



wwPDB EM Validation Summary Report ⓘ

Apr 29, 2025 – 12:54 PM EDT

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

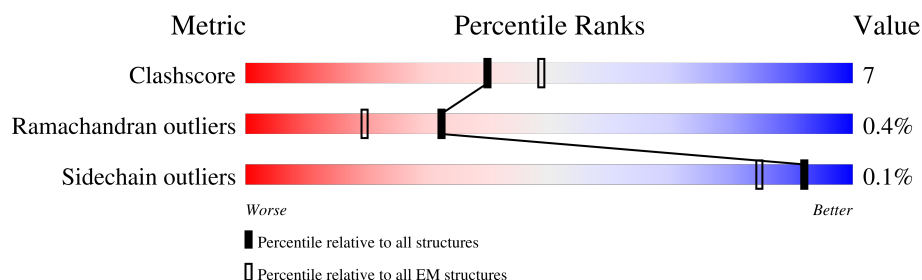
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.40 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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>•</div> <div>88%</div> <div>9%</div> <div>•</div> </div>
2	T	32	<div> <div>•</div> <div>91%</div> <div>6%</div> <div>•</div> </div>
2	m	32	<div> <div>6%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
3	B	749	<div> <div>10%</div> <div>85%</div> <div>15%</div> <div></div> </div>
3	H	749	<div> <div>10%</div> <div>83%</div> <div>16%</div> <div>•</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	
10	l	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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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		

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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

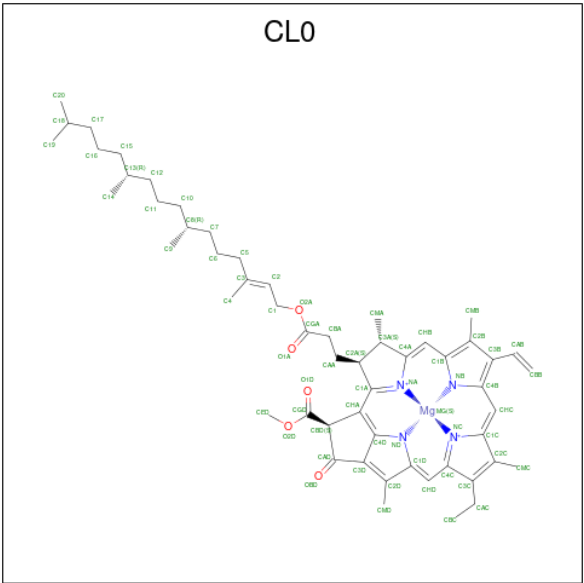
- Molecule 9 is a protein called Photosystem I reaction center subunit IX.

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.

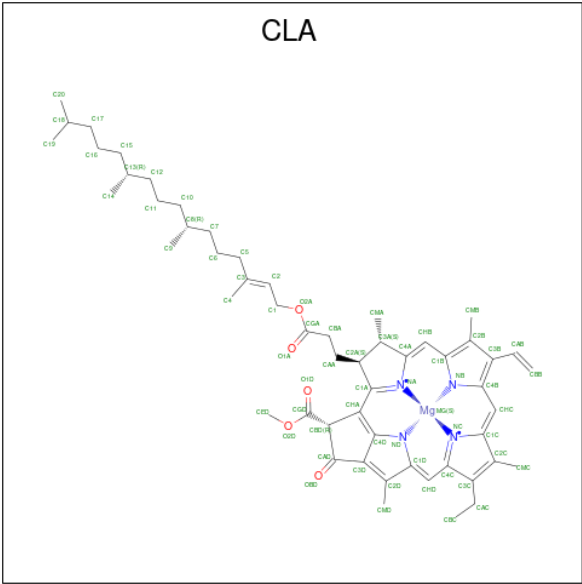
Mol	Chain	Residues	Atoms					AltConf	Trace
10	S	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	l	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		
10	L	154	Total	C	N	O	S	0	0
			1159	772	186	198	3		

- 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).



Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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
			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
			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	
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
			55	45	1	4	5	
12	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 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 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 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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

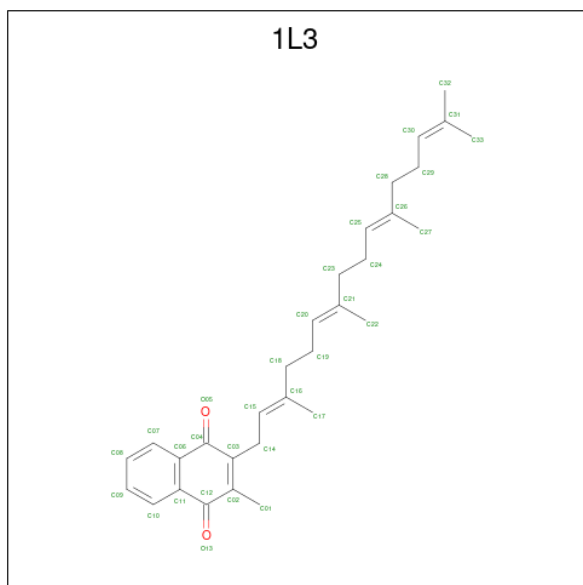
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total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

Continued on next page...

Continued from previous page...

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: $C_{31}H_{40}O_2$).



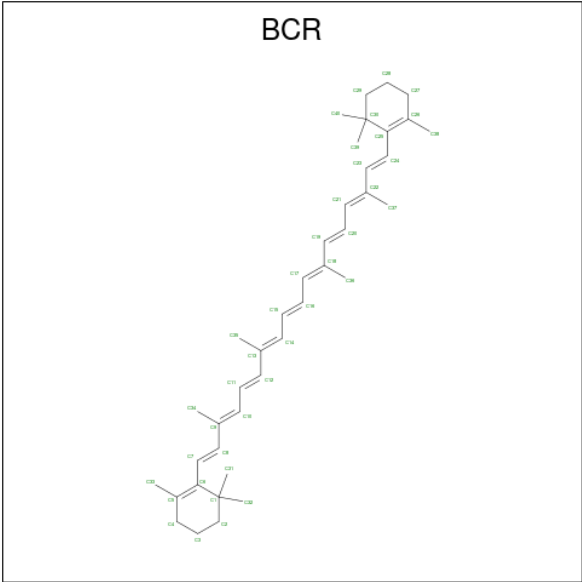
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			33	31	2	
13	H	1	Total	C	O	0
			33	31	2	
13	a	1	Total	C	O	0
			33	31	2	
13	b	1	Total	C	O	0
			33	31	2	
13	A	1	Total	C	O	0
			33	31	2	
13	B	1	Total	C	O	0
			33	31	2	

- 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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

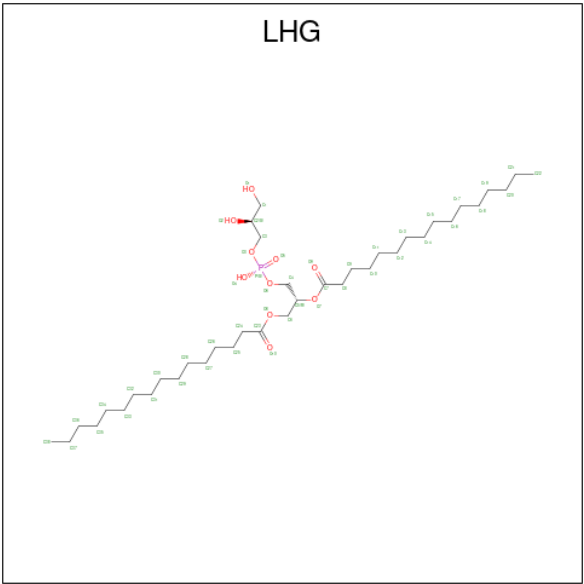
Mol	Chain	Residues	Atoms	AltConf
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	l	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C 40 40	0
15	A	1	Total C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

Continued on next page...

Continued from previous page...

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).



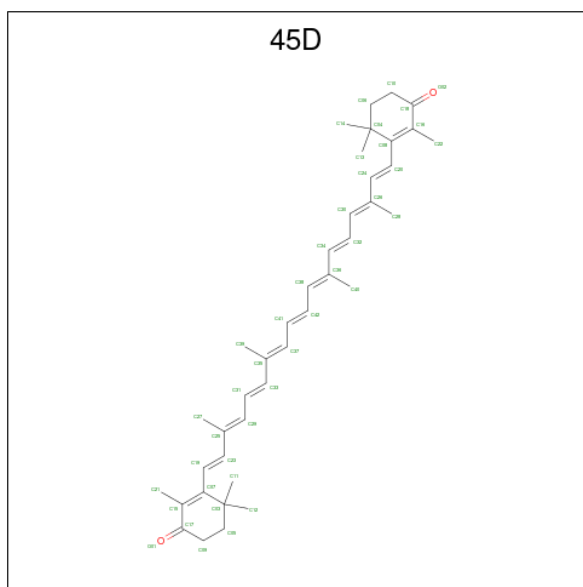
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			49	38	10	1	

Continued on next page...

Continued from previous page...

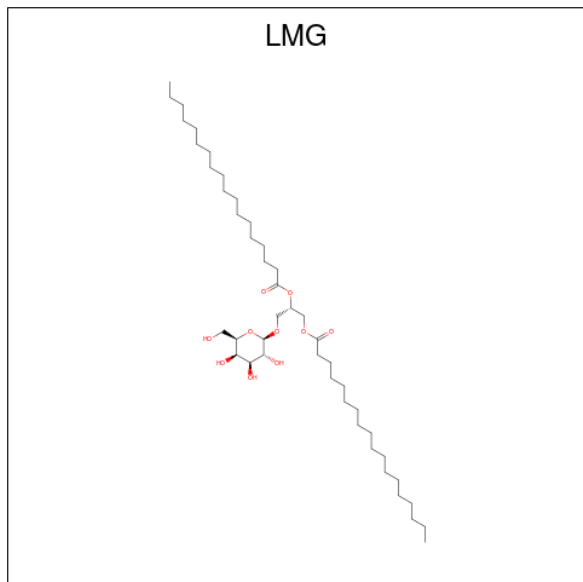
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			27	16	10	1	
16	G	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	a	1	Total	C	O	P	0
			27	16	10	1	
16	a	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			49	38	10	1	
16	A	1	Total	C	O	P	0
			27	16	10	1	
16	A	1	Total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

- Molecule 17 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂) (labeled as "Ligand of Interest" by depositor).



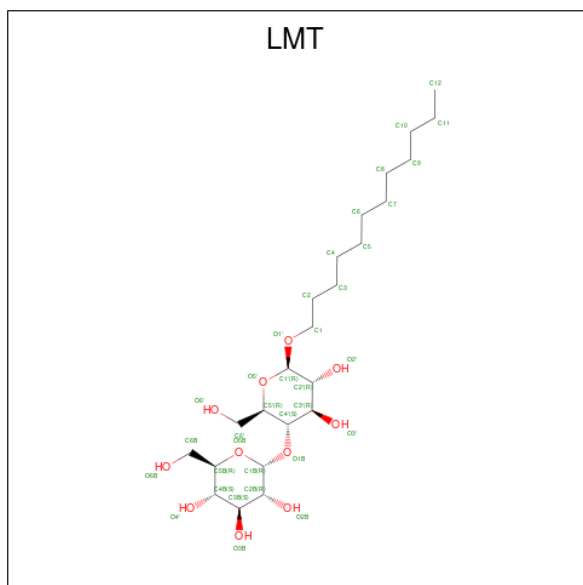
Mol	Chain	Residues	Atoms			AltConf
17	T	1	Total	C	O	0
			42	40	2	
17	m	1	Total	C	O	0
			42	40	2	
17	M	1	Total	C	O	0
			42	40	2	

- 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	

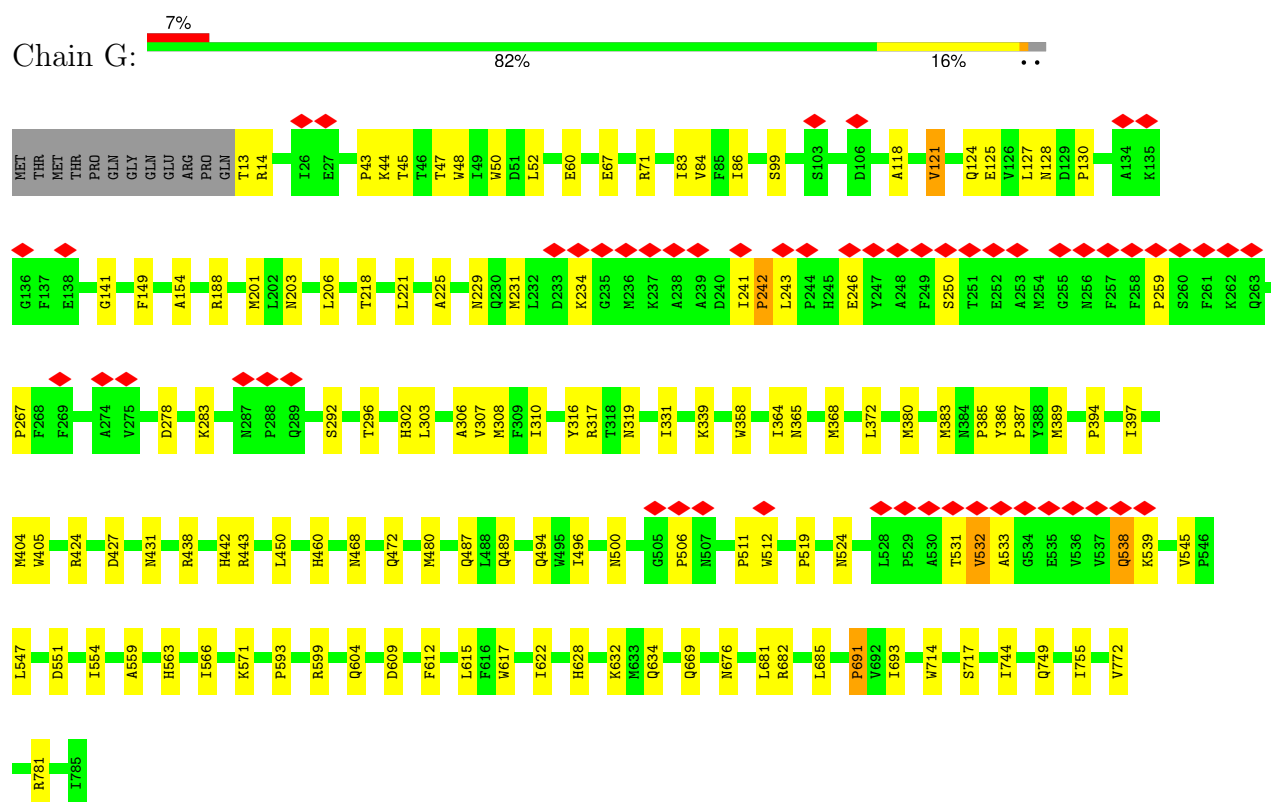
- Molecule 20 is water.

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	

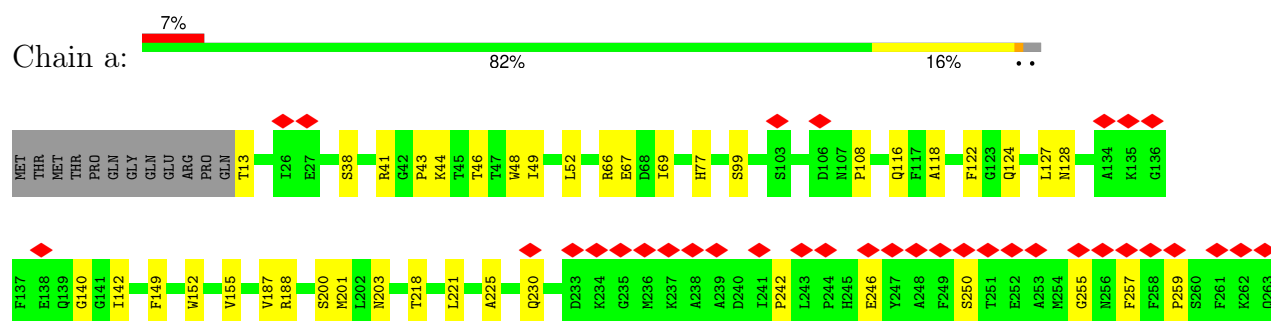
3 Residue-property plots

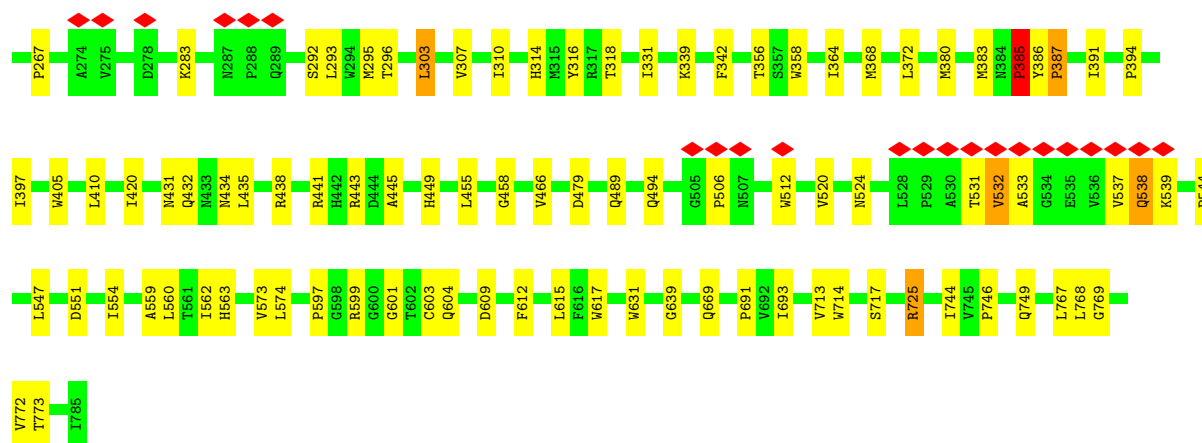
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

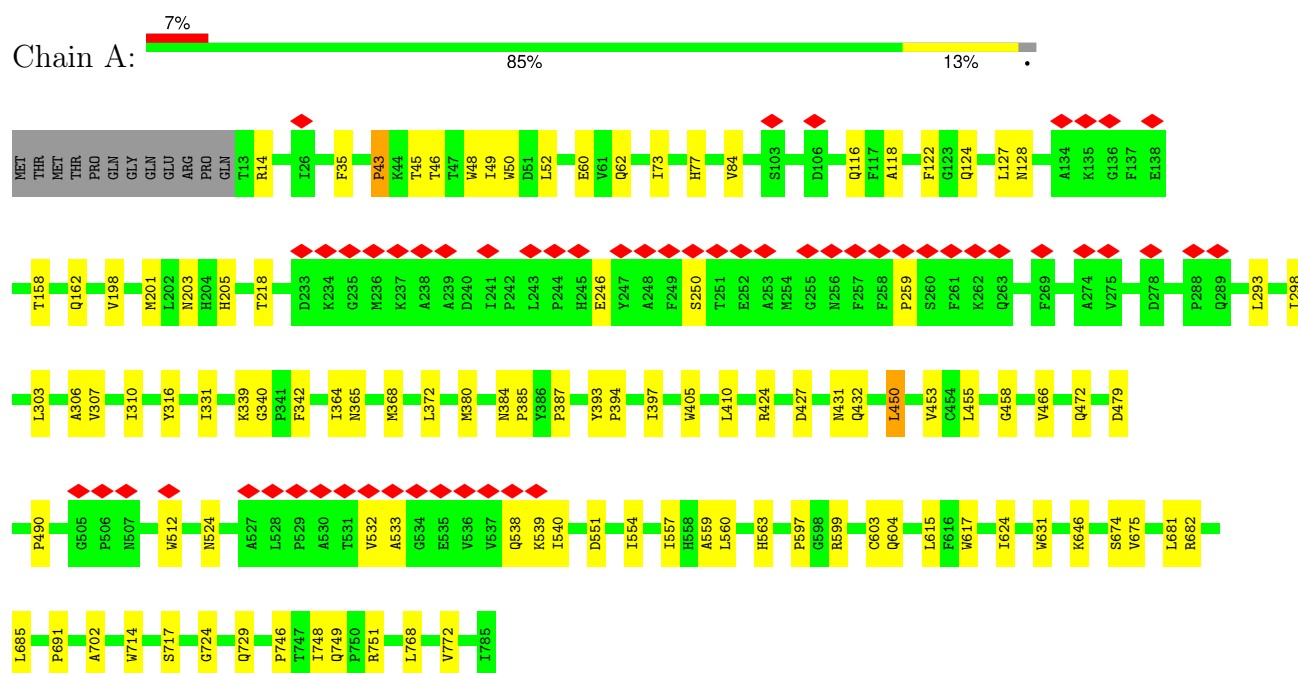


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

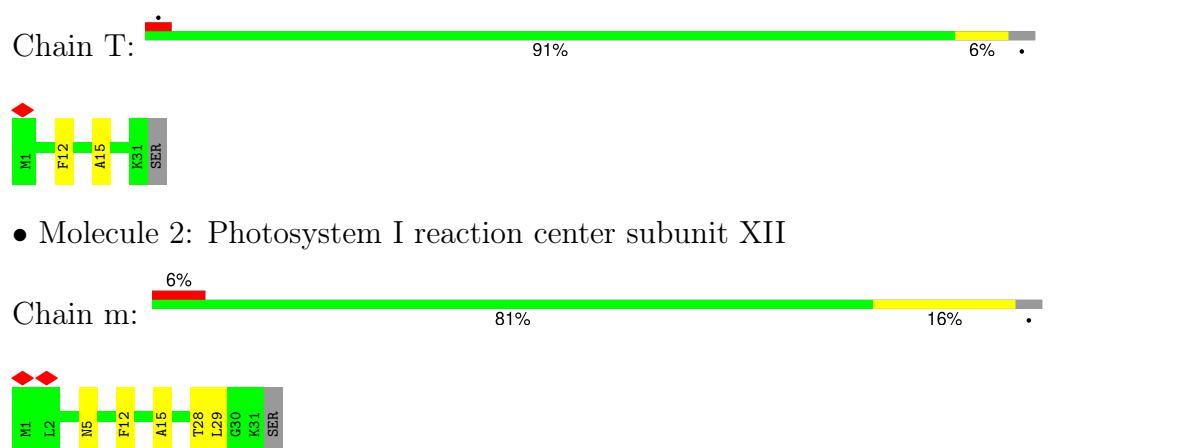




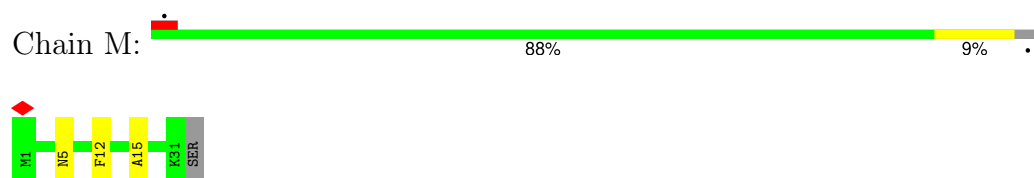
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



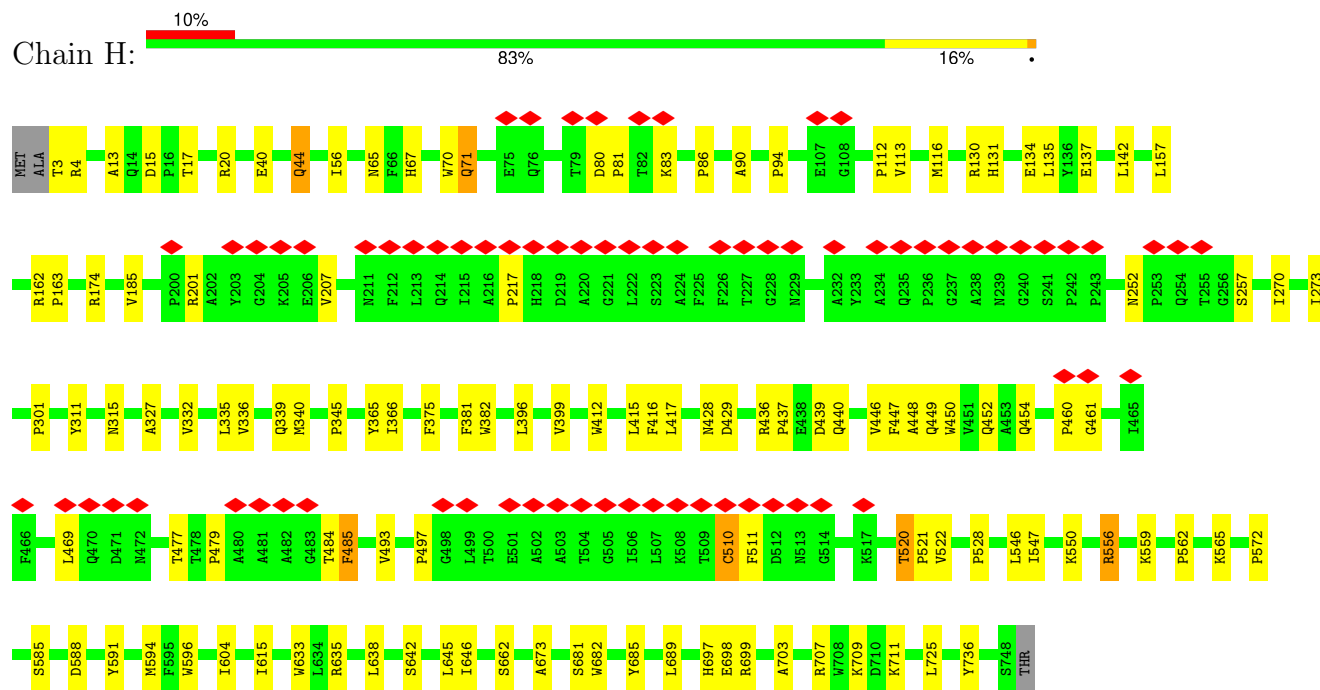
- Molecule 2: Photosystem I reaction center subunit XII



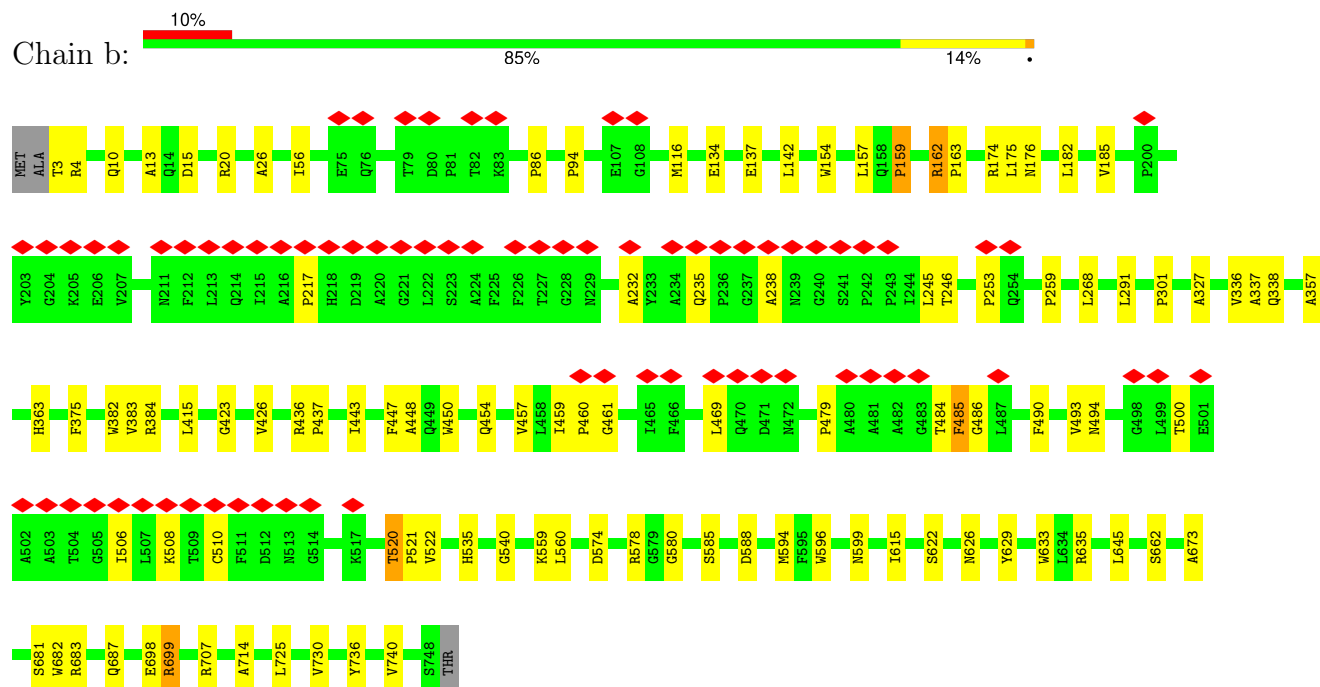
- Molecule 2: Photosystem I reaction center subunit XII



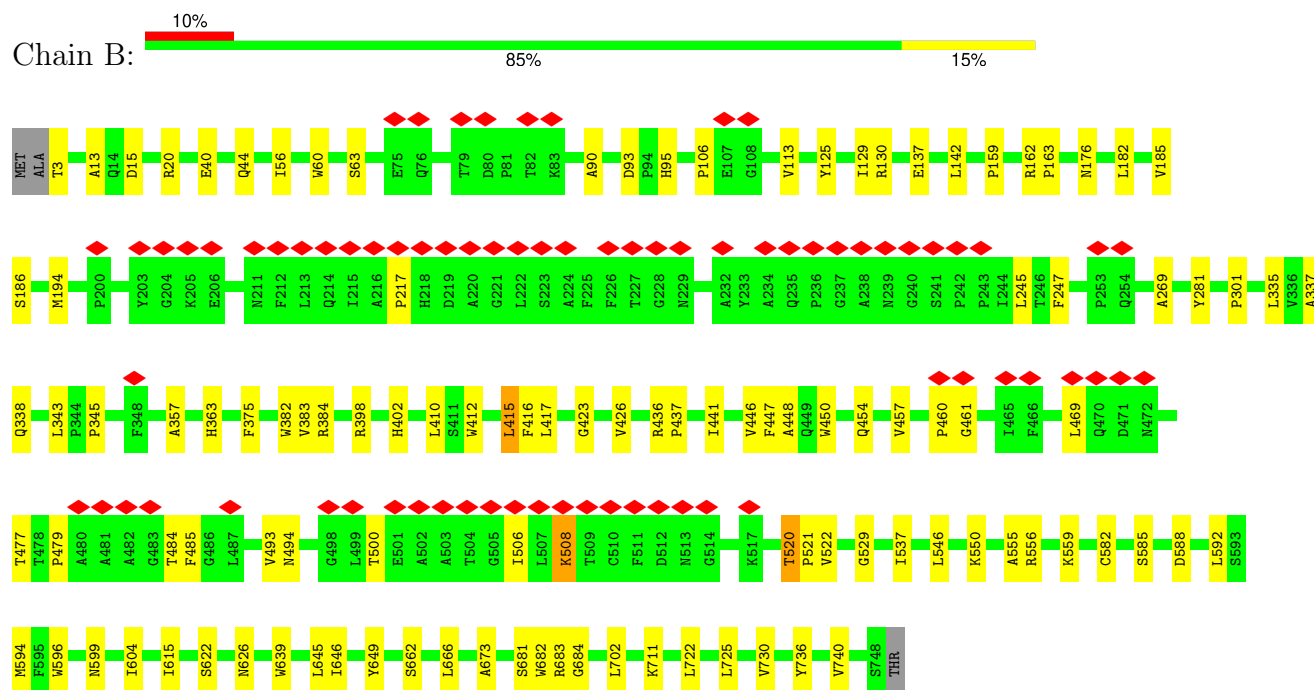
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



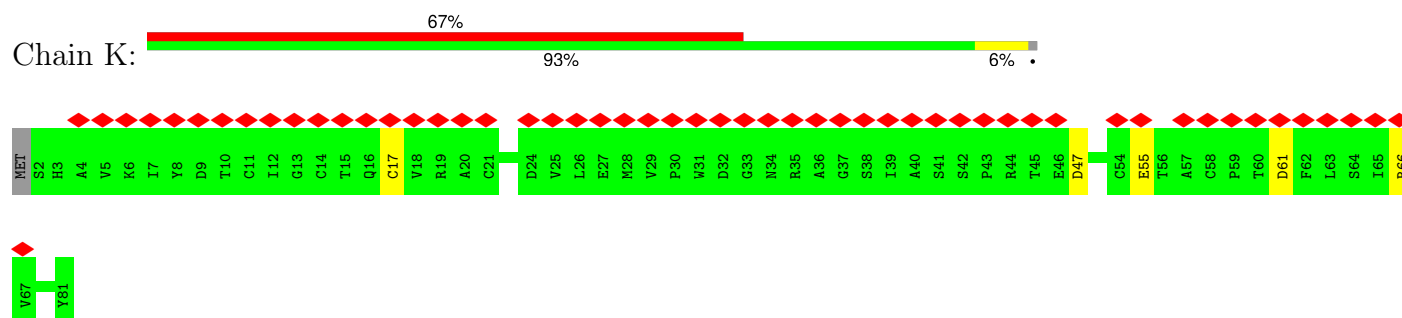
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



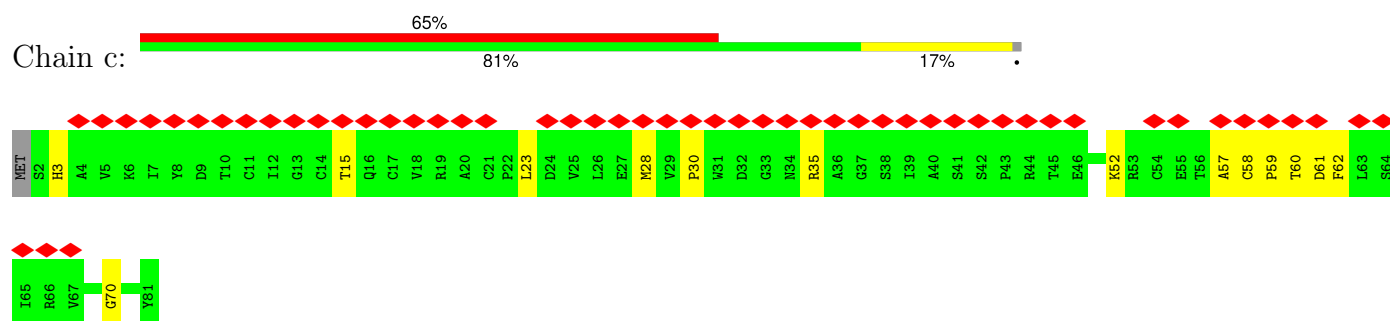
- Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



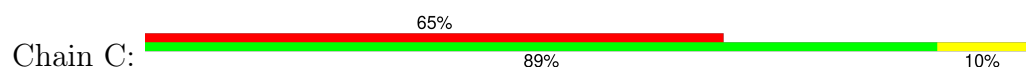
- Molecule 4: Photosystem I iron-sulfur center

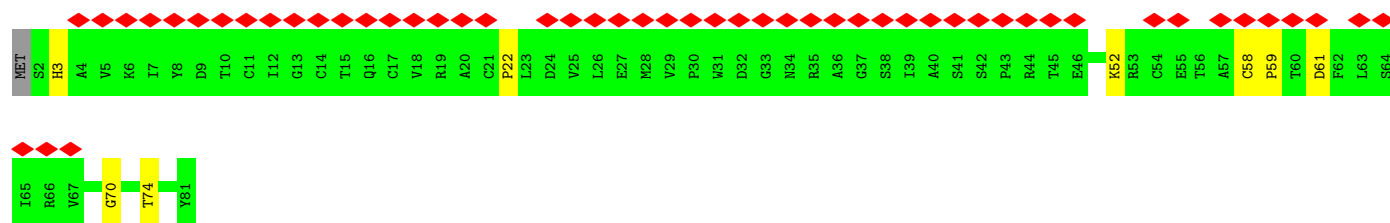


- Molecule 4: Photosystem I iron-sulfur center

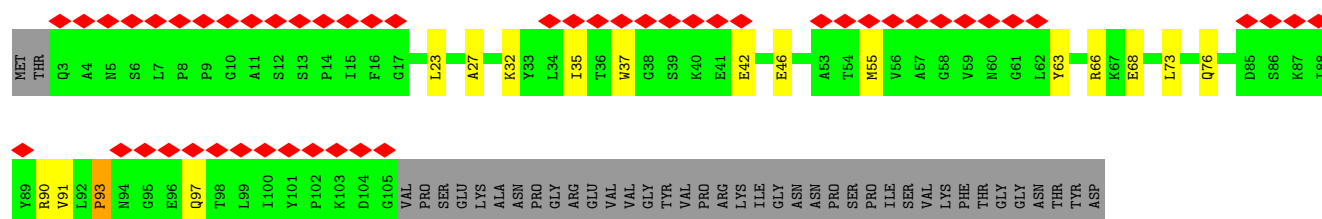


- Molecule 4: Photosystem I iron-sulfur center

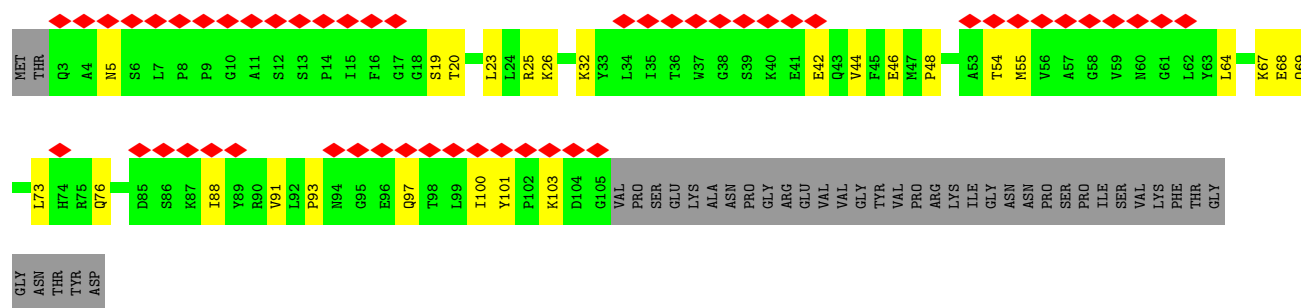




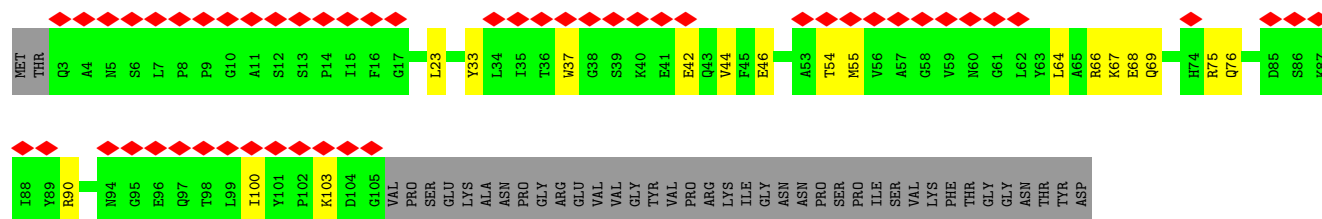
• Molecule 5: Photosystem I reaction center subunit II



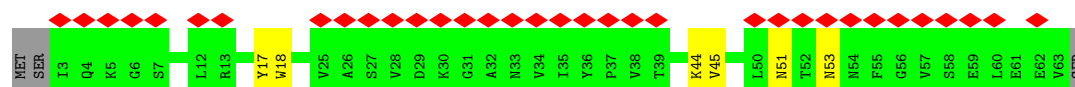
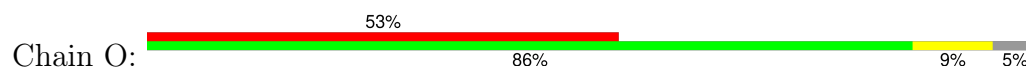
• Molecule 5: Photosystem I reaction center subunit II



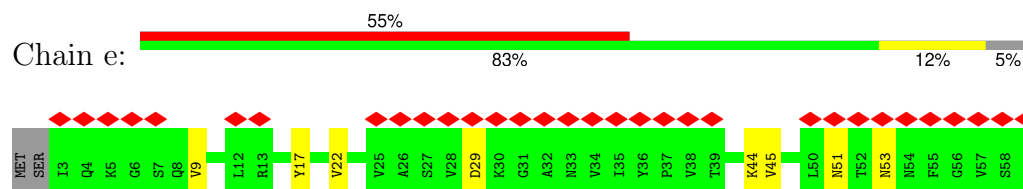
• Molecule 5: Photosystem I reaction center subunit II



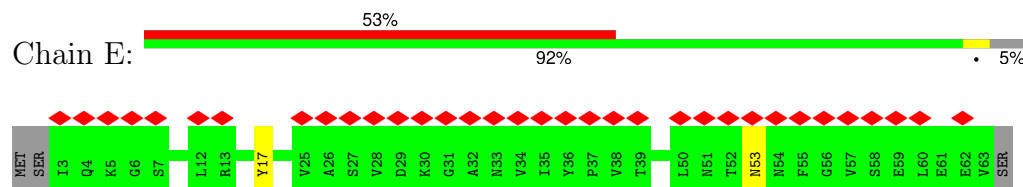
• Molecule 6: Photosystem I reaction center subunit IV



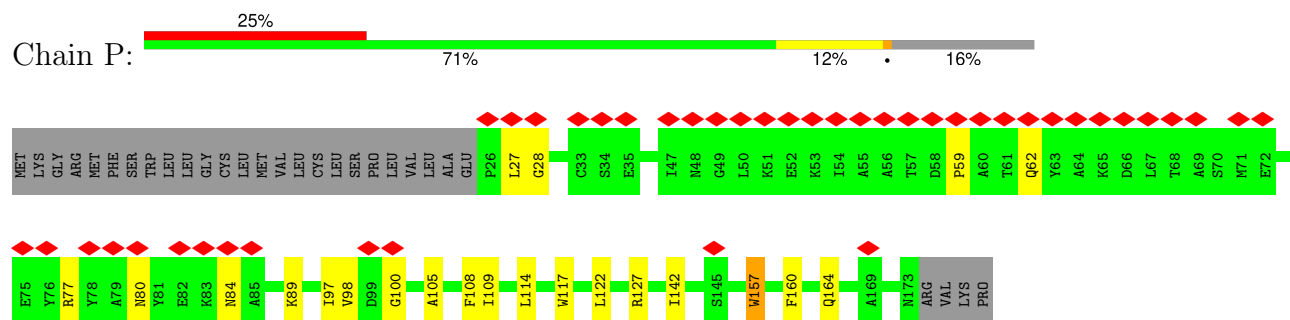
- Molecule 6: Photosystem I reaction center subunit IV



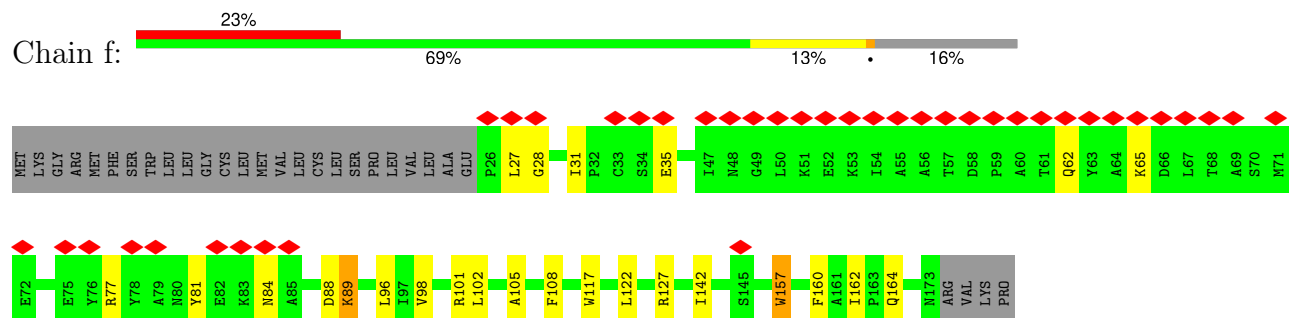
- Molecule 6: Photosystem I reaction center subunit IV



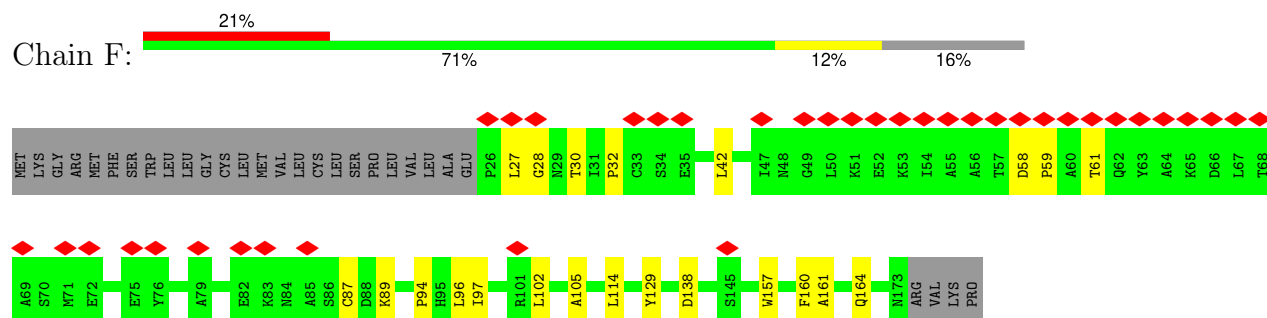
- Molecule 7: Photosystem I reaction center subunit III



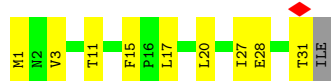
- Molecule 7: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit III



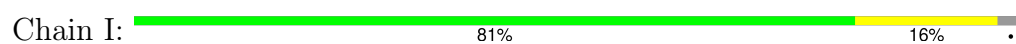
- Molecule 8: Photosystem I reaction center subunit VIII



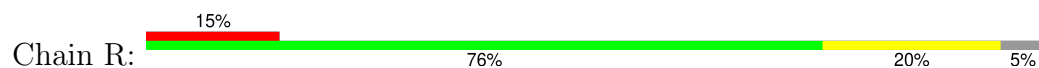
- Molecule 8: Photosystem I reaction center subunit VIII



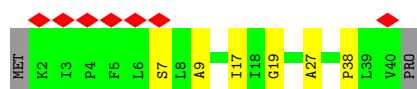
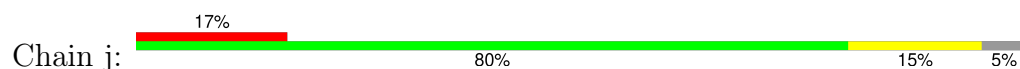
- Molecule 8: Photosystem I reaction center subunit VIII



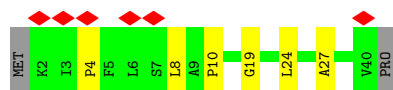
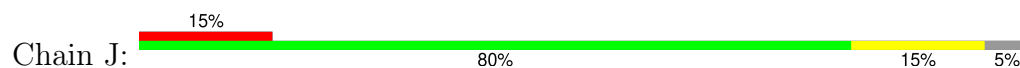
- Molecule 9: Photosystem I reaction center subunit IX



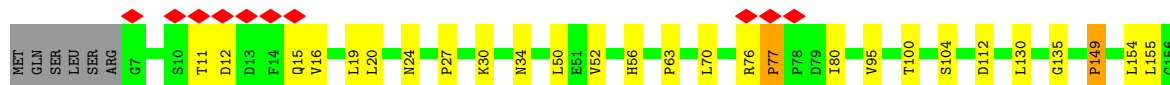
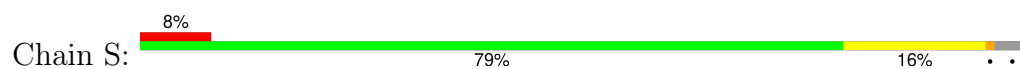
- Molecule 9: Photosystem I reaction center subunit IX



- Molecule 9: Photosystem I reaction center subunit IX

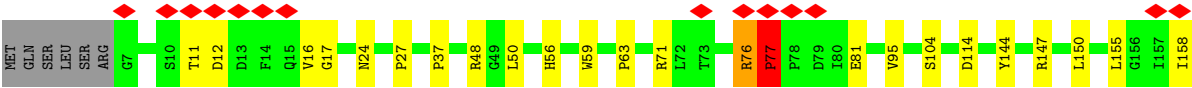
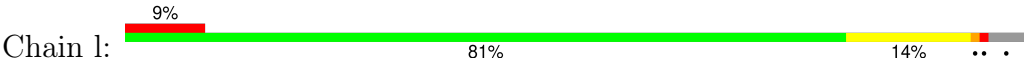


- Molecule 10: Photosystem I reaction center subunit XI

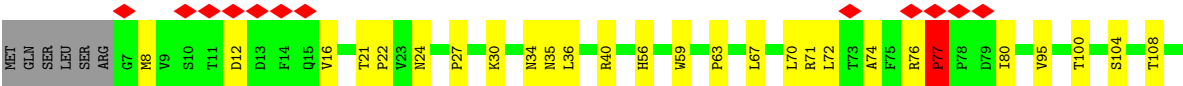




• Molecule 10: Photosystem I reaction center subunit XI



• 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 45D, LMG, SF4, BCR, CL0, 1L3, LMT, CLA, LHG

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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%)	22	33
1	G	771/785 (98%)	725 (94%)	40 (5%)	6 (1%)	16	26
1	a	771/785 (98%)	722 (94%)	45 (6%)	4 (0%)	25	38
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	65
3	H	744/749 (99%)	702 (94%)	41 (6%)	1 (0%)	48	65
3	b	744/749 (99%)	700 (94%)	43 (6%)	1 (0%)	48	65
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%)	19	29
7	P	146/177 (82%)	134 (92%)	11 (8%)	1 (1%)	19	29
7	f	146/177 (82%)	135 (92%)	10 (7%)	1 (1%)	19	29
8	I	29/32 (91%)	27 (93%)	2 (7%)	0	100	100

Continued on next page...

Continued from previous page...

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%)	10	15
10	S	152/160 (95%)	145 (95%)	5 (3%)	2 (1%)	10	15
10	l	152/160 (95%)	143 (94%)	7 (5%)	2 (1%)	10	15
All	All	6438/6792 (95%)	6065 (94%)	346 (5%)	27 (0%)	32	44

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%)	92	97
1	a	603/628 (96%)	601 (100%)	2 (0%)	91	96
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

Continued on next page...

Continued from previous page...

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%)	67	82
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%)	92	97

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
16	LHG	A	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.24	3 (10%)
15	BCR	S	205	-	41,41,41	2.67	6 (14%)	56,56,56	6.46	25 (44%)
12	CLA	b	815	-	58,68,73	2.26	19 (32%)	68,107,113	2.75	24 (35%)
12	CLA	G	813	1	48,58,73	2.60	20 (41%)	56,95,113	2.98	27 (48%)
14	SF4	G	844	1,3	0,12,12	-	-	-	-	-
17	45D	m	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.90	31 (57%)
12	CLA	S	203	10	63,73,73	2.27	19 (30%)	74,113,113	2.63	25 (33%)
12	CLA	H	819	-	43,53,73	2.73	20 (46%)	50,89,113	2.90	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	804	1	63,73,73	2.29	21 (33%)	74,113,113	2.50	25 (33%)
12	CLA	A	807	1	63,73,73	2.24	19 (30%)	74,113,113	2.65	25 (33%)
12	CLA	G	824	-	53,63,73	2.48	21 (39%)	62,101,113	2.67	23 (37%)
15	BCR	A	849	-	41,41,41	2.63	6 (14%)	56,56,56	6.81	25 (44%)
12	CLA	G	840	1	48,58,73	2.64	19 (39%)	56,95,113	2.78	25 (44%)
12	CLA	B	831	-	43,53,73	2.70	19 (44%)	50,89,113	2.80	22 (44%)
12	CLA	H	817	-	63,73,73	2.28	20 (31%)	74,113,113	2.28	23 (31%)
12	CLA	G	809	1	48,58,73	2.67	21 (43%)	56,95,113	2.91	24 (42%)
15	BCR	Q	101	-	41,41,41	2.62	6 (14%)	56,56,56	6.90	22 (39%)
12	CLA	B	827	3	43,53,73	2.66	18 (41%)	50,89,113	2.72	22 (44%)
12	CLA	G	807	1	63,73,73	2.23	19 (30%)	74,113,113	2.67	22 (29%)
12	CLA	G	828	-	58,68,73	2.34	19 (32%)	68,107,113	2.56	25 (36%)
12	CLA	A	815	-	43,53,73	2.62	19 (44%)	50,89,113	2.90	23 (46%)
15	BCR	B	844	-	41,41,41	2.64	6 (14%)	56,56,56	6.82	25 (44%)
15	BCR	G	850	-	41,41,41	2.65	6 (14%)	56,56,56	6.77	25 (44%)
15	BCR	b	844	-	41,41,41	2.57	6 (14%)	56,56,56	6.69	22 (39%)
12	CLA	a	806	-	63,73,73	2.23	18 (28%)	74,113,113	2.67	25 (33%)
14	SF4	C	102	4	0,12,12	-	-	-	-	-
12	CLA	P	201	20	63,73,73	2.31	20 (31%)	74,113,113	2.37	23 (31%)
12	CLA	B	819	-	43,53,73	2.66	20 (46%)	50,89,113	2.88	23 (46%)
15	BCR	H	844	-	25,25,41	2.21	2 (8%)	33,33,56	7.59	18 (54%)
12	CLA	a	827	-	58,68,73	2.35	19 (32%)	68,107,113	2.58	25 (36%)
16	LHG	G	851	-	48,48,48	0.91	2 (4%)	51,54,54	1.05	3 (5%)
12	CLA	S	202	10	53,63,73	2.49	19 (35%)	62,101,113	2.66	26 (41%)
12	CLA	a	841	20	63,73,73	2.22	20 (31%)	74,113,113	2.43	26 (35%)
15	BCR	b	842	-	25,25,41	2.19	2 (8%)	33,33,56	7.60	18 (54%)
12	CLA	B	802	-	63,73,73	2.24	21 (33%)	74,113,113	2.77	30 (40%)
15	BCR	H	846	-	41,41,41	2.59	6 (14%)	56,56,56	6.68	19 (33%)
12	CLA	H	822	20	63,73,73	2.26	19 (30%)	74,113,113	2.46	28 (37%)
15	BCR	R	101	-	41,41,41	2.67	6 (14%)	56,56,56	6.58	23 (41%)
12	CLA	H	802	-	63,73,73	2.26	20 (31%)	74,113,113	2.86	32 (43%)
12	CLA	a	810	1,12	48,58,73	2.59	20 (41%)	56,95,113	2.94	26 (46%)
12	CLA	G	808	1	63,73,73	2.22	19 (30%)	74,113,113	2.61	24 (32%)
15	BCR	G	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.69	22 (39%)
12	CLA	B	838	-	63,73,73	2.28	20 (31%)	74,113,113	2.60	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	815	-	43,53,73	2.67	20 (46%)	50,89,113	2.92	24 (48%)
12	CLA	S	204	20	63,73,73	2.30	20 (31%)	74,113,113	2.51	23 (31%)
12	CLA	L	206	20	63,73,73	2.30	19 (30%)	74,113,113	2.48	22 (29%)
12	CLA	B	801	-	58,68,73	2.34	18 (31%)	68,107,113	2.70	24 (35%)
12	CLA	a	835	1	43,53,73	2.61	20 (46%)	50,89,113	2.90	21 (42%)
12	CLA	H	839	-	63,73,73	2.27	20 (31%)	74,113,113	2.61	28 (37%)
12	CLA	H	826	-	63,73,73	2.31	20 (31%)	74,113,113	2.12	23 (31%)
12	CLA	a	832	1	63,73,73	2.29	19 (30%)	74,113,113	2.31	23 (31%)
12	CLA	B	803	-	63,73,73	2.30	21 (33%)	74,113,113	2.72	27 (36%)
12	CLA	B	829	3	63,73,73	2.32	22 (34%)	74,113,113	2.53	23 (31%)
15	BCR	F	202	-	41,41,41	2.79	6 (14%)	56,56,56	6.76	23 (41%)
12	CLA	b	825	-	63,73,73	2.30	20 (31%)	74,113,113	2.21	23 (31%)
12	CLA	F	203	-	43,53,73	2.68	20 (46%)	50,89,113	4.72	24 (48%)
12	CLA	G	826	20	53,63,73	2.49	18 (33%)	62,101,113	2.71	29 (46%)
16	LHG	A	853	-	48,48,48	0.93	2 (4%)	51,54,54	3.77	6 (11%)
15	BCR	b	841	-	41,41,41	2.55	6 (14%)	56,56,56	6.66	26 (46%)
12	CLA	A	833	-	63,73,73	2.24	20 (31%)	74,113,113	2.47	25 (33%)
12	CLA	H	825	-	63,73,73	2.22	17 (26%)	74,113,113	2.46	27 (36%)
12	CLA	a	807	-	63,73,73	2.27	20 (31%)	74,113,113	2.63	26 (35%)
12	CLA	G	816	-	43,53,73	2.66	20 (46%)	50,89,113	2.89	23 (46%)
12	CLA	A	812	-	48,58,73	2.63	21 (43%)	56,95,113	2.94	26 (46%)
17	45D	M	101	-	43,43,43	3.99	19 (44%)	54,60,60	7.88	31 (57%)
12	CLA	G	825	20	63,73,73	2.36	21 (33%)	74,113,113	2.42	28 (37%)
15	BCR	L	207	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	18 (32%)
12	CLA	b	833	3	63,73,73	2.26	20 (31%)	74,113,113	2.49	27 (36%)
12	CLA	G	806	-	63,73,73	2.24	20 (31%)	74,113,113	2.65	25 (33%)
12	CLA	b	810	3	63,73,73	2.25	18 (28%)	74,113,113	2.75	29 (39%)
12	CLA	A	818	-	63,73,73	2.23	20 (31%)	74,113,113	2.59	25 (33%)
12	CLA	B	805	3	63,73,73	2.26	20 (31%)	74,113,113	2.57	24 (32%)
11	CL0	A	801	1	63,73,73	2.28	20 (31%)	74,113,113	2.50	27 (36%)
12	CLA	A	809	1	43,53,73	2.68	21 (48%)	50,89,113	2.93	23 (46%)
12	CLA	A	838	1	43,53,73	2.63	20 (46%)	50,89,113	3.01	23 (46%)
12	CLA	A	855	-	63,73,73	2.18	19 (30%)	74,113,113	2.69	27 (36%)
15	BCR	j	101	-	41,41,41	2.69	6 (14%)	56,56,56	6.57	21 (37%)
12	CLA	B	833	3	58,68,73	2.34	20 (34%)	68,107,113	2.70	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	825	-	63,73,73	2.29	20 (31%)	74,113,113	2.16	23 (31%)
12	CLA	b	829	3	63,73,73	2.33	21 (33%)	74,113,113	2.58	24 (32%)
12	CLA	b	835	20	63,73,73	2.31	19 (30%)	74,113,113	2.48	27 (36%)
15	BCR	A	844	-	41,41,41	2.60	6 (14%)	56,56,56	6.59	21 (37%)
12	CLA	a	834	-	63,73,73	2.28	18 (28%)	74,113,113	2.40	27 (36%)
12	CLA	a	836	1	48,58,73	2.75	21 (43%)	56,95,113	3.04	29 (51%)
12	CLA	l	204	10	53,63,73	2.49	19 (35%)	62,101,113	2.69	24 (38%)
12	CLA	A	822	-	48,58,73	2.68	21 (43%)	56,95,113	2.75	25 (44%)
14	SF4	K	101	4	0,12,12	-	-	-	-	-
15	BCR	a	847	-	41,41,41	2.66	6 (14%)	56,56,56	6.76	26 (46%)
12	CLA	H	814	3	53,63,73	2.51	21 (39%)	62,101,113	2.65	22 (35%)
12	CLA	H	805	3	63,73,73	2.28	22 (34%)	74,113,113	2.60	26 (35%)
12	CLA	A	829	1	63,73,73	2.22	19 (30%)	74,113,113	2.44	26 (35%)
12	CLA	b	834	3	43,53,73	2.60	19 (44%)	50,89,113	3.04	21 (42%)
12	CLA	b	837	-	63,73,73	2.27	20 (31%)	74,113,113	2.61	27 (36%)
12	CLA	G	817	1	48,58,73	2.63	21 (43%)	56,95,113	2.83	30 (53%)
12	CLA	A	811	-	43,53,73	2.67	19 (44%)	50,89,113	2.74	20 (40%)
12	CLA	b	836	-	63,73,73	2.27	18 (28%)	74,113,113	2.70	31 (41%)
12	CLA	A	810	1,12	48,58,73	2.57	21 (43%)	56,95,113	3.00	25 (44%)
12	CLA	H	830	3	63,73,73	2.28	21 (33%)	74,113,113	2.59	22 (29%)
12	CLA	A	840	1	48,58,73	2.64	19 (39%)	56,95,113	2.76	25 (44%)
15	BCR	H	842	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	25 (44%)
15	BCR	P	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.51	23 (41%)
12	CLA	G	830	-	63,73,73	2.26	19 (30%)	74,113,113	2.47	23 (31%)
19	LMT	B	847	-	36,36,36	1.26	5 (13%)	47,47,47	1.11	3 (6%)
12	CLA	G	834	-	63,73,73	2.28	19 (30%)	74,113,113	2.46	26 (35%)
12	CLA	b	811	-	58,68,73	2.42	21 (36%)	68,107,113	2.62	25 (36%)
12	CLA	a	821	-	43,53,73	2.69	20 (46%)	50,89,113	2.99	22 (44%)
15	BCR	a	852	-	41,41,41	2.71	6 (14%)	56,56,56	6.46	20 (35%)
12	CLA	H	833	-	43,53,73	2.69	20 (46%)	50,89,113	2.89	22 (44%)
12	CLA	H	824	3	63,73,73	2.29	19 (30%)	74,113,113	2.55	30 (40%)
12	CLA	b	831	3	43,53,73	2.69	20 (46%)	50,89,113	2.91	23 (46%)
16	LHG	a	850	-	48,48,48	0.92	2 (4%)	51,54,54	0.93	2 (3%)
12	CLA	a	804	12	53,63,73	2.47	21 (39%)	62,101,113	2.81	28 (45%)
15	BCR	A	848	-	41,41,41	2.71	6 (14%)	56,56,56	6.77	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	820	-	43,53,73	2.66	20 (46%)	50,89,113	2.89	22 (44%)
12	CLA	A	824	20	63,73,73	2.34	20 (31%)	74,113,113	2.45	24 (32%)
12	CLA	G	805	1,12	53,63,73	2.47	21 (39%)	62,101,113	2.82	29 (46%)
12	CLA	B	822	20	63,73,73	2.30	20 (31%)	74,113,113	2.43	26 (35%)
12	CLA	G	831	1	48,58,73	2.62	19 (39%)	56,95,113	2.73	27 (48%)
12	CLA	G	810	1	43,53,73	2.64	20 (46%)	50,89,113	2.91	23 (46%)
12	CLA	a	808	1	48,58,73	2.67	20 (41%)	56,95,113	2.84	24 (42%)
12	CLA	A	820	-	63,73,73	2.25	18 (28%)	74,113,113	2.66	26 (35%)
12	CLA	A	825	20	53,63,73	2.50	19 (35%)	62,101,113	2.71	25 (40%)
18	LMG	B	846	-	55,55,55	1.48	8 (14%)	63,63,63	1.12	3 (4%)
12	CLA	b	824	3	63,73,73	2.19	19 (30%)	74,113,113	2.56	29 (39%)
12	CLA	b	809	3	43,53,73	2.67	20 (46%)	50,89,113	2.88	22 (44%)
12	CLA	A	839	1	63,73,73	2.33	20 (31%)	74,113,113	2.43	27 (36%)
12	CLA	A	828	-	63,73,73	2.35	20 (31%)	74,113,113	2.31	26 (35%)
12	CLA	a	818	-	63,73,73	2.26	21 (33%)	74,113,113	2.53	27 (36%)
12	CLA	B	820	3	43,53,73	2.66	19 (44%)	50,89,113	2.84	22 (44%)
12	CLA	G	841	20	63,73,73	2.24	18 (28%)	74,113,113	2.40	24 (32%)
16	LHG	a	851	12	26,26,48	1.25	2 (7%)	29,32,54	1.25	3 (10%)
11	CL0	a	801	1	63,73,73	2.37	19 (30%)	74,113,113	2.54	30 (40%)
12	CLA	b	821	20	63,73,73	2.23	18 (28%)	74,113,113	2.57	30 (40%)
12	CLA	A	802	20	63,73,73	2.21	18 (28%)	74,113,113	2.27	24 (32%)
12	CLA	H	807	3	63,73,73	2.27	19 (30%)	74,113,113	2.53	28 (37%)
15	BCR	A	847	-	41,41,41	2.71	6 (14%)	56,56,56	6.75	27 (48%)
12	CLA	G	823	1	48,58,73	2.67	21 (43%)	56,95,113	2.79	22 (39%)
12	CLA	a	833	-	63,73,73	2.24	20 (31%)	74,113,113	2.47	26 (35%)
12	CLA	H	837	20	63,73,73	2.32	19 (30%)	74,113,113	2.55	24 (32%)
12	CLA	L	202	3	63,73,73	2.30	19 (30%)	74,113,113	2.40	24 (32%)
12	CLA	H	810	3	43,53,73	2.66	20 (46%)	50,89,113	2.87	21 (42%)
12	CLA	A	836	1	48,58,73	2.75	20 (41%)	56,95,113	3.39	30 (53%)
12	CLA	B	814	-	53,63,73	2.42	20 (37%)	62,101,113	2.70	24 (38%)
12	CLA	A	814	-	43,53,73	2.68	19 (44%)	50,89,113	2.85	23 (46%)
12	CLA	B	815	-	58,68,73	2.40	20 (34%)	68,107,113	2.70	24 (35%)
12	CLA	j	104	-	43,53,73	2.71	21 (48%)	50,89,113	2.75	22 (44%)
14	SF4	a	843	1,3	0,12,12	-	-	-	-	-
12	CLA	b	827	3	43,53,73	2.67	19 (44%)	50,89,113	2.80	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
18	LMG	b	845	-	55,55,55	1.49	8 (14%)	63,63,63	1.11	3 (4%)
12	CLA	G	821	-	63,73,73	2.30	20 (31%)	74,113,113	2.44	28 (37%)
12	CLA	b	848	16	58,68,73	2.37	19 (32%)	68,107,113	2.58	23 (33%)
12	CLA	A	837	1	63,73,73	2.25	20 (31%)	74,113,113	2.59	28 (37%)
12	CLA	H	809	3	43,53,73	2.67	21 (48%)	50,89,113	2.88	25 (50%)
12	CLA	J	103	-	43,53,73	2.69	21 (48%)	50,89,113	2.80	21 (42%)
12	CLA	H	813	-	43,53,73	2.61	19 (44%)	50,89,113	3.12	25 (50%)
12	CLA	G	832	1	63,73,73	2.30	20 (31%)	74,113,113	2.31	23 (31%)
12	CLA	H	836	3	43,53,73	2.57	19 (44%)	50,89,113	3.04	21 (42%)
12	CLA	b	803	-	63,73,73	2.35	19 (30%)	74,113,113	2.59	25 (33%)
15	BCR	a	849	-	41,41,41	2.64	6 (14%)	56,56,56	6.77	26 (46%)
12	CLA	a	819	1	43,53,73	2.60	19 (44%)	50,89,113	2.91	24 (48%)
15	BCR	b	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.59	25 (44%)
17	45D	T	101	-	43,43,43	4.00	19 (44%)	54,60,60	7.84	31 (57%)
12	CLA	A	804	12	53,63,73	2.48	21 (39%)	62,101,113	2.81	28 (45%)
12	CLA	G	802	-	58,68,73	2.37	19 (32%)	68,107,113	2.75	27 (39%)
12	CLA	a	812	-	48,58,73	2.62	21 (43%)	56,95,113	2.92	27 (48%)
12	CLA	a	816	1	48,58,73	2.62	19 (39%)	56,95,113	2.80	29 (51%)
12	CLA	a	811	-	43,53,73	2.66	19 (44%)	50,89,113	2.77	21 (42%)
12	CLA	b	826	3	63,73,73	2.40	19 (30%)	74,113,113	2.69	28 (37%)
12	CLA	H	806	-	63,73,73	2.22	19 (30%)	74,113,113	2.76	27 (36%)
19	LMT	H	848	-	36,36,36	1.18	4 (11%)	47,47,47	0.96	1 (2%)
12	CLA	A	803	1	63,73,73	2.29	21 (33%)	74,113,113	2.52	25 (33%)
12	CLA	B	830	-	63,73,73	2.27	20 (31%)	74,113,113	2.38	24 (32%)
12	CLA	A	808	1	48,58,73	2.65	21 (43%)	56,95,113	2.92	23 (41%)
15	BCR	B	842	-	41,41,41	2.58	6 (14%)	56,56,56	6.62	21 (37%)
12	CLA	f	201	20	63,73,73	2.32	21 (33%)	74,113,113	2.33	24 (32%)
15	BCR	a	845	-	41,41,41	2.65	6 (14%)	56,56,56	6.65	23 (41%)
15	BCR	i	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	19 (33%)
15	BCR	A	852	-	41,41,41	2.70	6 (14%)	56,56,56	6.43	20 (35%)
12	CLA	b	816	-	63,73,73	2.26	20 (31%)	74,113,113	2.30	24 (32%)
13	1L3	b	838	-	34,34,34	2.67	12 (35%)	43,45,45	1.51	8 (18%)
12	CLA	a	817	-	53,63,73	2.56	21 (39%)	62,101,113	2.81	26 (41%)
12	CLA	H	821	-	43,53,73	2.63	18 (41%)	50,89,113	2.87	23 (46%)
12	CLA	A	806	1	63,73,73	2.24	19 (30%)	74,113,113	2.68	23 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	b	839	-	41,41,41	2.68	6 (14%)	56,56,56	6.58	20 (35%)
12	CLA	A	826	1	63,73,73	2.30	19 (30%)	74,113,113	2.60	27 (36%)
12	CLA	a	855	-	63,73,73	2.18	20 (31%)	74,113,113	2.73	27 (36%)
15	BCR	J	102	-	41,41,41	2.65	6 (14%)	56,56,56	6.86	19 (33%)
12	CLA	l	206	20	63,73,73	2.30	20 (31%)	74,113,113	2.50	23 (31%)
12	CLA	b	806	-	63,73,73	2.22	19 (30%)	74,113,113	2.75	28 (37%)
12	CLA	G	856	-	63,73,73	2.22	20 (31%)	74,113,113	2.54	26 (35%)
12	CLA	f	203	-	43,53,73	2.68	20 (46%)	50,89,113	4.70	23 (46%)
15	BCR	G	847	-	41,41,41	2.70	6 (14%)	56,56,56	6.50	21 (37%)
12	CLA	A	817	-	53,63,73	2.60	19 (35%)	62,101,113	2.66	29 (46%)
12	CLA	b	818	-	43,53,73	2.70	20 (46%)	50,89,113	2.91	22 (44%)
12	CLA	B	806	3	63,73,73	2.20	19 (30%)	74,113,113	2.77	27 (36%)
12	CLA	H	815	3	53,63,73	2.47	19 (35%)	62,101,113	2.74	26 (41%)
12	CLA	B	813	3	53,63,73	2.52	21 (39%)	62,101,113	2.68	22 (35%)
12	CLA	a	831	1	53,63,73	2.54	21 (39%)	62,101,113	2.65	25 (40%)
12	CLA	H	850	16	58,68,73	2.38	19 (32%)	68,107,113	2.56	27 (39%)
15	BCR	B	841	-	41,41,41	2.61	6 (14%)	56,56,56	6.61	25 (44%)
12	CLA	A	816	1	48,58,73	2.62	20 (41%)	56,95,113	2.83	28 (50%)
12	CLA	a	822	-	48,58,73	2.68	21 (43%)	56,95,113	2.80	24 (42%)
12	CLA	A	835	-	43,53,73	2.63	20 (46%)	50,89,113	2.91	22 (44%)
12	CLA	b	812	-	43,53,73	2.67	20 (46%)	50,89,113	3.10	25 (50%)
12	CLA	H	818	-	43,53,73	2.66	19 (44%)	50,89,113	2.89	21 (42%)
15	BCR	L	203	-	41,41,41	2.78	6 (14%)	56,56,56	6.44	21 (37%)
12	CLA	B	824	-	63,73,73	2.22	17 (26%)	74,113,113	2.44	29 (39%)
12	CLA	b	817	3	43,53,73	2.65	19 (44%)	50,89,113	2.91	22 (44%)
14	SF4	c	102	4	0,12,12	-	-	-	-	-
12	CLA	G	818	-	53,63,73	2.60	20 (37%)	62,101,113	2.75	31 (50%)
15	BCR	H	841	-	41,41,41	2.62	6 (14%)	56,56,56	6.61	20 (35%)
12	CLA	A	813	-	43,53,73	2.71	19 (44%)	50,89,113	3.06	23 (46%)
15	BCR	l	203	-	41,41,41	2.79	6 (14%)	56,56,56	6.50	22 (39%)
16	LHG	a	853	-	48,48,48	0.94	2 (4%)	51,54,54	1.09	3 (5%)
12	CLA	B	809	3	43,53,73	2.66	20 (46%)	50,89,113	2.86	22 (44%)
12	CLA	H	832	-	43,53,73	2.63	19 (44%)	50,89,113	2.80	22 (44%)
12	CLA	H	804	-	63,73,73	2.22	19 (30%)	74,113,113	2.69	24 (32%)
12	CLA	B	807	3	63,73,73	2.22	19 (30%)	74,113,113	2.52	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	855	20	63,73,73	2.29	19 (30%)	74,113,113	2.49	25 (33%)
12	CLA	G	833	1	63,73,73	2.25	19 (30%)	74,113,113	2.40	24 (32%)
15	BCR	b	843	-	41,41,41	2.63	6 (14%)	56,56,56	6.84	24 (42%)
12	CLA	L	205	10	63,73,73	2.27	19 (30%)	74,113,113	2.65	25 (33%)
12	CLA	B	810	3	63,73,73	2.26	20 (31%)	74,113,113	2.75	27 (36%)
12	CLA	H	808	3	63,73,73	2.30	18 (28%)	74,113,113	2.40	24 (32%)
12	CLA	a	823	-	53,63,73	2.47	20 (37%)	62,101,113	2.72	24 (38%)
12	CLA	b	830	-	43,53,73	2.65	19 (44%)	50,89,113	2.83	21 (42%)
12	CLA	B	818	-	43,53,73	2.70	20 (46%)	50,89,113	2.94	22 (44%)
15	BCR	i	101	-	41,41,41	2.60	6 (14%)	56,56,56	6.97	21 (37%)
12	CLA	B	835	3	43,53,73	2.58	18 (41%)	50,89,113	3.00	22 (44%)
12	CLA	G	812	-	43,53,73	2.65	19 (44%)	50,89,113	2.79	20 (40%)
15	BCR	G	853	-	41,41,41	2.71	6 (14%)	56,56,56	6.40	20 (35%)
12	CLA	a	803	1	63,73,73	2.28	21 (33%)	74,113,113	2.53	28 (37%)
12	CLA	A	854	20	63,73,73	2.32	20 (31%)	74,113,113	2.45	29 (39%)
12	CLA	A	831	1	53,63,73	2.52	19 (35%)	62,101,113	2.69	27 (43%)
12	CLA	b	823	3	63,73,73	2.28	19 (30%)	74,113,113	2.53	28 (37%)
15	BCR	A	845	-	41,41,41	2.62	6 (14%)	56,56,56	6.64	22 (39%)
12	CLA	R	103	-	43,53,73	2.70	20 (46%)	50,89,113	2.79	21 (42%)
12	CLA	B	832	3	43,53,73	2.69	20 (46%)	50,89,113	2.89	23 (46%)
15	BCR	f	202	-	41,41,41	2.80	6 (14%)	56,56,56	6.66	24 (42%)
12	CLA	a	838	1	43,53,73	2.63	20 (46%)	50,89,113	3.00	23 (46%)
12	CLA	A	830	1	48,58,73	2.60	19 (39%)	56,95,113	2.85	28 (50%)
12	CLA	B	836	20	63,73,73	2.31	19 (30%)	74,113,113	2.53	27 (36%)
12	CLA	G	819	-	63,73,73	2.25	21 (33%)	74,113,113	2.56	28 (37%)
12	CLA	b	822	20	63,73,73	2.29	21 (33%)	74,113,113	2.62	25 (33%)
12	CLA	a	809	1	43,53,73	2.59	19 (44%)	50,89,113	2.97	23 (46%)
11	CL0	G	801	1	63,73,73	2.32	20 (31%)	74,113,113	2.40	26 (35%)
15	BCR	a	846	-	41,41,41	2.68	6 (14%)	56,56,56	6.62	22 (39%)
12	CLA	j	102	-	63,73,73	2.27	20 (31%)	74,113,113	2.35	26 (35%)
16	LHG	G	852	12	26,26,48	1.24	2 (7%)	29,32,54	1.25	4 (13%)
12	CLA	G	811	1,12	48,58,73	2.58	21 (43%)	56,95,113	3.05	26 (46%)
19	LMT	b	846	-	36,36,36	1.17	4 (11%)	47,47,47	1.01	2 (4%)
12	CLA	G	822	1	43,53,73	2.69	20 (46%)	50,89,113	2.98	22 (44%)
12	CLA	H	835	3	63,73,73	2.24	19 (30%)	74,113,113	2.45	24 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	826	3	63,73,73	2.37	20 (31%)	74,113,113	2.70	28 (37%)
14	SF4	c	101	4	0,12,12	-	-	-		
12	CLA	A	841	20	63,73,73	2.25	20 (31%)	74,113,113	2.44	26 (35%)
12	CLA	F	201	20	63,73,73	2.31	21 (33%)	74,113,113	2.35	25 (33%)
12	CLA	H	827	3	63,73,73	2.34	20 (31%)	74,113,113	2.89	30 (40%)
12	CLA	A	834	-	63,73,73	2.28	20 (31%)	74,113,113	2.45	24 (32%)
14	SF4	K	102	4	0,12,12	-	-	-		
15	BCR	a	848	-	41,41,41	2.72	6 (14%)	56,56,56	6.78	21 (37%)
12	CLA	A	827	1	58,68,73	2.33	18 (31%)	68,107,113	2.56	25 (36%)
12	CLA	a	829	1	63,73,73	2.24	19 (30%)	74,113,113	2.47	24 (32%)
12	CLA	H	812	3	58,68,73	2.42	21 (36%)	68,107,113	2.59	25 (36%)
15	BCR	A	846	-	41,41,41	2.63	6 (14%)	56,56,56	6.91	19 (33%)
12	CLA	H	816	-	58,68,73	2.33	18 (31%)	68,107,113	2.96	26 (38%)
12	CLA	H	811	3	63,73,73	2.22	18 (28%)	74,113,113	2.62	29 (39%)
12	CLA	a	824	20	63,73,73	2.34	21 (33%)	74,113,113	2.55	30 (40%)
12	CLA	b	828	3	43,53,73	2.69	20 (46%)	50,89,113	2.91	25 (50%)
12	CLA	b	832	3	58,68,73	2.38	21 (36%)	68,107,113	2.61	25 (36%)
15	BCR	F	204	-	41,41,41	2.63	6 (14%)	56,56,56	6.47	22 (39%)
15	BCR	L	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.55	26 (46%)
15	BCR	H	845	-	41,41,41	2.64	6 (14%)	56,56,56	6.83	25 (44%)
12	CLA	b	804	-	63,73,73	2.23	19 (30%)	74,113,113	2.66	25 (33%)
13	1L3	A	842	-	34,34,34	2.63	14 (41%)	43,45,45	1.50	11 (25%)
12	CLA	a	820	-	63,73,73	2.31	20 (31%)	74,113,113	2.41	24 (32%)
12	CLA	b	802	-	63,73,73	2.20	20 (31%)	74,113,113	2.92	32 (43%)
12	CLA	l	202	3	63,73,73	2.30	20 (31%)	74,113,113	2.40	22 (29%)
12	CLA	a	828	-	63,73,73	2.31	19 (30%)	74,113,113	2.38	28 (37%)
12	CLA	B	837	3	63,73,73	2.24	20 (31%)	74,113,113	2.73	30 (40%)
12	CLA	G	839	1	63,73,73	2.32	21 (33%)	74,113,113	2.46	23 (31%)
12	CLA	b	814	3	53,63,73	2.45	19 (35%)	62,101,113	2.68	25 (40%)
12	CLA	G	827	-	63,73,73	2.30	20 (31%)	74,113,113	2.55	29 (39%)
12	CLA	B	804	-	63,73,73	2.21	19 (30%)	74,113,113	2.64	24 (32%)
15	BCR	G	849	-	41,41,41	2.75	6 (14%)	56,56,56	6.76	21 (37%)
12	CLA	B	811	-	58,68,73	2.41	21 (36%)	68,107,113	2.57	24 (35%)
12	CLA	A	832	1	63,73,73	2.29	19 (30%)	74,113,113	2.32	21 (28%)
12	CLA	a	837	1	63,73,73	2.25	20 (31%)	74,113,113	2.61	28 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	825	20	53,63,73	2.51	19 (35%)	62,101,113	2.69	25 (40%)
12	CLA	b	808	3	43,53,73	2.65	20 (46%)	50,89,113	2.90	26 (52%)
12	CLA	G	814	1	43,53,73	2.63	18 (41%)	50,89,113	3.03	22 (44%)
12	CLA	B	808	3	43,53,73	2.67	20 (46%)	50,89,113	2.90	25 (50%)
12	CLA	a	840	1	48,58,73	2.64	19 (39%)	56,95,113	2.79	25 (44%)
15	BCR	B	840	-	41,41,41	2.62	6 (14%)	56,56,56	6.68	20 (35%)
12	CLA	H	803	-	63,73,73	2.32	19 (30%)	74,113,113	2.54	24 (32%)
12	CLA	B	834	3	63,73,73	2.25	19 (30%)	74,113,113	2.50	25 (33%)
13	1L3	G	843	-	34,34,34	2.68	15 (44%)	43,45,45	1.48	10 (23%)
12	CLA	G	803	20	63,73,73	2.23	20 (31%)	74,113,113	2.26	24 (32%)
15	BCR	b	847	-	41,41,41	2.63	6 (14%)	56,56,56	6.61	22 (39%)
12	CLA	A	821	1	43,53,73	2.68	20 (46%)	50,89,113	2.99	21 (42%)
15	BCR	H	843	-	41,41,41	2.57	6 (14%)	56,56,56	6.64	24 (42%)
12	CLA	H	834	20	58,68,73	2.36	20 (34%)	68,107,113	2.56	23 (33%)
15	BCR	J	101	-	41,41,41	2.71	6 (14%)	56,56,56	6.56	22 (39%)
12	CLA	b	820	-	43,53,73	2.64	19 (44%)	50,89,113	2.89	20 (40%)
15	BCR	a	844	-	41,41,41	2.61	6 (14%)	56,56,56	6.65	21 (37%)
12	CLA	G	842	16	58,68,73	2.37	20 (34%)	68,107,113	2.58	25 (36%)
18	LMG	H	847	-	55,55,55	1.49	8 (14%)	63,63,63	1.10	4 (6%)
12	CLA	B	821	20	63,73,73	2.23	18 (28%)	74,113,113	2.57	29 (39%)
14	SF4	A	843	1,3	0,12,12	-	-	-	-	-
12	CLA	A	805	-	63,73,73	2.25	19 (30%)	74,113,113	2.67	26 (35%)
16	LHG	A	850	-	48,48,48	0.90	2 (4%)	51,54,54	1.00	4 (7%)
13	1L3	a	842	-	34,34,34	2.65	14 (41%)	43,45,45	1.51	11 (25%)
15	BCR	I	101	-	41,41,41	2.61	6 (14%)	56,56,56	6.86	21 (37%)
12	CLA	a	802	20	63,73,73	2.22	19 (30%)	74,113,113	2.28	23 (31%)
15	BCR	l	201	-	41,41,41	2.67	6 (14%)	56,56,56	6.52	24 (42%)
15	BCR	J	104	-	41,41,41	2.54	6 (14%)	56,56,56	6.56	23 (41%)
12	CLA	b	819	-	43,53,73	2.66	20 (46%)	50,89,113	2.86	21 (42%)
15	BCR	Q	102	-	41,41,41	2.71	6 (14%)	56,56,56	6.73	17 (30%)
15	BCR	f	204	-	41,41,41	2.61	6 (14%)	56,56,56	6.44	22 (39%)
12	CLA	b	805	3	63,73,73	2.25	19 (30%)	74,113,113	2.58	25 (33%)
12	CLA	H	838	-	63,73,73	2.27	19 (30%)	74,113,113	2.67	31 (41%)
12	CLA	L	204	10	53,63,73	2.48	19 (35%)	62,101,113	2.73	23 (37%)
12	CLA	l	205	10	63,73,73	2.26	19 (30%)	74,113,113	2.66	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	839	1	63,73,73	2.32	20 (31%)	74,113,113	2.46	22 (29%)
12	CLA	A	819	1	43,53,73	2.66	20 (46%)	50,89,113	2.89	23 (46%)
15	BCR	G	848	-	41,41,41	2.65	6 (14%)	56,56,56	6.74	25 (44%)
12	CLA	a	826	1	63,73,73	2.29	20 (31%)	74,113,113	2.59	26 (35%)
12	CLA	a	854	20	63,73,73	2.27	20 (31%)	74,113,113	2.45	26 (35%)
12	CLA	H	829	3	43,53,73	2.69	20 (46%)	50,89,113	2.89	25 (50%)
12	CLA	a	813	-	43,53,73	2.69	20 (46%)	50,89,113	2.85	25 (50%)
12	CLA	B	812	-	43,53,73	2.68	20 (46%)	50,89,113	2.93	23 (46%)
12	CLA	B	816	-	63,73,73	2.28	20 (31%)	74,113,113	2.32	25 (33%)
14	SF4	C	101	4	0,12,12	-	-	-	-	-
12	CLA	a	815	-	43,53,73	2.67	20 (46%)	50,89,113	2.87	21 (42%)
12	CLA	b	801	-	58,68,73	2.33	19 (32%)	68,107,113	2.67	24 (35%)
12	CLA	P	203	-	43,53,73	2.67	20 (46%)	50,89,113	4.70	23 (46%)
15	BCR	G	845	-	41,41,41	2.61	6 (14%)	56,56,56	6.63	21 (37%)
13	1L3	H	840	-	34,34,34	2.70	13 (38%)	43,45,45	1.46	8 (18%)
15	BCR	R	102	-	41,41,41	2.63	6 (14%)	56,56,56	6.83	17 (30%)
12	CLA	G	838	1	43,53,73	2.63	20 (46%)	50,89,113	2.99	23 (46%)
12	CLA	G	835	1	43,53,73	2.63	20 (46%)	50,89,113	2.90	22 (44%)
12	CLA	H	801	1	53,63,73	2.53	21 (39%)	62,101,113	2.68	26 (41%)
15	BCR	j	103	-	41,41,41	2.65	6 (14%)	56,56,56	6.80	16 (28%)
13	1L3	B	839	-	34,34,34	2.67	12 (35%)	43,45,45	1.54	9 (20%)
16	LHG	G	854	-	48,48,48	0.94	2 (4%)	51,54,54	3.78	6 (11%)
12	CLA	G	837	1	63,73,73	2.24	20 (31%)	74,113,113	2.61	29 (39%)
12	CLA	B	823	3	63,73,73	2.28	19 (30%)	74,113,113	2.54	30 (40%)
12	CLA	G	836	1	48,58,73	2.73	21 (43%)	56,95,113	3.00	25 (44%)
15	BCR	S	201	-	41,41,41	2.80	6 (14%)	56,56,56	6.51	23 (41%)
12	CLA	G	829	1	63,73,73	2.35	20 (31%)	74,113,113	2.32	24 (32%)
12	CLA	A	823	-	53,63,73	2.46	20 (37%)	62,101,113	2.70	23 (37%)
12	CLA	B	828	3	43,53,73	2.69	20 (46%)	50,89,113	2.91	26 (52%)
12	CLA	a	805	1	63,73,73	2.25	20 (31%)	74,113,113	2.58	25 (33%)
15	BCR	B	845	-	41,41,41	2.58	6 (14%)	56,56,56	6.68	18 (32%)
15	BCR	P	202	-	41,41,41	2.72	6 (14%)	56,56,56	6.71	23 (41%)
12	CLA	B	817	3	43,53,73	2.65	19 (44%)	50,89,113	3.02	21 (42%)
12	CLA	H	823	20	63,73,73	2.30	20 (31%)	74,113,113	2.47	25 (33%)
12	CLA	H	831	-	63,73,73	2.30	21 (33%)	74,113,113	2.52	25 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	814	-	43,53,73	2.67	19 (44%)	50,89,113	2.90	22 (44%)
12	CLA	H	828	3	43,53,73	2.65	19 (44%)	50,89,113	2.91	22 (44%)
12	CLA	b	813	3	53,63,73	2.52	22 (41%)	62,101,113	2.71	24 (38%)
12	CLA	a	830	1	48,58,73	2.61	19 (39%)	56,95,113	2.79	27 (48%)
12	CLA	G	820	1	43,53,73	2.62	19 (44%)	50,89,113	2.88	24 (48%)
12	CLA	b	807	-	63,73,73	2.21	20 (31%)	74,113,113	2.61	25 (33%)
15	BCR	H	849	-	41,41,41	2.57	6 (14%)	56,56,56	6.50	20 (35%)
15	BCR	B	843	-	25,25,41	2.18	2 (8%)	33,33,56	7.57	17 (51%)

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
16	LHG	A	851	12	-	14/31/31/53	-
15	BCR	S	205	-	-	9/29/63/63	0/2/2/2
12	CLA	b	815	-	1/1/14/20	8/31/109/115	-
12	CLA	G	813	1	1/1/12/20	8/19/97/115	-
14	SF4	G	844	1,3	-	-	0/6/5/5
17	45D	m	101	-	-	13/29/69/69	0/2/2/2
12	CLA	S	203	10	1/1/15/20	14/37/115/115	-
12	CLA	H	819	-	1/1/11/20	3/13/91/115	-
12	CLA	G	804	1	1/1/15/20	14/37/115/115	-
12	CLA	A	807	1	1/1/15/20	21/37/115/115	-
12	CLA	G	824	-	1/1/13/20	7/25/103/115	-
15	BCR	A	849	-	-	12/29/63/63	0/2/2/2
12	CLA	G	840	1	1/1/12/20	5/19/97/115	-
12	CLA	B	831	-	1/1/11/20	4/13/91/115	-
12	CLA	H	817	-	1/1/15/20	13/37/115/115	-
12	CLA	G	809	1	1/1/12/20	7/19/97/115	-
15	BCR	Q	101	-	-	8/29/63/63	0/2/2/2
12	CLA	B	827	3	1/1/11/20	4/13/91/115	-
12	CLA	G	807	1	1/1/15/20	13/37/115/115	-
12	CLA	G	828	-	1/1/14/20	13/31/109/115	-
12	CLA	A	815	-	1/1/11/20	3/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	844	-	-	8/29/63/63	0/2/2/2
15	BCR	G	850	-	-	12/29/63/63	0/2/2/2
15	BCR	b	844	-	-	6/29/63/63	0/2/2/2
12	CLA	a	806	-	1/1/15/20	13/37/115/115	-
14	SF4	C	102	4	-	-	0/6/5/5
12	CLA	P	201	20	1/1/15/20	14/37/115/115	-
12	CLA	B	819	-	1/1/11/20	5/13/91/115	-
15	BCR	H	844	-	-	3/18/35/63	0/1/1/2
12	CLA	a	827	-	1/1/14/20	12/31/109/115	-
16	LHG	G	851	-	-	31/53/53/53	-
12	CLA	S	202	10	1/1/13/20	7/25/103/115	-
12	CLA	a	841	20	1/1/15/20	13/37/115/115	-
15	BCR	b	842	-	-	3/18/35/63	0/1/1/2
12	CLA	B	802	-	1/1/15/20	15/37/115/115	-
15	BCR	H	846	-	-	9/29/63/63	0/2/2/2
12	CLA	H	822	20	1/1/15/20	15/37/115/115	-
15	BCR	R	101	-	-	11/29/63/63	0/2/2/2
12	CLA	H	802	-	1/1/15/20	13/37/115/115	-
12	CLA	a	810	1,12	1/1/12/20	7/19/97/115	-
12	CLA	G	808	1	1/1/15/20	19/37/115/115	-
15	BCR	G	846	-	-	3/29/63/63	0/2/2/2
12	CLA	B	838	-	1/1/15/20	19/37/115/115	-
12	CLA	G	815	-	1/1/11/20	7/13/91/115	-
12	CLA	S	204	20	1/1/15/20	10/37/115/115	-
12	CLA	L	206	20	1/1/15/20	10/37/115/115	-
12	CLA	B	801	-	1/1/14/20	6/31/109/115	-
12	CLA	a	835	1	1/1/11/20	5/13/91/115	-
12	CLA	H	839	-	1/1/15/20	14/37/115/115	-
12	CLA	H	826	-	1/1/15/20	11/37/115/115	-
12	CLA	a	832	1	1/1/15/20	13/37/115/115	-
12	CLA	B	803	-	1/1/15/20	17/37/115/115	-
12	CLA	B	829	3	1/1/15/20	18/37/115/115	-
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	b	825	-	1/1/15/20	12/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	F	203	-	1/1/11/20	6/13/91/115	-
12	CLA	G	826	20	1/1/13/20	5/25/103/115	-
16	LHG	A	853	-	-	39/53/53/53	-
15	BCR	b	841	-	-	9/29/63/63	0/2/2/2
12	CLA	A	833	-	1/1/15/20	13/37/115/115	-
12	CLA	H	825	-	1/1/15/20	20/37/115/115	-
12	CLA	a	807	-	1/1/15/20	20/37/115/115	-
12	CLA	G	816	-	1/1/11/20	3/13/91/115	-
12	CLA	A	812	-	1/1/12/20	8/19/97/115	-
17	45D	M	101	-	-	13/29/69/69	0/2/2/2
12	CLA	G	825	20	1/1/15/20	16/37/115/115	-
15	BCR	L	207	-	-	10/29/63/63	0/2/2/2
12	CLA	b	833	3	1/1/15/20	9/37/115/115	-
12	CLA	G	806	-	1/1/15/20	10/37/115/115	-
12	CLA	b	810	3	1/1/15/20	25/37/115/115	-
12	CLA	A	818	-	1/1/15/20	13/37/115/115	-
12	CLA	B	805	3	1/1/15/20	15/37/115/115	-
11	CL0	A	801	1	3/3/20/25	4/37/135/135	-
12	CLA	A	809	1	1/1/11/20	5/13/91/115	-
12	CLA	A	838	1	1/1/11/20	3/13/91/115	-
12	CLA	A	855	-	1/1/15/20	9/37/115/115	-
15	BCR	j	101	-	-	12/29/63/63	0/2/2/2
12	CLA	B	833	3	1/1/14/20	13/31/109/115	-
12	CLA	B	825	-	1/1/15/20	11/37/115/115	-
12	CLA	b	829	3	1/1/15/20	18/37/115/115	-
12	CLA	b	835	20	1/1/15/20	11/37/115/115	-
15	BCR	A	844	-	-	10/29/63/63	0/2/2/2
12	CLA	a	834	-	1/1/15/20	18/37/115/115	-
12	CLA	a	836	1	1/1/12/20	5/19/97/115	-
12	CLA	l	204	10	1/1/13/20	6/25/103/115	-
12	CLA	A	822	-	1/1/12/20	4/19/97/115	-
14	SF4	K	101	4	-	-	0/6/5/5
15	BCR	a	847	-	-	4/29/63/63	0/2/2/2
12	CLA	H	814	3	1/1/13/20	4/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	H	805	3	1/1/15/20	14/37/115/115	-
12	CLA	A	829	1	1/1/15/20	10/37/115/115	-
12	CLA	b	834	3	1/1/11/20	5/13/91/115	-
12	CLA	b	837	-	1/1/15/20	14/37/115/115	-
12	CLA	G	817	1	1/1/12/20	4/19/97/115	-
12	CLA	A	811	-	1/1/11/20	4/13/91/115	-
12	CLA	b	836	-	1/1/15/20	16/37/115/115	-
12	CLA	A	810	1,12	1/1/12/20	5/19/97/115	-
12	CLA	H	830	3	1/1/15/20	18/37/115/115	-
12	CLA	A	840	1	1/1/12/20	7/19/97/115	-
15	BCR	H	842	-	-	8/29/63/63	0/2/2/2
15	BCR	P	204	-	-	7/29/63/63	0/2/2/2
12	CLA	G	830	-	1/1/15/20	10/37/115/115	-
19	LMT	B	847	-	-	10/21/61/61	0/2/2/2
12	CLA	G	834	-	1/1/15/20	19/37/115/115	-
12	CLA	b	811	-	1/1/14/20	10/31/109/115	-
12	CLA	a	821	-	1/1/11/20	9/13/91/115	-
15	BCR	a	852	-	-	13/29/63/63	0/2/2/2
12	CLA	H	833	-	1/1/11/20	5/13/91/115	-
12	CLA	H	824	3	1/1/15/20	16/37/115/115	-
12	CLA	b	831	3	1/1/11/20	3/13/91/115	-
16	LHG	a	850	-	-	26/53/53/53	-
12	CLA	a	804	12	1/1/13/20	11/25/103/115	-
15	BCR	A	848	-	-	13/29/63/63	0/2/2/2
12	CLA	H	820	-	1/1/11/20	5/13/91/115	-
12	CLA	A	824	20	1/1/15/20	18/37/115/115	-
12	CLA	G	805	1,12	1/1/13/20	11/25/103/115	-
12	CLA	B	822	20	1/1/15/20	16/37/115/115	-
12	CLA	G	831	1	1/1/12/20	6/19/97/115	-
12	CLA	G	810	1	1/1/11/20	5/13/91/115	-
12	CLA	a	808	1	1/1/12/20	7/19/97/115	-
12	CLA	A	820	-	1/1/15/20	15/37/115/115	-
12	CLA	A	825	20	1/1/13/20	4/25/103/115	-
18	LMG	B	846	-	-	18/50/70/70	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	824	3	1/1/15/20	20/37/115/115	-
12	CLA	b	809	3	1/1/11/20	2/13/91/115	-
12	CLA	A	839	1	1/1/15/20	7/37/115/115	-
12	CLA	A	828	-	1/1/15/20	13/37/115/115	-
12	CLA	a	818	-	1/1/15/20	15/37/115/115	-
12	CLA	B	820	3	1/1/11/20	4/13/91/115	-
12	CLA	G	841	20	1/1/15/20	13/37/115/115	-
16	LHG	a	851	12	-	18/31/31/53	-
11	CL0	a	801	1	3/3/20/25	6/37/135/135	-
12	CLA	b	821	20	1/1/15/20	15/37/115/115	-
12	CLA	A	802	20	1/1/15/20	8/37/115/115	-
12	CLA	H	807	3	1/1/15/20	9/37/115/115	-
15	BCR	A	847	-	-	4/29/63/63	0/2/2/2
12	CLA	G	823	1	1/1/12/20	5/19/97/115	-
12	CLA	a	833	-	1/1/15/20	13/37/115/115	-
12	CLA	H	837	20	1/1/15/20	12/37/115/115	-
12	CLA	L	202	3	1/1/15/20	12/37/115/115	-
12	CLA	H	810	3	1/1/11/20	2/13/91/115	-
12	CLA	B	814	-	1/1/13/20	7/25/103/115	-
12	CLA	A	836	1	-	7/19/97/115	-
12	CLA	A	814	-	1/1/11/20	7/13/91/115	-
12	CLA	B	815	-	1/1/14/20	11/31/109/115	-
12	CLA	j	104	-	1/1/11/20	5/13/91/115	-
14	SF4	a	843	1,3	-	-	0/6/5/5
12	CLA	b	827	3	1/1/11/20	3/13/91/115	-
18	LMG	b	845	-	-	18/50/70/70	0/1/1/1
12	CLA	G	821	-	1/1/15/20	10/37/115/115	-
12	CLA	b	848	16	1/1/14/20	14/31/109/115	-
12	CLA	A	837	1	1/1/15/20	15/37/115/115	-
12	CLA	H	809	3	1/1/11/20	3/13/91/115	-
12	CLA	J	103	-	1/1/11/20	6/13/91/115	-
12	CLA	H	813	-	1/1/11/20	9/13/91/115	-
12	CLA	G	832	1	1/1/15/20	12/37/115/115	-
12	CLA	H	836	3	1/1/11/20	5/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	803	-	1/1/15/20	16/37/115/115	-
15	BCR	a	849	-	-	12/29/63/63	0/2/2/2
12	CLA	a	819	1	1/1/11/20	6/13/91/115	-
15	BCR	b	840	-	-	8/29/63/63	0/2/2/2
17	45D	T	101	-	-	13/29/69/69	0/2/2/2
12	CLA	A	804	12	1/1/13/20	12/25/103/115	-
12	CLA	G	802	-	1/1/14/20	7/31/109/115	-
12	CLA	a	812	-	1/1/12/20	8/19/97/115	-
12	CLA	a	816	1	1/1/12/20	7/19/97/115	-
12	CLA	a	811	-	1/1/11/20	4/13/91/115	-
12	CLA	b	826	3	1/1/15/20	10/37/115/115	-
12	CLA	H	806	-	1/1/15/20	11/37/115/115	-
19	LMT	H	848	-	-	11/21/61/61	0/2/2/2
12	CLA	A	803	1	1/1/15/20	14/37/115/115	-
12	CLA	B	830	-	1/1/15/20	11/37/115/115	-
12	CLA	A	808	1	1/1/12/20	7/19/97/115	-
15	BCR	B	842	-	-	9/29/63/63	0/2/2/2
12	CLA	f	201	20	1/1/15/20	15/37/115/115	-
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2
15	BCR	i	102	-	-	11/29/63/63	0/2/2/2
15	BCR	A	852	-	-	12/29/63/63	0/2/2/2
12	CLA	b	816	-	1/1/15/20	13/37/115/115	-
13	1L3	b	838	-	-	5/23/43/43	0/2/2/2
12	CLA	a	817	-	1/1/13/20	15/25/103/115	-
12	CLA	H	821	-	1/1/11/20	2/13/91/115	-
12	CLA	A	806	1	1/1/15/20	13/37/115/115	-
15	BCR	b	839	-	-	13/29/63/63	0/2/2/2
12	CLA	A	826	1	1/1/15/20	15/37/115/115	-
12	CLA	a	855	-	1/1/15/20	11/37/115/115	-
15	BCR	J	102	-	-	18/29/63/63	0/2/2/2
12	CLA	l	206	20	1/1/15/20	11/37/115/115	-
12	CLA	b	806	-	1/1/15/20	11/37/115/115	-
12	CLA	G	856	-	1/1/15/20	10/37/115/115	-
12	CLA	f	203	-	1/1/11/20	6/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	G	847	-	-	6/29/63/63	0/2/2/2
12	CLA	A	817	-	1/1/13/20	15/25/103/115	-
12	CLA	b	818	-	1/1/11/20	3/13/91/115	-
12	CLA	B	806	3	1/1/15/20	11/37/115/115	-
12	CLA	H	815	3	1/1/13/20	6/25/103/115	-
12	CLA	B	813	3	1/1/13/20	5/25/103/115	-
12	CLA	a	831	1	1/1/13/20	11/25/103/115	-
12	CLA	H	850	16	1/1/14/20	14/31/109/115	-
15	BCR	B	841	-	-	8/29/63/63	0/2/2/2
12	CLA	A	816	1	1/1/12/20	4/19/97/115	-
12	CLA	a	822	-	1/1/12/20	4/19/97/115	-
12	CLA	A	835	-	1/1/11/20	7/13/91/115	-
12	CLA	b	812	-	1/1/11/20	9/13/91/115	-
12	CLA	H	818	-	1/1/11/20	8/13/91/115	-
15	BCR	L	203	-	-	14/29/63/63	0/2/2/2
12	CLA	B	824	-	1/1/15/20	22/37/115/115	-
12	CLA	b	817	3	1/1/11/20	8/13/91/115	-
14	SF4	c	102	4	-	-	0/6/5/5
12	CLA	G	818	-	1/1/13/20	15/25/103/115	-
15	BCR	H	841	-	-	14/29/63/63	0/2/2/2
12	CLA	A	813	-	1/1/11/20	2/13/91/115	-
15	BCR	l	203	-	-	16/29/63/63	0/2/2/2
16	LHG	a	853	-	-	35/53/53/53	-
12	CLA	B	809	3	1/1/11/20	5/13/91/115	-
12	CLA	H	832	-	1/1/11/20	4/13/91/115	-
12	CLA	H	804	-	1/1/15/20	16/37/115/115	-
12	CLA	B	807	3	1/1/15/20	8/37/115/115	-
12	CLA	G	855	20	1/1/15/20	16/37/115/115	-
12	CLA	G	833	1	1/1/15/20	13/37/115/115	-
15	BCR	b	843	-	-	9/29/63/63	0/2/2/2
12	CLA	L	205	10	1/1/15/20	14/37/115/115	-
12	CLA	B	810	3	1/1/15/20	27/37/115/115	-
12	CLA	H	808	3	1/1/15/20	13/37/115/115	-
12	CLA	a	823	-	1/1/13/20	9/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	830	-	1/1/11/20	4/13/91/115	-
12	CLA	B	818	-	1/1/11/20	3/13/91/115	-
15	BCR	i	101	-	-	9/29/63/63	0/2/2/2
12	CLA	B	835	3	1/1/11/20	5/13/91/115	-
12	CLA	G	812	-	1/1/11/20	4/13/91/115	-
15	BCR	G	853	-	-	12/29/63/63	0/2/2/2
12	CLA	a	803	1	1/1/15/20	14/37/115/115	-
12	CLA	A	854	20	1/1/15/20	16/37/115/115	-
12	CLA	A	831	1	1/1/13/20	11/25/103/115	-
12	CLA	b	823	3	1/1/15/20	14/37/115/115	-
15	BCR	A	845	-	-	7/29/63/63	0/2/2/2
12	CLA	R	103	-	1/1/11/20	5/13/91/115	-
12	CLA	B	832	3	1/1/11/20	3/13/91/115	-
15	BCR	f	202	-	-	14/29/63/63	0/2/2/2
12	CLA	a	838	1	1/1/11/20	3/13/91/115	-
12	CLA	A	830	1	1/1/12/20	5/19/97/115	-
12	CLA	B	836	20	1/1/15/20	11/37/115/115	-
12	CLA	G	819	-	1/1/15/20	15/37/115/115	-
12	CLA	b	822	20	1/1/15/20	16/37/115/115	-
12	CLA	a	809	1	1/1/11/20	5/13/91/115	-
11	CL0	G	801	1	3/3/20/25	8/37/135/135	-
15	BCR	a	846	-	-	8/29/63/63	0/2/2/2
12	CLA	j	102	-	1/1/15/20	11/37/115/115	-
16	LHG	G	852	12	-	16/31/31/53	-
12	CLA	G	811	1,12	1/1/12/20	6/19/97/115	-
19	LMT	b	846	-	-	10/21/61/61	0/2/2/2
12	CLA	G	822	1	1/1/11/20	9/13/91/115	-
12	CLA	H	835	3	1/1/15/20	10/37/115/115	-
12	CLA	B	826	3	1/1/15/20	12/37/115/115	-
14	SF4	c	101	4	-	-	0/6/5/5
12	CLA	A	841	20	1/1/15/20	15/37/115/115	-
12	CLA	F	201	20	1/1/15/20	13/37/115/115	-
12	CLA	H	827	3	1/1/15/20	12/37/115/115	-
12	CLA	A	834	-	1/1/15/20	16/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	SF4	K	102	4	-	-	0/6/5/5
15	BCR	a	848	-	-	12/29/63/63	0/2/2/2
12	CLA	A	827	1	1/1/14/20	13/31/109/115	-
12	CLA	a	829	1	1/1/15/20	10/37/115/115	-
12	CLA	H	812	3	1/1/14/20	11/31/109/115	-
15	BCR	A	846	-	-	8/29/63/63	0/2/2/2
12	CLA	H	816	-	1/1/14/20	10/31/109/115	-
12	CLA	H	811	3	1/1/15/20	23/37/115/115	-
12	CLA	a	824	20	1/1/15/20	16/37/115/115	-
12	CLA	b	828	3	1/1/11/20	4/13/91/115	-
12	CLA	b	832	3	1/1/14/20	13/31/109/115	-
15	BCR	F	204	-	-	7/29/63/63	0/2/2/2
15	BCR	L	201	-	-	8/29/63/63	0/2/2/2
15	BCR	H	845	-	-	9/29/63/63	0/2/2/2
12	CLA	b	804	-	1/1/15/20	16/37/115/115	-
13	1L3	A	842	-	-	5/23/43/43	0/2/2/2
12	CLA	a	820	-	1/1/15/20	15/37/115/115	-
12	CLA	b	802	-	1/1/15/20	13/37/115/115	-
12	CLA	l	202	3	1/1/15/20	16/37/115/115	-
12	CLA	a	828	-	1/1/15/20	11/37/115/115	-
12	CLA	B	837	3	1/1/15/20	16/37/115/115	-
12	CLA	G	839	1	1/1/15/20	7/37/115/115	-
12	CLA	b	814	3	1/1/13/20	6/25/103/115	-
12	CLA	G	827	-	1/1/15/20	16/37/115/115	-
12	CLA	B	804	-	1/1/15/20	16/37/115/115	-
15	BCR	G	849	-	-	12/29/63/63	0/2/2/2
12	CLA	B	811	-	1/1/14/20	11/31/109/115	-
12	CLA	A	832	1	1/1/15/20	13/37/115/115	-
12	CLA	a	837	1	1/1/15/20	12/37/115/115	-
12	CLA	a	825	20	1/1/13/20	4/25/103/115	-
12	CLA	b	808	3	1/1/11/20	3/13/91/115	-
12	CLA	G	814	1	1/1/11/20	4/13/91/115	-
12	CLA	B	808	3	1/1/11/20	3/13/91/115	-
12	CLA	a	840	1	1/1/12/20	7/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	840	-	-	10/29/63/63	0/2/2/2
12	CLA	H	803	-	1/1/15/20	17/37/115/115	-
12	CLA	B	834	3	1/1/15/20	8/37/115/115	-
13	1L3	G	843	-	-	5/23/43/43	0/2/2/2
12	CLA	G	803	20	1/1/15/20	8/37/115/115	-
15	BCR	b	847	-	-	7/29/63/63	0/2/2/2
12	CLA	A	821	1	1/1/11/20	9/13/91/115	-
15	BCR	H	843	-	-	9/29/63/63	0/2/2/2
12	CLA	H	834	20	1/1/14/20	13/31/109/115	-
15	BCR	J	101	-	-	10/29/63/63	0/2/2/2
12	CLA	b	820	-	1/1/11/20	2/13/91/115	-
15	BCR	a	844	-	-	11/29/63/63	0/2/2/2
12	CLA	G	842	16	1/1/14/20	13/31/109/115	-
18	LMG	H	847	-	-	16/50/70/70	0/1/1/1
12	CLA	B	821	20	1/1/15/20	15/37/115/115	-
14	SF4	A	843	1,3	-	-	0/6/5/5
12	CLA	A	805	-	1/1/15/20	12/37/115/115	-
16	LHG	A	850	-	-	30/53/53/53	-
13	1L3	a	842	-	-	5/23/43/43	0/2/2/2
15	BCR	I	101	-	-	8/29/63/63	0/2/2/2
12	CLA	a	802	20	1/1/15/20	8/37/115/115	-
15	BCR	l	201	-	-	8/29/63/63	0/2/2/2
15	BCR	J	104	-	-	5/29/63/63	0/2/2/2
12	CLA	b	819	-	1/1/11/20	5/13/91/115	-
15	BCR	Q	102	-	-	11/29/63/63	0/2/2/2
15	BCR	f	204	-	-	7/29/63/63	0/2/2/2
12	CLA	b	805	3	1/1/15/20	18/37/115/115	-
12	CLA	H	838	-	1/1/15/20	18/37/115/115	-
12	CLA	L	204	10	1/1/13/20	7/25/103/115	-
12	CLA	l	205	10	1/1/15/20	13/37/115/115	-
12	CLA	a	839	1	1/1/15/20	11/37/115/115	-
12	CLA	A	819	1	1/1/11/20	7/13/91/115	-
15	BCR	G	848	-	-	4/29/63/63	0/2/2/2
12	CLA	a	826	1	1/1/15/20	15/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	854	20	1/1/15/20	17/37/115/115	-
12	CLA	H	829	3	1/1/11/20	4/13/91/115	-
12	CLA	a	813	-	1/1/11/20	2/13/91/115	-
12	CLA	B	812	-	1/1/11/20	9/13/91/115	-
12	CLA	B	816	-	1/1/15/20	13/37/115/115	-
14	SF4	C	101	4	-	-	0/6/5/5
12	CLA	a	815	-	1/1/11/20	3/13/91/115	-
12	CLA	b	801	-	1/1/14/20	7/31/109/115	-
12	CLA	P	203	-	1/1/11/20	6/13/91/115	-
15	BCR	G	845	-	-	10/29/63/63	0/2/2/2
13	1L3	H	840	-	-	5/23/43/43	0/2/2/2
15	BCR	R	102	-	-	19/29/63/63	0/2/2/2
12	CLA	G	838	1	1/1/11/20	3/13/91/115	-
12	CLA	G	835	1	1/1/11/20	7/13/91/115	-
12	CLA	H	801	1	1/1/13/20	11/25/103/115	-
15	BCR	j	103	-	-	17/29/63/63	0/2/2/2
13	1L3	B	839	-	-	5/23/43/43	0/2/2/2
16	LHG	G	854	-	-	37/53/53/53	-
12	CLA	G	837	1	1/1/15/20	12/37/115/115	-
12	CLA	B	823	3	1/1/15/20	15/37/115/115	-
12	CLA	G	836	1	1/1/12/20	5/19/97/115	-
15	BCR	S	201	-	-	16/29/63/63	0/2/2/2
12	CLA	G	829	1	1/1/15/20	14/37/115/115	-
12	CLA	A	823	-	1/1/13/20	11/25/103/115	-
12	CLA	B	828	3	1/1/11/20	4/13/91/115	-
12	CLA	a	805	1	1/1/15/20	14/37/115/115	-
15	BCR	B	845	-	-	6/29/63/63	0/2/2/2
15	BCR	P	202	-	-	13/29/63/63	0/2/2/2
12	CLA	B	817	3	1/1/11/20	8/13/91/115	-
12	CLA	H	823	20	1/1/15/20	17/37/115/115	-
12	CLA	H	831	-	1/1/15/20	11/37/115/115	-
12	CLA	a	814	-	1/1/11/20	7/13/91/115	-
12	CLA	H	828	3	1/1/11/20	3/13/91/115	-
12	CLA	b	813	3	1/1/13/20	7/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	830	1	-	8/19/97/115	-
12	CLA	G	820	1	1/1/11/20	6/13/91/115	-
12	CLA	b	807	-	1/1/15/20	10/37/115/115	-
15	BCR	H	849	-	-	8/29/63/63	0/2/2/2
15	BCR	B	843	-	-	3/18/35/63	0/1/1/2

The worst 5 of 5831 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 8303 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	NC
11	G	801	CL0	NA
11	G	801	CL0	ND
11	a	801	CL0	NC
11	a	801	CL0	NA

5 of 3726 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
16	A	851	LHG	3	0
15	S	205	BCR	3	0
12	b	815	CLA	2	0
12	G	813	CLA	1	0
17	m	101	45D	4	0
12	S	203	CLA	3	0
12	G	804	CLA	2	0
12	A	807	CLA	3	0
12	G	824	CLA	4	0
15	A	849	BCR	5	0
12	G	840	CLA	1	0
12	B	831	CLA	2	0
12	H	817	CLA	2	0
15	Q	101	BCR	4	0
12	B	827	CLA	2	0
12	G	807	CLA	2	0
12	G	828	CLA	1	0
15	B	844	BCR	4	0
15	G	850	BCR	3	0
15	b	844	BCR	3	0
12	a	806	CLA	3	0
12	P	201	CLA	5	0
15	H	844	BCR	4	0
12	a	827	CLA	2	0
16	G	851	LHG	3	0
12	S	202	CLA	1	0
12	a	841	CLA	2	0
15	b	842	BCR	4	0
12	B	802	CLA	2	0
15	H	846	BCR	2	0
12	H	822	CLA	2	0
15	R	101	BCR	2	0
12	H	802	CLA	3	0
12	G	808	CLA	3	0
15	G	846	BCR	1	0
12	S	204	CLA	3	0
12	L	206	CLA	4	0
12	B	801	CLA	5	0
12	a	835	CLA	2	0
12	H	826	CLA	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	832	CLA	3	0
12	B	803	CLA	1	0
12	B	829	CLA	1	0
15	F	202	BCR	3	0
12	b	825	CLA	4	0
12	F	203	CLA	1	0
12	G	826	CLA	2	0
15	b	841	BCR	1	0
12	A	833	CLA	3	0
12	H	825	CLA	5	0
12	a	807	CLA	5	0
12	A	812	CLA	1	0
17	M	101	45D	3	0
12	G	825	CLA	7	0
15	L	207	BCR	1	0
12	b	833	CLA	2	0
12	G	806	CLA	3	0
12	b	810	CLA	3	0
12	A	818	CLA	5	0
12	B	805	CLA	6	0
11	A	801	CL0	4	0
12	A	855	CLA	3	0
15	j	101	BCR	2	0
12	B	833	CLA	7	0
12	B	825	CLA	4	0
12	b	829	CLA	1	0
12	b	835	CLA	2	0
12	a	834	CLA	2	0
12	a	836	CLA	1	0
12	l	204	CLA	2	0
15	a	847	BCR	3	0
12	H	805	CLA	5	0
12	A	829	CLA	4	0
12	b	834	CLA	2	0
12	b	837	CLA	1	0
12	G	817	CLA	1	0
12	b	836	CLA	5	0
12	A	840	CLA	4	0
15	H	842	BCR	2	0
15	P	204	BCR	1	0
12	G	830	CLA	3	0
19	B	847	LMT	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	834	CLA	3	0
12	a	821	CLA	1	0
15	a	852	BCR	1	0
12	H	824	CLA	3	0
16	a	850	LHG	2	0
15	A	848	BCR	2	0
12	A	824	CLA	7	0
12	B	822	CLA	6	0
12	G	810	CLA	1	0
12	A	820	CLA	2	0
12	A	825	CLA	2	0
18	B	846	LMG	4	0
12	b	824	CLA	2	0
12	A	839	CLA	1	0
12	A	828	CLA	2	0
12	a	818	CLA	5	0
12	G	841	CLA	1	0
16	a	851	LHG	1	0
12	b	821	CLA	3	0
12	A	802	CLA	3	0
12	H	807	CLA	3	0
15	A	847	BCR	1	0
12	G	823	CLA	1	0
12	a	833	CLA	4	0
12	H	837	CLA	2	0
12	L	202	CLA	2	0
12	B	814	CLA	2	0
12	B	815	CLA	1	0
12	b	827	CLA	3	0
18	b	845	LMG	3	0
12	G	821	CLA	3	0
12	b	848	CLA	2	0
12	A	837	CLA	1	0
12	J	103	CLA	1	0
12	G	832	CLA	2	0
12	H	836	CLA	3	0
12	b	803	CLA	1	0
15	a	849	BCR	3	0
15	b	840	BCR	4	0
17	T	101	45D	3	0
12	A	804	CLA	2	0
12	G	802	CLA	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	812	CLA	2	0
12	a	816	CLA	1	0
12	b	826	CLA	2	0
12	H	806	CLA	2	0
19	H	848	LMT	1	0
12	A	803	CLA	3	0
12	B	830	CLA	4	0
12	A	808	CLA	1	0
15	B	842	BCR	1	0
12	f	201	CLA	3	0
15	a	845	BCR	2	0
15	A	852	BCR	2	0
12	b	816	CLA	2	0
12	a	817	CLA	3	0
12	A	806	CLA	2	0
15	b	839	BCR	1	0
12	A	826	CLA	2	0
12	a	855	CLA	6	0
15	J	102	BCR	2	0
12	l	206	CLA	3	0
12	b	806	CLA	3	0
12	G	856	CLA	4	0
12	f	203	CLA	2	0
15	G	847	BCR	3	0
12	A	817	CLA	1	0
12	B	806	CLA	3	0
12	H	815	CLA	2	0
12	a	831	CLA	2	0
12	H	850	CLA	3	0
15	B	841	BCR	3	0
12	A	816	CLA	1	0
12	a	822	CLA	1	0
12	A	835	CLA	1	0
12	b	812	CLA	2	0
15	L	203	BCR	2	0
12	B	824	CLA	1	0
12	b	817	CLA	1	0
12	G	818	CLA	4	0
15	H	841	BCR	1	0
15	l	203	BCR	2	0
16	a	853	LHG	1	0
12	H	832	CLA	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	804	CLA	3	0
12	B	807	CLA	4	0
12	G	855	CLA	3	0
12	G	833	CLA	2	0
15	b	843	BCR	6	0
12	L	205	CLA	3	0
12	B	810	CLA	1	0
12	H	808	CLA	4	0
12	a	823	CLA	1	0
12	b	830	CLA	1	0
15	i	101	BCR	3	0
12	B	835	CLA	2	0
15	G	853	BCR	1	0
12	a	803	CLA	1	0
12	A	854	CLA	4	0
12	A	831	CLA	2	0
12	b	823	CLA	2	0
15	A	845	BCR	3	0
12	R	103	CLA	1	0
15	f	202	BCR	2	0
12	B	836	CLA	1	0
12	G	819	CLA	4	0
12	b	822	CLA	8	0
12	a	809	CLA	2	0
11	G	801	CL0	1	0
15	a	846	BCR	4	0
12	j	102	CLA	2	0
16	G	852	LHG	1	0
19	b	846	LMT	1	0
12	G	822	CLA	1	0
12	H	835	CLA	4	0
12	A	841	CLA	1	0
12	F	201	CLA	3	0
12	H	827	CLA	1	0
12	A	834	CLA	2	0
14	K	102	SF4	1	0
15	a	848	BCR	2	0
12	A	827	CLA	3	0
12	a	829	CLA	3	0
12	H	812	CLA	1	0
15	A	846	BCR	3	0
12	H	816	CLA	3	0

Continued on next page...

Continued from previous page...

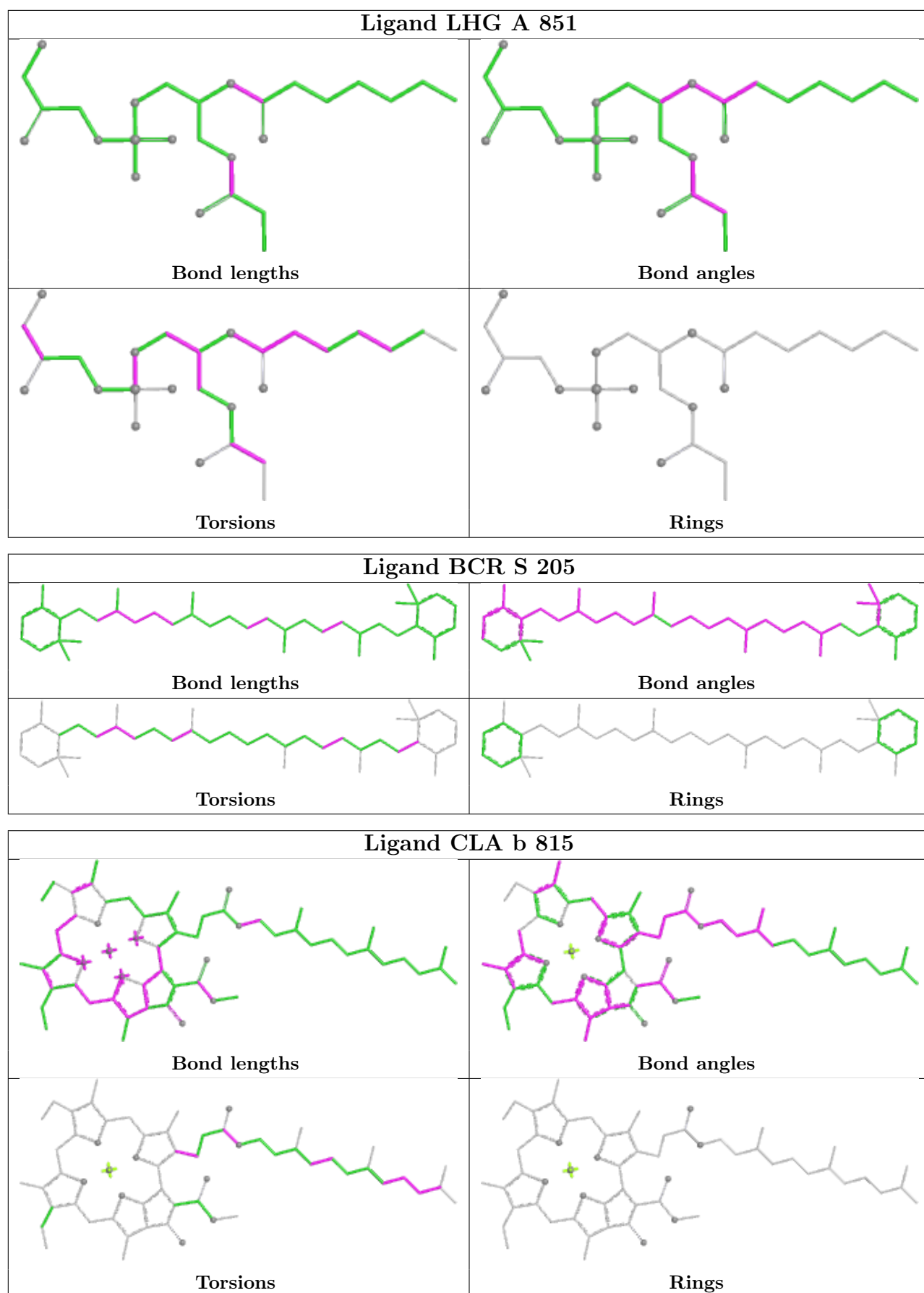
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	811	CLA	2	0
12	a	824	CLA	5	0
12	b	828	CLA	2	0
12	b	832	CLA	5	0
15	F	204	BCR	2	0
15	L	201	BCR	2	0
15	H	845	BCR	6	0
12	b	804	CLA	3	0
12	a	820	CLA	1	0
12	b	802	CLA	3	0
12	l	202	CLA	5	0
12	a	828	CLA	6	0
12	B	837	CLA	3	0
12	G	839	CLA	2	0
12	G	827	CLA	3	0
12	B	804	CLA	3	0
15	G	849	BCR	3	0
12	A	832	CLA	3	0
12	a	825	CLA	1	0
12	a	840	CLA	1	0
12	B	834	CLA	2	0
12	G	803	CLA	2	0
15	b	847	BCR	4	0
12	A	821	CLA	1	0
15	H	843	BCR	4	0
12	H	834	CLA	4	0
15	J	101	BCR	2	0
12	G	842	CLA	2	0
18	H	847	LMG	5	0
12	A	805	CLA	2	0
15	I	101	BCR	4	0
12	a	802	CLA	3	0
15	l	201	BCR	2	0
15	J	104	BCR	2	0
15	Q	102	BCR	1	0
15	f	204	BCR	2	0
12	b	805	CLA	7	0
12	H	838	CLA	4	0
12	L	204	CLA	2	0
12	l	205	CLA	4	0
12	a	839	CLA	2	0
15	G	848	BCR	2	0

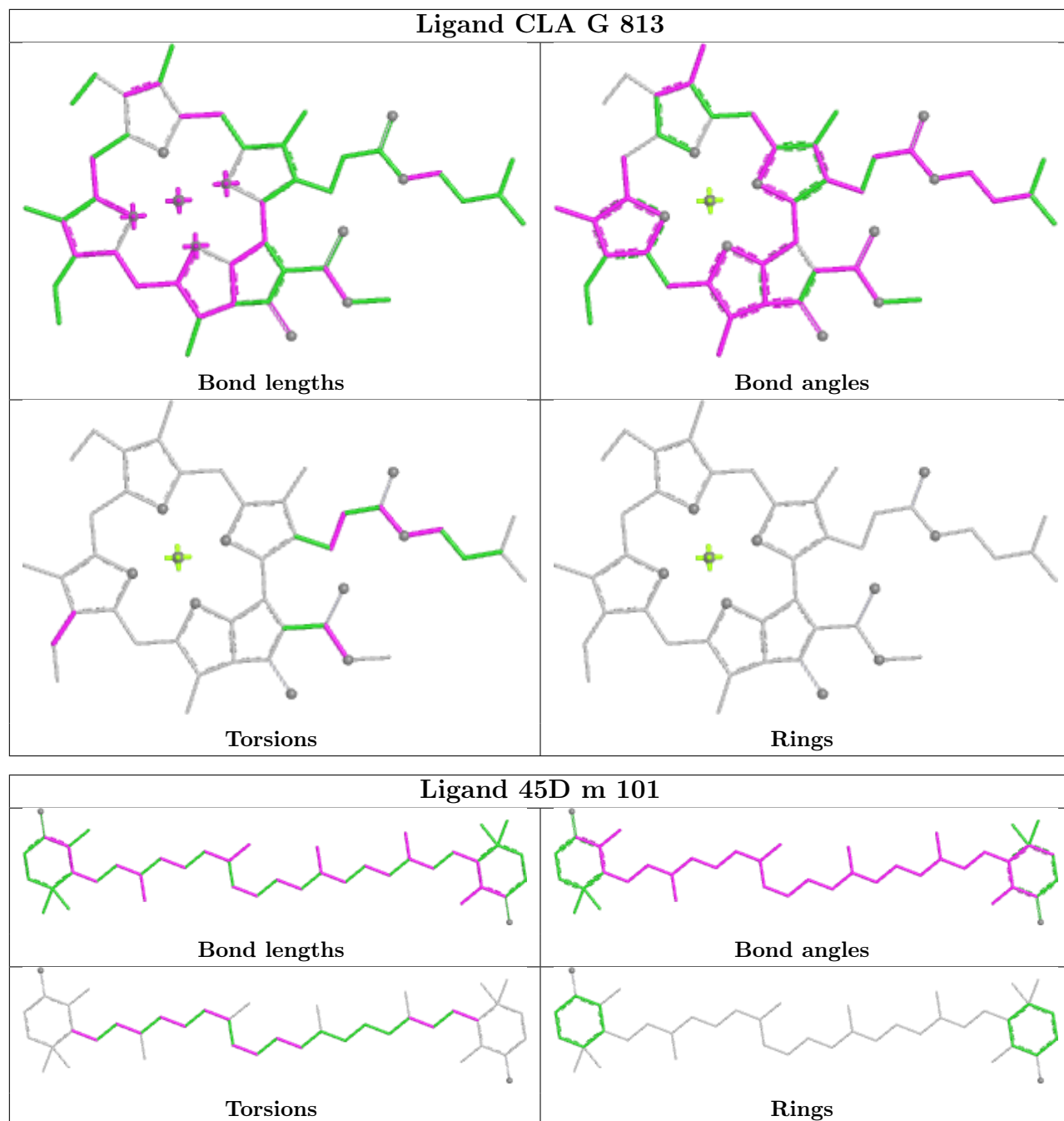
Continued on next page...

Continued from previous page...

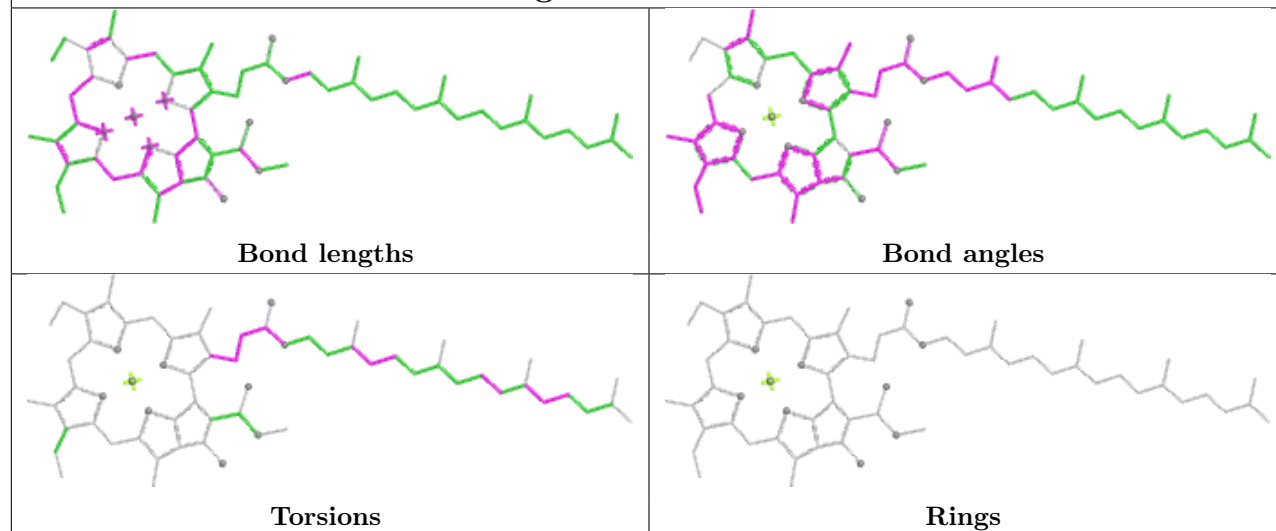
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	826	CLA	3	0
12	a	854	CLA	5	0
12	H	829	CLA	1	0
12	B	812	CLA	1	0
12	b	801	CLA	1	0
15	G	845	BCR	1	0
15	R	102	BCR	3	0
12	G	835	CLA	2	0
12	H	801	CLA	1	0
15	j	103	BCR	3	0
16	G	854	LHG	1	0
12	G	837	CLA	1	0
12	B	823	CLA	2	0
15	S	201	BCR	2	0
12	G	829	CLA	5	0
12	A	823	CLA	2	0
12	B	828	CLA	2	0
12	a	805	CLA	4	0
15	B	845	BCR	3	0
15	P	202	BCR	4	0
12	H	823	CLA	6	0
12	H	831	CLA	3	0
12	a	814	CLA	1	0
12	H	828	CLA	3	0
12	b	813	CLA	1	0
12	b	807	CLA	2	0
15	H	849	BCR	3	0
15	B	843	BCR	3	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.

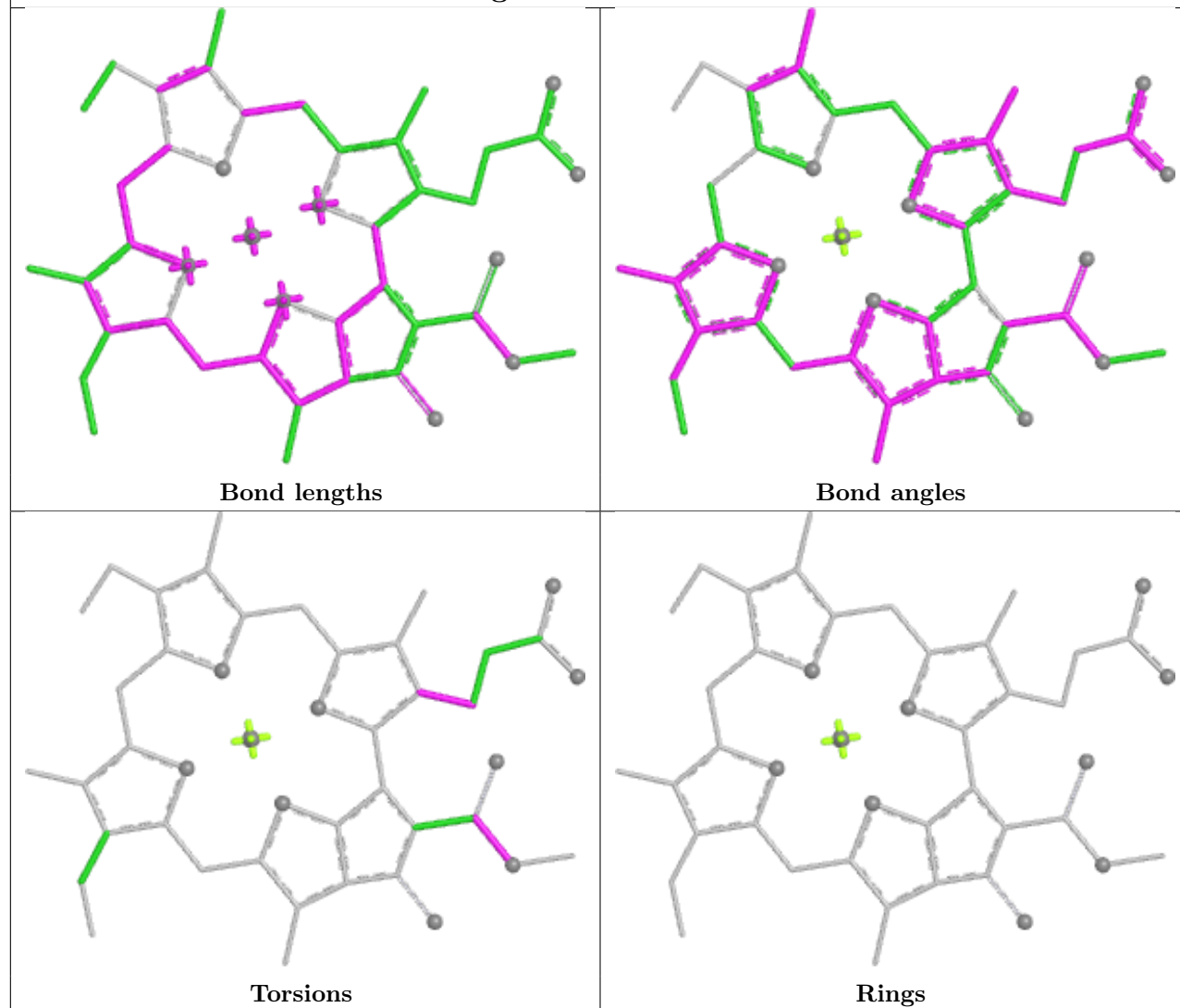


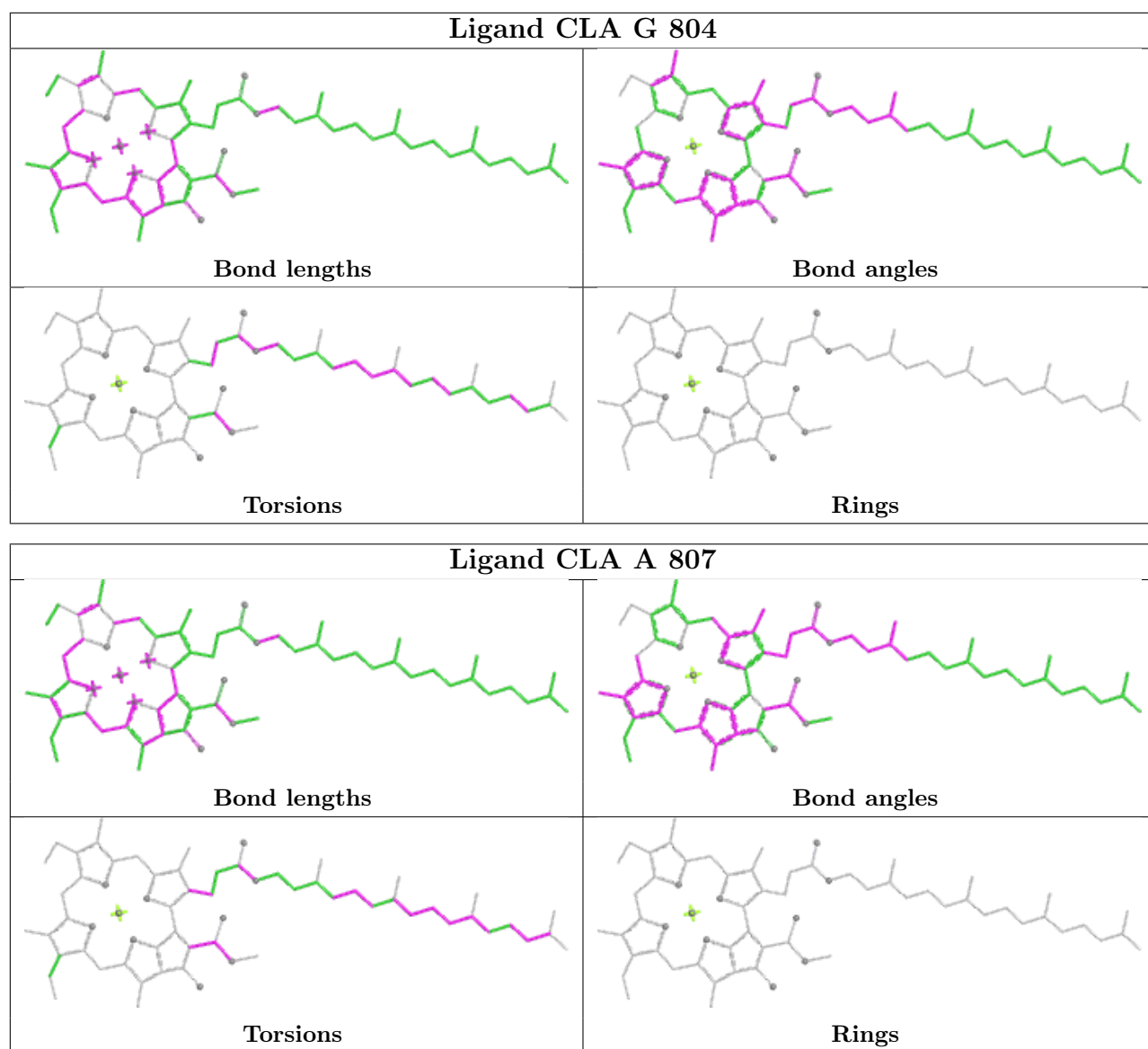


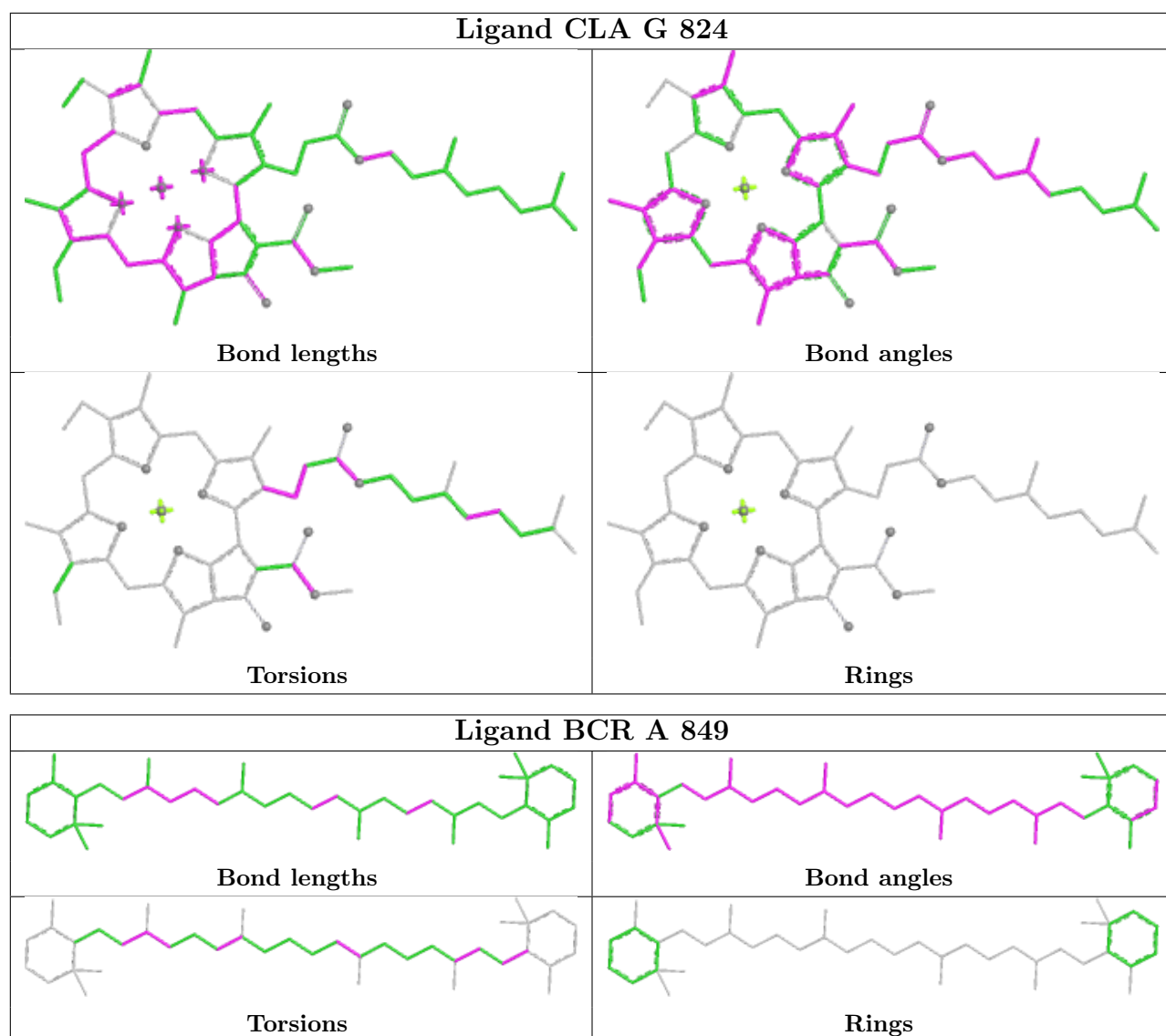
Ligand CLA S 203

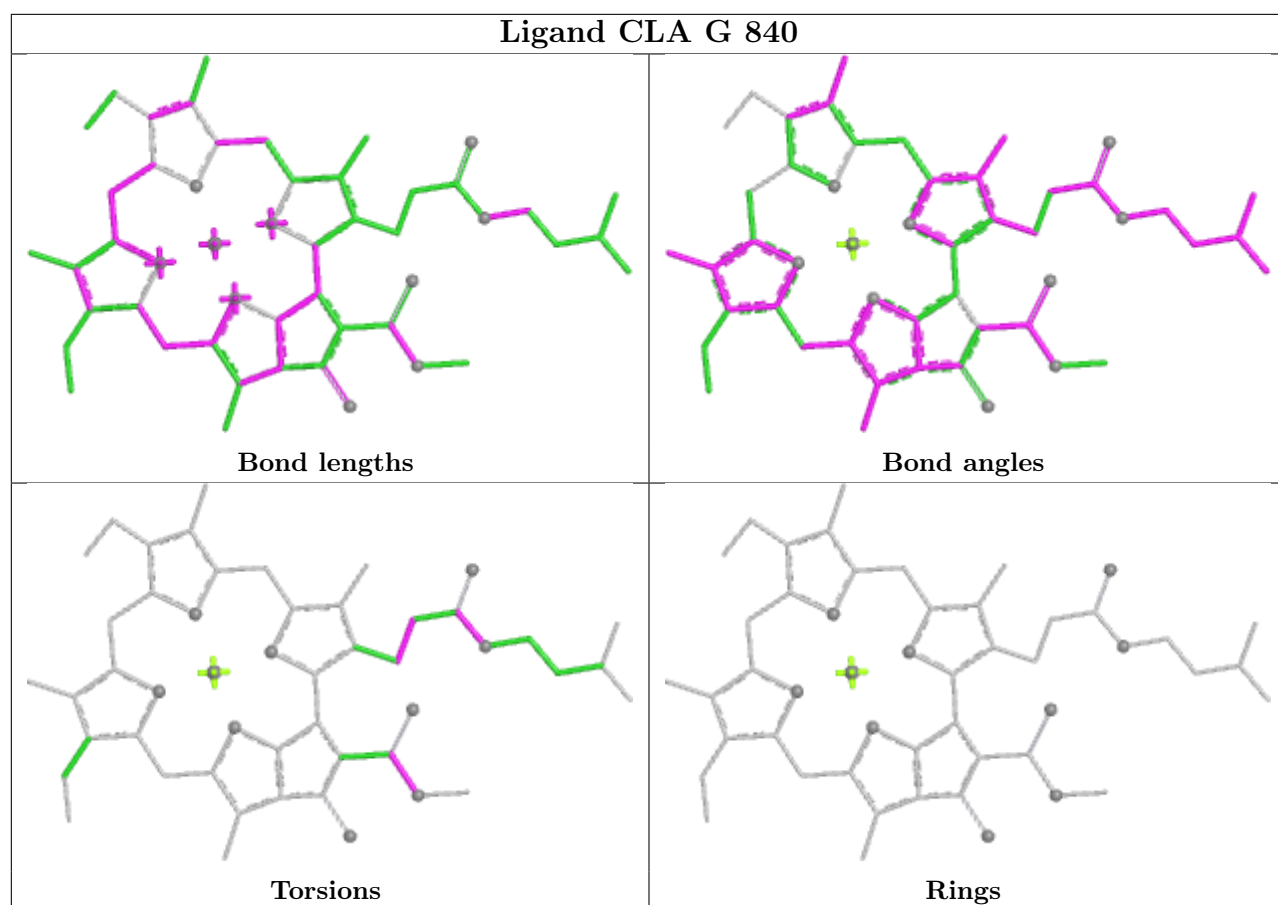


Ligand CLA H 819

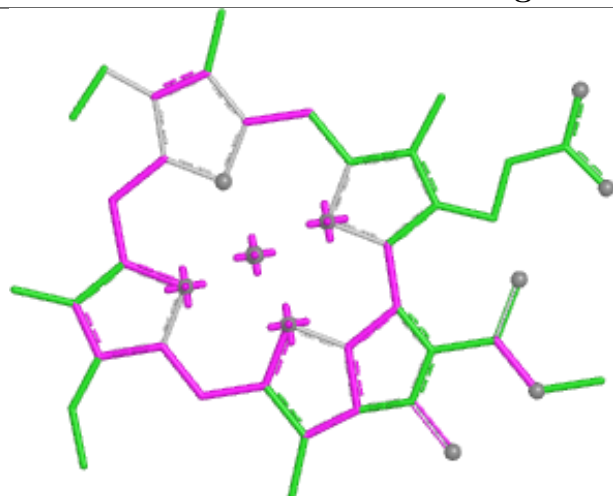




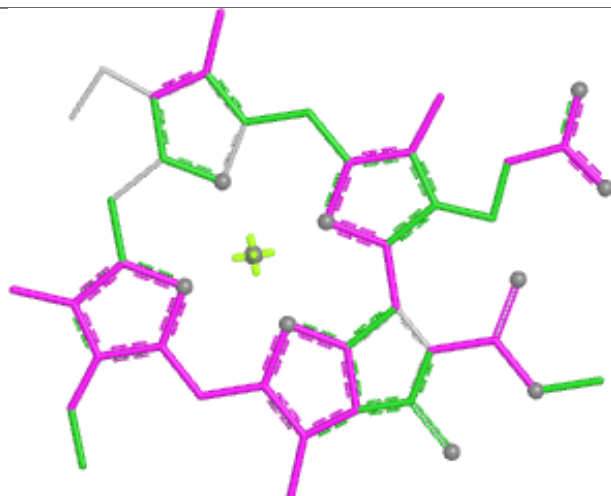




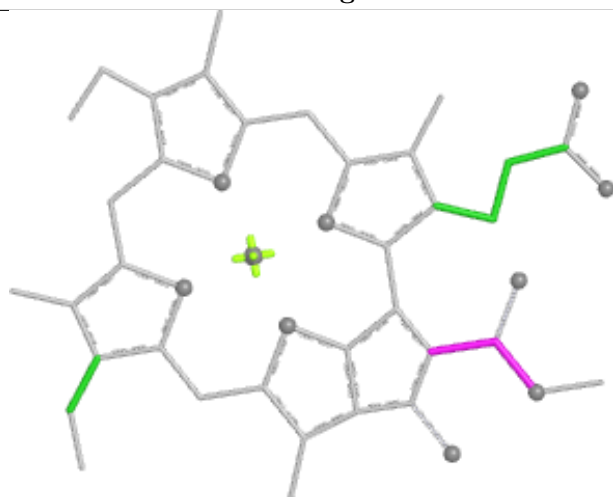
Ligand CLA B 831



Bond lengths



Bond angles

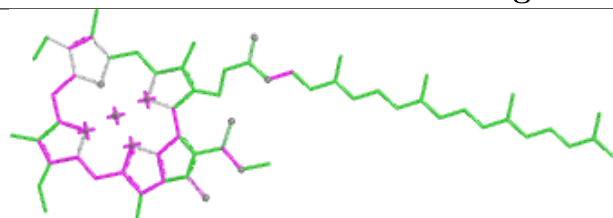


Torsions

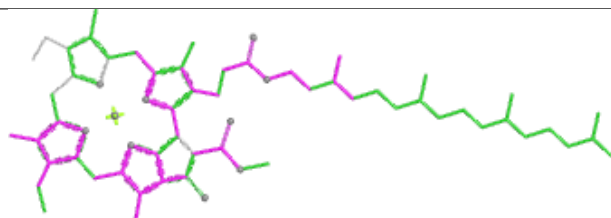


Rings

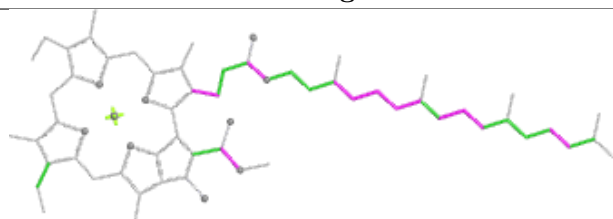
Ligand CLA H 817



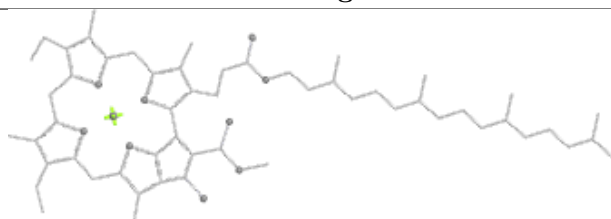
Bond lengths



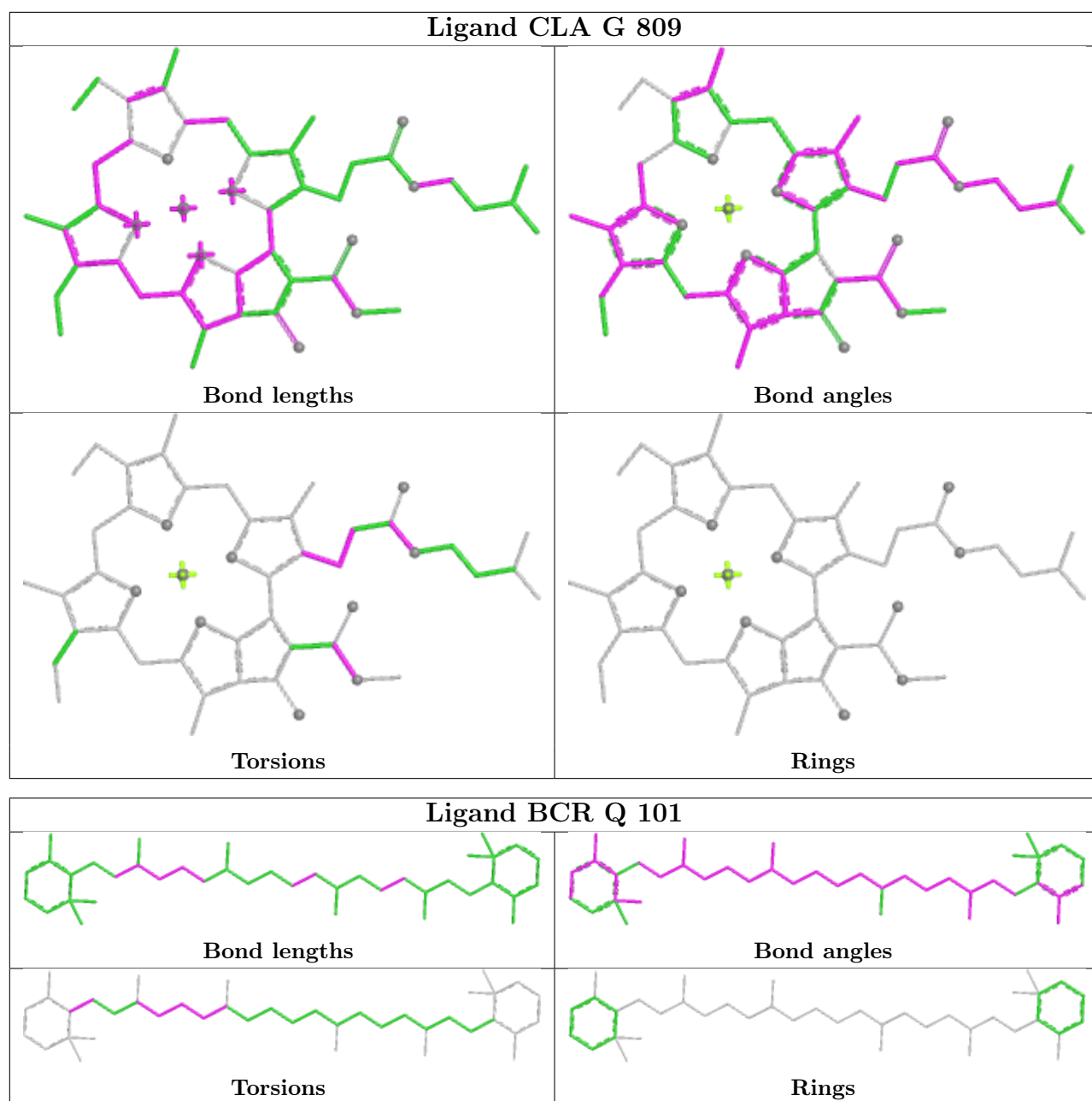
Bond angles



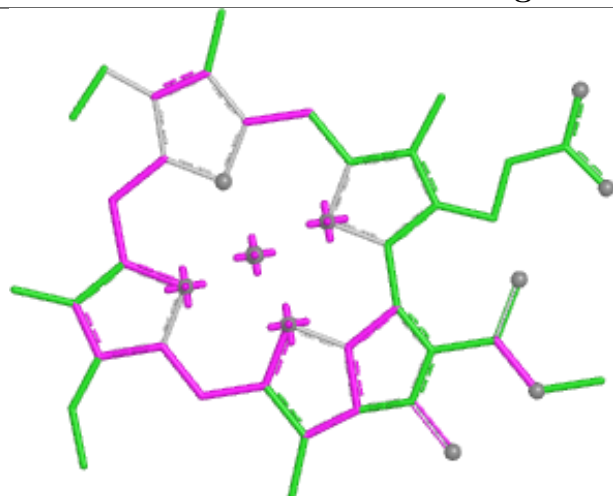
Torsions



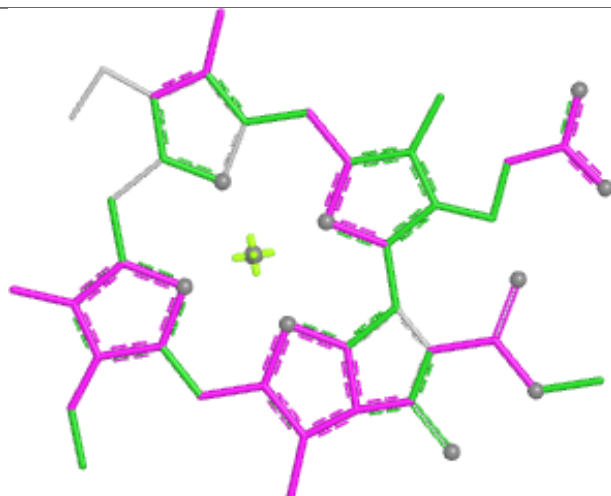
Rings



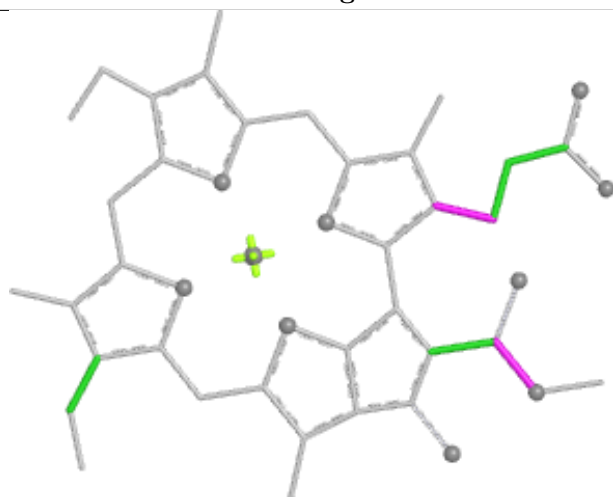
Ligand CLA B 827



Bond lengths



Bond angles

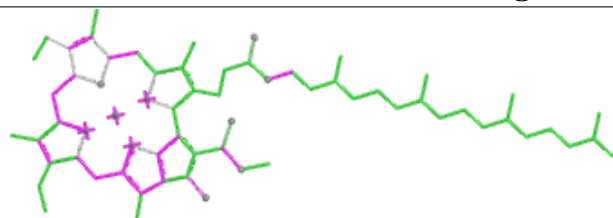


Torsions

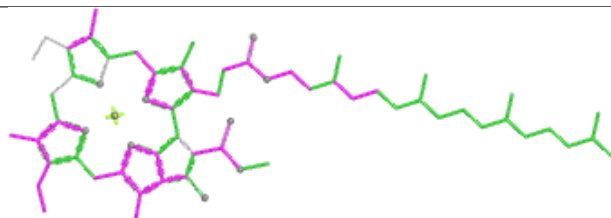


Rings

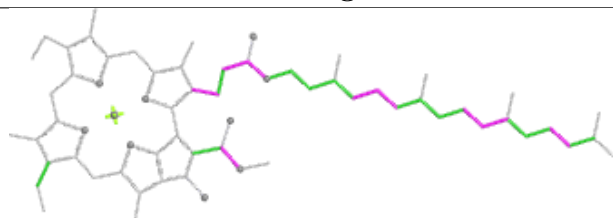
Ligand CLA G 807



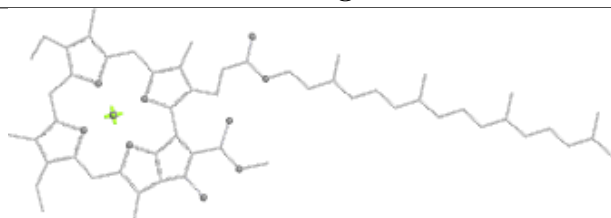
Bond lengths



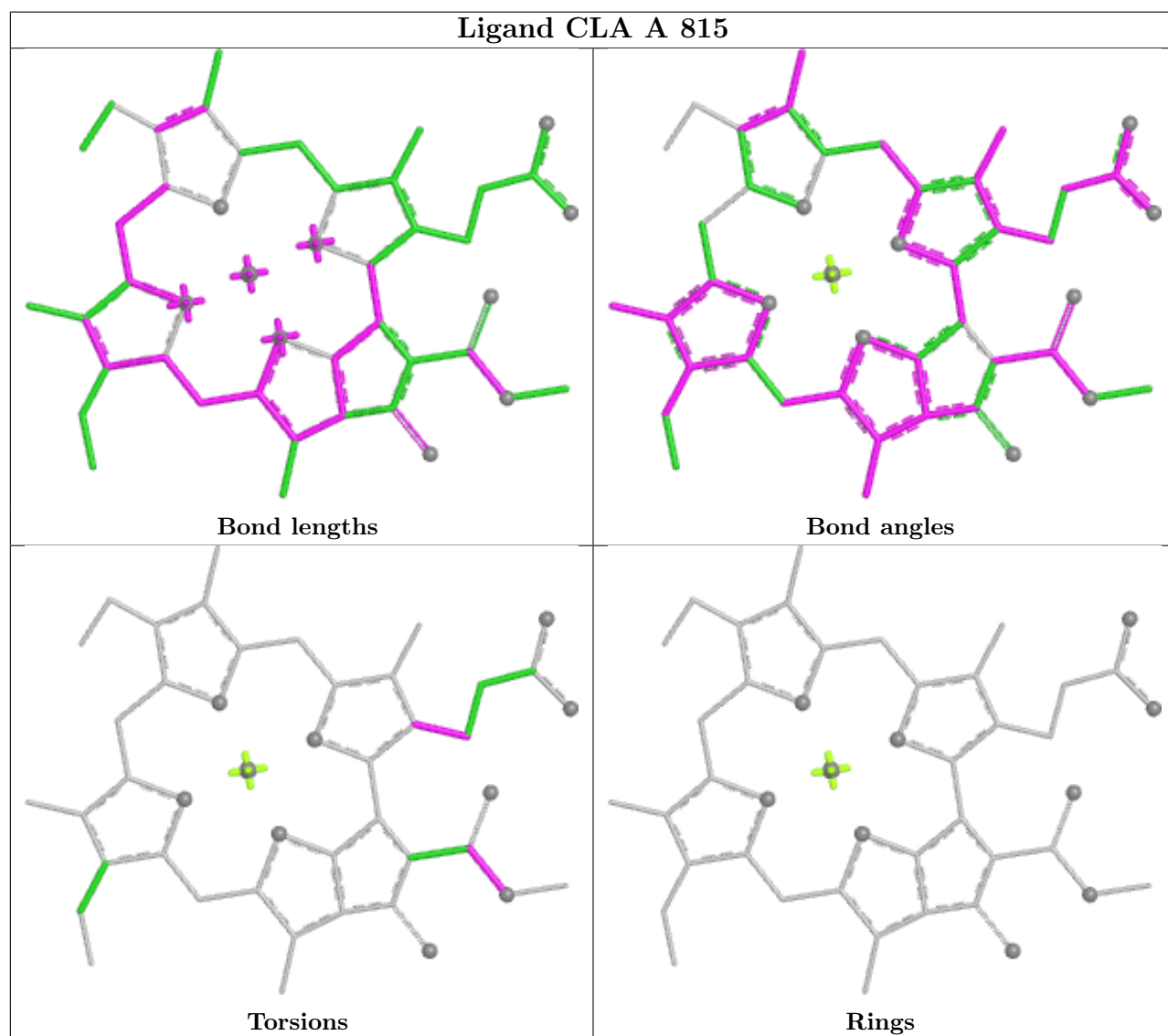
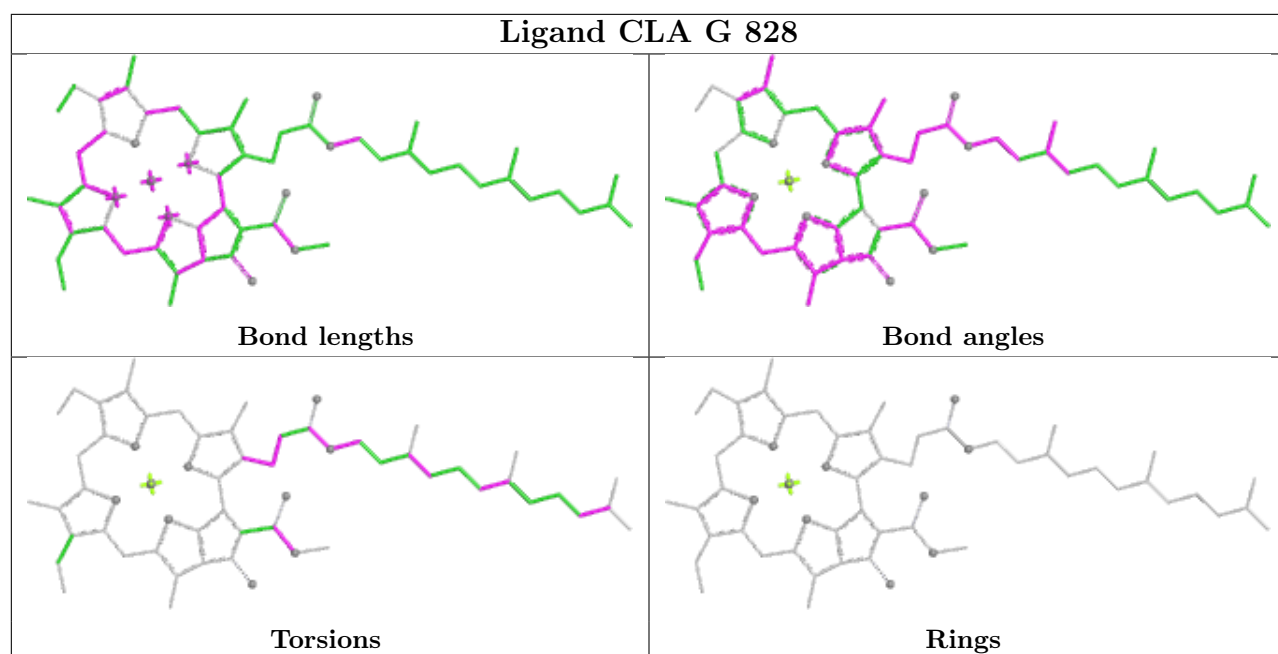
Bond angles

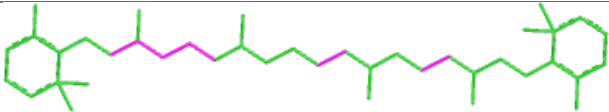
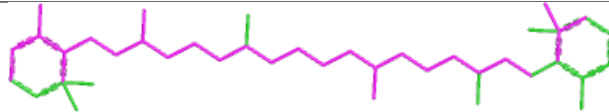
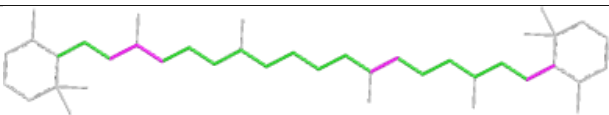
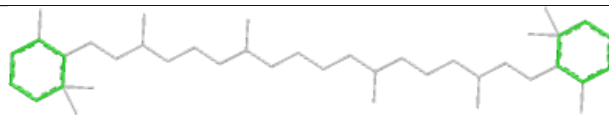



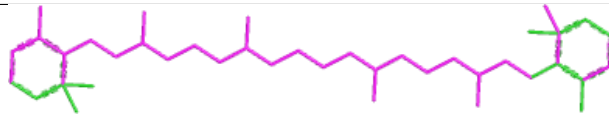
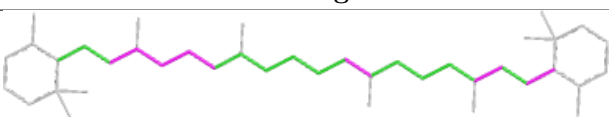
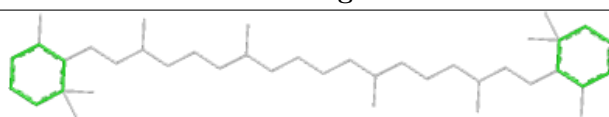
Torsions

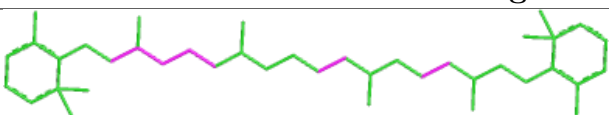
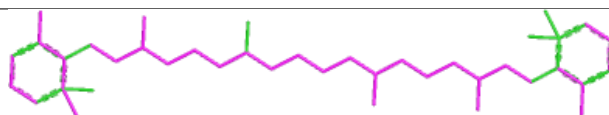
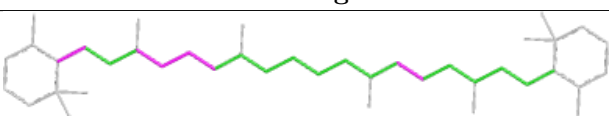
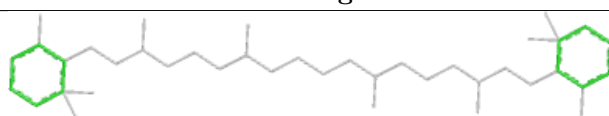


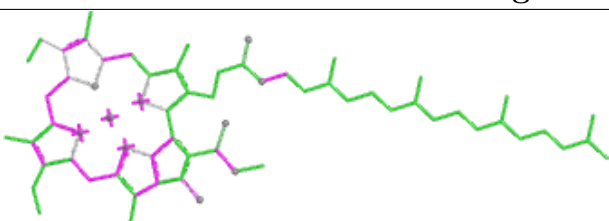
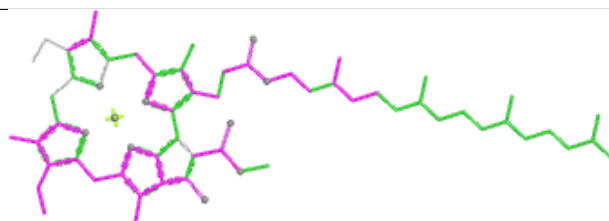
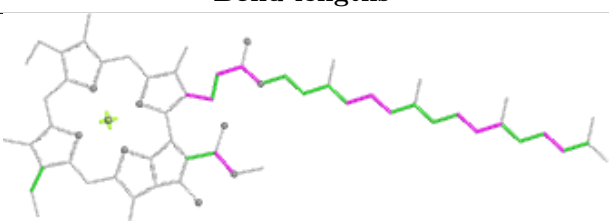
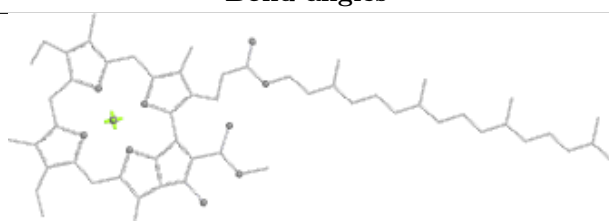
Rings

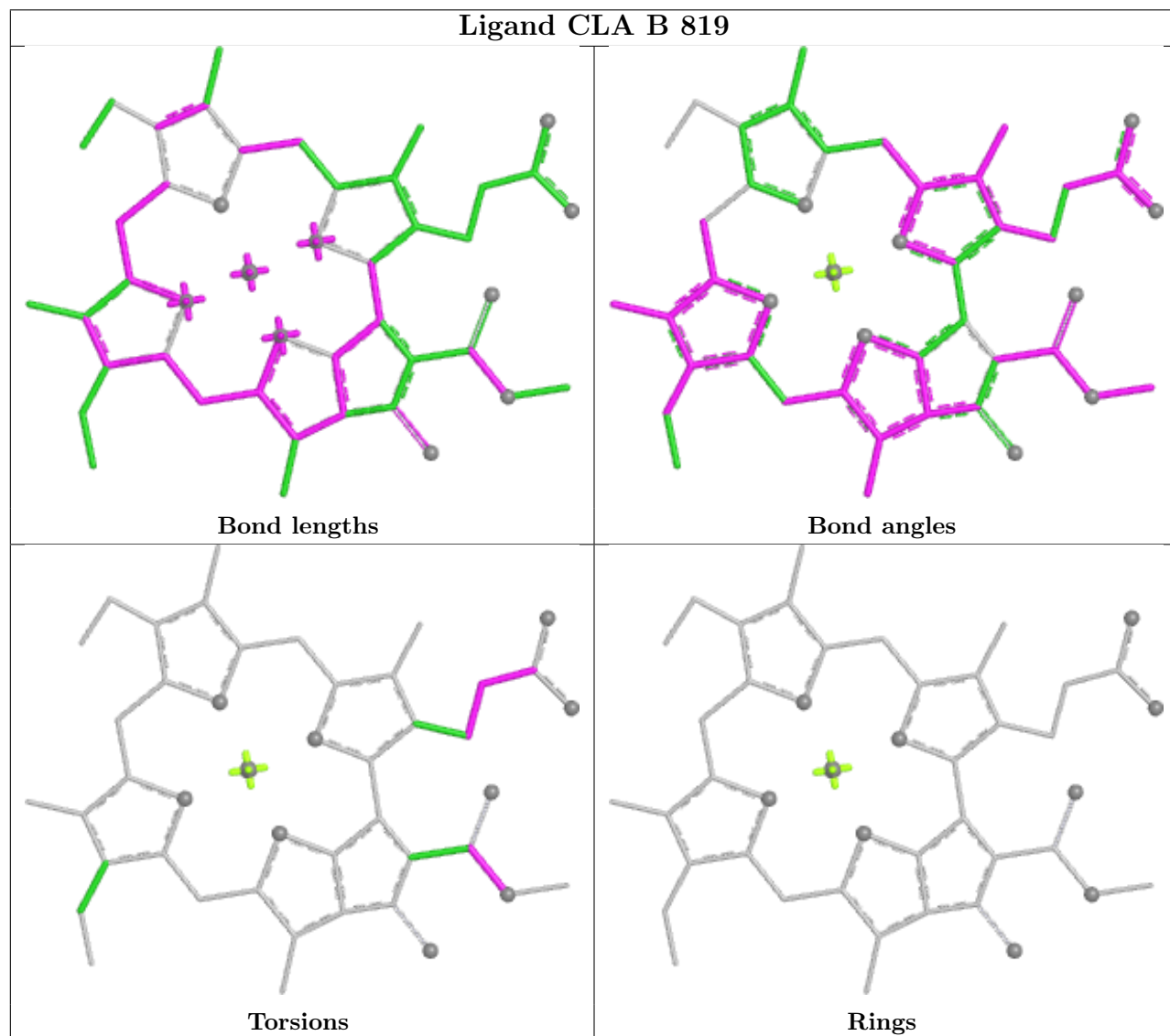
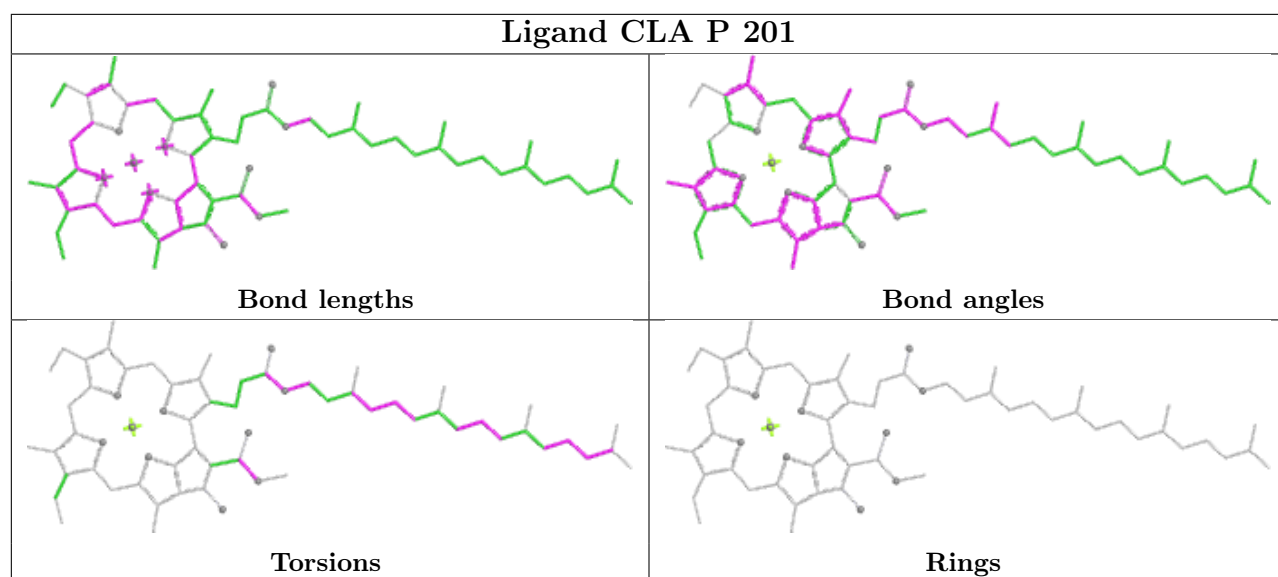


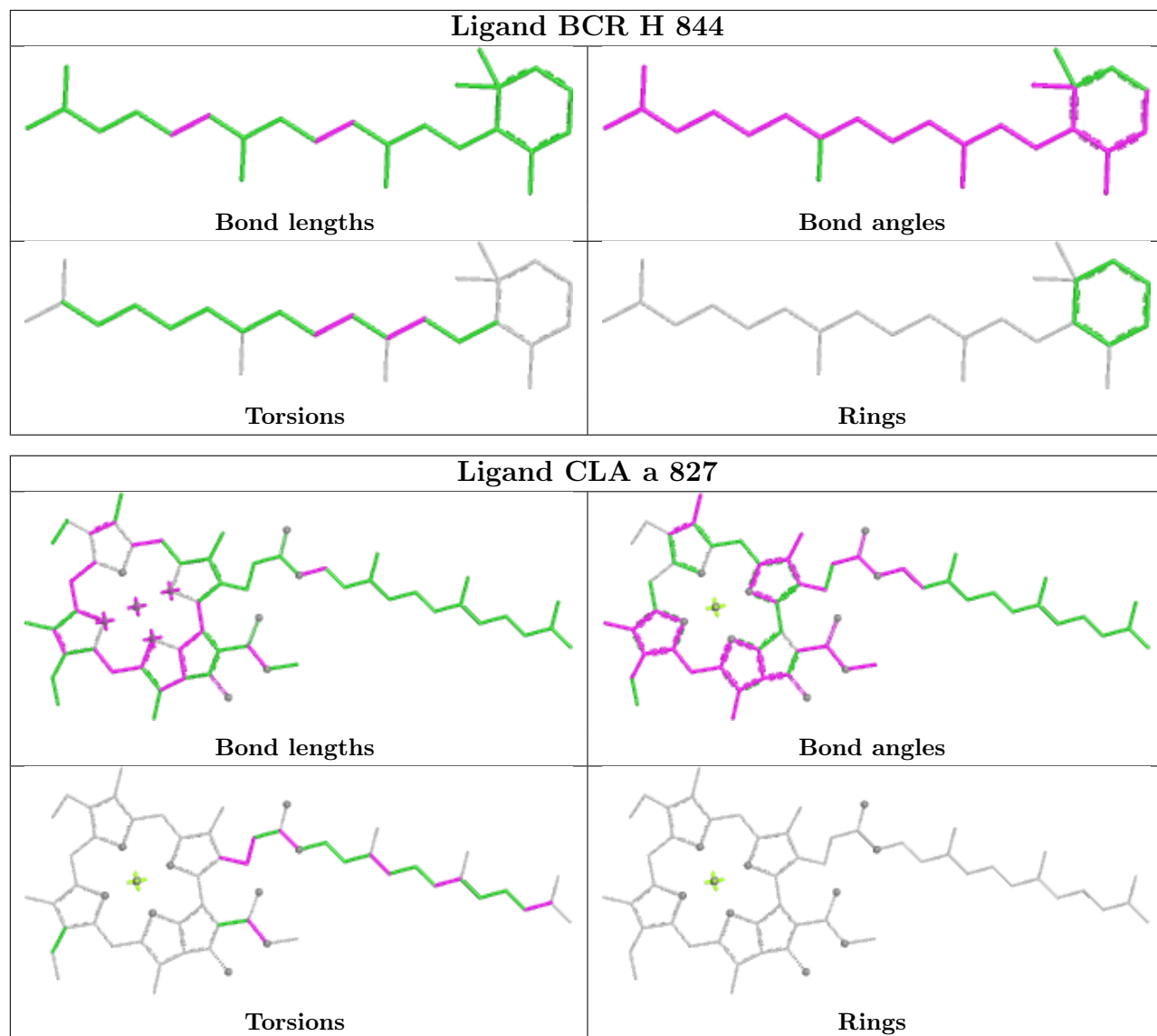
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

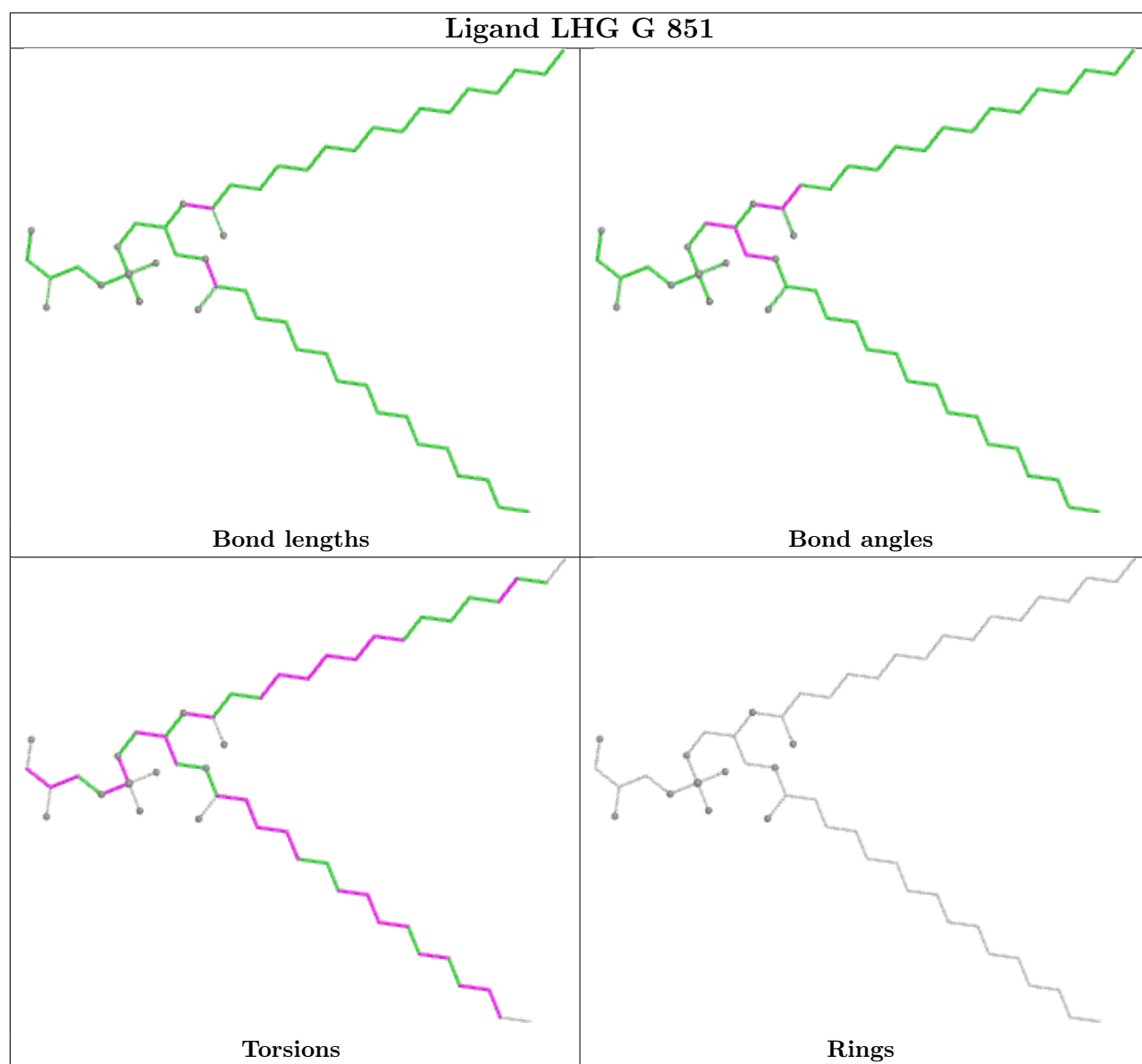
Ligand BCR G 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

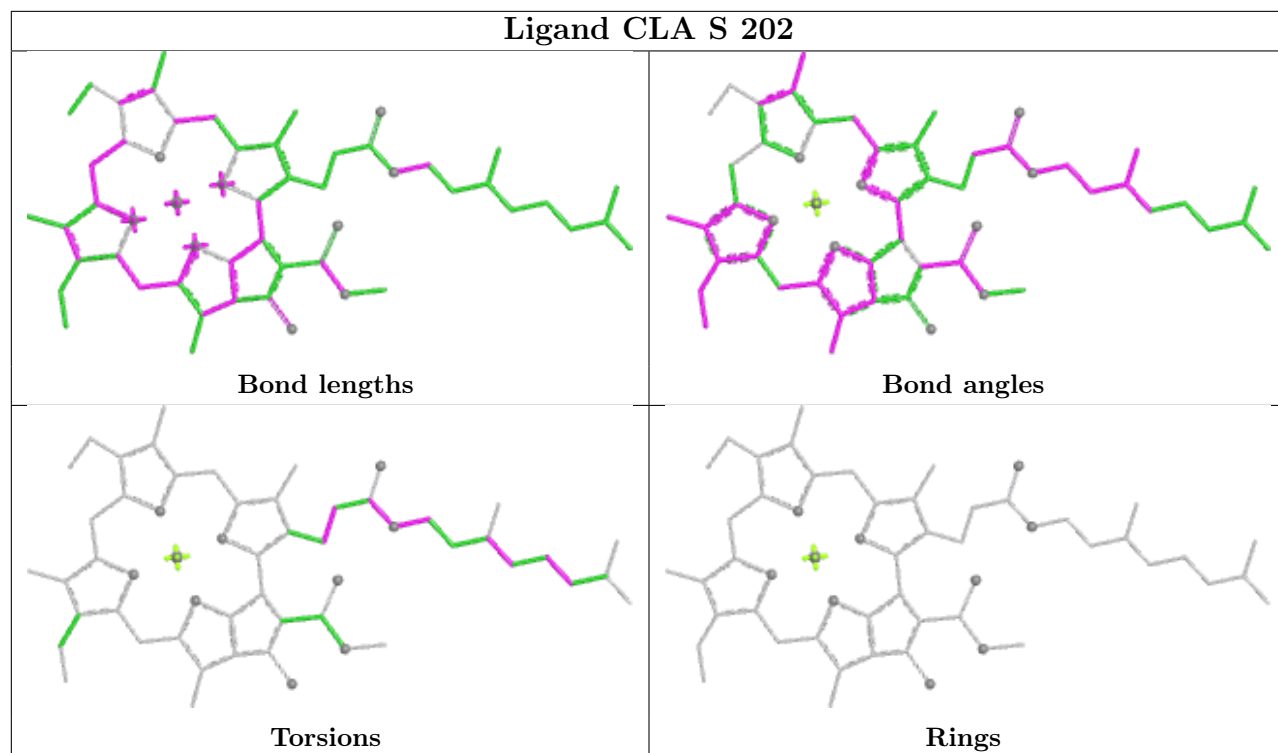
Ligand CLA a 806	
	
Bond lengths	Bond angles
	
Torsions	Rings



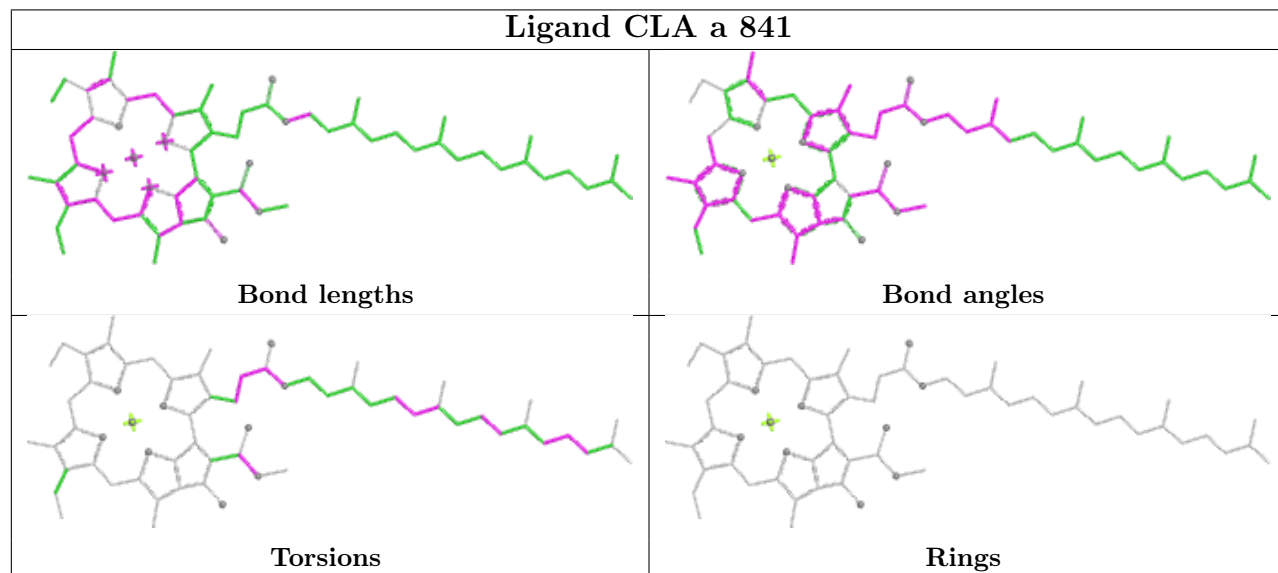


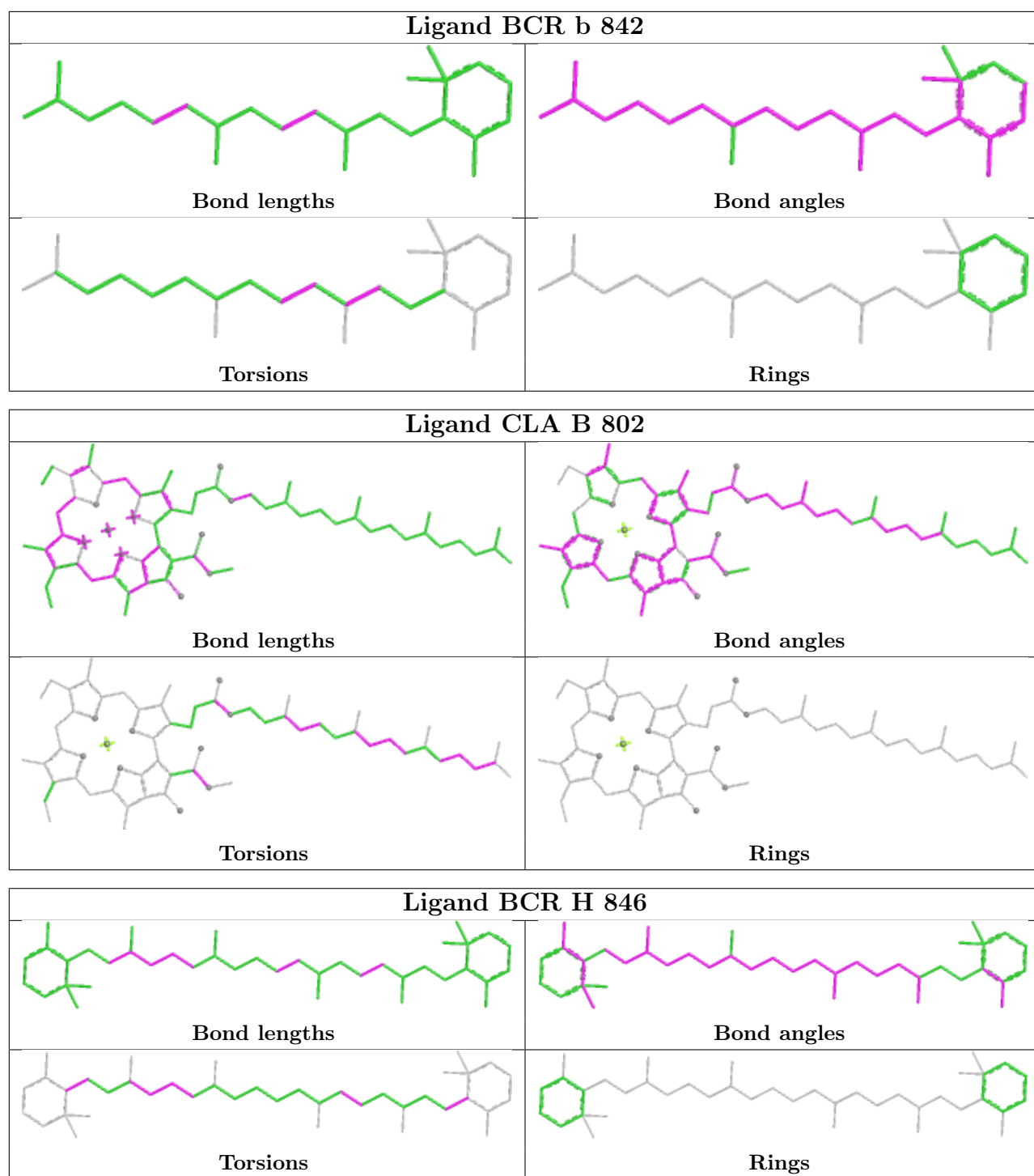


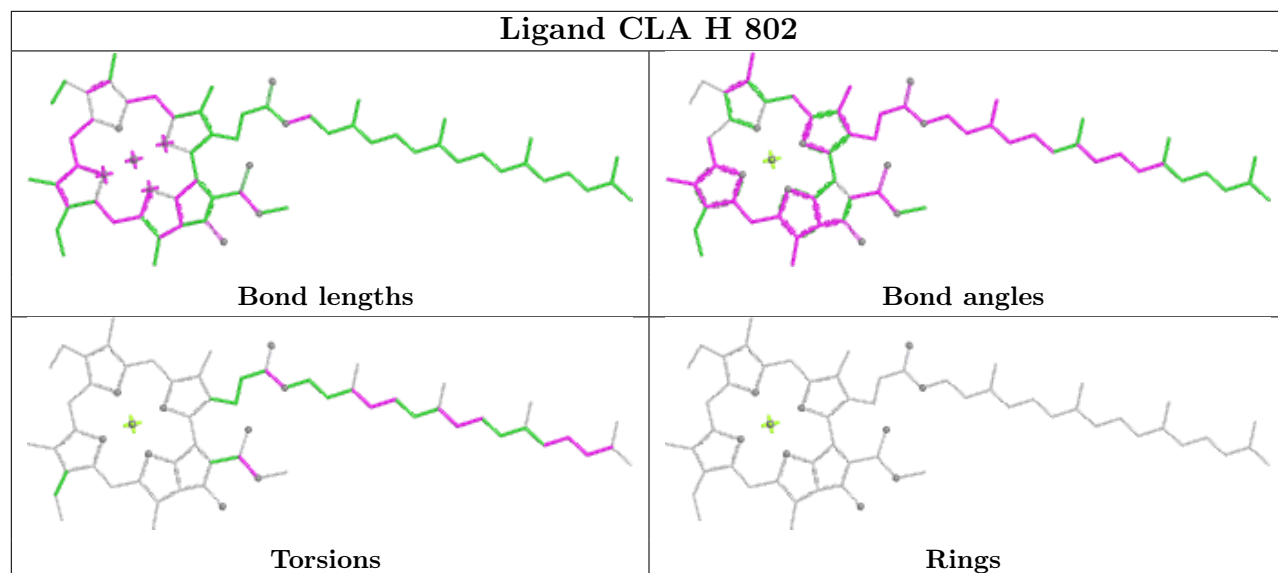
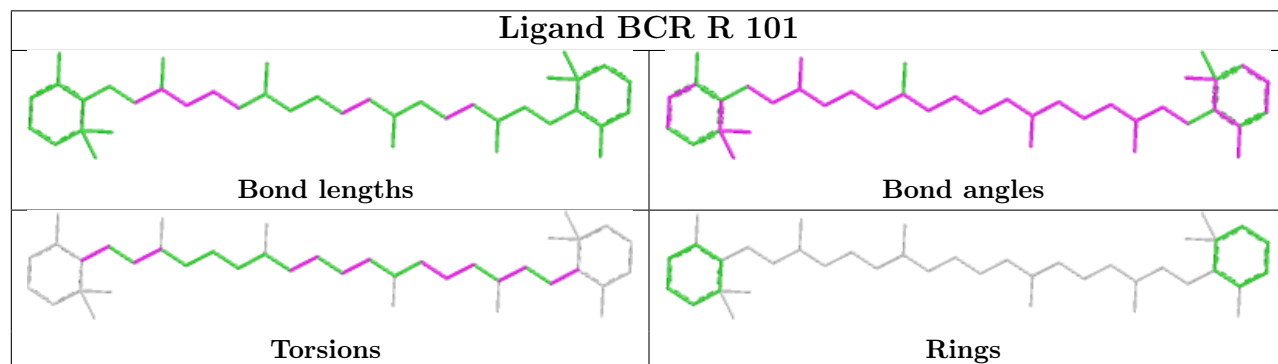
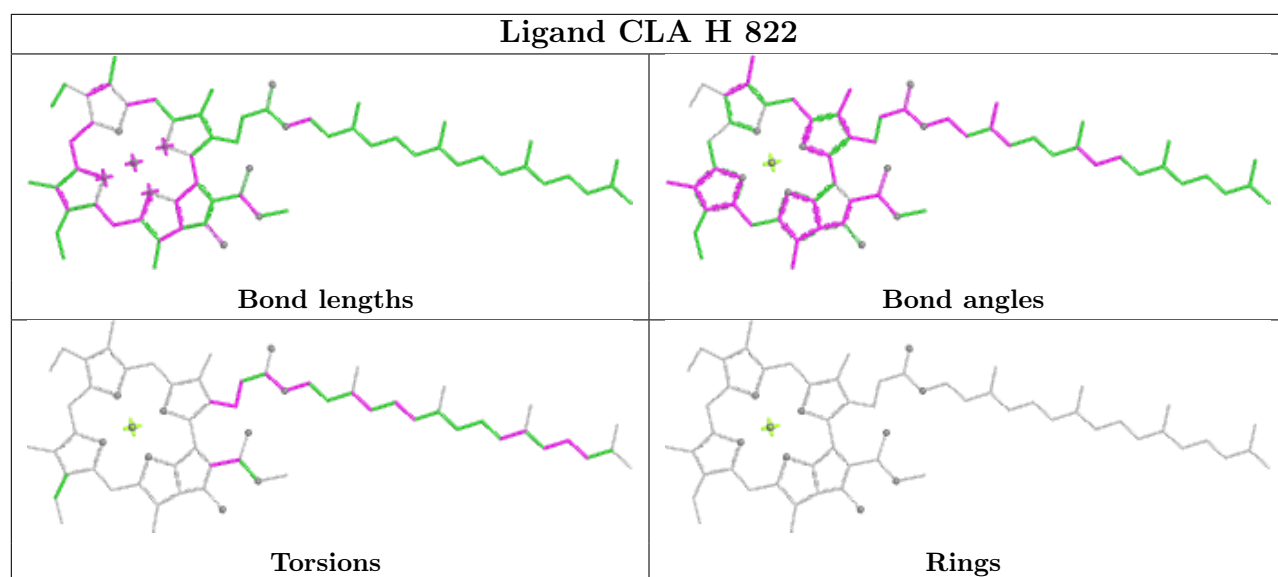
Ligand CLA S 202



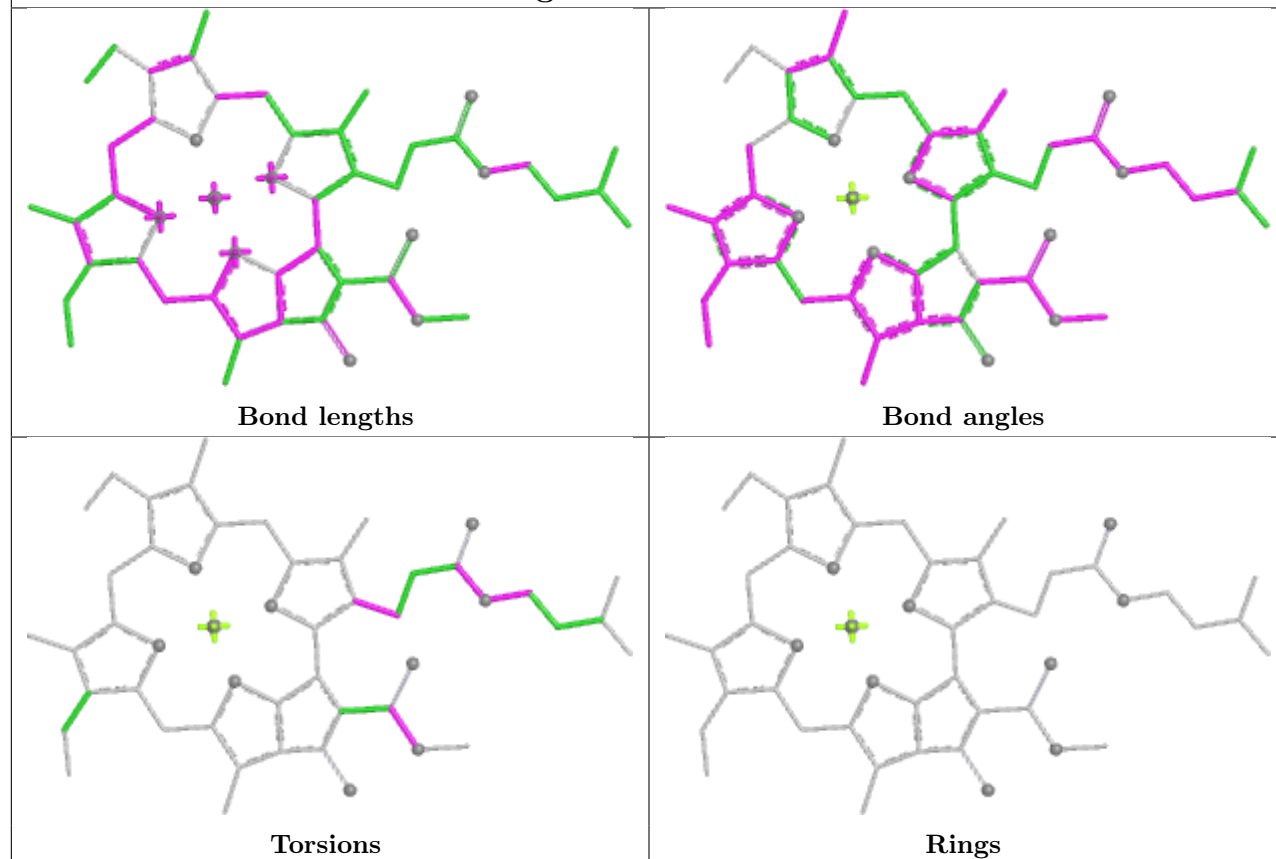
Ligand CLA a 841



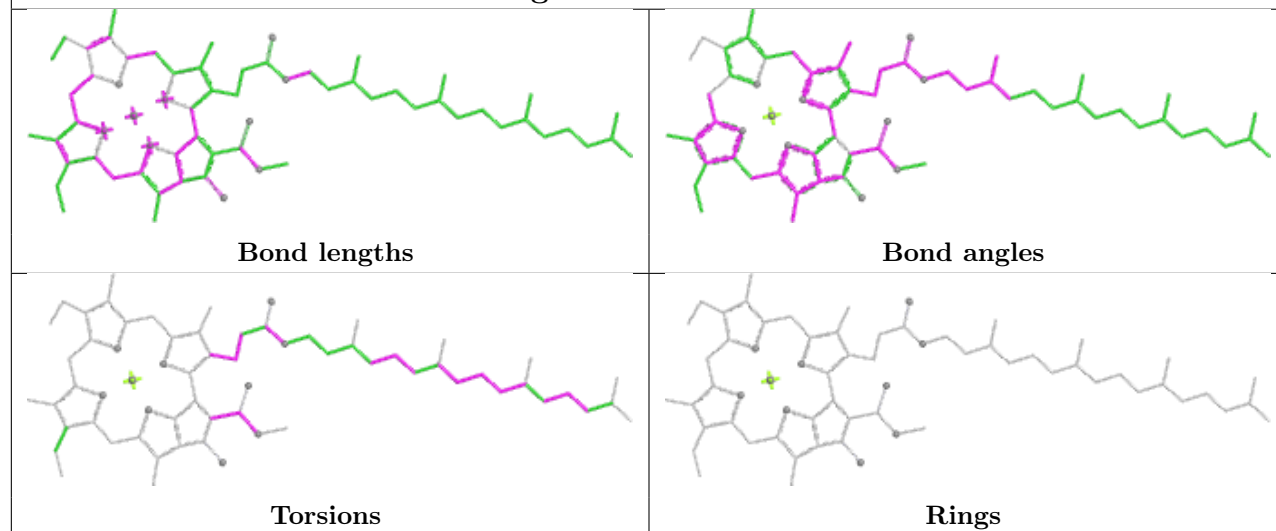


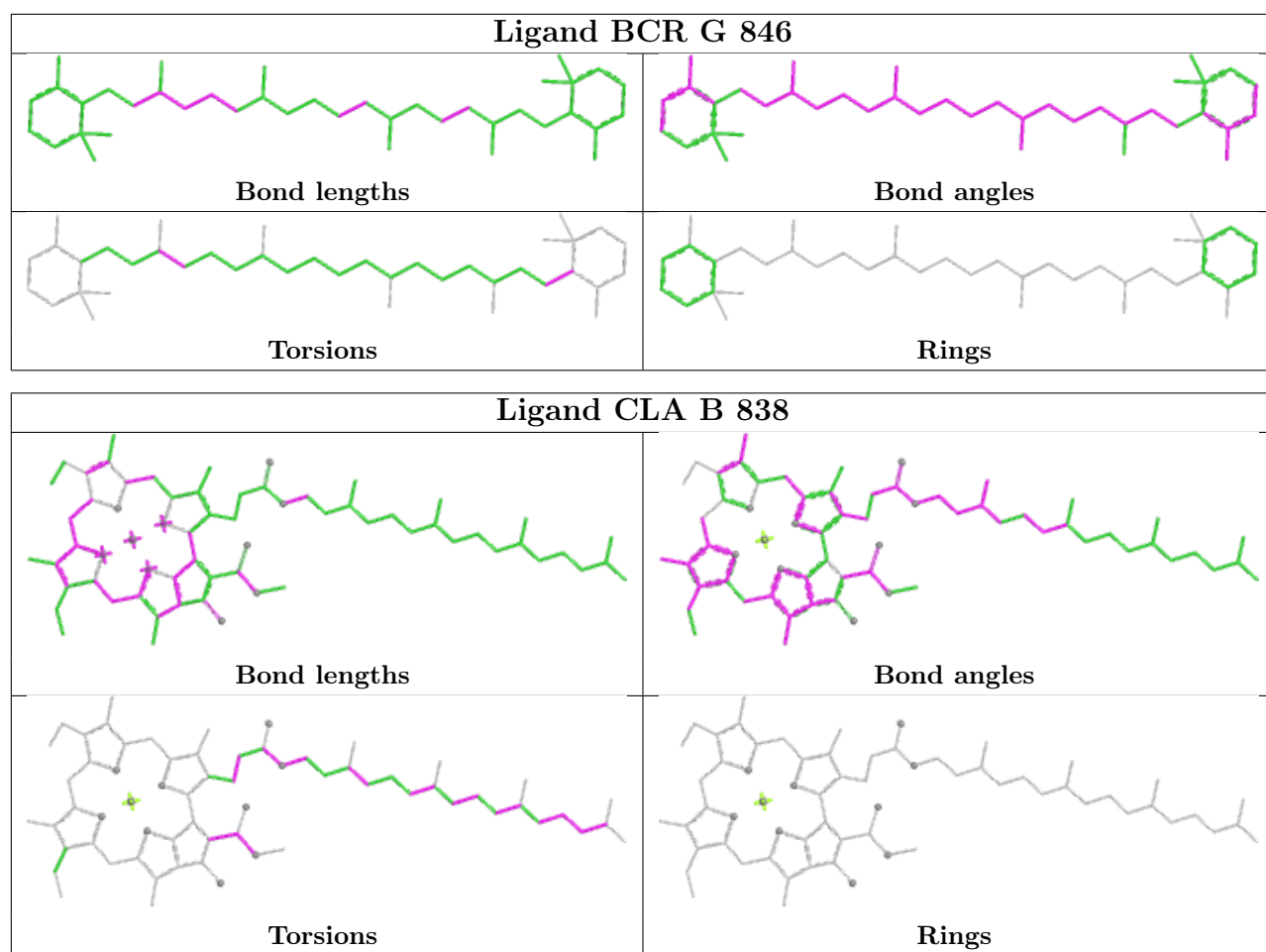


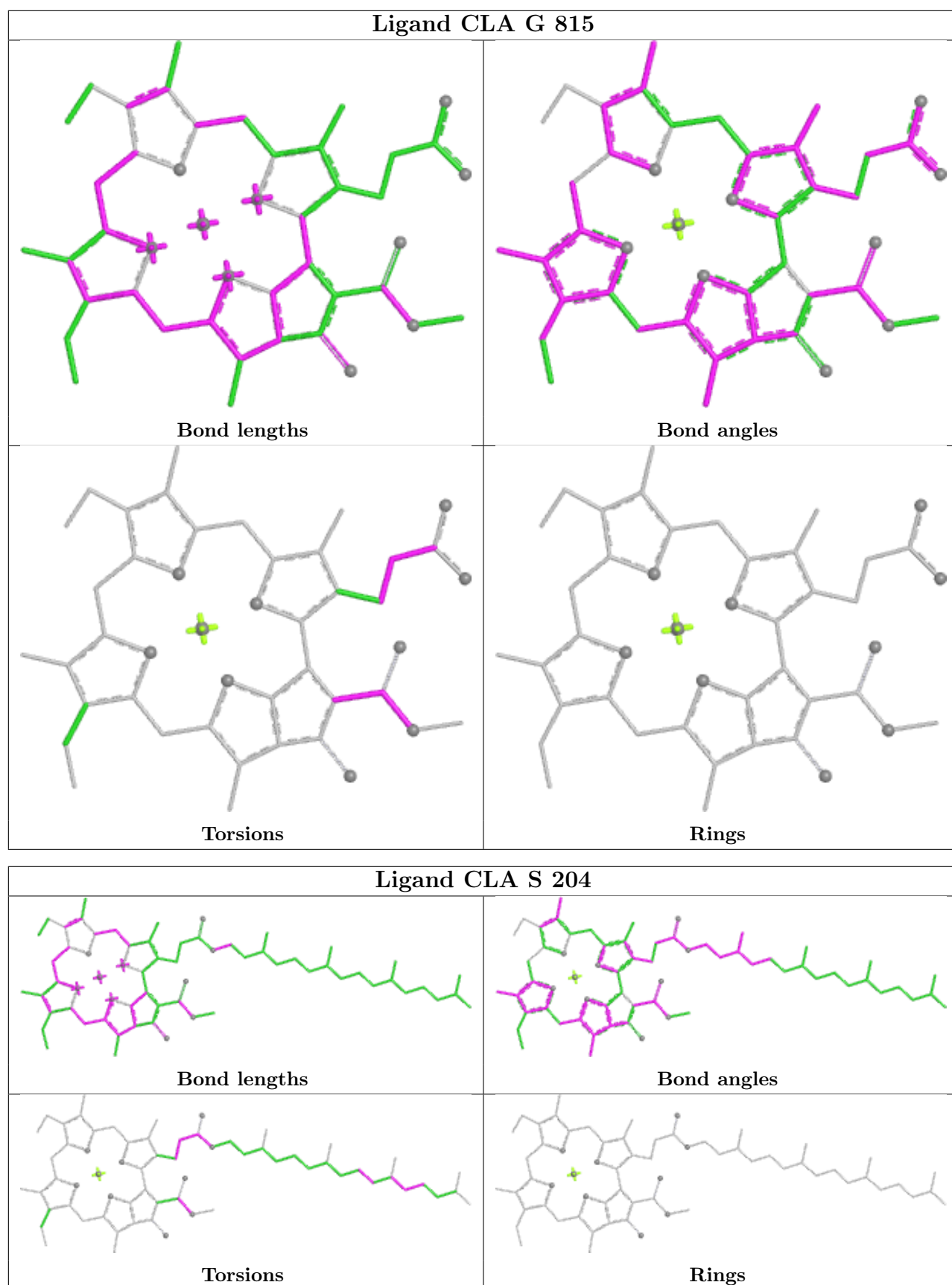
Ligand CLA a 810

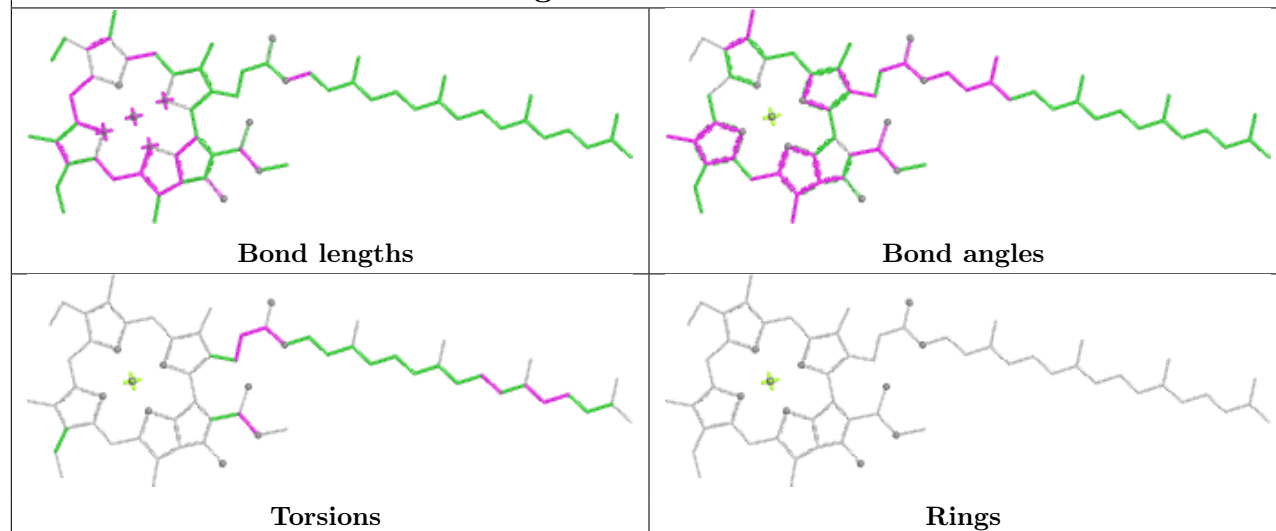
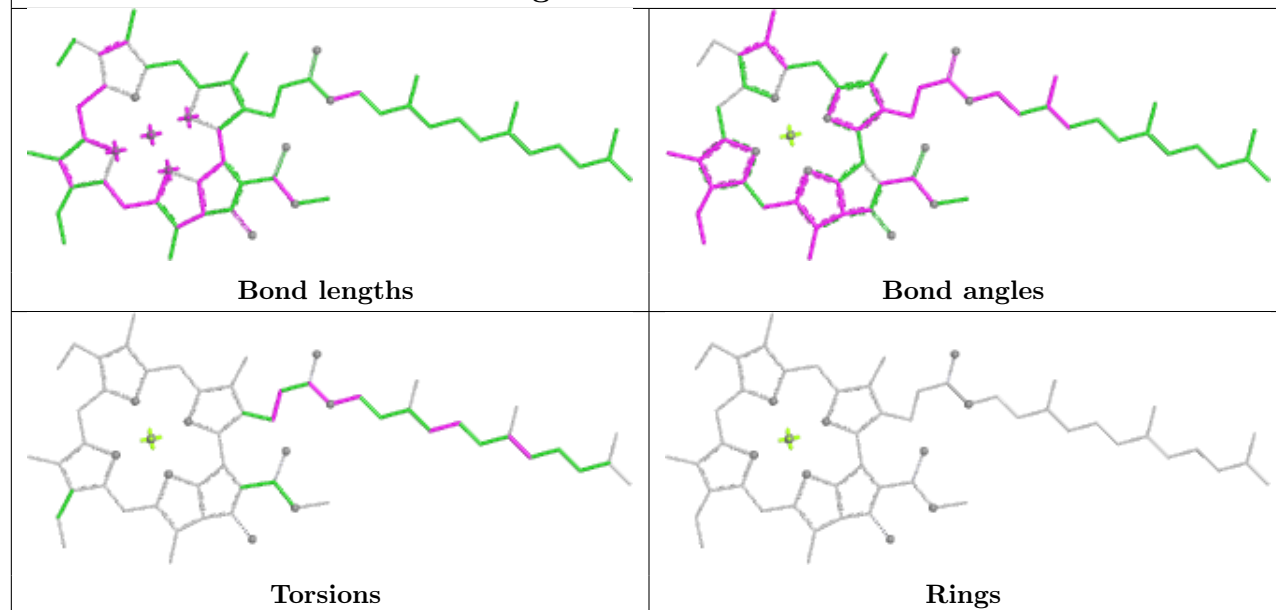


Ligand CLA G 808

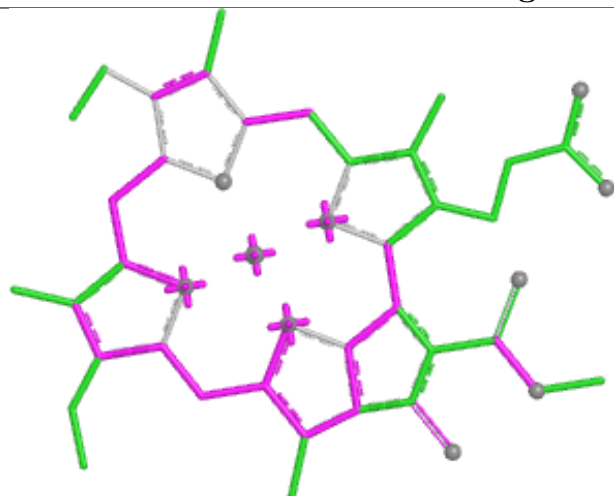




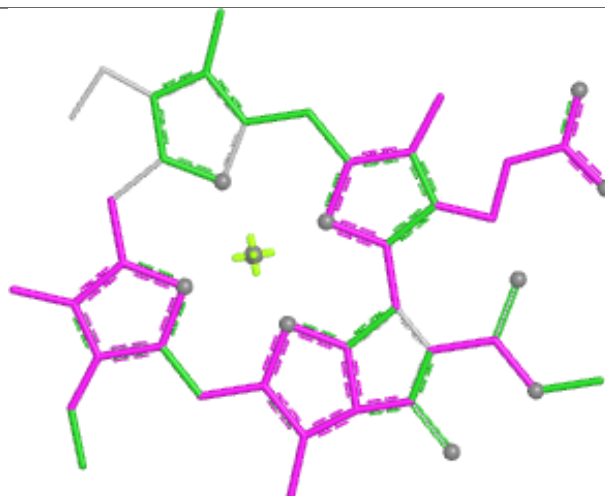


Ligand CLA L 206**Ligand CLA B 801**

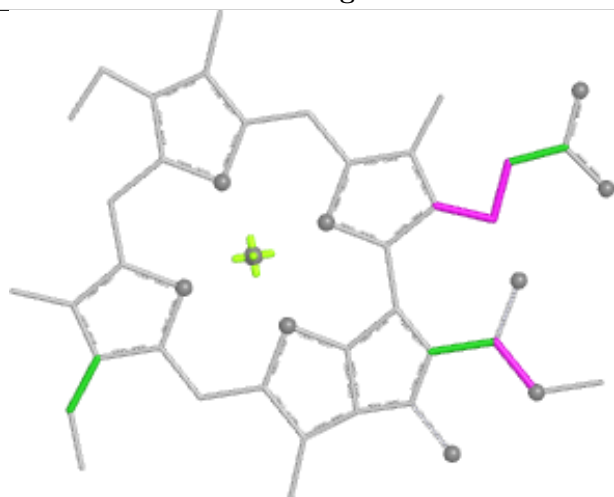
Ligand CLA a 835



Bond lengths



Bond angles

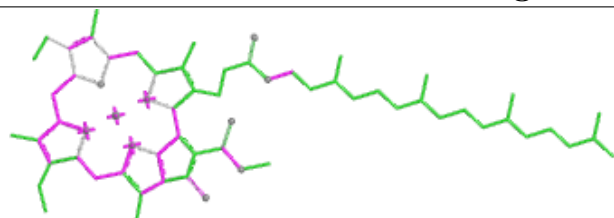


Torsions

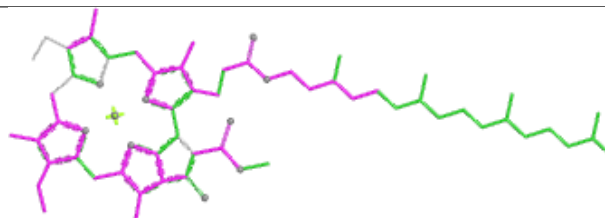


Rings

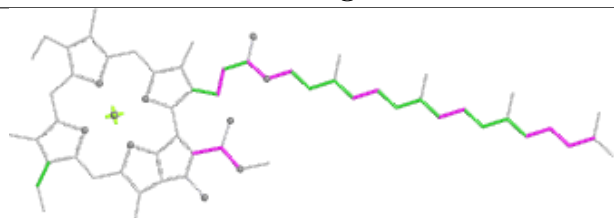
Ligand CLA H 839



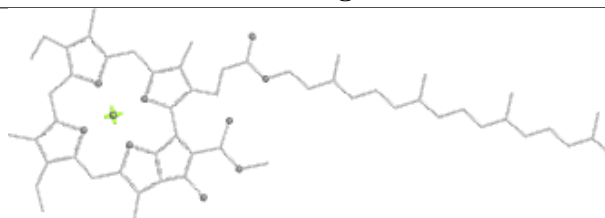
Bond lengths



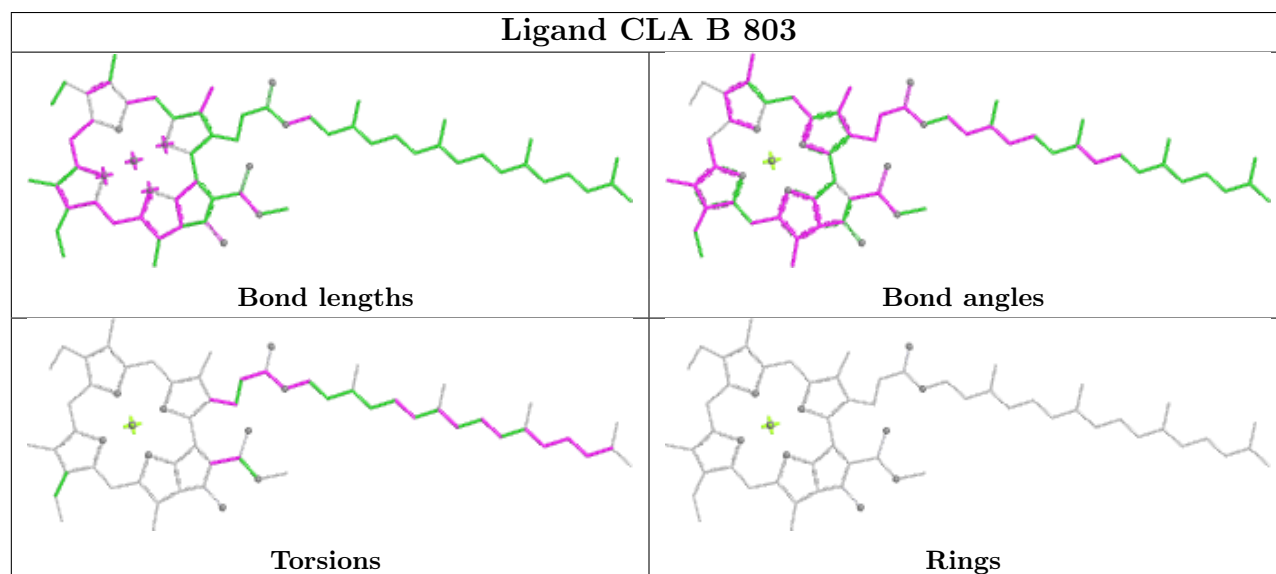
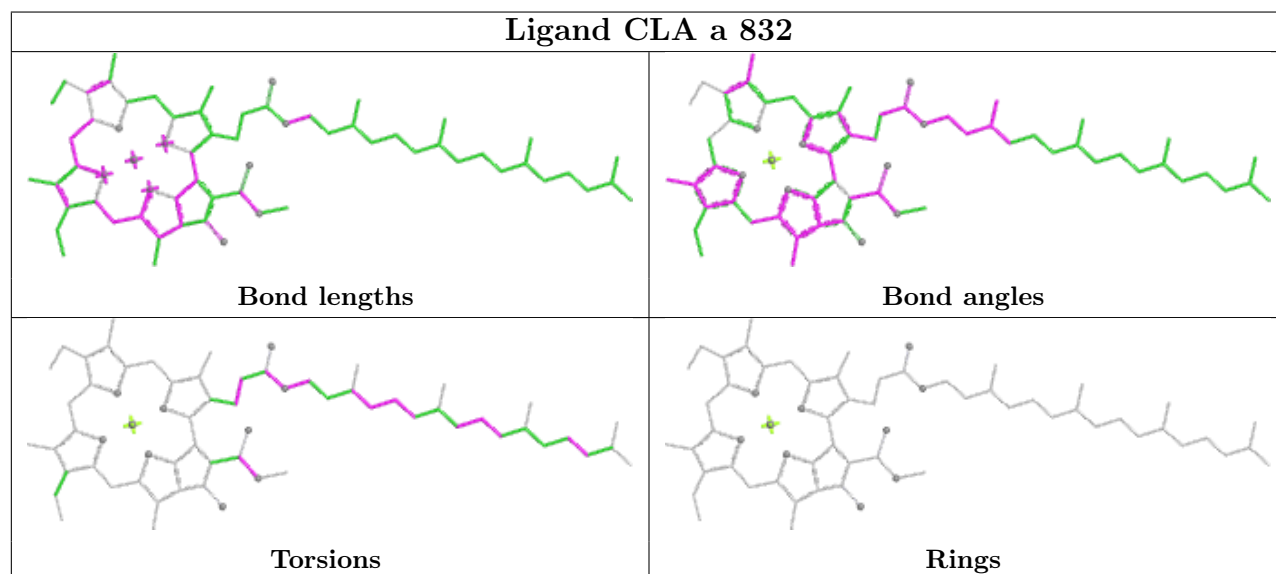
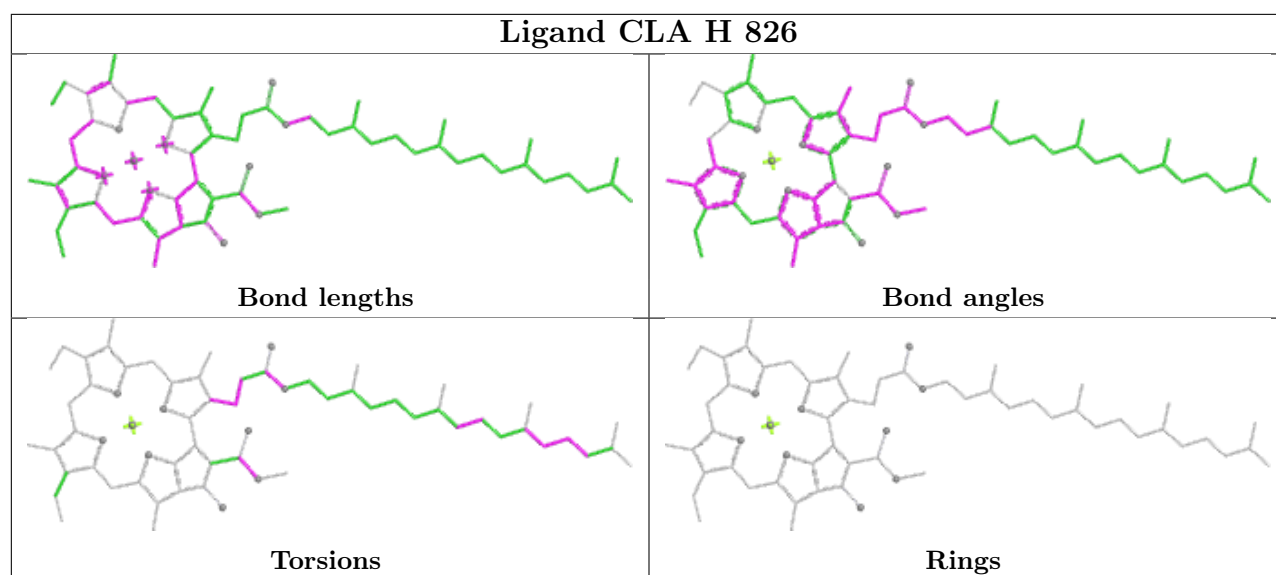
Bond angles

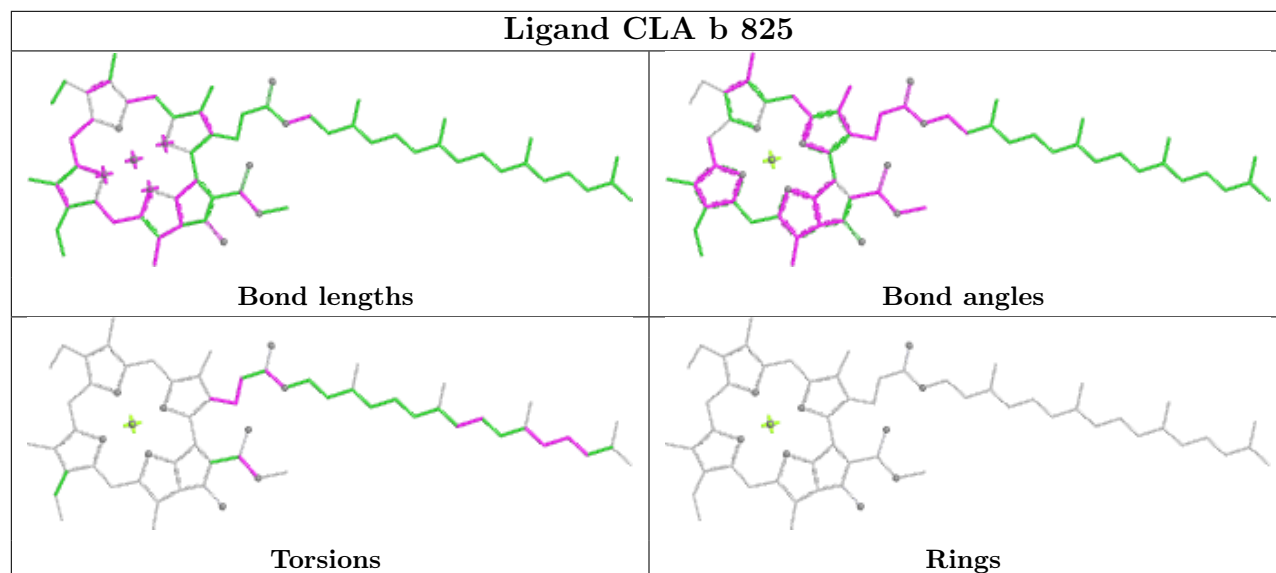
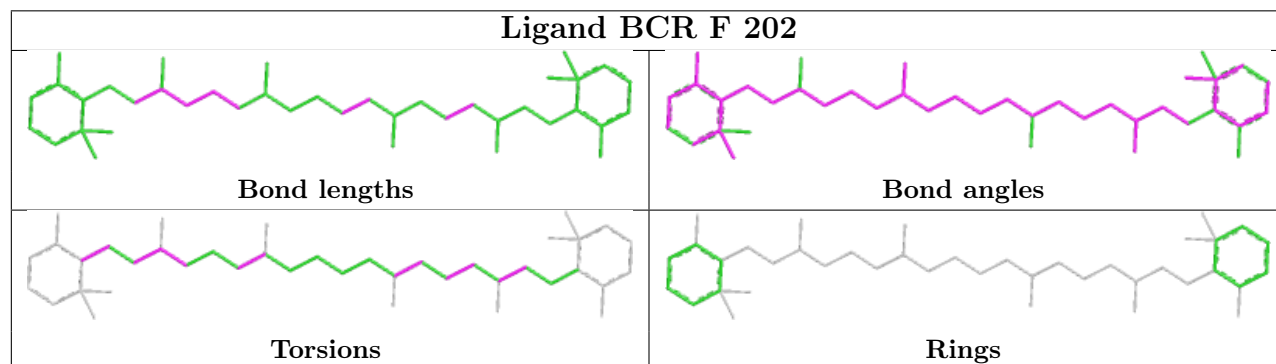
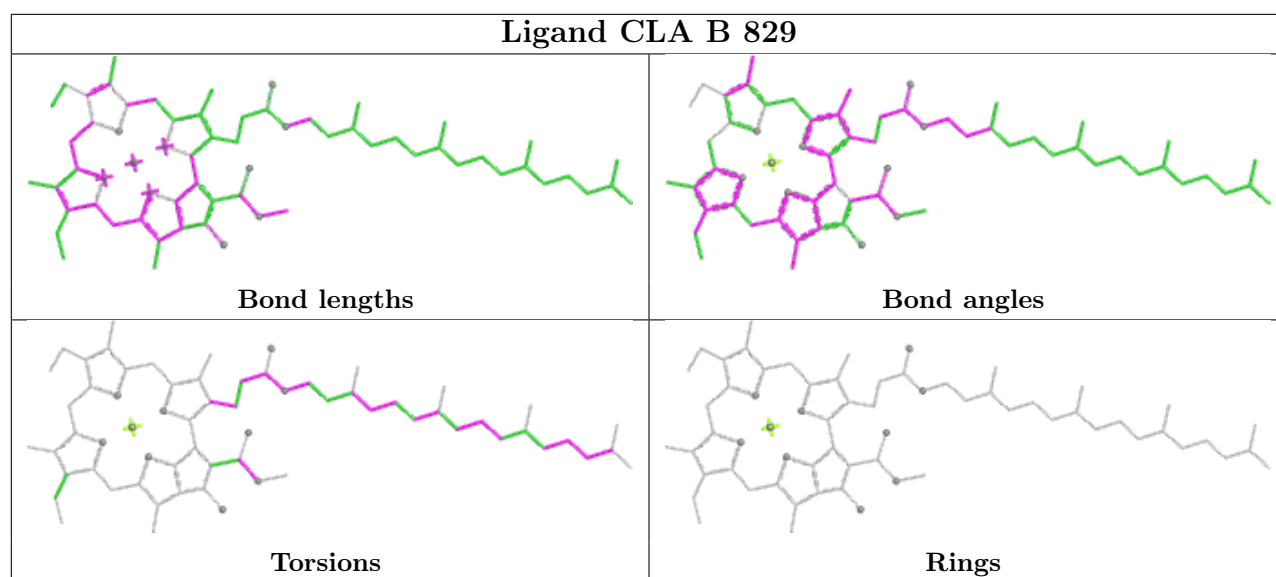


Torsions

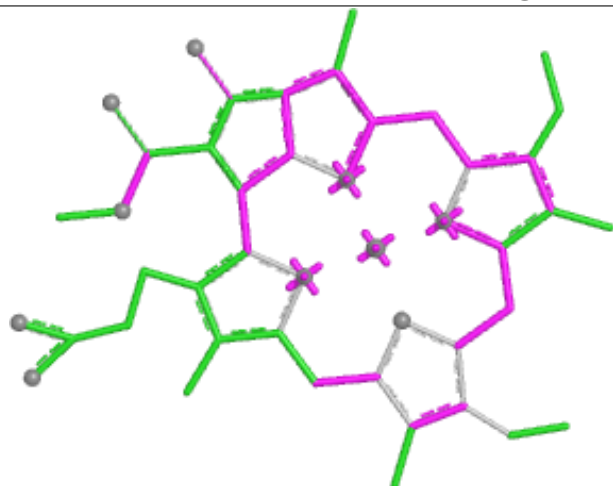


Rings

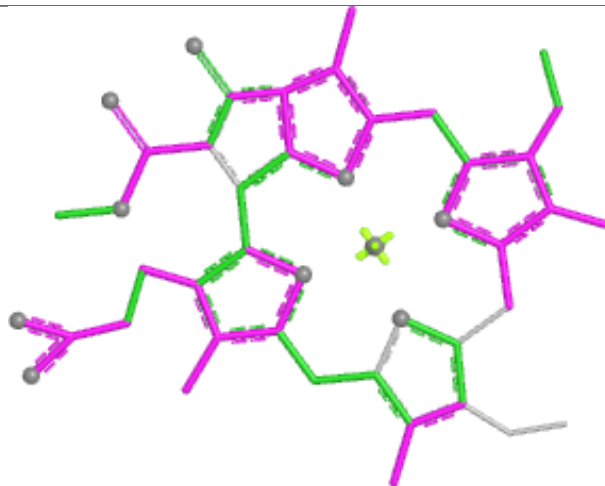




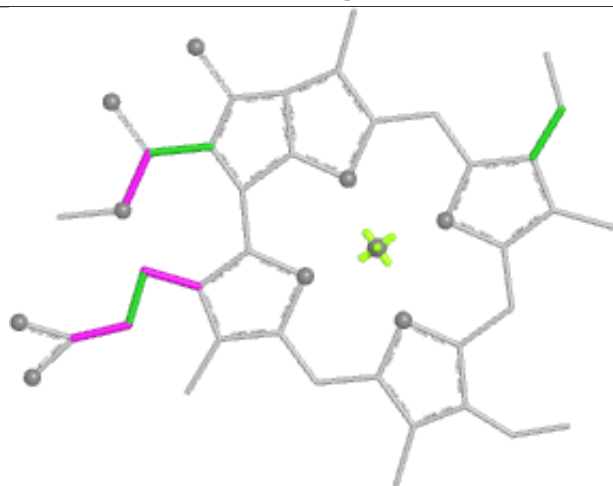
Ligand CLA F 203



Bond lengths



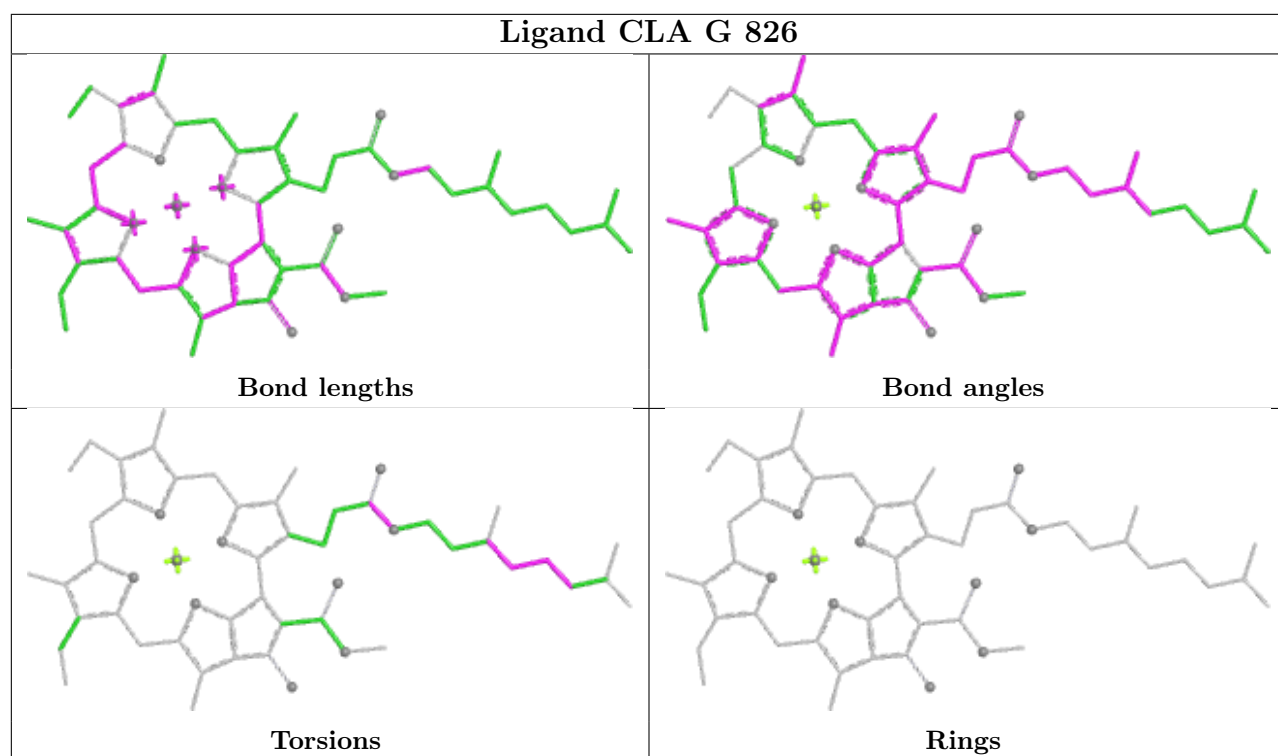
Bond angles

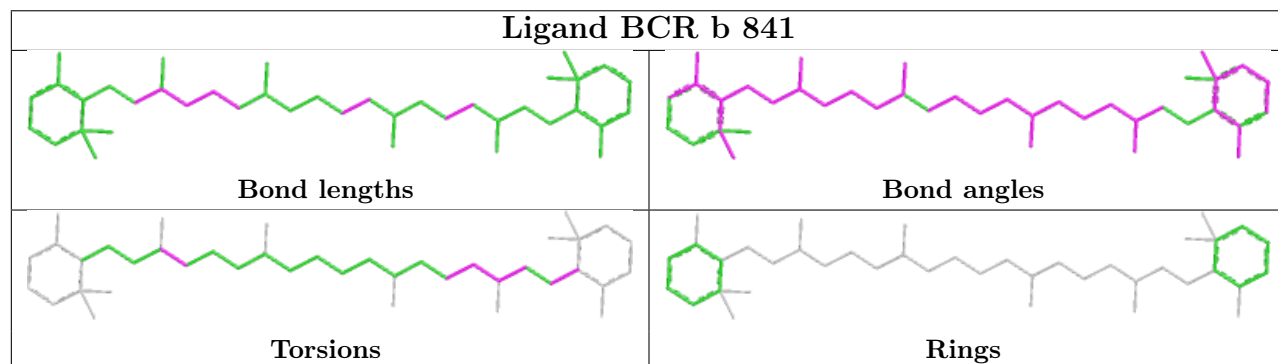
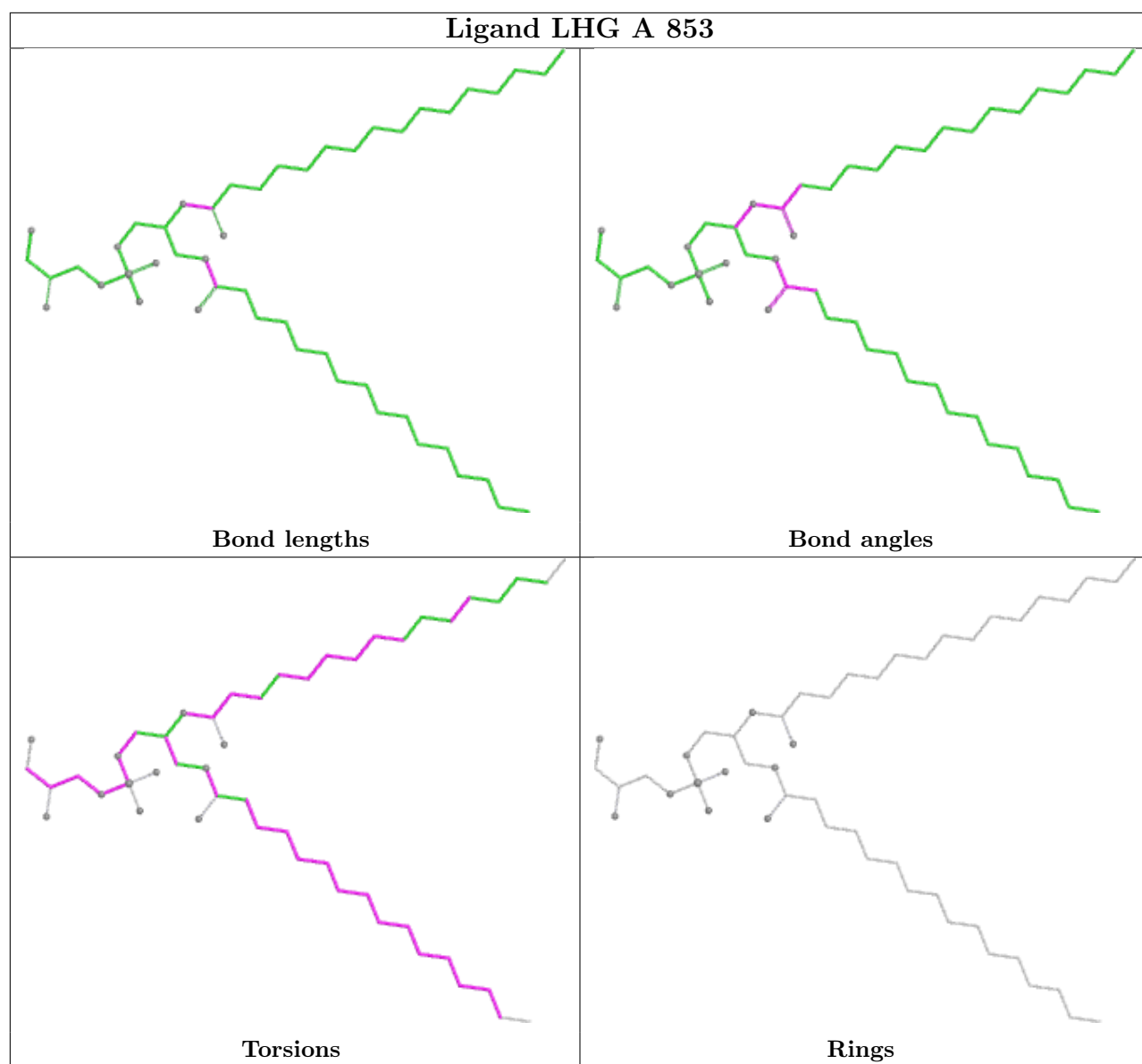


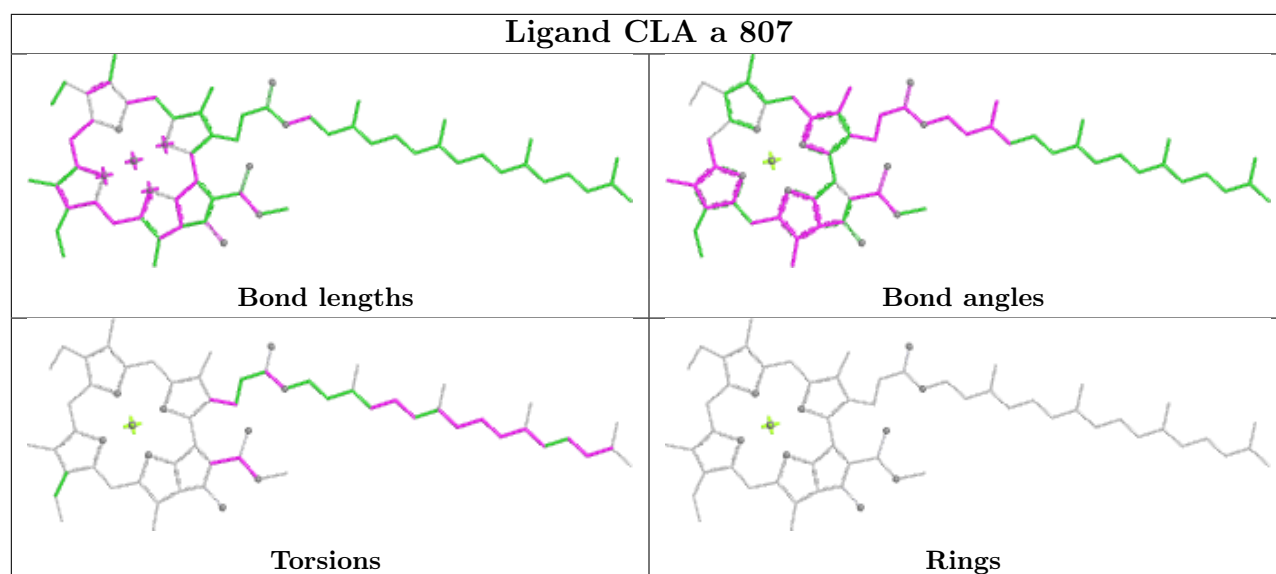
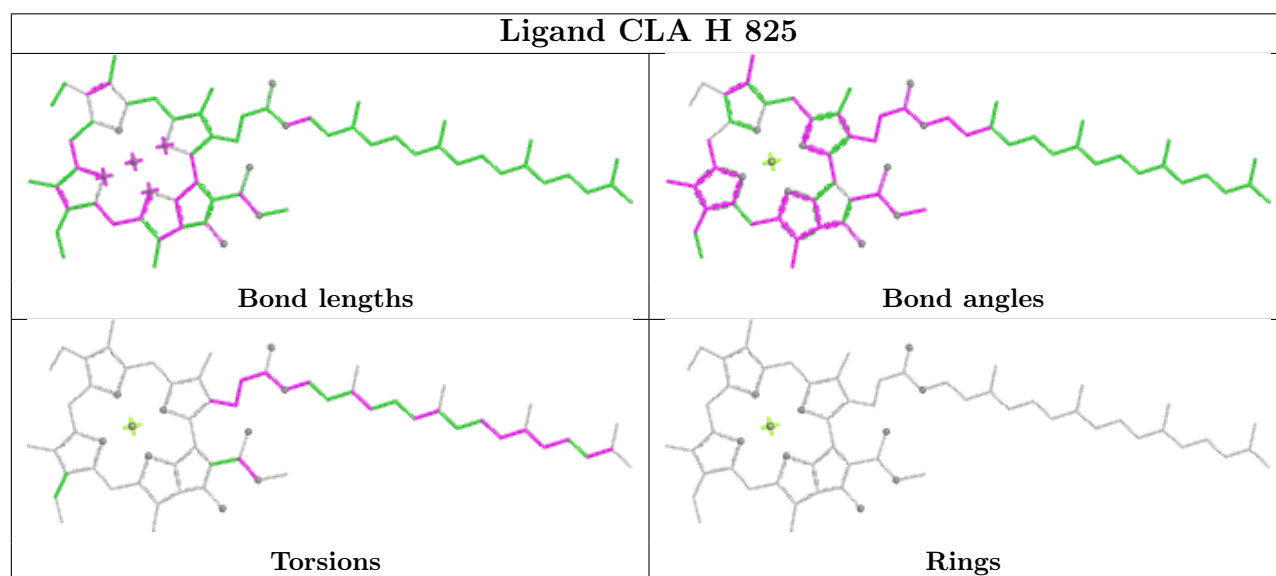
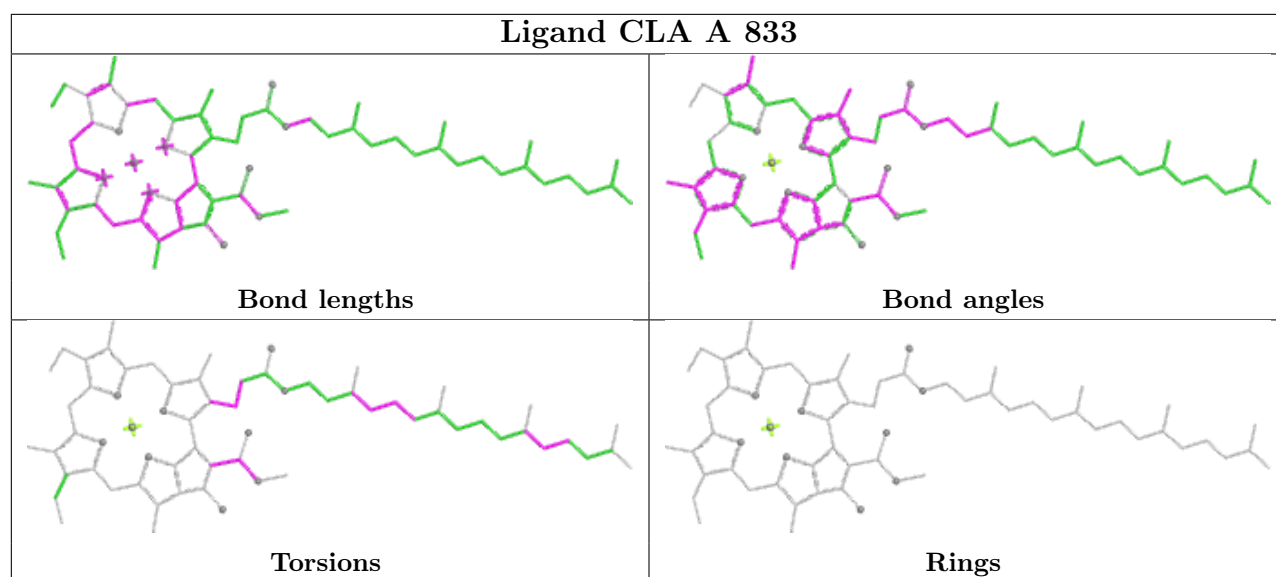
Torsions



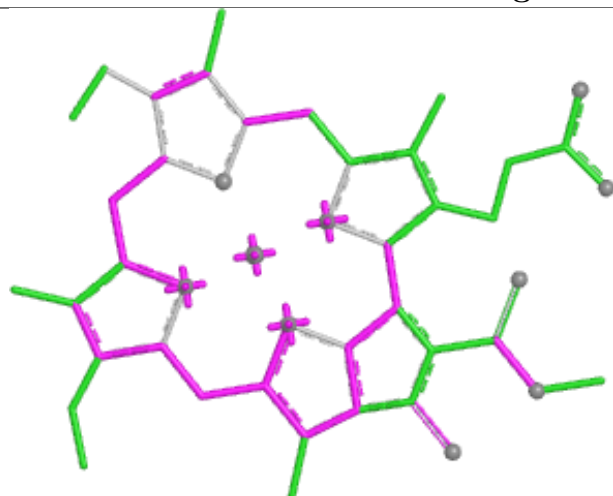
Rings



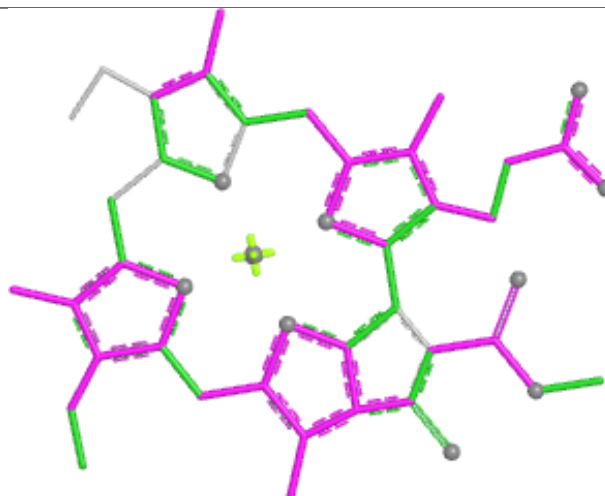




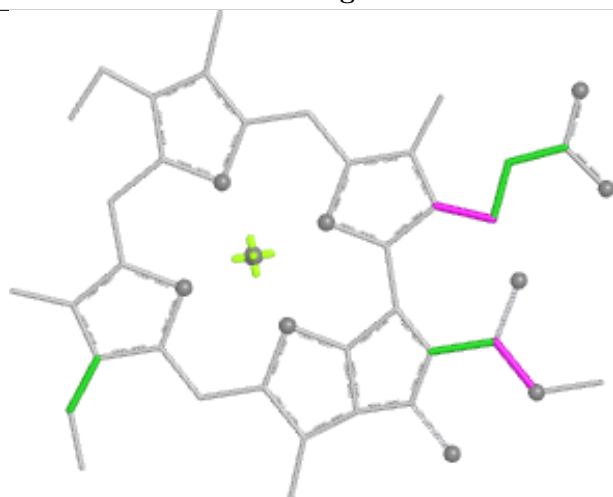
Ligand CLA G 816



Bond lengths



Bond angles

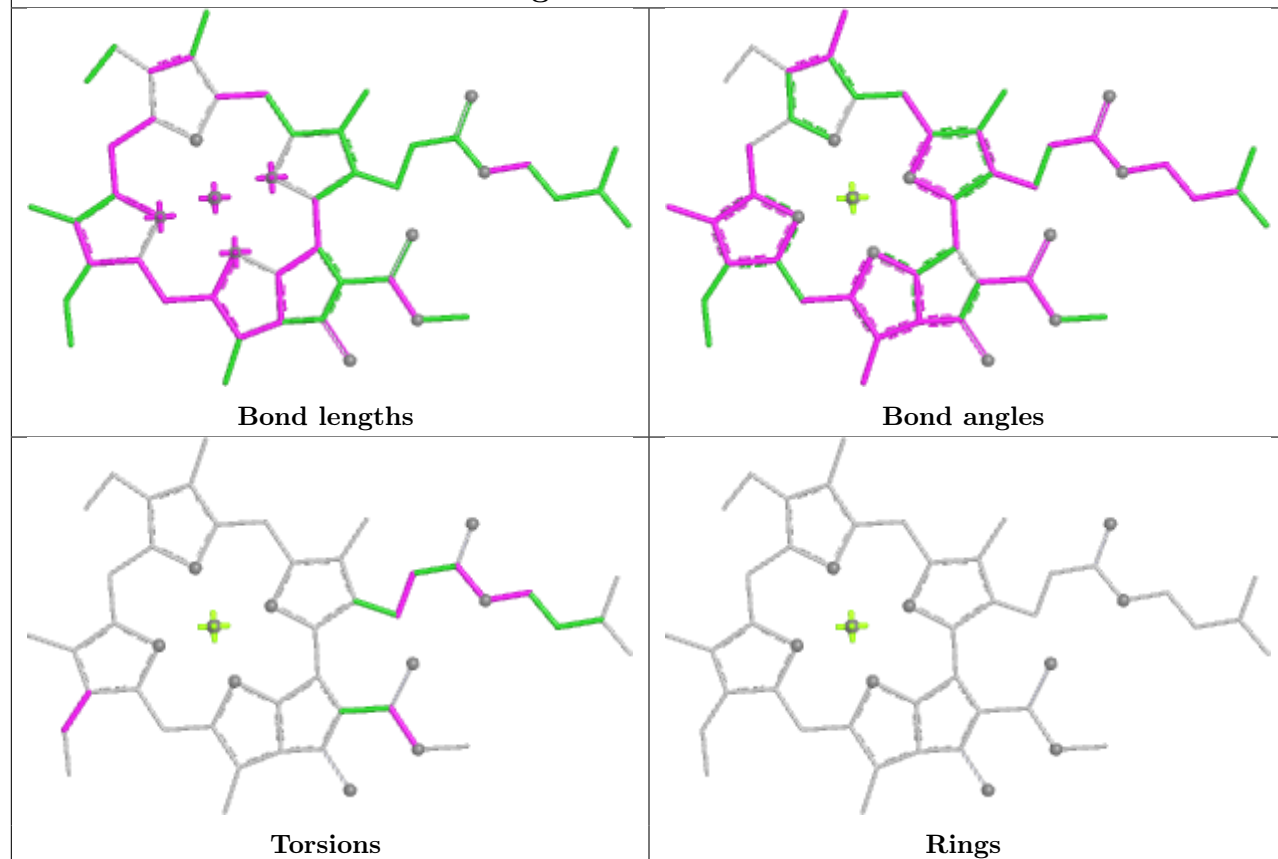


Torsions

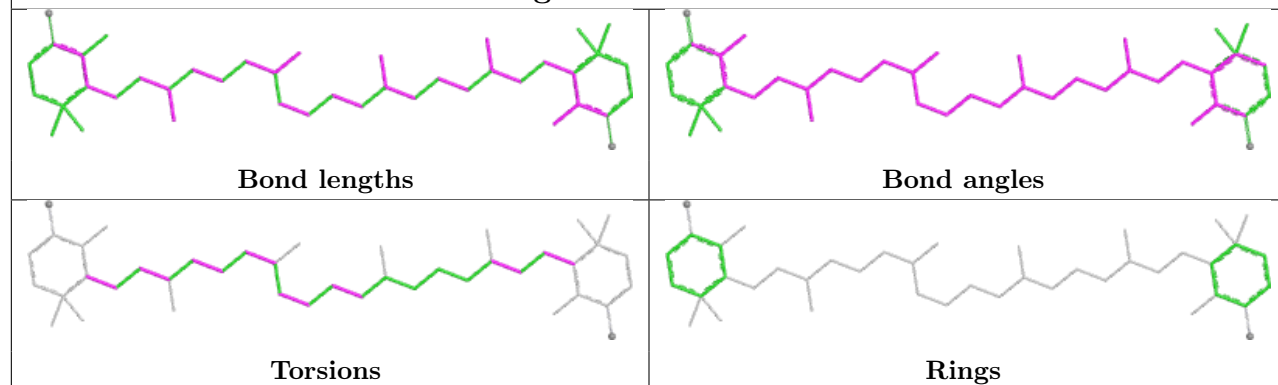


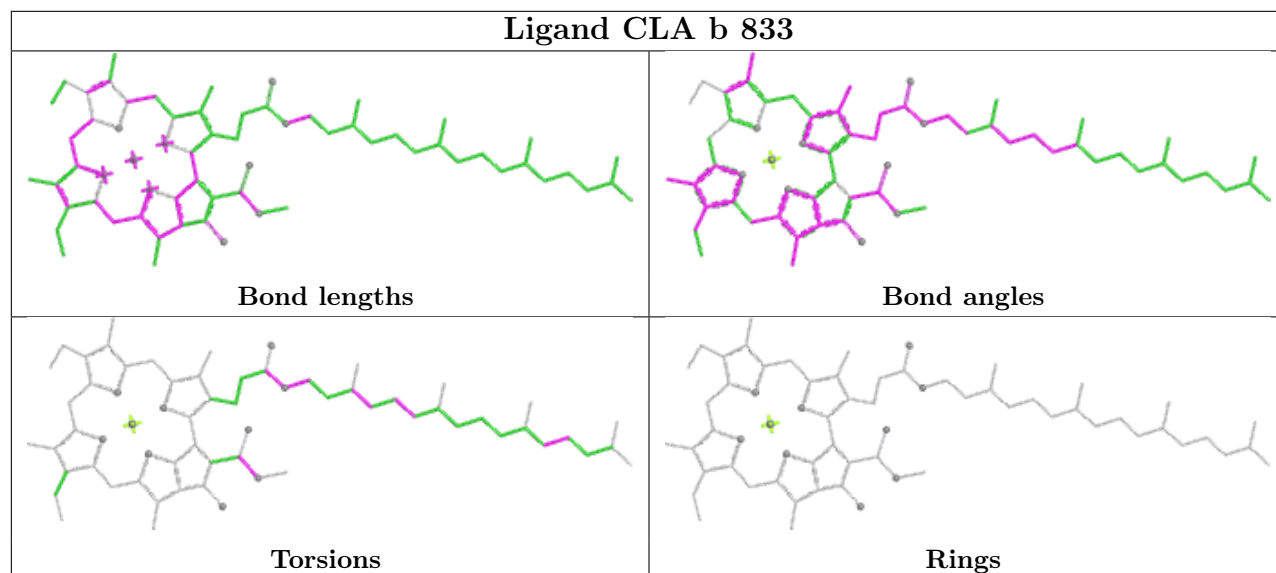
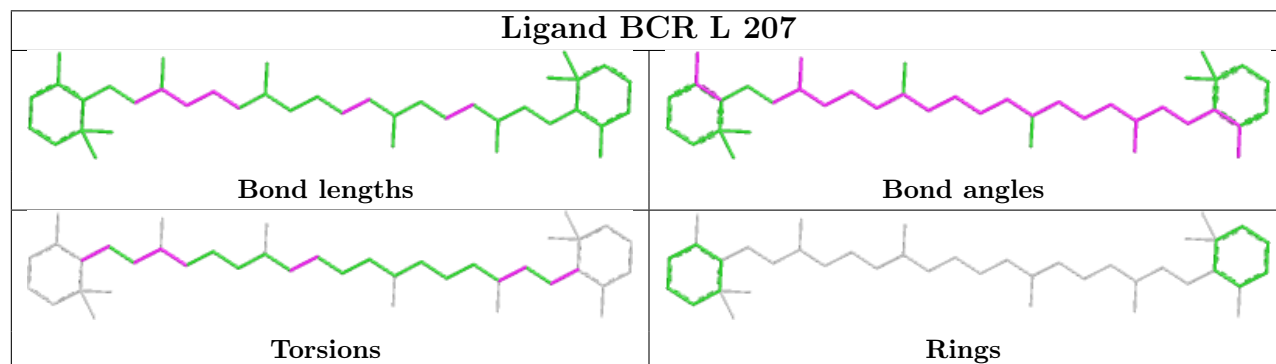
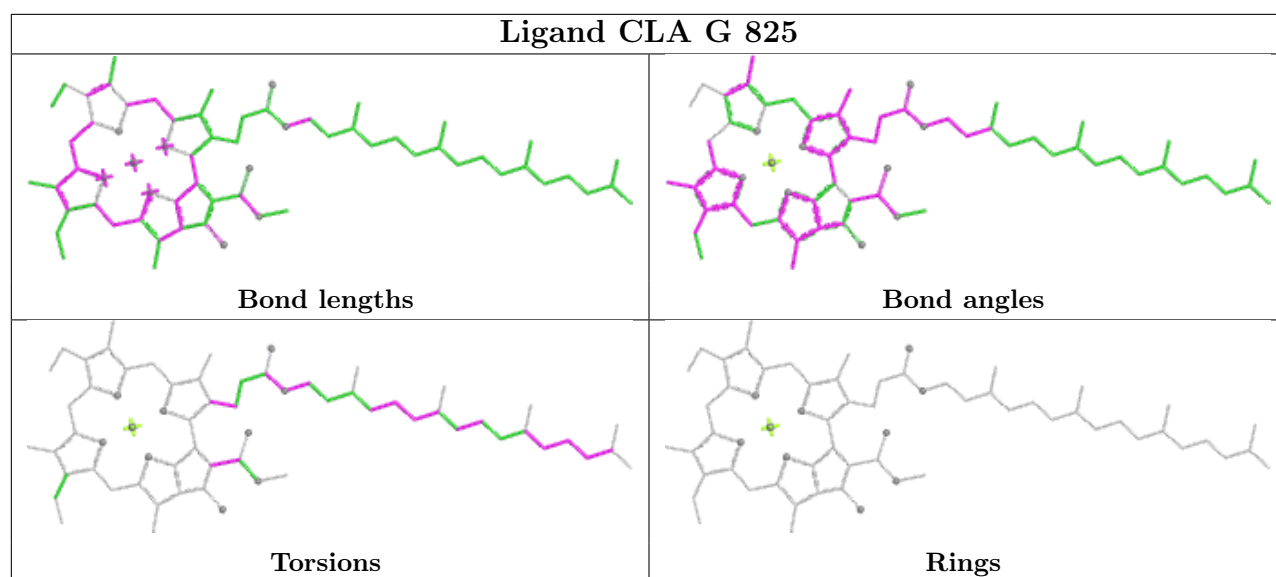
Rings

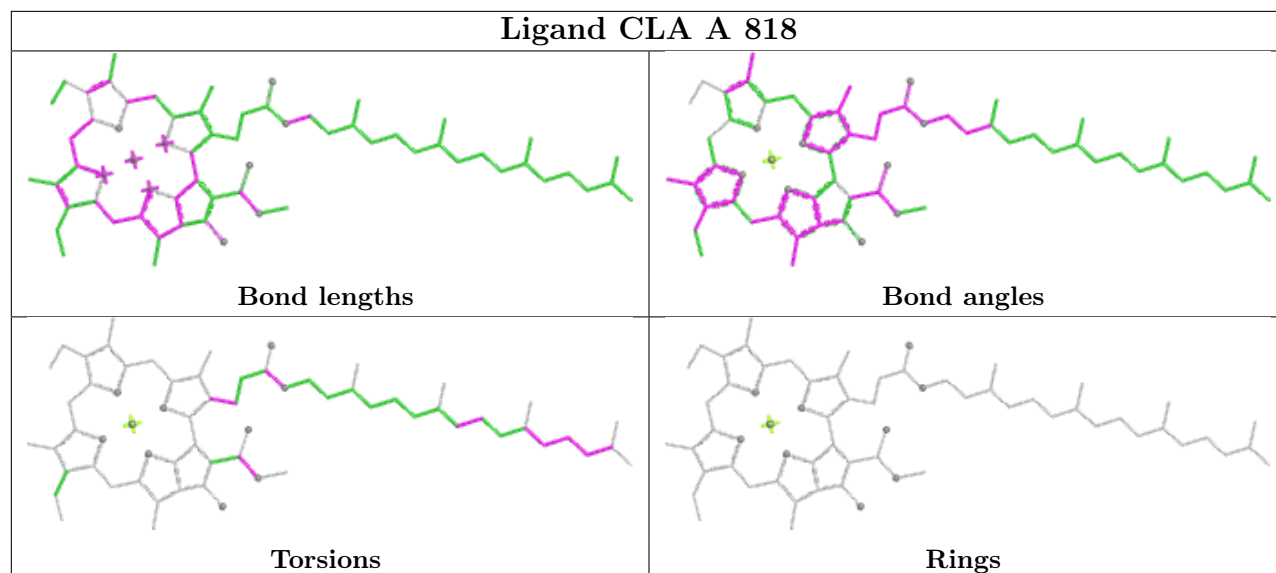
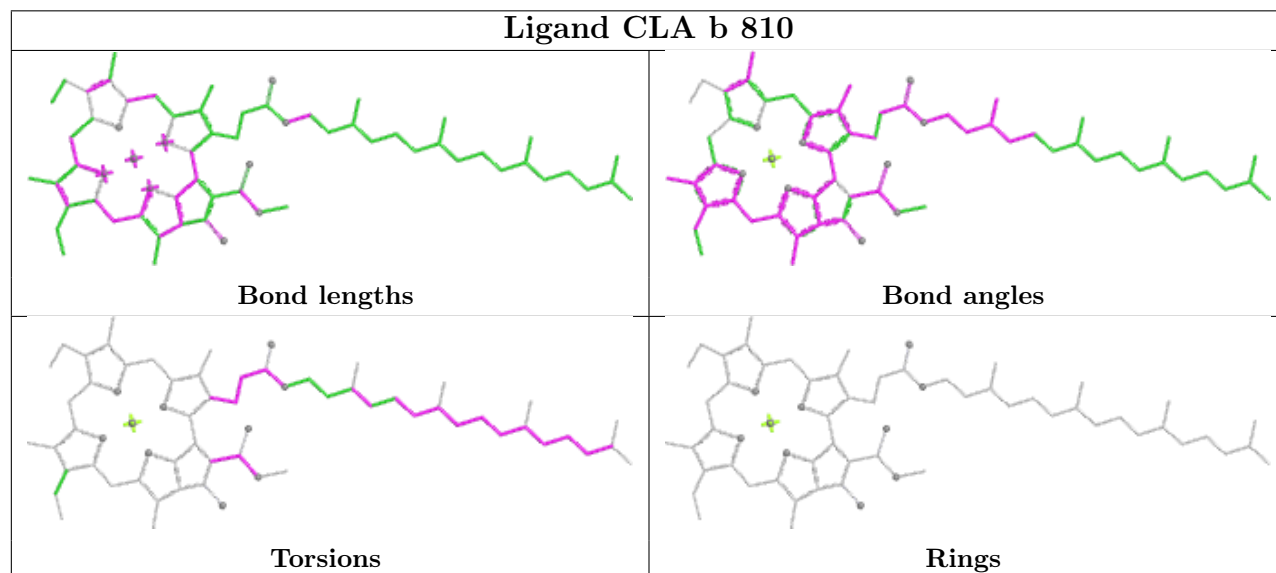
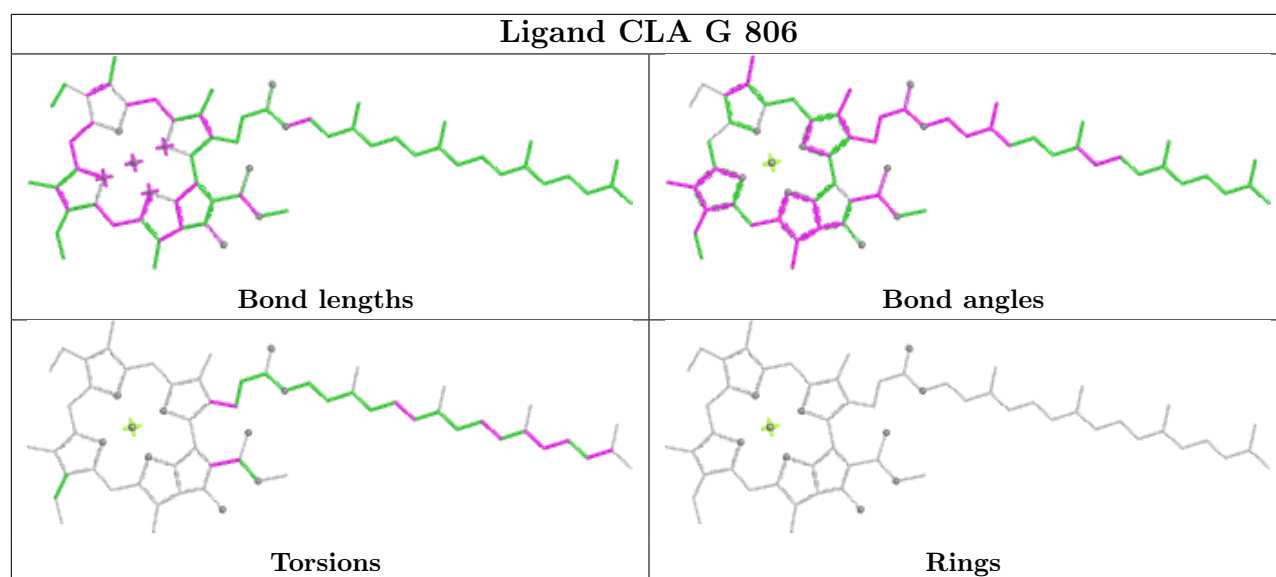
Ligand CLA A 812

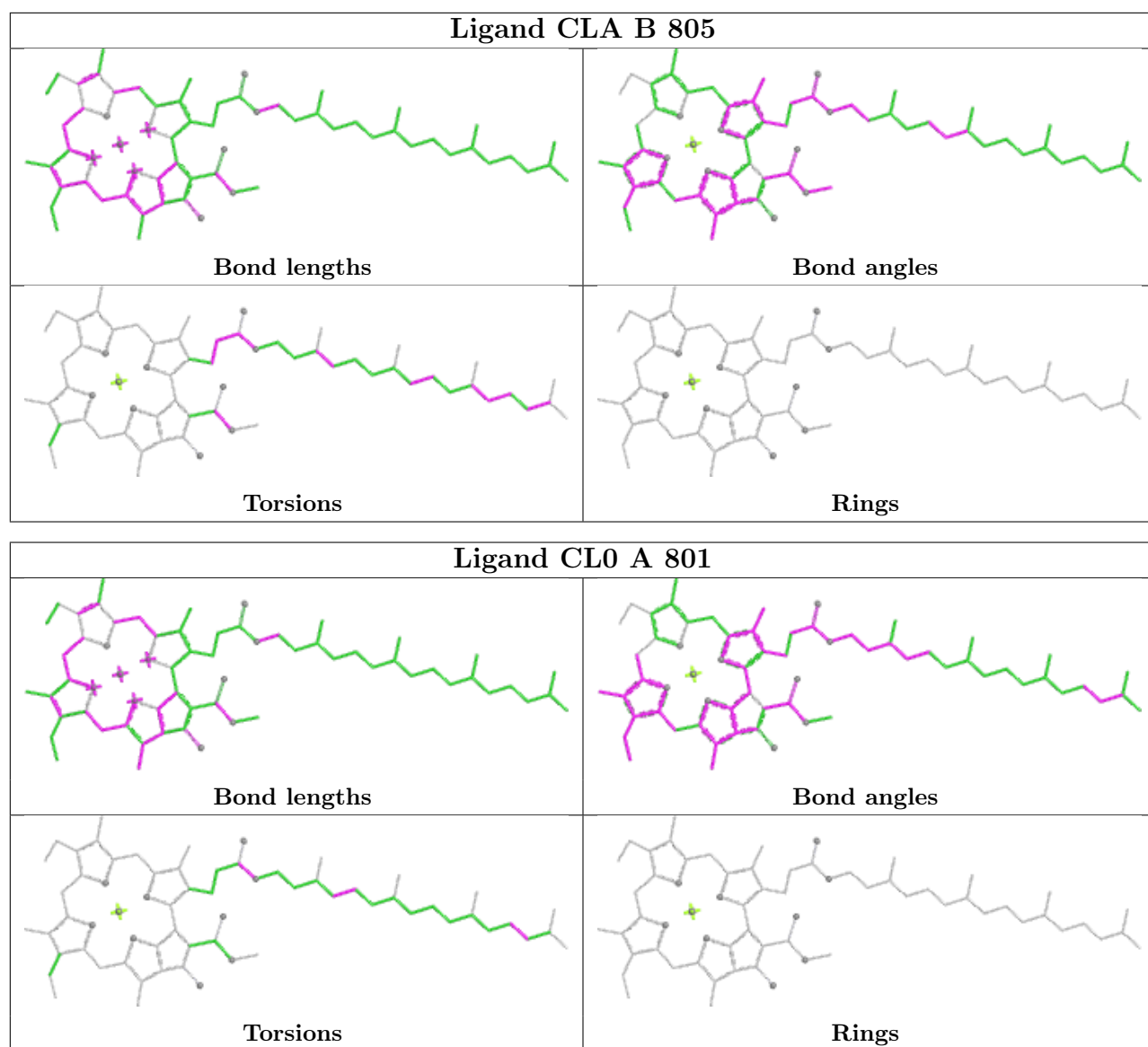


Ligand 45D M 101

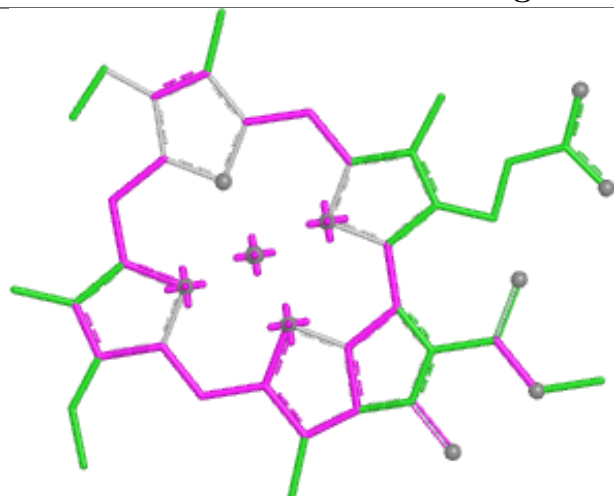




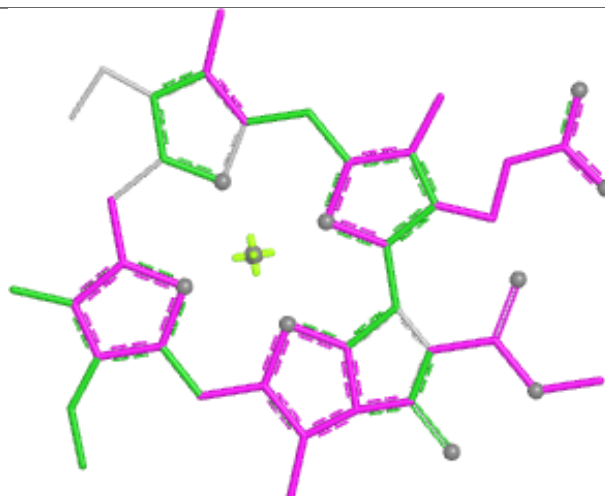




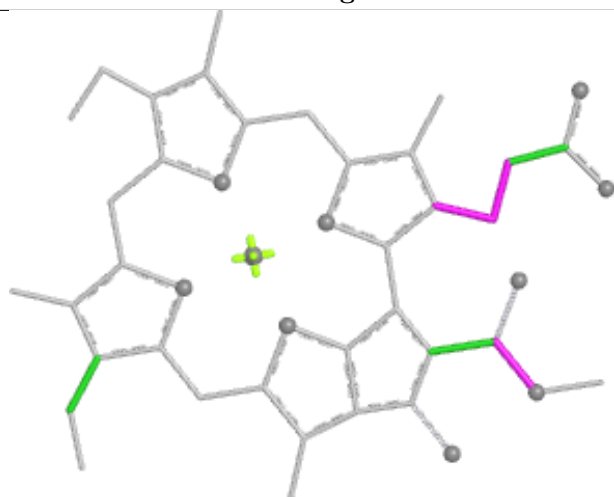
Ligand CLA A 809



Bond lengths



Bond angles

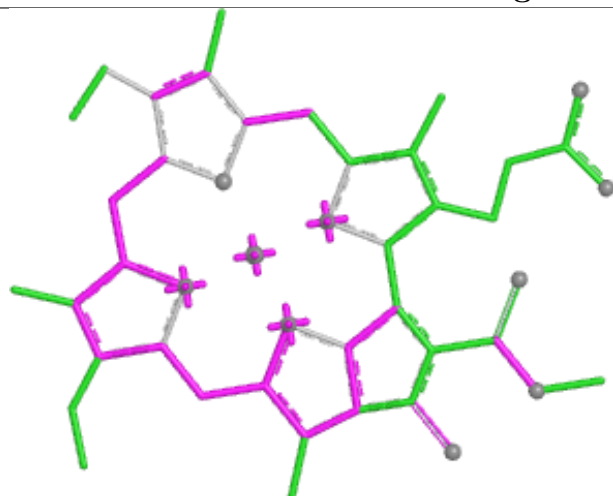


Torsions

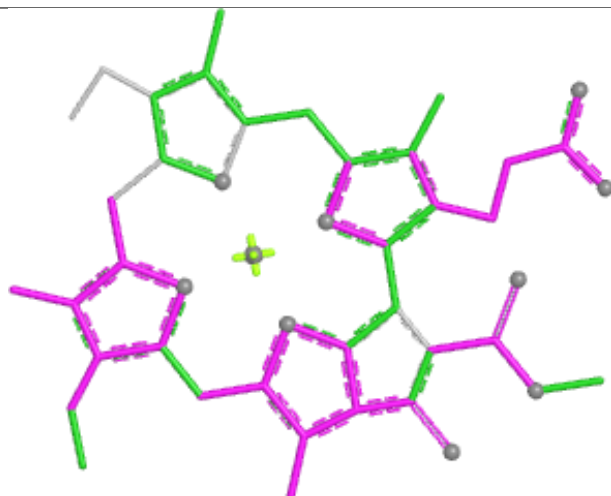


Rings

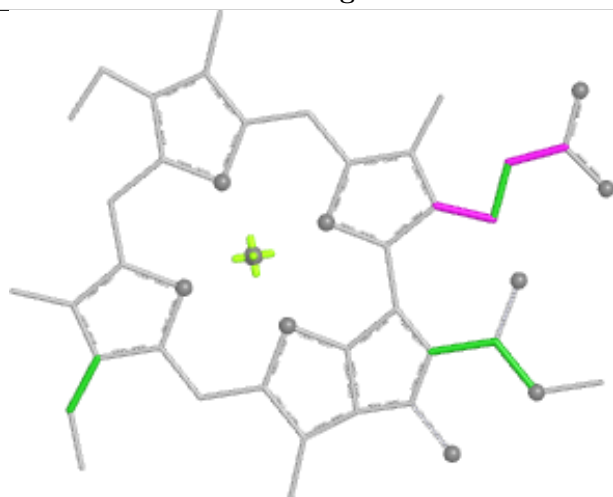
Ligand CLA A 838



Bond lengths



Bond angles

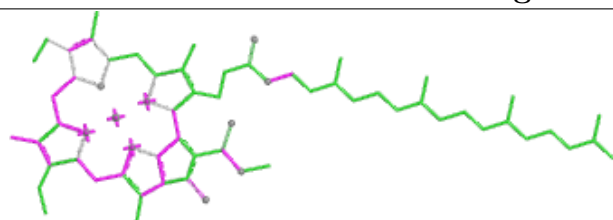


Torsions

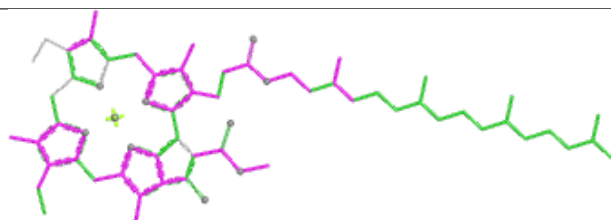


Rings

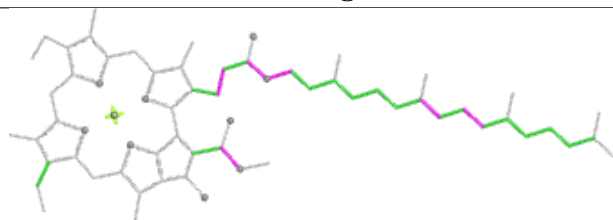
Ligand CLA A 855



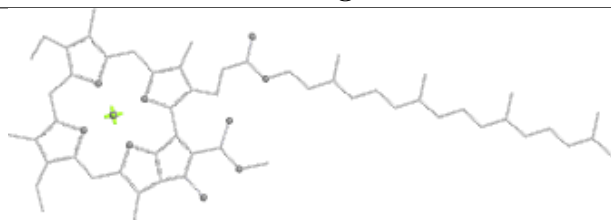
Bond lengths



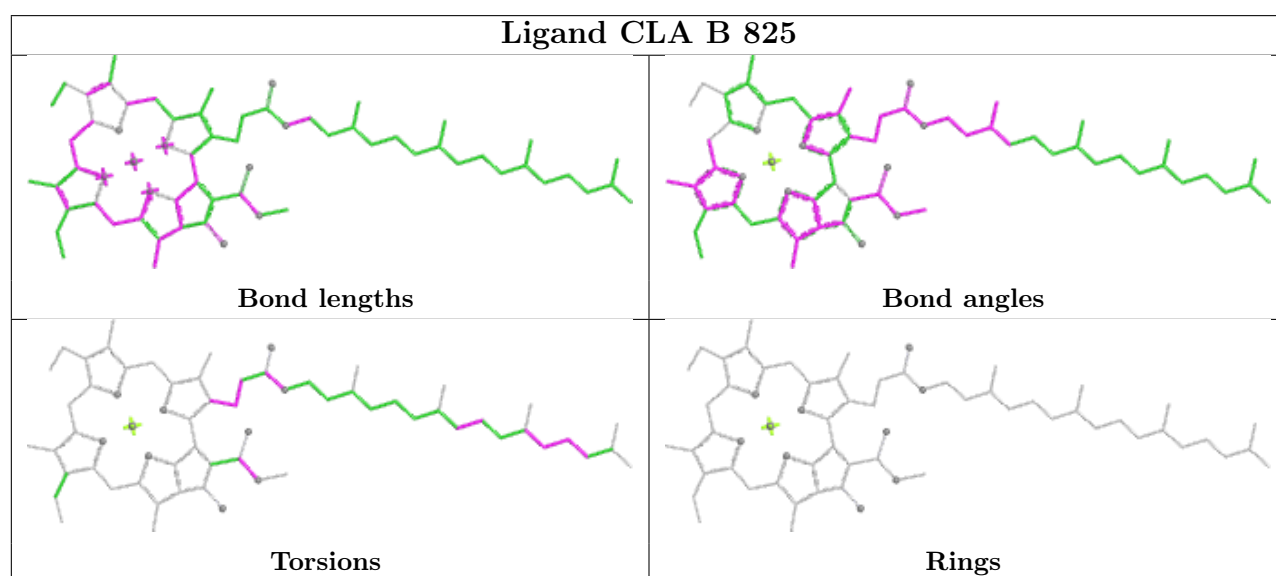
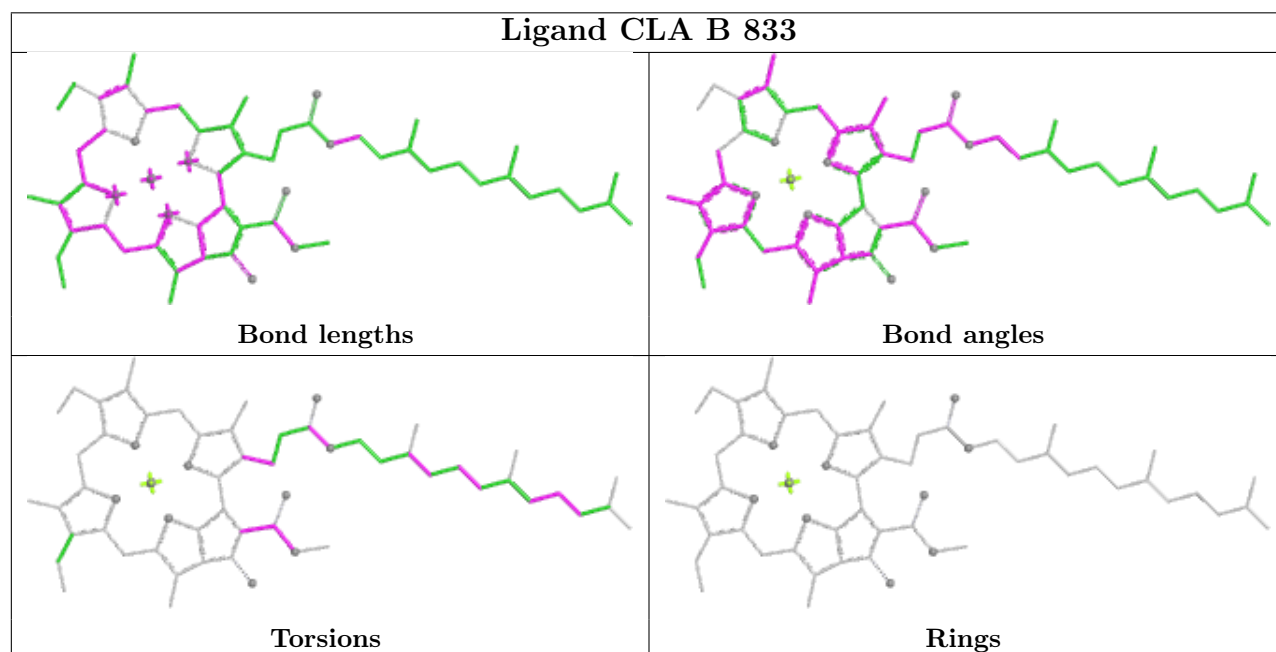
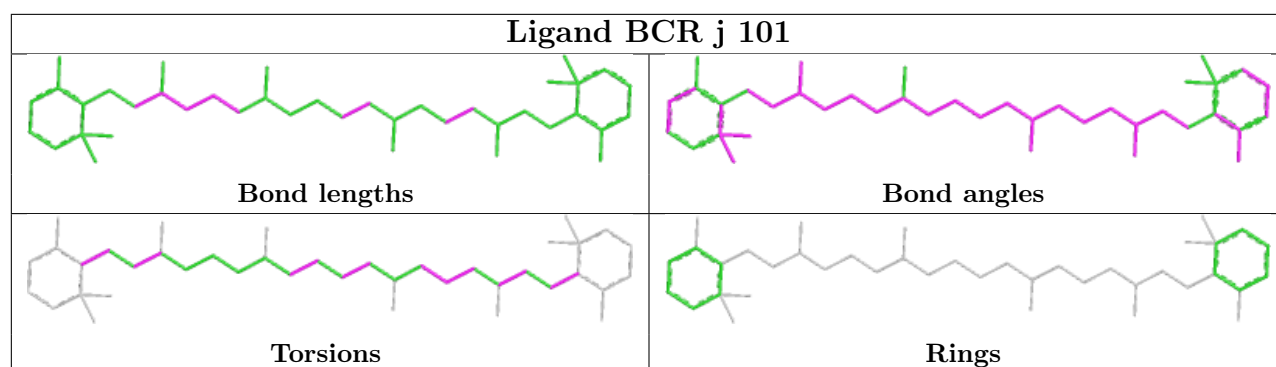
Bond angles

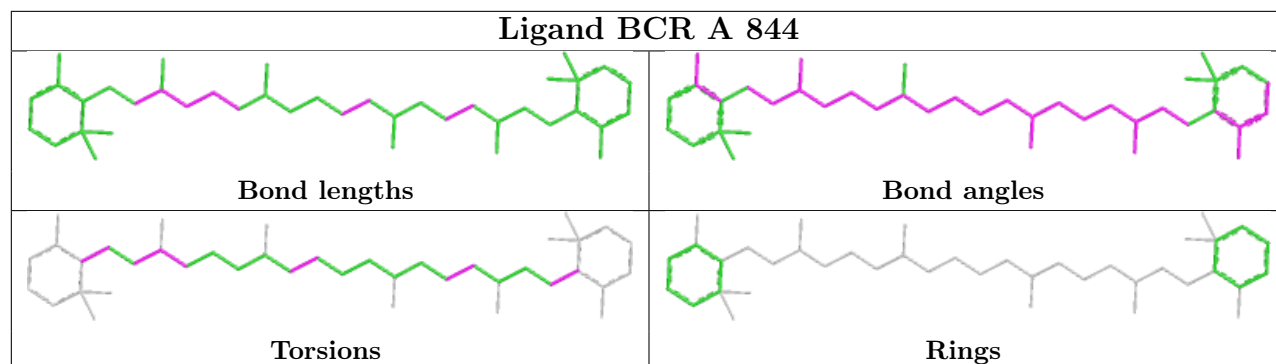
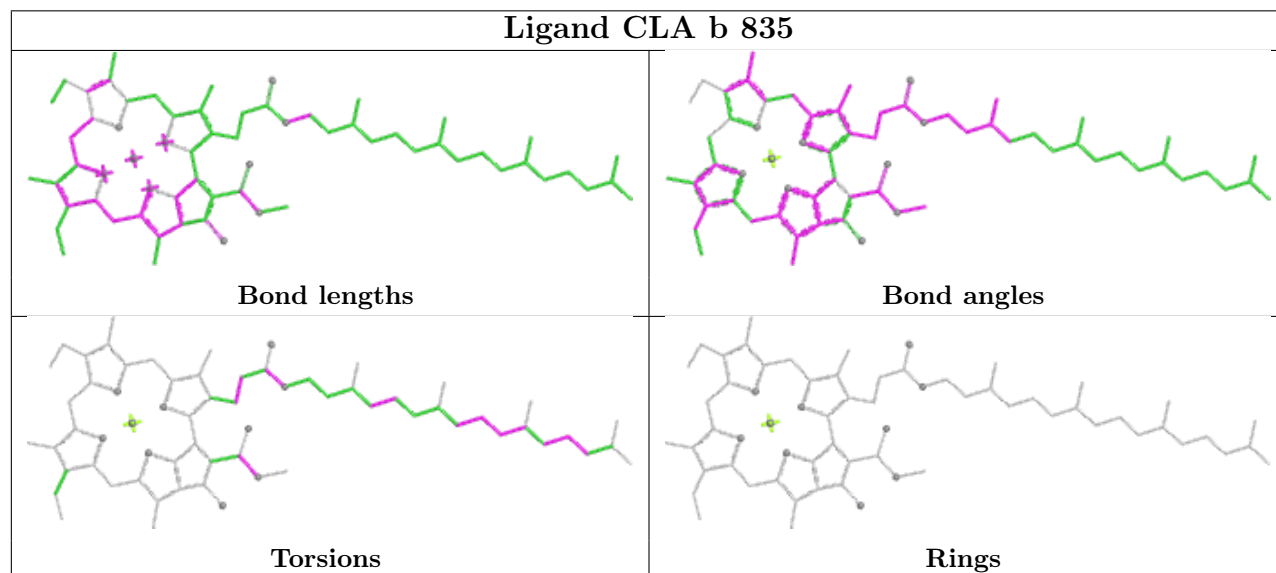
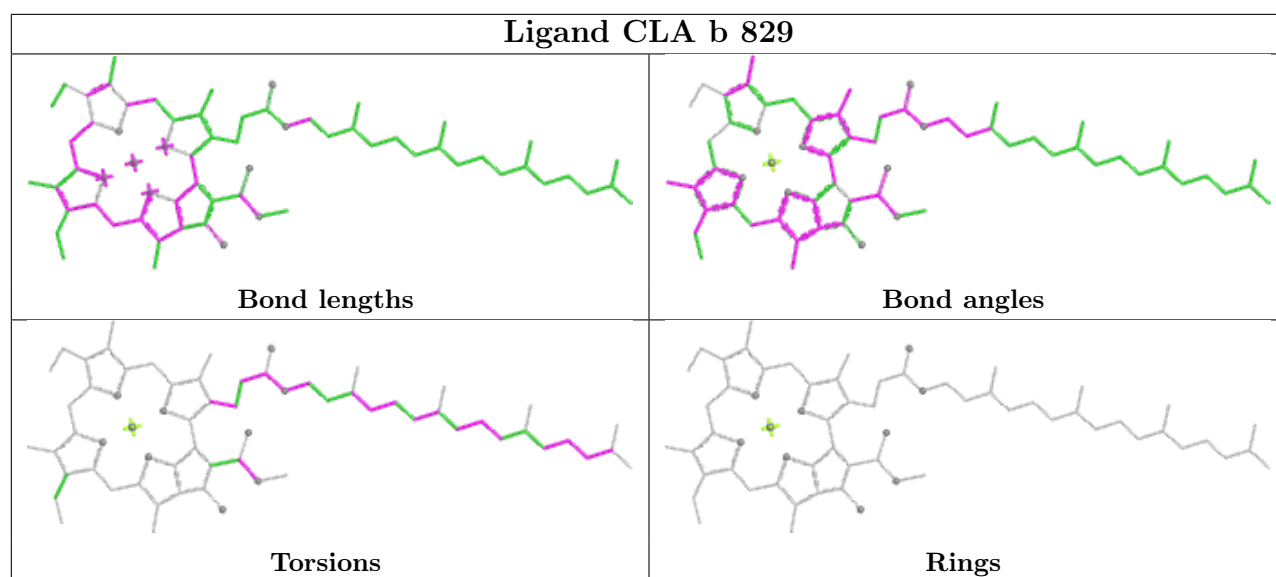


Torsions

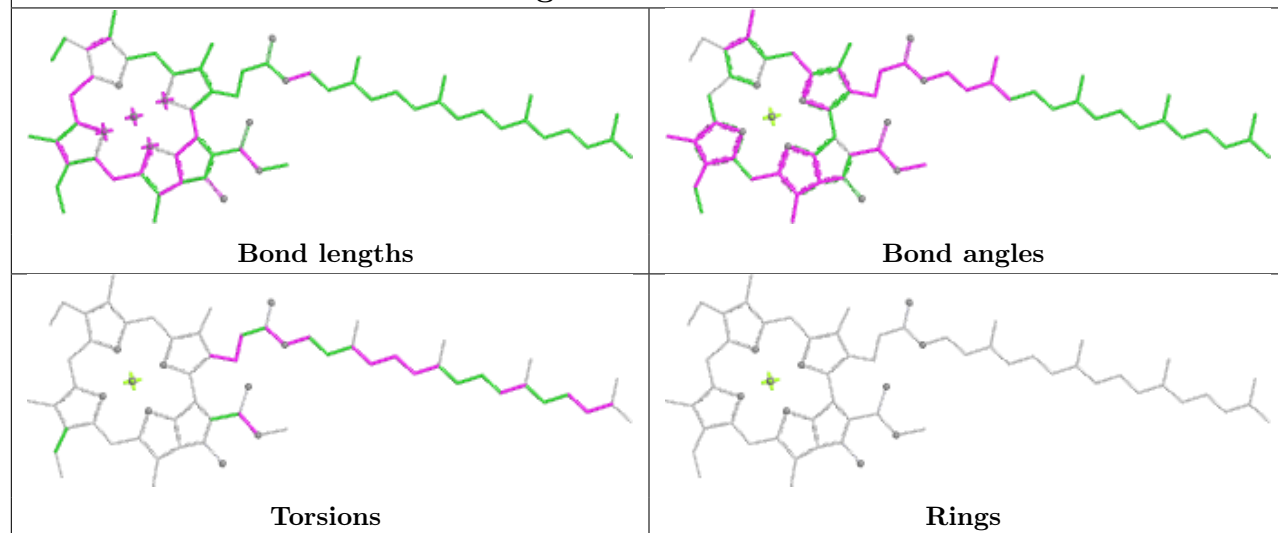


Rings

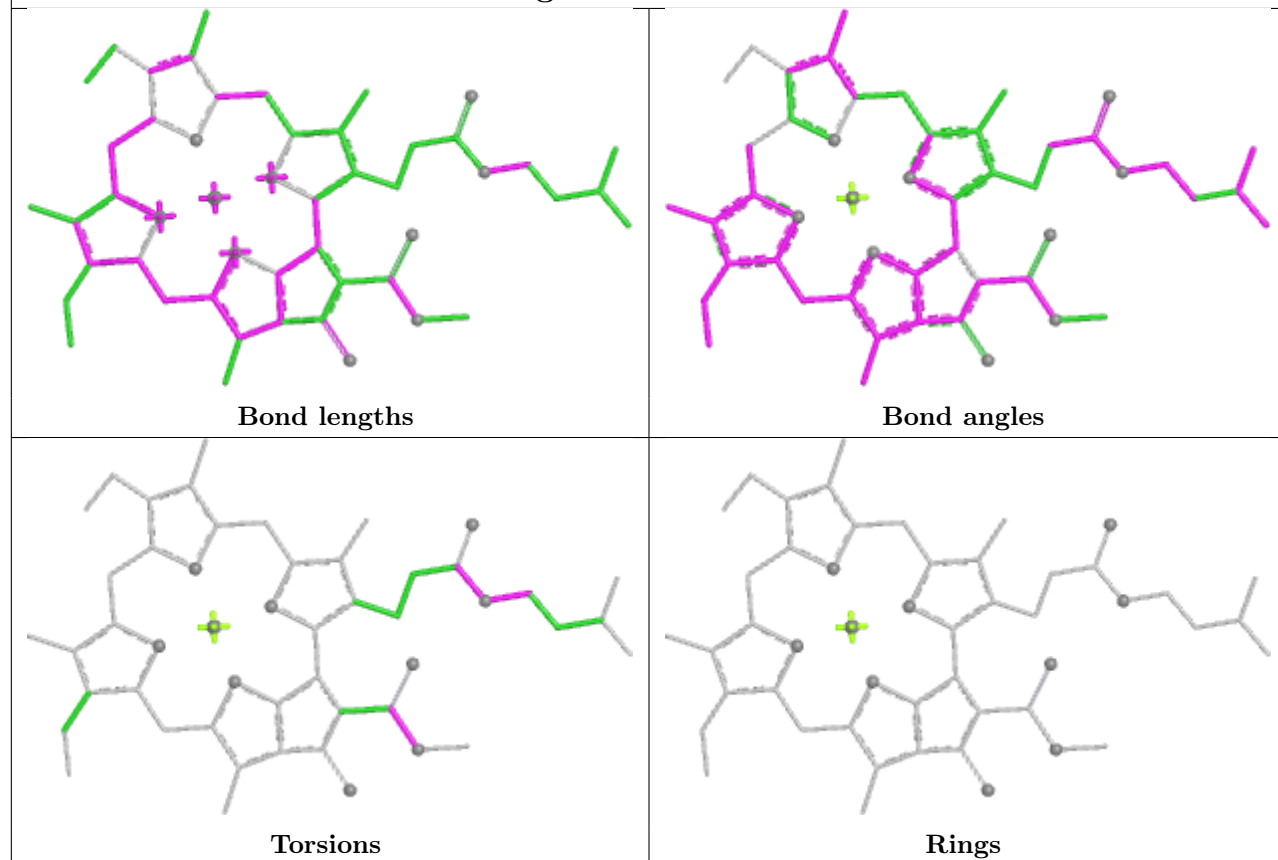




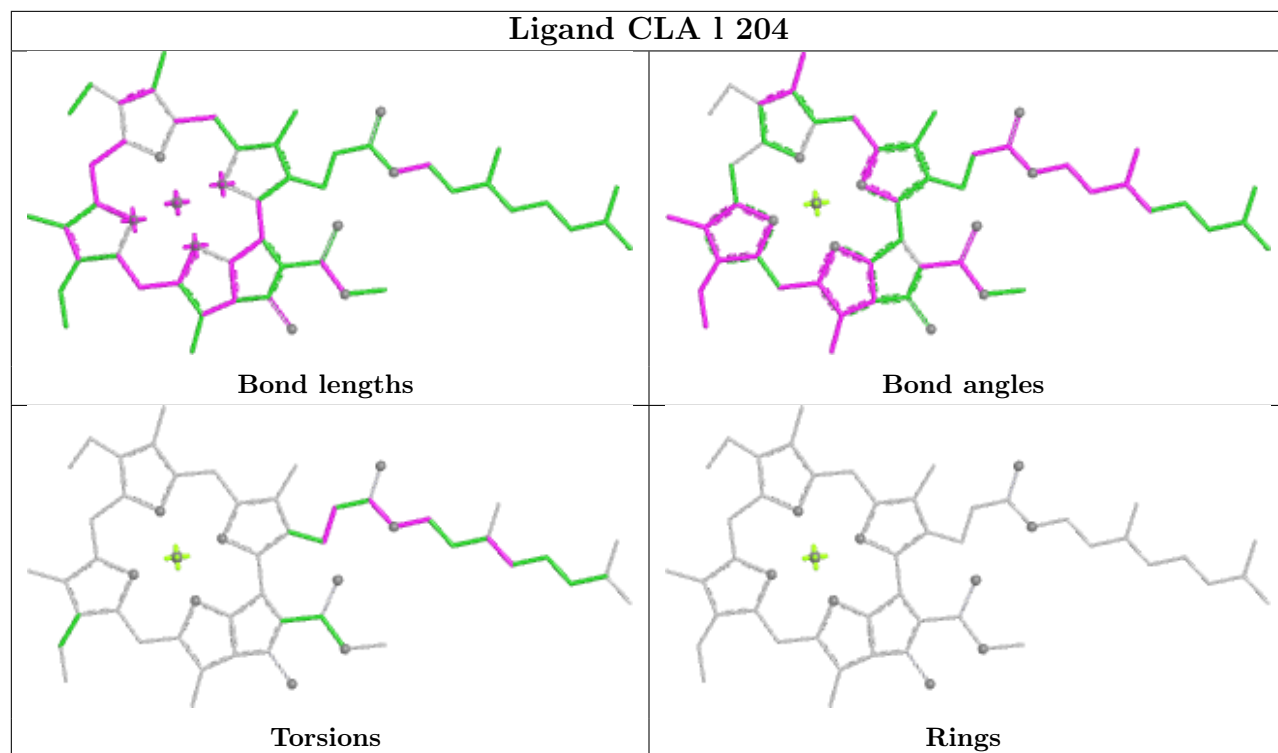
Ligand CLA a 834



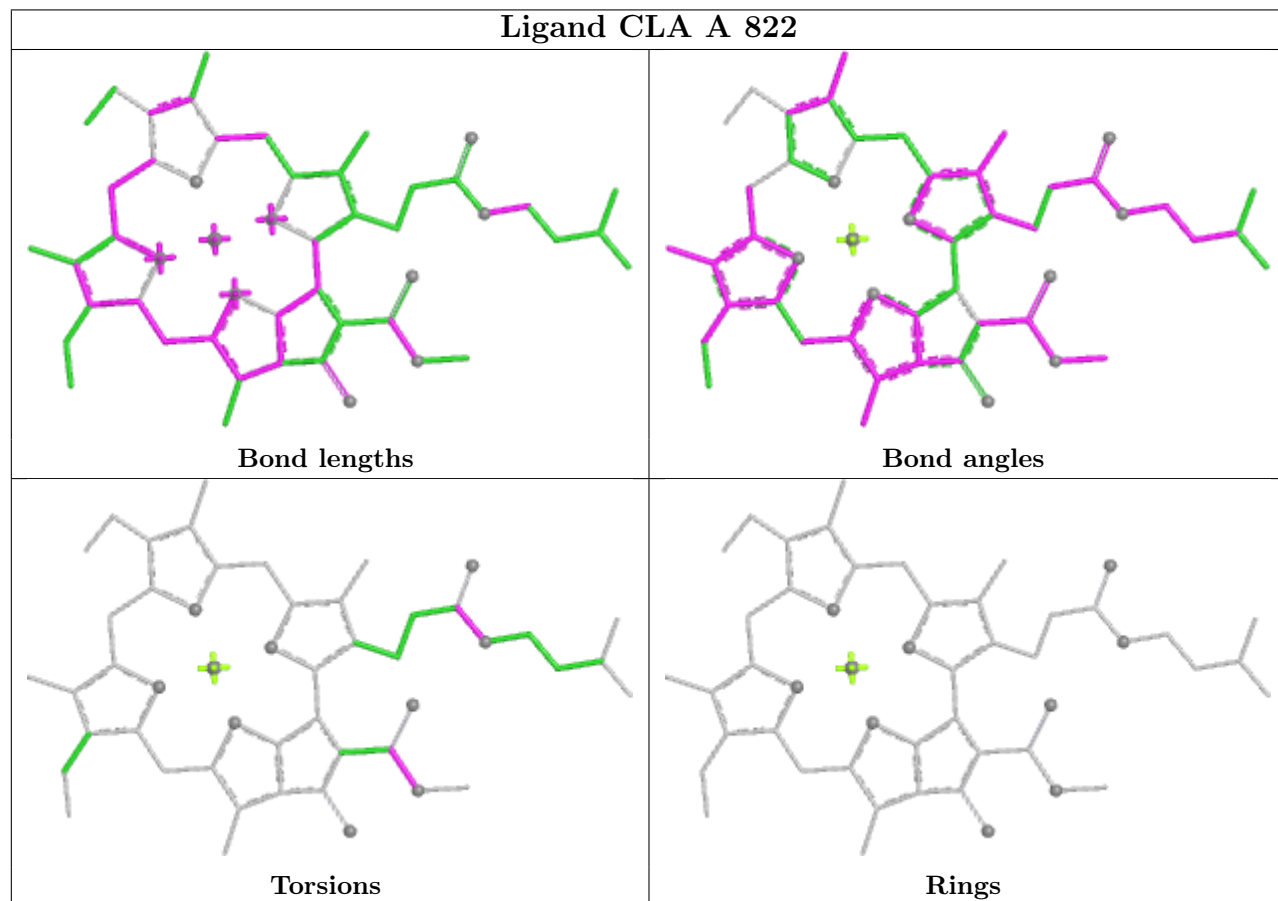
Ligand CLA a 836

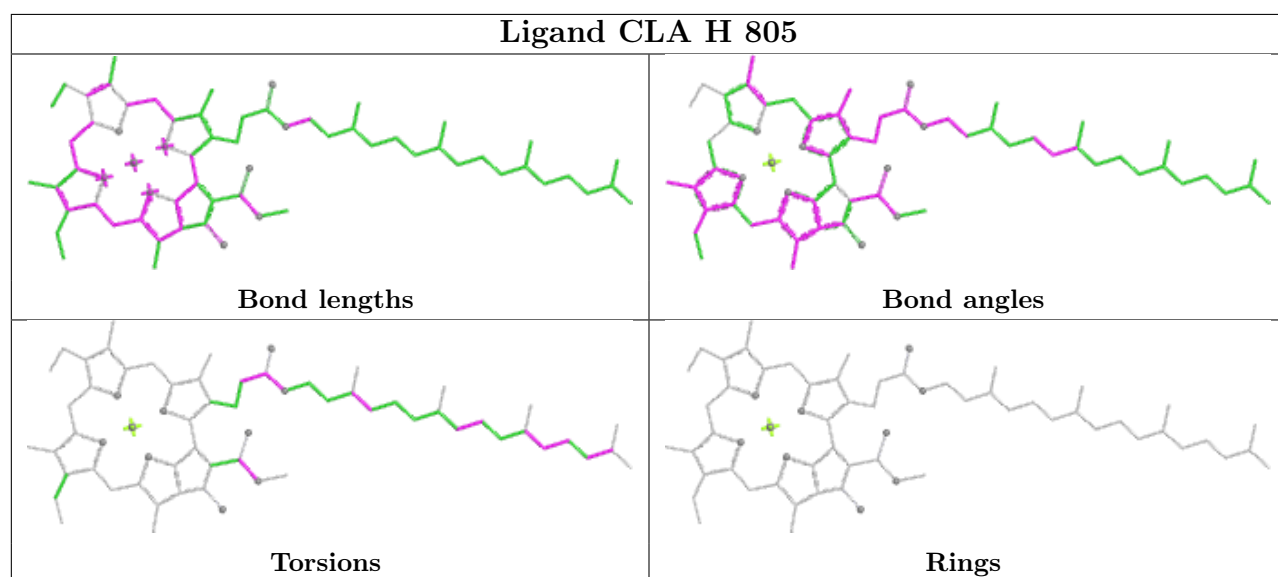
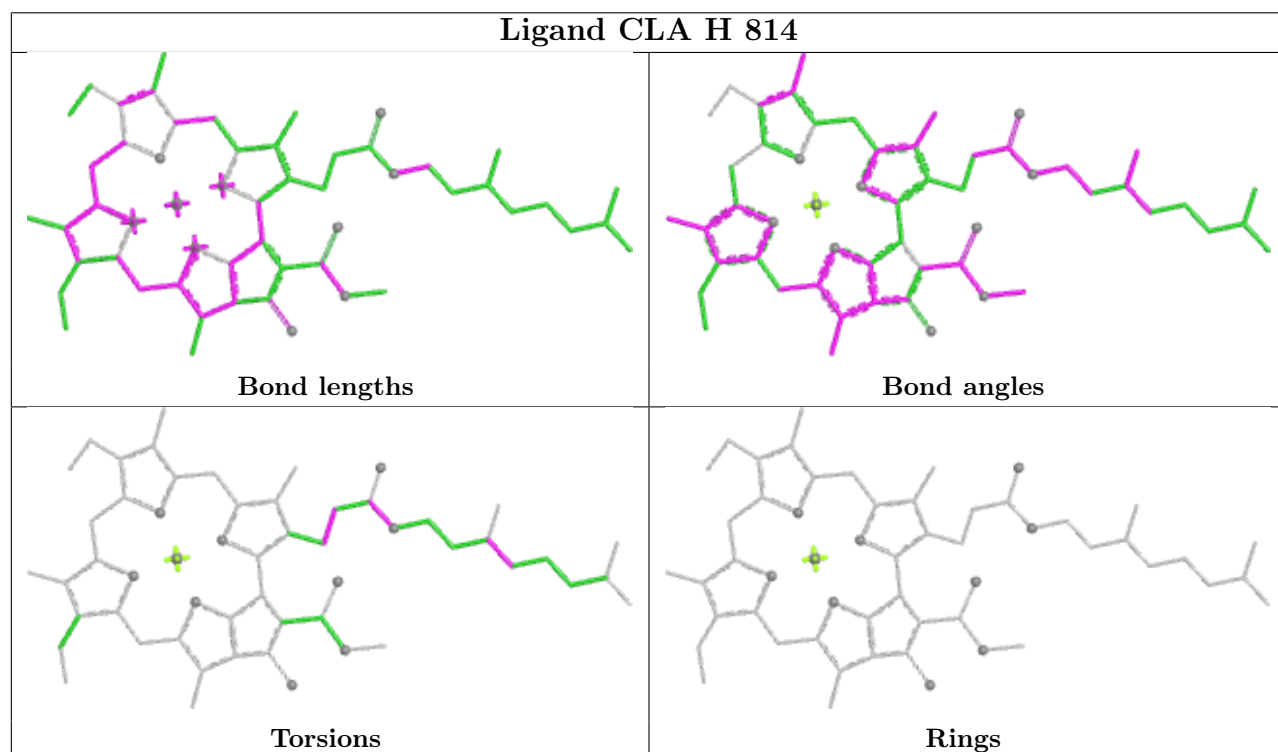
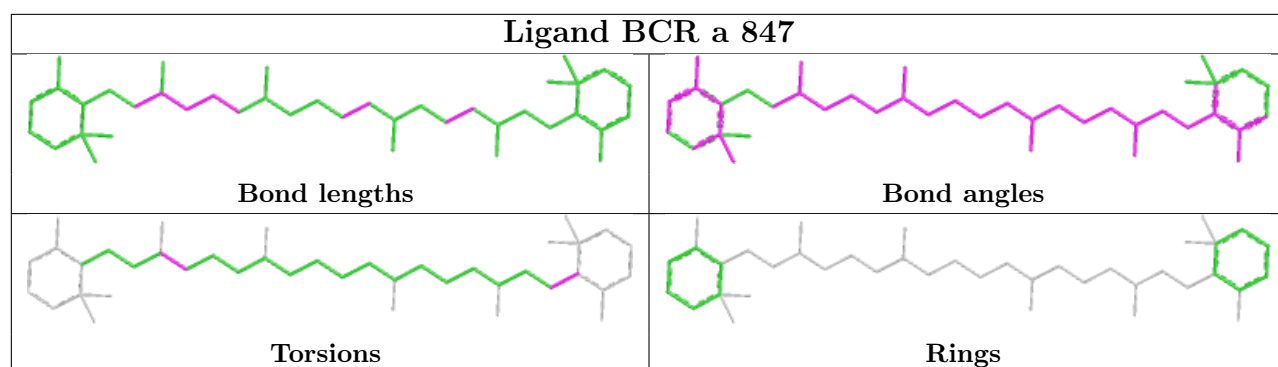


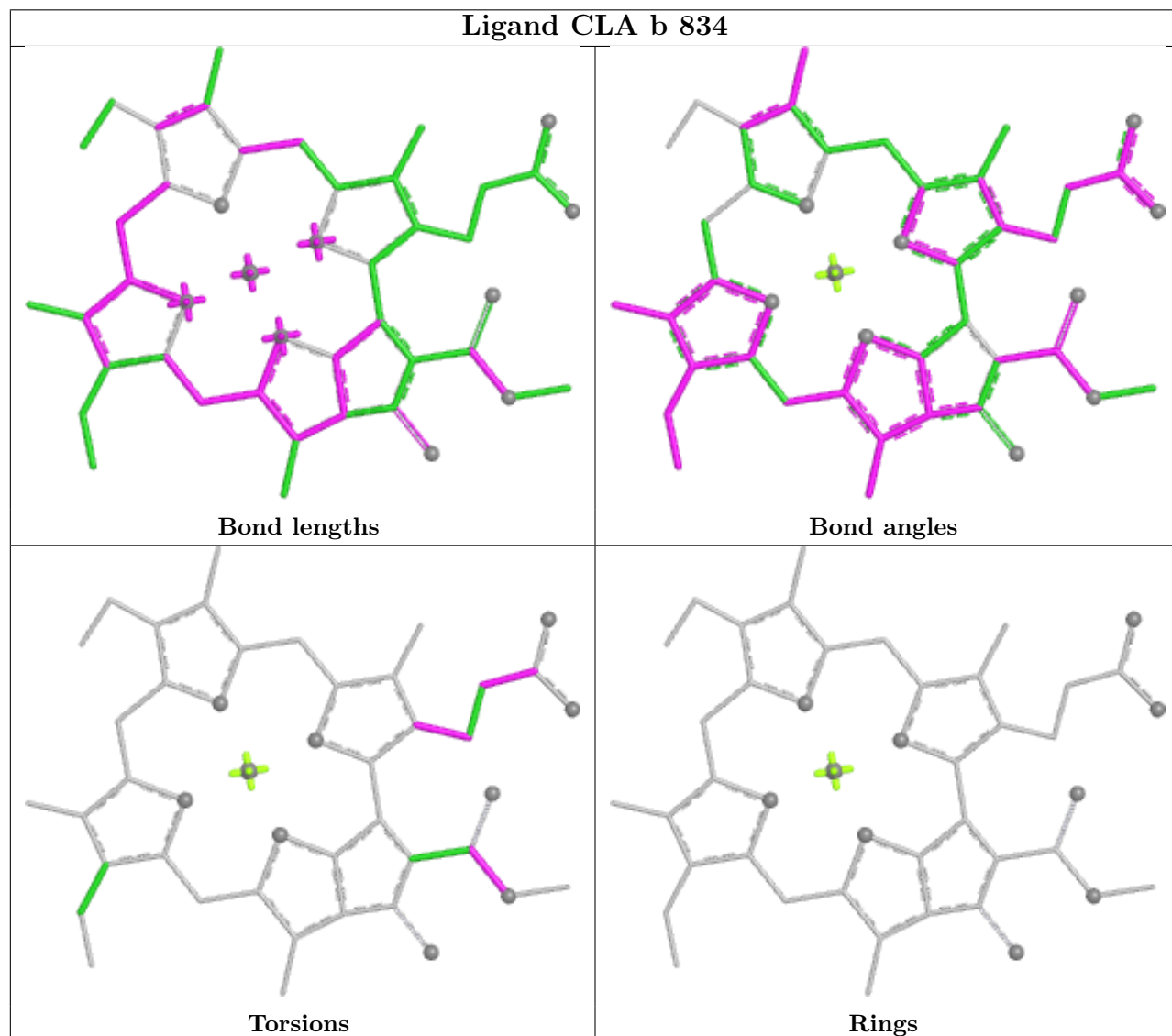
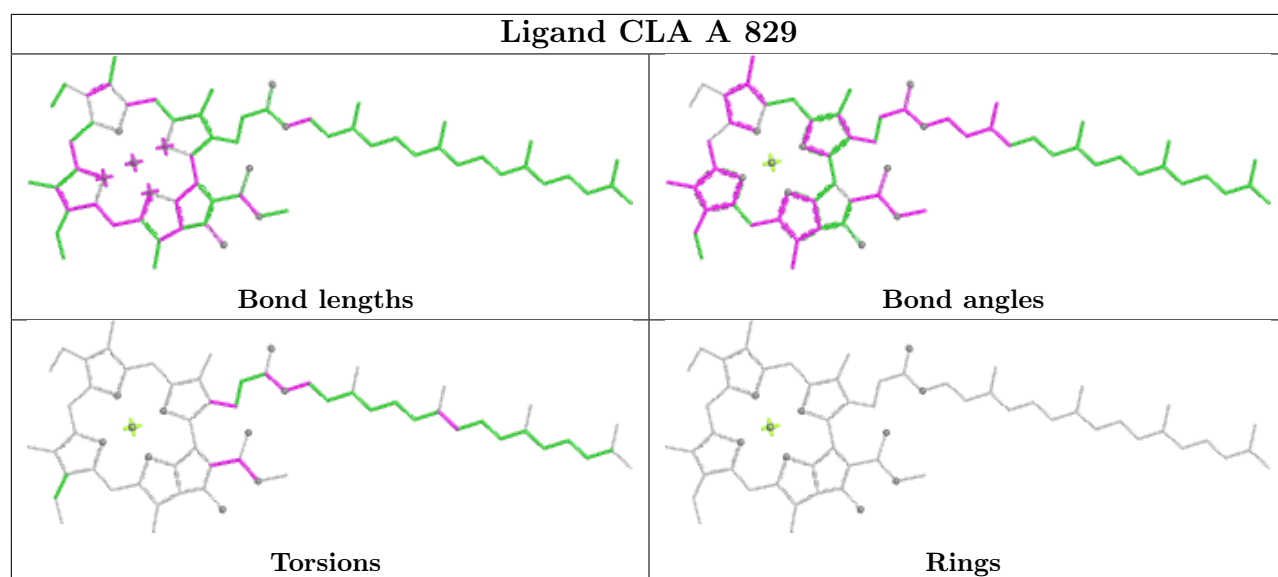
Ligand CLA 1 204



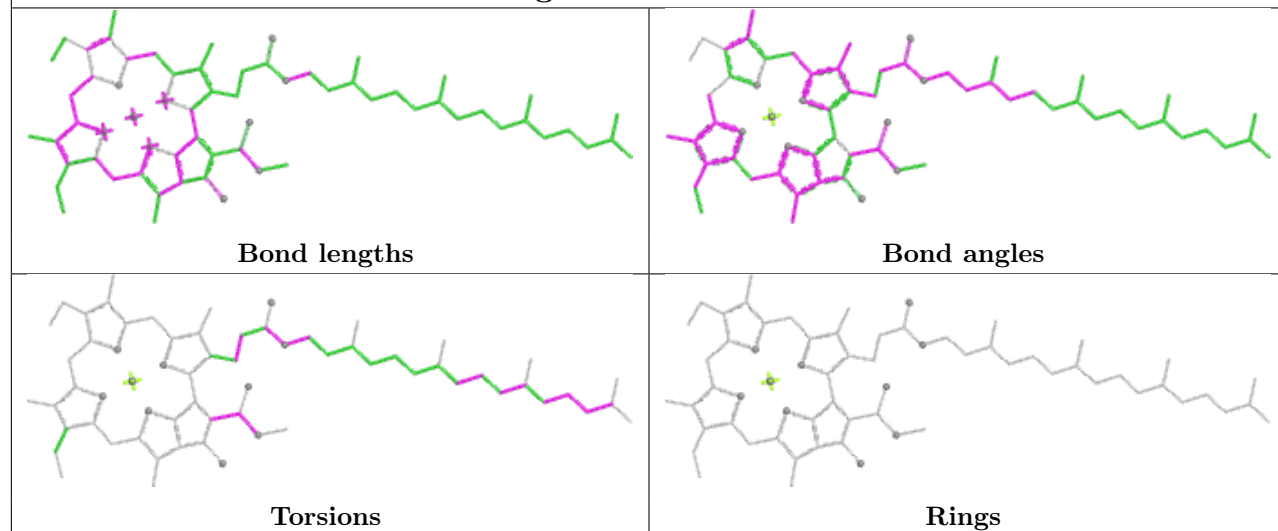
Ligand CLA A 822



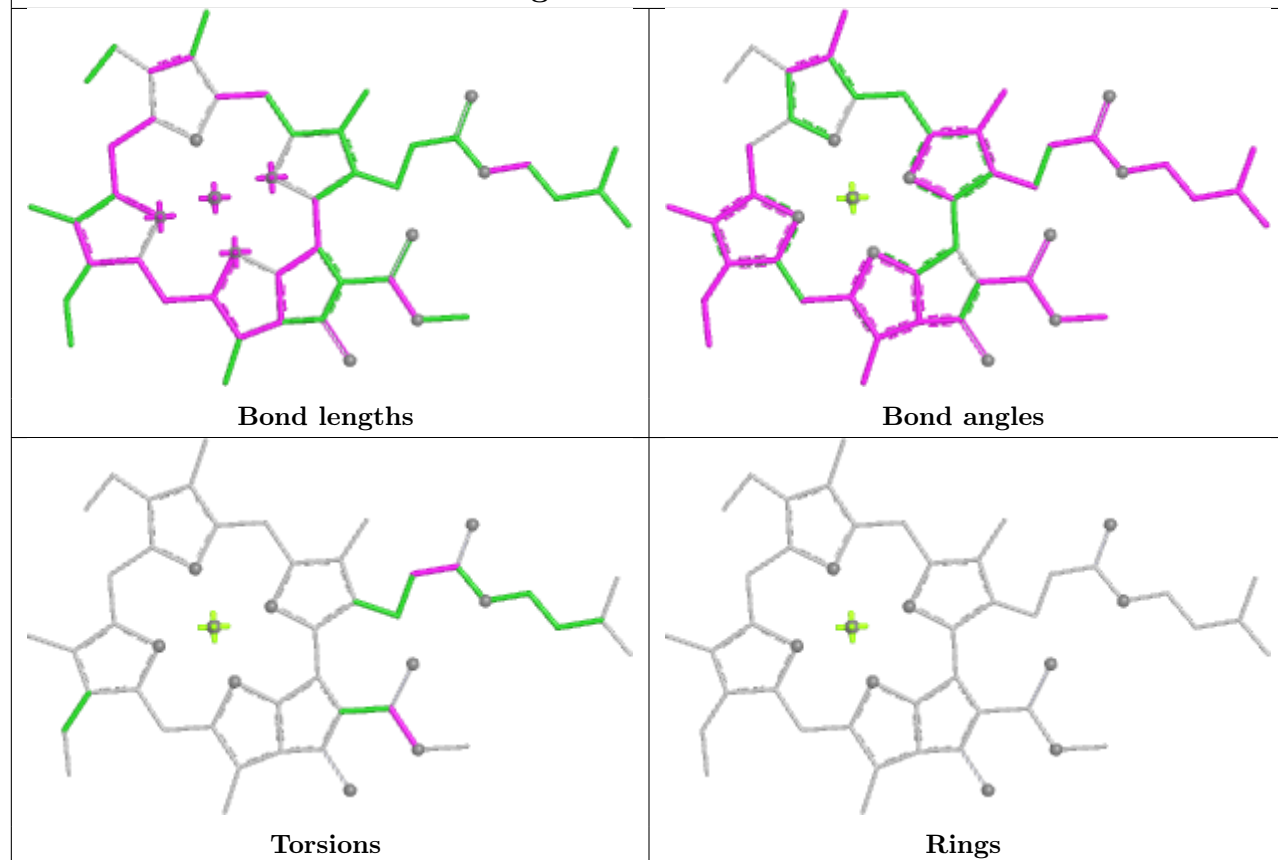




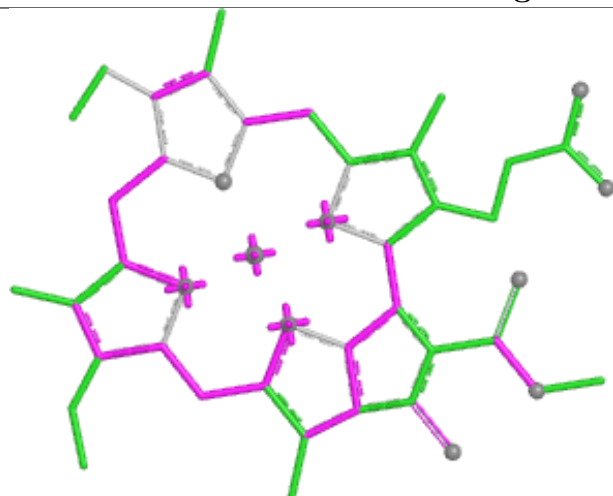
Ligand CLA b 837



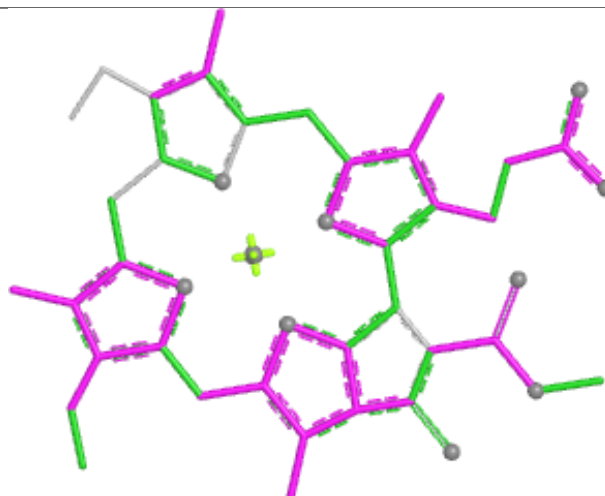
Ligand CLA G 817



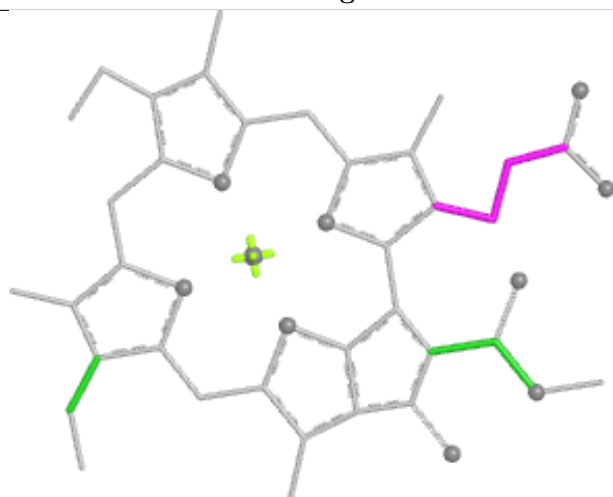
Ligand CLA A 811



Bond lengths



Bond angles

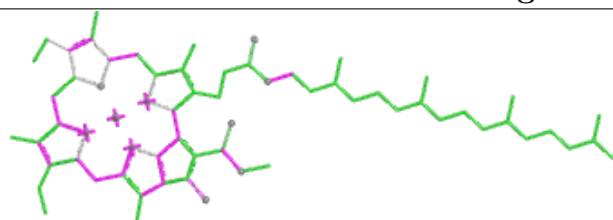


Torsions

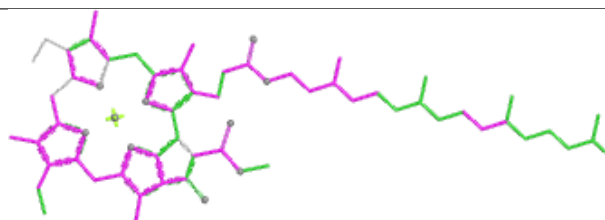


Rings

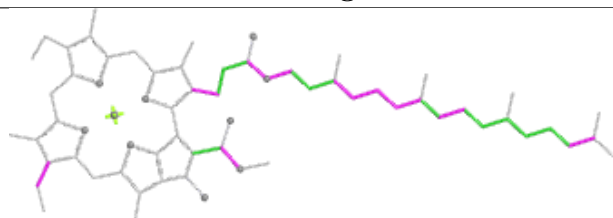
Ligand CLA b 836



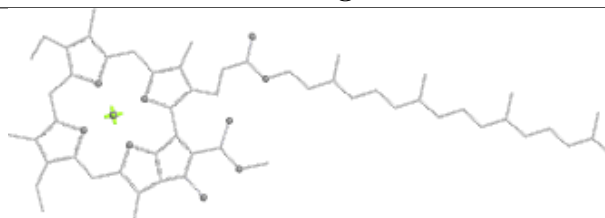
Bond lengths



Bond angles

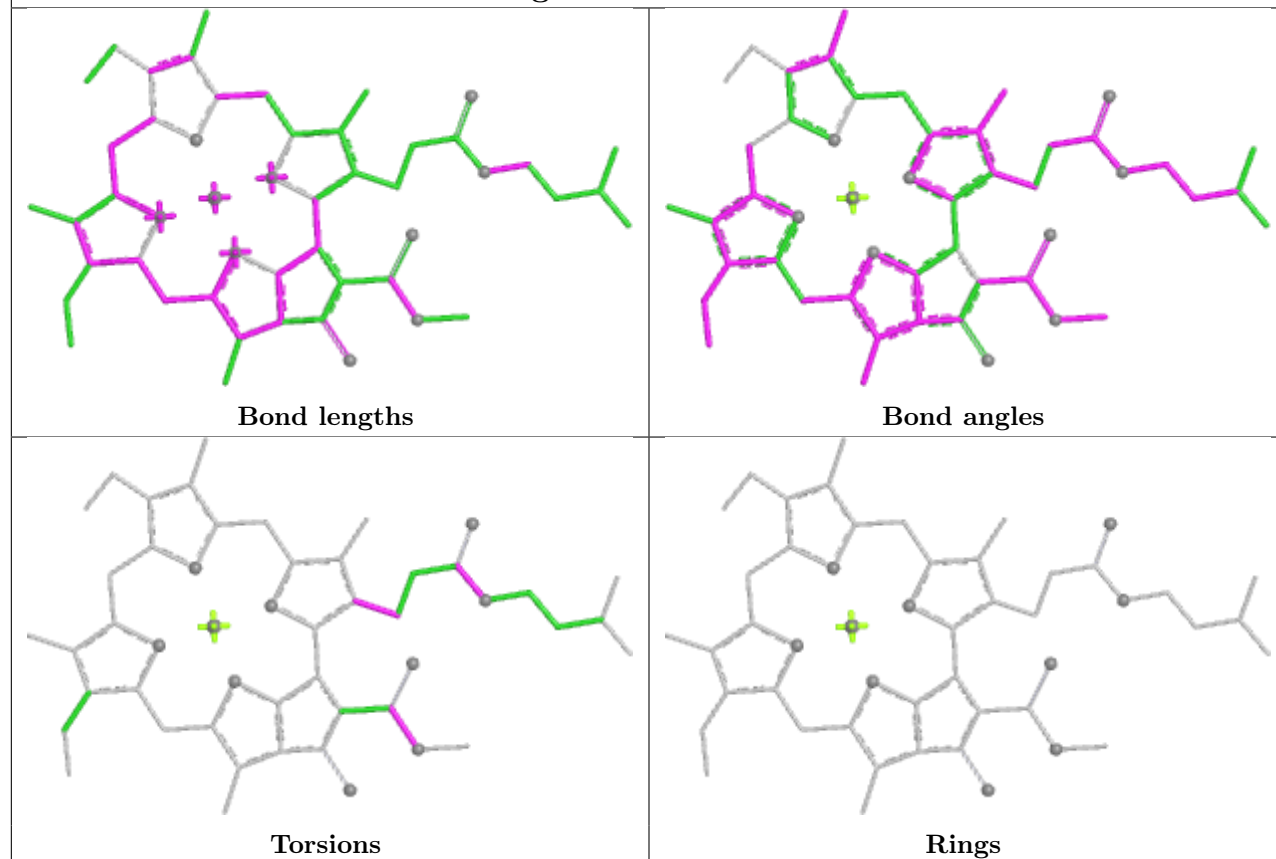


Torsions

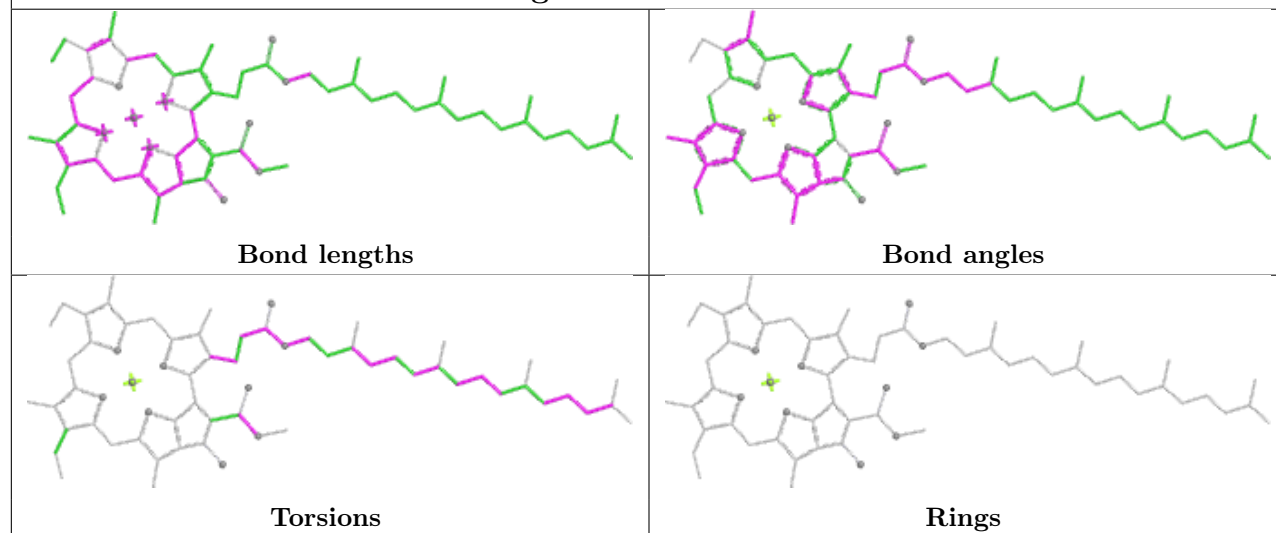


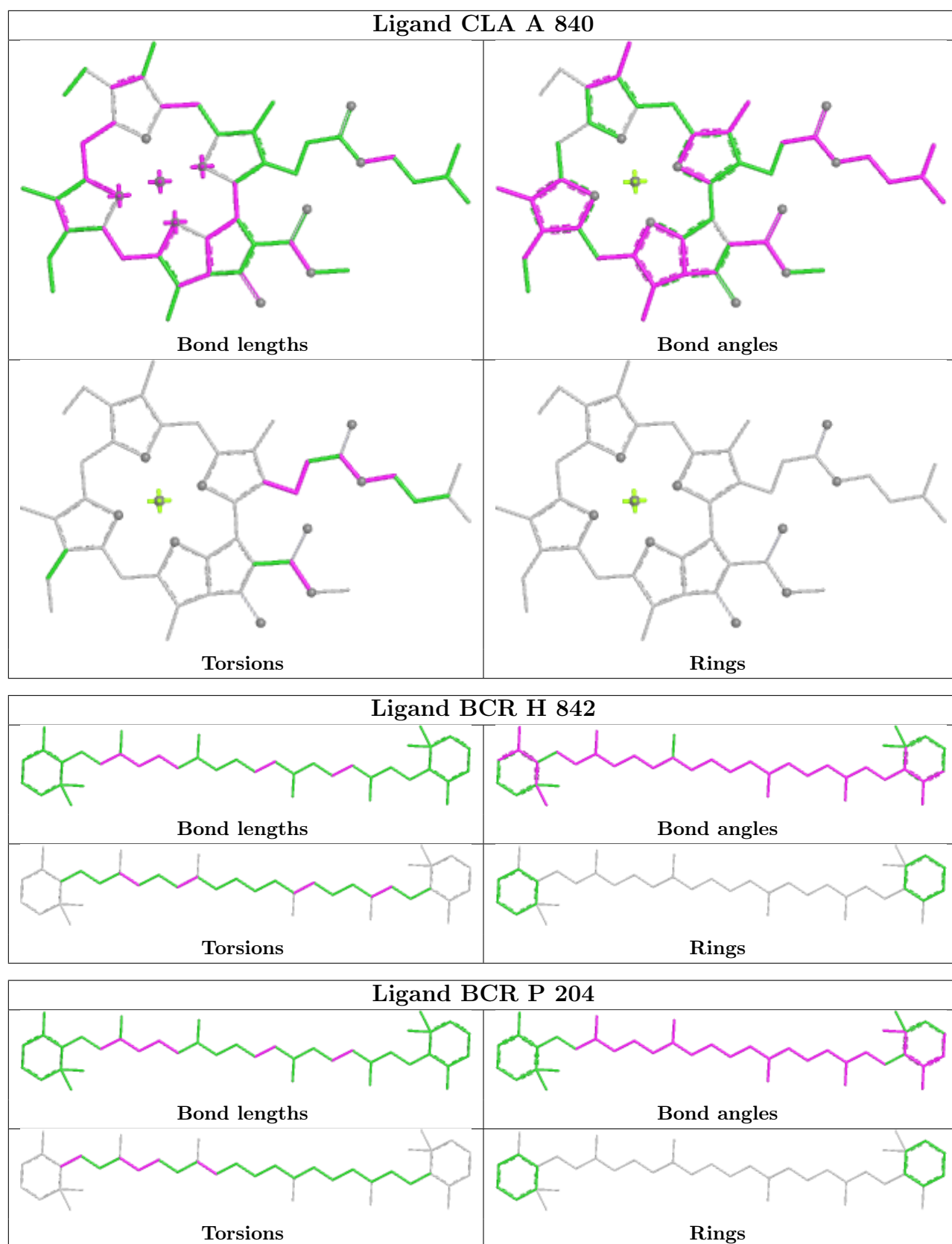
Rings

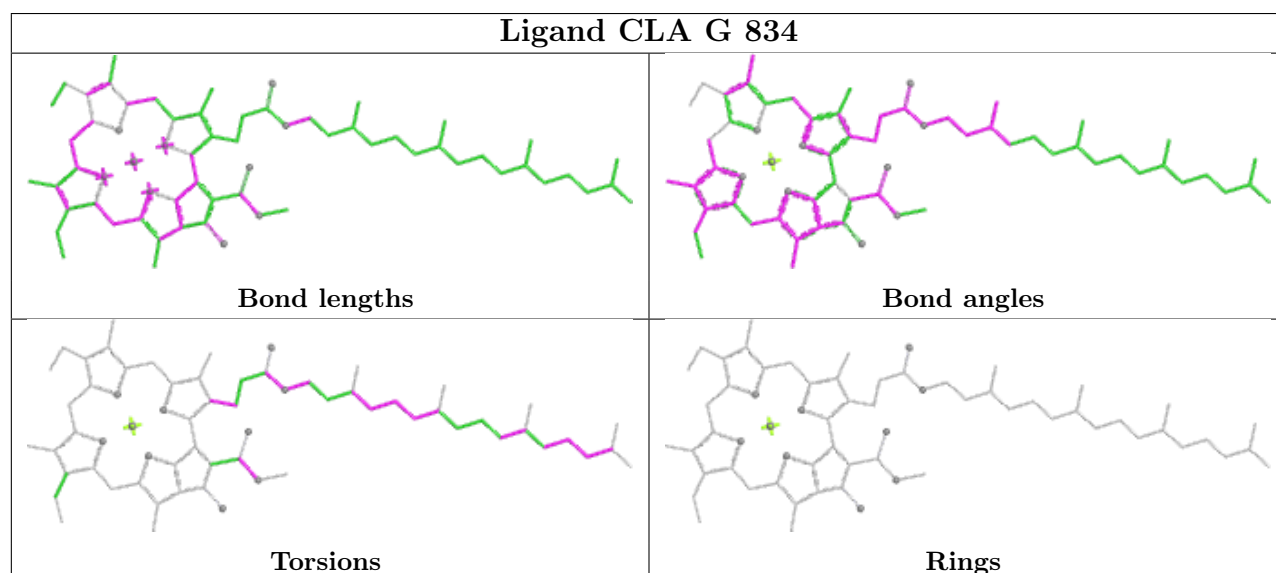
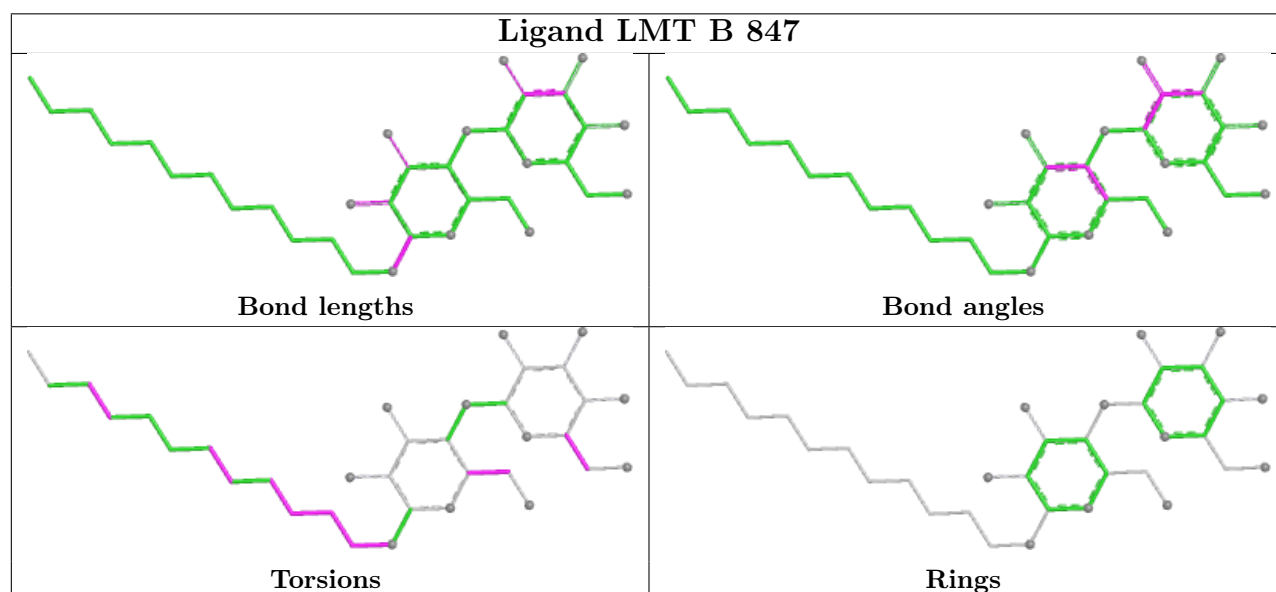
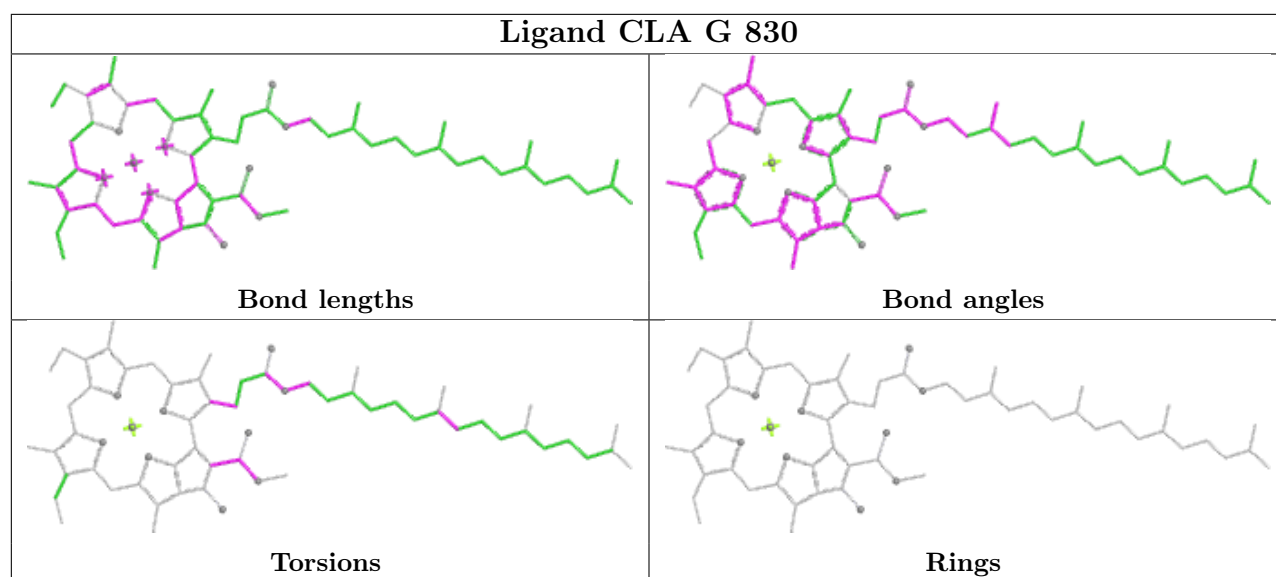
Ligand CLA A 810



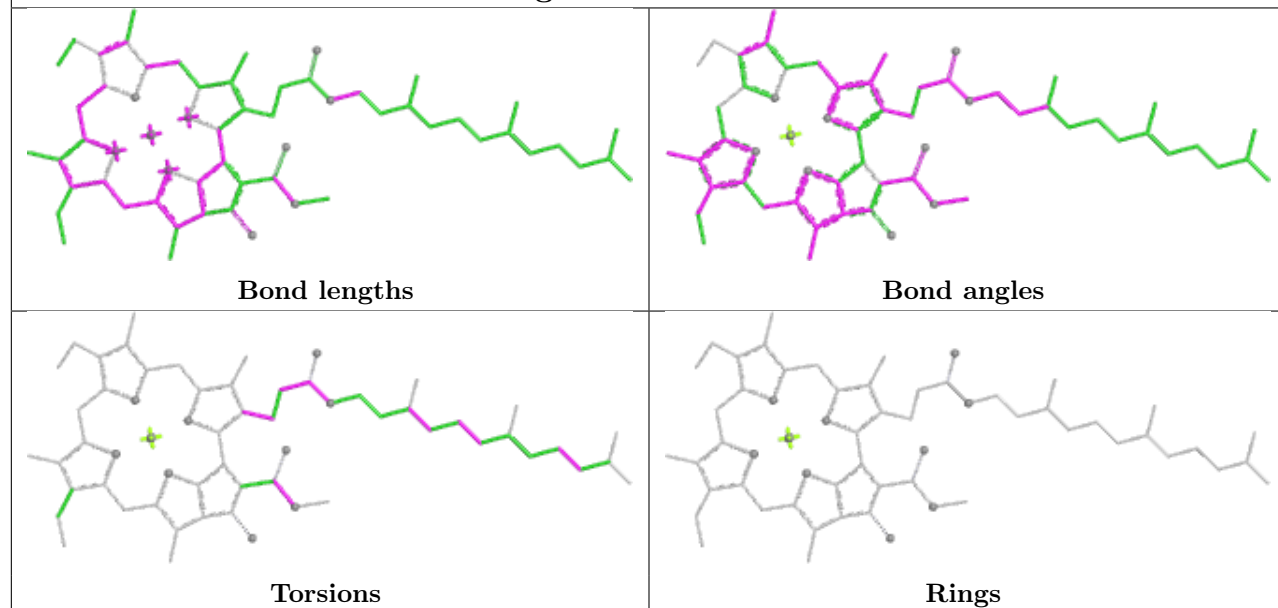
Ligand CLA H 830



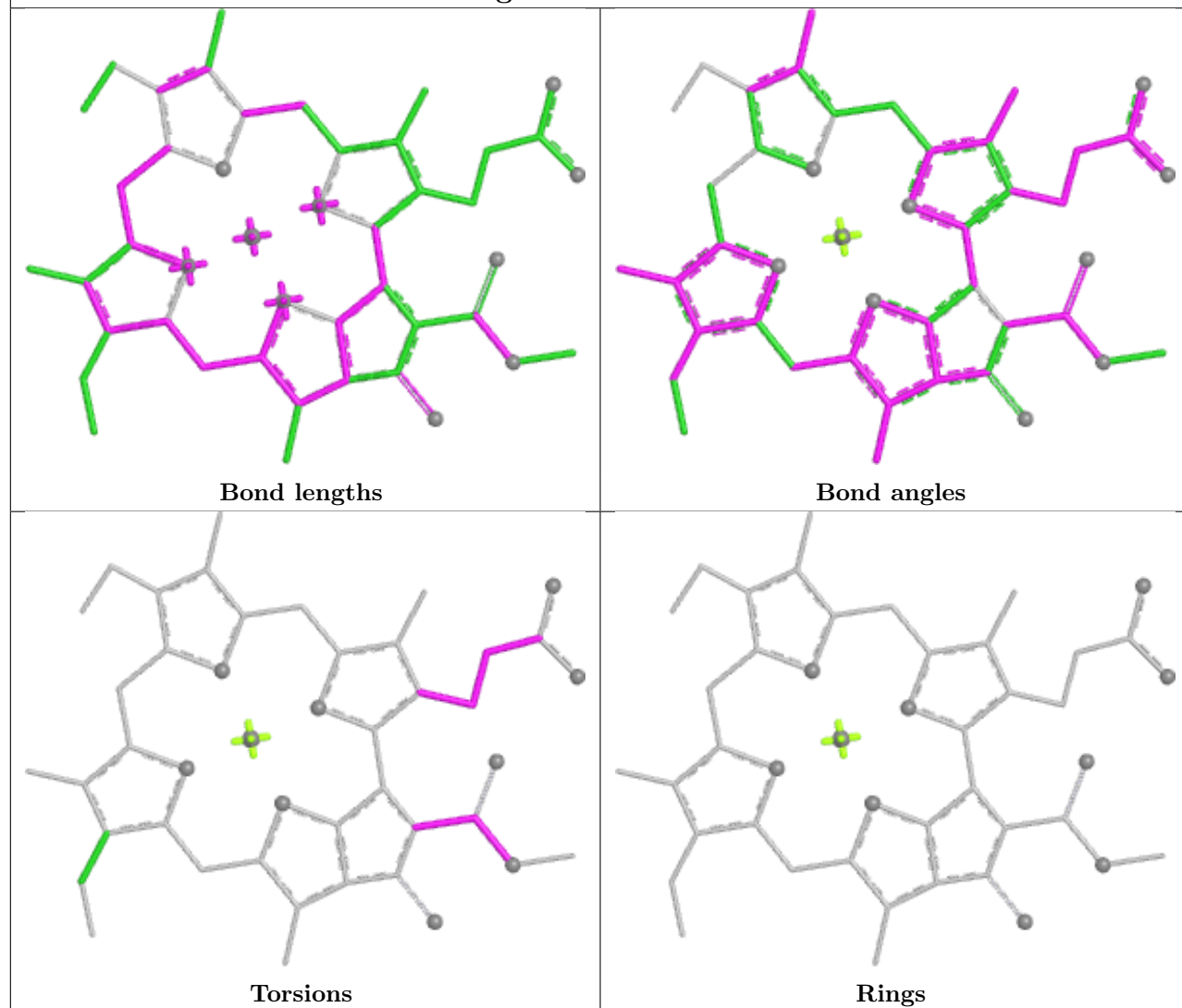


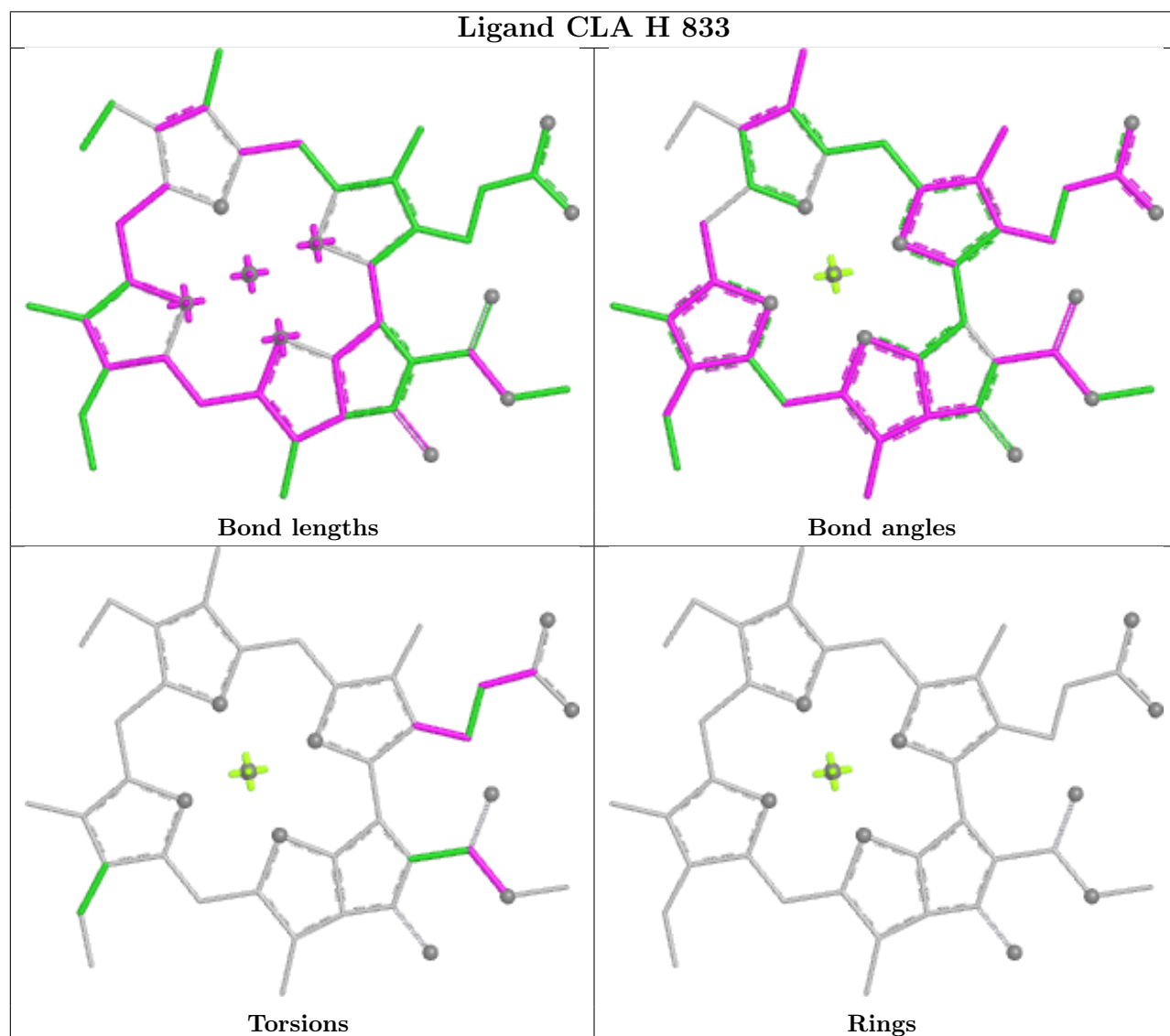
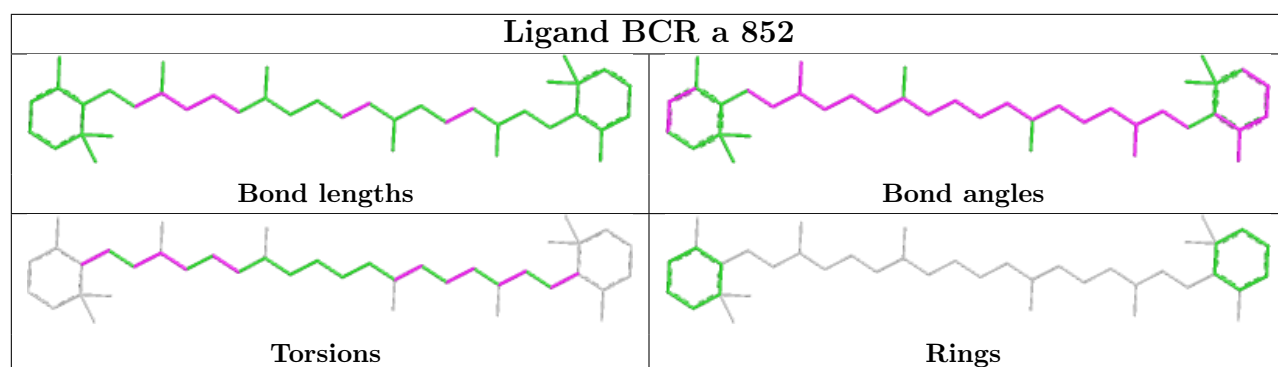


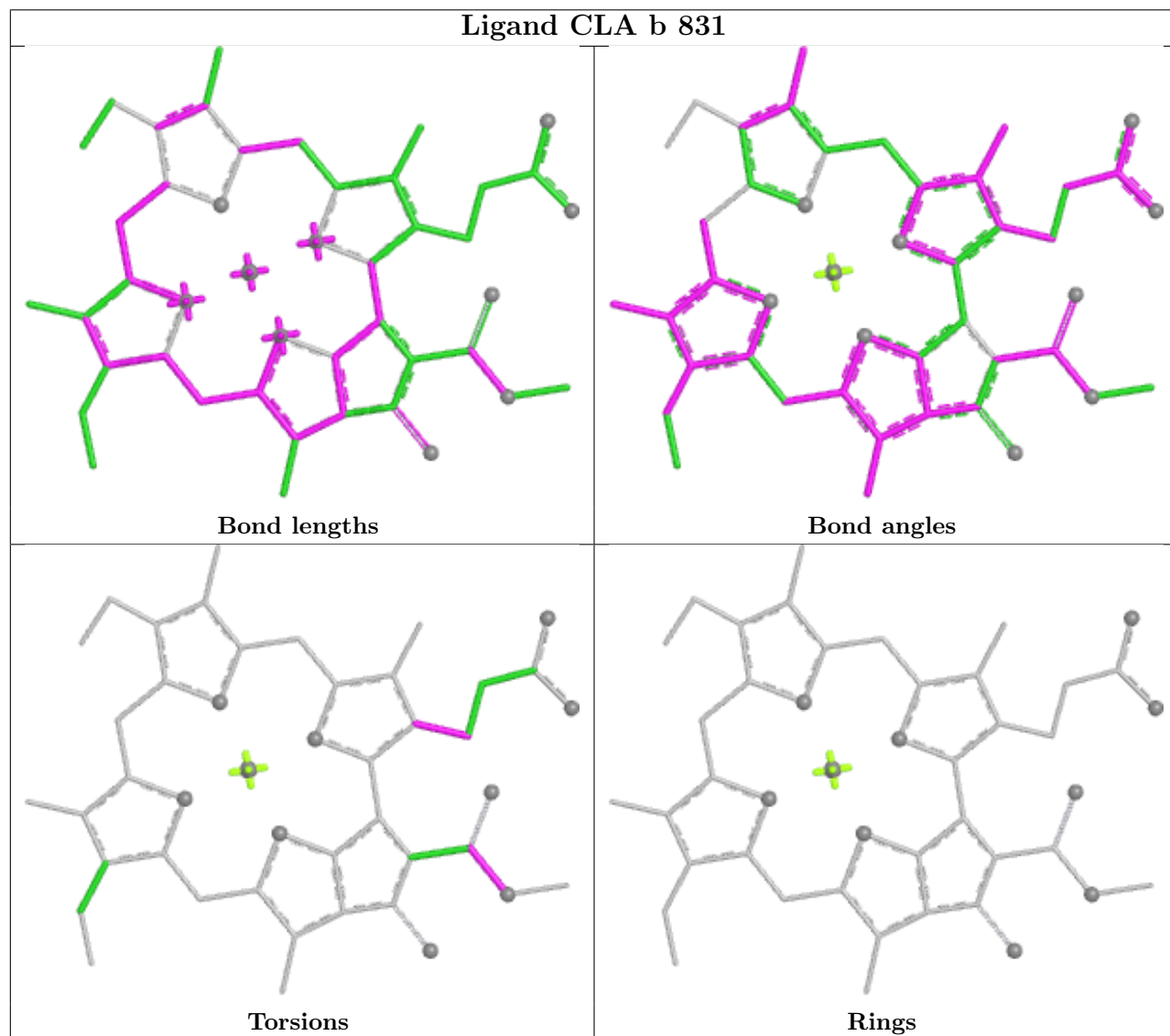
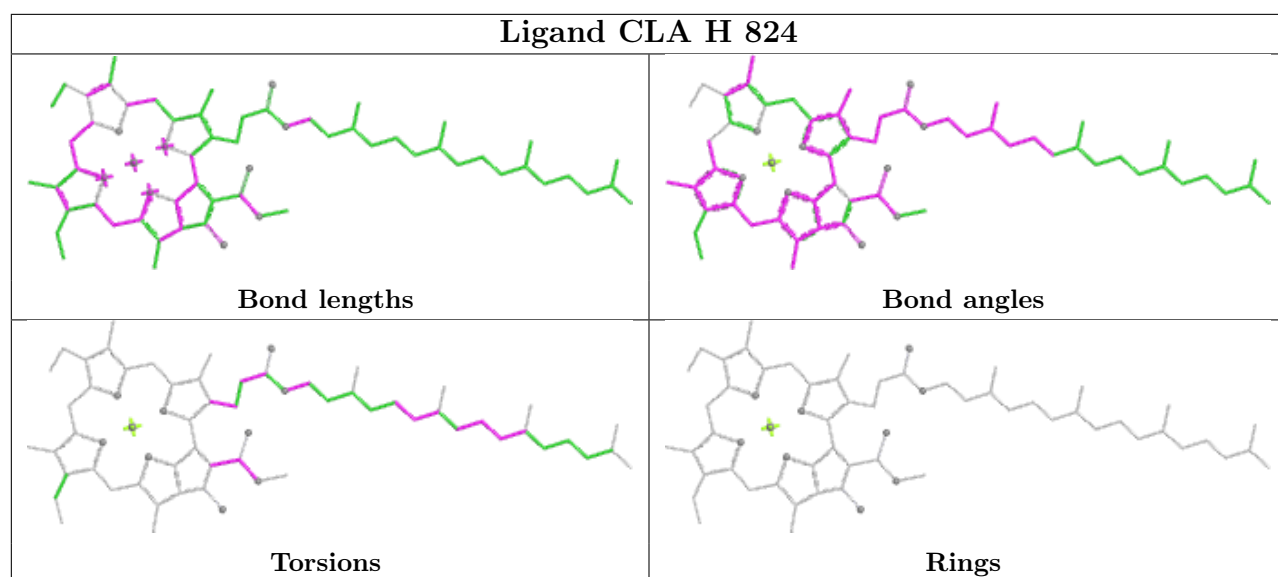
Ligand CLA b 811

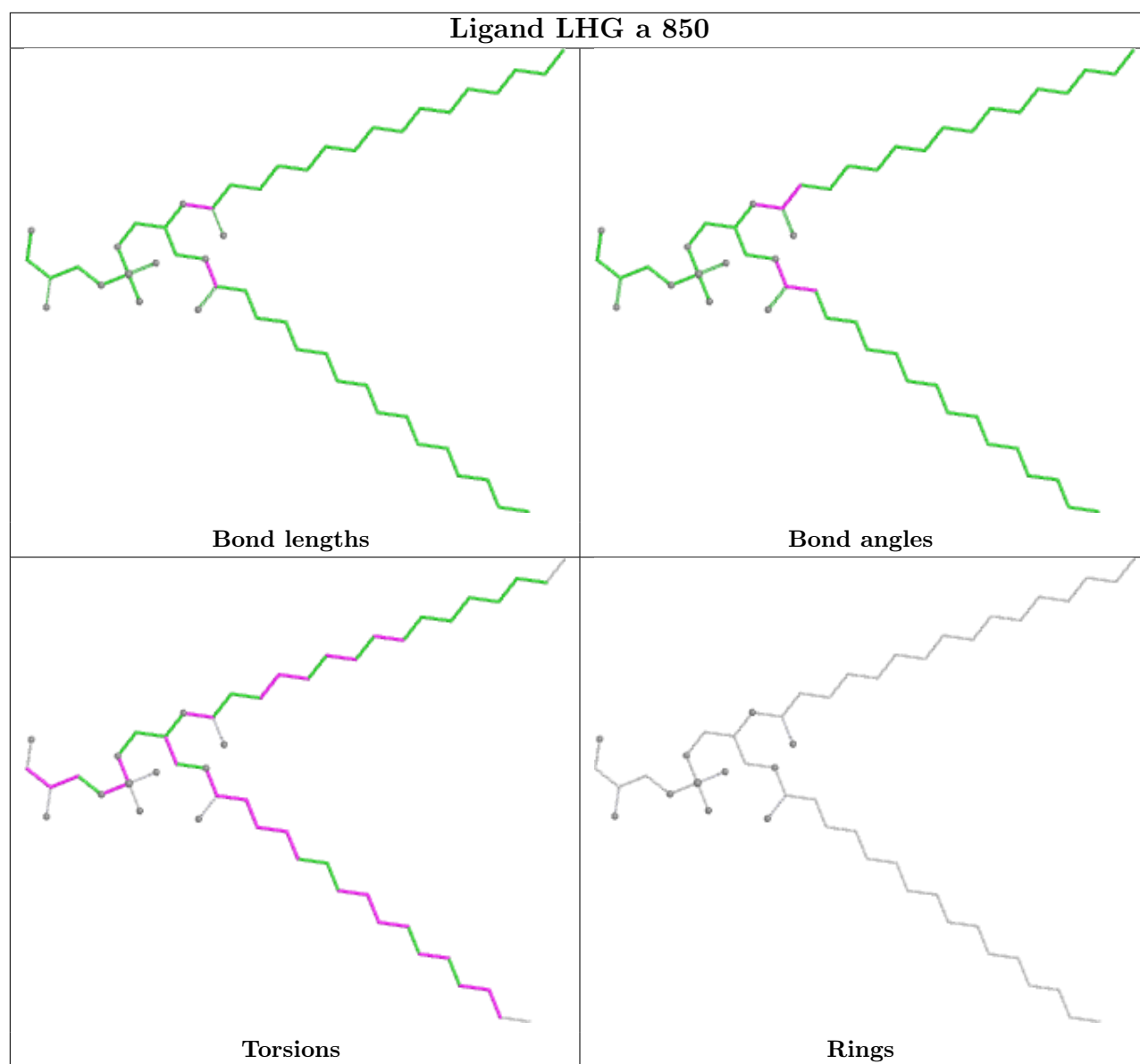


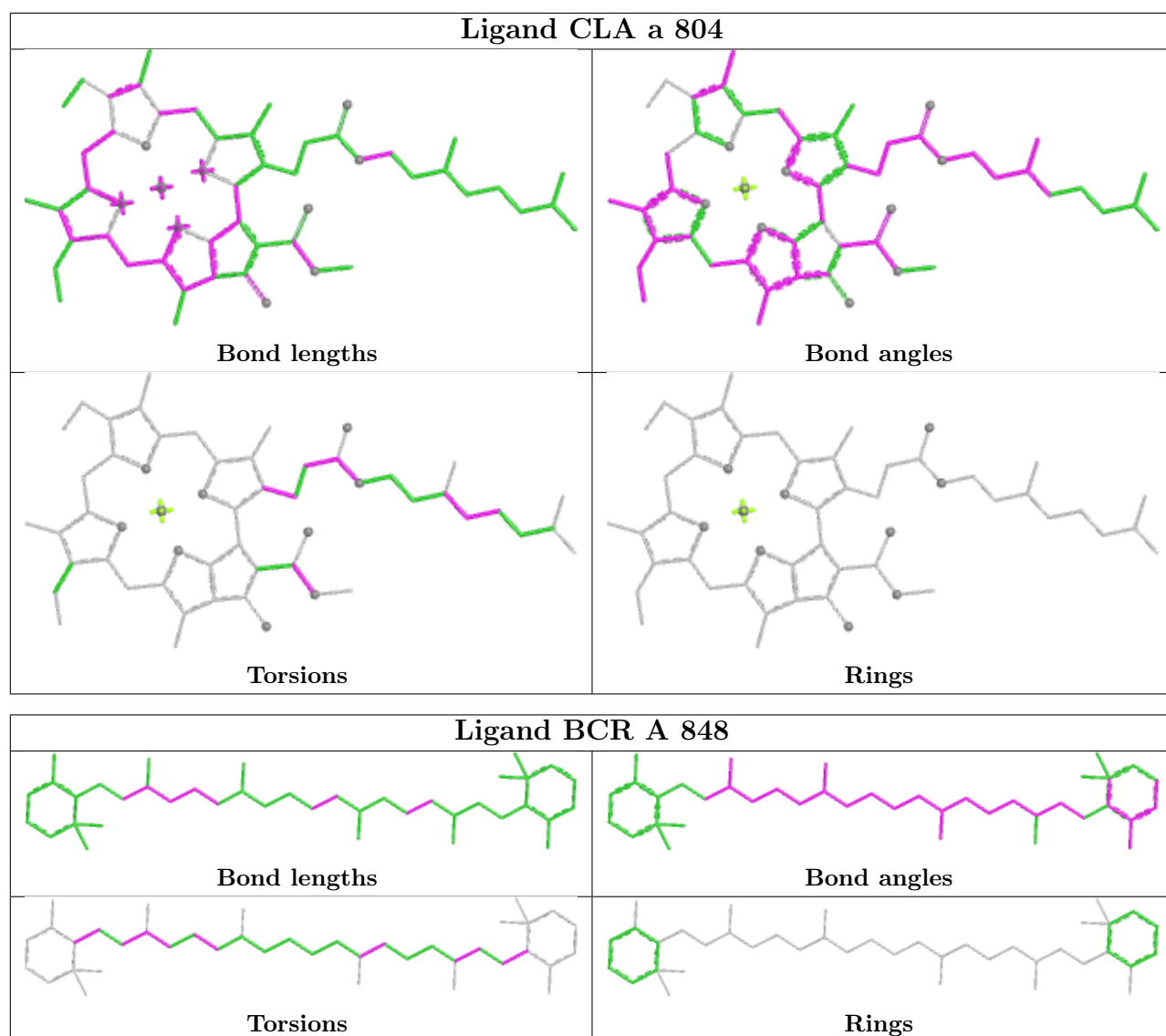
Ligand CLA a 821

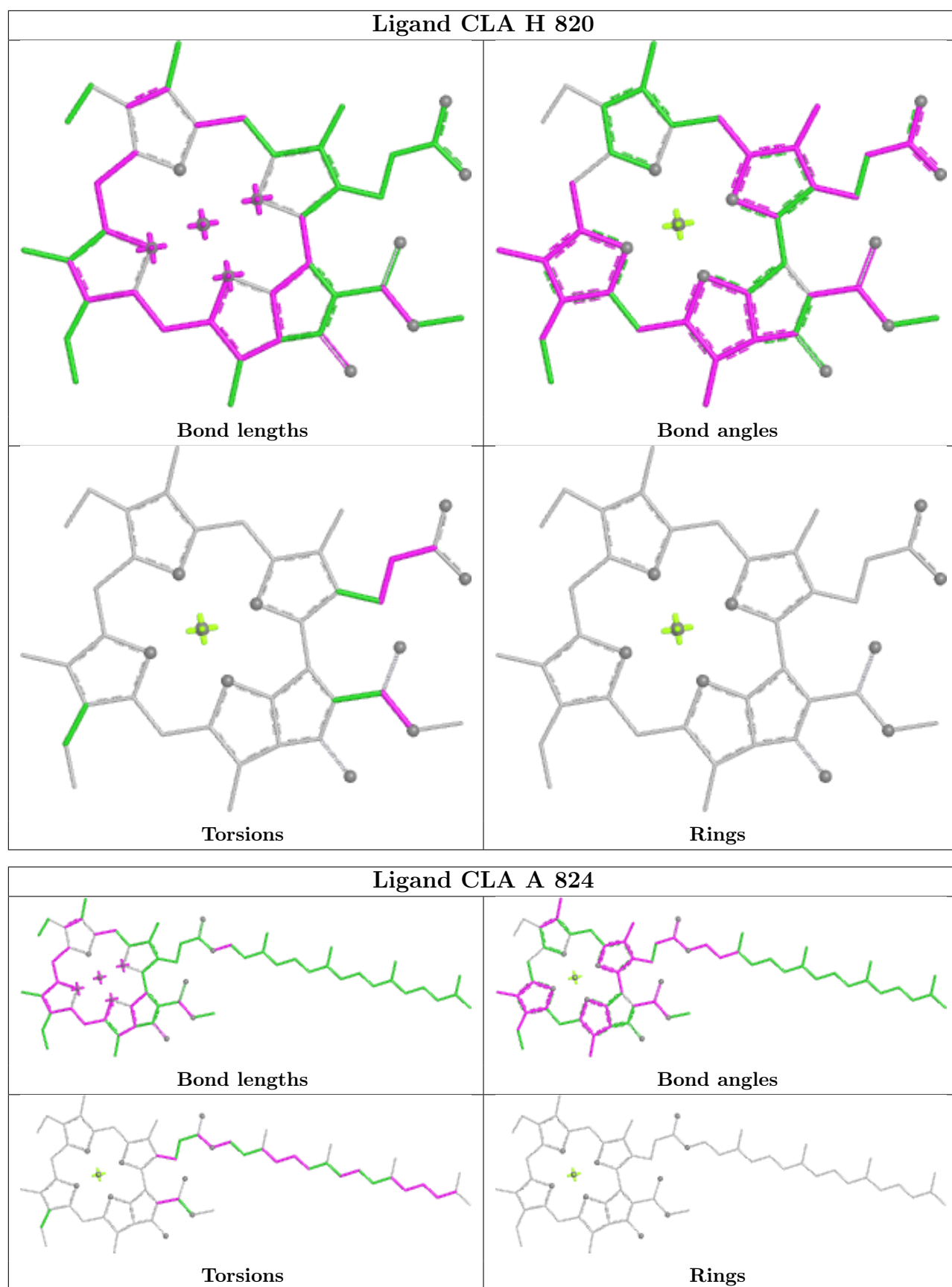


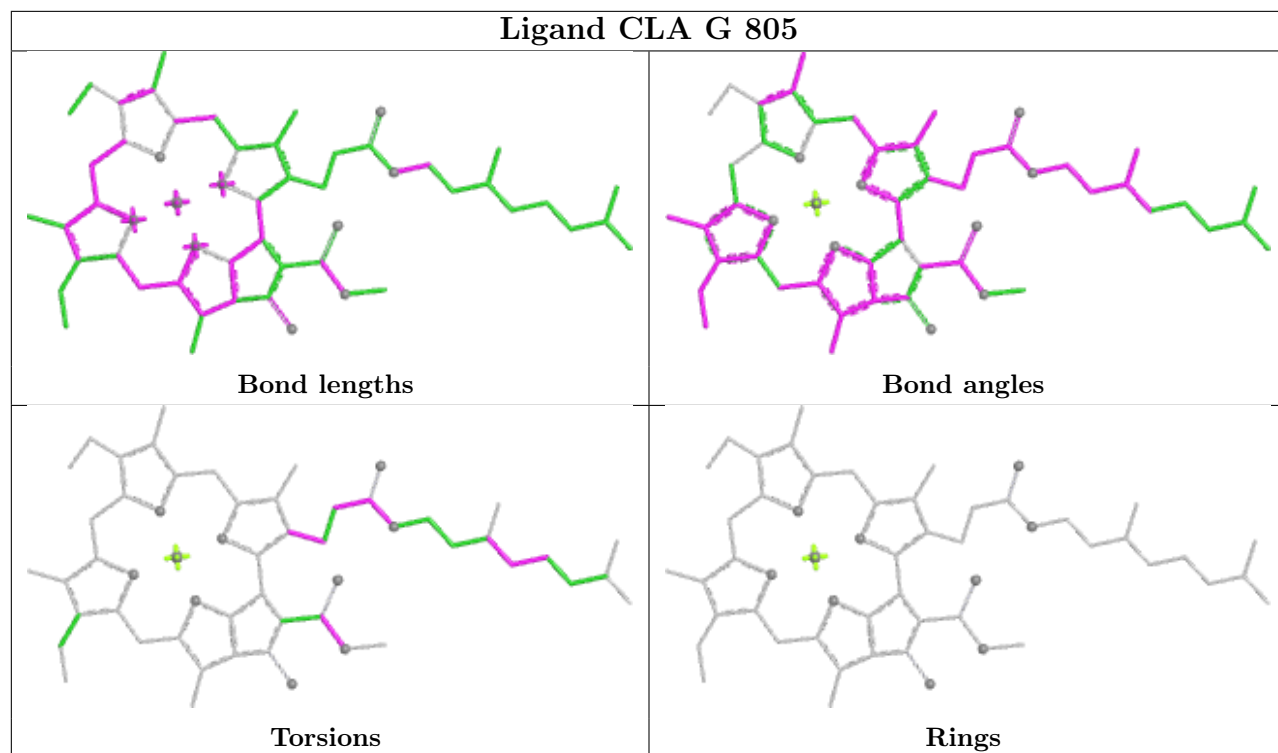
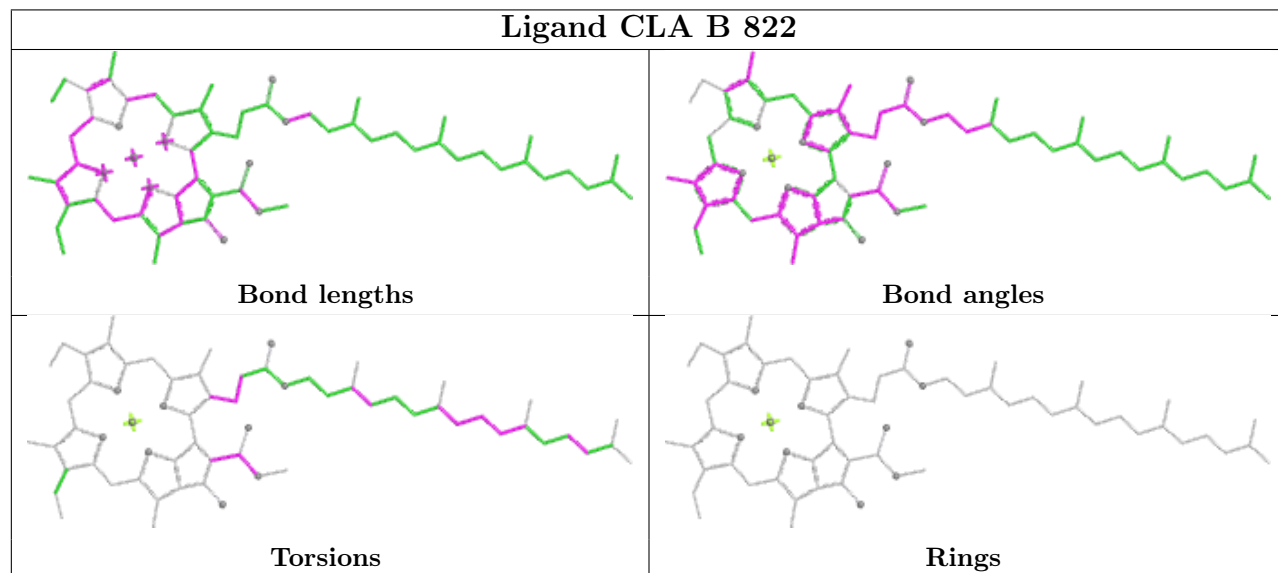


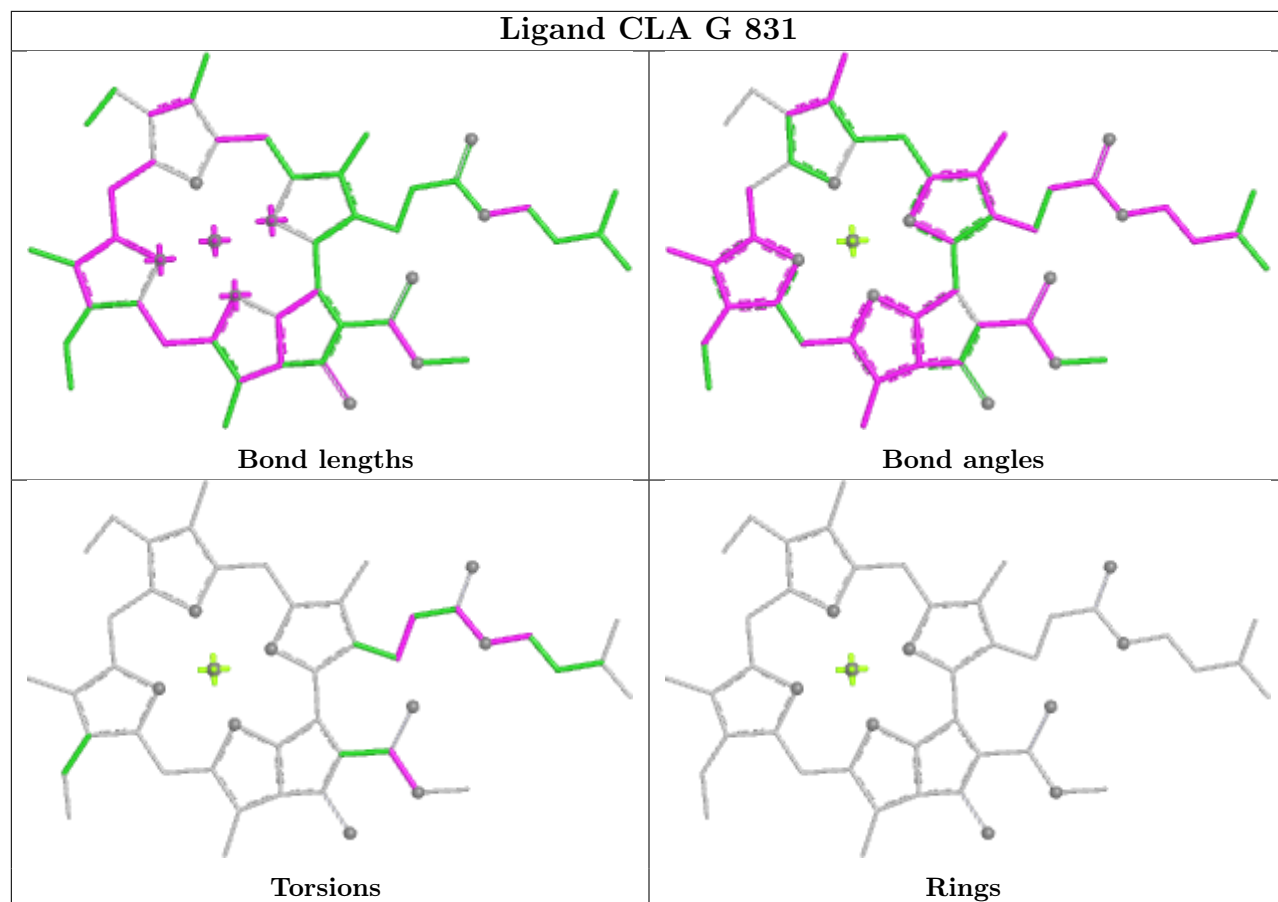


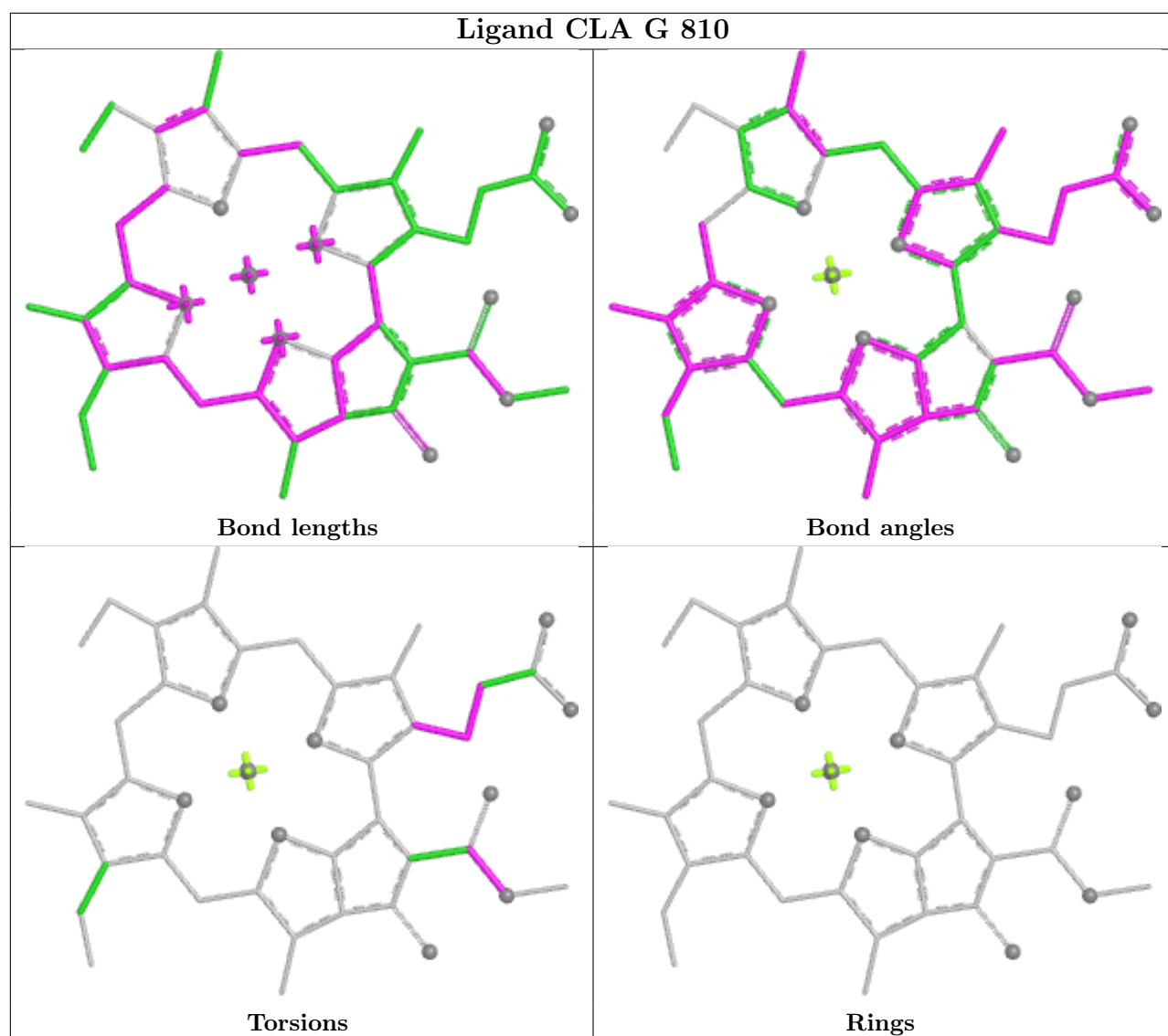




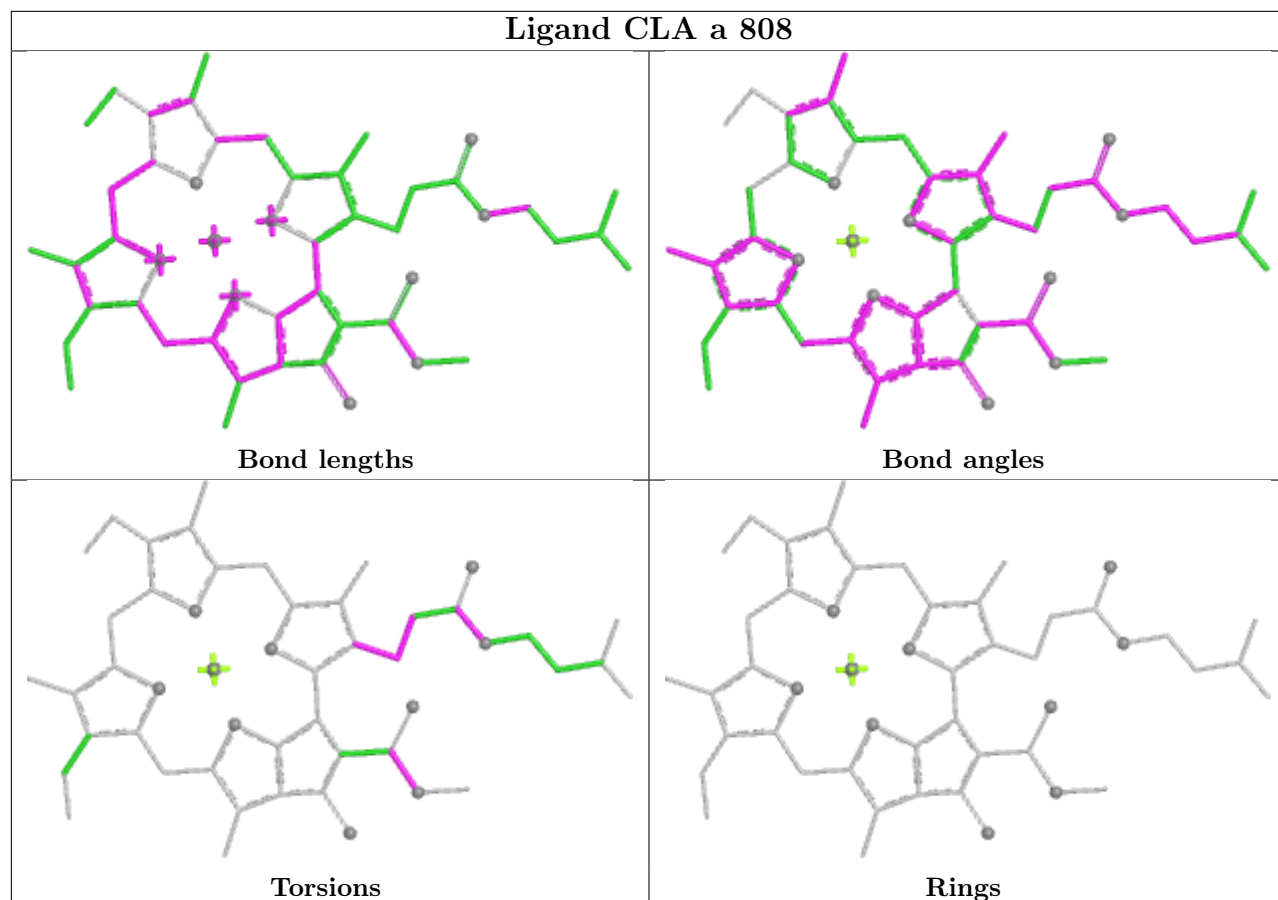


Ligand CLA G 805**Ligand CLA B 822**

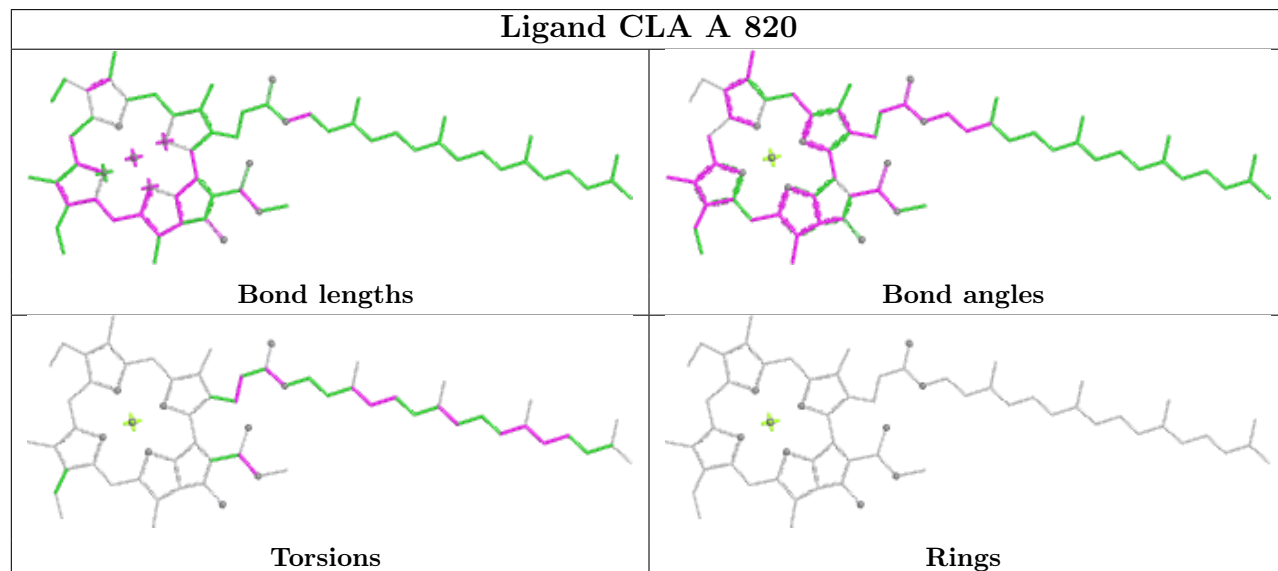


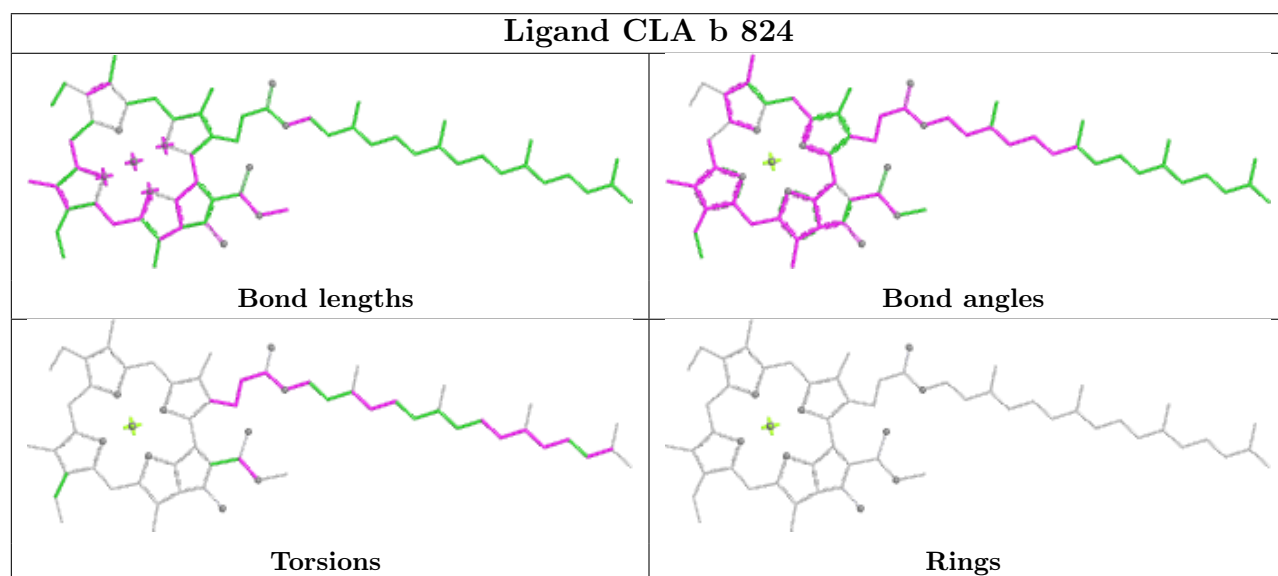
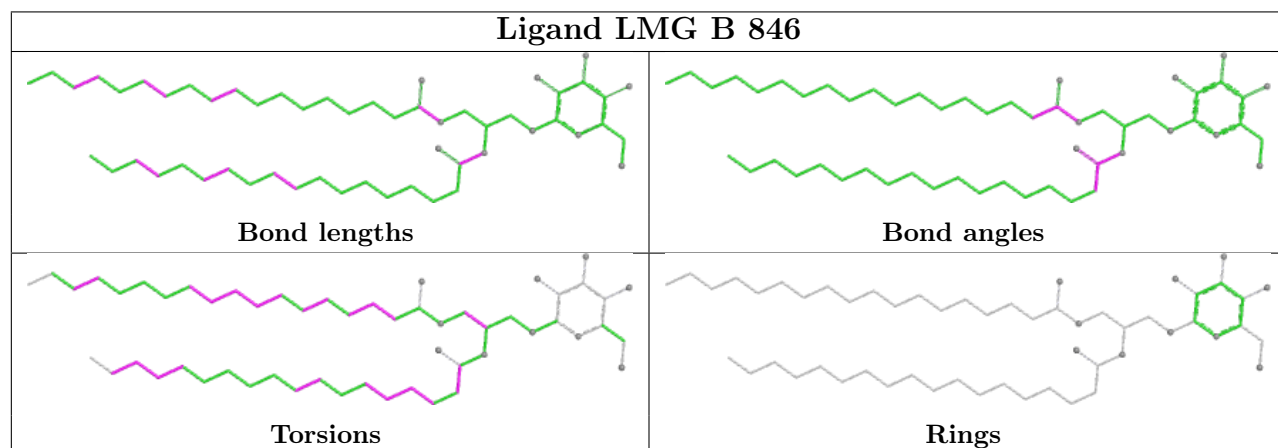
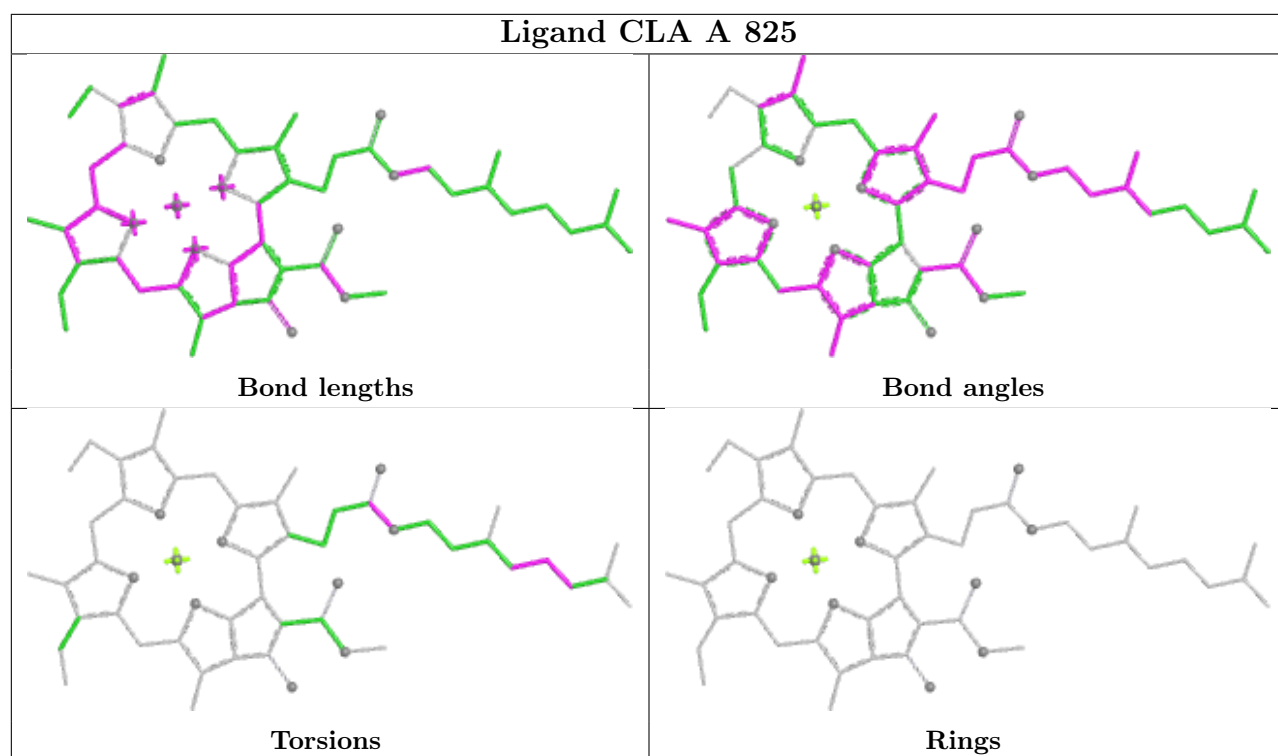


Ligand CLA a 808

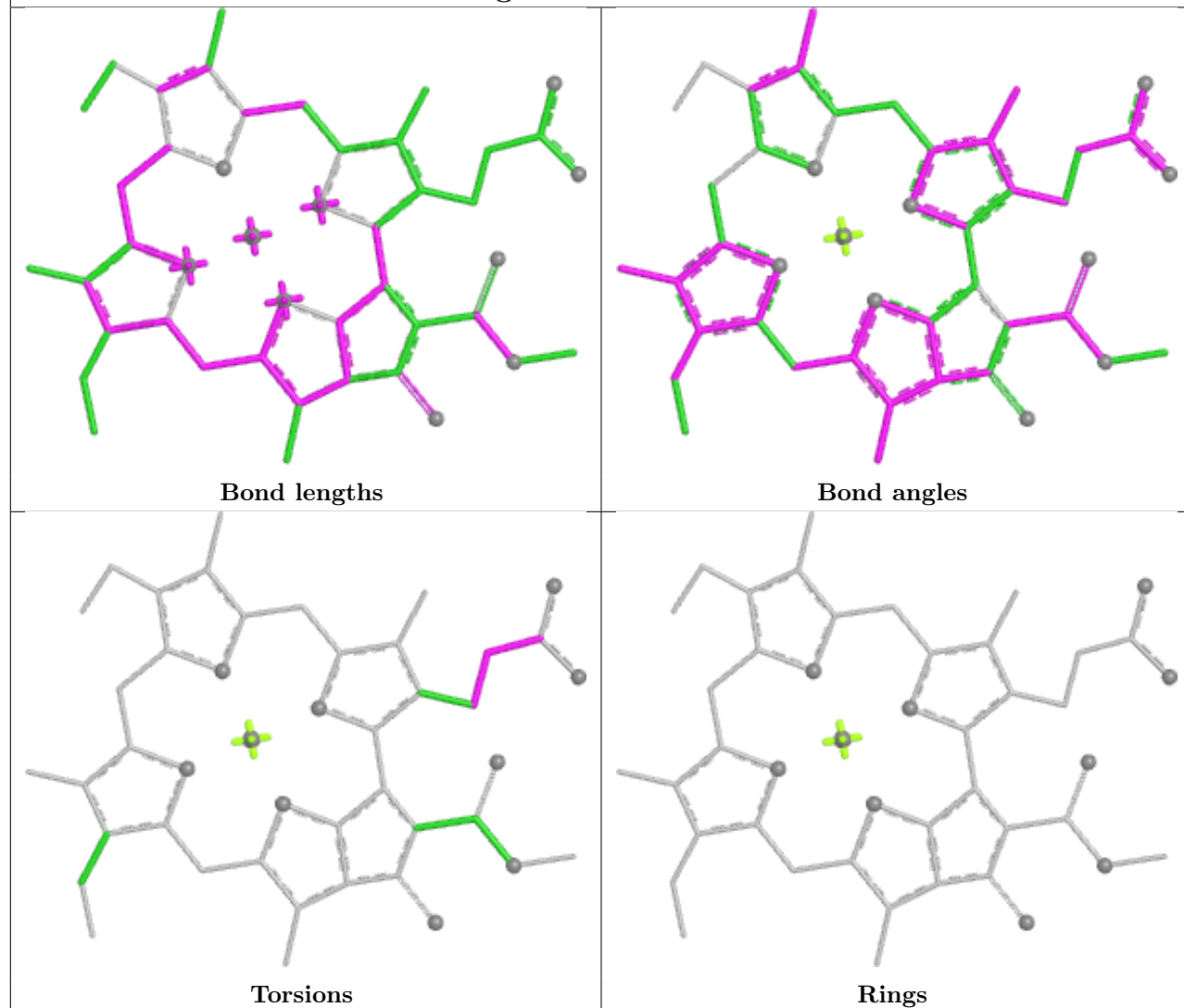


Ligand CLA A 820

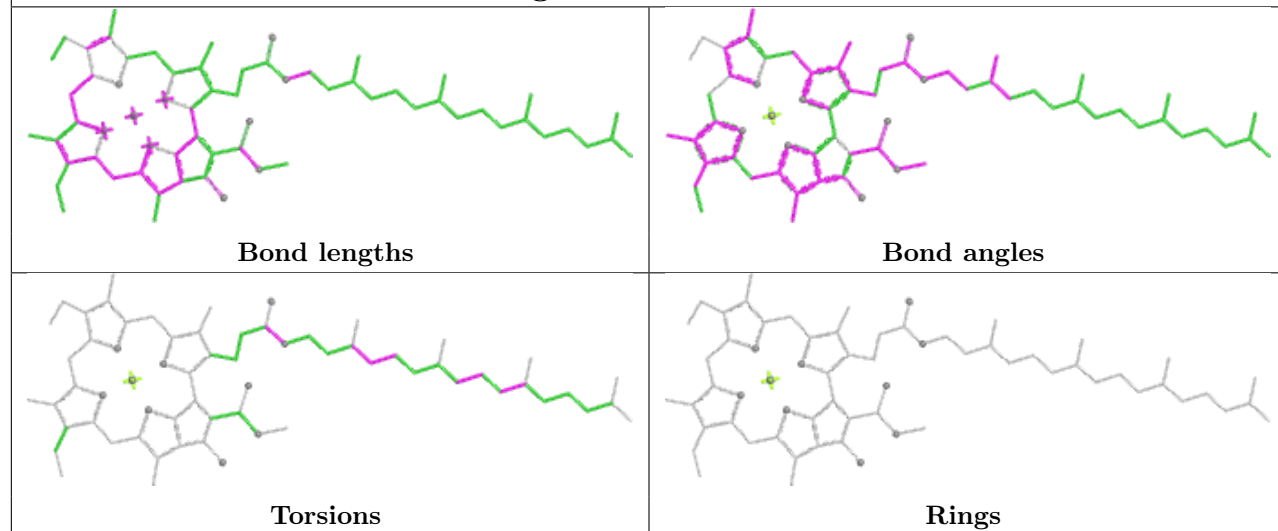


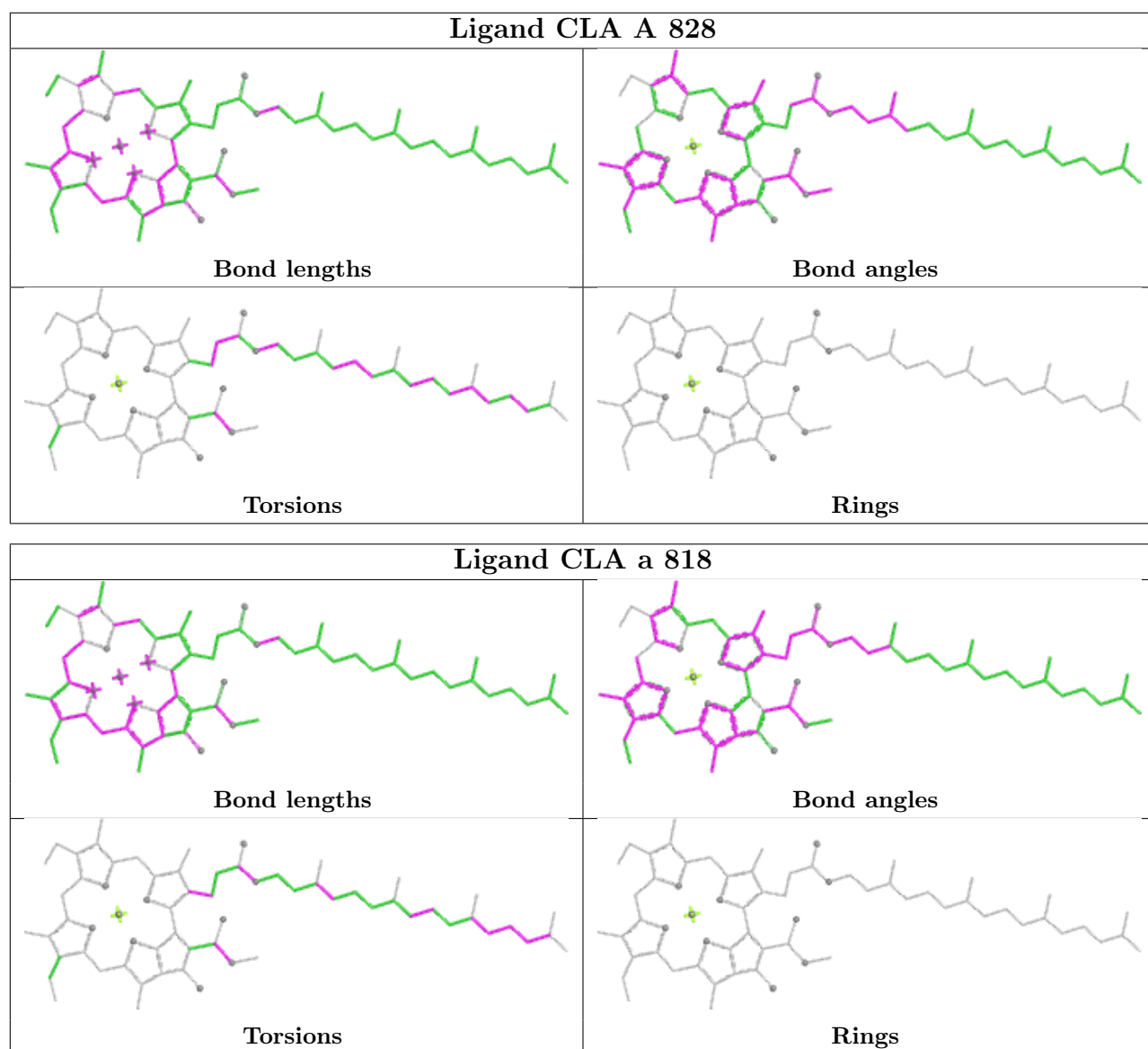


Ligand CLA b 809

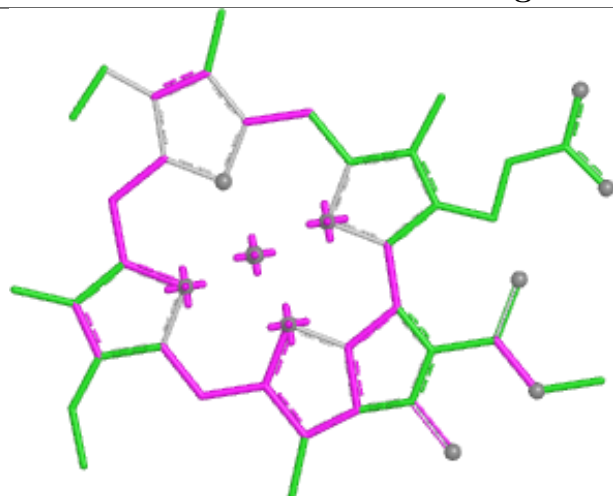


Ligand CLA A 839

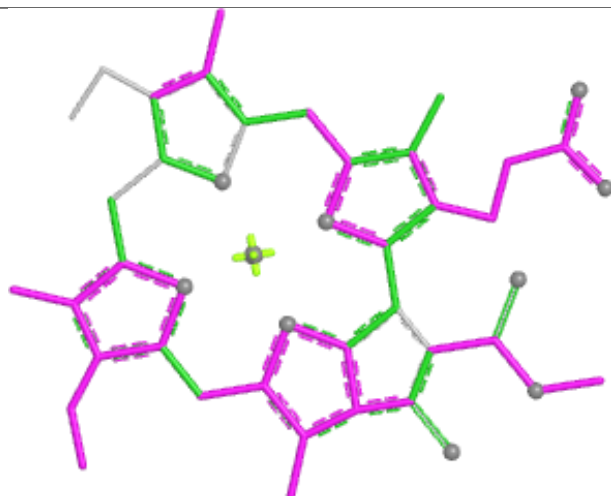




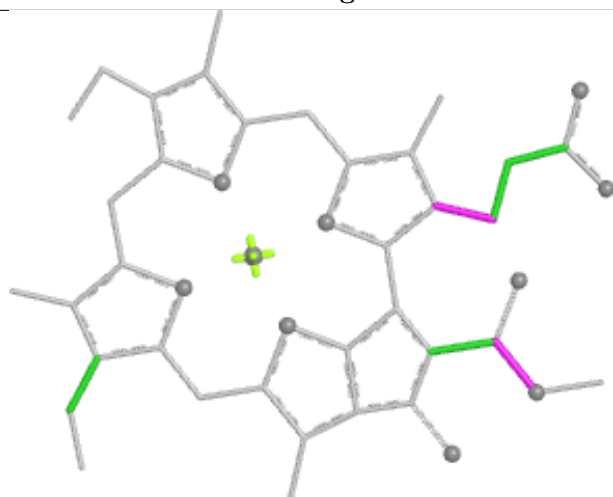
Ligand CLA B 820



Bond lengths



Bond angles

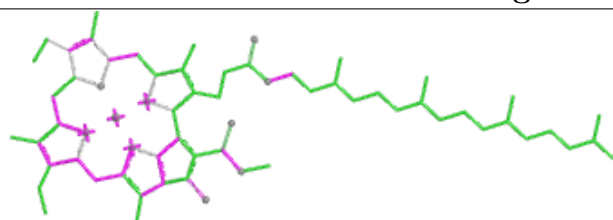


Torsions

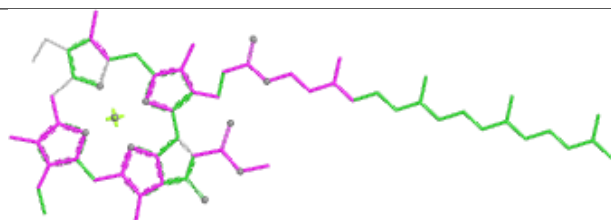


Rings

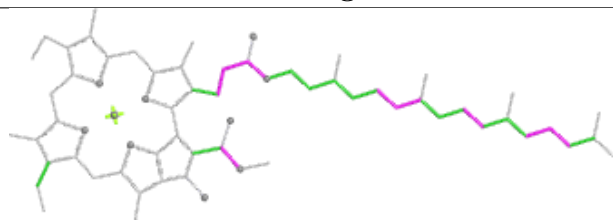
Ligand CLA G 841



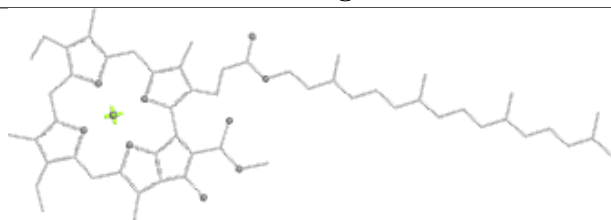
Bond lengths



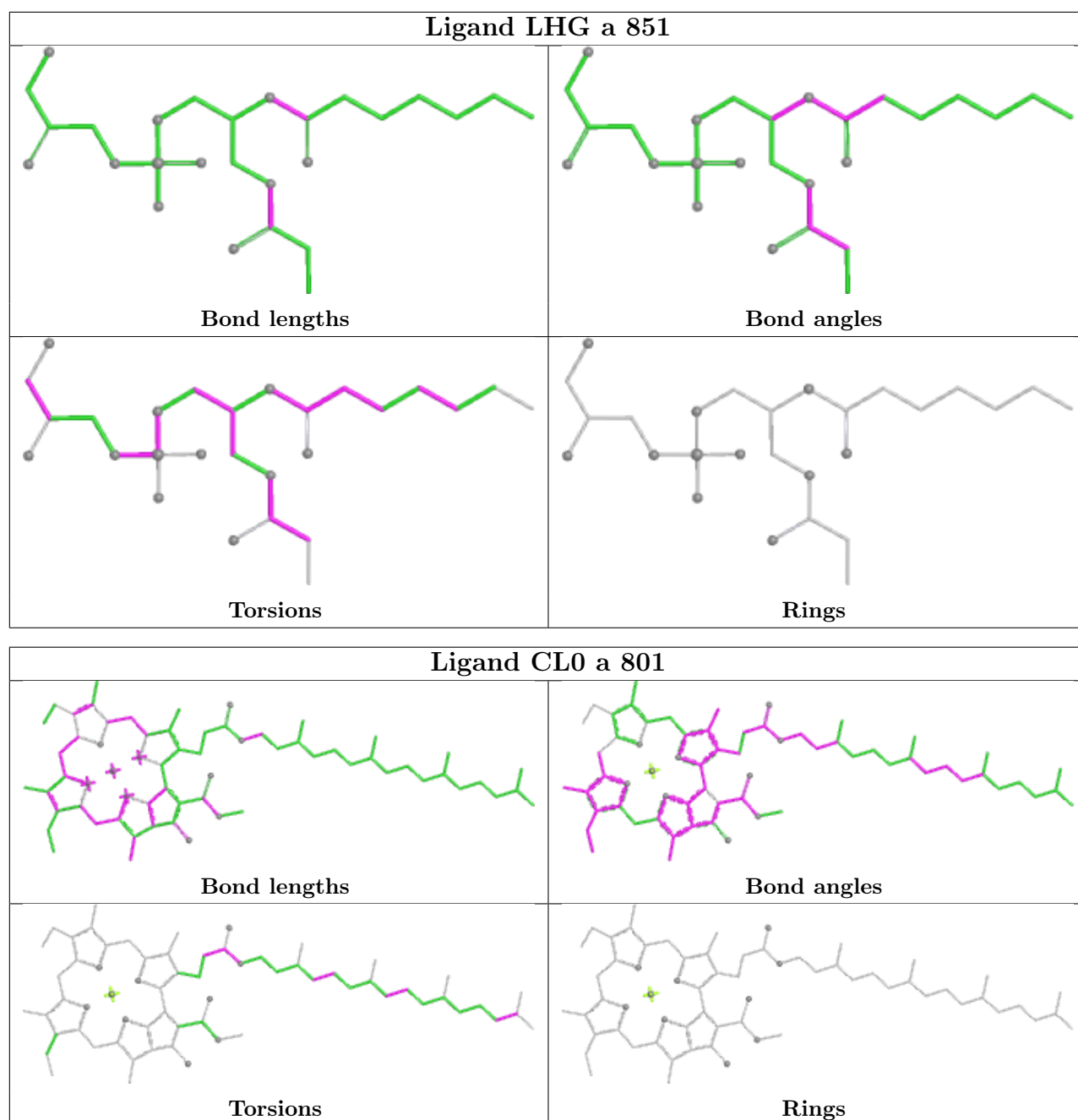
Bond angles

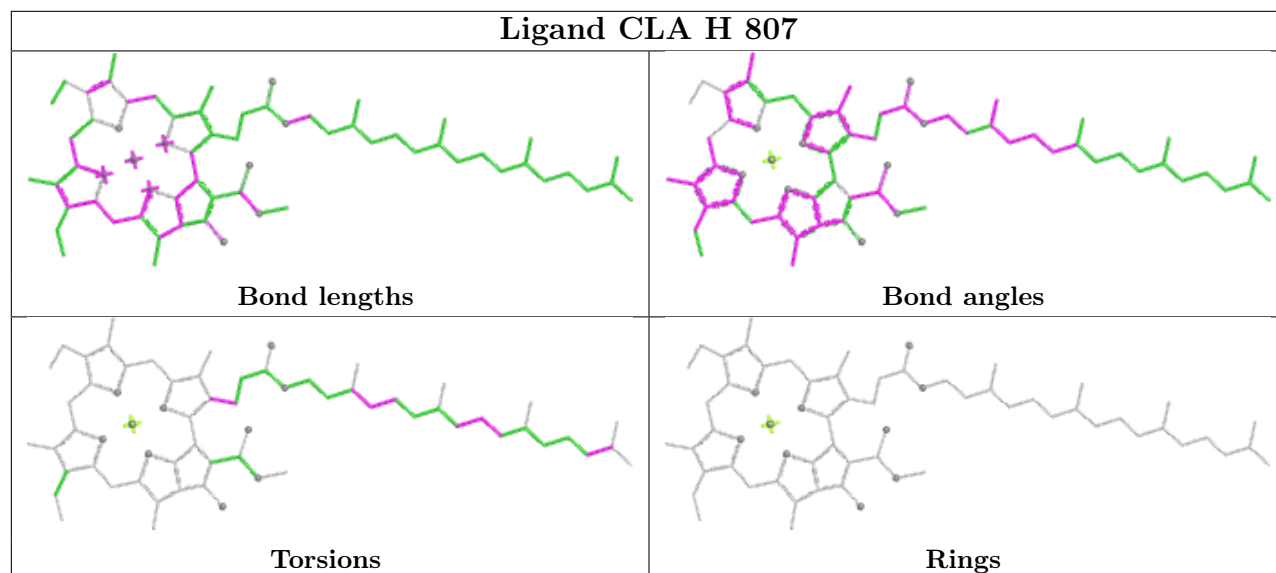
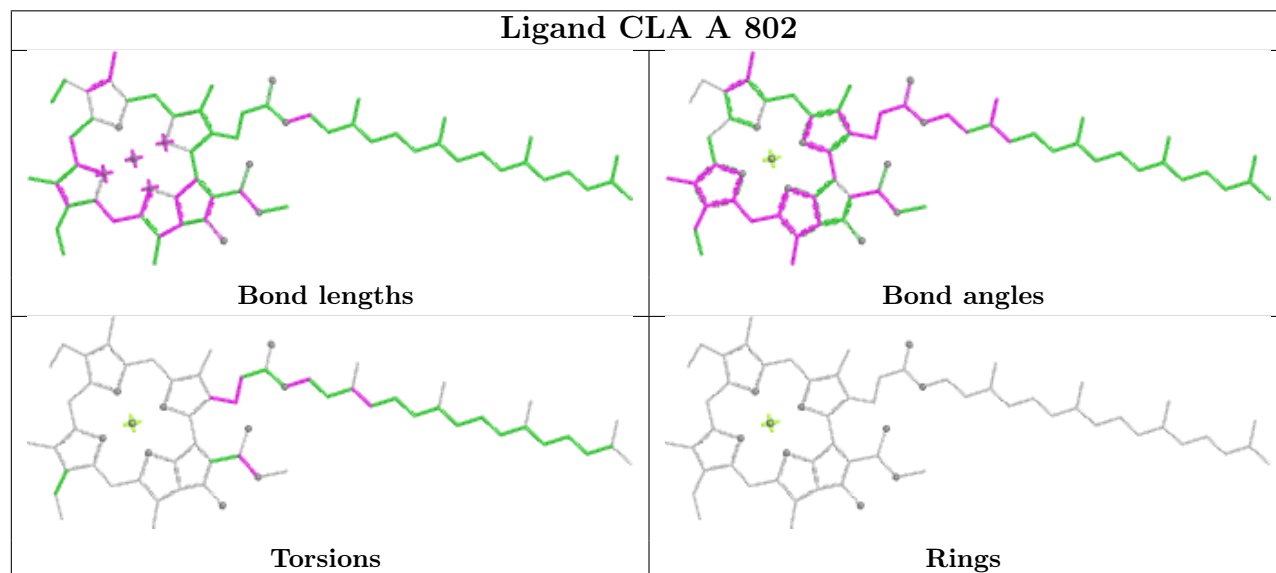
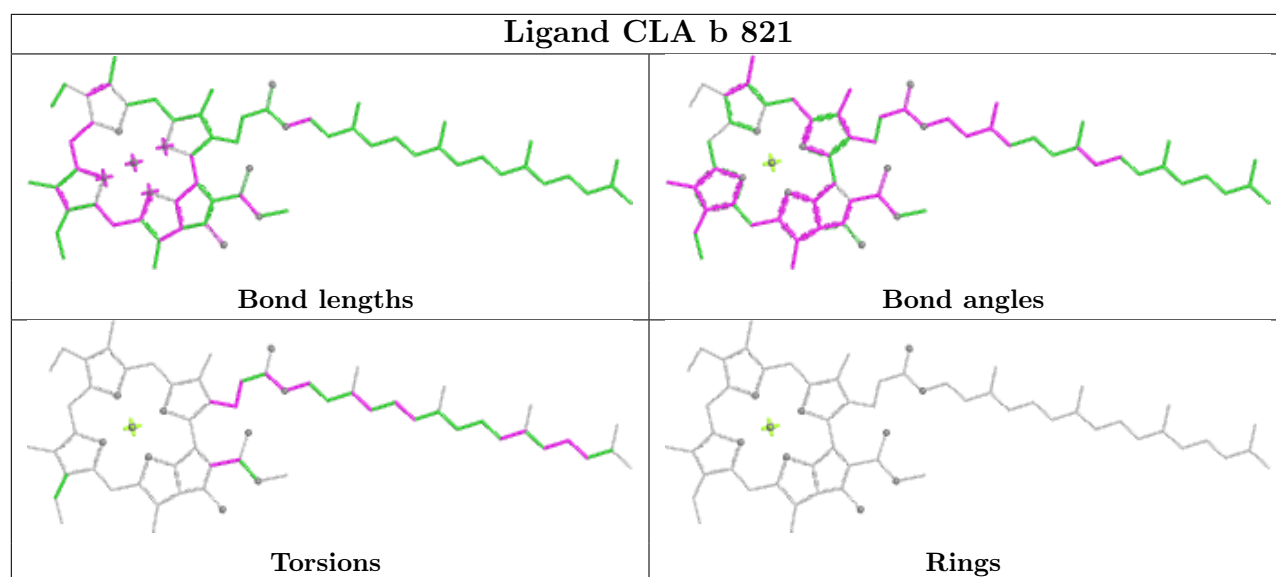


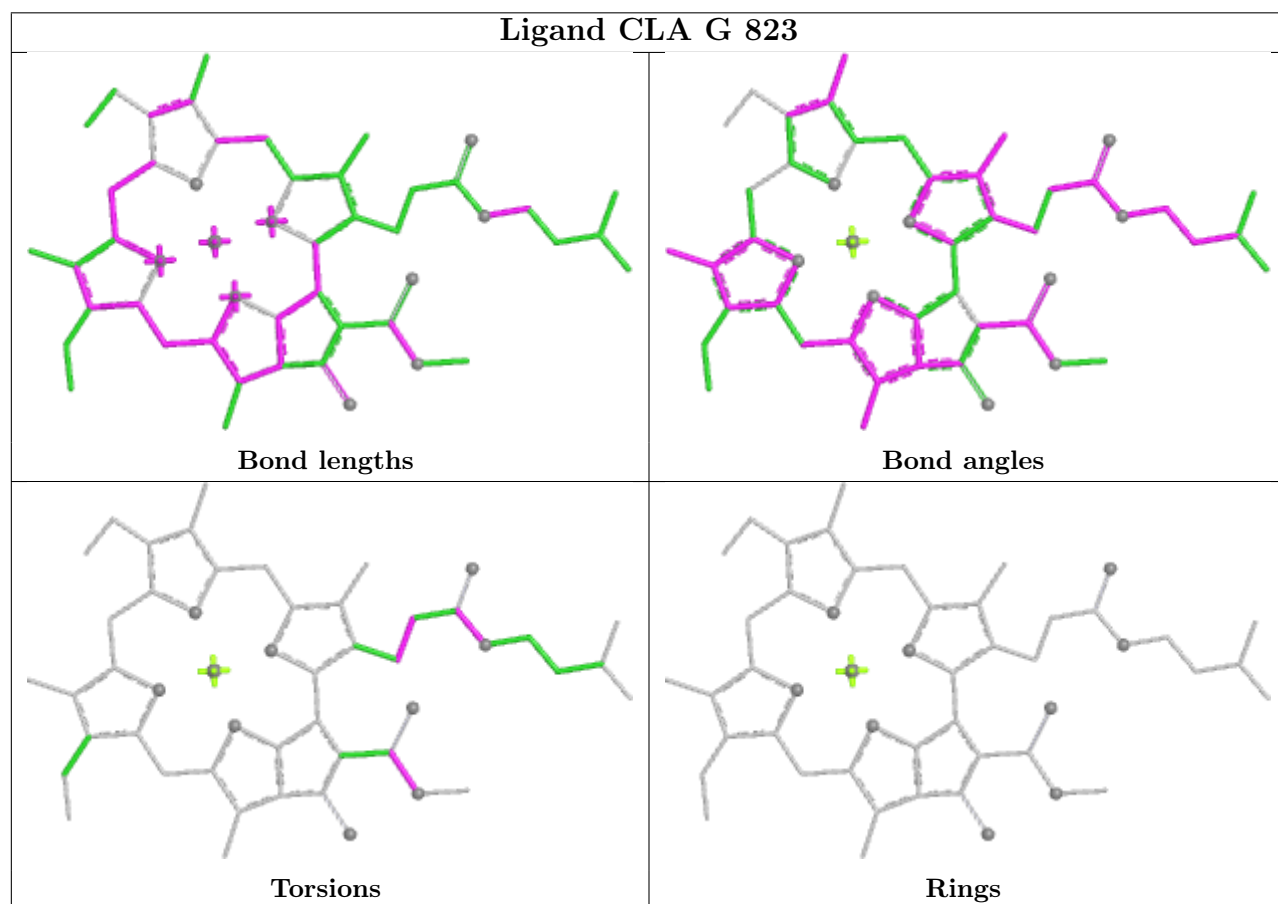
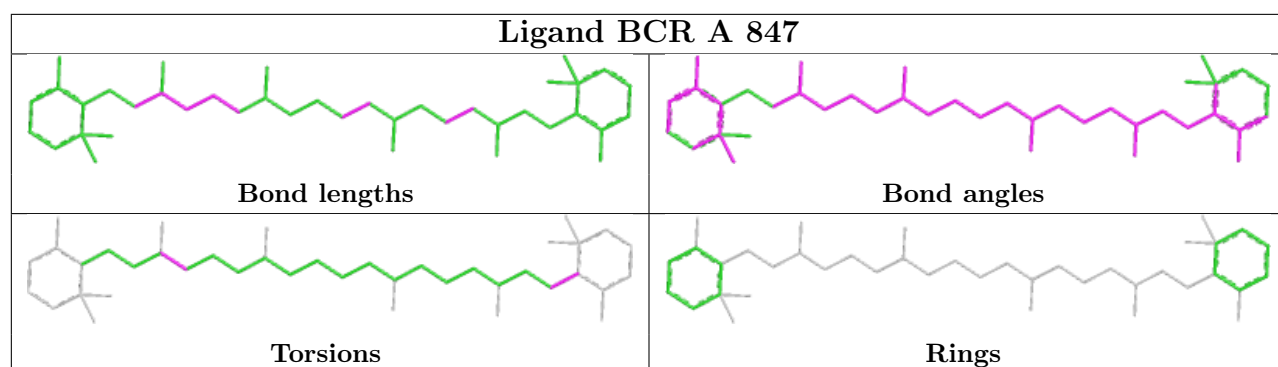
Torsions

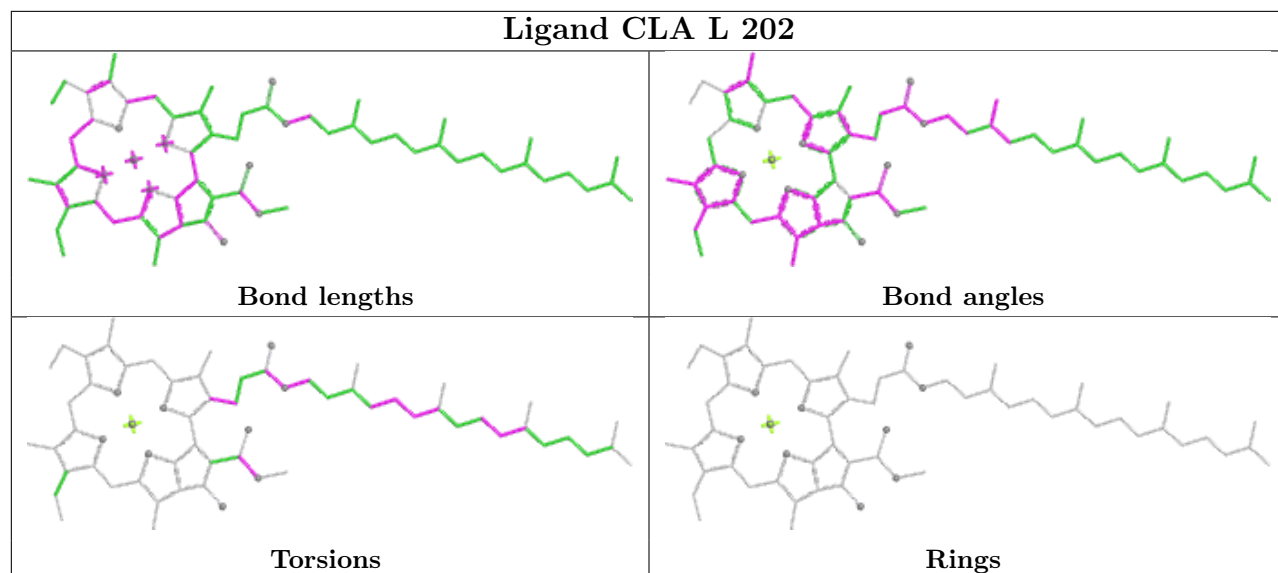
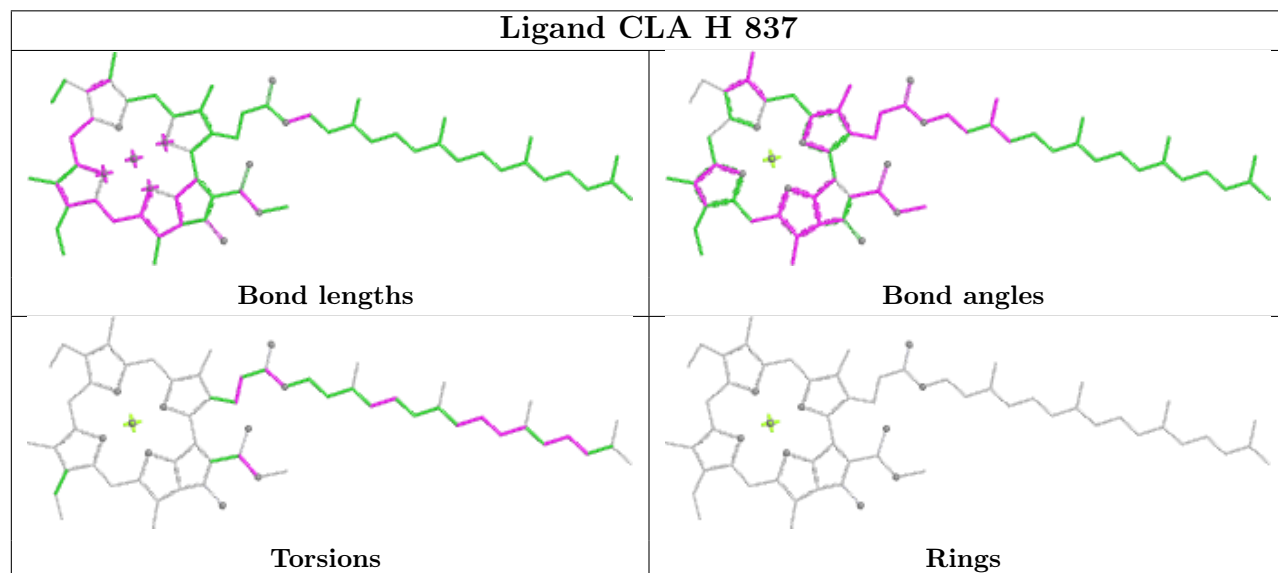
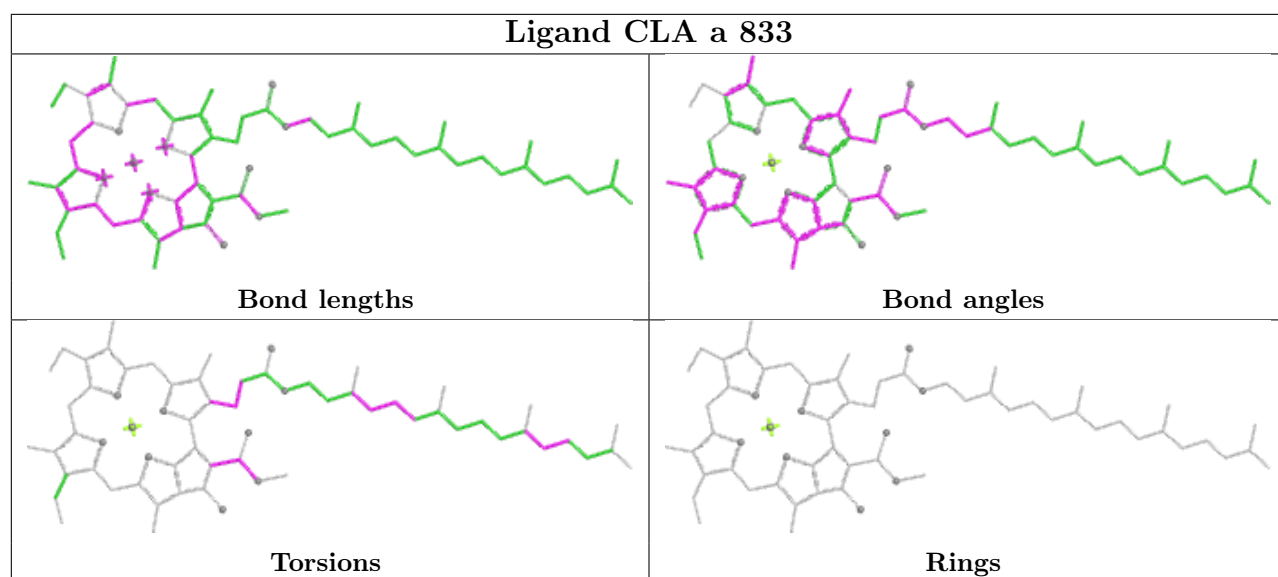


Rings

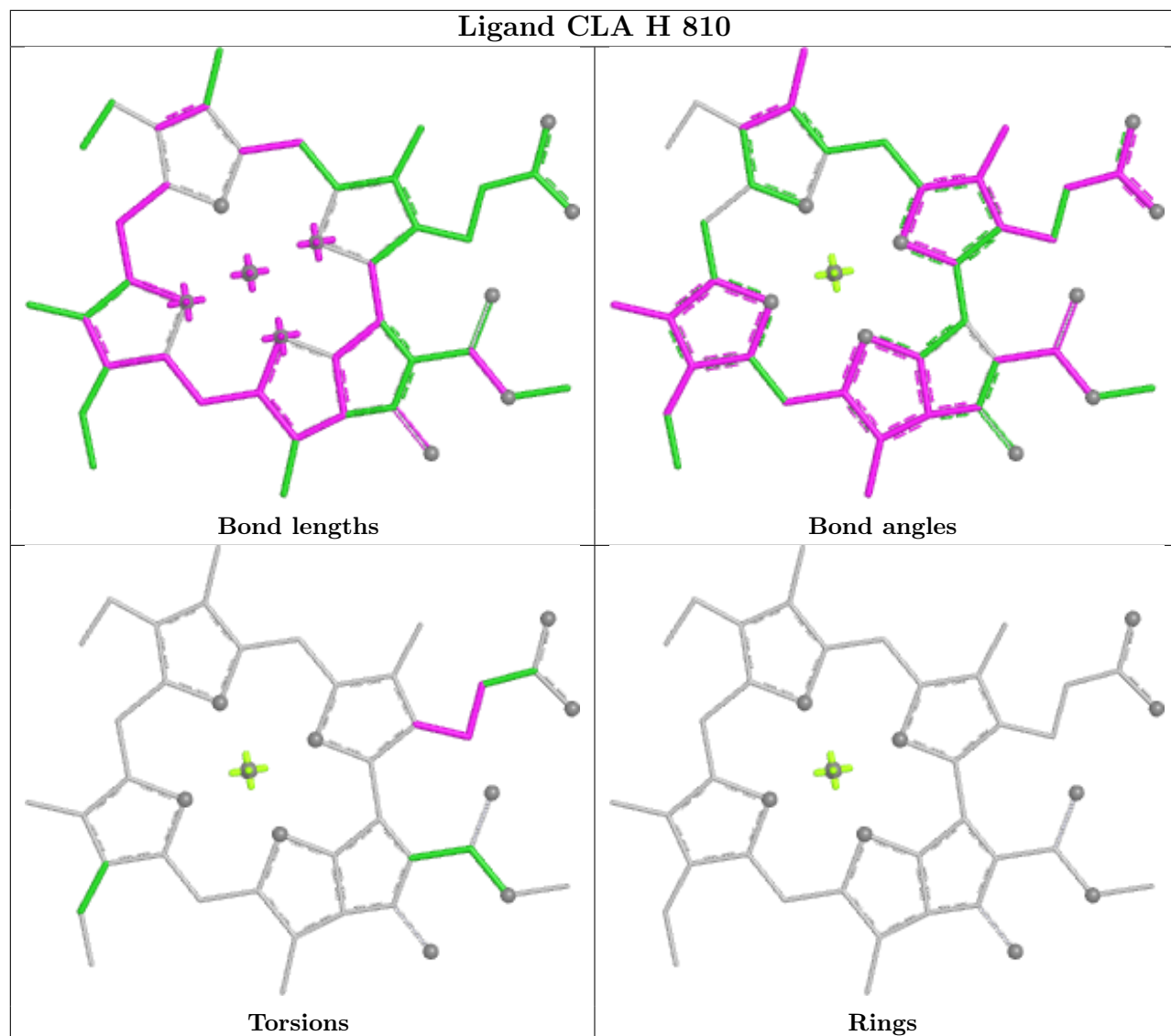




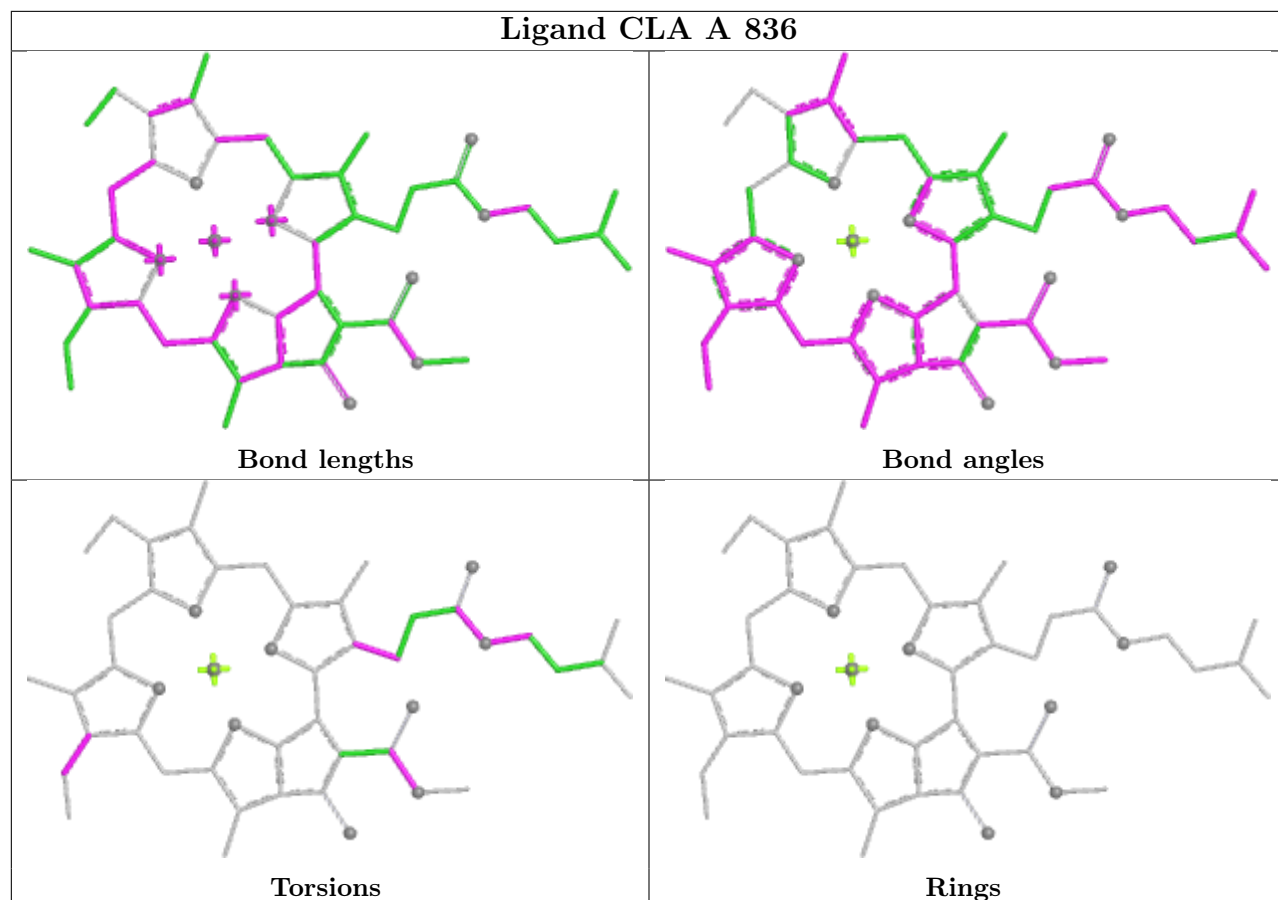




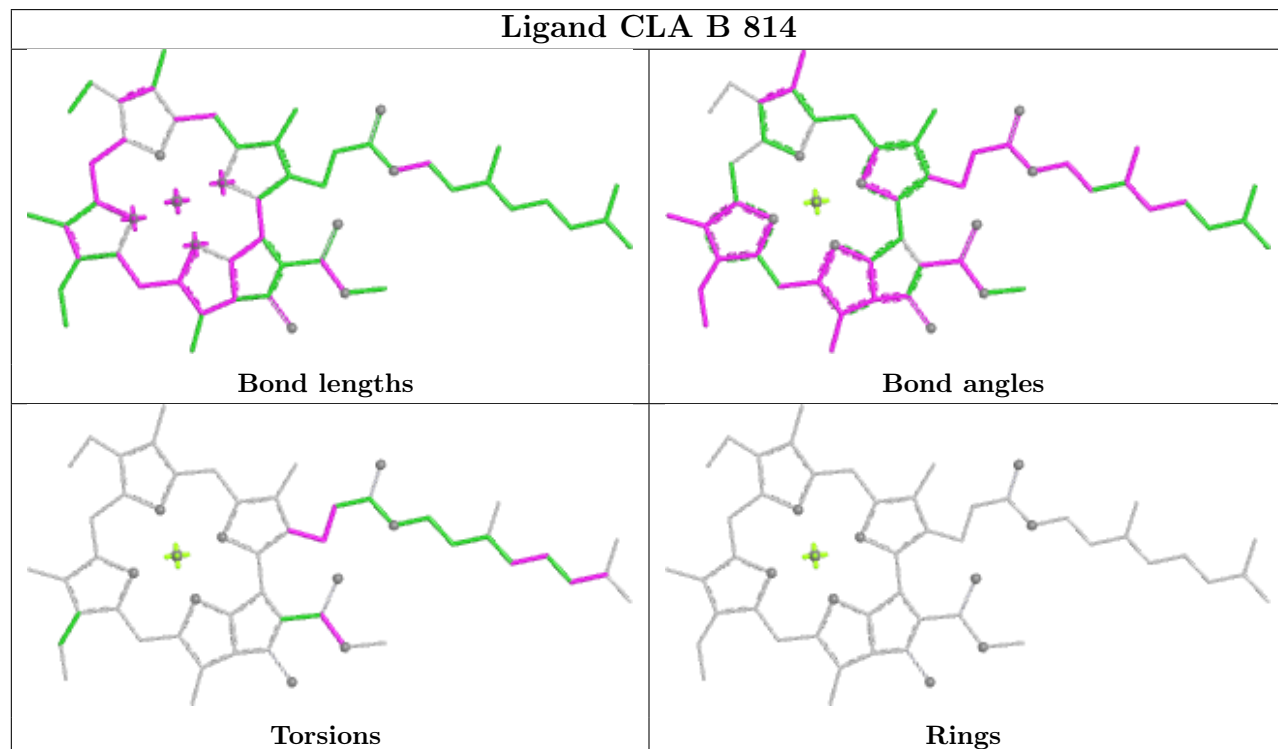
Ligand CLA H 810



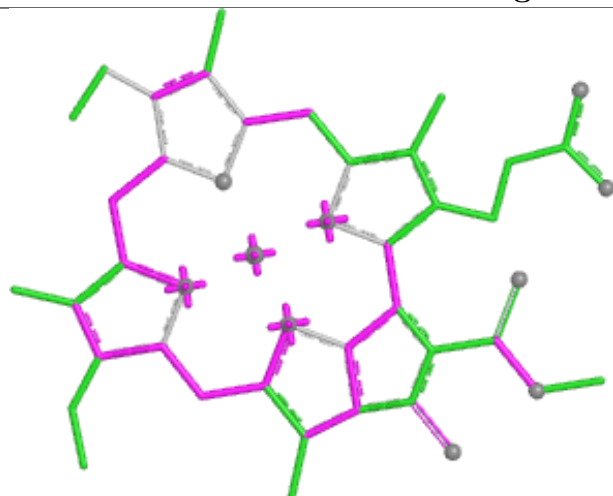
Ligand CLA A 836



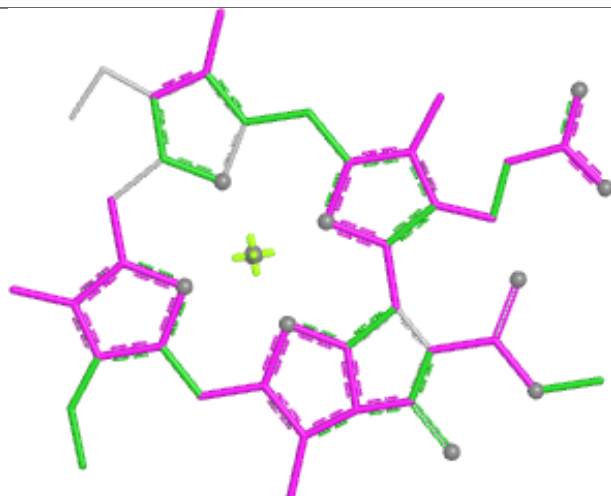
Ligand CLA B 814



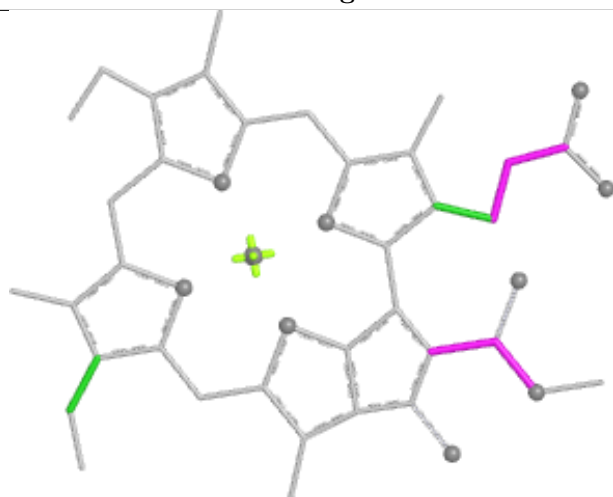
Ligand CLA A 814



Bond lengths



Bond angles

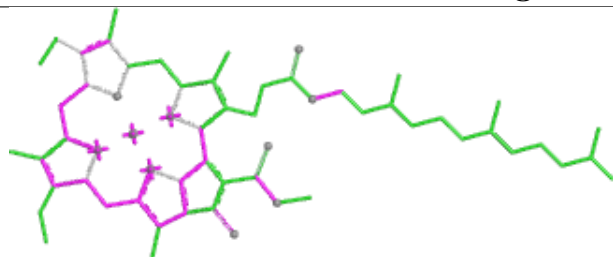


Torsions

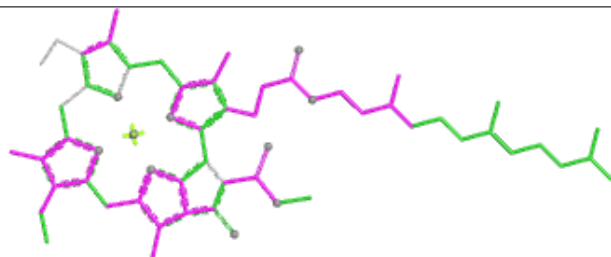


Rings

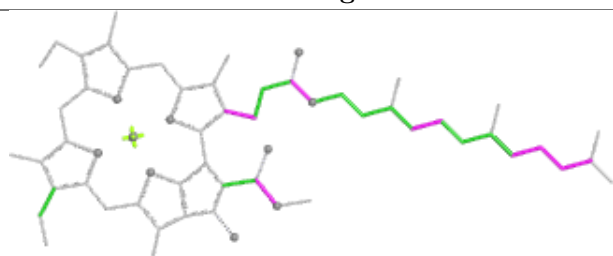
Ligand CLA B 815



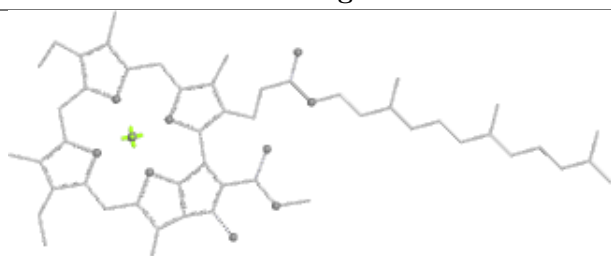
Bond lengths



Bond angles

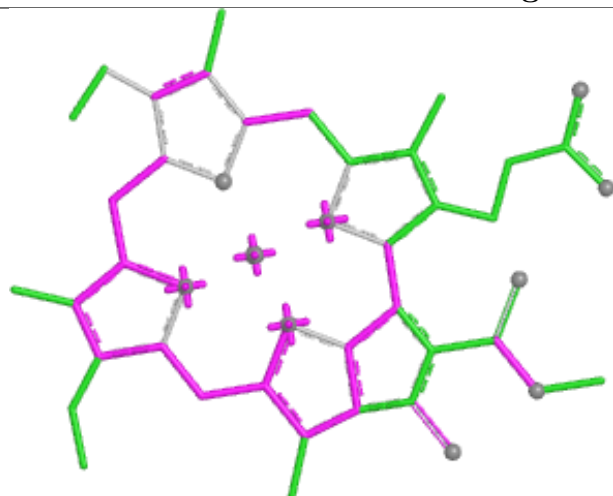


Torsions

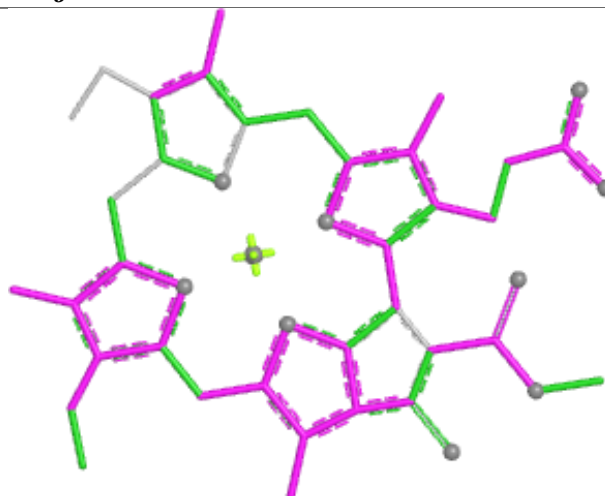


Rings

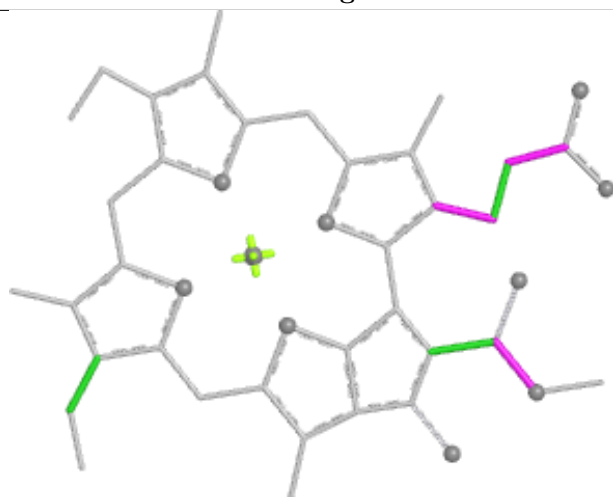
Ligand CLA j 104



Bond lengths



Bond angles

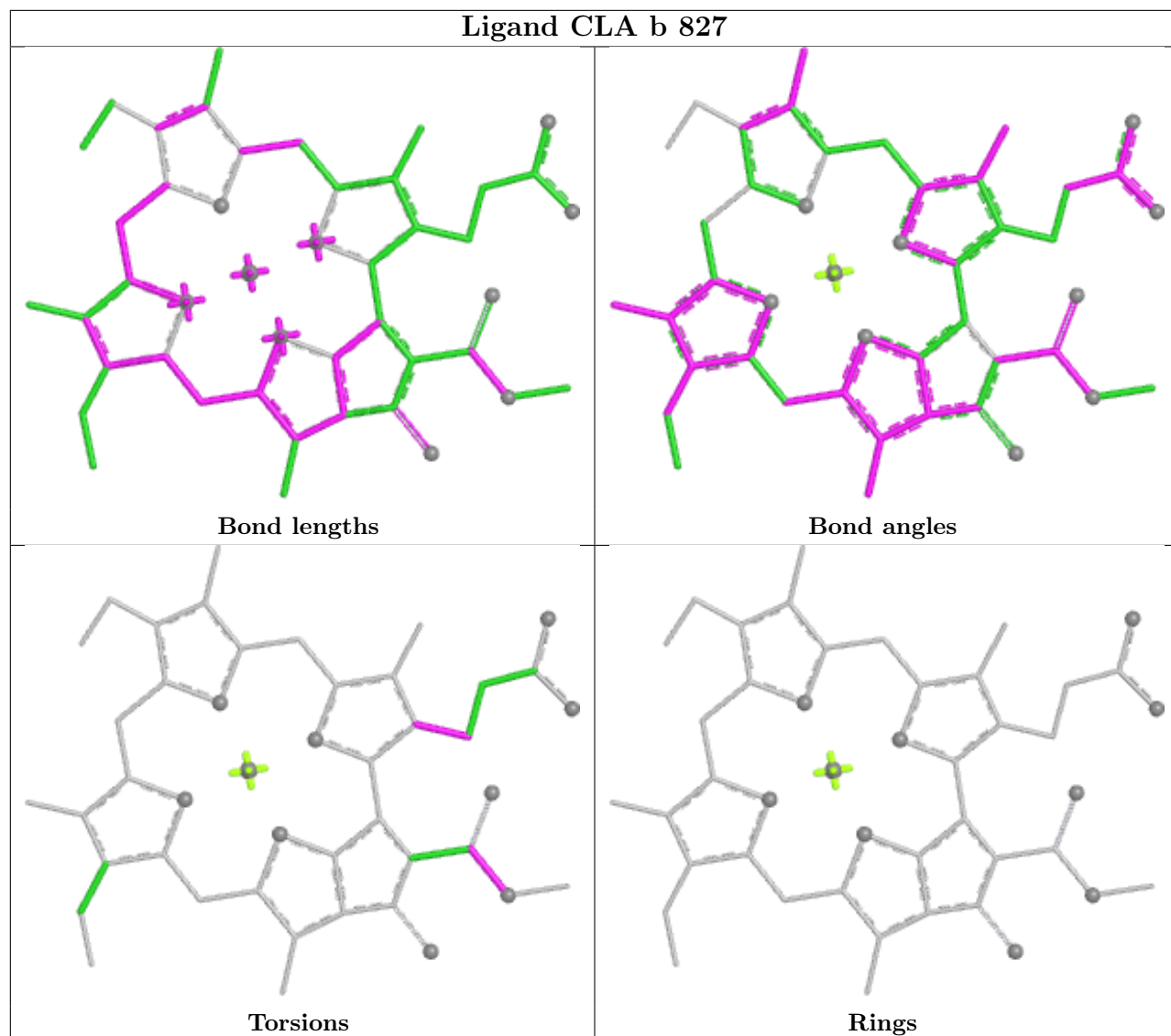


Torsions

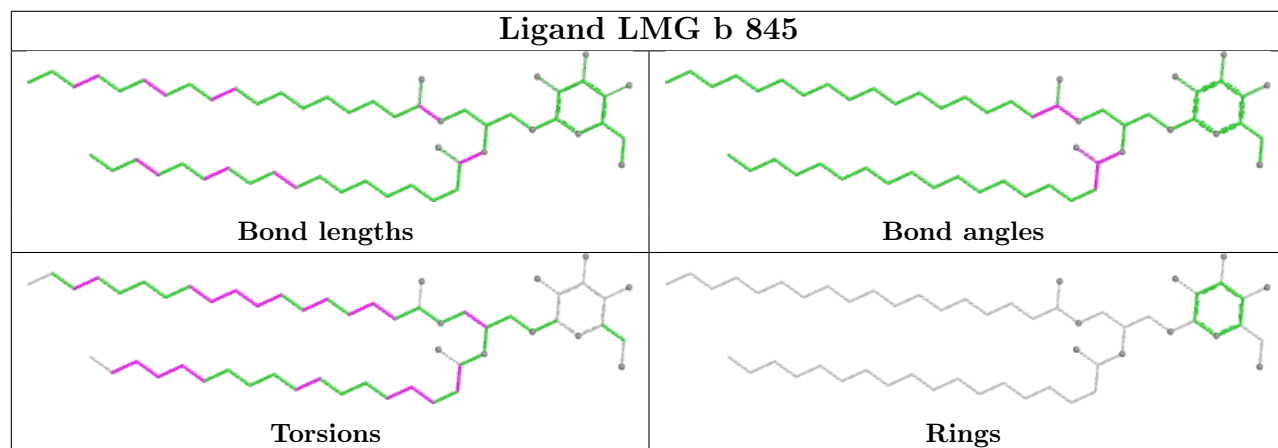


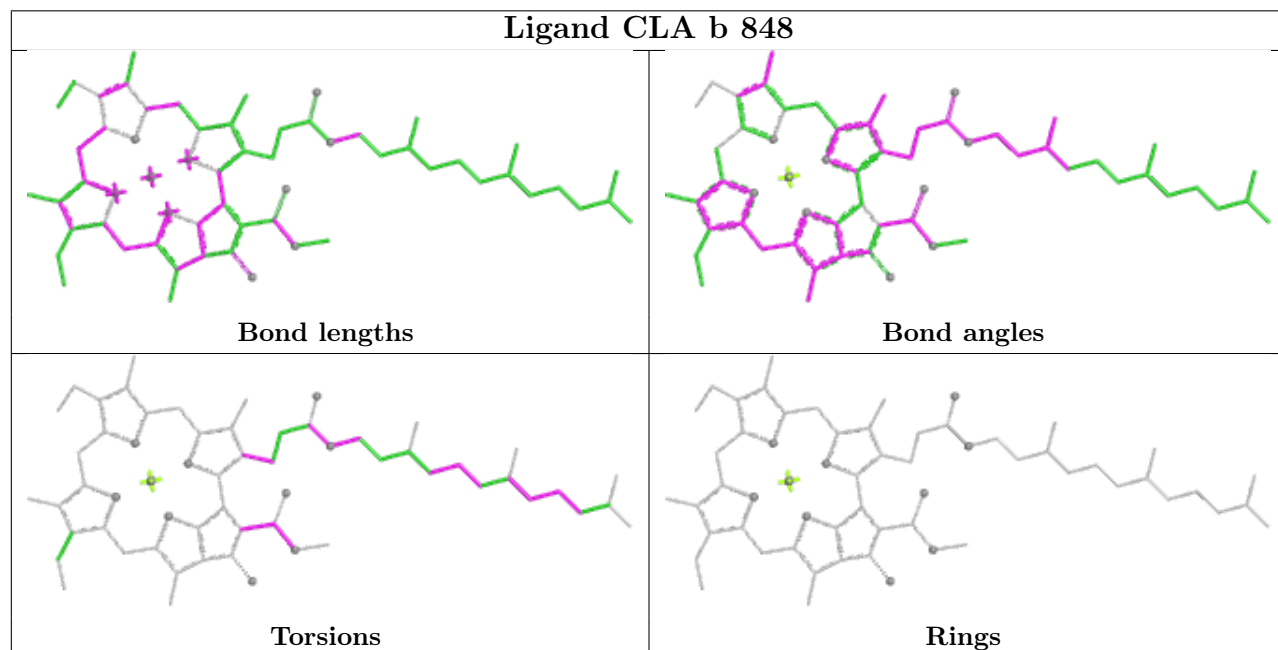
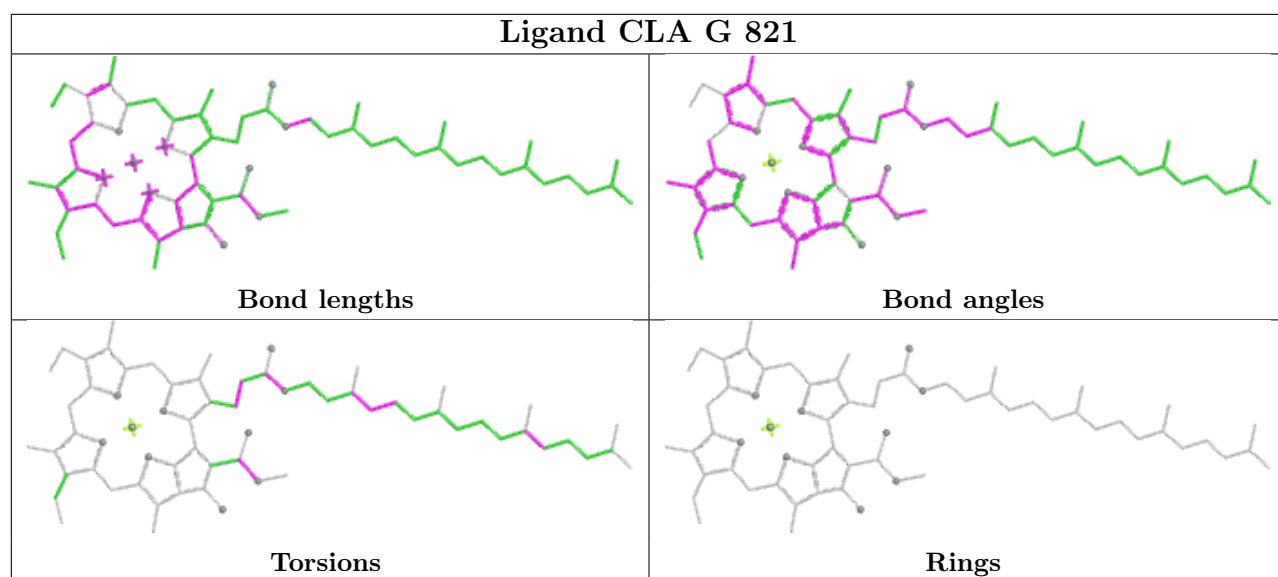
Rings

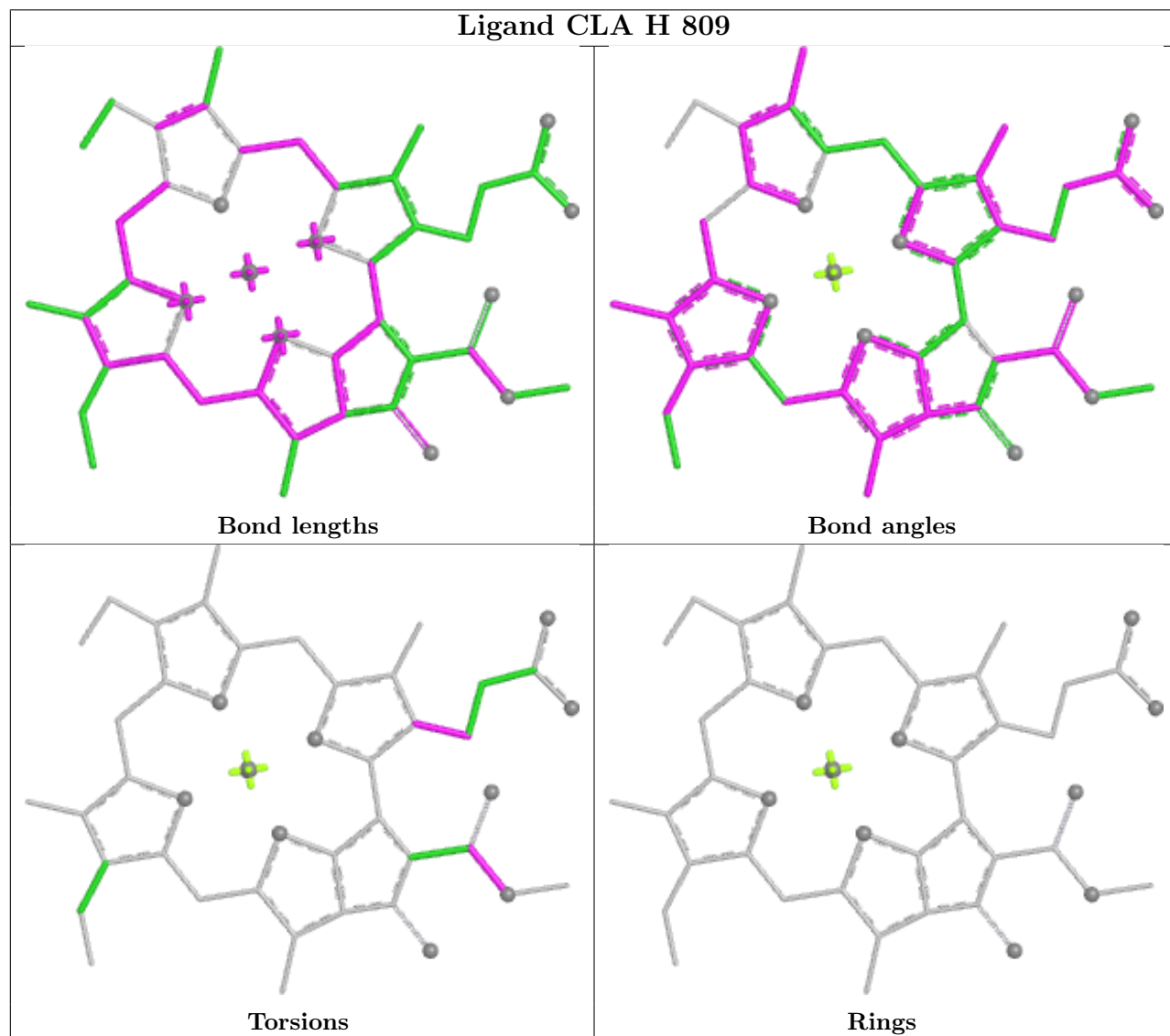
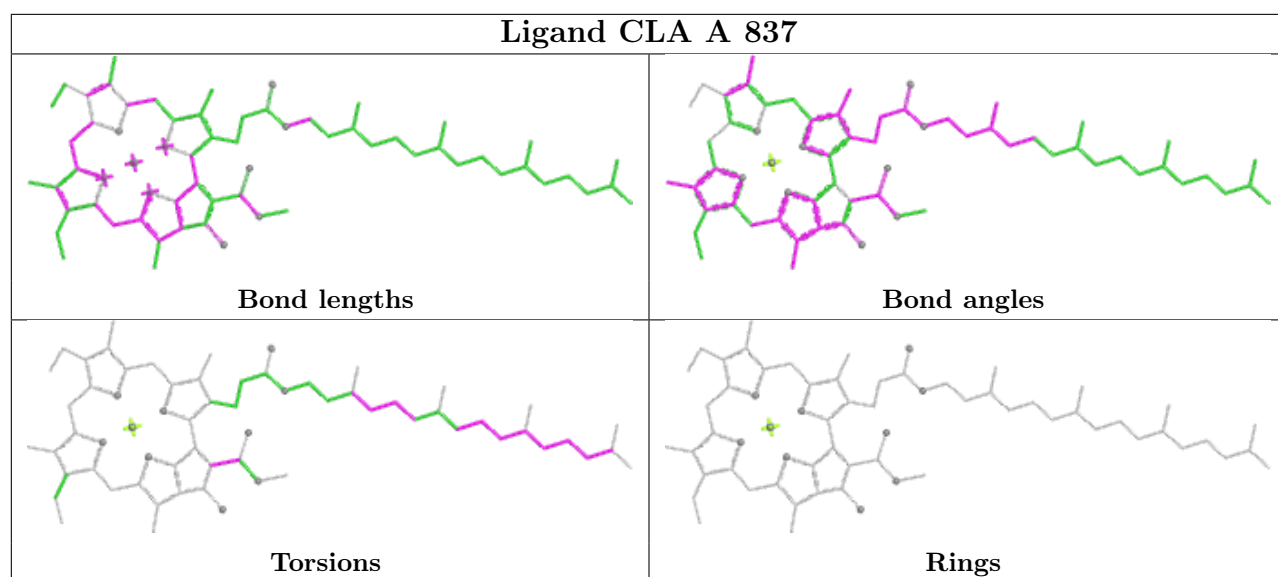
Ligand CLA b 827



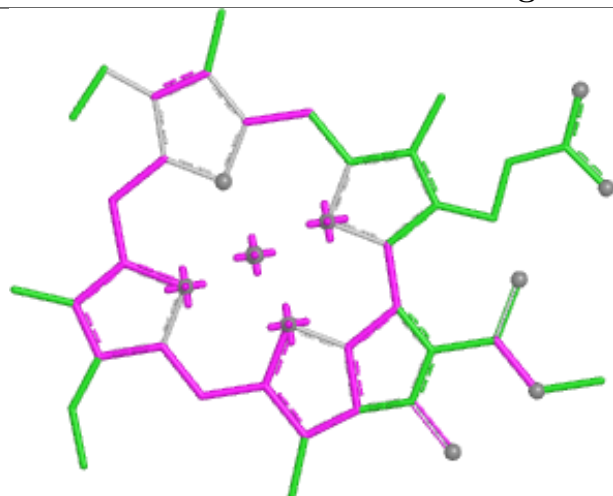
Ligand LMG b 845



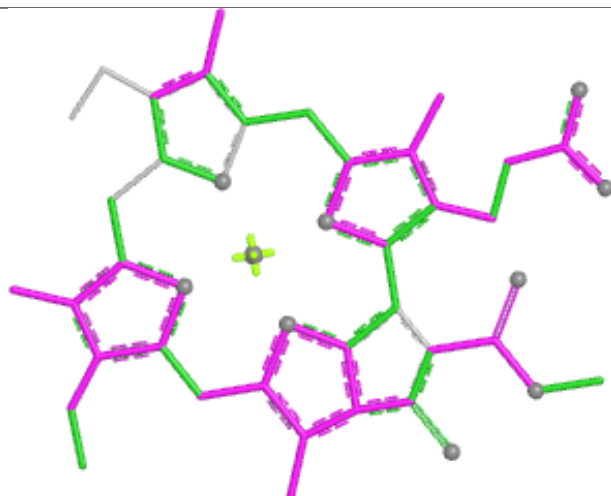




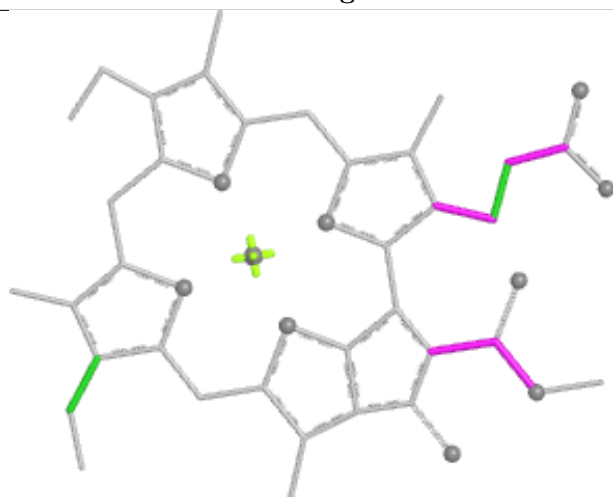
Ligand CLA J 103



Bond lengths



Bond angles

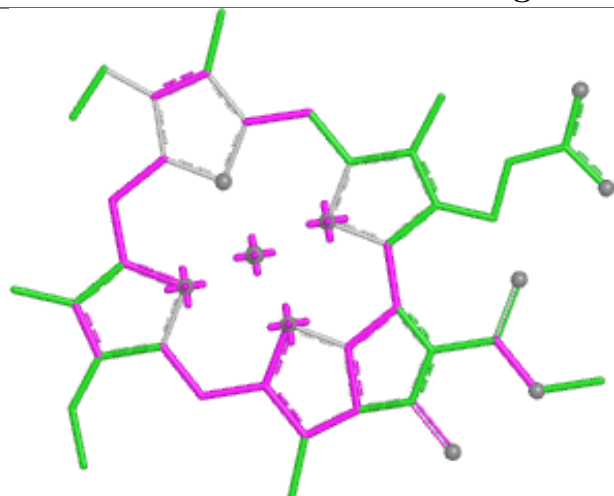


Torsions

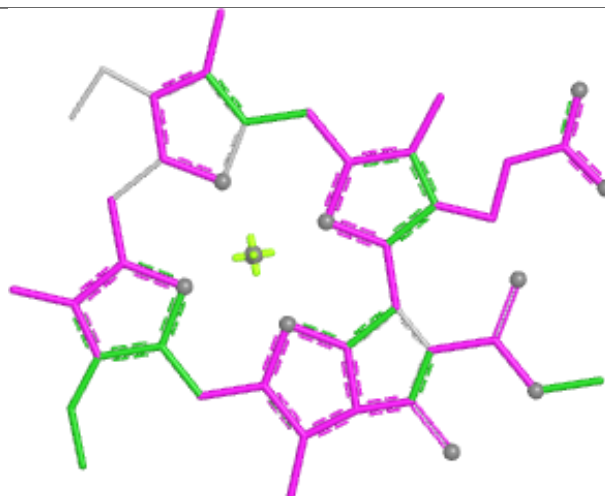


Rings

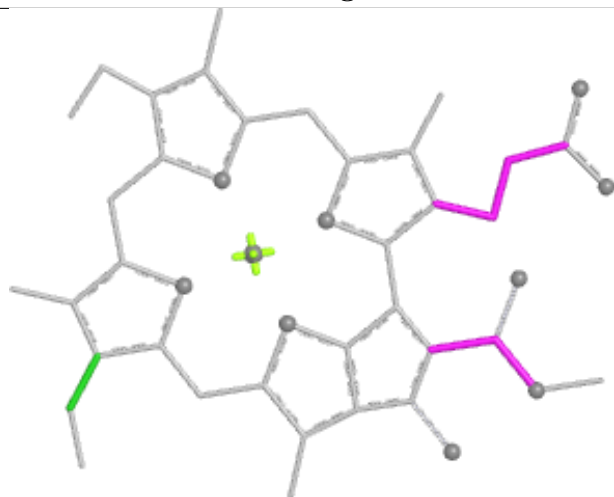
Ligand CLA H 813



Bond lengths



Bond angles

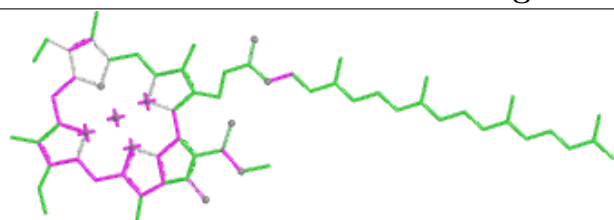


Torsions

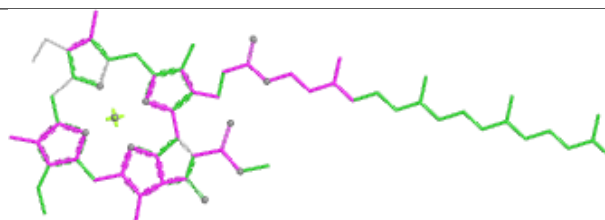


Rings

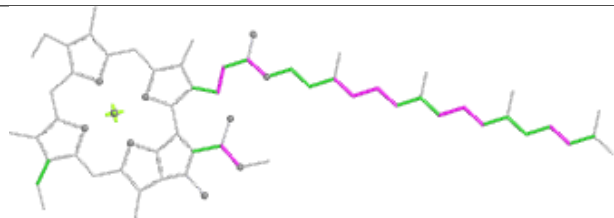
Ligand CLA G 832



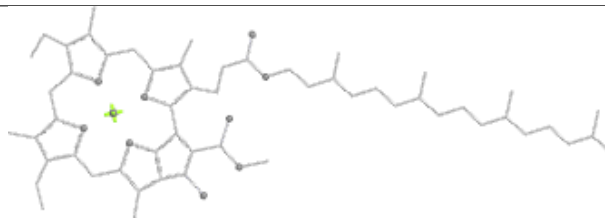
Bond lengths



Bond angles

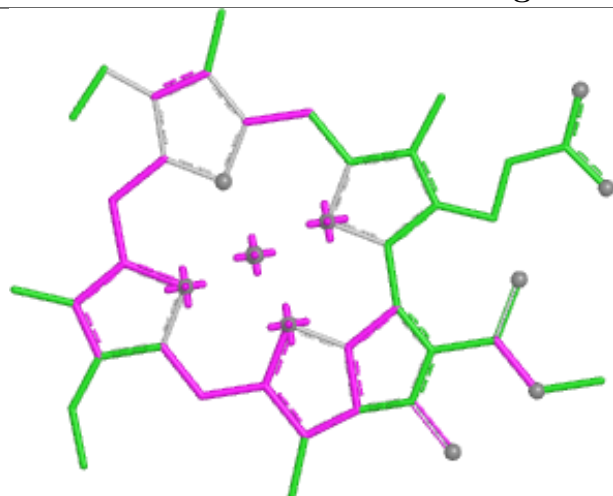


Torsions

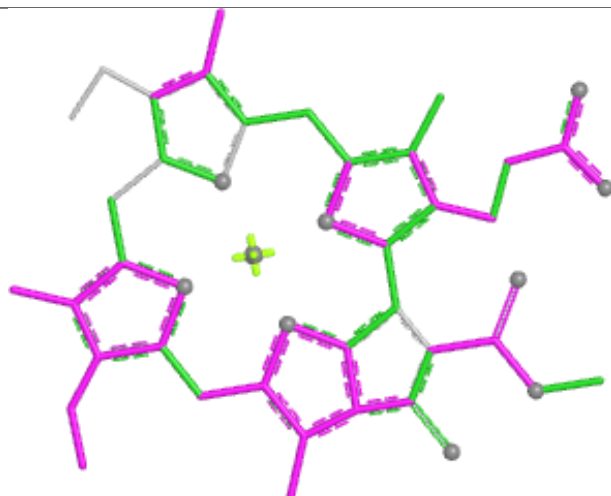


Rings

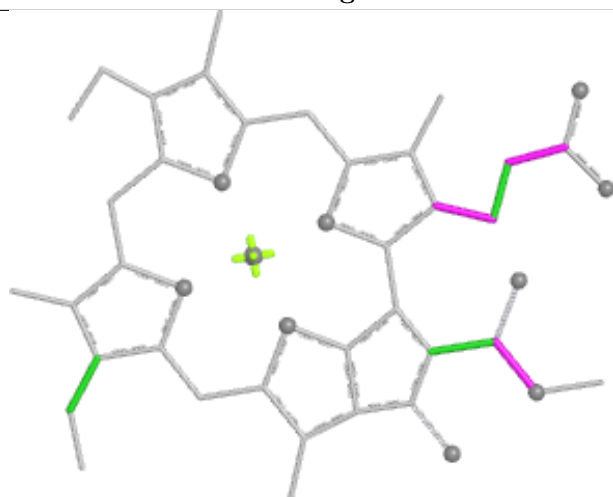
Ligand CLA H 836



Bond lengths



Bond angles

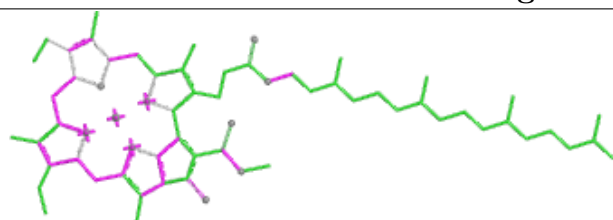


Torsions

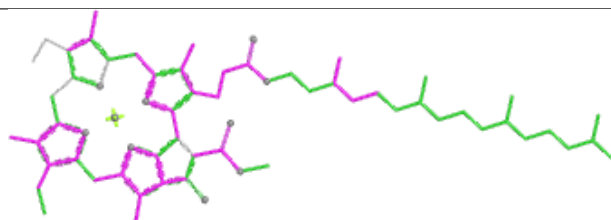


Rings

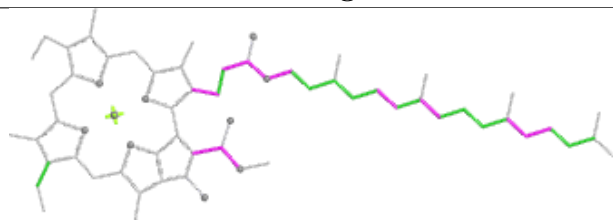
Ligand CLA b 803



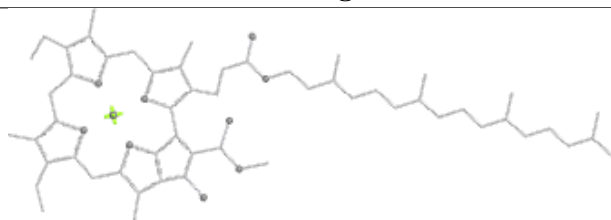
Bond lengths



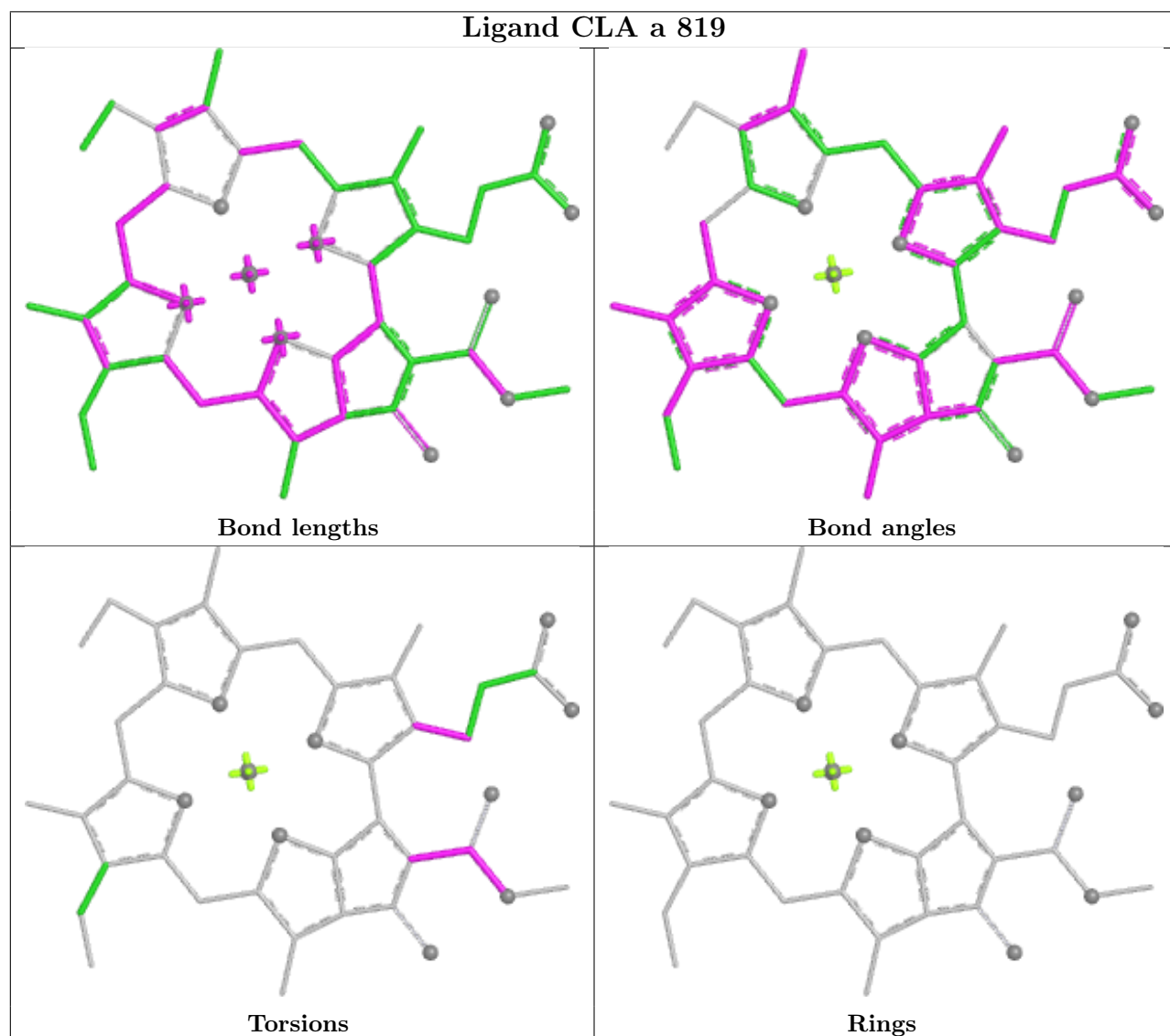
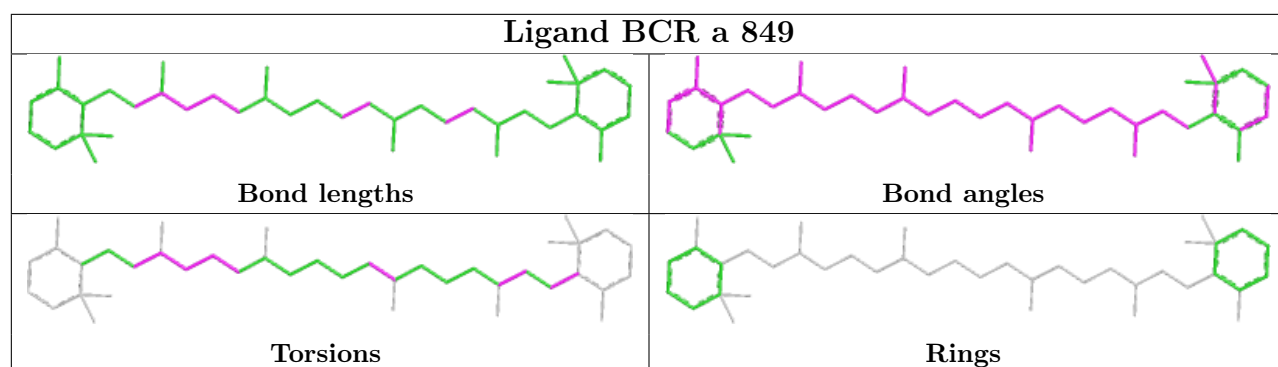
Bond angles

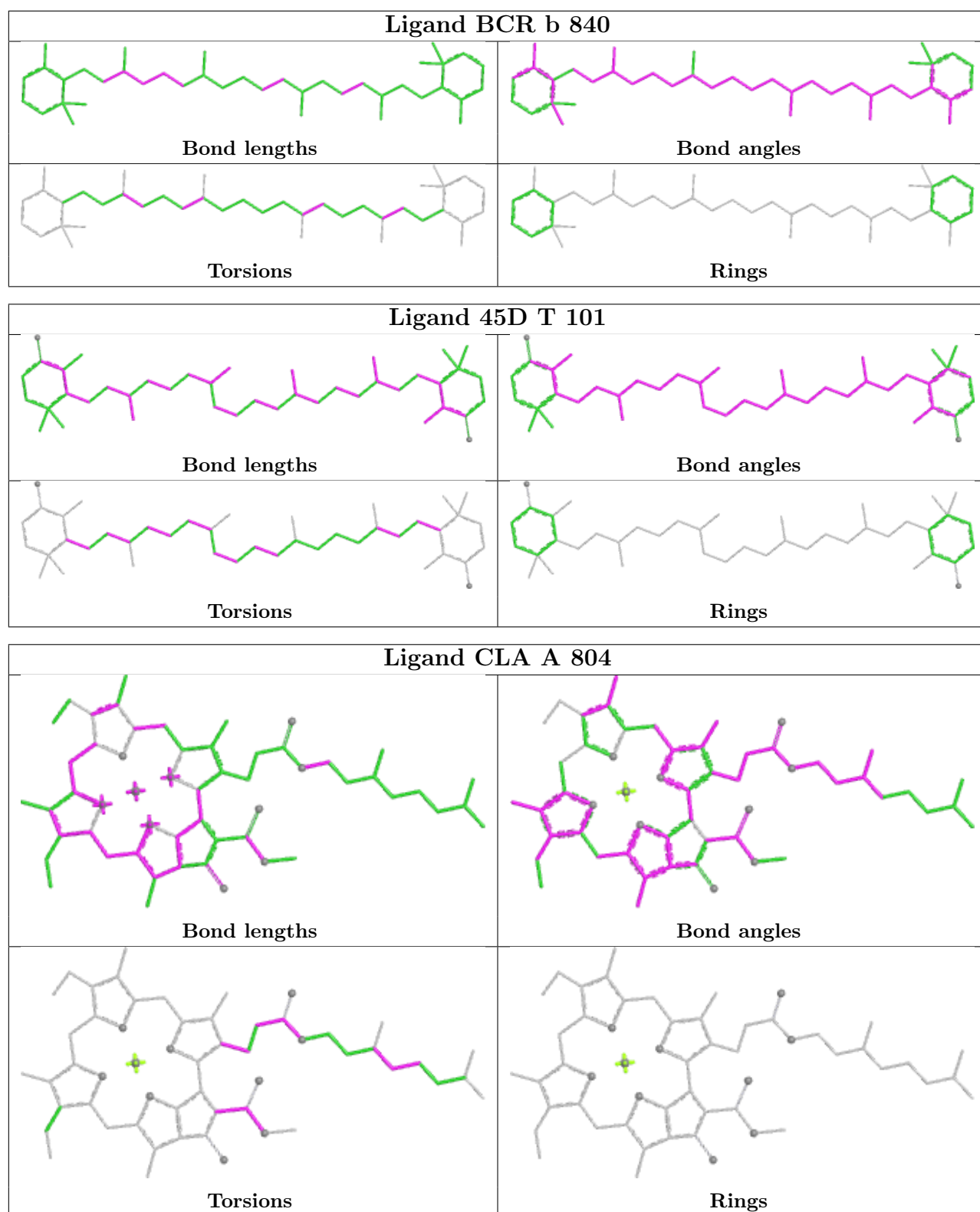


Torsions

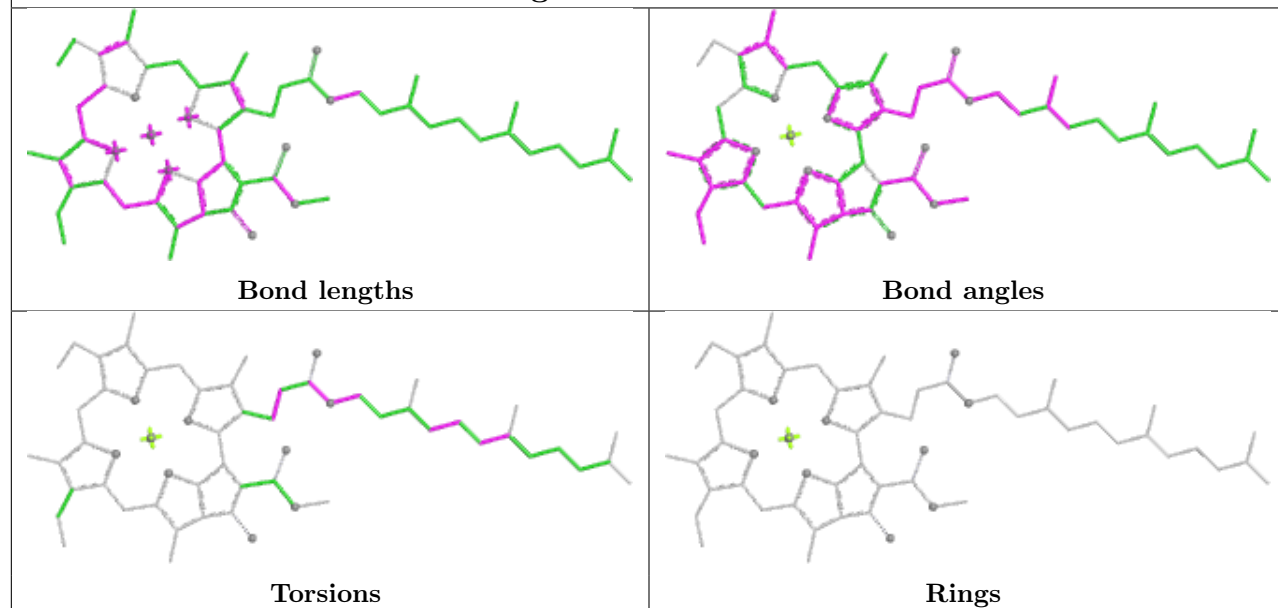


Rings

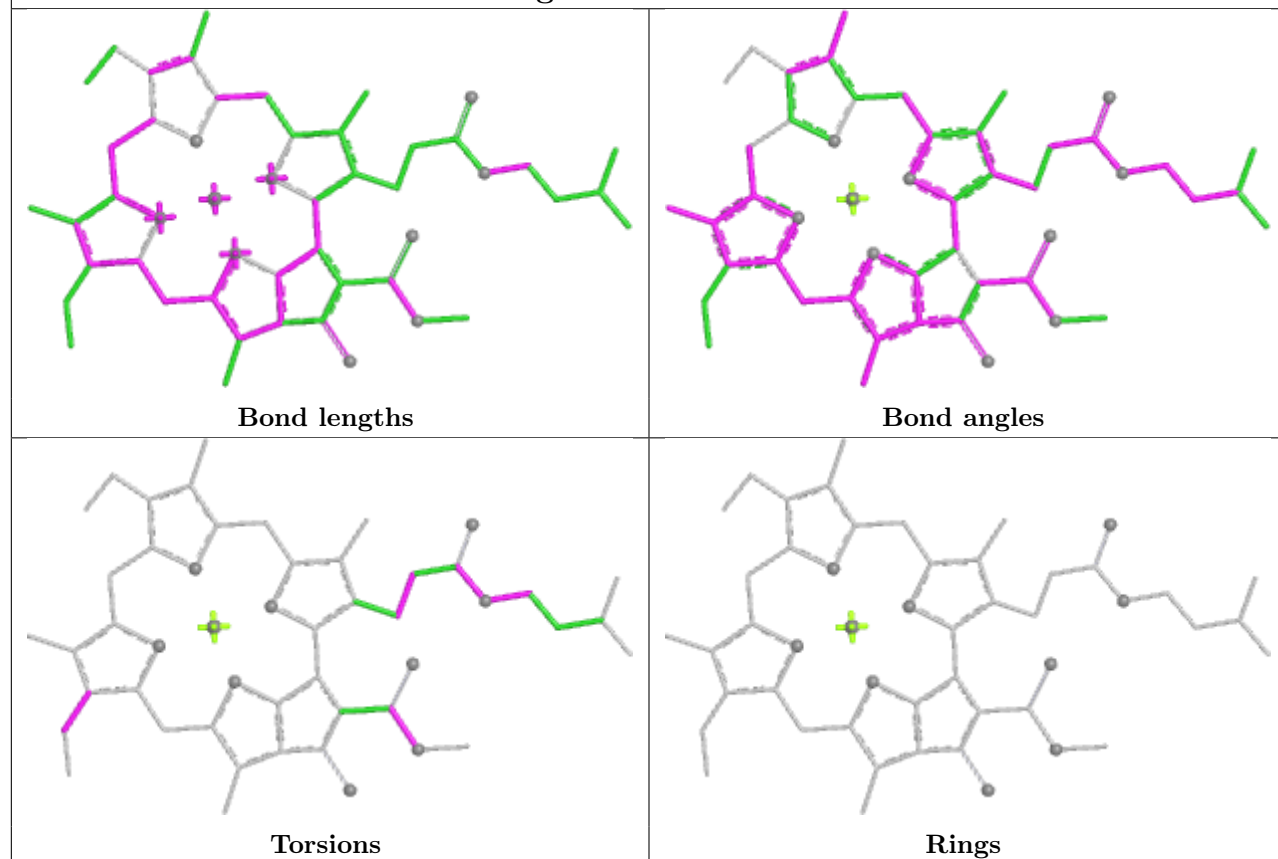




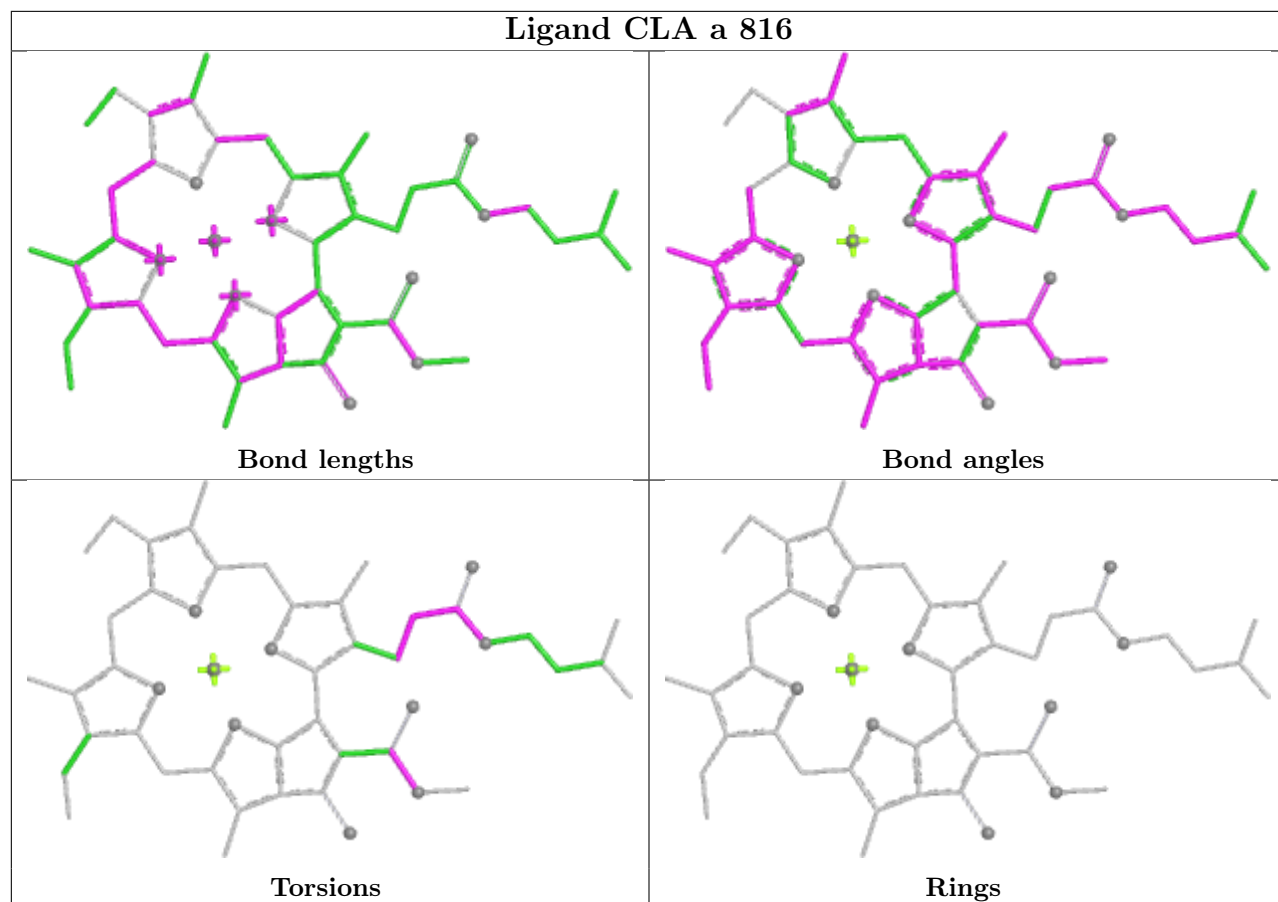
Ligand CLA G 802



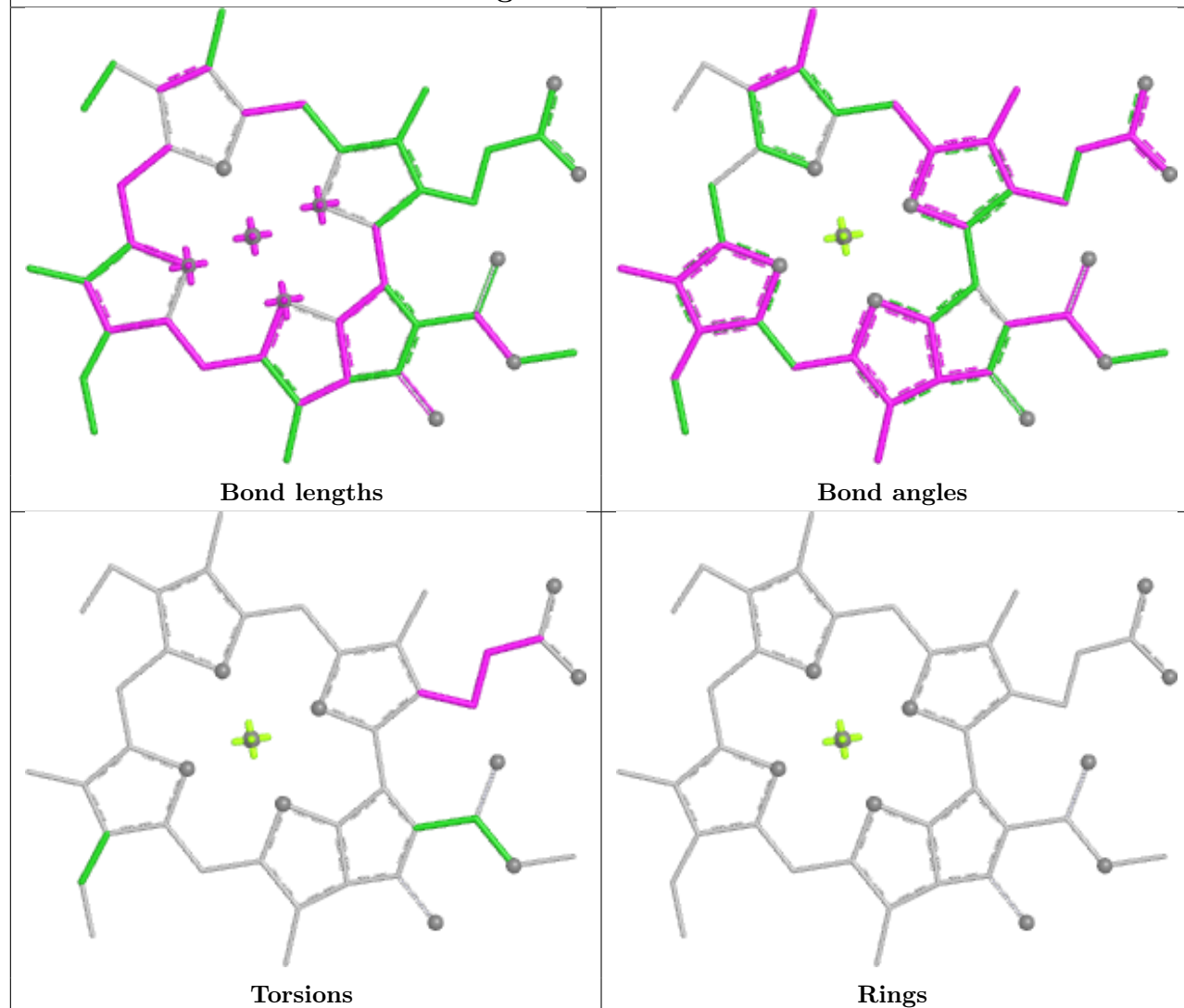
Ligand CLA a 812



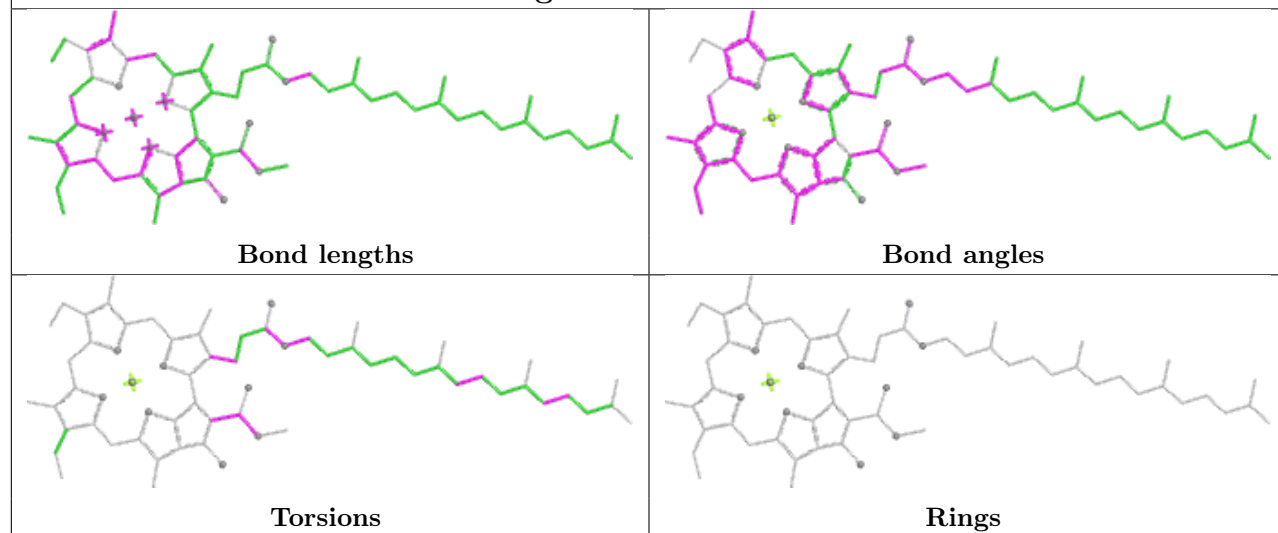
Ligand CLA a 816

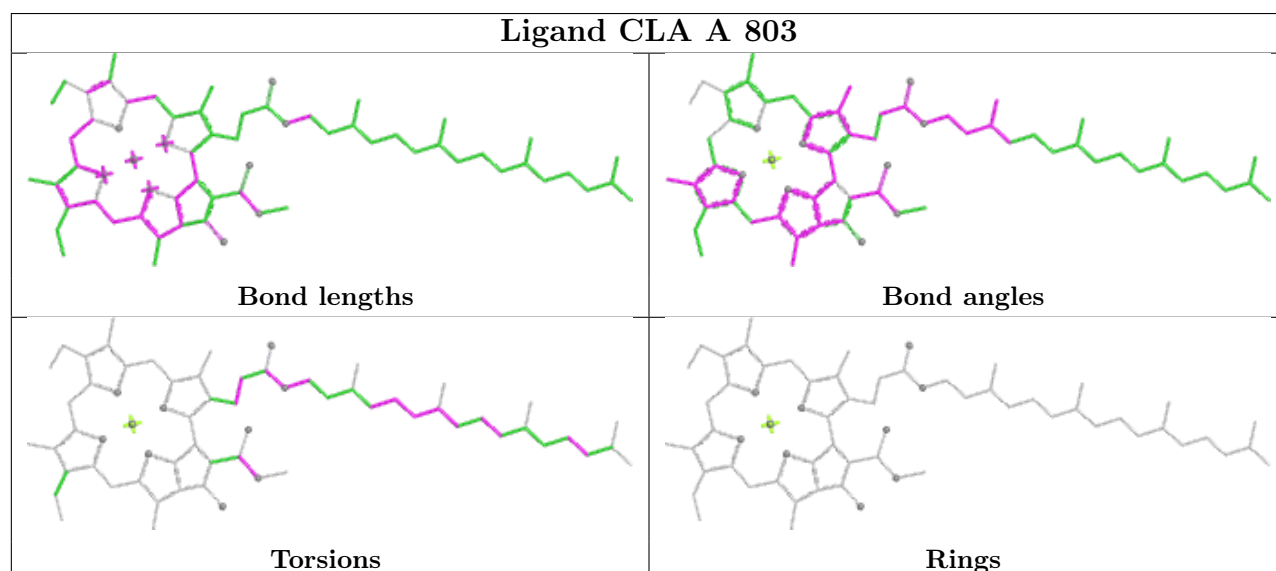
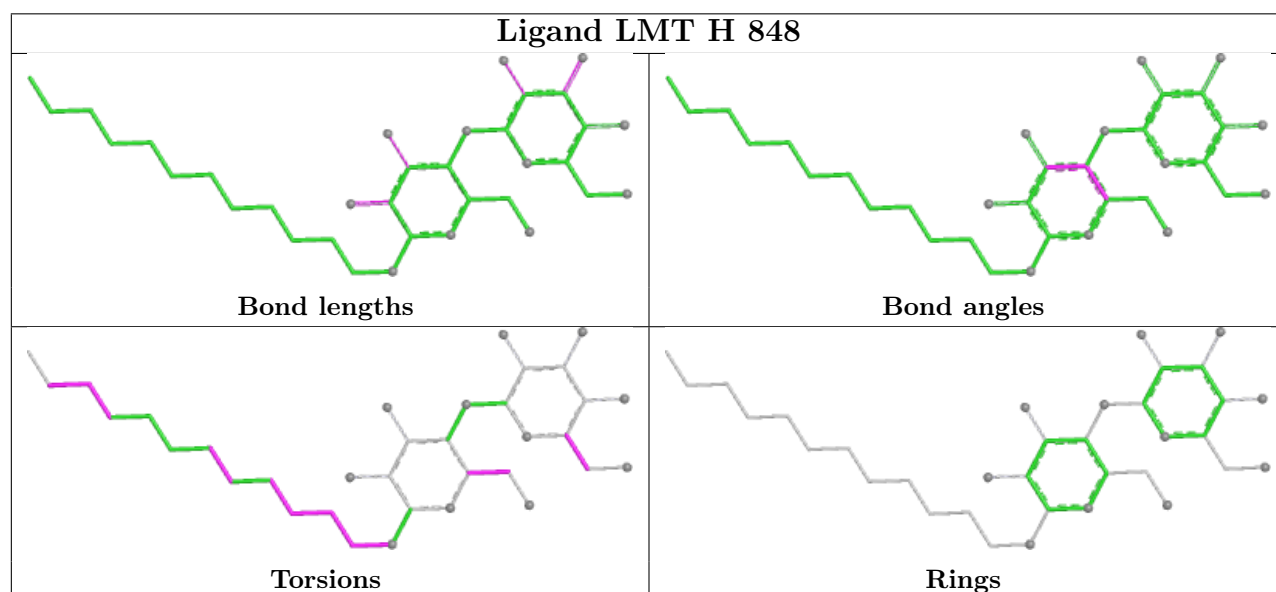
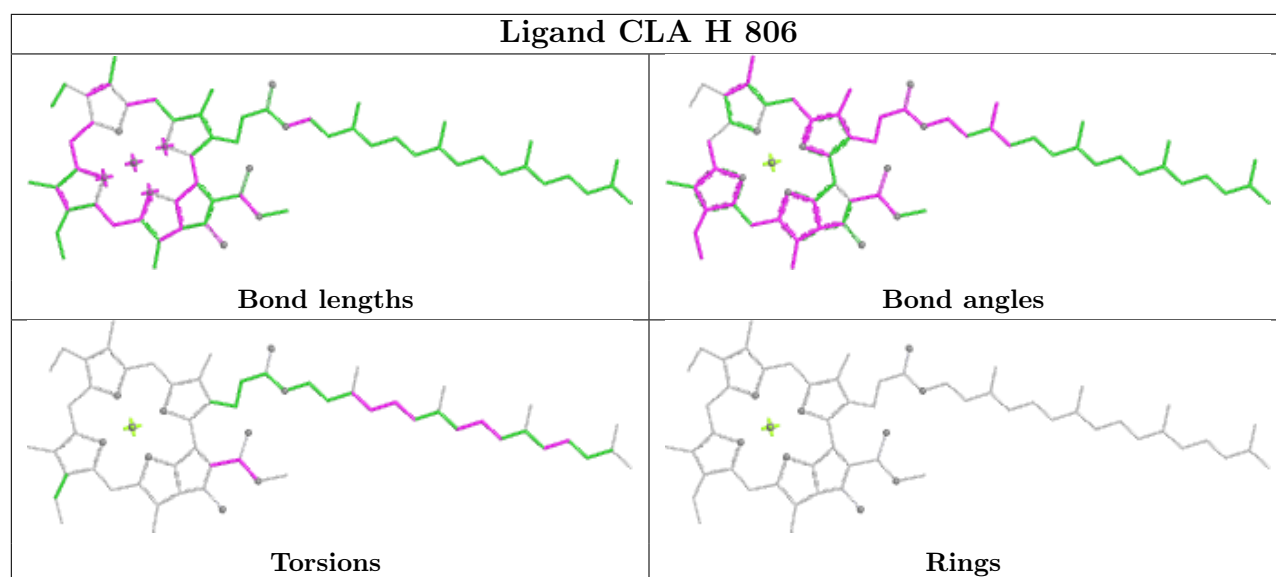


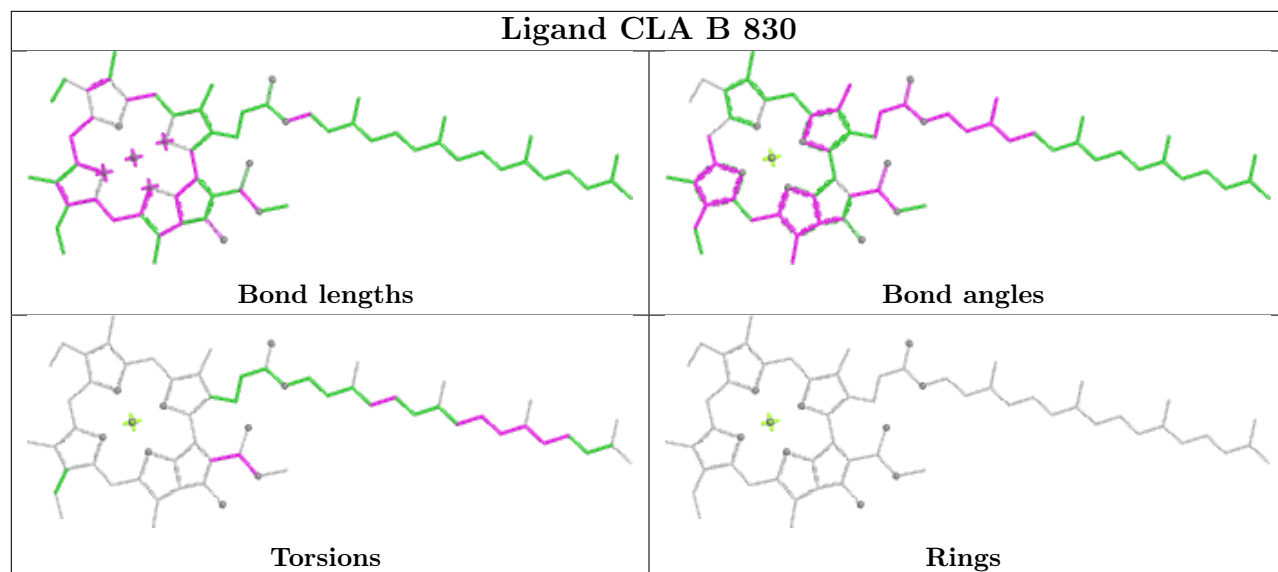
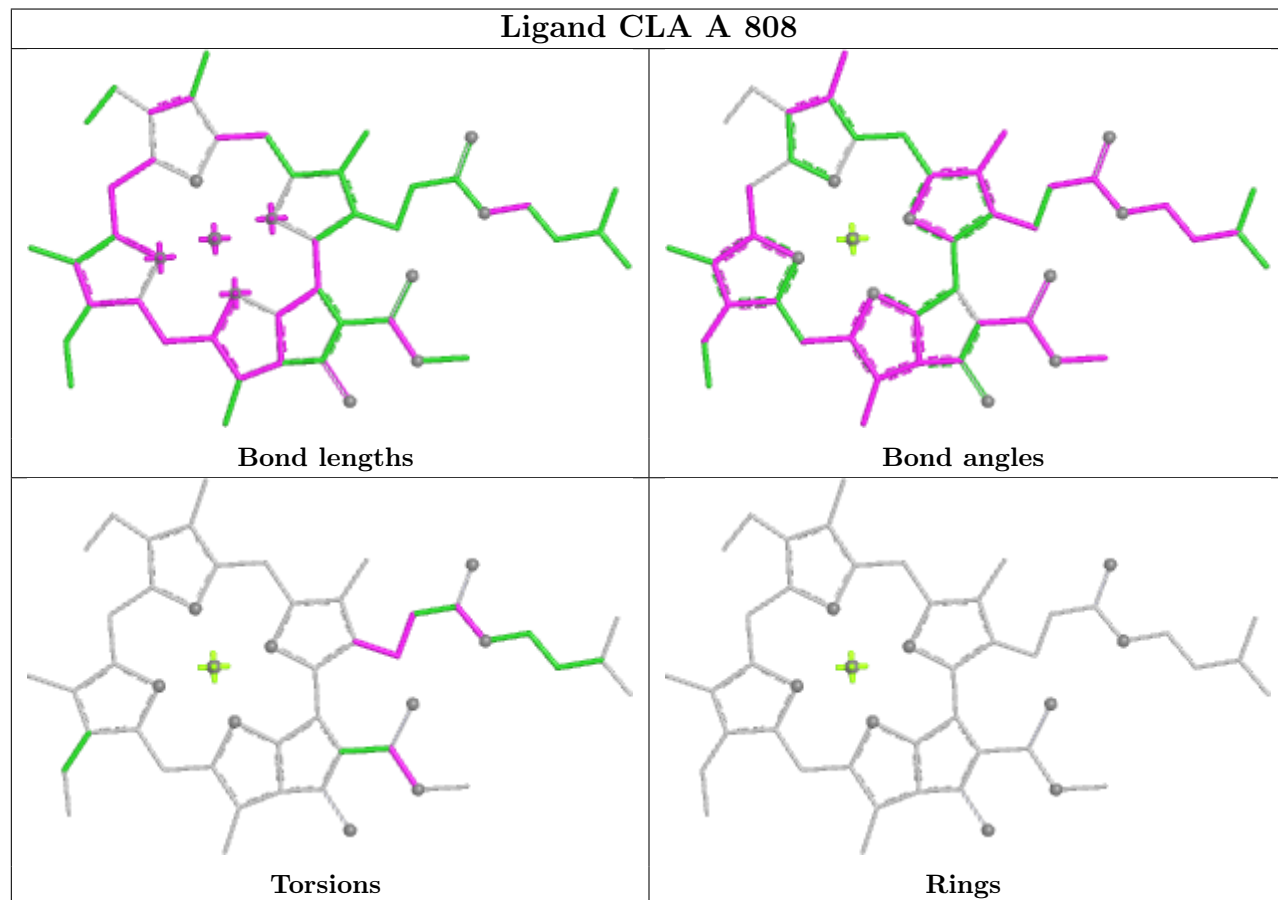
Ligand CLA a 811

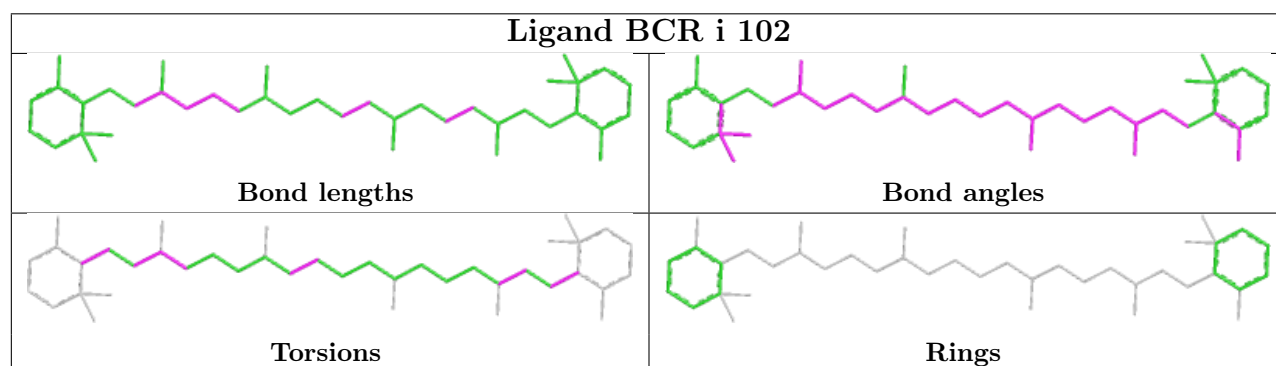
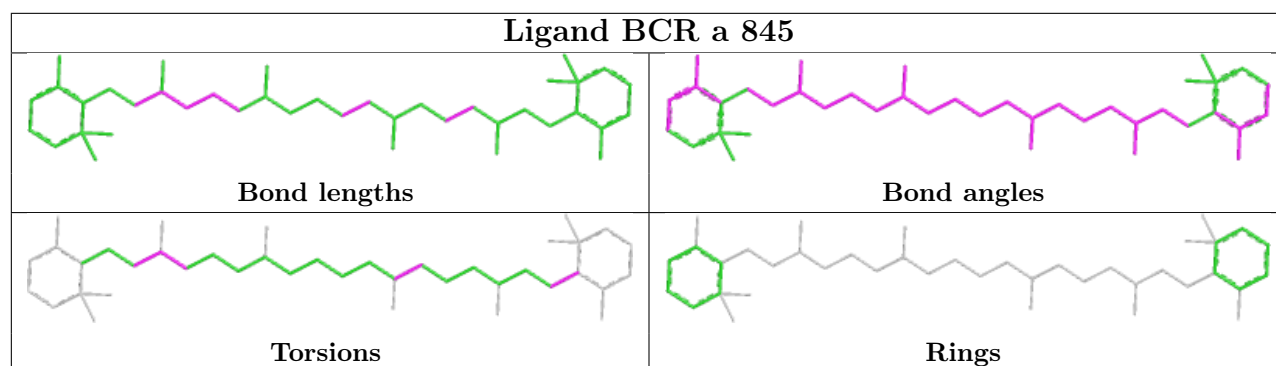
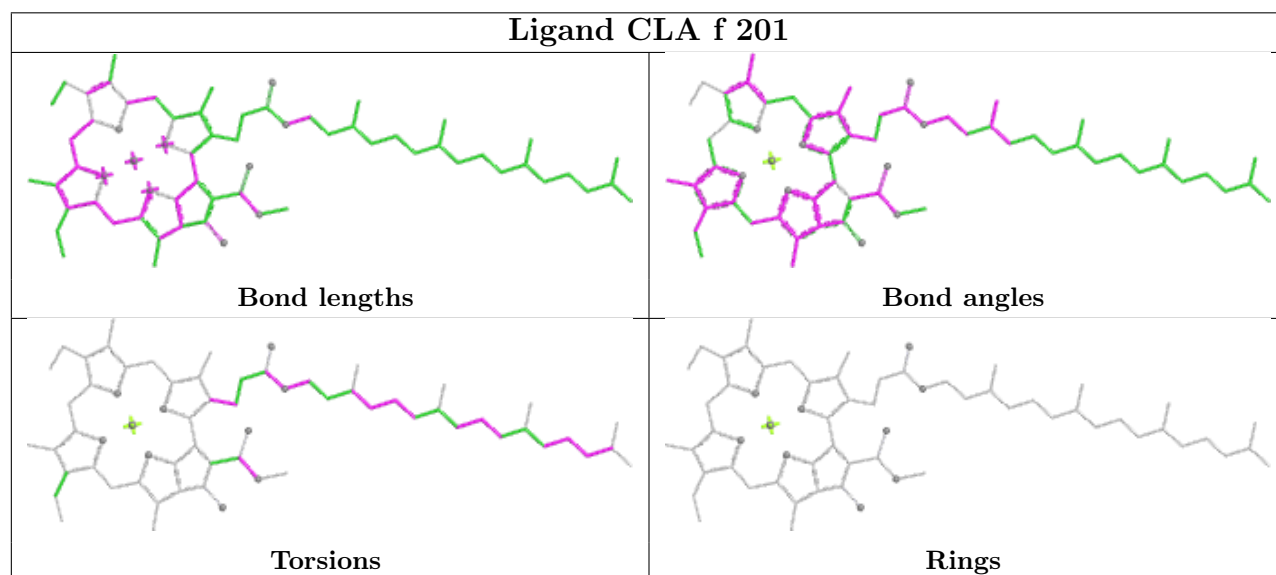
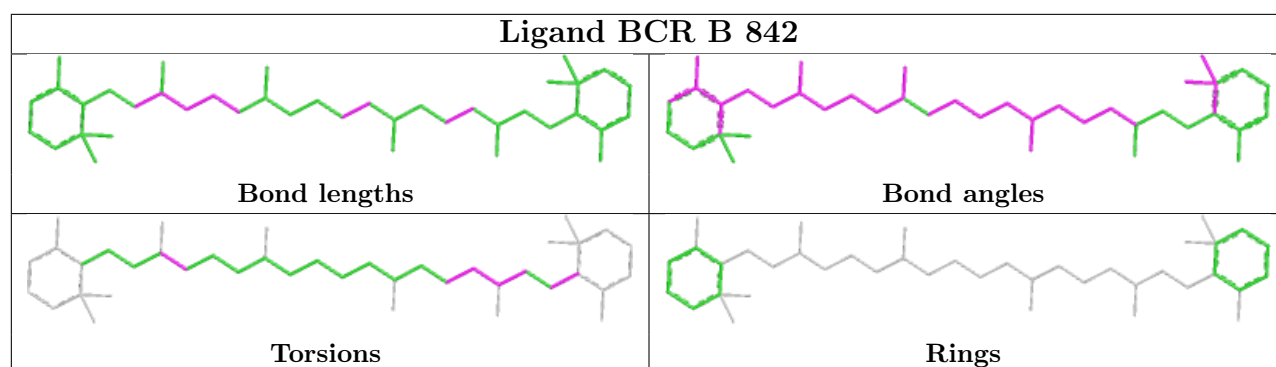


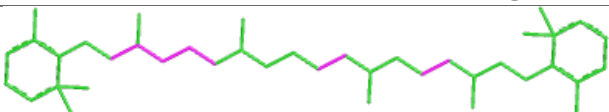
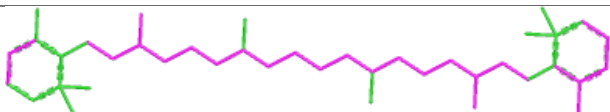
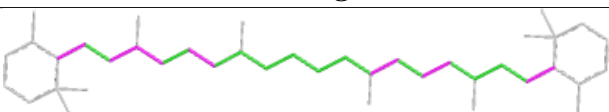
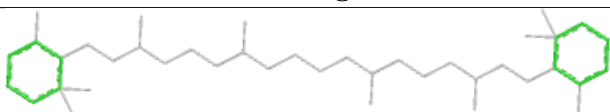
Ligand CLA b 826

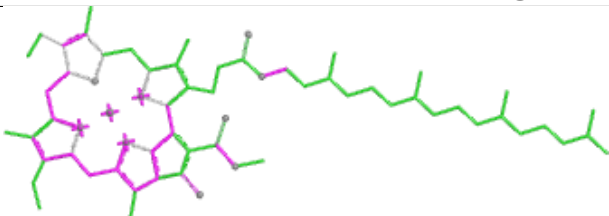
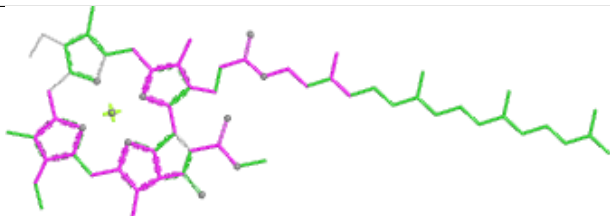
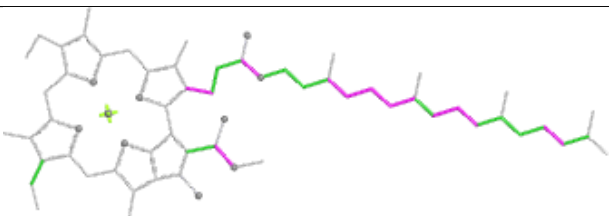
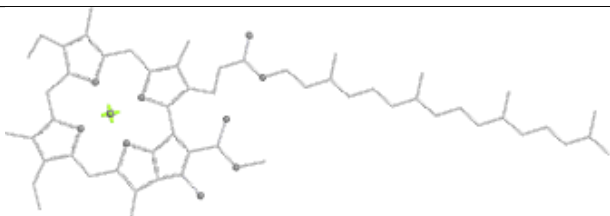


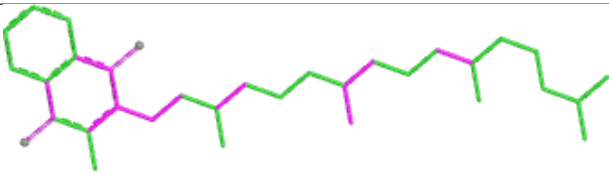
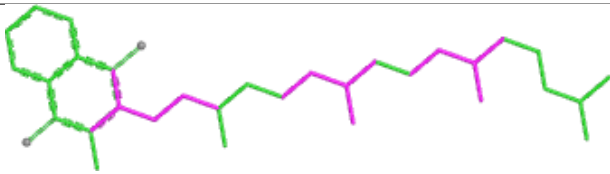
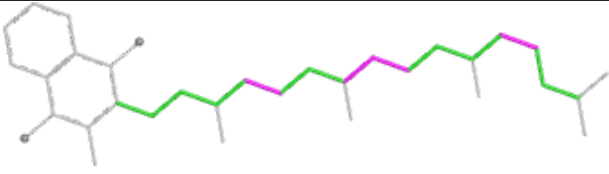
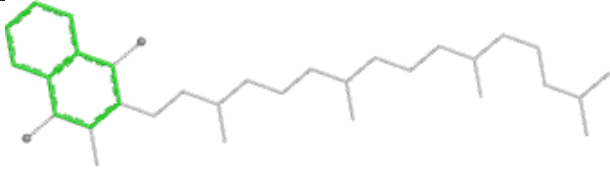


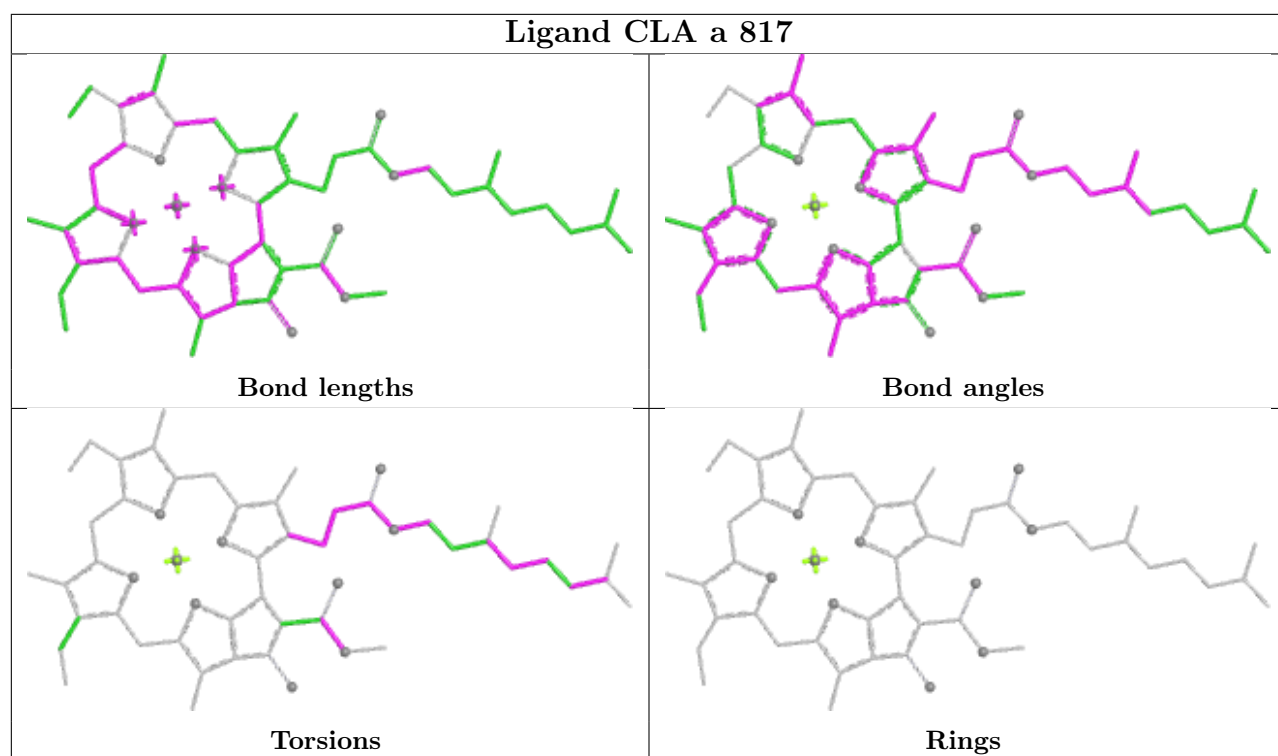
Ligand CLA B 830**Ligand CLA A 808**



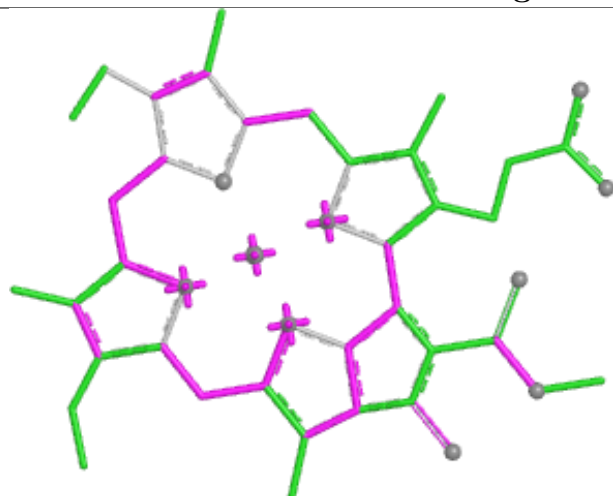
Ligand BCR A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 816	
	
Bond lengths	Bond angles
	
Torsions	Rings

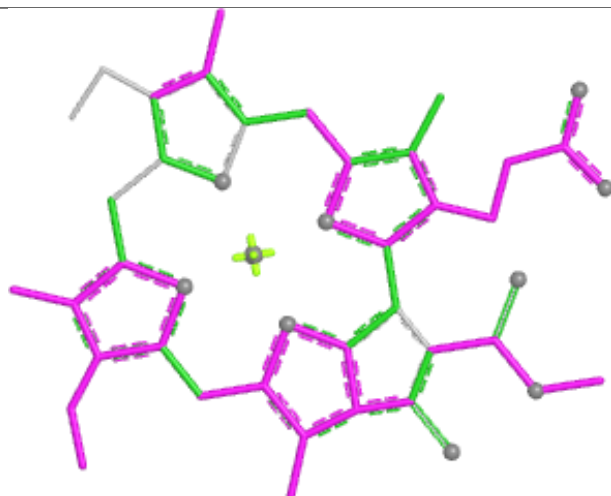
Ligand 1L3 b 838	
	
Bond lengths	Bond angles
	
Torsions	Rings



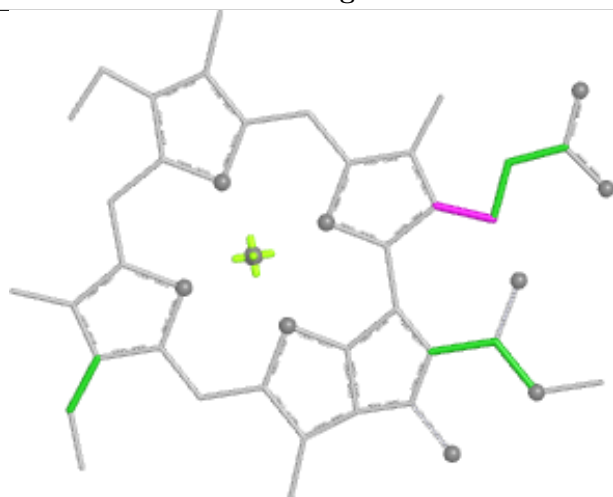
Ligand CLA H 821



Bond lengths



Bond angles

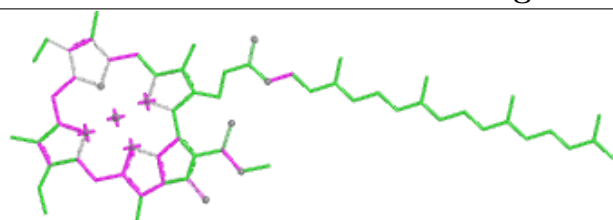


Torsions

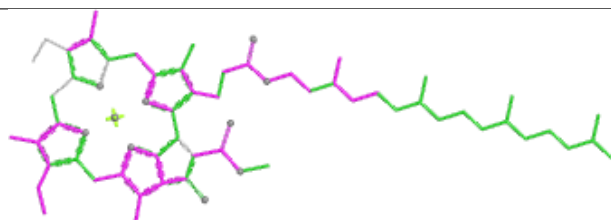


Rings

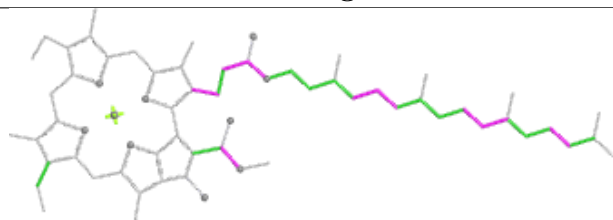
Ligand CLA A 806



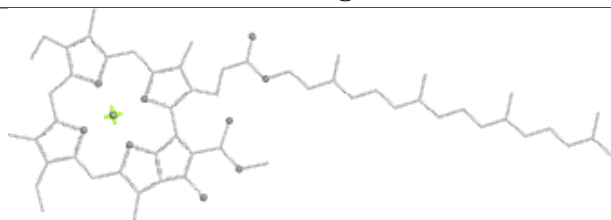
Bond lengths



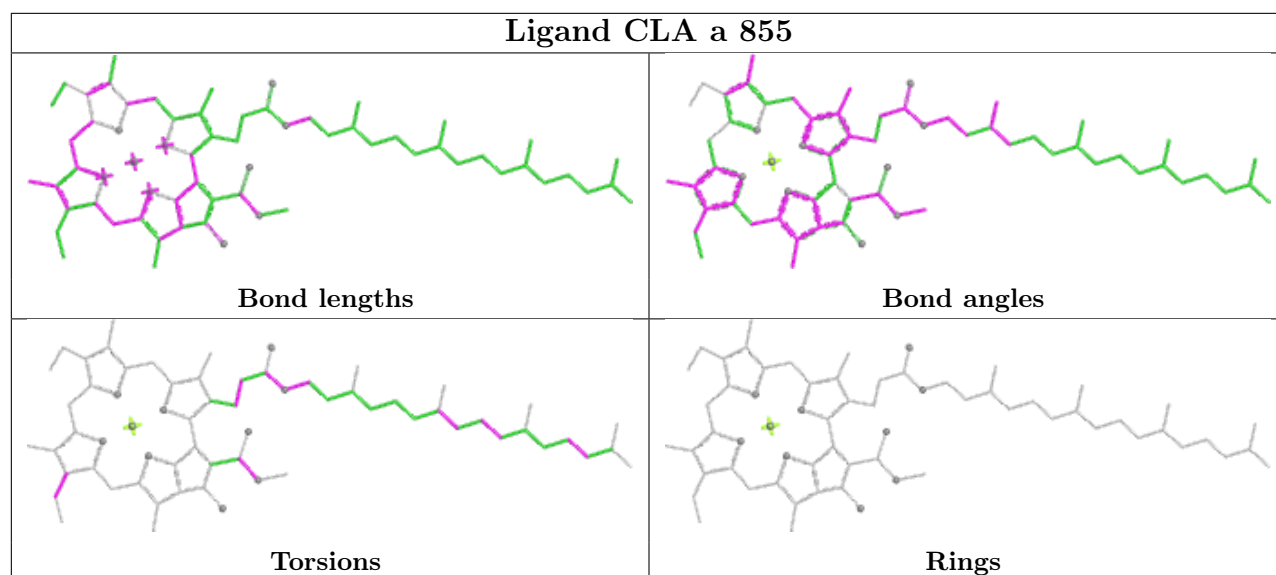
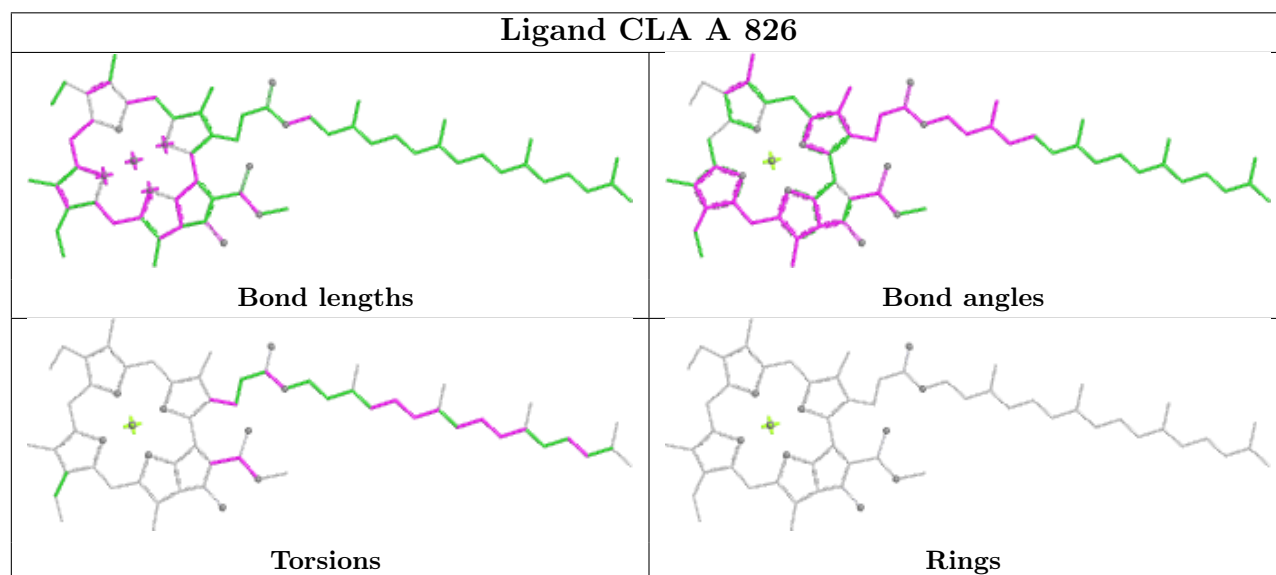
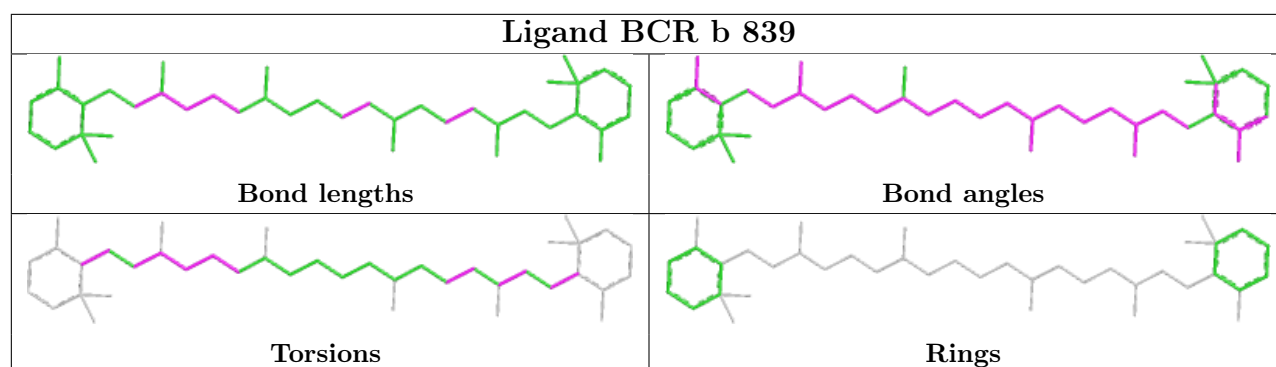
Bond angles

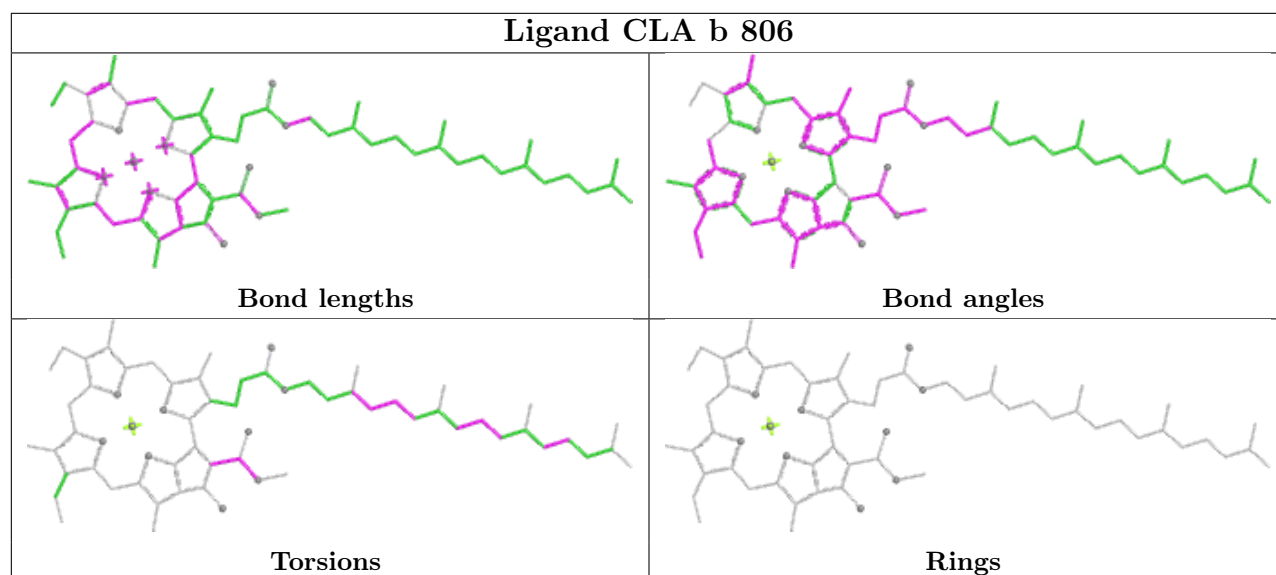
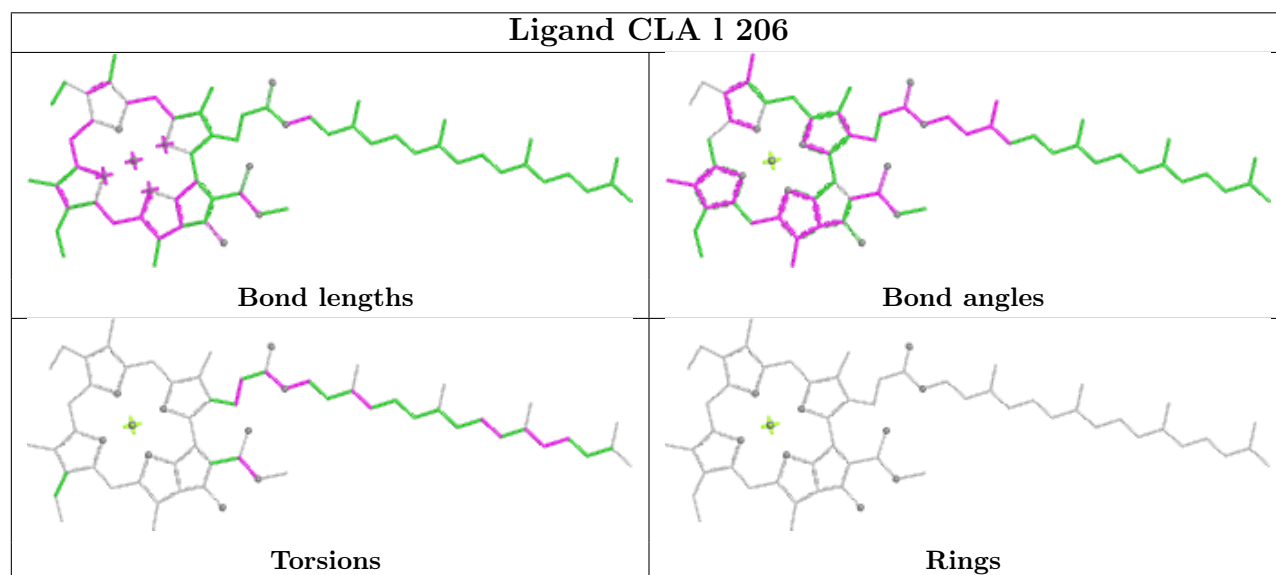
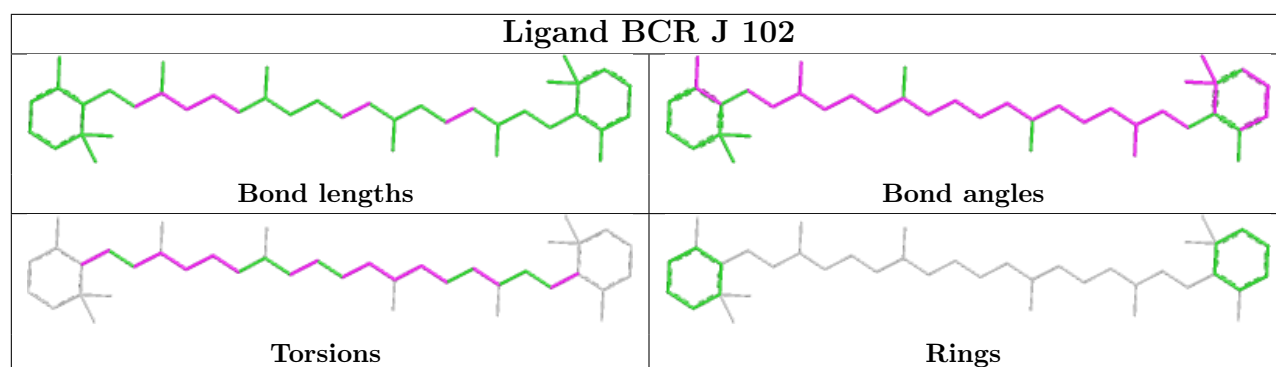


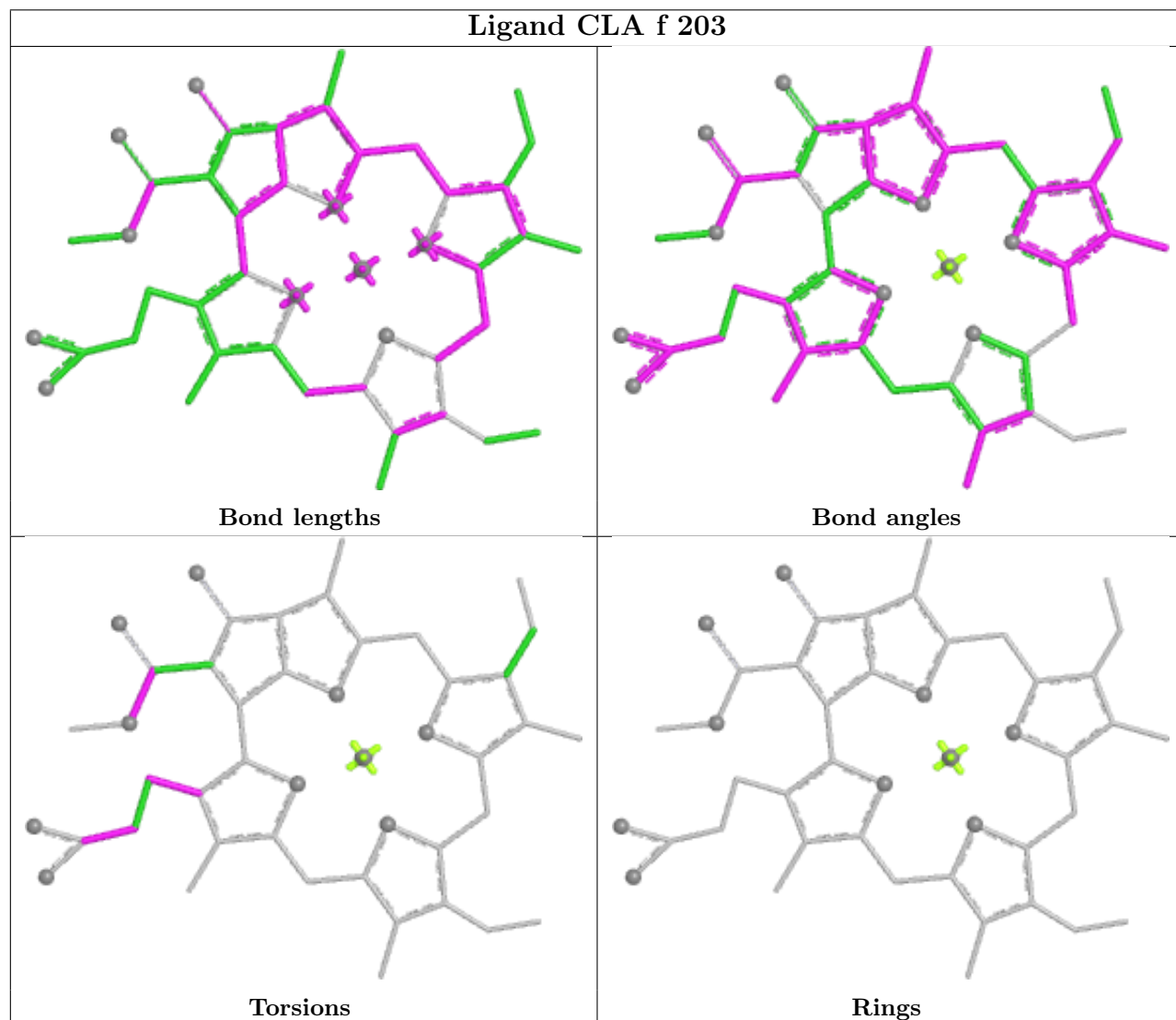
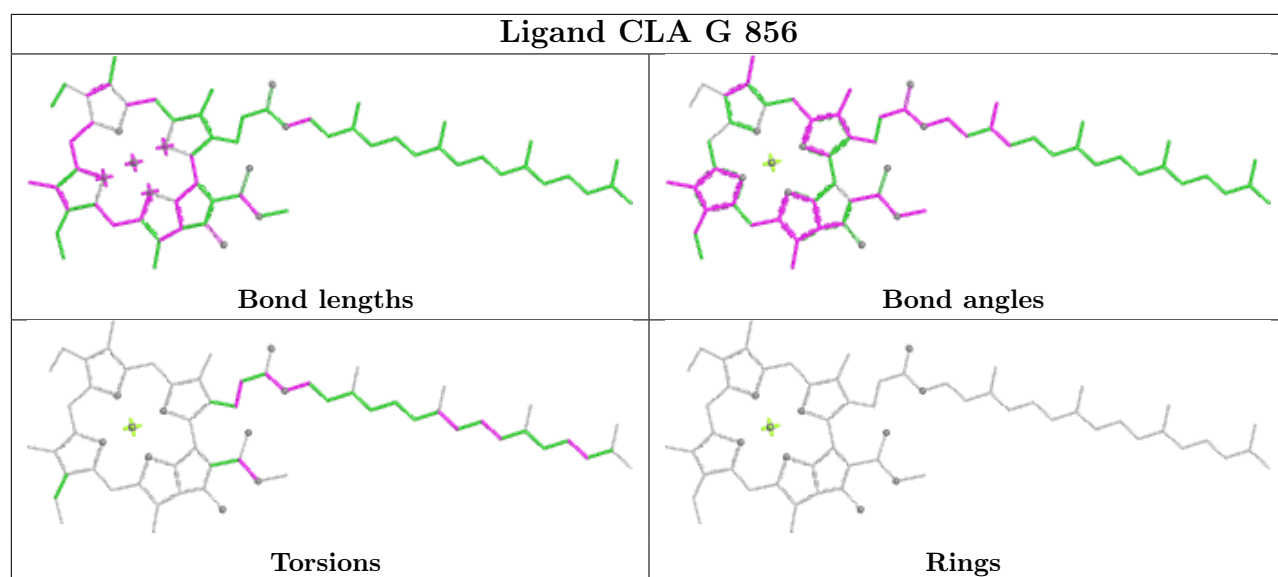
Torsions

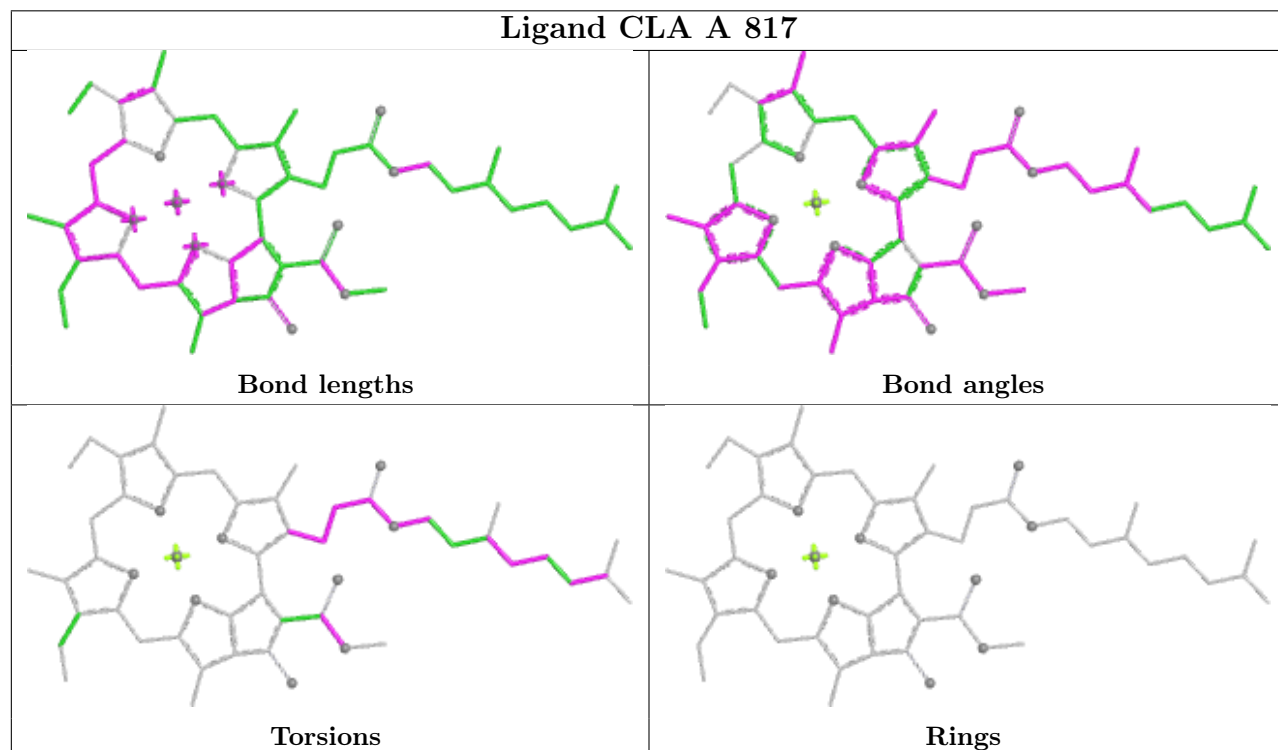
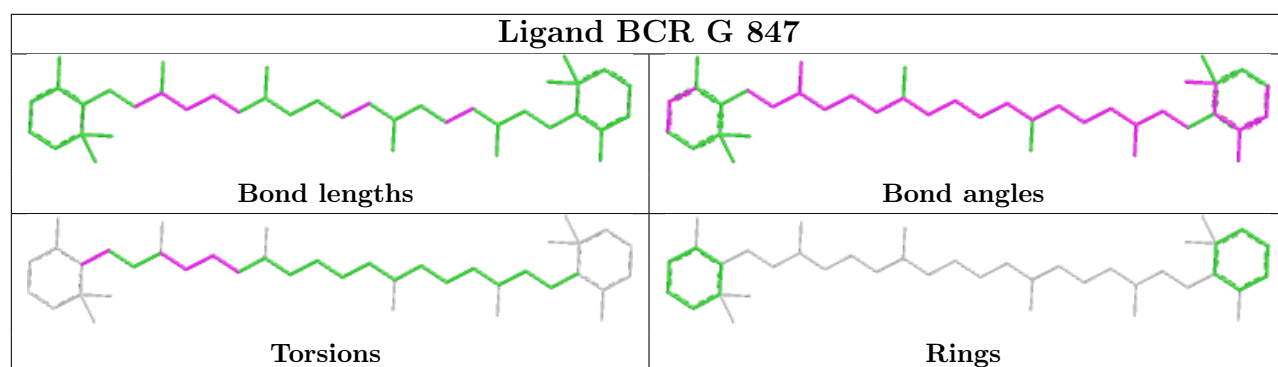


Rings

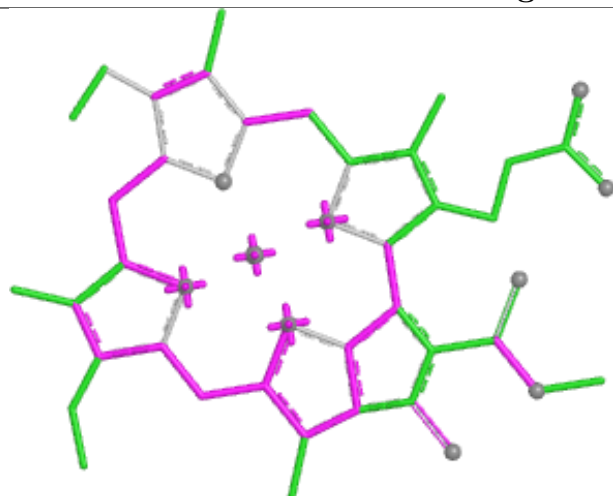




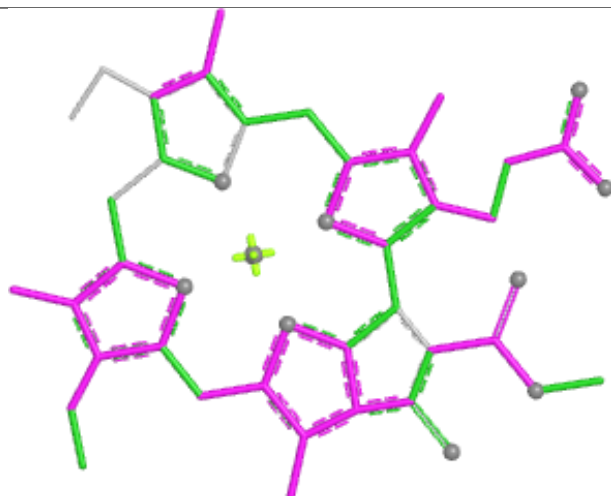




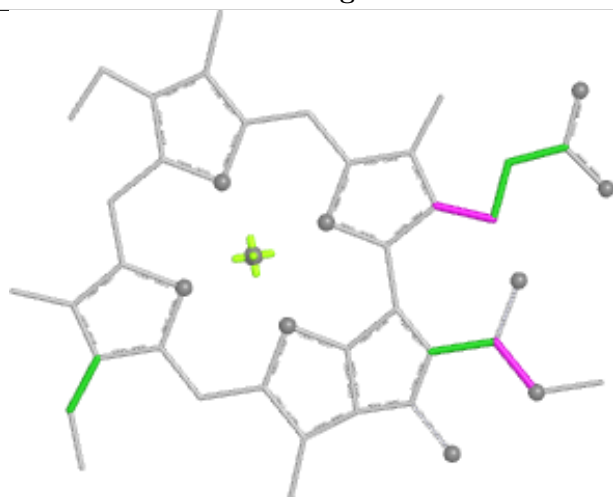
Ligand CLA b 818



Bond lengths



Bond angles

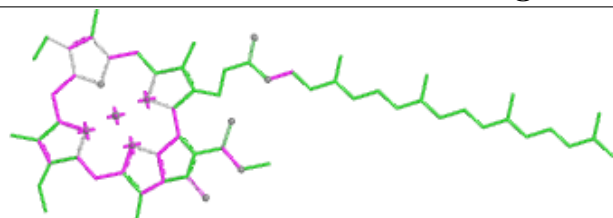


Torsions

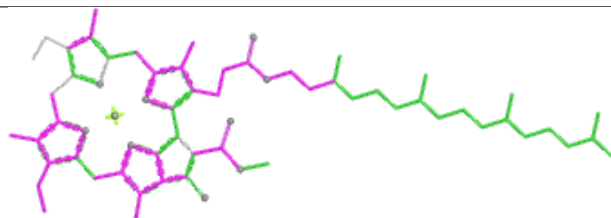


Rings

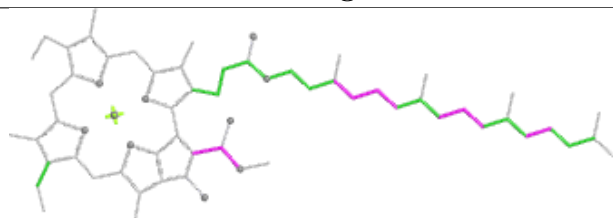
Ligand CLA B 806



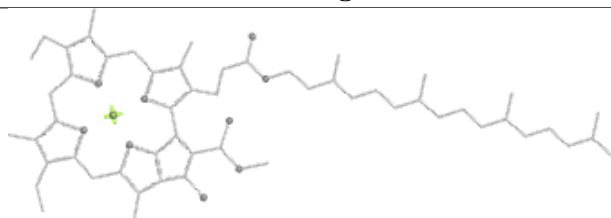
Bond lengths



Bond angles

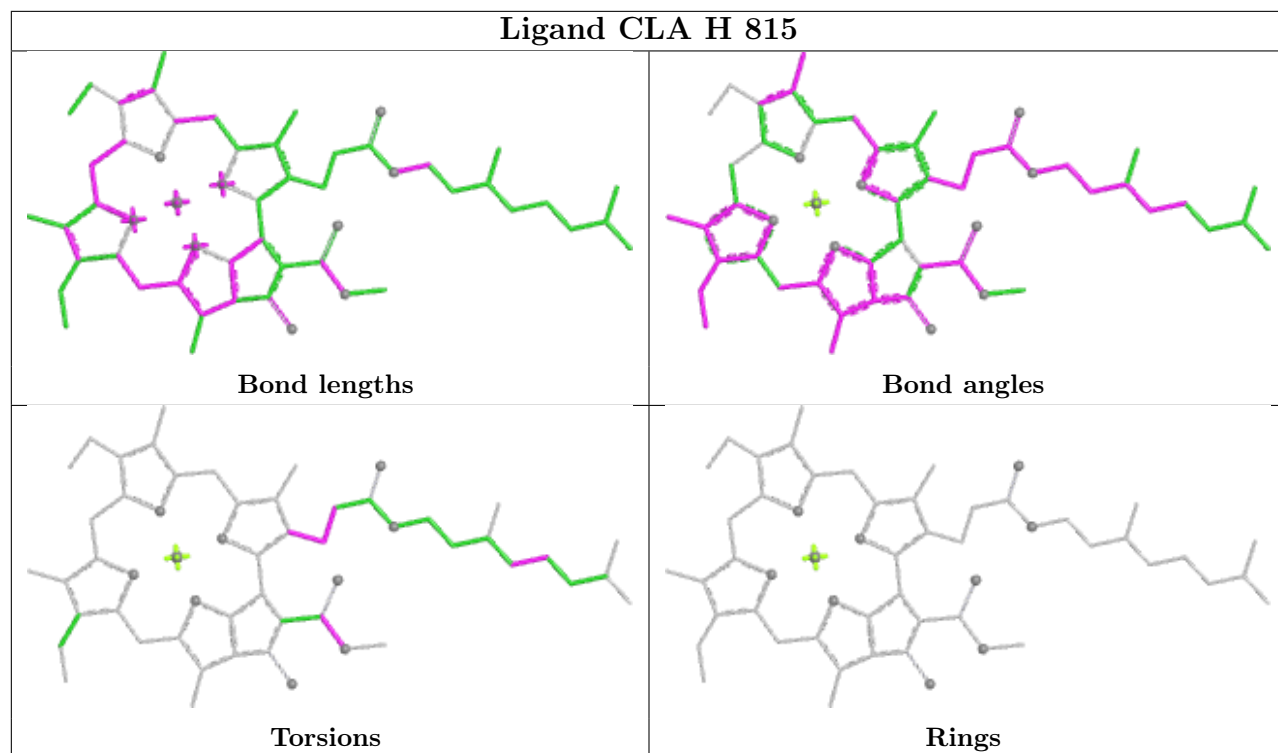


Torsions

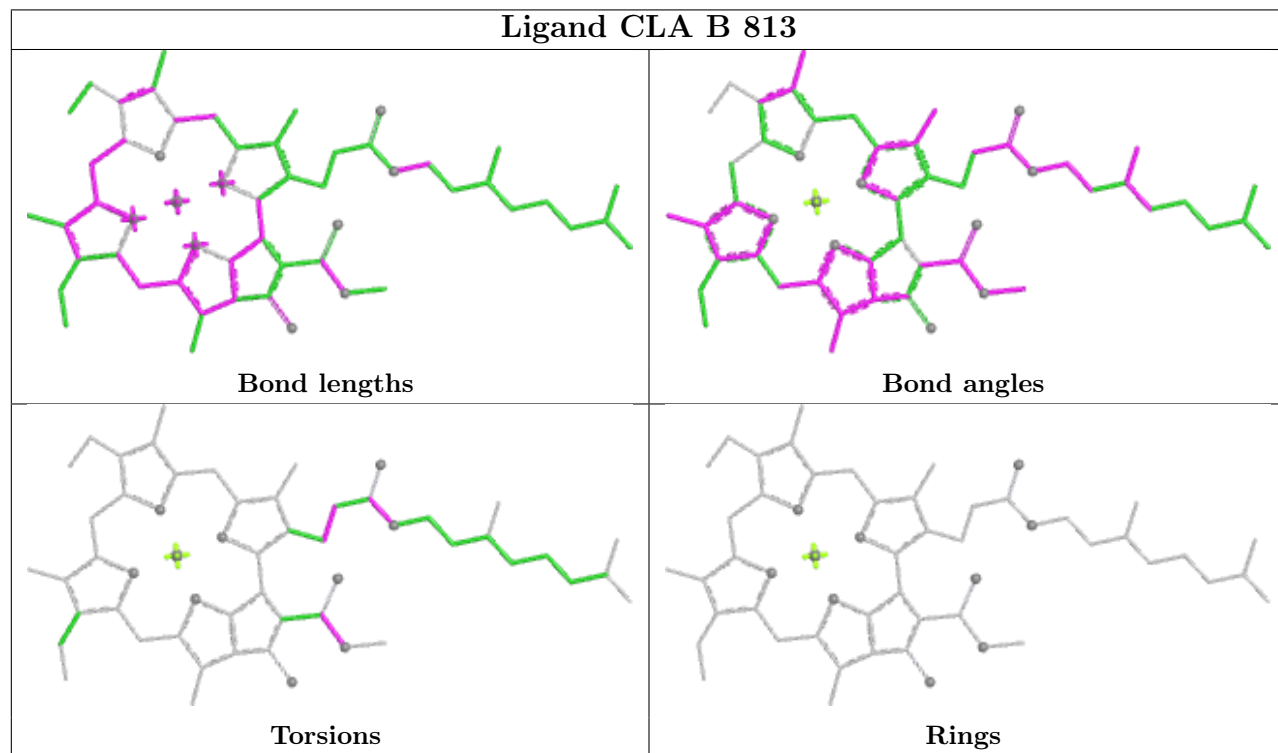


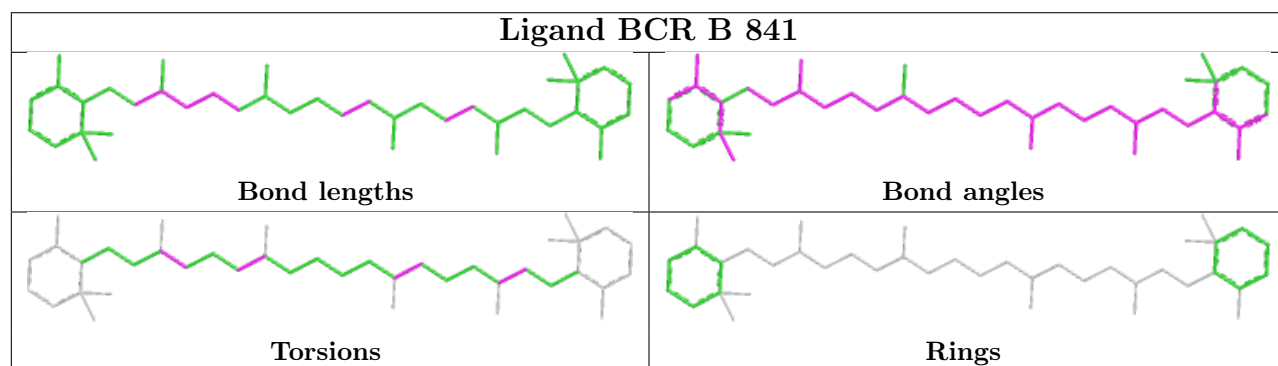
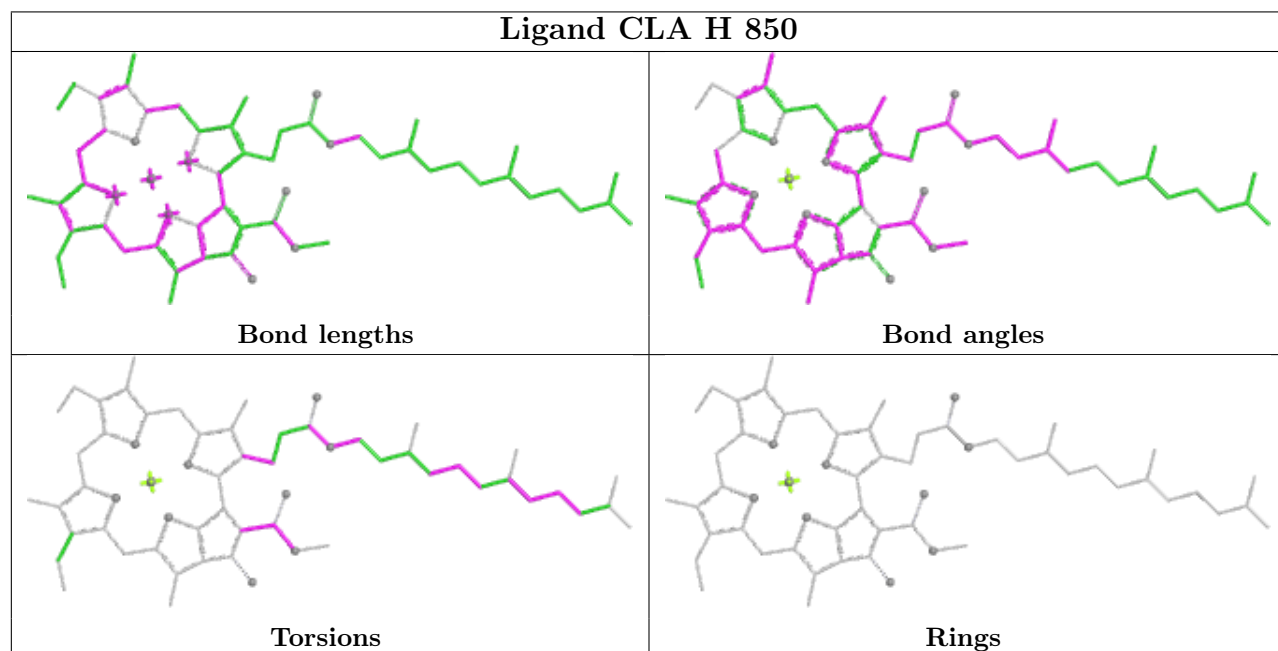
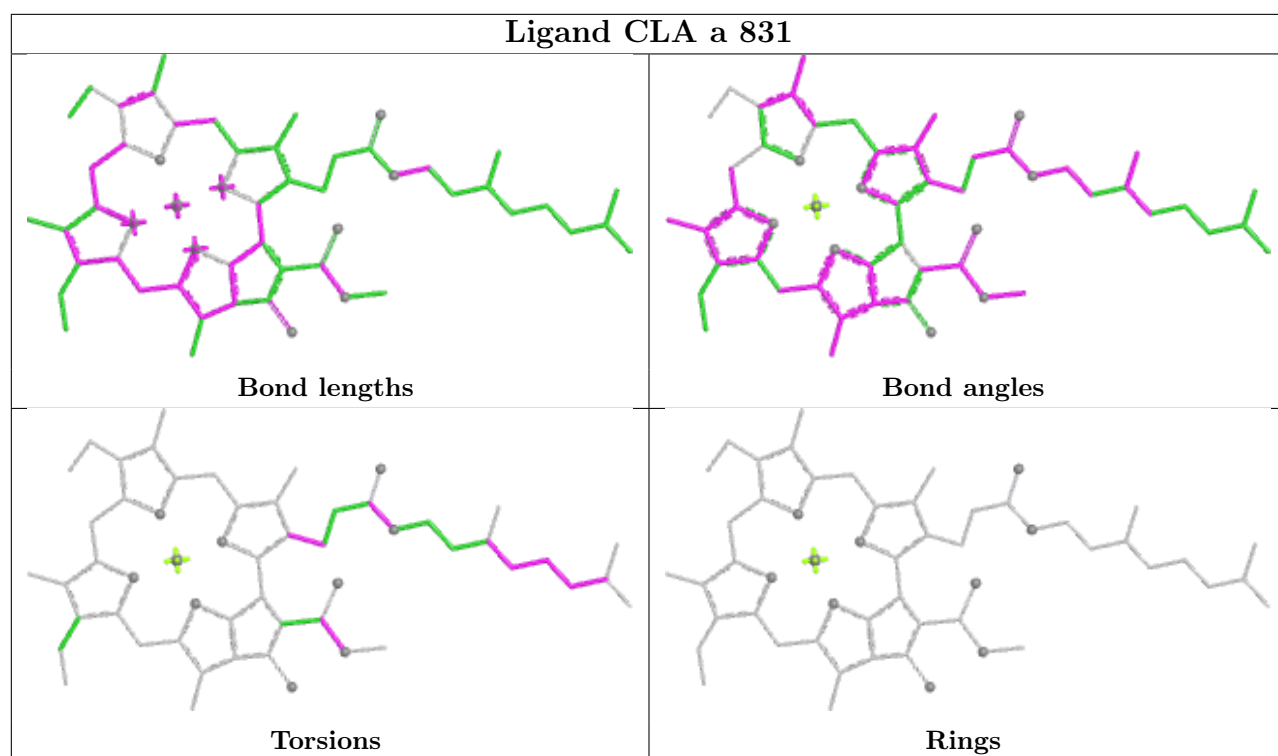
Rings

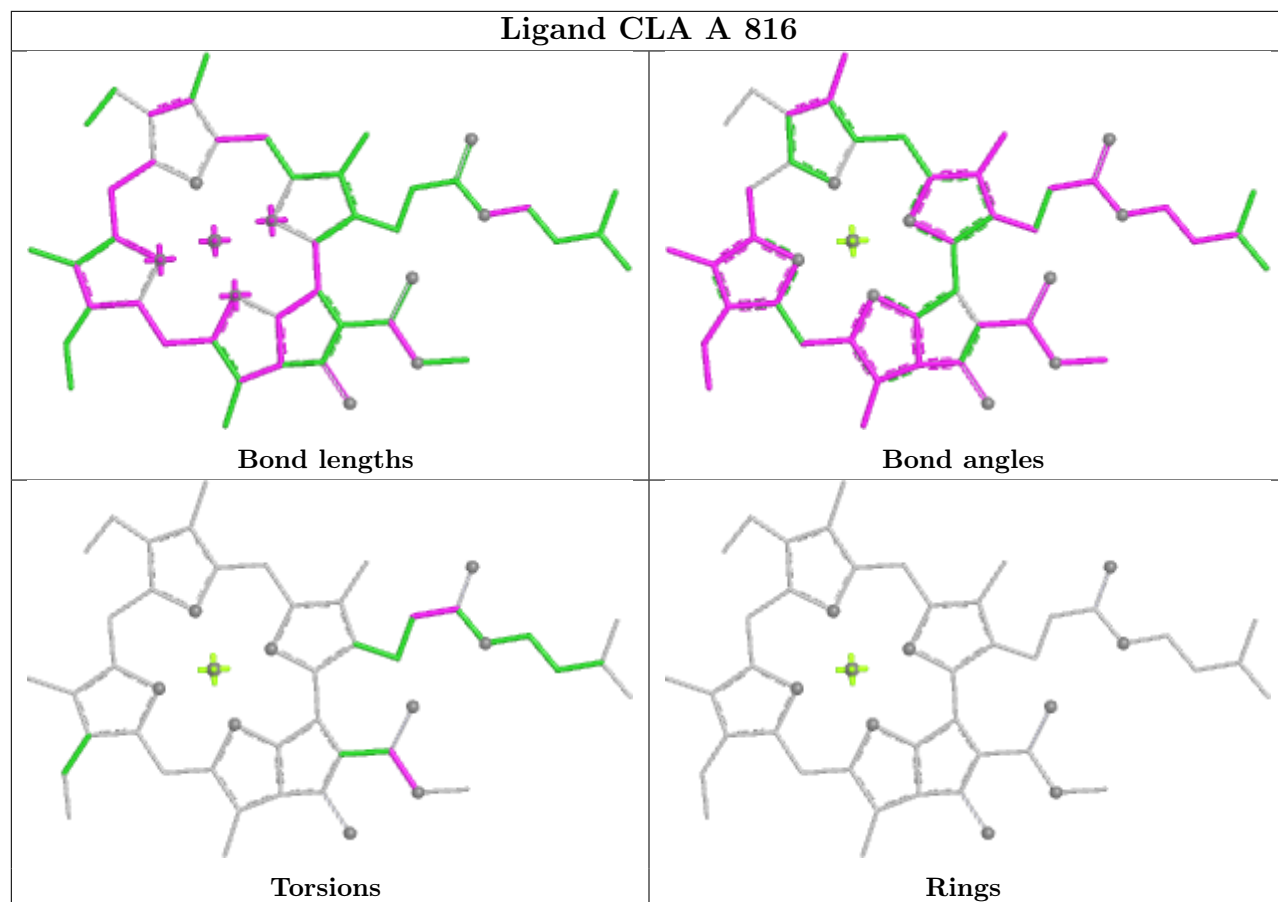
Ligand CLA H 815



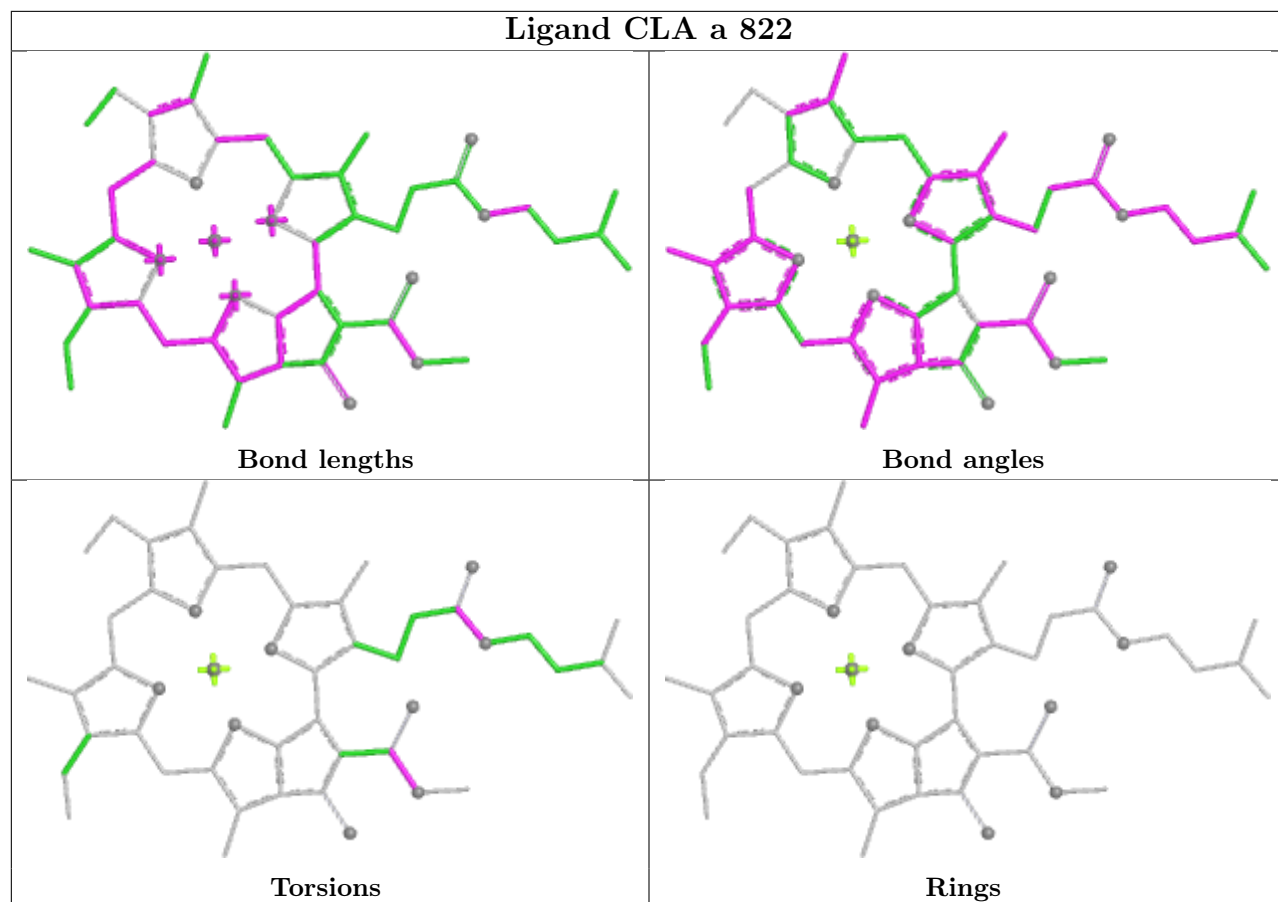
Ligand CLA B 813



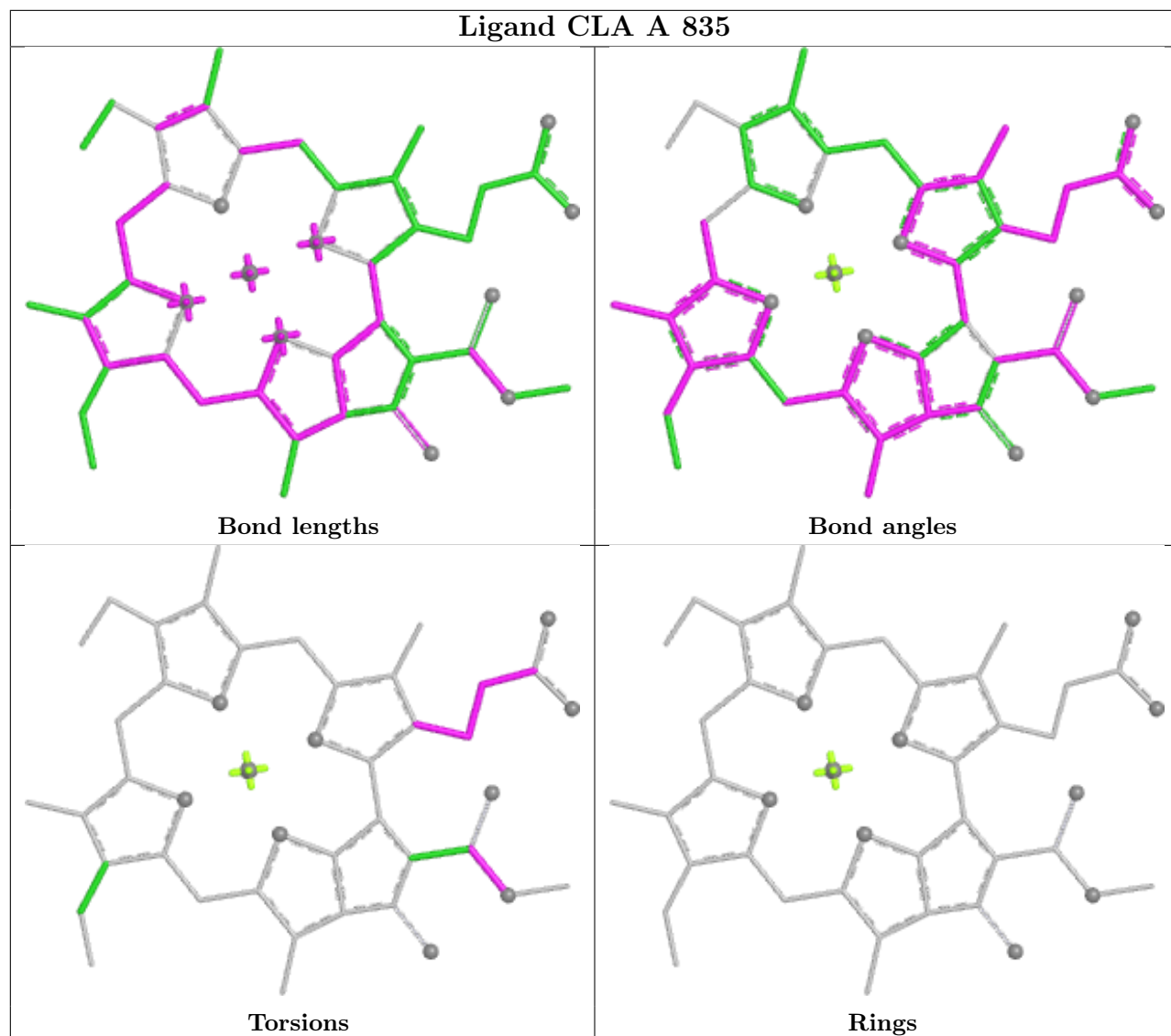




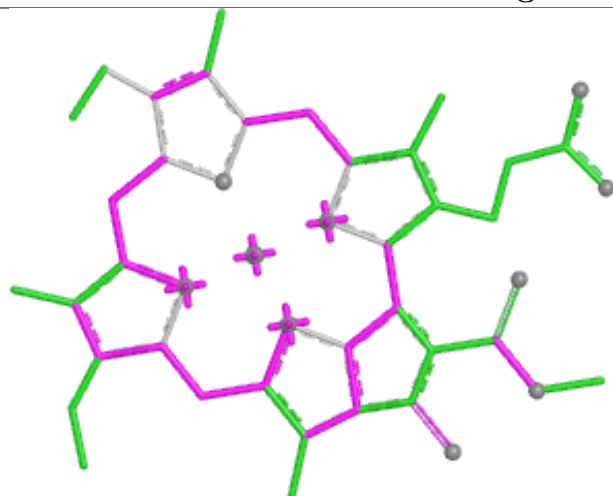
Ligand CLA a 822



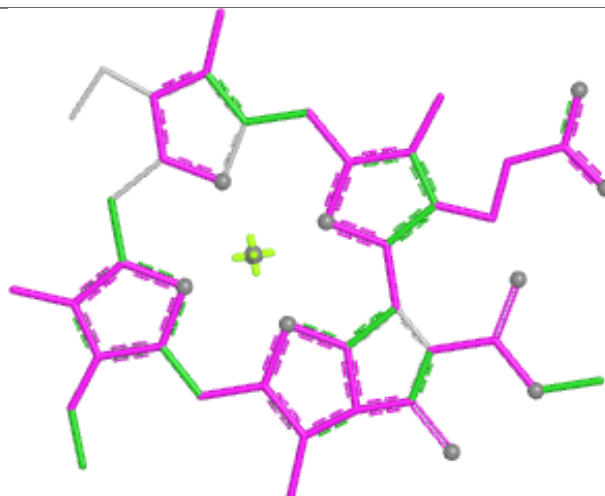
Ligand CLA A 835



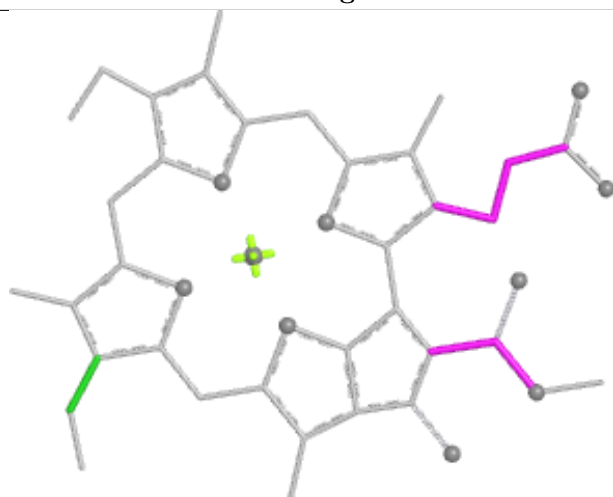
Ligand CLA b 812



Bond lengths



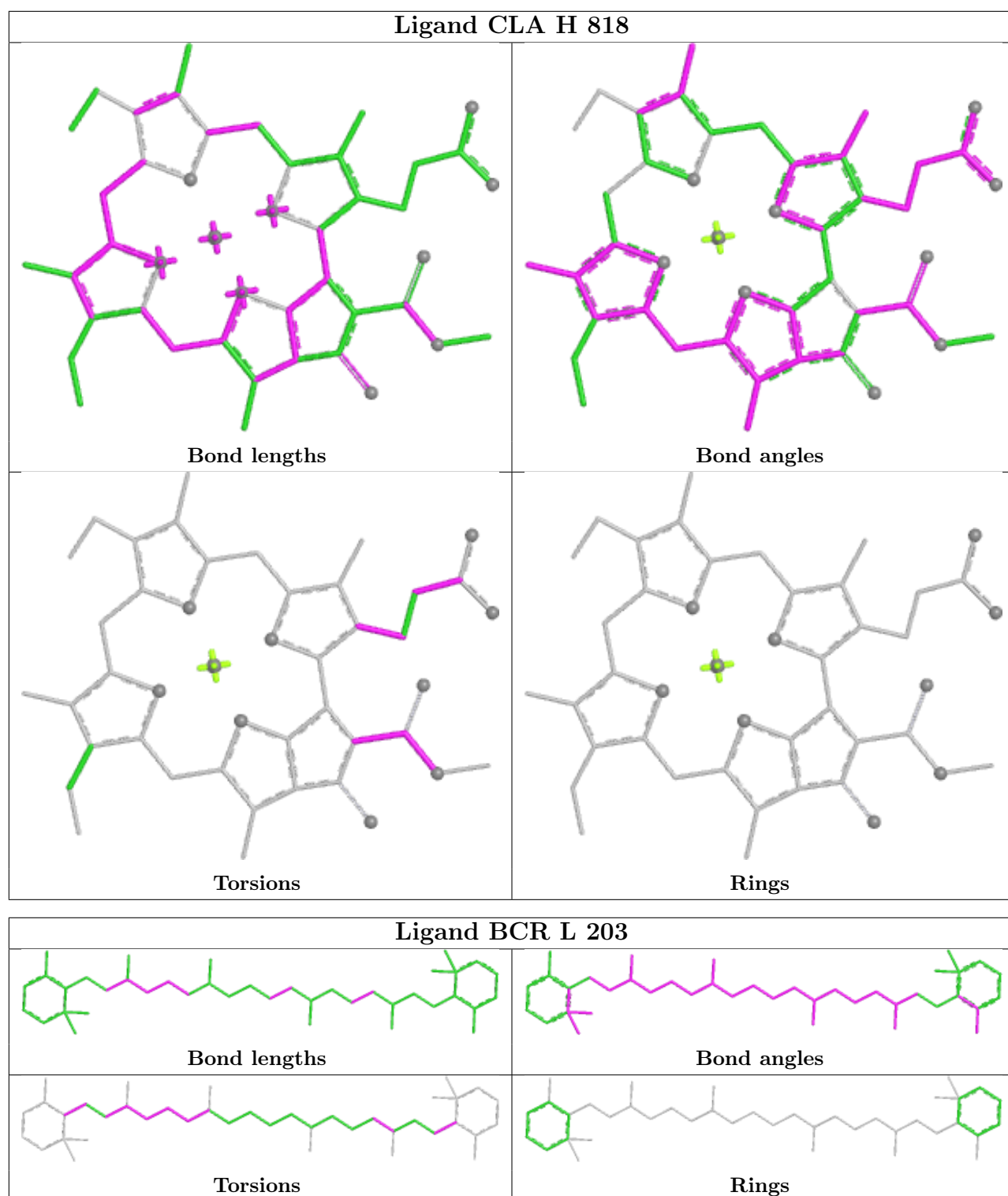
Bond angles

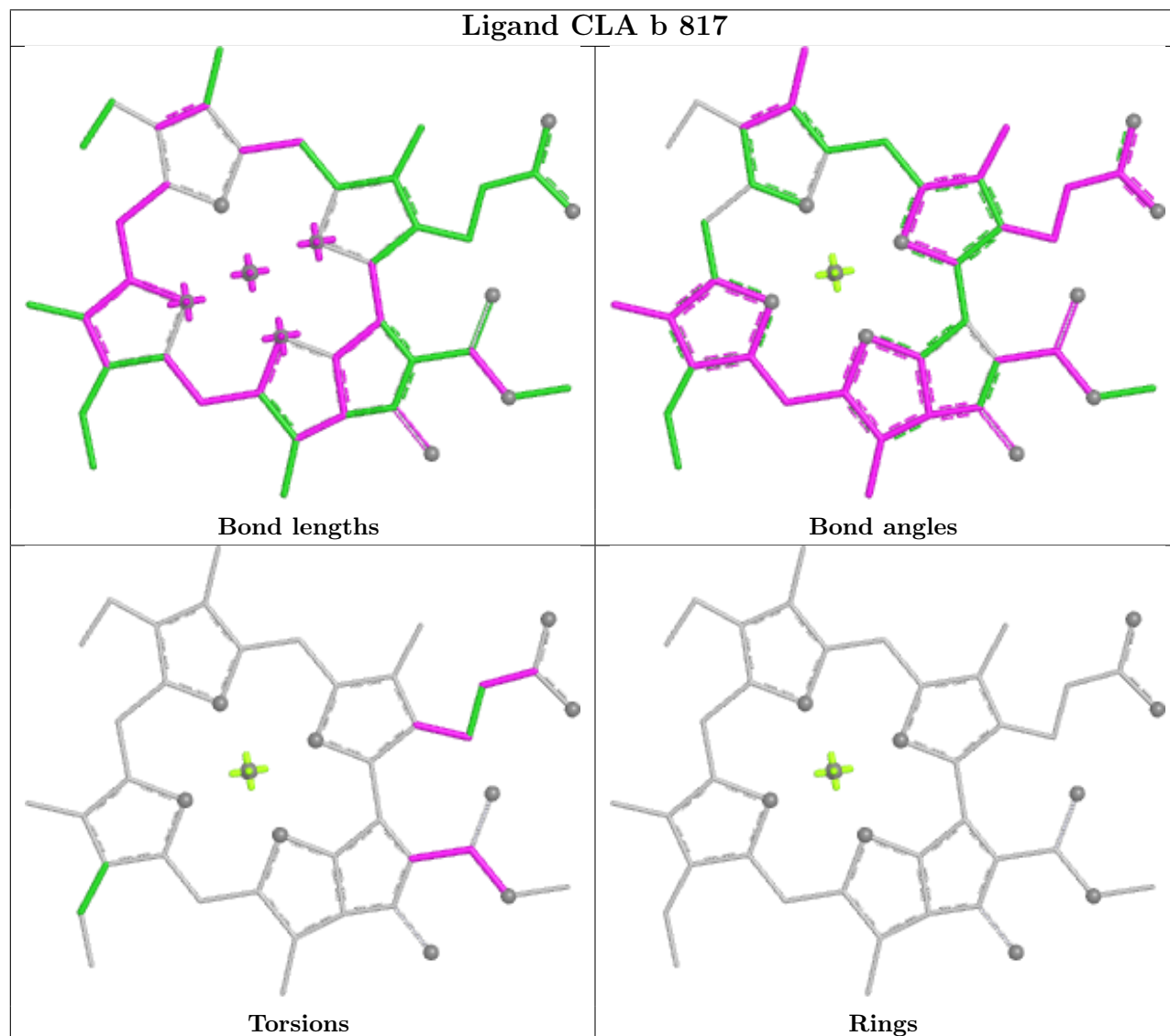
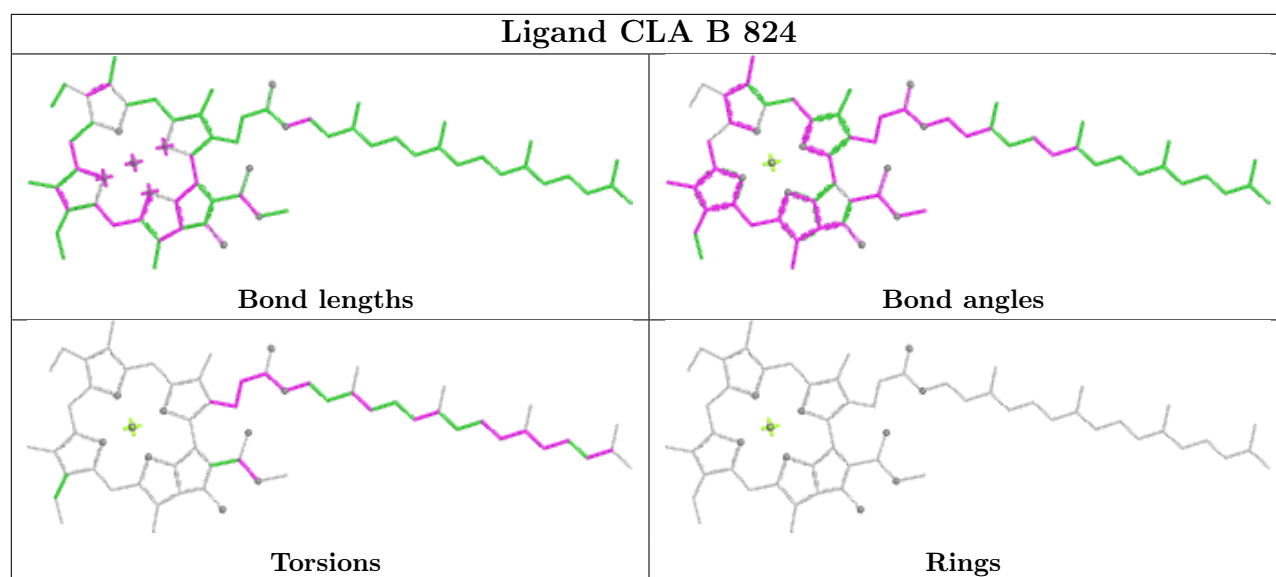


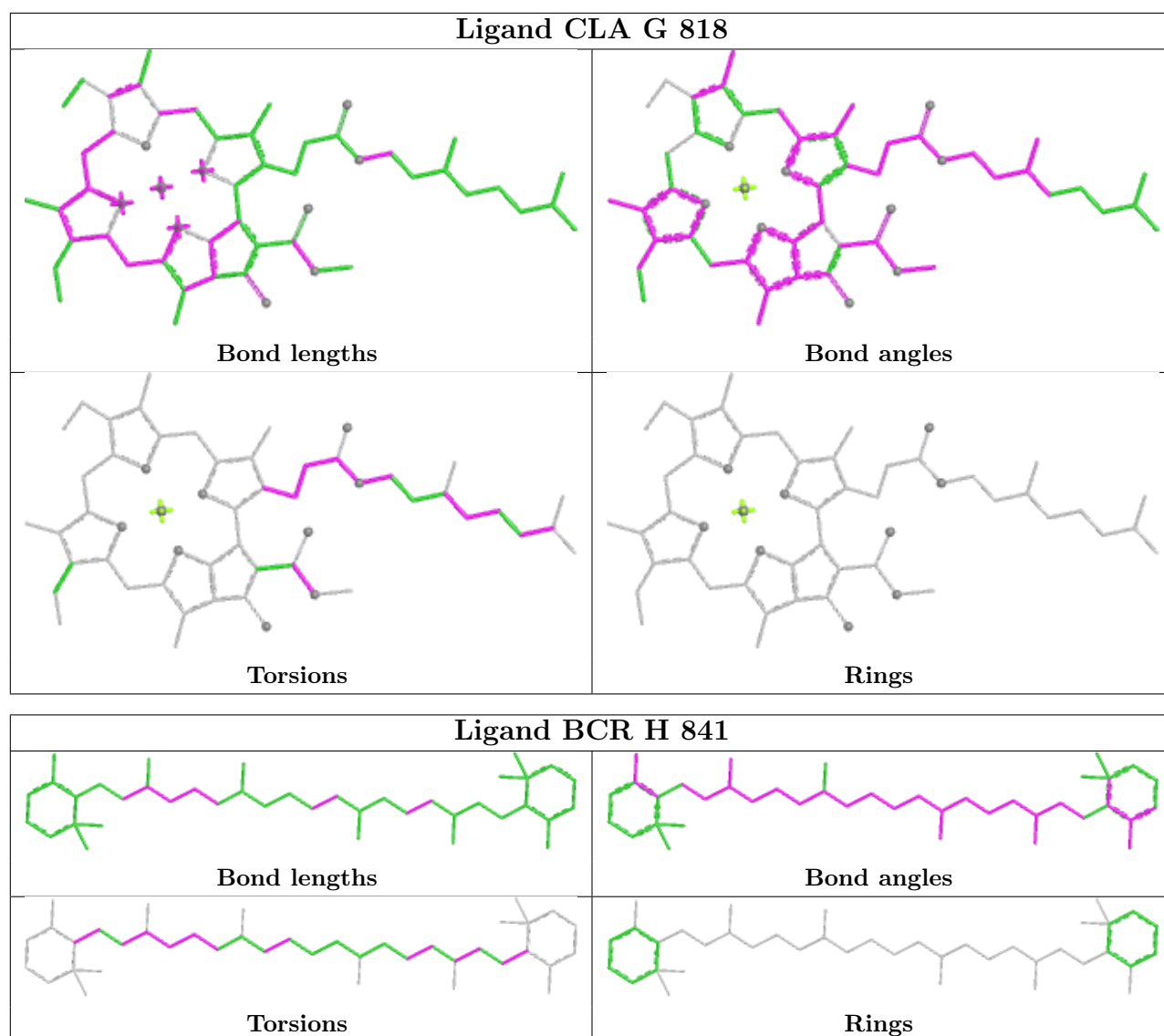
Torsions



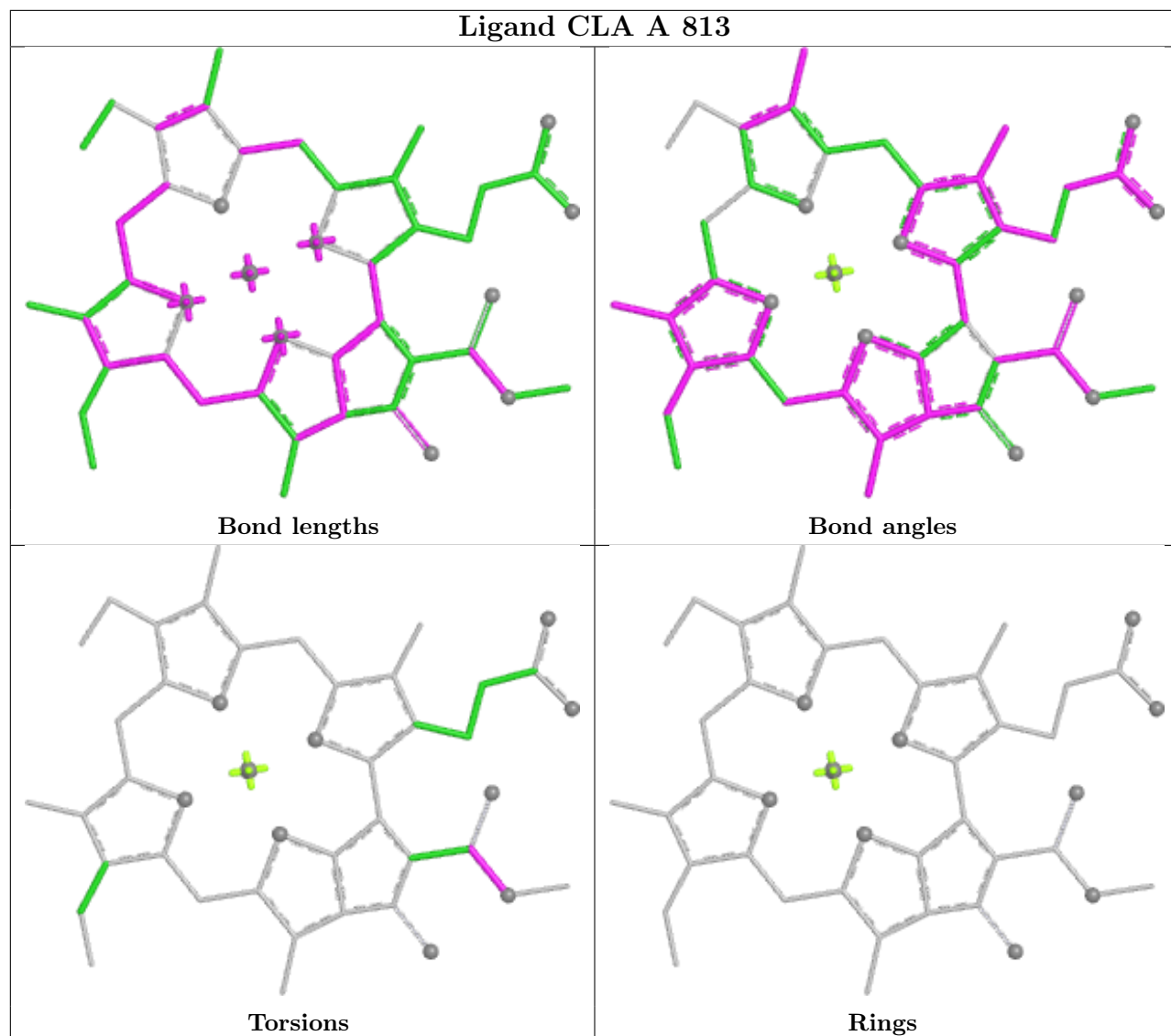
Rings



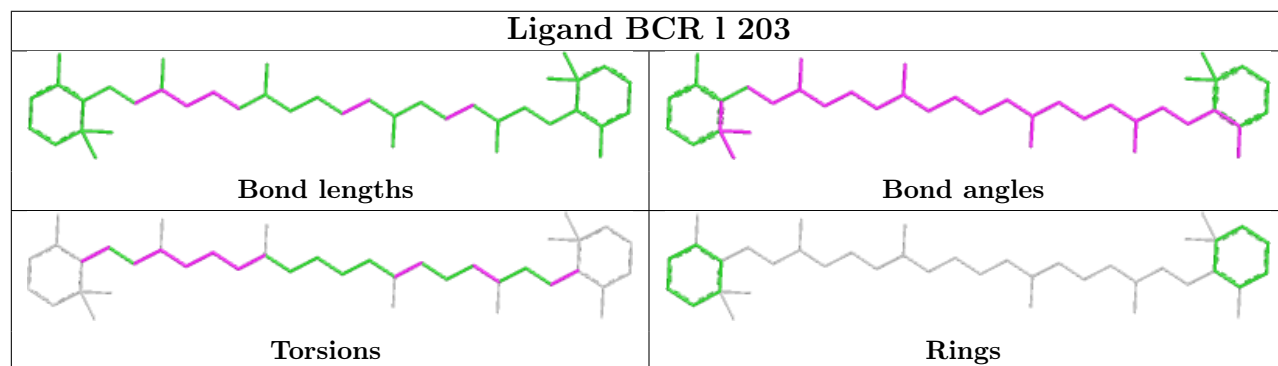


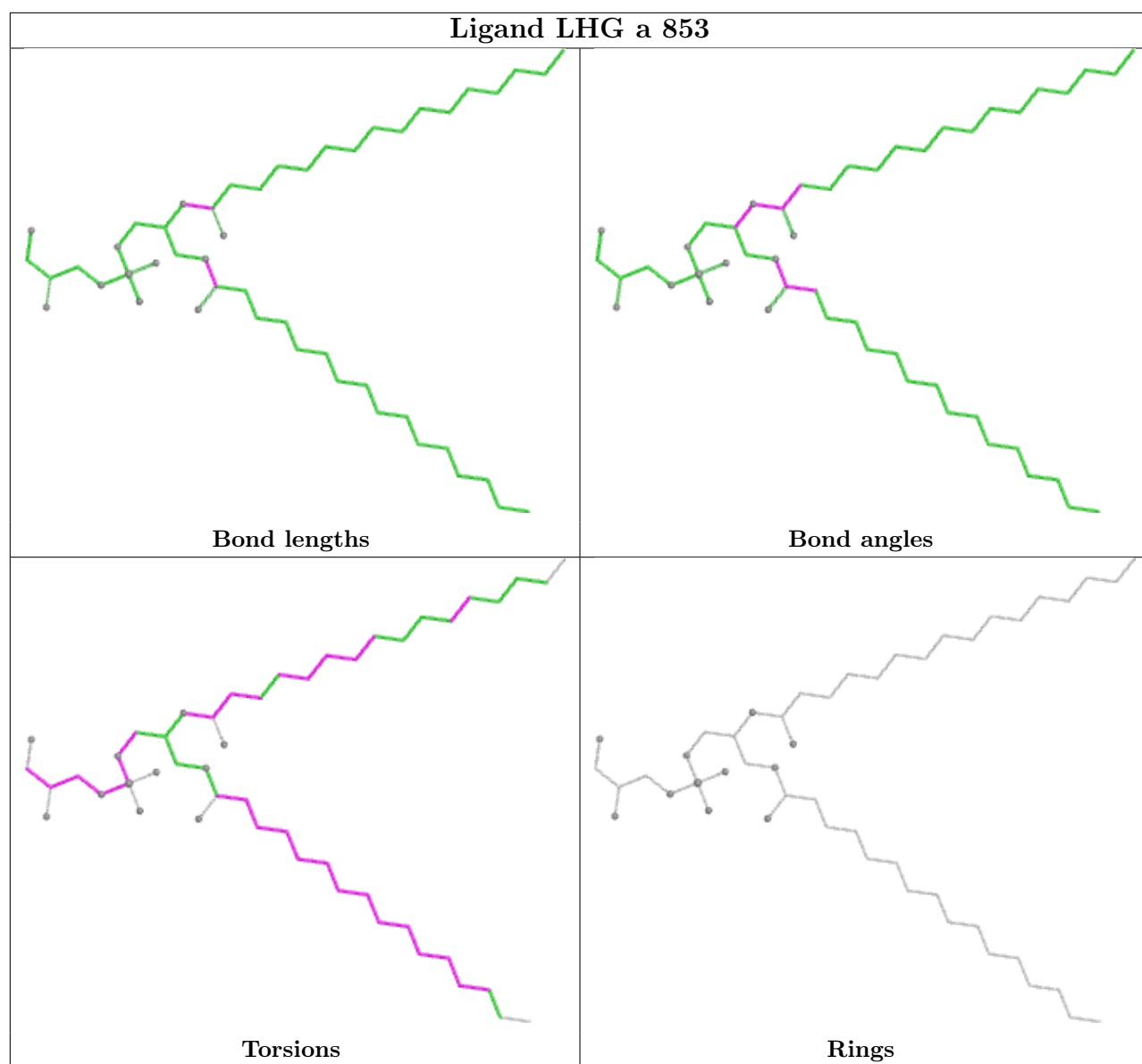


Ligand CLA A 813

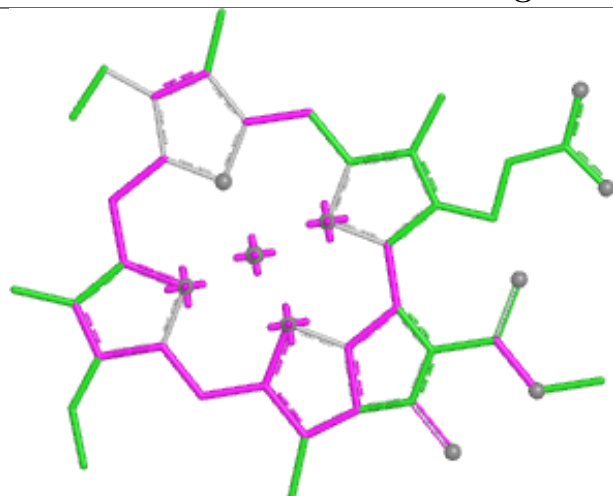


Ligand BCR 1 203

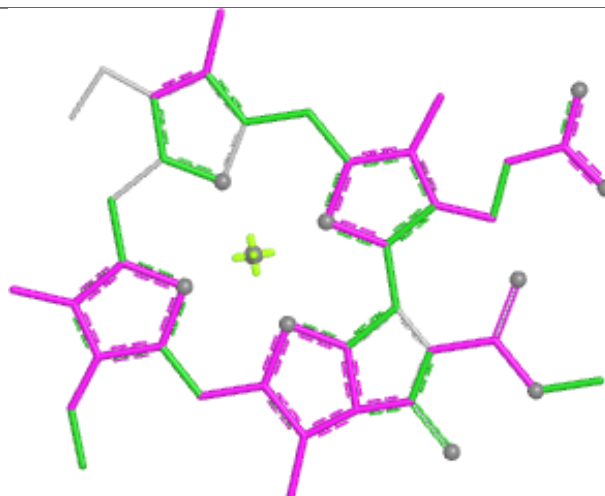




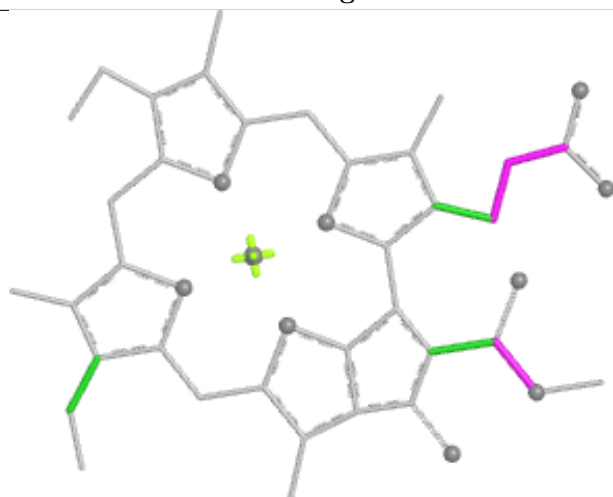
Ligand CLA B 809



Bond lengths



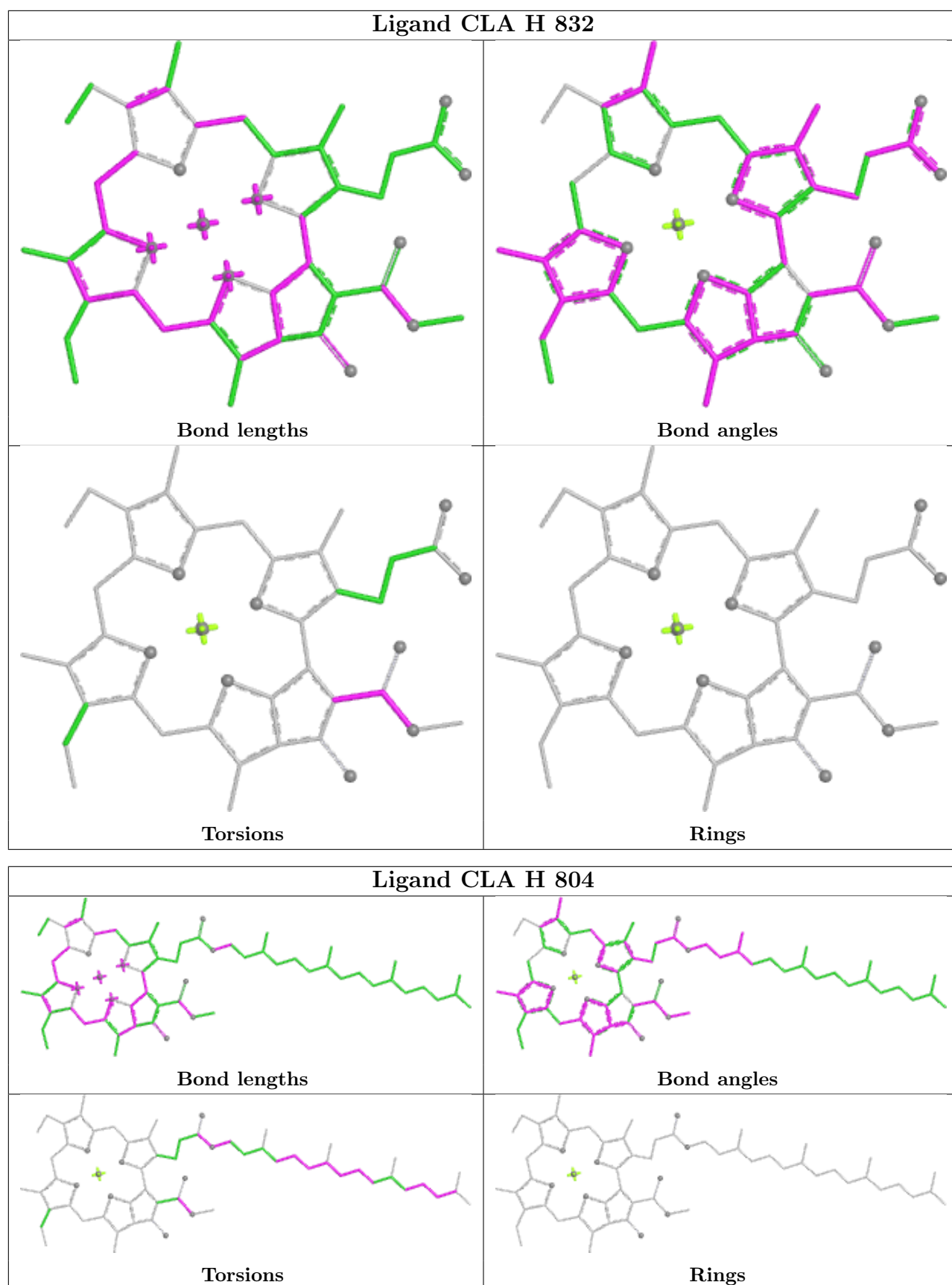
Bond angles

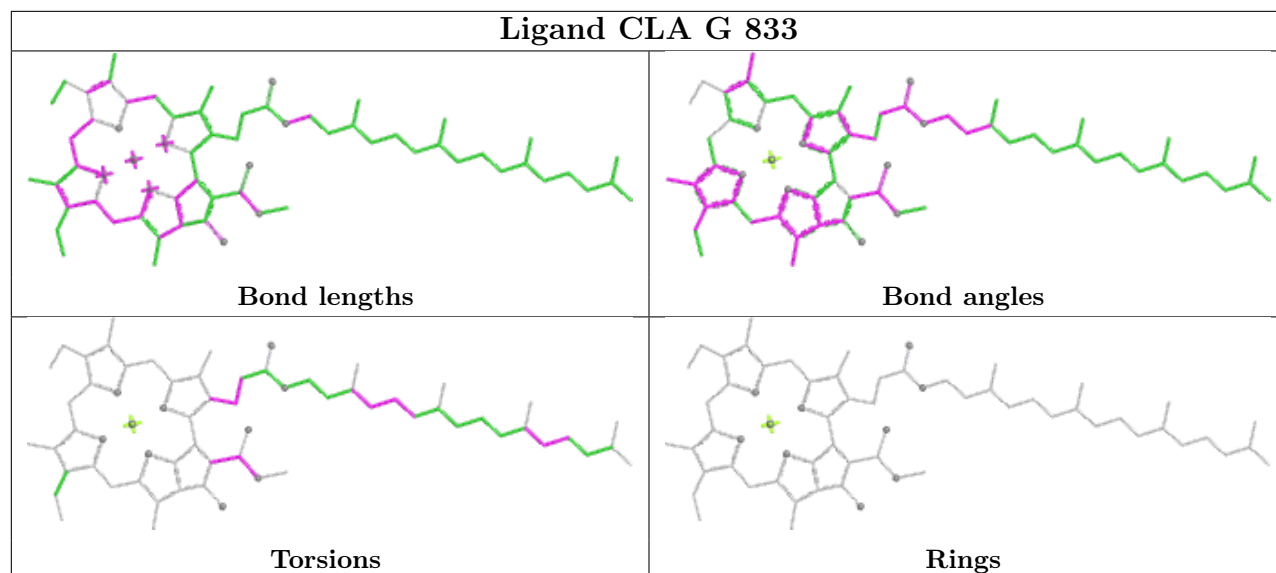
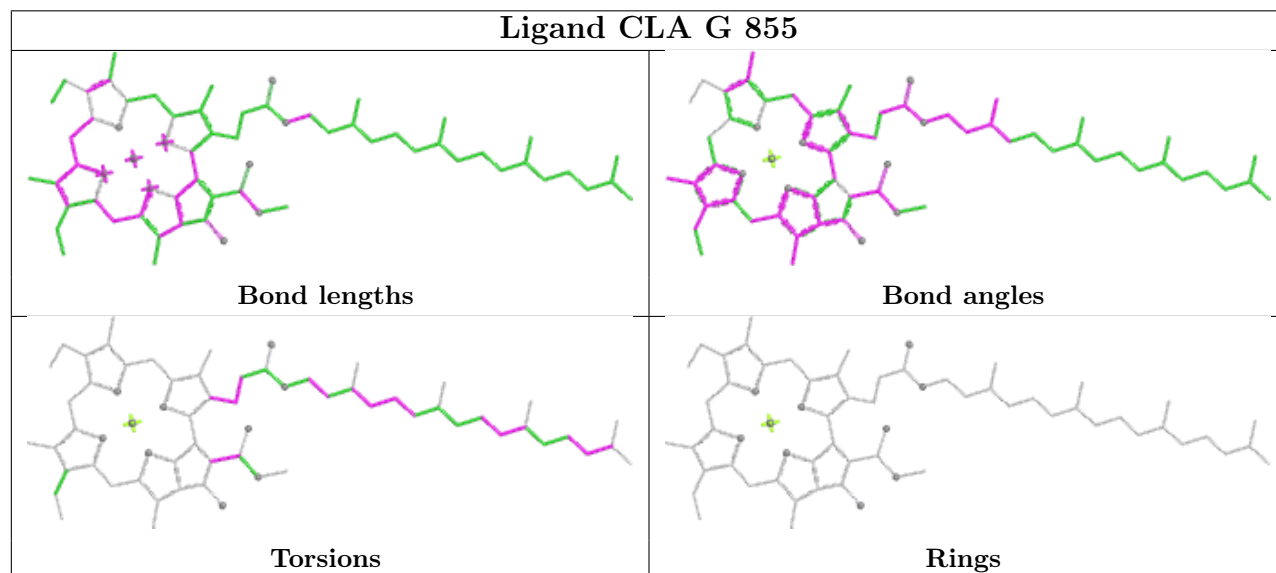
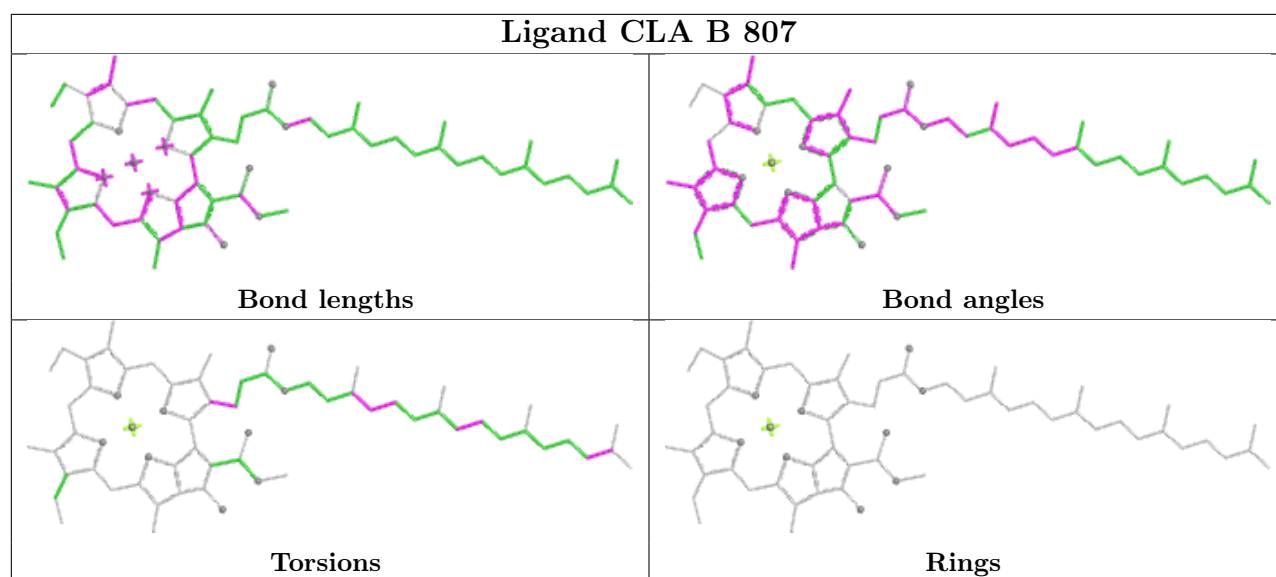


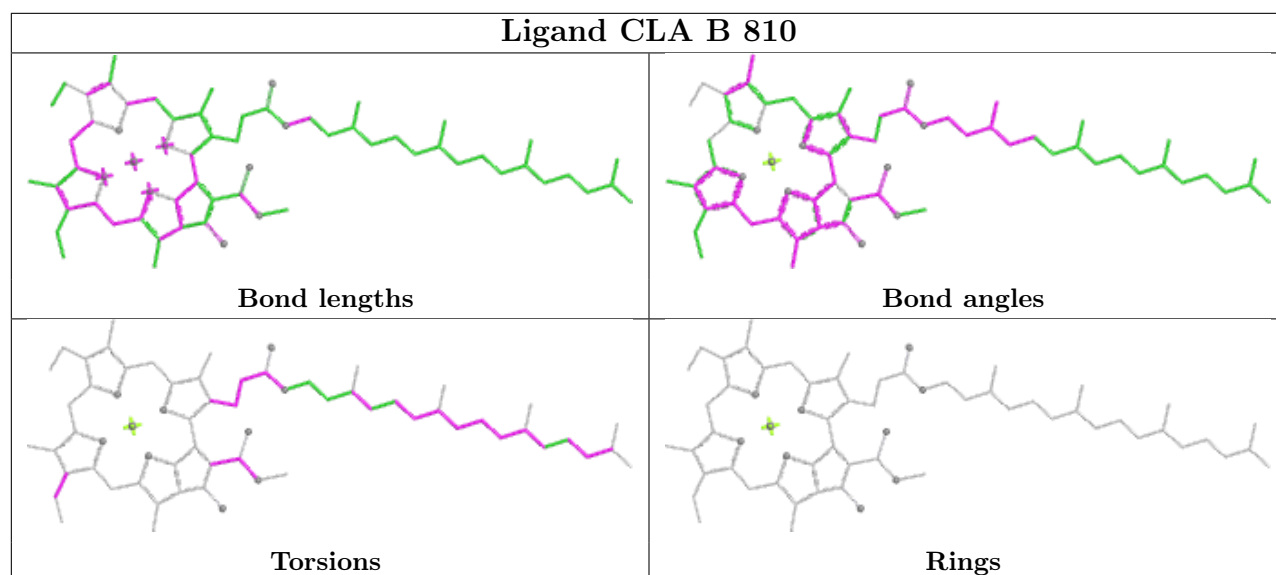
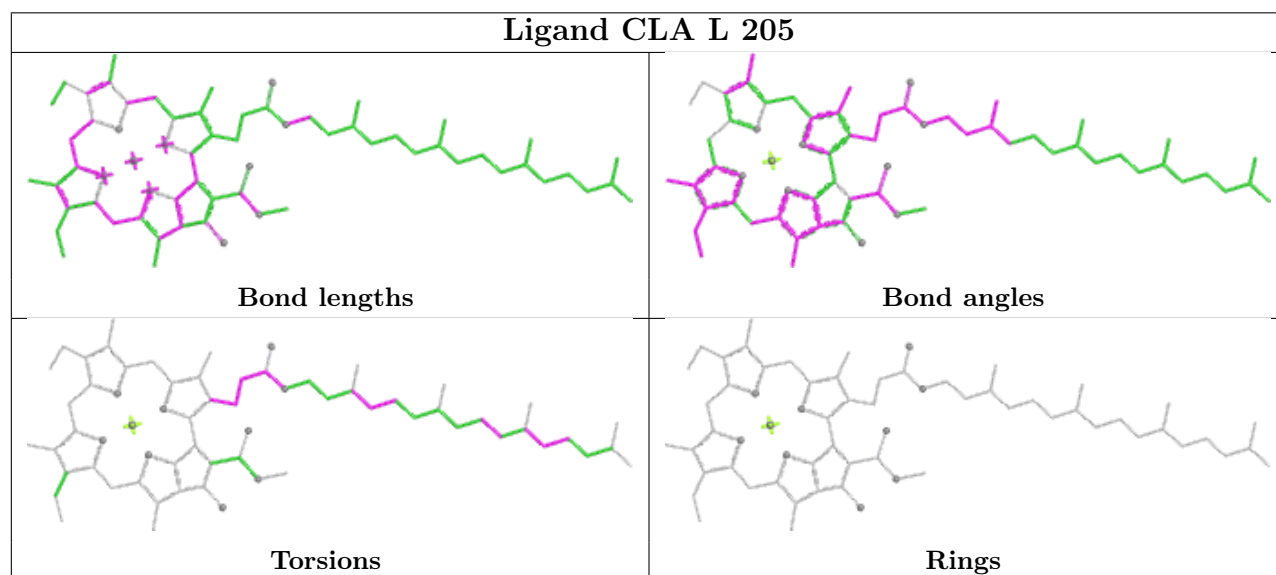
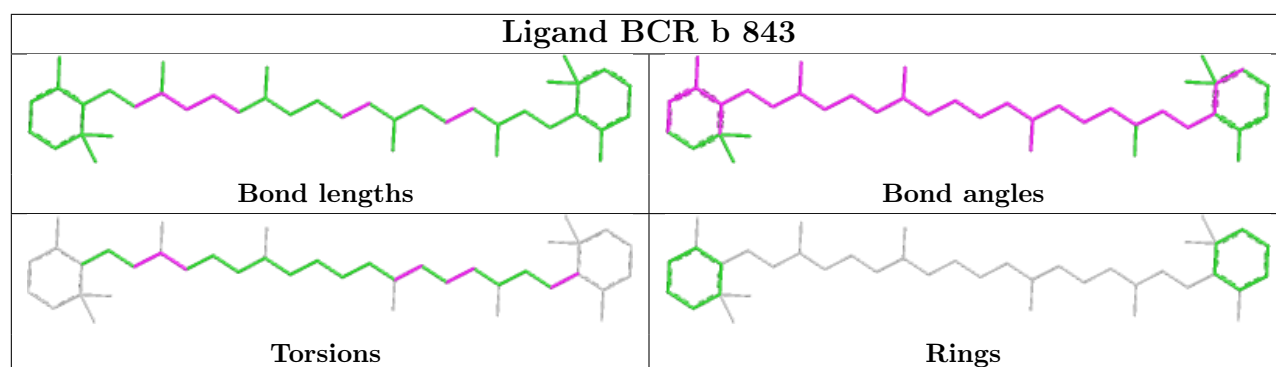
Torsions

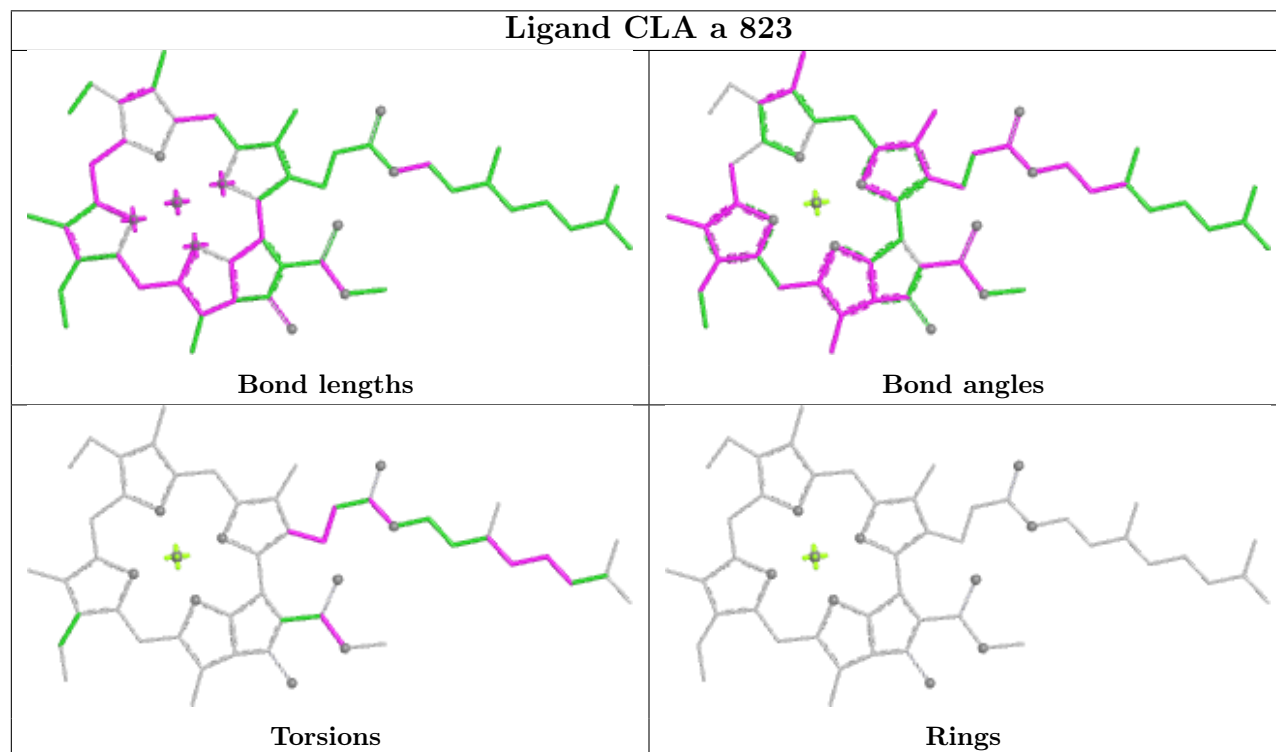
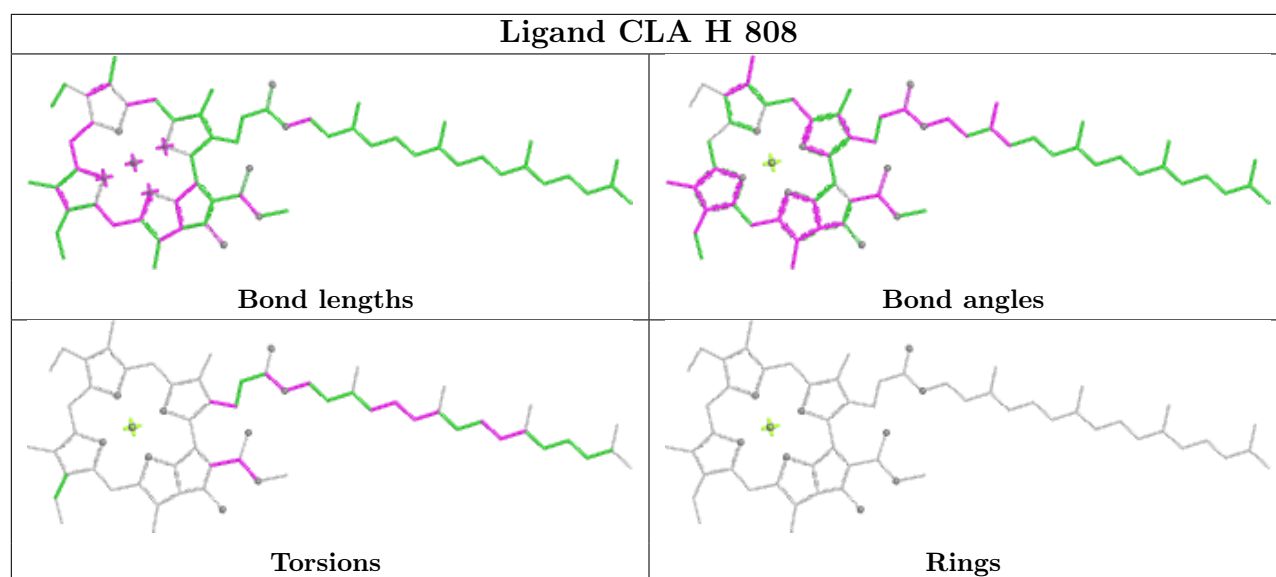


Rings

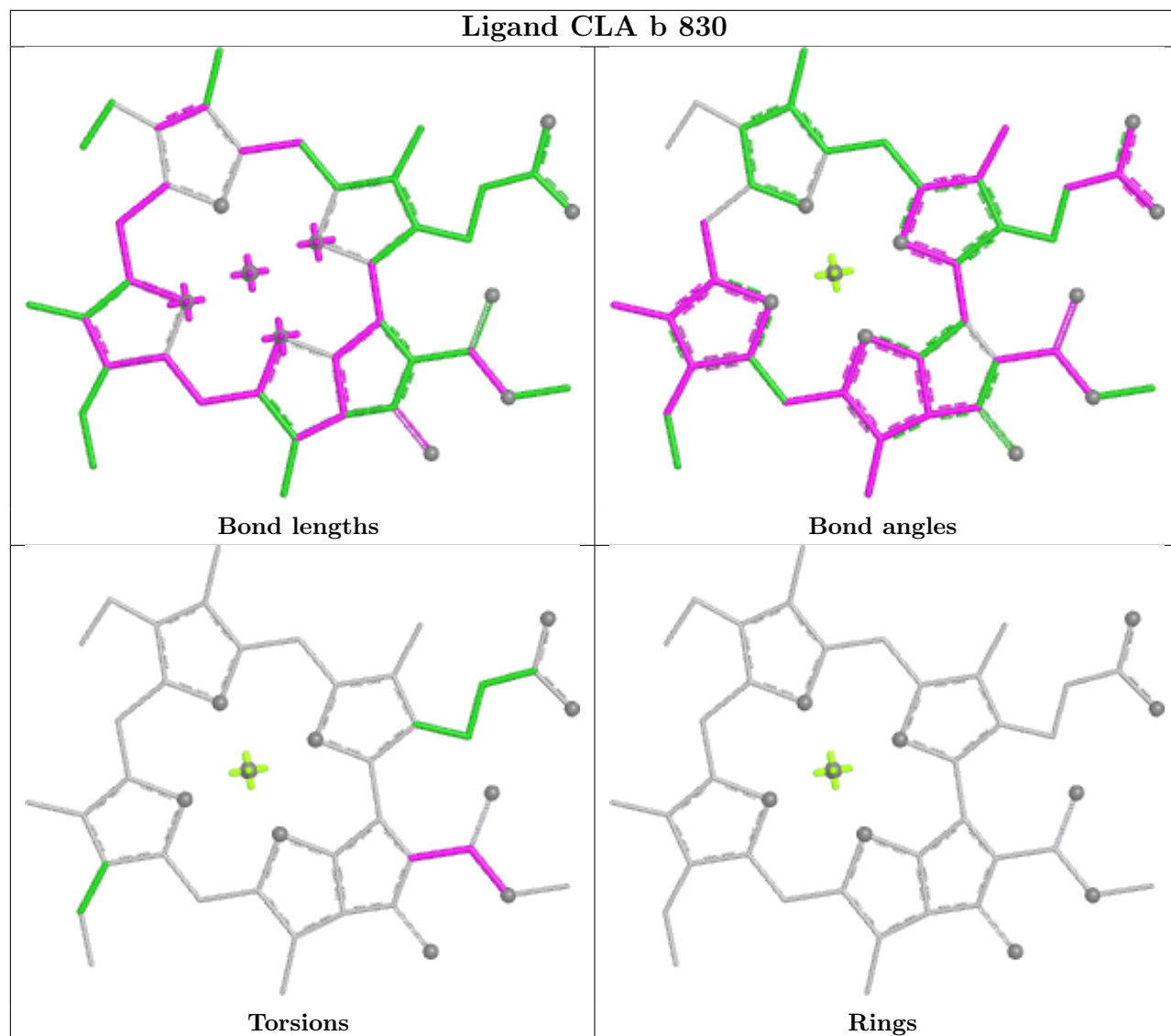




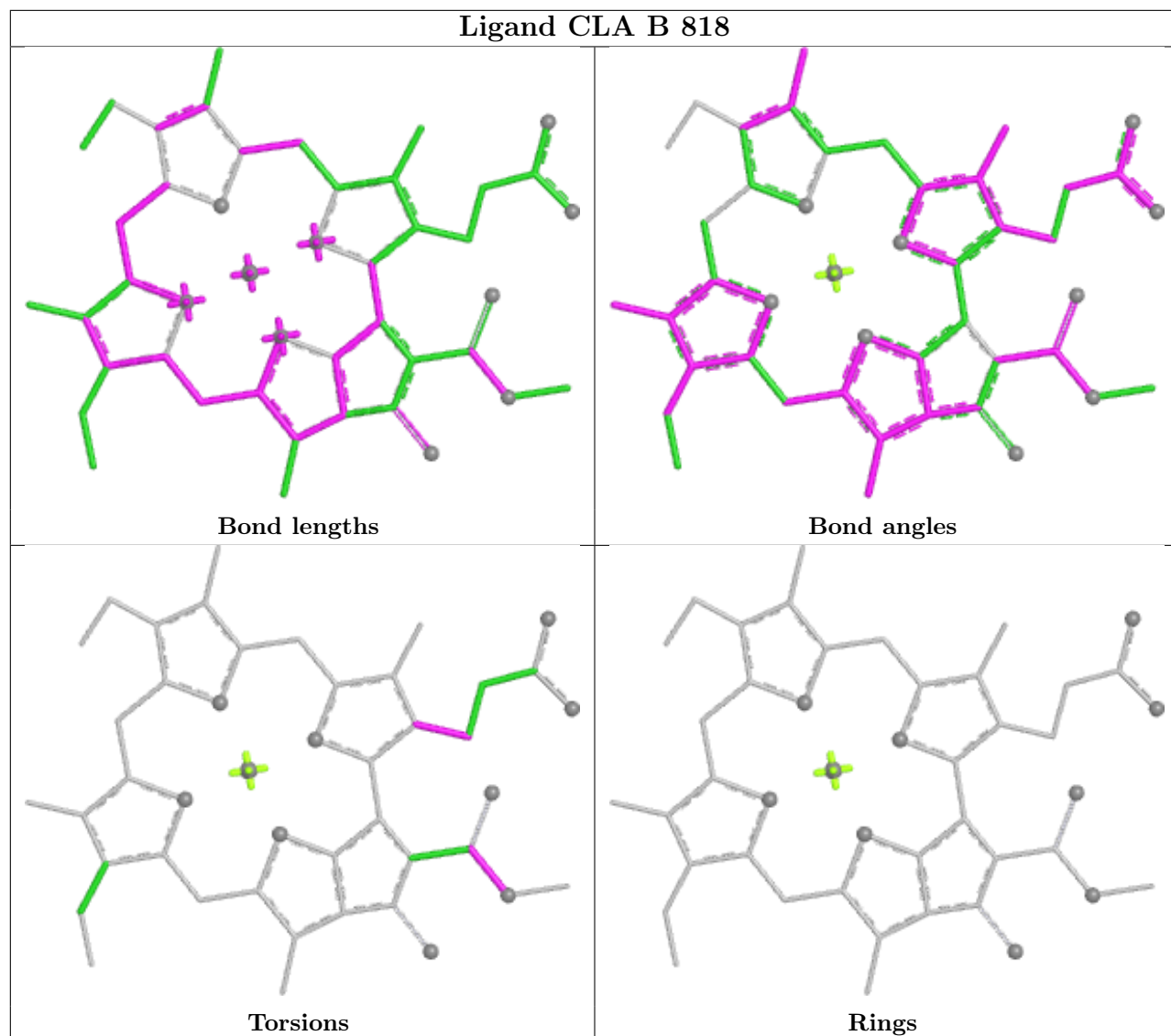




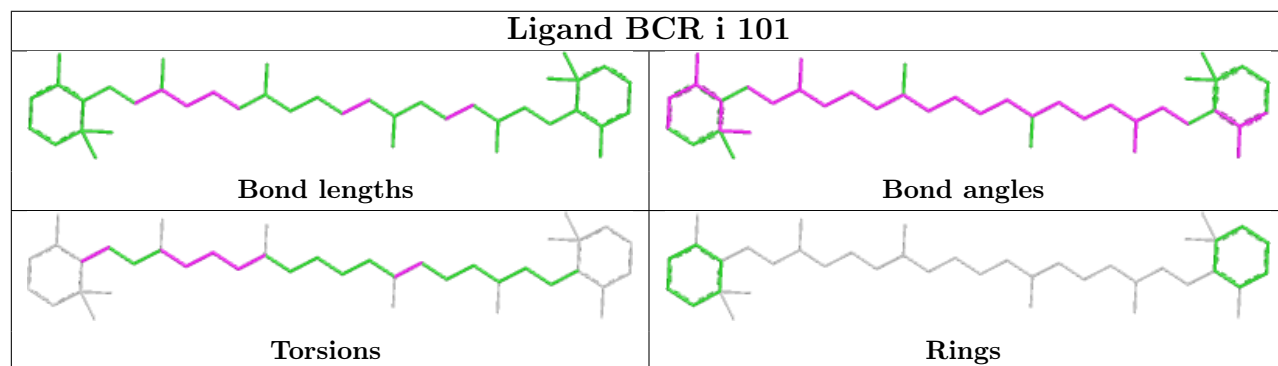
Ligand CLA b 830



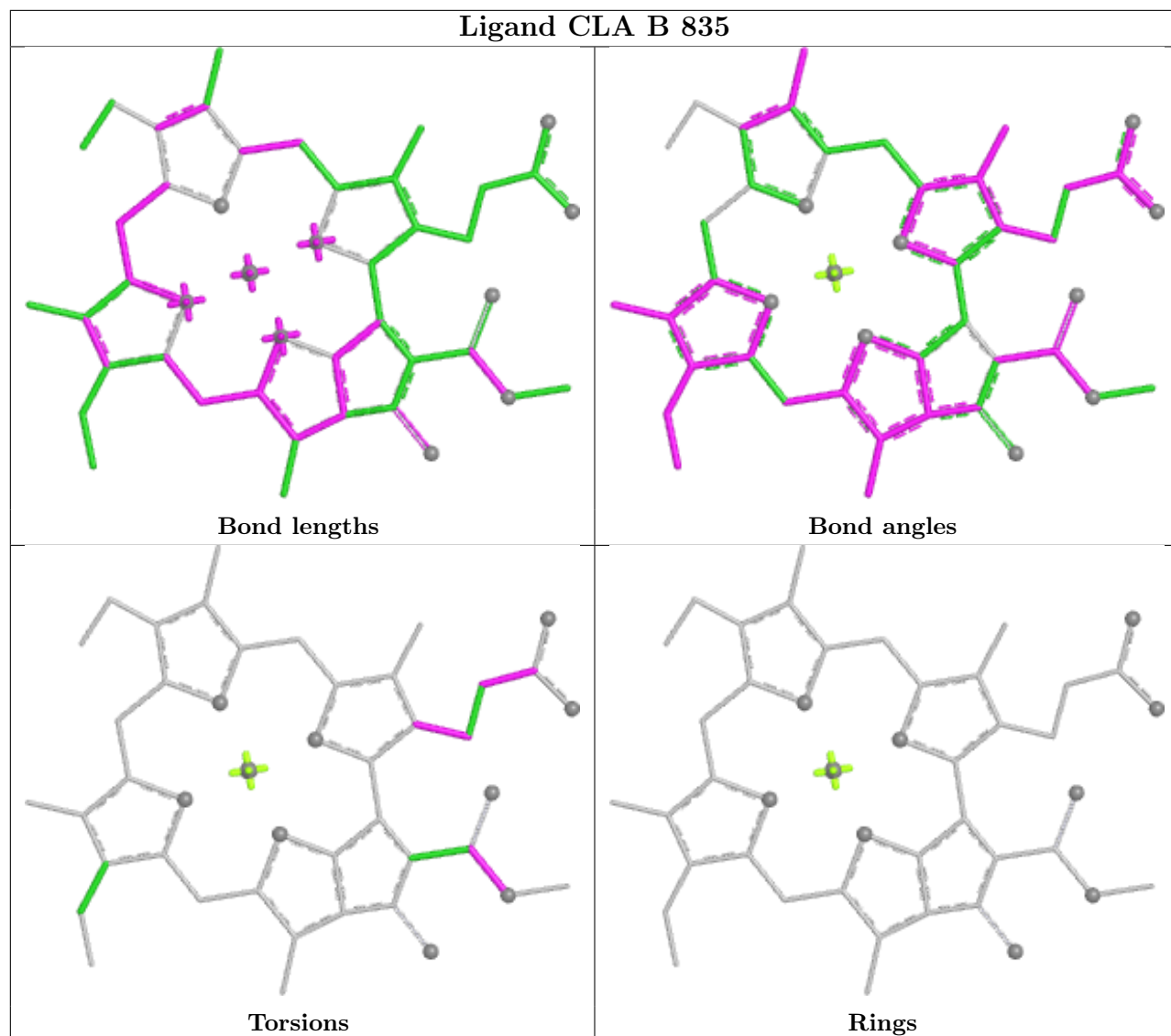
Ligand CLA B 818

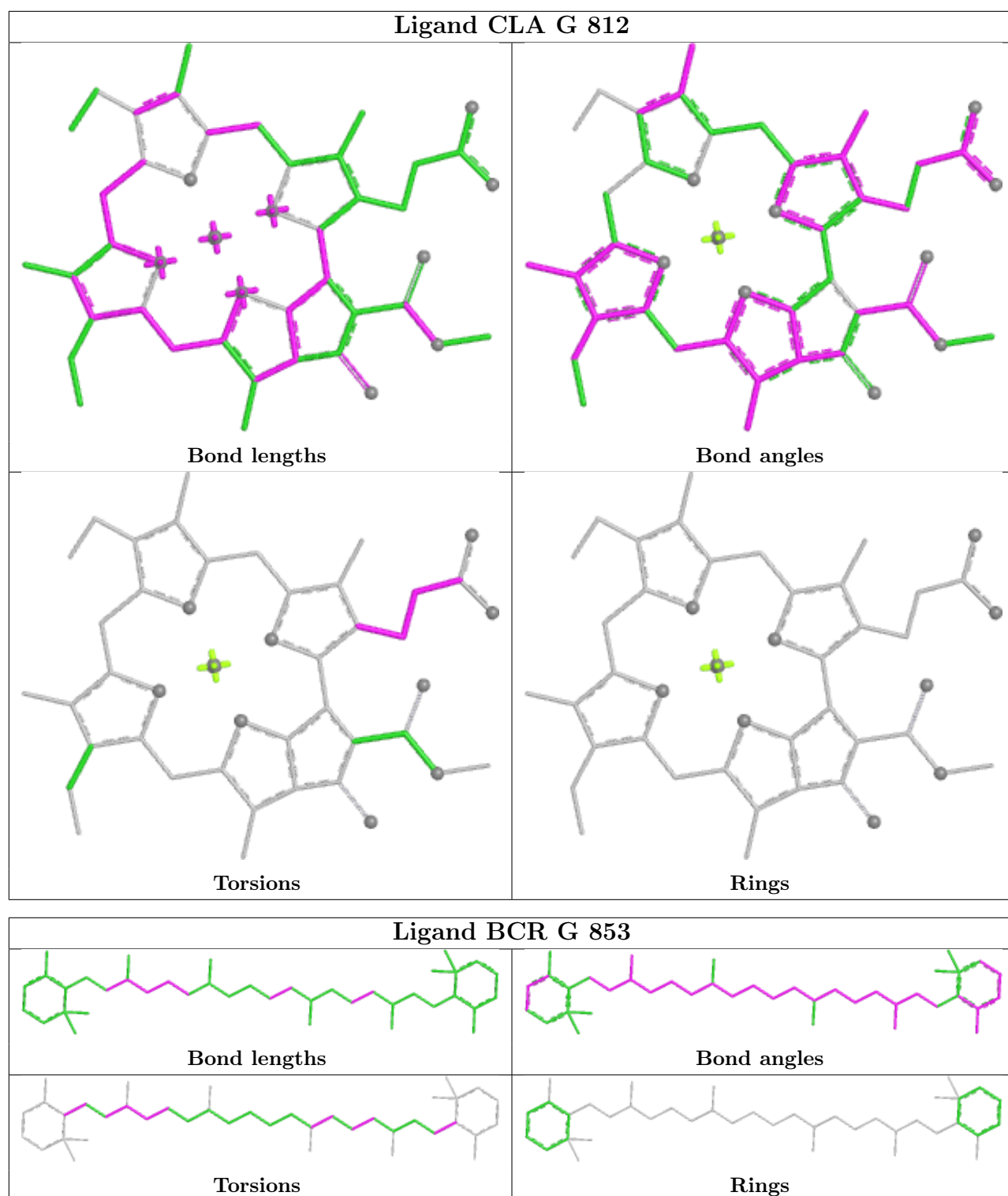


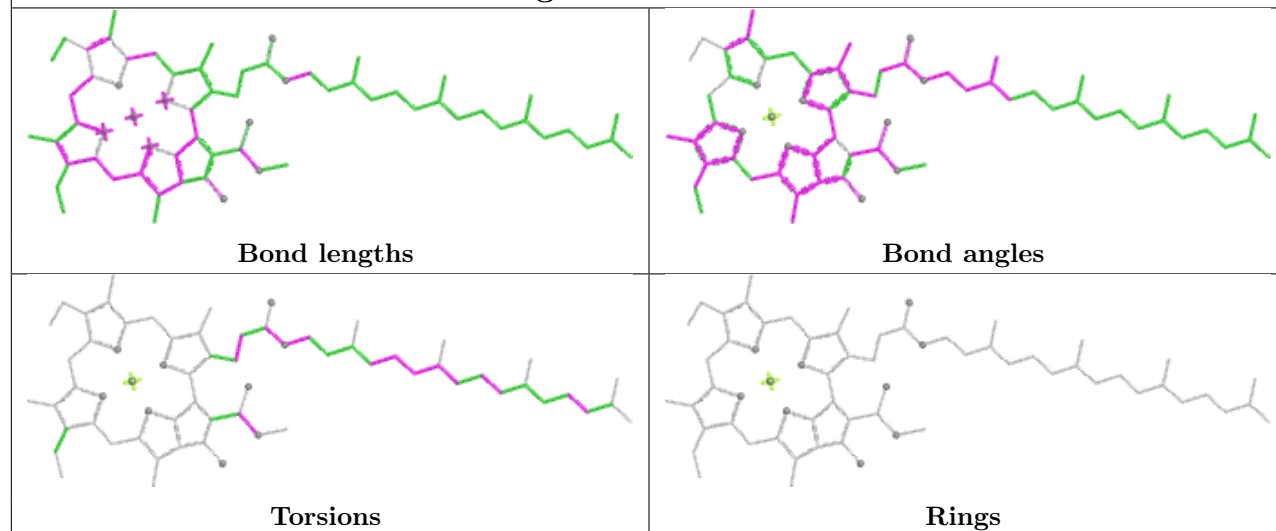
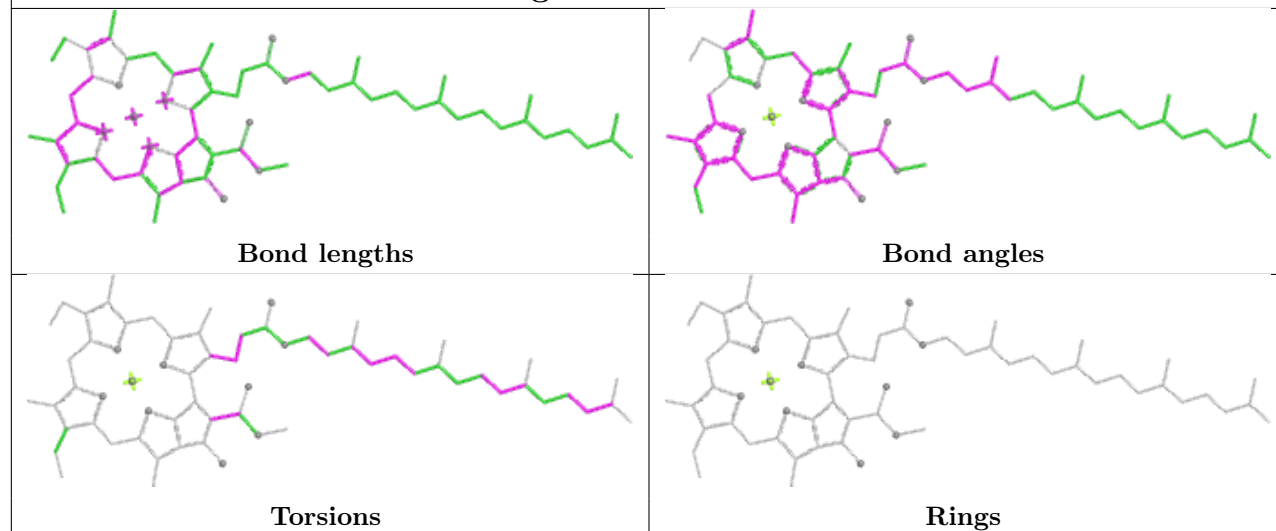
Ligand BCR i 101

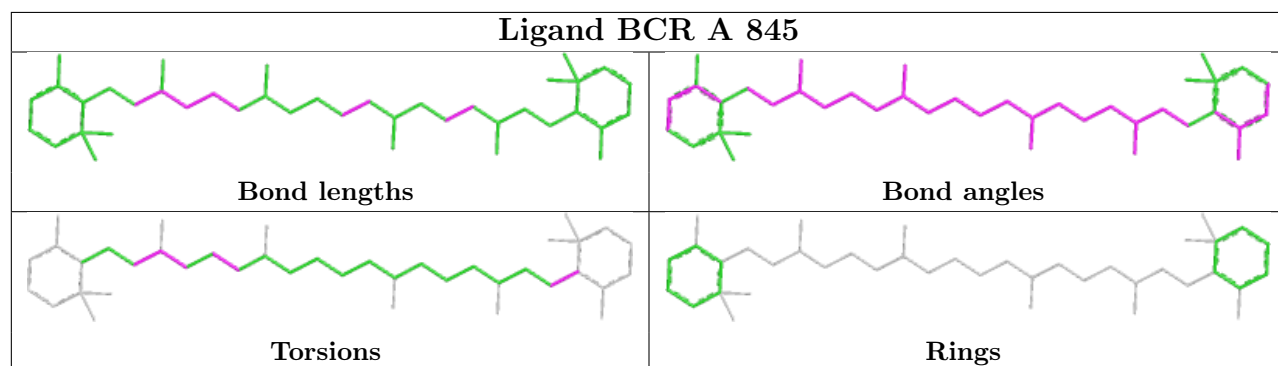
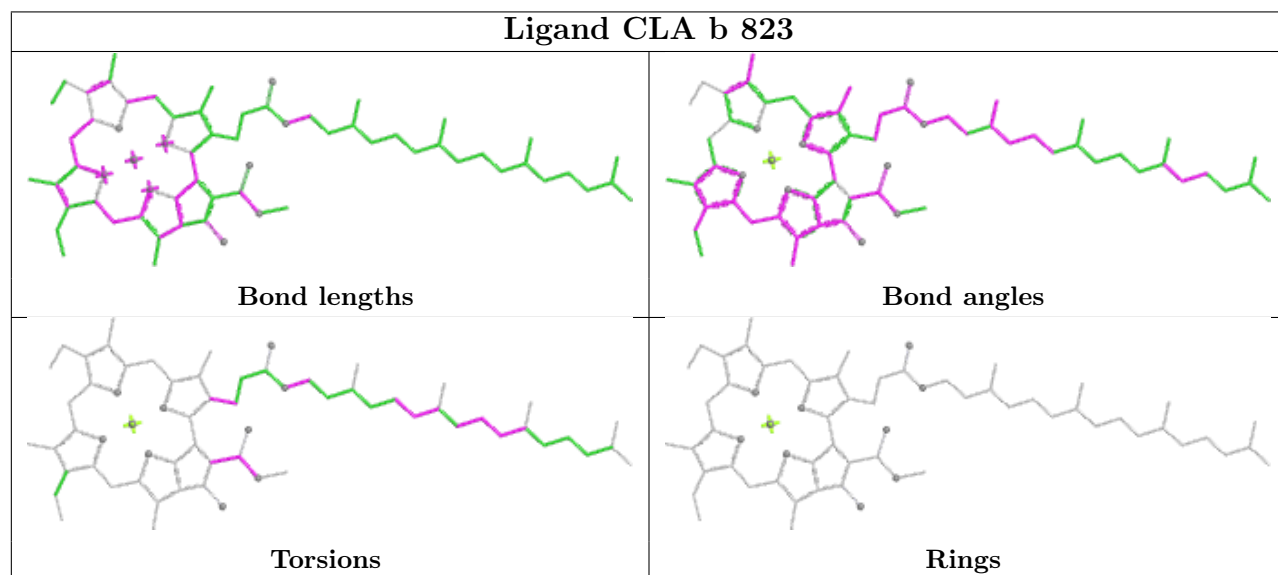
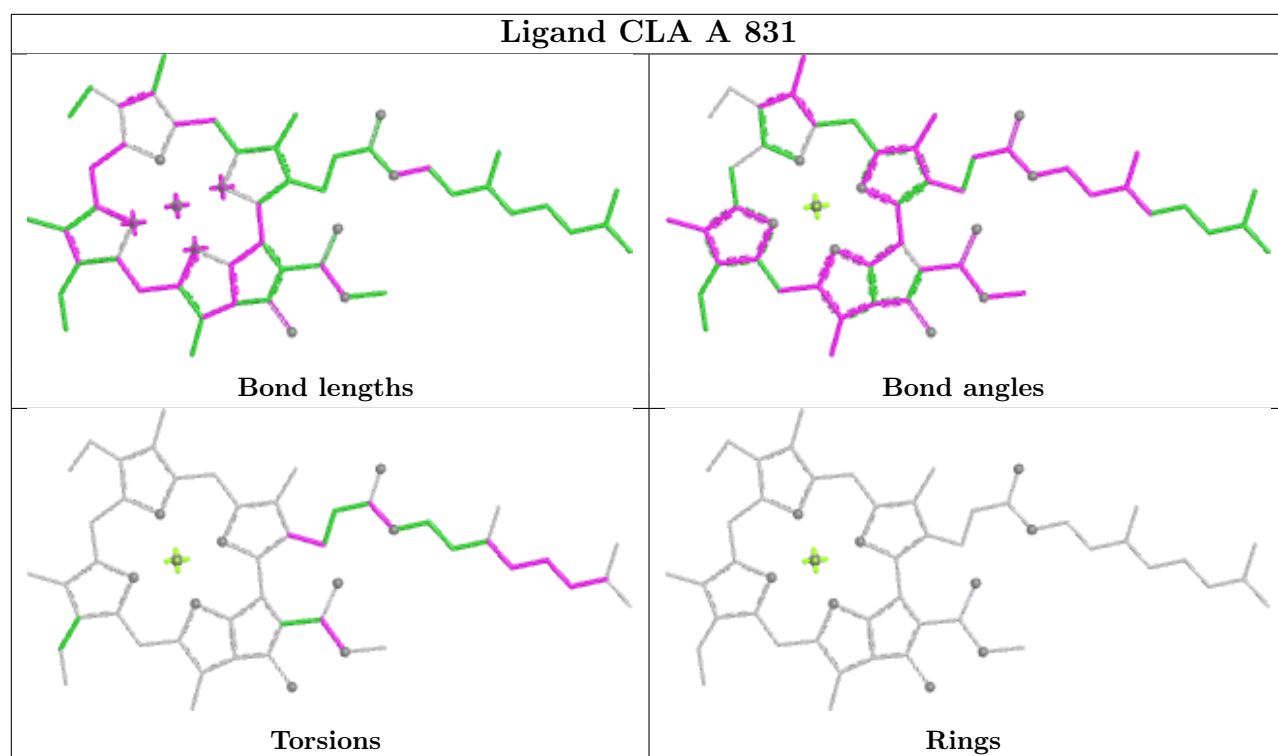


Ligand CLA B 835

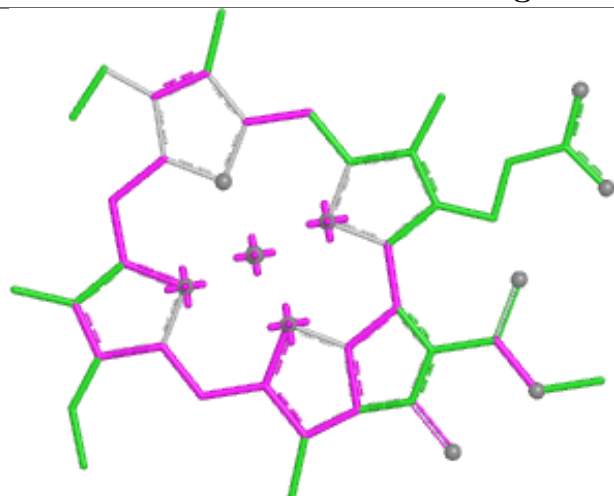




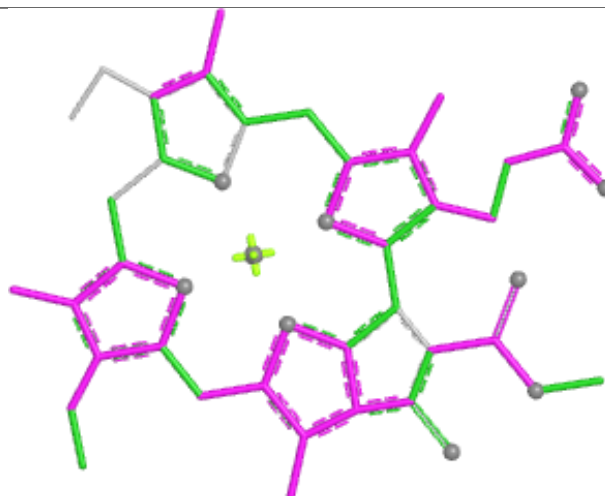
Ligand CLA a 803**Ligand CLA A 854**



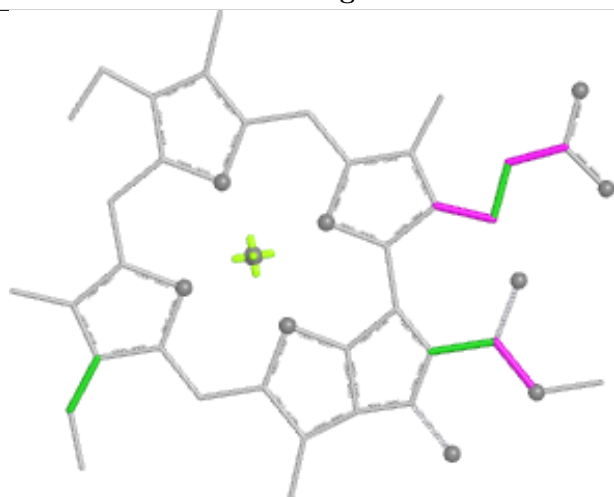
Ligand CLA R 103



Bond lengths



Bond angles

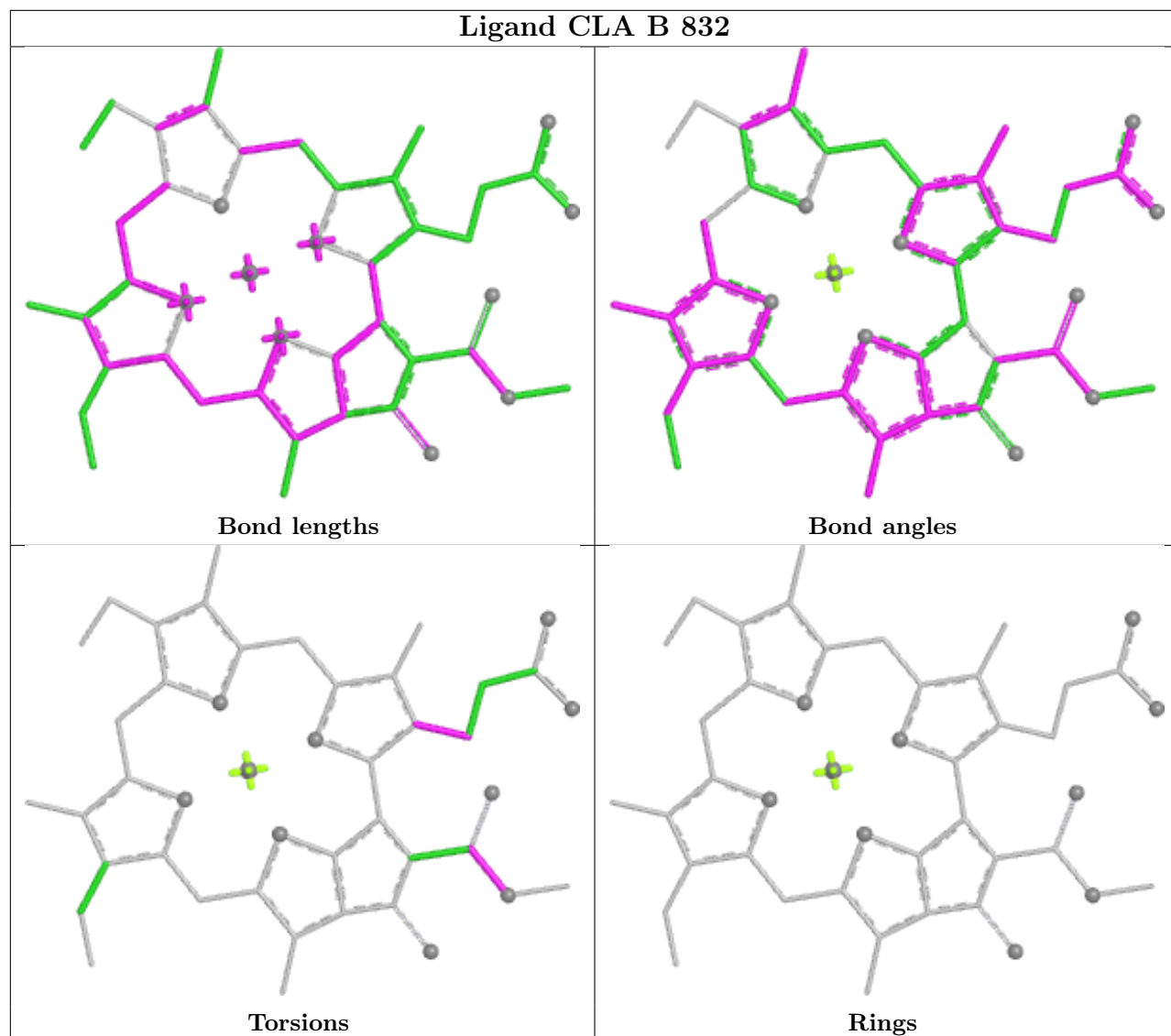


Torsions

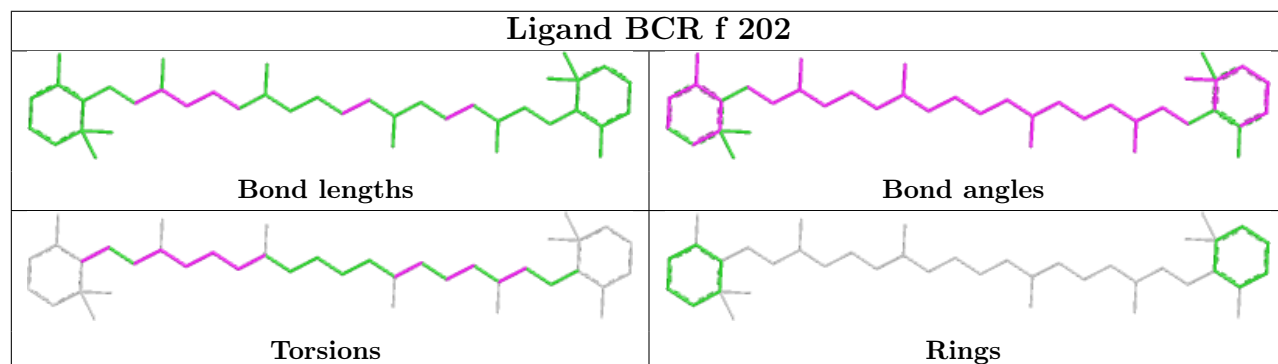


Rings

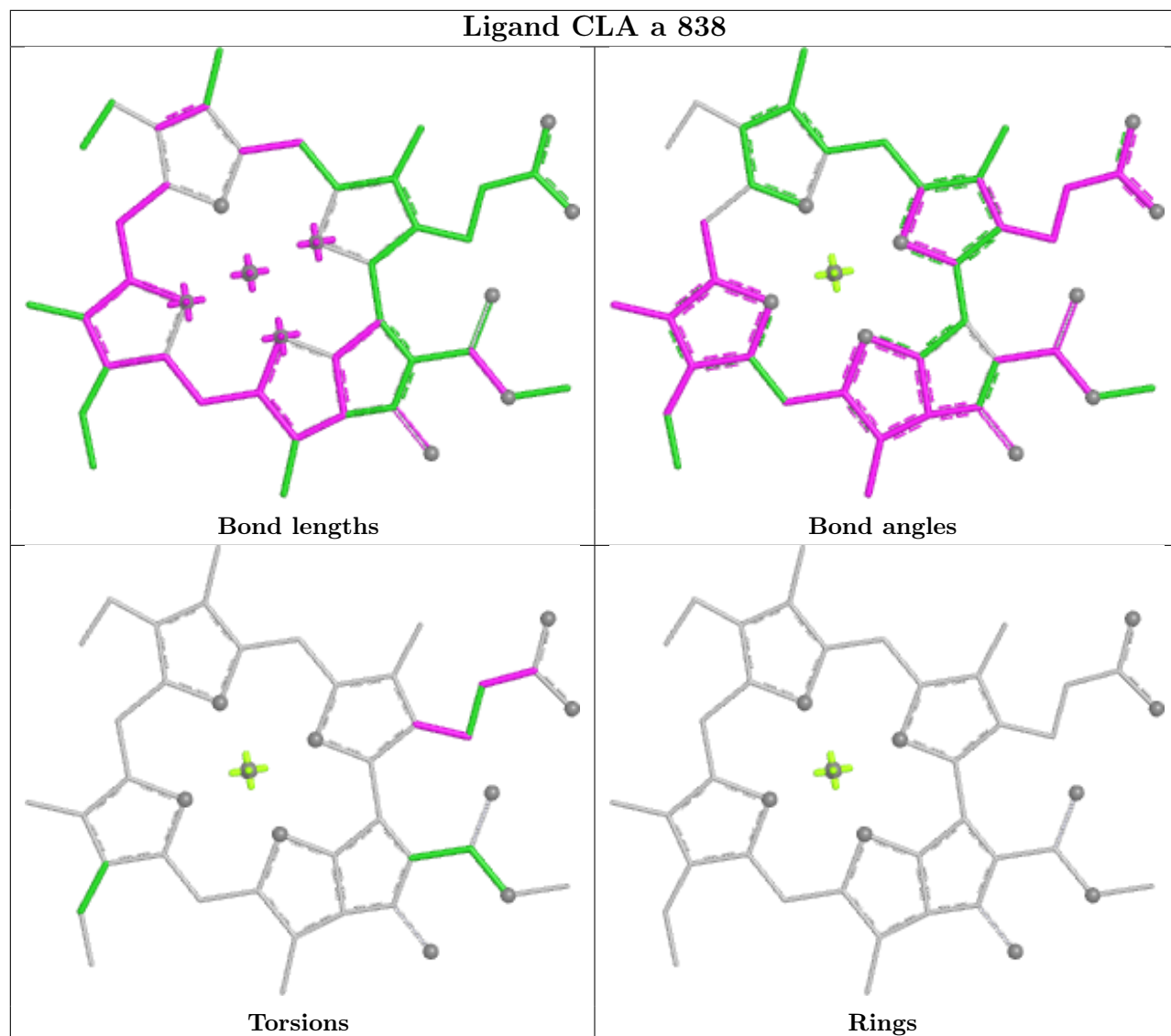
Ligand CLA B 832



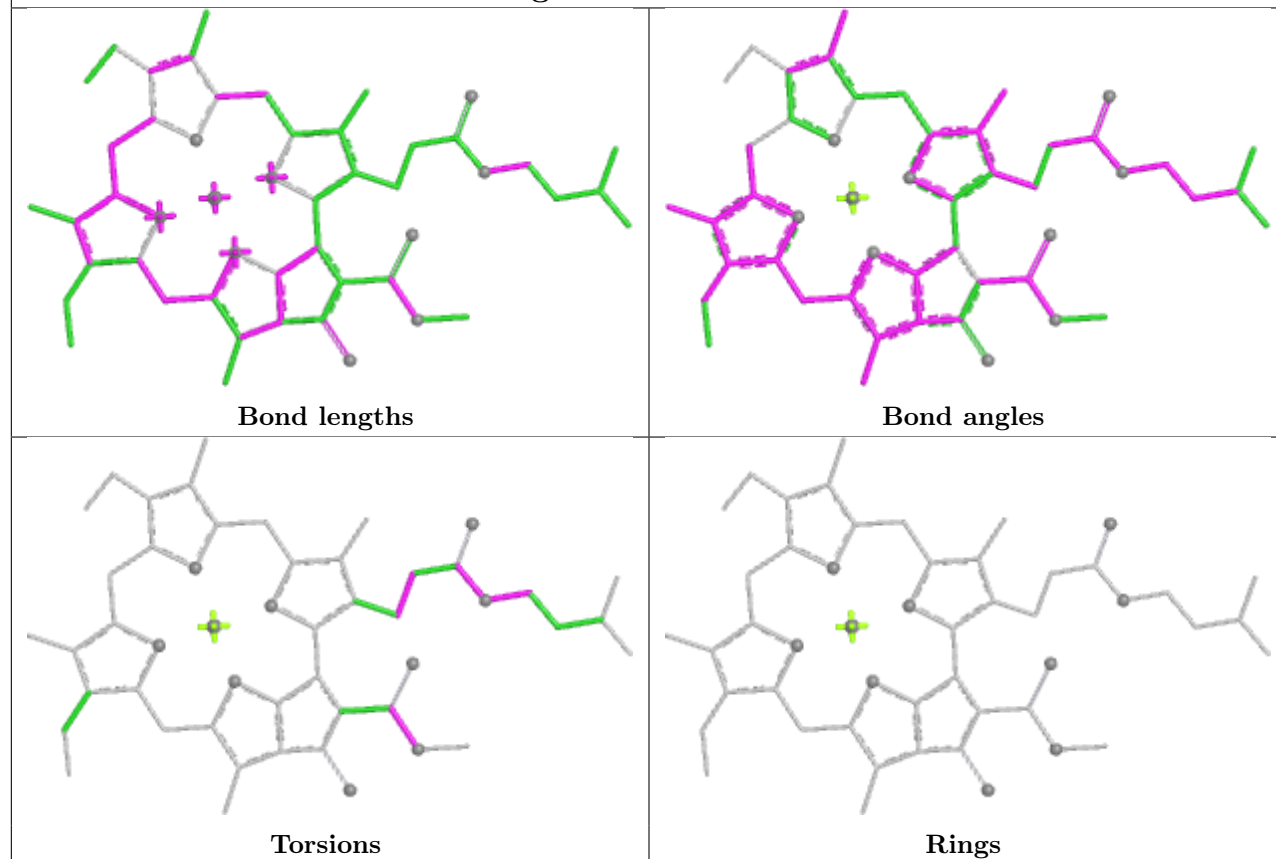
Ligand BCR f 202



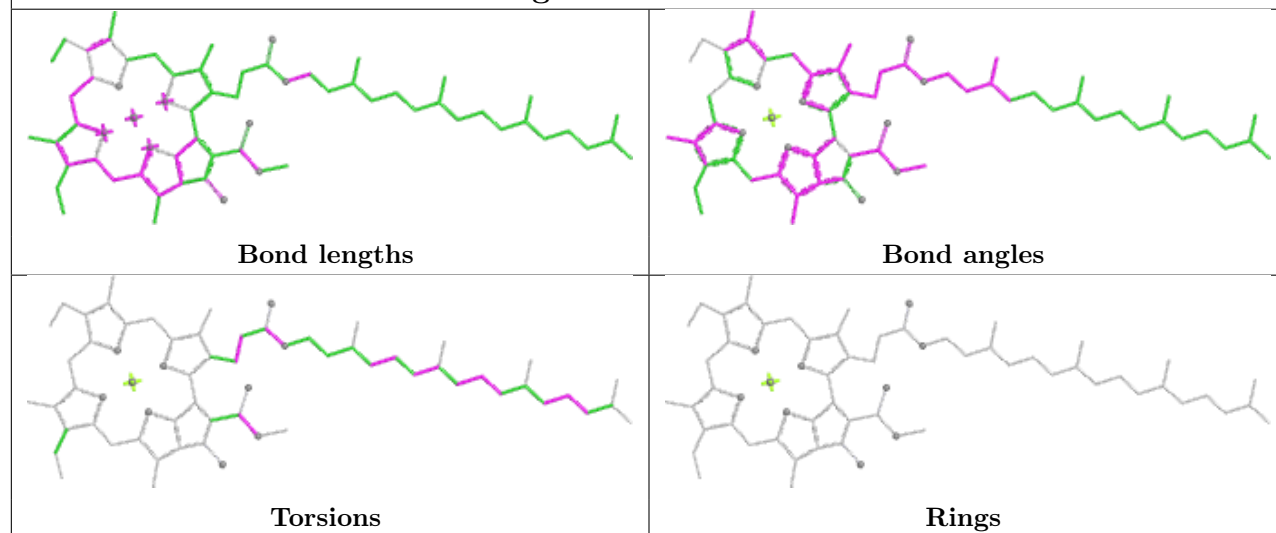
Ligand CLA a 838

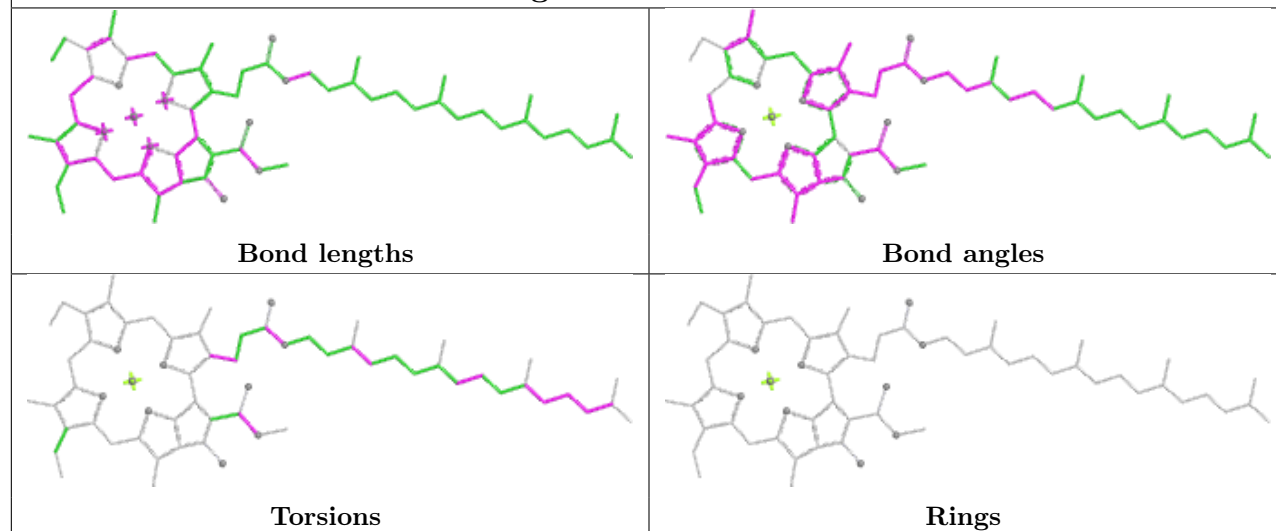
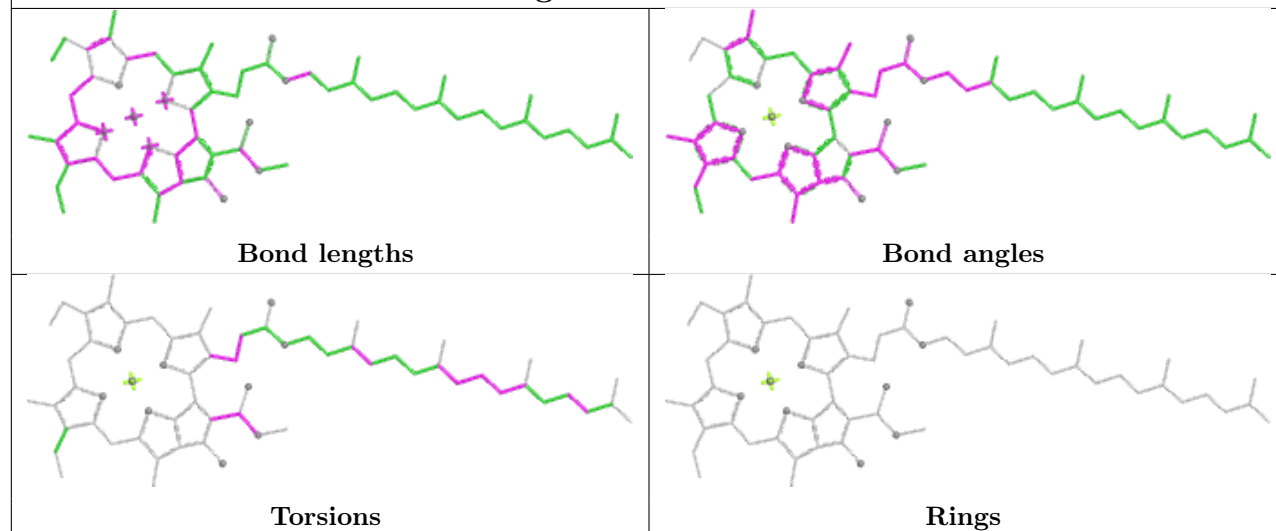


Ligand CLA A 830

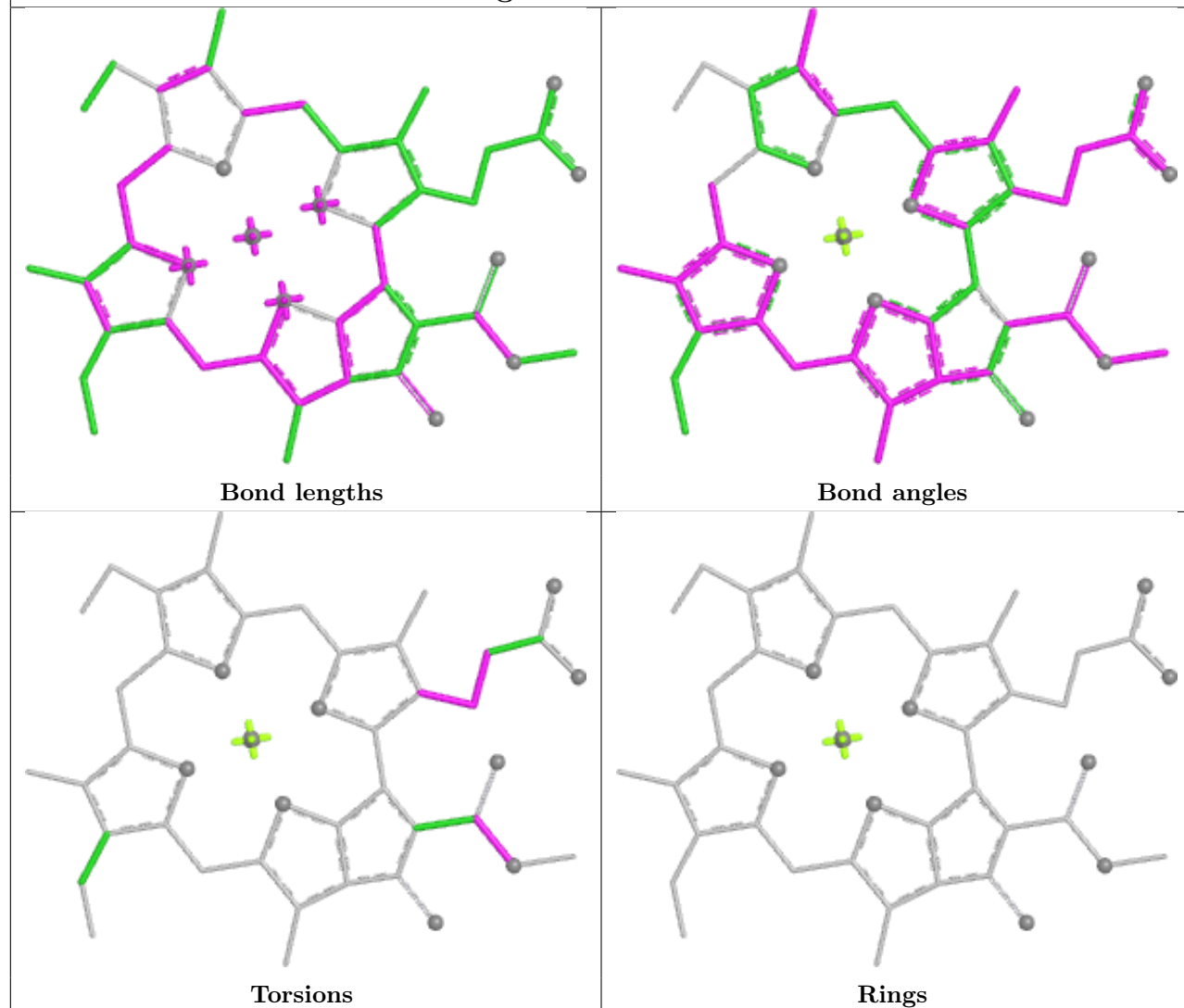


Ligand CLA B 836

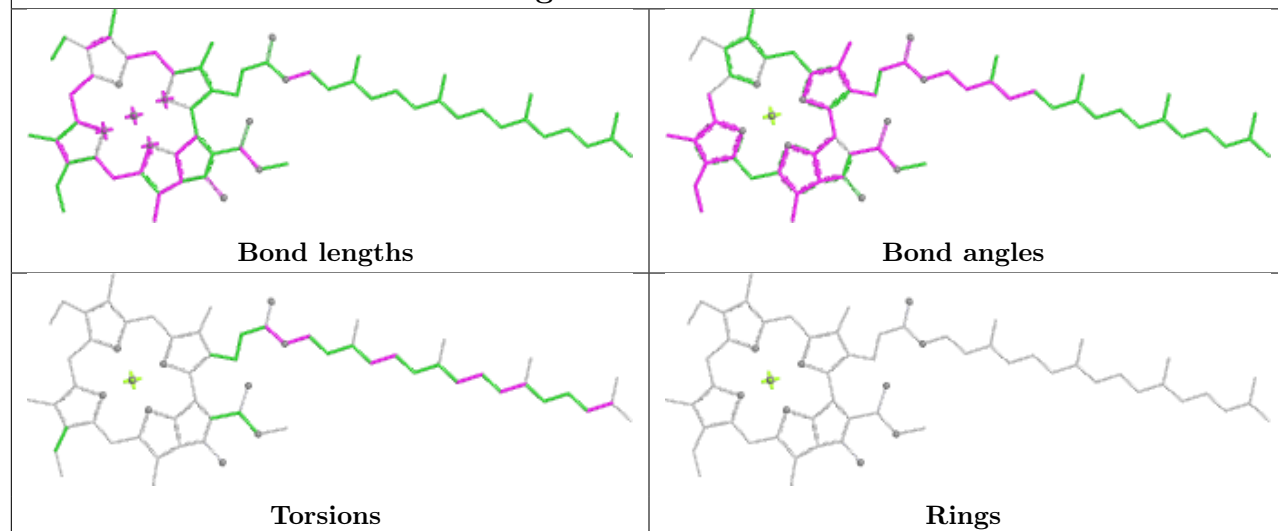


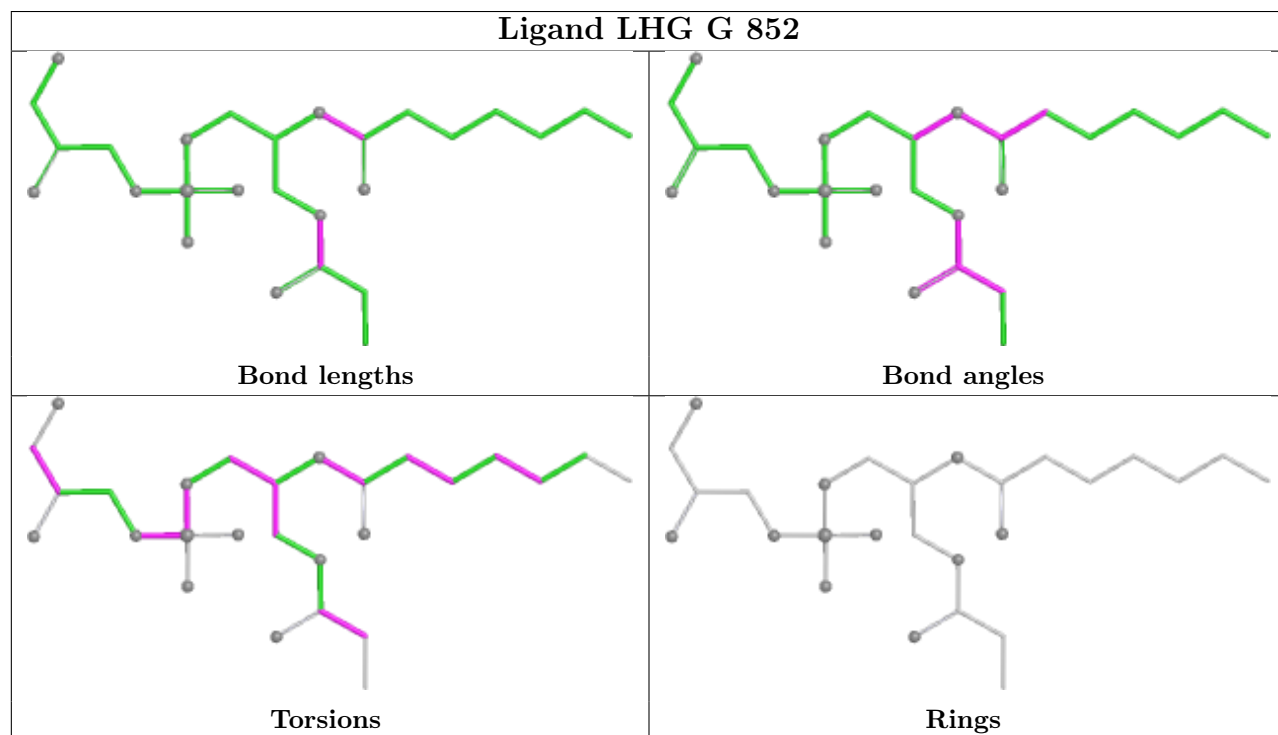
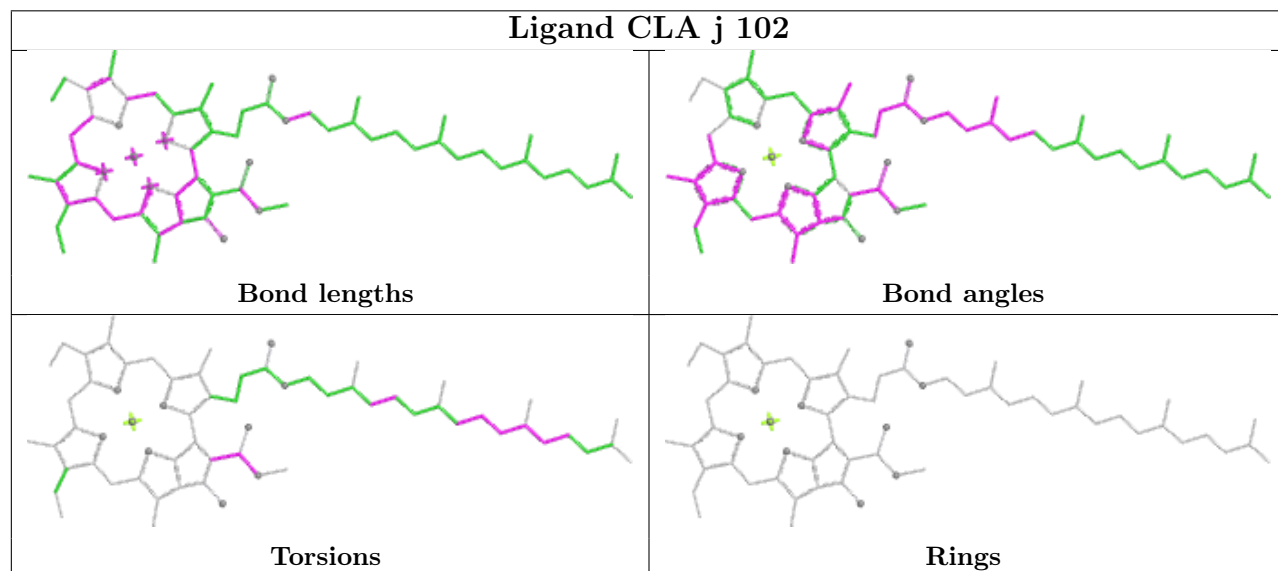
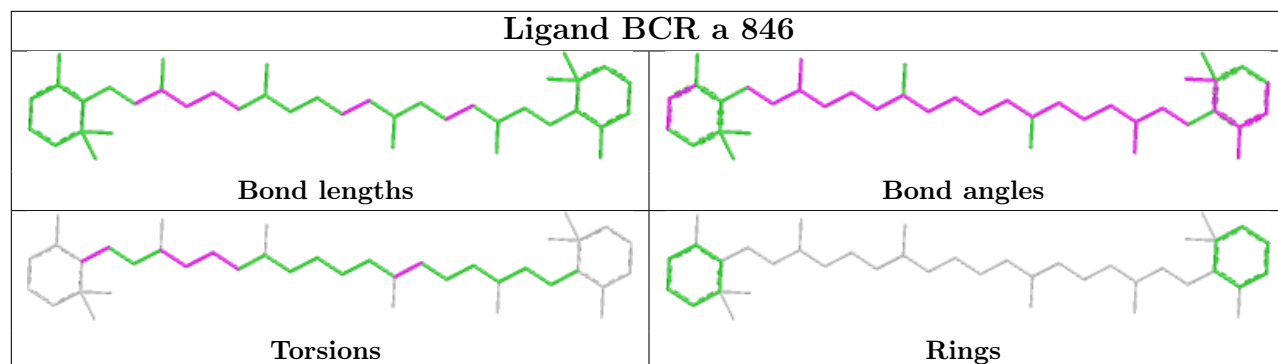
Ligand CLA G 819**Ligand CLA b 822**

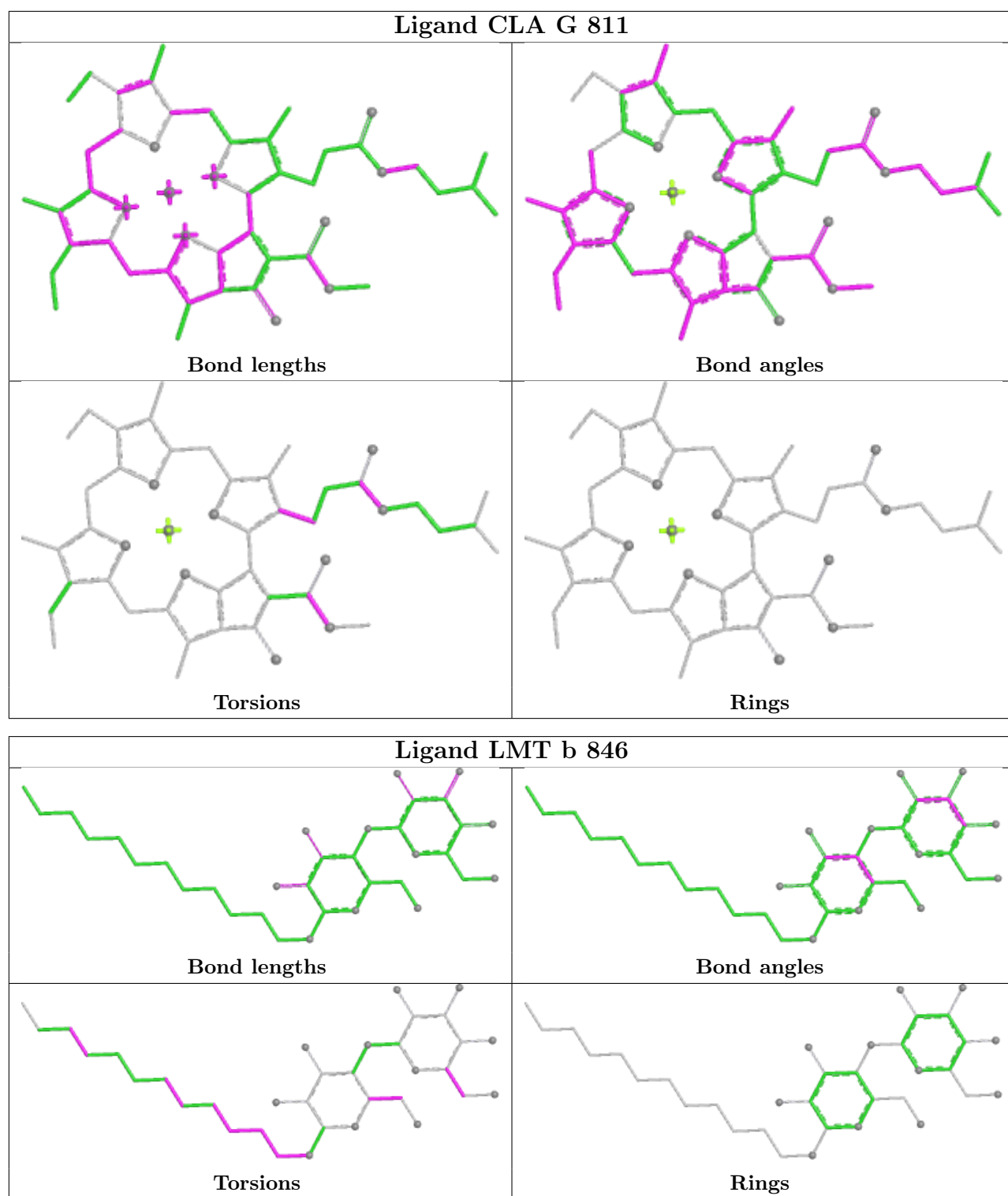
Ligand CLA a 809

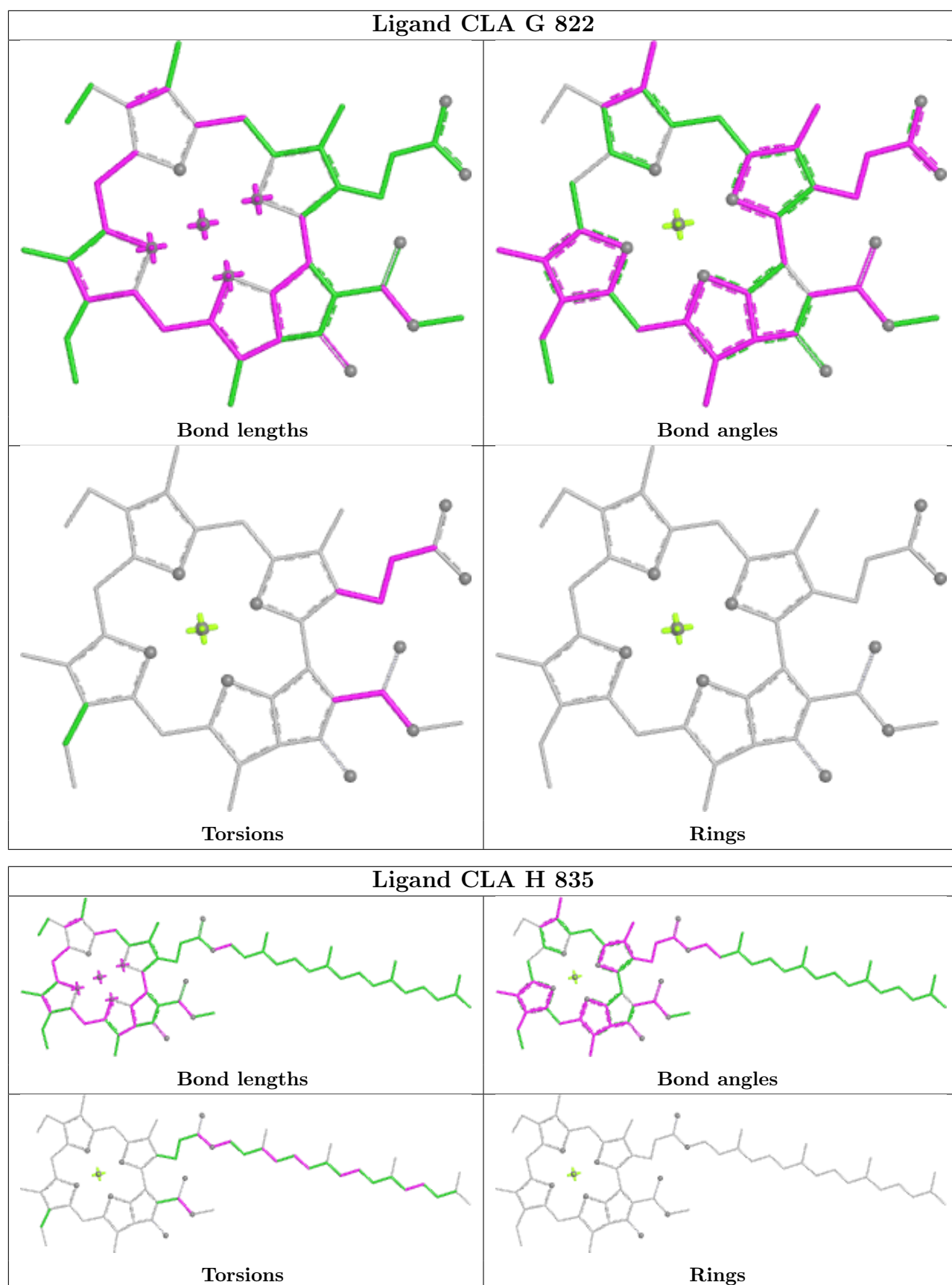


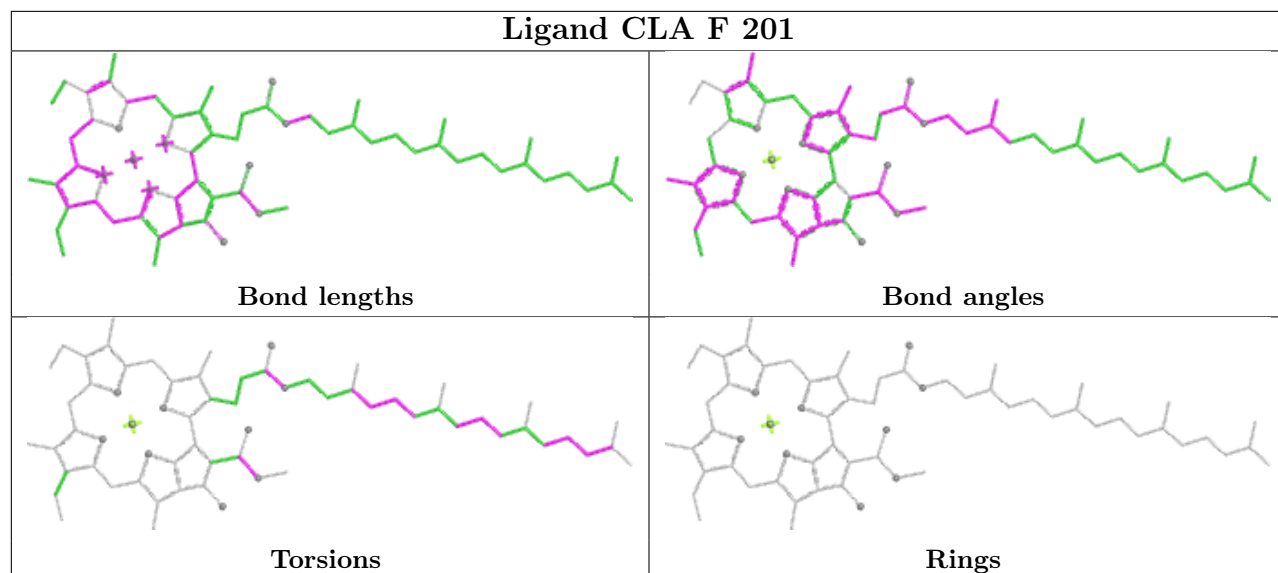
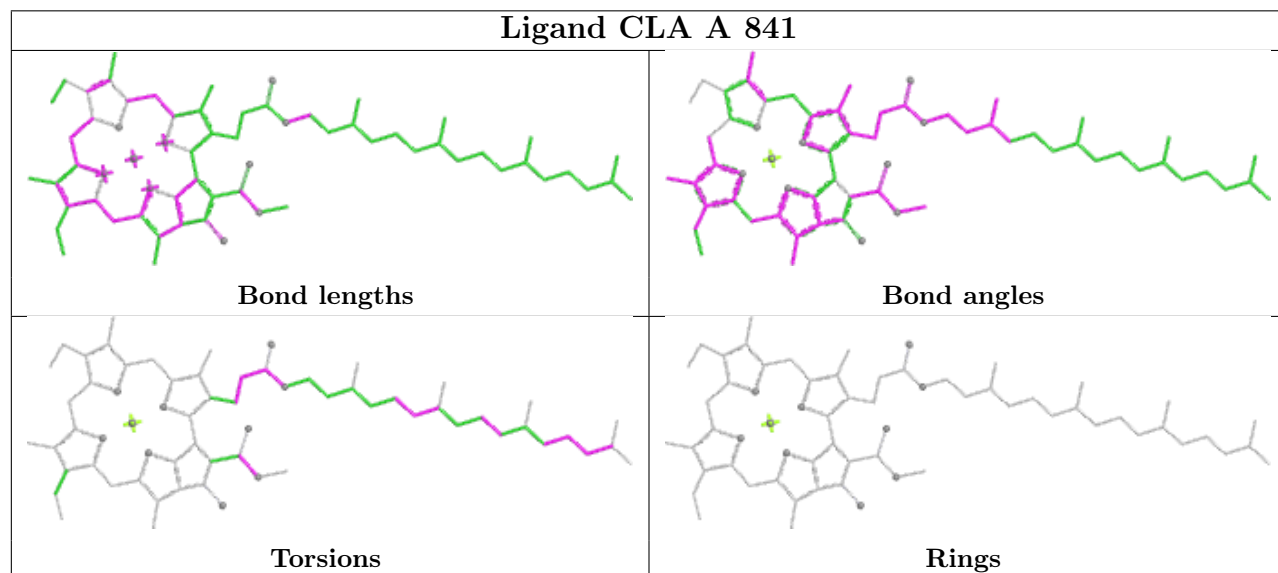
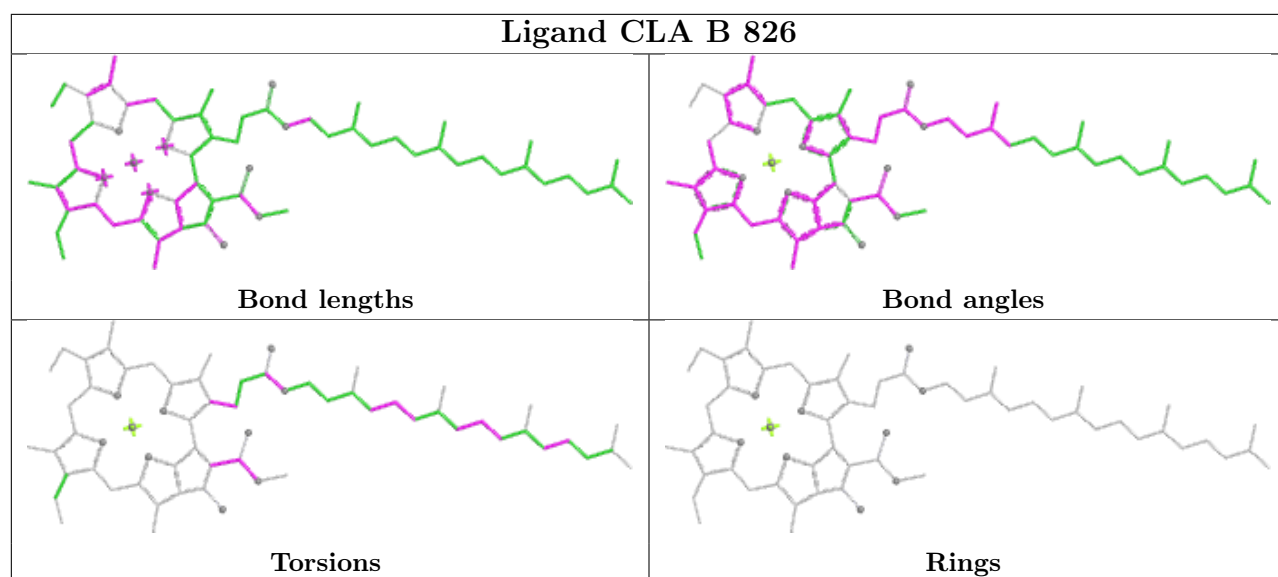
Ligand CL0 G 801

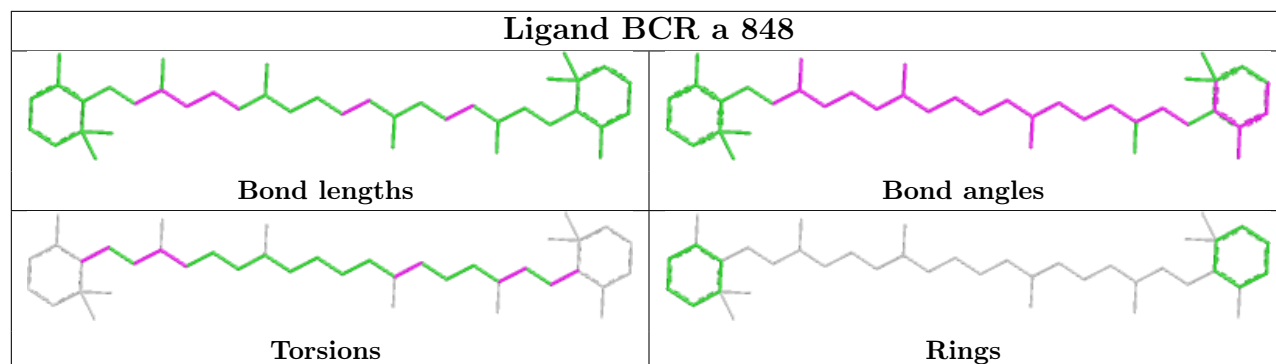
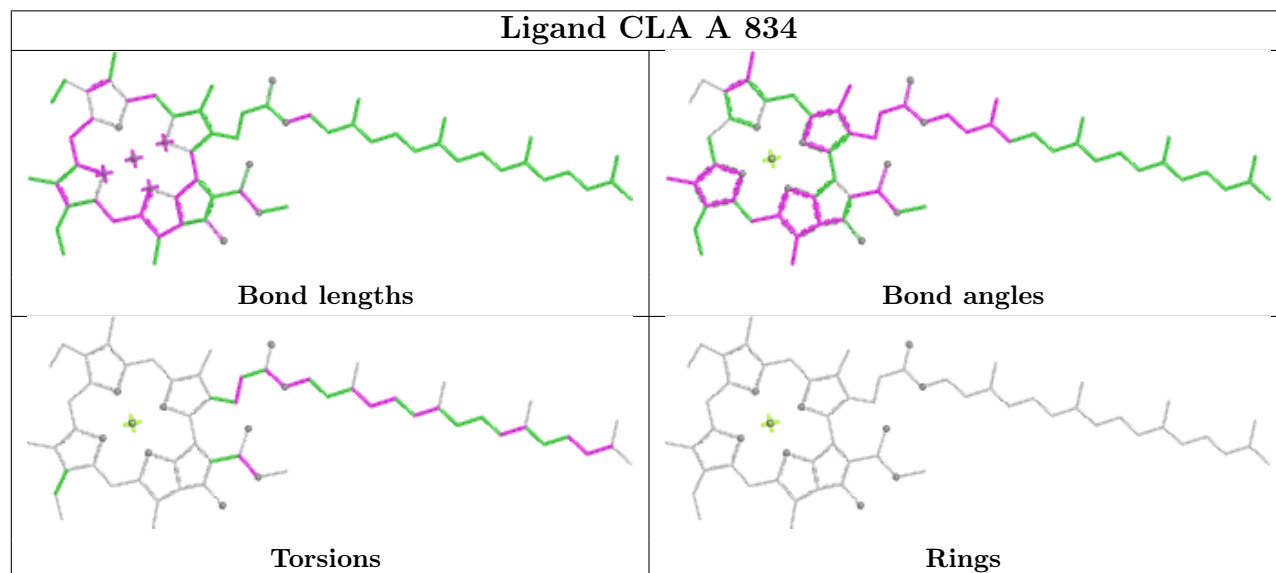
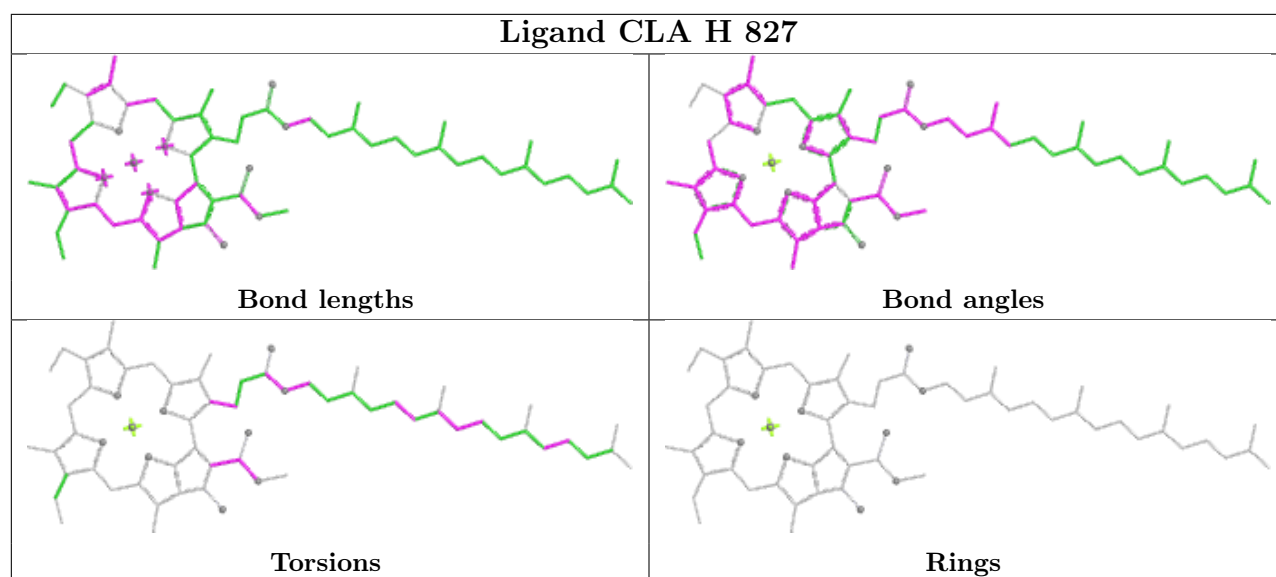


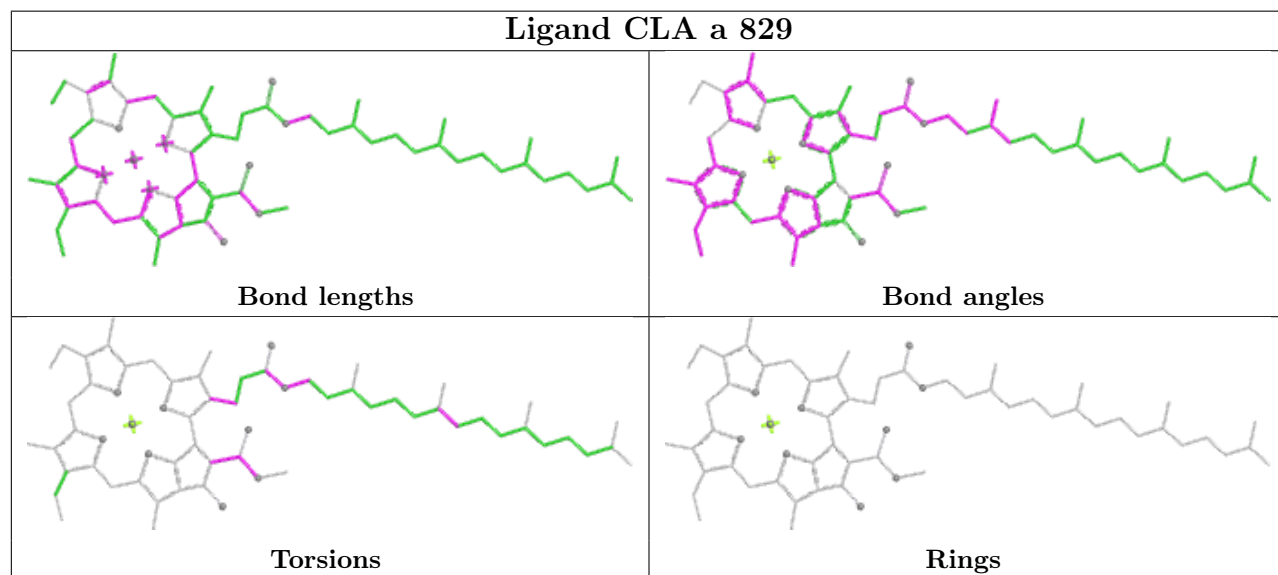
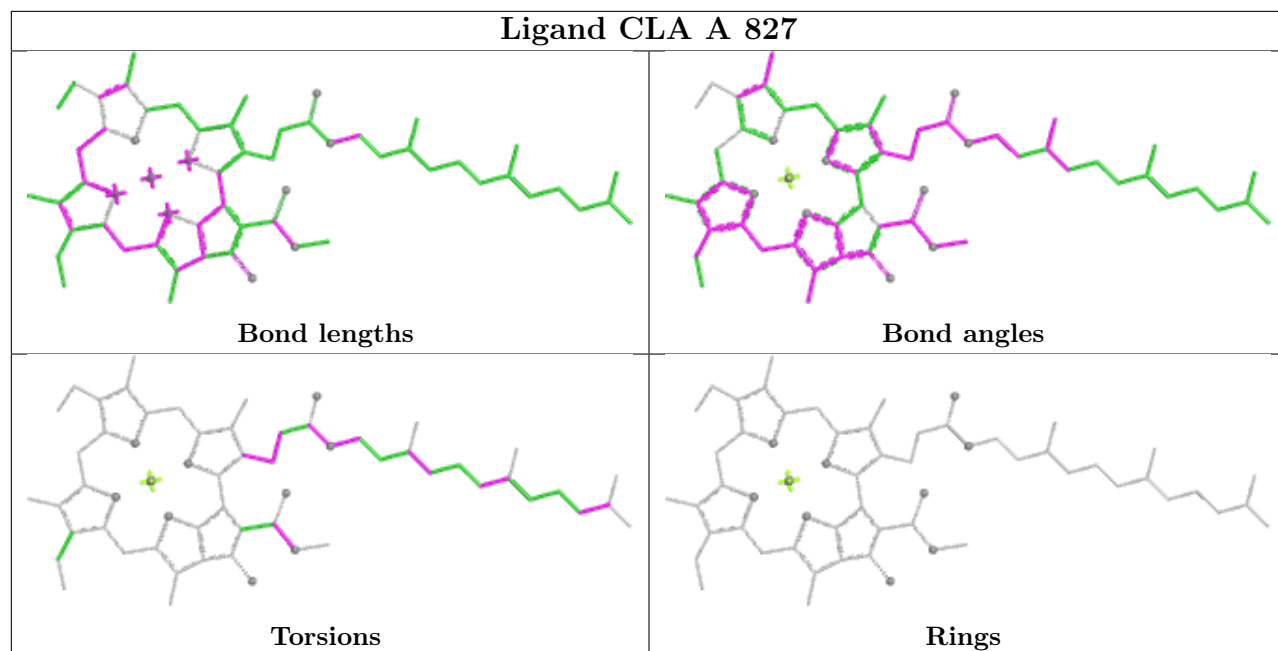


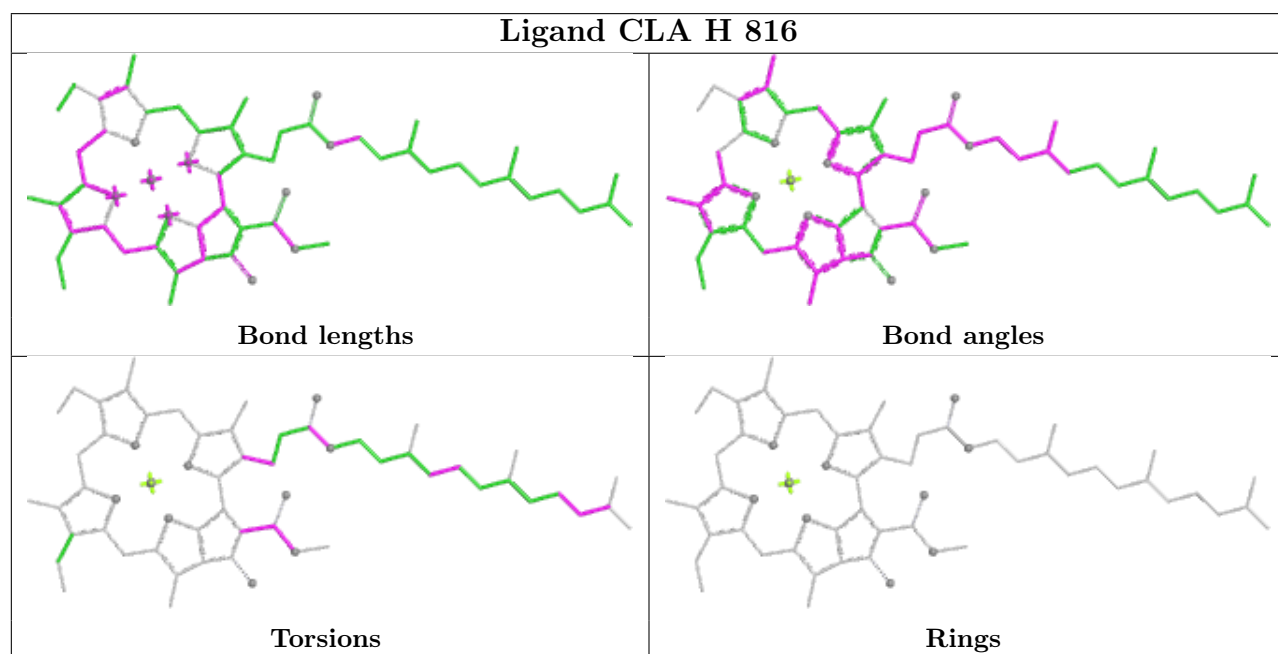
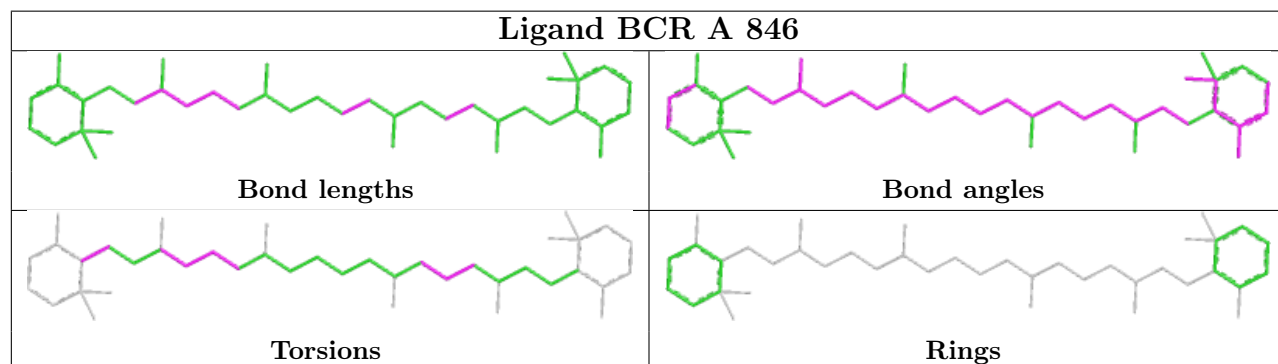
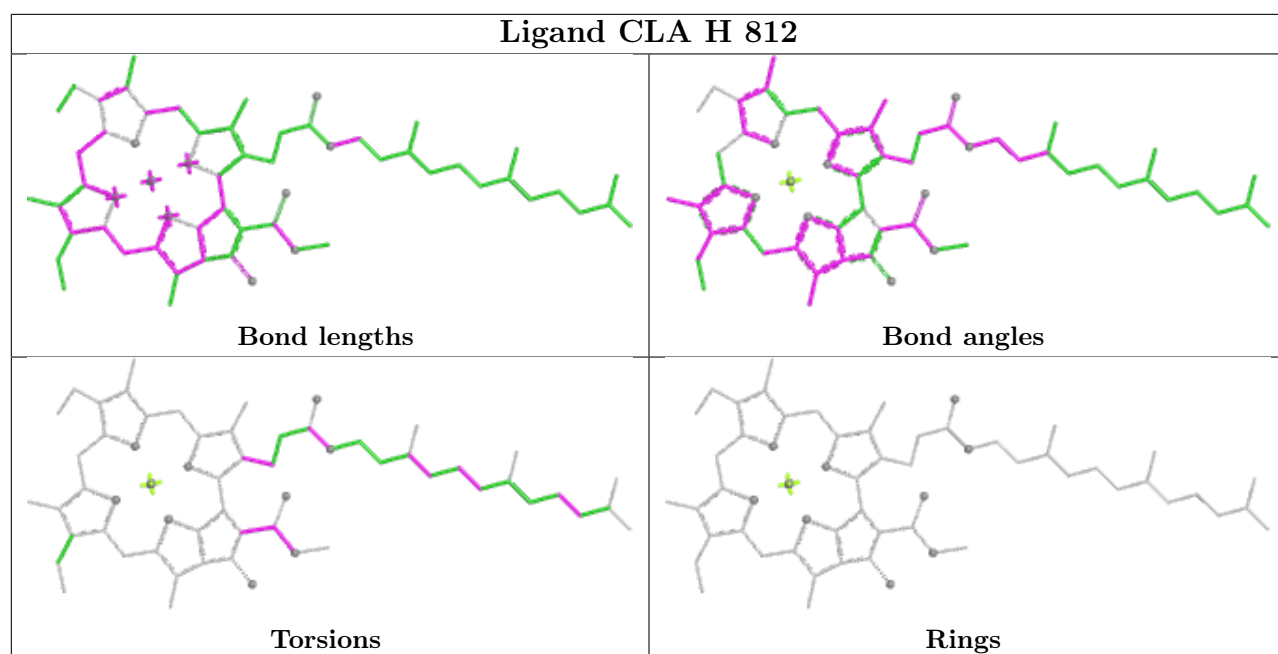


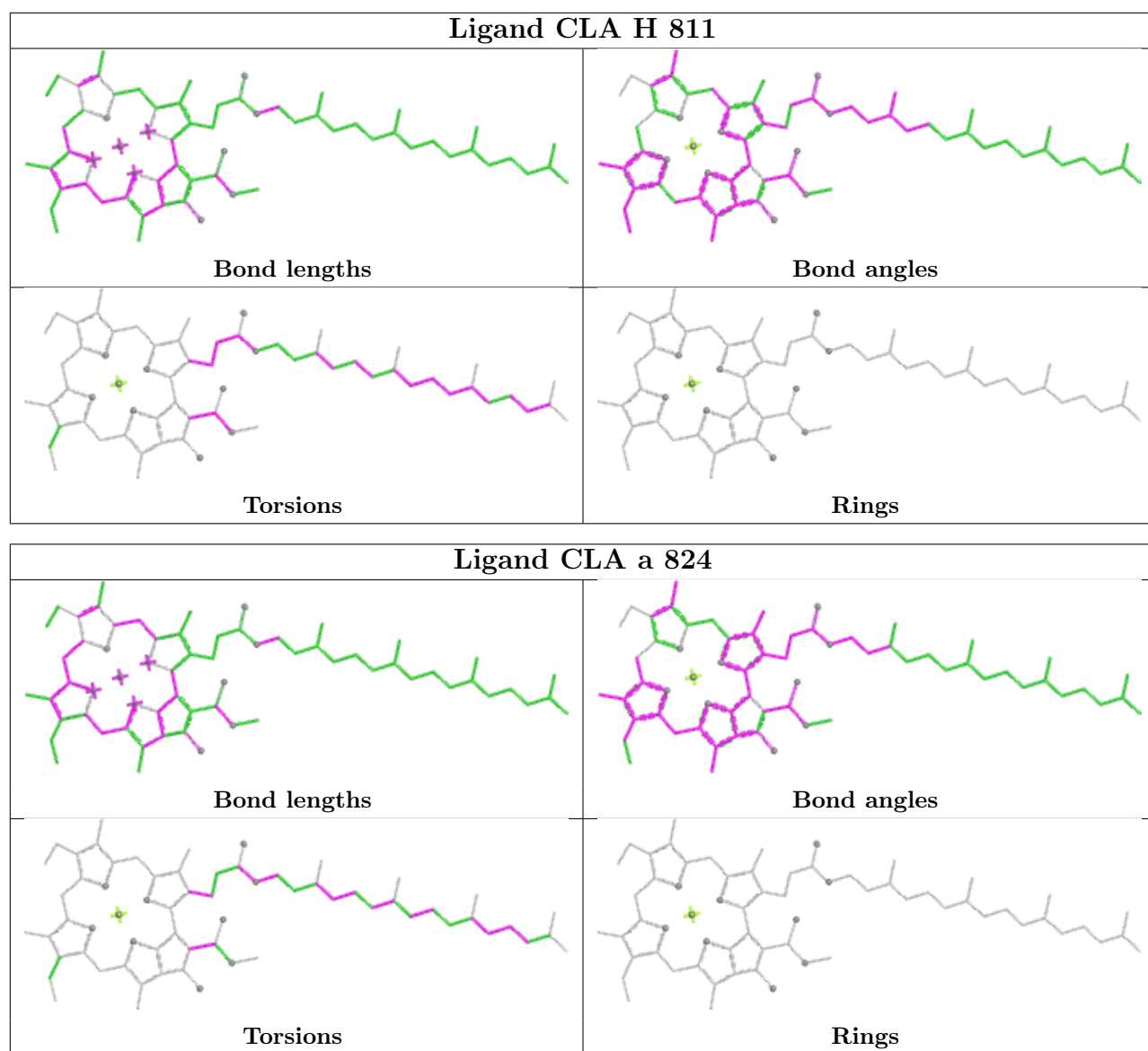




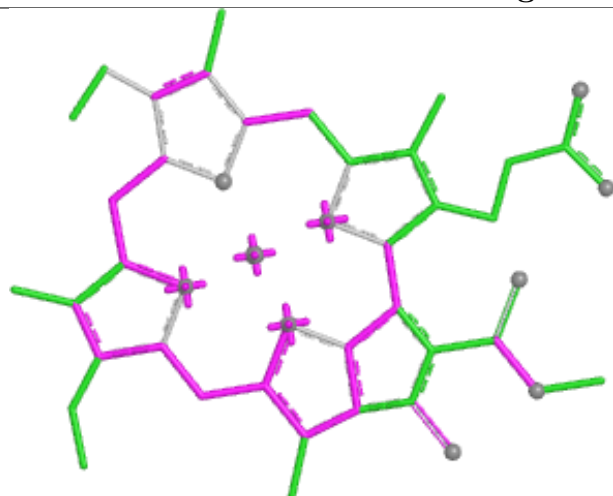




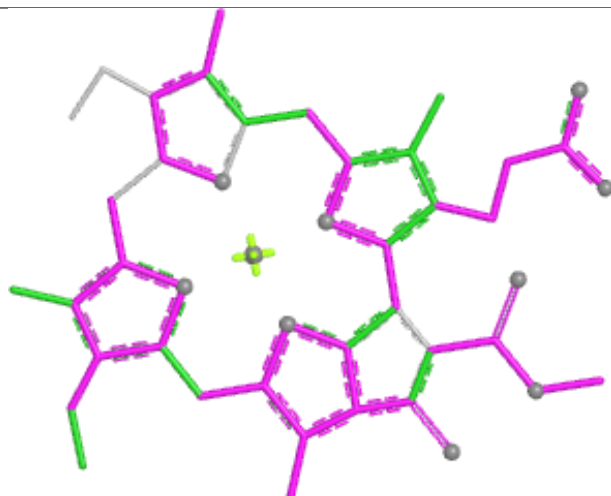




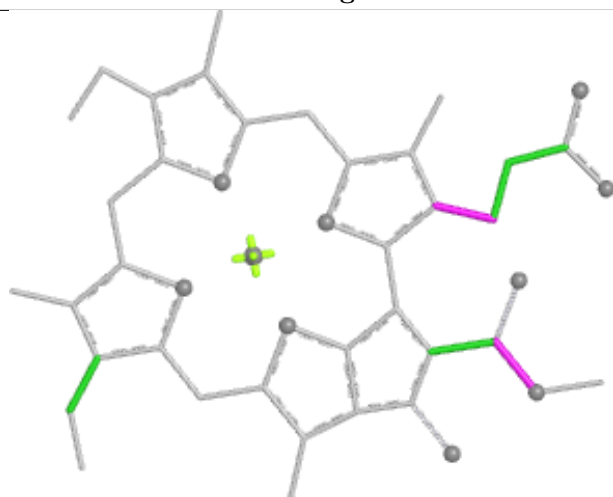
Ligand CLA b 828



Bond lengths



Bond angles

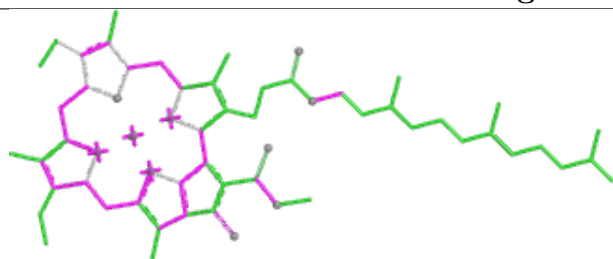


Torsions

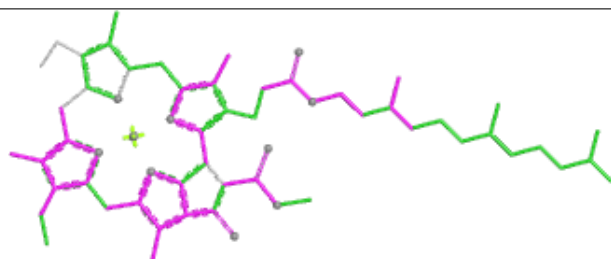


Rings

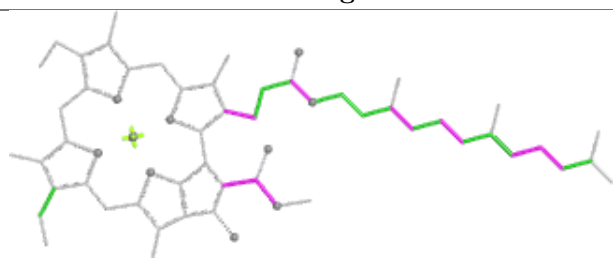
Ligand CLA b 832



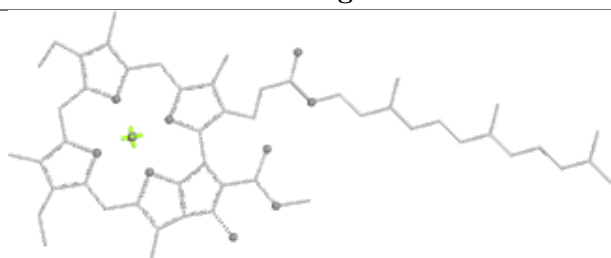
Bond lengths



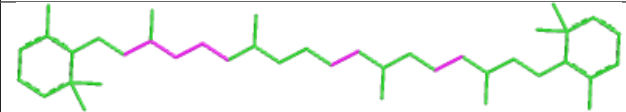
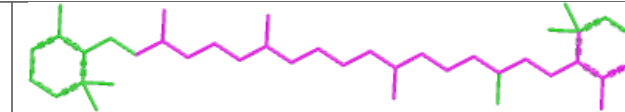
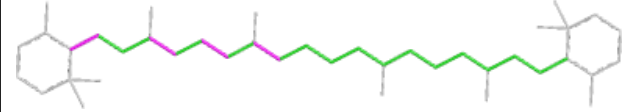
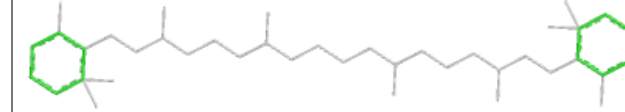
Bond angles

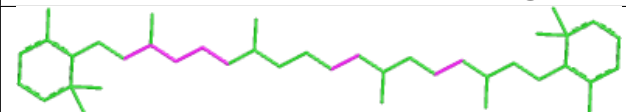
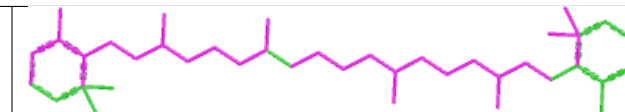
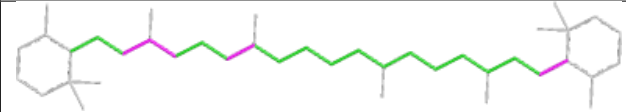
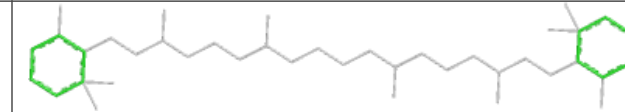


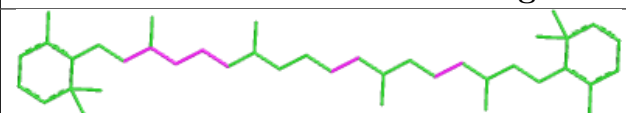
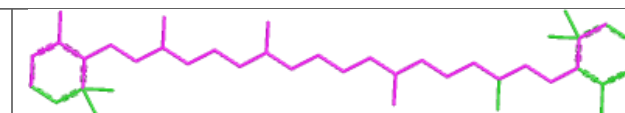
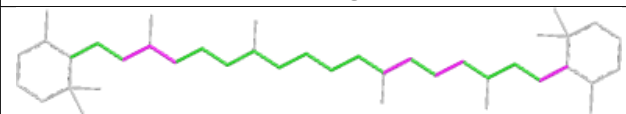
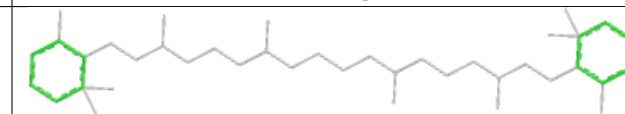
Torsions

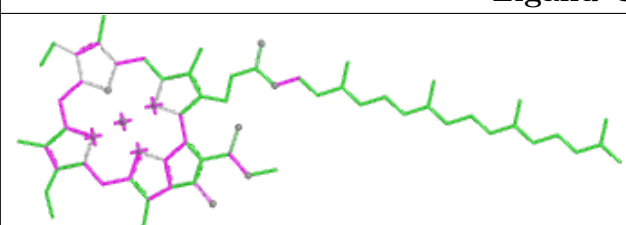
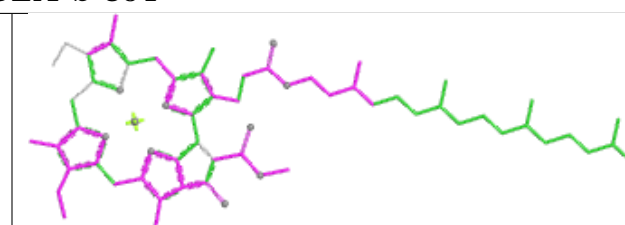
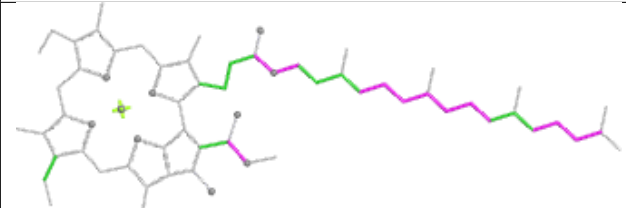
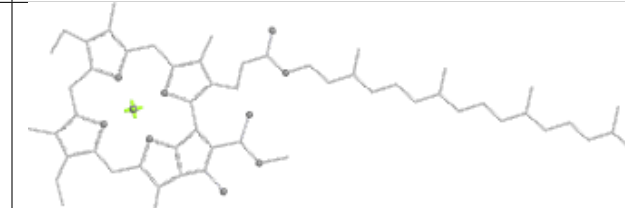


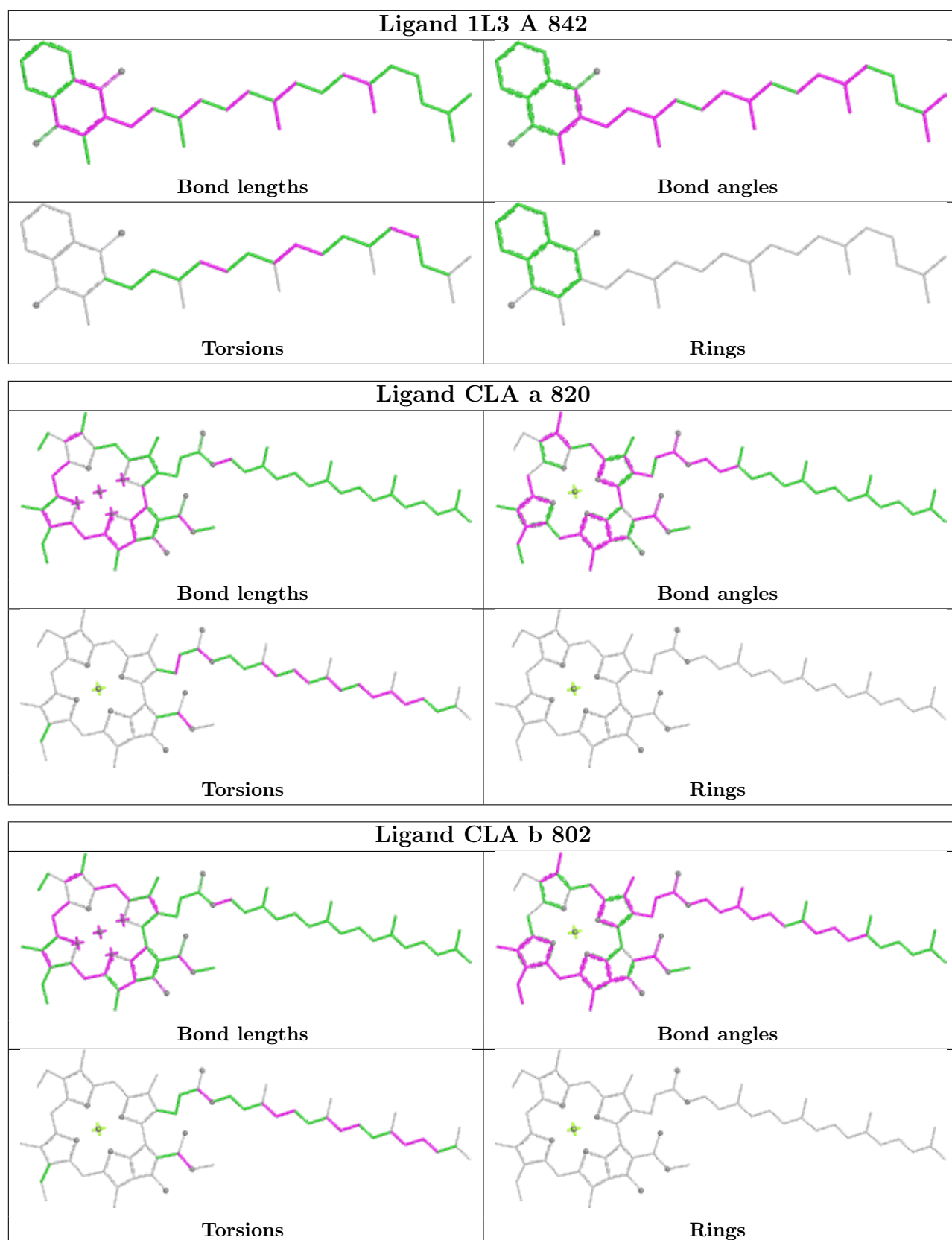
Rings

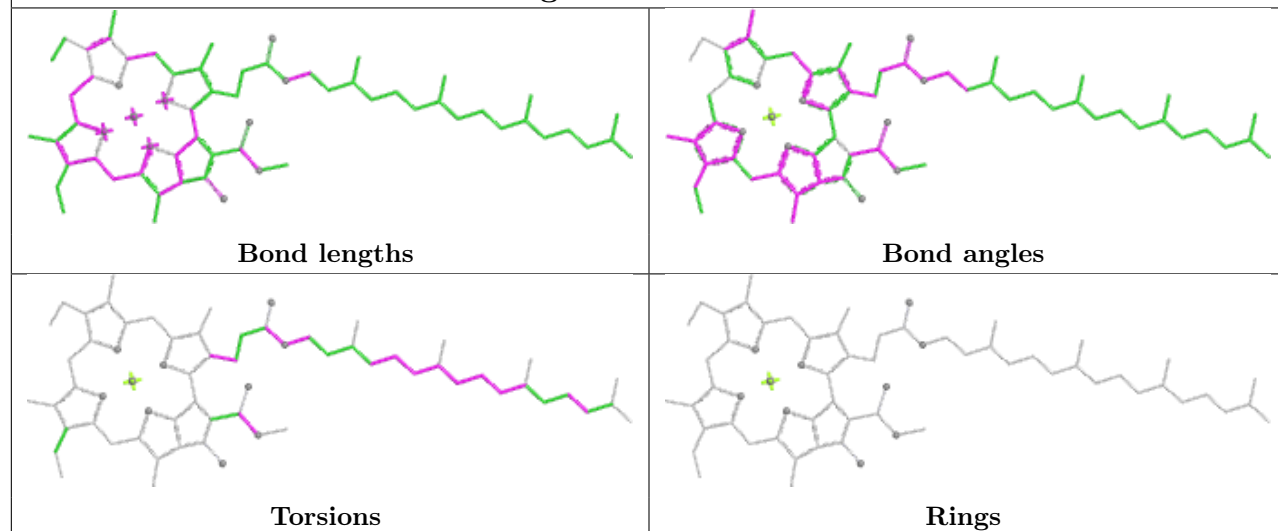
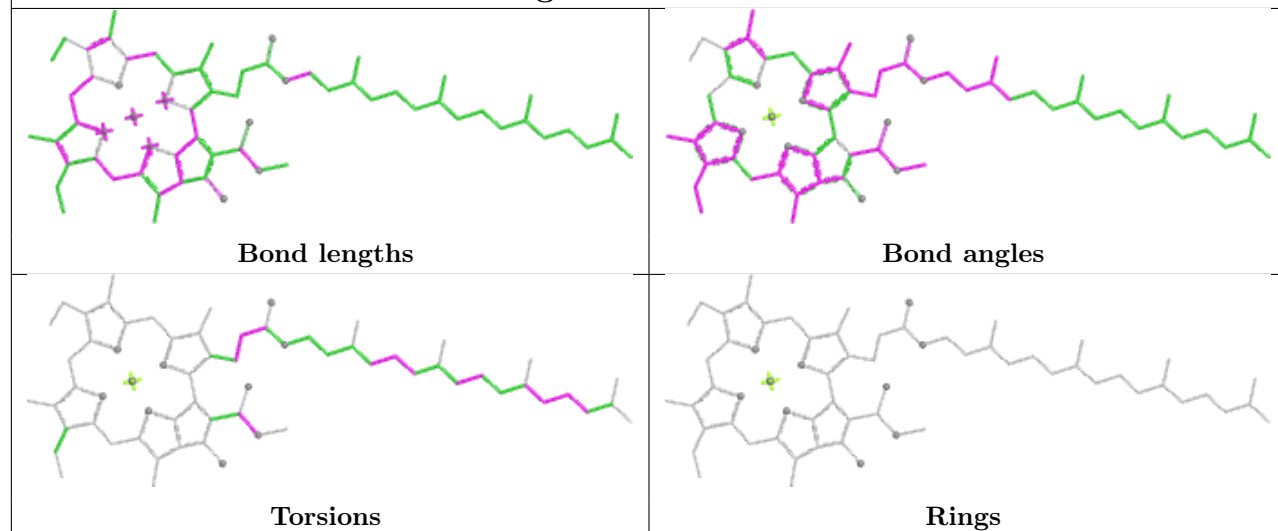
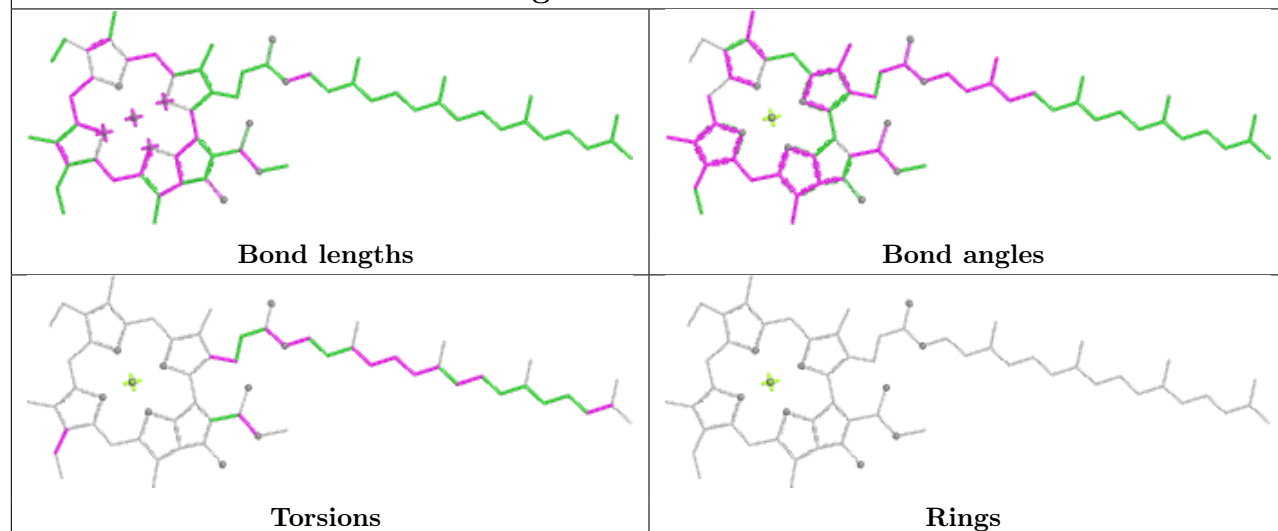
Ligand BCR F 204	
	
Bond lengths	Bond angles
	
Torsions	Rings

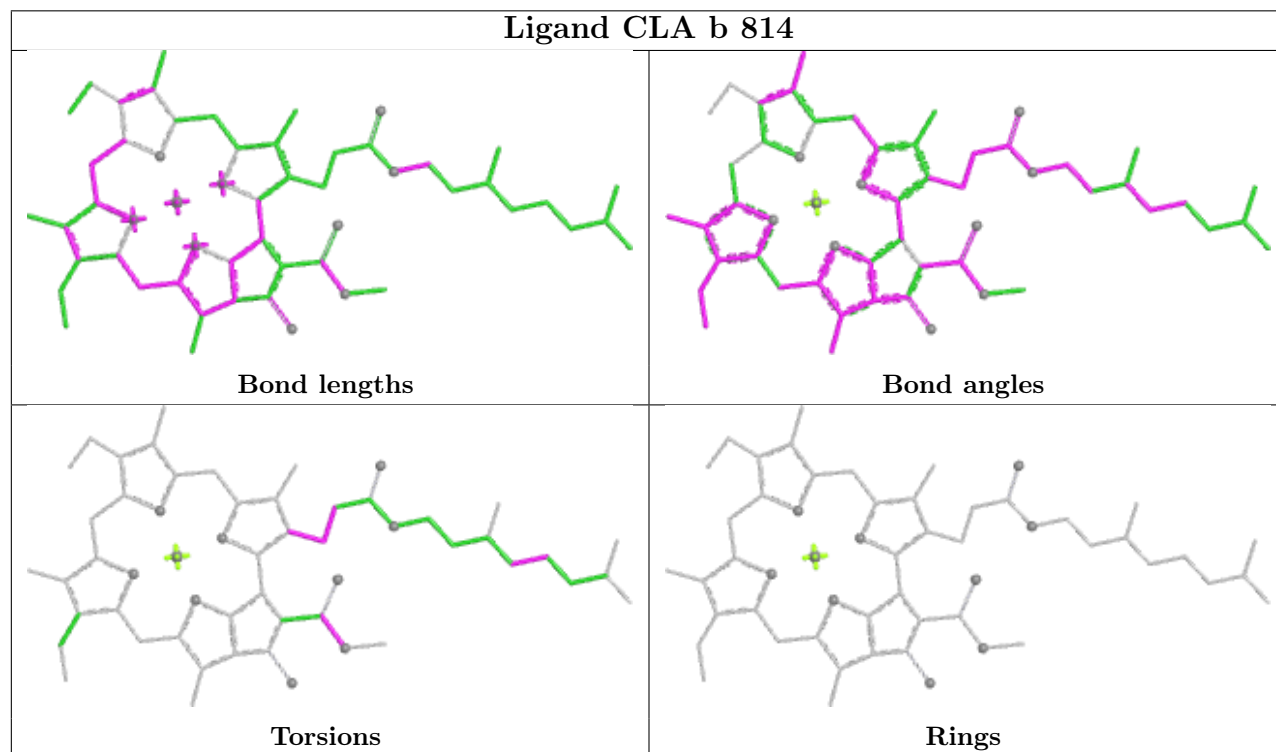
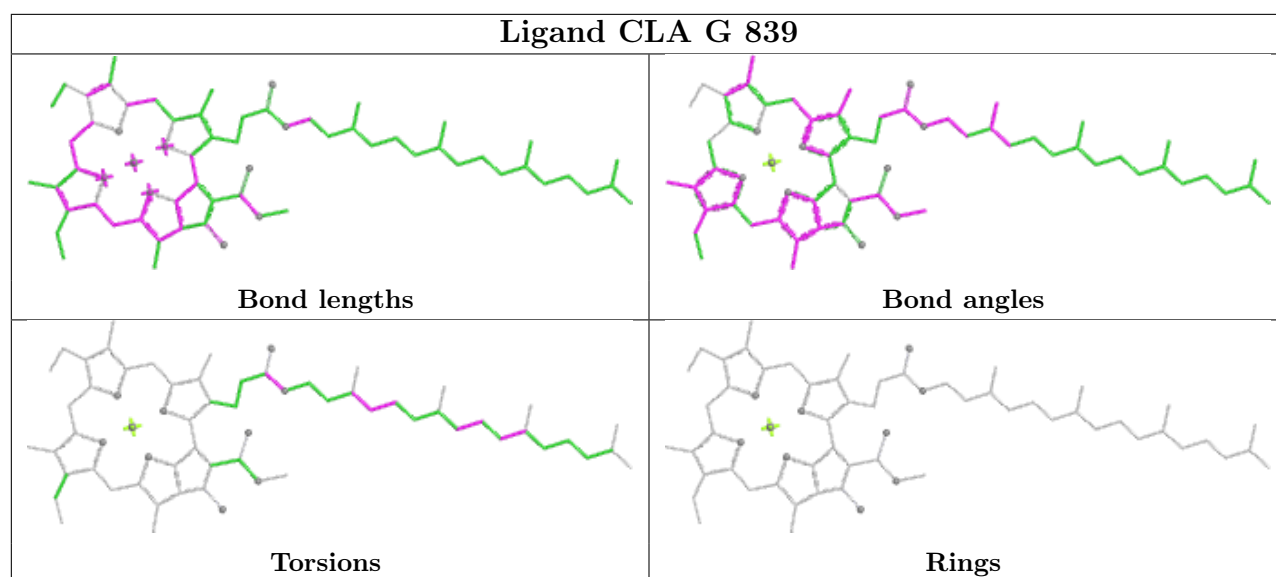
Ligand BCR L 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

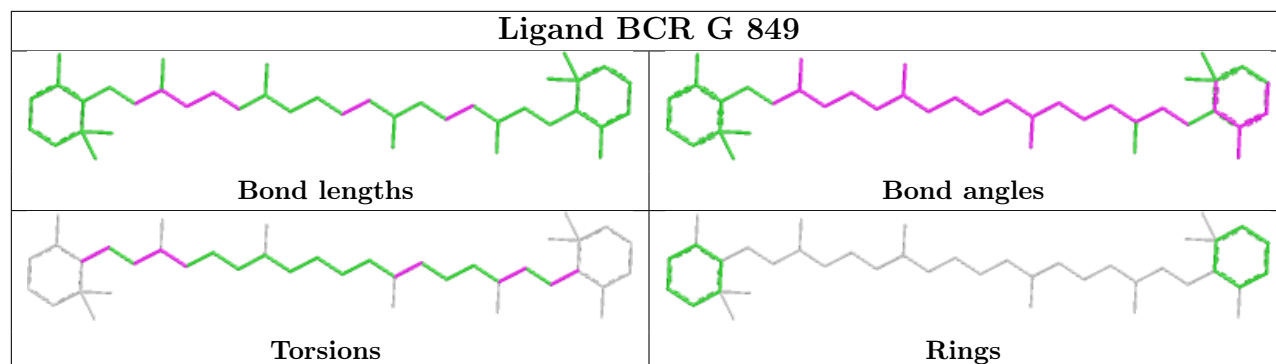
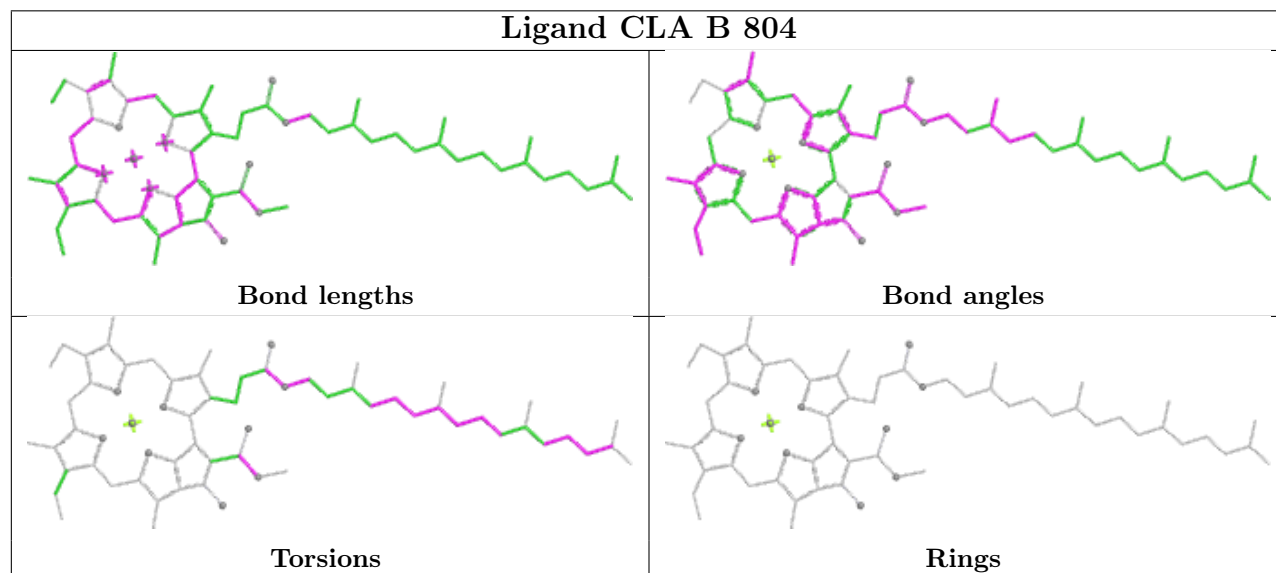
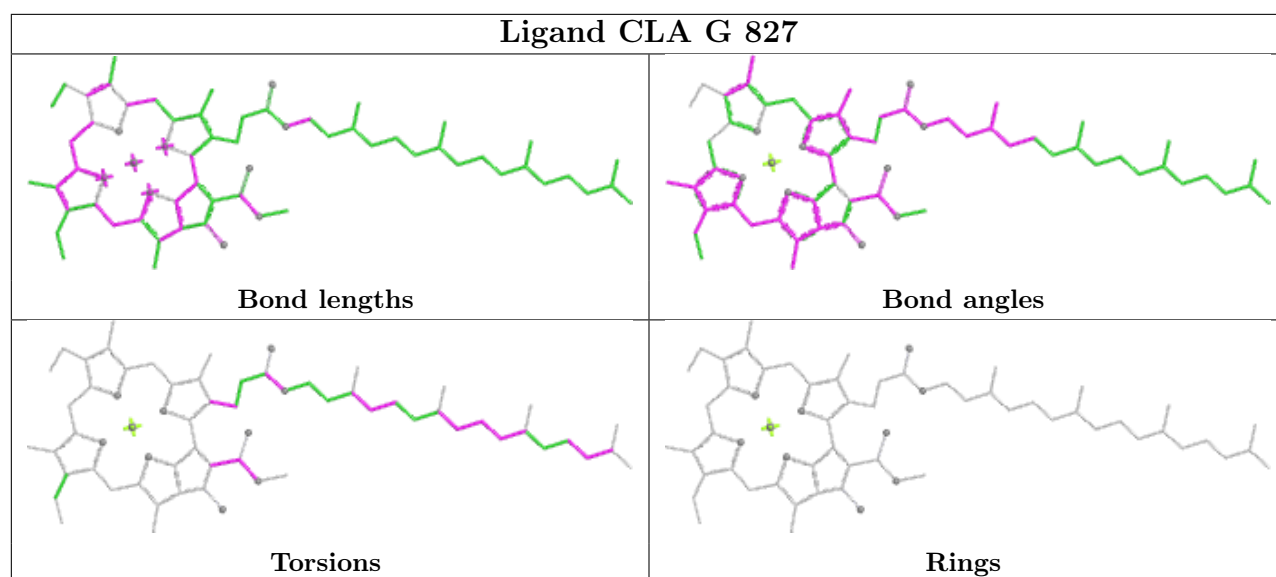
Ligand BCR H 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

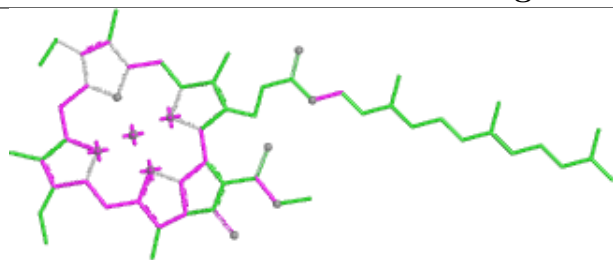
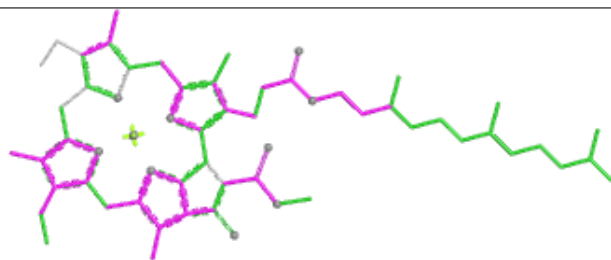
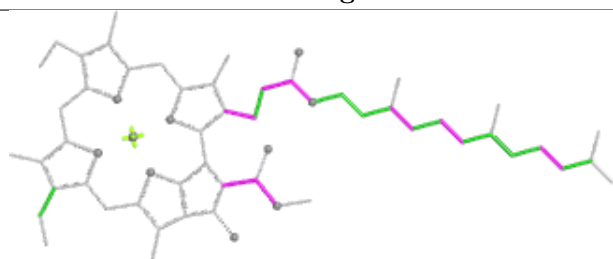
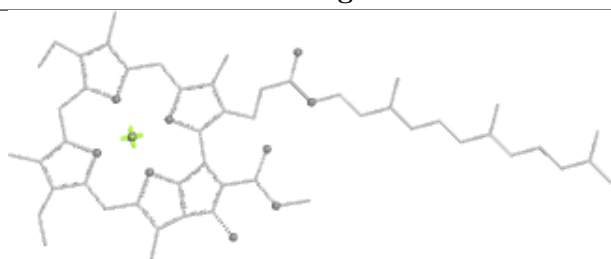
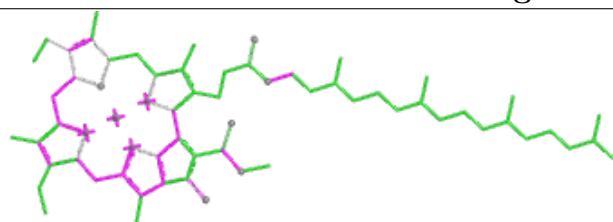
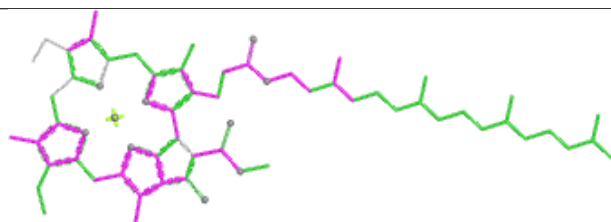
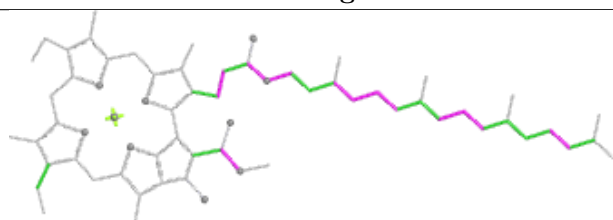
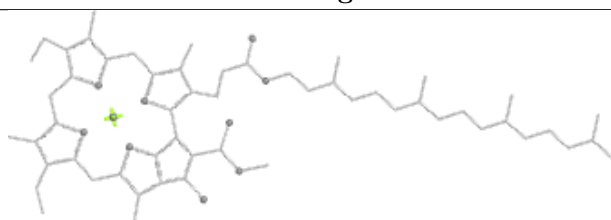
Ligand CLA b 804	
	
Bond lengths	Bond angles
	
Torsions	Rings



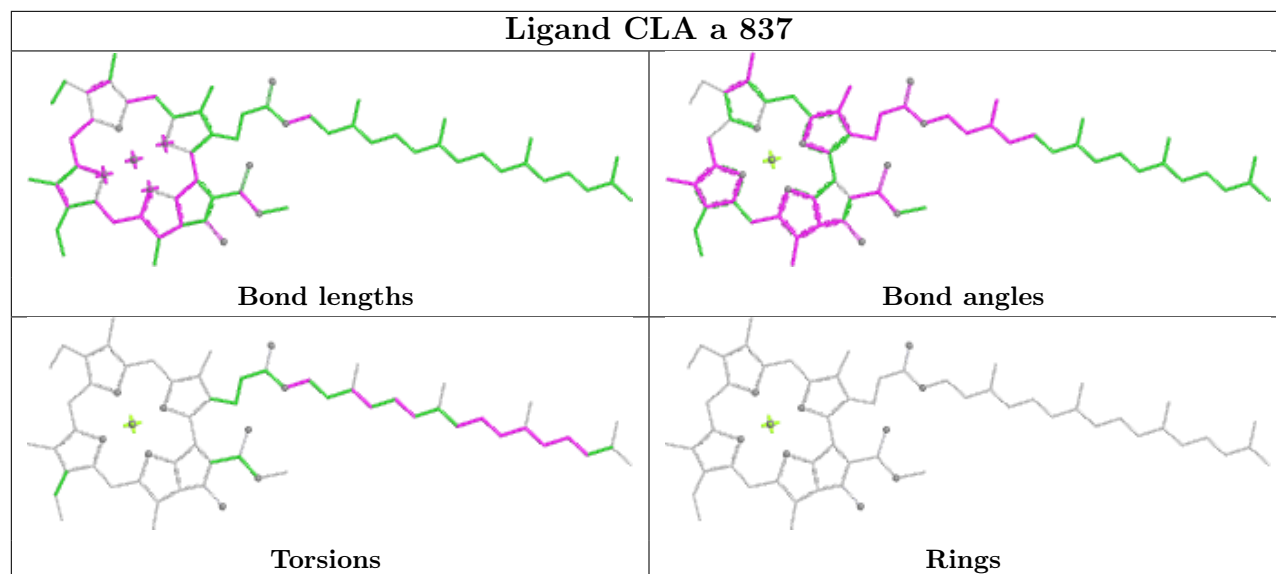
Ligand CLA 1 202**Ligand CLA a 828****Ligand CLA B 837**



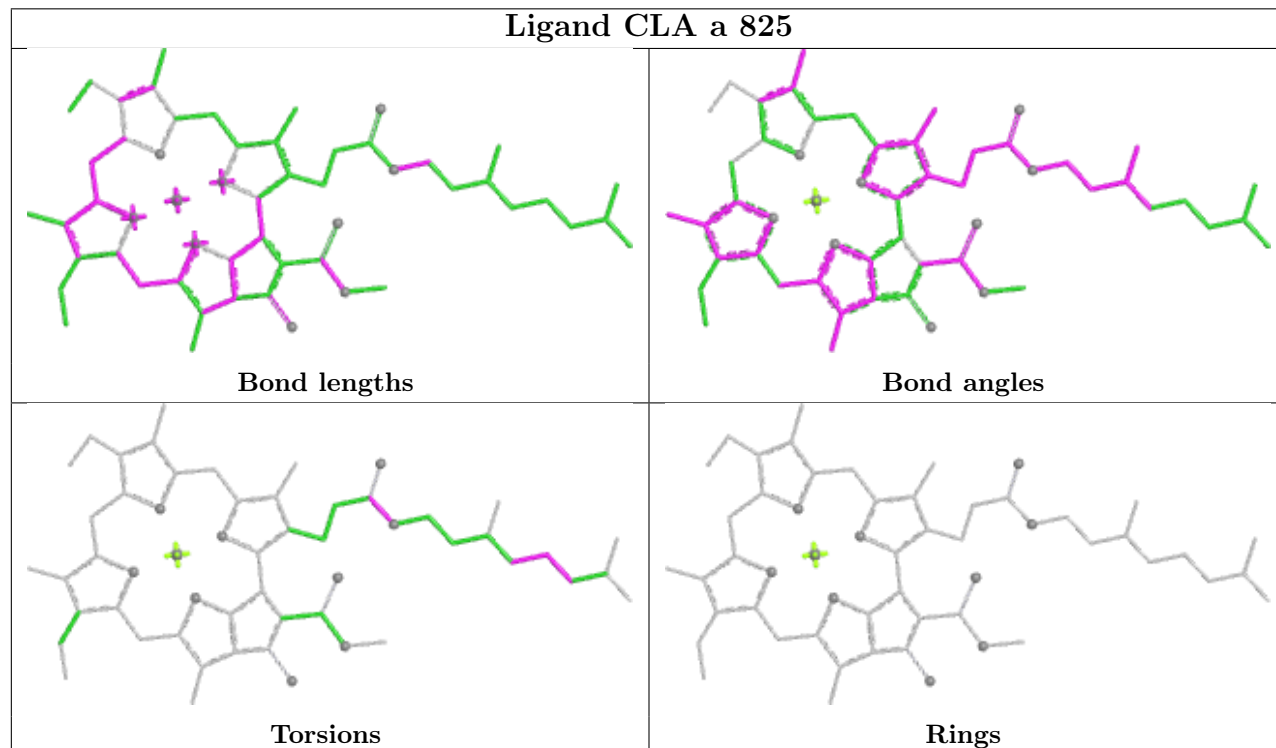


Ligand CLA B 811**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 832****Bond lengths****Bond angles****Torsions****Rings**

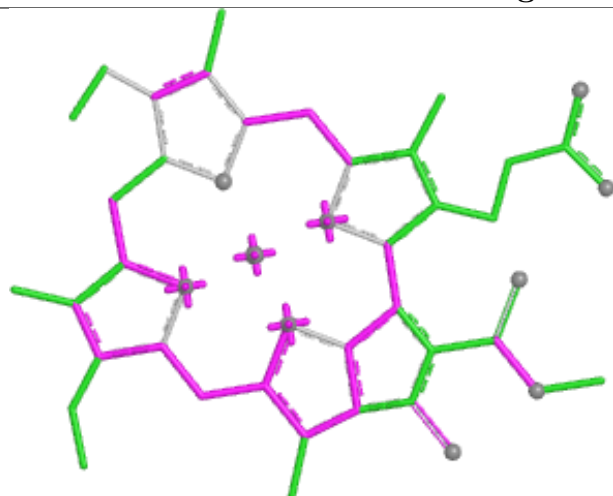
Ligand CLA a 837



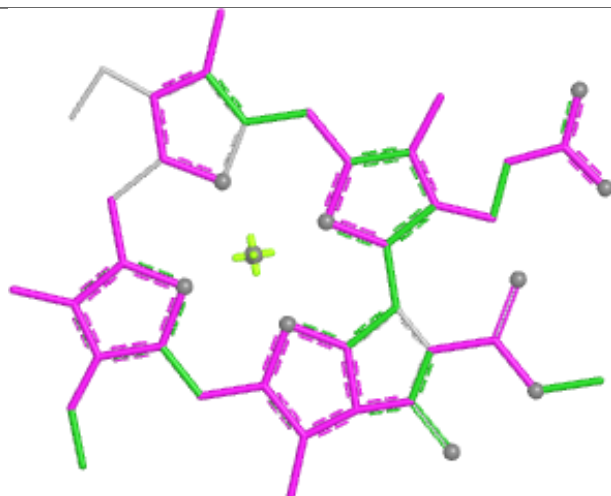
Ligand CLA a 825



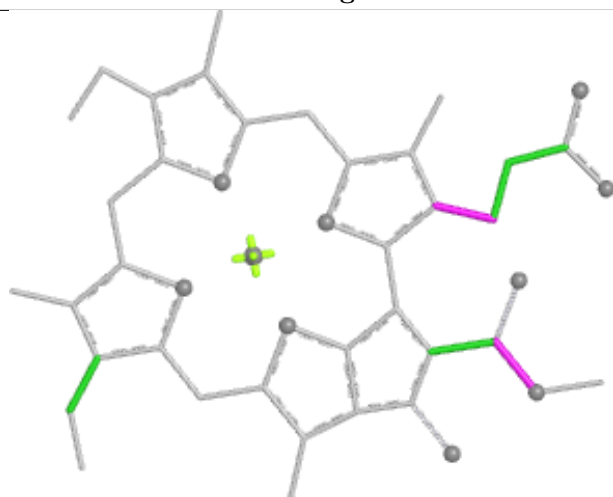
Ligand CLA b 808



Bond lengths



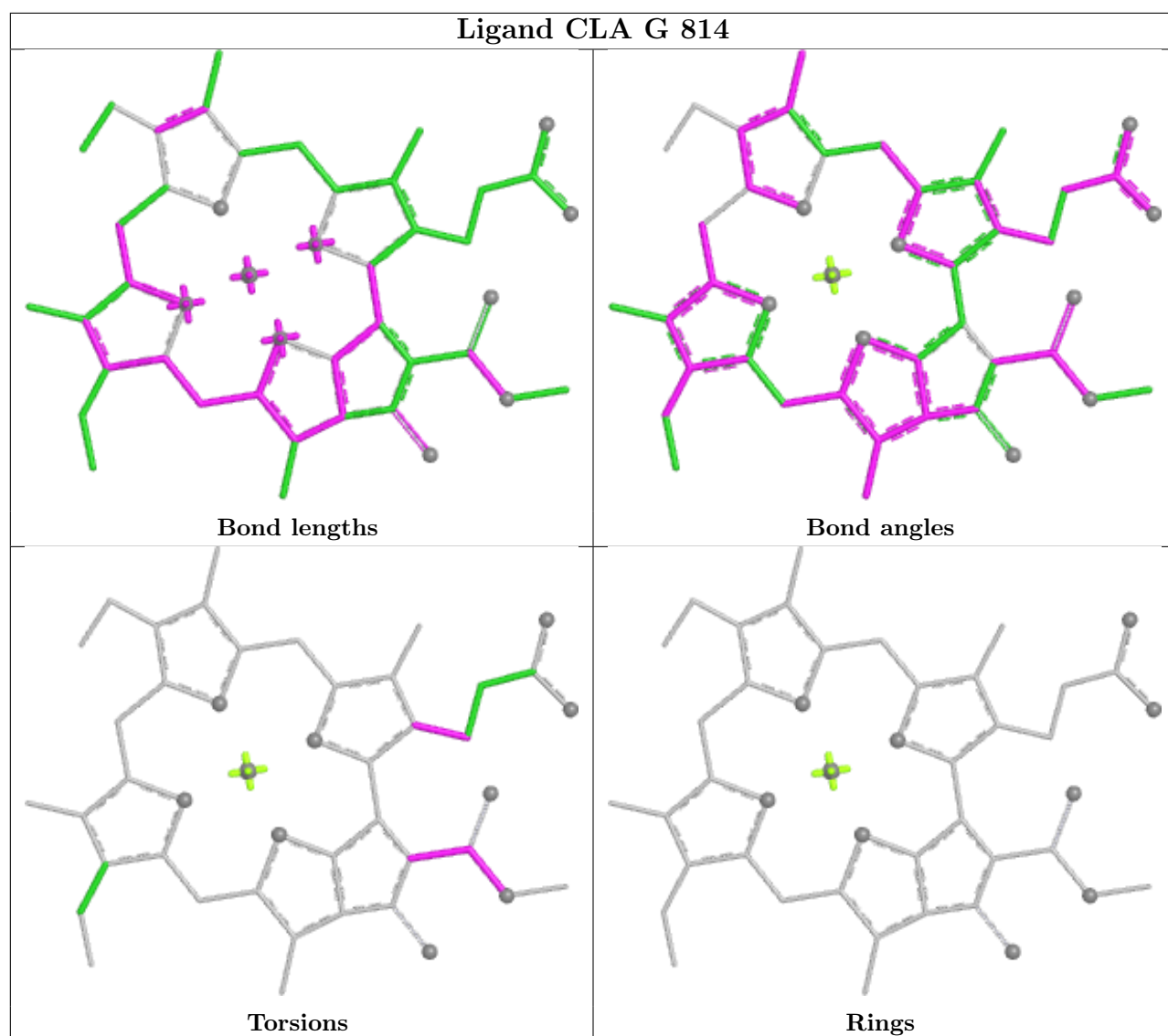
Bond angles



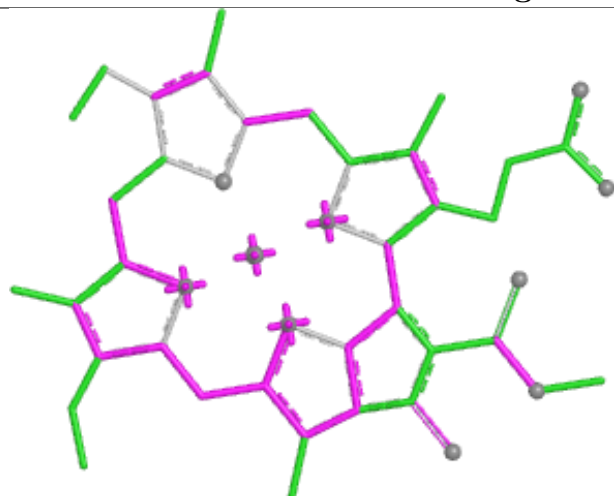
Torsions



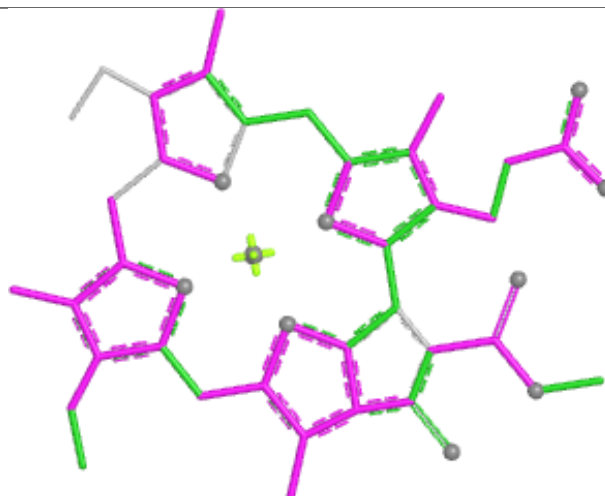
Rings



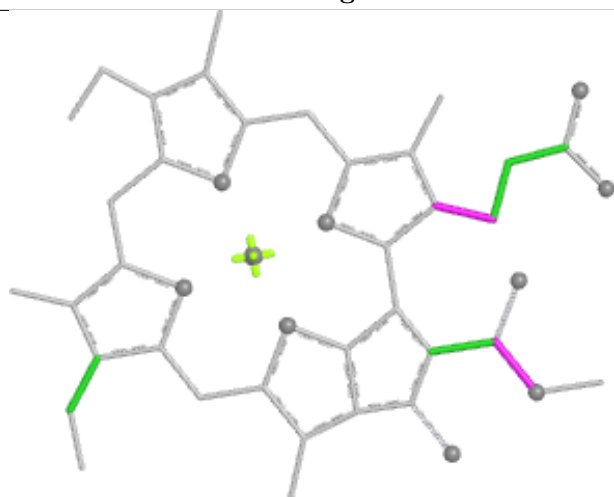
Ligand CLA B 808



Bond lengths



Bond angles

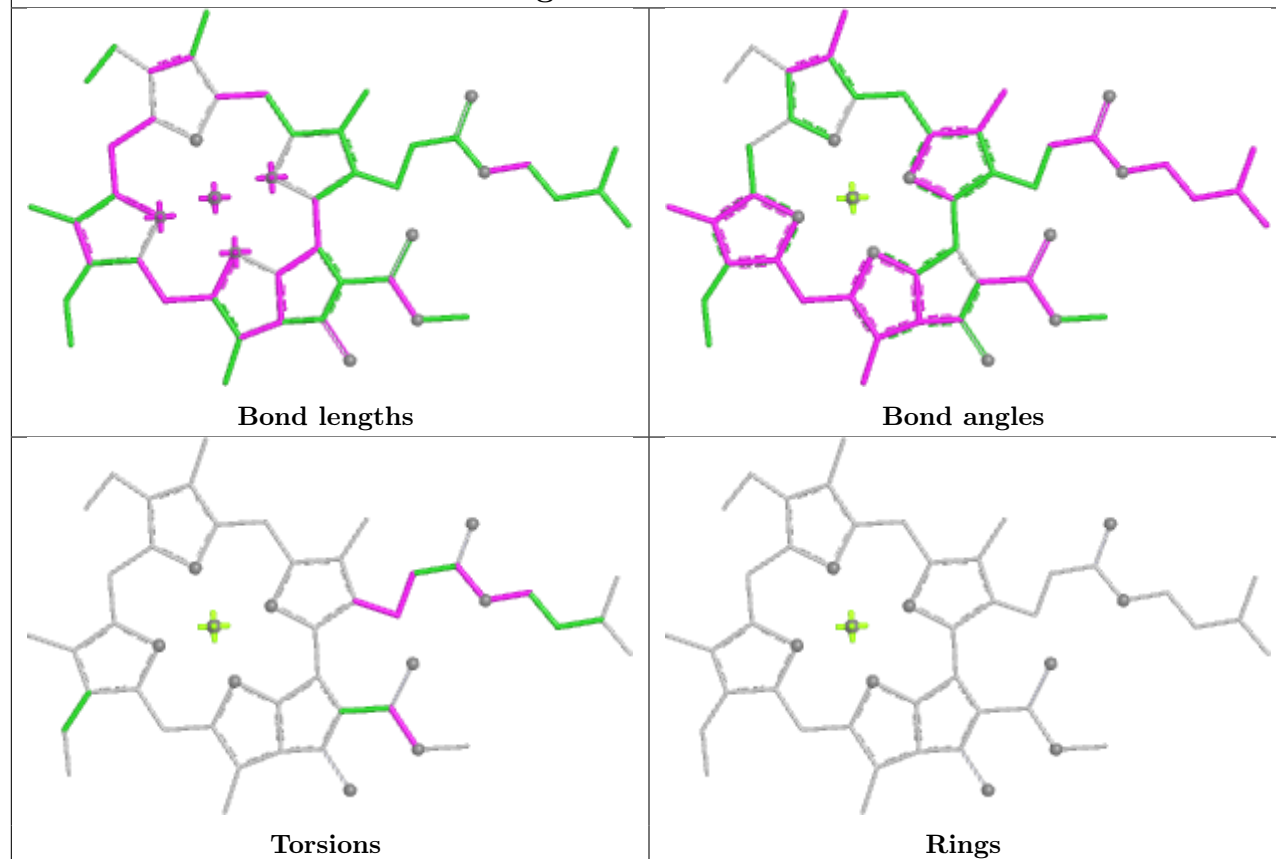


Torsions

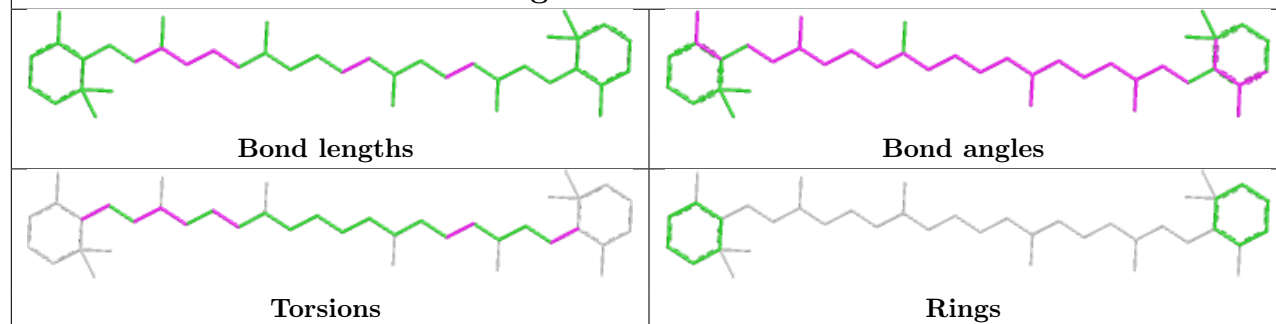


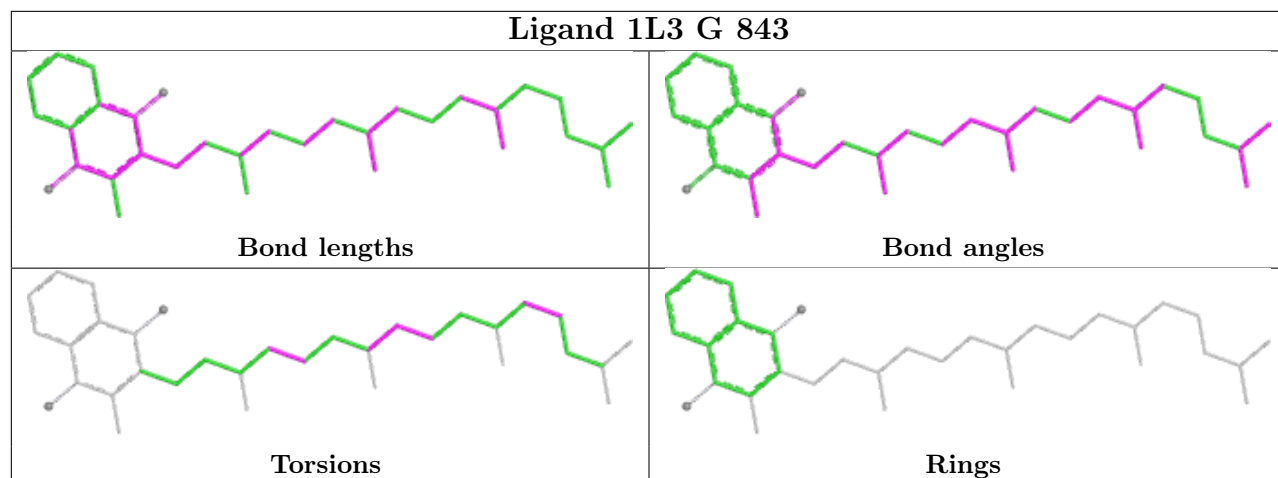
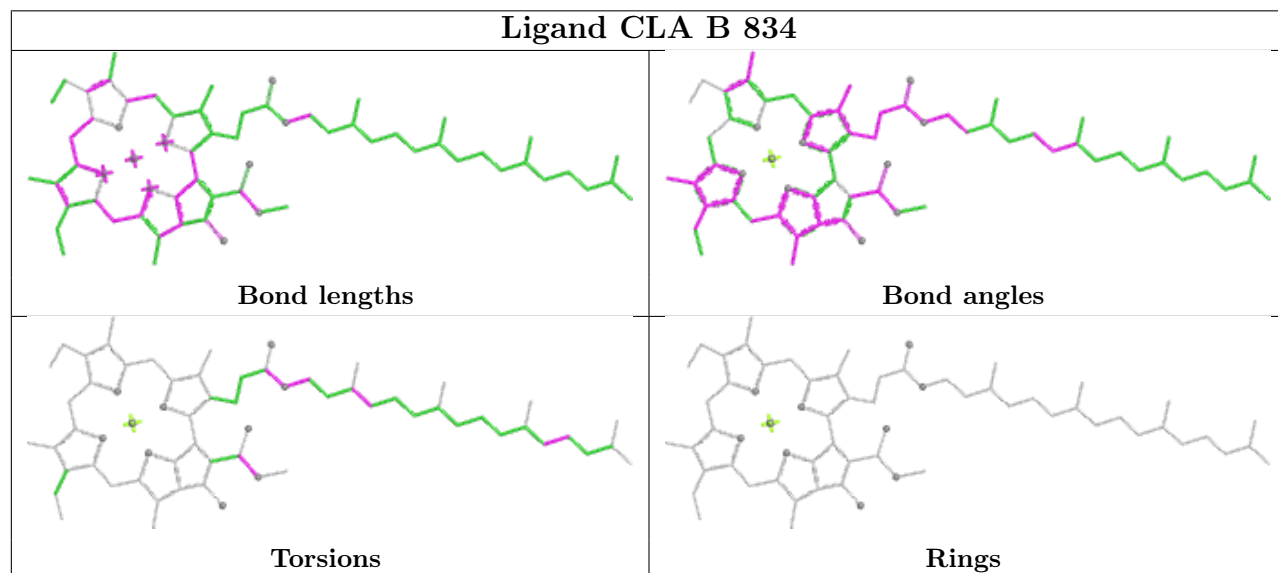
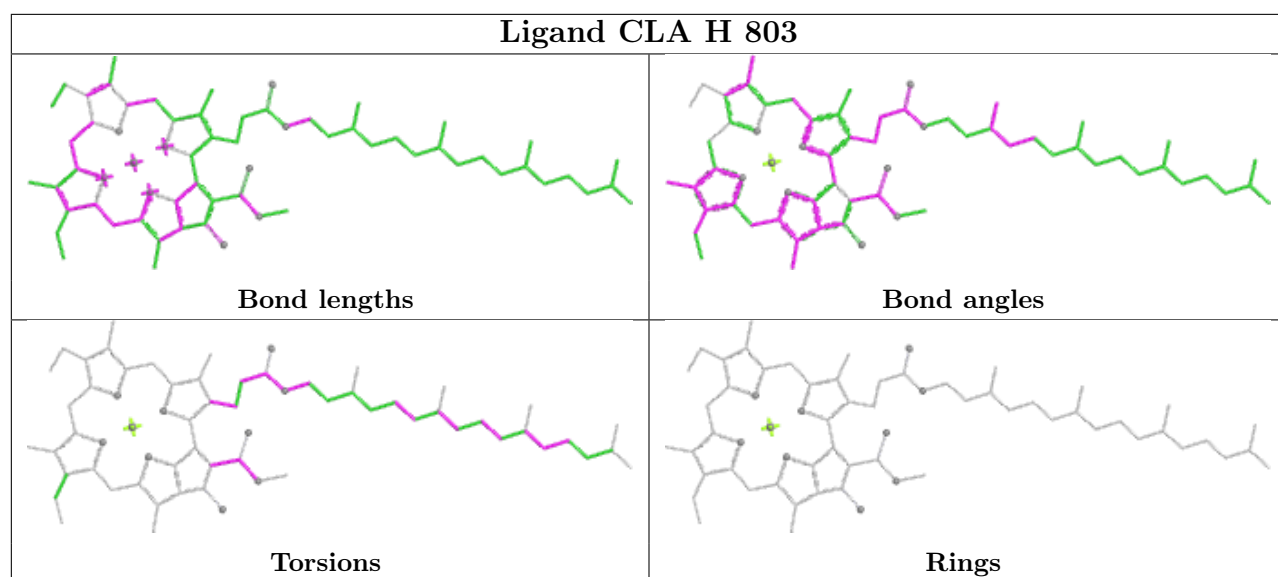
Rings

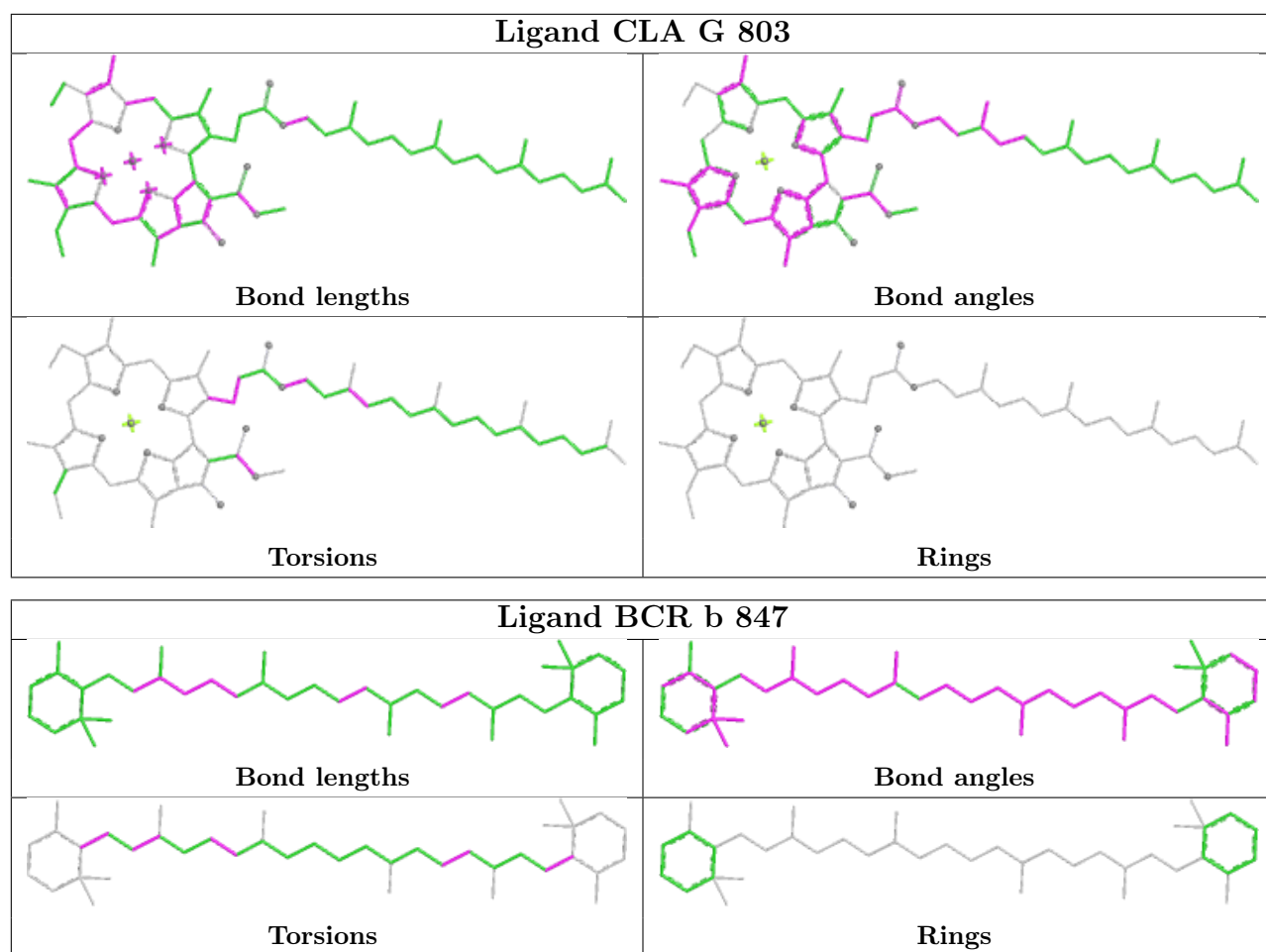
Ligand CLA a 840



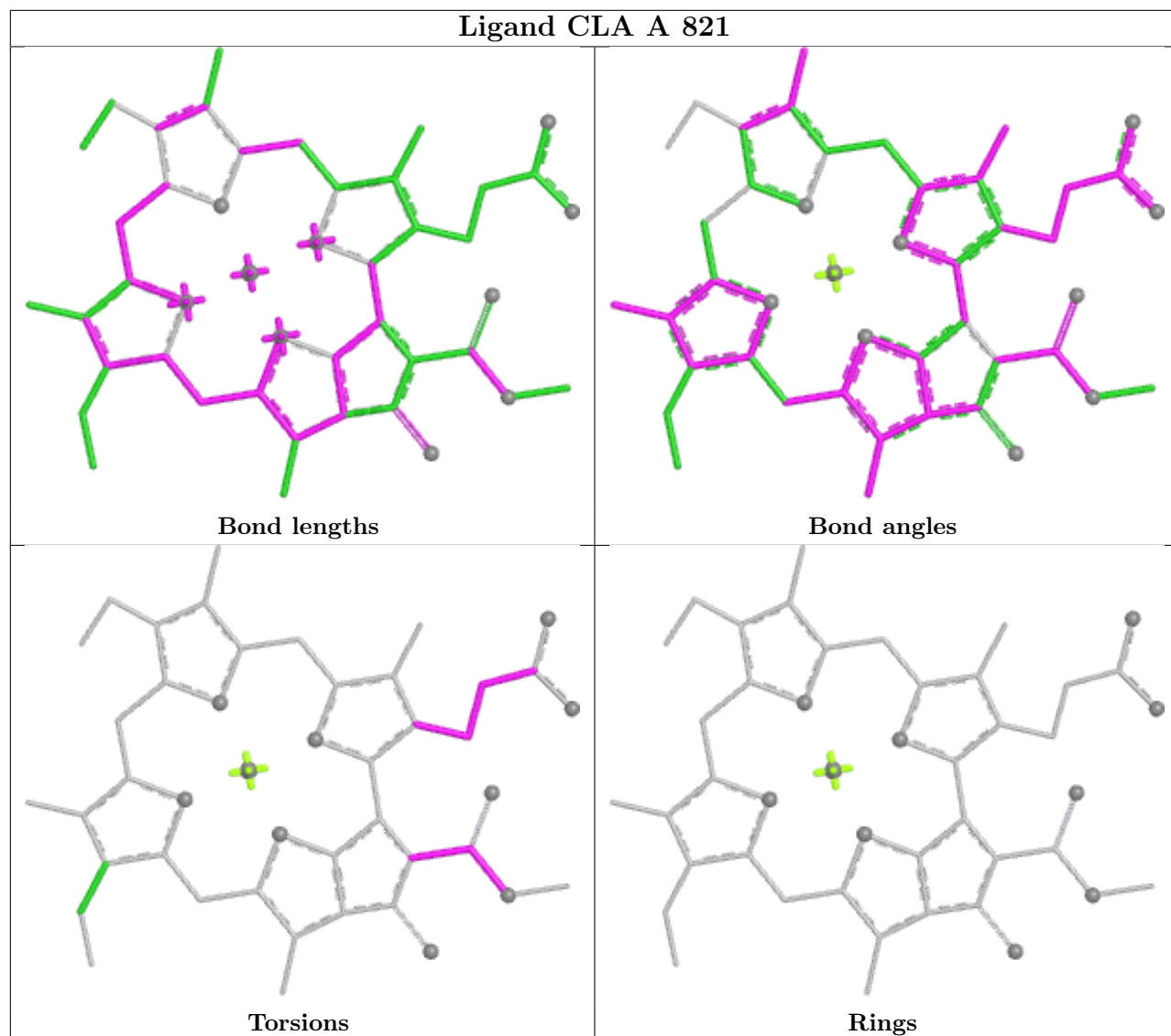
Ligand BCR B 840



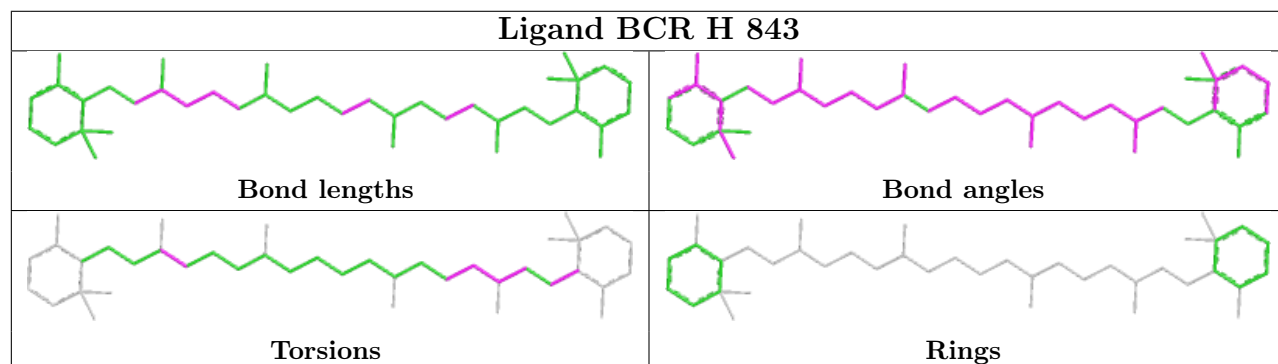


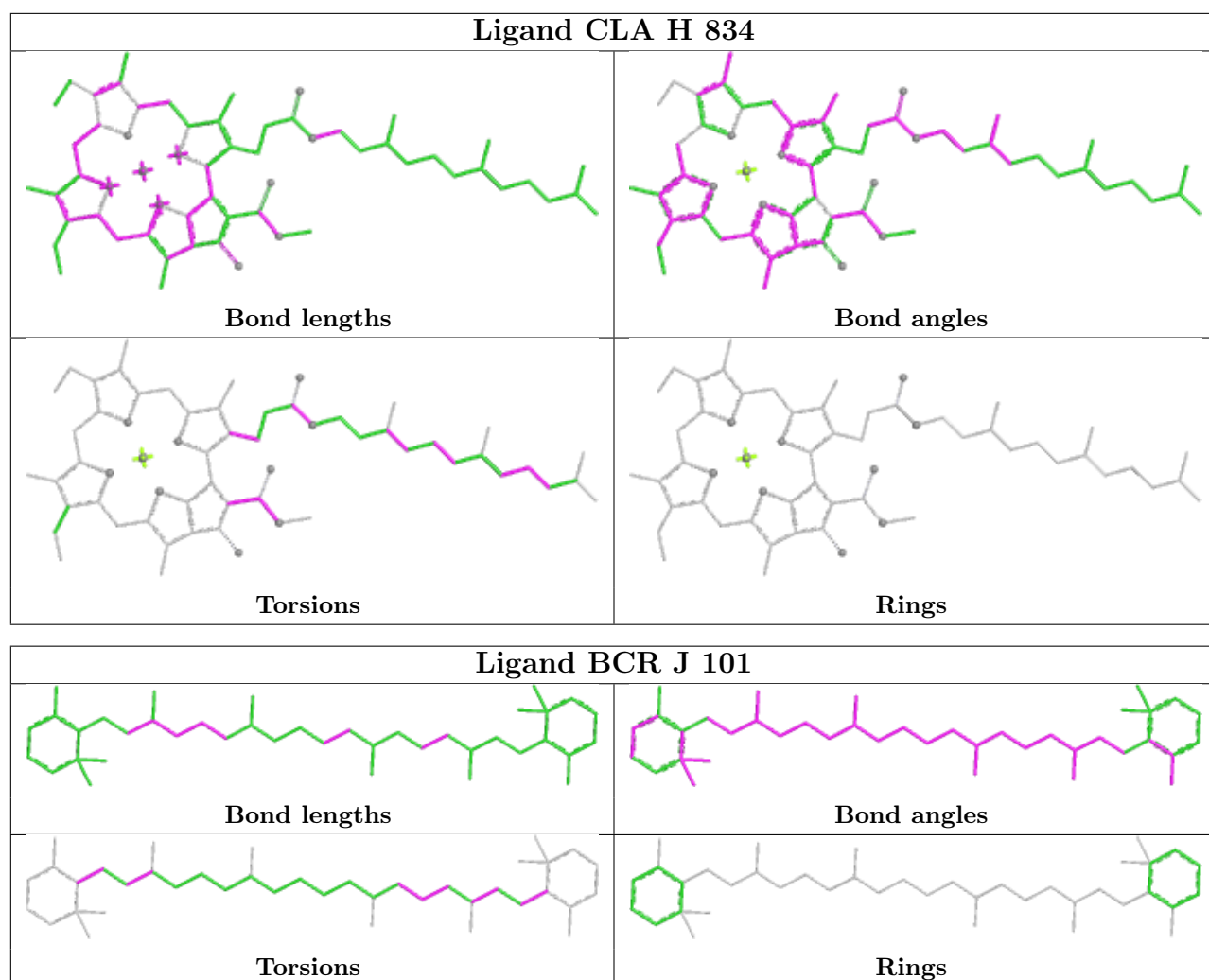


Ligand CLA A 821

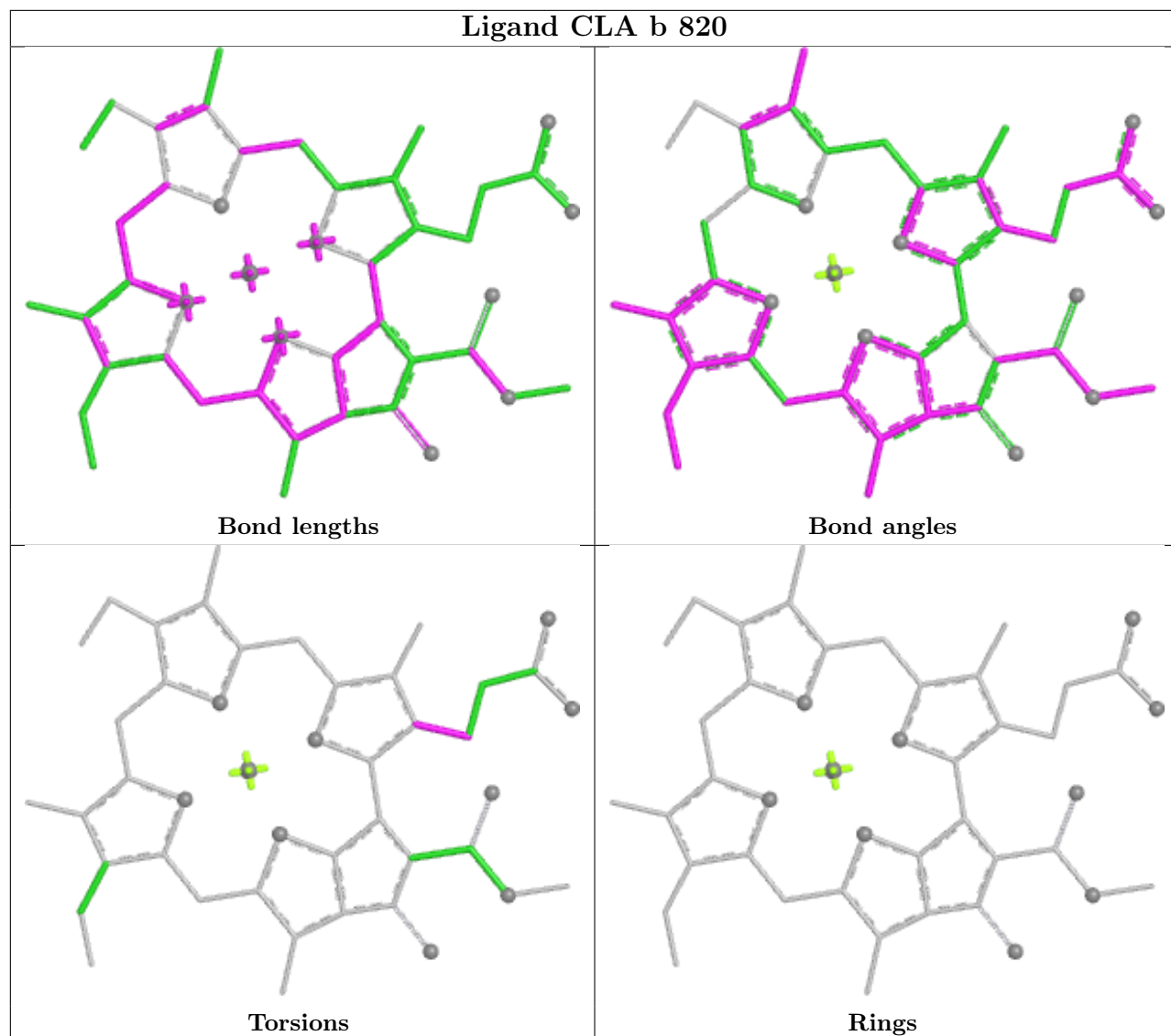


Ligand BCR H 843

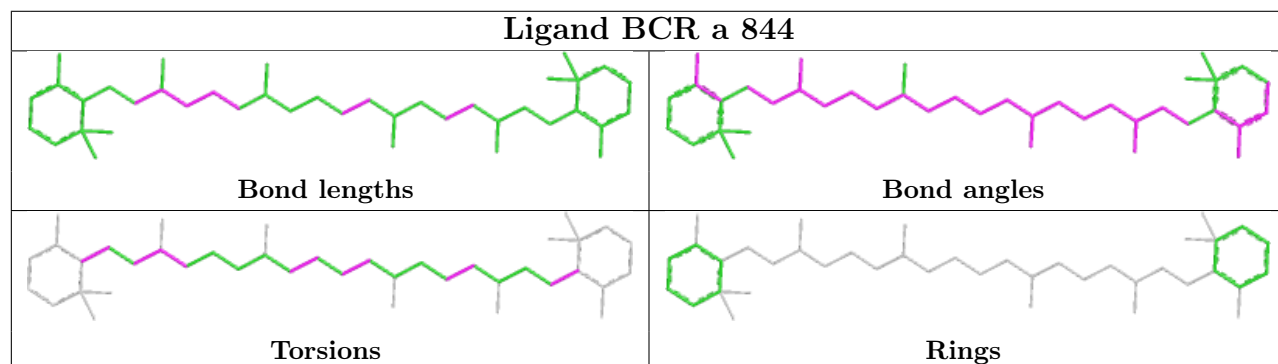


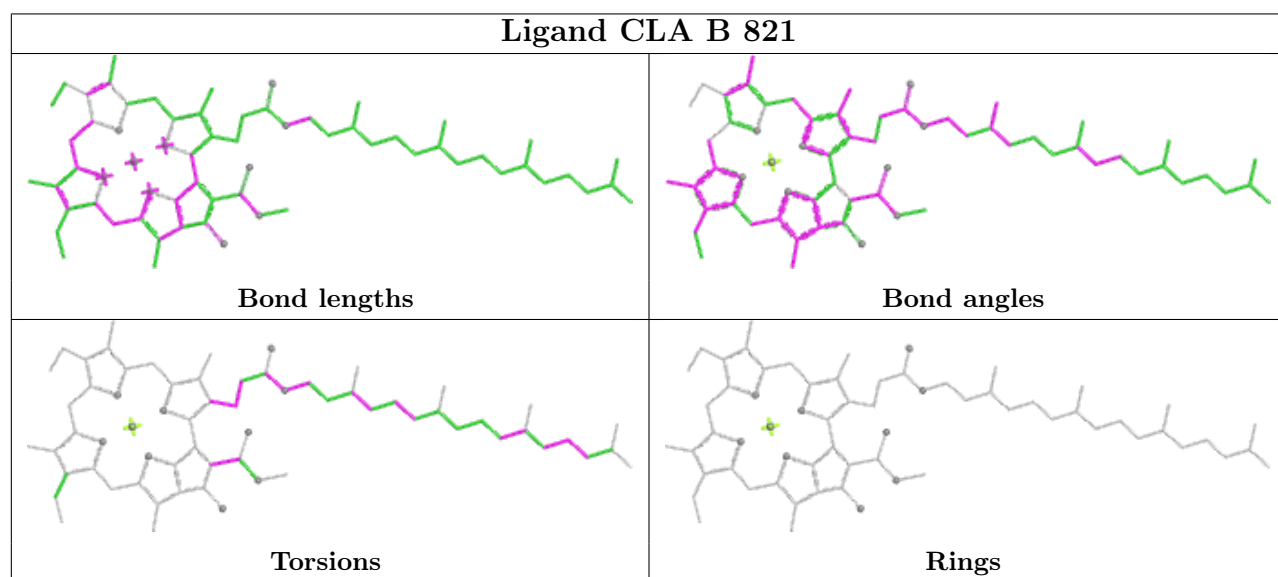
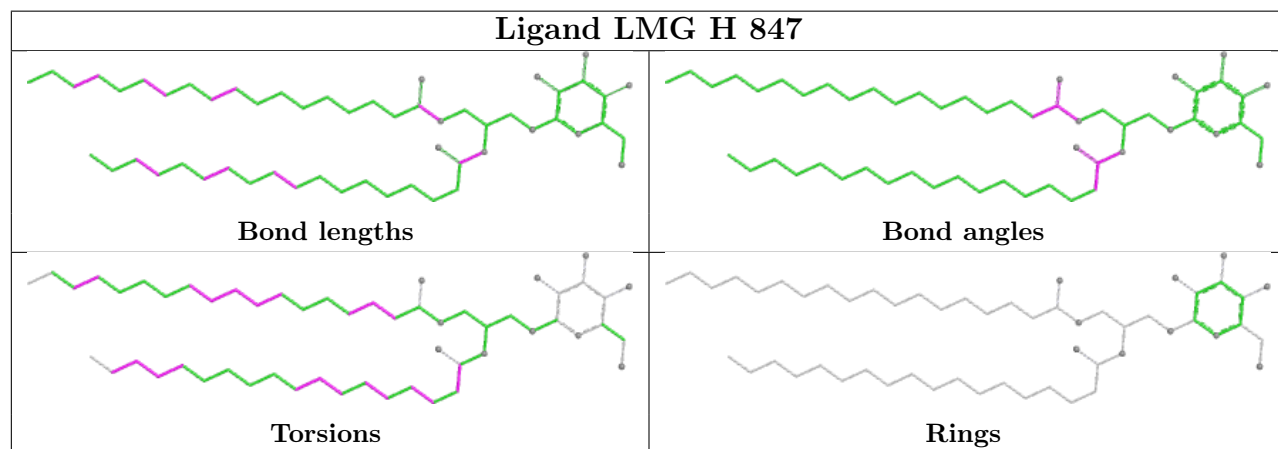
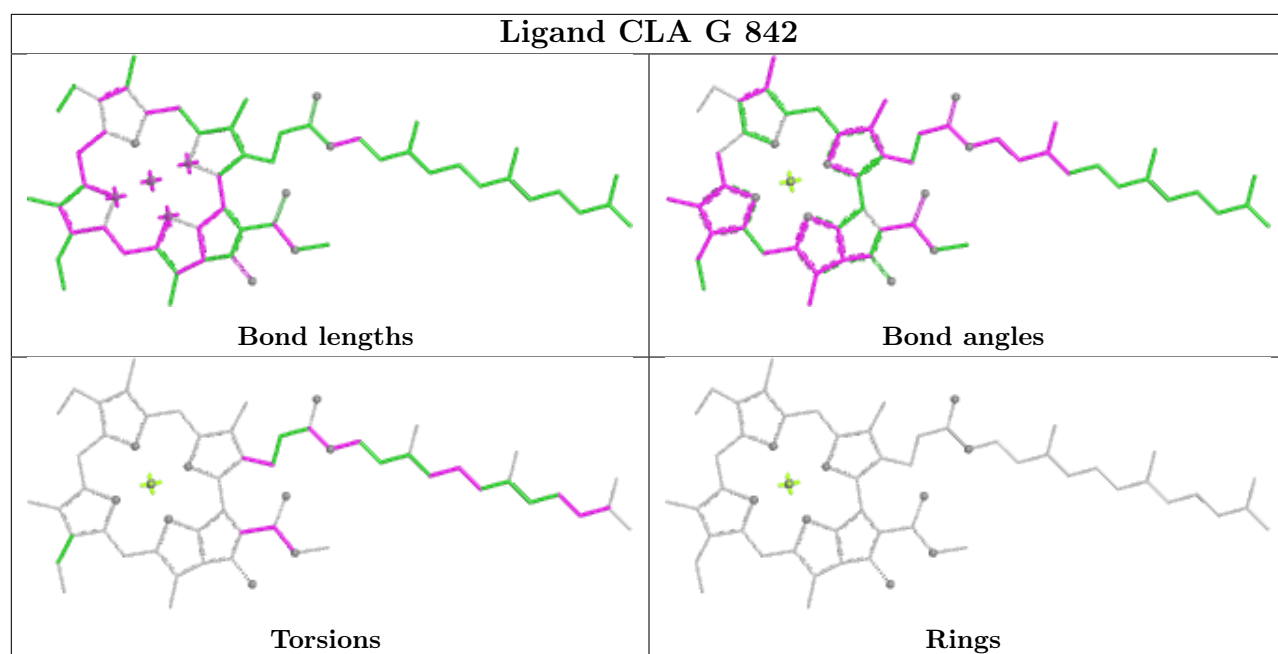


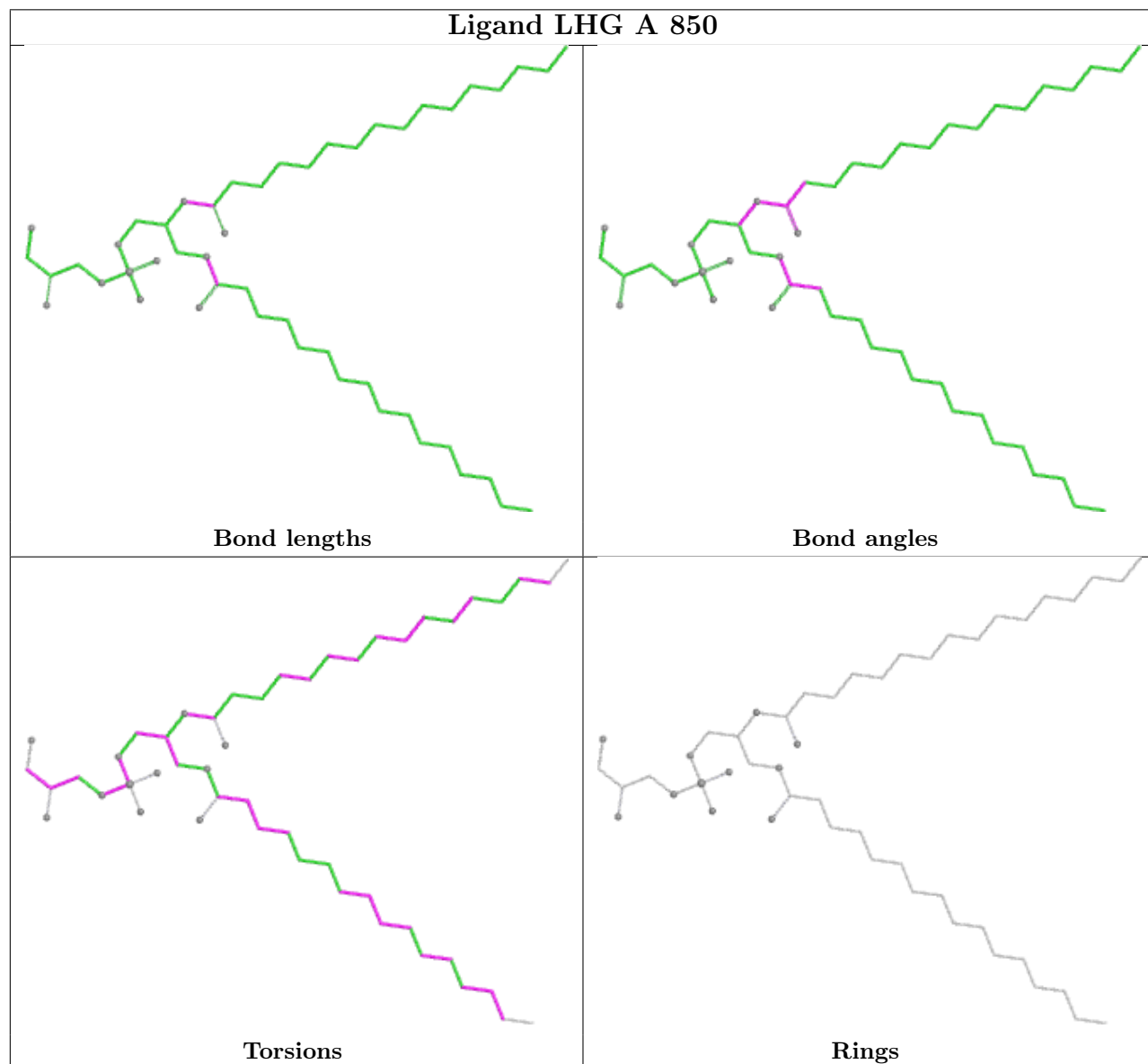
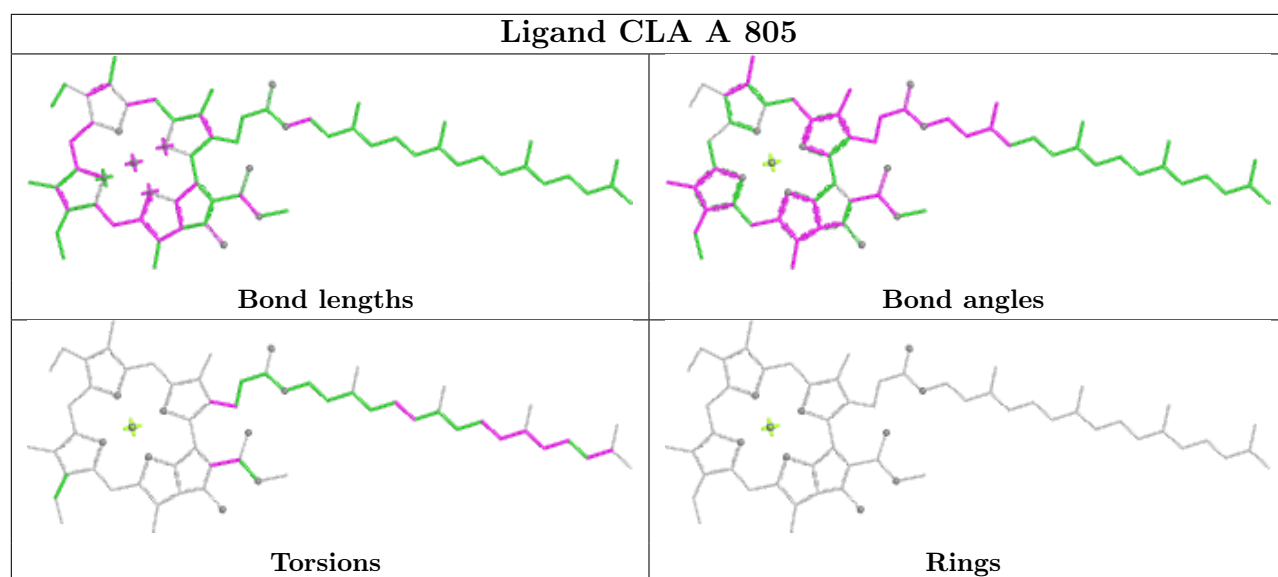
Ligand CLA b 820

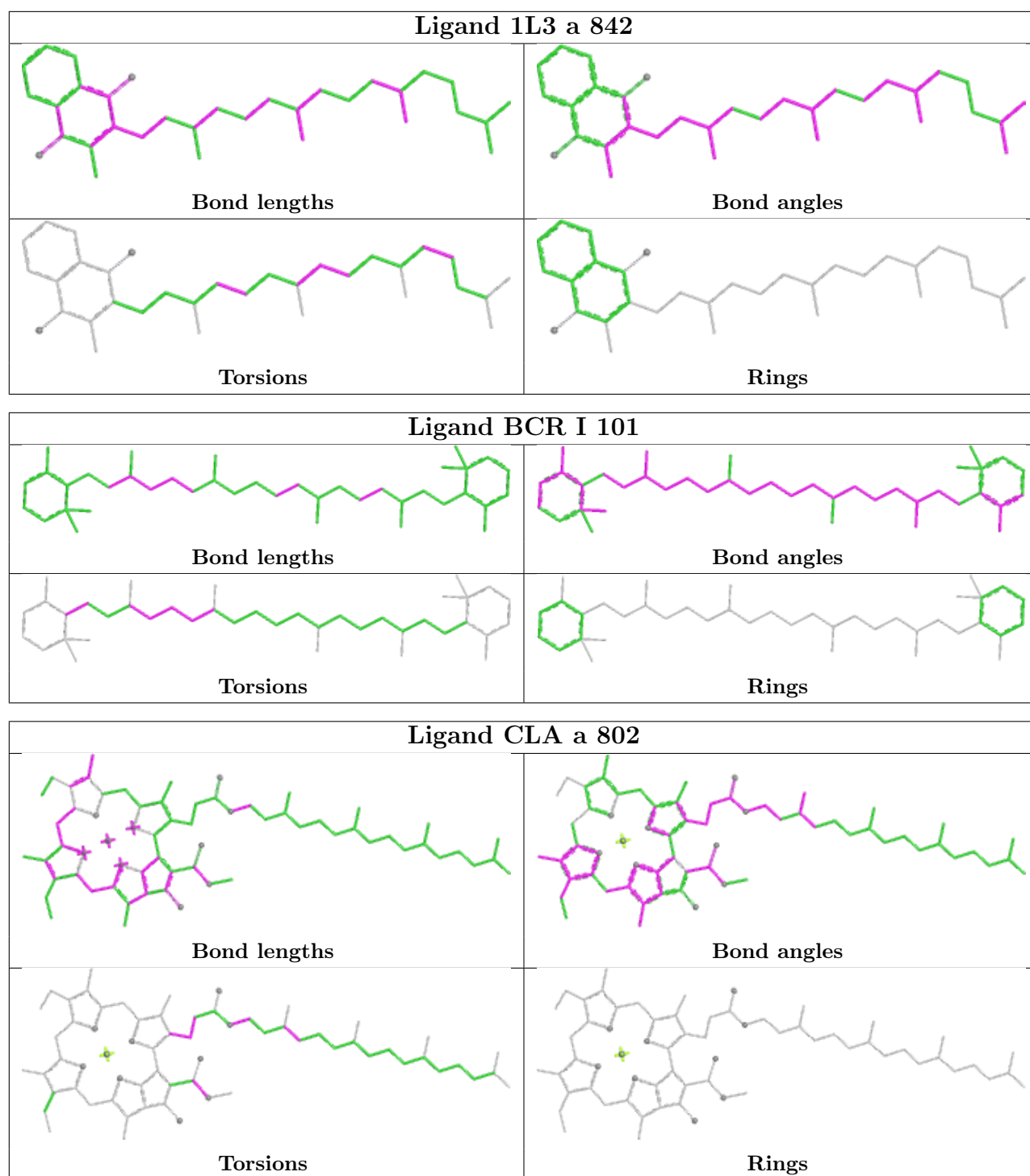


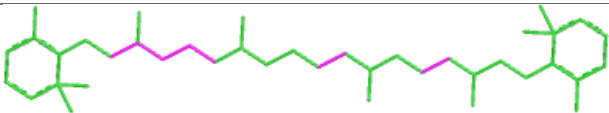
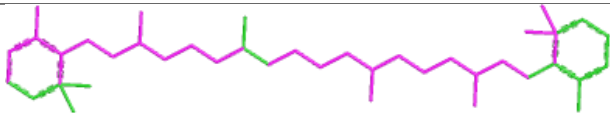
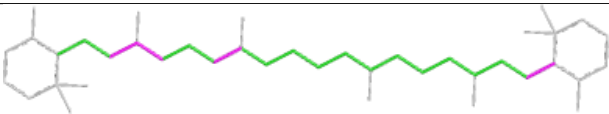
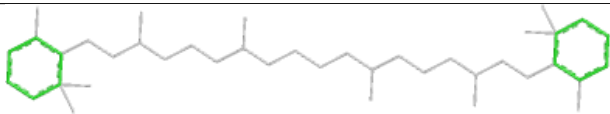
Ligand BCR a 844


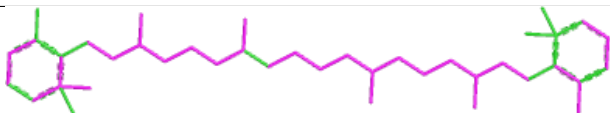
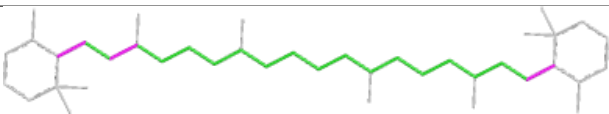
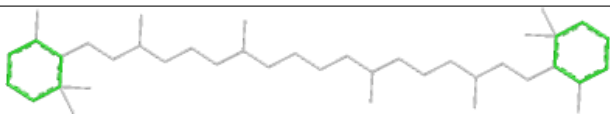




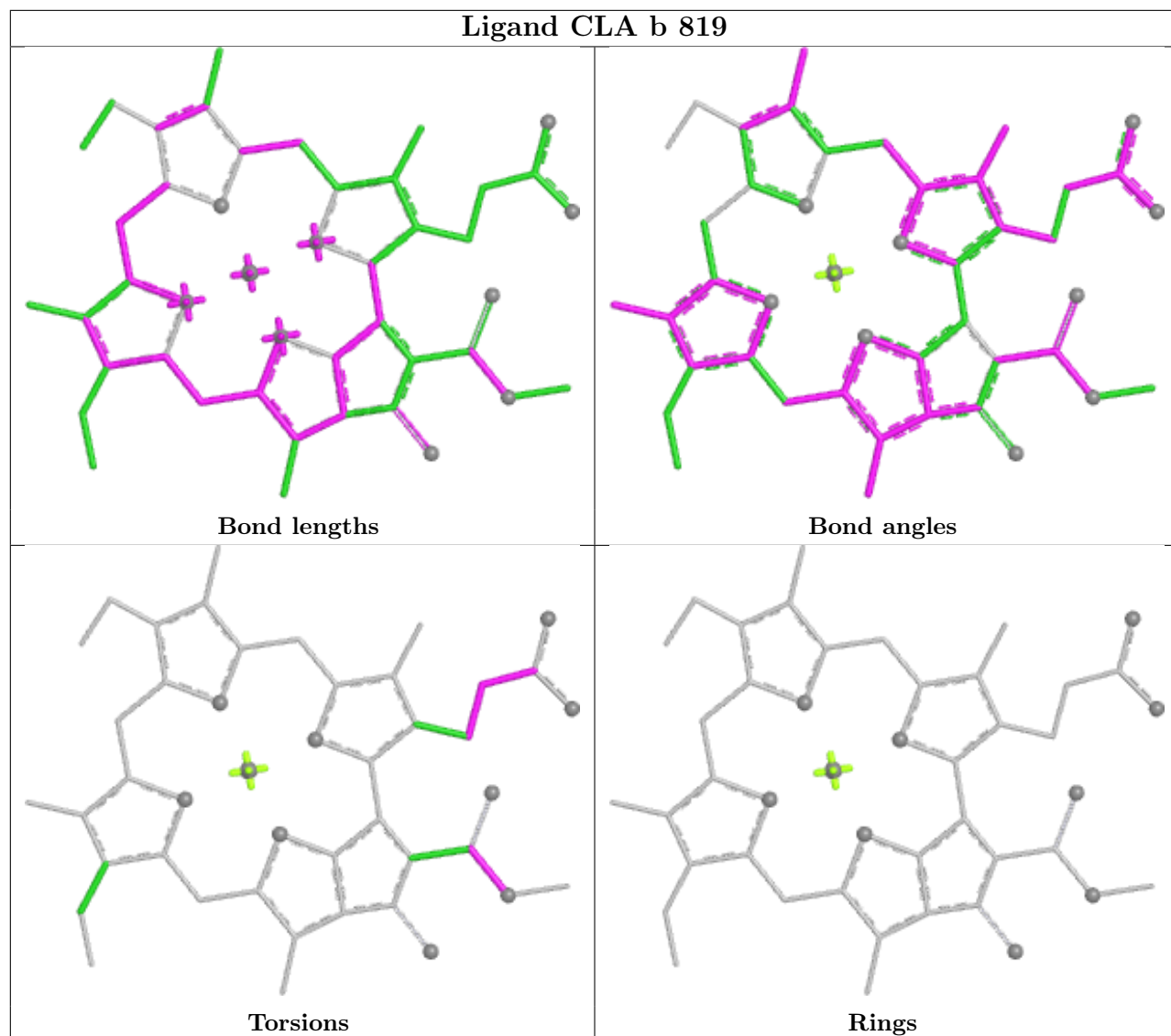




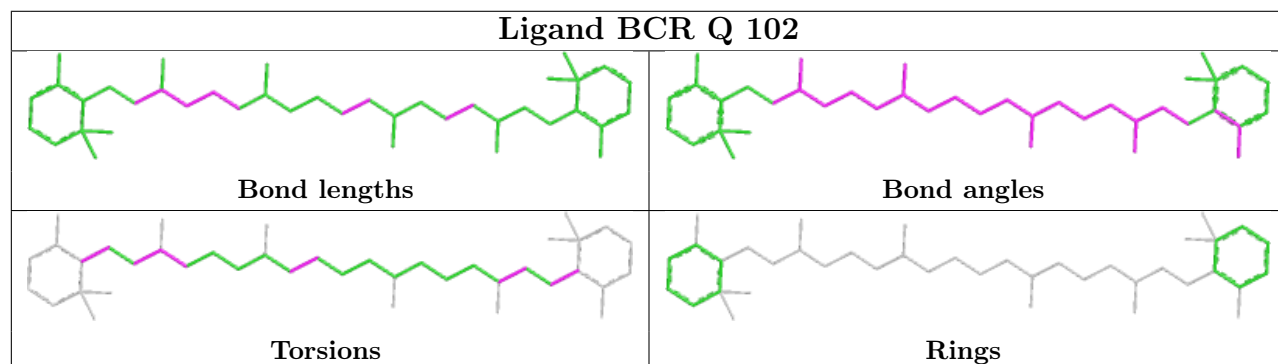
Ligand BCR I 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

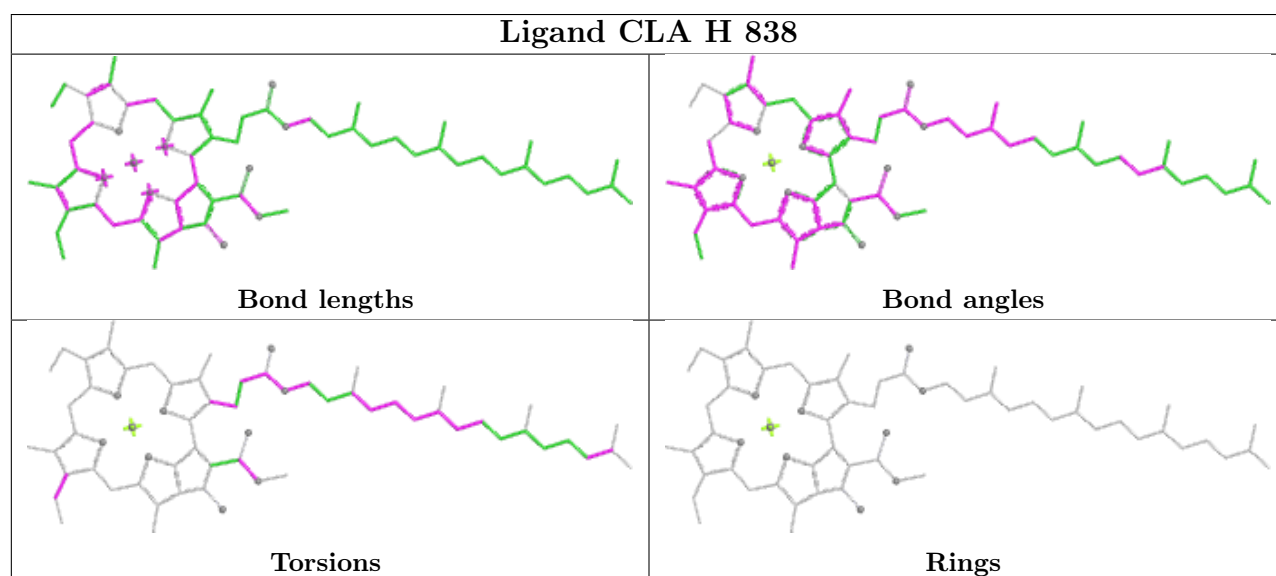
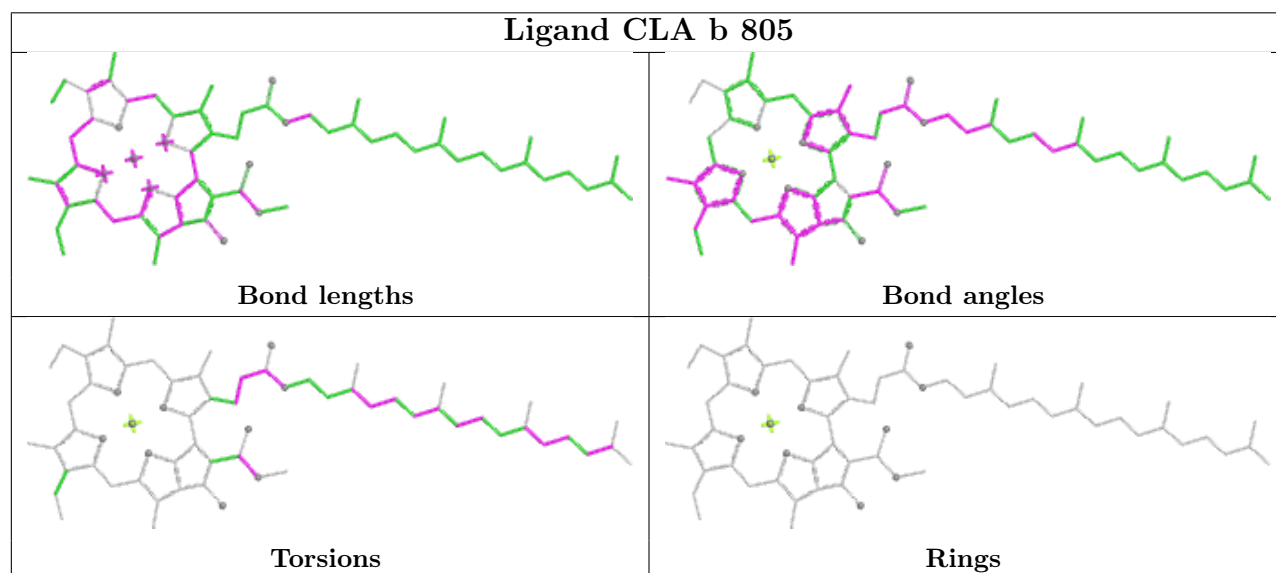
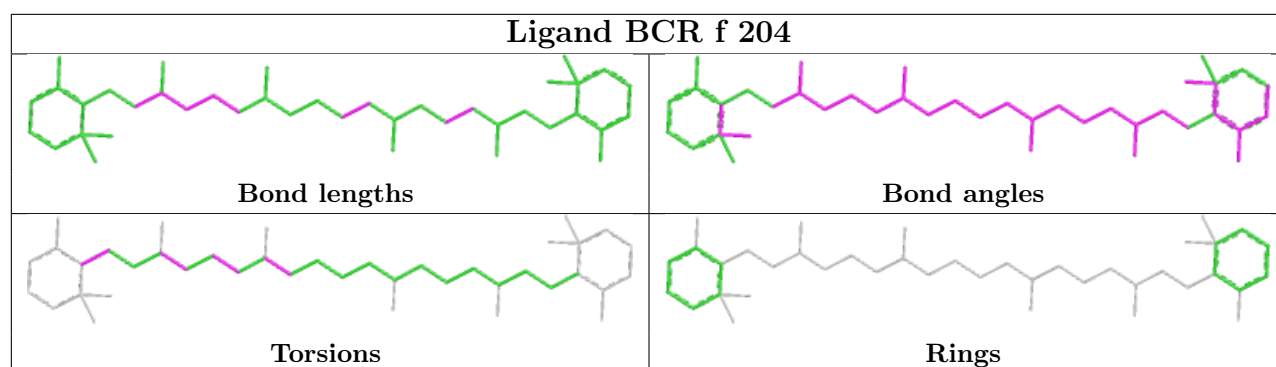
Ligand BCR J 104	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 819

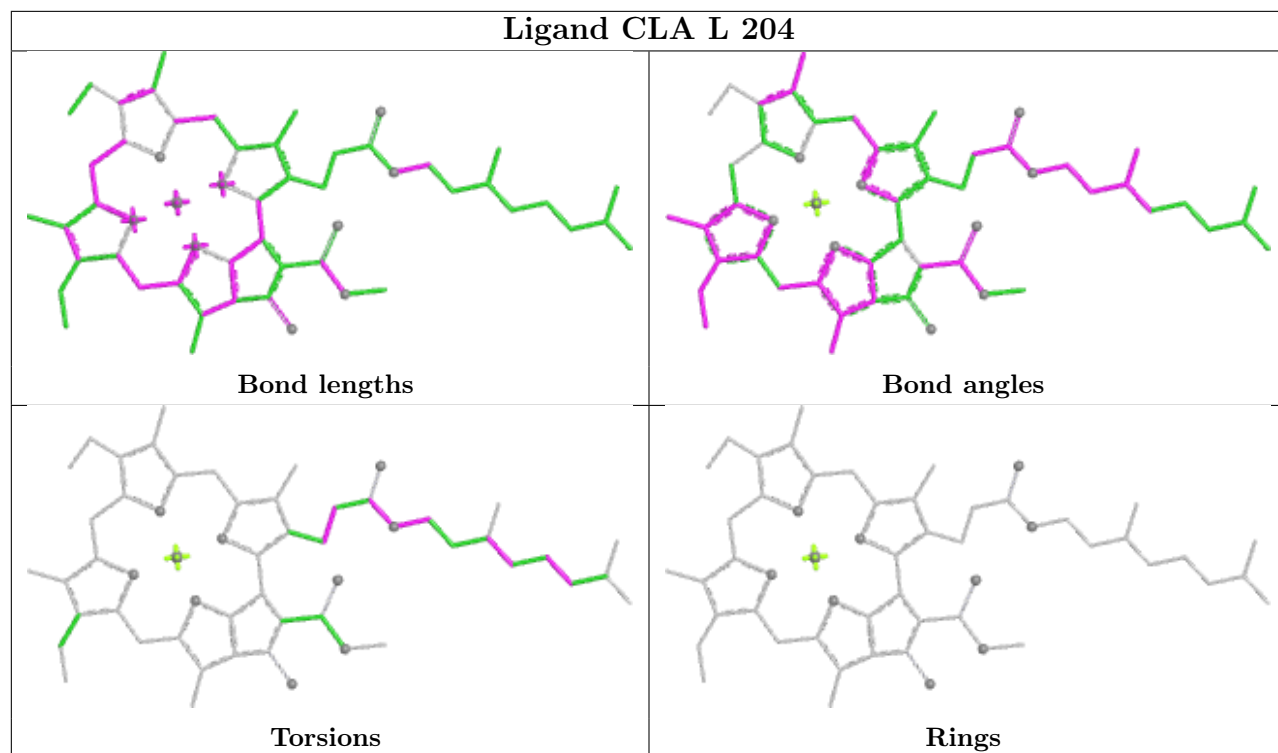


Ligand BCR Q 102

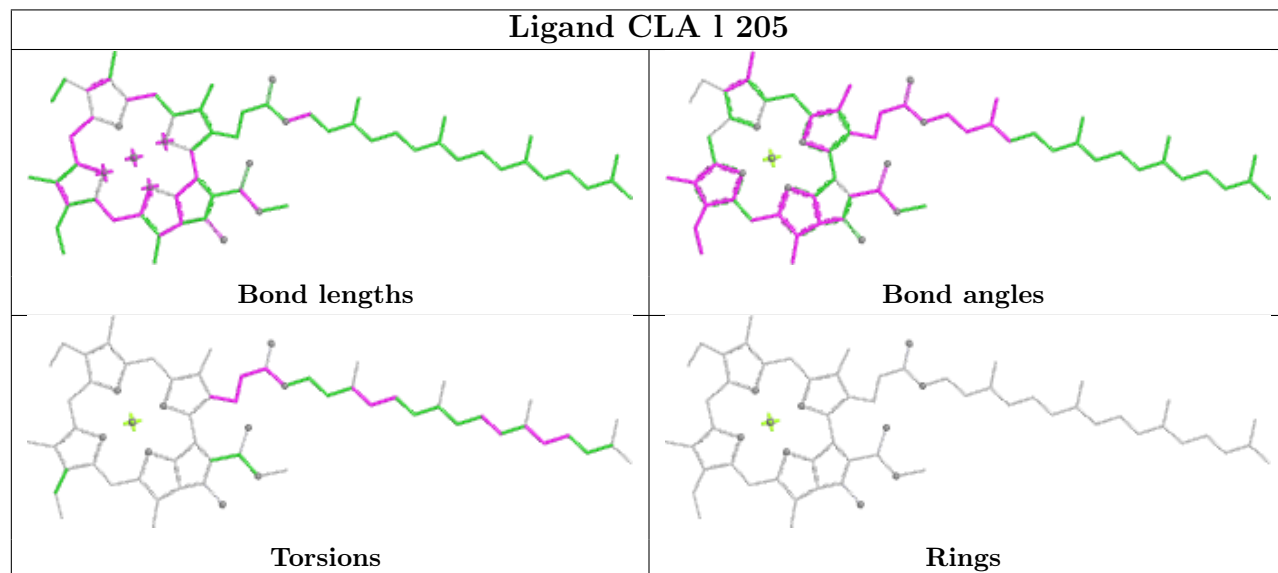


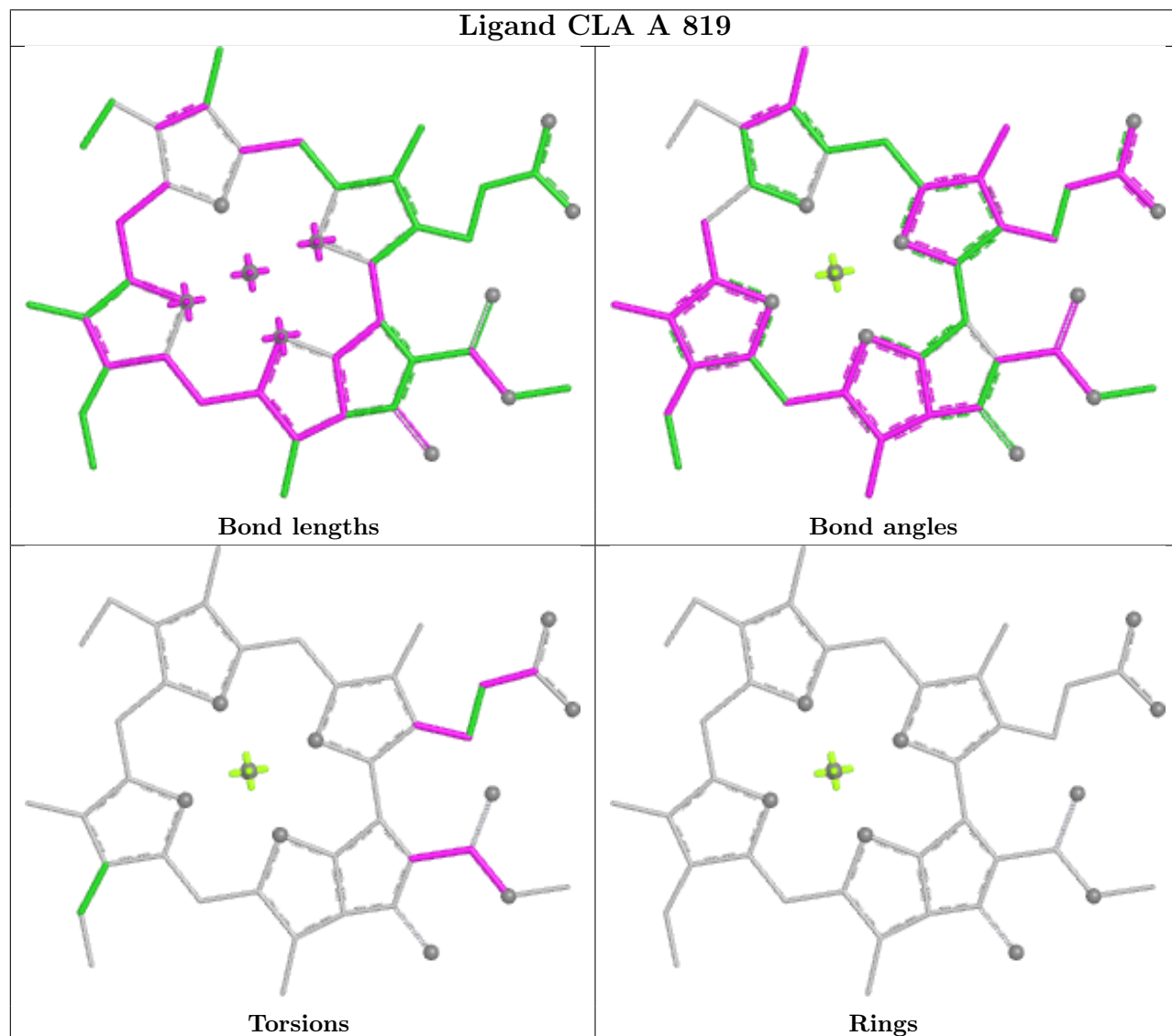
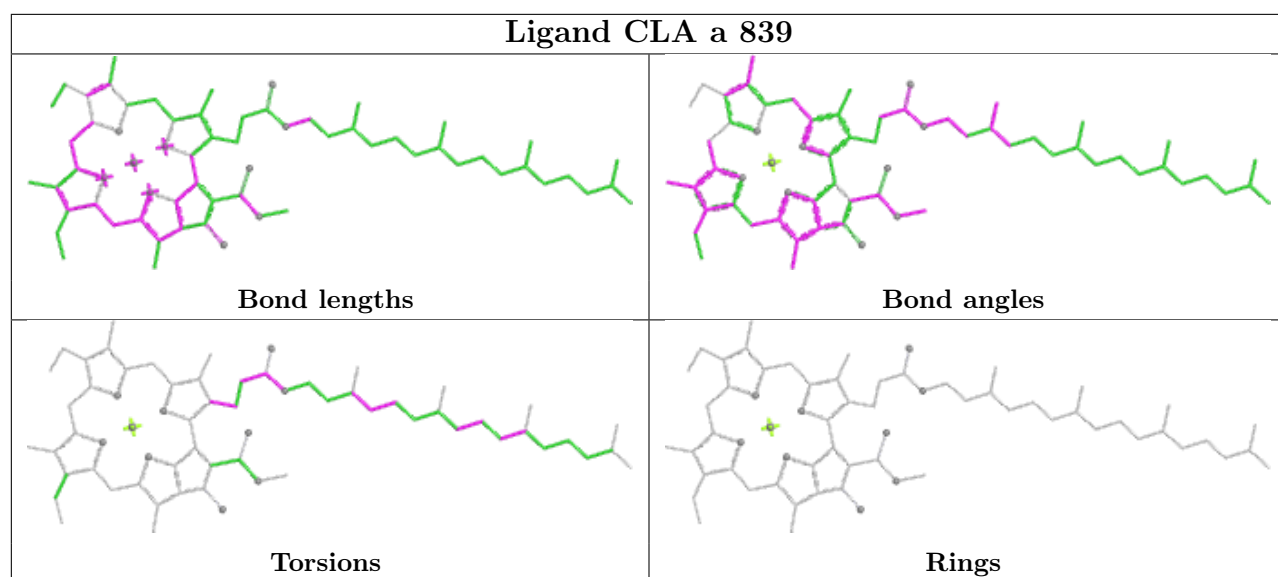


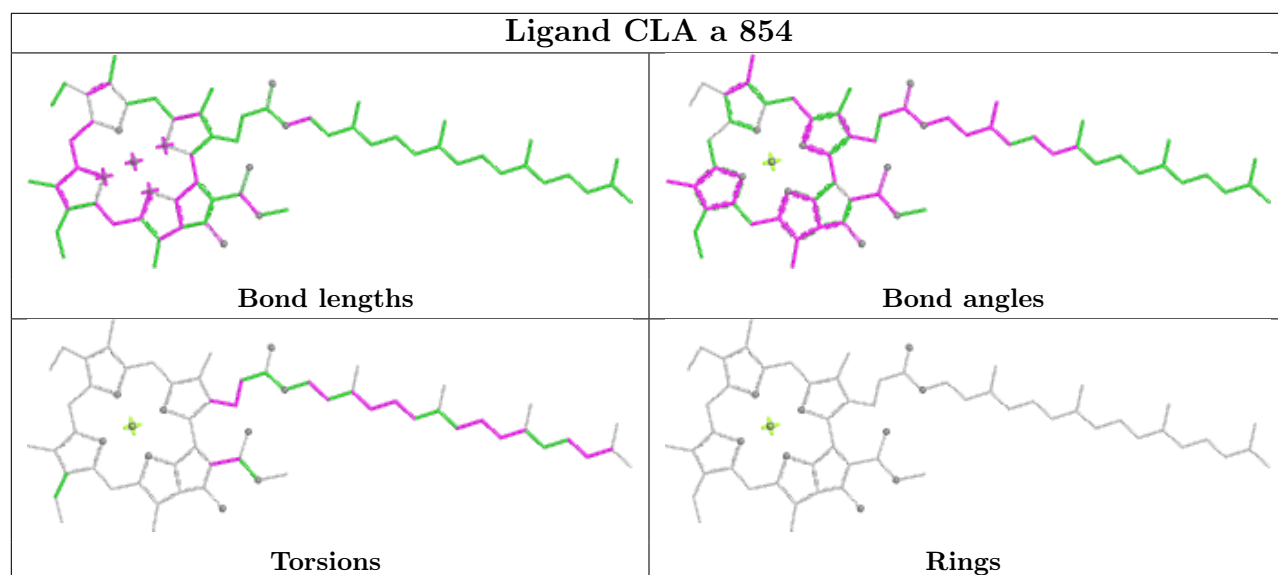
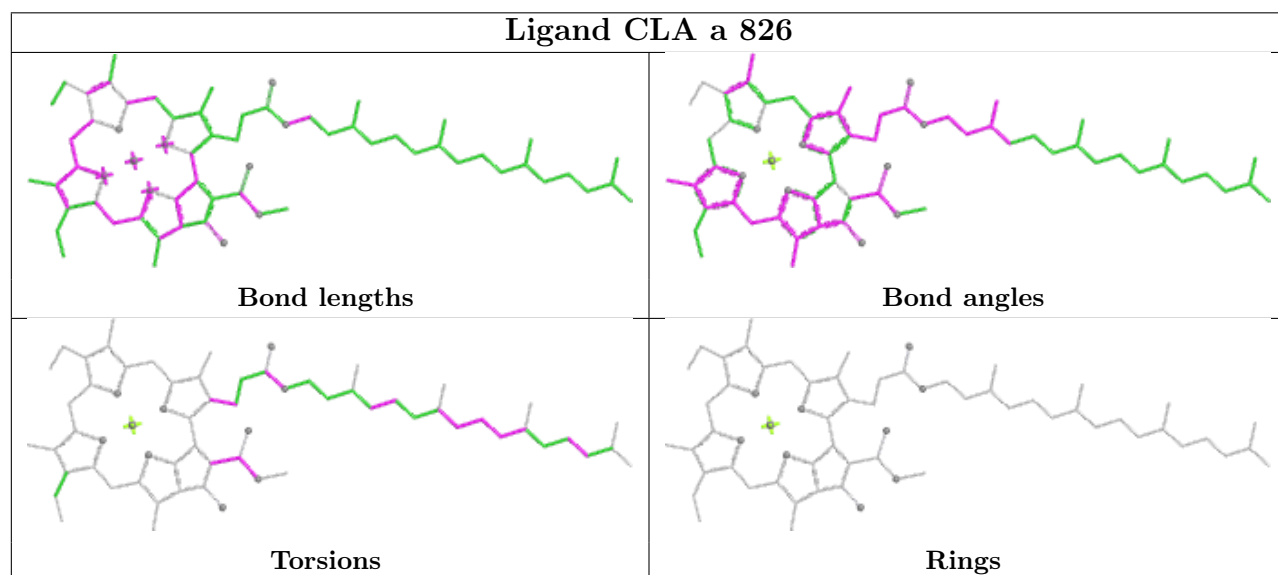
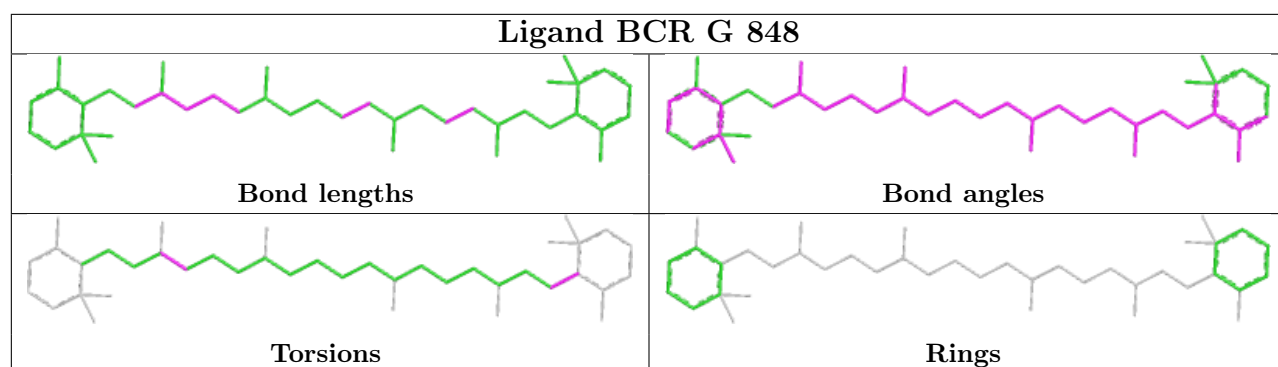
Ligand CLA L 204



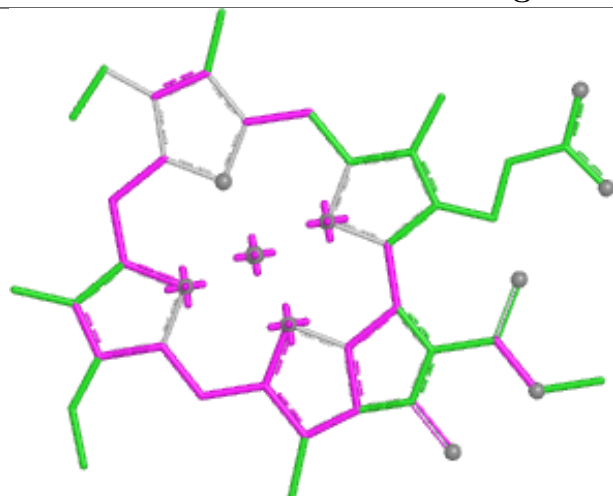
Ligand CLA I 205



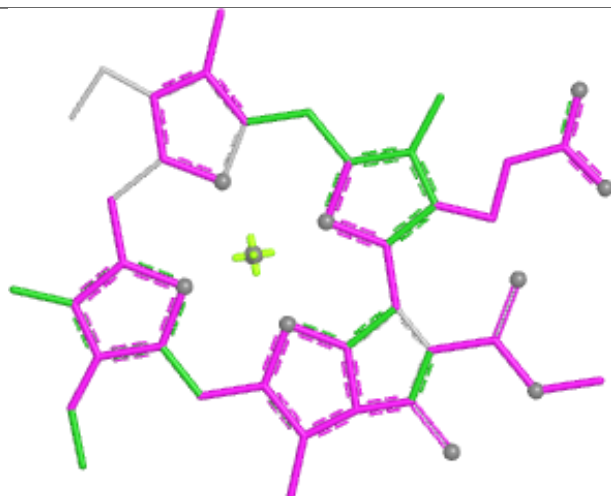




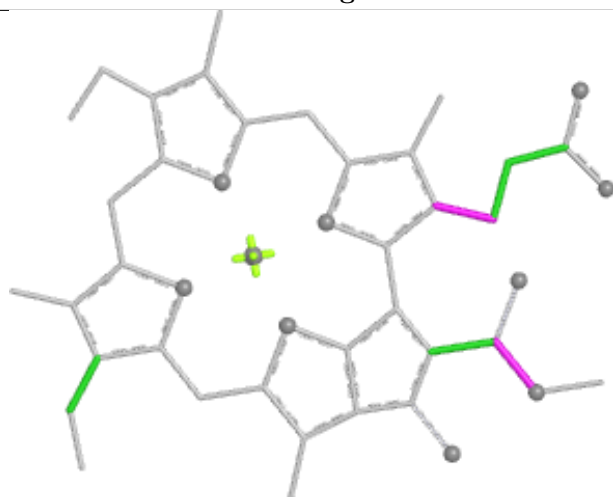
Ligand CLA H 829



Bond lengths



Bond angles

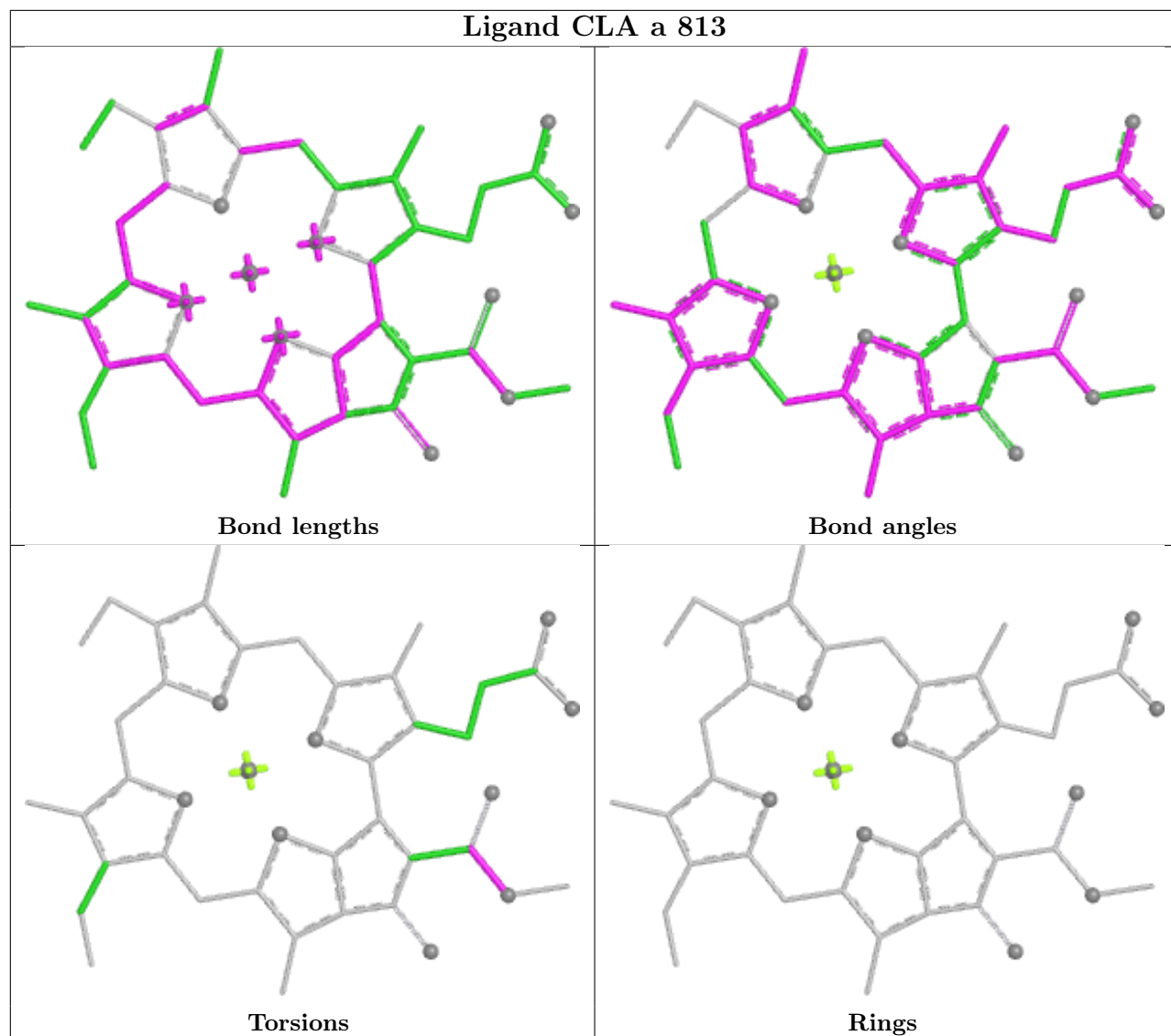


Torsions

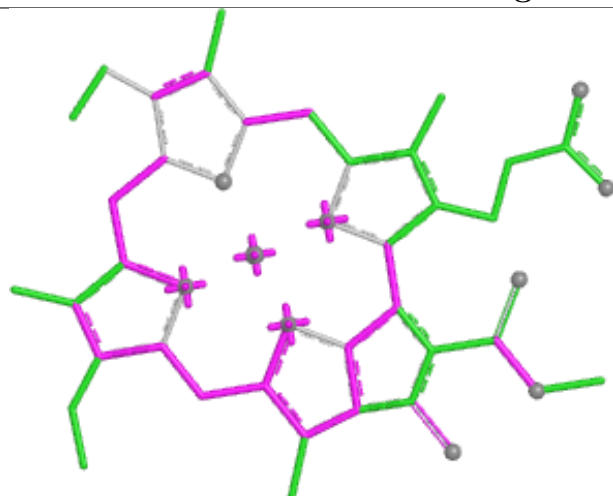


Rings

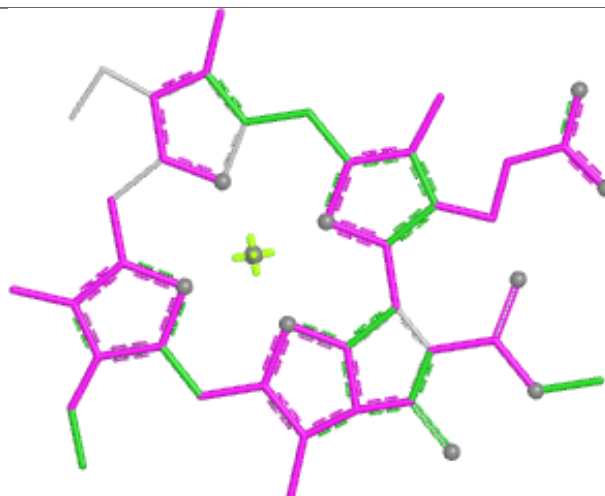
Ligand CLA a 813



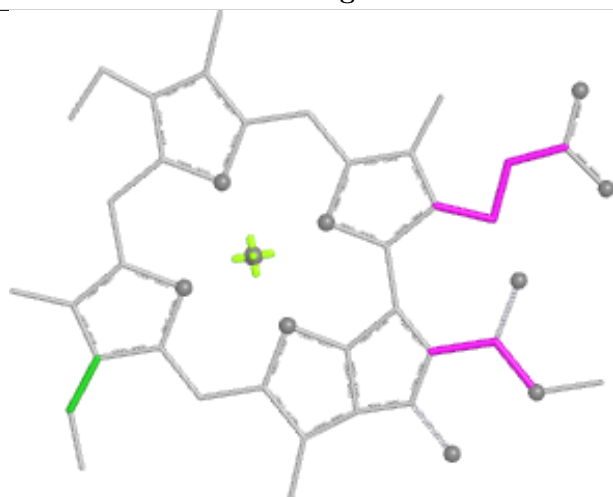
Ligand CLA B 812



Bond lengths



Bond angles

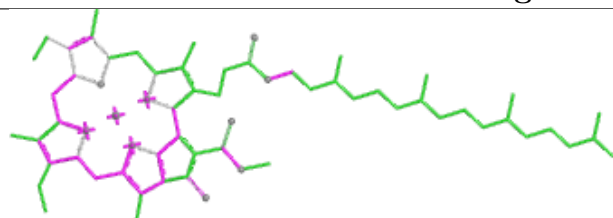


Torsions

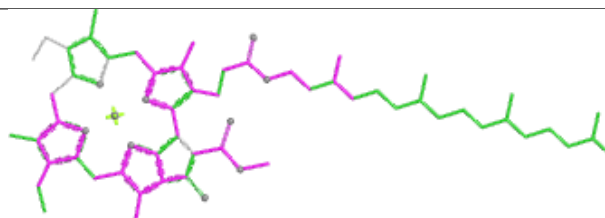


Rings

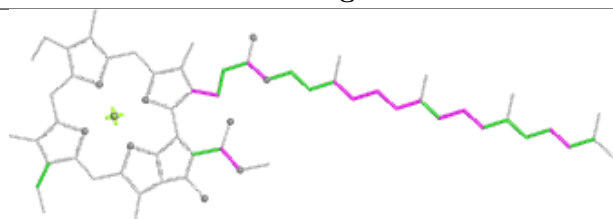
Ligand CLA B 816



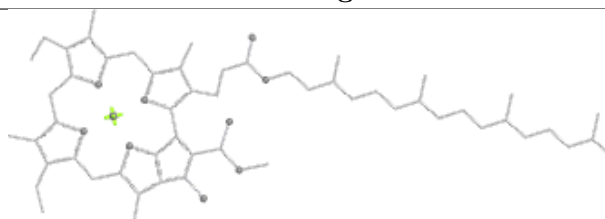
Bond lengths



Bond angles

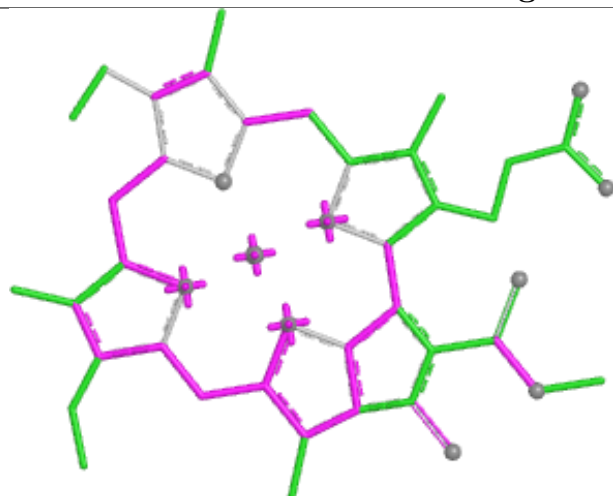


Torsions

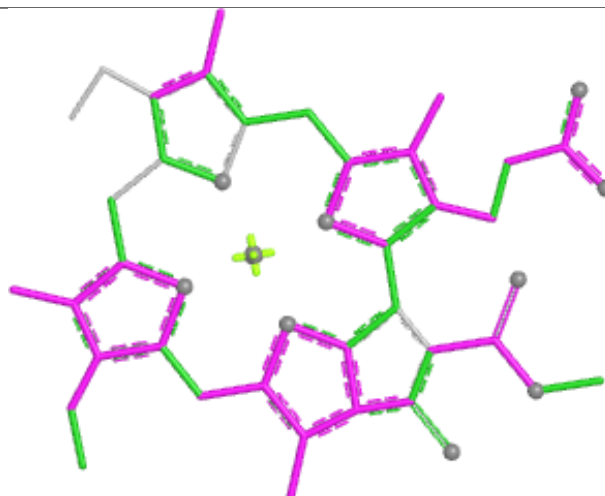


Rings

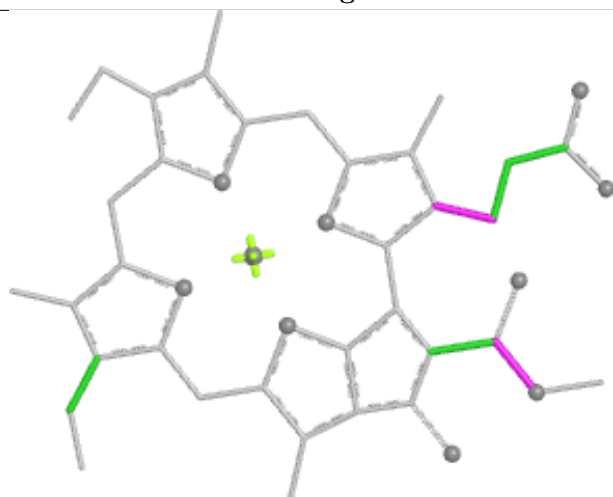
Ligand CLA a 815



Bond lengths



Bond angles

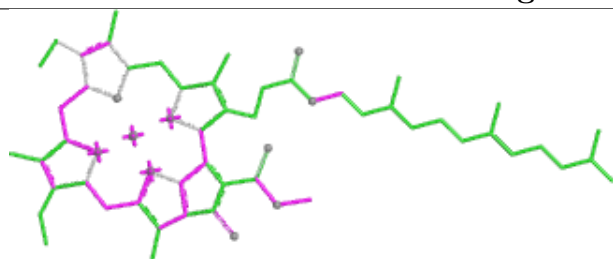


Torsions

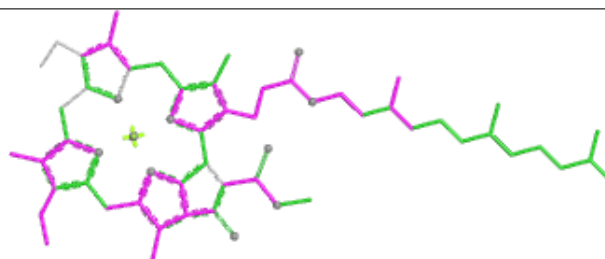


Rings

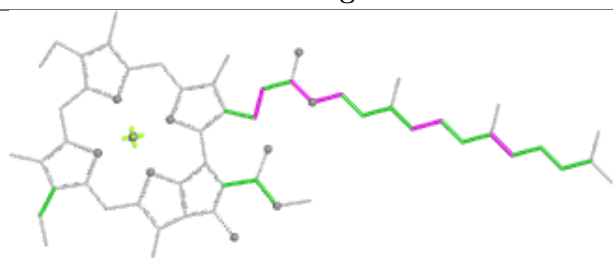
Ligand CLA b 801



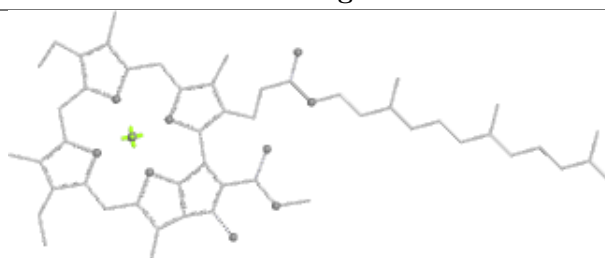
Bond lengths



Bond angles

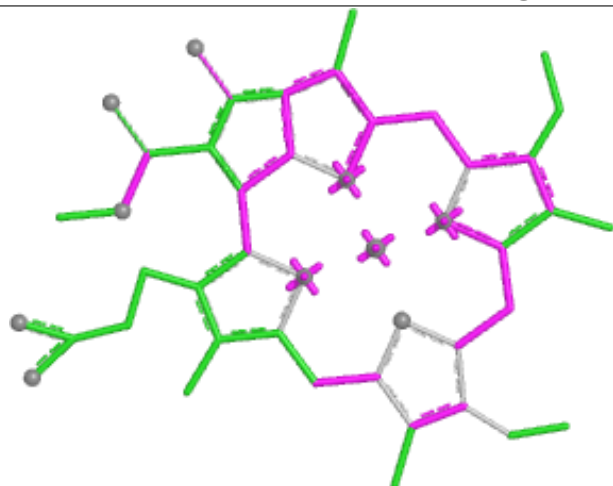


Torsions

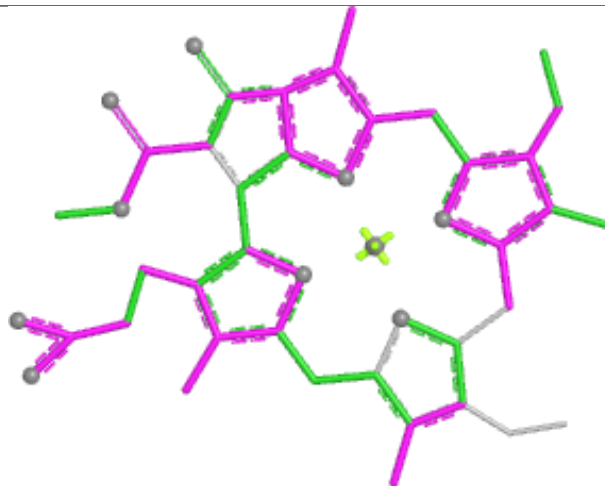


Rings

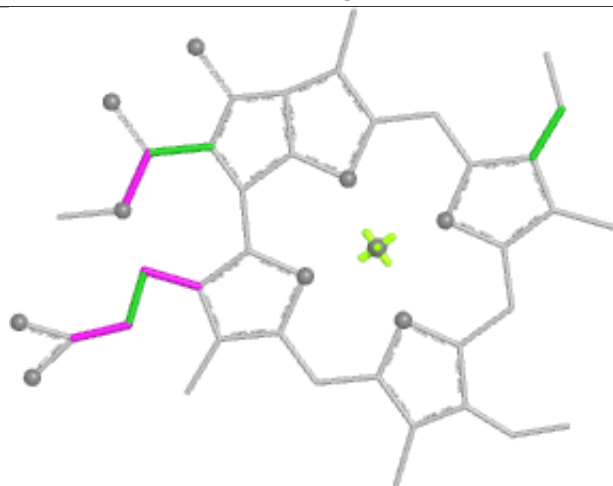
Ligand CLA P 203



Bond lengths



Bond angles

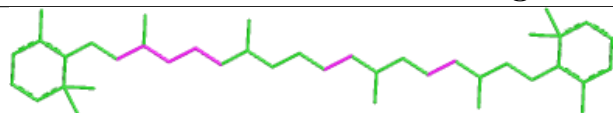


Torsions

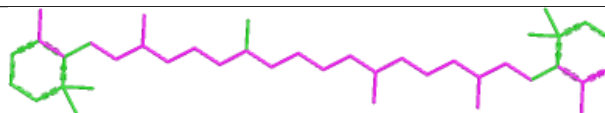


Rings

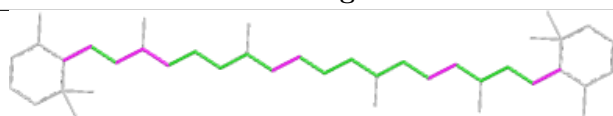
Ligand BCR G 845



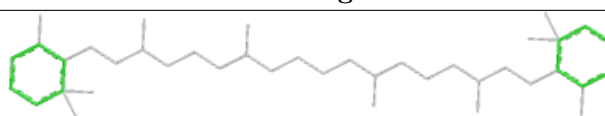
Bond lengths



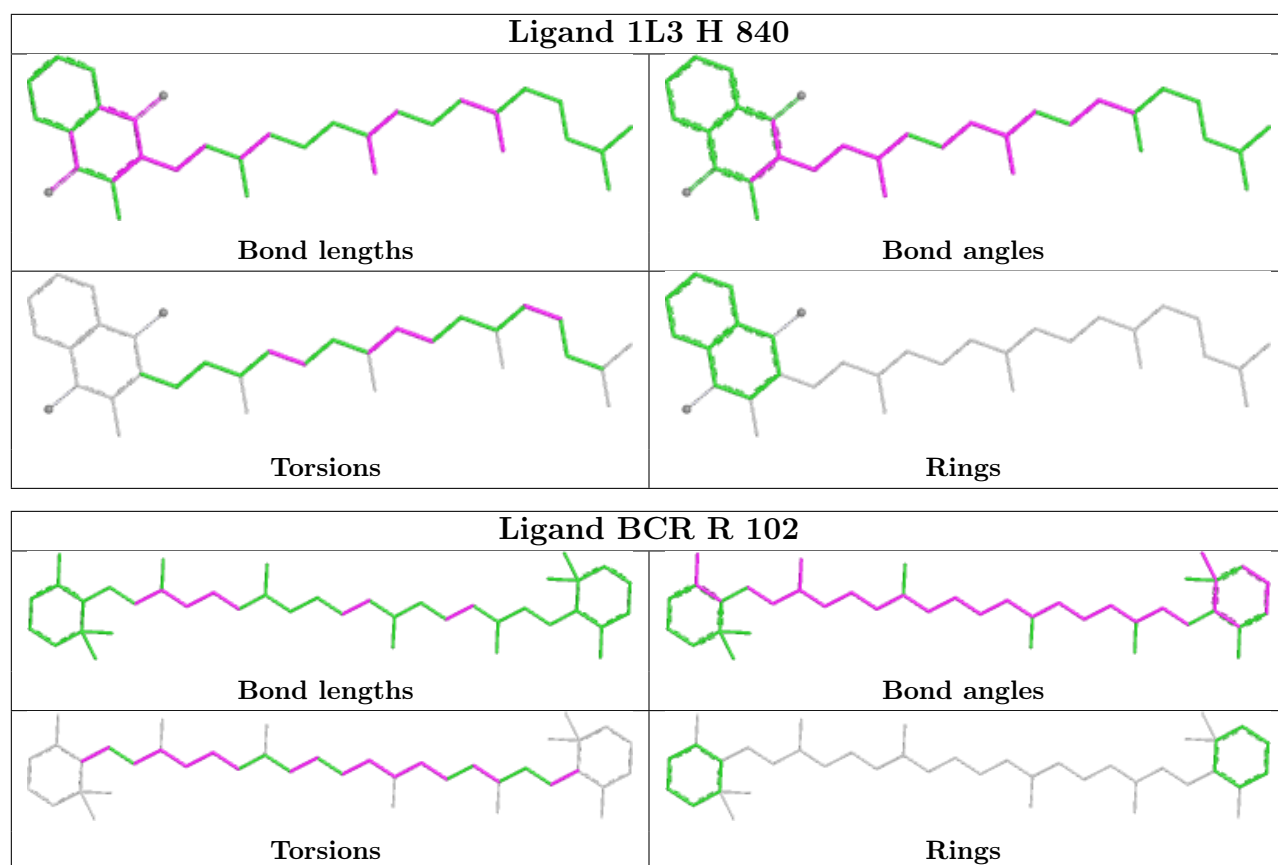
Bond angles



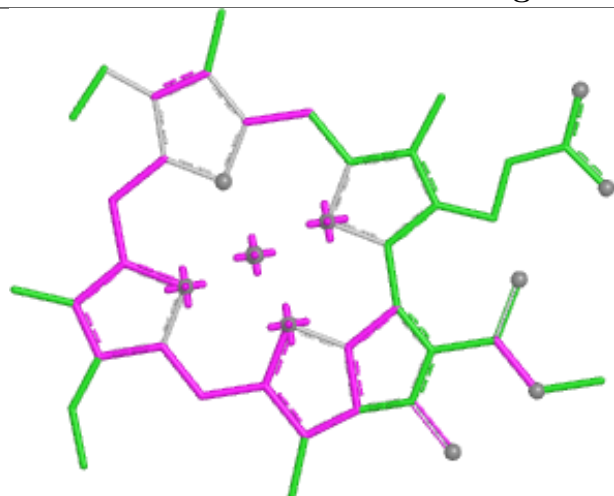
Torsions



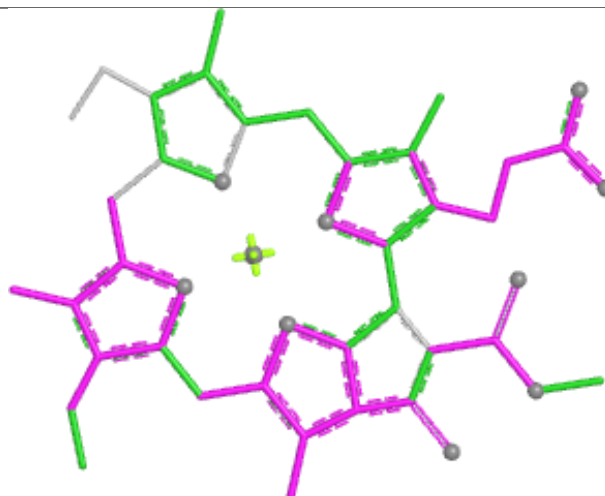
Rings



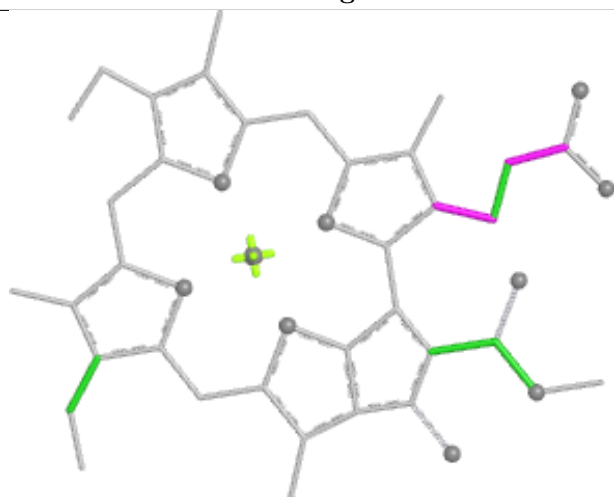
Ligand CLA G 838



Bond lengths



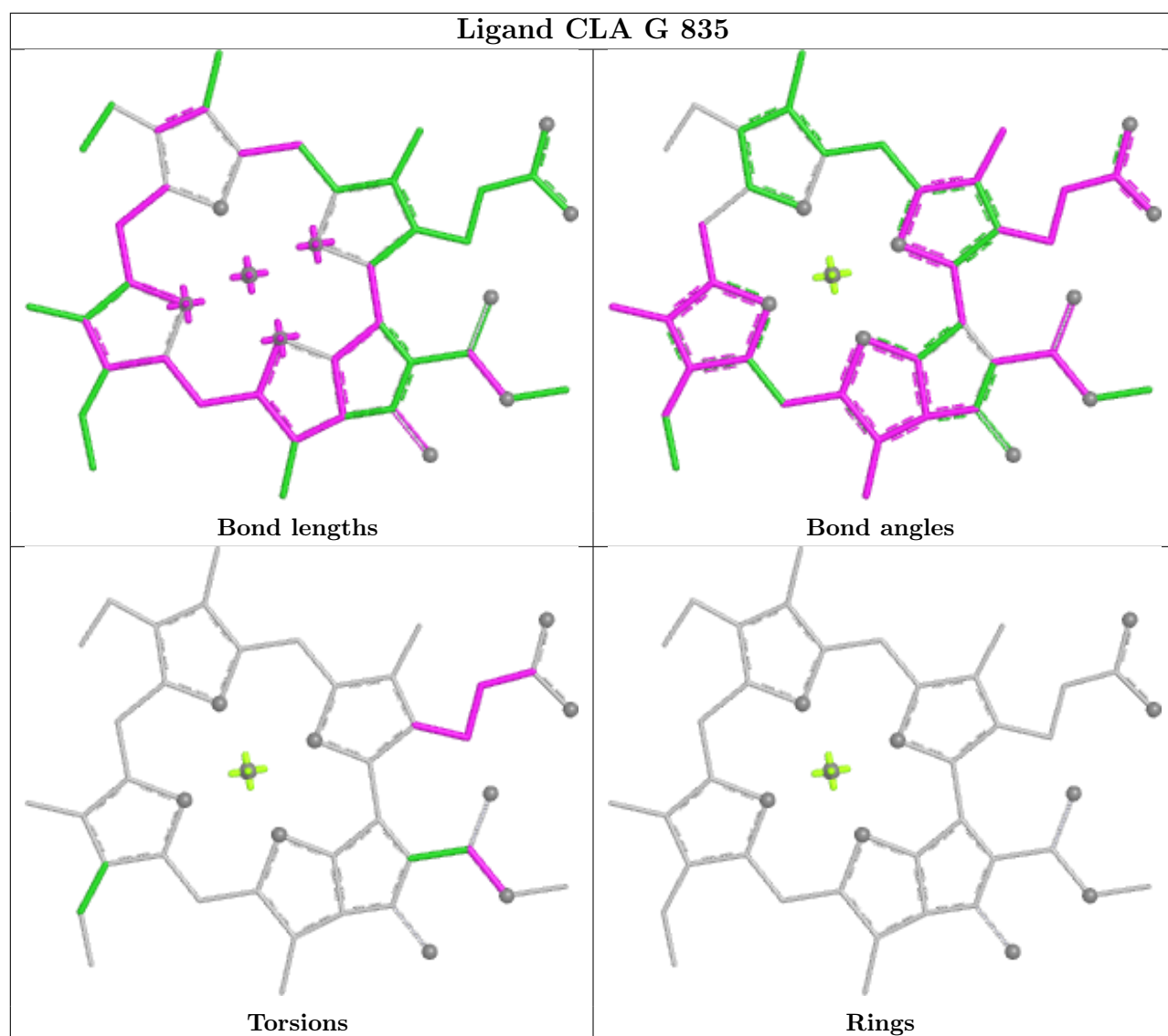
Bond angles

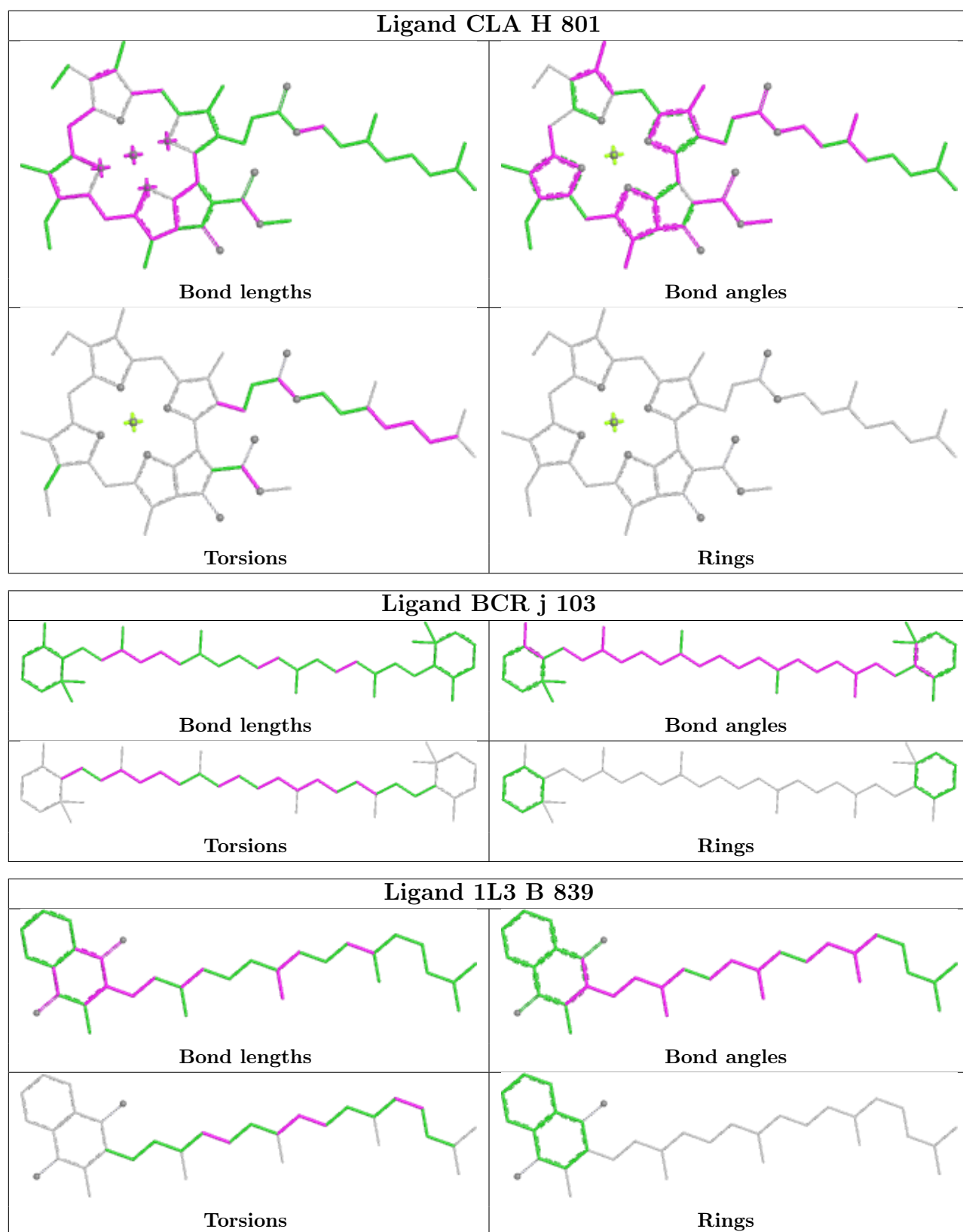


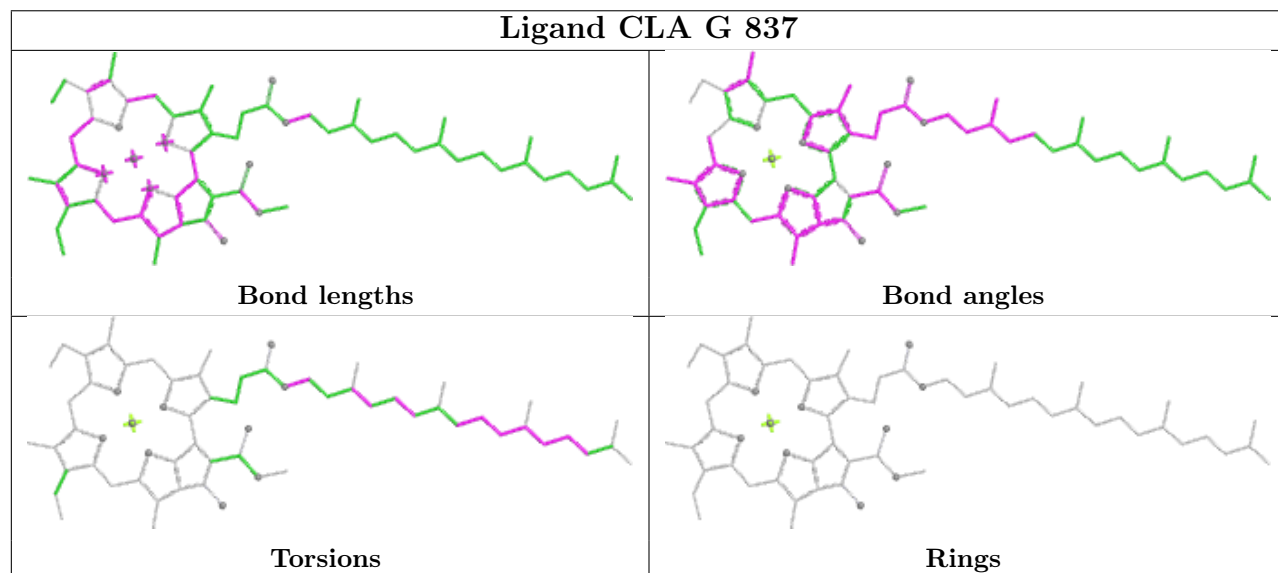
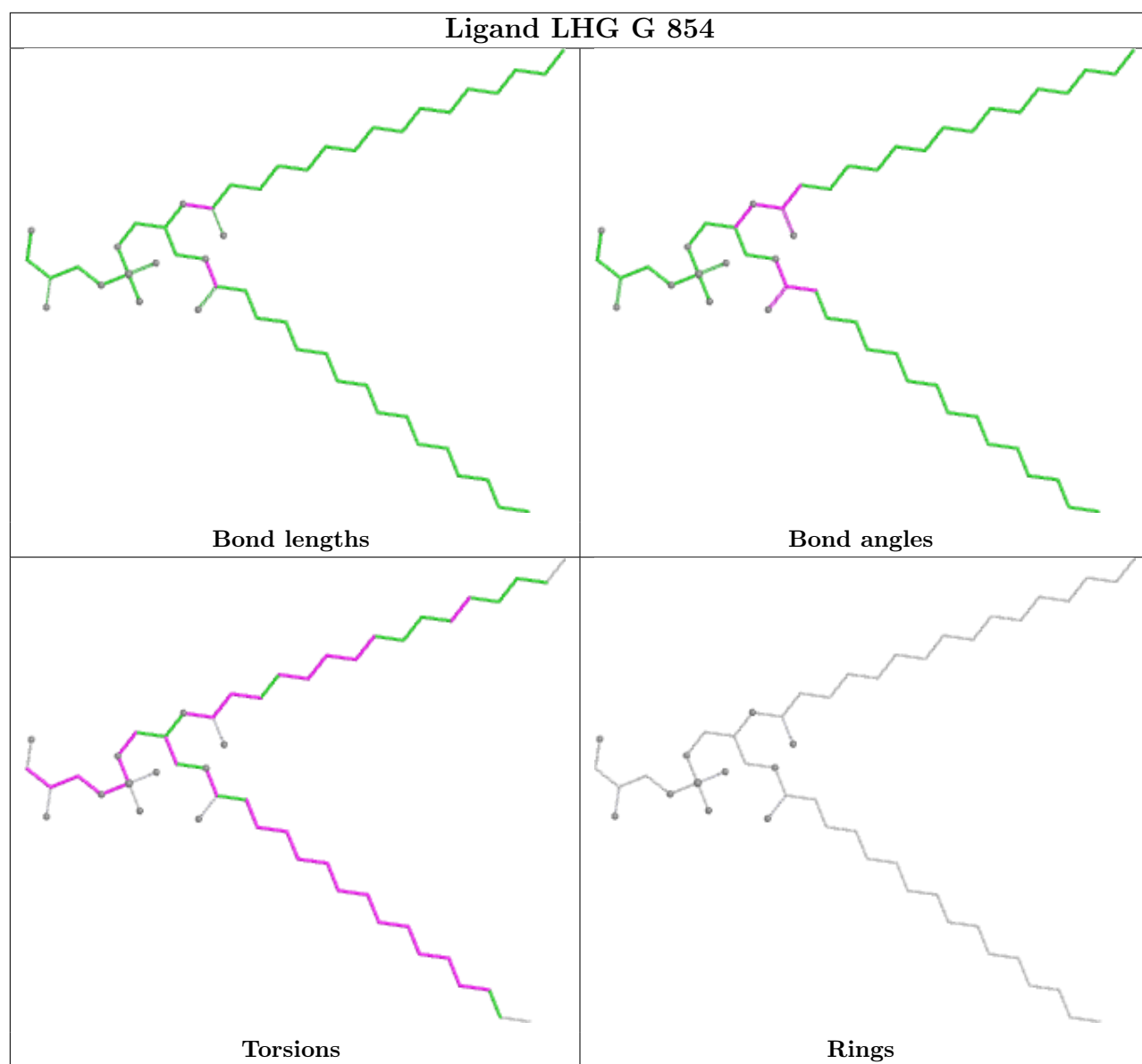
Torsions

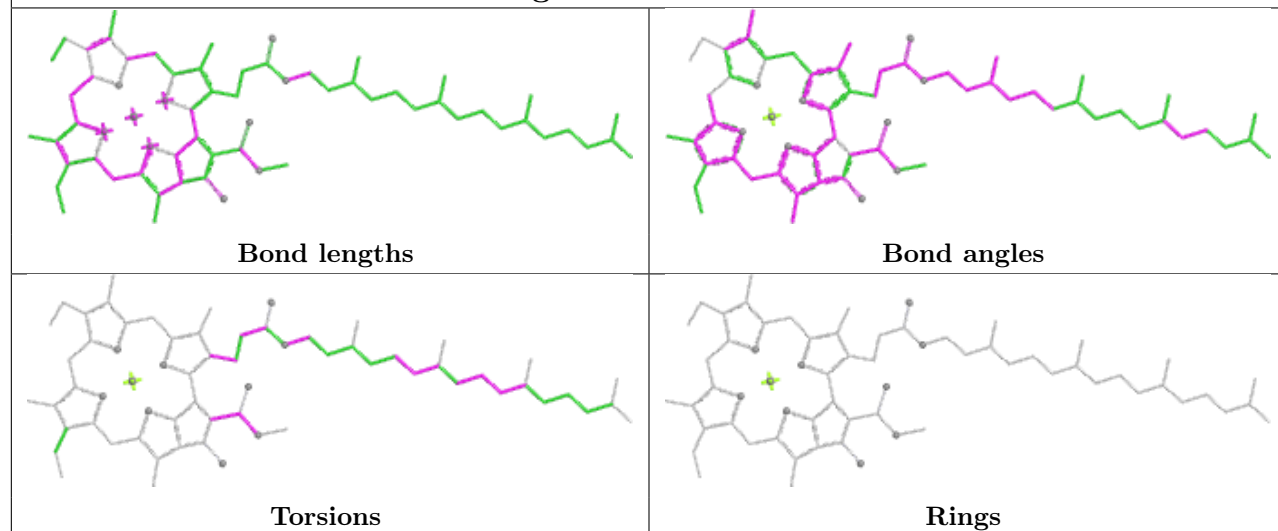
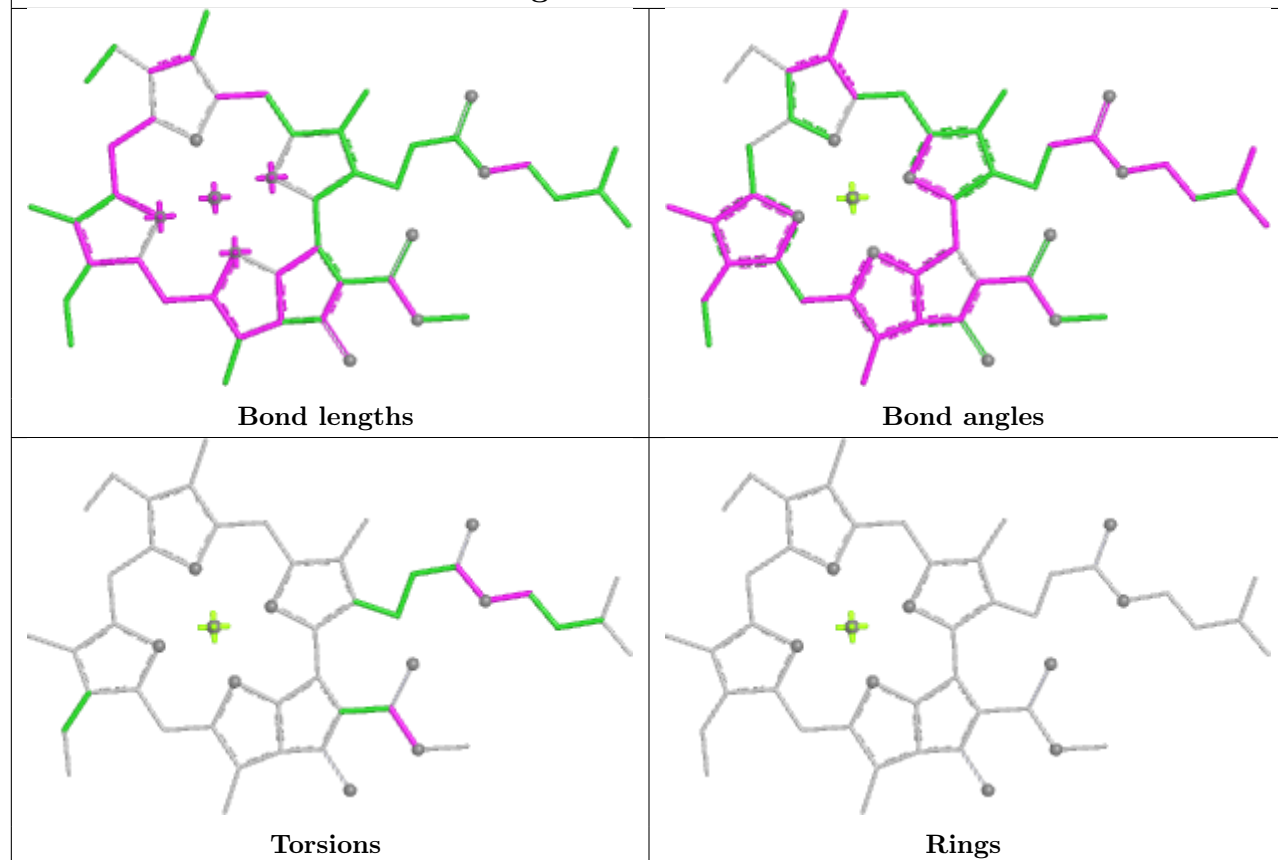


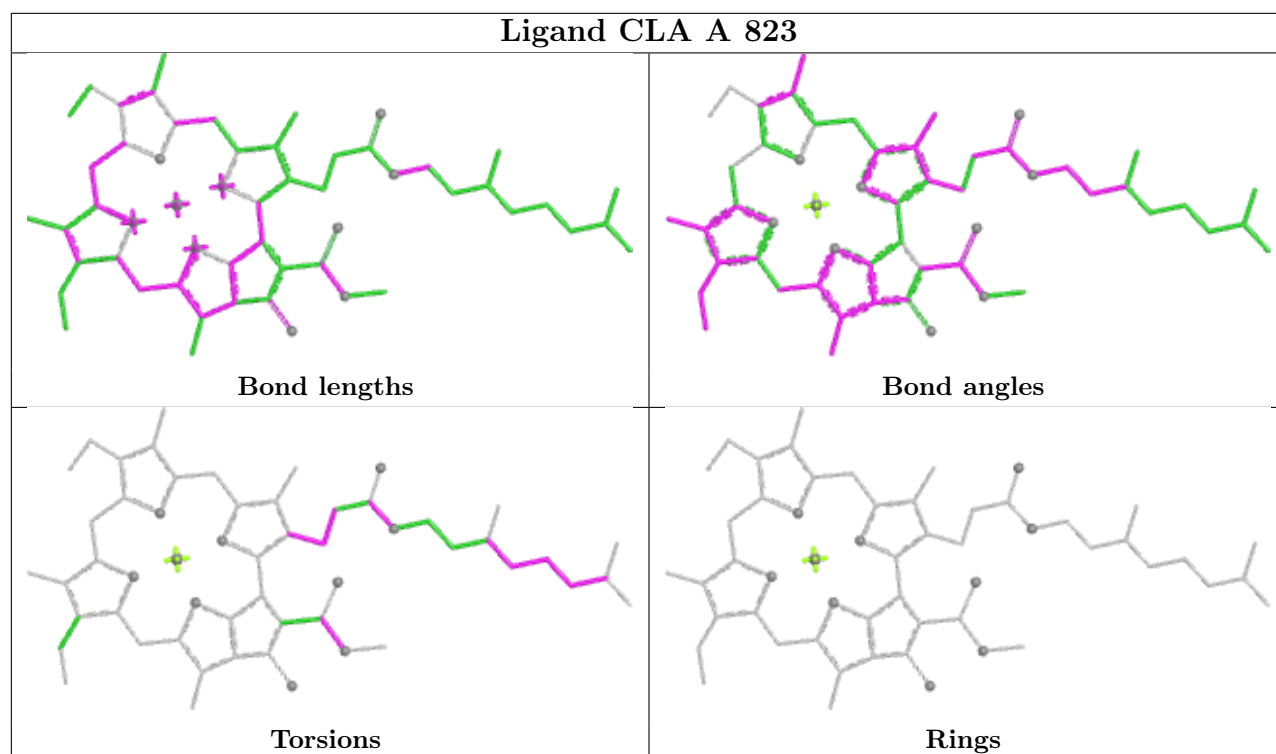
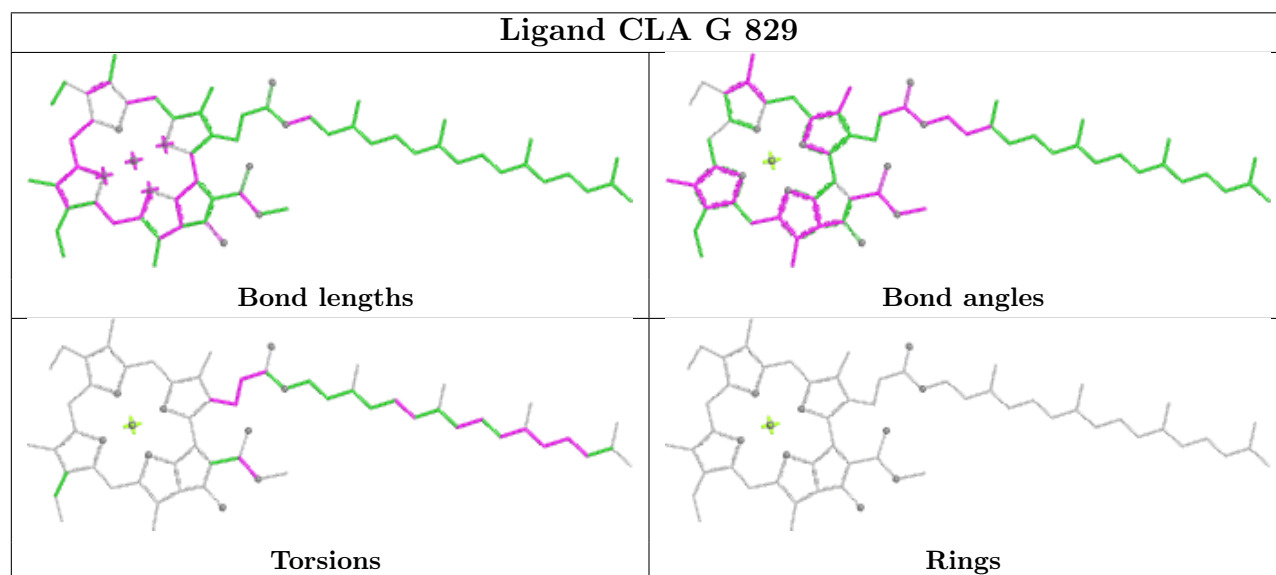
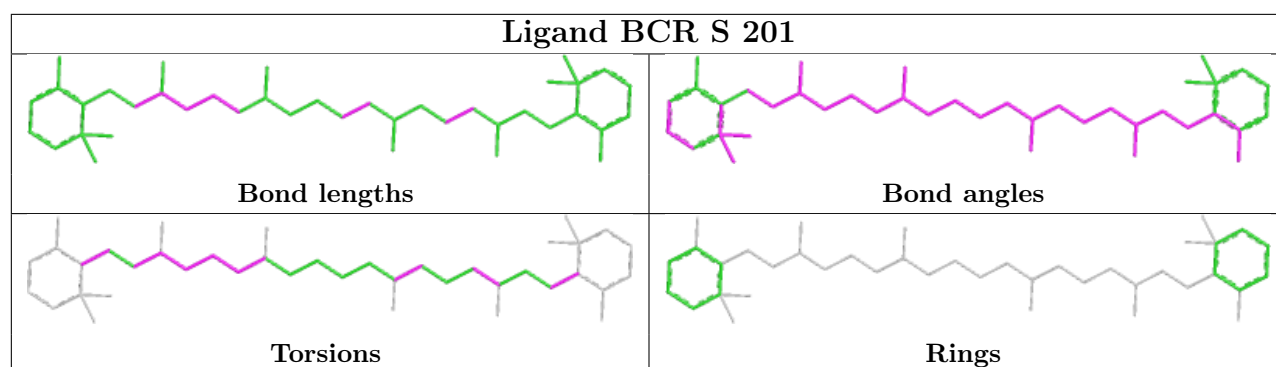
Rings



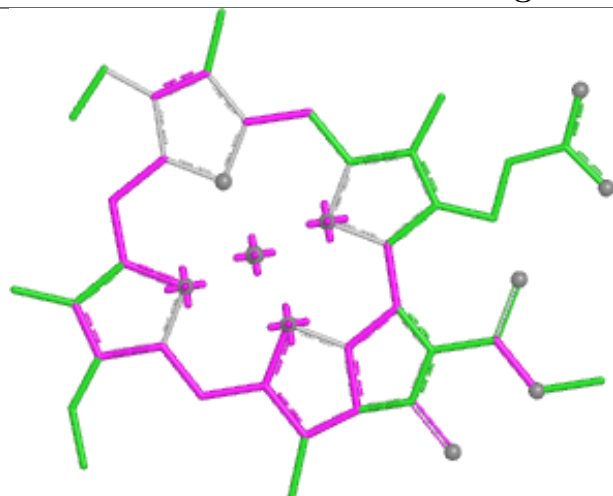




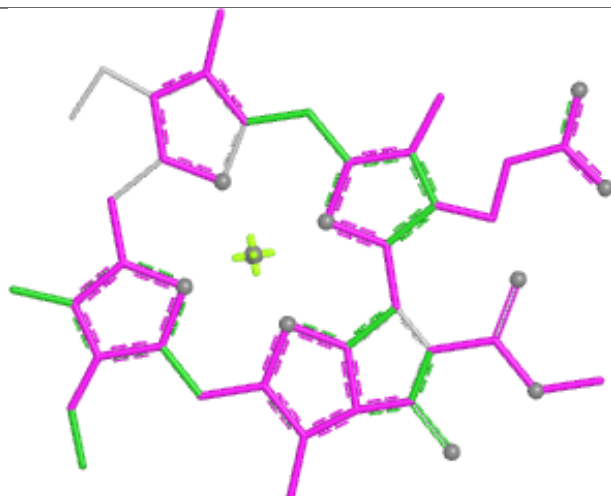
Ligand CLA B 823**Ligand CLA G 836**



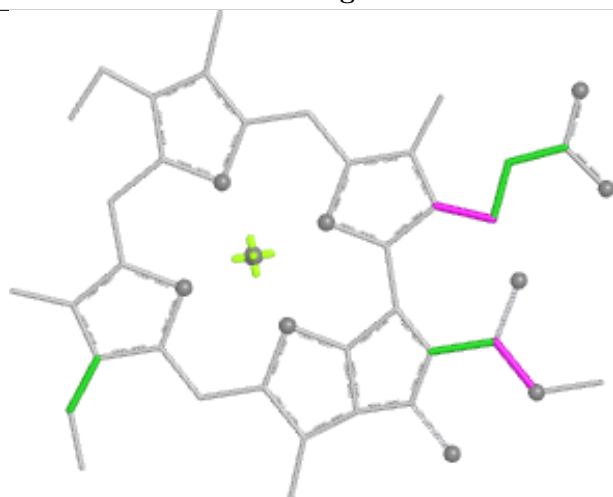
Ligand CLA B 828



Bond lengths



Bond angles

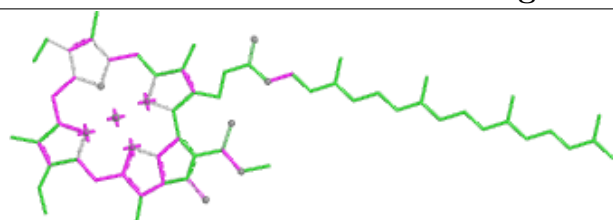


Torsions

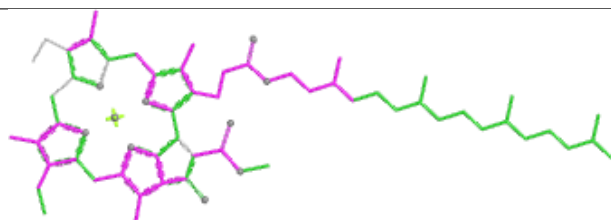


Rings

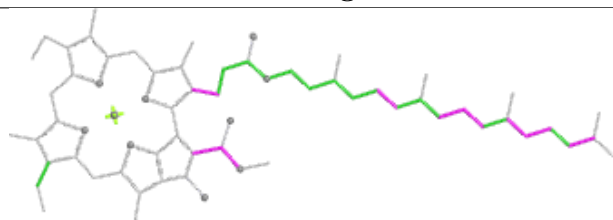
Ligand CLA a 805



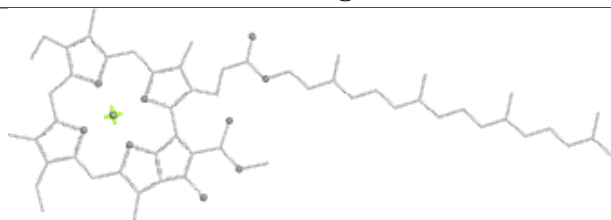
Bond lengths



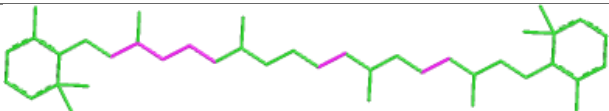
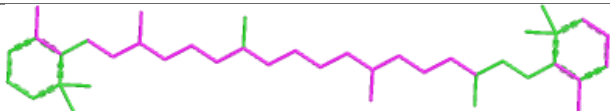
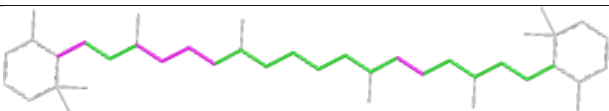
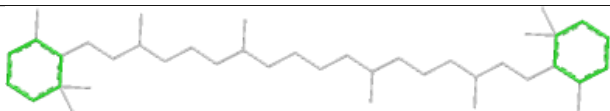
Bond angles



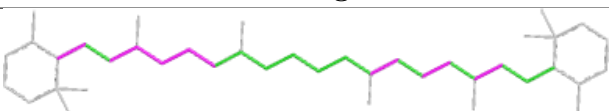
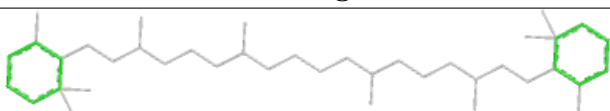


Torsions

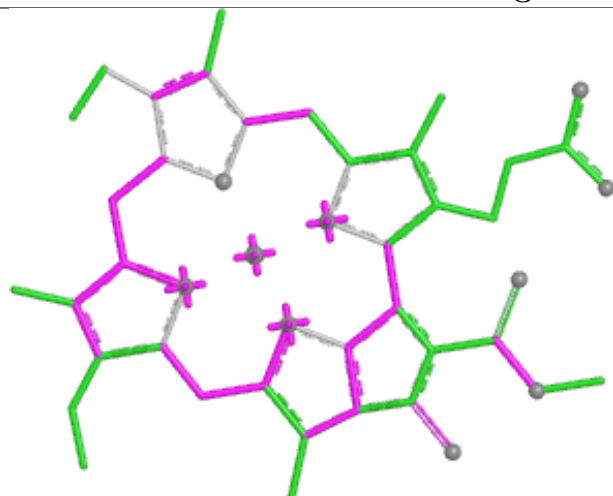


Rings

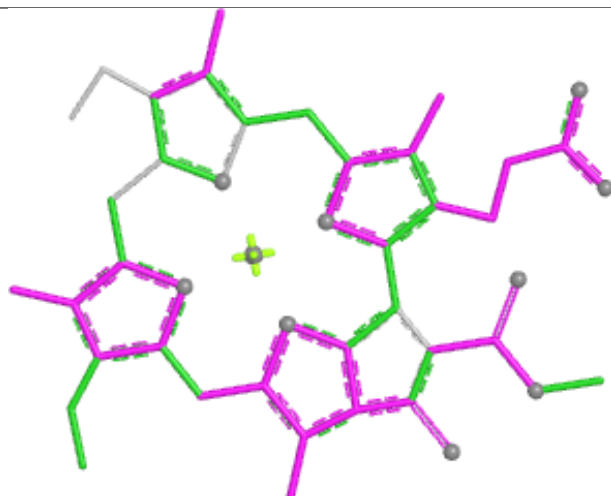
Ligand BCR B 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR P 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

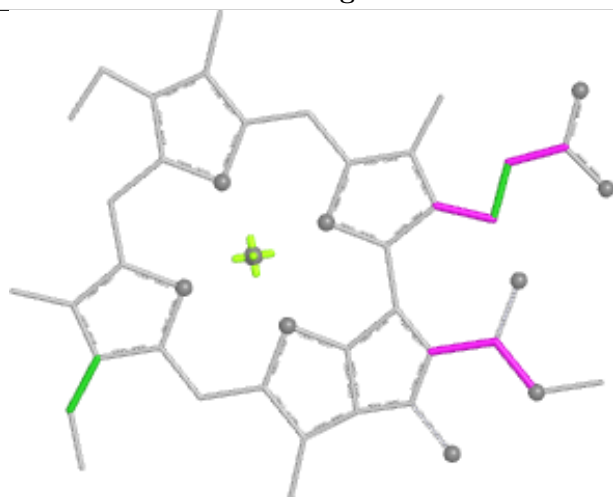
Ligand CLA B 817



Bond lengths



Bond angles

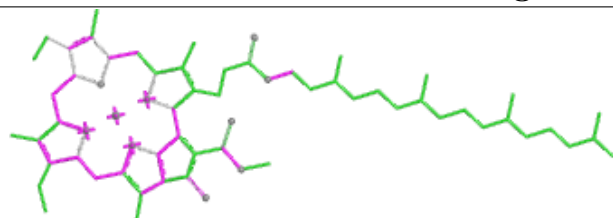


Torsions

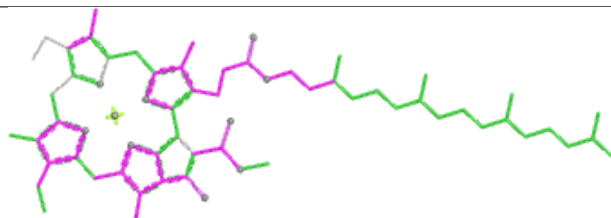


Rings

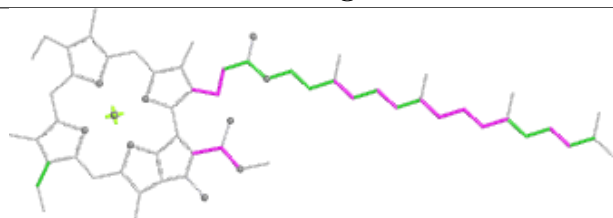
Ligand CLA H 823



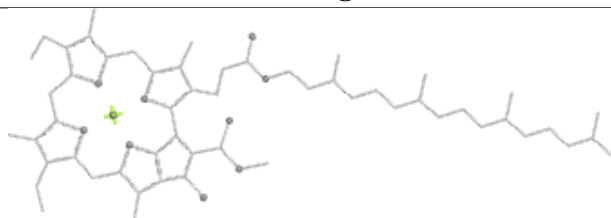
Bond lengths



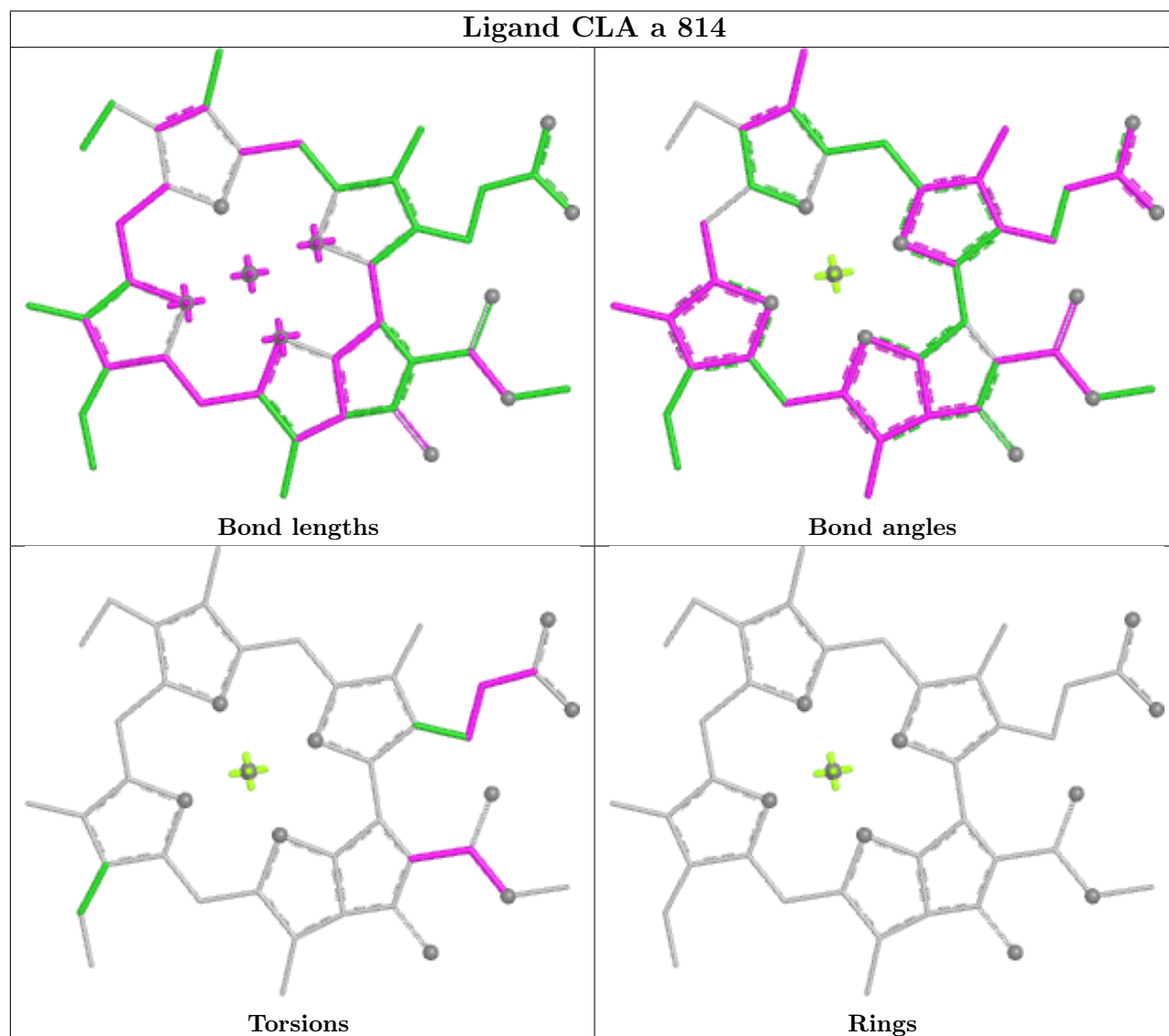
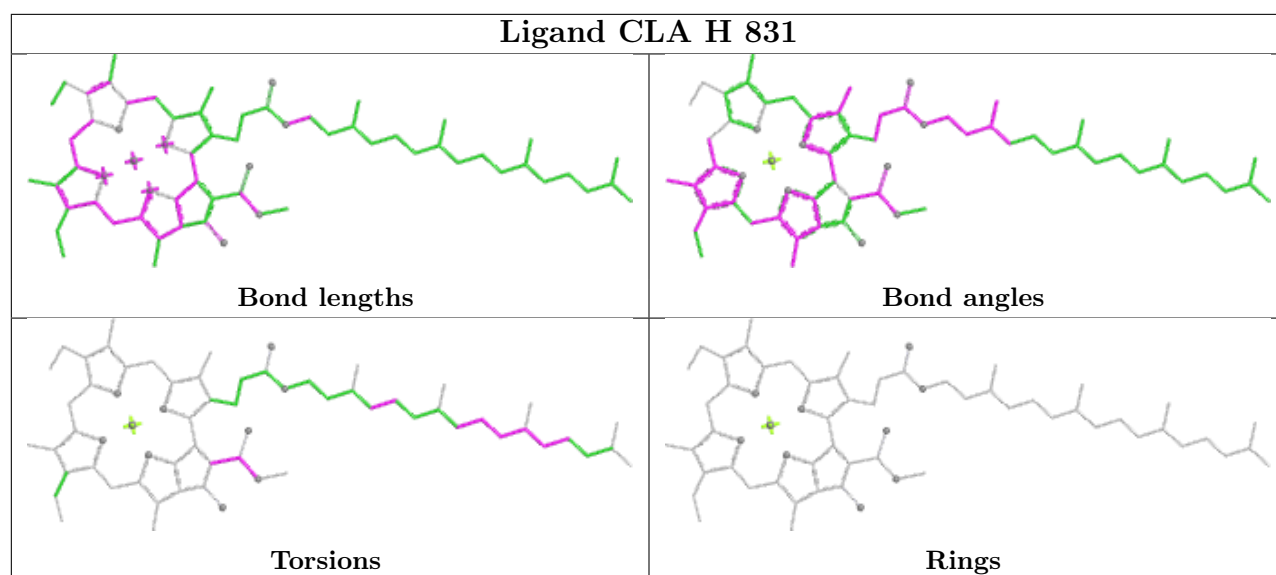
Bond angles



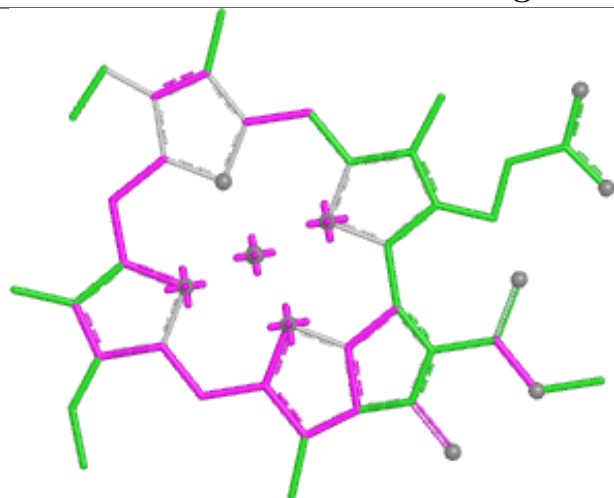
Torsions



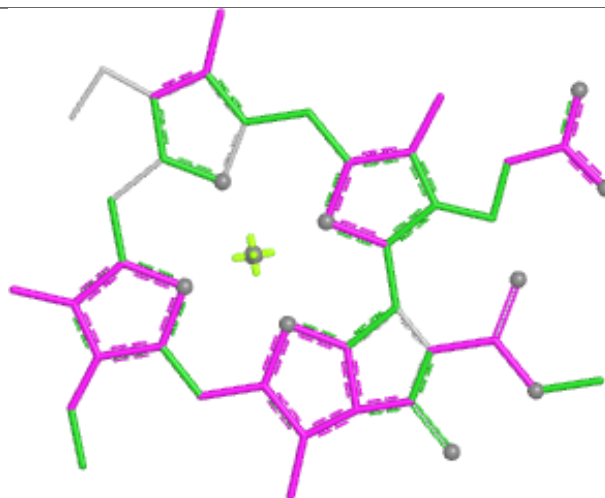
Rings



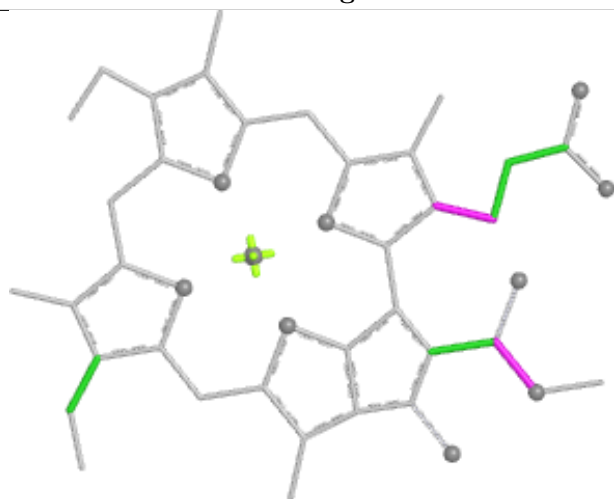
Ligand CLA H 828



Bond lengths



Bond angles

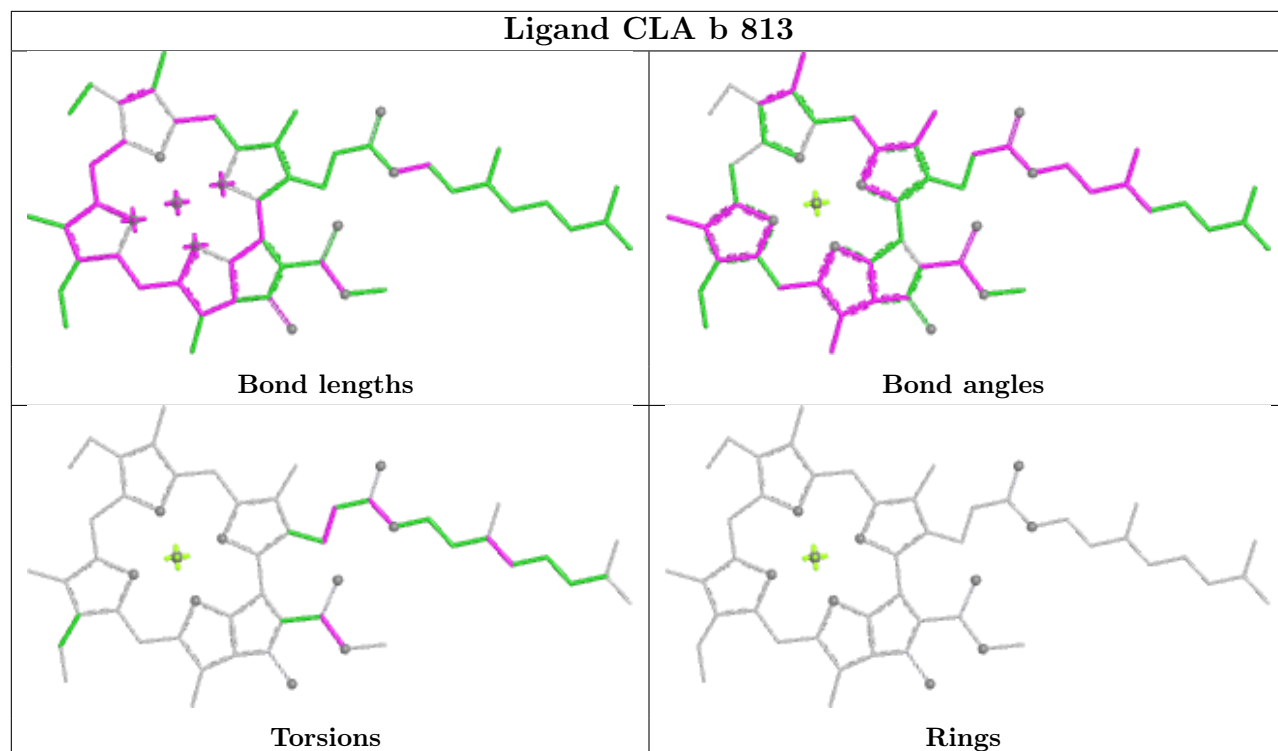


Torsions

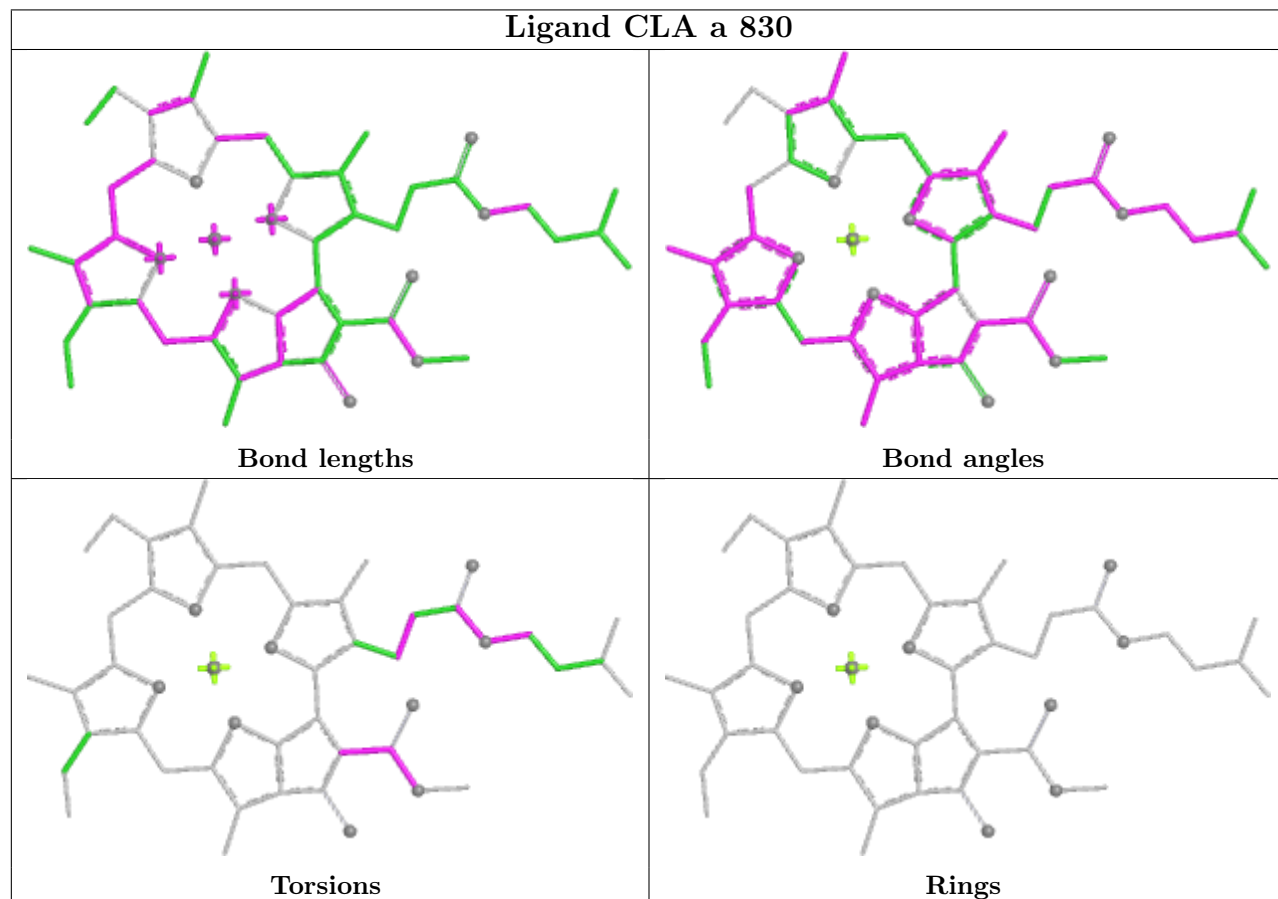


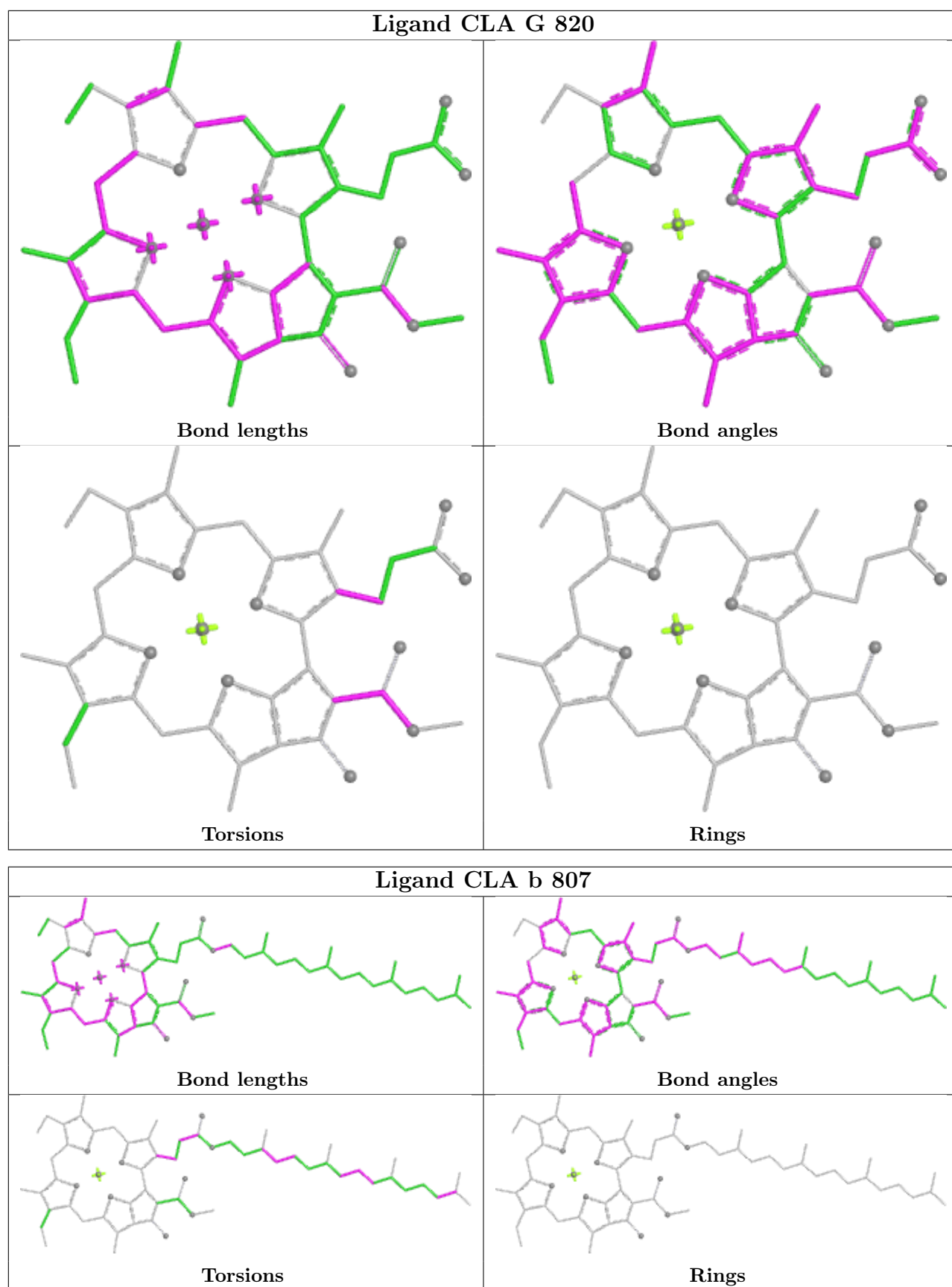
Rings

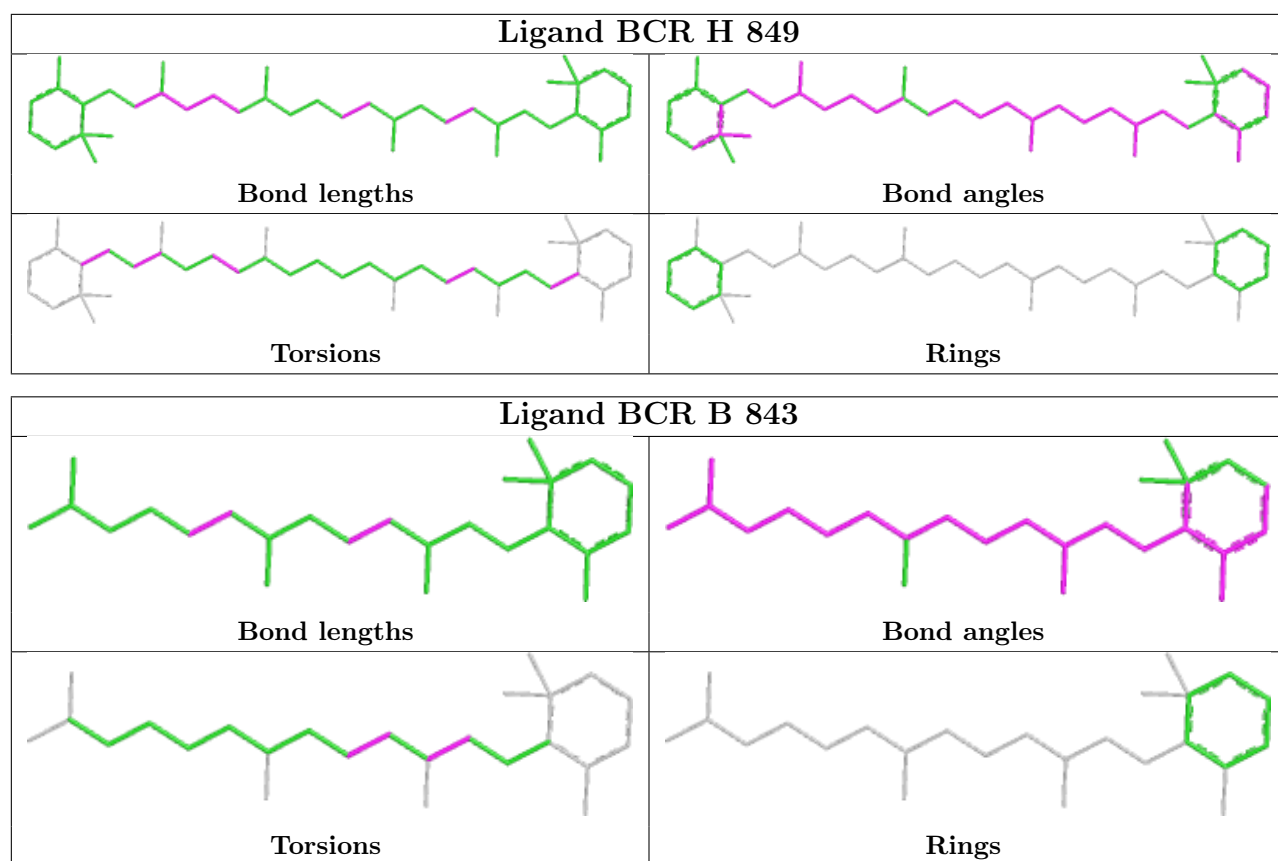
Ligand CLA b 813



Ligand CLA a 830







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.

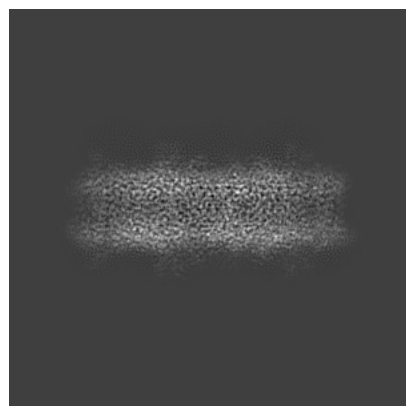
6 Map visualisation [i](#)

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.

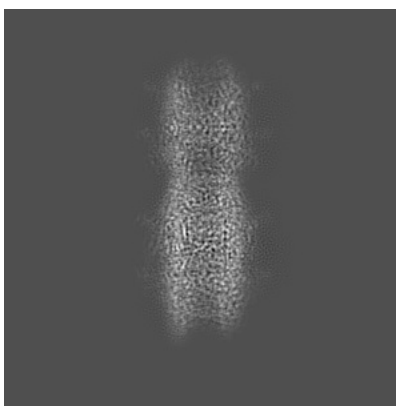
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

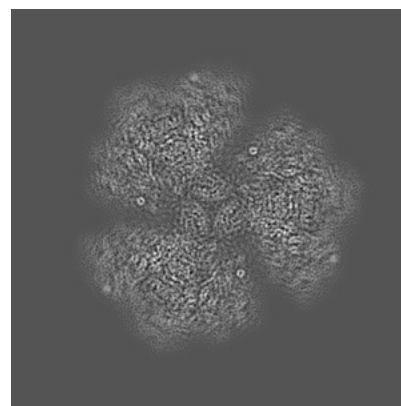
6.1.1 Primary map



X

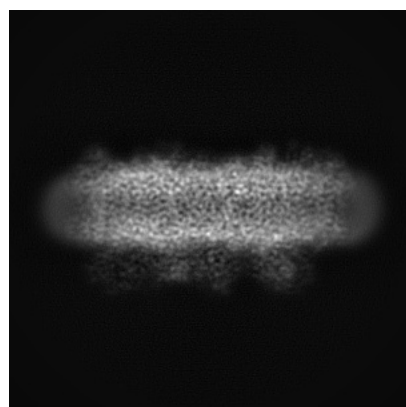


Y

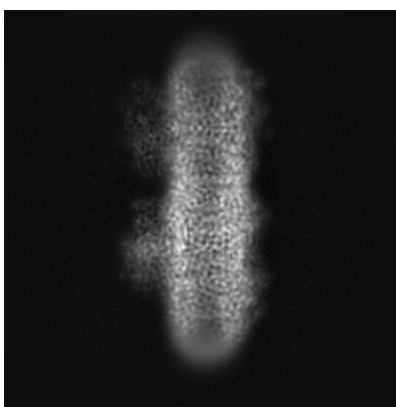


Z

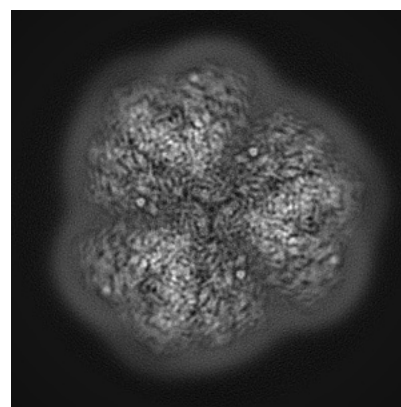
6.1.2 Raw map



X



Y

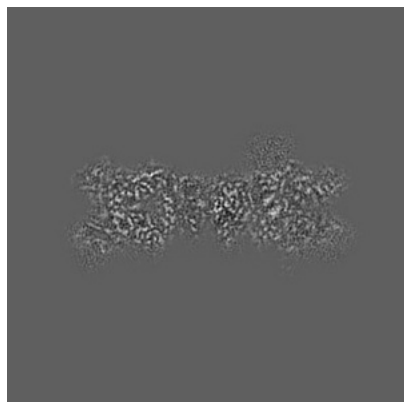


Z

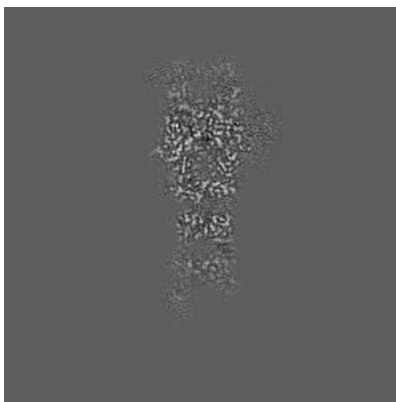
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

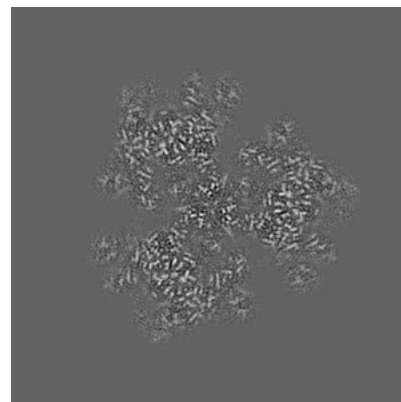
6.2.1 Primary map



X Index: 160

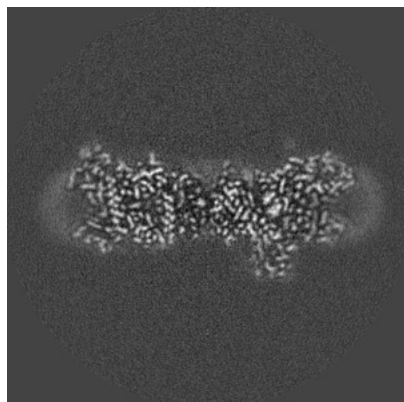


Y Index: 160

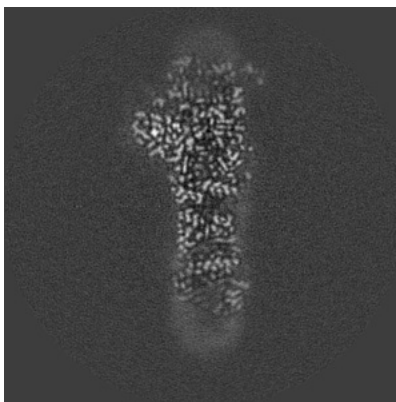


Z Index: 160

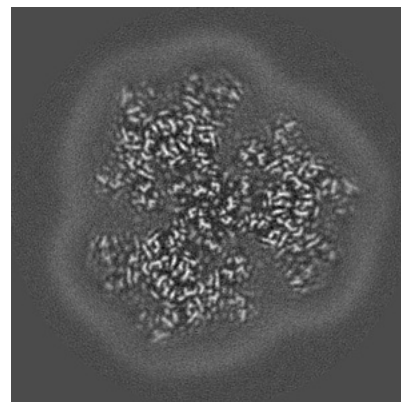
6.2.2 Raw map



X Index: 160



Y Index: 160

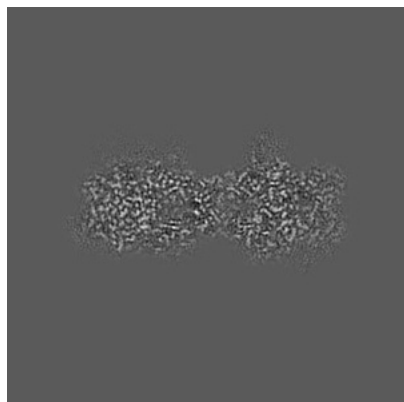


Z Index: 160

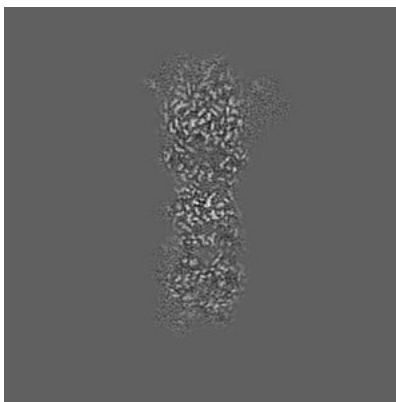
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

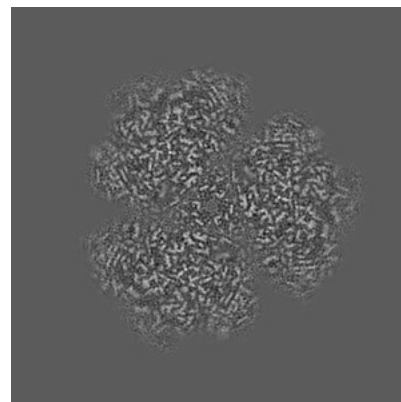
6.3.1 Primary map



X Index: 142

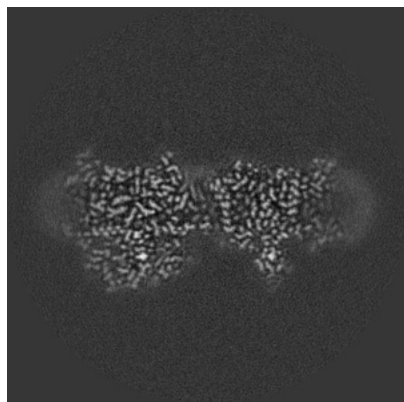


Y Index: 175

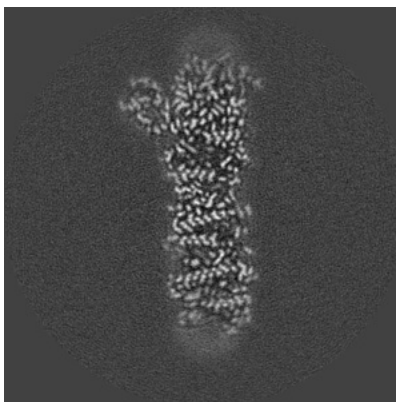


Z Index: 174

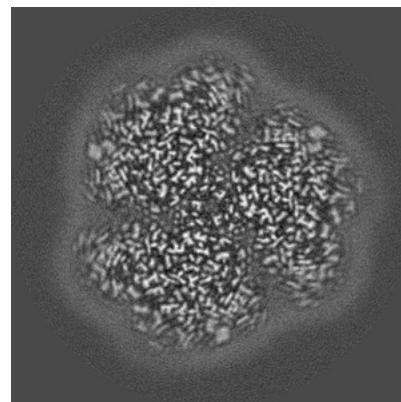
6.3.2 Raw map



X Index: 131



Y Index: 175

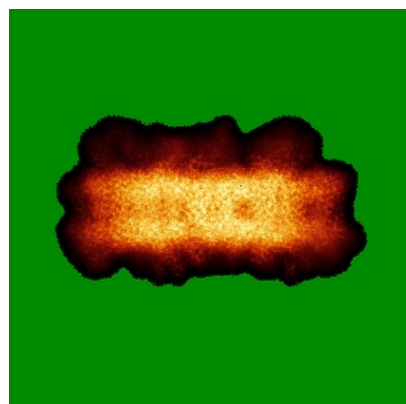


Z Index: 175

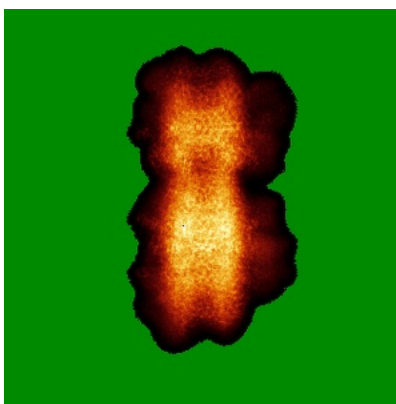
The images above show the largest variance slices of the map in three orthogonal directions.

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

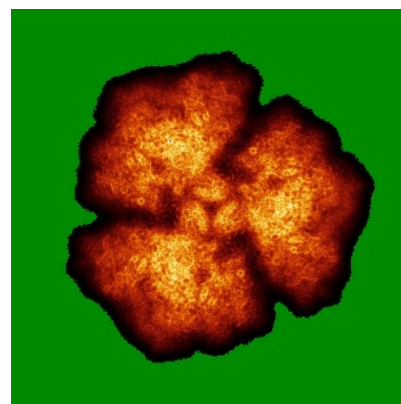
6.4.1 Primary map



X

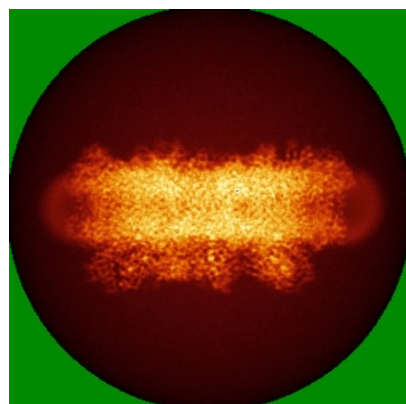


Y

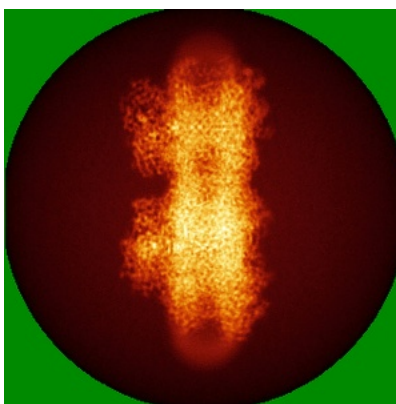


Z

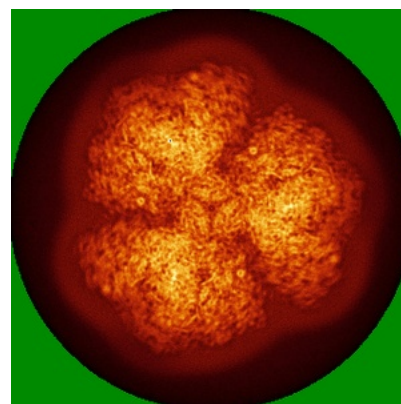
6.4.2 Raw map



X



Y

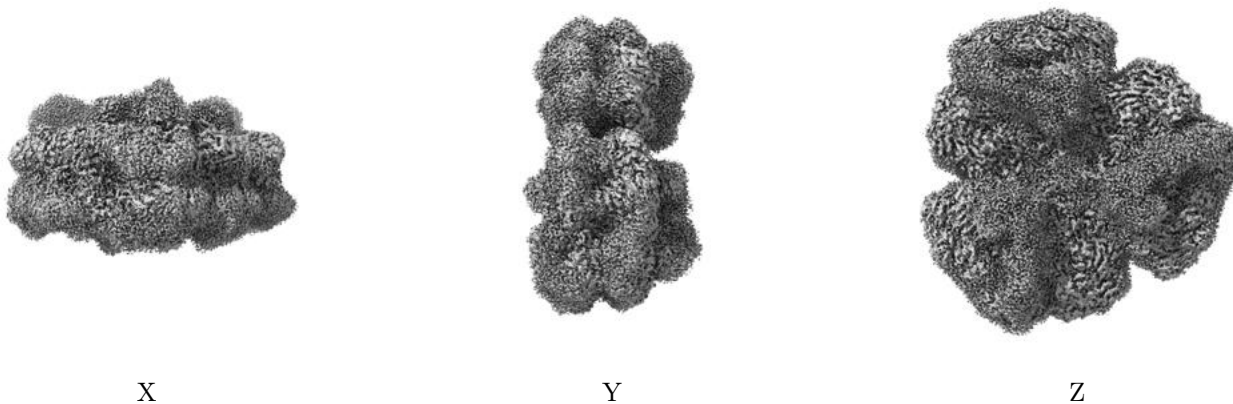


Z

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.

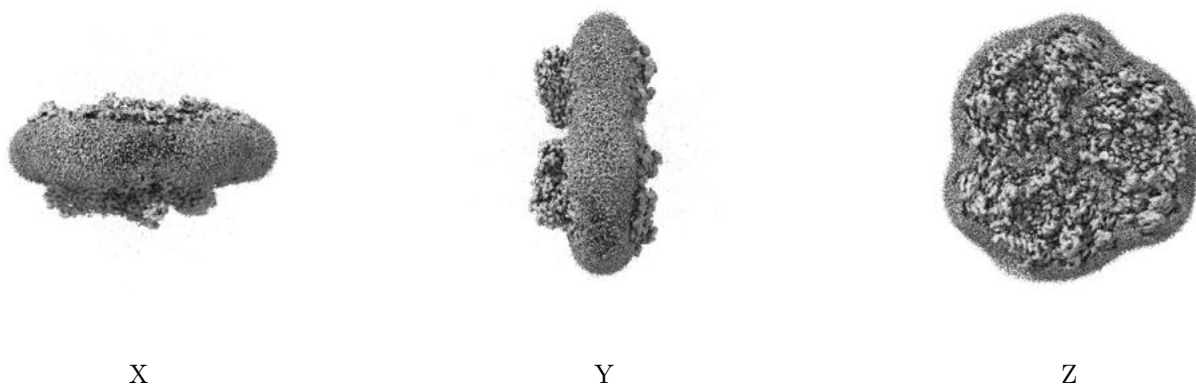
6.5 Orthogonal surface views [i](#)

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.

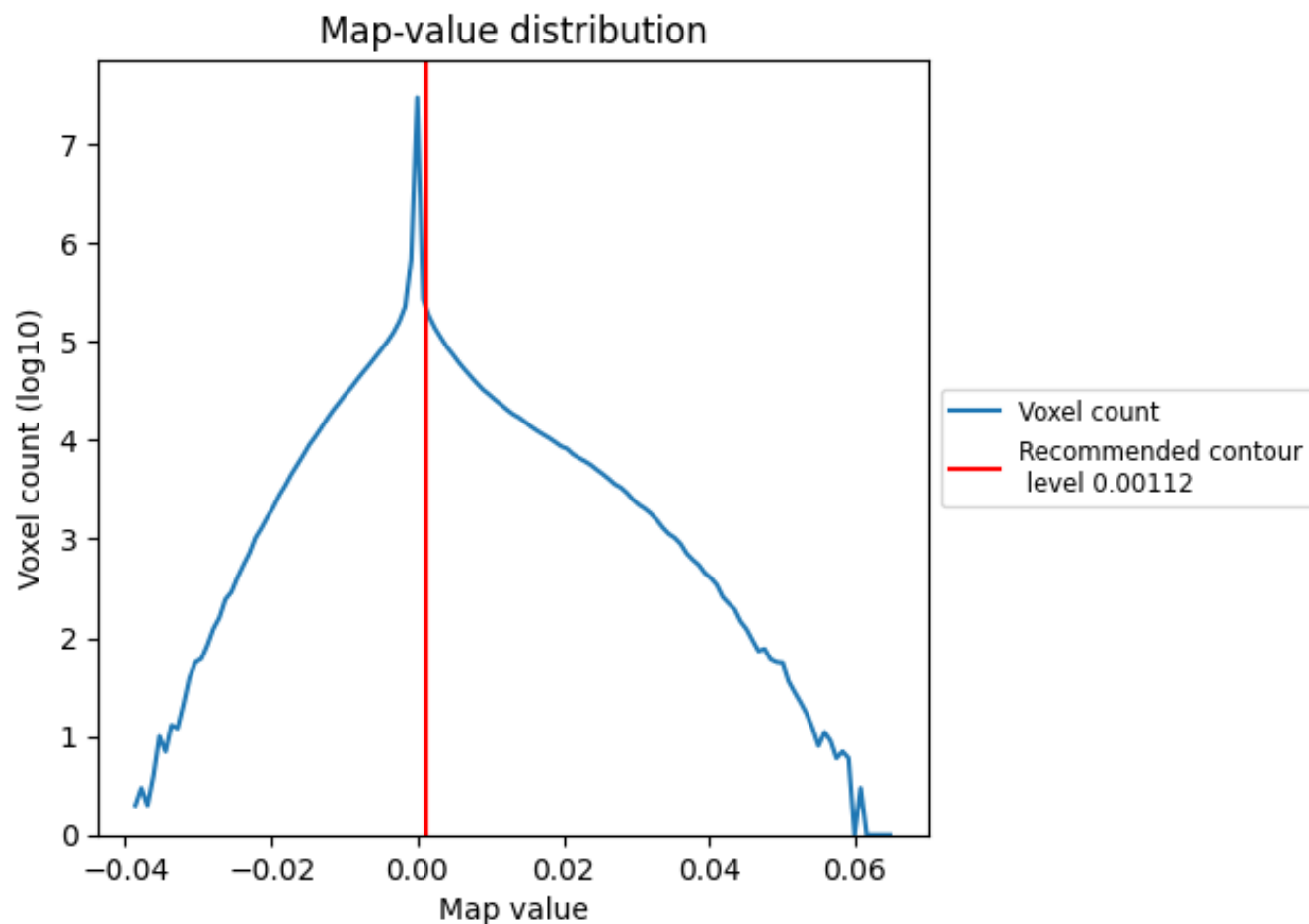
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

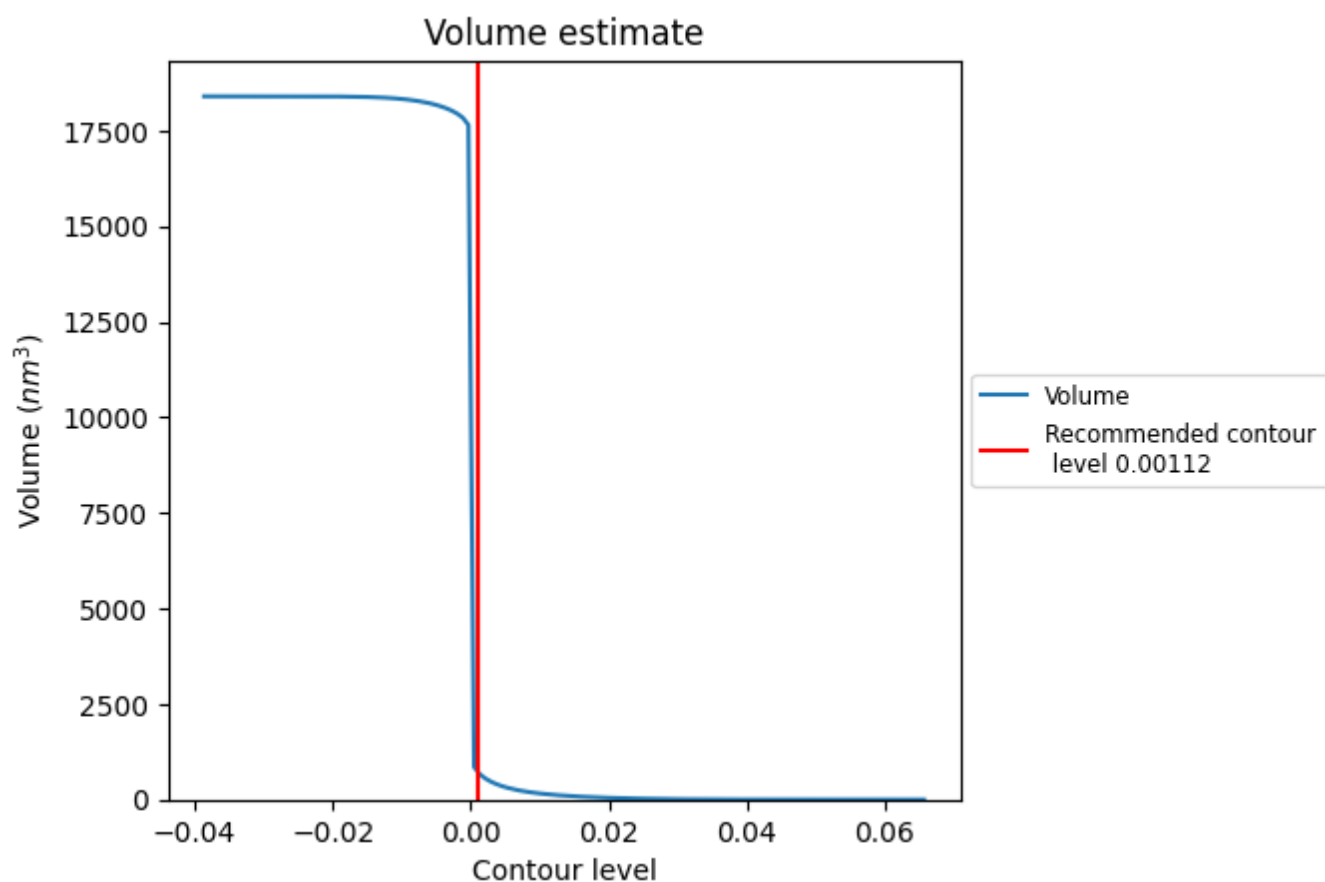
This section contains the results of statistical analysis of the map.

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.

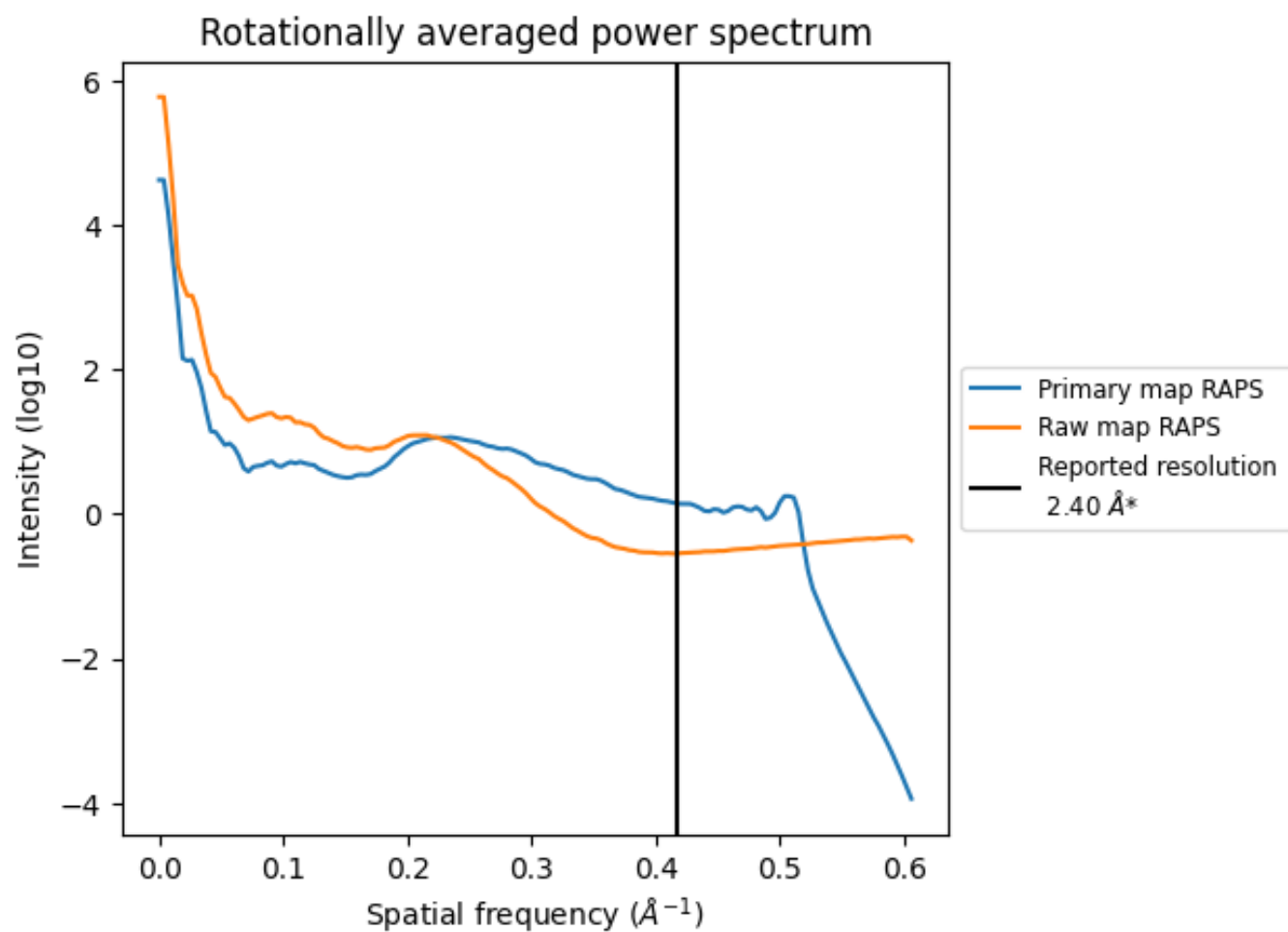
7.2 Volume estimate [i](#)



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 ⓘ

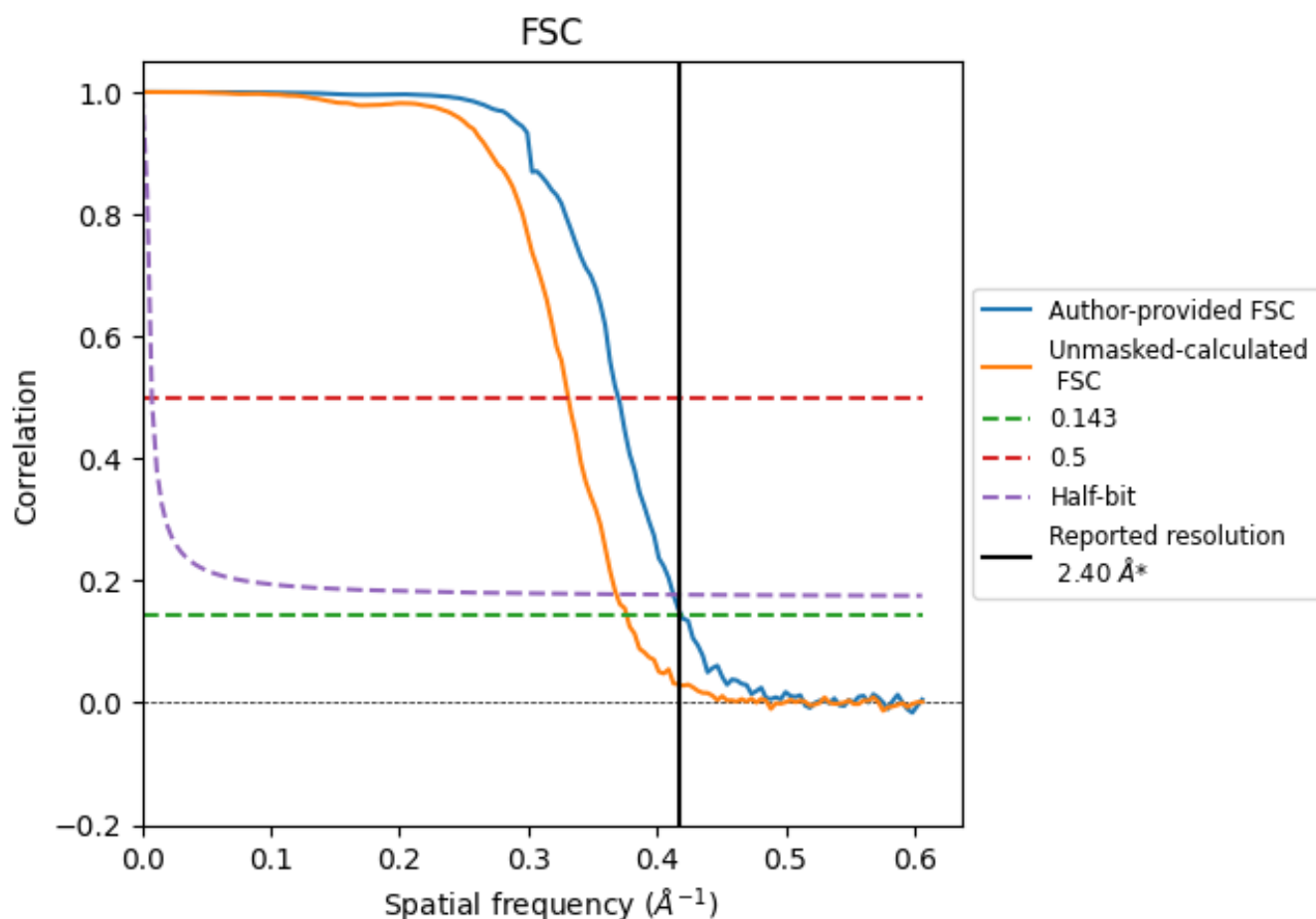


*Reported resolution corresponds to spatial frequency of 0.417 Å⁻¹

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](#)

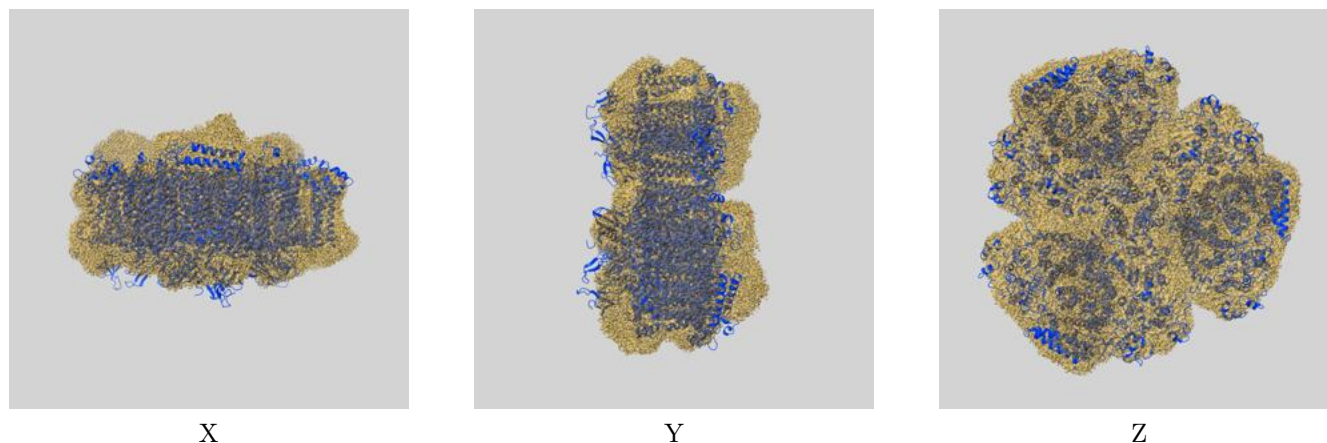
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.40	-	-
Author-provided FSC curve	2.39	2.70	2.42
Unmasked-calculated*	2.66	3.02	2.71

*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](#)

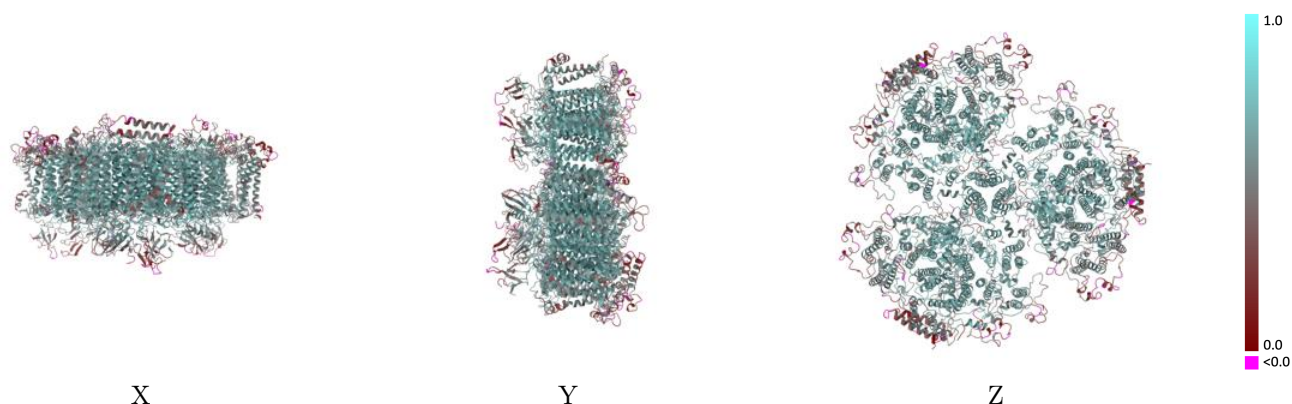
This section contains information regarding the fit between EMDB map EMD-47359 and PDB model 9E0J. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



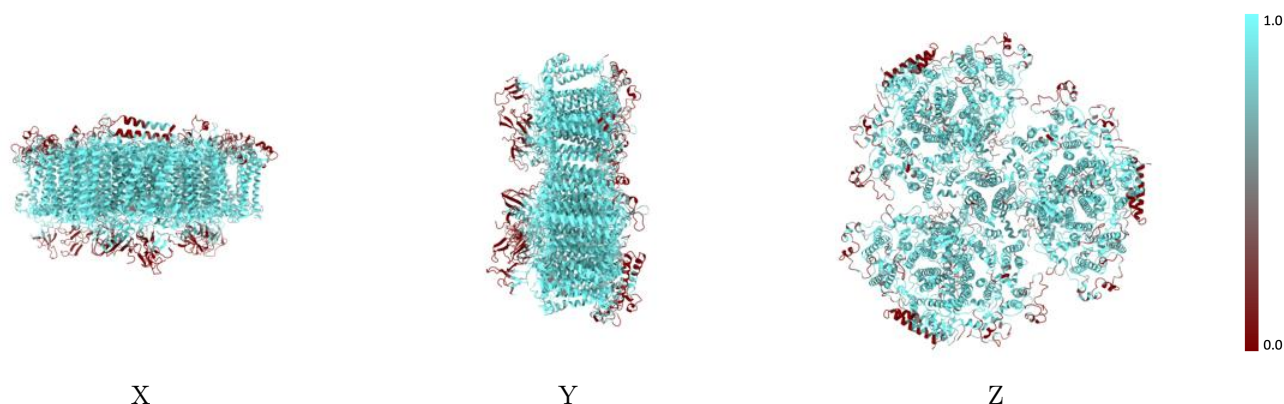
The images above show the 3D surface view of the map at the recommended contour level 0.00112 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



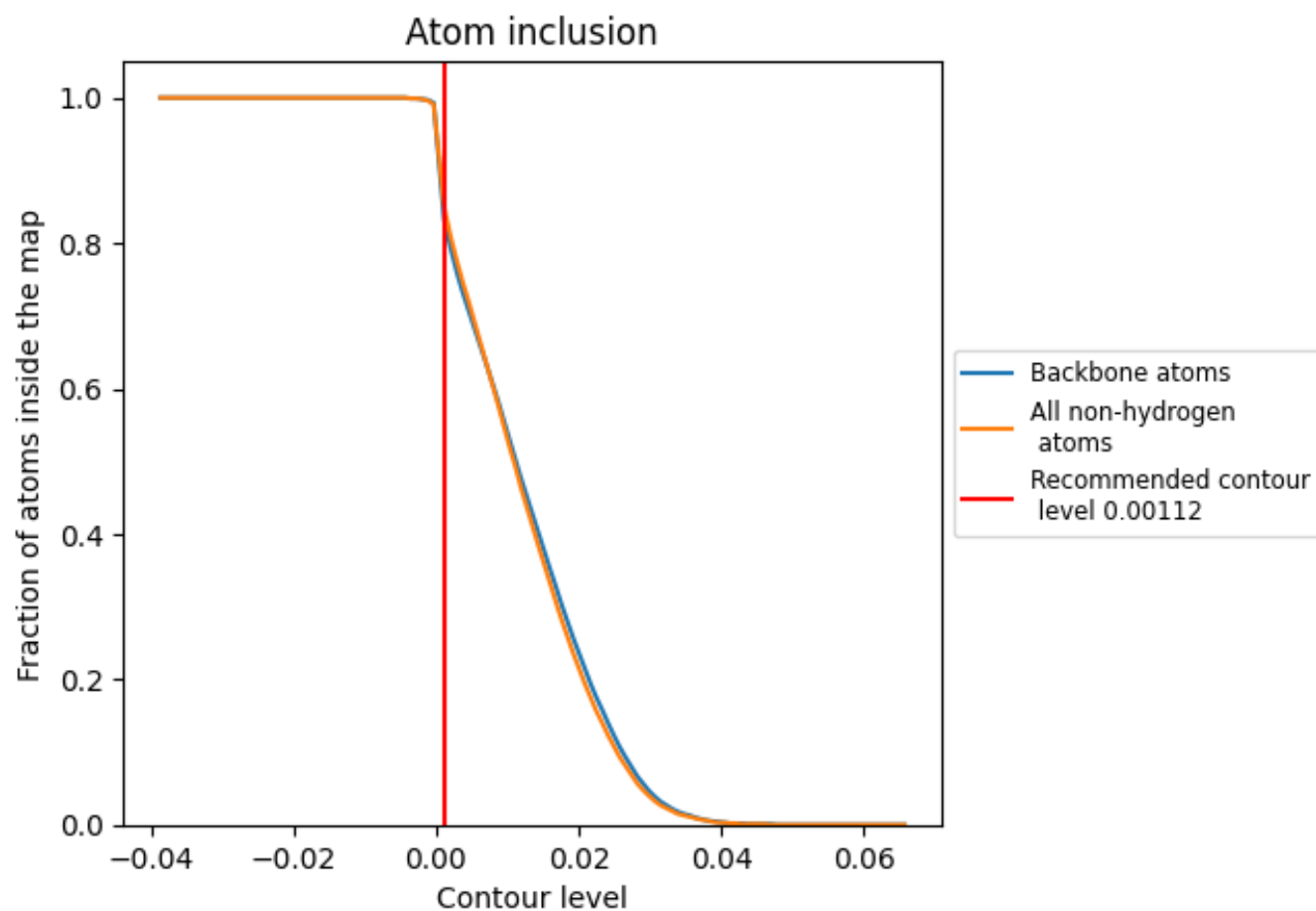
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.00112).































































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	 0.4450
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

