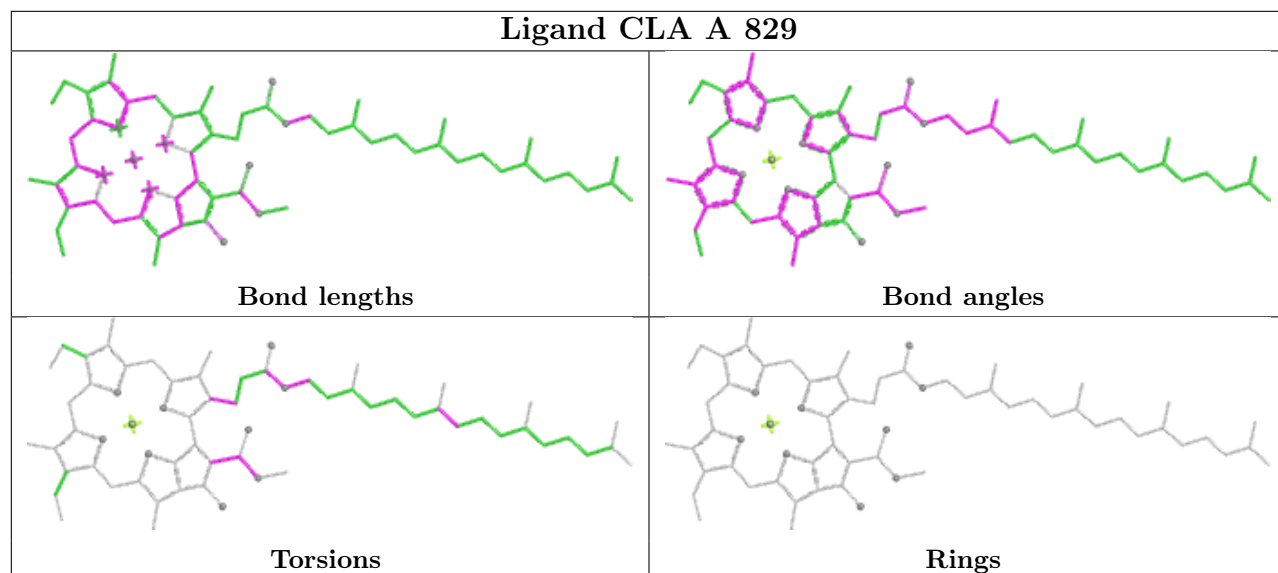
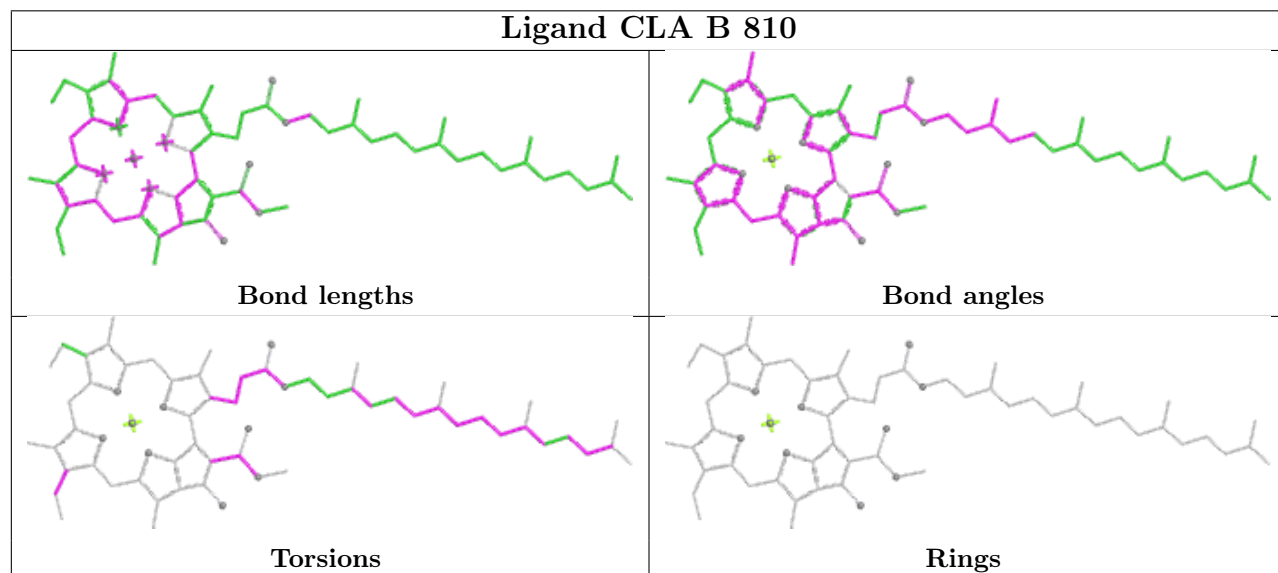
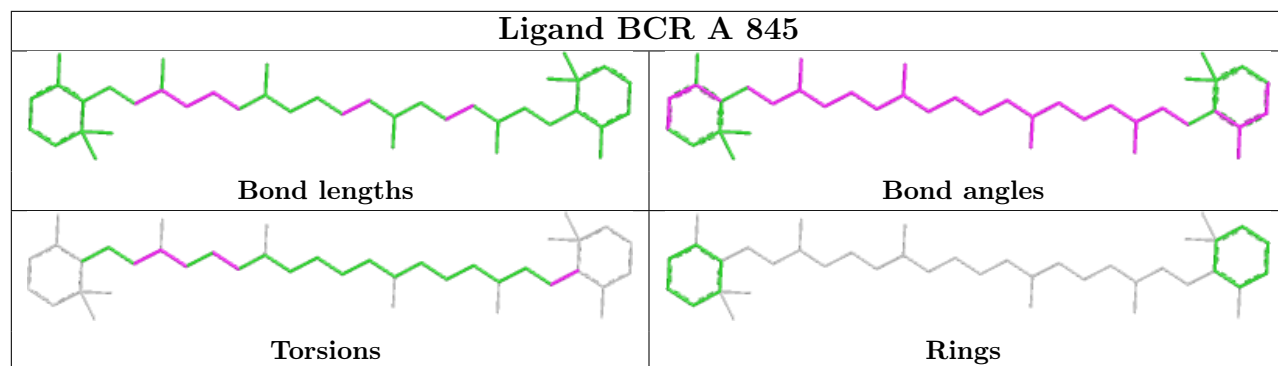


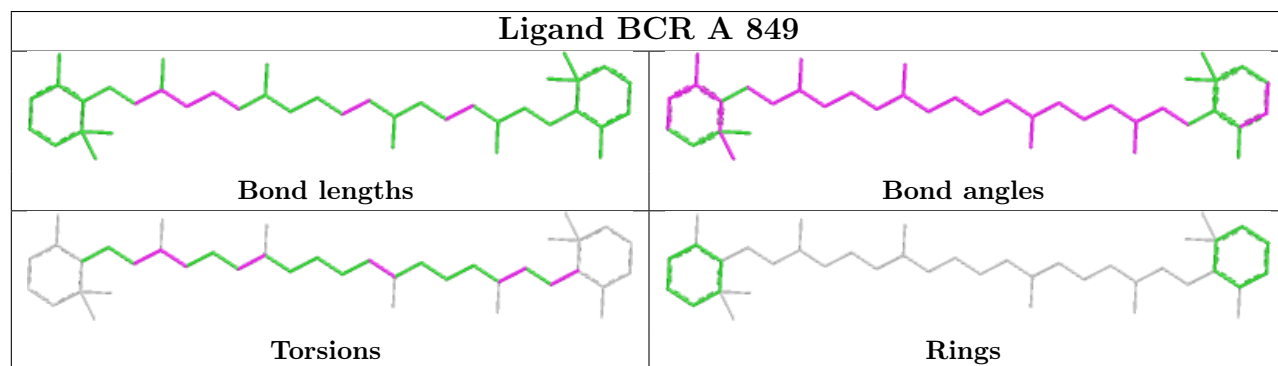
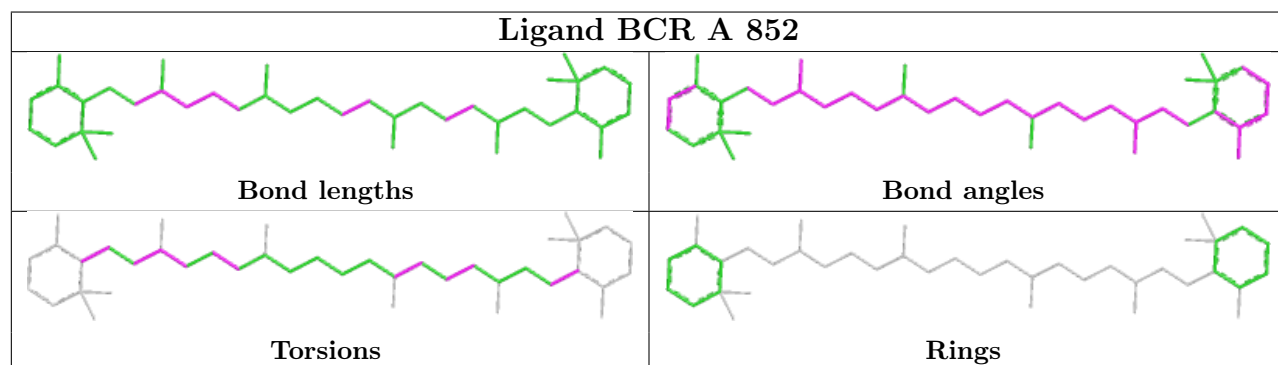
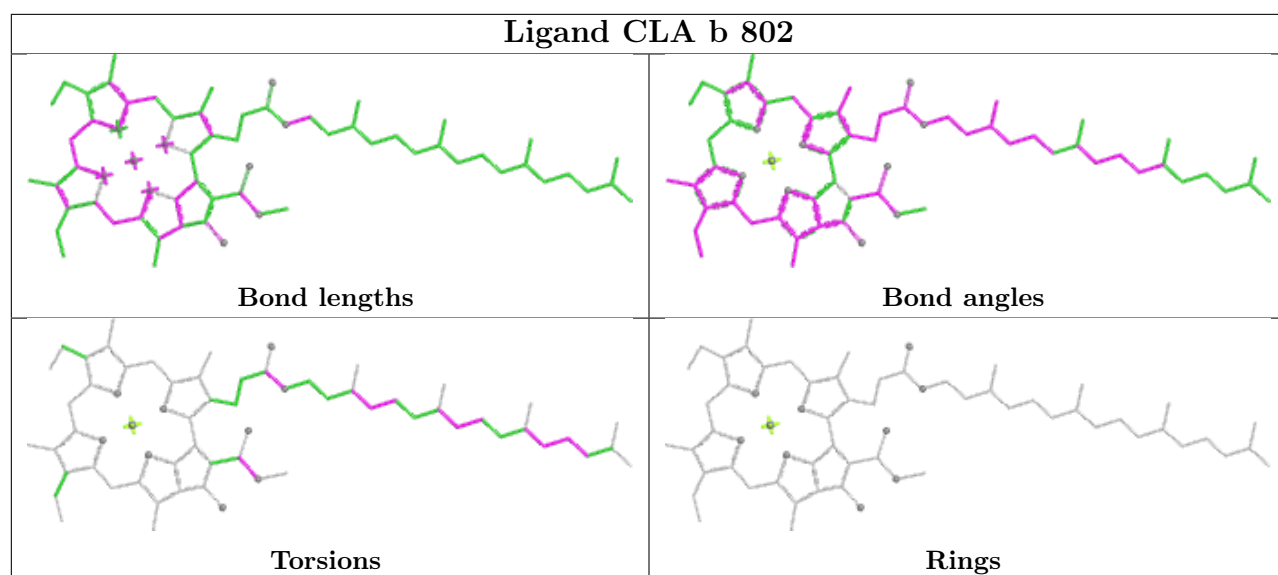


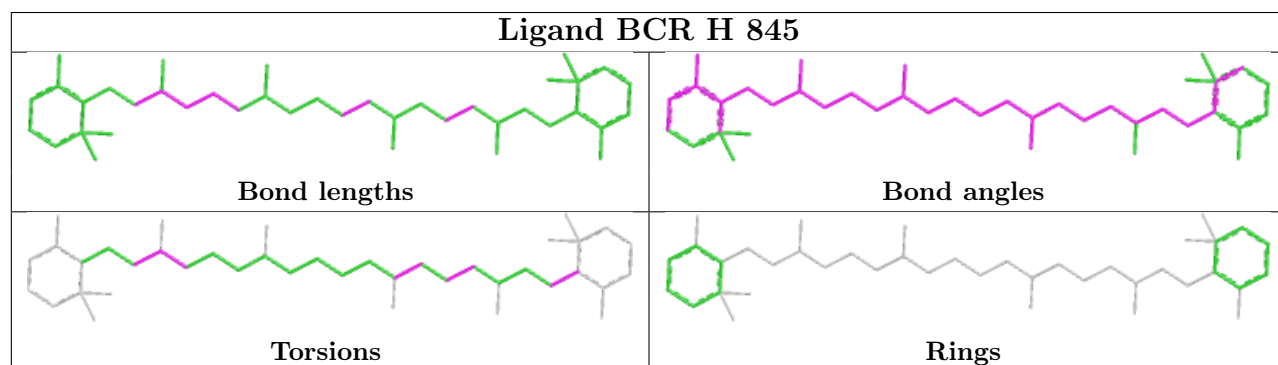
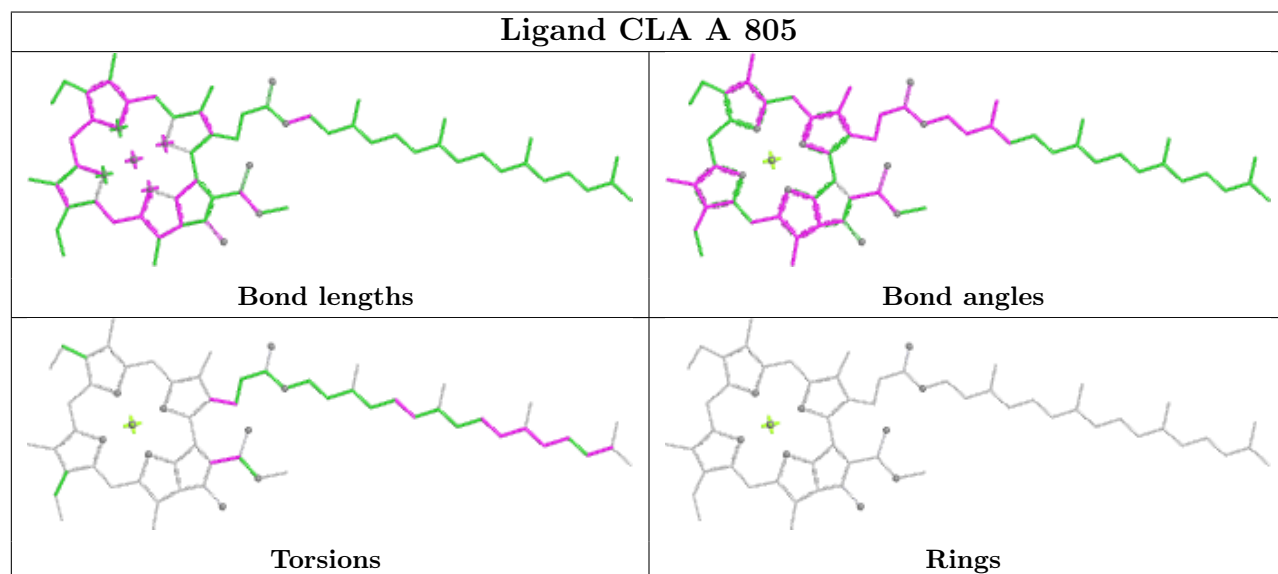
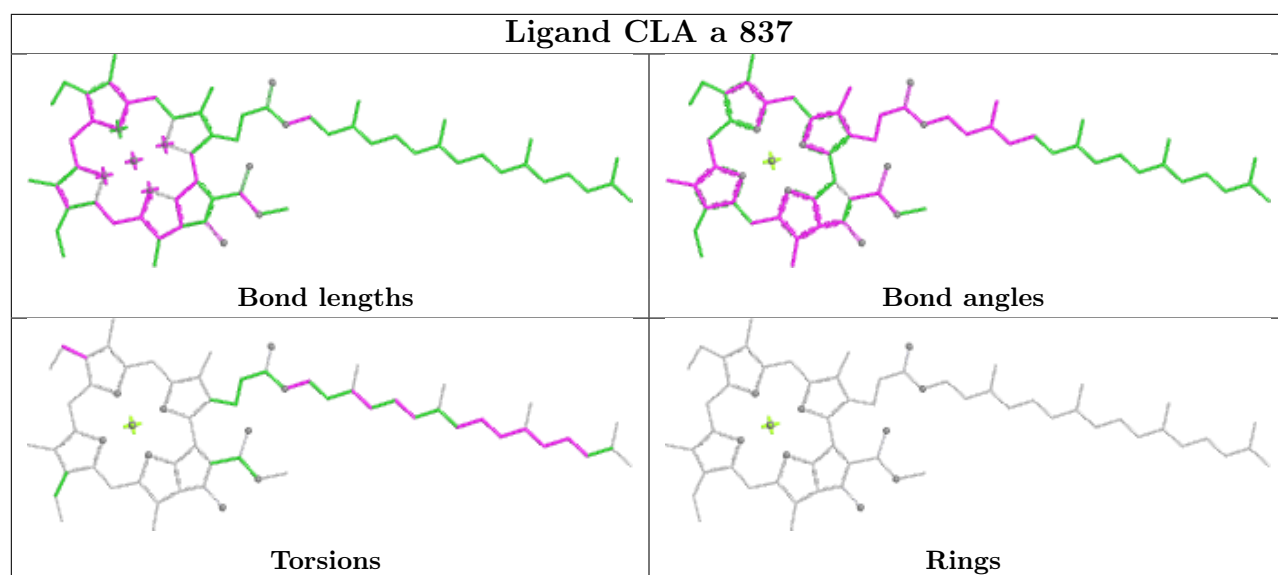




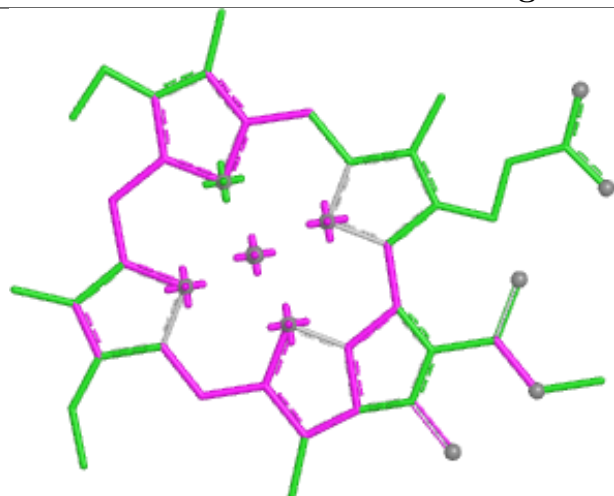




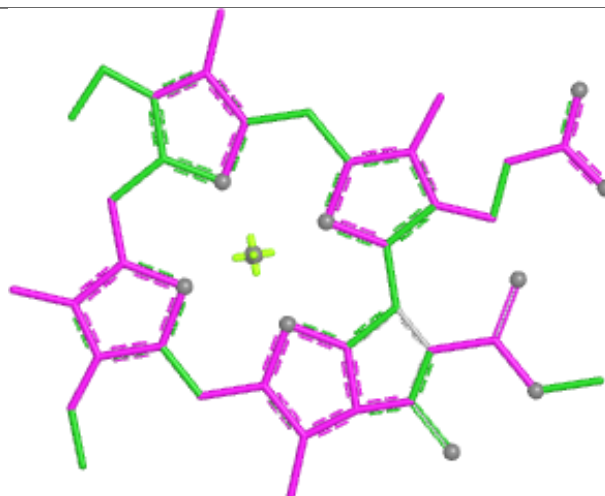




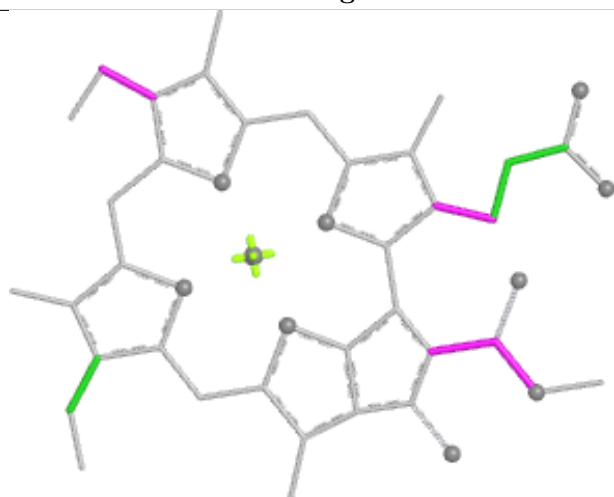
Ligand CLA a 819



Bond lengths



Bond angles

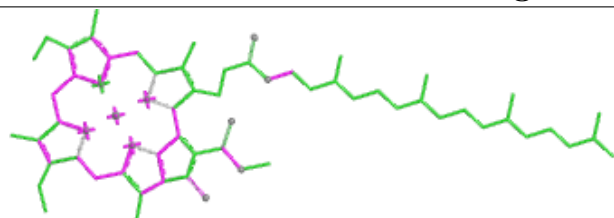


Torsions

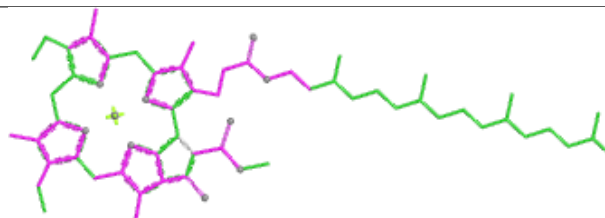


Rings

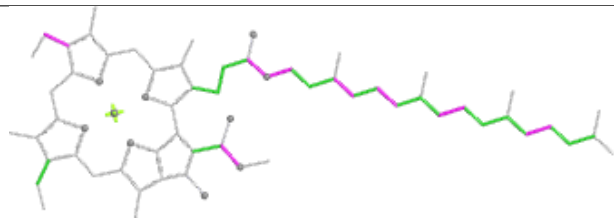
Ligand CLA H 835



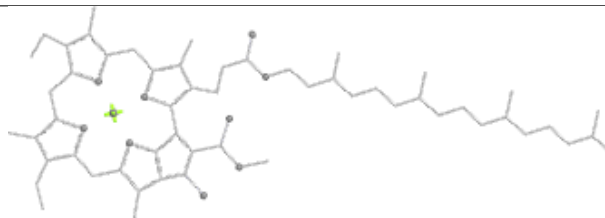
Bond lengths



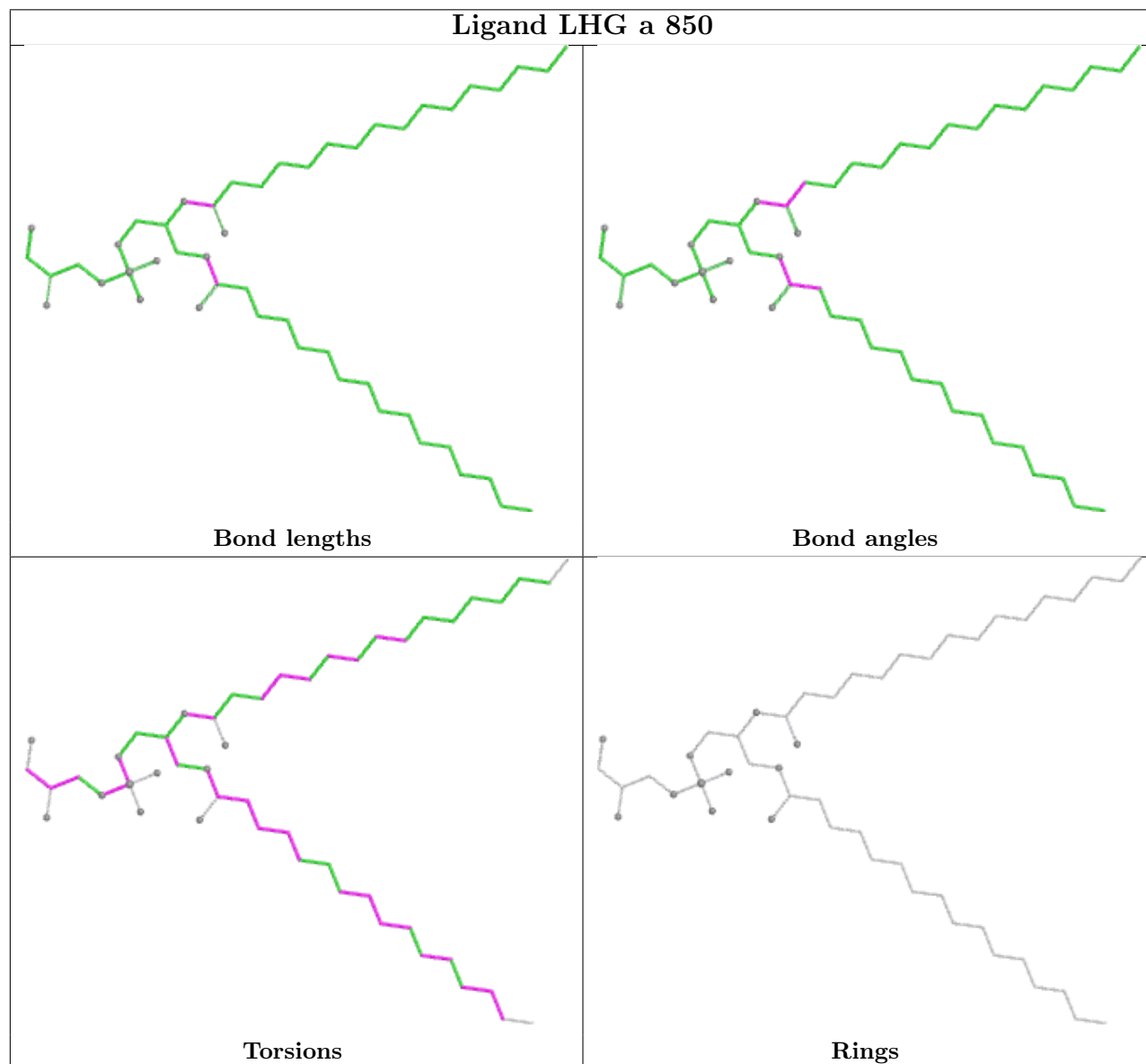
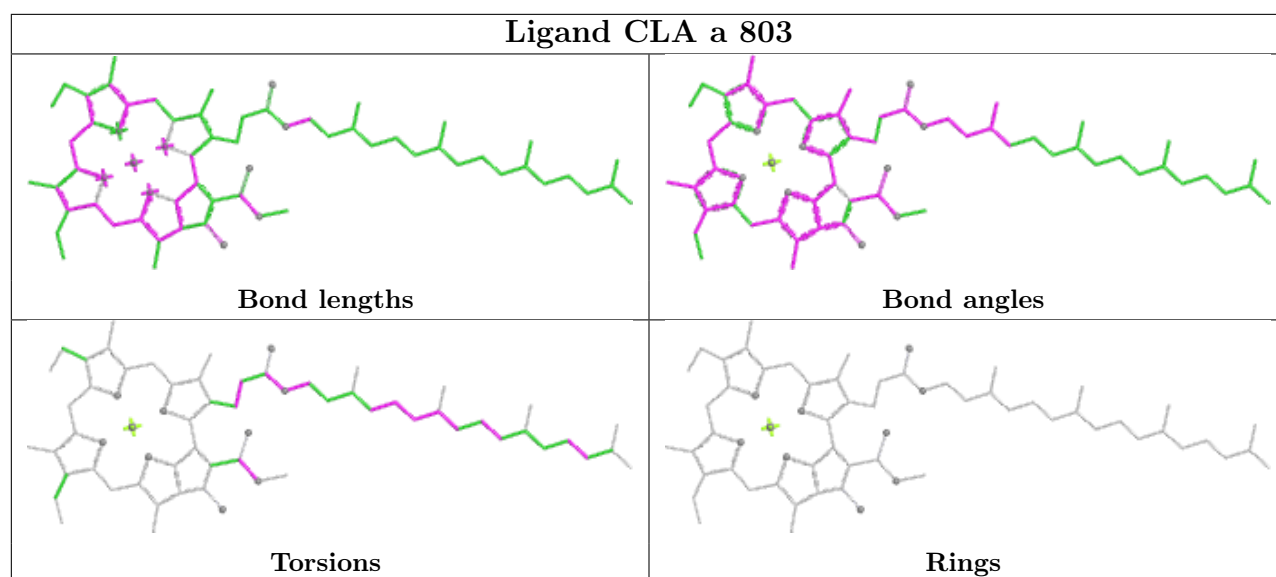
Bond angles

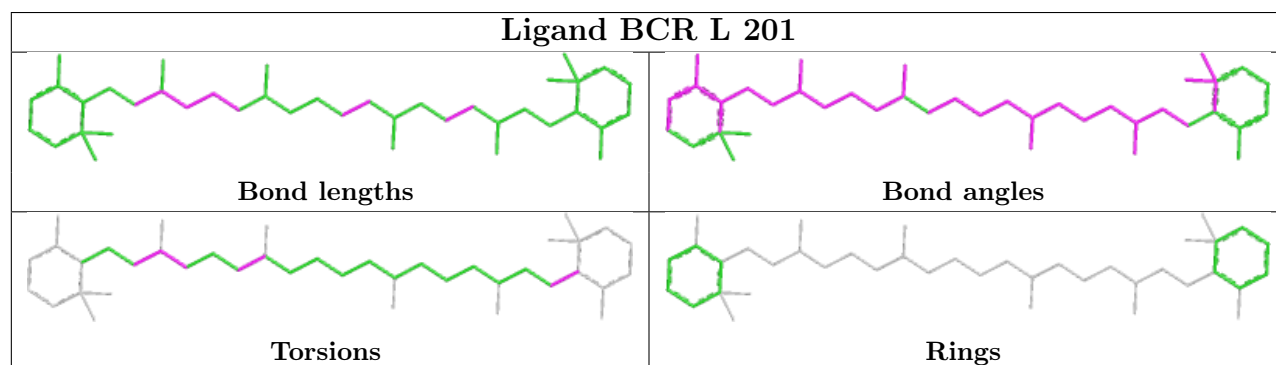
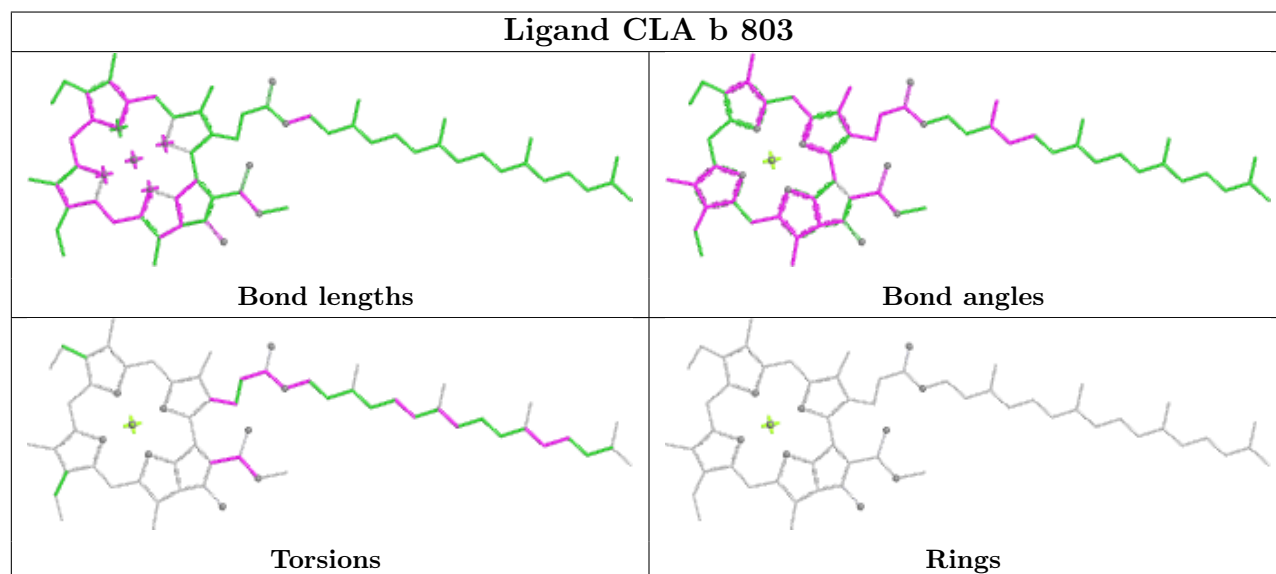
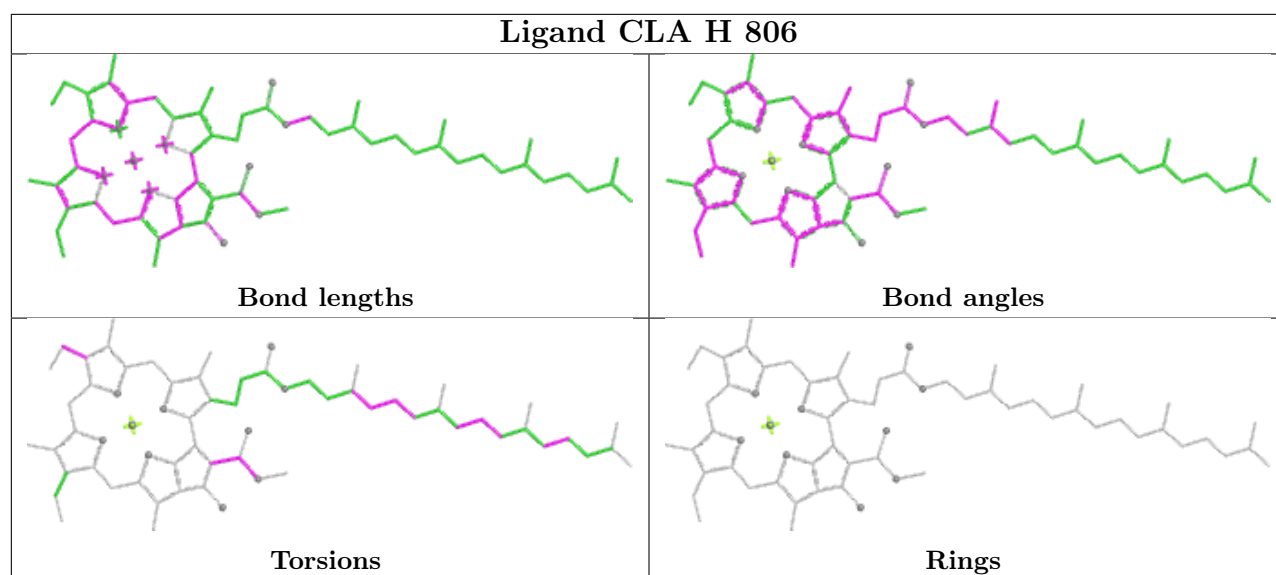


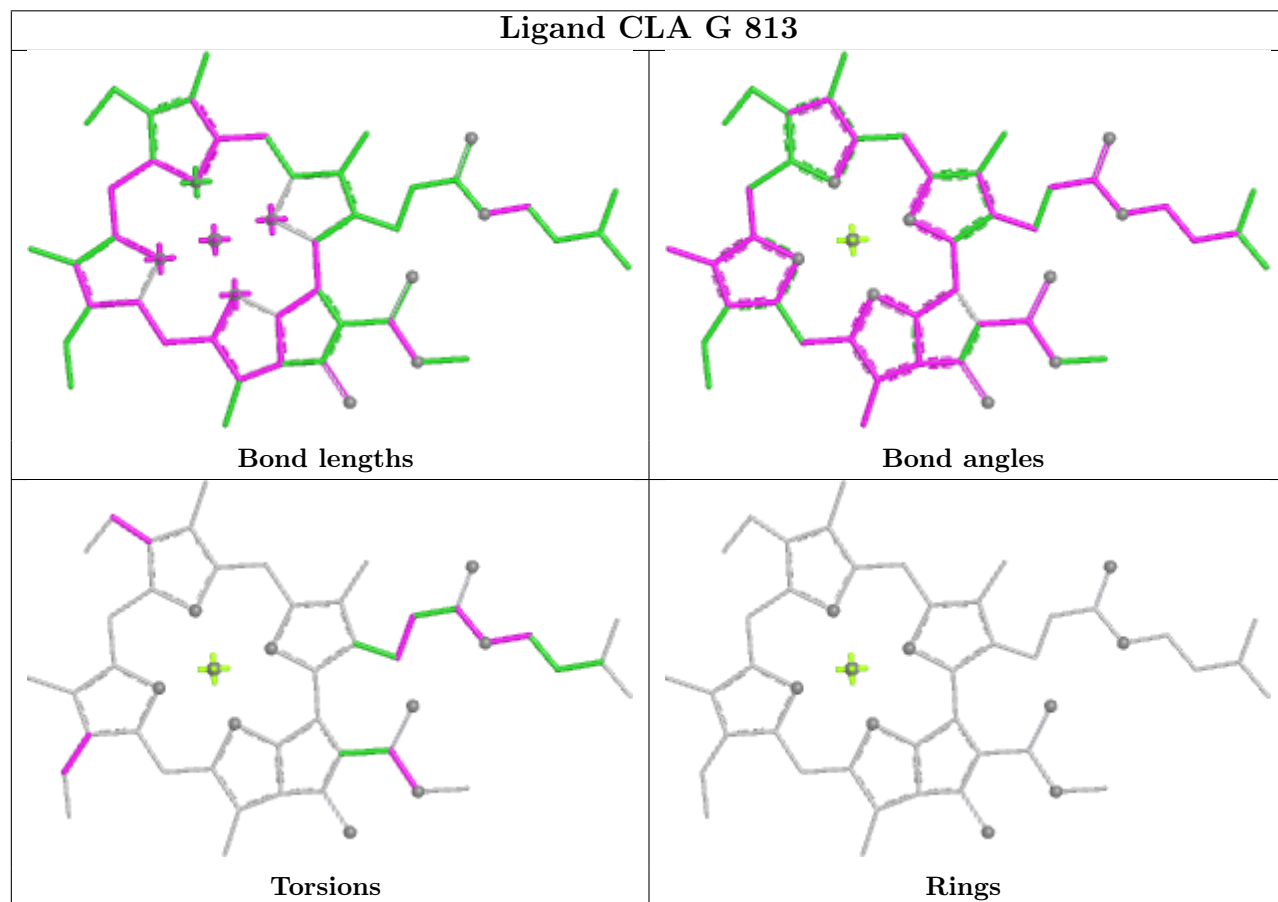
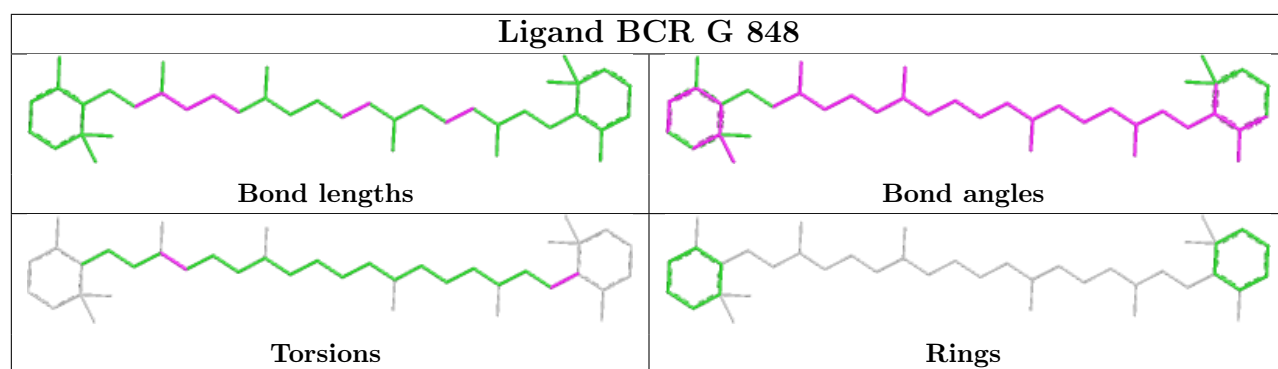
Torsions

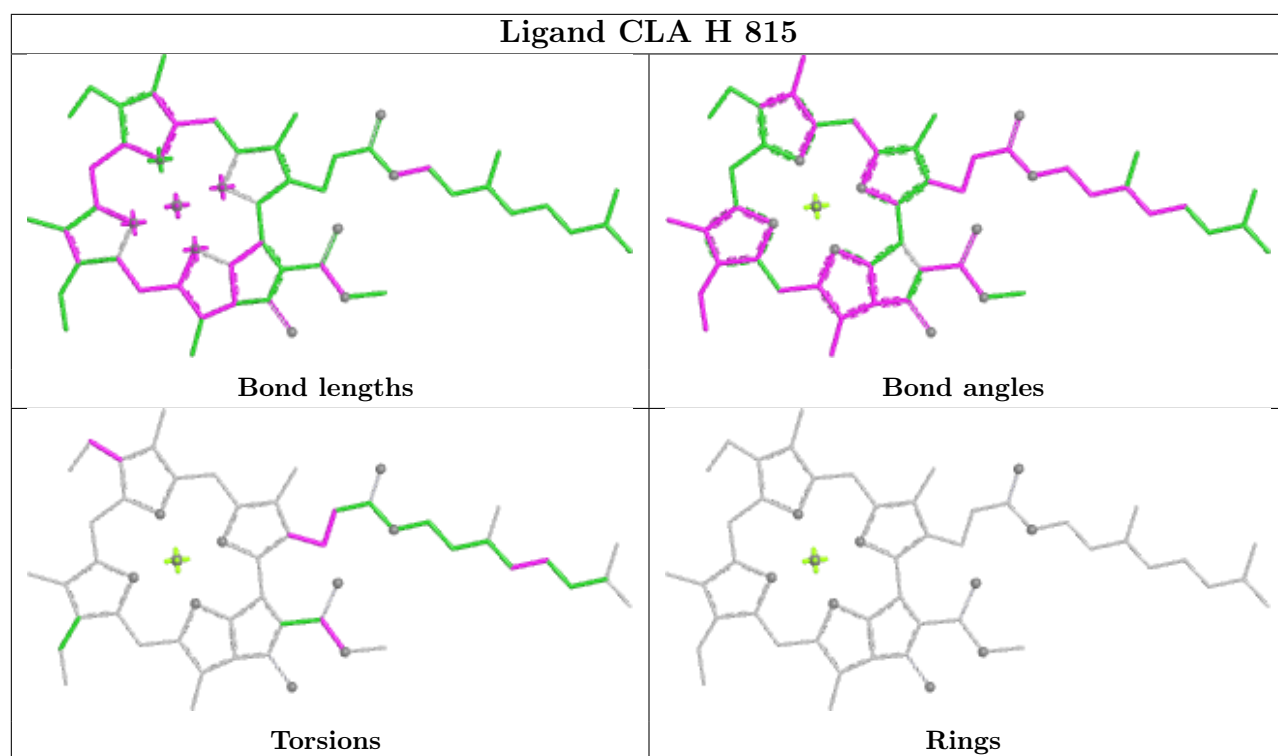


Rings

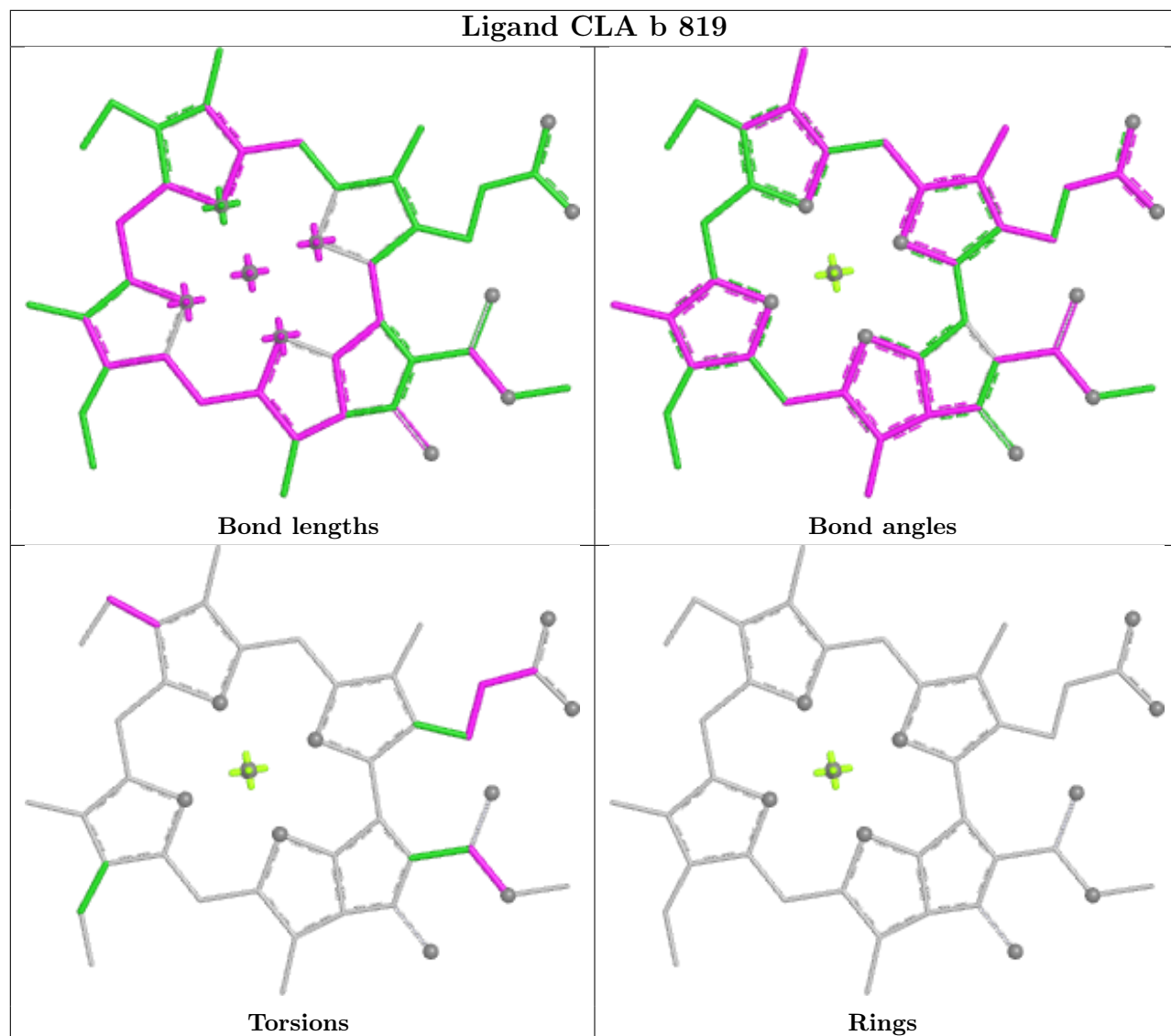


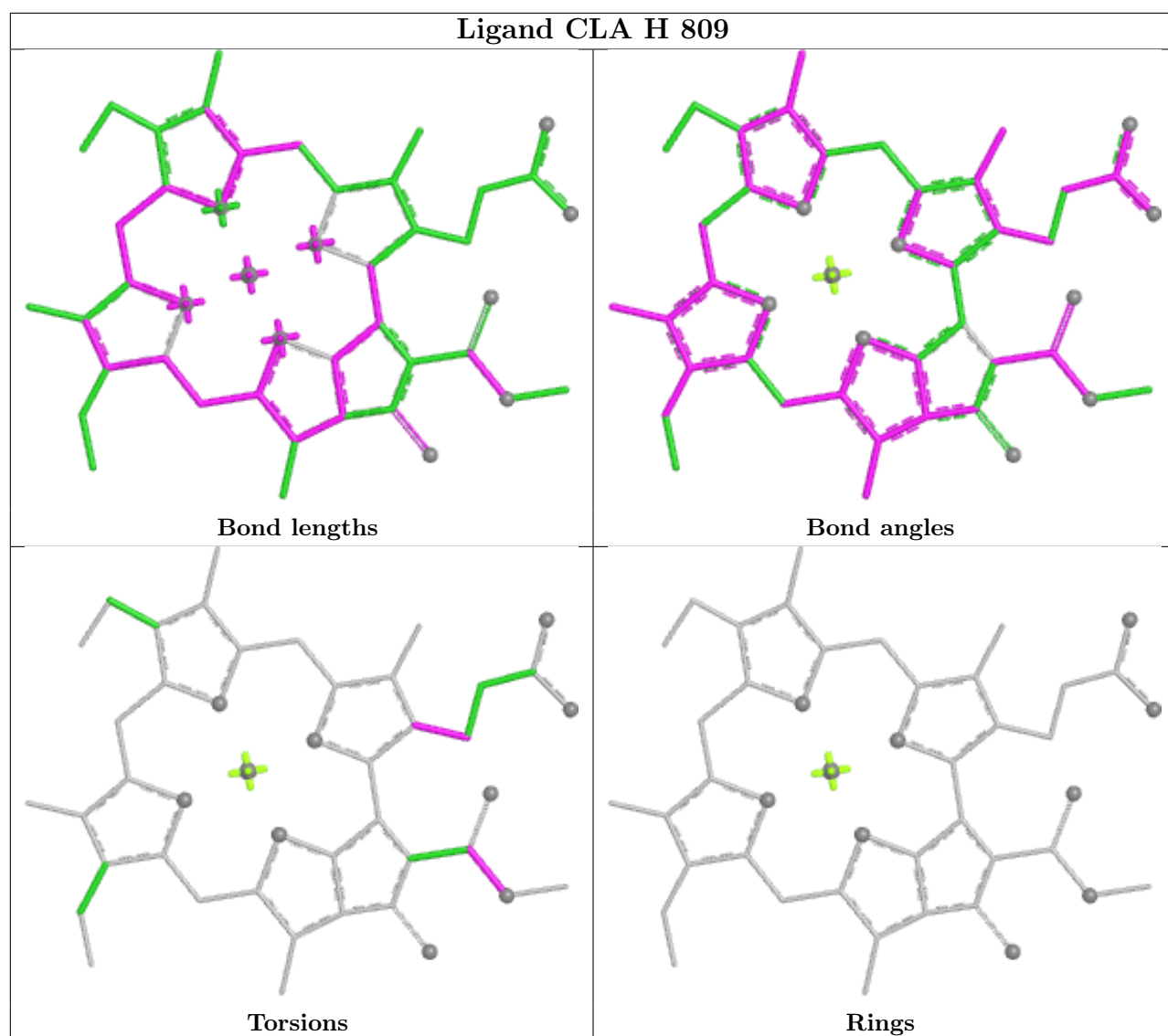


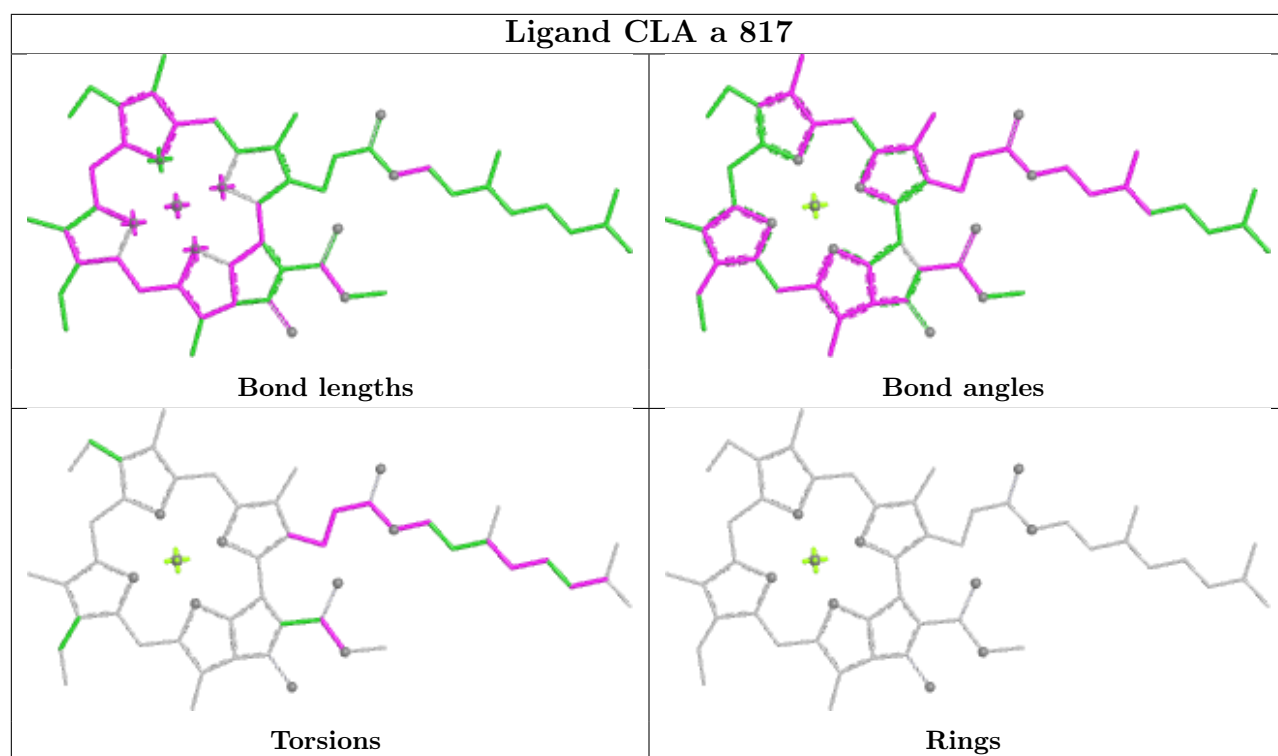




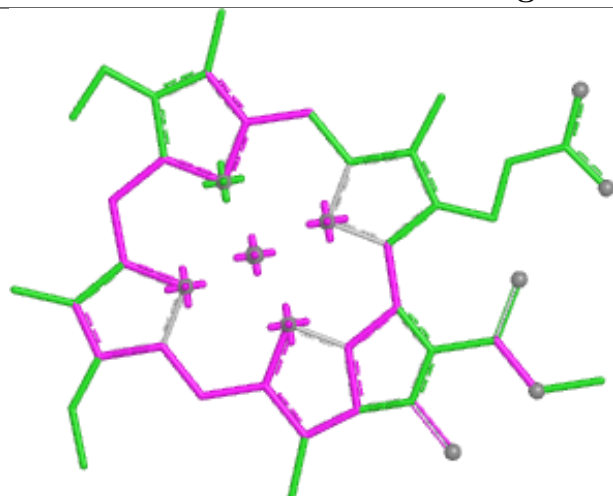
Ligand CLA b 819



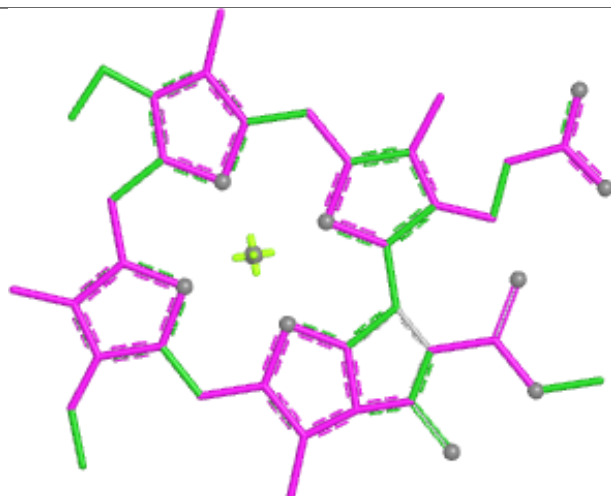




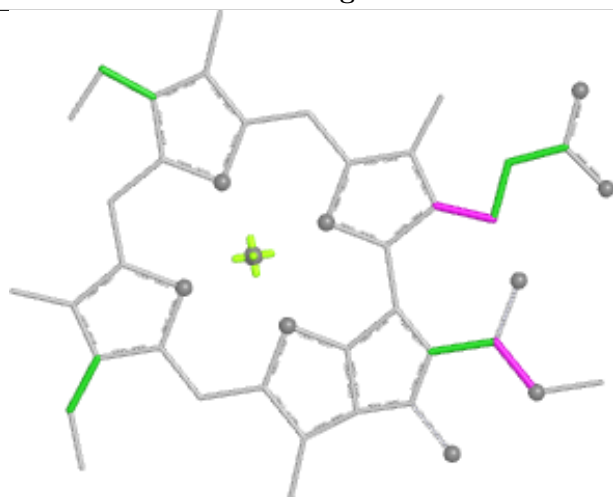
Ligand CLA b 808



Bond lengths



Bond angles

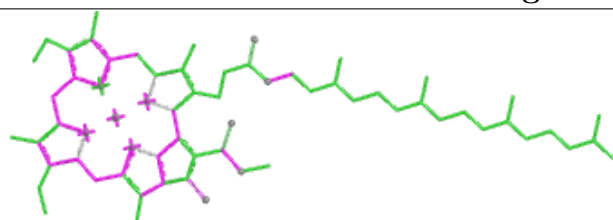


Torsions

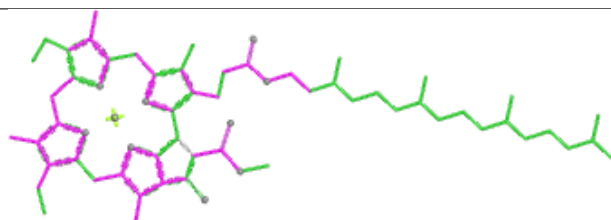


Rings

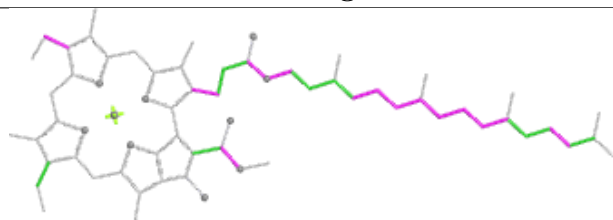
Ligand CLA l 202



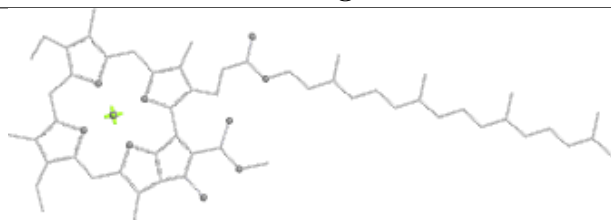
Bond lengths



Bond angles

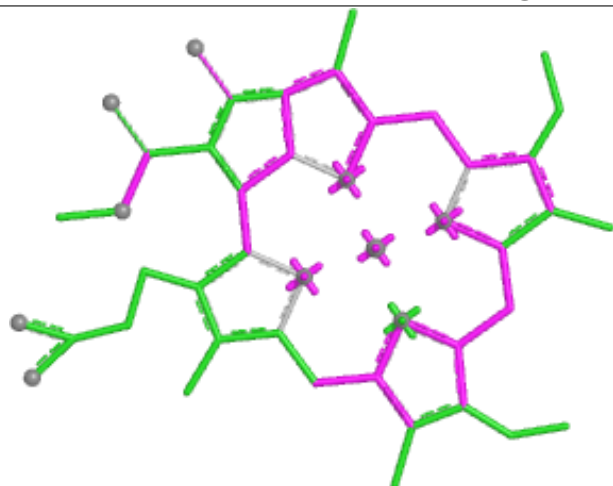


Torsions

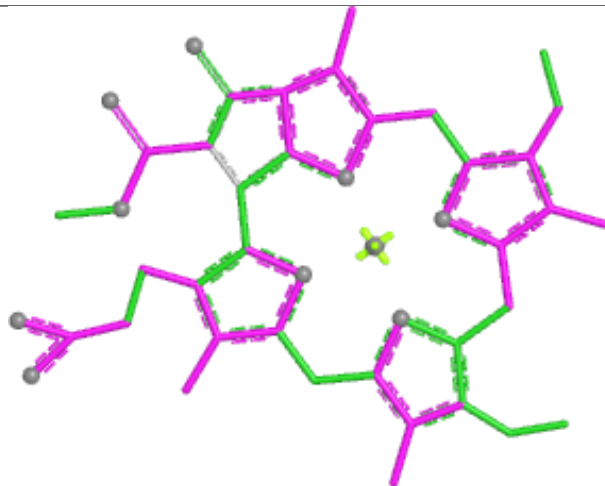


Rings

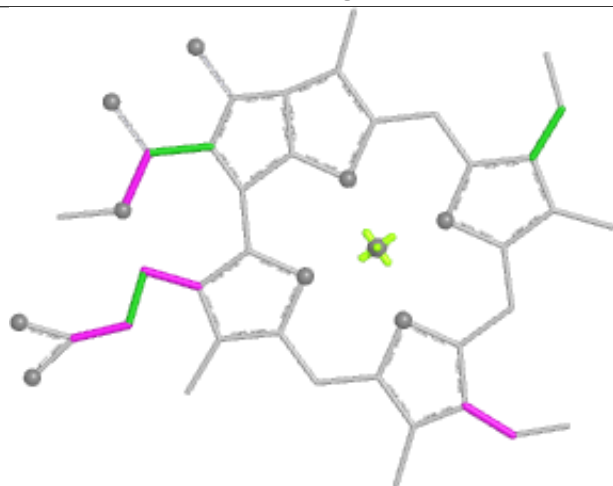
Ligand CLA F 203



Bond lengths



Bond angles

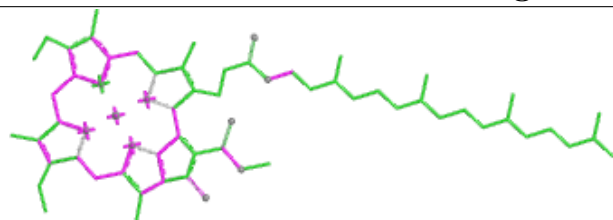


Torsions

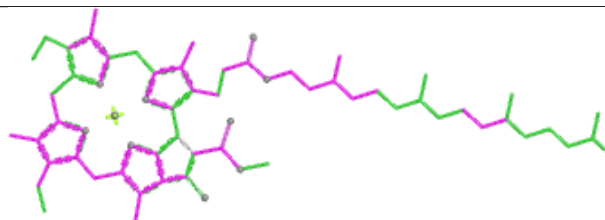


Rings

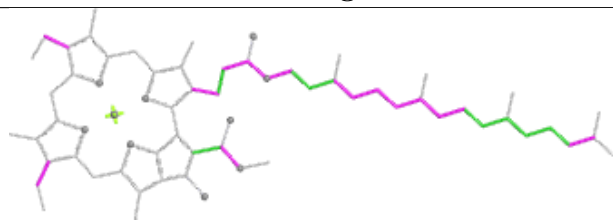
Ligand CLA H 838



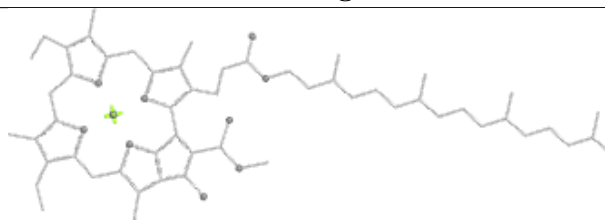
Bond lengths



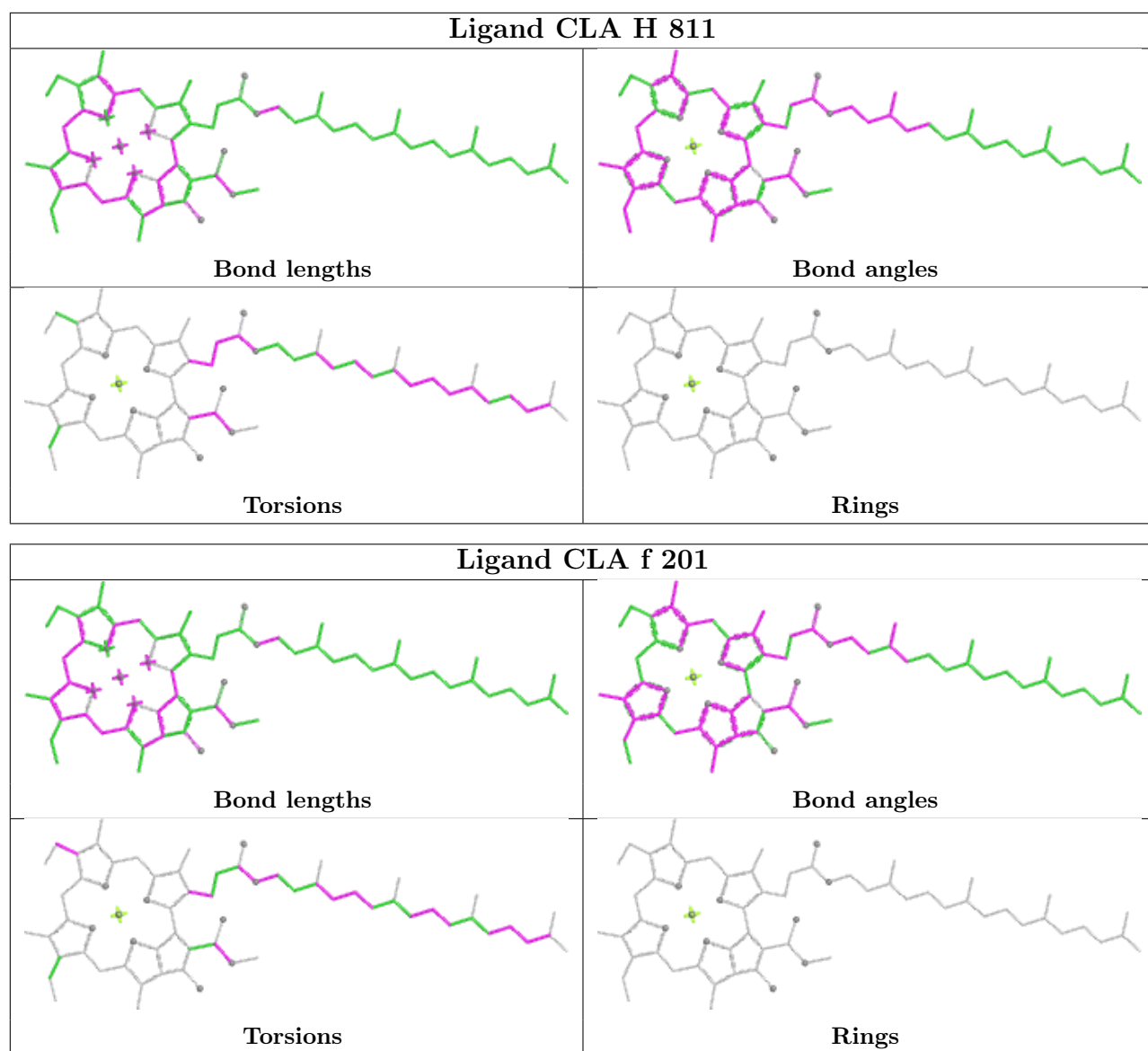
Bond angles

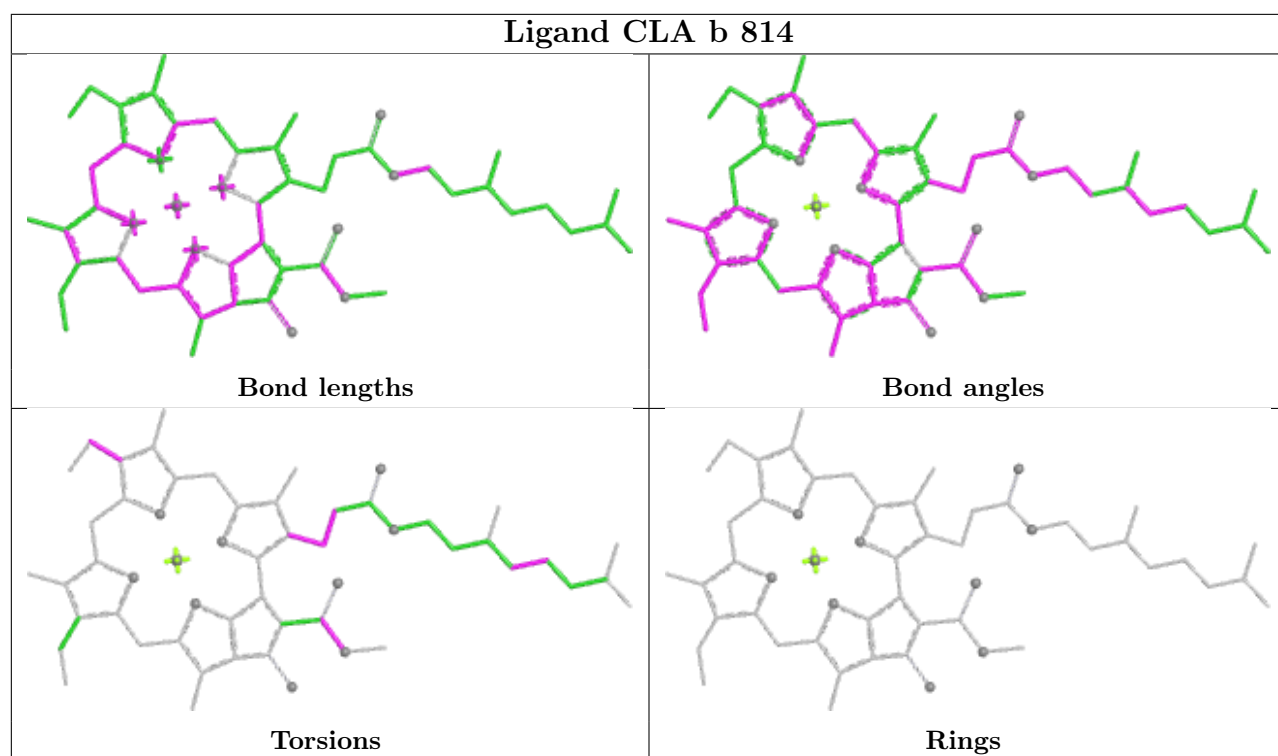


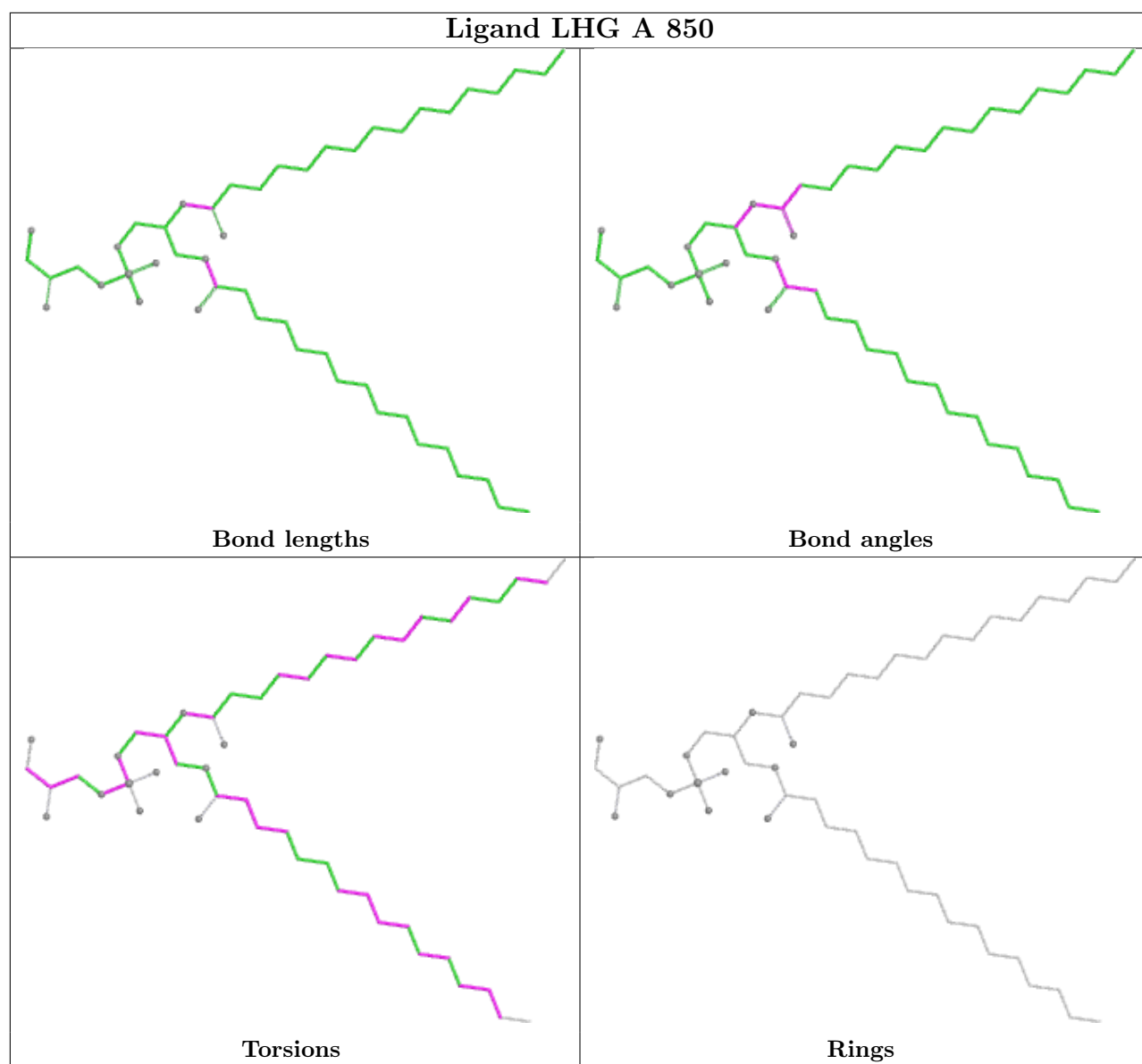
Torsions



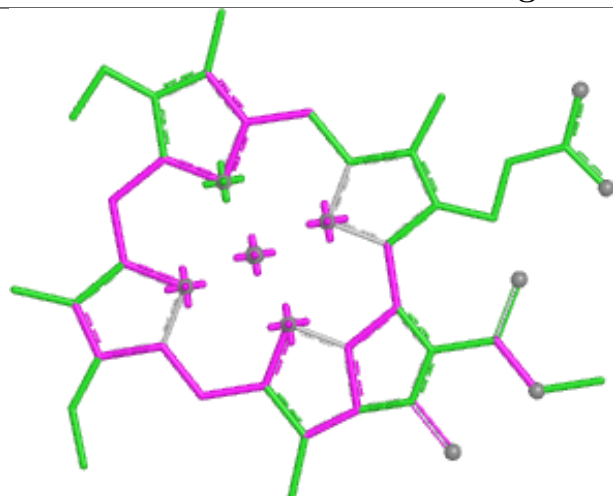
Rings



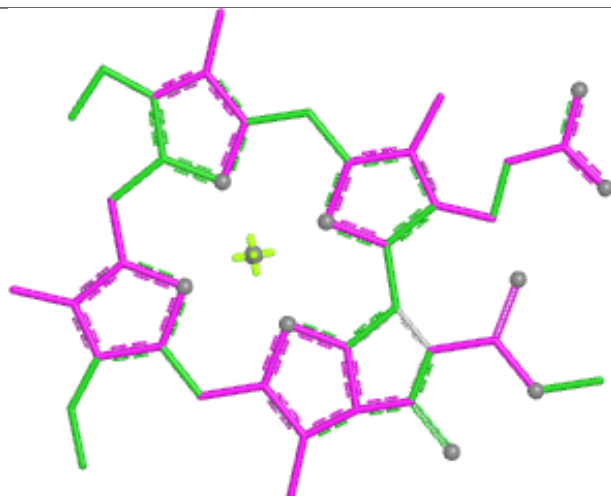




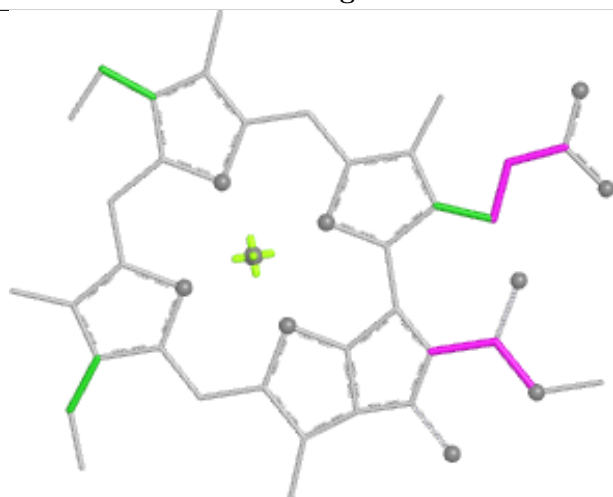
Ligand CLA a 814



Bond lengths



Bond angles

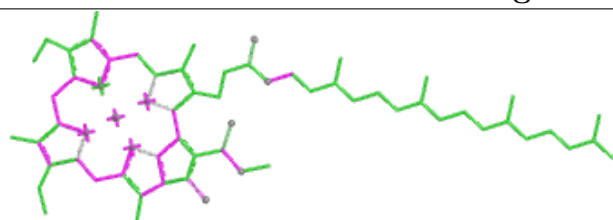


Torsions

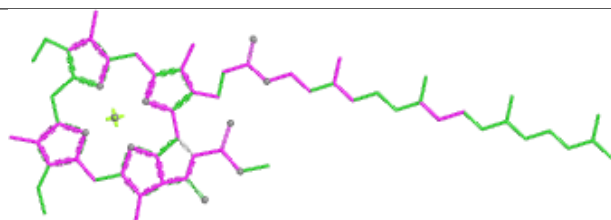


Rings

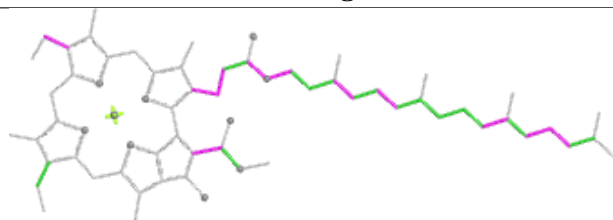
Ligand CLA H 822



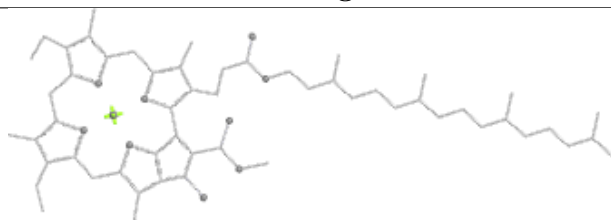
Bond lengths



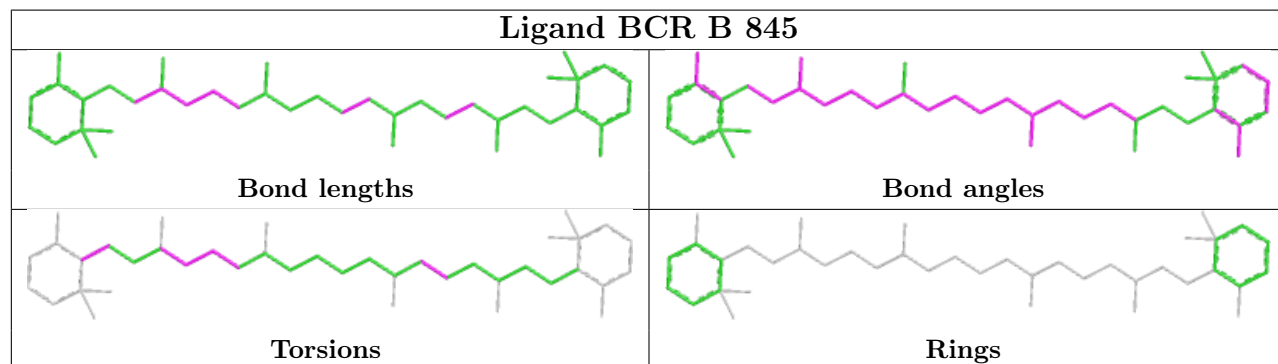
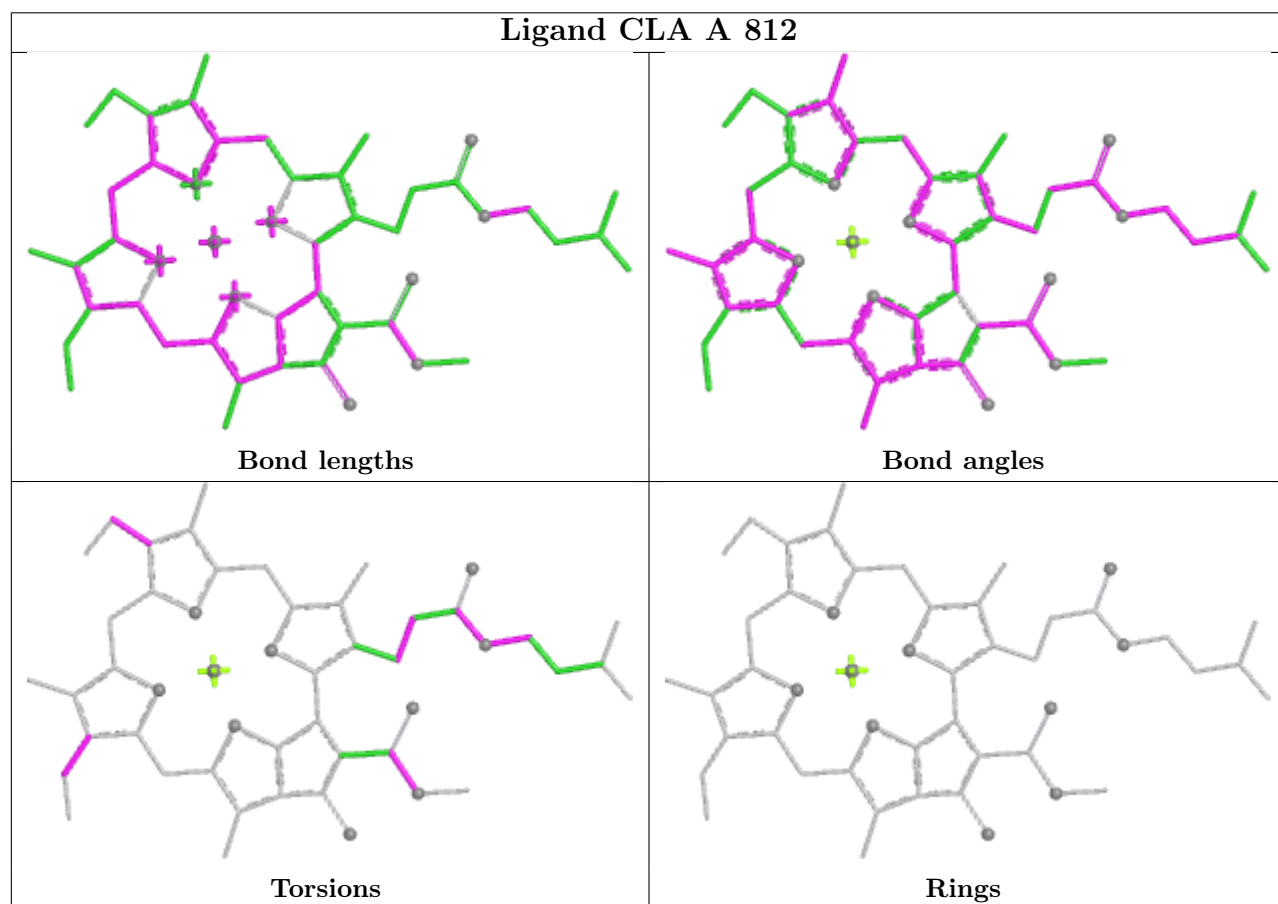
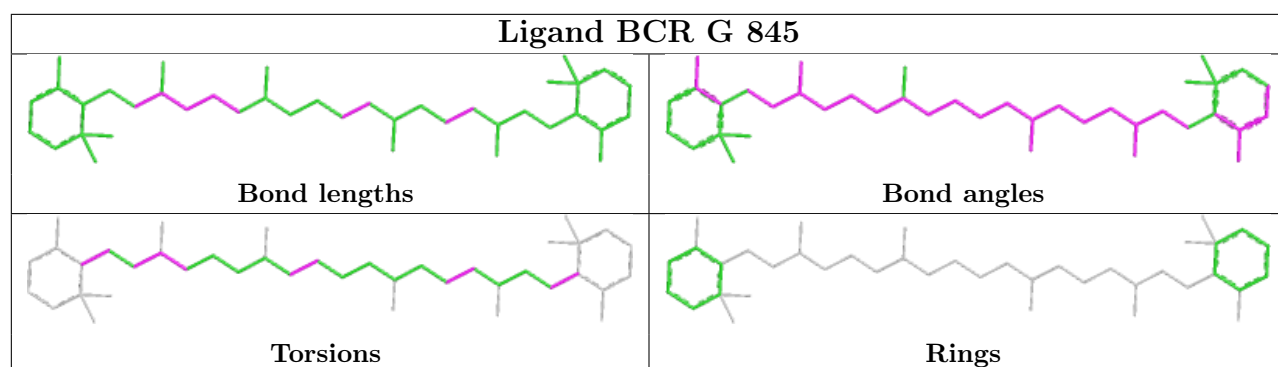
Bond angles

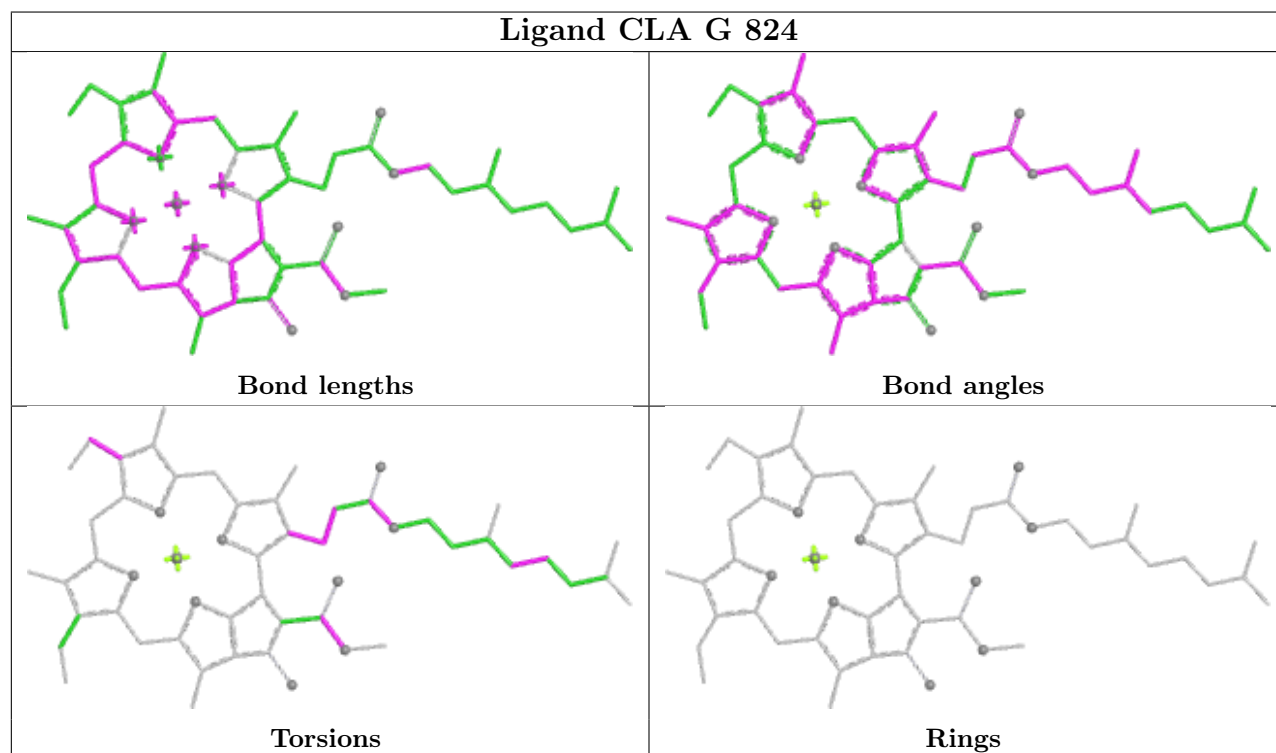
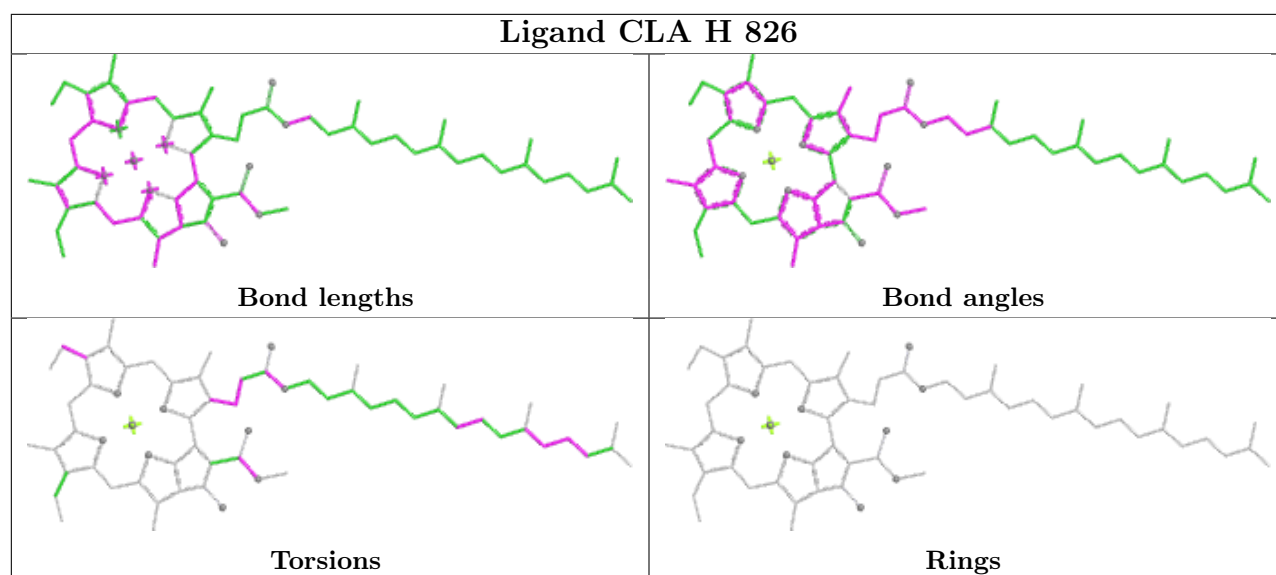


Torsions

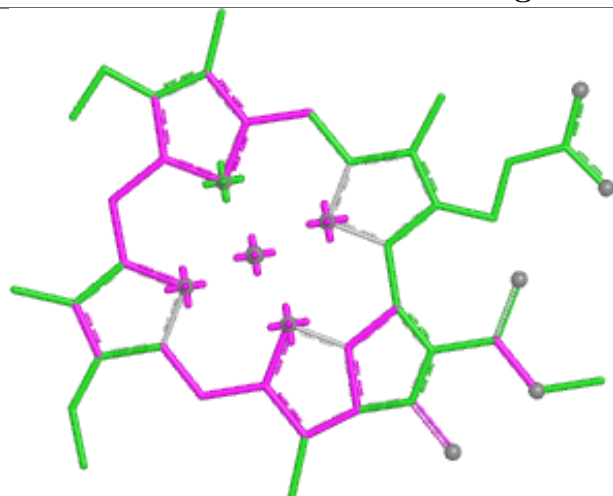


Rings

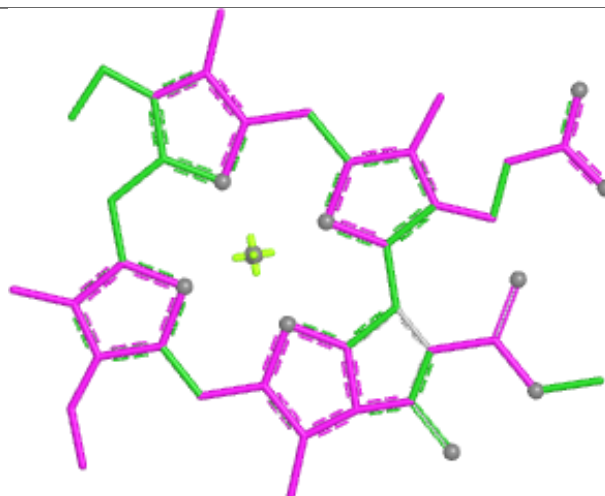




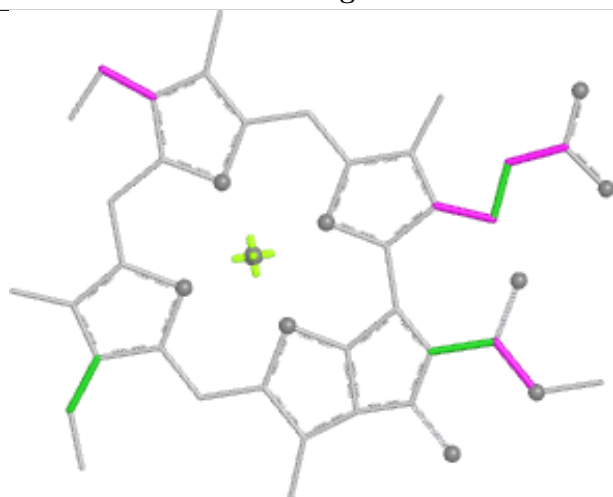
Ligand CLA B 835



Bond lengths



Bond angles

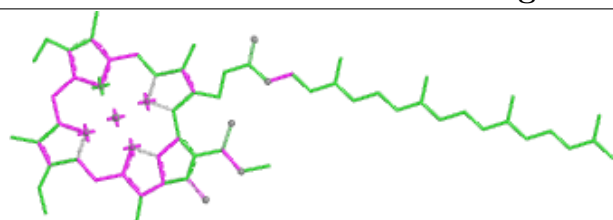


Torsions

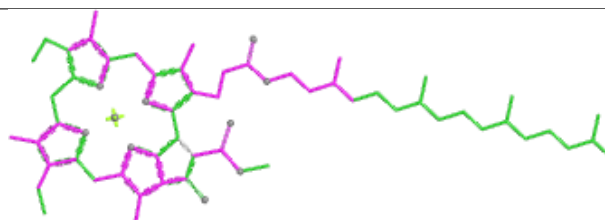


Rings

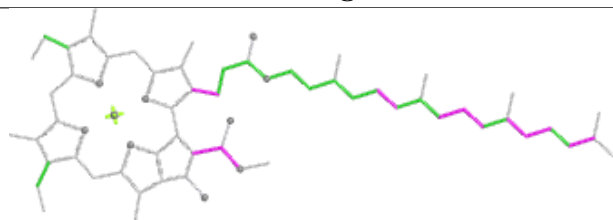
Ligand CLA a 805



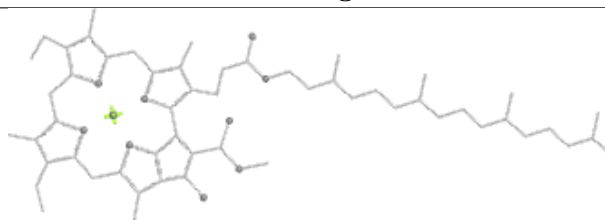
Bond lengths



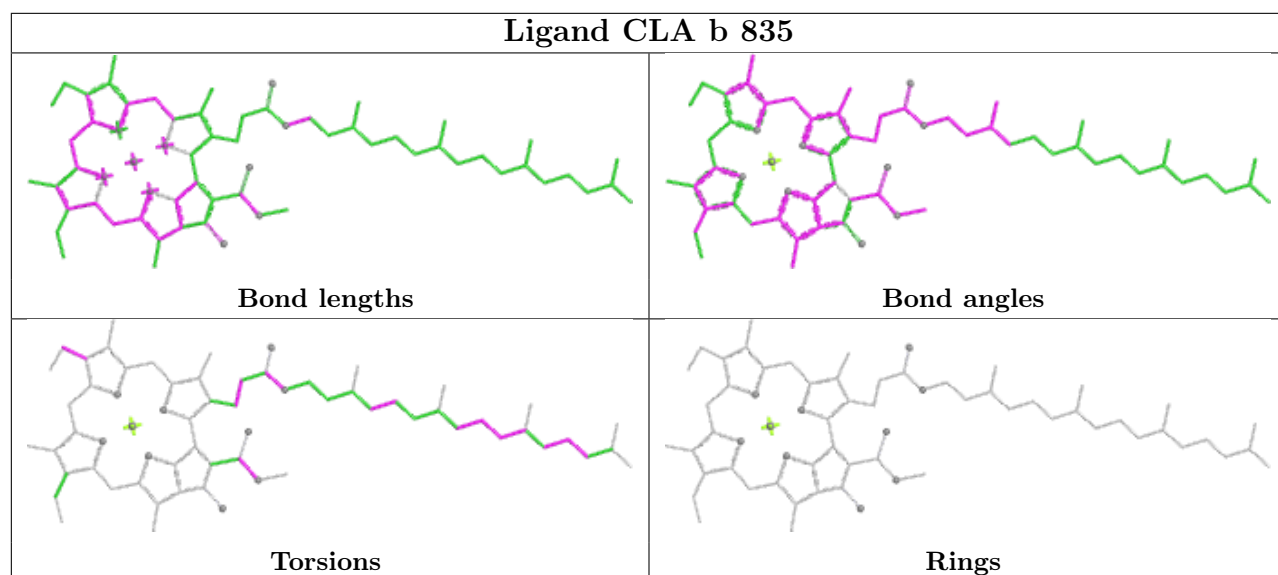
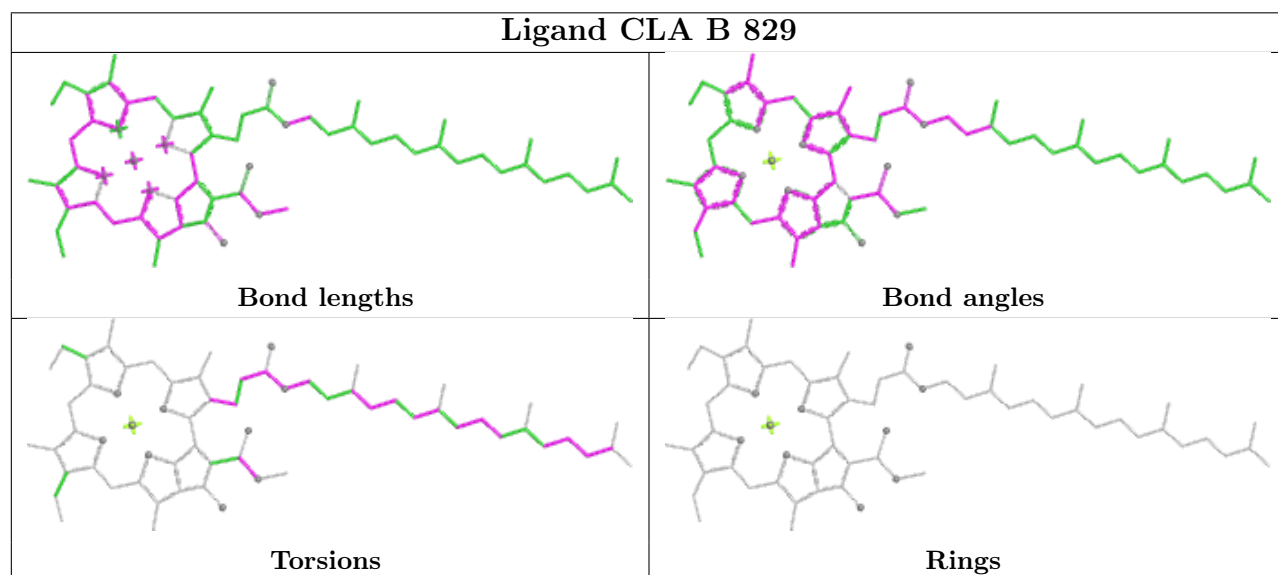
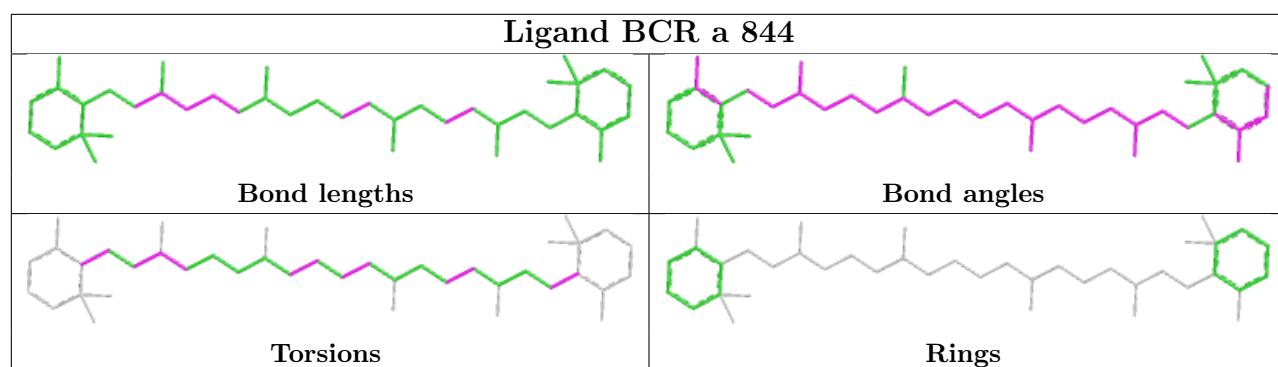
Bond angles

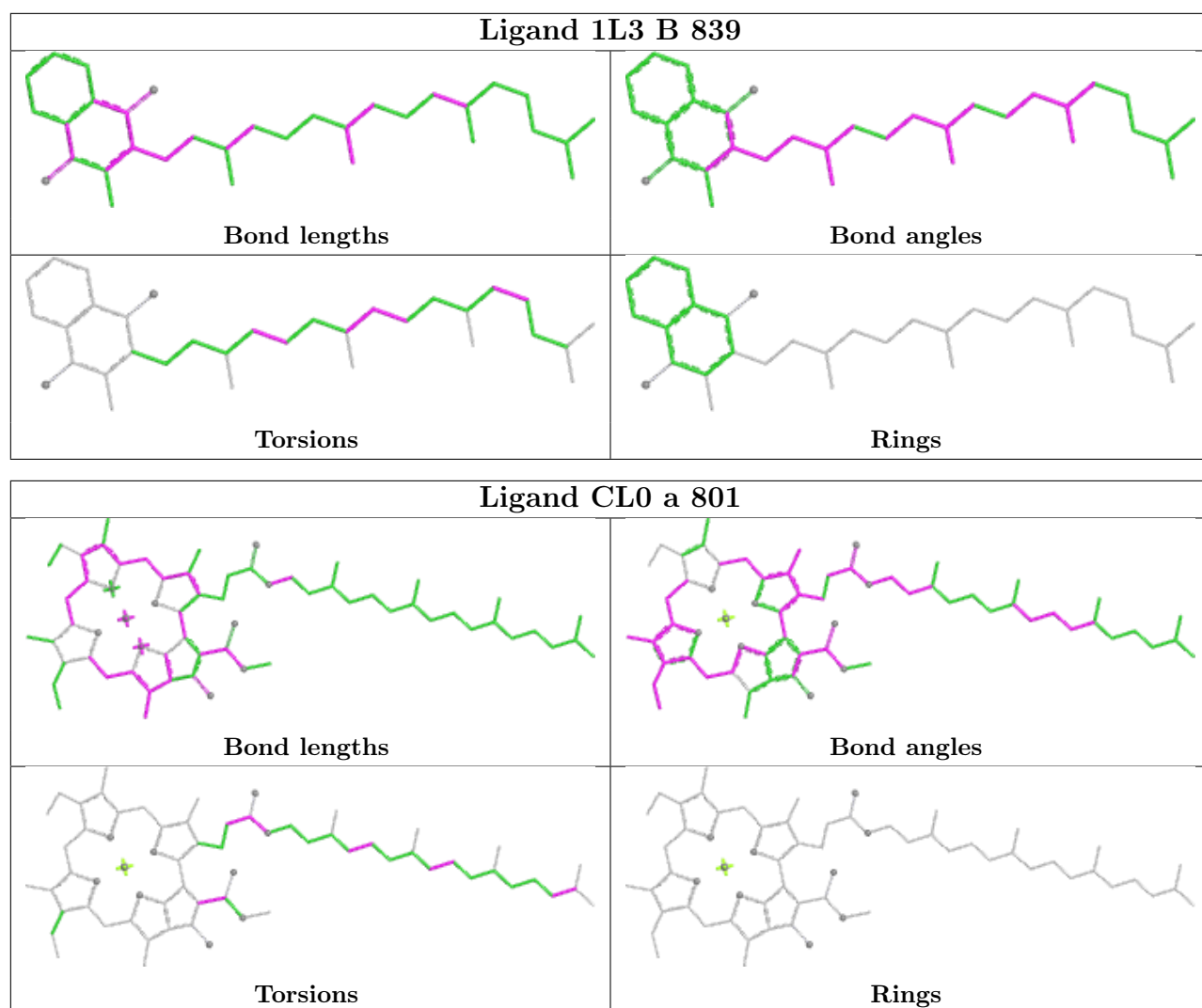


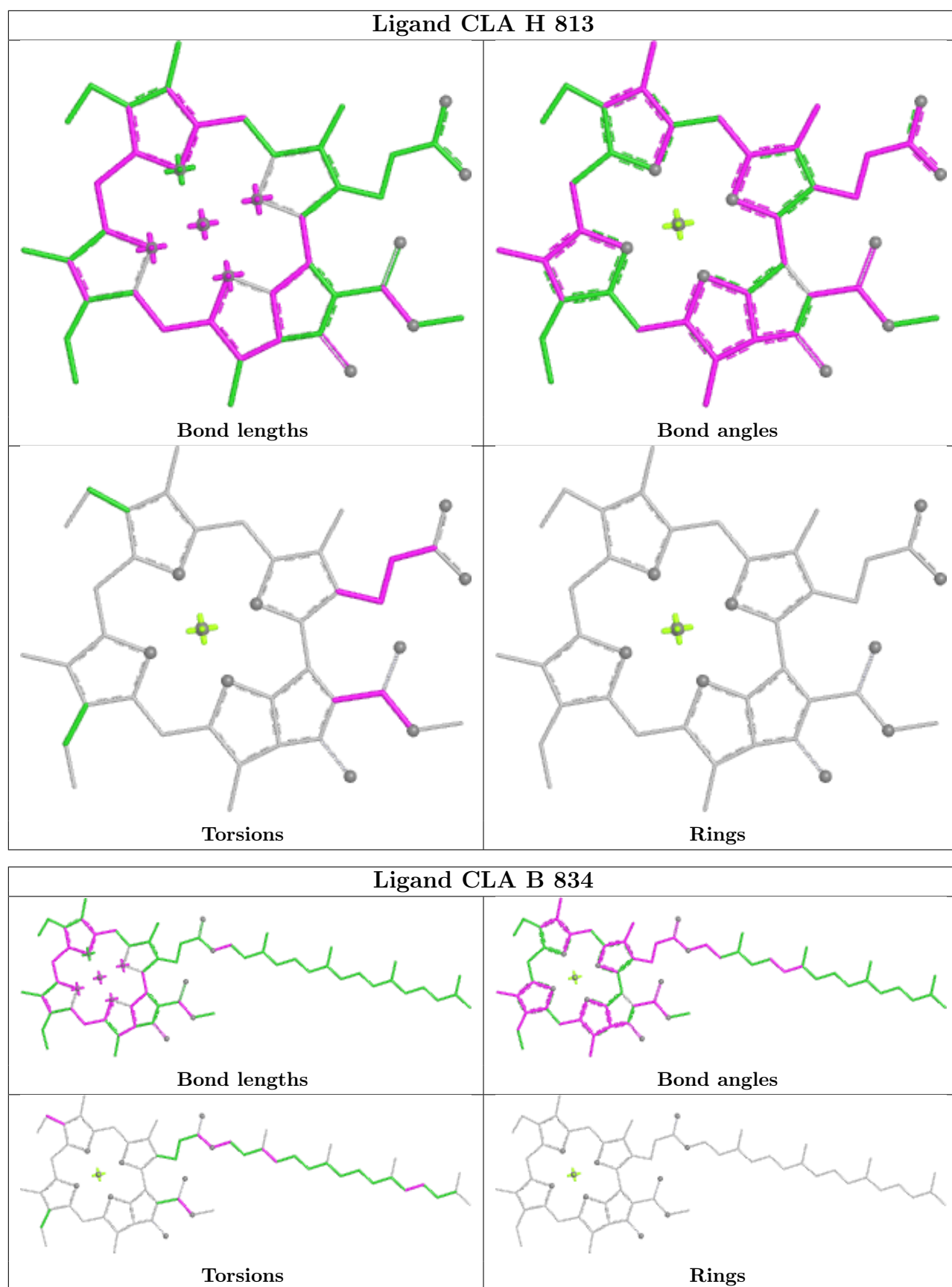
Torsions

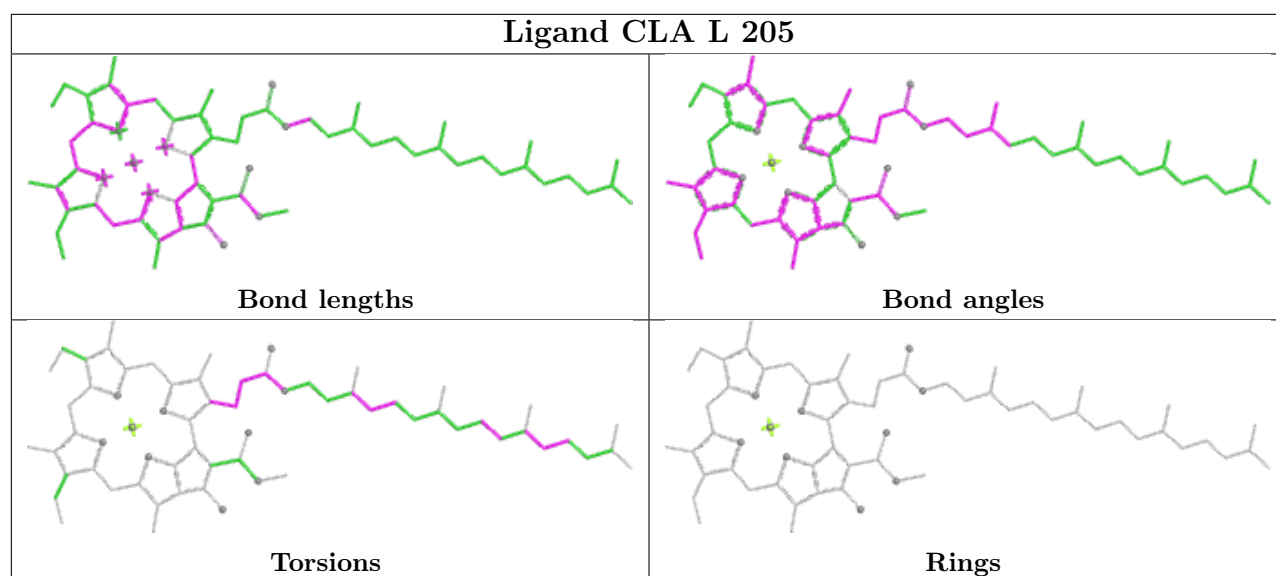
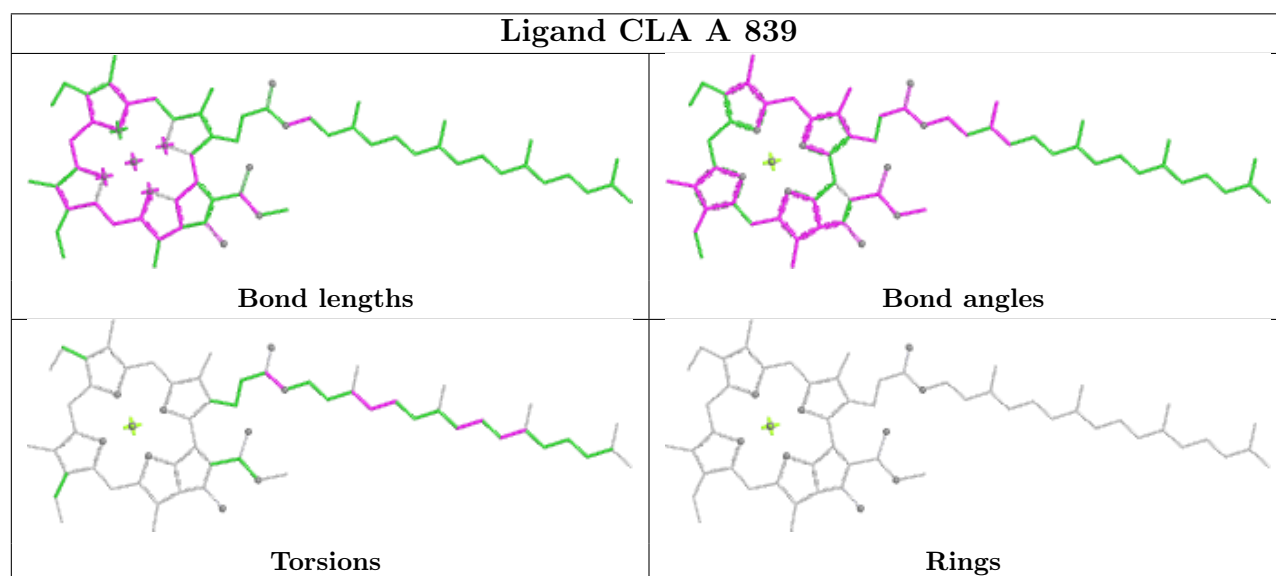
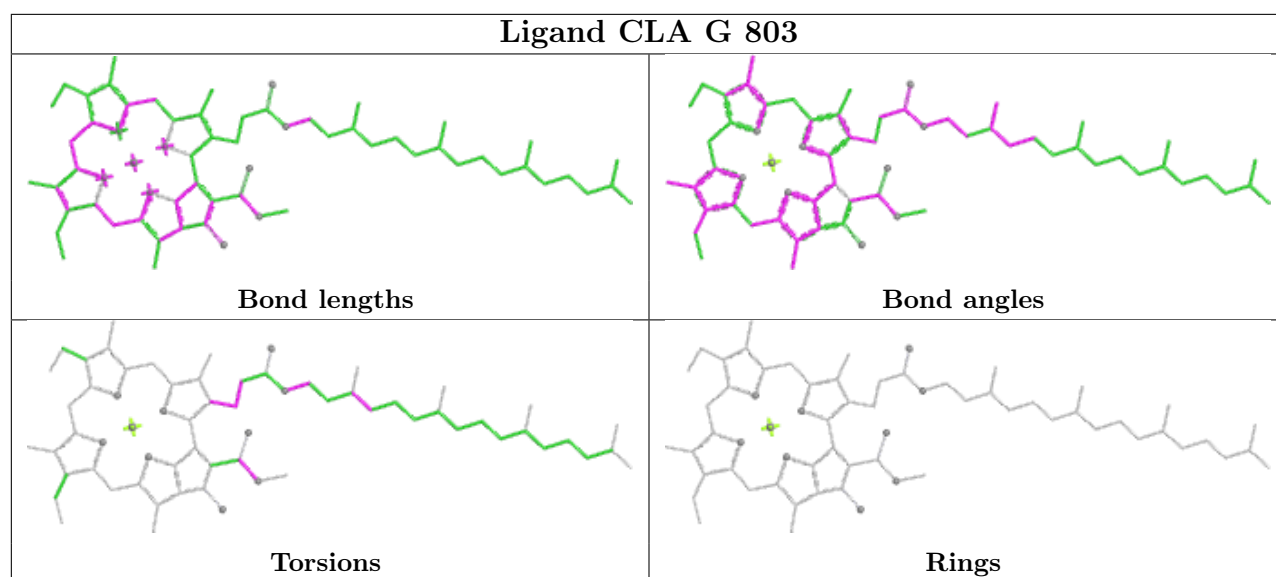


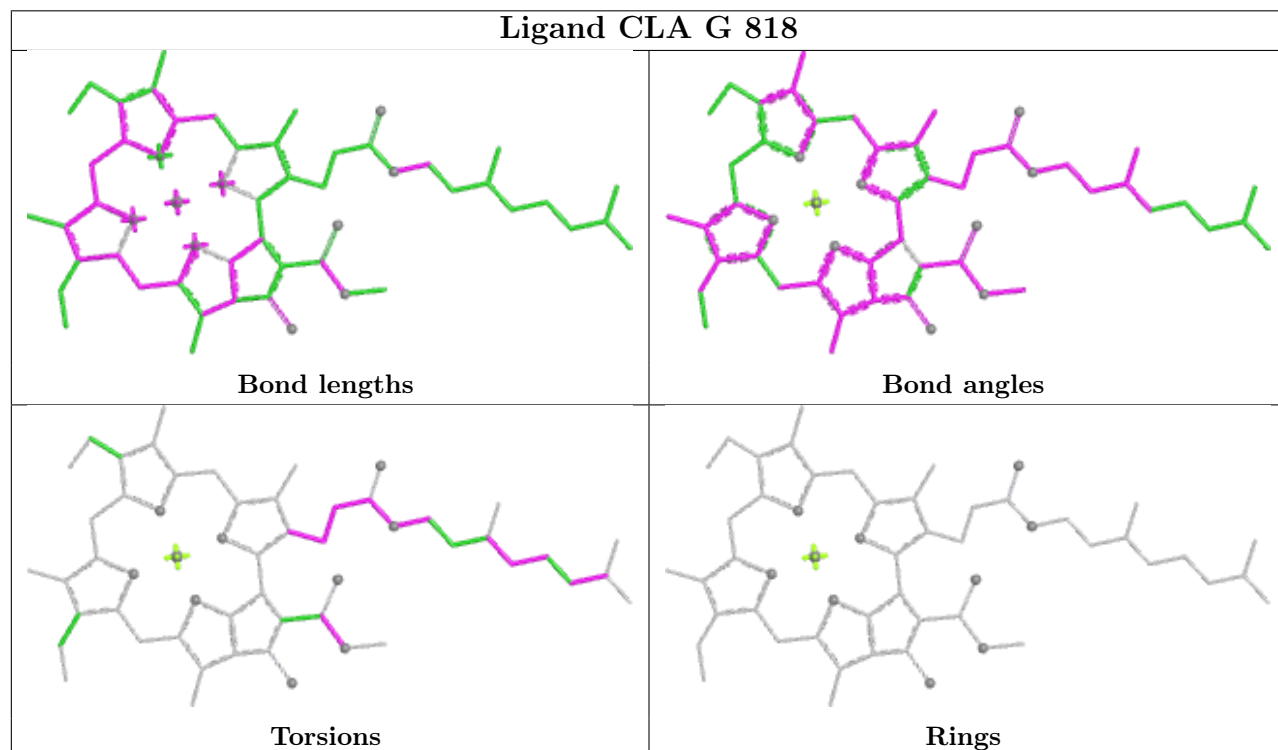
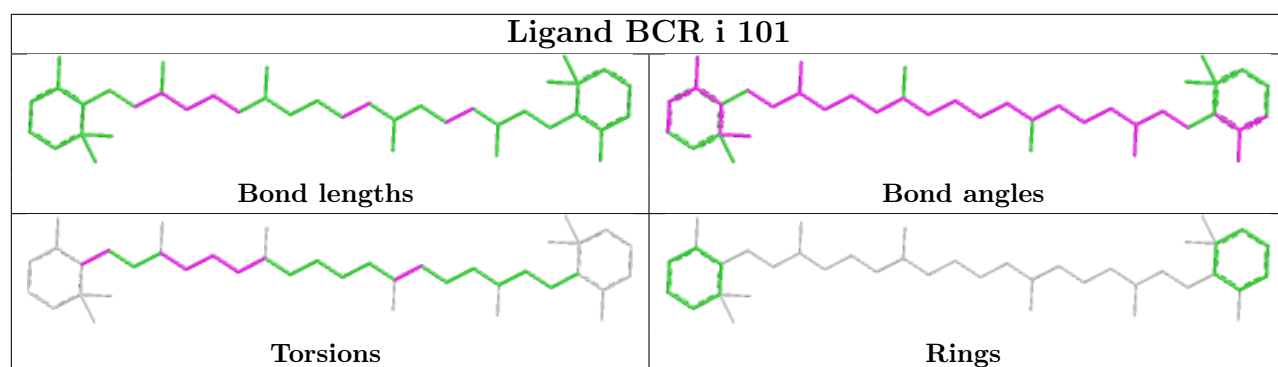
Rings



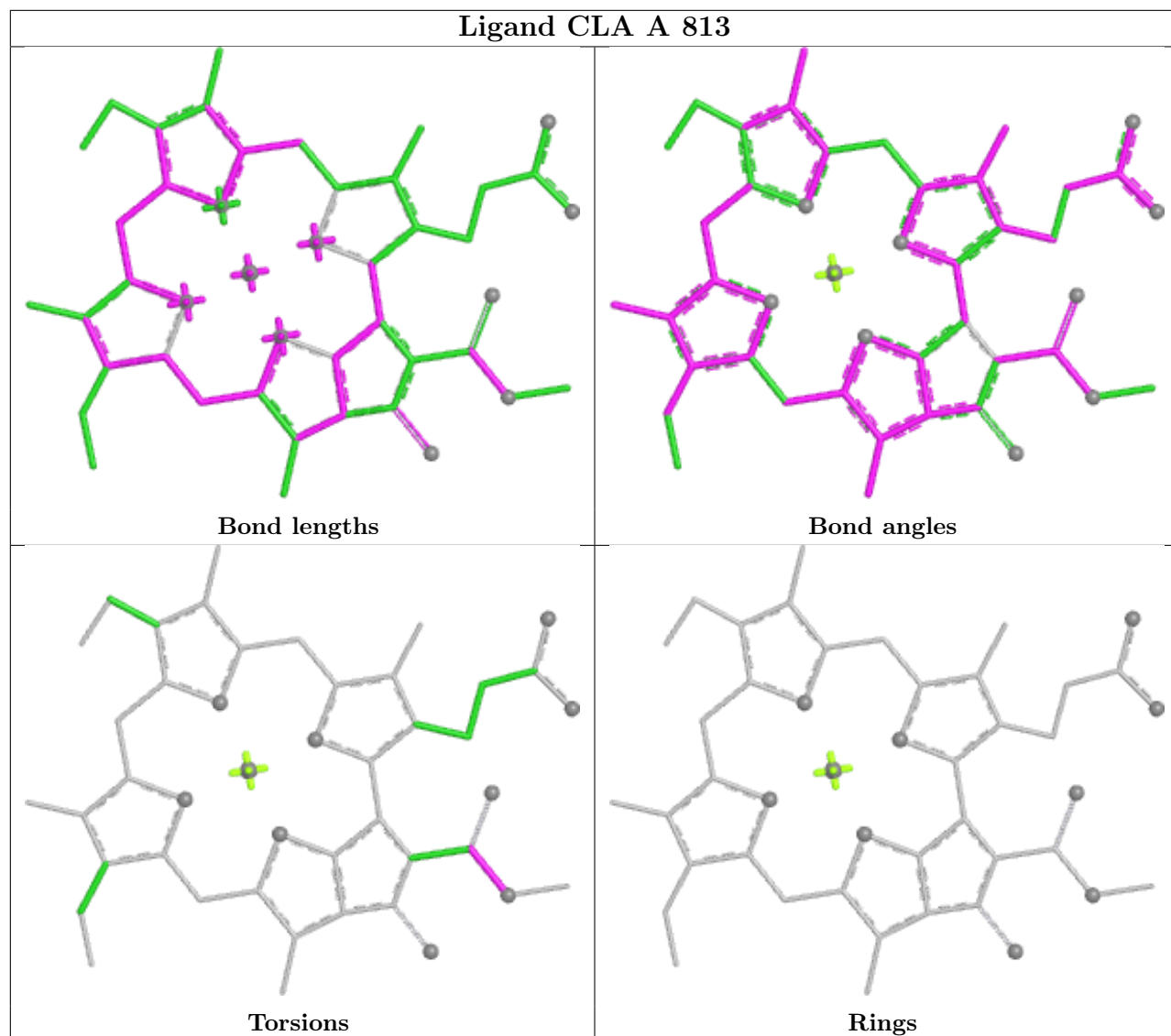




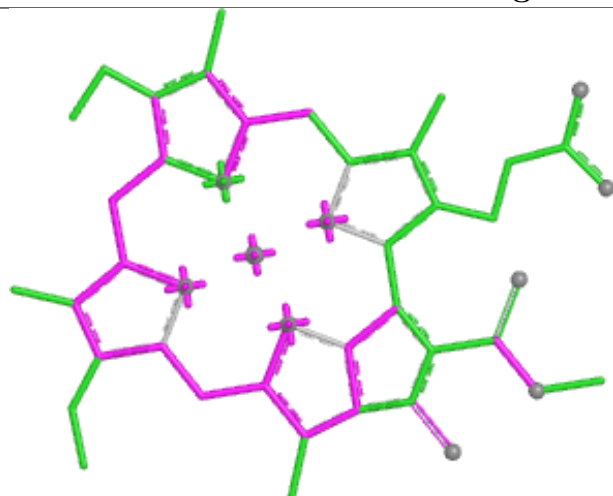




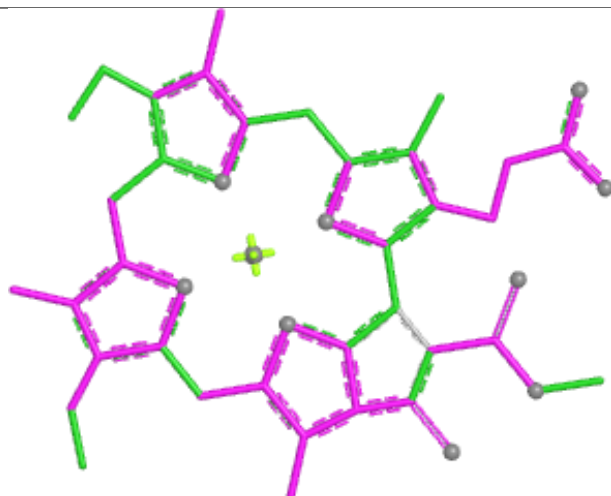
Ligand CLA A 813



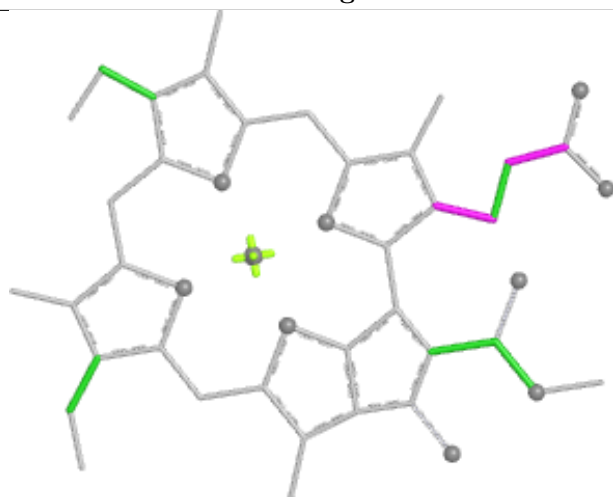
Ligand CLA G 838



Bond lengths



Bond angles

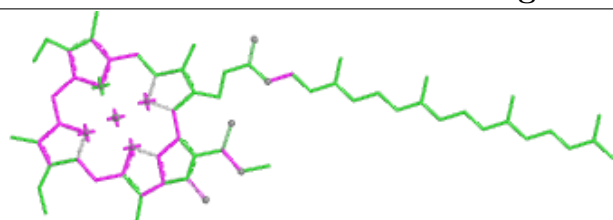


Torsions

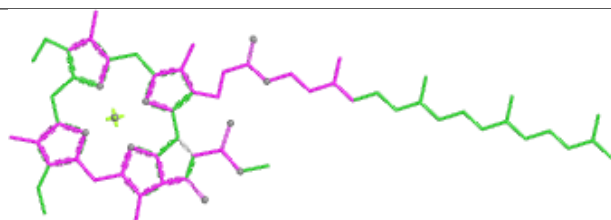


Rings

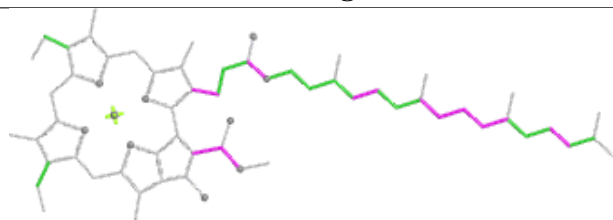
Ligand CLA a 826



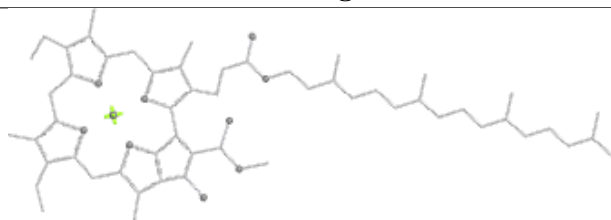
Bond lengths



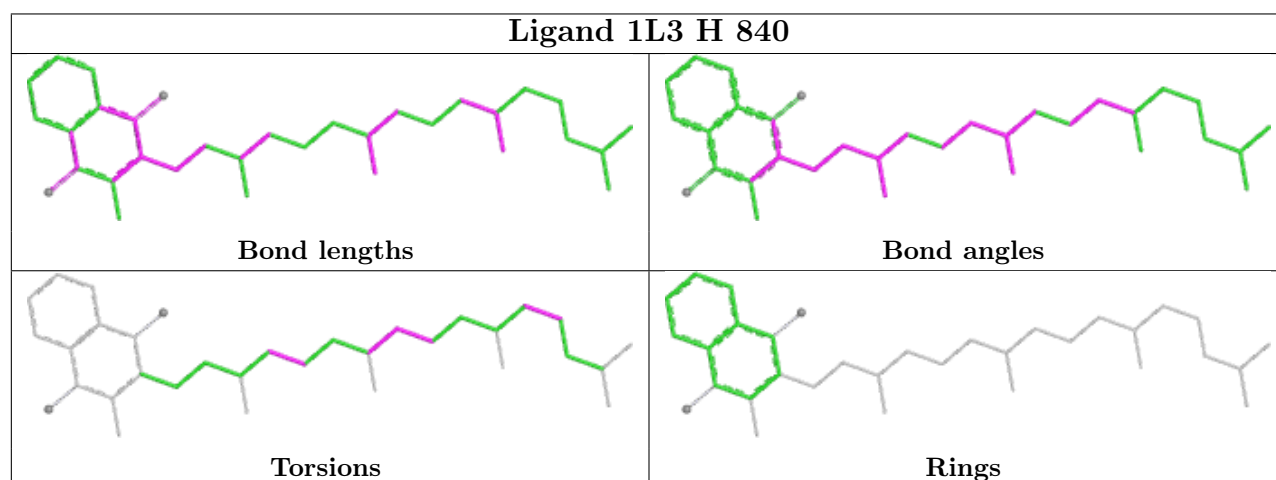
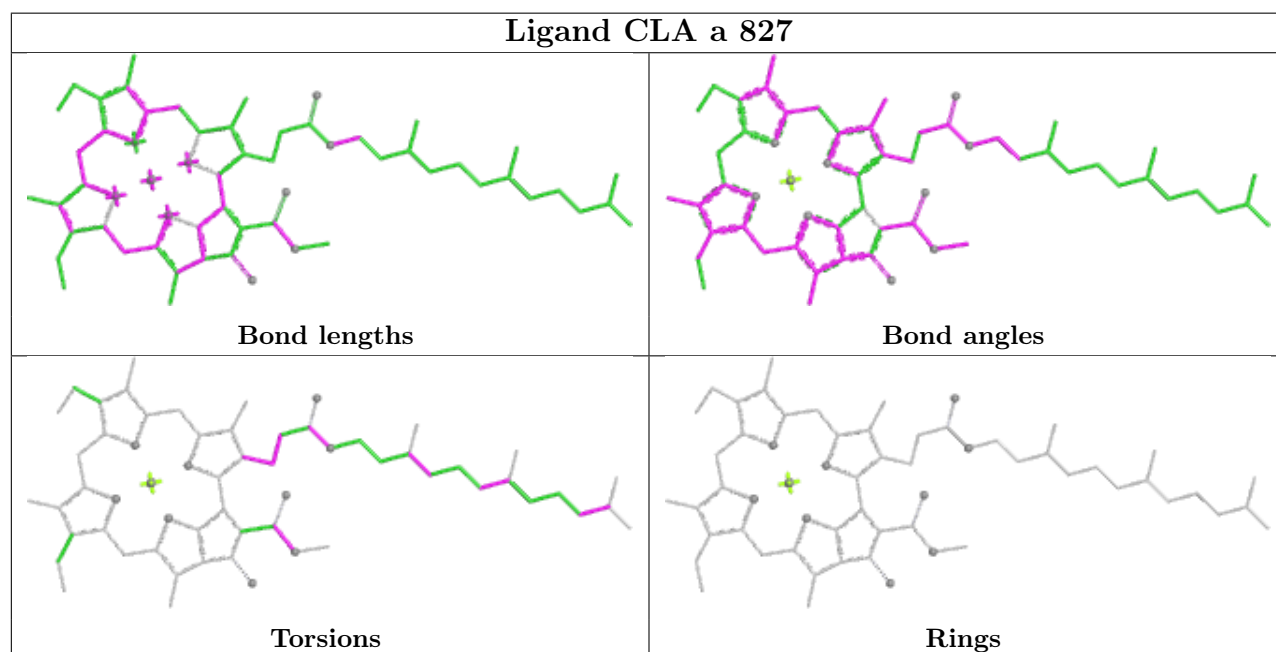
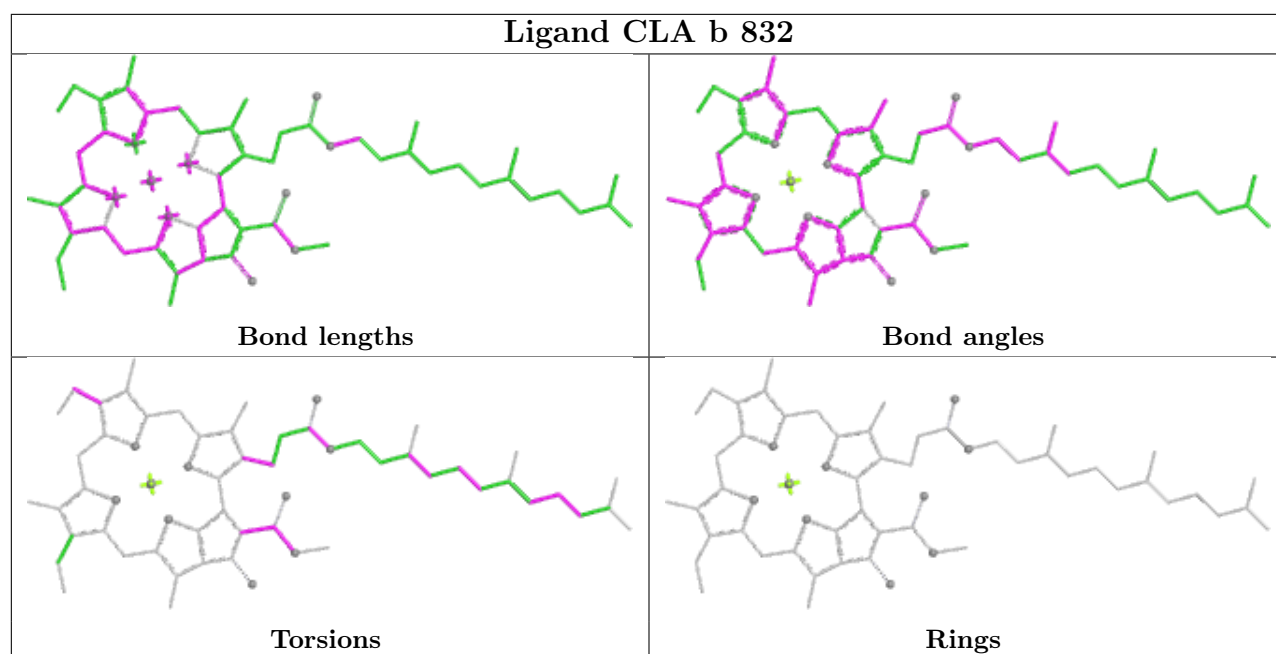
Bond angles

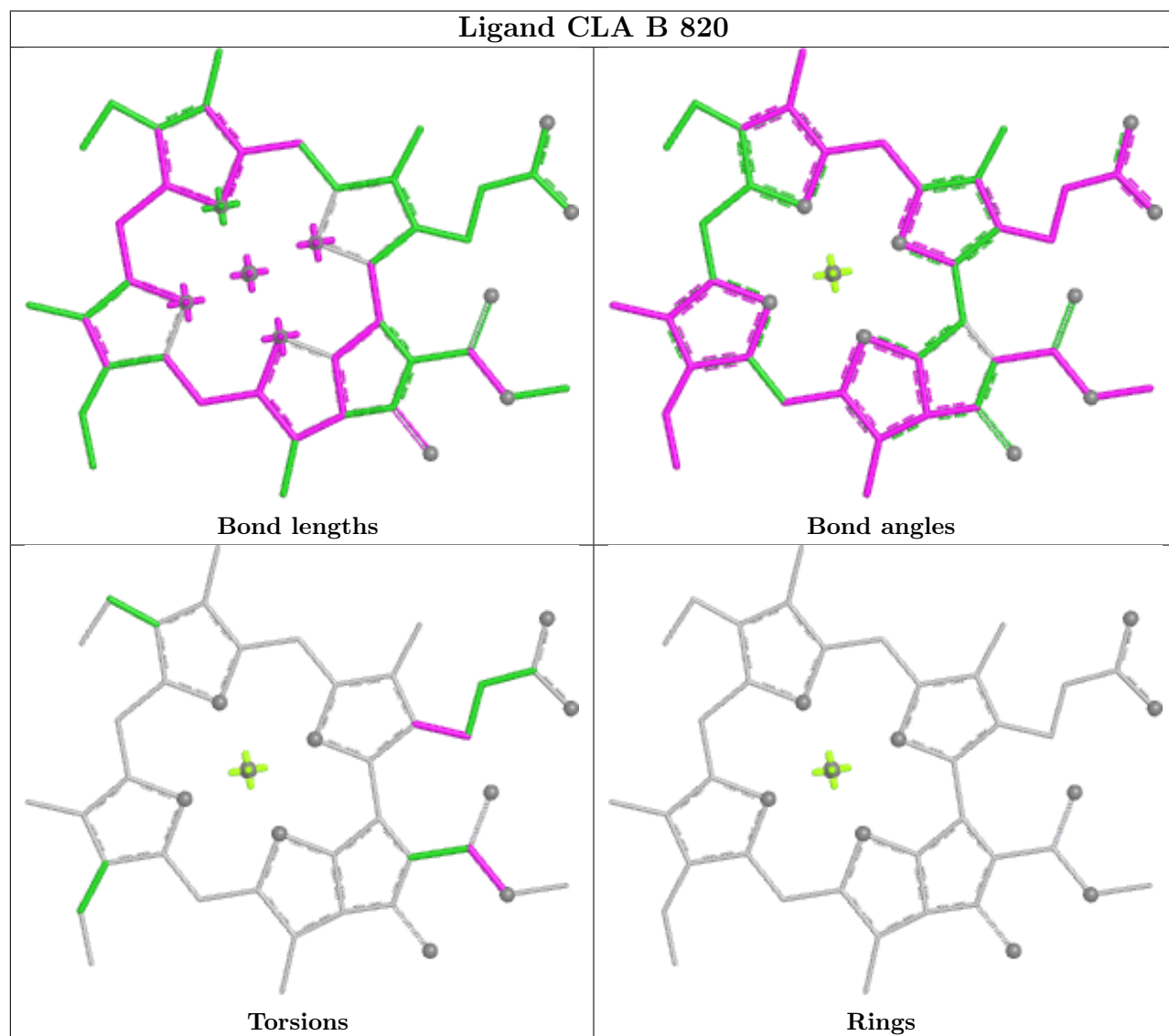
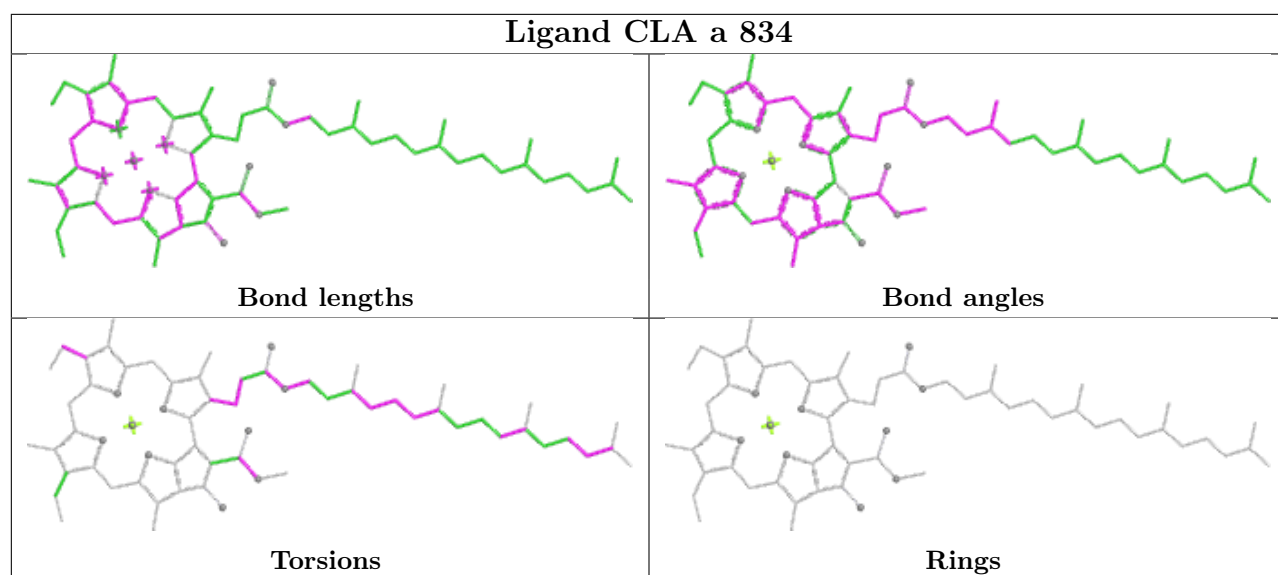


Torsions

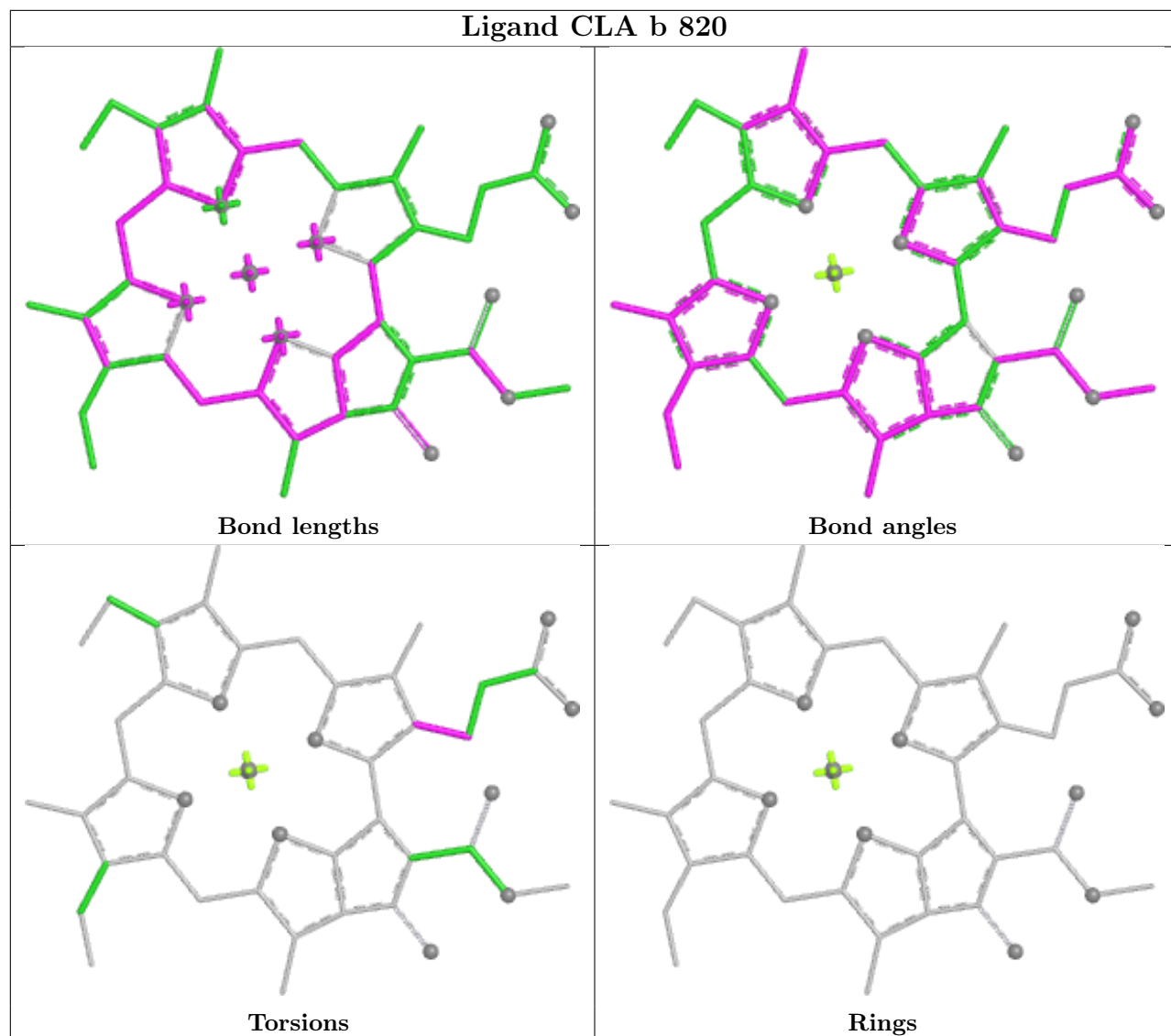


Rings

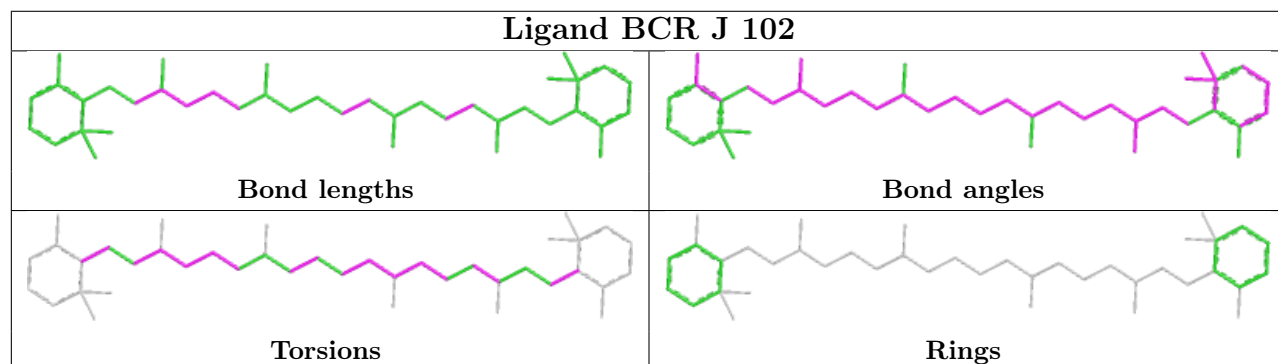


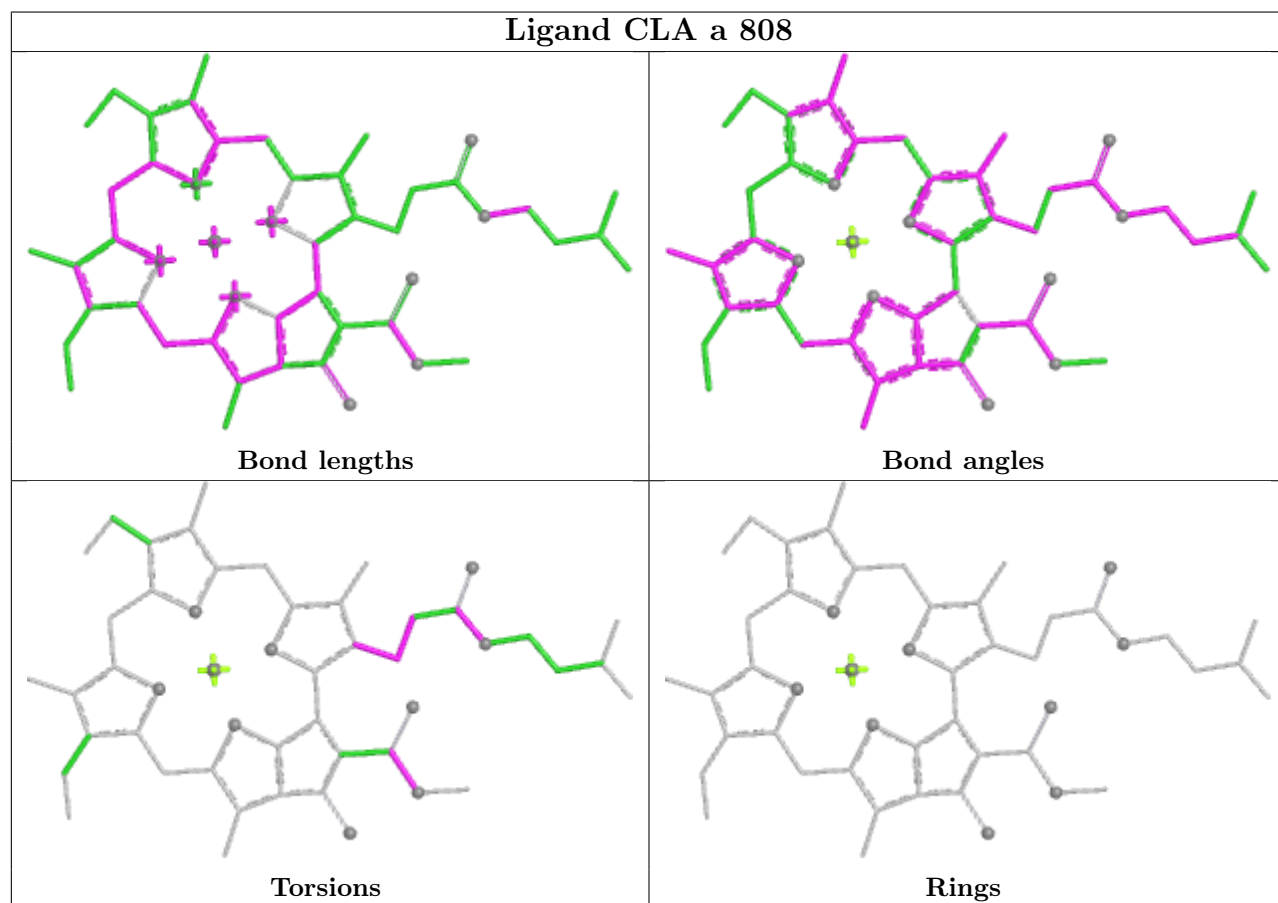
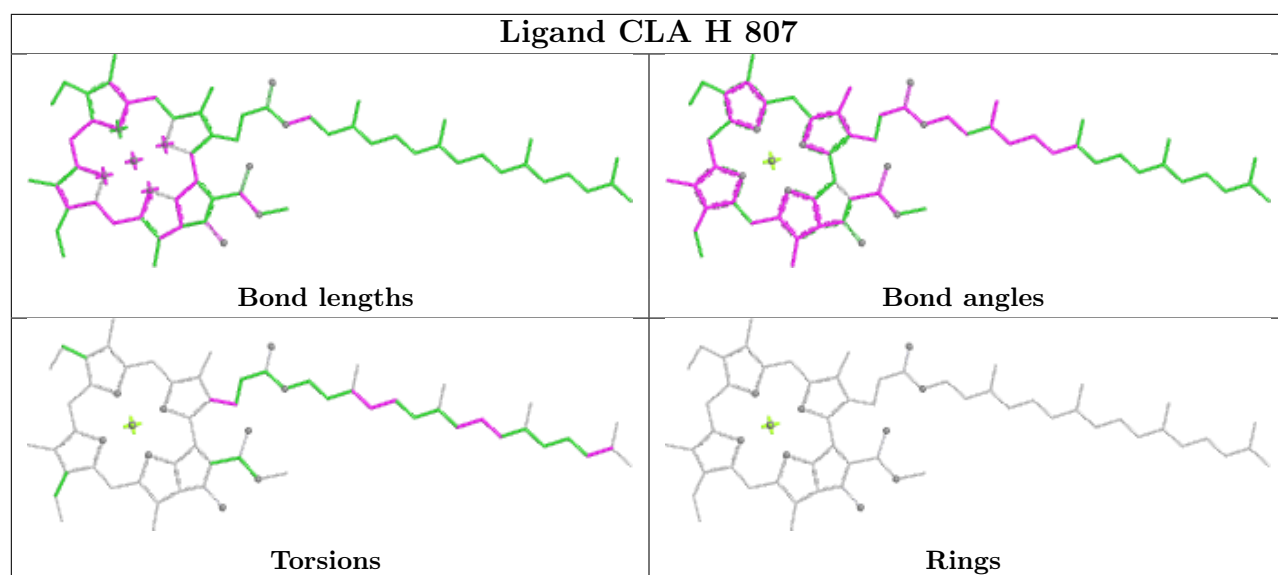


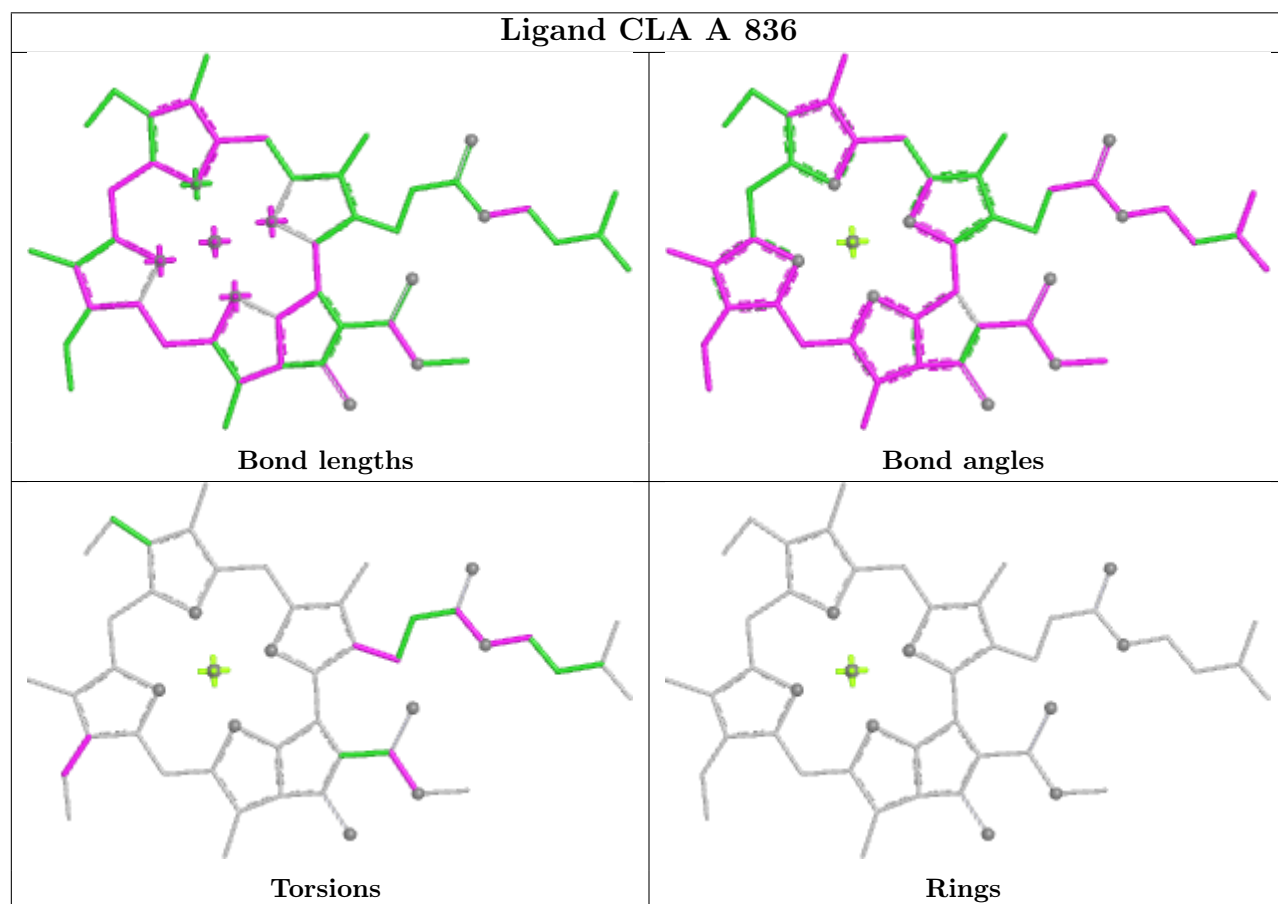
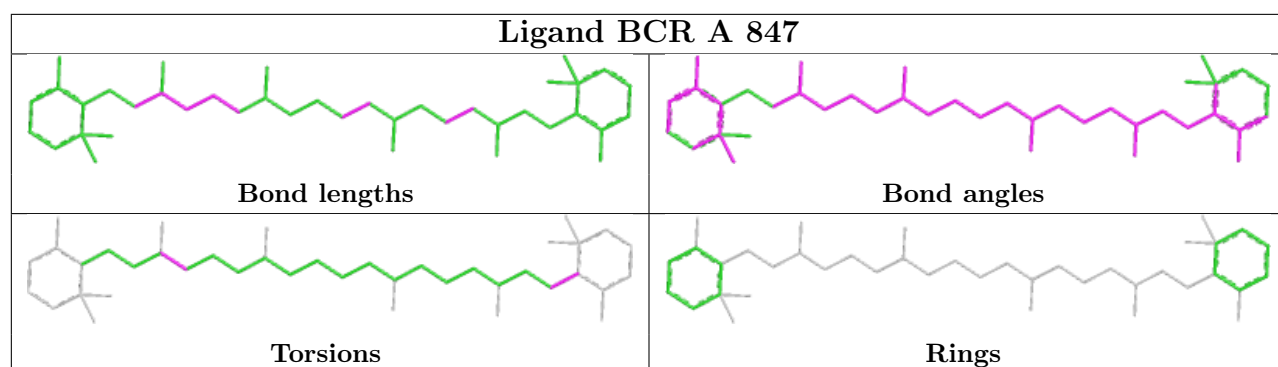
Ligand CLA b 820

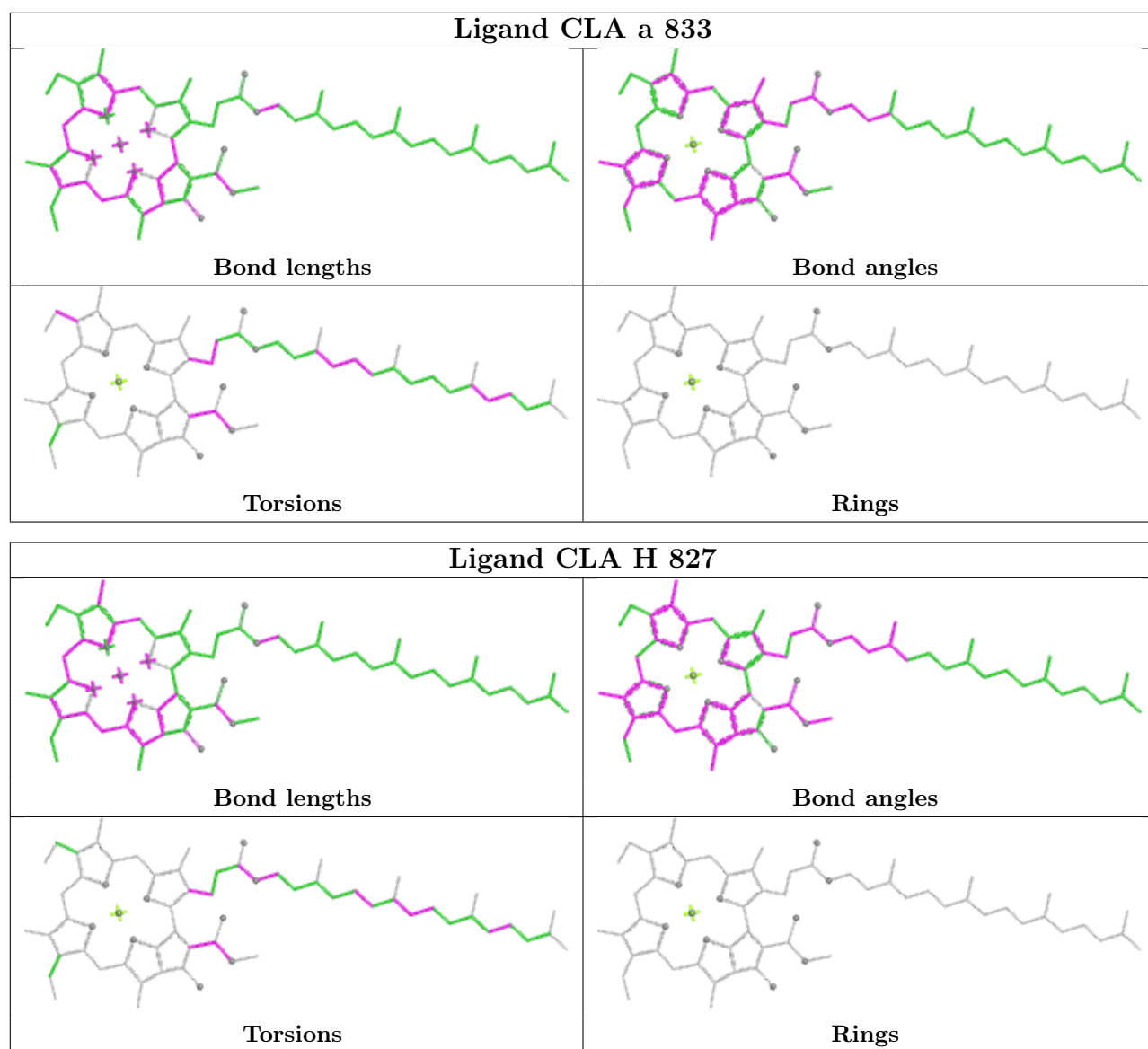


Ligand BCR J 102

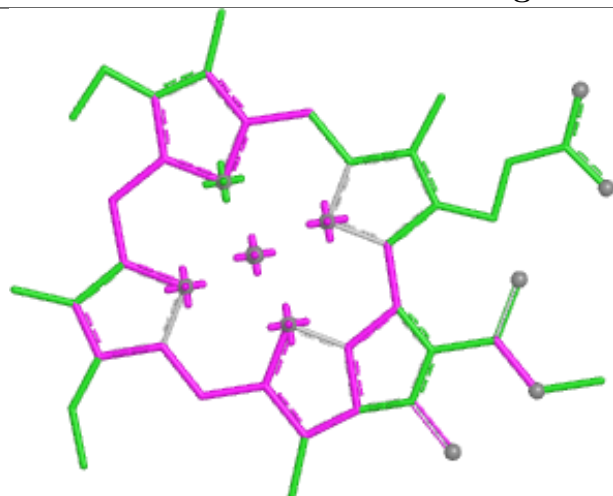




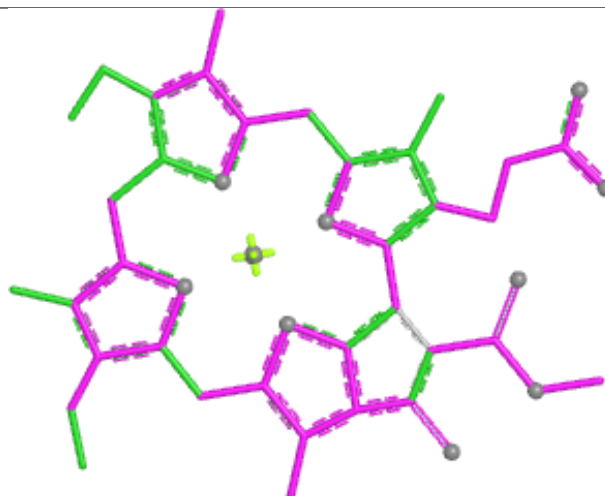




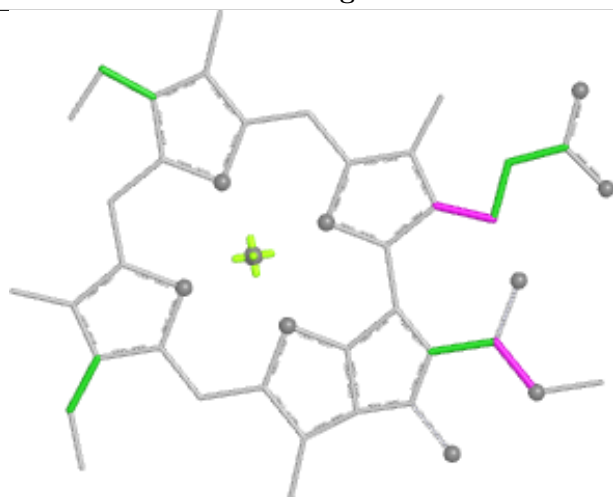
Ligand CLA H 829



Bond lengths



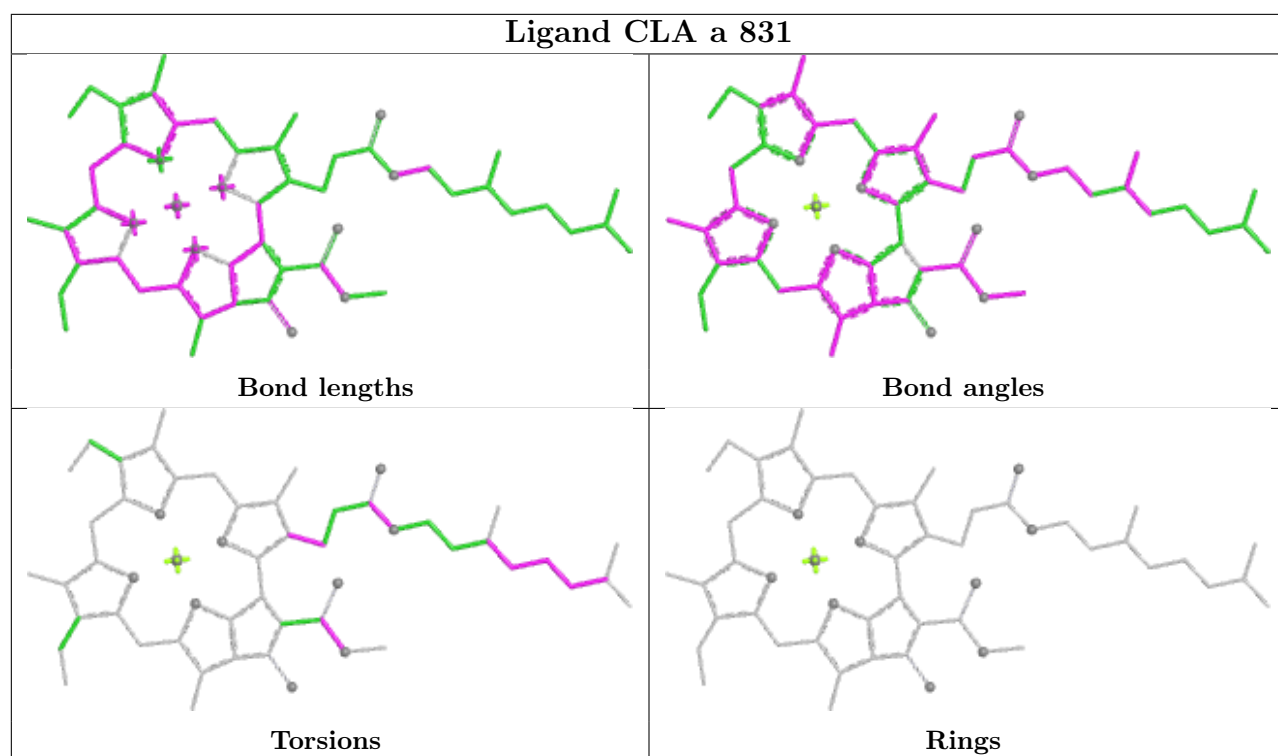
Bond angles



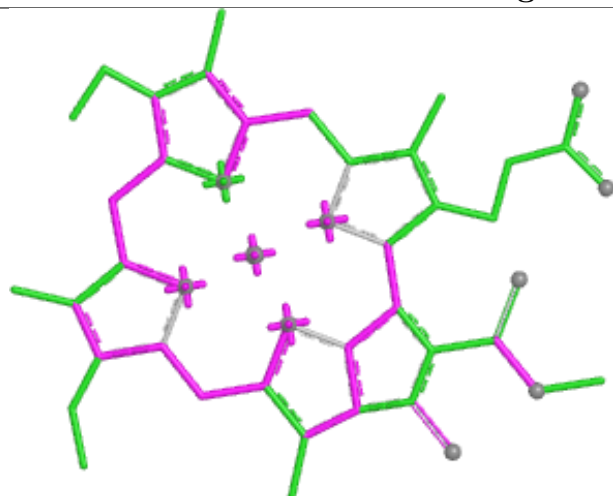
Torsions



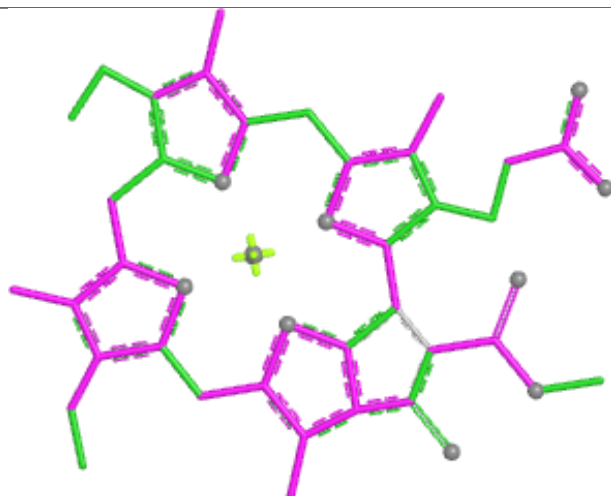
Rings



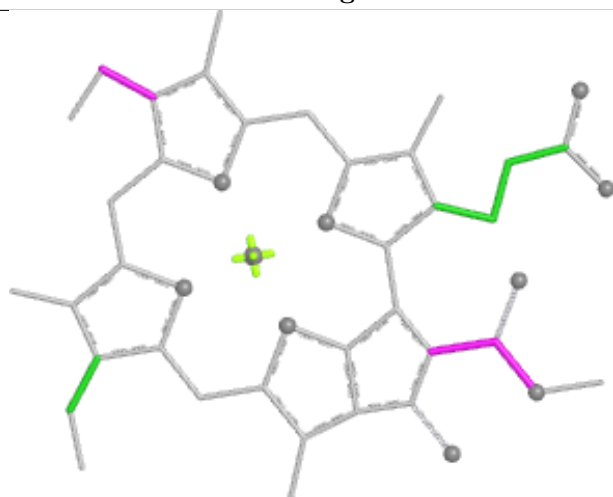
Ligand CLA b 830



Bond lengths



Bond angles

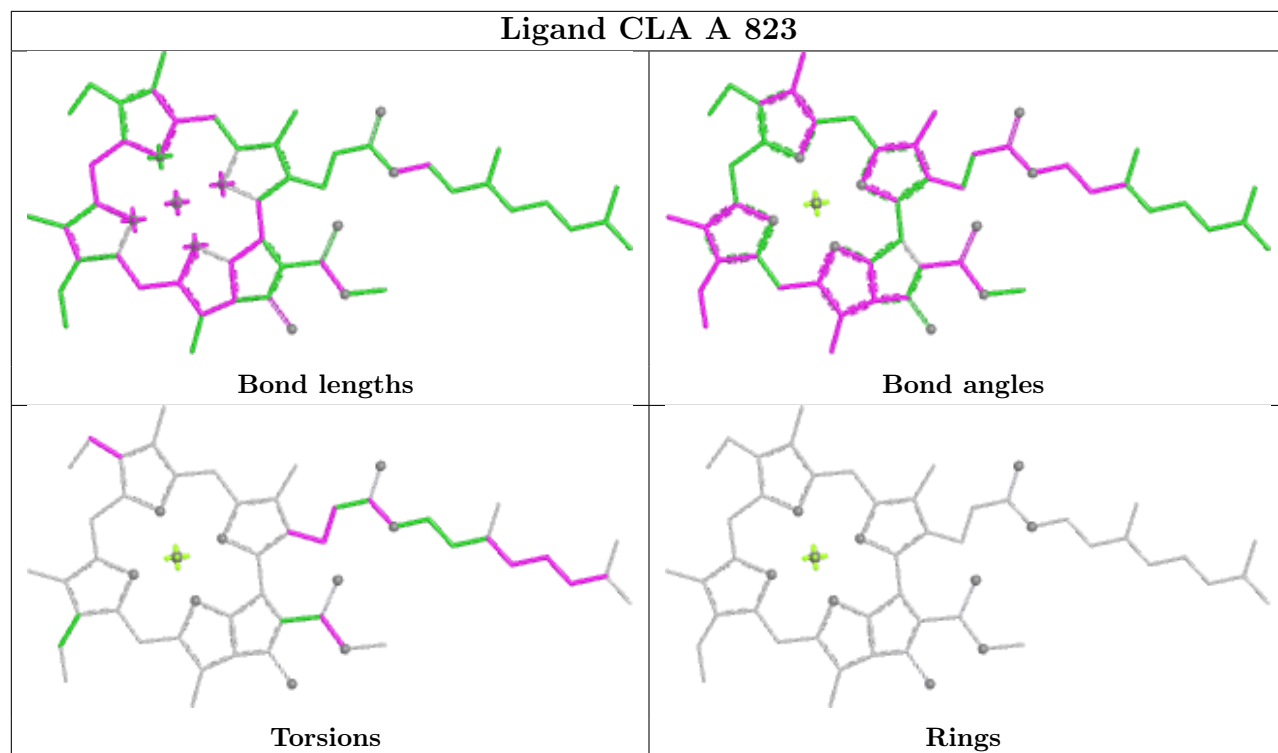


Torsions

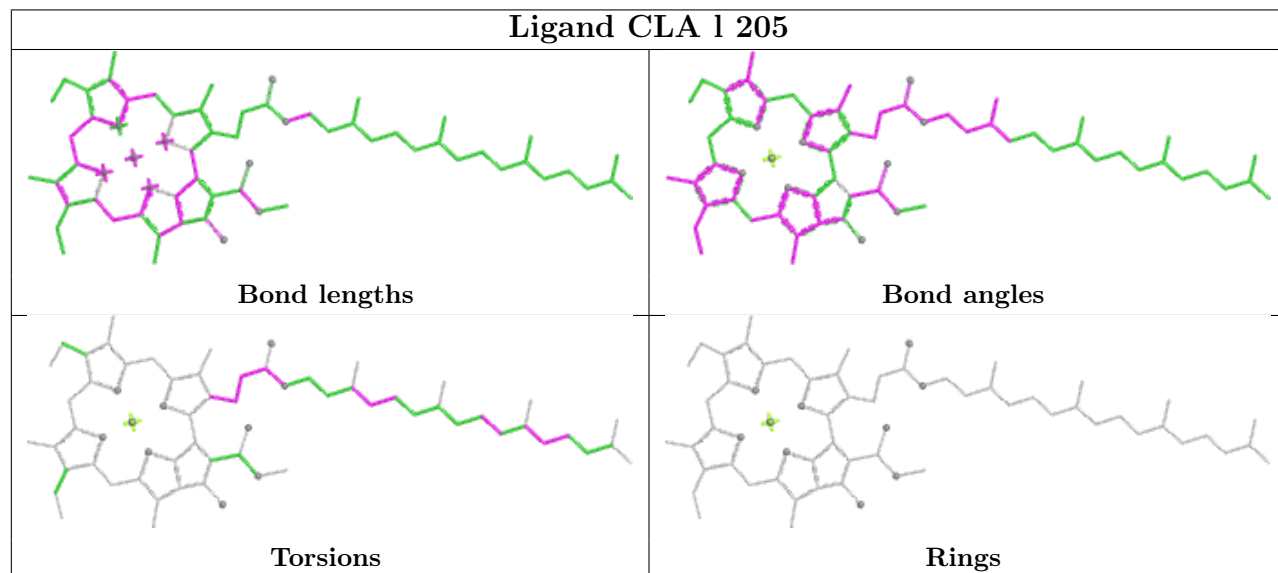


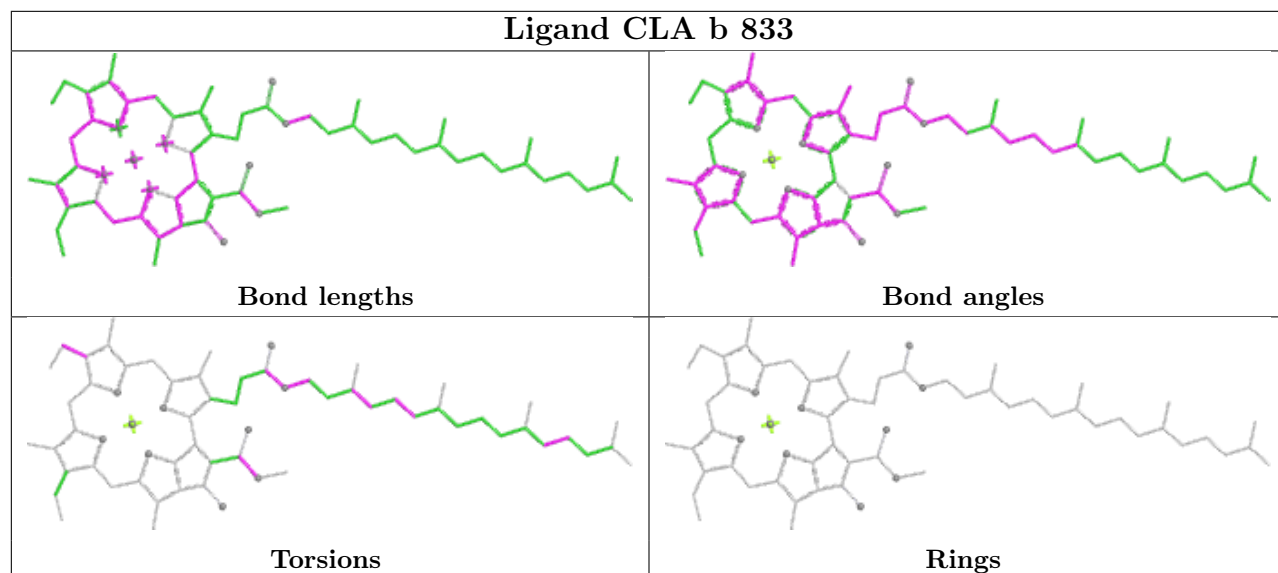
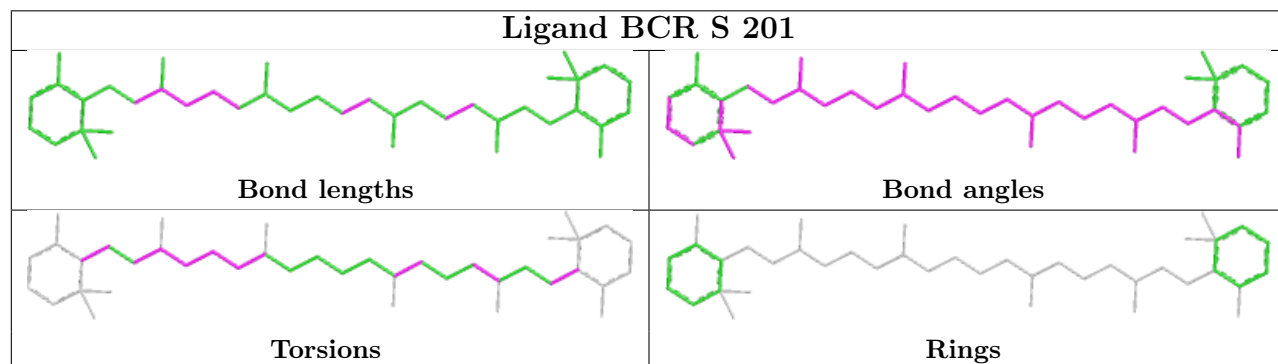
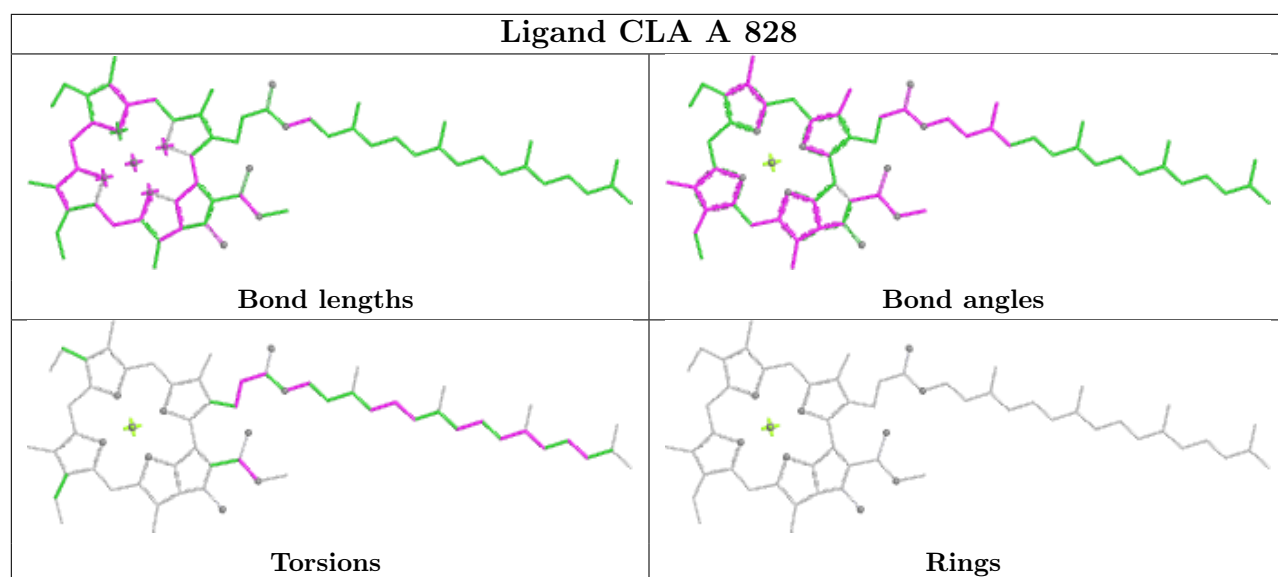
Rings

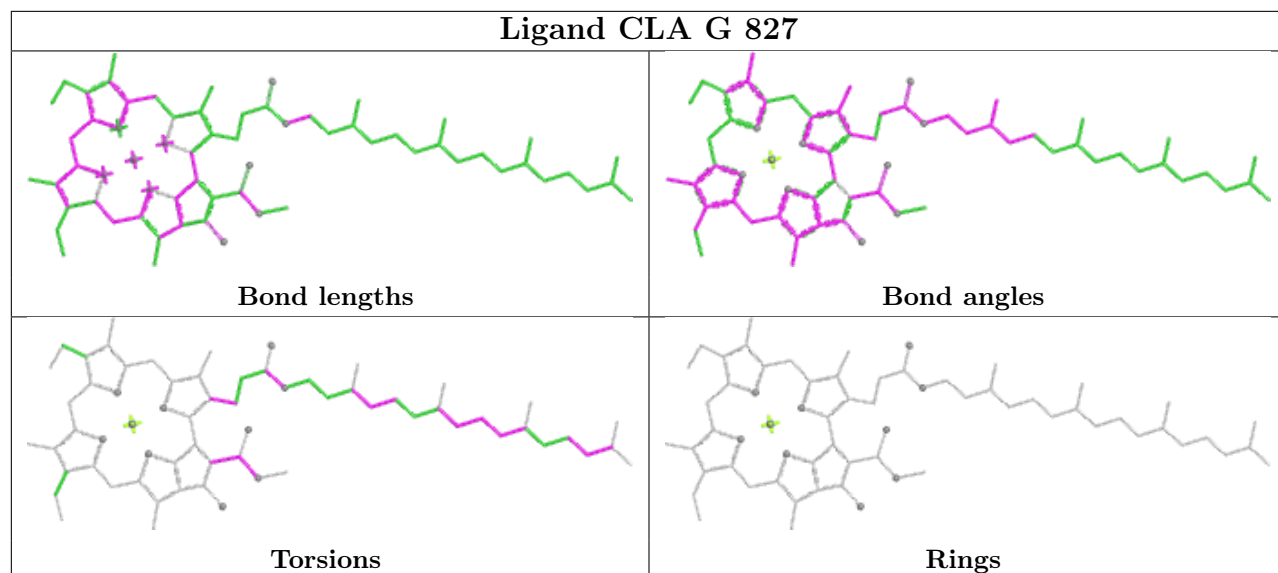
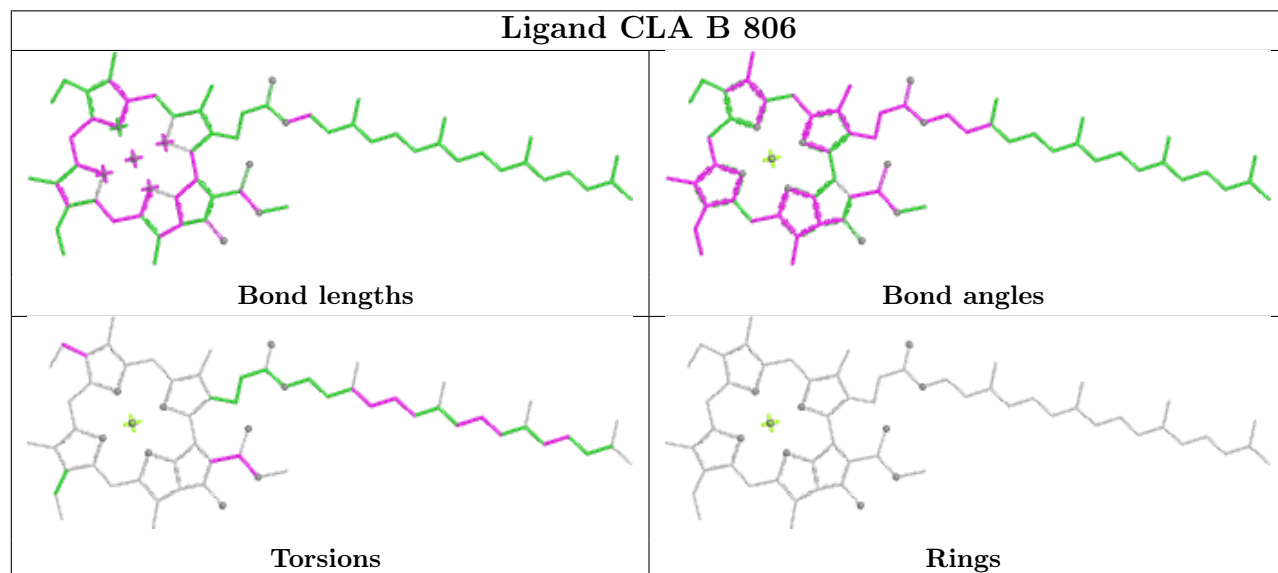
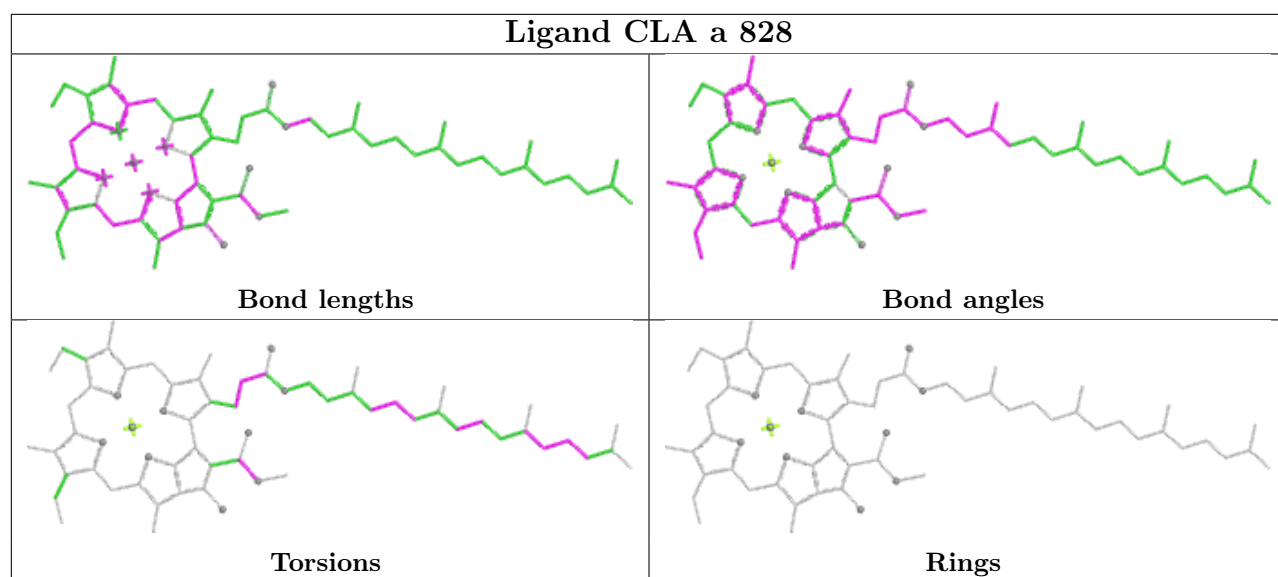
Ligand CLA A 823



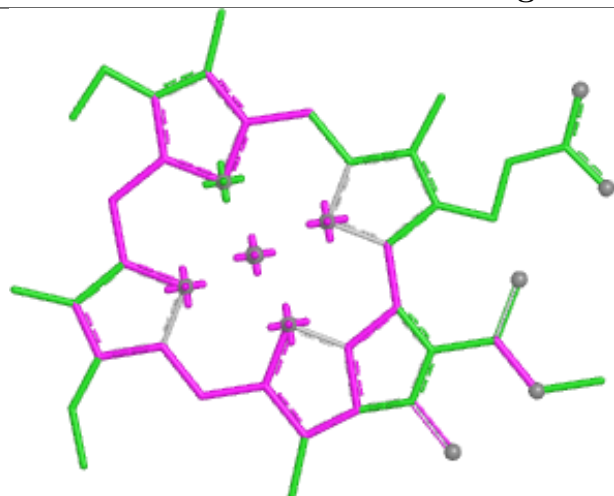
Ligand CLA I 205



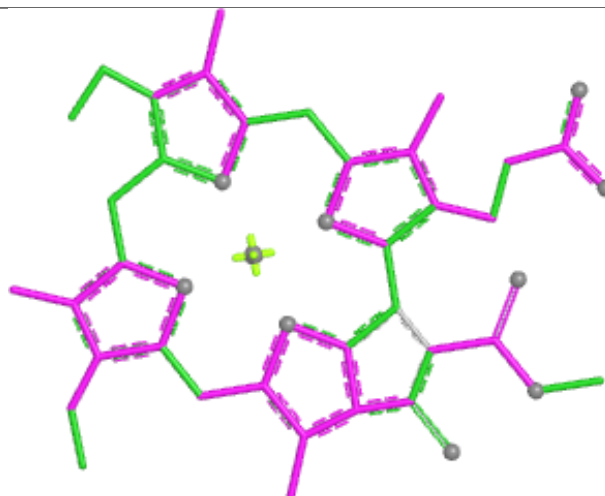




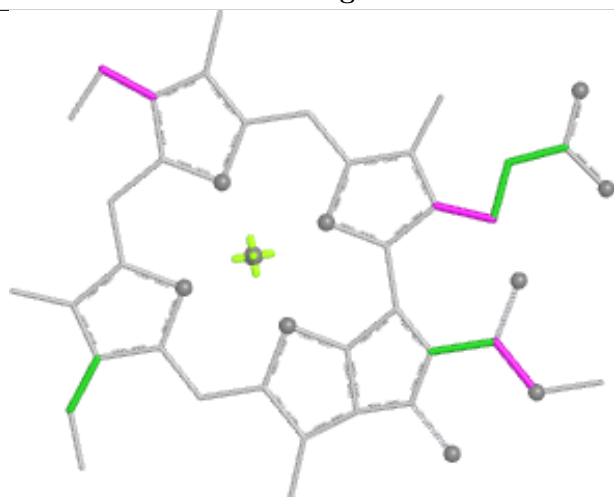
Ligand CLA b 818



Bond lengths



Bond angles

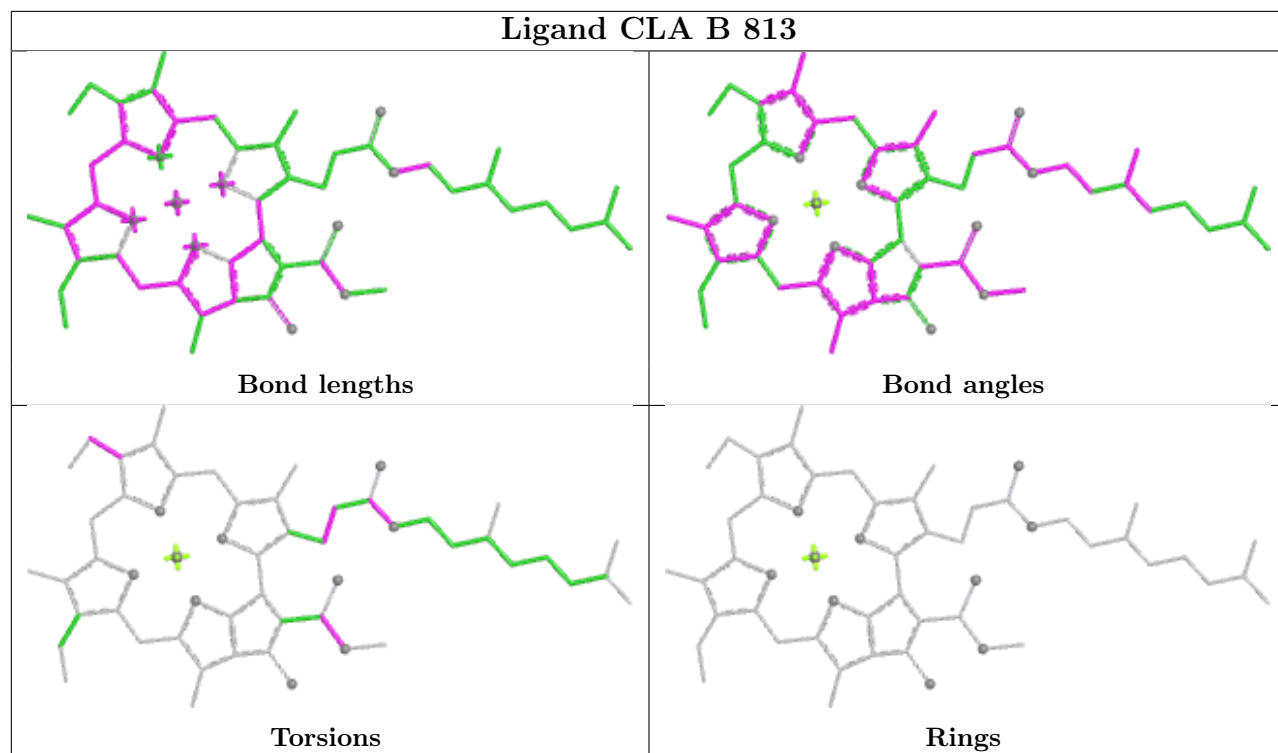


Torsions

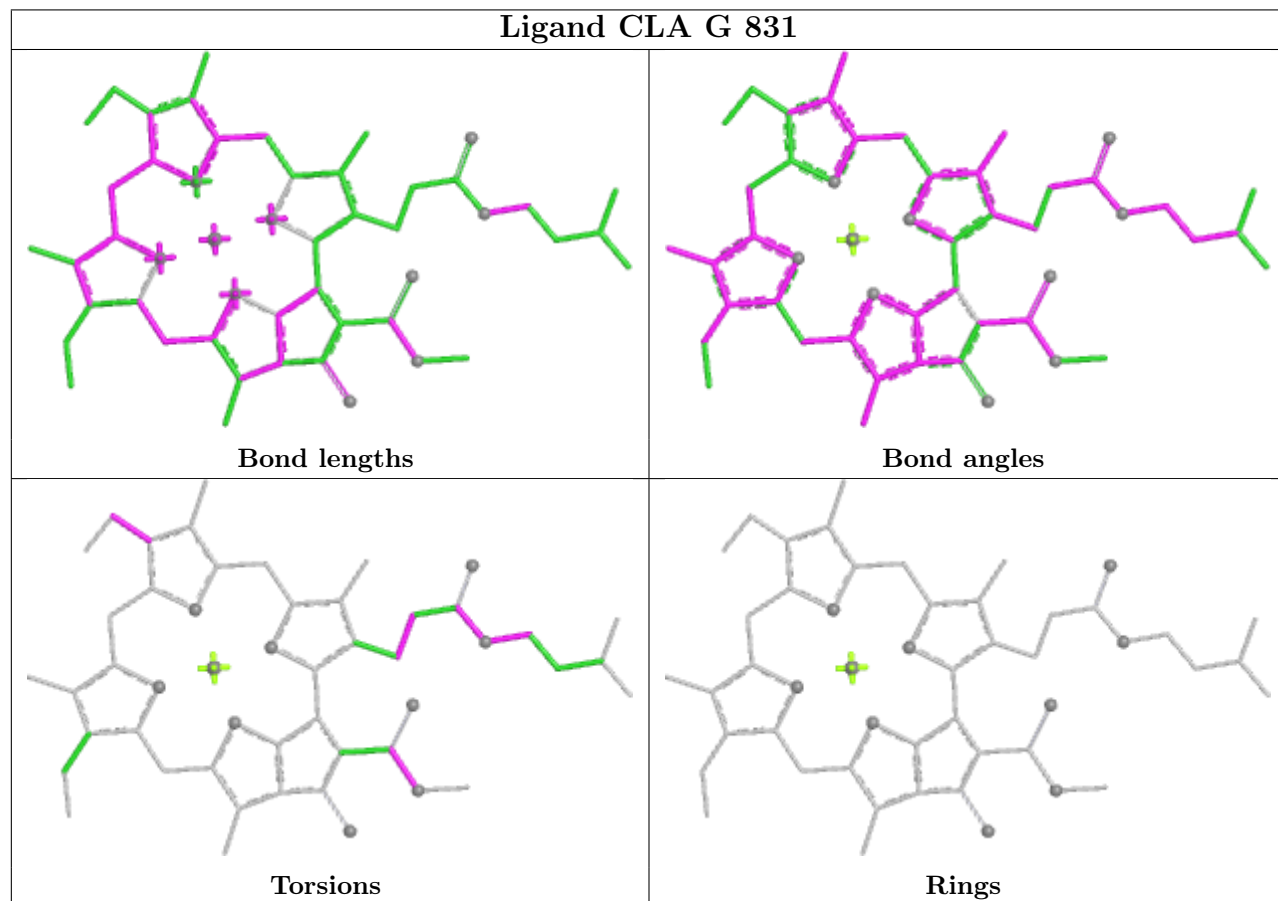


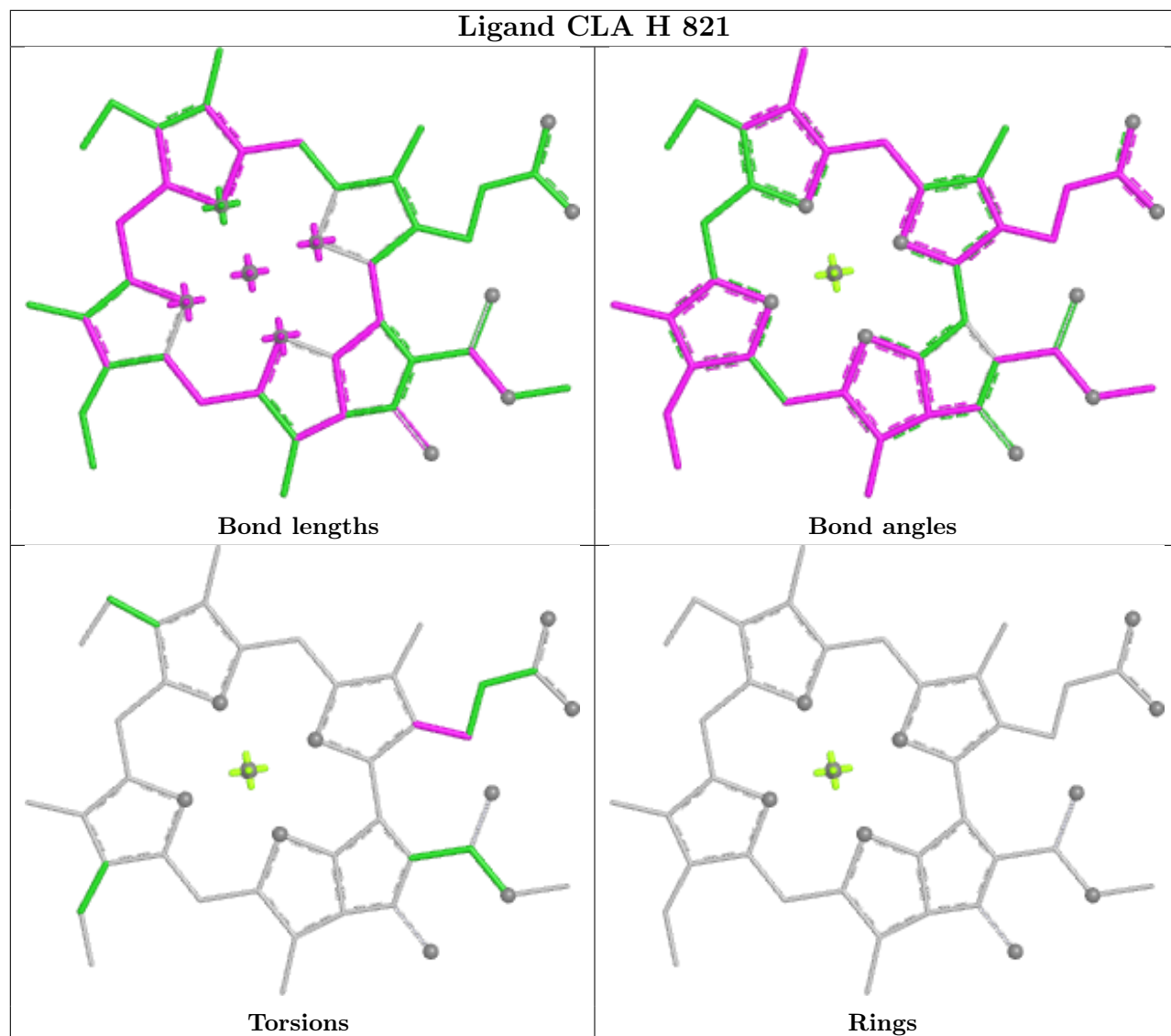
Rings

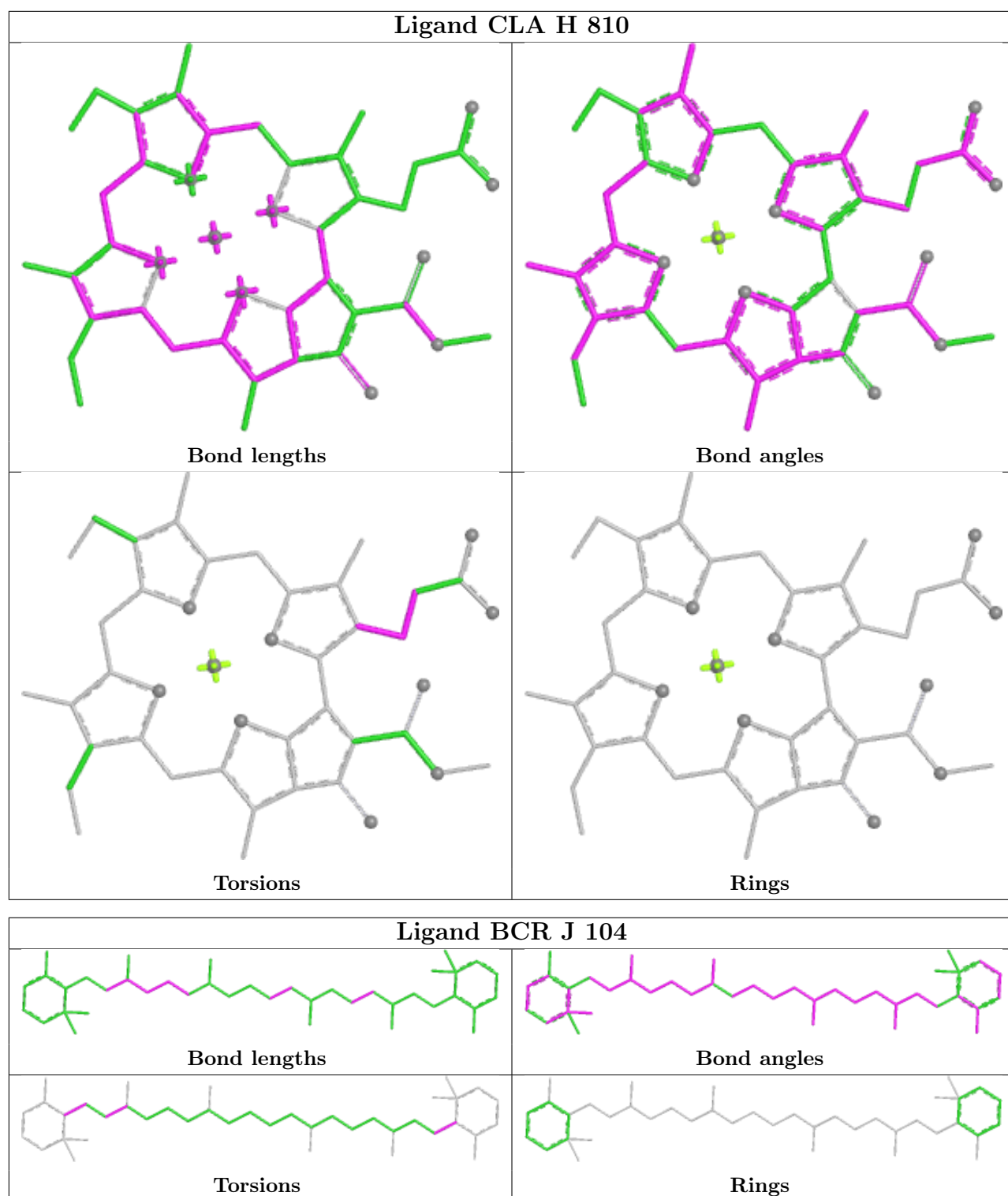
Ligand CLA B 813

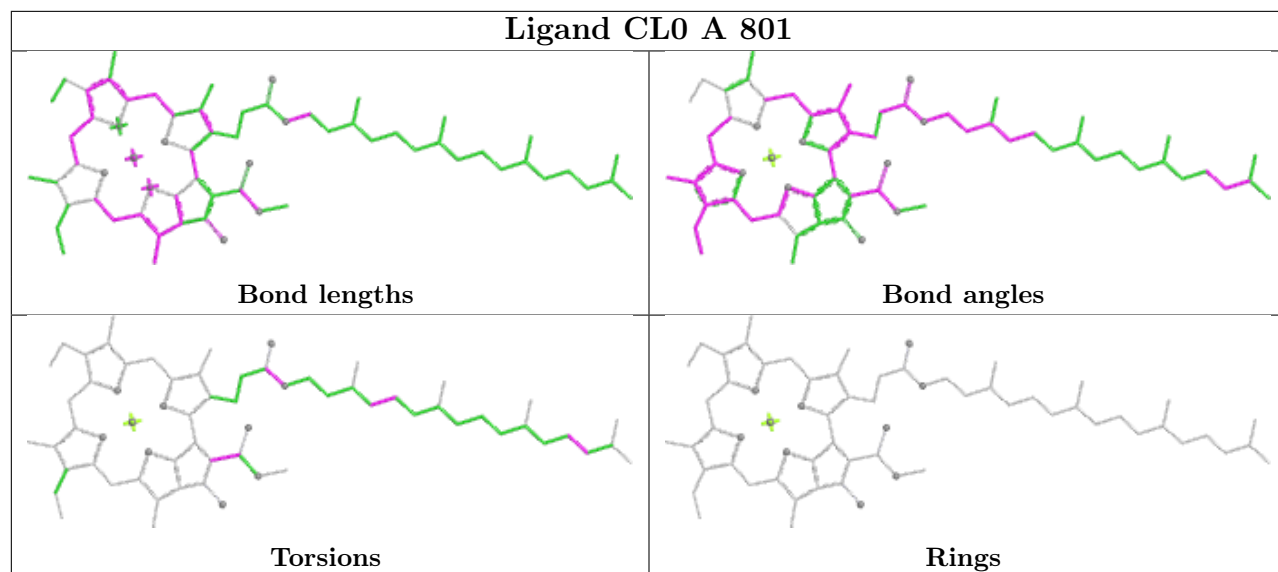
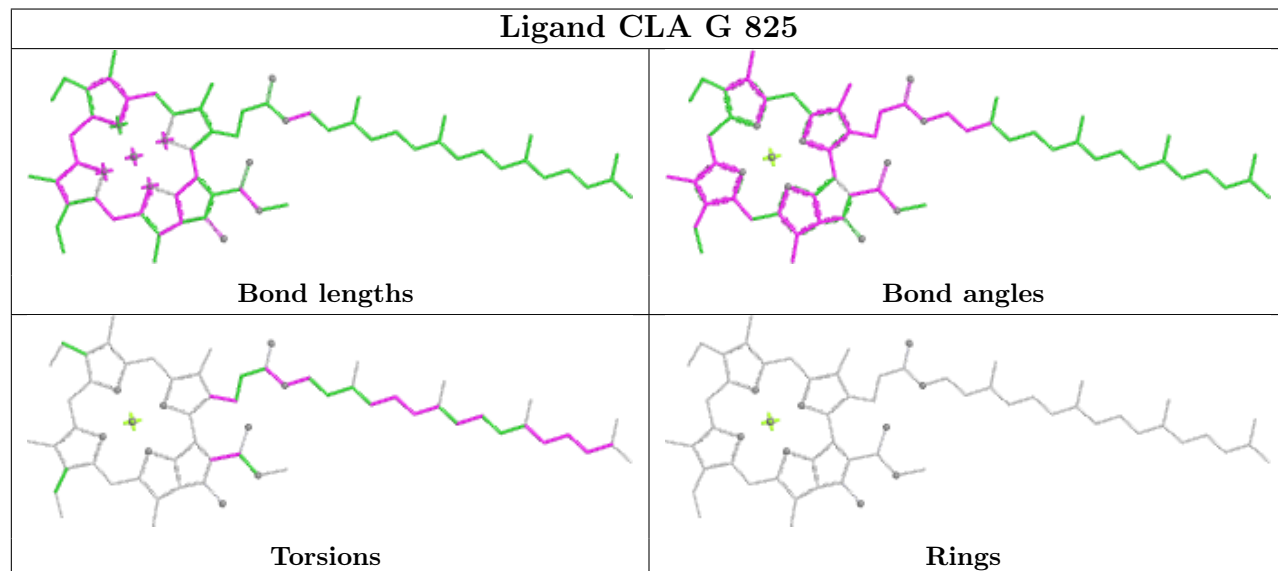


Ligand CLA G 831

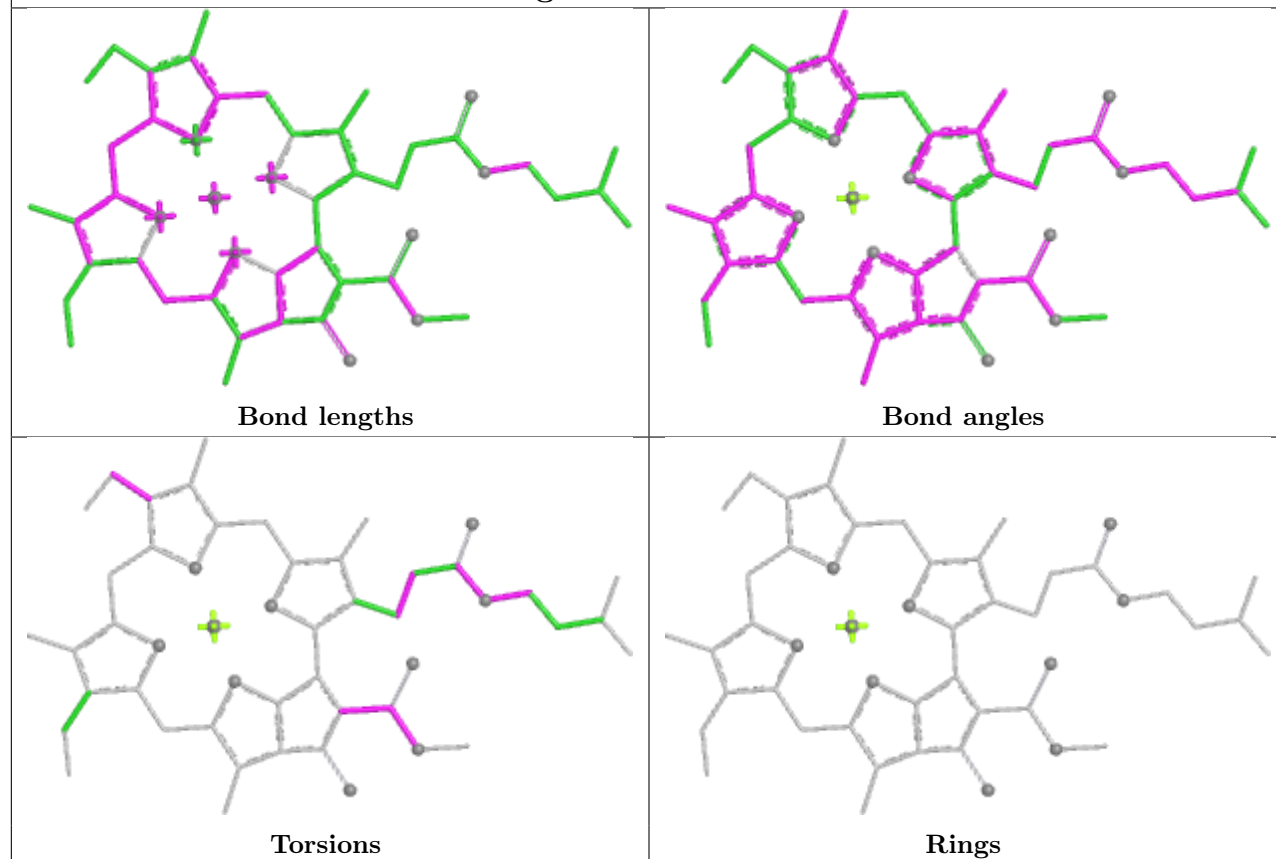




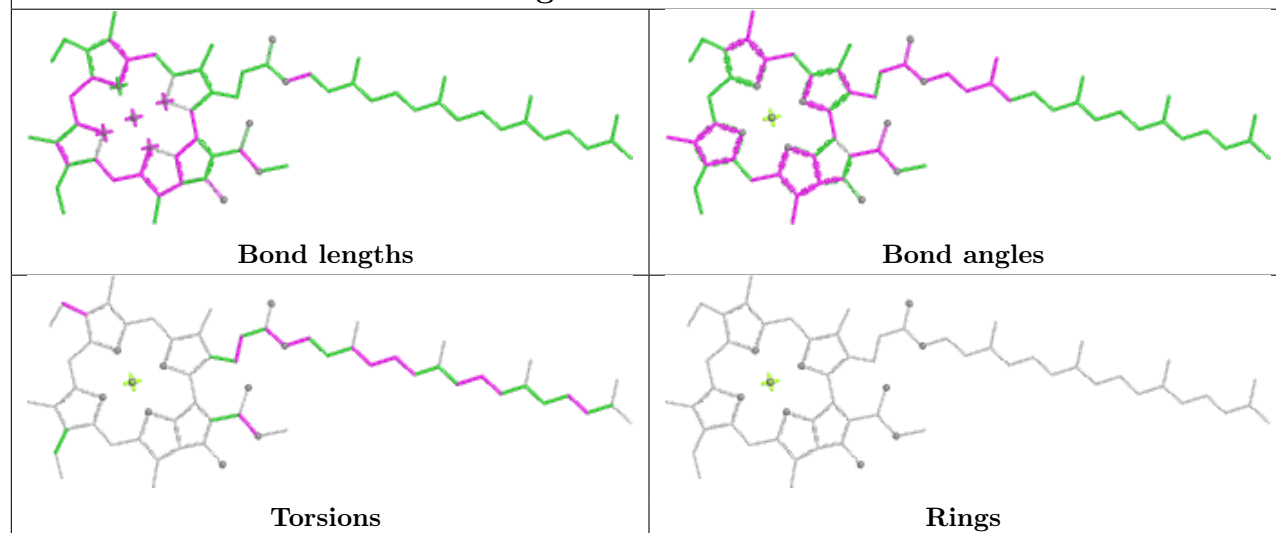


Ligand CL0 A 801**Ligand CLA G 825**

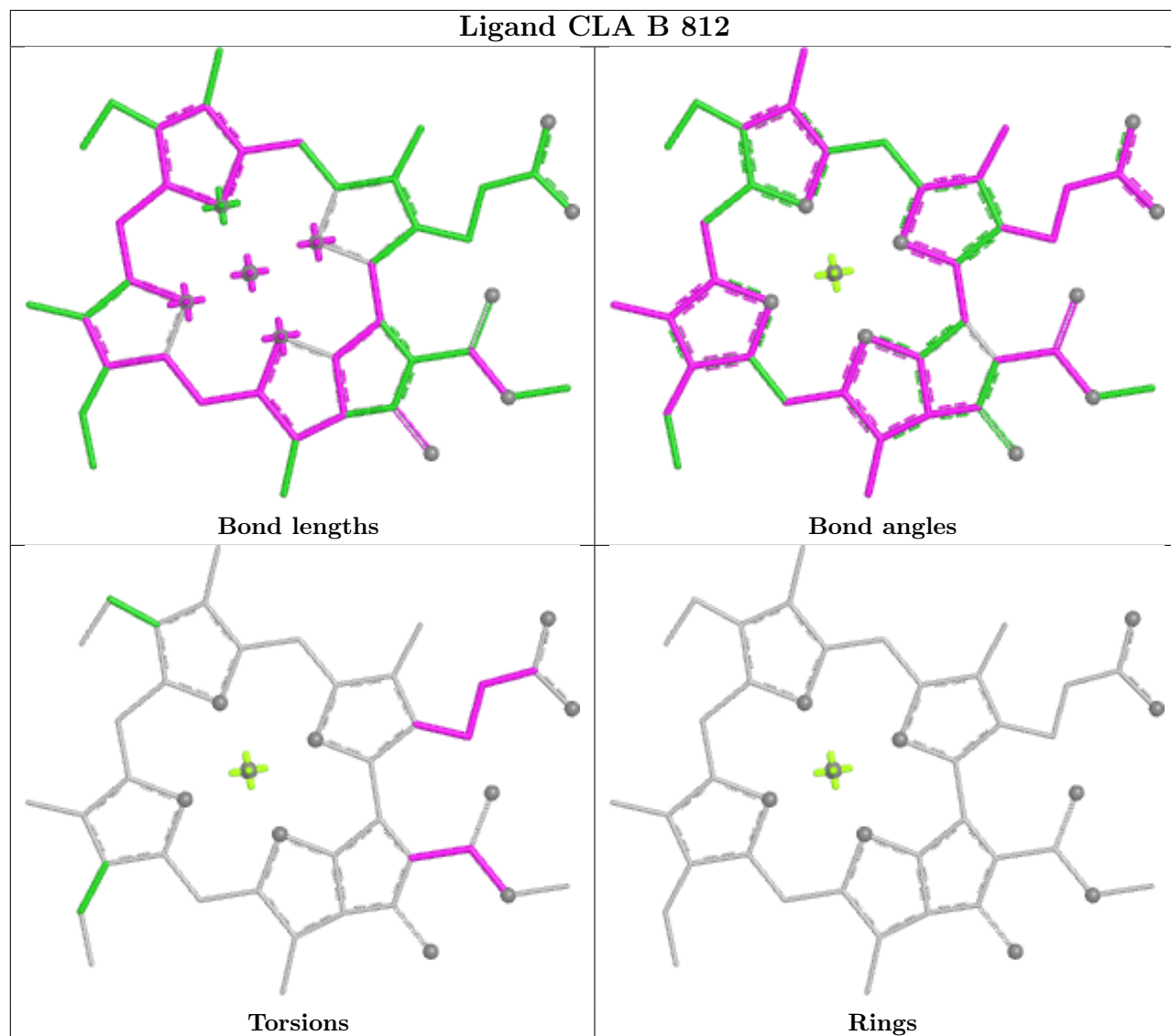
Ligand CLA a 830



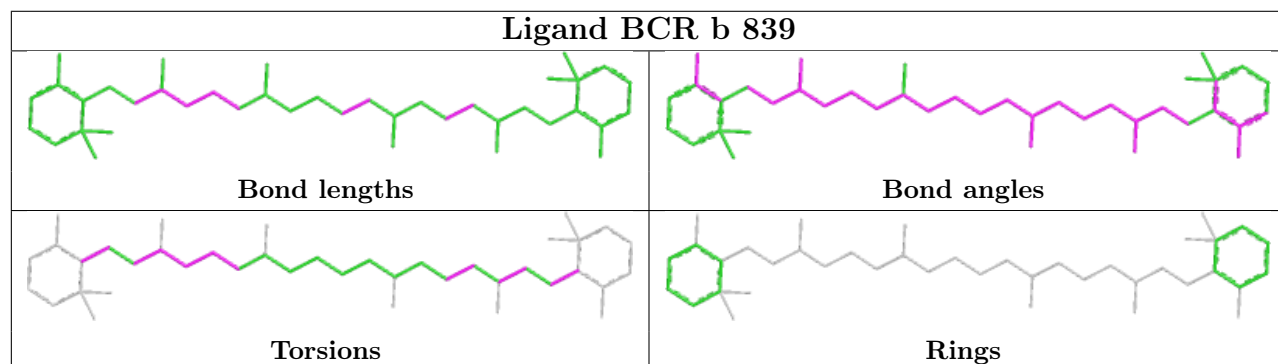
Ligand CLA a 832



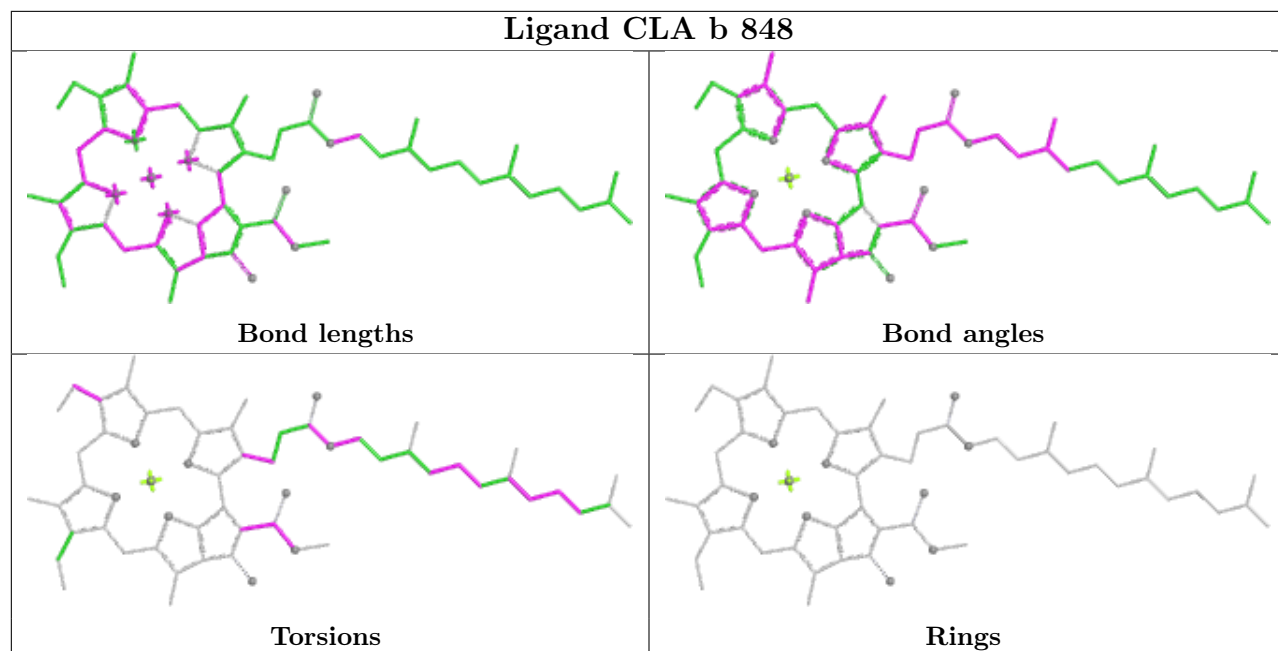
Ligand CLA B 812



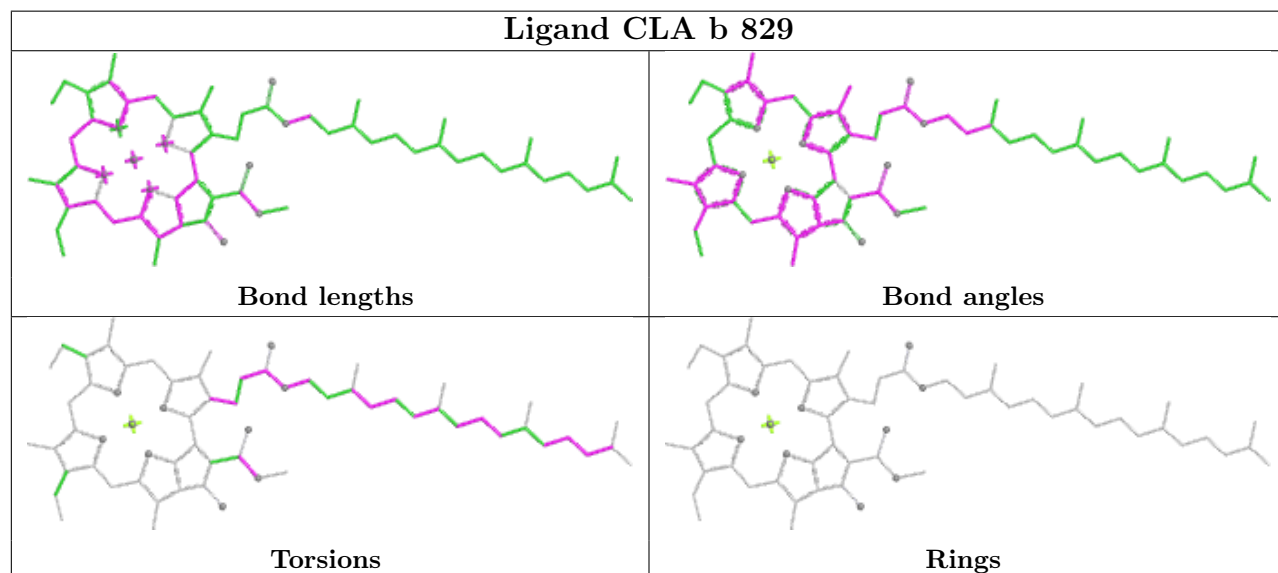
Ligand BCR b 839



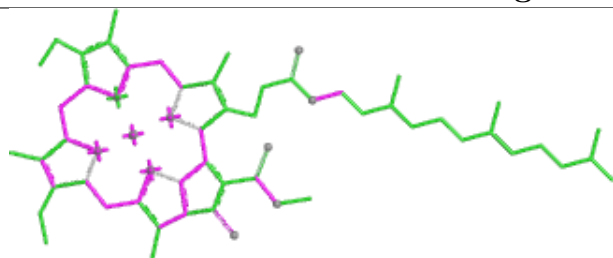
Ligand CLA b 848



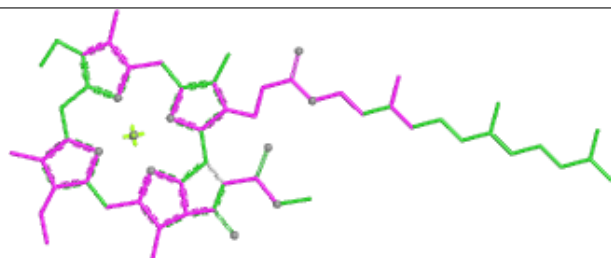
Ligand CLA b 829



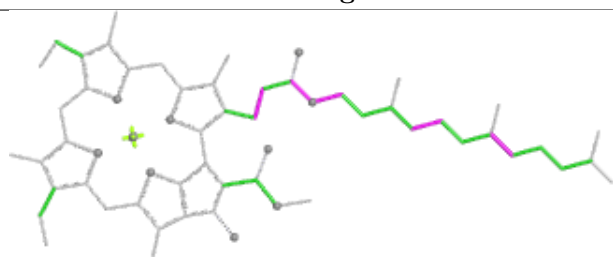
Ligand CLA B 801



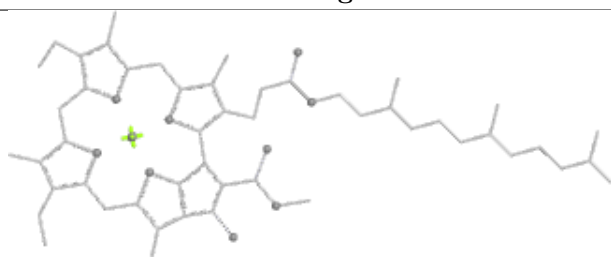
Bond lengths



Bond angles

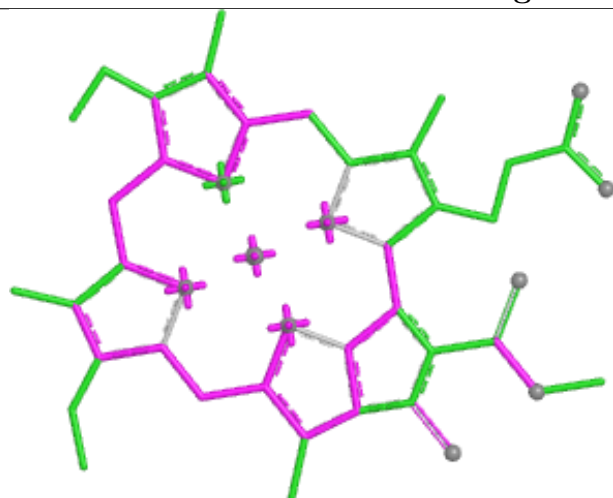


Torsions

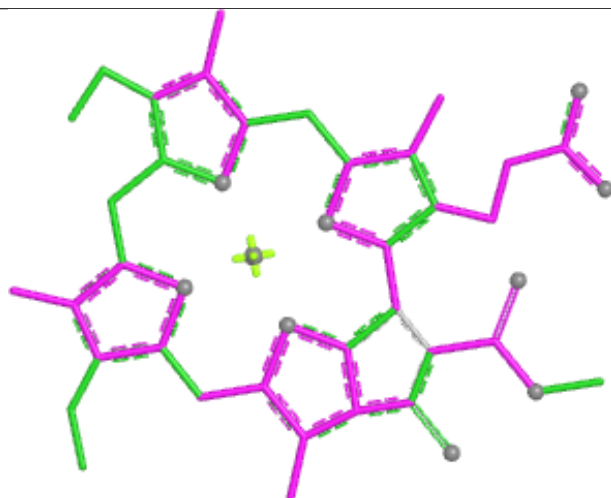


Rings

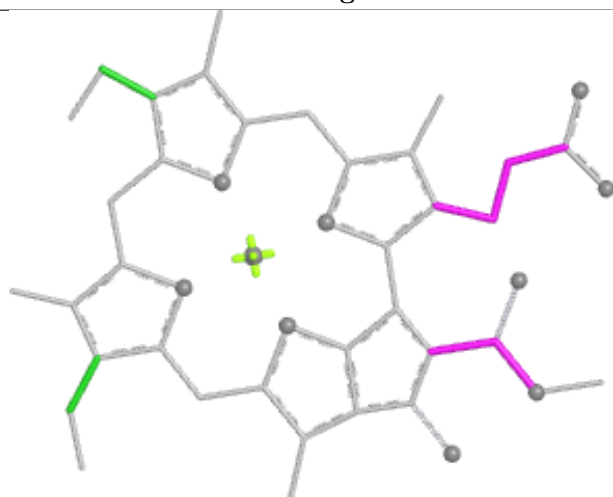
Ligand CLA A 821



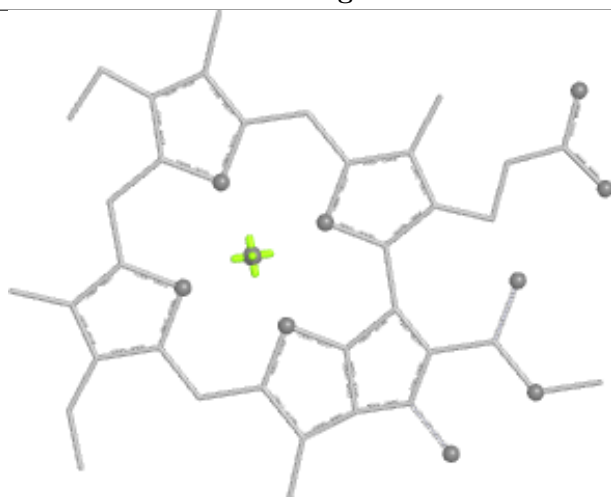
Bond lengths



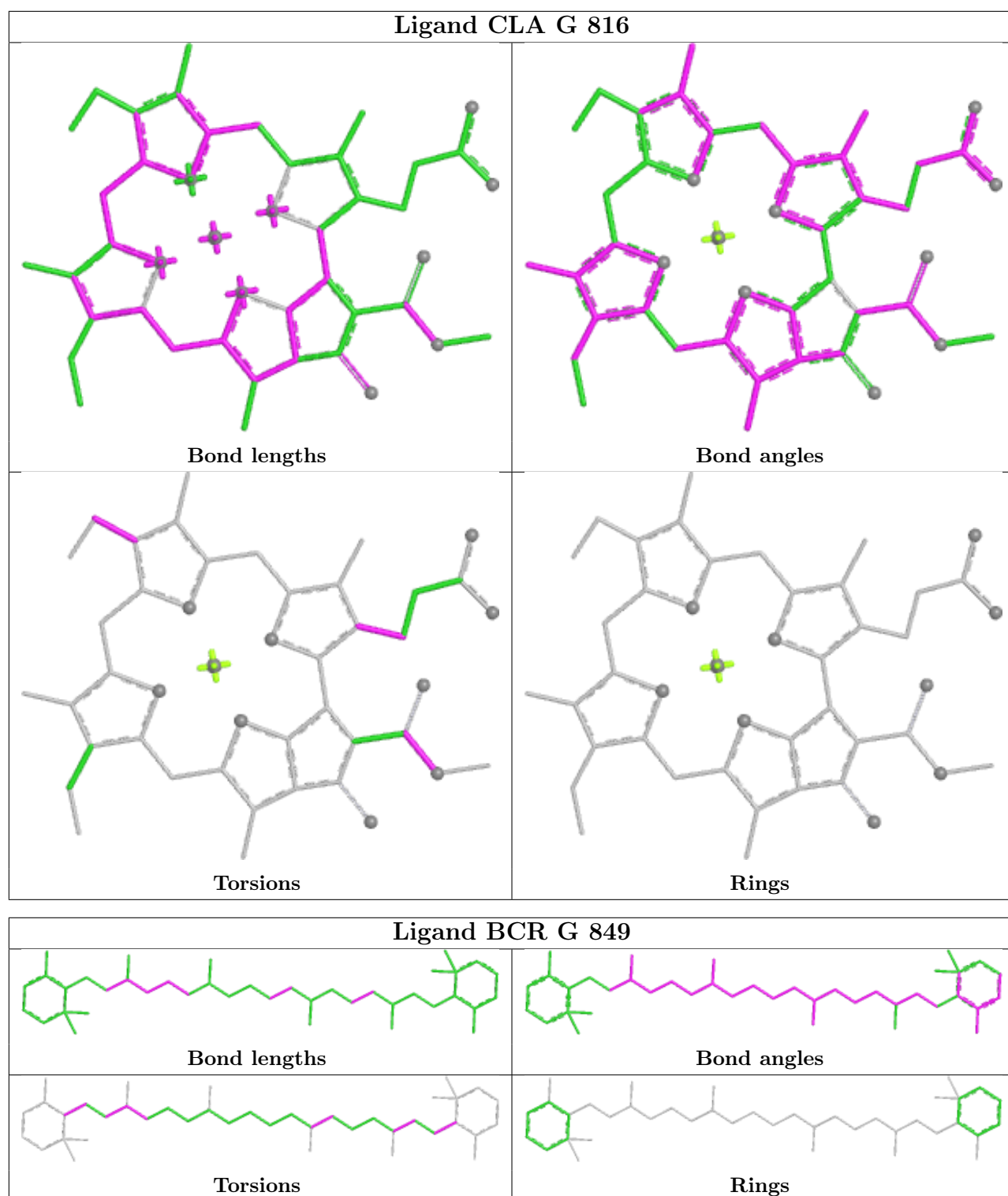
Bond angles

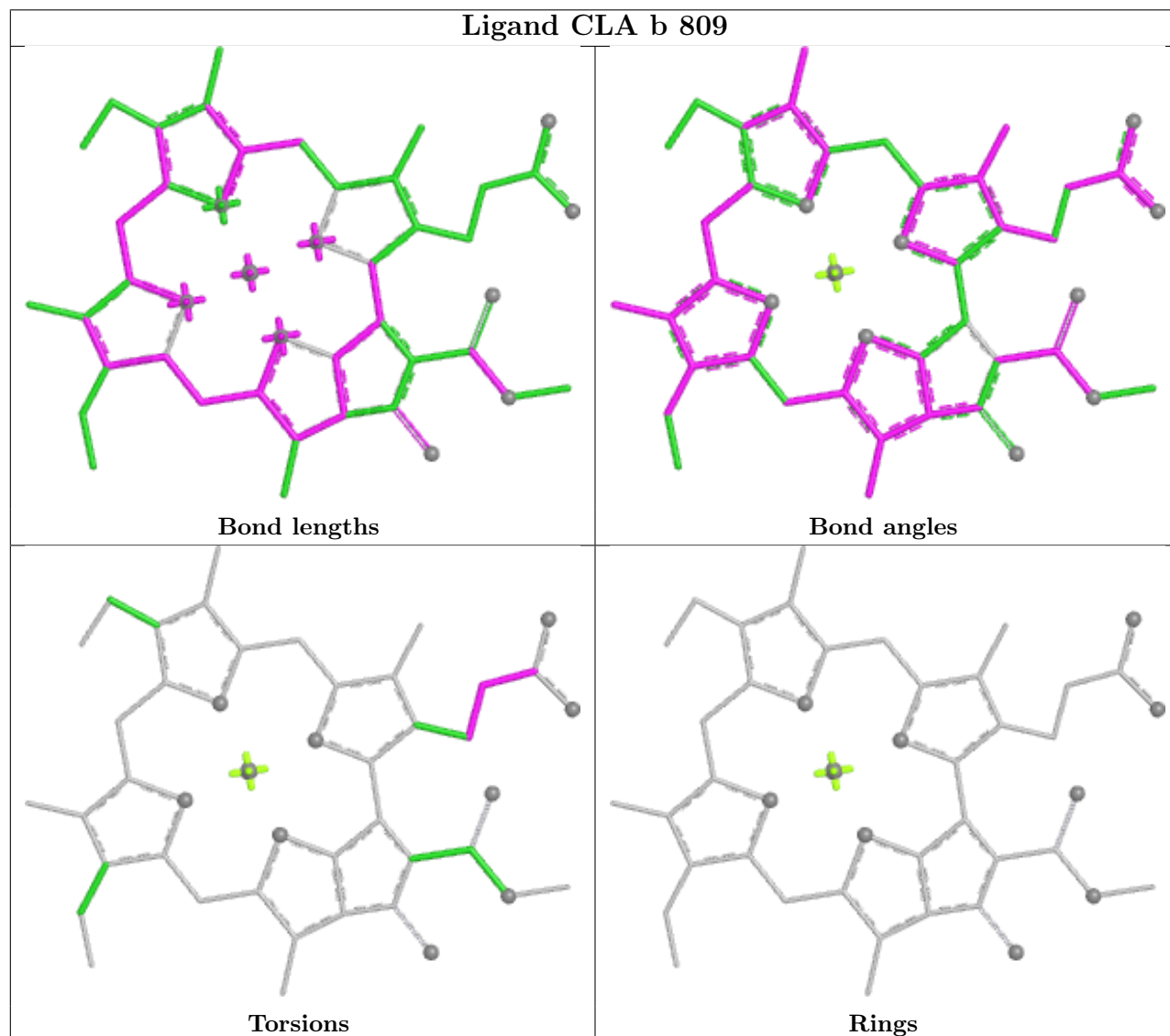
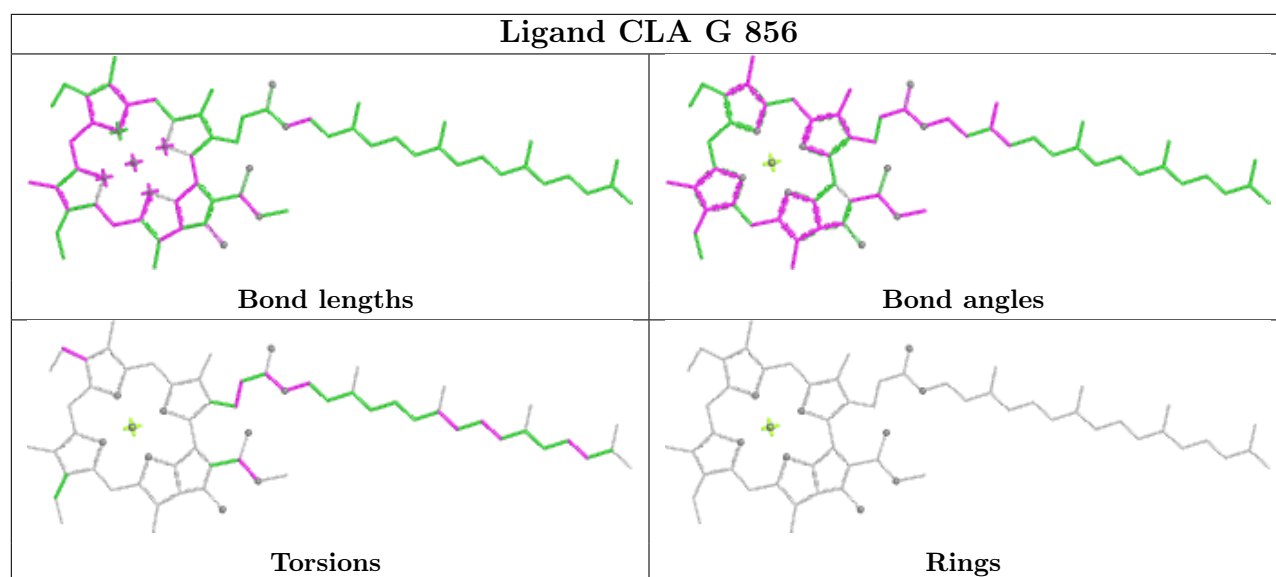


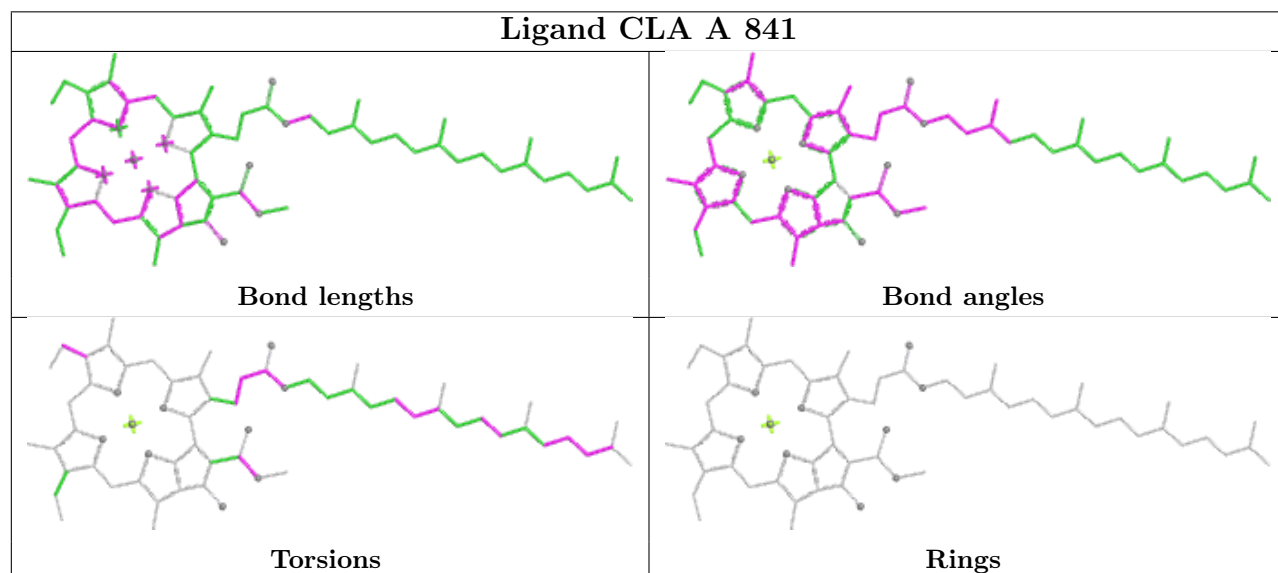
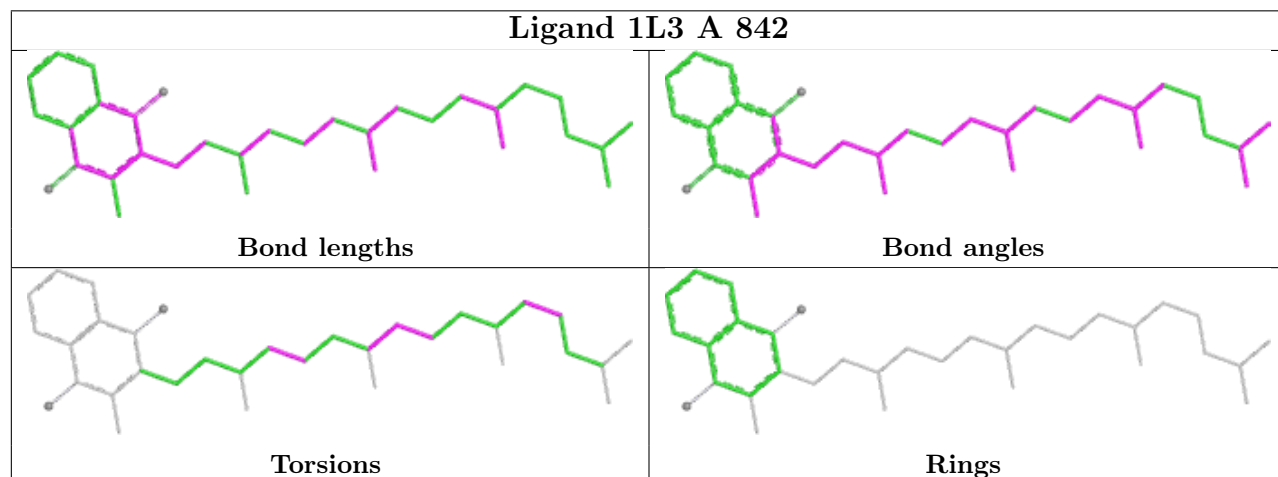
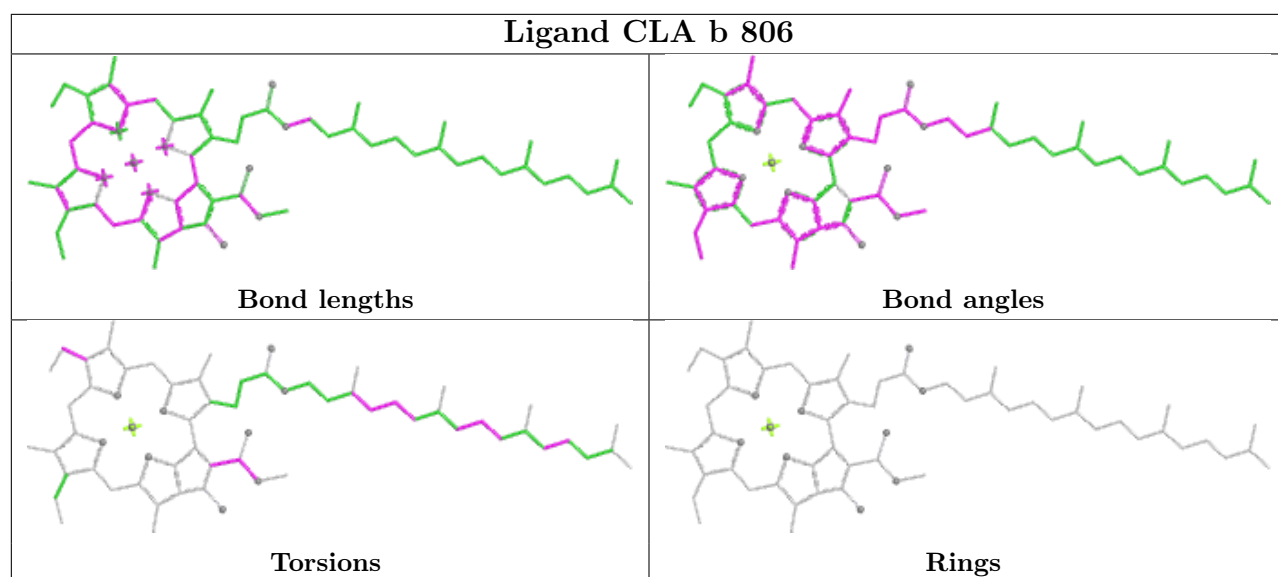
Torsions

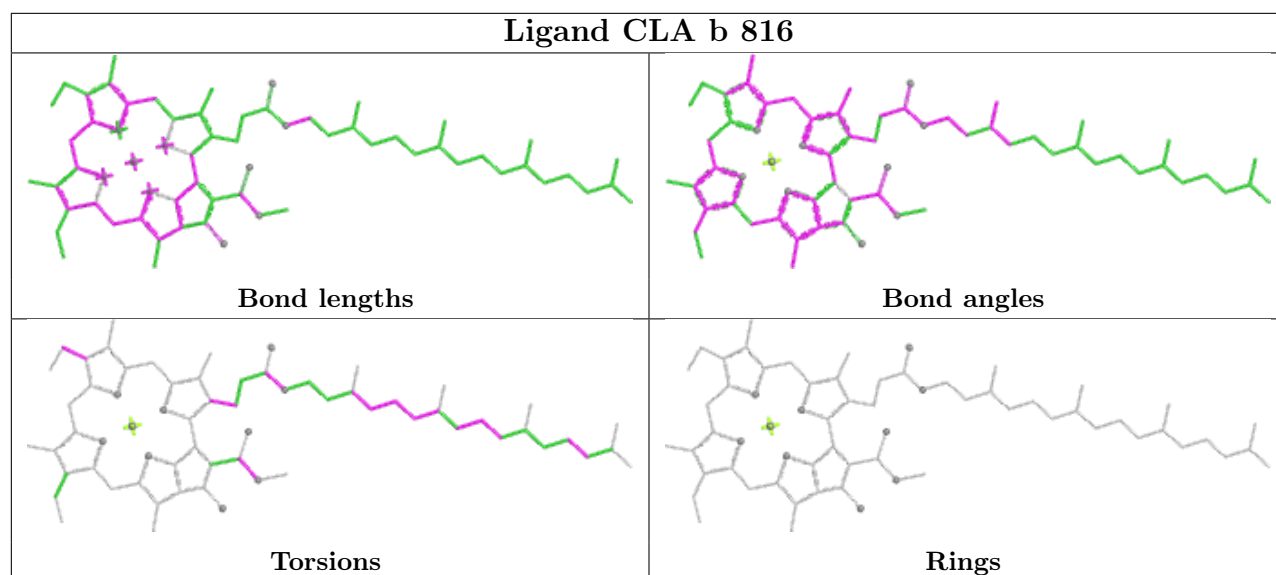
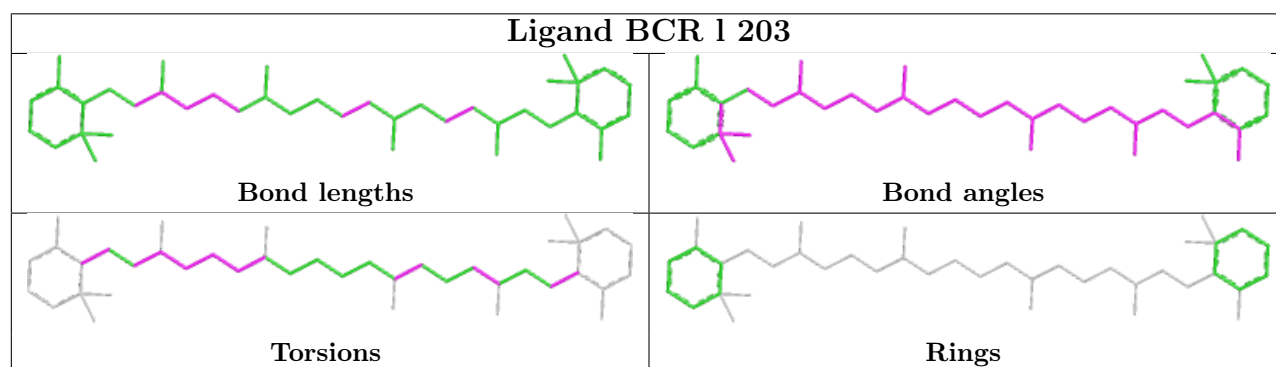
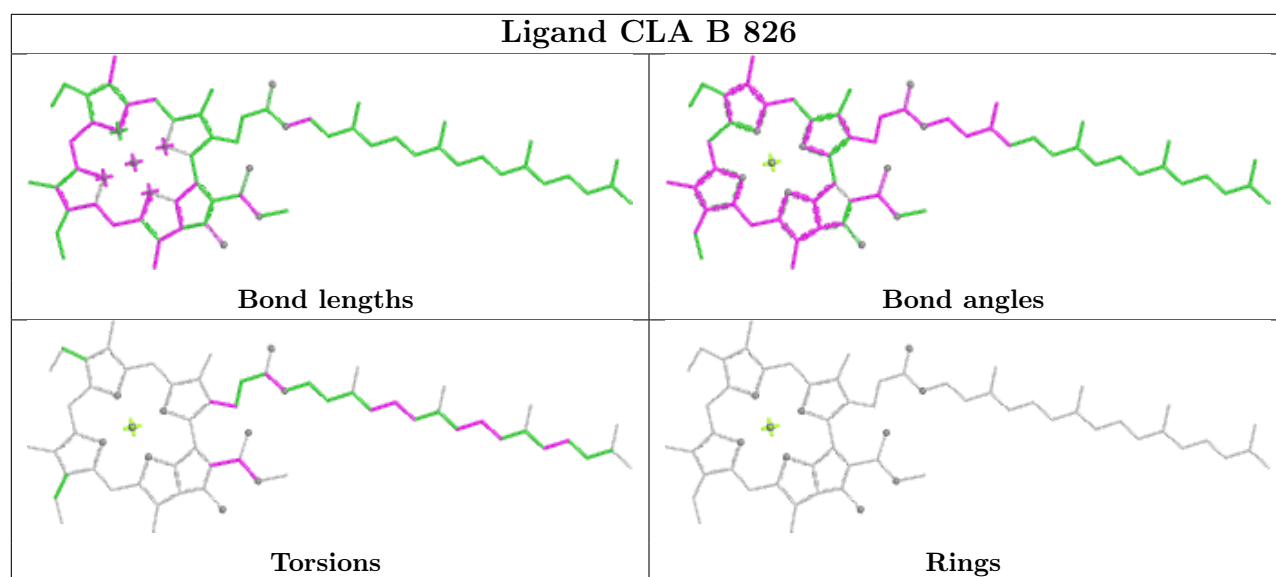


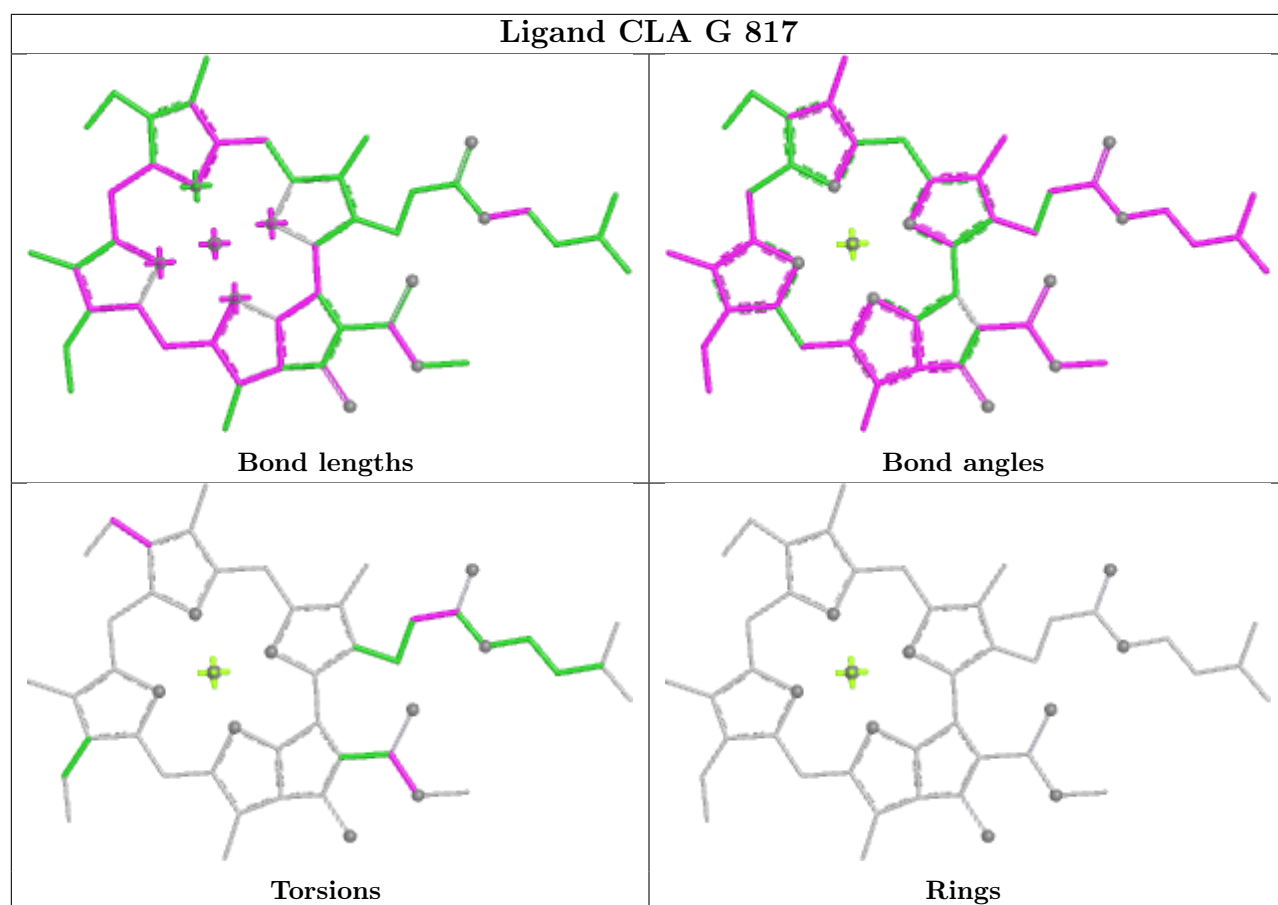
Rings



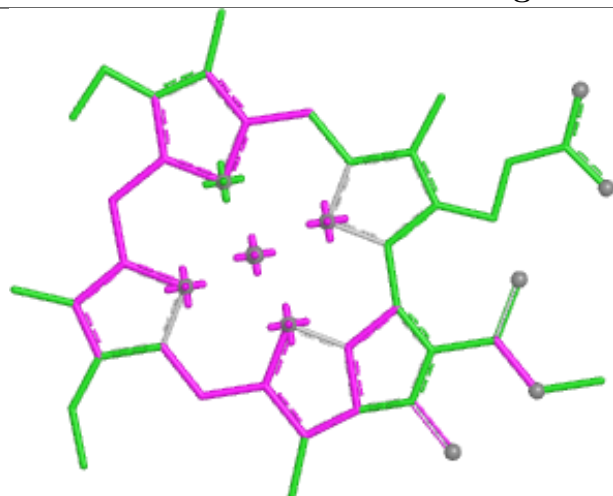




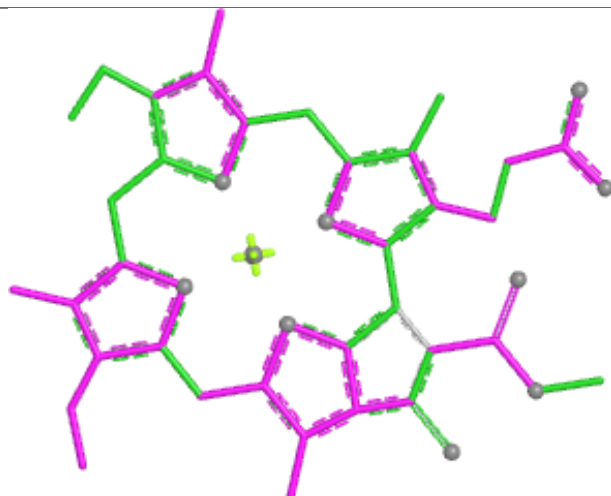




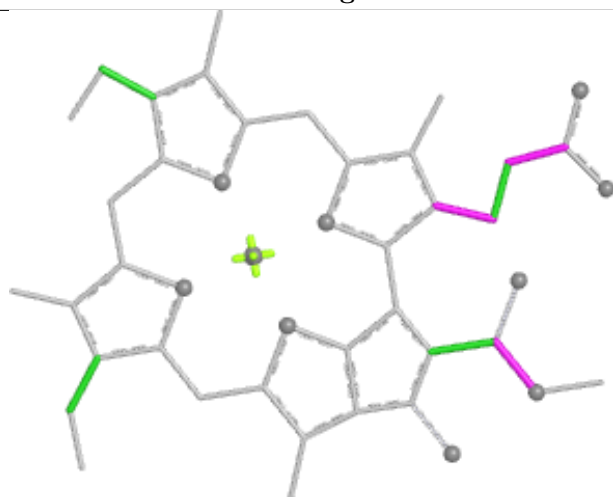
Ligand CLA H 836



Bond lengths



Bond angles

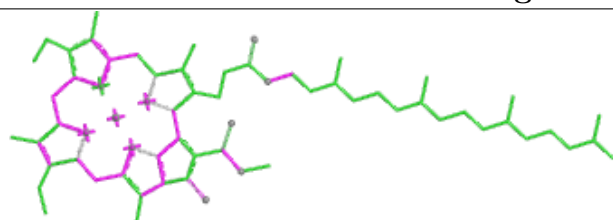


Torsions

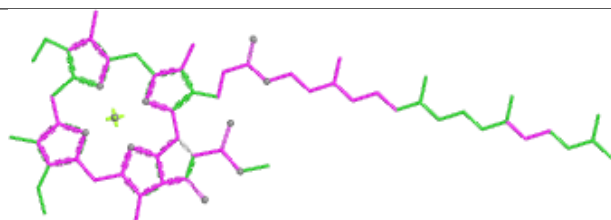


Rings

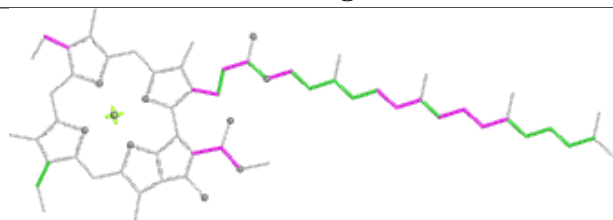
Ligand CLA B 823



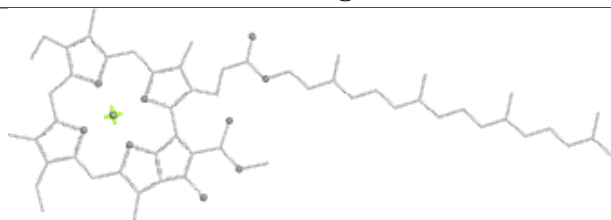
Bond lengths



Bond angles

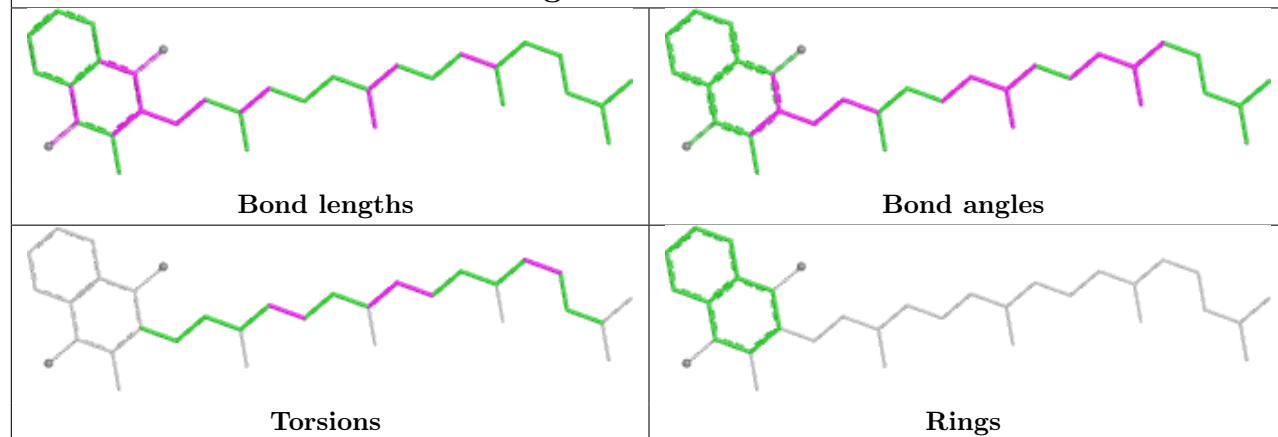


Torsions

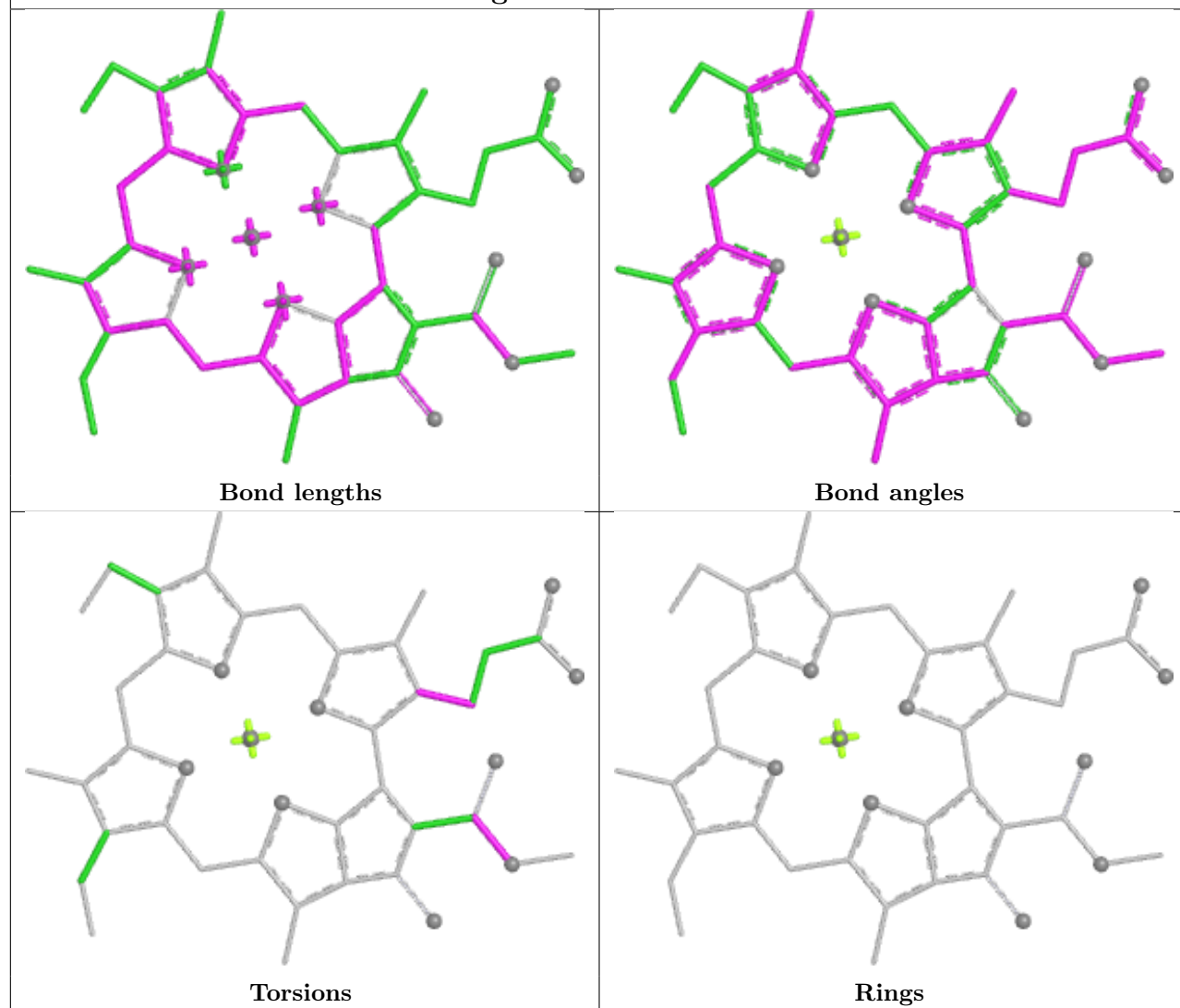


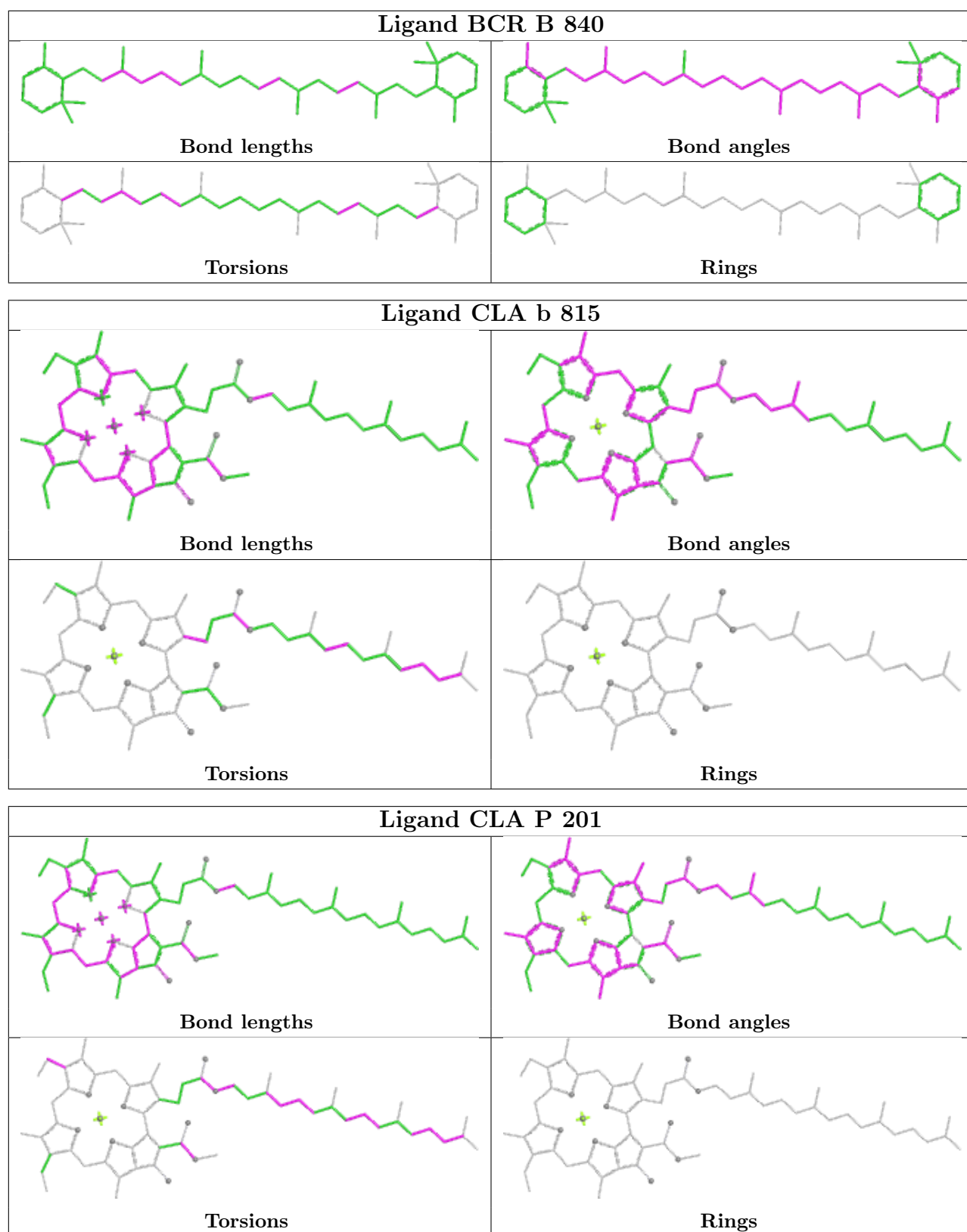
Rings

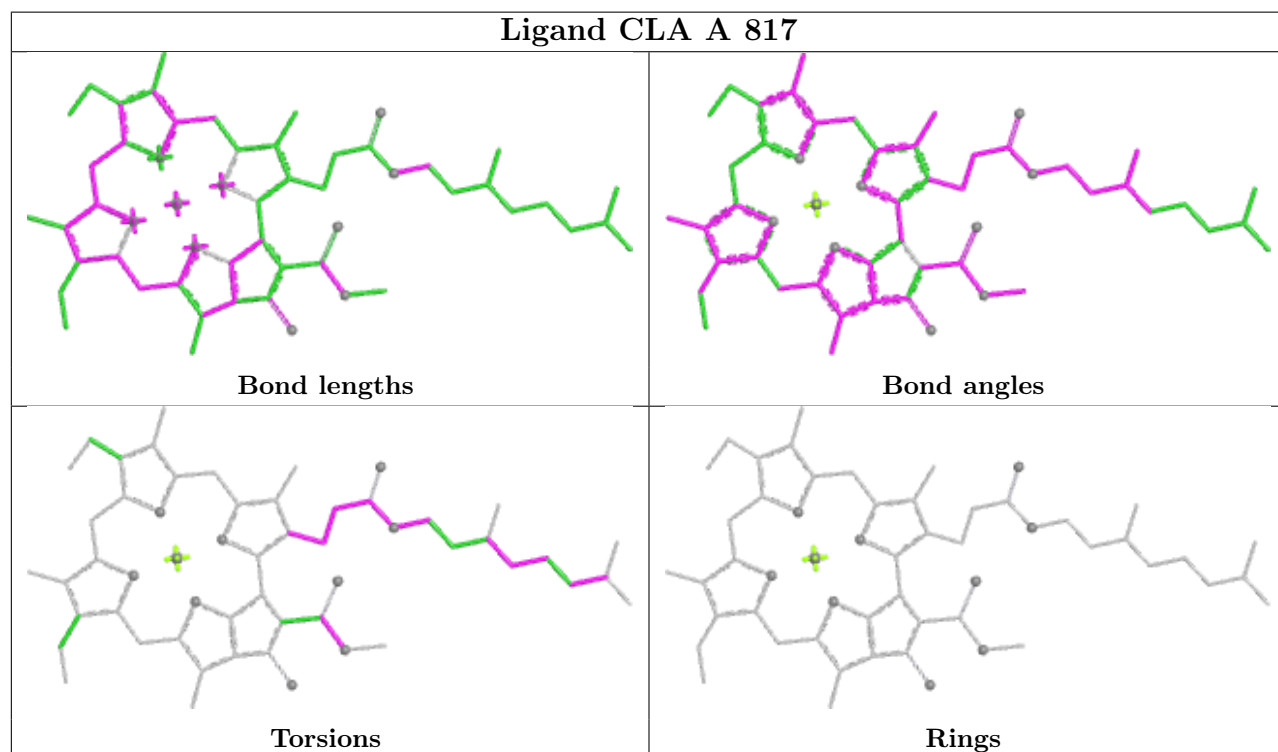
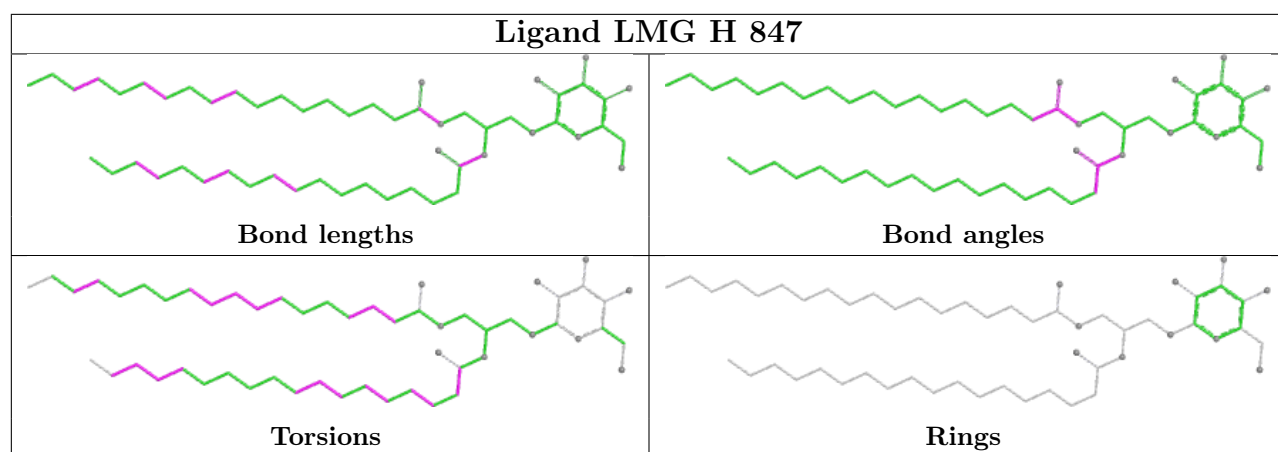
Ligand 1L3 b 838



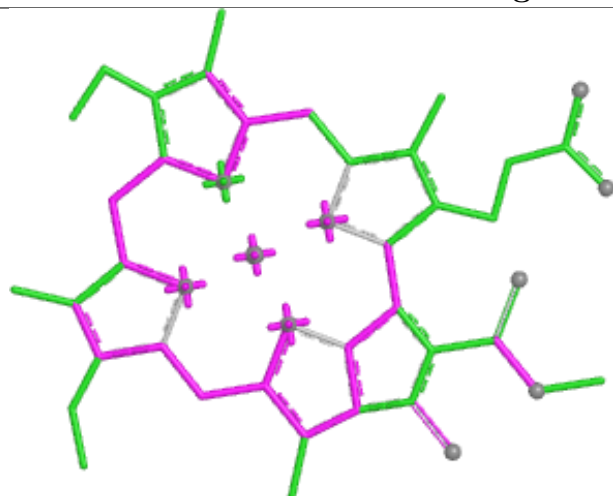
Ligand CLA B 828



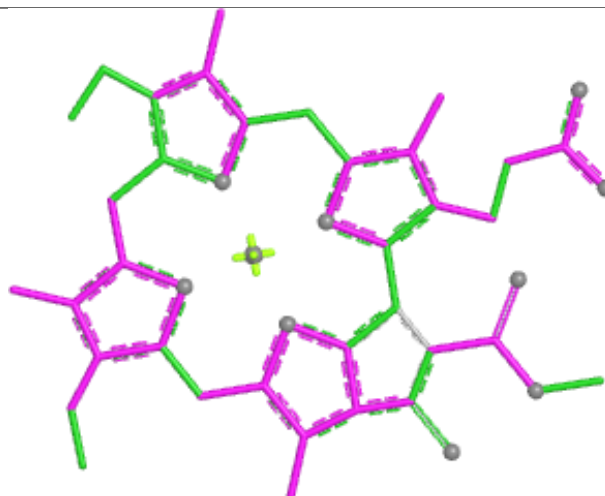




Ligand CLA G 815



Bond lengths



Bond angles

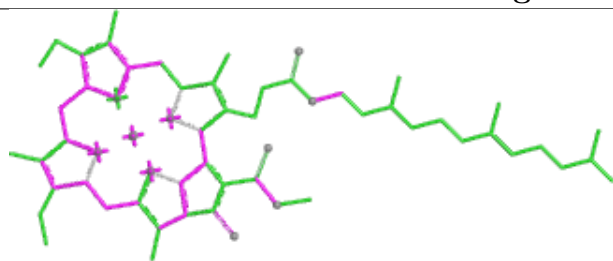


Torsions

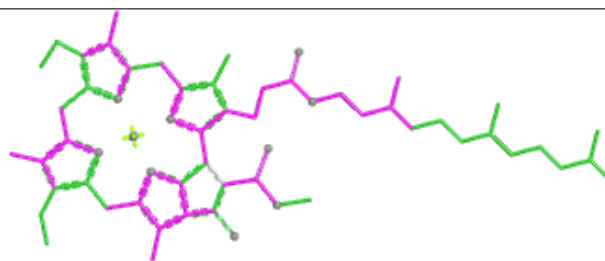


Rings

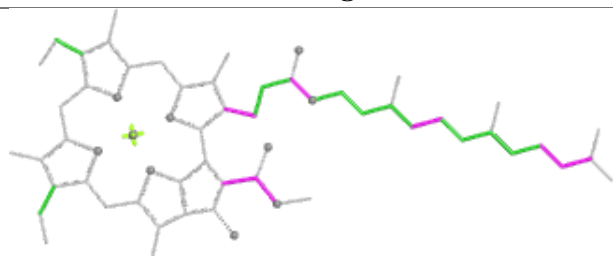
Ligand CLA H 816



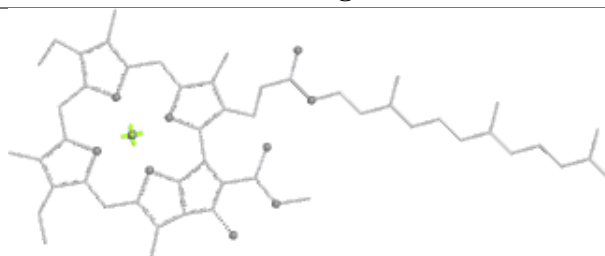
Bond lengths



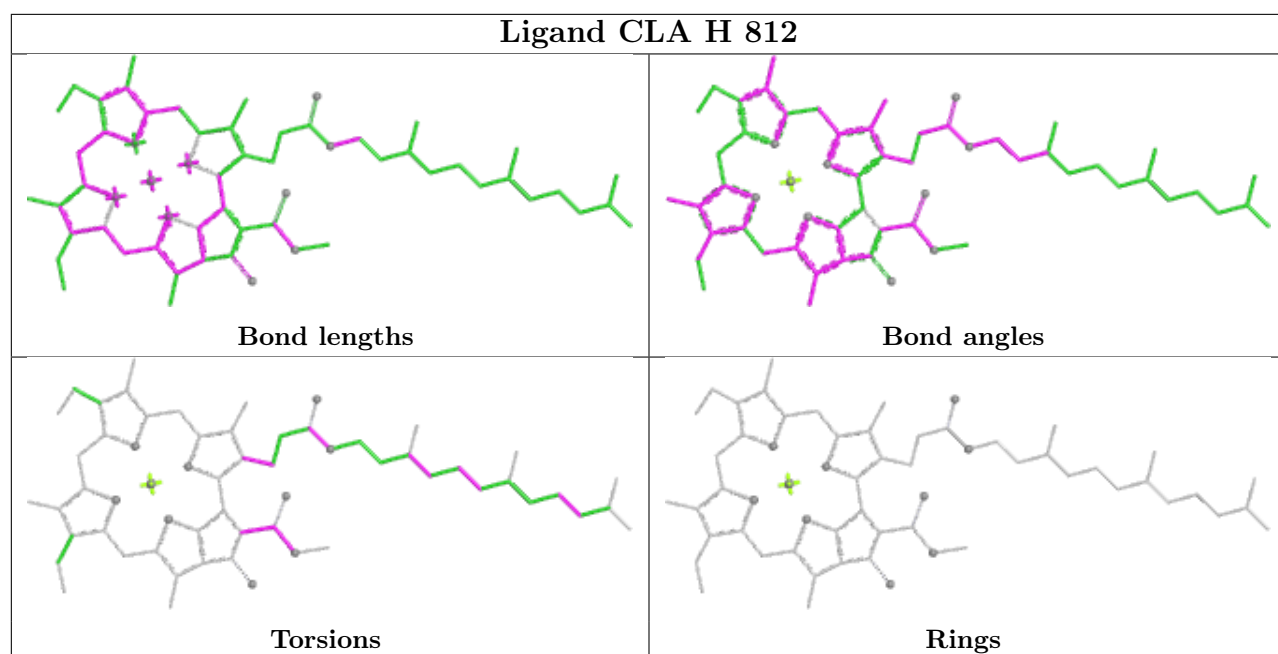
Bond angles

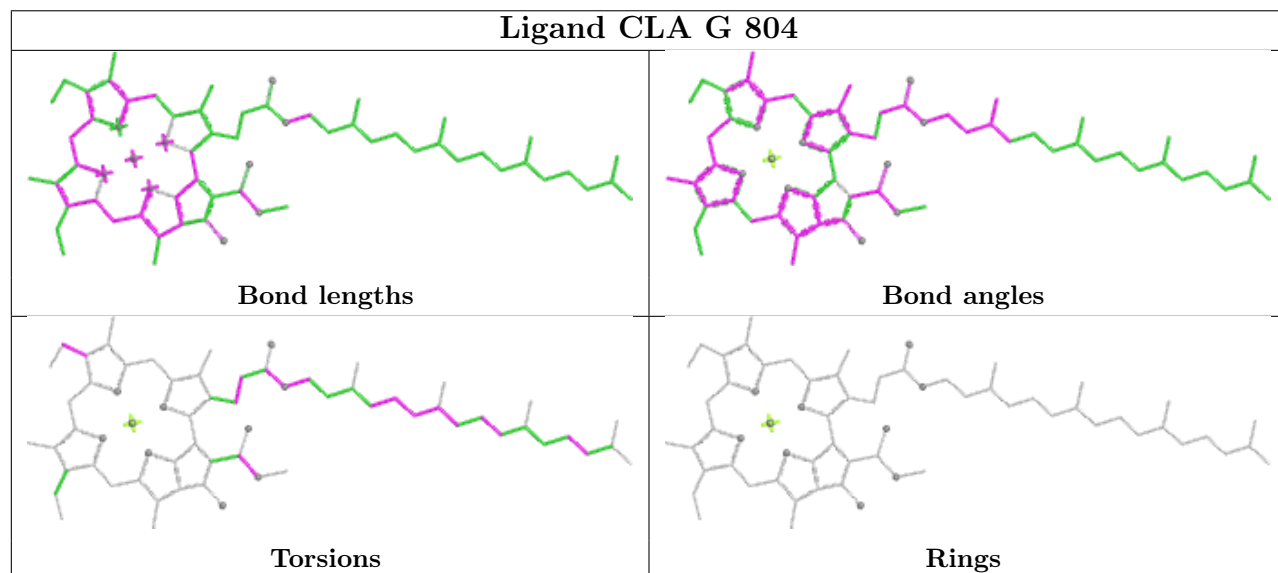
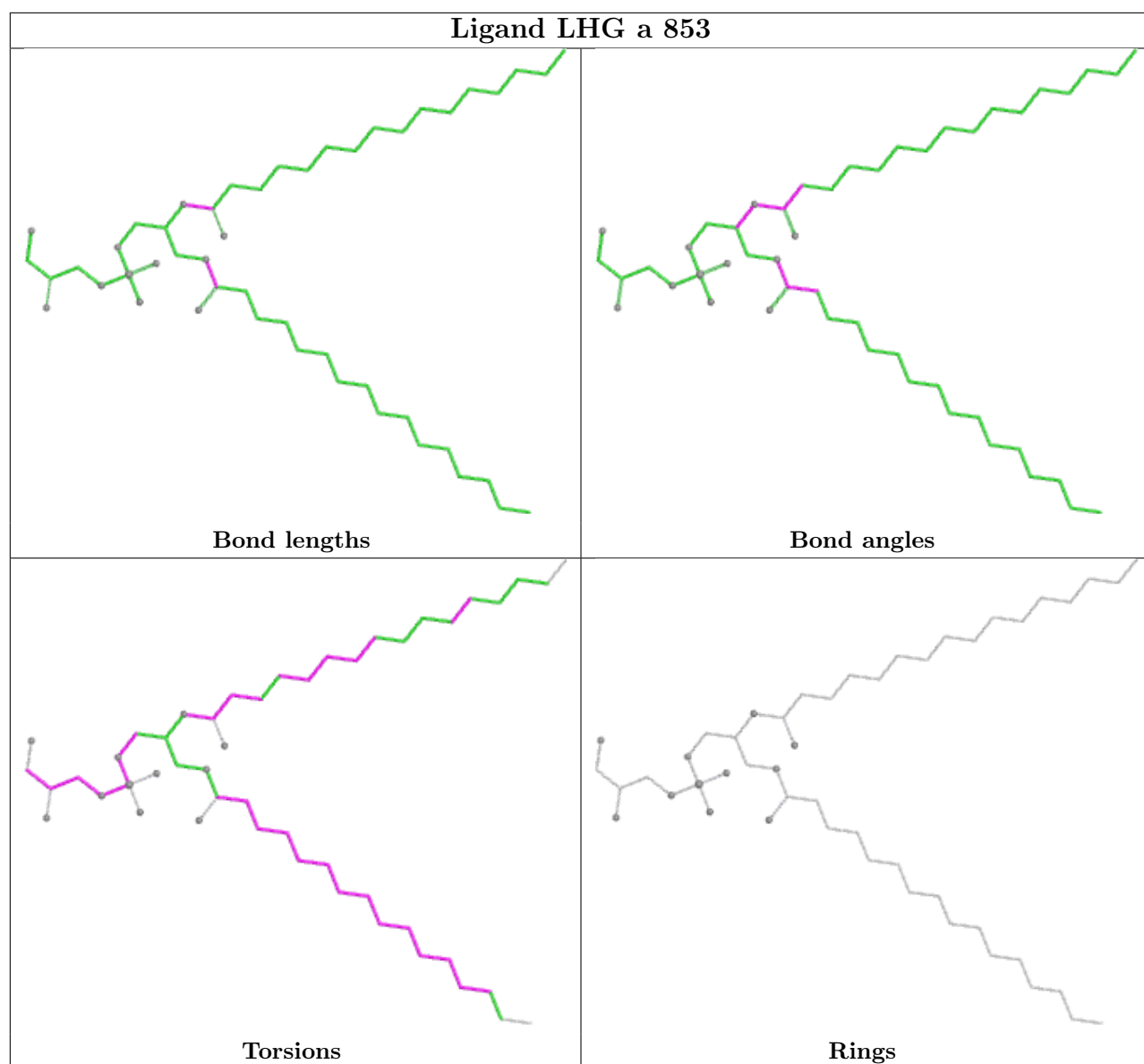


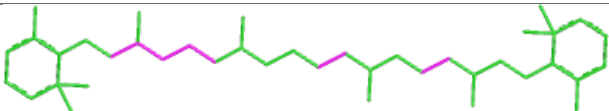
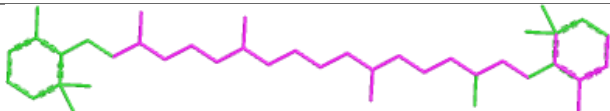
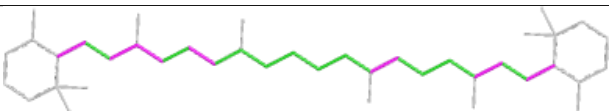
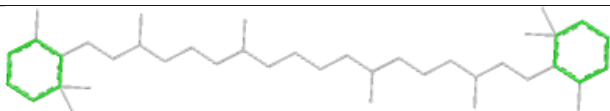
Torsions



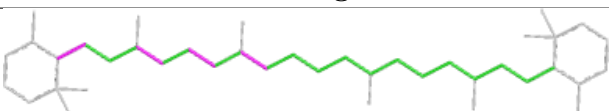
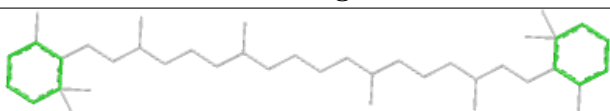


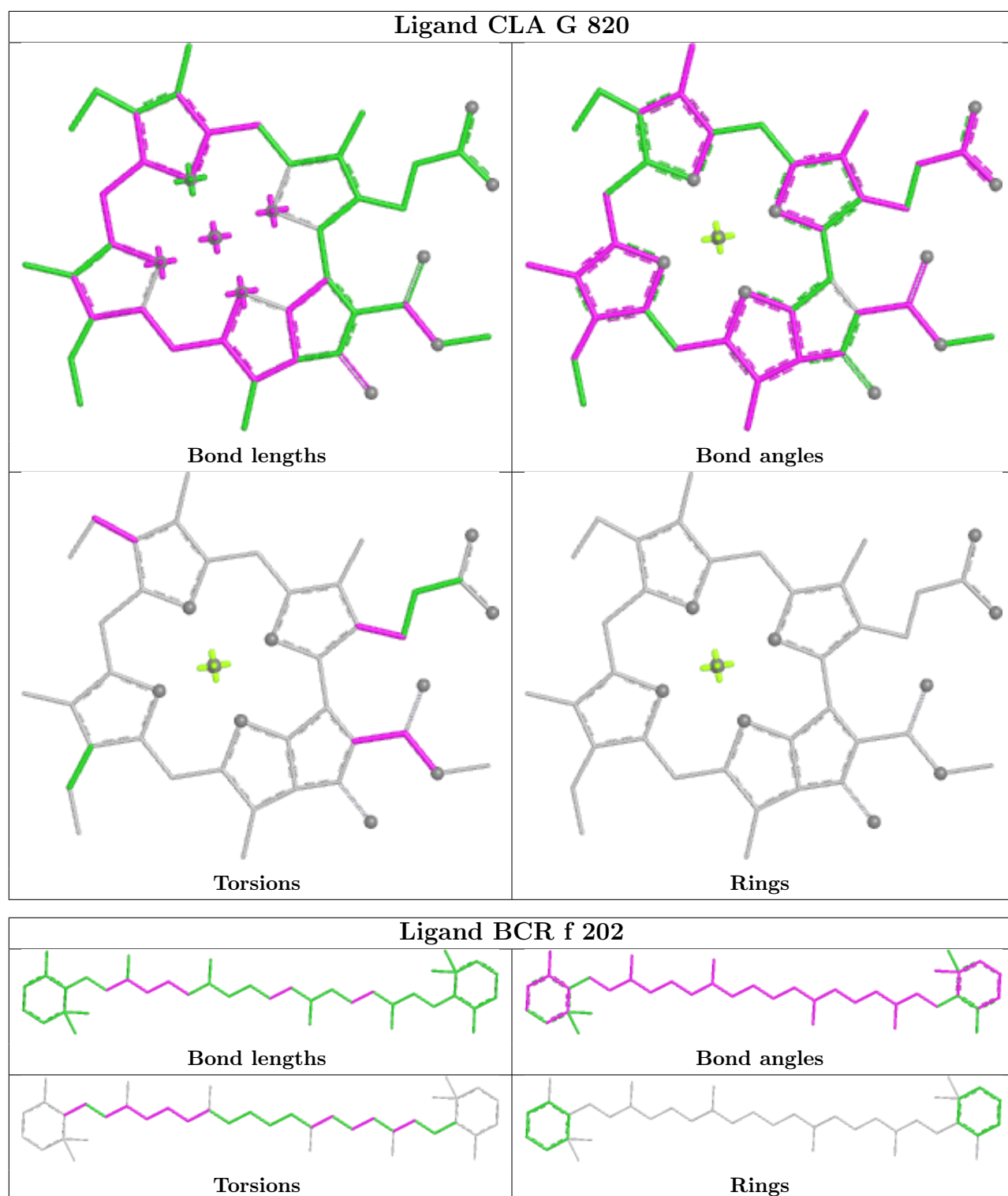
Rings

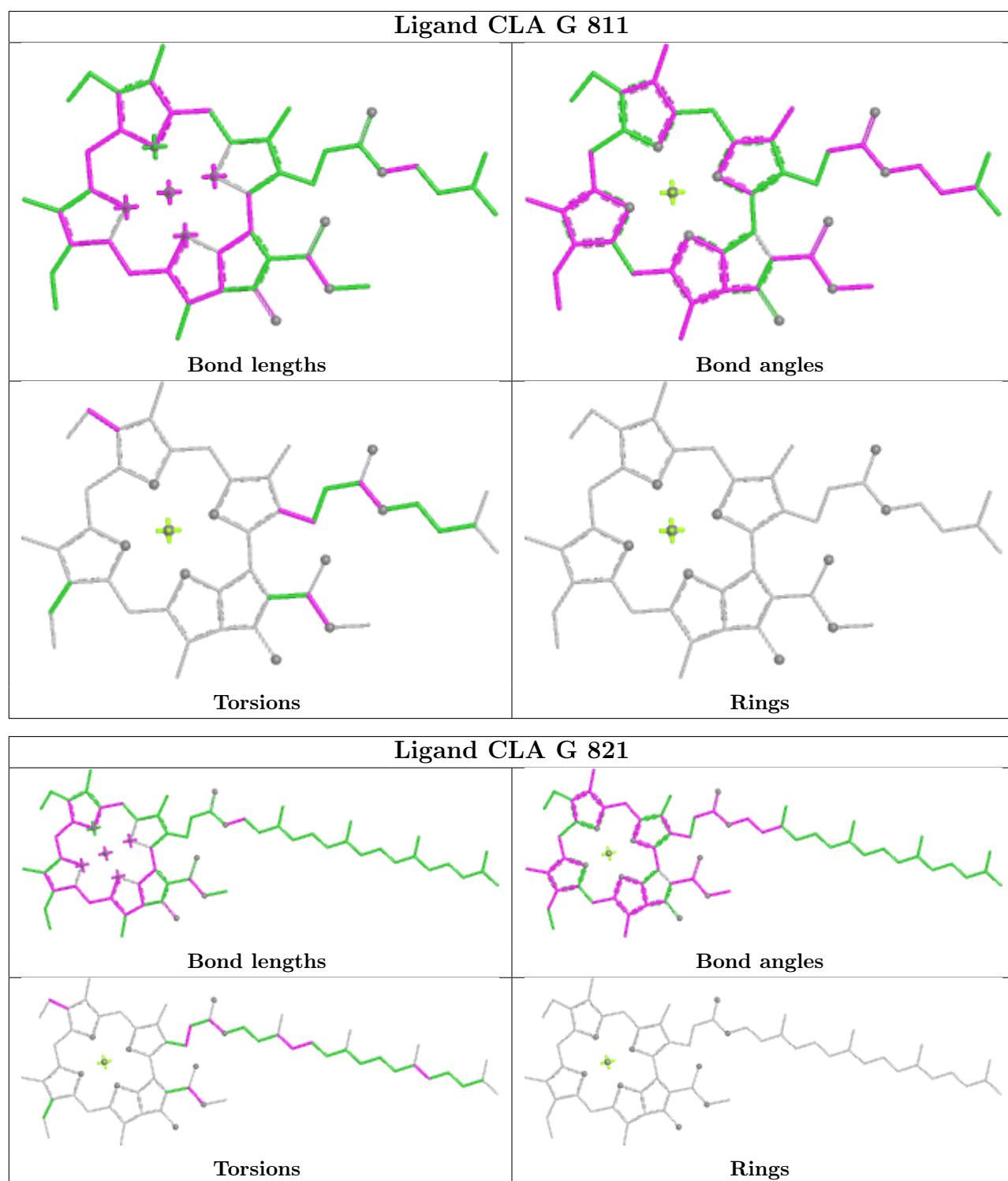


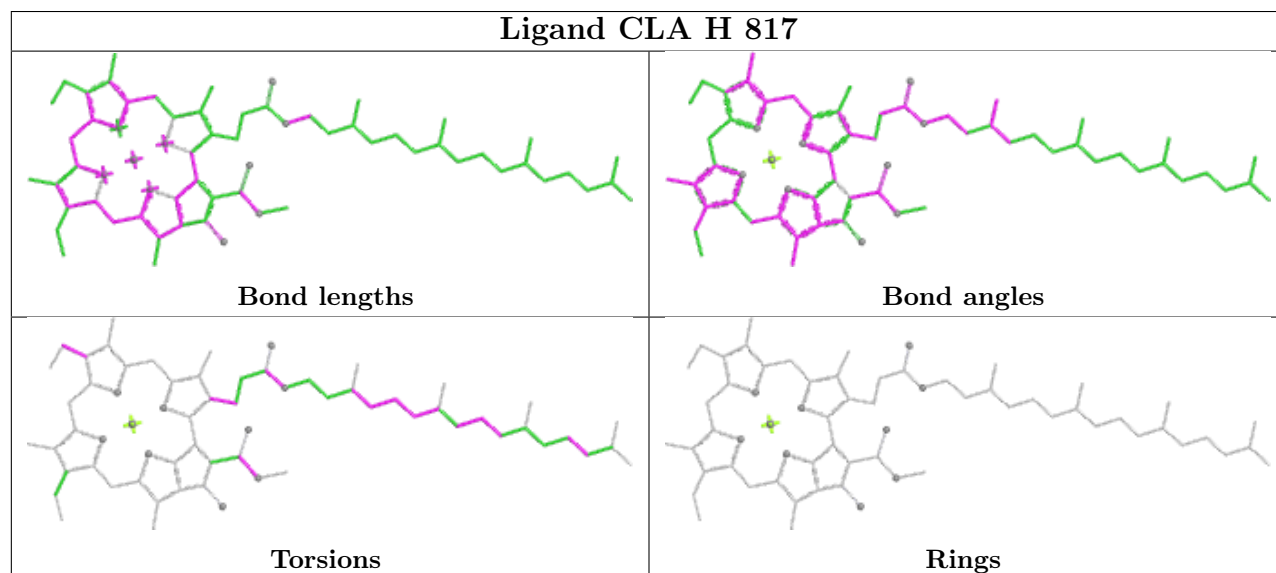
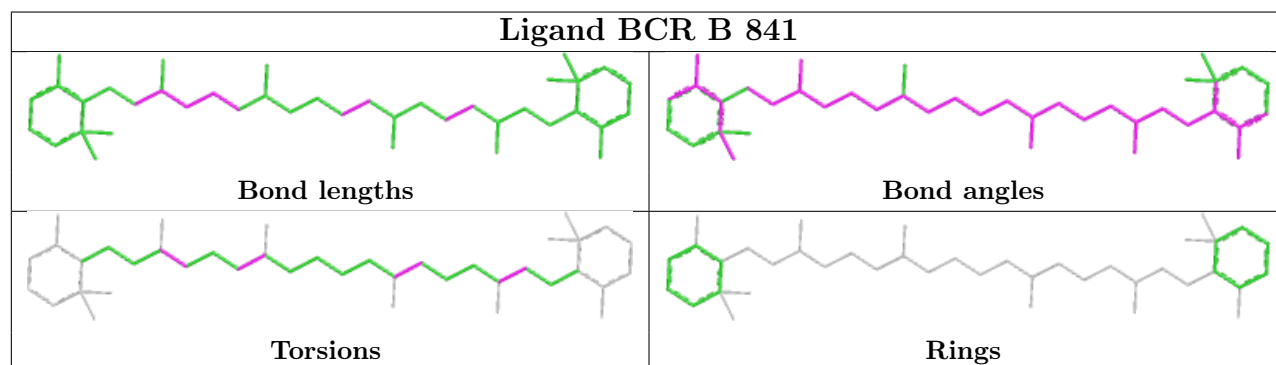
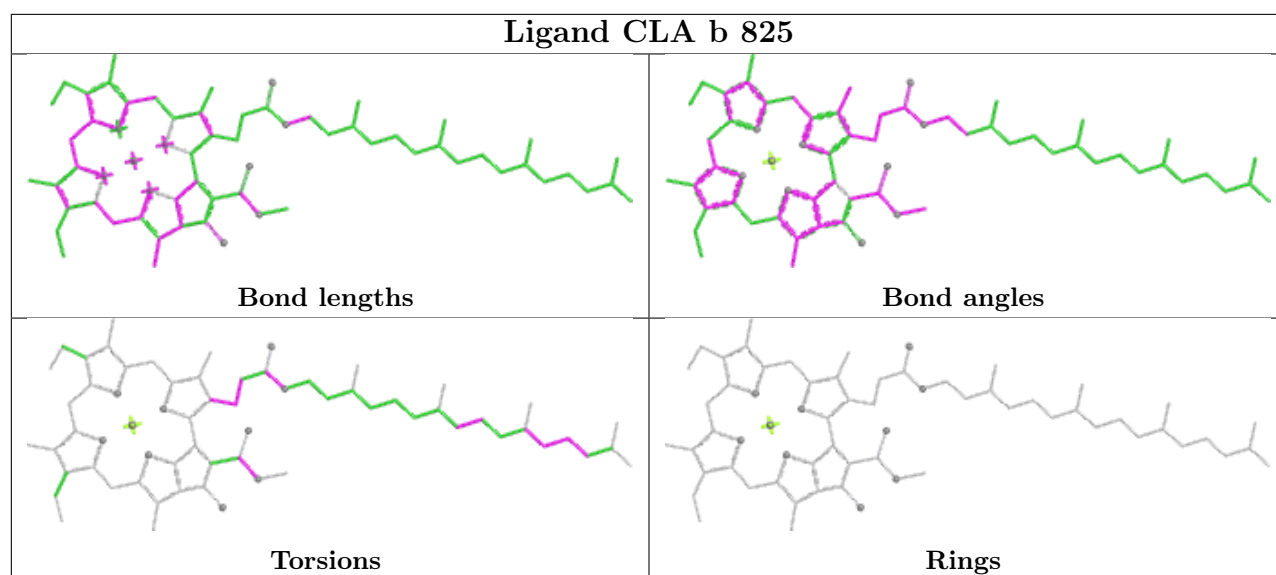


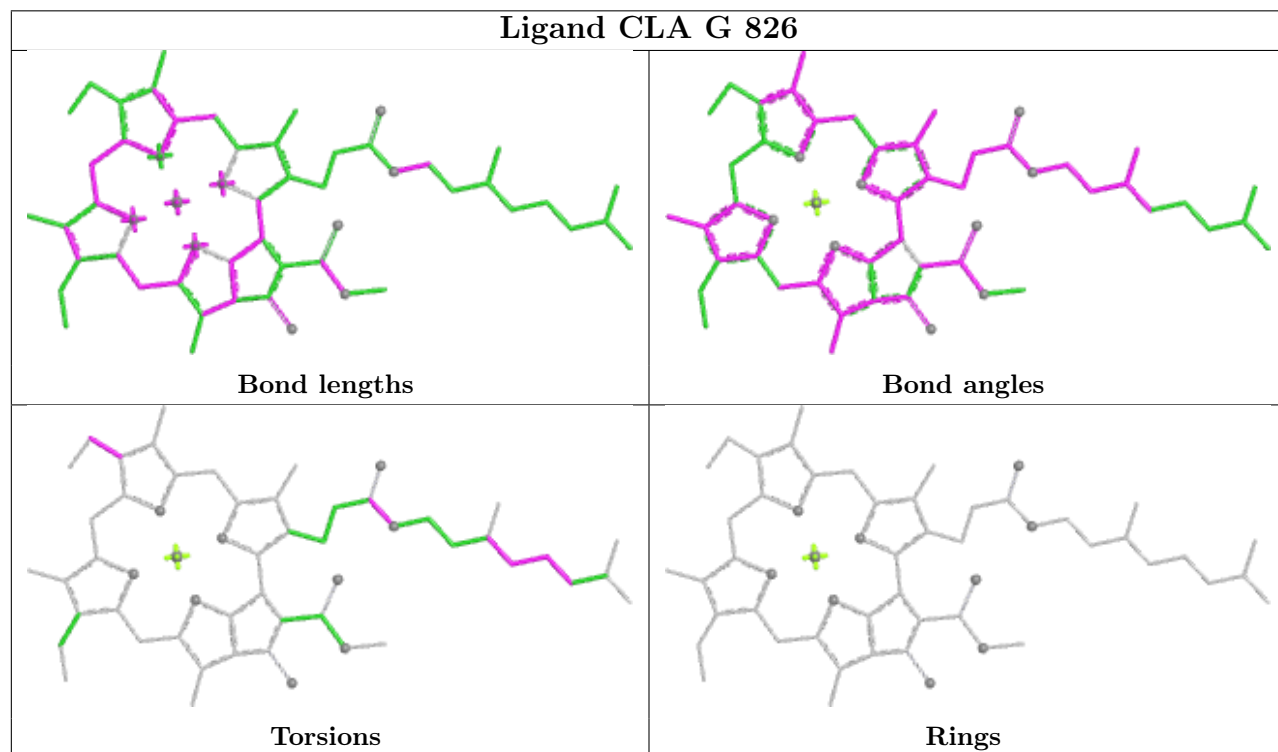
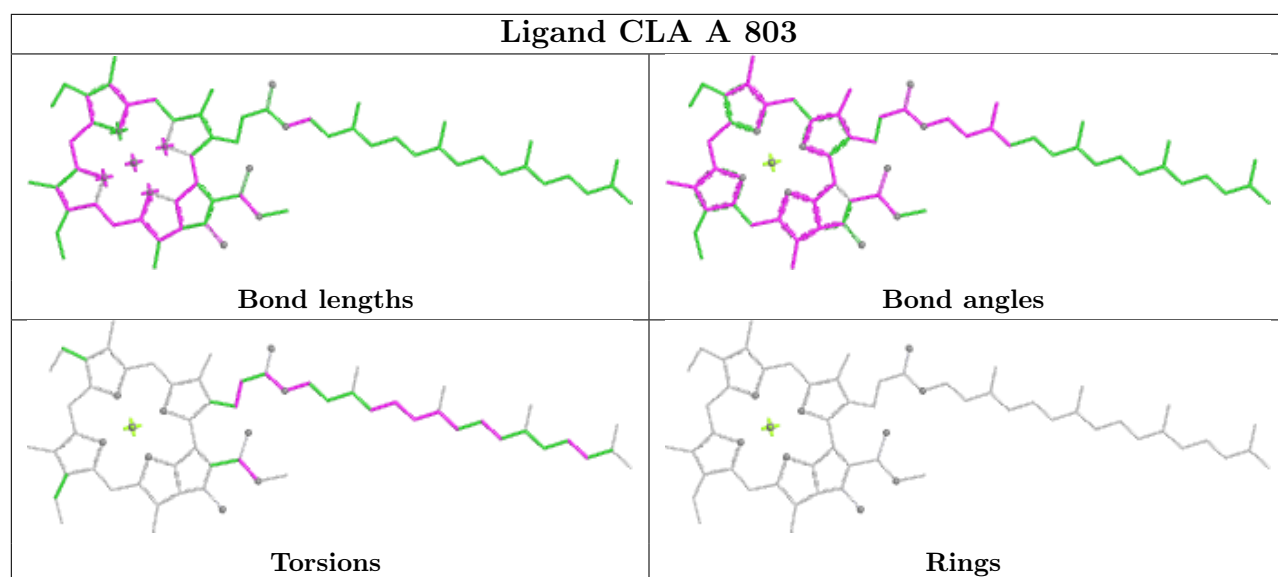
Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

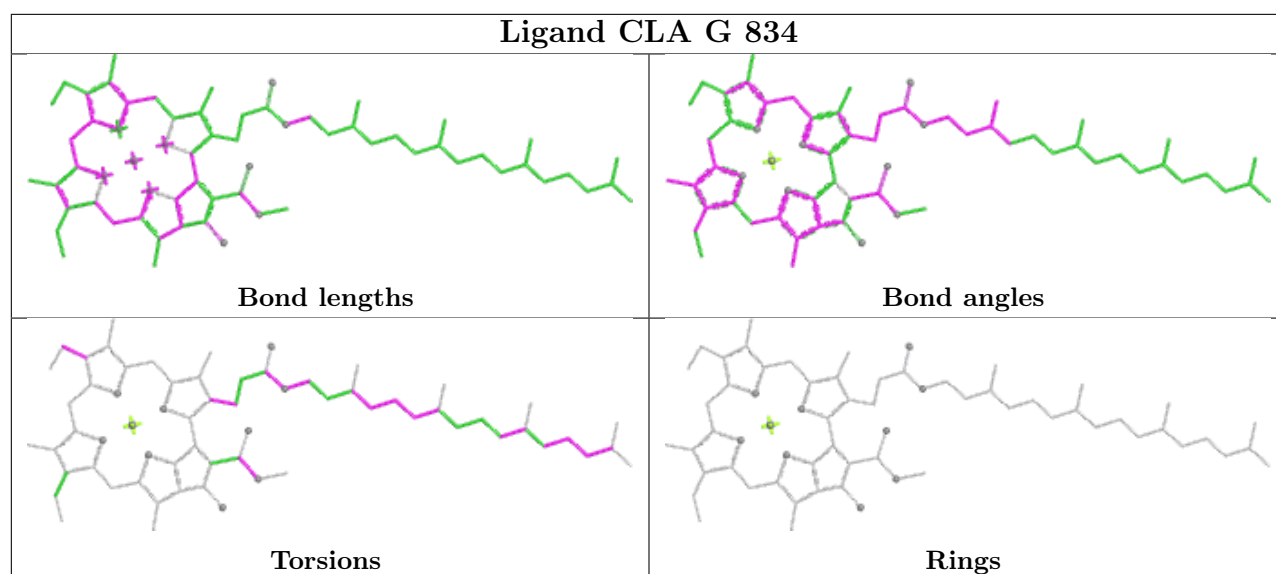
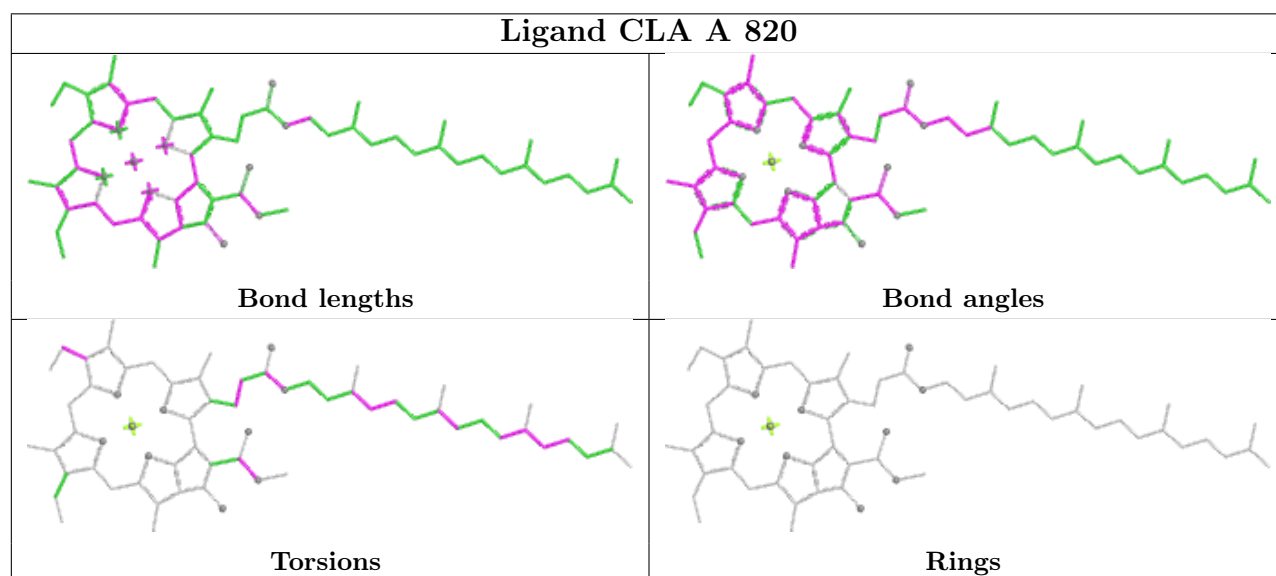
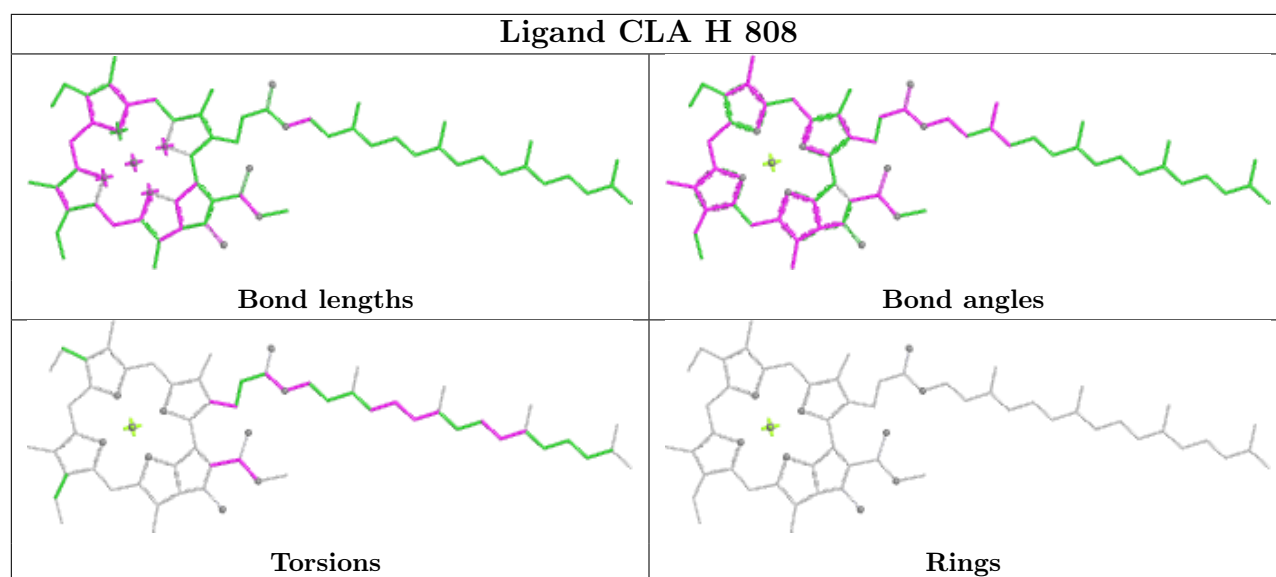
Ligand BCR f 204	
	
Bond lengths	Bond angles
	
Torsions	Rings



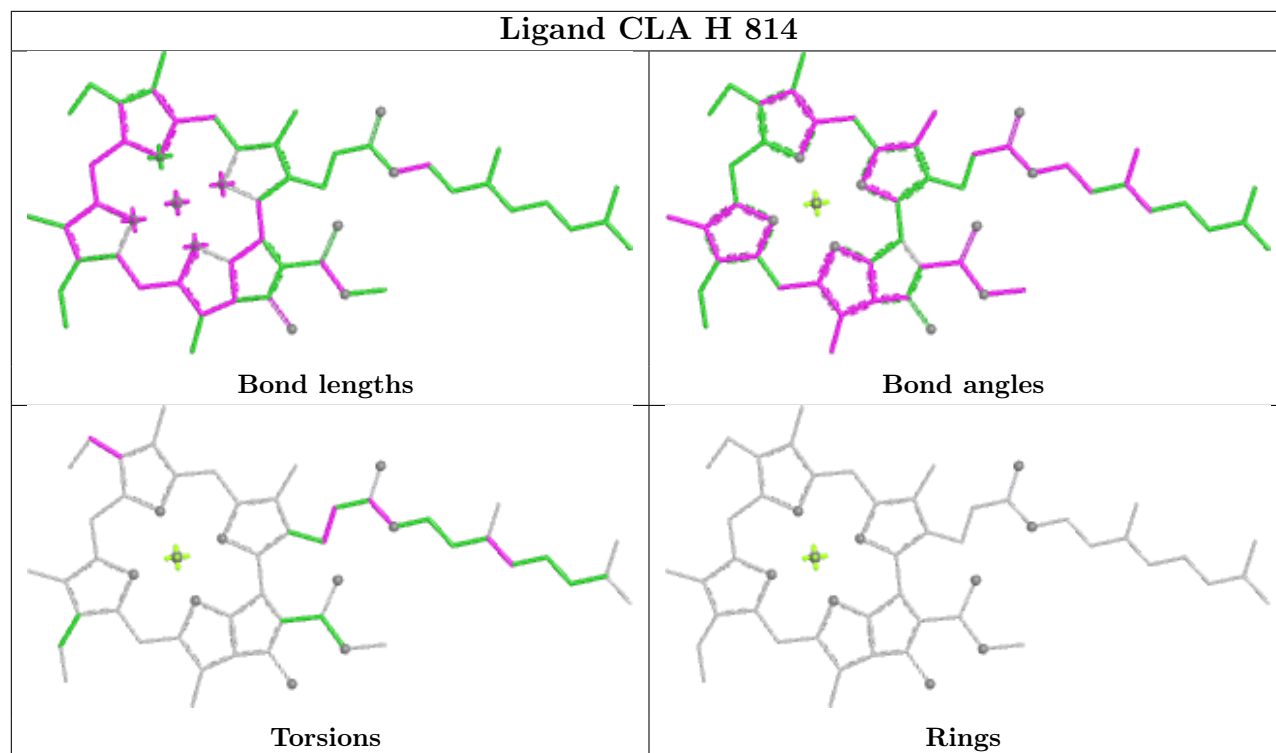




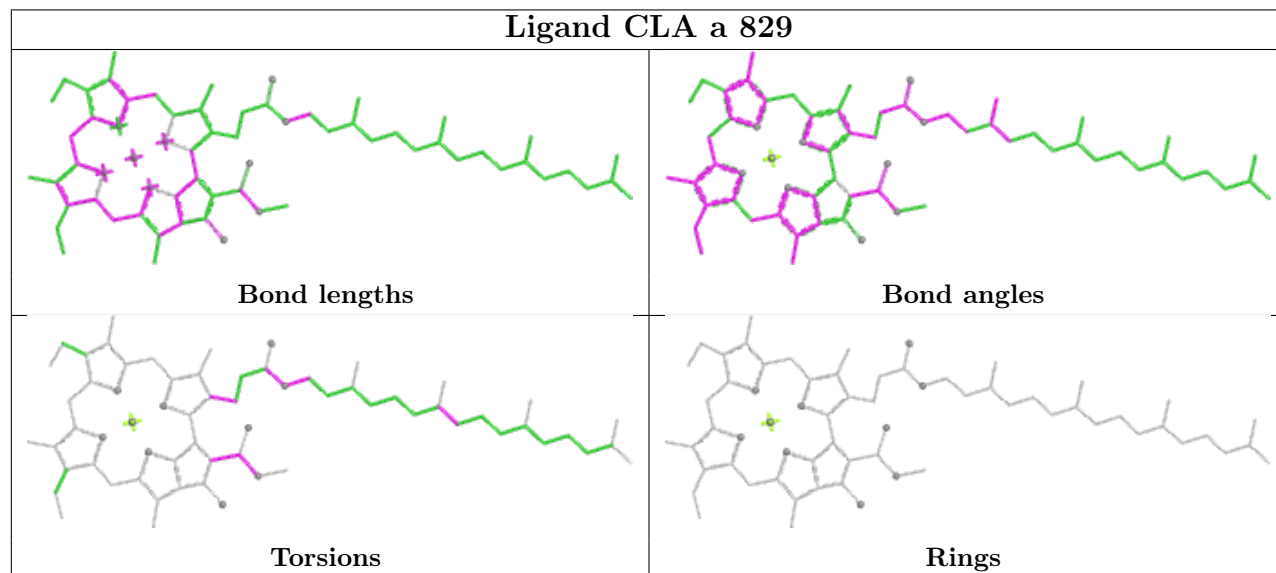


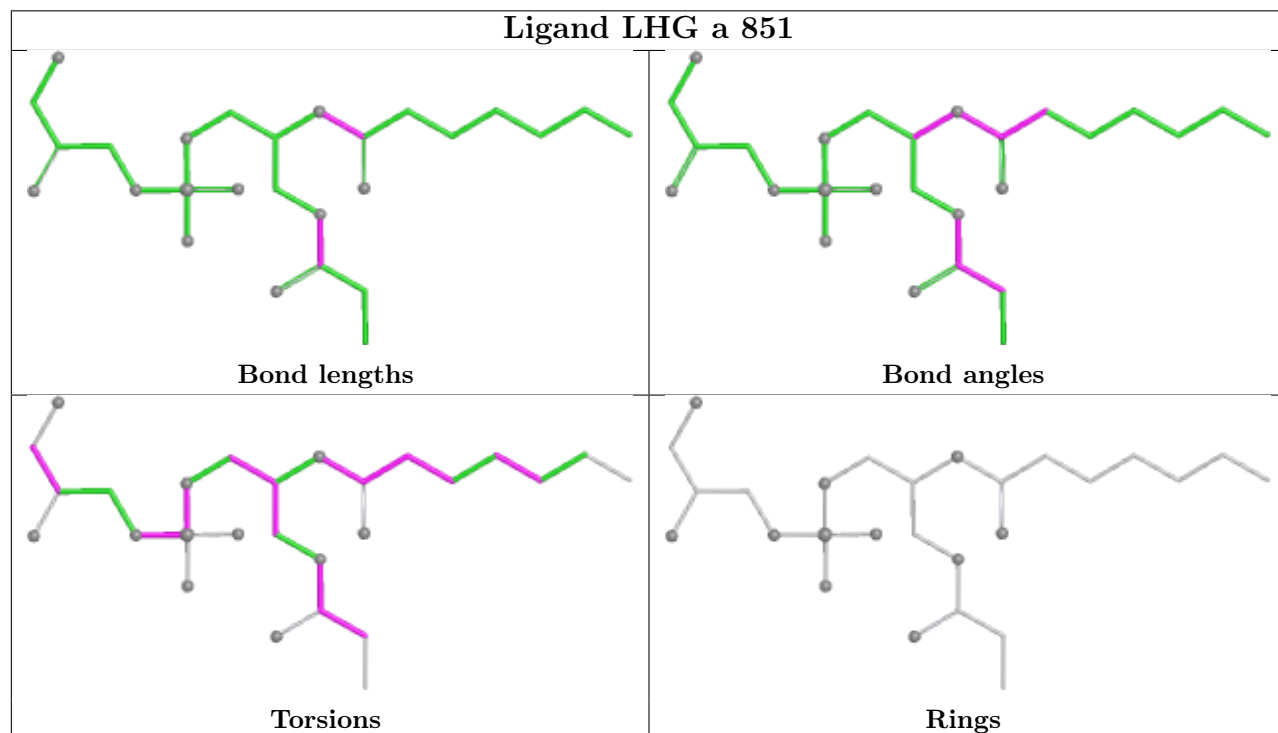
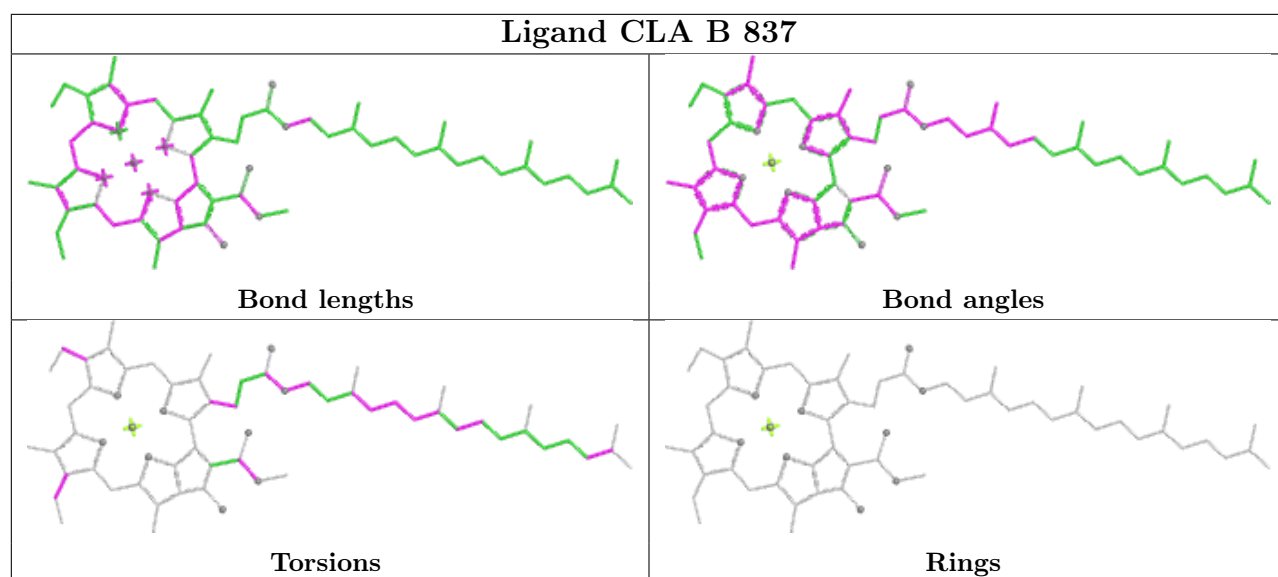


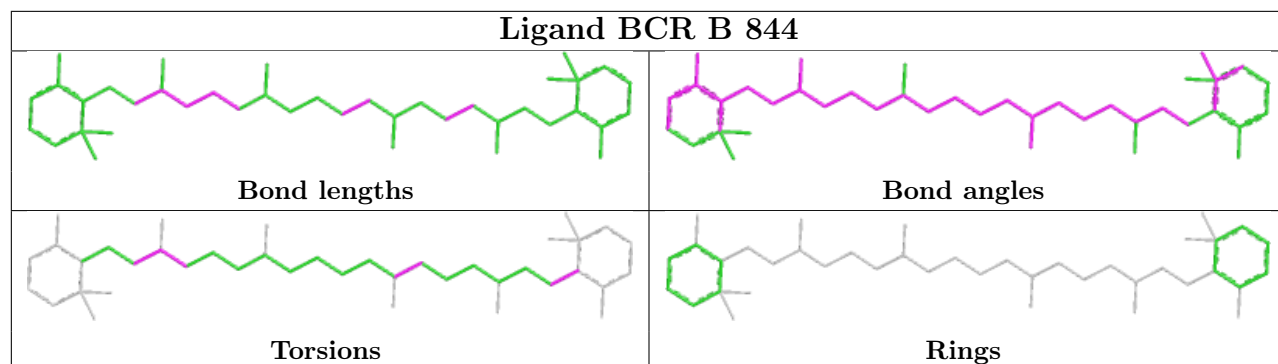
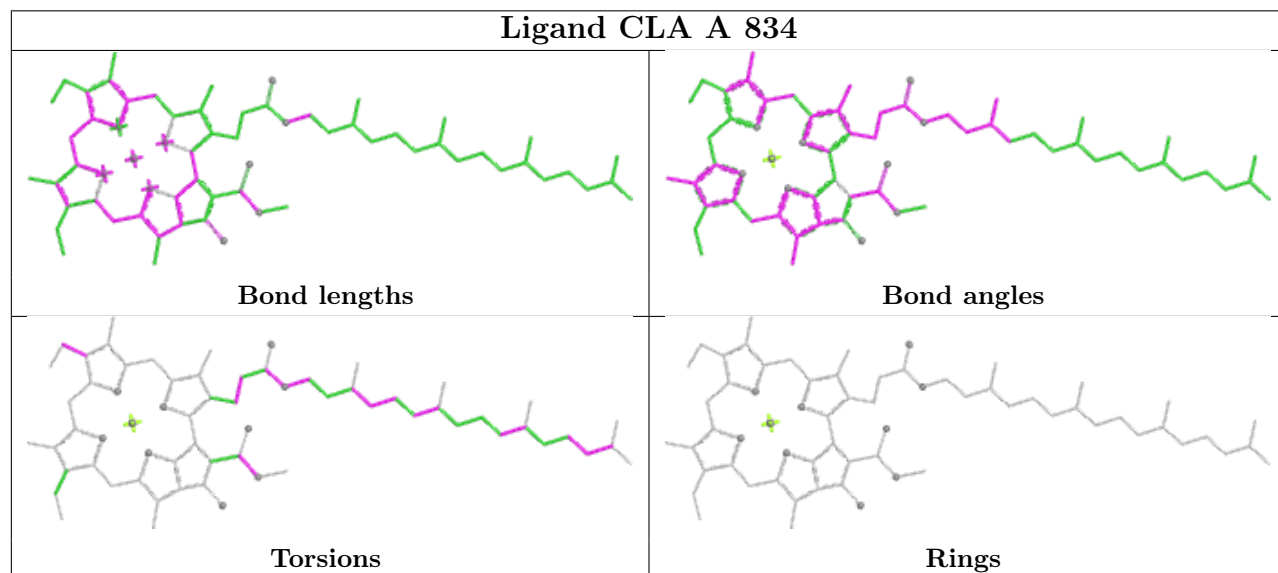
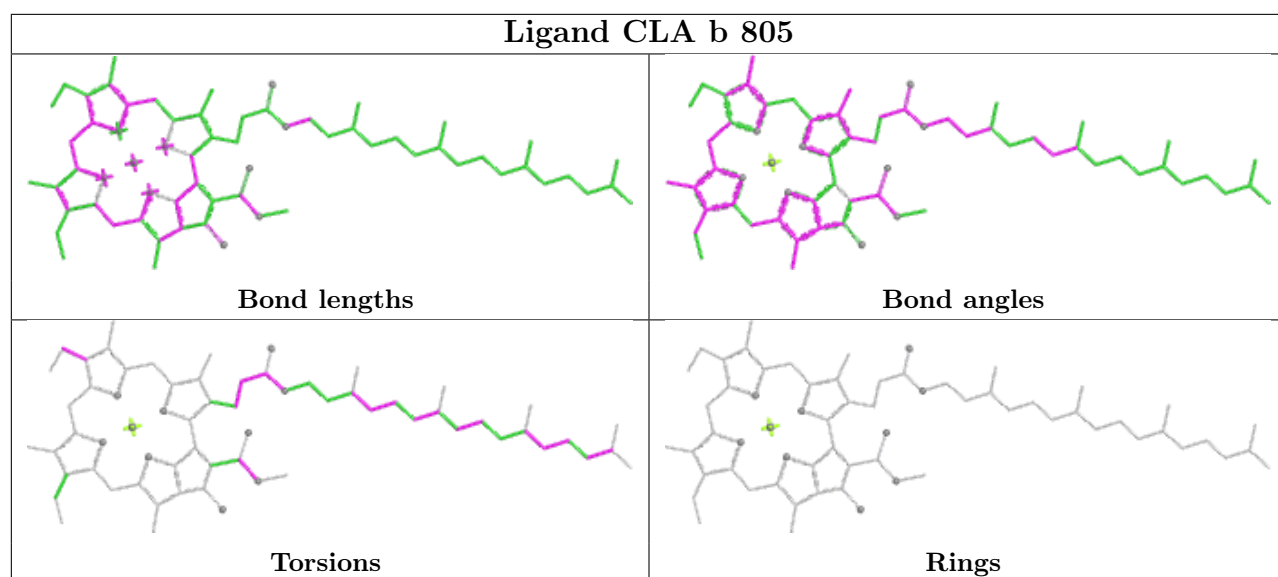
Ligand CLA H 814



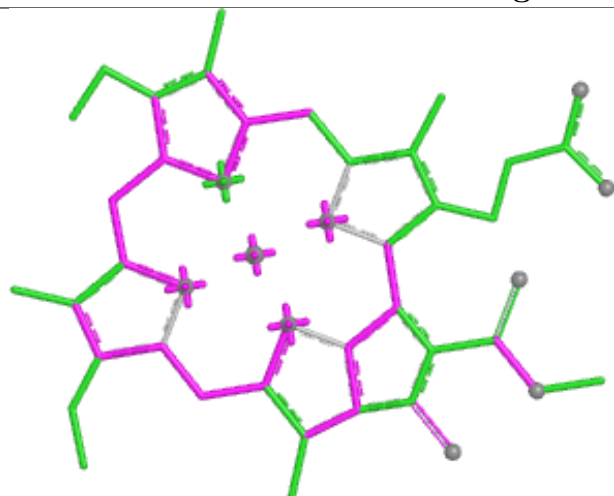
Ligand CLA a 829



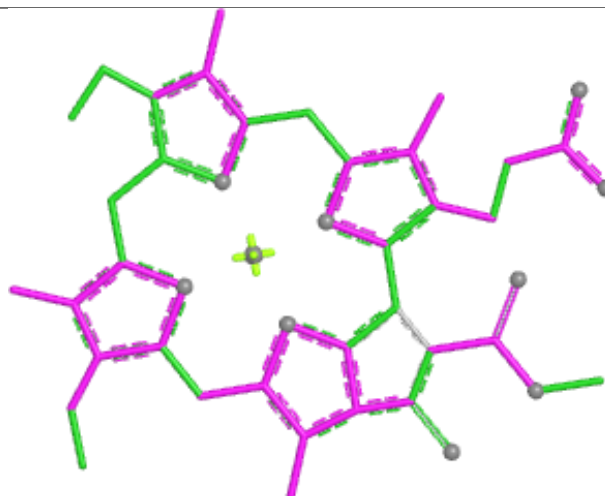




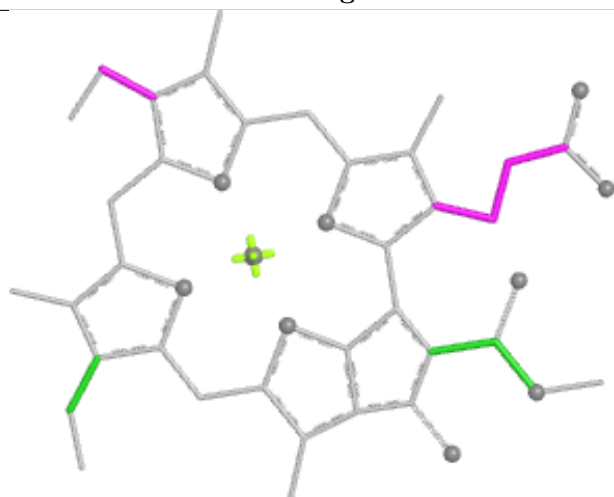
Ligand CLA G 812



Bond lengths



Bond angles

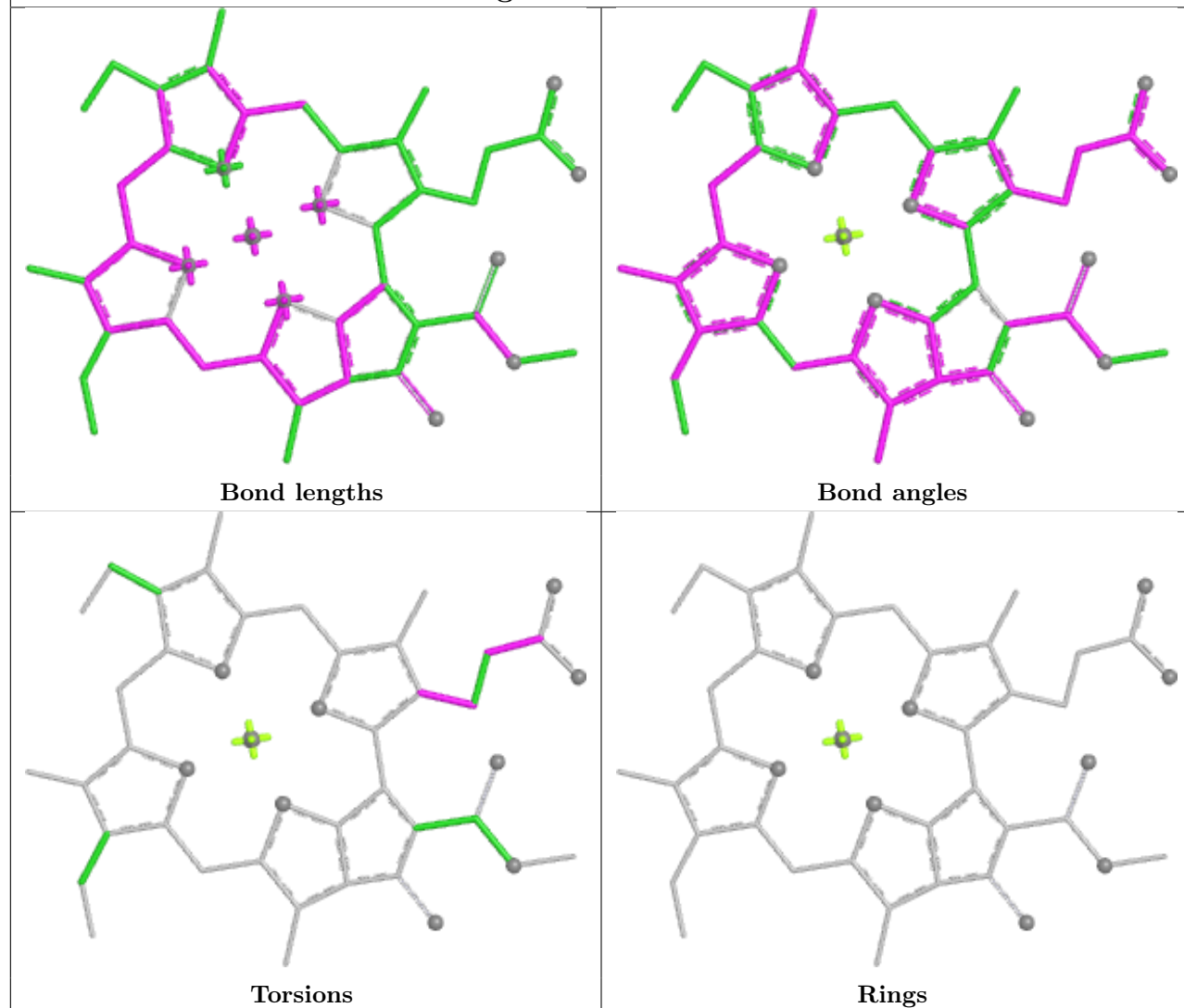


Torsions

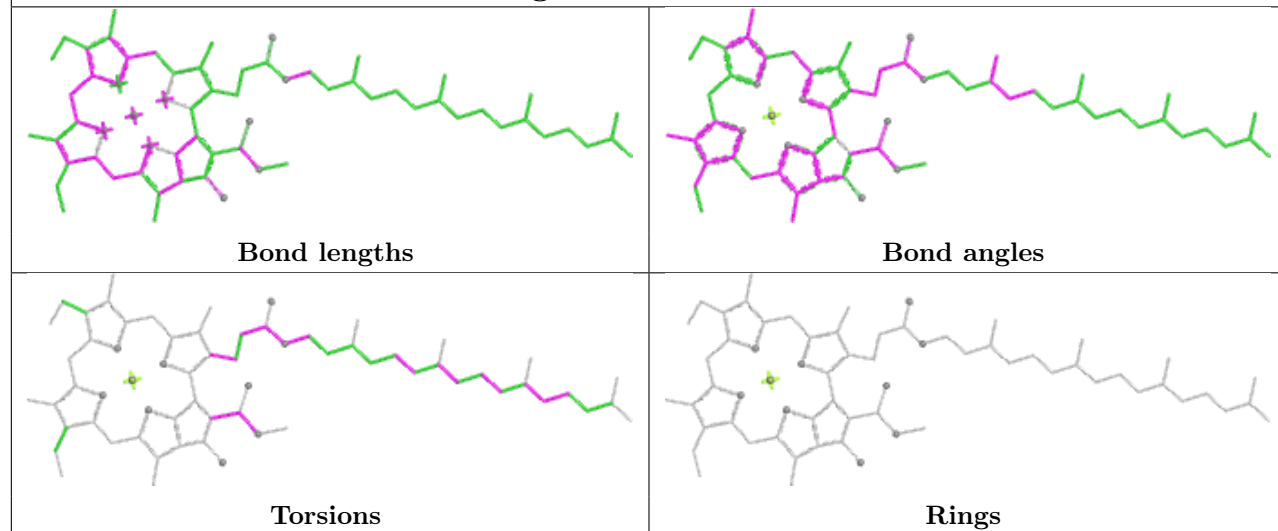


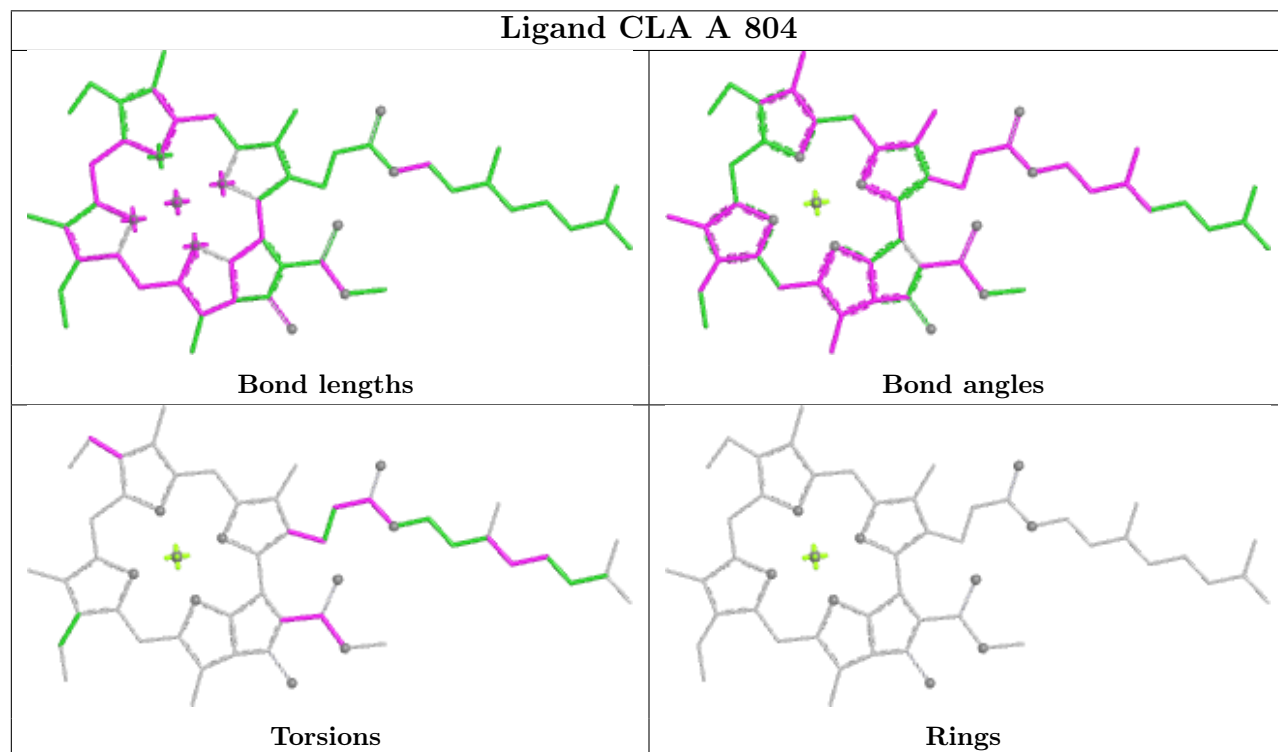
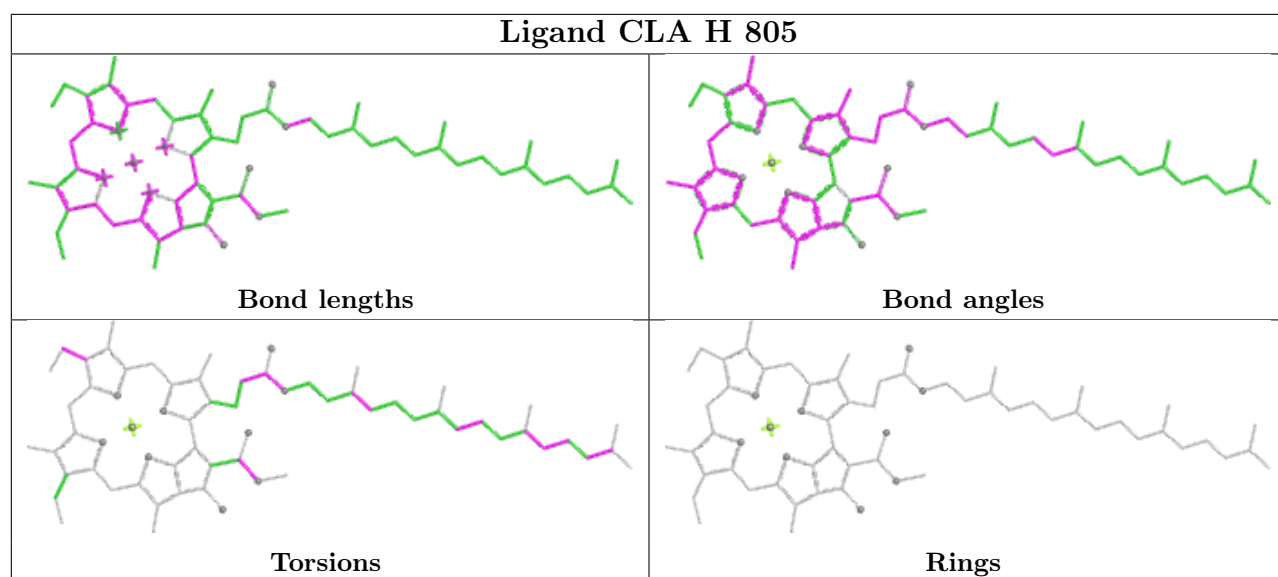
Rings

Ligand CLA a 838

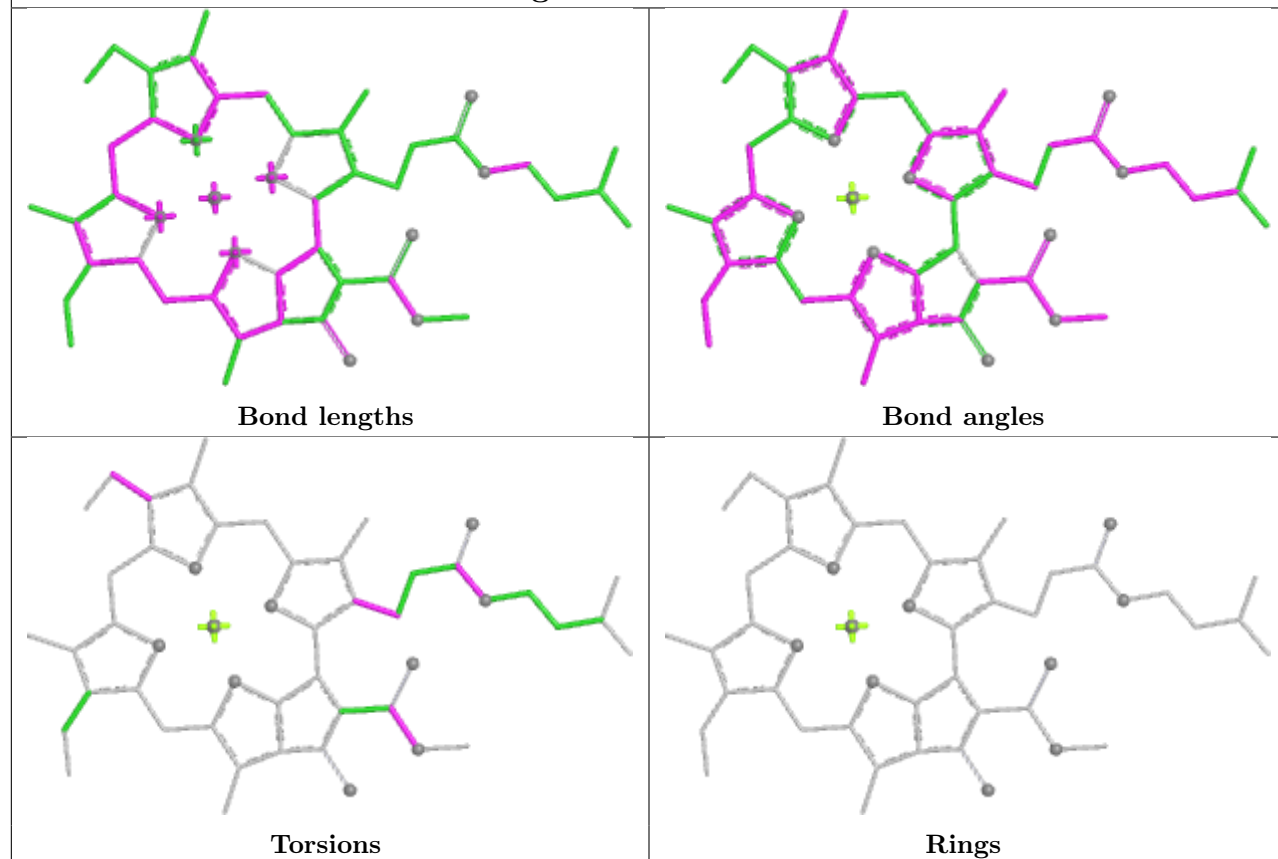


Ligand CLA H 803

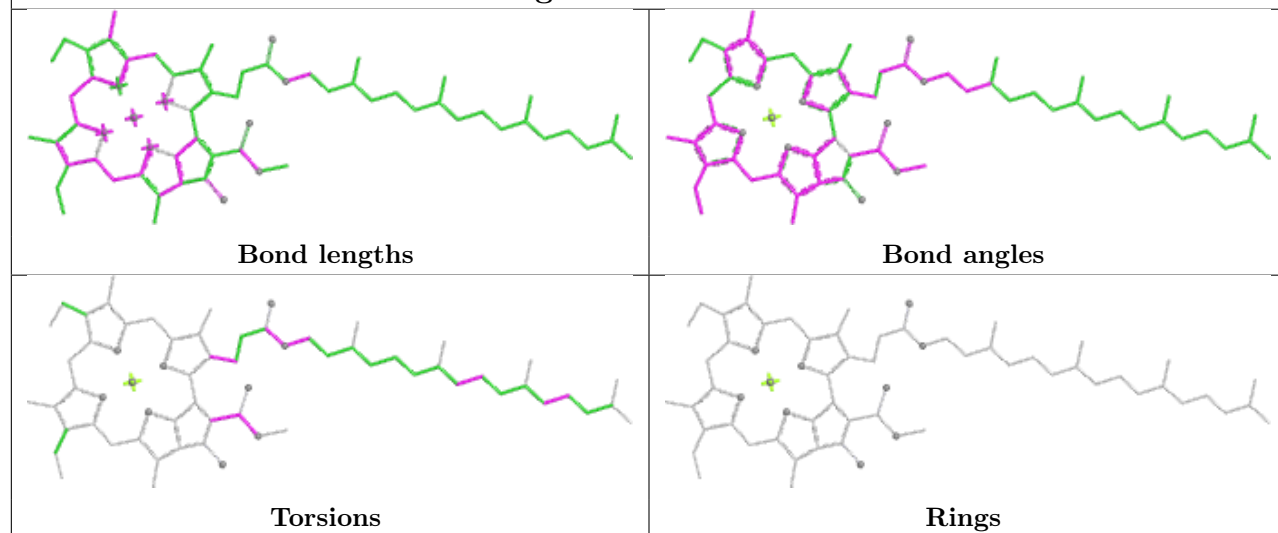


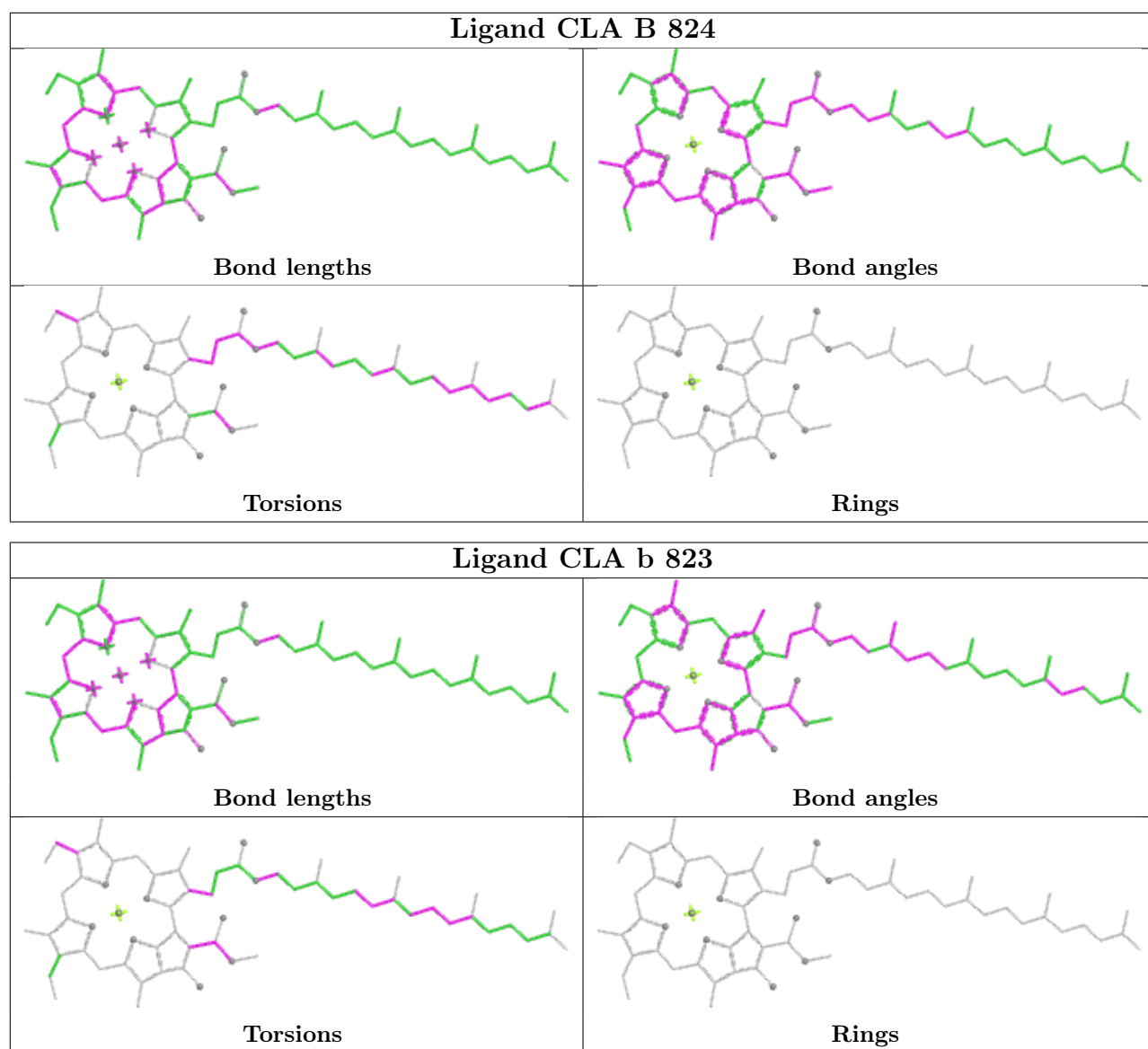


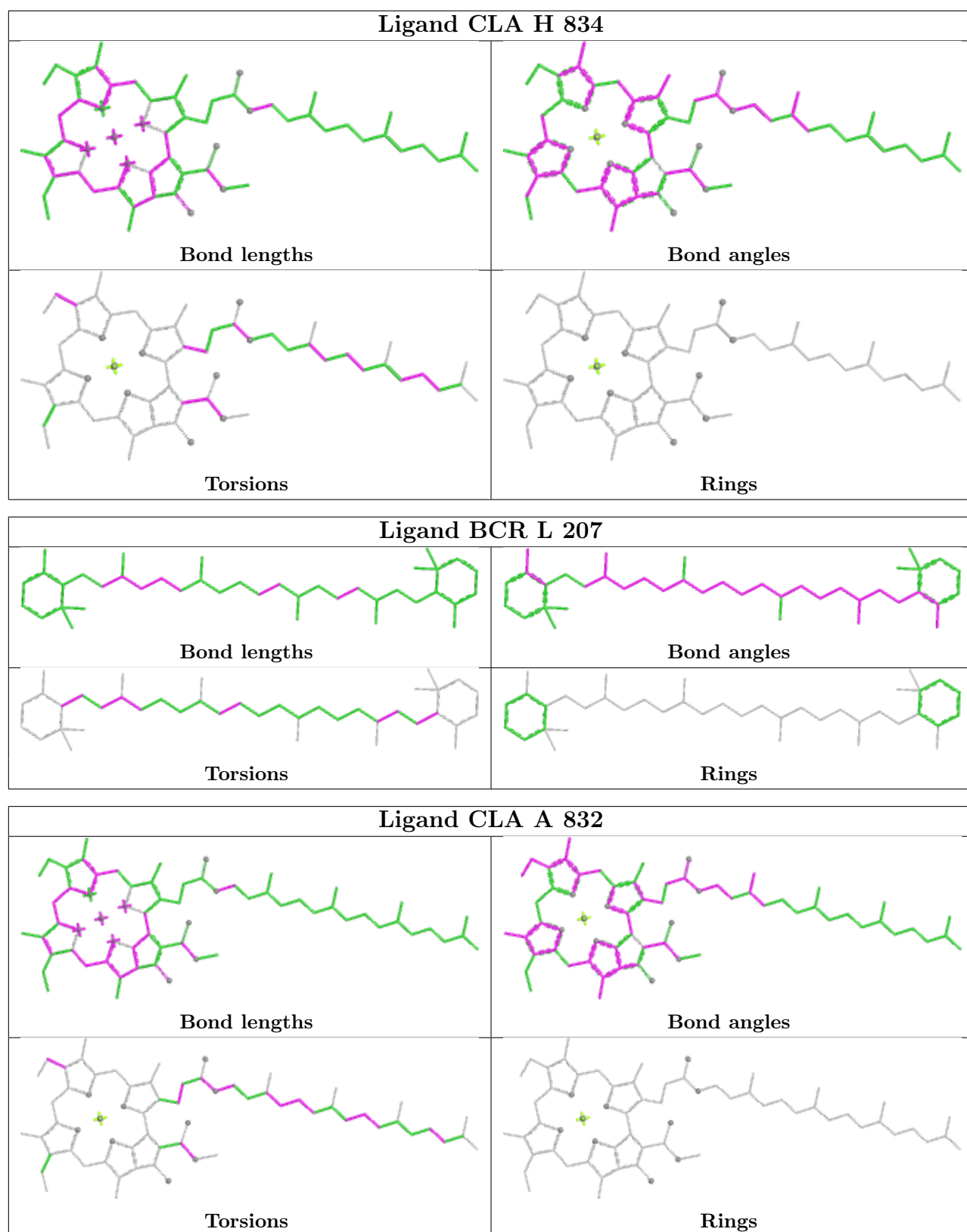
Ligand CLA A 810

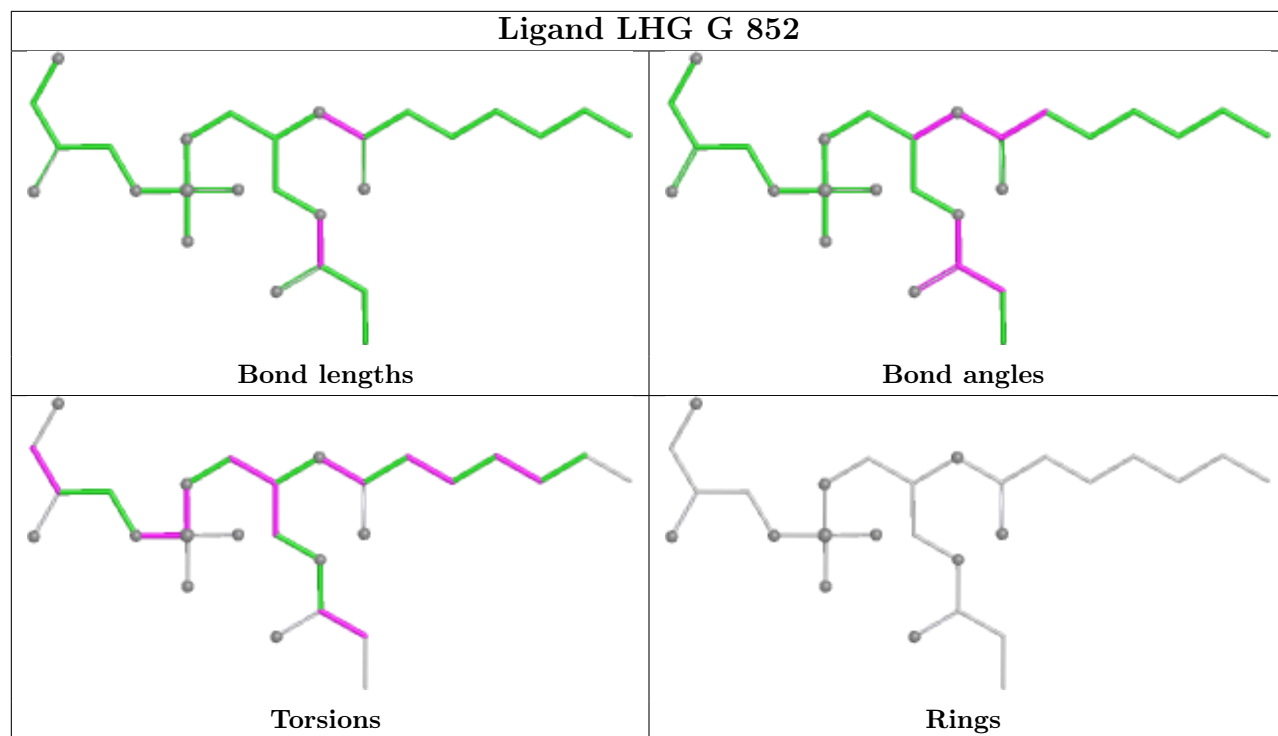


Ligand CLA b 826

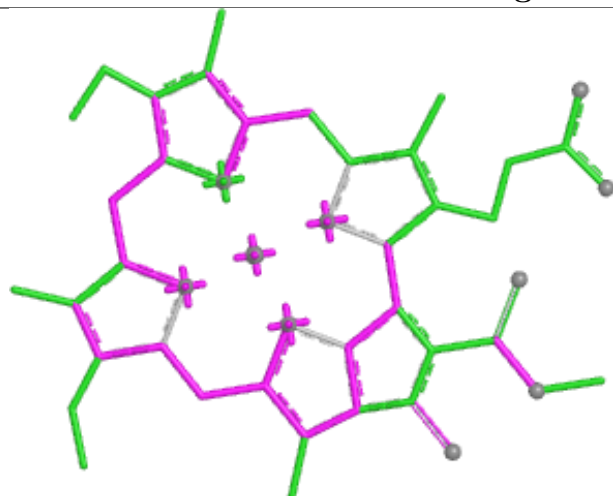




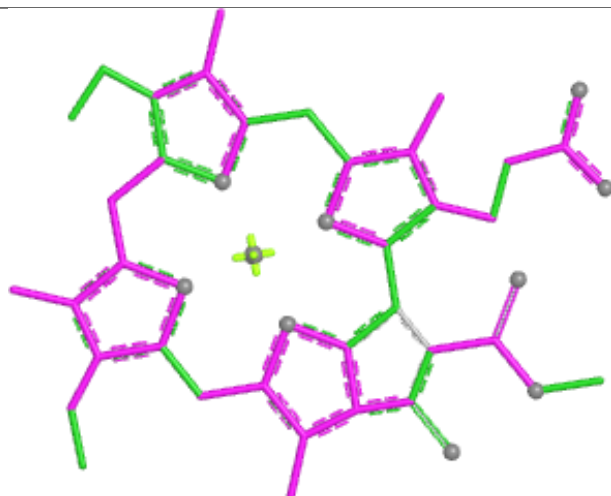




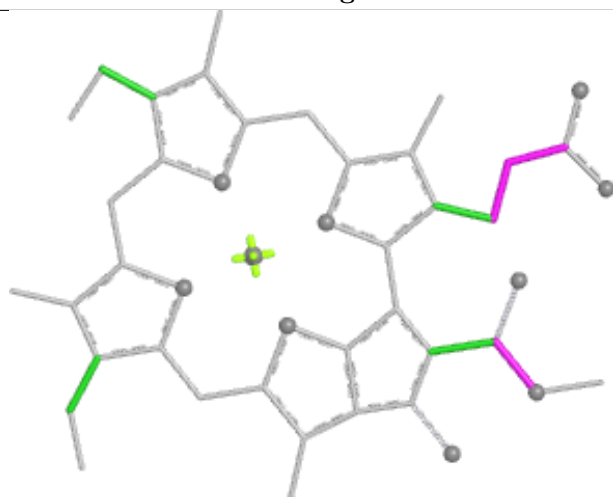
Ligand CLA B 809



Bond lengths



Bond angles

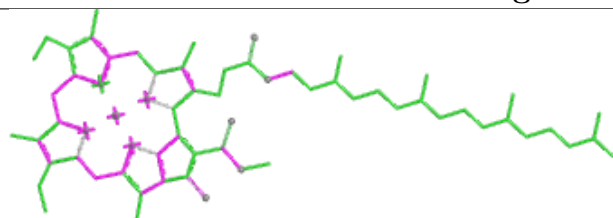


Torsions

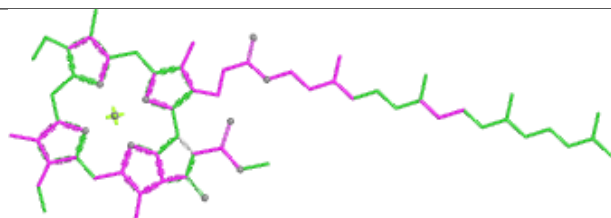


Rings

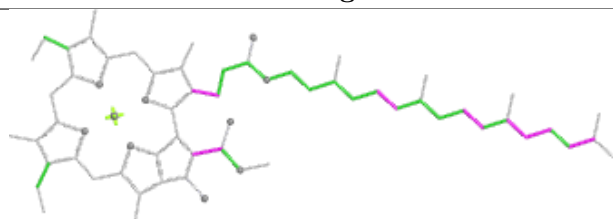
Ligand CLA G 806



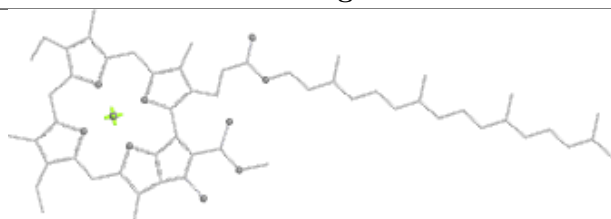
Bond lengths



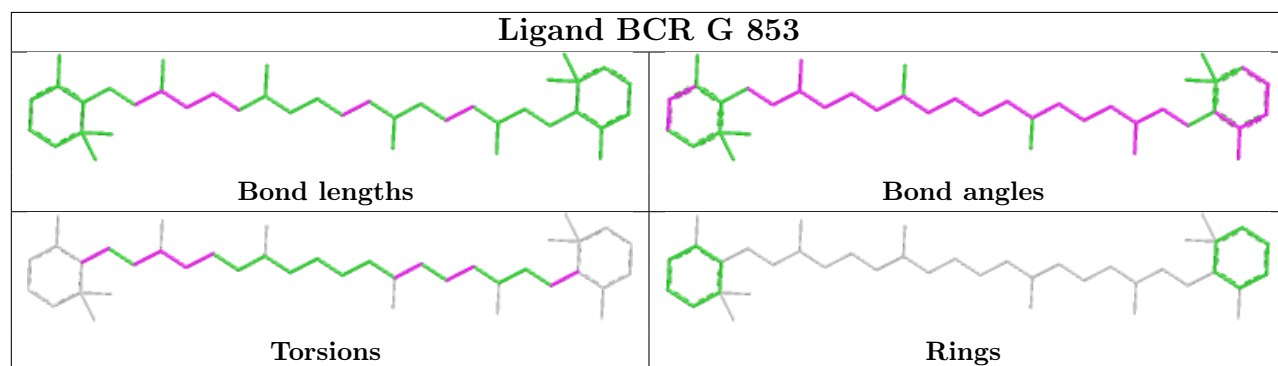
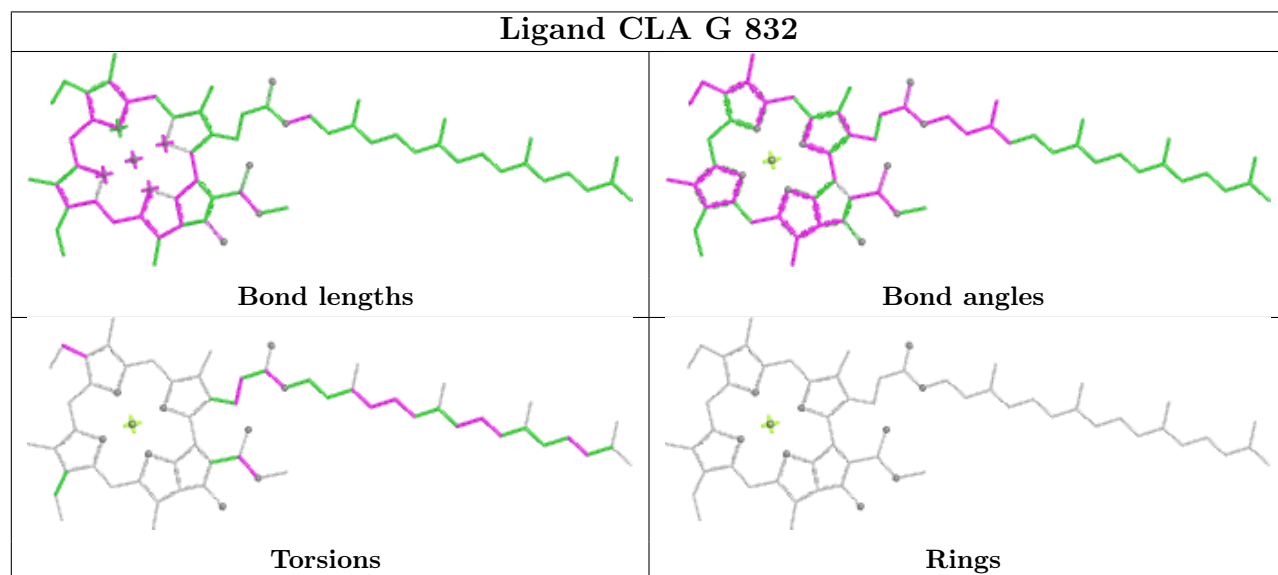
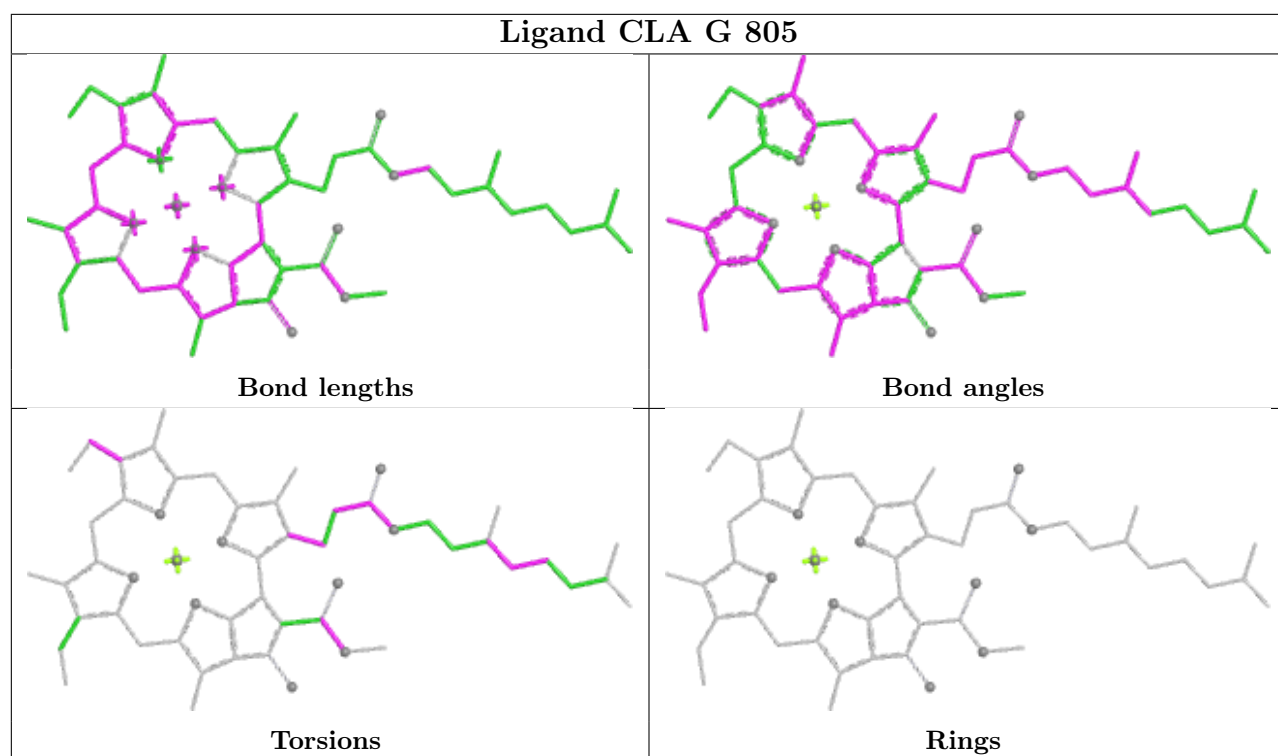
Bond angles

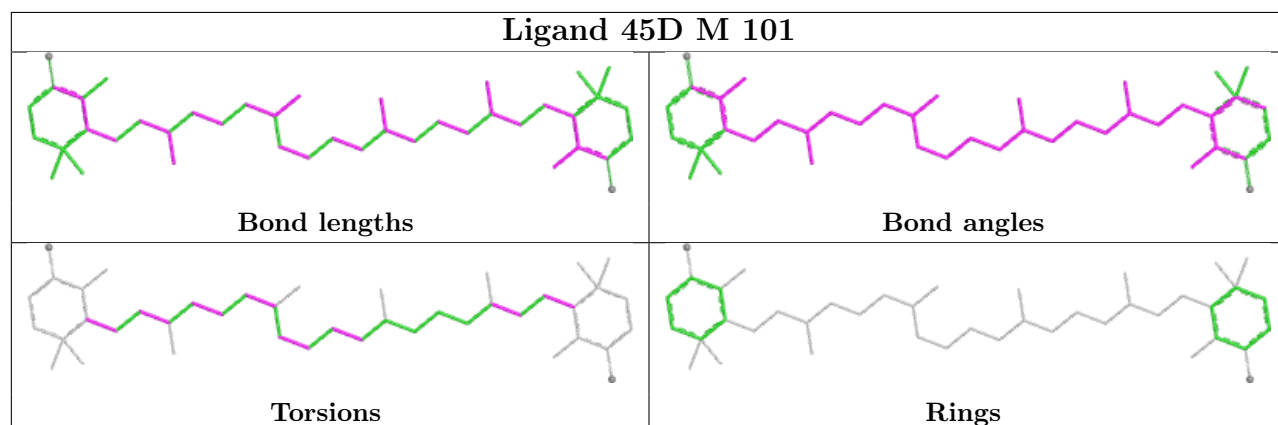
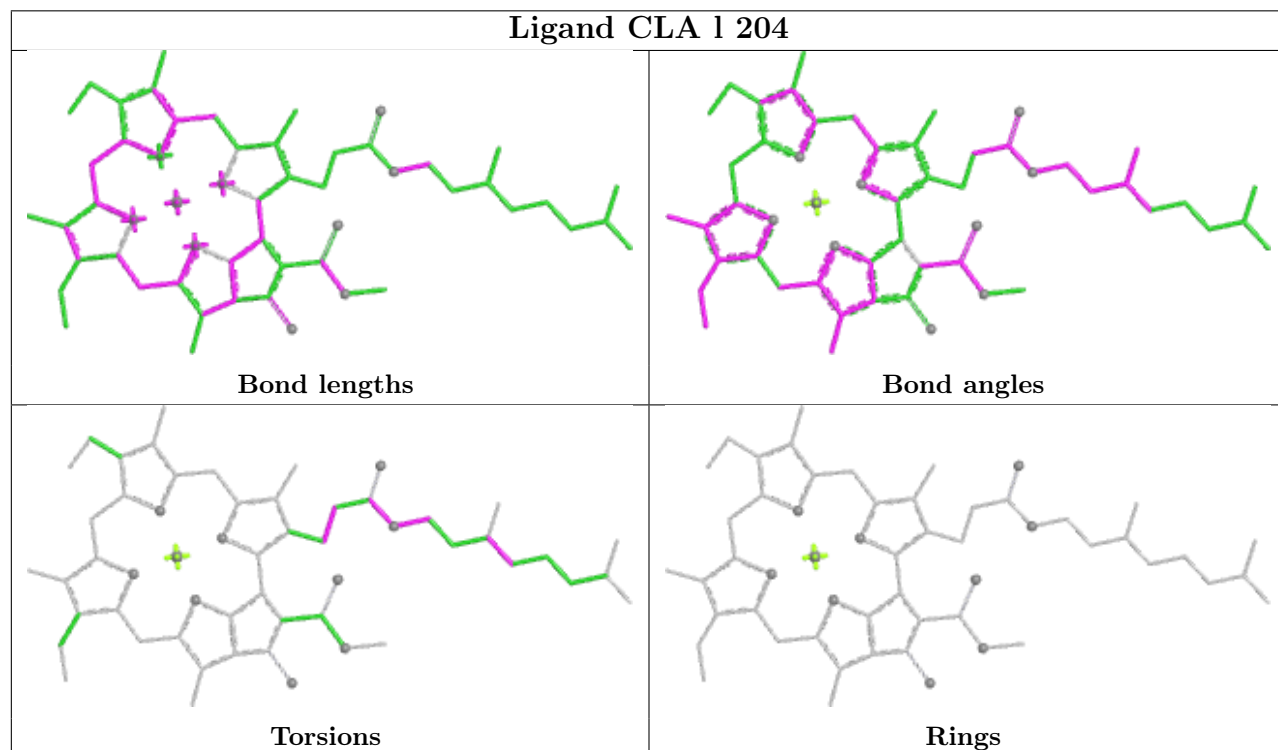
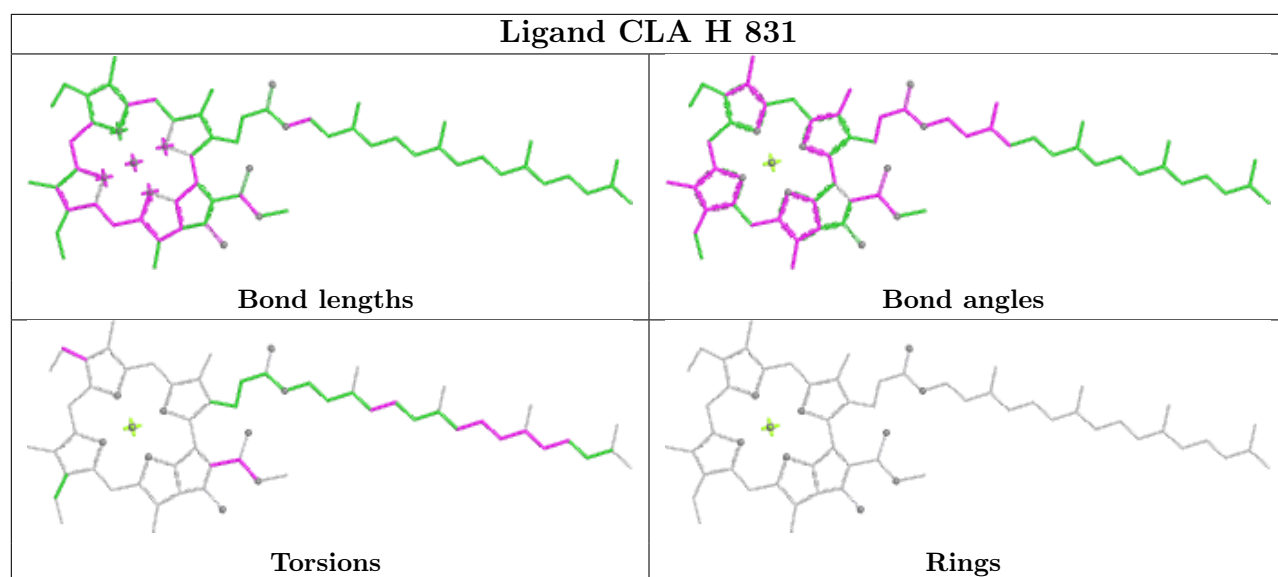


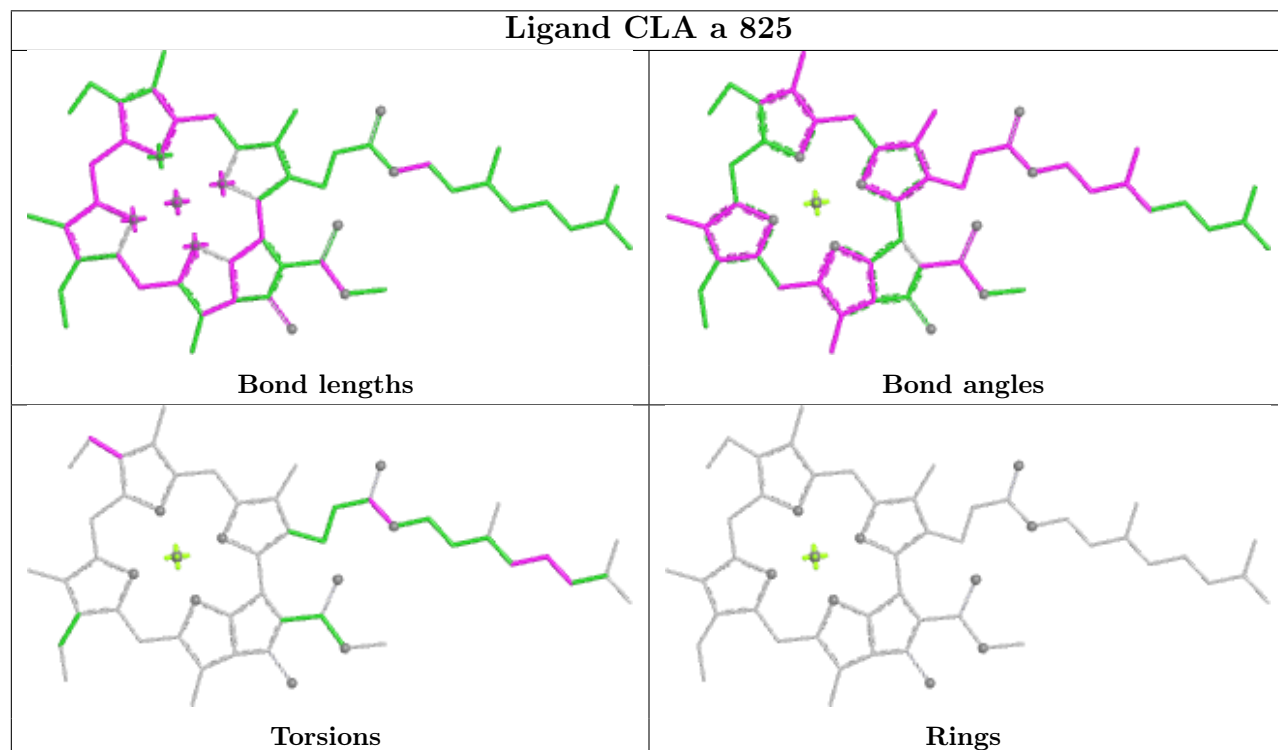
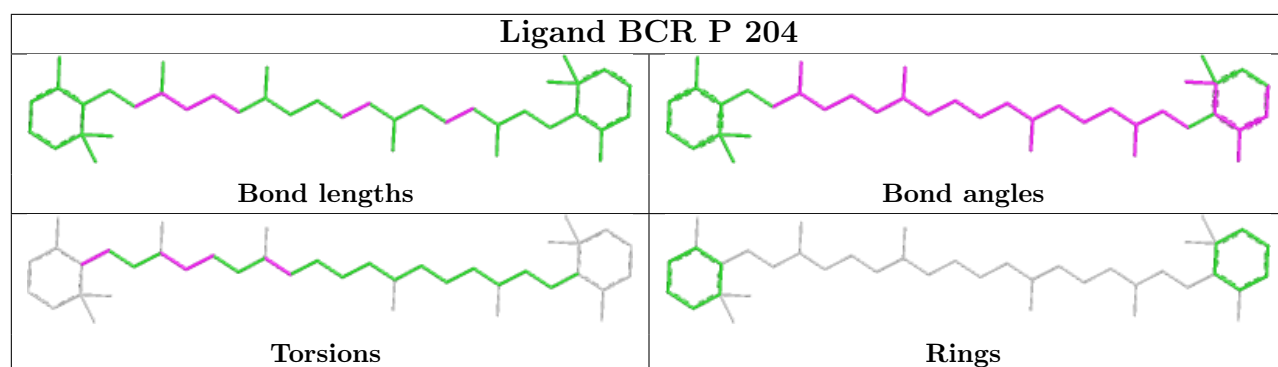
Torsions

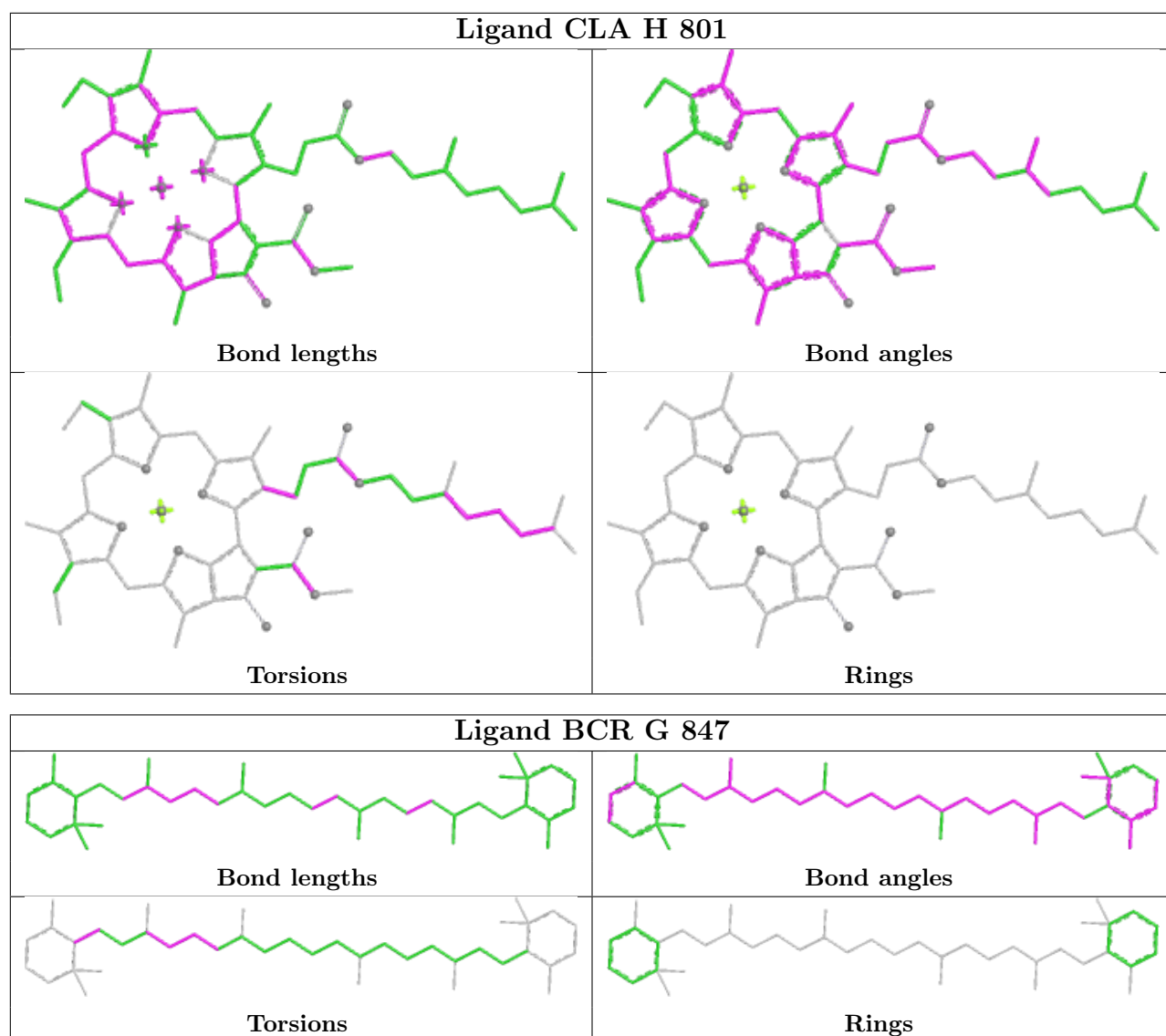


Rings

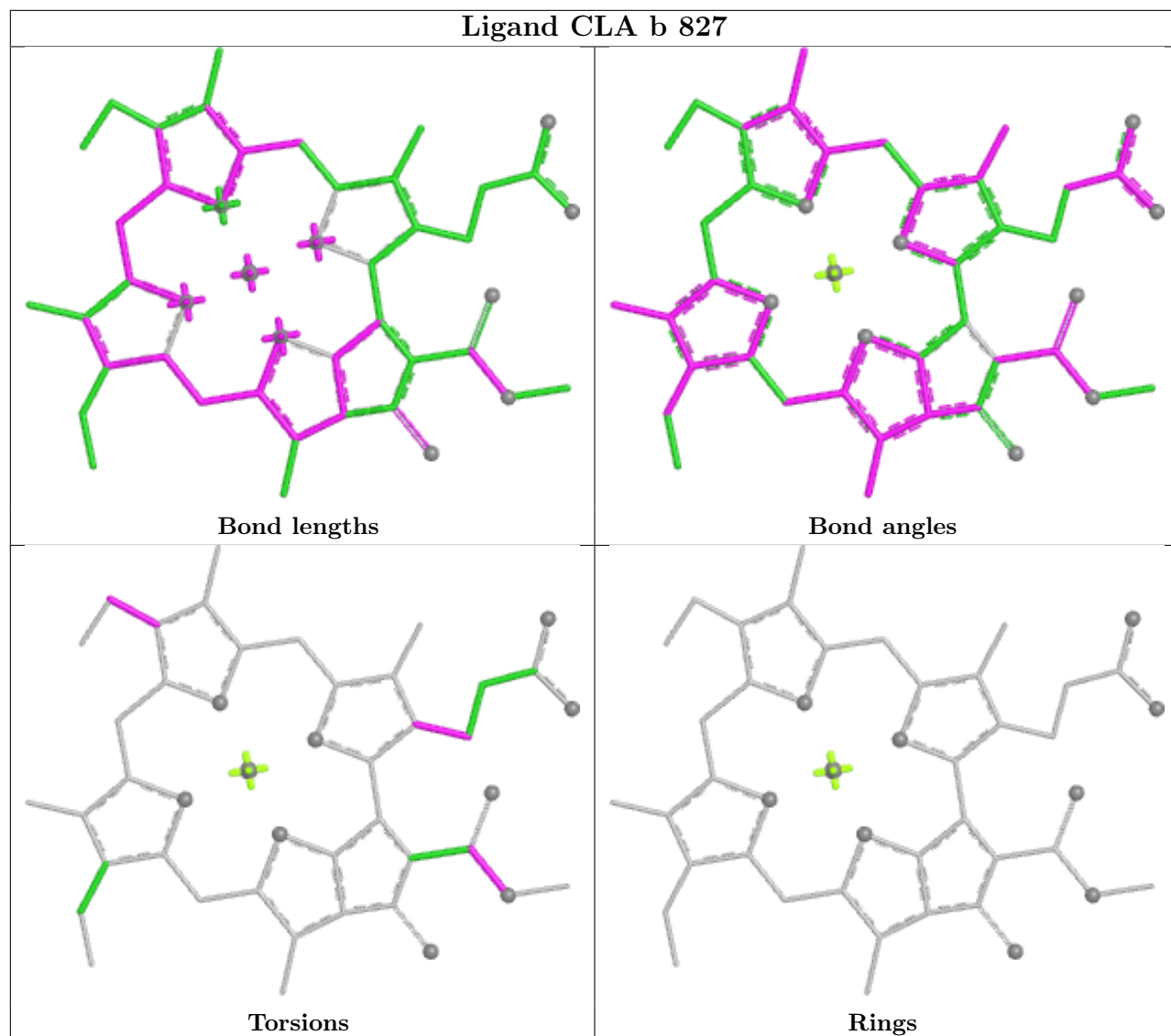




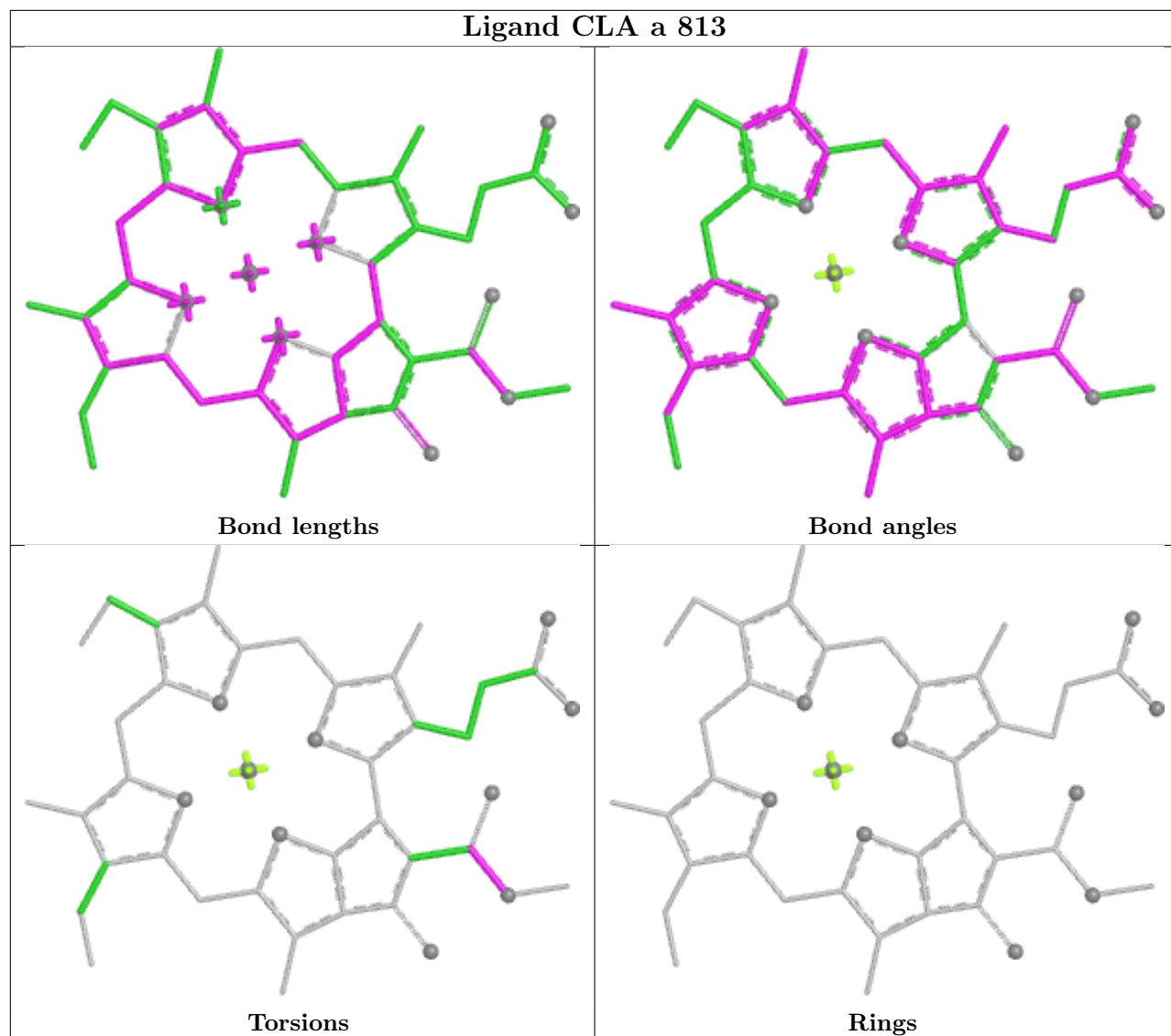




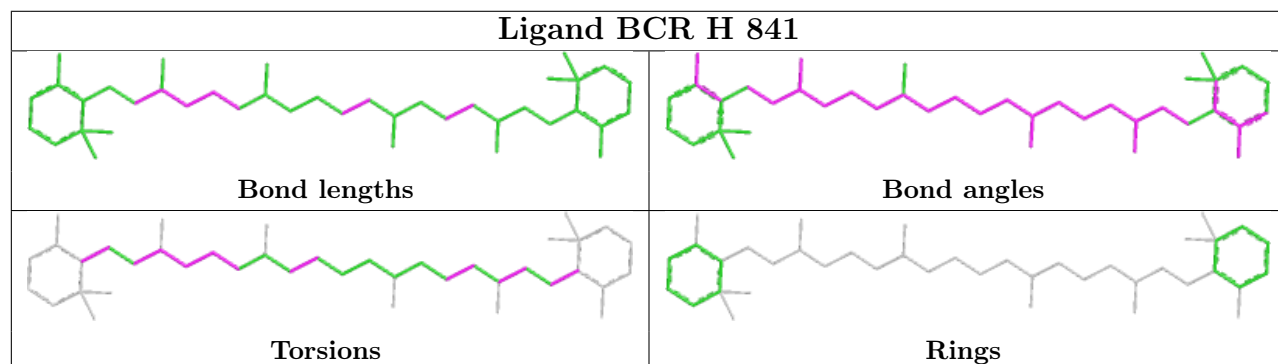
Ligand CLA b 827

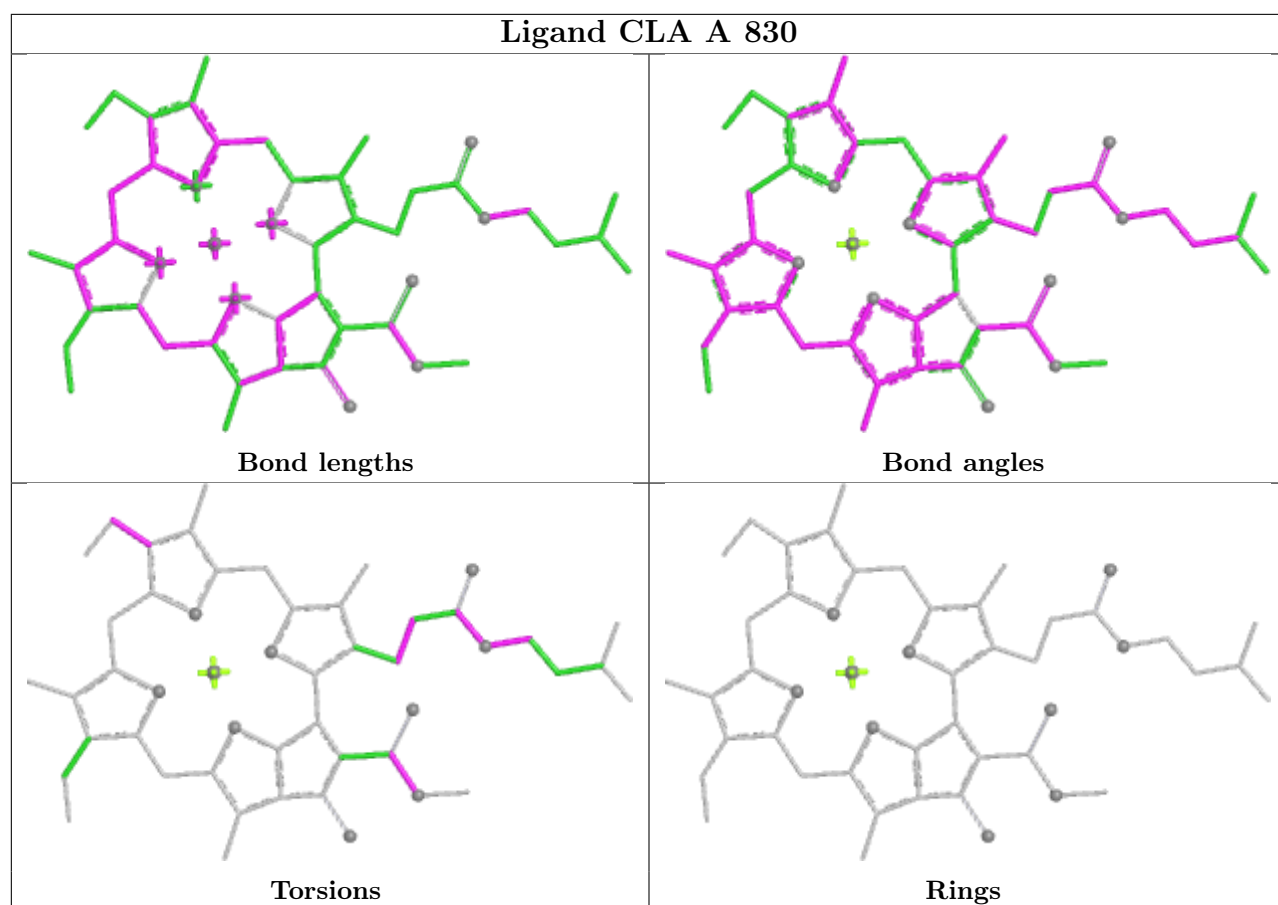


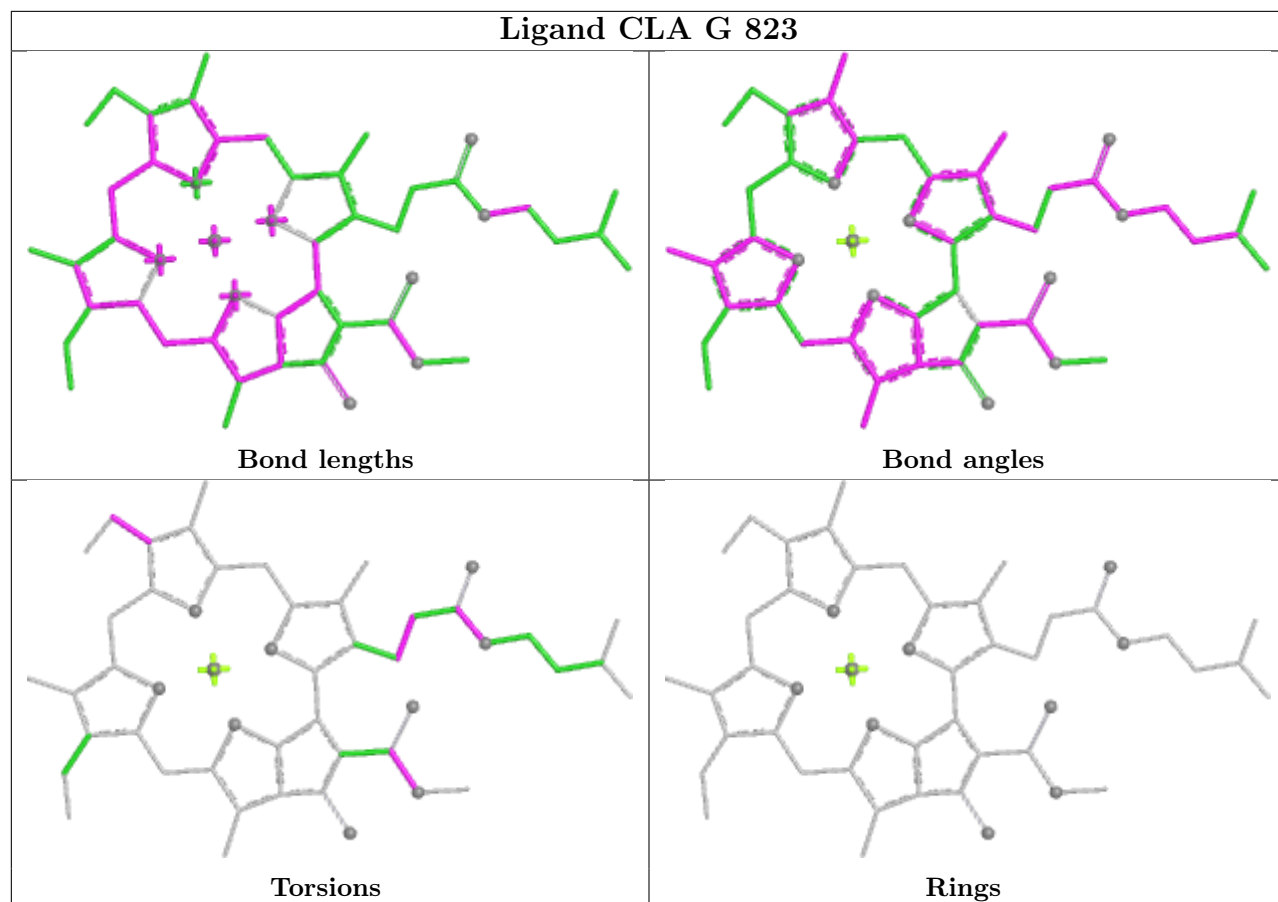
Ligand CLA a 813



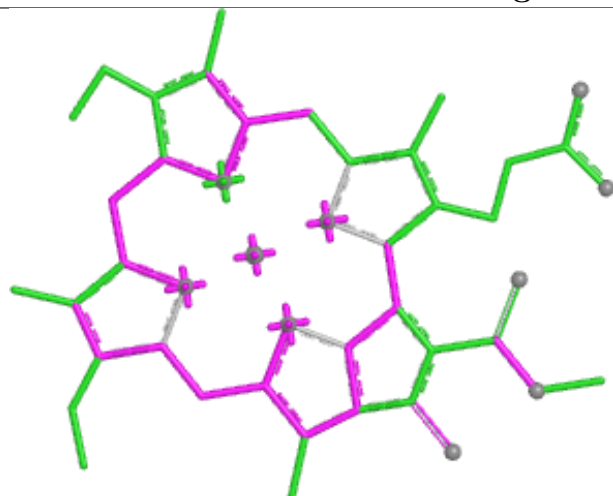
Ligand BCR H 841



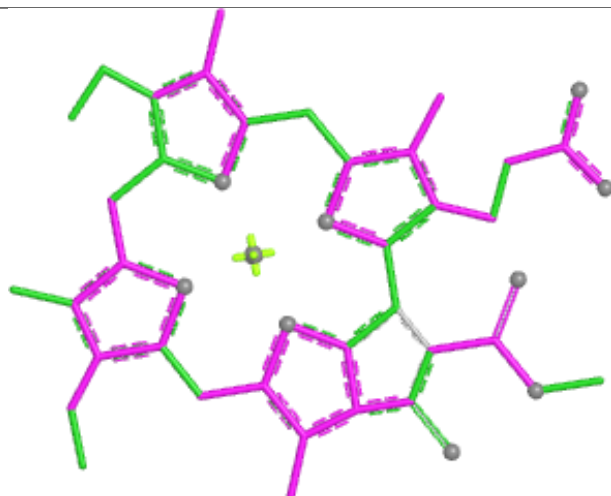




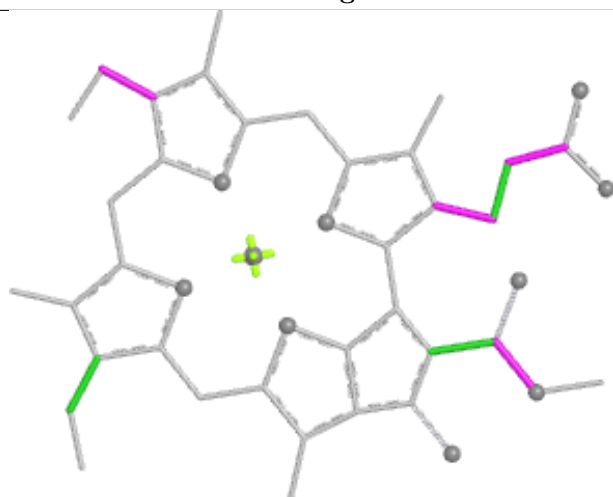
Ligand CLA H 833



Bond lengths



Bond angles

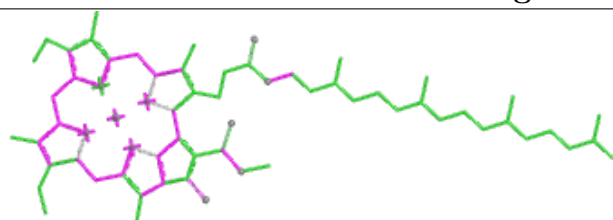


Torsions

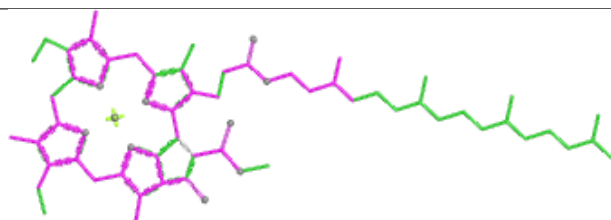


Rings

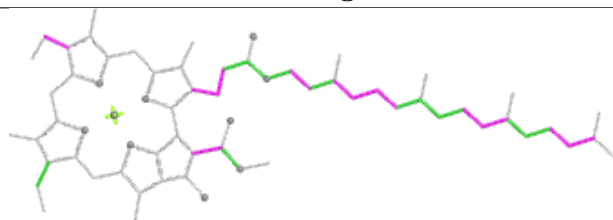
Ligand CLA A 854



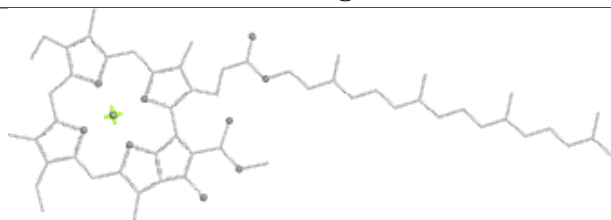
Bond lengths



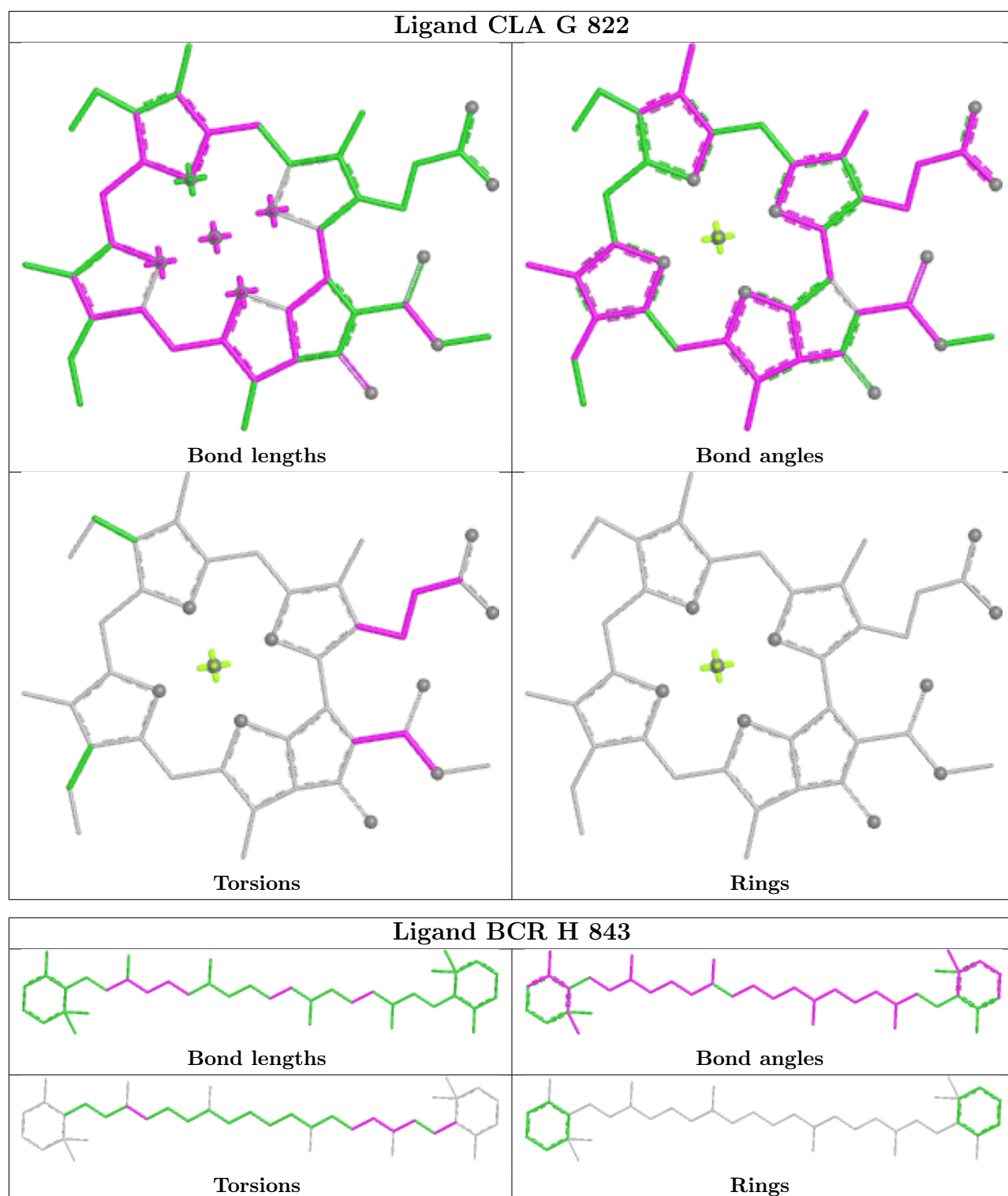
Bond angles

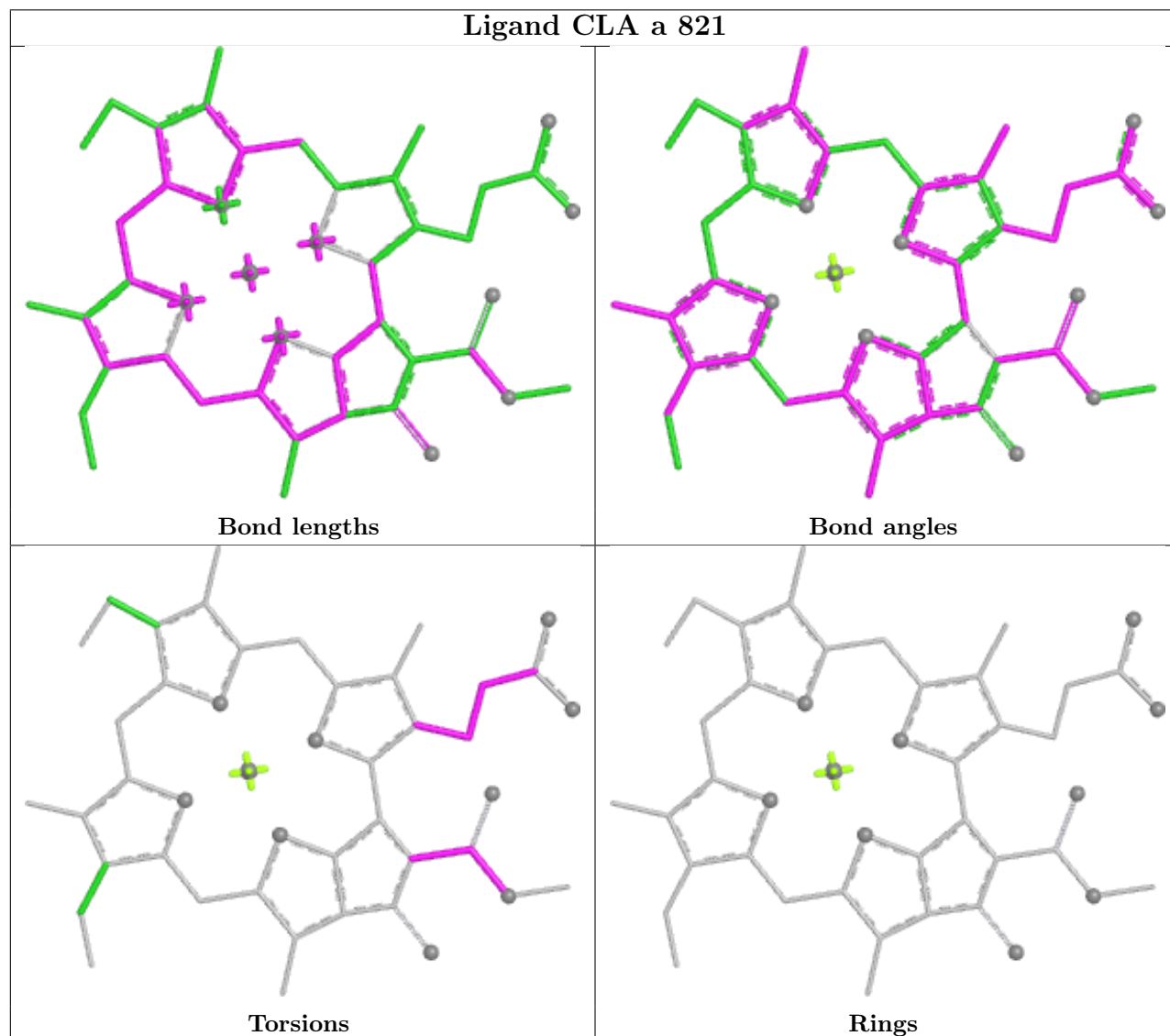
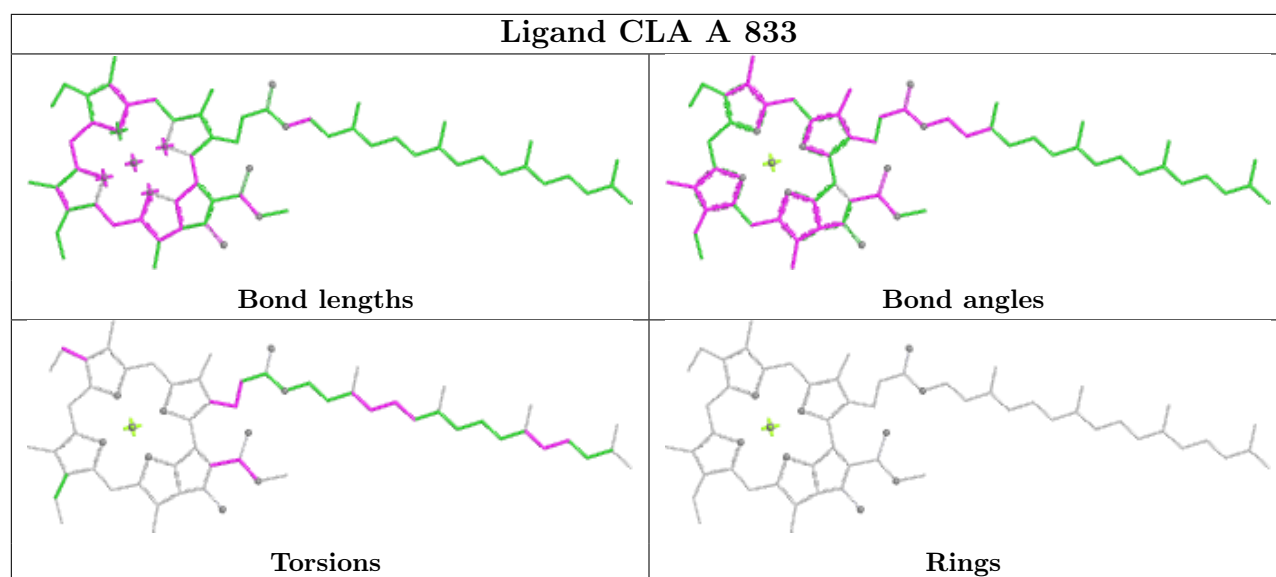


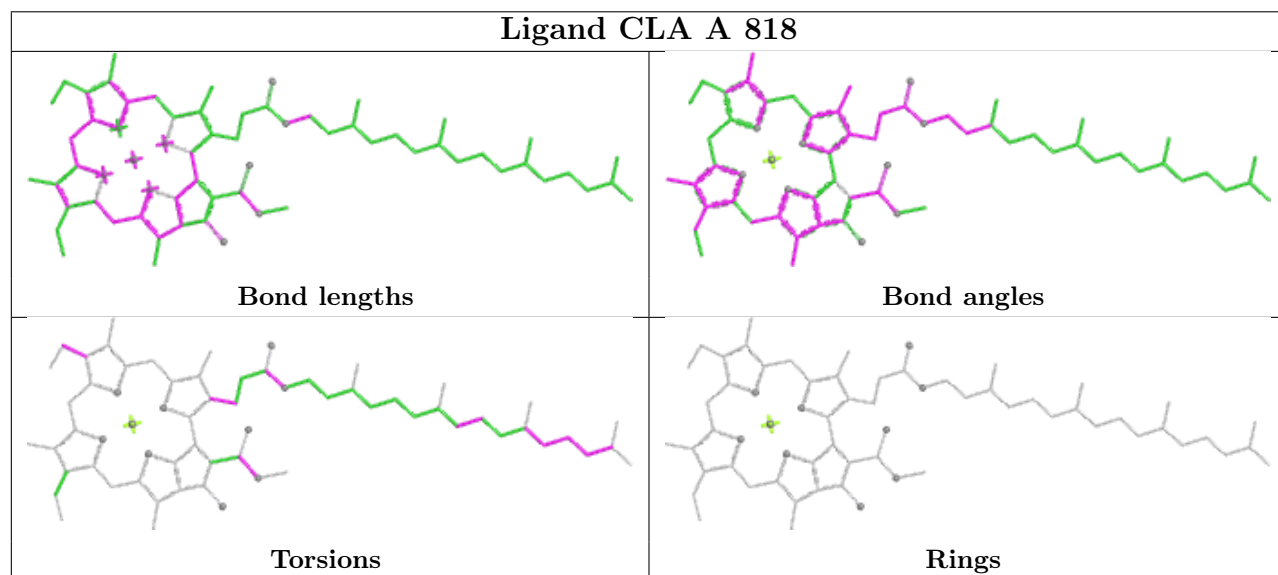
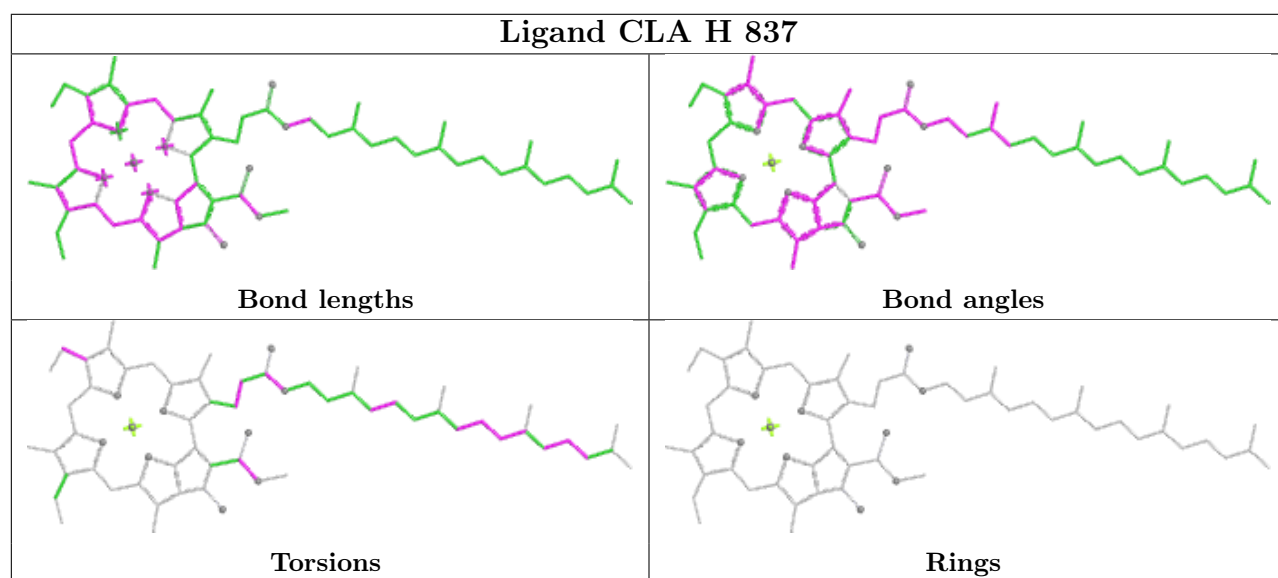
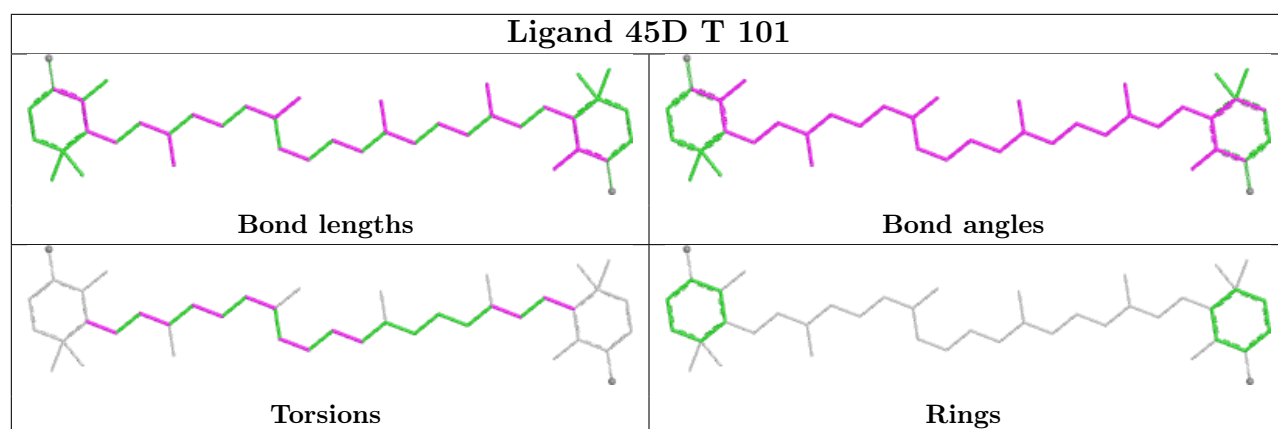
Torsions

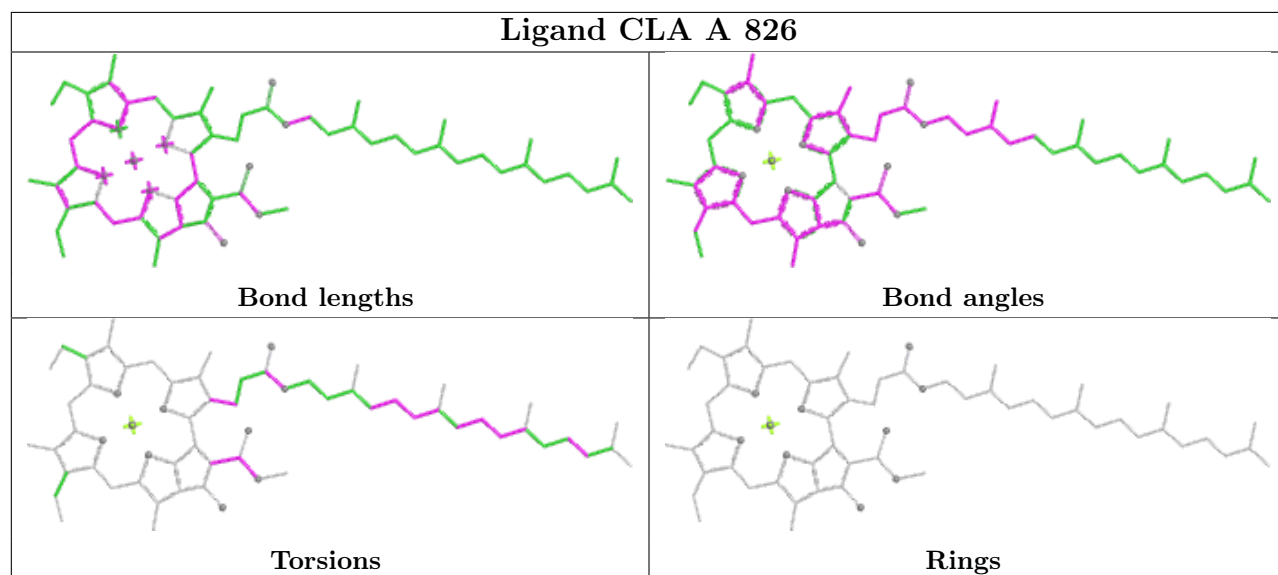
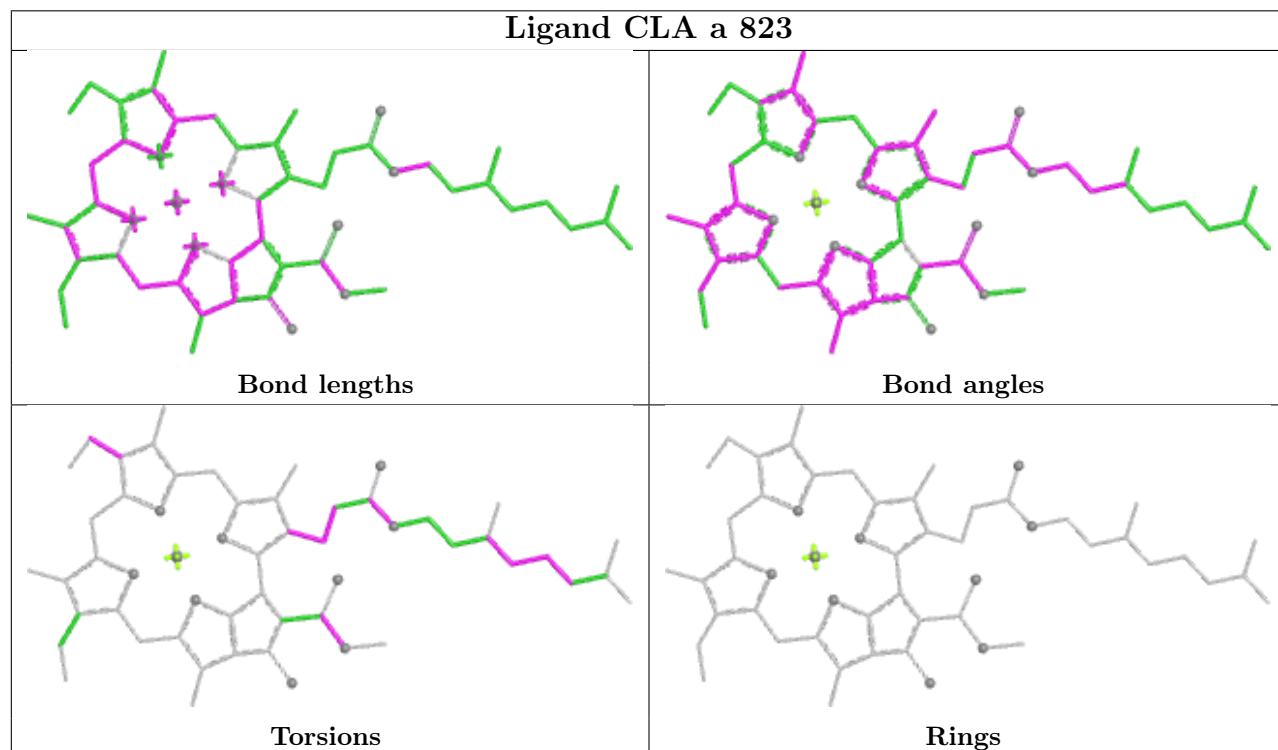
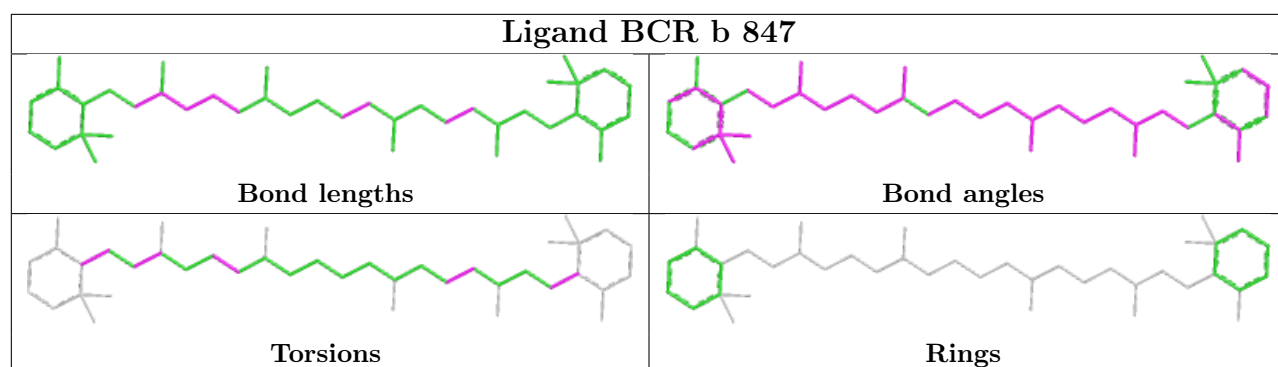


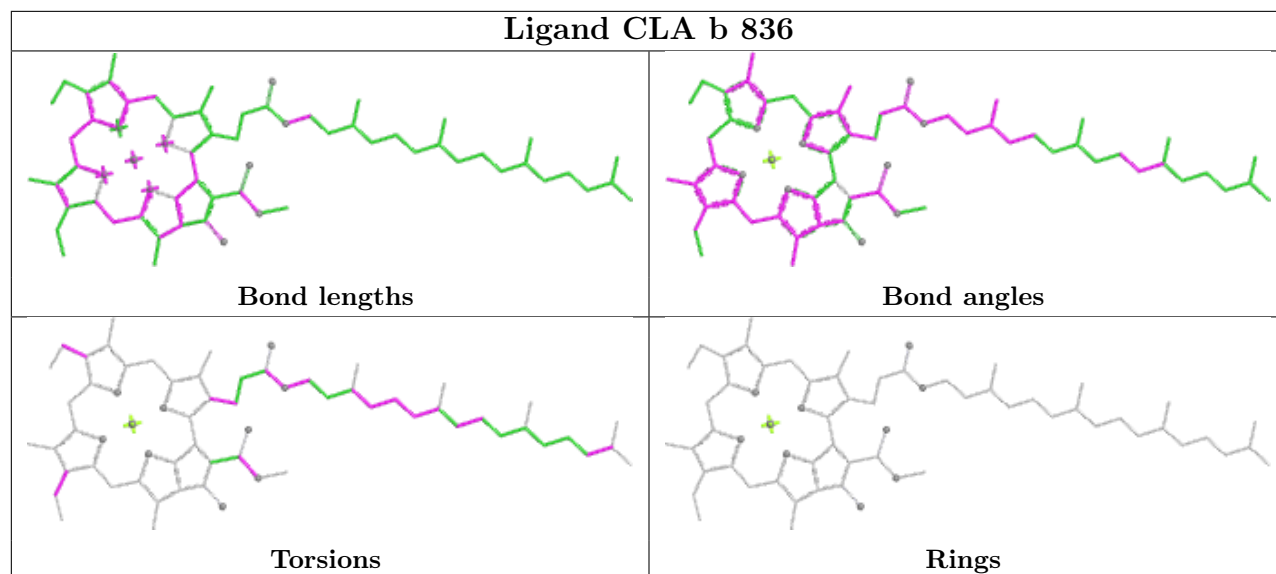
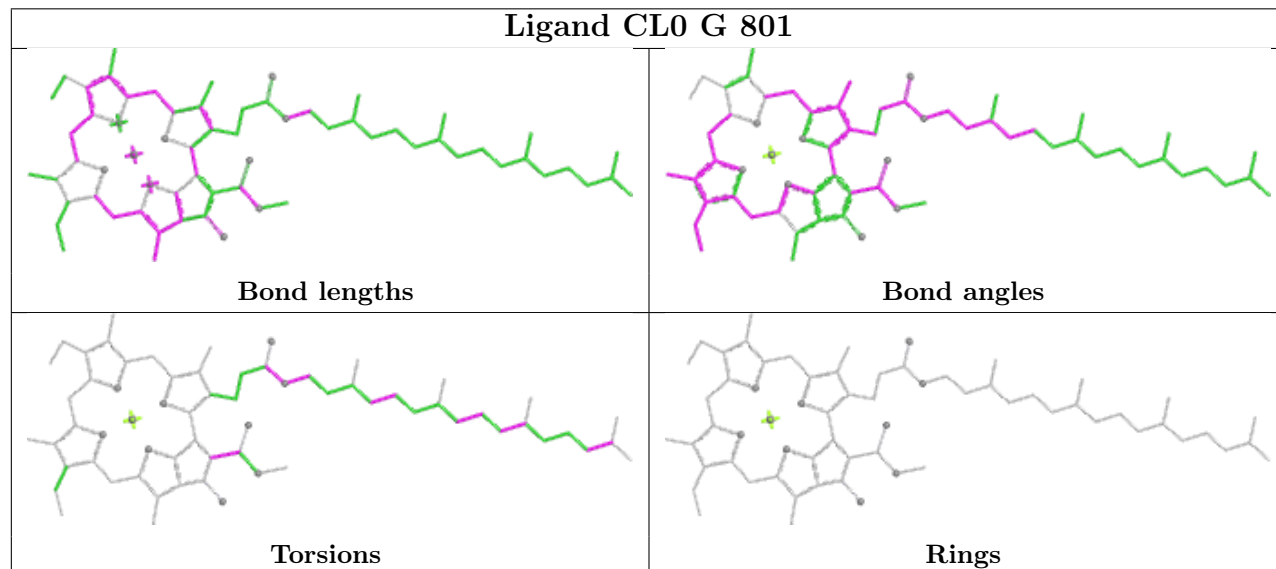
Rings



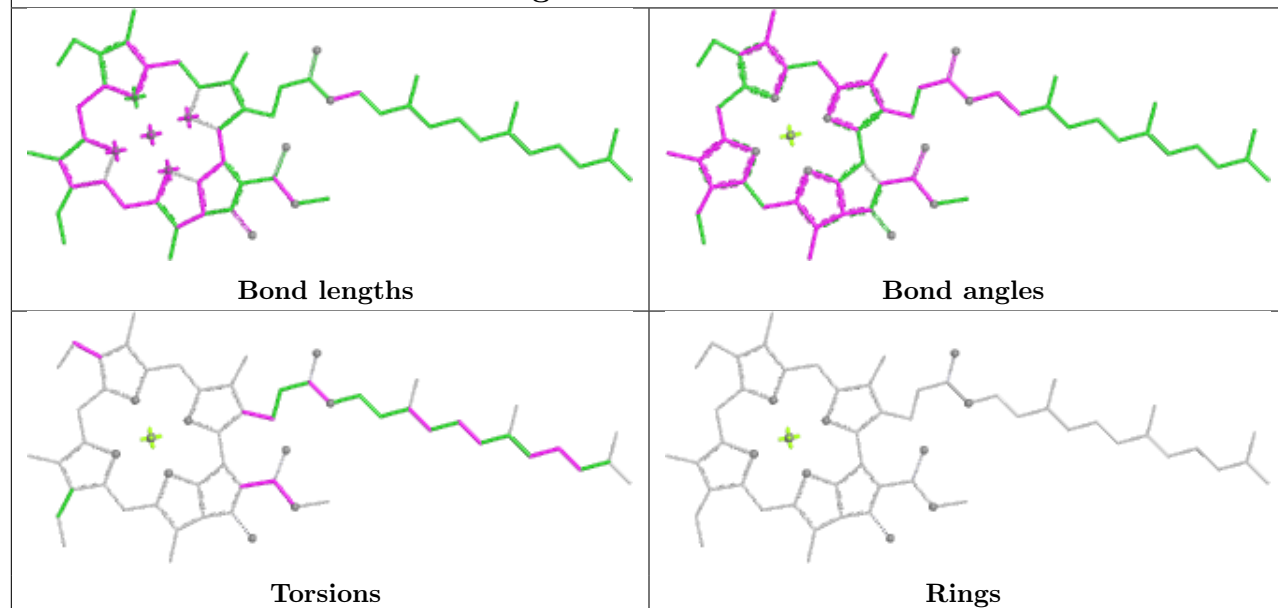




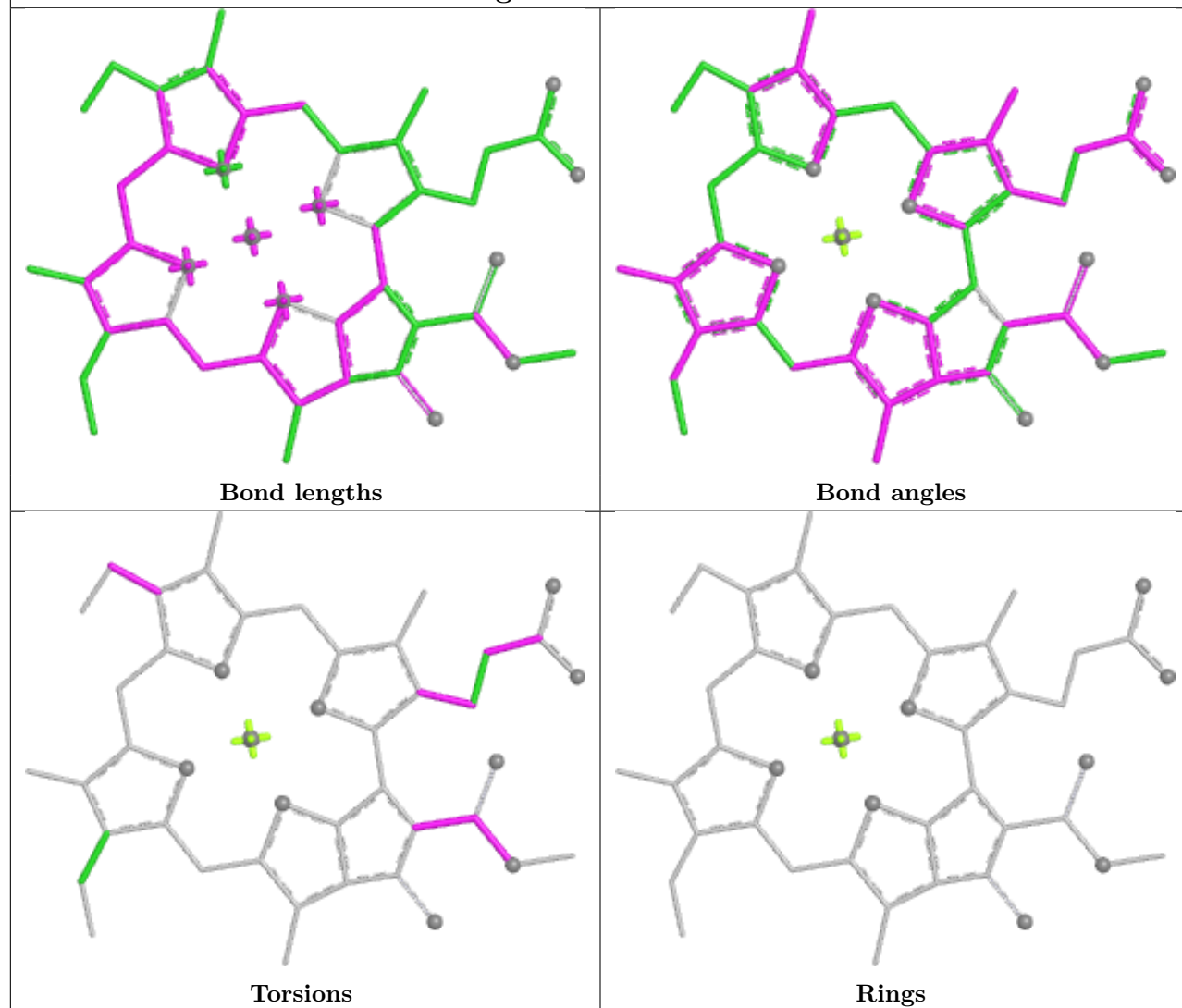


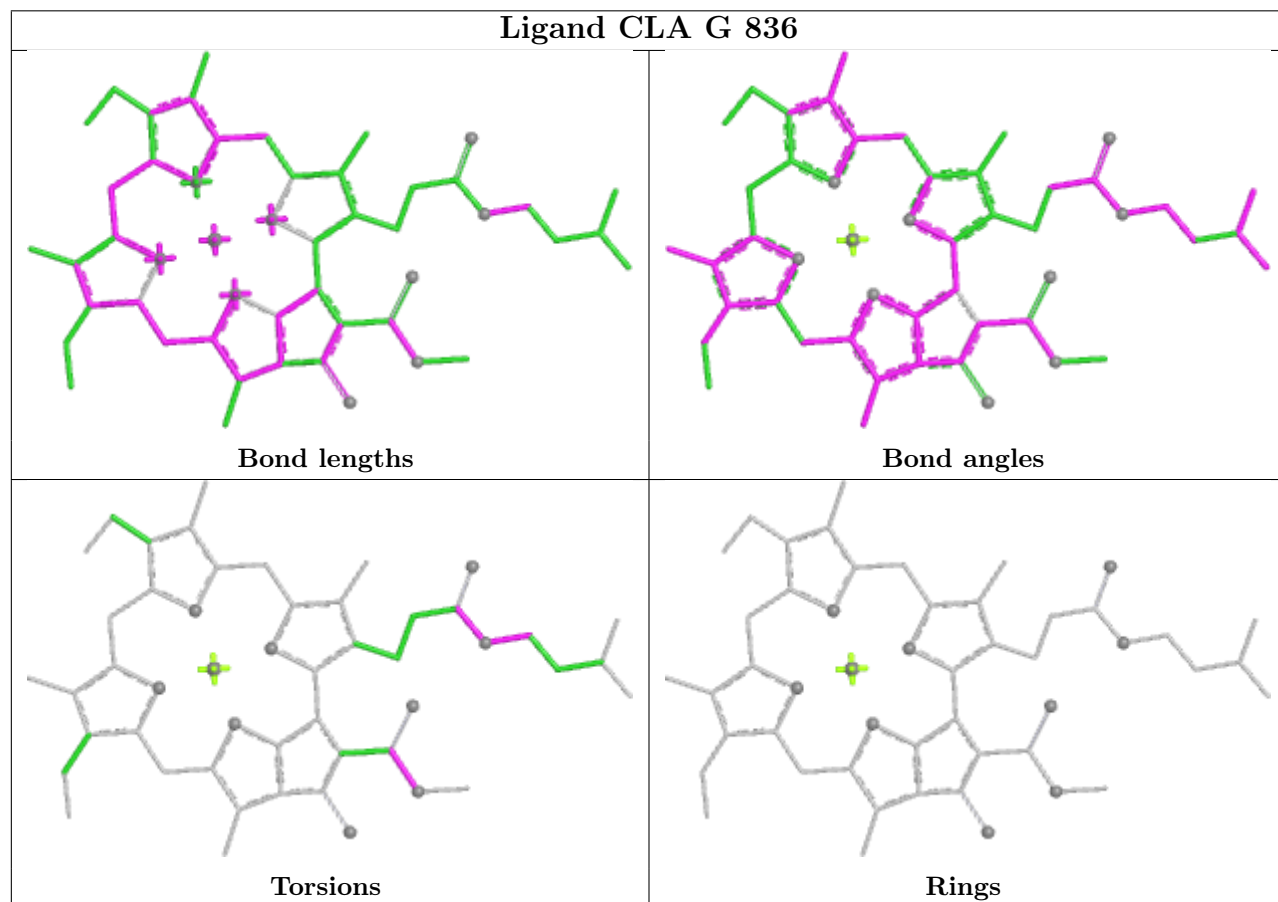
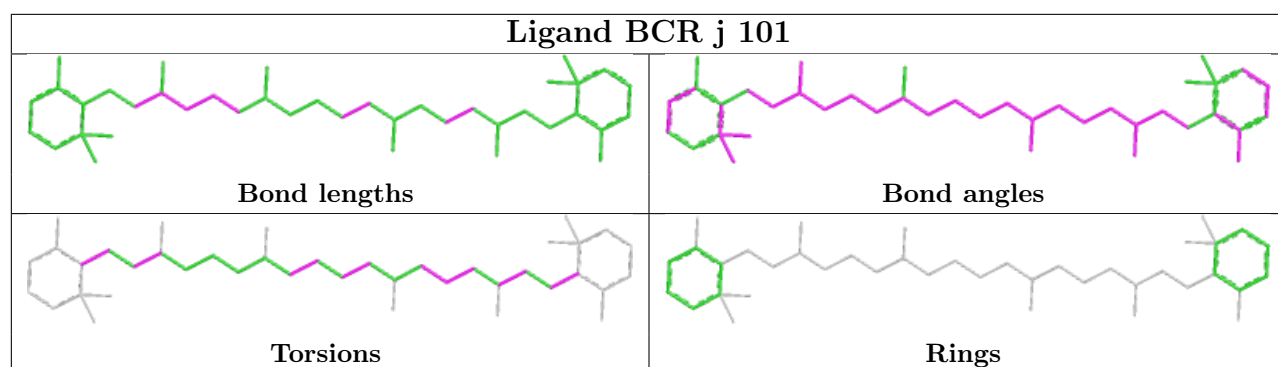
Ligand CLA b 836**Ligand CL0 G 801**

Ligand CLA B 833

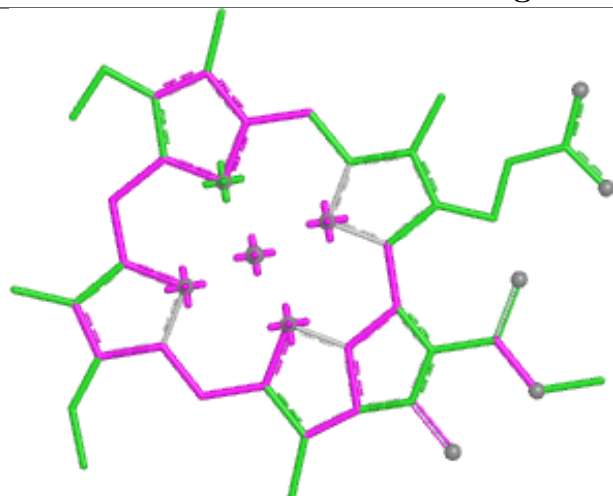


Ligand CLA J 103

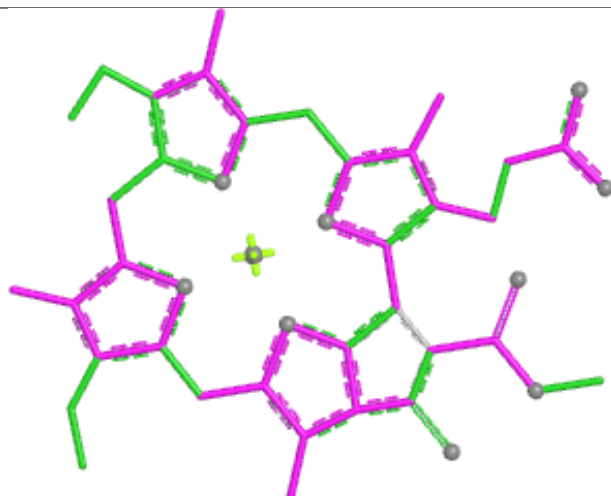




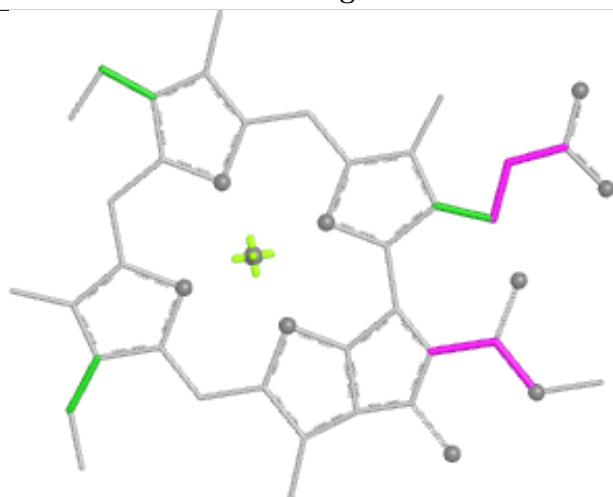
Ligand CLA A 814



Bond lengths



Bond angles

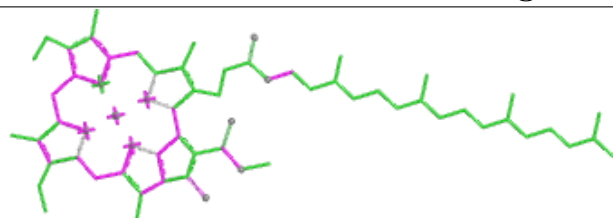


Torsions

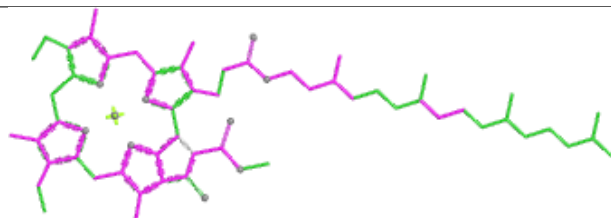


Rings

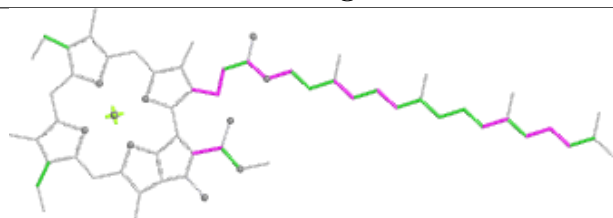
Ligand CLA b 821



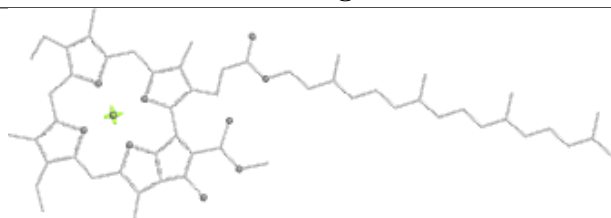
Bond lengths



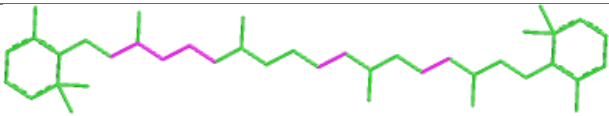
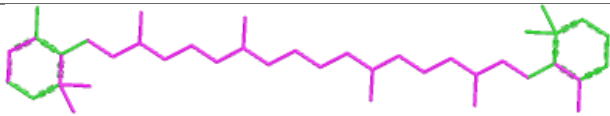
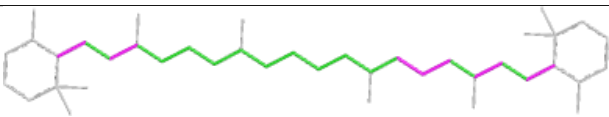
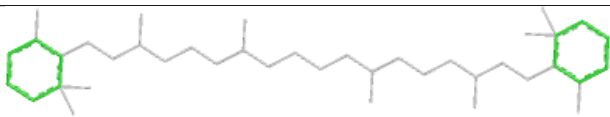
Bond angles

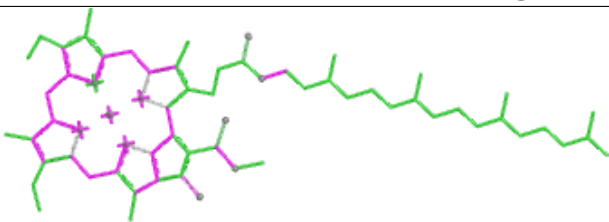
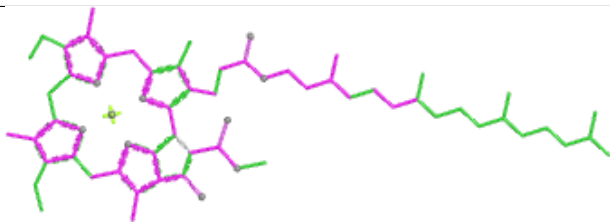
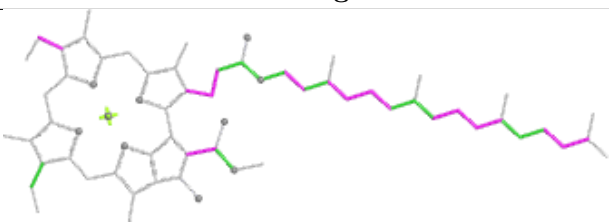
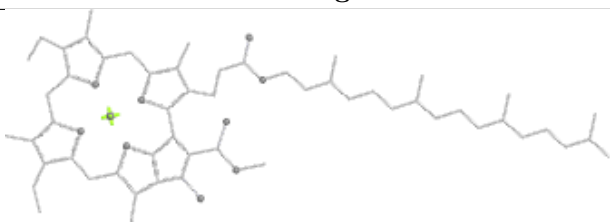


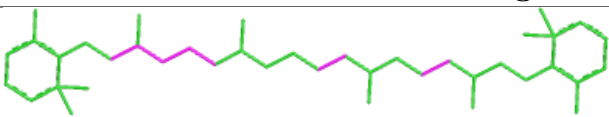
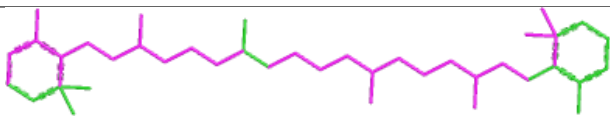
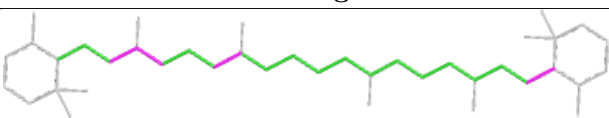
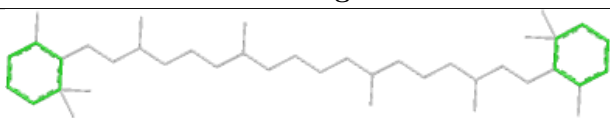
Torsions

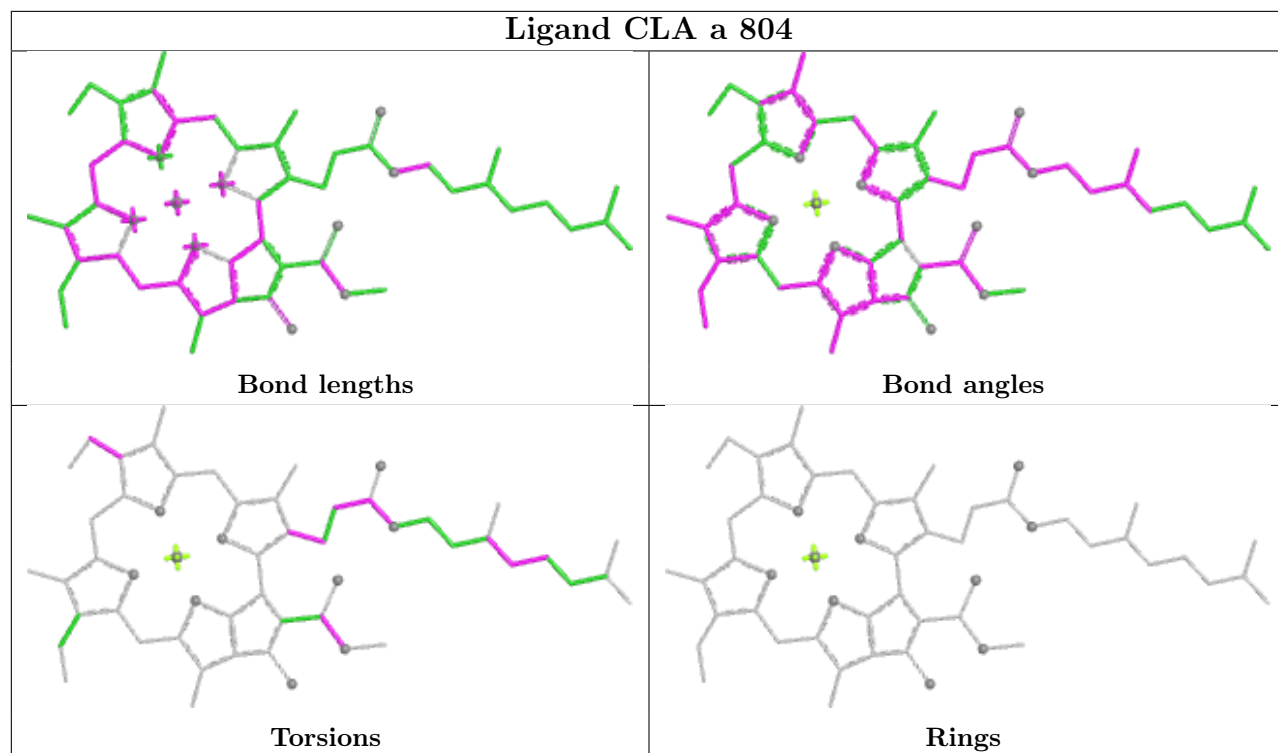
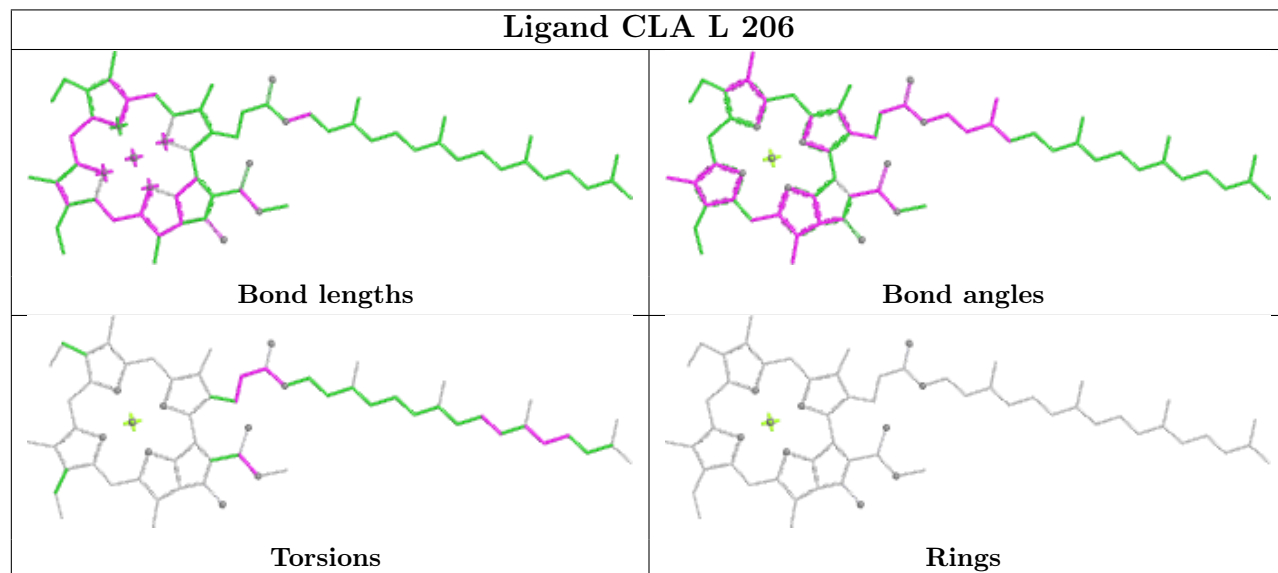


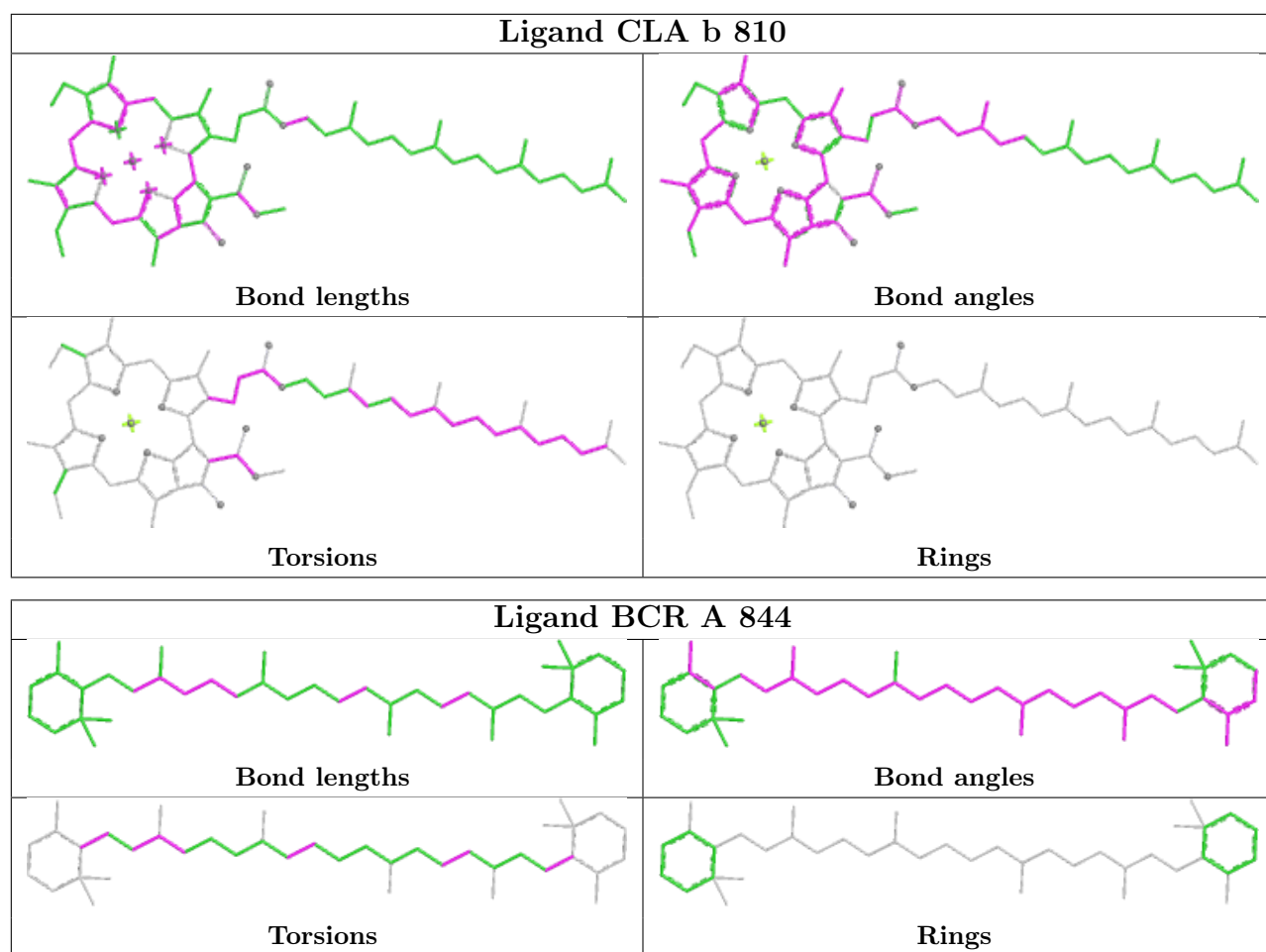
Rings

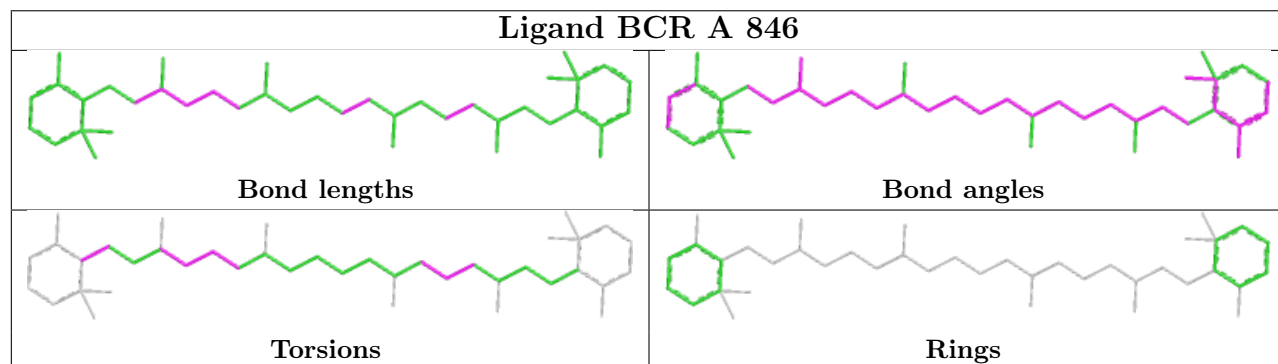
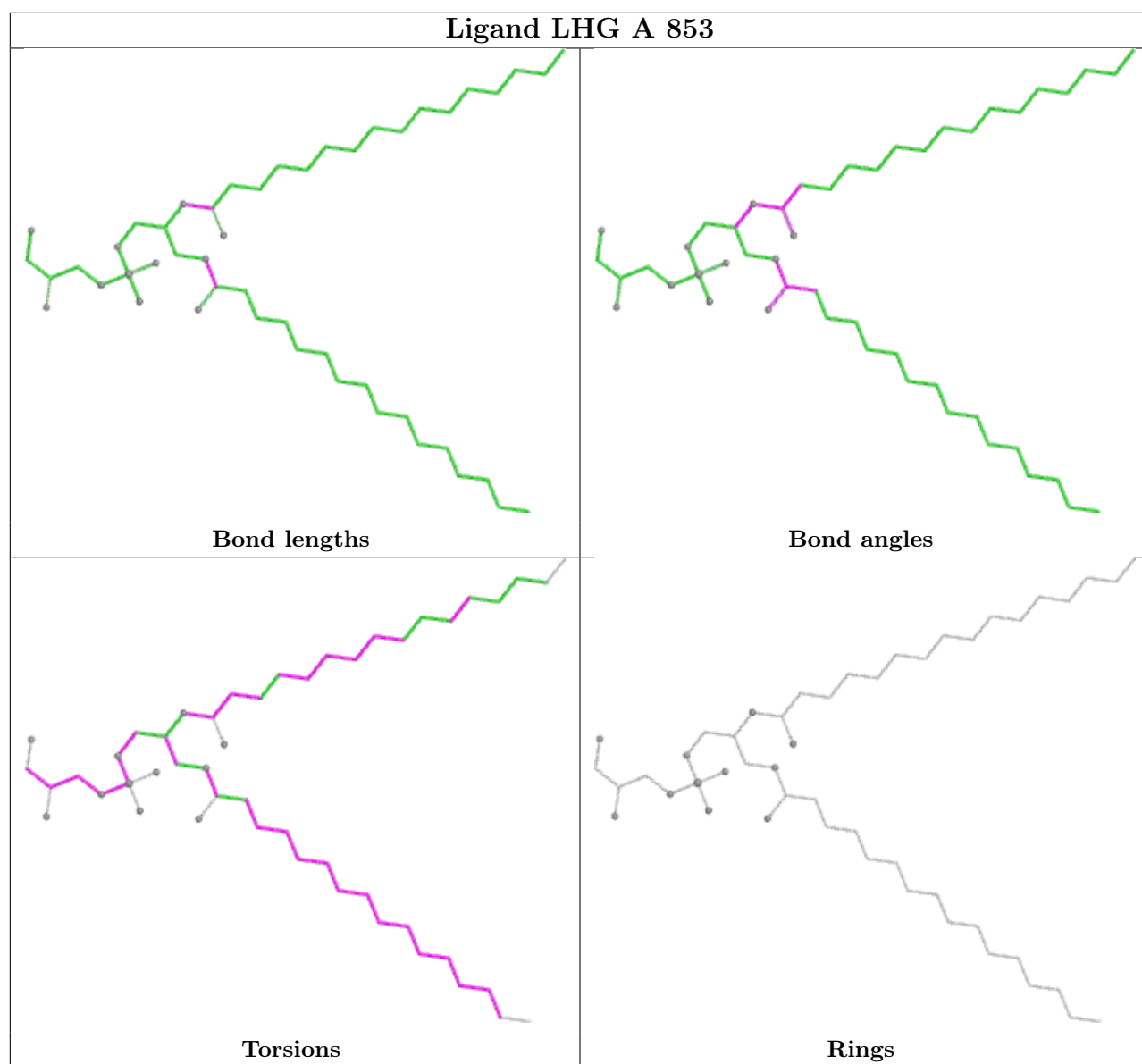
Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

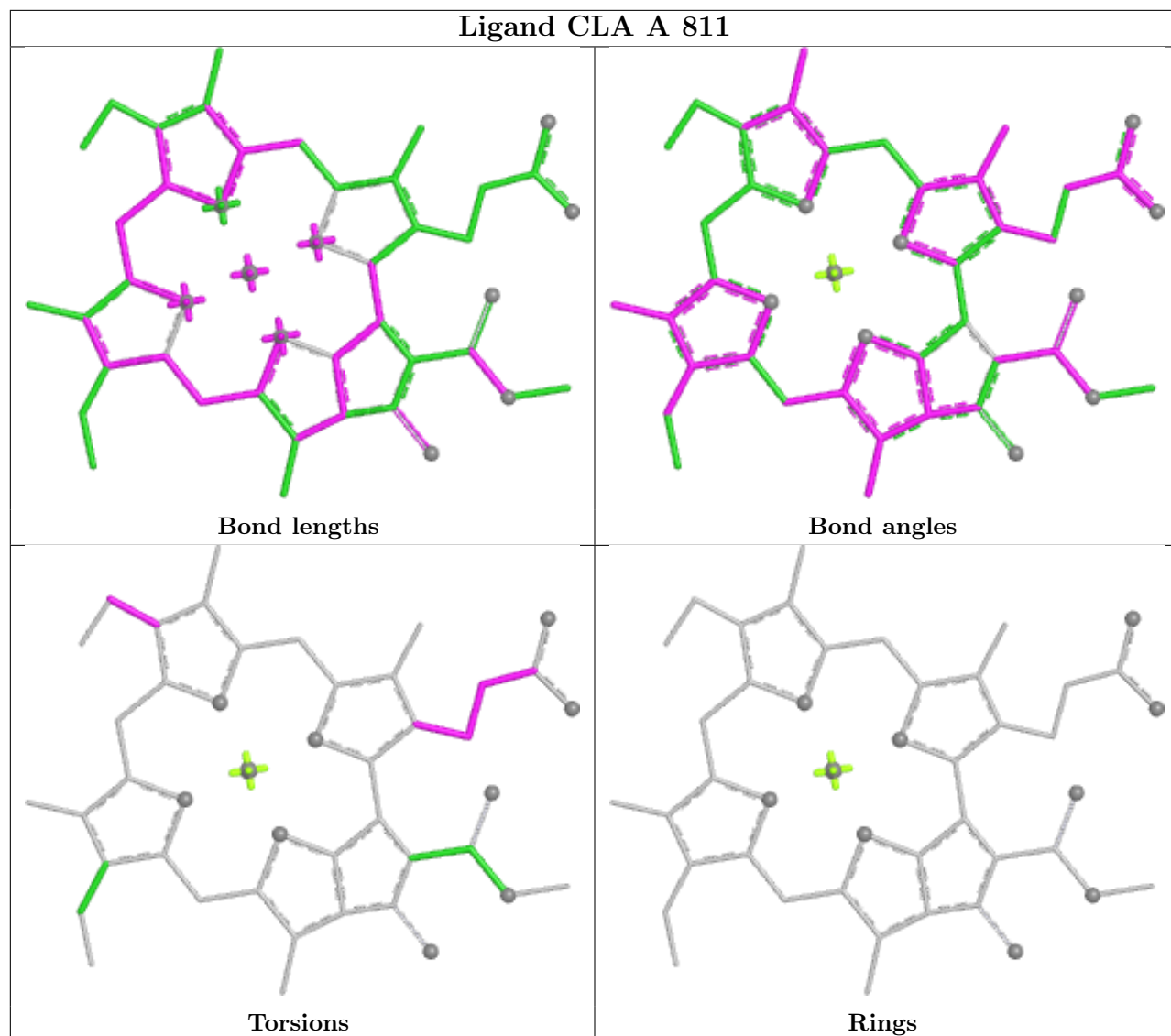
Ligand BCR I 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA a 804**Ligand CLA L 206**

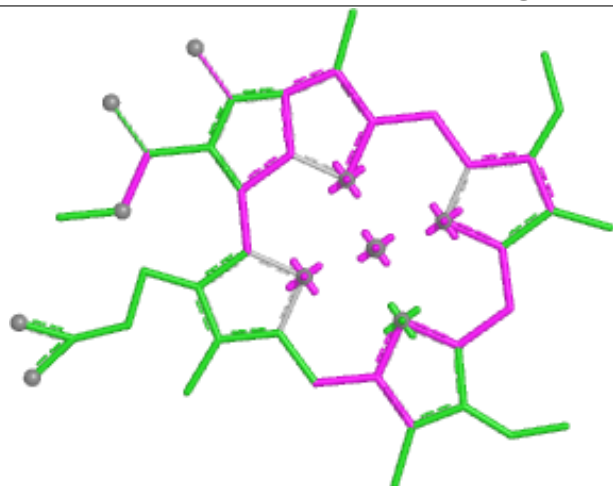




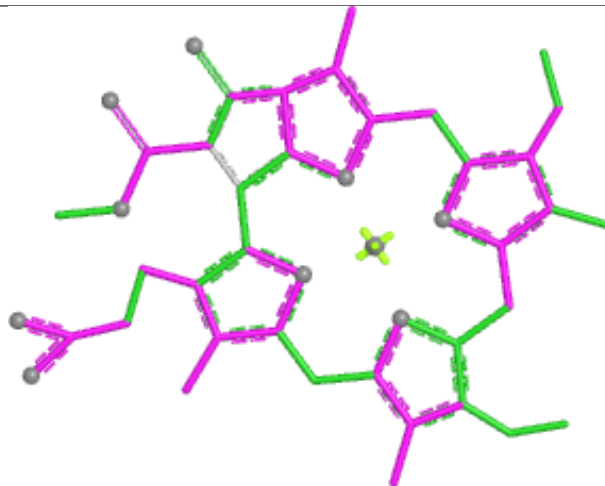
Ligand CLA A 811



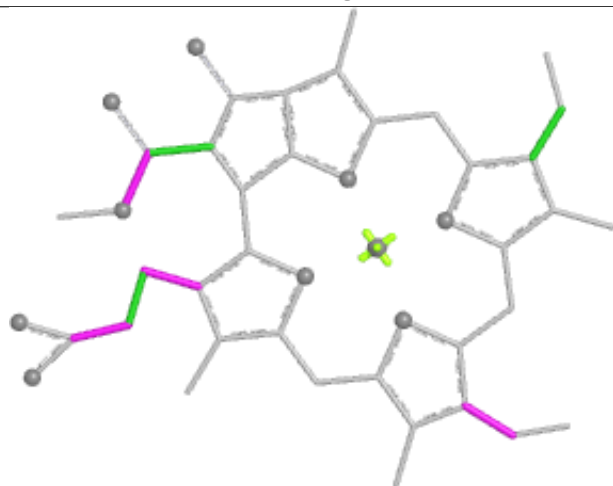
Ligand CLA P 203



Bond lengths



Bond angles

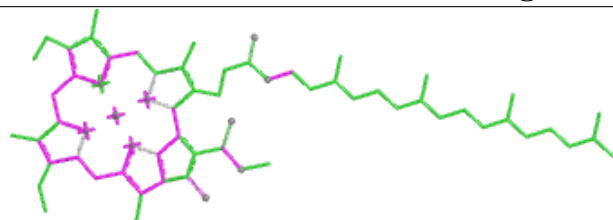


Torsions

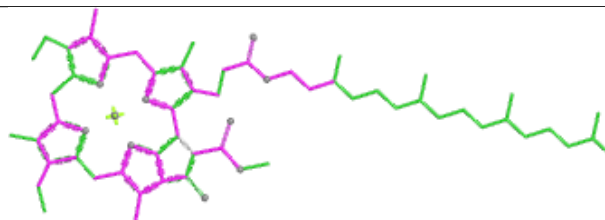


Rings

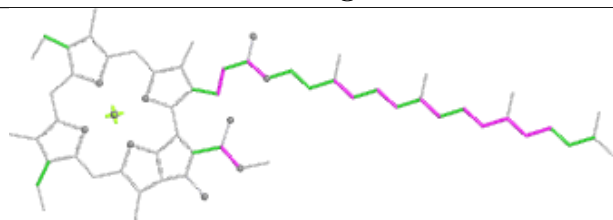
Ligand CLA a 820



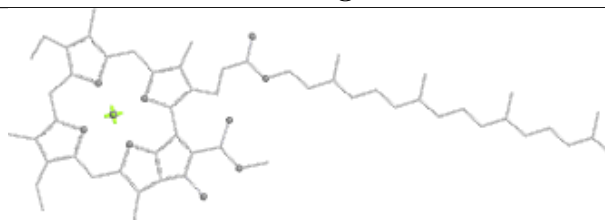
Bond lengths



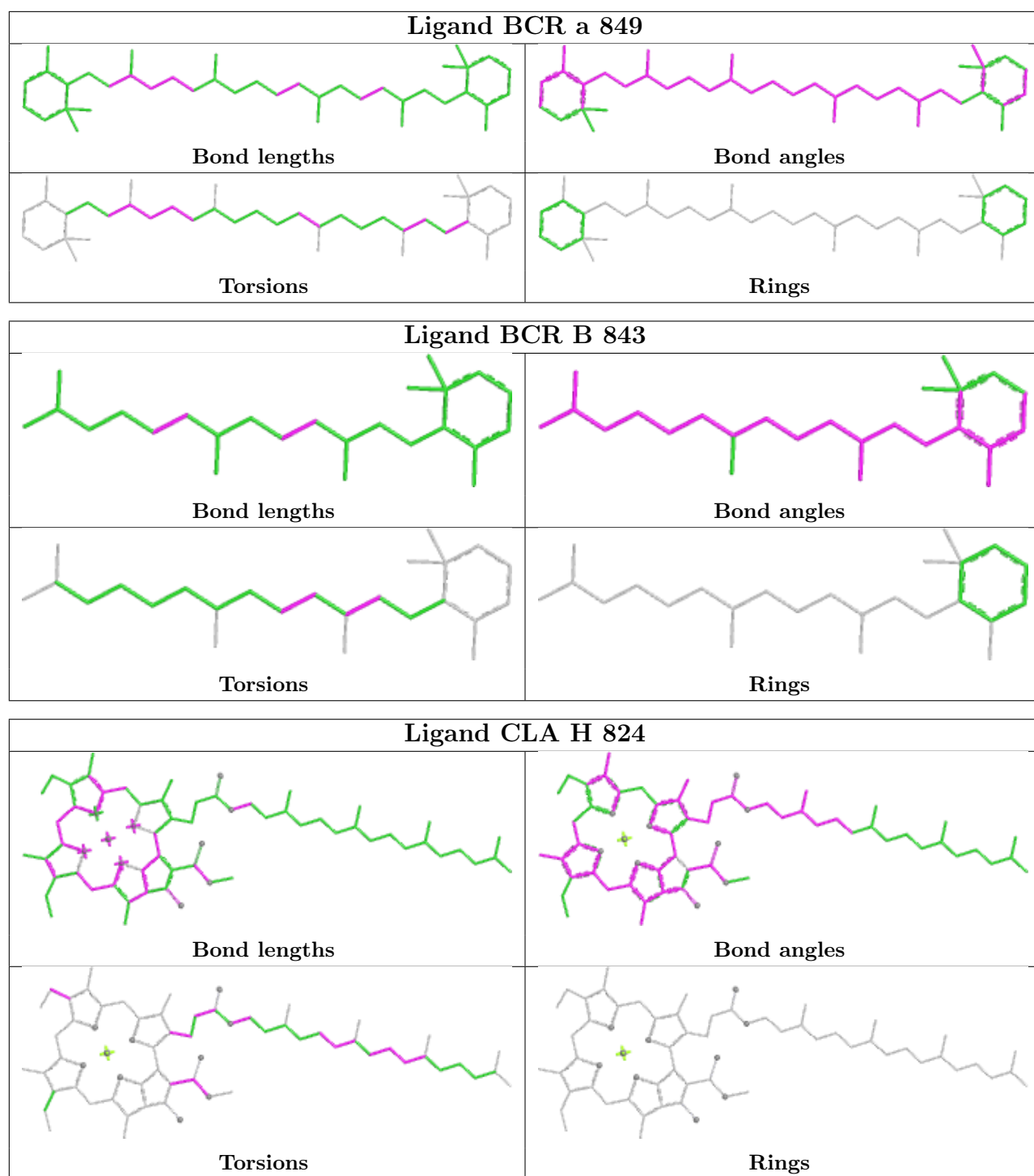
Bond angles

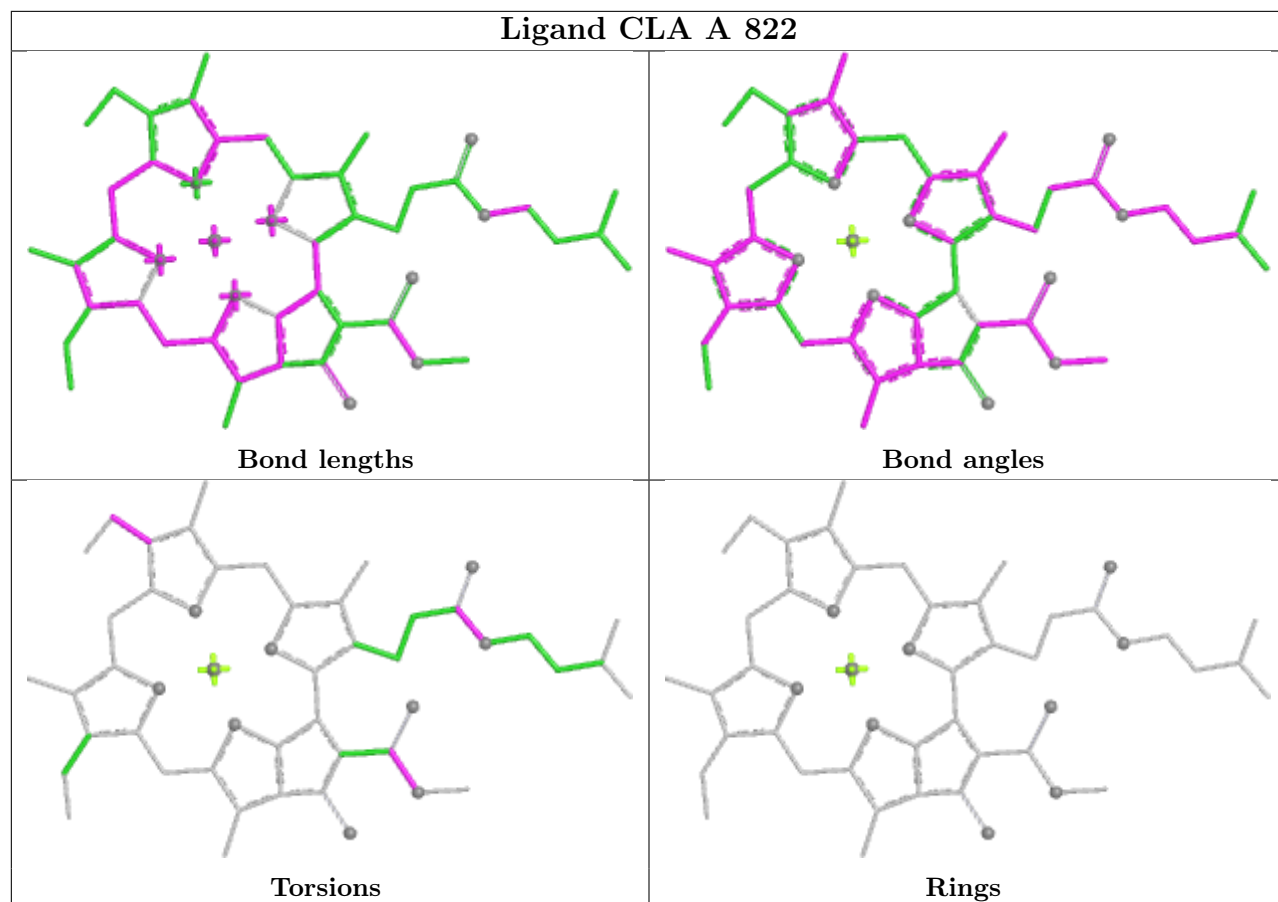


Torsions

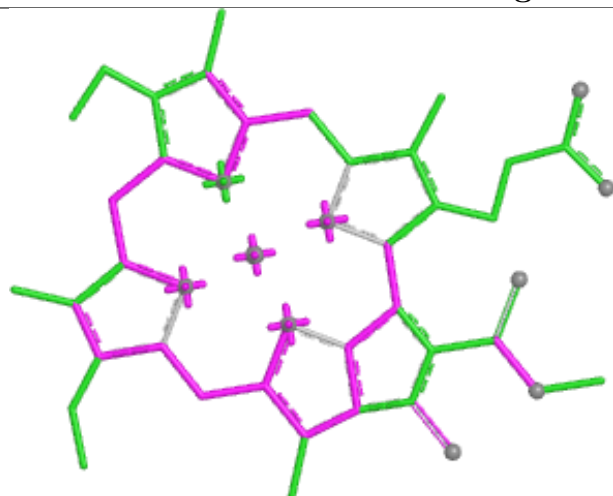


Rings

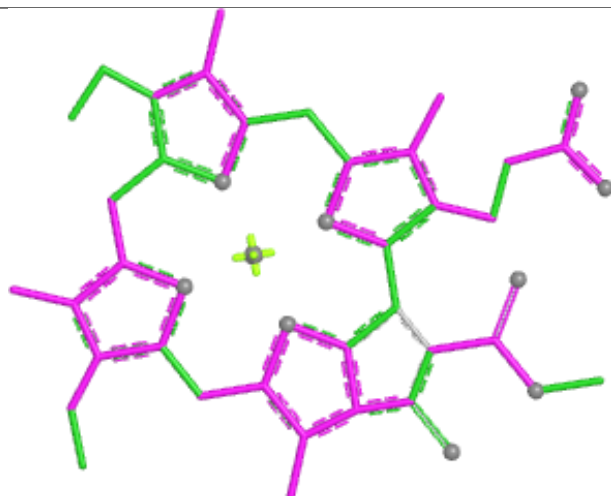




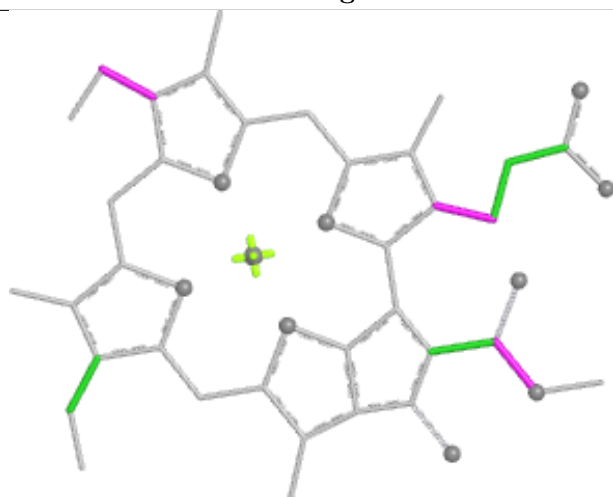
Ligand CLA B 832



Bond lengths



Bond angles

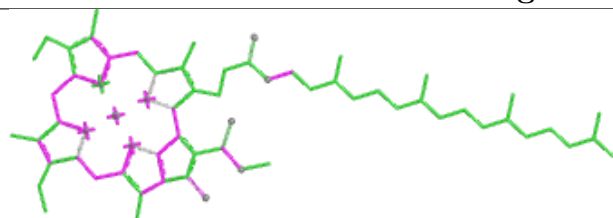


Torsions

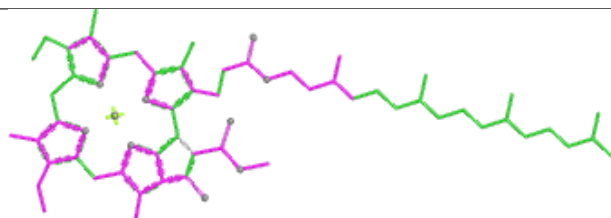


Rings

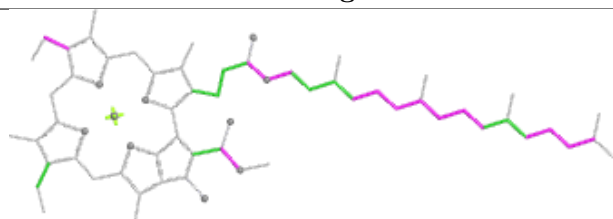
Ligand CLA b 804



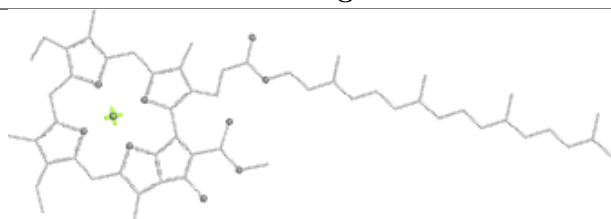
Bond lengths



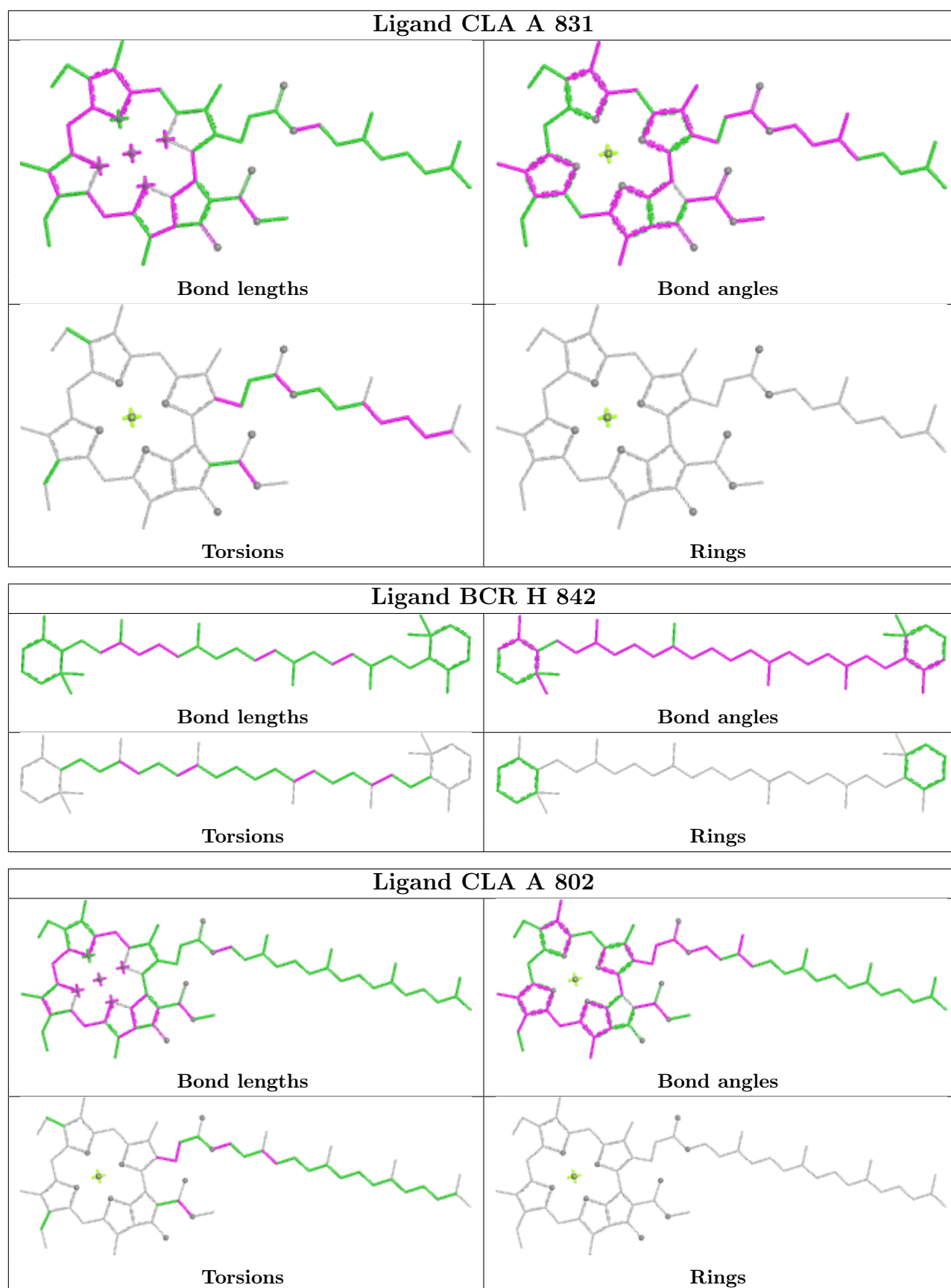
Bond angles

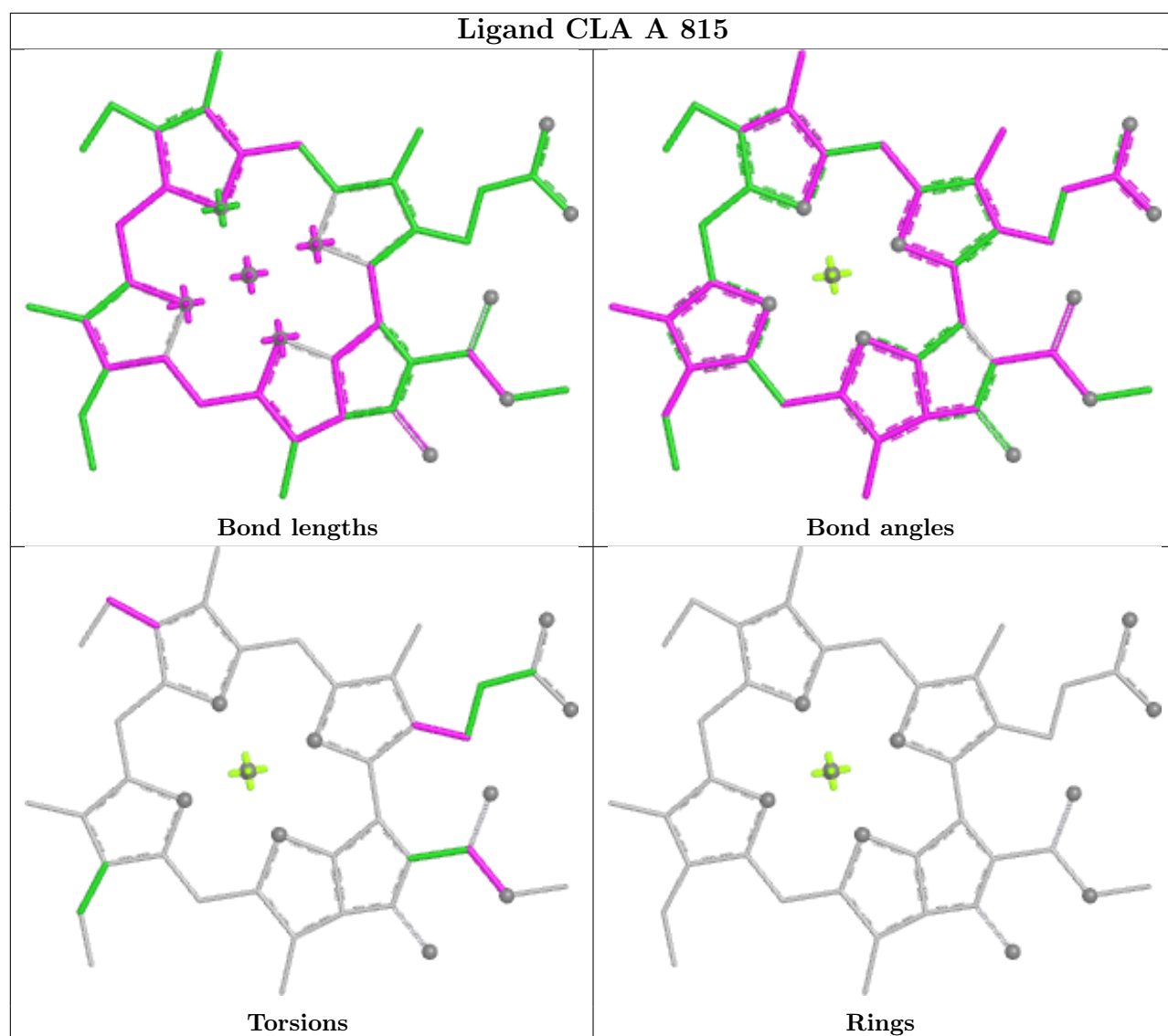


Torsions

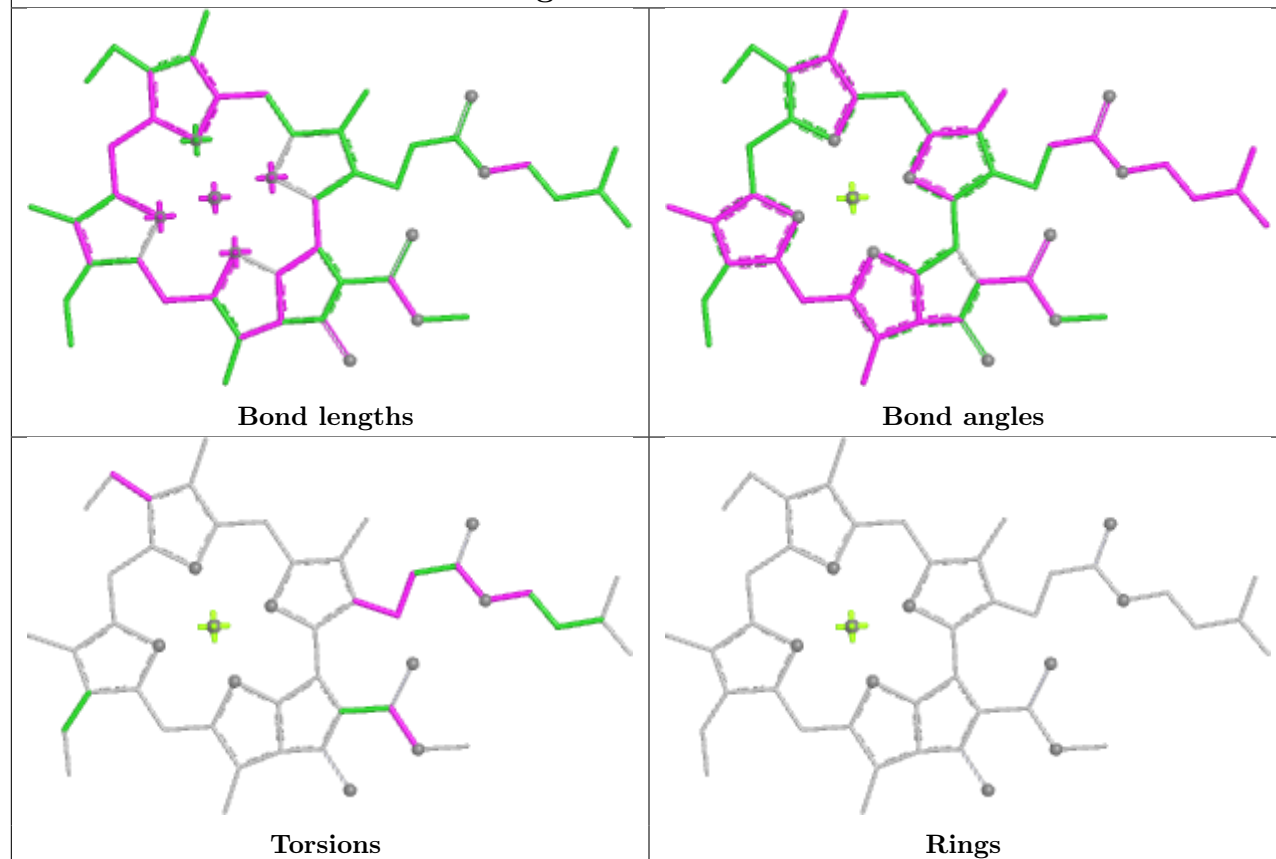


Rings

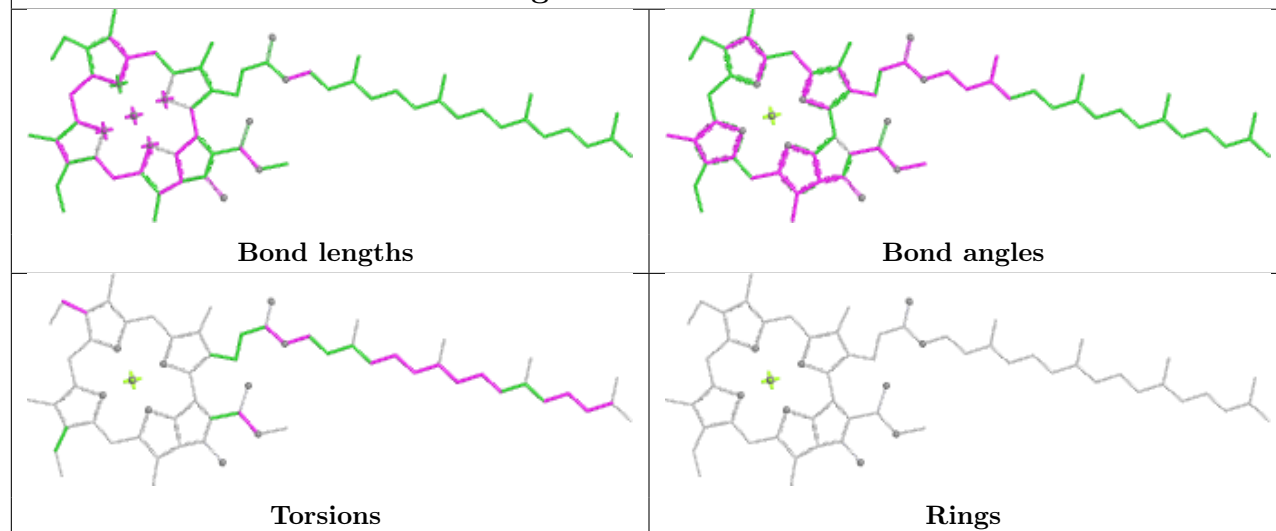


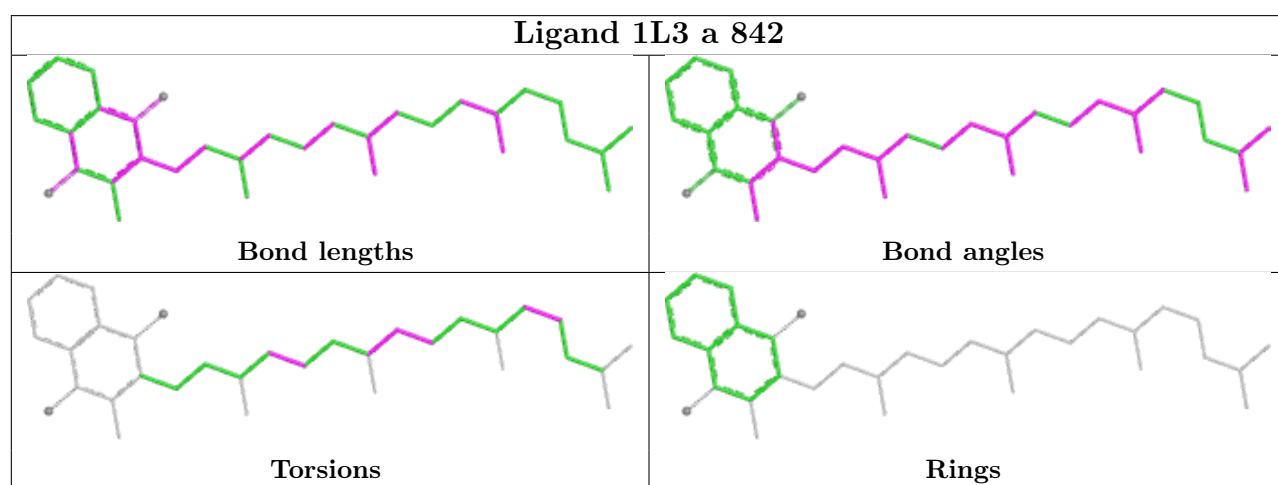
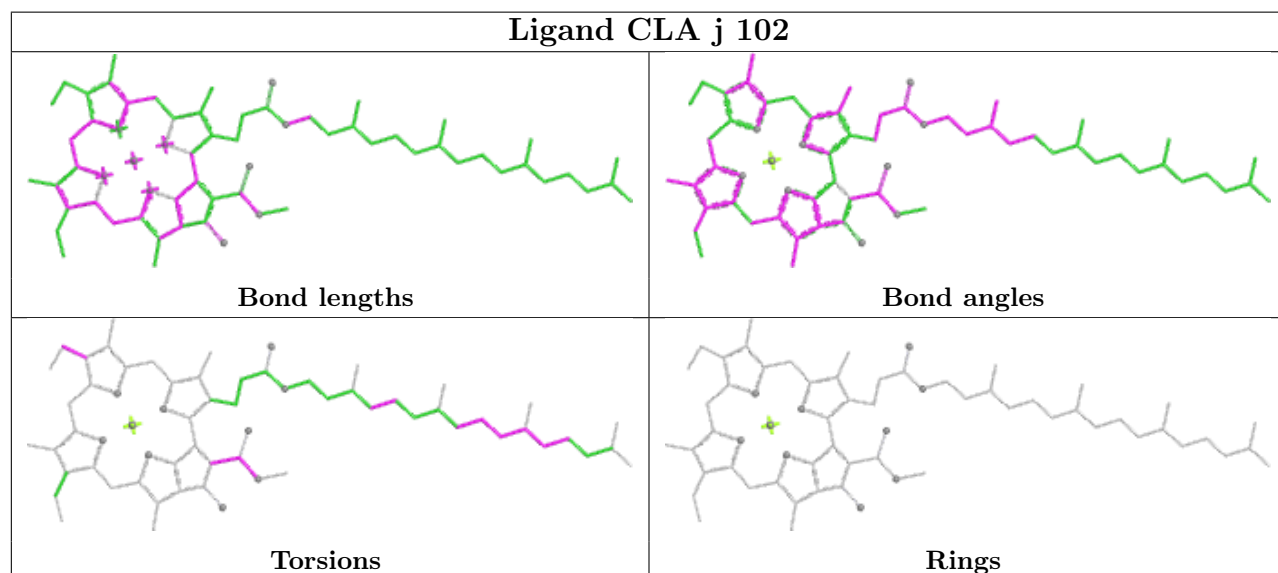
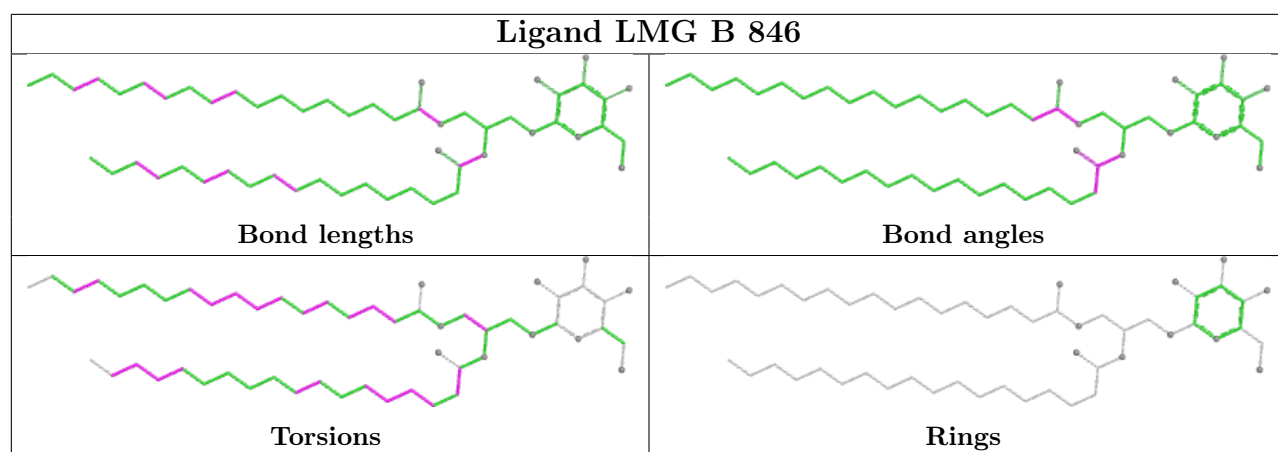


Ligand CLA a 840

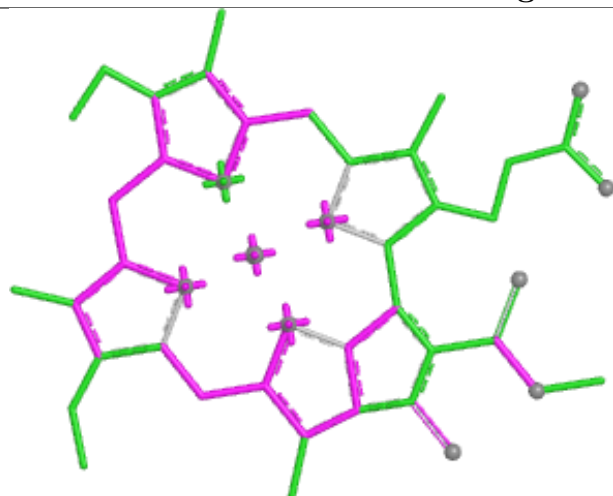


Ligand CLA H 804

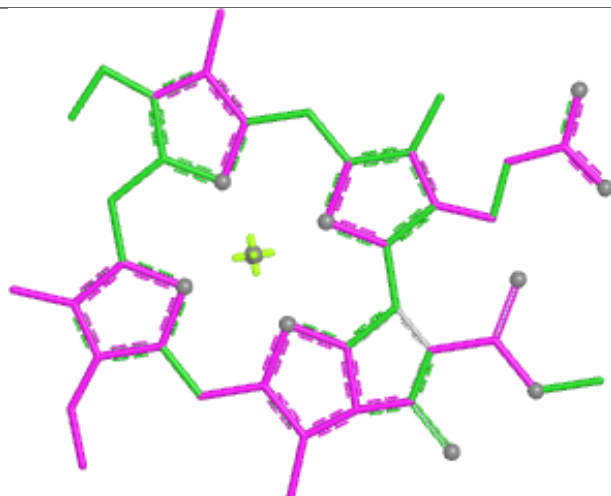




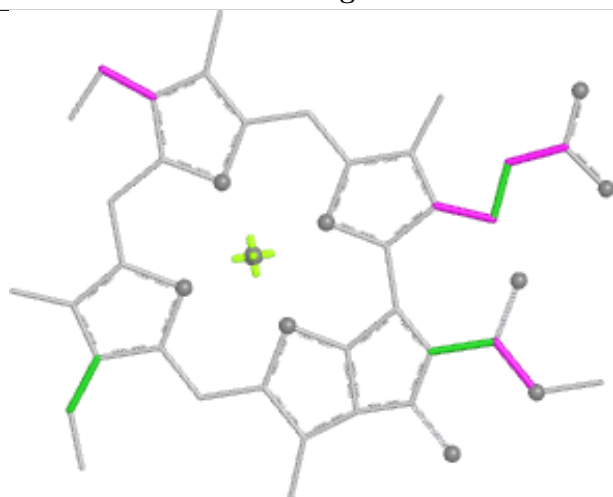
Ligand CLA b 834



Bond lengths



Bond angles

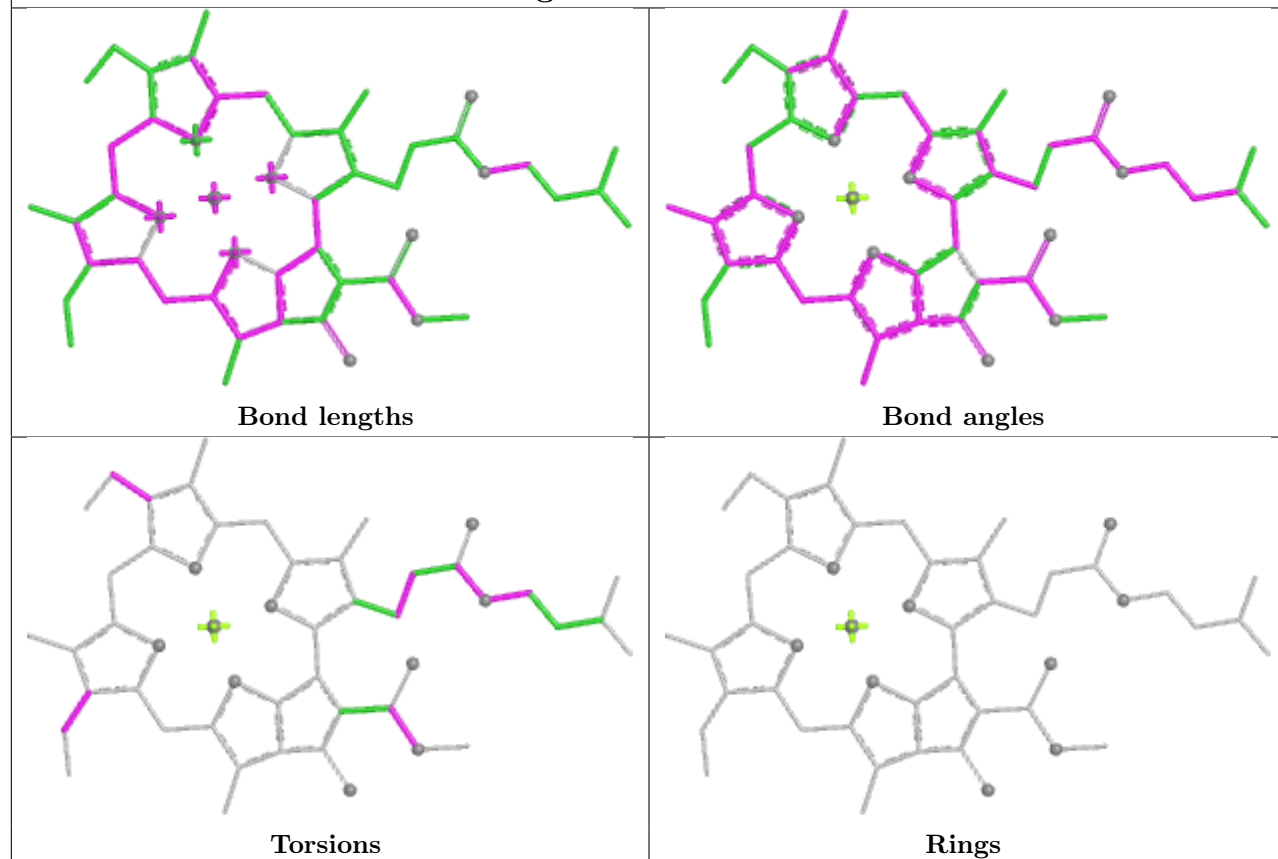


Torsions

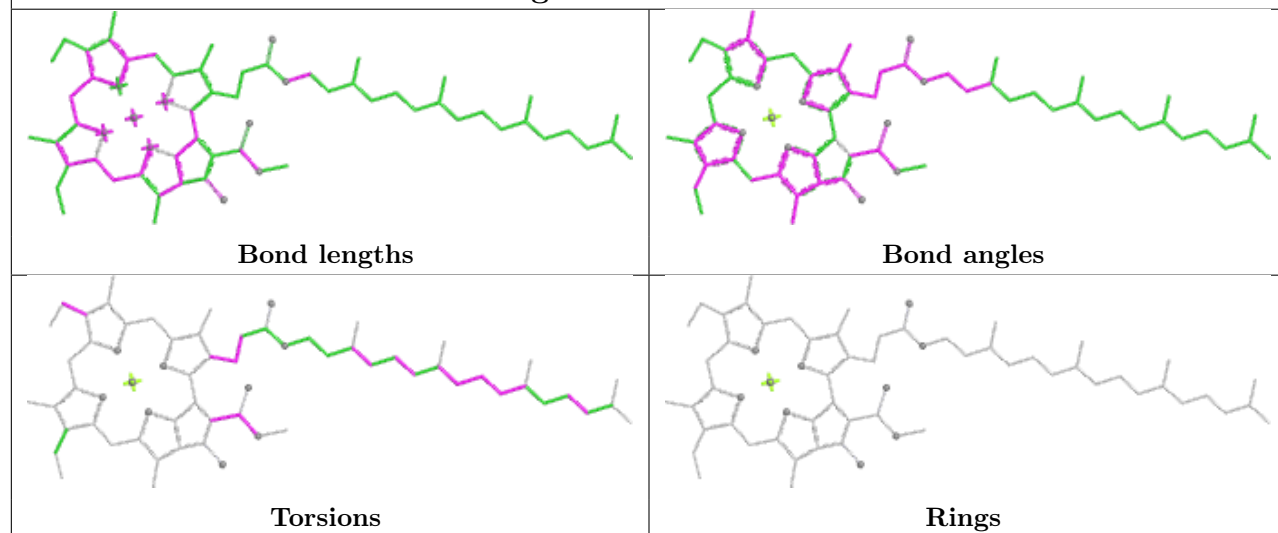


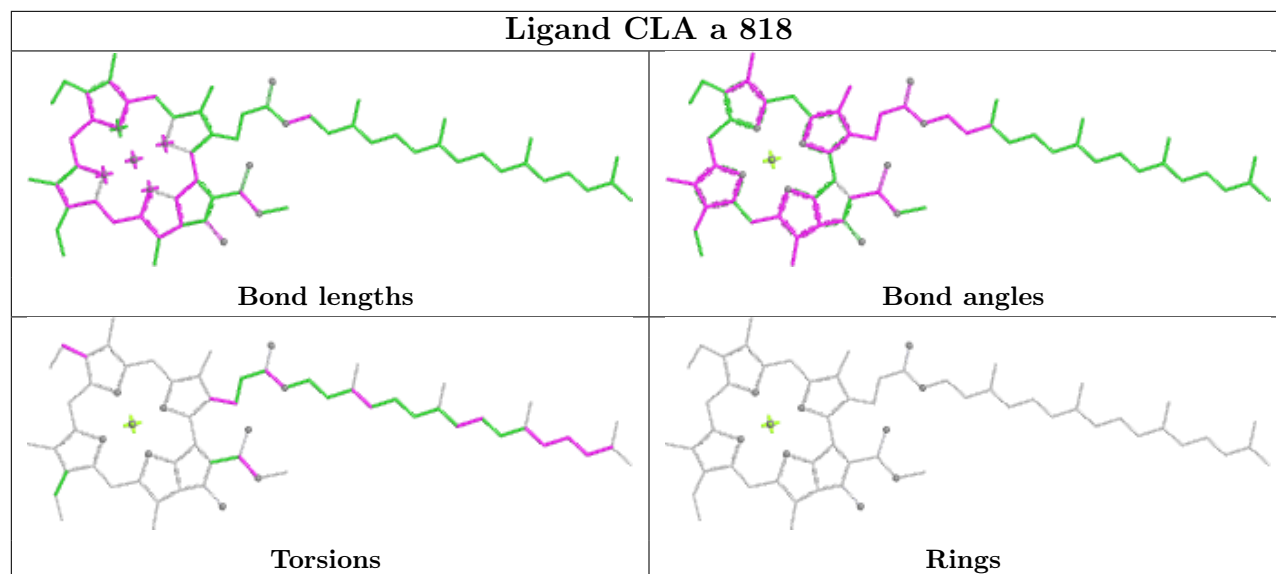
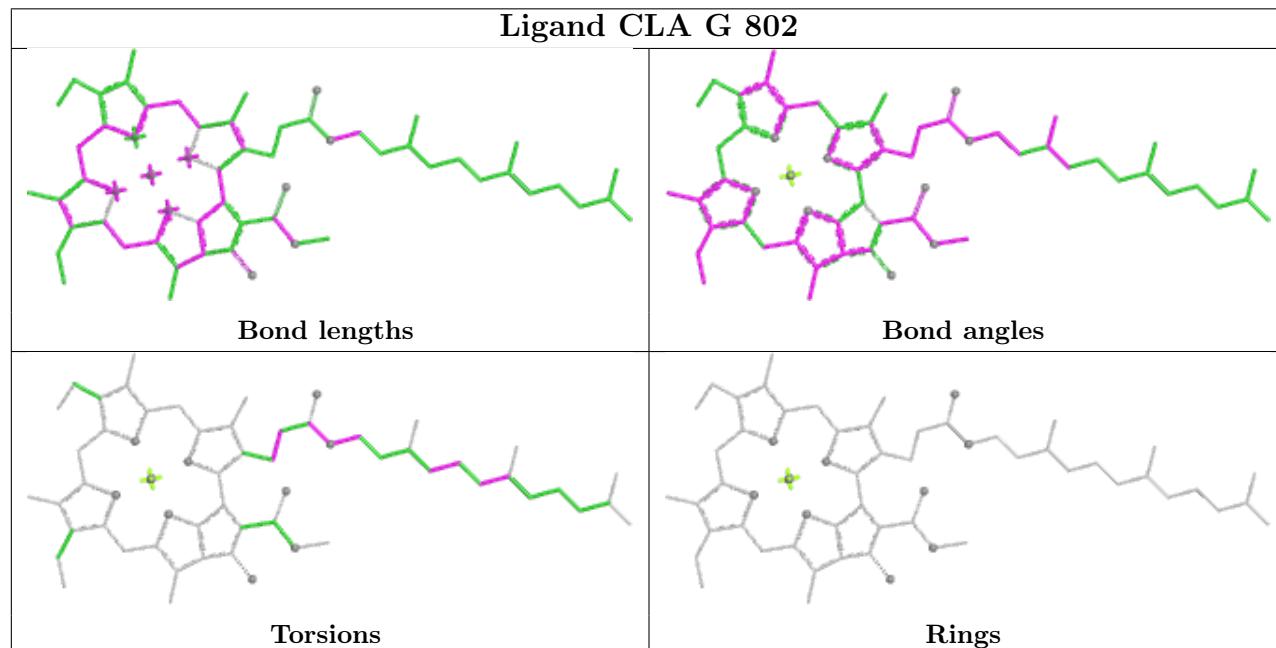
Rings

Ligand CLA a 812

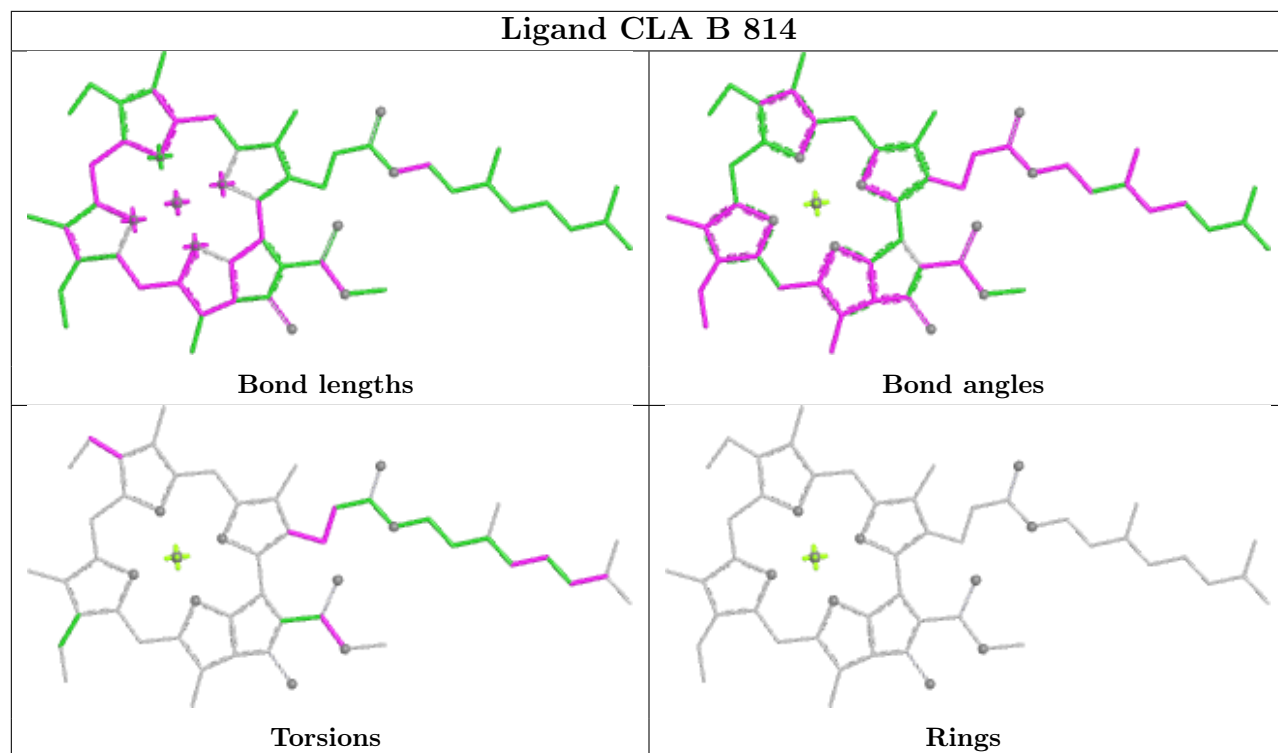


Ligand CLA H 823

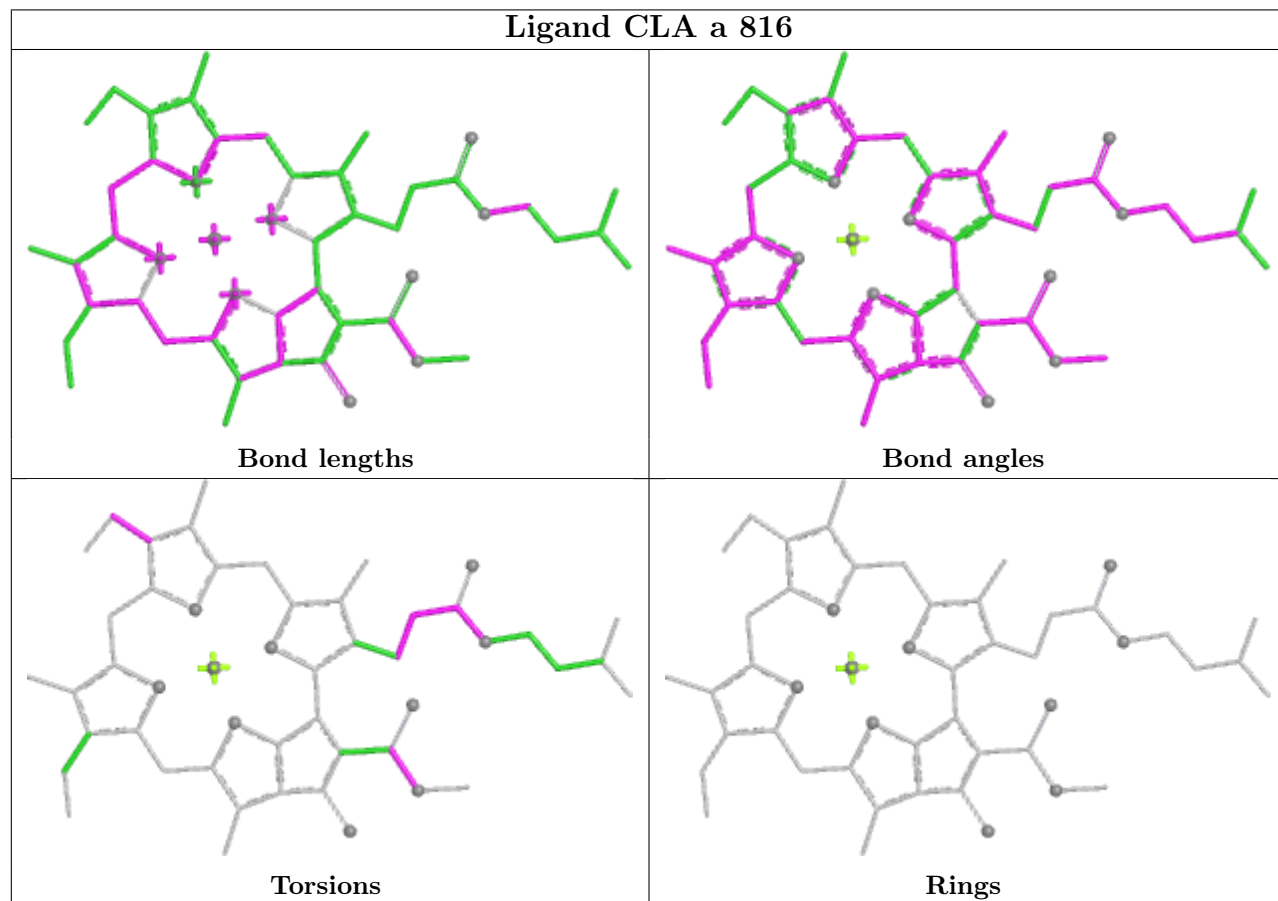


Ligand CLA a 818**Ligand CLA G 802**

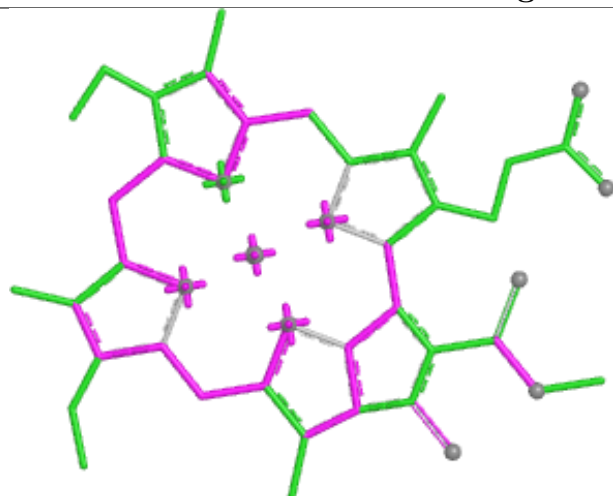
Ligand CLA B 814



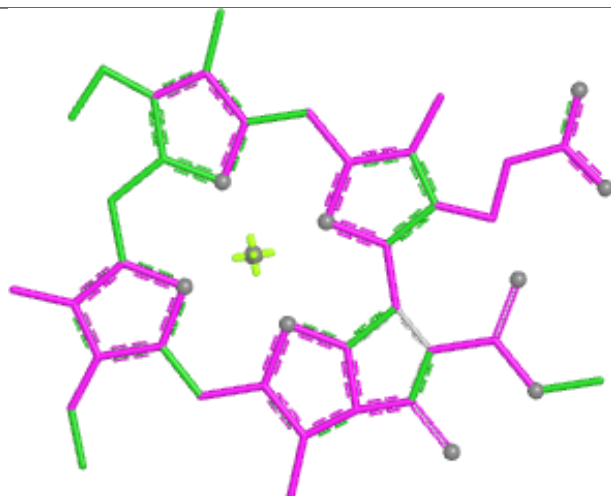
Ligand CLA a 816



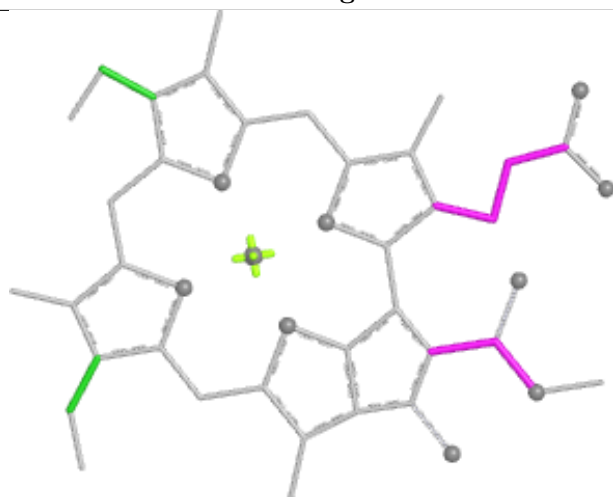
Ligand CLA b 812



Bond lengths



Bond angles

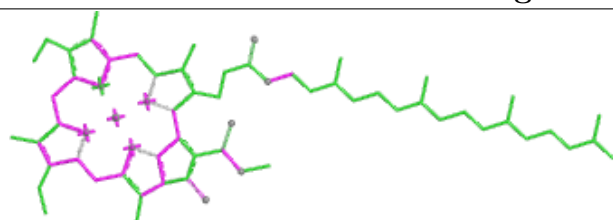


Torsions

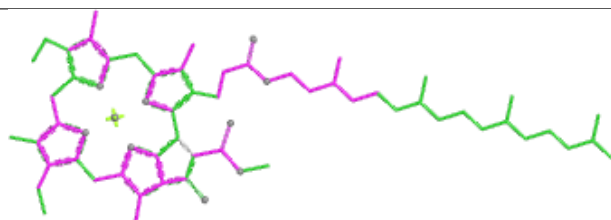


Rings

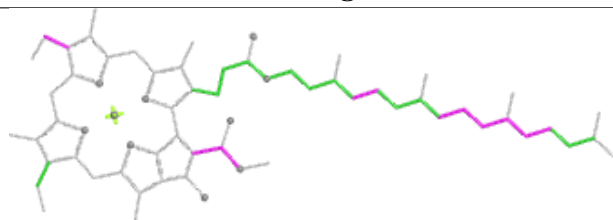
Ligand CLA B 830



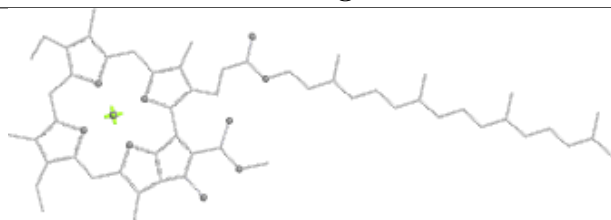
Bond lengths



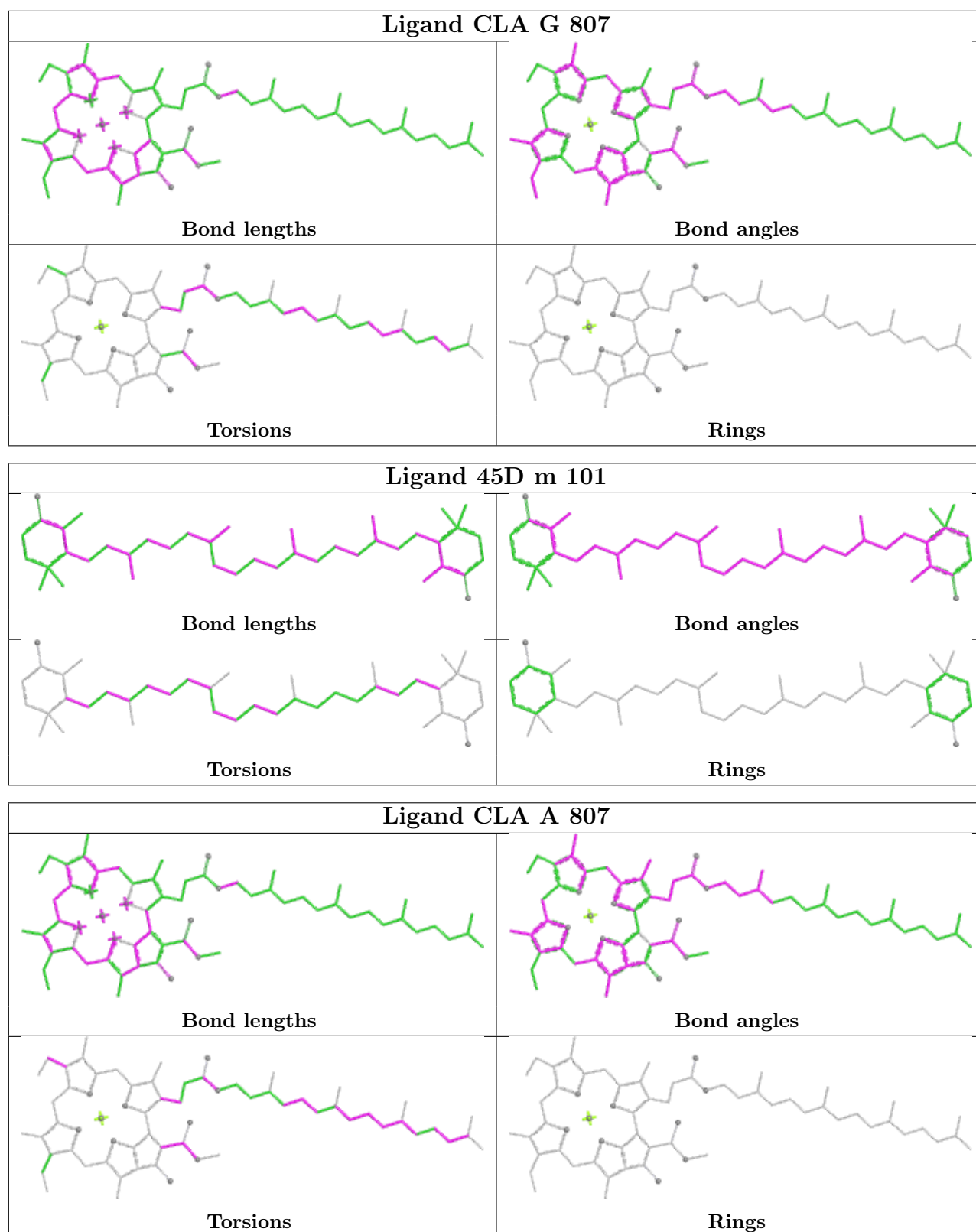
Bond angles



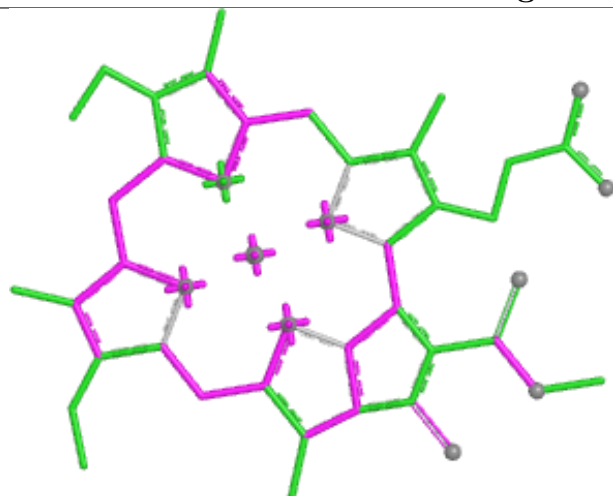
Torsions



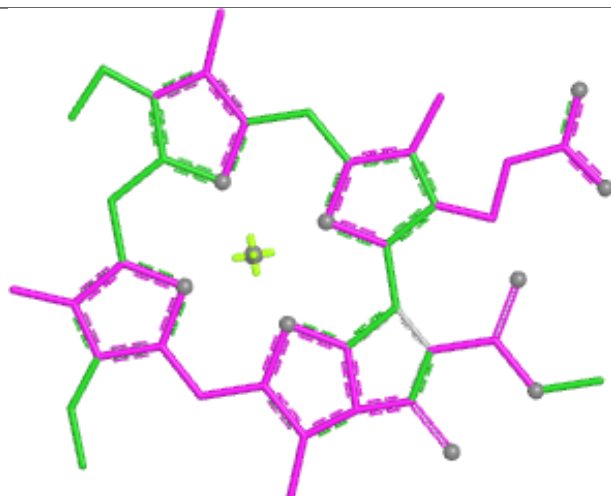
Rings



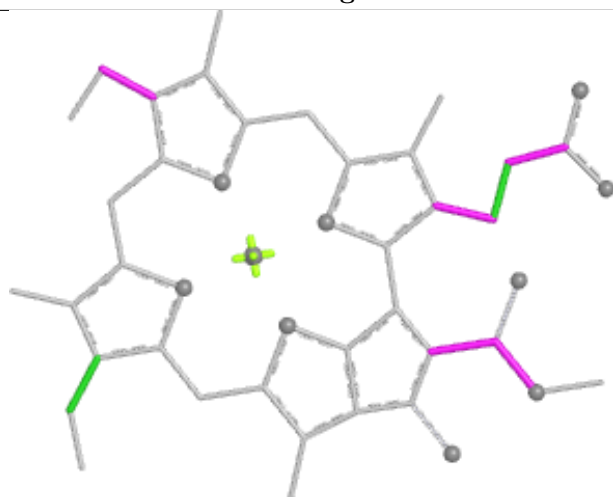
Ligand CLA b 817



Bond lengths



Bond angles

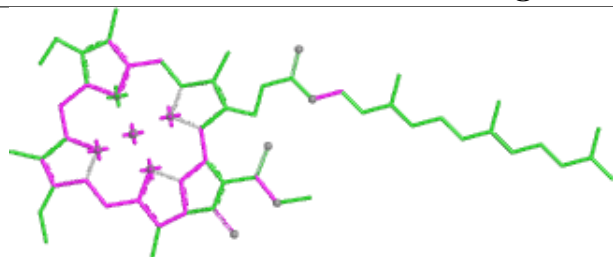


Torsions

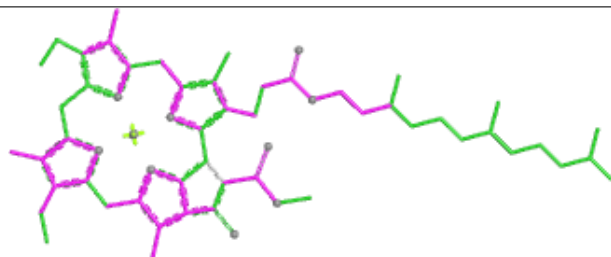


Rings

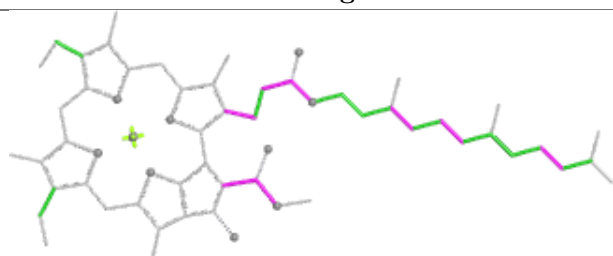
Ligand CLA B 811



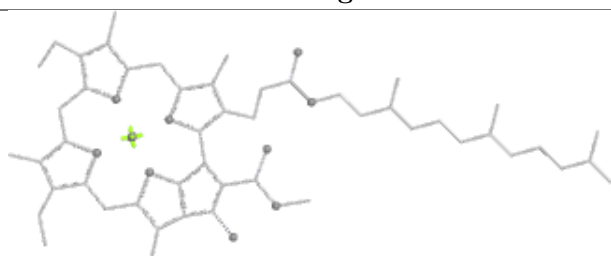
Bond lengths



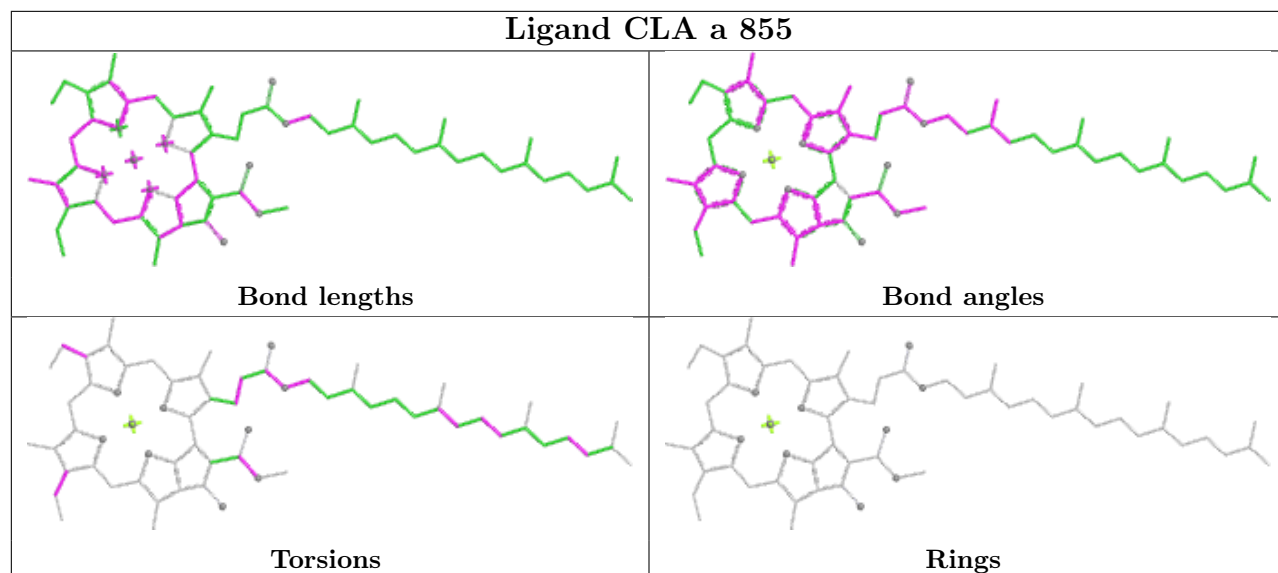
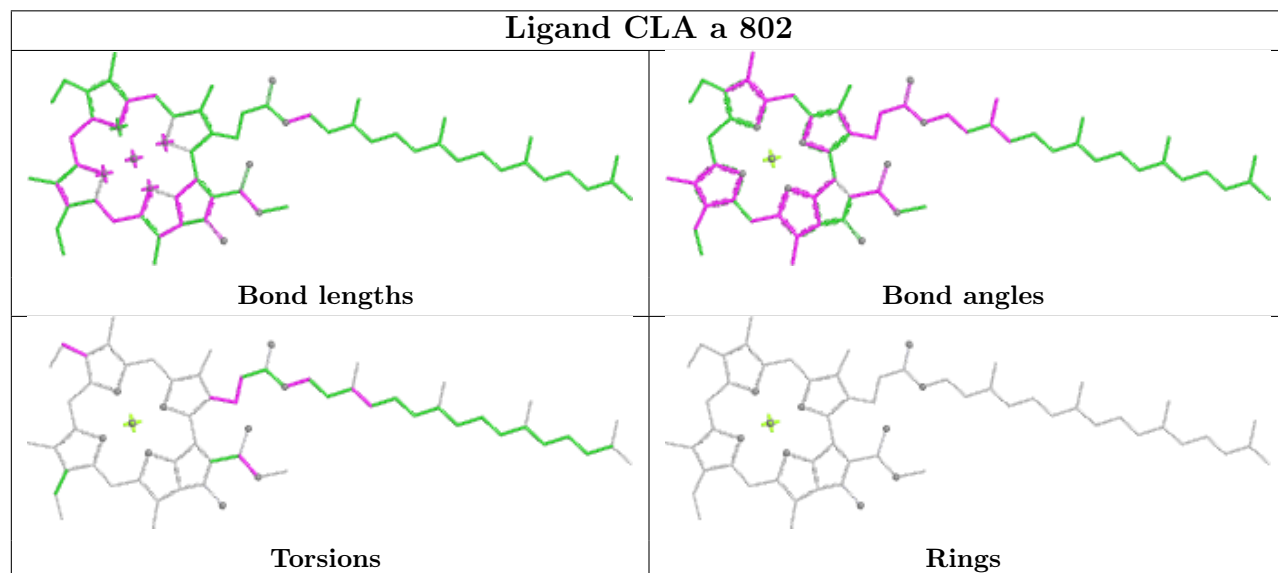
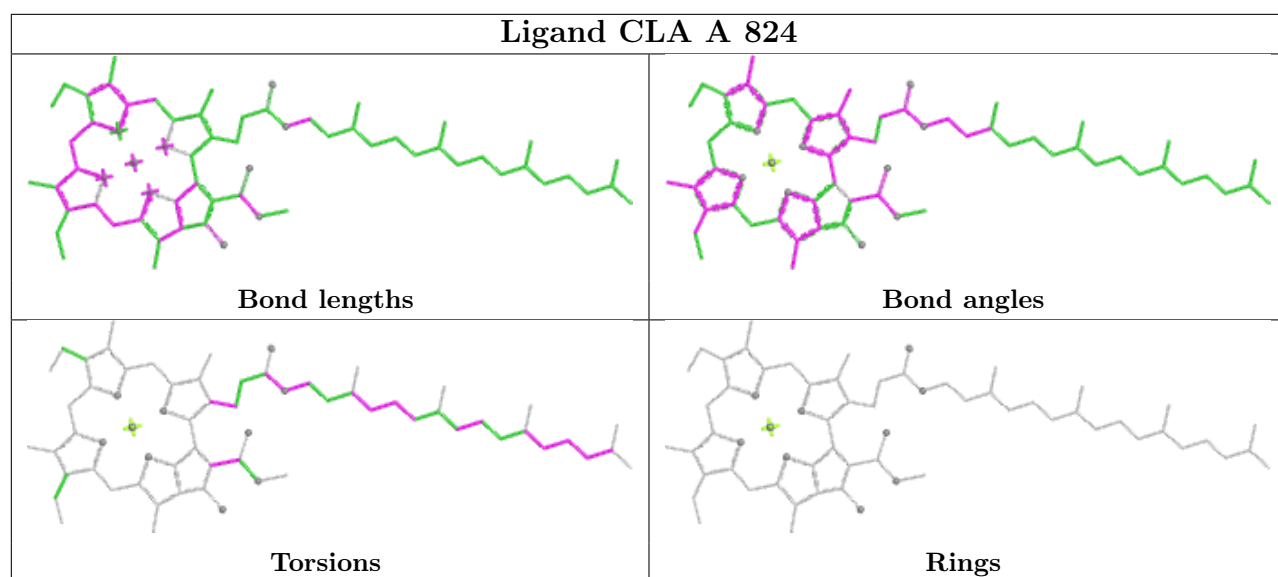
Bond angles

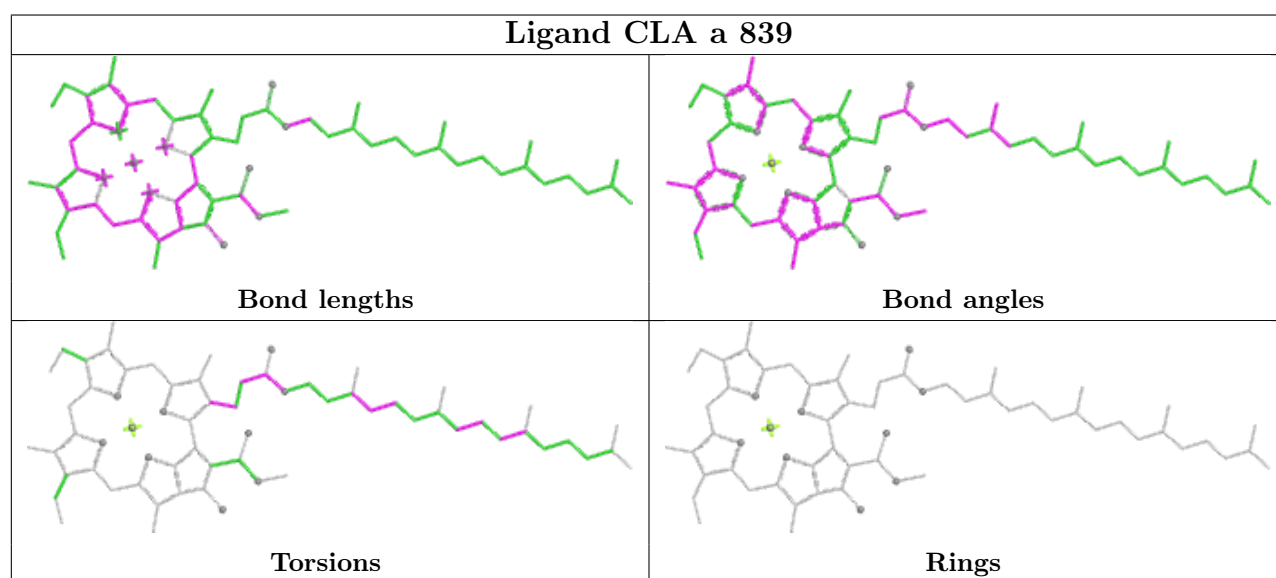
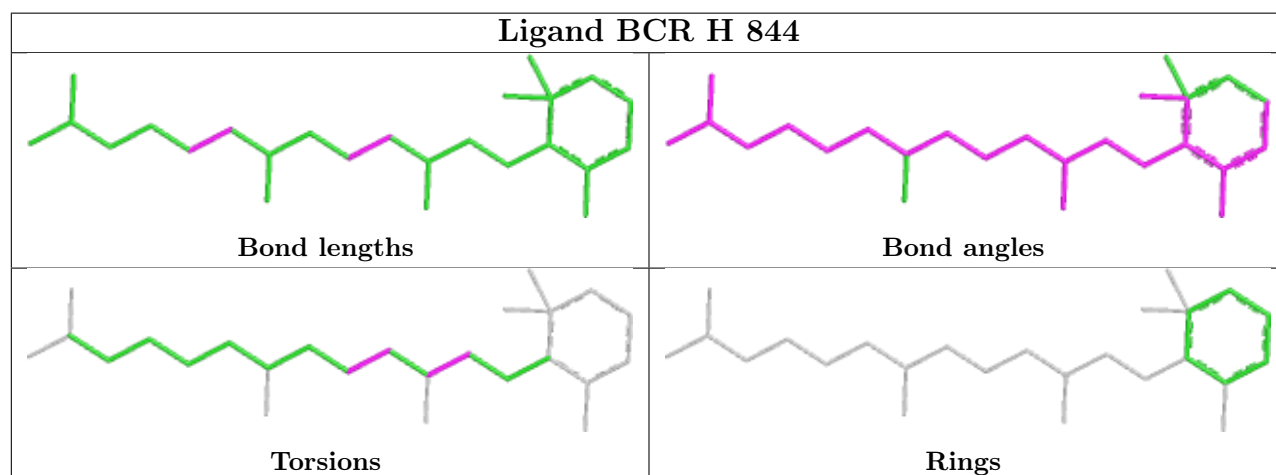
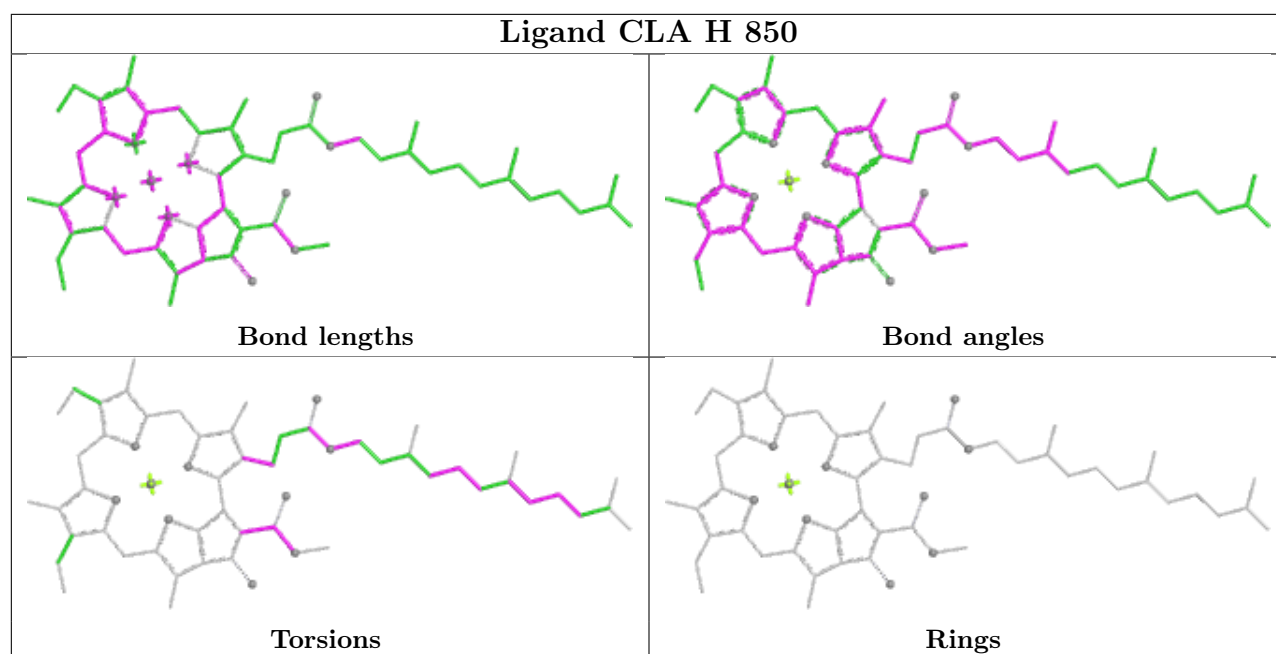


Torsions

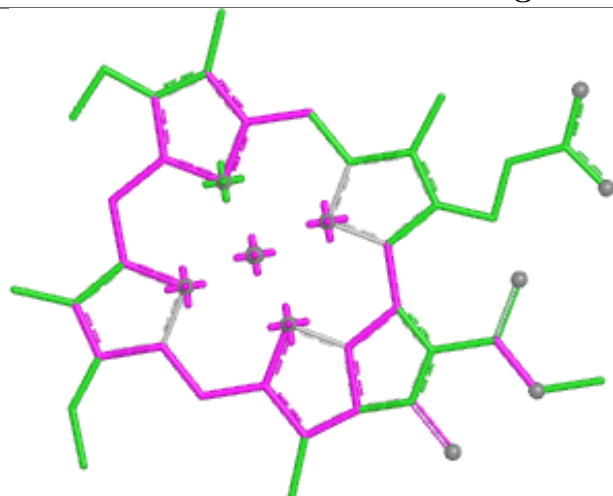


Rings

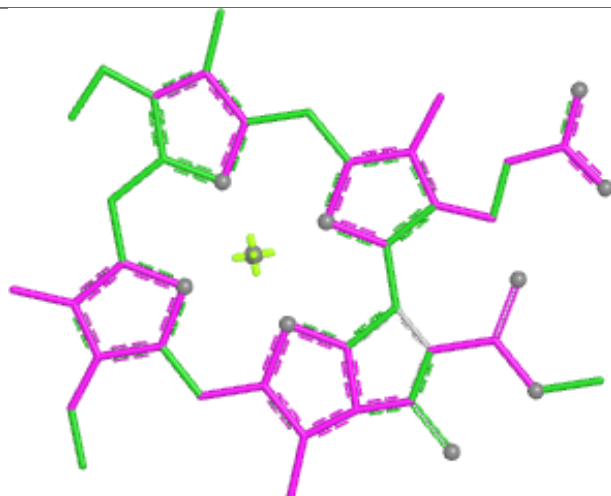




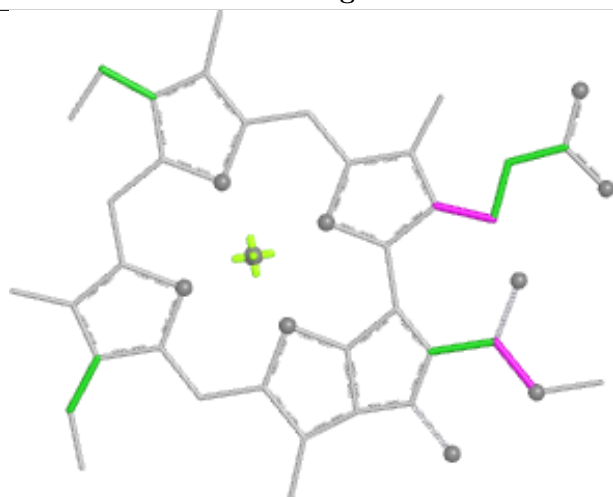
Ligand CLA B 818



Bond lengths



Bond angles

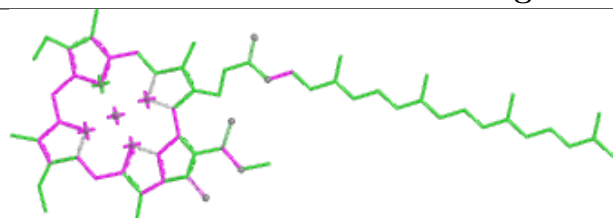


Torsions

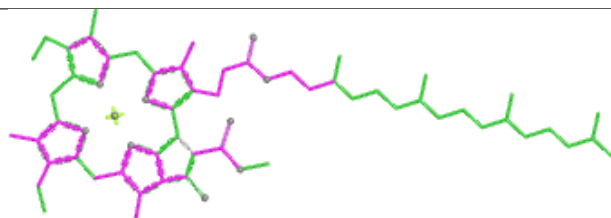


Rings

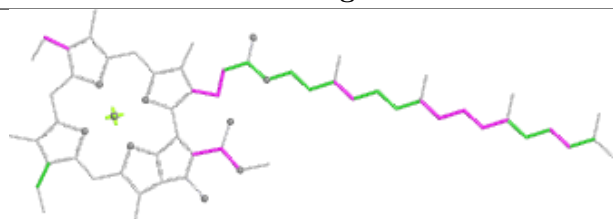
Ligand CLA B 822



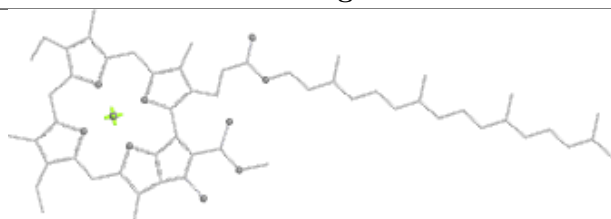
Bond lengths



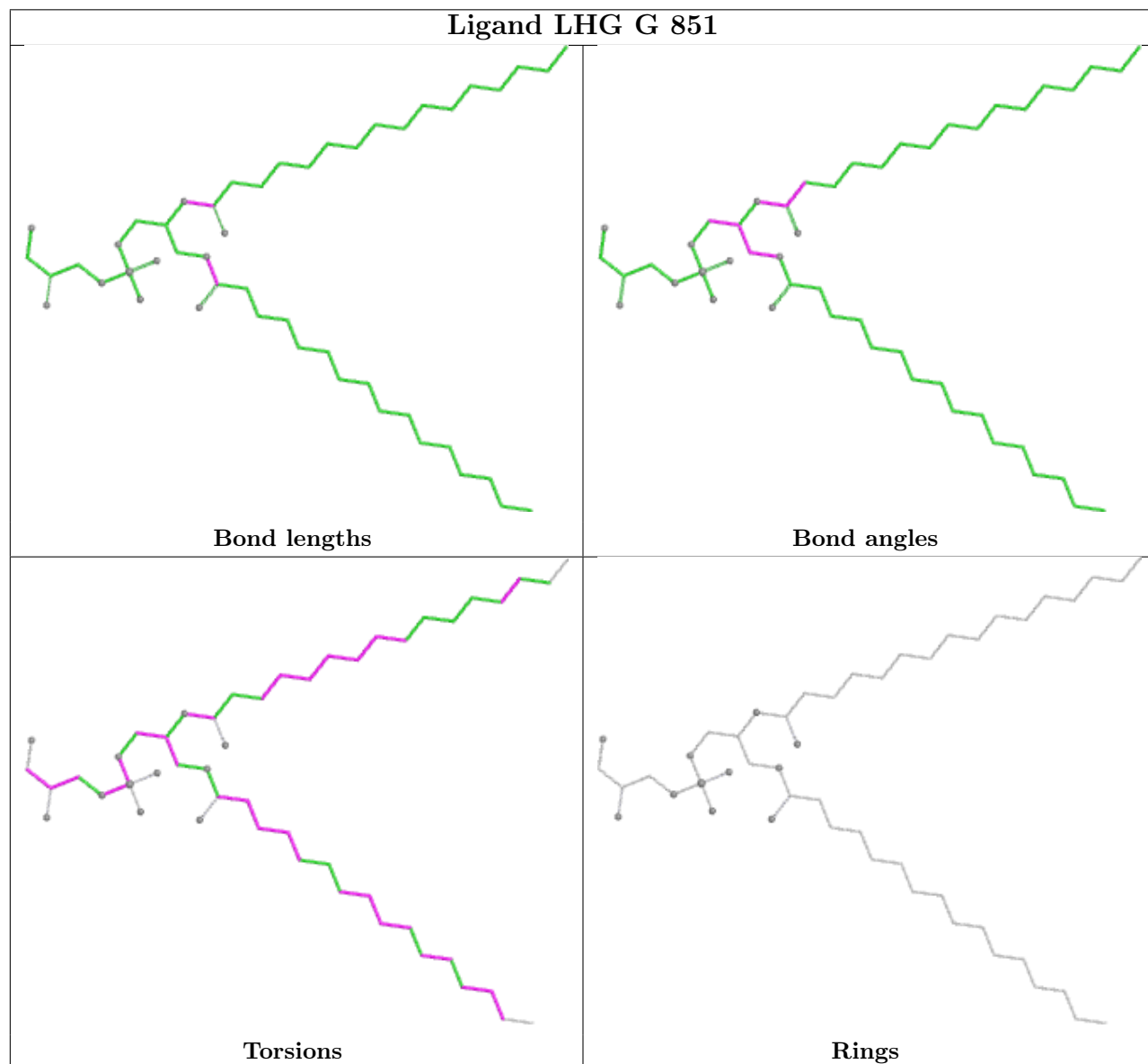
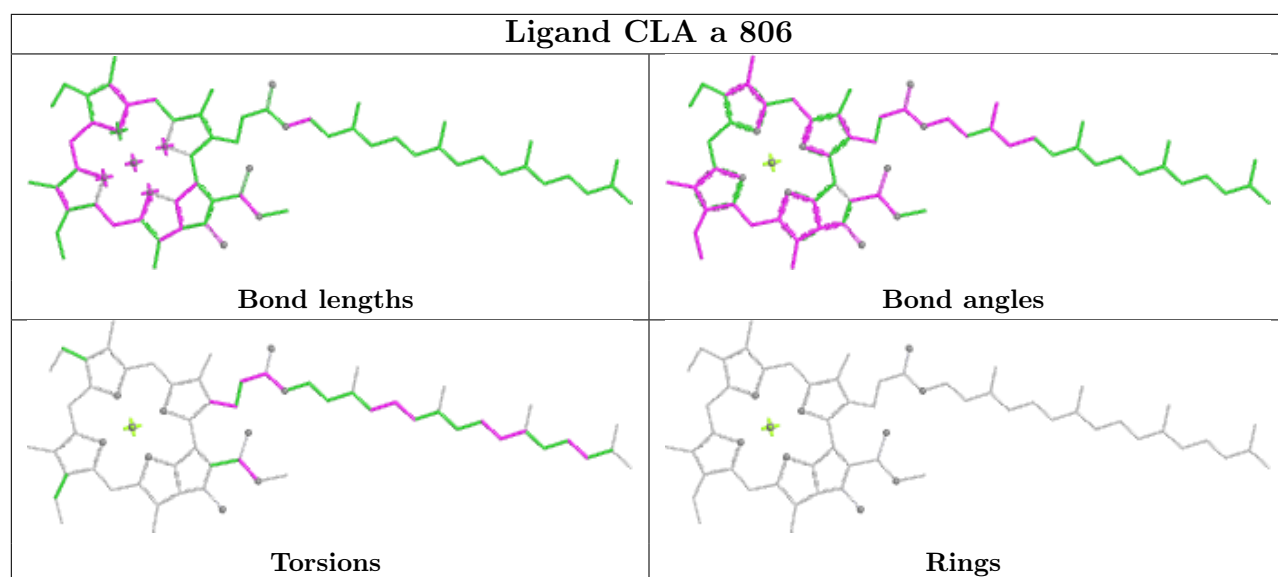
Bond angles

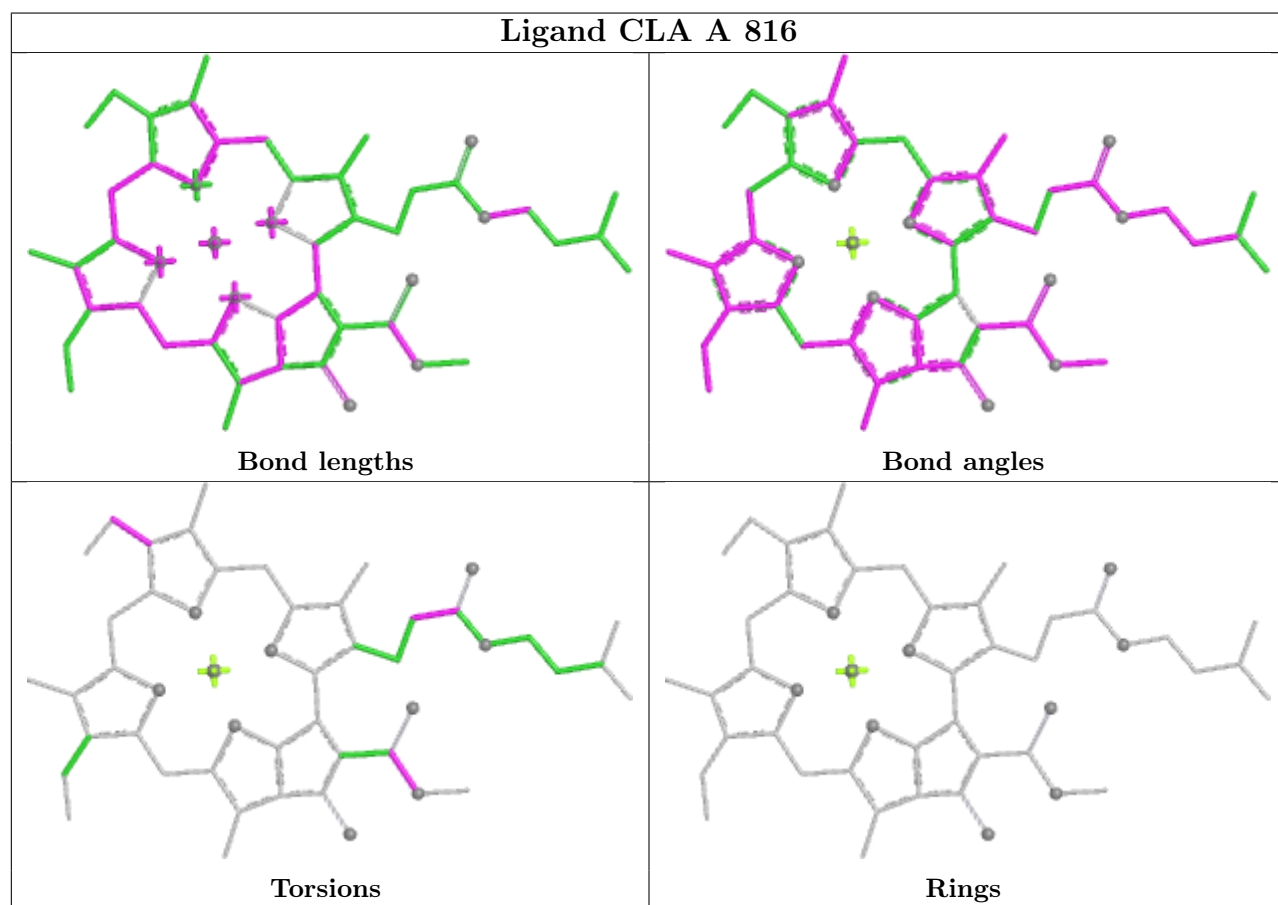
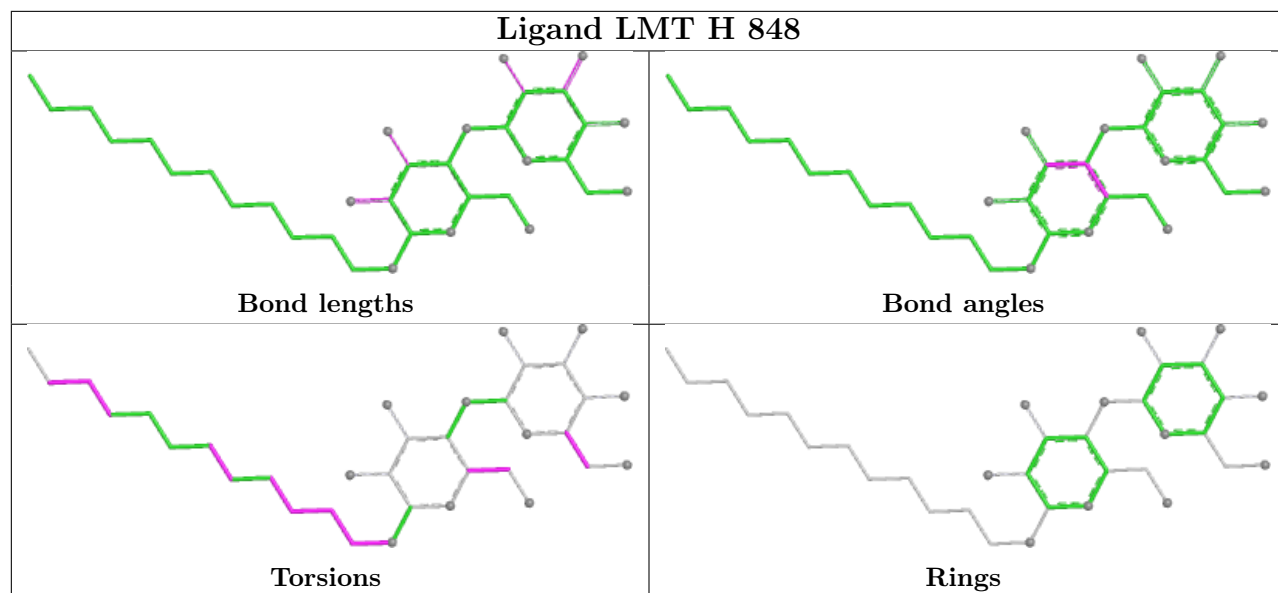


Torsions

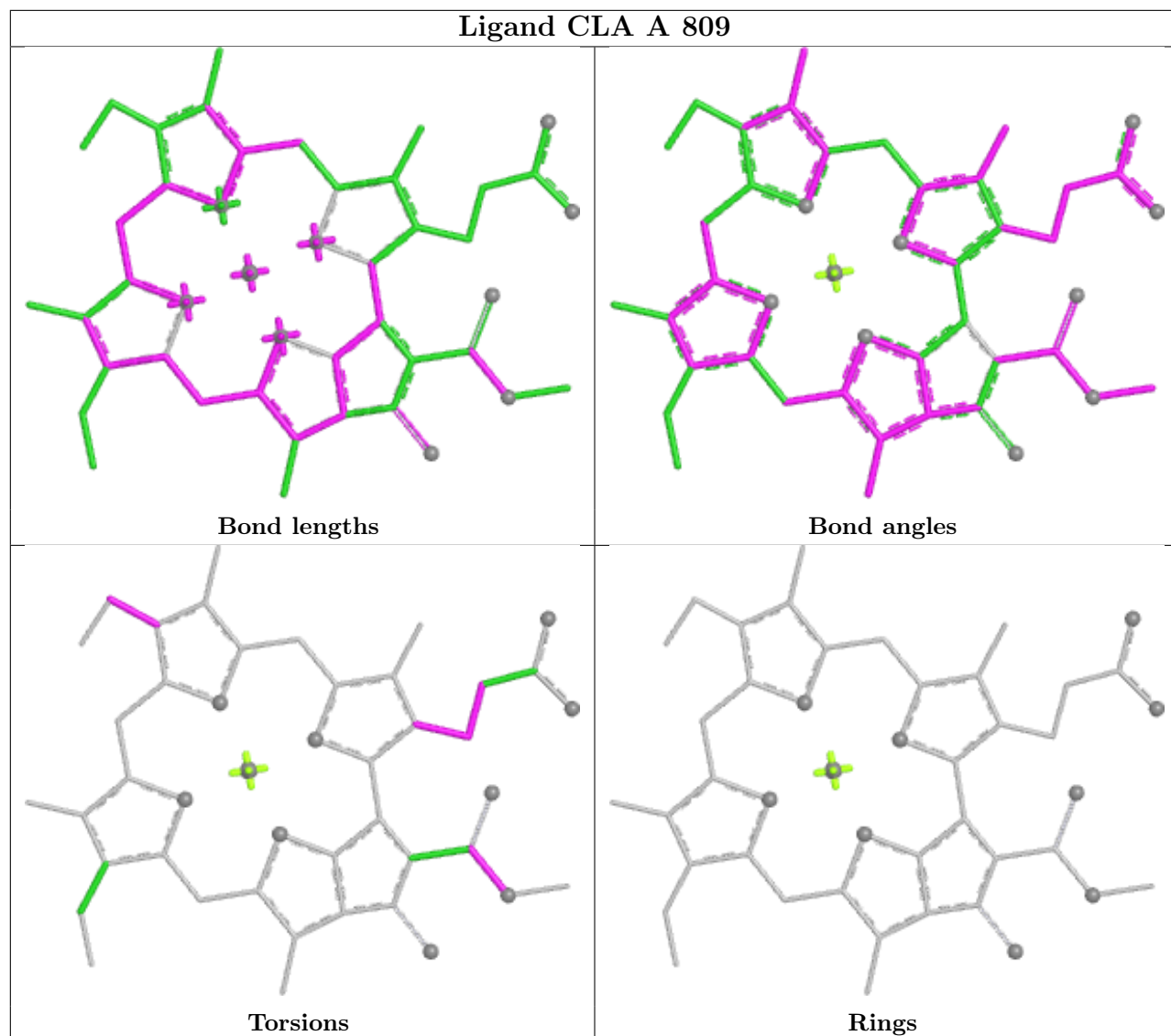


Rings

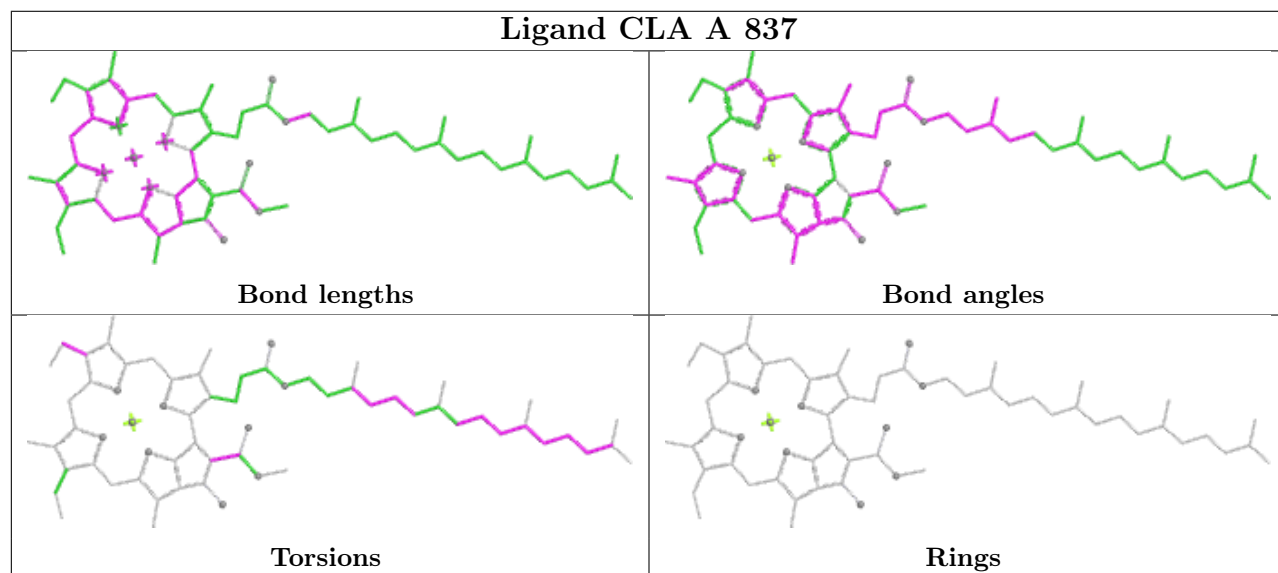


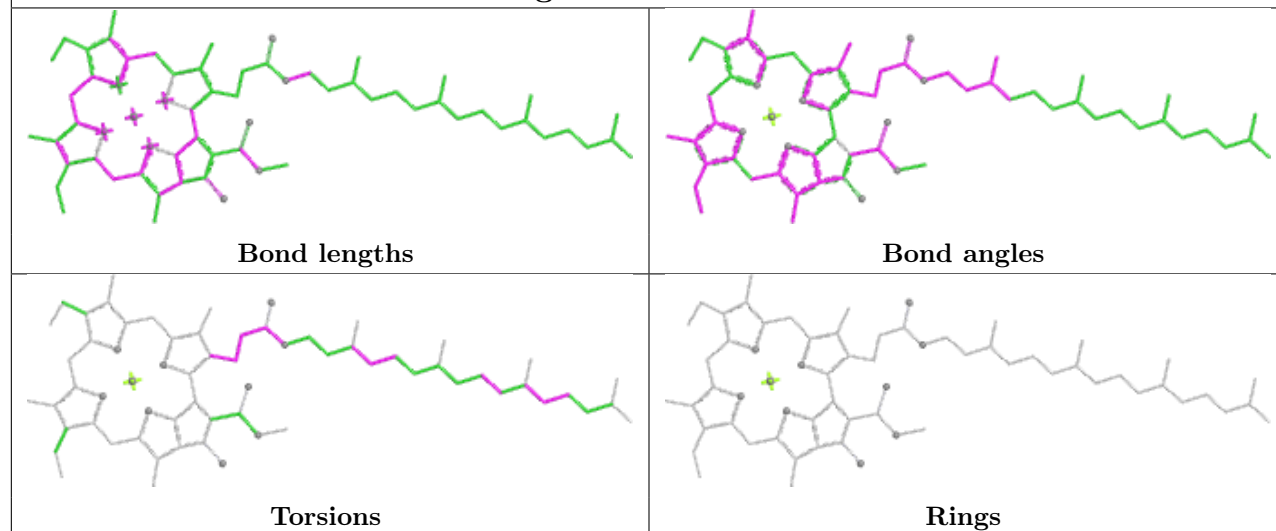
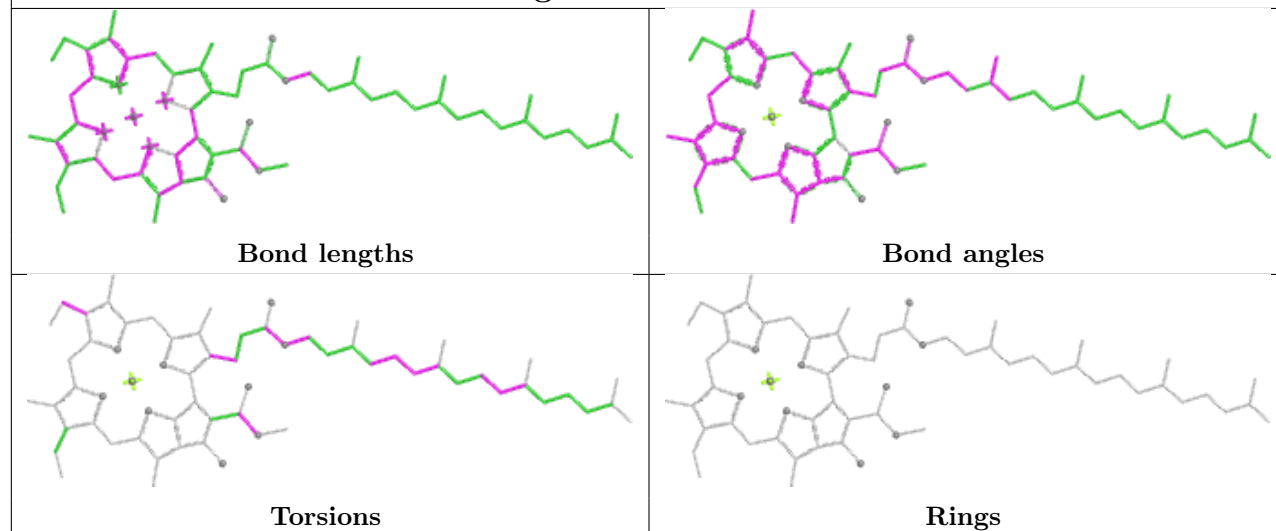


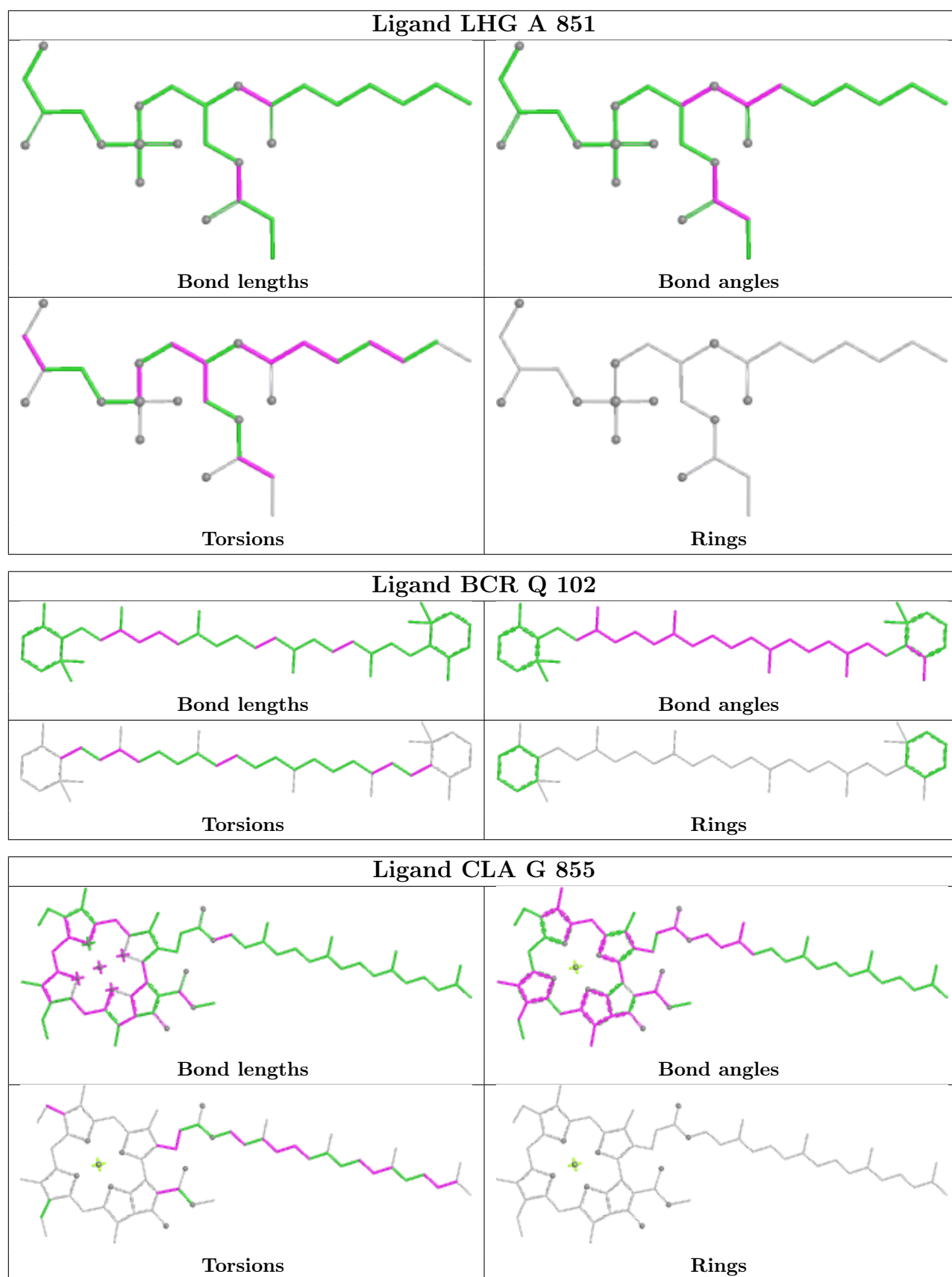
Ligand CLA A 809

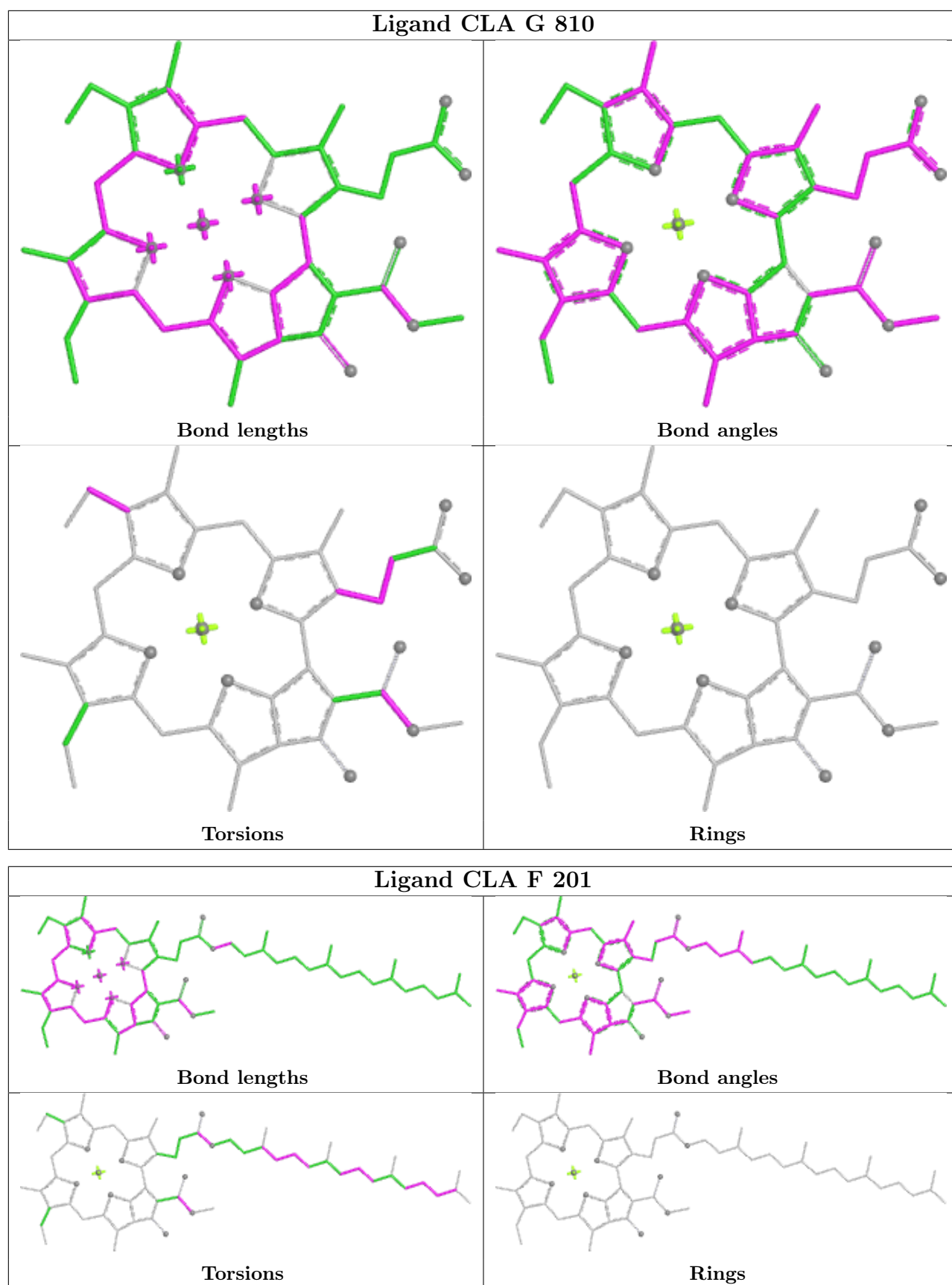


Ligand CLA A 837

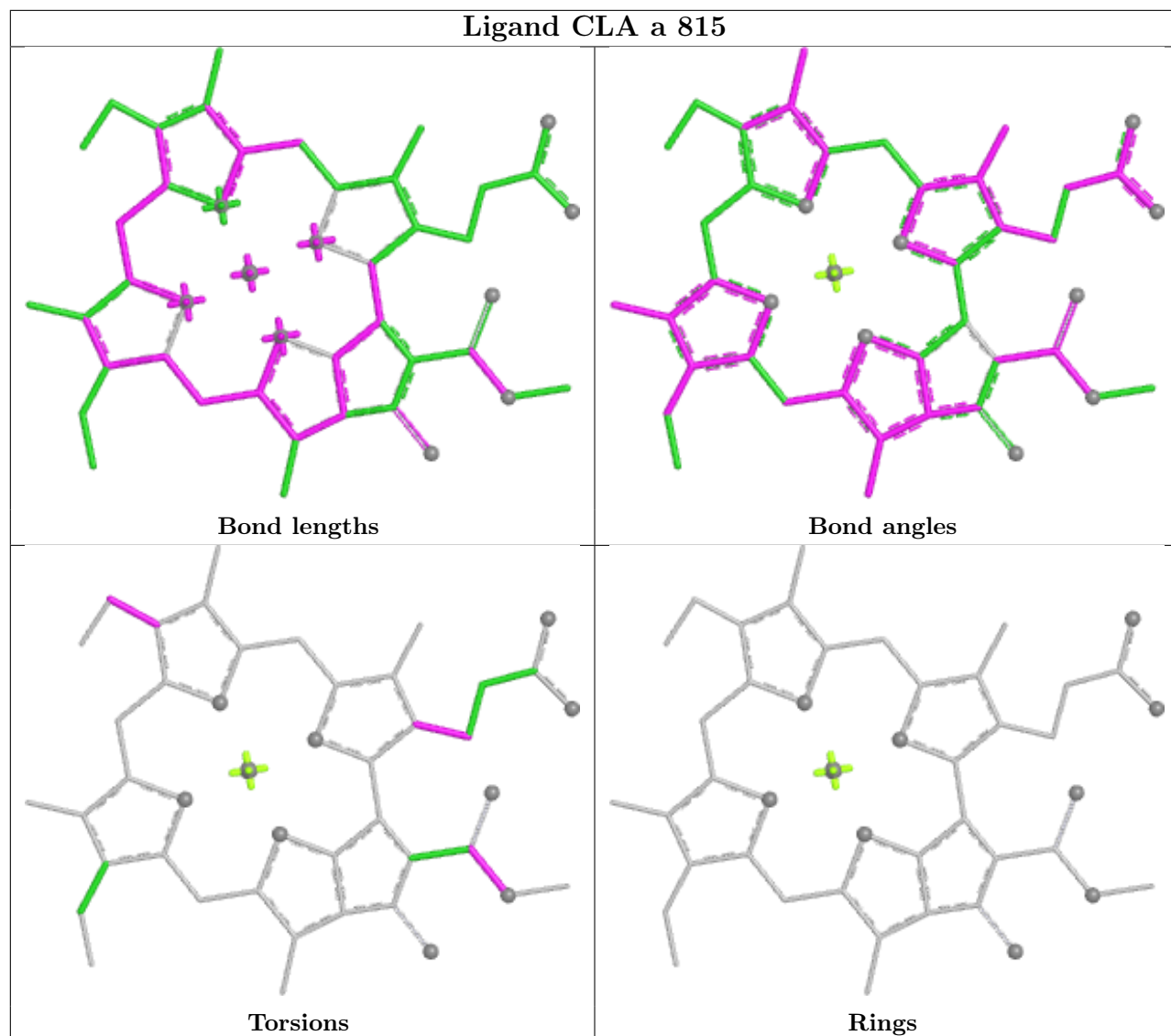


Ligand CLA S 203**Ligand CLA L 202**

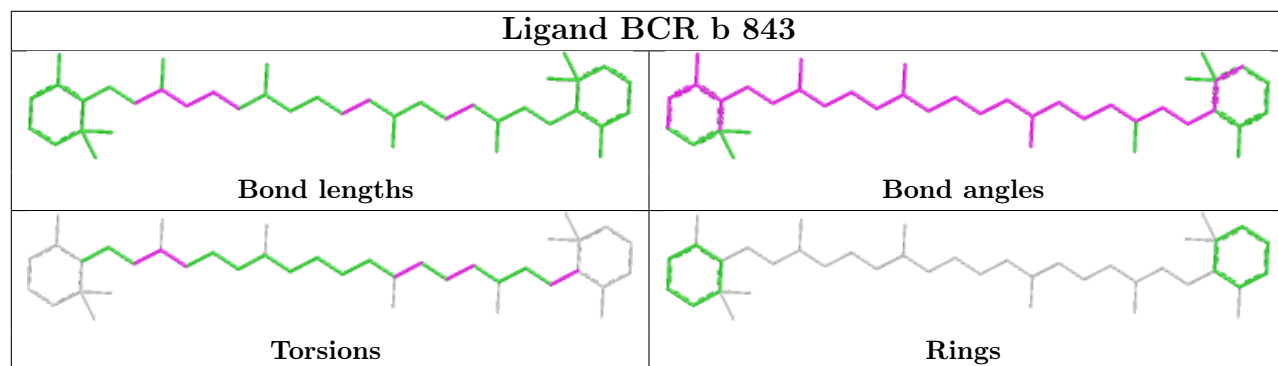




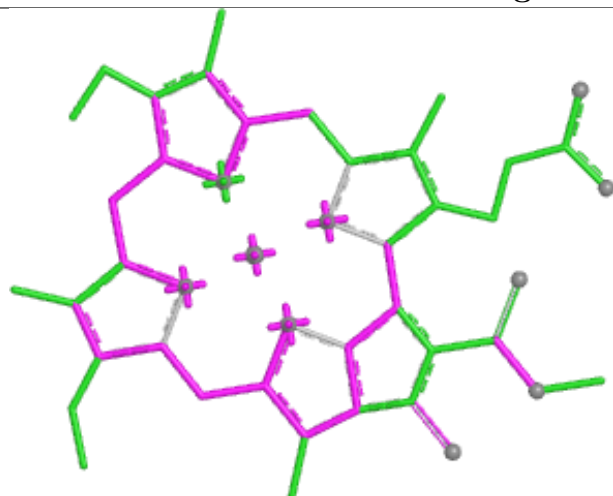
Ligand CLA a 815



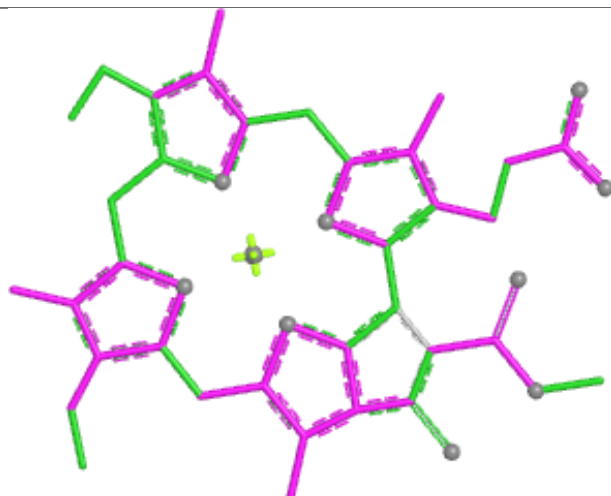
Ligand BCR b 843



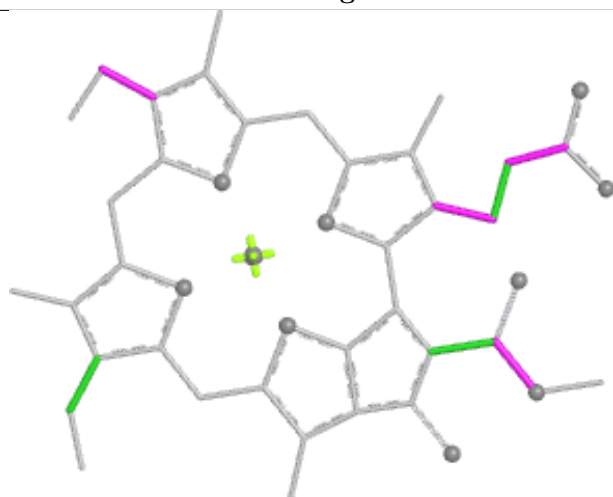
Ligand CLA R 103



Bond lengths



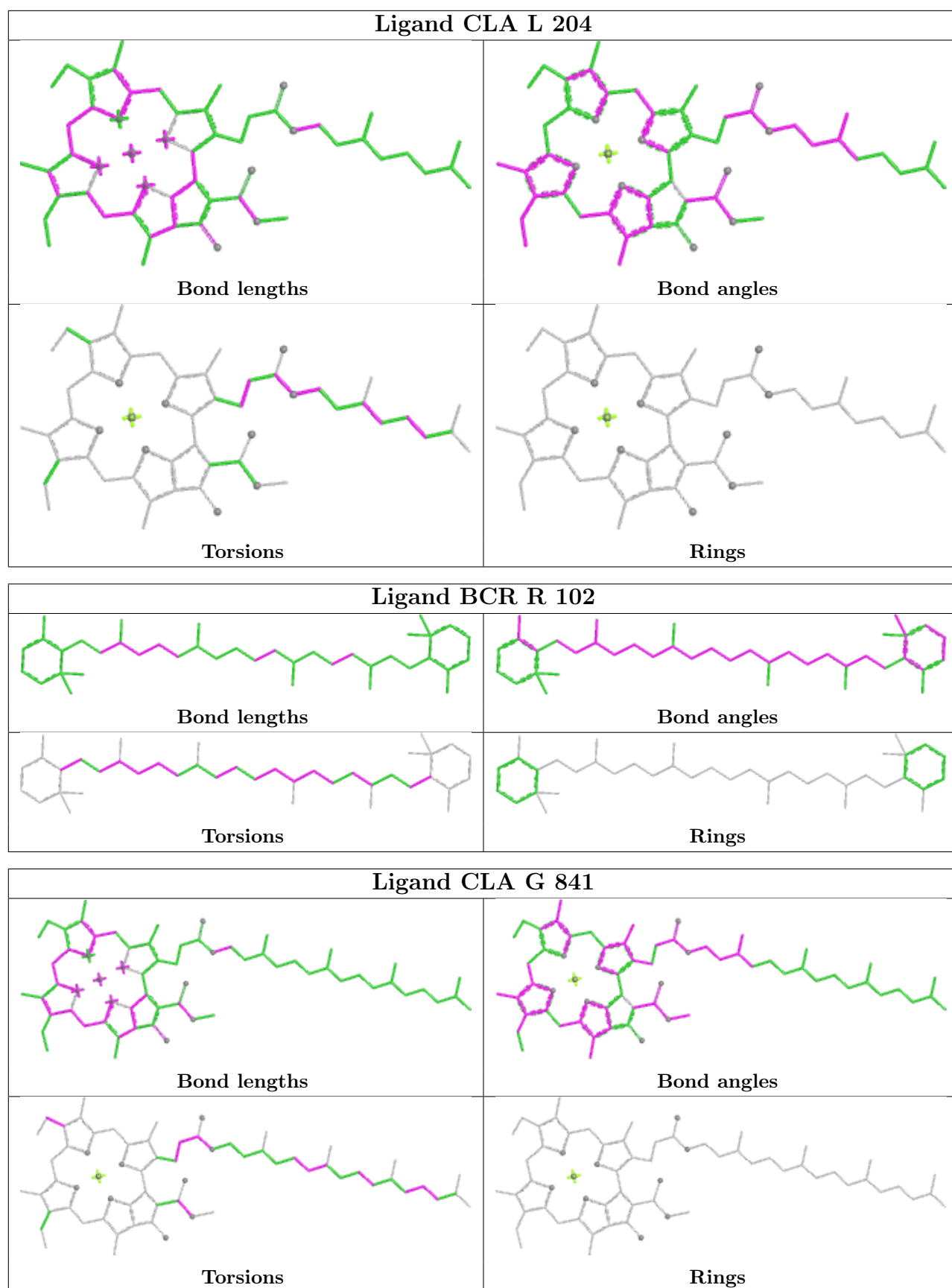
Bond angles



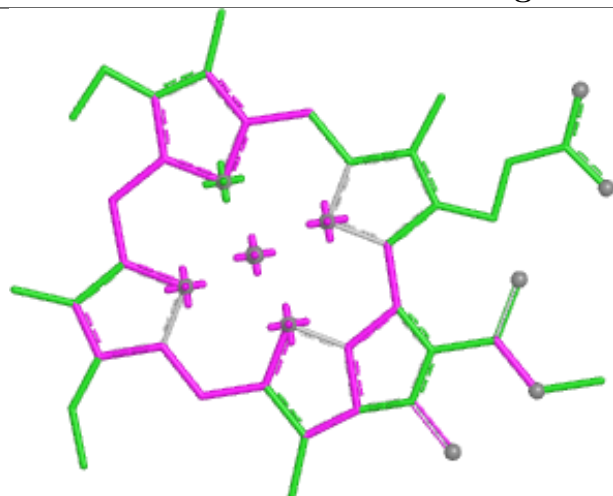
Torsions



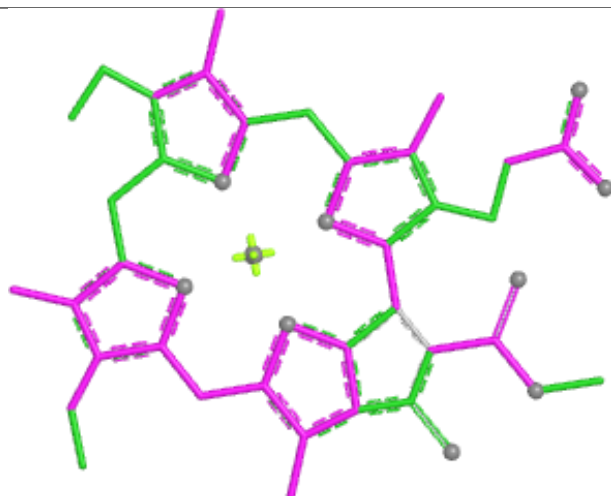
Rings



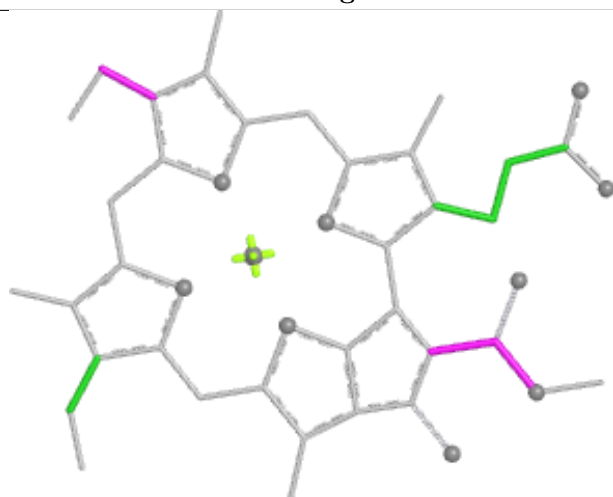
Ligand CLA B 831



Bond lengths



Bond angles

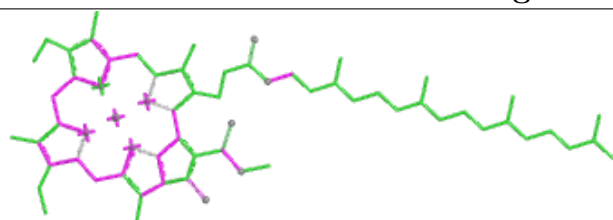


Torsions

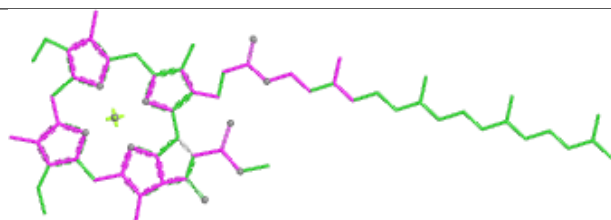


Rings

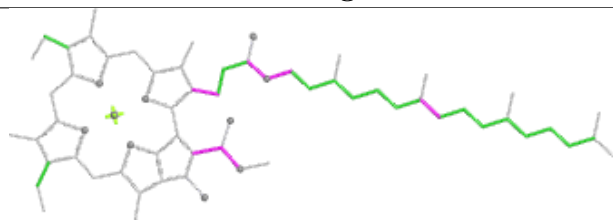
Ligand CLA G 830



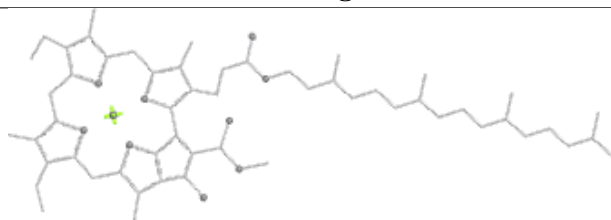
Bond lengths



Bond angles

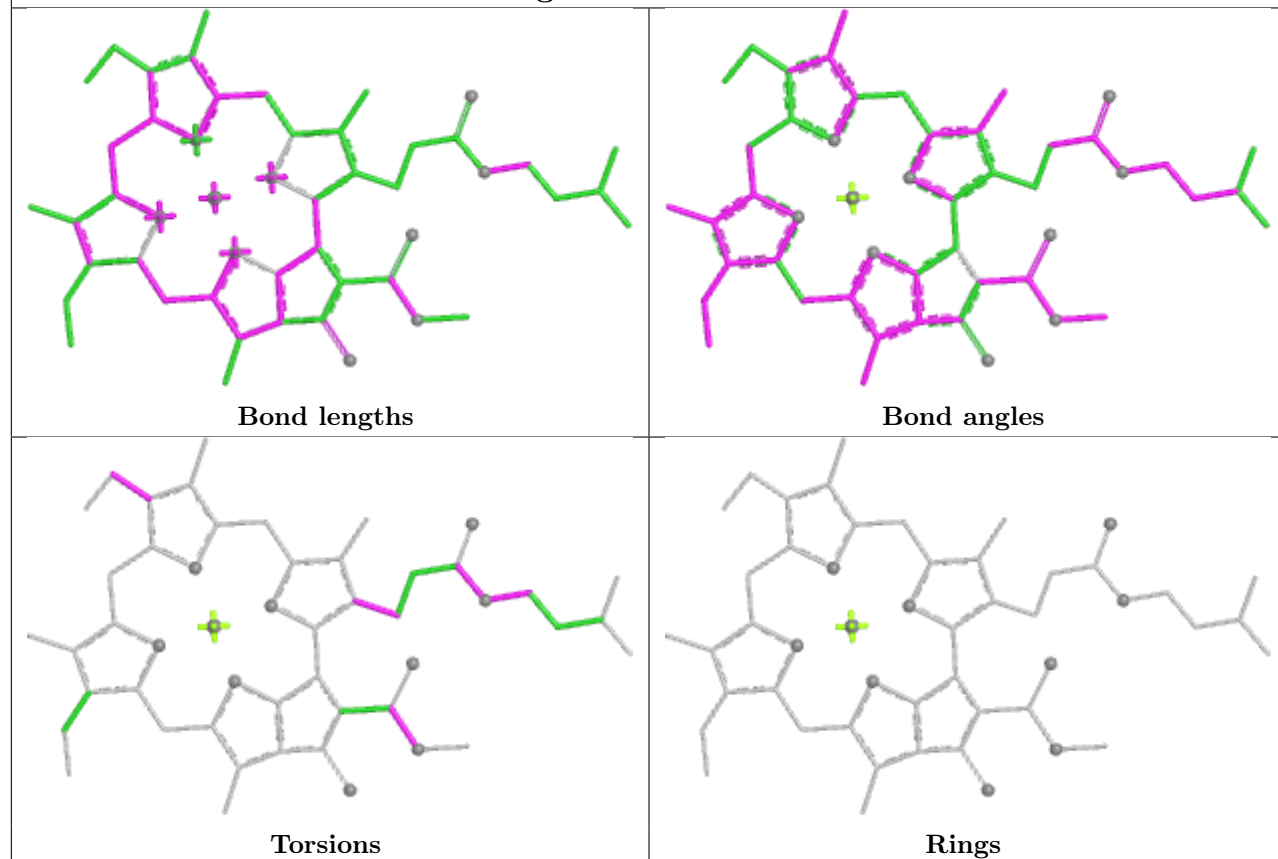


Torsions

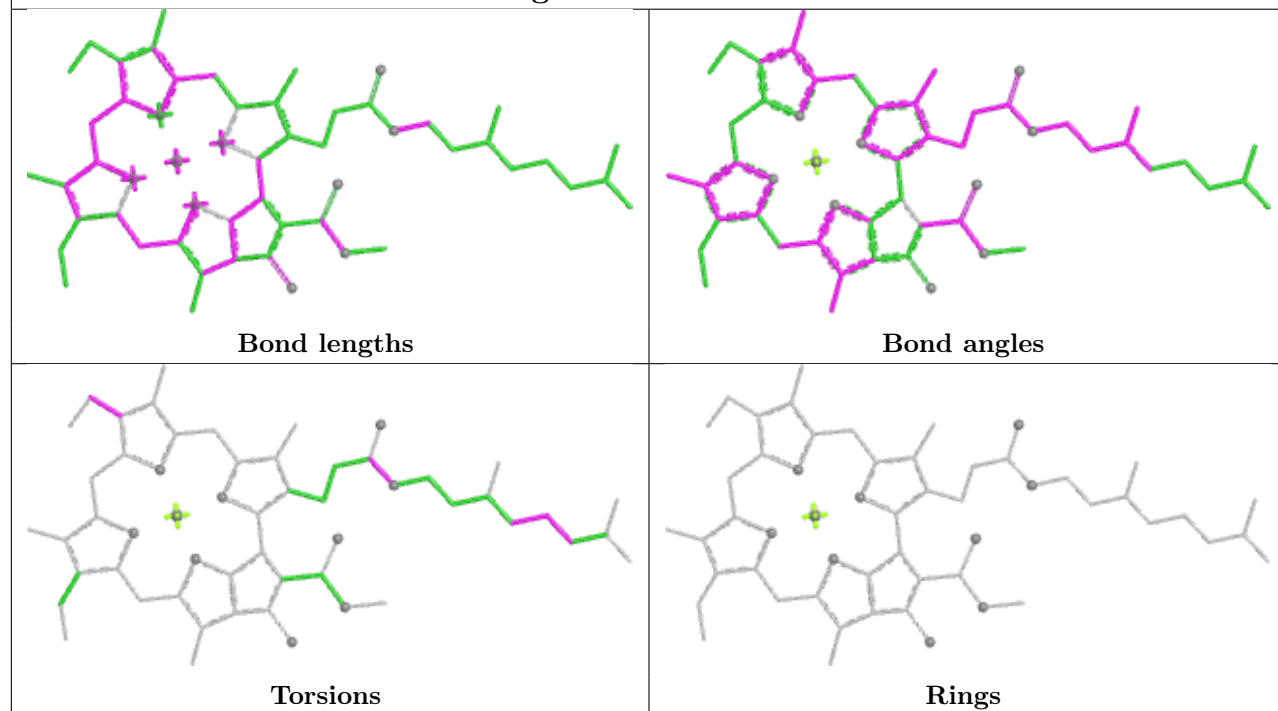


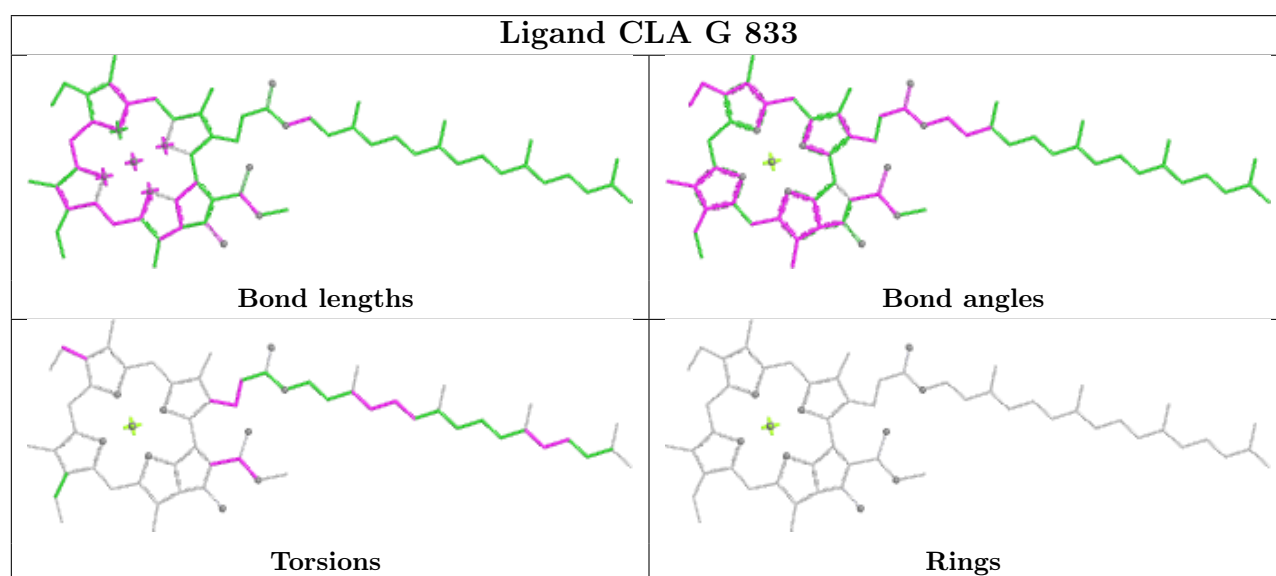
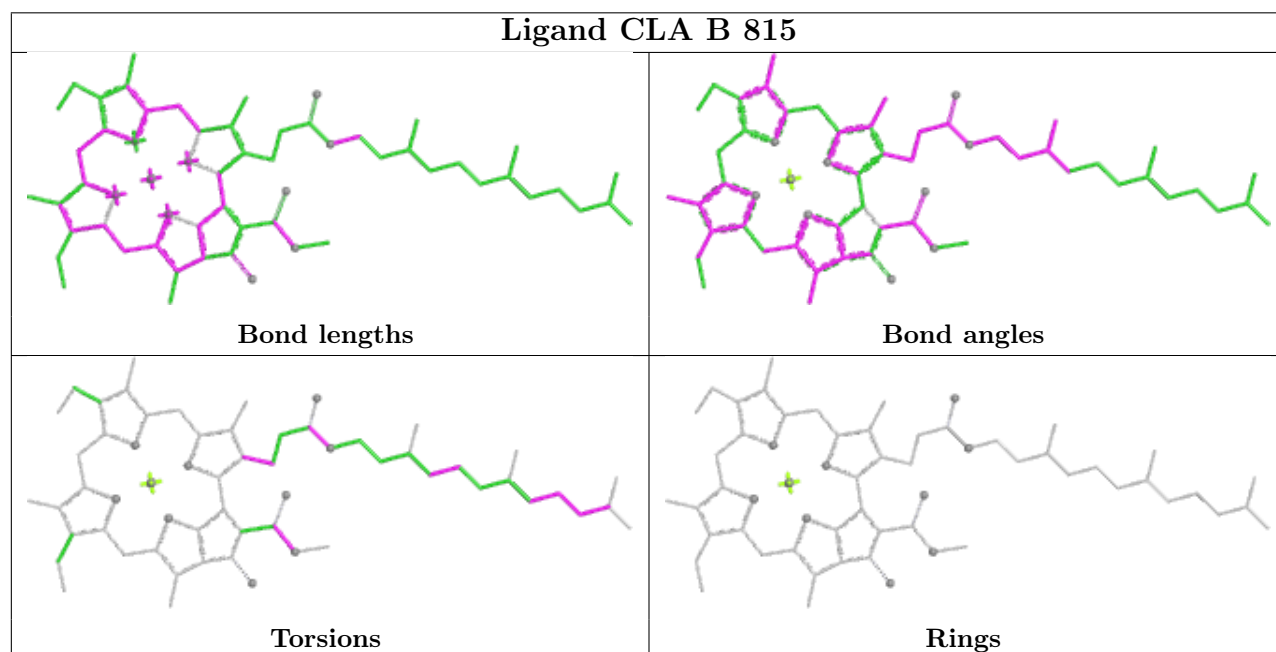
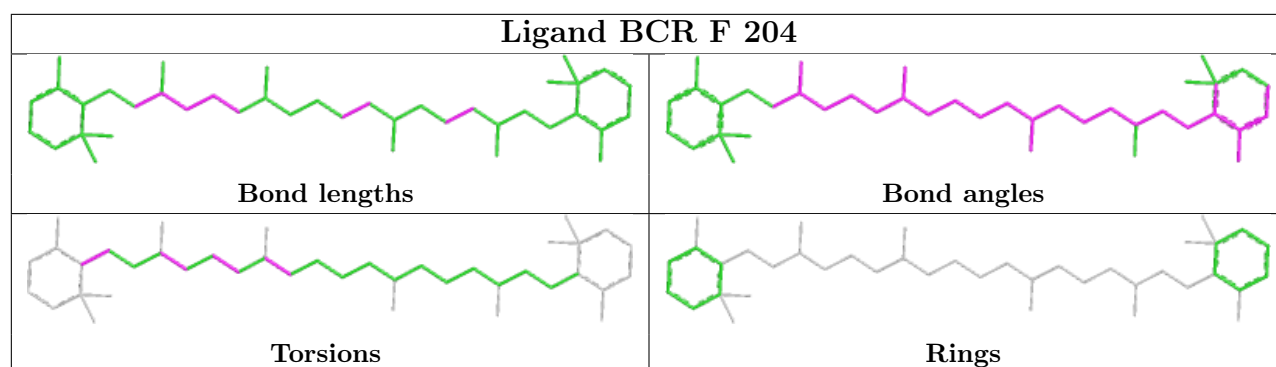
Rings

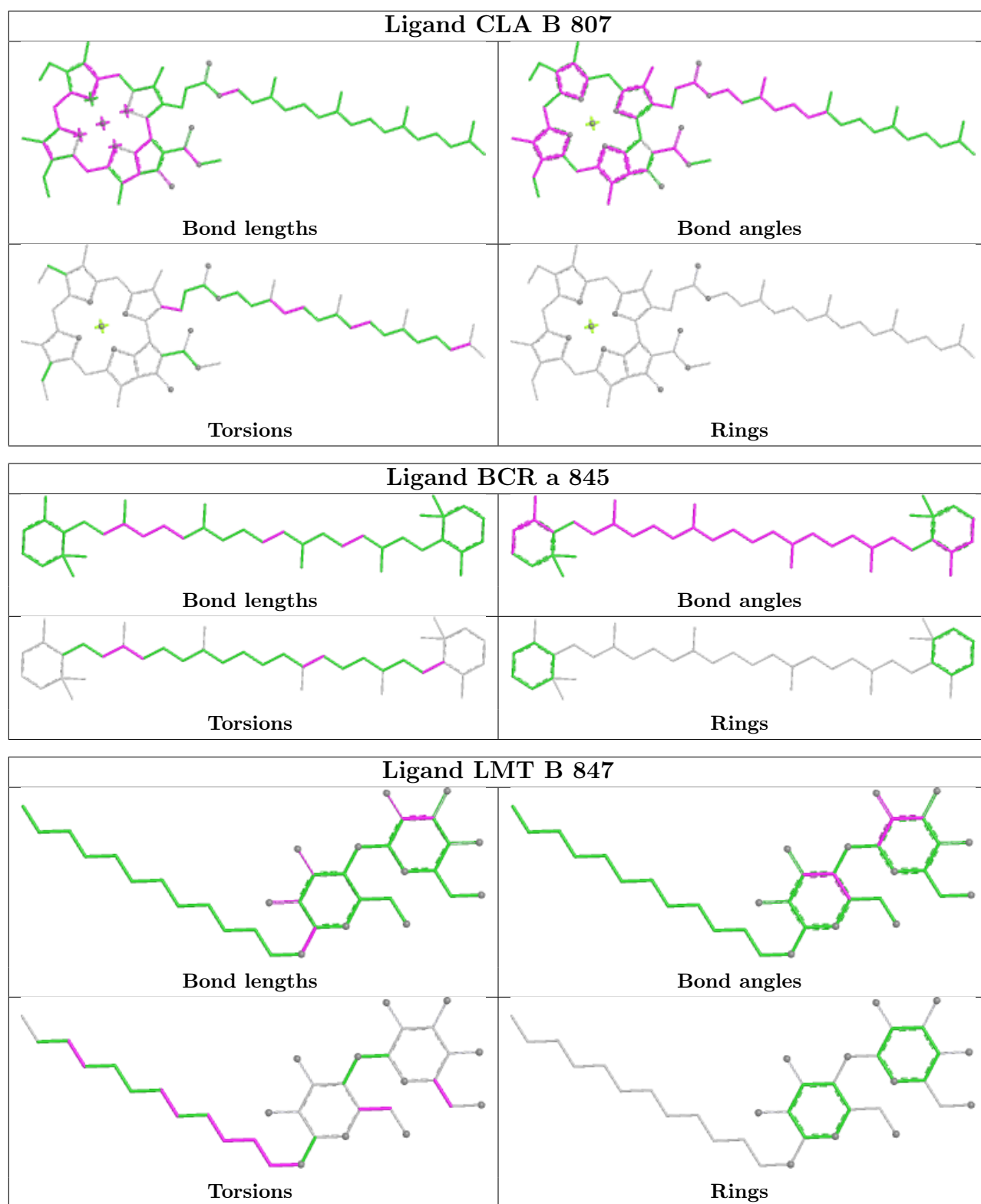
Ligand CLA a 810



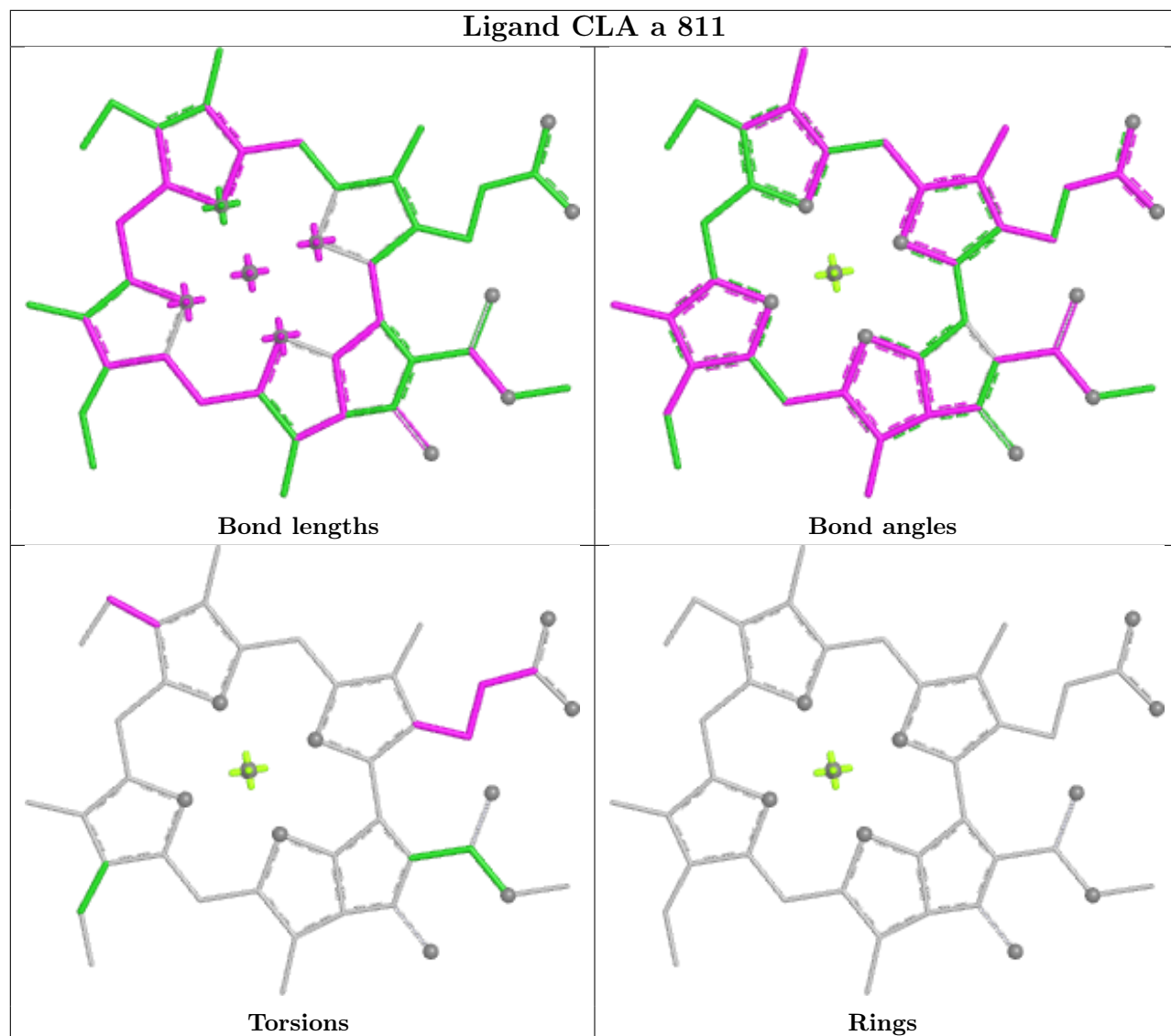
Ligand CLA A 825



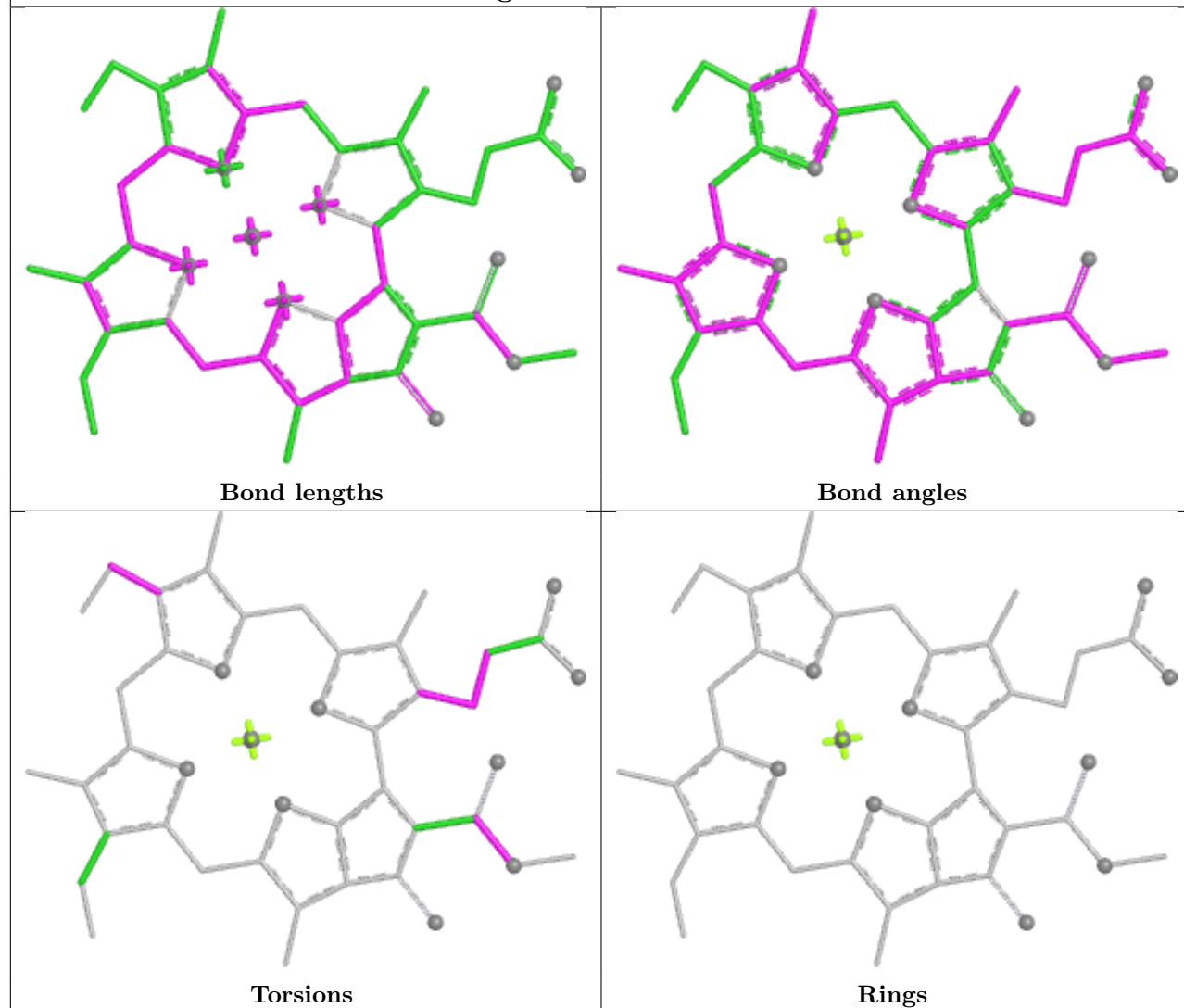




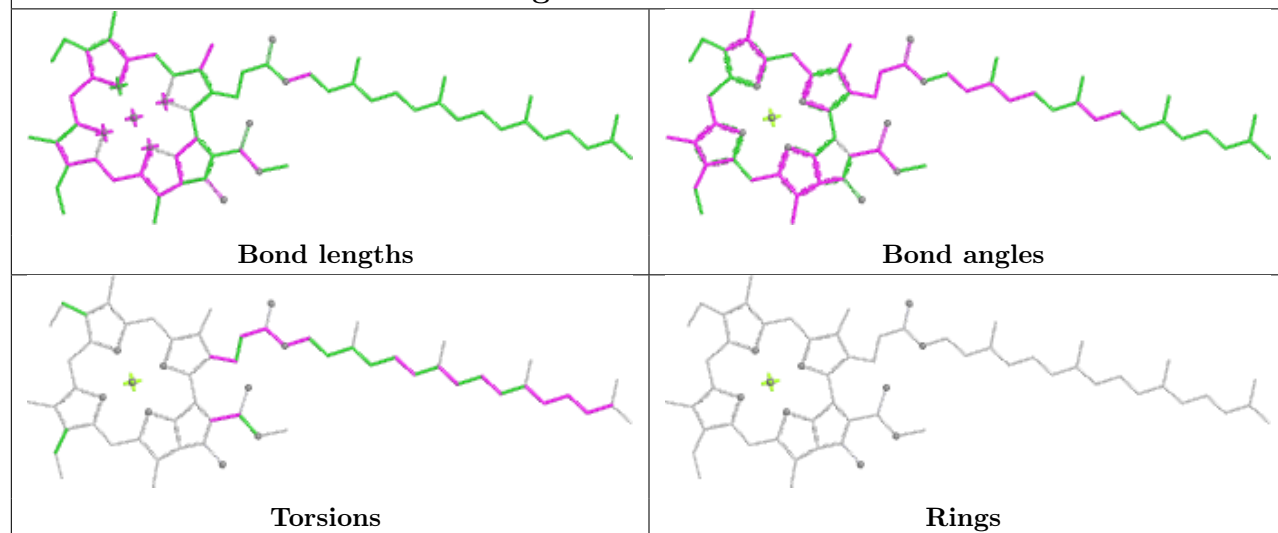
Ligand CLA a 811

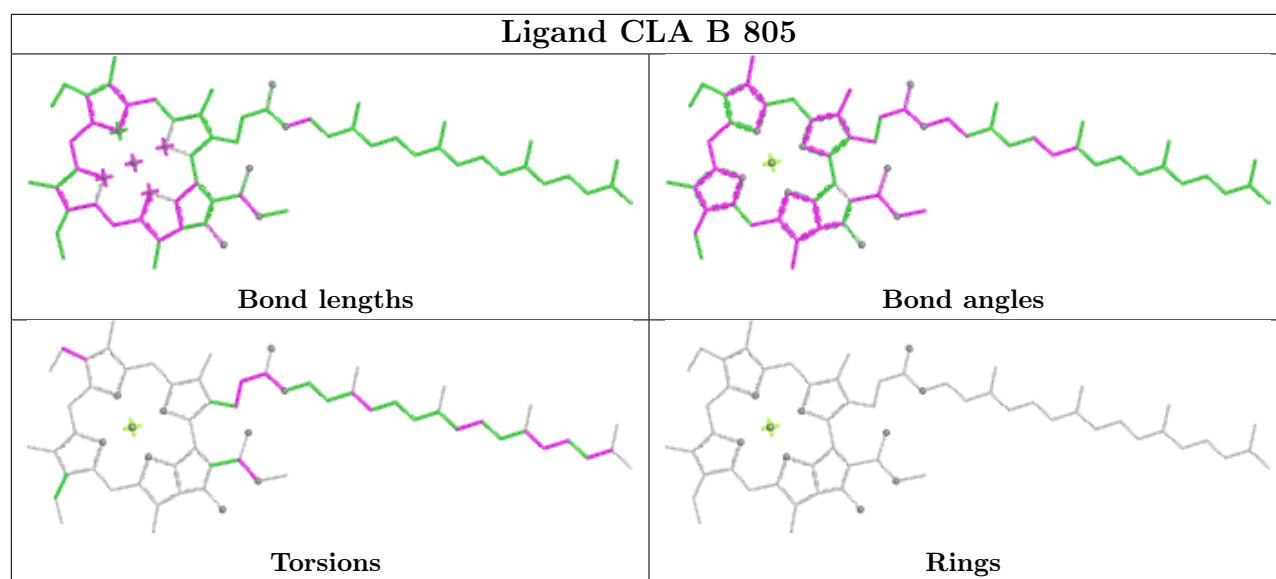


Ligand CLA a 809



Ligand CLA B 803





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.

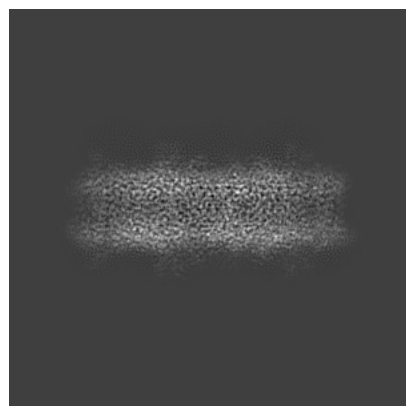
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47359. These allow visual inspection of the internal detail of the map and identification of artifacts.

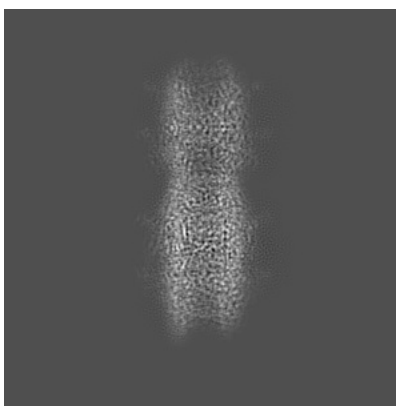
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

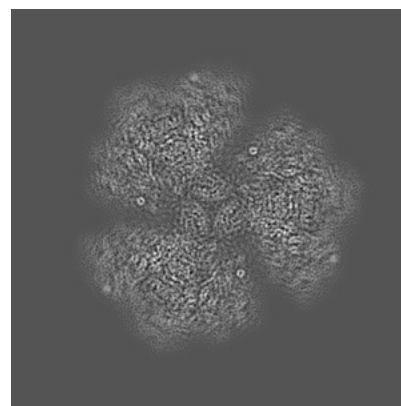
6.1.1 Primary map



X

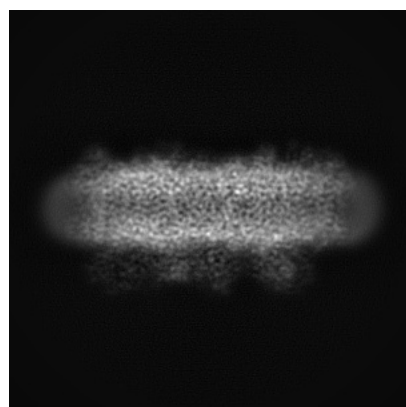


Y

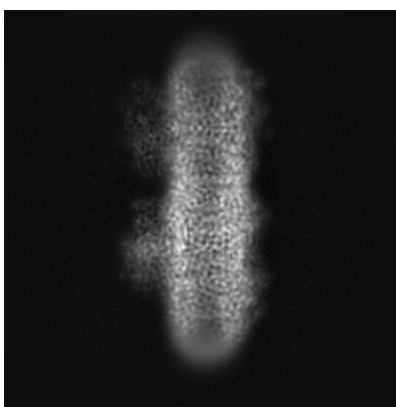


Z

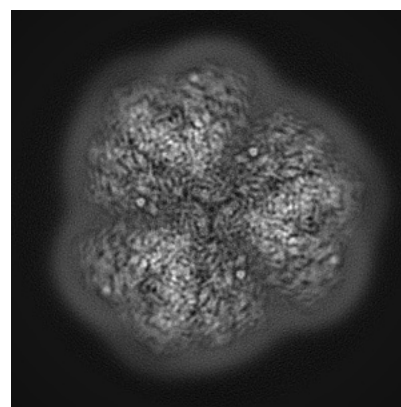
6.1.2 Raw map



X



Y

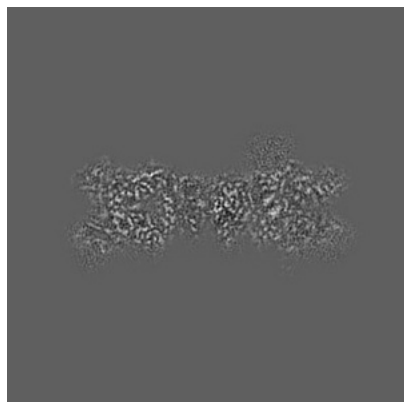


Z

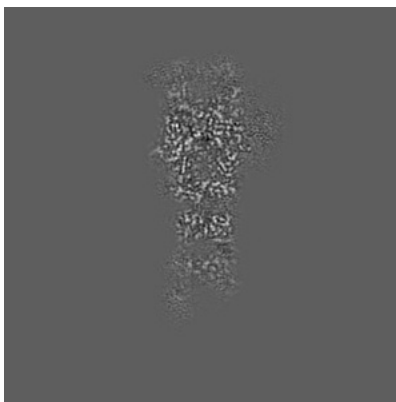
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

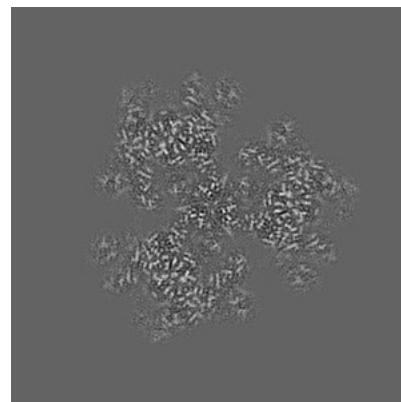
6.2.1 Primary map



X Index: 160

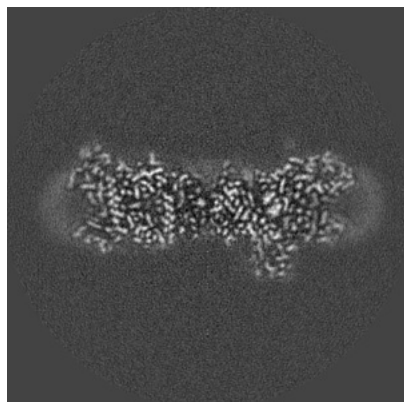


Y Index: 160

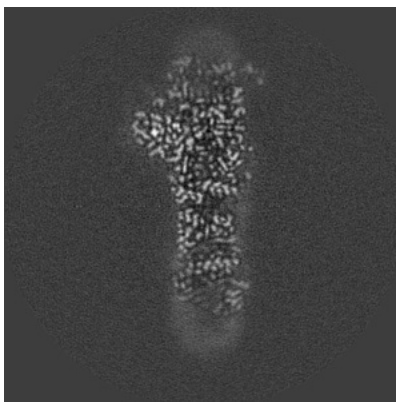


Z Index: 160

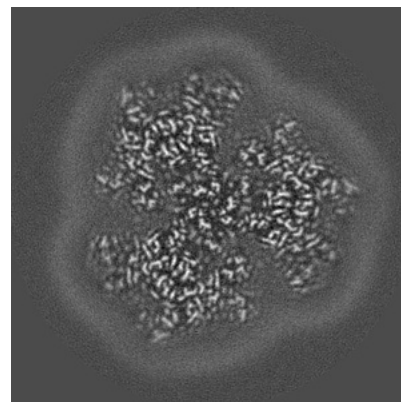
6.2.2 Raw map



X Index: 160



Y Index: 160

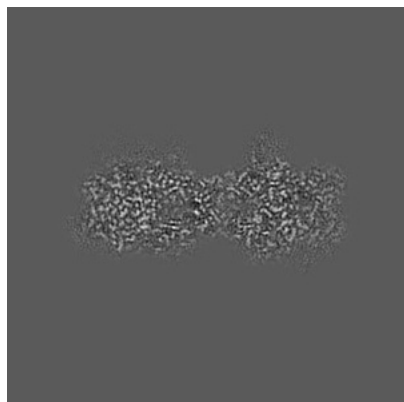


Z Index: 160

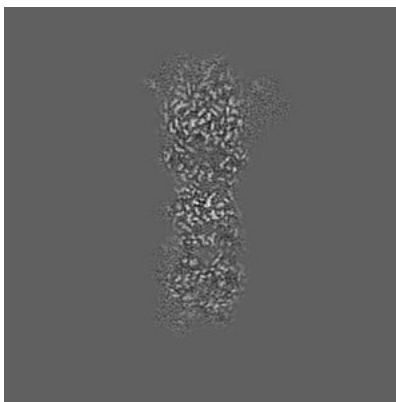
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

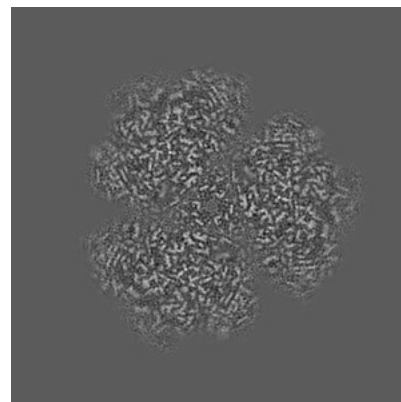
6.3.1 Primary map



X Index: 142

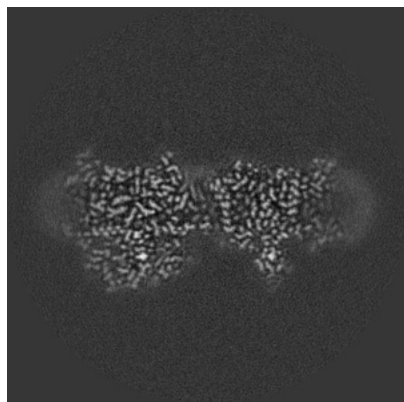


Y Index: 175

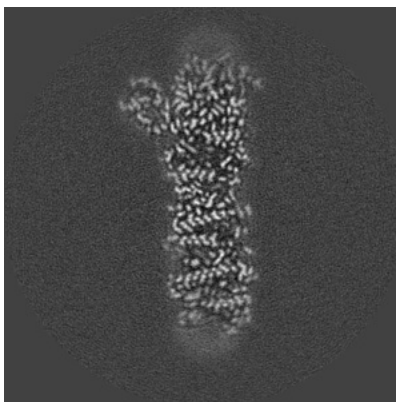


Z Index: 174

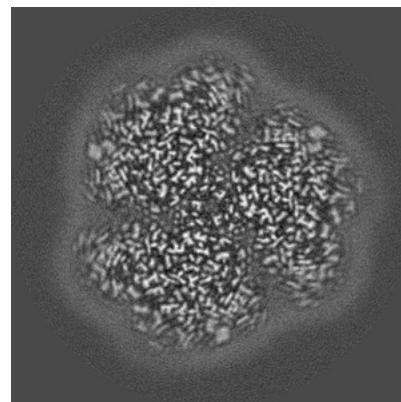
6.3.2 Raw map



X Index: 131



Y Index: 175

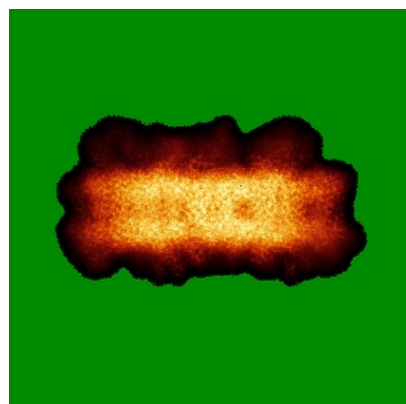


Z Index: 175

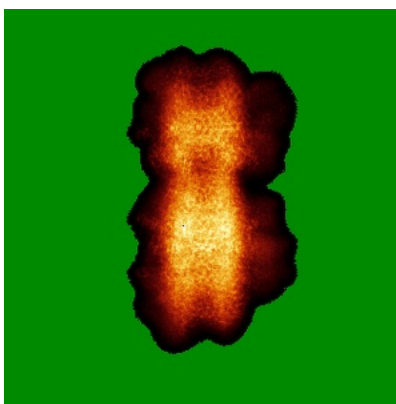
The images above show the largest variance slices of the map in three orthogonal directions.

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

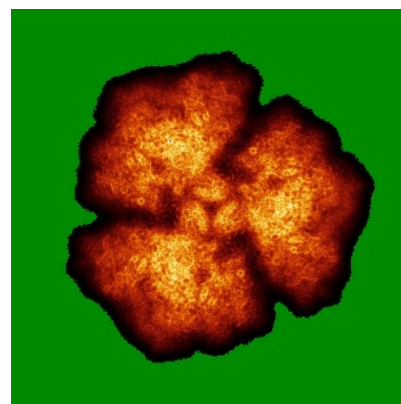
6.4.1 Primary map



X

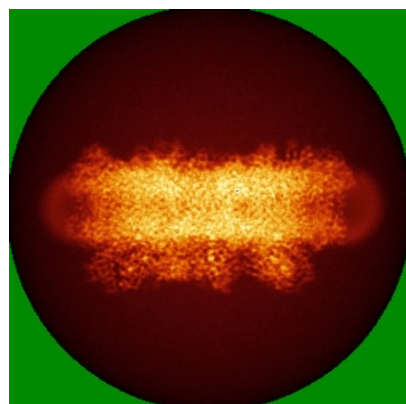


Y

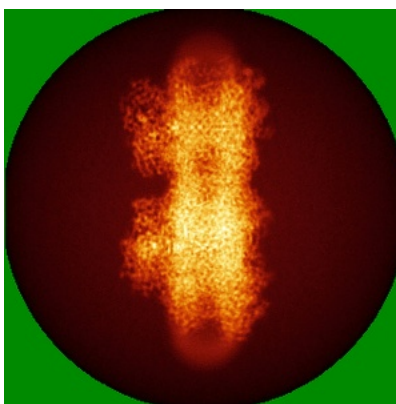


Z

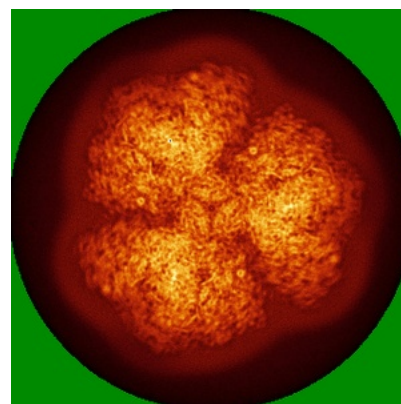
6.4.2 Raw map



X



Y

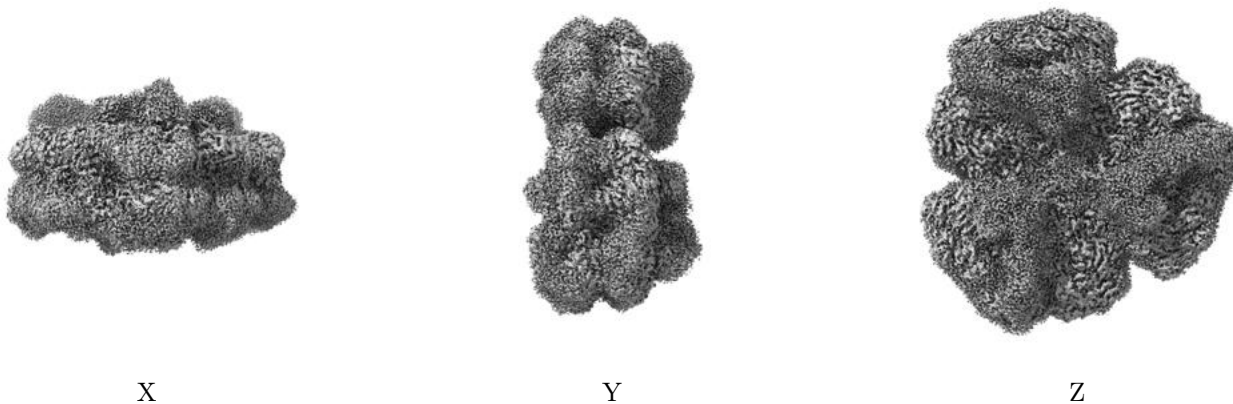


Z

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.

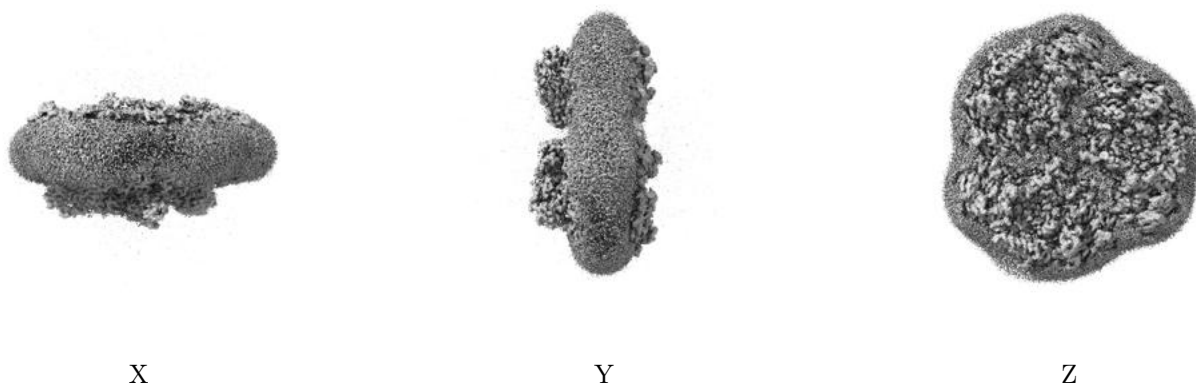
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.00112. 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.

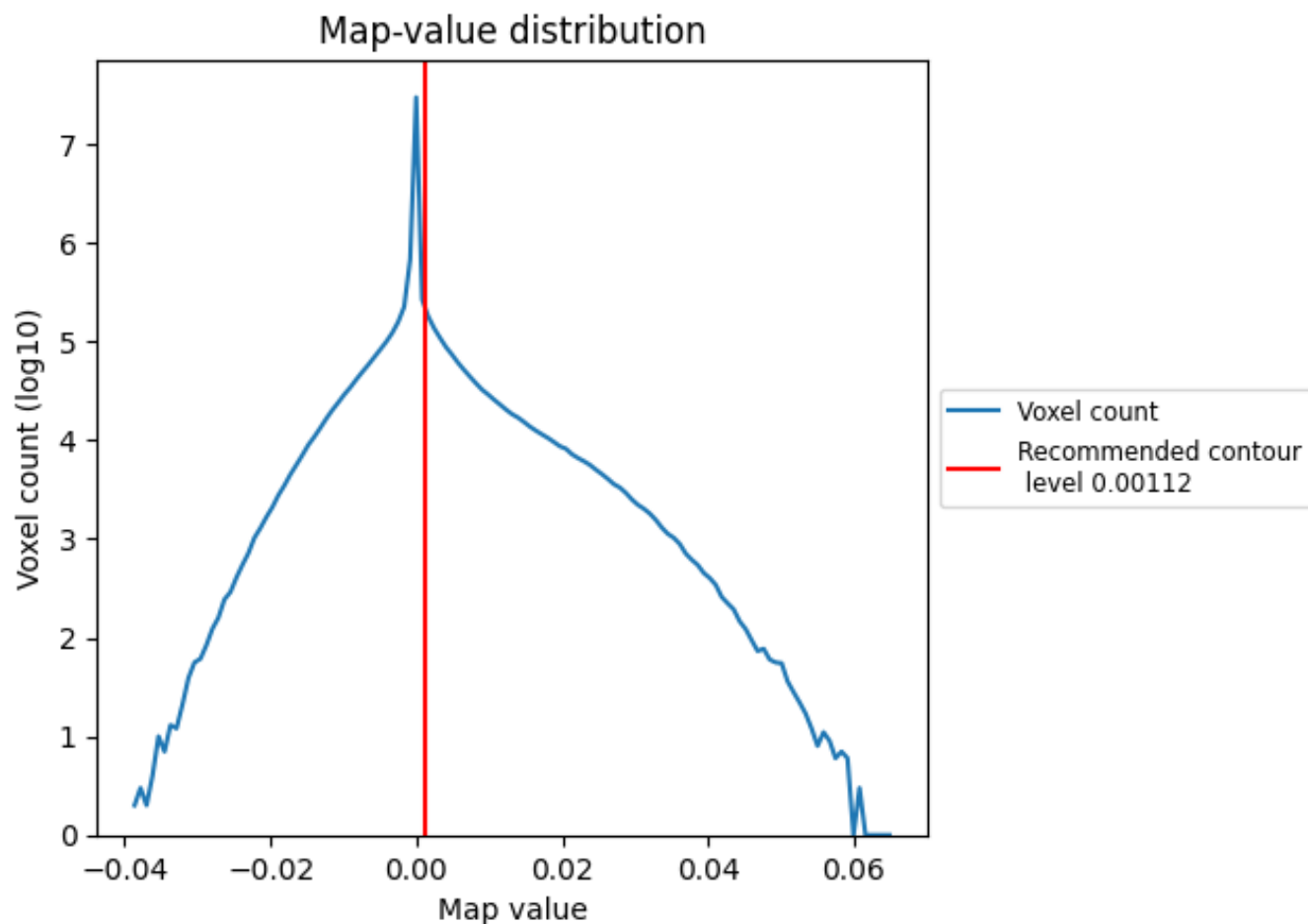
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

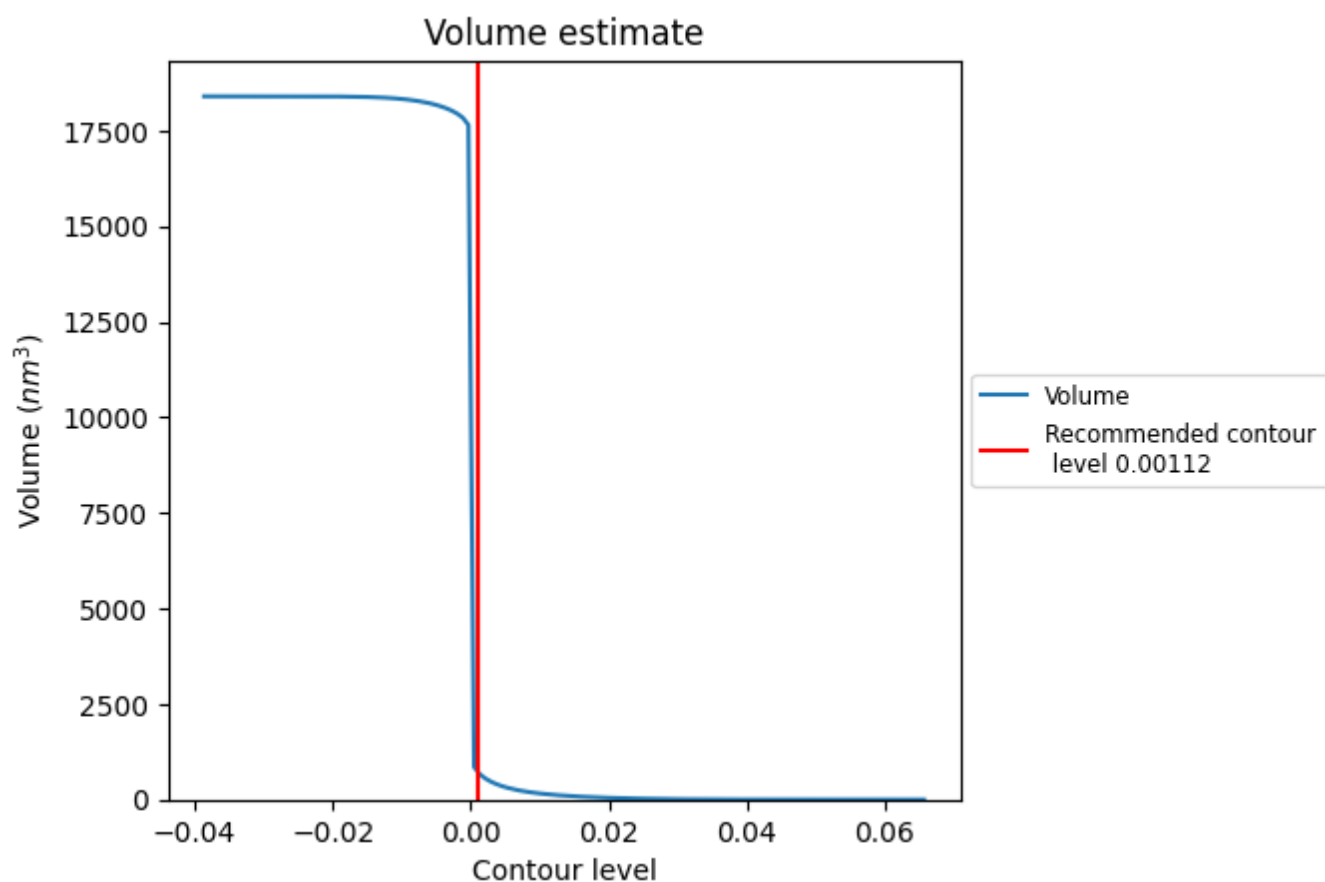
This section contains the results of statistical analysis of the map.

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.

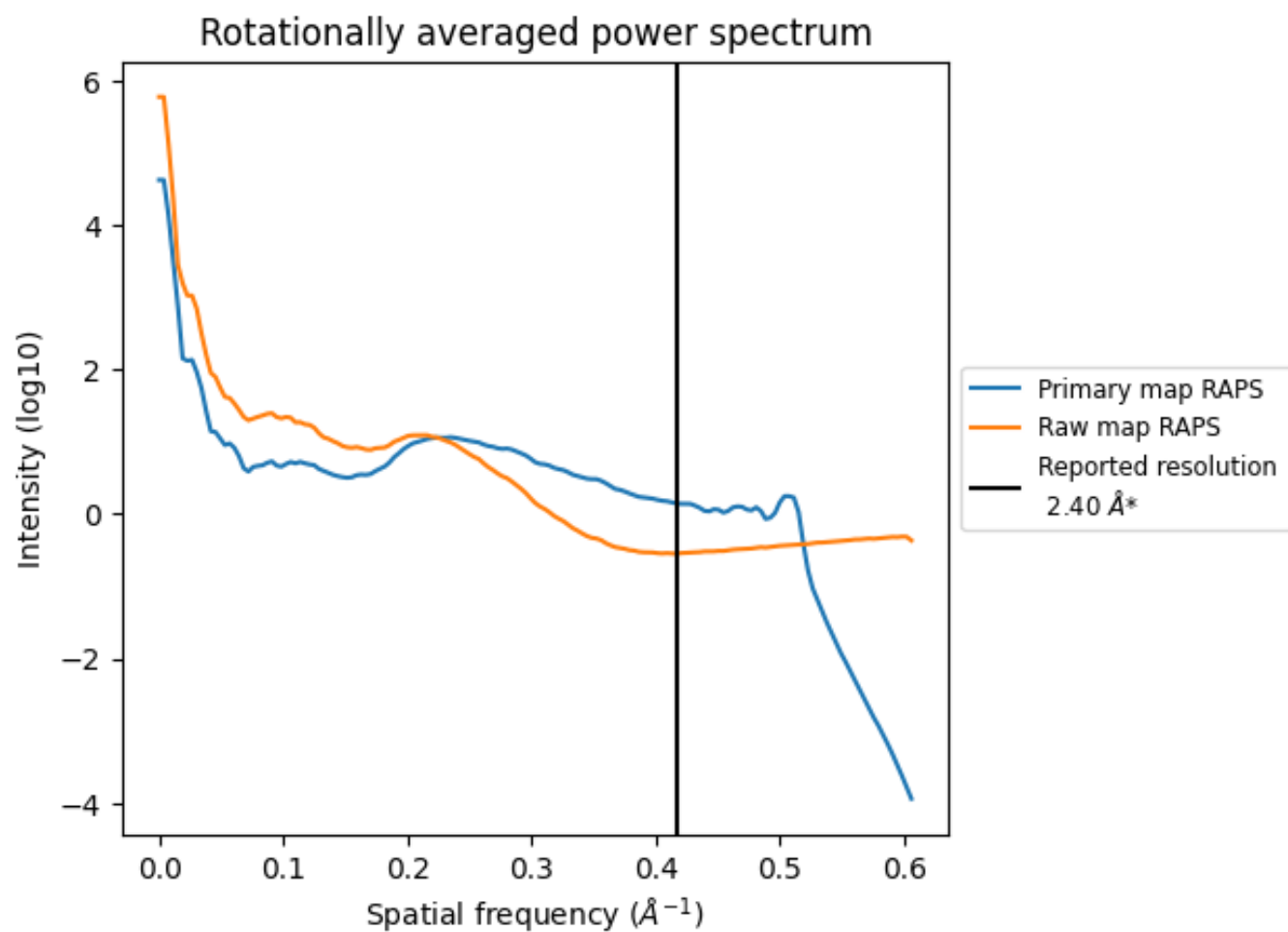
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 708 nm³; this corresponds to an approximate mass of 640 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 ⓘ

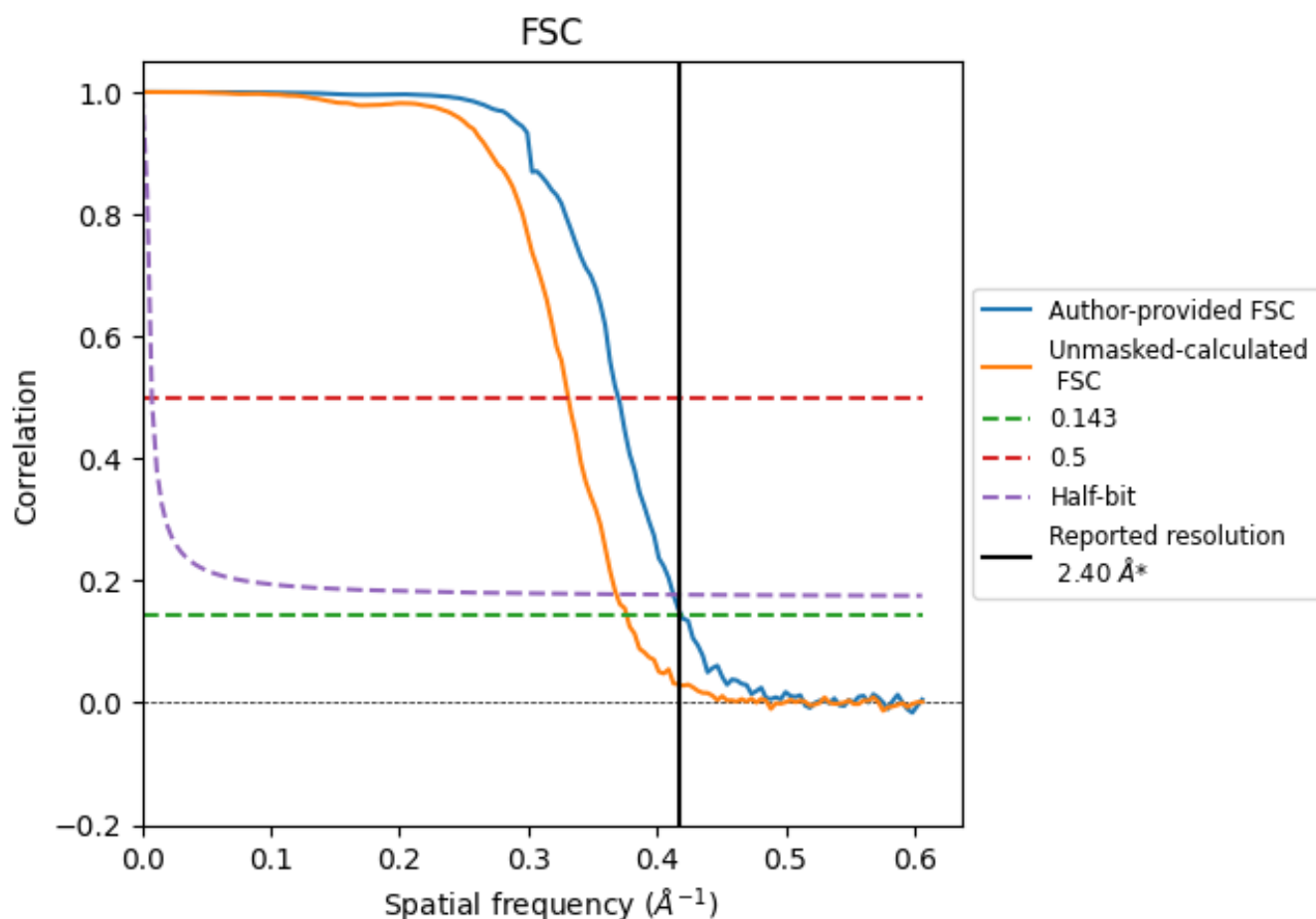


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

8.2 Resolution estimates [i](#)

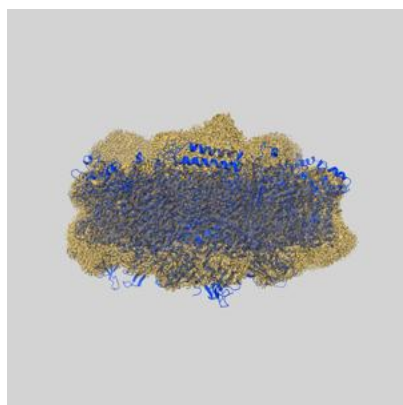
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.70	2.42
Unmasked-calculated*	2.66	3.02	2.71

*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 2.66 differs from the reported value 2.4 by more than 10 %

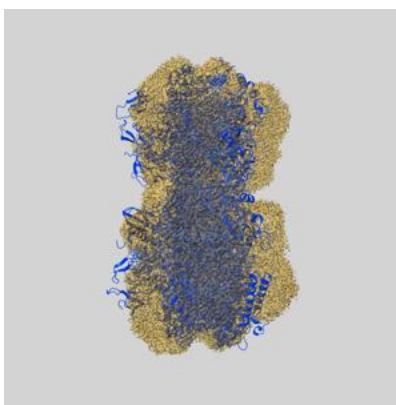
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47359 and PDB model 9E0J. Per-residue inclusion information can be found in section [3](#) on page [36](#).

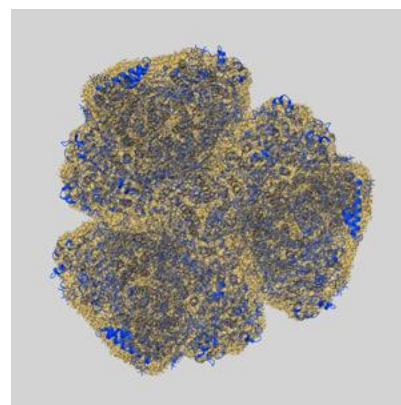
9.1 Map-model overlay [i](#)



X



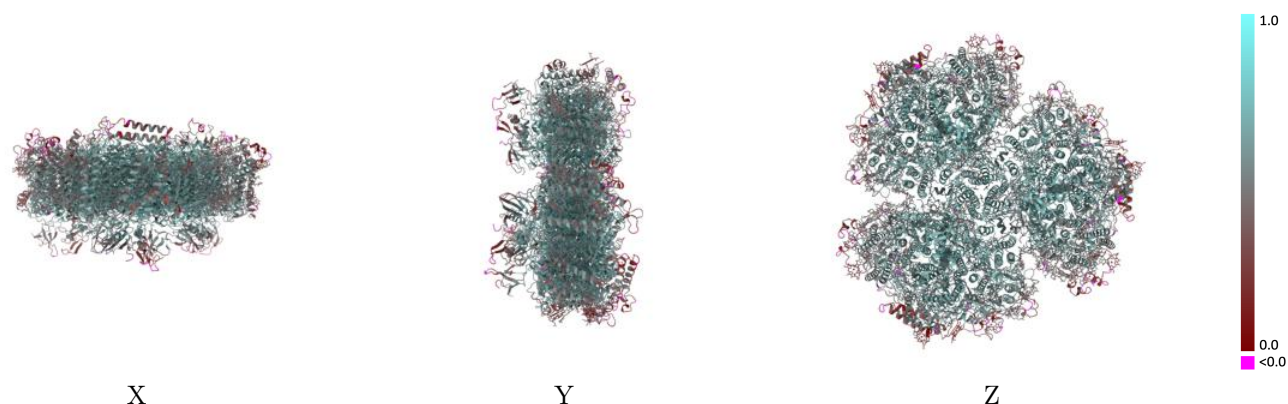
Y



Z

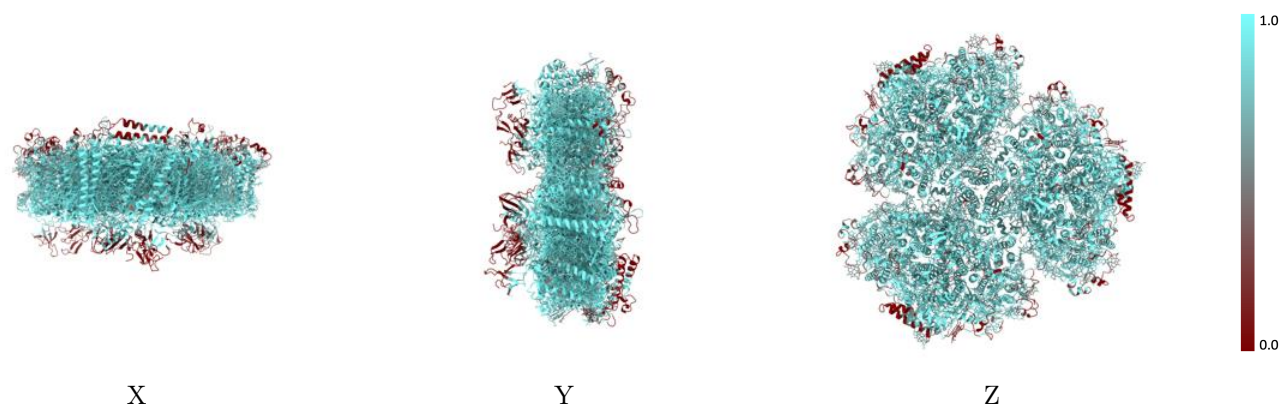
The images above show the 3D surface view of the map at the recommended contour level 0.00112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



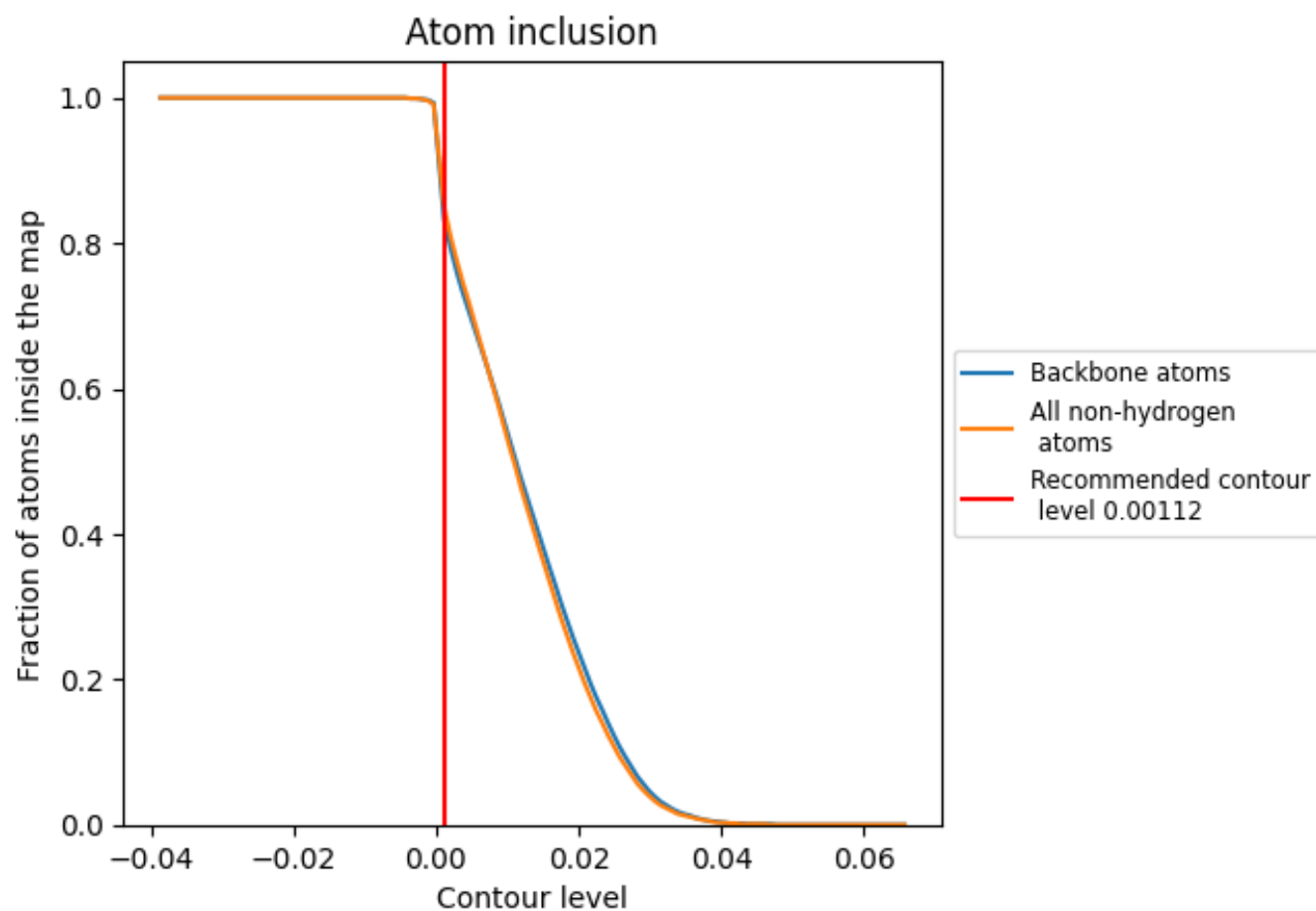
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.00112).































































9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 85% 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 (0.00112) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8510	 0.5700
A	 0.9120	 0.5760
B	 0.9030	 0.6090
C	 0.3140	 0.4440
D	 0.4860	 0.4910
E	 0.4120	 0.3990
F	 0.6840	 0.4230
G	 0.9130	 0.5760
H	 0.8980	 0.6030
I	 0.9590	 0.6510
J	 0.7760	 0.4280
K	 0.3120	 0.4410
L	 0.9010	 0.6240
M	 0.9370	 0.6550
N	 0.4850	 0.5060
O	 0.4290	 0.4260
P	 0.6600	 0.4140
Q	 0.9450	 0.6480
R	 0.7480	 0.3910
S	 0.8980	 0.6210
T	 0.9400	 0.6400
a	 0.9100	 0.5760
b	 0.9000	 0.6050
c	 0.3170	 0.4490
d	 0.4840	 0.4930
e	 0.4100	 0.4110
f	 0.6690	 0.4100
i	 0.9670	 0.6570
j	 0.7930	 0.4330
l	 0.9000	 0.6200
m	 0.9370	 0.6320

