



wwPDB EM Validation Summary Report ⓘ

Aug 5, 2026 – 11:44 AM EDT

PDB ID : 9AU4 / pdb_00009au4
EMDB ID : EMD-43843
Title : Cryo-EM structure of a photosystem I variant containing an unusual plastoquinone derivative in its electron transfer chain
Authors : Gisriel, C.J.; Vasily, K.; Iwig, D.F.; Russell, B.P.; Vinyard, D.J.; Golbeck, J.H.; Brudvig, G.W.; Lakshmi, K.V.
Deposited on : 2024-02-28
Resolution : 2.03 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:

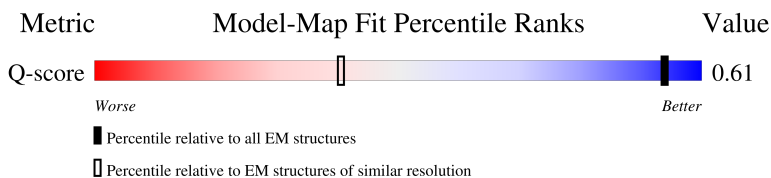
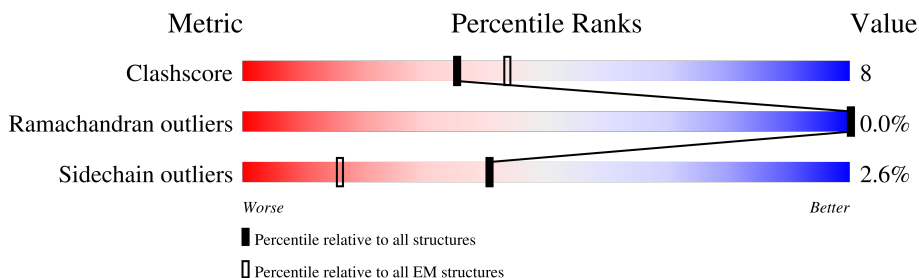
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 2.03 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1771 (1.55 - 2.53)

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	751	
1	G	751	
1	a	751	
2	B	730	

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Mol	Chain	Length	Quality of chain
2	H	730	
2	b	730	
3	C	81	
3	N	81	
3	c	81	
4	D	141	
4	O	141	
4	d	141	
5	E	74	
5	P	74	
5	e	74	
6	F	165	
6	Q	165	
6	f	165	
7	I	40	
7	R	40	
7	i	40	
8	J	40	
8	S	40	
8	j	40	
9	K	90	
9	T	90	
9	k	90	
10	L	157	
10	U	157	

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Mol	Chain	Length	Quality of chain
10	l	157	 85% 13% •
11	M	31	 84% 13% •
11	V	31	 84% 13% •
11	m	31	 84% 13% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	A1AGD	A	840	X	-	-	-
13	A1AGD	B	2153	X	-	-	-
13	A1AGD	G	840	X	-	-	-
13	A1AGD	H	2153	X	-	-	-
13	A1AGD	a	840	X	-	-	-
13	A1AGD	b	2153	X	-	-	-
23	ZEX	F	205	-	X	-	-
23	ZEX	Q	205	-	X	-	-
23	ZEX	f	205	-	X	-	-

2 Entry composition

There are 27 unique types of molecules in this entry. The entry contains 73866 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	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		
1	a	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		
1	A	737	Total	C	N	O	S	0	0
			5770	3780	980	983	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		
2	b	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		
2	B	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	O	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		
4	D	139	Total	C	N	O	S	0	0
			1087	688	188	208	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	P	69	Total	C	N	O		0	0
			542	340	96	106			
5	e	69	Total	C	N	O		0	0
			542	340	96	106			
5	E	69	Total	C	N	O		0	0
			542	340	96	106			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	f	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		
6	F	141	Total	C	N	O	S	0	0
			1100	711	183	201	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	40	Total	C	N	O	S	0	0
			311	209	44	55	3		
7	i	40	Total	C	N	O	S	0	0
			311	209	44	55	3		
7	I	40	Total	C	N	O	S	0	0
			311	209	44	55	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	S	39	Total	C	N	O	S	0	0
			311	210	46	53	2		
8	j	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O	S	0	0
			311	210	46	53	2		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	T	67	Total	C	N	O	S	0	0
			484	320	77	82	5		
9	k	67	Total	C	N	O	S	0	0
			484	320	77	82	5		
9	K	67	Total	C	N	O	S	0	0
			484	320	77	82	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
10	l	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		
10	L	154	Total	C	N	O	S	0	0
			1156	753	188	213	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

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



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

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

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

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Mol	Chain	Residues	Atoms					AltConf
12	H	1	Total 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 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 45	C 35	Mg 1	N 4	O 5	0
12	H	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	Q	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	Q	1	Total 46	C 36	Mg 1	N 4	O 5	0
12	Q	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	T	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	U	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	a	1	Total 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 51	C 41	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 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 45	C 35	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 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 60	C 50	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 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 60	C 50	Mg 1	N 4	O 5	0

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

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

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Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	b	1	Total 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 55	C 45	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 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 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 50	C 40	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 46	C 36	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

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Mol	Chain	Residues	Atoms					AltConf
12	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	k	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 65	C 55	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
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 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 51	C 41	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 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 45	C 35	Mg 1	N 4	O 5	0

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

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

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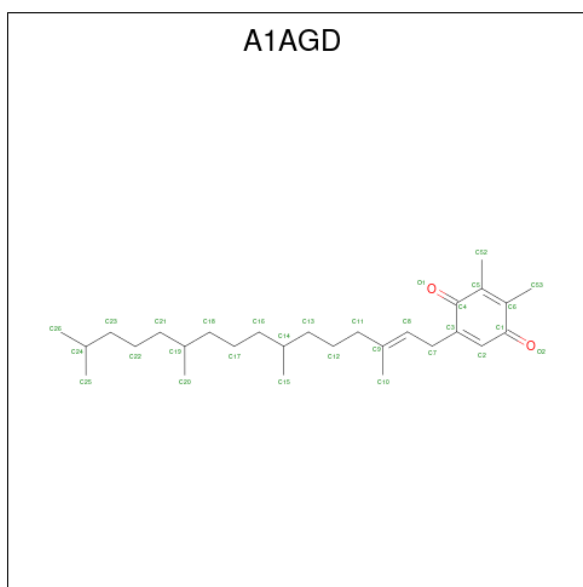
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
12	B	1	Total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

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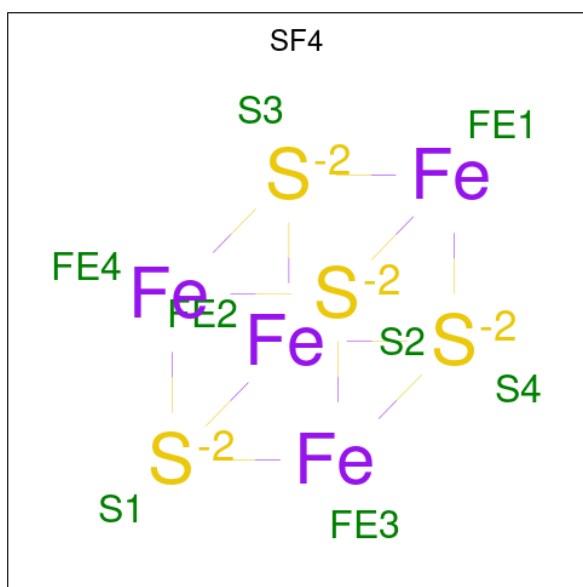
Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	F	1	Total 65	C 55	Mg 1	N 4	O 5	0
12	F	1	Total 46	C 36	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	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	K	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 65	C 55	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

- Molecule 13 is 2,3-dimethyl-5-[(2E,7R,11R)-3,7,11,15-tetramethylhexadec-2-en-1-yl]cyclohexa-2,5-diene-1,4-dione (CCD ID: A1AGD) (formula: C₂₈H₄₆O₂).



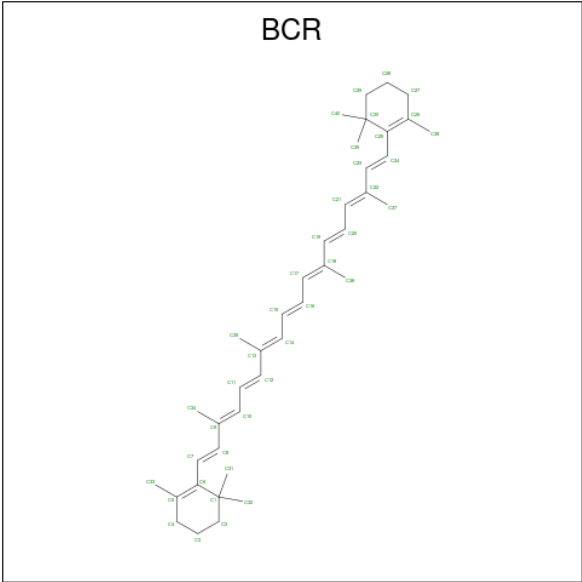
Mol	Chain	Residues	Atoms			AltConf
13	G	1	Total	C	O	0
			30	28	2	
13	H	1	Total	C	O	0
			30	28	2	
13	a	1	Total	C	O	0
			30	28	2	
13	b	1	Total	C	O	0
			30	28	2	
13	A	1	Total	C	O	0
			30	28	2	
13	B	1	Total	C	O	0
			30	28	2	

- Molecule 14 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
14	G	1	Total	Fe	S	0
			8	4	4	
14	N	1	Total	Fe	S	0
			8	4	4	
14	N	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	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
			40	40	
15	Q	1	Total	C	0
			40	40	
15	R	1	Total	C	0
			40	40	
15	S	1	Total	C	0
			40	40	
15	S	1	Total	C	0
			40	40	
15	T	1	Total	C	0
			40	40	
15	U	1	Total	C	0
			40	40	

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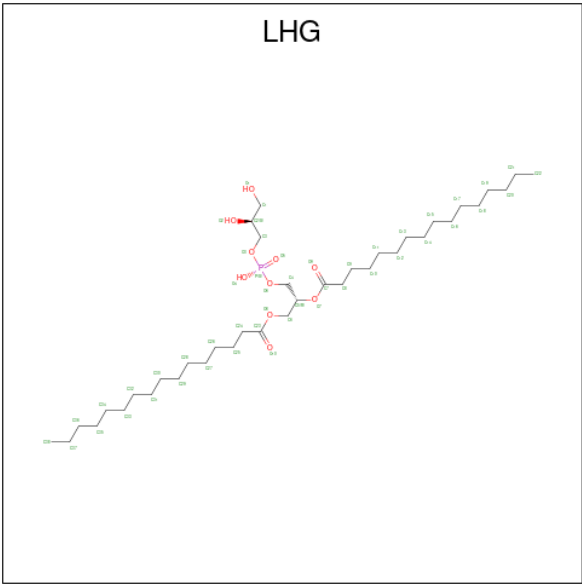
Mol	Chain	Residues	Atoms	AltConf
15	U	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	a	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	b	1	Total C 40 40	0
15	f	1	Total C 40 40	0
15	i	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	j	1	Total C 40 40	0
15	k	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	B	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms		AltConf
15	B	1	Total	C	0
			40	40	
15	B	1	Total	C	0
			40	40	
15	B	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	K	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	
15	L	1	Total	C	0
			40	40	

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



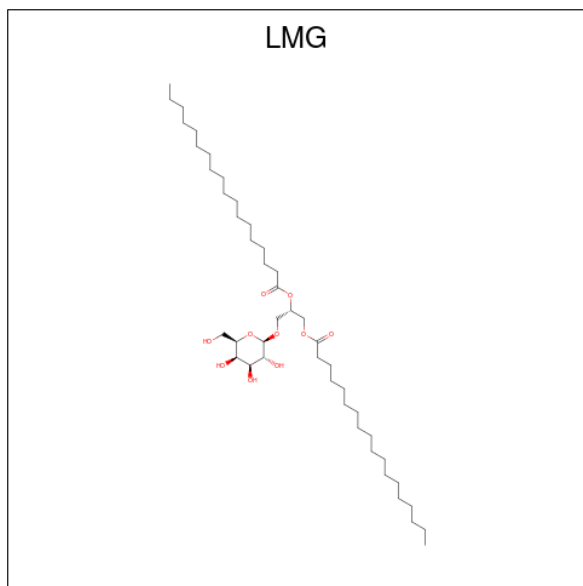
Mol	Chain	Residues	Atoms				AltConf
16	G	1	Total	C	O	P	0
			49	38	10	1	

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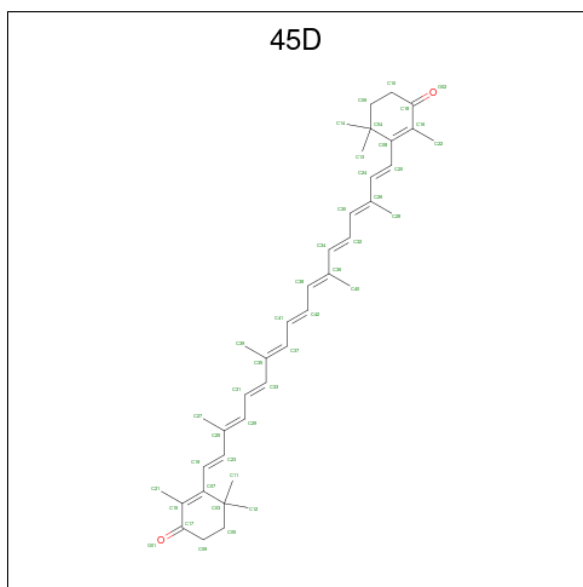
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
16	G	1	Total 49	38	10	1	0
16	H	1	Total 43	32	10	1	0
16	V	1	Total 44	33	10	1	0
16	a	1	Total 49	38	10	1	0
16	a	1	Total 49	38	10	1	0
16	b	1	Total 43	32	10	1	0
16	m	1	Total 44	33	10	1	0
16	A	1	Total 49	38	10	1	0
16	A	1	Total 49	38	10	1	0
16	B	1	Total 43	32	10	1	0
16	M	1	Total 44	33	10	1	0

- Molecule 17 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
17	G	1	Total	C	O	0
			50	40	10	
17	G	1	Total	C	O	0
			32	22	10	
17	H	1	Total	C	O	0
			51	41	10	
17	a	1	Total	C	O	0
			50	40	10	
17	a	1	Total	C	O	0
			32	22	10	
17	b	1	Total	C	O	0
			51	41	10	
17	A	1	Total	C	O	0
			50	40	10	
17	A	1	Total	C	O	0
			32	22	10	
17	B	1	Total	C	O	0
			51	41	10	

- Molecule 18 is beta,beta-carotene-4,4'-dione (CCD ID: 45D) (formula: C₄₀H₅₂O₂).

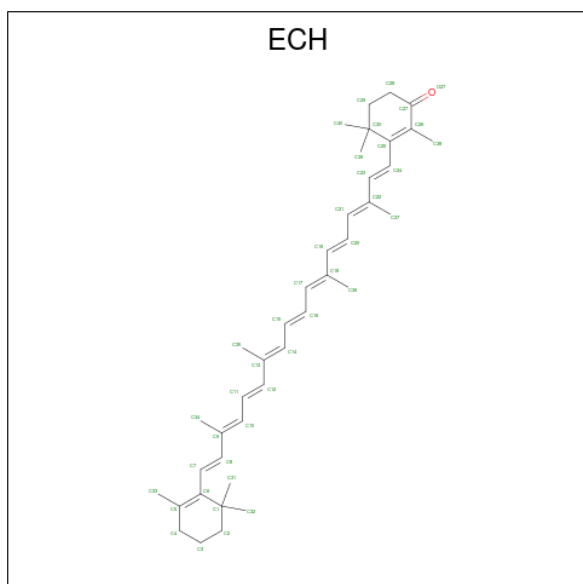


Mol	Chain	Residues	Atoms			AltConf
18	G	1	Total	C	O	0
			42	40	2	
18	a	1	Total	C	O	0
			42	40	2	
18	A	1	Total	C	O	0
			42	40	2	

- Molecule 19 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
19	G	1	Total	Cl	0
			1	1	
19	a	1	Total	Cl	0
			1	1	
19	A	1	Total	Cl	0
			1	1	

- Molecule 20 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: C₄₀H₅₄O).

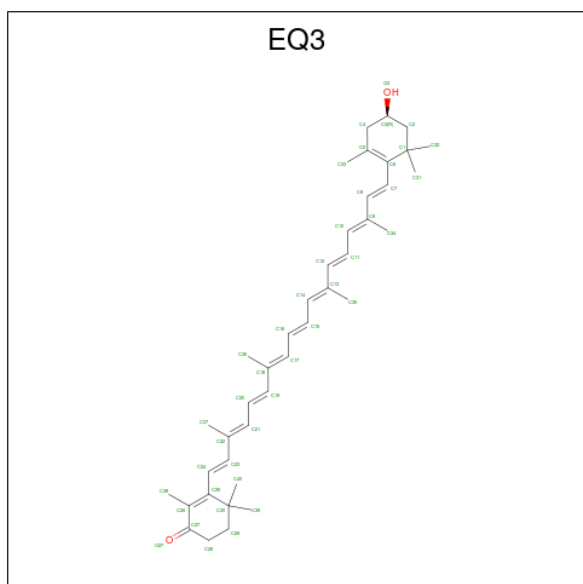


Mol	Chain	Residues	Atoms			AltConf
20	H	1	Total	C	O	0
			41	40	1	
20	V	1	Total	C	O	0
			41	40	1	
20	b	1	Total	C	O	0
			41	40	1	
20	m	1	Total	C	O	0
			41	40	1	
20	B	1	Total	C	O	0
			41	40	1	
20	M	1	Total	C	O	0
			41	40	1	

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca).

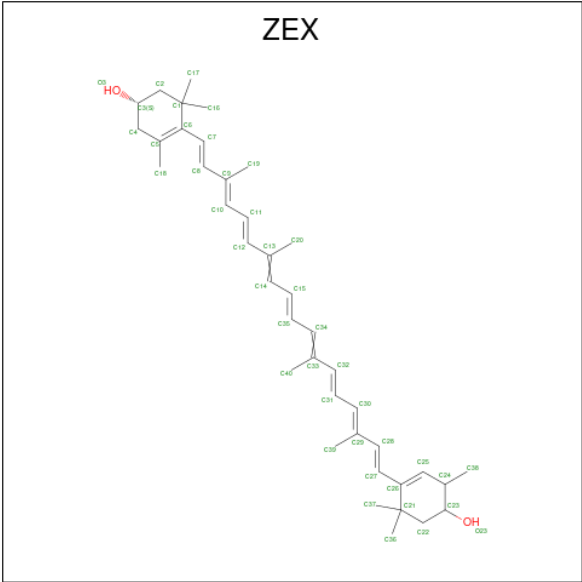
Mol	Chain	Residues	Atoms		AltConf
21	H	1	Total	Ca	0
			1	1	
21	U	1	Total	Ca	0
			1	1	
21	b	1	Total	Ca	0
			1	1	
21	l	1	Total	Ca	0
			1	1	
21	B	1	Total	Ca	0
			1	1	
21	L	1	Total	Ca	0
			1	1	

- Molecule 22 is (3'R)-3'-hydroxy-beta,beta-caroten-4-one (CCD ID: EQ3) (formula: $C_{40}H_{54}O_2$).



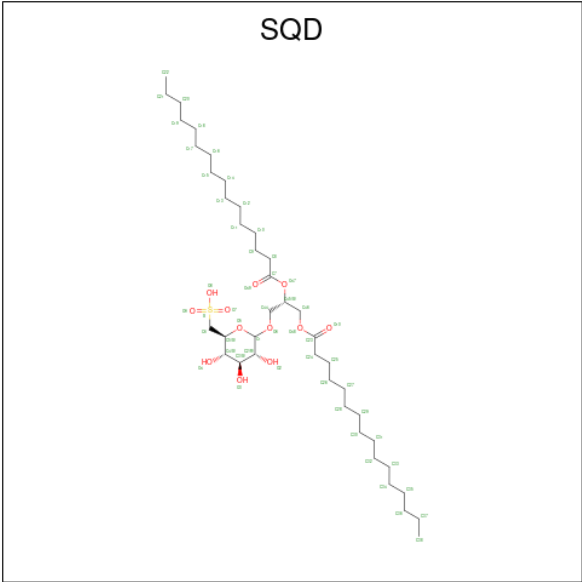
Mol	Chain	Residues	Atoms			AltConf
22	H	1	Total	C	O	0
			42	40	2	
22	b	1	Total	C	O	0
			42	40	2	
22	B	1	Total	C	O	0
			42	40	2	

- Molecule 23 is (1R,2S)-4-{(1E,3E,5E,7E,9E,11E,13E,15E,17E)-18-[(4S)-4-hydroxy-2,6,6-trimethylcyclohex-1-en-1-yl]-3,7,12,16-tetramethyloctadeca-1,3,5,7,9,11,13,15,17-nonaen-1-yl}-2,5,5-trimethylcyclohex-3-en-1-ol (CCD ID: ZEX) (formula: $C_{40}H_{56}O_2$).



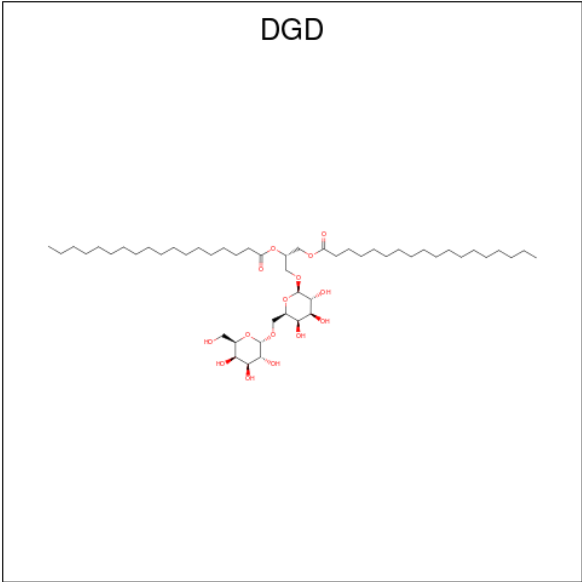
Mol	Chain	Residues	Atoms			AltConf
23	H	1	Total	C	O	0
			42	40	2	
23	Q	1	Total	C	O	0
			42	40	2	
23	b	1	Total	C	O	0
			42	40	2	
23	f	1	Total	C	O	0
			42	40	2	
23	B	1	Total	C	O	0
			42	40	2	
23	F	1	Total	C	O	0
			42	40	2	

- Molecule 24 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



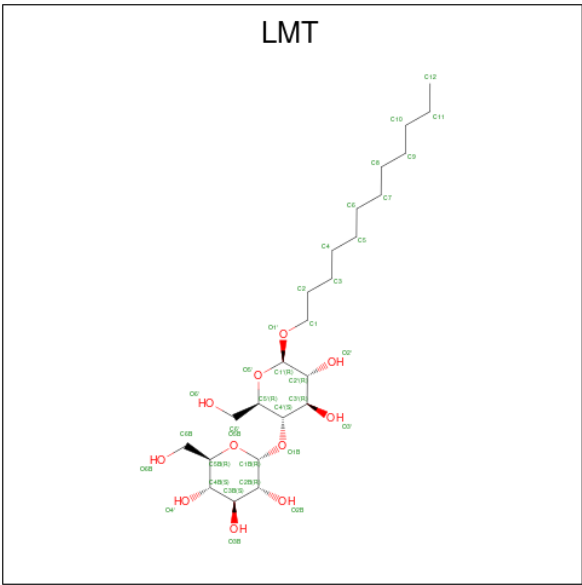
Mol	Chain	Residues	Atoms				AltConf
24	U	1	Total	C	O	S	0
			45	32	12	1	
24	V	1	Total	C	O	S	0
			54	41	12	1	
24	l	1	Total	C	O	S	0
			45	32	12	1	
24	m	1	Total	C	O	S	0
			54	41	12	1	
24	L	1	Total	C	O	S	0
			45	32	12	1	
24	M	1	Total	C	O	S	0
			54	41	12	1	

- Molecule 25 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅).



Mol	Chain	Residues	Atoms			AltConf
25	U	1	Total	C	O	0
			49	39	10	
25	I	1	Total	C	O	0
			49	39	10	
25	L	1	Total	C	O	0
			49	39	10	

- Molecule 26 is DODECYL-BETA-D-MALTOSE (CCD ID: LMT) (formula: C₂₄H₄₆O₁₁).



Mol	Chain	Residues	Atoms			AltConf
26	U	1	Total	C	O	0
			35	24	11	

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Mol	Chain	Residues	Atoms			AltConf
26	l	1	Total	C	O	0
			35	24	11	
26	L	1	Total	C	O	0
			35	24	11	

- Molecule 27 is water.

Mol	Chain	Residues	Atoms			AltConf
27	G	90	Total	O		0
			90	90		
27	H	112	Total	O		0
			112	112		
27	N	36	Total	O		0
			36	36		
27	O	28	Total	O		0
			28	28		
27	P	7	Total	O		0
			7	7		
27	Q	2	Total	O		0
			2	2		
27	R	4	Total	O		0
			4	4		
27	U	24	Total	O		0
			24	24		
27	a	90	Total	O		0
			90	90		
27	b	112	Total	O		0
			112	112		
27	c	36	Total	O		0
			36	36		
27	d	28	Total	O		0
			28	28		
27	e	7	Total	O		0
			7	7		
27	f	2	Total	O		0
			2	2		
27	i	4	Total	O		0
			4	4		
27	l	24	Total	O		0
			24	24		
27	A	90	Total	O		0
			90	90		

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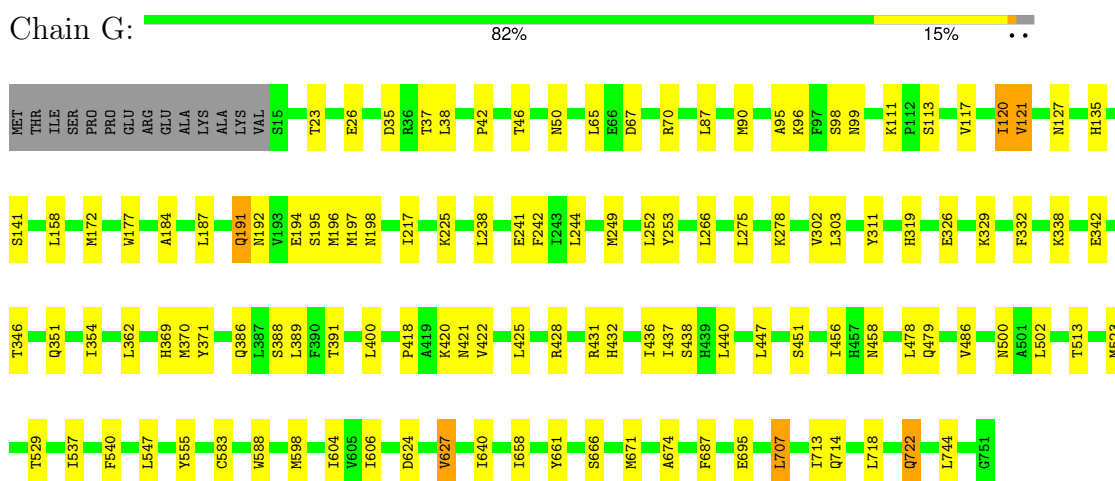
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Mol	Chain	Residues	Atoms		AltConf
27	B	112	Total 112	O 112	0
27	C	36	Total 36	O 36	0
27	D	28	Total 28	O 28	0
27	E	7	Total 7	O 7	0
27	F	2	Total 2	O 2	0
27	I	4	Total 4	O 4	0
27	L	24	Total 24	O 24	0

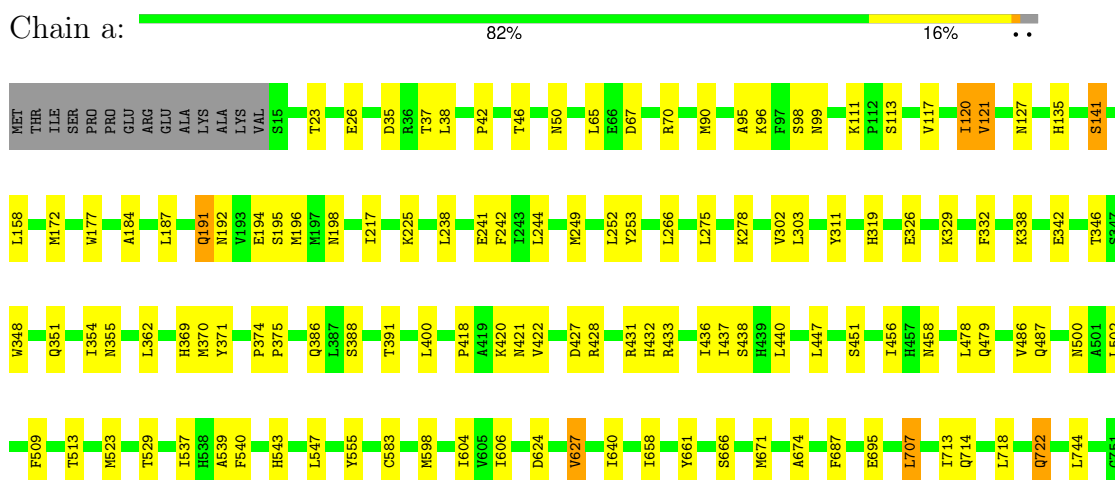
3 Residue-property plots [i](#)

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

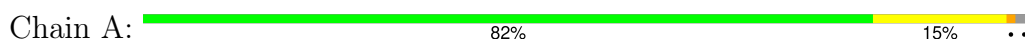
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

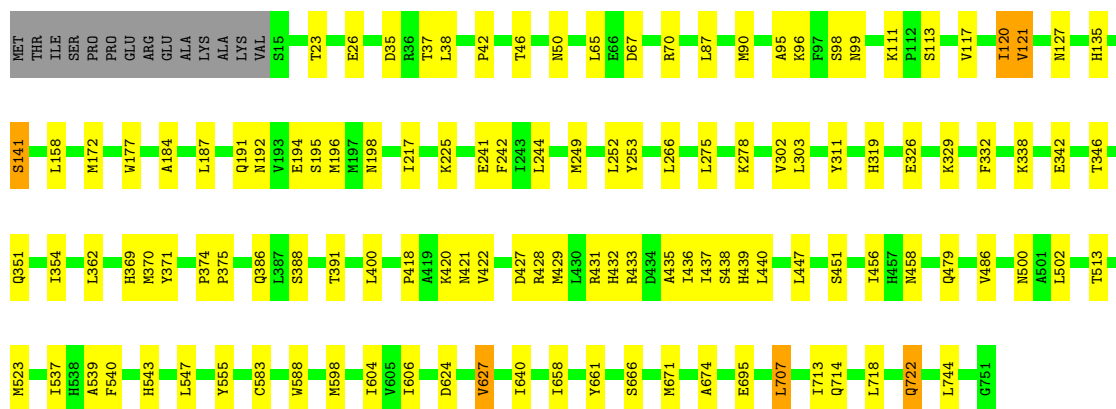


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



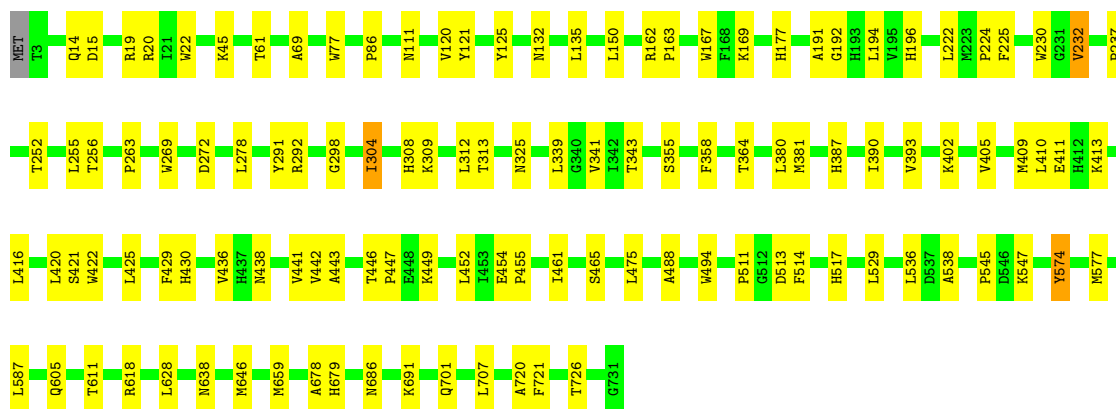
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





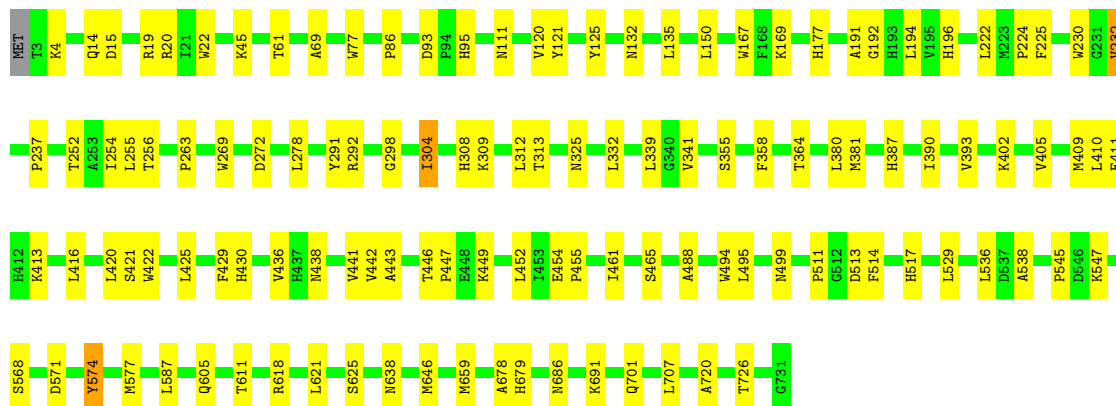
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain H: 84% 15%



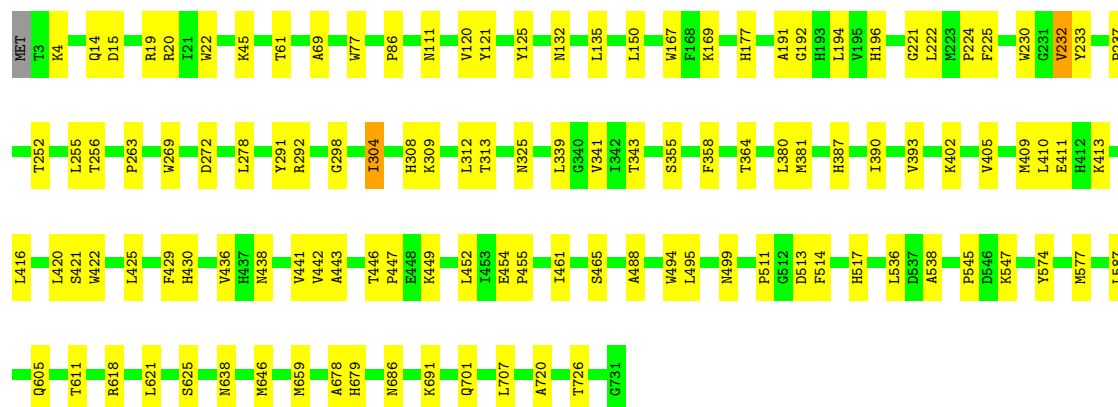
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 83% 16%

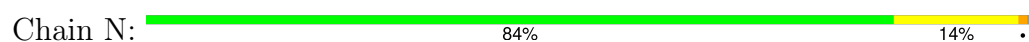


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

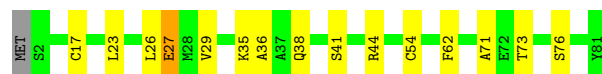
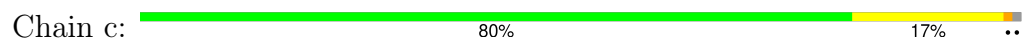
Chain B: 84% 16%



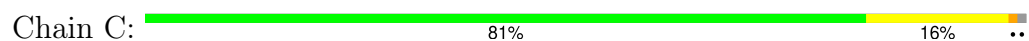
• Molecule 3: Photosystem I iron-sulfur center



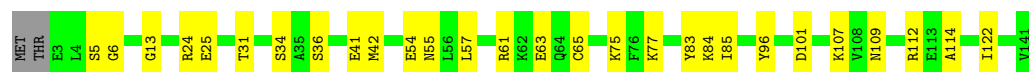
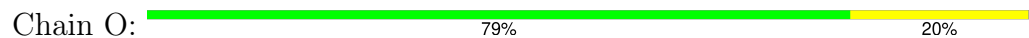
• Molecule 3: Photosystem I iron-sulfur center



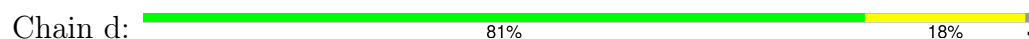
• Molecule 3: Photosystem I iron-sulfur center



• Molecule 4: Photosystem I reaction center subunit II



• Molecule 4: Photosystem I reaction center subunit II



• Molecule 4: Photosystem I reaction center subunit II

MT	THR	E3	L4	S5	G6		R24	E25		T31		S34	A35	S36		E41	M42		E54	N55	L56	L57		R61	K62	G63	Q64	G65		K75	F76	K77		Y83	K84	L85		Y96			D101		K107	V108	N109		R112	E113	A114		I122		V141
----	-----	----	----	----	----	--	-----	-----	--	-----	--	-----	-----	-----	--	-----	-----	--	-----	-----	-----	-----	--	-----	-----	-----	-----	-----	--	-----	-----	-----	--	-----	-----	-----	--	-----	--	--	------	--	------	------	------	--	------	------	------	--	------	--	------

- | | | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | A2 | V9 | K12 | R13 | Y17 | G20 | V28 | E29 | K30 | P36 | V56 | A62 | L66 | E67 | L68 | V69 | Q70 | ALA | ALA | ALA | LYS |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

- [illegible]

- | | | | | | | | | | | | | | | | | | | | |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|
| MET | A2 | V9 | K12 | R13 | Y17 | G20 | V28 | P36 | V56 | A62 | L66 | E67 | L68 | V69 | Q70 | ALA | ALA | ALA | LYS |
|-----|----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|

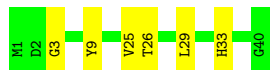
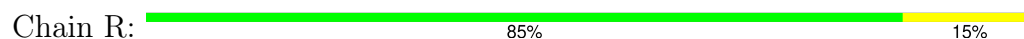
- | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|-----|------|------|------|------|------|------|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|-----|------|------|------|------|
| | K130 | L131 | V132 | P139 | P142 | R143 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| MET | LYS | HIS | LEU | ALA | LEU | LEU | LEU | ALA | THR | TRP | PHE | ASN | PHE | ALA | PRO | SER | SER | ALA | ASP | D3 | P14 | L17 | I86 | R39 | F50 | F51 | H52 | D56 | G57 | R58 | F59 | T60 | W81 | R84 | S85 | E86 | L87 | E92 | V101 | N104 | A122 | C12E |

-
- | Category | Count |
|----------|-------|
| MET | 1 |
| LYS | 1 |
| HIS | 1 |
| LEU | 1 |
| LEU | 1 |
| ALA | 1 |
| LEU | 1 |
| LEU | 1 |
| LEU | 1 |
| ALA | 1 |
| PHE | 1 |
| THR | 1 |
| TRP | 1 |
| PHE | 1 |
| ASN | 1 |
| PHE | 1 |
| ALA | 1 |
| PRO | 1 |
| SER | 1 |
| SER | 1 |
| ALA | 1 |
| ASP | 1 |
| D3 | 1 |
| P14 | 1 |
| L17 | 1 |
| L35 | 1 |
| R39 | 1 |
| Y50 | 1 |
| F51 | 1 |
| H52 | 1 |
| D56 | 1 |
| G57 | 1 |
| R58 | 1 |
| F59 | 1 |
| T60 | 1 |
| R84 | 1 |
| S85 | 1 |
| E92 | 1 |
| V101 | 1 |
| N104 | 1 |
| A122 | 1 |
| E125 | 1 |
| K130 | 1 |
| L131 | 1 |
| H122 | 1 |

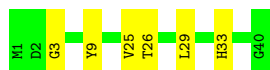
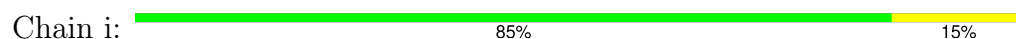
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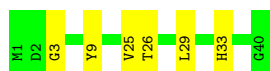
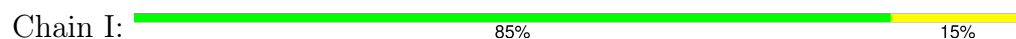
- Molecule 7: Photosystem I reaction center subunit VIII



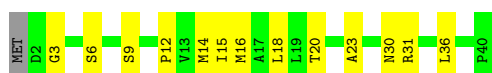
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



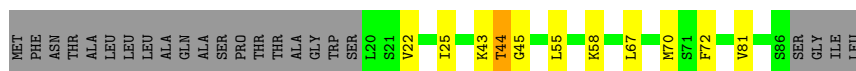
- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain T:  62% 11% 26%



- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain k:  62% 11% 26%



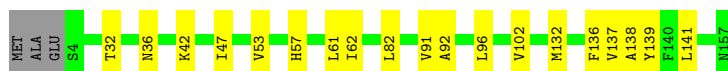
- Molecule 9: Photosystem I reaction center subunit PsaK 2

Chain K:  61% 12% 26%



- Molecule 10: Photosystem I reaction center subunit XI

Chain U:  86% 12%



- Molecule 10: Photosystem I reaction center subunit XI

Chain l:  85% 13%



- Molecule 10: Photosystem I reaction center subunit XI

Chain L:  87% 11%



- Molecule 11: Photosystem I reaction center subunit XII

Chain V:  84% 13%



- Molecule 11: Photosystem I reaction center subunit XII

Chain m:  84% 13% •



- Molecule 11: Photosystem I reaction center subunit XII

Chain M:  84% 13% •



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	375816	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	59.972	Depositor
Minimum map value	-21.826	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	0.0149	Depositor
Map size (Å)	266.24, 266.24, 266.24	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83199996, 0.83199996, 0.83199996	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, SQD, ZEX, CLA, LMT, EQ3, A1AGD, DGD, BCR, LMG, ECH, SF4, CL, CA, 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	0.26	0/5967	0.57	3/8133 (0.0%)
1	G	0.26	0/5967	0.57	3/8133 (0.0%)
1	a	0.26	0/5967	0.57	3/8133 (0.0%)
2	B	0.26	0/5981	0.59	3/8178 (0.0%)
2	H	0.26	0/5981	0.59	3/8178 (0.0%)
2	b	0.26	0/5981	0.59	3/8178 (0.0%)
3	C	0.22	0/610	0.63	2/826 (0.2%)
3	N	0.23	0/610	0.63	2/826 (0.2%)
3	c	0.22	0/610	0.63	2/826 (0.2%)
4	D	0.19	0/1111	0.51	0/1497
4	O	0.20	0/1111	0.51	0/1497
4	d	0.19	0/1111	0.51	0/1497
5	E	0.23	0/551	0.59	2/745 (0.3%)
5	P	0.23	0/551	0.59	2/745 (0.3%)
5	e	0.23	0/551	0.59	2/745 (0.3%)
6	F	0.23	0/1130	0.58	2/1535 (0.1%)
6	Q	0.23	0/1130	0.58	2/1535 (0.1%)
6	f	0.23	0/1130	0.58	2/1535 (0.1%)
7	I	0.28	0/322	0.62	0/438
7	R	0.28	0/322	0.62	0/438
7	i	0.28	0/322	0.62	0/438
8	J	0.25	0/320	0.63	1/433 (0.2%)
8	S	0.25	0/320	0.63	1/433 (0.2%)
8	j	0.26	0/320	0.63	1/433 (0.2%)
9	K	0.27	0/492	0.71	0/661
9	T	0.27	0/492	0.71	0/661
9	k	0.27	0/492	0.71	0/661
10	L	0.25	0/1186	0.56	0/1611
10	U	0.25	0/1186	0.56	0/1611
10	l	0.25	0/1186	0.56	0/1611
11	M	0.27	0/241	0.54	0/326
11	V	0.27	0/241	0.54	0/326

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	m	0.27	0/241	0.54	0/326
All	All	0.25	0/53733	0.58	39/73149 (0.1%)

There are no bond length outliers.

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	263	PRO	N-CD-CG	-6.99	92.72	103.20
2	B	263	PRO	N-CD-CG	-6.99	92.72	103.20
2	H	263	PRO	N-CD-CG	-6.98	92.73	103.20
2	b	263	PRO	CA-N-CD	-6.42	103.01	112.00
2	H	263	PRO	CA-N-CD	-6.41	103.02	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5770	0	5622	82	0
1	G	5770	0	5622	82	0
1	a	5770	0	5622	83	0
2	B	5770	0	5547	80	0
2	H	5770	0	5547	84	0
2	b	5770	0	5547	85	0
3	C	600	0	581	7	0
3	N	600	0	581	6	0
3	c	600	0	581	8	0
4	D	1087	0	1082	15	0
4	O	1087	0	1082	16	0
4	d	1087	0	1082	14	0
5	E	542	0	525	6	0
5	P	542	0	525	7	0
5	e	542	0	525	7	0
6	F	1100	0	1096	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	Q	1100	0	1096	14	0
6	f	1100	0	1096	11	0
7	I	311	0	304	6	0
7	R	311	0	304	6	0
7	i	311	0	304	6	0
8	J	311	0	316	8	0
8	S	311	0	316	10	0
8	j	311	0	316	7	0
9	K	484	0	514	7	0
9	T	484	0	514	6	0
9	k	484	0	514	6	0
10	L	1156	0	1127	14	0
10	U	1156	0	1127	15	0
10	l	1156	0	1127	16	0
11	M	238	0	260	8	0
11	V	238	0	260	7	0
11	m	238	0	260	8	0
12	A	2536	0	2594	84	0
12	B	2425	0	2404	79	0
12	F	156	0	138	5	0
12	G	2536	0	2594	84	0
12	H	2425	0	2404	82	0
12	J	90	0	66	1	0
12	K	45	0	33	0	0
12	L	260	0	288	12	0
12	Q	156	0	138	6	0
12	S	90	0	66	1	0
12	T	45	0	33	0	0
12	U	260	0	288	12	0
12	a	2536	0	2594	83	0
12	b	2425	0	2404	82	0
12	f	156	0	138	5	0
12	j	90	0	66	1	0
12	k	45	0	33	0	0
12	l	260	0	288	12	0
13	A	30	0	0	1	0
13	B	30	0	0	2	0
13	G	30	0	0	1	0
13	H	30	0	0	2	0
13	a	30	0	0	1	0
13	b	30	0	0	2	0
14	A	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	C	16	0	0	0	0
14	G	8	0	0	0	0
14	N	16	0	0	0	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
15	A	160	0	224	8	0
15	B	160	0	224	10	0
15	F	40	0	56	2	0
15	G	160	0	224	11	0
15	H	160	0	224	11	0
15	I	40	0	56	2	0
15	J	80	0	112	9	0
15	K	40	0	56	2	0
15	L	80	0	112	7	0
15	Q	40	0	56	2	0
15	R	40	0	56	2	0
15	S	80	0	112	9	0
15	T	40	0	56	2	0
15	U	80	0	112	5	0
15	a	160	0	224	11	0
15	b	160	0	224	8	0
15	f	40	0	56	2	0
15	i	40	0	56	1	0
15	j	80	0	112	10	0
15	k	40	0	56	2	0
15	l	80	0	112	7	0
16	A	98	0	148	8	0
16	B	43	0	59	4	0
16	G	98	0	148	8	0
16	H	43	0	59	4	0
16	M	44	0	61	2	0
16	V	44	0	61	3	0
16	a	98	0	148	8	0
16	b	43	0	59	4	0
16	m	44	0	61	2	0
17	A	82	0	107	6	0
17	B	51	0	75	0	0
17	G	82	0	107	7	0
17	H	51	0	75	0	0
17	a	82	0	107	6	0
17	b	51	0	75	0	0
18	A	42	0	52	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	G	42	0	52	1	0
18	a	42	0	52	1	0
19	A	1	0	0	0	0
19	G	1	0	0	0	0
19	a	1	0	0	0	0
20	B	41	0	54	7	0
20	H	41	0	54	6	0
20	M	41	0	54	1	0
20	V	41	0	54	2	0
20	b	41	0	54	7	0
20	m	41	0	54	1	0
21	B	1	0	0	0	0
21	H	1	0	0	0	0
21	L	1	0	0	0	0
21	U	1	0	0	0	0
21	b	1	0	0	0	0
21	l	1	0	0	0	0
22	B	42	0	0	0	0
22	H	42	0	0	0	0
22	b	42	0	0	0	0
23	B	42	0	56	2	0
23	F	42	0	55	2	0
23	H	42	0	56	3	0
23	Q	42	0	55	2	0
23	b	42	0	56	2	0
23	f	42	0	55	2	0
24	L	45	0	54	4	0
24	M	54	0	78	9	0
24	U	45	0	54	4	0
24	V	54	0	78	8	0
24	l	45	0	54	4	0
24	m	54	0	78	8	0
25	L	49	0	70	3	0
25	U	49	0	70	3	0
25	l	49	0	70	3	0
26	L	35	0	45	3	0
26	U	35	0	45	3	0
26	l	35	0	45	3	0
27	A	90	0	0	3	0
27	B	112	0	0	2	0
27	C	36	0	0	0	0
27	D	28	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	E	7	0	0	0	0
27	F	2	0	0	0	0
27	G	90	0	0	4	0
27	H	112	0	0	2	0
27	I	4	0	0	0	0
27	L	24	0	0	1	0
27	N	36	0	0	0	0
27	O	28	0	0	0	0
27	P	7	0	0	0	0
27	Q	2	0	0	0	0
27	R	4	0	0	0	0
27	U	24	0	0	1	0
27	a	90	0	0	3	0
27	b	112	0	0	2	0
27	c	36	0	0	0	0
27	d	28	0	0	0	0
27	e	7	0	0	0	0
27	f	2	0	0	0	0
27	i	4	0	0	0	0
27	l	24	0	0	1	0
All	All	73866	0	72915	1156	0

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

The worst 5 of 1156 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)
20:H:2143:ECH:H33B	12:a:854:CLA:HBB1	1.35	1.08
20:b:2143:ECH:H33B	12:A:854:CLA:HBB1	1.35	1.08
12:G:854:CLA:HBB1	20:B:2144:ECH:H33B	1.33	1.06
12:G:854:CLA:CBB	20:B:2144:ECH:H33B	1.86	1.05
20:b:2143:ECH:H33B	12:A:854:CLA:CBB	1.87	1.03

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	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
1	G	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
1	a	735/751 (98%)	701 (95%)	33 (4%)	1 (0%)	48	45
2	B	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	H	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
2	b	727/730 (100%)	692 (95%)	35 (5%)	0	100	100
3	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	N	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
3	c	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
4	D	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	O	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
4	d	137/141 (97%)	134 (98%)	3 (2%)	0	100	100
5	E	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	P	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
5	e	67/74 (90%)	62 (92%)	5 (8%)	0	100	100
6	F	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	Q	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
6	f	139/165 (84%)	136 (98%)	3 (2%)	0	100	100
7	I	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	R	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
7	i	38/40 (95%)	35 (92%)	3 (8%)	0	100	100
8	J	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	S	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
8	j	37/40 (92%)	36 (97%)	1 (3%)	0	100	100
9	K	65/90 (72%)	58 (89%)	7 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	T	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
9	k	65/90 (72%)	58 (89%)	7 (11%)	0	100	100
10	L	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	U	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
10	l	152/157 (97%)	146 (96%)	6 (4%)	0	100	100
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	V	29/31 (94%)	29 (100%)	0	0	100	100
11	m	29/31 (94%)	29 (100%)	0	0	100	100
All	All	6612/6900 (96%)	6312 (96%)	297 (4%)	3 (0%)	100	100

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	121	VAL
1	a	121	VAL
1	A	121	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	591/603 (98%)	578 (98%)	13 (2%)	45	45
1	G	591/603 (98%)	577 (98%)	14 (2%)	43	41
1	a	591/603 (98%)	577 (98%)	14 (2%)	43	41
2	B	582/583 (100%)	570 (98%)	12 (2%)	47	47
2	H	582/583 (100%)	570 (98%)	12 (2%)	47	47
2	b	582/583 (100%)	570 (98%)	12 (2%)	47	47
3	C	68/69 (99%)	66 (97%)	2 (3%)	37	34
3	N	68/69 (99%)	66 (97%)	2 (3%)	37	34
3	c	68/69 (99%)	66 (97%)	2 (3%)	37	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	D	114/116 (98%)	112 (98%)	2 (2%)	51	52
4	O	114/116 (98%)	112 (98%)	2 (2%)	51	52
4	d	114/116 (98%)	112 (98%)	2 (2%)	51	52
5	E	58/60 (97%)	55 (95%)	3 (5%)	21	13
5	P	58/60 (97%)	55 (95%)	3 (5%)	21	13
5	e	58/60 (97%)	55 (95%)	3 (5%)	21	13
6	F	118/137 (86%)	112 (95%)	6 (5%)	21	14
6	Q	118/137 (86%)	112 (95%)	6 (5%)	21	14
6	f	118/137 (86%)	112 (95%)	6 (5%)	21	14
7	I	32/32 (100%)	32 (100%)	0	100	100
7	R	32/32 (100%)	32 (100%)	0	100	100
7	i	32/32 (100%)	32 (100%)	0	100	100
8	J	34/35 (97%)	33 (97%)	1 (3%)	37	34
8	S	34/35 (97%)	33 (97%)	1 (3%)	37	34
8	j	34/35 (97%)	33 (97%)	1 (3%)	37	34
9	K	50/68 (74%)	47 (94%)	3 (6%)	17	10
9	T	50/68 (74%)	47 (94%)	3 (6%)	17	10
9	k	50/68 (74%)	47 (94%)	3 (6%)	17	10
10	L	116/118 (98%)	114 (98%)	2 (2%)	53	53
10	U	116/118 (98%)	114 (98%)	2 (2%)	53	53
10	l	116/118 (98%)	114 (98%)	2 (2%)	53	53
11	M	25/25 (100%)	23 (92%)	2 (8%)	11	5
11	V	25/25 (100%)	23 (92%)	2 (8%)	11	5
11	m	25/25 (100%)	23 (92%)	2 (8%)	11	5
All	All	5364/5538 (97%)	5224 (97%)	140 (3%)	41	38

5 of 140 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	429	PHE
3	C	23	LEU
6	F	130	LYS
1	a	120	ILE
1	a	37	THR

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

Mol	Chain	Res	Type
2	b	325	ASN
2	B	686	ASN
4	d	23	ASN
2	B	627	GLN
8	J	30	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 9 are monoatomic - leaving 393 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	CLA	a	819	1	69,73,73	1.18	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	Q	204	-	49,53,73	1.40	6 (12%)	58,89,113	1.42	4 (6%)
12	CLA	a	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
12	CLA	b	2124	27	69,73,73	1.17	7 (10%)	82,113,113	1.31	8 (9%)
12	CLA	B	2122	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
12	CLA	G	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	2110	2	69,73,73	1.21	7 (10%)	82,113,113	1.34	5 (6%)
12	CLA	A	801	1	69,73,73	1.20	8 (11%)	82,113,113	1.30	7 (8%)
12	CLA	H	2133	2	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	B	2132	2	59,63,73	1.26	8 (13%)	70,101,113	1.38	7 (10%)
15	BCR	j	104	-	41,41,41	1.07	3 (7%)	56,56,56	1.27	7 (12%)
12	CLA	b	2135	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
12	CLA	H	2141	16	49,53,73	1.39	6 (12%)	58,89,113	1.54	7 (12%)
12	CLA	b	2140	2	69,73,73	1.18	6 (8%)	82,113,113	1.35	5 (6%)
12	CLA	H	2129	2	69,73,73	1.20	10 (14%)	82,113,113	1.36	7 (8%)
24	SQD	L	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	G	804	1	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	H	2139	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
24	SQD	l	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	H	2124	27	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
24	SQD	m	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	B	2131	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	b	2112	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
12	CLA	G	836	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	J	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
12	CLA	b	2125	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	8 (12%)
12	CLA	B	2106	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)
15	BCR	B	2143	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	A	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	T	4002	9	49,53,73	1.40	8 (16%)	58,89,113	1.49	4 (6%)
12	CLA	G	829	1	69,73,73	1.18	8 (11%)	82,113,113	1.42	5 (6%)
12	CLA	H	2126	2	69,73,73	1.19	8 (11%)	82,113,113	1.28	4 (4%)
12	CLA	G	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
13	A1AGD	a	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.93	12 (31%)
12	CLA	A	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.47	6 (9%)
12	CLA	G	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	832	1	69,73,73	1.18	6 (8%)	82,113,113	1.21	5 (6%)
12	CLA	a	805	1	69,73,73	1.16	9 (13%)	82,113,113	1.40	9 (10%)
12	CLA	A	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
15	BCR	i	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.32	6 (10%)
15	BCR	H	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	2127	2	69,73,73	1.16	7 (10%)	82,113,113	1.27	7 (8%)
12	CLA	G	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
12	CLA	S	102	-	49,53,73	1.41	6 (12%)	58,89,113	1.51	6 (10%)
12	CLA	K	4002	9	49,53,73	1.40	7 (14%)	58,89,113	1.49	4 (6%)
16	LHG	B	2149	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
12	CLA	a	836	1	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
14	SF4	c	102	3	0,12,12	-	-	-		
12	CLA	b	2121	-	59,63,73	1.27	7 (11%)	70,101,113	1.33	7 (10%)
12	CLA	j	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
17	LMG	B	2148	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
12	CLA	H	2130	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	F	204	-	49,53,73	1.40	6 (12%)	58,89,113	1.43	4 (6%)
12	CLA	a	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
20	ECH	B	2144	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	a	829	1	69,73,73	1.18	7 (10%)	82,113,113	1.43	5 (6%)
12	CLA	G	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.37	7 (9%)
12	CLA	B	2135	-	49,53,73	1.38	6 (12%)	58,89,113	1.49	6 (10%)
12	CLA	l	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.32	8 (9%)
12	CLA	H	2106	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	H	2152	16	54,58,73	1.28	7 (12%)	64,95,113	1.49	5 (7%)
12	CLA	A	837	1	69,73,73	1.17	7 (10%)	82,113,113	1.33	6 (7%)
25	DGD	l	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
16	LHG	m	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	b	2115	2	49,53,73	1.42	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	b	2106	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	A	805	1	69,73,73	1.16	8 (11%)	82,113,113	1.40	9 (10%)
15	BCR	J	104	-	41,41,41	1.06	3 (7%)	56,56,56	1.27	7 (12%)
25	DGD	U	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.36	7 (12%)
12	CLA	H	2108	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
12	CLA	a	832	1	69,73,73	1.17	7 (10%)	82,113,113	1.20	5 (6%)
12	CLA	A	804	1	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	a	802	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
12	CLA	A	829	1	69,73,73	1.18	8 (11%)	82,113,113	1.42	5 (6%)
23	ZEX	B	2152	-	43,43,43	5.84	26 (60%)	51,60,60	10.37	30 (58%)
12	CLA	B	2120	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	2136	2	49,53,73	1.38	9 (18%)	58,89,113	1.54	6 (10%)
12	CLA	H	2121	-	59,63,73	1.26	7 (11%)	70,101,113	1.33	7 (10%)
12	CLA	b	2132	2	69,73,73	1.15	5 (7%)	82,113,113	1.47	8 (9%)
12	CLA	H	2114	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	7 (8%)
12	CLA	H	2134	-	49,53,73	1.37	6 (12%)	58,89,113	1.48	6 (10%)
12	CLA	A	815	-	49,53,73	1.40	7 (14%)	58,89,113	1.48	4 (6%)
12	CLA	J	102	-	49,53,73	1.40	6 (12%)	58,89,113	1.52	6 (10%)
15	BCR	A	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
16	LHG	G	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.29	7 (13%)
14	SF4	a	841	1,2	0,12,12	-	-	-	-	-
12	CLA	A	819	1	69,73,73	1.19	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	a	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
14	SF4	C	101	3	0,12,12	-	-	-	-	-
12	CLA	Q	201	27	69,73,73	1.17	8 (11%)	82,113,113	1.26	4 (4%)
17	LMG	A	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	B	2142	16	49,53,73	1.39	6 (12%)	58,89,113	1.55	7 (12%)
12	CLA	B	2133	2	69,73,73	1.16	5 (7%)	82,113,113	1.47	9 (10%)
15	BCR	j	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	8 (14%)
12	CLA	G	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	7 (10%)
12	CLA	A	813	1	69,73,73	1.18	5 (7%)	82,113,113	1.34	5 (6%)
22	EQ3	H	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
12	CLA	A	831	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
12	CLA	B	2121	-	59,63,73	1.28	8 (13%)	70,101,113	1.40	5 (7%)
12	CLA	b	2123	2	59,63,73	1.27	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	A	809	1	54,58,73	1.33	7 (12%)	64,95,113	1.46	9 (14%)
12	CLA	B	2114	-	49,53,73	1.42	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	A	824	27	69,73,73	1.20	7 (10%)	82,113,113	1.38	10 (12%)
12	CLA	H	2137	2	69,73,73	1.14	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	b	2127	2	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)
12	CLA	G	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.36	5 (6%)
12	CLA	G	850	27	69,73,73	1.16	9 (13%)	82,113,113	1.26	5 (6%)
16	LHG	a	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	H	2118	2	54,58,73	1.34	8 (14%)	64,95,113	1.49	6 (9%)
12	CLA	B	2116	2	49,53,73	1.41	8 (16%)	58,89,113	1.49	4 (6%)
12	CLA	L	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	l	204	10	69,73,73	1.14	9 (13%)	82,113,113	1.33	6 (7%)
12	CLA	k	4002	9	49,53,73	1.40	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	B	2138	2	69,73,73	1.15	8 (11%)	82,113,113	1.31	7 (8%)
14	SF4	G	841	1,2	0,12,12	-	-	-		
17	LMG	H	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
15	BCR	G	843	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	8 (14%)
12	CLA	a	818	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
12	CLA	A	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	7 (10%)
20	ECH	m	101	-	42,42,42	0.39	0	55,58,58	0.74	0
15	BCR	S	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	H	2104	-	69,73,73	1.13	8 (11%)	82,113,113	1.53	8 (9%)
12	CLA	b	2120	-	59,63,73	1.28	8 (13%)	70,101,113	1.41	5 (7%)
12	CLA	H	2131	2	59,63,73	1.26	8 (13%)	70,101,113	1.37	7 (10%)
17	LMG	b	2147	-	51,51,55	0.75	0	59,59,63	1.30	8 (13%)
15	BCR	B	2145	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
15	BCR	l	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	B	2140	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
12	CLA	b	2134	-	49,53,73	1.38	6 (12%)	58,89,113	1.49	6 (10%)
12	CLA	G	801	1	69,73,73	1.20	8 (11%)	82,113,113	1.30	7 (8%)
15	BCR	U	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2109	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
12	CLA	H	2138	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
15	BCR	b	2145	-	41,41,41	1.05	2 (4%)	56,56,56	1.14	3 (5%)
15	BCR	F	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.21	5 (8%)
12	CLA	H	2102	-	69,73,73	1.13	9 (13%)	82,113,113	1.47	9 (10%)
12	CLA	B	2137	2	49,53,73	1.38	8 (16%)	58,89,113	1.54	6 (10%)
23	ZEX	F	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
17	LMG	a	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.28	6 (10%)
12	CLA	a	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
16	LHG	A	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)
17	LMG	G	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
12	CLA	G	854	-	59,63,73	1.27	8 (13%)	70,101,113	1.40	9 (12%)
12	CLA	F	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
12	CLA	b	2128	2	69,73,73	1.18	8 (11%)	82,113,113	1.18	6 (7%)
12	CLA	A	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.32	4 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	803	1,12	59,63,73	1.27	6 (10%)	70,101,113	1.39	7 (10%)
12	CLA	a	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
15	BCR	G	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	4 (7%)
12	CLA	G	837	1	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	H	2110	2	69,73,73	1.21	6 (8%)	82,113,113	1.33	5 (6%)
12	CLA	A	850	27	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
14	SF4	A	841	1,2	0,12,12	-	-	-	-	-
15	BCR	T	4001	-	41,41,41	1.02	3 (7%)	56,56,56	1.31	6 (10%)
12	CLA	H	2116	-	49,53,73	1.39	7 (14%)	58,89,113	1.49	5 (8%)
12	CLA	B	2102	27	69,73,73	1.14	8 (11%)	82,113,113	1.28	7 (8%)
15	BCR	H	2145	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	A	836	1	69,73,73	1.16	8 (11%)	82,113,113	1.27	4 (4%)
12	CLA	B	2129	2	69,73,73	1.18	8 (11%)	82,113,113	1.18	5 (6%)
14	SF4	C	102	3	0,12,12	-	-	-	-	-
13	A1AGD	H	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
12	CLA	B	2105	-	69,73,73	1.13	8 (11%)	82,113,113	1.53	8 (9%)
12	CLA	b	2141	16	49,53,73	1.39	6 (12%)	58,89,113	1.55	7 (12%)
12	CLA	a	801	1	69,73,73	1.20	9 (13%)	82,113,113	1.30	7 (8%)
12	CLA	H	2140	2	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
12	CLA	b	2107	2	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	B	2108	2	69,73,73	1.18	9 (13%)	82,113,113	1.27	4 (4%)
12	CLA	B	2126	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	8 (12%)
12	CLA	G	817	1	64,68,73	1.21	9 (14%)	76,107,113	1.29	8 (10%)
12	CLA	G	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
15	BCR	K	4001	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	G	825	27	64,68,73	1.21	8 (12%)	76,107,113	1.39	10 (13%)
12	CLA	B	2134	2	69,73,73	1.18	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	B	2104	2	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	A	832	1	69,73,73	1.17	7 (10%)	82,113,113	1.21	4 (4%)
12	CLA	G	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
12	CLA	A	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
23	ZEX	f	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
15	BCR	R	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)
15	BCR	k	4001	-	41,41,41	1.01	2 (4%)	56,56,56	1.31	5 (8%)
12	CLA	a	803	1,12	59,63,73	1.27	6 (10%)	70,101,113	1.39	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LMG	A	847	-	50,50,55	1.00	5 (10%)	58,58,63	1.29	6 (10%)
15	BCR	B	2147	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	B	2136	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
12	CLA	B	2141	2	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
12	CLA	a	813	1	69,73,73	1.18	6 (8%)	82,113,113	1.34	5 (6%)
23	ZEX	b	2151	-	43,43,43	5.85	26 (60%)	51,60,60	10.37	30 (58%)
16	LHG	b	2148	12	42,42,48	0.63	0	45,48,54	1.22	4 (8%)
15	BCR	f	202	-	41,41,41	1.04	2 (4%)	56,56,56	1.20	5 (8%)
15	BCR	a	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2105	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)
12	CLA	a	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
24	SQD	U	208	-	43,45,54	1.67	8 (18%)	53,56,65	1.58	7 (13%)
12	CLA	G	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
16	LHG	M	102	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	b	2108	2	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
12	CLA	B	2111	2	69,73,73	1.21	7 (10%)	82,113,113	1.33	5 (6%)
22	EQ3	b	2150	-	43,43,43	4.23	24 (55%)	55,60,60	5.22	27 (49%)
12	CLA	A	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
16	LHG	V	103	-	43,43,48	0.66	1 (2%)	46,49,54	1.23	4 (8%)
12	CLA	G	820	27	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
12	CLA	B	2107	-	69,73,73	1.16	5 (7%)	82,113,113	1.33	8 (9%)
12	CLA	H	2115	2	49,53,73	1.41	7 (14%)	58,89,113	1.49	4 (6%)
12	CLA	B	2123	-	49,53,73	1.40	8 (16%)	58,89,113	1.37	4 (6%)
12	CLA	B	2113	2	69,73,73	1.18	7 (10%)	82,113,113	1.27	5 (6%)
12	CLA	A	812	1	69,73,73	1.19	8 (11%)	82,113,113	1.26	7 (8%)
13	A1AGD	B	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
12	CLA	A	811	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
12	CLA	H	2103	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	G	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
12	CLA	G	828	-	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
12	CLA	A	807	1	69,73,73	1.15	8 (11%)	82,113,113	1.35	8 (9%)
12	CLA	B	2139	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
12	CLA	H	2136	2	49,53,73	1.38	8 (16%)	58,89,113	1.53	6 (10%)
16	LHG	a	848	12	48,48,48	0.64	1 (2%)	51,54,54	1.26	6 (11%)
15	BCR	I	101	-	41,41,41	1.02	2 (4%)	56,56,56	1.31	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
15	BCR	b	2144	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	G	830	1	59,63,73	1.26	8 (13%)	70,101,113	1.44	10 (14%)
12	CLA	B	2124	2	59,63,73	1.26	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	U	204	10	69,73,73	1.13	8 (11%)	82,113,113	1.34	6 (7%)
15	BCR	G	842	-	41,41,41	1.04	2 (4%)	56,56,56	1.23	5 (8%)
24	SQD	V	102	-	52,54,54	1.56	7 (13%)	62,65,65	1.37	8 (12%)
18	45D	a	852	-	43,43,43	0.39	0	54,60,60	0.85	0
12	CLA	B	2119	2	54,58,73	1.34	8 (14%)	64,95,113	1.49	6 (9%)
12	CLA	a	850	27	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
12	CLA	A	818	1	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
12	CLA	a	820	27	69,73,73	1.15	8 (11%)	82,113,113	1.38	8 (9%)
22	EQ3	B	2151	-	43,43,43	4.23	23 (53%)	55,60,60	5.22	27 (49%)
15	BCR	a	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
16	LHG	A	846	-	48,48,48	0.67	2 (4%)	51,54,54	1.28	7 (13%)
12	CLA	G	807	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	8 (9%)
25	DGD	L	209	-	49,49,67	0.95	5 (10%)	57,57,81	1.37	7 (12%)
12	CLA	G	818	1	69,73,73	1.15	9 (13%)	82,113,113	1.33	8 (9%)
12	CLA	b	2111	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
12	CLA	a	808	1	54,58,73	1.30	8 (14%)	64,95,113	1.54	8 (12%)
12	CLA	l	203	10	69,73,73	1.14	8 (11%)	82,113,113	1.36	8 (9%)
12	CLA	H	2107	2	69,73,73	1.18	9 (13%)	82,113,113	1.27	5 (6%)
15	BCR	B	2146	-	41,41,41	1.06	2 (4%)	56,56,56	1.14	3 (5%)
12	CLA	a	828	-	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
12	CLA	G	823	1	64,68,73	1.21	9 (14%)	76,107,113	1.38	7 (9%)
12	CLA	H	2123	2	59,63,73	1.26	7 (11%)	70,101,113	1.45	8 (11%)
12	CLA	A	828	-	69,73,73	1.15	7 (10%)	82,113,113	1.28	6 (7%)
12	CLA	b	2119	2	69,73,73	1.17	8 (11%)	82,113,113	1.29	8 (9%)
12	CLA	B	2112	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
20	ECH	M	103	-	42,42,42	0.39	0	55,58,58	0.74	0
12	CLA	b	2113	-	49,53,73	1.42	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	B	2125	27	69,73,73	1.18	7 (10%)	82,113,113	1.31	8 (9%)
12	CLA	b	2137	2	69,73,73	1.14	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	f	204	-	49,53,73	1.39	6 (12%)	58,89,113	1.43	4 (6%)
12	CLA	a	830	1	59,63,73	1.25	8 (13%)	70,101,113	1.45	10 (14%)
12	CLA	L	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	2129	2	69,73,73	1.21	11 (15%)	82,113,113	1.36	7 (8%)
12	CLA	a	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	a	854	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	9 (12%)
12	CLA	U	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
18	45D	A	852	-	43,43,43	0.38	0	54,60,60	0.86	0
12	CLA	b	2139	27	69,73,73	1.14	8 (11%)	82,113,113	1.35	7 (8%)
15	BCR	H	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
12	CLA	b	2105	2	69,73,73	1.16	7 (10%)	82,113,113	1.32	7 (8%)
12	CLA	b	2101	27	69,73,73	1.14	8 (11%)	82,113,113	1.28	8 (9%)
12	CLA	H	2119	2	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	G	839	1	69,73,73	1.18	8 (11%)	82,113,113	1.31	6 (7%)
12	CLA	a	824	27	69,73,73	1.19	7 (10%)	82,113,113	1.37	10 (12%)
12	CLA	a	821	1	64,68,73	1.20	8 (12%)	76,107,113	1.32	4 (5%)
12	CLA	a	811	-	49,53,73	1.39	7 (14%)	58,89,113	1.44	4 (6%)
12	CLA	G	824	27	69,73,73	1.19	7 (10%)	82,113,113	1.38	10 (12%)
12	CLA	A	825	27	64,68,73	1.20	8 (12%)	76,107,113	1.39	10 (13%)
12	CLA	H	2120	-	59,63,73	1.28	8 (13%)	70,101,113	1.40	5 (7%)
15	BCR	A	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	a	817	1	64,68,73	1.22	9 (14%)	76,107,113	1.29	8 (10%)
12	CLA	a	807	1	69,73,73	1.14	8 (11%)	82,113,113	1.36	8 (9%)
12	CLA	B	2127	2	69,73,73	1.18	8 (11%)	82,113,113	1.28	4 (4%)
15	BCR	G	844	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
12	CLA	A	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
12	CLA	H	2113	-	49,53,73	1.42	6 (12%)	58,89,113	1.43	4 (6%)
17	LMG	G	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.27	4 (10%)
12	CLA	G	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.46	6 (9%)
12	CLA	b	2126	2	69,73,73	1.19	8 (11%)	82,113,113	1.27	4 (4%)
12	CLA	G	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.56	6 (10%)
23	ZEX	H	2151	-	43,43,43	5.84	26 (60%)	51,60,60	10.36	30 (58%)
12	CLA	A	834	1	59,63,73	1.26	7 (11%)	70,101,113	1.47	11 (15%)
12	CLA	a	825	27	64,68,73	1.21	8 (12%)	76,107,113	1.39	10 (13%)
13	A1AGD	b	2153	-	30,30,30	2.73	6 (20%)	38,39,39	2.83	13 (34%)
15	BCR	b	2146	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	6 (10%)
12	CLA	H	2112	2	69,73,73	1.18	8 (11%)	82,113,113	1.27	4 (4%)
16	LHG	G	848	12	48,48,48	0.63	1 (2%)	51,54,54	1.26	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	ECH	V	101	-	42,42,42	0.39	0	55,58,58	0.74	0
12	CLA	G	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.41	6 (9%)
12	CLA	b	2117	2	49,53,73	1.39	5 (10%)	58,89,113	1.54	6 (10%)
12	CLA	A	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	811	-	49,53,73	1.39	6 (12%)	58,89,113	1.44	4 (6%)
12	CLA	G	819	1	69,73,73	1.19	7 (10%)	82,113,113	1.32	6 (7%)
12	CLA	G	803	1,12	59,63,73	1.27	5 (8%)	70,101,113	1.39	8 (11%)
12	CLA	L	203	10	69,73,73	1.15	8 (11%)	82,113,113	1.37	9 (10%)
12	CLA	A	810	1,12	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
12	CLA	B	2103	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	10 (12%)
15	BCR	S	104	-	41,41,41	1.07	2 (4%)	56,56,56	1.28	7 (12%)
12	CLA	U	201	1	69,73,73	1.13	7 (10%)	82,113,113	1.31	7 (8%)
12	CLA	b	2133	2	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
12	CLA	a	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	5 (6%)
15	BCR	H	2144	-	41,41,41	1.00	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	b	2102	-	69,73,73	1.14	9 (13%)	82,113,113	1.47	10 (12%)
12	CLA	H	2125	27	54,58,73	1.31	8 (14%)	64,95,113	1.45	7 (10%)
15	BCR	b	2142	-	41,41,41	1.09	2 (4%)	56,56,56	1.19	5 (8%)
12	CLA	f	203	-	49,53,73	1.40	8 (16%)	58,89,113	1.41	5 (8%)
12	CLA	A	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.36	6 (7%)
12	CLA	H	2117	2	49,53,73	1.39	5 (10%)	58,89,113	1.55	6 (10%)
12	CLA	B	2110	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	7 (8%)
12	CLA	G	802	1	69,73,73	1.16	8 (11%)	82,113,113	1.26	6 (7%)
20	ECH	H	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	B	2128	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	6 (7%)
12	CLA	b	2114	-	69,73,73	1.18	9 (13%)	82,113,113	1.33	7 (8%)
15	BCR	Q	202	-	41,41,41	1.05	2 (4%)	56,56,56	1.21	5 (8%)
15	BCR	a	843	-	41,41,41	1.03	2 (4%)	56,56,56	1.27	8 (14%)
12	CLA	B	2101	16	54,58,73	1.28	7 (12%)	64,95,113	1.49	5 (7%)
12	CLA	S	103	8	49,53,73	1.40	6 (12%)	58,89,113	1.47	5 (8%)
12	CLA	B	2115	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	7 (8%)
12	CLA	a	823	1	64,68,73	1.21	8 (12%)	76,107,113	1.38	7 (9%)
12	CLA	a	806	1	54,58,73	1.31	7 (12%)	64,95,113	1.47	6 (9%)
12	CLA	U	203	10	69,73,73	1.15	8 (11%)	82,113,113	1.38	9 (10%)
12	CLA	b	2116	-	49,53,73	1.39	7 (14%)	58,89,113	1.48	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	H	2135	-	49,53,73	1.39	8 (16%)	58,89,113	1.43	5 (8%)
14	SF4	N	101	3	0,12,12	-	-	-		
12	CLA	G	813	1	69,73,73	1.18	6 (8%)	82,113,113	1.34	6 (7%)
12	CLA	G	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.36	7 (8%)
15	BCR	L	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
15	BCR	U	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	L	204	10	69,73,73	1.14	8 (11%)	82,113,113	1.33	6 (7%)
12	CLA	A	833	1	69,73,73	1.14	8 (11%)	82,113,113	1.35	5 (6%)
12	CLA	A	802	1	69,73,73	1.17	8 (11%)	82,113,113	1.26	6 (7%)
12	CLA	A	830	1	59,63,73	1.26	8 (13%)	70,101,113	1.45	10 (14%)
12	CLA	B	2117	-	49,53,73	1.39	7 (14%)	58,89,113	1.48	5 (8%)
12	CLA	a	837	1	69,73,73	1.17	7 (10%)	82,113,113	1.31	6 (7%)
12	CLA	G	815	-	49,53,73	1.39	6 (12%)	58,89,113	1.49	4 (6%)
26	LMT	L	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0
12	CLA	B	2118	2	49,53,73	1.39	5 (10%)	58,89,113	1.55	6 (10%)
12	CLA	H	2122	-	49,53,73	1.40	7 (14%)	58,89,113	1.37	4 (6%)
12	CLA	b	2131	2	59,63,73	1.26	8 (13%)	70,101,113	1.37	7 (10%)
15	BCR	l	206	-	41,41,41	1.02	2 (4%)	56,56,56	1.23	5 (8%)
12	CLA	H	2128	2	69,73,73	1.18	8 (11%)	82,113,113	1.17	5 (6%)
12	CLA	a	816	1	59,63,73	1.25	8 (13%)	70,101,113	1.46	7 (10%)
14	SF4	N	102	3	0,12,12	-	-	-		
18	45D	G	852	-	43,43,43	0.38	0	54,60,60	0.86	0
12	CLA	Q	203	-	49,53,73	1.41	8 (16%)	58,89,113	1.40	5 (8%)
12	CLA	H	2101	27	69,73,73	1.15	8 (11%)	82,113,113	1.29	7 (8%)
15	BCR	A	845	-	41,41,41	1.11	2 (4%)	56,56,56	1.29	4 (7%)
15	BCR	J	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.33	8 (14%)
12	CLA	B	2109	2	69,73,73	1.17	7 (10%)	82,113,113	1.33	5 (6%)
12	CLA	G	809	1	54,58,73	1.34	7 (12%)	64,95,113	1.45	9 (14%)
24	SQD	M	101	-	52,54,54	1.55	7 (13%)	62,65,65	1.37	8 (12%)
12	CLA	a	804	1	69,73,73	1.16	8 (11%)	82,113,113	1.44	6 (7%)
12	CLA	f	201	27	69,73,73	1.18	8 (11%)	82,113,113	1.27	5 (6%)
12	CLA	H	2132	2	69,73,73	1.16	5 (7%)	82,113,113	1.47	8 (9%)
12	CLA	G	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
16	LHG	H	2148	12	42,42,48	0.64	0	45,48,54	1.22	4 (8%)
12	CLA	l	205	27	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	838	1	69,73,73	1.18	8 (11%)	82,113,113	1.37	6 (7%)
12	CLA	A	820	27	69,73,73	1.16	8 (11%)	82,113,113	1.38	8 (9%)
12	CLA	b	2118	2	54,58,73	1.34	8 (14%)	64,95,113	1.48	6 (9%)
12	CLA	B	2130	2	69,73,73	1.20	11 (15%)	82,113,113	1.36	7 (8%)
20	ECH	b	2143	-	42,42,42	0.40	0	55,58,58	1.59	7 (12%)
12	CLA	b	2130	-	49,53,73	1.39	8 (16%)	58,89,113	1.47	4 (6%)
12	CLA	b	2103	2	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
26	LMT	l	210	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	0
17	LMG	a	849	-	32,32,55	1.00	1 (3%)	40,40,63	1.26	4 (10%)
12	CLA	a	815	-	49,53,73	1.40	6 (12%)	58,89,113	1.49	4 (6%)
12	CLA	A	826	1	69,73,73	1.19	8 (11%)	82,113,113	1.28	6 (7%)
12	CLA	A	854	-	59,63,73	1.26	7 (11%)	70,101,113	1.40	9 (12%)
12	CLA	F	201	27	69,73,73	1.17	8 (11%)	82,113,113	1.27	5 (6%)
23	ZEX	Q	205	-	43,43,43	5.82	27 (62%)	51,60,60	10.43	30 (58%)
12	CLA	b	2104	-	69,73,73	1.13	9 (13%)	82,113,113	1.52	8 (9%)
15	BCR	a	844	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
12	CLA	a	851	27	69,73,73	1.16	7 (10%)	82,113,113	1.33	6 (7%)
12	CLA	G	821	1	64,68,73	1.21	8 (12%)	76,107,113	1.32	4 (5%)
12	CLA	b	2122	-	49,53,73	1.41	7 (14%)	58,89,113	1.38	4 (6%)
12	CLA	H	2111	2	69,73,73	1.18	8 (11%)	82,113,113	1.57	13 (15%)
12	CLA	a	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.28	8 (9%)
12	CLA	a	809	1	54,58,73	1.34	8 (14%)	64,95,113	1.45	9 (14%)
15	BCR	L	207	-	41,41,41	1.07	2 (4%)	56,56,56	1.35	8 (14%)
12	CLA	b	2152	16	54,58,73	1.28	8 (14%)	64,95,113	1.49	5 (7%)
12	CLA	a	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)
13	A1AGD	A	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
12	CLA	A	823	1	64,68,73	1.21	8 (12%)	76,107,113	1.37	6 (7%)
12	CLA	A	817	1	64,68,73	1.22	9 (14%)	76,107,113	1.30	8 (10%)
13	A1AGD	G	840	-	30,30,30	1.80	8 (26%)	38,39,39	1.94	12 (31%)
14	SF4	c	101	3	0,12,12	-	-	-	-	-
12	CLA	j	102	-	49,53,73	1.41	6 (12%)	58,89,113	1.51	6 (10%)
12	CLA	b	2109	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	7 (8%)
12	CLA	b	2138	-	49,53,73	1.36	8 (16%)	58,89,113	1.42	5 (8%)
12	CLA	A	835	1	69,73,73	1.16	9 (13%)	82,113,113	1.28	8 (9%)
12	CLA	A	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	822	-	54,58,73	1.31	7 (12%)	64,95,113	1.40	6 (9%)
26	LMT	U	210	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	0

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
12	CLA	a	819	1	-	18/39/115/115	-
12	CLA	Q	204	-	-	5/15/91/115	-
12	CLA	a	810	1,12	-	15/39/115/115	-
12	CLA	b	2124	27	-	6/39/115/115	-
12	CLA	B	2122	-	-	10/27/103/115	-
12	CLA	G	805	1	-	14/39/115/115	-
12	CLA	b	2110	2	-	14/39/115/115	-
12	CLA	A	801	1	-	5/39/115/115	-
12	CLA	H	2133	2	-	18/39/115/115	-
12	CLA	B	2132	2	-	7/27/103/115	-
15	BCR	j	104	-	-	9/29/63/63	0/2/2/2
12	CLA	b	2135	-	-	9/15/91/115	-
12	CLA	H	2141	16	-	7/15/91/115	-
12	CLA	b	2140	2	-	16/39/115/115	-
12	CLA	H	2129	2	-	13/39/115/115	-
24	SQD	L	208	-	-	15/40/60/69	0/1/1/1
12	CLA	G	804	1	-	16/39/115/115	-
12	CLA	H	2139	27	-	10/39/115/115	-
24	SQD	l	208	-	-	15/40/60/69	0/1/1/1
12	CLA	H	2124	27	-	6/39/115/115	-
24	SQD	m	102	-	-	28/49/69/69	0/1/1/1
12	CLA	B	2131	-	-	2/15/91/115	-
12	CLA	b	2112	2	-	8/39/115/115	-
12	CLA	G	836	1	-	14/39/115/115	-
12	CLA	J	103	8	-	10/15/91/115	-
12	CLA	b	2125	27	-	4/21/97/115	-
12	CLA	B	2106	2	-	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	B	2143	-	-	6/29/63/63	0/2/2/2
15	BCR	A	843	-	-	15/29/63/63	0/2/2/2
12	CLA	T	4002	9	-	9/15/91/115	-
12	CLA	G	829	1	-	12/39/115/115	-
12	CLA	H	2126	2	-	11/39/115/115	-
12	CLA	G	810	1,12	-	15/39/115/115	-
13	A1AGD	a	840	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	A	806	1	-	7/21/97/115	-
12	CLA	G	851	27	-	13/39/115/115	-
12	CLA	G	832	1	-	12/39/115/115	-
12	CLA	a	805	1	-	14/39/115/115	-
12	CLA	A	808	1	-	3/21/97/115	-
15	BCR	i	101	-	-	7/29/63/63	0/2/2/2
15	BCR	H	2146	-	-	17/29/63/63	0/2/2/2
12	CLA	H	2127	2	-	16/39/115/115	-
12	CLA	G	808	1	-	3/21/97/115	-
12	CLA	S	102	-	-	9/15/91/115	-
12	CLA	K	4002	9	-	9/15/91/115	-
16	LHG	B	2149	12	-	18/47/47/53	-
12	CLA	a	836	1	-	14/39/115/115	-
14	SF4	c	102	3	-	-	0/6/5/5
12	CLA	b	2121	-	-	10/27/103/115	-
12	CLA	j	103	8	-	10/15/91/115	-
17	LMG	B	2148	-	-	14/46/66/70	0/1/1/1
12	CLA	H	2130	-	-	2/15/91/115	-
12	CLA	F	204	-	-	5/15/91/115	-
12	CLA	a	812	1	-	13/39/115/115	-
20	ECH	B	2144	-	-	12/29/66/66	0/2/2/2
12	CLA	a	829	1	-	12/39/115/115	-
12	CLA	G	831	1	-	9/33/109/115	-
12	CLA	B	2135	-	-	4/15/91/115	-
12	CLA	l	201	1	-	15/39/115/115	-
12	CLA	H	2106	-	-	16/39/115/115	-
12	CLA	H	2152	16	-	5/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	837	1	-	11/39/115/115	-
25	DGD	l	209	-	-	21/44/64/95	0/1/1/2
16	LHG	m	103	-	-	24/48/48/53	-
12	CLA	b	2115	2	-	4/15/91/115	-
12	CLA	b	2106	-	-	16/39/115/115	-
12	CLA	A	805	1	-	14/39/115/115	-
15	BCR	J	104	-	-	9/29/63/63	0/2/2/2
25	DGD	U	209	-	-	21/44/64/95	0/1/1/2
12	CLA	H	2108	2	-	11/39/115/115	-
12	CLA	a	832	1	-	12/39/115/115	-
12	CLA	A	804	1	-	16/39/115/115	-
12	CLA	a	802	1	-	9/39/115/115	-
12	CLA	A	829	1	-	12/39/115/115	-
23	ZEX	B	2152	-	-	11/29/67/67	0/2/2/2
12	CLA	B	2120	2	-	16/39/115/115	-
12	CLA	b	2136	2	-	7/15/91/115	-
12	CLA	H	2121	-	-	10/27/103/115	-
12	CLA	b	2132	2	-	18/39/115/115	-
12	CLA	H	2114	-	-	18/39/115/115	-
12	CLA	H	2134	-	-	4/15/91/115	-
12	CLA	A	815	-	-	5/15/91/115	-
12	CLA	J	102	-	-	9/15/91/115	-
15	BCR	A	842	-	-	12/29/63/63	0/2/2/2
16	LHG	G	846	-	-	28/53/53/53	-
14	SF4	a	841	1,2	-	-	0/6/5/5
12	CLA	A	819	1	-	18/39/115/115	-
12	CLA	a	831	1	-	9/33/109/115	-
14	SF4	C	101	3	-	-	0/6/5/5
12	CLA	Q	201	27	-	21/39/115/115	-
17	LMG	A	849	-	-	14/26/46/70	0/1/1/1
12	CLA	B	2142	16	-	7/15/91/115	-
12	CLA	B	2133	2	-	18/39/115/115	-
15	BCR	j	101	-	-	13/29/63/63	0/2/2/2
12	CLA	G	816	1	-	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	813	1	-	14/39/115/115	-
22	EQ3	H	2150	-	-	14/29/68/68	0/2/2/2
12	CLA	A	831	1	-	9/33/109/115	-
12	CLA	B	2121	-	-	8/27/103/115	-
12	CLA	b	2123	2	-	12/27/103/115	-
12	CLA	A	809	1	-	10/21/97/115	-
12	CLA	B	2114	-	-	10/15/91/115	-
12	CLA	A	824	27	-	19/39/115/115	-
12	CLA	H	2137	2	-	7/39/115/115	-
12	CLA	b	2127	2	-	16/39/115/115	-
12	CLA	G	833	1	-	15/39/115/115	-
12	CLA	G	850	27	-	6/39/115/115	-
16	LHG	a	846	-	-	27/53/53/53	-
12	CLA	H	2118	2	-	7/21/97/115	-
12	CLA	B	2116	2	-	4/15/91/115	-
12	CLA	L	201	1	-	15/39/115/115	-
12	CLA	l	204	10	-	8/39/115/115	-
12	CLA	k	4002	9	-	9/15/91/115	-
12	CLA	B	2138	2	-	7/39/115/115	-
14	SF4	G	841	1,2	-	-	0/6/5/5
17	LMG	H	2147	-	-	14/46/66/70	0/1/1/1
15	BCR	G	843	-	-	15/29/63/63	0/2/2/2
12	CLA	a	818	1	-	11/39/115/115	-
12	CLA	A	816	1	-	4/27/103/115	-
20	ECH	m	101	-	-	10/29/66/66	0/2/2/2
15	BCR	S	101	-	-	13/29/63/63	0/2/2/2
12	CLA	H	2104	-	-	8/39/115/115	-
12	CLA	b	2120	-	-	8/27/103/115	-
12	CLA	H	2131	2	-	7/27/103/115	-
17	LMG	b	2147	-	-	14/46/66/70	0/1/1/1
15	BCR	B	2145	-	-	8/29/63/63	0/2/2/2
15	BCR	l	207	-	-	6/29/63/63	0/2/2/2
12	CLA	B	2140	27	-	10/39/115/115	-
12	CLA	b	2134	-	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	801	1	-	5/39/115/115	-
15	BCR	U	206	-	-	10/29/63/63	0/2/2/2
12	CLA	H	2109	-	-	13/39/115/115	-
12	CLA	H	2138	-	-	6/15/91/115	-
15	BCR	b	2145	-	-	7/29/63/63	0/2/2/2
15	BCR	F	202	-	-	13/29/63/63	0/2/2/2
12	CLA	H	2102	-	-	12/39/115/115	-
12	CLA	B	2137	2	-	7/15/91/115	-
23	ZEX	F	205	-	-	14/29/67/67	0/2/2/2
17	LMG	a	847	-	-	20/45/65/70	0/1/1/1
12	CLA	a	814	-	-	4/15/91/115	-
16	LHG	A	848	12	-	19/53/53/53	-
17	LMG	G	847	-	-	20/45/65/70	0/1/1/1
12	CLA	G	854	-	-	7/27/103/115	-
12	CLA	F	203	-	-	6/15/91/115	-
12	CLA	b	2128	2	-	12/39/115/115	-
12	CLA	A	821	1	-	9/33/109/115	-
12	CLA	A	803	1,12	-	2/27/103/115	-
15	BCR	T	4001	-	-	8/29/63/63	0/2/2/2
15	BCR	G	845	-	-	8/29/63/63	0/2/2/2
12	CLA	a	834	1	-	12/27/103/115	-
12	CLA	G	837	1	-	11/39/115/115	-
12	CLA	H	2110	2	-	14/39/115/115	-
12	CLA	A	850	27	-	6/39/115/115	-
14	SF4	A	841	1,2	-	-	0/6/5/5
12	CLA	H	2116	-	-	9/15/91/115	-
12	CLA	B	2102	27	-	14/39/115/115	-
15	BCR	H	2145	-	-	7/29/63/63	0/2/2/2
12	CLA	A	836	1	-	14/39/115/115	-
12	CLA	B	2129	2	-	12/39/115/115	-
14	SF4	C	102	3	-	-	0/6/5/5
13	A1AGD	H	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	B	2105	-	-	8/39/115/115	-
12	CLA	b	2141	16	-	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	801	1	-	5/39/115/115	-
12	CLA	H	2140	2	-	16/39/115/115	-
12	CLA	b	2107	2	-	16/39/115/115	-
12	CLA	B	2108	2	-	16/39/115/115	-
12	CLA	B	2126	27	-	4/21/97/115	-
12	CLA	G	817	1	-	17/33/109/115	-
12	CLA	G	835	1	-	13/39/115/115	-
15	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	G	825	27	-	7/33/109/115	-
12	CLA	B	2134	2	-	18/39/115/115	-
12	CLA	B	2104	2	-	17/39/115/115	-
12	CLA	A	832	1	-	12/39/115/115	-
12	CLA	G	812	1	-	13/39/115/115	-
12	CLA	A	839	1	-	10/39/115/115	-
23	ZEX	f	205	-	-	14/29/67/67	0/2/2/2
15	BCR	R	101	-	-	7/29/63/63	0/2/2/2
15	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
12	CLA	a	803	1,12	-	2/27/103/115	-
17	LMG	A	847	-	-	20/45/65/70	0/1/1/1
15	BCR	B	2147	-	-	17/29/63/63	0/2/2/2
12	CLA	B	2136	-	-	9/15/91/115	-
12	CLA	B	2141	2	-	16/39/115/115	-
12	CLA	a	813	1	-	14/39/115/115	-
23	ZEX	b	2151	-	-	11/29/67/67	0/2/2/2
16	LHG	b	2148	12	-	18/47/47/53	-
15	BCR	f	202	-	-	13/29/63/63	0/2/2/2
15	BCR	a	842	-	-	11/29/63/63	0/2/2/2
12	CLA	H	2105	2	-	9/39/115/115	-
12	CLA	a	839	1	-	10/39/115/115	-
24	SQD	U	208	-	-	15/40/60/69	0/1/1/1
12	CLA	G	826	1	-	15/39/115/115	-
16	LHG	M	102	-	-	24/48/48/53	-
12	CLA	b	2108	2	-	11/39/115/115	-
12	CLA	B	2111	2	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	EQ3	b	2150	-	-	14/29/68/68	0/2/2/2
12	CLA	A	822	-	-	8/21/97/115	-
16	LHG	V	103	-	-	24/48/48/53	-
12	CLA	G	820	27	-	7/39/115/115	-
12	CLA	B	2107	-	-	16/39/115/115	-
12	CLA	H	2115	2	-	4/15/91/115	-
12	CLA	B	2123	-	-	7/15/91/115	-
12	CLA	B	2113	2	-	8/39/115/115	-
12	CLA	A	812	1	-	13/39/115/115	-
13	A1AGD	B	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	A	811	-	-	8/15/91/115	-
12	CLA	H	2103	2	-	17/39/115/115	-
12	CLA	G	834	1	-	12/27/103/115	-
12	CLA	G	828	-	-	12/39/115/115	-
12	CLA	A	807	1	-	14/39/115/115	-
12	CLA	B	2139	-	-	6/15/91/115	-
12	CLA	H	2136	2	-	7/15/91/115	-
16	LHG	a	848	12	-	19/53/53/53	-
15	BCR	I	101	-	-	7/29/63/63	0/2/2/2
15	BCR	b	2144	-	-	8/29/63/63	0/2/2/2
12	CLA	G	830	1	-	9/27/103/115	-
12	CLA	B	2124	2	-	12/27/103/115	-
12	CLA	U	204	10	-	8/39/115/115	-
15	BCR	G	842	-	-	12/29/63/63	0/2/2/2
24	SQD	V	102	-	-	28/49/69/69	0/1/1/1
18	45D	a	852	-	-	8/29/69/69	0/2/2/2
12	CLA	B	2119	2	-	7/21/97/115	-
12	CLA	a	850	27	-	6/39/115/115	-
12	CLA	A	818	1	-	11/39/115/115	-
12	CLA	a	820	27	-	7/39/115/115	-
22	EQ3	B	2151	-	-	14/29/68/68	0/2/2/2
15	BCR	a	845	-	-	8/29/63/63	0/2/2/2
16	LHG	A	846	-	-	27/53/53/53	-
12	CLA	G	807	1	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	DGD	L	209	-	-	21/44/64/95	0/1/1/2
12	CLA	G	818	1	-	11/39/115/115	-
12	CLA	b	2111	2	-	14/39/115/115	-
12	CLA	a	808	1	-	3/21/97/115	-
12	CLA	l	203	10	-	12/39/115/115	-
12	CLA	H	2107	2	-	16/39/115/115	-
15	BCR	B	2146	-	-	7/29/63/63	0/2/2/2
12	CLA	a	828	-	-	12/39/115/115	-
12	CLA	G	823	1	-	10/33/109/115	-
12	CLA	H	2123	2	-	12/27/103/115	-
12	CLA	A	828	-	-	12/39/115/115	-
12	CLA	b	2119	2	-	16/39/115/115	-
12	CLA	B	2112	2	-	14/39/115/115	-
20	ECH	M	103	-	-	10/29/66/66	0/2/2/2
12	CLA	b	2113	-	-	10/15/91/115	-
12	CLA	B	2125	27	-	6/39/115/115	-
12	CLA	b	2137	2	-	7/39/115/115	-
12	CLA	f	204	-	-	5/15/91/115	-
12	CLA	a	830	1	-	9/27/103/115	-
12	CLA	L	205	27	-	6/39/115/115	-
12	CLA	b	2129	2	-	13/39/115/115	-
12	CLA	a	826	1	-	15/39/115/115	-
12	CLA	a	854	-	-	7/27/103/115	-
12	CLA	U	205	27	-	6/39/115/115	-
18	45D	A	852	-	-	8/29/69/69	0/2/2/2
12	CLA	b	2139	27	-	10/39/115/115	-
15	BCR	H	2142	-	-	6/29/63/63	0/2/2/2
12	CLA	b	2105	2	-	9/39/115/115	-
12	CLA	b	2101	27	-	14/39/115/115	-
12	CLA	H	2119	2	-	16/39/115/115	-
12	CLA	G	839	1	-	10/39/115/115	-
12	CLA	a	824	27	-	19/39/115/115	-
12	CLA	a	821	1	-	9/33/109/115	-
12	CLA	a	811	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	824	27	-	19/39/115/115	-
12	CLA	A	825	27	-	7/33/109/115	-
12	CLA	H	2120	-	-	8/27/103/115	-
15	BCR	A	844	-	-	8/29/63/63	0/2/2/2
12	CLA	a	817	1	-	17/33/109/115	-
12	CLA	a	807	1	-	14/39/115/115	-
12	CLA	B	2127	2	-	11/39/115/115	-
15	BCR	G	844	-	-	8/29/63/63	0/2/2/2
12	CLA	A	814	-	-	4/15/91/115	-
12	CLA	H	2113	-	-	10/15/91/115	-
17	LMG	G	849	-	-	14/26/46/70	0/1/1/1
12	CLA	G	806	1	-	7/21/97/115	-
12	CLA	b	2126	2	-	11/39/115/115	-
12	CLA	G	814	-	-	4/15/91/115	-
23	ZEX	H	2151	-	-	11/29/67/67	0/2/2/2
12	CLA	A	834	1	-	12/27/103/115	-
12	CLA	a	825	27	-	7/33/109/115	-
13	A1AGD	b	2153	-	2/2/9/11	8/23/43/43	0/1/1/1
15	BCR	b	2146	-	-	17/29/63/63	0/2/2/2
12	CLA	H	2112	2	-	8/39/115/115	-
16	LHG	G	848	12	-	18/53/53/53	-
20	ECH	V	101	-	-	10/29/66/66	0/2/2/2
12	CLA	G	822	-	-	8/21/97/115	-
12	CLA	b	2117	2	-	10/15/91/115	-
12	CLA	A	851	27	-	13/39/115/115	-
12	CLA	G	811	-	-	8/15/91/115	-
12	CLA	G	819	1	-	18/39/115/115	-
12	CLA	G	803	1,12	-	2/27/103/115	-
12	CLA	L	203	10	-	12/39/115/115	-
12	CLA	A	810	1,12	-	15/39/115/115	-
12	CLA	B	2103	-	-	12/39/115/115	-
15	BCR	S	104	-	-	9/29/63/63	0/2/2/2
12	CLA	U	201	1	-	15/39/115/115	-
12	CLA	b	2133	2	-	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	833	1	-	15/39/115/115	-
15	BCR	H	2144	-	-	8/29/63/63	0/2/2/2
12	CLA	b	2102	-	-	12/39/115/115	-
12	CLA	H	2125	27	-	4/21/97/115	-
15	BCR	b	2142	-	-	6/29/63/63	0/2/2/2
12	CLA	f	203	-	-	6/15/91/115	-
12	CLA	A	838	1	-	5/39/115/115	-
12	CLA	H	2117	2	-	10/15/91/115	-
12	CLA	B	2110	-	-	13/39/115/115	-
12	CLA	G	802	1	-	9/39/115/115	-
20	ECH	H	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	B	2128	2	-	16/39/115/115	-
12	CLA	b	2114	-	-	18/39/115/115	-
15	BCR	Q	202	-	-	13/29/63/63	0/2/2/2
15	BCR	a	843	-	-	15/29/63/63	0/2/2/2
12	CLA	B	2101	16	-	5/21/97/115	-
12	CLA	S	103	8	-	10/15/91/115	-
12	CLA	B	2115	-	-	18/39/115/115	-
12	CLA	a	823	1	-	10/33/109/115	-
12	CLA	a	806	1	-	7/21/97/115	-
12	CLA	U	203	10	-	12/39/115/115	-
12	CLA	b	2116	-	-	9/15/91/115	-
12	CLA	H	2135	-	-	9/15/91/115	-
14	SF4	N	101	3	-	-	0/6/5/5
12	CLA	G	813	1	-	14/39/115/115	-
12	CLA	G	838	1	-	5/39/115/115	-
15	BCR	L	206	-	-	10/29/63/63	0/2/2/2
15	BCR	U	207	-	-	6/29/63/63	0/2/2/2
12	CLA	L	204	10	-	8/39/115/115	-
12	CLA	A	833	1	-	15/39/115/115	-
12	CLA	A	802	1	-	9/39/115/115	-
12	CLA	A	830	1	-	9/27/103/115	-
12	CLA	B	2117	-	-	9/15/91/115	-
12	CLA	a	837	1	-	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	815	-	-	5/15/91/115	-
26	LMT	L	210	-	-	12/21/61/61	0/2/2/2
12	CLA	B	2118	2	-	10/15/91/115	-
12	CLA	H	2122	-	-	7/15/91/115	-
12	CLA	b	2131	2	-	7/27/103/115	-
15	BCR	l	206	-	-	10/29/63/63	0/2/2/2
12	CLA	H	2128	2	-	12/39/115/115	-
12	CLA	a	816	1	-	4/27/103/115	-
14	SF4	N	102	3	-	-	0/6/5/5
18	45D	G	852	-	-	8/29/69/69	0/2/2/2
12	CLA	Q	203	-	-	6/15/91/115	-
12	CLA	H	2101	27	-	14/39/115/115	-
15	BCR	A	845	-	-	8/29/63/63	0/2/2/2
15	BCR	J	101	-	-	13/29/63/63	0/2/2/2
12	CLA	B	2109	2	-	11/39/115/115	-
12	CLA	G	809	1	-	10/21/97/115	-
24	SQD	M	101	-	-	28/49/69/69	0/1/1/1
12	CLA	a	804	1	-	16/39/115/115	-
12	CLA	f	201	27	-	22/39/115/115	-
12	CLA	H	2132	2	-	18/39/115/115	-
12	CLA	G	827	-	-	6/39/115/115	-
16	LHG	H	2148	12	-	18/47/47/53	-
12	CLA	l	205	27	-	6/39/115/115	-
12	CLA	a	838	1	-	5/39/115/115	-
12	CLA	A	820	27	-	7/39/115/115	-
12	CLA	b	2118	2	-	7/21/97/115	-
12	CLA	B	2130	2	-	13/39/115/115	-
20	ECH	b	2143	-	-	12/29/66/66	0/2/2/2
12	CLA	b	2130	-	-	2/15/91/115	-
12	CLA	b	2103	2	-	17/39/115/115	-
26	LMT	l	210	-	-	12/21/61/61	0/2/2/2
17	LMG	a	849	-	-	14/26/46/70	0/1/1/1
12	CLA	a	815	-	-	5/15/91/115	-
12	CLA	A	826	1	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	854	-	-	7/27/103/115	-
12	CLA	F	201	27	-	22/39/115/115	-
23	ZEX	Q	205	-	-	14/29/67/67	0/2/2/2
12	CLA	b	2104	-	-	8/39/115/115	-
15	BCR	a	844	-	-	8/29/63/63	0/2/2/2
12	CLA	a	851	27	-	13/39/115/115	-
12	CLA	G	821	1	-	9/33/109/115	-
12	CLA	b	2122	-	-	7/15/91/115	-
12	CLA	H	2111	2	-	14/39/115/115	-
12	CLA	a	835	1	-	13/39/115/115	-
12	CLA	a	809	1	-	10/21/97/115	-
15	BCR	L	207	-	-	6/29/63/63	0/2/2/2
12	CLA	b	2152	16	-	5/21/97/115	-
13	A1AGD	A	840	-	2/2/9/11	8/23/43/43	0/1/1/1
12	CLA	a	827	-	-	6/39/115/115	-
12	CLA	A	823	1	-	10/33/109/115	-
12	CLA	A	817	1	-	17/33/109/115	-
13	A1AGD	G	840	-	2/2/9/11	8/23/43/43	0/1/1/1
14	SF4	c	101	3	-	-	0/6/5/5
12	CLA	j	102	-	-	9/15/91/115	-
12	CLA	b	2109	-	-	13/39/115/115	-
12	CLA	b	2138	-	-	6/15/91/115	-
12	CLA	A	835	1	-	13/39/115/115	-
12	CLA	A	827	-	-	6/39/115/115	-
12	CLA	a	822	-	-	8/21/97/115	-
26	LMT	U	210	-	-	12/21/61/61	0/2/2/2

The worst 5 of 2582 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	205	ZEX	C25-C26	17.19	1.60	1.34
23	Q	205	ZEX	C25-C26	17.19	1.60	1.34
23	f	205	ZEX	C25-C26	17.17	1.60	1.34
23	b	2151	ZEX	C25-C26	17.17	1.60	1.34
23	B	2152	ZEX	C25-C26	17.12	1.60	1.34

The worst 5 of 2630 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	205	ZEX	C39-C29-C28	-32.45	68.51	118.09
23	F	205	ZEX	C39-C29-C28	-32.45	68.52	118.09
23	f	205	ZEX	C39-C29-C28	-32.44	68.54	118.09
23	b	2151	ZEX	C39-C29-C28	-32.08	69.09	118.09
23	B	2152	ZEX	C39-C29-C28	-32.07	69.10	118.09

5 of 12 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	G	840	A1AGD	C14
13	G	840	A1AGD	C19
13	H	2153	A1AGD	C14
13	H	2153	A1AGD	C19
13	a	840	A1AGD	C14

5 of 4249 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	G	802	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C1A-C2A-CAA-CBA
12	G	804	CLA	C3A-C2A-CAA-CBA
12	G	804	CLA	CAD-CBD-CGD-O1D
12	G	804	CLA	CAD-CBD-CGD-O2D

There are no ring outliers.

344 monomers are involved in 685 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	819	CLA	3	0
12	Q	204	CLA	2	0
12	a	810	CLA	5	0
12	b	2124	CLA	3	0
12	G	805	CLA	4	0
12	b	2110	CLA	1	0
12	A	801	CLA	1	0
12	H	2133	CLA	1	0
12	B	2132	CLA	6	0
15	j	104	BCR	6	0
12	b	2135	CLA	1	0
12	H	2141	CLA	4	0
12	b	2140	CLA	3	0
12	H	2129	CLA	2	0
24	L	208	SQD	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	804	CLA	2	0
12	H	2139	CLA	3	0
24	l	208	SQD	4	0
12	H	2124	CLA	3	0
24	m	102	SQD	8	0
12	B	2131	CLA	3	0
12	b	2112	CLA	1	0
12	G	836	CLA	2	0
12	b	2125	CLA	2	0
12	B	2106	CLA	2	0
15	B	2143	BCR	5	0
15	A	843	BCR	2	0
12	G	829	CLA	3	0
12	H	2126	CLA	4	0
12	G	810	CLA	3	0
13	a	840	A1AGD	1	0
12	A	806	CLA	1	0
12	G	851	CLA	4	0
12	G	832	CLA	1	0
12	a	805	CLA	3	0
12	A	808	CLA	1	0
15	i	101	BCR	1	0
15	H	2146	BCR	2	0
12	H	2127	CLA	3	0
12	G	808	CLA	1	0
12	S	102	CLA	1	0
16	B	2149	LHG	4	0
12	a	836	CLA	1	0
12	H	2130	CLA	3	0
12	F	204	CLA	1	0
12	a	812	CLA	6	0
20	B	2144	ECH	7	0
12	a	829	CLA	2	0
12	G	831	CLA	1	0
12	B	2135	CLA	3	0
12	l	201	CLA	2	0
12	H	2106	CLA	2	0
12	H	2152	CLA	1	0
12	A	837	CLA	1	0
25	l	209	DGD	3	0
16	m	103	LHG	2	0
12	b	2115	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	b	2106	CLA	2	0
12	A	805	CLA	3	0
15	J	104	BCR	6	0
25	U	209	DGD	3	0
12	H	2108	CLA	4	0
12	A	804	CLA	2	0
12	a	802	CLA	2	0
12	A	829	CLA	3	0
23	B	2152	ZEX	2	0
12	B	2120	CLA	4	0
12	b	2136	CLA	2	0
12	b	2132	CLA	2	0
12	H	2114	CLA	2	0
12	H	2134	CLA	3	0
12	J	102	CLA	1	0
15	A	842	BCR	1	0
16	G	846	LHG	2	0
12	A	819	CLA	3	0
12	Q	201	CLA	3	0
17	A	849	LMG	1	0
12	B	2142	CLA	4	0
12	B	2133	CLA	2	0
15	j	101	BCR	4	0
12	G	816	CLA	1	0
12	A	831	CLA	1	0
12	B	2121	CLA	3	0
12	b	2123	CLA	1	0
12	B	2114	CLA	1	0
12	A	824	CLA	2	0
12	H	2137	CLA	3	0
12	b	2127	CLA	3	0
12	G	833	CLA	4	0
16	a	846	LHG	2	0
12	H	2118	CLA	3	0
12	B	2116	CLA	1	0
12	L	201	CLA	2	0
12	l	204	CLA	1	0
12	B	2138	CLA	3	0
15	G	843	BCR	3	0
12	a	818	CLA	5	0
12	A	816	CLA	2	0
20	m	101	ECH	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	S	101	BCR	3	0
12	H	2104	CLA	3	0
12	b	2120	CLA	3	0
12	H	2131	CLA	5	0
15	l	207	BCR	4	0
12	B	2140	CLA	3	0
12	b	2134	CLA	3	0
12	G	801	CLA	1	0
15	U	206	BCR	2	0
12	H	2109	CLA	1	0
12	H	2138	CLA	5	0
15	b	2145	BCR	3	0
15	F	202	BCR	2	0
12	H	2102	CLA	1	0
12	B	2137	CLA	2	0
23	F	205	ZEX	2	0
17	a	847	LMG	5	0
16	A	848	LHG	6	0
17	G	847	LMG	5	0
12	G	854	CLA	3	0
12	F	203	CLA	1	0
12	b	2128	CLA	6	0
12	A	821	CLA	1	0
12	A	803	CLA	3	0
12	a	834	CLA	2	0
15	G	845	BCR	4	0
12	G	837	CLA	1	0
15	T	4001	BCR	2	0
12	H	2116	CLA	2	0
12	B	2102	CLA	2	0
15	H	2145	BCR	4	0
12	A	836	CLA	1	0
12	B	2129	CLA	7	0
13	H	2153	A1AGD	2	0
12	B	2105	CLA	3	0
12	b	2141	CLA	4	0
12	a	801	CLA	1	0
12	H	2140	CLA	2	0
12	b	2107	CLA	3	0
12	B	2108	CLA	3	0
12	B	2126	CLA	1	0
12	G	817	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	835	CLA	3	0
15	K	4001	BCR	2	0
12	G	825	CLA	3	0
12	B	2134	CLA	2	0
12	A	832	CLA	1	0
12	G	812	CLA	5	0
12	A	839	CLA	4	0
23	f	205	ZEX	2	0
15	R	101	BCR	2	0
15	k	4001	BCR	2	0
12	a	803	CLA	4	0
17	A	847	LMG	5	0
15	B	2147	BCR	2	0
12	B	2136	CLA	2	0
12	B	2141	CLA	2	0
23	b	2151	ZEX	2	0
16	b	2148	LHG	4	0
15	f	202	BCR	2	0
15	a	842	BCR	2	0
12	H	2105	CLA	2	0
12	a	839	CLA	3	0
24	U	208	SQD	4	0
12	G	826	CLA	3	0
16	M	102	LHG	2	0
12	b	2108	CLA	4	0
12	B	2111	CLA	1	0
16	V	103	LHG	3	0
12	G	820	CLA	5	0
12	B	2107	CLA	2	0
12	H	2115	CLA	1	0
12	B	2123	CLA	1	0
12	B	2113	CLA	1	0
12	A	812	CLA	6	0
13	B	2153	A1AGD	2	0
12	A	811	CLA	3	0
12	G	834	CLA	2	0
12	G	828	CLA	2	0
12	A	807	CLA	8	0
12	B	2139	CLA	5	0
12	H	2136	CLA	2	0
16	a	848	LHG	6	0
15	I	101	BCR	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	b	2144	BCR	1	0
12	G	830	CLA	3	0
12	B	2124	CLA	1	0
12	U	204	CLA	1	0
15	G	842	BCR	1	0
24	V	102	SQD	8	0
18	a	852	45D	1	0
12	B	2119	CLA	2	0
12	A	818	CLA	5	0
12	a	820	CLA	4	0
15	a	845	BCR	3	0
16	A	846	LHG	2	0
12	G	807	CLA	8	0
25	L	209	DGD	3	0
12	G	818	CLA	3	0
12	b	2111	CLA	2	0
12	a	808	CLA	1	0
12	l	203	CLA	3	0
12	H	2107	CLA	3	0
15	B	2146	BCR	3	0
12	a	828	CLA	2	0
12	G	823	CLA	5	0
12	H	2123	CLA	2	0
12	A	828	CLA	2	0
12	b	2119	CLA	5	0
12	B	2112	CLA	2	0
20	M	103	ECH	1	0
12	b	2113	CLA	1	0
12	B	2125	CLA	3	0
12	b	2137	CLA	3	0
12	f	204	CLA	1	0
12	a	830	CLA	3	0
12	L	205	CLA	5	0
12	b	2129	CLA	2	0
12	a	826	CLA	3	0
12	a	854	CLA	3	0
12	U	205	CLA	6	0
18	A	852	45D	1	0
12	b	2139	CLA	4	0
15	H	2142	BCR	4	0
12	b	2105	CLA	2	0
12	b	2101	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	H	2119	CLA	4	0
12	G	839	CLA	4	0
12	a	824	CLA	1	0
12	a	821	CLA	2	0
12	a	811	CLA	4	0
12	G	824	CLA	2	0
12	A	825	CLA	3	0
12	H	2120	CLA	3	0
15	A	844	BCR	2	0
12	a	817	CLA	4	0
12	a	807	CLA	7	0
12	B	2127	CLA	4	0
15	G	844	BCR	3	0
12	H	2113	CLA	1	0
17	G	849	LMG	2	0
12	G	806	CLA	1	0
12	b	2126	CLA	4	0
23	H	2151	ZEX	3	0
12	A	834	CLA	2	0
12	a	825	CLA	3	0
13	b	2153	A1AGD	2	0
15	b	2146	BCR	1	0
12	H	2112	CLA	2	0
16	G	848	LHG	6	0
20	V	101	ECH	2	0
12	b	2117	CLA	2	0
12	A	851	CLA	3	0
12	G	811	CLA	4	0
12	G	819	CLA	3	0
12	G	803	CLA	4	0
12	L	203	CLA	4	0
12	A	810	CLA	2	0
12	B	2103	CLA	1	0
15	S	104	BCR	6	0
12	U	201	CLA	2	0
12	b	2133	CLA	1	0
12	a	833	CLA	4	0
15	H	2144	BCR	1	0
12	b	2102	CLA	1	0
12	H	2125	CLA	2	0
15	b	2142	BCR	3	0
12	f	203	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	838	CLA	2	0
12	H	2117	CLA	2	0
12	B	2110	CLA	1	0
12	G	802	CLA	2	0
20	H	2143	ECH	6	0
12	B	2128	CLA	3	0
12	b	2114	CLA	2	0
15	Q	202	BCR	2	0
15	a	843	BCR	3	0
12	B	2101	CLA	1	0
12	B	2115	CLA	2	0
12	a	823	CLA	4	0
12	a	806	CLA	1	0
12	U	203	CLA	3	0
12	b	2116	CLA	2	0
12	H	2135	CLA	2	0
12	G	838	CLA	1	0
15	L	206	BCR	2	0
15	U	207	BCR	3	0
12	L	204	CLA	1	0
12	A	833	CLA	4	0
12	A	802	CLA	2	0
12	A	830	CLA	3	0
12	B	2117	CLA	1	0
12	a	837	CLA	2	0
26	L	210	LMT	3	0
12	B	2118	CLA	2	0
12	H	2122	CLA	1	0
12	b	2131	CLA	5	0
15	l	206	BCR	3	0
12	H	2128	CLA	7	0
12	a	816	CLA	1	0
18	G	852	45D	1	0
12	Q	203	CLA	1	0
12	H	2101	CLA	2	0
15	A	845	BCR	3	0
15	J	101	BCR	3	0
12	B	2109	CLA	3	0
24	M	101	SQD	9	0
12	a	804	CLA	4	0
12	f	201	CLA	3	0
12	H	2132	CLA	2	0

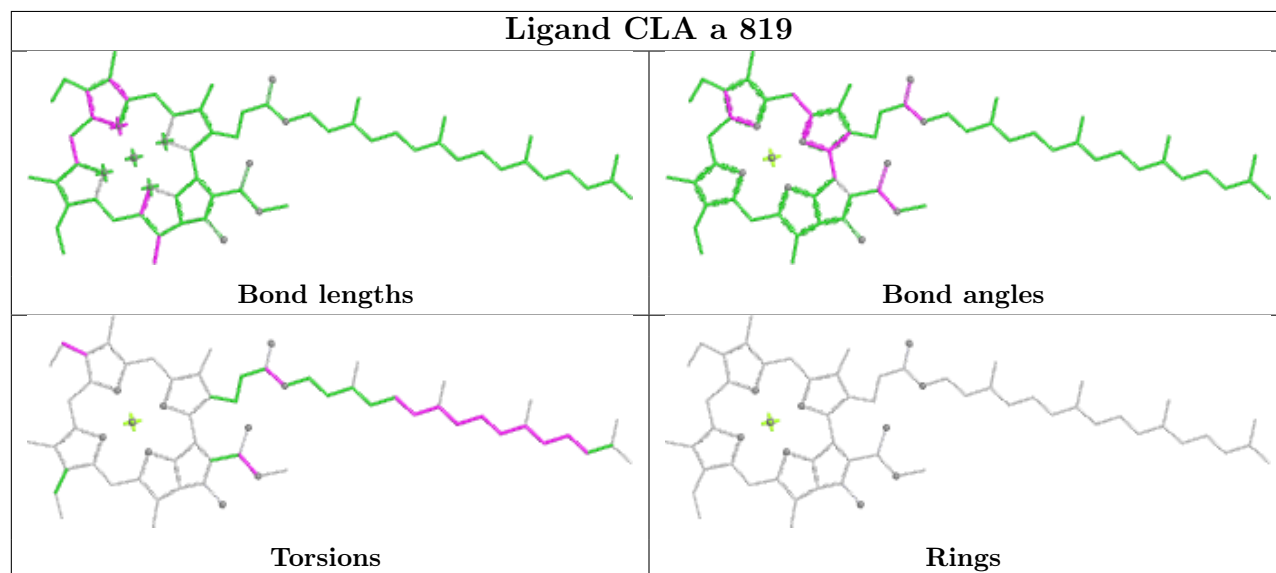
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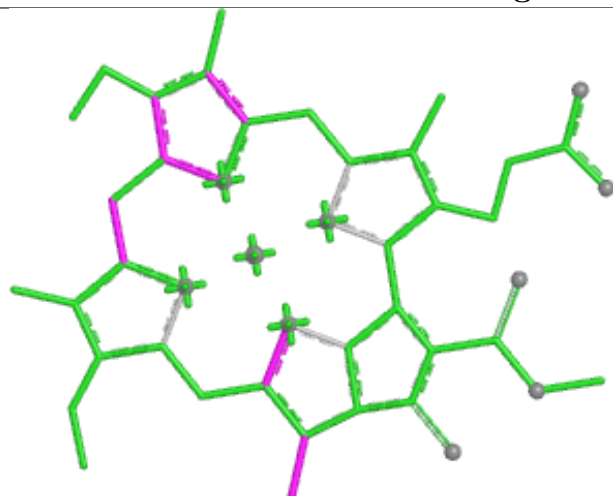
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	827	CLA	2	0
16	H	2148	LHG	4	0
12	l	205	CLA	6	0
12	a	838	CLA	2	0
12	A	820	CLA	5	0
12	b	2118	CLA	3	0
12	B	2130	CLA	1	0
20	b	2143	ECH	7	0
12	b	2130	CLA	3	0
26	l	210	LMT	3	0
17	a	849	LMG	1	0
12	A	826	CLA	3	0
12	A	854	CLA	3	0
12	F	201	CLA	3	0
23	Q	205	ZEX	2	0
12	b	2104	CLA	3	0
15	a	844	BCR	3	0
12	a	851	CLA	3	0
12	G	821	CLA	2	0
12	b	2122	CLA	1	0
12	H	2111	CLA	2	0
12	a	835	CLA	3	0
15	L	207	BCR	5	0
12	b	2152	CLA	1	0
12	a	827	CLA	3	0
13	A	840	A1AGD	1	0
12	A	823	CLA	5	0
12	A	817	CLA	4	0
13	G	840	A1AGD	1	0
12	j	102	CLA	1	0
12	b	2109	CLA	1	0
12	b	2138	CLA	5	0
12	A	835	CLA	3	0
12	A	827	CLA	3	0
26	U	210	LMT	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

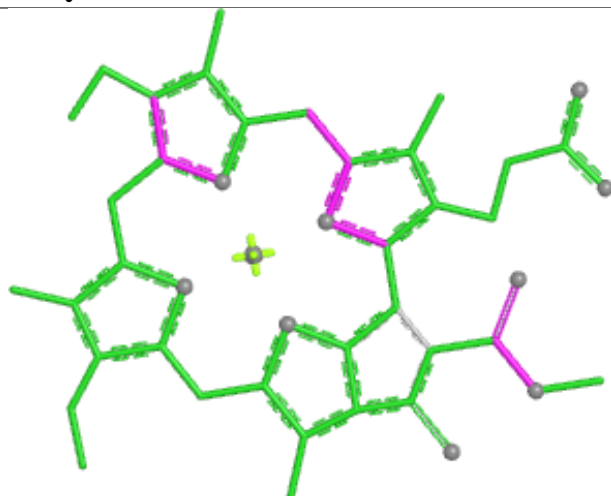
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



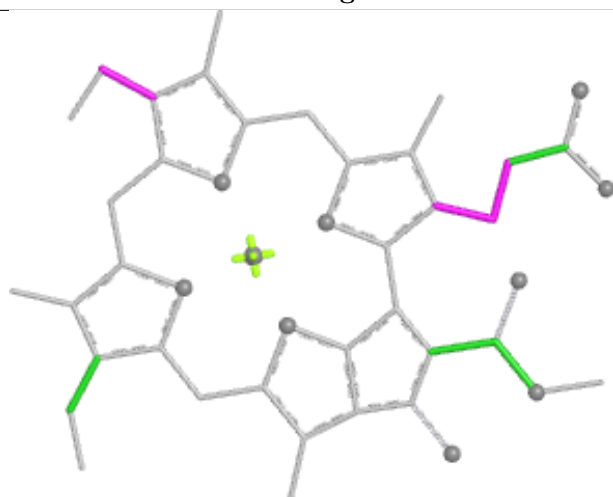
Ligand CLA Q 204



Bond lengths



Bond angles

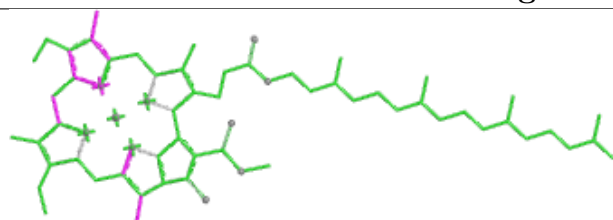


Torsions

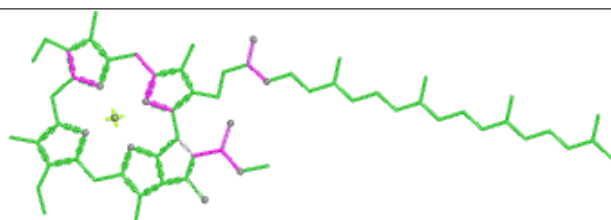


Rings

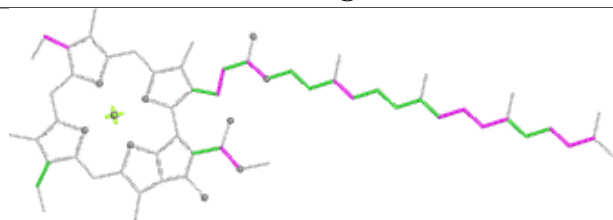
Ligand CLA a 810



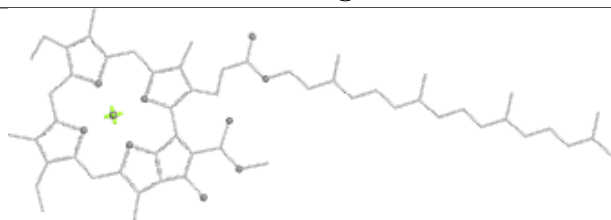
Bond lengths



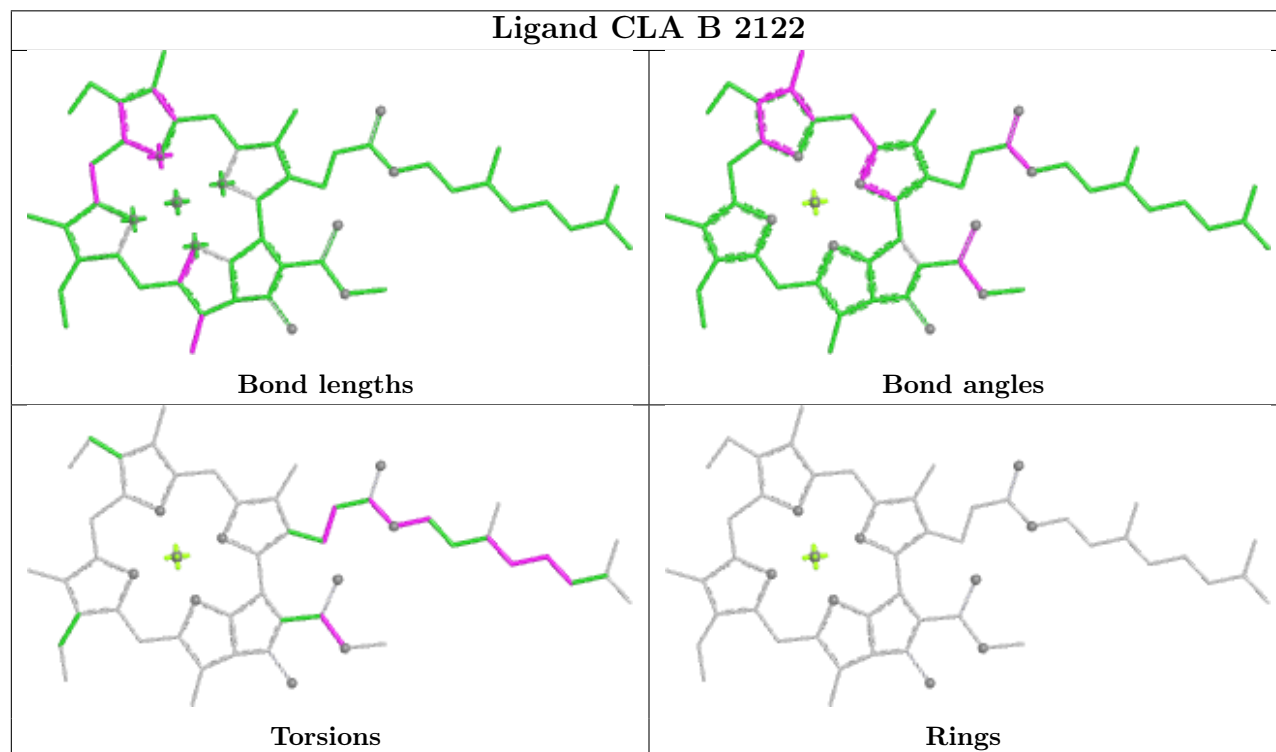
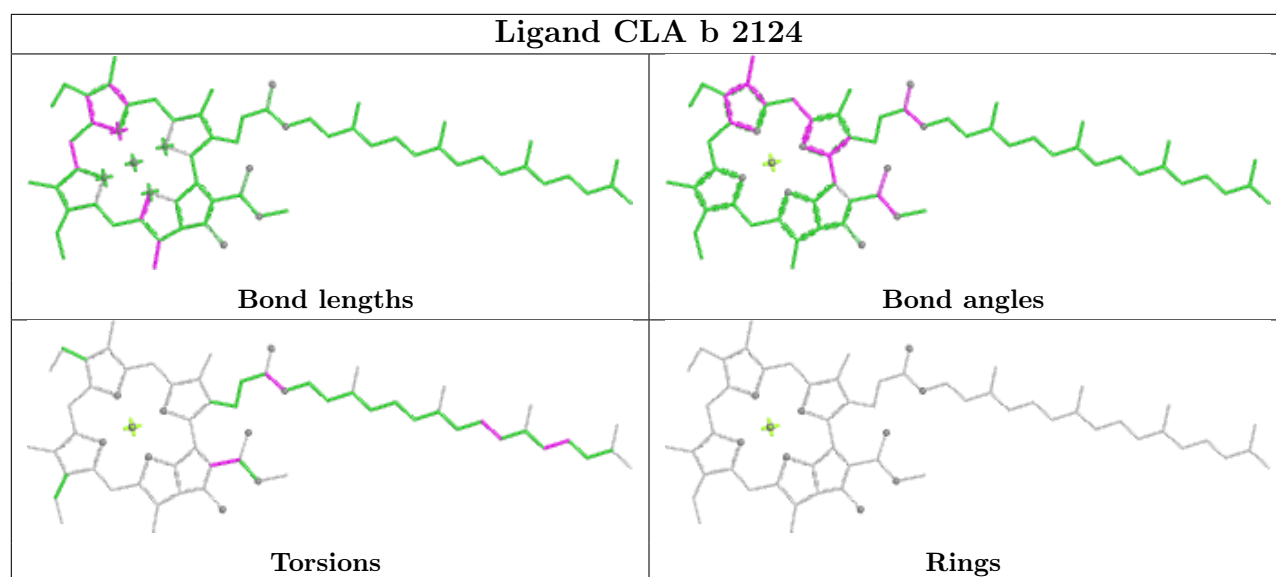
Bond angles

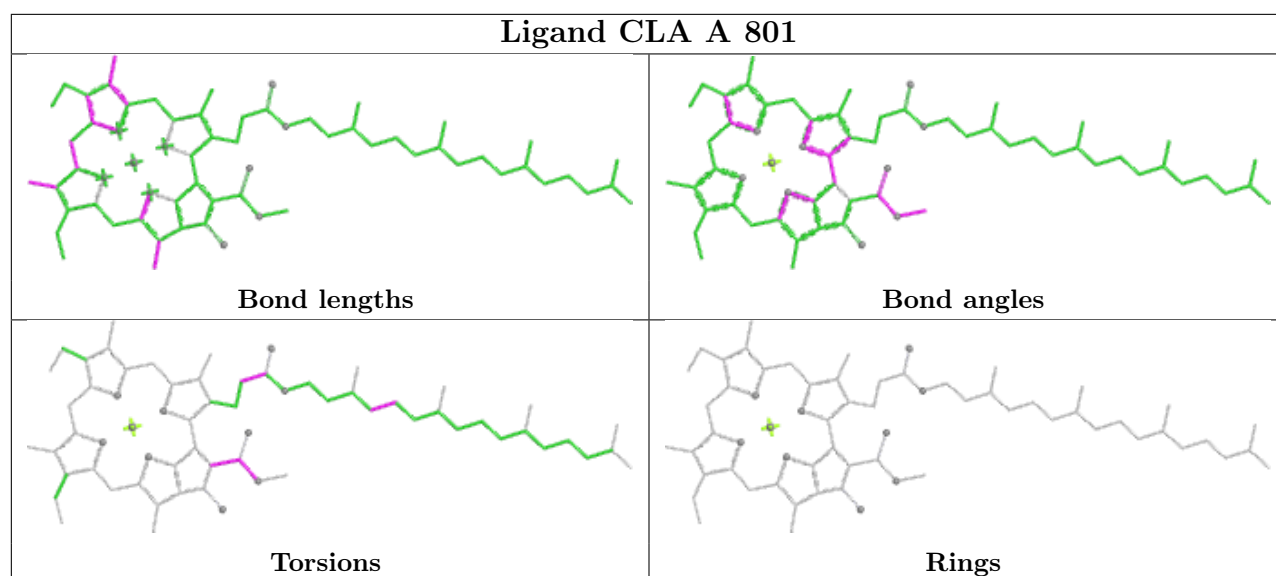
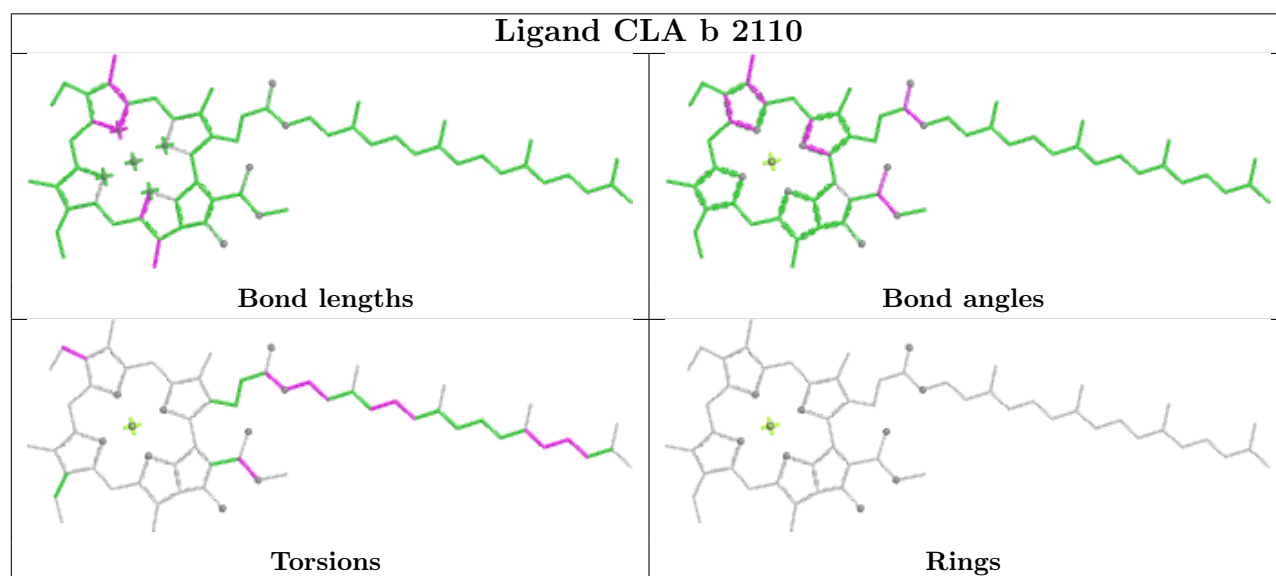
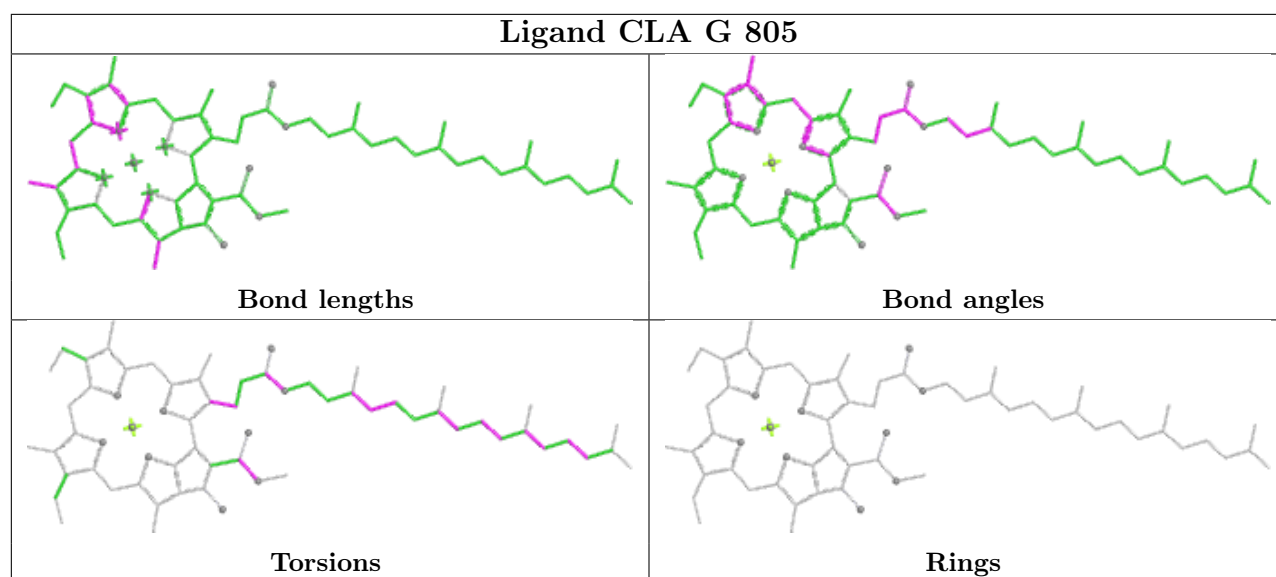


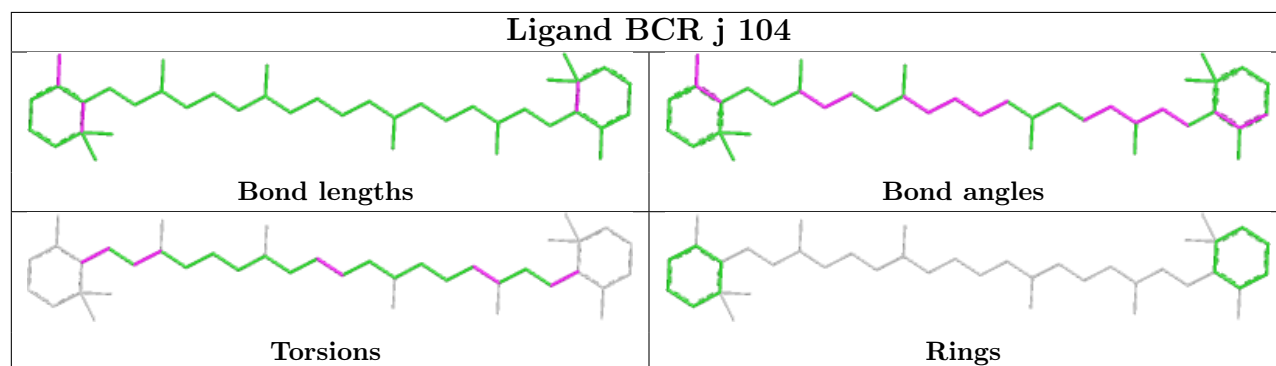
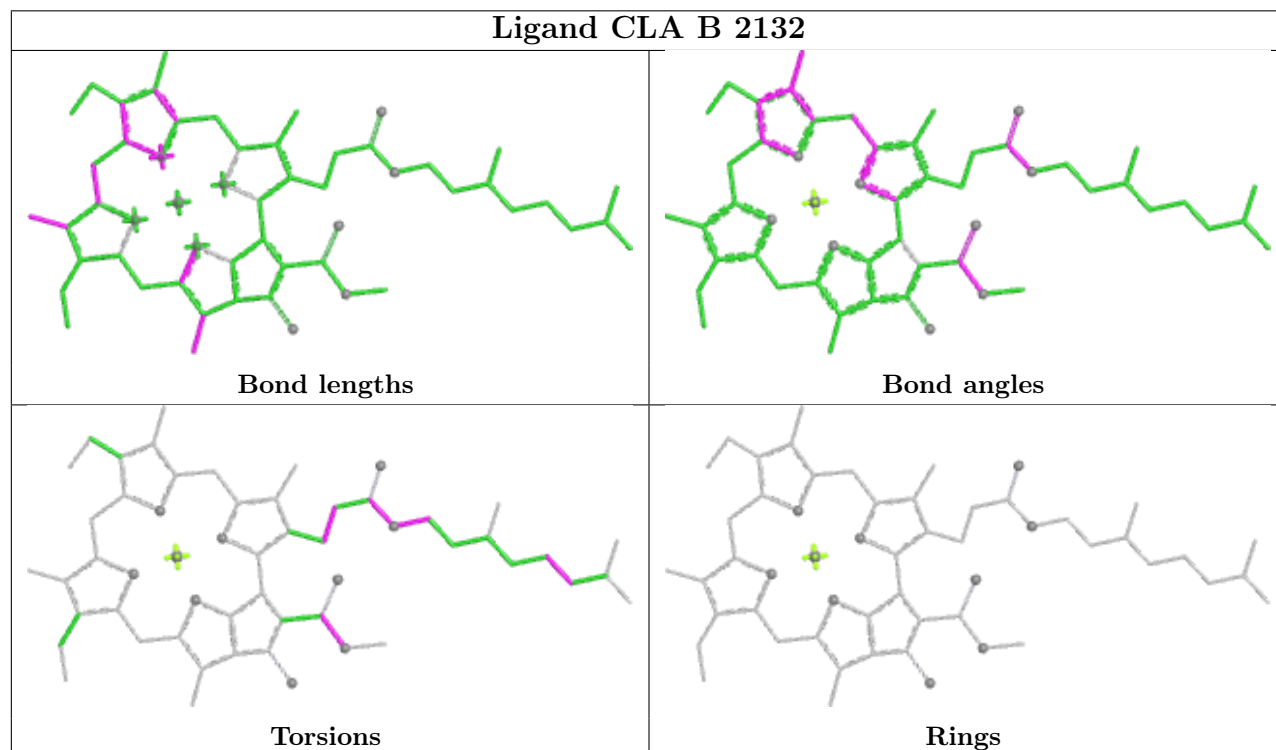
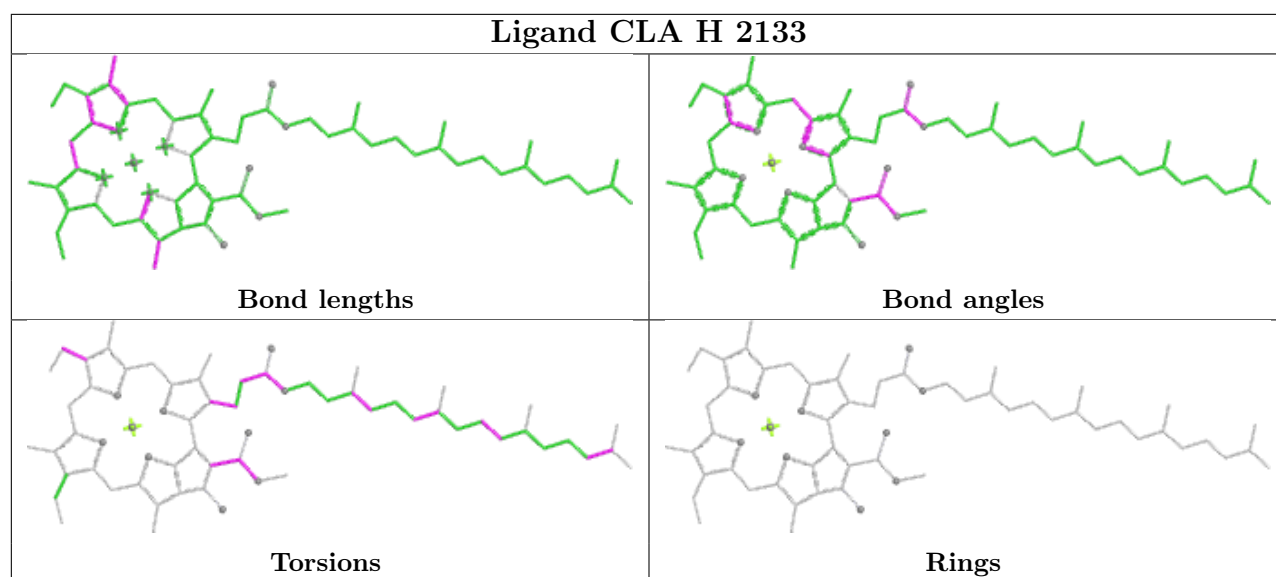
Torsions

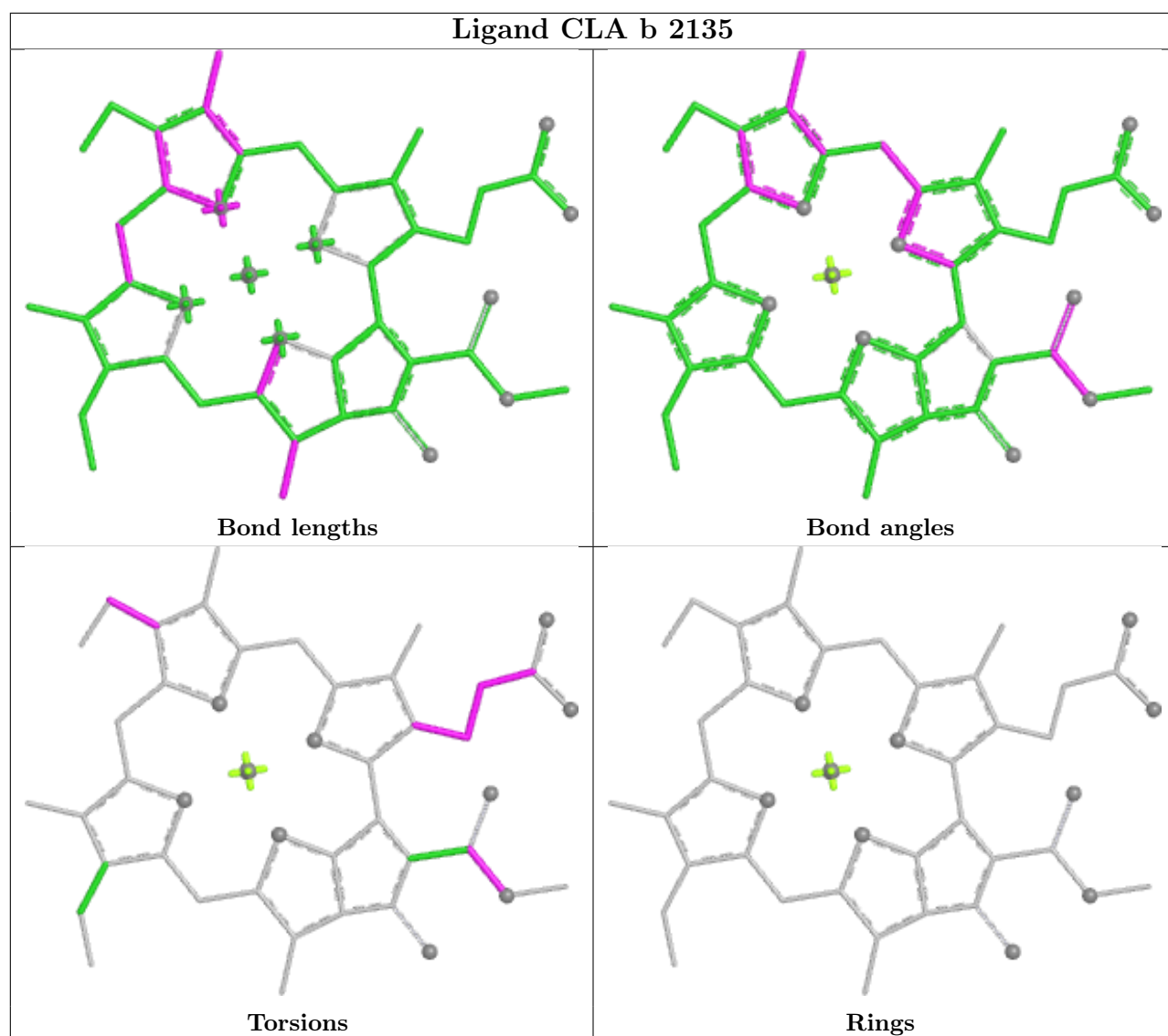


Rings

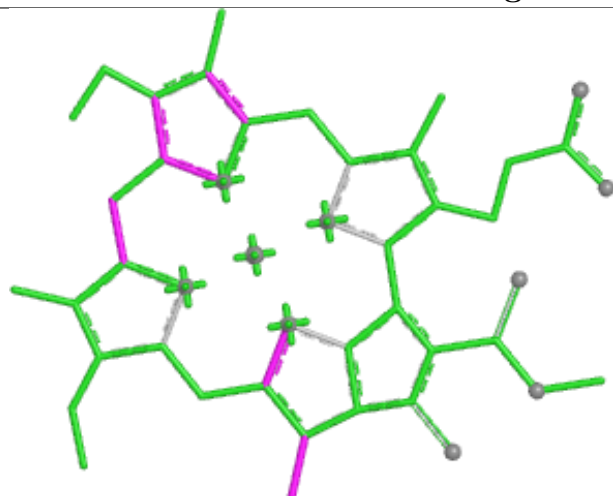




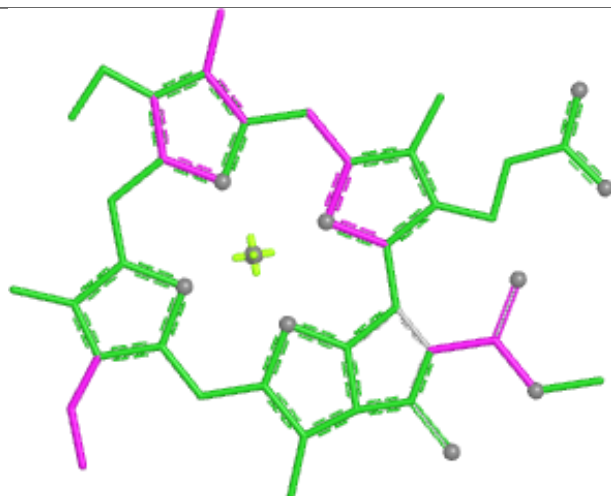




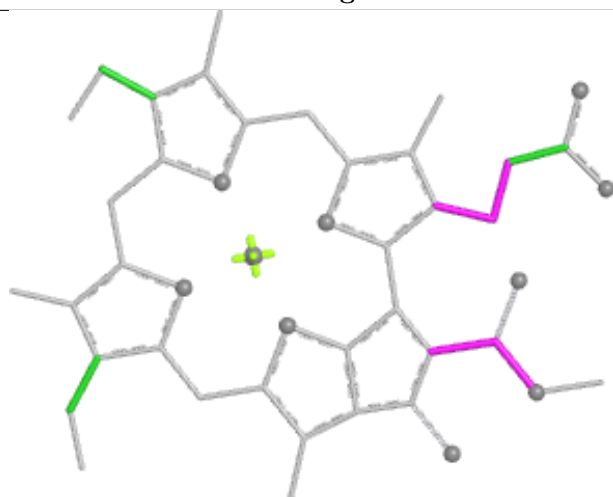
Ligand CLA H 2141



Bond lengths



Bond angles

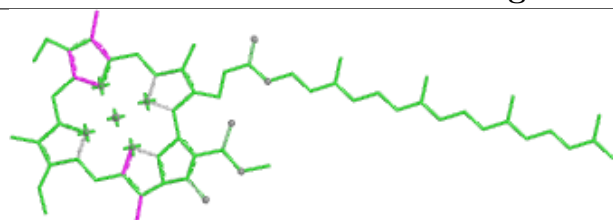


Torsions

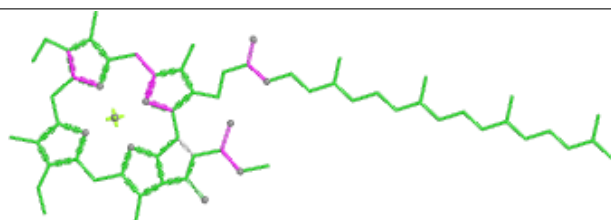


Rings

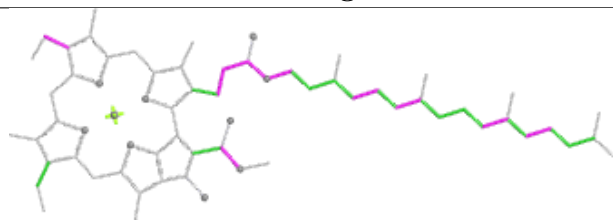
Ligand CLA b 2140



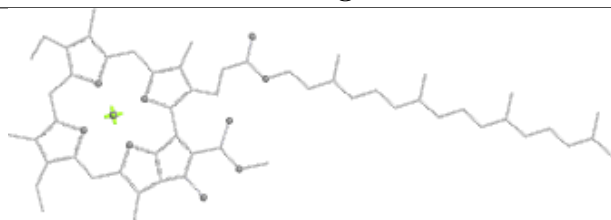
Bond lengths



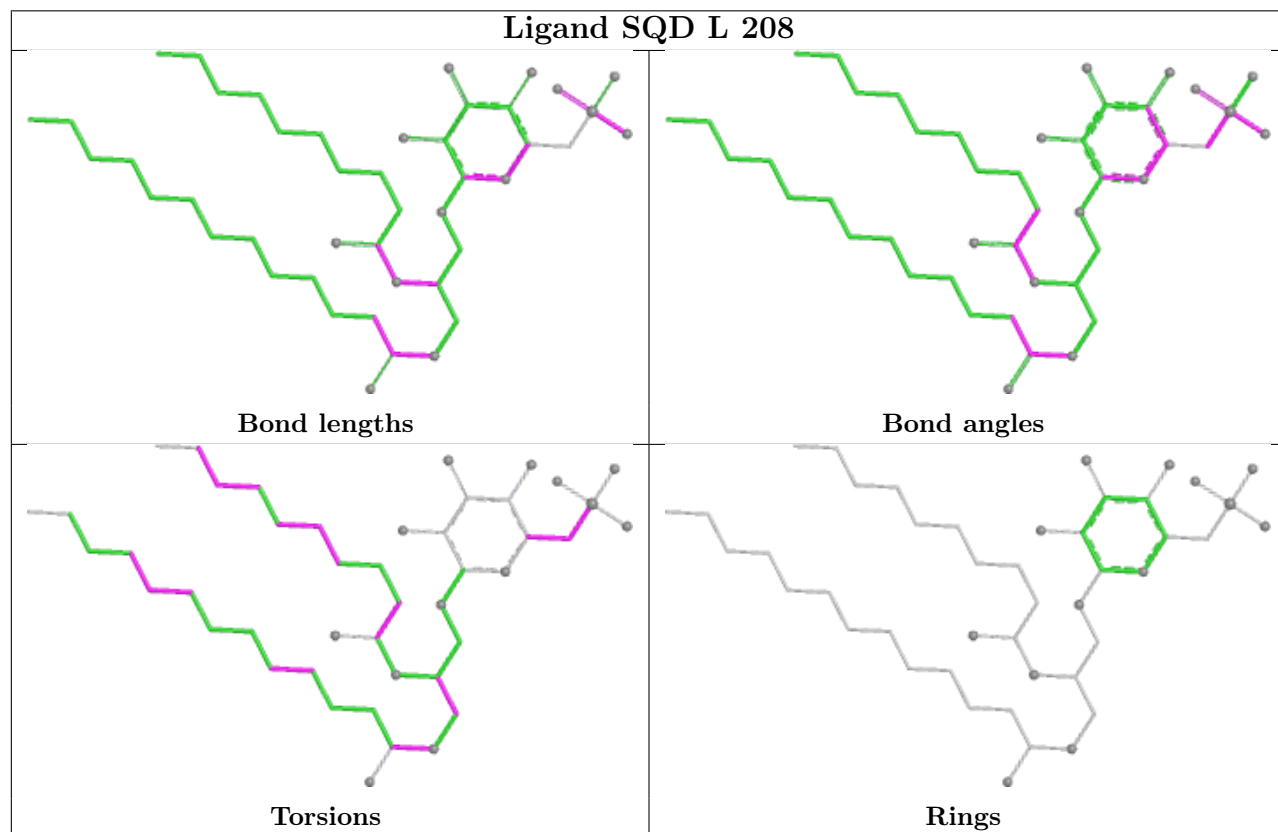
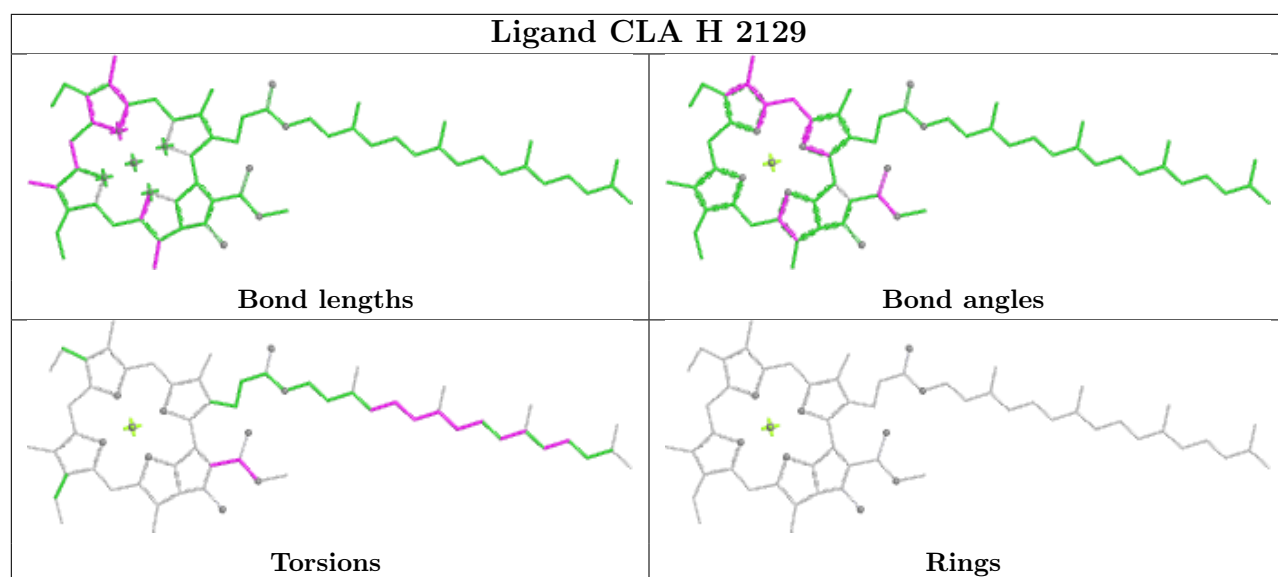
Bond angles

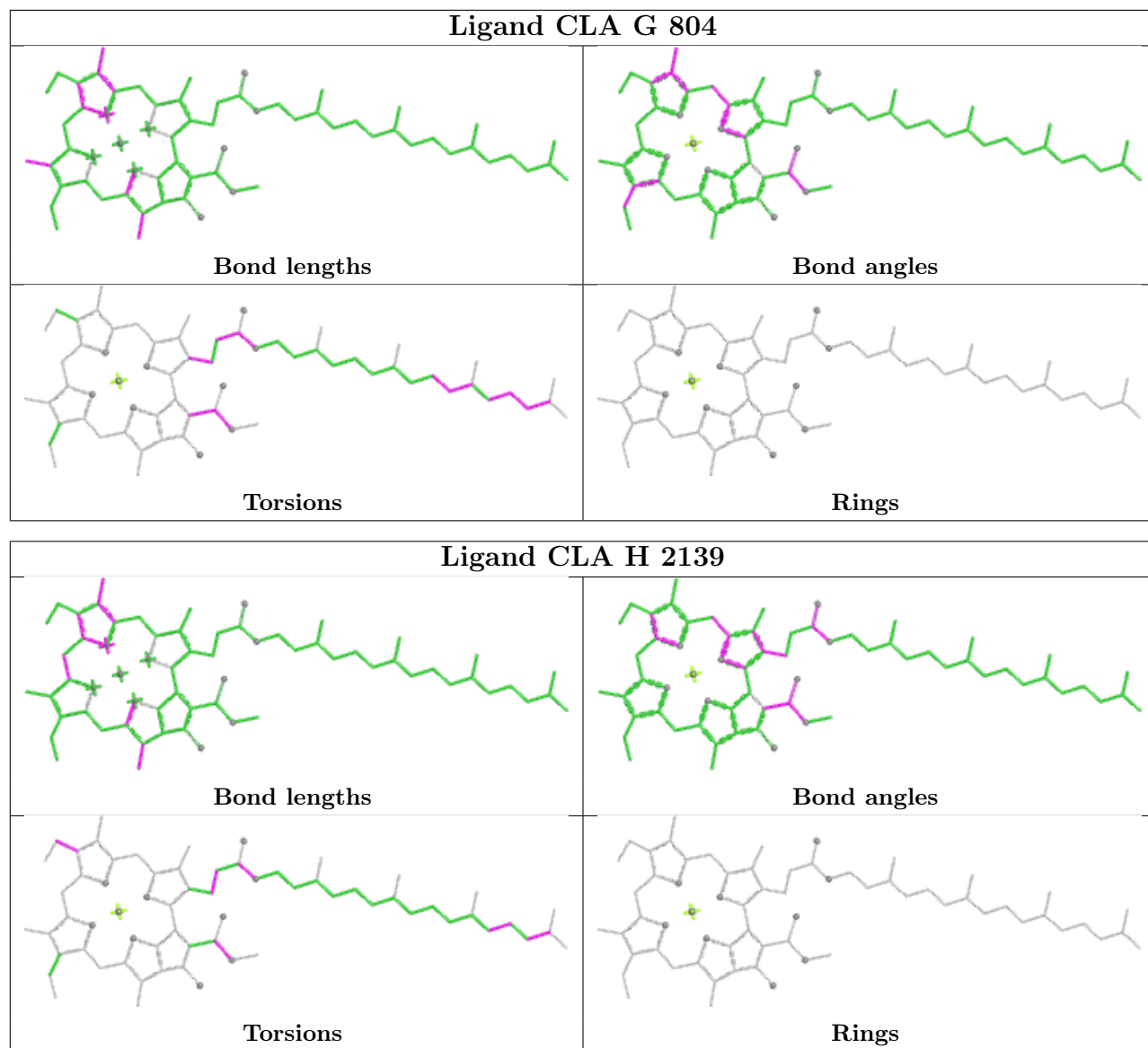


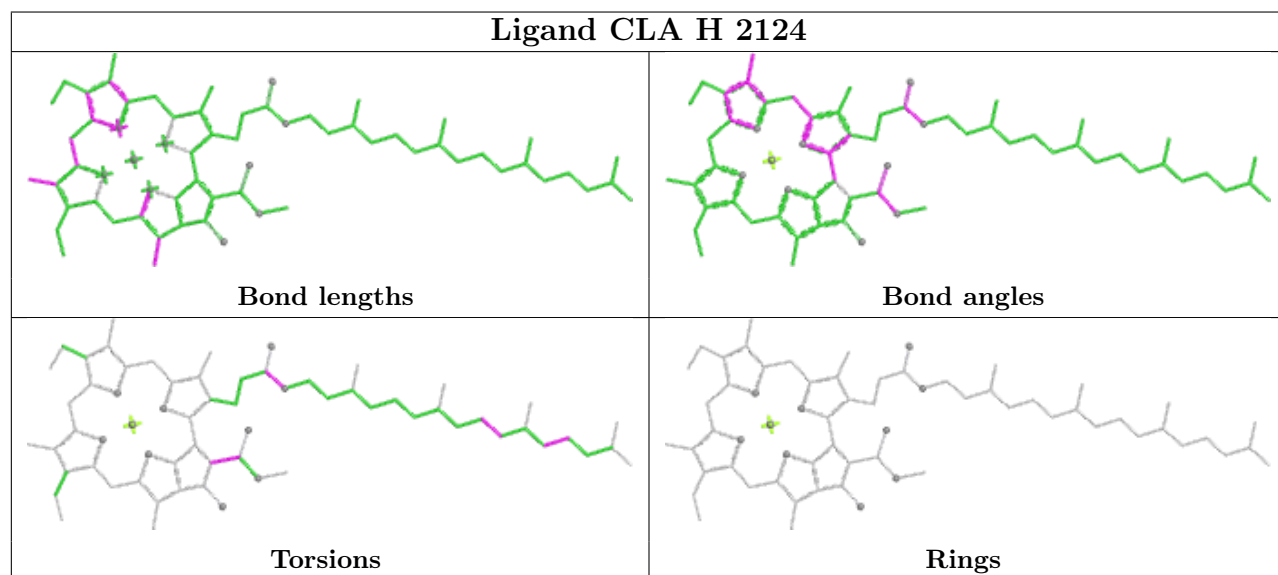
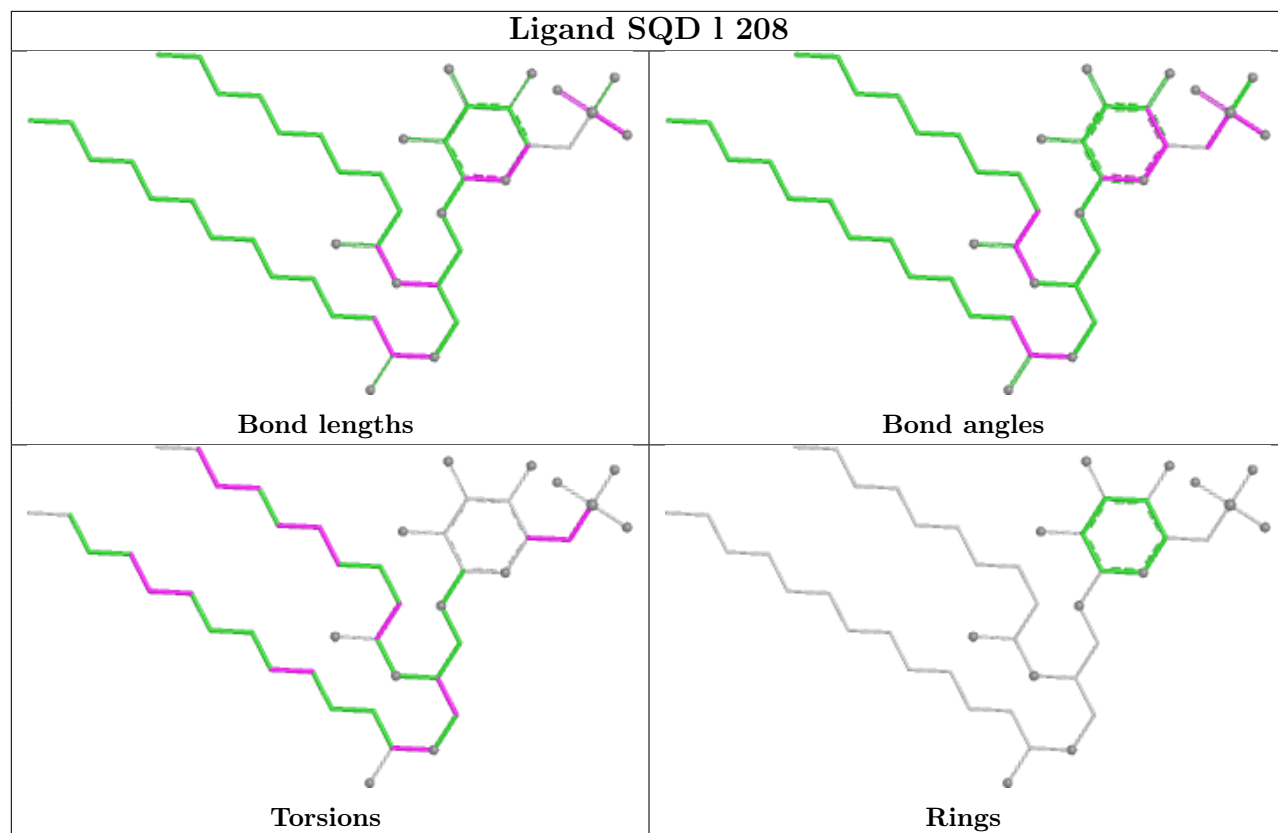
Torsions

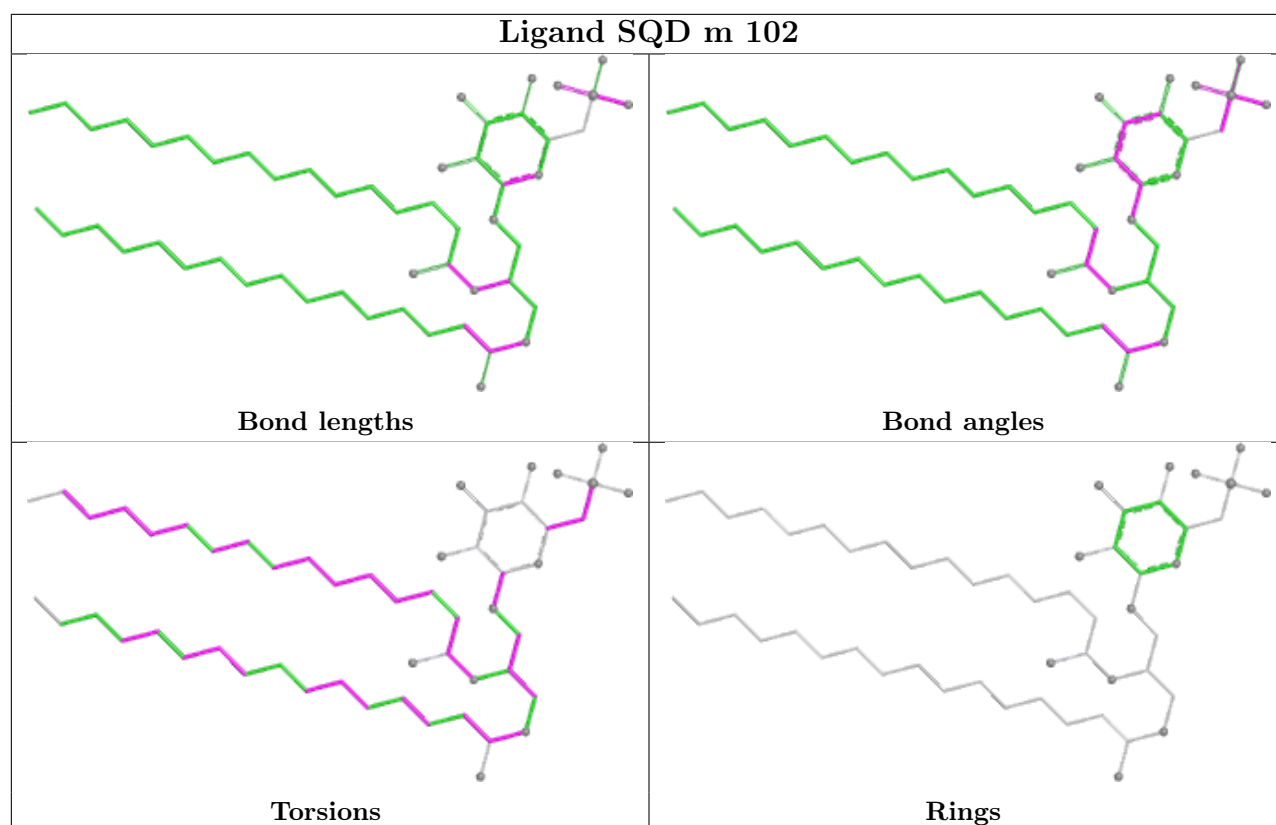


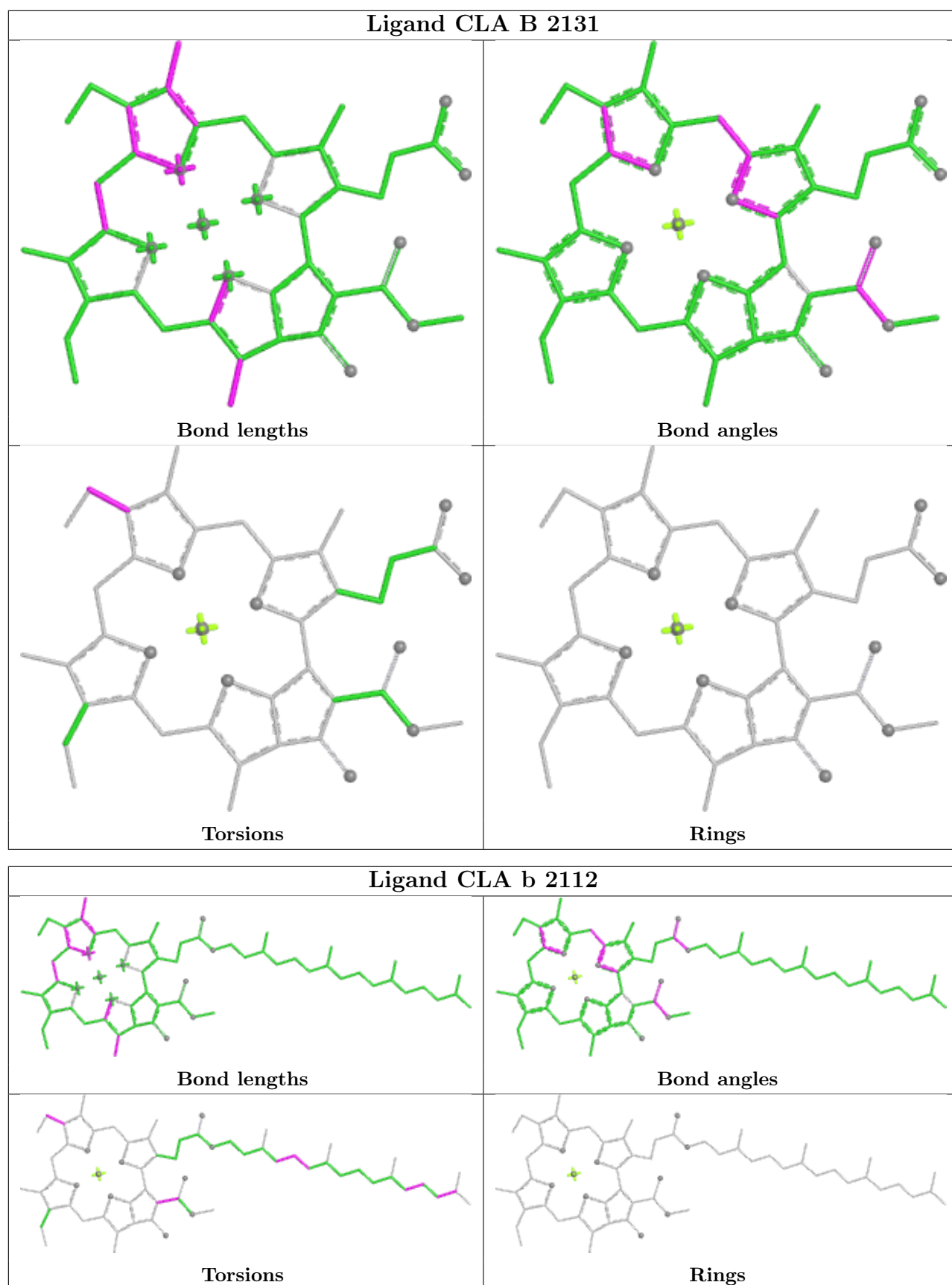
Rings



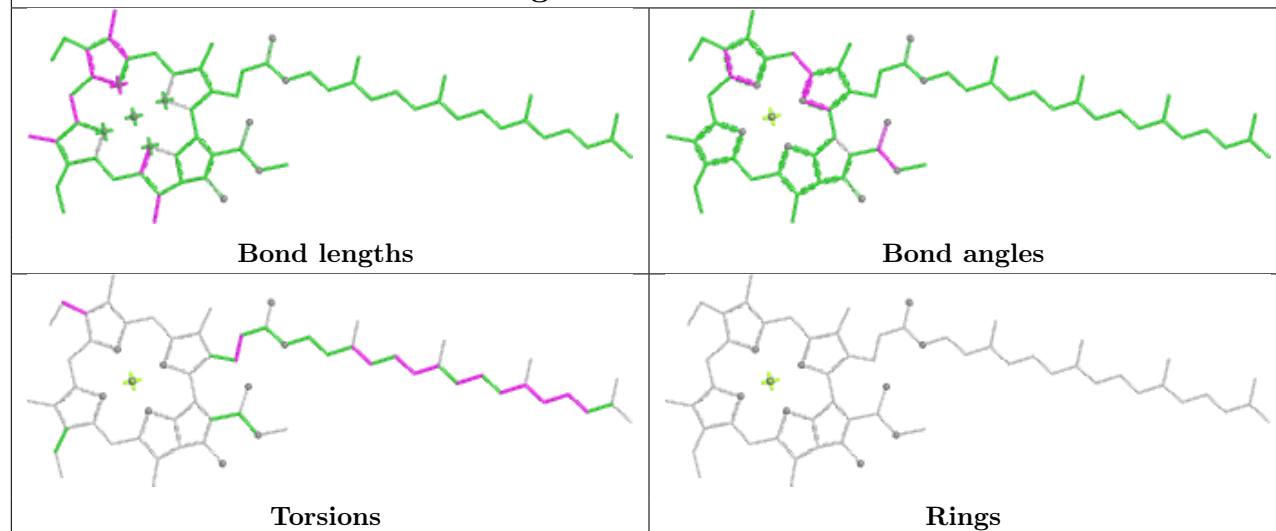




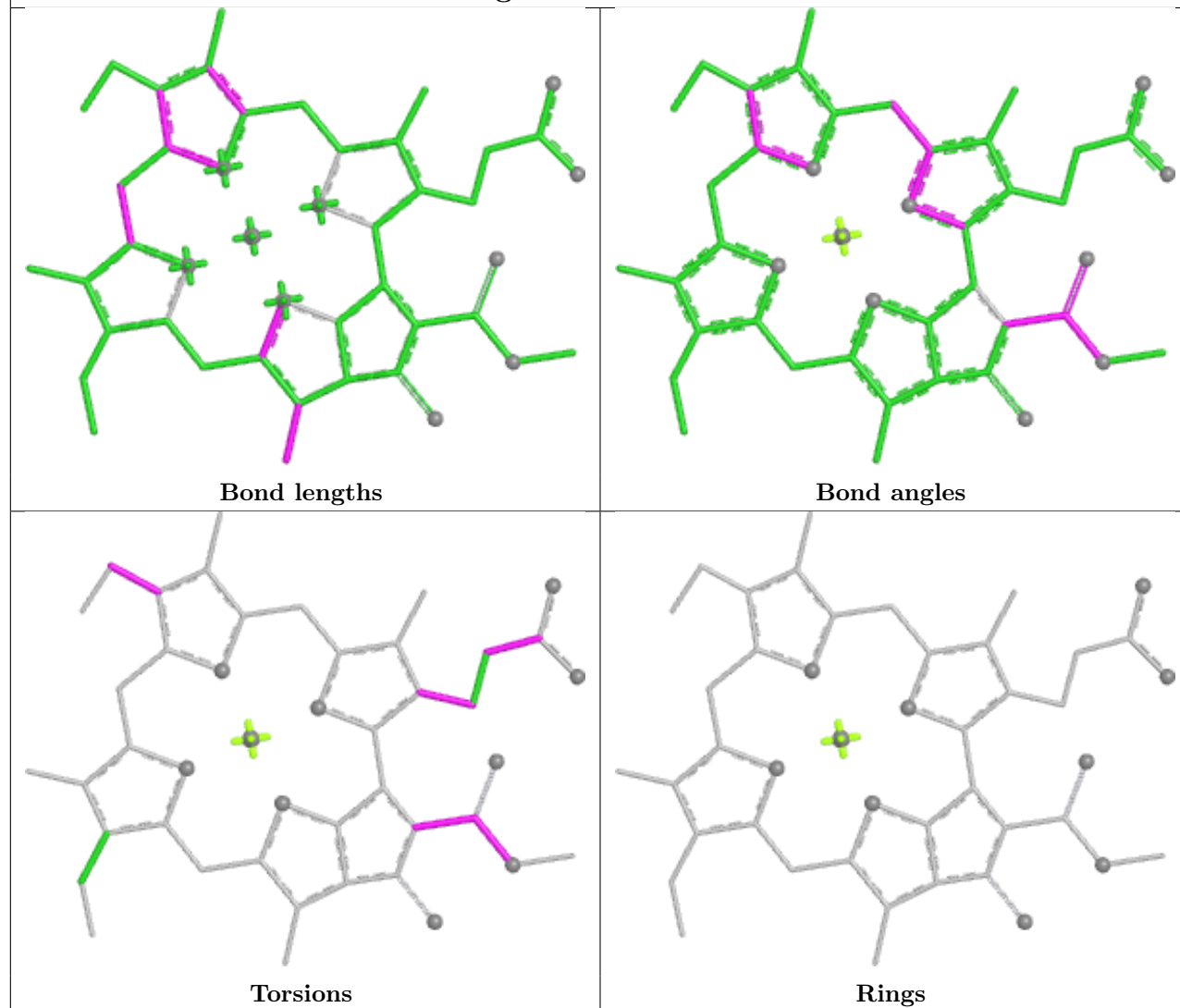




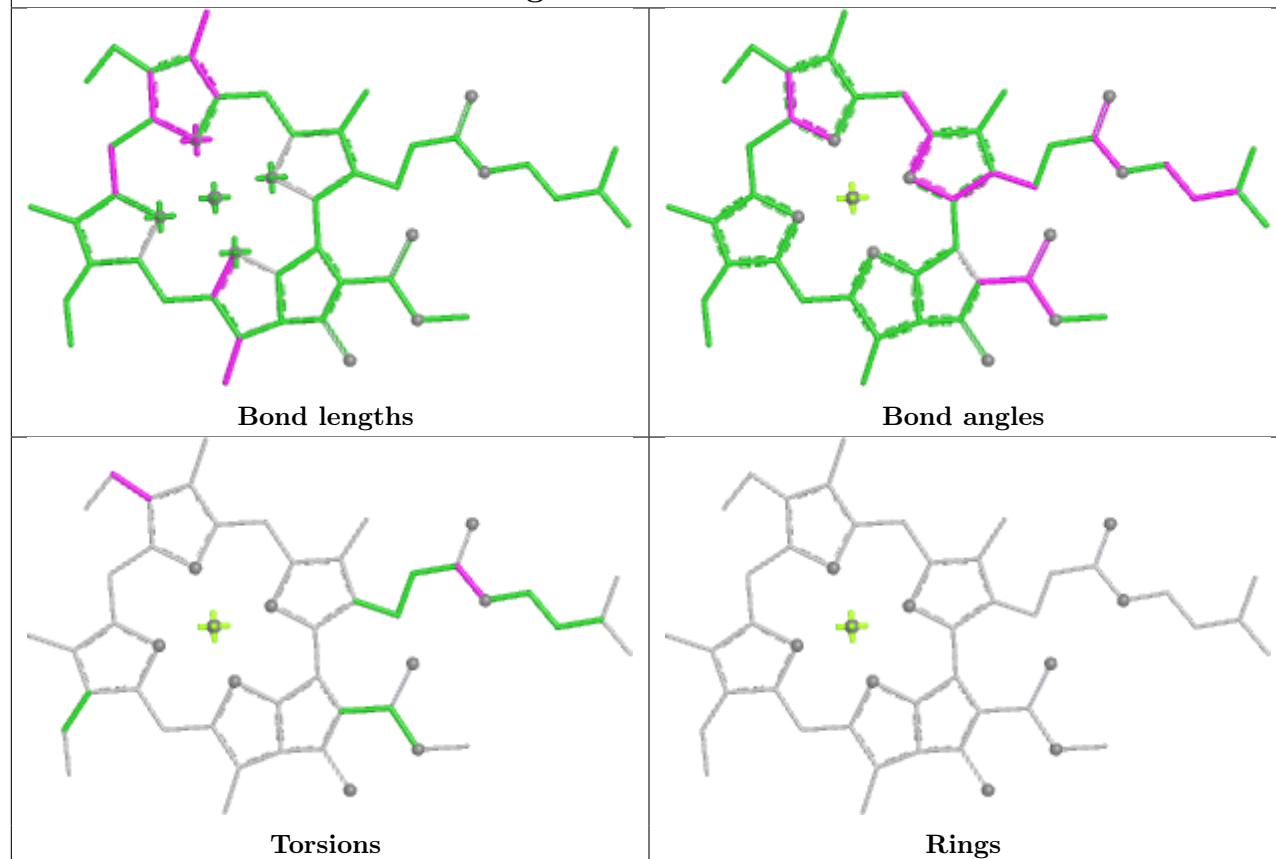
Ligand CLA G 836



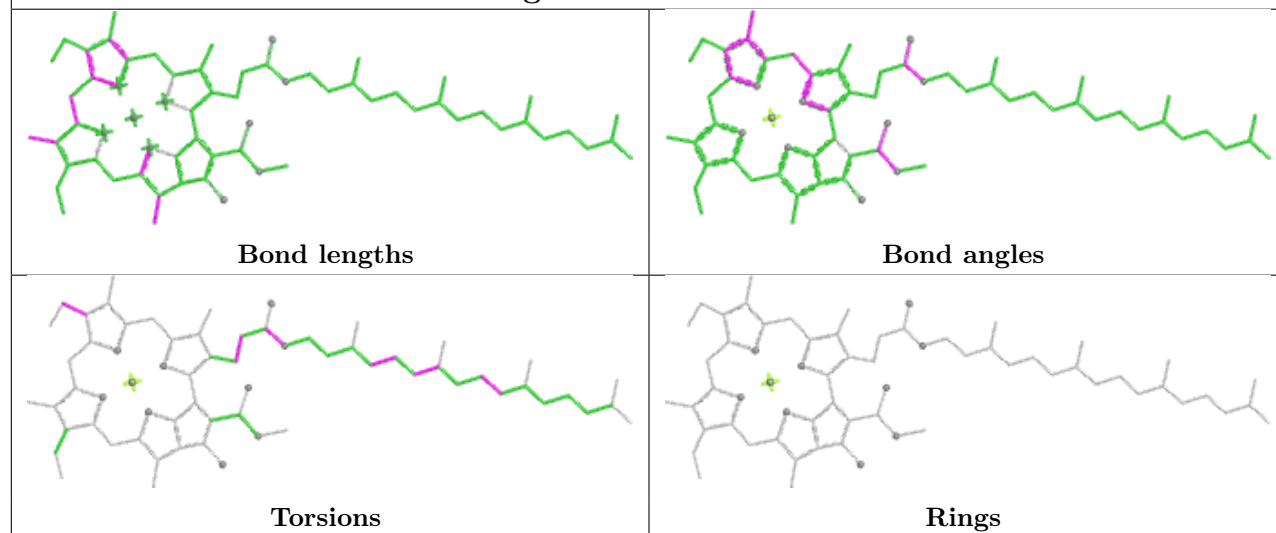
Ligand CLA J 103

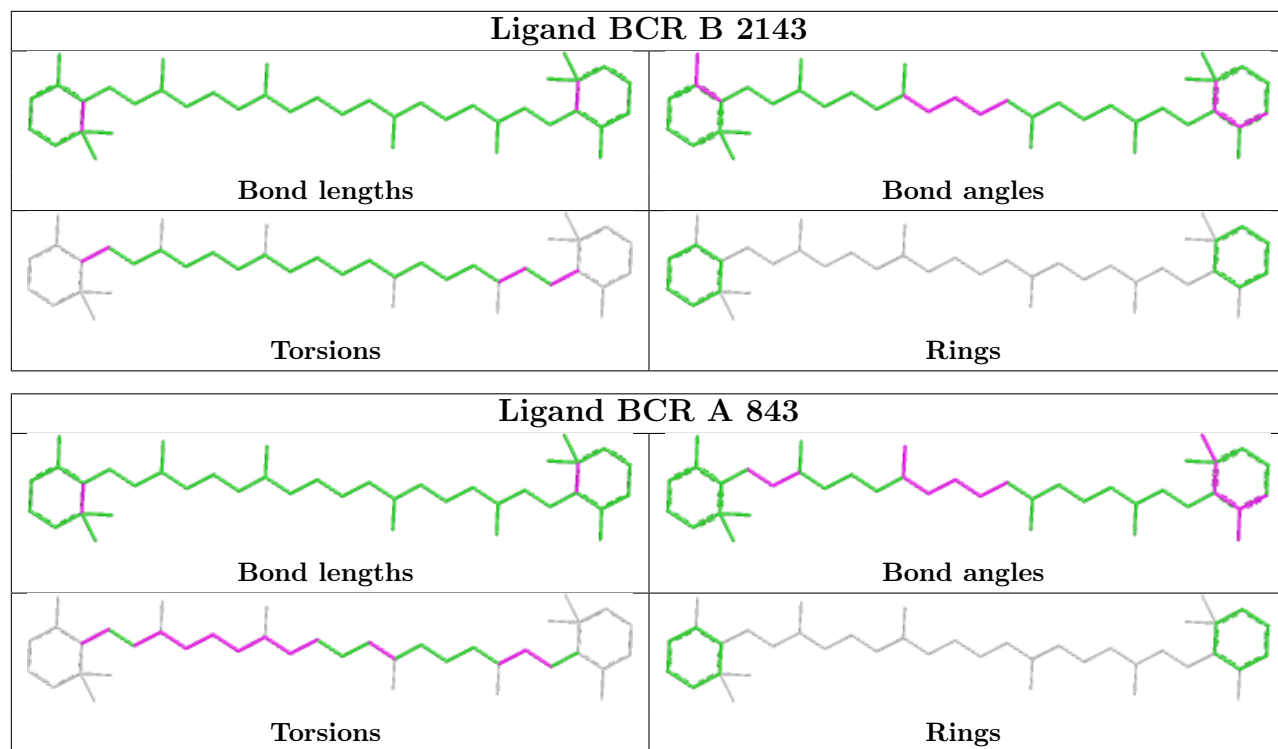


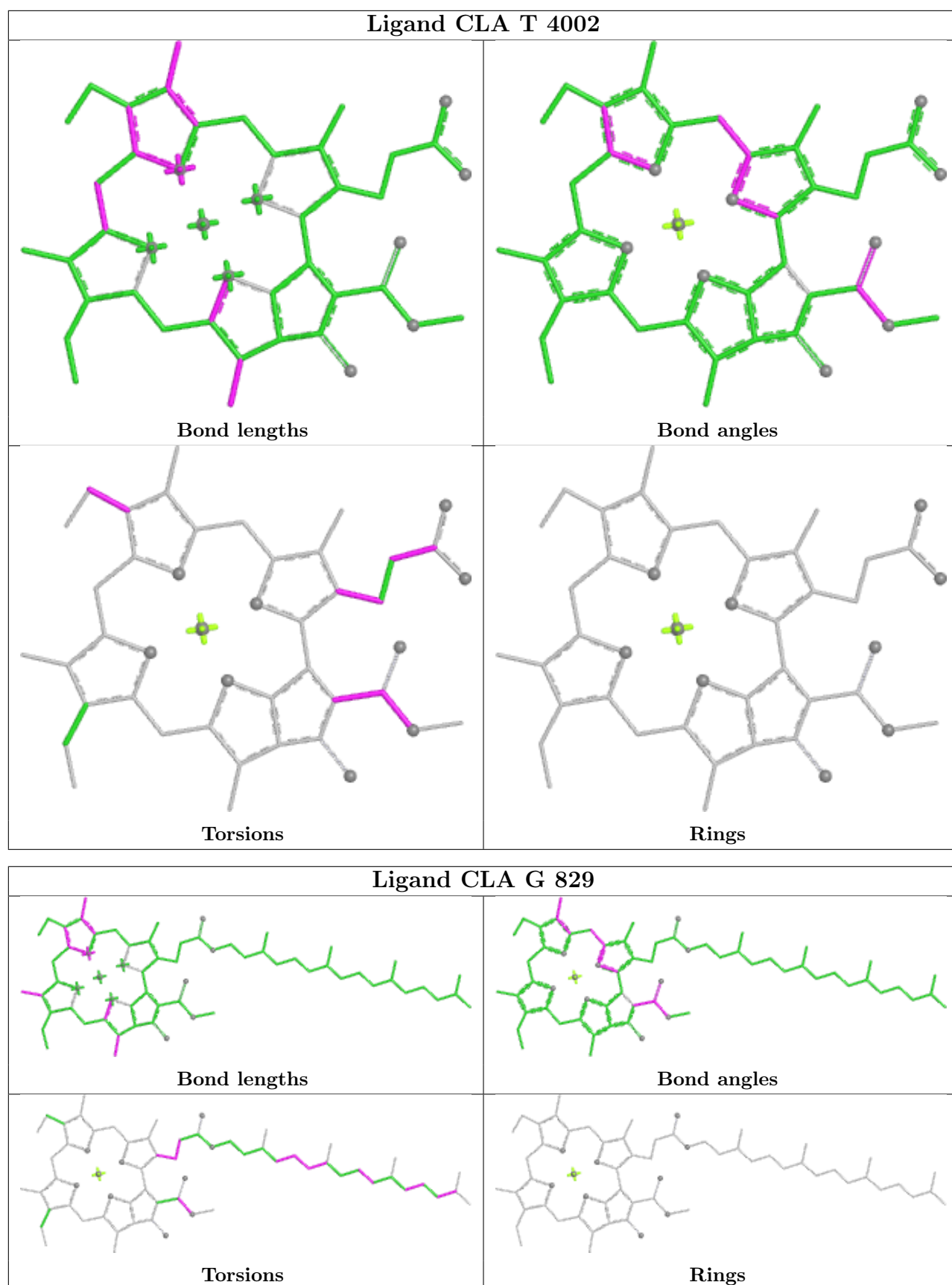
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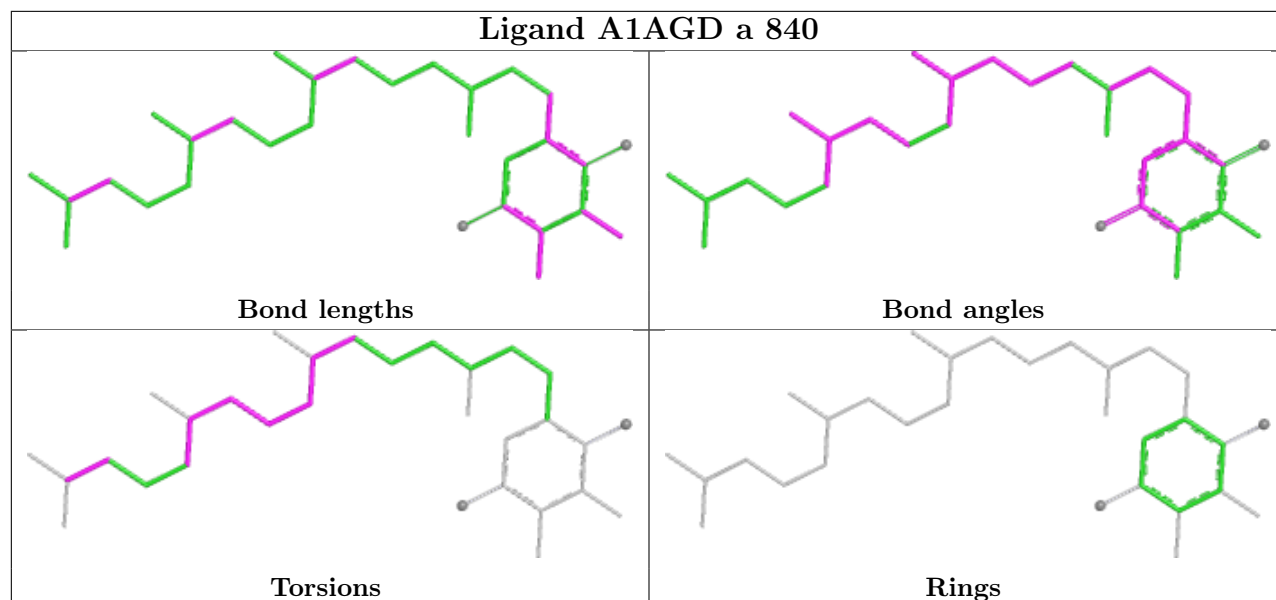
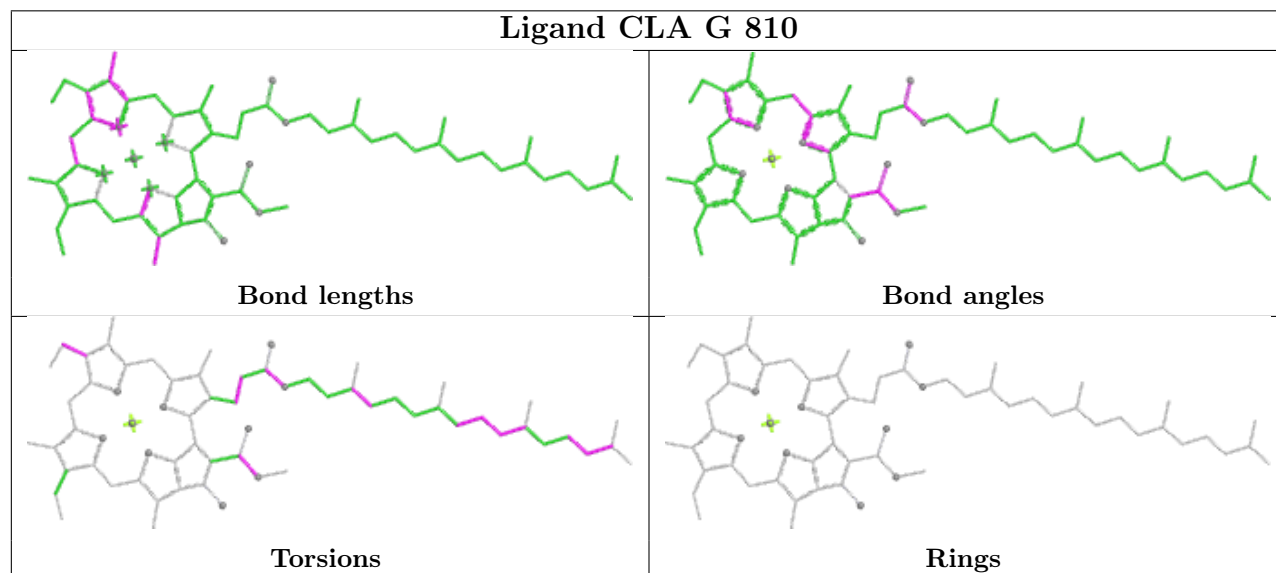
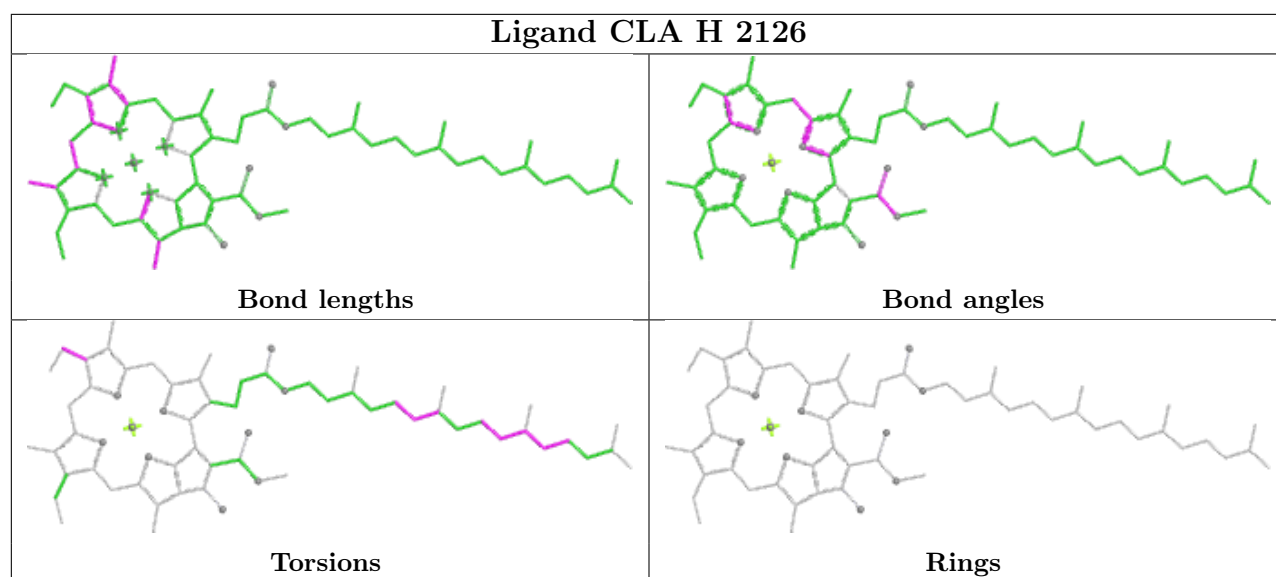


Ligand CLA B 2106

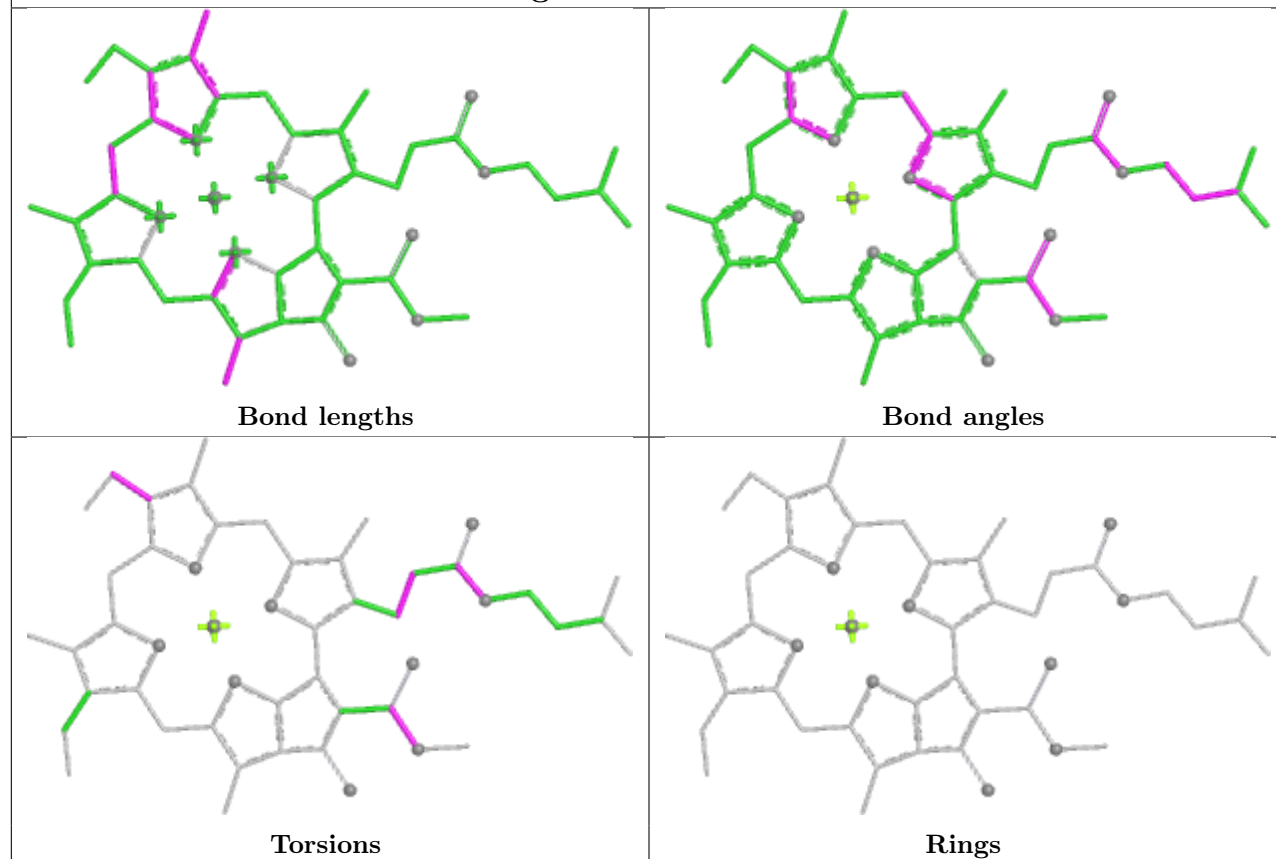




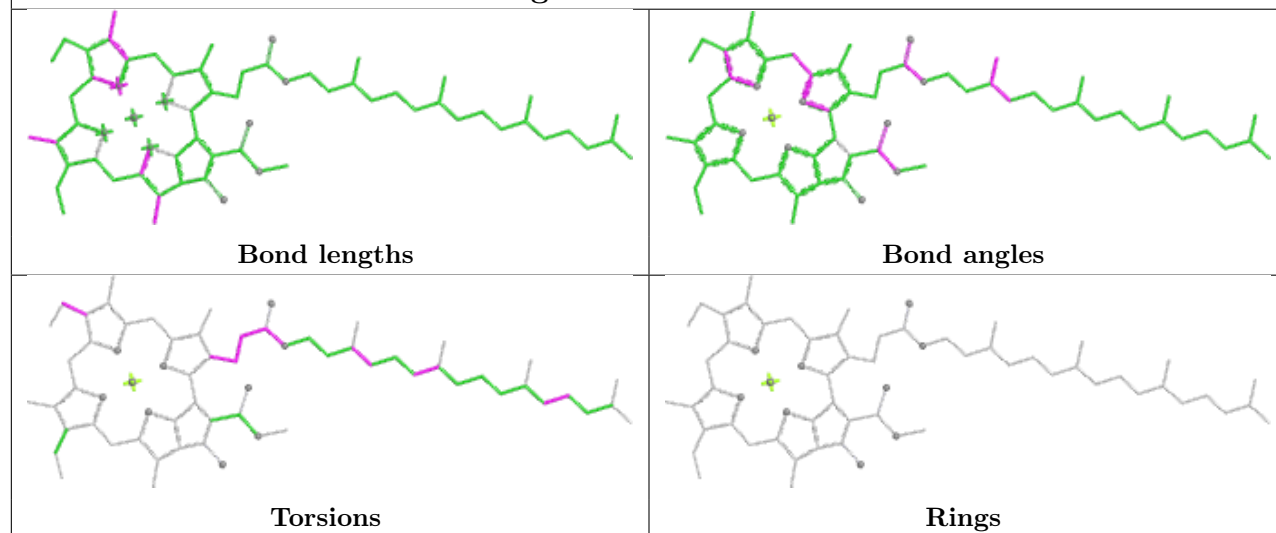


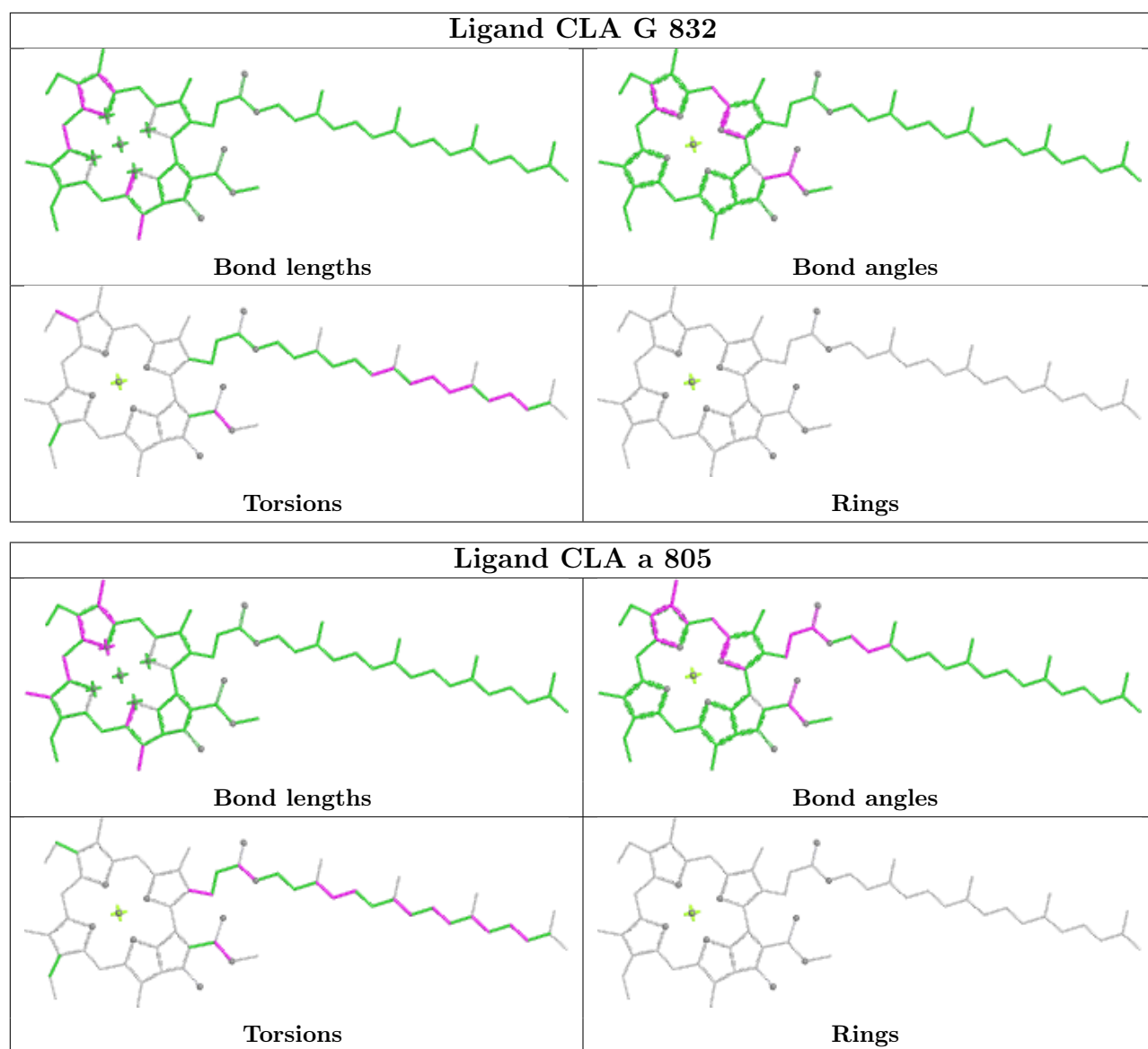


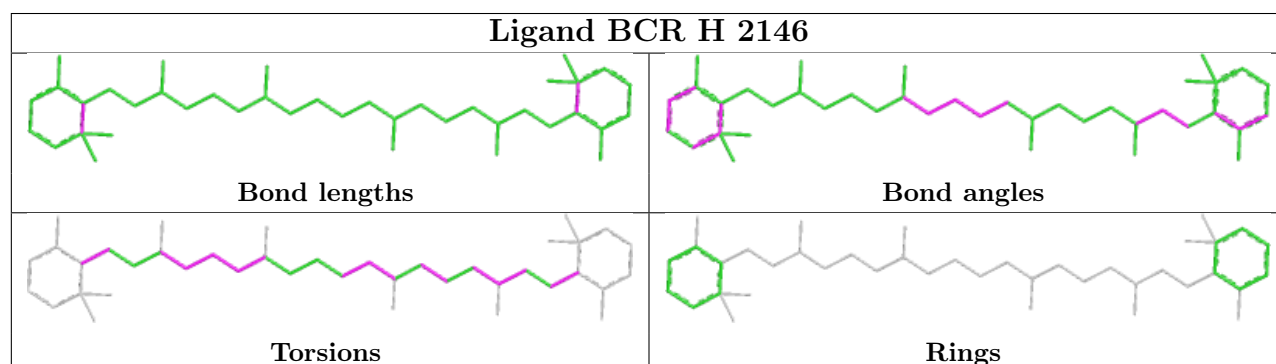
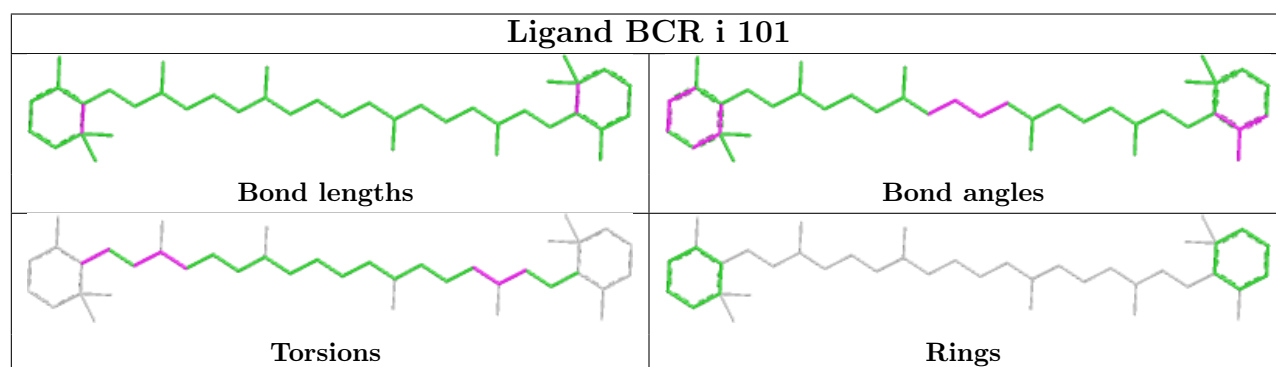
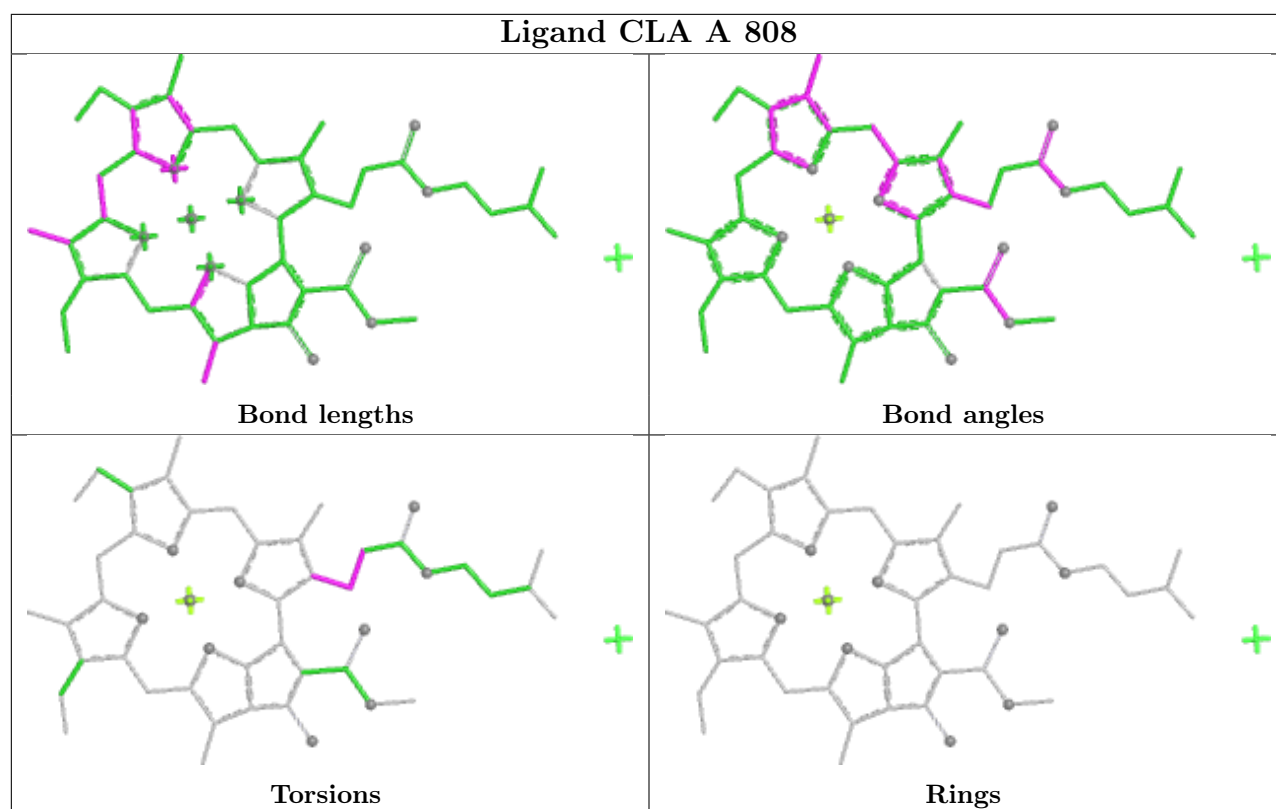
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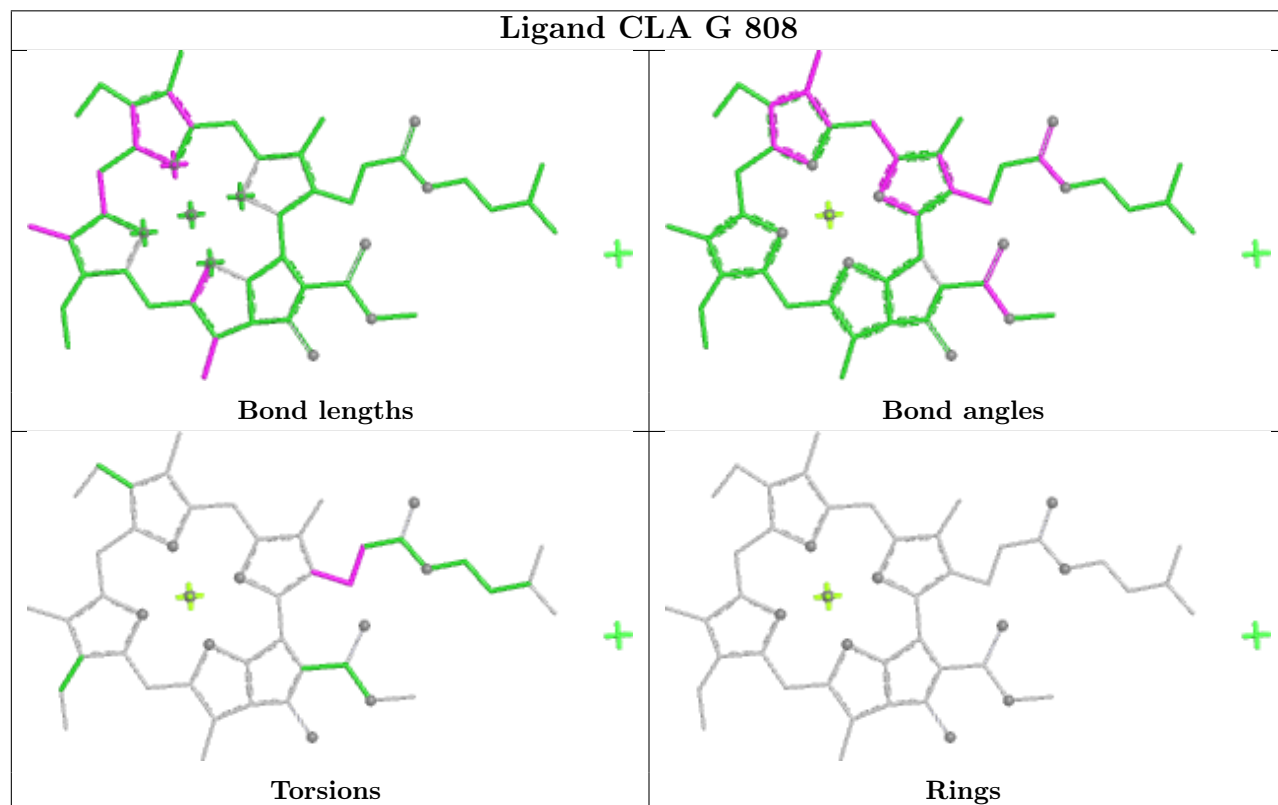
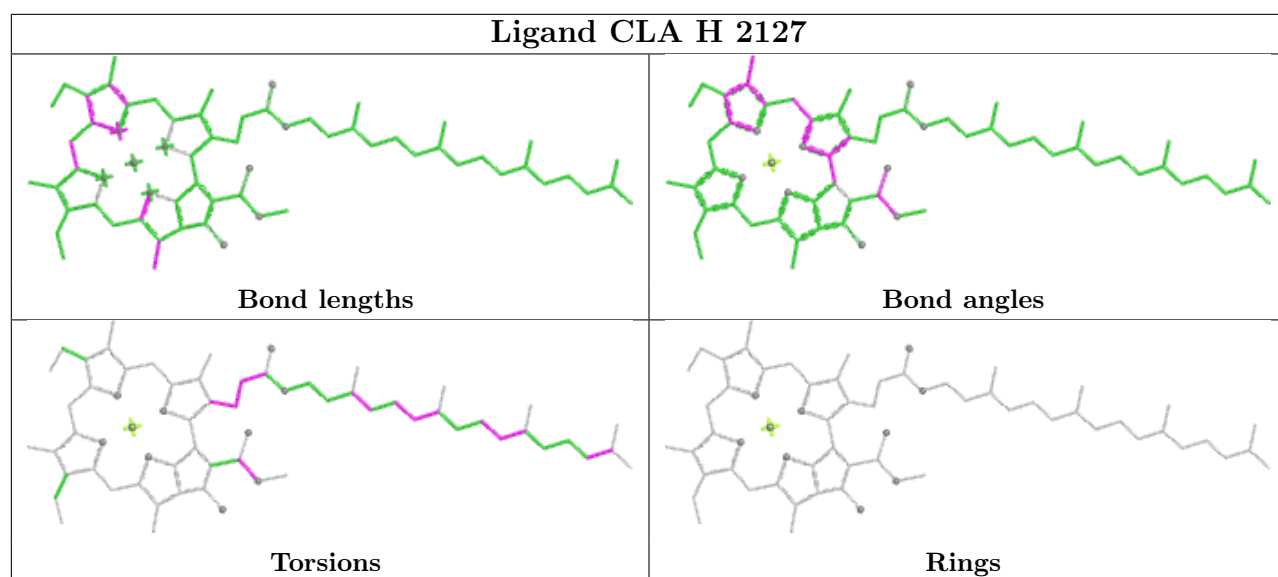


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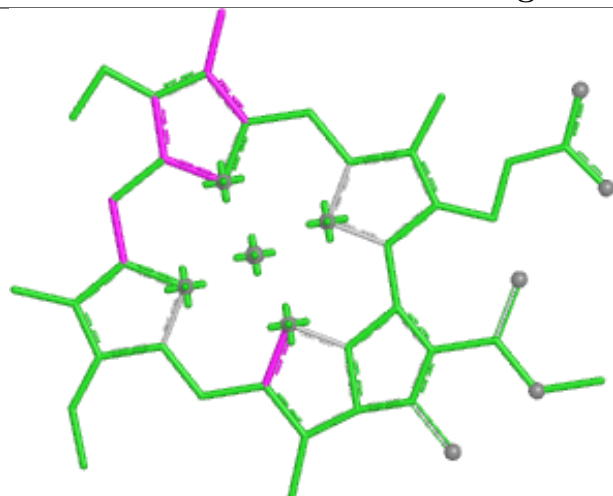




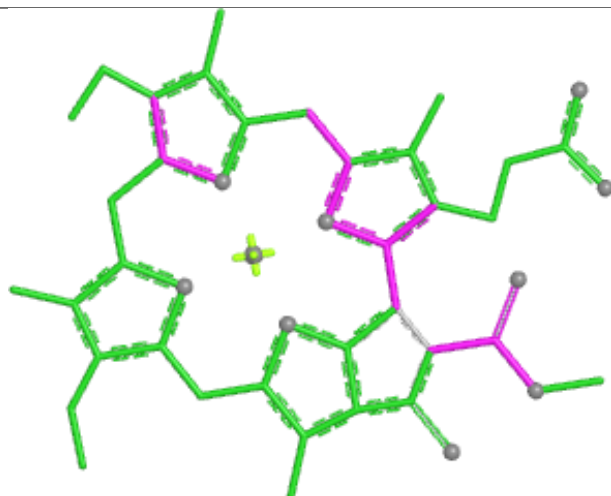




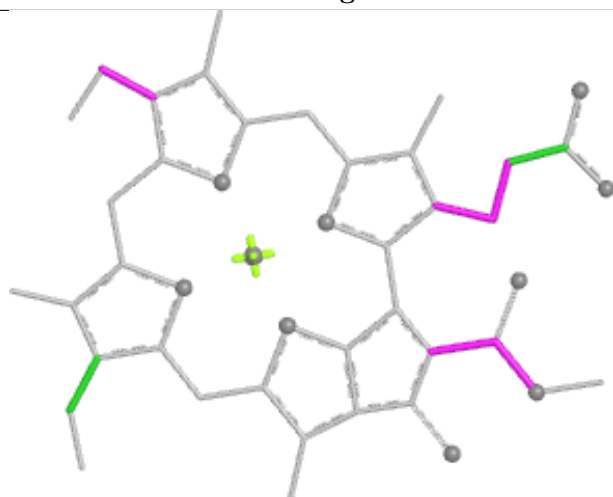
Ligand CLA S 102



Bond lengths



Bond angles

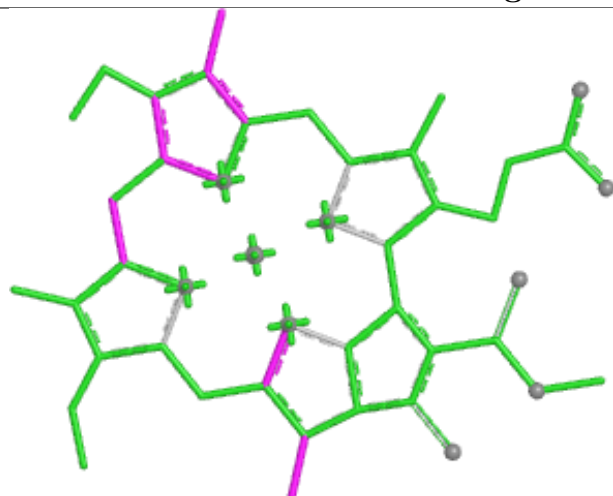


Torsions

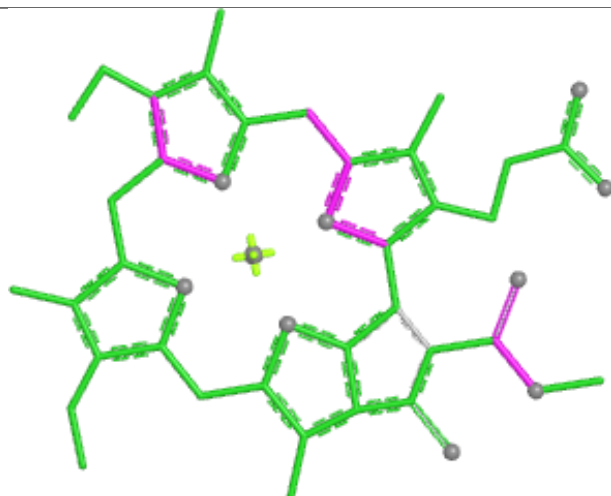


Rings

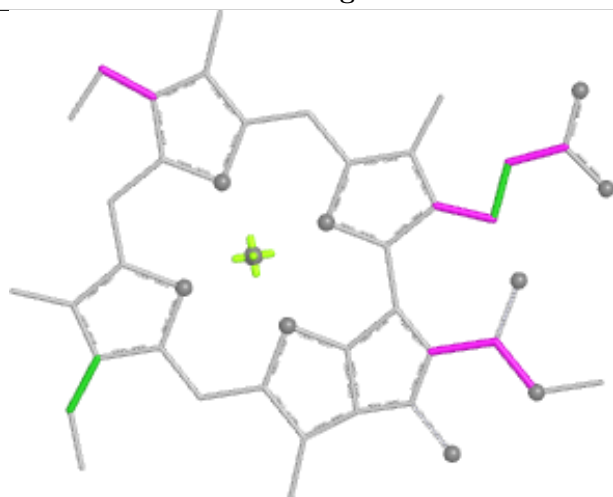
Ligand CLA K 4002



Bond lengths



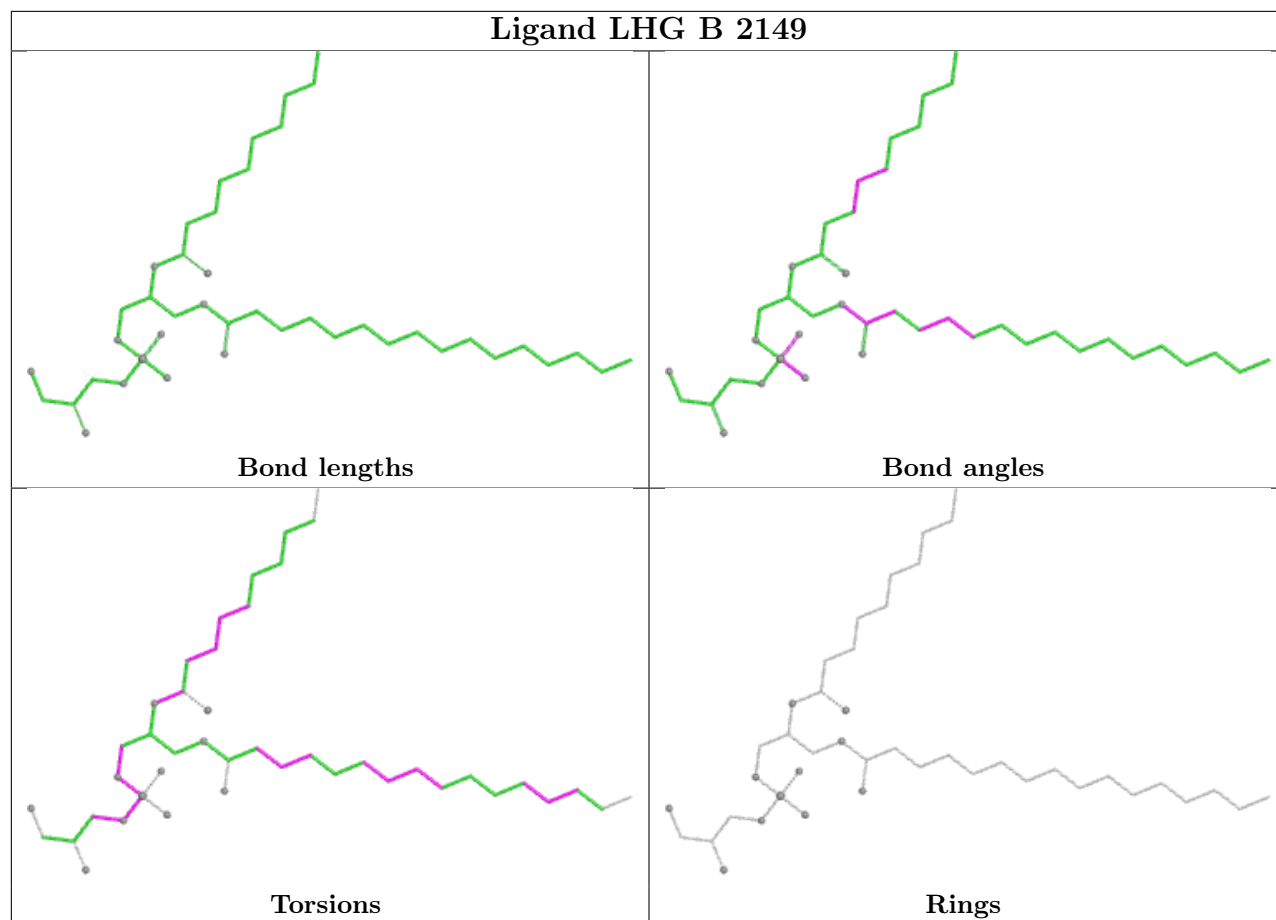
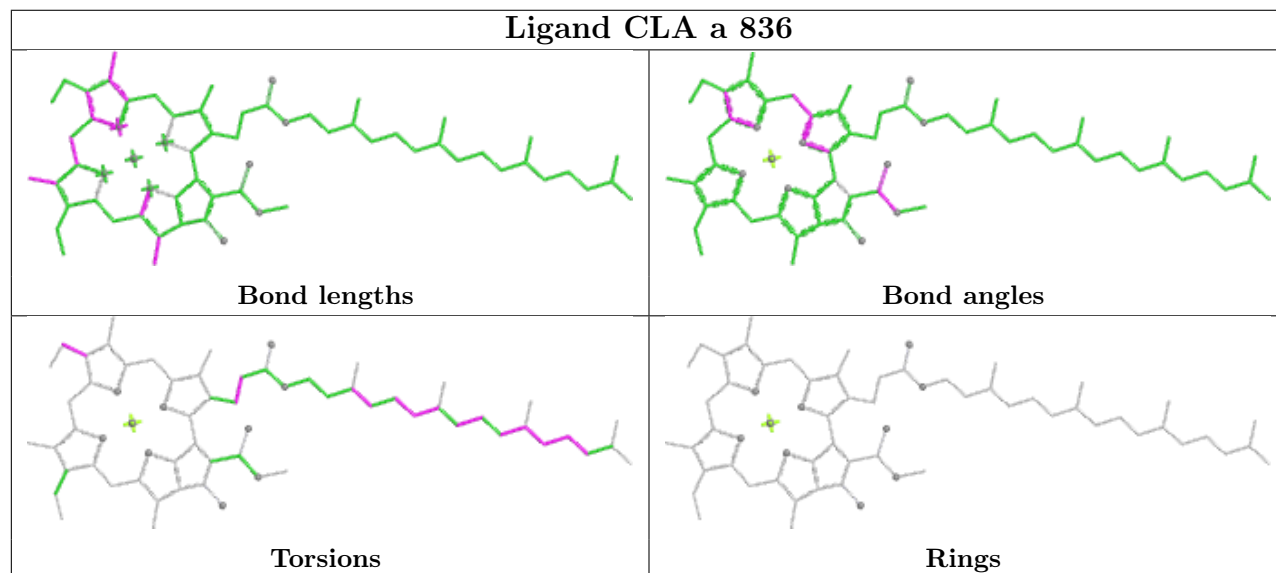
Bond angles

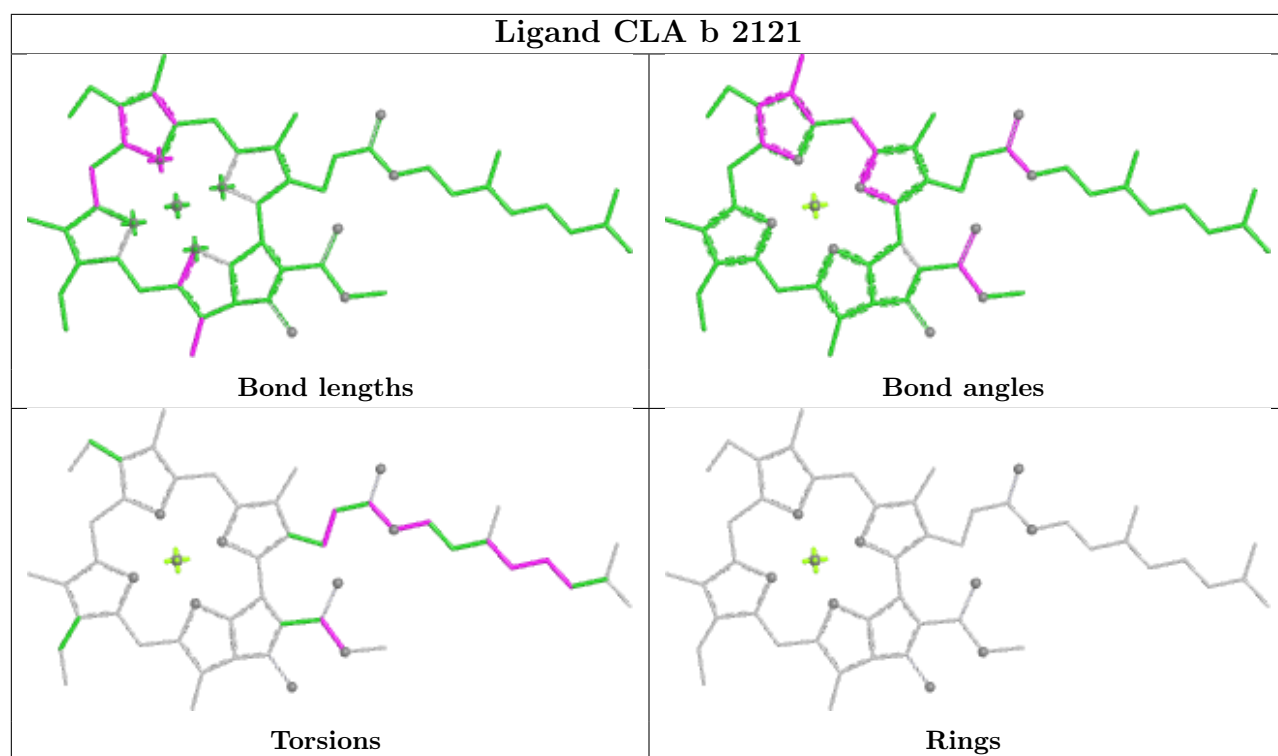


Torsions

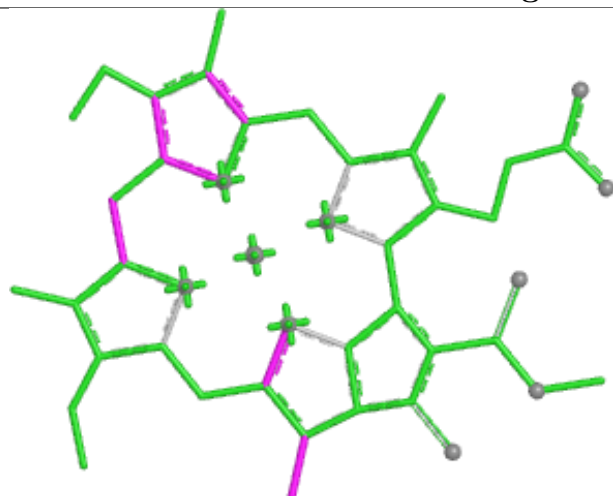


Rings

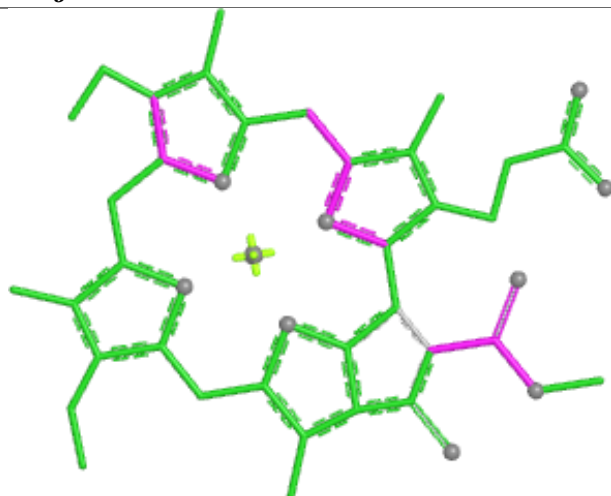
Ligand LHG B 2149**Ligand CLA a 836**



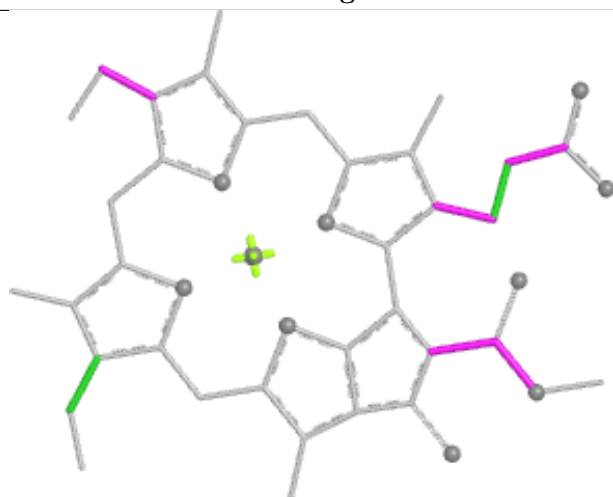
Ligand CLA j 103



Bond lengths



Bond angles

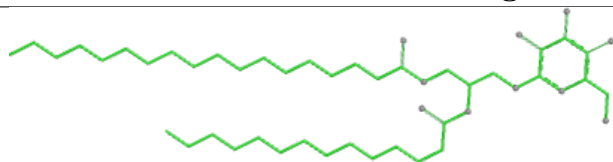


Torsions

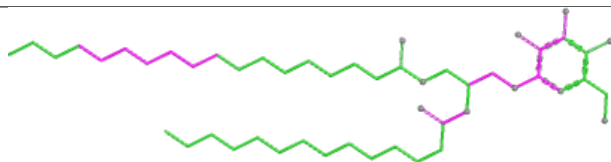


Rings

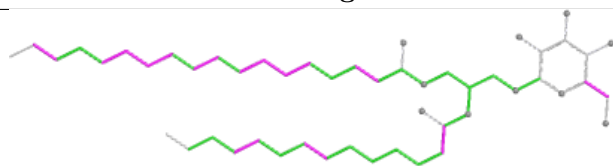
Ligand LMG B 2148



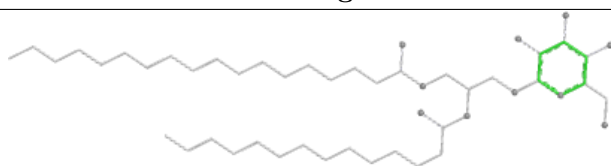
Bond lengths



Bond angles

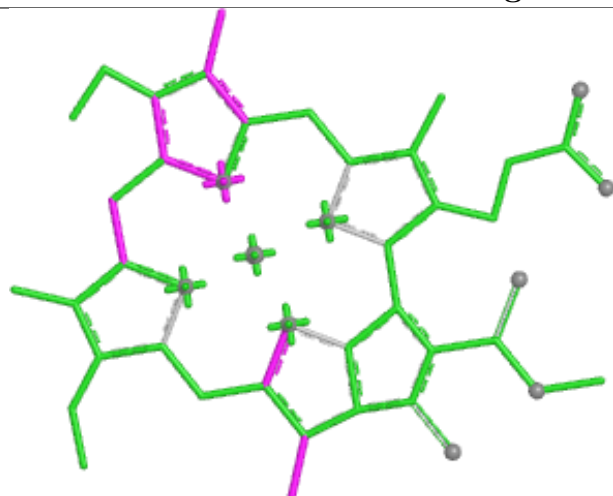


Torsions

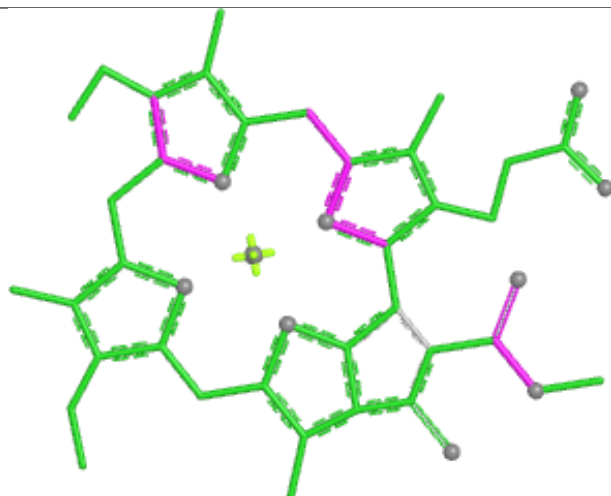


Rings

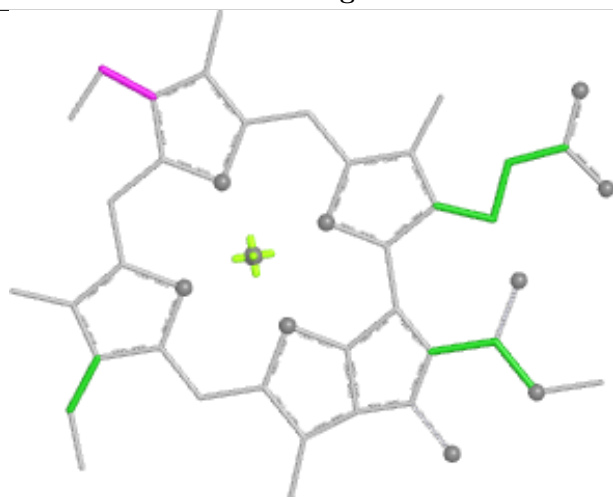
Ligand CLA H 2130



Bond lengths



Bond angles

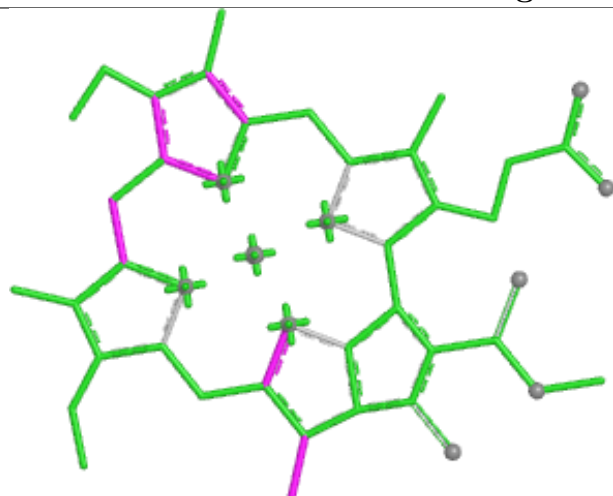


Torsions

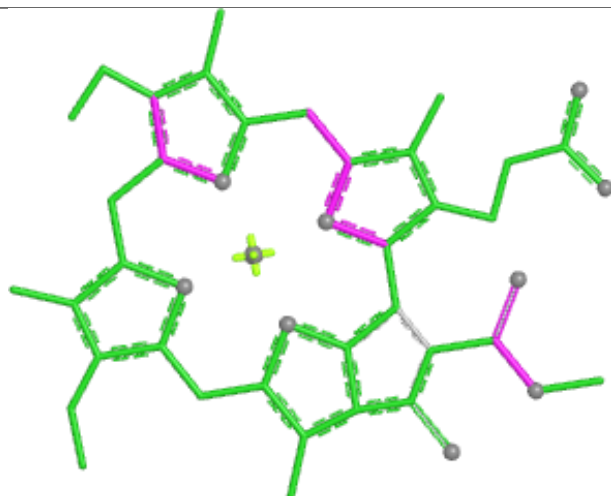


Rings

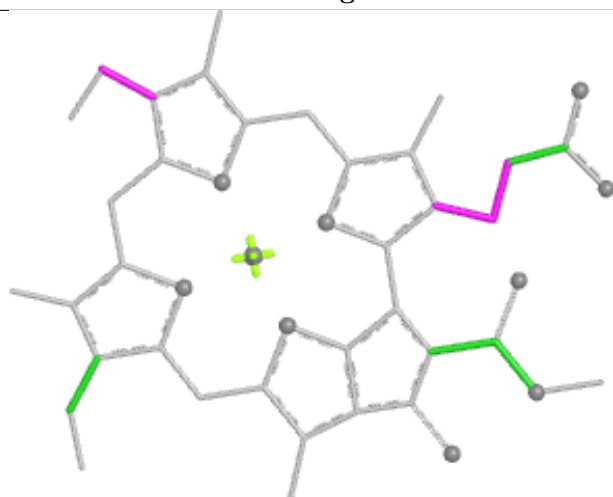
Ligand CLA F 204



Bond lengths



Bond angles

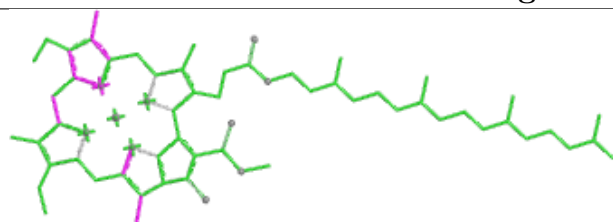


Torsions

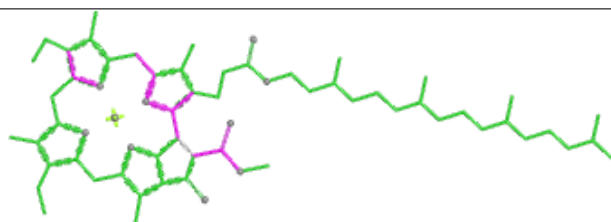


Rings

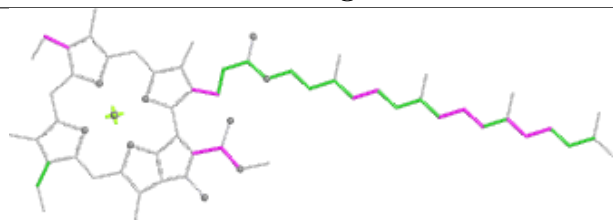
Ligand CLA a 812



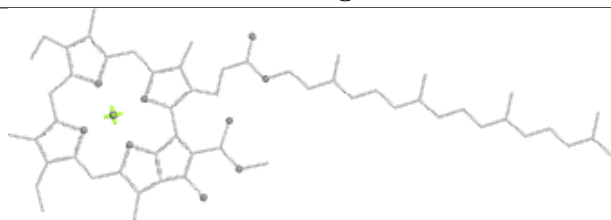
Bond lengths



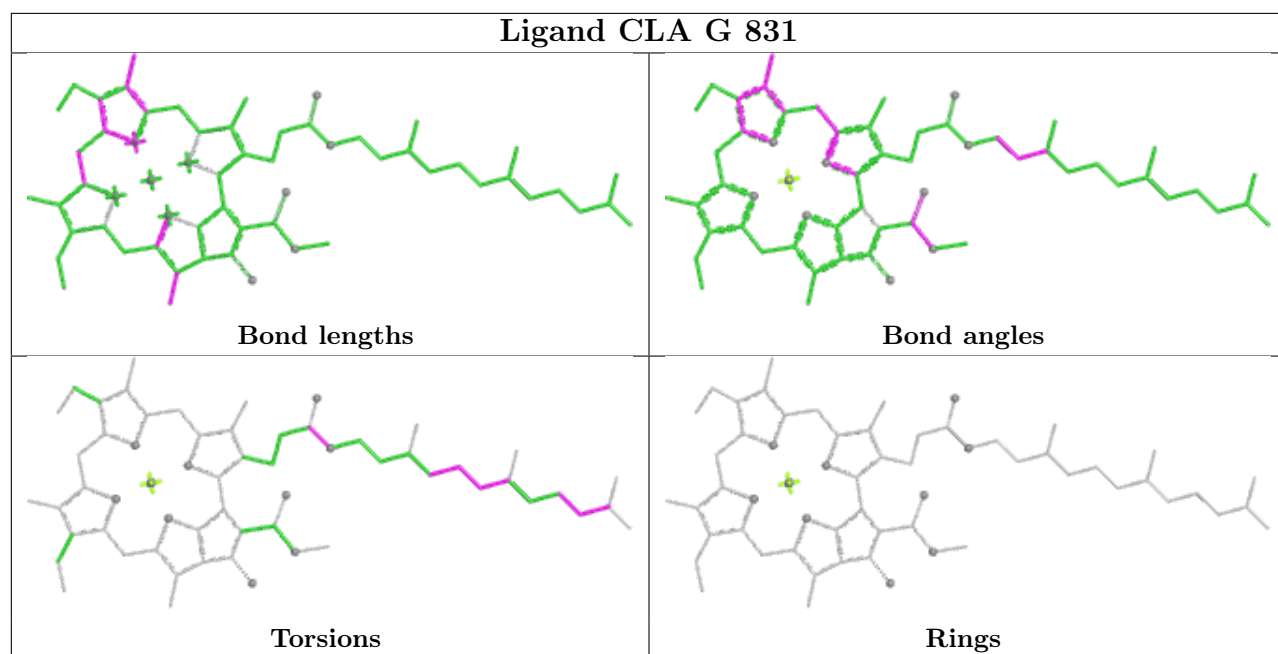
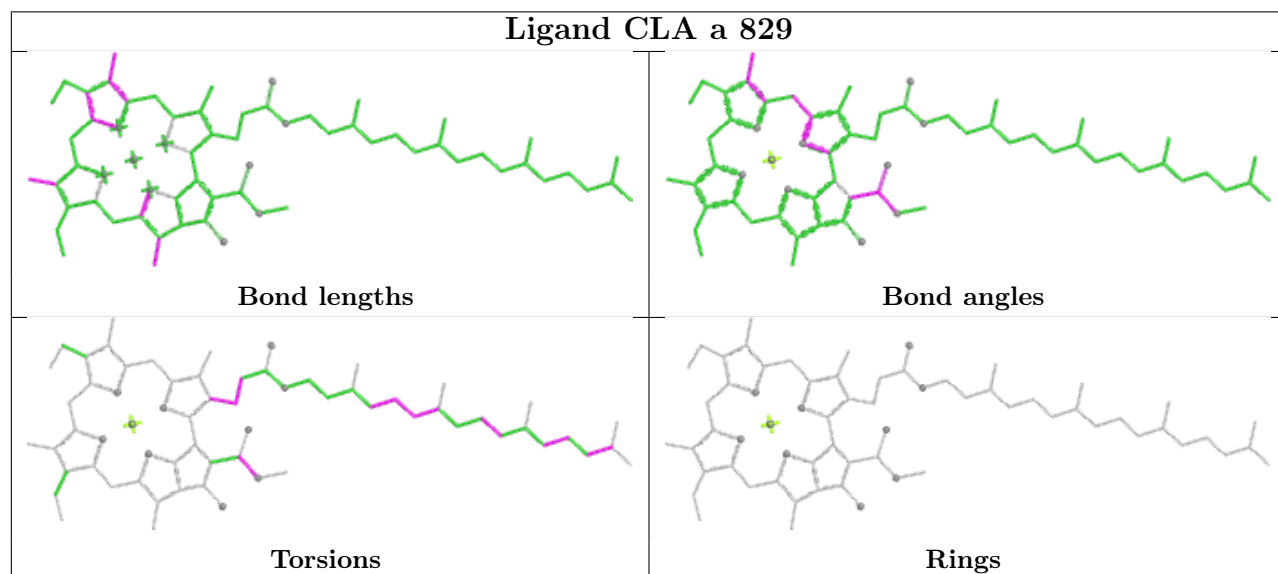
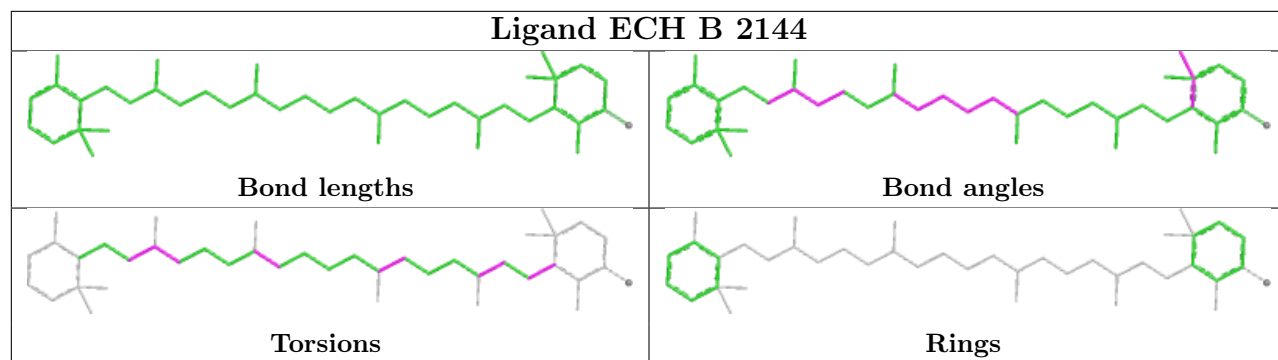
Bond angles

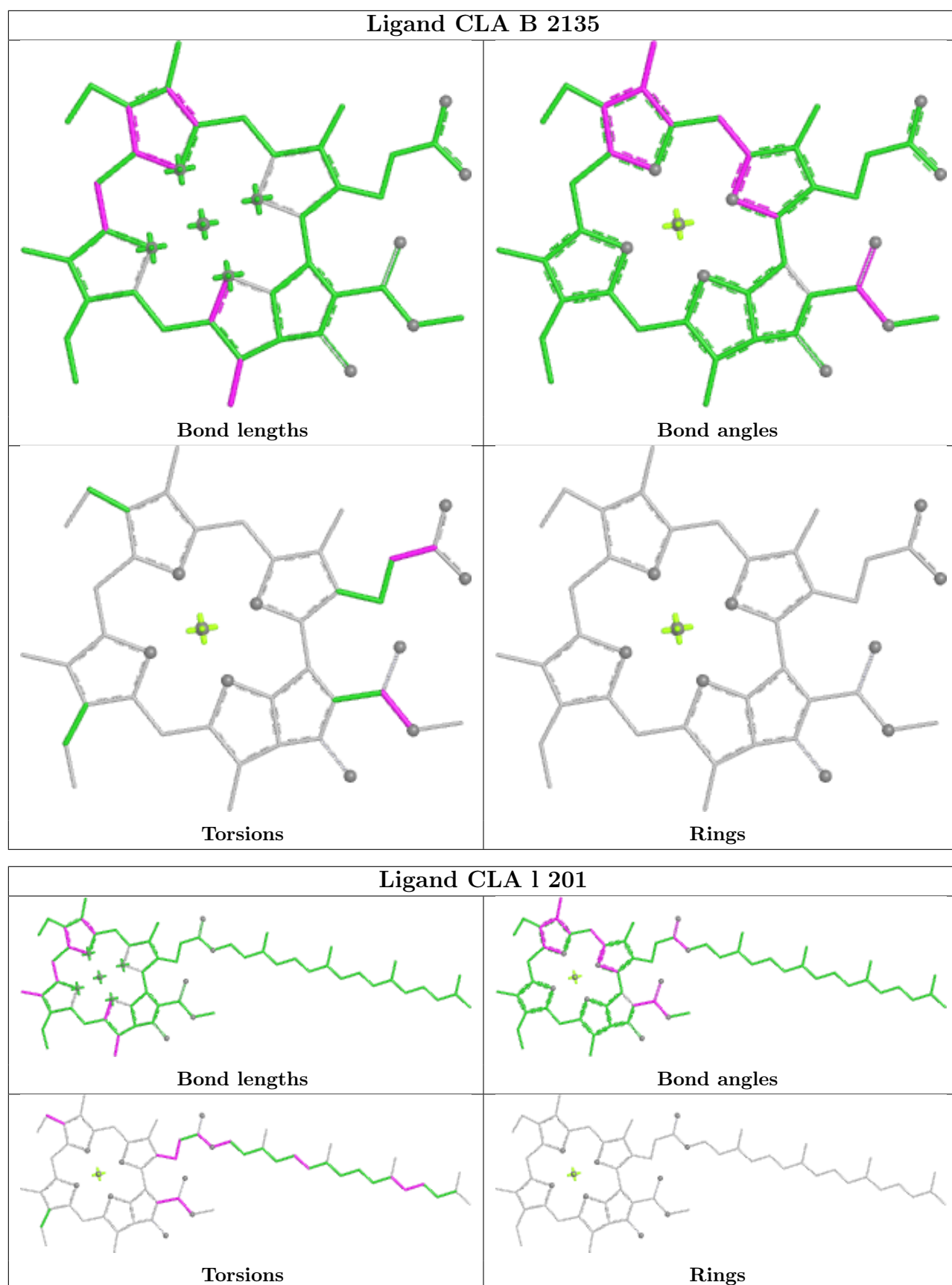


Torsions

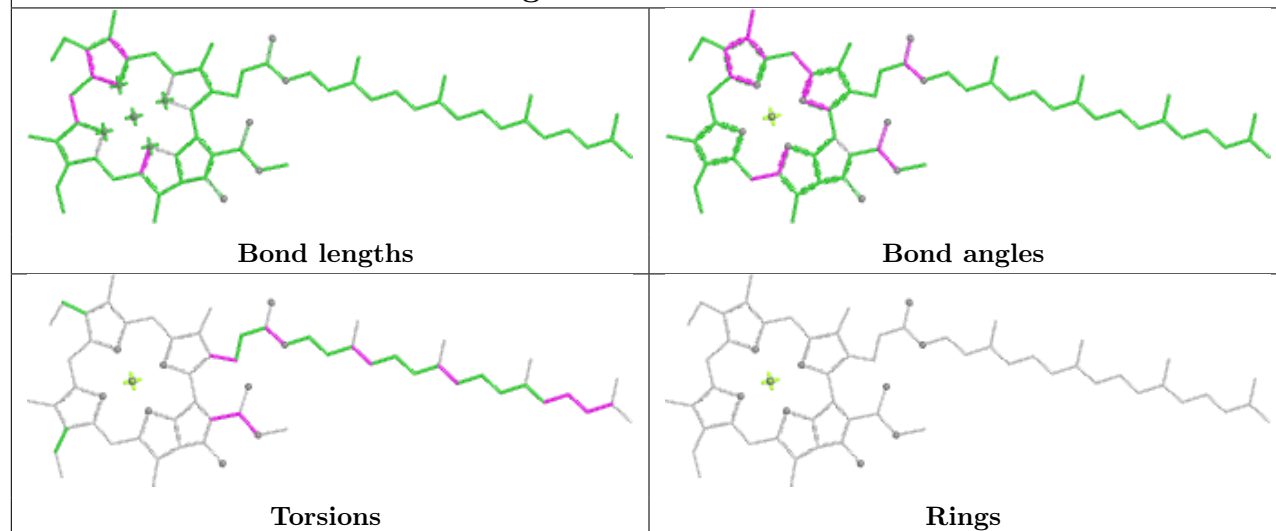


Rings

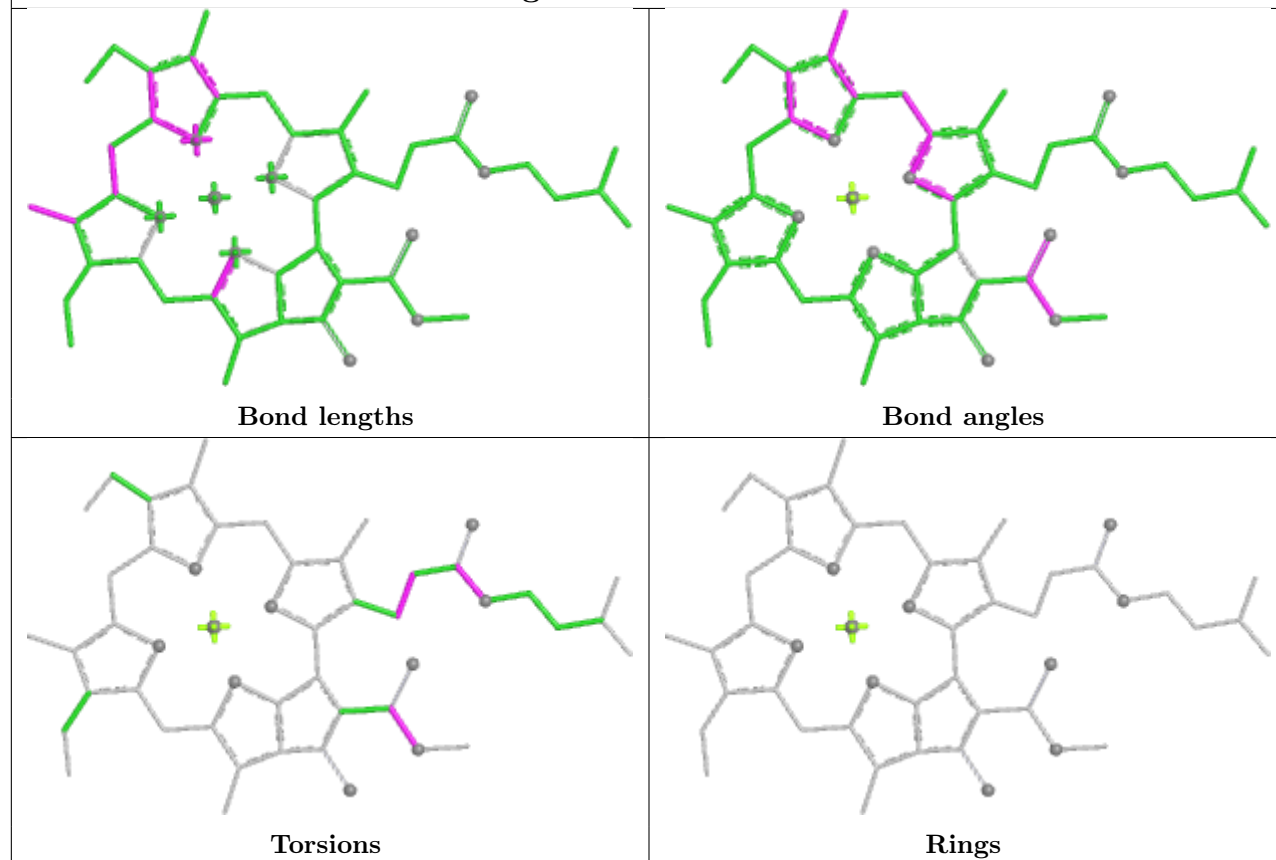


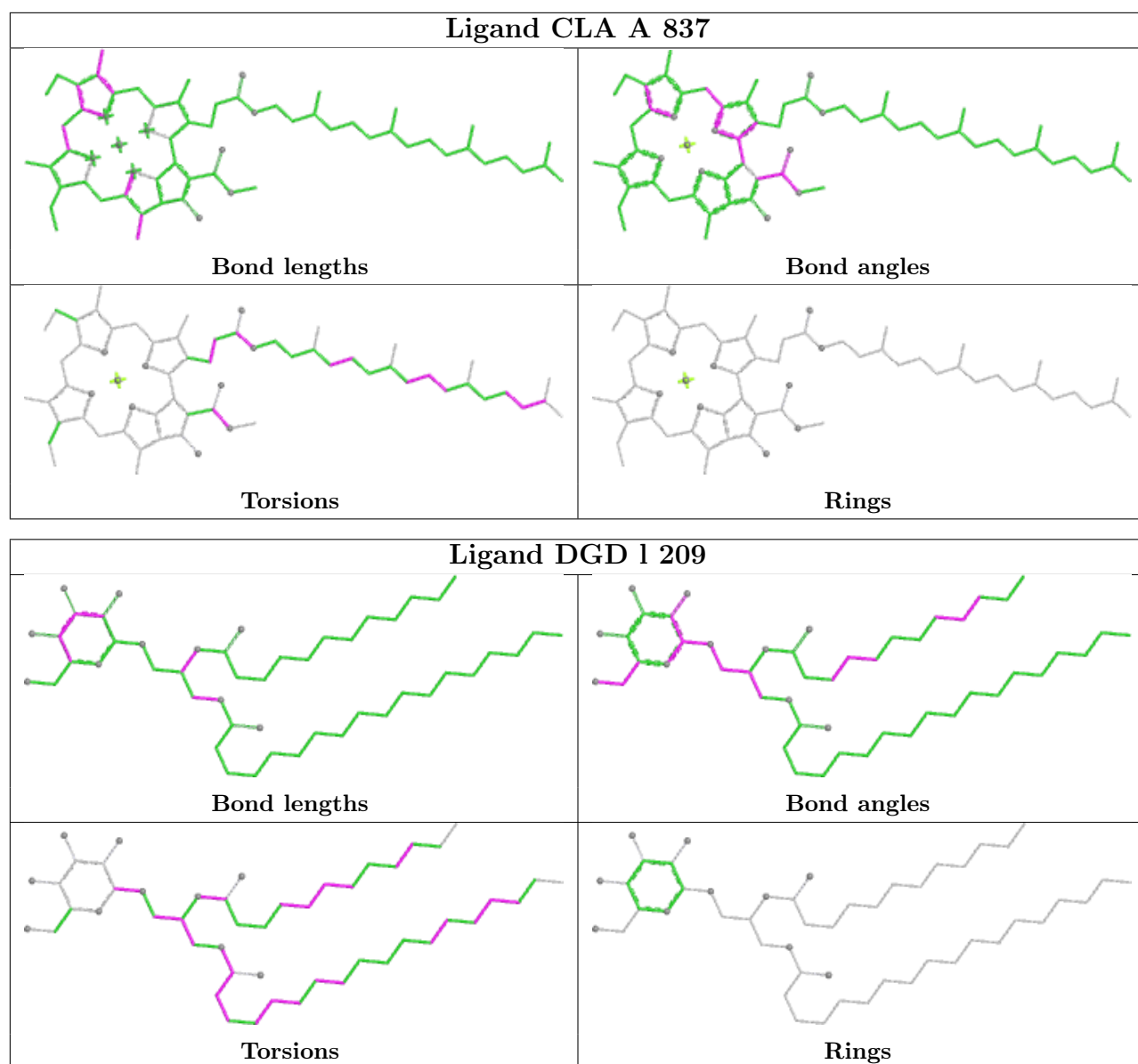


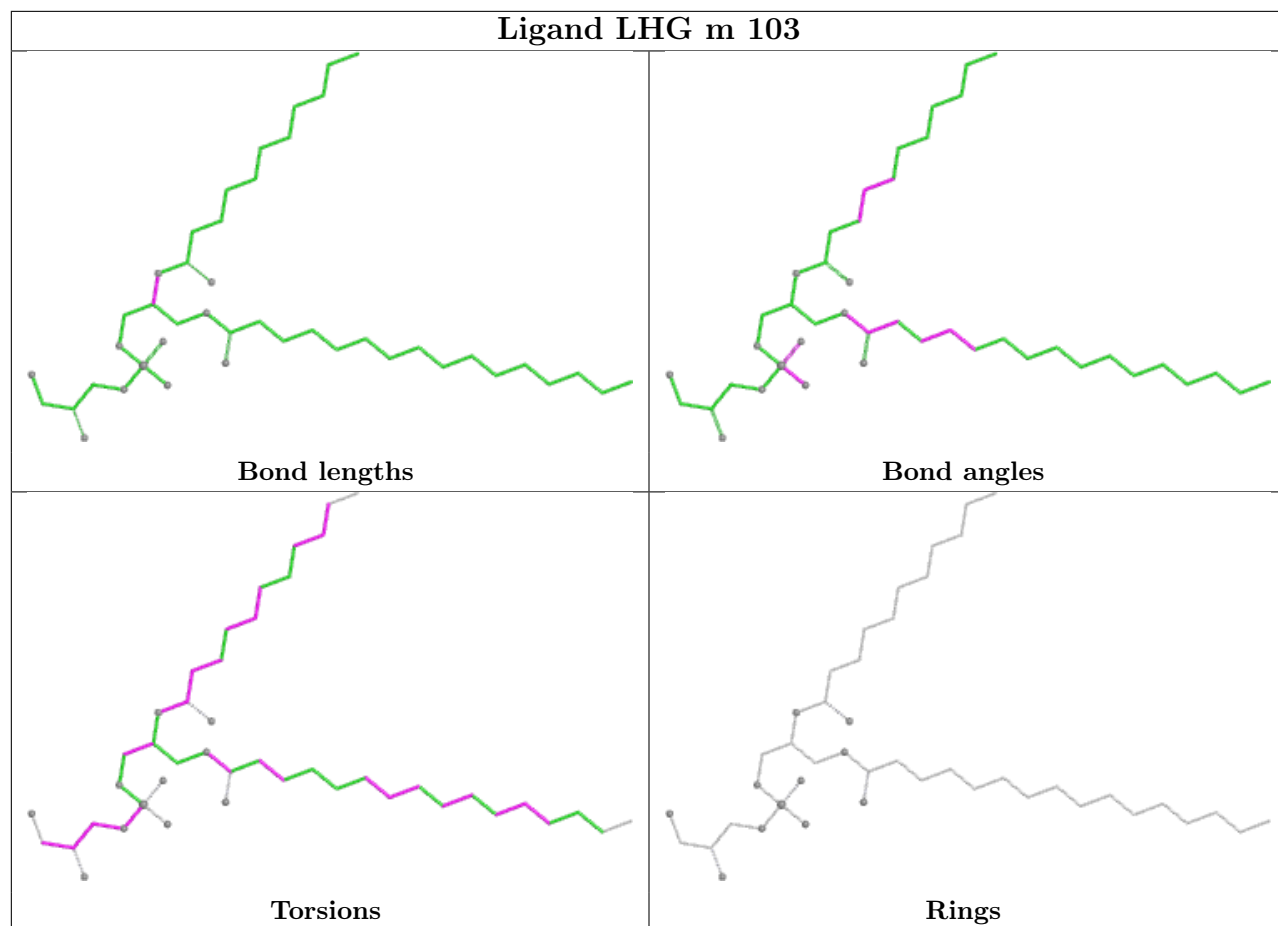
Ligand CLA H 2106

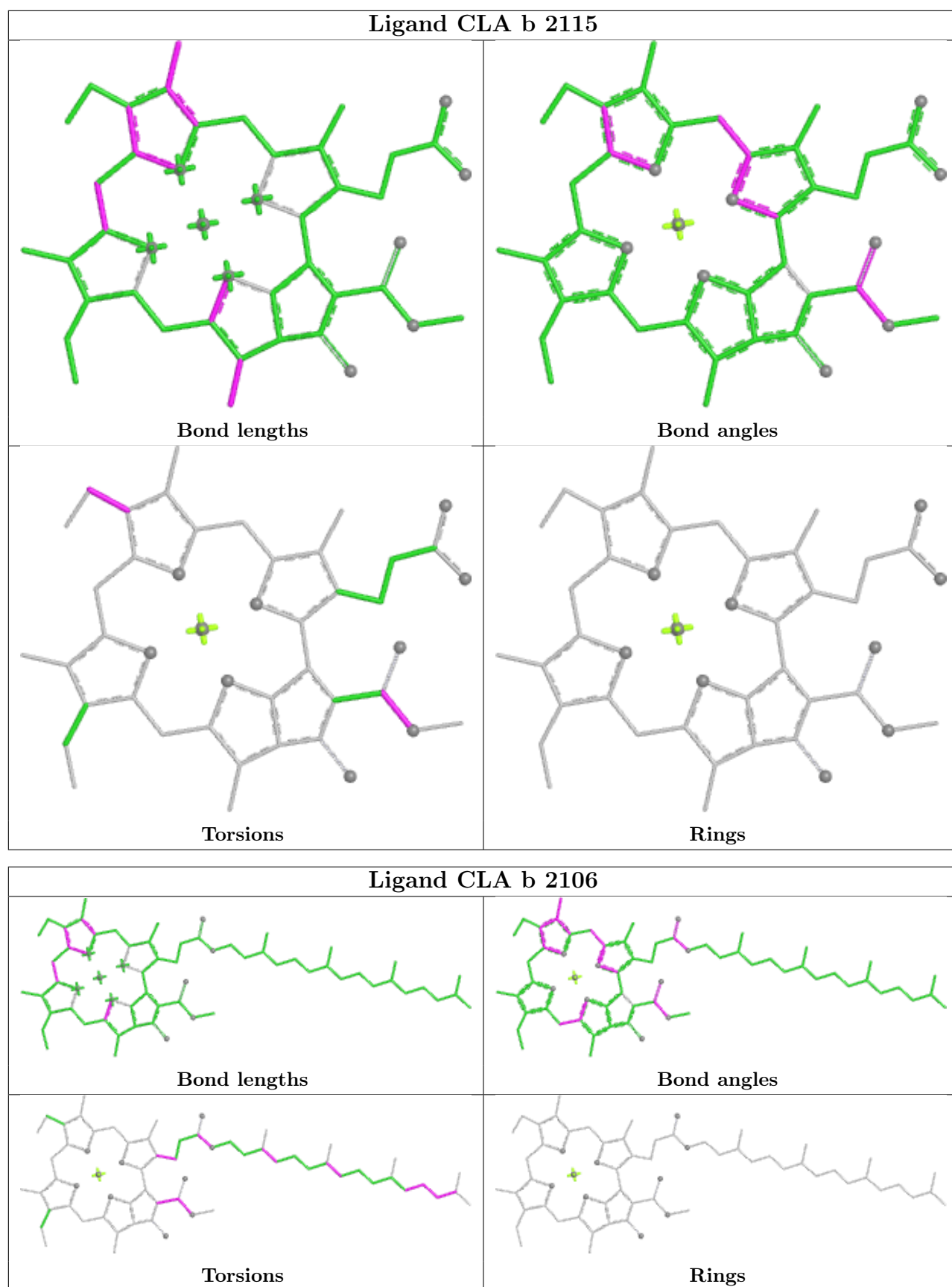


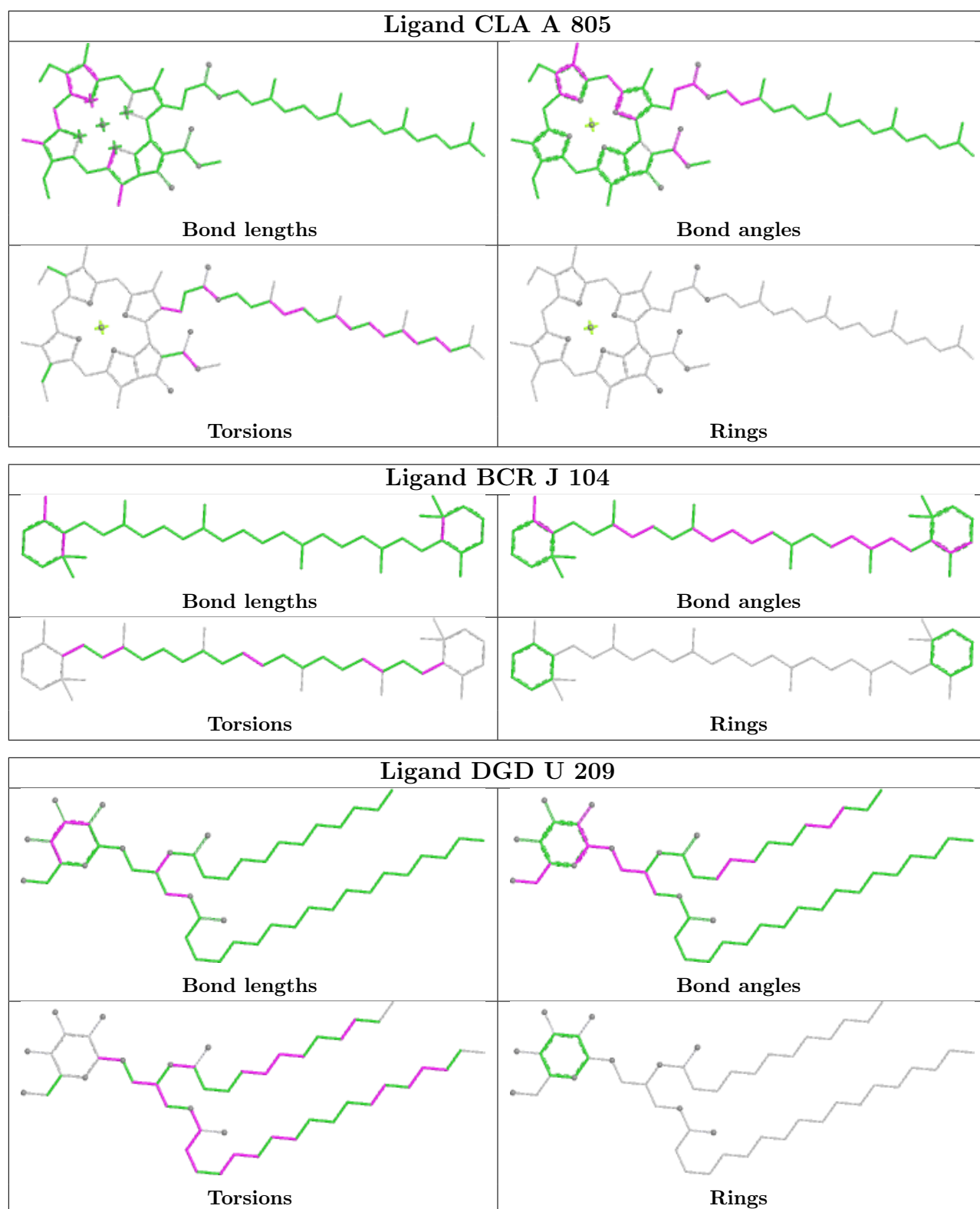
Ligand CLA H 2152

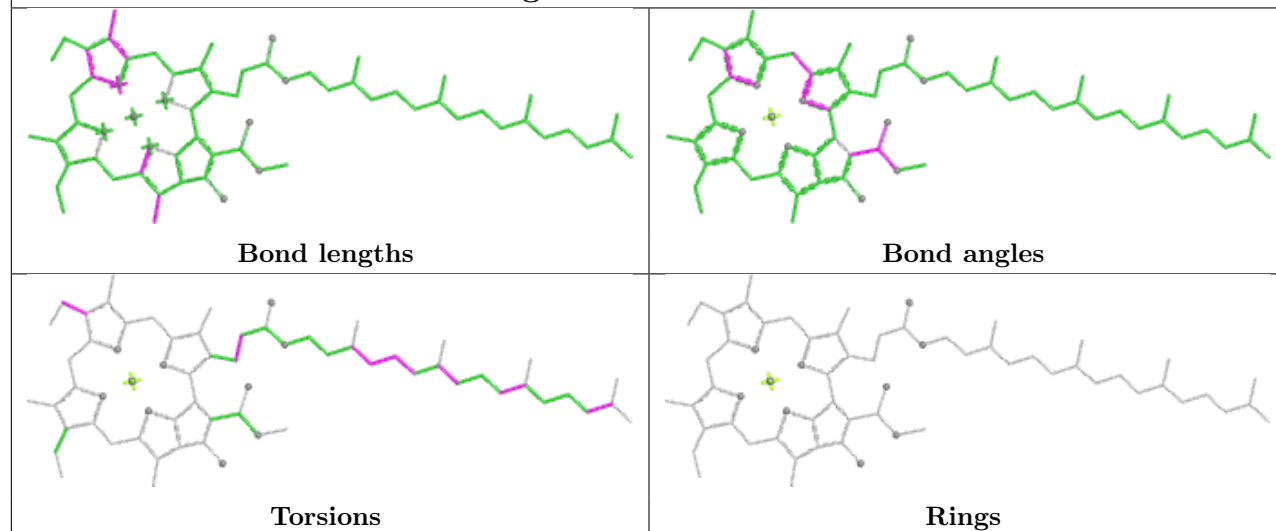
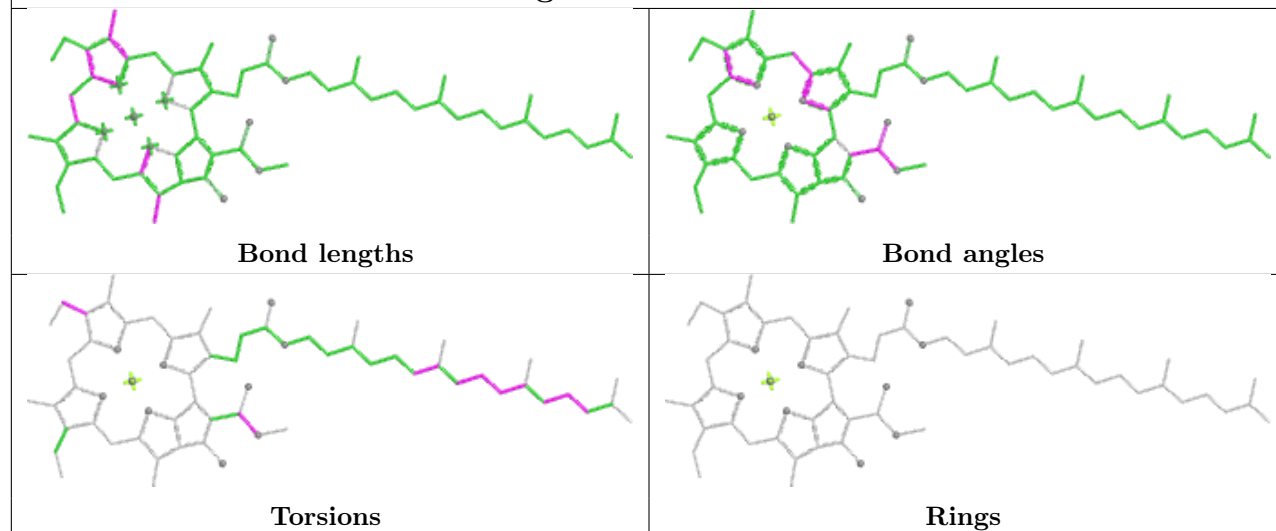
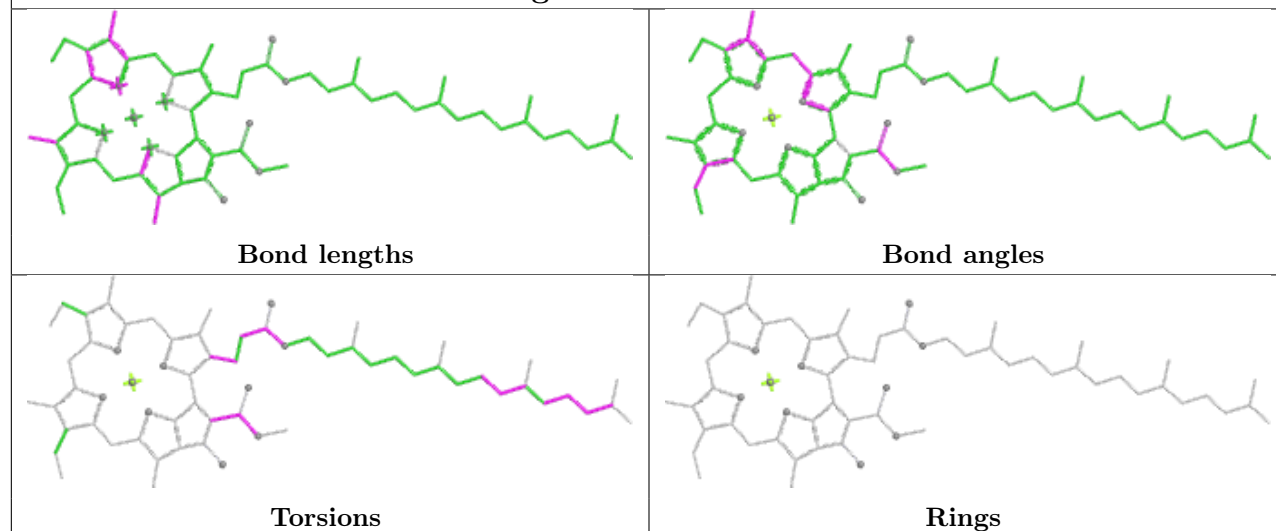


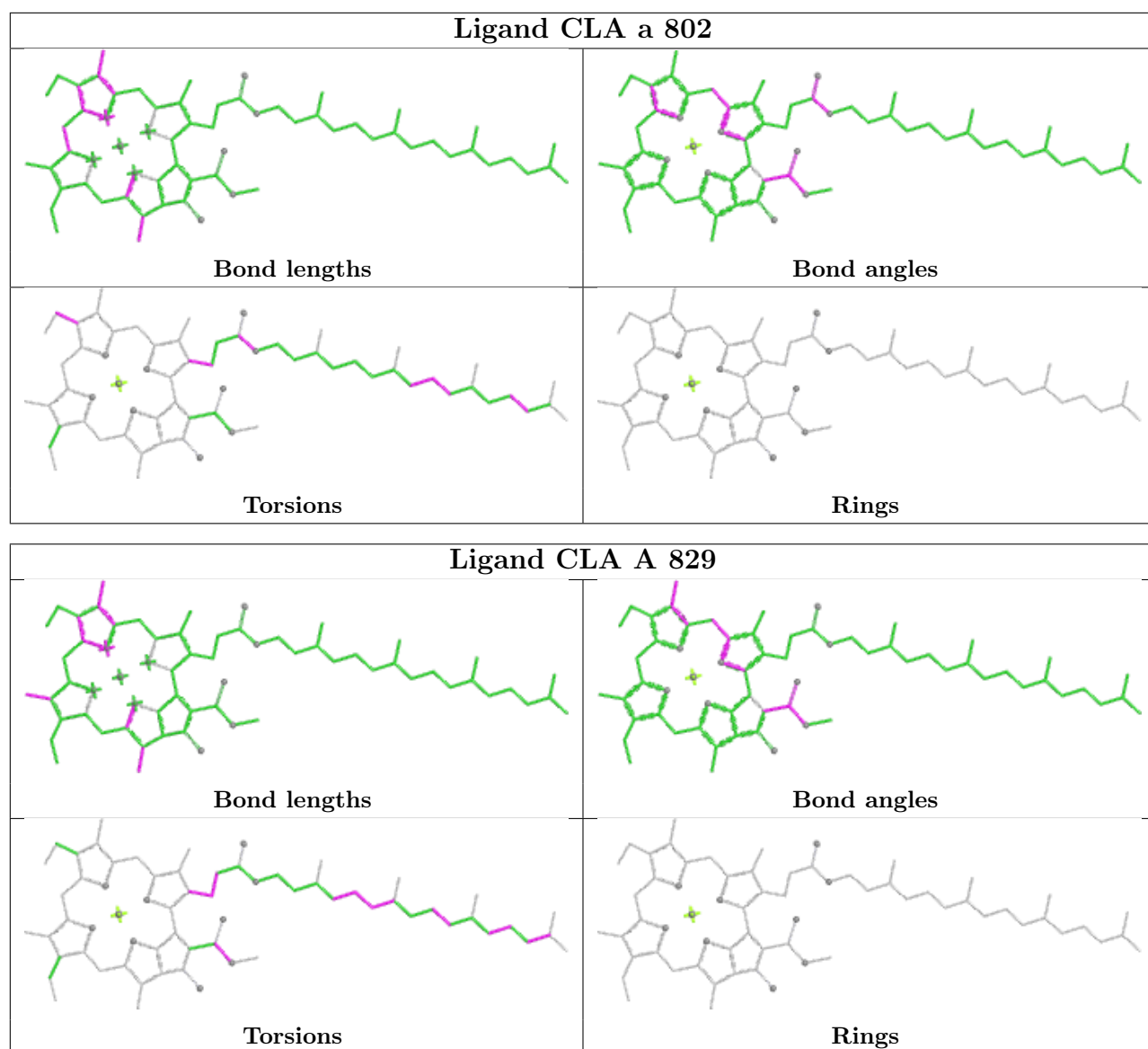


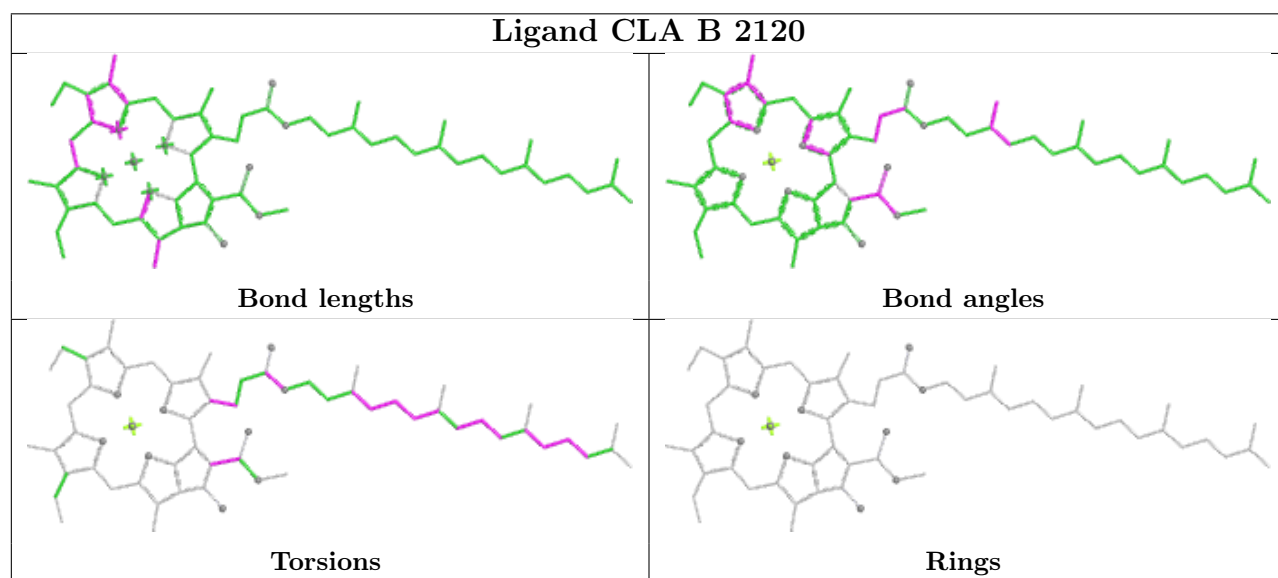
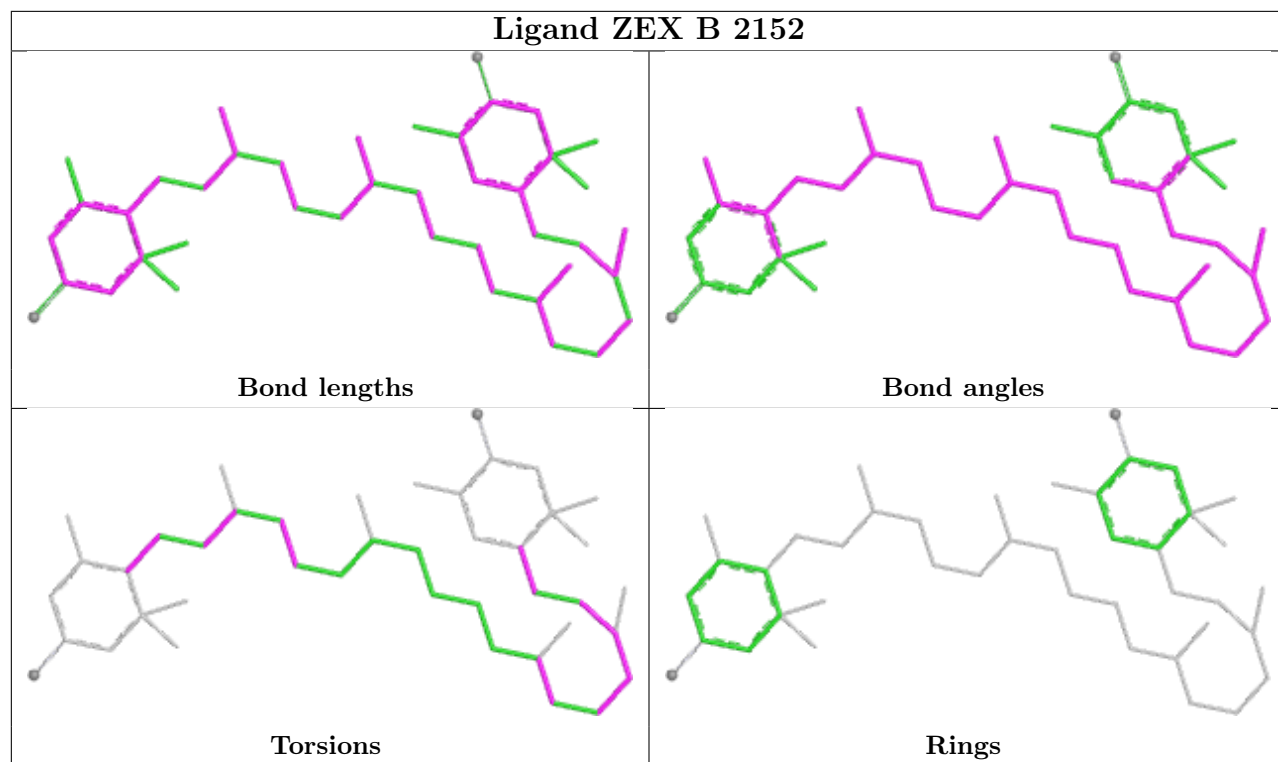


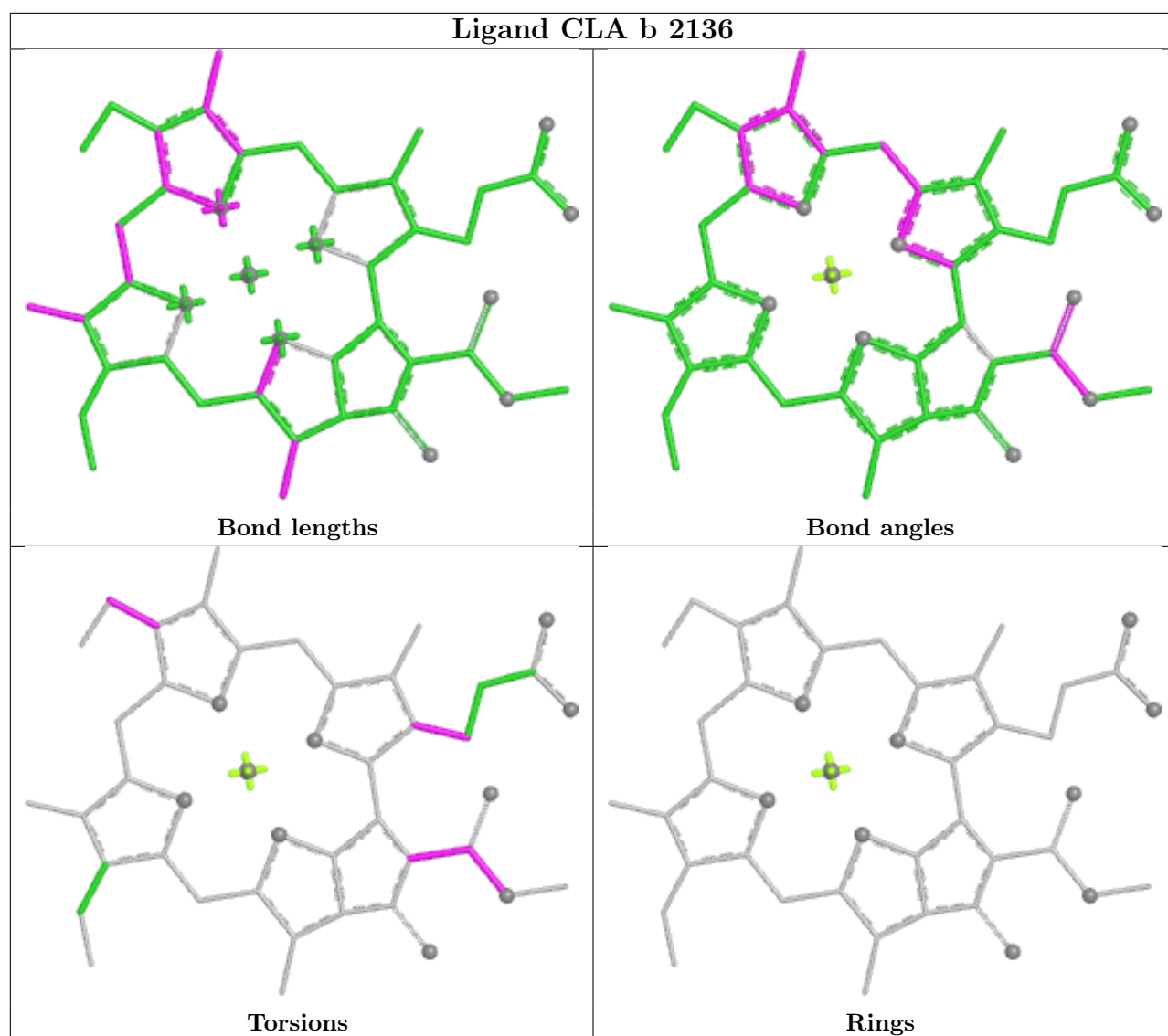




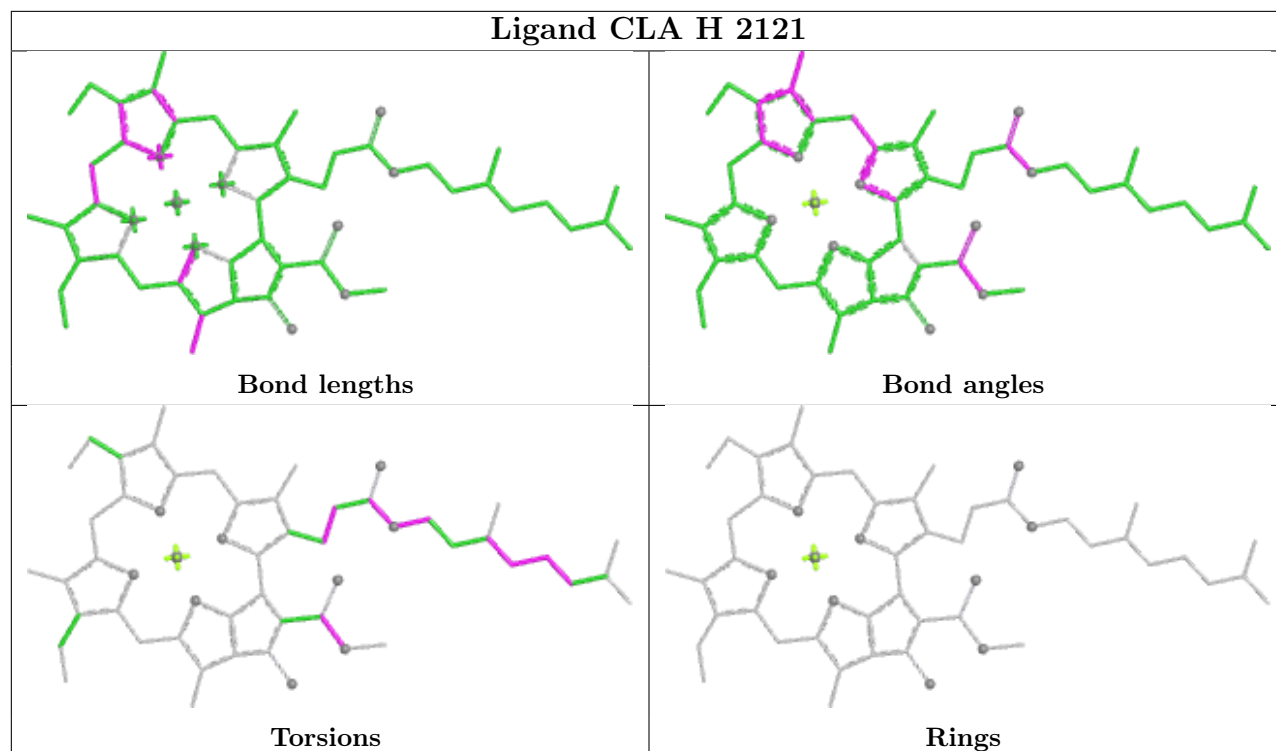
Ligand CLA H 2108**Ligand CLA a 832****Ligand CLA A 804**



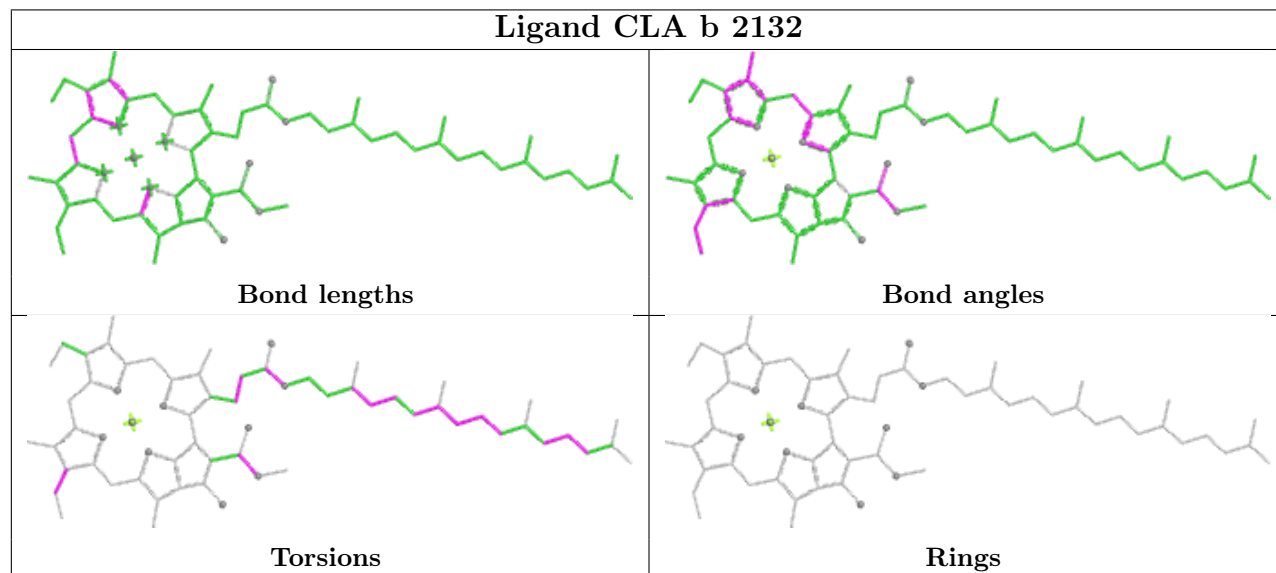




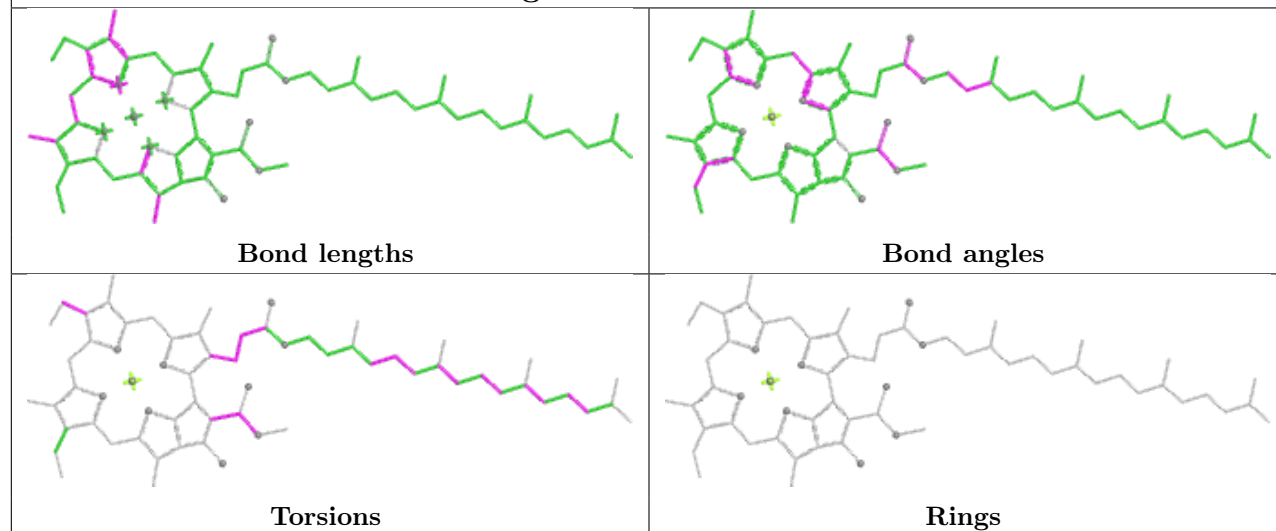
Ligand CLA H 2121



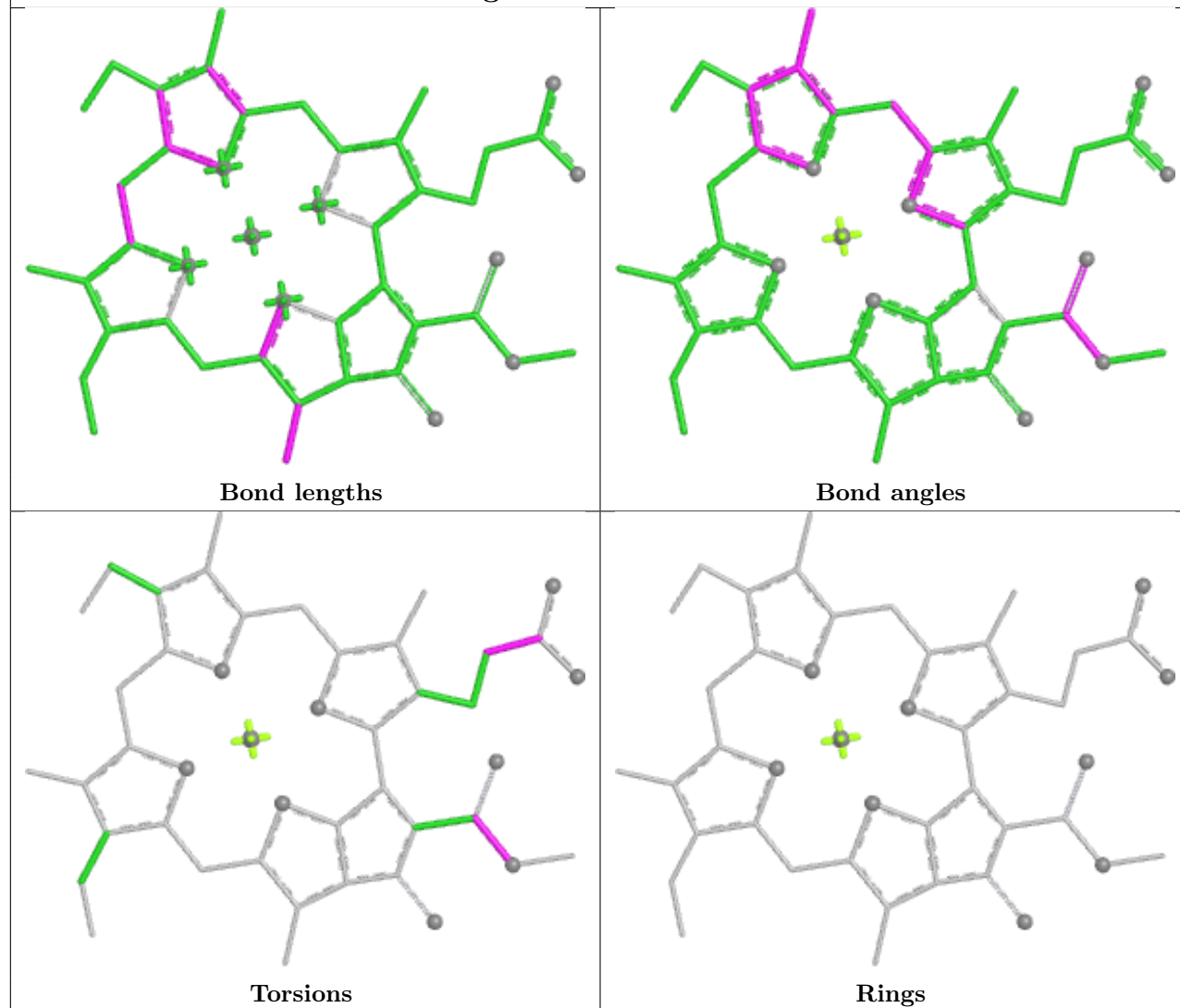
Ligand CLA b 2132



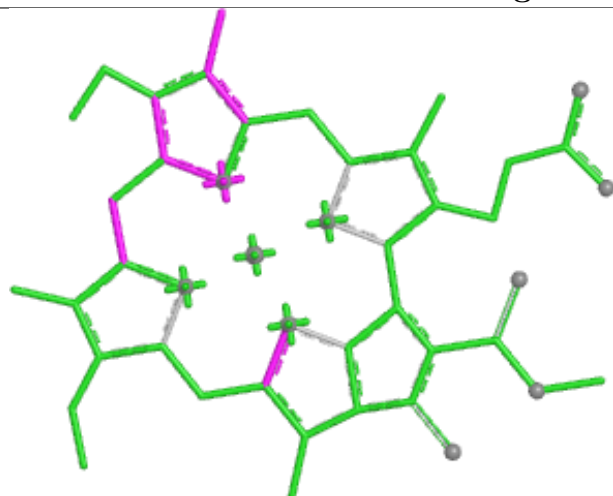
Ligand CLA H 2114



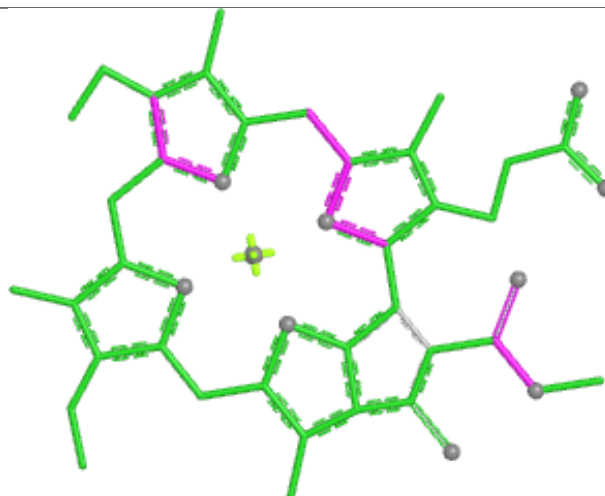
Ligand CLA H 2134



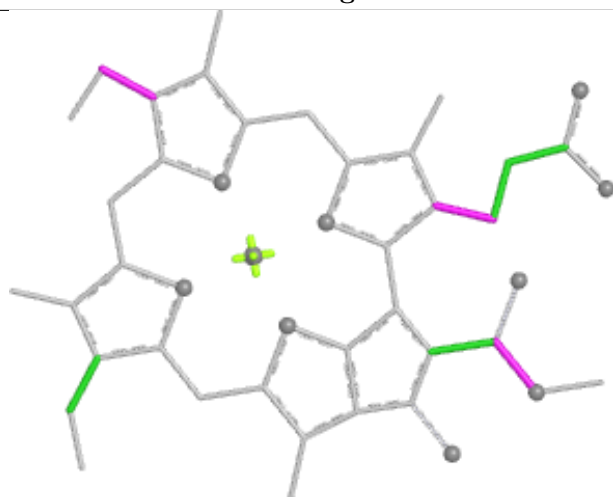
Ligand CLA A 815



Bond lengths



Bond angles

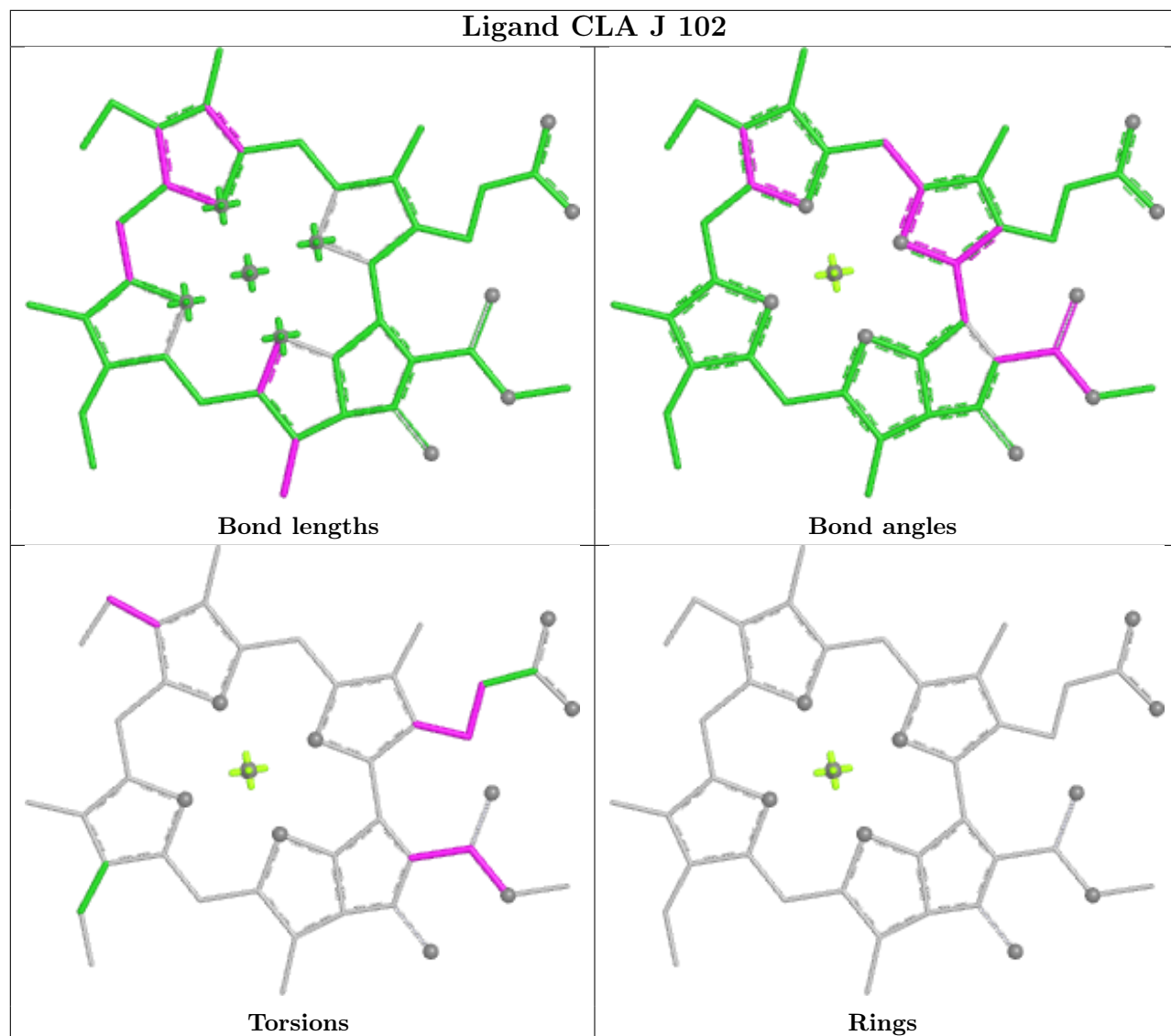


Torsions

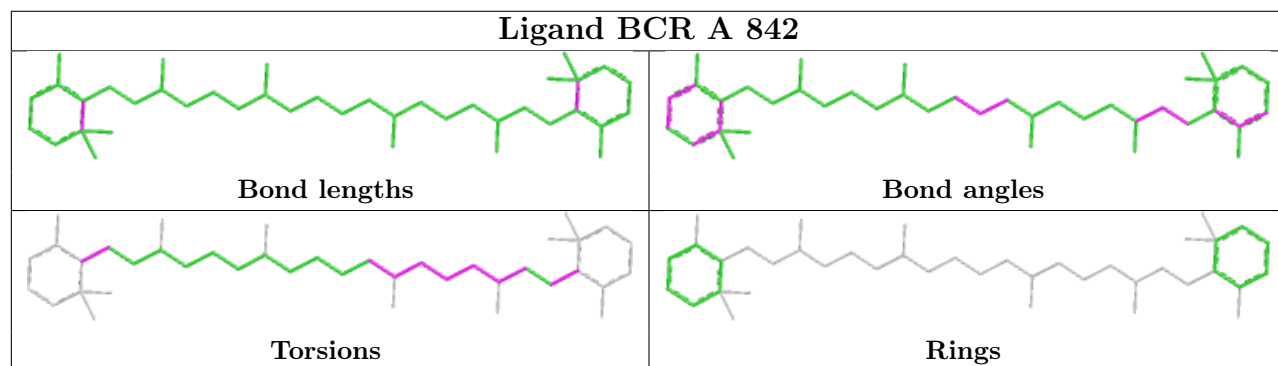


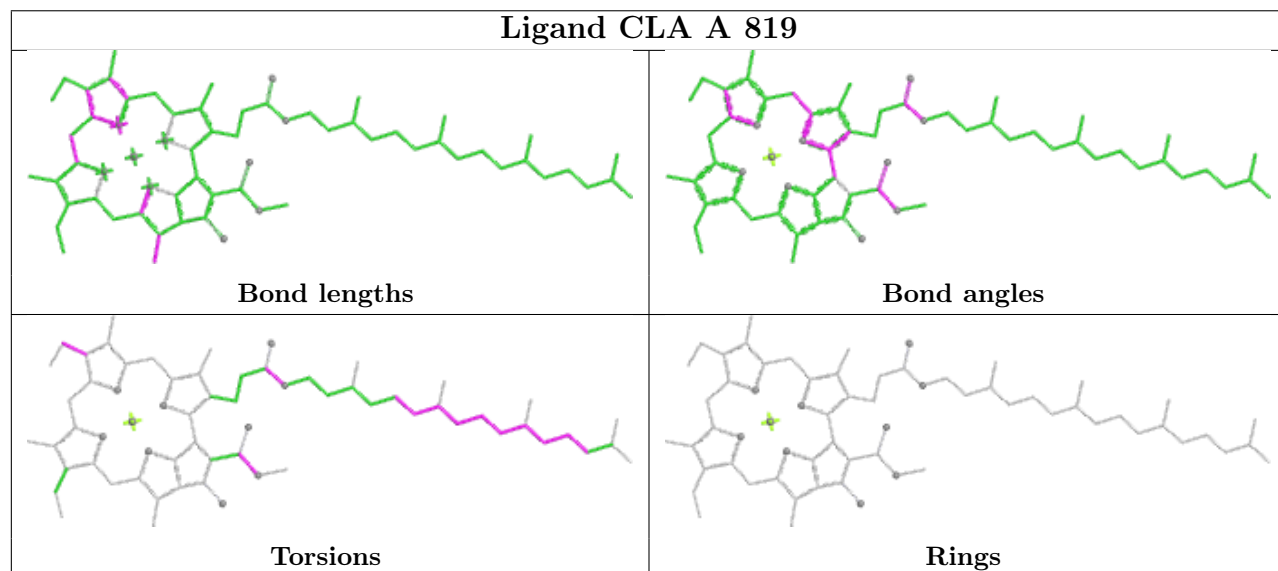
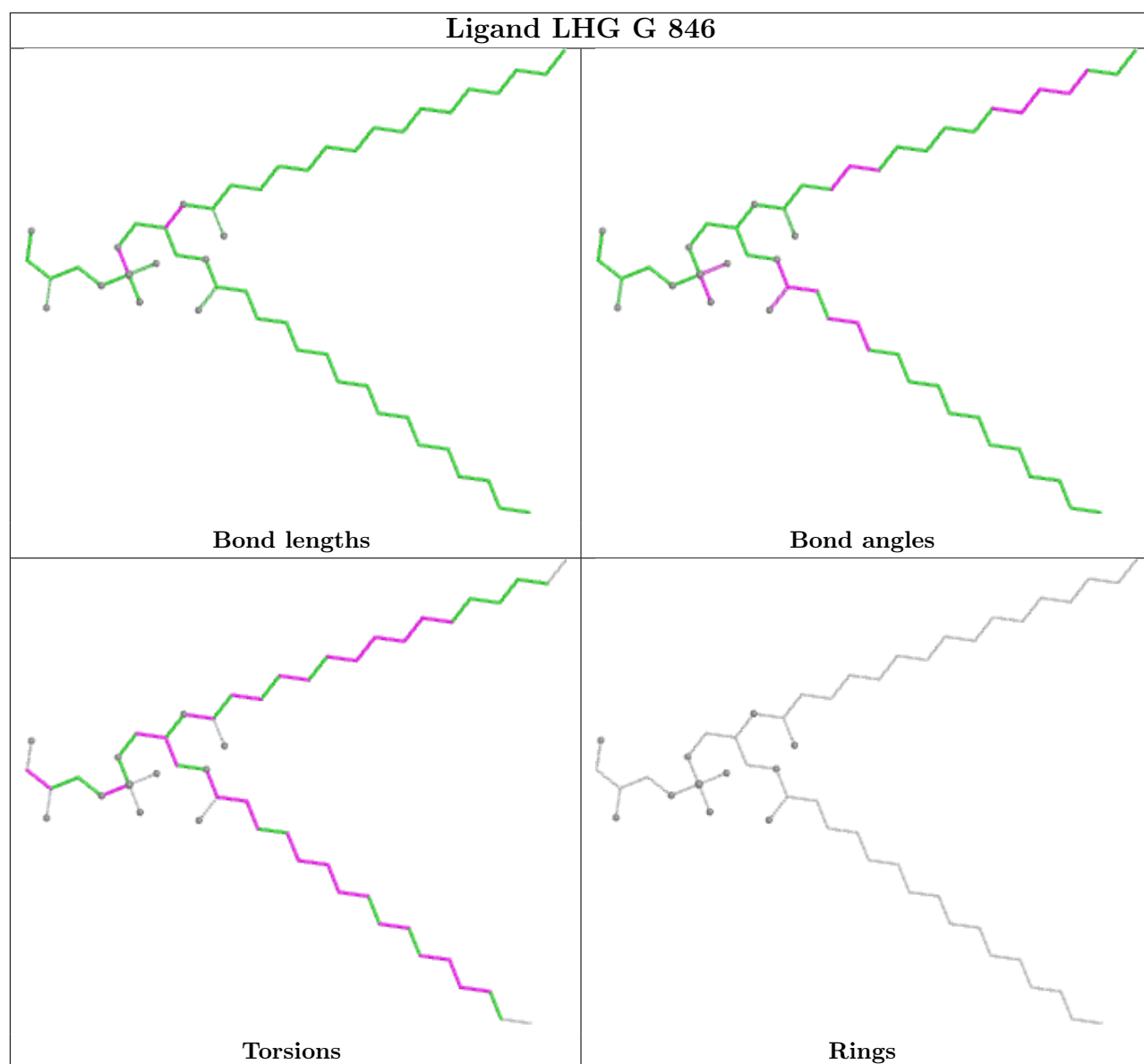
Rings

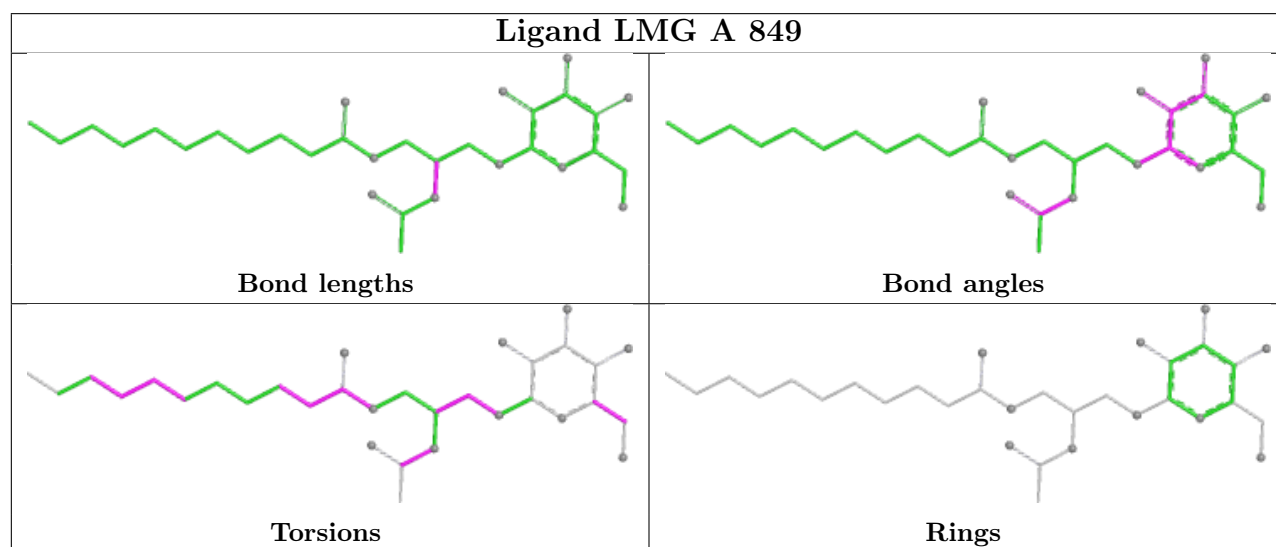
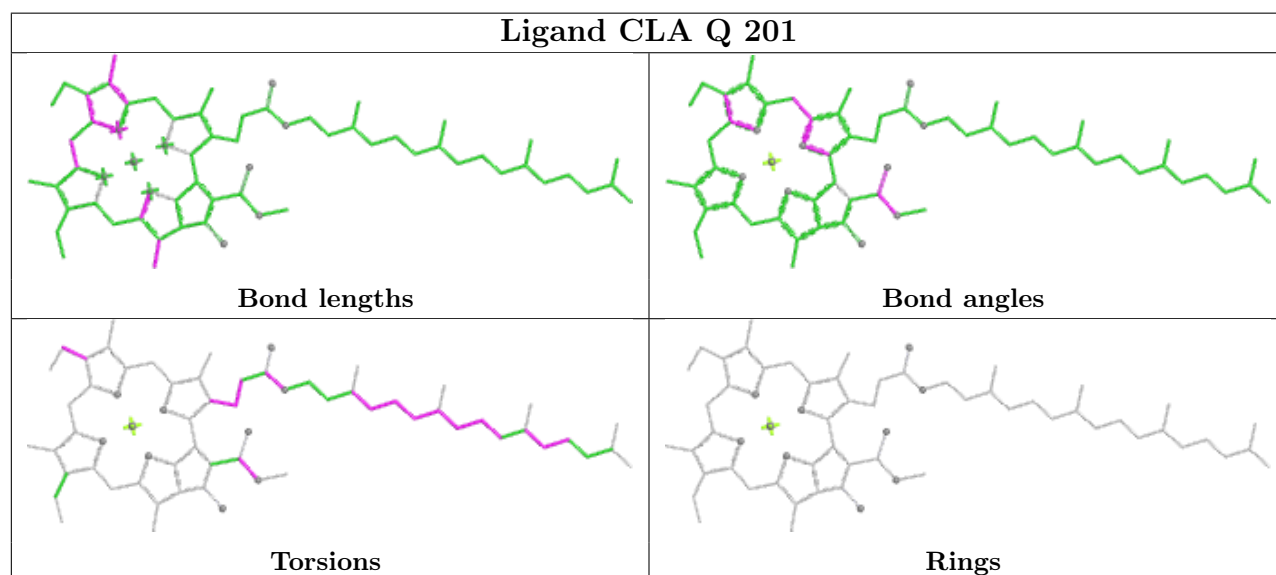
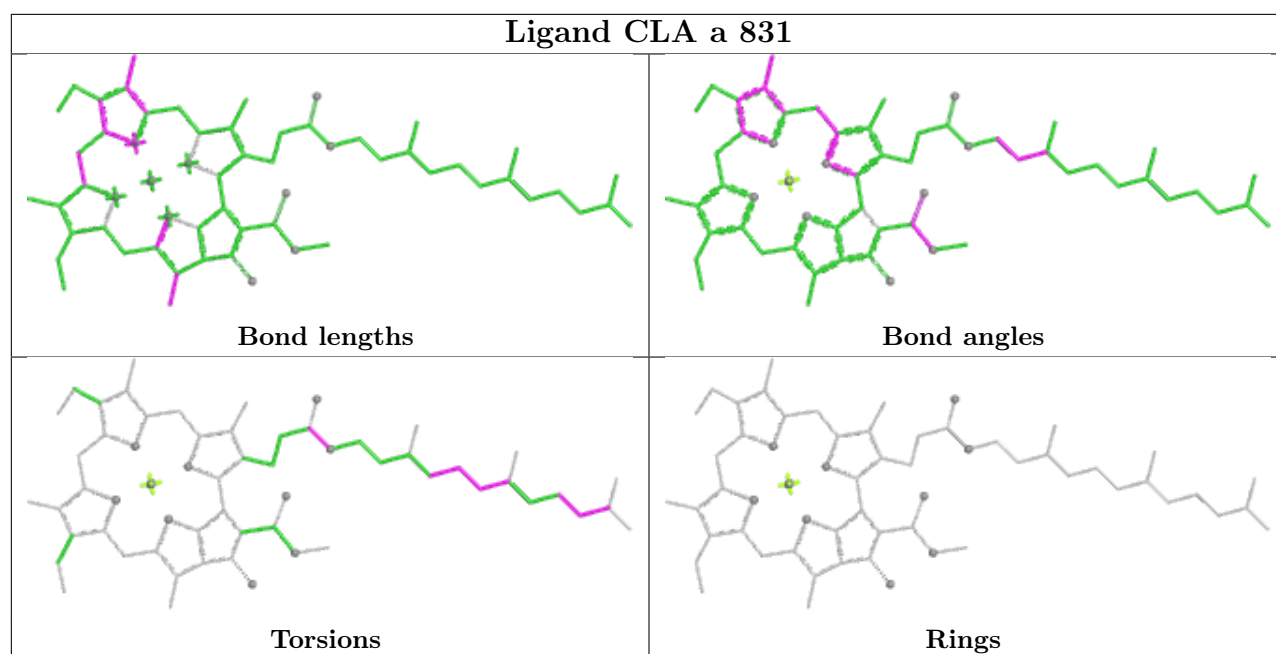
Ligand CLA J 102

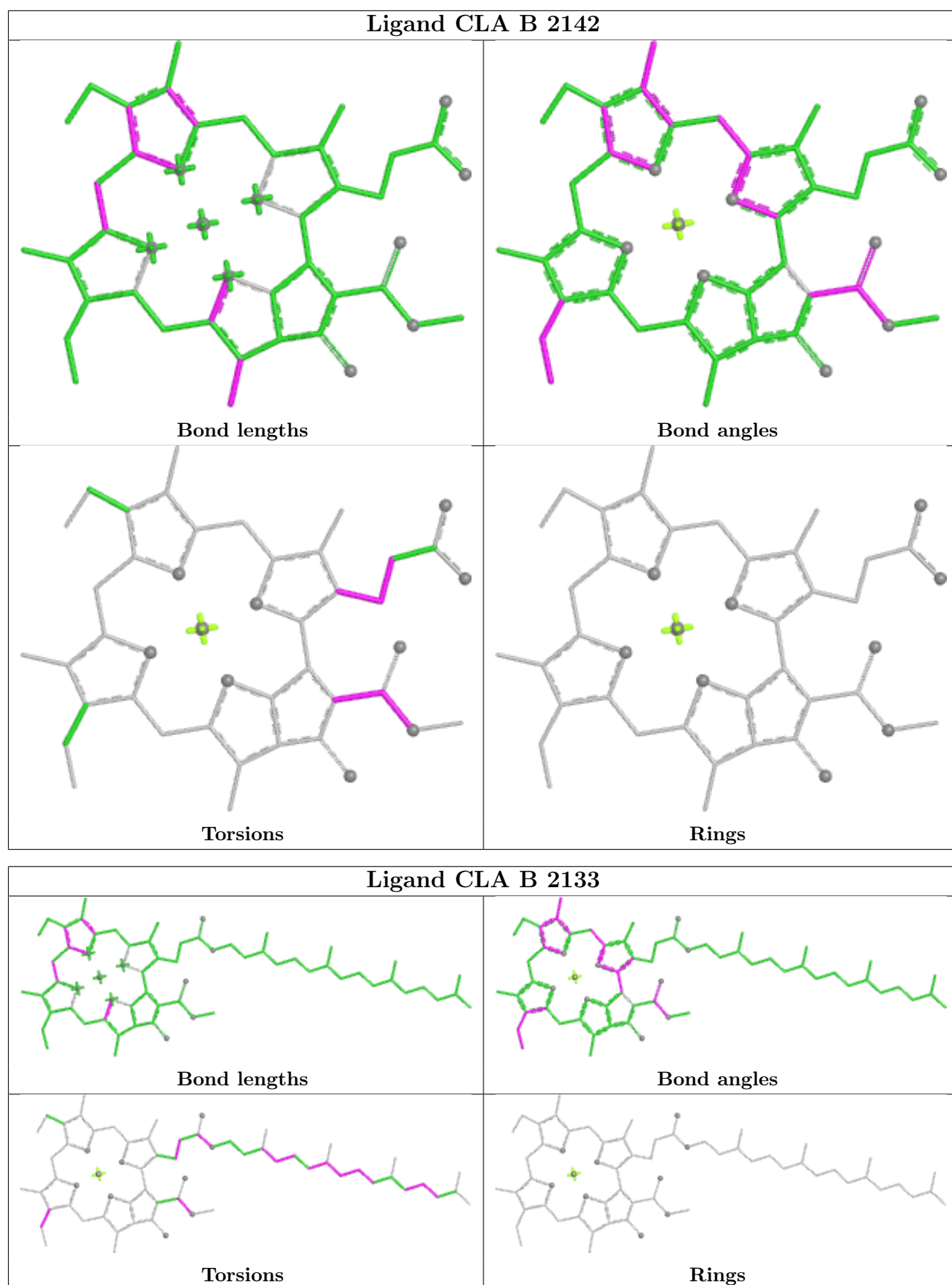


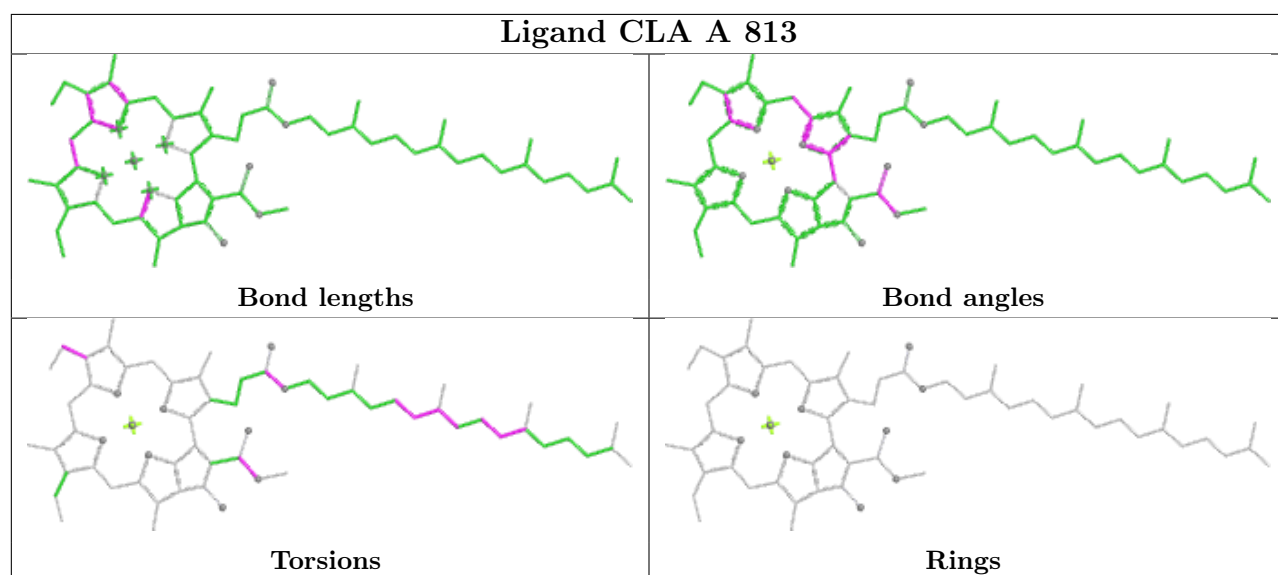
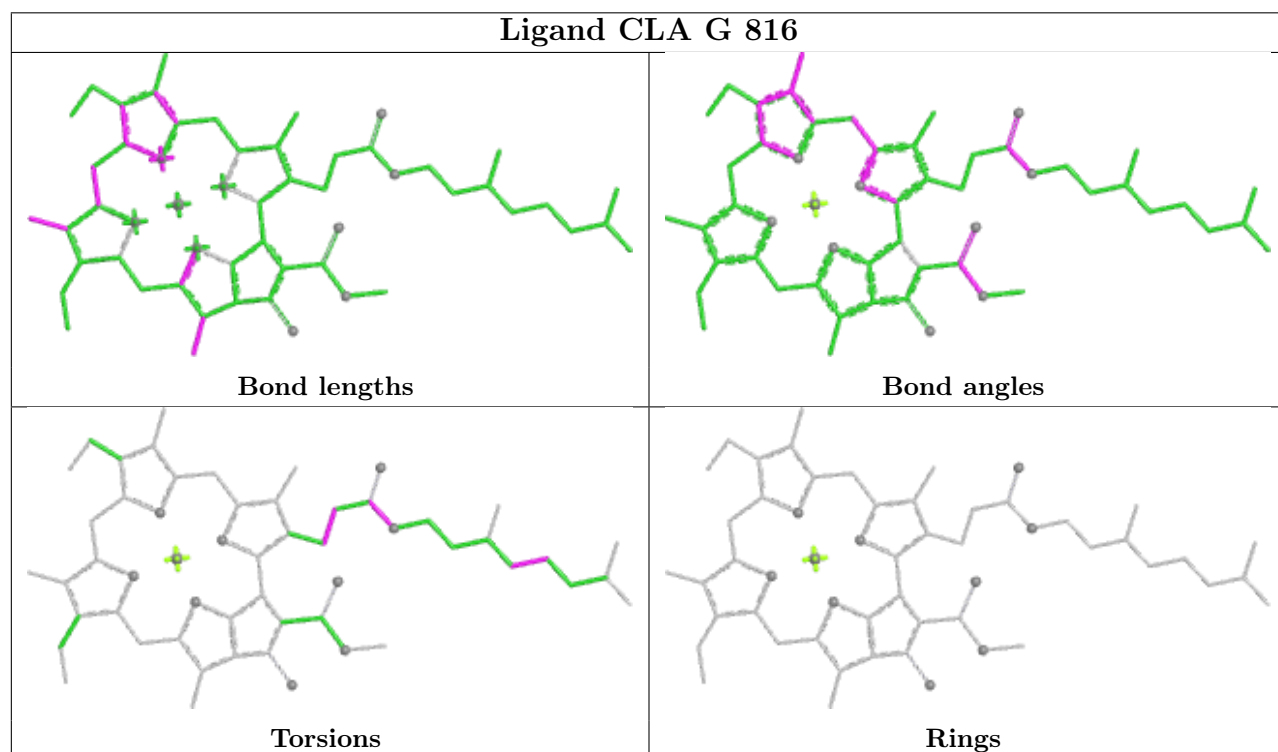
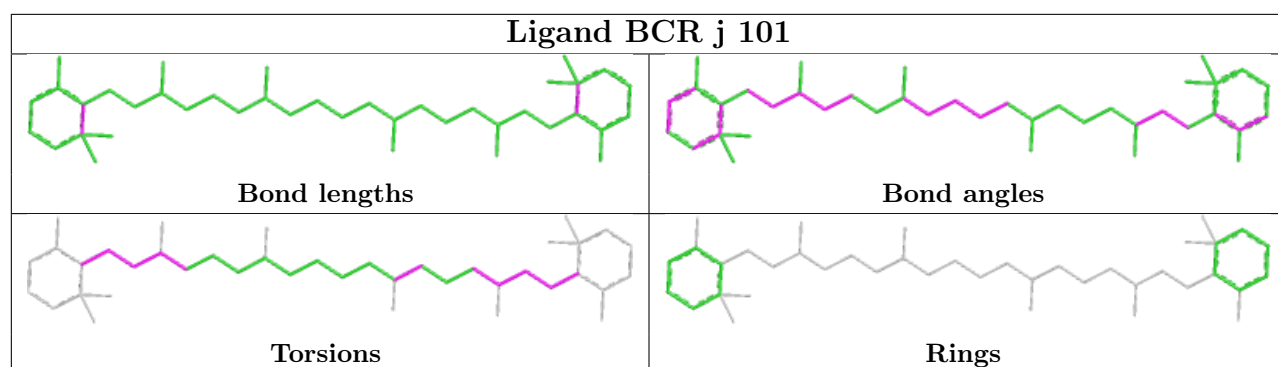
Ligand BCR A 842

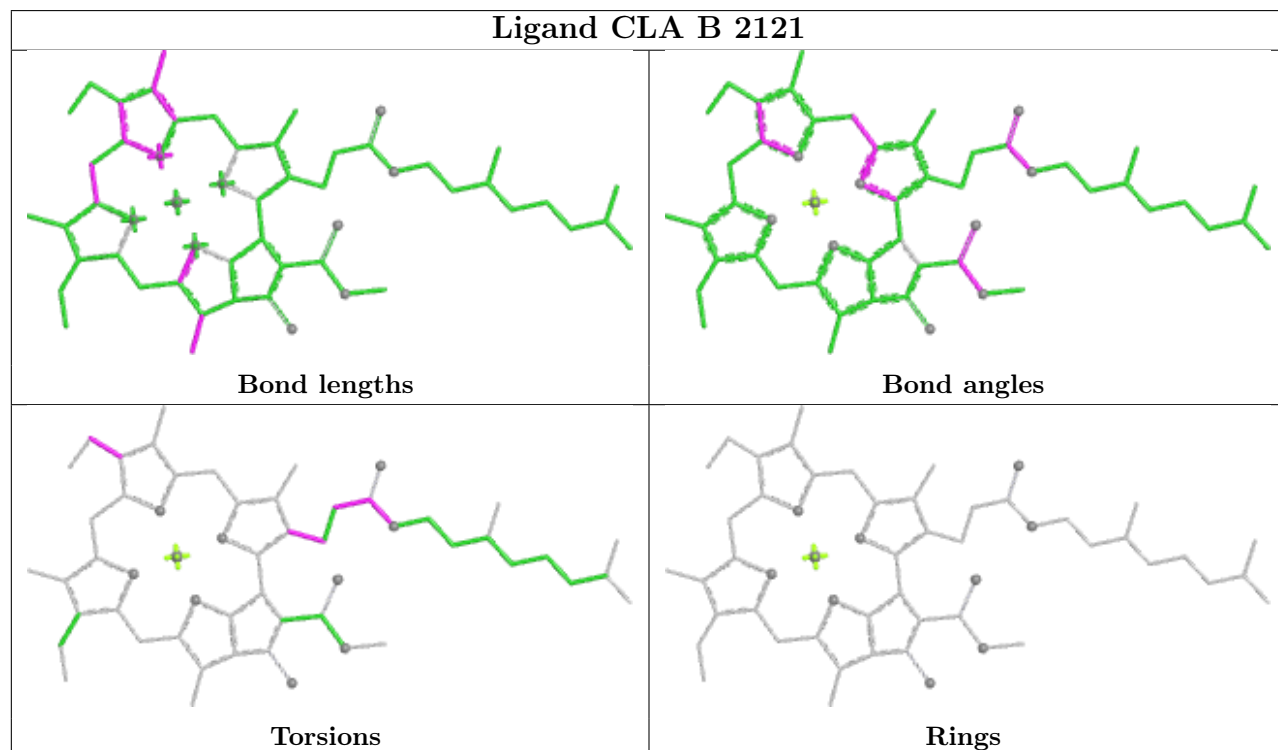
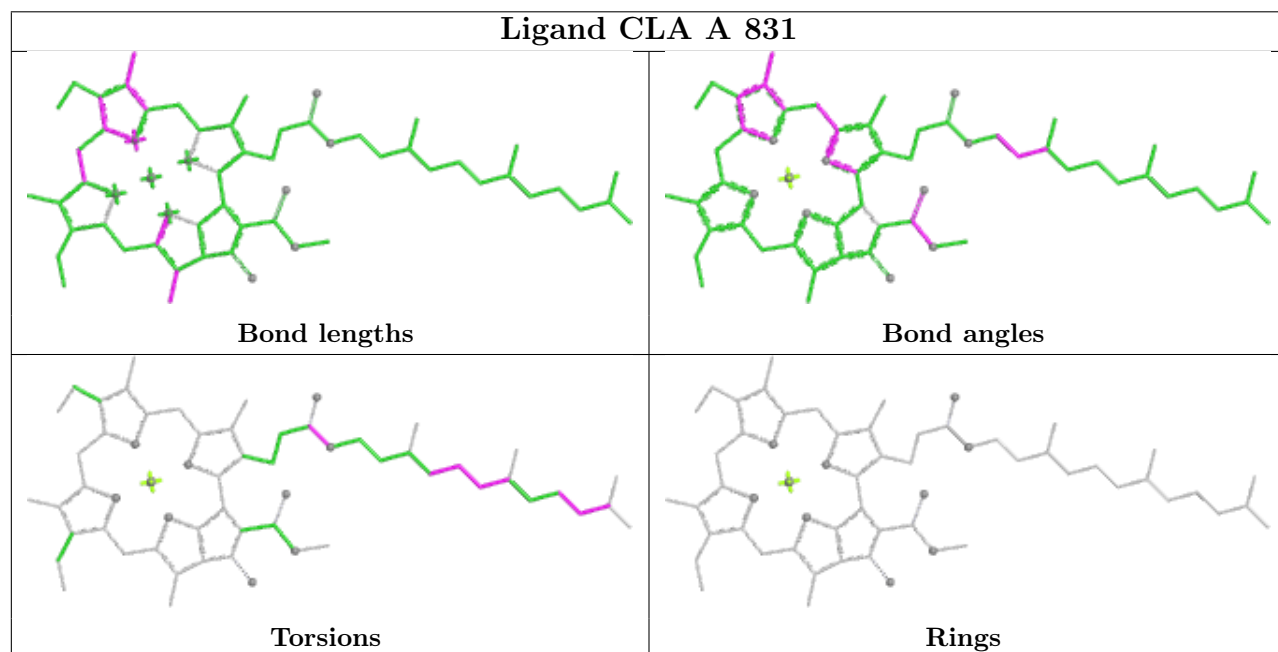
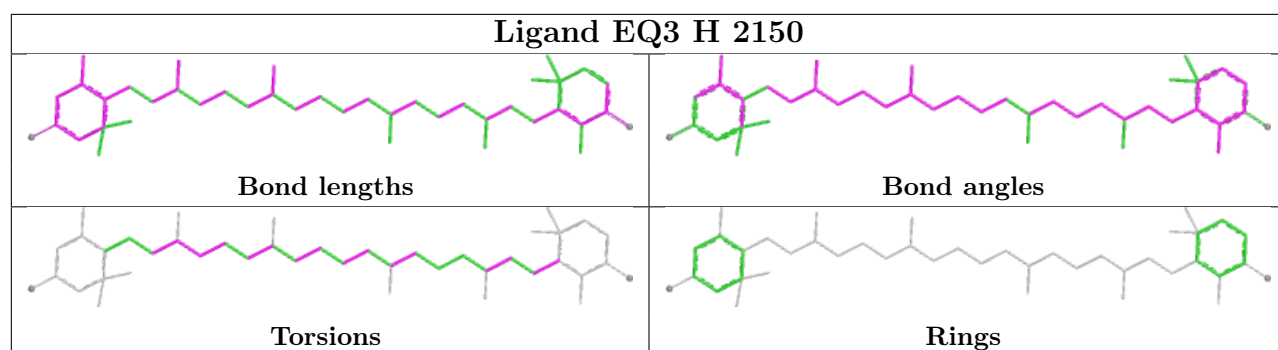


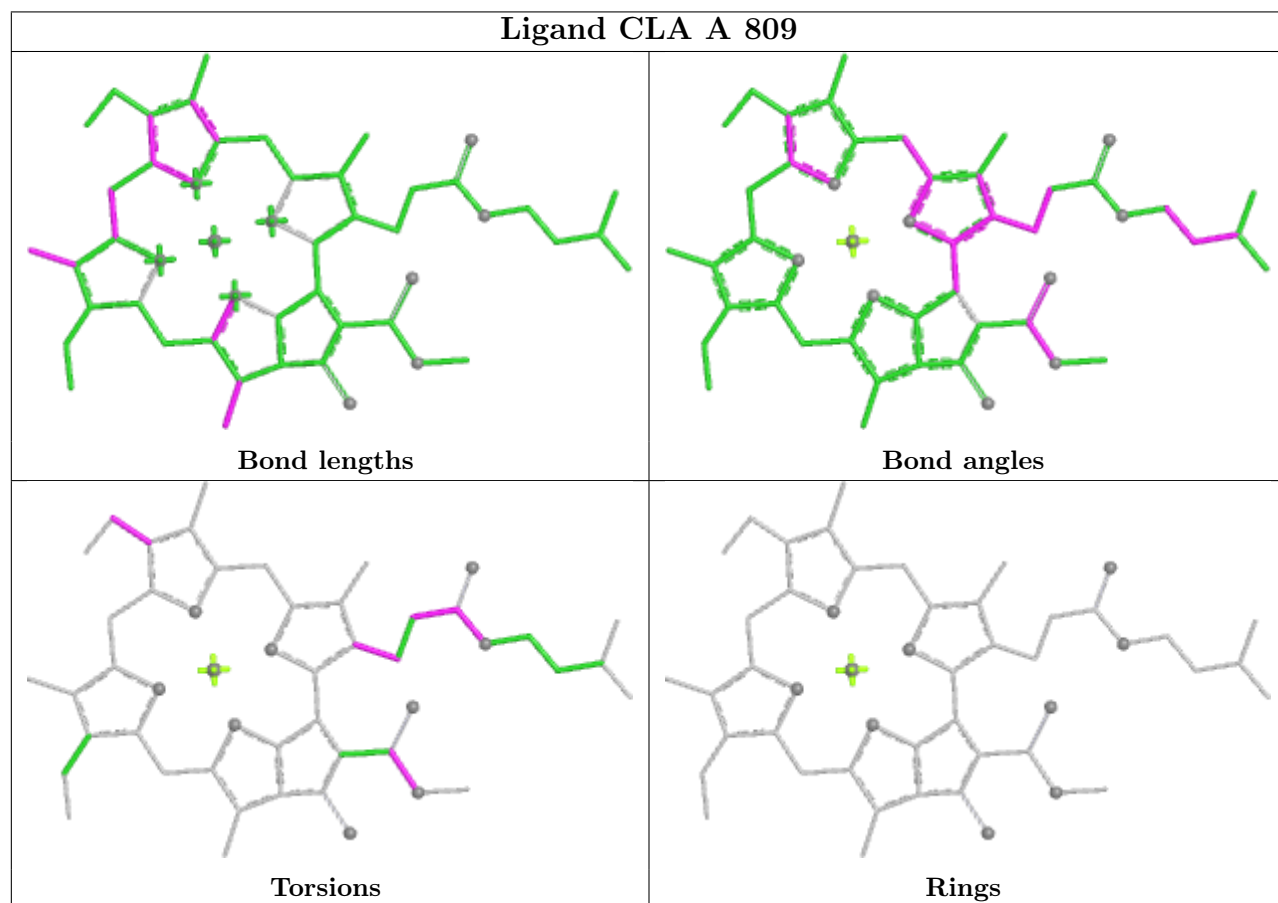
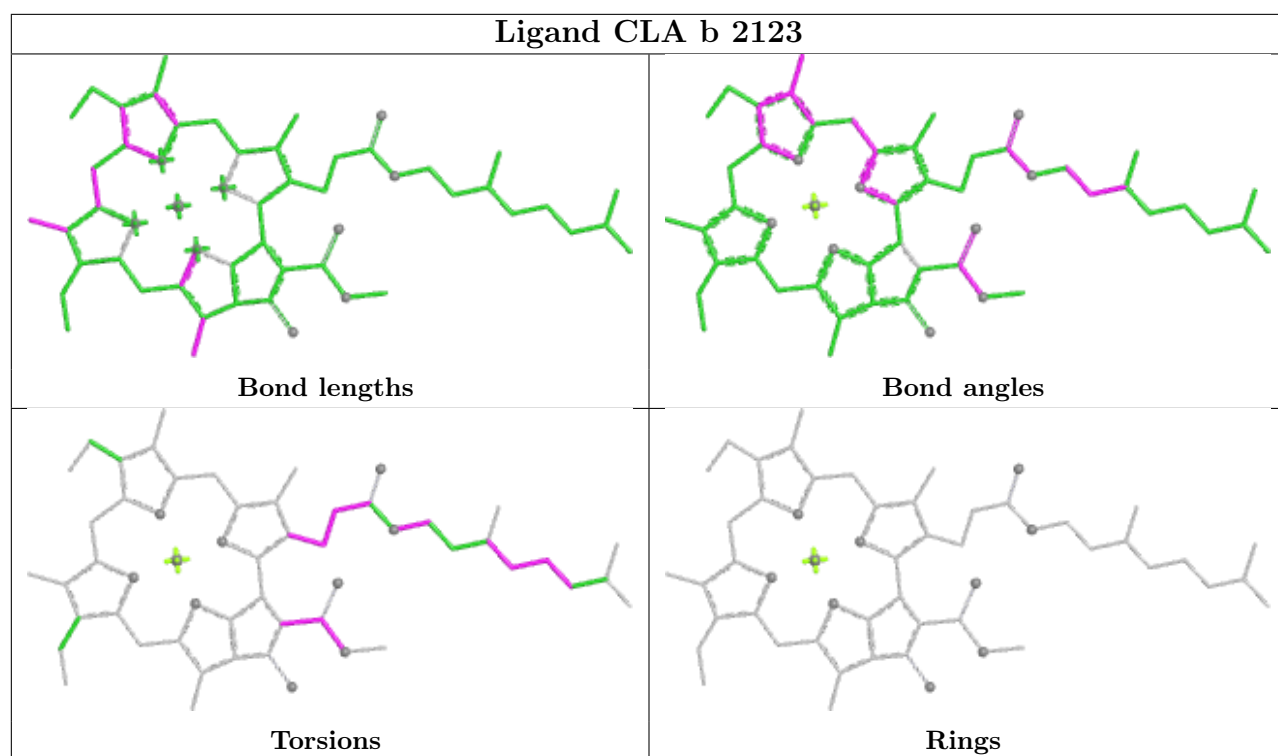


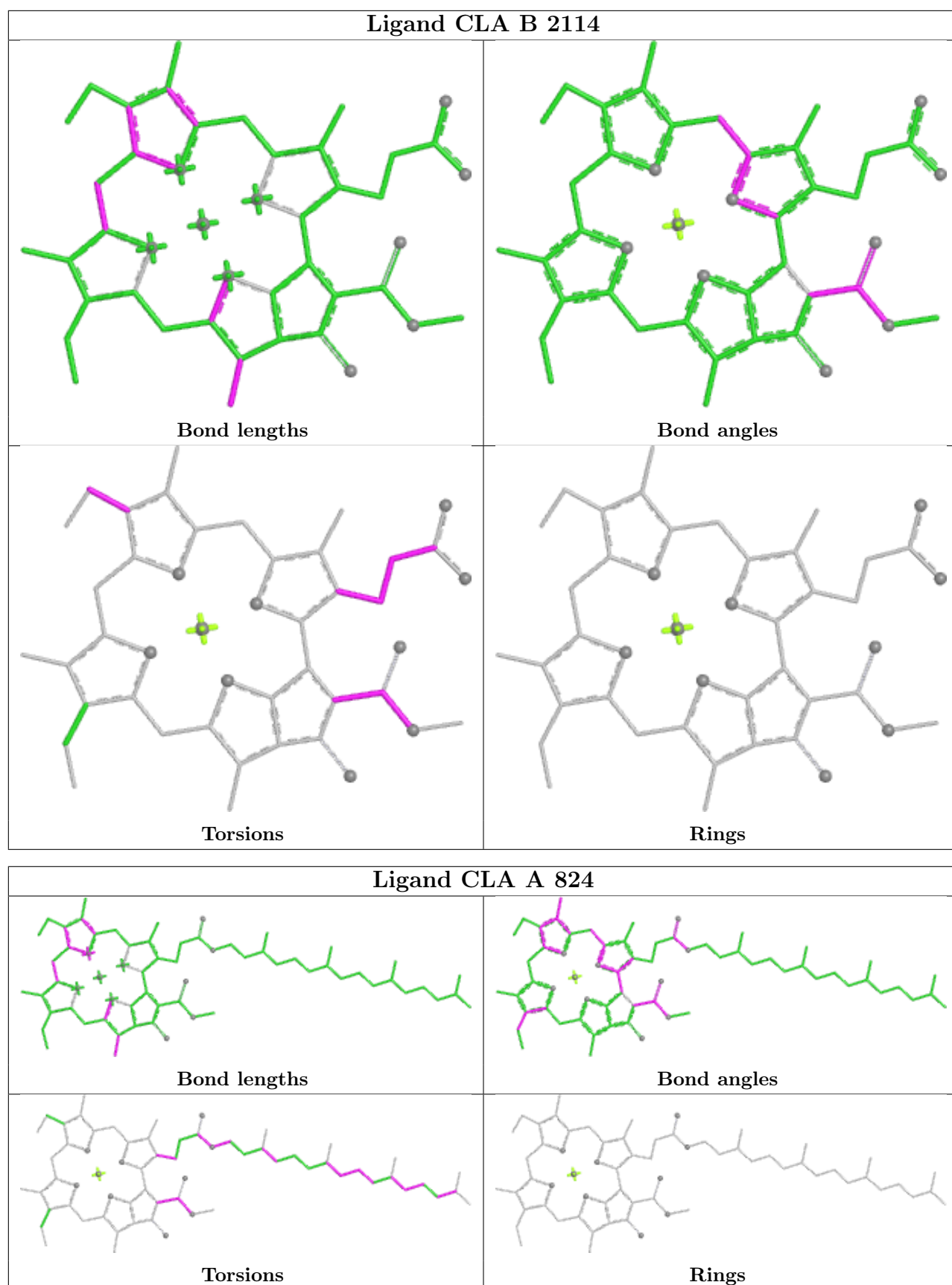


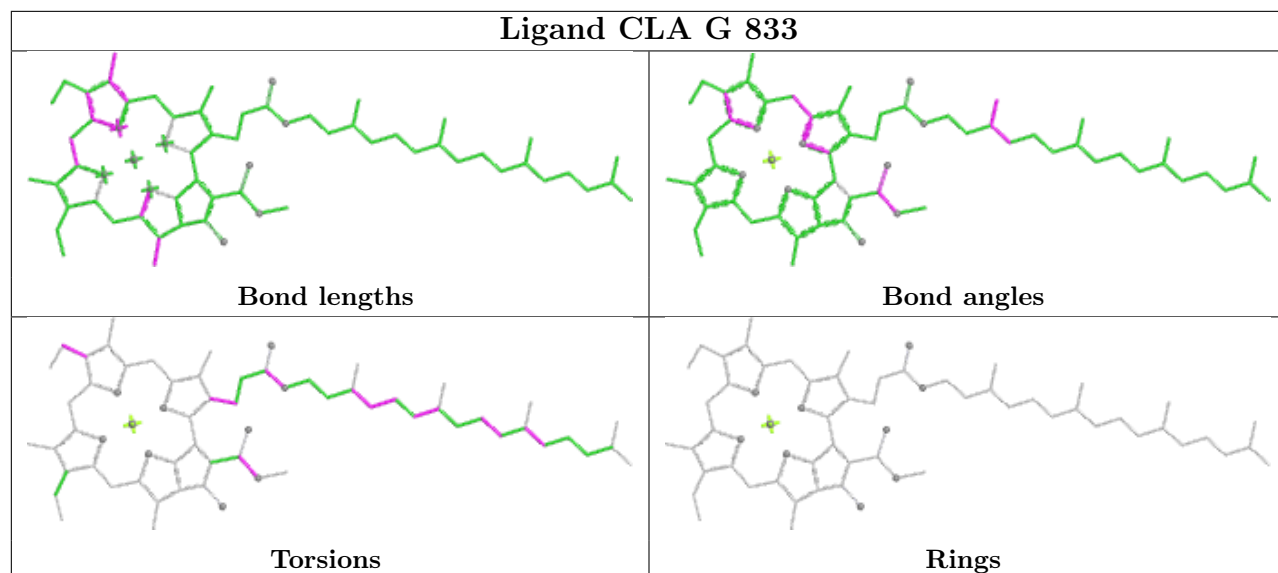
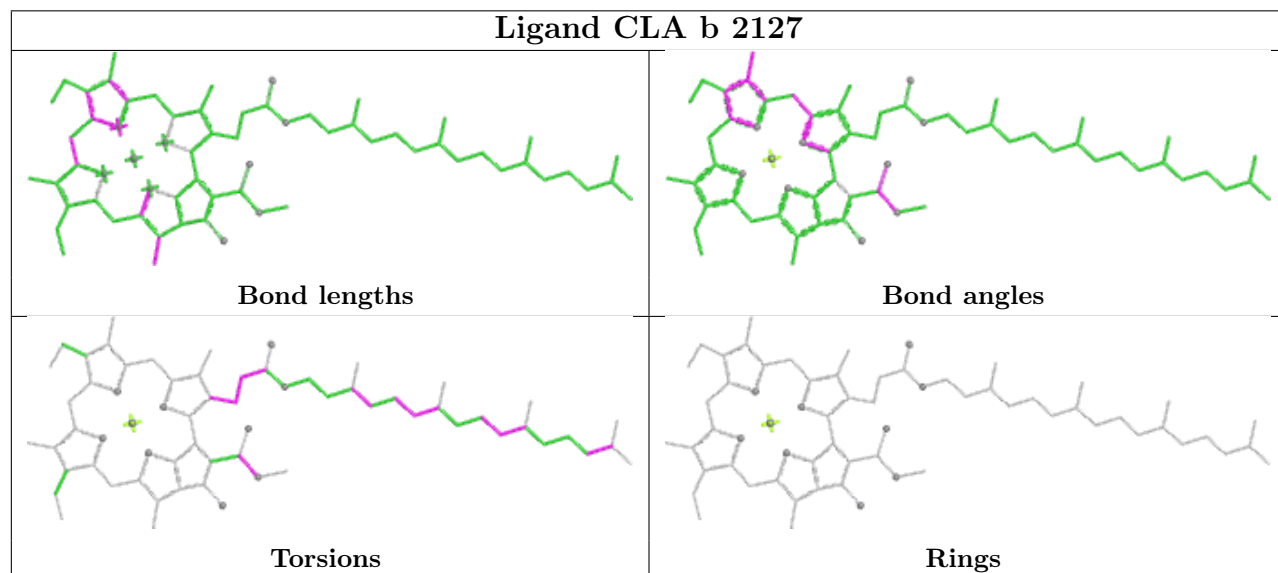
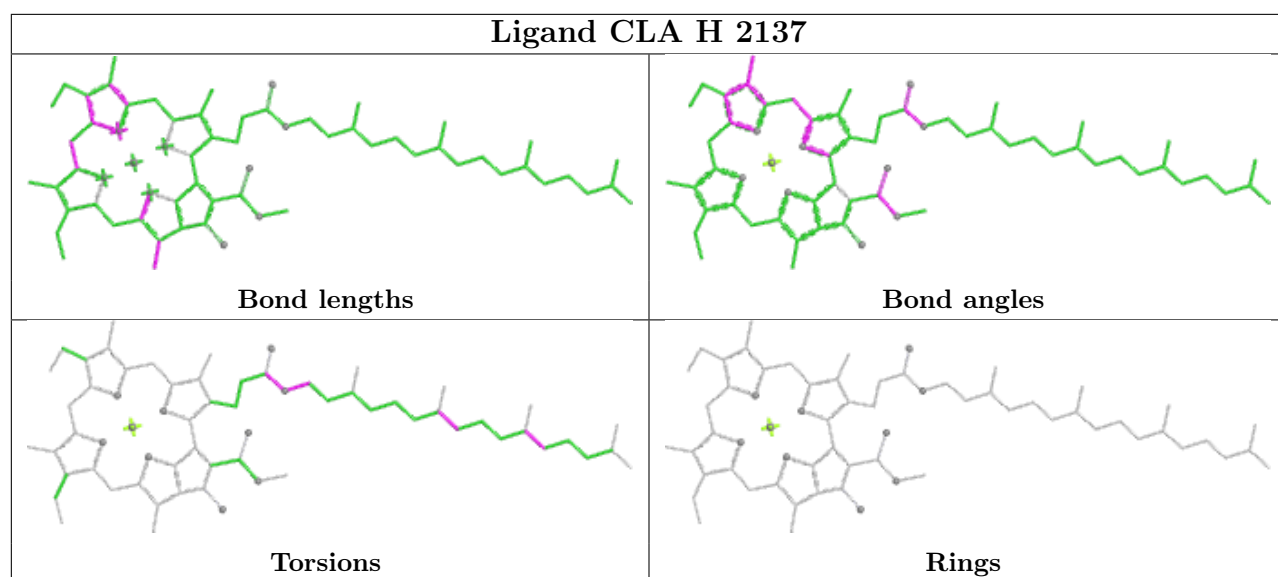


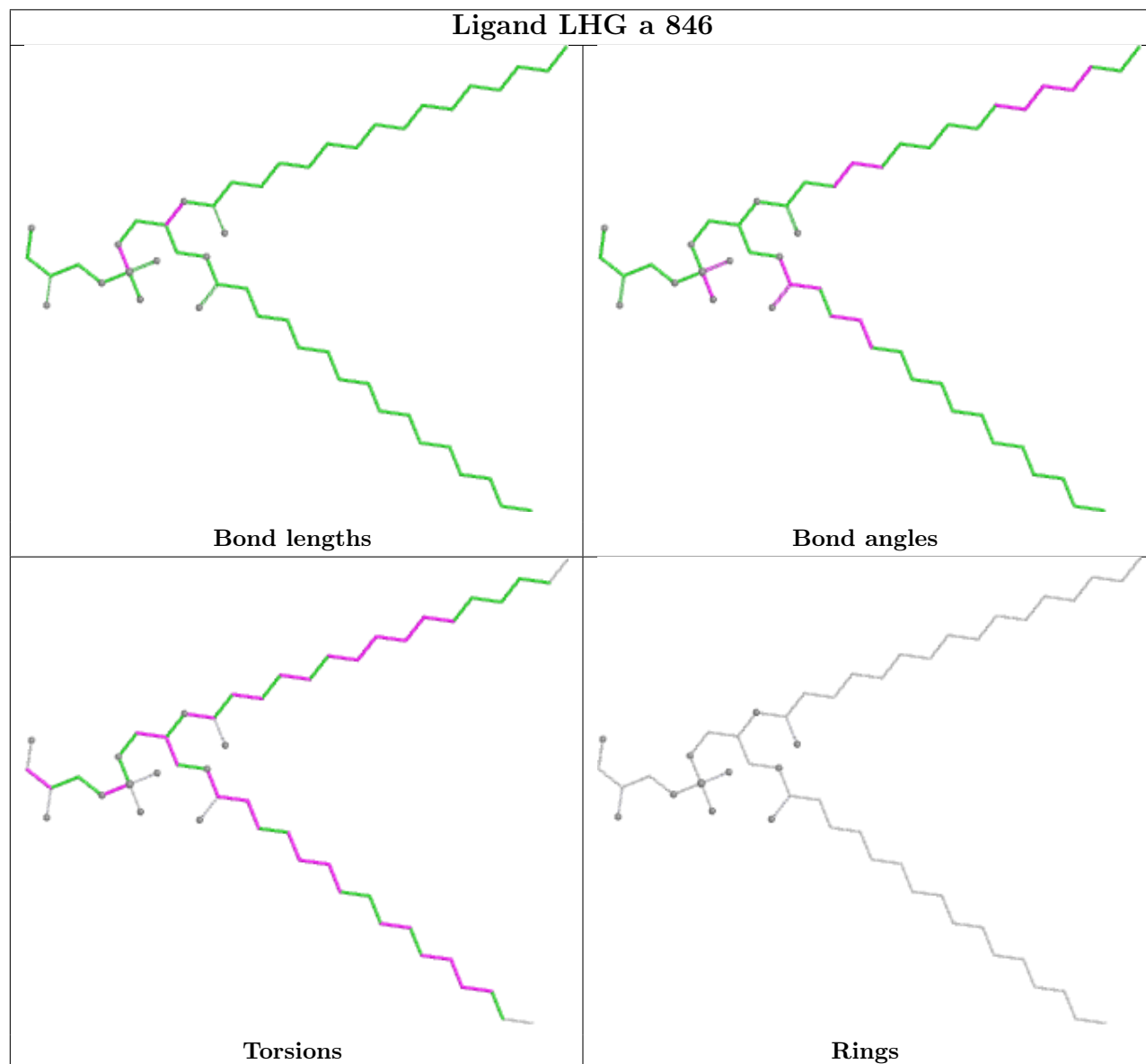
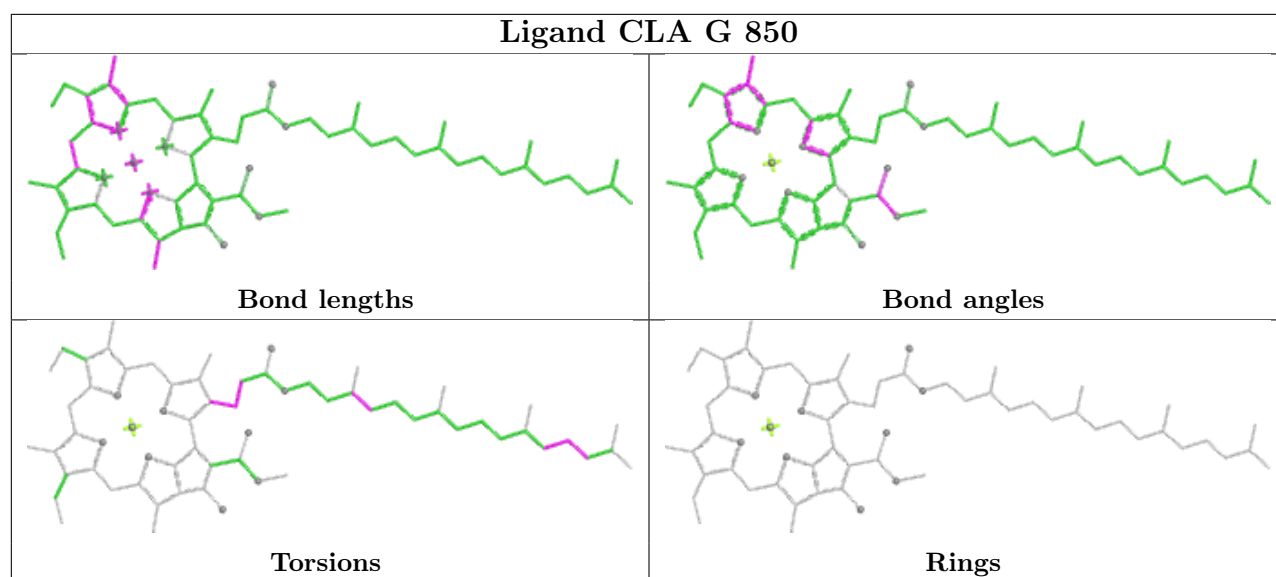


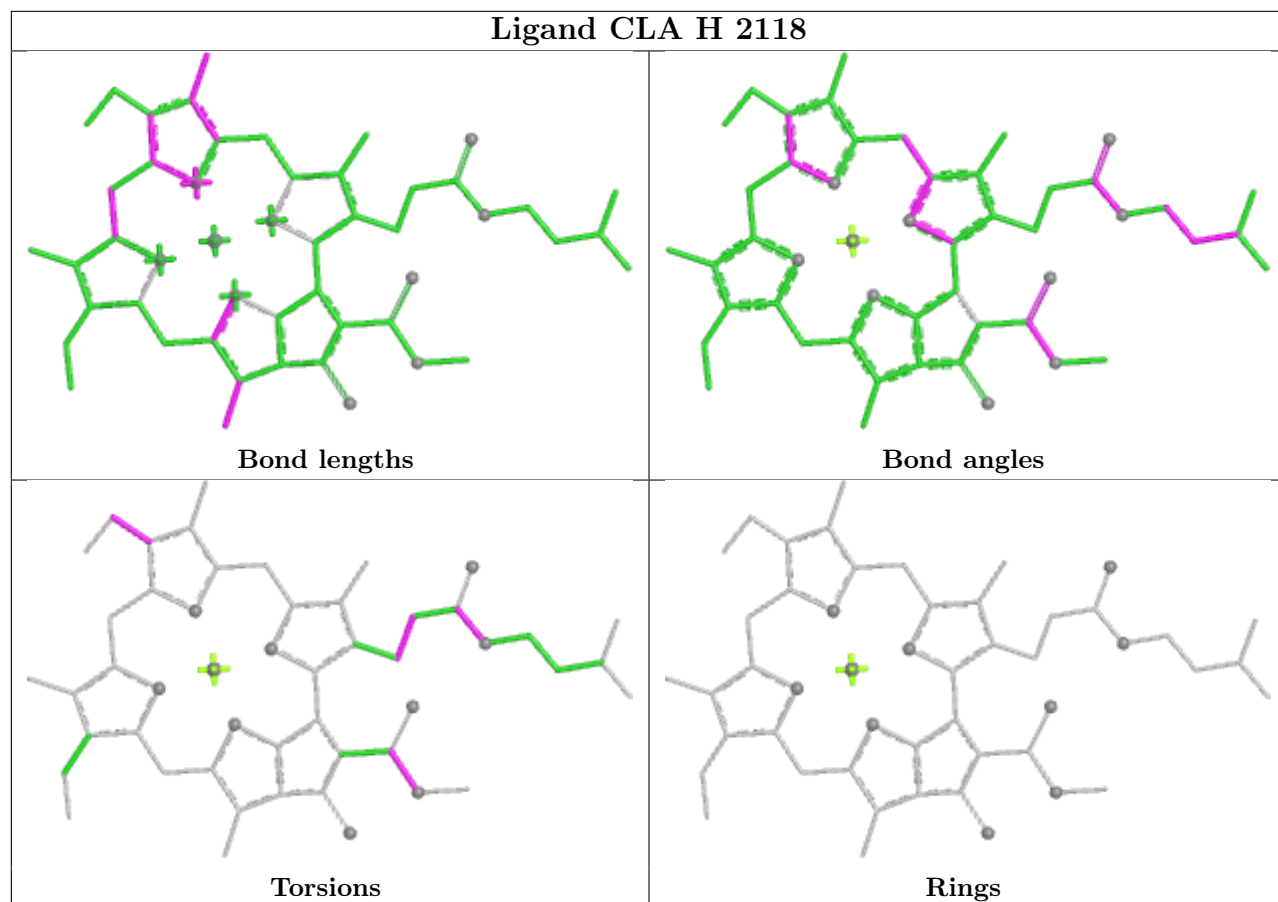




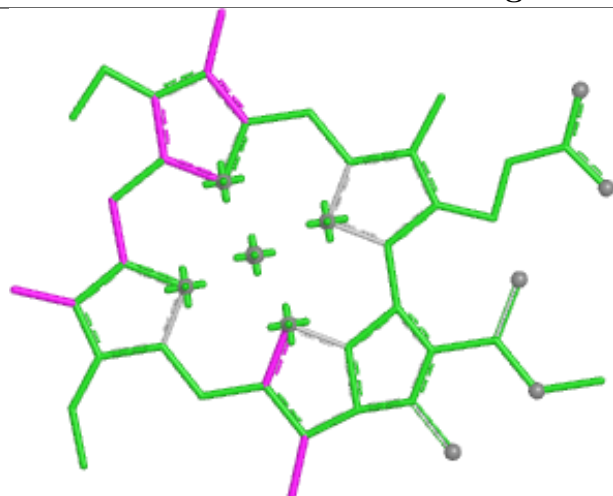




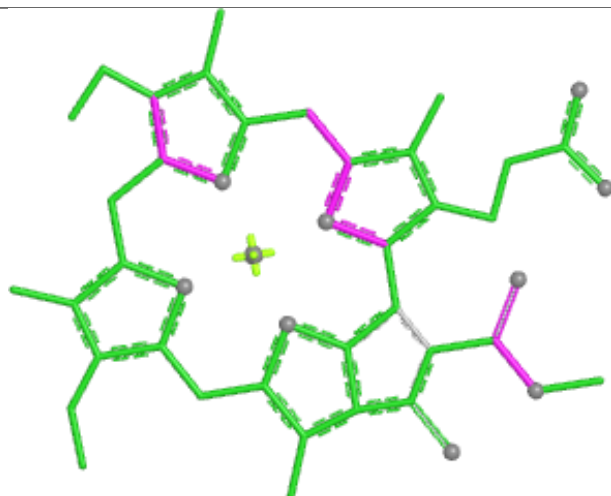




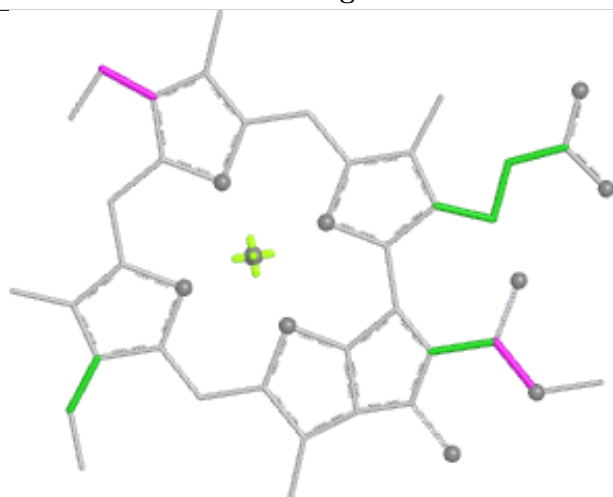
Ligand CLA B 2116



Bond lengths



Bond angles

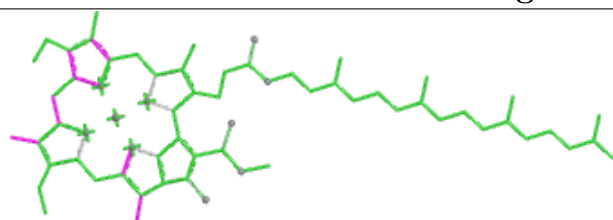


Torsions

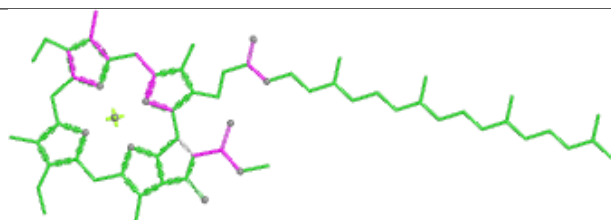


Rings

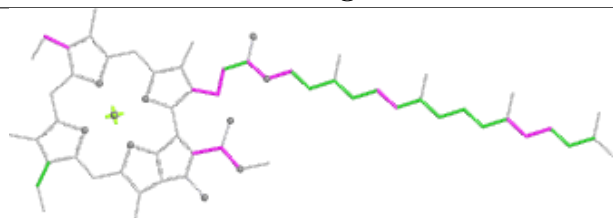
Ligand CLA L 201



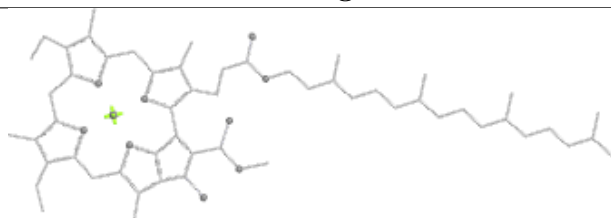
Bond lengths



Bond angles

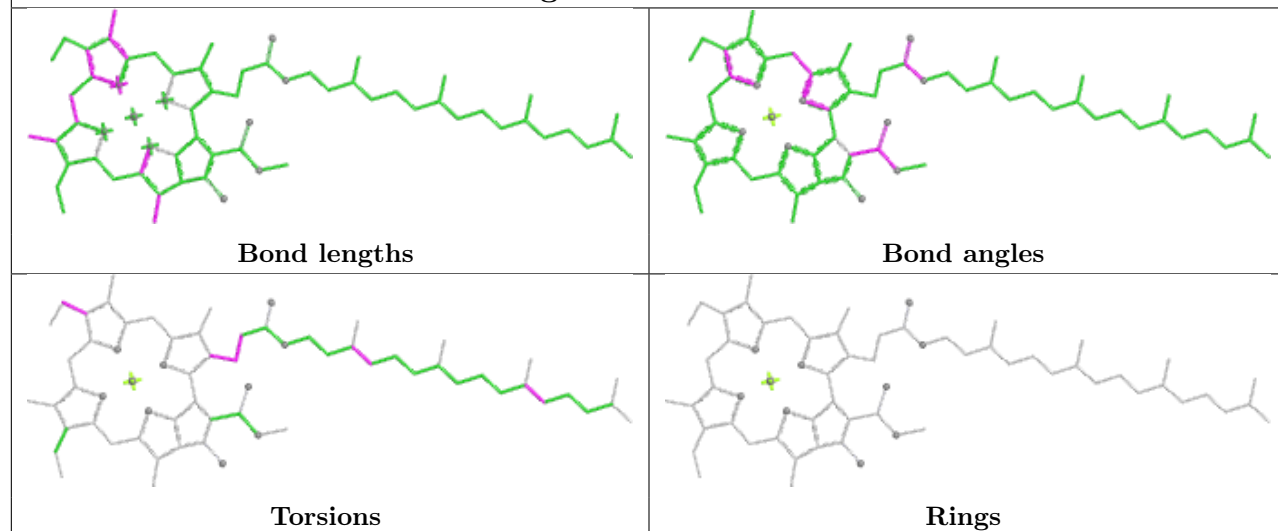


Torsions

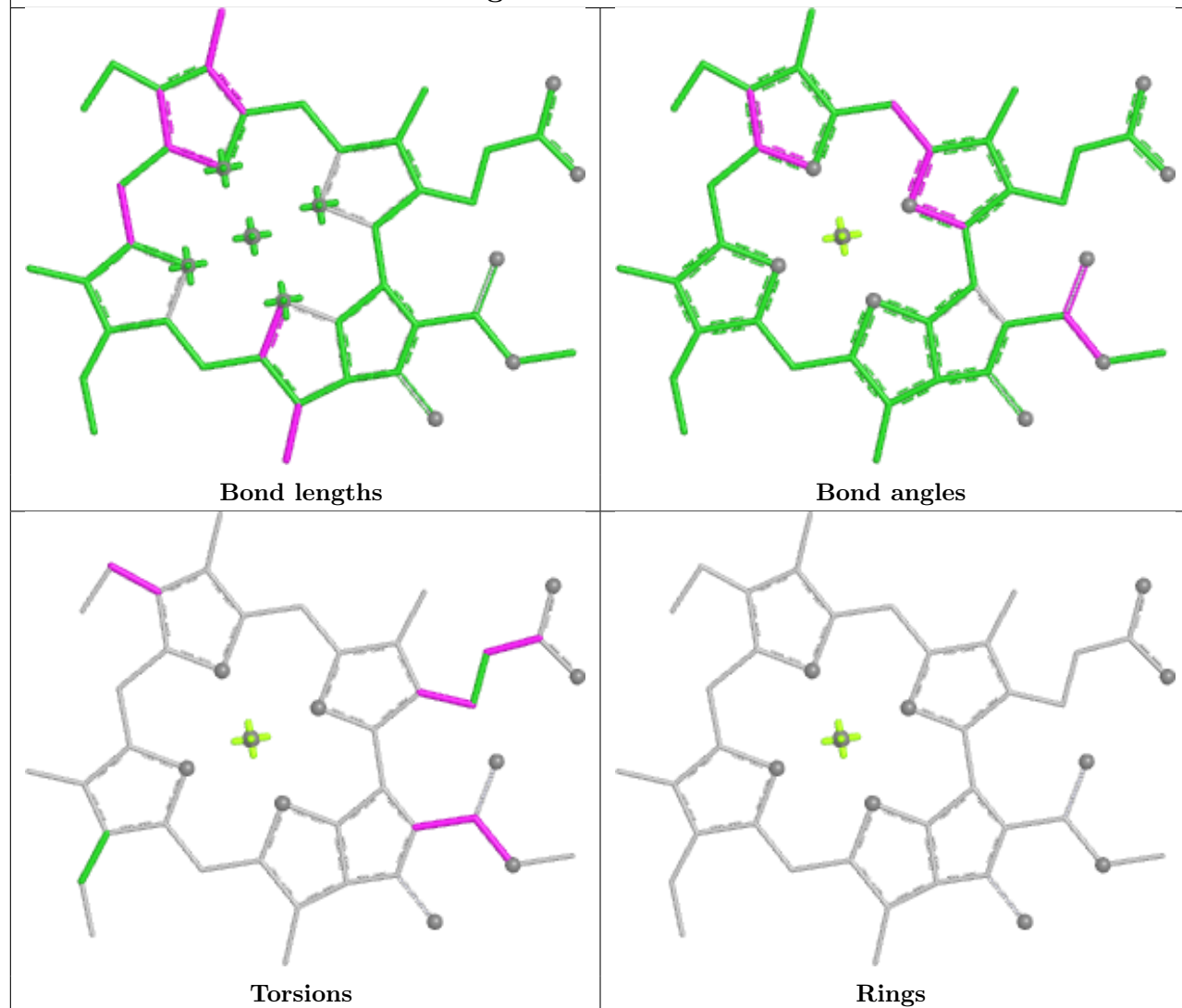


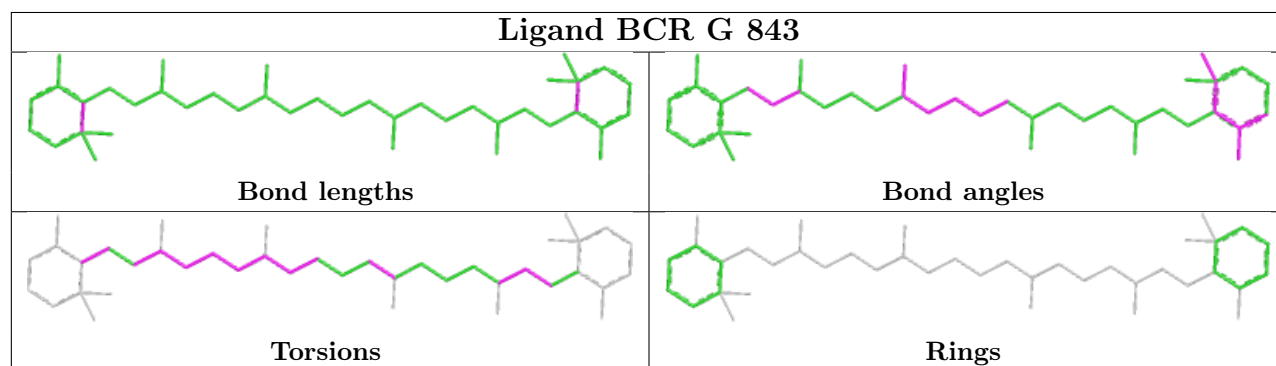
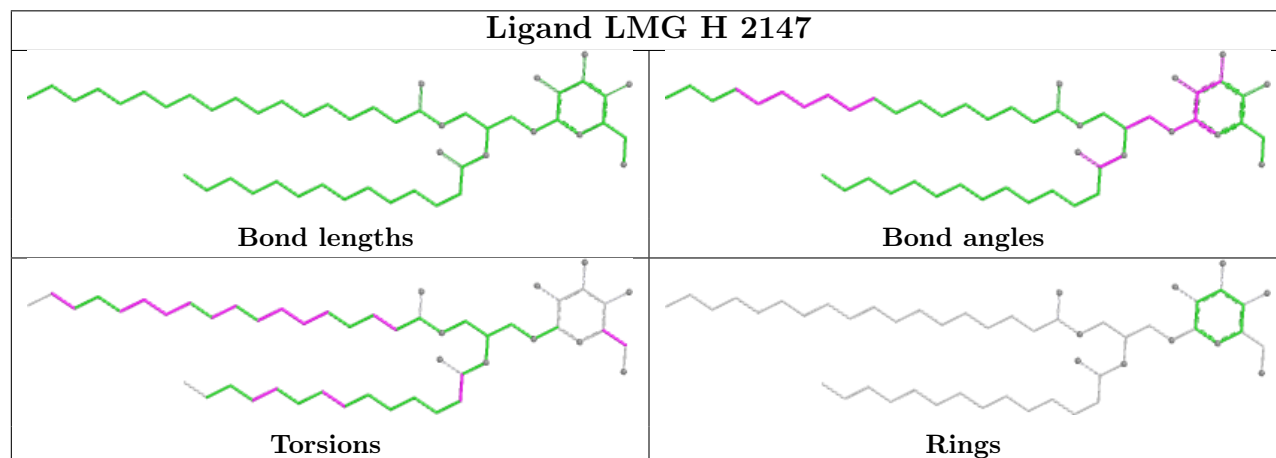
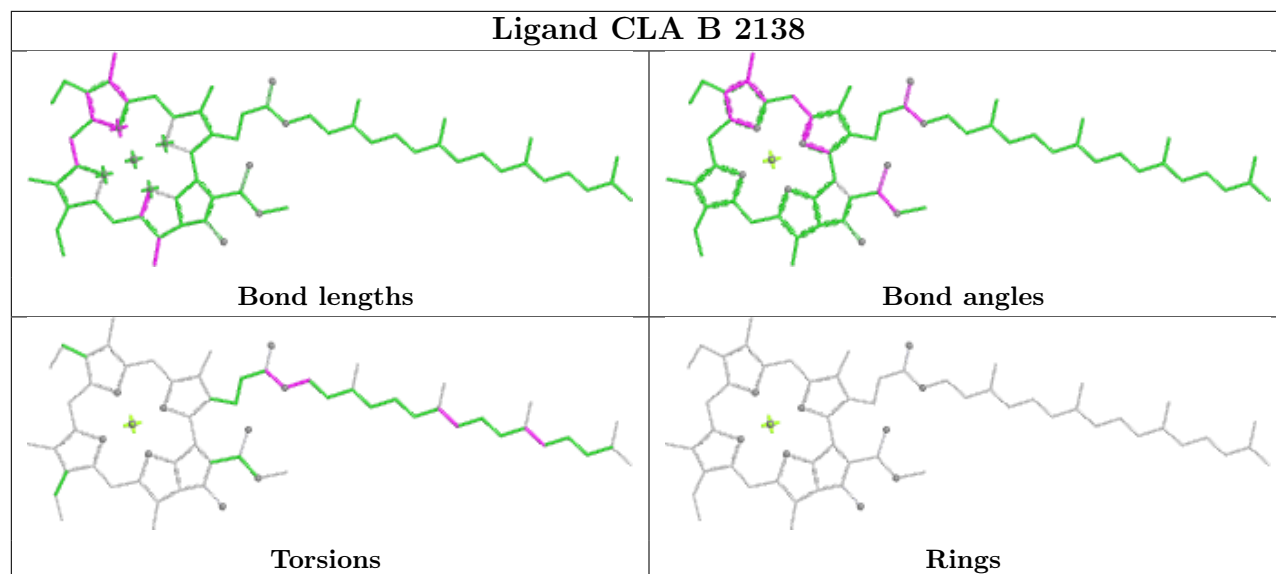
Rings

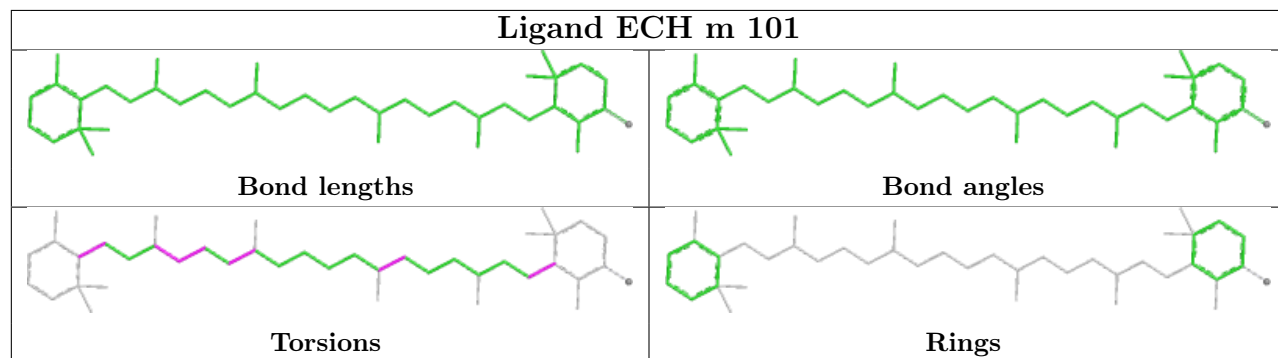
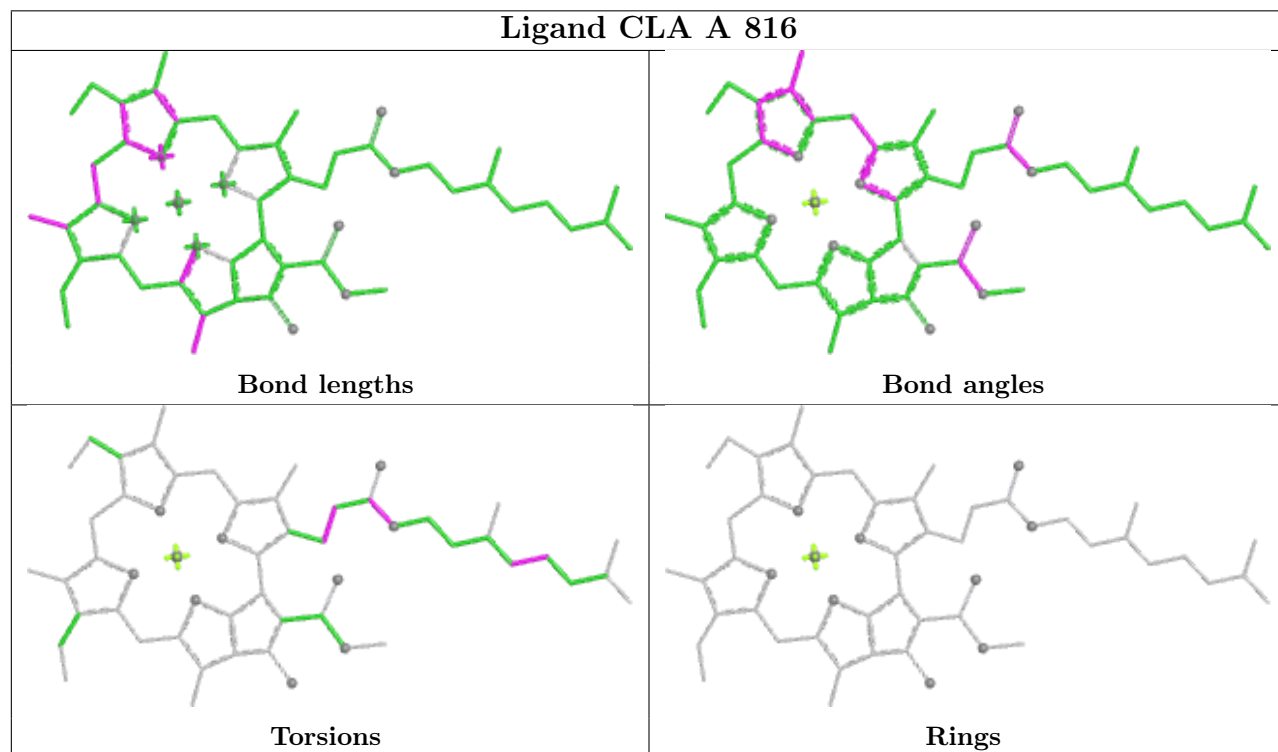
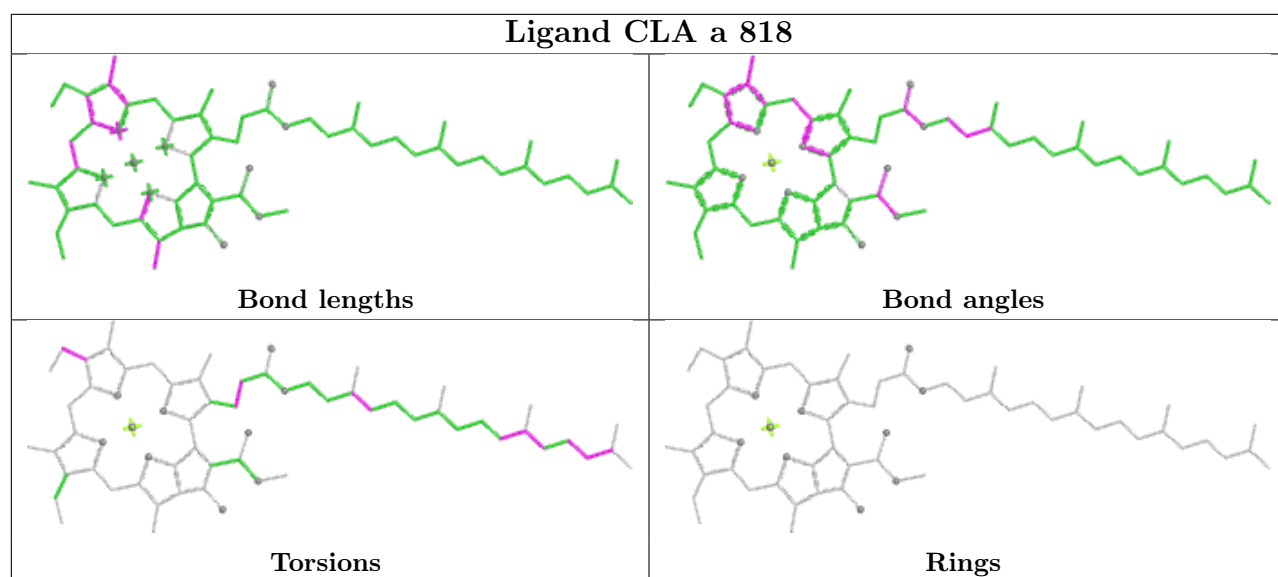
Ligand CLA l 204

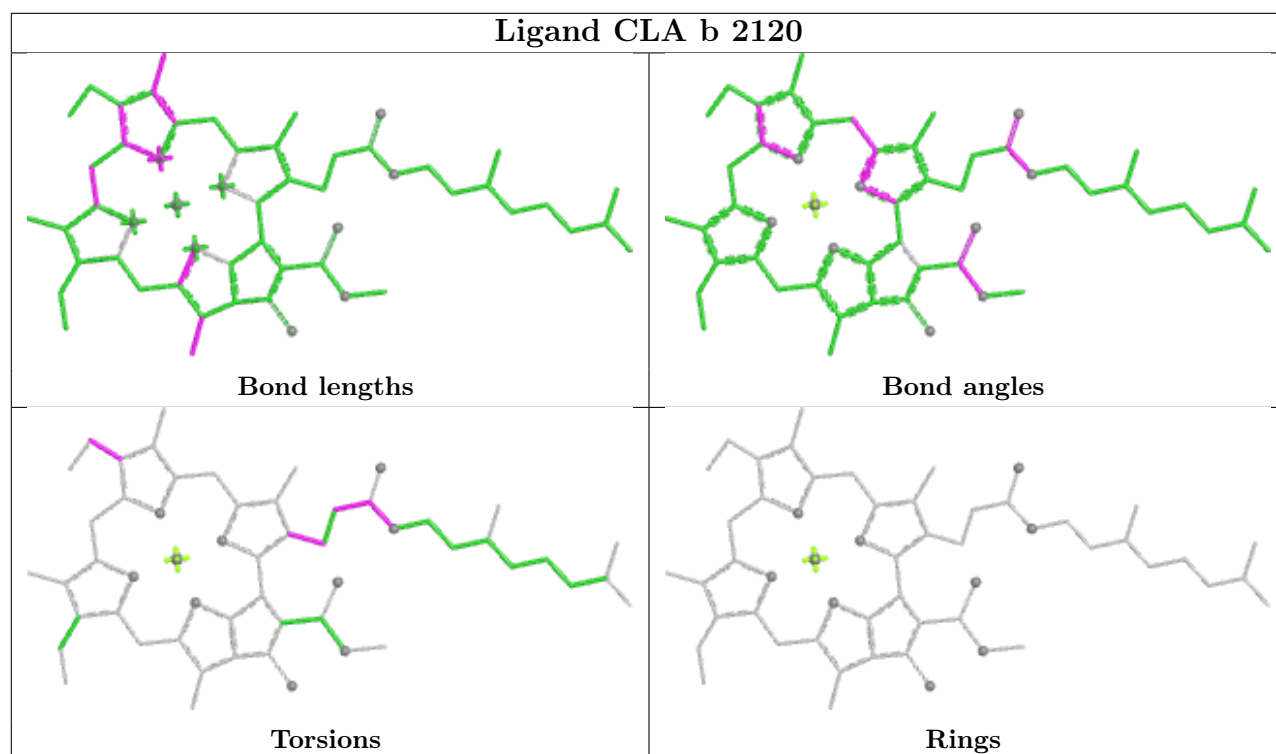
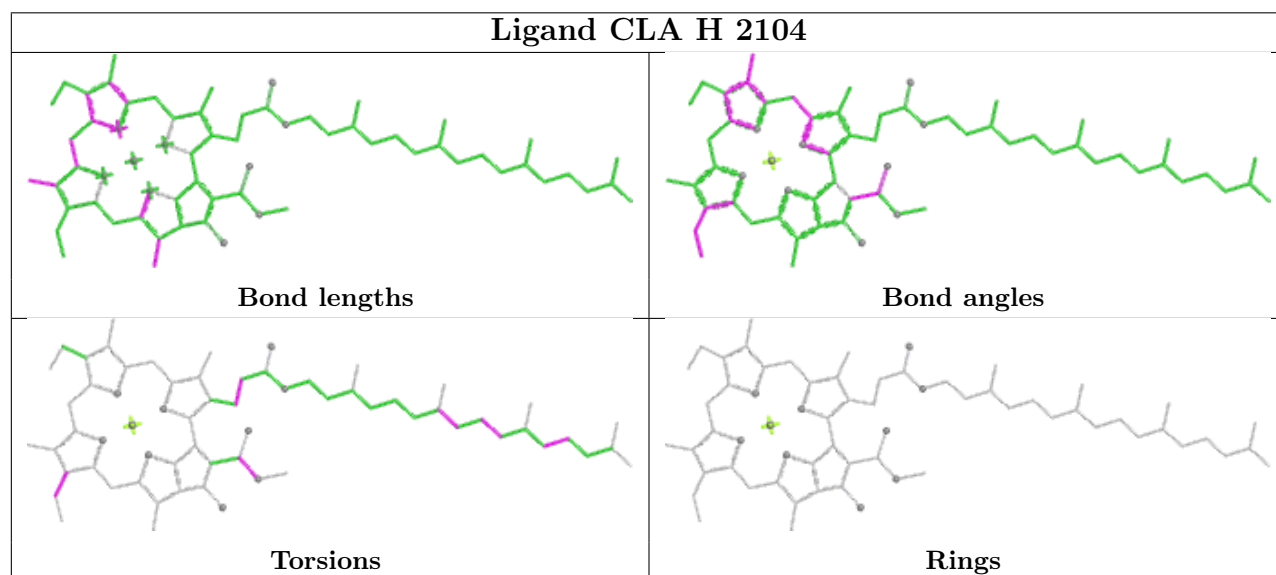
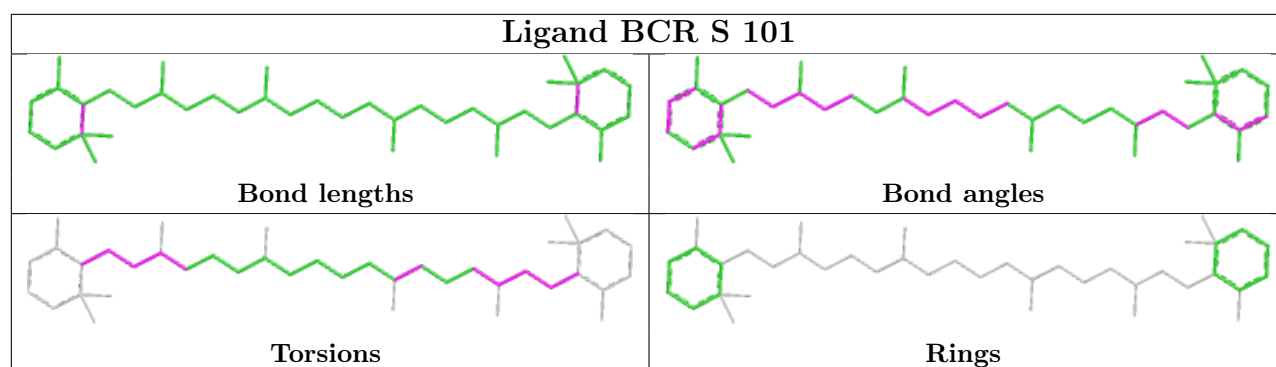


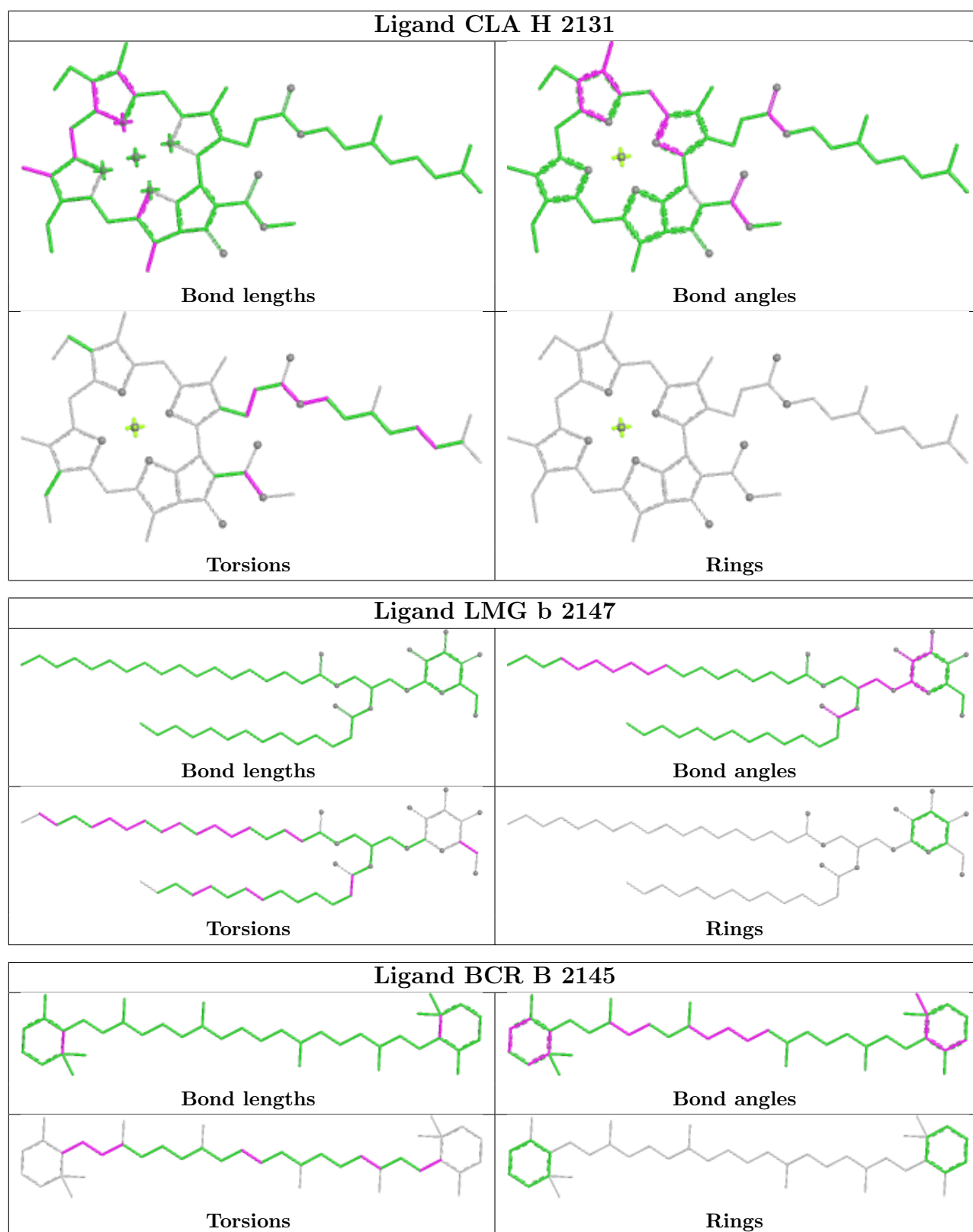
Ligand CLA k 4002

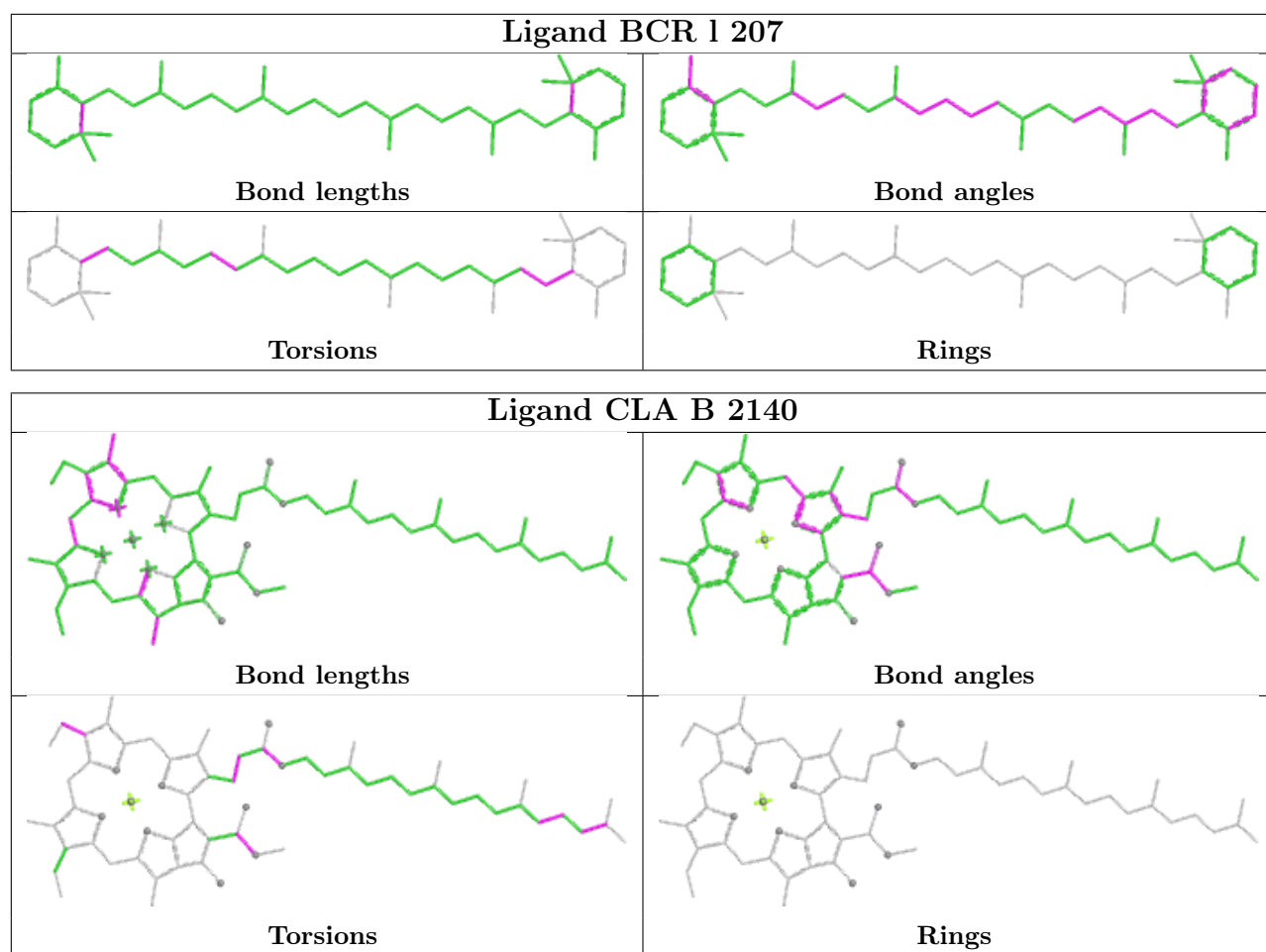


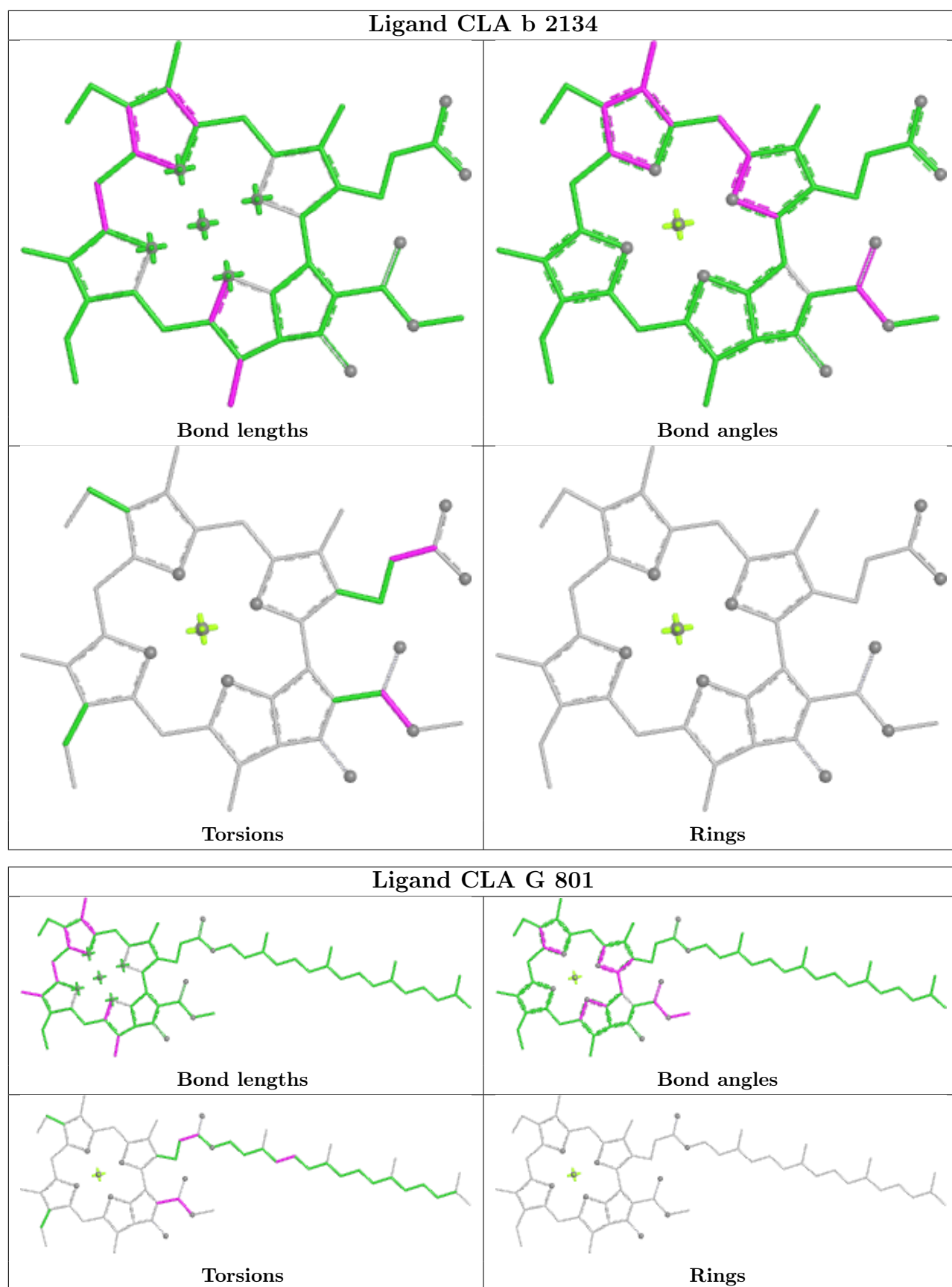


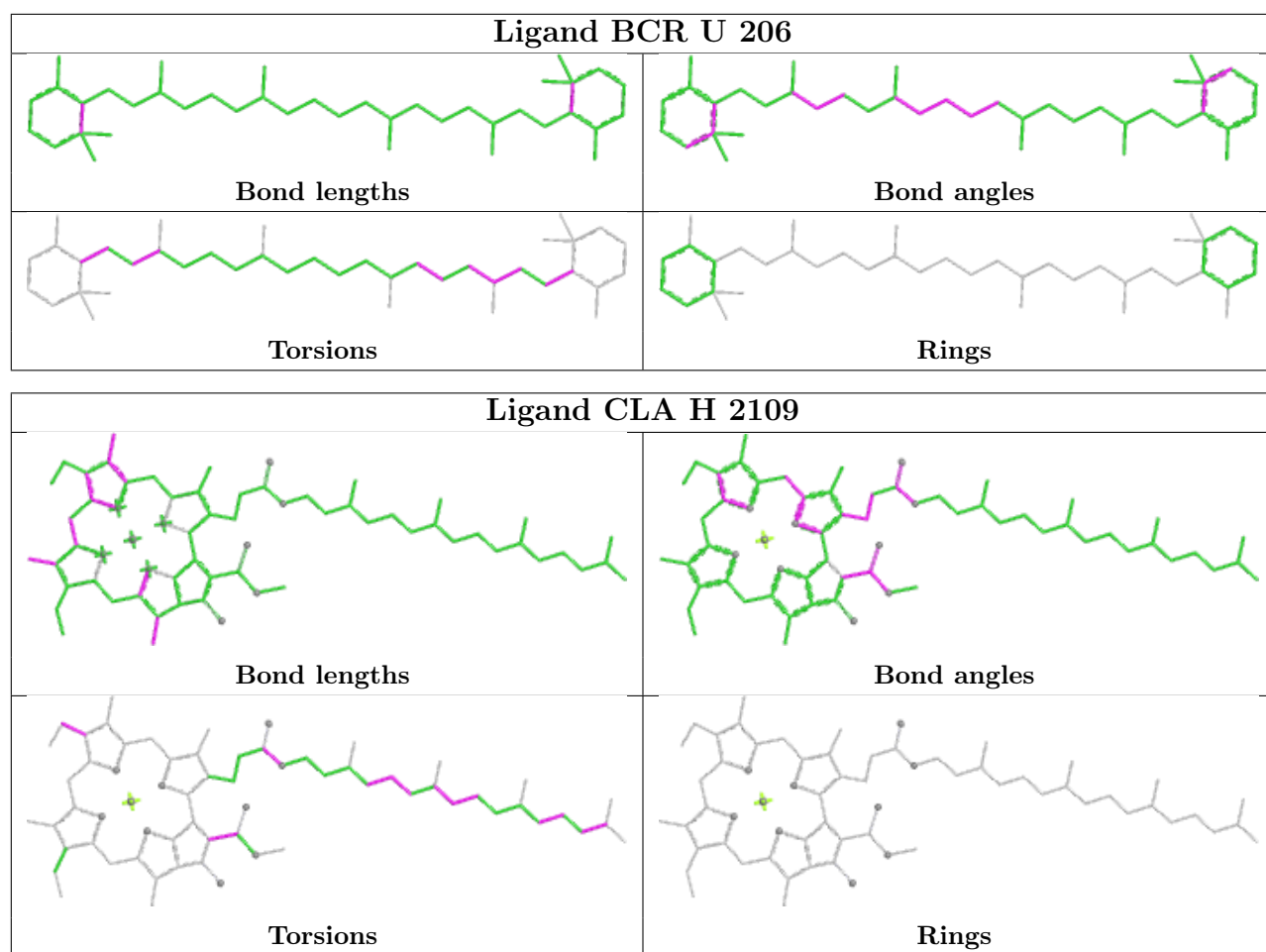




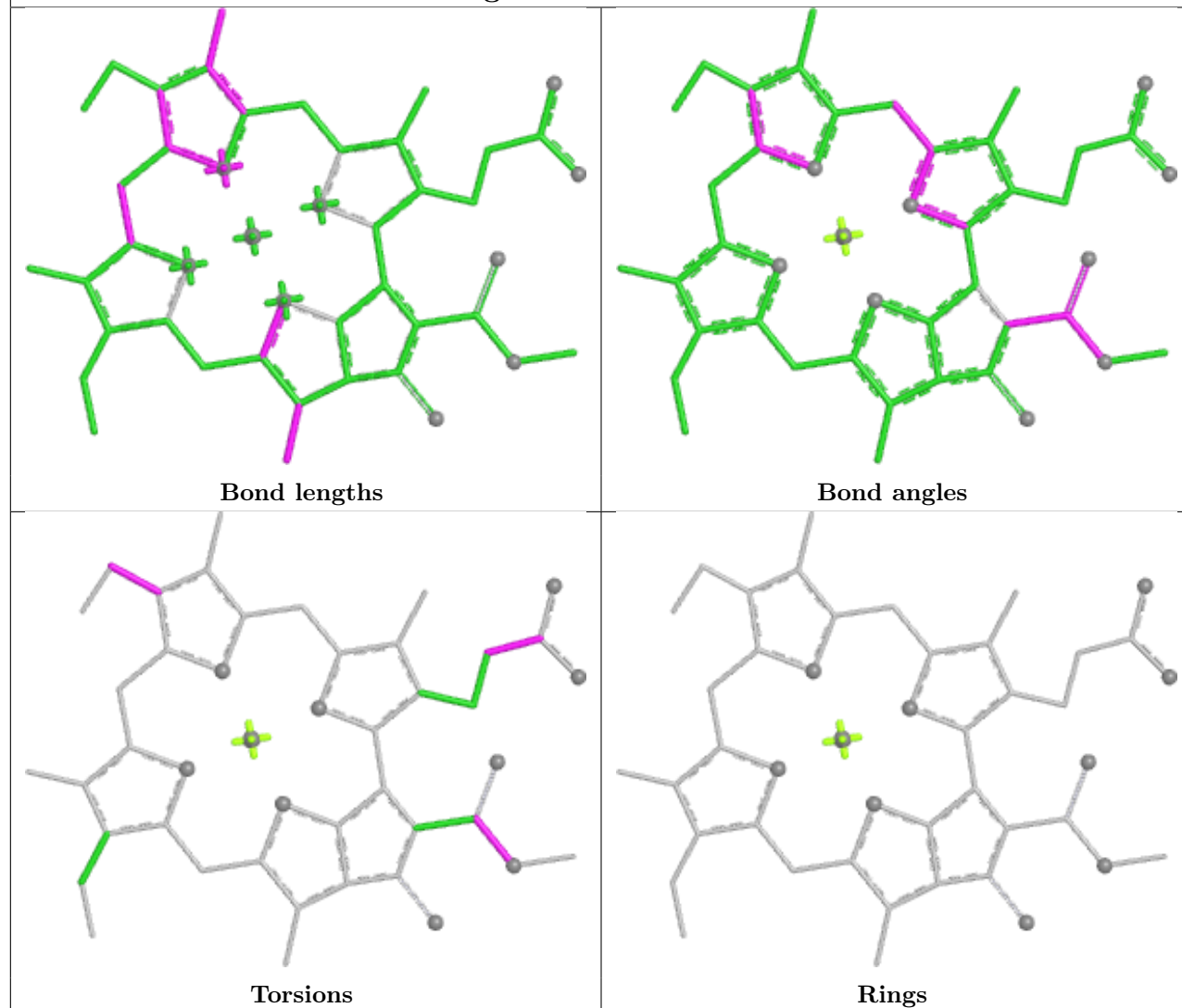




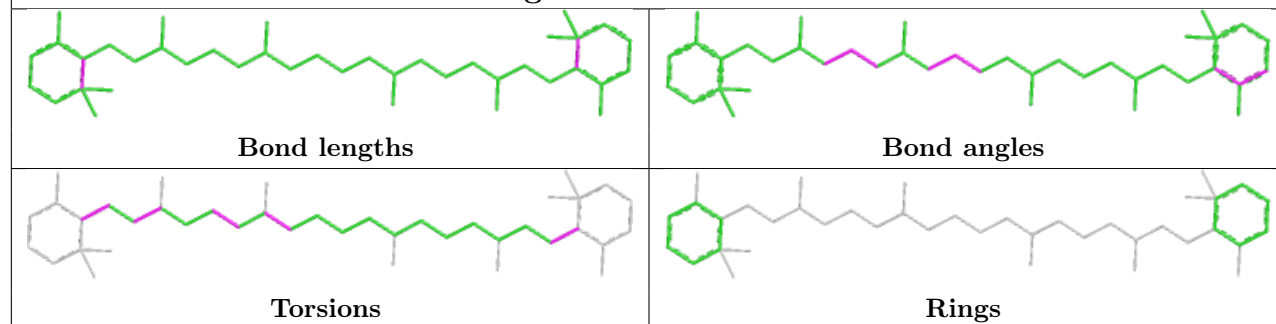


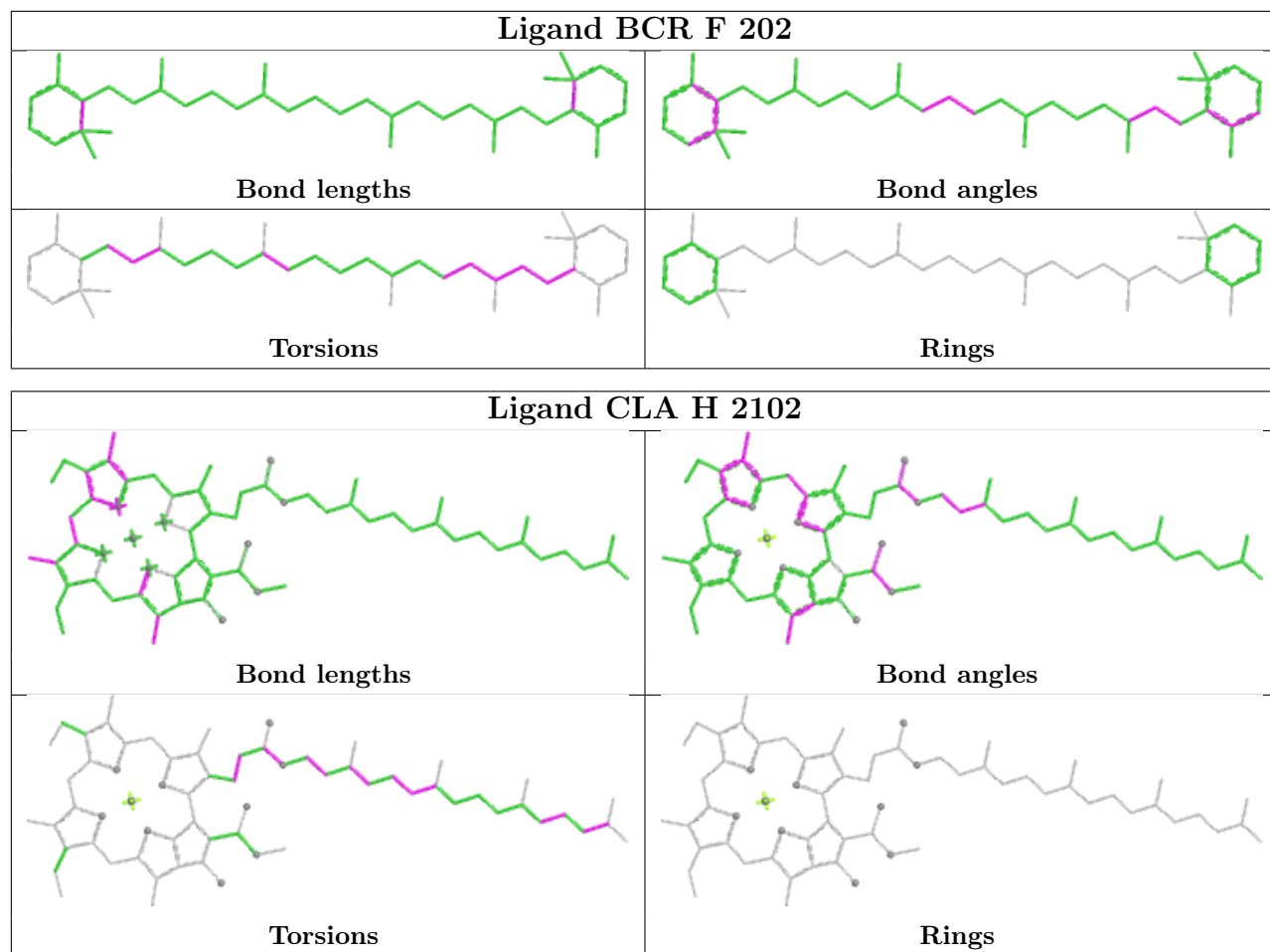


Ligand CLA H 2138

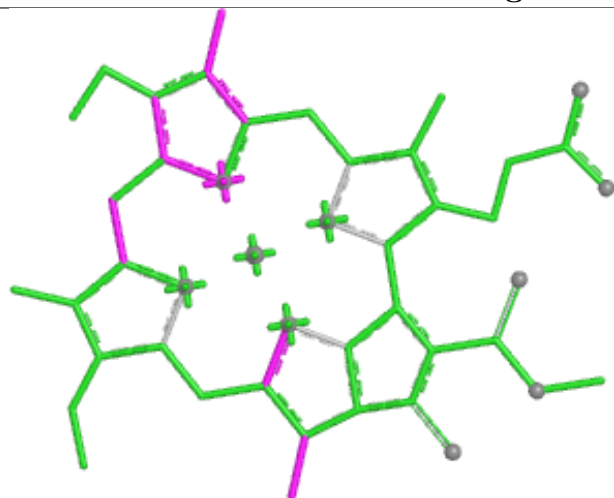


Ligand BCR b 2145

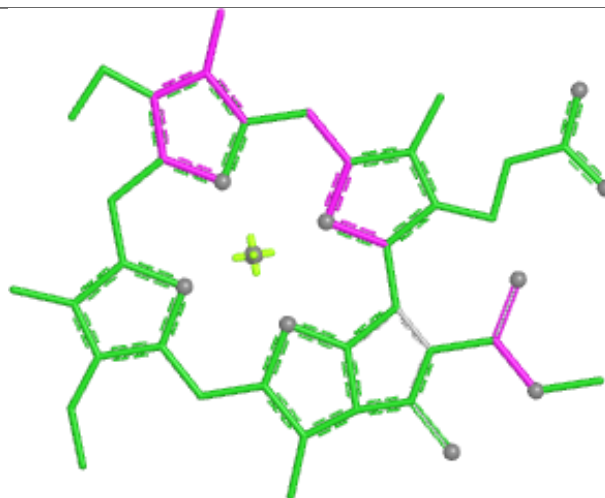




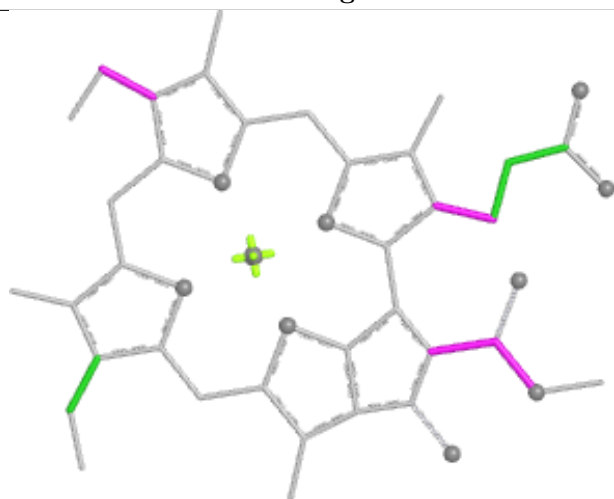
Ligand CLA B 2137



Bond lengths



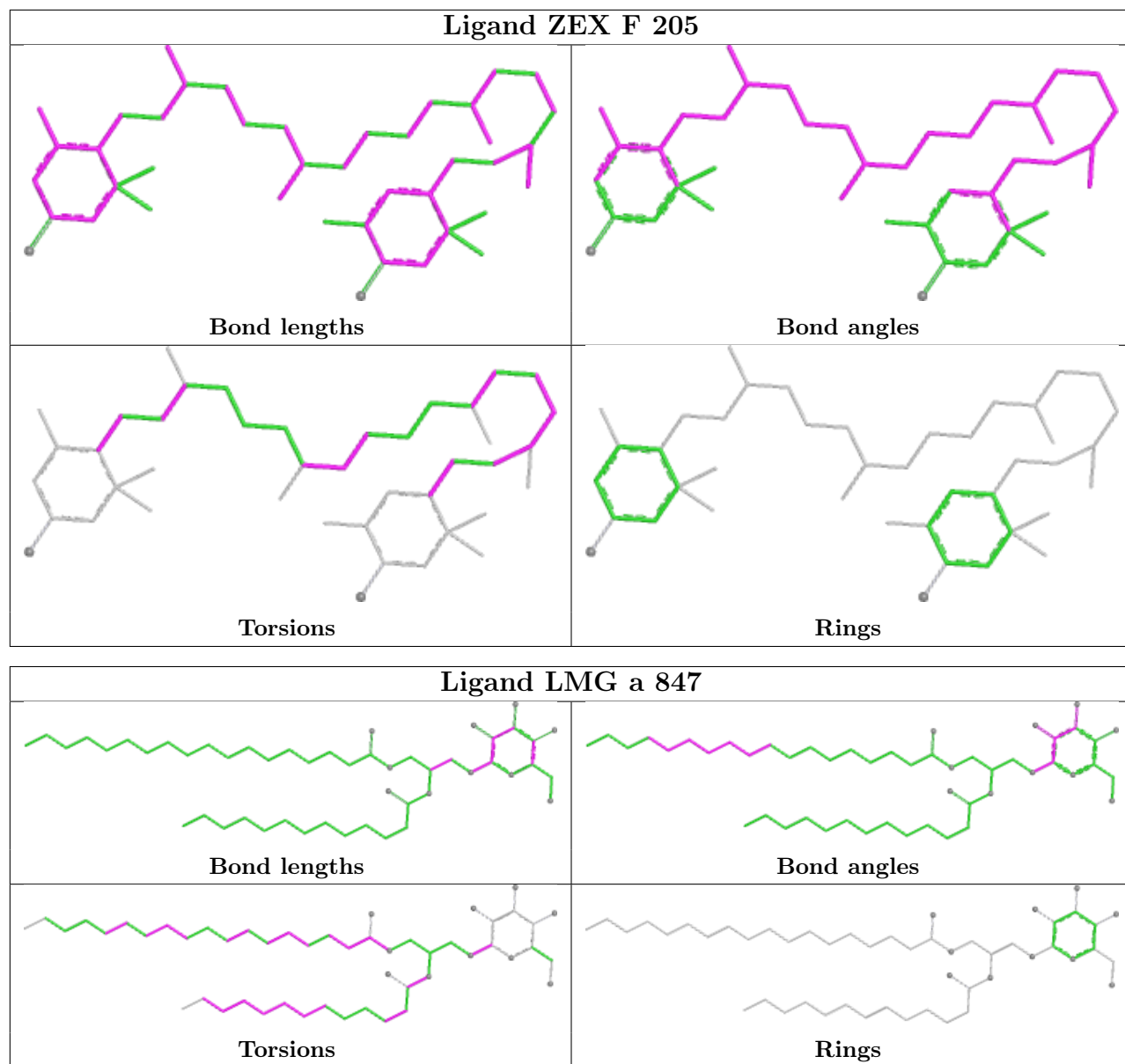
Bond angles



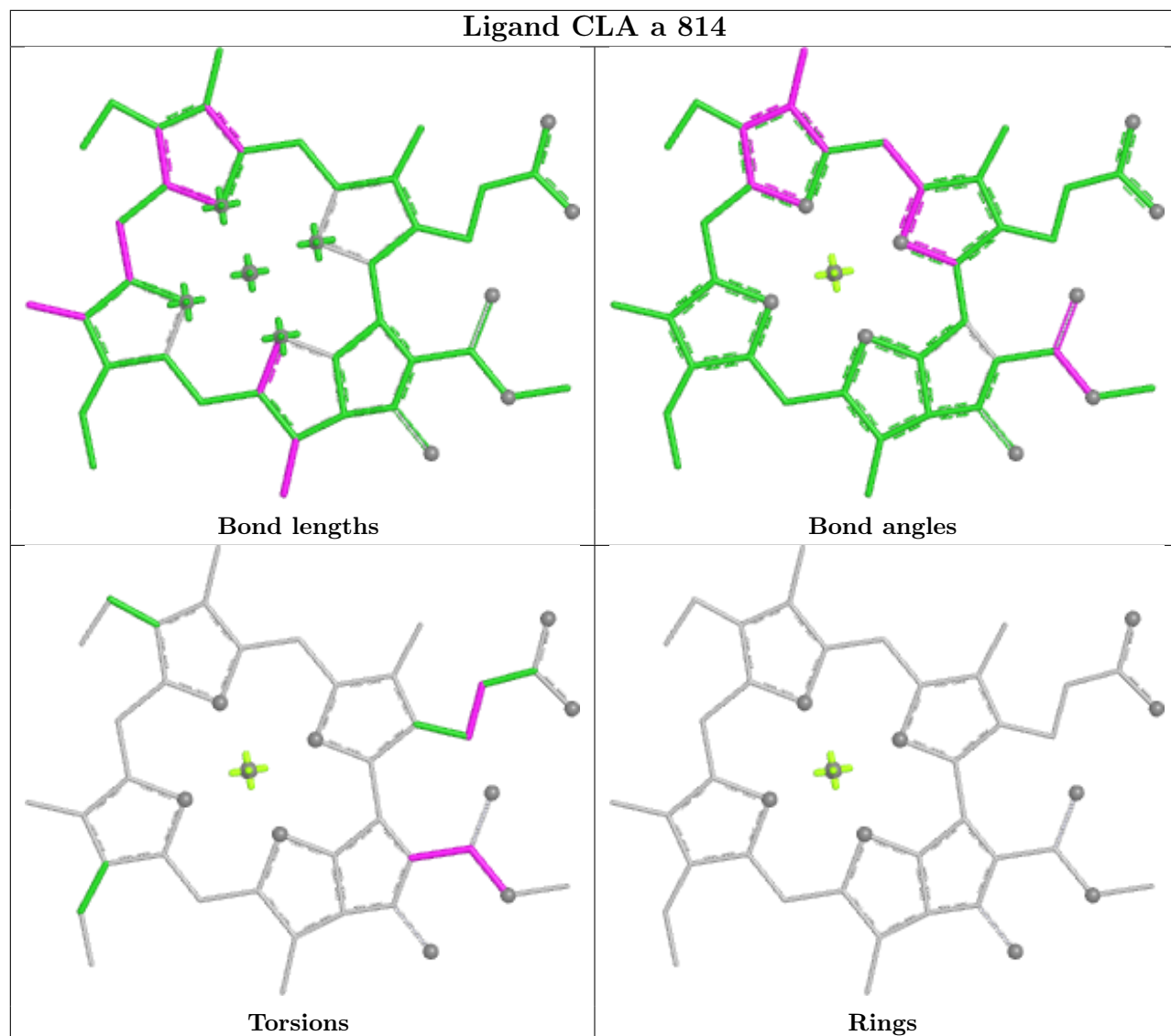
Torsions

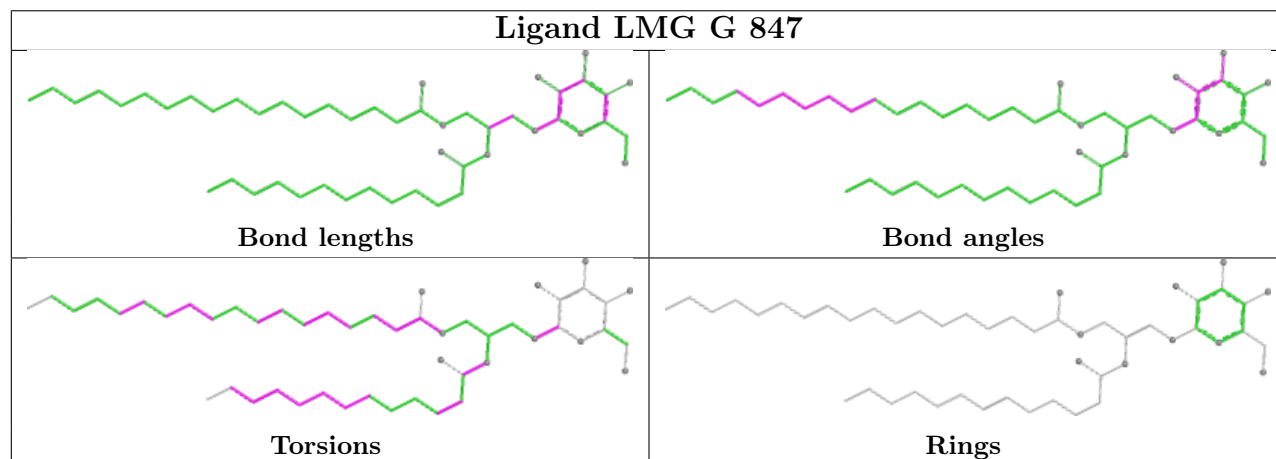
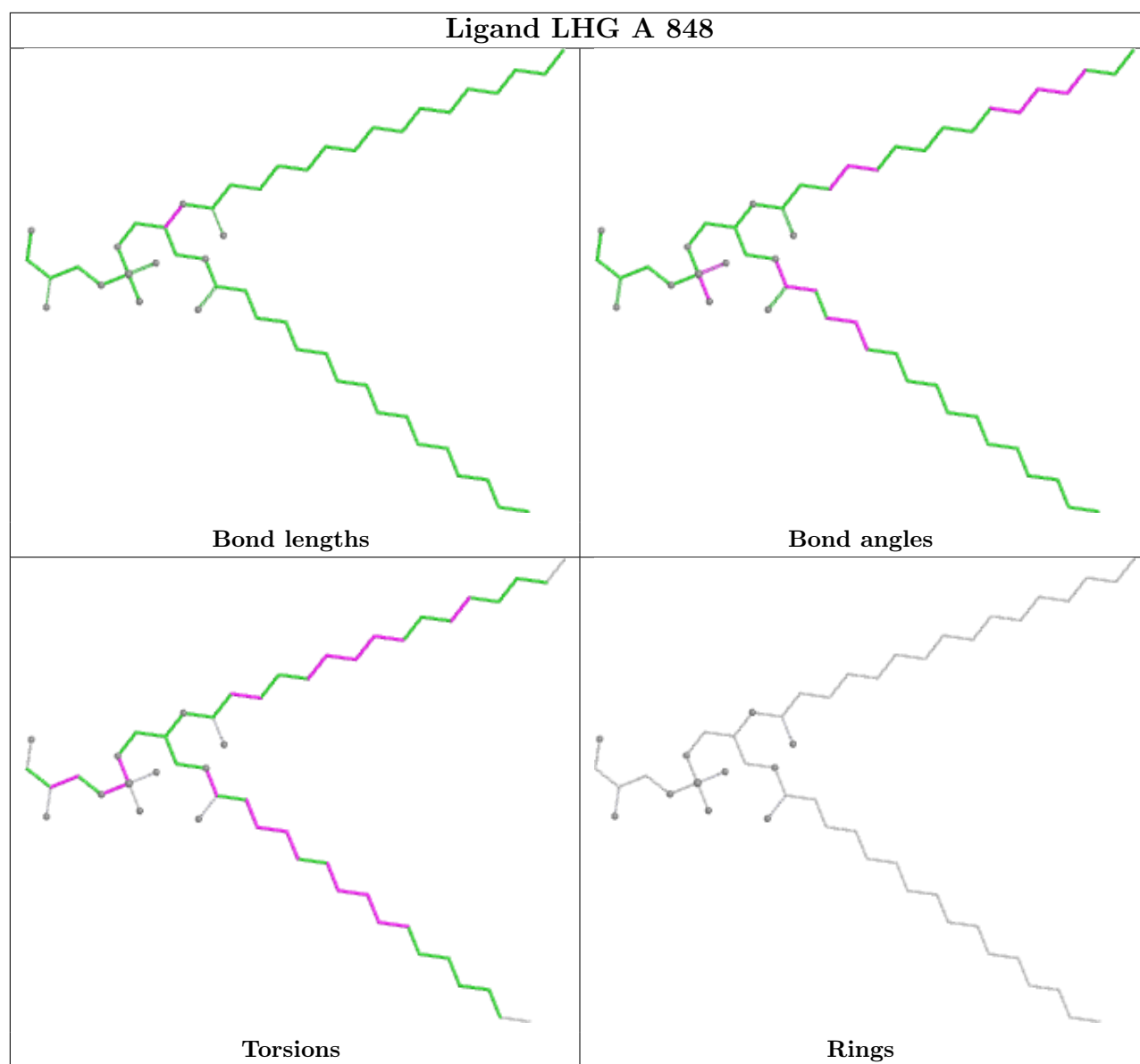


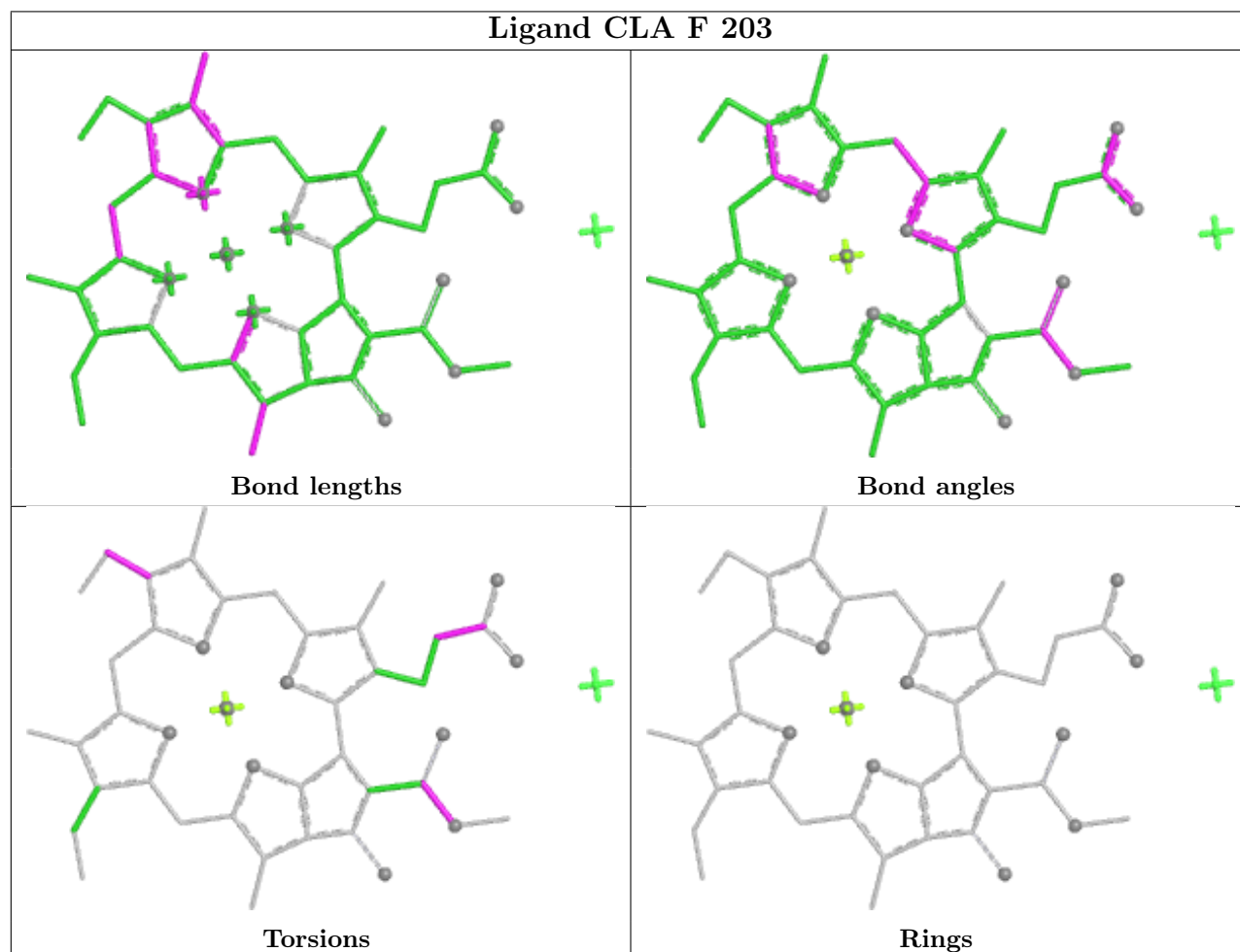
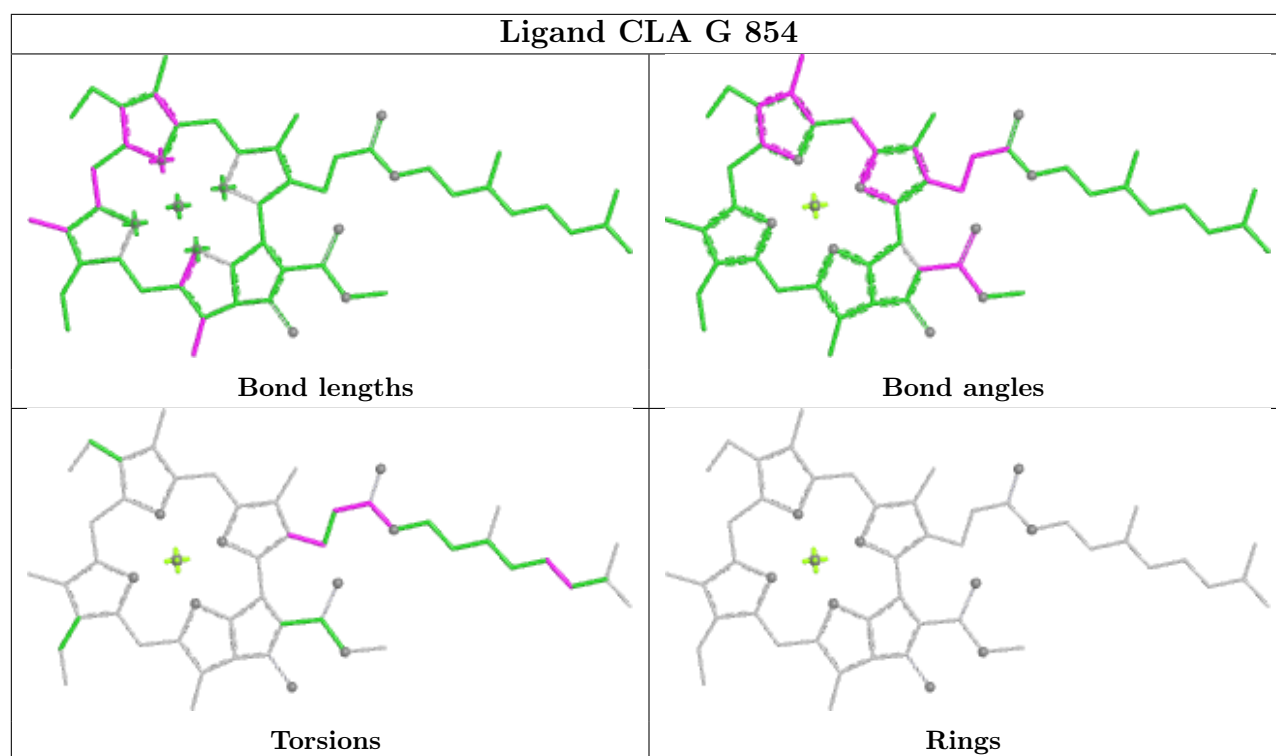
Rings

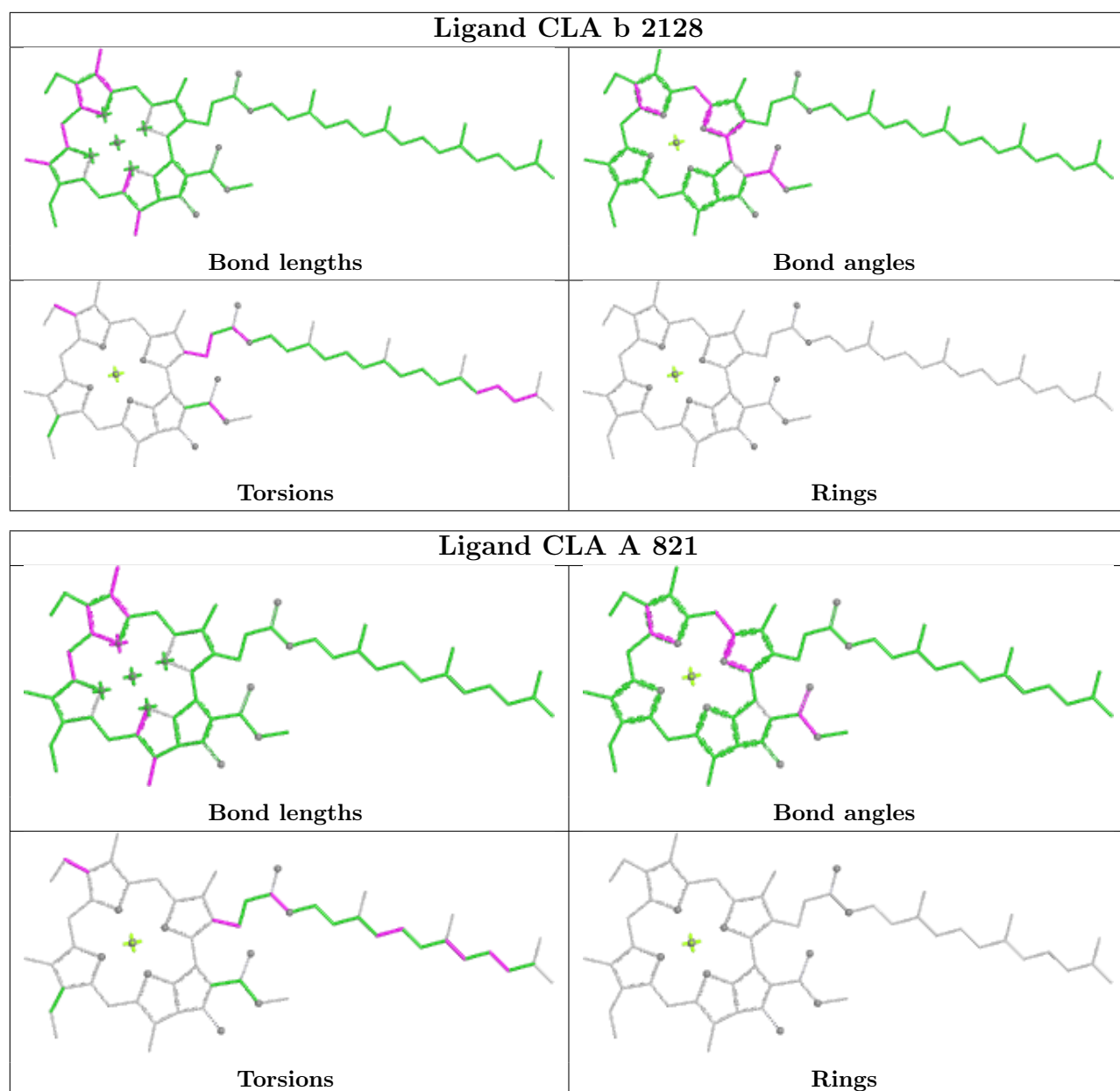


Ligand CLA a 814

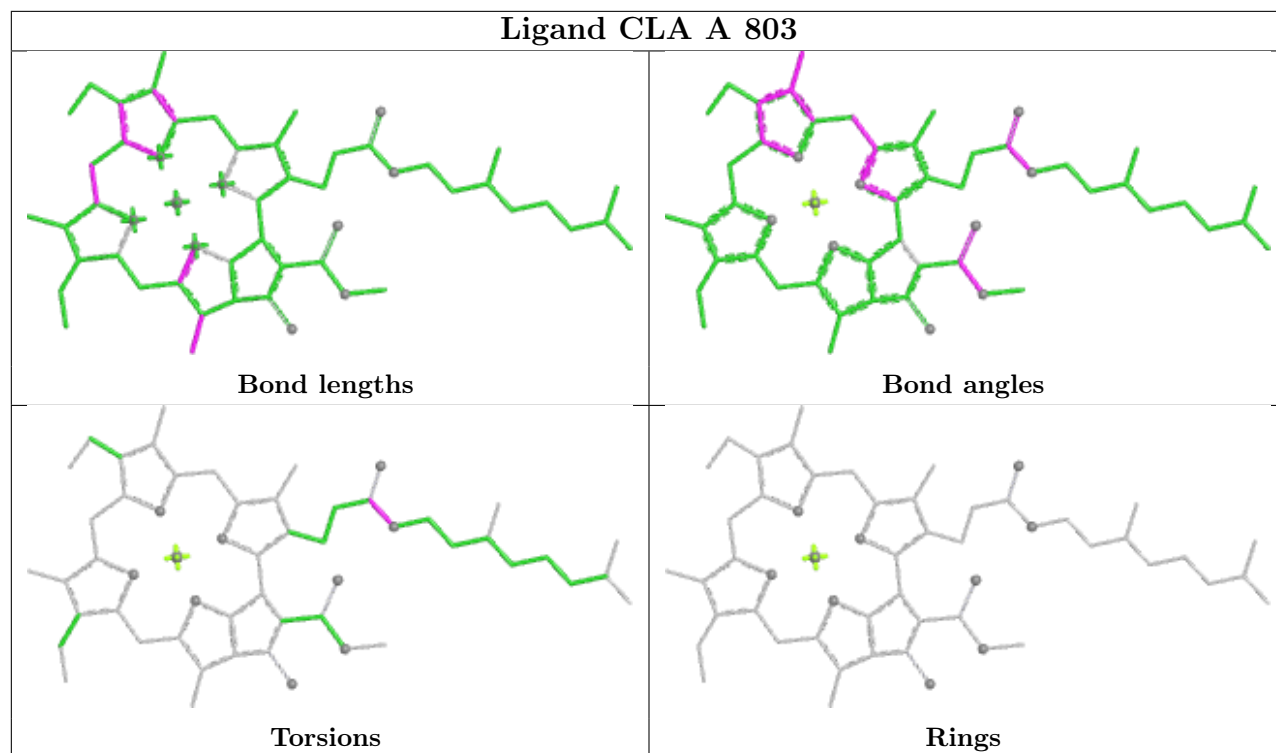




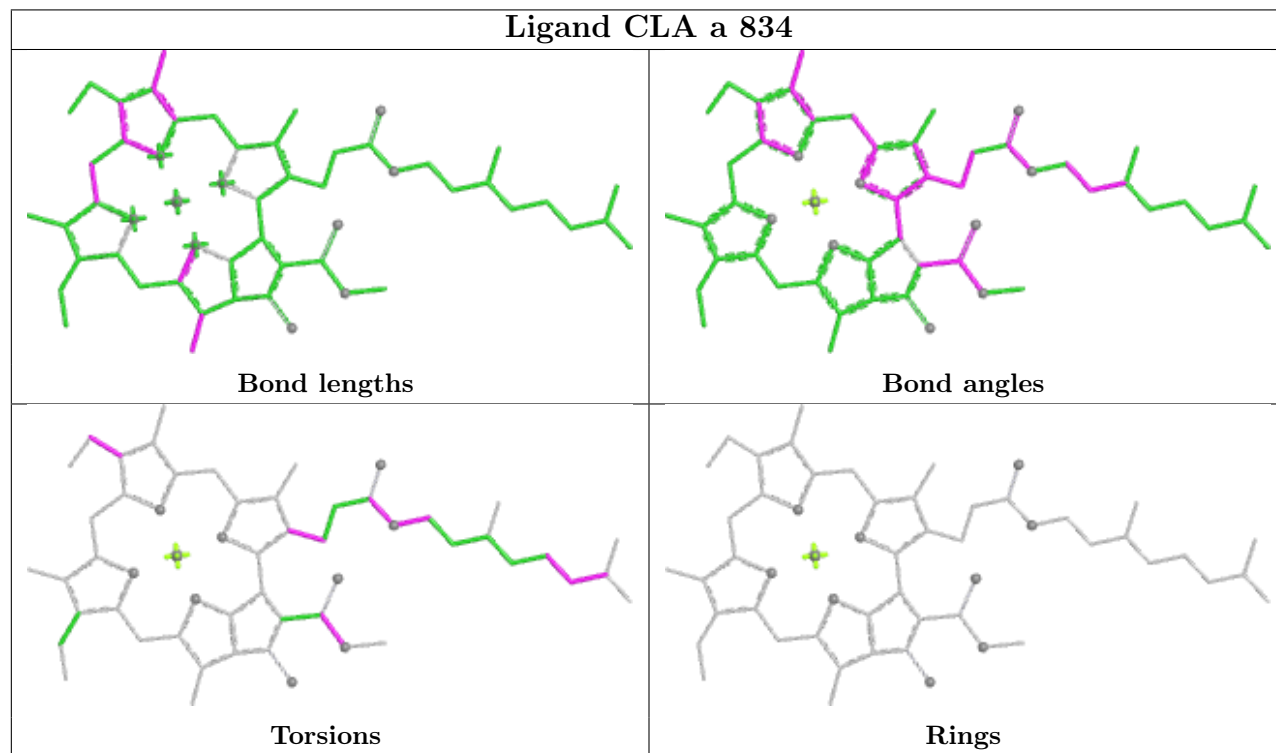


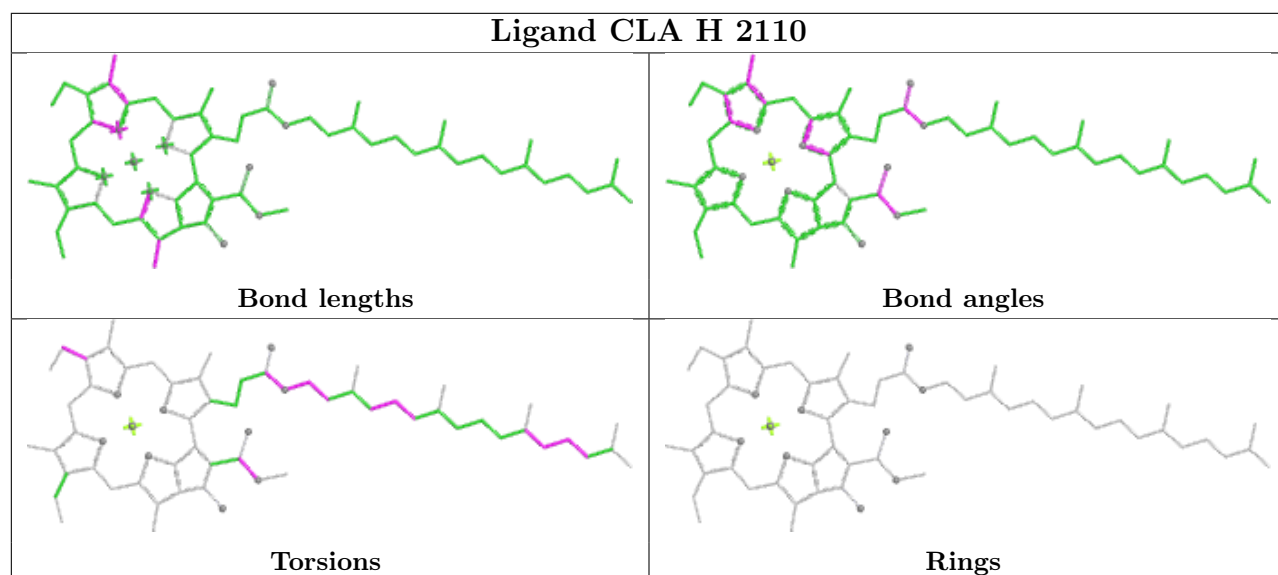
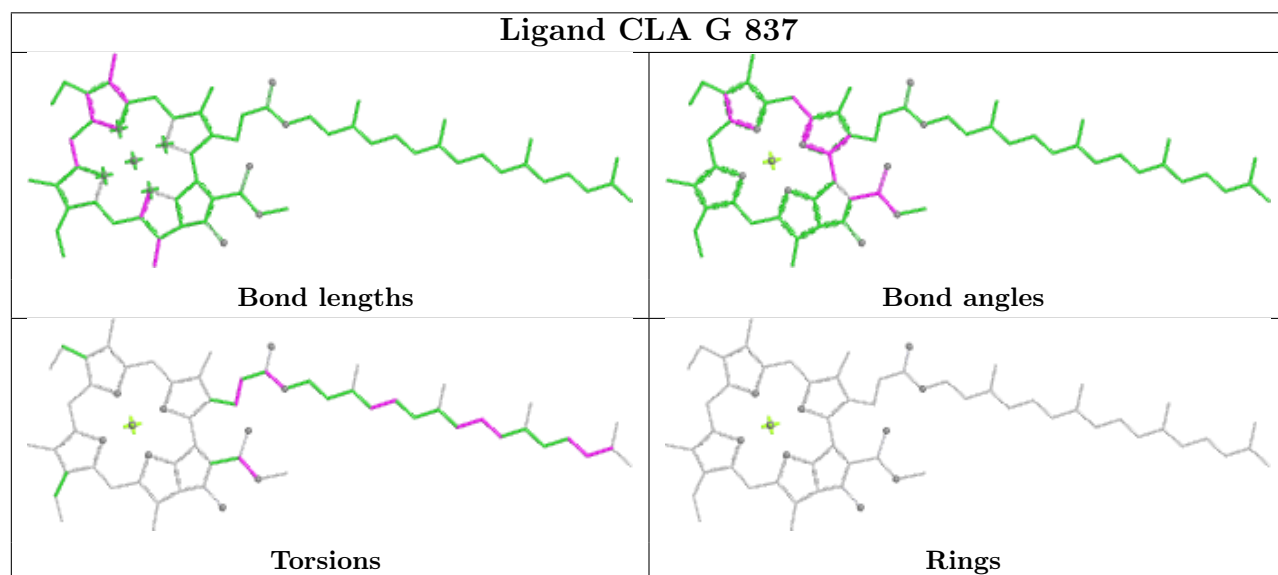
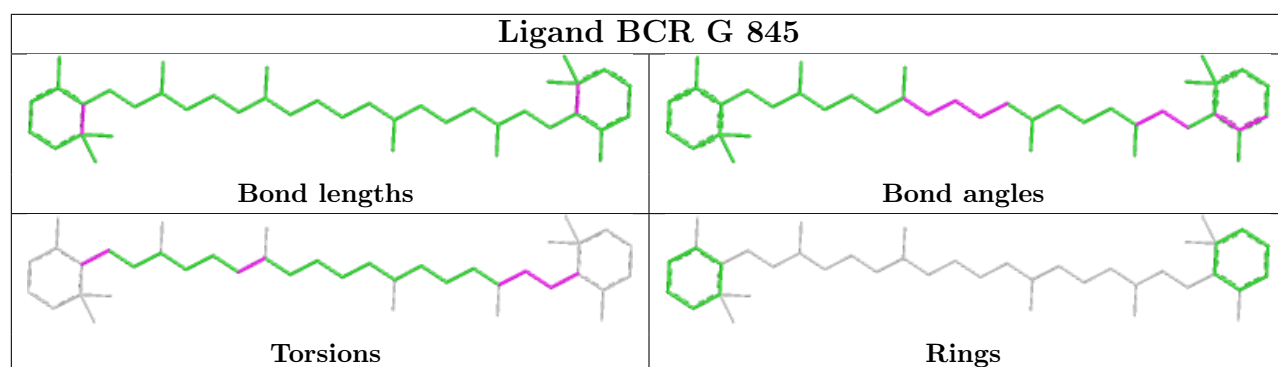


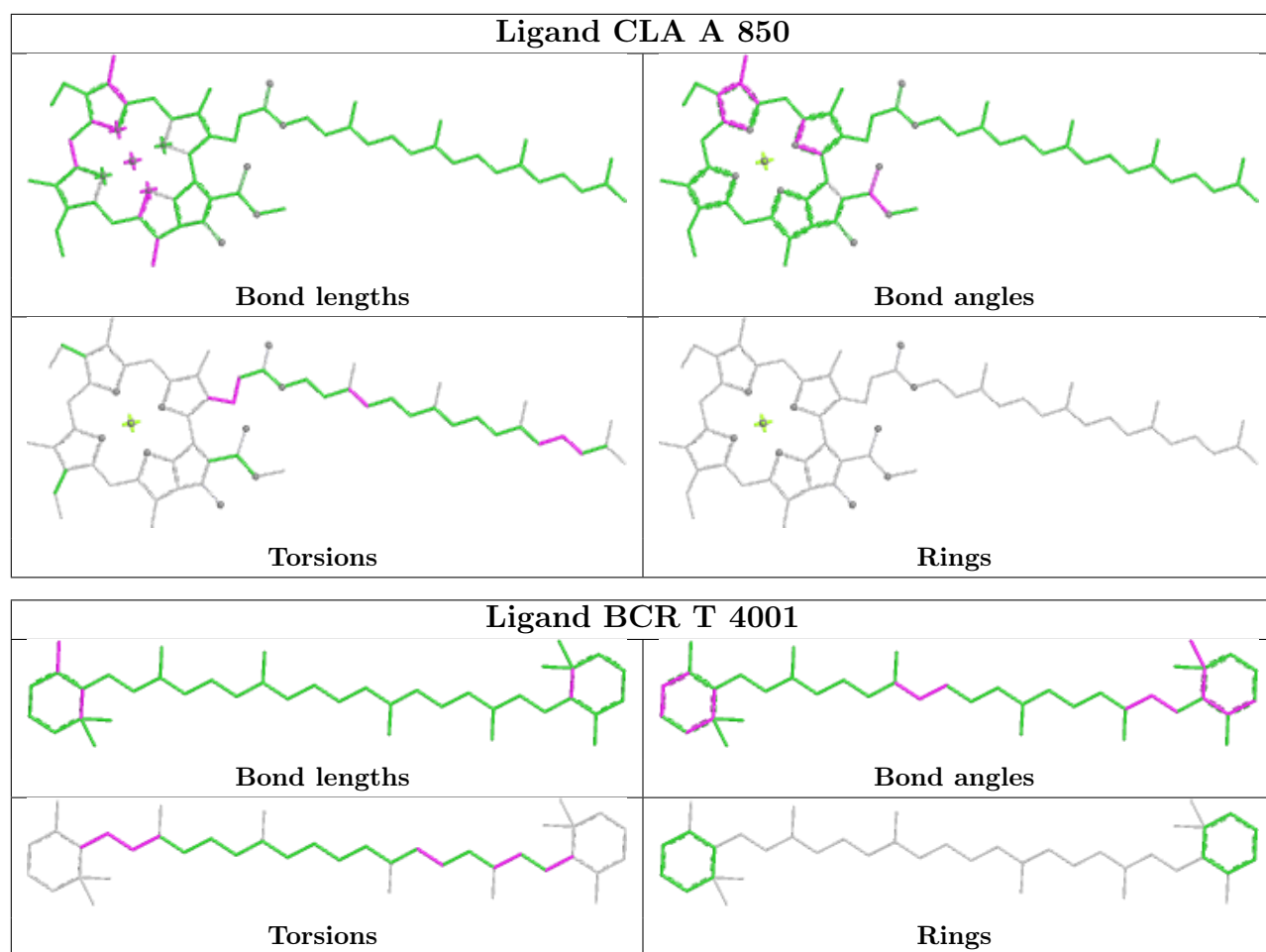
Ligand CLA A 803



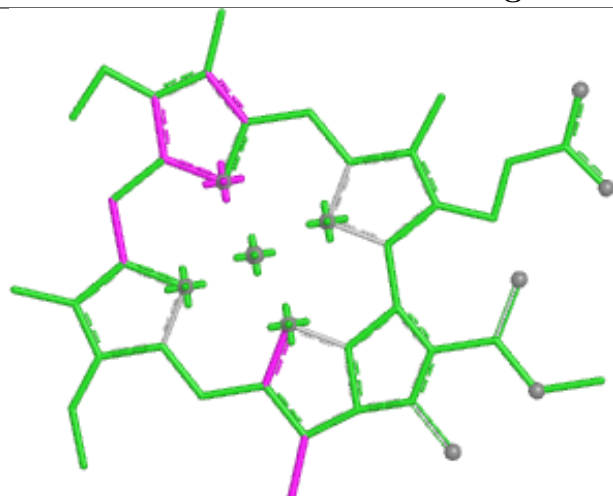
Ligand CLA a 834



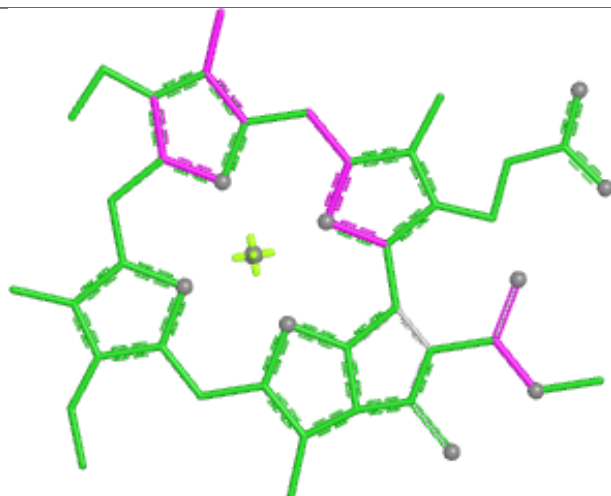




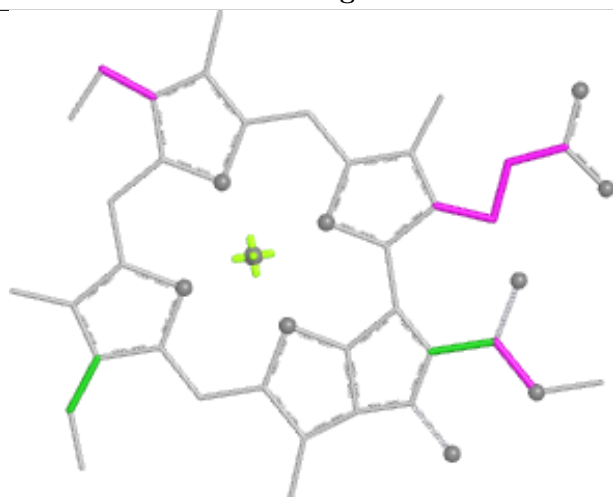
Ligand CLA H 2116



Bond lengths



Bond angles

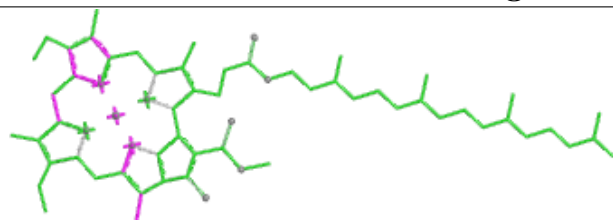


Torsions

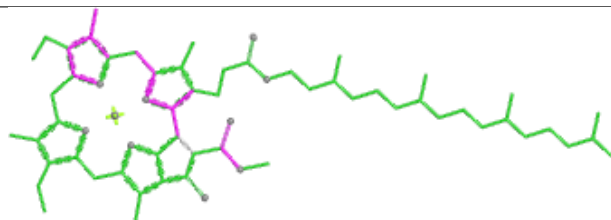


Rings

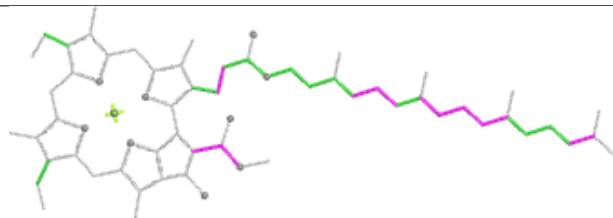
Ligand CLA B 2102



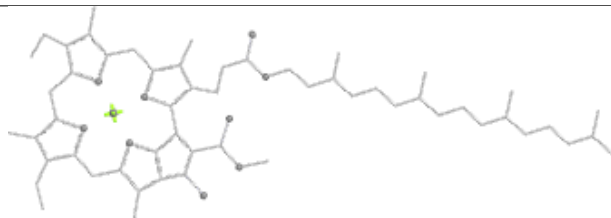
Bond lengths



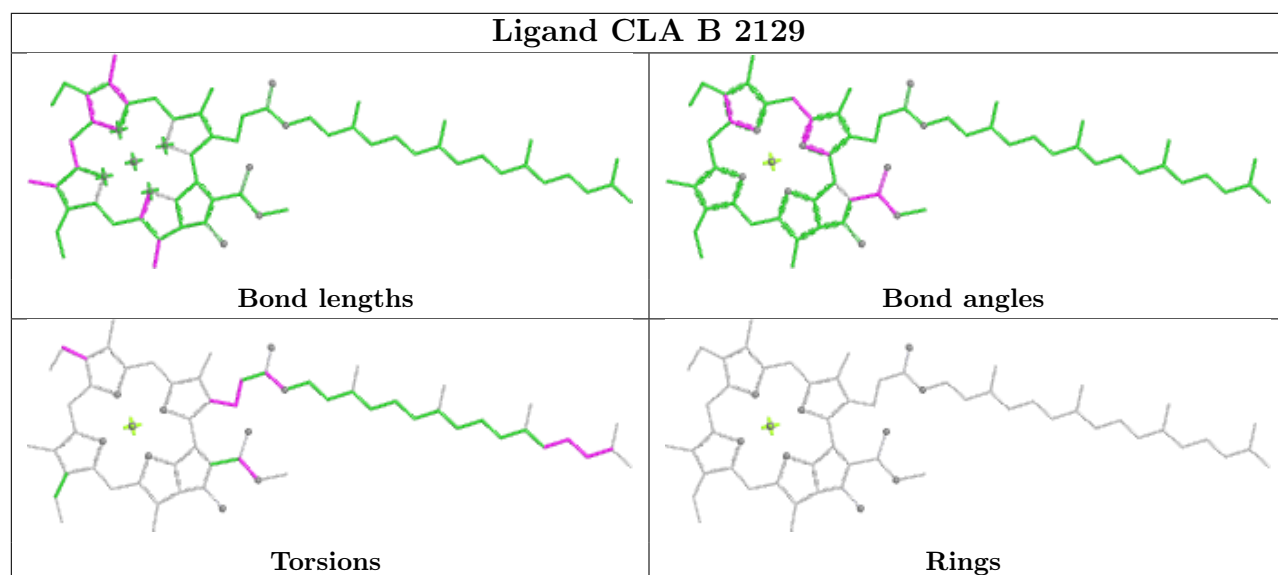
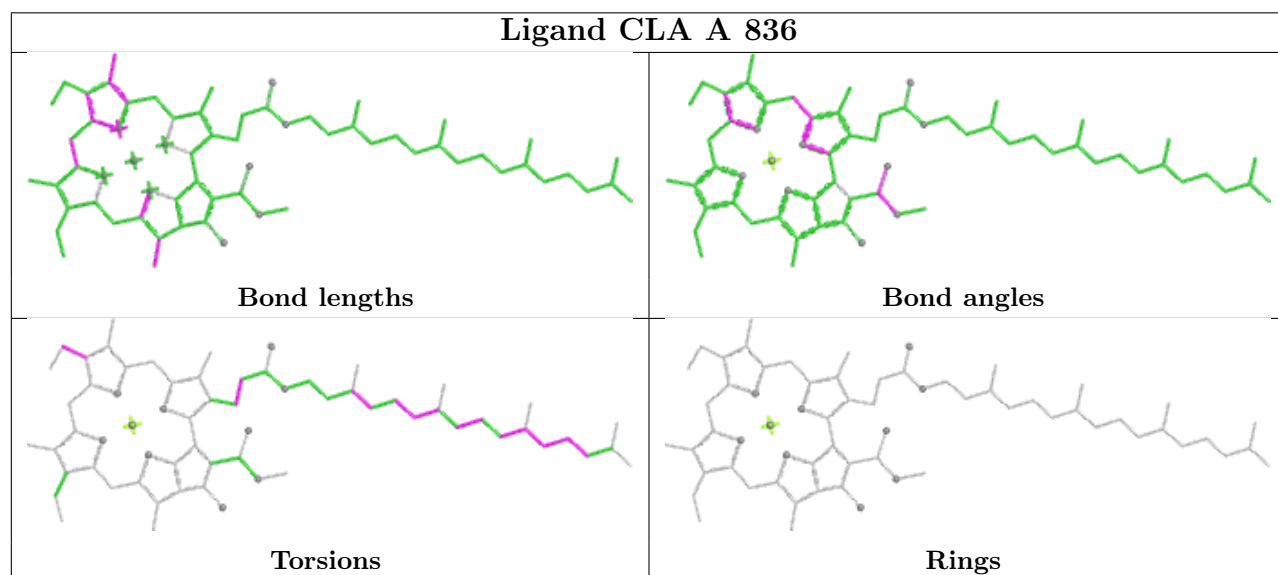
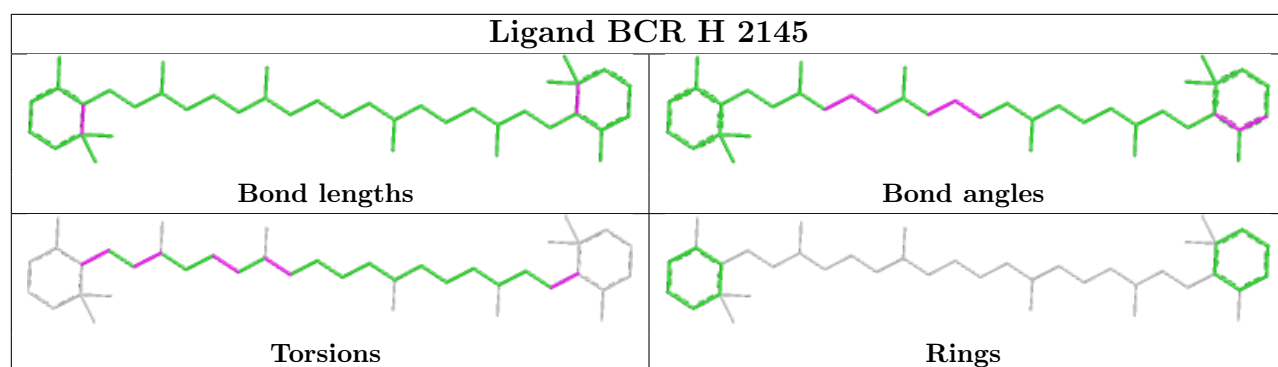
Bond angles

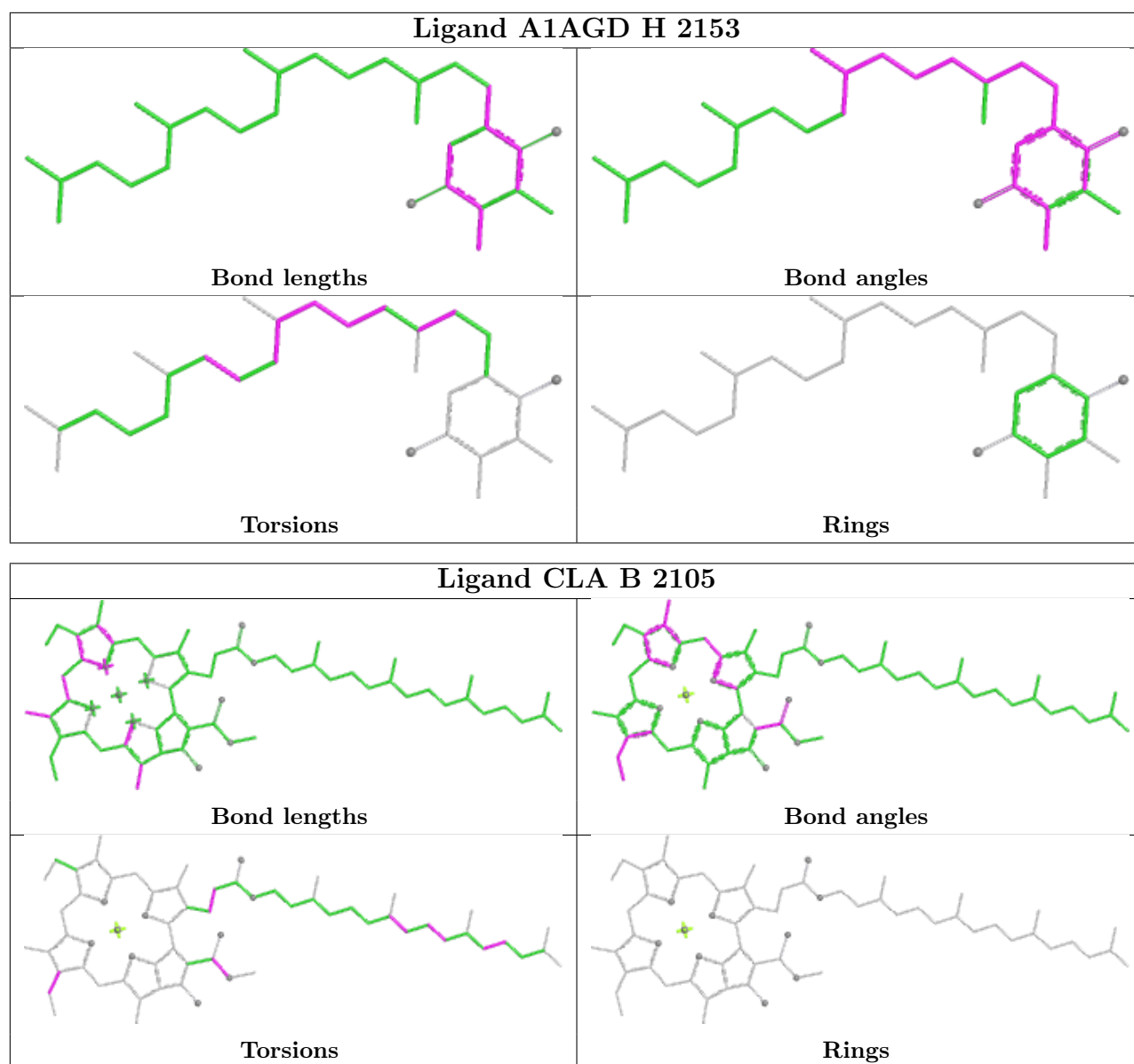


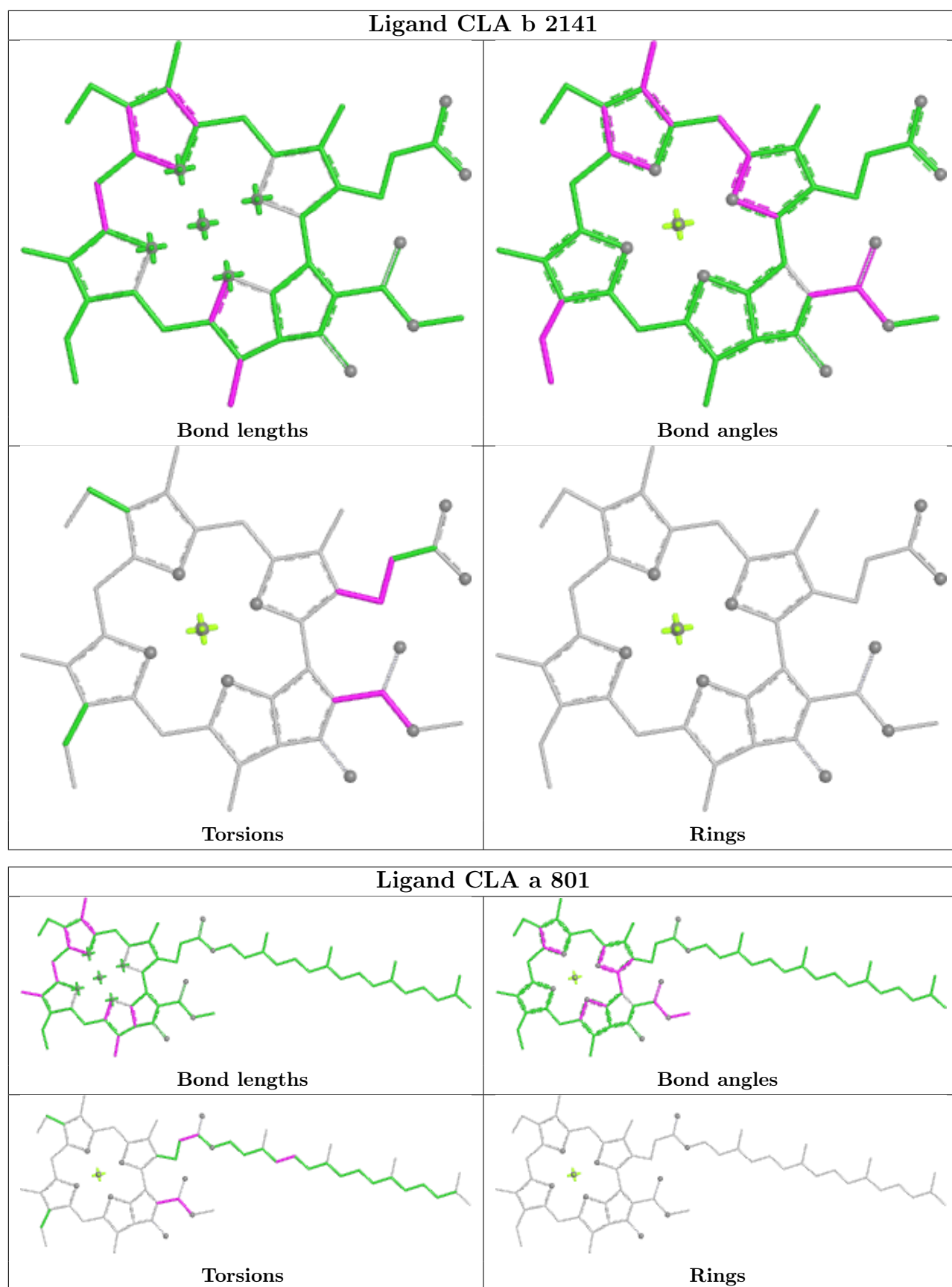
Torsions

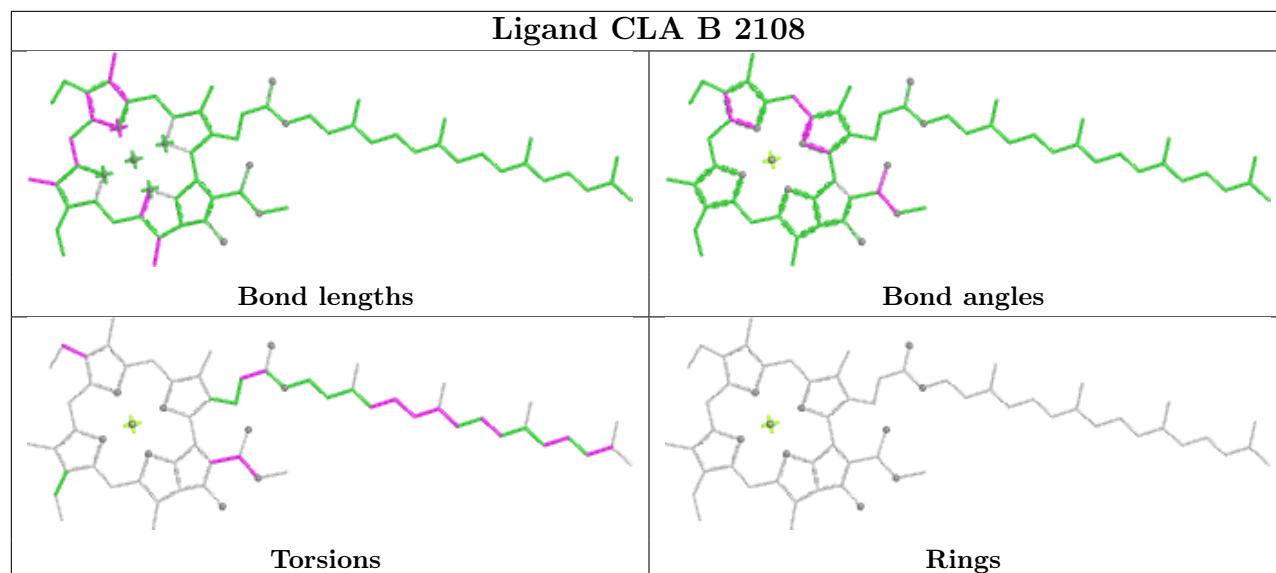
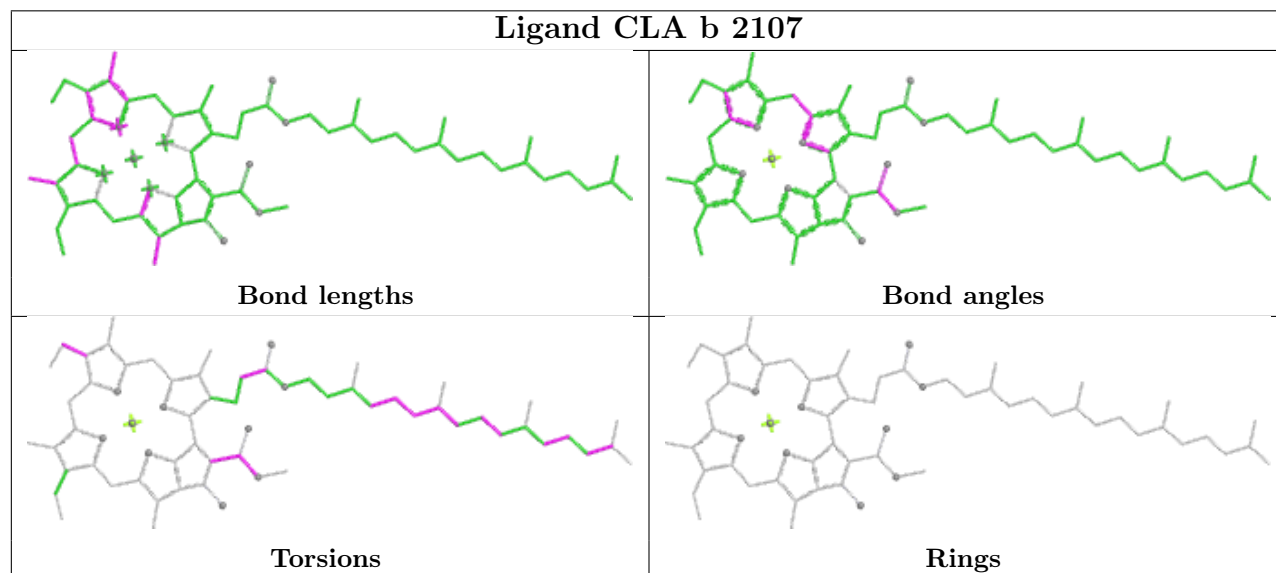
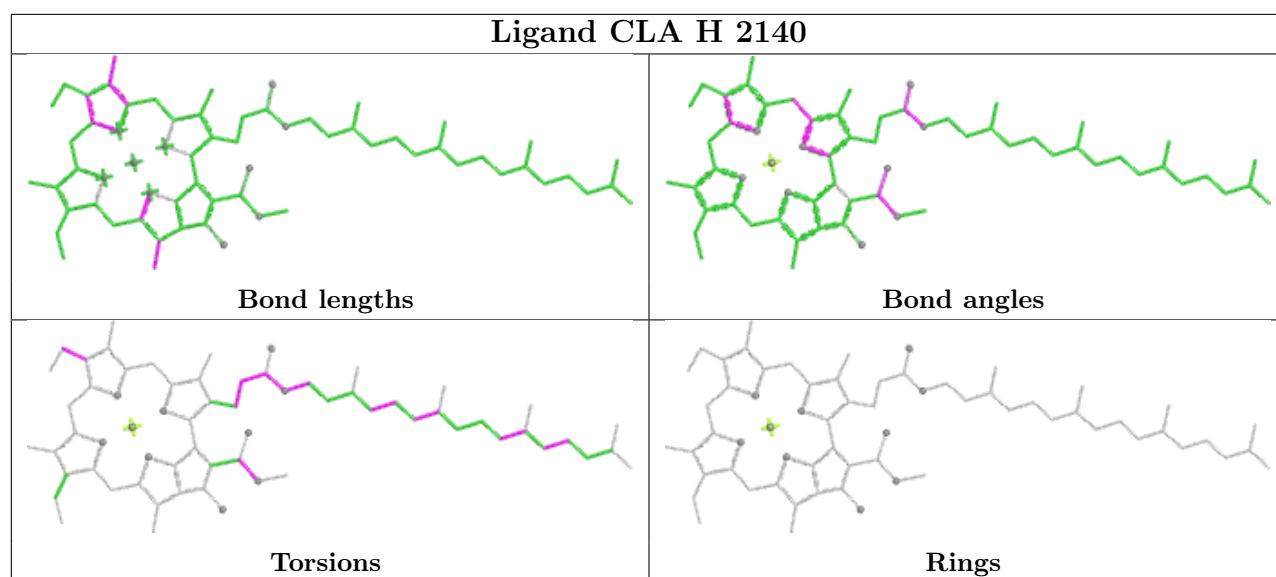


Rings

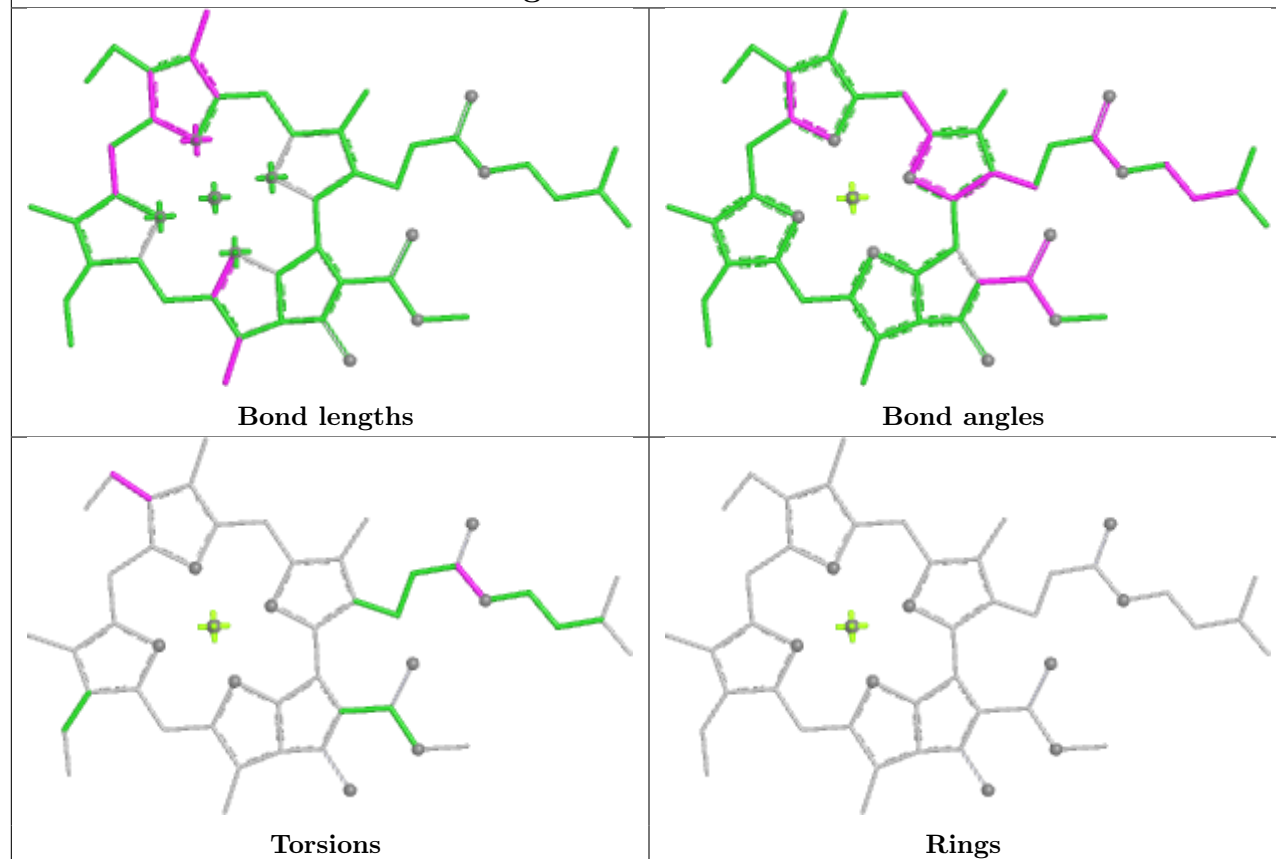




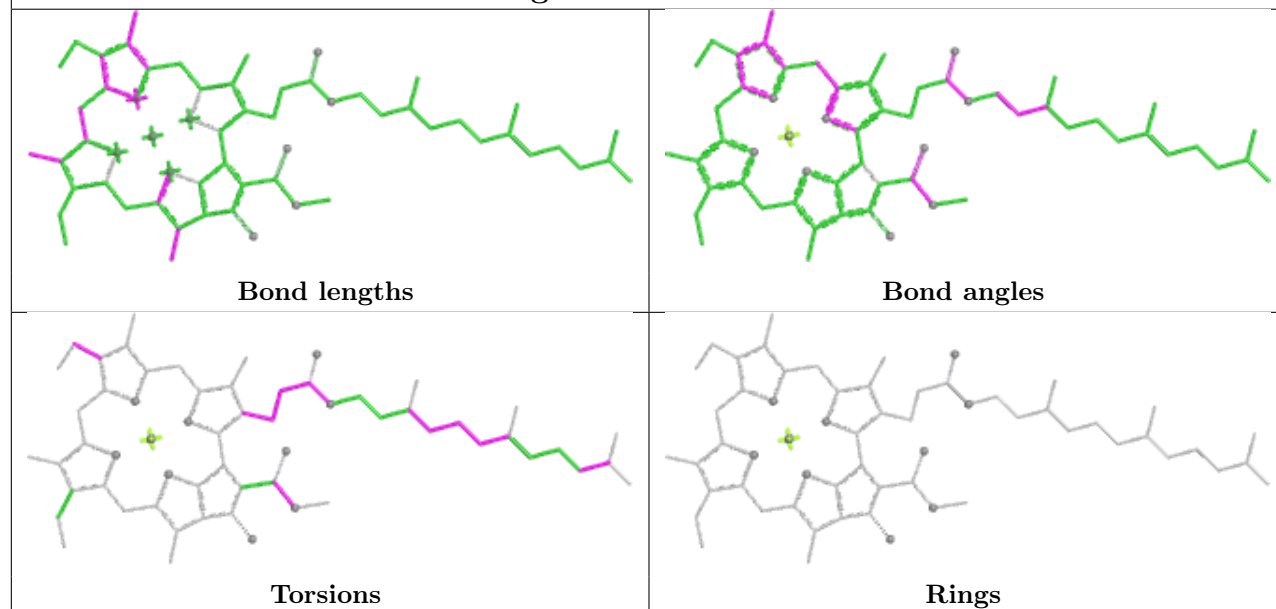


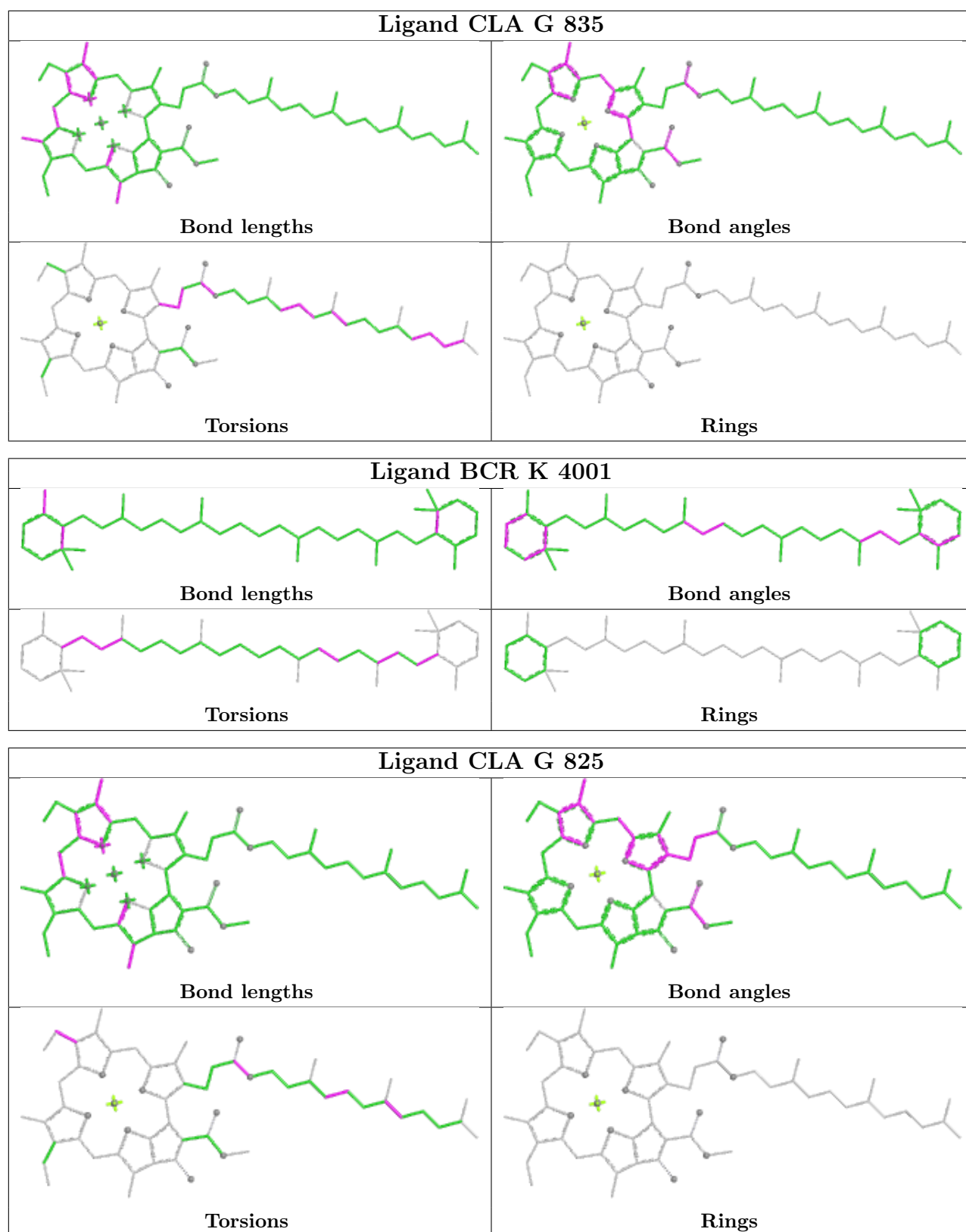


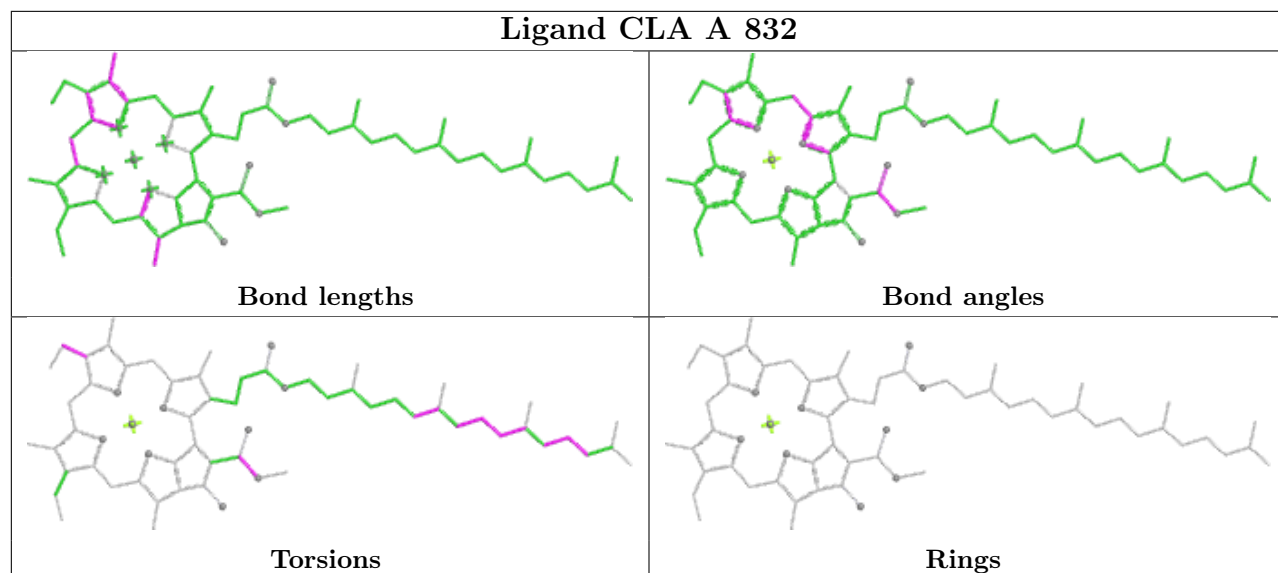
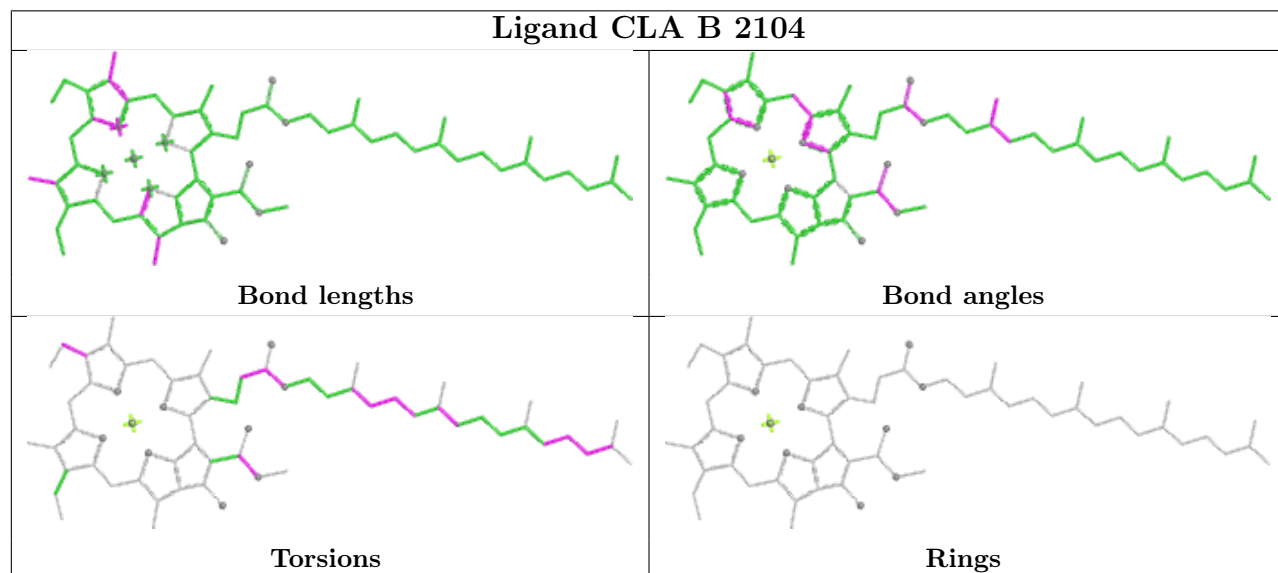
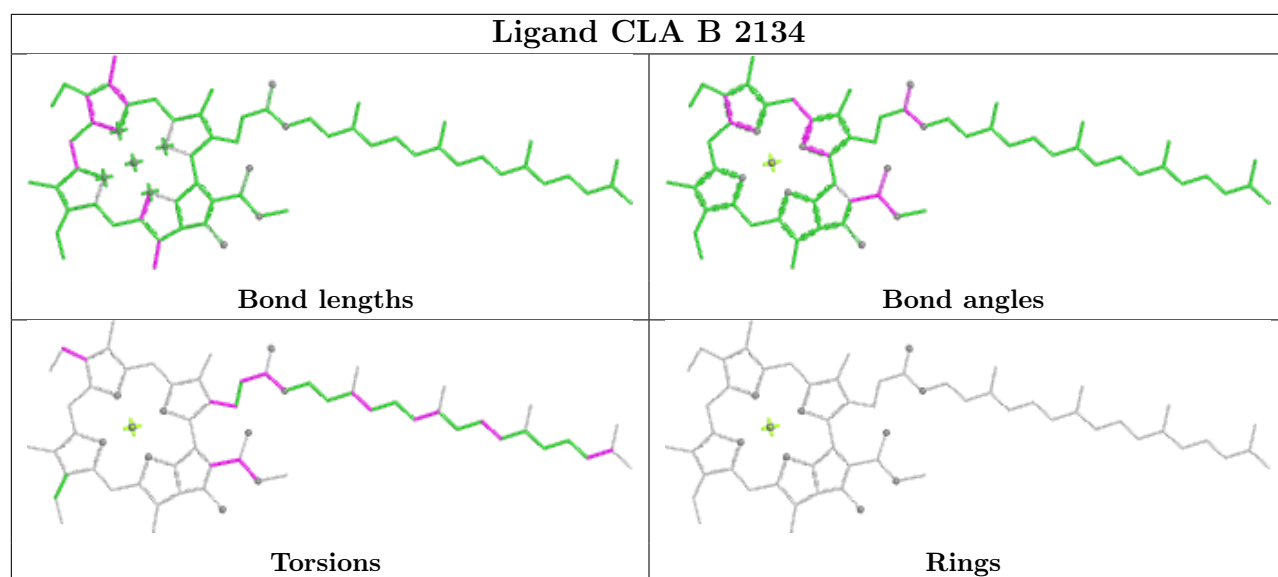
Ligand CLA B 2126

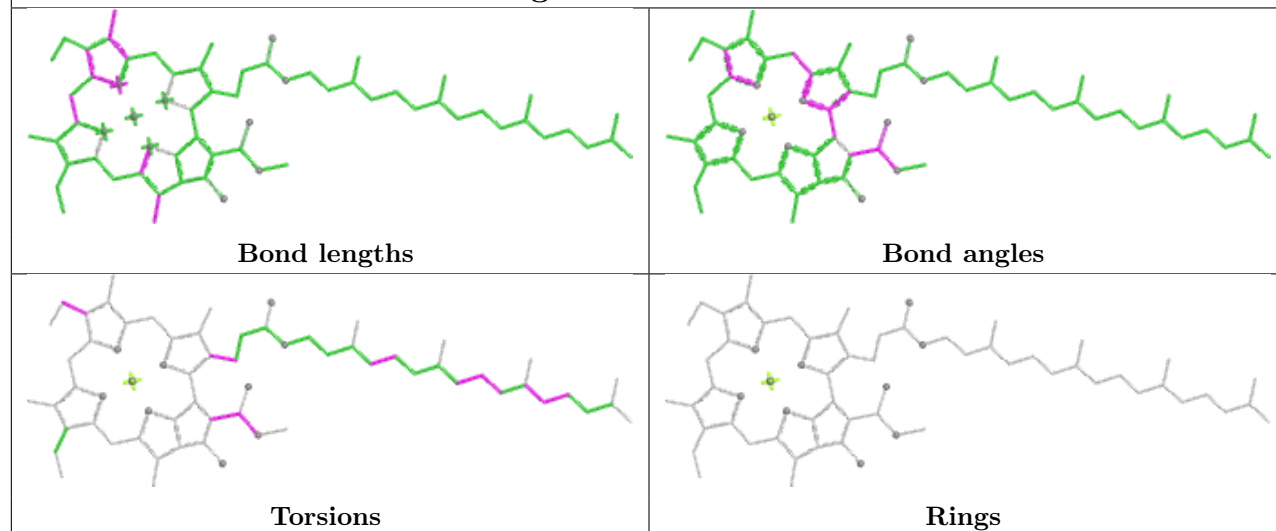
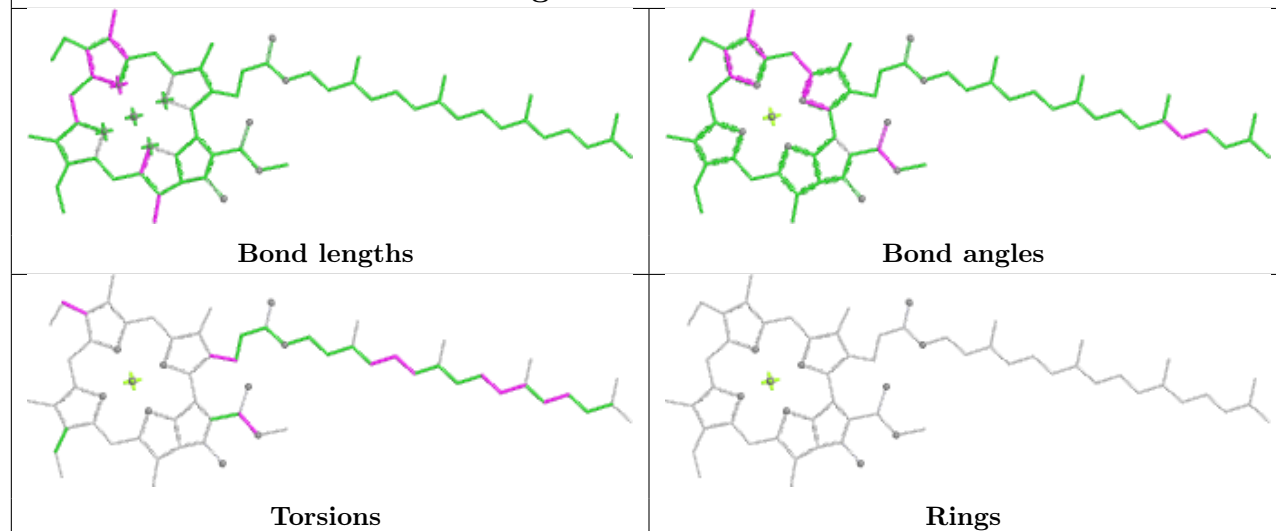


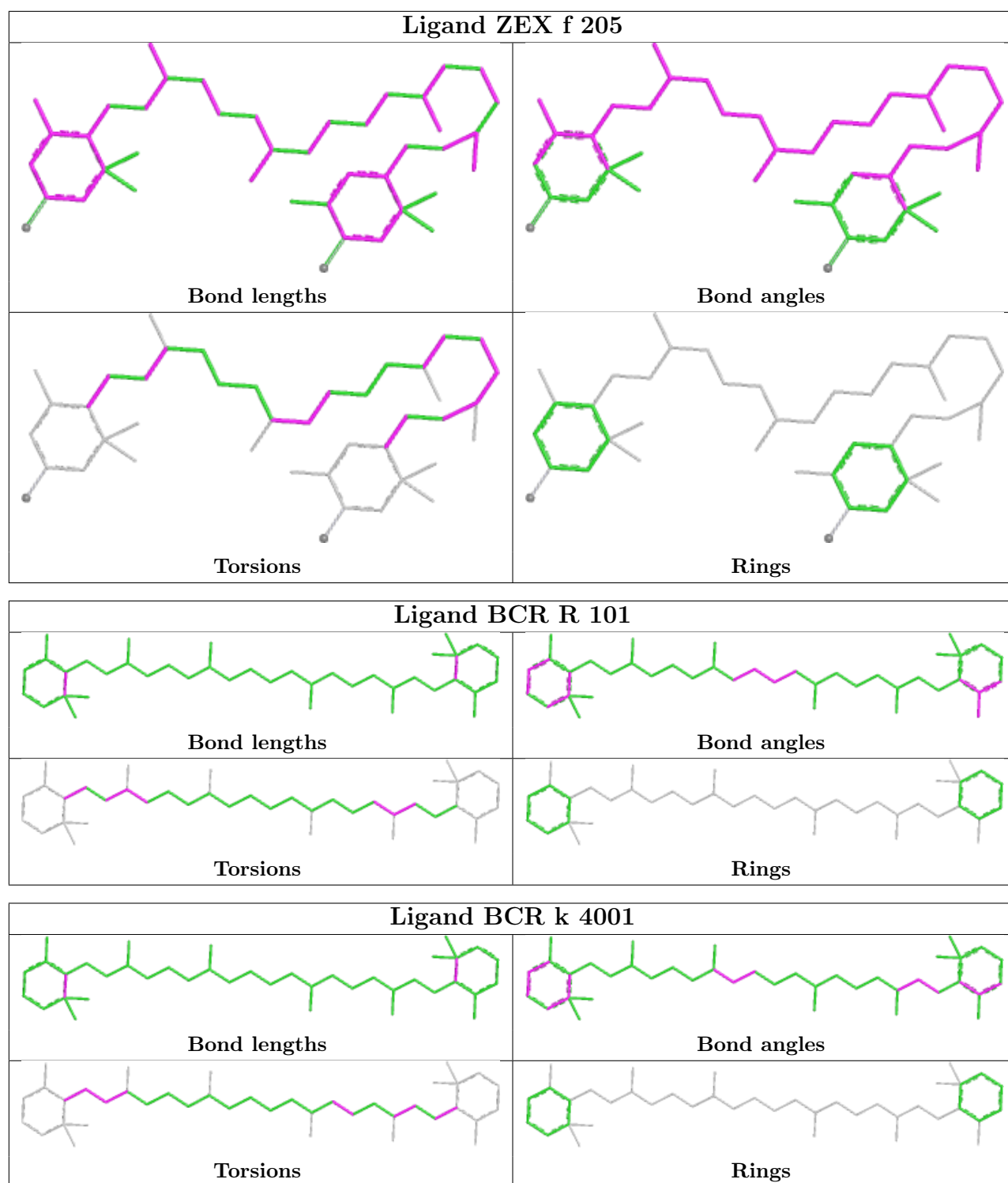
Ligand CLA G 817

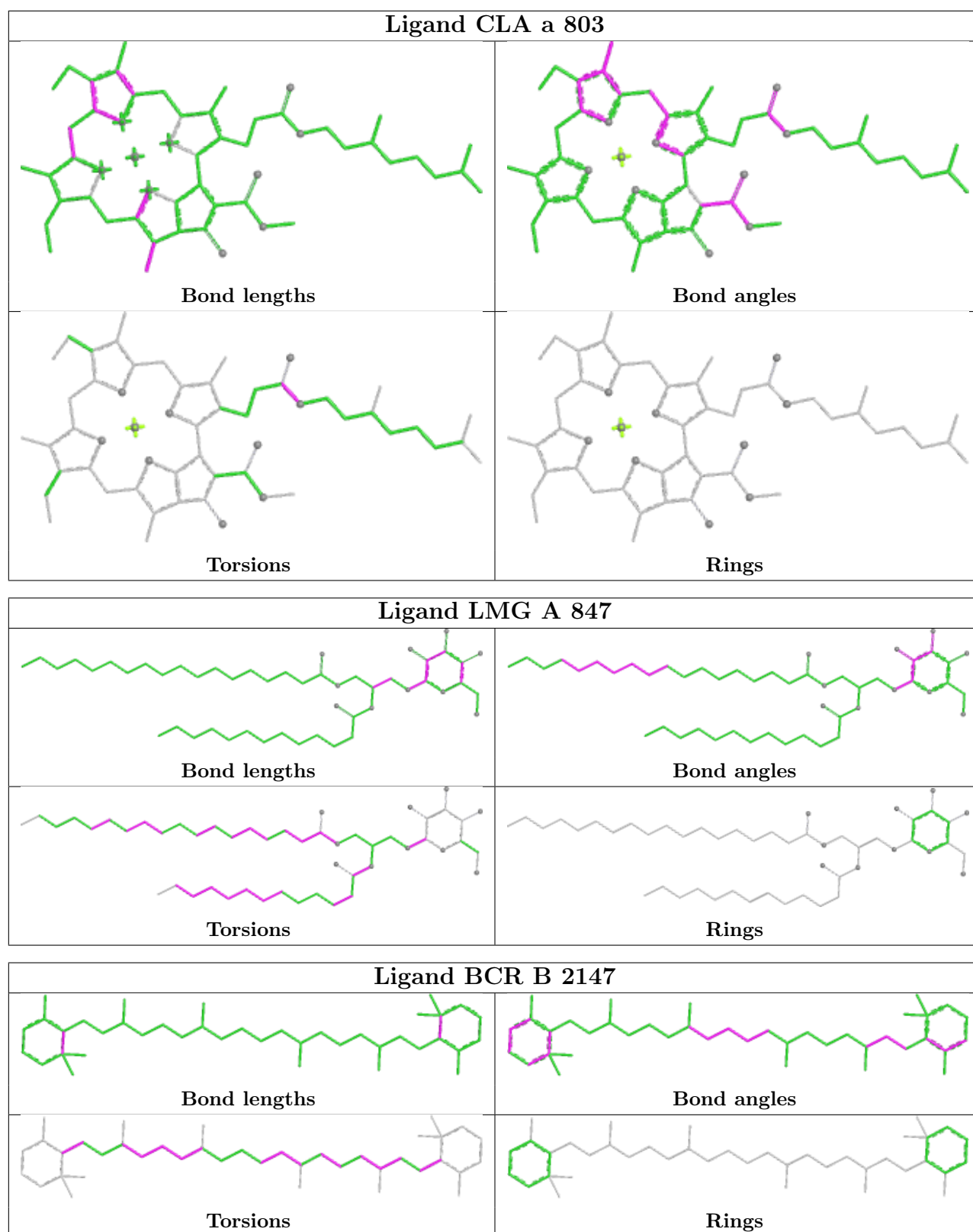




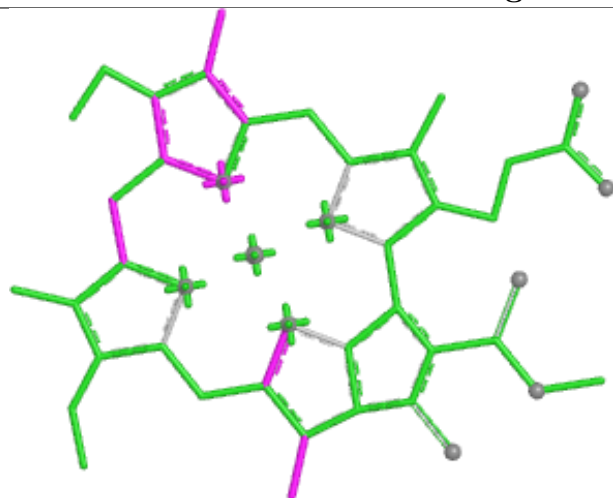


Ligand CLA G 812**Ligand CLA A 839**

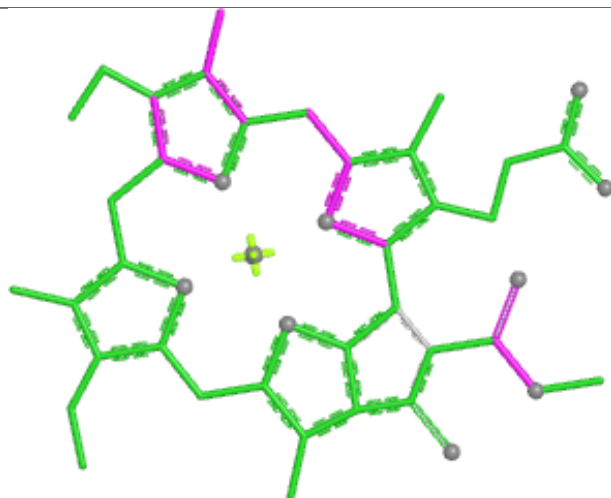




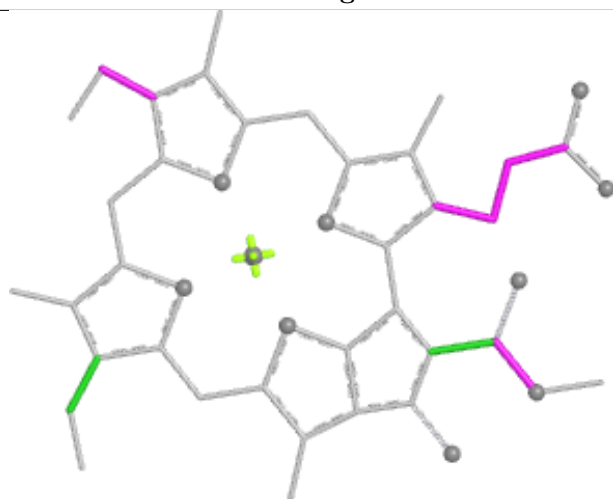
Ligand CLA B 2136



Bond lengths



Bond angles

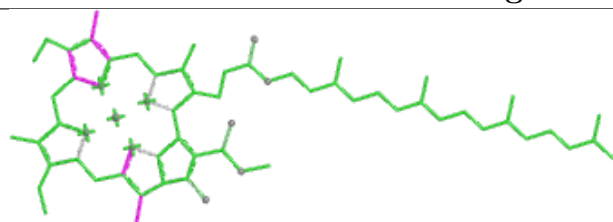


Torsions

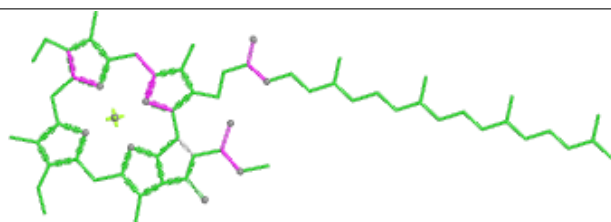


Rings

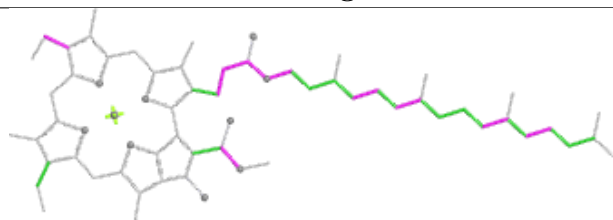
Ligand CLA B 2141



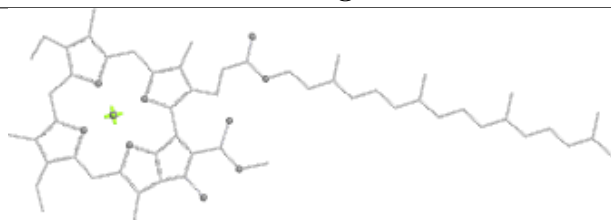
Bond lengths



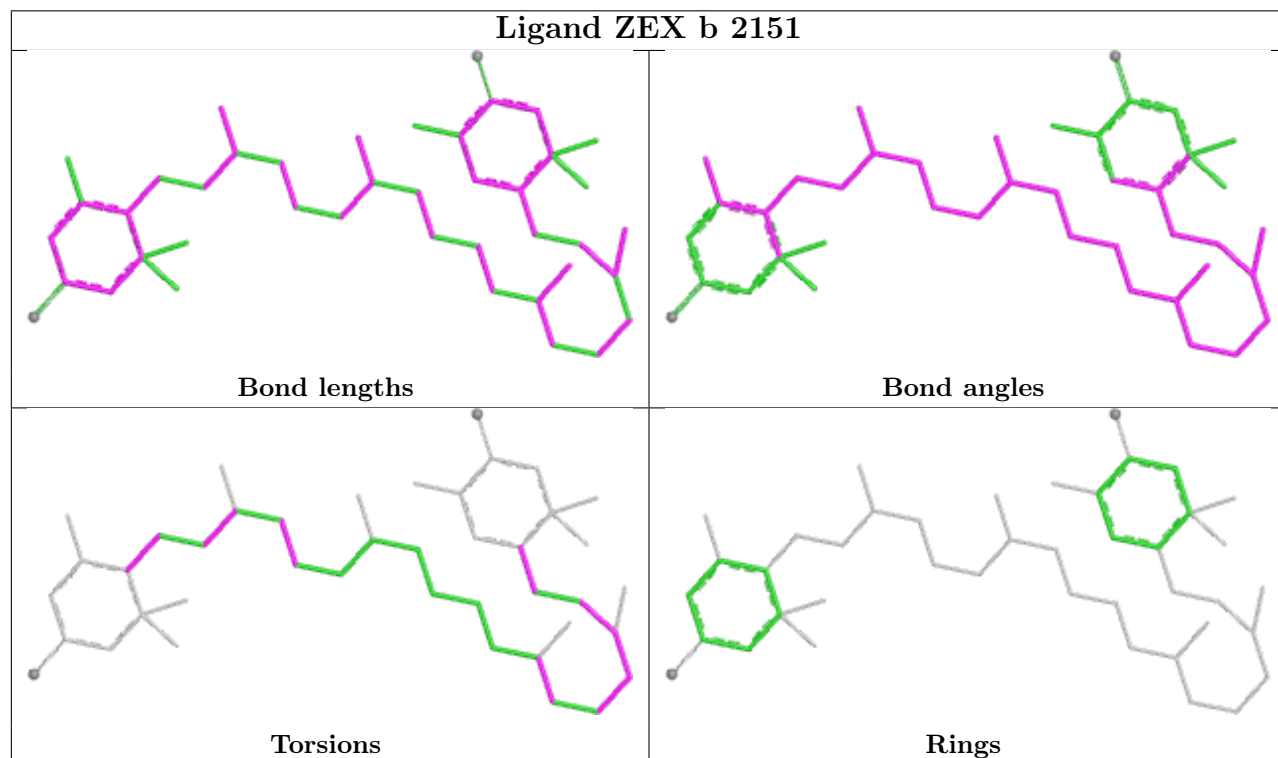
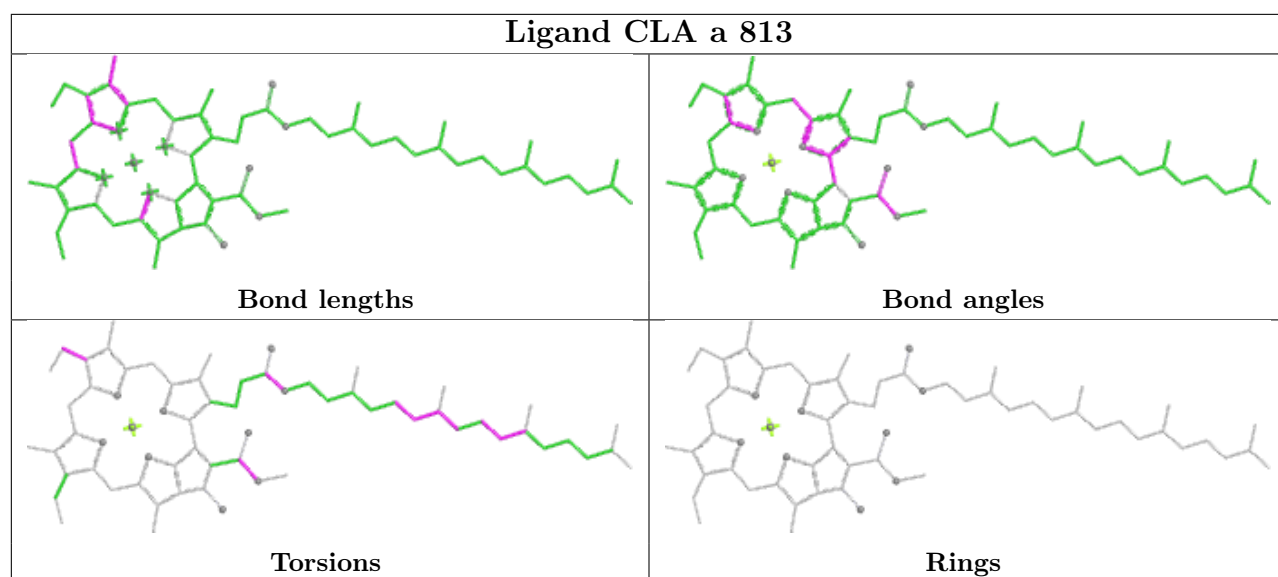
Bond angles

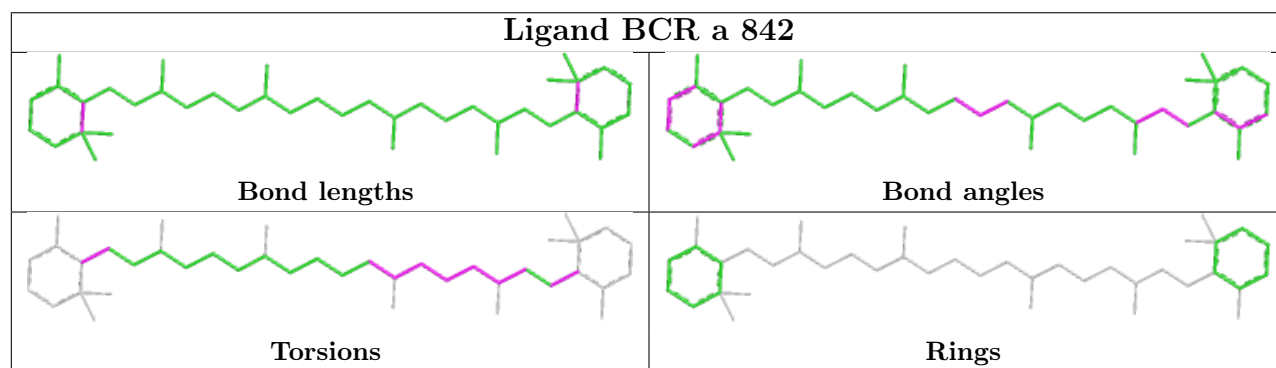
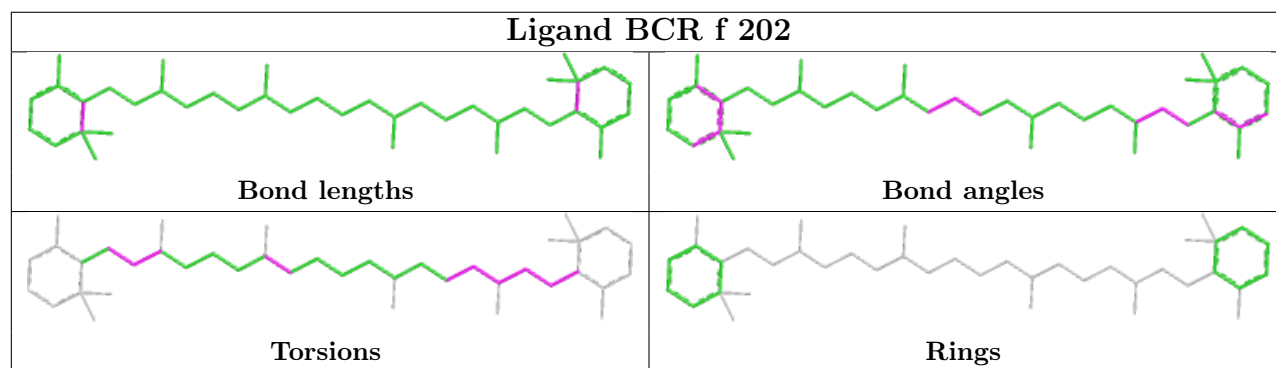
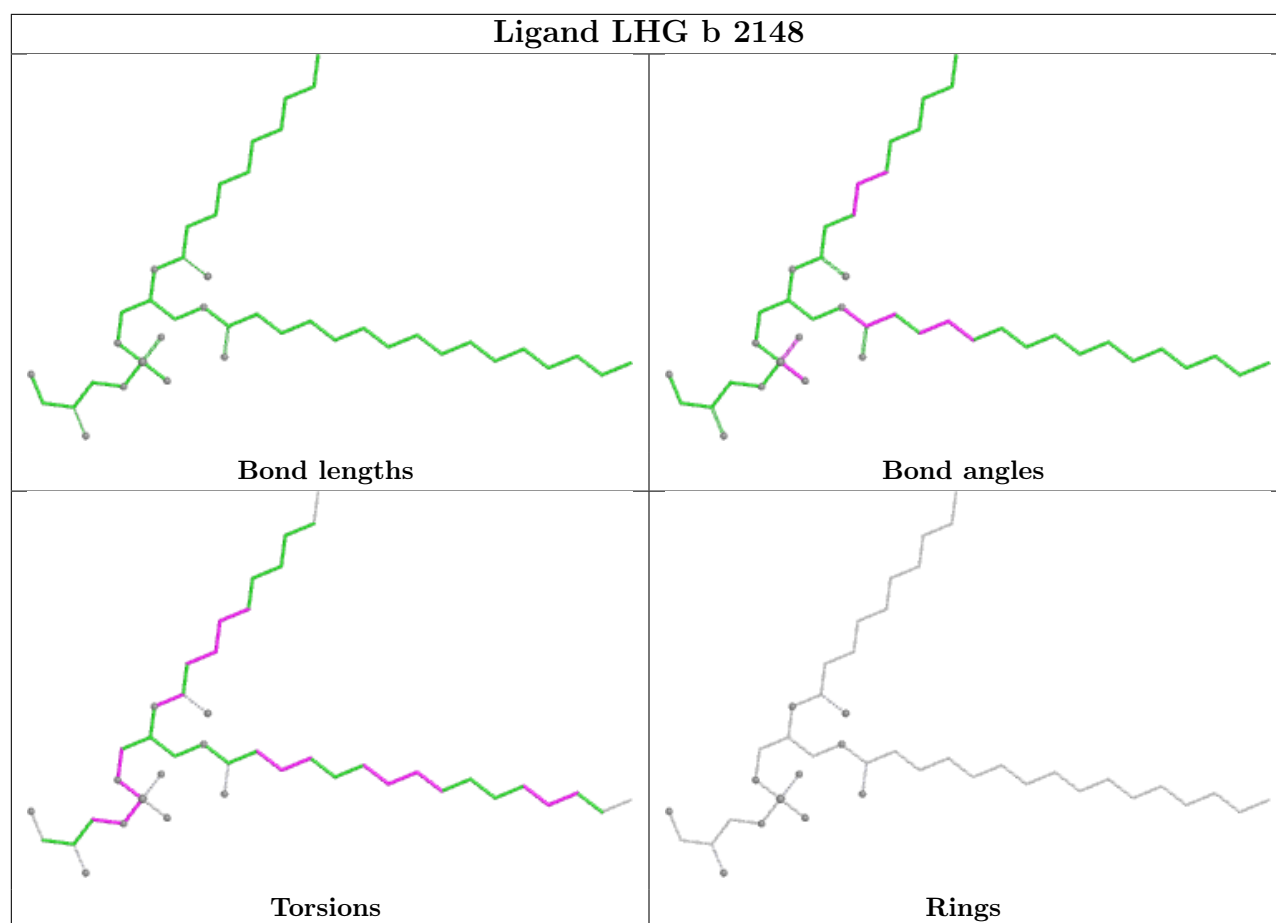


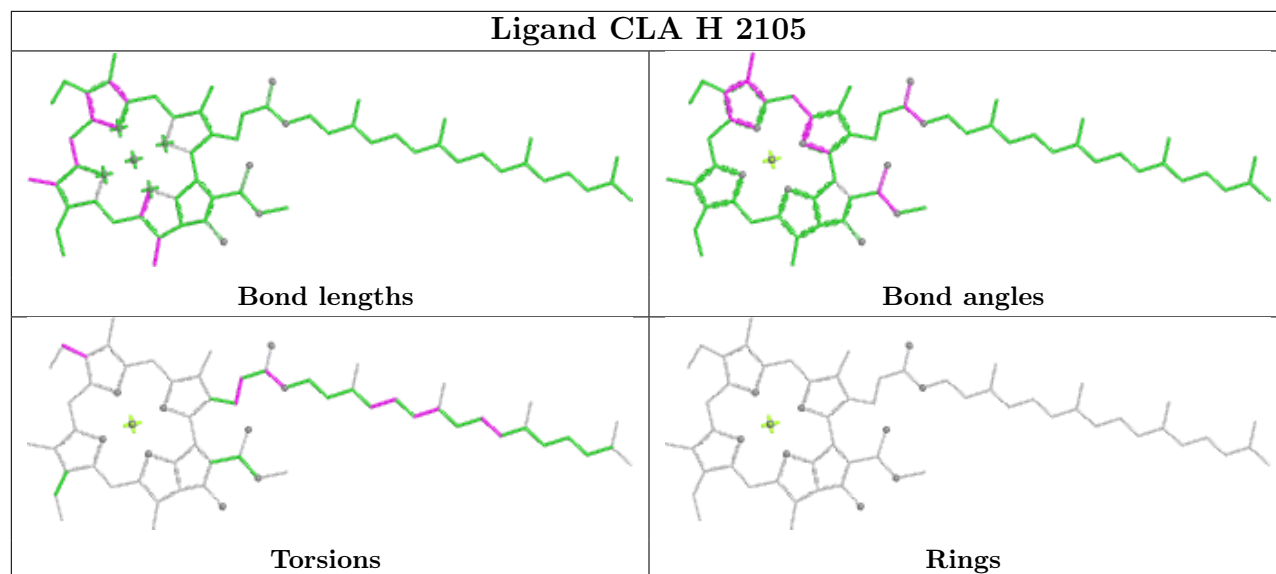
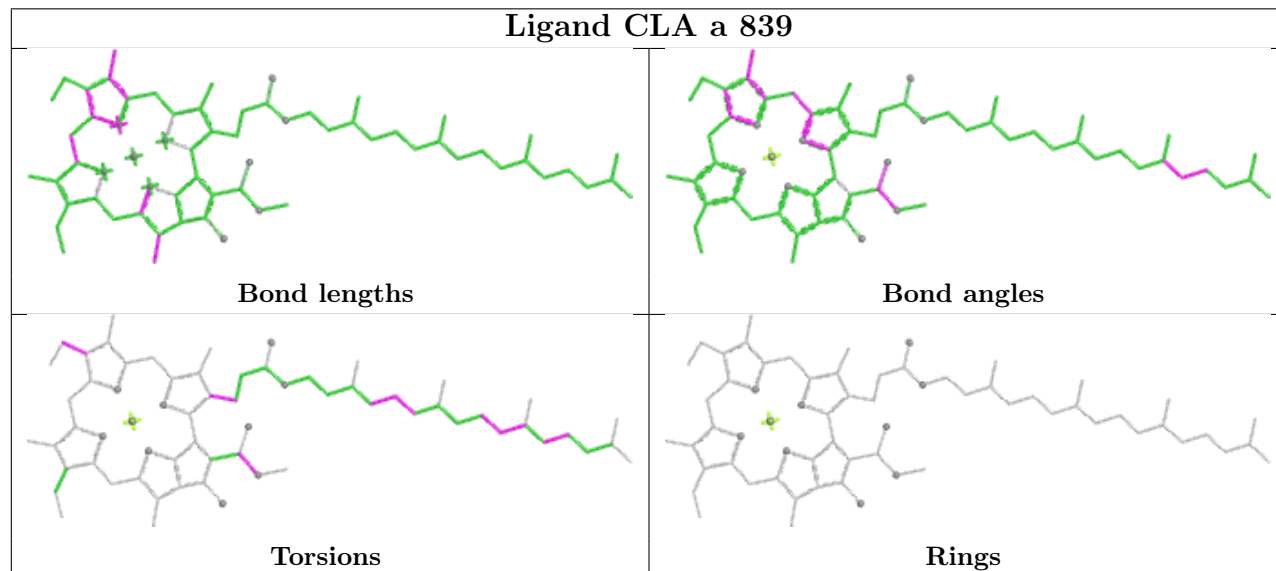
Torsions

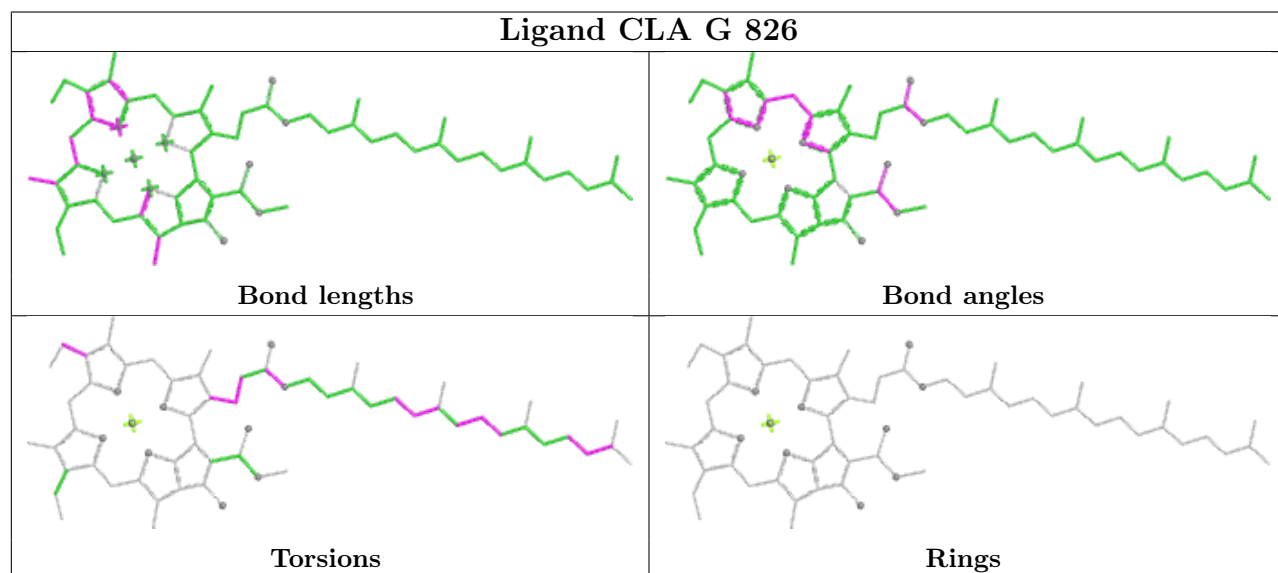
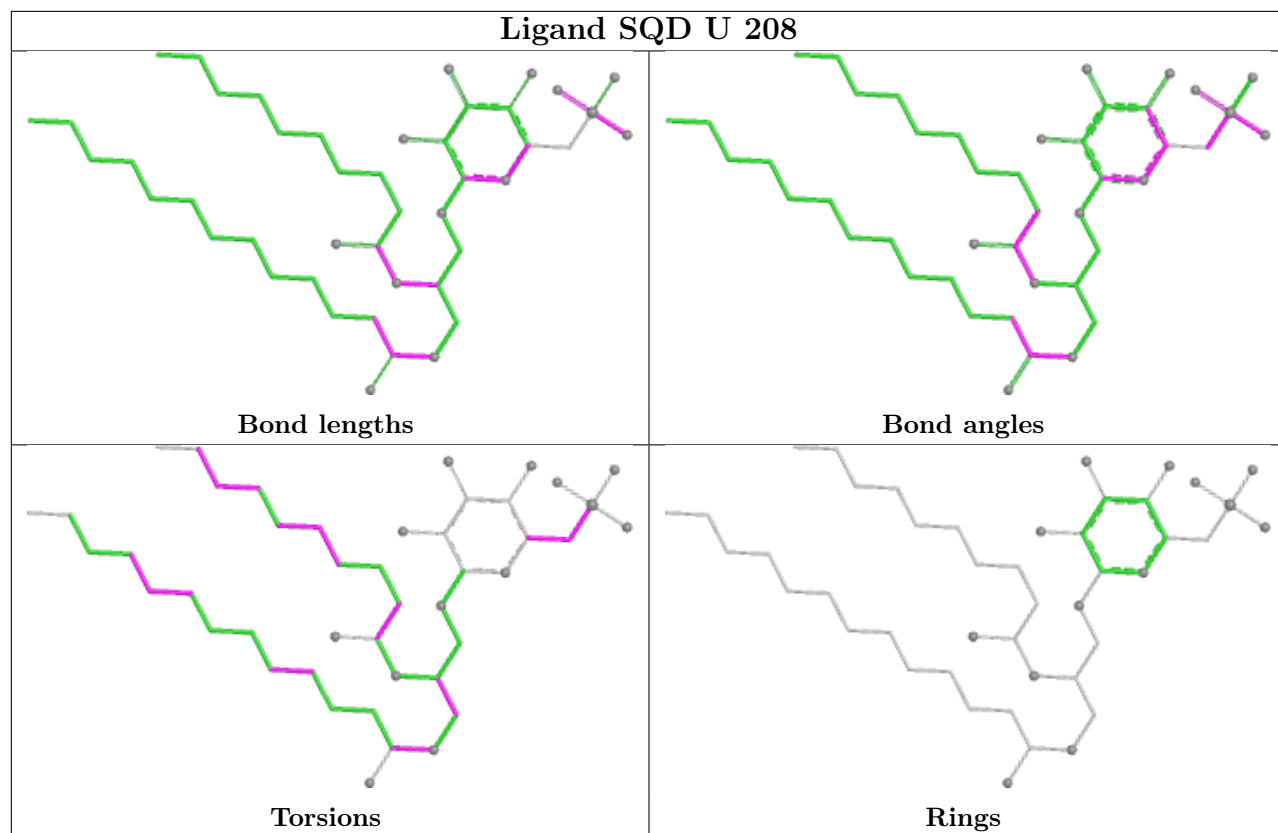


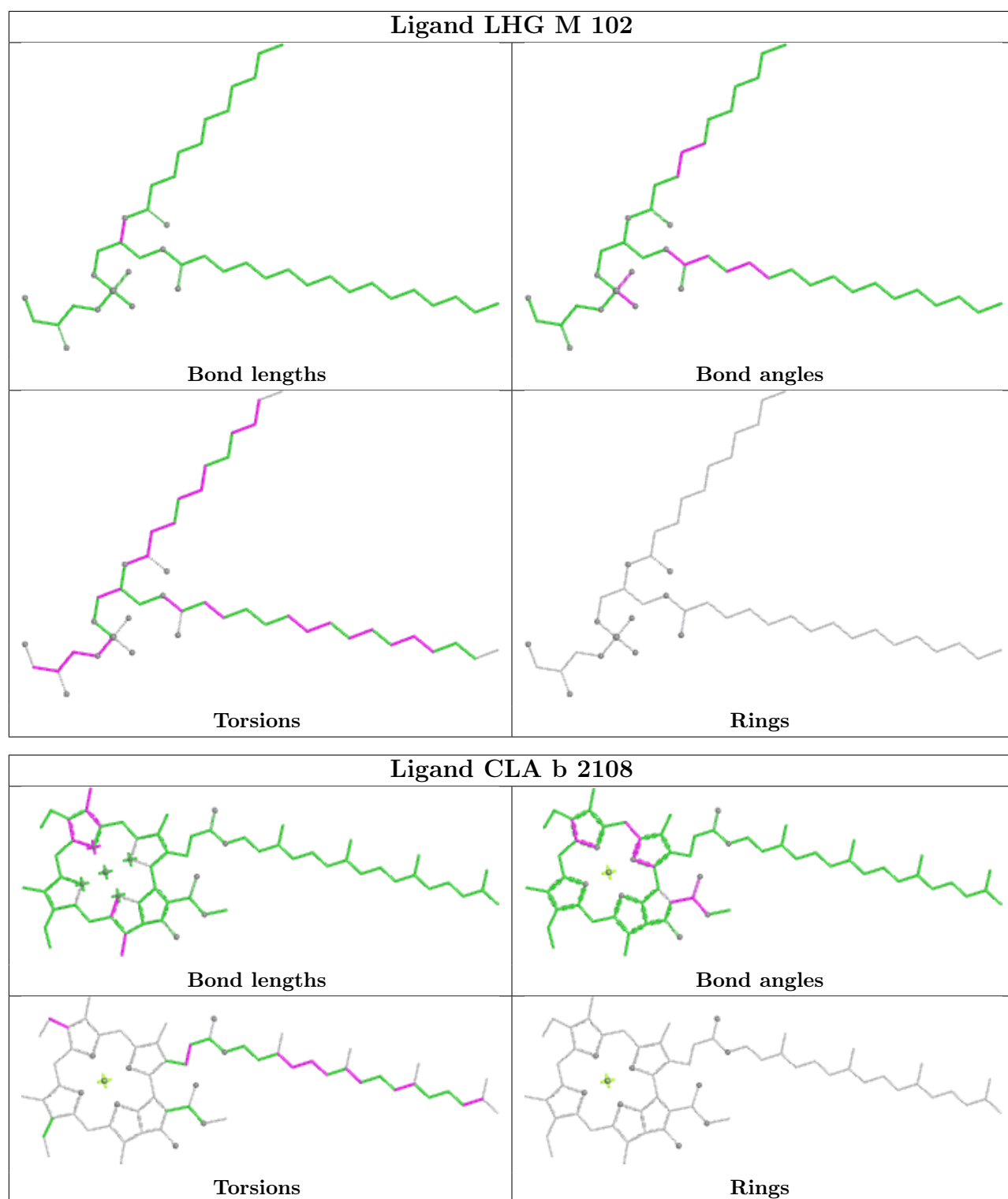
Rings

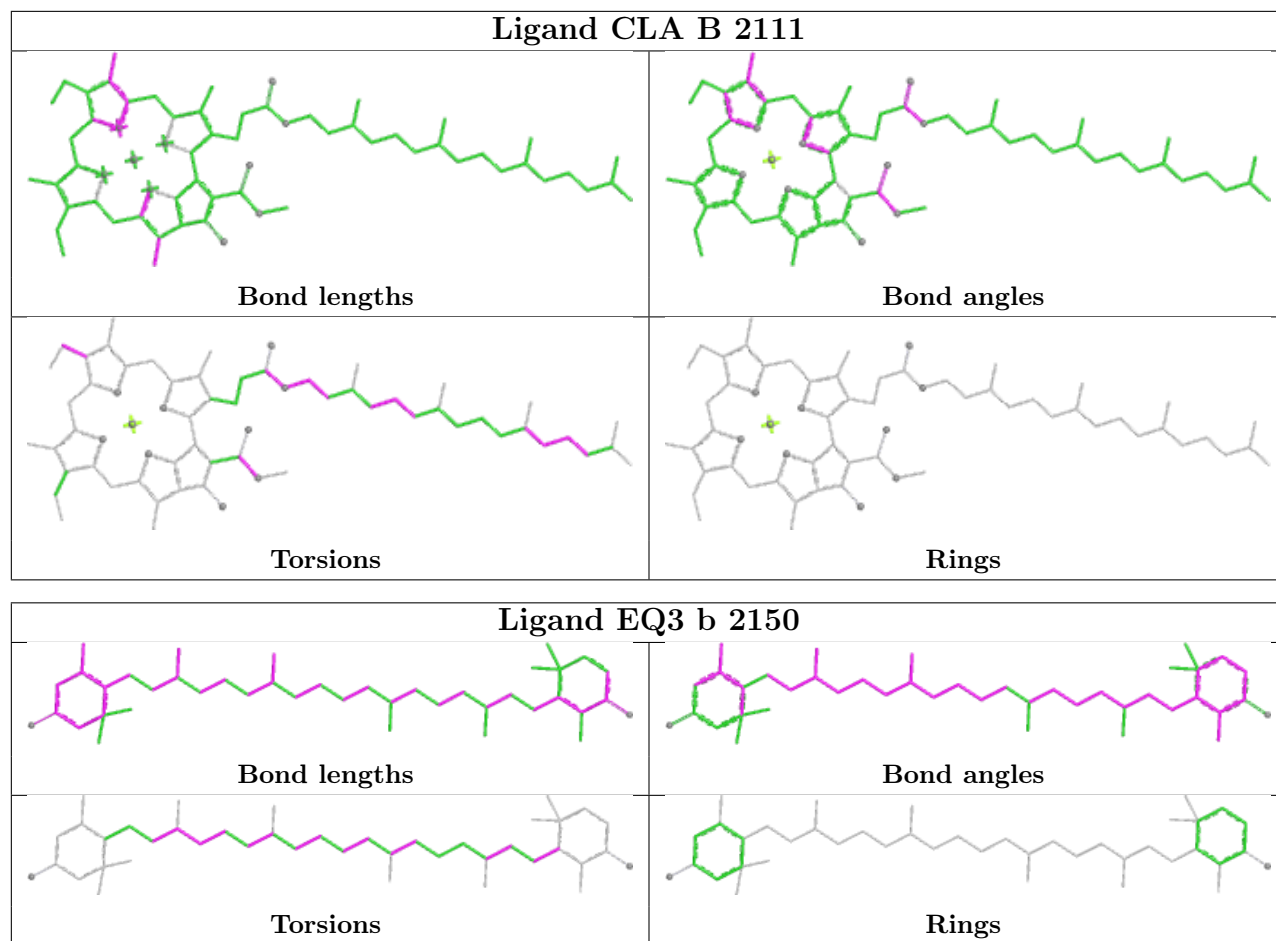


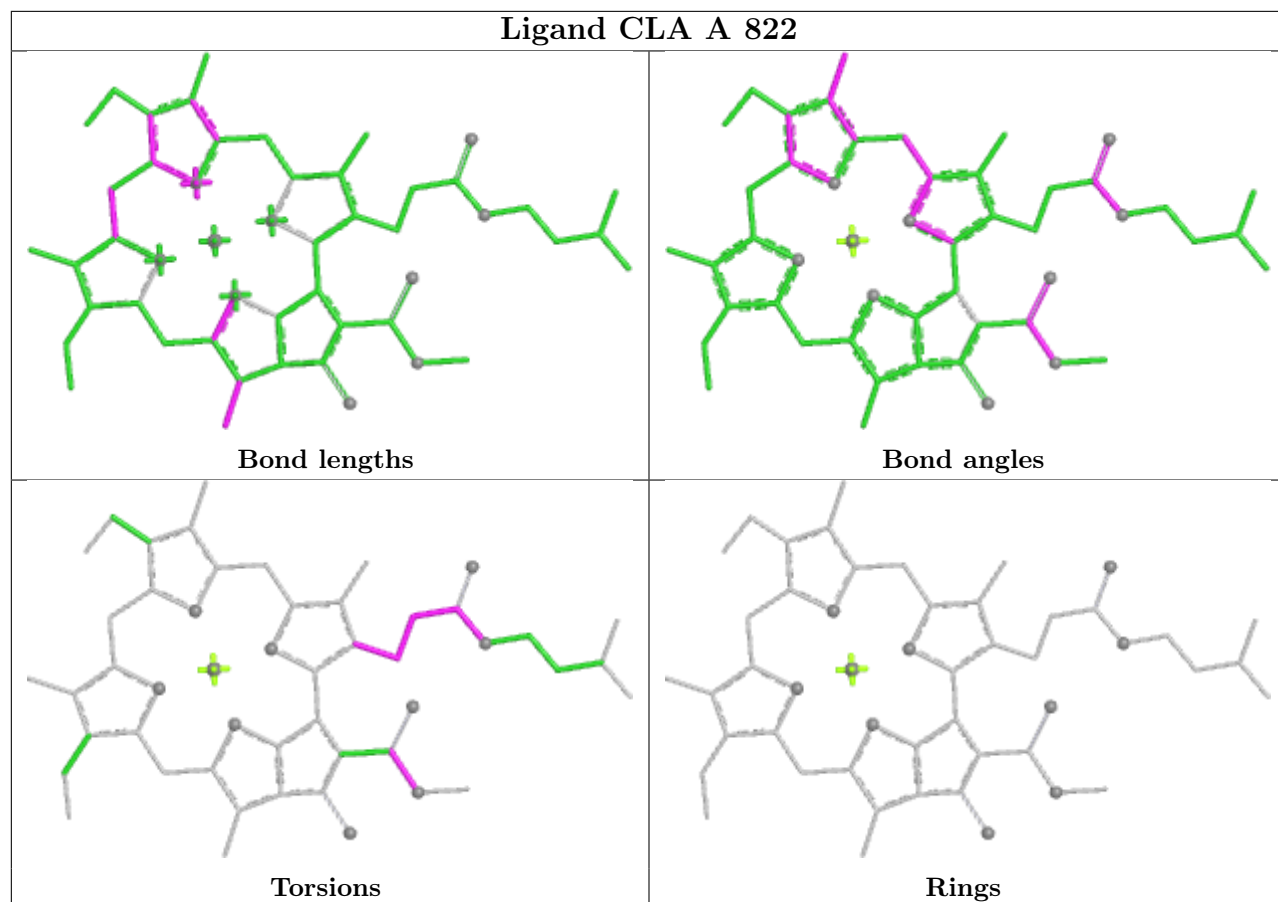


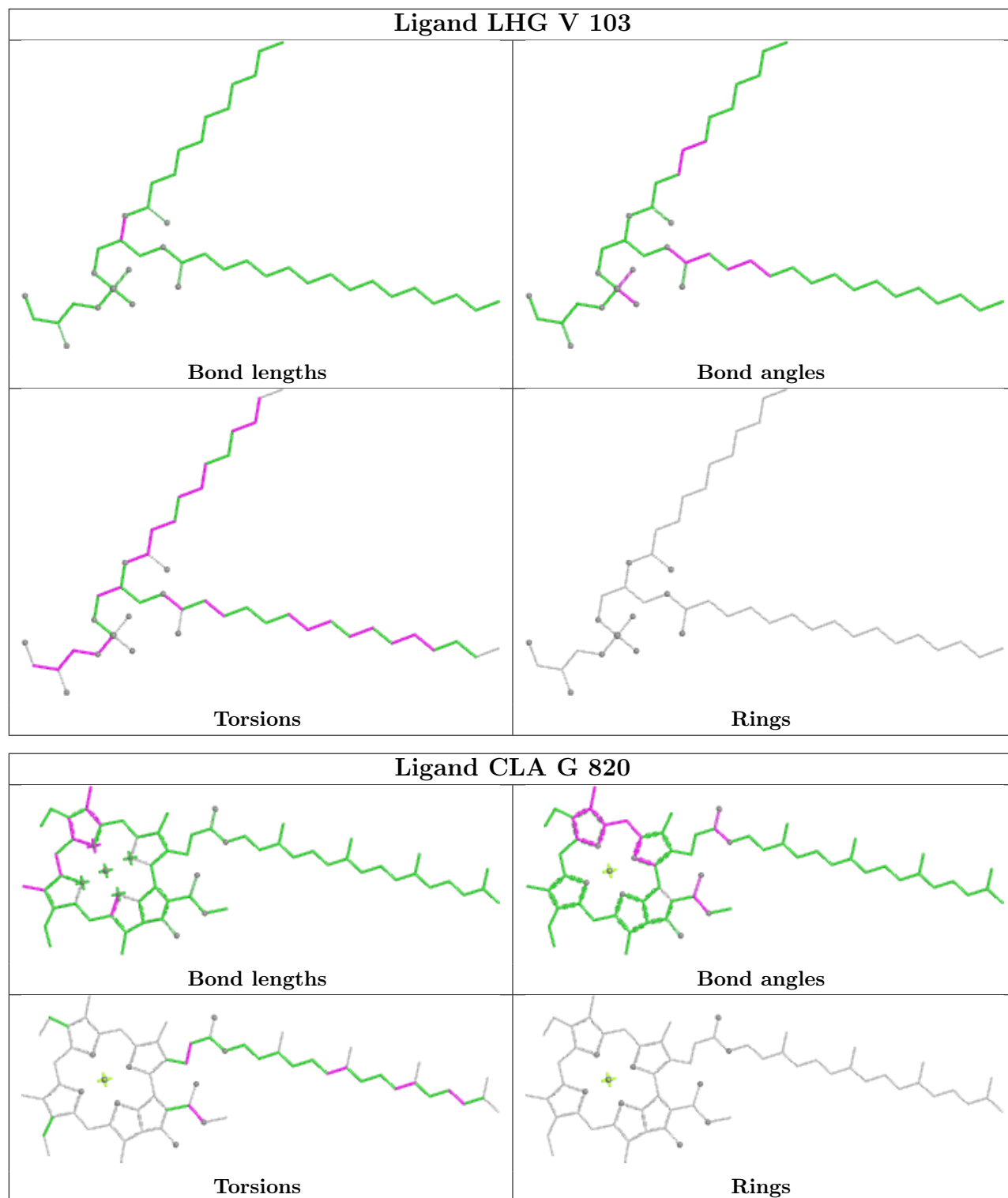
Ligand CLA H 2105**Ligand CLA a 839**

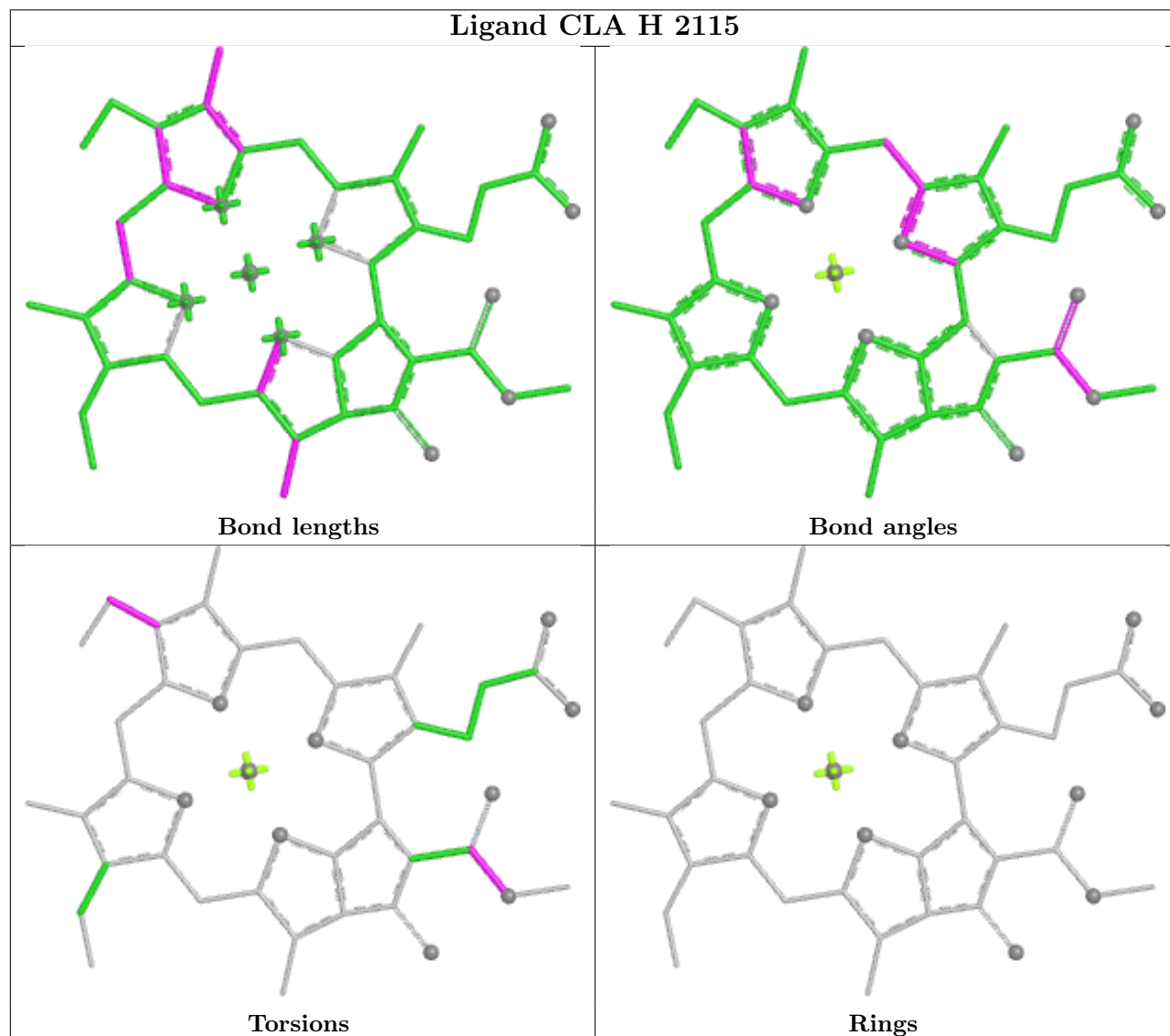
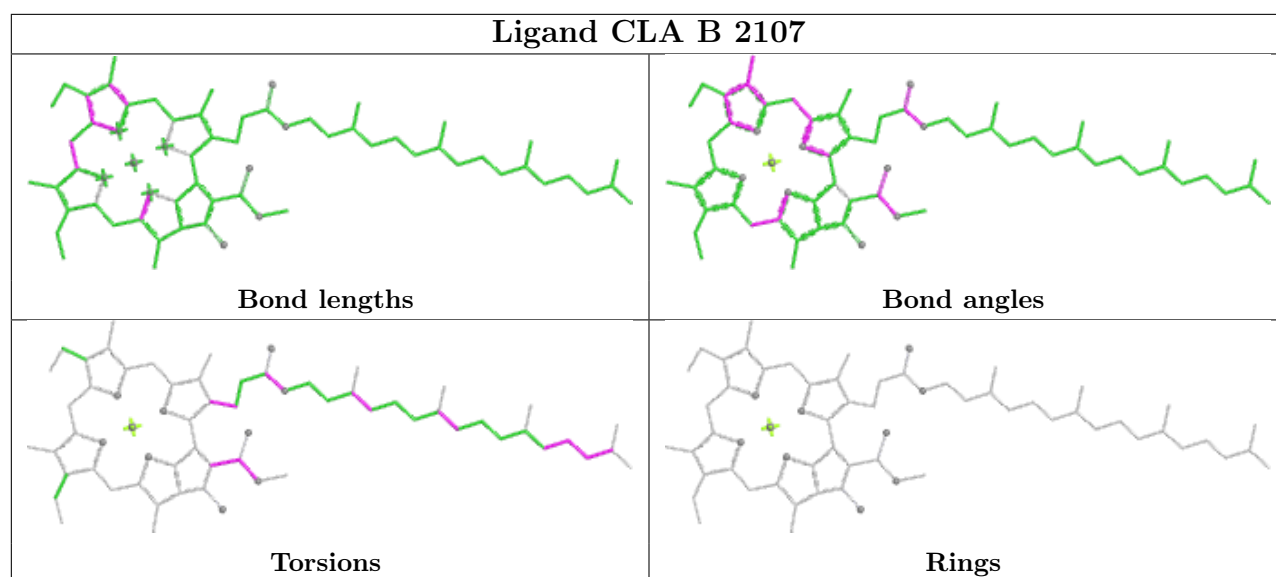


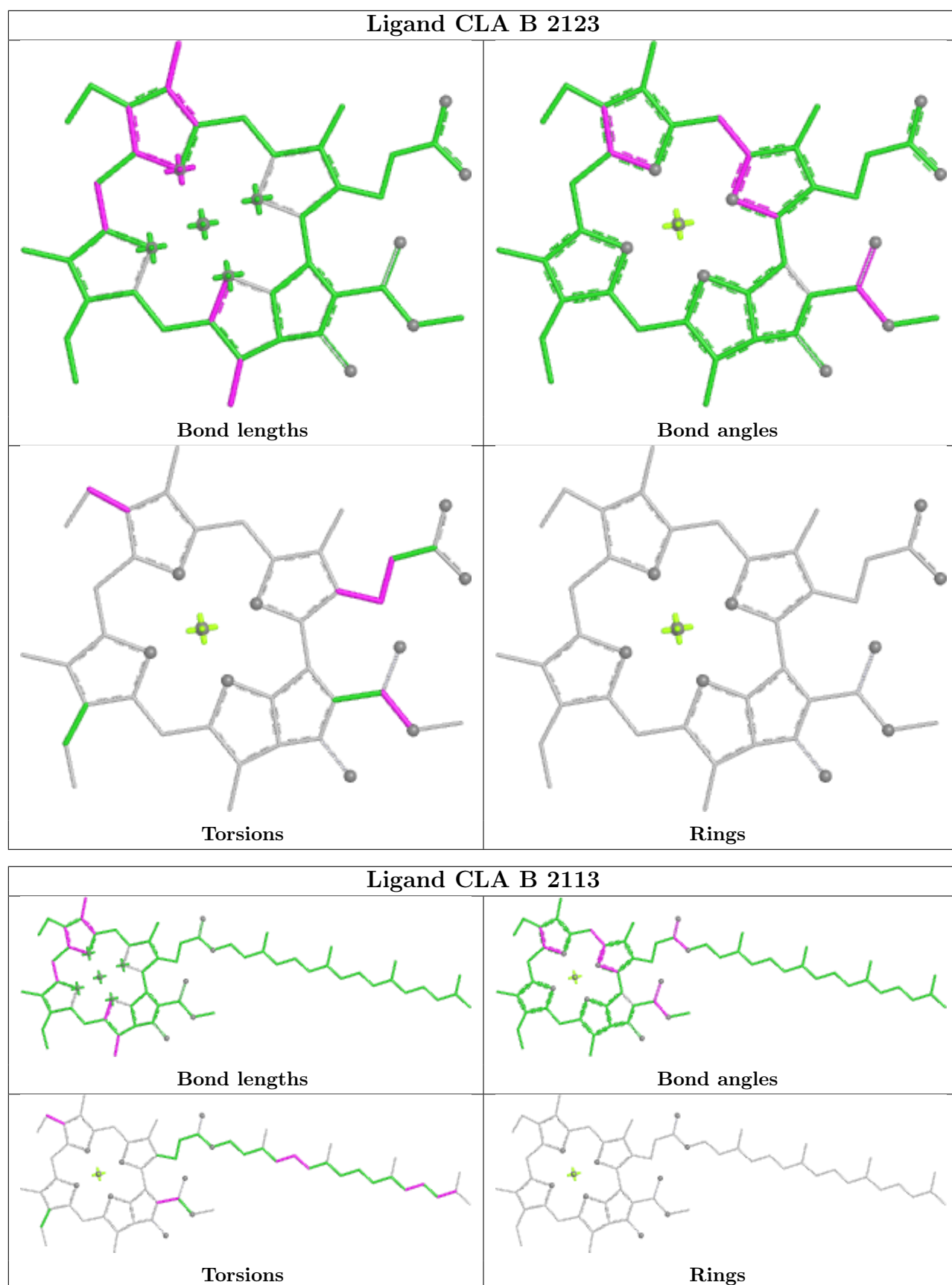


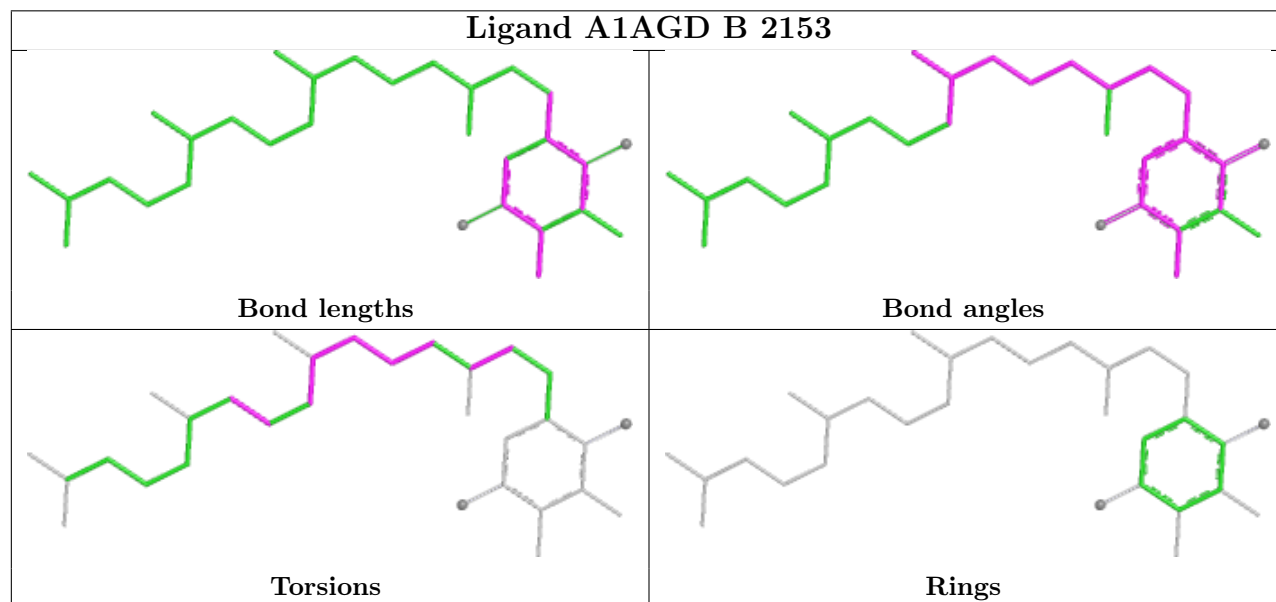
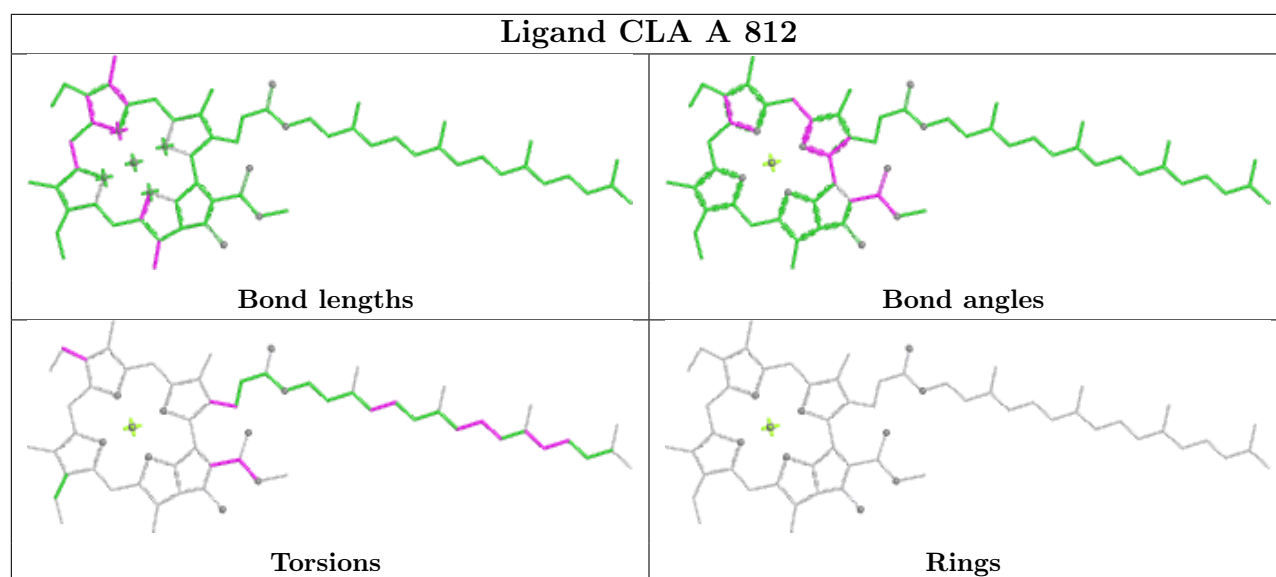




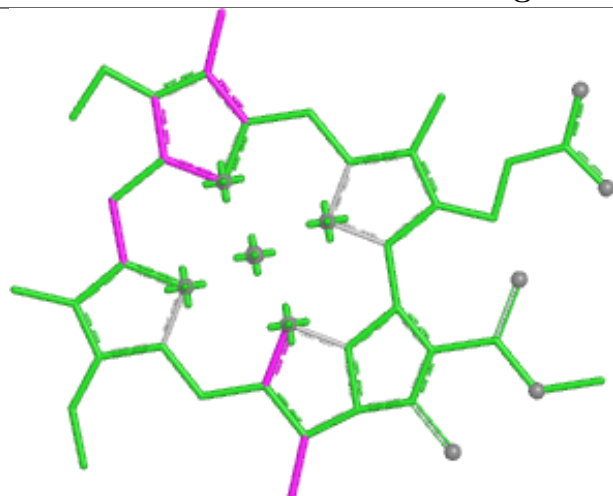




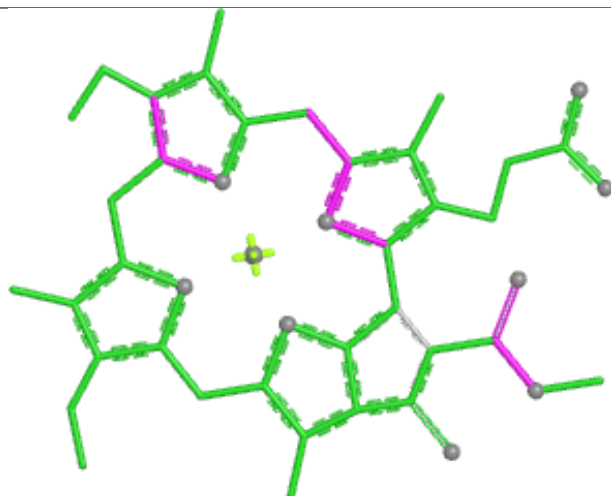




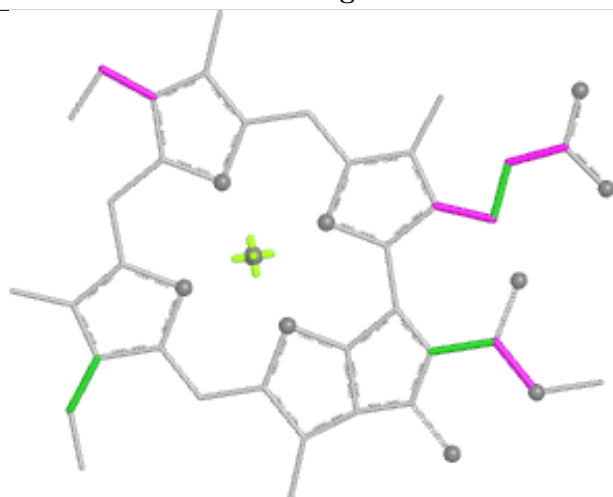
Ligand CLA A 811



Bond lengths



Bond angles

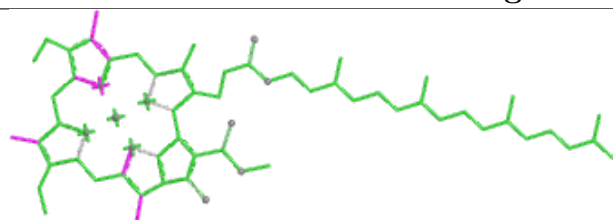


Torsions

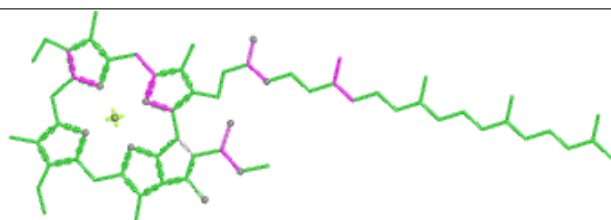


Rings

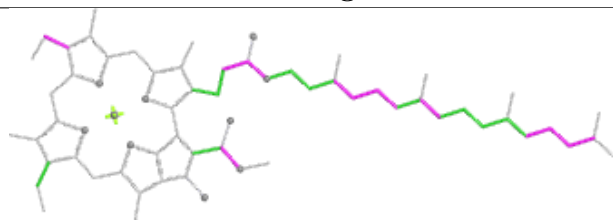
Ligand CLA H 2103



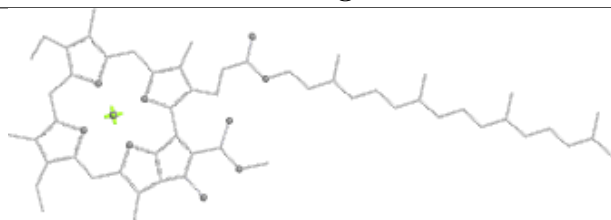
Bond lengths



Bond angles

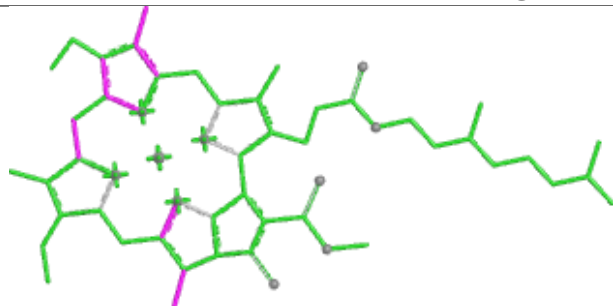


Torsions

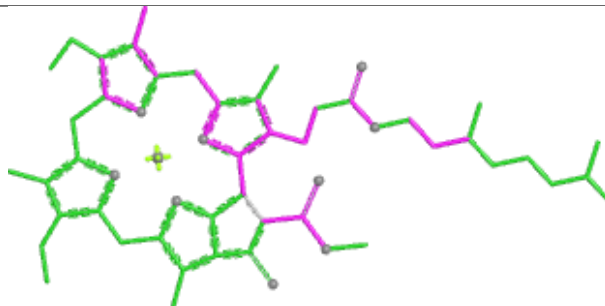


Rings

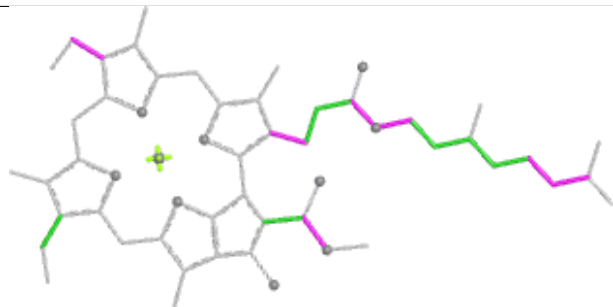
Ligand CLA G 834



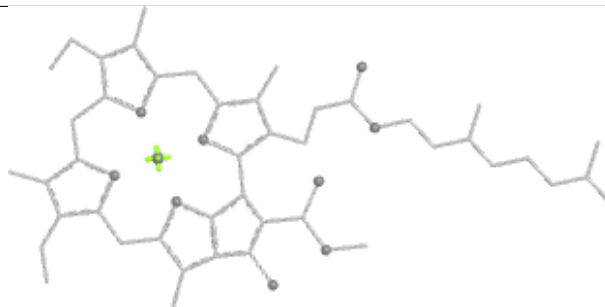
Bond lengths



Bond angles

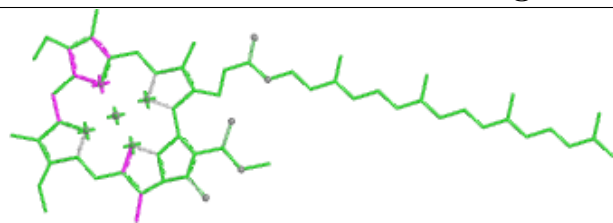


Torsions

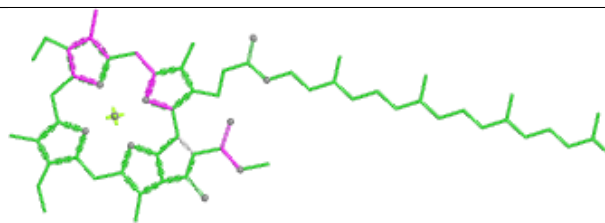


Rings

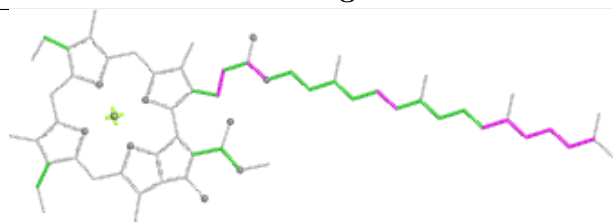
Ligand CLA G 828



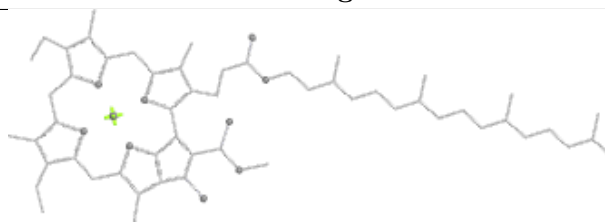
Bond lengths



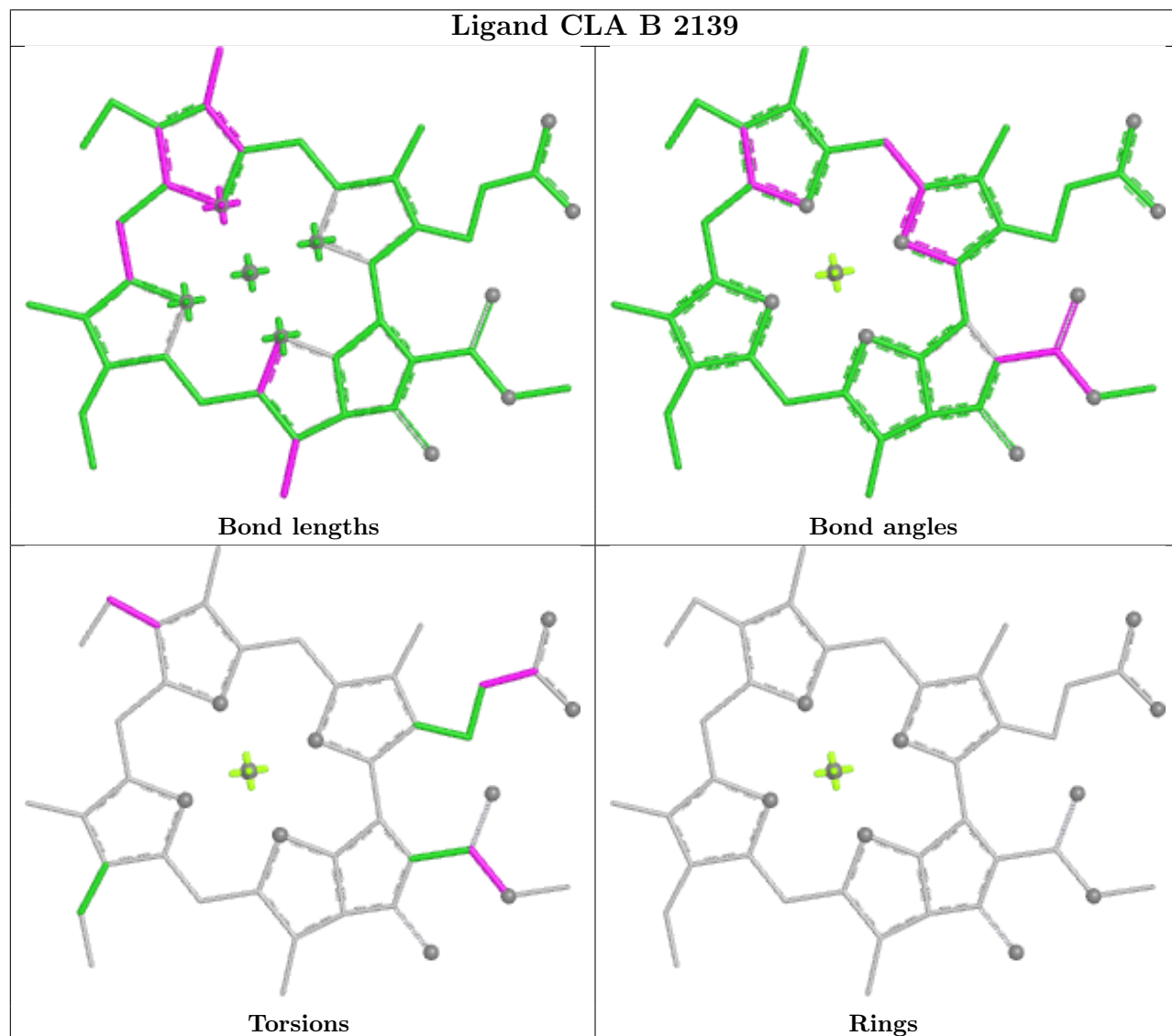
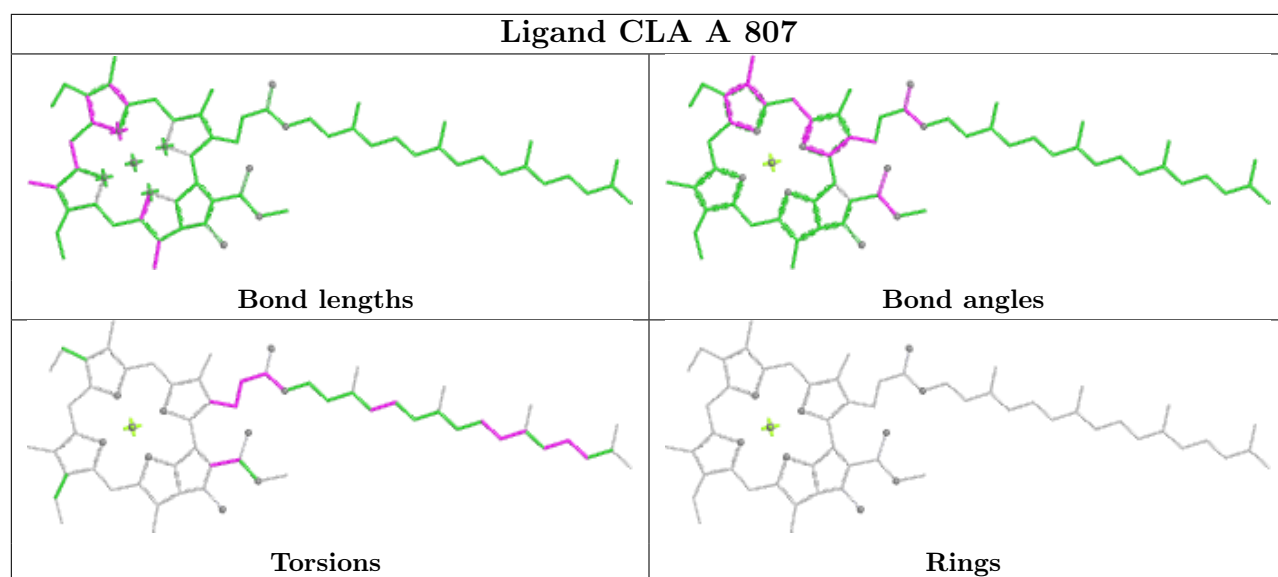
Bond angles



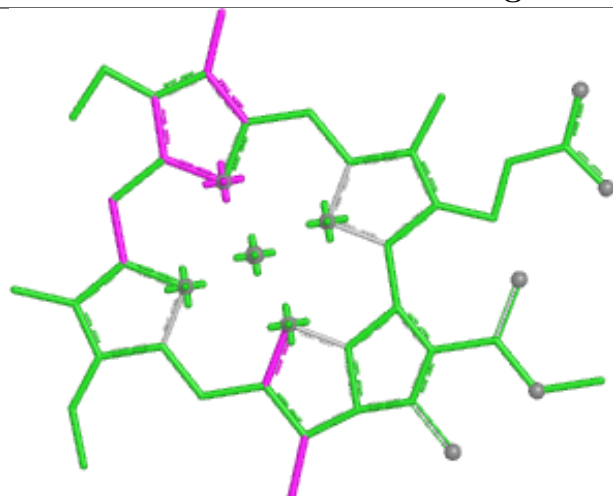
Torsions



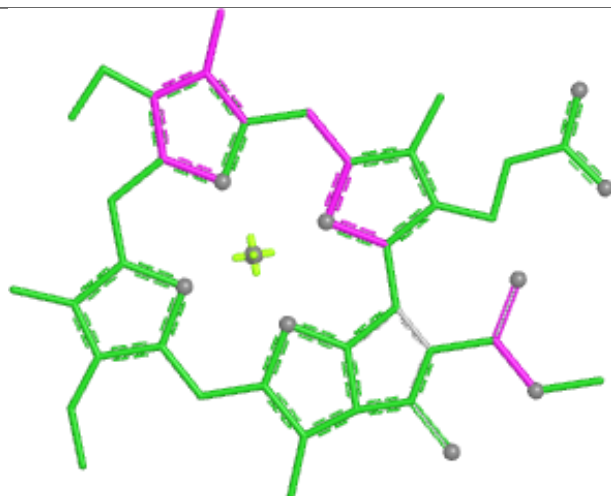
Rings



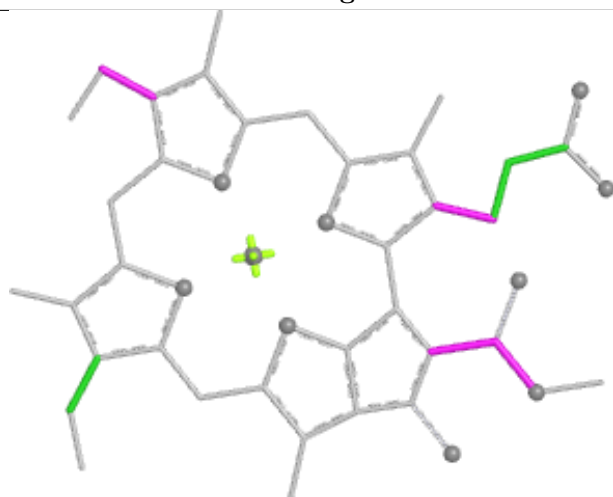
Ligand CLA H 2136



Bond lengths



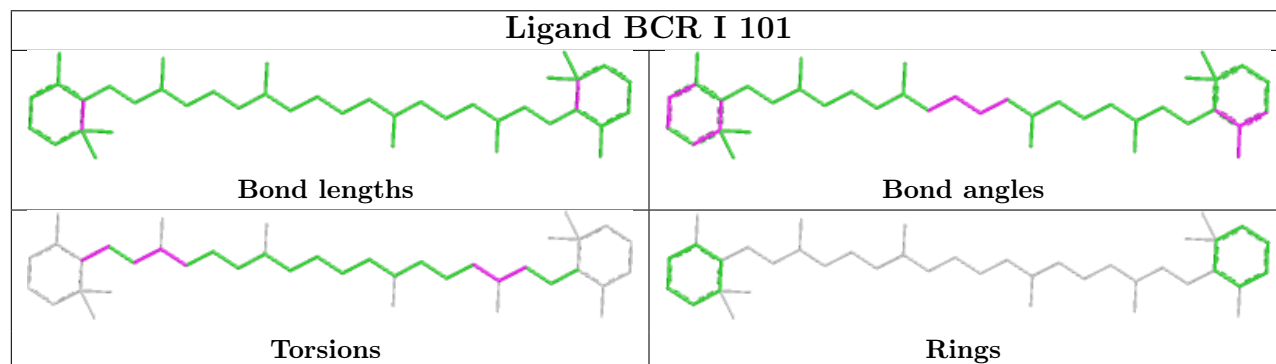
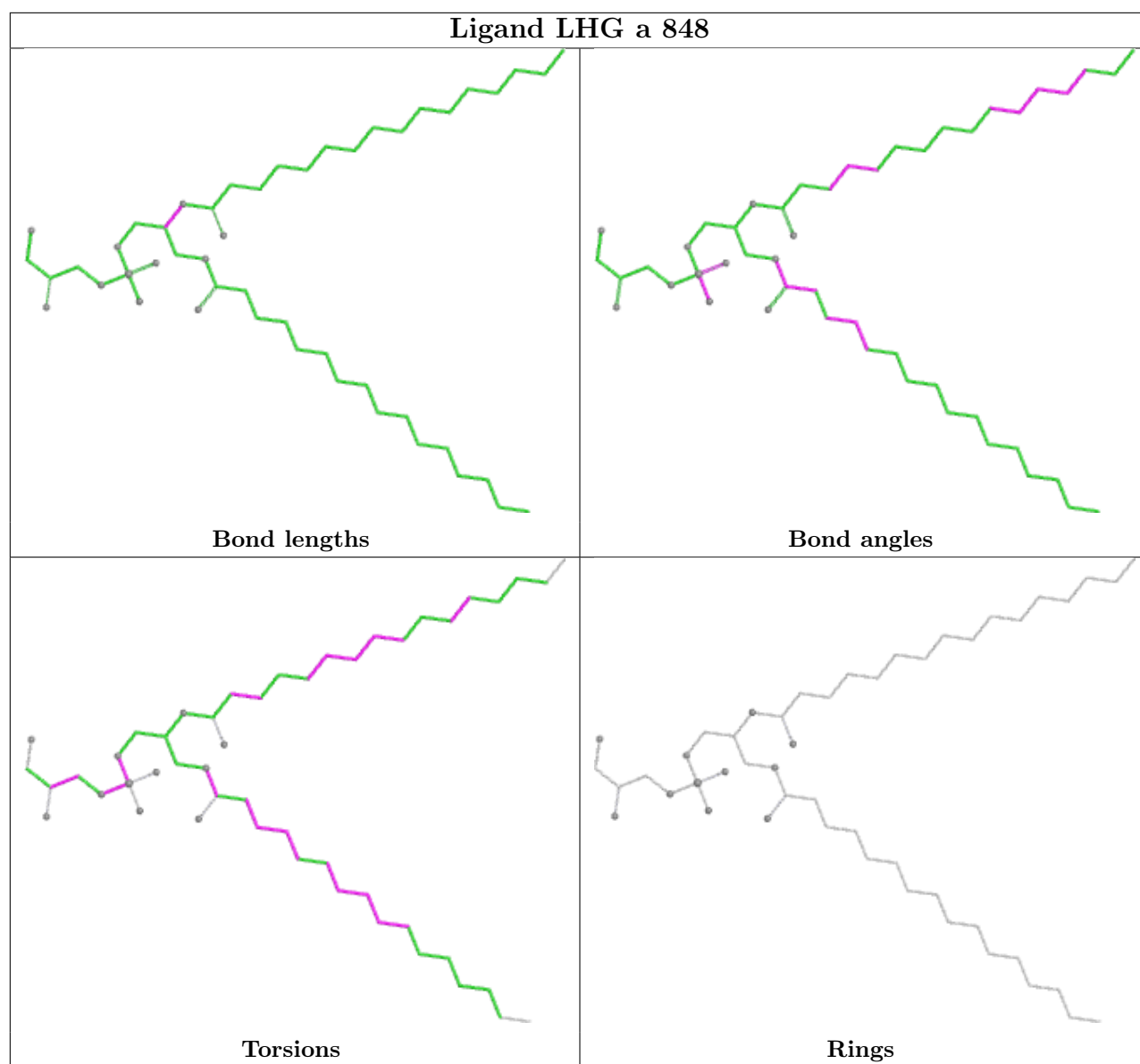
Bond angles

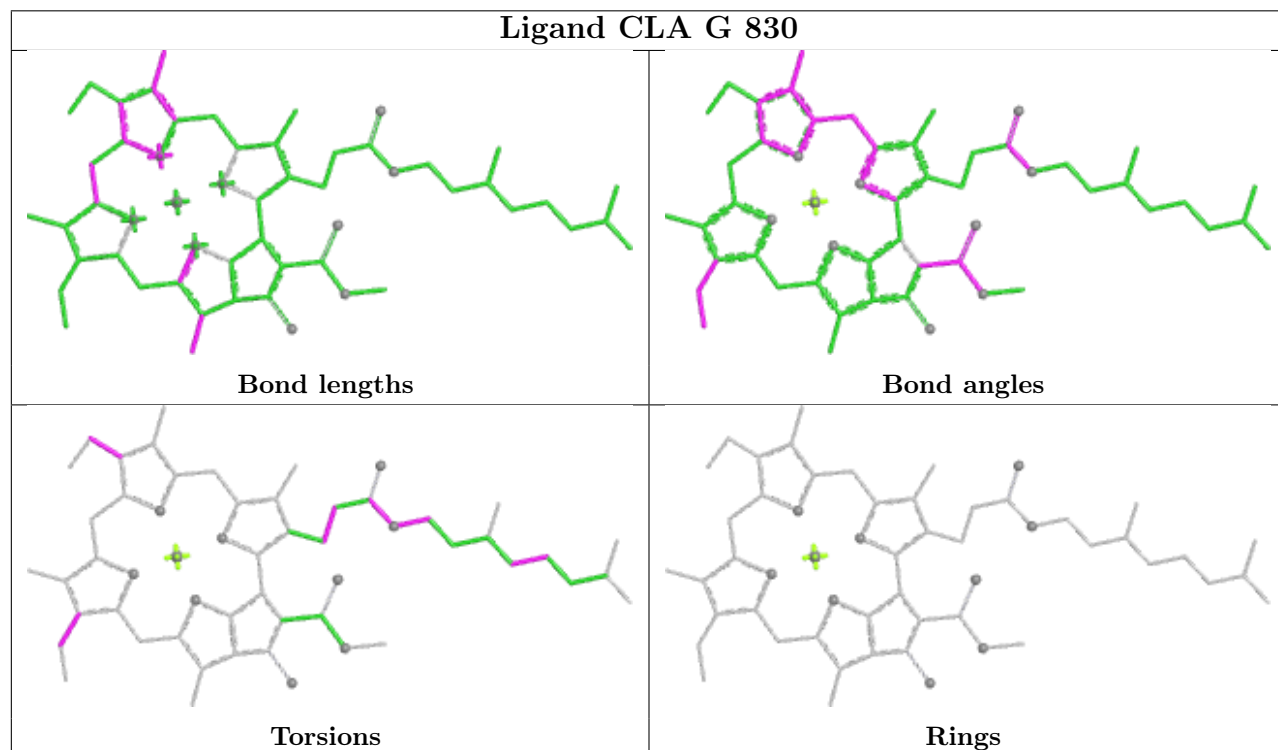
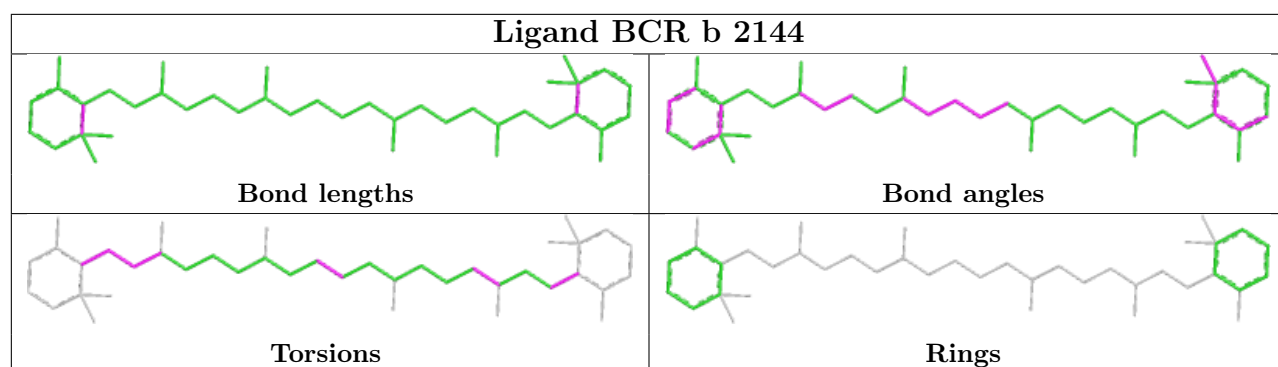


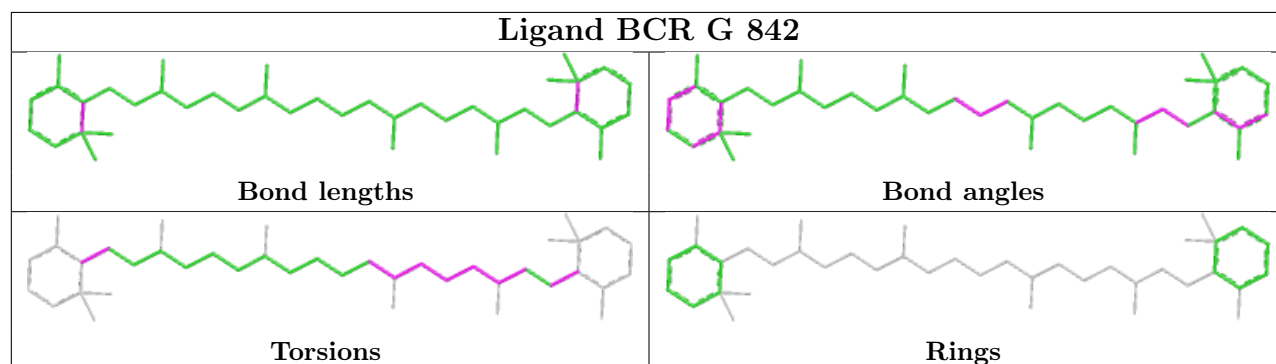
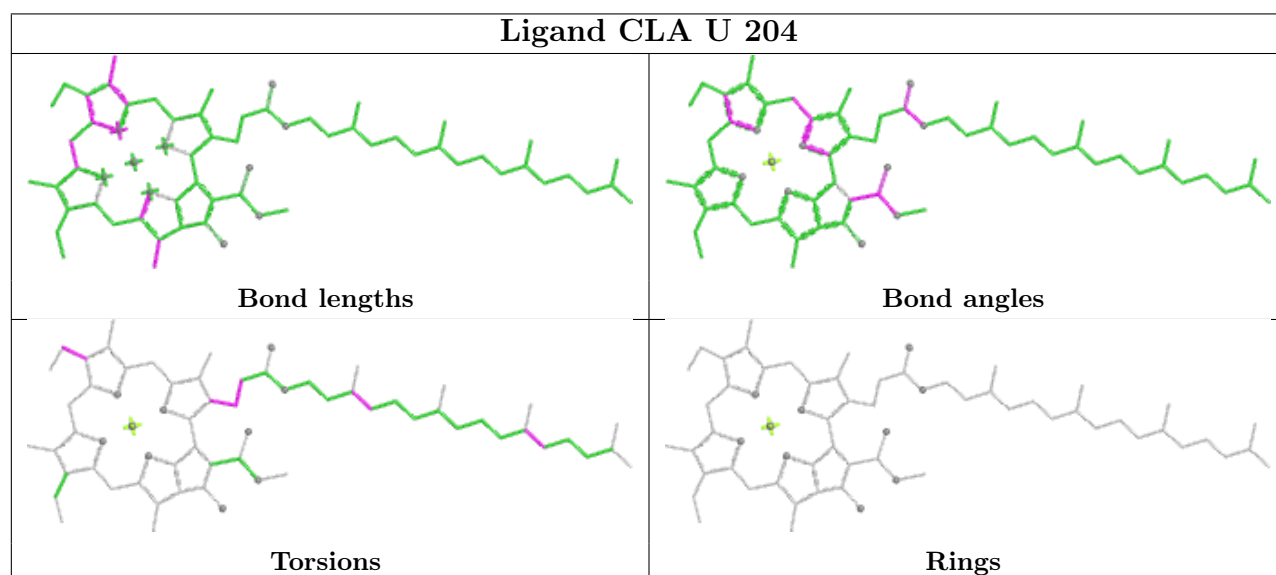
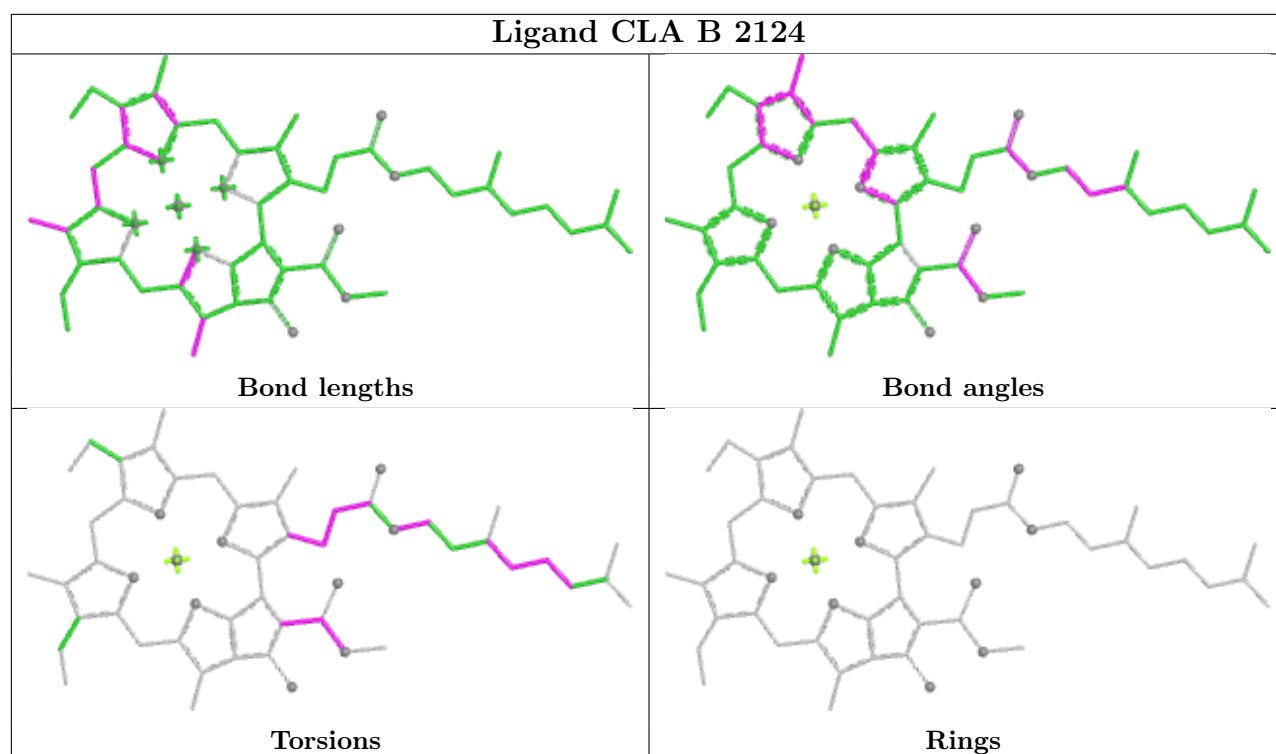
Torsions

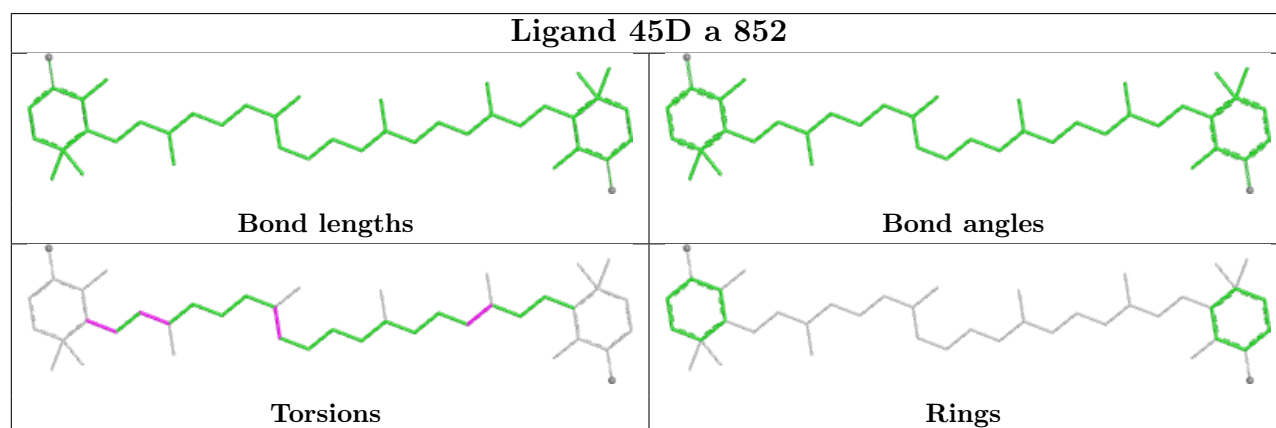
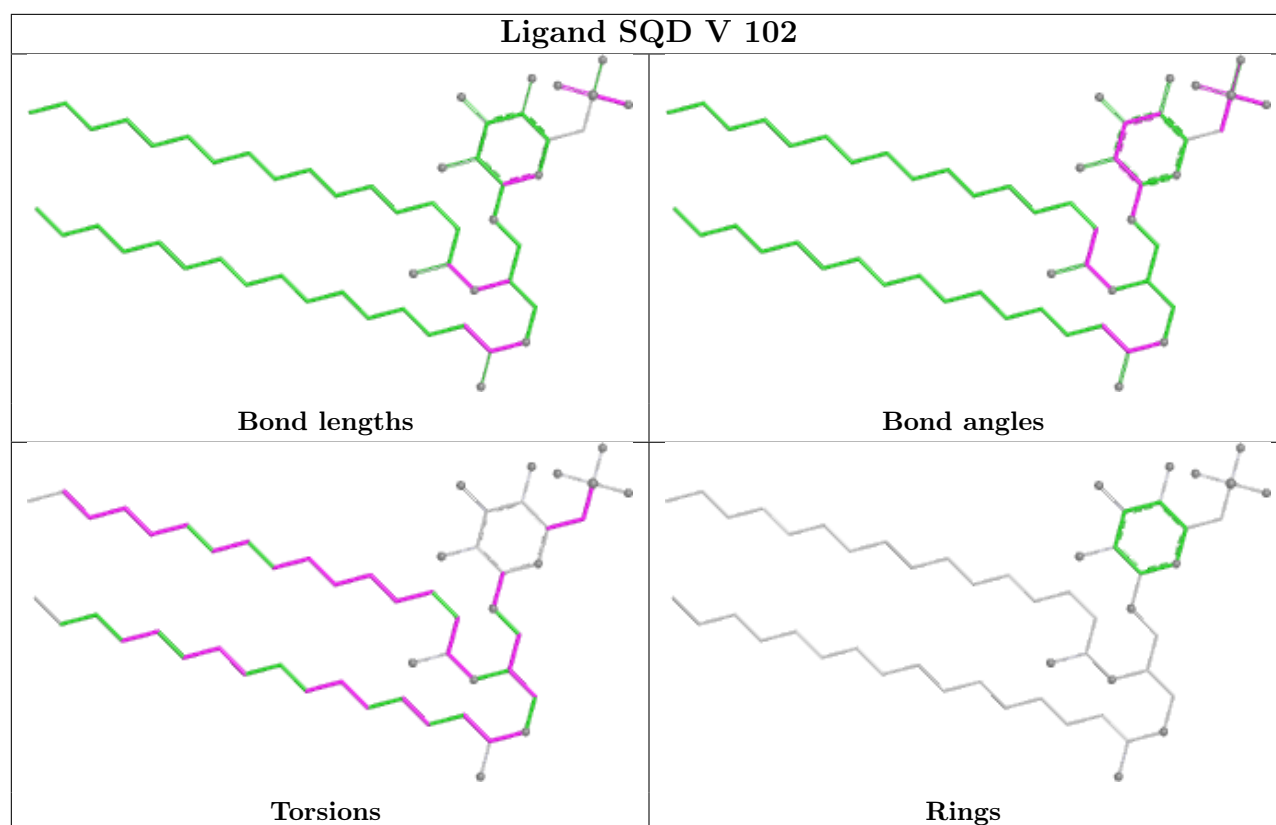


Rings

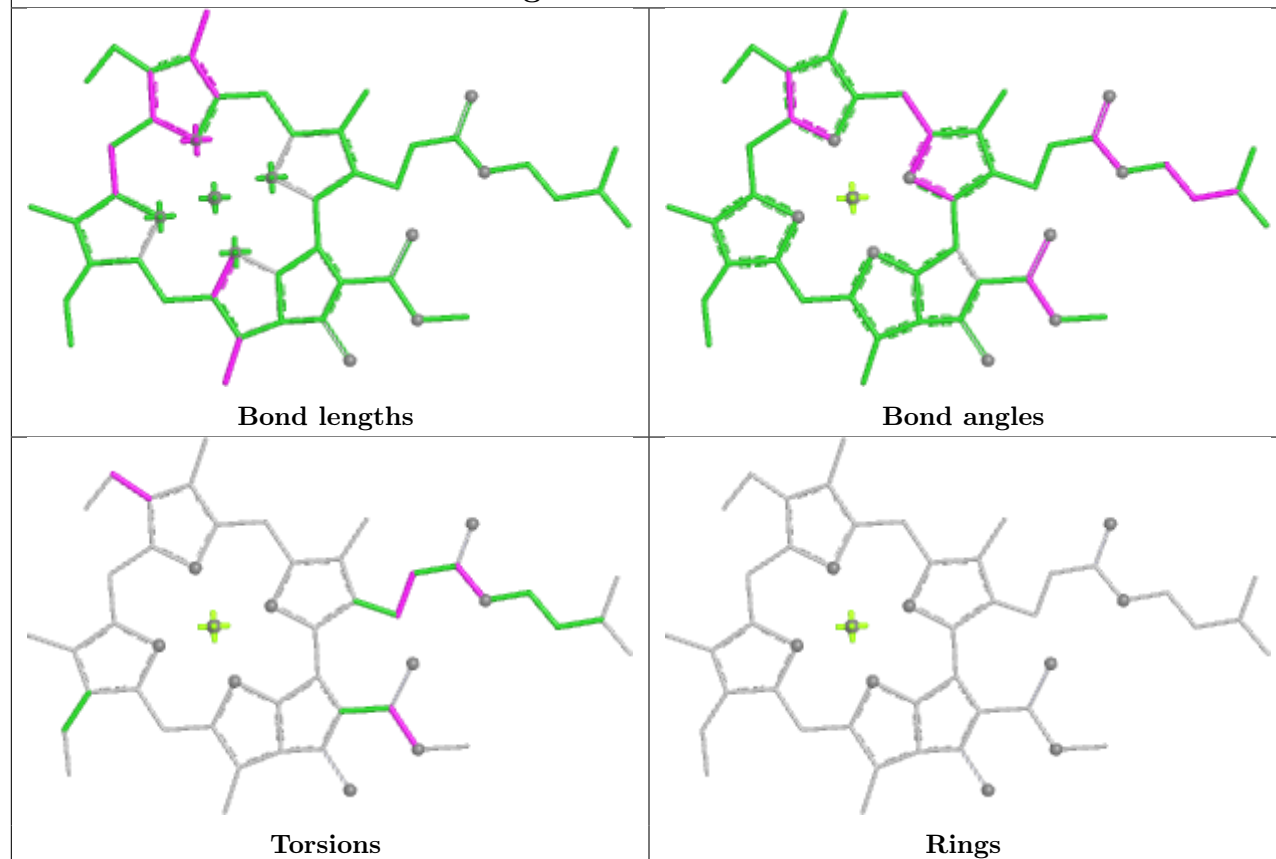




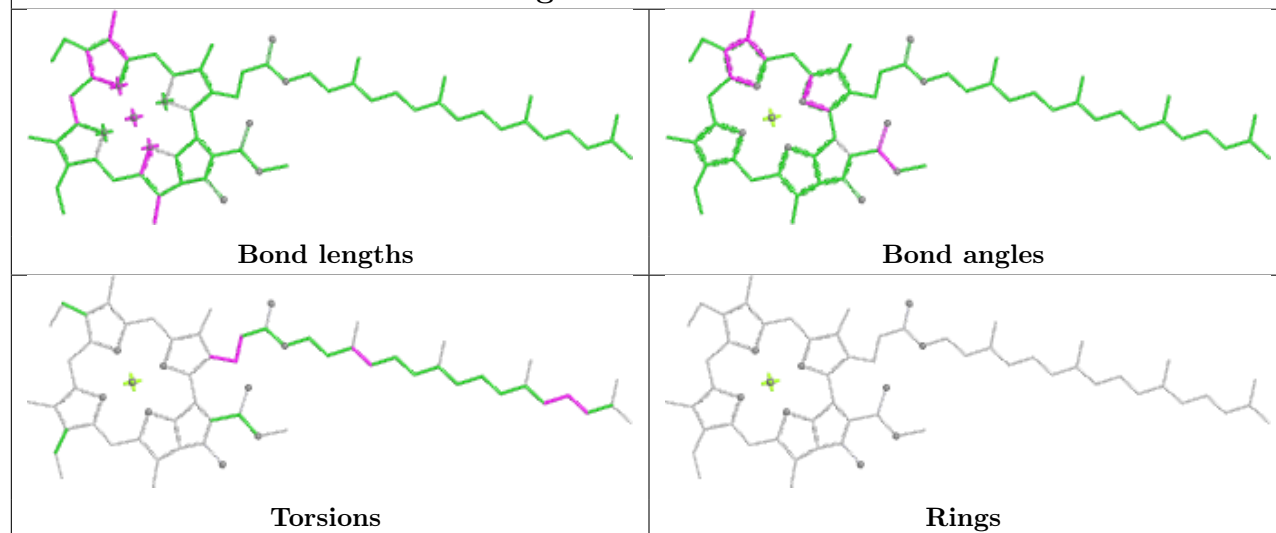


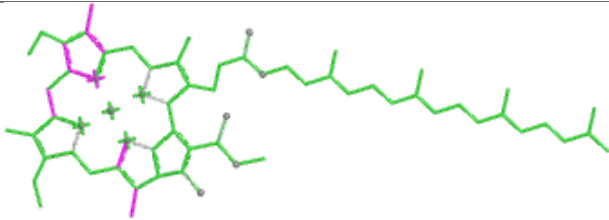
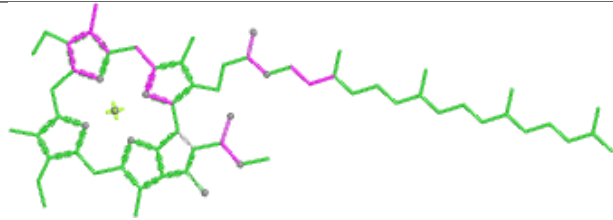
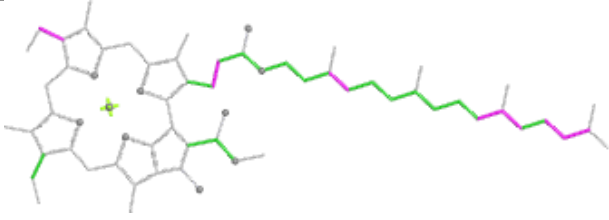
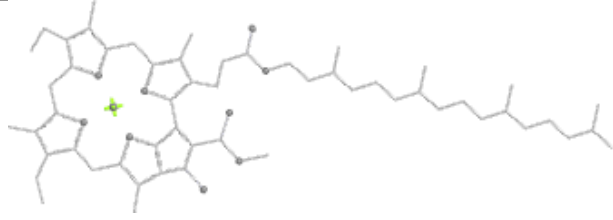


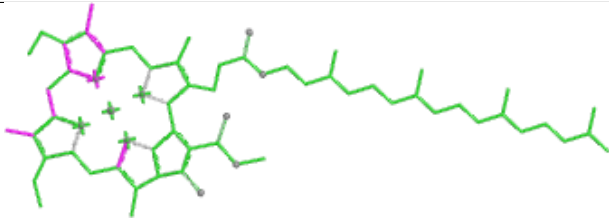
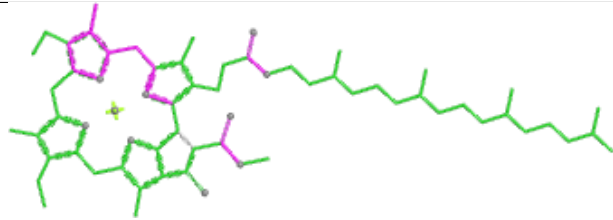
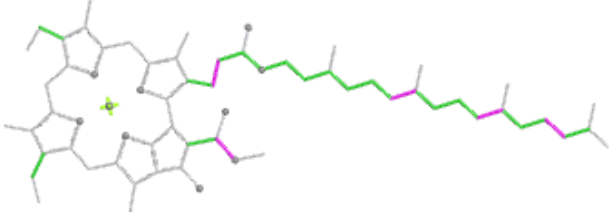
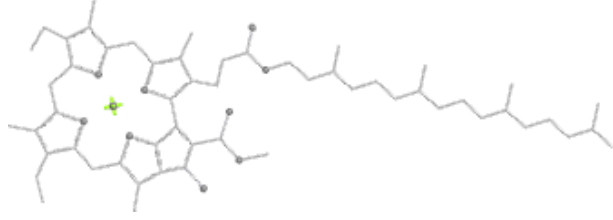
Ligand CLA B 2119

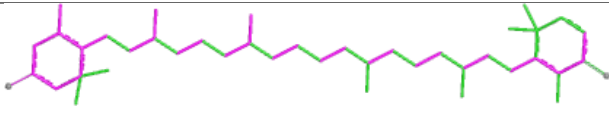
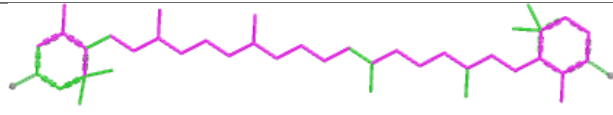
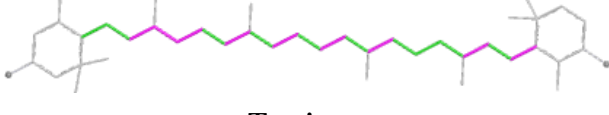
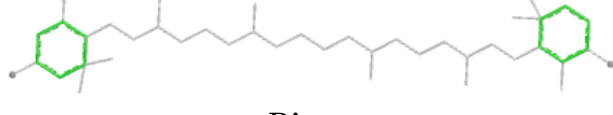


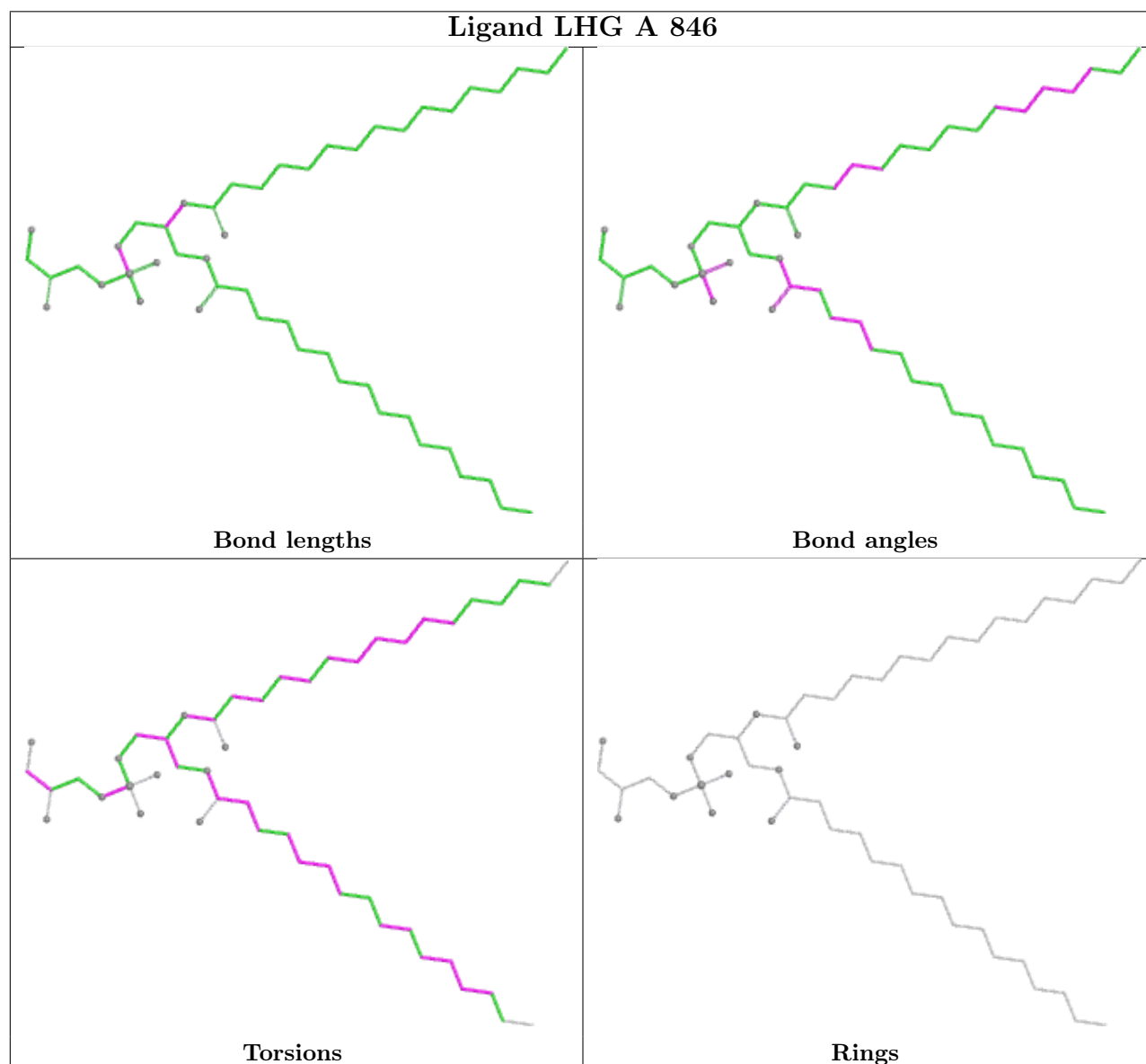
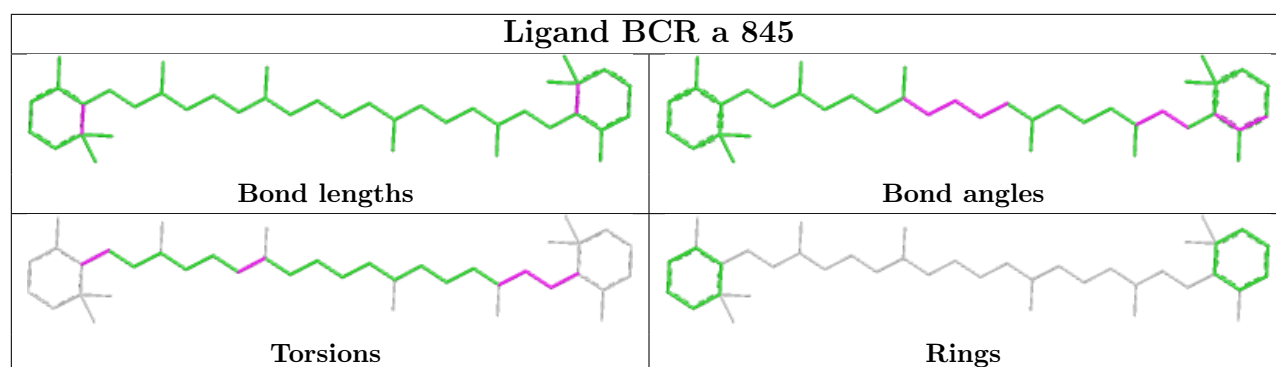
Ligand CLA a 850

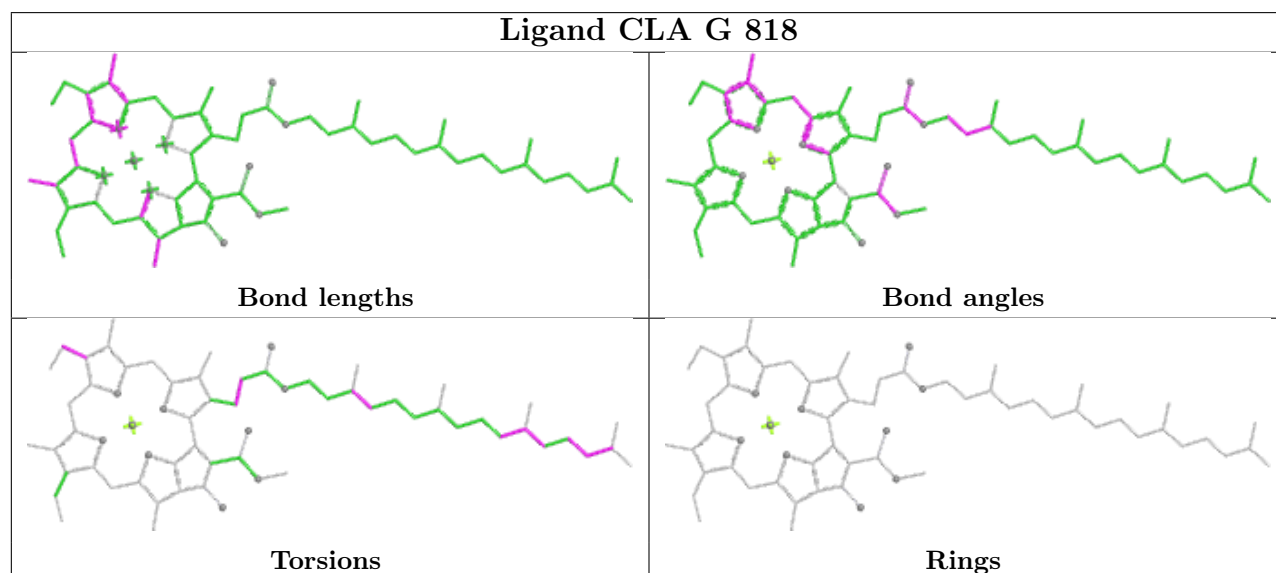
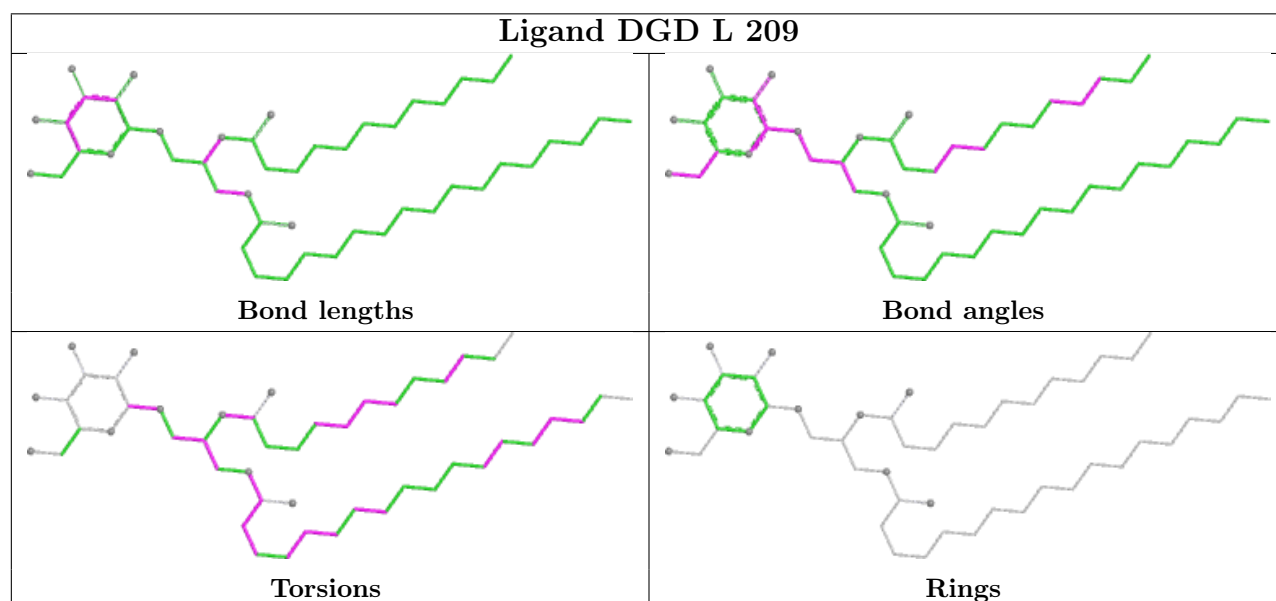
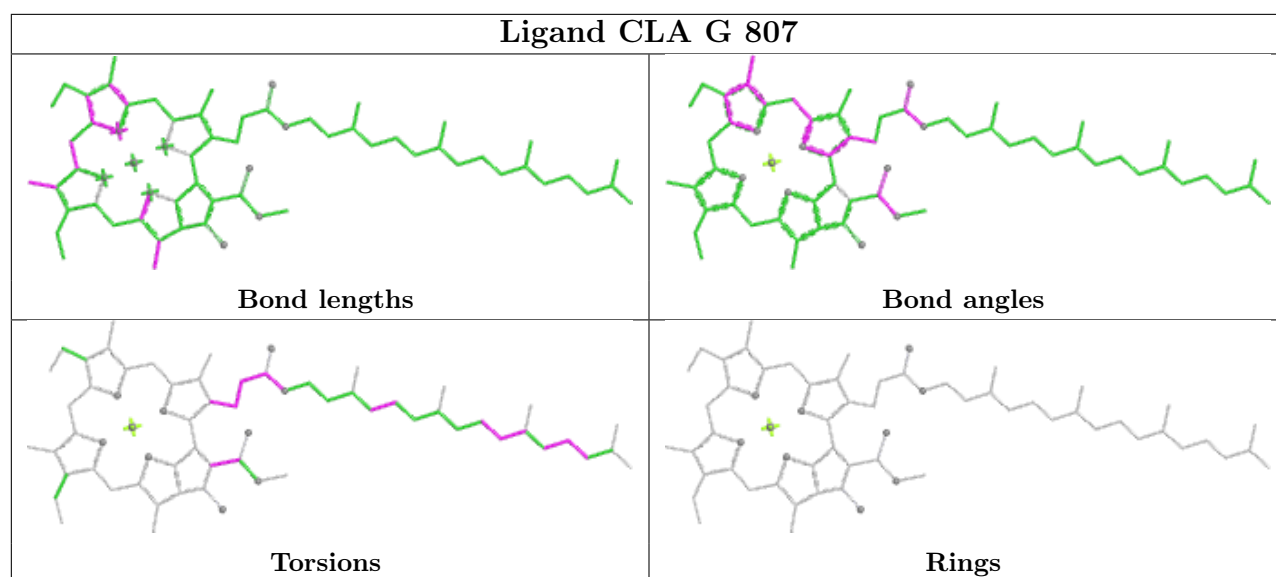


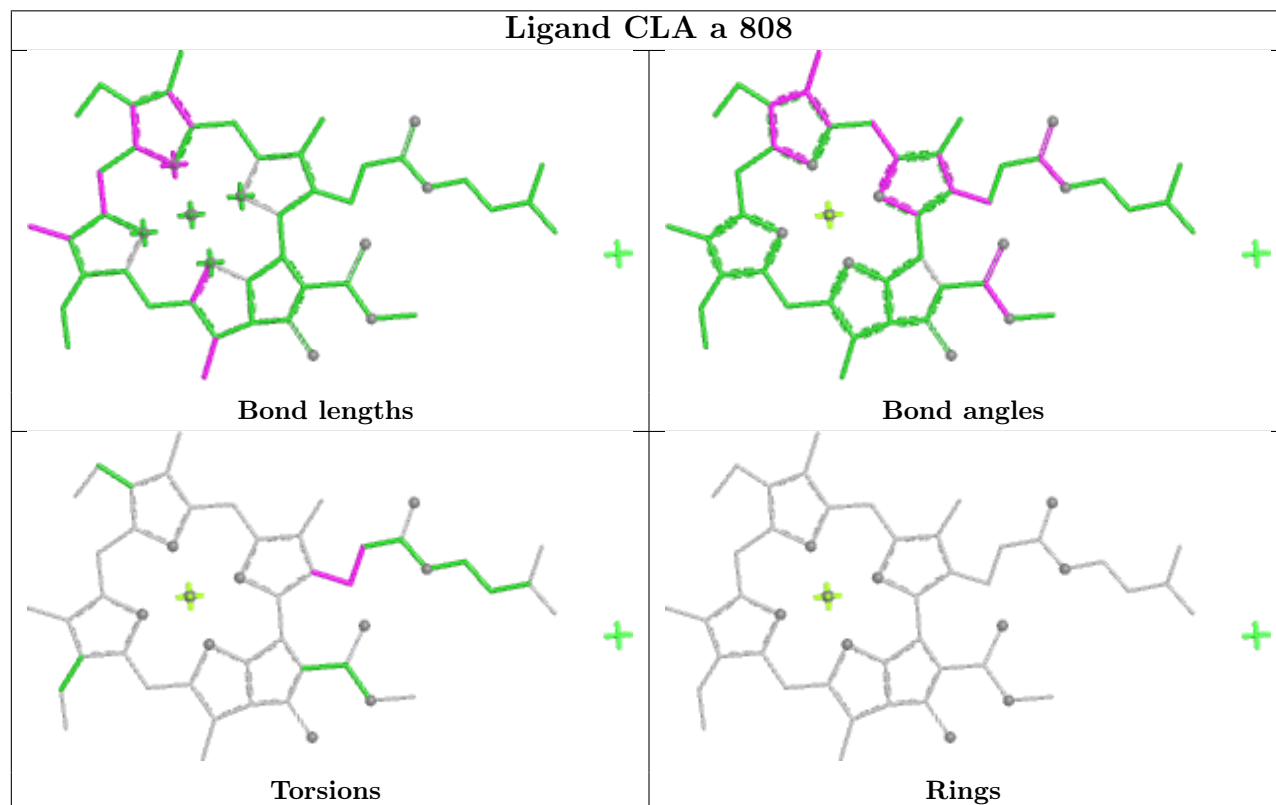
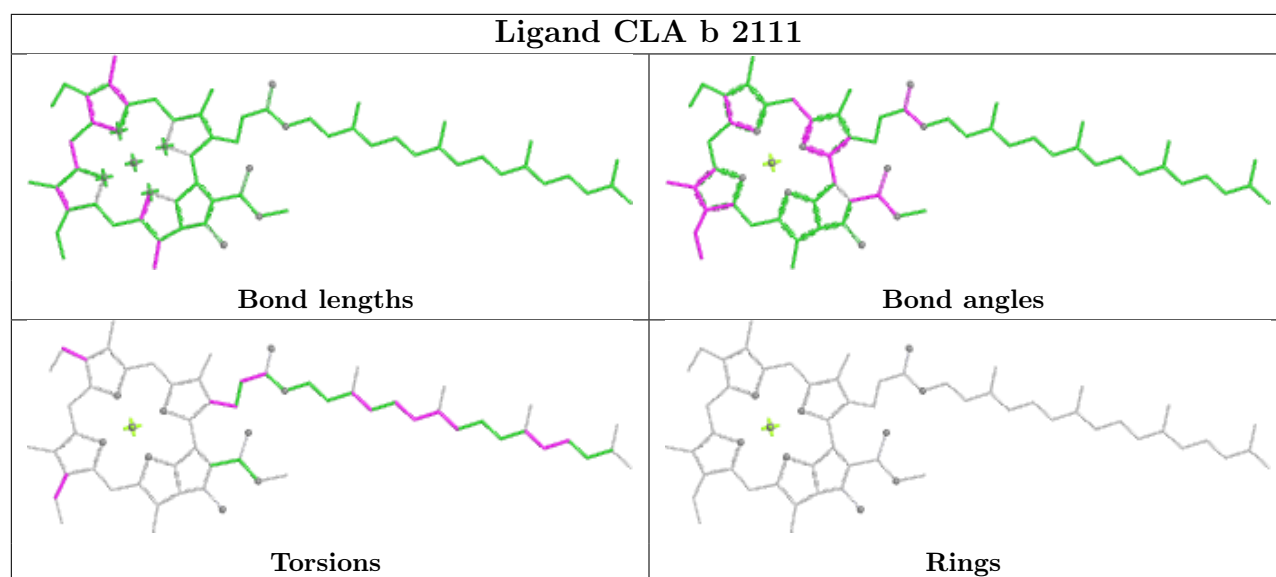
Ligand CLA A 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

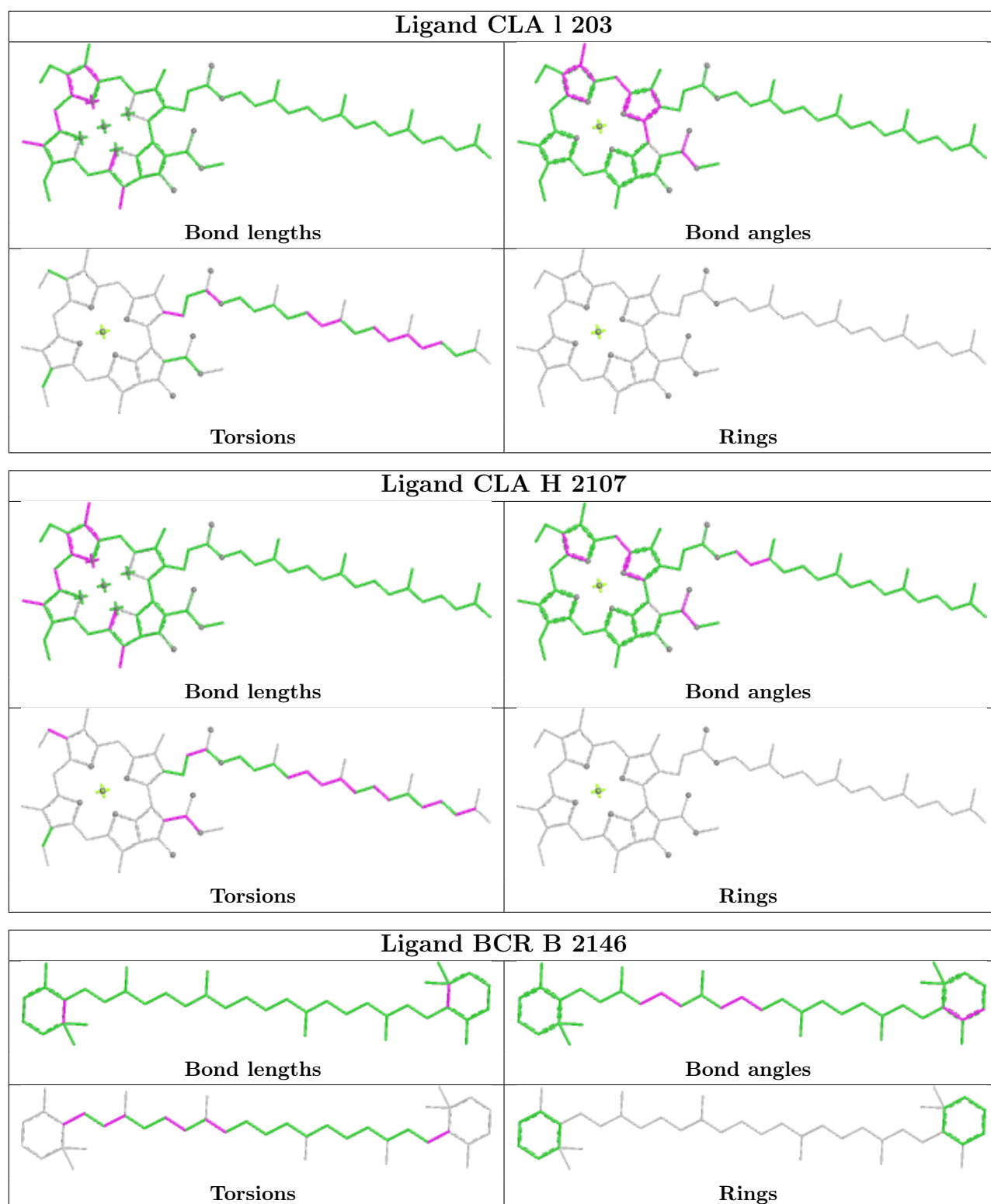
Ligand CLA a 820	
	
Bond lengths	Bond angles
	
Torsions	Rings

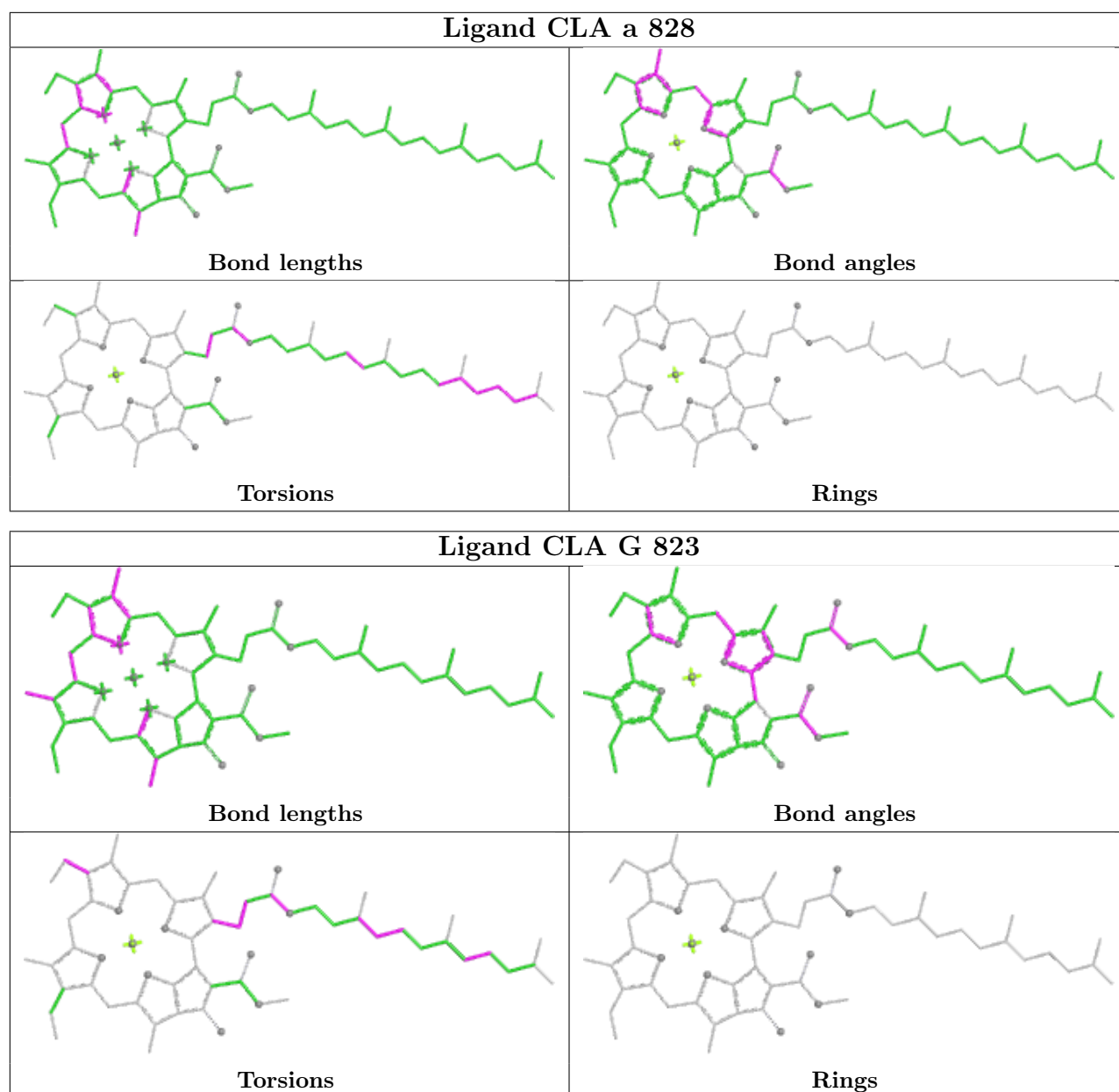
Ligand EQ3 B 2151	
	
Bond lengths	Bond angles
	
Torsions	Rings

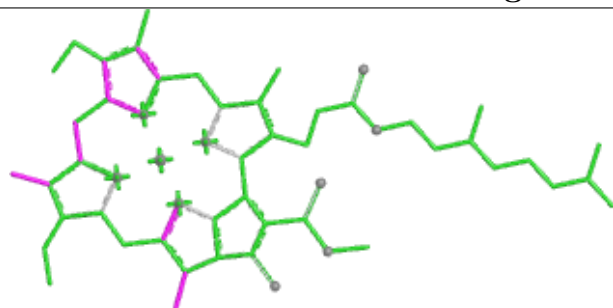




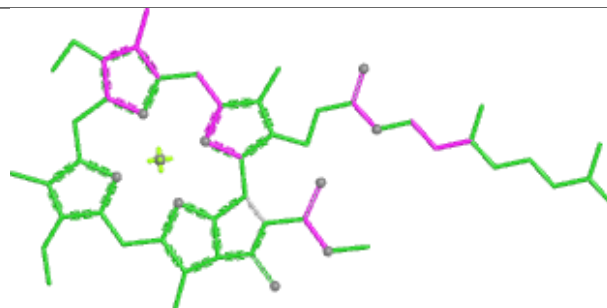




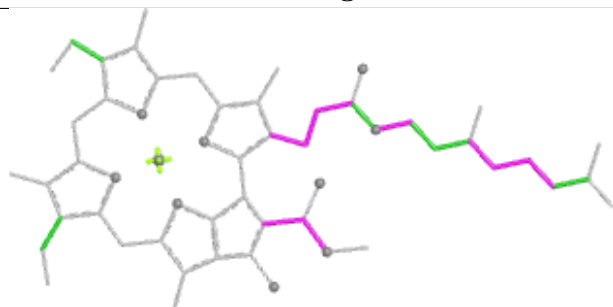


Ligand CLA H 2123

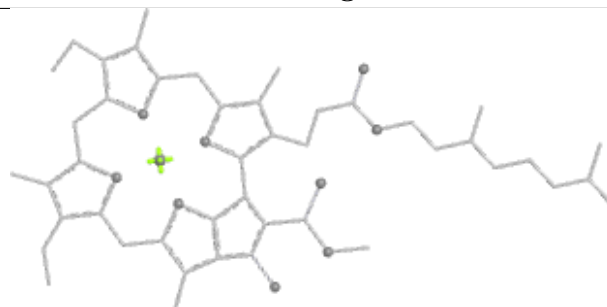
Bond lengths



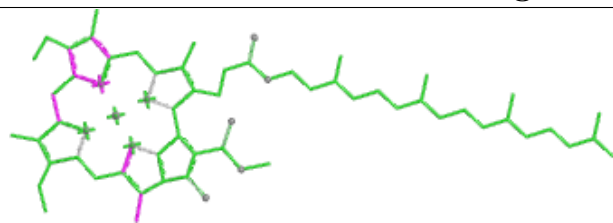
Bond angles



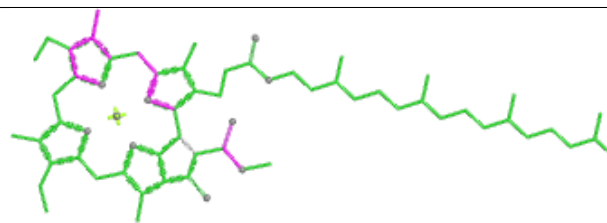
Torsions



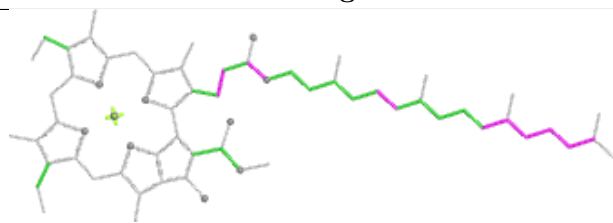
Rings

Ligand CLA A 828

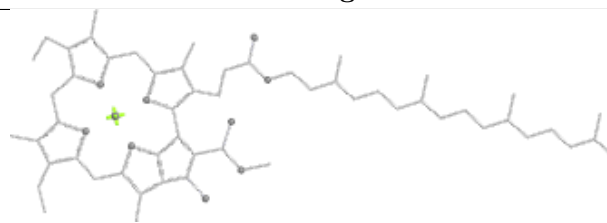
Bond lengths



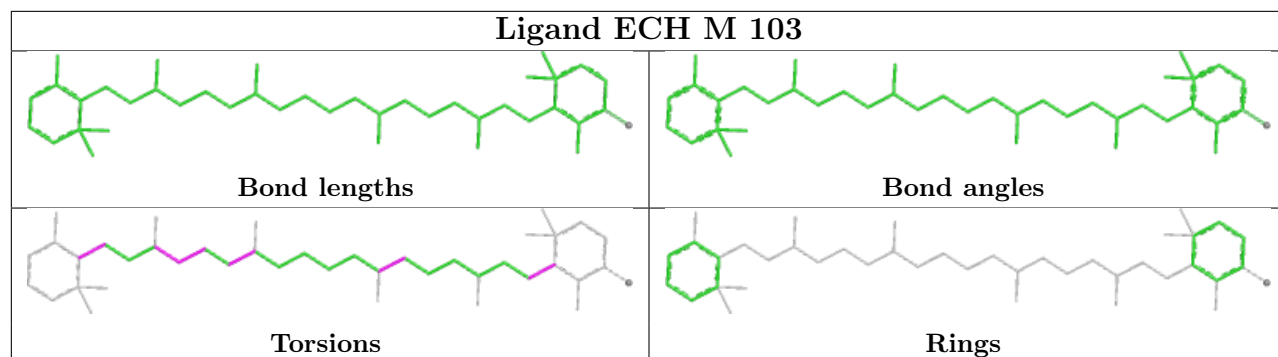
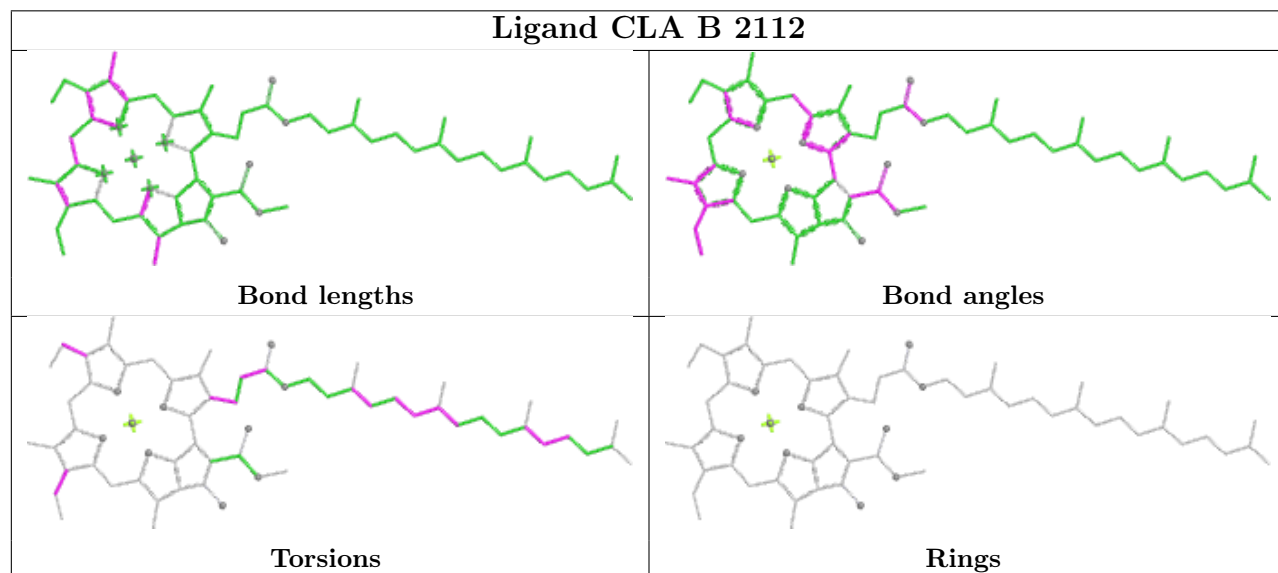
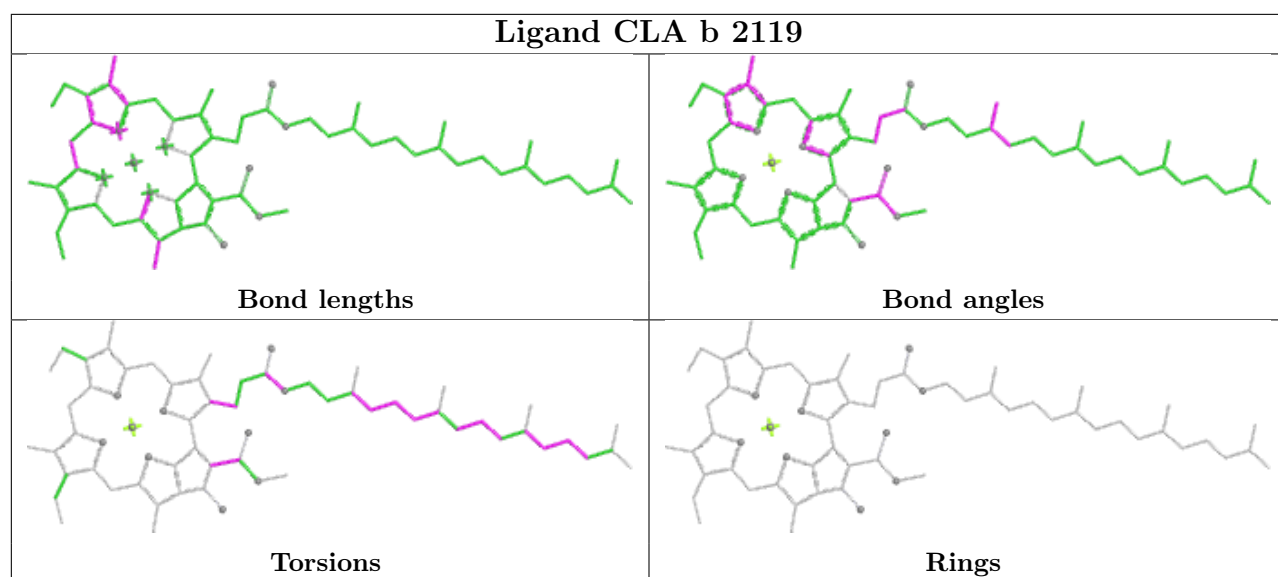
Bond angles

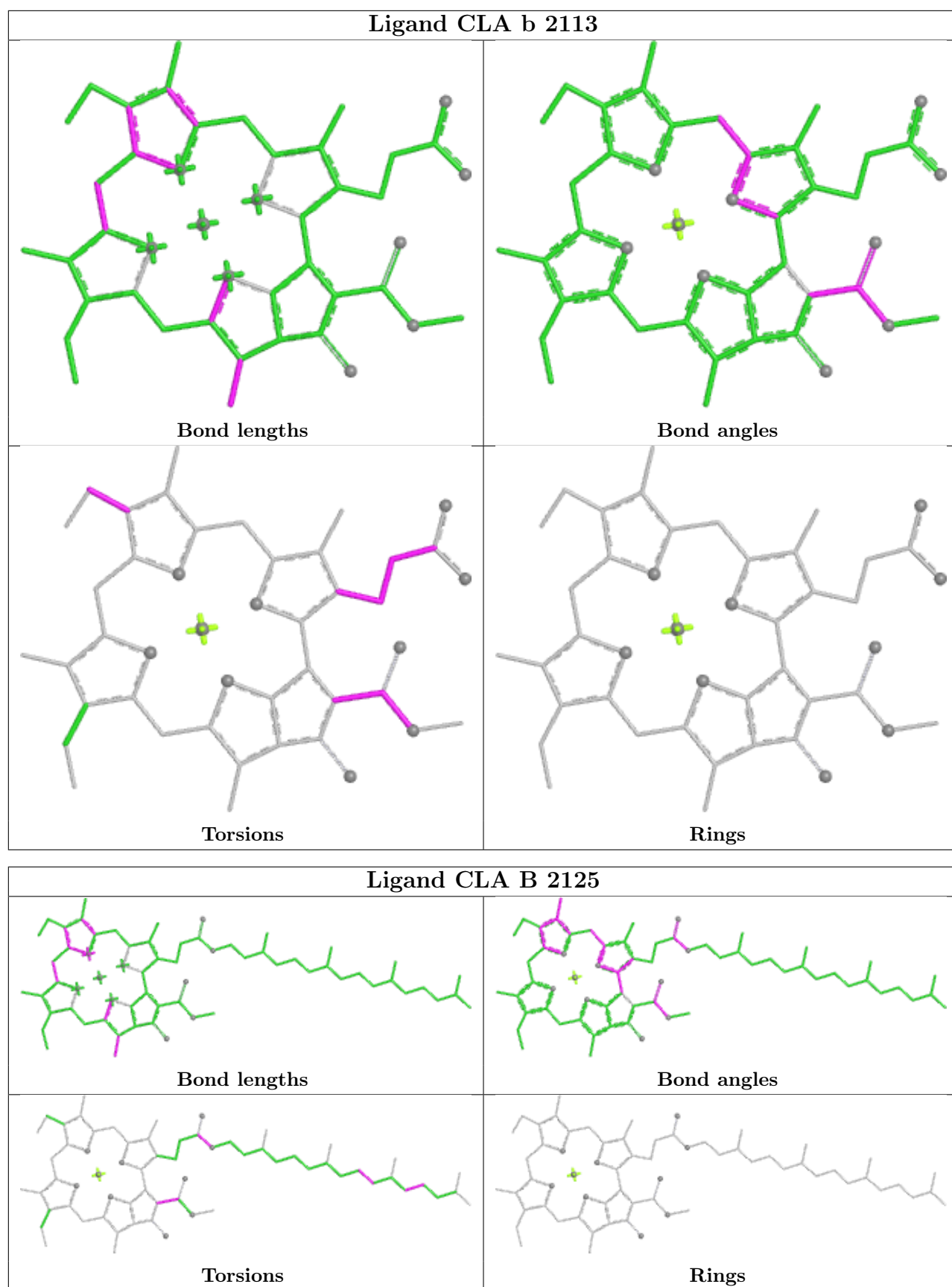


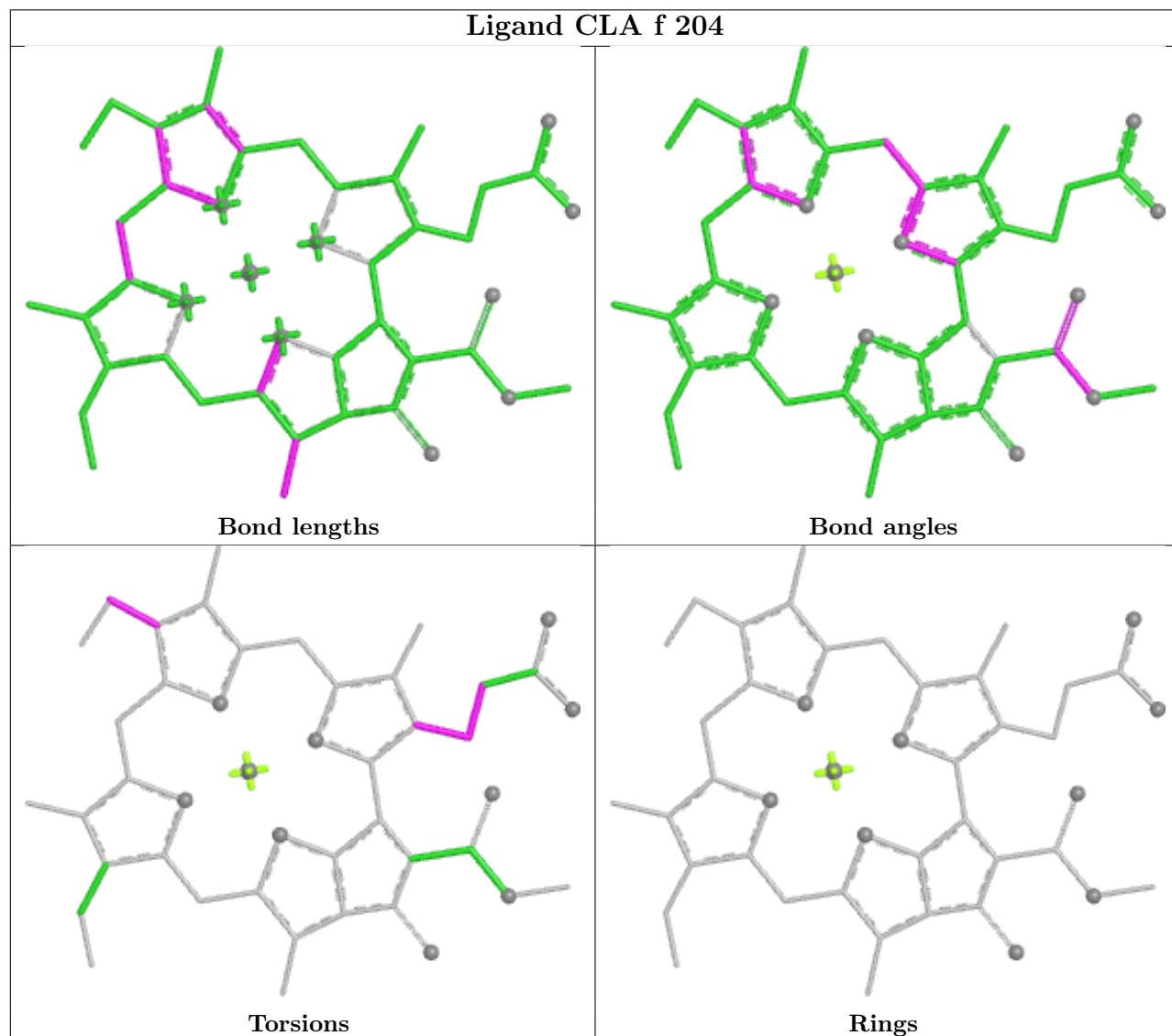
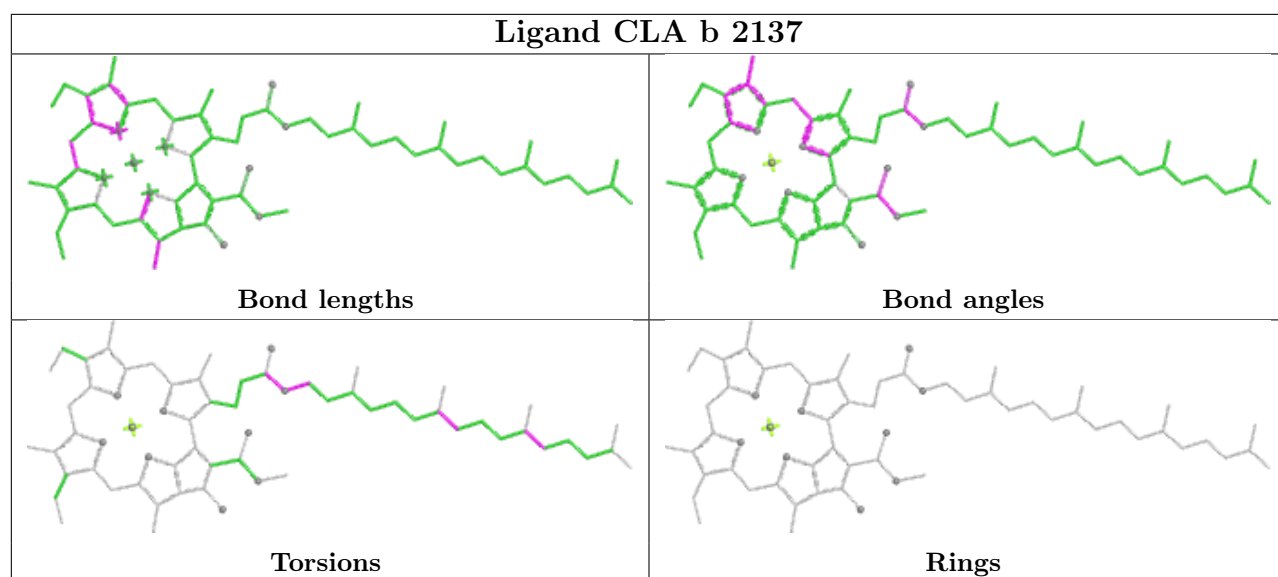
Torsions

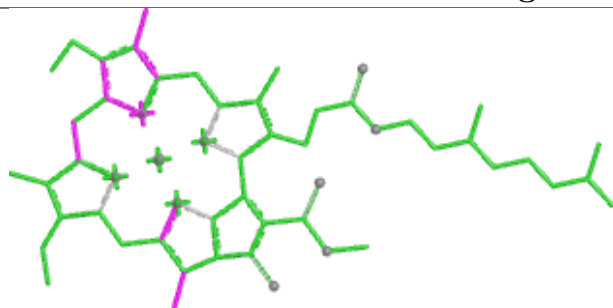


Rings

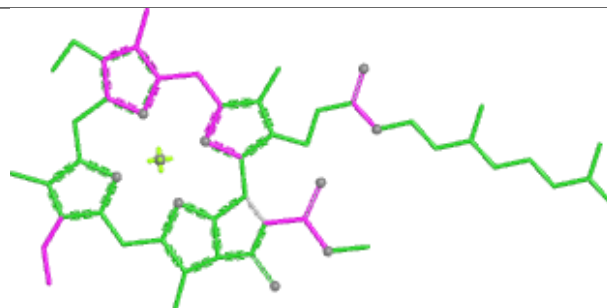




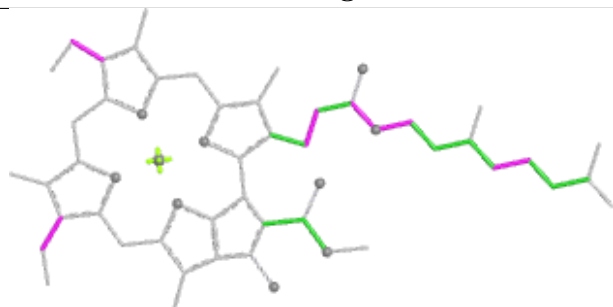


Ligand CLA a 830

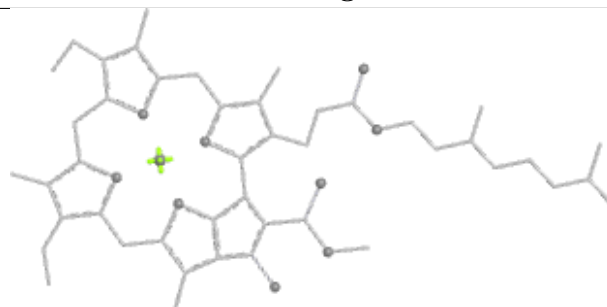
Bond lengths



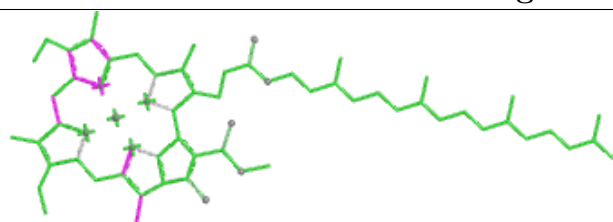
Bond angles



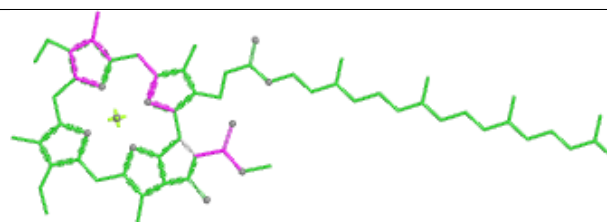
Torsions



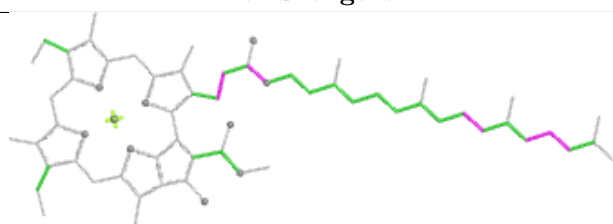
Rings

Ligand CLA L 205

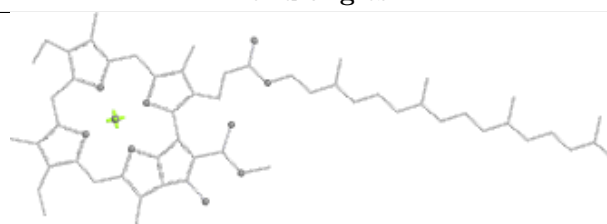
Bond lengths



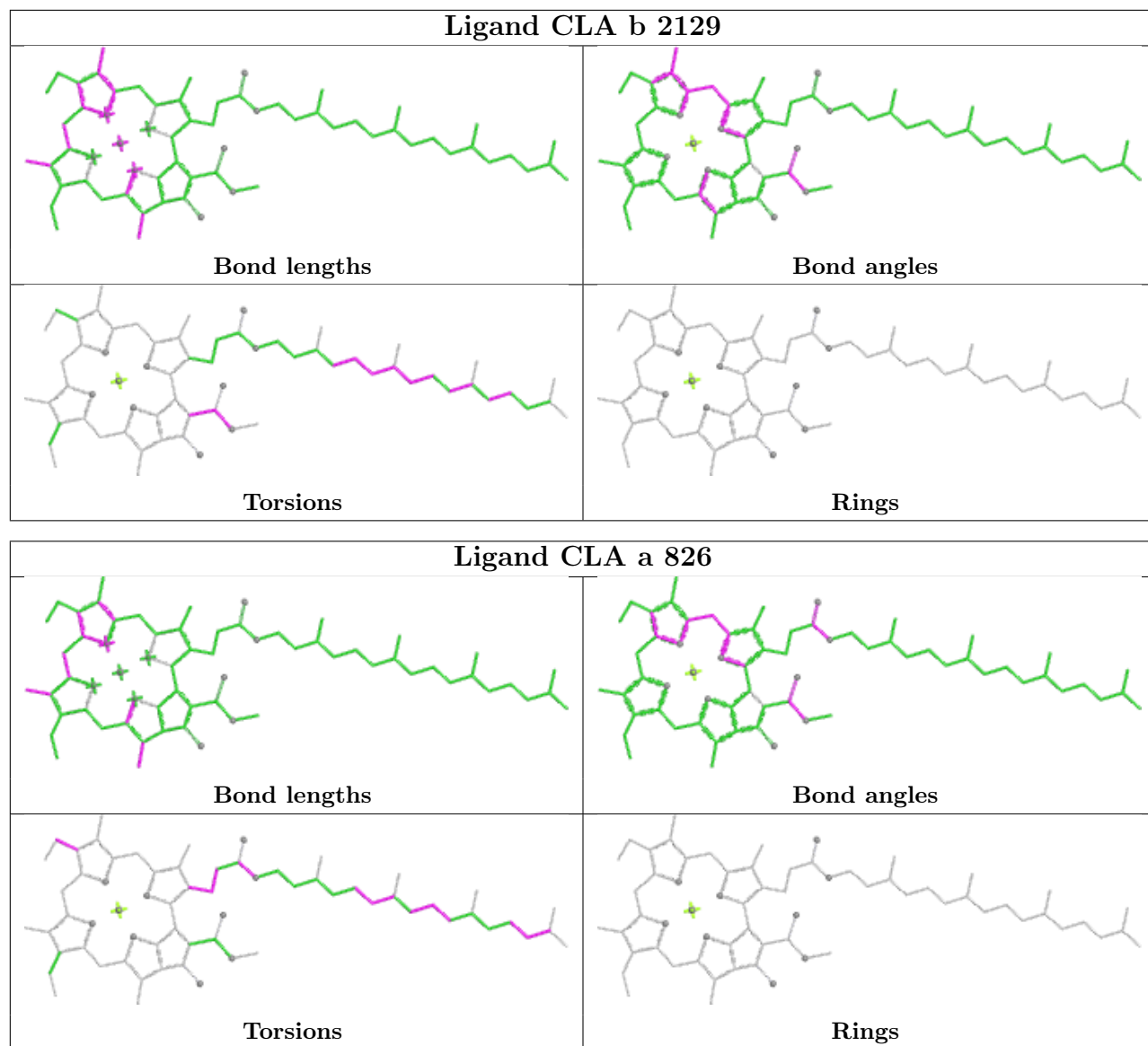
Bond angles

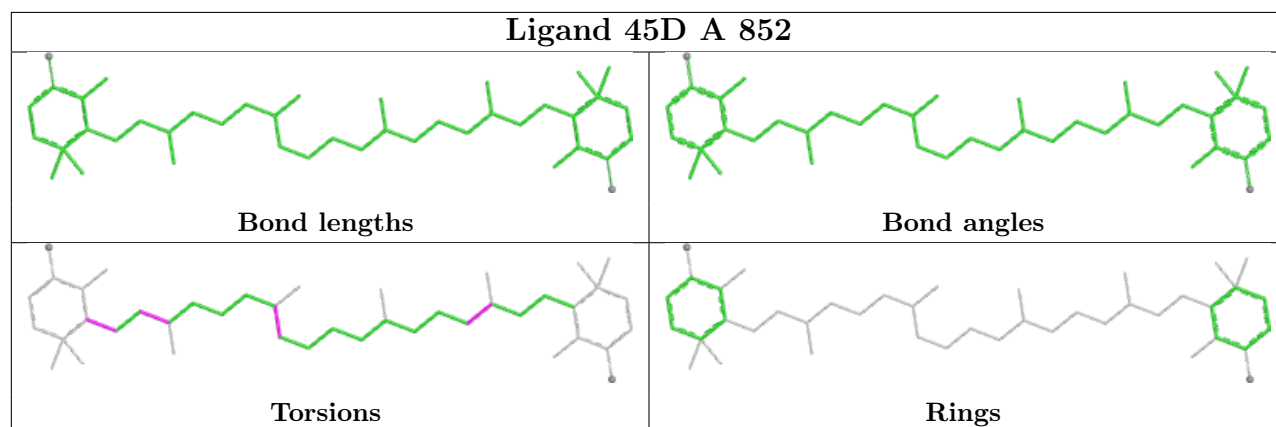
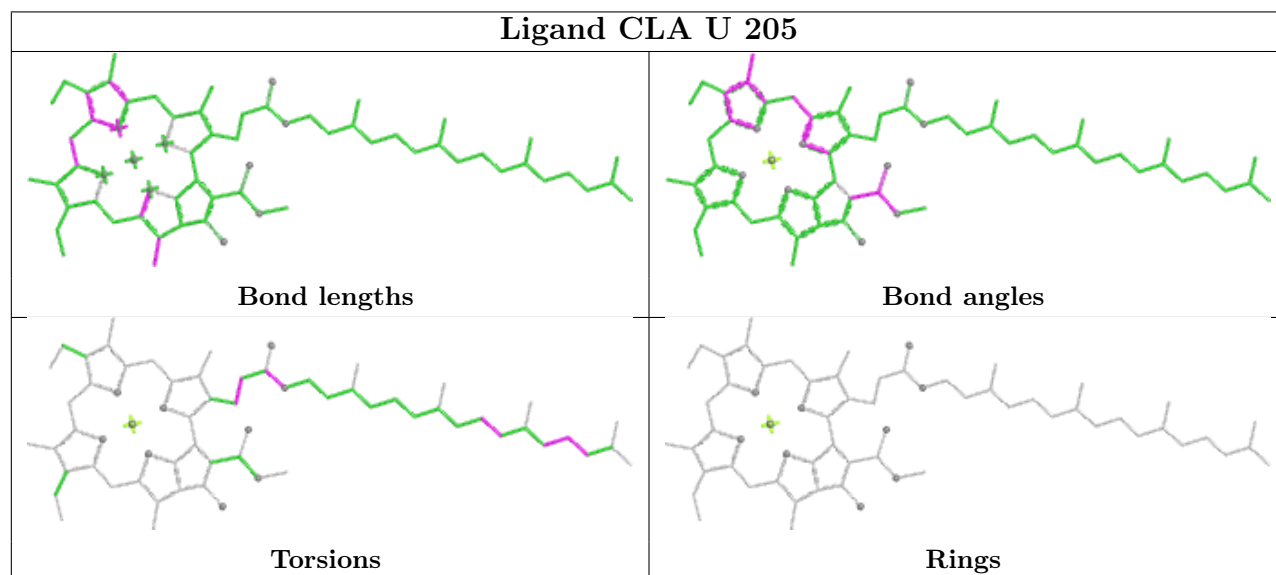
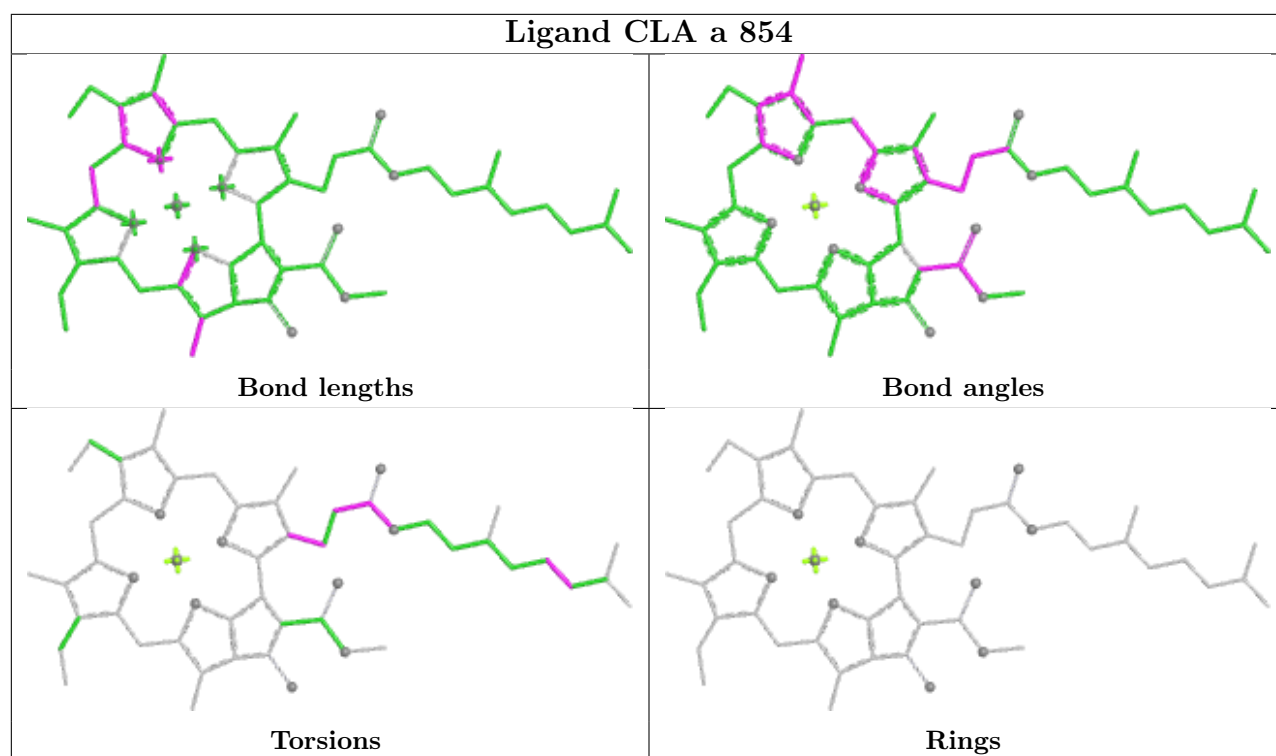


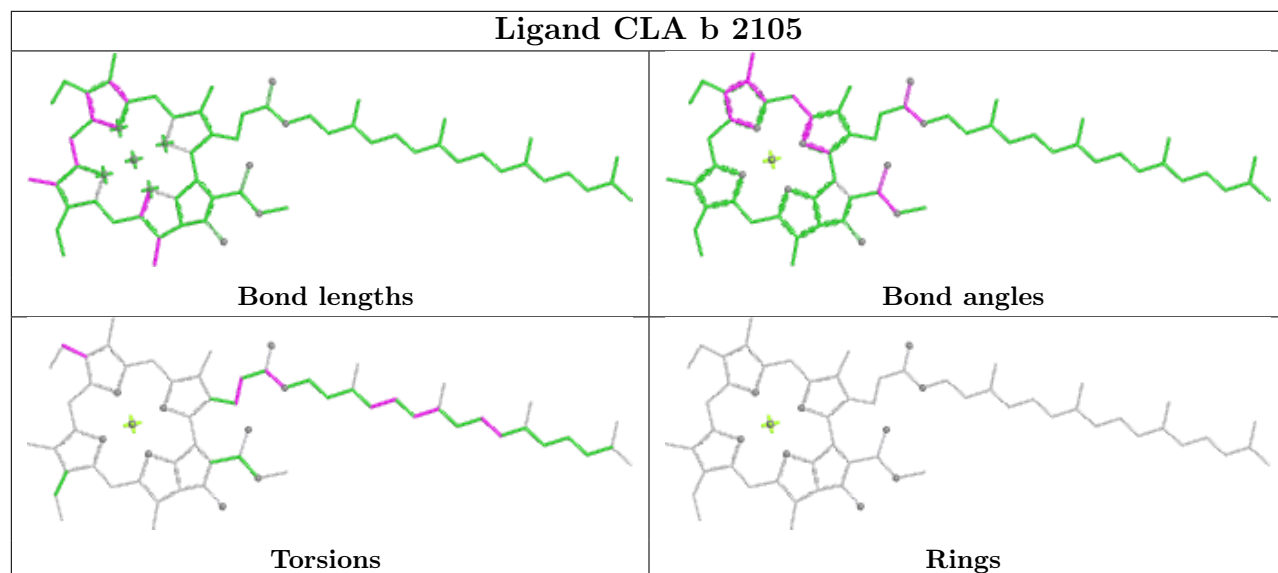
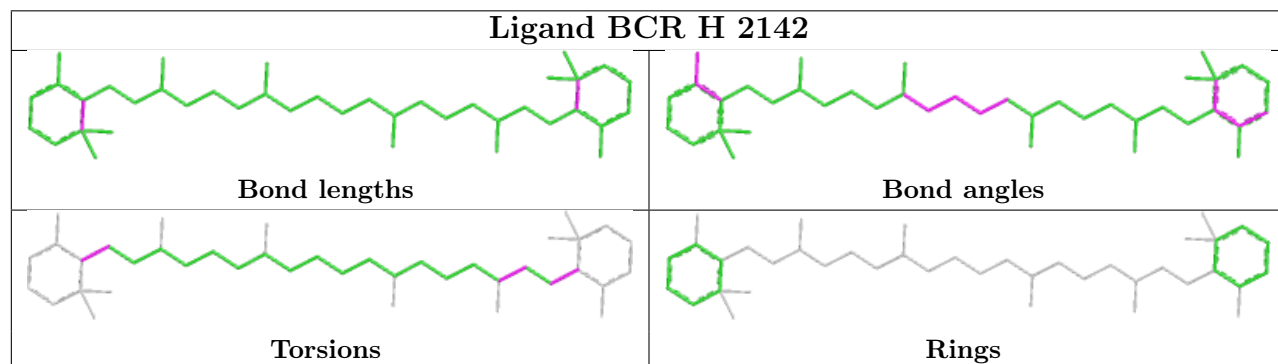
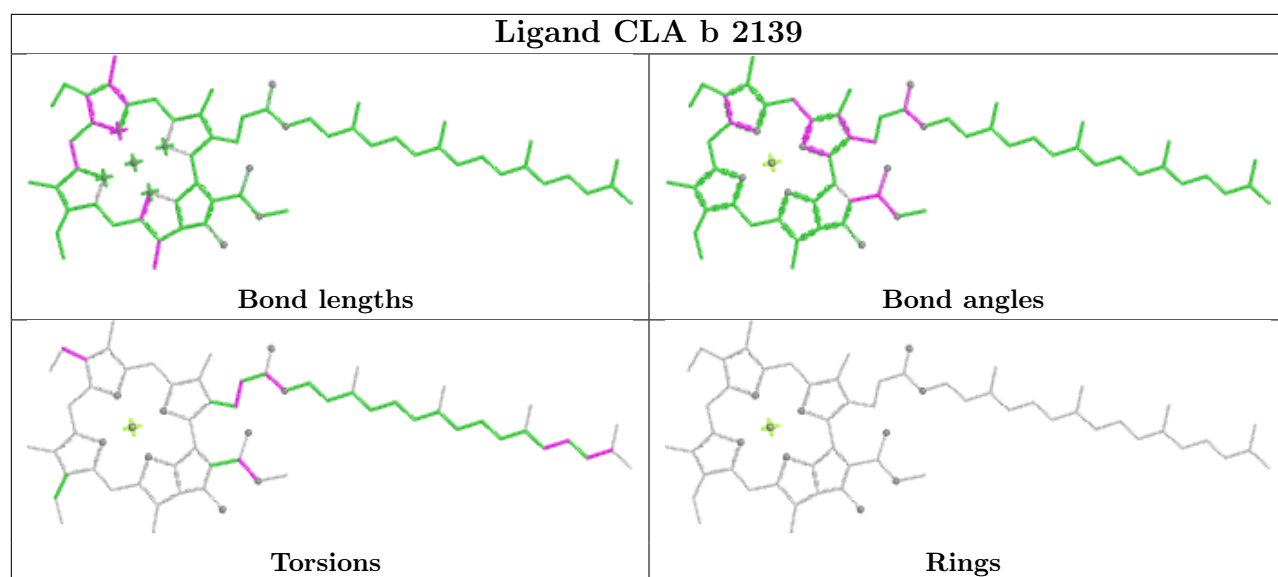
Torsions

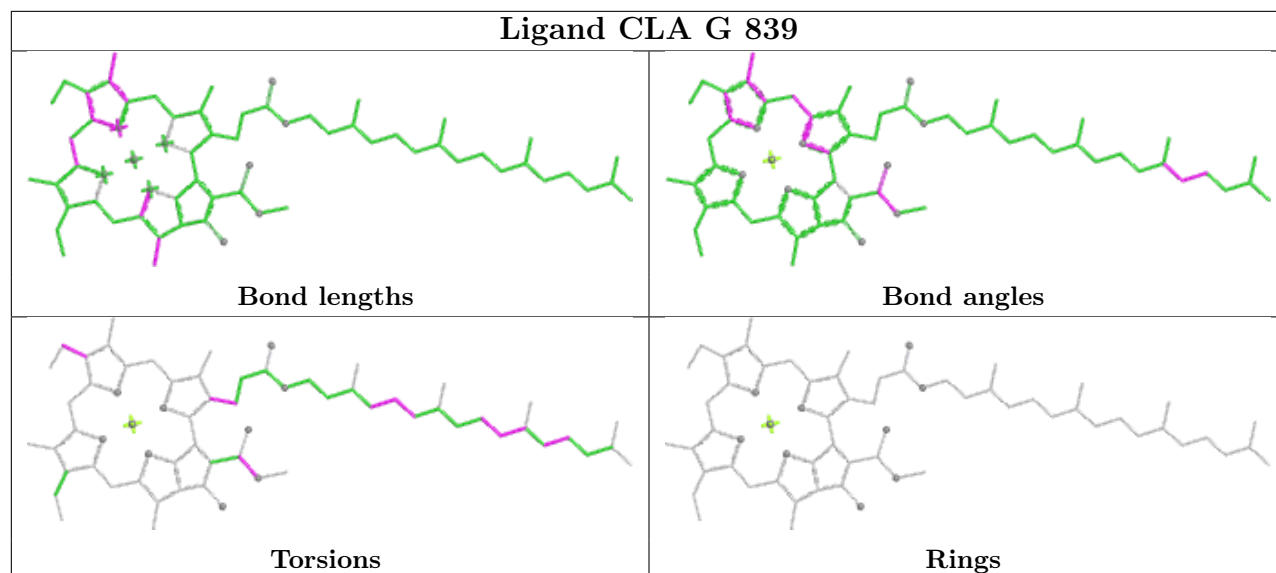
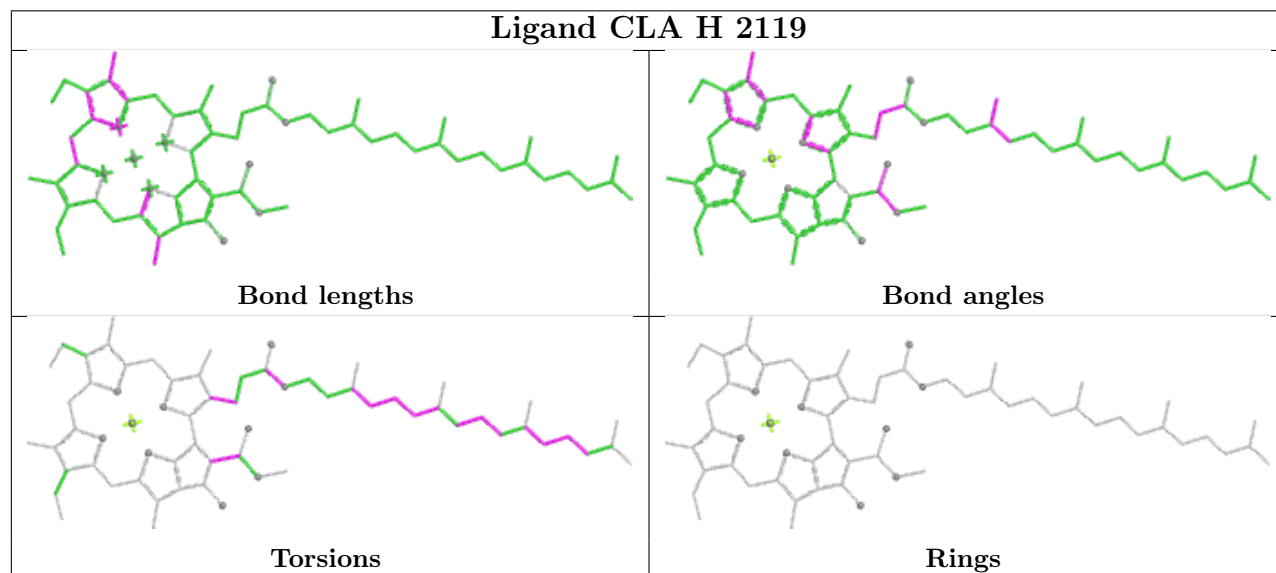
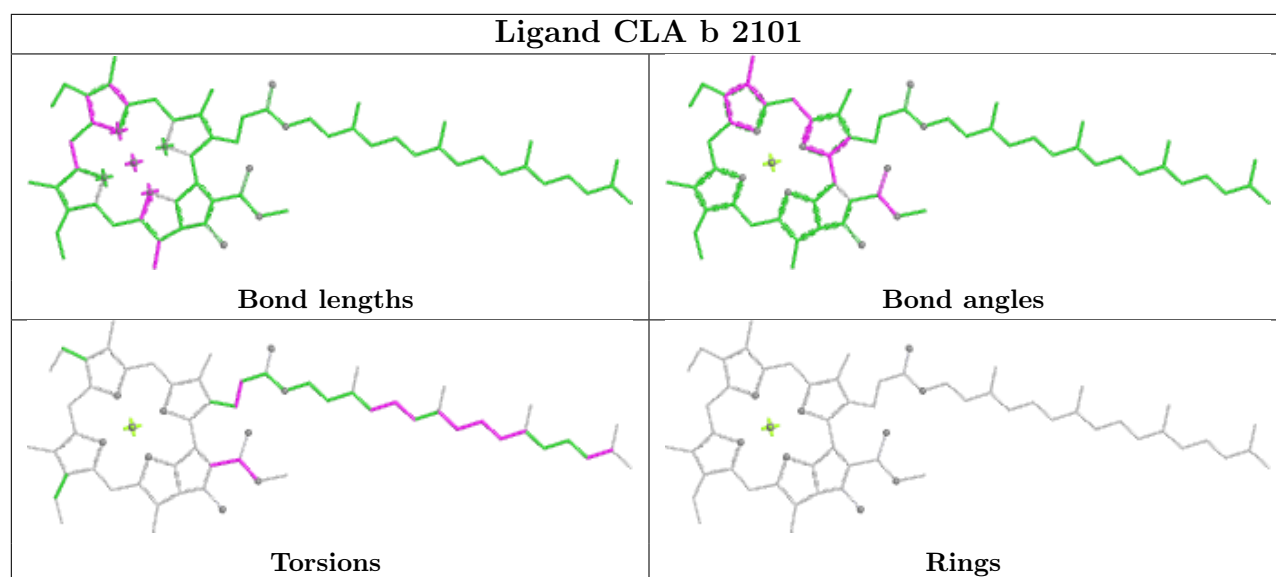


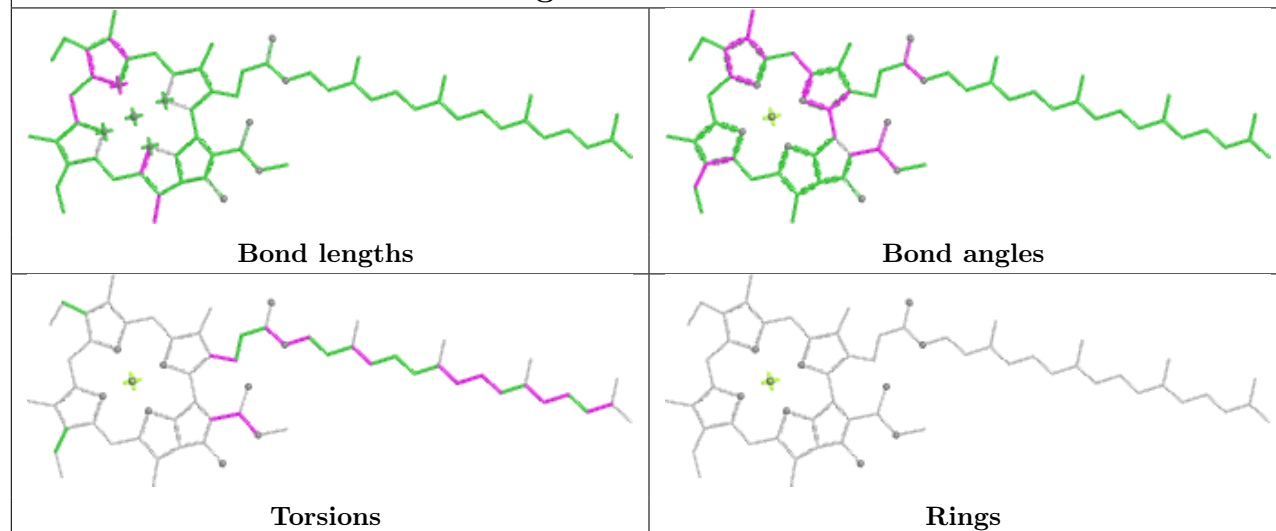
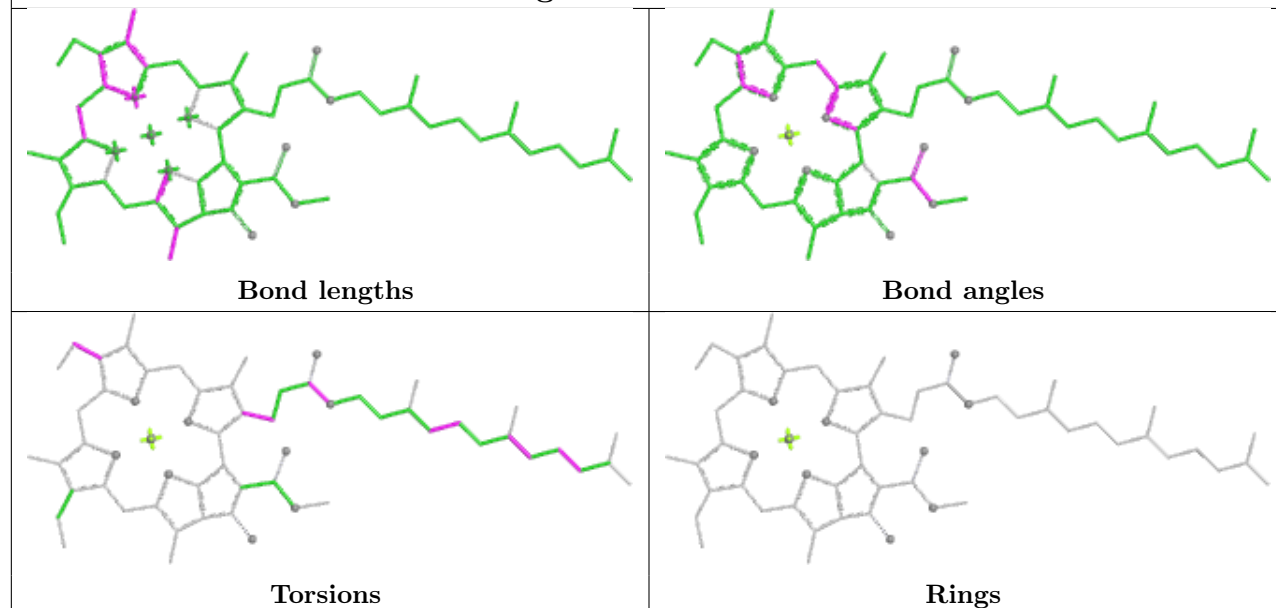
Rings



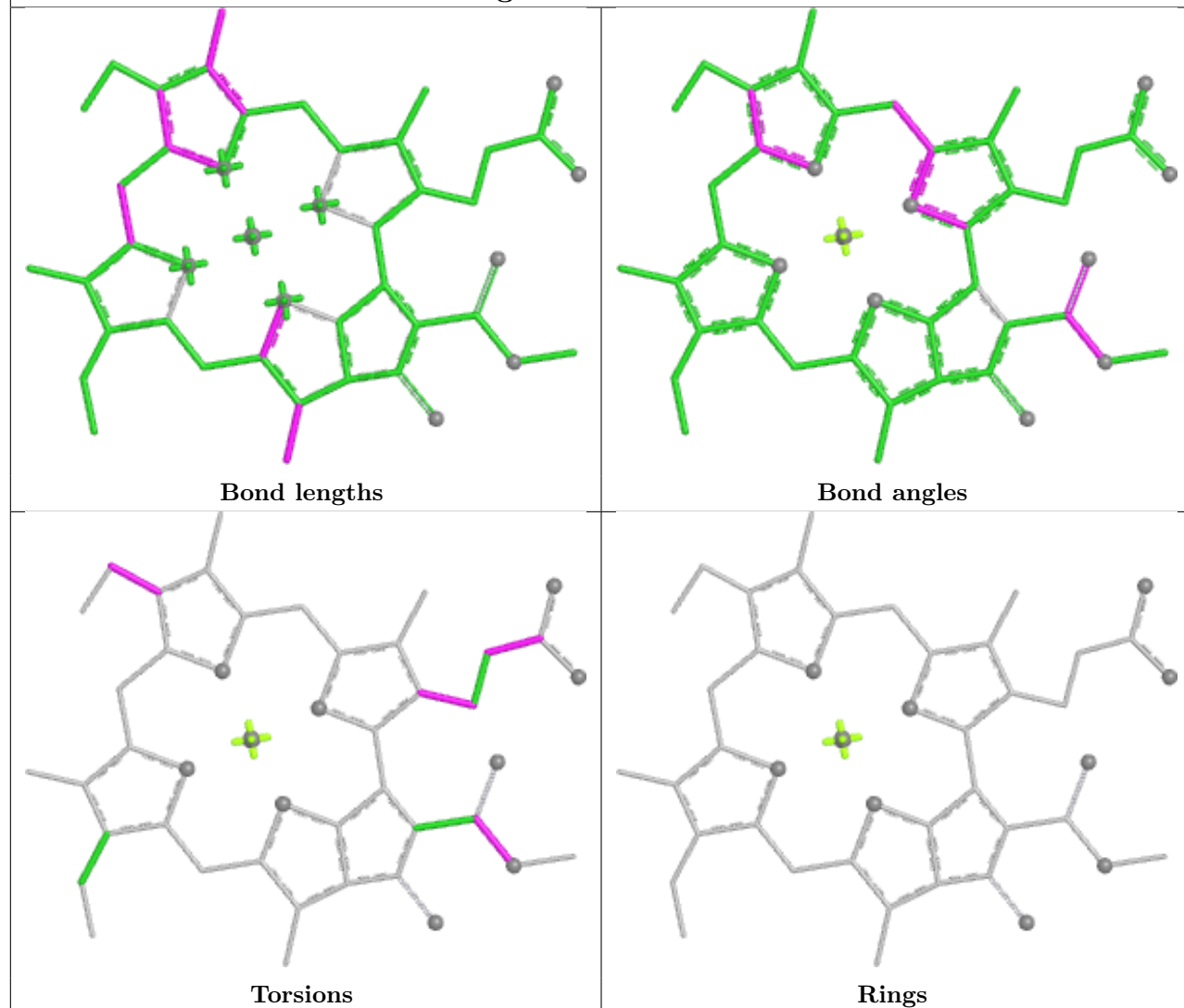




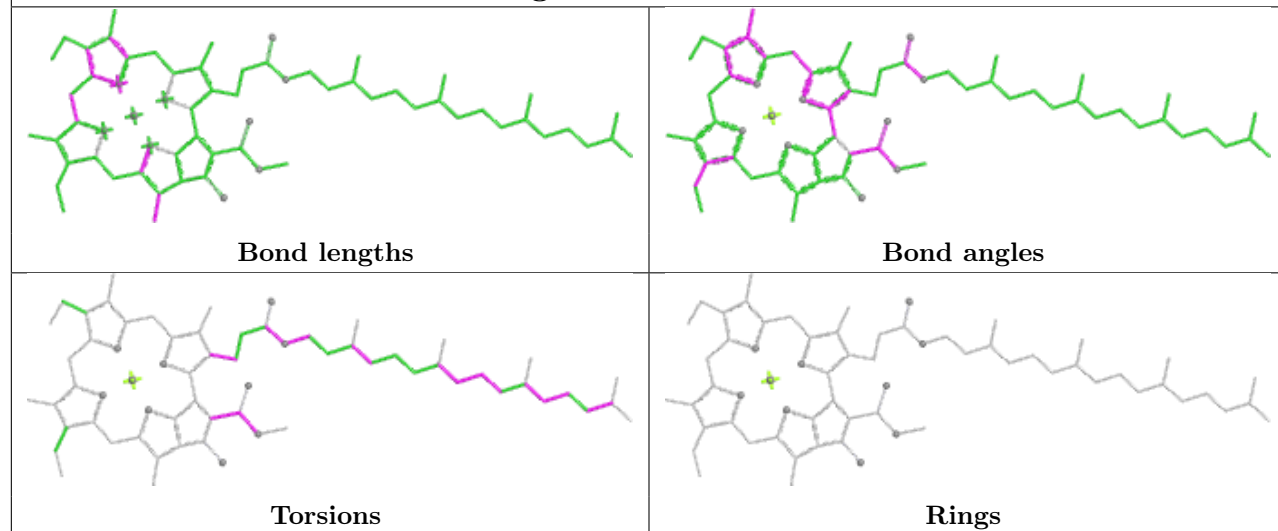


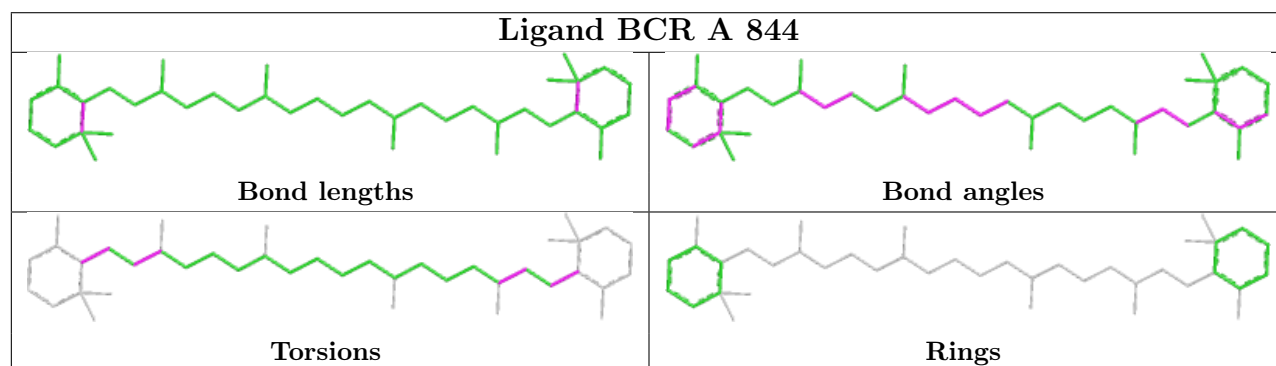
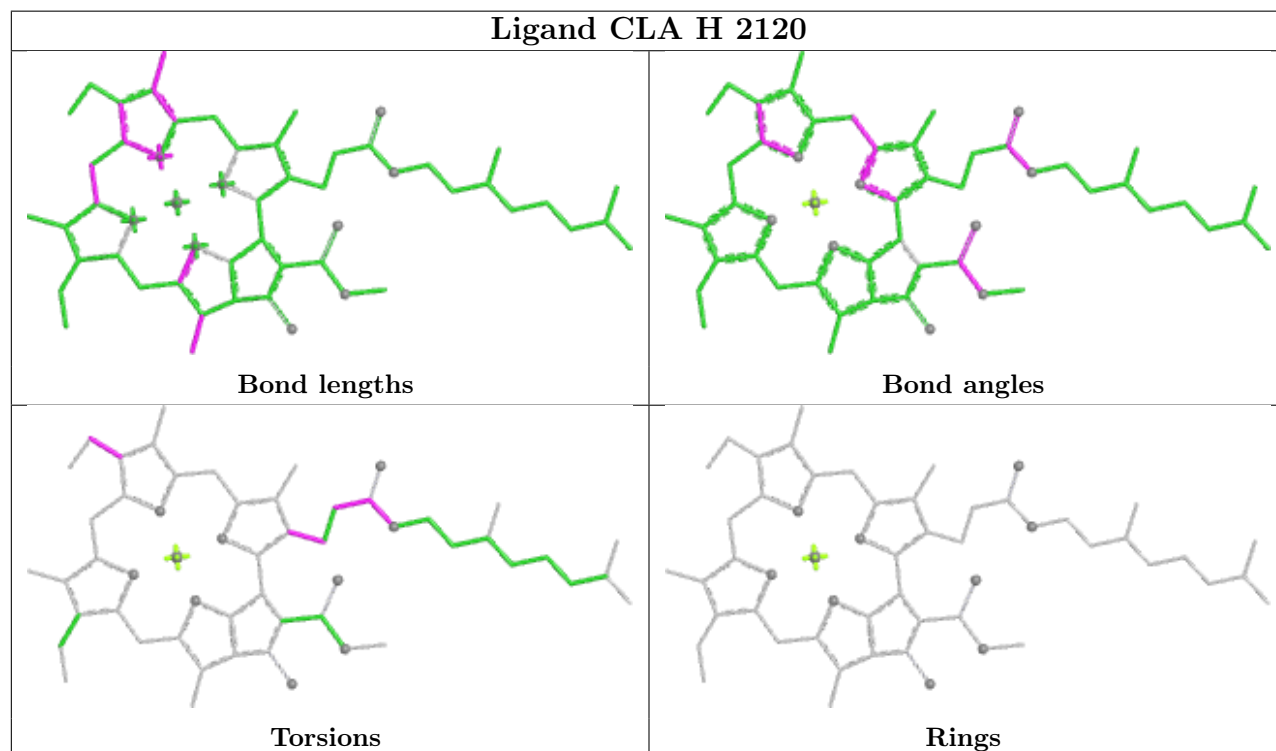
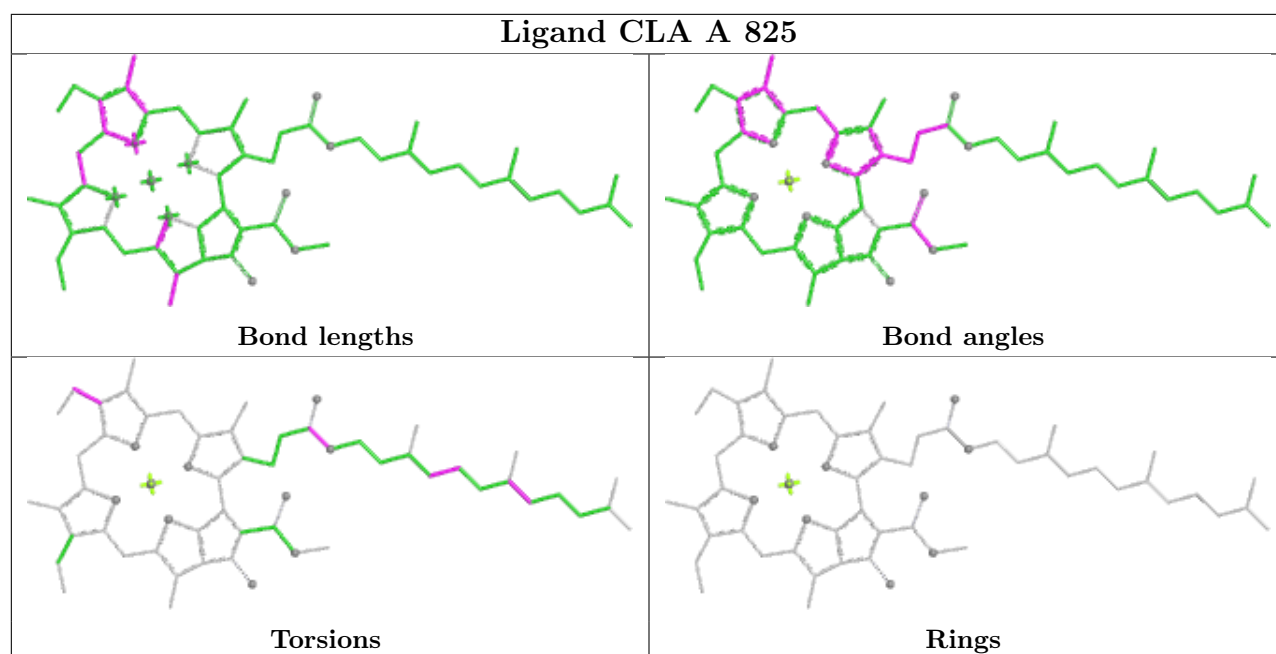
Ligand CLA a 824**Ligand CLA a 821**

Ligand CLA a 811

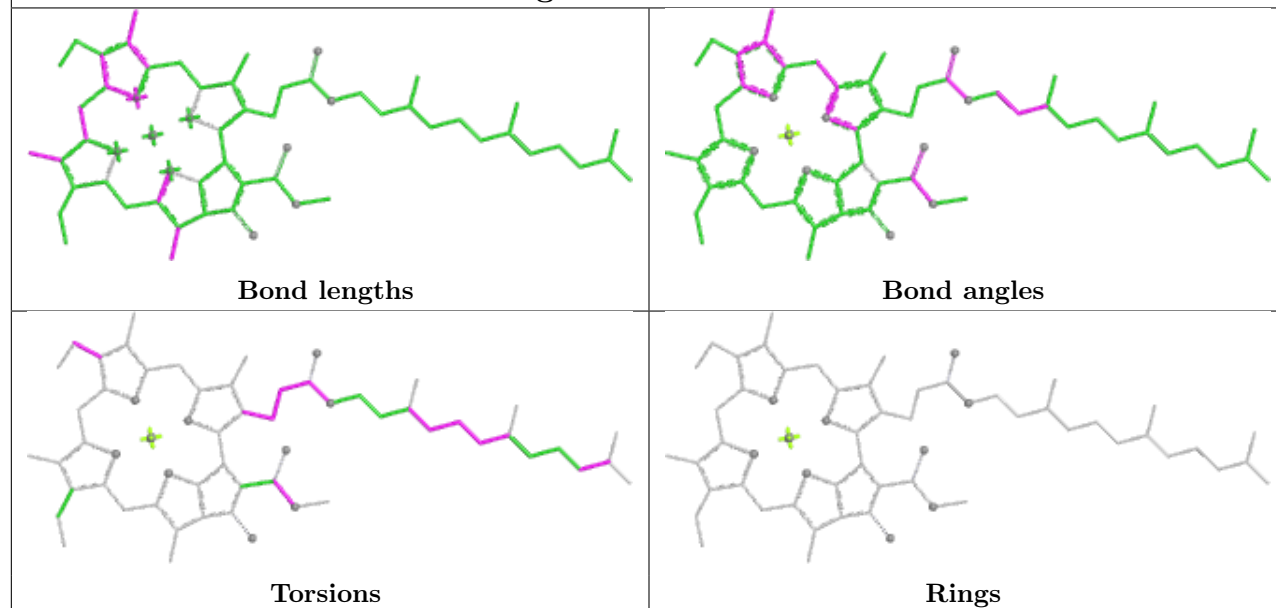


Ligand CLA G 824

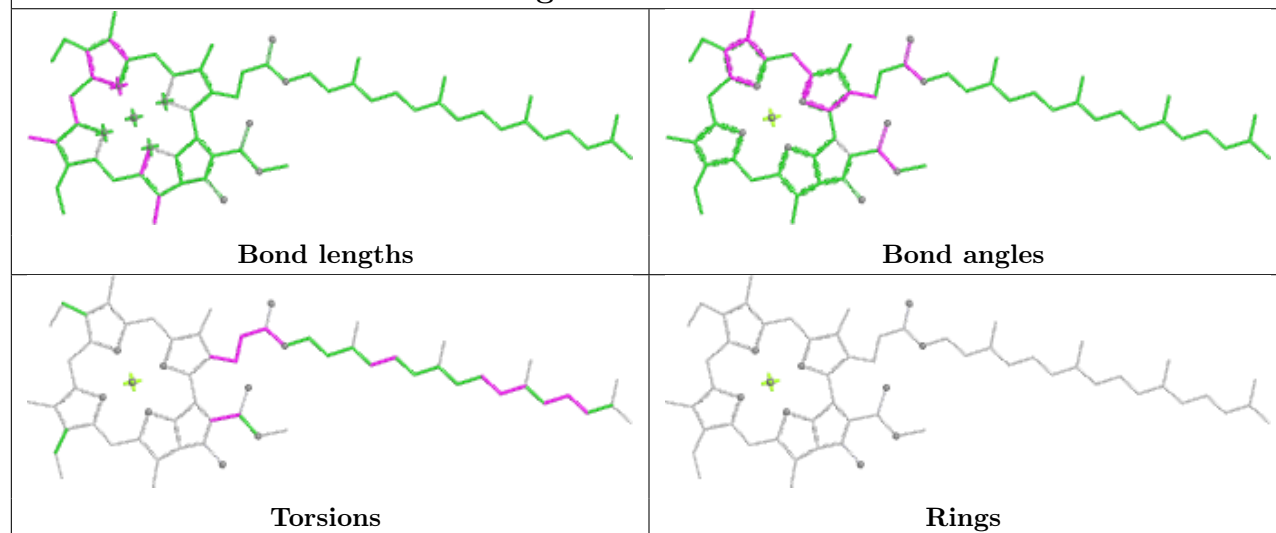


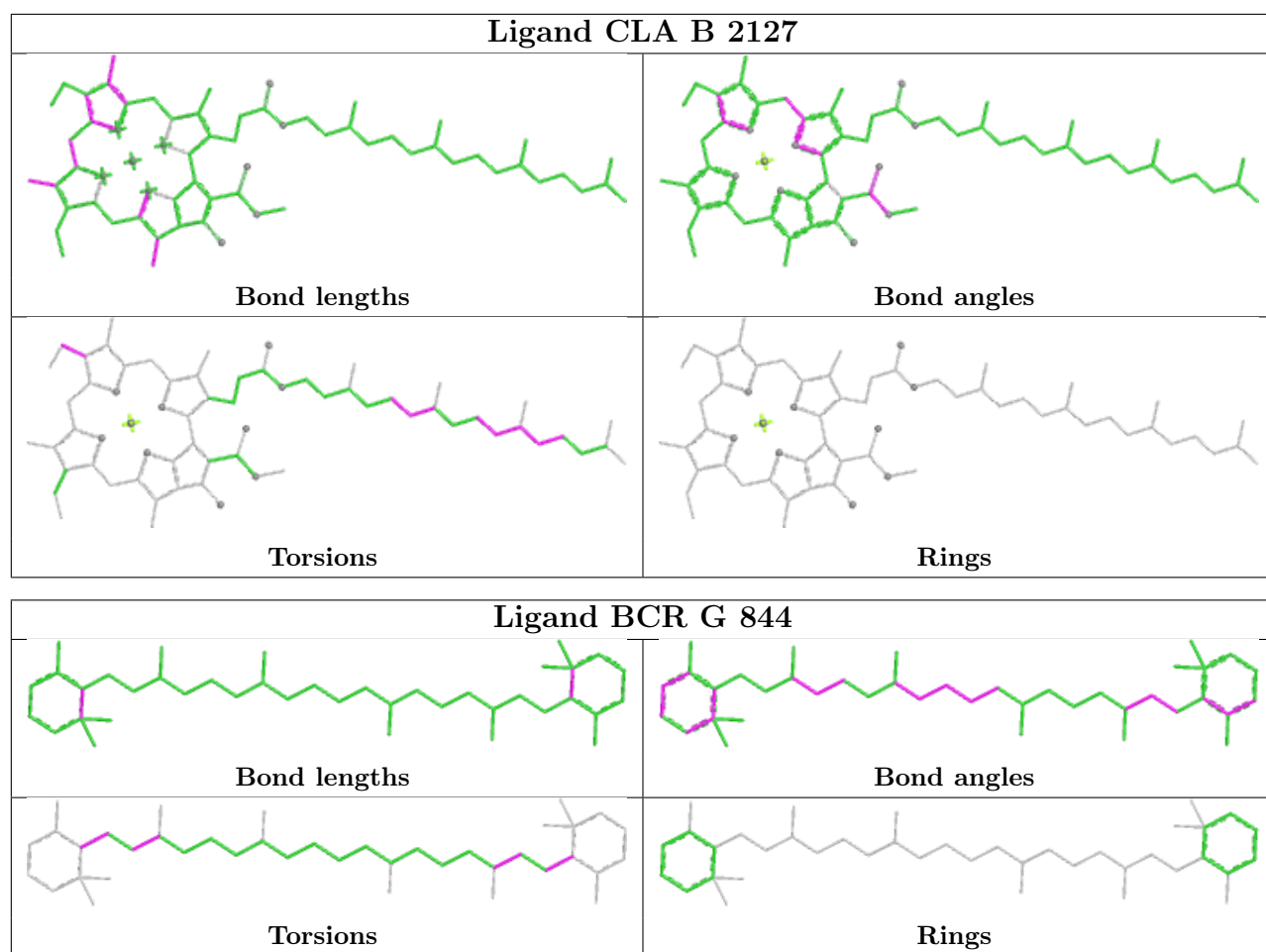


Ligand CLA a 817

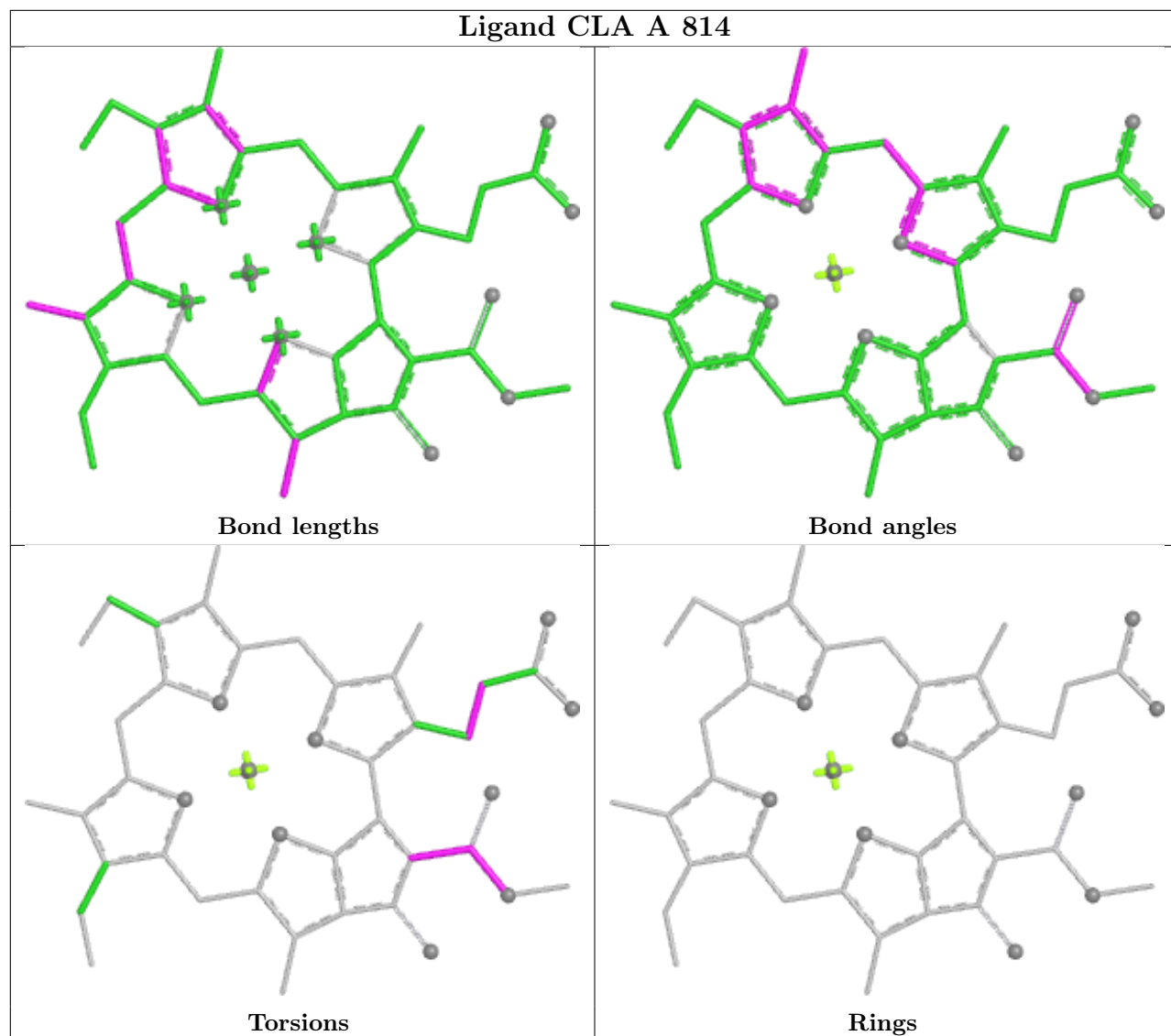


Ligand CLA a 807

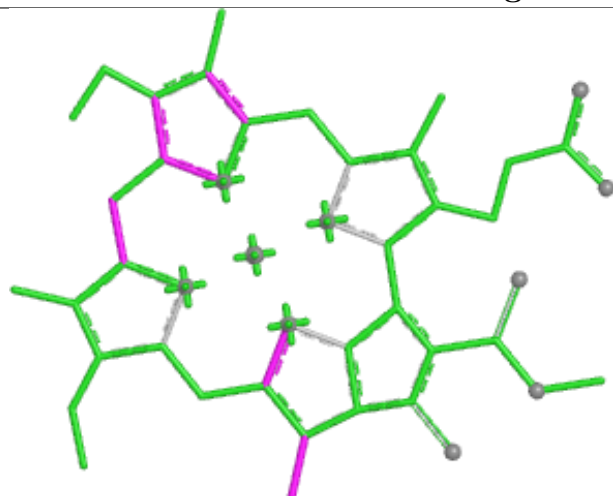




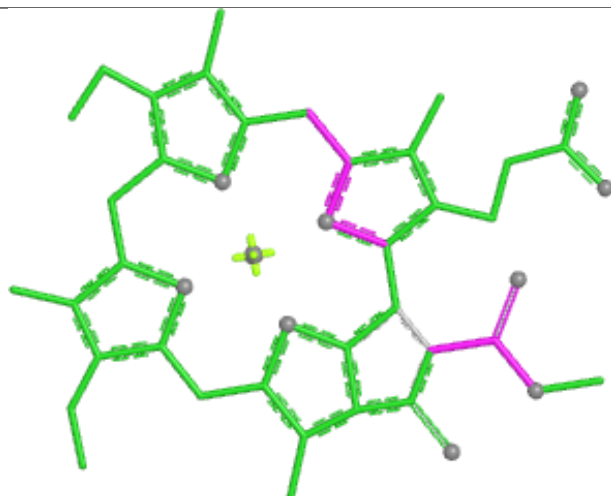
Ligand CLA A 814



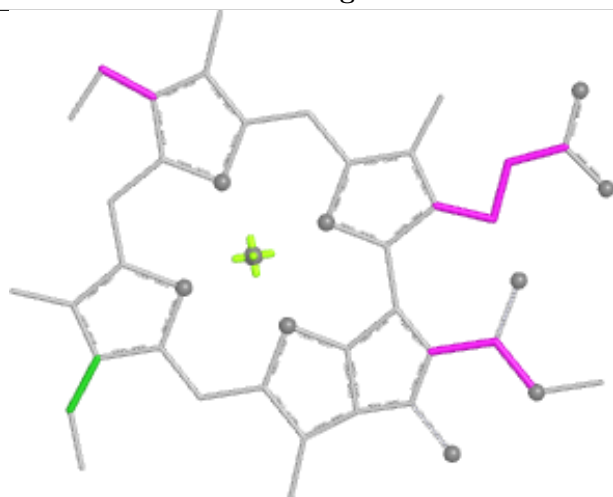
Ligand CLA H 2113



Bond lengths



Bond angles

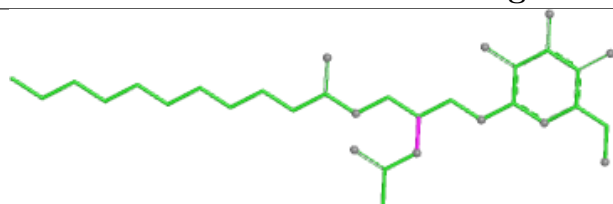


Torsions

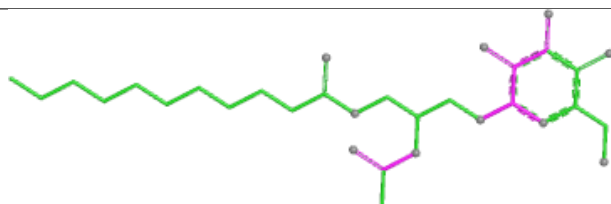


Rings

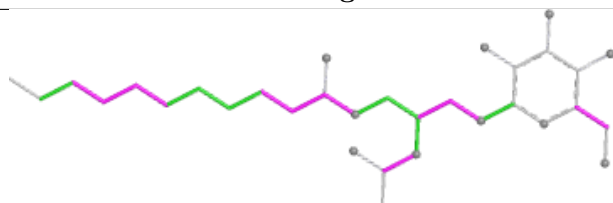
Ligand LMG G 849



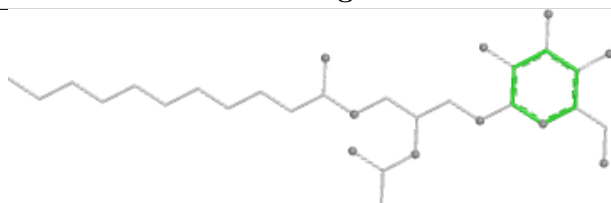
Bond lengths



Bond angles

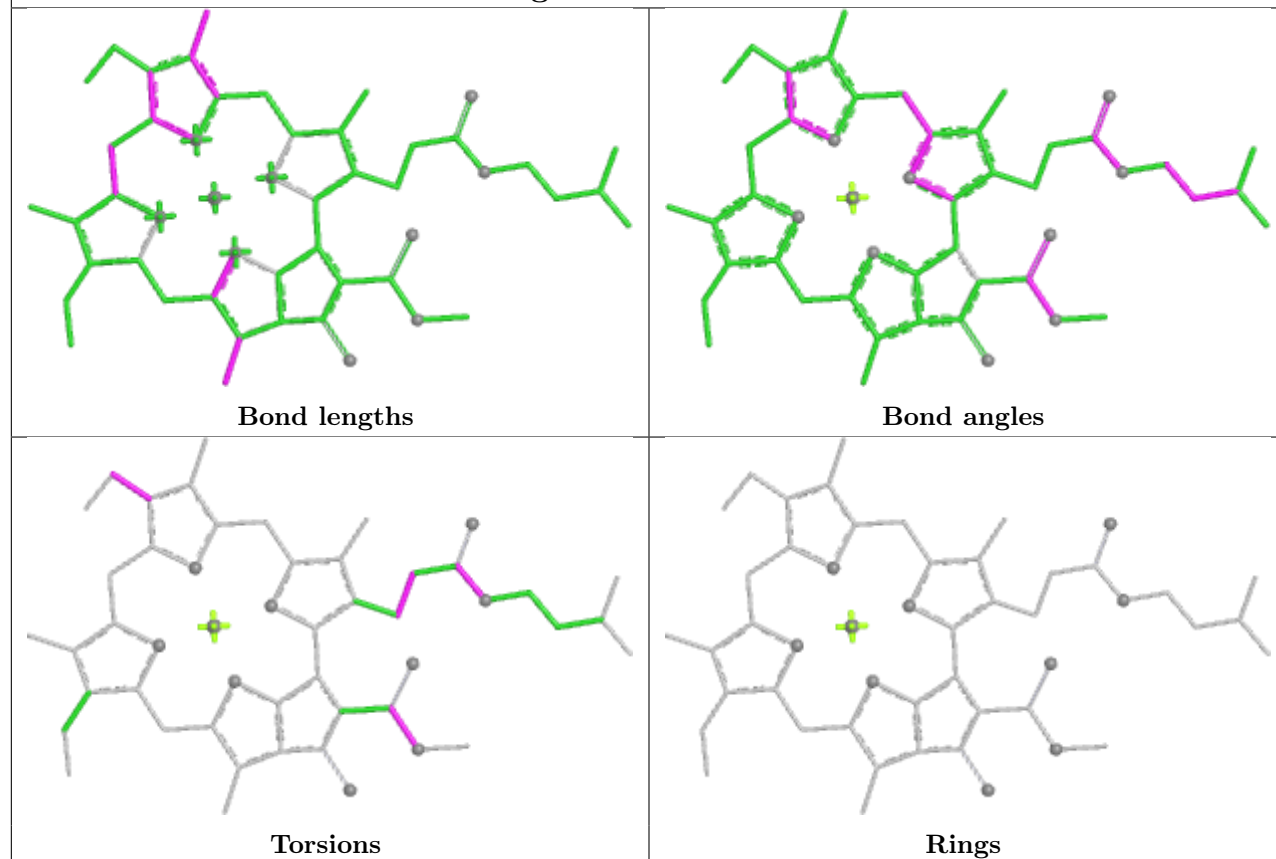


Torsions

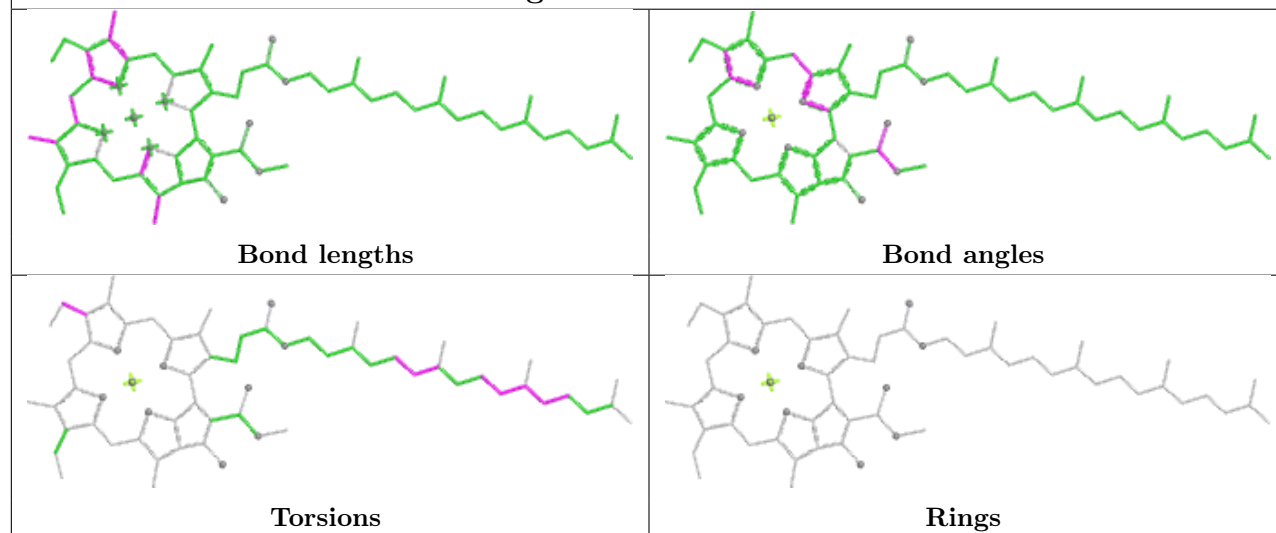


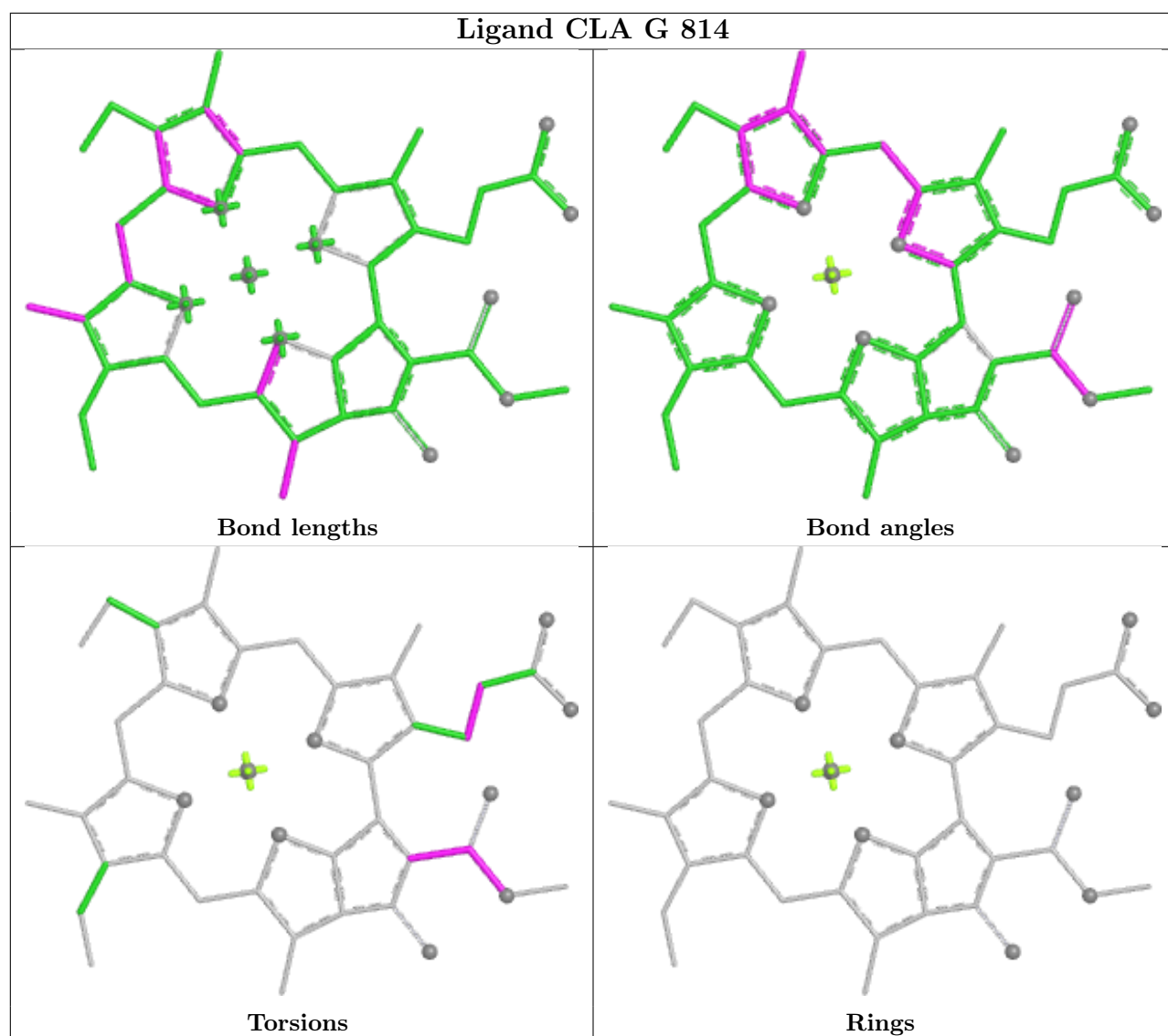
Rings

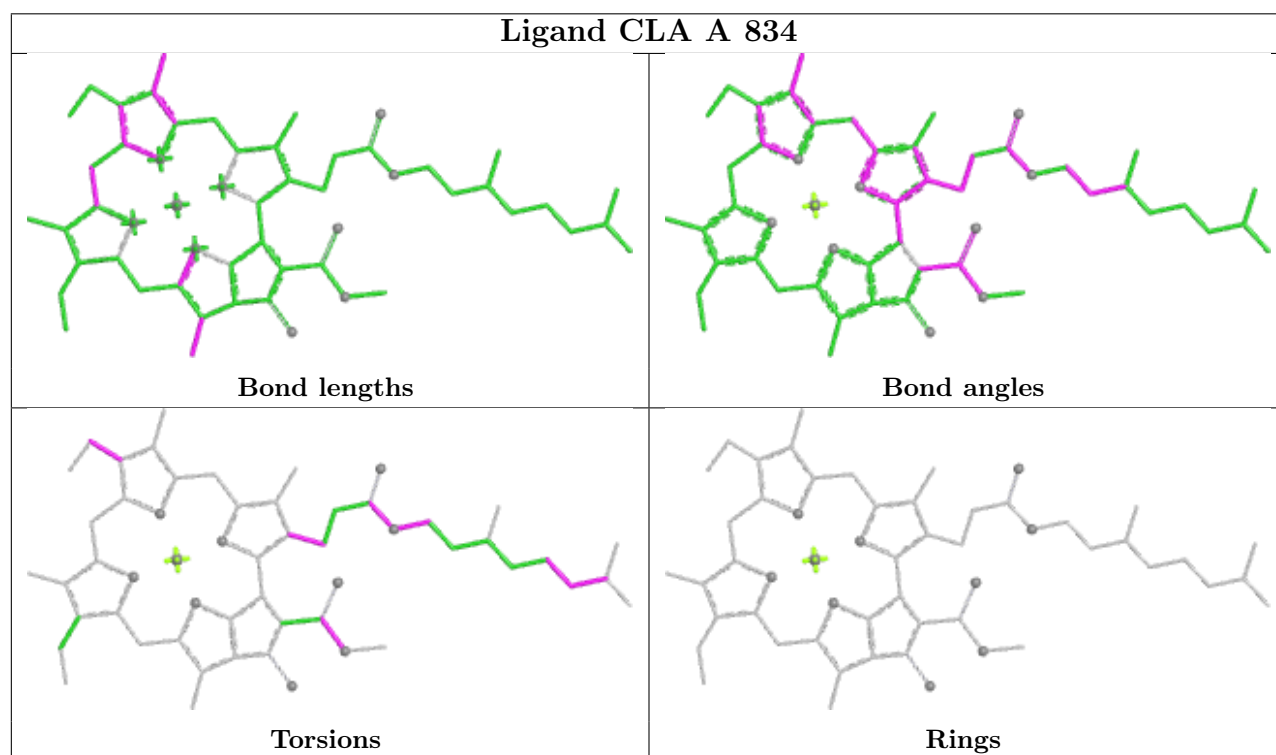
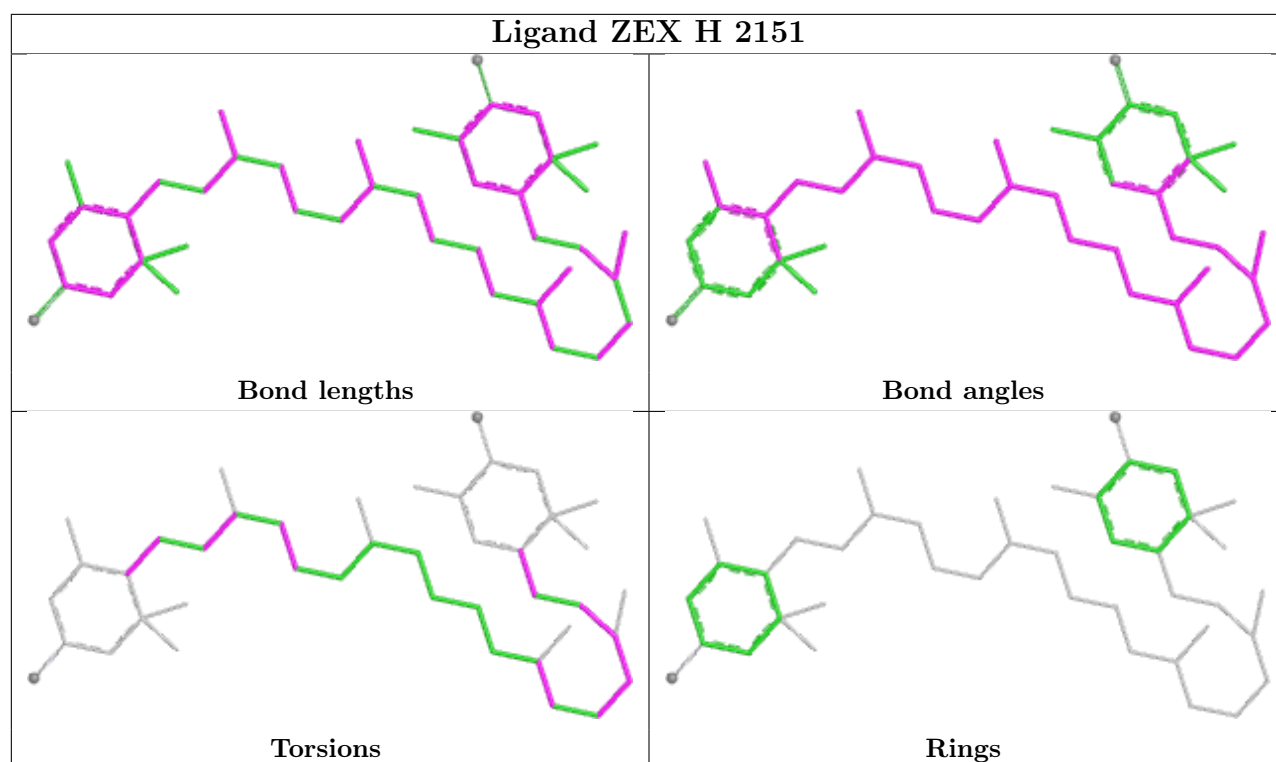
Ligand CLA G 806

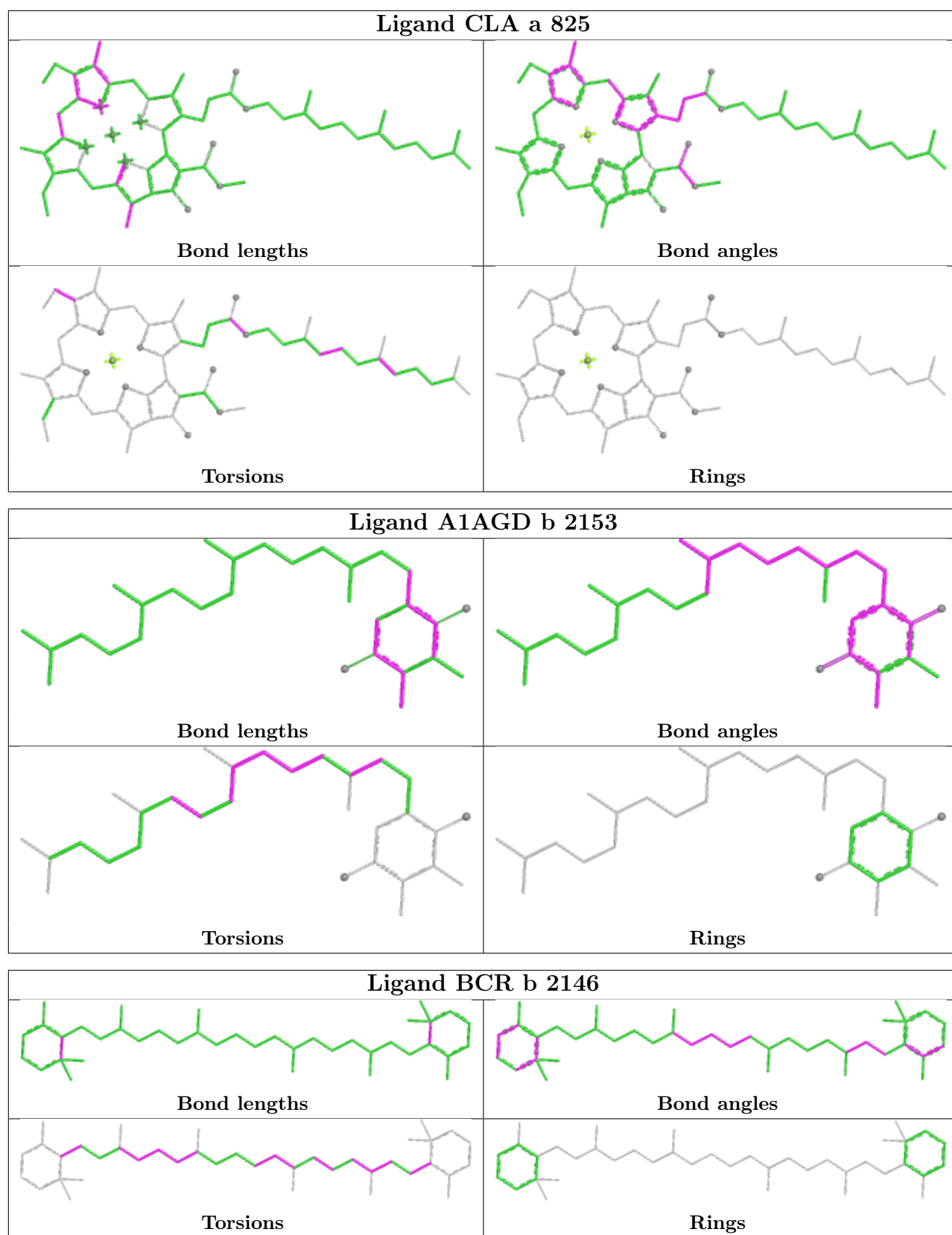


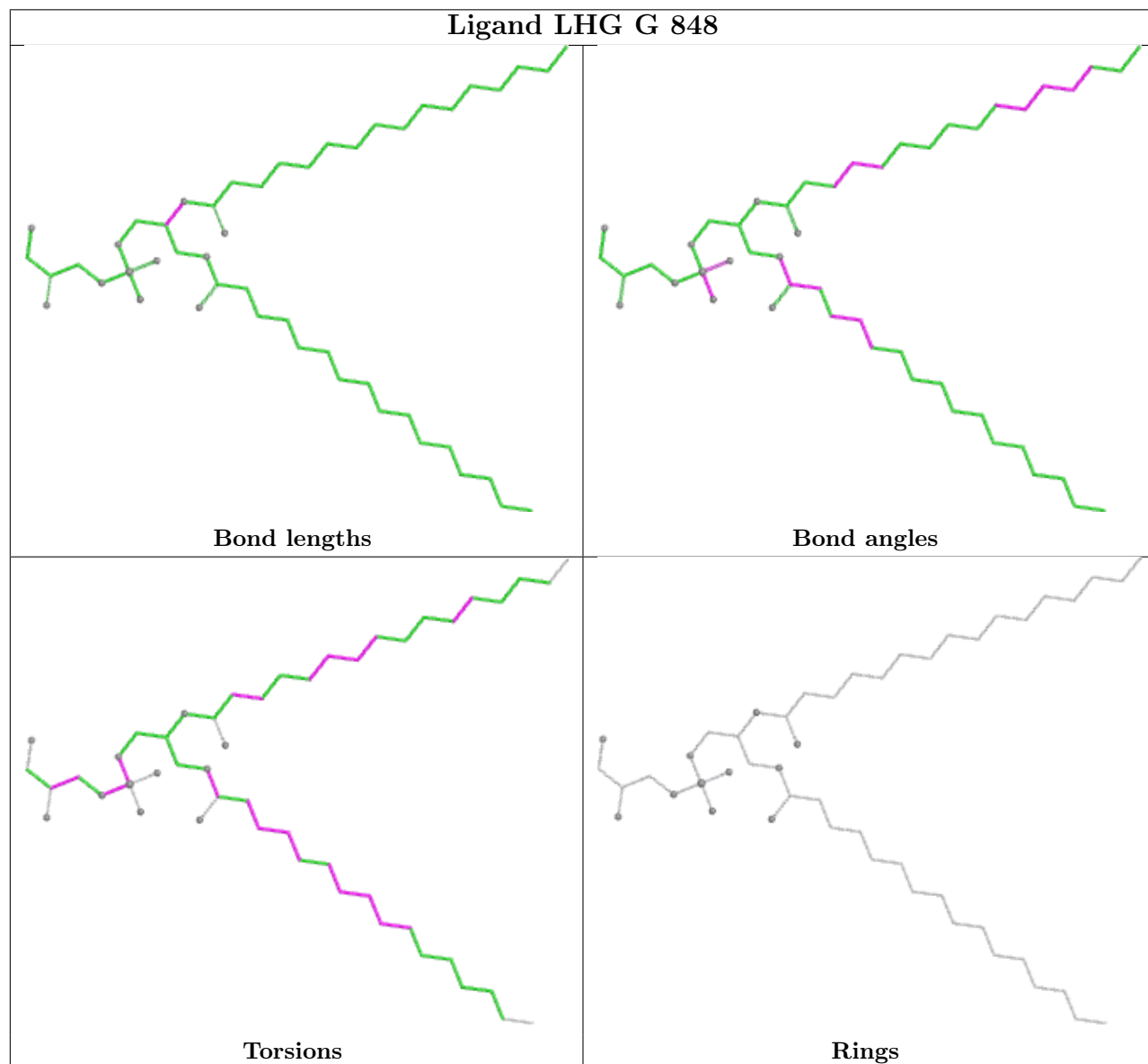
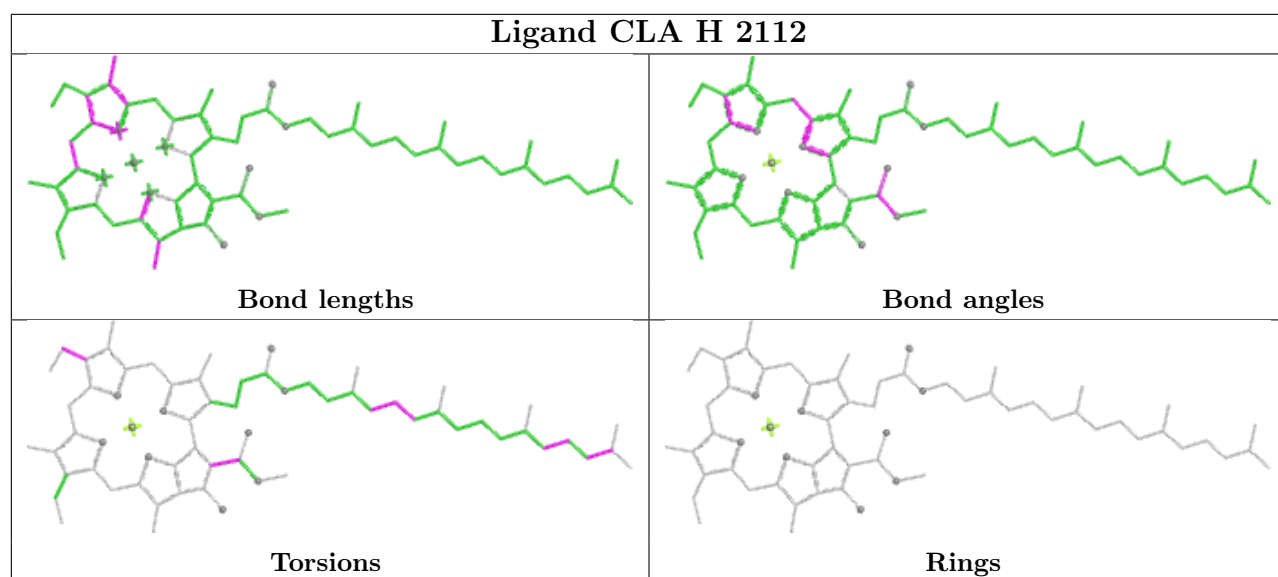
Ligand CLA b 2126

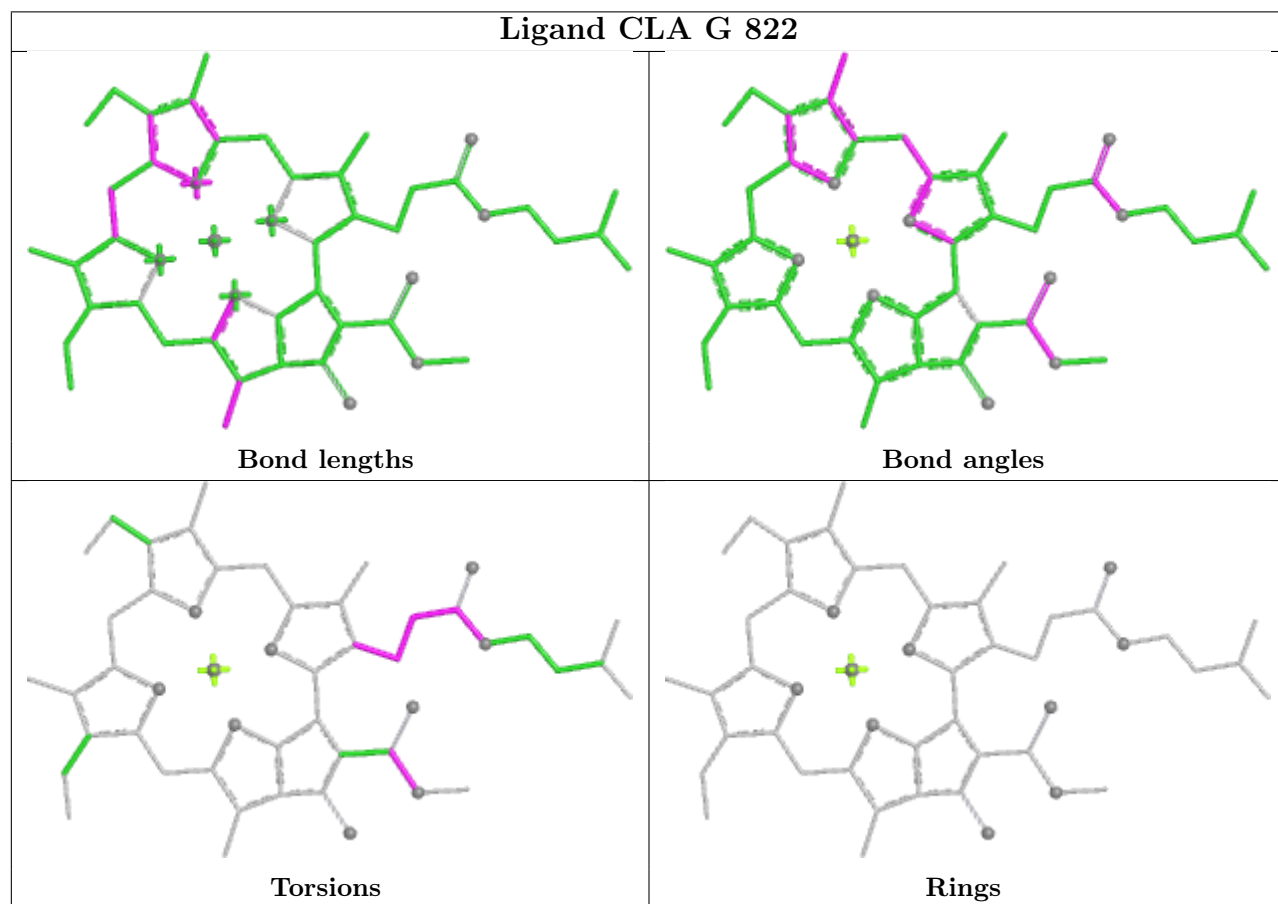
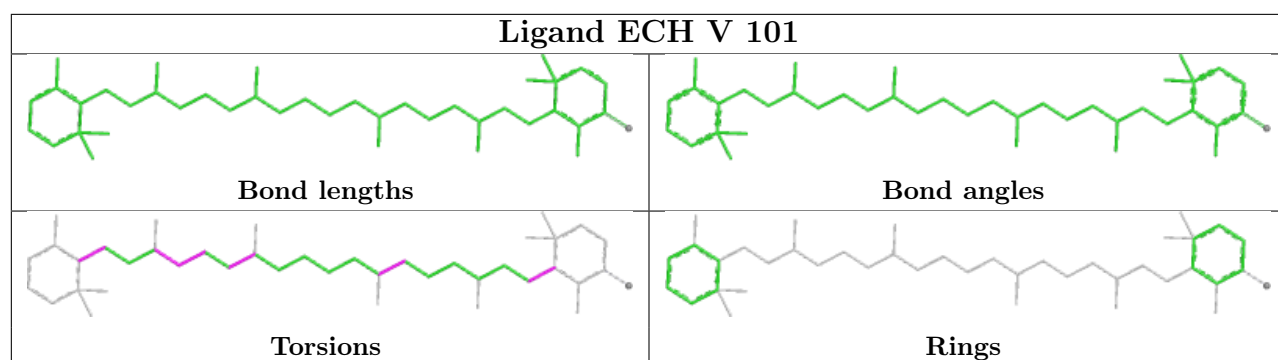


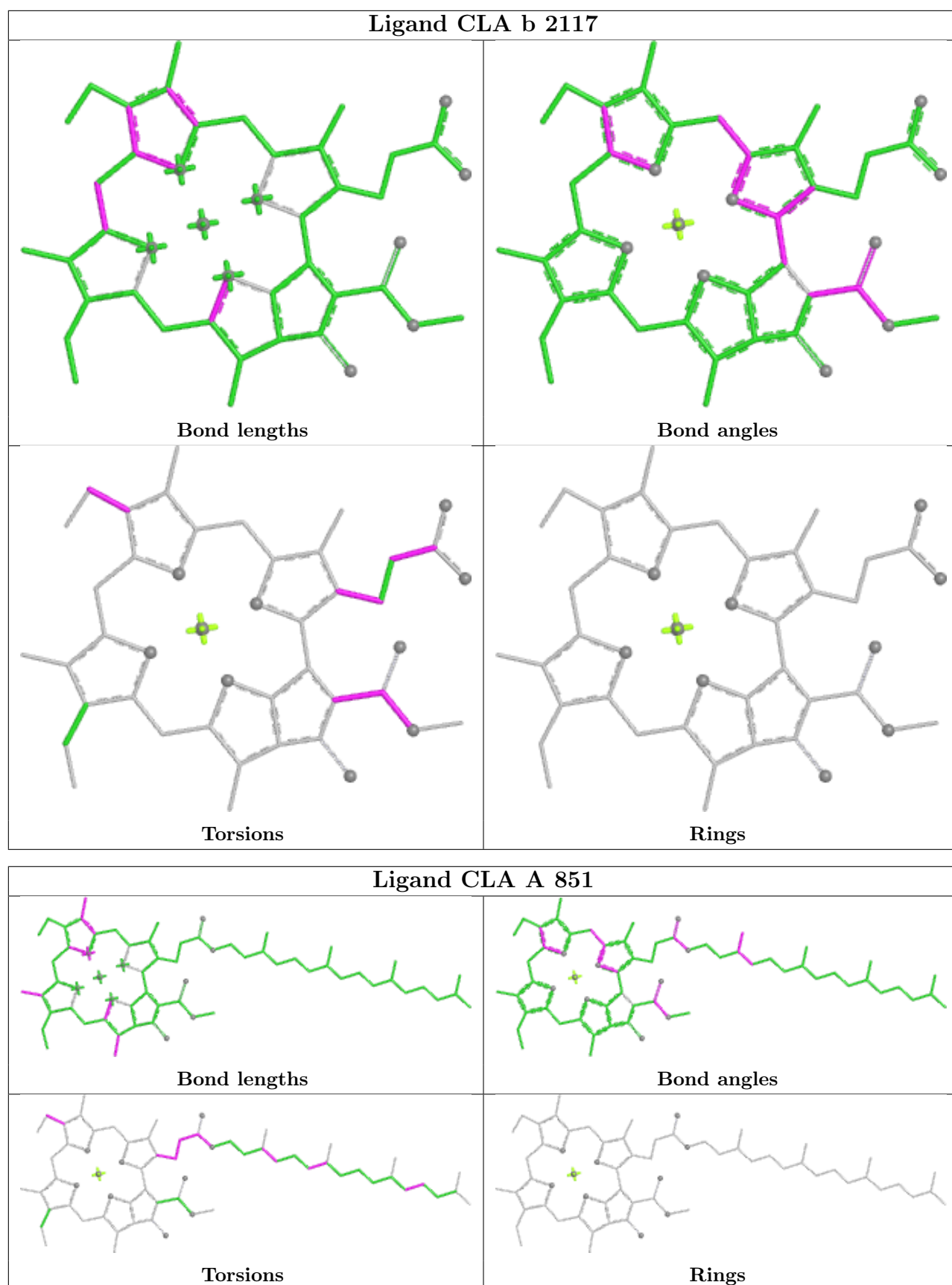




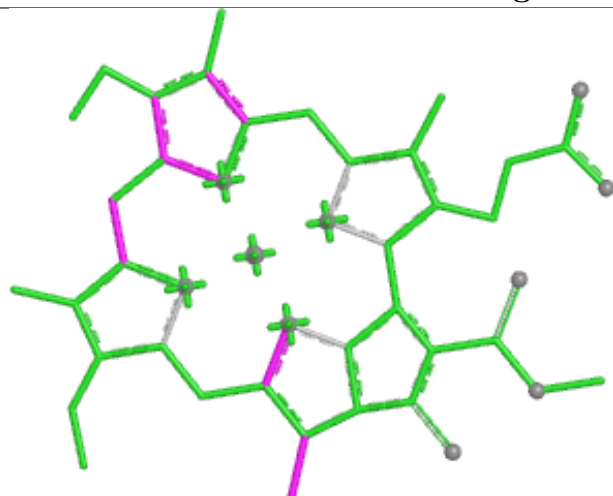




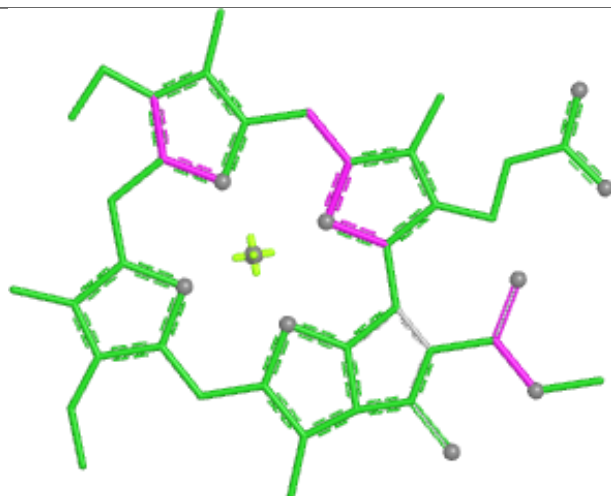




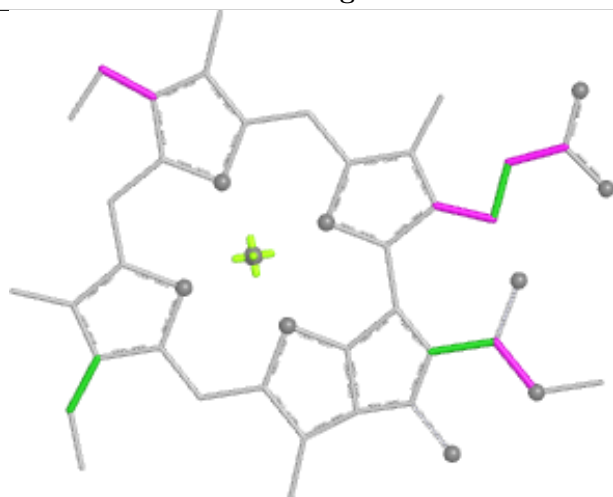
Ligand CLA G 811



Bond lengths



Bond angles

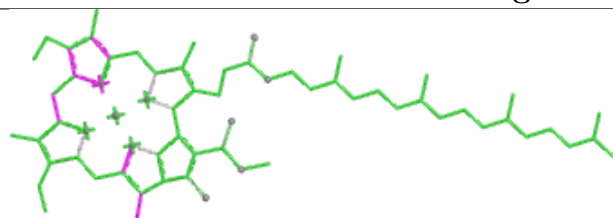


Torsions

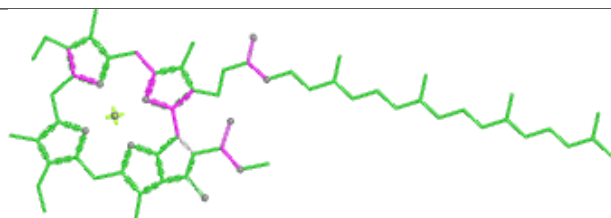


Rings

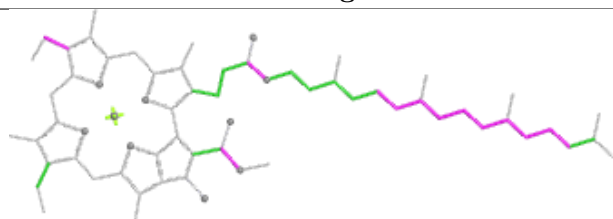
Ligand CLA G 819



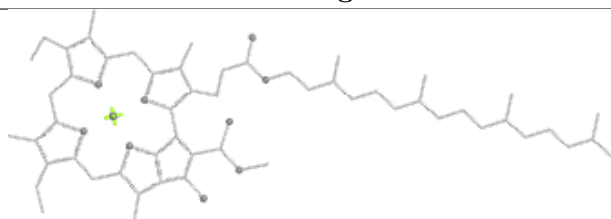
Bond lengths



Bond angles

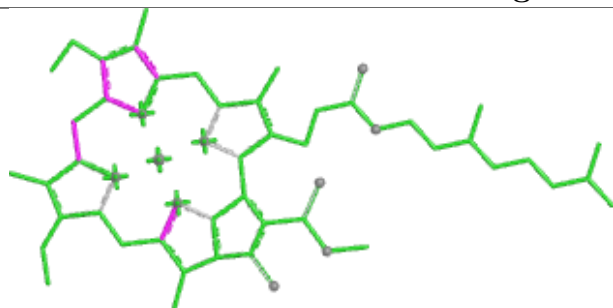


Torsions

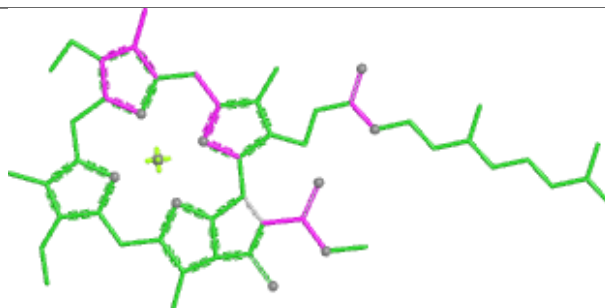


Rings

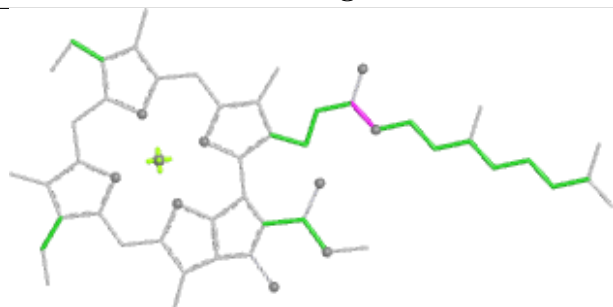
Ligand CLA G 803



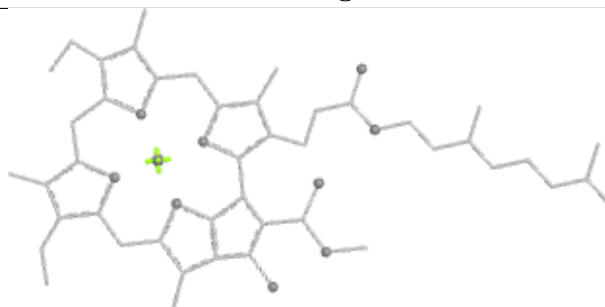
Bond lengths



Bond angles

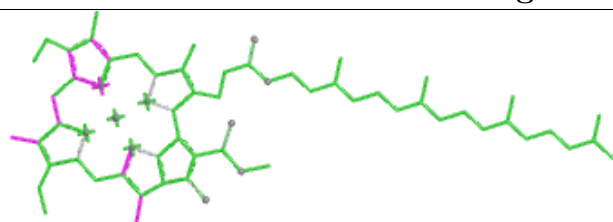


Torsions

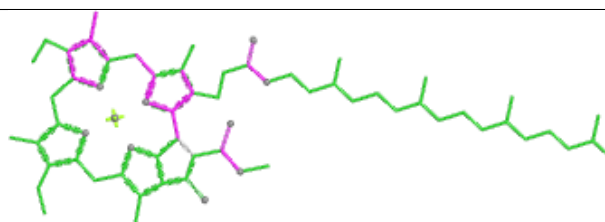


Rings

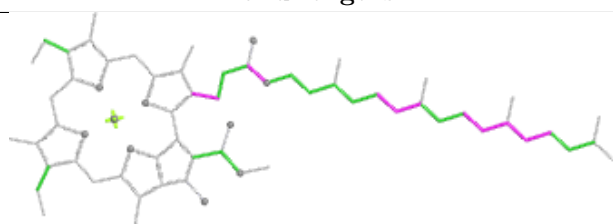
Ligand CLA L 203



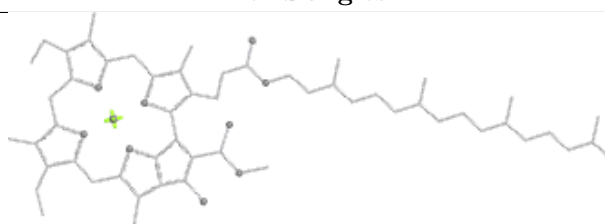
Bond lengths



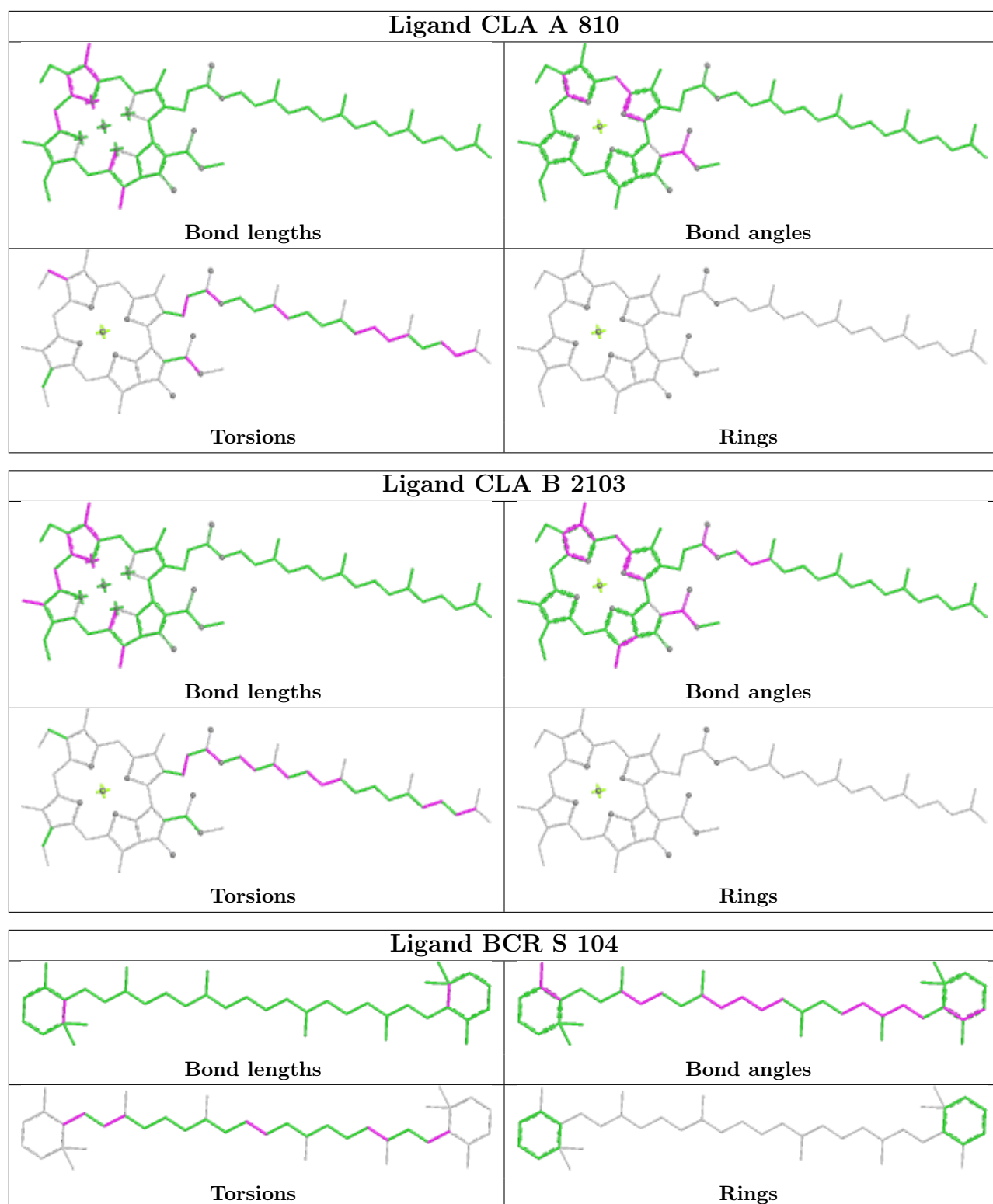
Bond angles

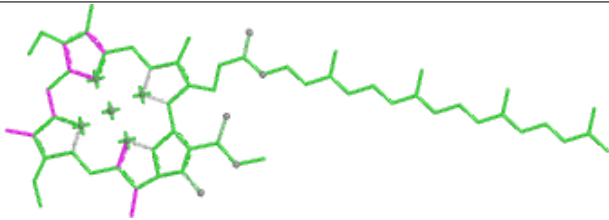
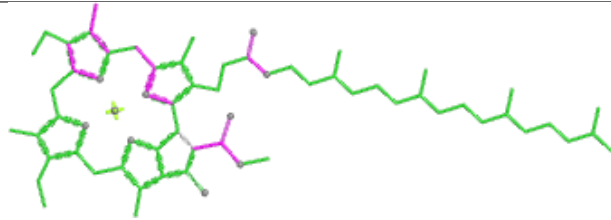
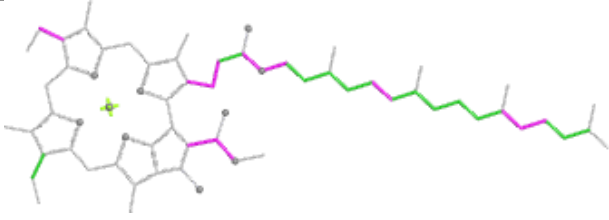
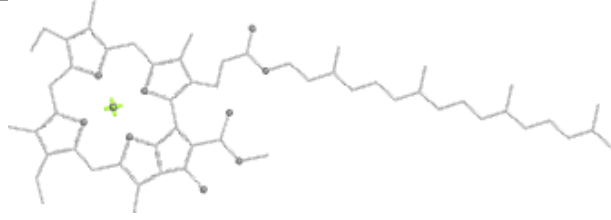


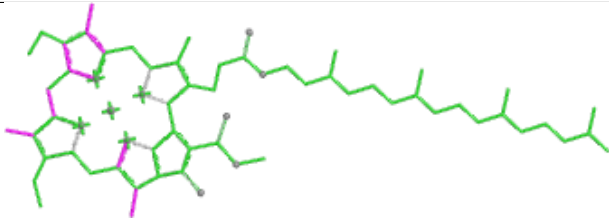
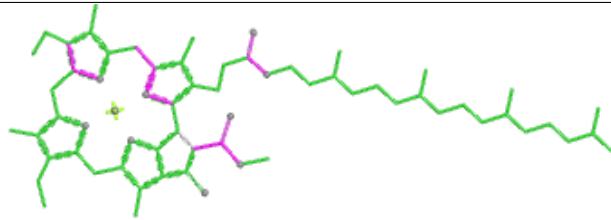
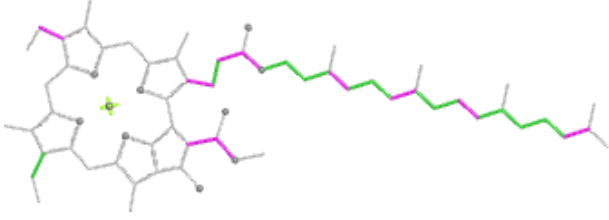
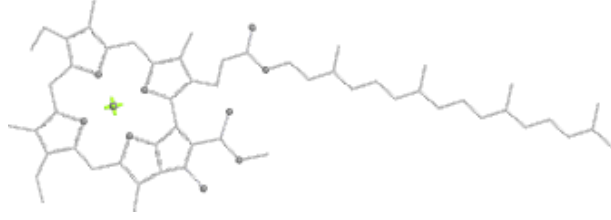
Torsions

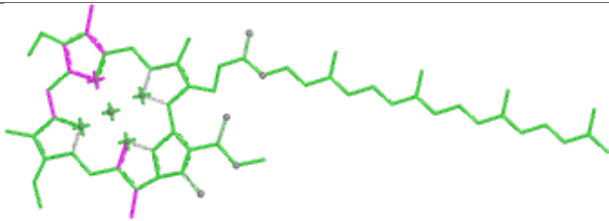
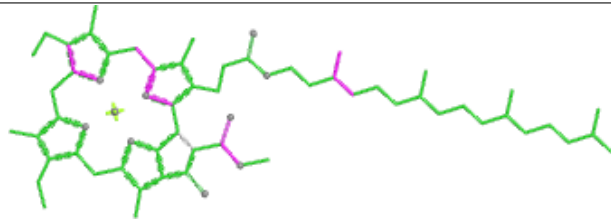
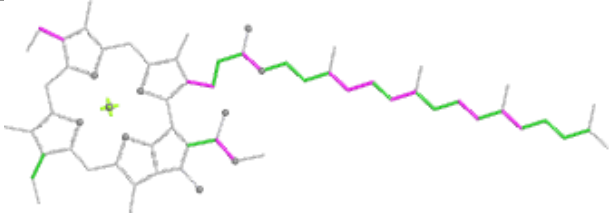
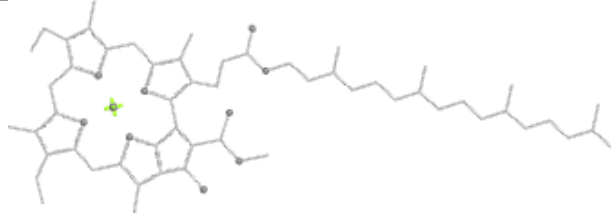


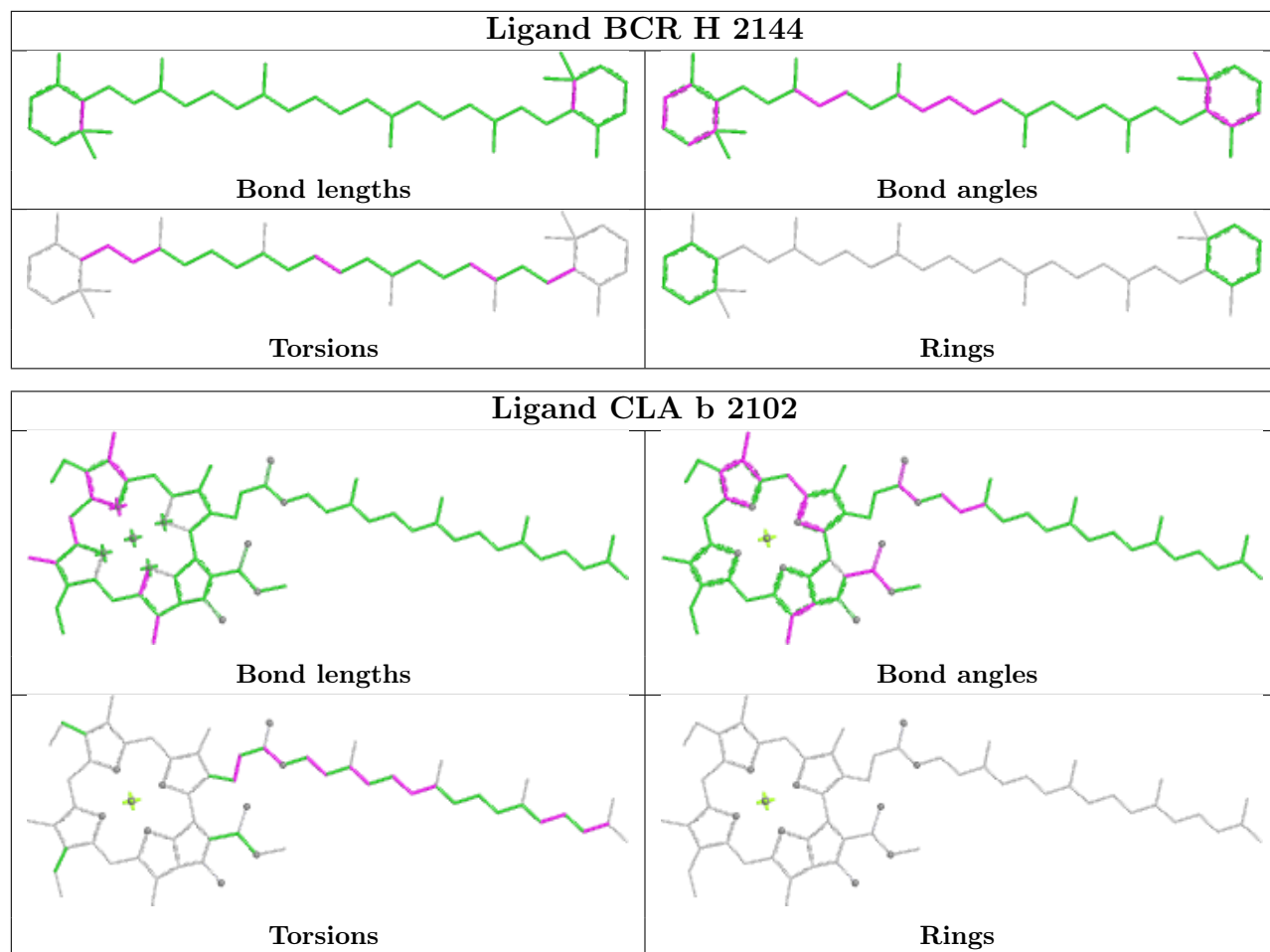
Rings



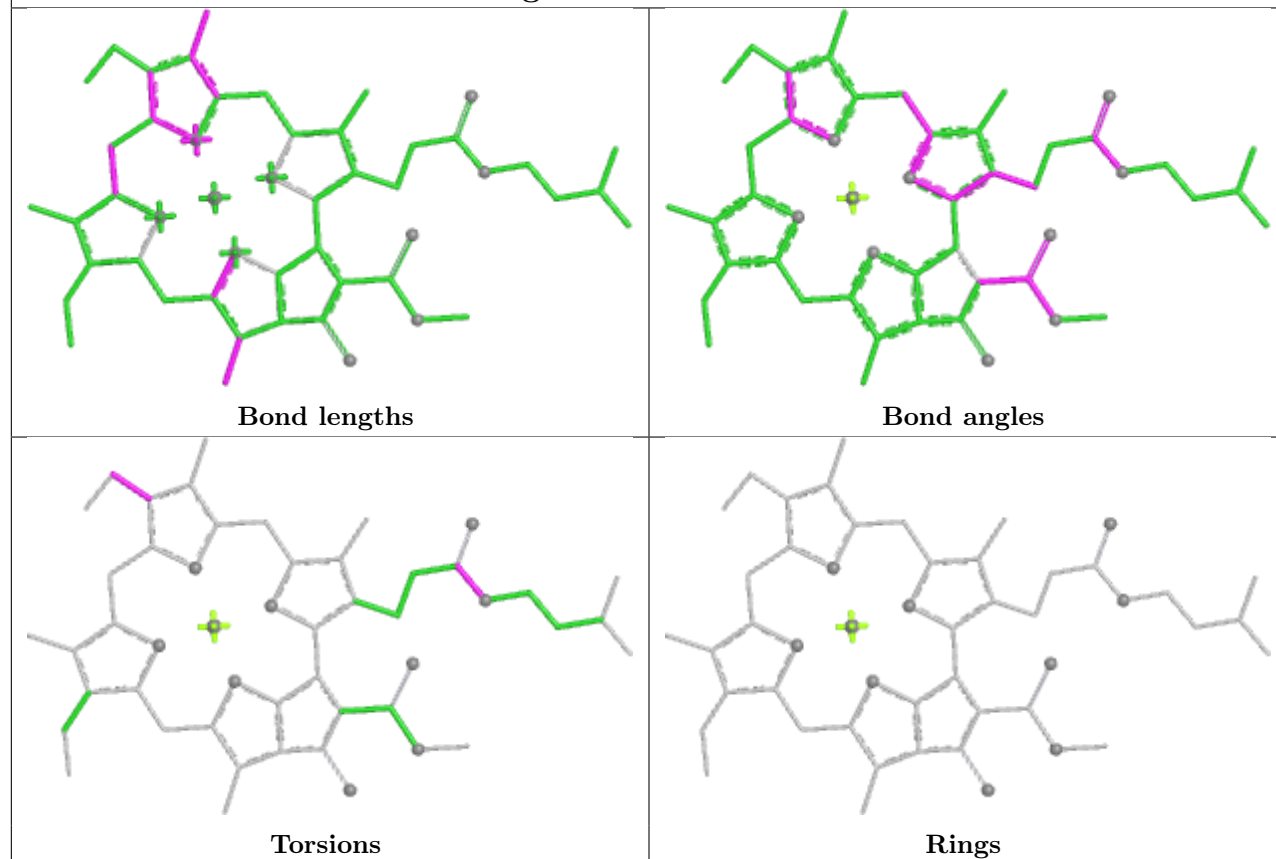
Ligand CLA U 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 2133	
	
Bond lengths	Bond angles
	
Torsions	Rings

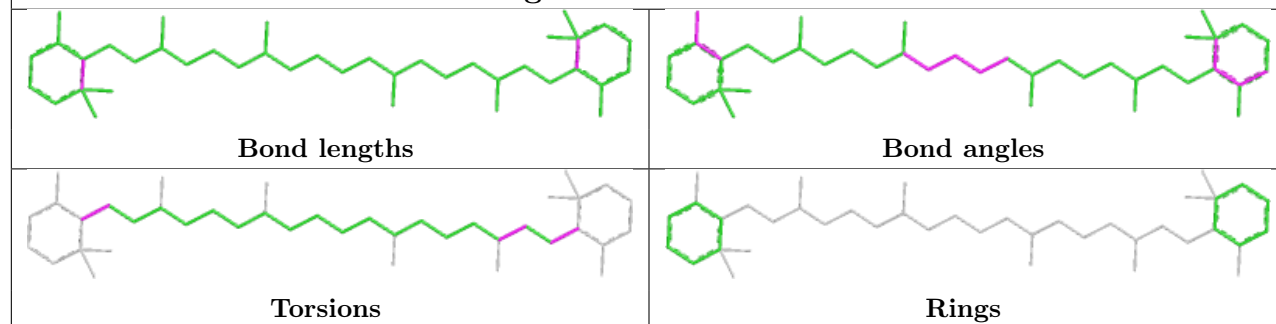
Ligand CLA a 833	
	
Bond lengths	Bond angles
	
Torsions	Rings



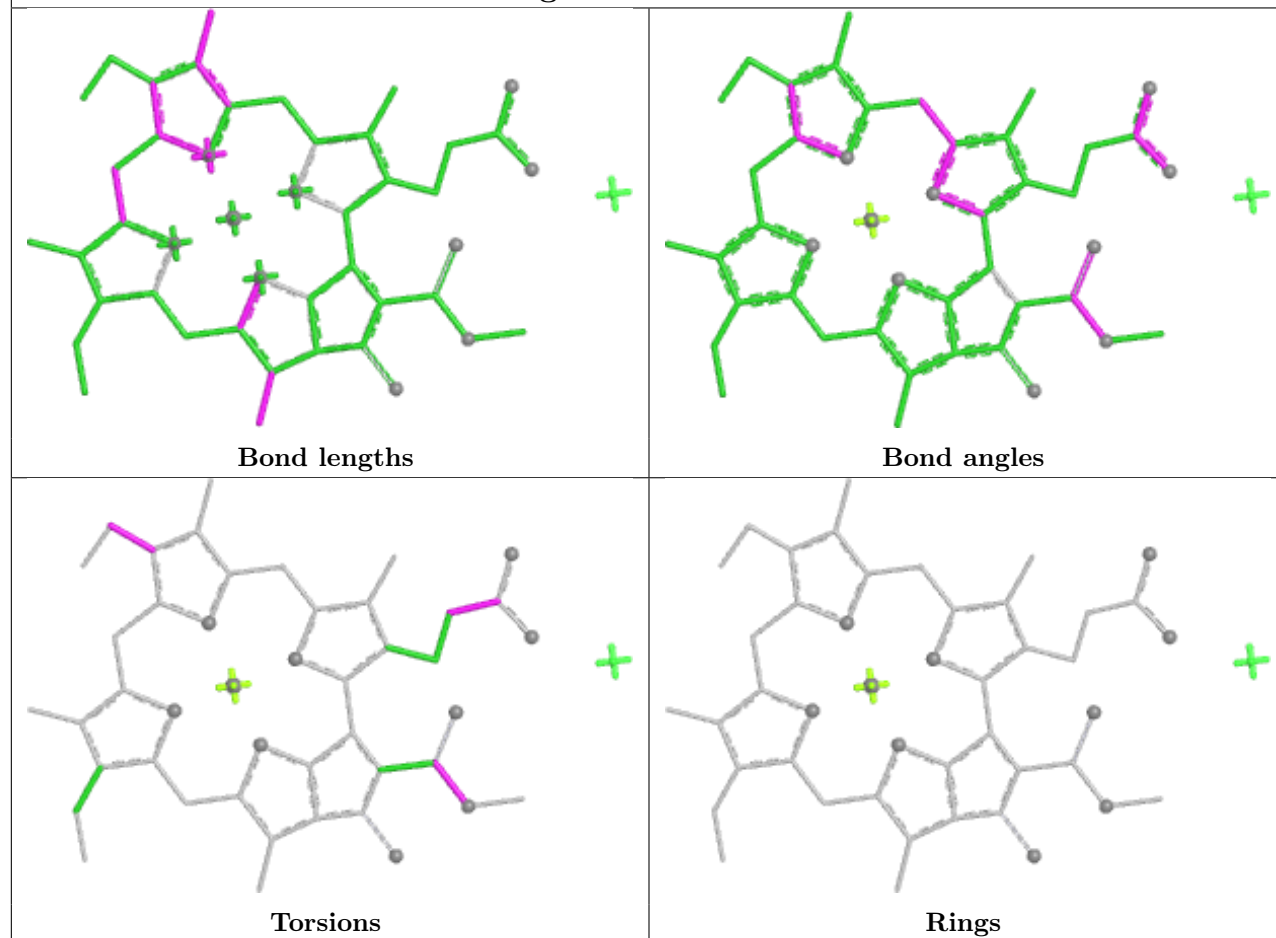
Ligand CLA H 2125



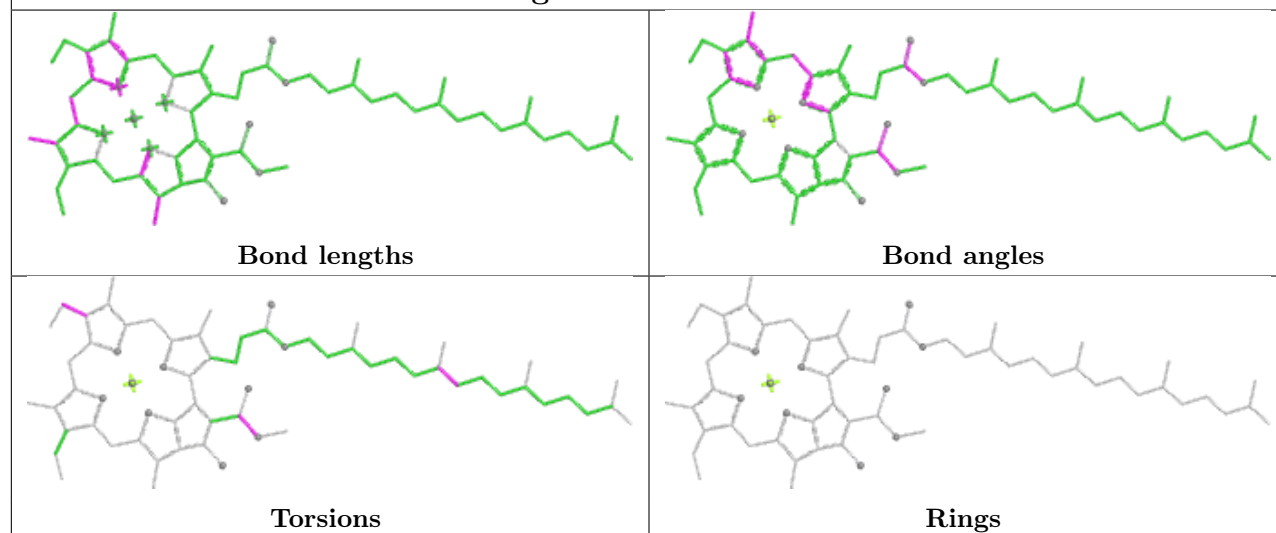
Ligand BCR b 2142



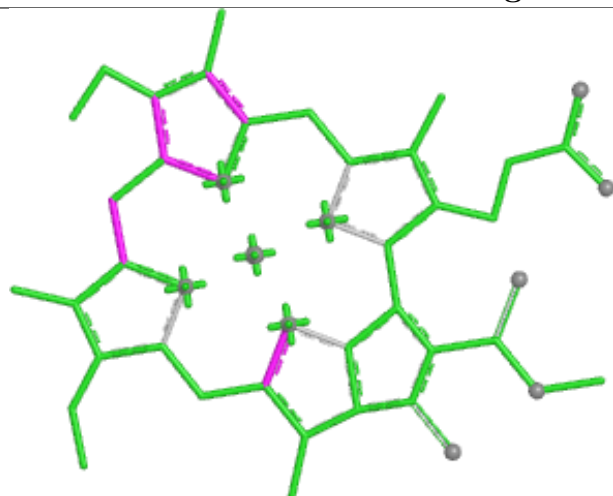
Ligand CLA f 203



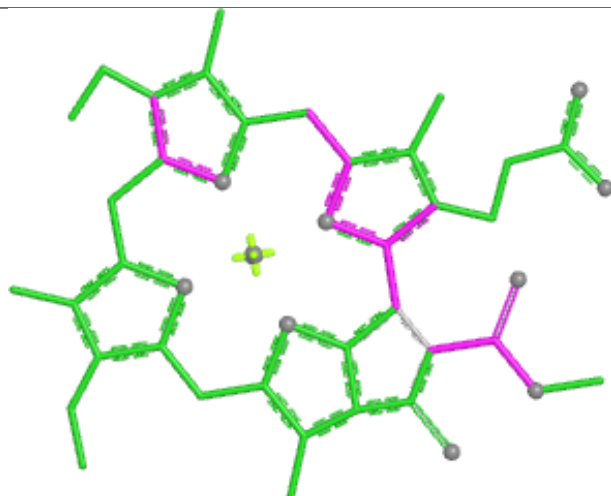
Ligand CLA A 838



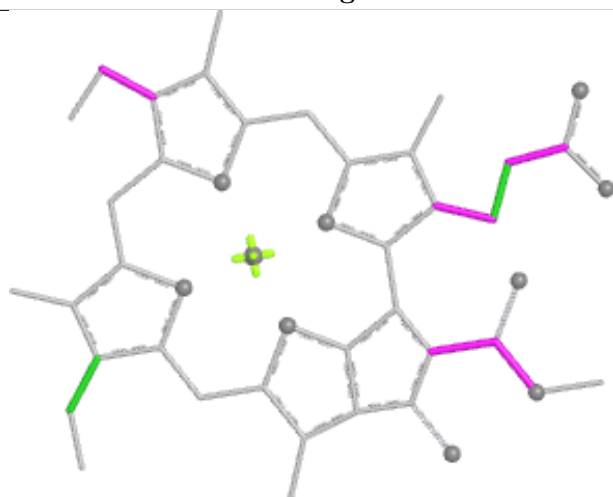
Ligand CLA H 2117



Bond lengths



Bond angles

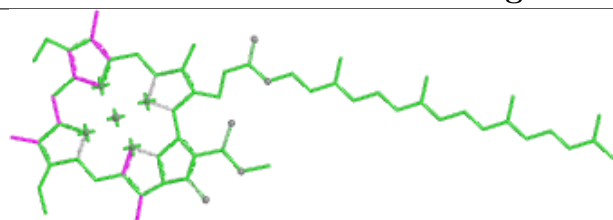


Torsions

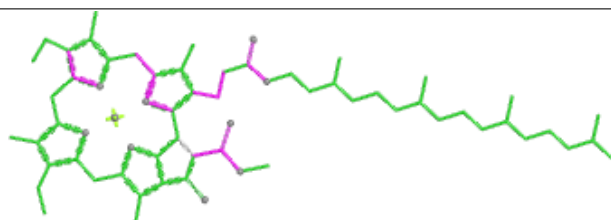


Rings

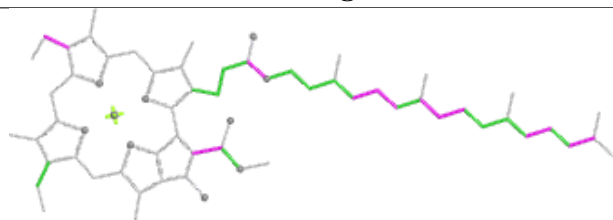
Ligand CLA B 2110



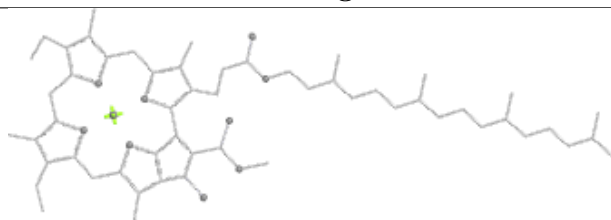
Bond lengths



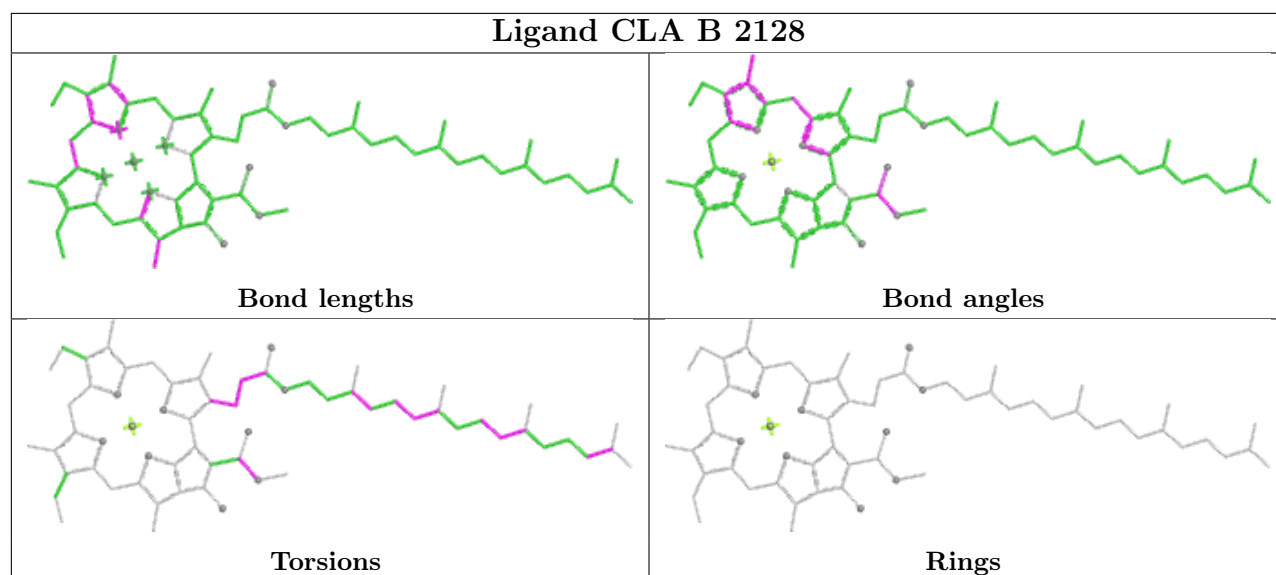
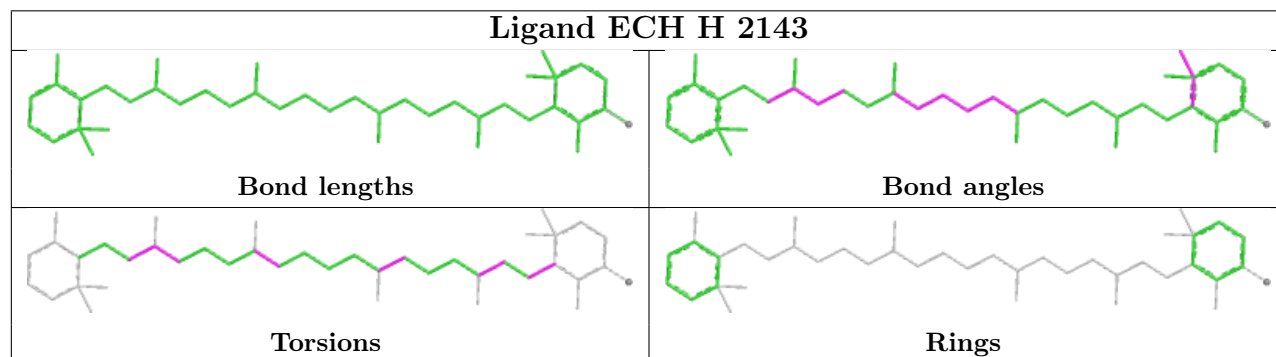
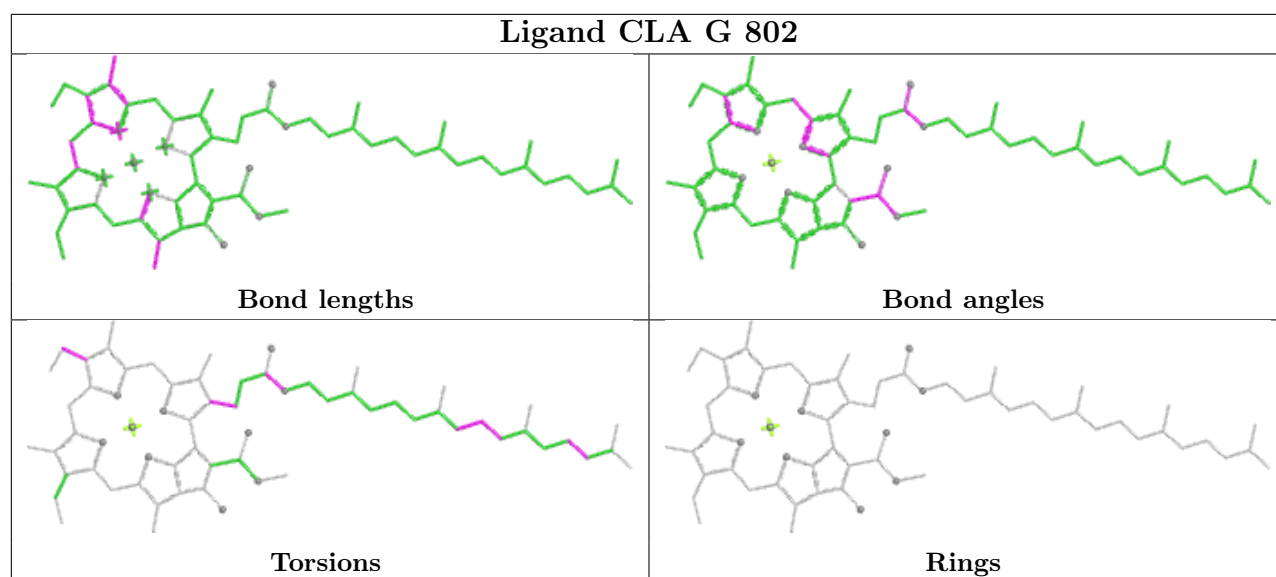
Bond angles

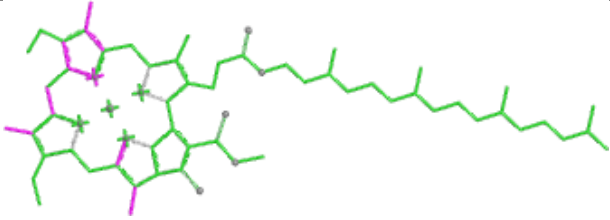
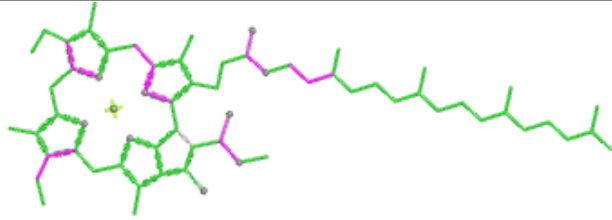
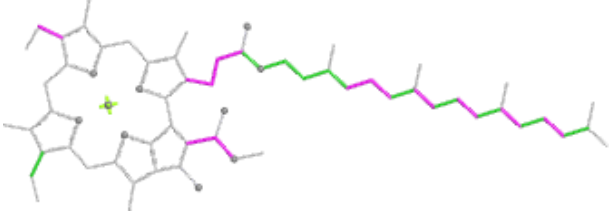
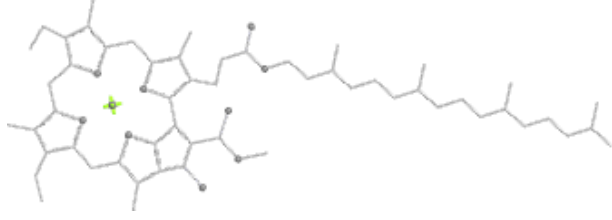
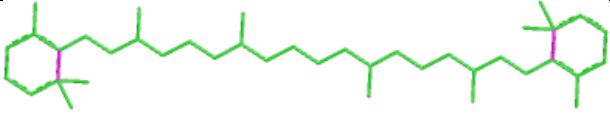
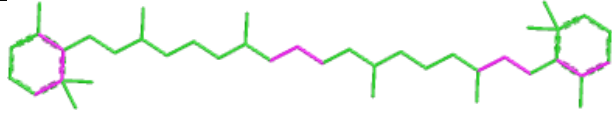
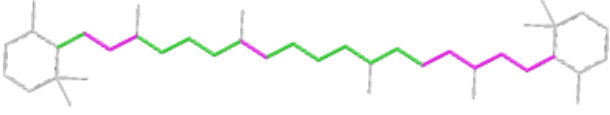
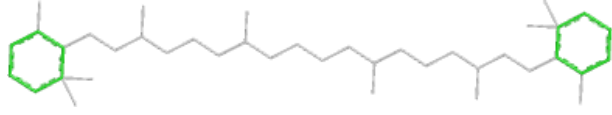
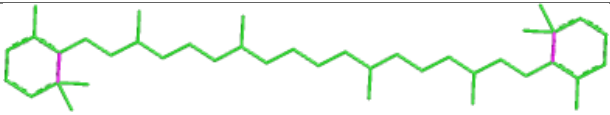
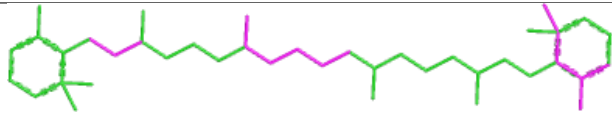
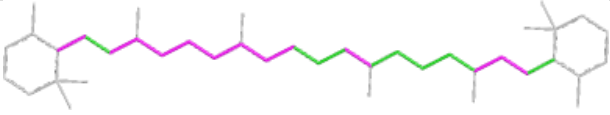
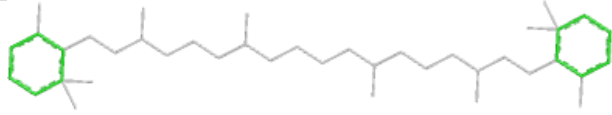


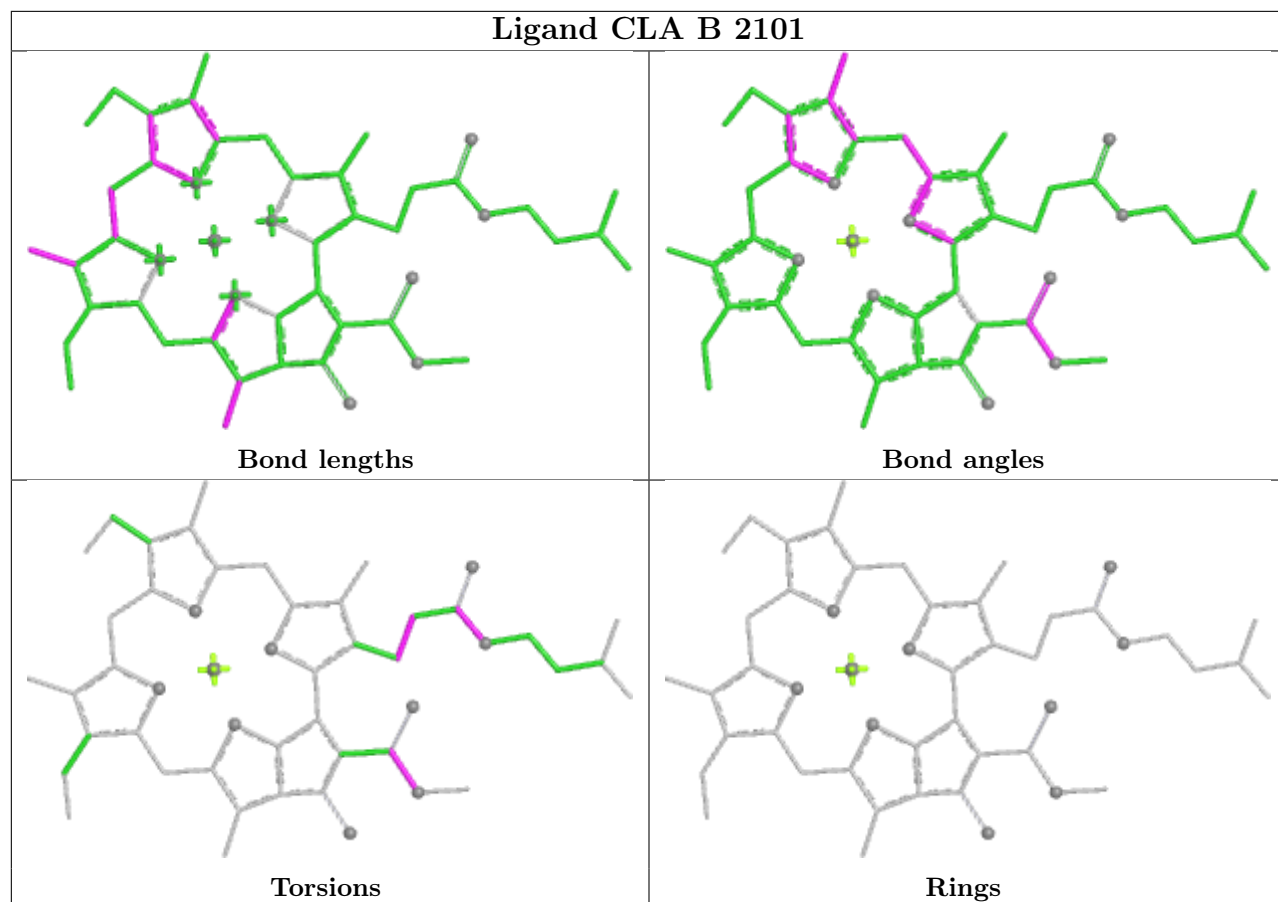
Torsions



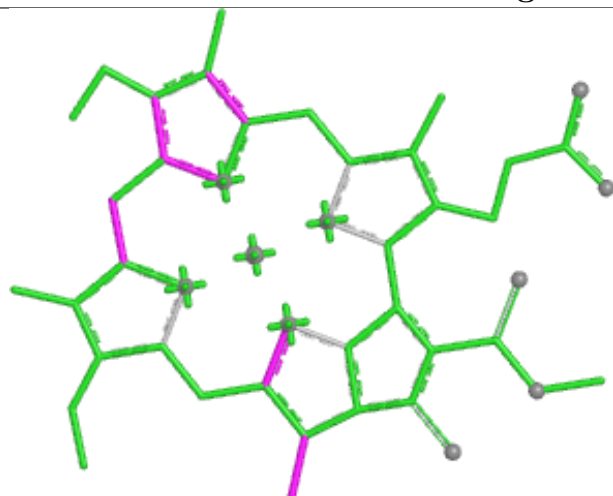
Rings



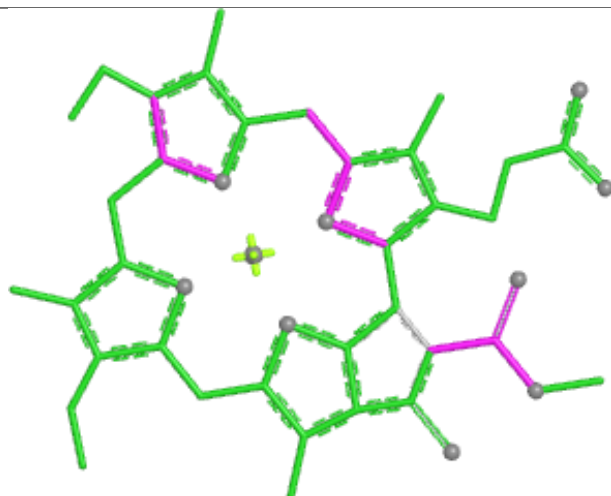
Ligand CLA b 2114	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR Q 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR a 843	
 Bond lengths	 Bond angles
 Torsions	 Rings



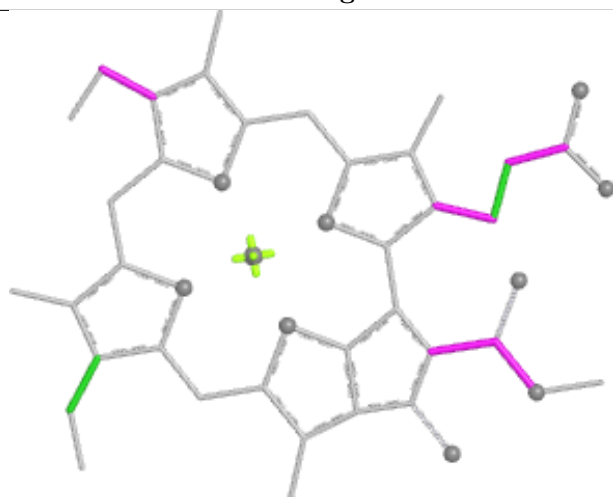
Ligand CLA S 103



Bond lengths



Bond angles

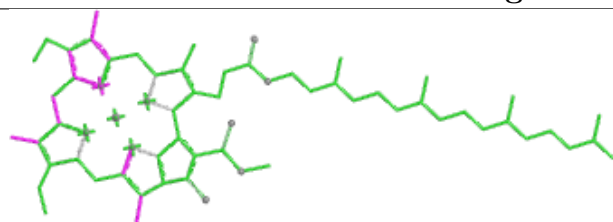


Torsions

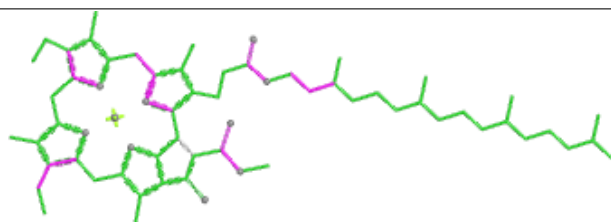


Rings

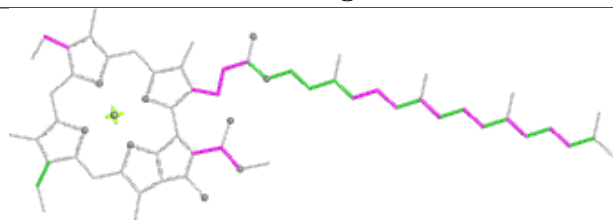
Ligand CLA B 2115



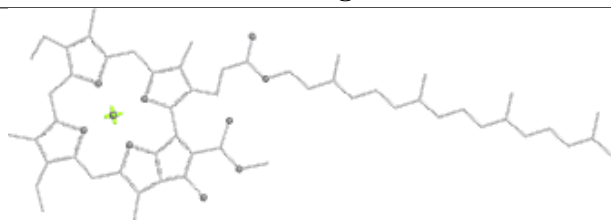
Bond lengths



Bond angles

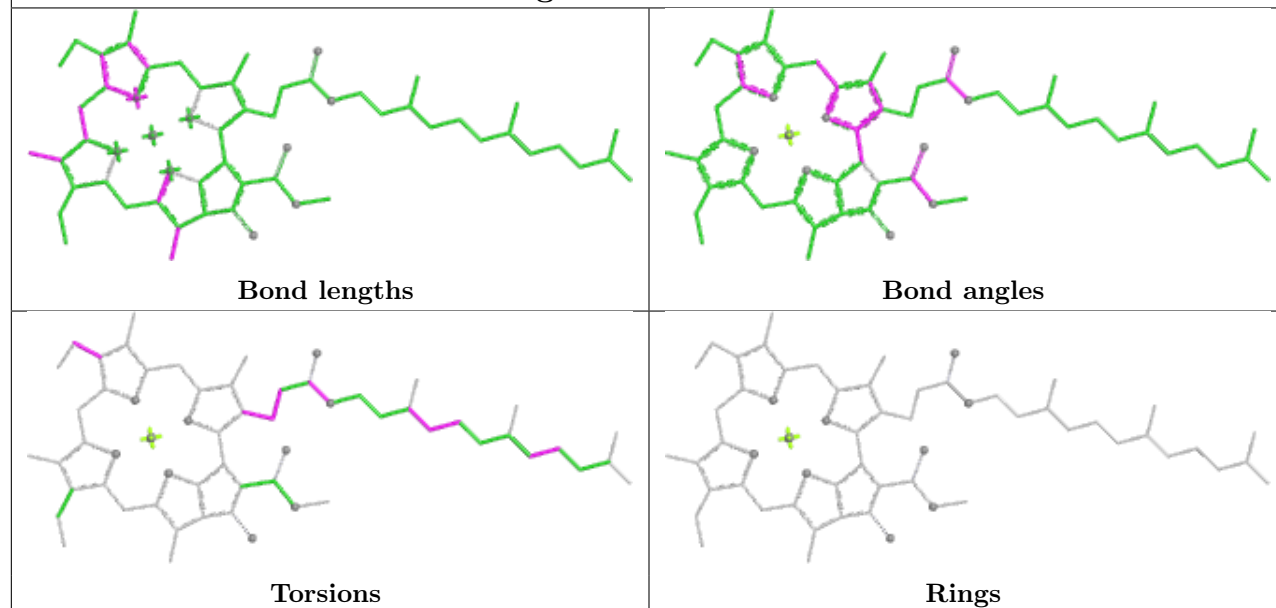


Torsions

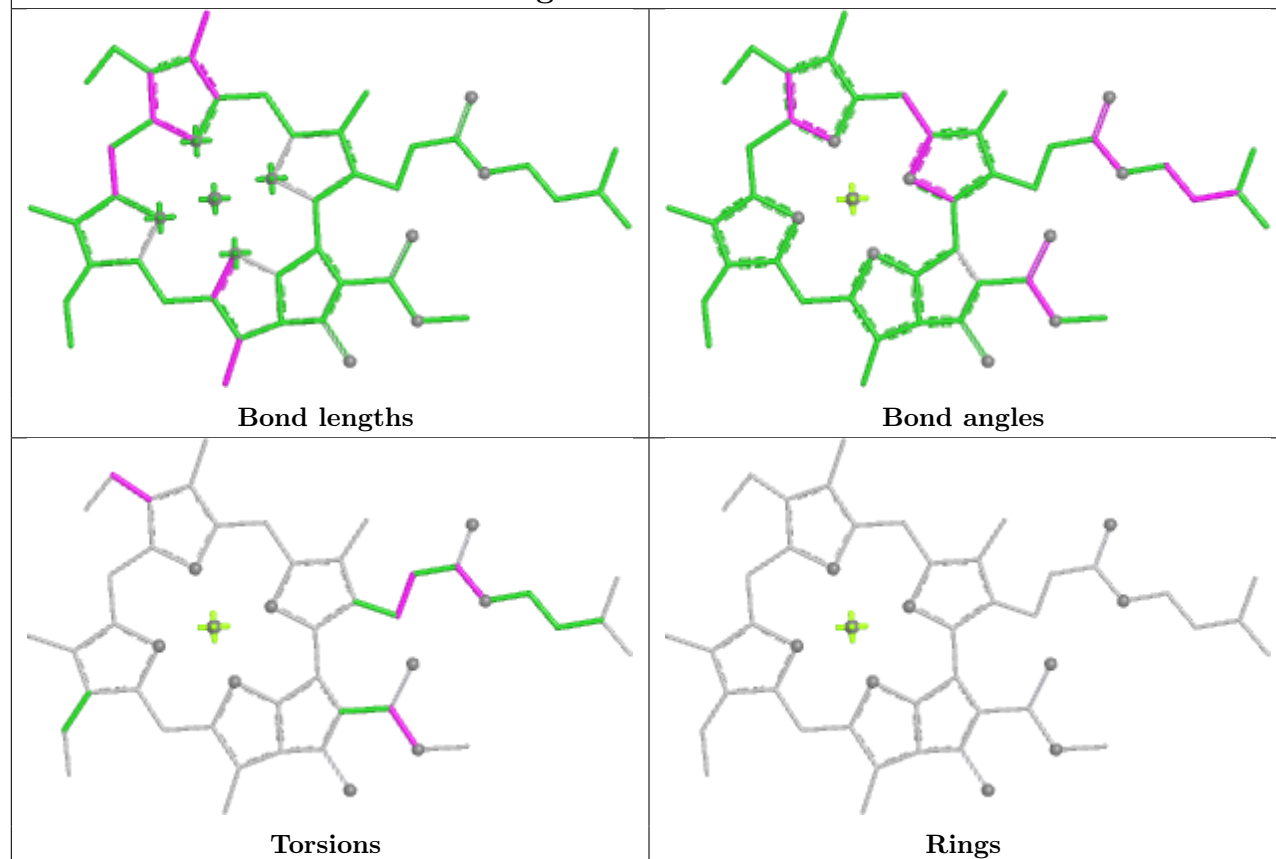


Rings

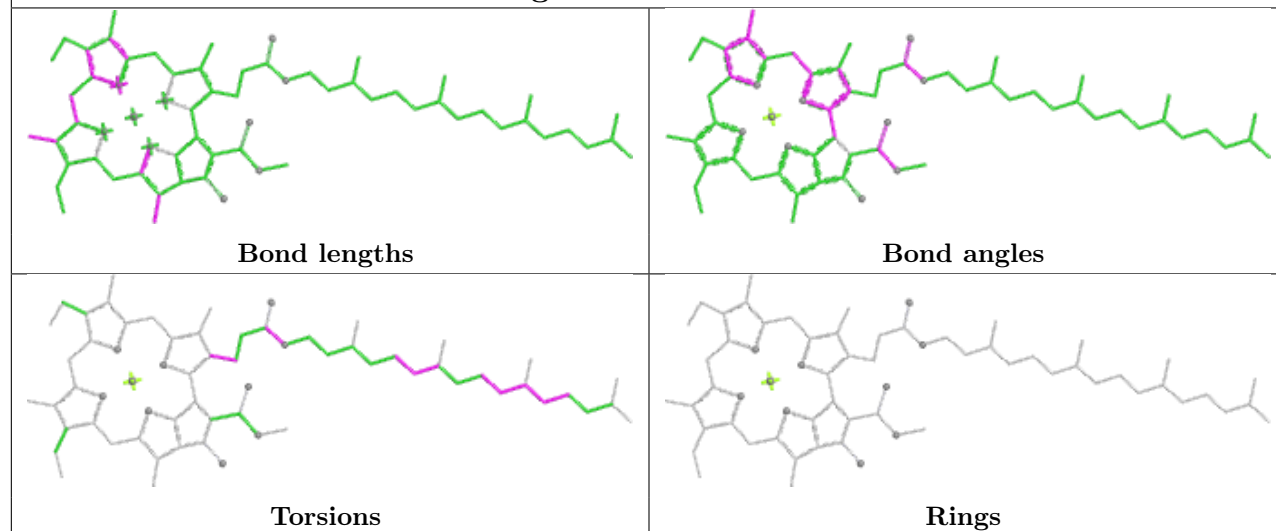
Ligand CLA a 823



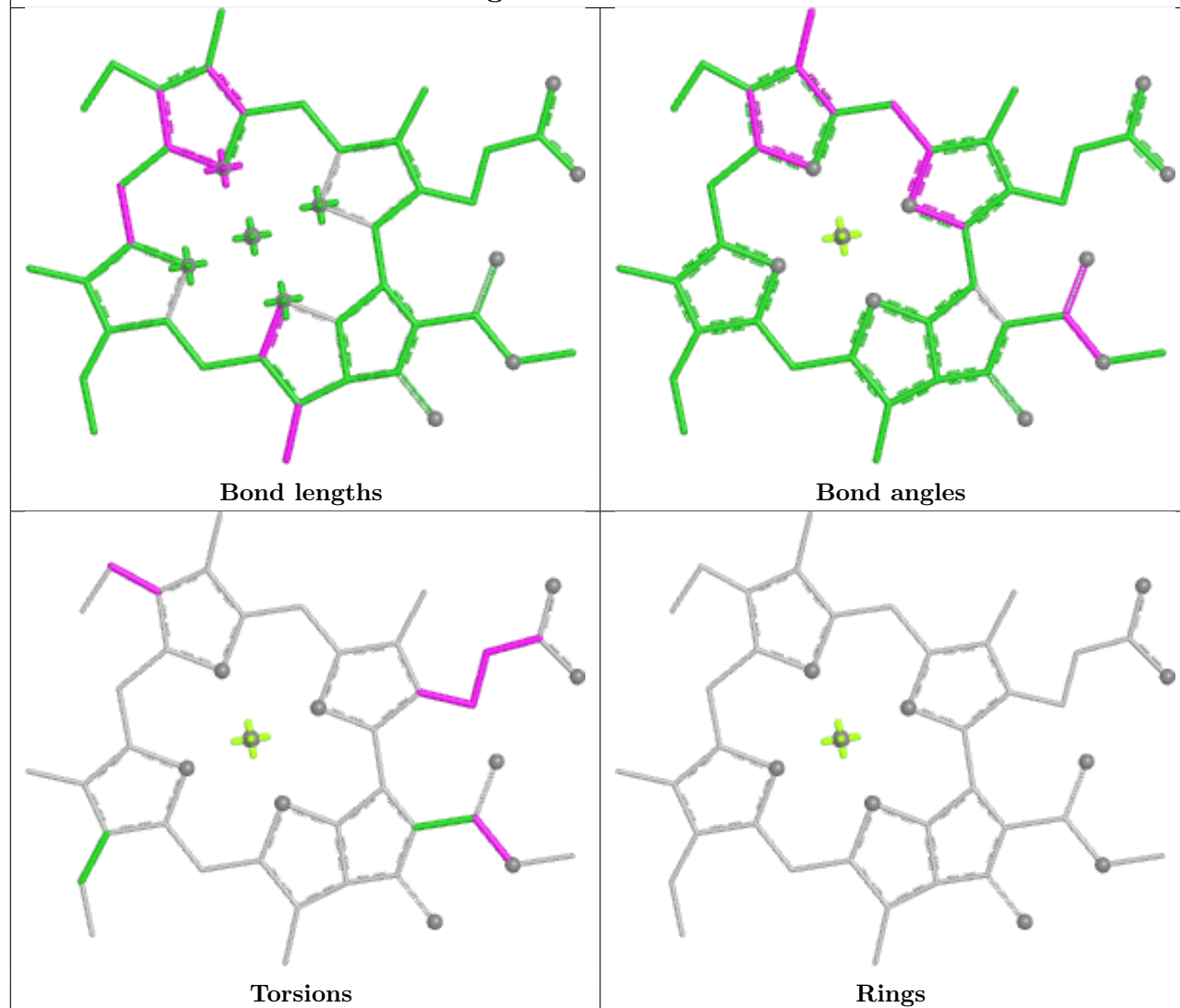
Ligand CLA a 806



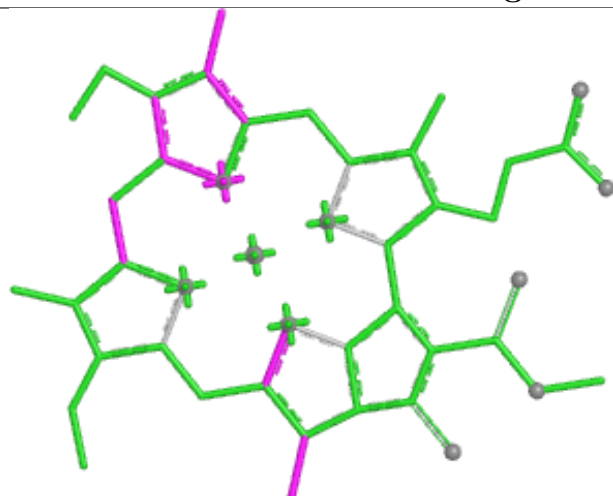
Ligand CLA U 203



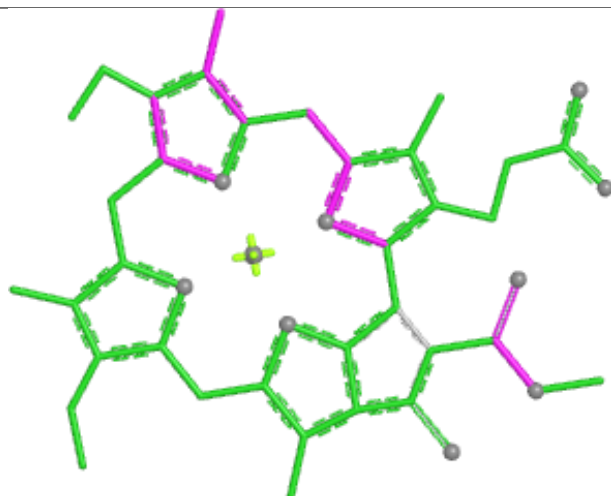
Ligand CLA b 2116



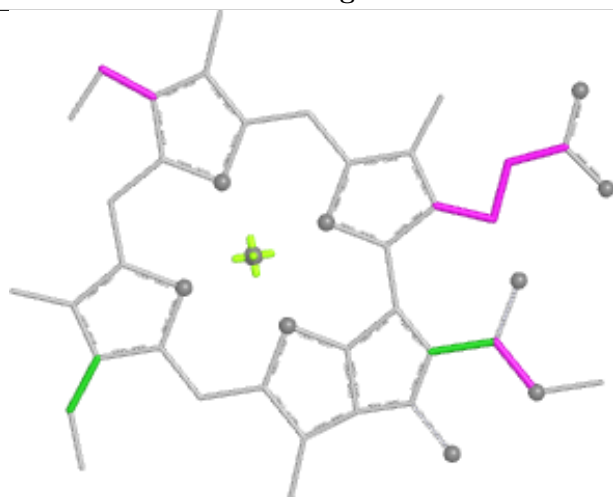
Ligand CLA H 2135



Bond lengths



Bond angles

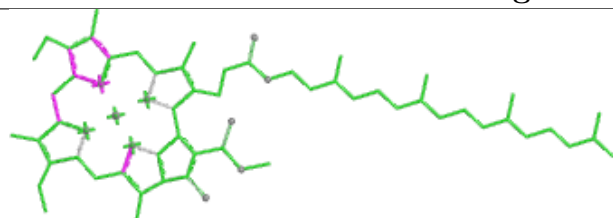


Torsions

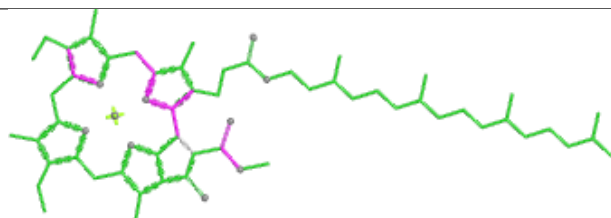


Rings

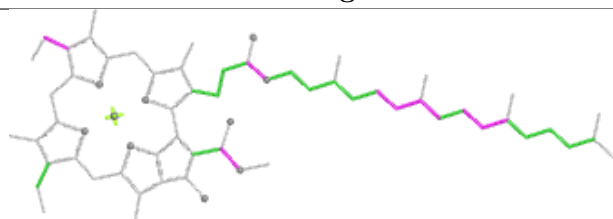
Ligand CLA G 813



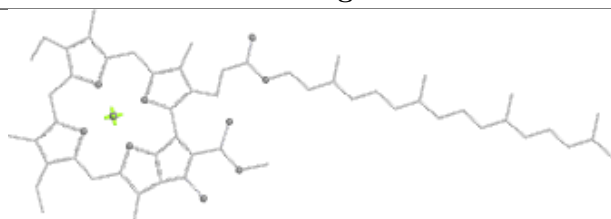
Bond lengths



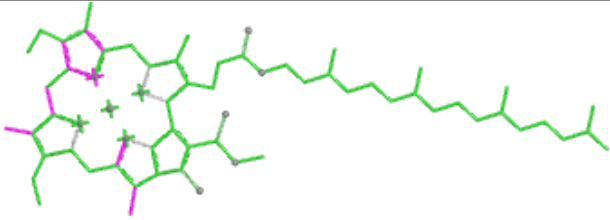
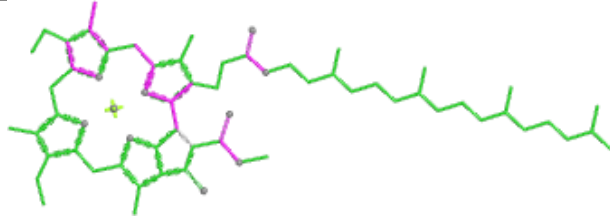
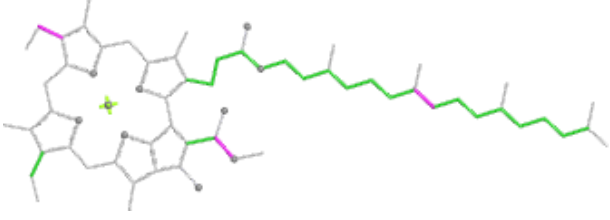
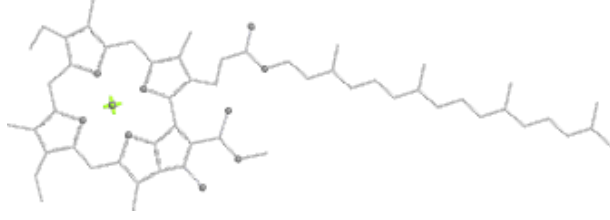
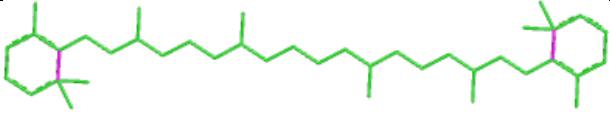
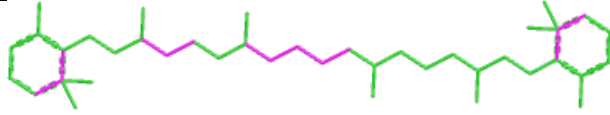
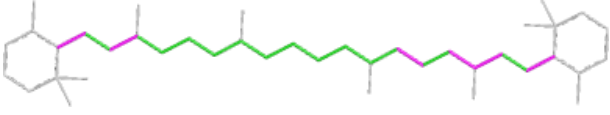
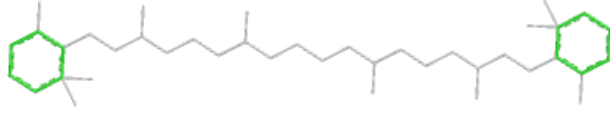
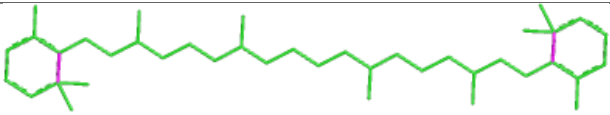
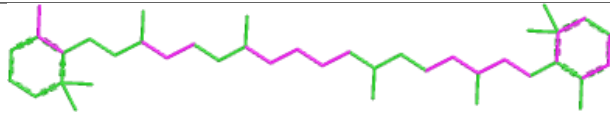
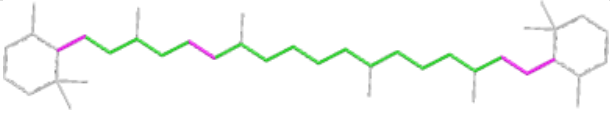
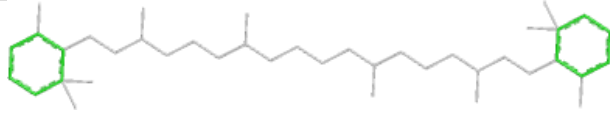
Bond angles

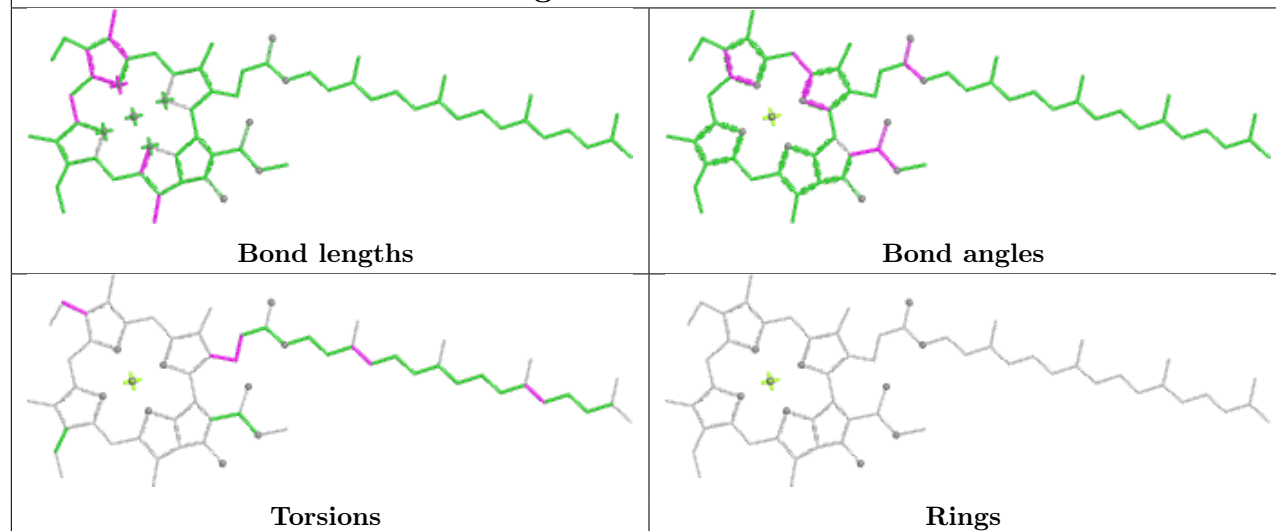
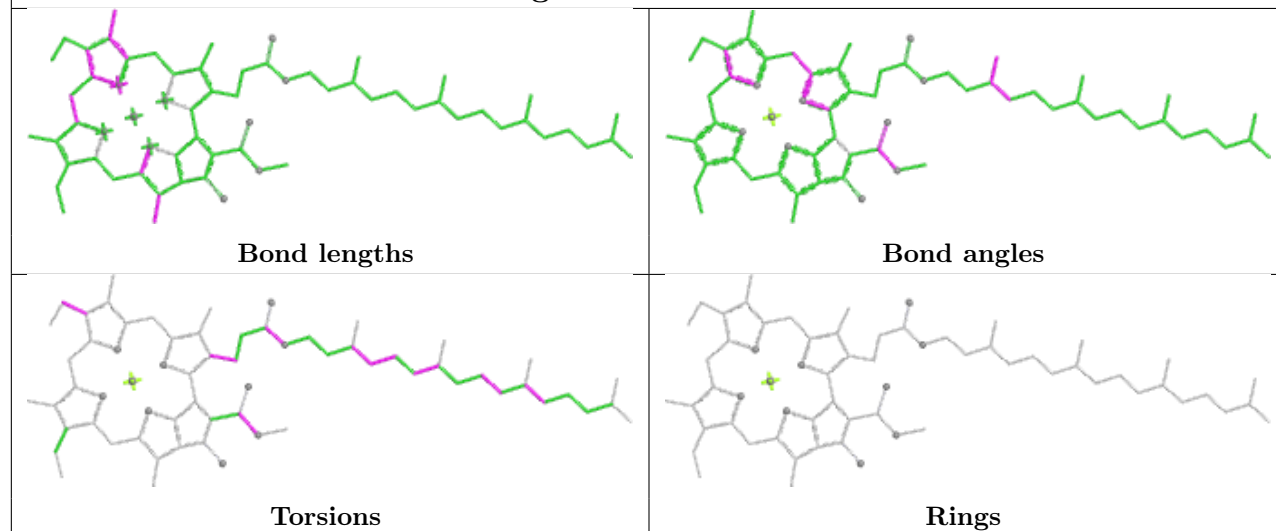
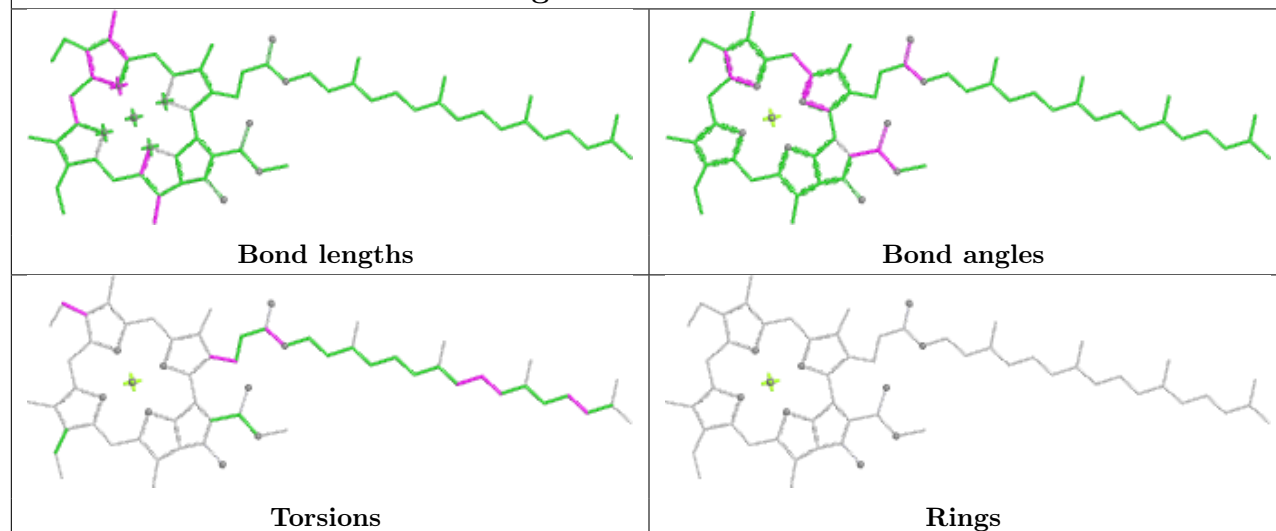


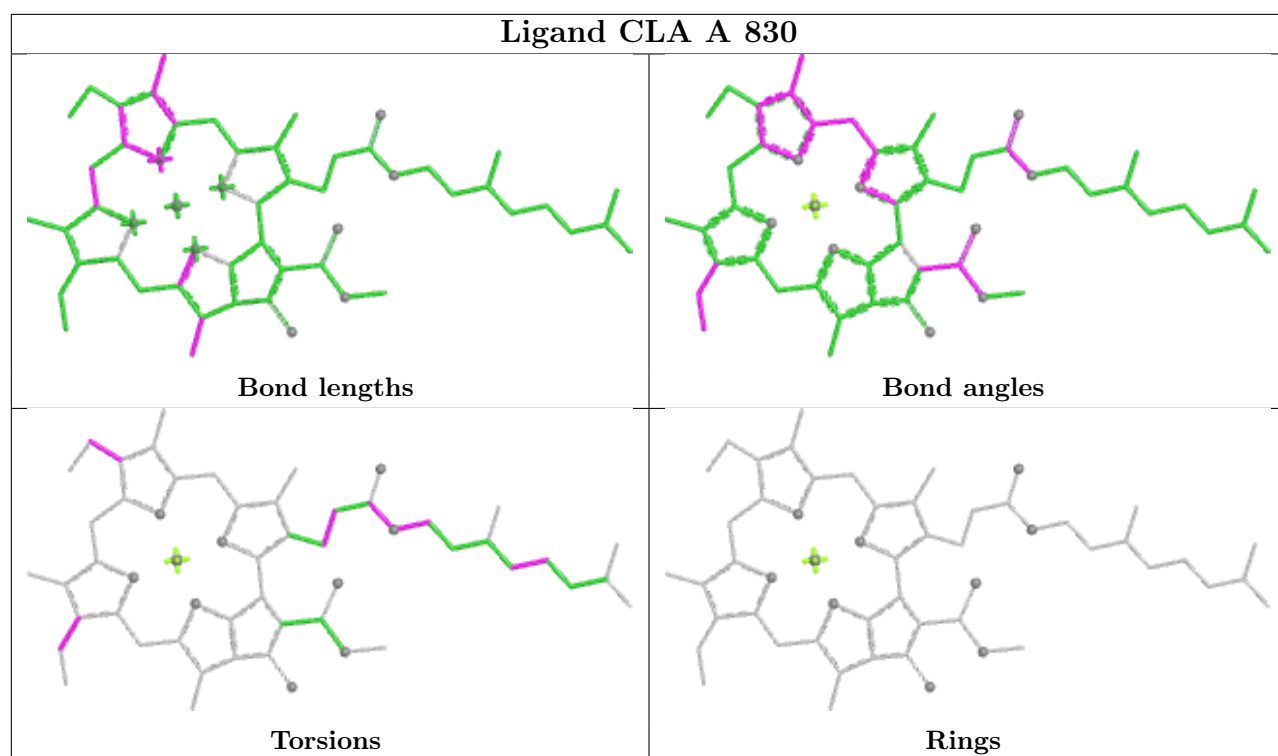
Torsions



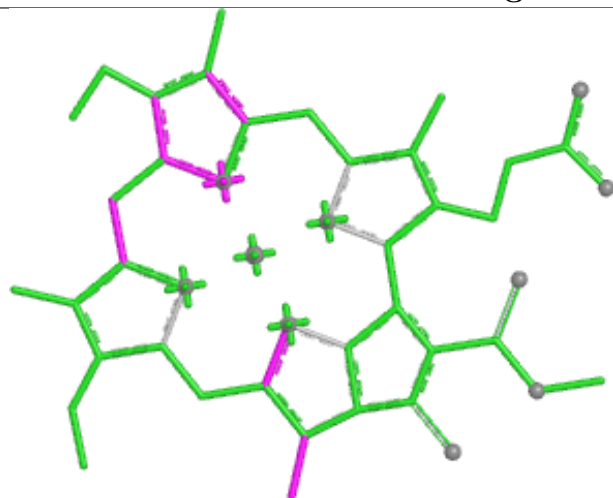
Rings

Ligand CLA G 838	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR L 206	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR U 207	
 Bond lengths	 Bond angles
 Torsions	 Rings

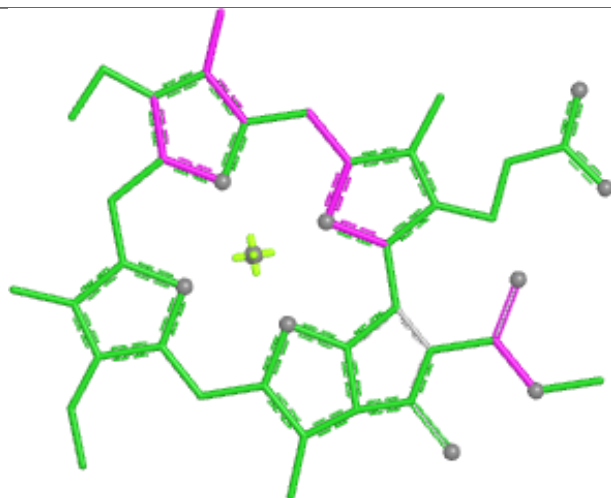
Ligand CLA L 204**Ligand CLA A 833****Ligand CLA A 802**



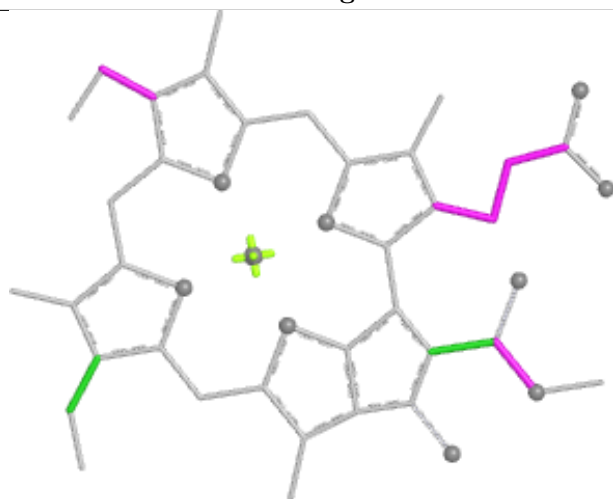
Ligand CLA B 2117



Bond lengths



Bond angles

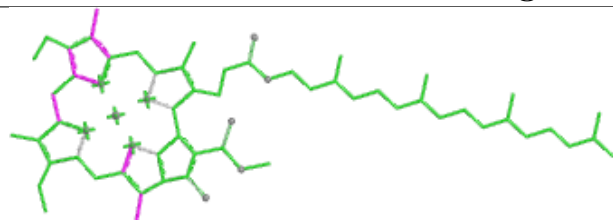


Torsions

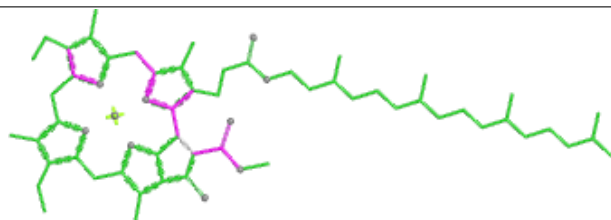


Rings

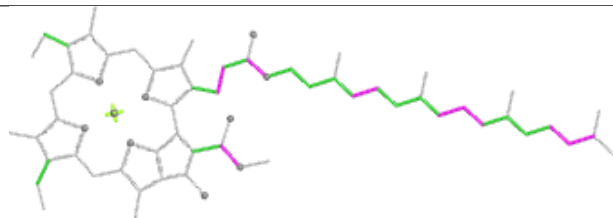
Ligand CLA a 837



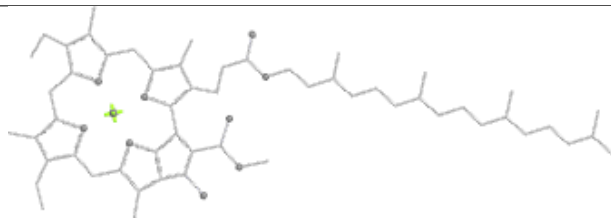
Bond lengths



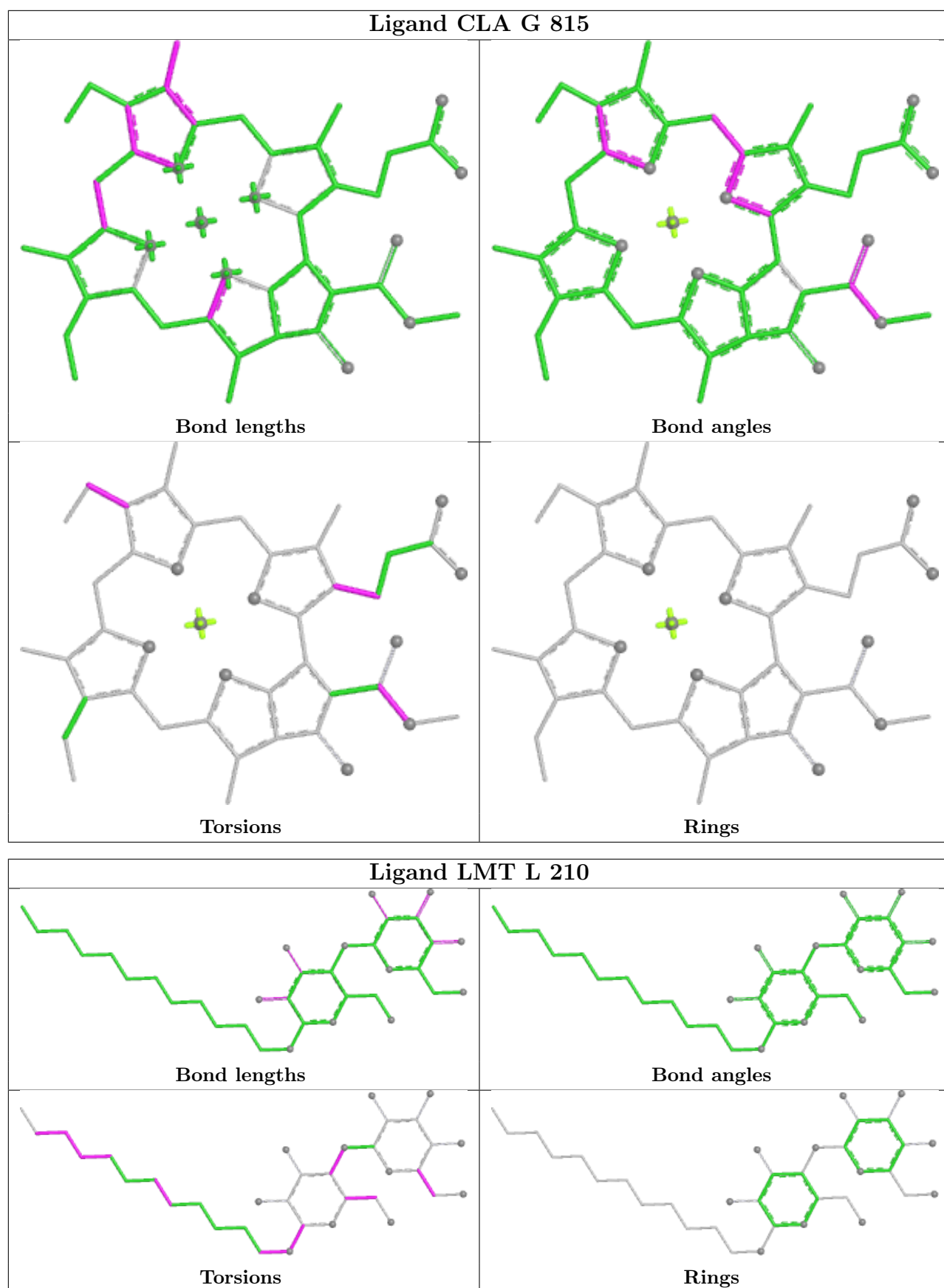
Bond angles



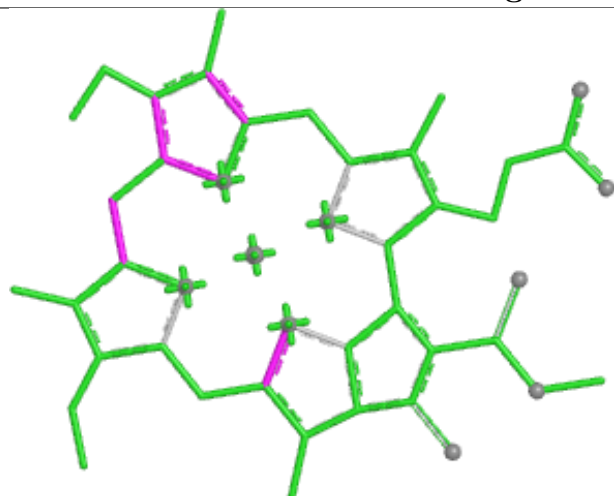
Torsions



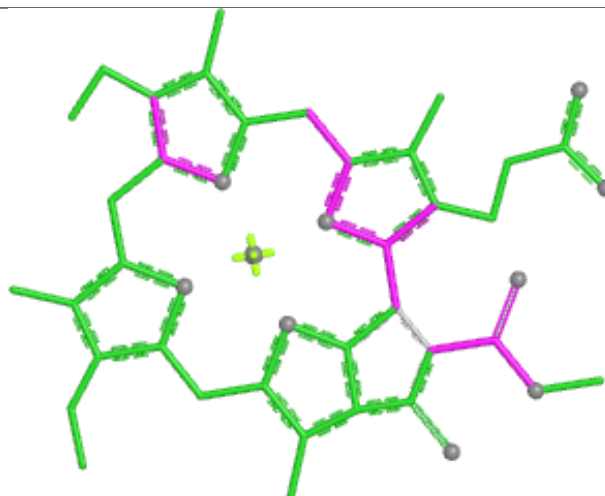
Rings



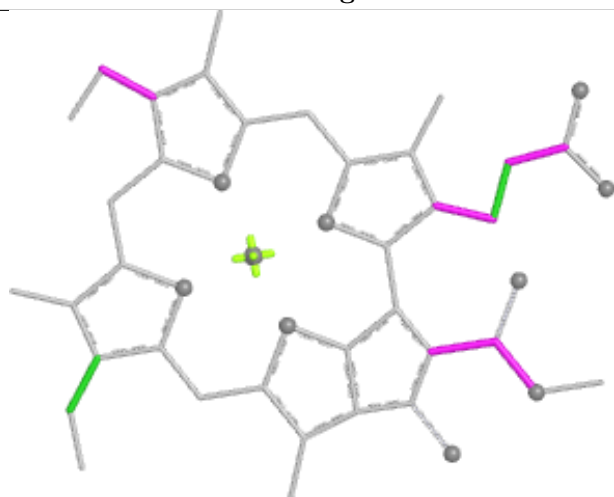
Ligand CLA B 2118



Bond lengths



Bond angles

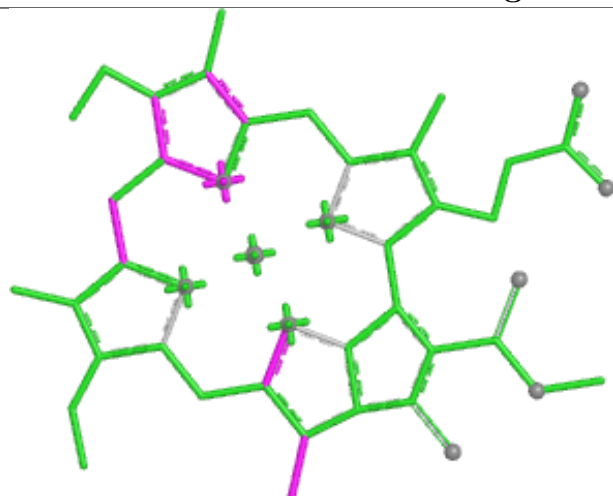


Torsions

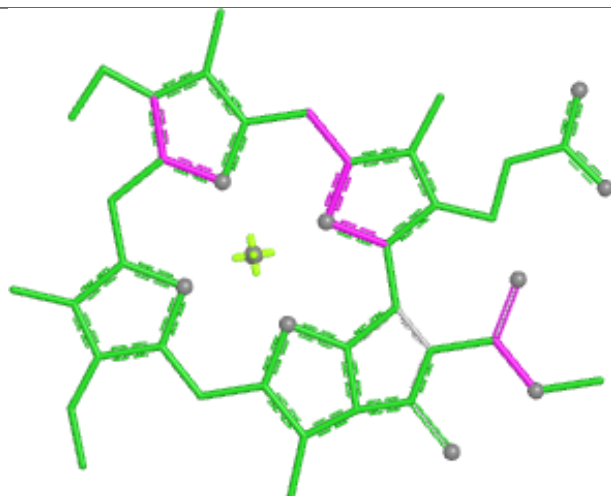


Rings

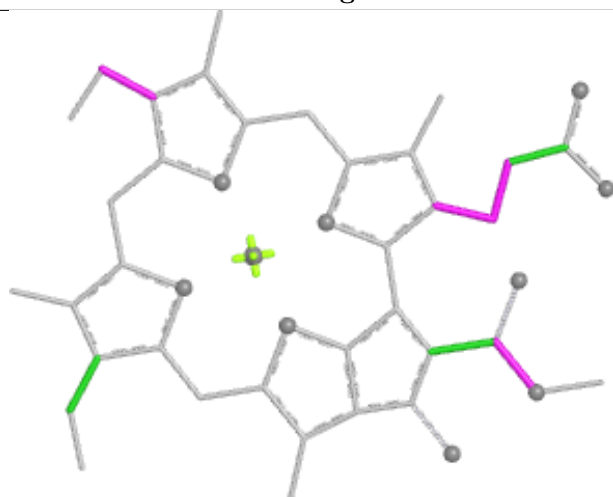
Ligand CLA H 2122



Bond lengths



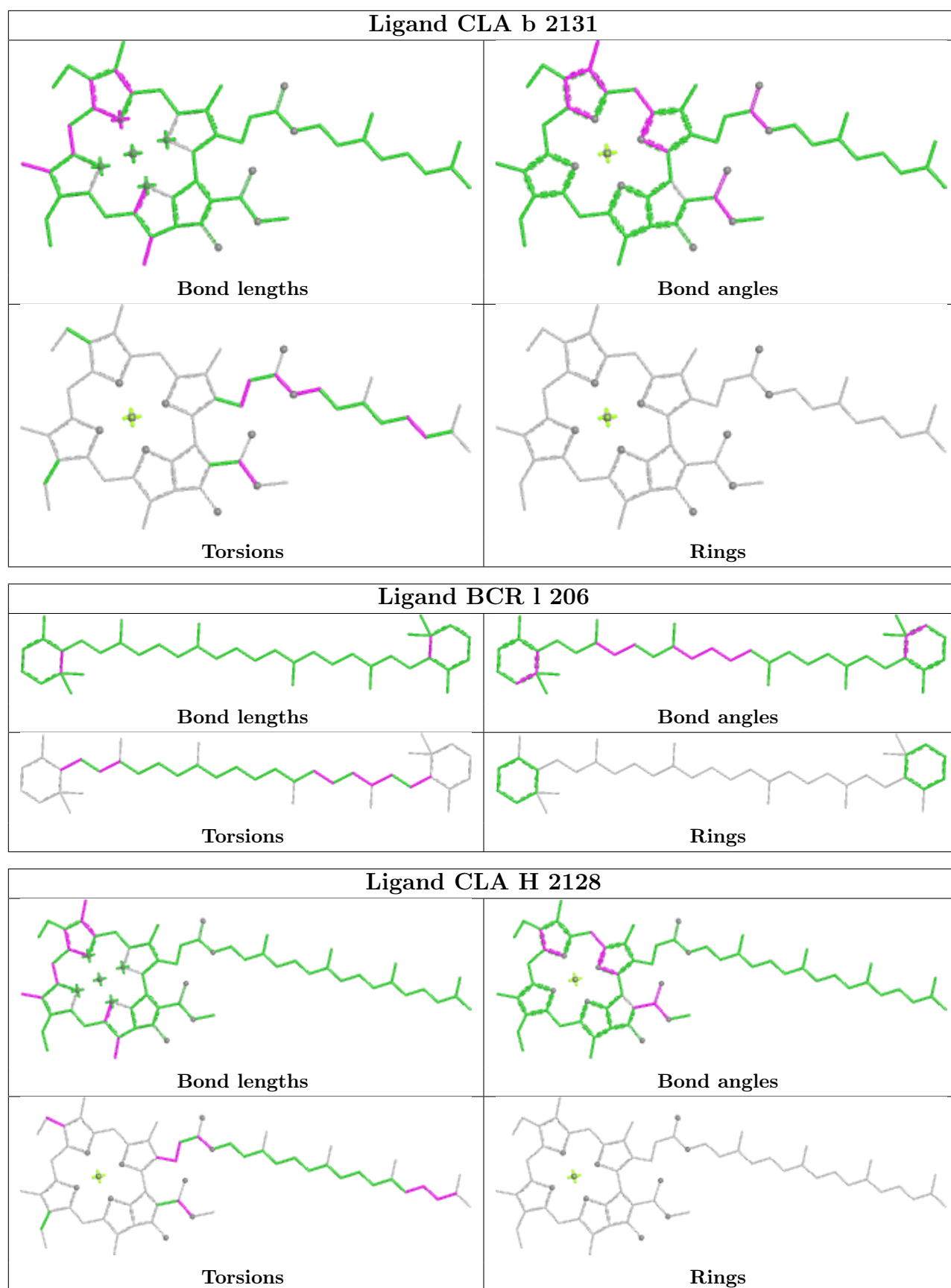
Bond angles

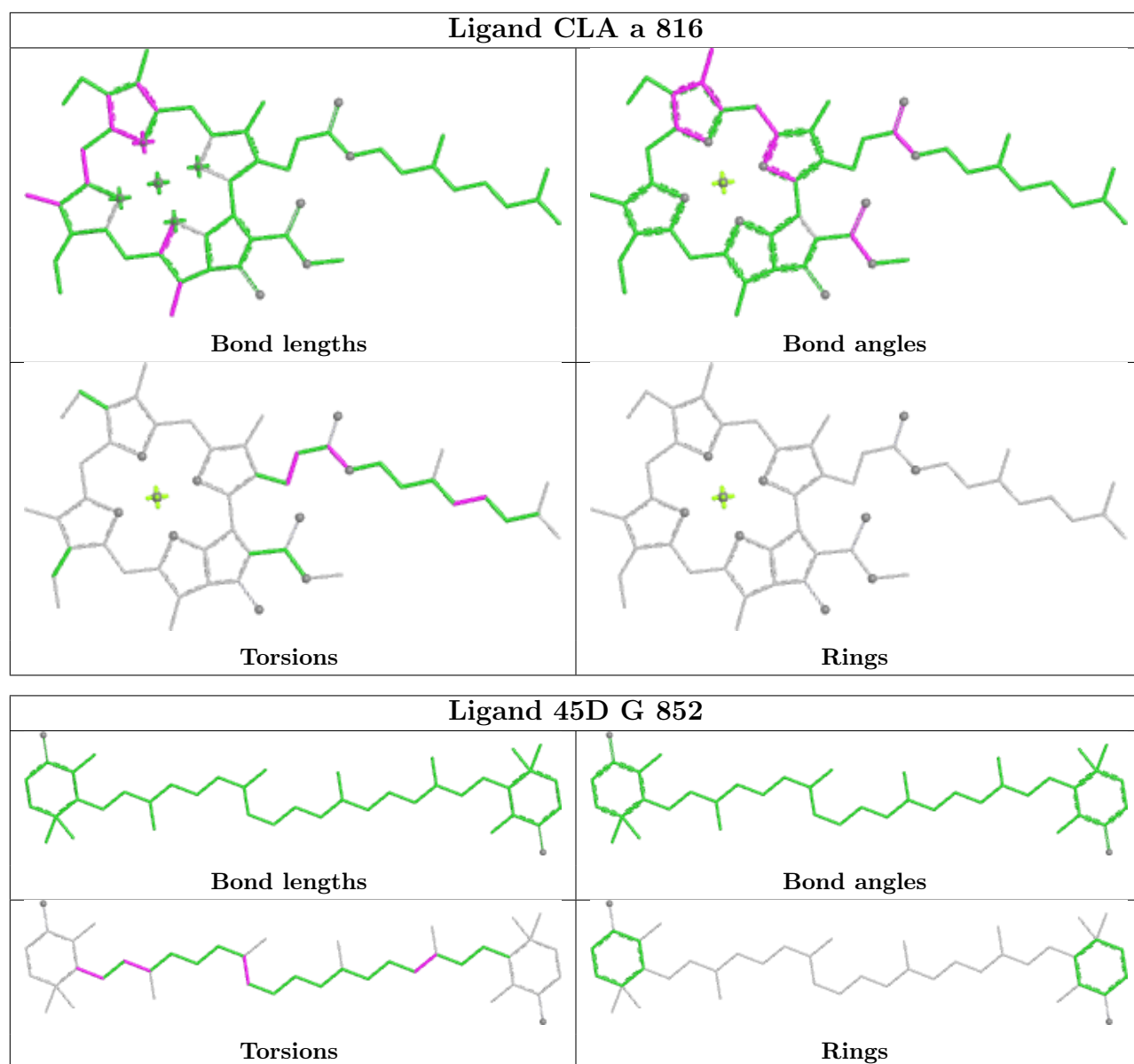


Torsions

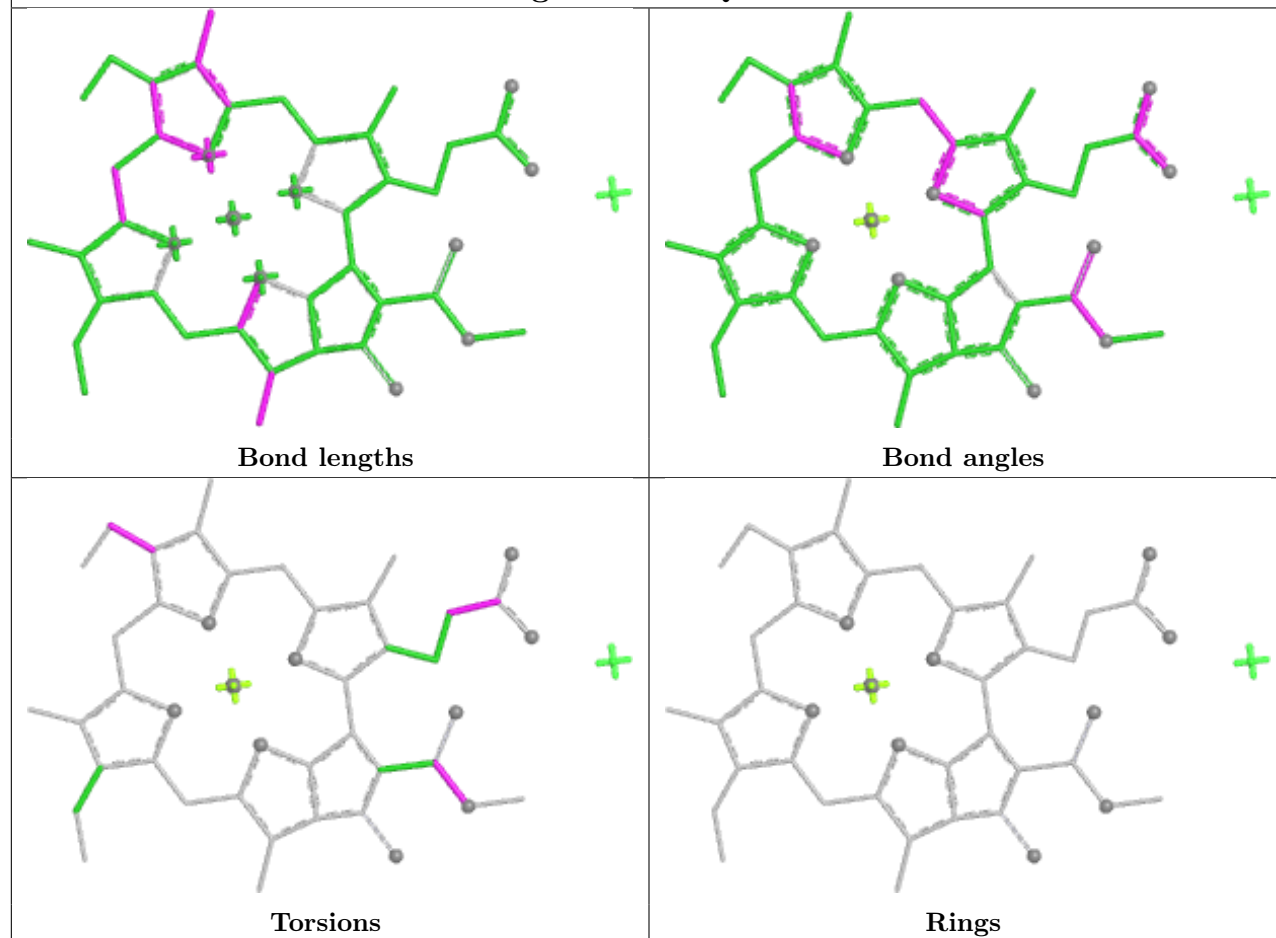


Rings

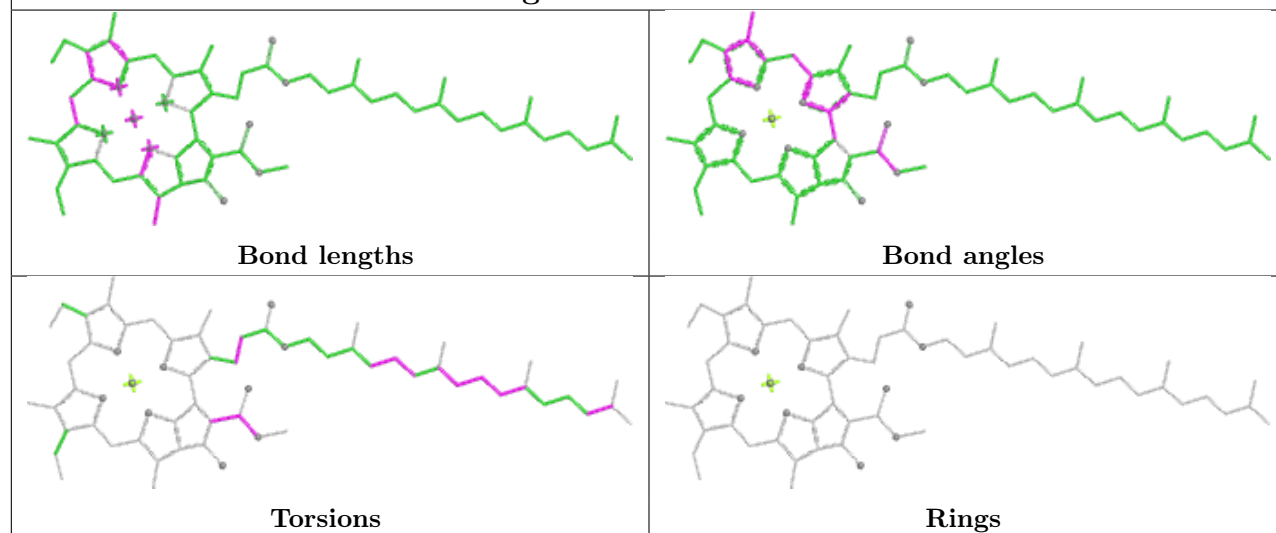


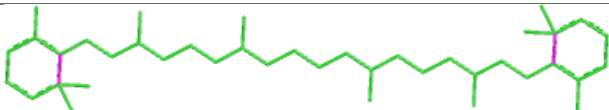
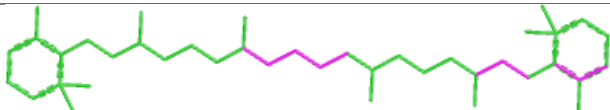
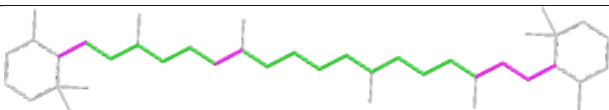
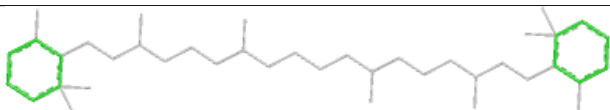


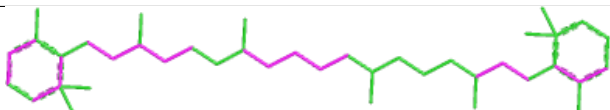
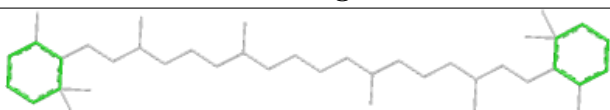
Ligand CLA Q 203

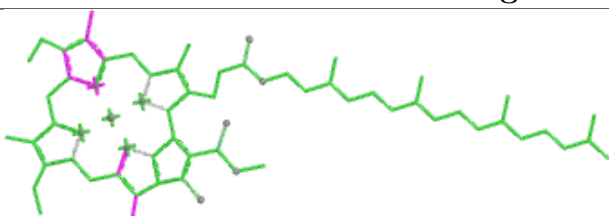
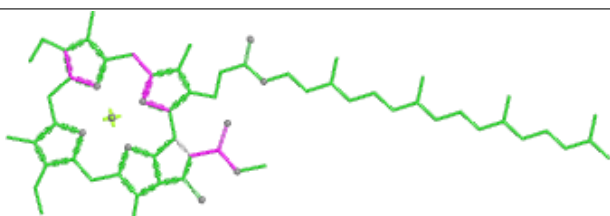
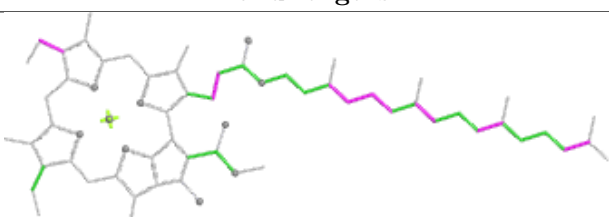
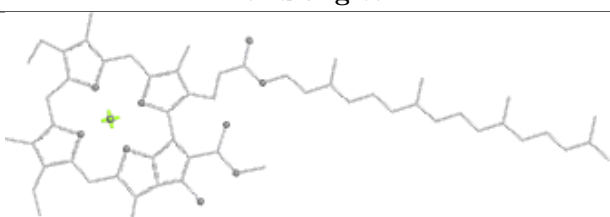


Ligand CLA H 2101

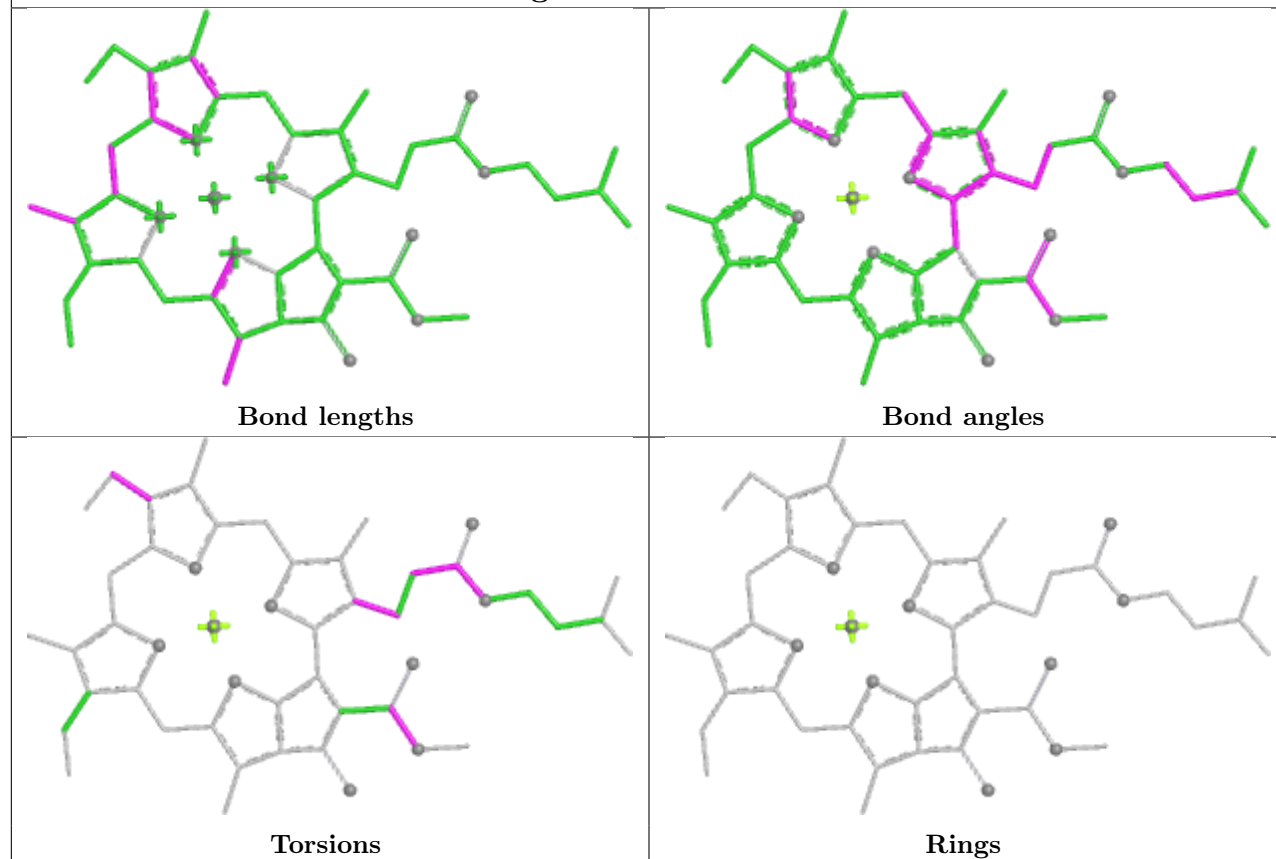


Ligand BCR A 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

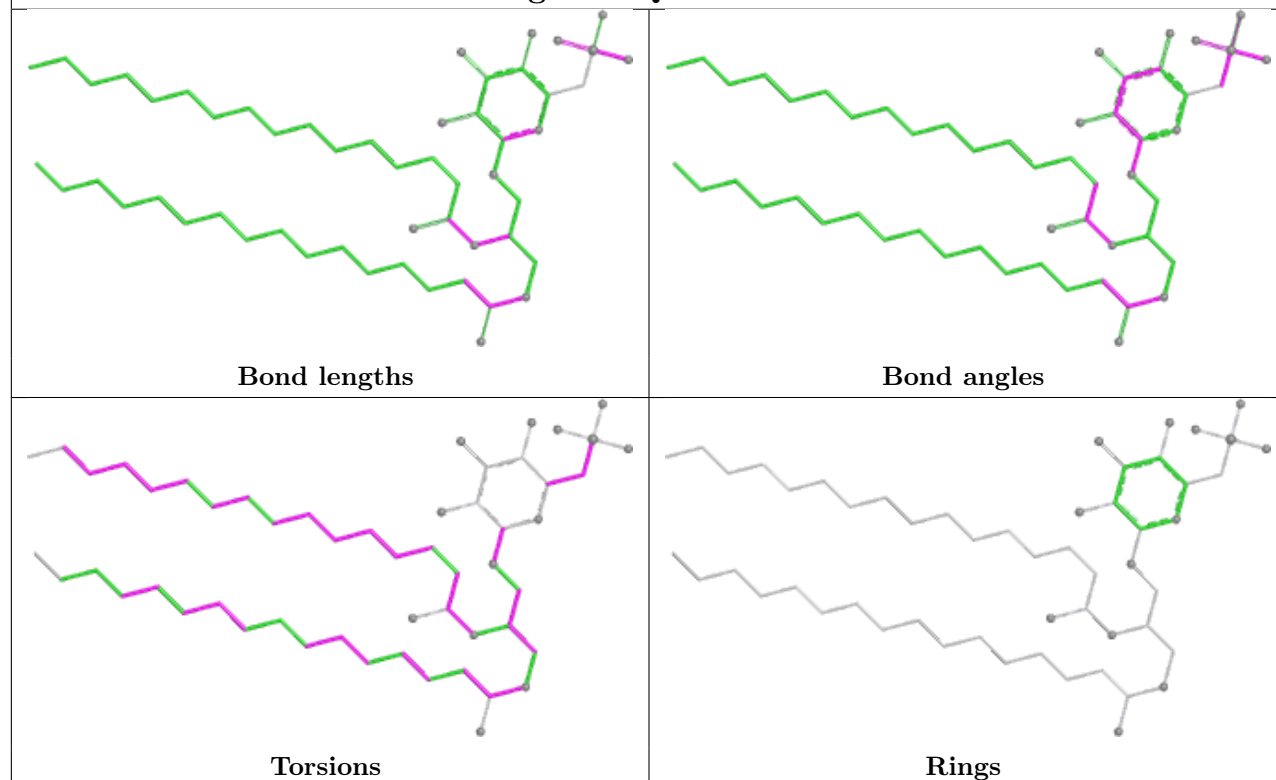
Ligand BCR J 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

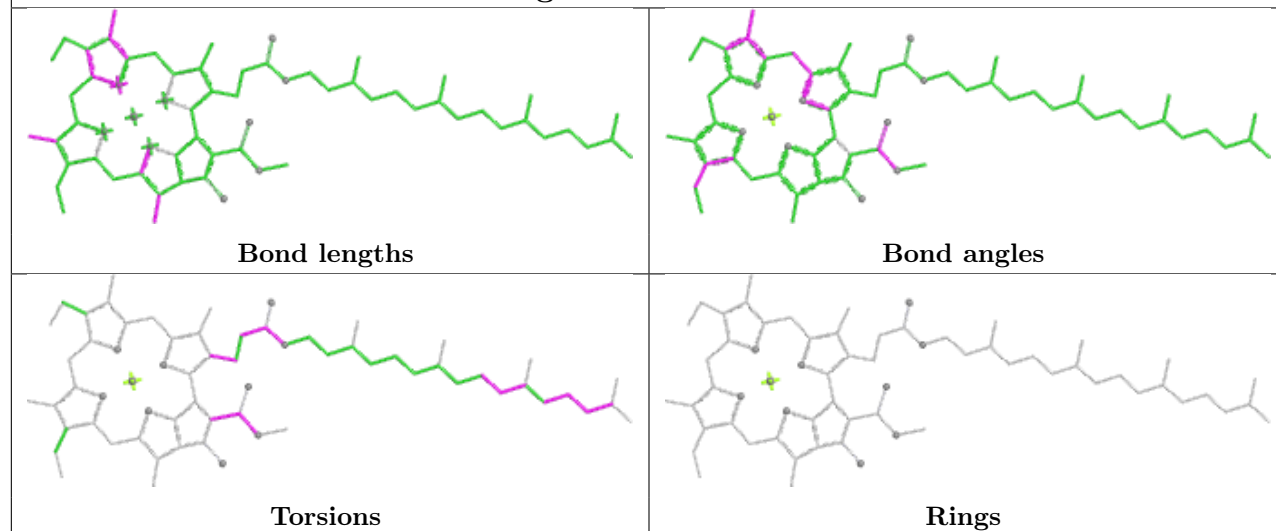
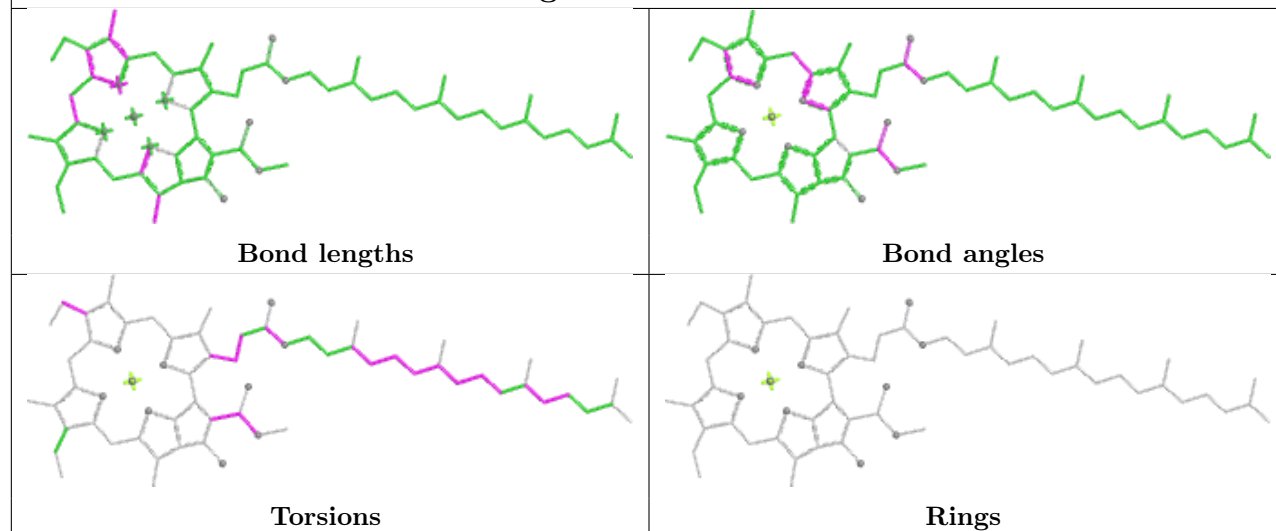
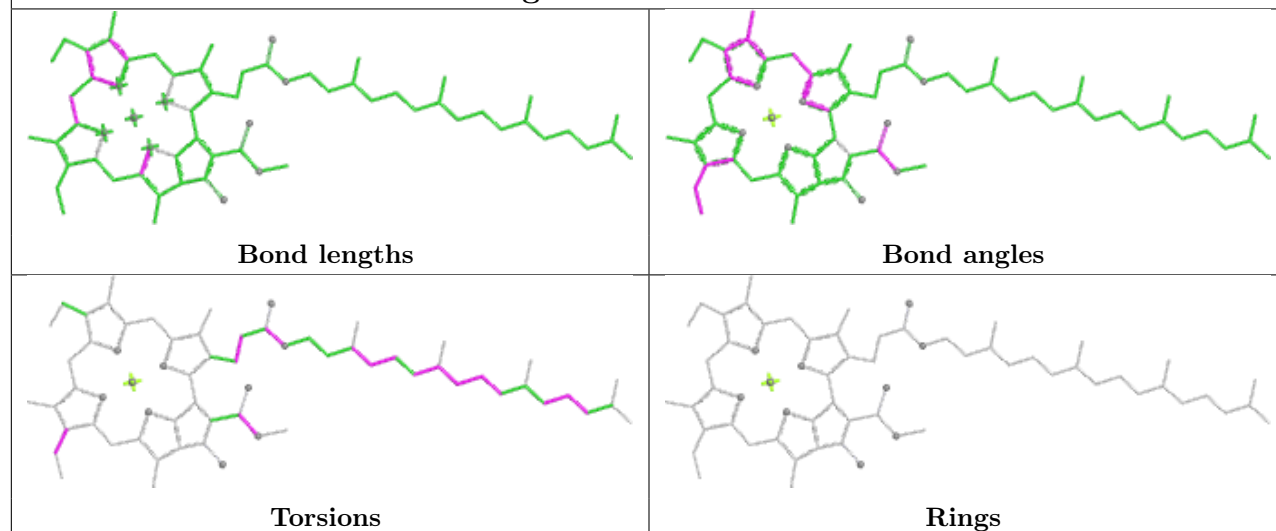
Ligand CLA B 2109	
	
Bond lengths	Bond angles
	
Torsions	Rings

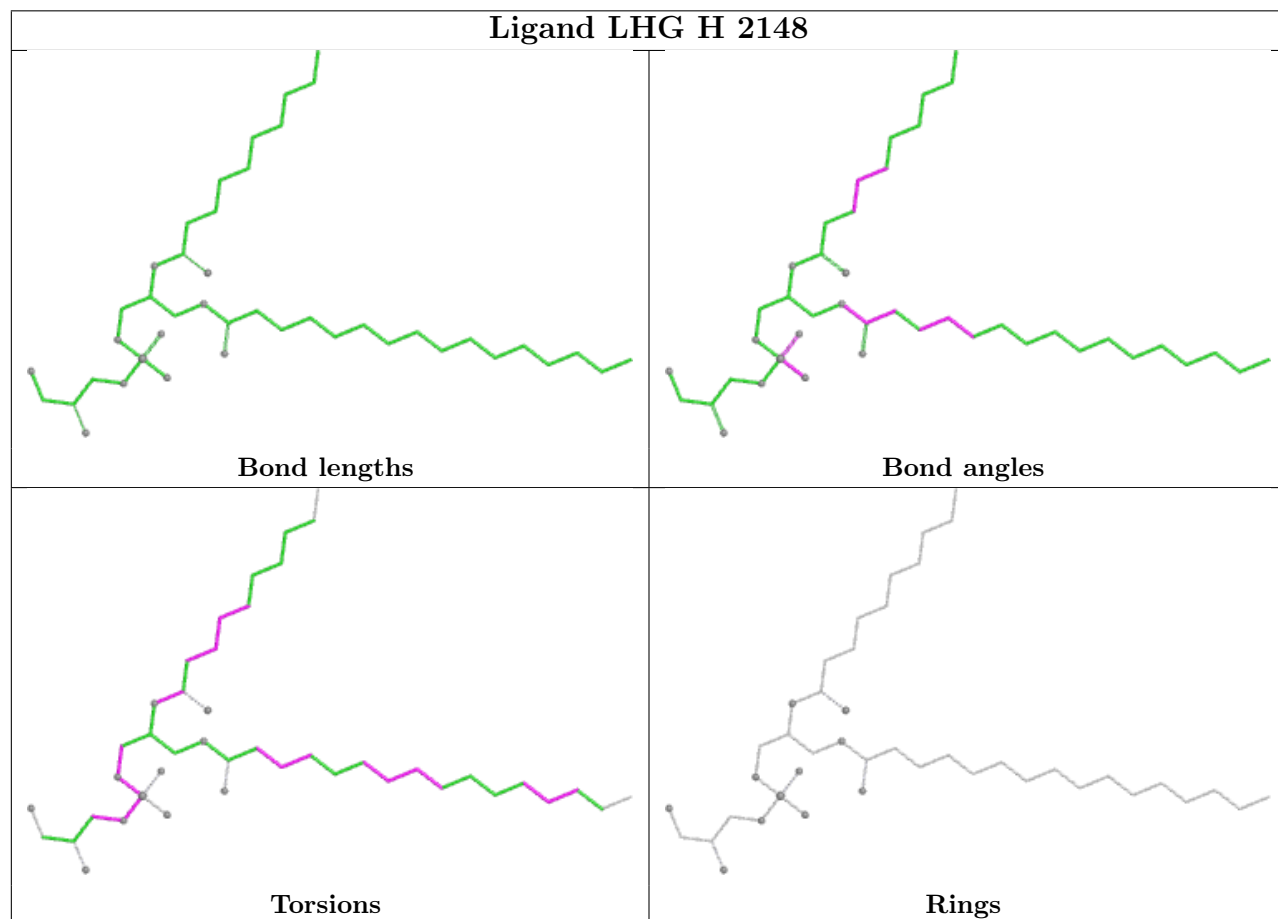
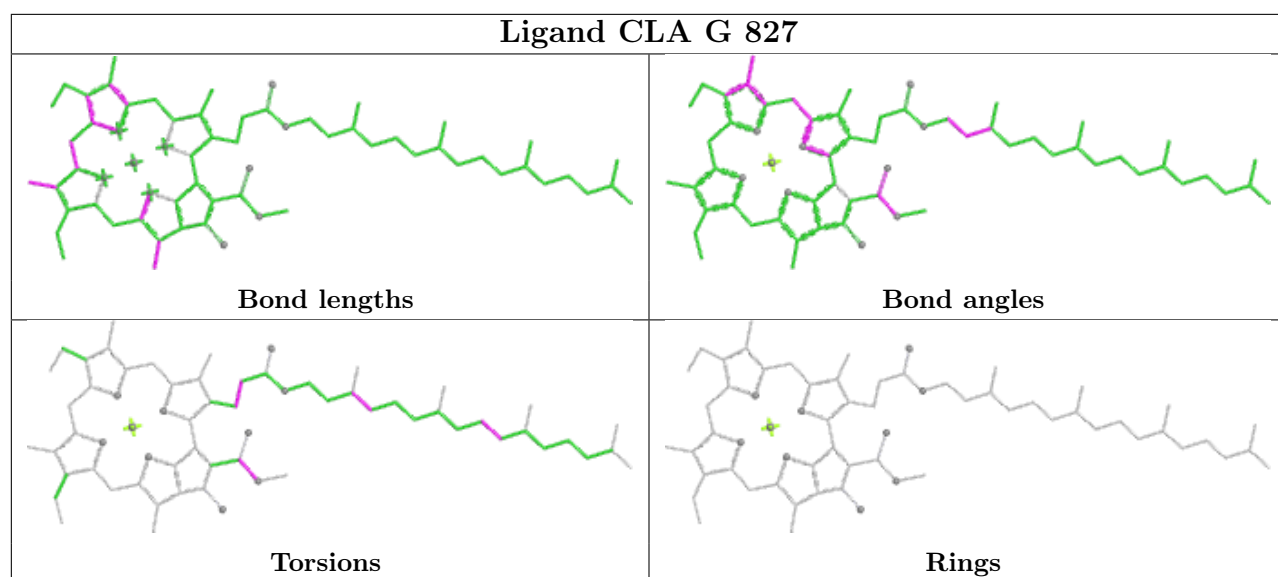
Ligand CLA G 809

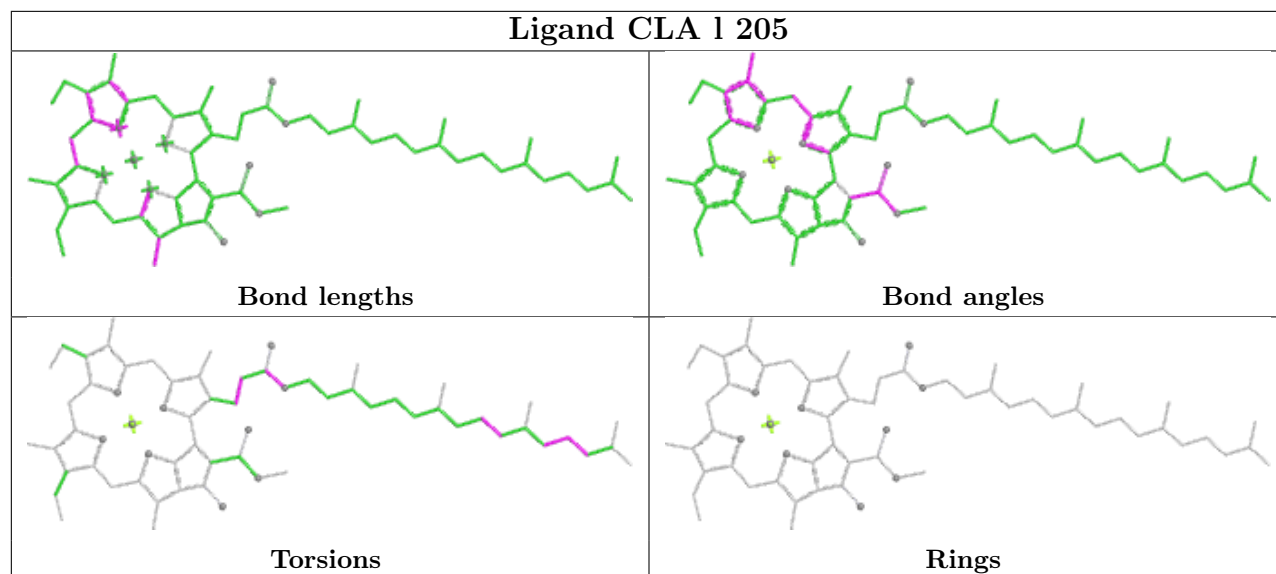
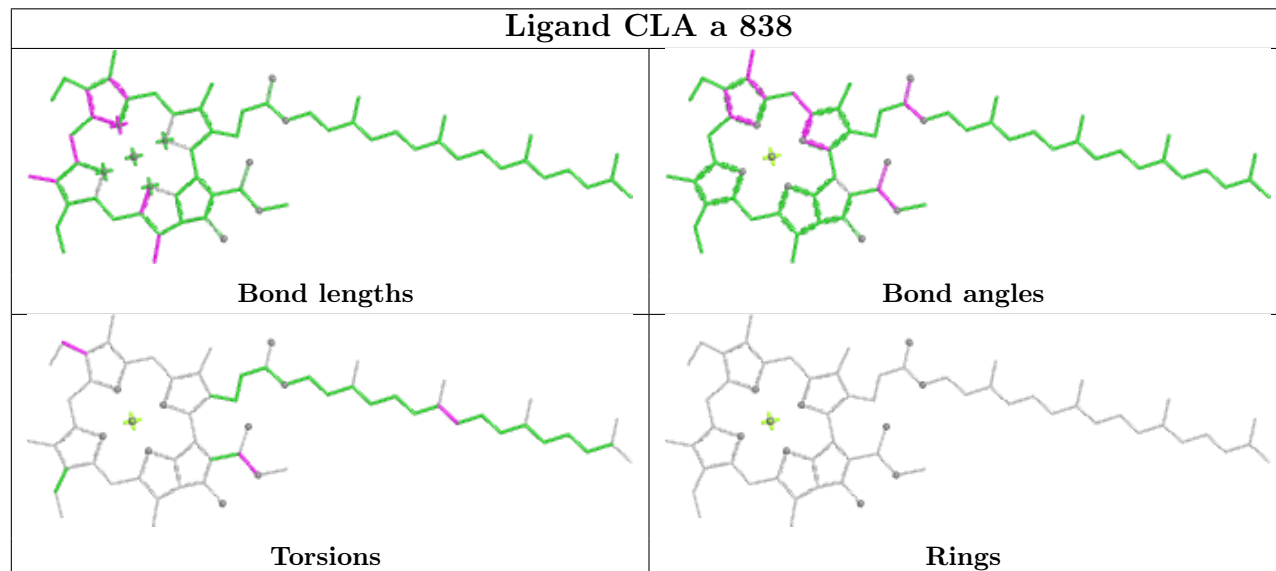
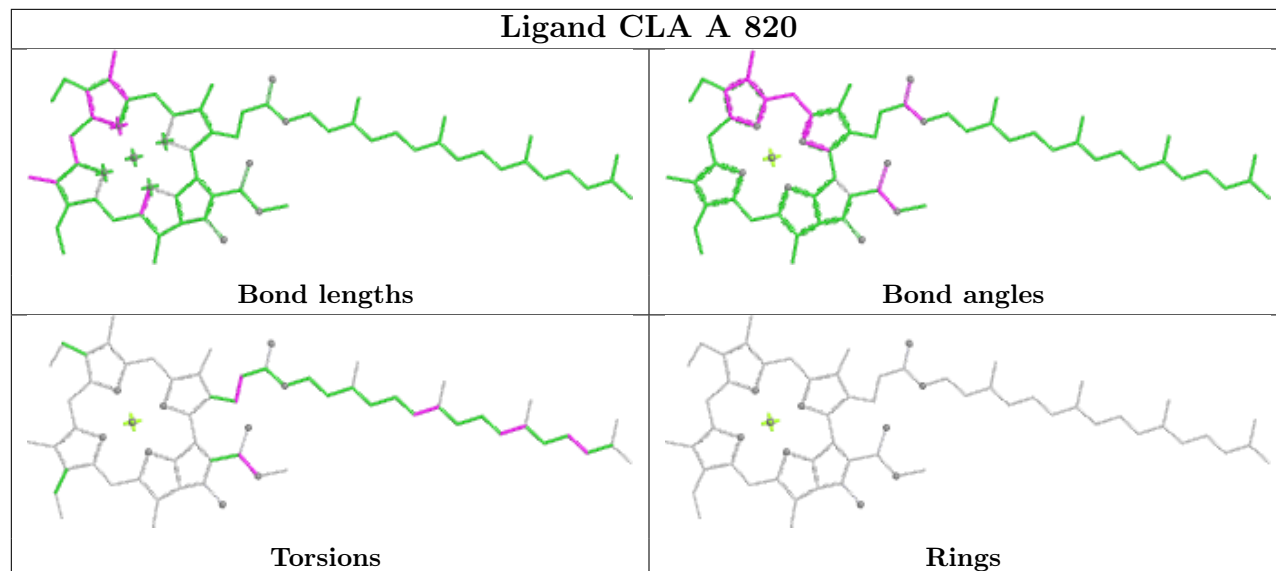


Ligand SQD M 101

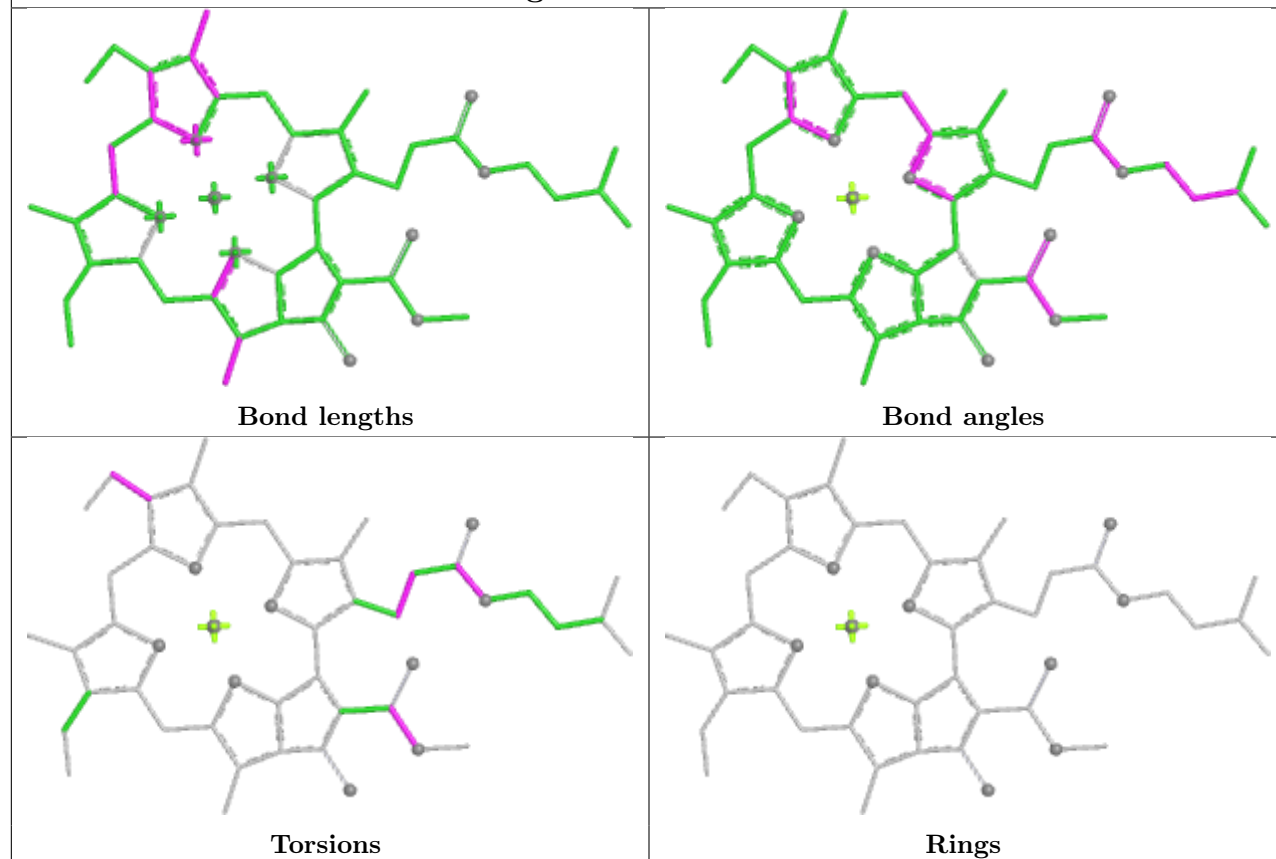


Ligand CLA a 804**Ligand CLA f 201****Ligand CLA H 2132**

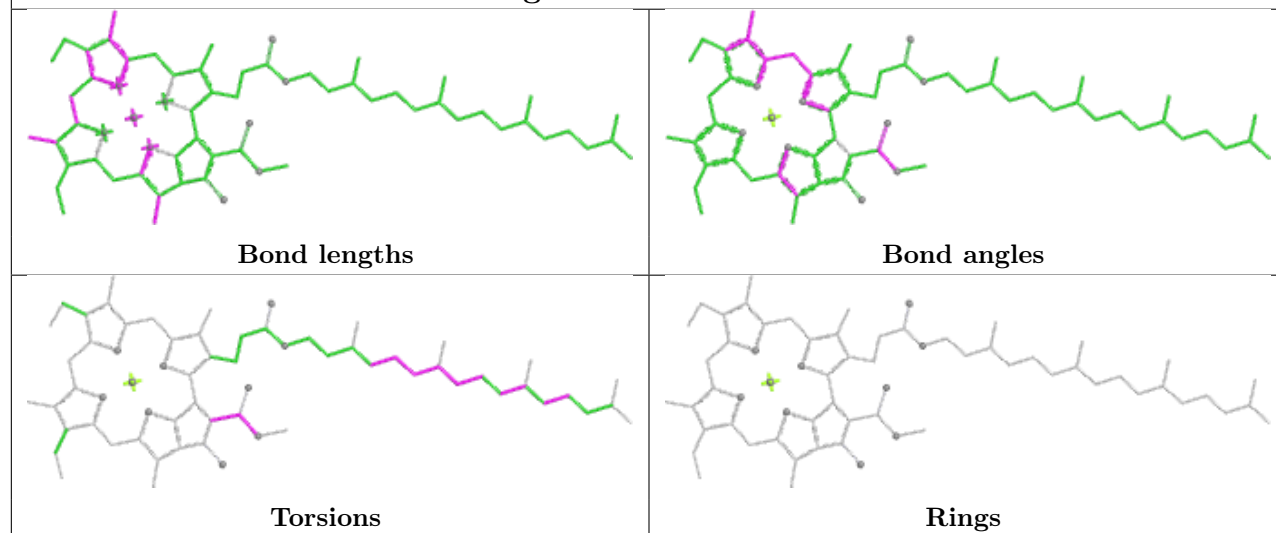


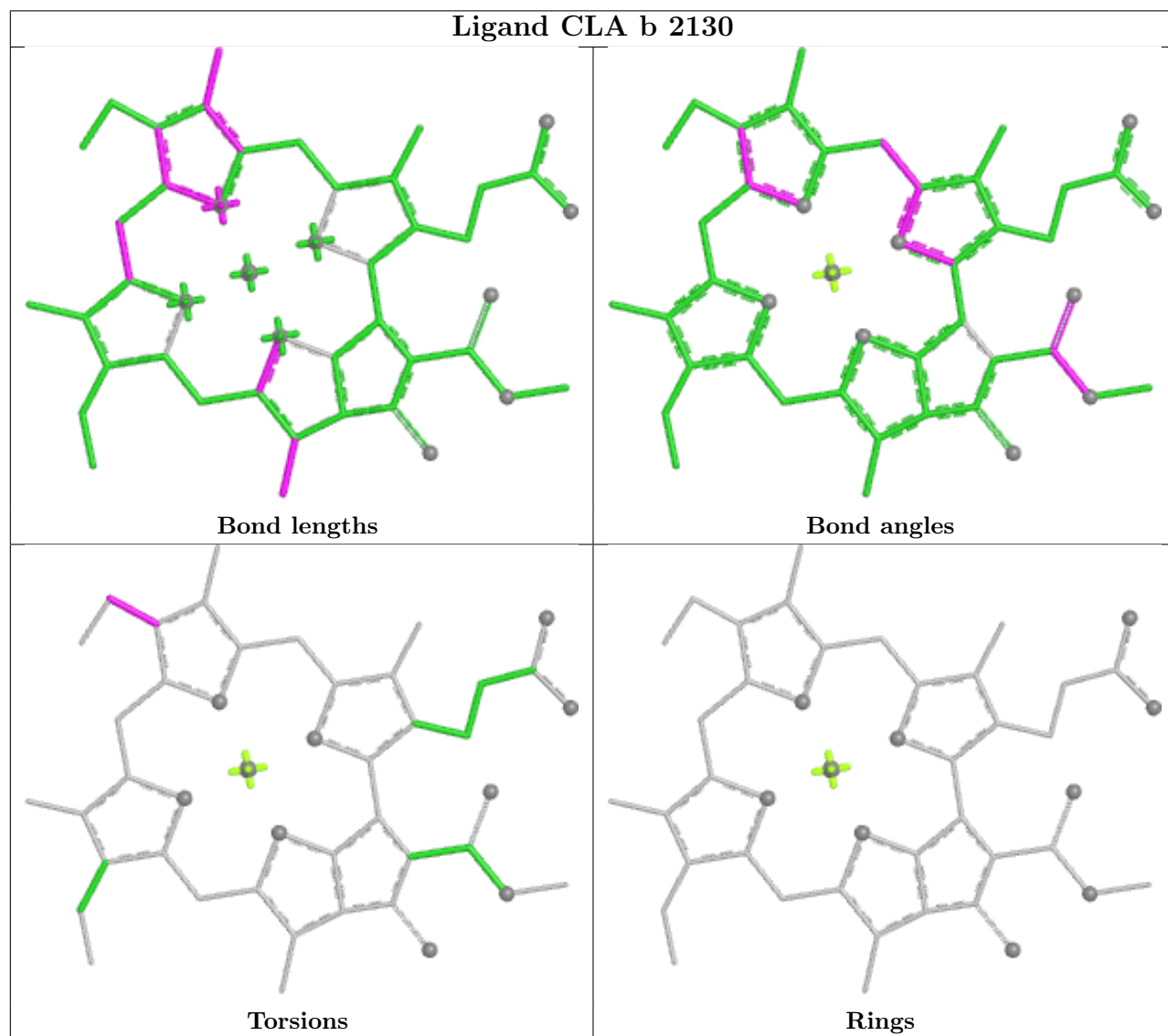
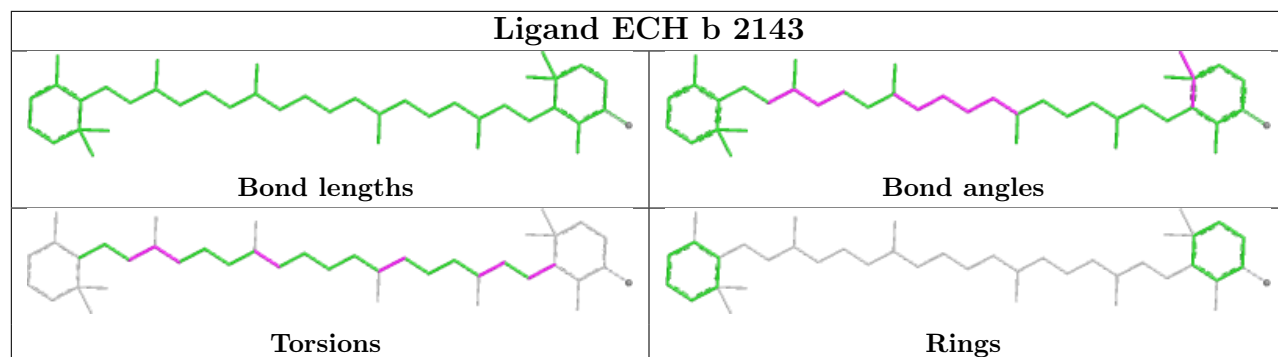
Ligand CLA 1 205**Ligand CLA a 838****Ligand CLA A 820**

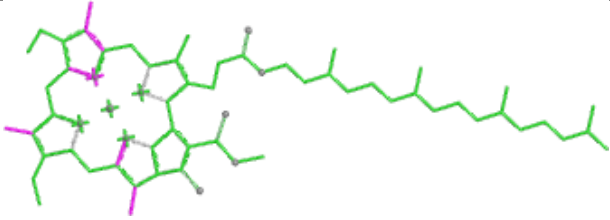
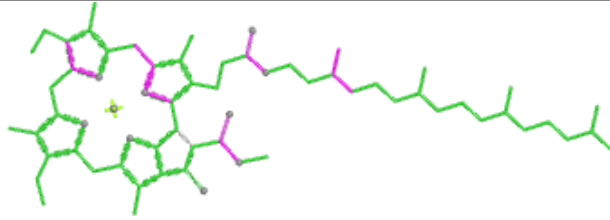
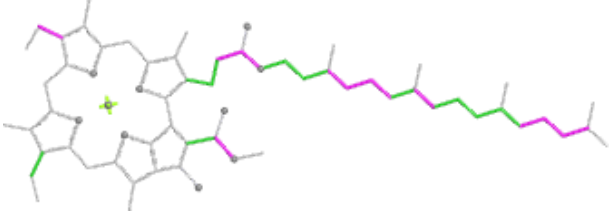
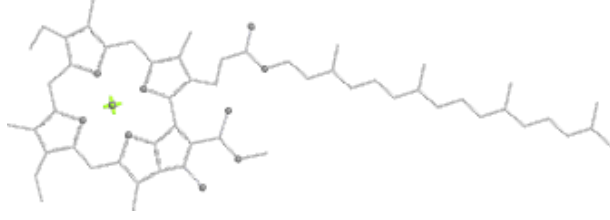
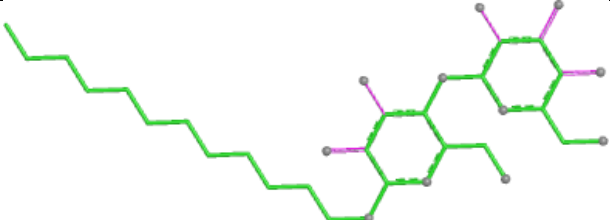
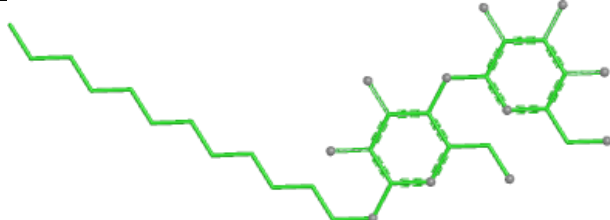
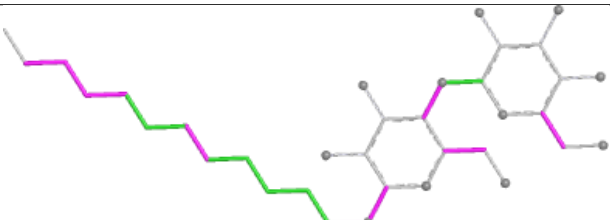
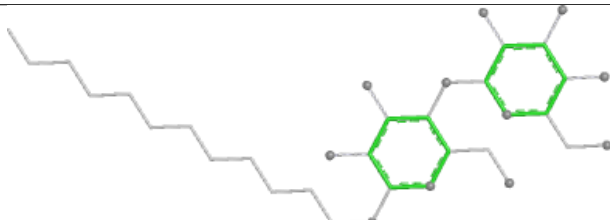
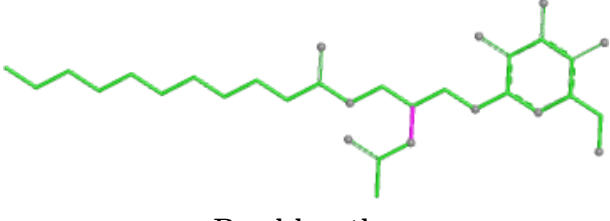
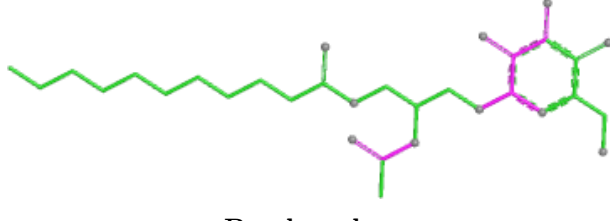
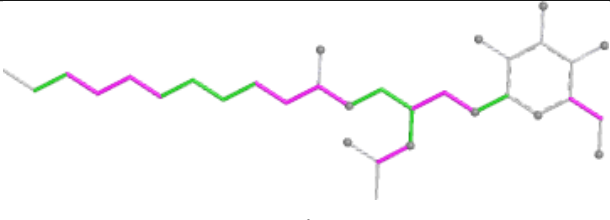
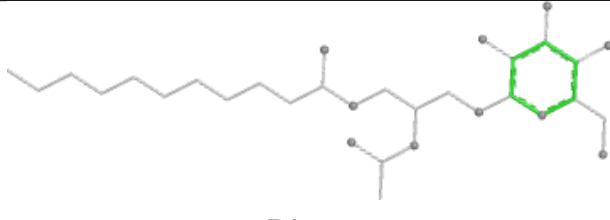
Ligand CLA b 2118



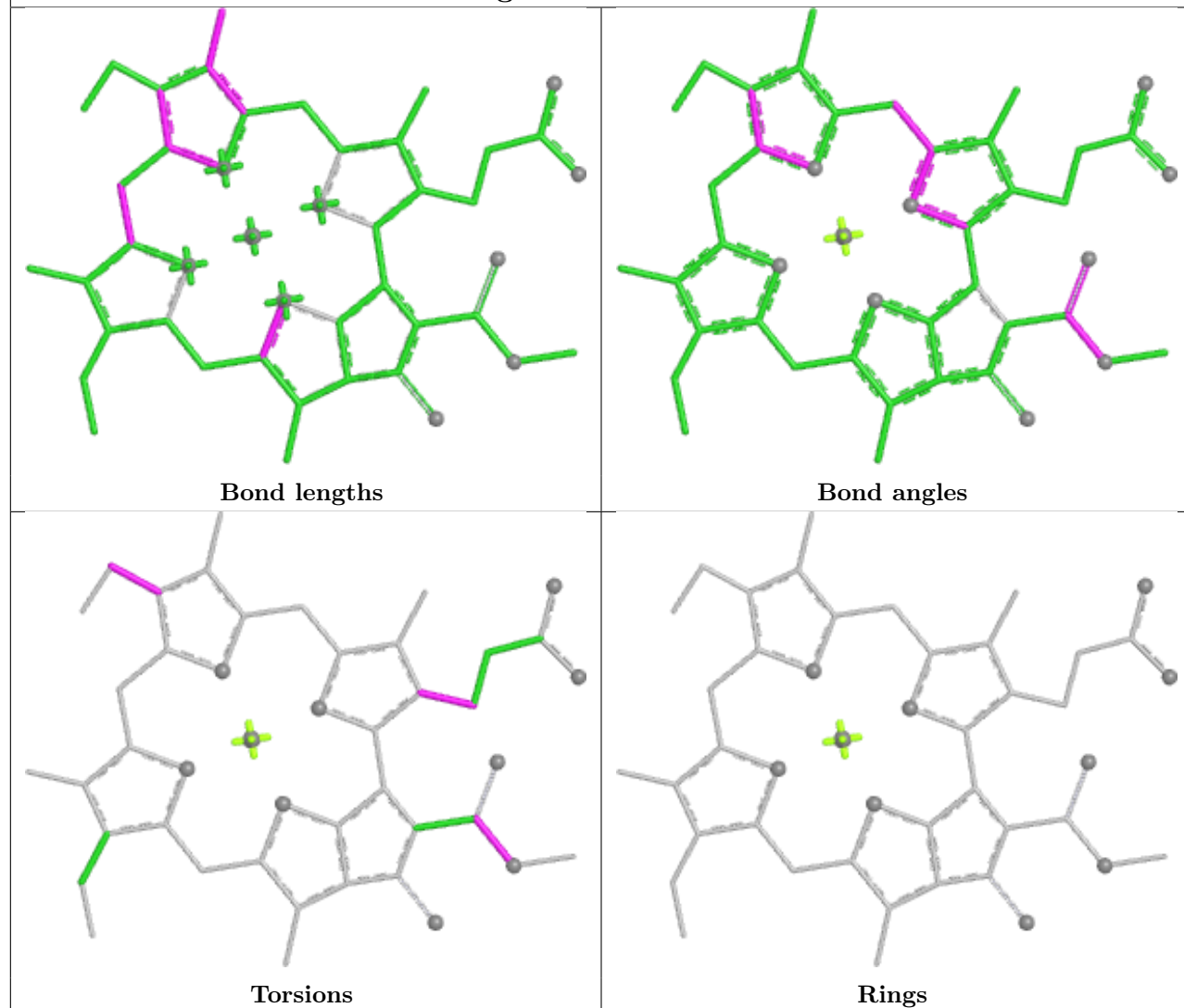
Ligand CLA B 2130



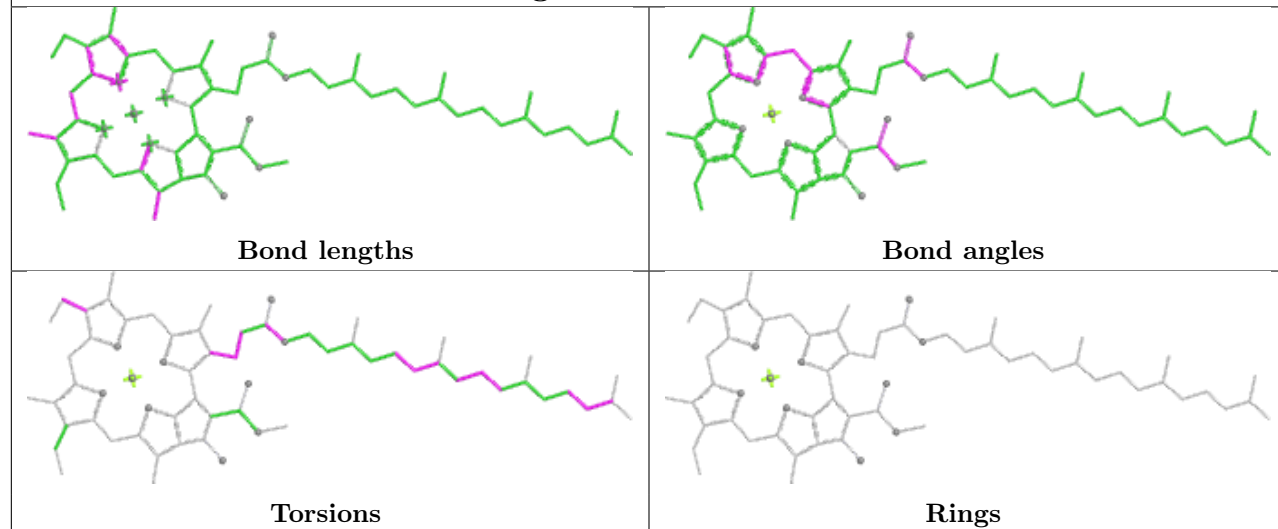


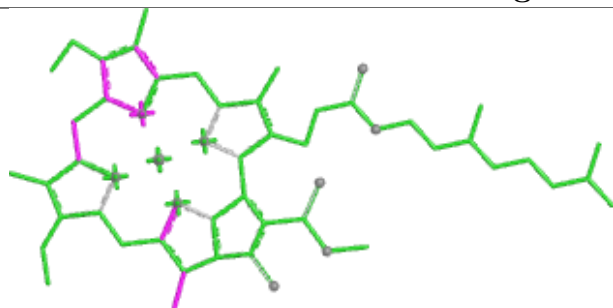
Ligand CLA b 2103	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMT l 210	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG a 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA a 815

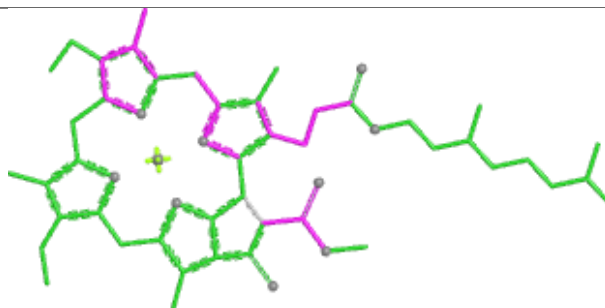


Ligand CLA A 826

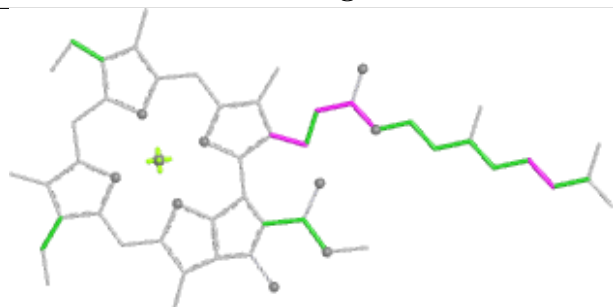


Ligand CLA A 854

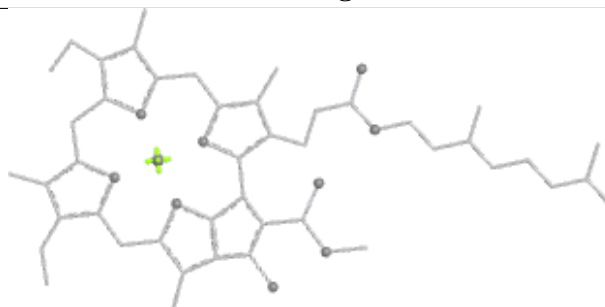
Bond lengths



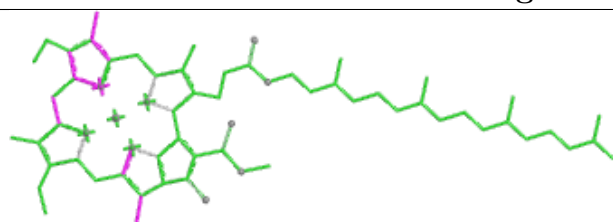
Bond angles



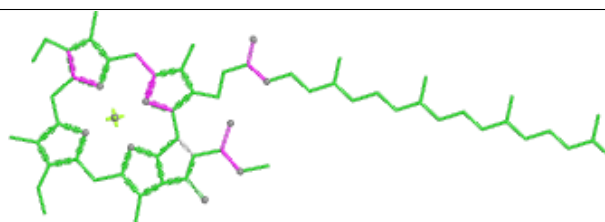
Torsions



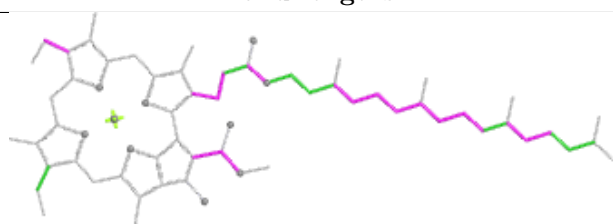
Rings

Ligand CLA F 201

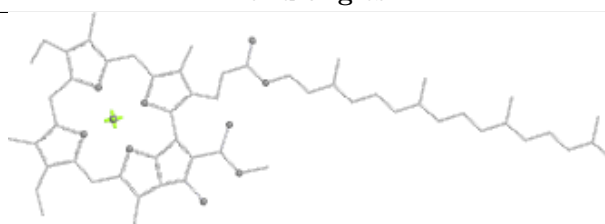
Bond lengths



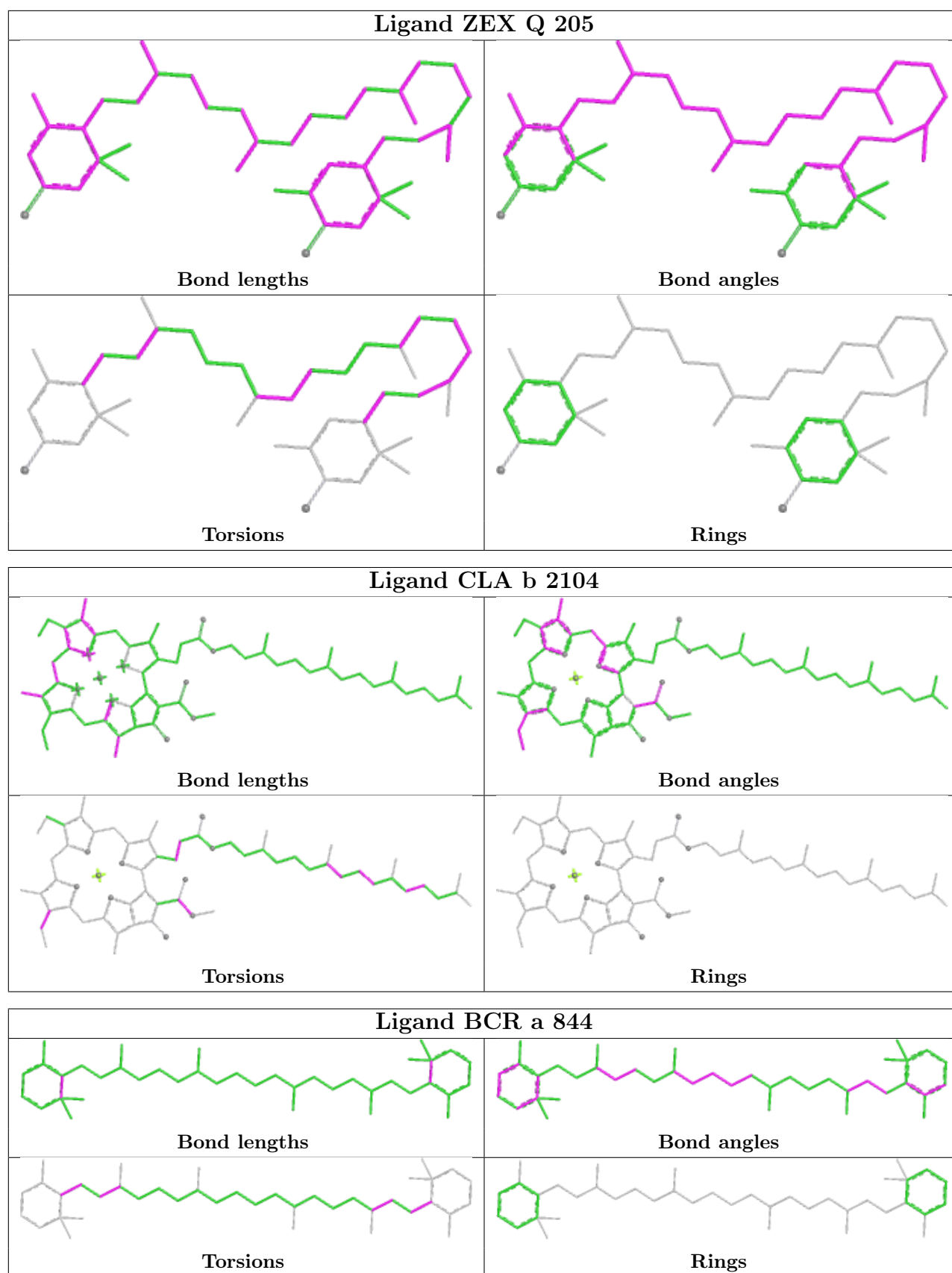
Bond angles

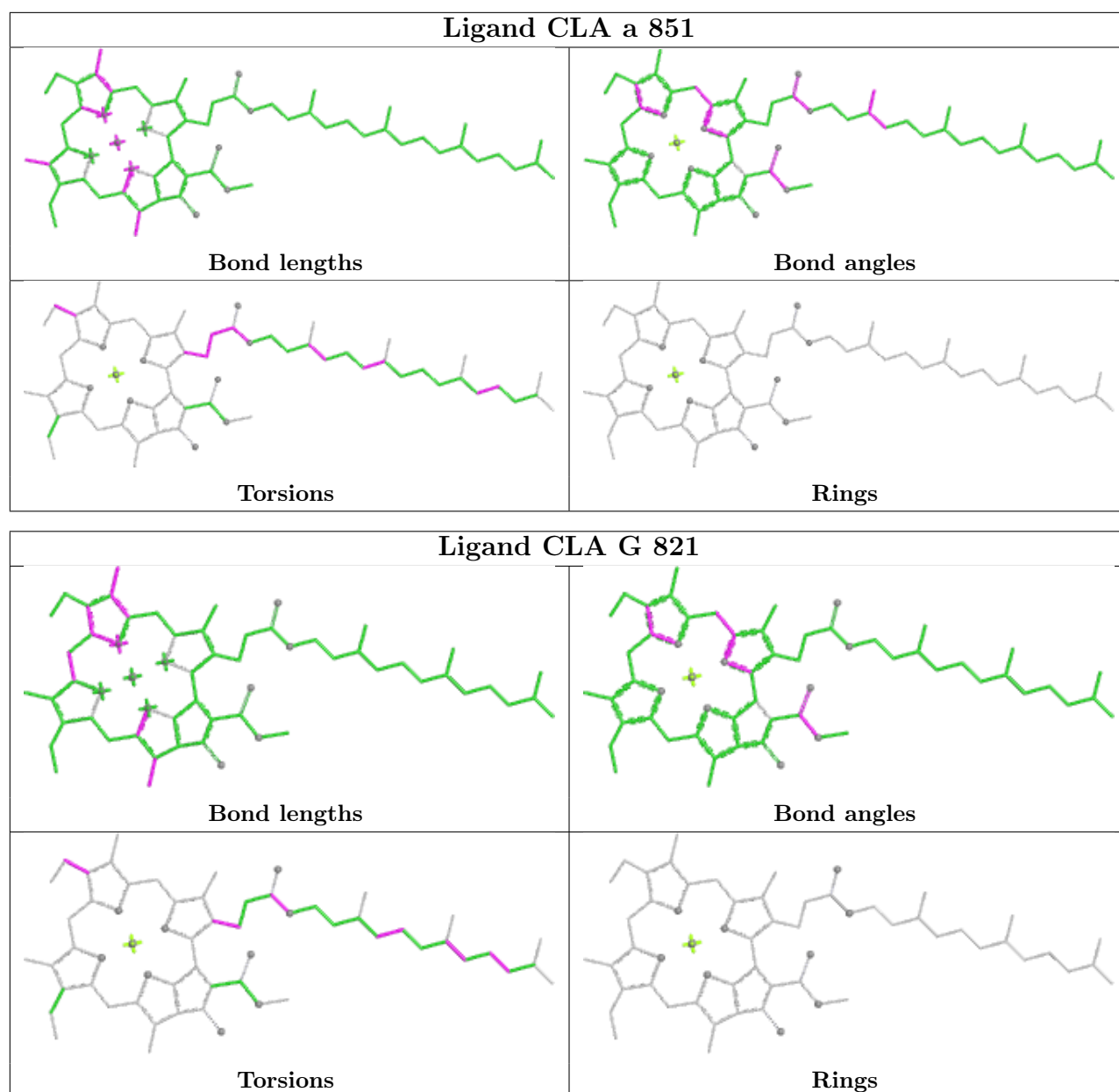


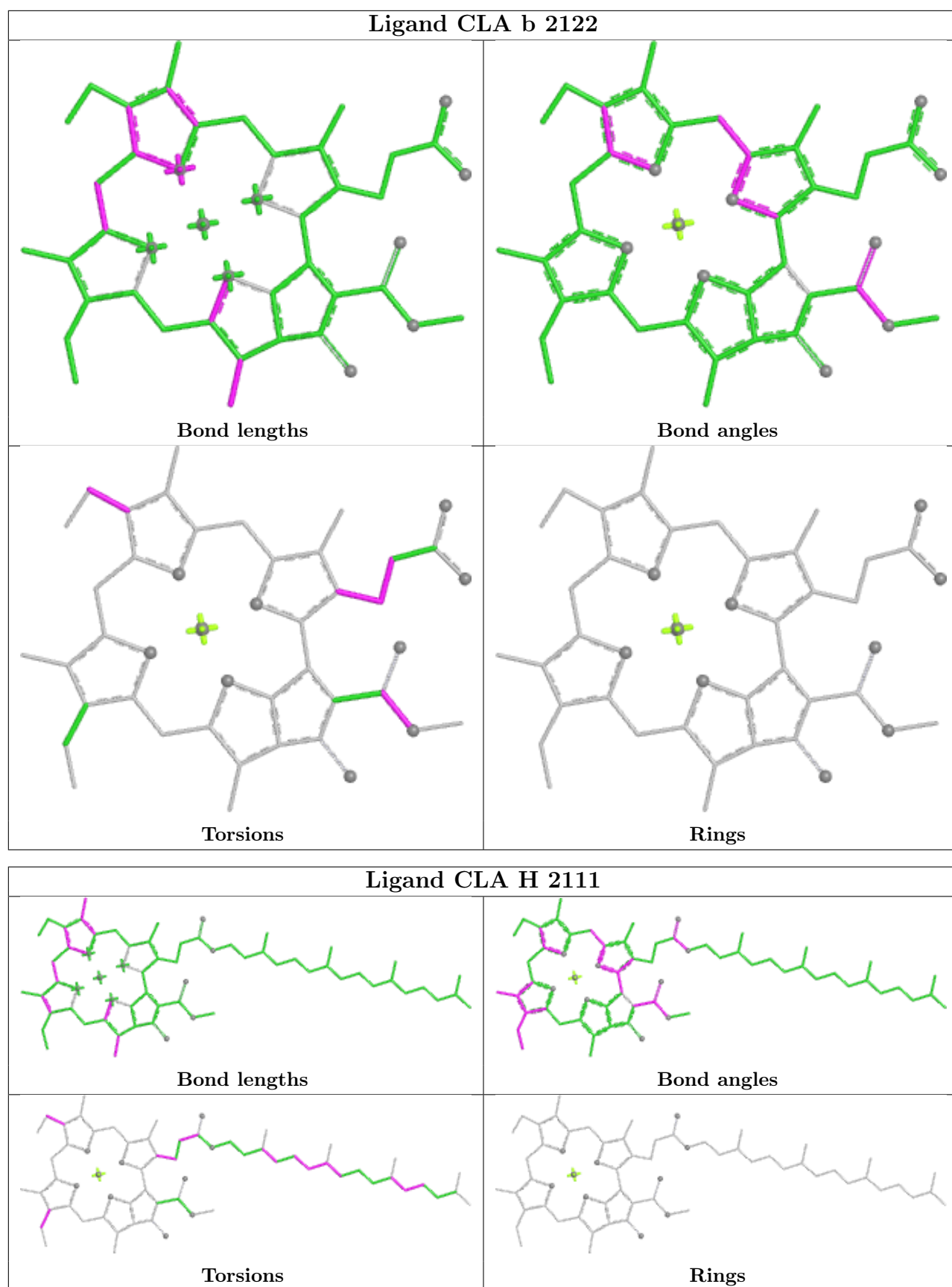
Torsions



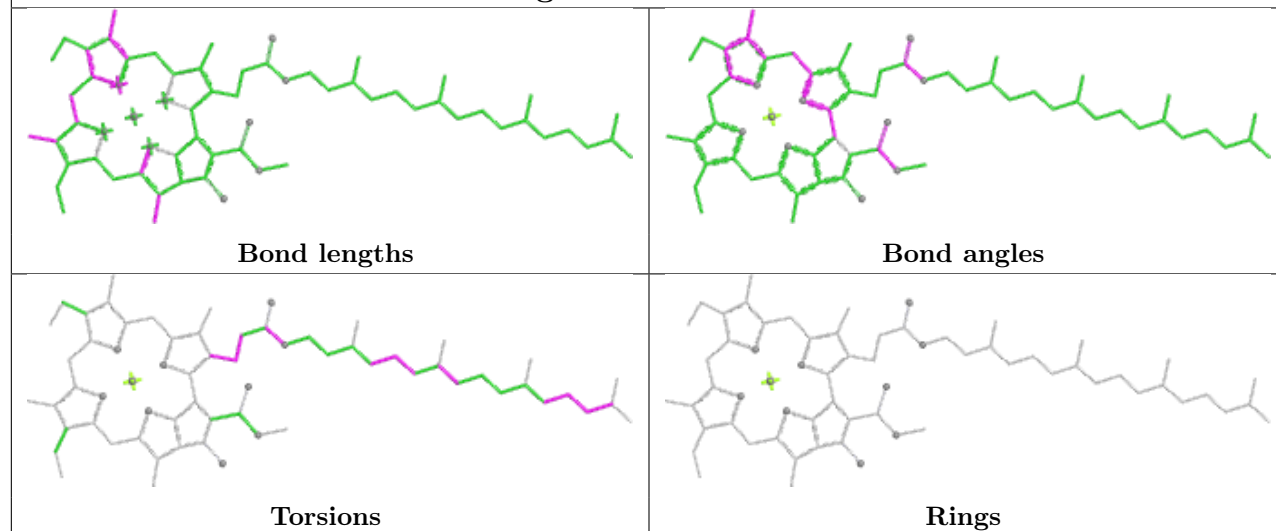
Rings



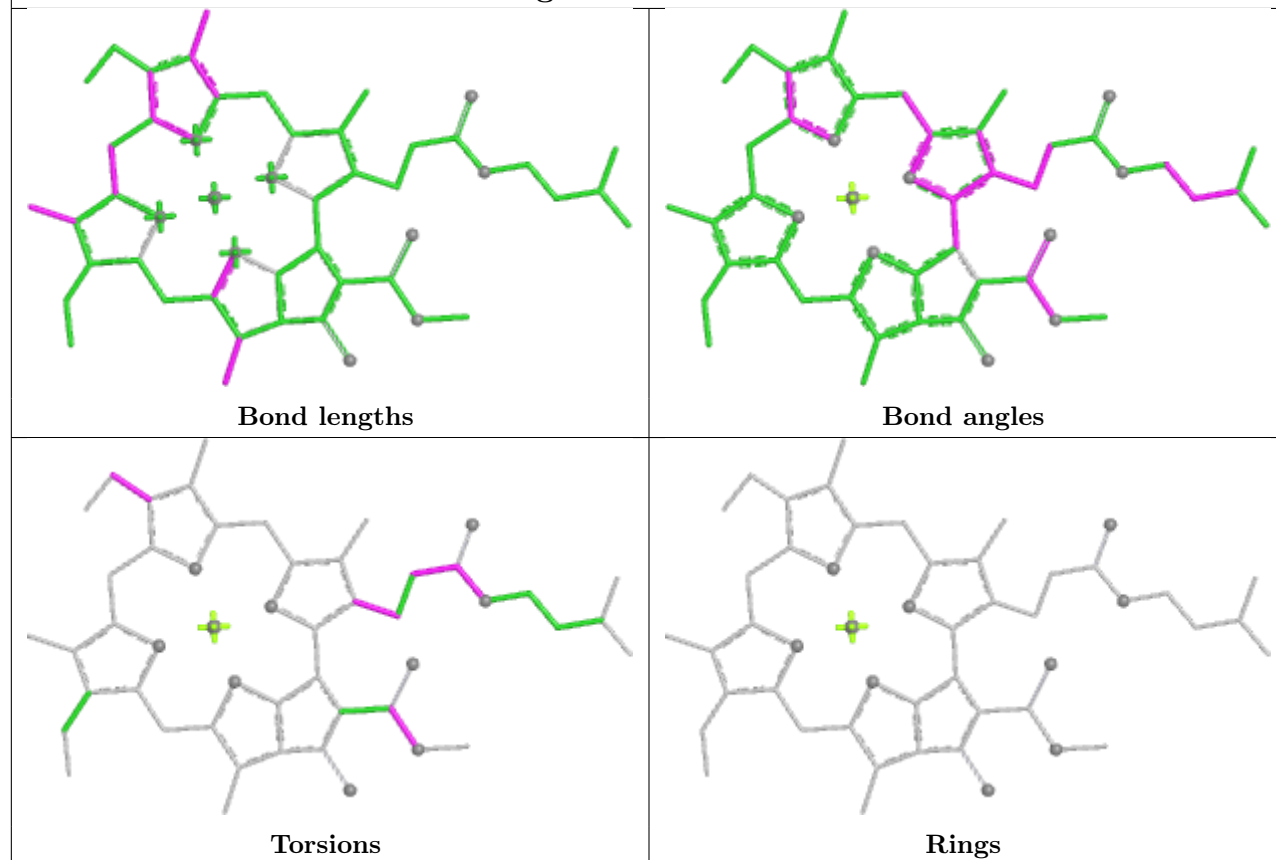


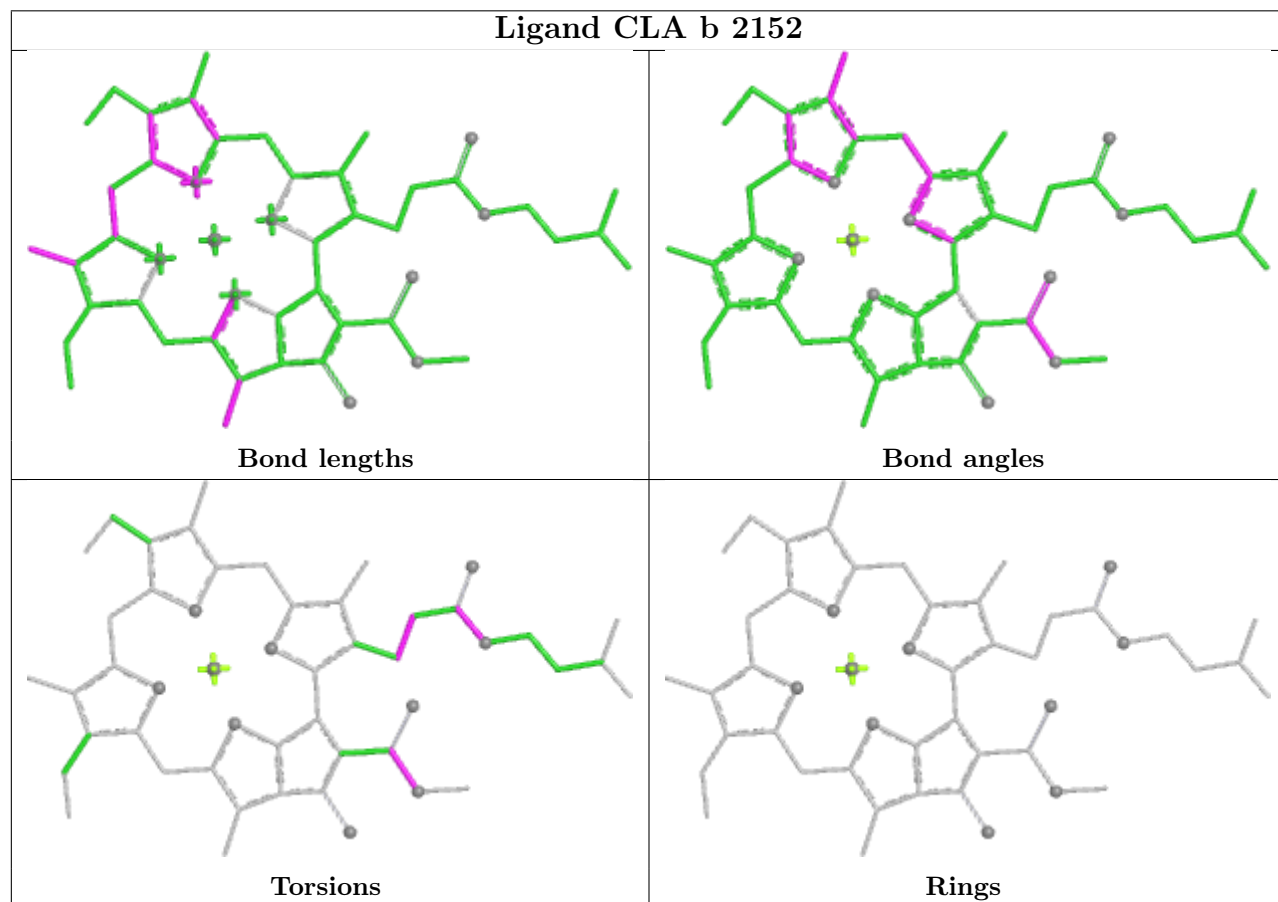
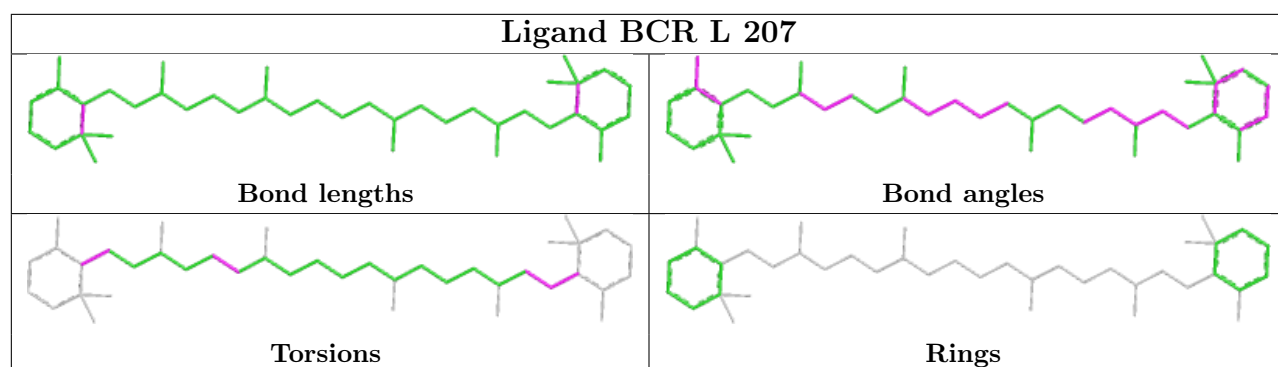


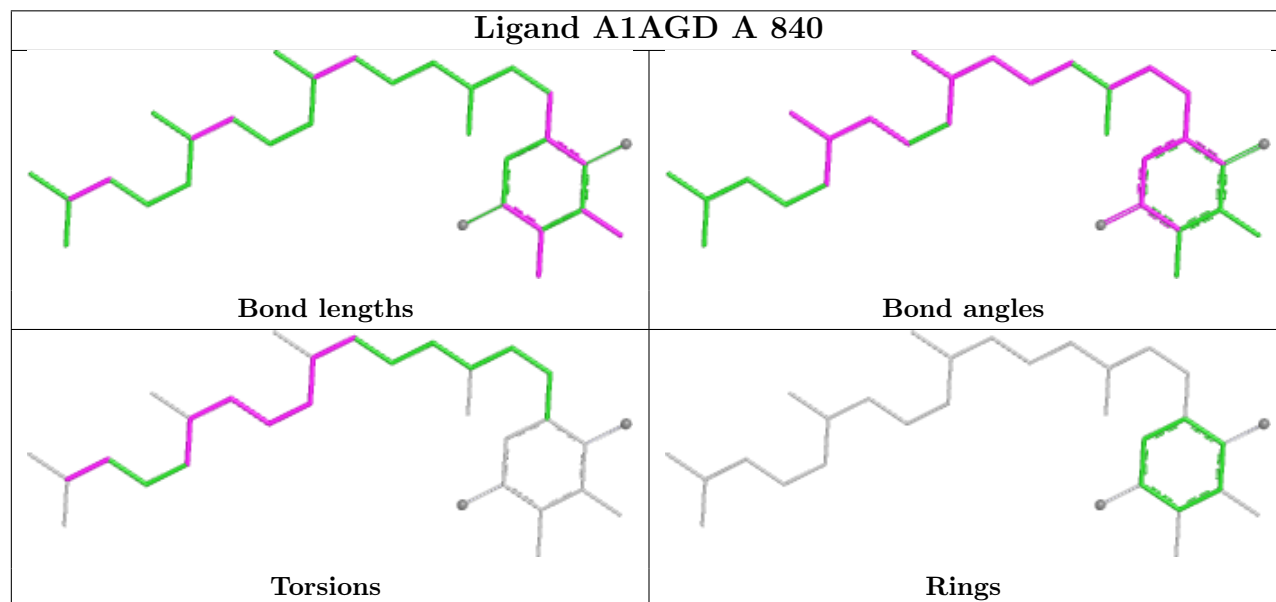
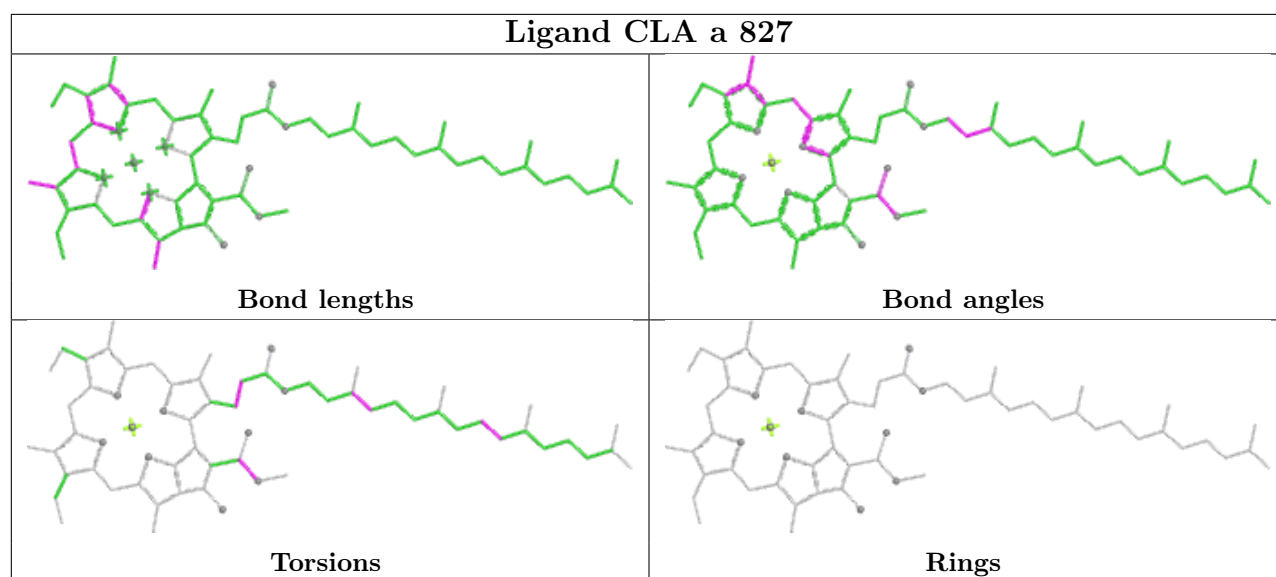
Ligand CLA a 835



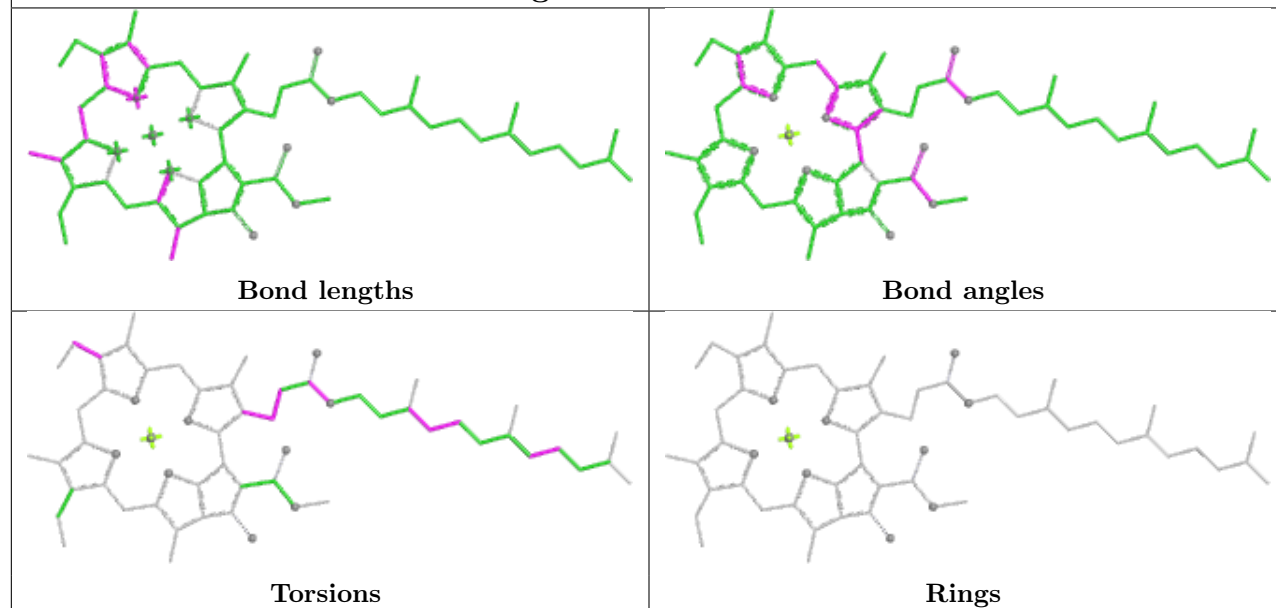
Ligand CLA a 809



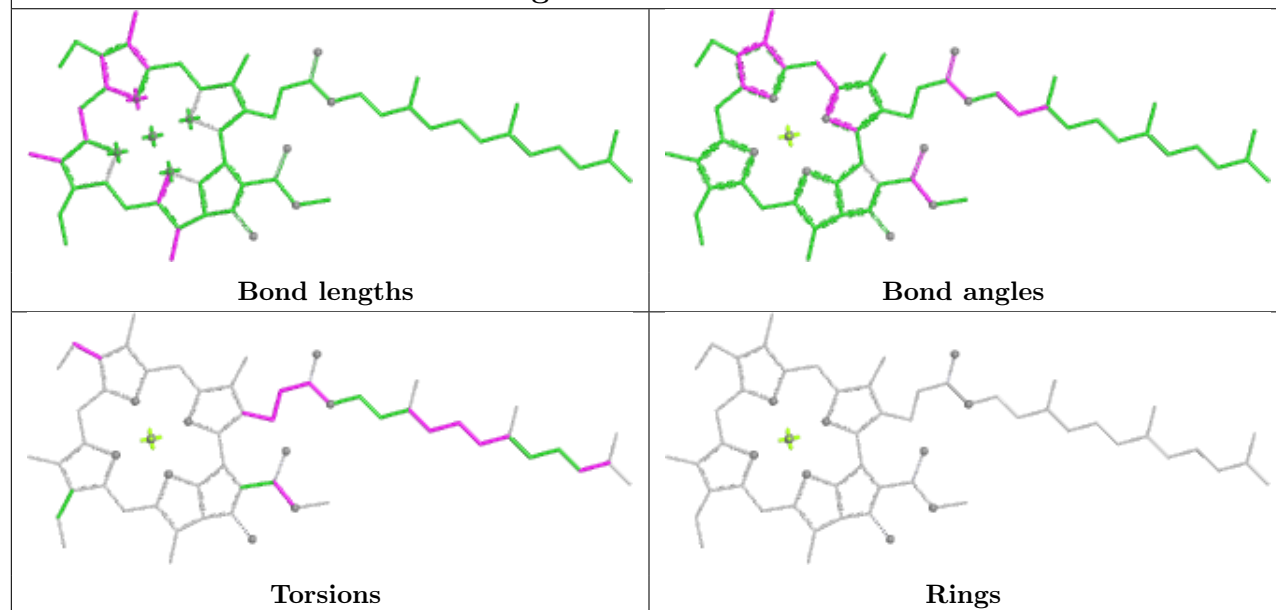


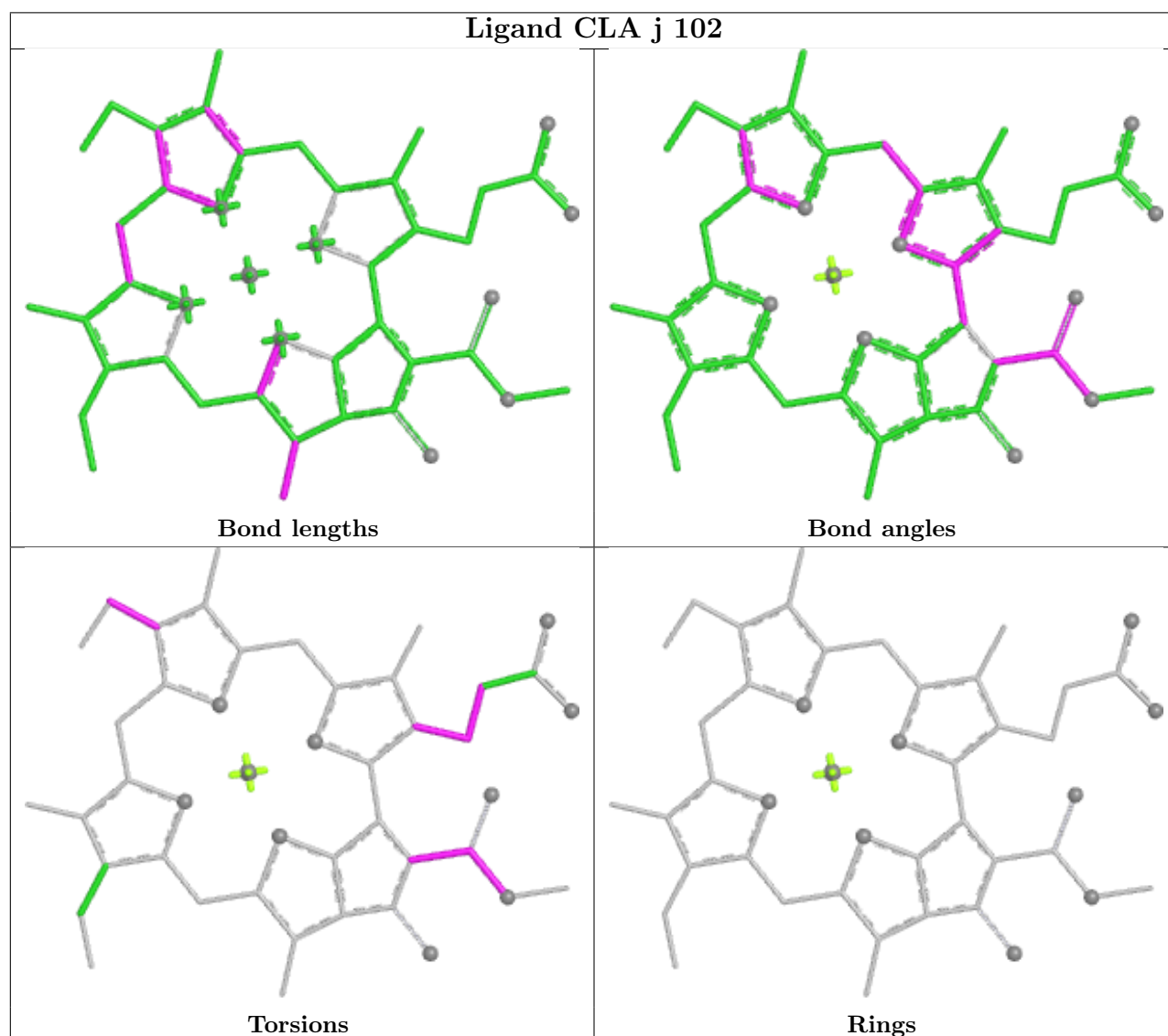
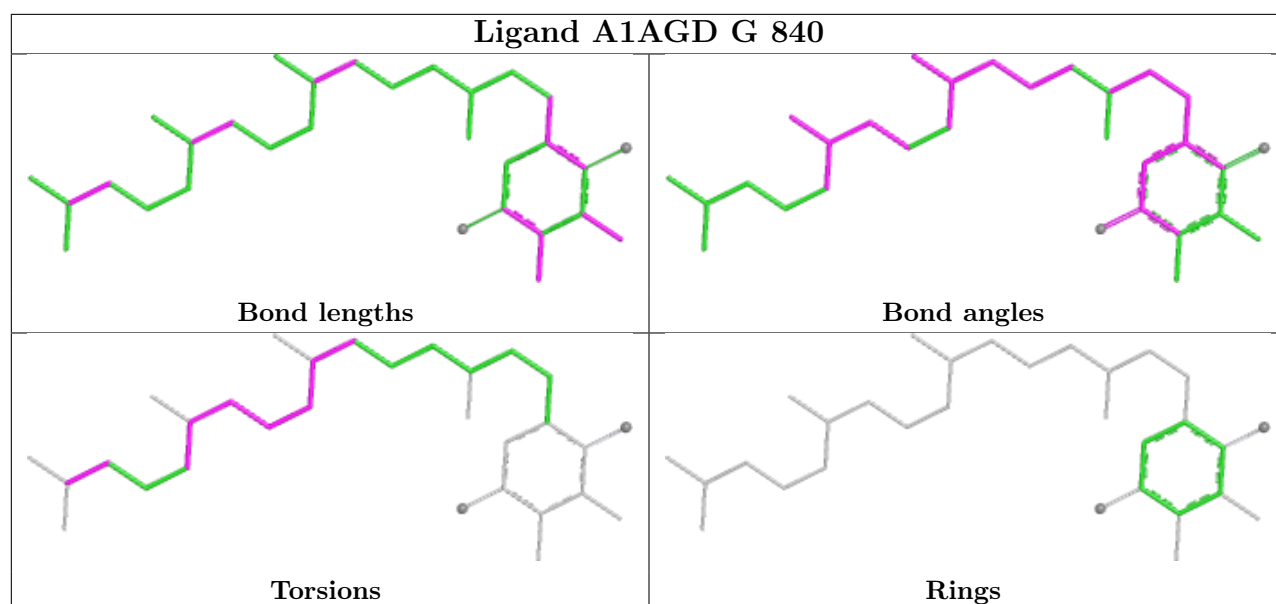


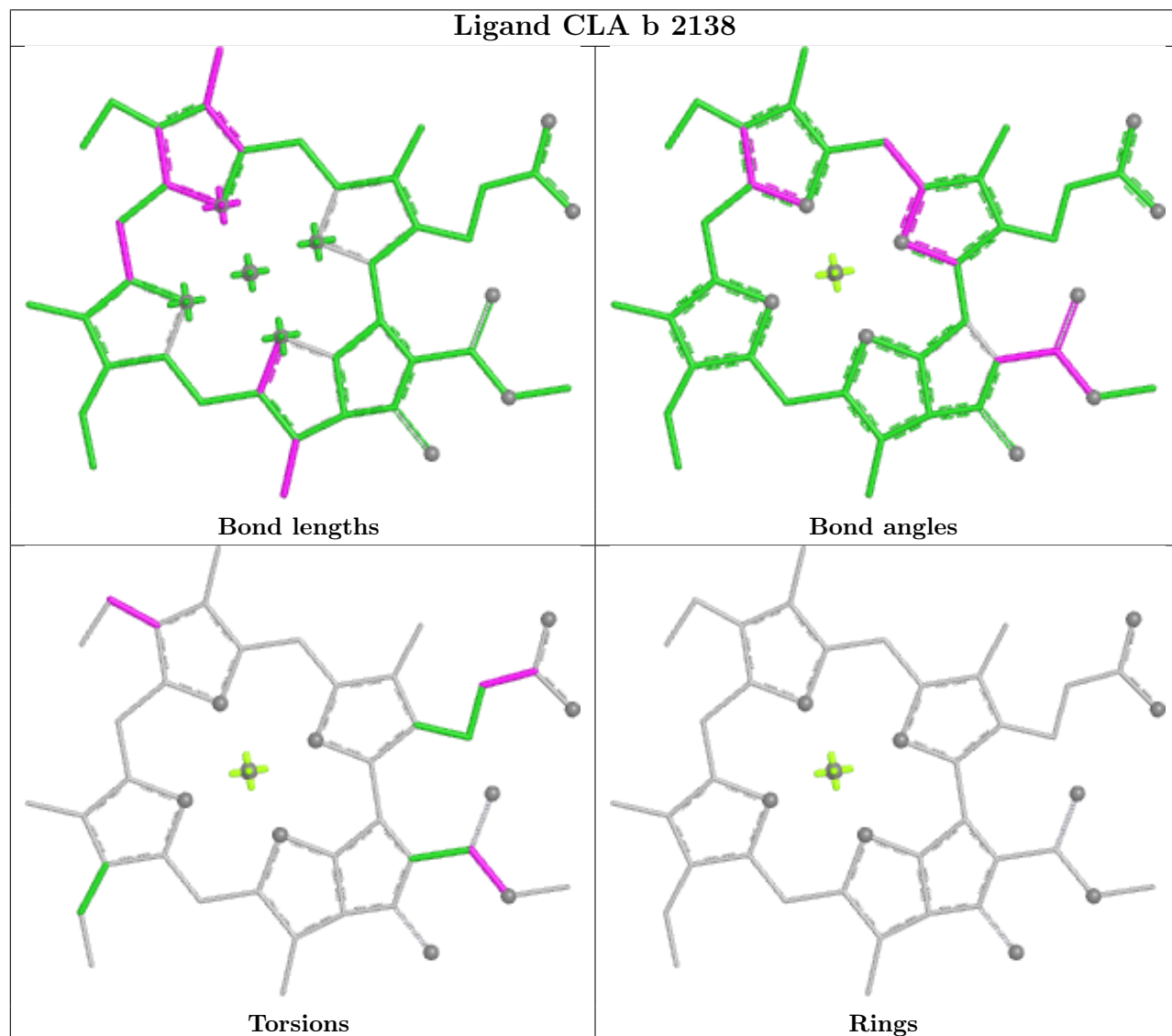
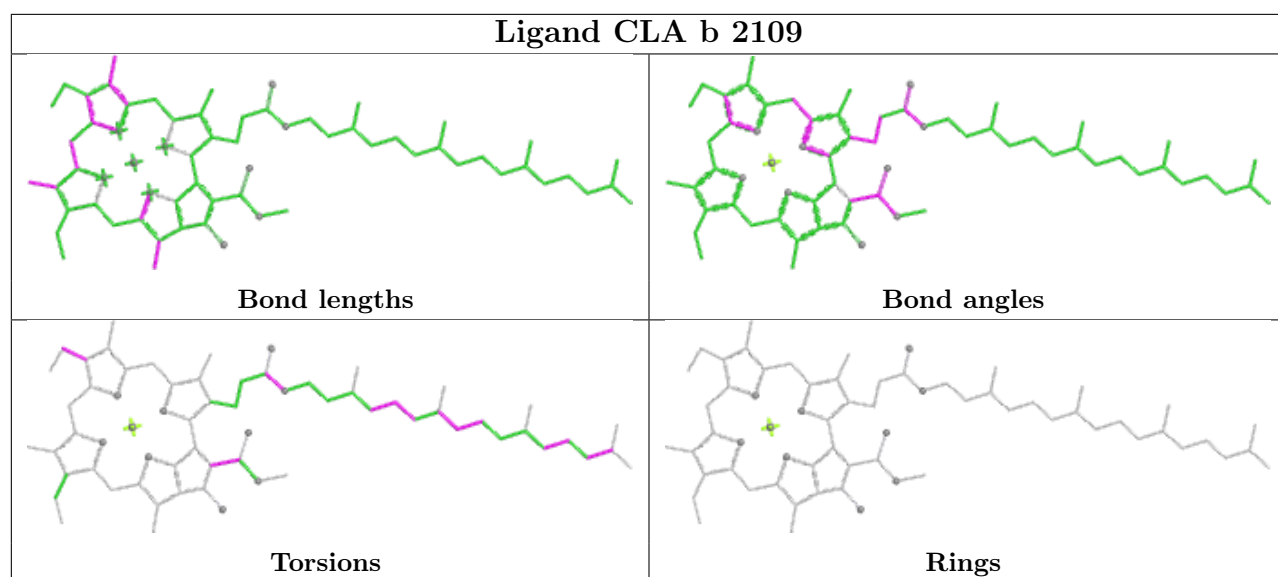
Ligand CLA A 823

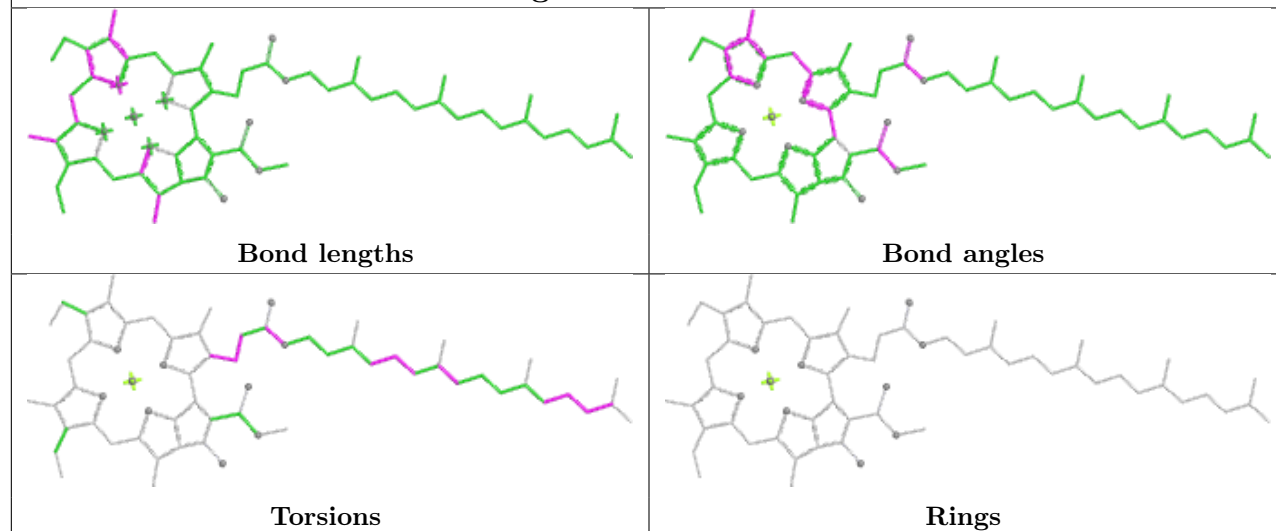
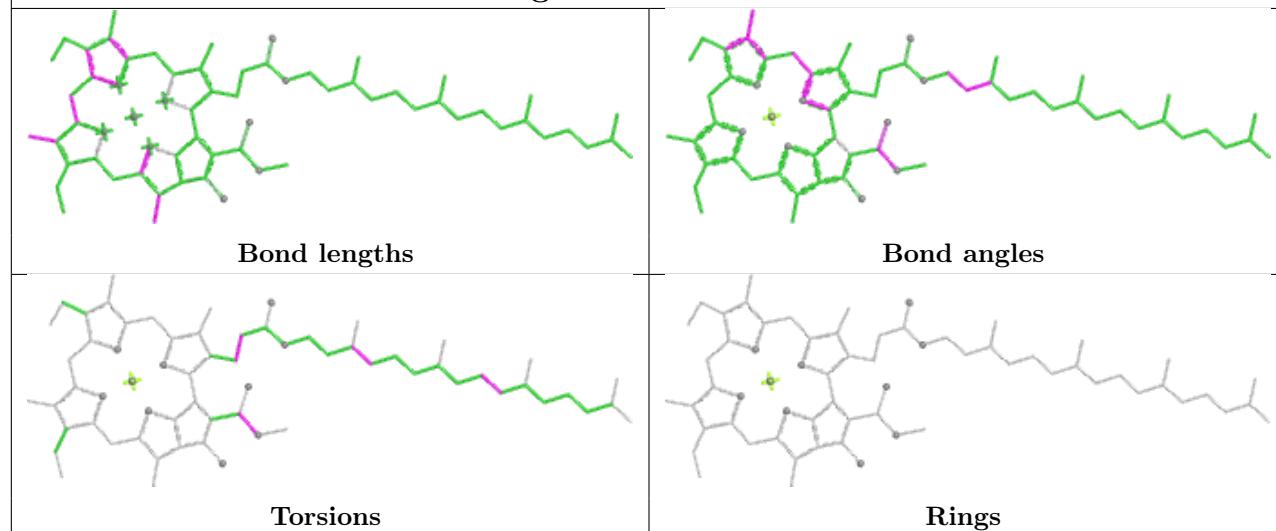


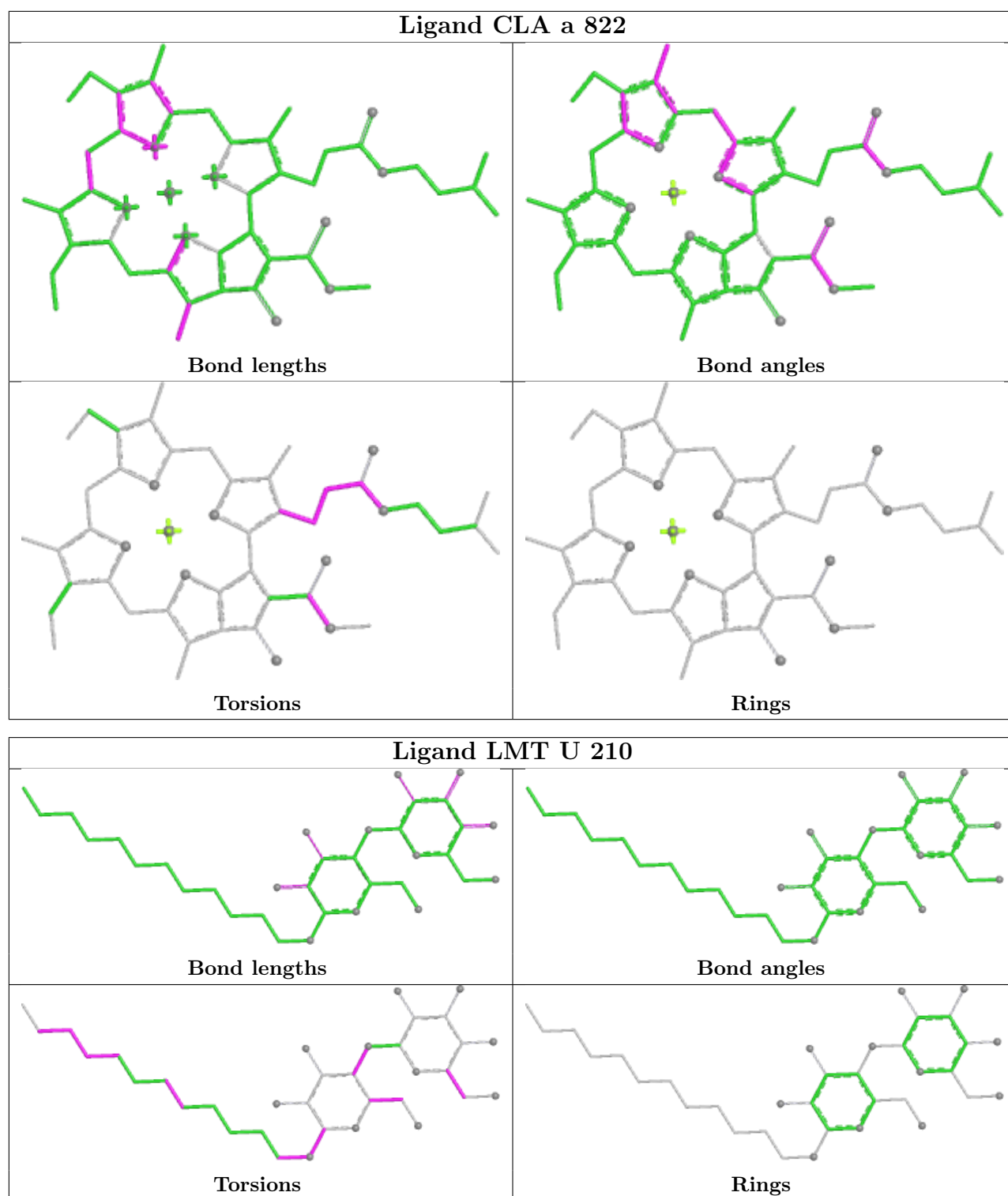
Ligand CLA A 817







Ligand CLA A 835**Ligand CLA A 827**



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

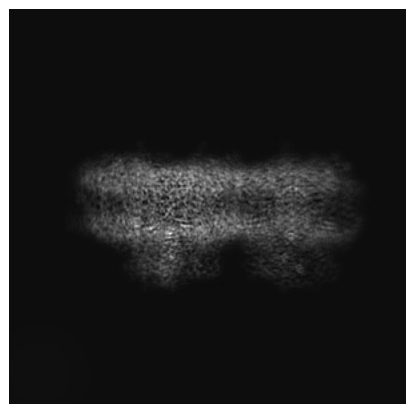
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43843. These allow visual inspection of the internal detail of the map and identification of artifacts.

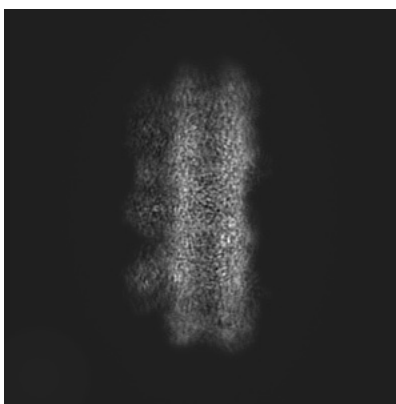
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

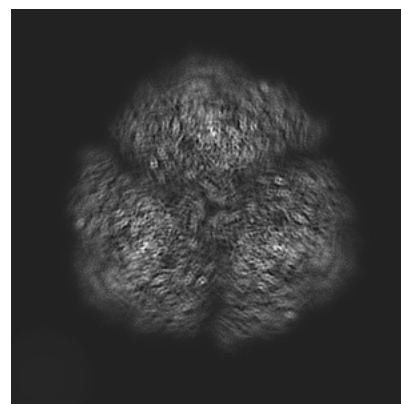
6.1.1 Primary map



X

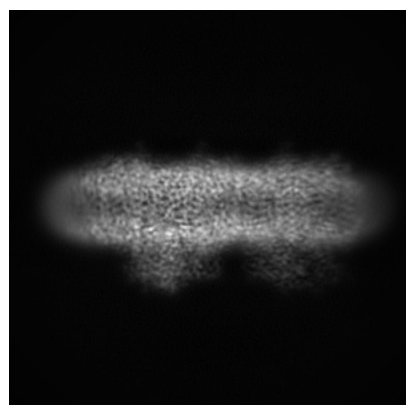


Y

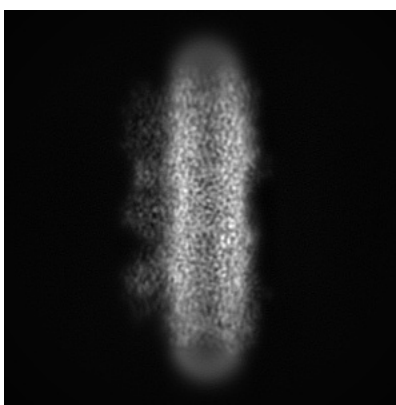


Z

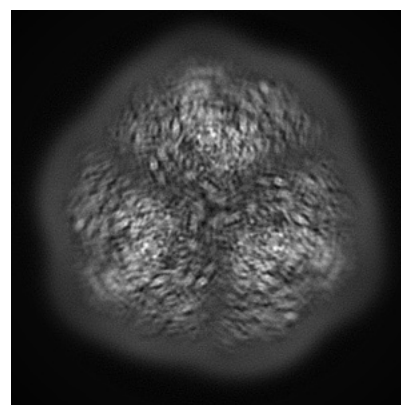
6.1.2 Raw map



X



Y



Z

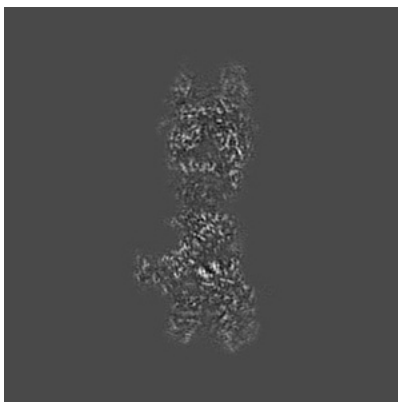
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

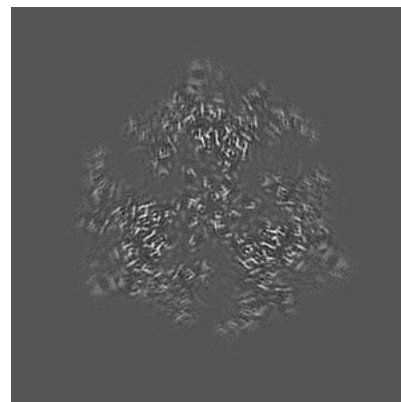
6.2.1 Primary map



X Index: 160

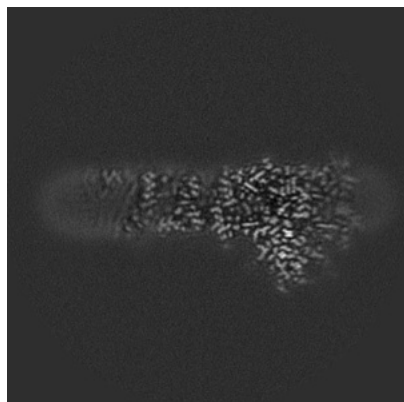


Y Index: 160

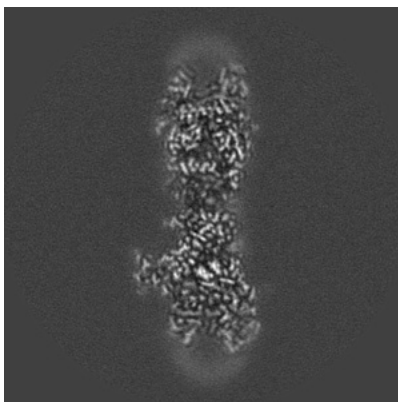


Z Index: 160

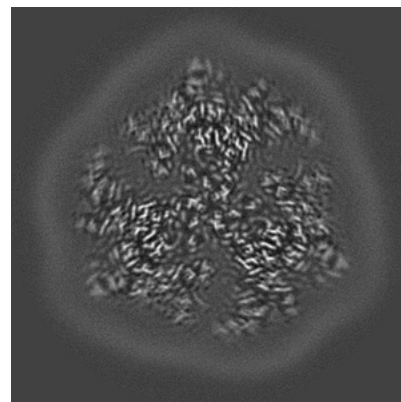
6.2.2 Raw map



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](#)

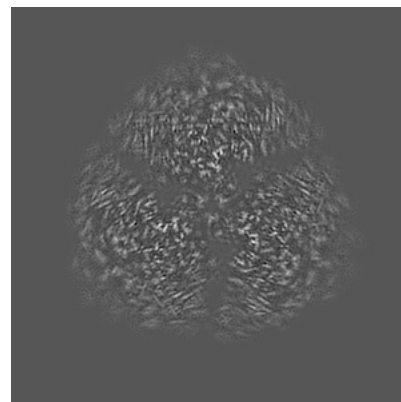
6.3.1 Primary map



X Index: 107

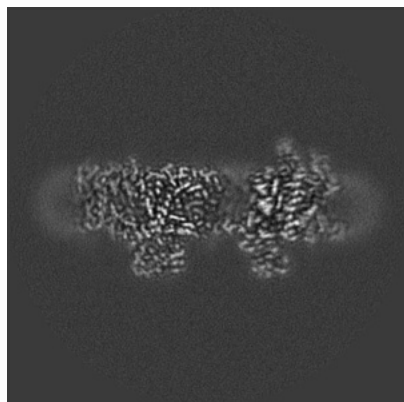


Y Index: 128

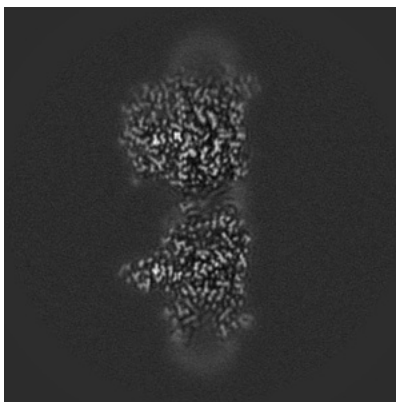


Z Index: 176

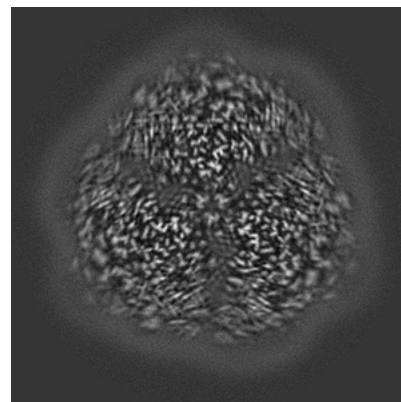
6.3.2 Raw map



X Index: 187



Y Index: 129

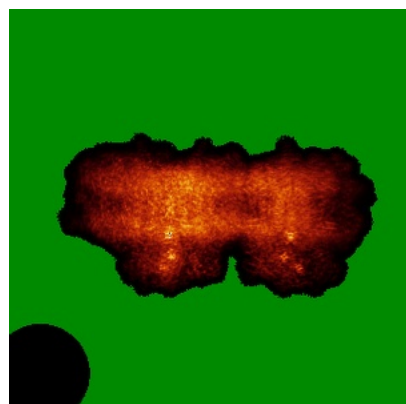


Z Index: 176

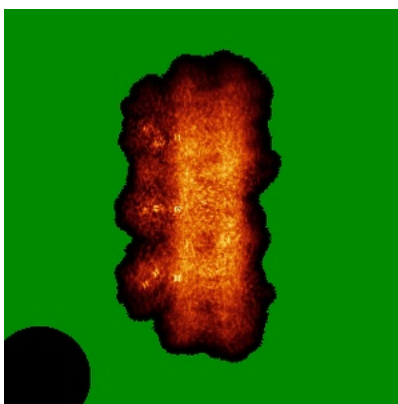
The images above show the largest variance slices of the map in three orthogonal directions.

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

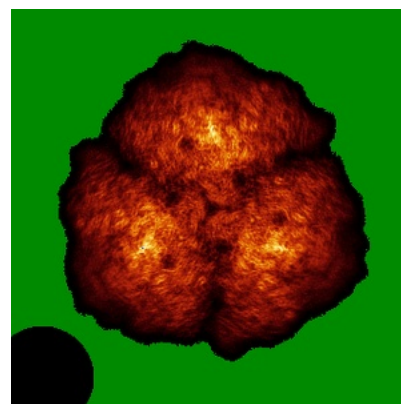
6.4.1 Primary map



X

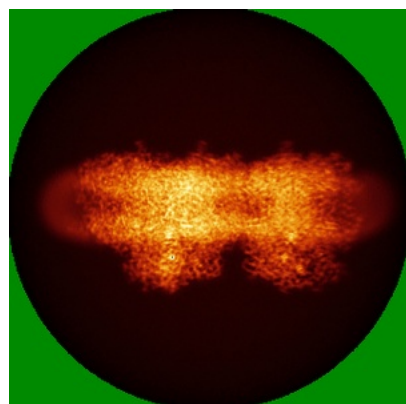


Y

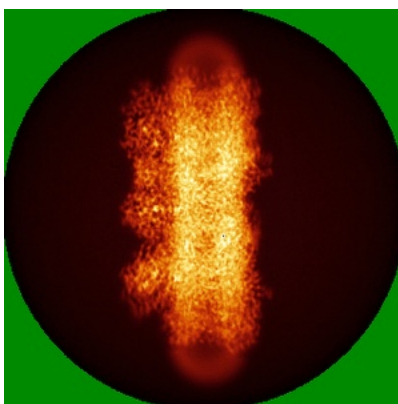


Z

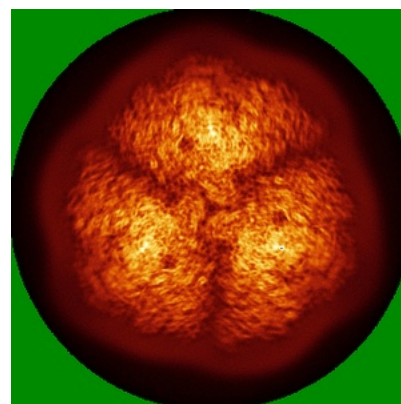
6.4.2 Raw map



X



Y

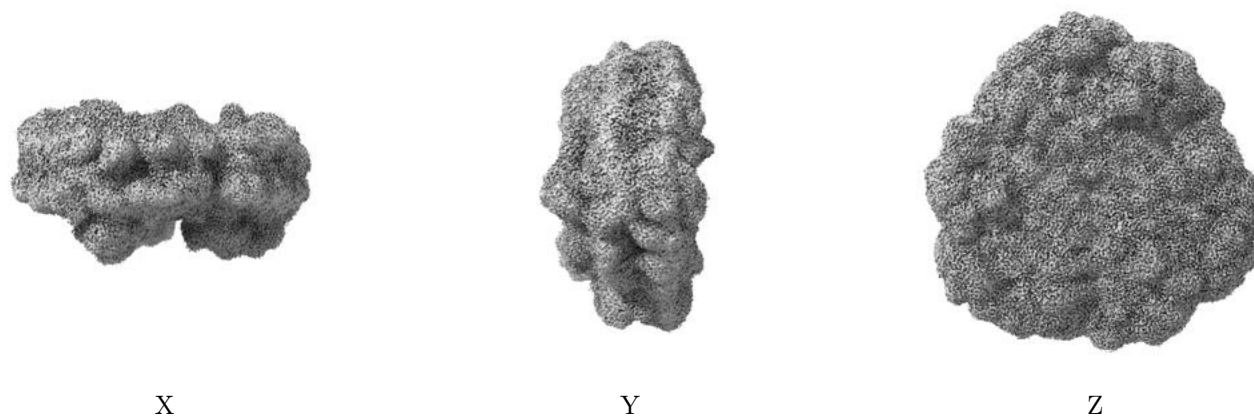


Z

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.

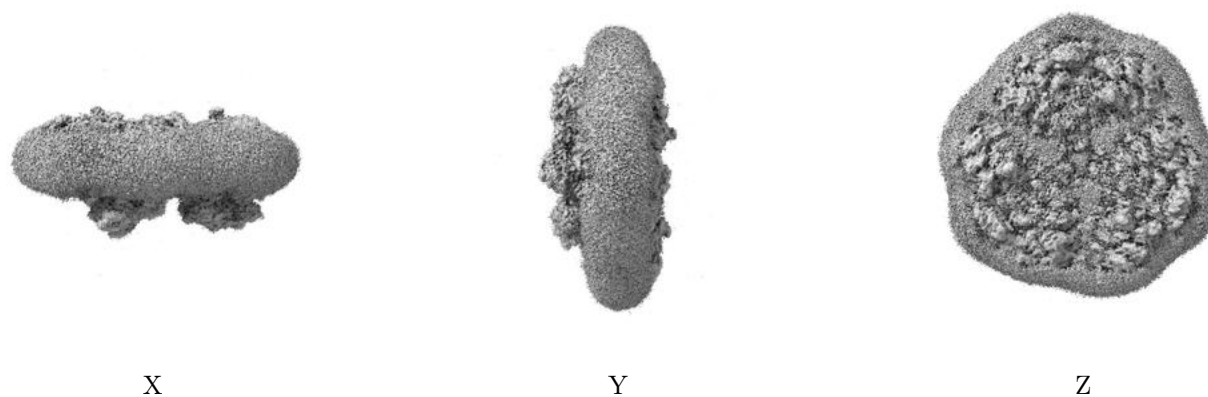
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0149. 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.

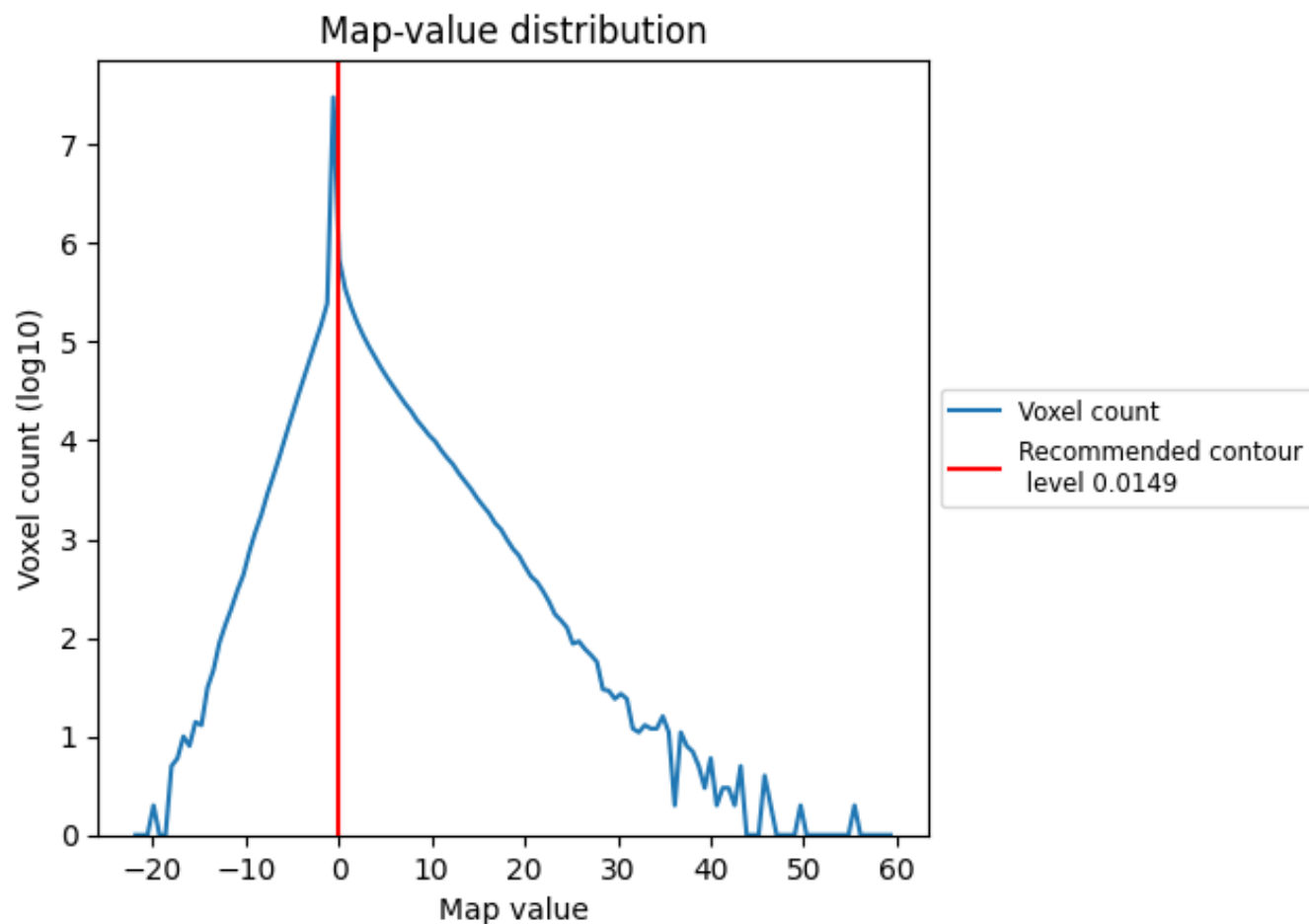
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

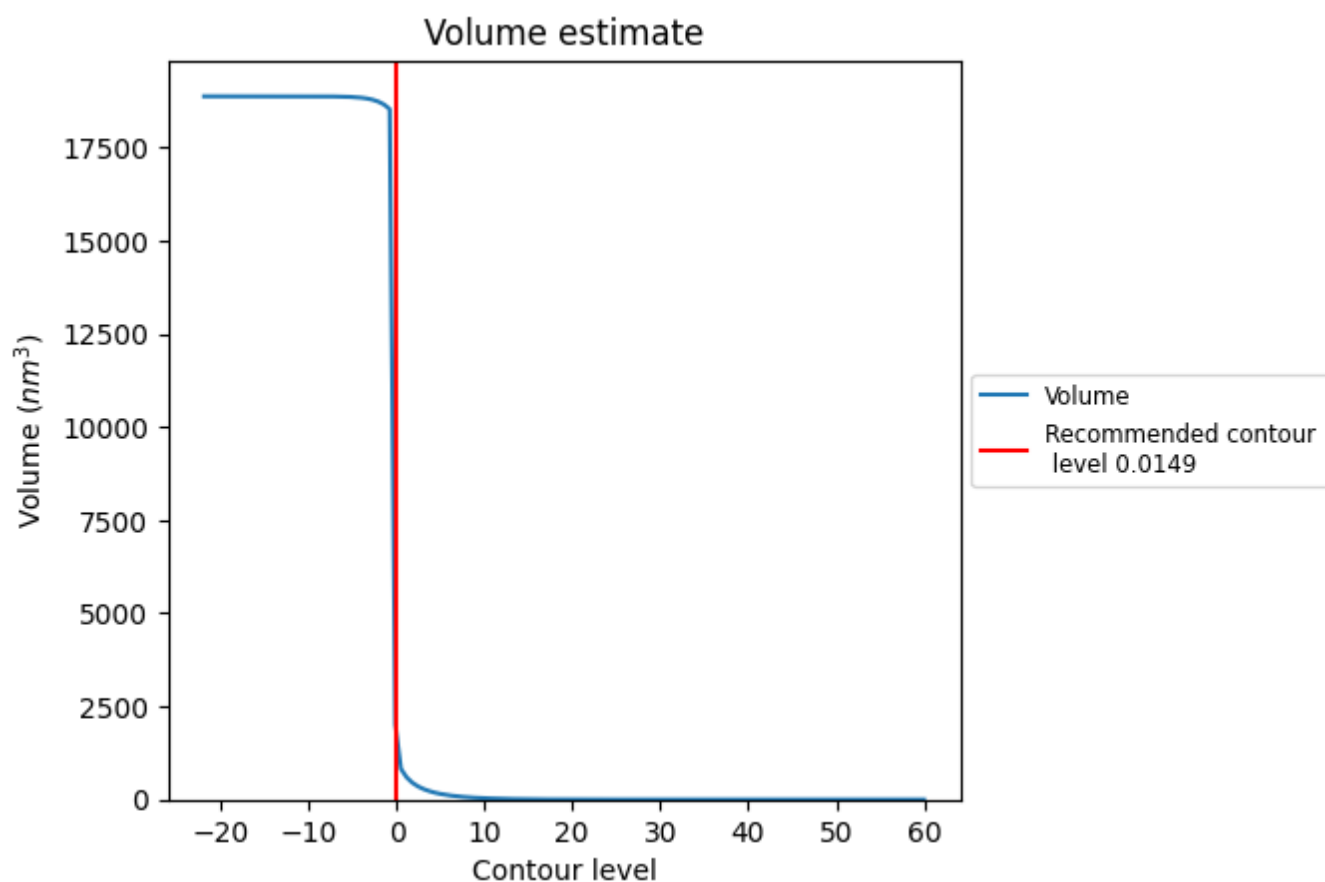
This section contains the results of statistical analysis of the map.

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.

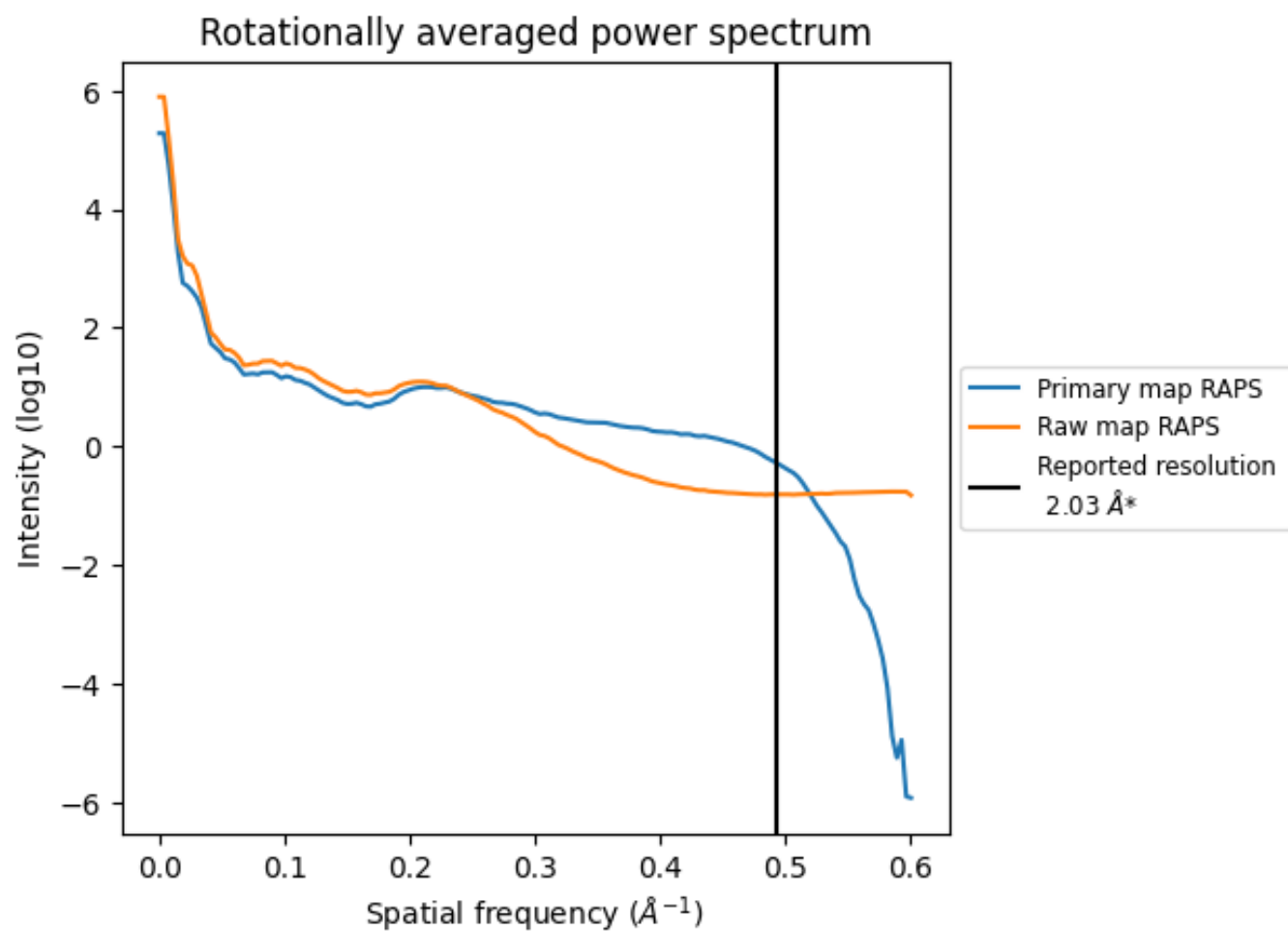
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1809 nm³; this corresponds to an approximate mass of 1634 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 ⓘ

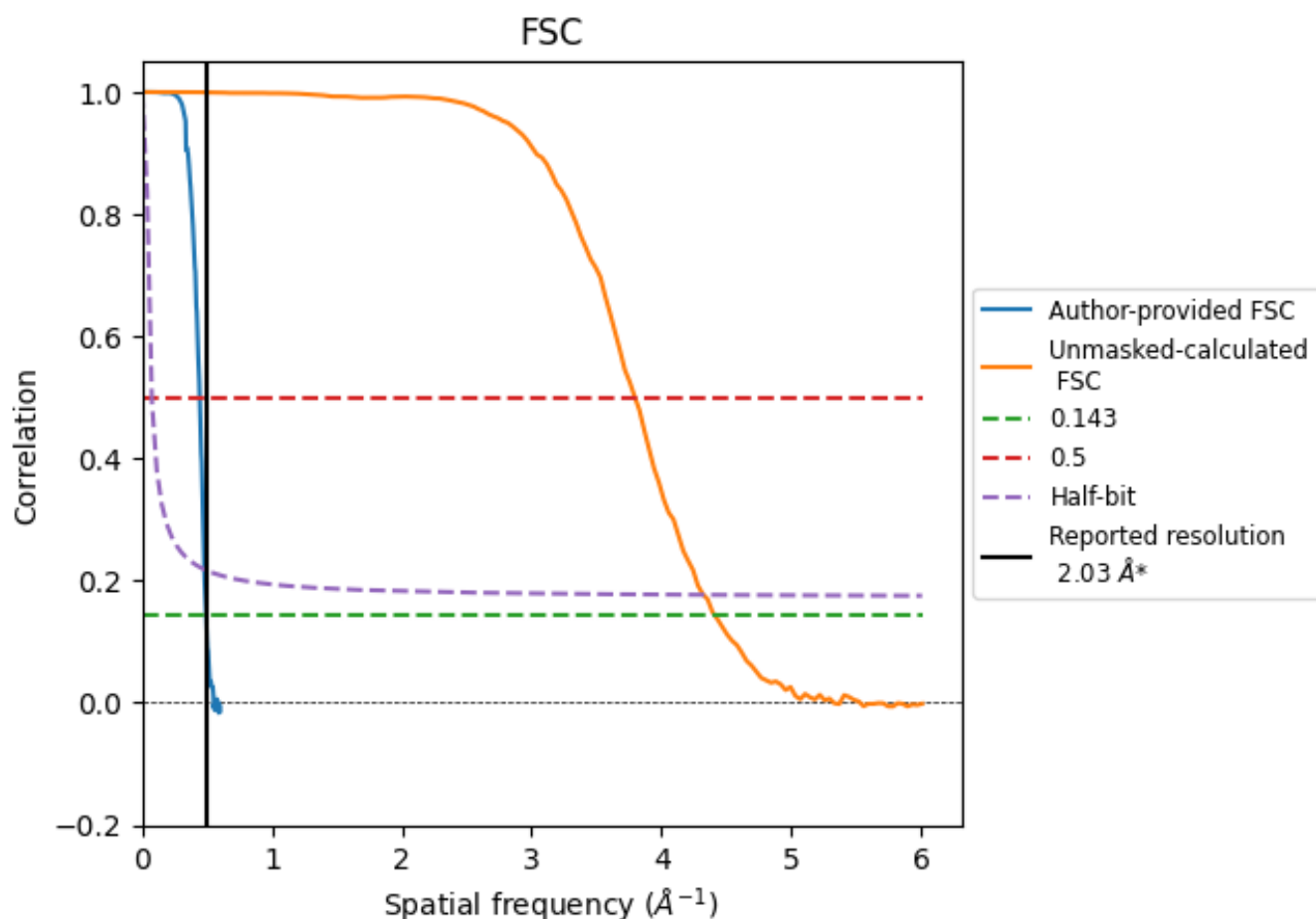


*Reported resolution corresponds to spatial frequency of 0.493 Å⁻¹

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 0.493 Å⁻¹

8.2 Resolution estimates [i](#)

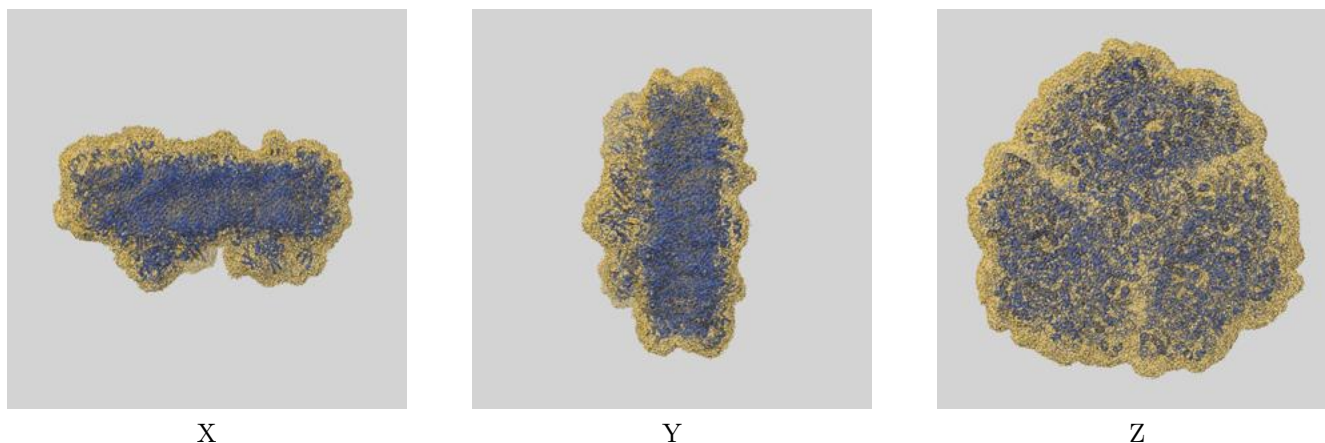
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.03	-	-
Author-provided FSC curve	2.03	2.26	2.06
Unmasked-calculated*	0.23	0.26	0.23

*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 0.23 differs from the reported value 2.03 by more than 10 %

9 Map-model fit [i](#)

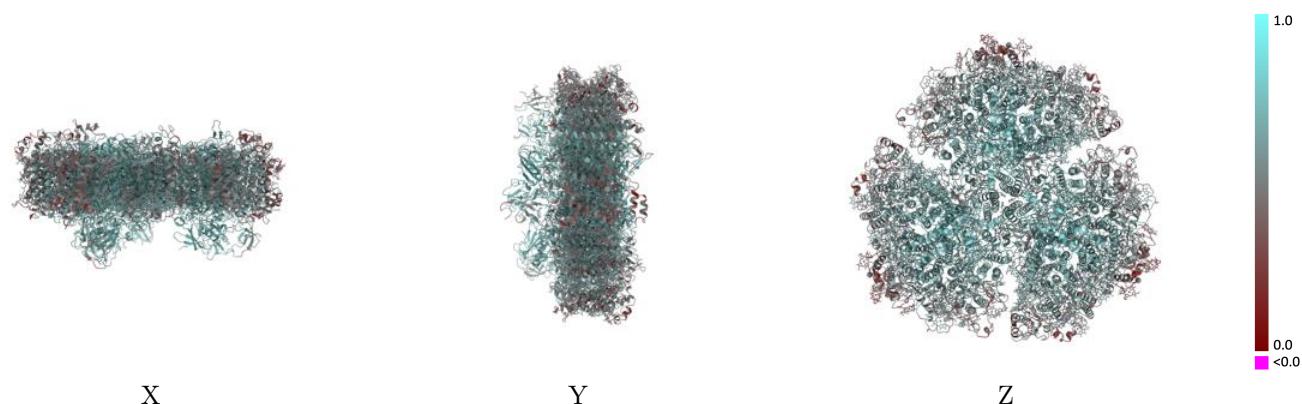
This section contains information regarding the fit between EMDB map EMD-43843 and PDB model 9AU4. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



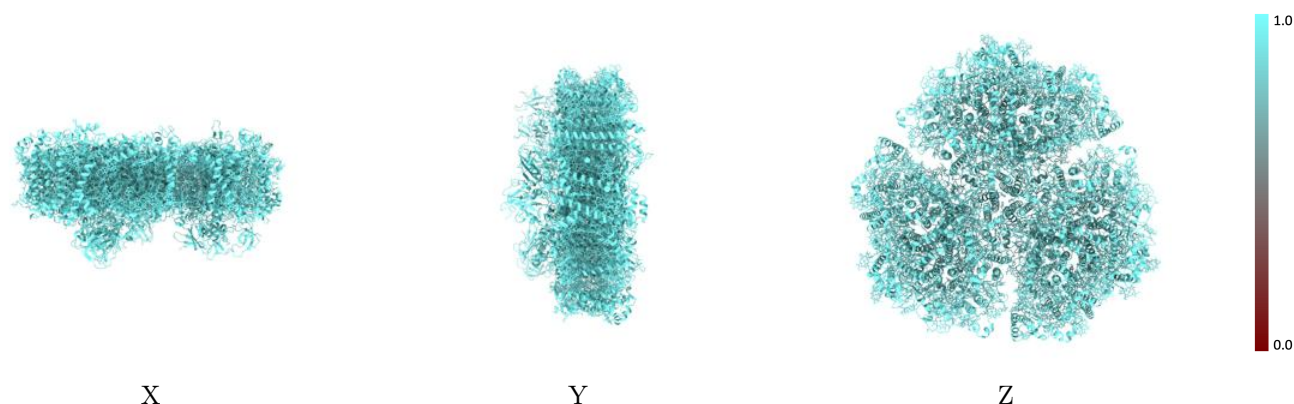
The images above show the 3D surface view of the map at the recommended contour level 0.0149 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



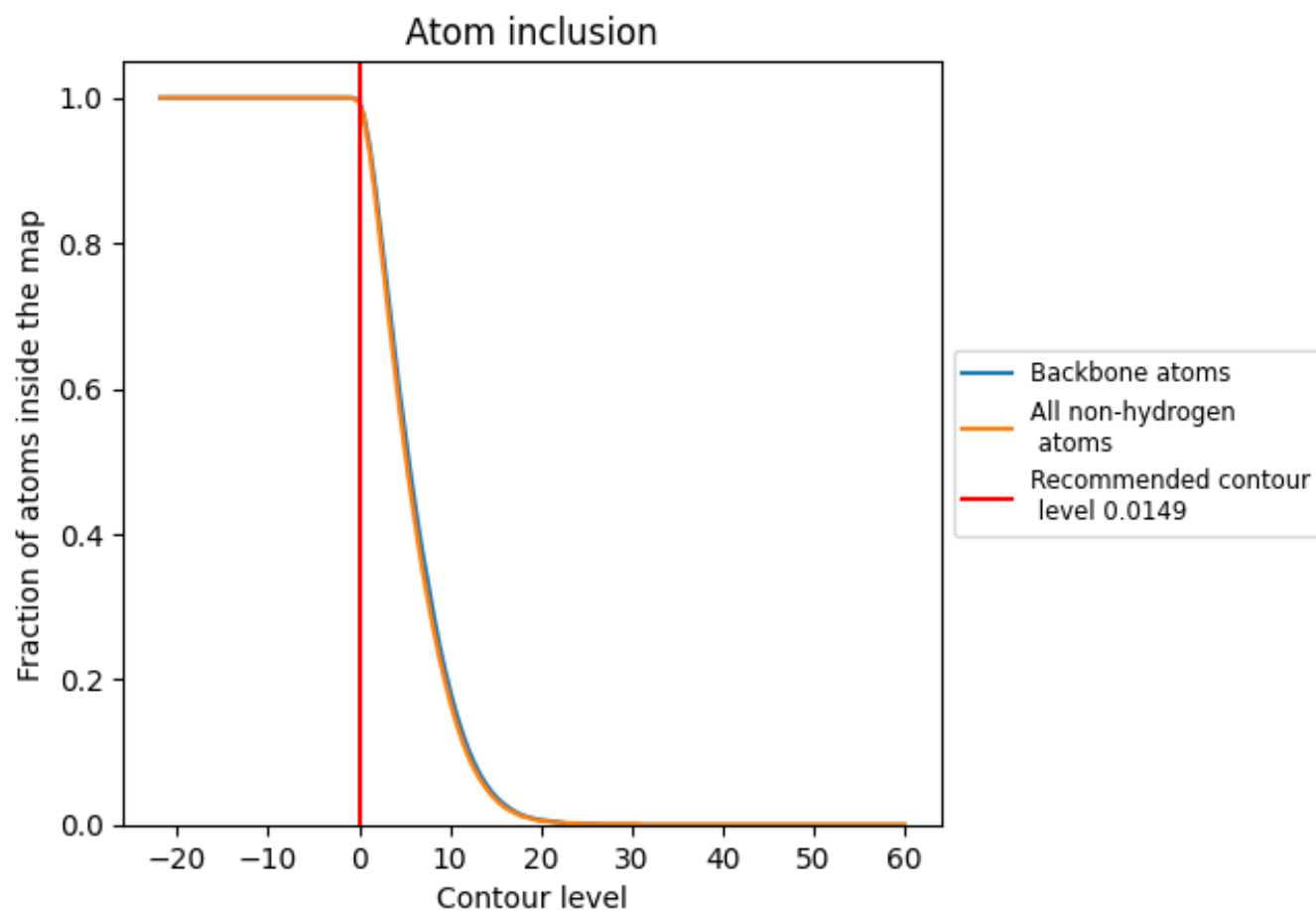
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0149).

9.4 Atom inclusion [i](#)



At the recommended contour level, 100% of all backbone atoms, 100% 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 (0.0149) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9950	 0.6100
A	 0.9960	 0.6240
B	 0.9960	 0.6230
C	 0.9970	 0.7170
D	 1.0000	 0.6860
E	 0.9940	 0.5800
F	 0.9880	 0.4410
G	 0.9950	 0.6180
H	 0.9960	 0.6180
I	 1.0000	 0.6990
J	 0.9870	 0.3880
K	 0.9860	 0.4140
L	 0.9990	 0.6850
M	 1.0000	 0.6520
N	 0.9980	 0.7120
O	 0.9990	 0.6740
P	 0.9850	 0.5580
Q	 0.9810	 0.4280
R	 0.9970	 0.6950
S	 0.9830	 0.3800
T	 0.9820	 0.3930
U	 0.9980	 0.6810
V	 1.0000	 0.6530
a	 0.9960	 0.6200
b	 0.9960	 0.6190
c	 0.9970	 0.7150
d	 1.0000	 0.6820
e	 0.9960	 0.5720
f	 0.9880	 0.4310
i	 1.0000	 0.6950
j	 0.9810	 0.3820
k	 0.9880	 0.3970
l	 0.9980	 0.6810
m	 1.0000	 0.6510

