



wwPDB EM Validation Summary Report ⓘ

Aug 4, 2026 – 11:07 PM EDT

PDB ID : 6VPV / pdb_00006vpv
EMDB ID : EMD-21320
Title : Trimeric Photosystem I from the High-Light Tolerant Cyanobacteria
Cyanobacterium Aponinum
Authors : Dobson, Z.; Toporik, H.; Vaughn, N.; Lin, S.; Williams, D.; Fromme, P.;
Mazor, Y.
Deposited on : 2020-02-04
Resolution : 2.70 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

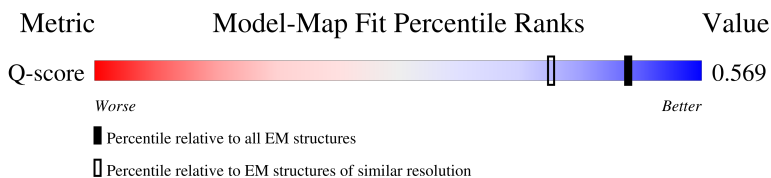
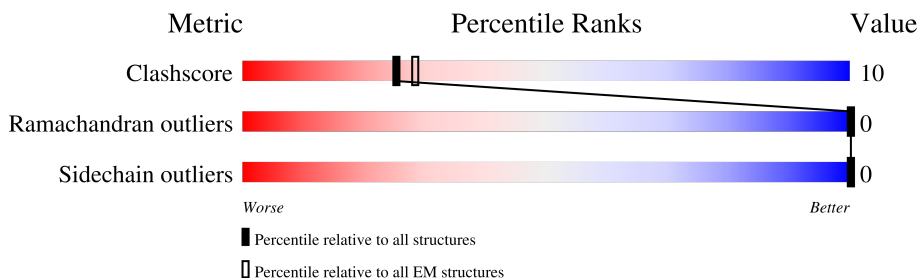
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

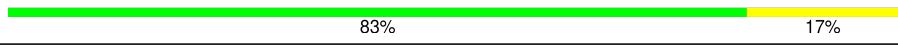
The reported resolution of this entry is 2.70 Å.

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.



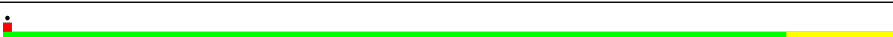
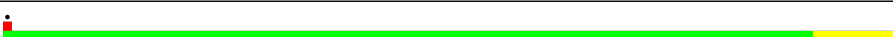
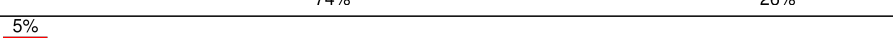
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	1	741	
1	A	741	
1	a	741	
2	2	737	

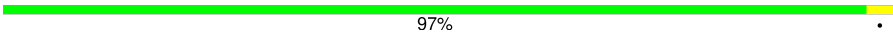
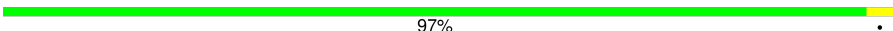
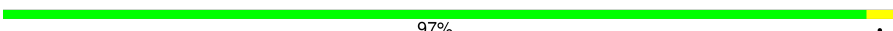
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Mol	Chain	Length	Quality of chain
2	B	737	
2	b	737	
3	3	80	
3	C	80	
3	c	80	
4	4	139	
4	D	139	
4	d	139	
5	5	68	
5	E	68	
5	e	68	
6	6	141	
6	F	141	
6	f	141	
7	7	38	
7	I	38	
7	i	38	
8	8	39	
8	J	39	
8	j	39	
9	9	78	
9	K	78	
9	k	78	
10	0	160	
10	L	160	

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Mol	Chain	Length	Quality of chain
10	l	160	 72% 28%
11	M	30	 97% •
11	m	30	 97% •
11	z	30	 97% •

2 Entry composition

There are 19 unique types of molecules in this entry. The entry contains 72192 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		
1	a	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		
1	1	741	Total	C	N	O	S	0	0
			5790	3797	983	984	26		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	320	ASN	SER	conflict	UNP A0A2G3P9X3
A	512	GLU	ASP	conflict	UNP A0A2G3P9X3
a	320	ASN	SER	conflict	UNP A0A2G3P9X3
a	512	GLU	ASP	conflict	UNP A0A2G3P9X3
1	320	ASN	SER	conflict	UNP A0A2G3P9X3
1	512	GLU	ASP	conflict	UNP A0A2G3P9X3

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		
2	b	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		
2	2	737	Total	C	N	O	S	0	0
			5815	3823	978	1000	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	80	Total	C	N	O	S	0	0
			599	368	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			599	368	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		
4	d	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		
4	4	139	Total	C	N	O	S	0	0
			1097	699	185	209	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	68	Total	C	N	O	0	0
			539	342	94	103		
5	e	68	Total	C	N	O	0	0
			539	342	94	103		
5	5	68	Total	C	N	O	0	0
			539	342	94	103		

- Molecule 6 is a protein called PSI-F.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		
6	f	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		
6	6	141	Total	C	N	O	S	0	0
			1100	708	180	207	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			275	186	39	48	2		
7	i	38	Total	C	N	O	S	0	0
			275	186	39	48	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	7	38	Total	C	N	O	S	0	0
			275	186	39	48	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	39	Total	C	N	O		0	0
			309	212	46	51			
8	j	39	Total	C	N	O		0	0
			309	212	46	51			
8	8	39	Total	C	N	O		0	0
			309	212	46	51			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	78	Total	C	N	O	S	0	0
			544	358	85	97	4		
9	k	78	Total	C	N	O	S	0	0
			544	358	85	97	4		
9	9	78	Total	C	N	O	S	0	0
			544	358	85	97	4		

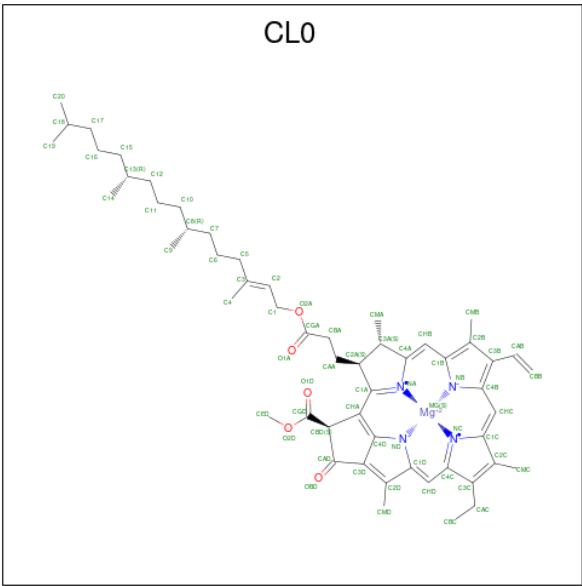
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		
10	l	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		
10	0	160	Total	C	N	O	S	0	0
			1183	770	193	215	5		

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

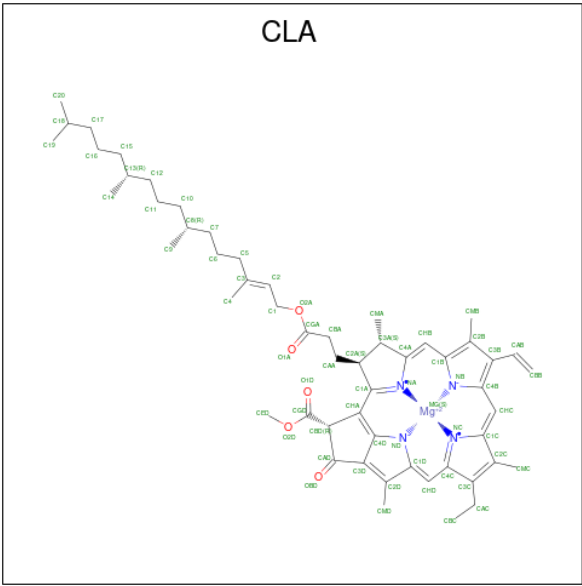
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	30	Total	C	N	O		0	0
			232	156	35	41			
11	m	30	Total	C	N	O		0	0
			232	156	35	41			
11	z	30	Total	C	N	O		0	0
			232	156	35	41			

- Molecule 12 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	B	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	F	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	F	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	I	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	J	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	J	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	K	1	Total 44	C 34	Mg 1	N 4	O 5	0
13	L	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	L	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	L	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	a	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 56	C 46	Mg 1	N 4	O 5	0
13	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 46	C 36	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 41	C 33	Mg 1	N 4	O 3	0
13	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	b	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	b	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 40	C 32	Mg 1	N 4	O 3	0

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Mol	Chain	Residues	Atoms					AltConf
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	i	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	j	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	j	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	k	1	Total 44	C 34	Mg 1	N 4	O 5	0
13	l	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	l	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	l	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	l	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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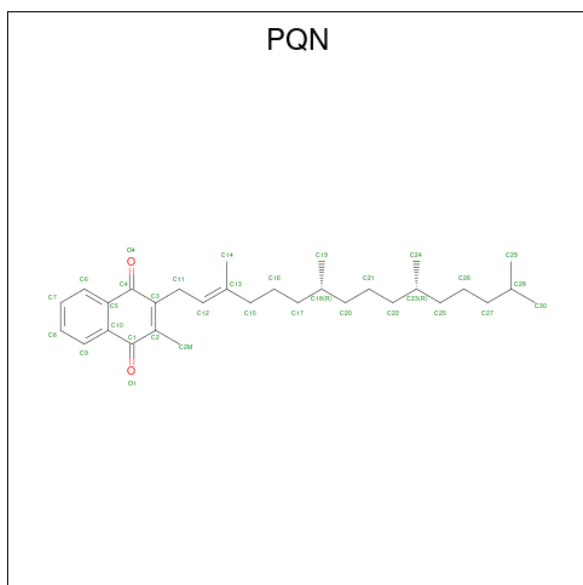
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 40	C 32	Mg 1	N 4	O 3	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	6	1	Total 46	C 36	Mg 1	N 4	O 5	0
13	7	1	Total 65	C 55	Mg 1	N 4	O 5	0

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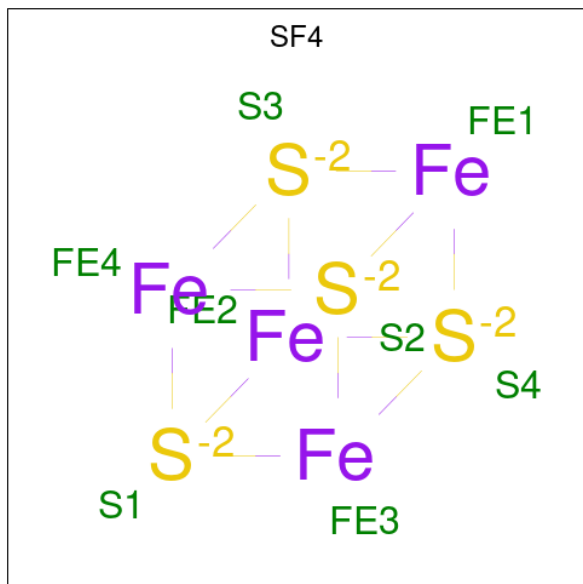
Mol	Chain	Residues	Atoms					AltConf
13	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms			AltConf
14	A	1	Total	C	O	0
			33	31	2	
14	B	1	Total	C	O	0
			33	31	2	
14	a	1	Total	C	O	0
			33	31	2	
14	b	1	Total	C	O	0
			33	31	2	
14	1	1	Total	C	O	0
			33	31	2	
14	2	1	Total	C	O	0
			33	31	2	

- Molecule 15 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



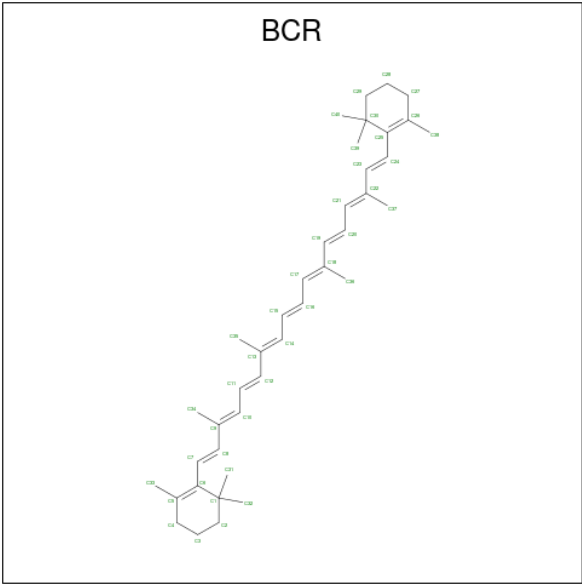
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	a	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	

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Mol	Chain	Residues	Atoms			AltConf
15	1	1	Total	Fe	S	0
			8	4	4	
15	3	1	Total	Fe	S	0
			8	4	4	
15	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	K	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	b	1	Total C 40 40	0

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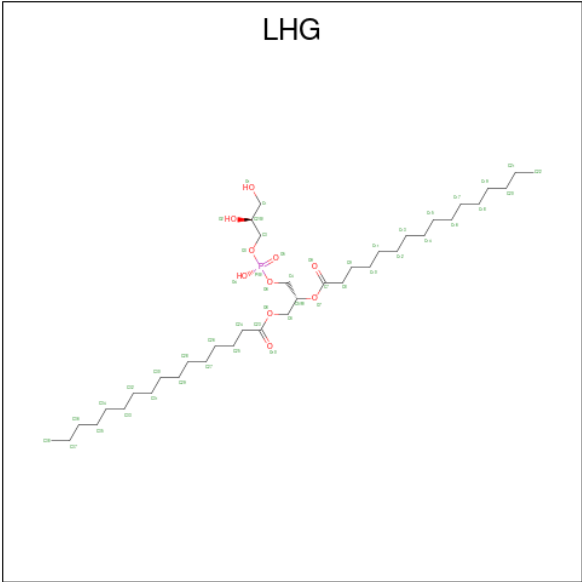
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	k	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0

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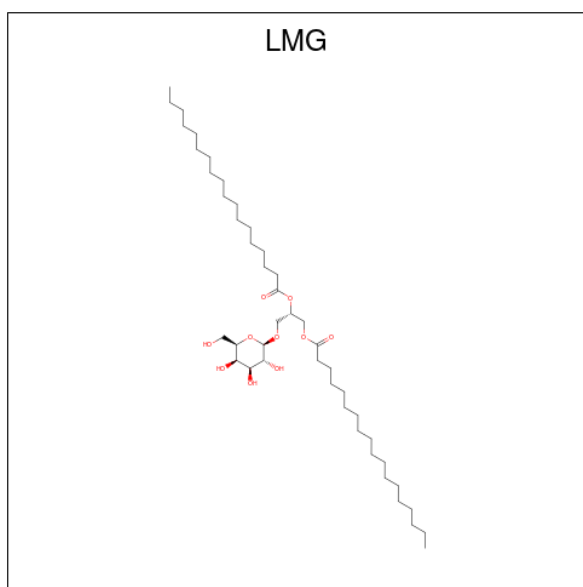
Mol	Chain	Residues	Atoms	AltConf
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	z	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



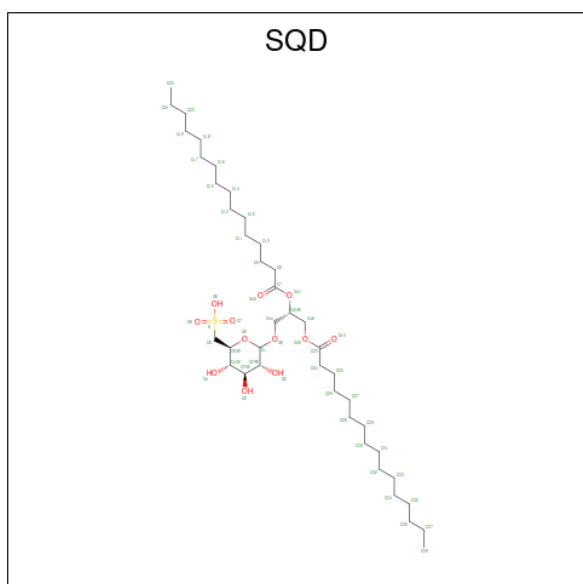
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	a	1	Total	C	O	P	0
			36	25	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	1	1	Total	C	O	P	0
			36	25	10	1	
17	1	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
18	B	1	41	31	10	0
18	b	1	41	31	10	0
18	2	1	41	31	10	0

- Molecule 19 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

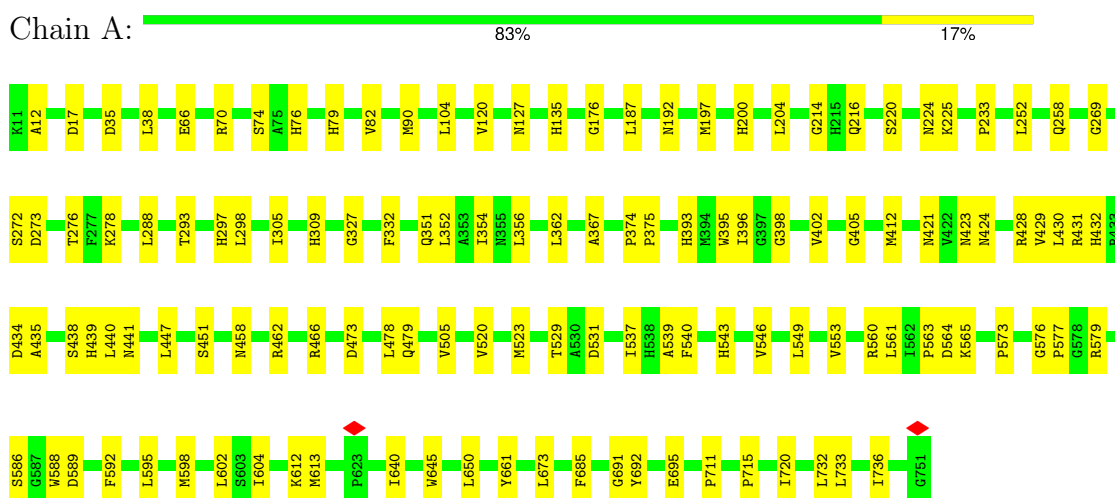


Mol	Chain	Residues	Atoms				AltConf
19	I	1	Total 50	C 37	O 12	S 1	0
19	i	1	Total 50	C 37	O 12	S 1	0
19	7	1	Total 50	C 37	O 12	S 1	0

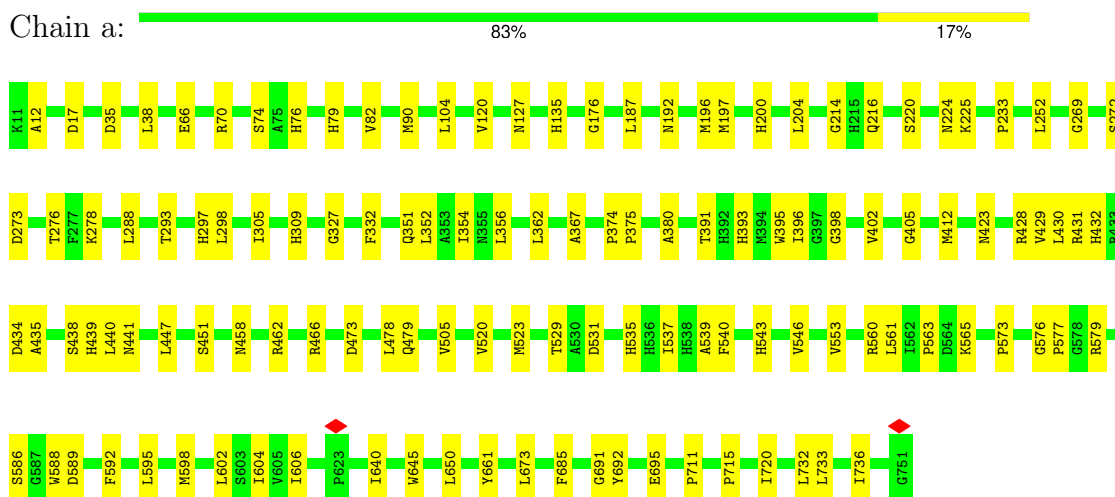
3 Residue-property plots

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

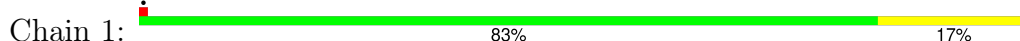
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

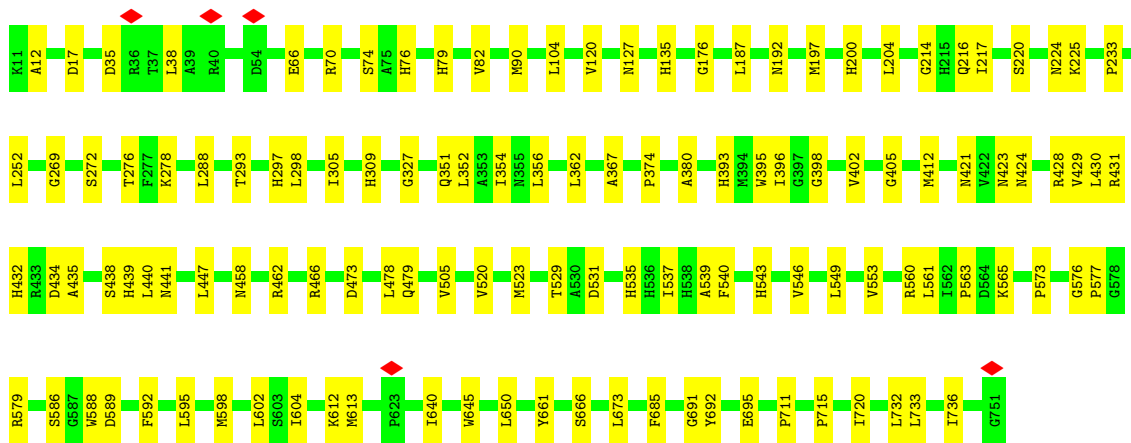


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



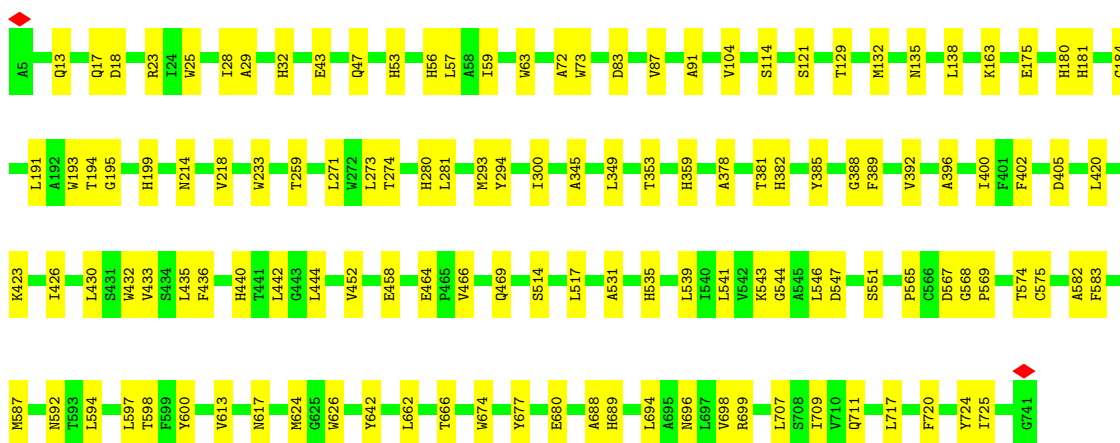
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





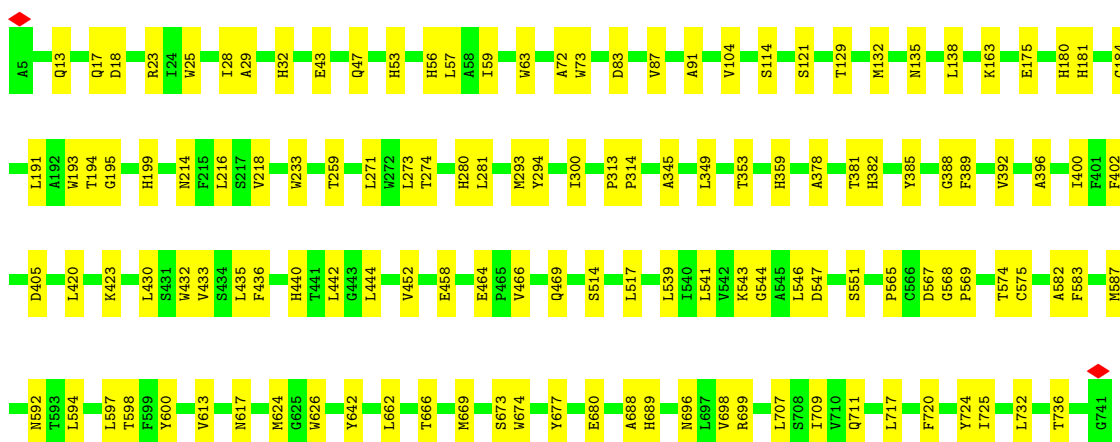
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 83% 17%



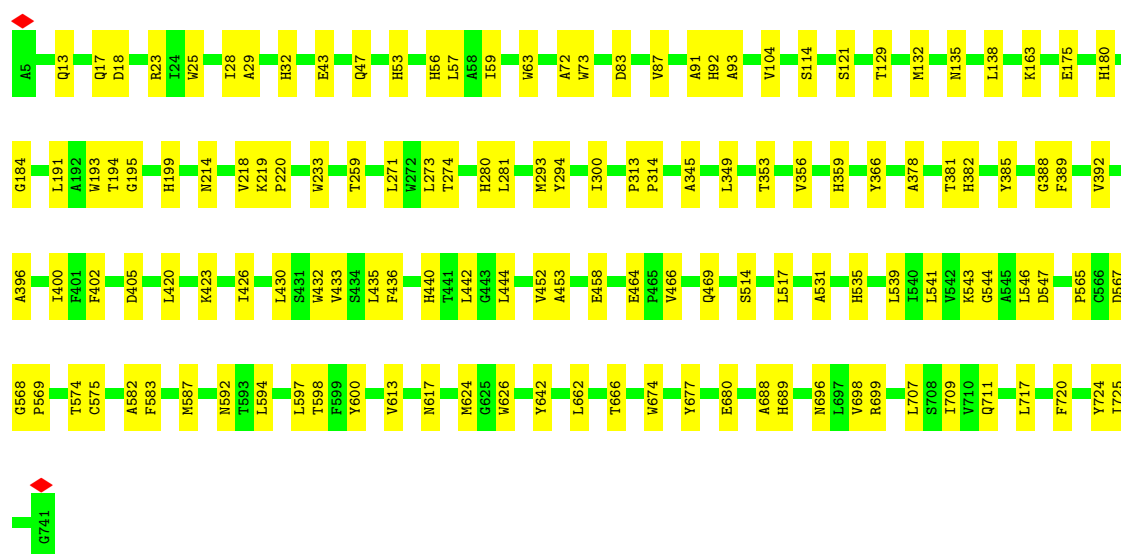
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 82% 18%



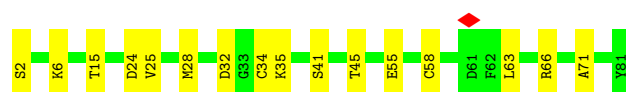
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  82% 18%



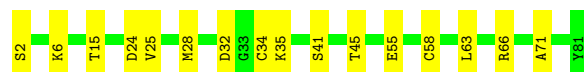
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  80% 20%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  80% 20%



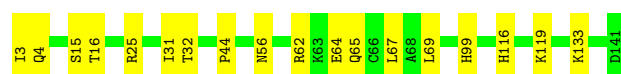
- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  79% 21%



- Molecule 4: Photosystem I reaction center subunit II

Chain D:  87% 13%



- Molecule 4: Photosystem I reaction center subunit II

Chain d:  87% 13%



- Molecule 4: Photosystem I reaction center subunit II

Chain 4:  88% 12%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  87% 13%



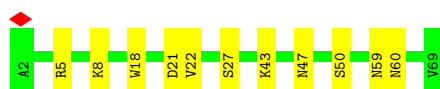
- Molecule 5: Photosystem I reaction center subunit IV

Chain e:  88% 12%



- Molecule 5: Photosystem I reaction center subunit IV

Chain 5:  84% 16%



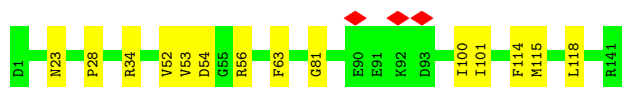
- Molecule 6: PSI-F

Chain F:  89% 11%



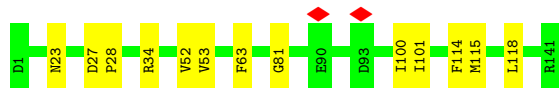
- Molecule 6: PSI-F

Chain f:  90% 10%



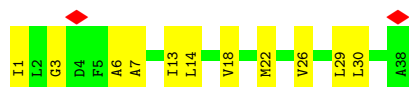
- Molecule 6: PSI-F

Chain 6:  91% 9%



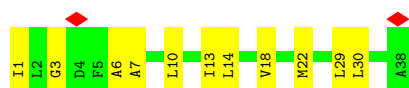
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  5% 71% 29%



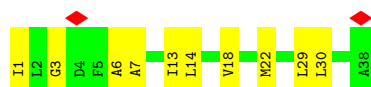
- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  5% 71% 29%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain 7:  5% 74% 26%



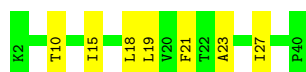
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  82% 18%



- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  82% 18%

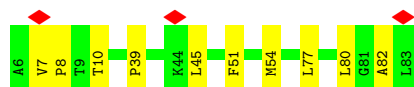
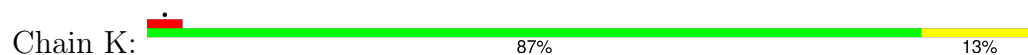


- Molecule 8: Photosystem I reaction center subunit IX

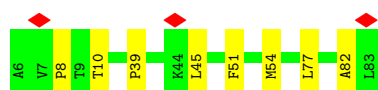
Chain 8:  82% 18%



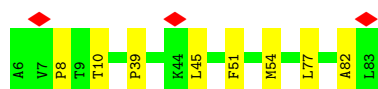
- Molecule 9: Photosystem I reaction center subunit PsaK



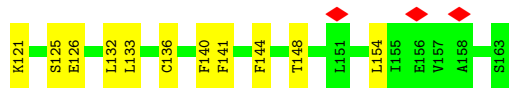
- Molecule 9: Photosystem I reaction center subunit PsaK



- Molecule 9: Photosystem I reaction center subunit PsaK



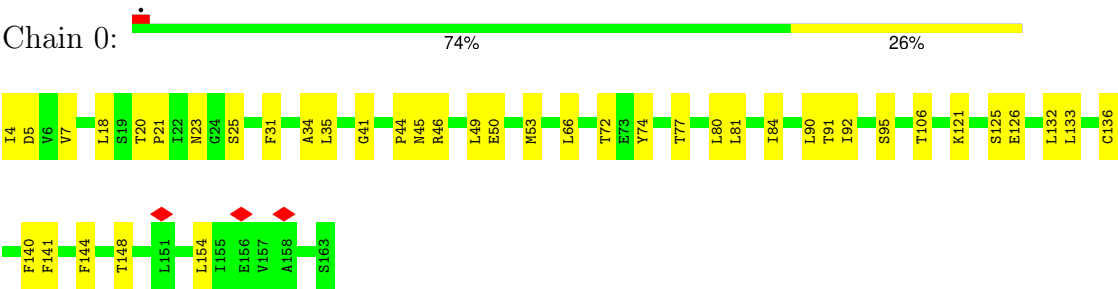
- Molecule 10: Photosystem I reaction center subunit XI



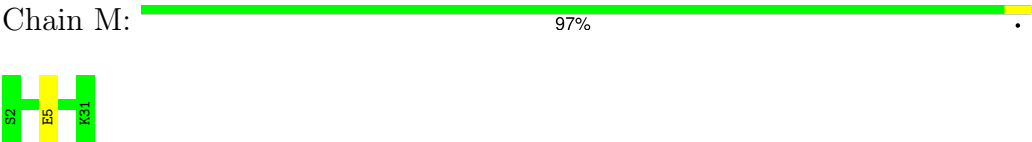
- Molecule 10: Photosystem I reaction center subunit XI



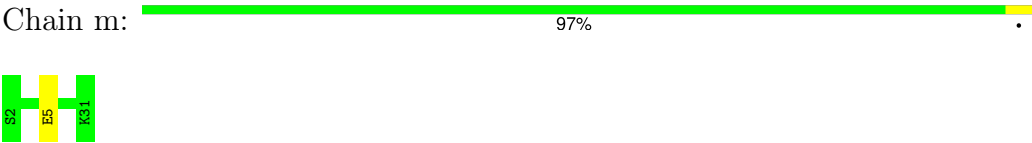
- Molecule 10: Photosystem I reaction center subunit XI



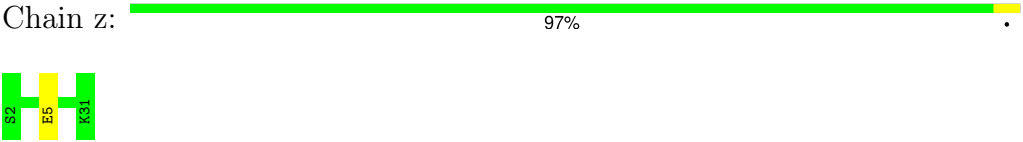
• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



• Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	75290	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.53	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	37.813	Depositor
Minimum map value	-24.049	Depositor
Average map value	0.001	Depositor
Map value standard deviation	1.148	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	315.19998, 315.19998, 315.19998	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0506666, 1.0506666, 1.0506666	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, BCR, SQD, LMG, CL0, CLA, SF4, PQN

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	1	0.26	0/5986	0.49	0/8157
1	A	0.26	0/5986	0.49	0/8157
1	a	0.26	0/5986	0.49	0/8157
2	2	0.27	0/6026	0.53	0/8237
2	B	0.26	0/6026	0.53	0/8237
2	b	0.27	0/6026	0.53	0/8237
3	3	0.26	0/609	0.54	0/824
3	C	0.26	0/609	0.54	0/824
3	c	0.26	0/609	0.54	0/824
4	4	0.24	0/1123	0.61	0/1514
4	D	0.24	0/1123	0.61	0/1514
4	d	0.25	0/1123	0.61	0/1514
5	5	0.21	0/549	0.48	0/741
5	E	0.21	0/549	0.48	0/741
5	e	0.21	0/549	0.48	0/741
6	6	0.25	0/1130	0.59	0/1533
6	F	0.24	0/1130	0.59	0/1533
6	f	0.25	0/1130	0.59	0/1533
7	7	0.26	0/280	0.66	0/381
7	I	0.26	0/280	0.66	0/381
7	i	0.26	0/280	0.66	0/381
8	8	0.28	0/318	0.43	0/435
8	J	0.28	0/318	0.43	0/435
8	j	0.28	0/318	0.43	0/435
9	9	0.28	0/556	0.67	0/759
9	K	0.28	0/556	0.67	0/759
9	k	0.28	0/556	0.67	0/759
10	0	0.27	0/1215	0.71	0/1659
10	L	0.27	0/1215	0.71	0/1659
10	l	0.27	0/1215	0.71	0/1659
11	M	0.16	0/235	0.37	0/318
11	m	0.16	0/235	0.37	0/318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	z	0.16	0/235	0.37	0/318
All	All	0.26	0/54081	0.54	0/73674

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	674	TRP	Peptide
2	B	674	TRP	Peptide
2	b	674	TRP	Peptide

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	1	5790	0	5666	97	0
1	A	5790	0	5666	102	0
1	a	5790	0	5666	98	0
2	2	5815	0	5585	111	0
2	B	5815	0	5585	110	0
2	b	5815	0	5585	109	0
3	3	599	0	579	13	0
3	C	599	0	579	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	c	599	0	579	12	0
4	4	1097	0	1080	15	0
4	D	1097	0	1080	16	0
4	d	1097	0	1080	16	0
5	5	539	0	530	7	0
5	E	539	0	530	6	0
5	e	539	0	530	5	0
6	6	1100	0	1075	19	0
6	F	1100	0	1075	19	0
6	f	1100	0	1075	20	0
7	7	275	0	296	22	0
7	I	275	0	296	23	0
7	i	275	0	296	24	0
8	8	309	0	323	7	0
8	J	309	0	323	7	0
8	j	309	0	323	7	0
9	9	544	0	556	5	0
9	K	544	0	556	7	0
9	k	544	0	556	5	0
10	0	1183	0	1186	111	0
10	L	1183	0	1186	123	0
10	l	1183	0	1186	114	0
11	M	232	0	252	1	0
11	m	232	0	252	1	0
11	z	232	0	252	1	0
12	1	65	0	72	5	0
12	A	65	0	72	5	0
12	a	65	0	72	5	0
13	0	286	0	275	16	0
13	1	2387	0	2270	113	0
13	2	2184	0	2136	88	0
13	6	146	0	115	3	0
13	7	65	0	72	8	0
13	8	135	0	100	3	0
13	9	135	0	96	1	0
13	A	2387	0	2270	107	0
13	B	2249	0	2208	90	0
13	F	146	0	115	6	0
13	I	65	0	72	9	0
13	J	135	0	100	3	0
13	K	135	0	96	0	0
13	L	221	0	203	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	a	2387	0	2270	109	0
13	b	2249	0	2208	90	0
13	f	146	0	115	6	0
13	i	65	0	72	9	0
13	j	135	0	100	3	0
13	k	135	0	96	0	0
13	l	221	0	203	15	0
14	1	33	0	46	2	0
14	2	33	0	46	7	0
14	A	33	0	46	4	0
14	B	33	0	46	7	0
14	a	33	0	46	4	0
14	b	33	0	46	6	0
15	1	8	0	0	0	0
15	3	16	0	0	1	0
15	A	8	0	0	0	0
15	C	16	0	0	0	0
15	a	8	0	0	0	0
15	c	16	0	0	0	0
16	0	120	0	168	10	0
16	1	200	0	280	18	0
16	2	280	0	392	23	0
16	6	80	0	112	4	0
16	7	40	0	56	3	0
16	8	80	0	112	5	0
16	9	80	0	112	5	0
16	A	200	0	280	20	0
16	B	280	0	392	19	0
16	F	80	0	112	5	0
16	I	40	0	56	5	0
16	J	80	0	112	3	0
16	K	80	0	112	2	0
16	L	120	0	168	16	0
16	M	40	0	56	2	0
16	a	200	0	280	17	0
16	b	280	0	392	21	0
16	f	80	0	112	4	0
16	i	40	0	56	5	0
16	j	80	0	112	4	0
16	k	80	0	112	2	0
16	l	120	0	168	12	0
16	m	40	0	56	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	z	40	0	56	3	0
17	1	77	0	97	2	0
17	A	77	0	97	2	0
17	a	77	0	97	1	0
18	2	41	0	52	3	0
18	B	41	0	52	3	0
18	b	41	0	52	3	0
19	7	50	0	64	12	0
19	I	50	0	64	13	0
19	i	50	0	64	12	0
All	All	72192	0	71571	1491	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 10.

The worst 5 of 1491 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)
6:6:115:MET:CE	6:6:118:LEU:HD12	1.29	1.59
6:F:115:MET:CE	6:F:118:LEU:HD12	1.29	1.58
6:f:115:MET:CE	6:f:118:LEU:HD12	1.29	1.56
7:i:30:LEU:HD21	19:i:101:SQD:C29	1.37	1.52
7:I:30:LEU:HD21	19:I:103:SQD:C29	1.40	1.46

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
1	A	739/741 (100%)	719 (97%)	20 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	739/741 (100%)	720 (97%)	19 (3%)	0	100	100
2	2	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
2	B	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
2	b	735/737 (100%)	712 (97%)	23 (3%)	0	100	100
3	3	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	c	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	4	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	D	137/139 (99%)	125 (91%)	12 (9%)	0	100	100
4	d	137/139 (99%)	126 (92%)	11 (8%)	0	100	100
5	5	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
5	E	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
5	e	66/68 (97%)	64 (97%)	2 (3%)	0	100	100
6	6	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
6	F	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
6	f	139/141 (99%)	128 (92%)	11 (8%)	0	100	100
7	7	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	I	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
7	i	36/38 (95%)	34 (94%)	2 (6%)	0	100	100
8	8	37/39 (95%)	37 (100%)	0	0	100	100
8	J	37/39 (95%)	37 (100%)	0	0	100	100
8	j	37/39 (95%)	37 (100%)	0	0	100	100
9	9	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
9	K	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
9	k	76/78 (97%)	69 (91%)	7 (9%)	0	100	100
10	0	158/160 (99%)	144 (91%)	14 (9%)	0	100	100
10	L	158/160 (99%)	144 (91%)	14 (9%)	0	100	100
10	l	158/160 (99%)	145 (92%)	13 (8%)	0	100	100
11	M	28/30 (93%)	28 (100%)	0	0	100	100
11	m	28/30 (93%)	28 (100%)	0	0	100	100
11	z	28/30 (93%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	6687/6753 (99%)	6412 (96%)	275 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	593/593 (100%)	593 (100%)	0	100	100
1	A	593/593 (100%)	593 (100%)	0	100	100
1	a	593/593 (100%)	593 (100%)	0	100	100
2	2	587/588 (100%)	587 (100%)	0	100	100
2	B	587/588 (100%)	587 (100%)	0	100	100
2	b	587/588 (100%)	587 (100%)	0	100	100
3	3	68/68 (100%)	68 (100%)	0	100	100
3	C	68/68 (100%)	68 (100%)	0	100	100
3	c	68/68 (100%)	68 (100%)	0	100	100
4	4	115/116 (99%)	115 (100%)	0	100	100
4	D	115/116 (99%)	115 (100%)	0	100	100
4	d	115/116 (99%)	115 (100%)	0	100	100
5	5	58/58 (100%)	58 (100%)	0	100	100
5	E	58/58 (100%)	58 (100%)	0	100	100
5	e	58/58 (100%)	58 (100%)	0	100	100
6	6	117/118 (99%)	117 (100%)	0	100	100
6	F	117/118 (99%)	117 (100%)	0	100	100
6	f	117/118 (99%)	117 (100%)	0	100	100
7	7	29/29 (100%)	29 (100%)	0	100	100
7	I	29/29 (100%)	29 (100%)	0	100	100
7	i	29/29 (100%)	29 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	8	34/34 (100%)	34 (100%)	0	100	100
8	J	34/34 (100%)	34 (100%)	0	100	100
8	j	34/34 (100%)	34 (100%)	0	100	100
9	9	53/55 (96%)	53 (100%)	0	100	100
9	K	53/55 (96%)	53 (100%)	0	100	100
9	k	53/55 (96%)	53 (100%)	0	100	100
10	0	124/124 (100%)	124 (100%)	0	100	100
10	L	124/124 (100%)	124 (100%)	0	100	100
10	l	124/124 (100%)	124 (100%)	0	100	100
11	M	25/25 (100%)	25 (100%)	0	100	100
11	m	25/25 (100%)	25 (100%)	0	100	100
11	z	25/25 (100%)	25 (100%)	0	100	100
All	All	5409/5424 (100%)	5409 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
2	b	711	GLN
1	1	240	HIS
10	0	150	HIS
5	e	64	HIS
10	l	45	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

384 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
13	CLA	B	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
13	CLA	B	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	7 (8%)
16	BCR	8	1105	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	7 (12%)
16	BCR	9	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	2	811	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	1	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.26	6 (7%)
13	CLA	1	827	-	69,73,73	1.14	10 (14%)	82,113,113	1.20	6 (7%)
13	CLA	B	828	-	59,63,73	1.26	9 (15%)	70,101,113	1.37	5 (7%)
13	CLA	2	808	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	6 (10%)
13	CLA	b	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
19	SQD	7	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.46	10 (17%)
13	CLA	b	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	B	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.38	4 (6%)
13	CLA	1	818	-	58,62,73	1.26	9 (15%)	68,99,113	1.45	7 (10%)
13	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	b	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
16	BCR	9	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	818	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)
13	CLA	F	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.26	3 (5%)
13	CLA	a	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
16	BCR	J	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	2	827	-	59,63,73	1.26	8 (13%)	70,101,113	1.37	5 (7%)
16	BCR	b	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
13	CLA	j	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.47	5 (9%)
13	CLA	a	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	6 (8%)
16	BCR	J	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
13	CLA	6	204	-	50,54,73	1.36	7 (14%)	59,90,113	1.27	3 (5%)
13	CLA	L	204	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	A	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.27	6 (8%)
16	BCR	A	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	8	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	b	847	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	b	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
19	SQD	I	103	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
16	BCR	z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	1	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	0	206	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
17	LHG	a	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
16	BCR	1	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	2	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	2	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.43	8 (10%)
16	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	B	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	A	824	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	B	823	-	69,73,73	1.17	9 (13%)	82,113,113	1.18	6 (7%)
13	CLA	B	829	-	66,70,73	1.17	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	A	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	2	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
16	BCR	1	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
16	BCR	2	839	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
18	LMG	2	845	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	K	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
13	CLA	1	822	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	8 (12%)
12	CL0	1	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.16	6 (7%)
13	CLA	f	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
16	BCR	k	4001	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)
16	BCR	1	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	b	834	-	64,68,73	1.21	9 (14%)	76,107,113	1.22	6 (7%)
13	CLA	A	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	A	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	A	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
13	CLA	f	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	b	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
13	CLA	2	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	b	817	-	45,49,73	1.40	8 (17%)	54,84,113	1.16	4 (7%)
15	SF4	3	102	3	0,12,12	-	-	-	-	-
16	BCR	i	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	10 (17%)
16	BCR	A	851	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	7 (12%)
13	CLA	1	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	5 (7%)
13	CLA	1	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	B	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	A	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)
13	CLA	A	807	-	59,63,73	1.25	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	A	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	a	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)
16	BCR	a	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	b	830	-	62,66,73	1.26	9 (14%)	73,104,113	1.43	5 (6%)
13	CLA	2	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
13	CLA	a	823	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	4 (6%)
13	CLA	A	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	a	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)
13	CLA	i	102	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
13	CLA	L	203	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
13	CLA	a	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
14	PQN	1	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	A	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	A	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
13	CLA	1	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	b	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.39	4 (6%)
13	CLA	b	818	-	50,54,73	1.35	7 (14%)	59,90,113	1.41	6 (10%)
13	CLA	1	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.22	6 (8%)
14	PQN	2	838	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	826	-	59,63,73	1.25	9 (15%)	70,101,113	1.23	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	0	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	6 (10%)
16	BCR	A	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	a	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
19	SQD	i	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
13	CLA	a	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	6 (10%)
13	CLA	a	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
16	BCR	j	1104	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	9 (16%)
13	CLA	B	834	-	64,68,73	1.20	9 (14%)	76,107,113	1.22	5 (6%)
13	CLA	b	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.56	10 (12%)
13	CLA	A	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.23	6 (8%)
16	BCR	0	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	F	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
17	LHG	A	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	b	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	7 (8%)
13	CLA	L	206	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
16	BCR	6	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
17	LHG	1	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
16	BCR	2	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.30	6 (10%)
16	BCR	L	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	9 (16%)
13	CLA	A	819	-	64,68,73	1.19	9 (14%)	76,107,113	1.52	7 (9%)
13	CLA	l	205	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	0	202	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	7	102	-	69,73,73	1.14	8 (11%)	82,113,113	1.27	6 (7%)
13	CLA	9	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
13	CLA	L	201	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	B	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.55	10 (12%)
16	BCR	2	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	1	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.41	5 (8%)
13	CLA	a	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	8 (11%)
13	CLA	2	836	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	830	-	62,66,73	1.25	9 (14%)	73,104,113	1.41	5 (6%)
13	CLA	1	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
13	CLA	2	831	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	a	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	M	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
16	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	A	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	7 (10%)
13	CLA	B	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	817	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
13	CLA	B	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
13	CLA	A	809	-	54,58,73	1.31	8 (14%)	64,95,113	1.34	7 (10%)
13	CLA	2	810	-	50,54,73	1.33	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	a	838	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
13	CLA	6	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
16	BCR	b	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	B	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
16	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	9 (16%)
13	CLA	b	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	b	822	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	2	813	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
13	CLA	B	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
16	BCR	l	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	B	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	a	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
16	BCR	7	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	2	828	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	9 (11%)
13	CLA	1	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	b	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	b	828	-	59,63,73	1.27	9 (15%)	70,101,113	1.38	4 (5%)
13	CLA	A	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	a	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
13	CLA	1	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	5 (7%)
13	CLA	A	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
13	CLA	b	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.18	6 (7%)
13	CLA	1	821	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	5 (6%)
13	CLA	1	813	-	59,63,73	1.25	9 (15%)	70,101,113	1.29	8 (11%)
16	BCR	b	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	k	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	m	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	a	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	9	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.36	4 (6%)
13	CLA	a	809	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
13	CLA	2	833	-	64,68,73	1.20	9 (14%)	76,107,113	1.22	5 (6%)
16	BCR	K	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	9	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
16	BCR	l	206	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
13	CLA	A	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.24	6 (7%)
13	CLA	B	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	A	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
13	CLA	a	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	8 (9%)
13	CLA	A	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)
13	CLA	1	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
13	CLA	a	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
16	BCR	b	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	1	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
16	BCR	8	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	a	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	A	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
13	CLA	a	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	6 (7%)
16	BCR	b	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	l	204	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	9 (14%)
13	CLA	B	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	10 (14%)
13	CLA	1	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	a	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	I	101	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	6 (7%)
12	CL0	a	801	-	69,73,73	1.18	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	1	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	7 (8%)
16	BCR	F	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	1	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.35	7 (10%)
16	BCR	2	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	a	837	-	64,68,73	1.21	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	A	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
16	BCR	1	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	2	825	-	64,68,73	1.24	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	A	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	9 (10%)
13	CLA	B	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	2	826	-	49,53,73	1.40	9 (18%)	58,89,113	1.30	6 (10%)
13	CLA	b	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	2	846	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
16	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	3 (5%)
14	PQN	A	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
17	LHG	A	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
15	SF4	a	844	1,2	0,12,12	-	-	-	-	-
13	CLA	0	203	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	1	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
13	CLA	b	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	1	829	-	69,73,73	1.15	10 (14%)	82,113,113	1.46	7 (8%)
14	PQN	b	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	B	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	a	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	8 (9%)
13	CLA	b	803	-	64,68,73	1.18	9 (14%)	76,107,113	1.42	8 (10%)
13	CLA	J	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	2	822	-	69,73,73	1.17	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	b	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	b	829	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	b	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	b	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
13	CLA	1	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	1	839	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
13	CLA	2	823	-	59,63,73	1.26	10 (16%)	70,101,113	1.57	10 (14%)
13	CLA	a	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	8	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.35	5 (8%)
13	CLA	a	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
16	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	B	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	k	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
13	CLA	B	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	1	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
16	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
13	CLA	a	804	-	59,63,73	1.24	9 (15%)	70,101,113	1.32	6 (8%)
13	CLA	A	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
17	LHG	1	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	1	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.53	7 (9%)
16	BCR	l	203	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	9 (16%)
13	CLA	A	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	a	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.51	7 (9%)
13	CLA	b	813	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	F	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	1	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
16	BCR	B	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
12	CL0	A	801	-	69,73,73	1.19	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	a	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	8 (10%)
16	BCR	6	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	A	834	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
14	PQN	B	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	B	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.42	8 (10%)
13	CLA	2	834	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
16	BCR	I	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	B	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	2	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.29	4 (5%)
13	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	B	847	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	B	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	7 (8%)
13	CLA	2	817	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)
13	CLA	a	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	2	837	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
16	BCR	1	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.42	9 (16%)
13	CLA	2	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.41	7 (8%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	1	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.38	5 (6%)
16	BCR	a	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.43	9 (16%)
13	CLA	b	836	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	2	821	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	b	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
13	CLA	a	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	5 (6%)
13	CLA	2	809	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	A	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	2	818	-	50,54,73	1.36	9 (18%)	59,90,113	1.38	4 (6%)
13	CLA	A	840	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	A	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	8 (12%)
13	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	K	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
16	BCR	k	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	b	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.29	6 (10%)
13	CLA	J	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	b	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	9 (12%)
16	BCR	B	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	b	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)
13	CLA	A	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.41	6 (7%)
16	BCR	b	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	a	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	9 (14%)
13	CLA	b	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	l	207	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
13	CLA	B	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	a	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	a	836	-	55,59,73	1.28	8 (14%)	64,96,113	1.39	8 (12%)
16	BCR	f	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
15	SF4	3	101	3	0,12,12	-	-	-	-	-
16	BCR	f	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	b	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	A	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.35	5 (7%)
18	LMG	b	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	a	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	1	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	6 (7%)
16	BCR	L	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
13	CLA	2	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	1	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	9 (14%)
13	CLA	A	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	1	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	4 (5%)
13	CLA	1	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	a	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	5 (7%)
13	CLA	b	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	a	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	6	201	-	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
13	CLA	2	816	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
13	CLA	1	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.25	4 (6%)
13	CLA	A	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	l	202	-	64,68,73	1.19	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	A	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	6 (8%)
13	CLA	j	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	6 (9%)
13	CLA	a	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
16	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	1	831	-	54,58,73	1.29	9 (16%)	64,95,113	1.44	9 (14%)
16	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
16	BCR	L	205	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	2	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	f	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
16	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	2	832	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	j	1103	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	1	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	1	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	2	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
13	CLA	2	829	-	62,66,73	1.25	9 (14%)	73,104,113	1.42	5 (6%)
13	CLA	1	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.54	11 (14%)
15	SF4	A	844	1,2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PQN	a	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
13	CLA	A	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	F	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.33	6 (10%)
13	CLA	A	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	5 (8%)
13	CLA	0	205	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
16	BCR	a	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	b	825	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
13	CLA	b	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
15	SF4	c	101	3	0,12,12	-	-	-	-	-
16	BCR	K	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	1	808	-	54,58,73	1.29	8 (14%)	64,95,113	1.73	6 (9%)
15	SF4	1	844	1,2	0,12,12	-	-	-	-	-
13	CLA	b	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	1	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
15	SF4	c	102	3	0,12,12	-	-	-	-	-
16	BCR	2	841	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
13	CLA	a	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	2	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	2	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	b	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	2	824	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
16	BCR	j	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
17	LHG	a	850	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	B	813	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	2	815	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
16	BCR	b	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
18	LMG	B	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	A	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
13	CLA	b	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	K	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	a	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	2	820	-	69,73,73	1.20	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	A	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	A	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	J	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	2	801	-	69,73,73	1.17	9 (13%)	82,113,113	1.56	11 (13%)
13	CLA	0	208	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	A	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	8	1102	-	44,48,73	1.45	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	1	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.34	6 (8%)
13	CLA	k	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	B	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)

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
13	CLA	B	838	-	-	7/39/115/115	-
13	CLA	B	802	-	-	9/39/115/115	-
16	BCR	8	1105	-	-	11/29/63/63	0/2/2/2
16	BCR	9	4001	-	-	9/29/63/63	0/2/2/2
13	CLA	2	811	-	-	4/15/91/115	-
13	CLA	1	837	-	-	8/33/109/115	-
13	CLA	1	827	-	-	13/39/115/115	-
13	CLA	B	828	-	-	9/27/103/115	-
13	CLA	2	808	-	-	5/15/91/115	-
13	CLA	b	816	-	-	7/33/109/115	-
19	SQD	7	101	-	-	19/45/65/69	0/1/1/1
13	CLA	b	833	-	-	6/21/97/115	-
13	CLA	B	819	-	-	6/17/93/115	-
13	CLA	1	818	-	-	7/26/102/115	-
13	CLA	B	831	-	-	7/39/115/115	-
13	CLA	b	835	-	-	3/21/97/115	-
16	BCR	9	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	B	818	-	-	10/17/93/115	-
13	CLA	F	204	-	-	8/17/93/115	-
13	CLA	a	810	-	-	8/15/91/115	-
16	BCR	J	1104	-	-	8/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	827	-	-	9/27/103/115	-
16	BCR	b	842	-	-	14/29/63/63	0/2/2/2
13	CLA	j	1102	-	-	6/10/82/115	-
13	CLA	a	835	-	-	14/29/105/115	-
16	BCR	J	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	a	821	-	-	11/39/115/115	-
13	CLA	6	204	-	-	8/17/93/115	-
13	CLA	L	204	-	-	4/17/93/115	-
13	CLA	A	835	-	-	14/29/105/115	-
16	BCR	A	846	-	-	6/29/63/63	0/2/2/2
13	CLA	8	1101	-	-	9/21/97/115	-
13	CLA	b	847	-	-	9/39/115/115	-
13	CLA	b	838	-	-	7/39/115/115	-
19	SQD	I	103	-	-	19/45/65/69	0/1/1/1
16	BCR	z	101	-	-	7/29/63/63	0/2/2/2
13	CLA	1	817	-	-	8/27/103/115	-
13	CLA	0	206	-	-	4/17/93/115	-
17	LHG	a	849	-	-	16/40/40/53	-
16	BCR	1	846	-	-	6/29/63/63	0/2/2/2
13	CLA	2	814	-	-	12/39/115/115	-
13	CLA	2	803	-	-	11/33/109/115	-
16	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	B	816	-	-	7/33/109/115	-
13	CLA	A	824	-	-	16/33/109/115	-
13	CLA	B	823	-	-	12/39/115/115	-
13	CLA	B	829	-	-	17/36/112/115	-
13	CLA	A	830	-	-	13/39/115/115	-
13	CLA	2	806	-	-	17/39/115/115	-
16	BCR	1	848	-	-	15/29/63/63	0/2/2/2
16	BCR	2	839	-	-	11/29/63/63	0/2/2/2
18	LMG	2	845	-	-	17/36/56/70	0/1/1/1
13	CLA	K	4003	-	-	8/17/93/115	-
13	CLA	1	822	-	-	8/21/97/115	-
12	CL0	1	801	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	f	204	-	-	8/17/93/115	-
16	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	1	851	-	-	13/29/63/63	0/2/2/2
13	CLA	b	834	-	-	6/33/109/115	-
13	CLA	A	822	-	-	8/21/97/115	-
13	CLA	A	831	-	-	8/21/97/115	-
13	CLA	1	812	-	-	6/17/93/115	-
13	CLA	A	816	-	-	8/17/93/115	-
13	CLA	f	201	-	-	6/27/103/115	-
13	CLA	b	814	-	-	8/21/97/115	-
13	CLA	2	804	-	-	17/39/115/115	-
13	CLA	b	817	-	-	2/10/86/115	-
16	BCR	i	103	-	-	8/29/63/63	0/2/2/2
15	SF4	3	102	3	-	-	0/6/5/5
16	BCR	A	851	-	-	13/29/63/63	0/2/2/2
13	CLA	1	805	-	-	12/27/103/115	-
13	CLA	1	828	-	-	9/39/115/115	-
13	CLA	B	833	-	-	6/21/97/115	-
13	CLA	A	802	-	-	10/33/109/115	-
13	CLA	A	807	-	-	4/27/103/115	-
13	CLA	A	812	-	-	6/17/93/115	-
13	CLA	a	831	-	-	8/21/97/115	-
16	BCR	a	851	-	-	13/29/63/63	0/2/2/2
13	CLA	b	830	-	-	10/31/107/115	-
13	CLA	2	802	-	-	9/39/115/115	-
15	SF4	C	101	3	-	-	0/6/5/5
13	CLA	a	823	-	-	7/21/97/115	-
13	CLA	A	806	-	-	12/39/115/115	-
13	CLA	a	802	-	-	10/33/109/115	-
13	CLA	i	102	-	-	14/39/115/115	-
13	CLA	L	203	-	-	7/21/97/115	-
13	CLA	a	828	-	-	9/39/115/115	-
14	PQN	1	843	-	-	10/23/43/43	0/2/2/2
13	CLA	A	823	-	-	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	841	-	-	12/33/109/115	-
13	CLA	1	806	-	-	12/39/115/115	-
13	CLA	b	819	-	-	6/17/93/115	-
13	CLA	b	818	-	-	10/17/93/115	-
13	CLA	1	826	-	-	7/27/103/115	-
14	PQN	2	838	-	-	10/23/43/43	0/2/2/2
13	CLA	a	826	-	-	7/27/103/115	-
16	BCR	0	201	-	-	7/29/63/63	0/2/2/2
16	BCR	A	845	-	-	8/29/63/63	0/2/2/2
13	CLA	a	816	-	-	8/17/93/115	-
19	SQD	i	101	-	-	19/45/65/69	0/1/1/1
13	CLA	a	815	-	-	3/15/91/115	-
13	CLA	a	825	-	-	15/36/112/115	-
16	BCR	j	1104	-	-	8/29/63/63	0/2/2/2
13	CLA	B	834	-	-	6/33/109/115	-
13	CLA	b	801	-	-	6/39/115/115	-
13	CLA	A	826	-	-	7/27/103/115	-
16	BCR	0	207	-	-	11/29/63/63	0/2/2/2
16	BCR	F	202	-	-	12/29/63/63	0/2/2/2
17	LHG	A	849	-	-	16/40/40/53	-
13	CLA	b	804	-	-	17/39/115/115	-
13	CLA	L	206	-	-	9/39/115/115	-
16	BCR	6	202	-	-	12/29/63/63	0/2/2/2
17	LHG	1	849	-	-	16/40/40/53	-
16	BCR	2	840	-	-	8/29/63/63	0/2/2/2
13	CLA	B	827	-	-	8/15/91/115	-
16	BCR	L	202	-	-	10/29/63/63	0/2/2/2
13	CLA	A	819	-	-	12/33/109/115	-
13	CLA	l	205	-	-	4/17/93/115	-
13	CLA	0	202	-	-	10/33/109/115	-
13	CLA	7	102	-	-	14/39/115/115	-
13	CLA	9	4005	-	-	6/13/89/115	-
13	CLA	L	201	-	-	10/33/109/115	-
13	CLA	B	801	-	-	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	2	844	-	-	15/29/63/63	0/2/2/2
13	CLA	1	815	-	-	3/15/91/115	-
13	CLA	a	813	-	-	10/27/103/115	-
13	CLA	2	836	-	-	14/39/115/115	-
13	CLA	B	830	-	-	10/31/107/115	-
13	CLA	1	838	-	-	10/39/115/115	-
13	CLA	2	831	-	-	4/10/82/115	-
13	CLA	a	827	-	-	13/39/115/115	-
16	BCR	M	101	-	-	7/29/63/63	0/2/2/2
16	BCR	2	847	-	-	10/29/63/63	0/2/2/2
13	CLA	A	813	-	-	10/27/103/115	-
13	CLA	B	837	-	-	14/39/115/115	-
13	CLA	B	817	-	-	2/10/86/115	-
13	CLA	B	820	-	-	8/27/103/115	-
13	CLA	A	809	-	-	9/21/97/115	-
13	CLA	2	810	-	-	8/17/93/115	-
13	CLA	a	838	-	-	10/39/115/115	-
13	CLA	6	203	-	-	1/15/91/115	-
16	BCR	b	844	-	-	6/29/63/63	0/2/2/2
13	CLA	B	822	-	-	2/21/97/115	-
16	BCR	0	204	-	-	10/29/63/63	0/2/2/2
13	CLA	b	811	-	-	8/17/93/115	-
13	CLA	b	822	-	-	2/21/97/115	-
13	CLA	2	813	-	-	8/21/97/115	-
13	CLA	B	807	-	-	15/39/115/115	-
16	BCR	l	201	-	-	7/29/63/63	0/2/2/2
13	CLA	B	836	-	-	5/39/115/115	-
13	CLA	a	818	-	-	7/26/102/115	-
16	BCR	7	103	-	-	8/29/63/63	0/2/2/2
13	CLA	2	828	-	-	17/36/112/115	-
13	CLA	1	810	-	-	8/15/91/115	-
13	CLA	b	805	-	-	13/39/115/115	-
13	CLA	b	828	-	-	9/27/103/115	-
13	CLA	A	836	-	-	6/23/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	834	-	-	12/39/115/115	-
13	CLA	1	835	-	-	14/29/105/115	-
13	CLA	A	808	-	-	5/21/97/115	-
13	CLA	b	823	-	-	12/39/115/115	-
13	CLA	1	821	-	-	11/39/115/115	-
13	CLA	1	813	-	-	10/27/103/115	-
16	BCR	b	841	-	-	8/29/63/63	0/2/2/2
13	CLA	k	4005	-	-	6/13/89/115	-
16	BCR	A	847	-	-	15/29/63/63	0/2/2/2
16	BCR	m	101	-	-	7/29/63/63	0/2/2/2
13	CLA	a	830	-	-	13/39/115/115	-
13	CLA	9	4002	-	-	7/15/91/115	-
13	CLA	a	809	-	-	9/21/97/115	-
13	CLA	2	833	-	-	6/33/109/115	-
16	BCR	K	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	9	4003	-	-	8/17/93/115	-
16	BCR	l	206	-	-	11/29/63/63	0/2/2/2
13	CLA	A	852	-	-	13/33/109/115	-
13	CLA	B	826	-	-	14/33/109/115	-
13	CLA	A	818	-	-	7/26/102/115	-
13	CLA	a	803	-	-	11/39/115/115	-
13	CLA	A	827	-	-	13/39/115/115	-
13	CLA	1	834	-	-	12/39/115/115	-
13	CLA	a	852	-	-	13/33/109/115	-
16	BCR	b	843	-	-	9/29/63/63	0/2/2/2
13	CLA	1	842	-	-	7/15/91/115	-
16	BCR	8	1104	-	-	9/29/63/63	0/2/2/2
13	CLA	a	829	-	-	12/39/115/115	-
13	CLA	A	825	-	-	15/36/112/115	-
13	CLA	a	833	-	-	13/39/115/115	-
16	BCR	b	840	-	-	11/29/63/63	0/2/2/2
13	CLA	l	204	-	-	7/21/97/115	-
13	CLA	B	824	-	-	7/27/103/115	-
13	CLA	1	852	-	-	13/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	822	-	-	8/21/97/115	-
13	CLA	I	101	-	-	14/39/115/115	-
12	CL0	a	801	-	-	14/39/115/115	-
13	CLA	1	830	-	-	13/39/115/115	-
16	BCR	F	205	-	-	12/29/63/63	0/2/2/2
13	CLA	1	809	-	-	9/21/97/115	-
16	BCR	2	842	-	-	9/29/63/63	0/2/2/2
13	CLA	a	837	-	-	8/33/109/115	-
13	CLA	A	838	-	-	10/39/115/115	-
16	BCR	1	845	-	-	8/29/63/63	0/2/2/2
13	CLA	2	825	-	-	14/33/109/115	-
13	CLA	A	839	-	-	9/39/115/115	-
13	CLA	B	832	-	-	4/10/82/115	-
13	CLA	2	826	-	-	8/15/91/115	-
13	CLA	b	807	-	-	15/39/115/115	-
13	CLA	2	846	-	-	9/39/115/115	-
16	BCR	a	845	-	-	8/29/63/63	0/2/2/2
14	PQN	A	843	-	-	10/23/43/43	0/2/2/2
17	LHG	A	850	-	-	19/45/45/53	-
15	SF4	a	844	1,2	-	-	0/6/5/5
13	CLA	0	203	-	-	15/39/115/115	-
13	CLA	1	816	-	-	8/17/93/115	-
13	CLA	b	812	-	-	4/15/91/115	-
13	CLA	1	829	-	-	12/39/115/115	-
14	PQN	b	839	-	-	10/23/43/43	0/2/2/2
13	CLA	B	805	-	-	13/39/115/115	-
13	CLA	a	839	-	-	9/39/115/115	-
13	CLA	b	803	-	-	11/33/109/115	-
13	CLA	J	1101	-	-	9/21/97/115	-
13	CLA	2	822	-	-	12/39/115/115	-
13	CLA	b	815	-	-	12/39/115/115	-
13	CLA	b	829	-	-	17/36/112/115	-
13	CLA	b	837	-	-	14/39/115/115	-
13	CLA	B	812	-	-	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	802	-	-	9/39/115/115	-
13	CLA	1	823	-	-	7/21/97/115	-
13	CLA	1	839	-	-	9/39/115/115	-
13	CLA	2	823	-	-	7/27/103/115	-
13	CLA	a	807	-	-	4/27/103/115	-
13	CLA	8	1103	-	-	8/15/91/115	-
16	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	a	832	-	-	9/39/115/115	-
13	CLA	B	811	-	-	8/17/93/115	-
13	CLA	k	4003	-	-	8/17/93/115	-
13	CLA	B	806	-	-	16/39/115/115	-
16	BCR	B	840	-	-	11/29/63/63	0/2/2/2
13	CLA	1	841	-	-	12/33/109/115	-
16	BCR	B	841	-	-	8/29/63/63	0/2/2/2
13	CLA	B	814	-	-	8/21/97/115	-
13	CLA	a	804	-	-	3/27/103/115	-
13	CLA	A	832	-	-	9/39/115/115	-
17	LHG	1	850	-	-	20/45/45/53	-
13	CLA	1	819	-	-	12/33/109/115	-
16	BCR	l	203	-	-	10/29/63/63	0/2/2/2
13	CLA	A	829	-	-	12/39/115/115	-
13	CLA	a	819	-	-	12/33/109/115	-
13	CLA	b	813	-	-	15/39/115/115	-
13	CLA	F	201	-	-	6/27/103/115	-
13	CLA	1	825	-	-	15/36/112/115	-
16	BCR	B	842	-	-	14/29/63/63	0/2/2/2
12	CL0	A	801	-	-	14/39/115/115	-
13	CLA	a	841	-	-	12/33/109/115	-
16	BCR	6	205	-	-	12/29/63/63	0/2/2/2
13	CLA	A	834	-	-	12/39/115/115	-
14	PQN	B	839	-	-	10/23/43/43	0/2/2/2
13	CLA	a	820	-	-	5/17/93/115	-
13	CLA	B	803	-	-	11/33/109/115	-
13	CLA	2	834	-	-	3/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	I	102	-	-	8/29/63/63	0/2/2/2
13	CLA	B	835	-	-	3/21/97/115	-
13	CLA	2	819	-	-	8/27/103/115	-
13	CLA	B	815	-	-	12/39/115/115	-
13	CLA	B	847	-	-	9/39/115/115	-
13	CLA	B	821	-	-	19/39/115/115	-
13	CLA	2	817	-	-	10/17/93/115	-
13	CLA	a	805	-	-	12/27/103/115	-
13	CLA	2	837	-	-	7/39/115/115	-
16	BCR	1	847	-	-	15/29/63/63	0/2/2/2
13	CLA	2	830	-	-	7/39/115/115	-
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	A	803	-	-	11/39/115/115	-
13	CLA	B	808	-	-	14/39/115/115	-
13	CLA	1	824	-	-	16/33/109/115	-
16	BCR	a	847	-	-	15/29/63/63	0/2/2/2
13	CLA	b	836	-	-	5/39/115/115	-
13	CLA	2	821	-	-	2/21/97/115	-
13	CLA	b	820	-	-	8/27/103/115	-
13	CLA	a	824	-	-	16/33/109/115	-
13	CLA	2	809	-	-	15/39/115/115	-
13	CLA	A	810	-	-	8/15/91/115	-
13	CLA	2	818	-	-	6/17/93/115	-
13	CLA	A	840	-	-	13/39/115/115	-
13	CLA	A	814	-	-	4/21/97/115	-
13	CLA	B	804	-	-	17/39/115/115	-
13	CLA	K	4005	-	-	6/13/89/115	-
16	BCR	k	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	b	827	-	-	8/15/91/115	-
13	CLA	J	1103	-	-	8/15/91/115	-
13	CLA	b	824	-	-	7/27/103/115	-
16	BCR	B	848	-	-	10/29/63/63	0/2/2/2
13	CLA	b	809	-	-	5/15/91/115	-
13	CLA	A	833	-	-	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	b	845	-	-	15/29/63/63	0/2/2/2
13	CLA	a	814	-	-	4/21/97/115	-
13	CLA	b	821	-	-	19/39/115/115	-
13	CLA	l	207	-	-	9/39/115/115	-
13	CLA	B	810	-	-	15/39/115/115	-
13	CLA	a	817	-	-	8/27/103/115	-
13	CLA	a	836	-	-	6/23/99/115	-
16	BCR	f	205	-	-	12/29/63/63	0/2/2/2
15	SF4	3	101	3	-	-	0/6/5/5
16	BCR	f	202	-	-	12/29/63/63	0/2/2/2
13	CLA	b	808	-	-	14/39/115/115	-
13	CLA	A	811	-	-	10/29/105/115	-
18	LMG	b	846	-	-	17/36/56/70	0/1/1/1
13	CLA	1	803	-	-	11/39/115/115	-
13	CLA	a	812	-	-	6/17/93/115	-
13	CLA	1	833	-	-	13/39/115/115	-
16	BCR	L	207	-	-	7/29/63/63	0/2/2/2
13	CLA	2	835	-	-	5/39/115/115	-
13	CLA	1	814	-	-	4/21/97/115	-
13	CLA	A	820	-	-	5/17/93/115	-
13	CLA	1	811	-	-	10/29/105/115	-
13	CLA	1	836	-	-	6/23/99/115	-
13	CLA	a	811	-	-	10/29/105/115	-
13	CLA	b	826	-	-	14/33/109/115	-
13	CLA	a	840	-	-	13/39/115/115	-
13	CLA	6	201	-	-	6/27/103/115	-
13	CLA	2	816	-	-	2/10/86/115	-
13	CLA	1	820	-	-	5/17/93/115	-
13	CLA	A	828	-	-	9/39/115/115	-
13	CLA	l	202	-	-	10/33/109/115	-
13	CLA	A	804	-	-	3/27/103/115	-
13	CLA	j	1101	-	-	9/21/97/115	-
13	CLA	a	808	-	-	5/21/97/115	-
16	BCR	B	845	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	831	-	-	8/21/97/115	-
16	BCR	A	848	-	-	15/29/63/63	0/2/2/2
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
16	BCR	2	843	-	-	6/29/63/63	0/2/2/2
13	CLA	f	203	-	-	1/15/91/115	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	2	832	-	-	6/21/97/115	-
13	CLA	j	1103	-	-	8/15/91/115	-
13	CLA	1	840	-	-	13/39/115/115	-
13	CLA	1	832	-	-	10/39/115/115	-
13	CLA	2	805	-	-	13/39/115/115	-
13	CLA	2	829	-	-	10/31/107/115	-
13	CLA	1	802	-	-	10/33/109/115	-
15	SF4	A	844	1,2	-	-	0/6/5/5
14	PQN	a	843	-	-	10/23/43/43	0/2/2/2
13	CLA	B	825	-	-	8/39/115/115	-
13	CLA	A	842	-	-	7/15/91/115	-
13	CLA	F	203	-	-	1/15/91/115	-
13	CLA	A	815	-	-	3/15/91/115	-
13	CLA	0	205	-	-	7/21/97/115	-
16	BCR	a	848	-	-	15/29/63/63	0/2/2/2
13	CLA	b	825	-	-	8/39/115/115	-
13	CLA	b	806	-	-	16/39/115/115	-
15	SF4	c	101	3	-	-	0/6/5/5
16	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	1	808	-	-	5/21/97/115	-
15	SF4	1	844	1,2	-	-	0/6/5/5
13	CLA	b	832	-	-	4/10/82/115	-
13	CLA	1	807	-	-	4/27/103/115	-
16	BCR	2	841	-	-	14/29/63/63	0/2/2/2
15	SF4	c	102	3	-	-	0/6/5/5
13	CLA	a	842	-	-	7/15/91/115	-
13	CLA	2	807	-	-	14/39/115/115	-
13	CLA	2	812	-	-	16/39/115/115	-
13	CLA	b	810	-	-	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	824	-	-	8/39/115/115	-
16	BCR	j	1105	-	-	11/29/63/63	0/2/2/2
17	LHG	a	850	-	-	19/45/45/53	-
13	CLA	B	813	-	-	15/39/115/115	-
13	CLA	2	815	-	-	7/33/109/115	-
16	BCR	b	848	-	-	10/29/63/63	0/2/2/2
18	LMG	B	846	-	-	17/36/56/70	0/1/1/1
13	CLA	A	821	-	-	11/39/115/115	-
13	CLA	b	831	-	-	7/39/115/115	-
13	CLA	K	4002	-	-	7/15/91/115	-
13	CLA	a	806	-	-	12/39/115/115	-
13	CLA	2	820	-	-	19/39/115/115	-
13	CLA	A	805	-	-	12/27/103/115	-
13	CLA	A	817	-	-	8/27/103/115	-
13	CLA	J	1102	-	-	6/10/82/115	-
13	CLA	2	801	-	-	6/39/115/115	-
13	CLA	0	208	-	-	9/39/115/115	-
13	CLA	A	837	-	-	8/33/109/115	-
13	CLA	8	1102	-	-	6/10/82/115	-
13	CLA	1	804	-	-	3/27/103/115	-
13	CLA	k	4002	-	-	7/15/91/115	-
13	CLA	B	809	-	-	5/15/91/115	-

The worst 5 of 2696 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	842	BCR	C30-C25	-3.74	1.49	1.53
16	b	842	BCR	C30-C25	-3.73	1.49	1.53
16	2	841	BCR	C30-C25	-3.73	1.49	1.53
16	2	847	BCR	C1-C6	-3.64	1.49	1.53
16	B	848	BCR	C1-C6	-3.62	1.49	1.53

The worst 5 of 2345 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	808	CLA	C4A-NA-C1A	9.75	111.13	106.68
13	A	808	CLA	C4A-NA-C1A	9.65	111.08	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	808	CLA	C4A-NA-C1A	9.64	111.08	106.68
13	b	801	CLA	C4A-NA-C1A	8.88	110.73	106.68
13	1	819	CLA	C4A-NA-C1A	8.76	110.67	106.68

There are no chirality outliers.

5 of 3615 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	805	CLA	CBA-CGA-O2A-C1
13	A	805	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	808	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

336 monomers are involved in 858 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	838	CLA	1	0
13	B	802	CLA	5	0
16	8	1105	BCR	2	0
16	9	4001	BCR	4	0
13	2	811	CLA	1	0
13	1	837	CLA	3	0
13	1	827	CLA	3	0
13	B	828	CLA	2	0
13	2	808	CLA	1	0
13	b	816	CLA	1	0
19	7	101	SQD	12	0
13	b	833	CLA	2	0
13	1	818	CLA	4	0
13	B	831	CLA	2	0
13	b	835	CLA	2	0
16	9	4004	BCR	1	0
13	B	818	CLA	1	0
13	a	810	CLA	1	0
16	J	1104	BCR	2	0
13	2	827	CLA	2	0
16	b	842	BCR	1	0
13	a	835	CLA	1	0
16	J	1105	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	821	CLA	6	0
13	L	204	CLA	1	0
13	A	835	CLA	1	0
16	A	846	BCR	5	0
13	8	1101	CLA	1	0
13	b	847	CLA	2	0
13	b	838	CLA	1	0
19	I	103	SQD	13	0
16	z	101	BCR	3	0
13	1	817	CLA	3	0
16	1	846	BCR	3	0
13	2	814	CLA	4	0
13	2	803	CLA	1	0
16	a	846	BCR	4	0
13	B	816	CLA	1	0
13	A	824	CLA	3	0
13	B	823	CLA	4	0
13	B	829	CLA	4	0
13	A	830	CLA	4	0
13	2	806	CLA	9	0
16	1	848	BCR	6	0
16	2	839	BCR	4	0
18	2	845	LMG	3	0
13	1	822	CLA	1	0
12	1	801	CL0	5	0
16	k	4001	BCR	1	0
16	1	851	BCR	2	0
13	A	822	CLA	1	0
13	A	831	CLA	4	0
13	f	201	CLA	5	0
13	b	814	CLA	3	0
13	2	804	CLA	5	0
13	b	817	CLA	1	0
15	3	102	SF4	1	0
16	i	103	BCR	5	0
16	A	851	BCR	2	0
13	1	805	CLA	4	0
13	1	828	CLA	9	0
13	B	833	CLA	2	0
13	A	802	CLA	5	0
13	A	807	CLA	1	0
13	a	831	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	a	851	BCR	2	0
13	b	830	CLA	2	0
13	2	802	CLA	4	0
13	a	823	CLA	2	0
13	A	806	CLA	6	0
13	a	802	CLA	5	0
13	i	102	CLA	9	0
13	L	203	CLA	9	0
13	a	828	CLA	9	0
14	1	843	PQN	2	0
13	A	823	CLA	2	0
13	A	841	CLA	5	0
13	1	806	CLA	7	0
13	b	818	CLA	1	0
13	1	826	CLA	4	0
14	2	838	PQN	7	0
13	a	826	CLA	4	0
16	0	201	BCR	6	0
16	A	845	BCR	3	0
19	i	101	SQD	12	0
13	a	815	CLA	2	0
13	a	825	CLA	4	0
16	j	1104	BCR	2	0
13	b	801	CLA	1	0
13	A	826	CLA	3	0
16	0	207	BCR	1	0
16	F	202	BCR	2	0
13	b	804	CLA	7	0
13	L	206	CLA	7	0
16	6	202	BCR	1	0
16	2	840	BCR	5	0
13	B	827	CLA	2	0
16	L	202	BCR	2	0
13	A	819	CLA	5	0
13	l	205	CLA	1	0
13	0	202	CLA	2	0
13	7	102	CLA	8	0
13	L	201	CLA	2	0
13	B	801	CLA	1	0
16	2	844	BCR	3	0
13	1	815	CLA	2	0
13	a	813	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	836	CLA	3	0
13	B	830	CLA	2	0
13	1	838	CLA	5	0
13	2	831	CLA	1	0
13	a	827	CLA	2	0
16	M	101	BCR	2	0
16	2	847	BCR	4	0
13	A	813	CLA	3	0
13	B	837	CLA	3	0
13	B	817	CLA	1	0
13	B	820	CLA	2	0
13	A	809	CLA	2	0
13	2	810	CLA	2	0
13	a	838	CLA	5	0
16	b	844	BCR	4	0
16	0	204	BCR	3	0
13	b	811	CLA	2	0
13	2	813	CLA	2	0
16	l	201	BCR	7	0
13	B	836	CLA	4	0
13	a	818	CLA	4	0
16	7	103	BCR	3	0
13	2	828	CLA	4	0
13	1	810	CLA	1	0
13	b	805	CLA	6	0
13	b	828	CLA	2	0
13	A	836	CLA	1	0
13	a	834	CLA	4	0
13	1	835	CLA	1	0
13	A	808	CLA	4	0
13	b	823	CLA	3	0
13	1	821	CLA	6	0
13	1	813	CLA	3	0
16	b	841	BCR	4	0
16	A	847	BCR	4	0
16	m	101	BCR	2	0
13	a	830	CLA	4	0
13	a	809	CLA	1	0
16	K	4004	BCR	1	0
13	9	4003	CLA	1	0
16	l	206	BCR	3	0
13	A	852	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	826	CLA	3	0
13	A	818	CLA	4	0
13	a	803	CLA	2	0
13	A	827	CLA	2	0
13	1	834	CLA	4	0
13	a	852	CLA	9	0
16	b	843	BCR	2	0
13	1	842	CLA	1	0
16	8	1104	BCR	3	0
13	a	829	CLA	3	0
13	A	825	CLA	4	0
13	a	833	CLA	3	0
16	b	840	BCR	4	0
13	l	204	CLA	7	0
13	B	824	CLA	6	0
13	1	852	CLA	8	0
13	a	822	CLA	1	0
13	I	101	CLA	9	0
12	a	801	CL0	5	0
13	1	830	CLA	4	0
16	F	205	BCR	3	0
13	1	809	CLA	2	0
16	2	842	BCR	2	0
13	a	837	CLA	4	0
13	A	838	CLA	5	0
16	1	845	BCR	2	0
13	2	825	CLA	3	0
13	A	839	CLA	3	0
13	B	832	CLA	1	0
13	2	826	CLA	1	0
13	b	807	CLA	1	0
13	2	846	CLA	2	0
16	a	845	BCR	2	0
14	A	843	PQN	4	0
17	A	850	LHG	2	0
13	0	203	CLA	1	0
13	1	829	CLA	3	0
14	b	839	PQN	6	0
13	B	805	CLA	6	0
13	a	839	CLA	4	0
13	b	803	CLA	2	0
13	J	1101	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	822	CLA	3	0
13	b	815	CLA	4	0
13	b	829	CLA	4	0
13	b	837	CLA	3	0
13	B	812	CLA	1	0
13	b	802	CLA	3	0
13	1	823	CLA	2	0
13	1	839	CLA	3	0
13	2	823	CLA	7	0
13	8	1103	CLA	2	0
13	a	832	CLA	3	0
16	B	843	BCR	1	0
13	B	811	CLA	2	0
13	B	806	CLA	8	0
16	B	840	BCR	4	0
13	1	841	CLA	5	0
16	B	841	BCR	5	0
13	B	814	CLA	2	0
13	a	804	CLA	3	0
13	A	832	CLA	3	0
17	1	850	LHG	2	0
13	1	819	CLA	5	0
16	l	203	BCR	2	0
13	A	829	CLA	3	0
13	a	819	CLA	5	0
13	b	813	CLA	2	0
13	F	201	CLA	5	0
13	1	825	CLA	5	0
16	B	842	BCR	1	0
12	A	801	CL0	5	0
13	a	841	CLA	5	0
16	6	205	BCR	3	0
13	A	834	CLA	4	0
14	B	839	PQN	7	0
13	a	820	CLA	1	0
13	B	803	CLA	2	0
13	2	834	CLA	3	0
16	I	102	BCR	5	0
13	B	835	CLA	3	0
13	2	819	CLA	2	0
13	B	815	CLA	5	0
13	B	847	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	821	CLA	6	0
13	2	817	CLA	1	0
13	a	805	CLA	2	0
13	2	837	CLA	1	0
16	1	847	BCR	5	0
13	2	830	CLA	2	0
13	A	803	CLA	2	0
13	B	808	CLA	3	0
13	1	824	CLA	3	0
16	a	847	BCR	3	0
13	b	836	CLA	3	0
13	b	820	CLA	3	0
13	a	824	CLA	4	0
13	2	809	CLA	7	0
13	A	810	CLA	2	0
13	A	840	CLA	3	0
13	B	804	CLA	6	0
16	k	4004	BCR	1	0
13	b	827	CLA	2	0
13	J	1103	CLA	2	0
13	b	824	CLA	7	0
16	B	848	BCR	2	0
13	b	809	CLA	1	0
13	A	833	CLA	2	0
16	b	845	BCR	3	0
13	b	821	CLA	6	0
13	l	207	CLA	5	0
13	B	810	CLA	7	0
13	a	817	CLA	3	0
13	a	836	CLA	1	0
16	f	205	BCR	2	0
16	f	202	BCR	2	0
13	b	808	CLA	3	0
13	A	811	CLA	2	0
18	b	846	LMG	3	0
13	1	803	CLA	3	0
13	1	833	CLA	3	0
16	L	207	BCR	10	0
13	2	835	CLA	4	0
13	A	820	CLA	1	0
13	1	811	CLA	2	0
13	1	836	CLA	1	0

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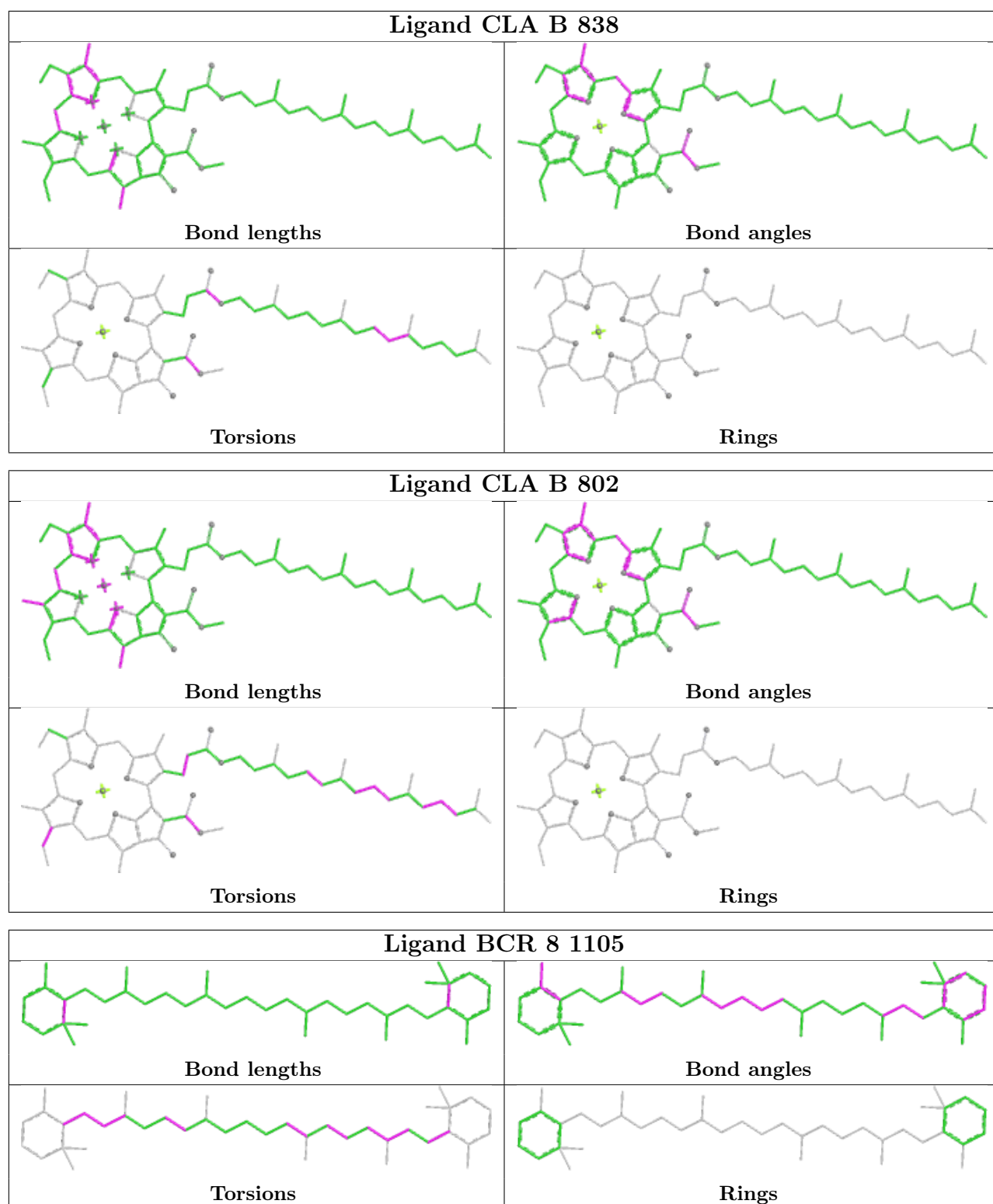
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	a	811	CLA	2	0
13	b	826	CLA	4	0
13	a	840	CLA	3	0
13	6	201	CLA	3	0
13	2	816	CLA	1	0
13	1	820	CLA	1	0
13	A	828	CLA	10	0
13	l	202	CLA	2	0
13	A	804	CLA	3	0
13	j	1101	CLA	1	0
13	a	808	CLA	4	0
16	B	845	BCR	3	0
13	1	831	CLA	4	0
16	A	848	BCR	6	0
16	L	205	BCR	4	0
16	2	843	BCR	5	0
13	f	203	CLA	1	0
16	B	844	BCR	4	0
13	2	832	CLA	2	0
13	j	1103	CLA	2	0
13	1	840	CLA	5	0
13	1	832	CLA	3	0
13	2	805	CLA	5	0
13	2	829	CLA	2	0
13	1	802	CLA	5	0
14	a	843	PQN	4	0
13	B	825	CLA	2	0
13	A	842	CLA	1	0
13	F	203	CLA	1	0
13	A	815	CLA	2	0
13	0	205	CLA	8	0
16	a	848	BCR	6	0
13	b	825	CLA	4	0
13	b	806	CLA	8	0
16	K	4001	BCR	1	0
13	1	808	CLA	4	0
13	b	832	CLA	1	0
13	1	807	CLA	1	0
16	2	841	BCR	1	0
13	a	842	CLA	1	0
13	2	807	CLA	3	0
13	2	812	CLA	2	0

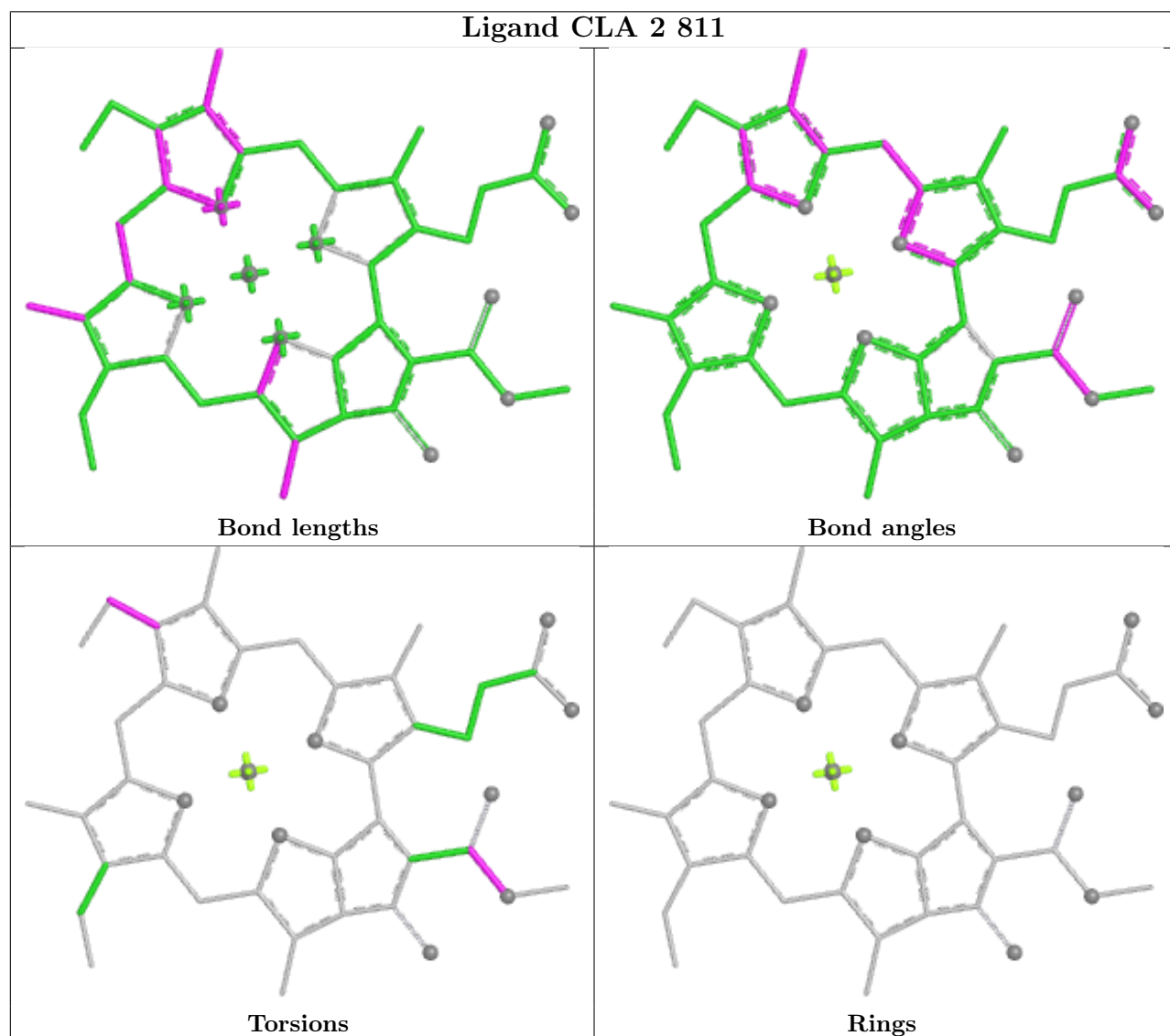
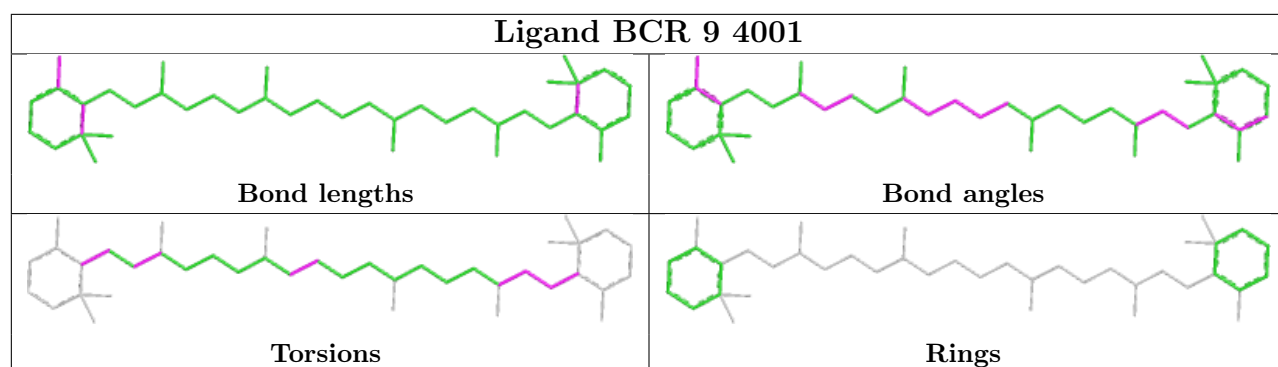
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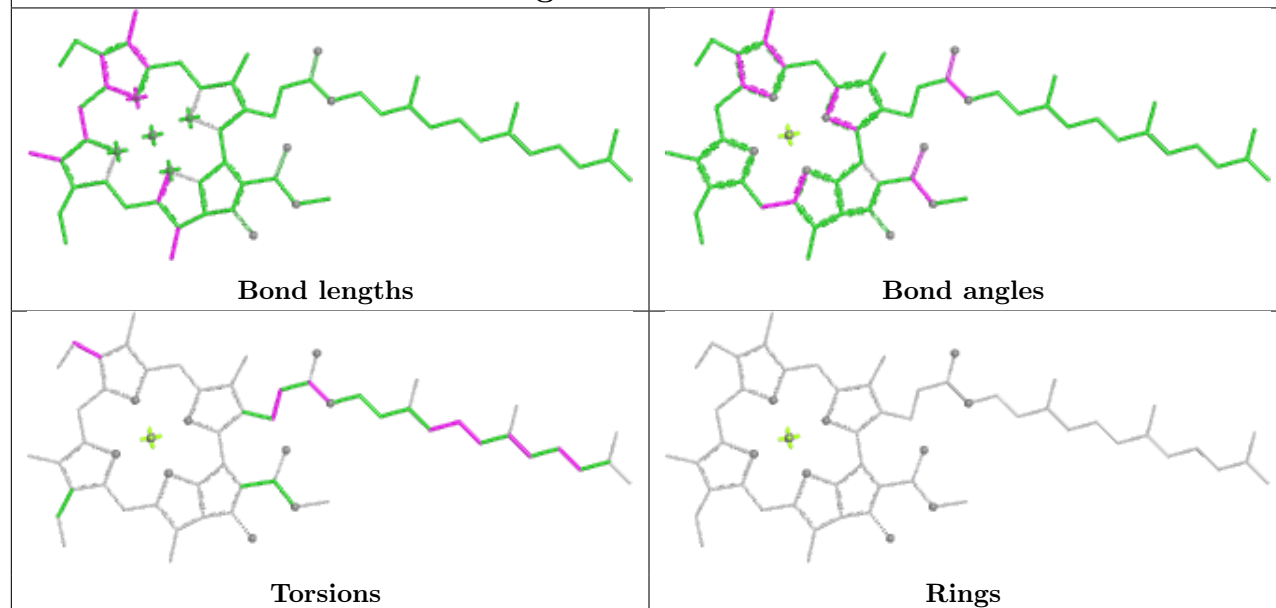
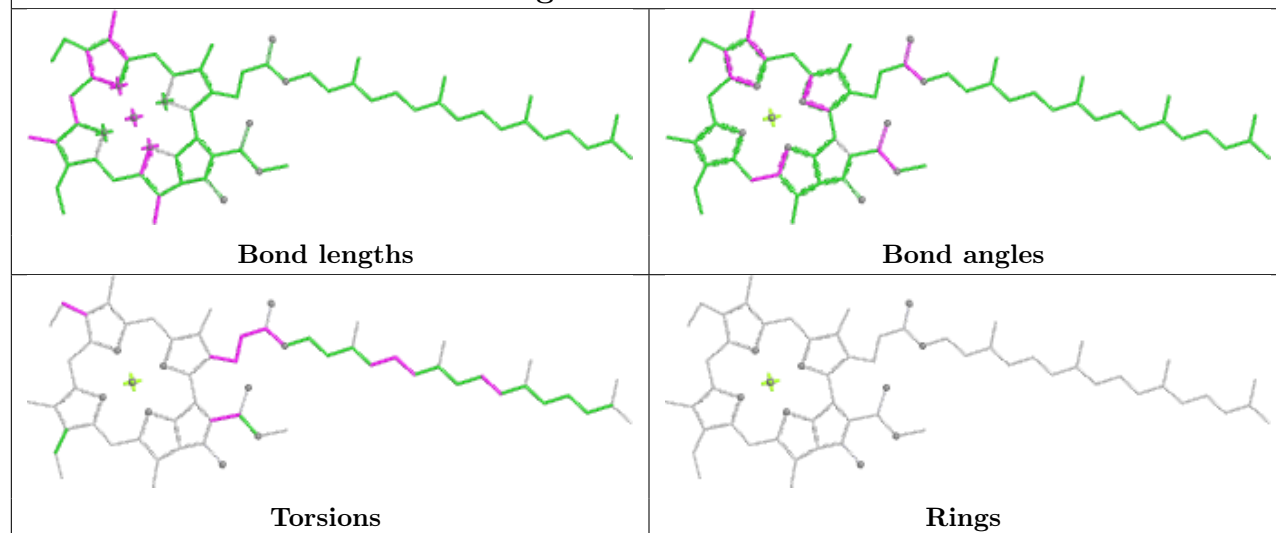
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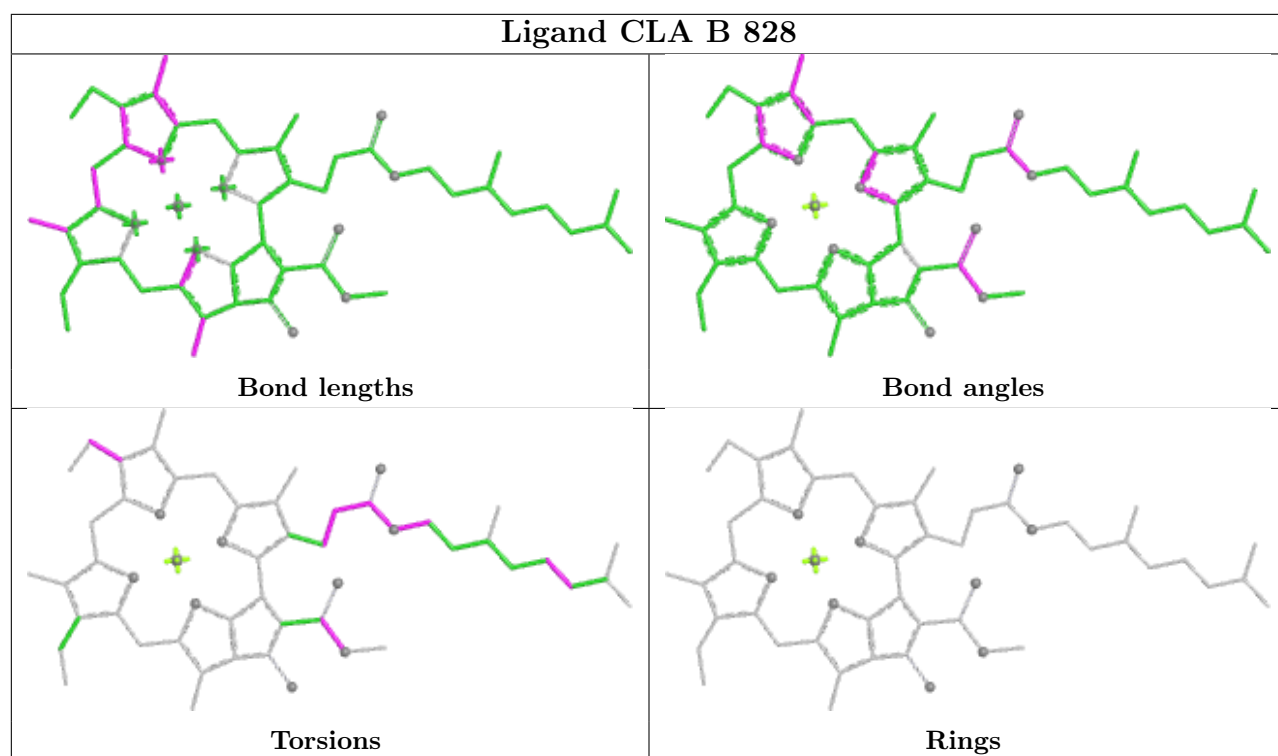
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	b	810	CLA	7	0
13	2	824	CLA	4	0
16	j	1105	BCR	2	0
17	a	850	LHG	1	0
13	B	813	CLA	1	0
13	2	815	CLA	1	0
16	b	848	BCR	4	0
18	B	846	LMG	3	0
13	A	821	CLA	6	0
13	b	831	CLA	2	0
13	a	806	CLA	5	0
13	2	820	CLA	7	0
13	A	805	CLA	2	0
13	A	817	CLA	3	0
13	2	801	CLA	1	0
13	0	208	CLA	5	0
13	A	837	CLA	4	0
13	1	804	CLA	3	0
13	B	809	CLA	1	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.

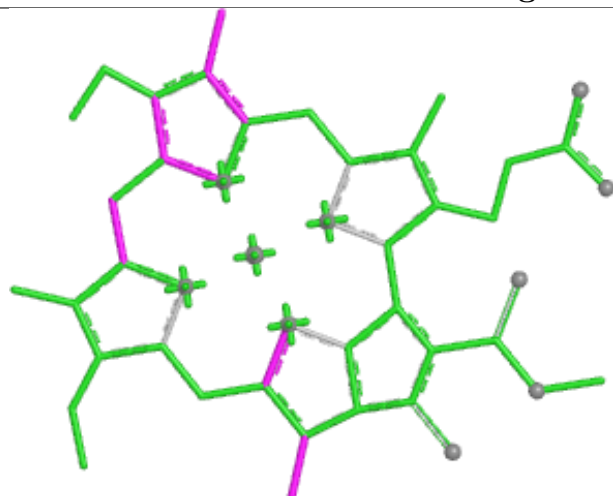




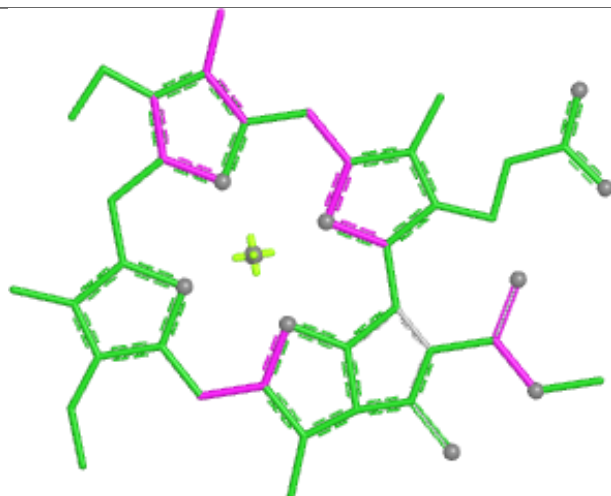
Ligand CLA 1 837**Ligand CLA 1 827**



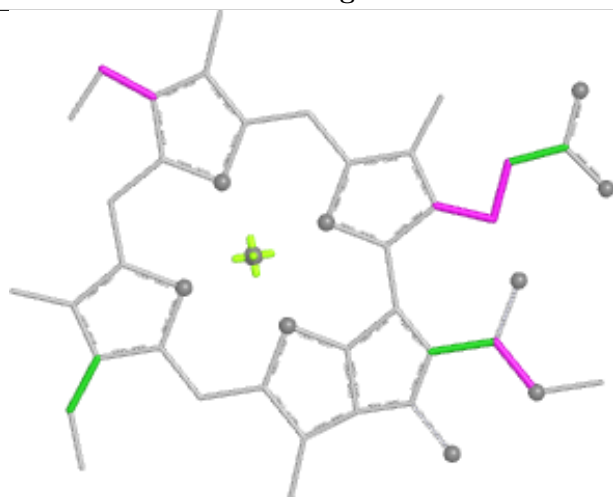
Ligand CLA 2 808



Bond lengths



Bond angles

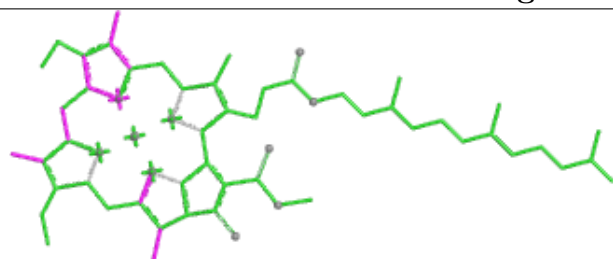


Torsions

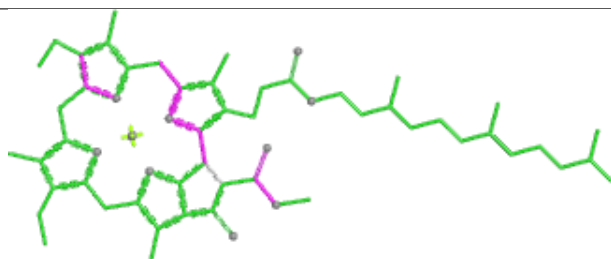


Rings

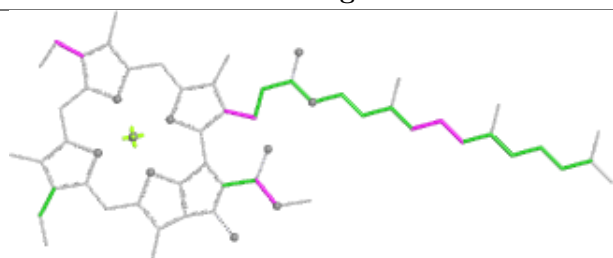
Ligand CLA b 816



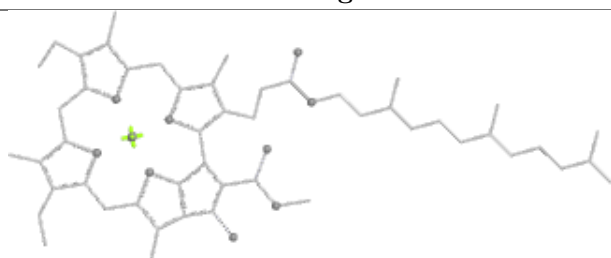
Bond lengths



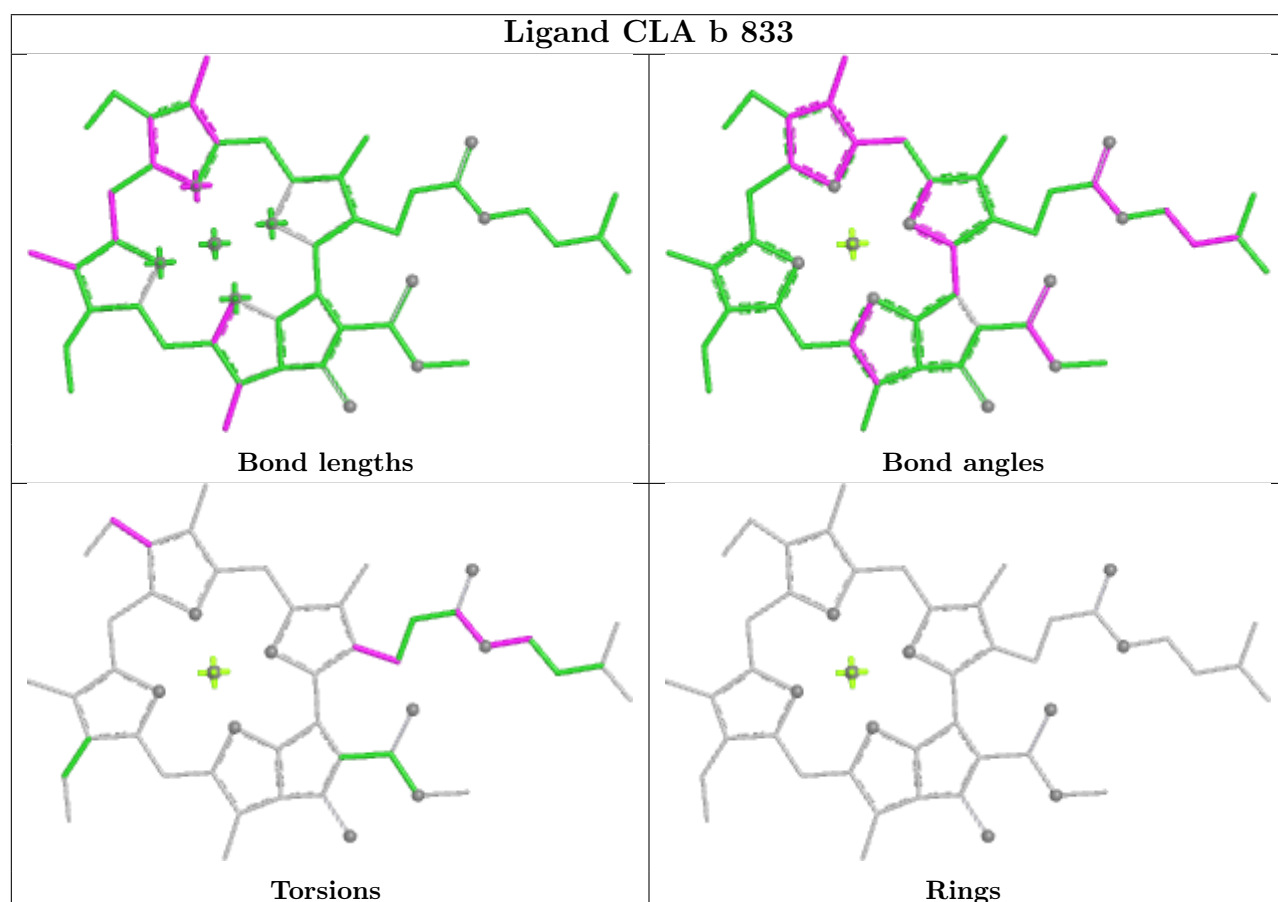
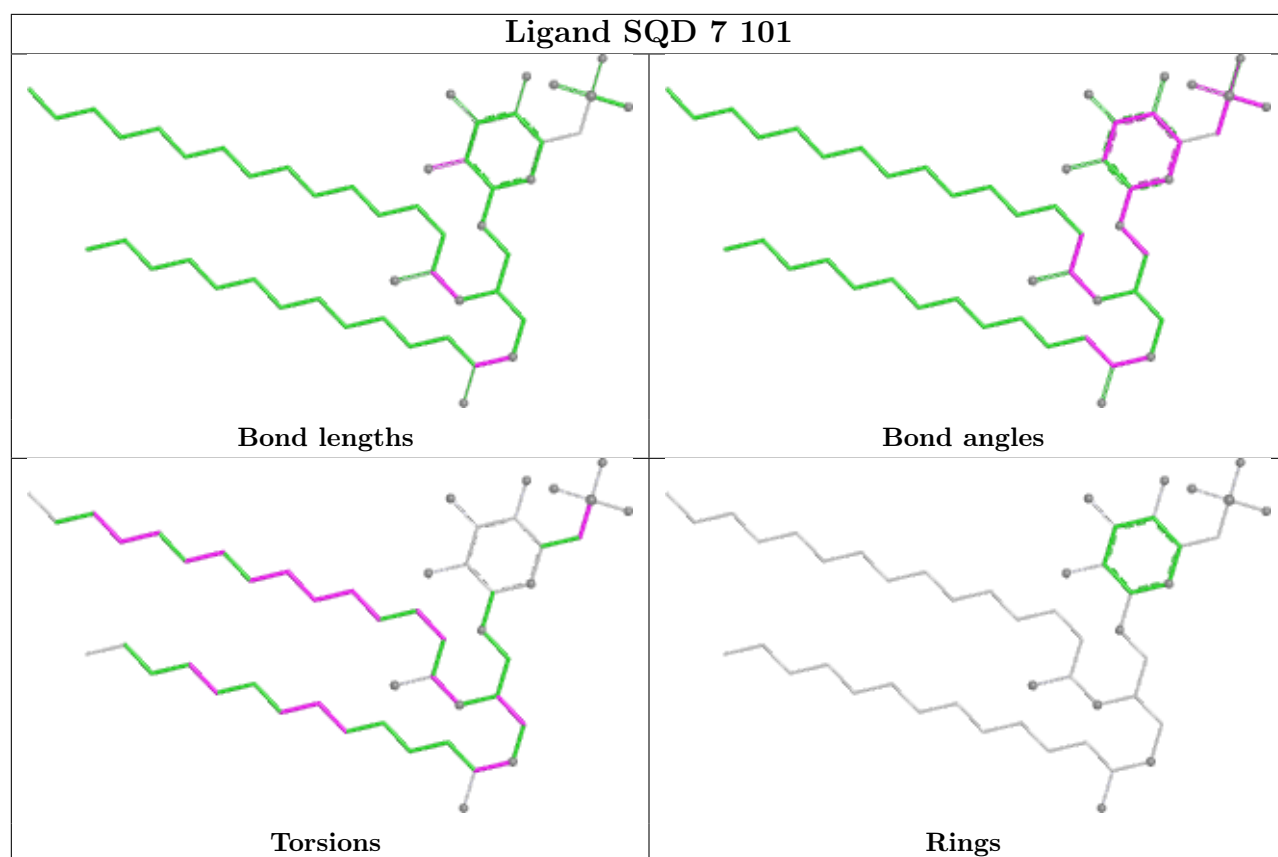
Bond angles



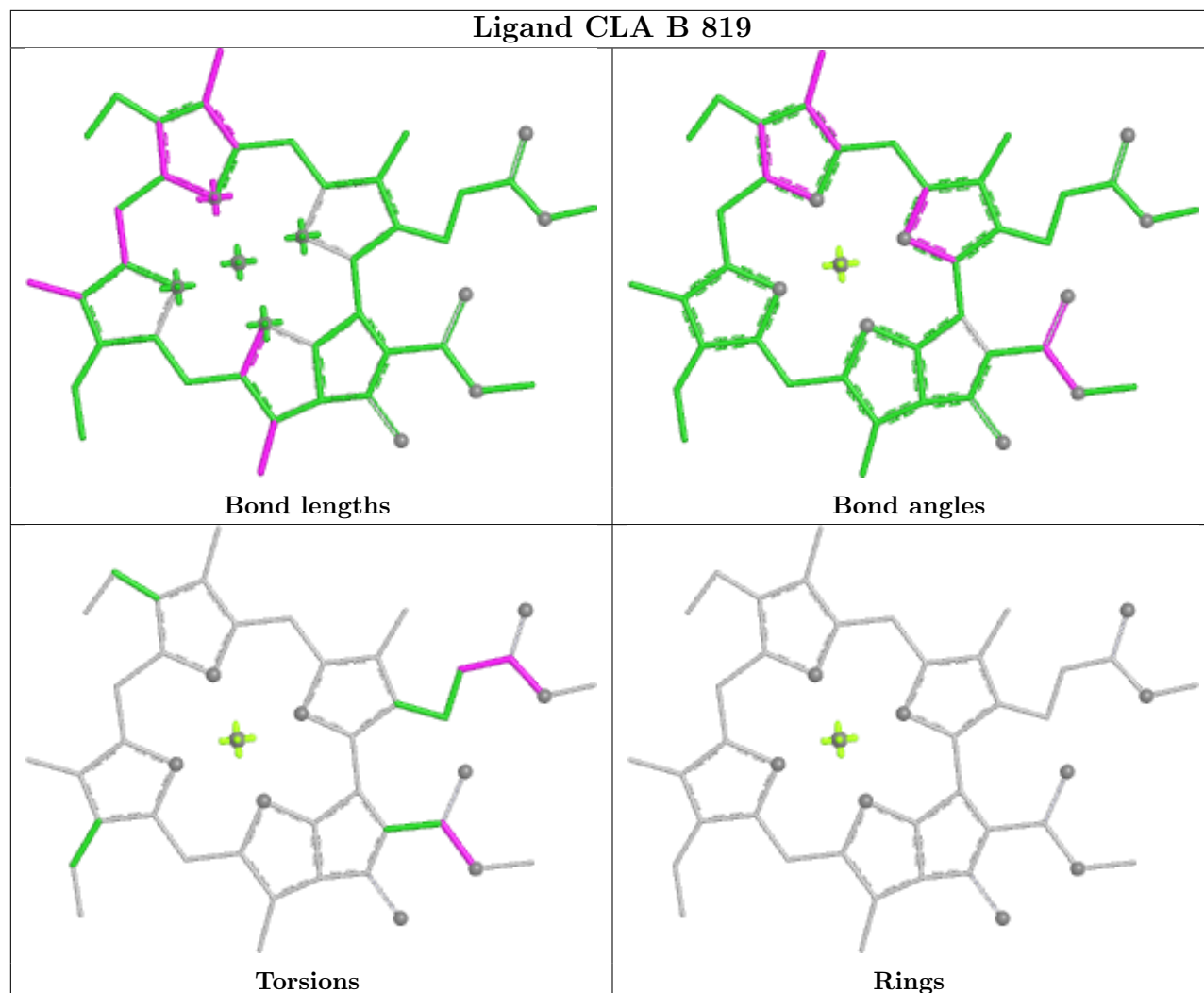
Torsions

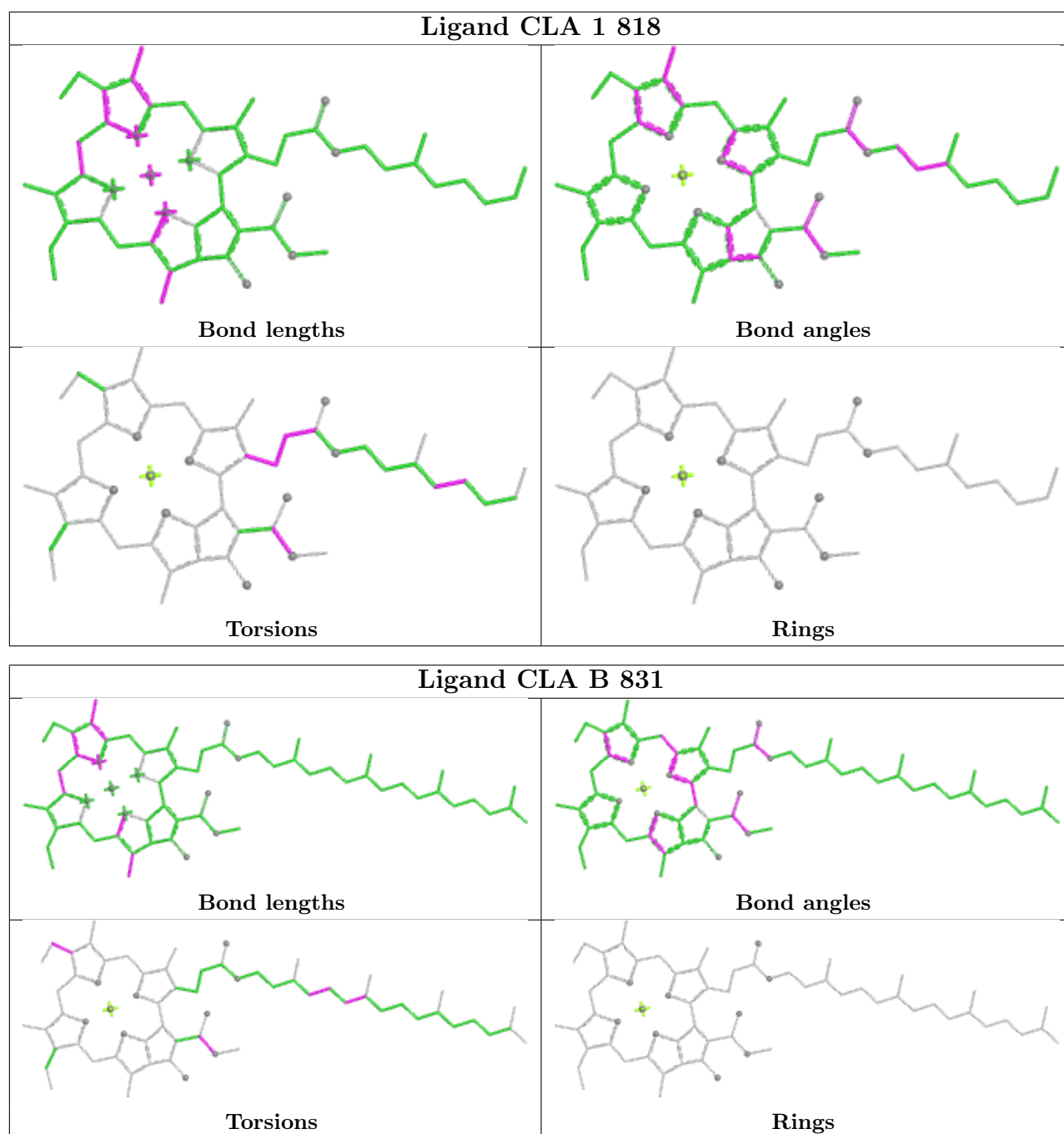


Rings

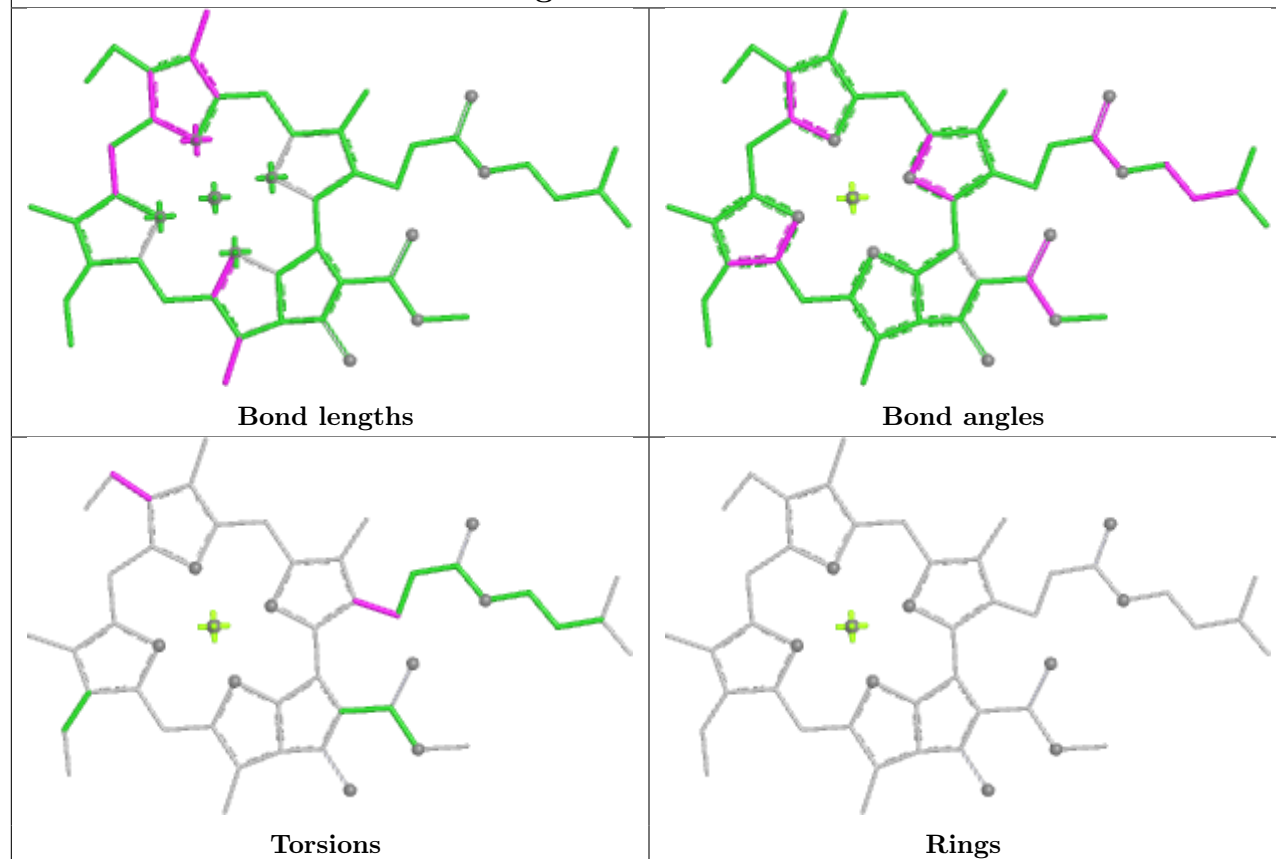


Ligand CLA B 819

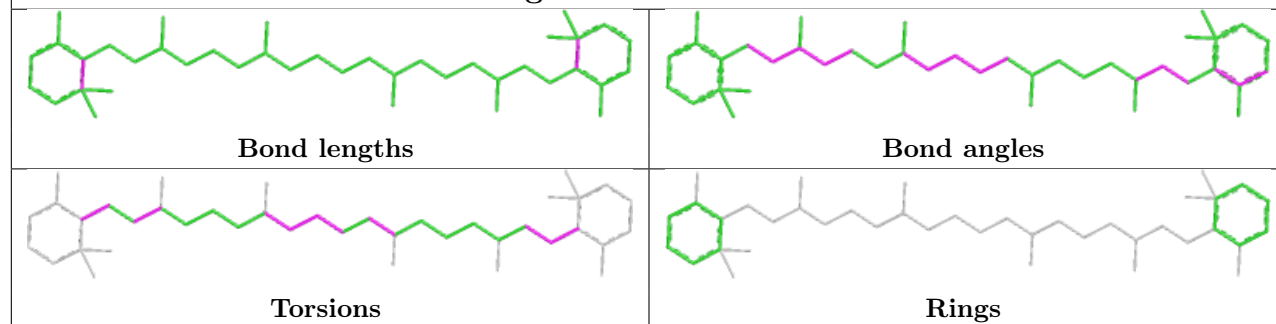


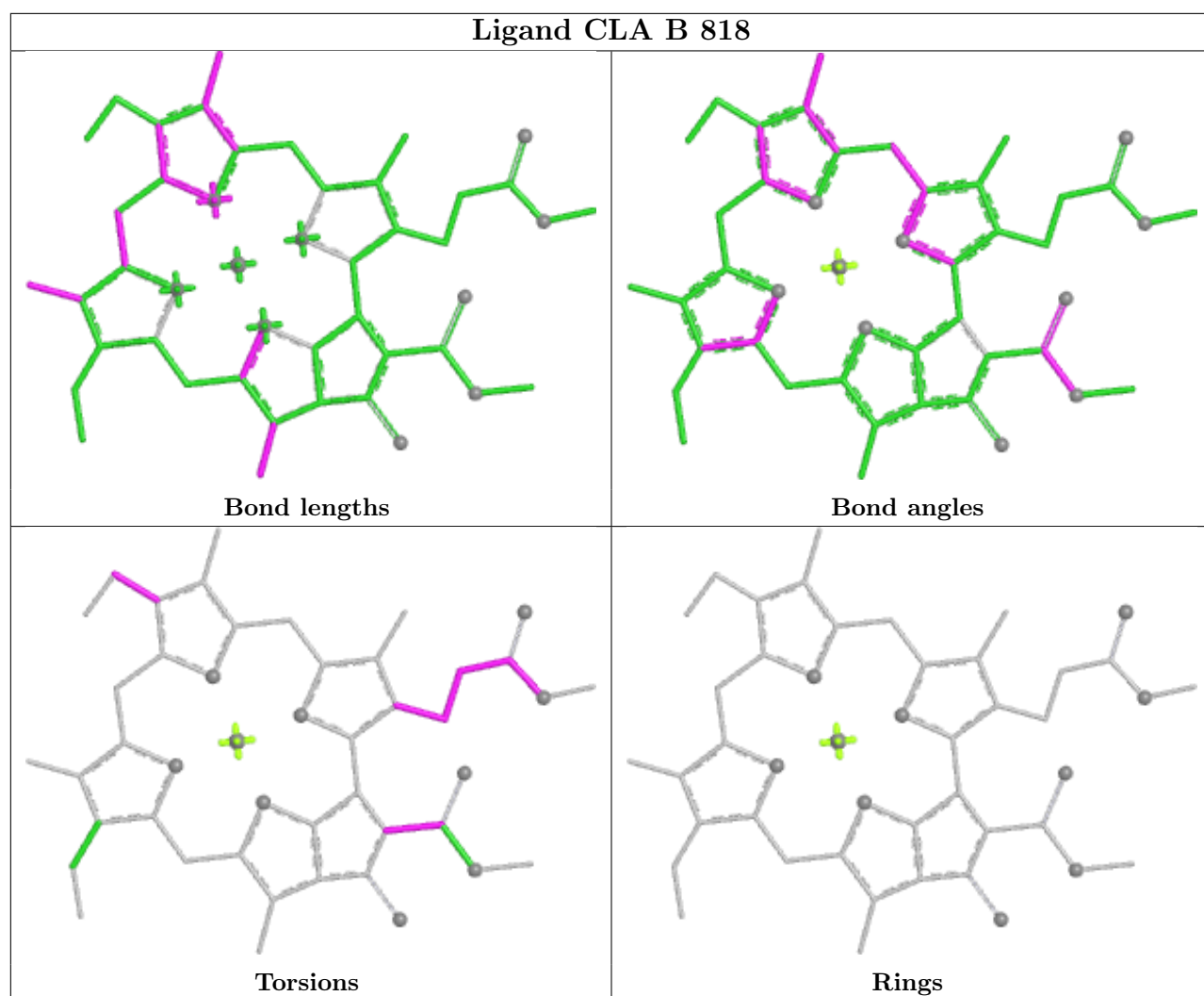


Ligand CLA b 835

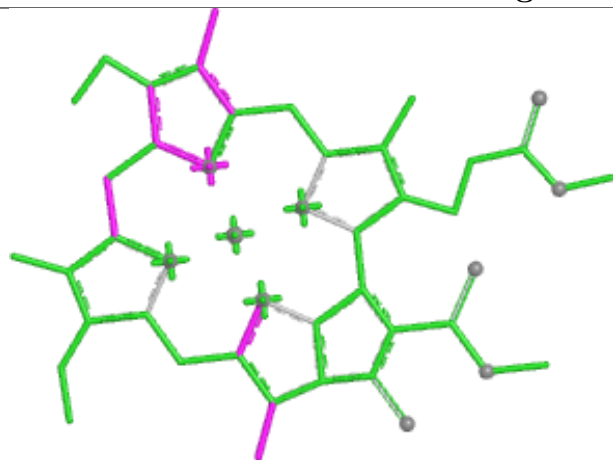


Ligand BCR 9 4004

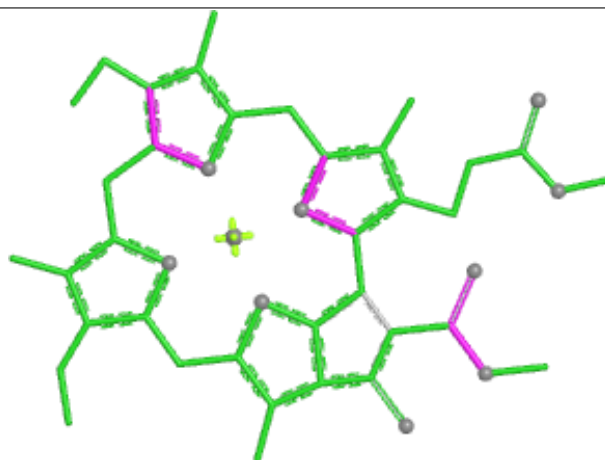




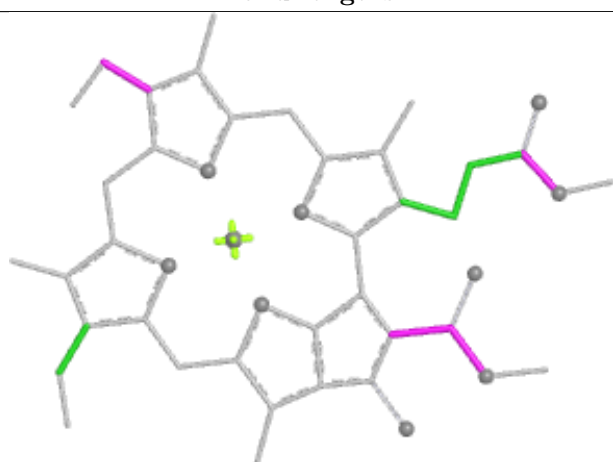
Ligand CLA F 204



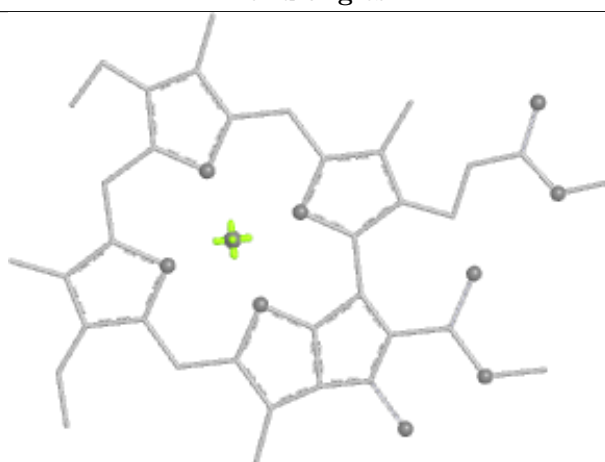
Bond lengths



Bond angles

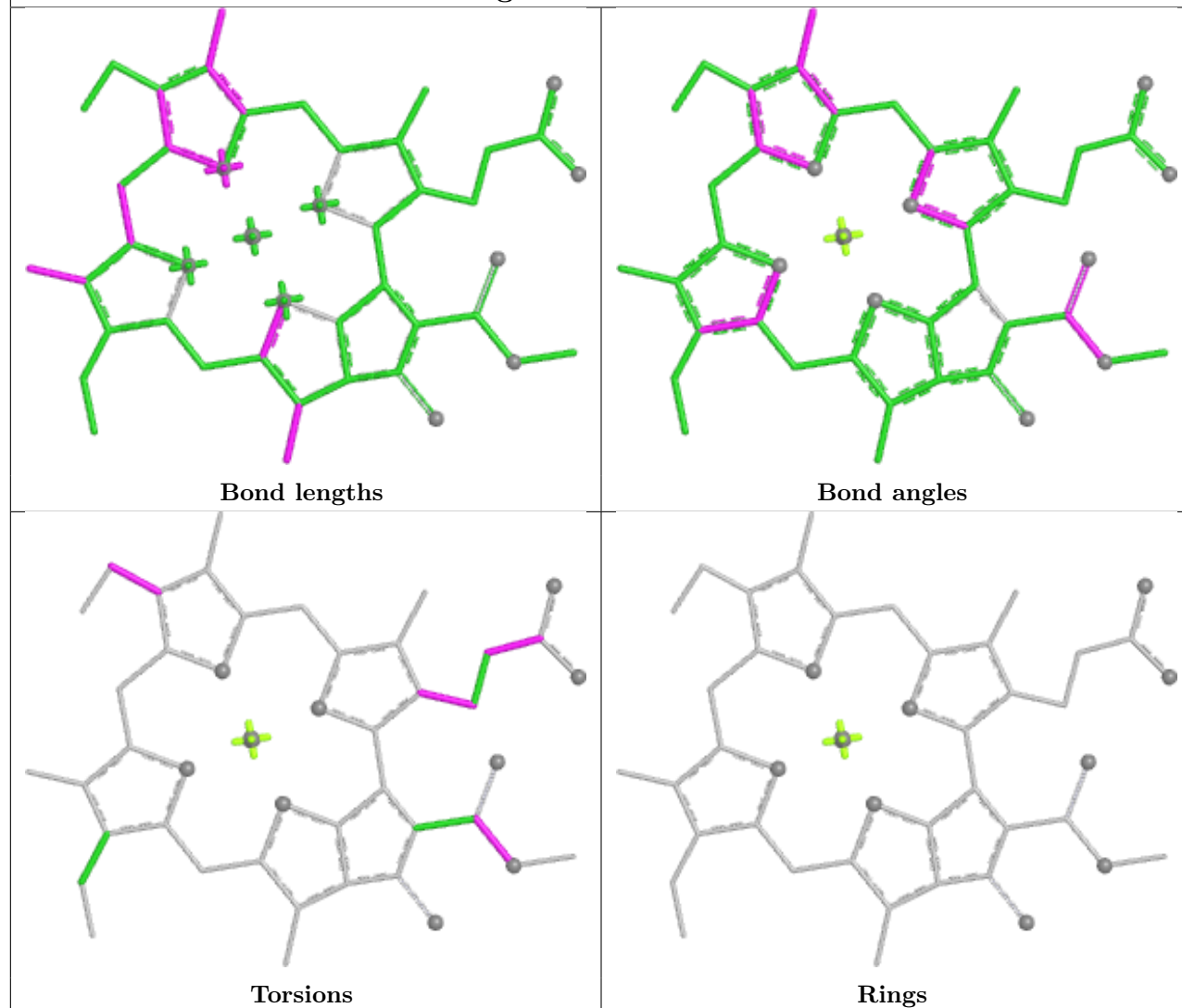


Torsions

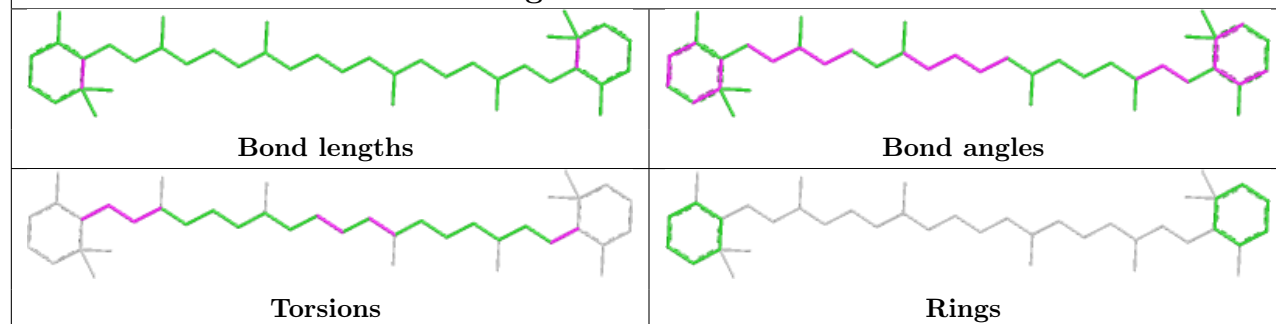


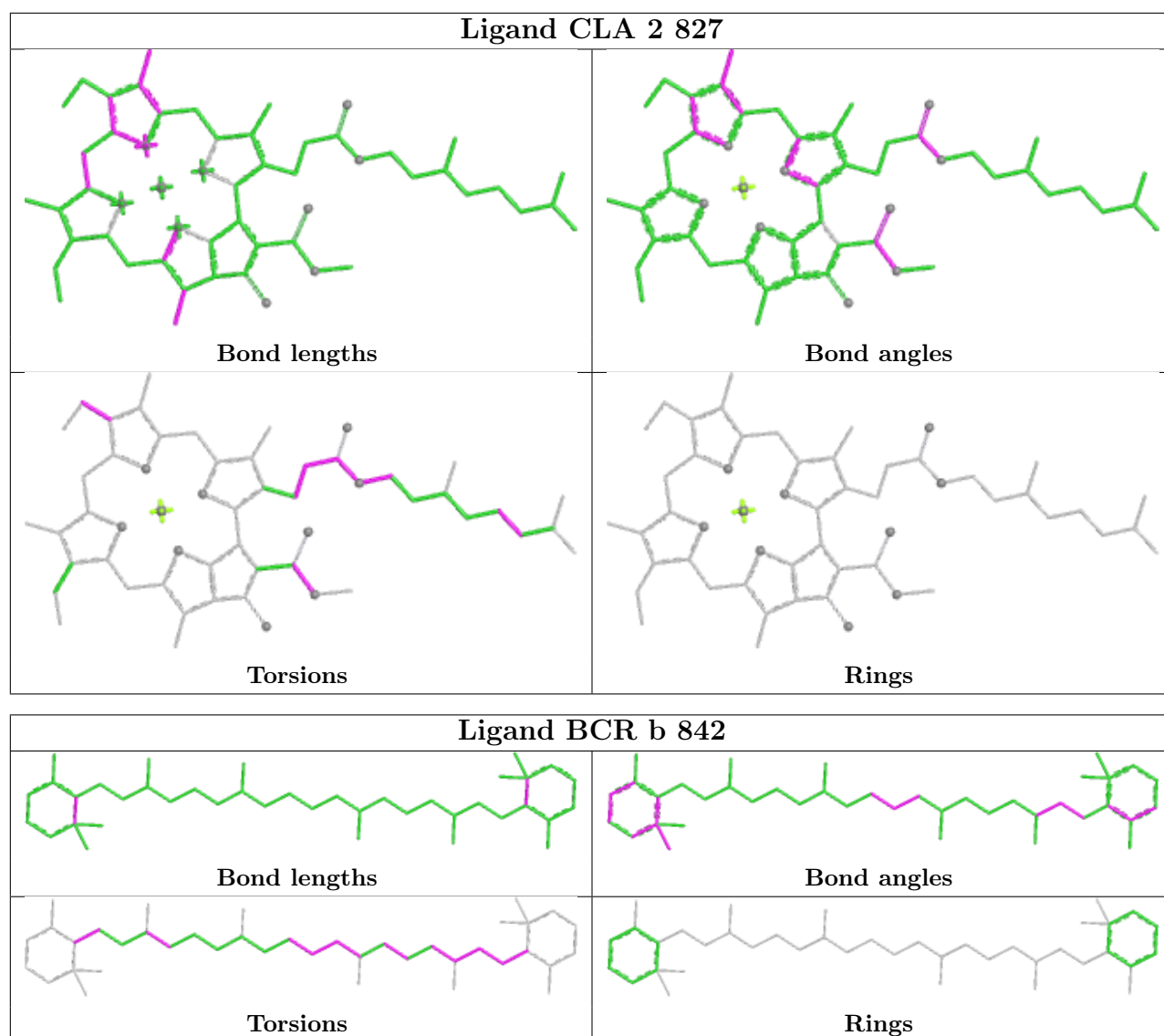
Rings

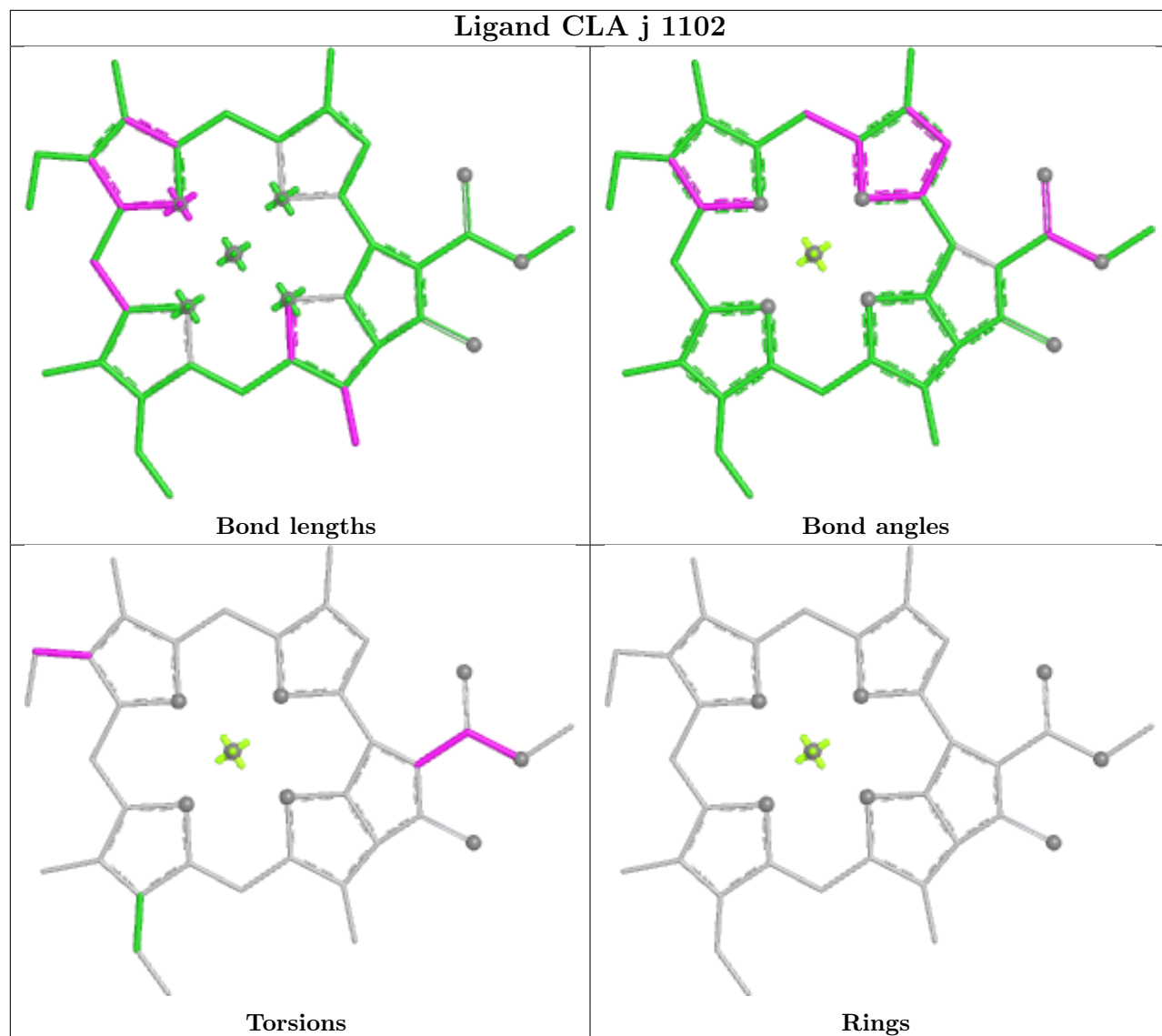
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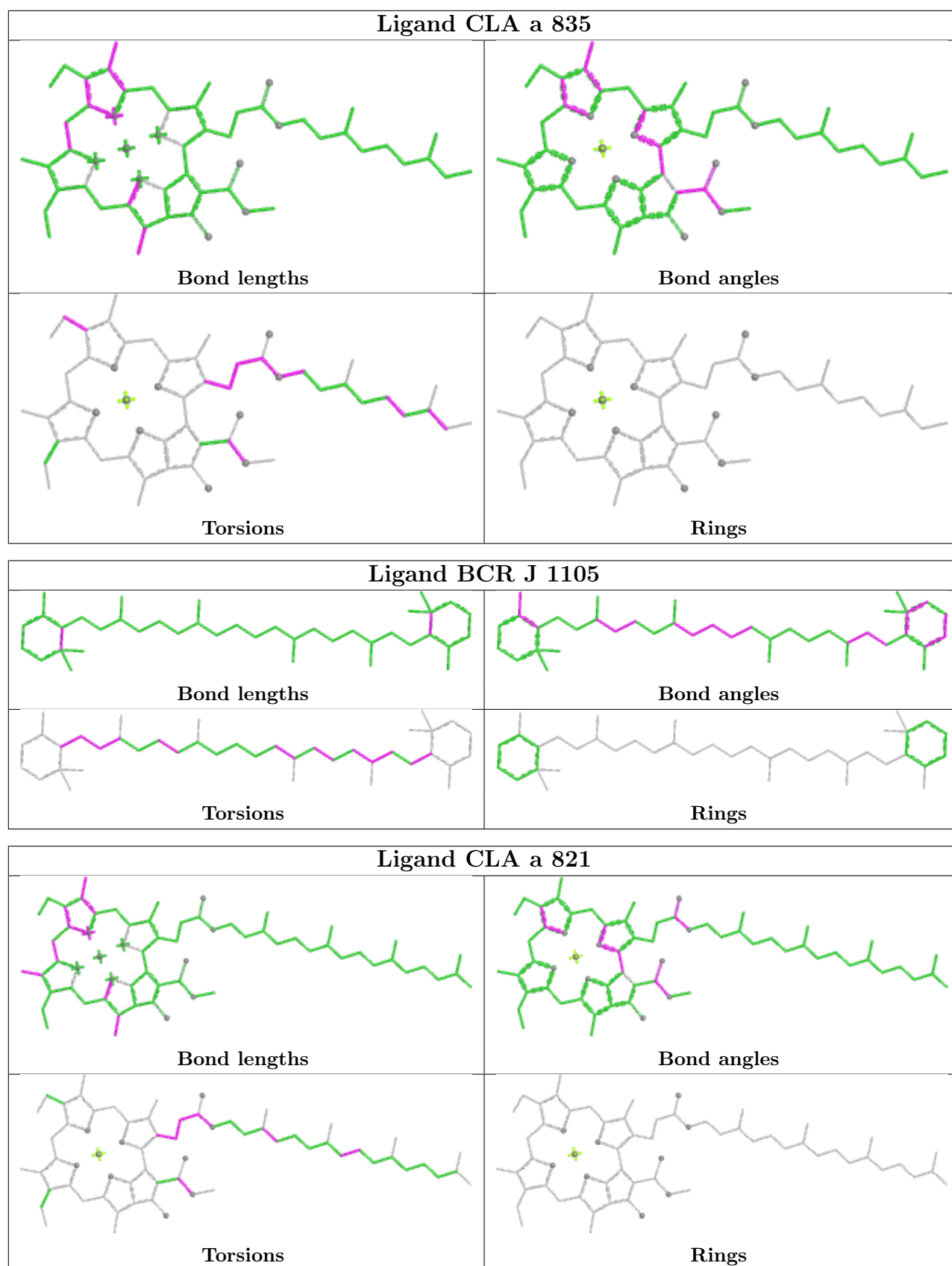


Ligand BCR J 1104

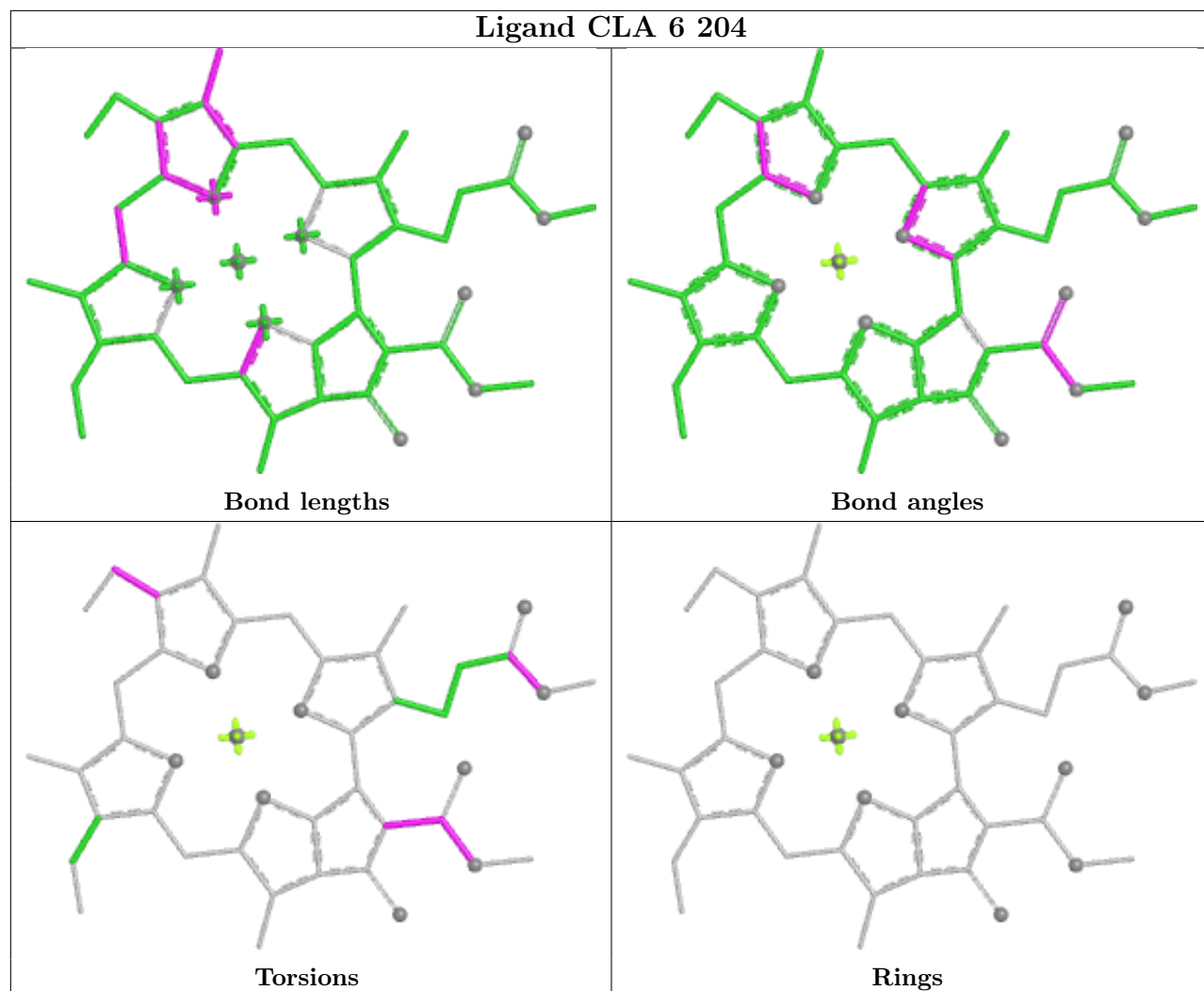




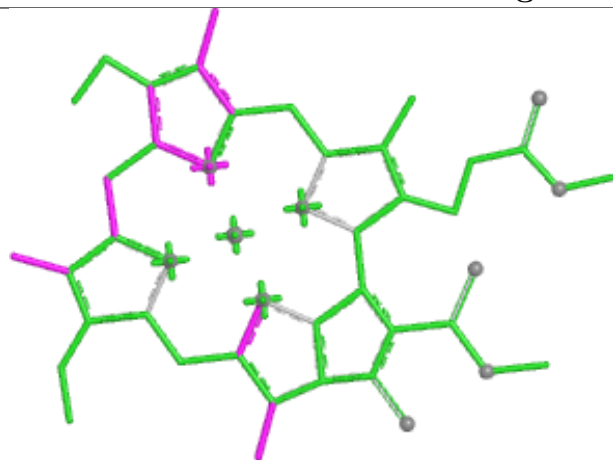




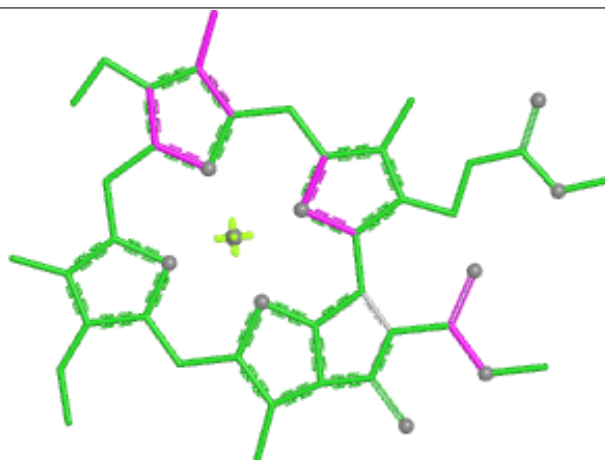
Ligand CLA 6 204



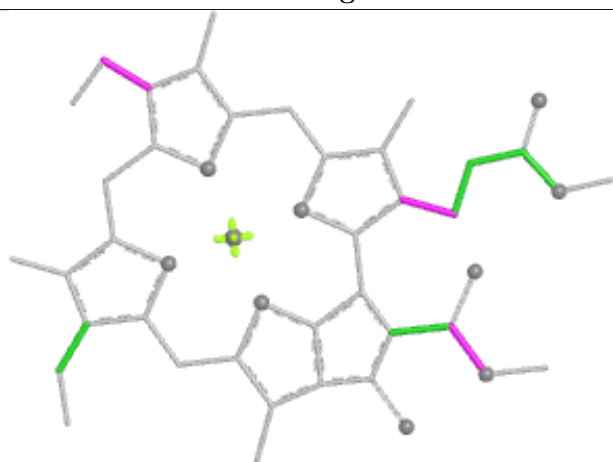
Ligand CLA L 204



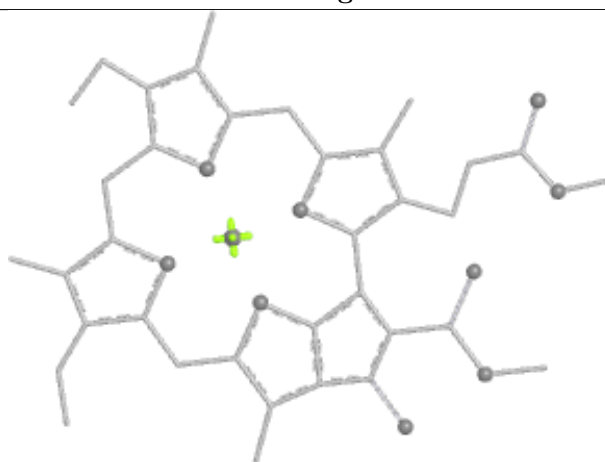
Bond lengths



Bond angles

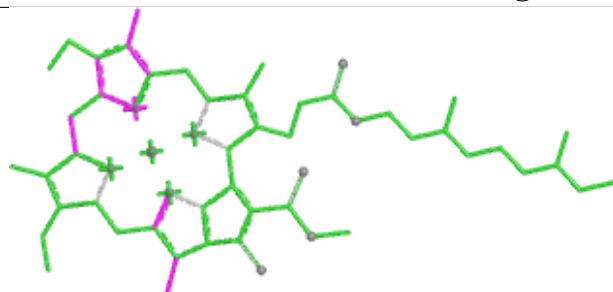


Torsions

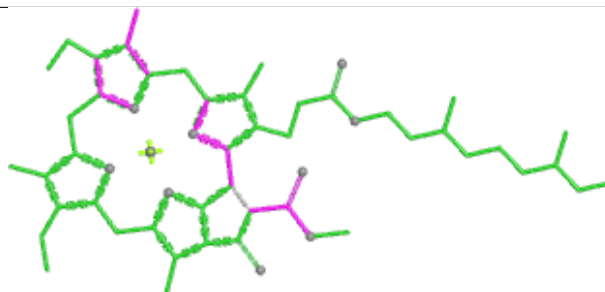


Rings

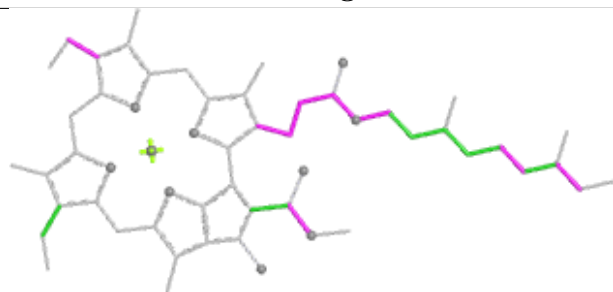
Ligand CLA A 835



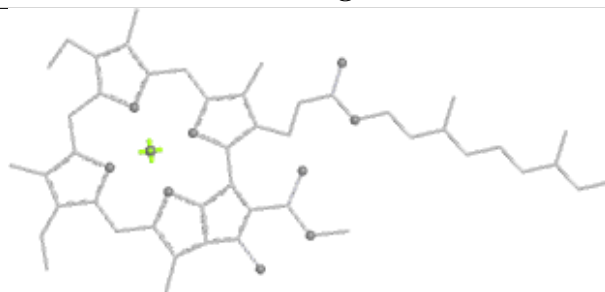
Bond lengths



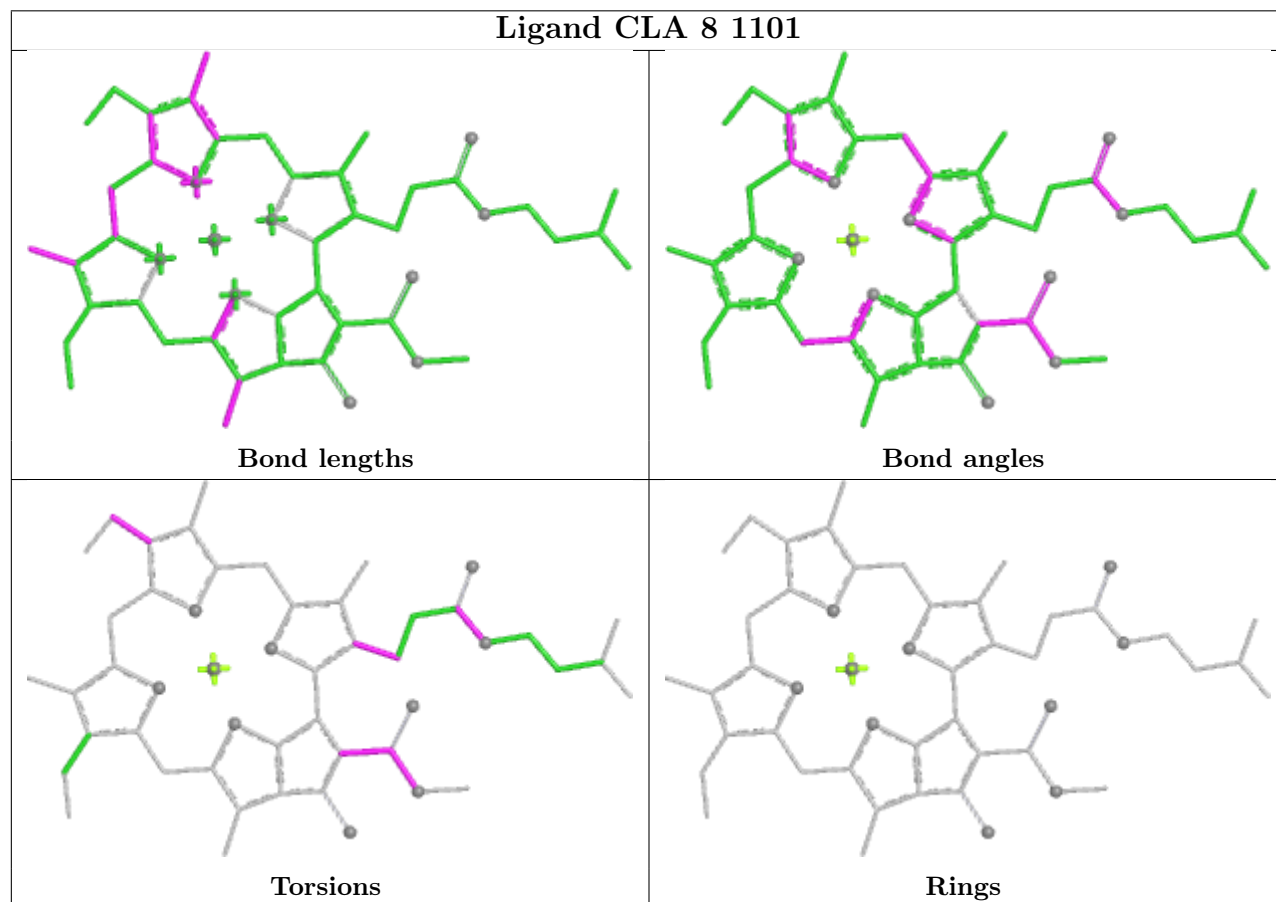
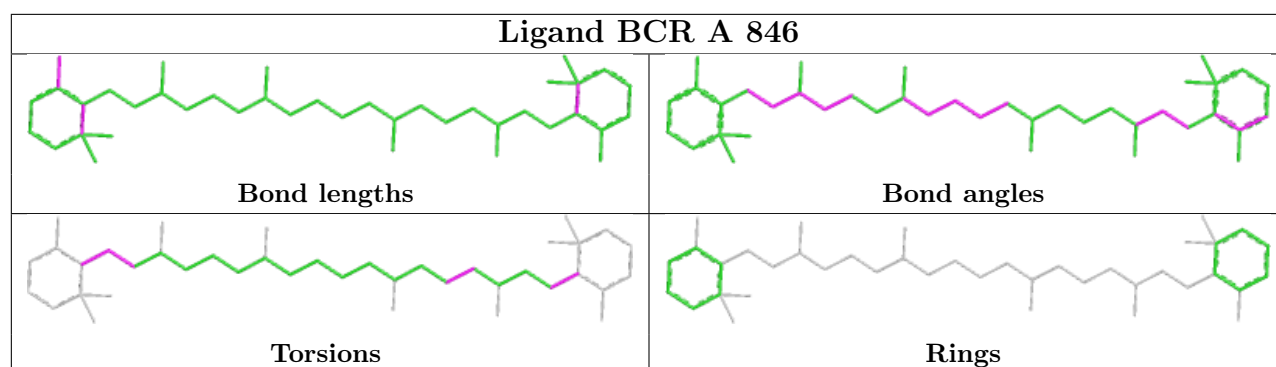
Bond angles

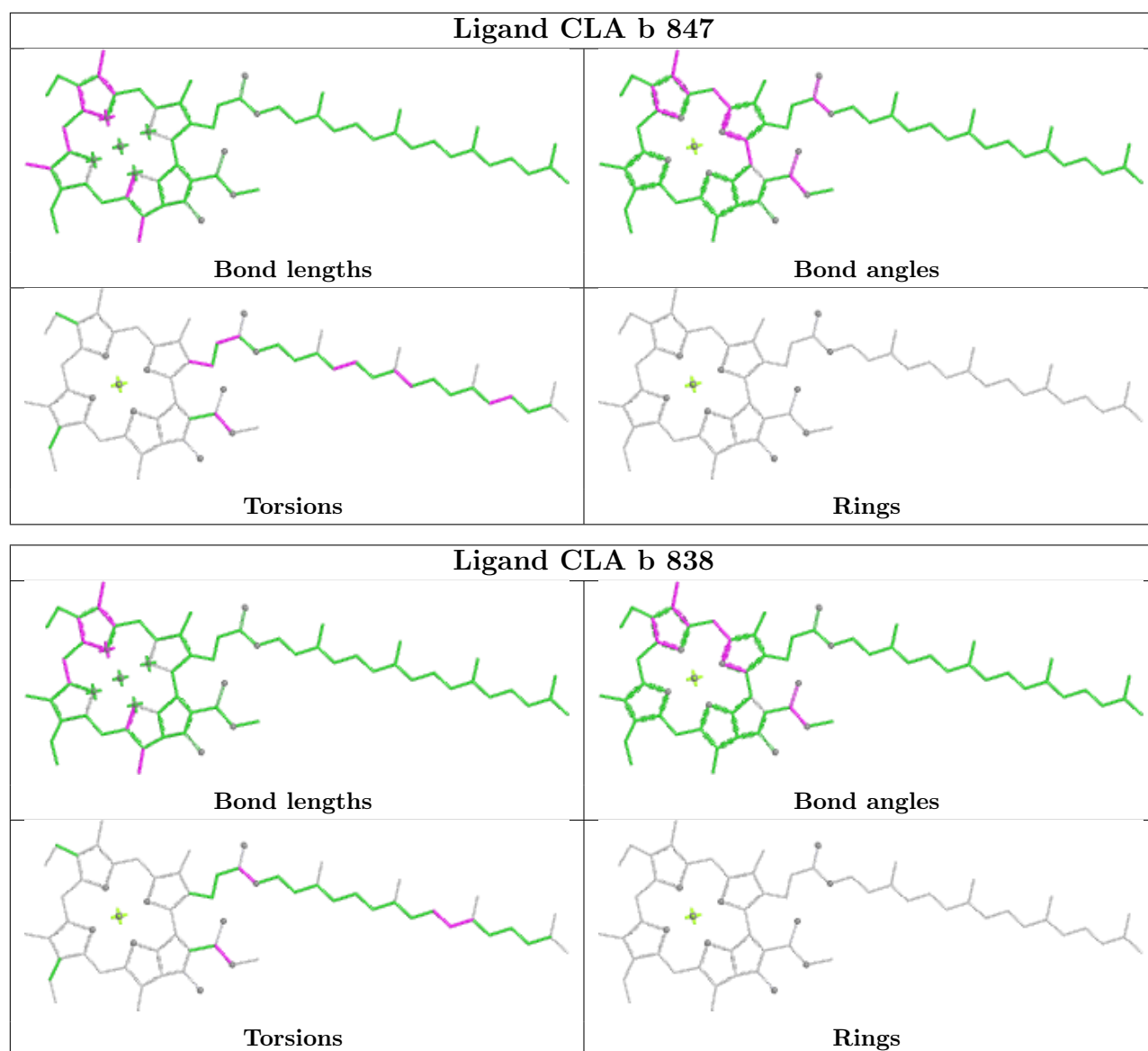


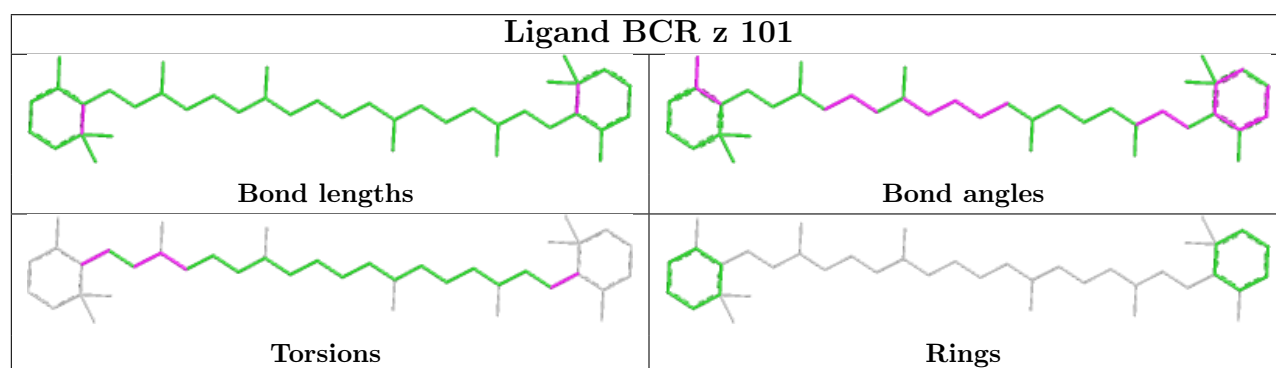
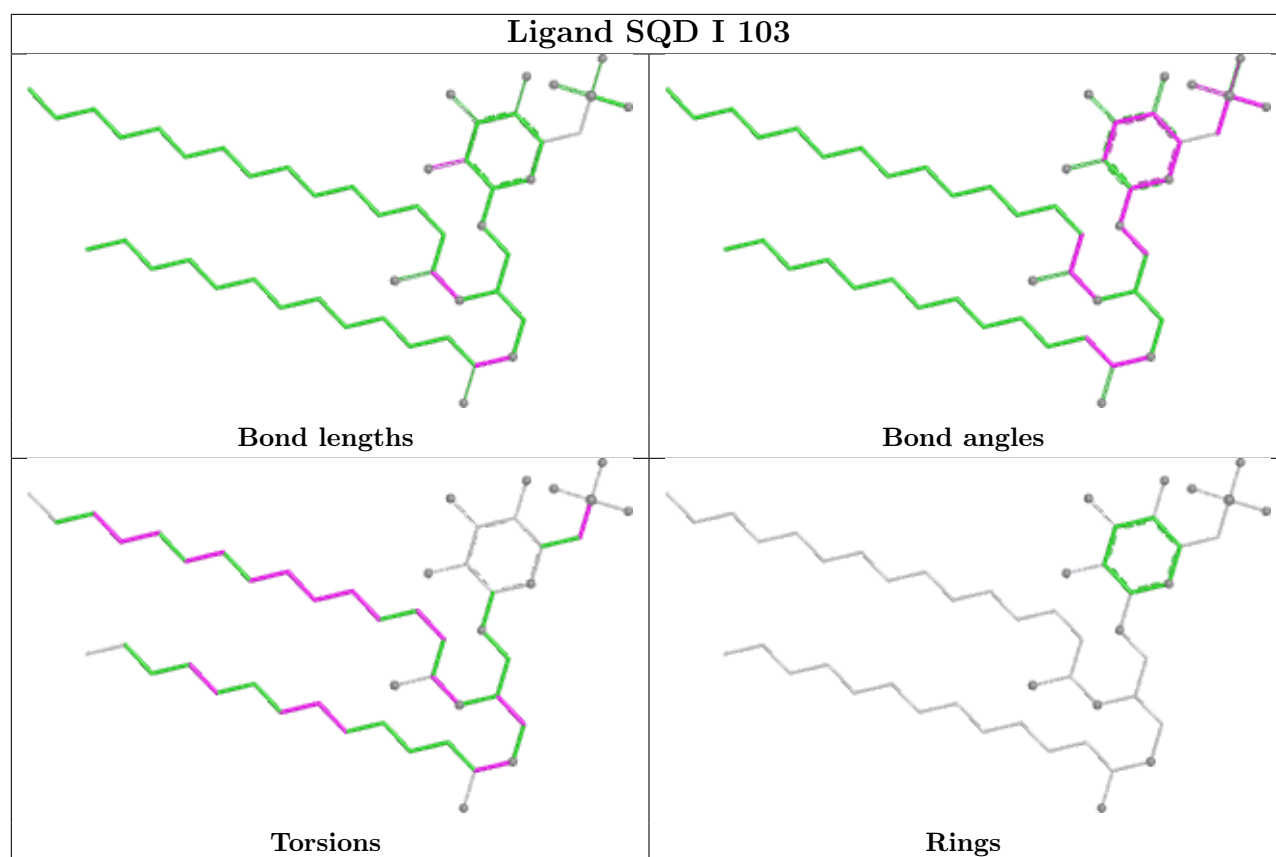
Torsions

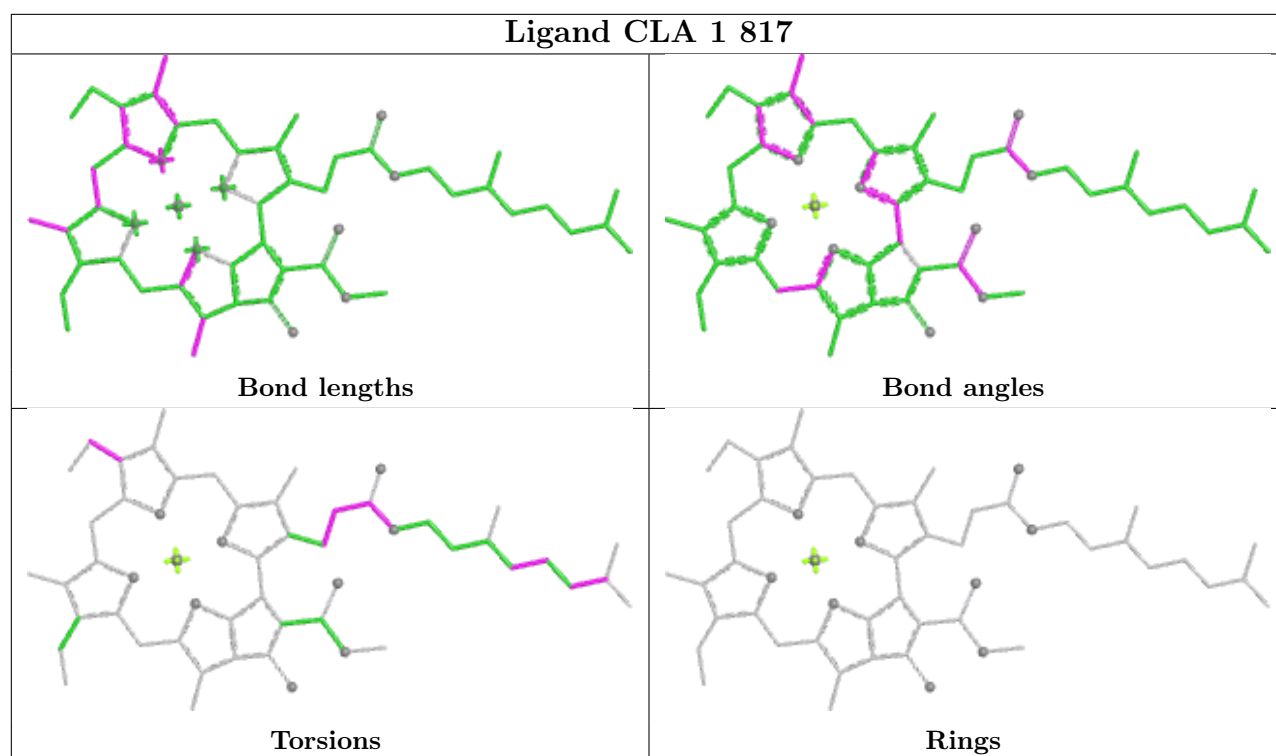


Rings

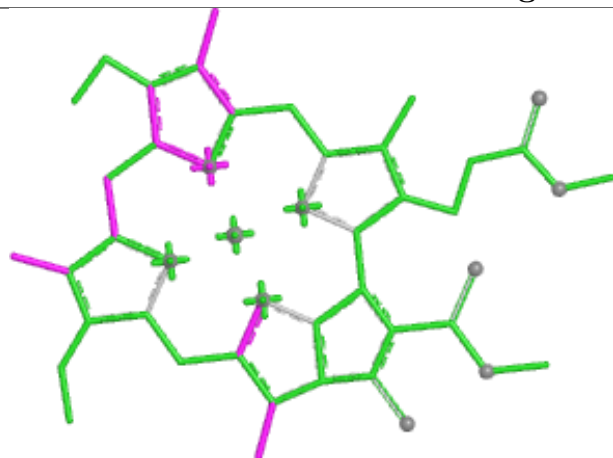




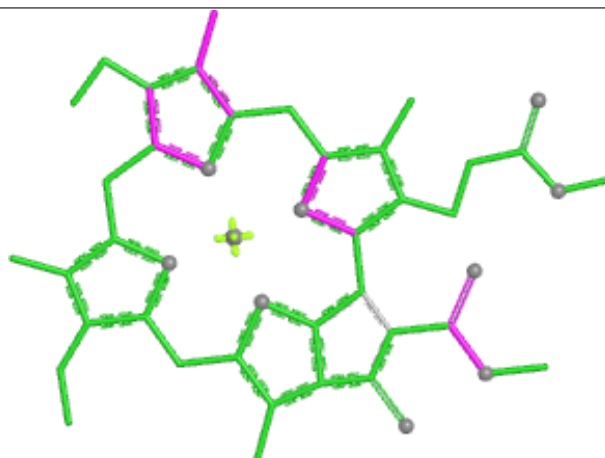




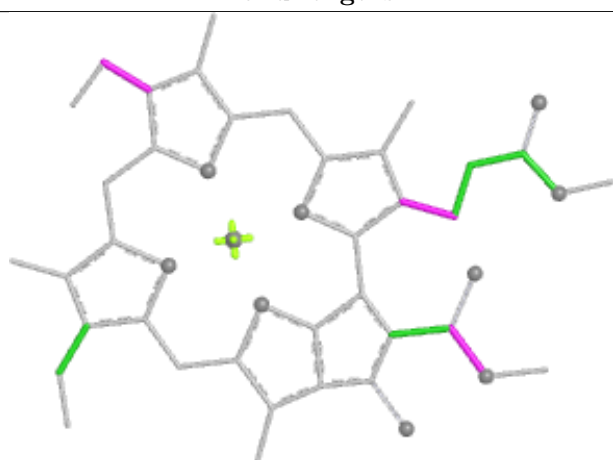
Ligand CLA 0 206



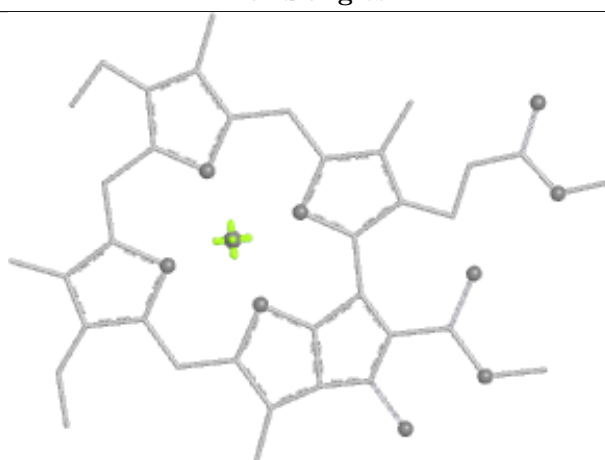
Bond lengths



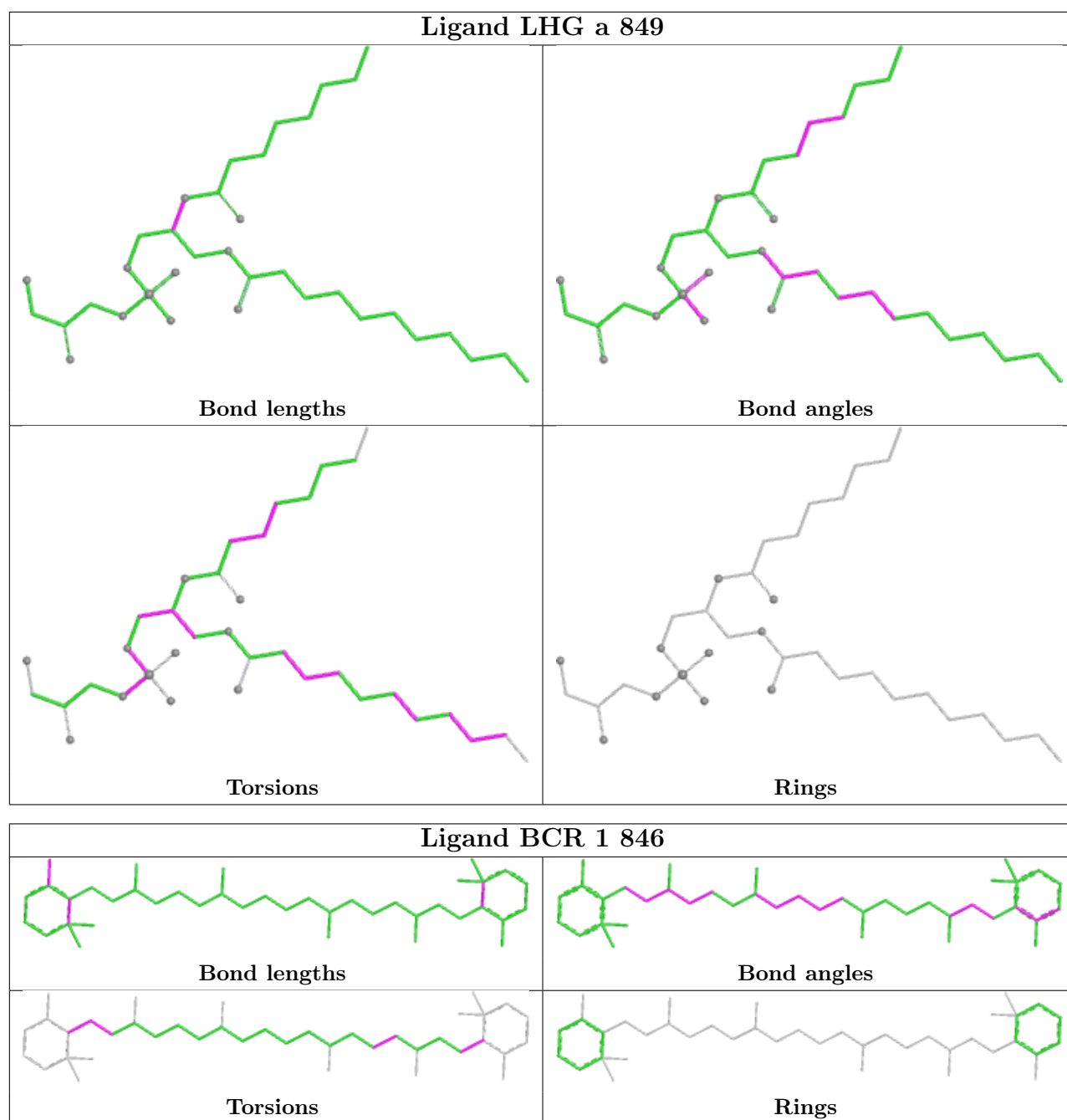
Bond angles

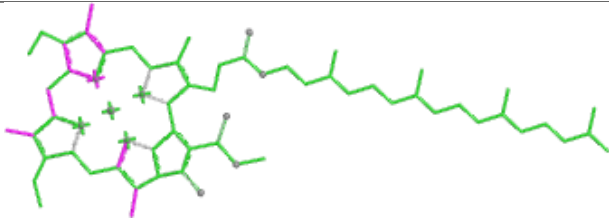
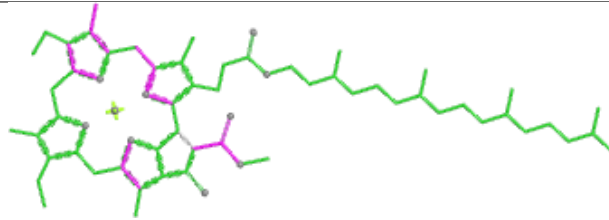
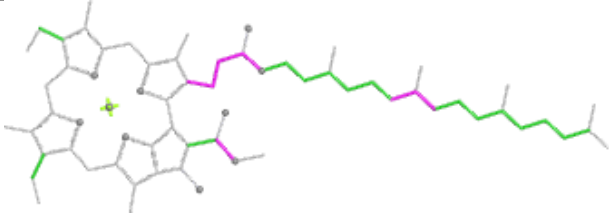
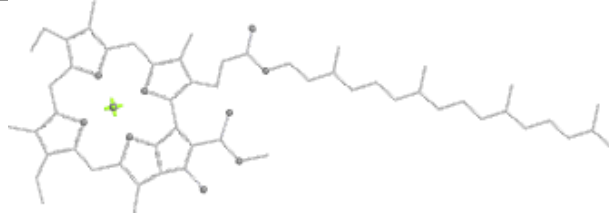
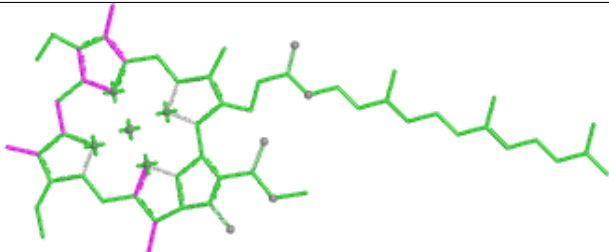
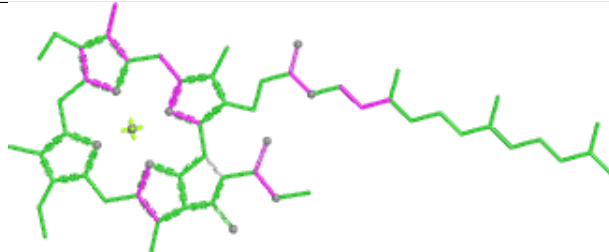
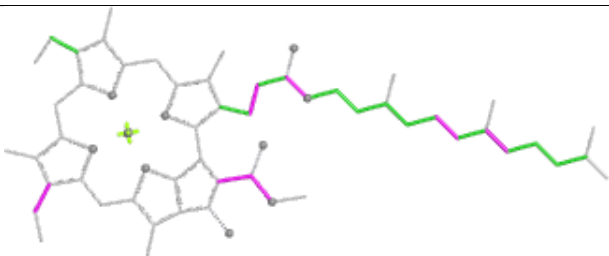
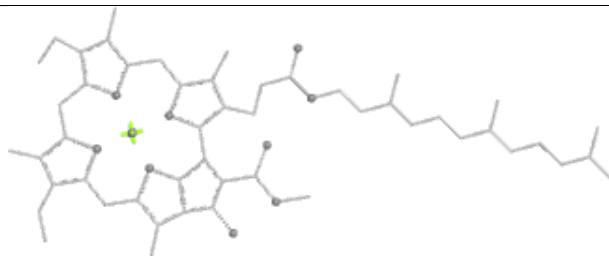
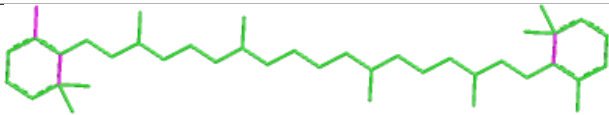
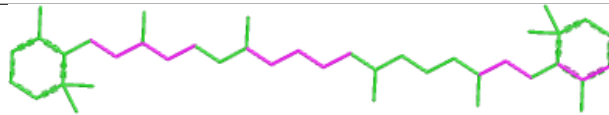
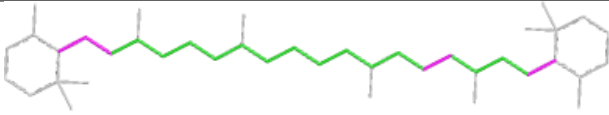
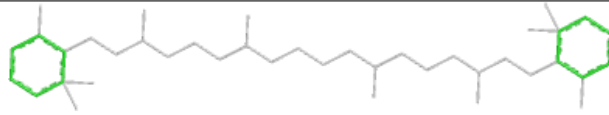


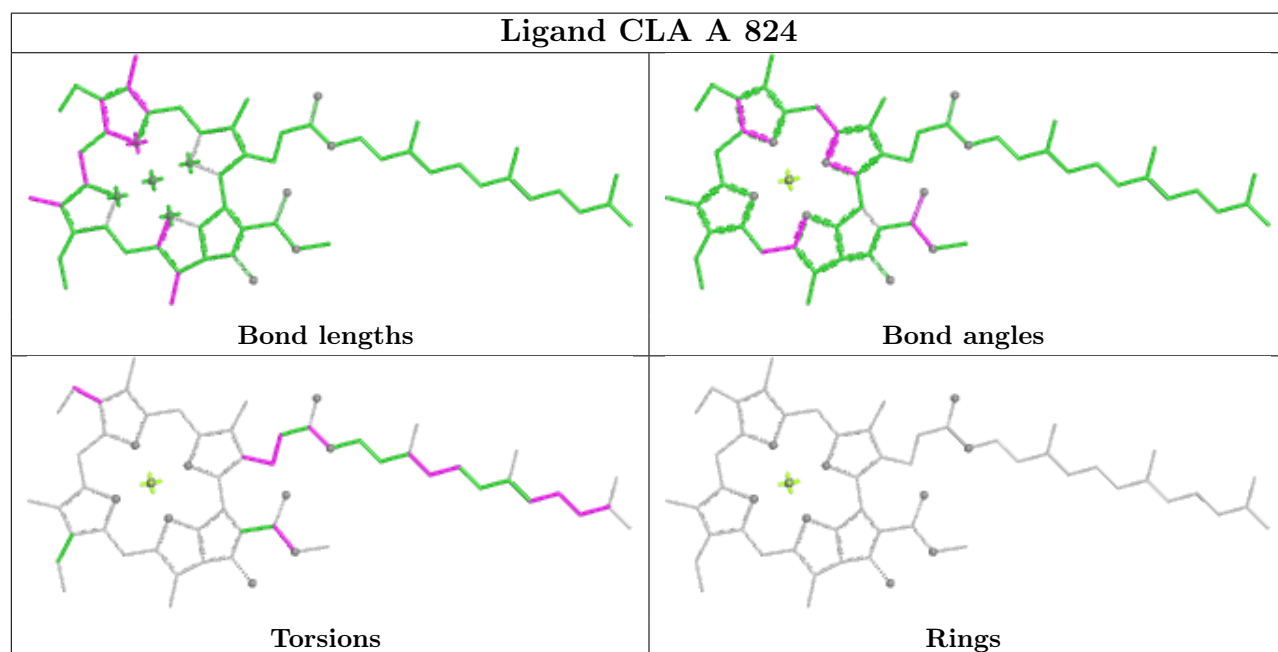
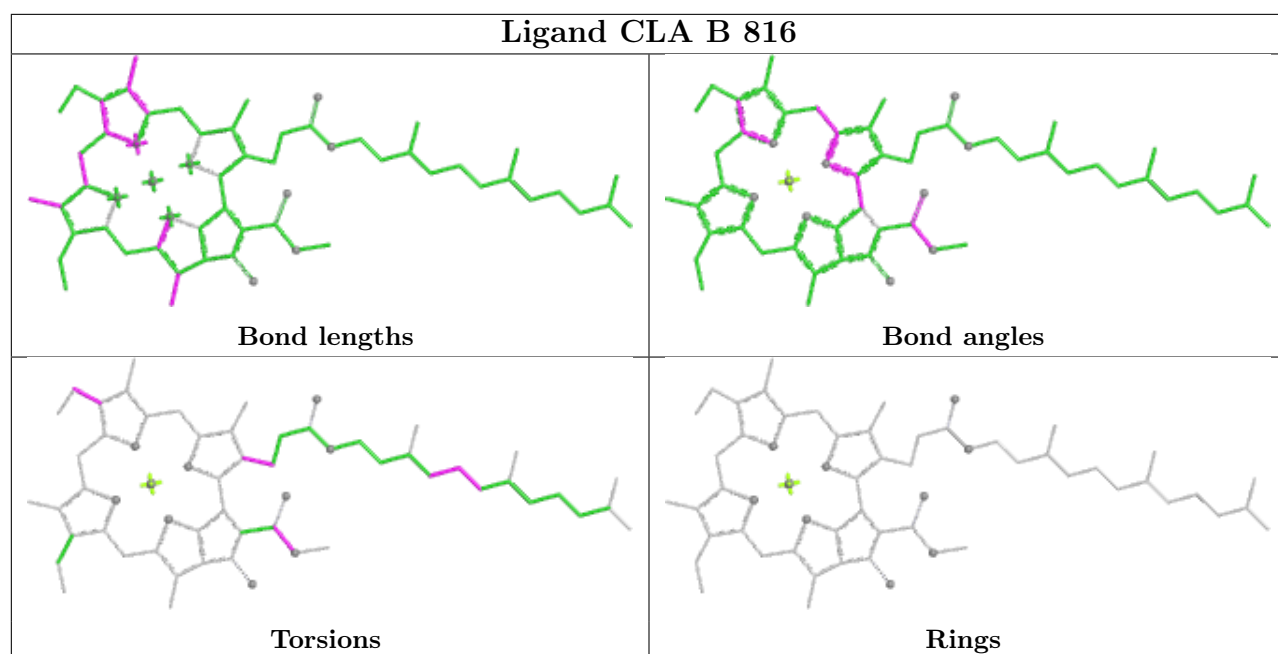
Torsions

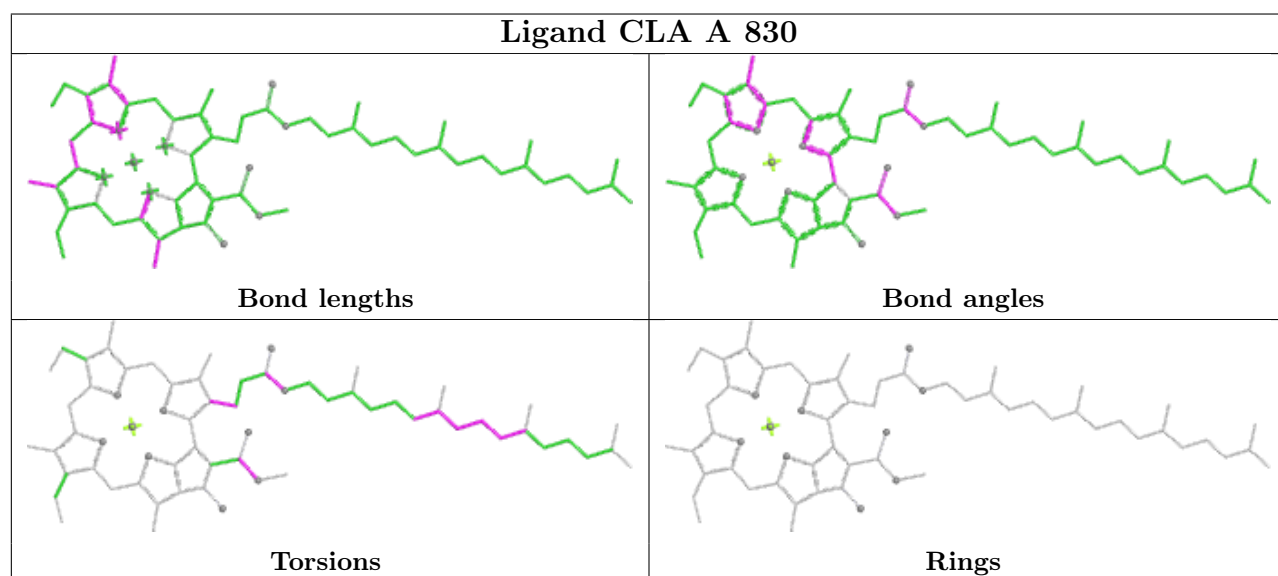
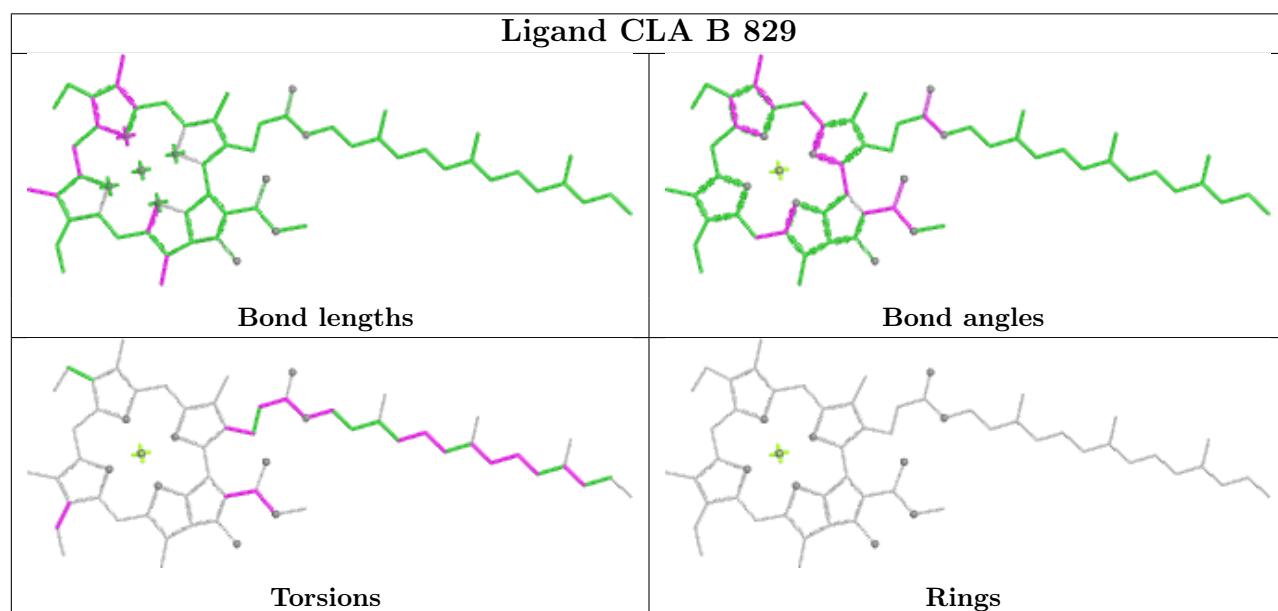
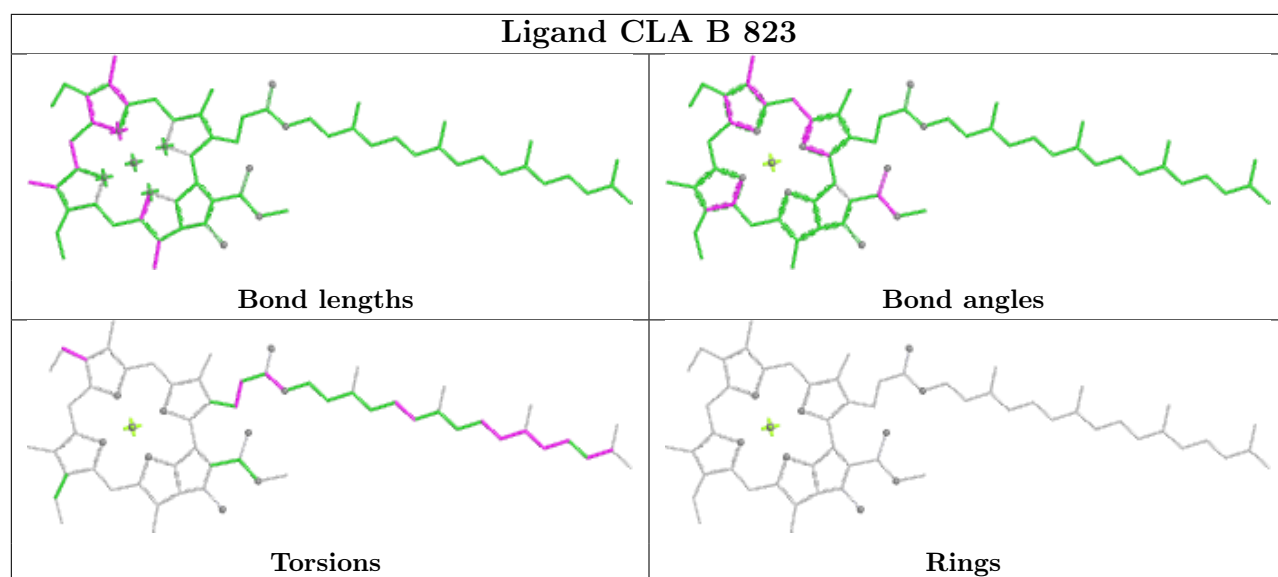


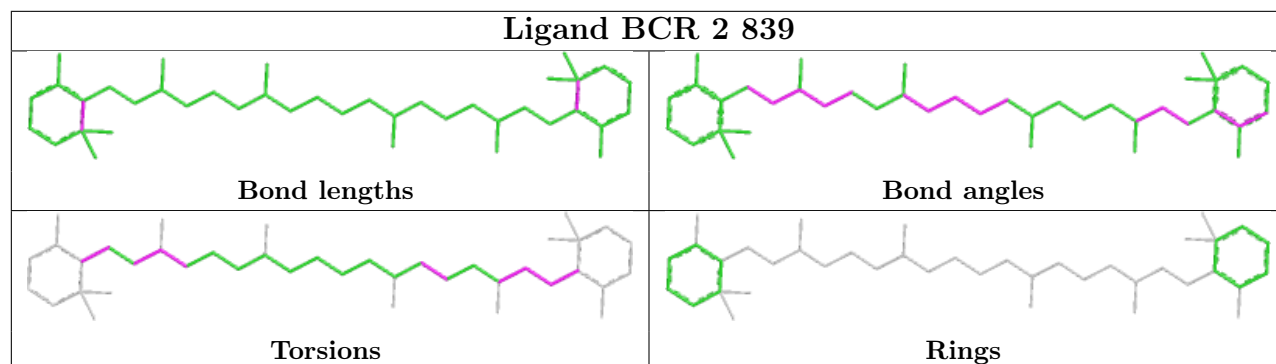
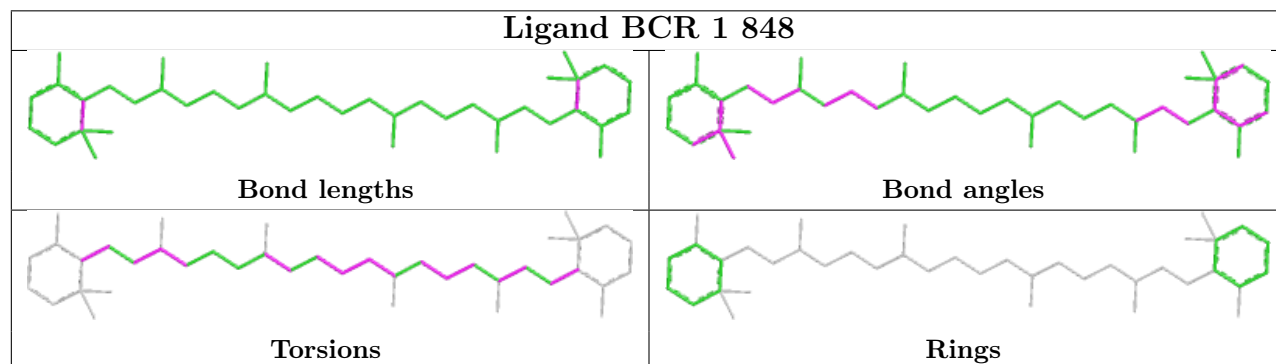
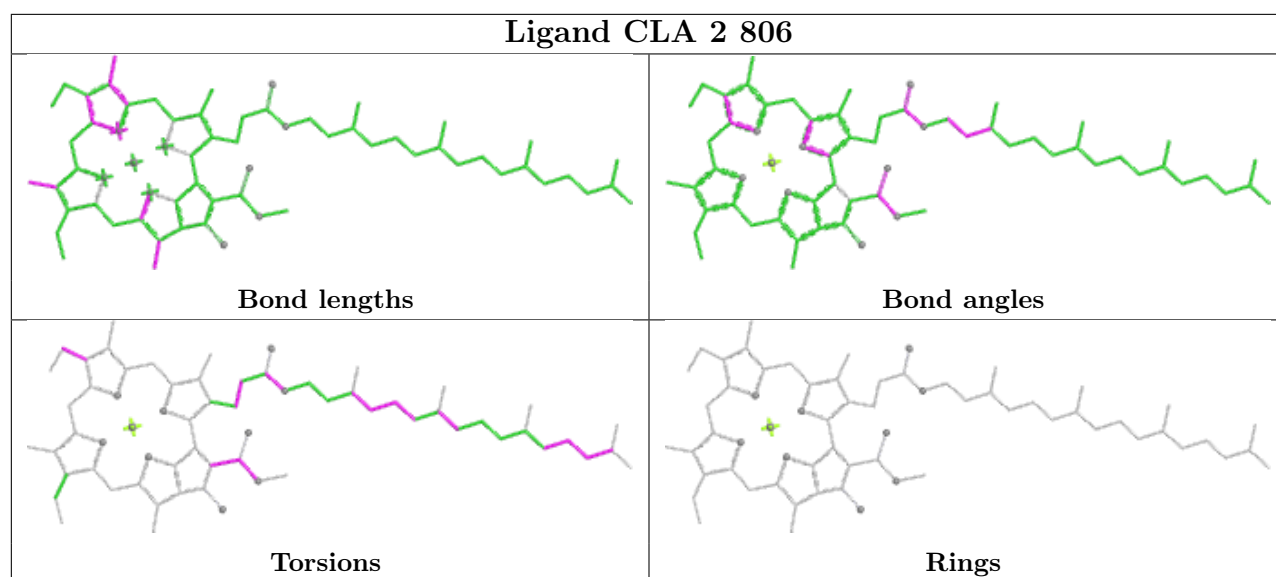
Rings

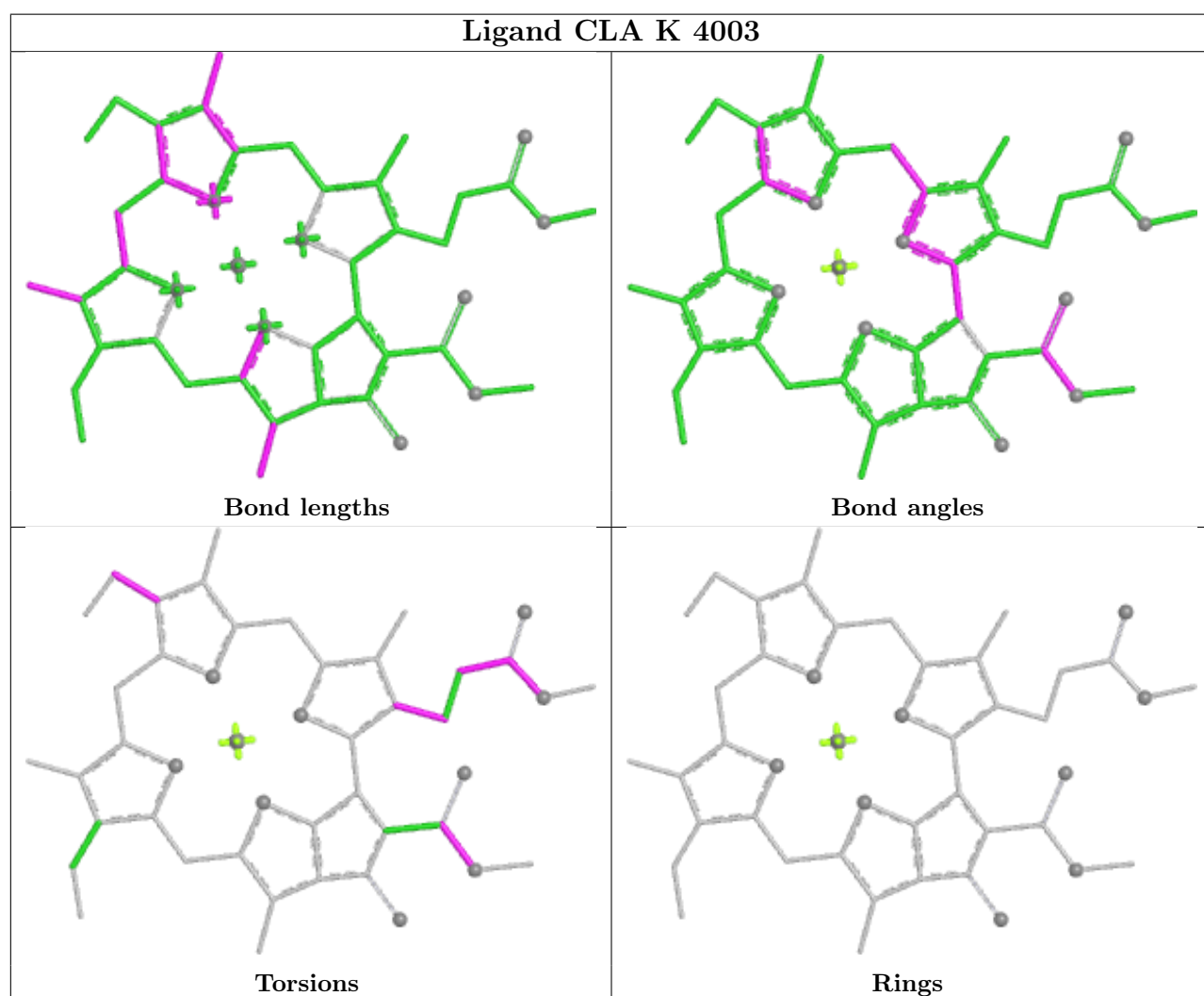
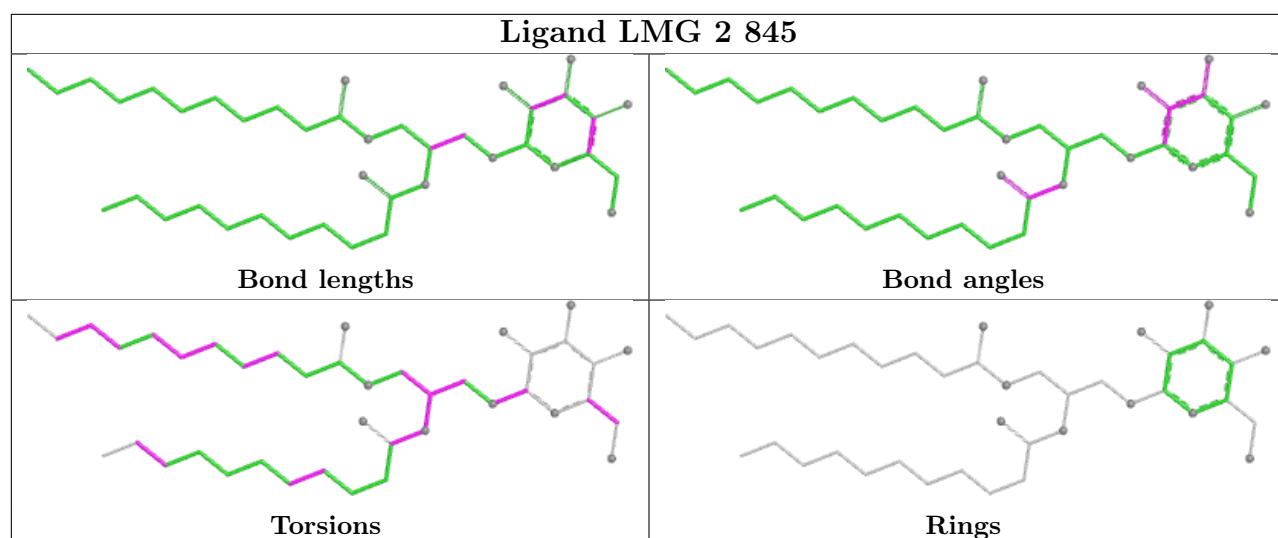


Ligand CLA 2 814	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA 2 803	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR a 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

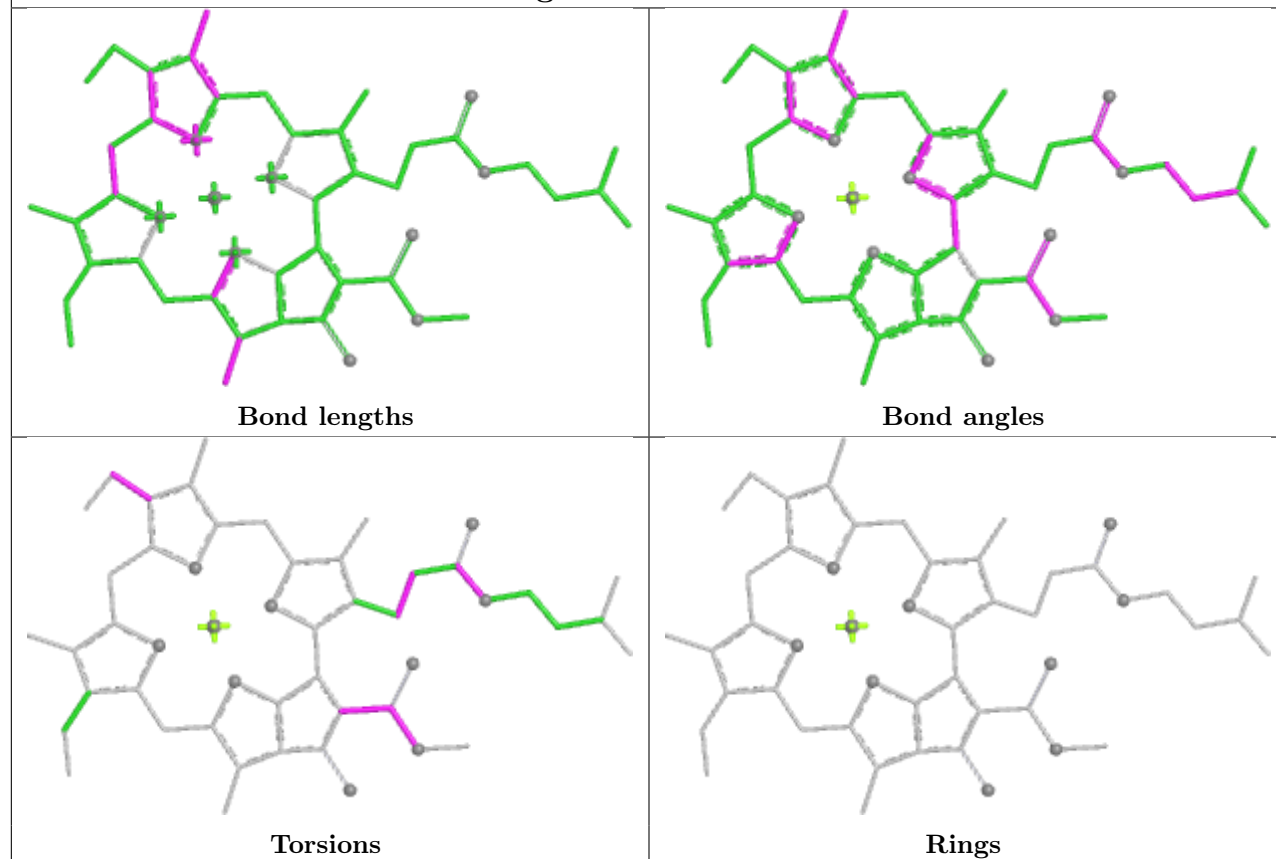




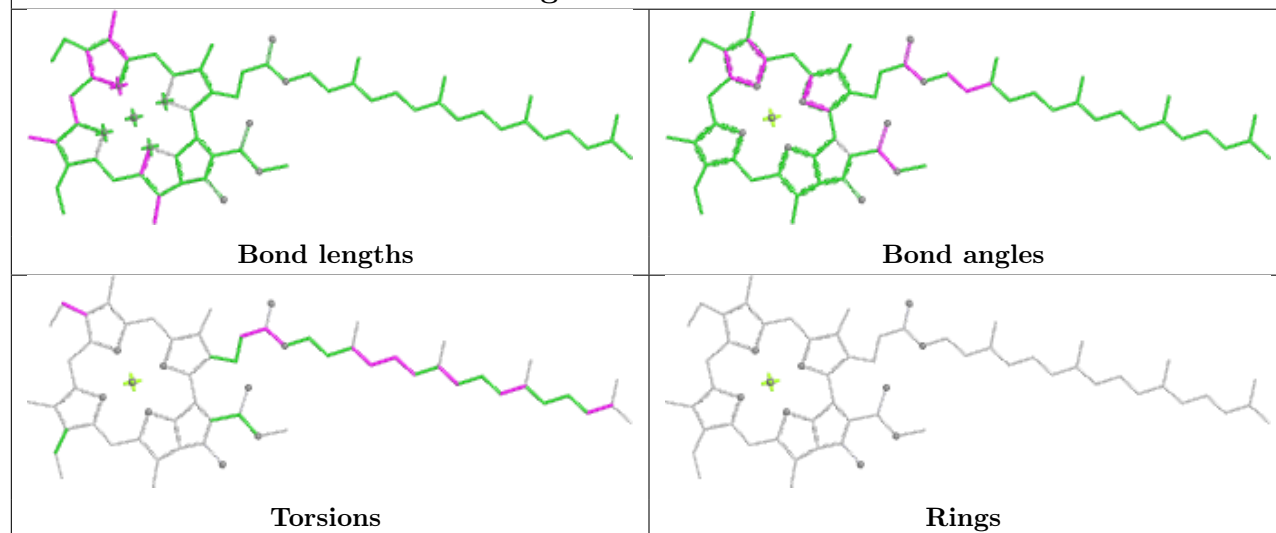


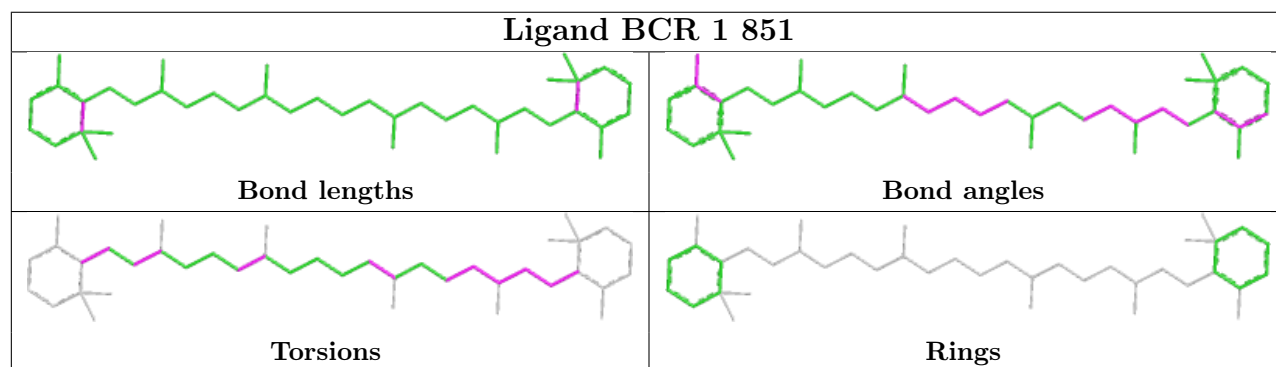
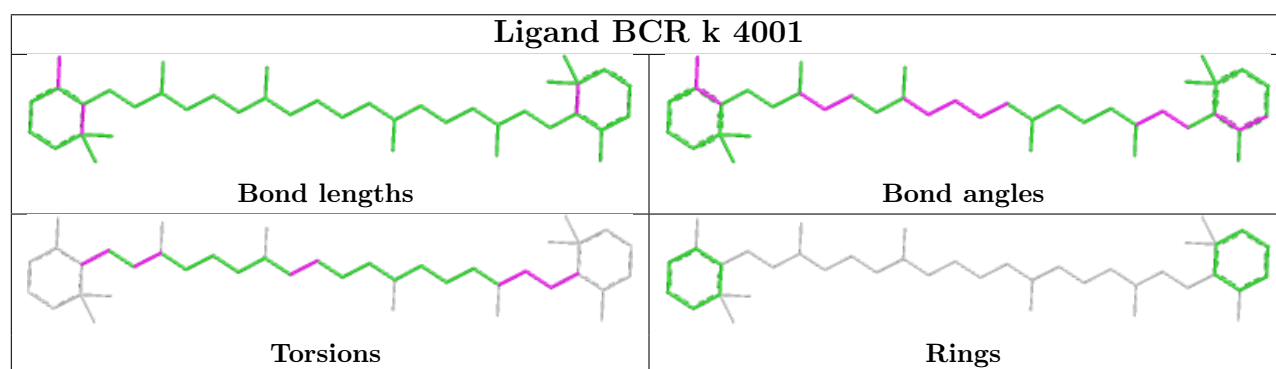
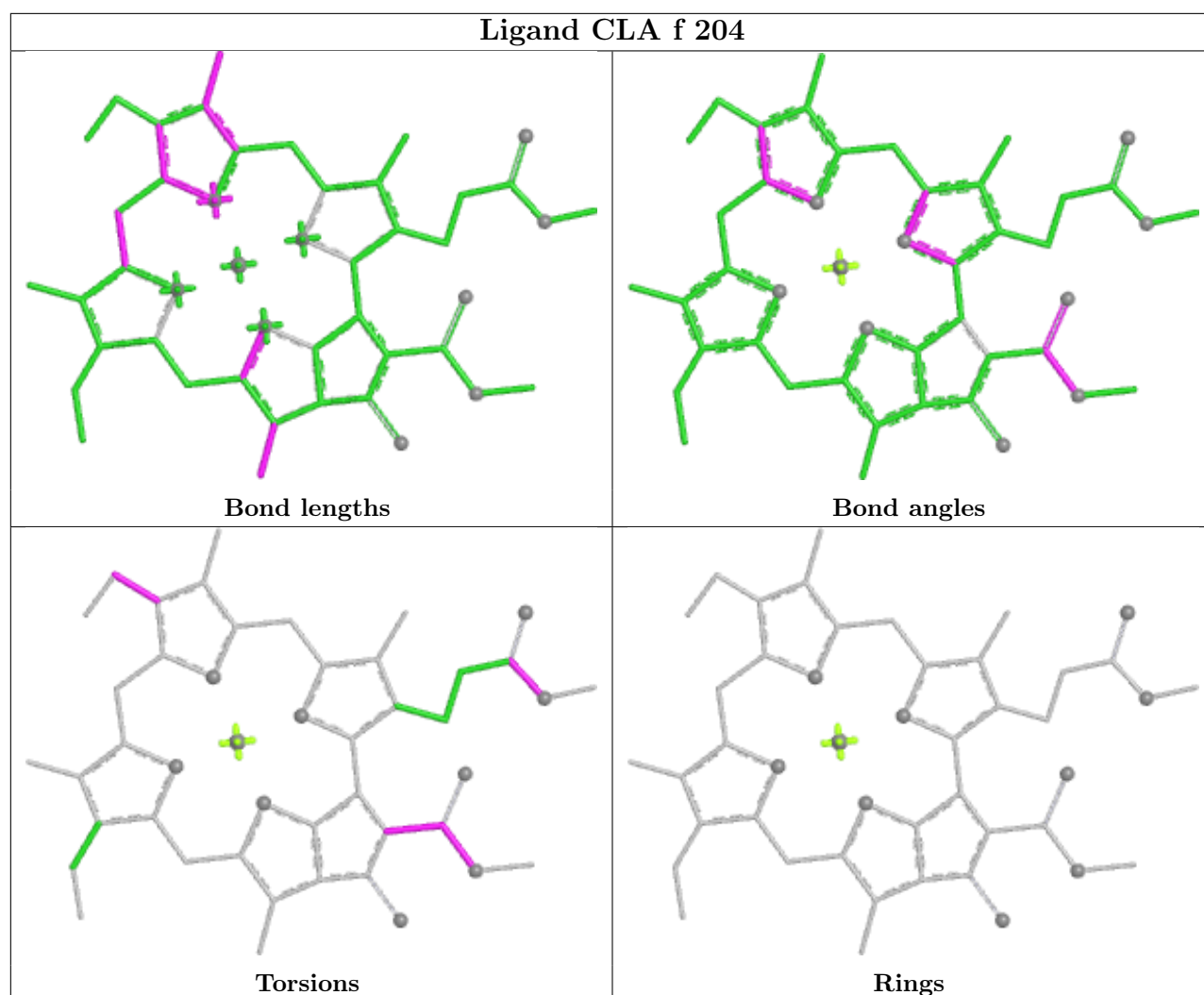


Ligand CLA 1 822

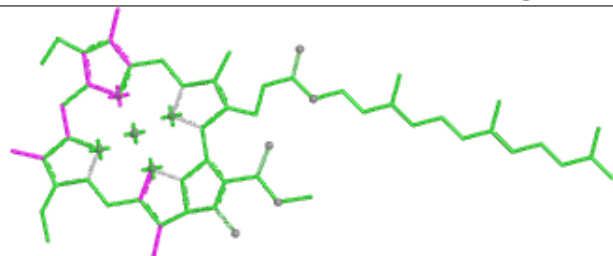


Ligand CL0 1 801

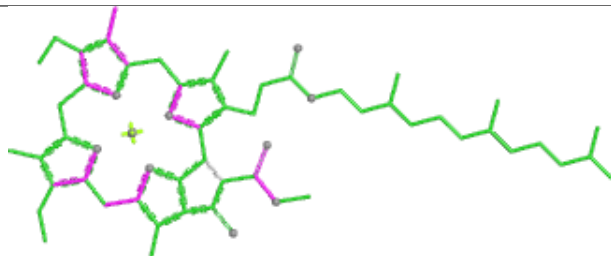




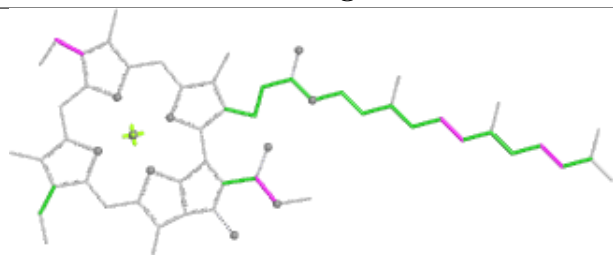
Ligand CLA b 834



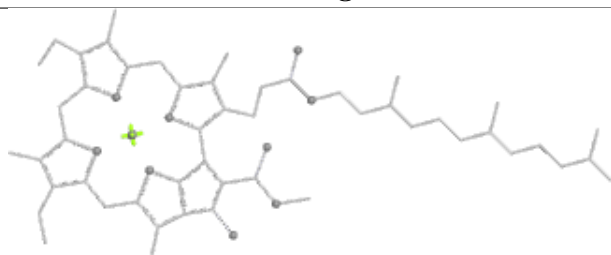
Bond lengths



Bond angles

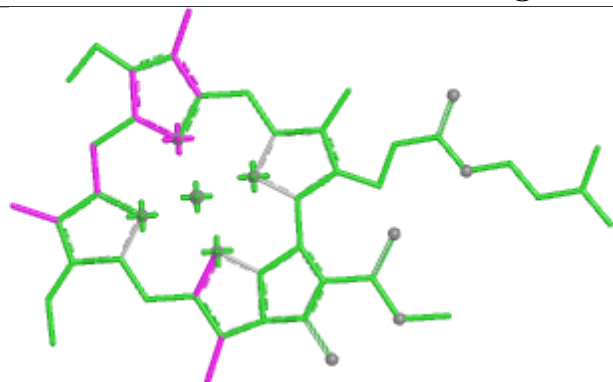


Torsions

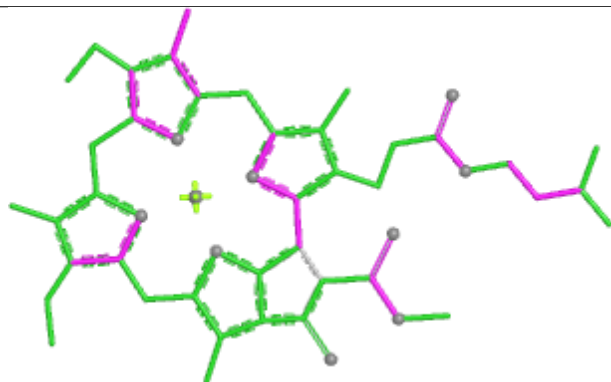


Rings

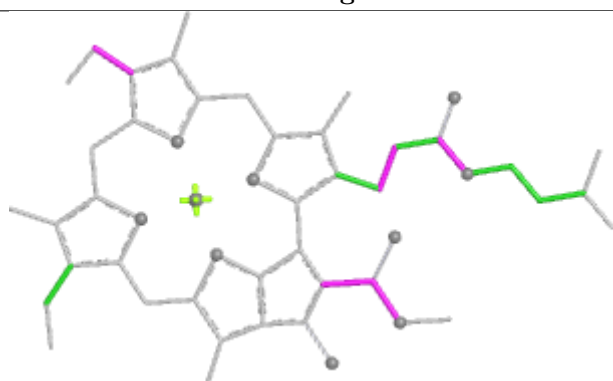
Ligand CLA A 822



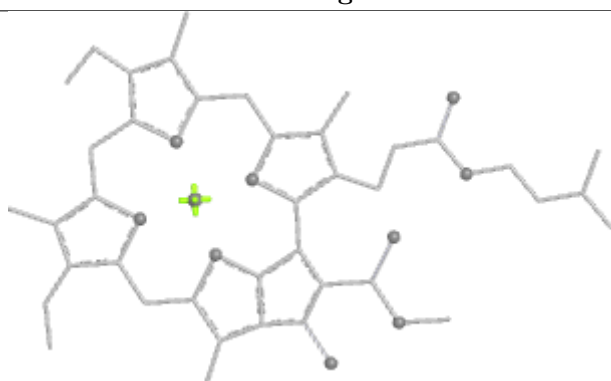
Bond lengths



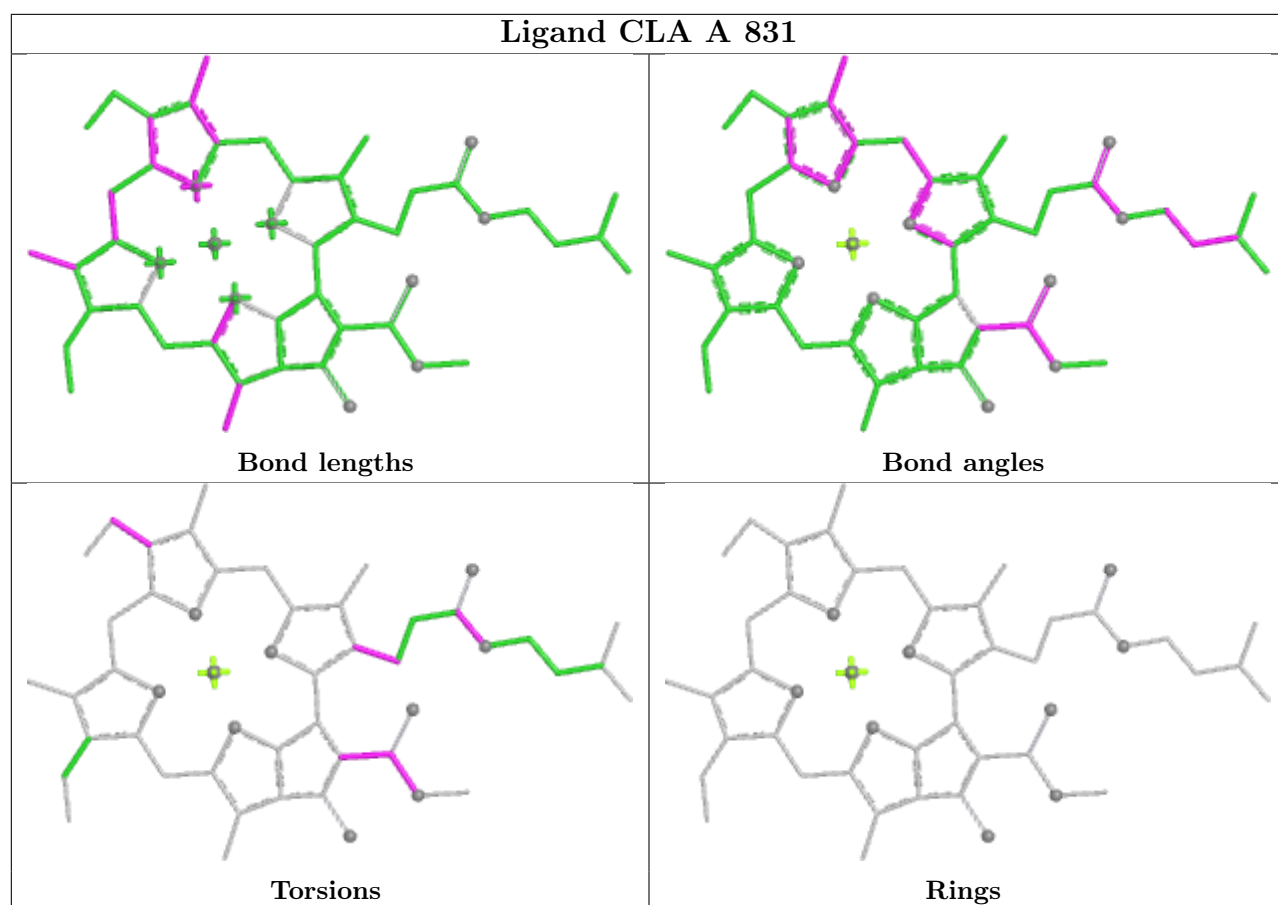
Bond angles



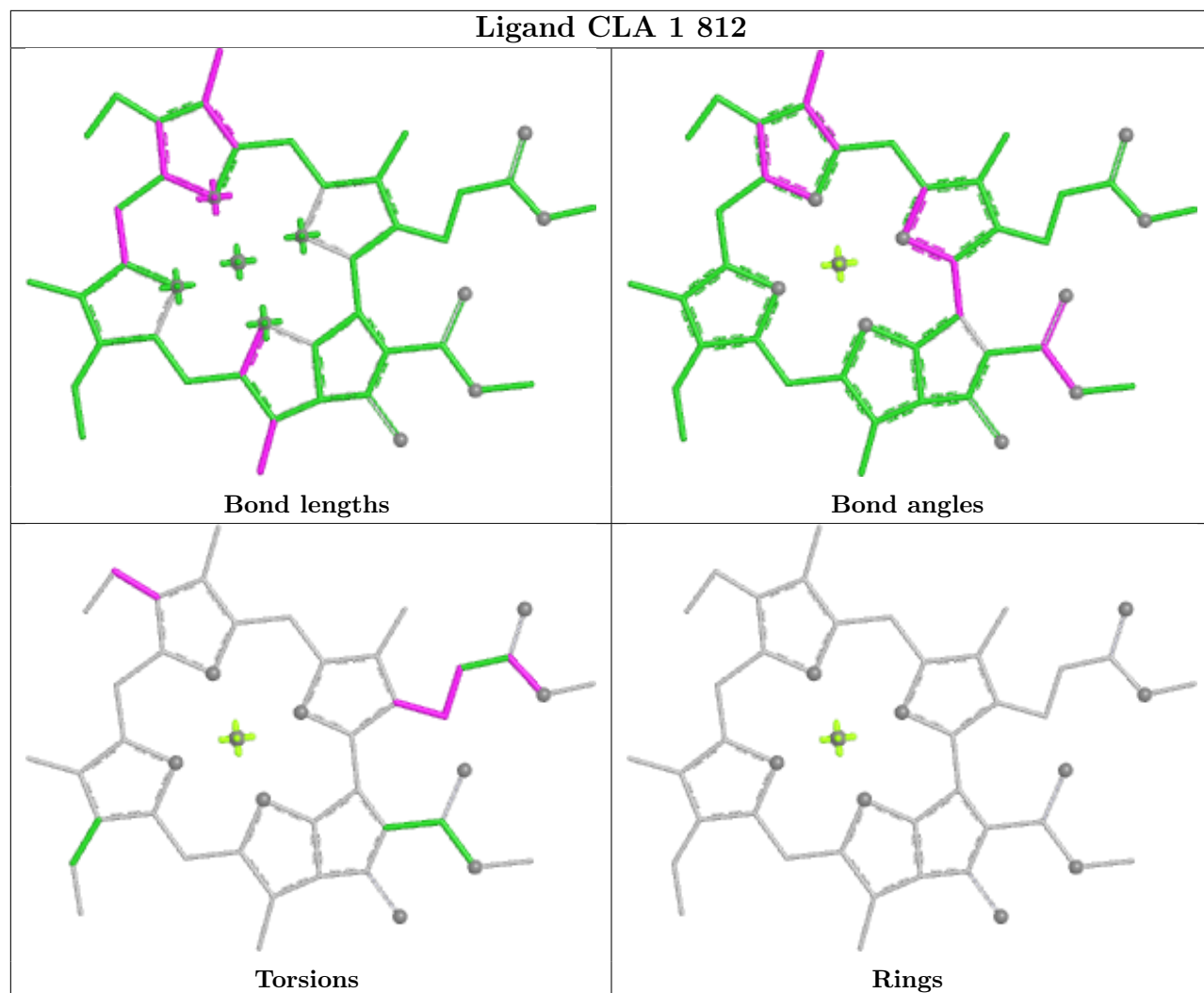
Torsions



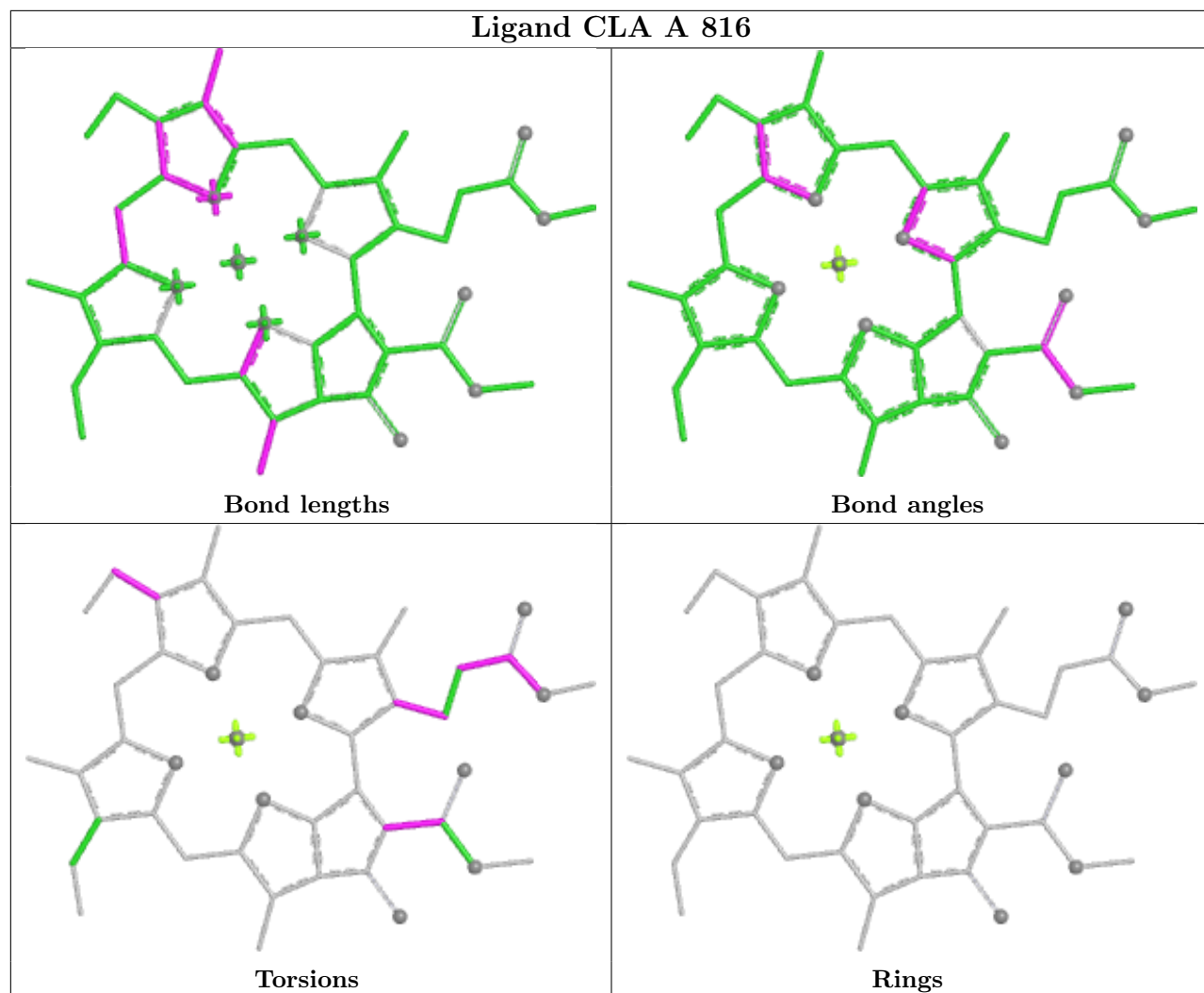
Rings



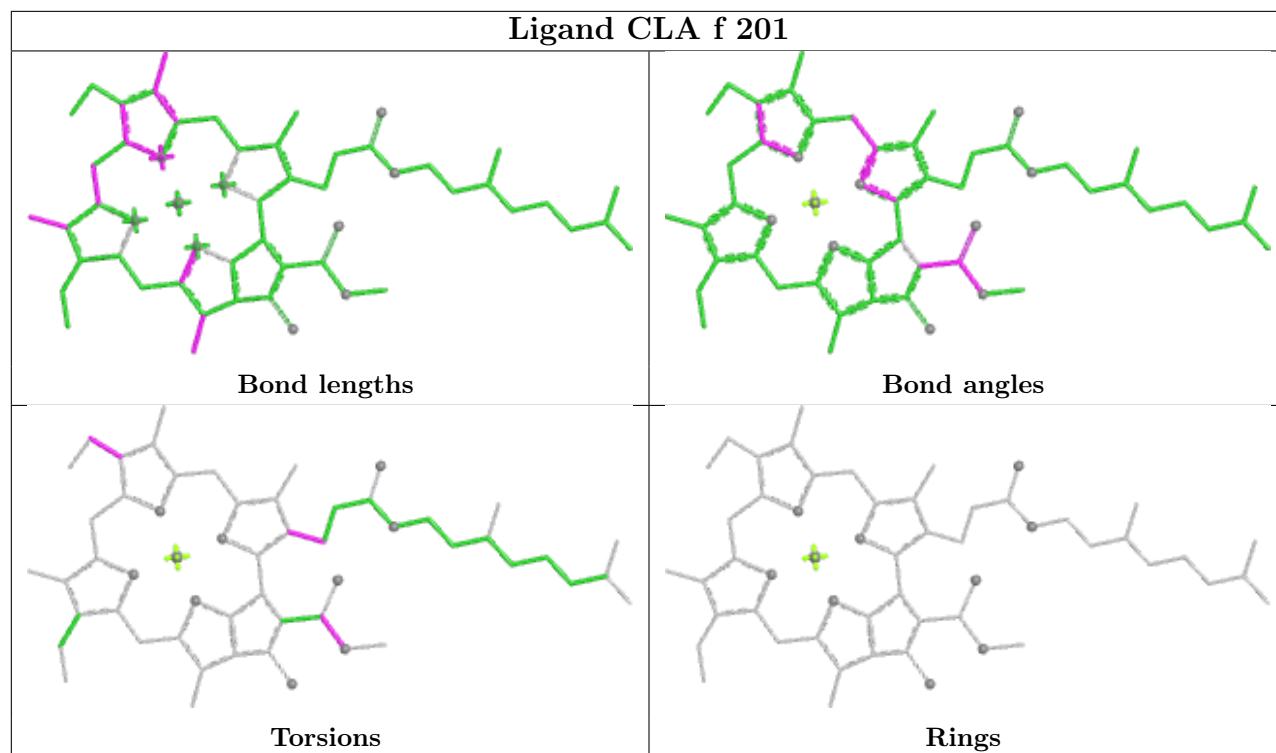
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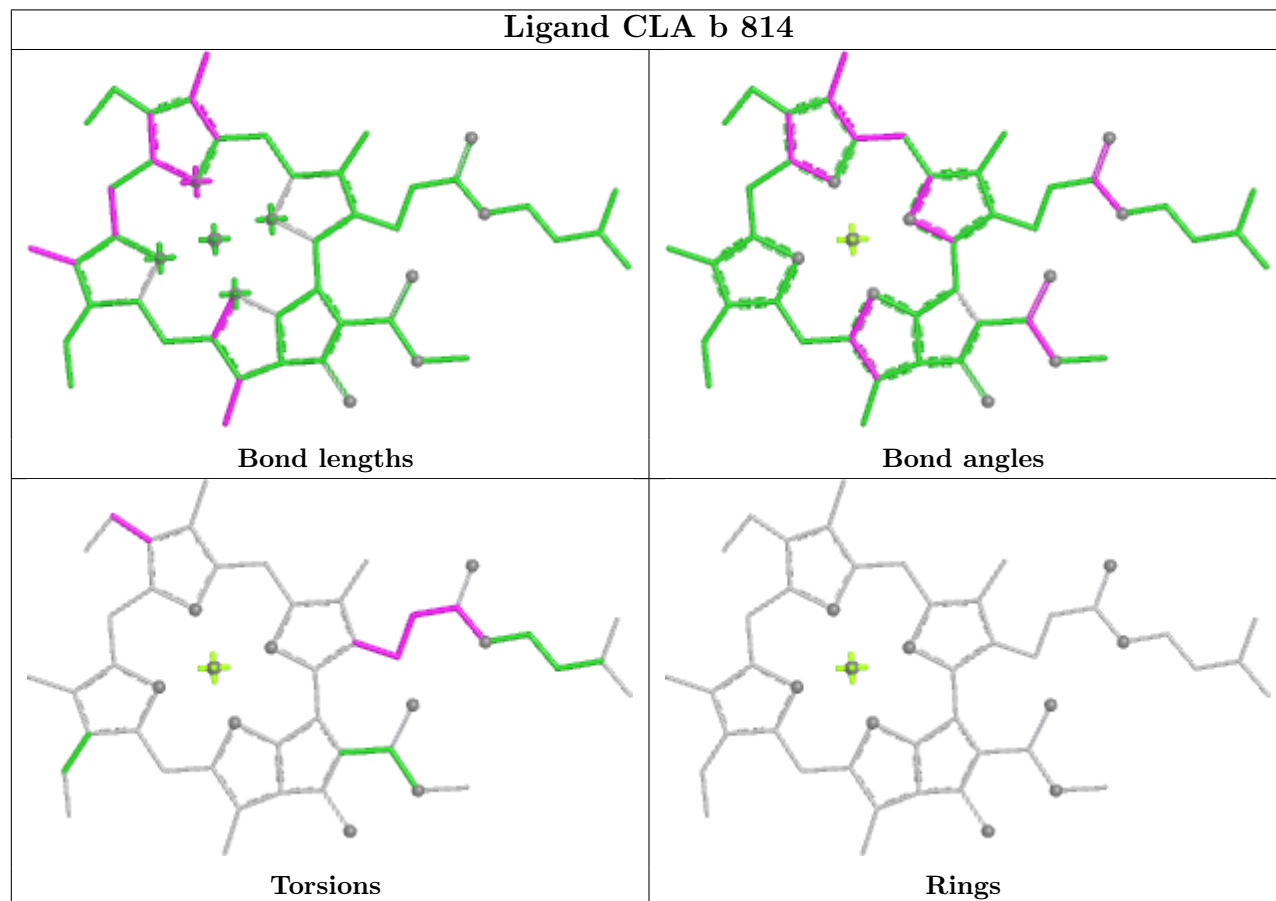
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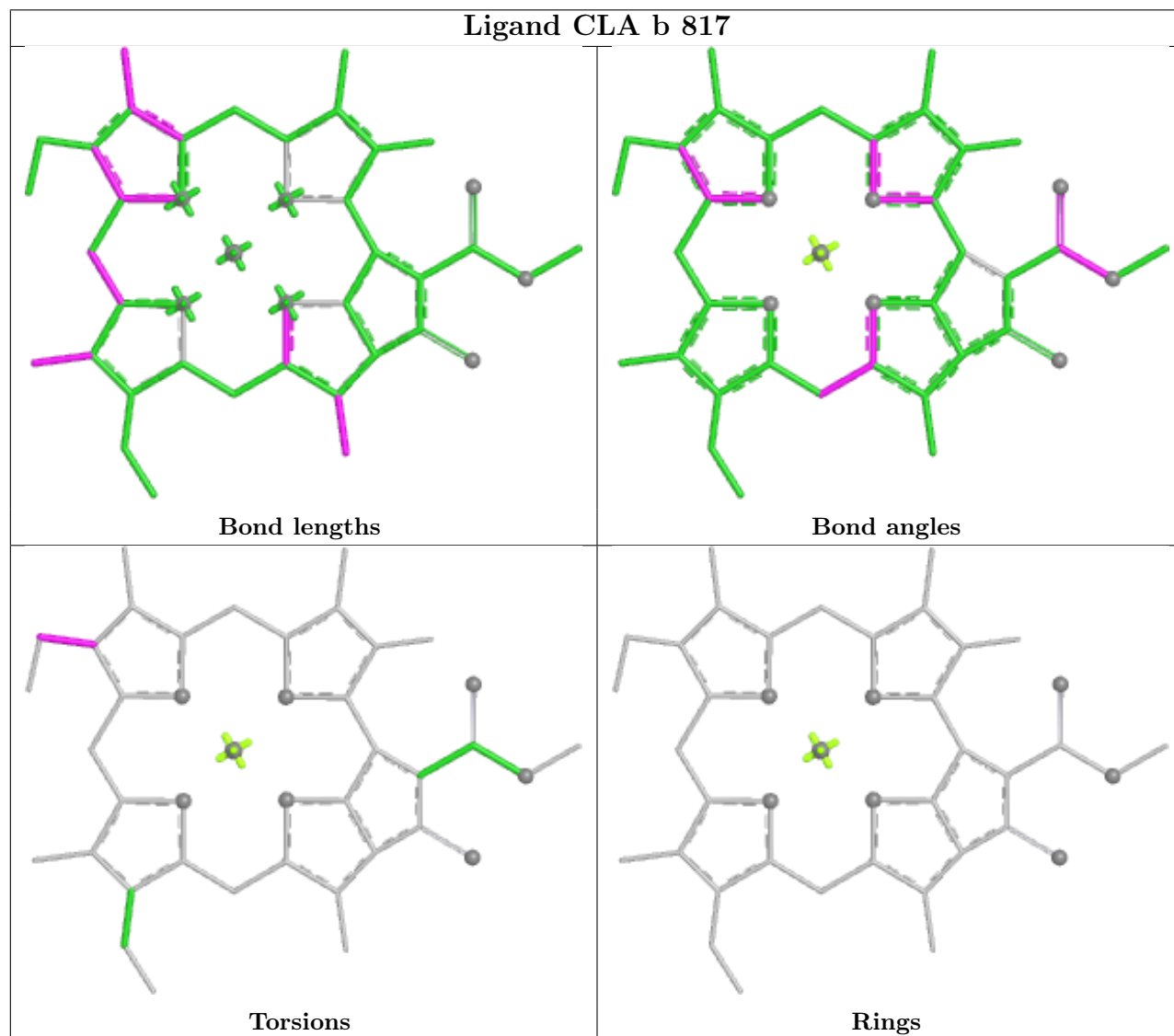
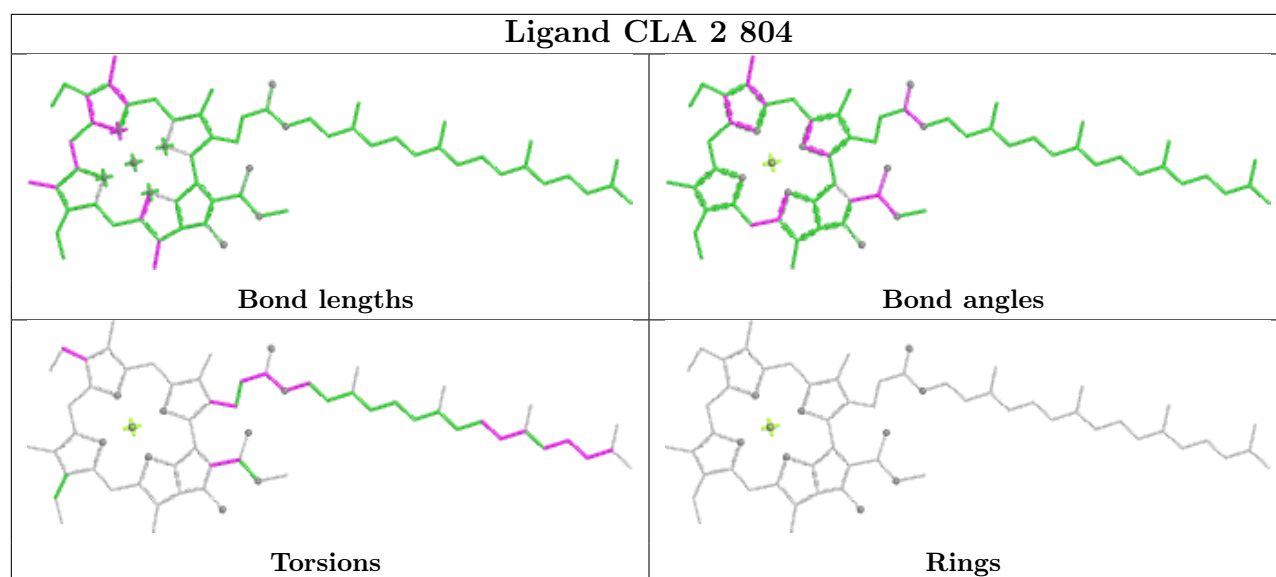


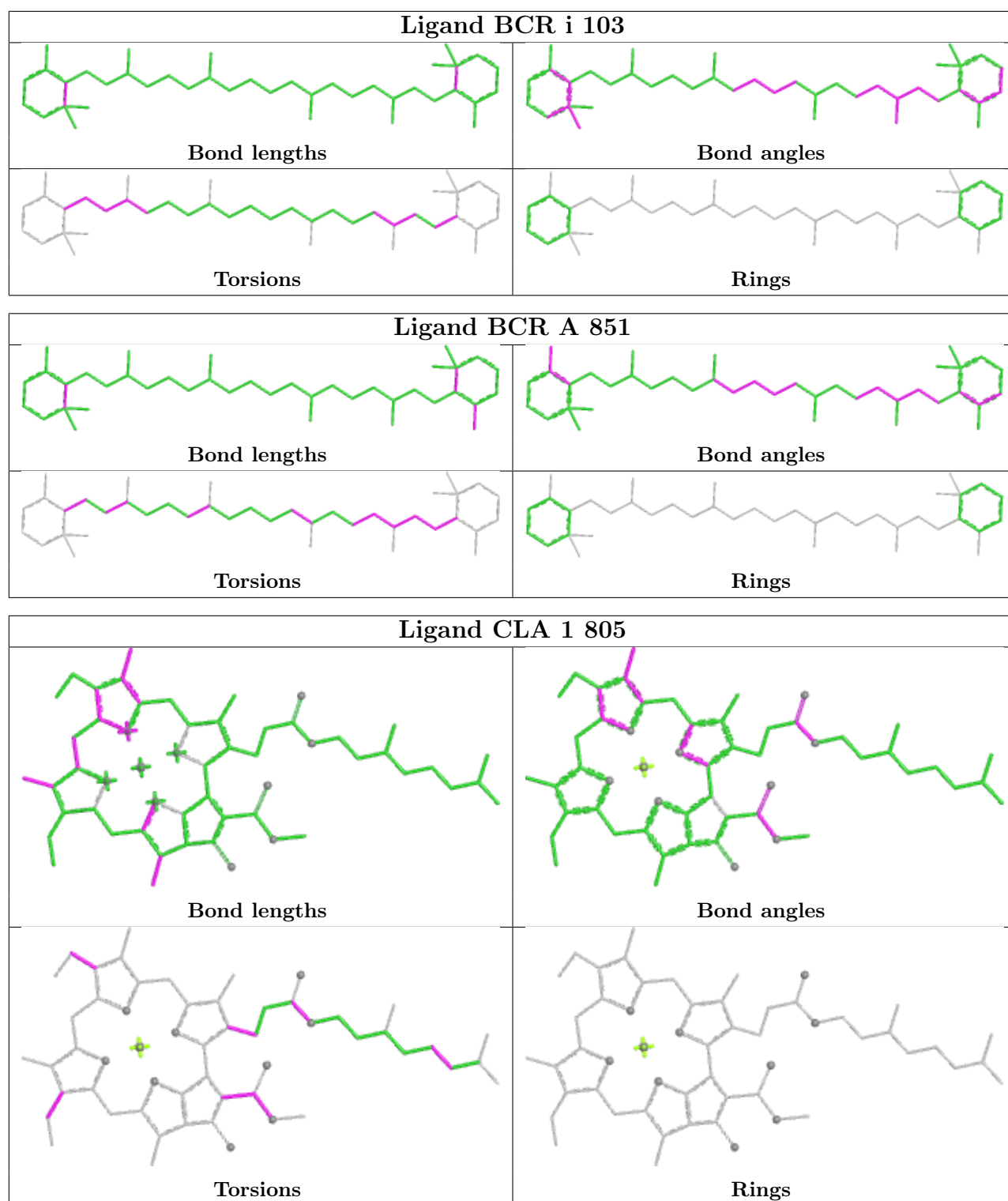
Ligand CLA f 201

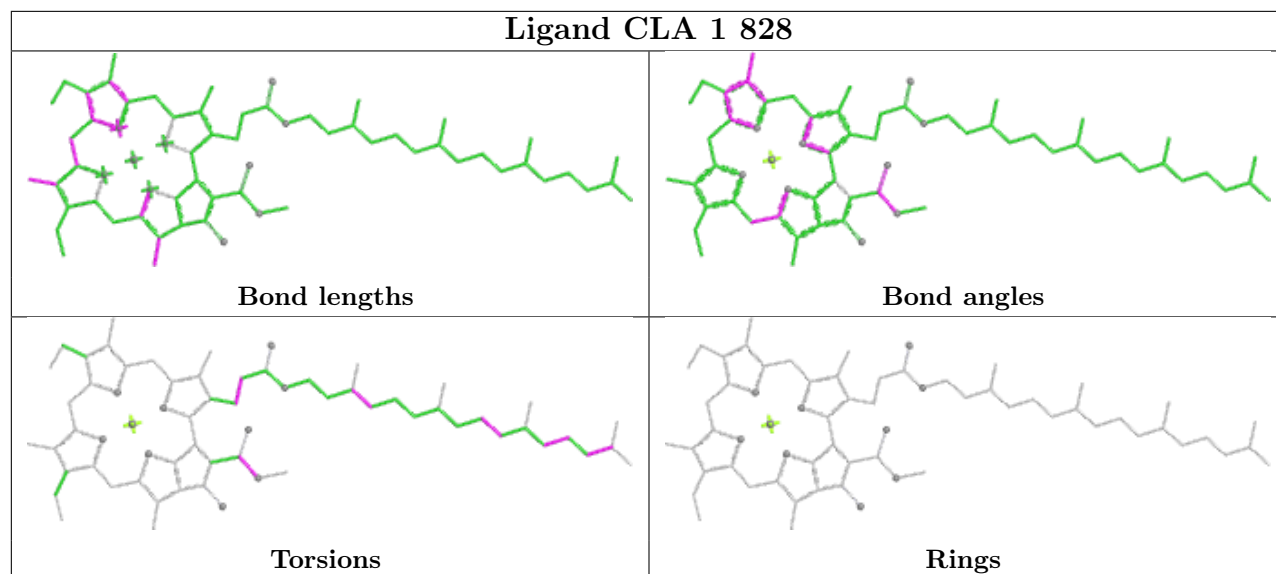
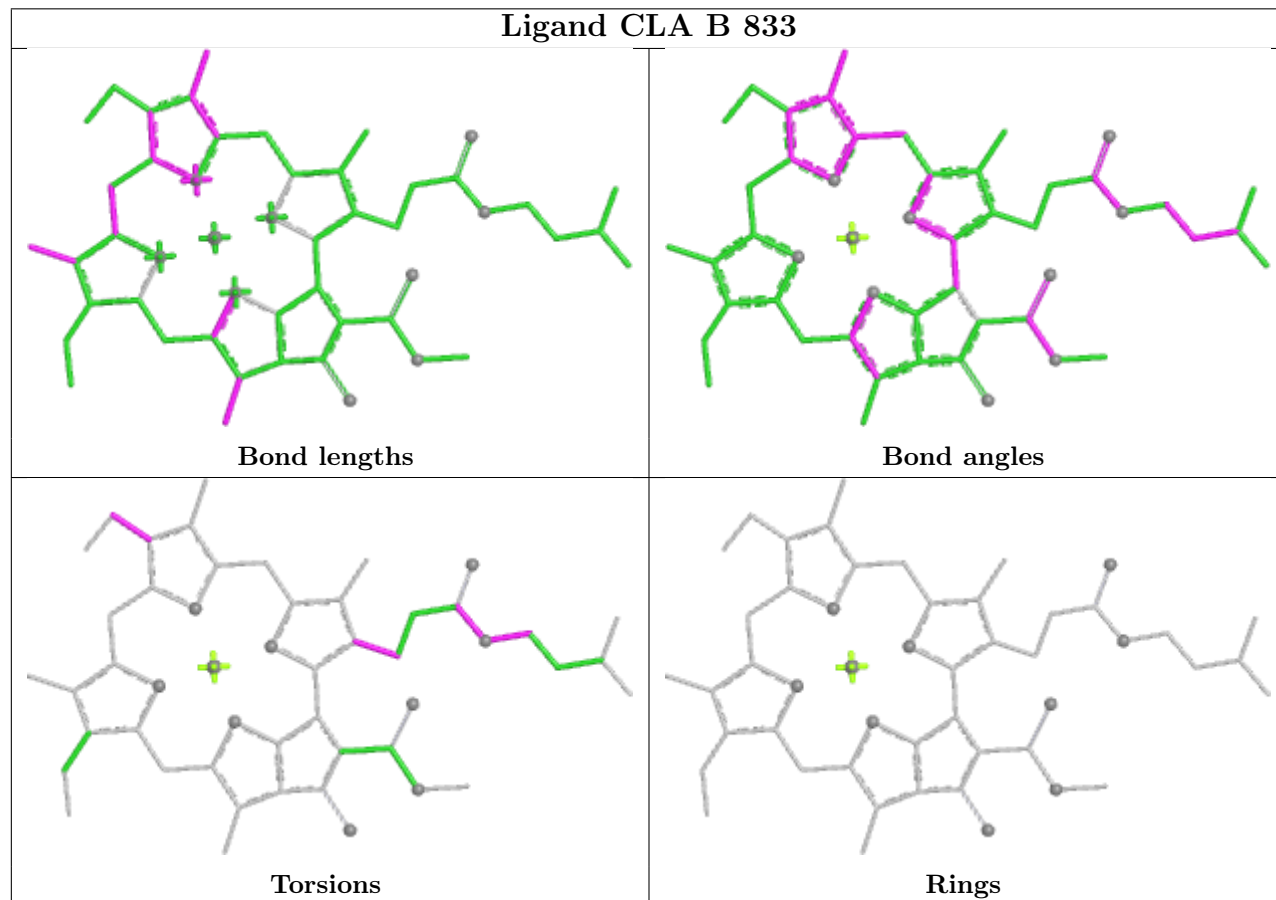


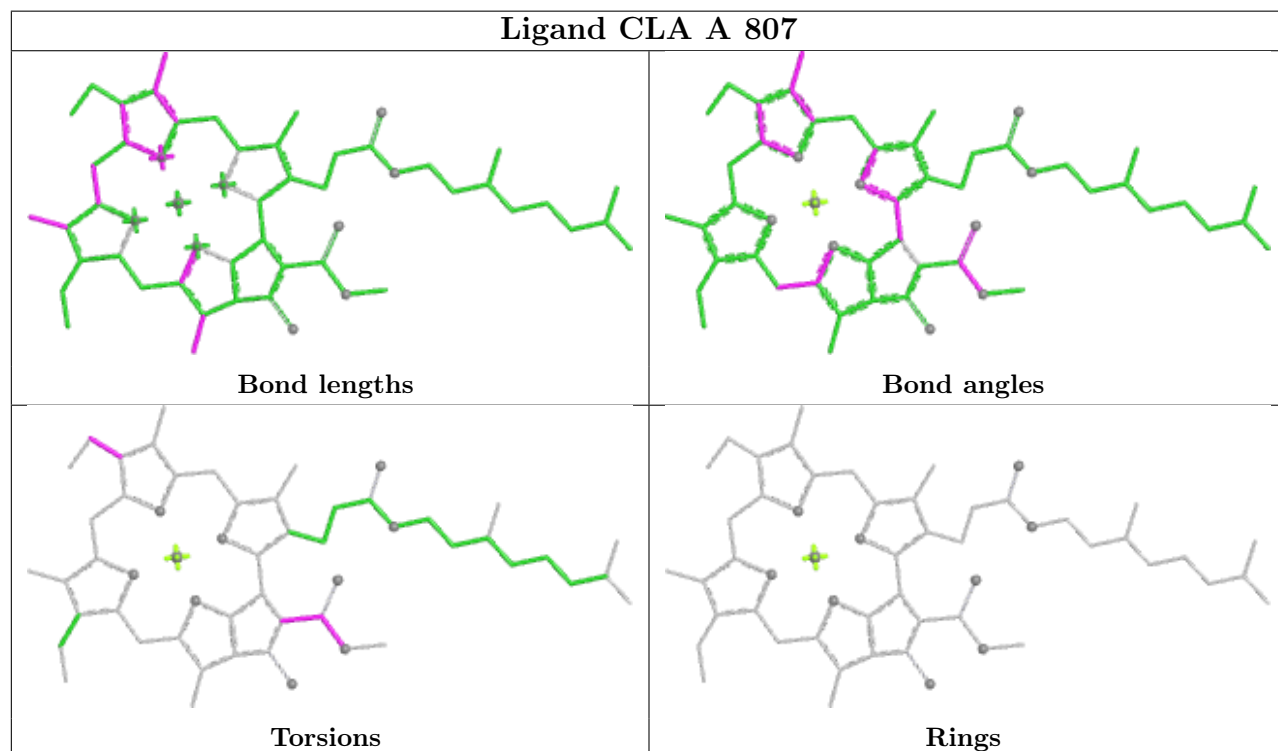
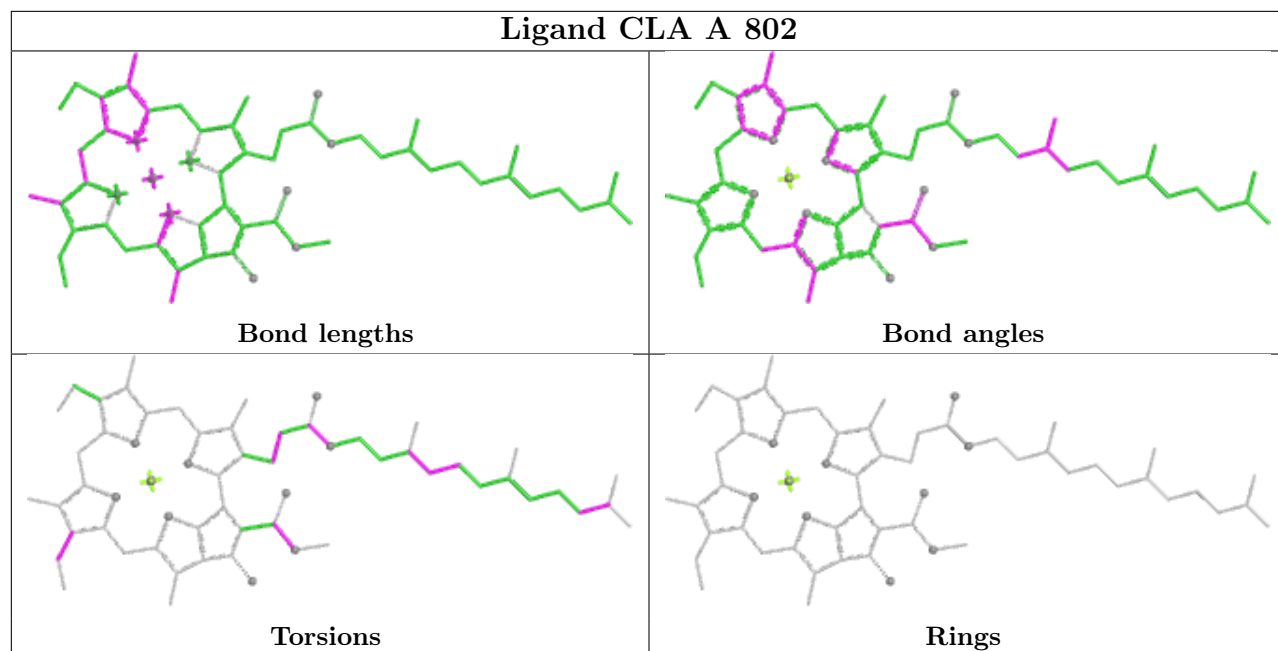
Ligand CLA b 814



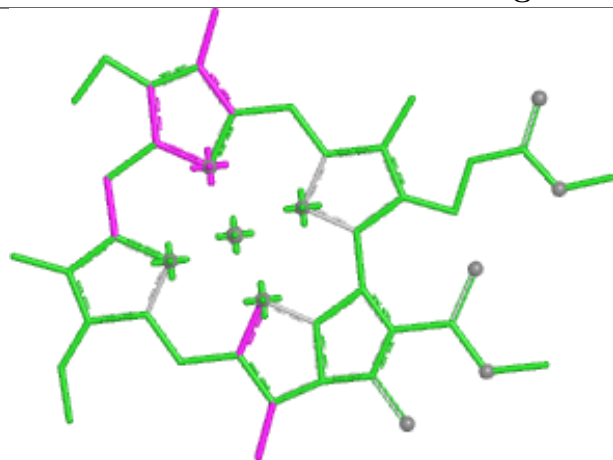




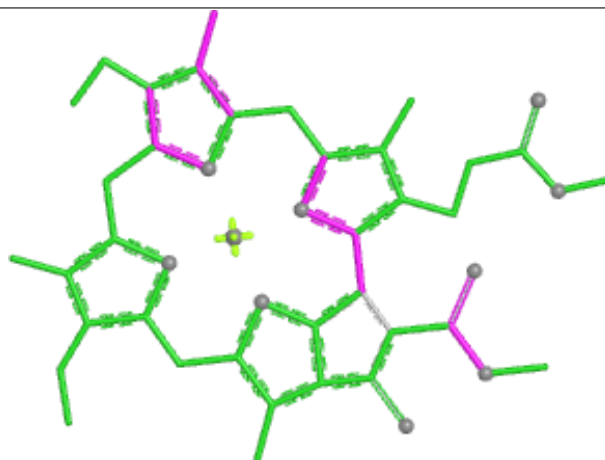
Ligand CLA 1 828**Ligand CLA B 833**



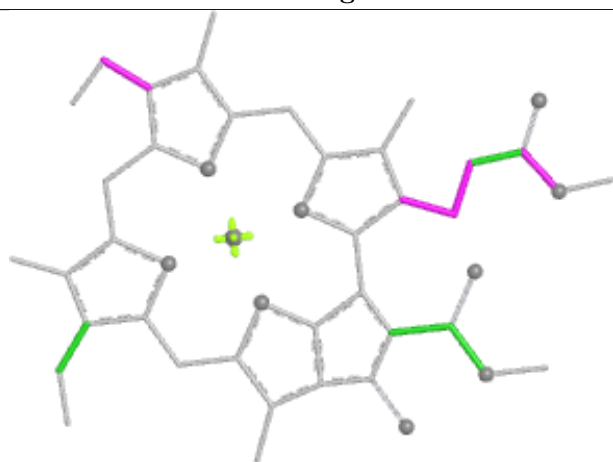
Ligand CLA A 812



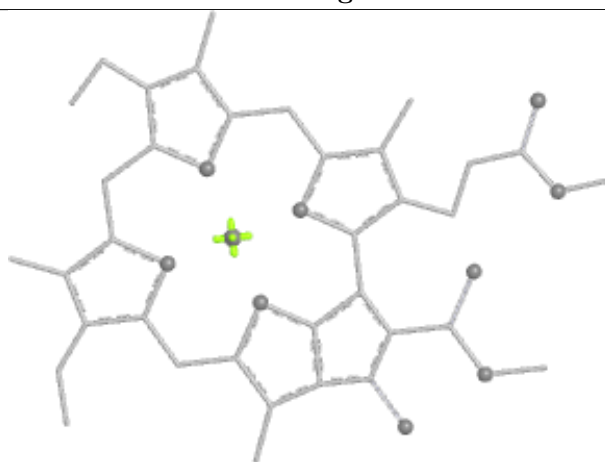
Bond lengths



Bond angles

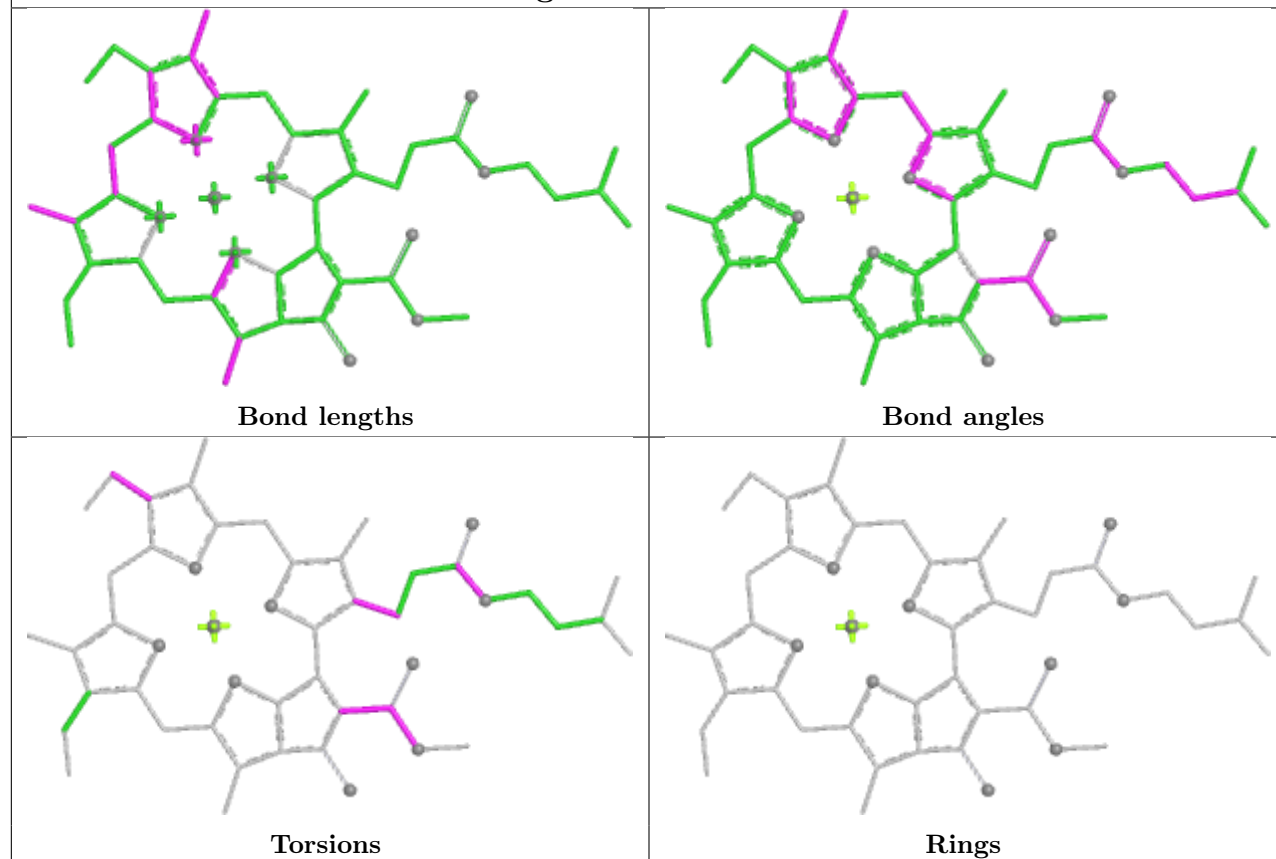


Torsions

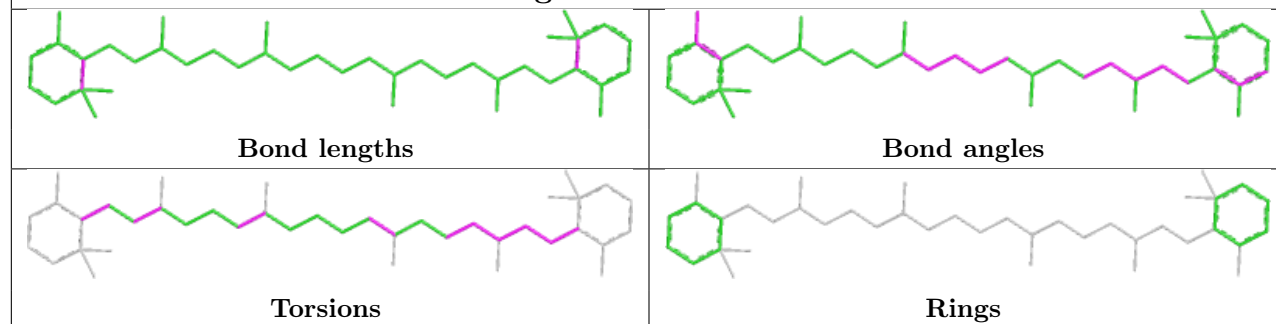


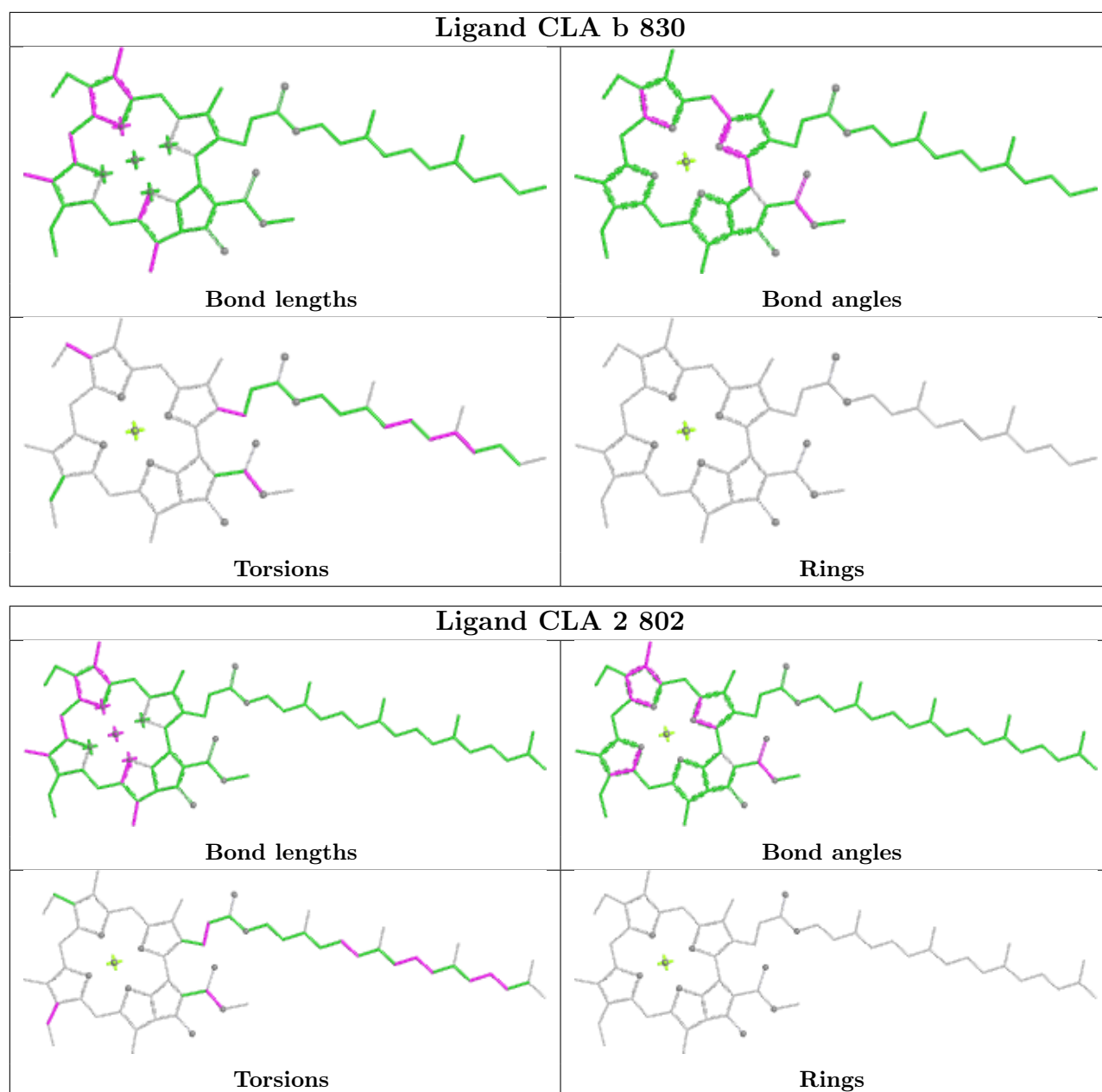
Rings

Ligand CLA a 831

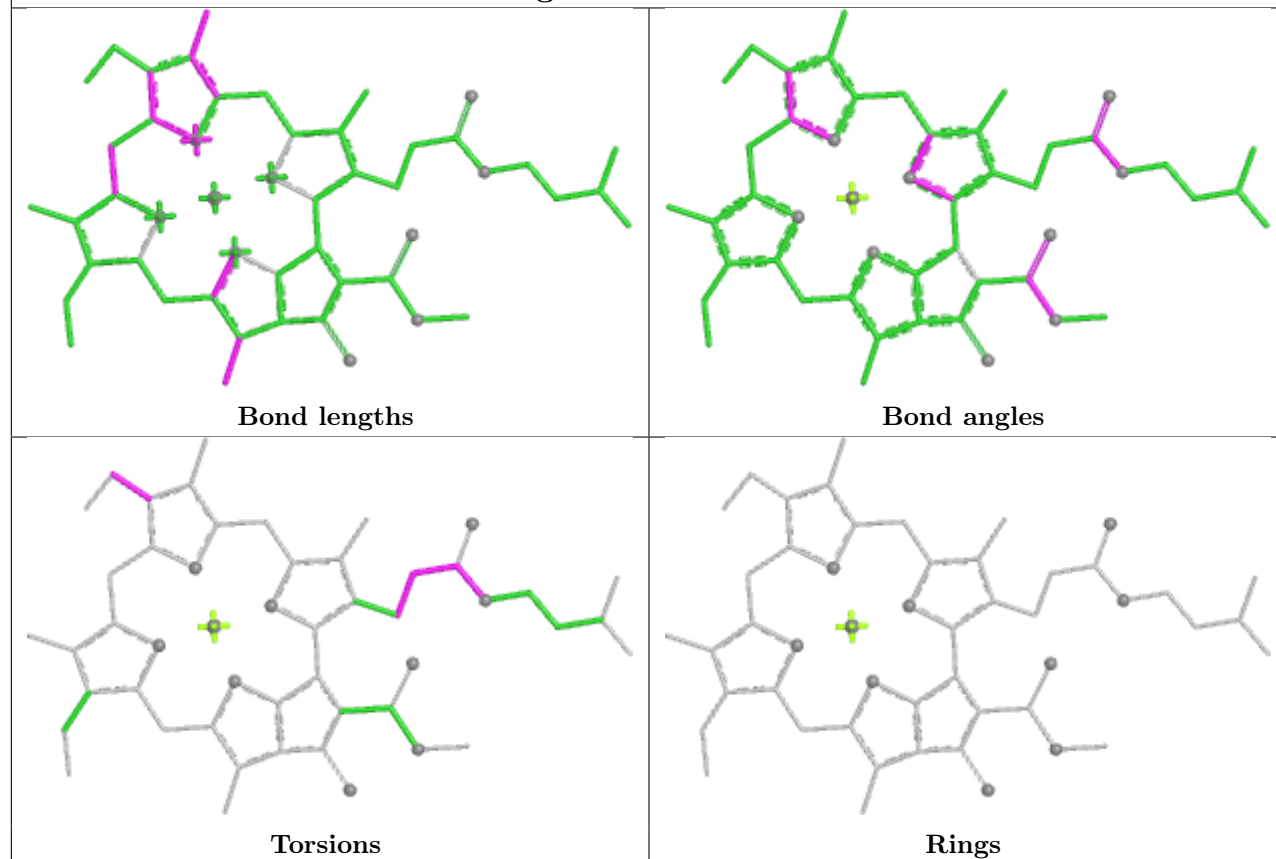


Ligand BCR a 851

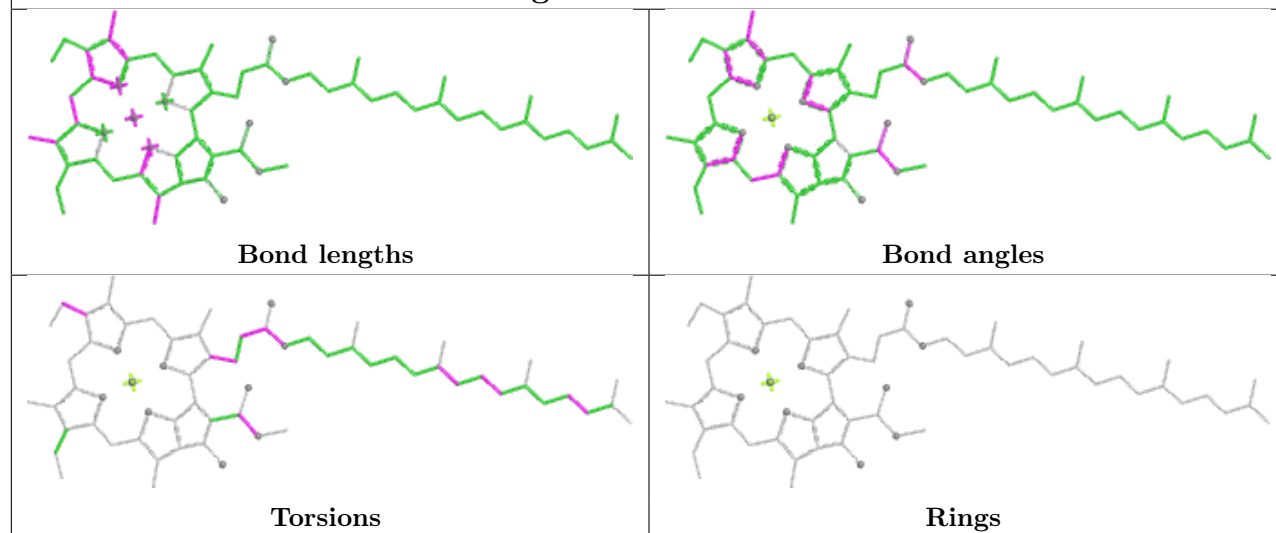


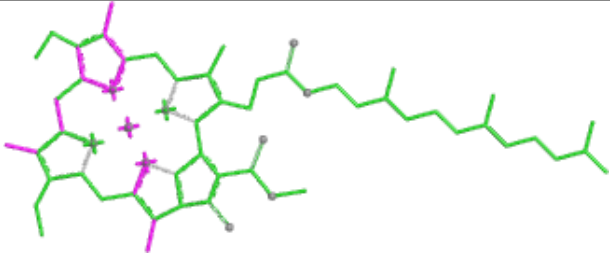
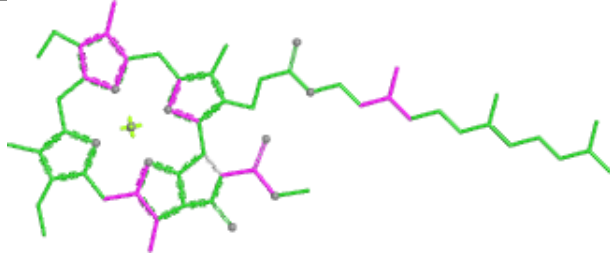
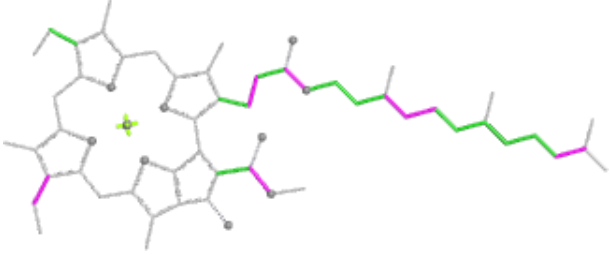
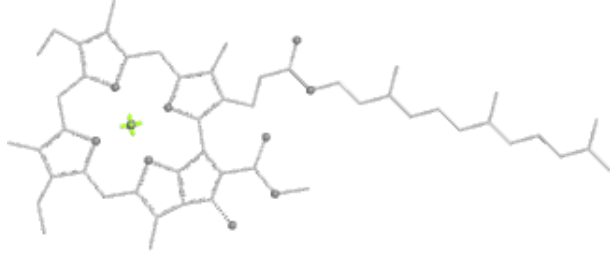
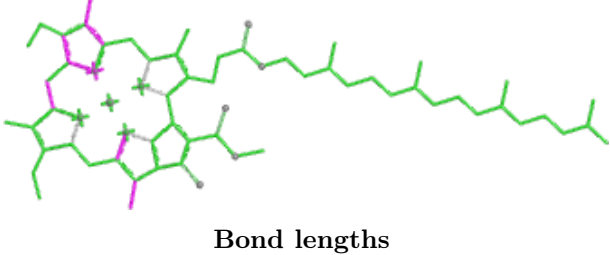
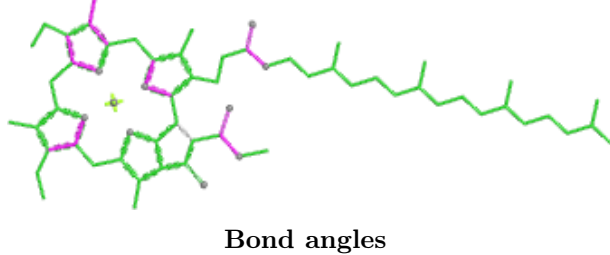
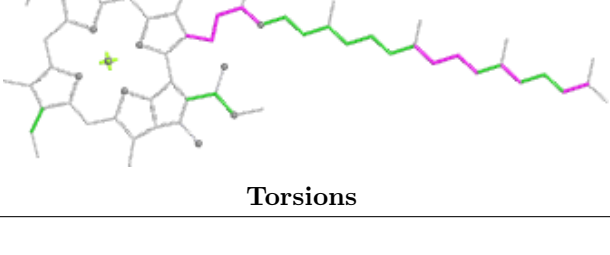
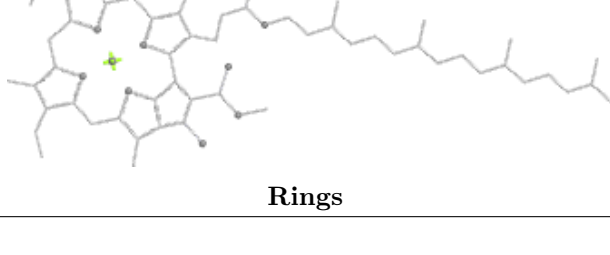


Ligand CLA a 823

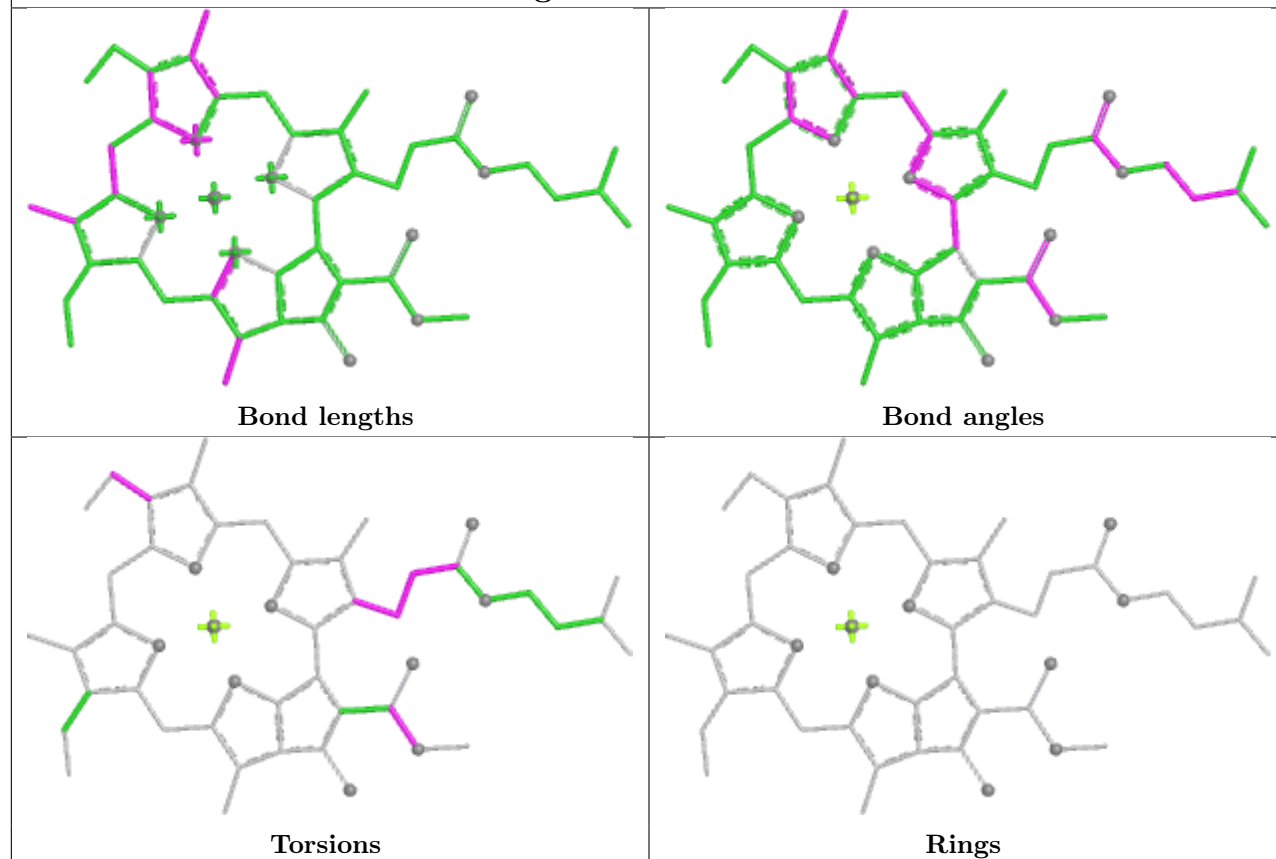


Ligand CLA A 806

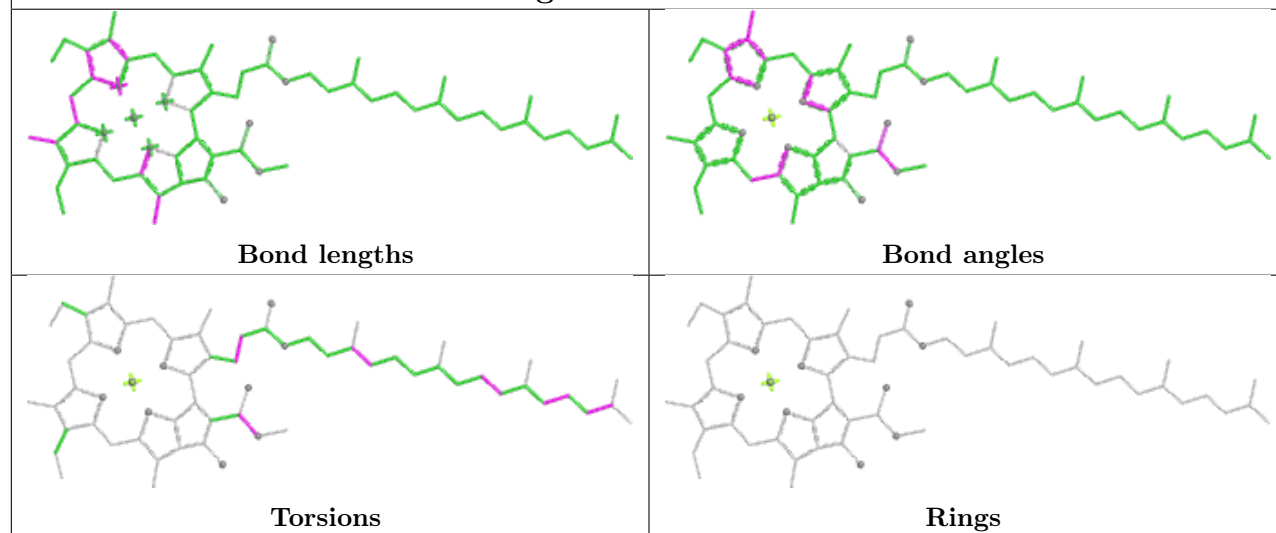


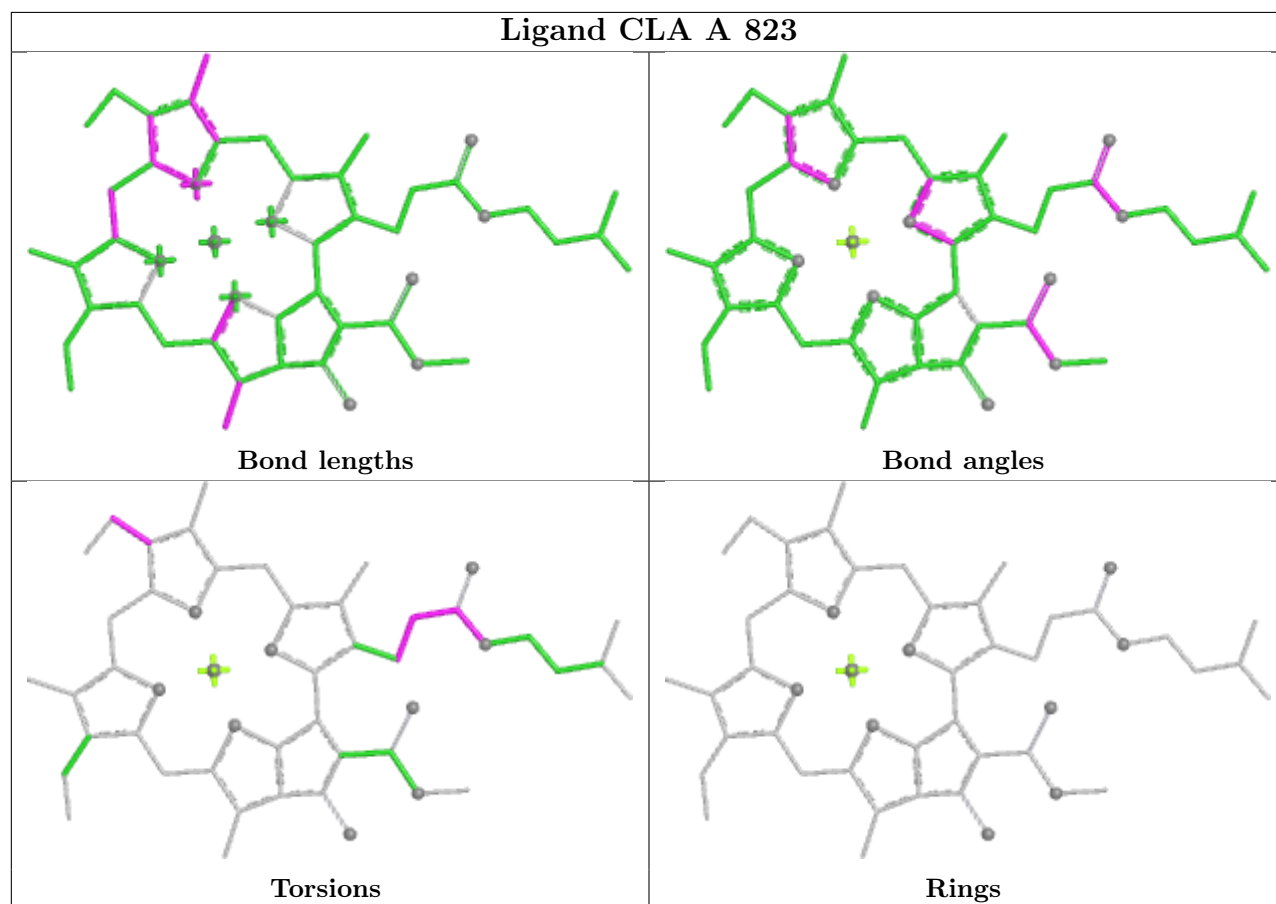
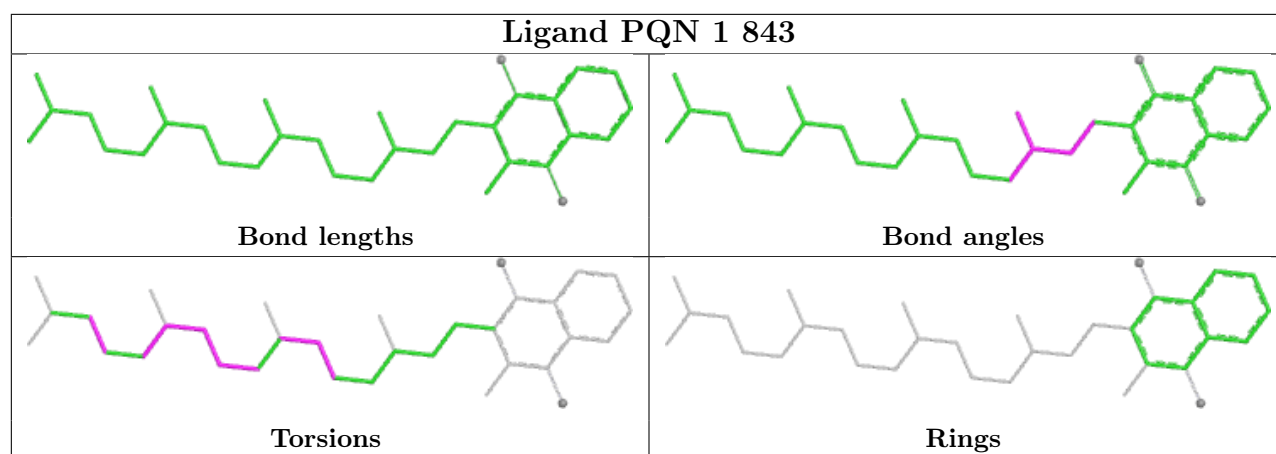
Ligand CLA a 802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA i 102	
 Bond lengths	 Bond angles
 Torsions	 Rings

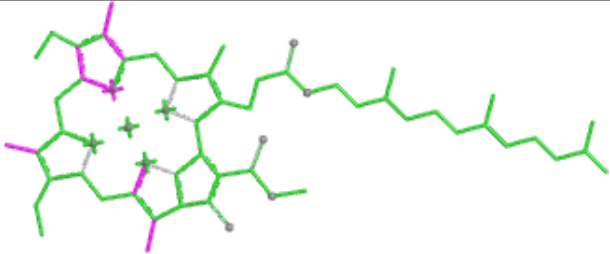
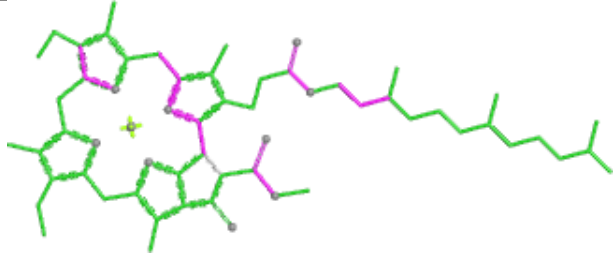
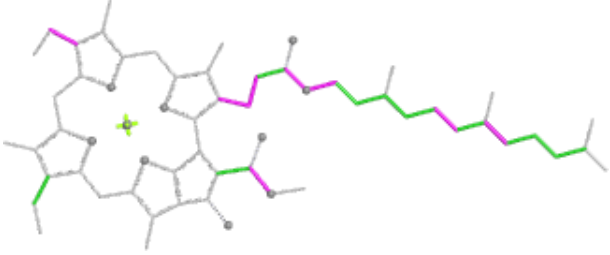
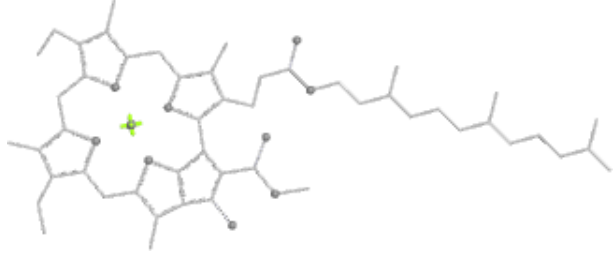
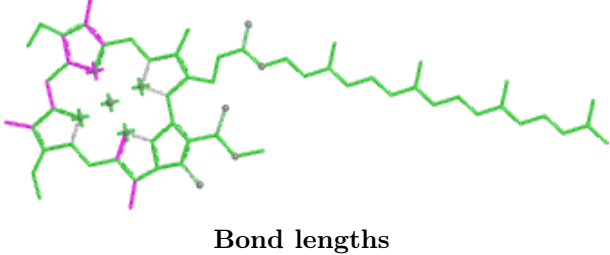
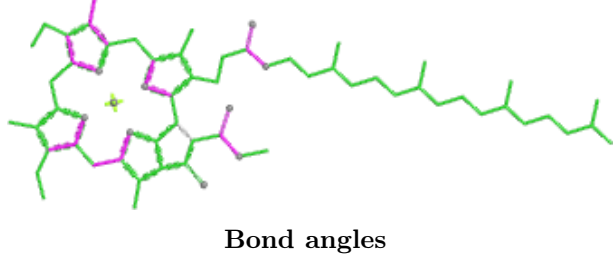
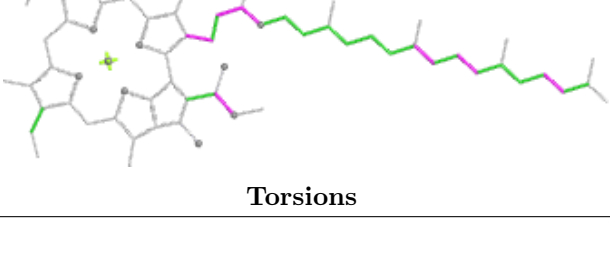
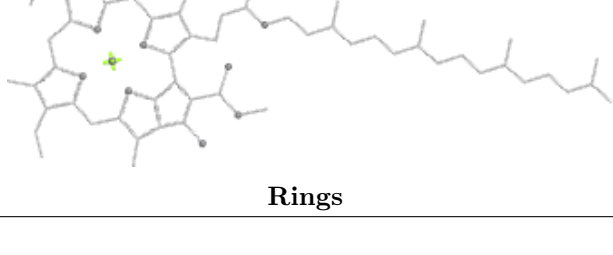
Ligand CLA L 203



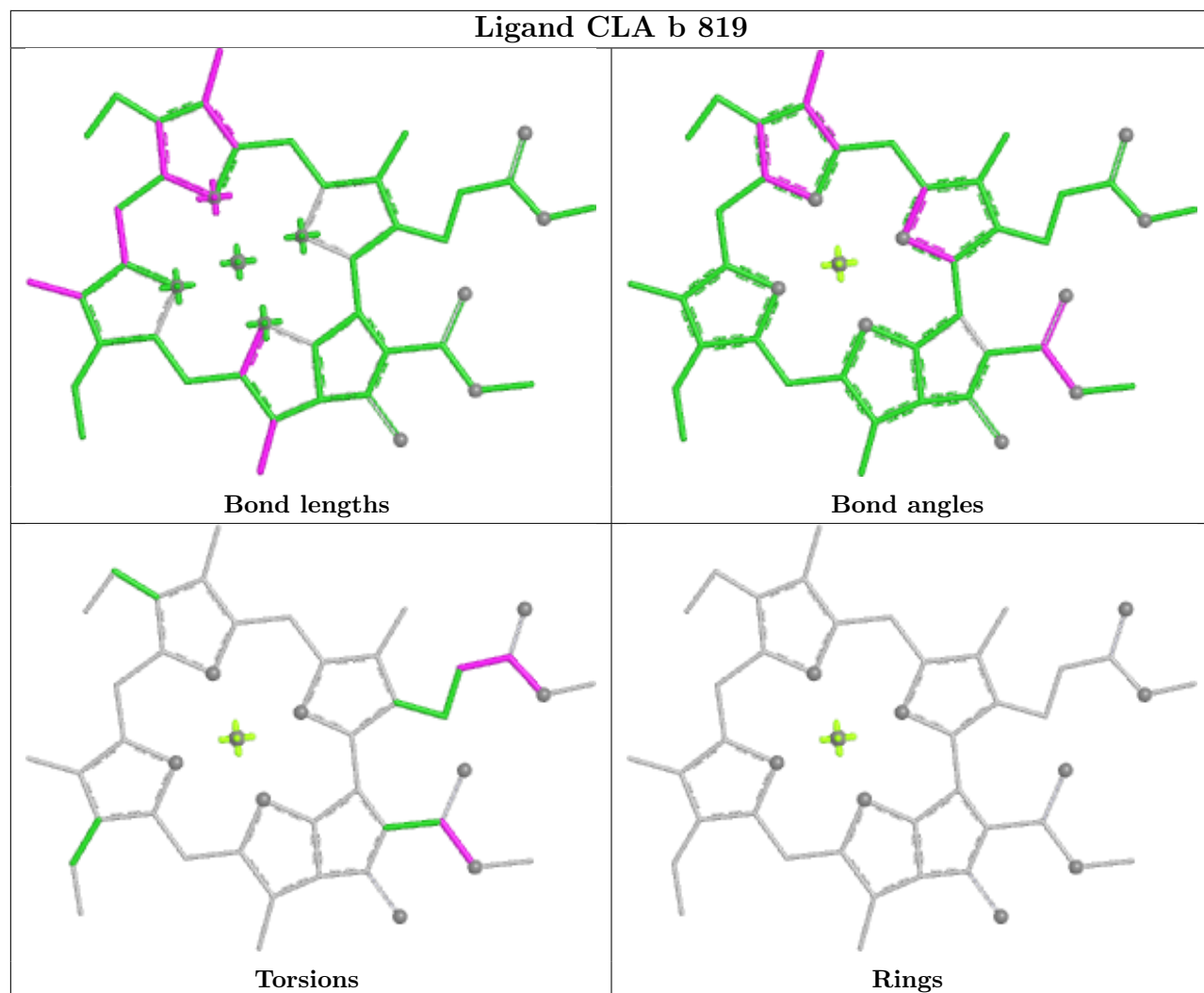
Ligand CLA a 828



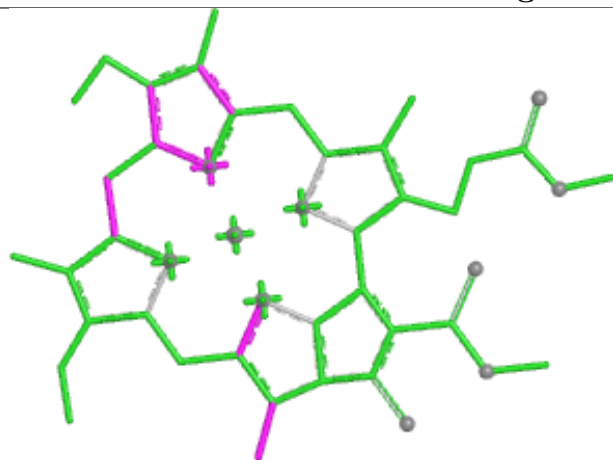


Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

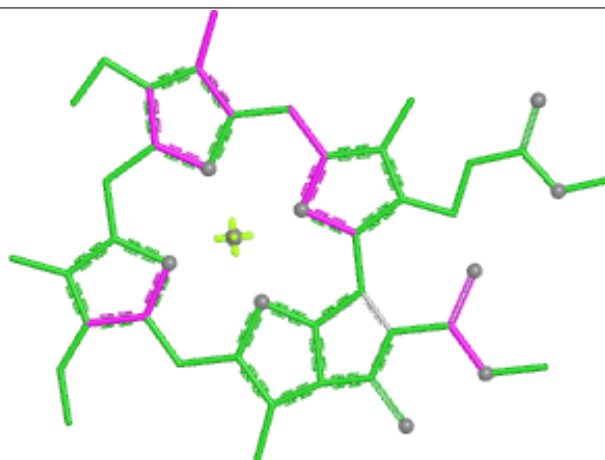
Ligand CLA b 819



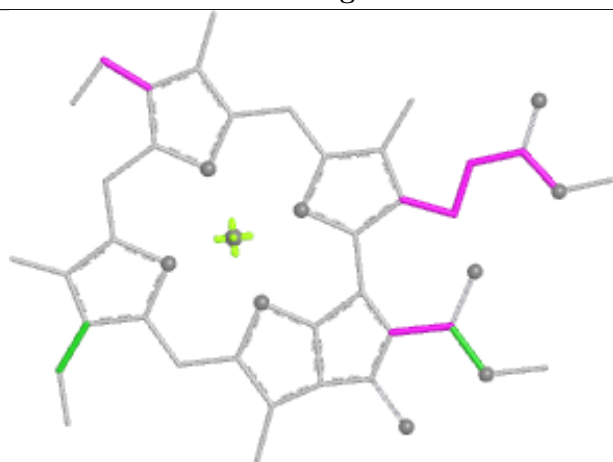
Ligand CLA b 818



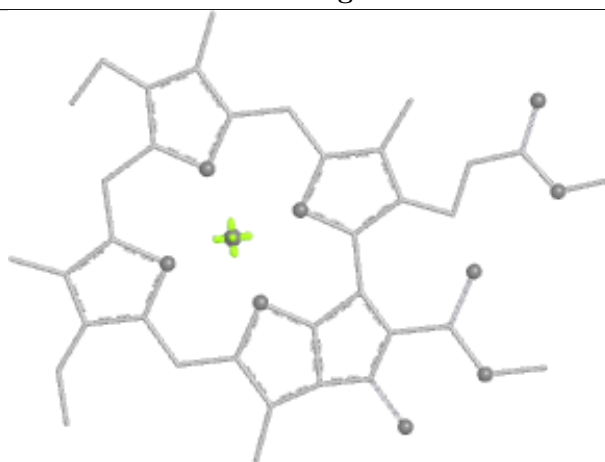
Bond lengths



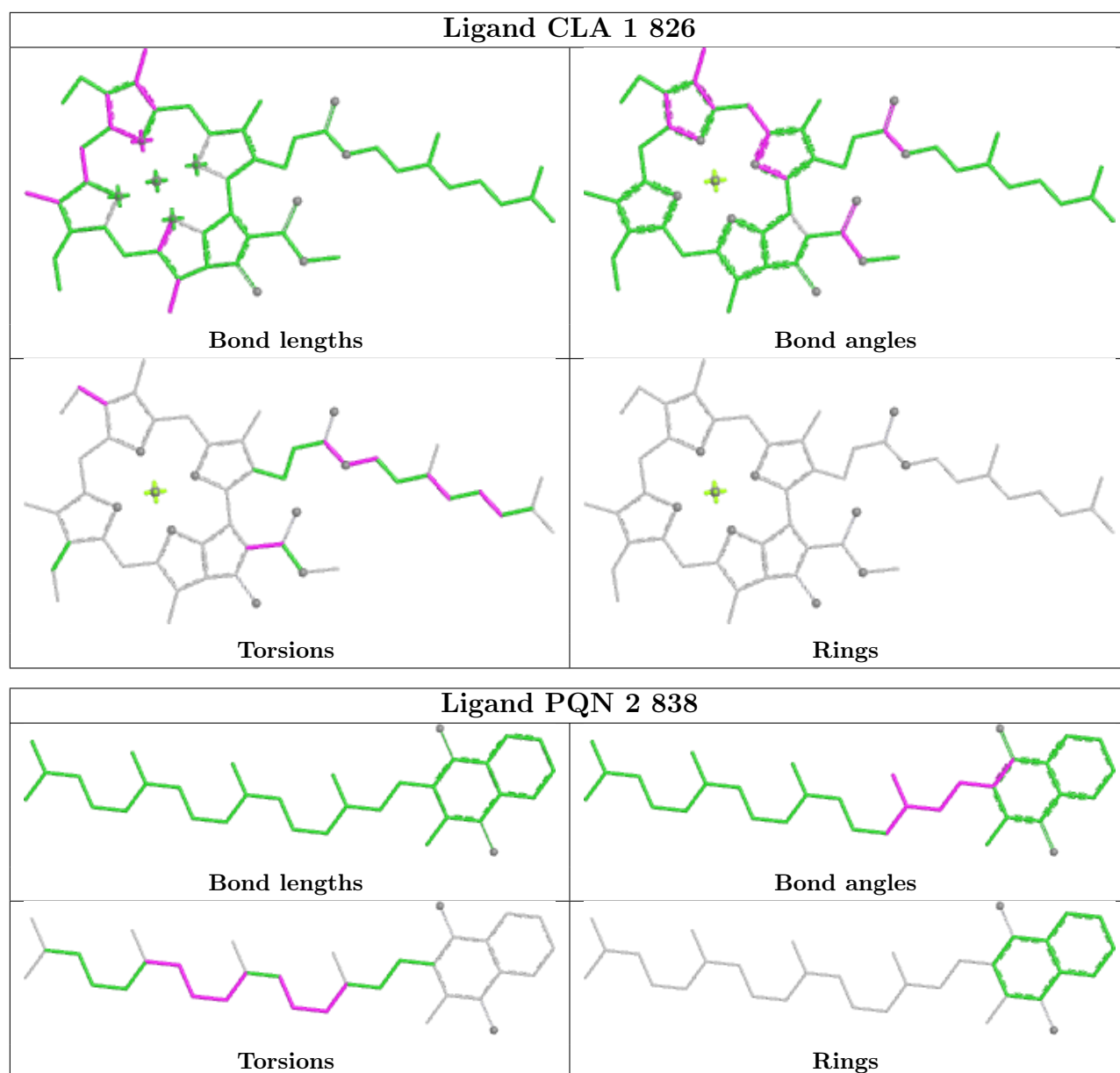
Bond angles

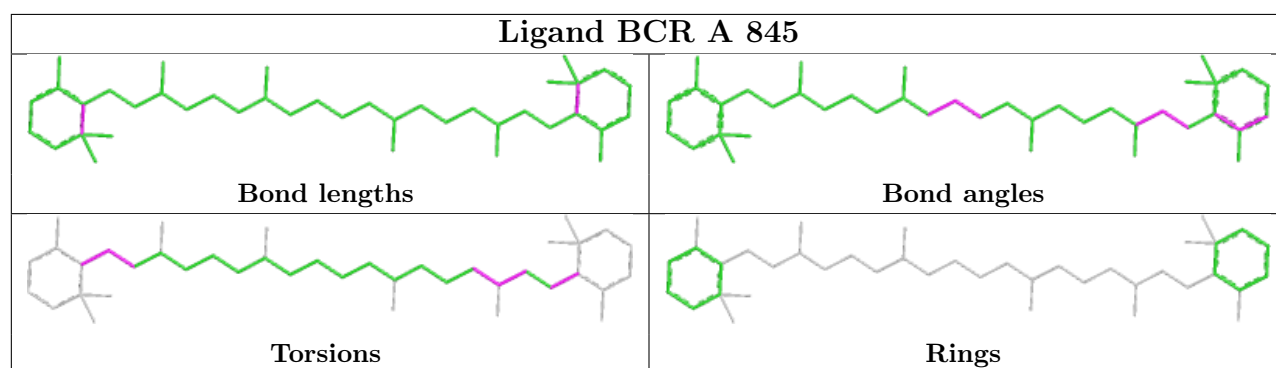
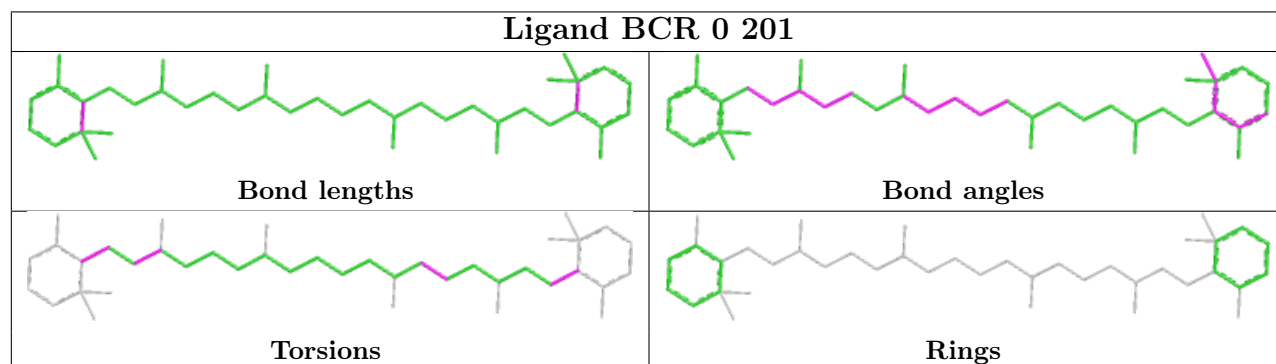
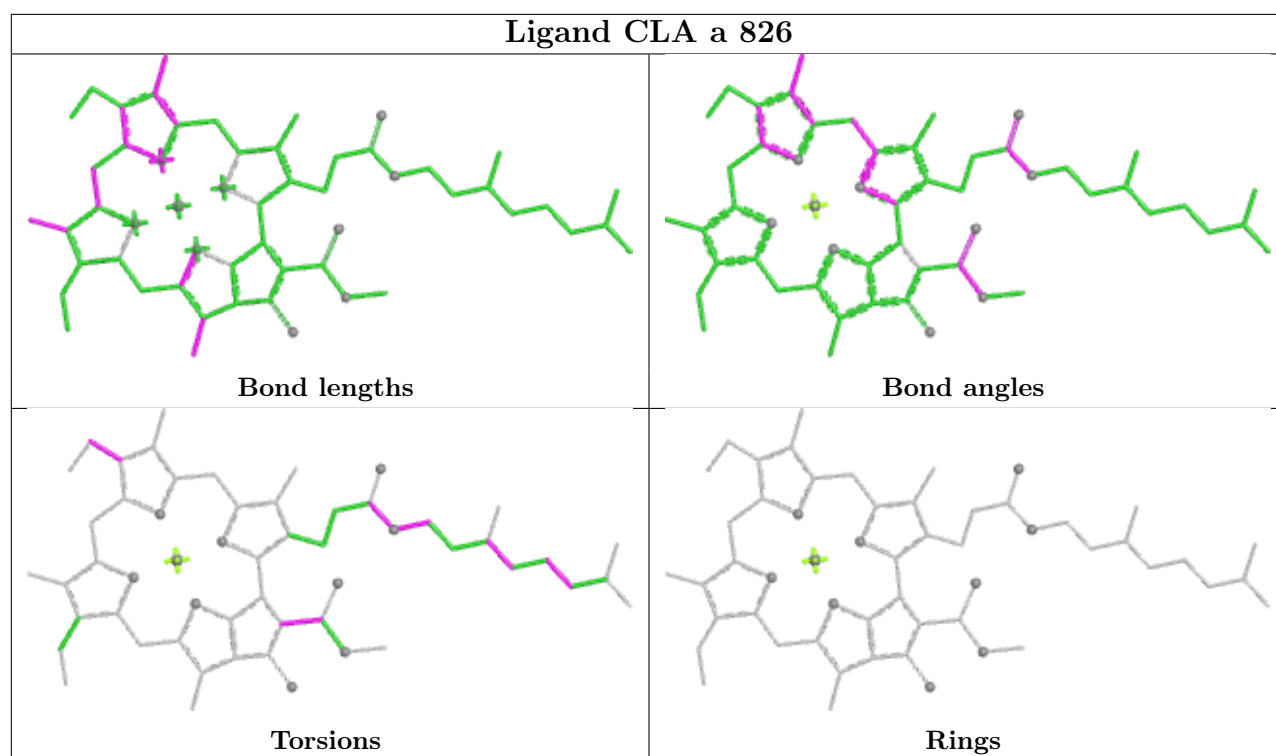


Torsions

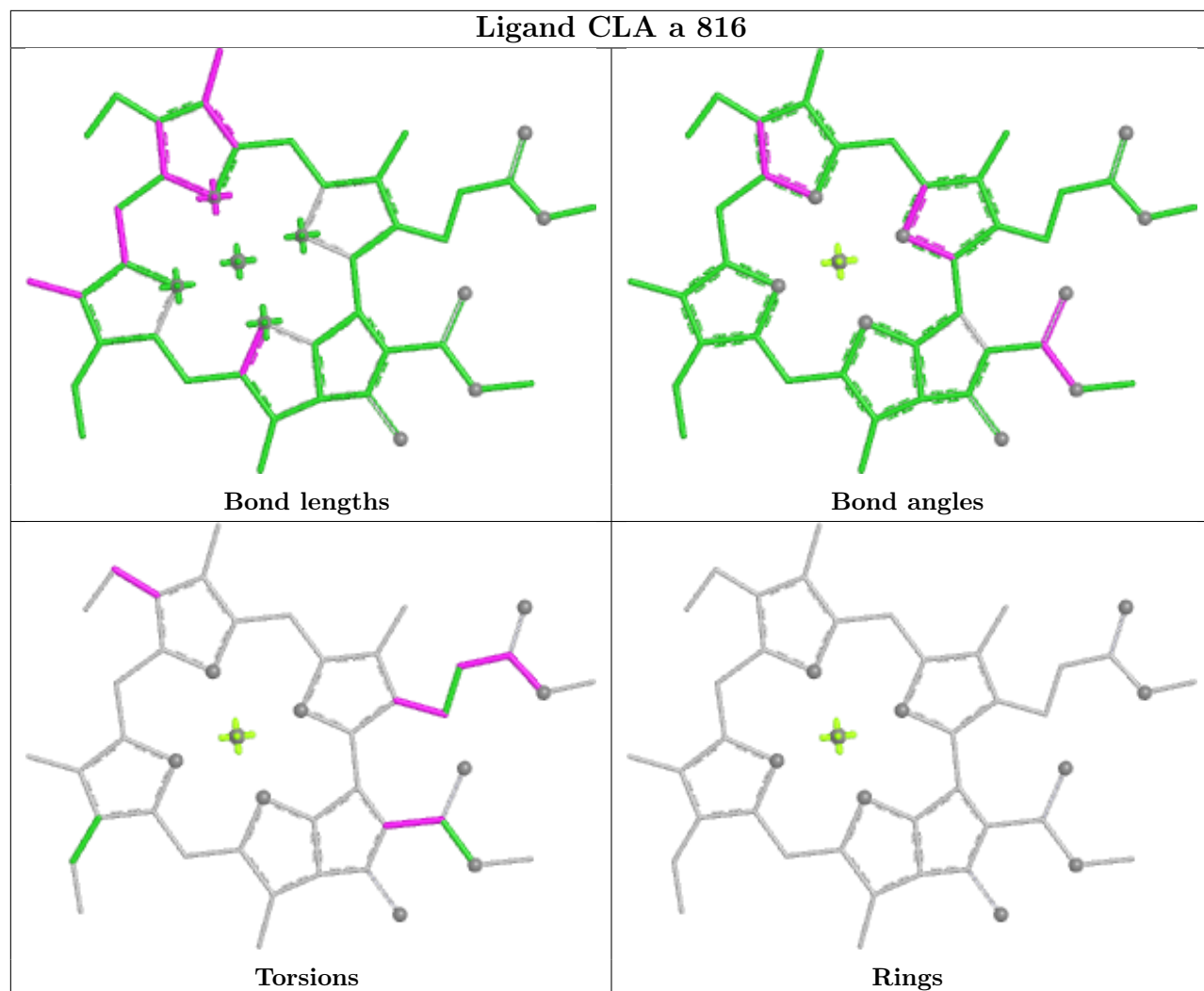


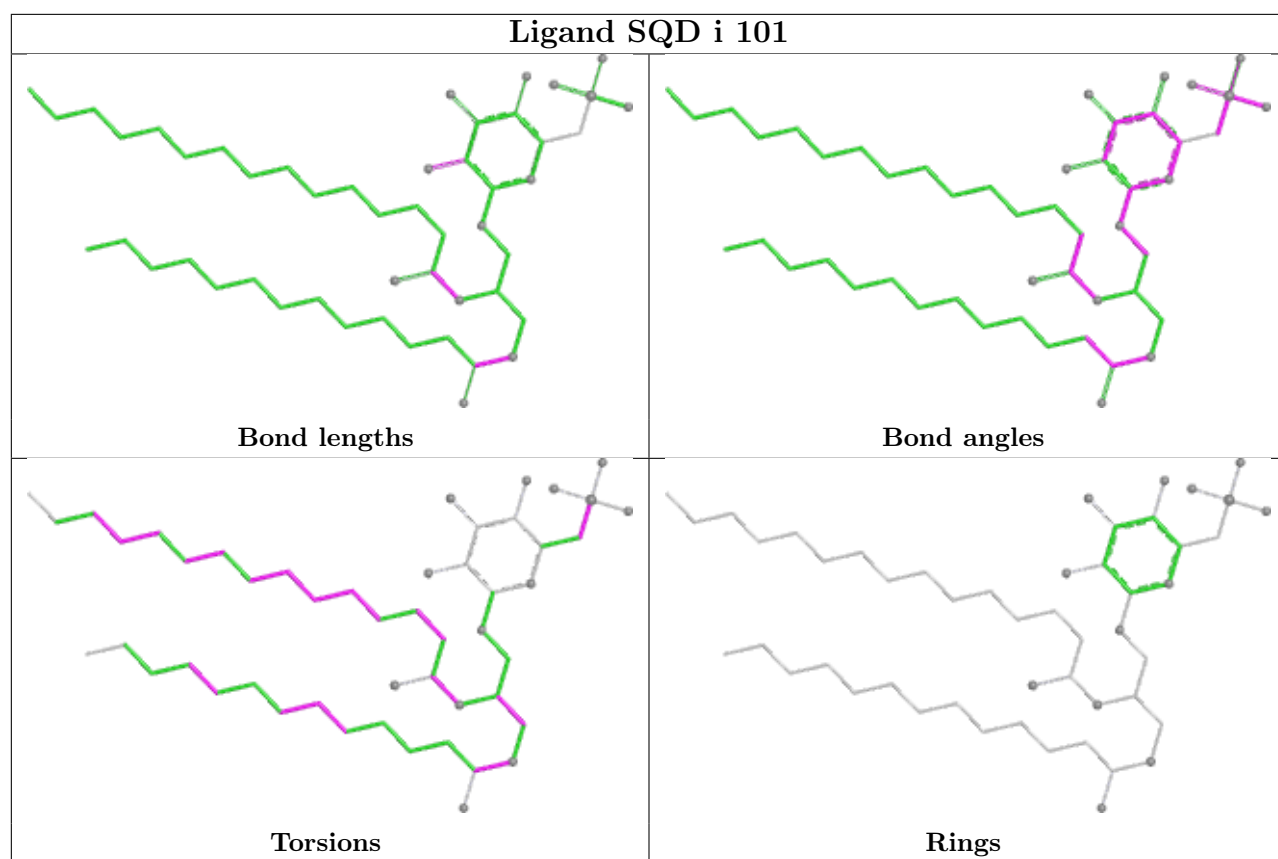
Rings



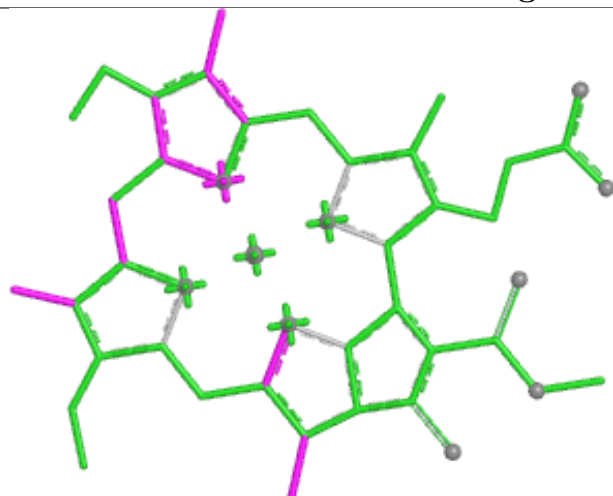


Ligand CLA a 816

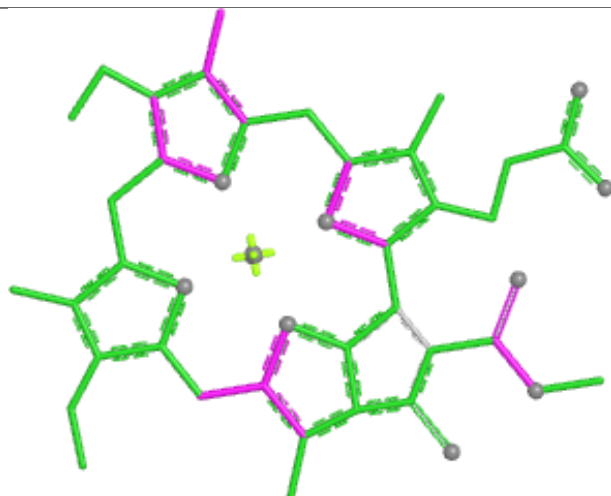




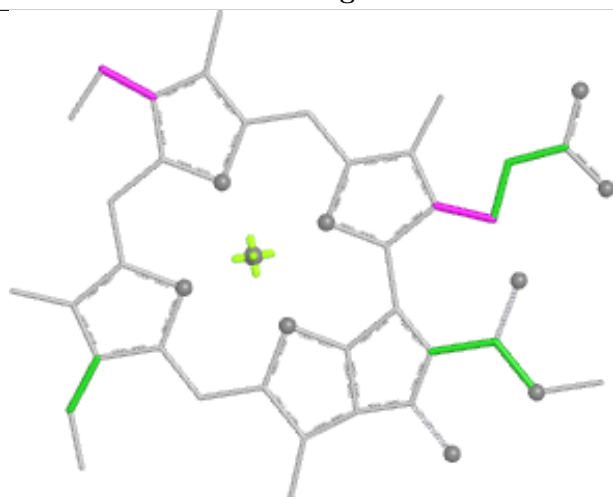
Ligand CLA a 815



Bond lengths



Bond angles

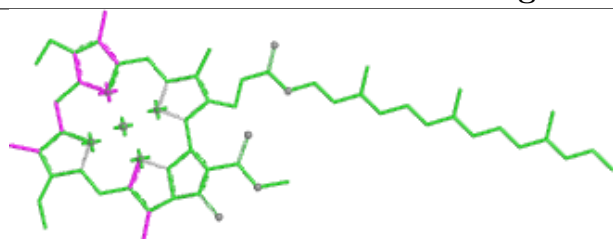


Torsions

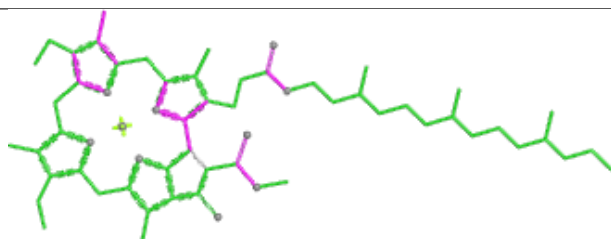


Rings

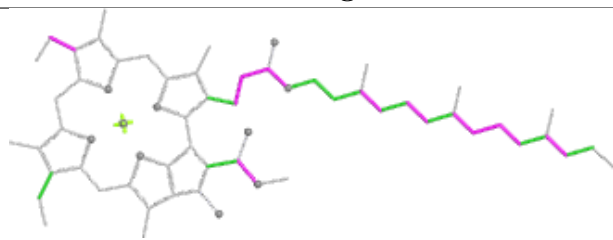
Ligand CLA a 825



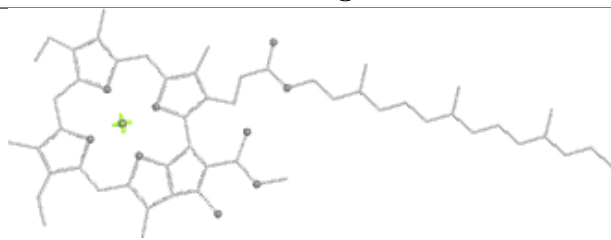
Bond lengths



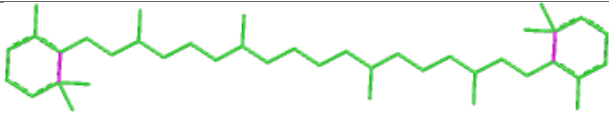
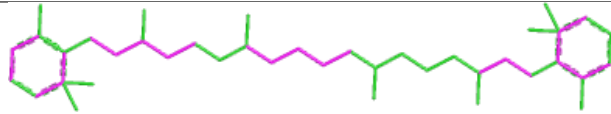
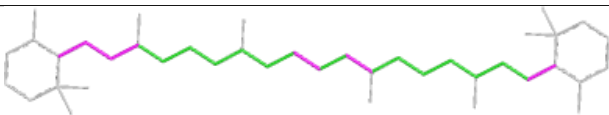
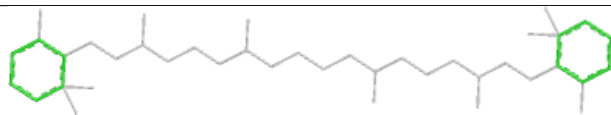
Bond angles

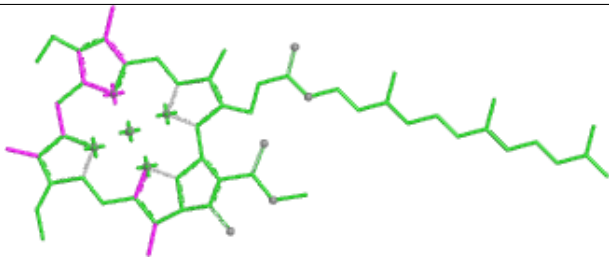
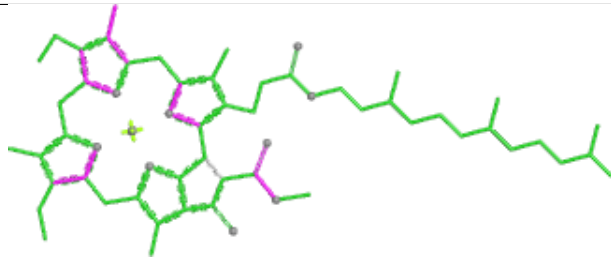
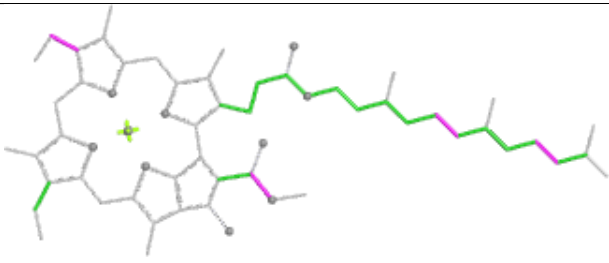
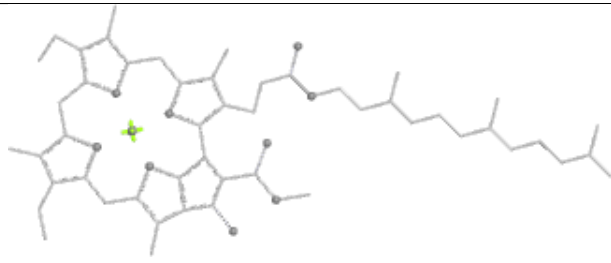


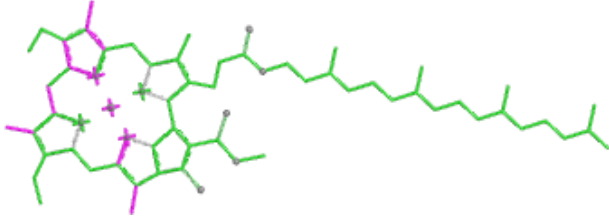
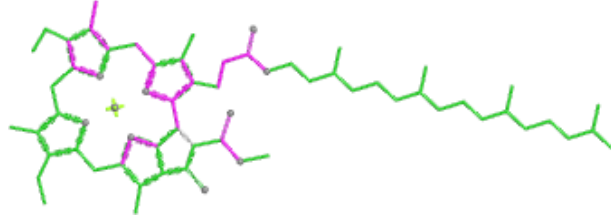
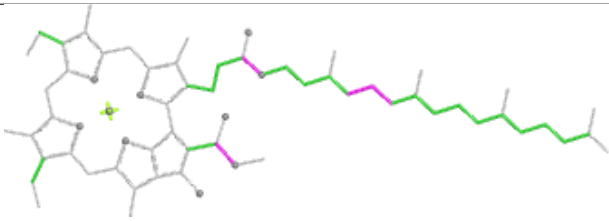
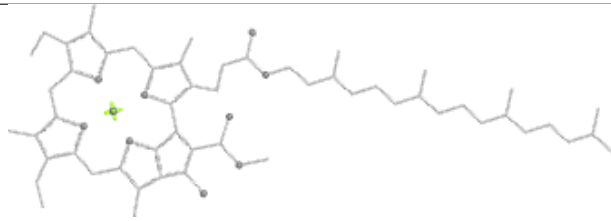
Torsions

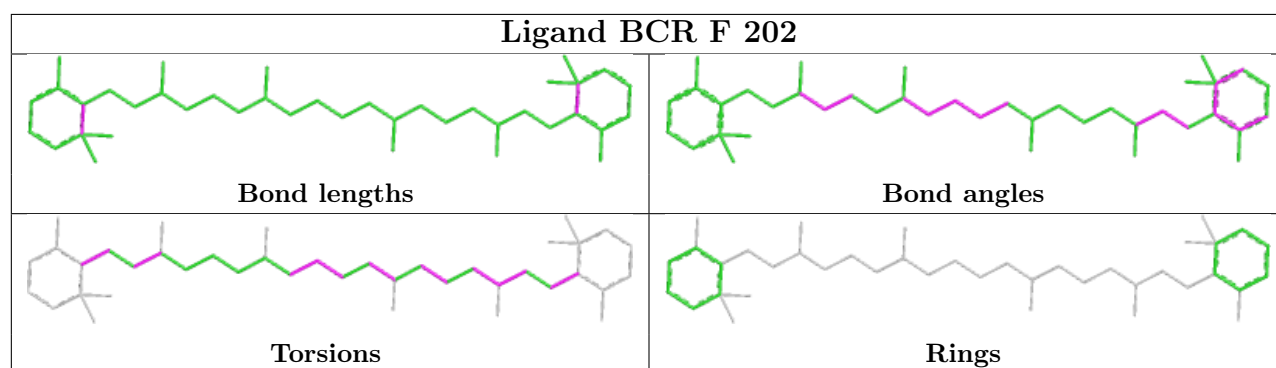
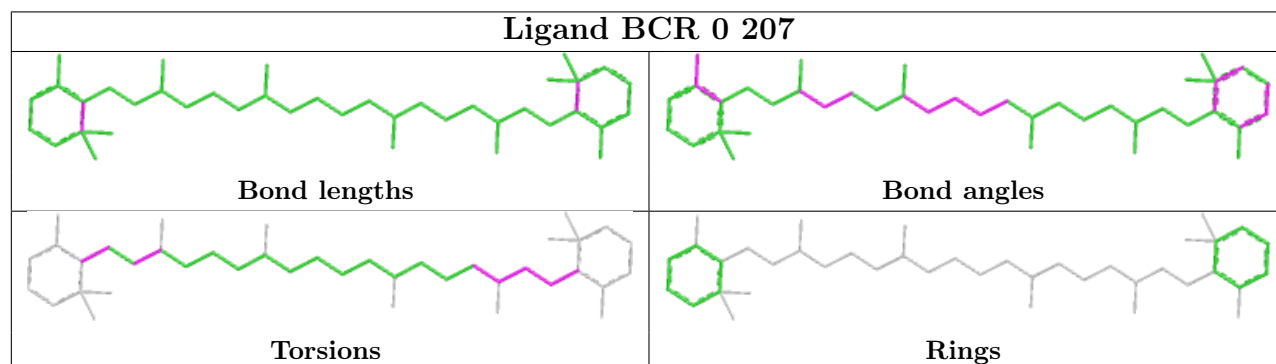
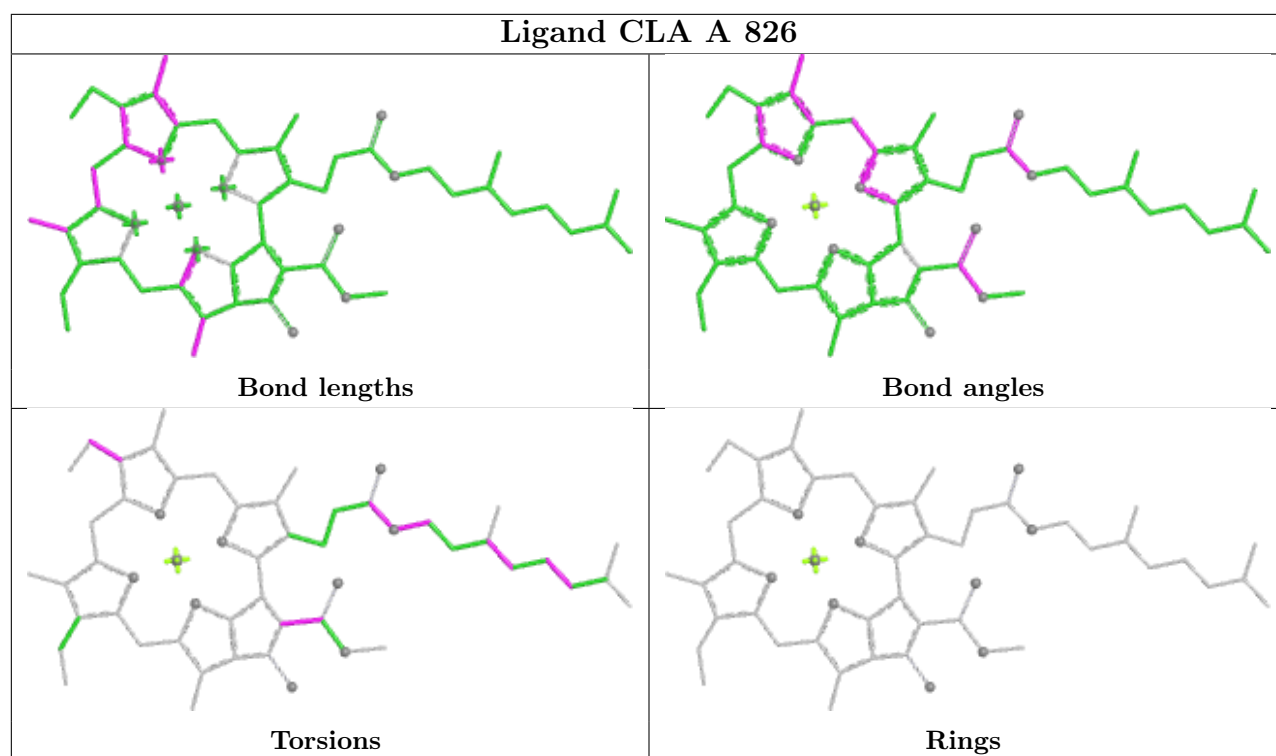


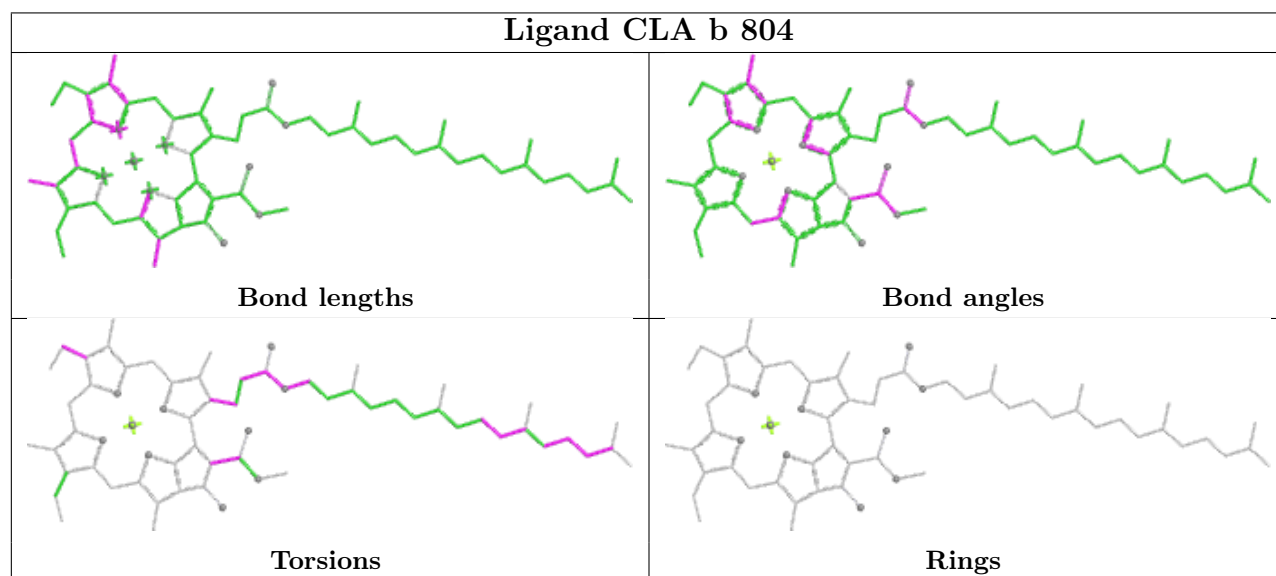
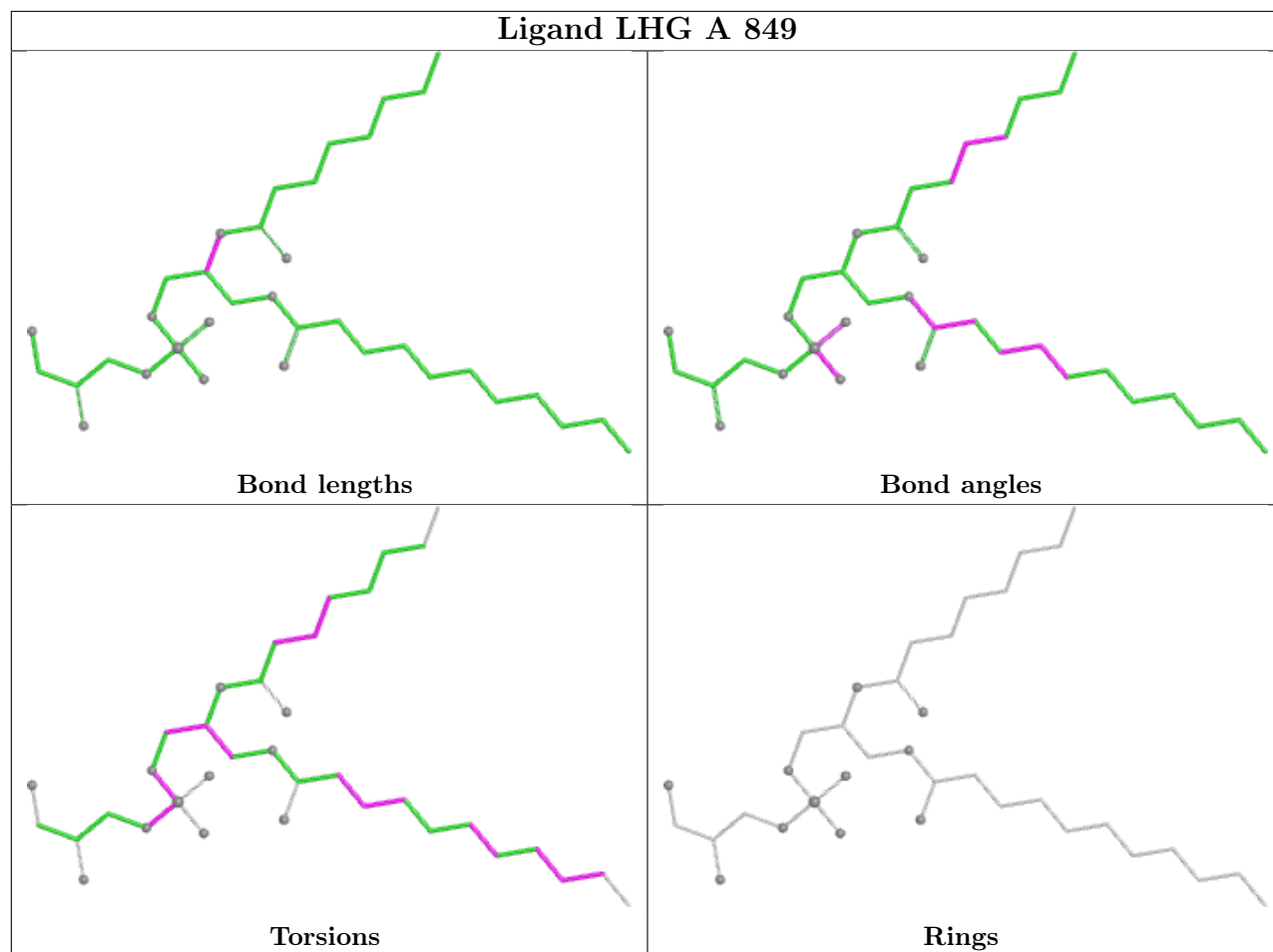
Rings

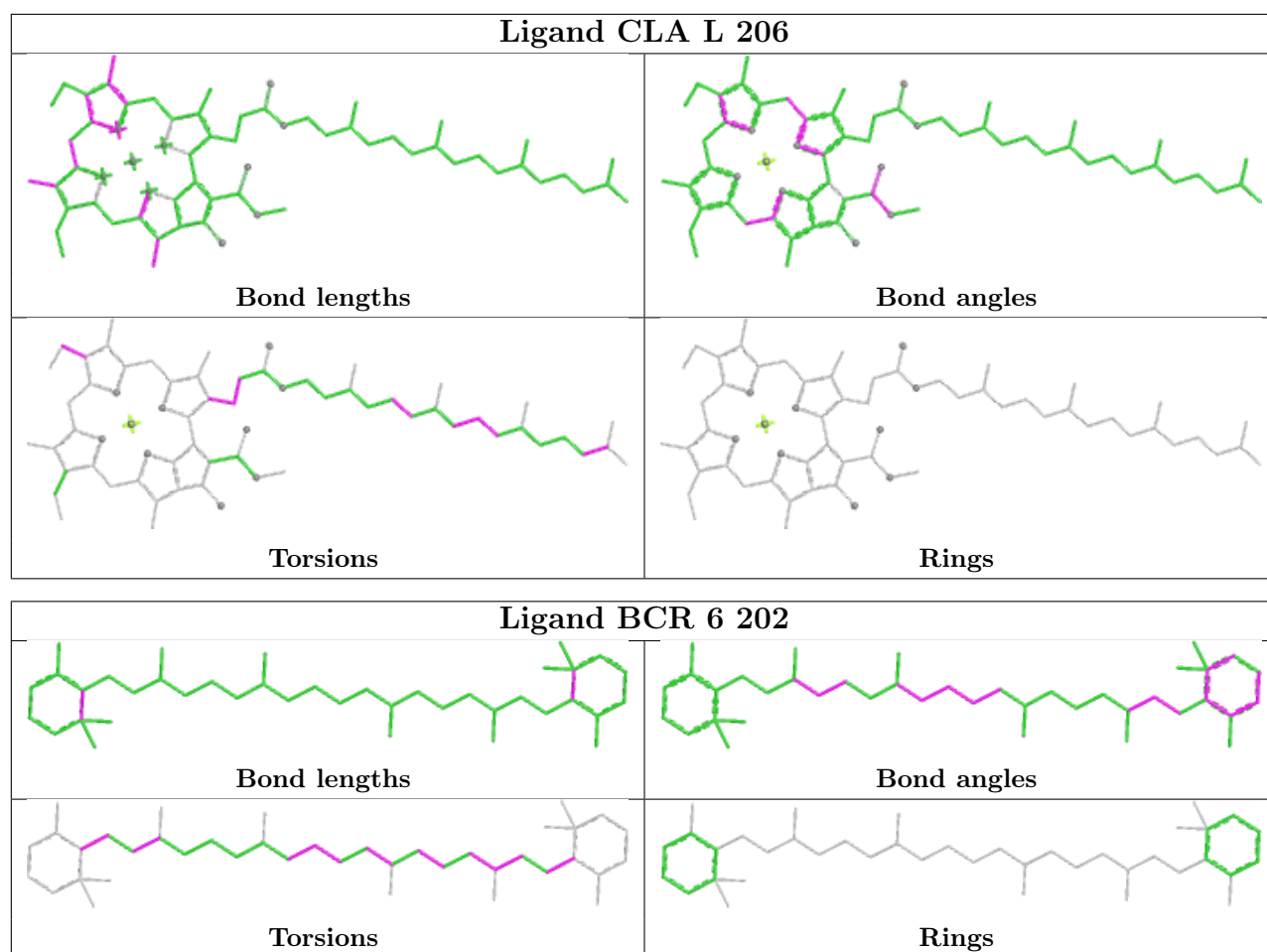
Ligand BCR j 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

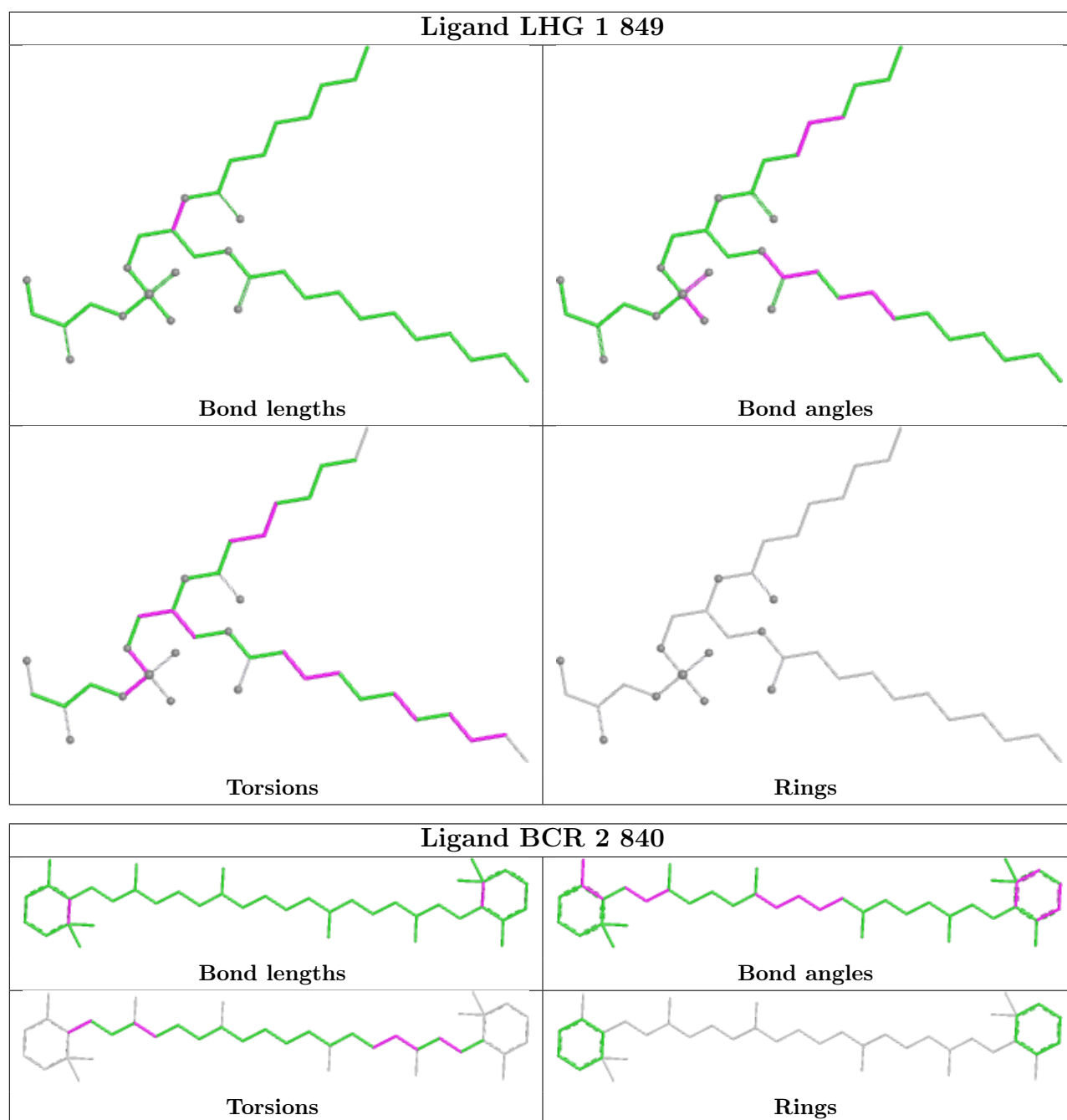
Ligand CLA B 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

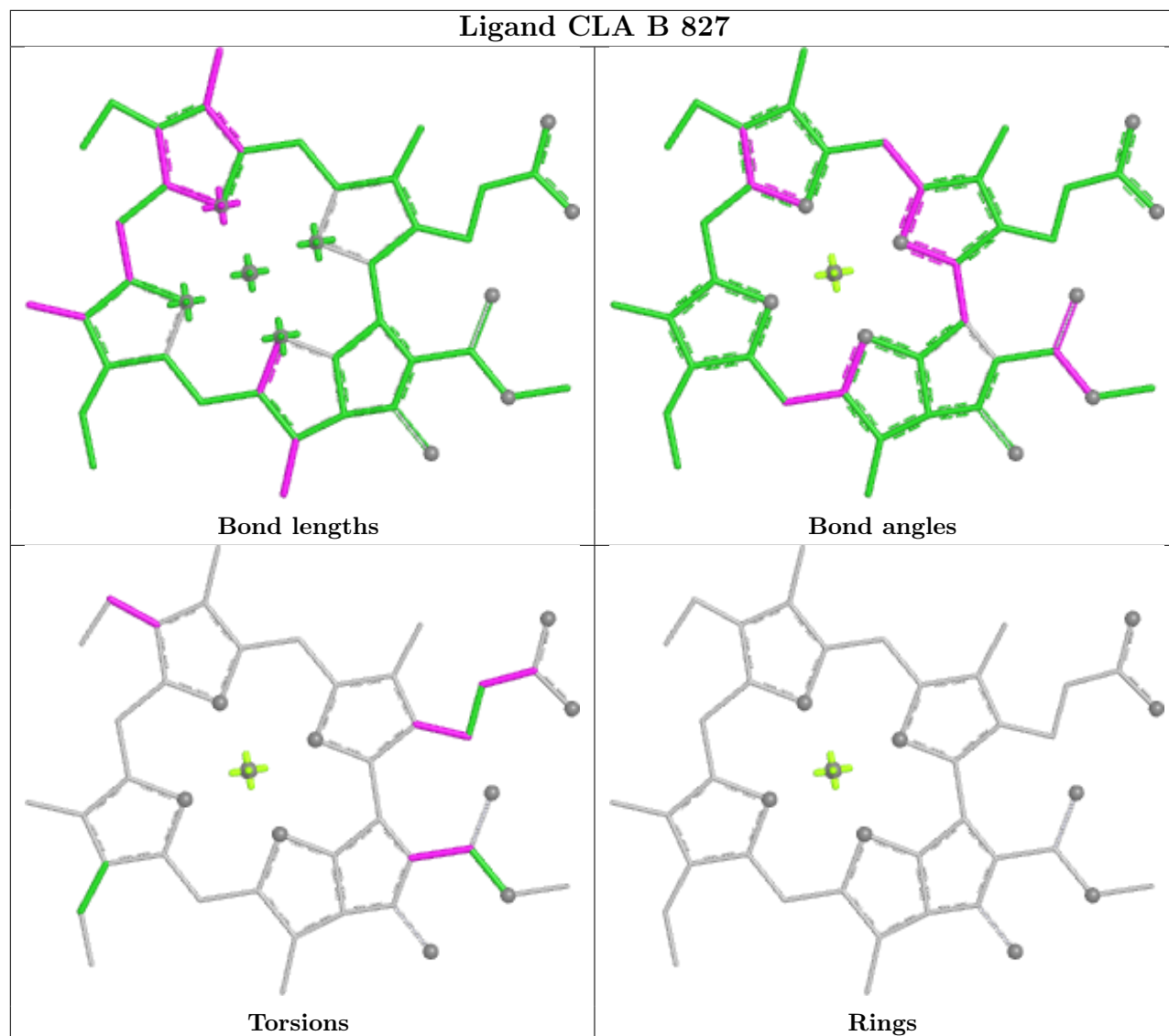




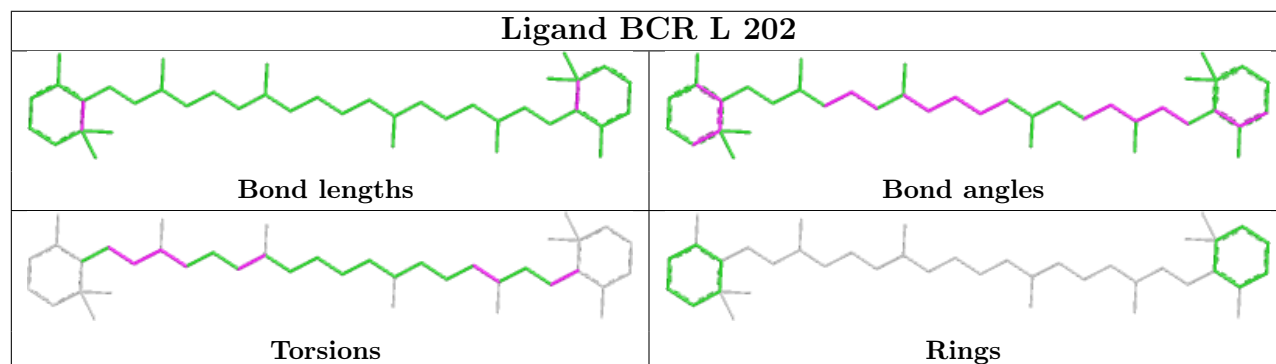


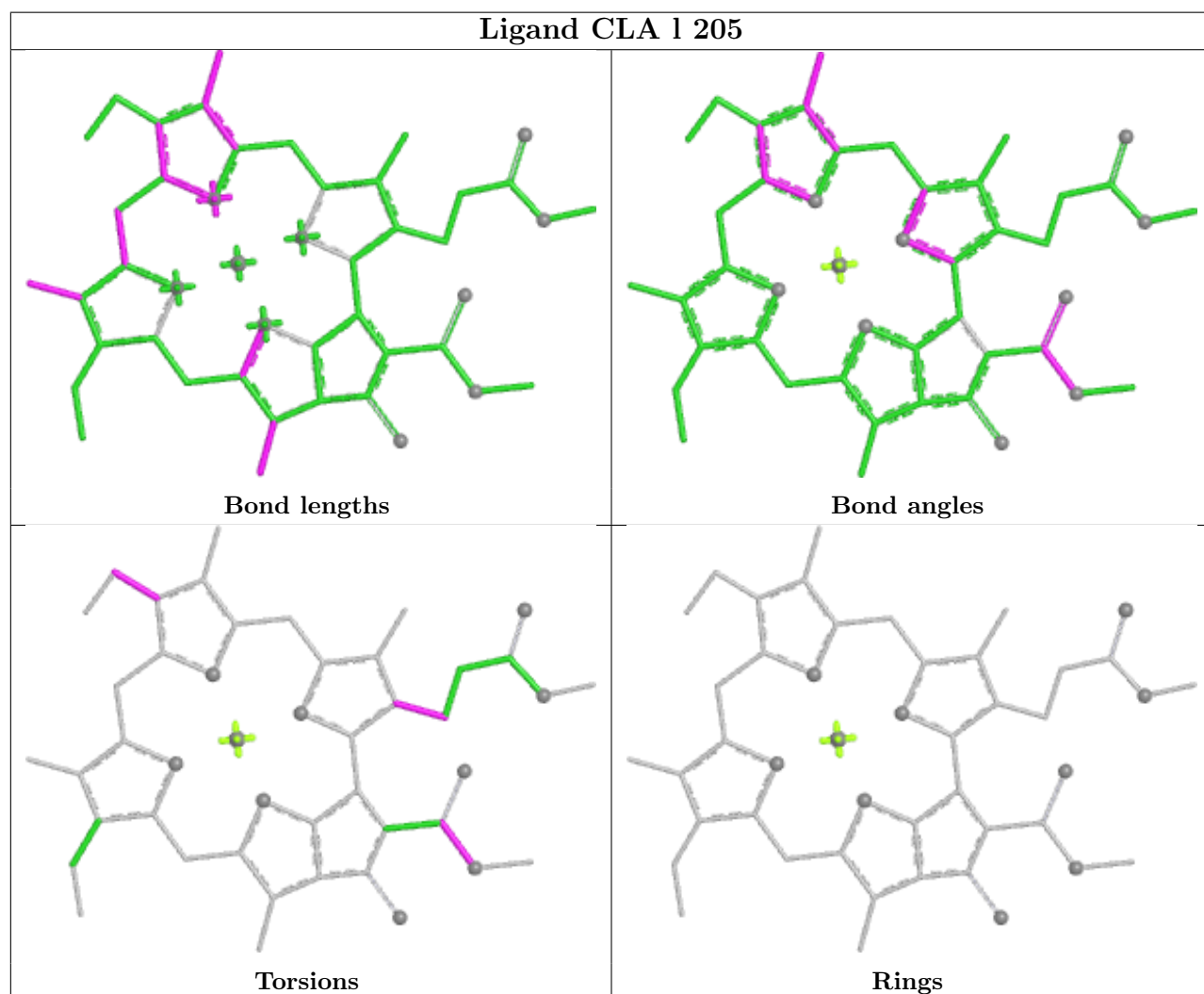
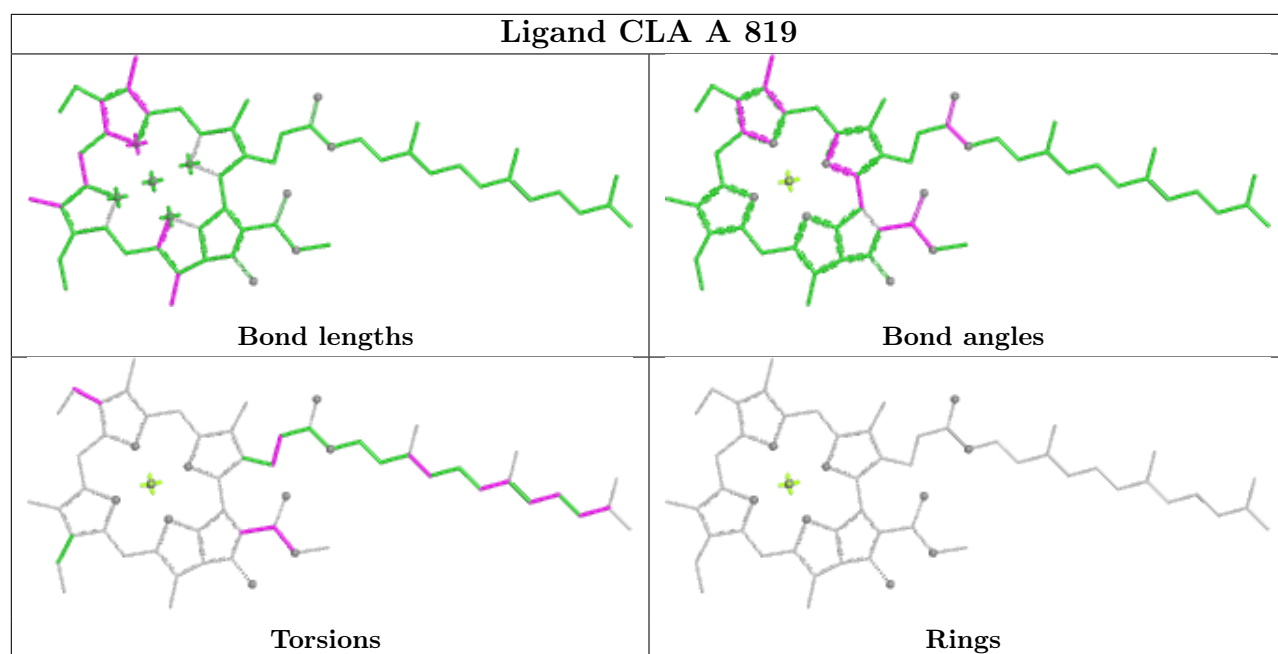


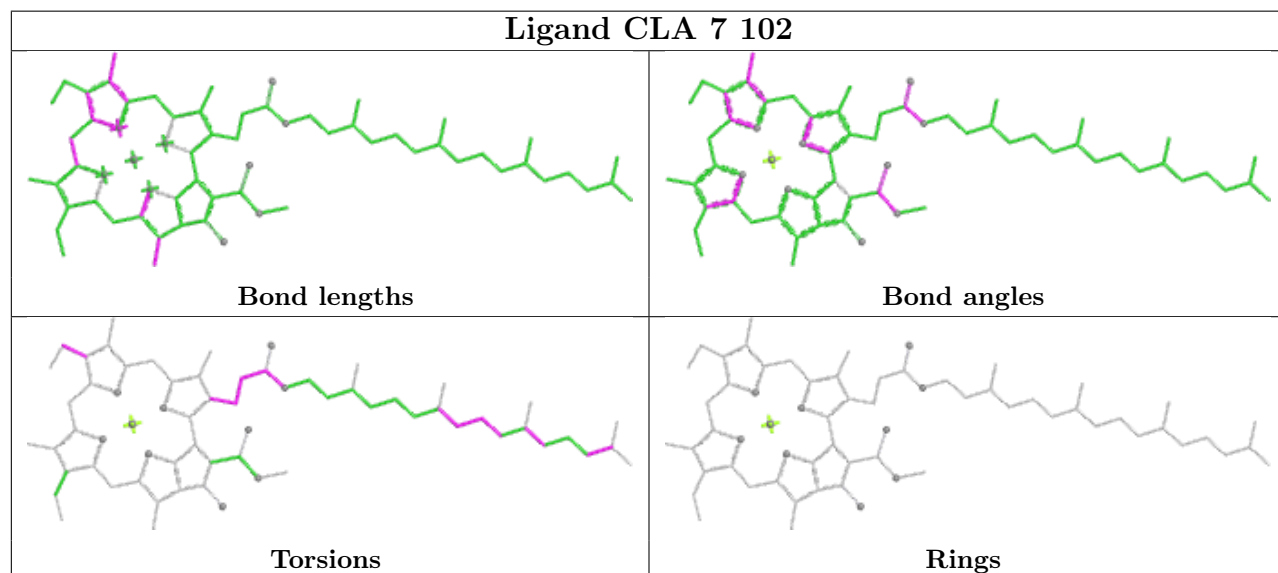
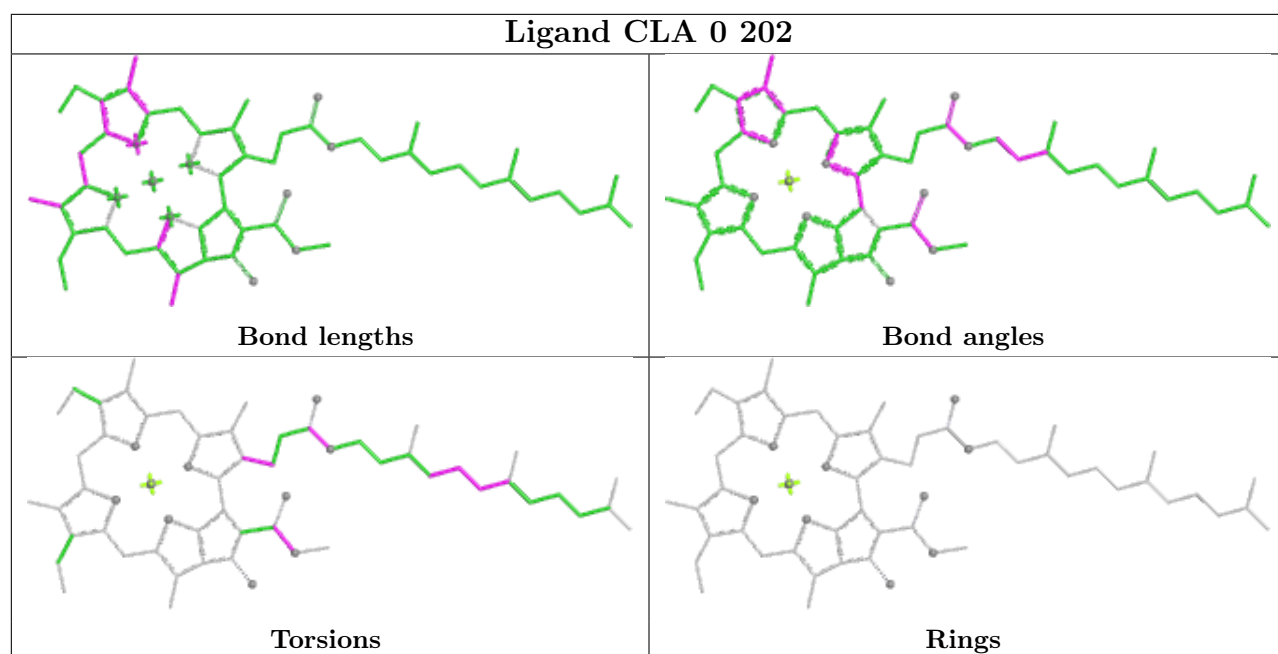
Ligand CLA B 827

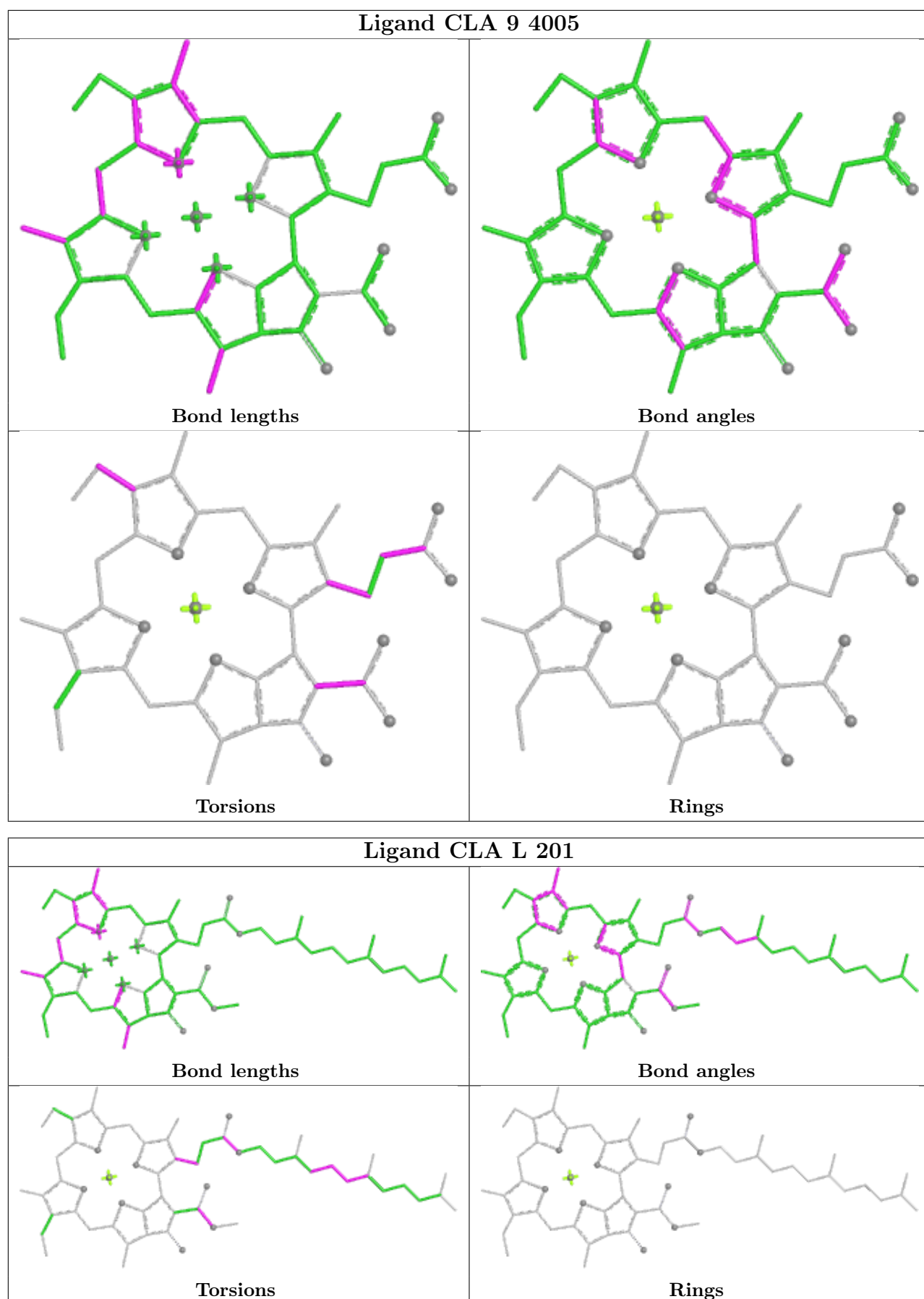


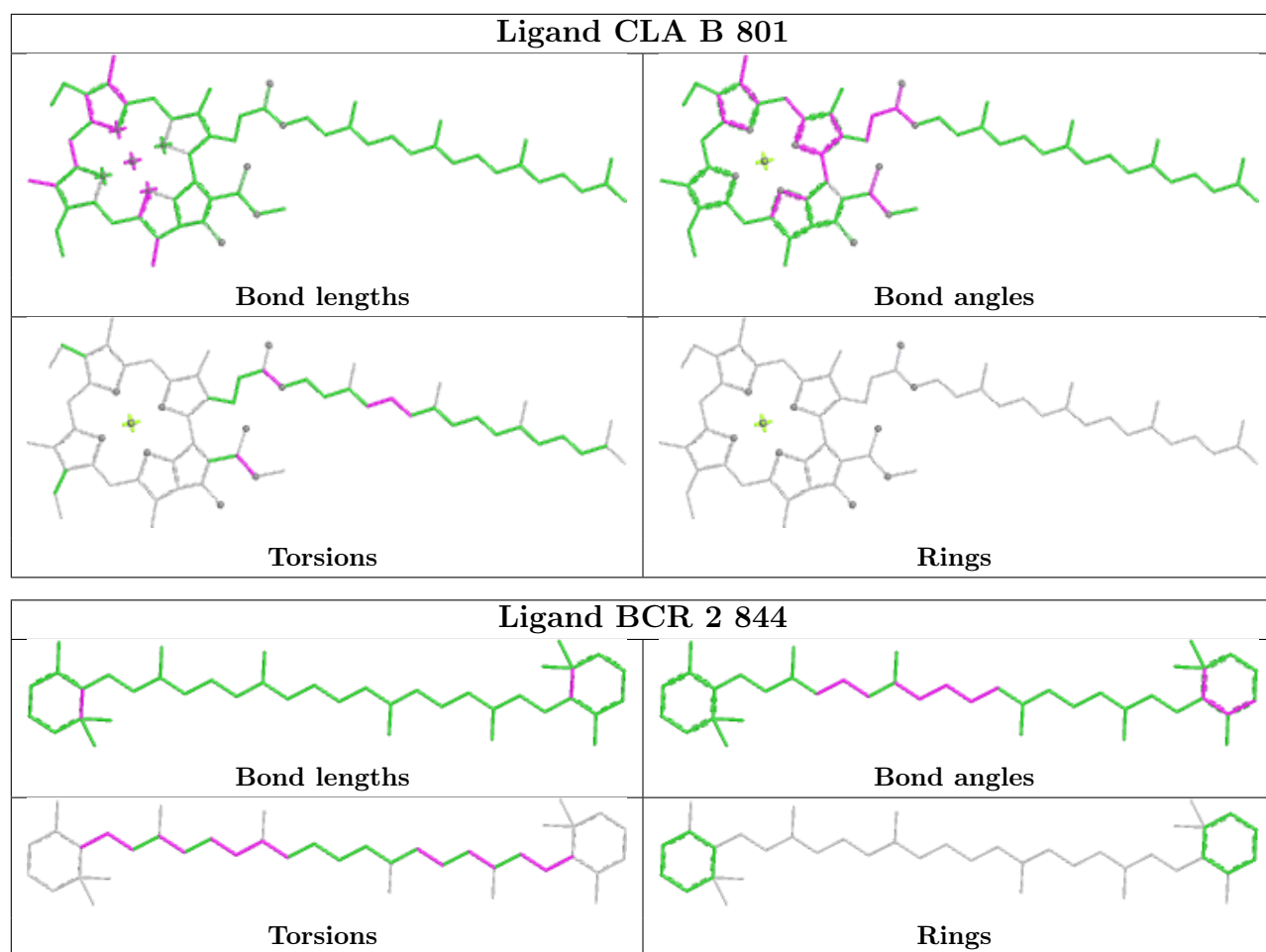
Ligand BCR L 202



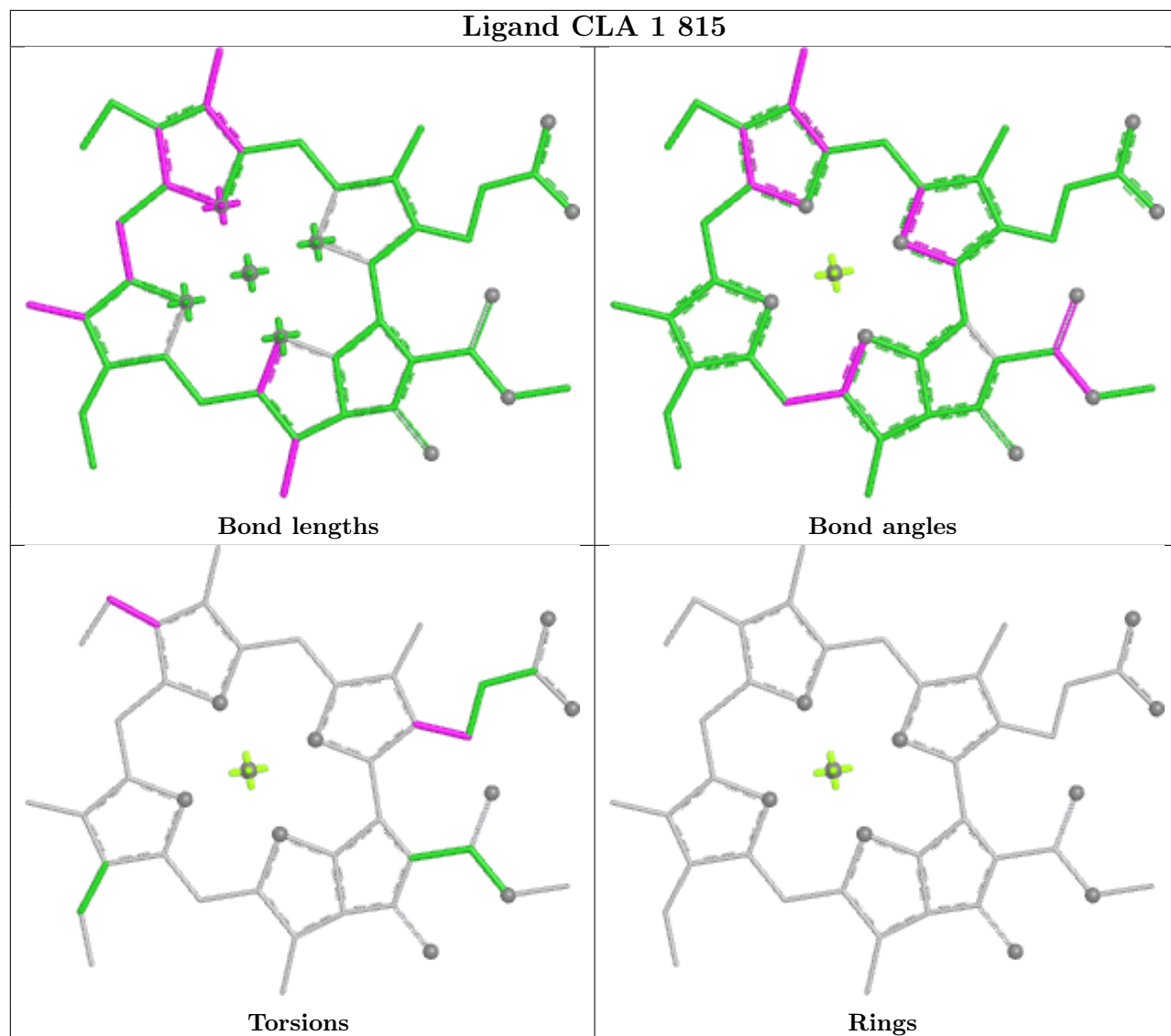


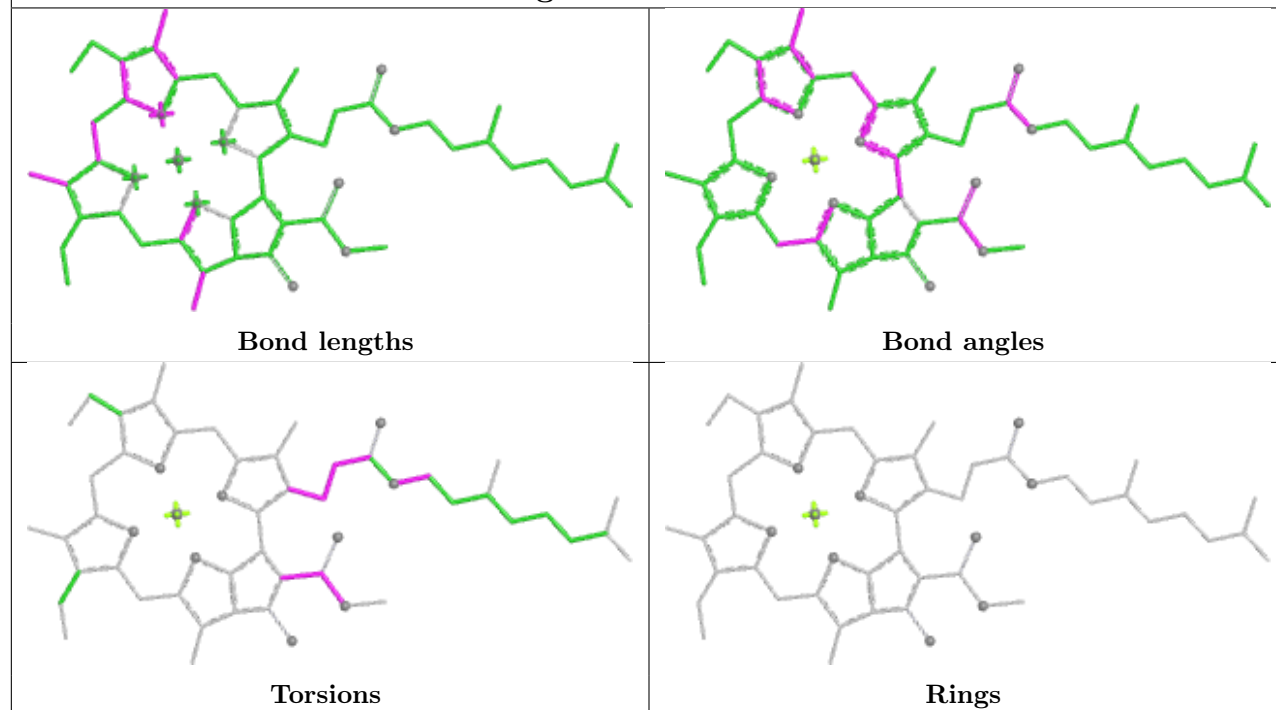
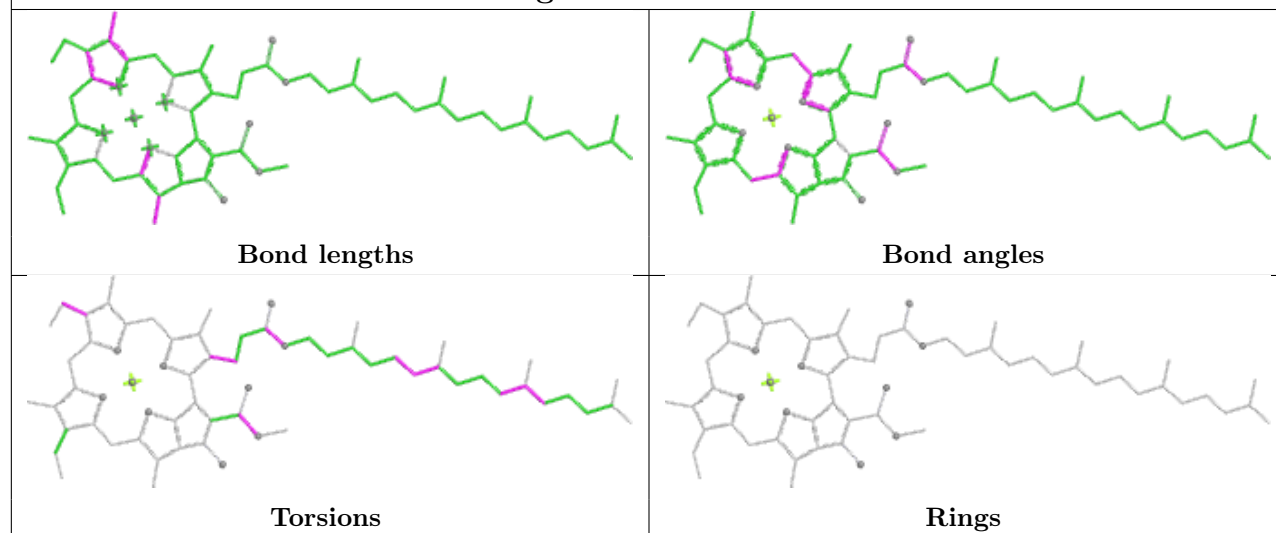


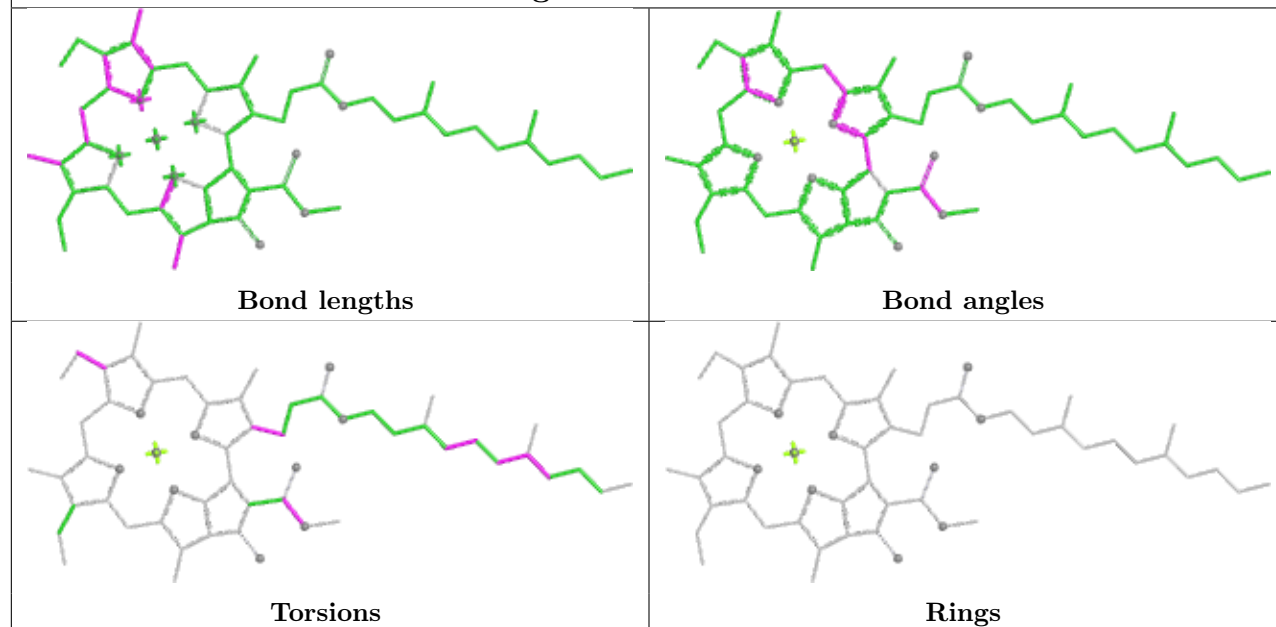
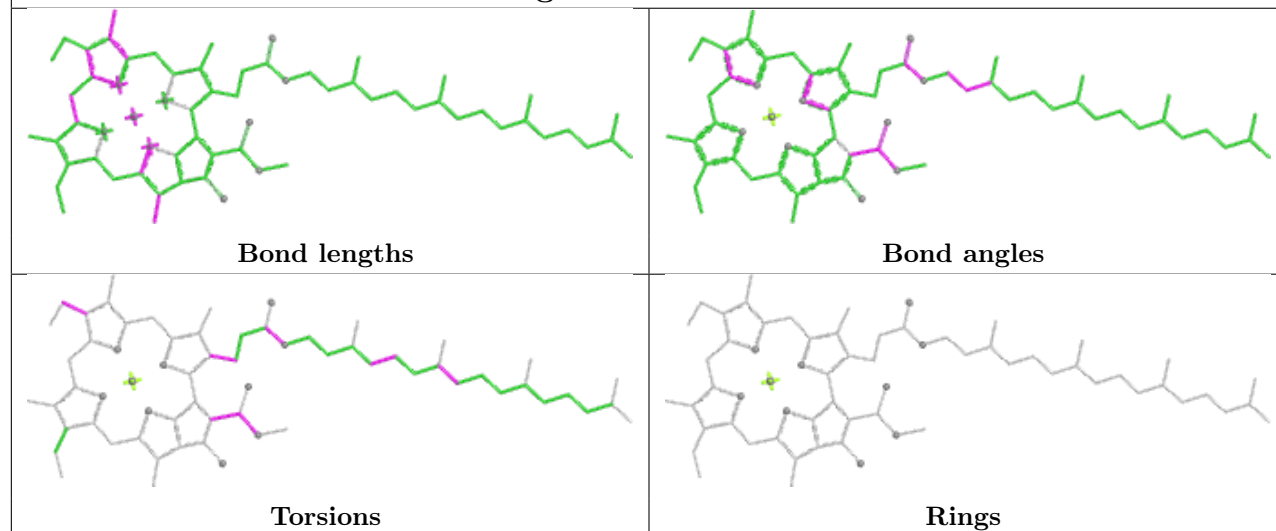




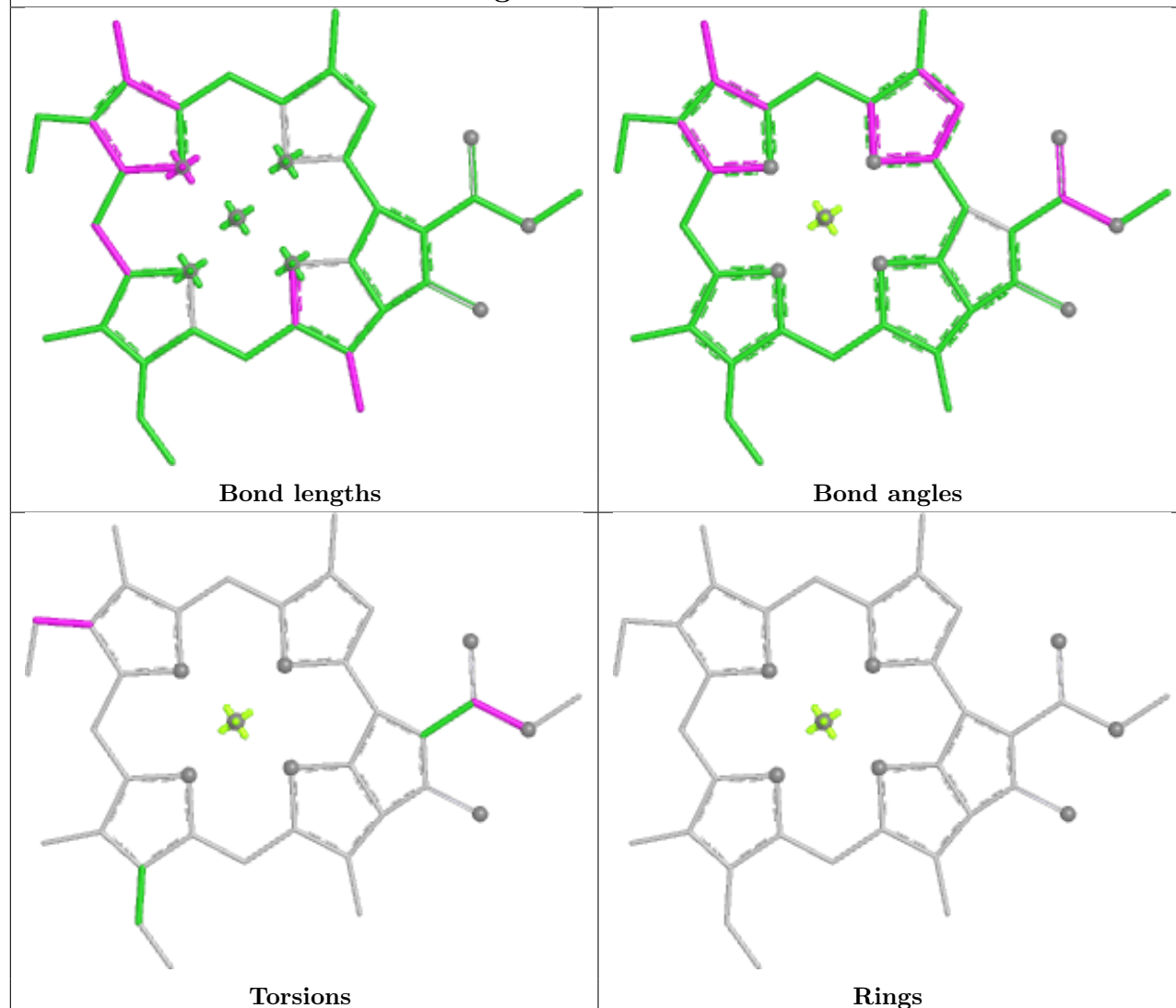
Ligand CLA 1 815



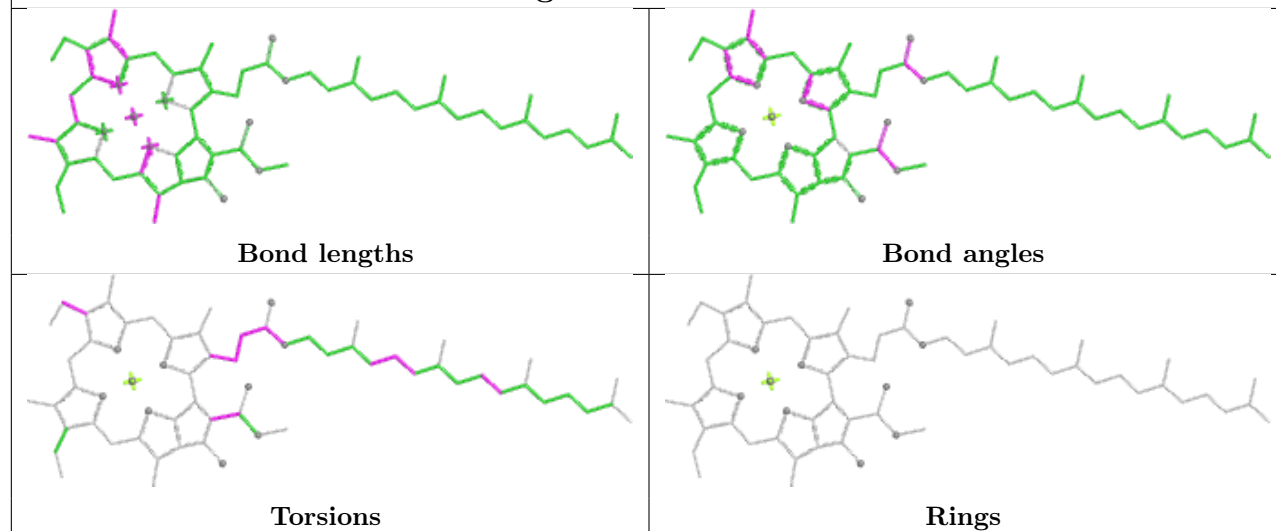
Ligand CLA a 813**Ligand CLA 2 836**

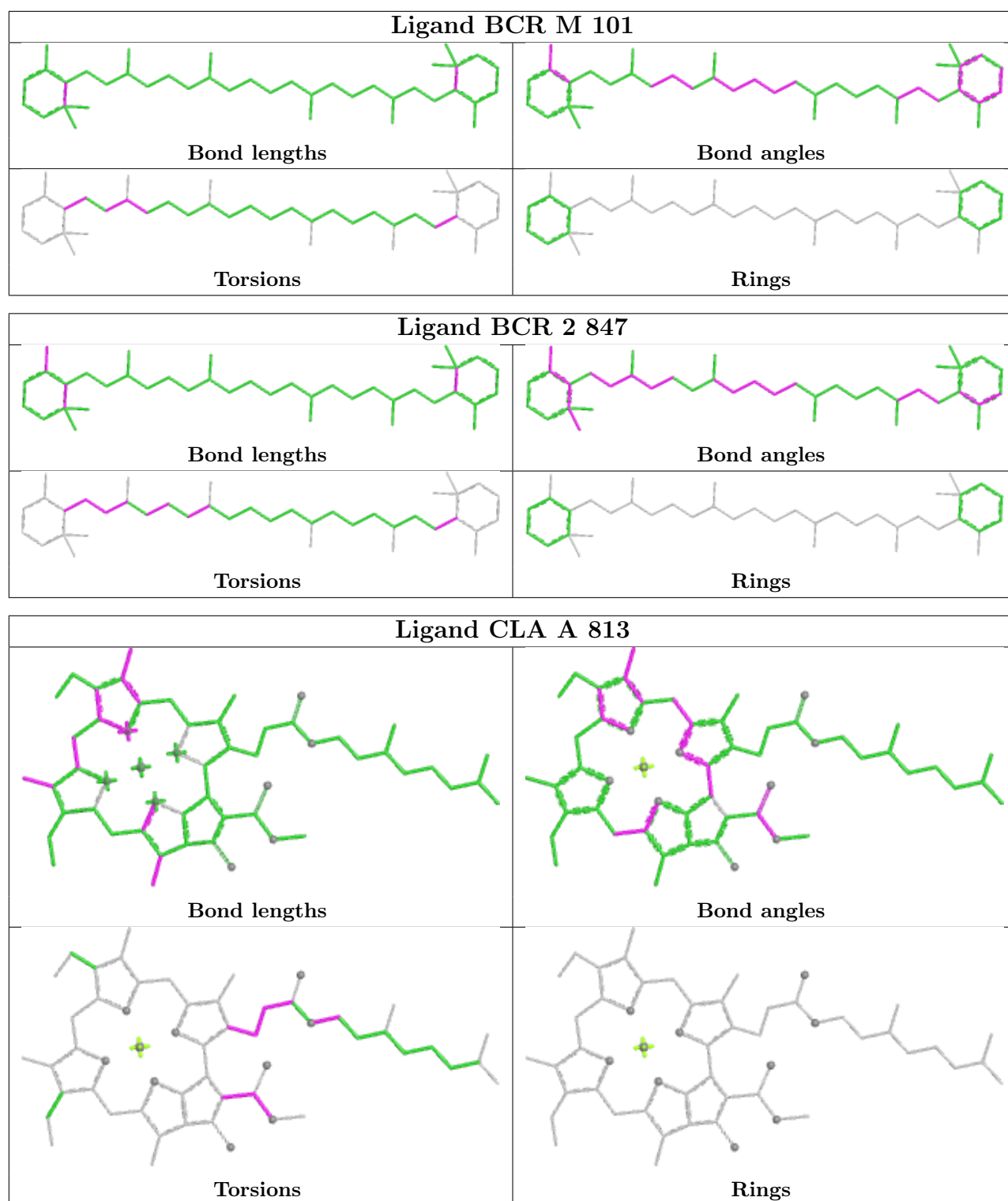
Ligand CLA B 830**Ligand CLA 1 838**

Ligand CLA 2 831

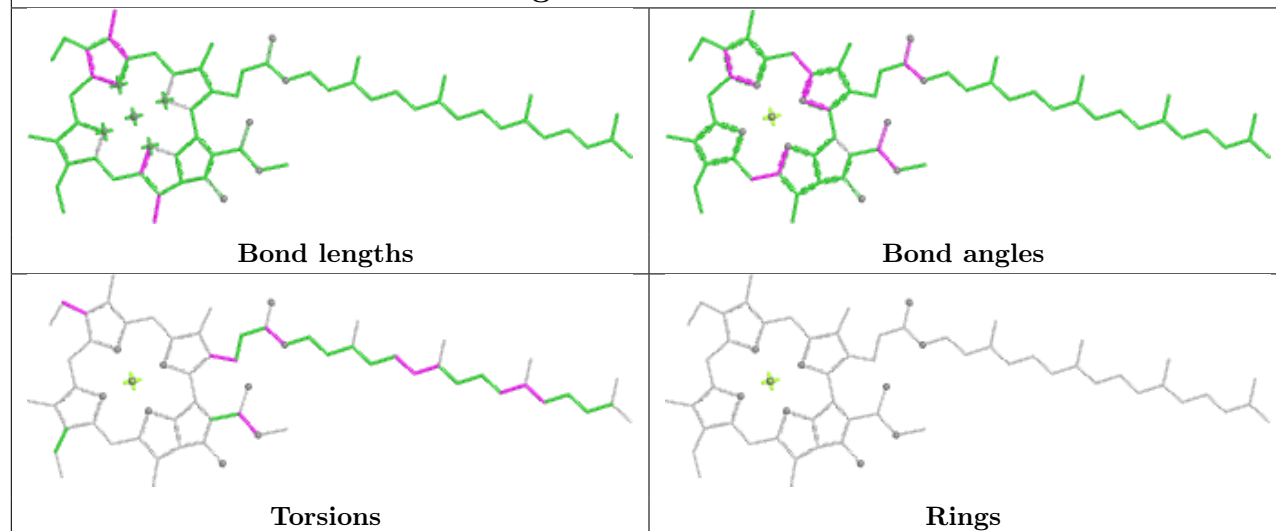


Ligand CLA a 827

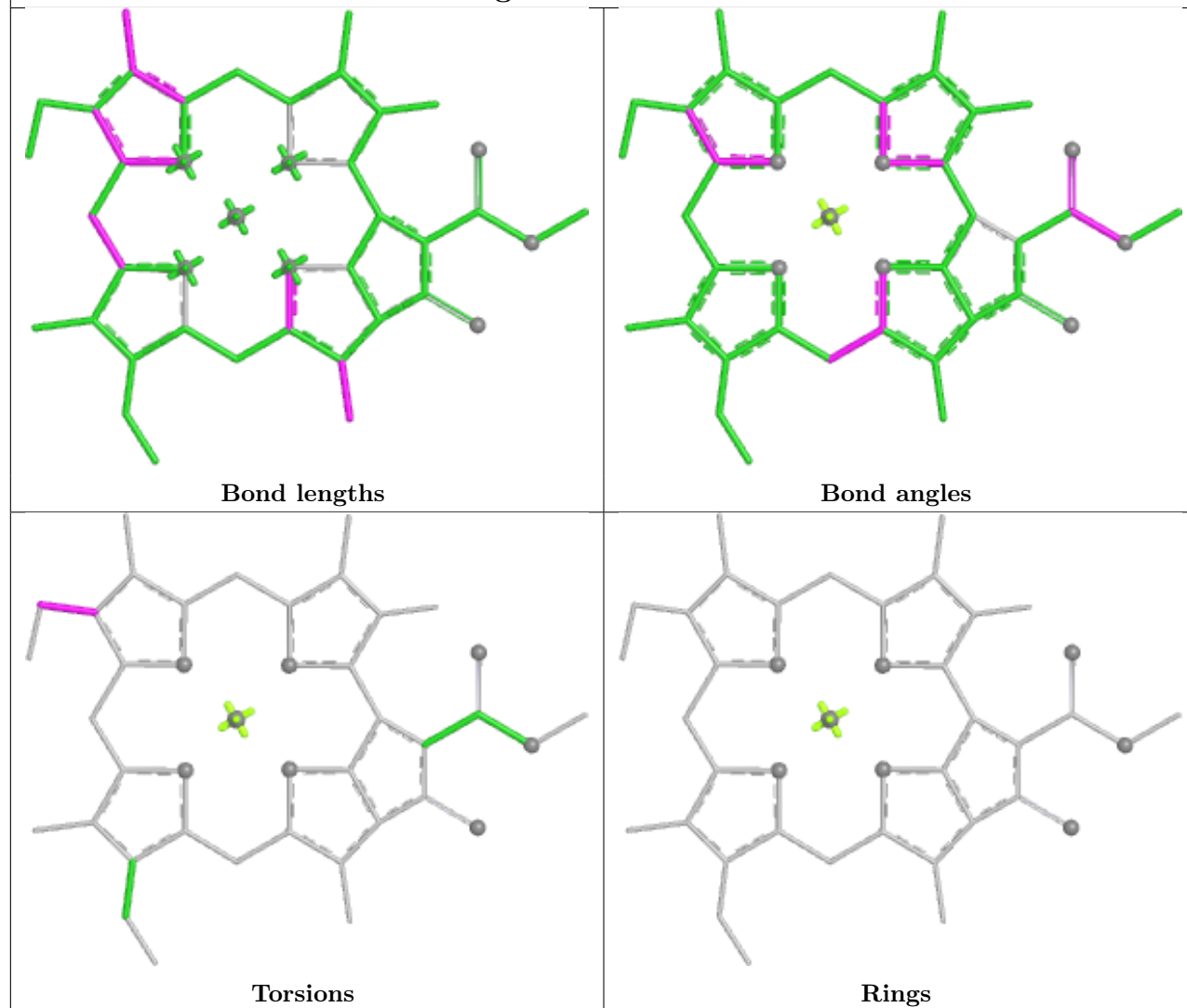




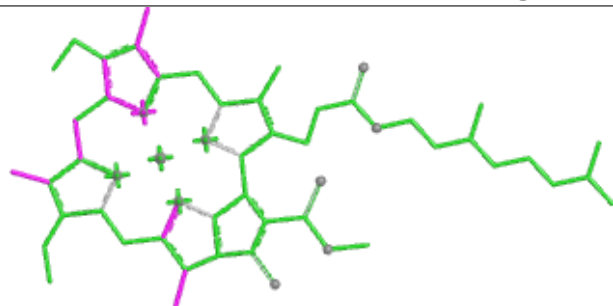
Ligand CLA B 837



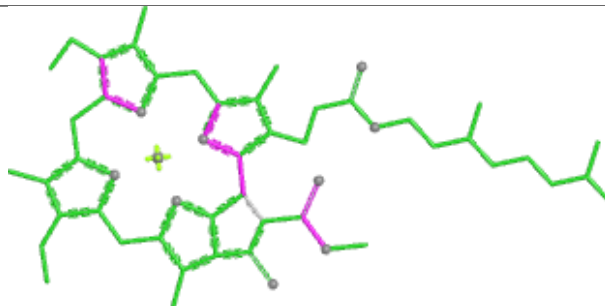
Ligand CLA B 817



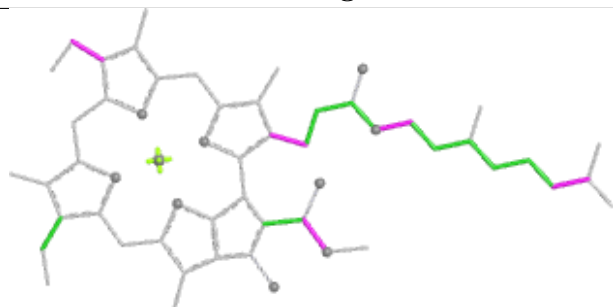
Ligand CLA B 820



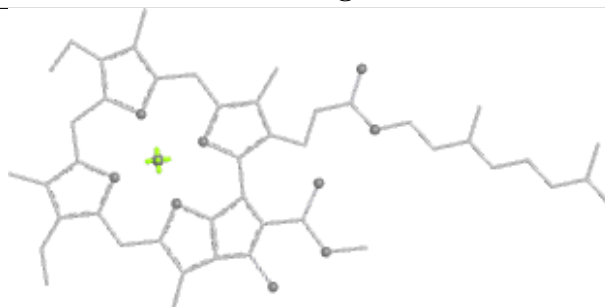
Bond lengths



Bond angles

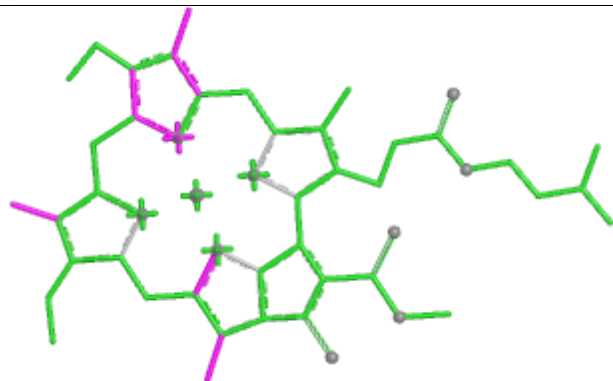


Torsions

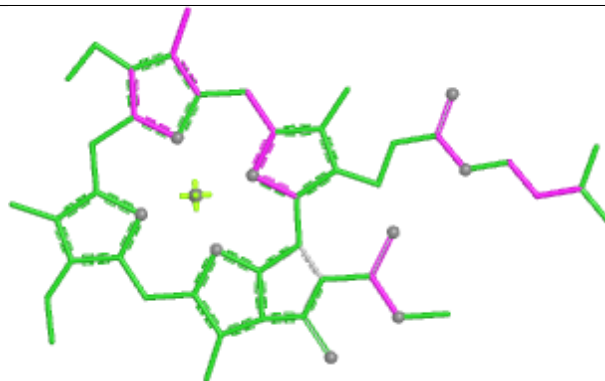


Rings

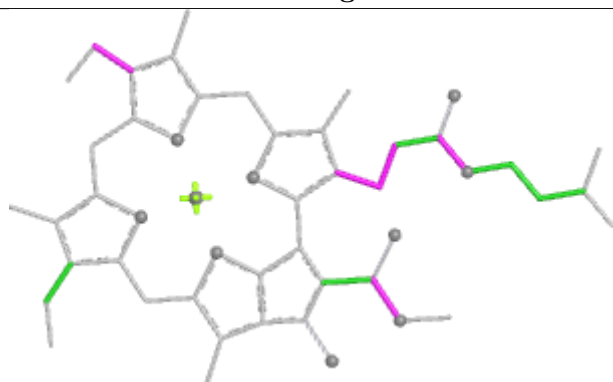
Ligand CLA A 809



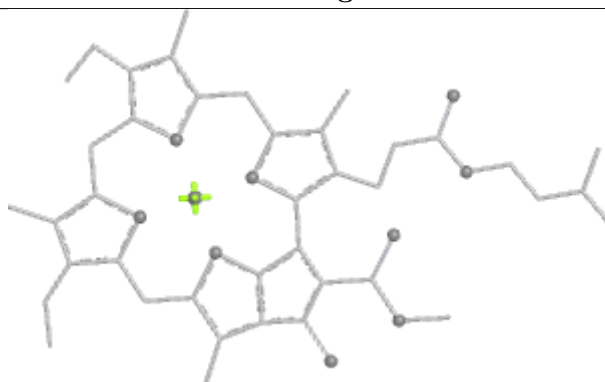
Bond lengths



Bond angles

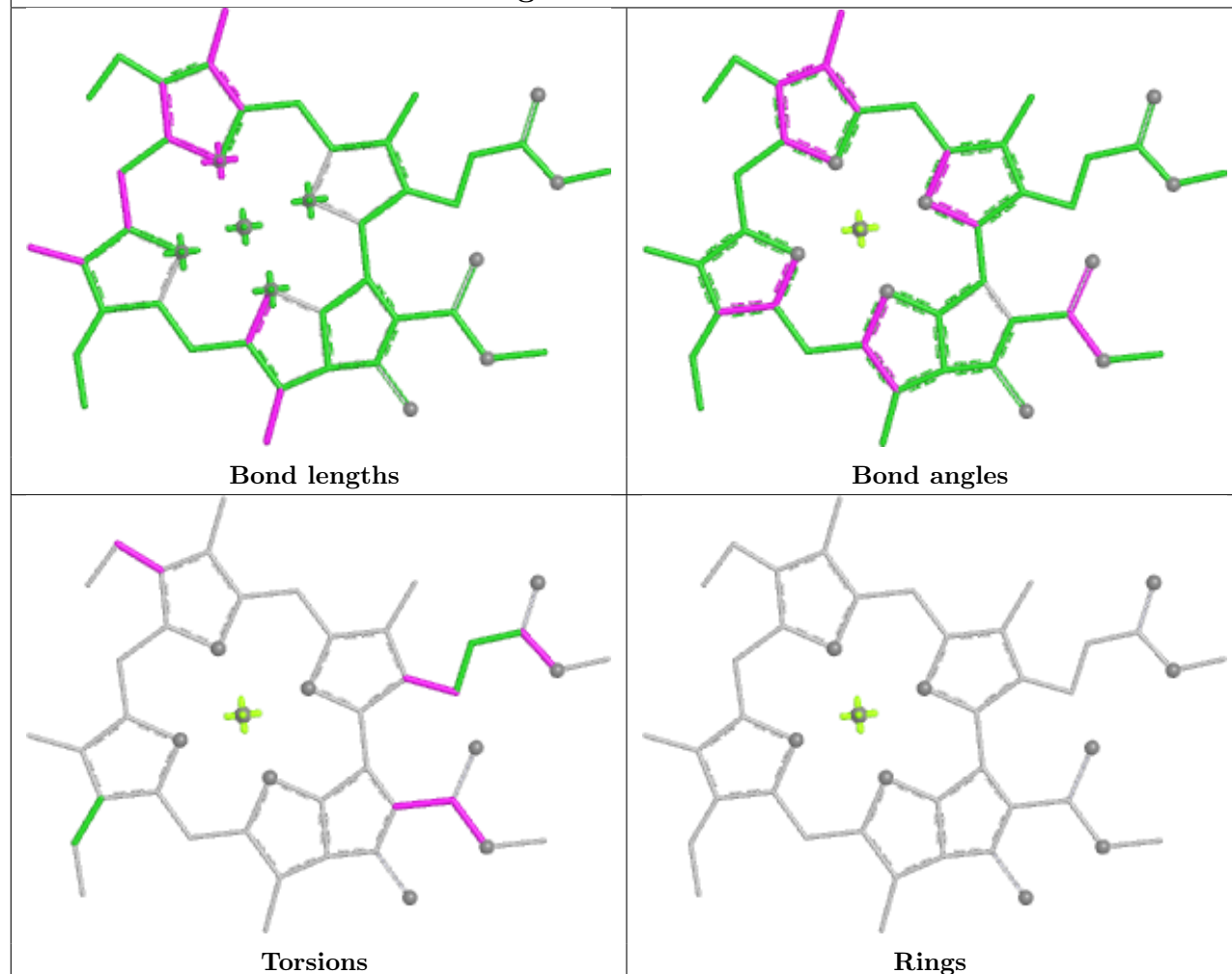


Torsions

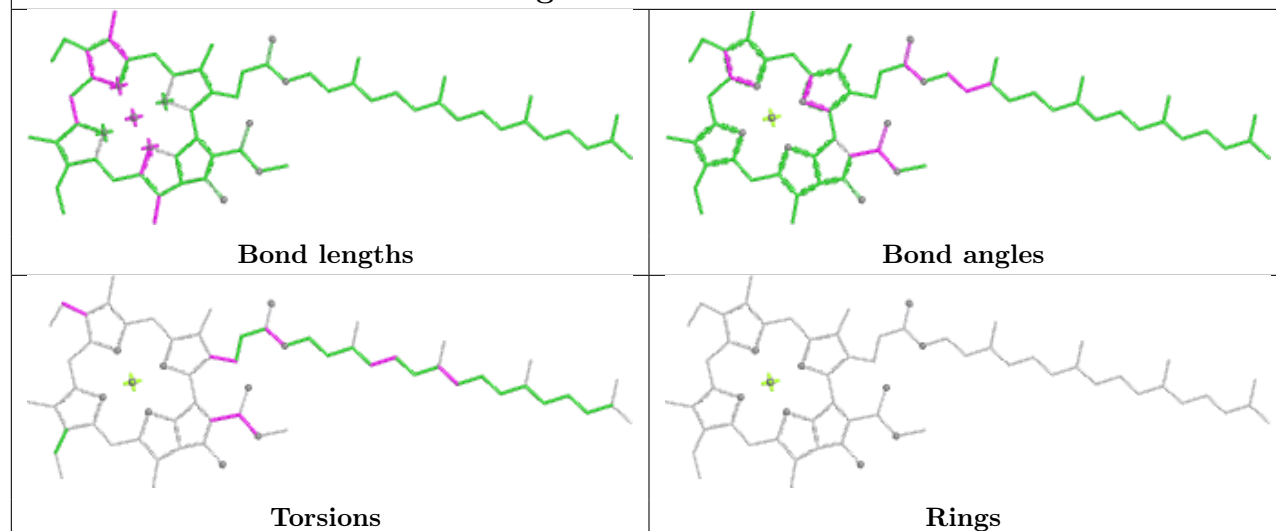


Rings

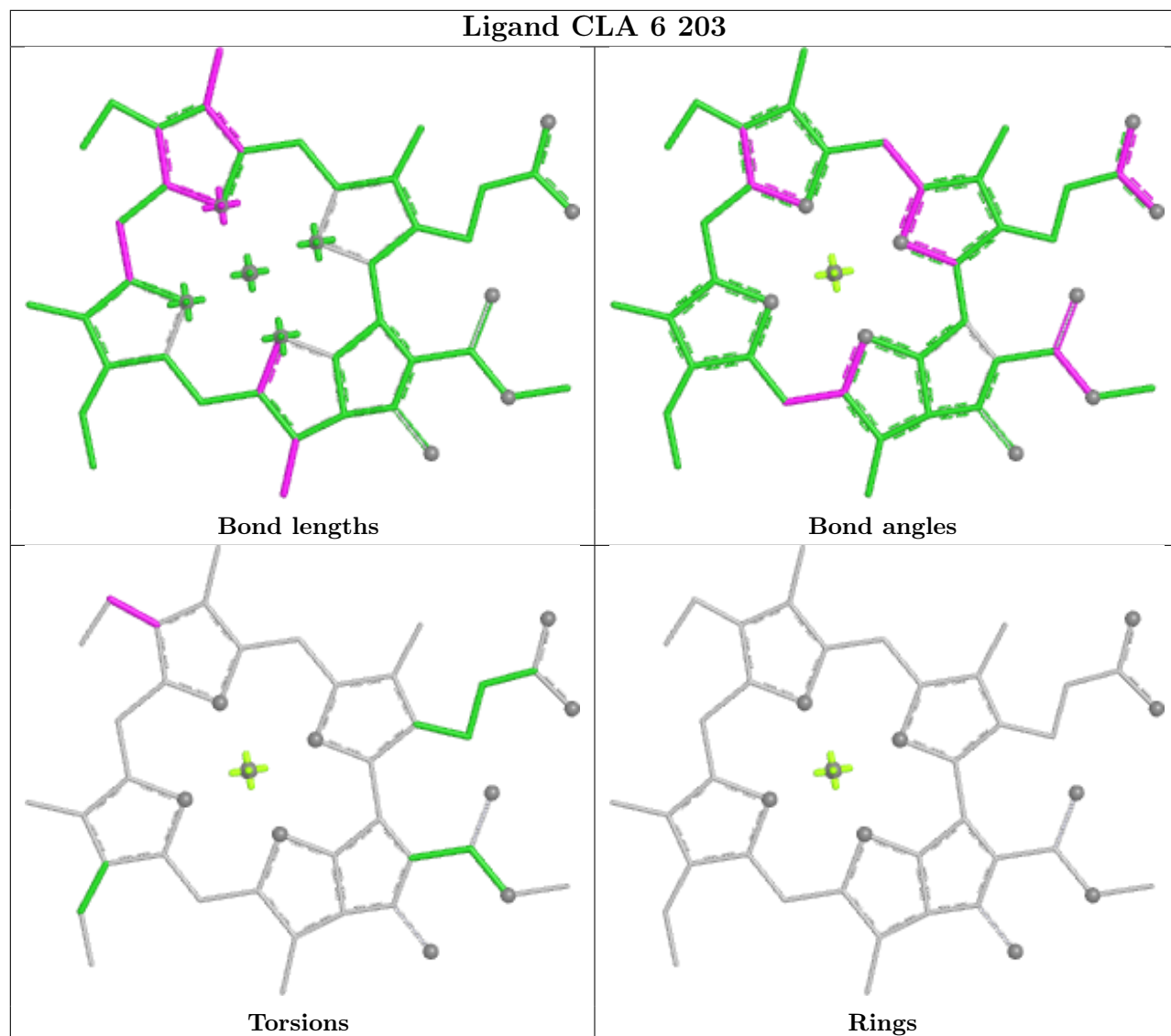
Ligand CLA 2 810



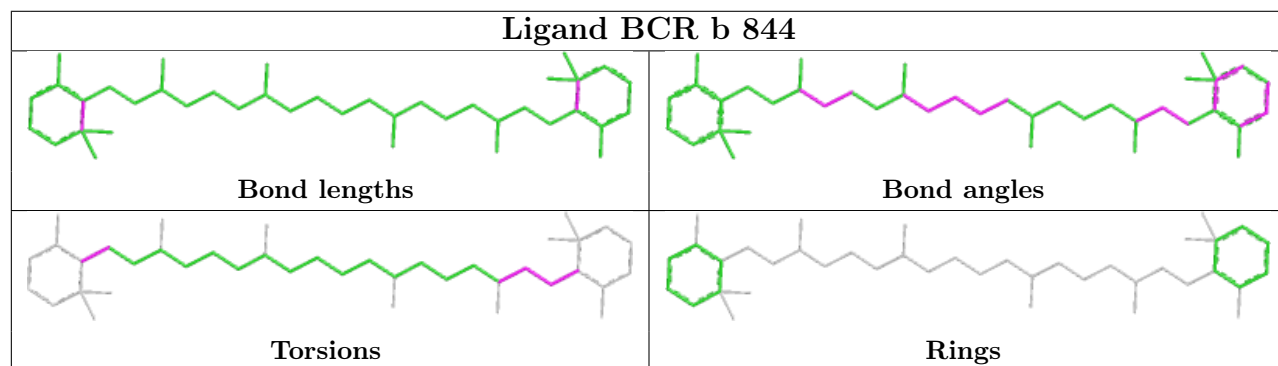
Ligand CLA a 838

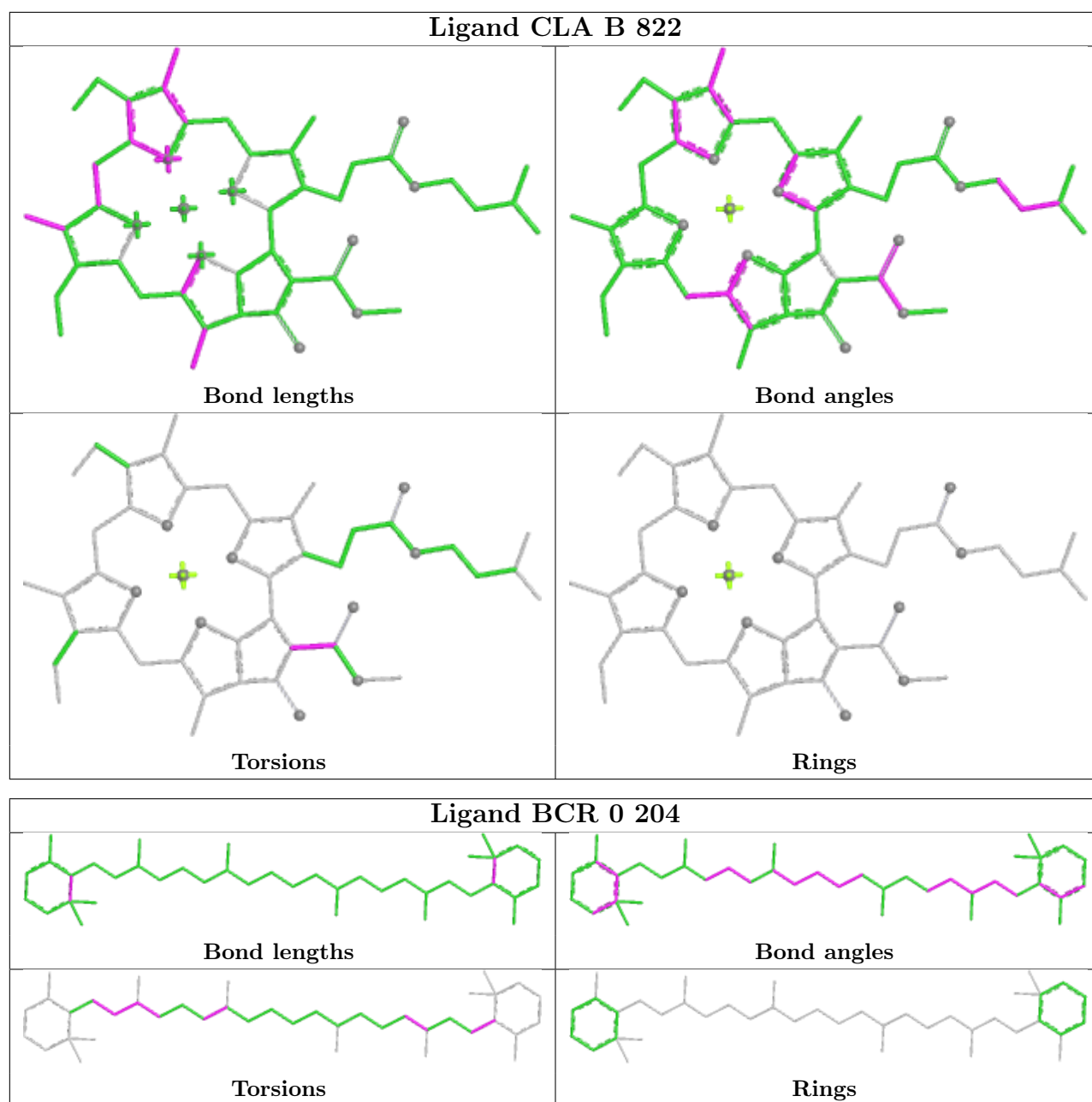


Ligand CLA 6 203

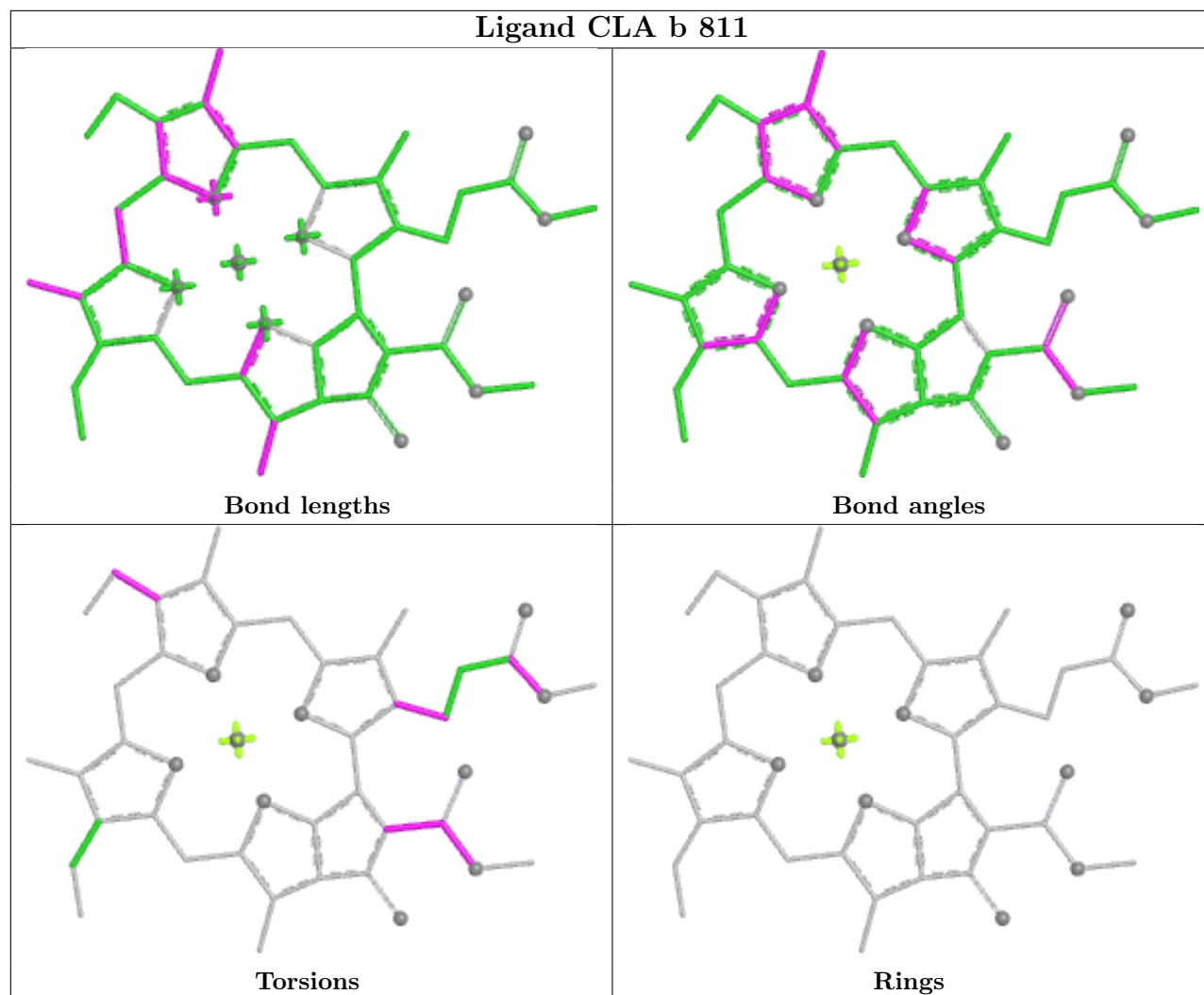


Ligand BCR b 844

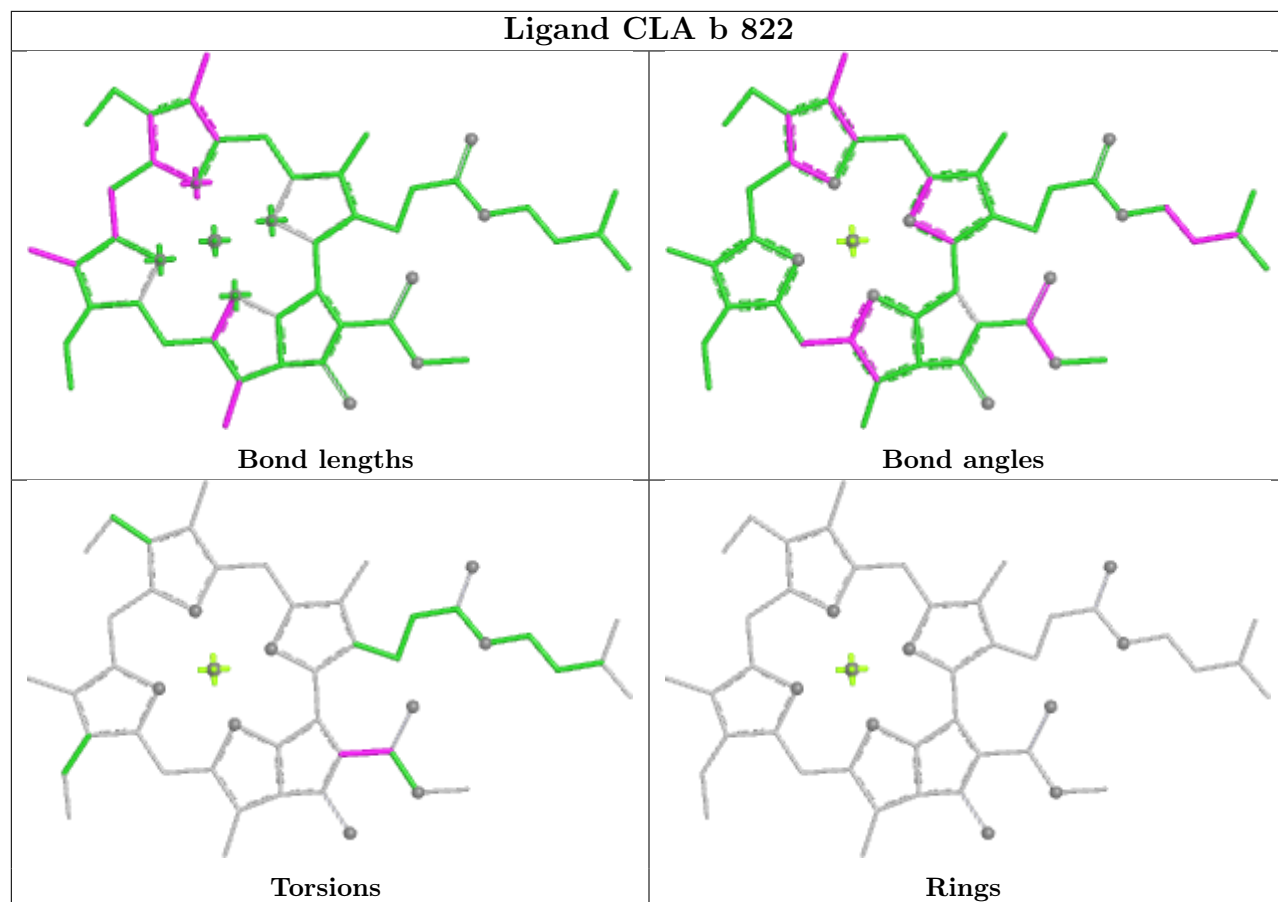




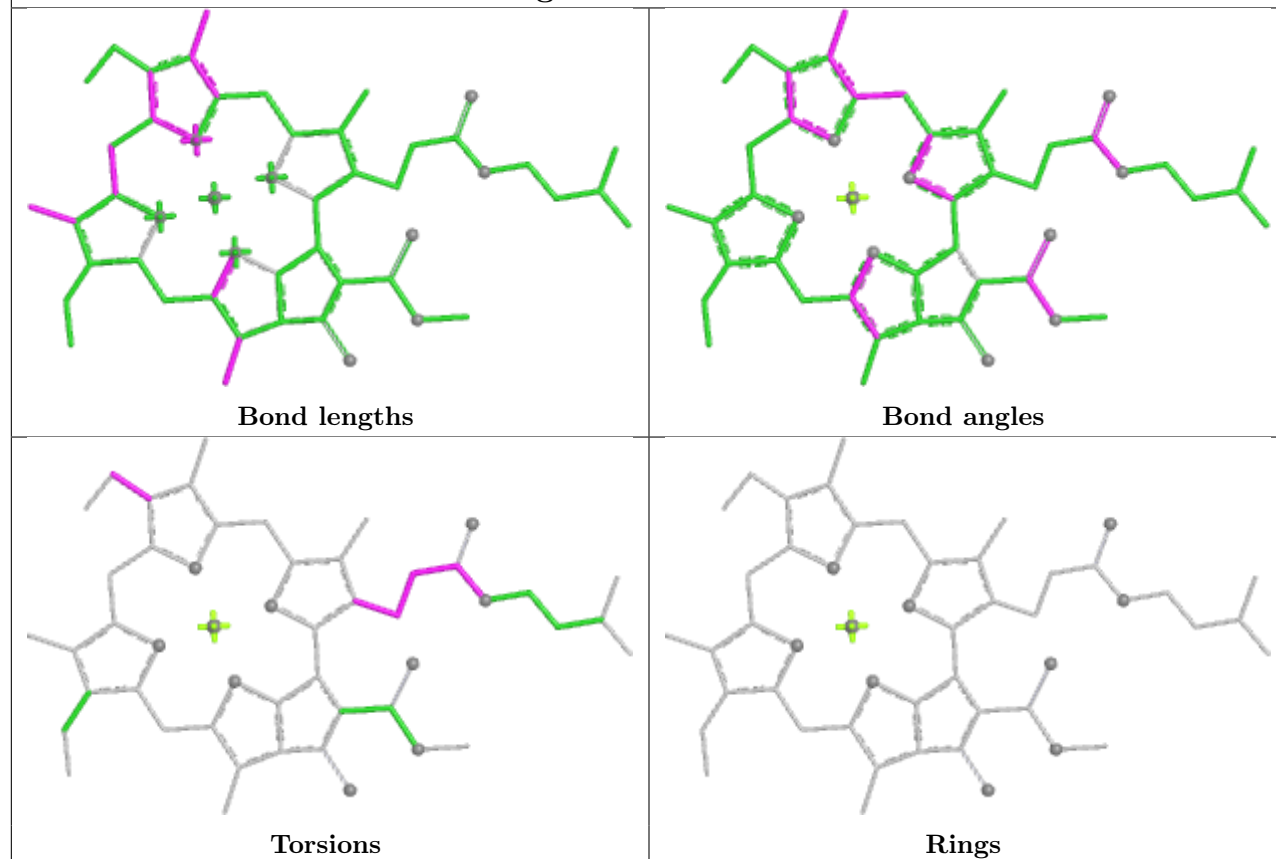
Ligand CLA b 811



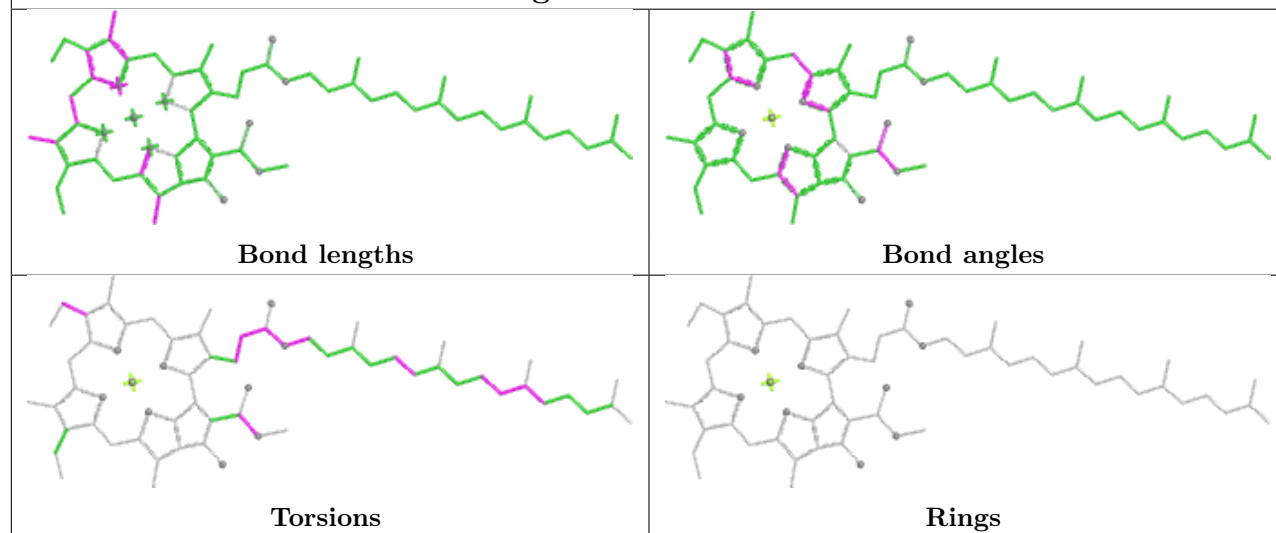
Ligand CLA b 822

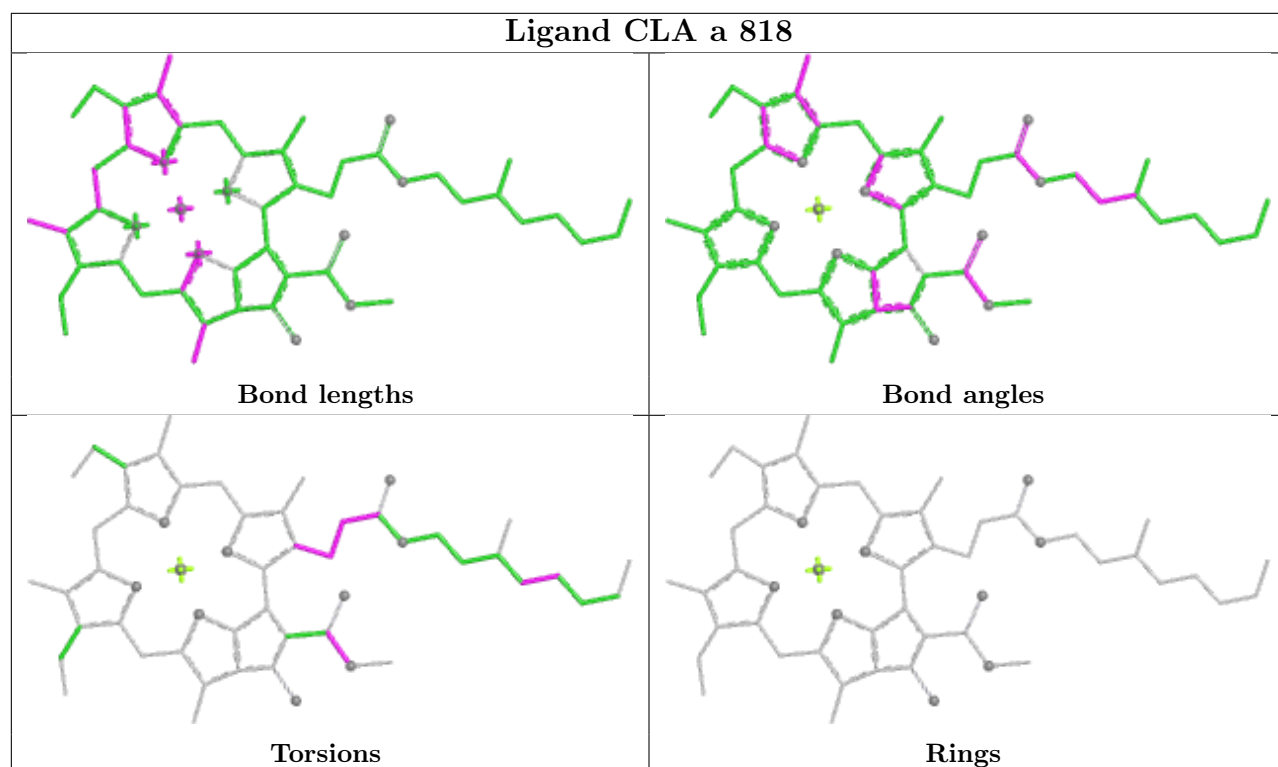
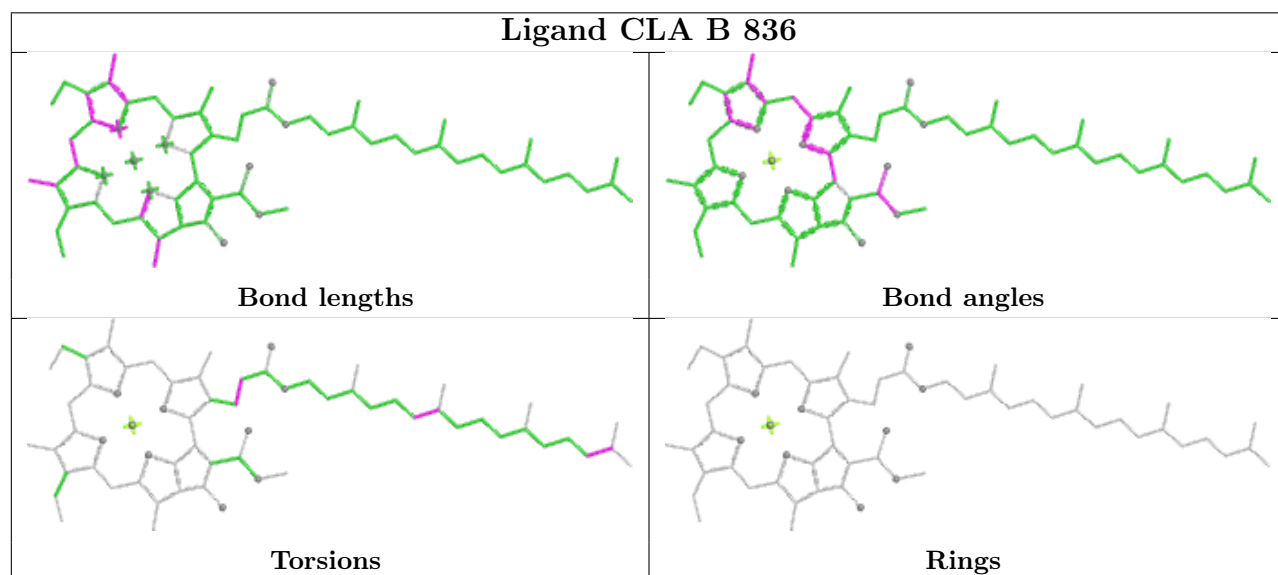
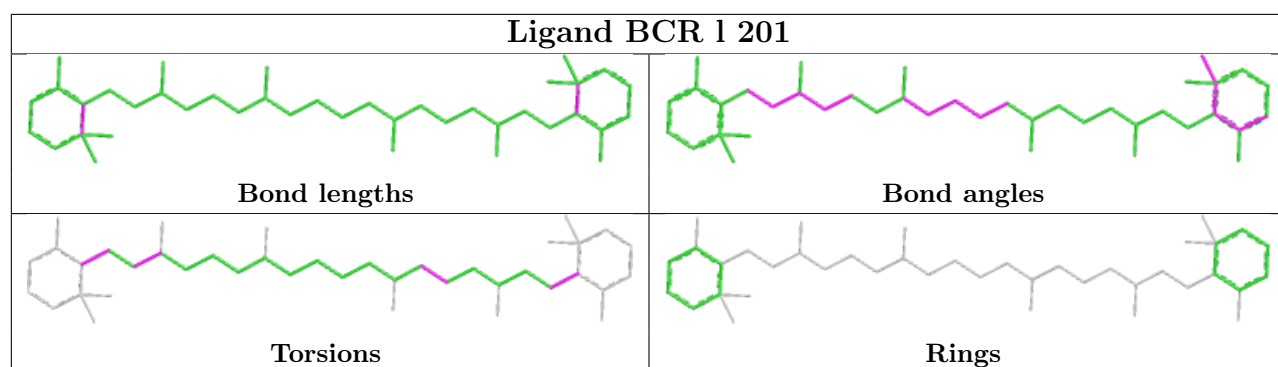


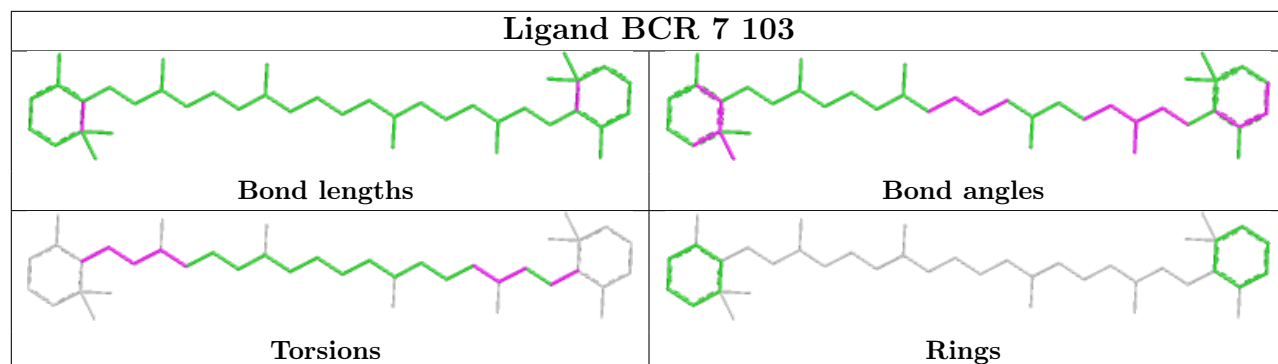
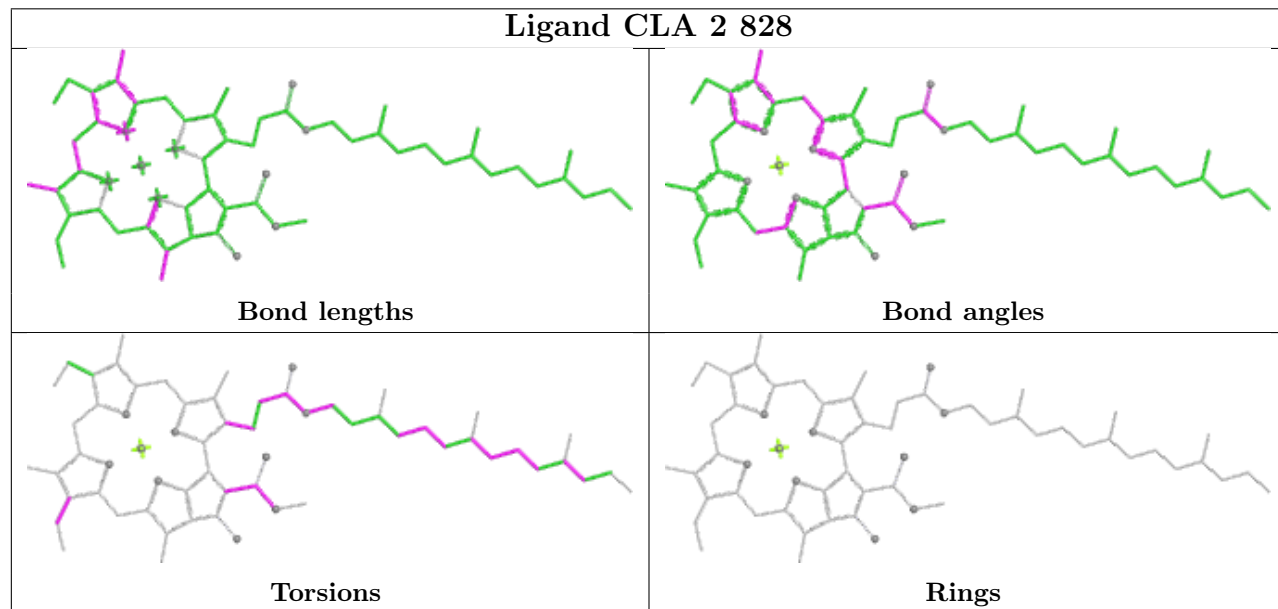
Ligand CLA 2 813



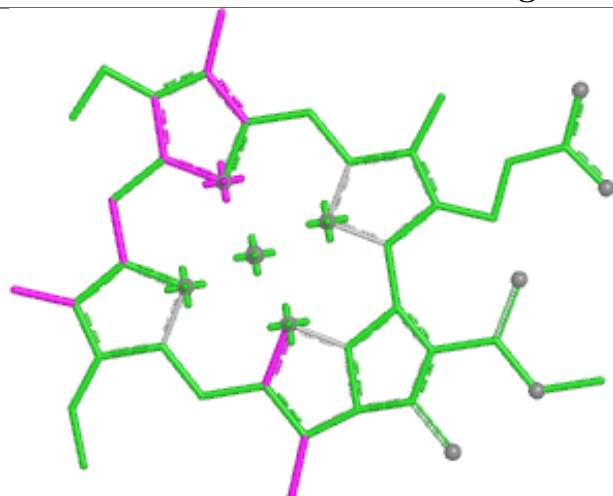
Ligand CLA B 807



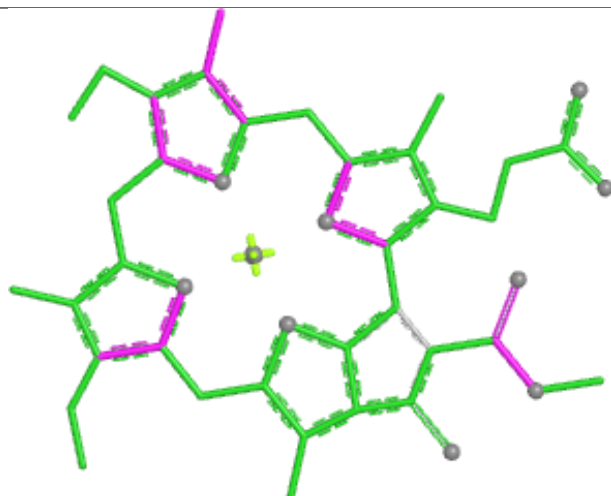


Ligand BCR 7 103**Ligand CLA 2 828**

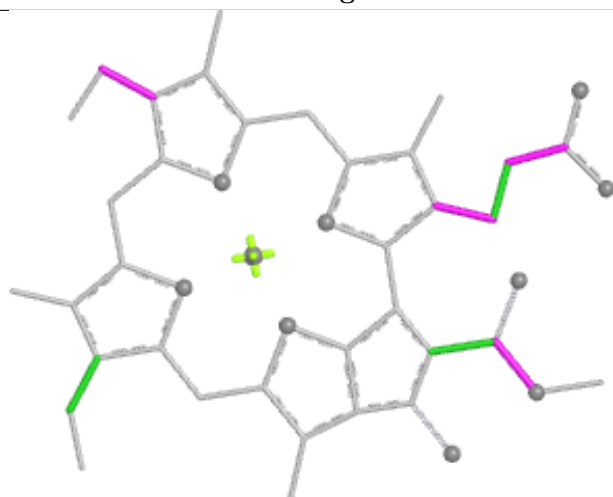
Ligand CLA 1 810



Bond lengths



Bond angles

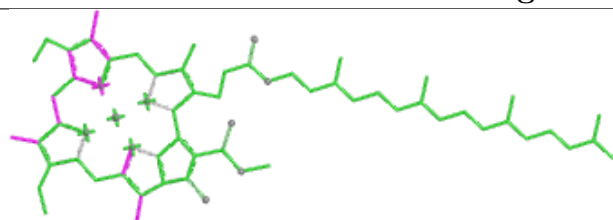


Torsions

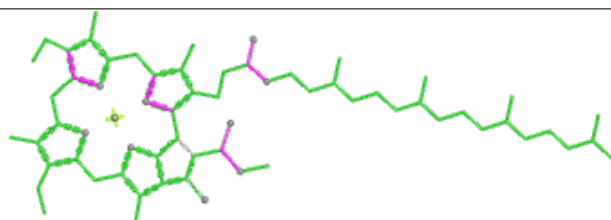


Rings

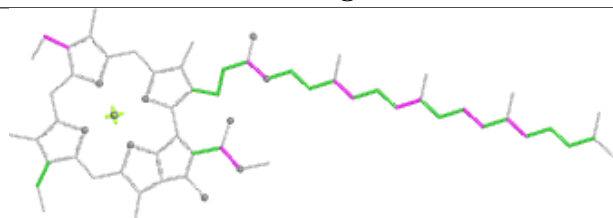
Ligand CLA b 805



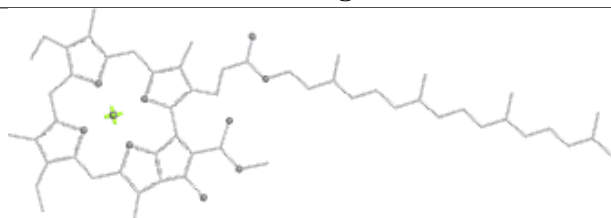
Bond lengths



Bond angles

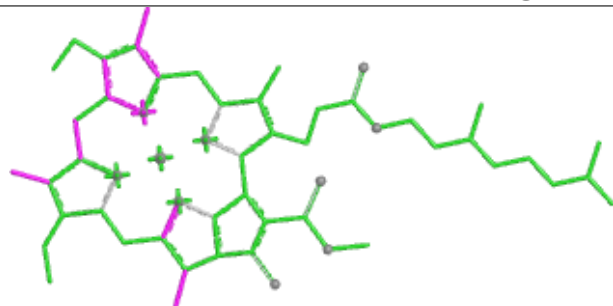


Torsions

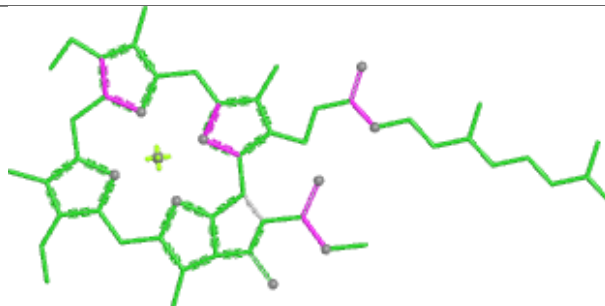


Rings

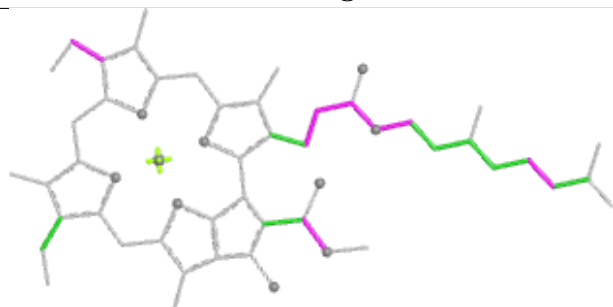
Ligand CLA b 828



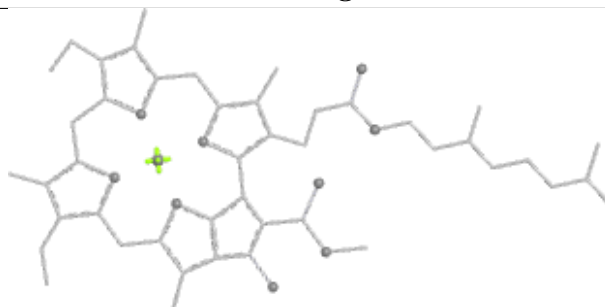
Bond lengths



Bond angles

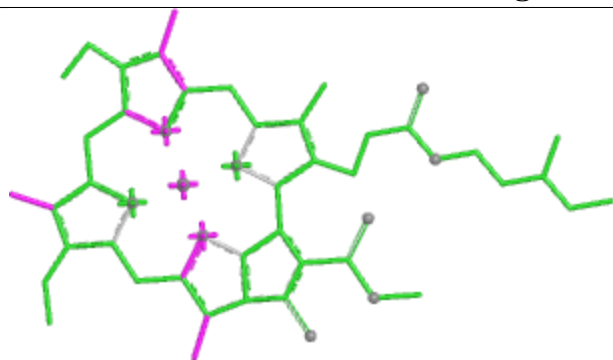


Torsions

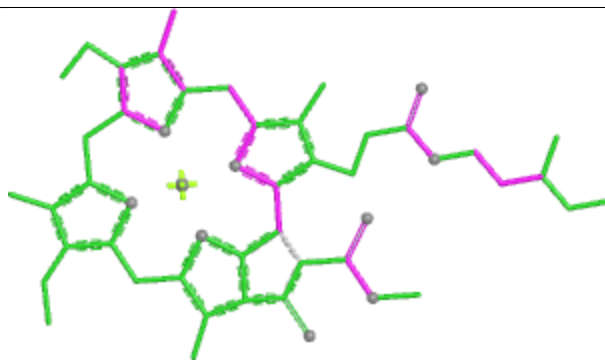


Rings

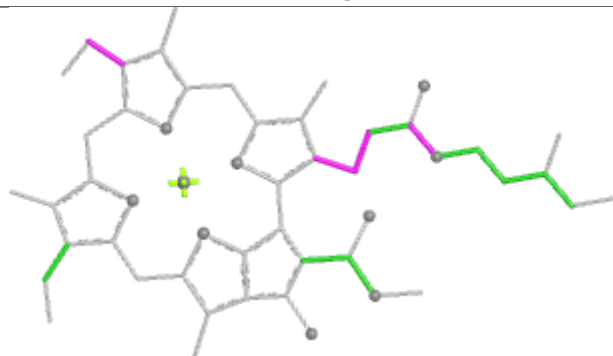
Ligand CLA A 836



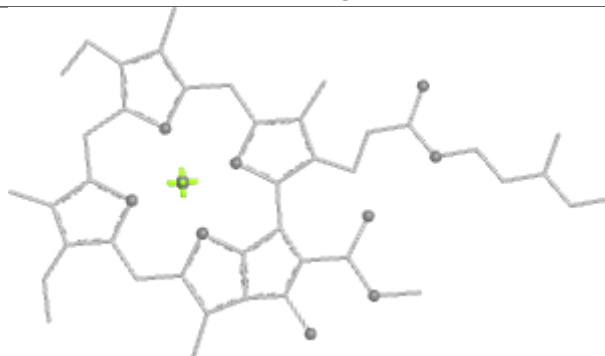
Bond lengths



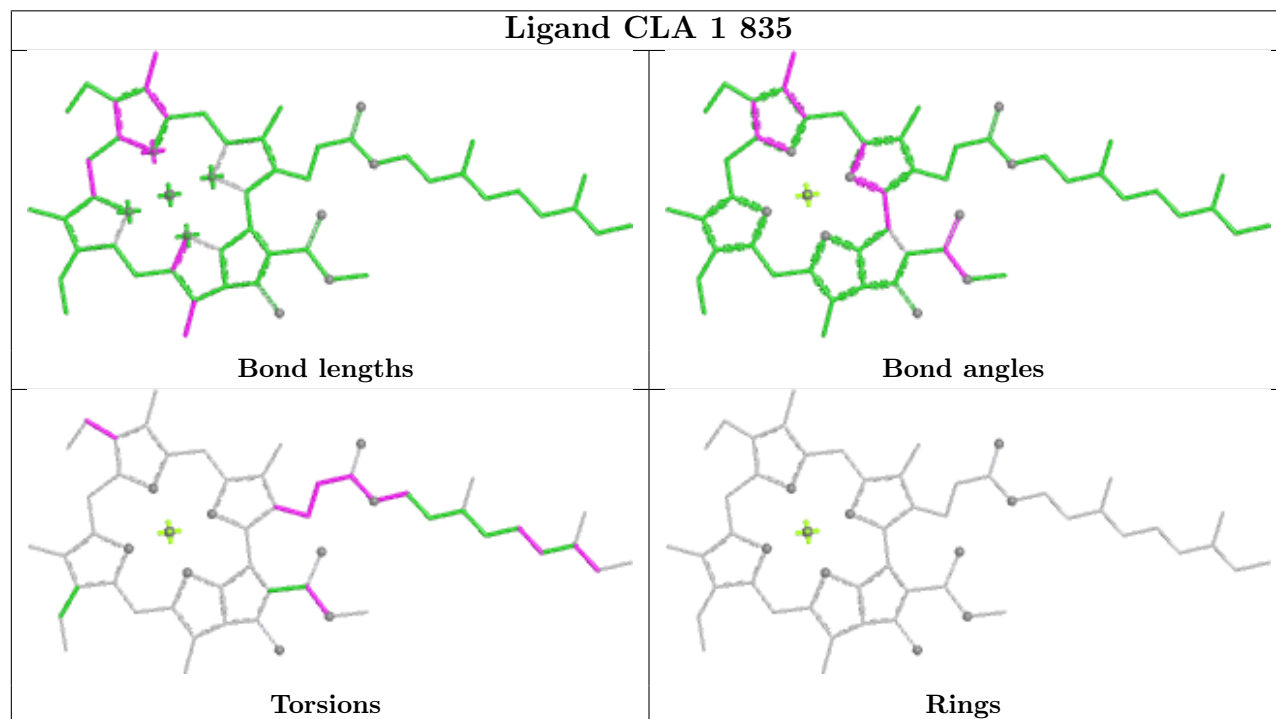
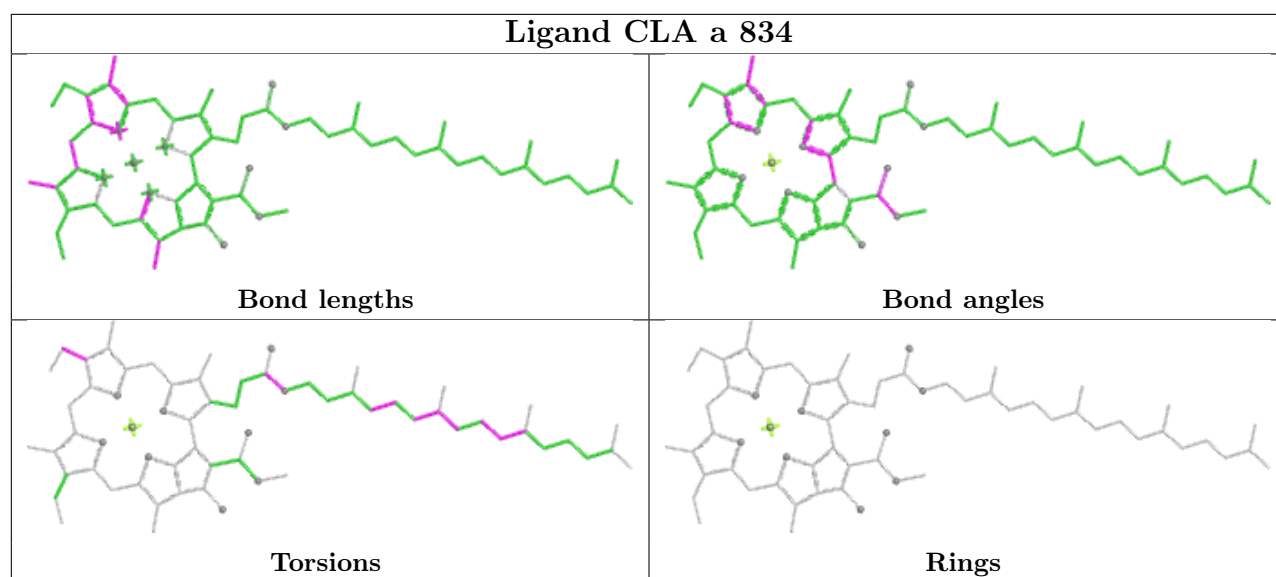
Bond angles



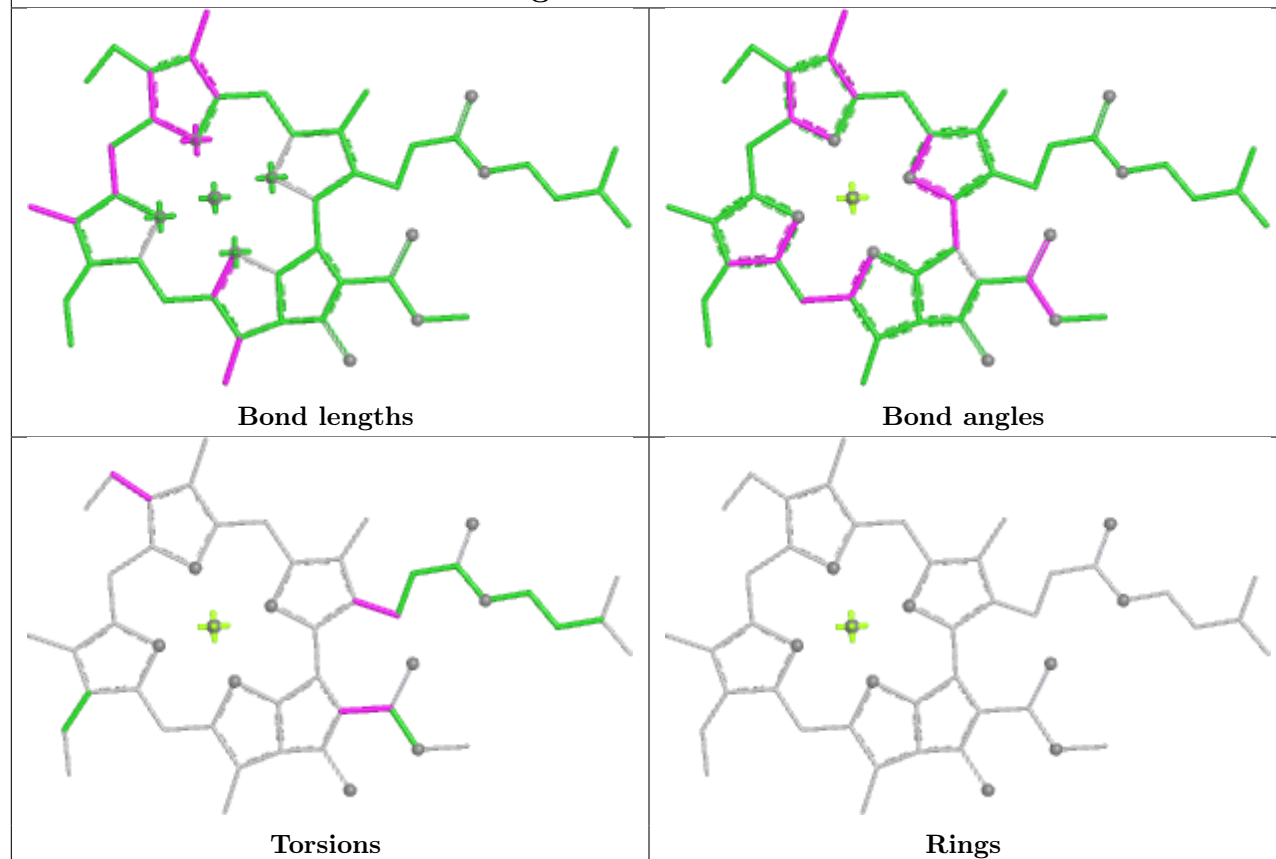
Torsions



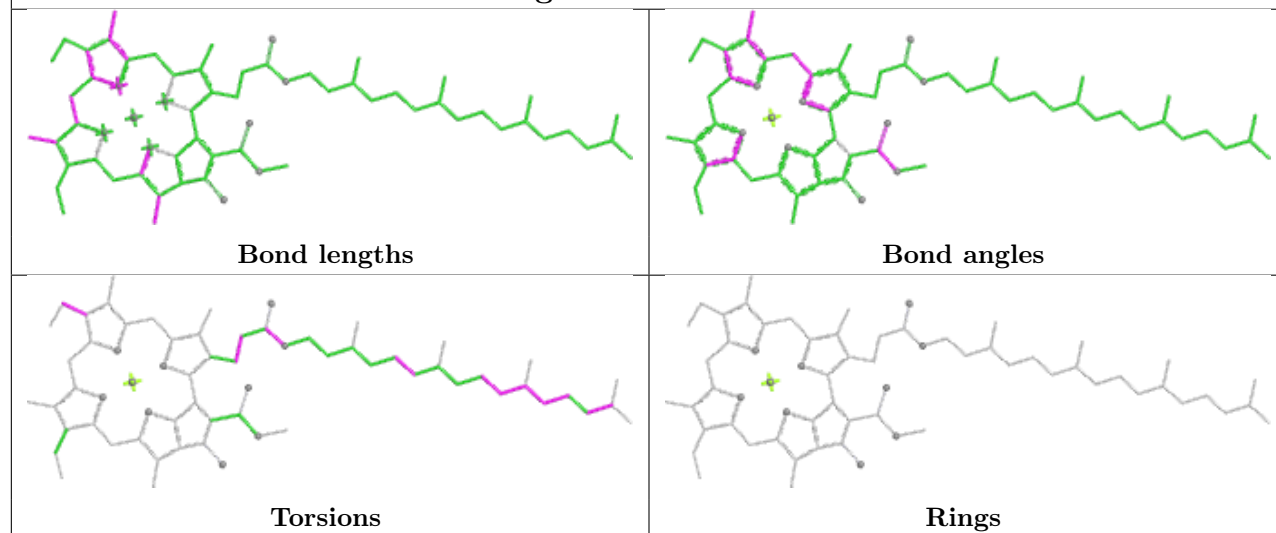
Rings

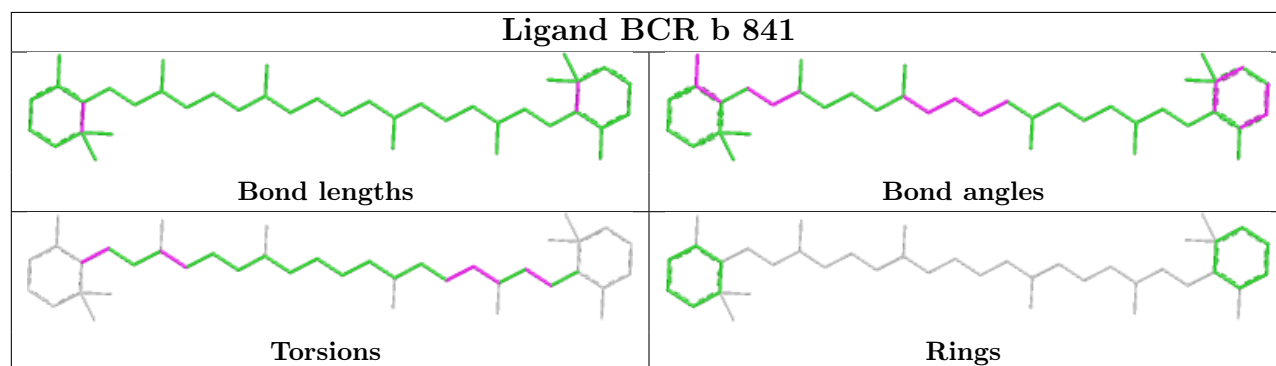
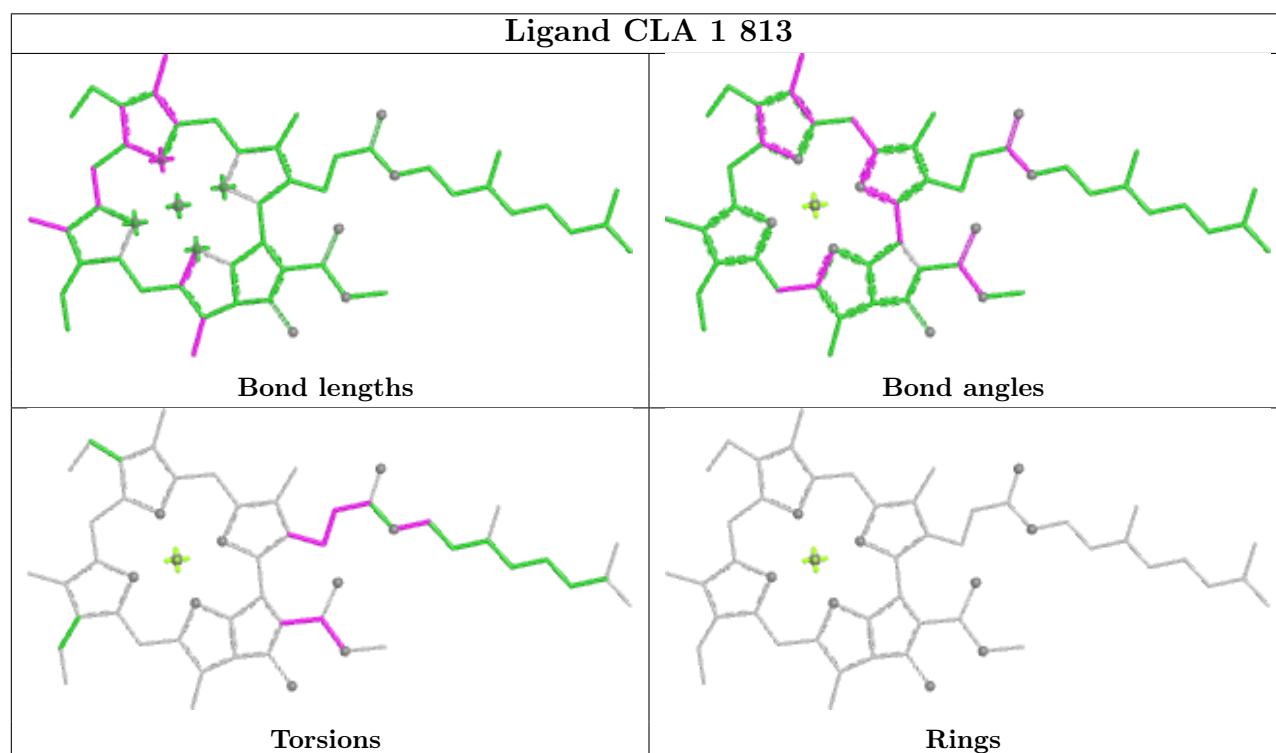
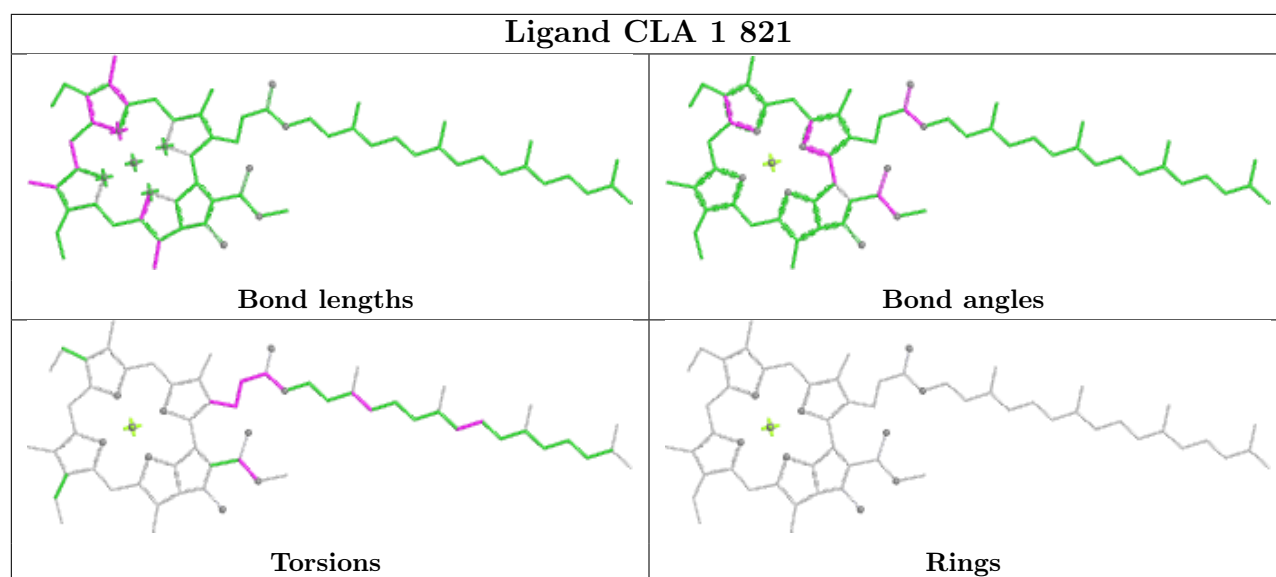


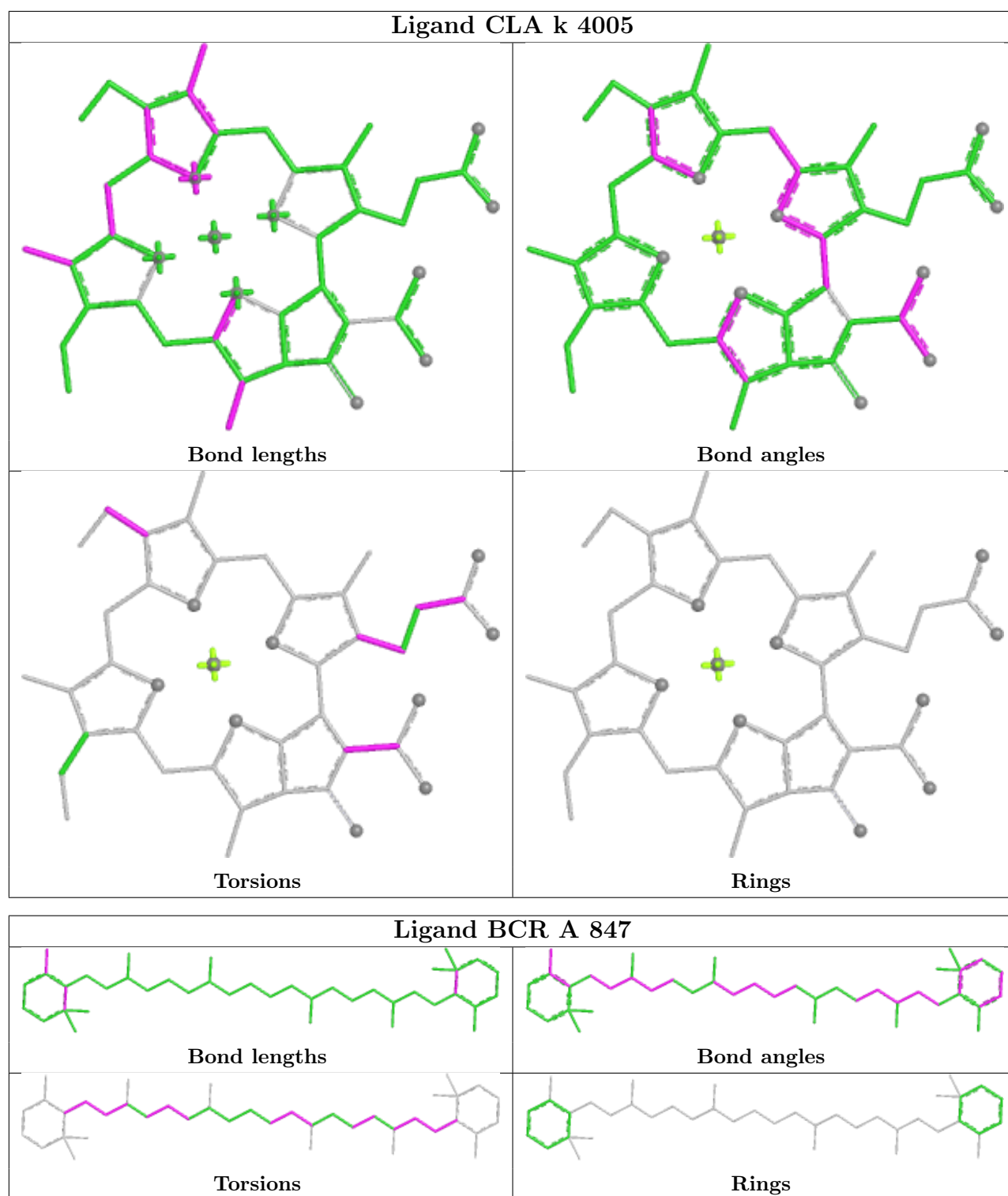
Ligand CLA A 808

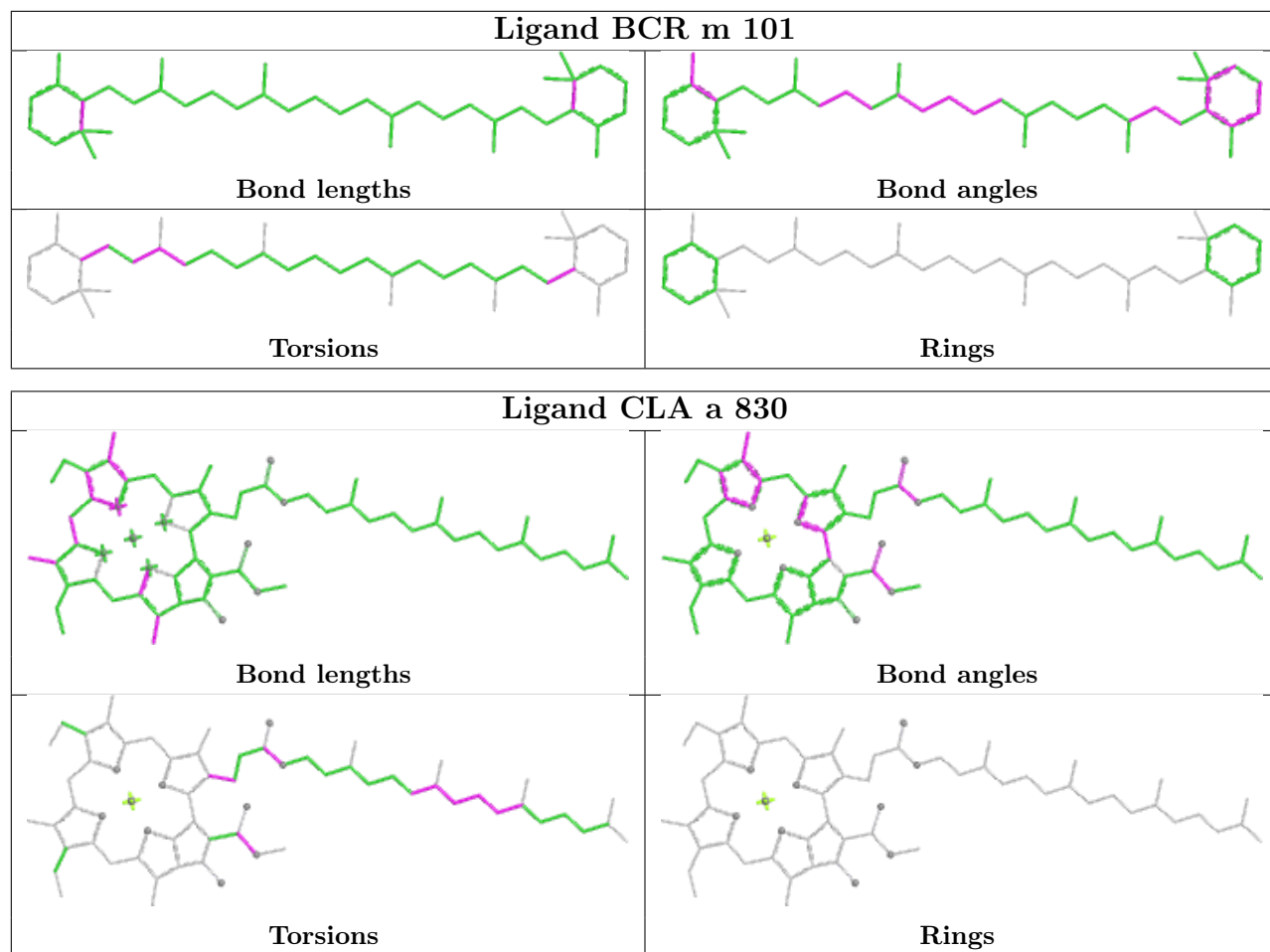


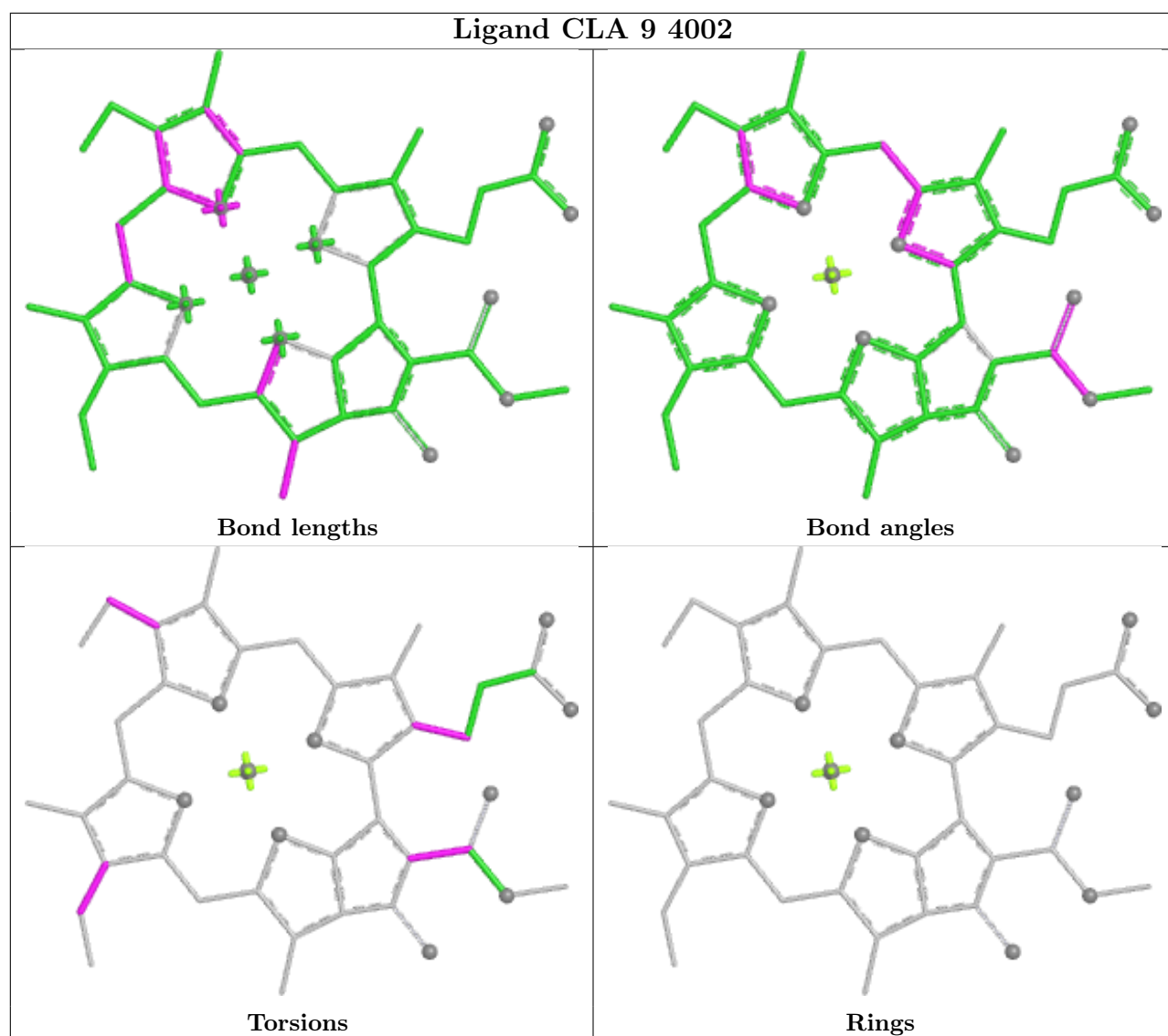
Ligand CLA b 823



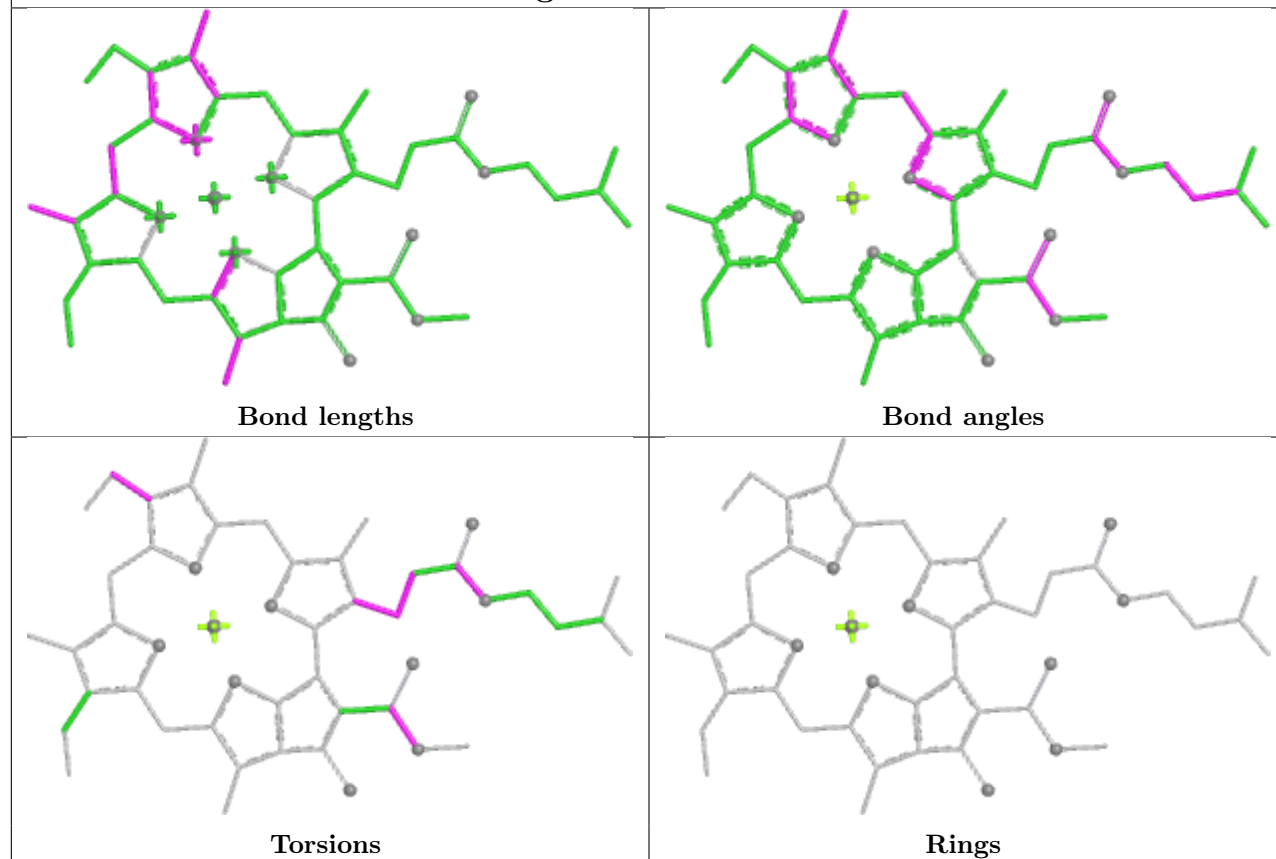




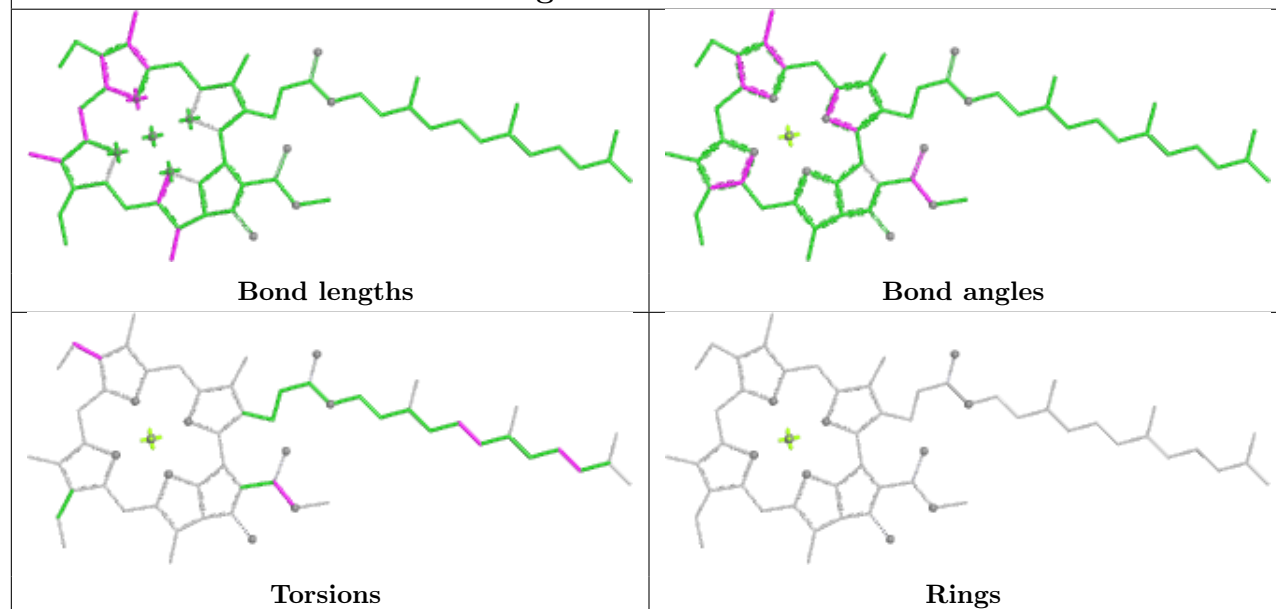


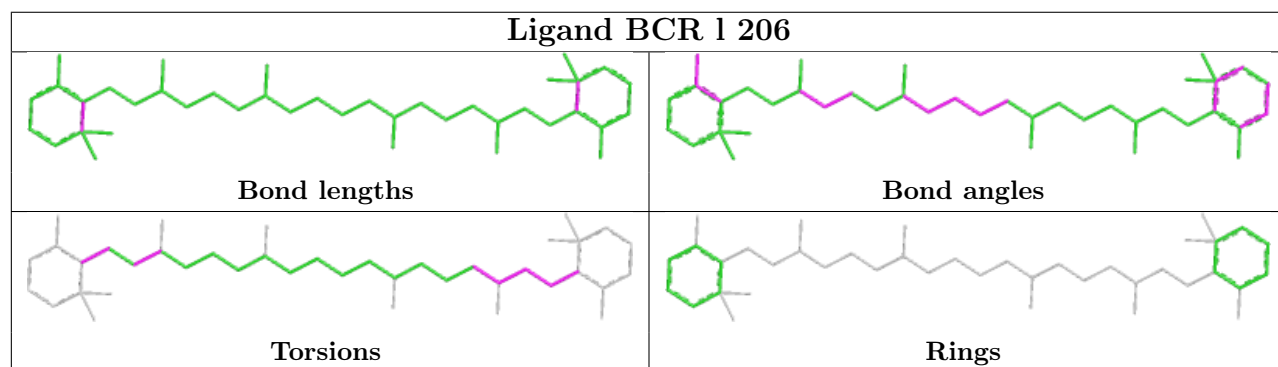
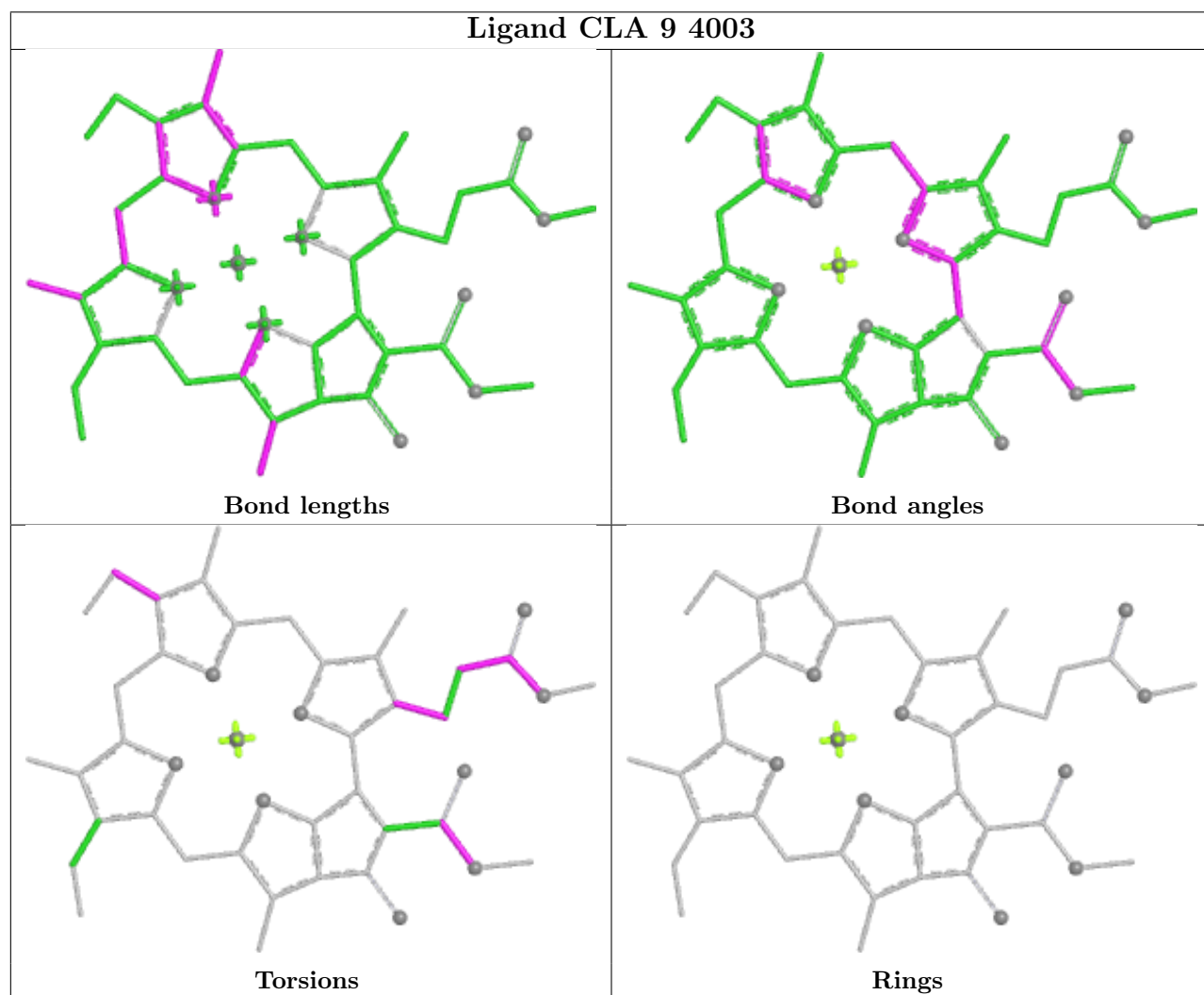
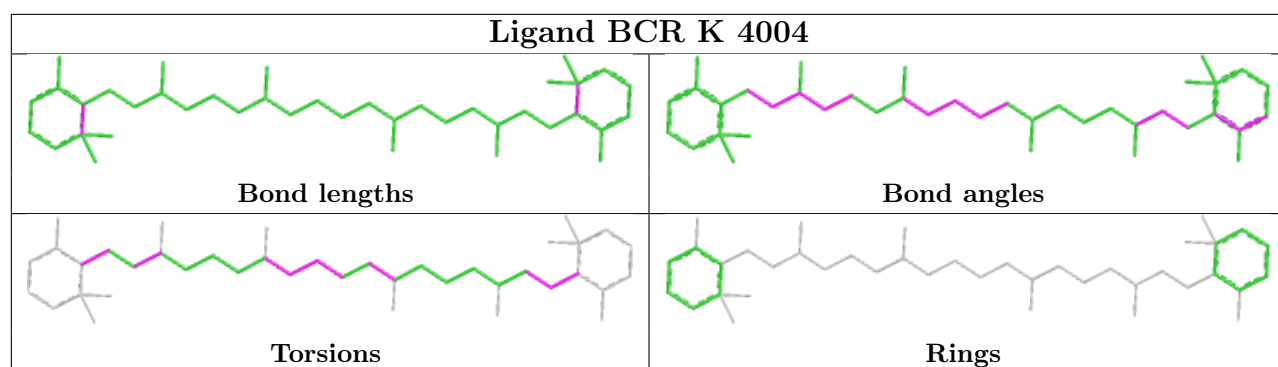


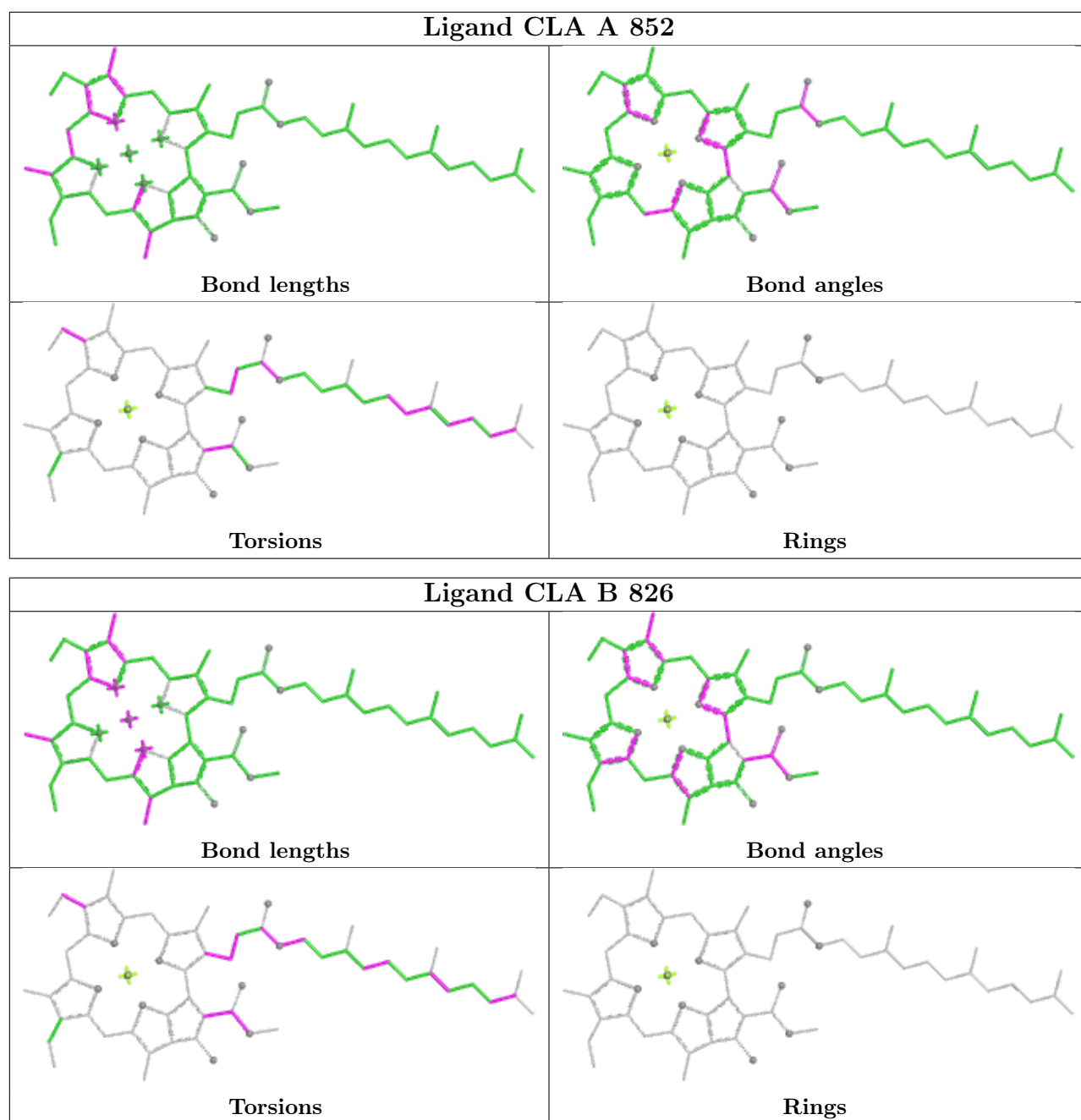
Ligand CLA a 809

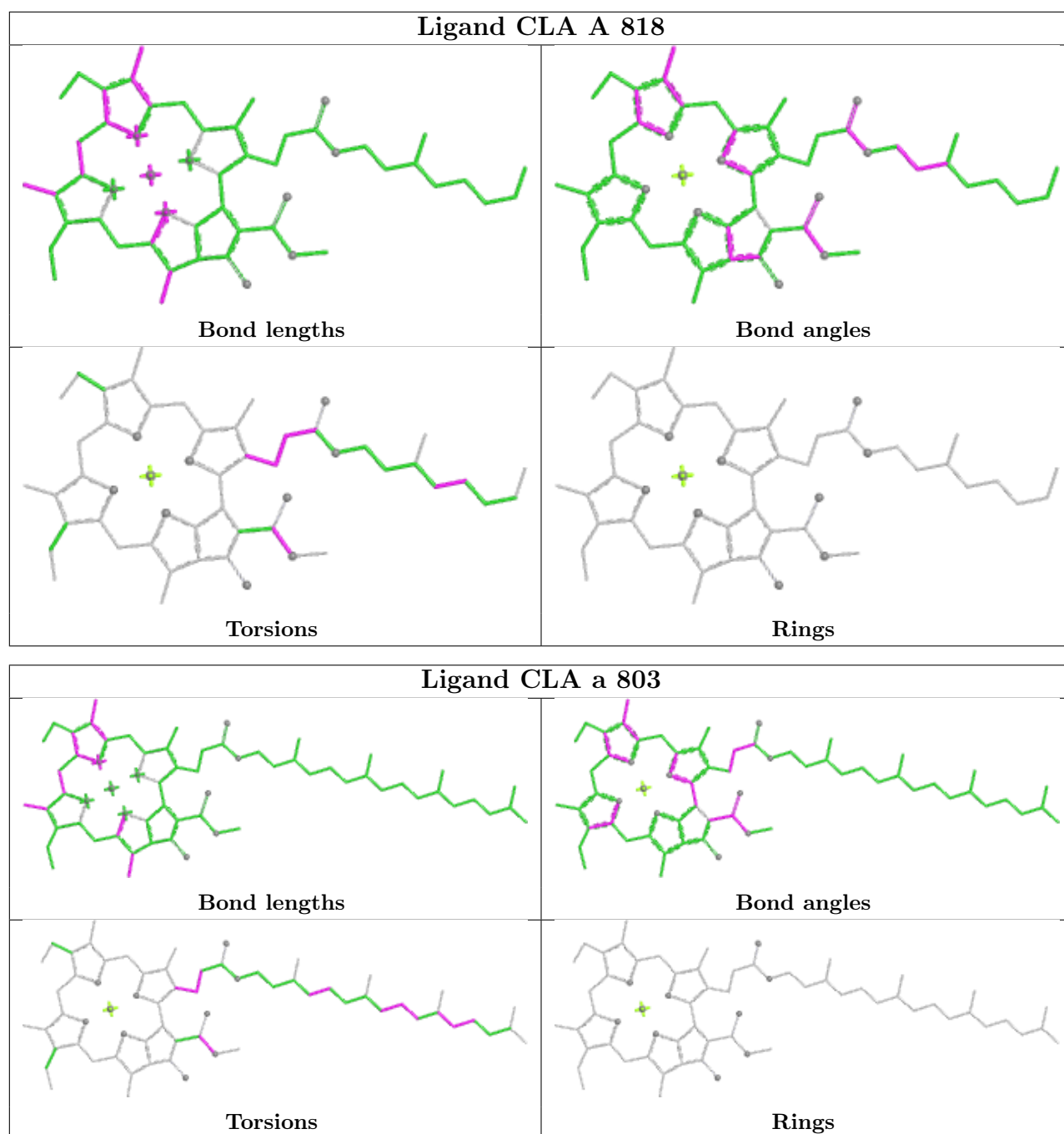


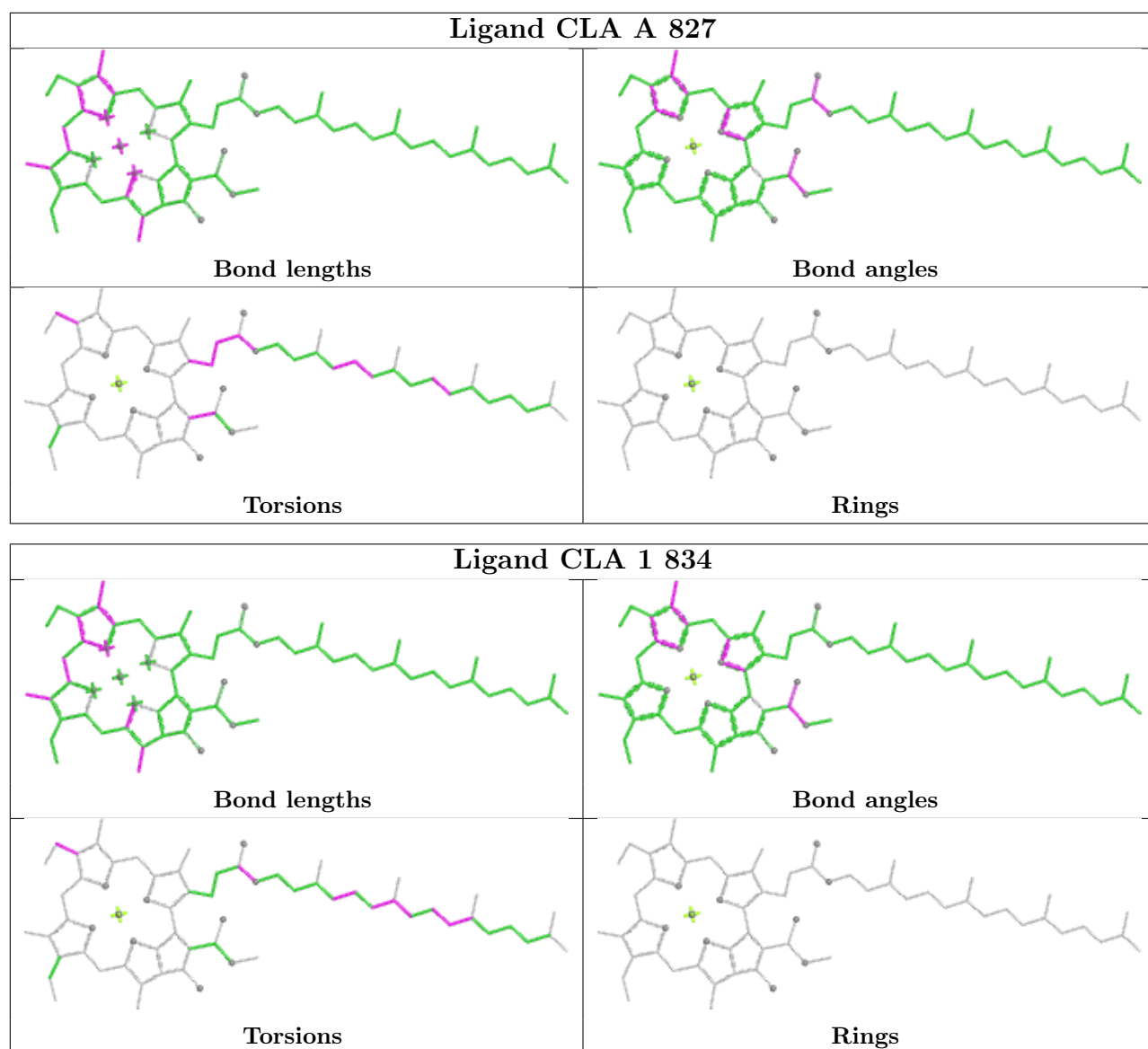
Ligand CLA 2 833

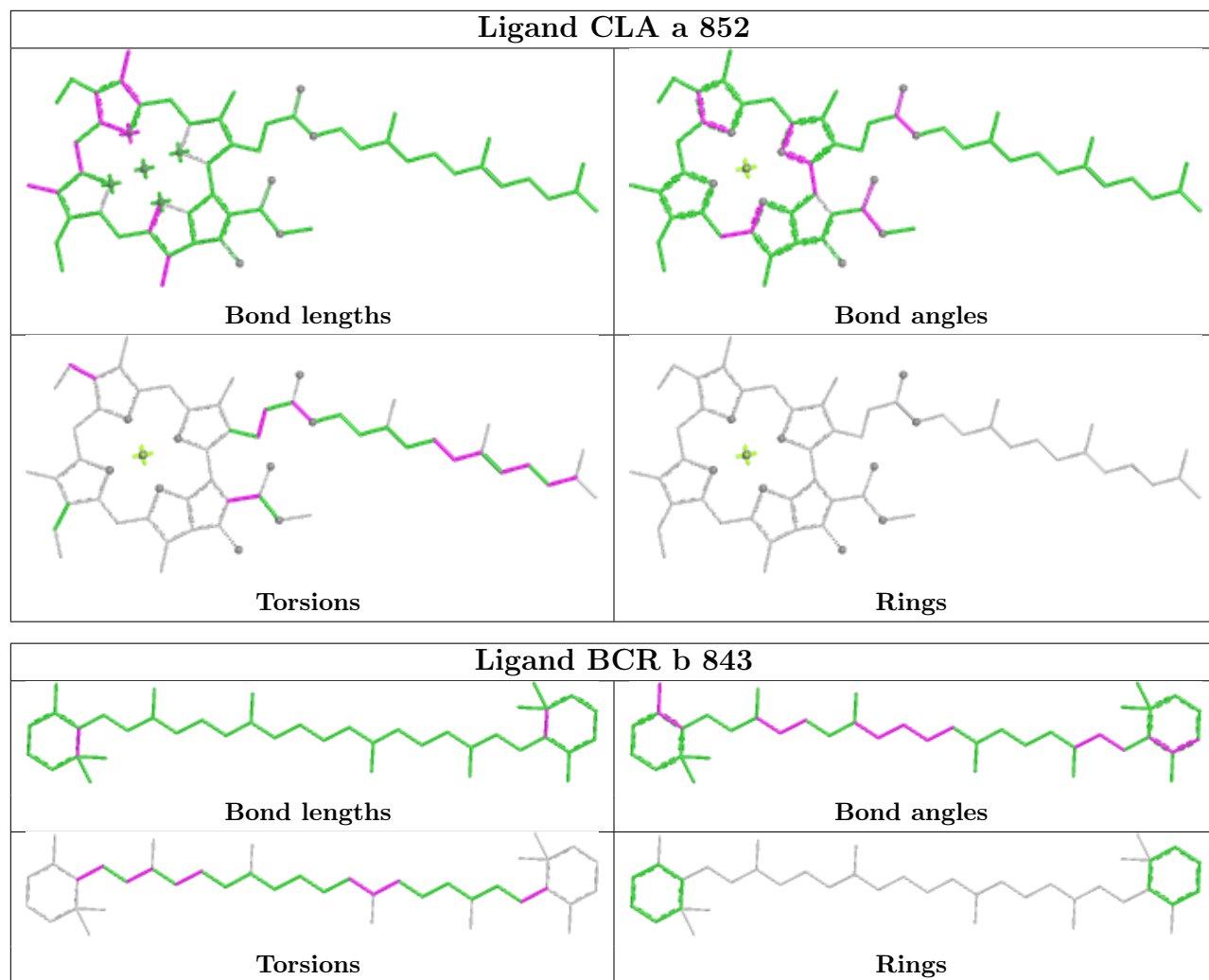




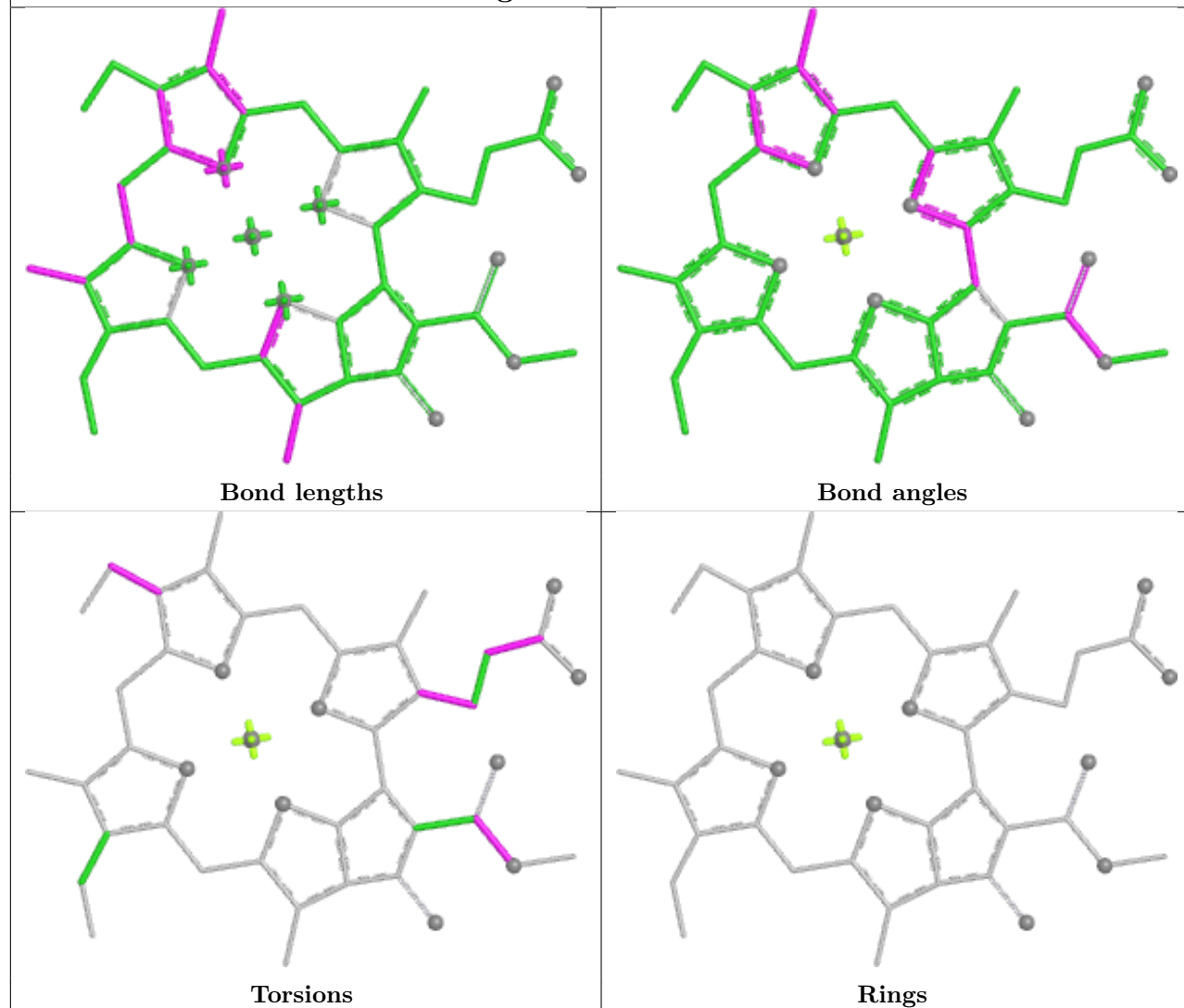




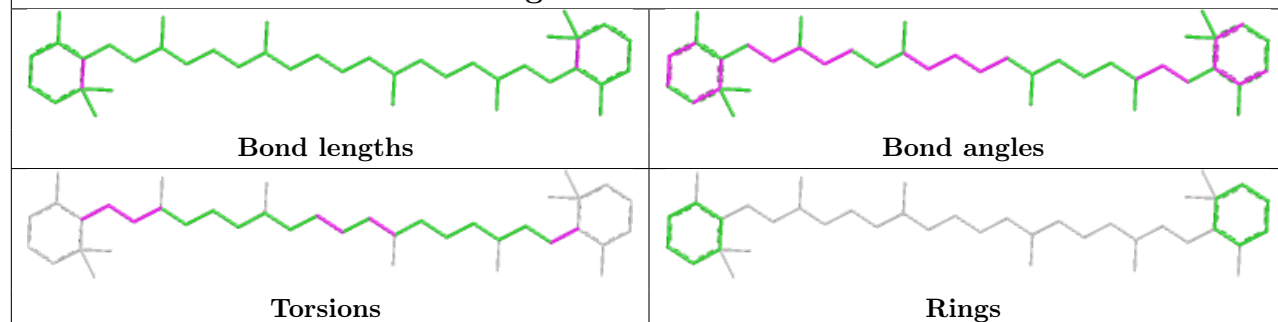


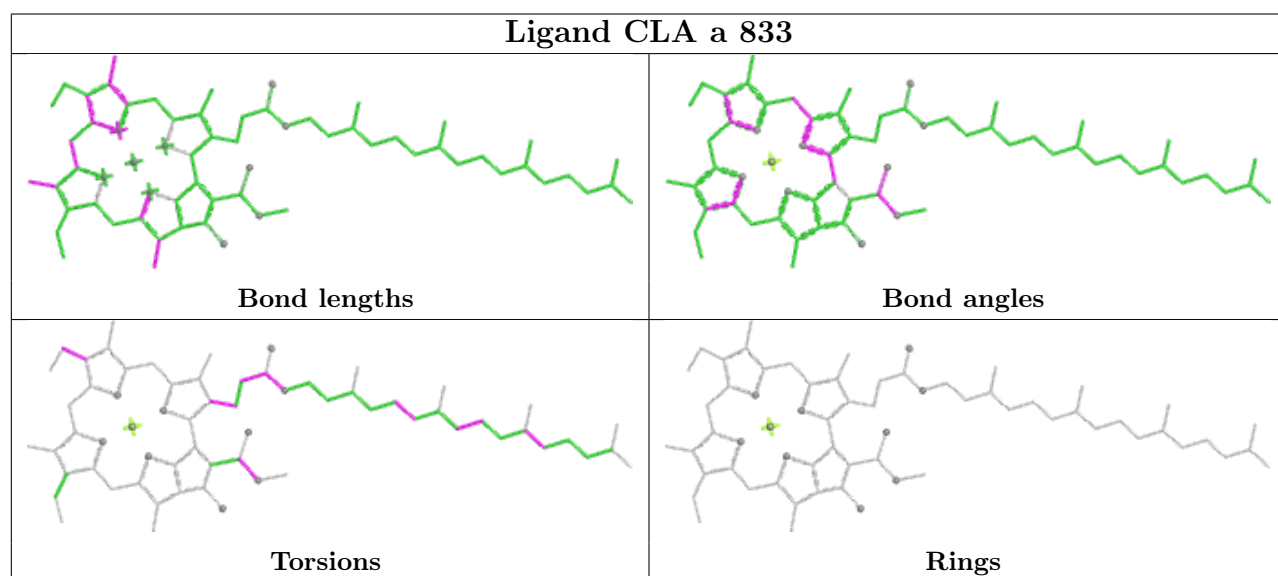
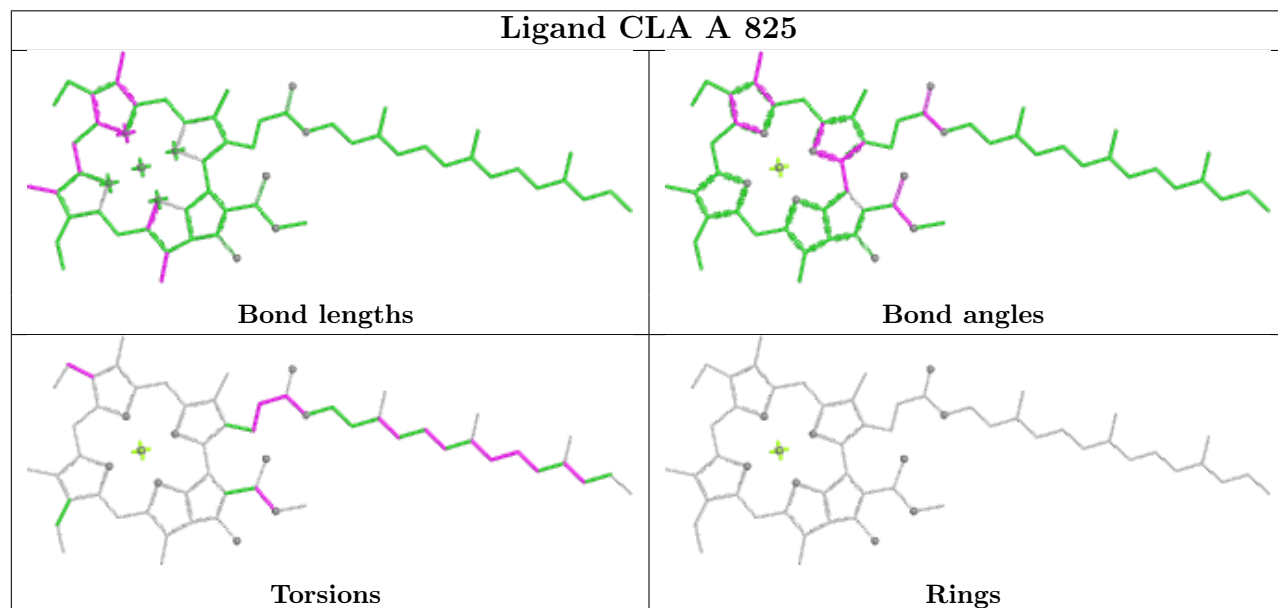
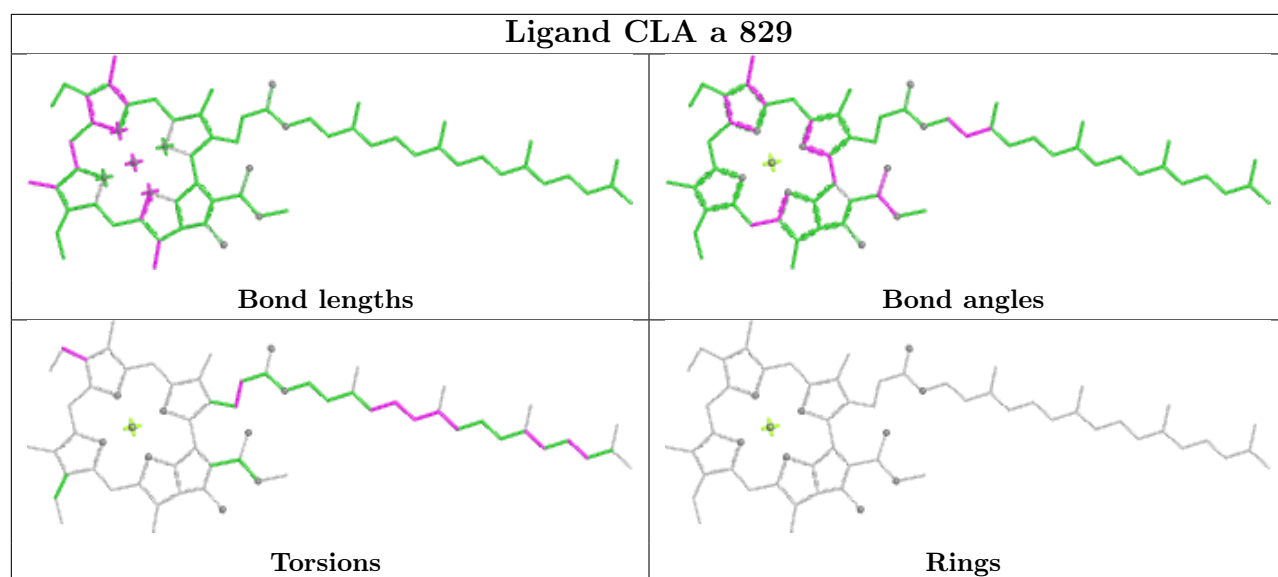


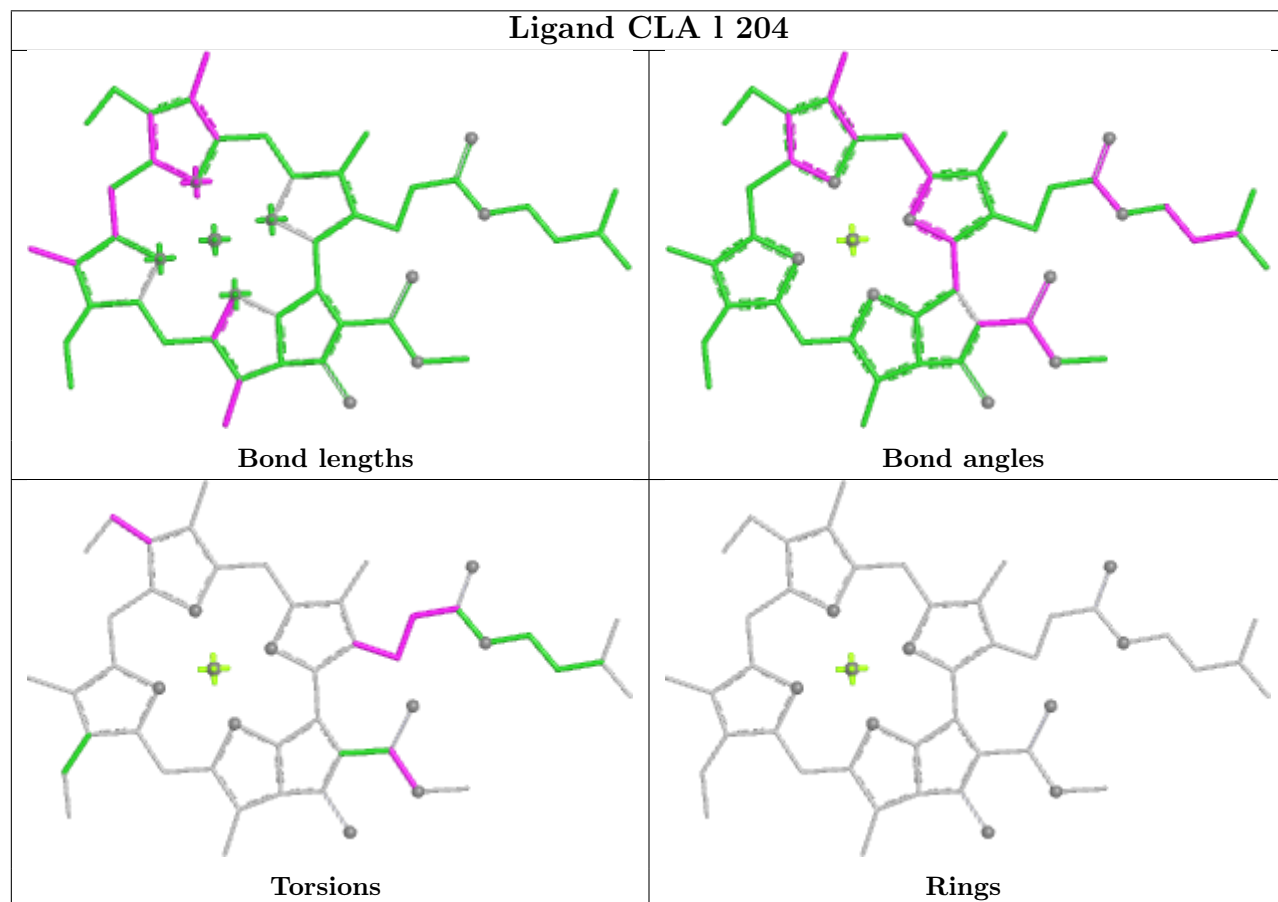
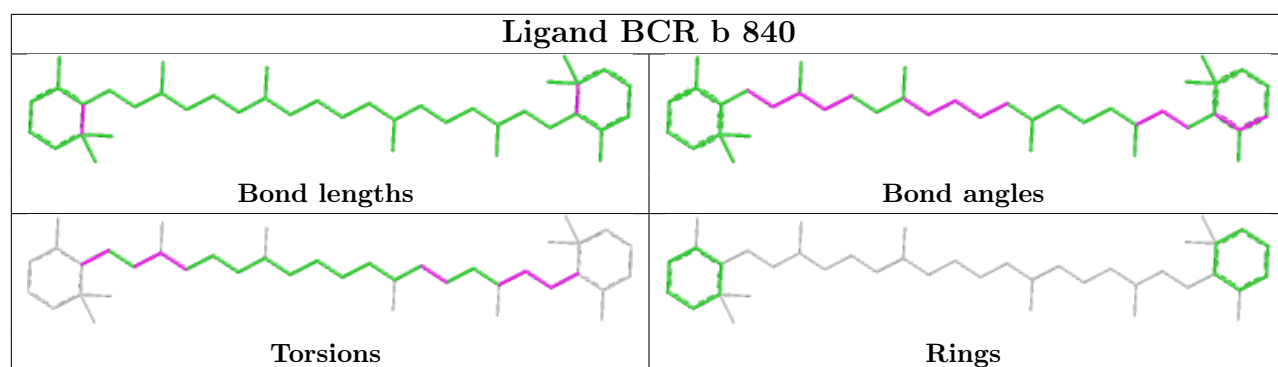
Ligand CLA 1 842



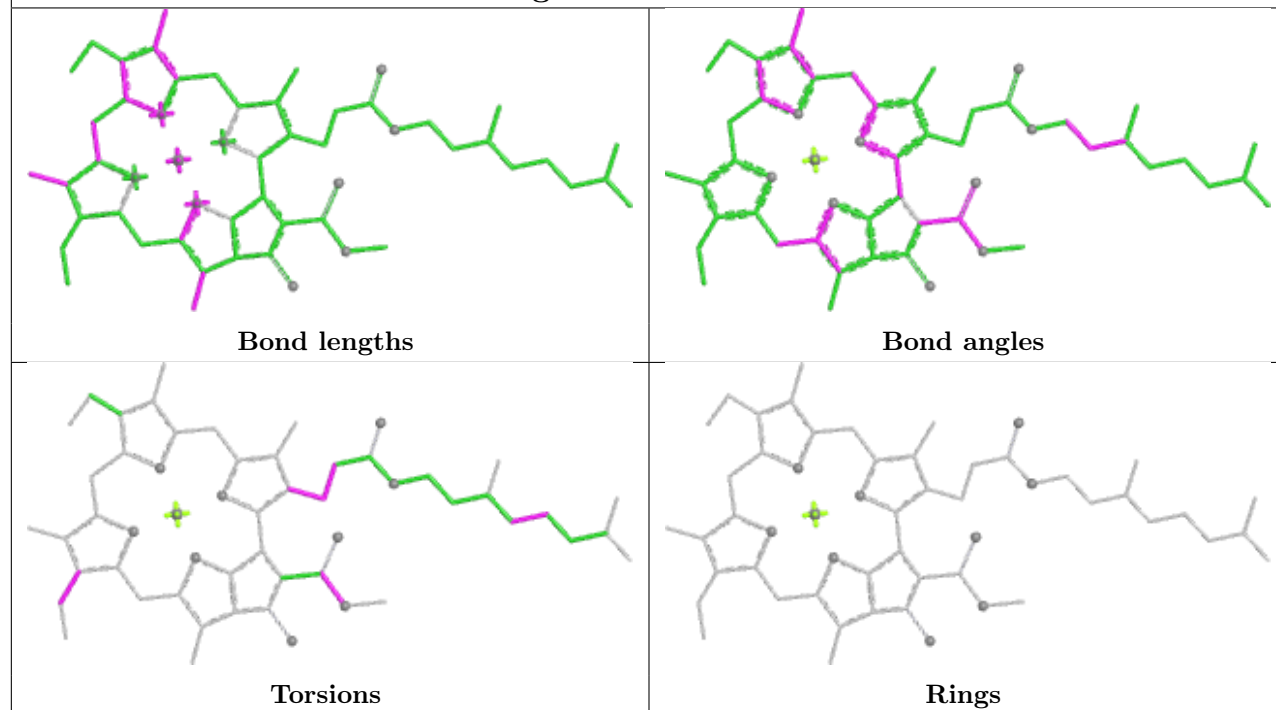
Ligand BCR 8 1104



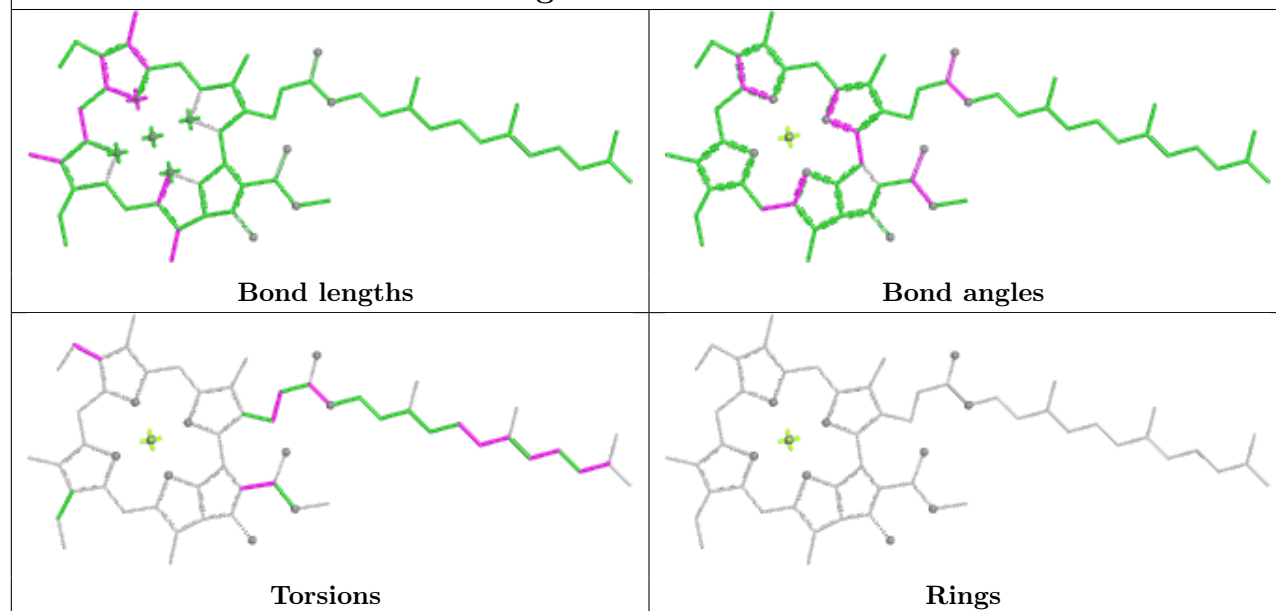




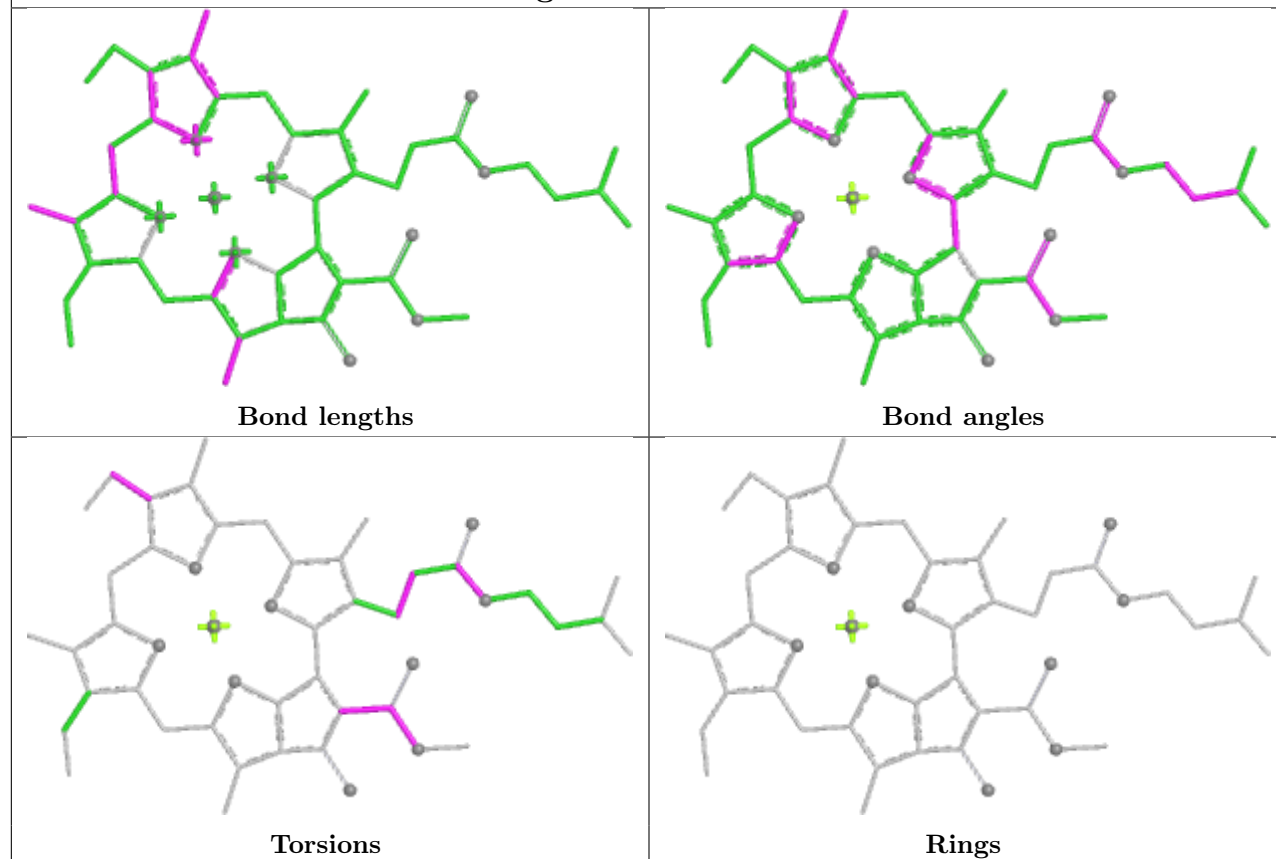
Ligand CLA B 824



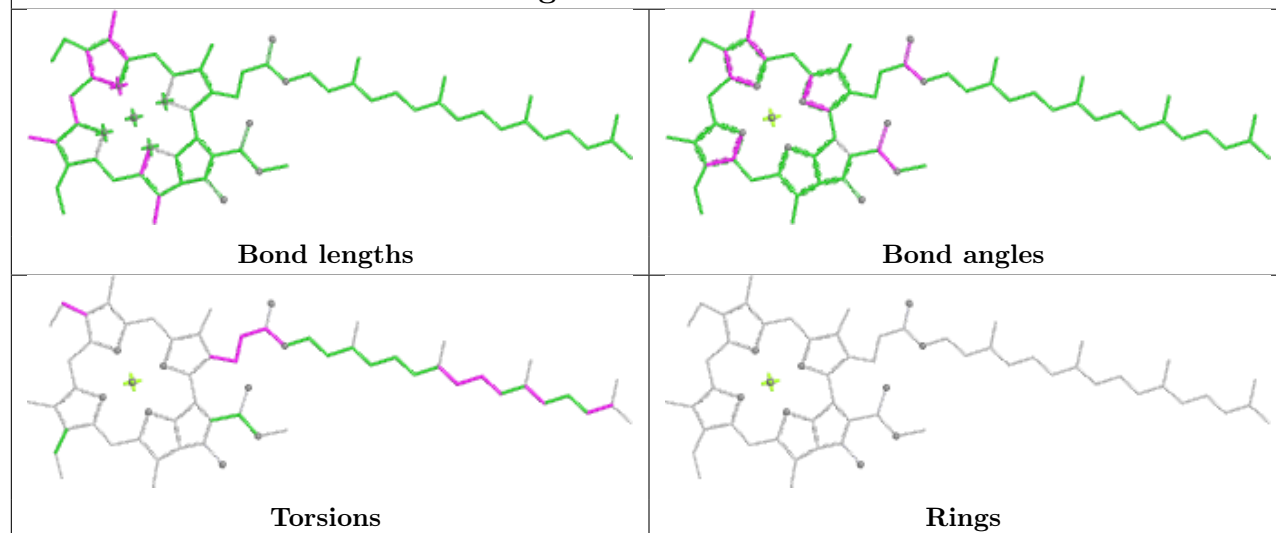
Ligand CLA 1 852

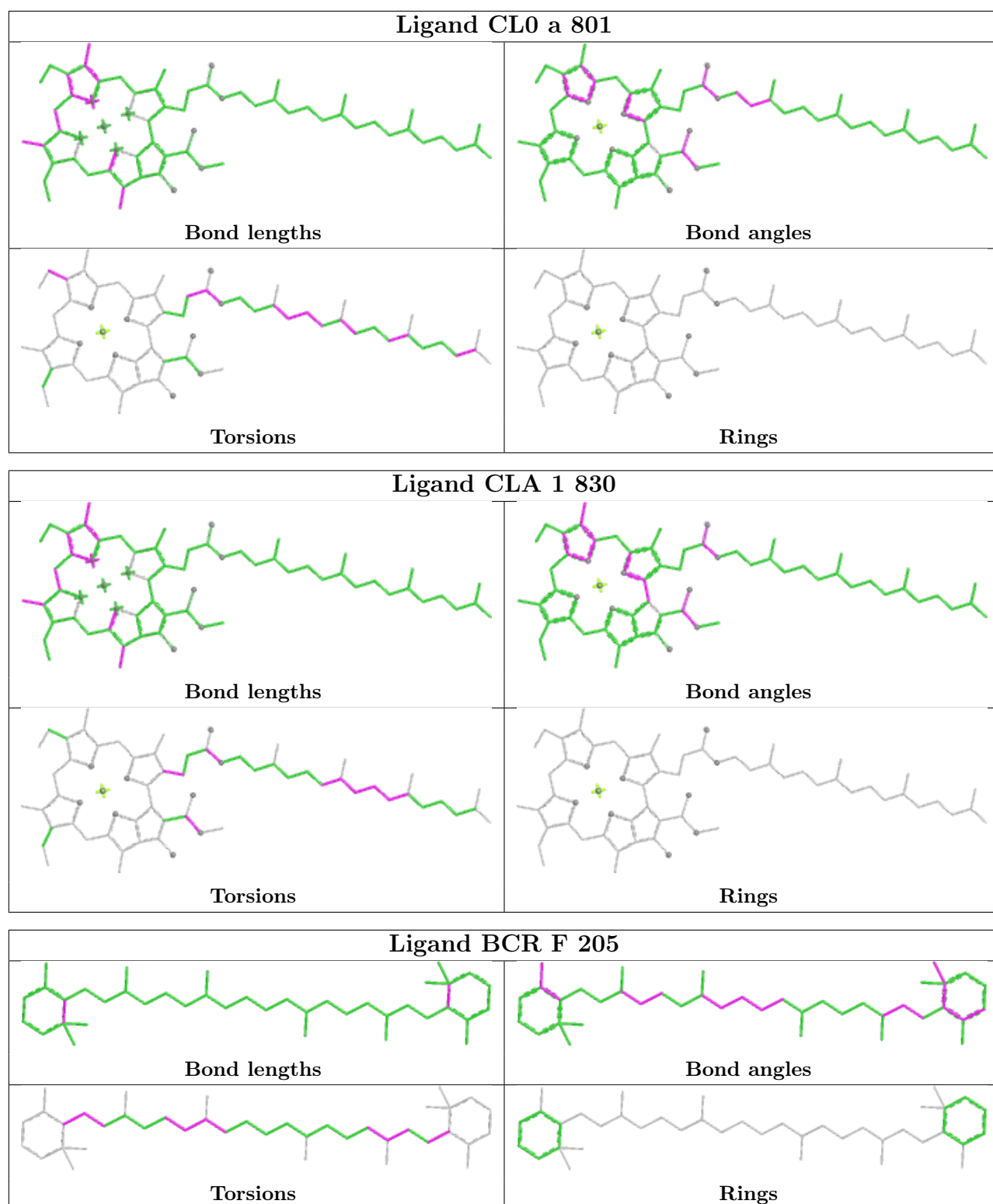


Ligand CLA a 822

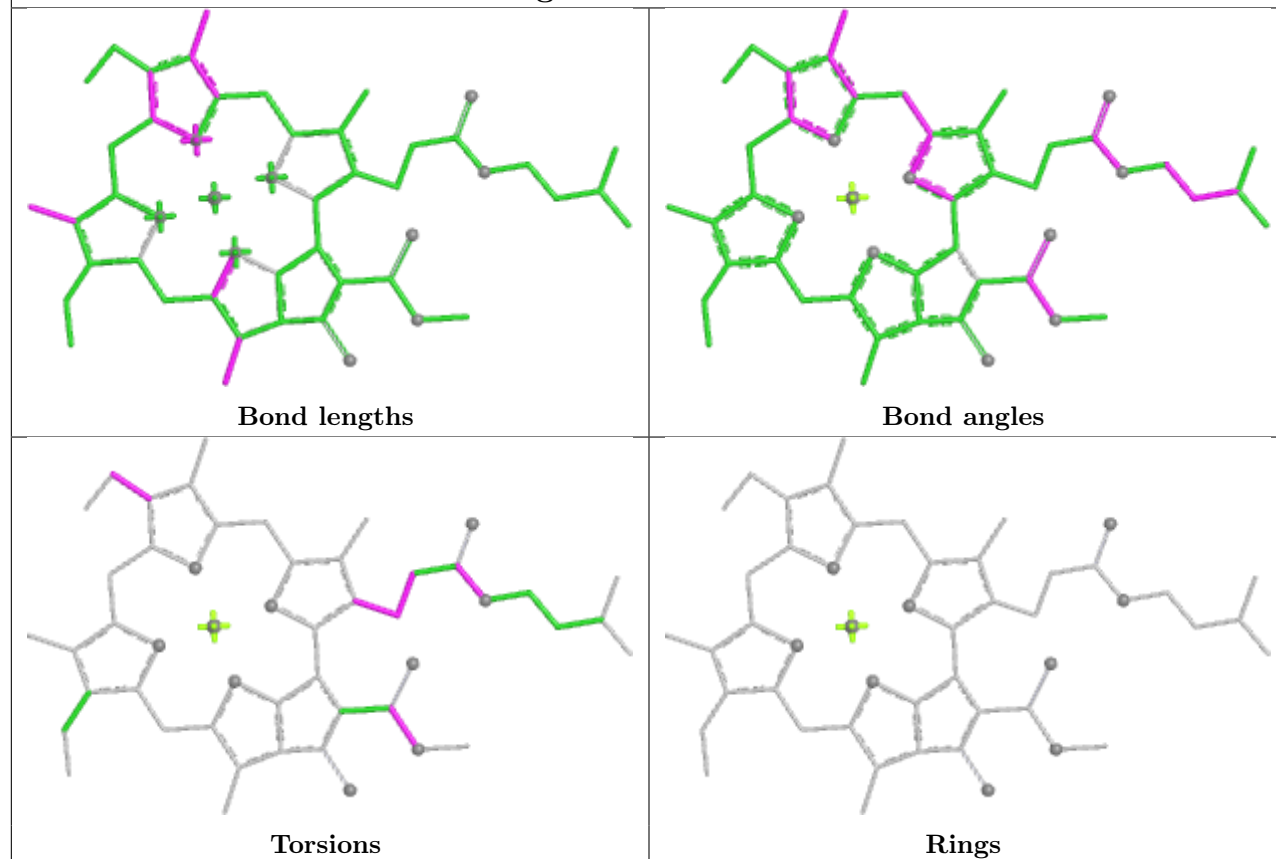


Ligand CLA I 101

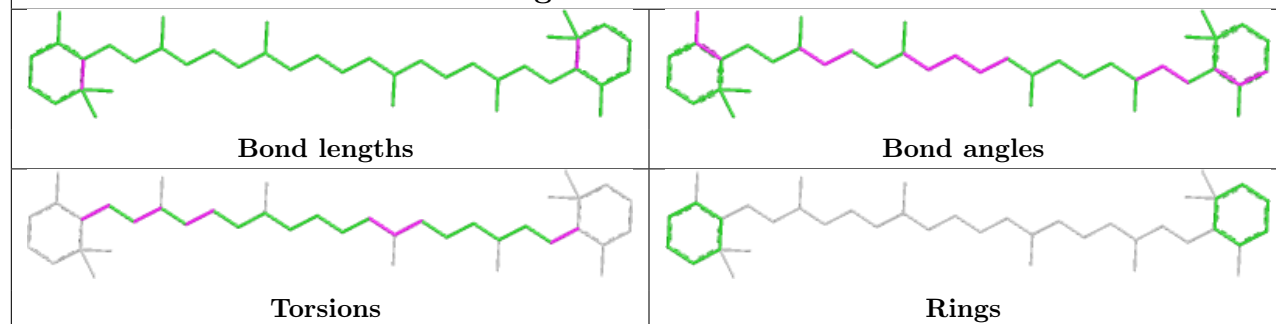


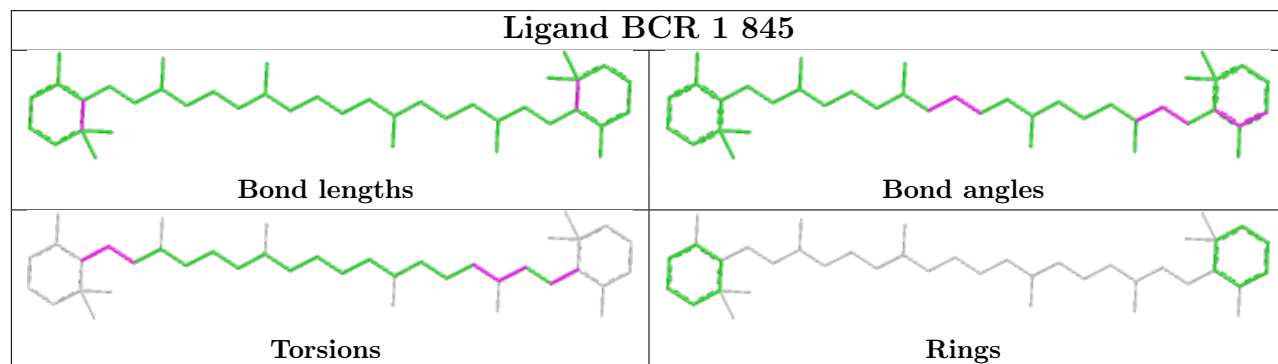
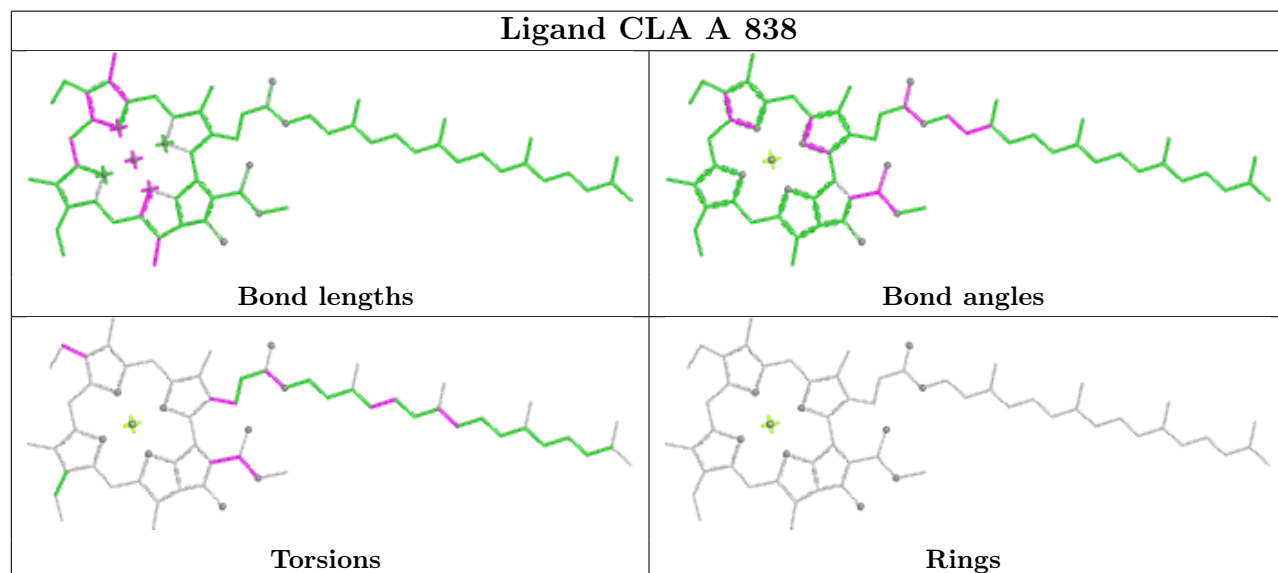
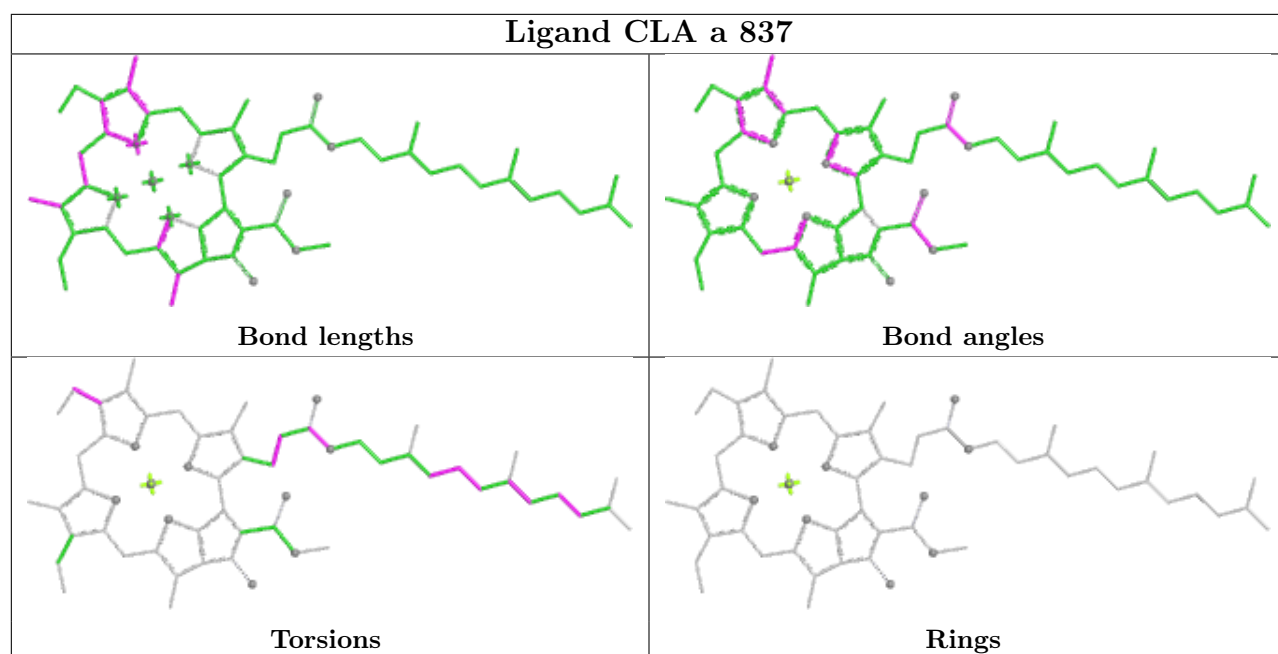


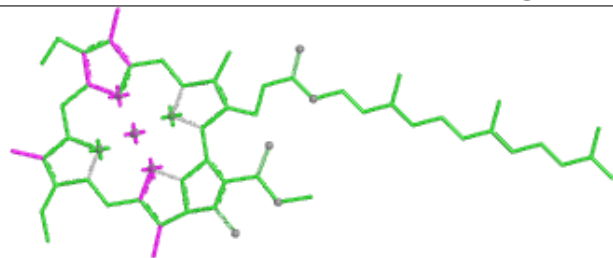
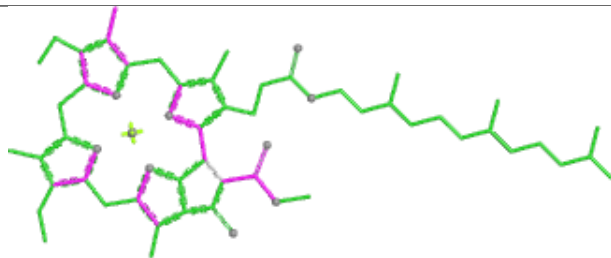
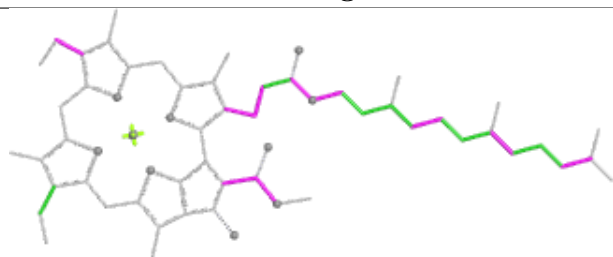
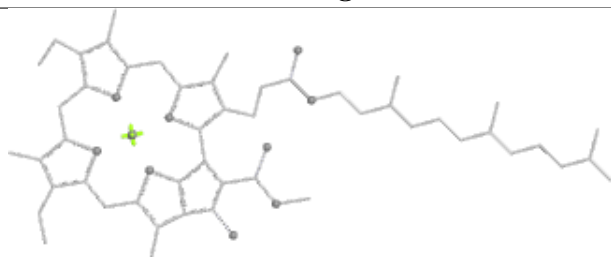
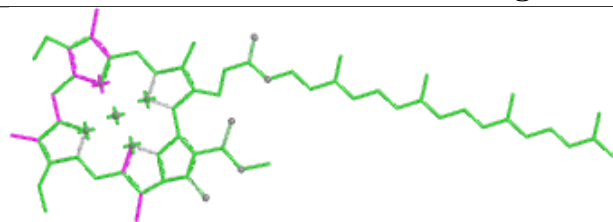
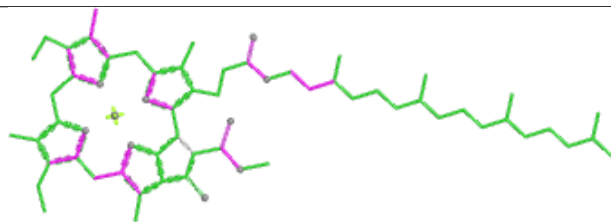
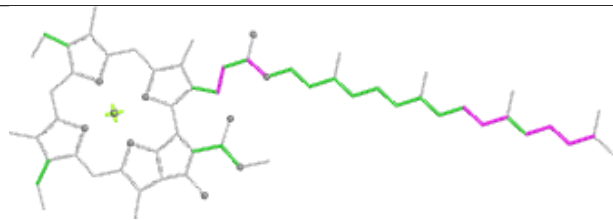
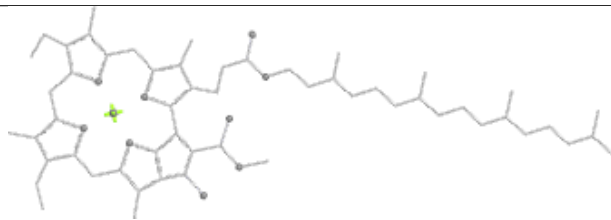
Ligand CLA 1 809

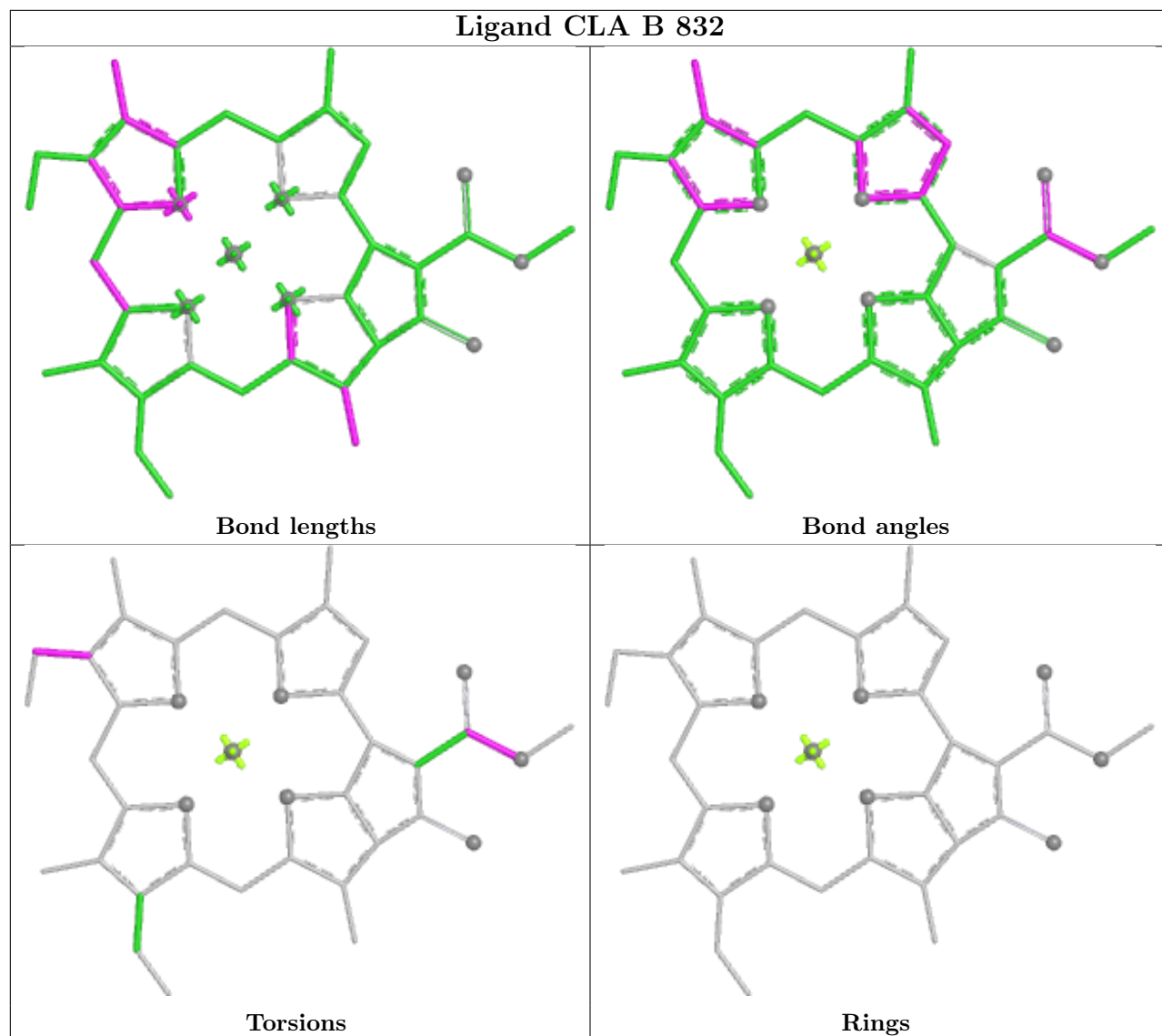


Ligand BCR 2 842

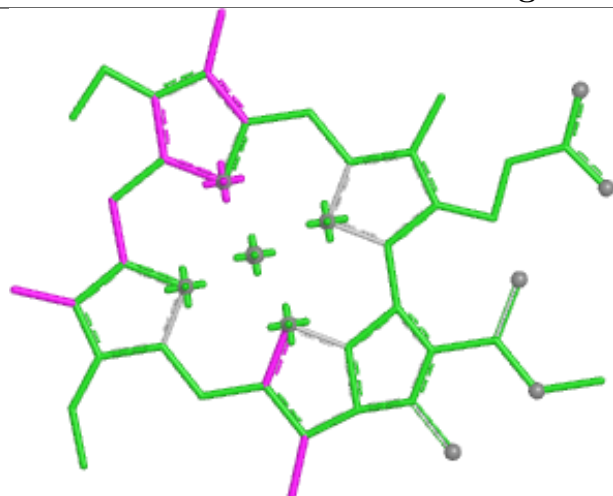




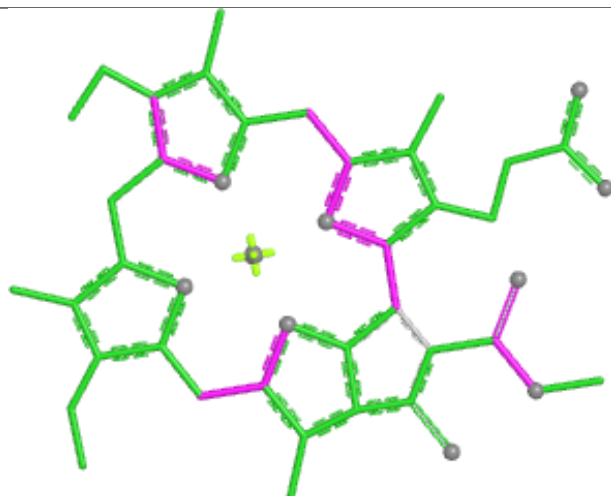
Ligand CLA 2 825**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 839****Bond lengths****Bond angles****Torsions****Rings**



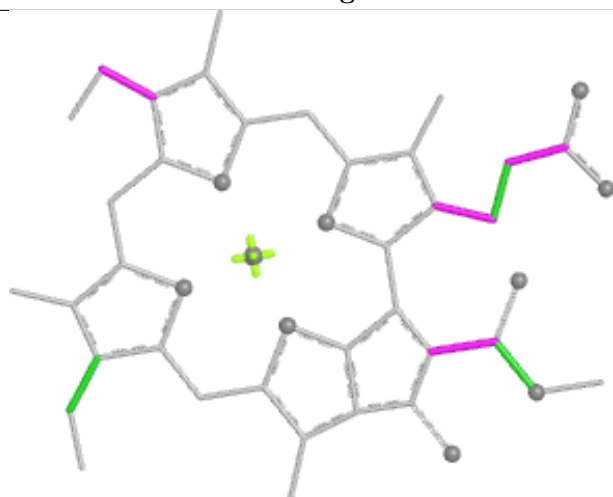
Ligand CLA 2 826



Bond lengths



Bond angles

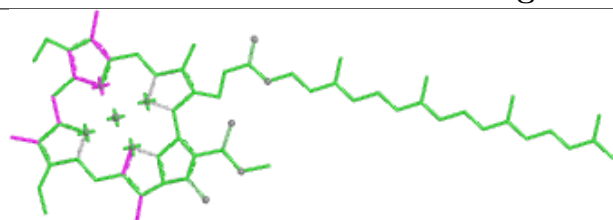


Torsions

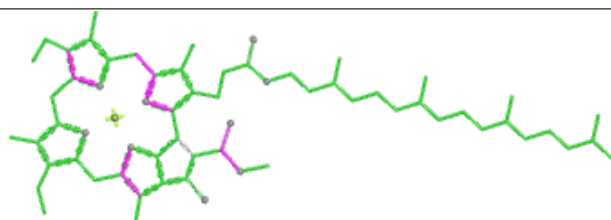


Rings

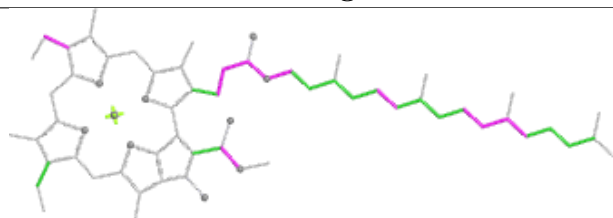
Ligand CLA b 807



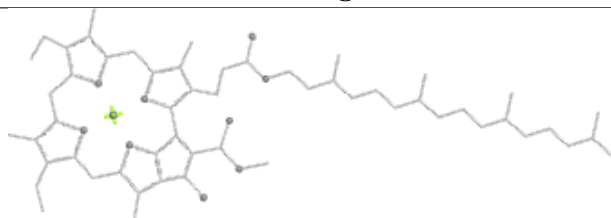
Bond lengths



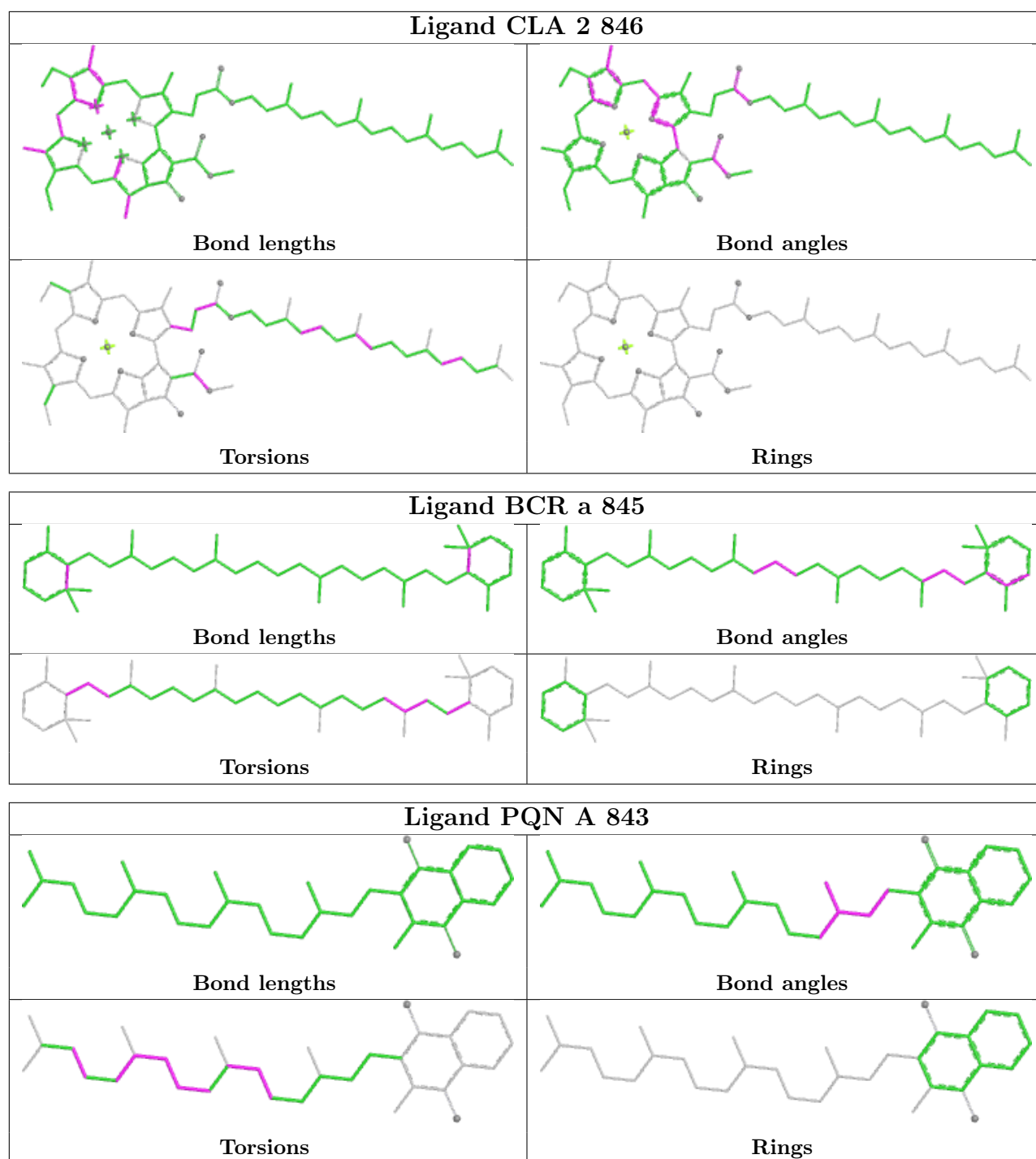
Bond angles

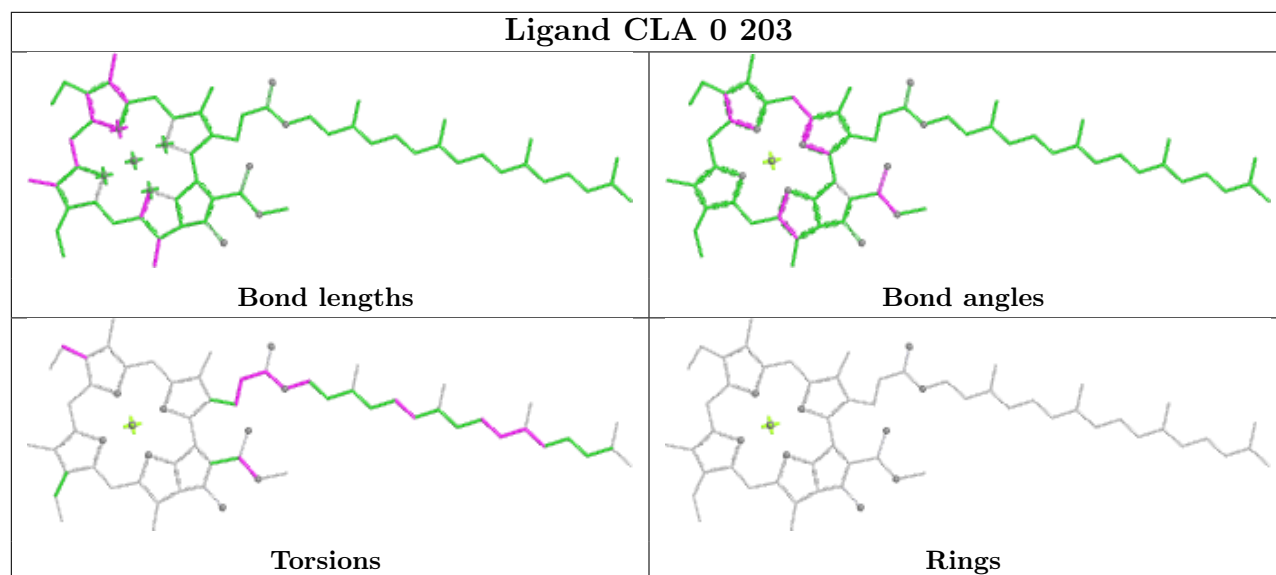
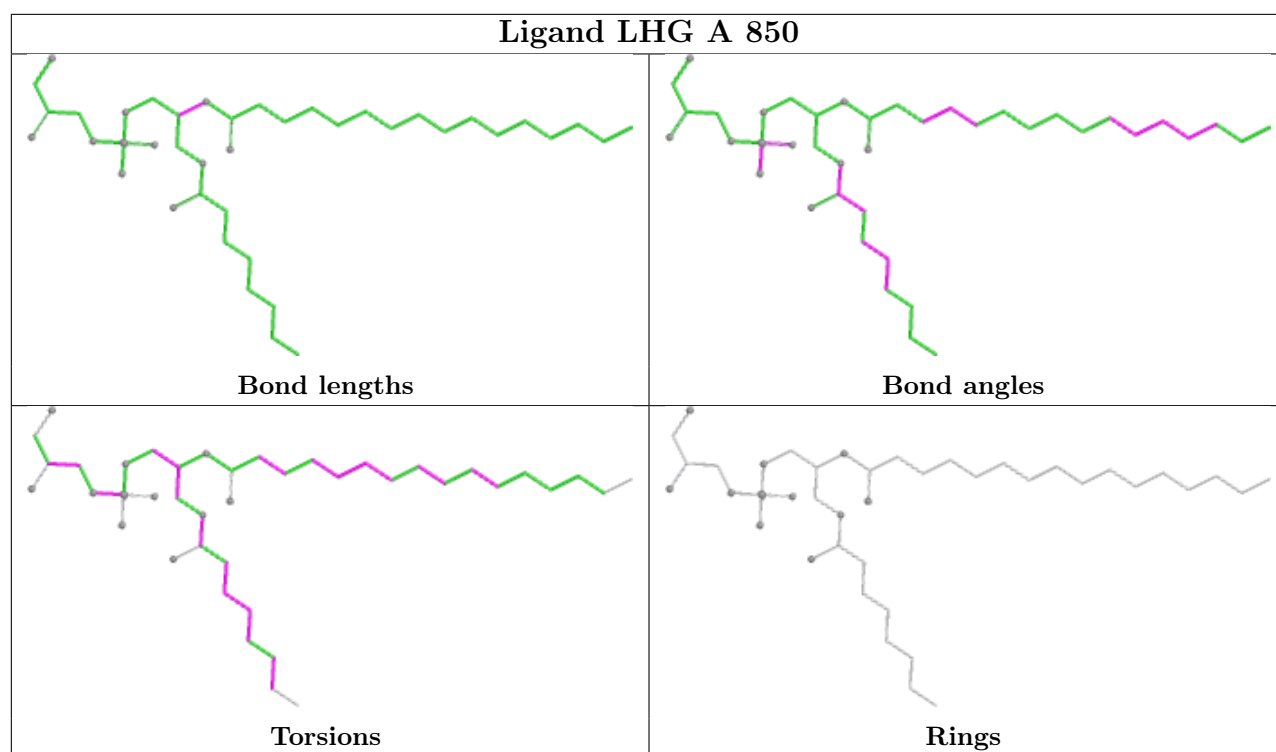


Torsions

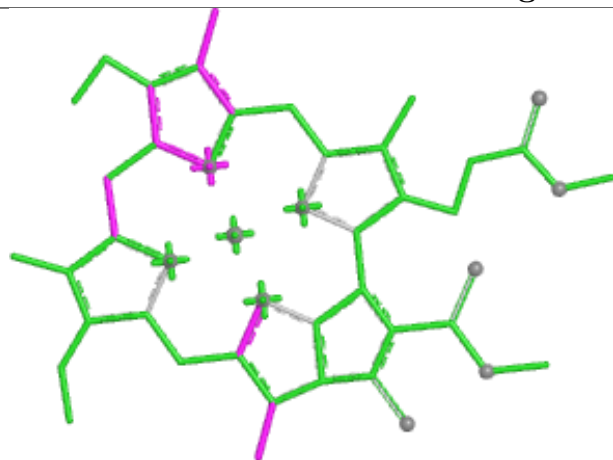


Rings

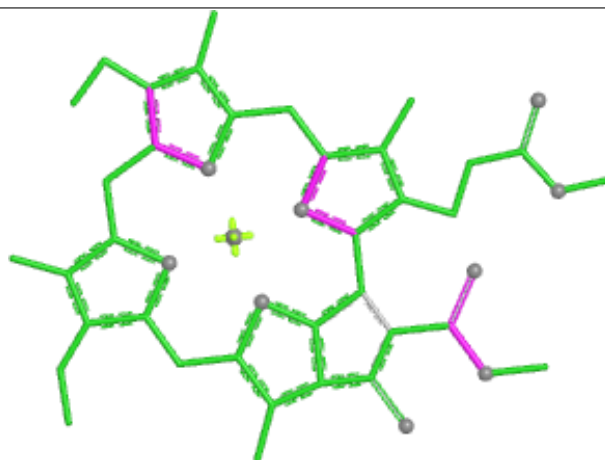




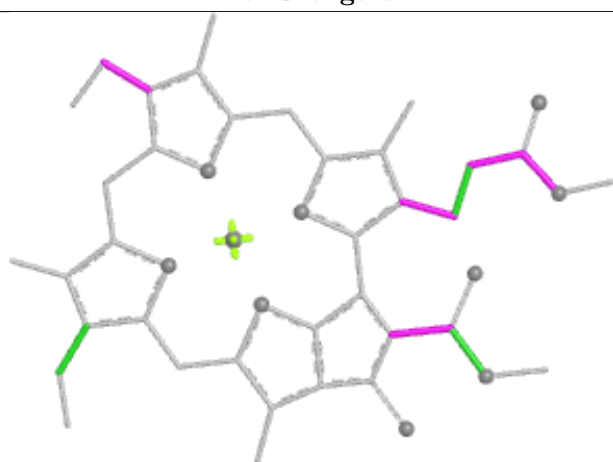
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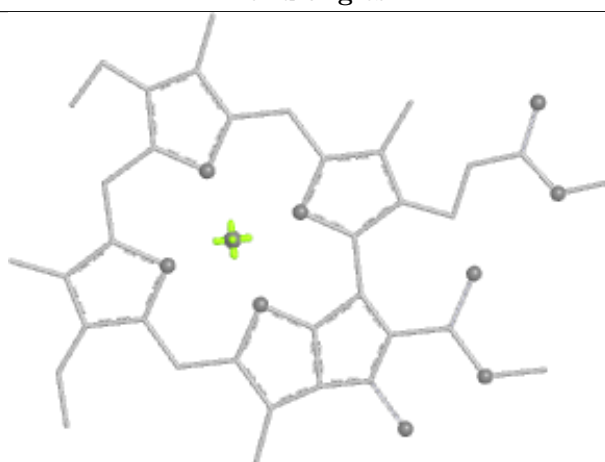
Bond lengths



Bond angles

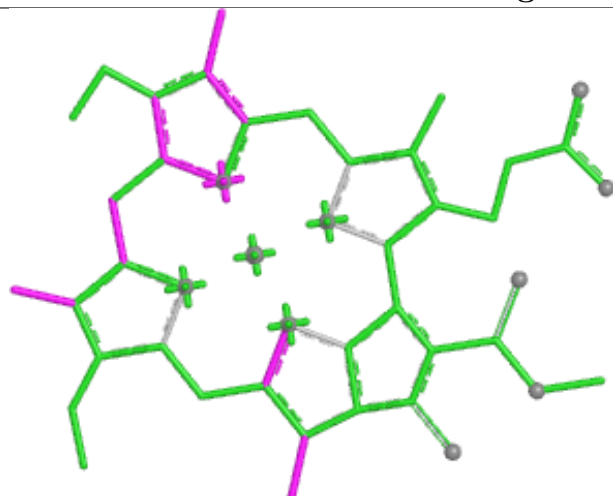


Torsions

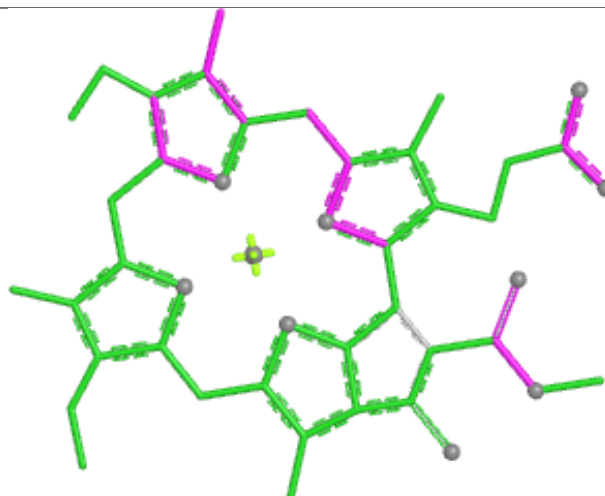


Rings

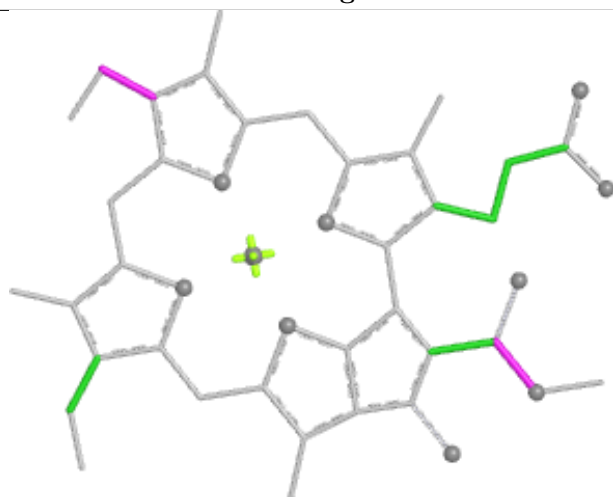
Ligand CLA b 812



Bond lengths



Bond angles

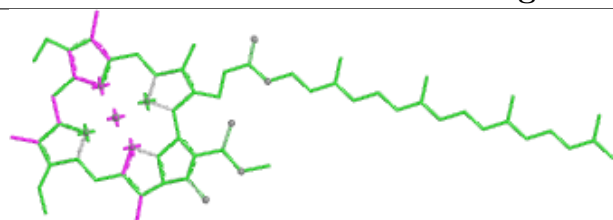


Torsions

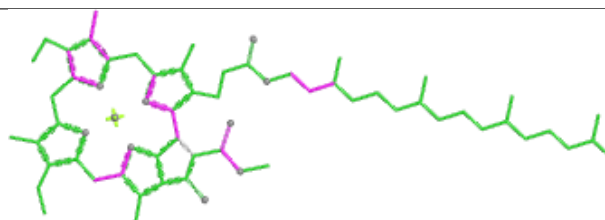


Rings

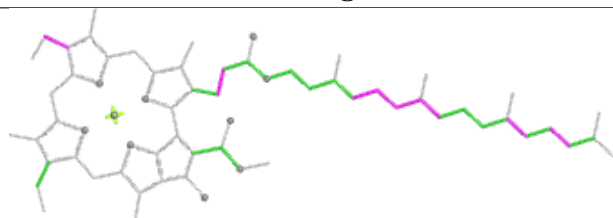
Ligand CLA 1 829



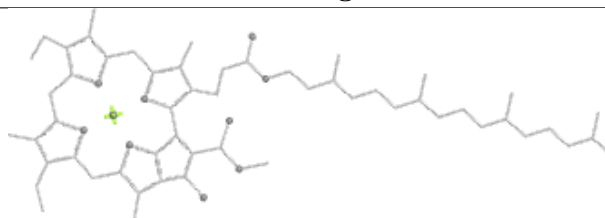
Bond lengths



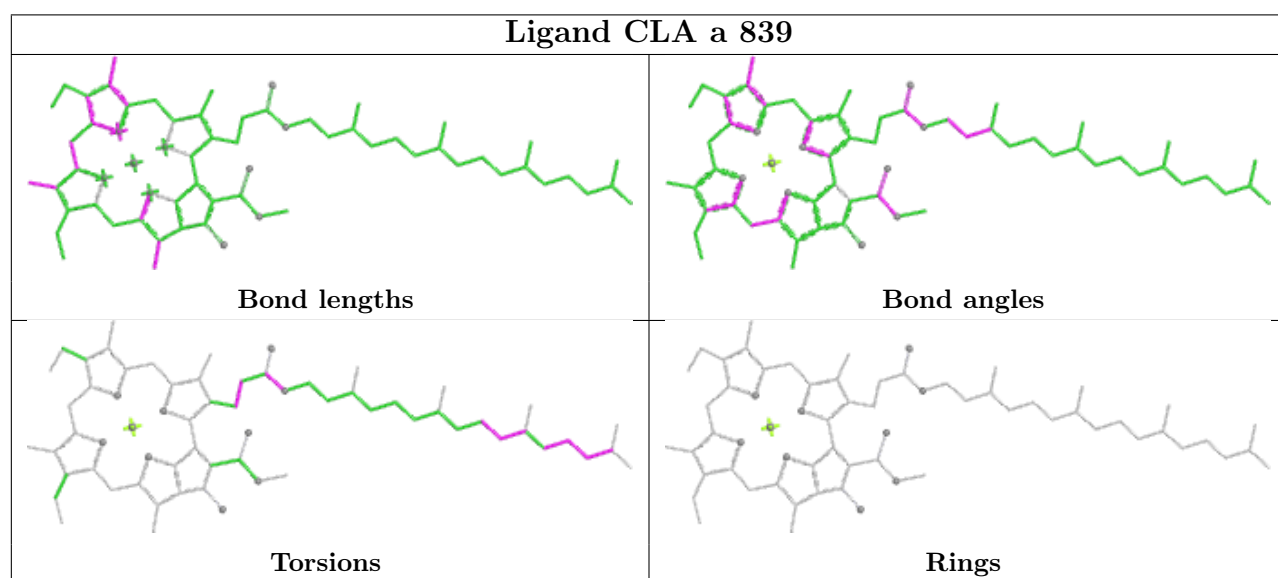
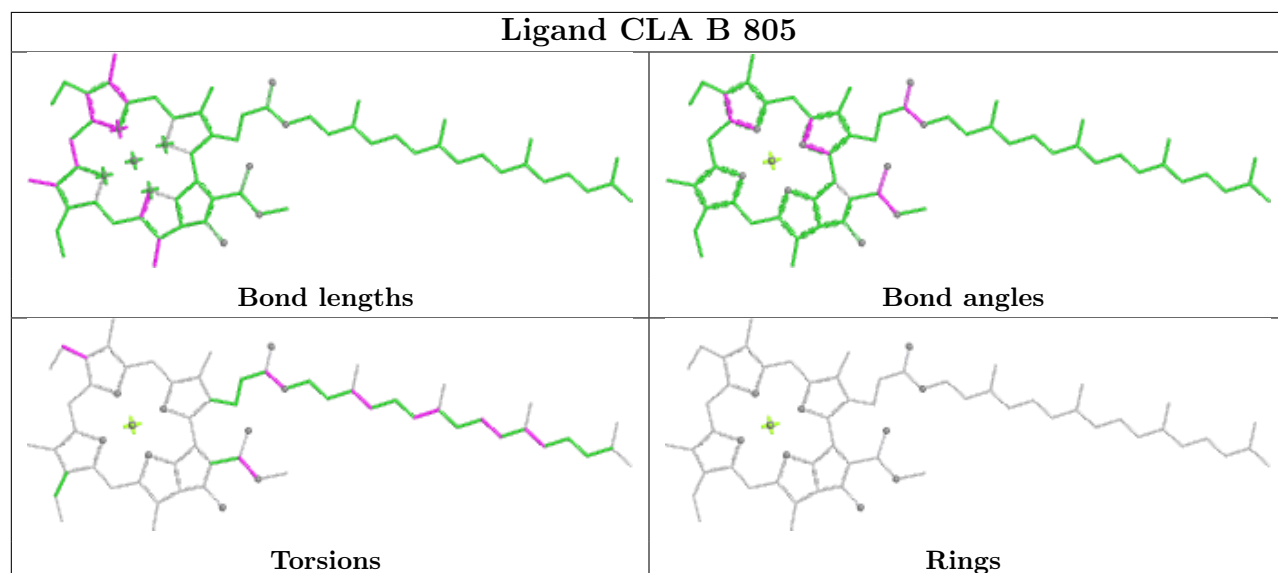
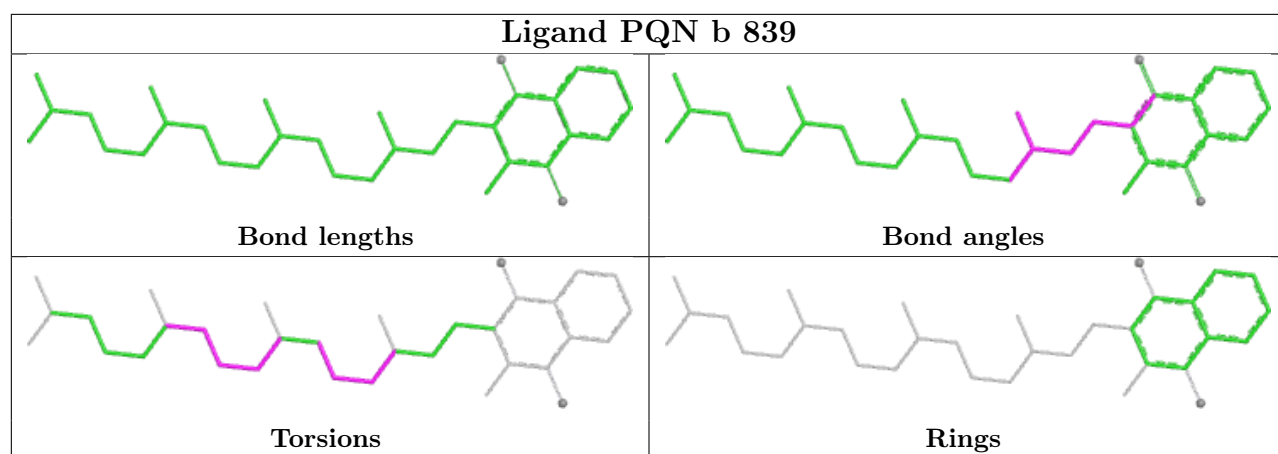
Bond angles



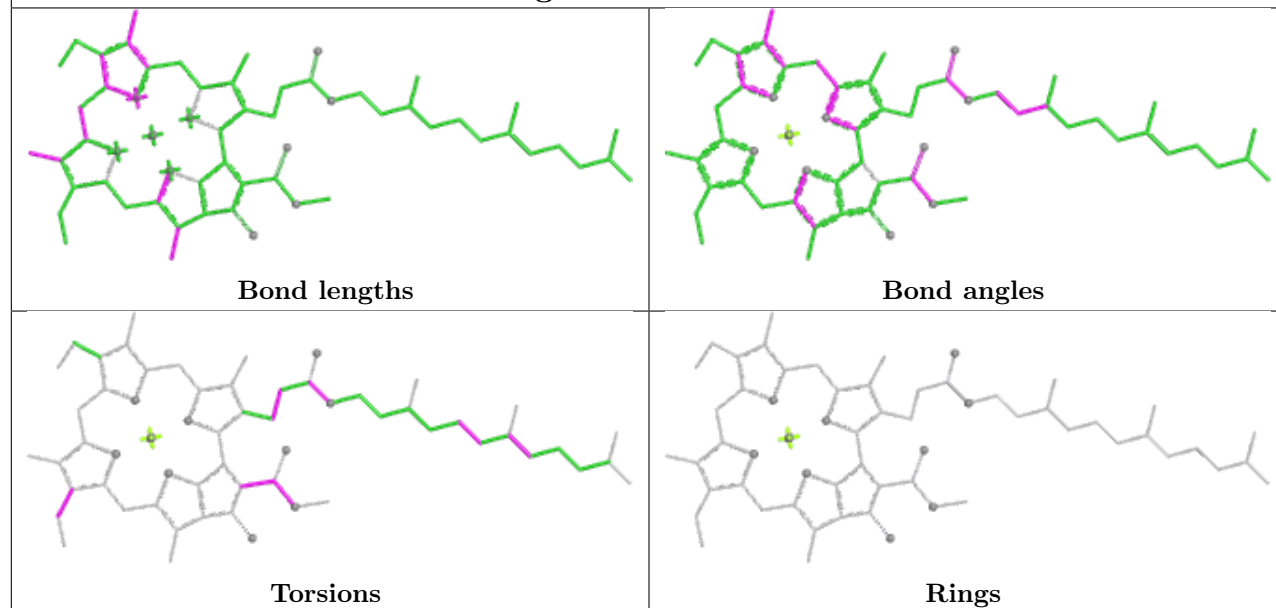
Torsions



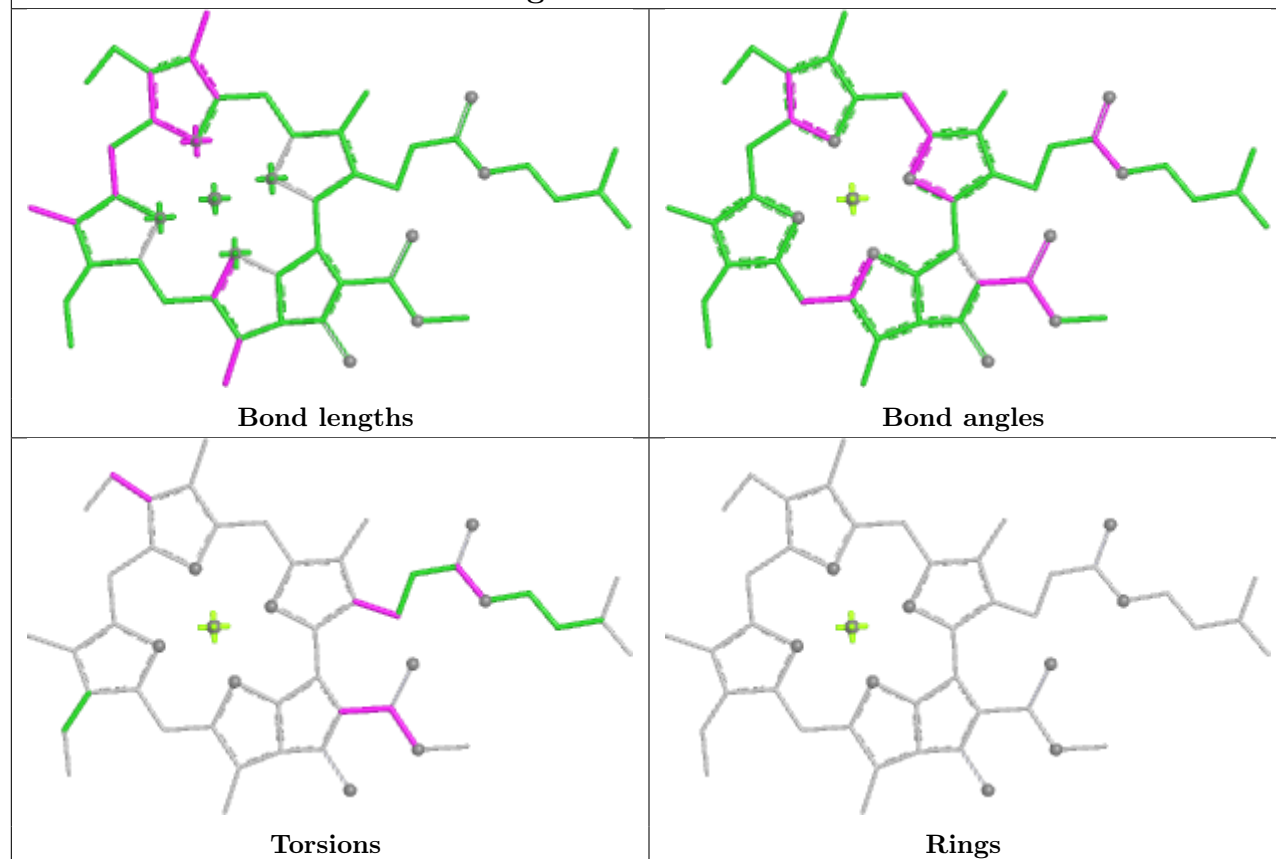
Rings

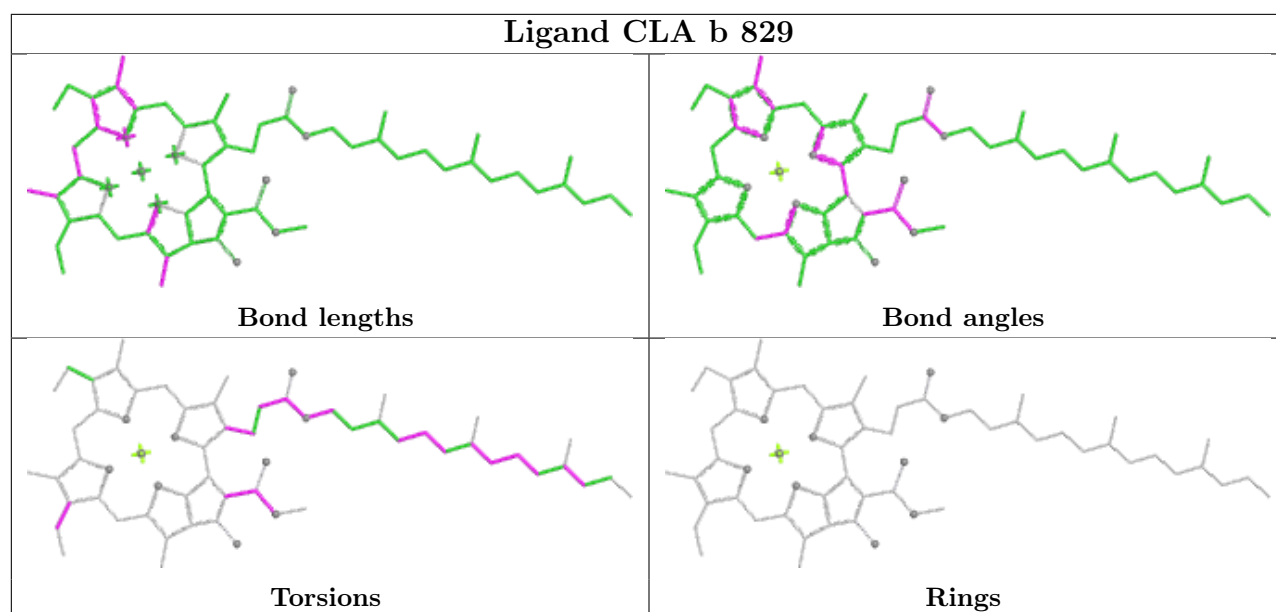
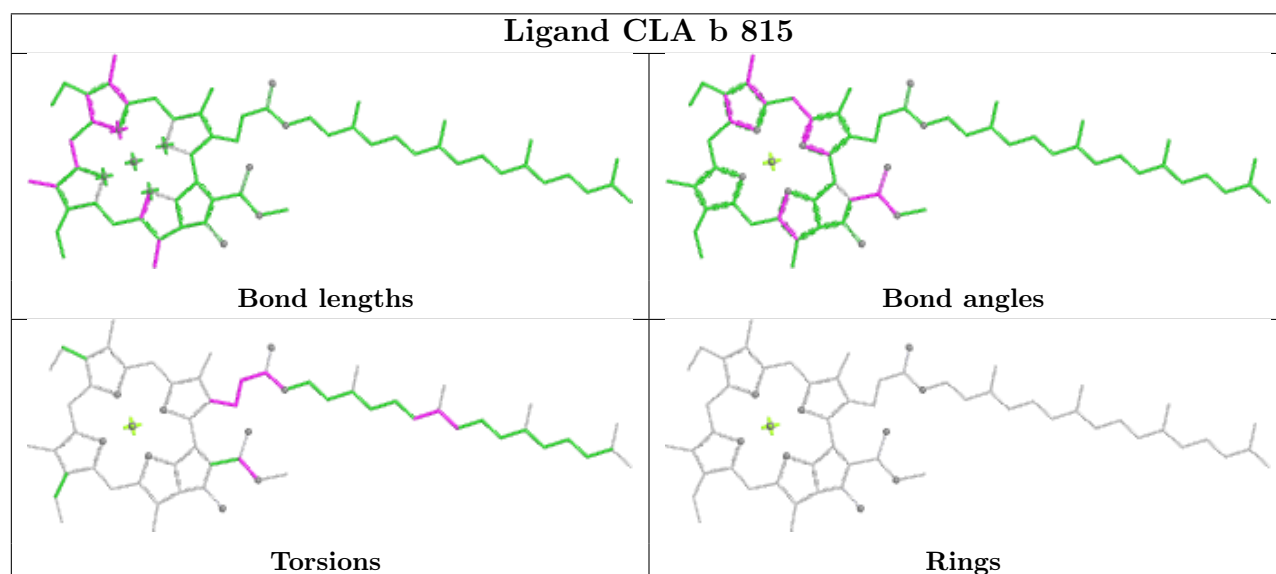
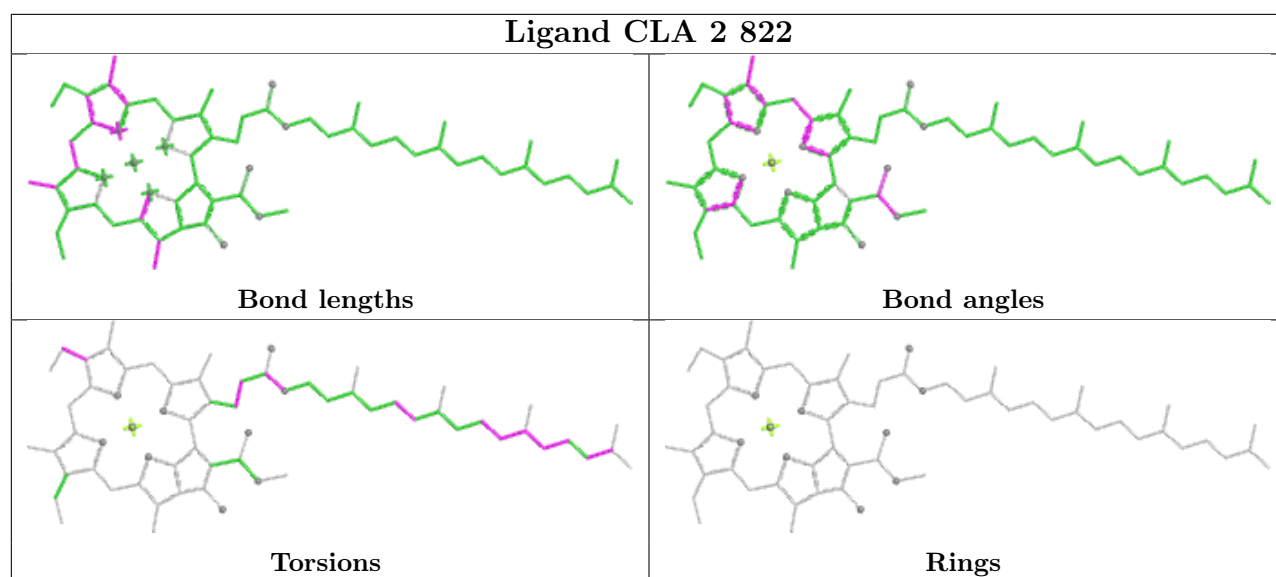


Ligand CLA b 803

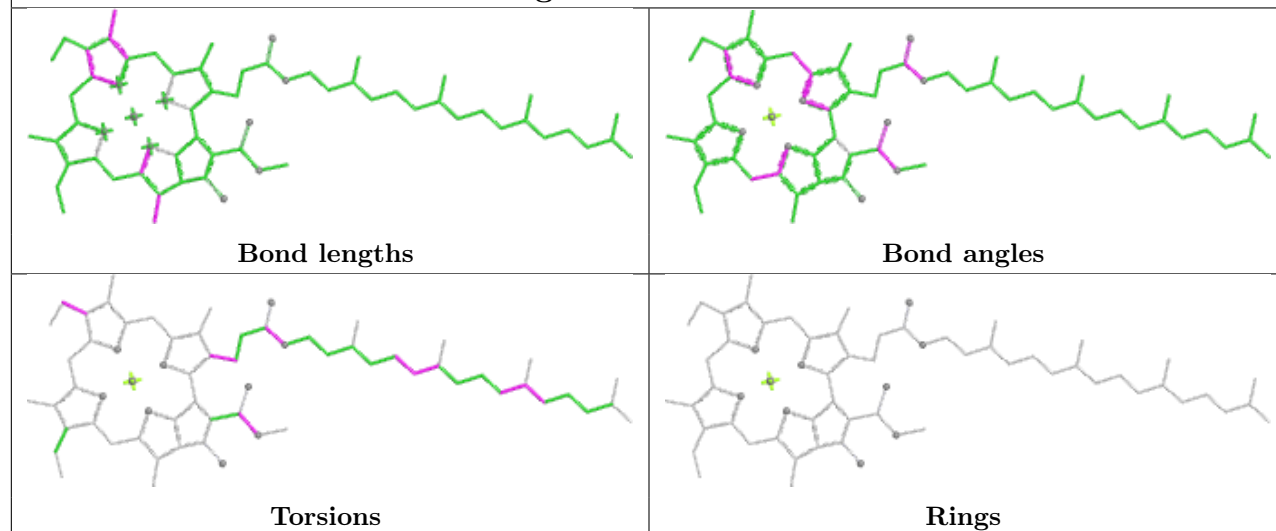


Ligand CLA J 1101

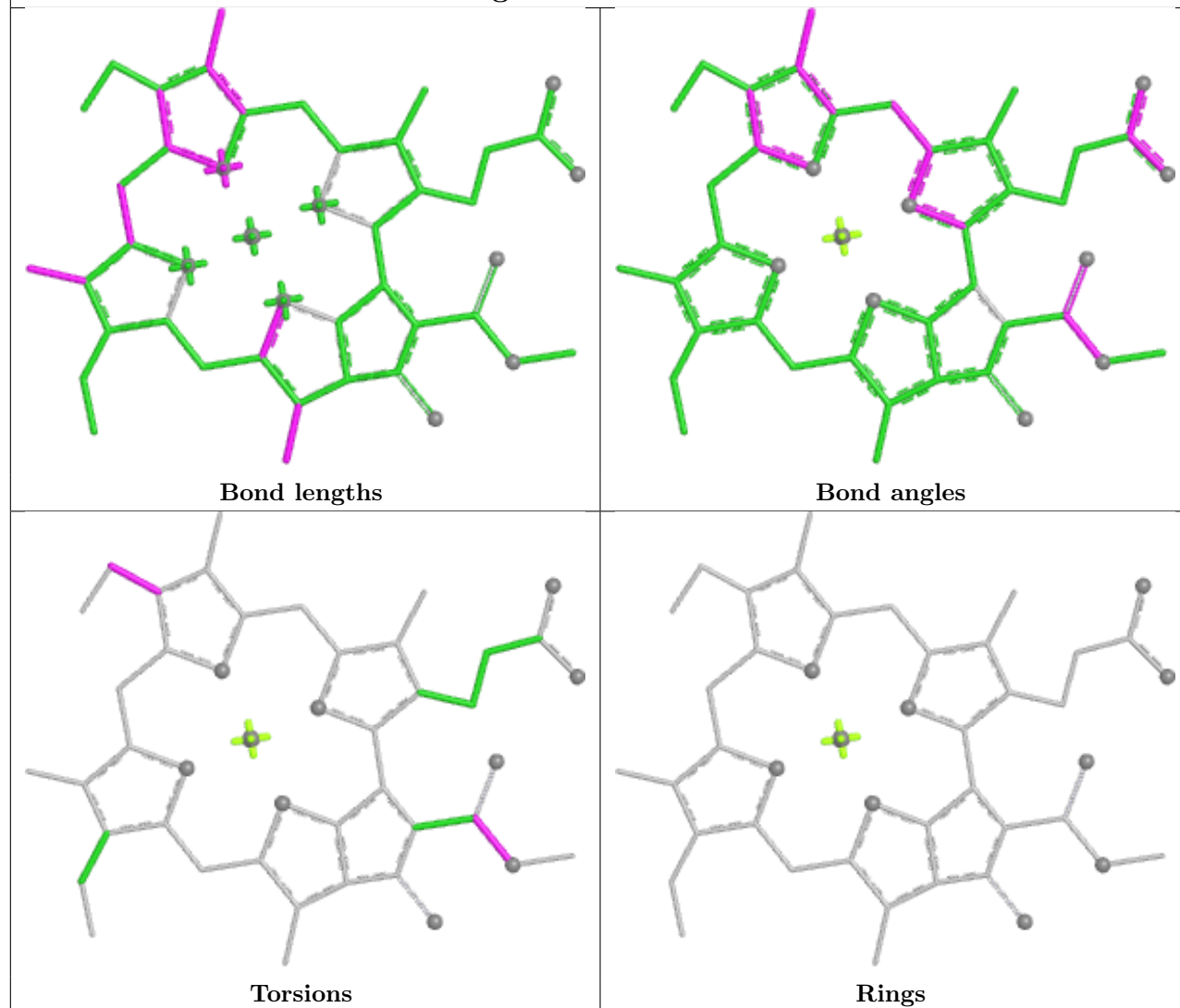




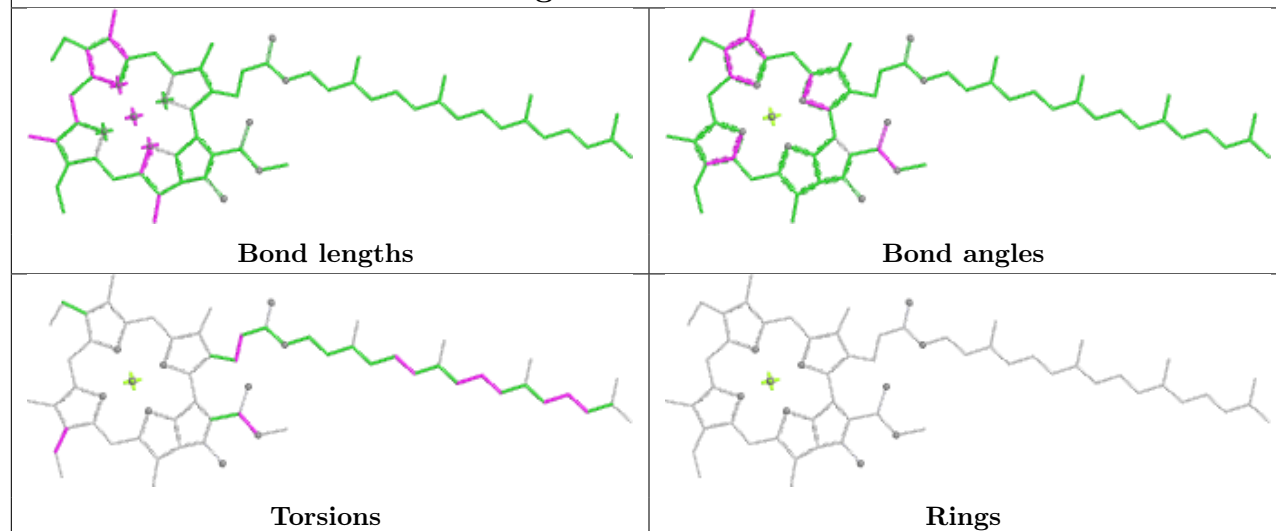
Ligand CLA b 837



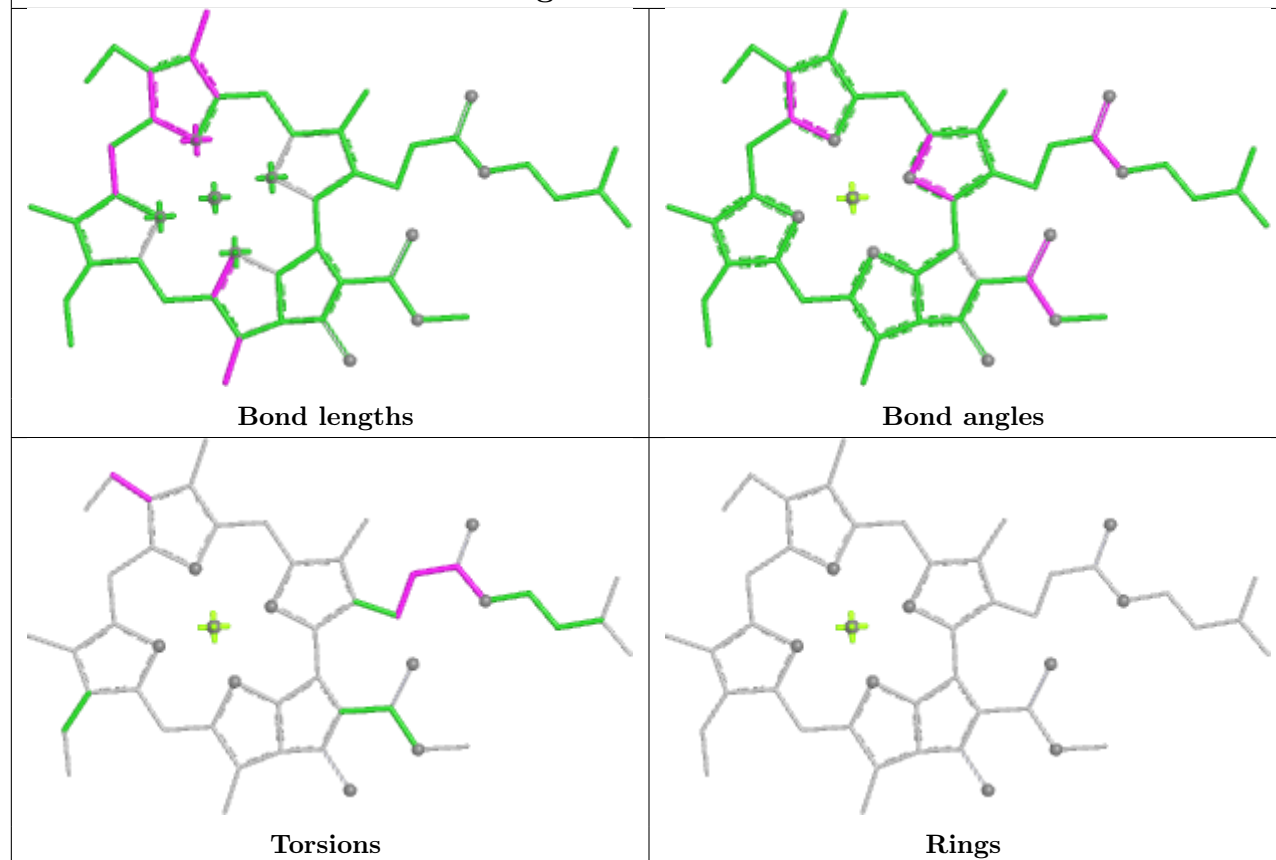
Ligand CLA B 812

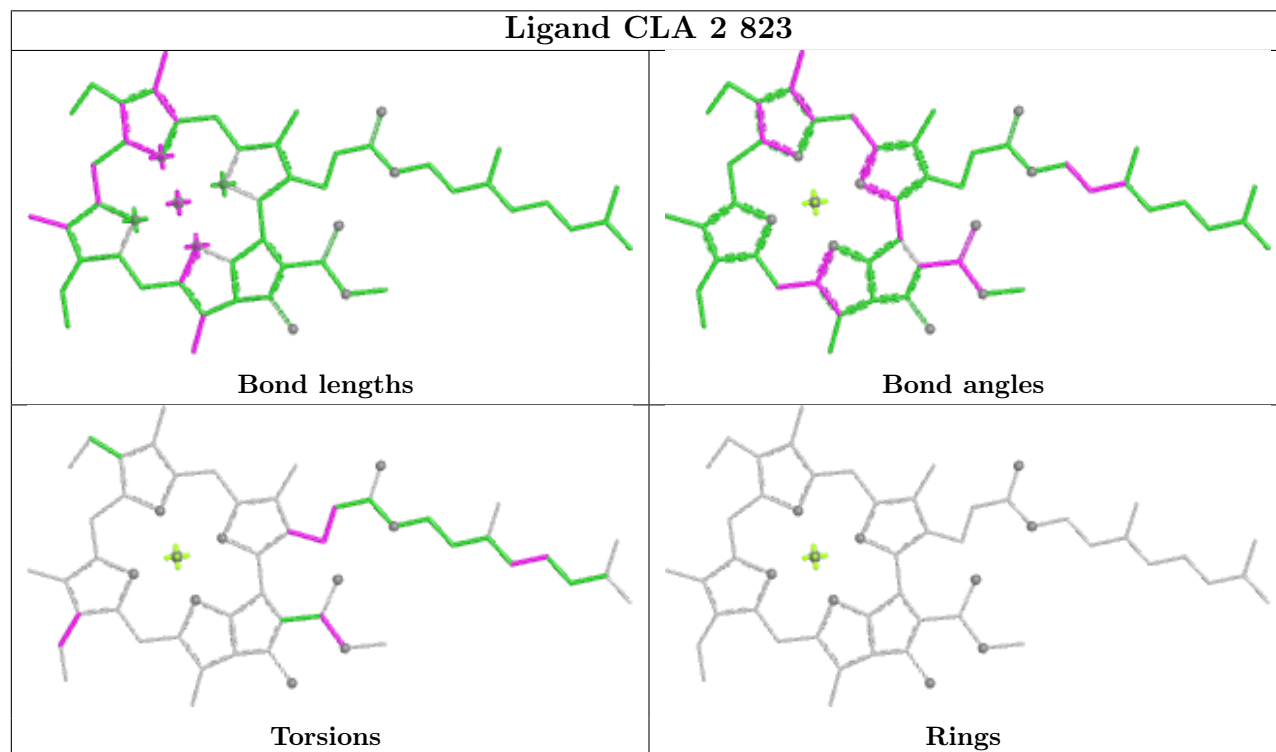
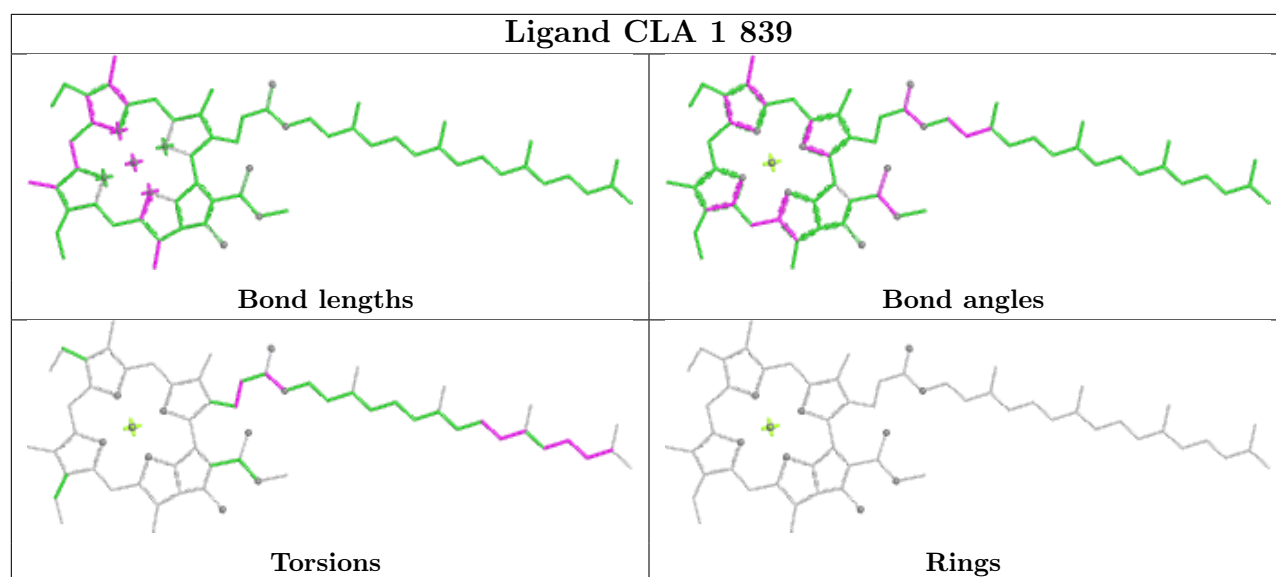


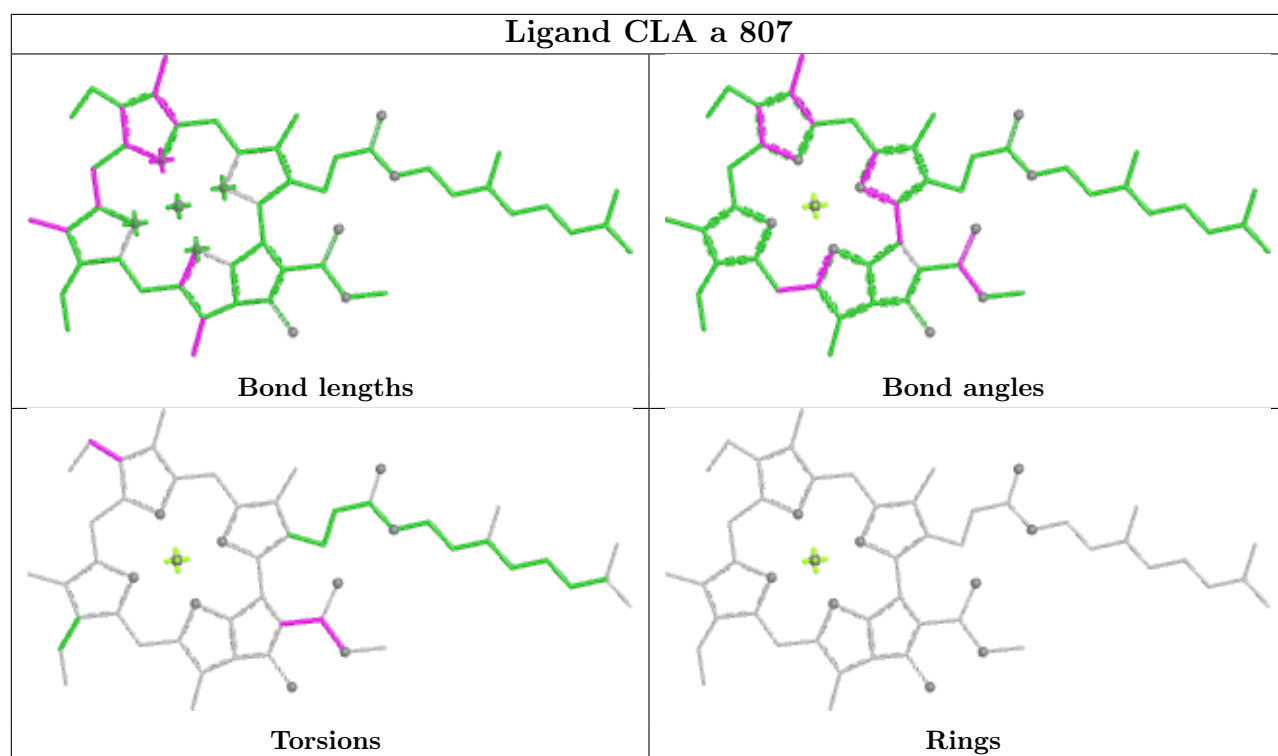
Ligand CLA b 802

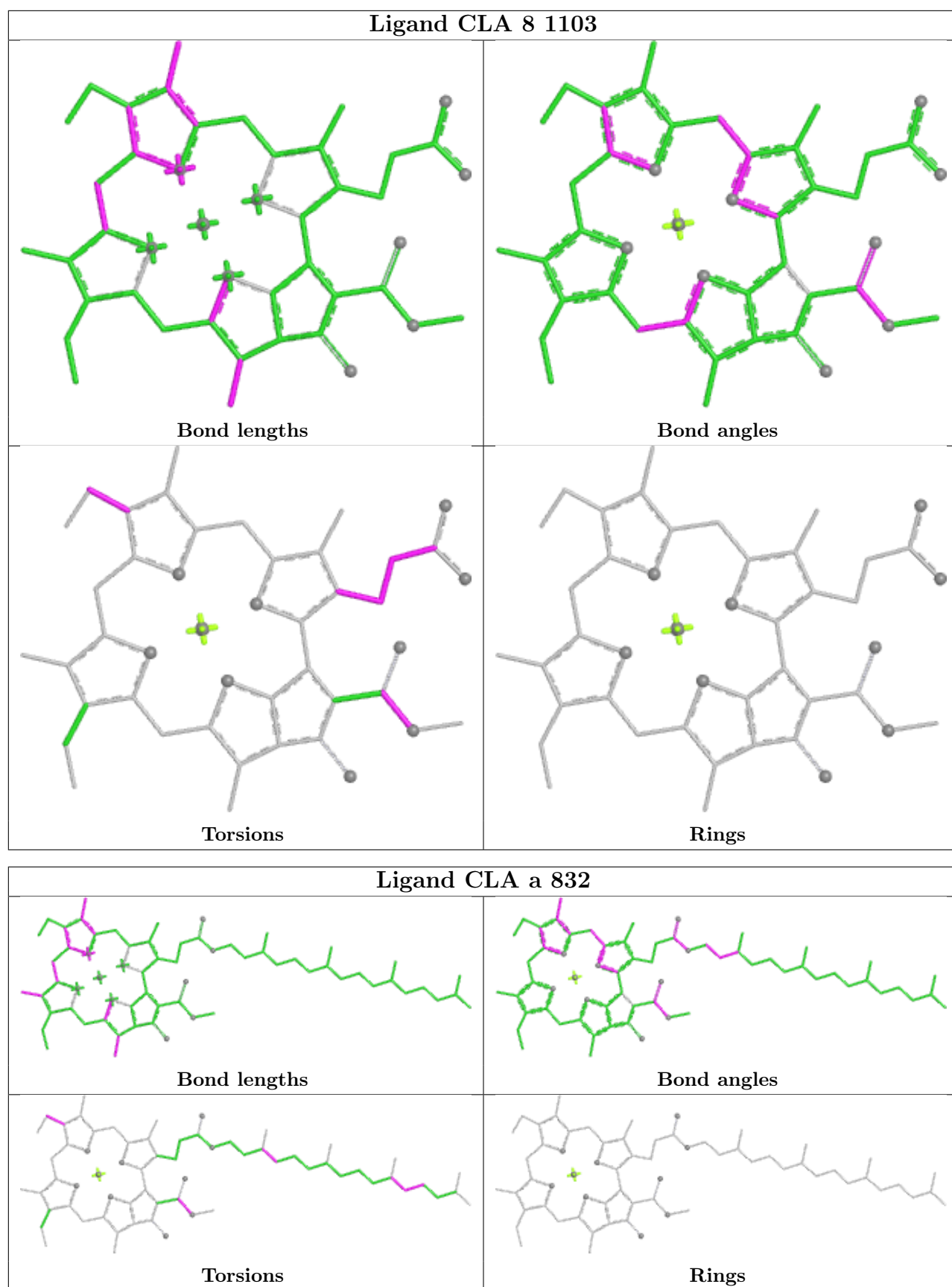


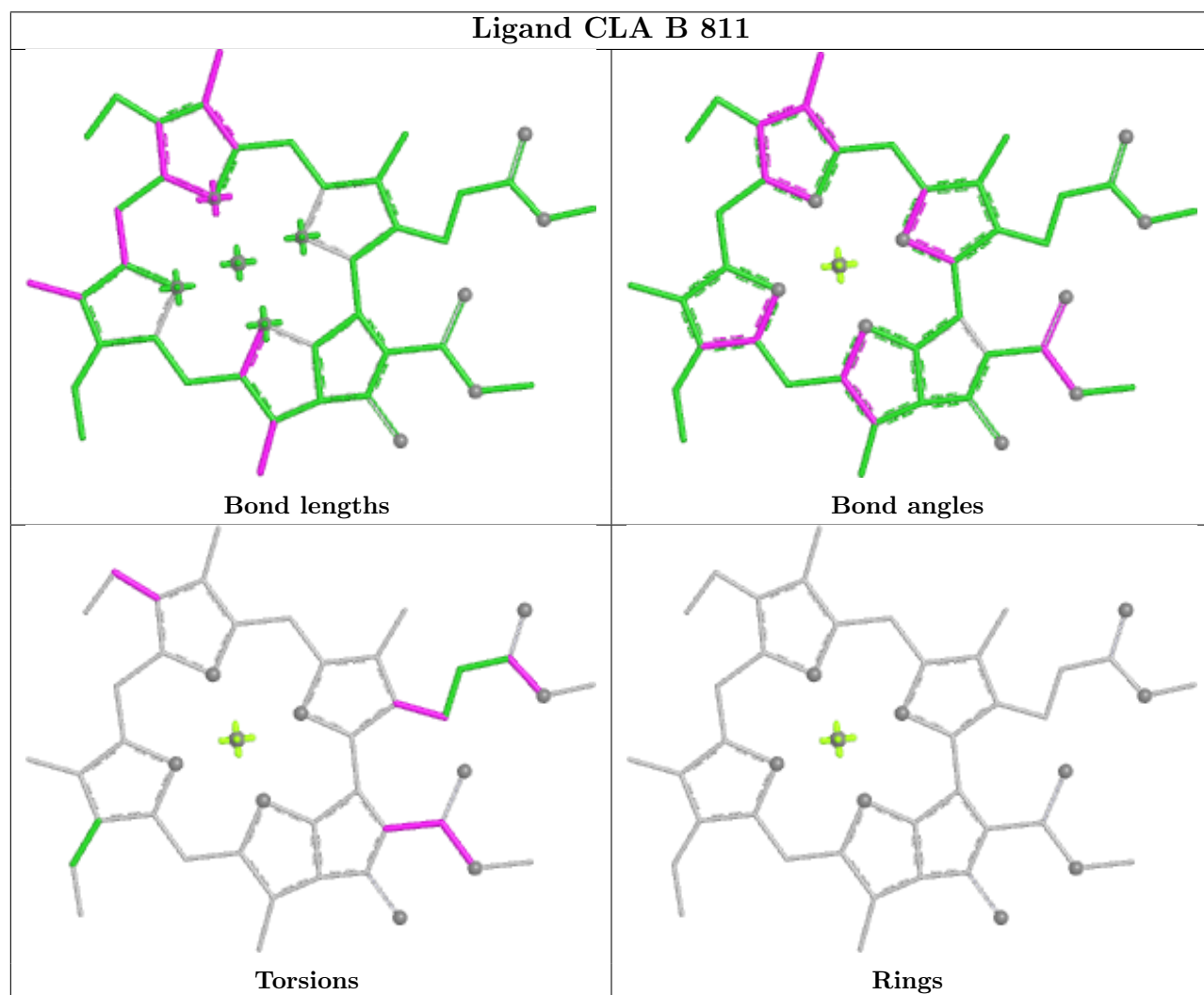
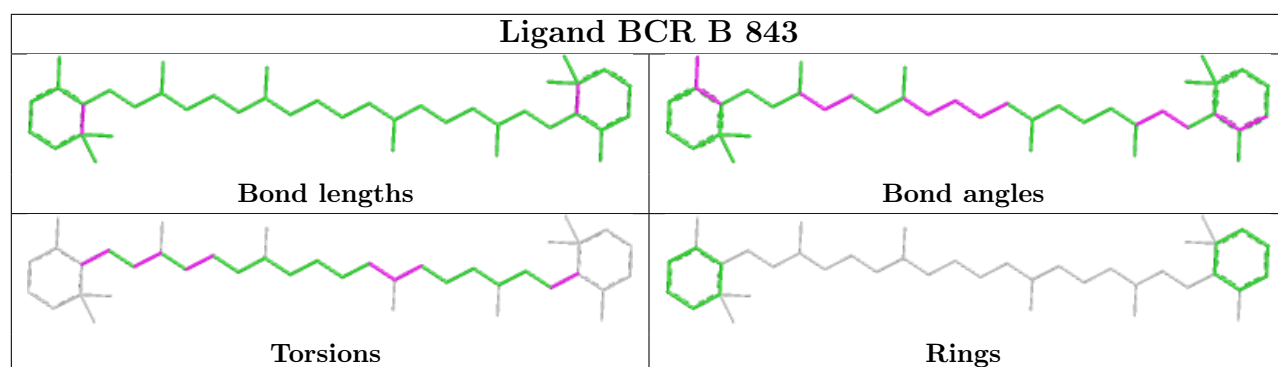
Ligand CLA 1 823

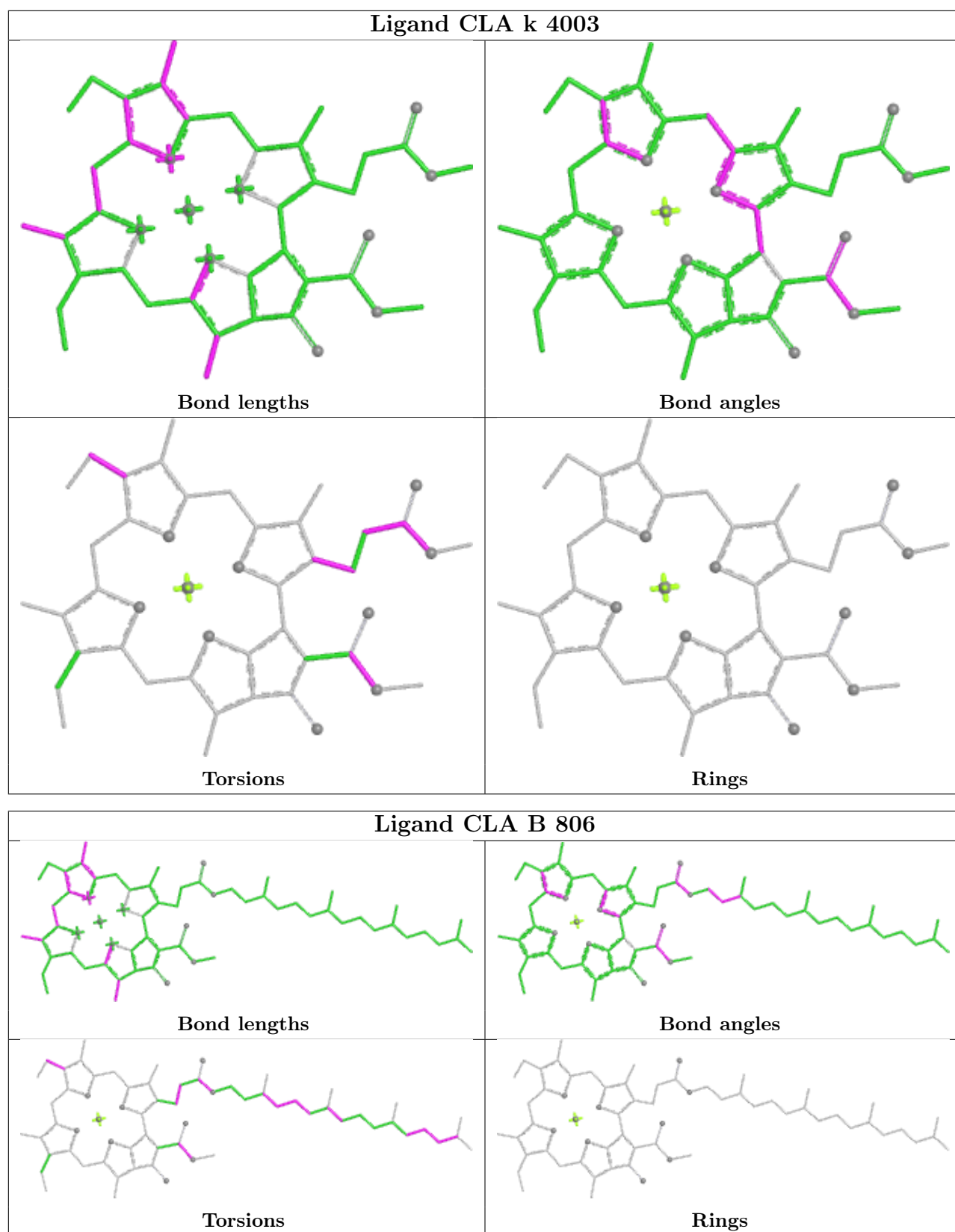


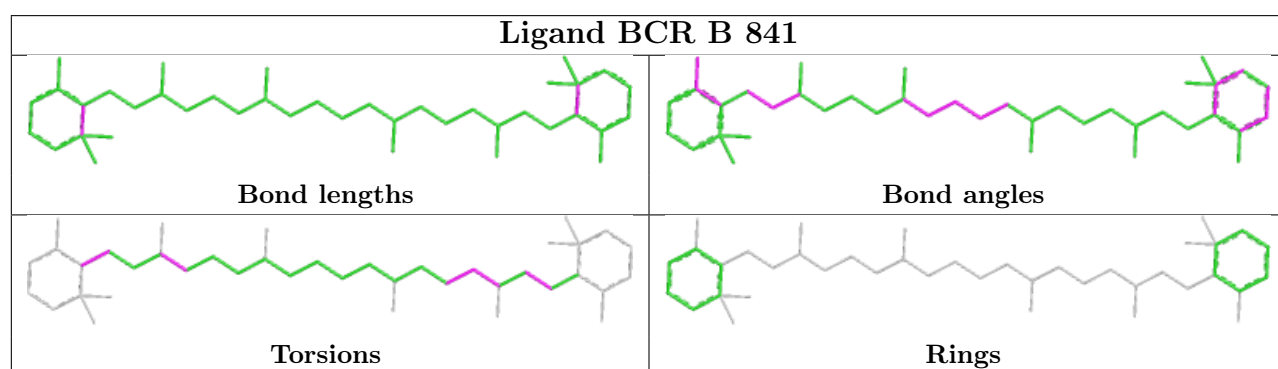
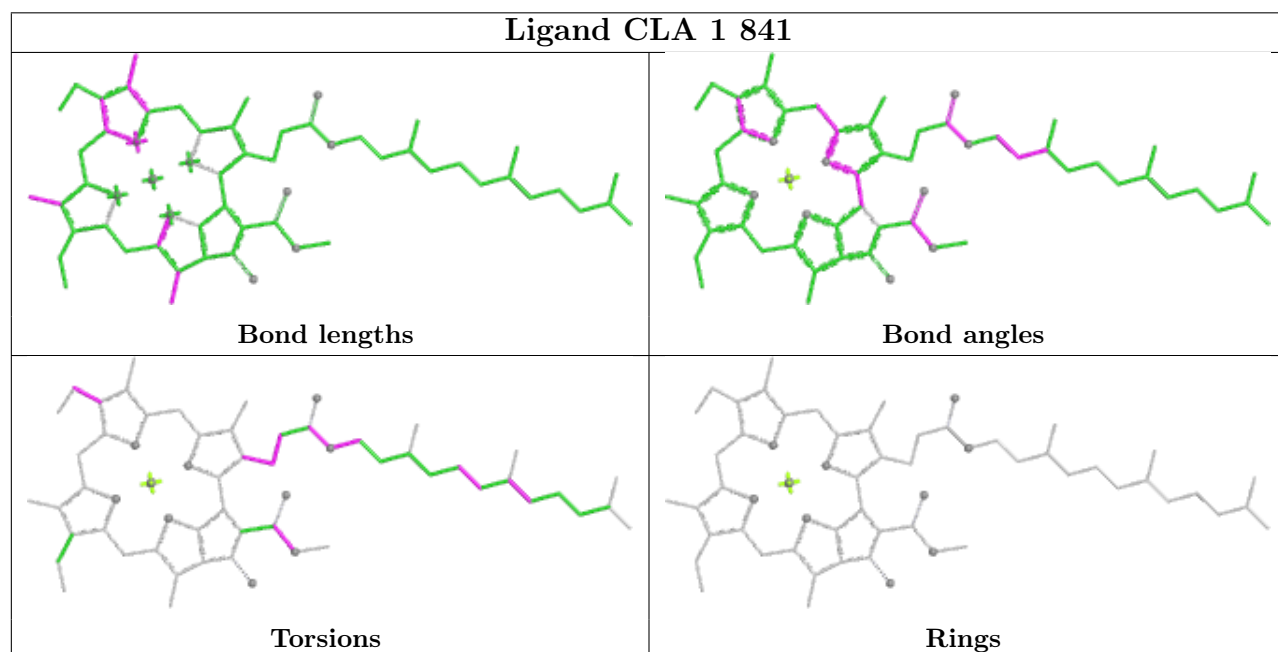
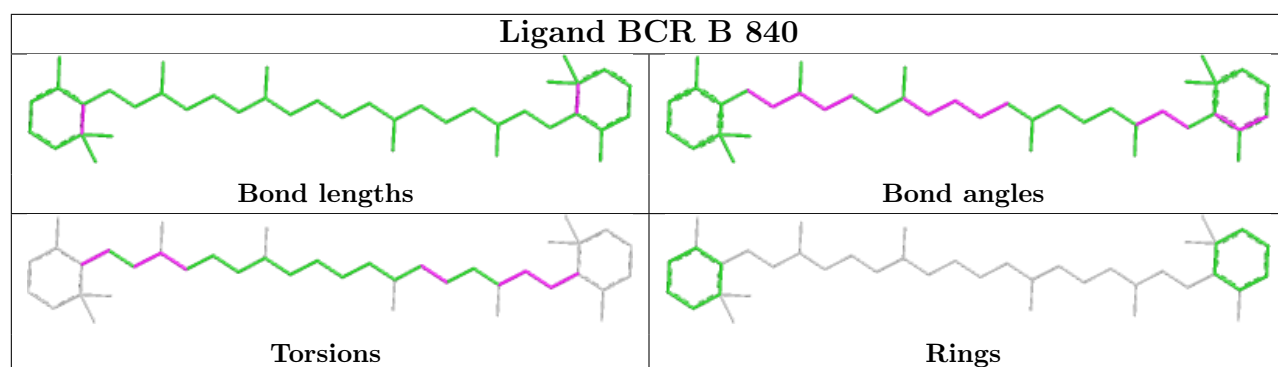




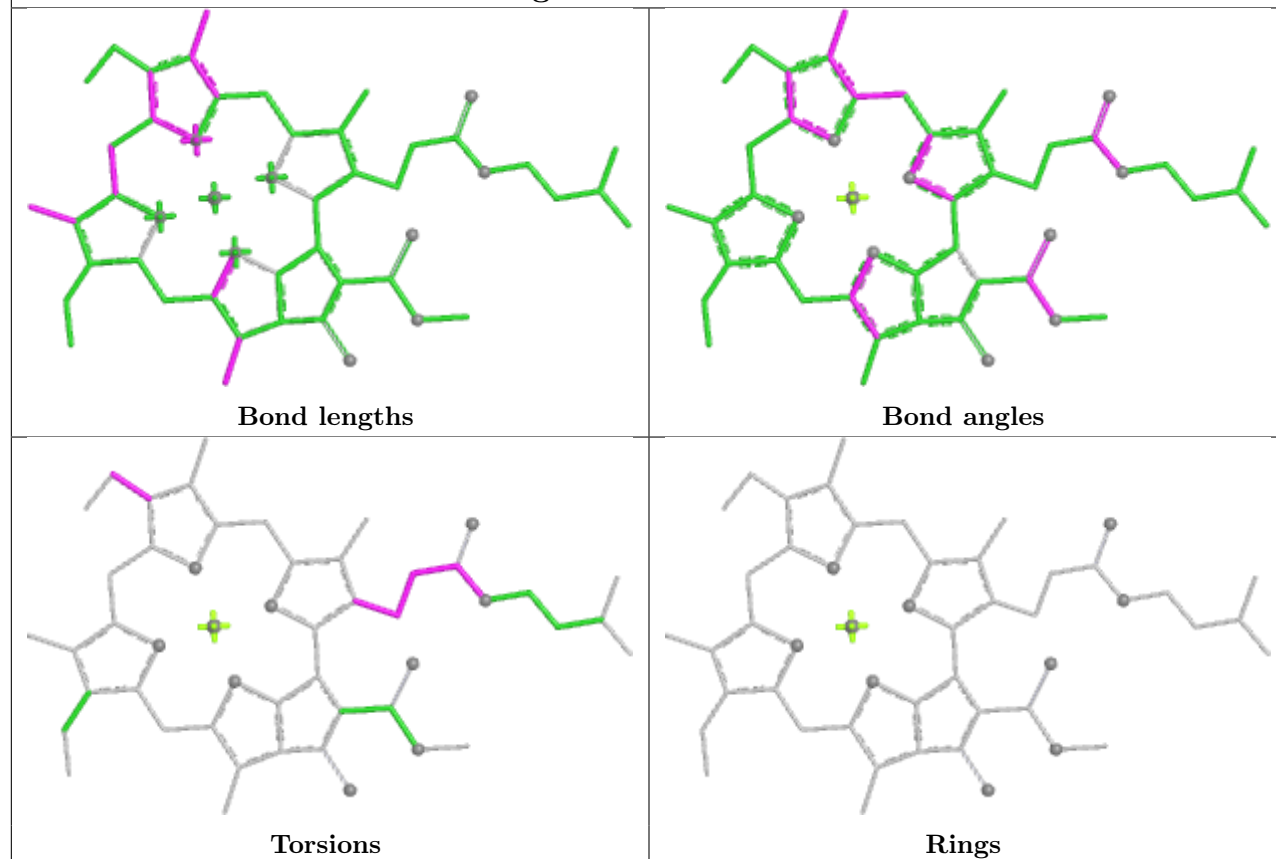




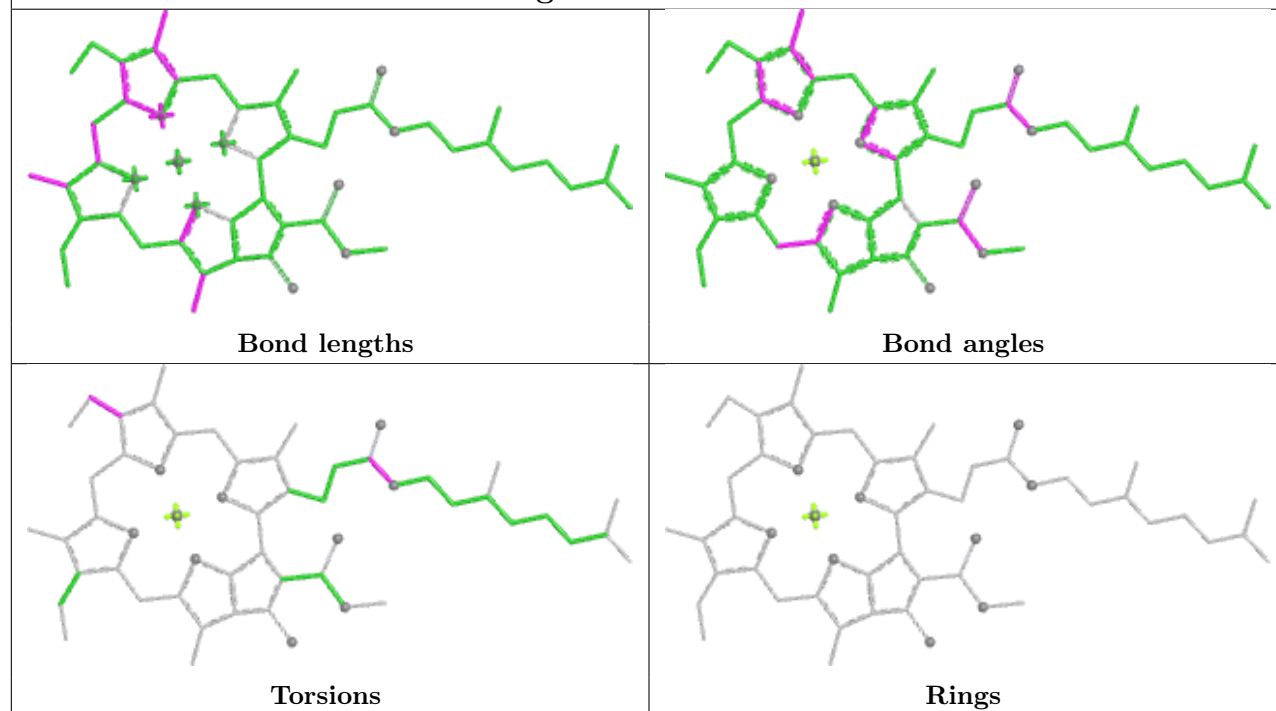


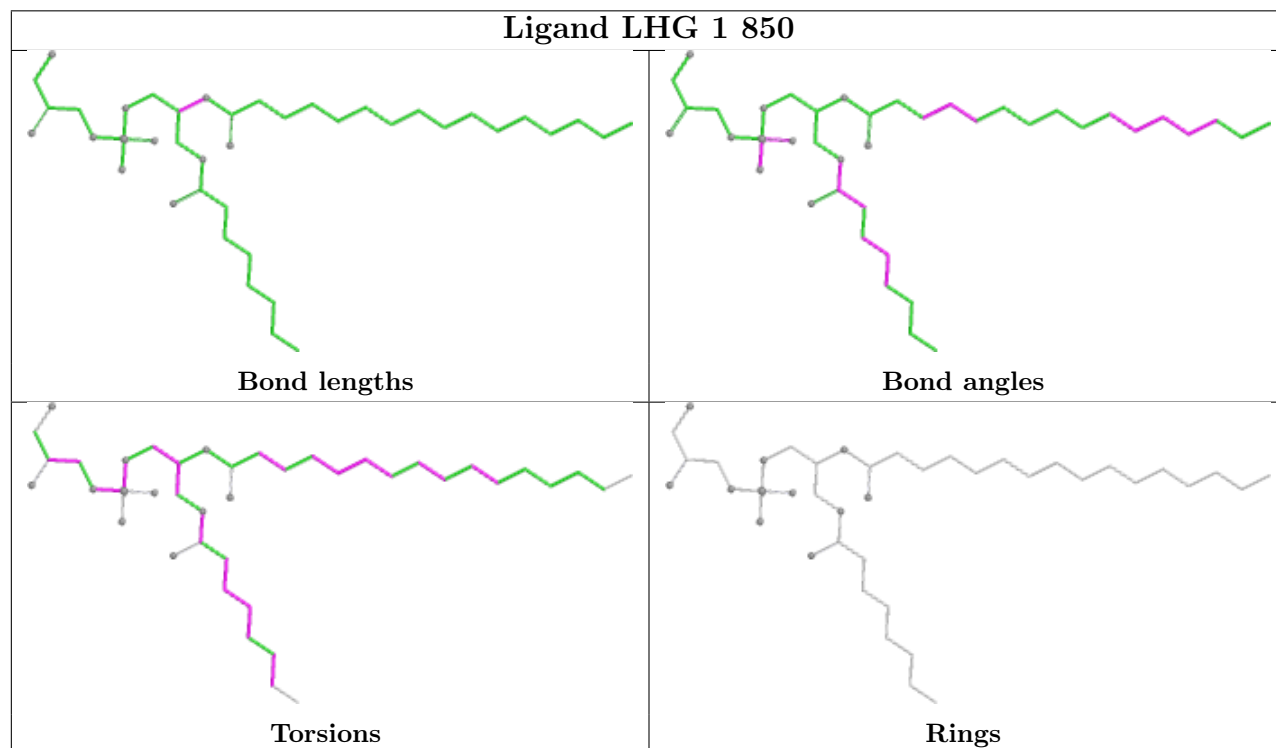
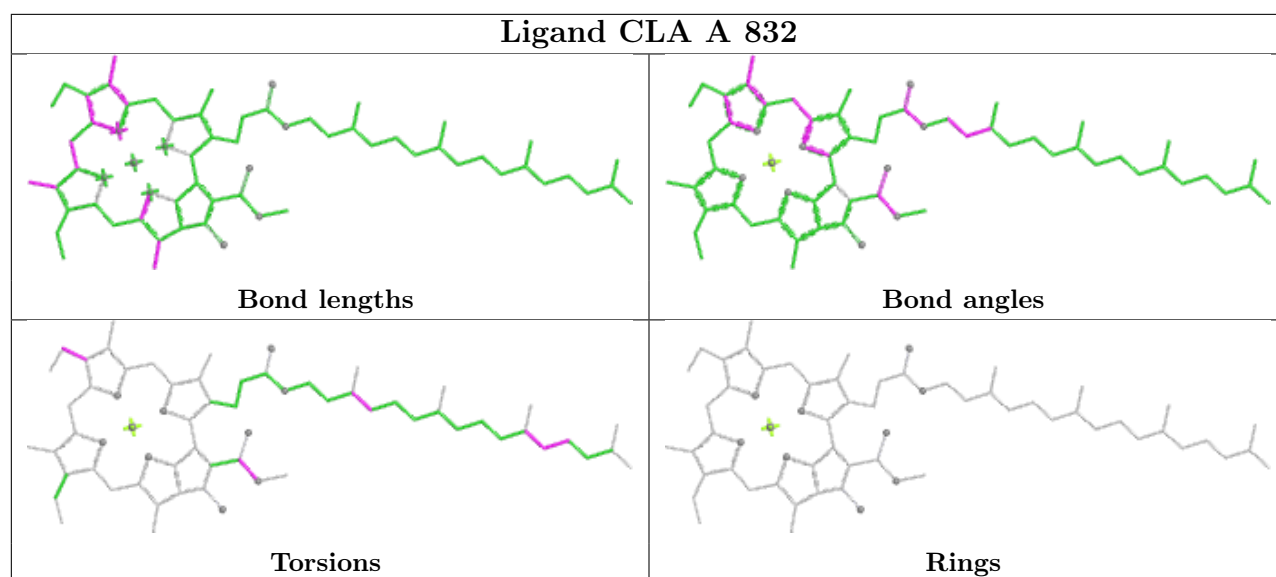


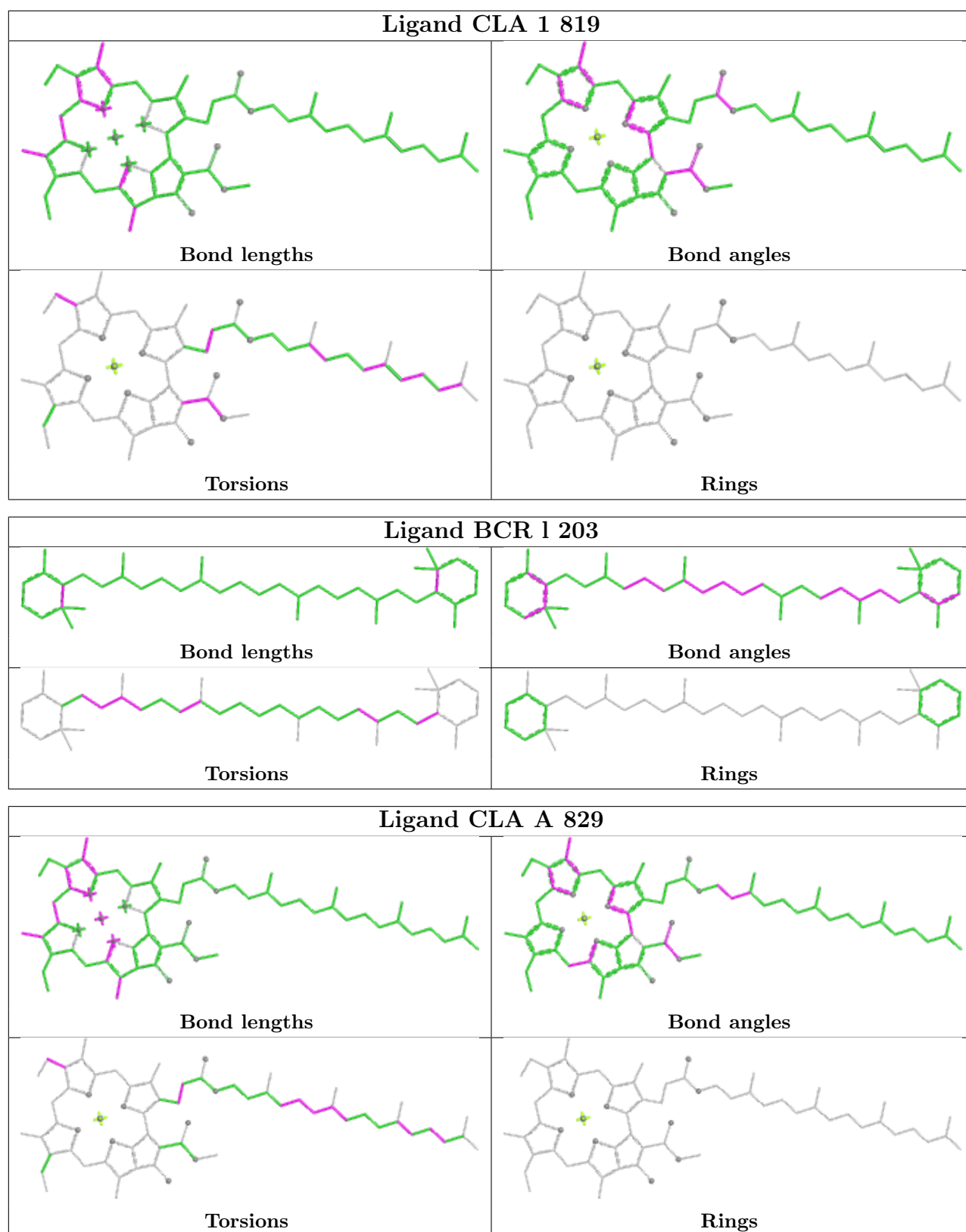
Ligand CLA B 814

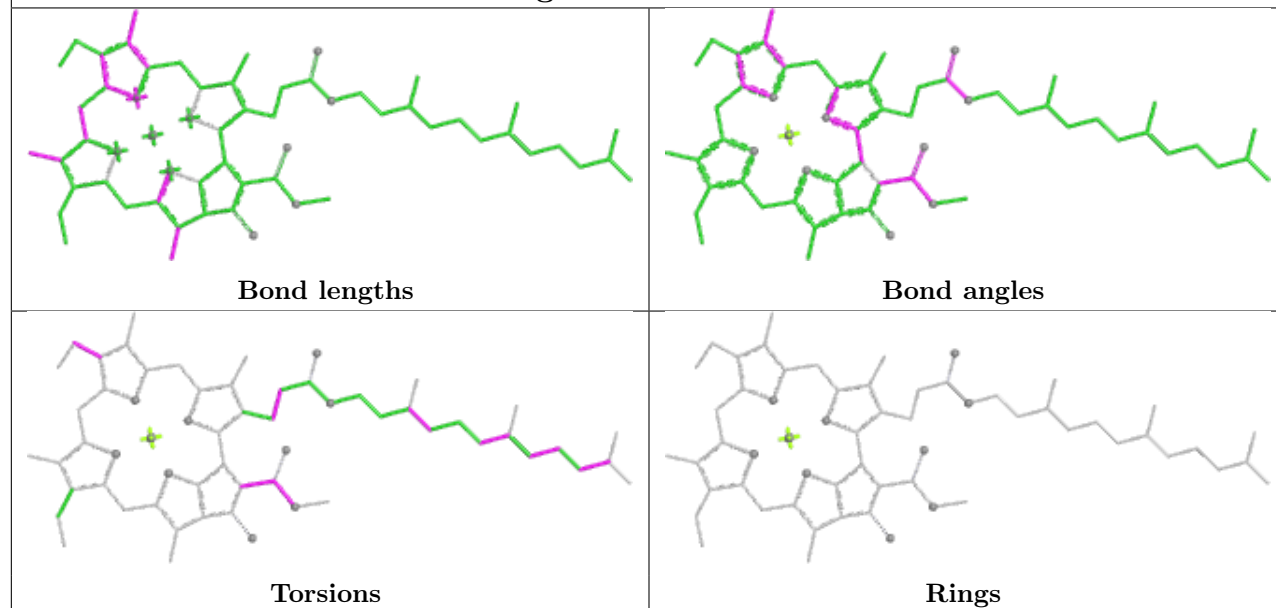
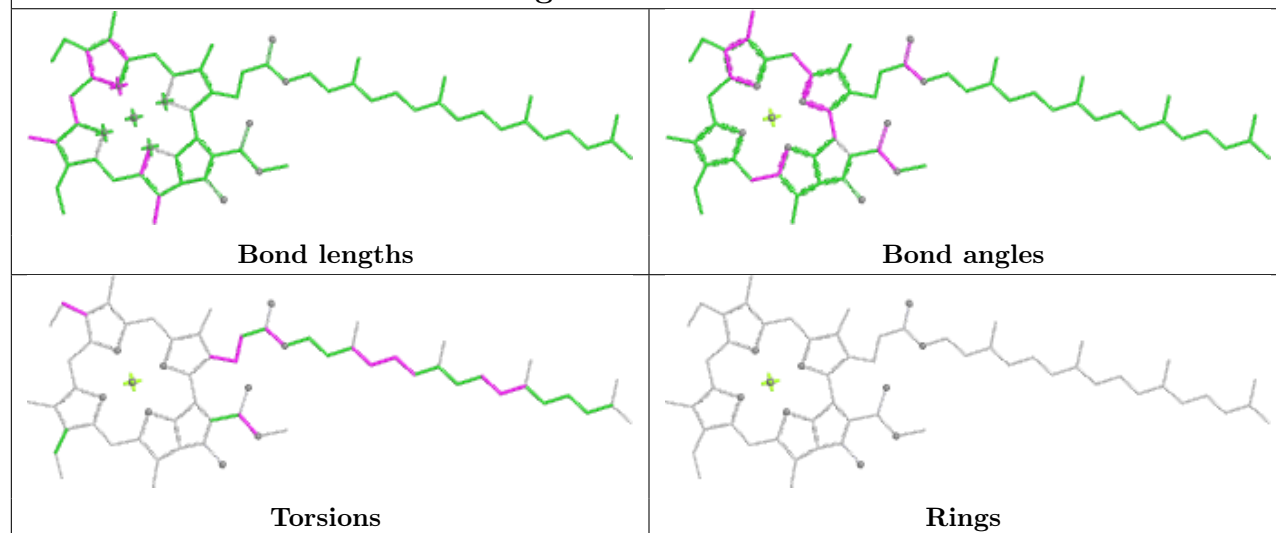


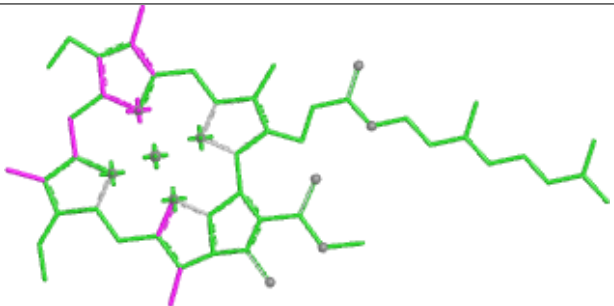
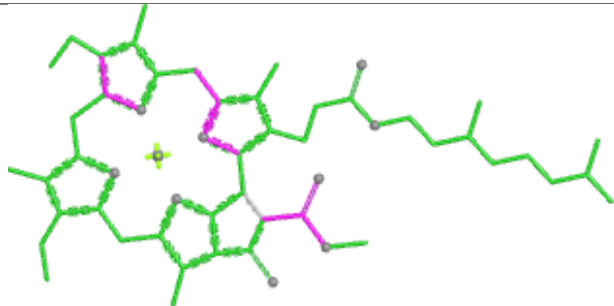
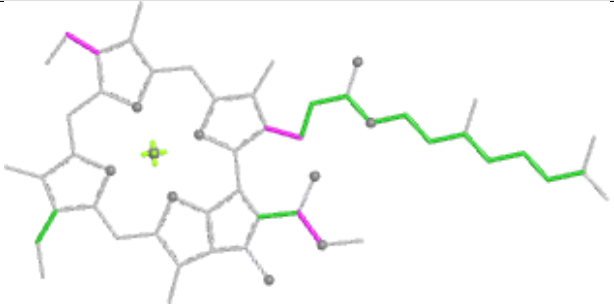
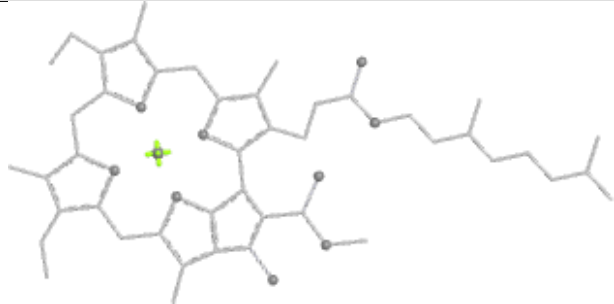
Ligand CLA a 804

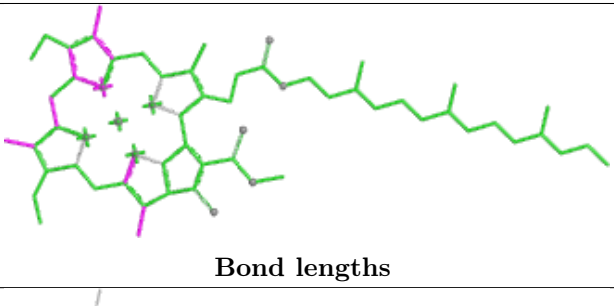
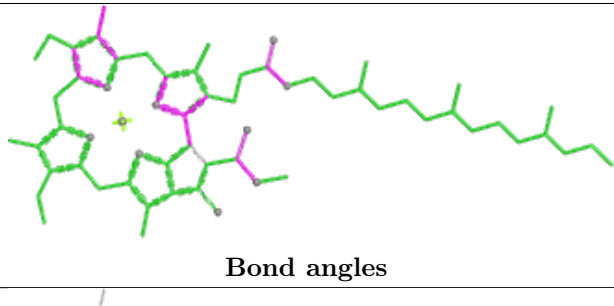
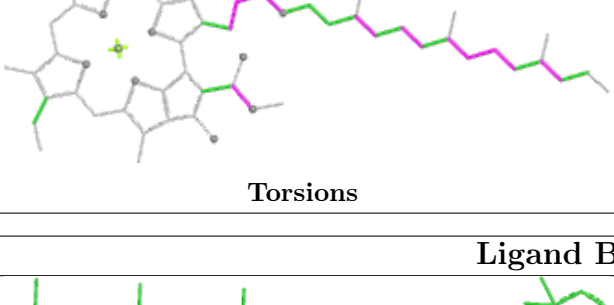
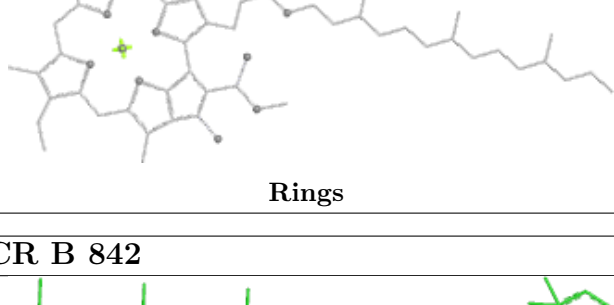


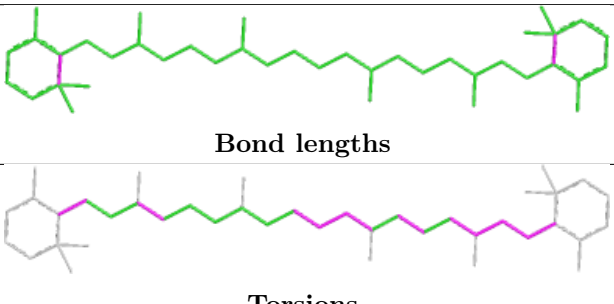
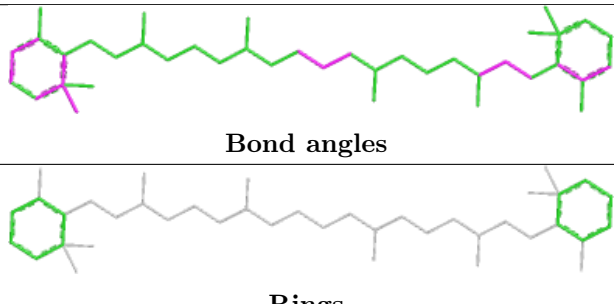


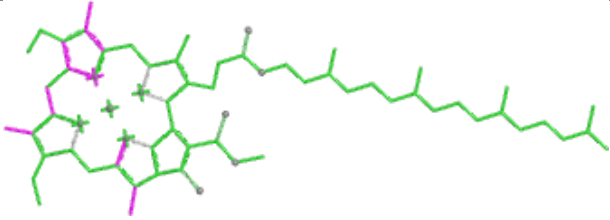
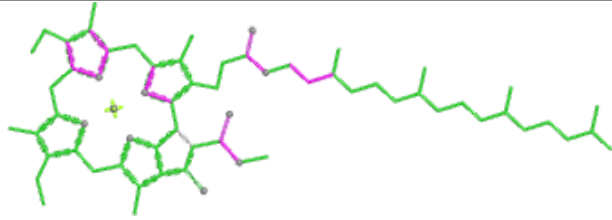
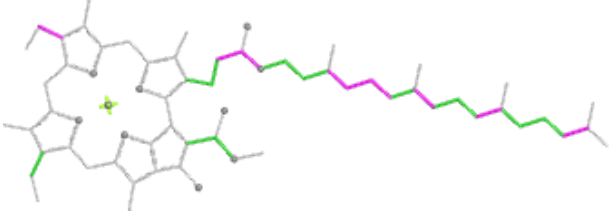
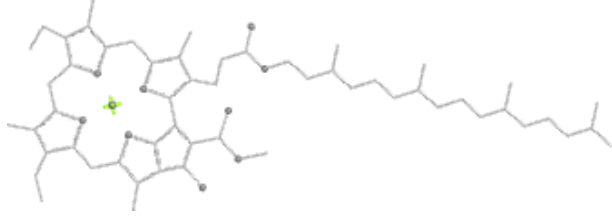
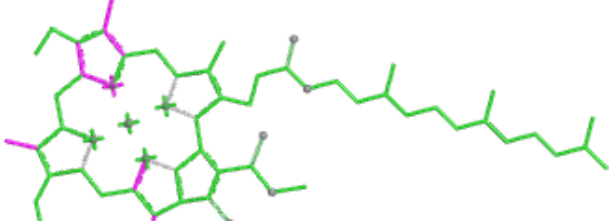
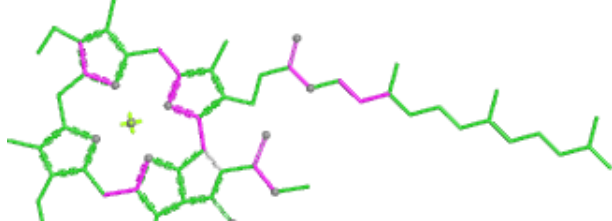
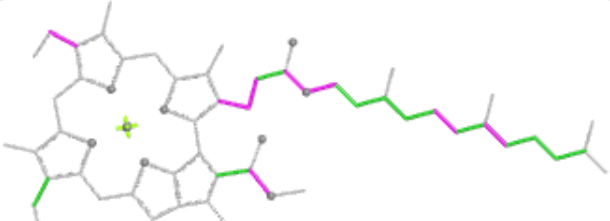
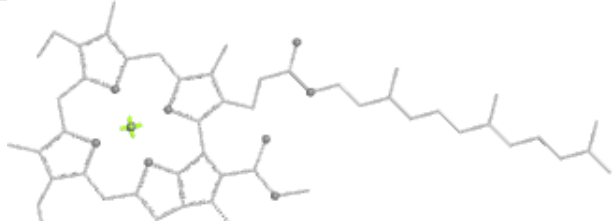
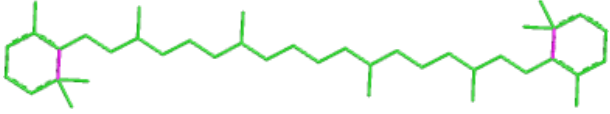
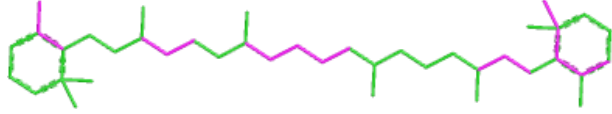
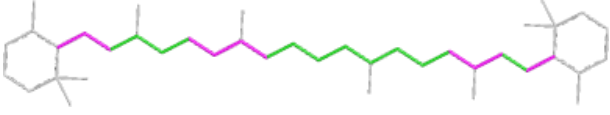
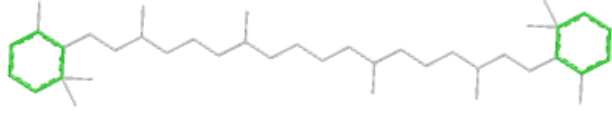


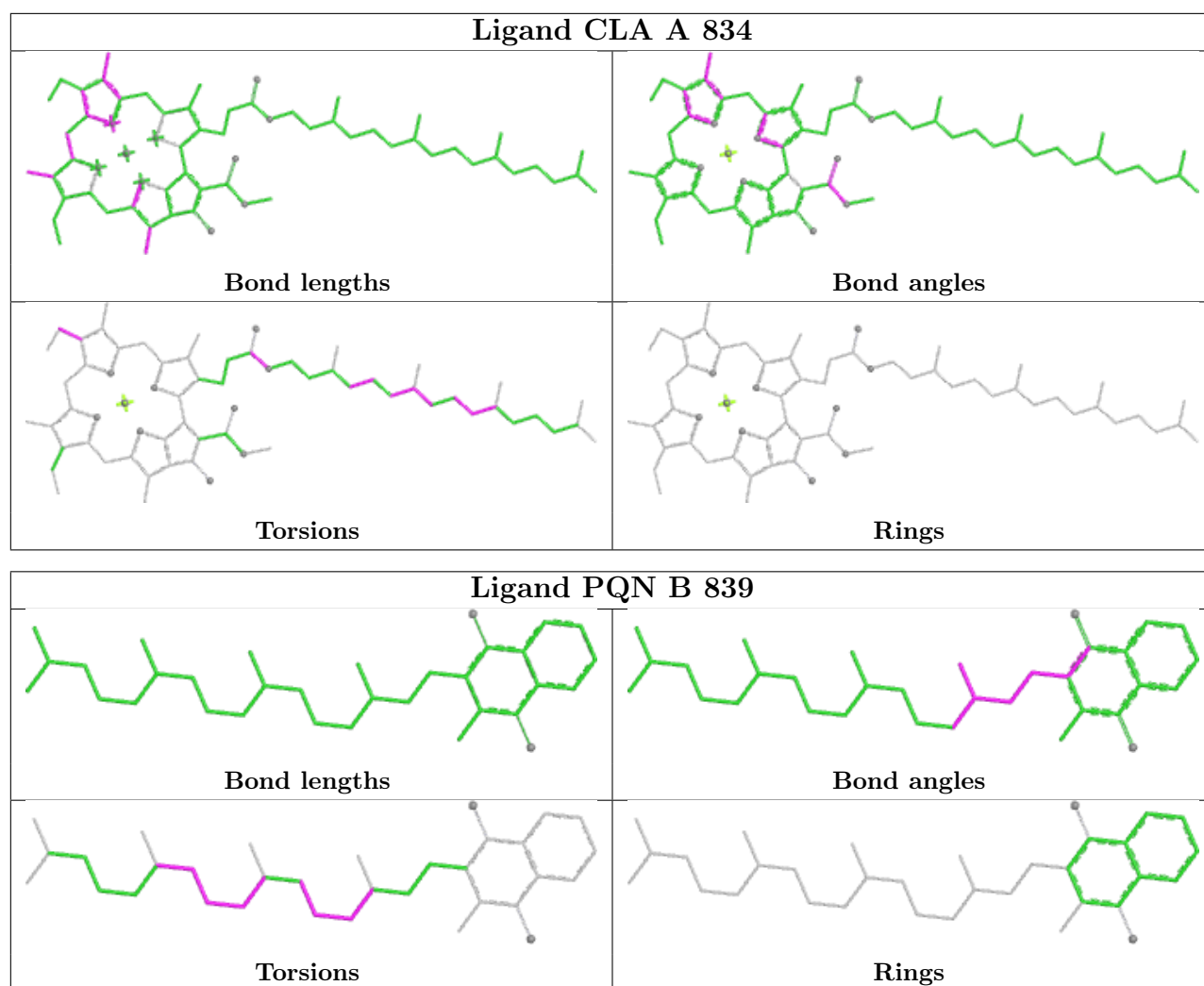
Ligand CLA a 819**Ligand CLA b 813**

Ligand CLA F 201	
	
Bond lengths	Bond angles
	
Torsions	Rings

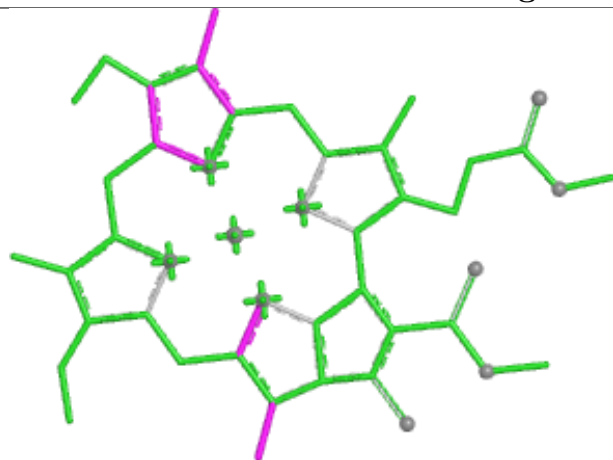
Ligand CLA 1 825	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR B 842	
	
Bond lengths	Bond angles
Torsions	Rings

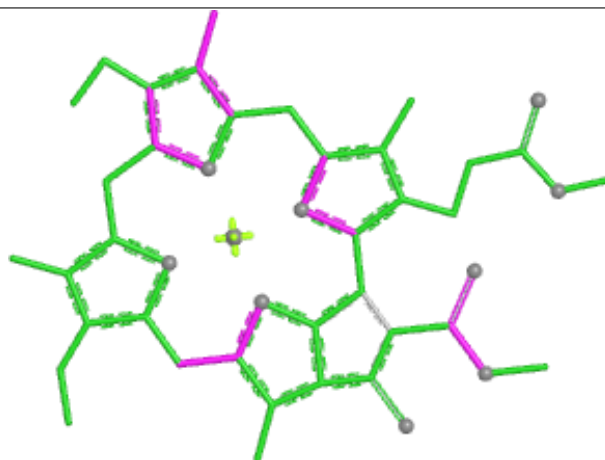
Ligand CL0 A 801	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA a 841	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 6 205	
 Bond lengths	 Bond angles
 Torsions	 Rings



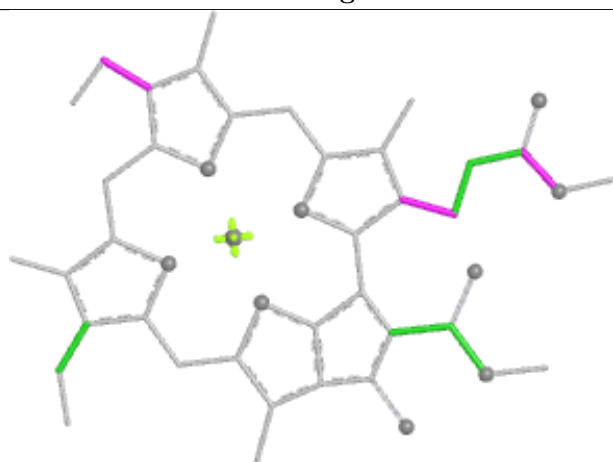
Ligand CLA a 820



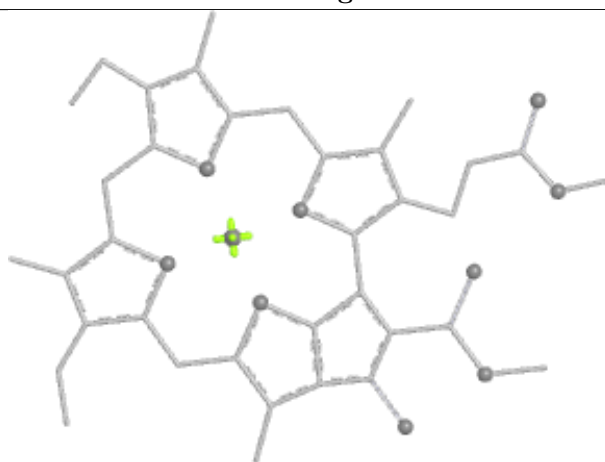
Bond lengths



Bond angles

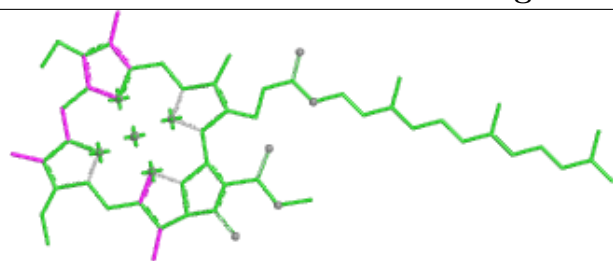


Torsions

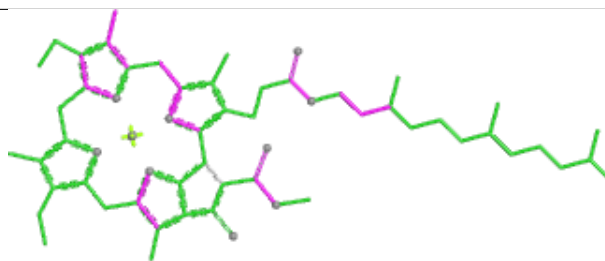


Rings

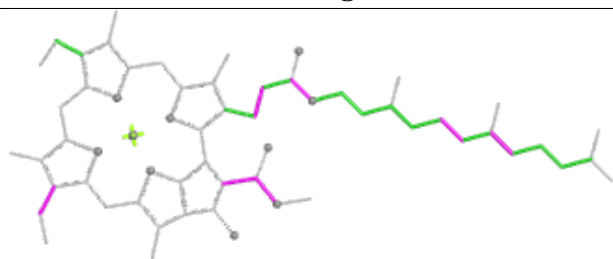
Ligand CLA B 803



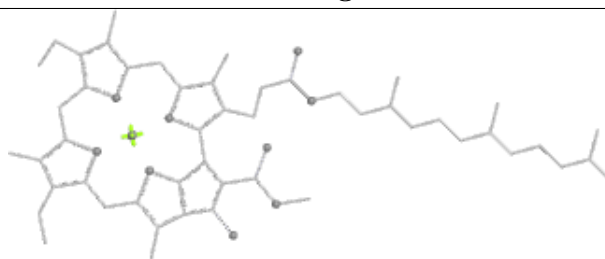
Bond lengths



Bond angles

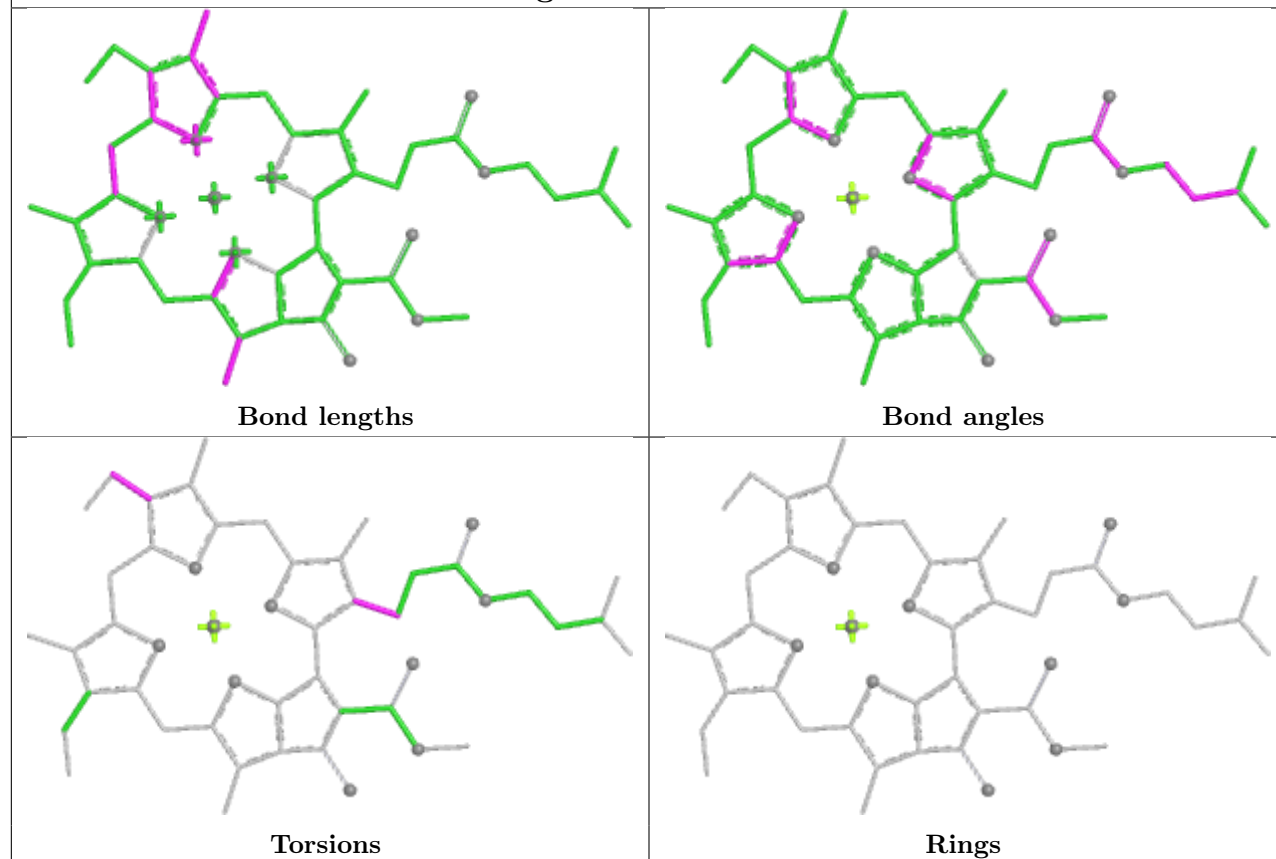


Torsions

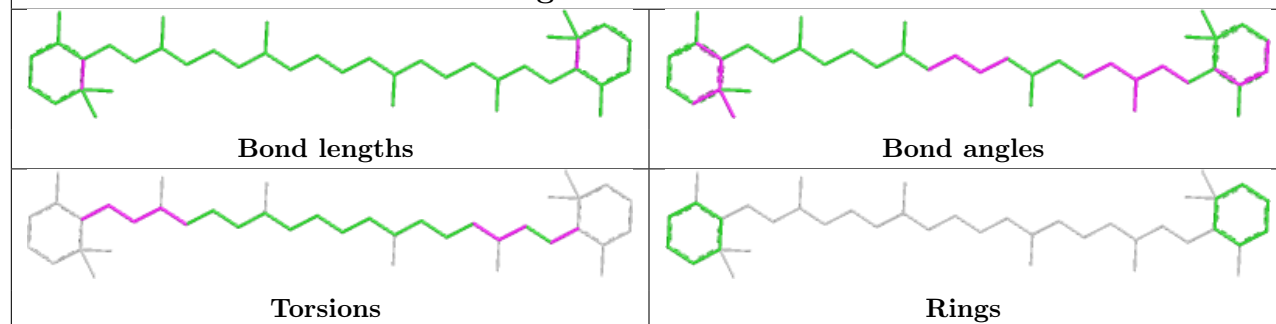


Rings

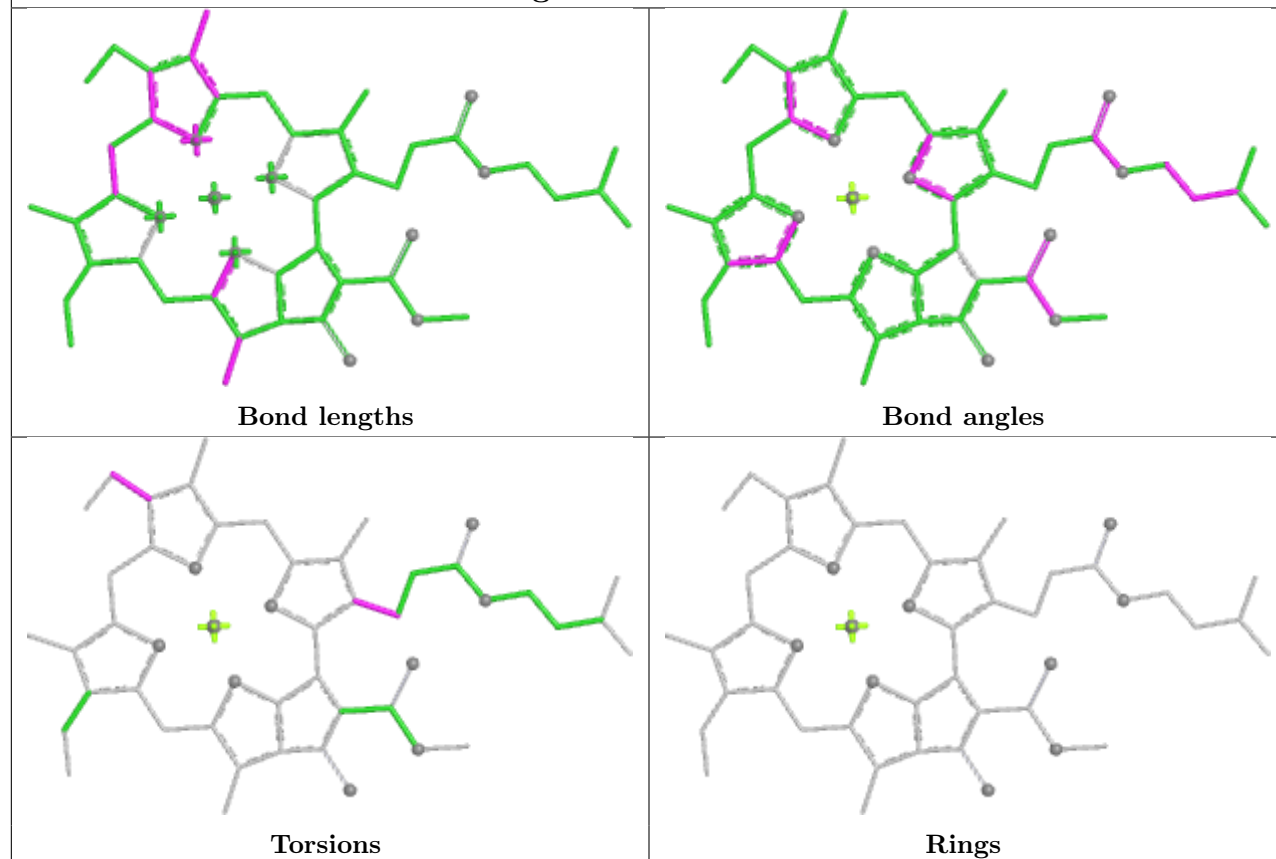
Ligand CLA 2 834



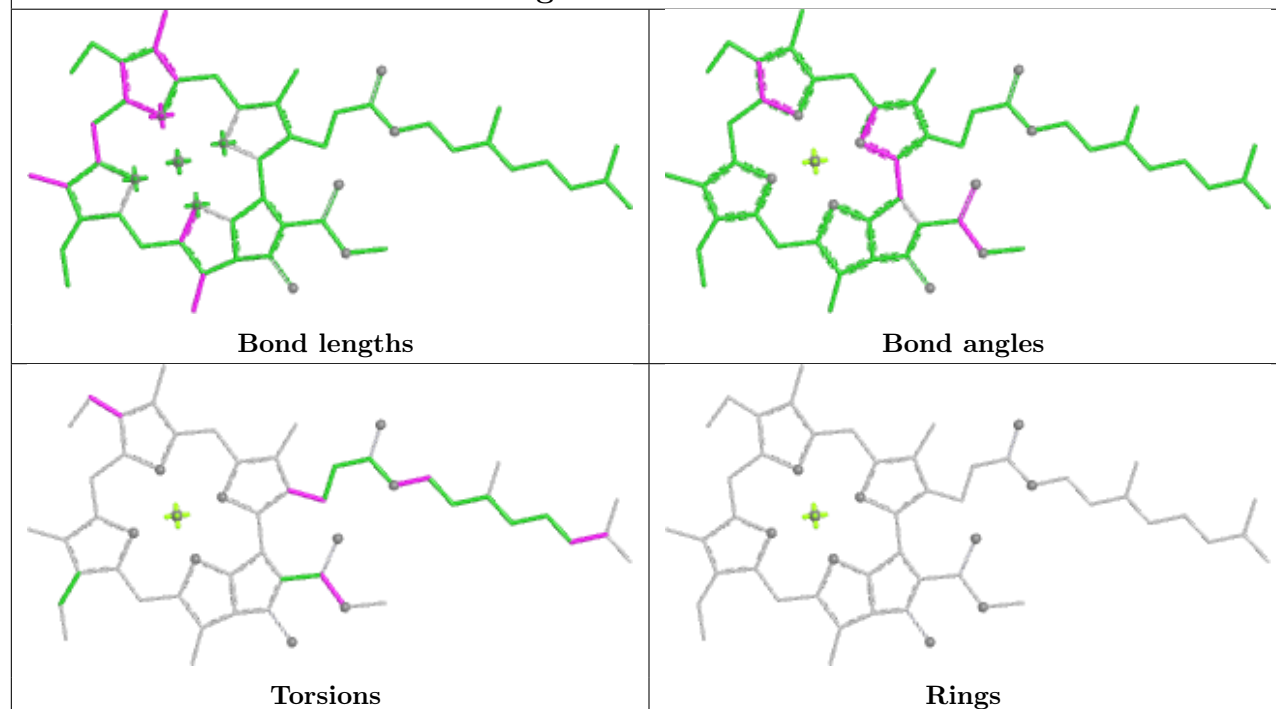
Ligand BCR I 102

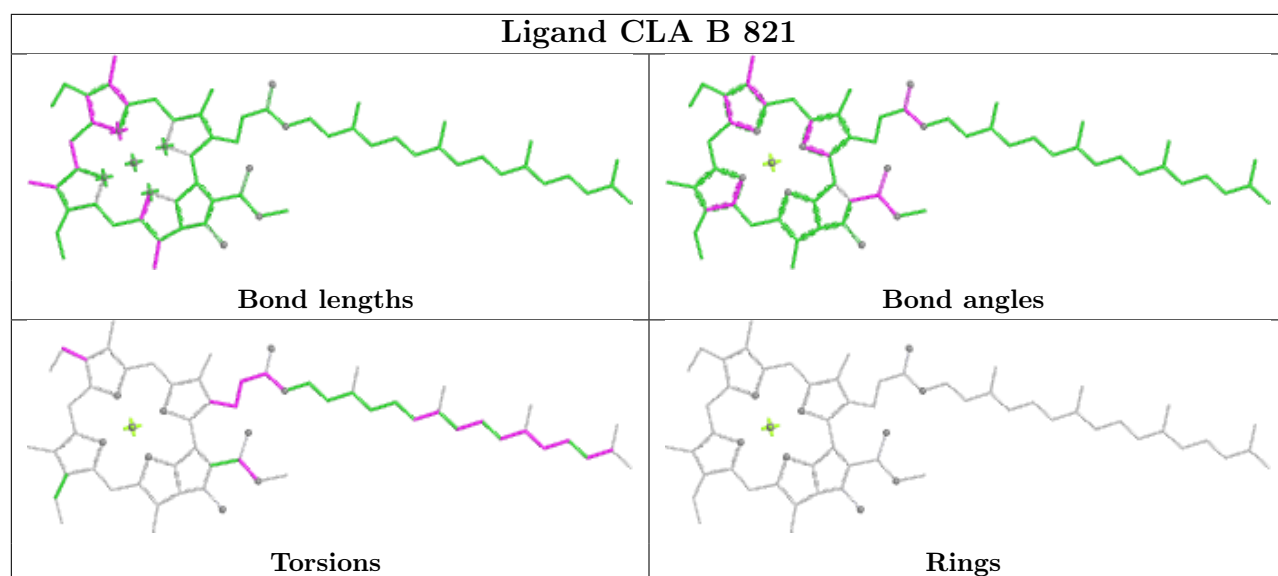
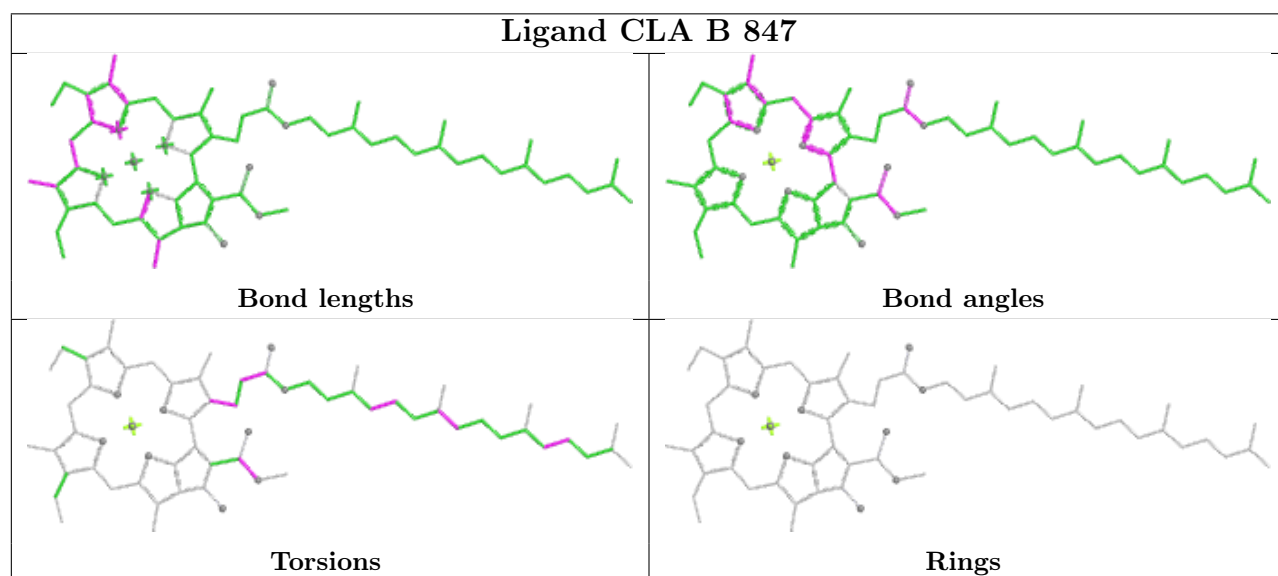
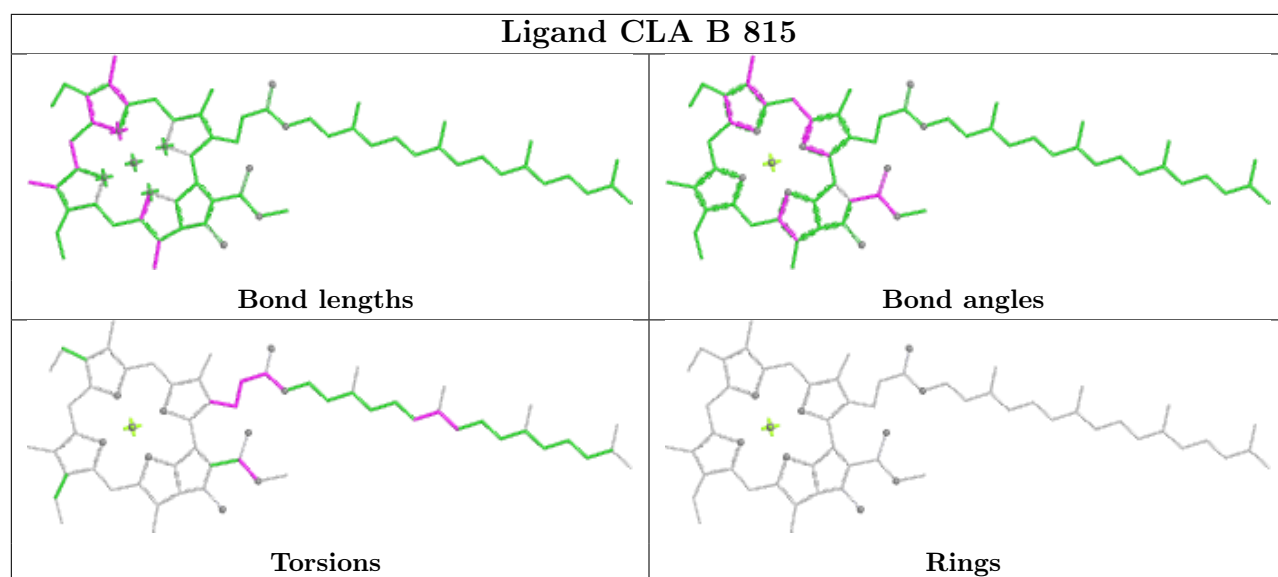


Ligand CLA B 835

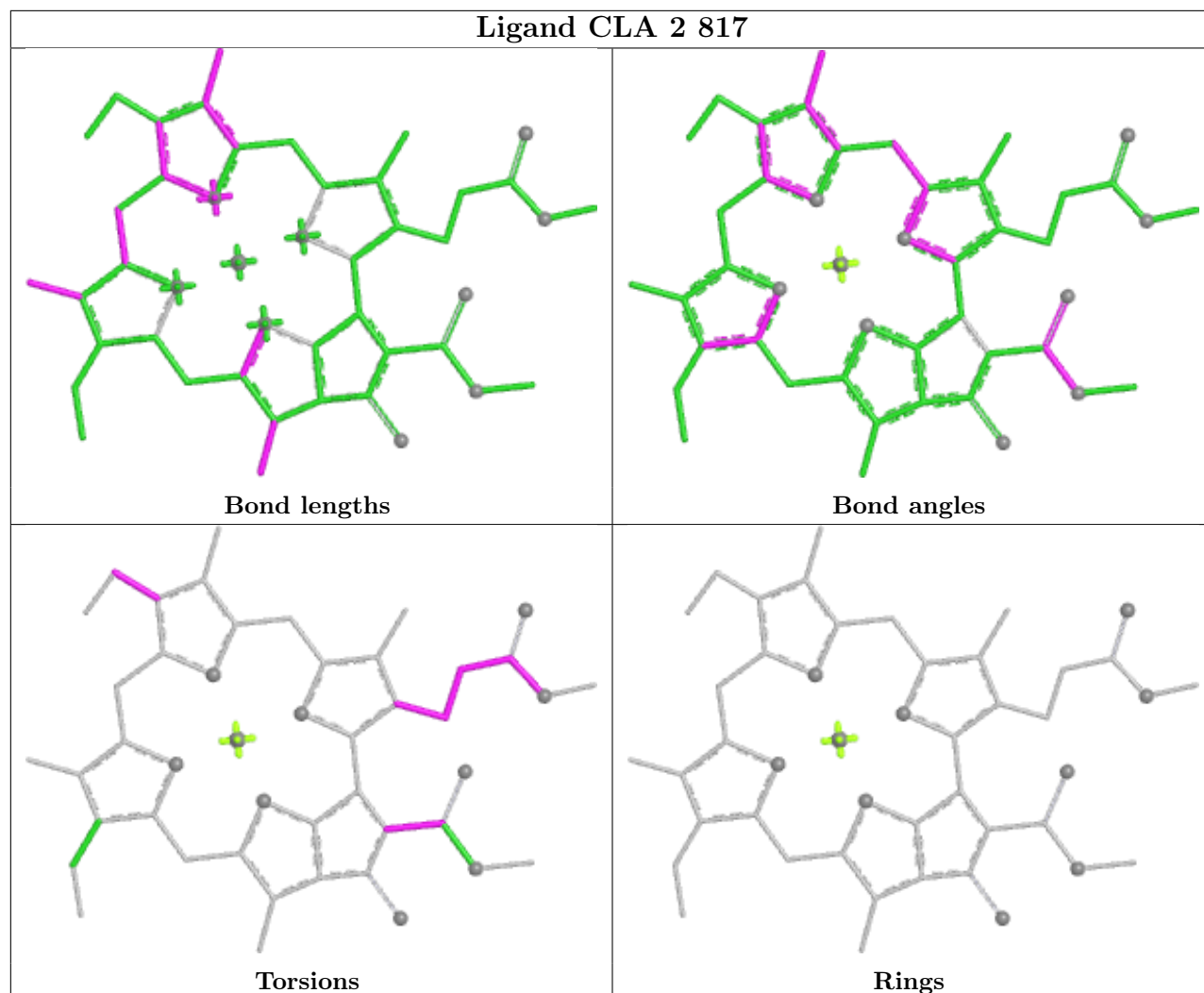


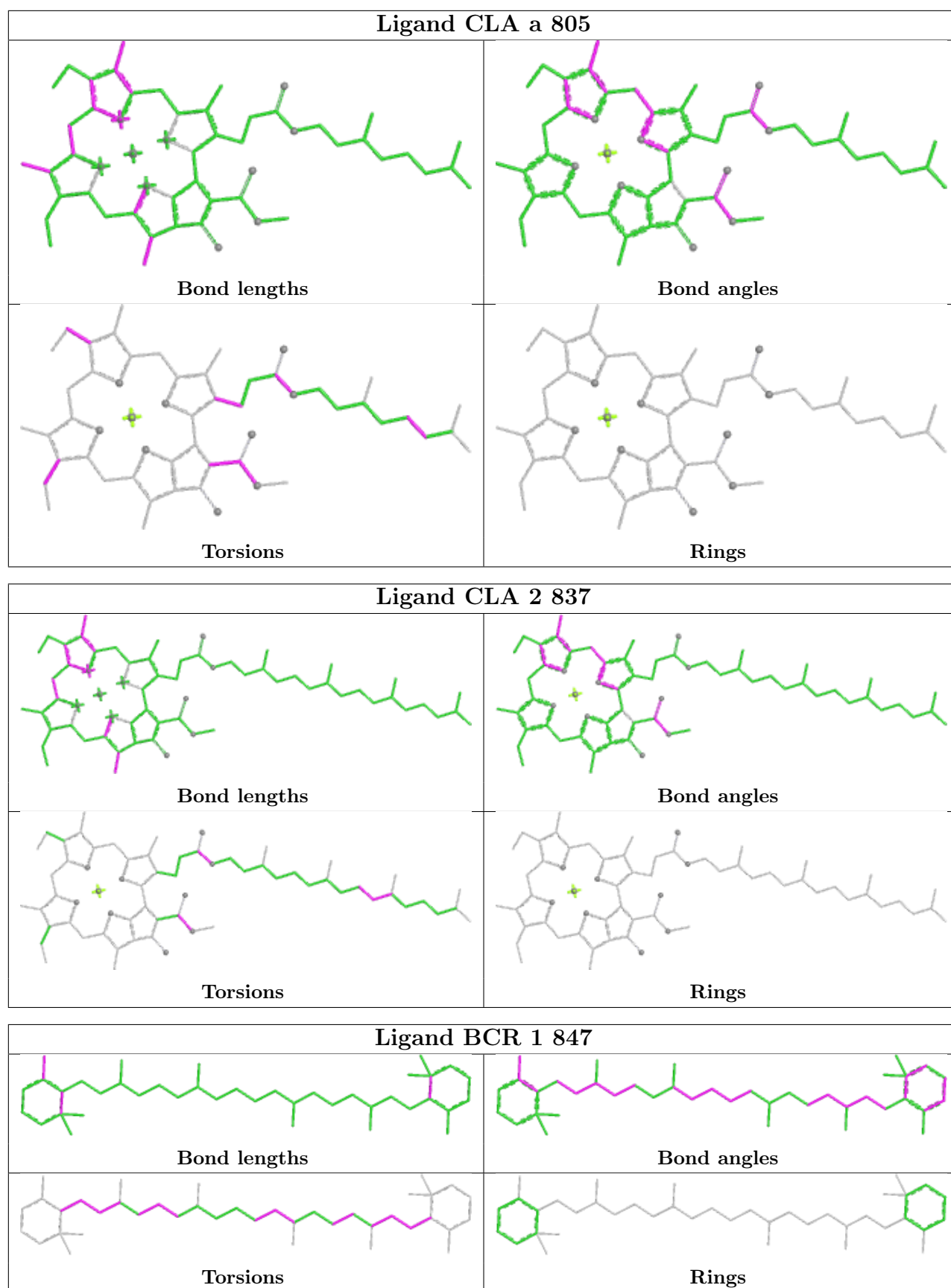
Ligand CLA 2 819

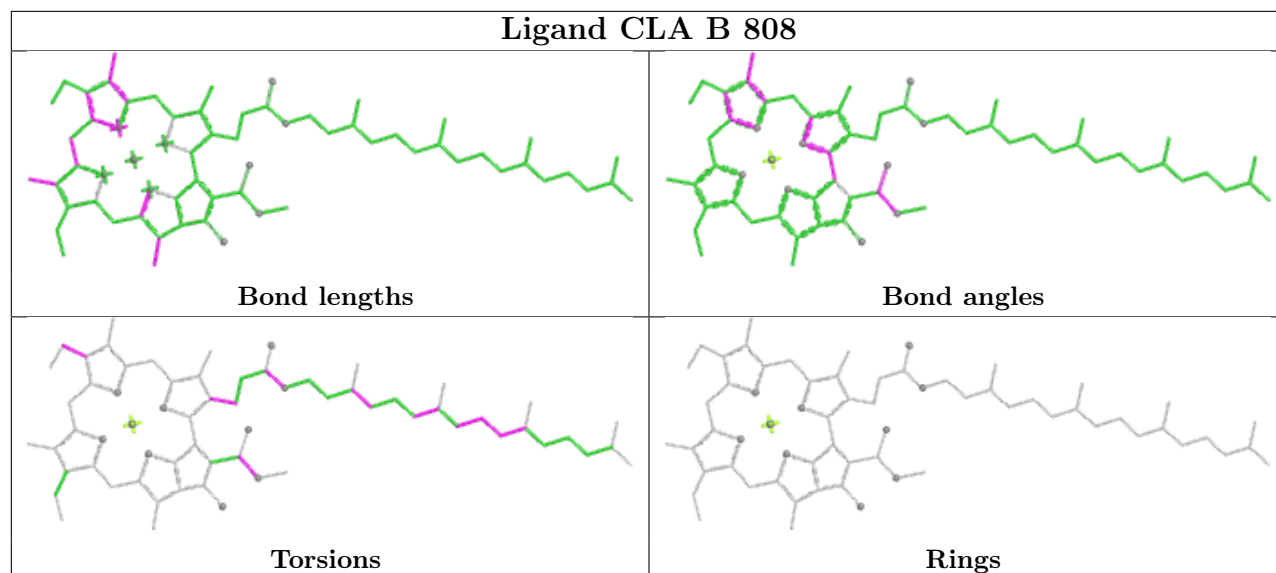
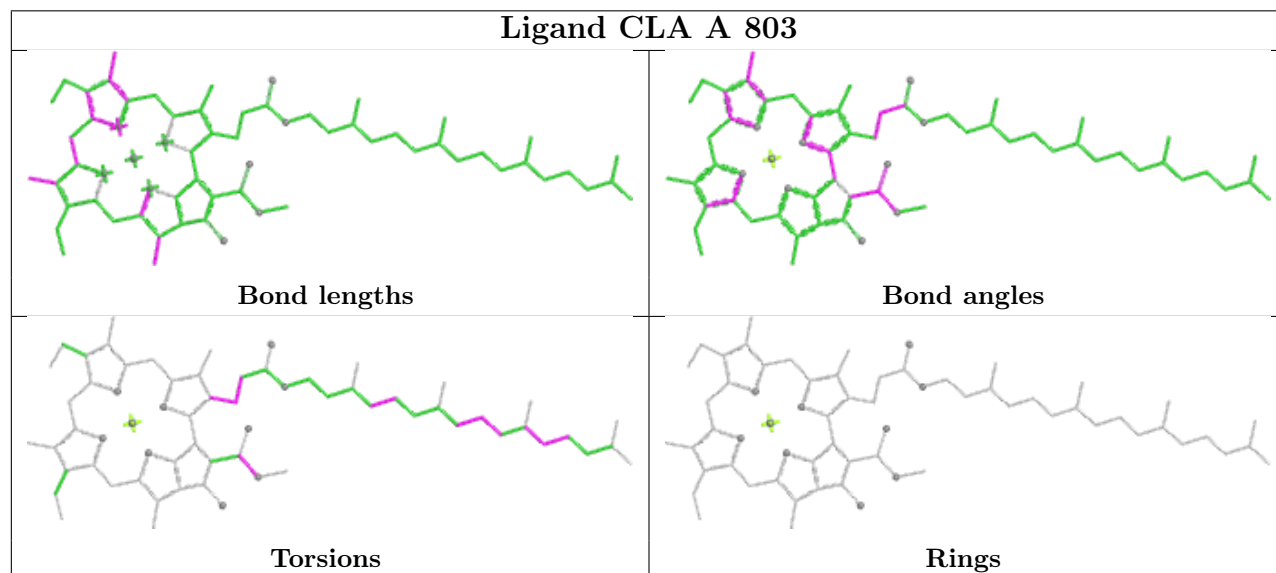
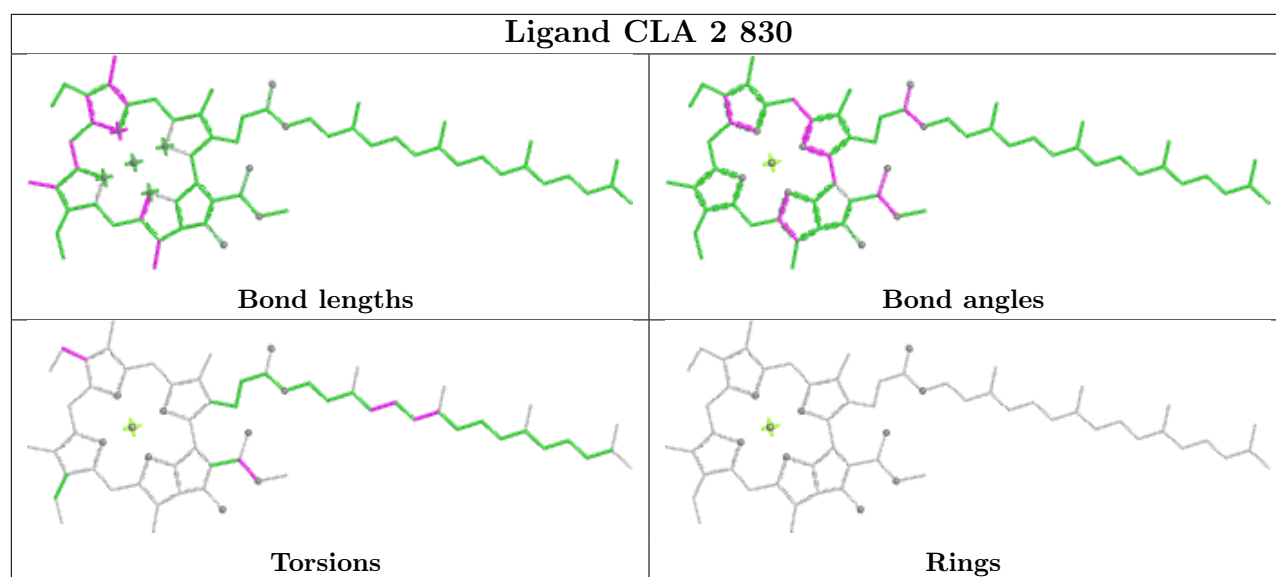


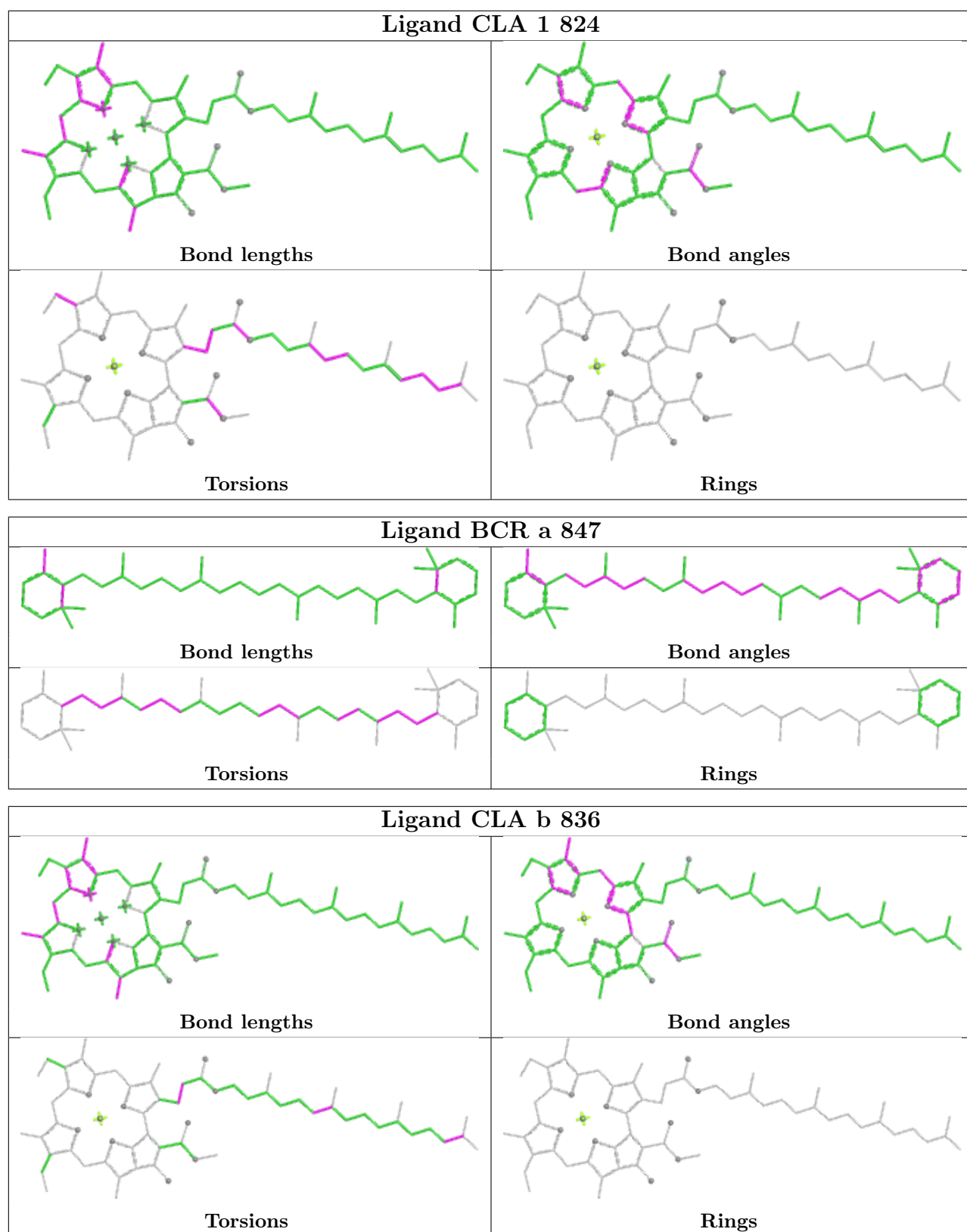


Ligand CLA 2 817

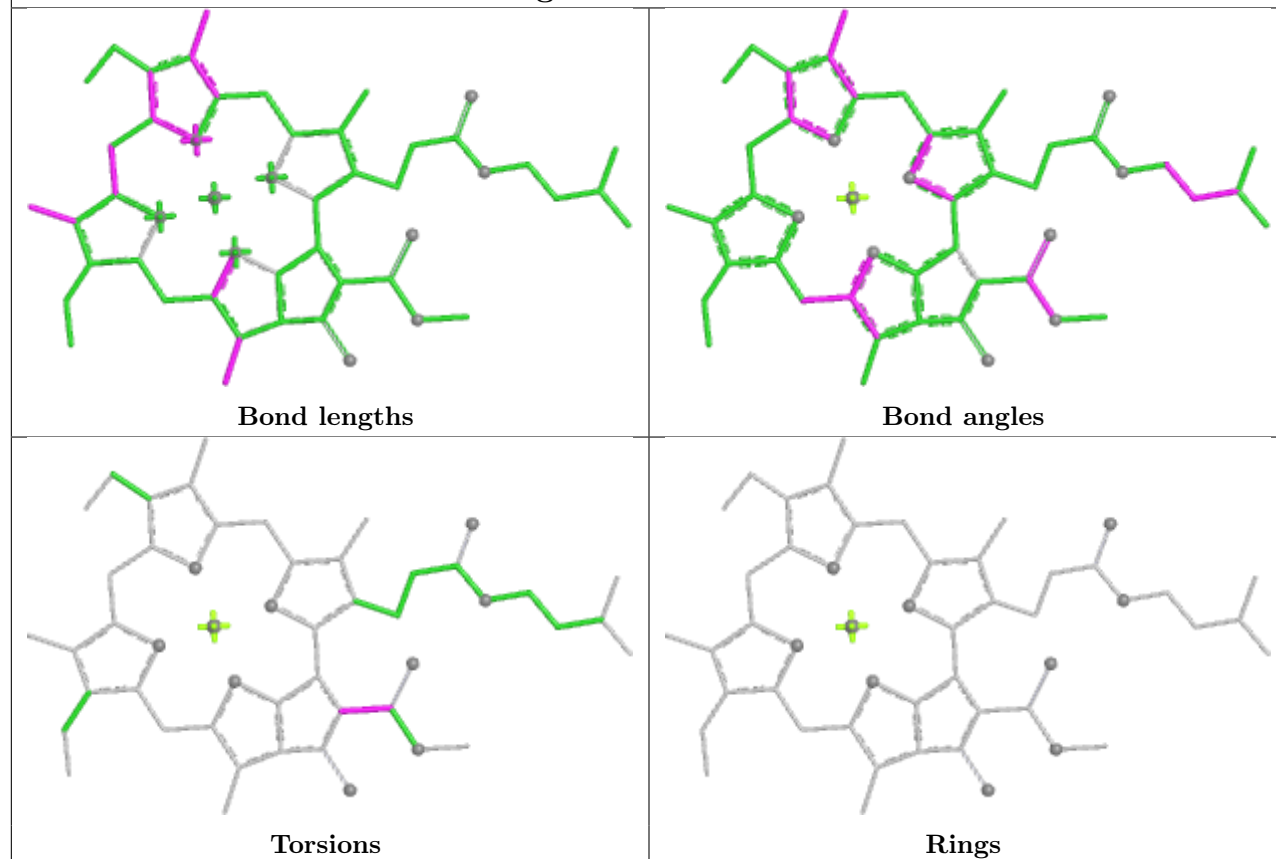




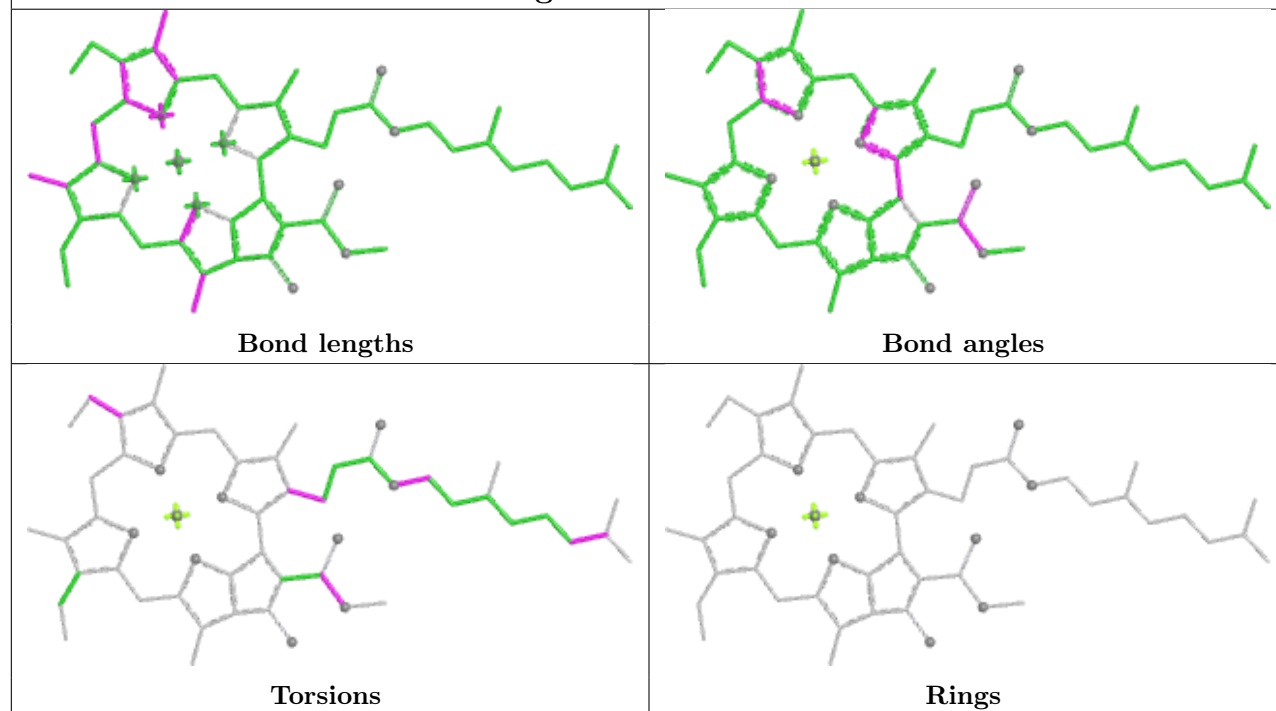


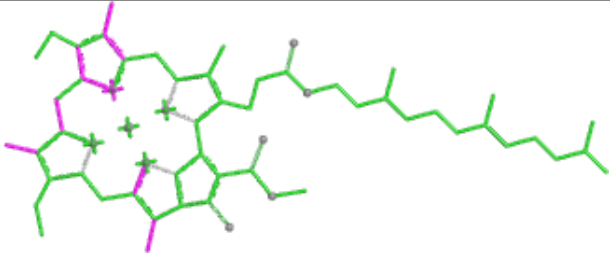
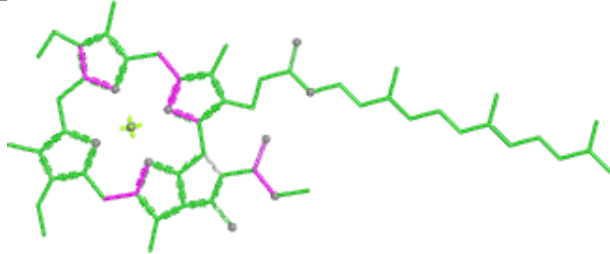
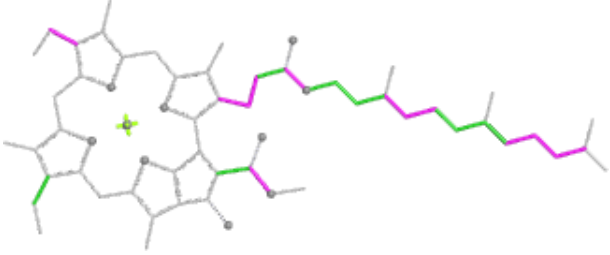
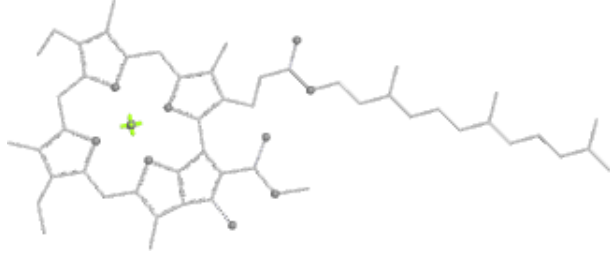
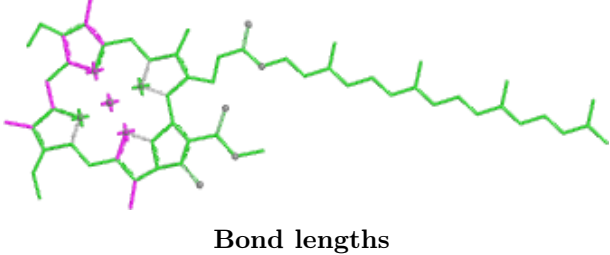
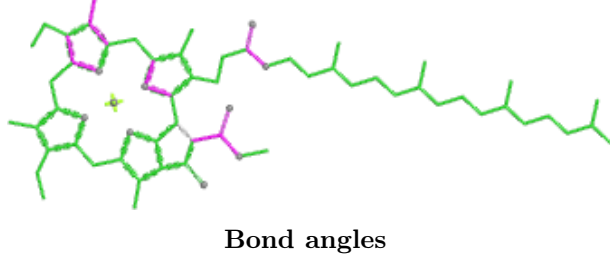
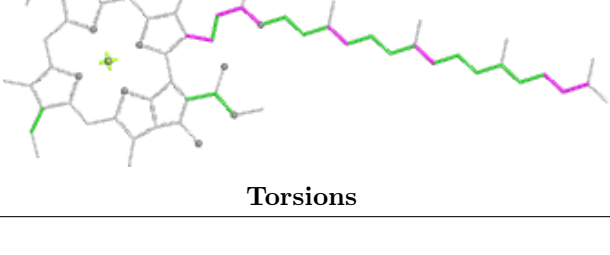
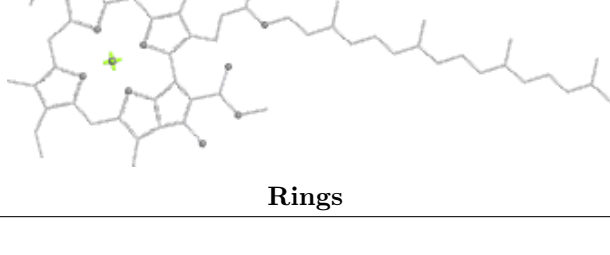


Ligand CLA 2 821

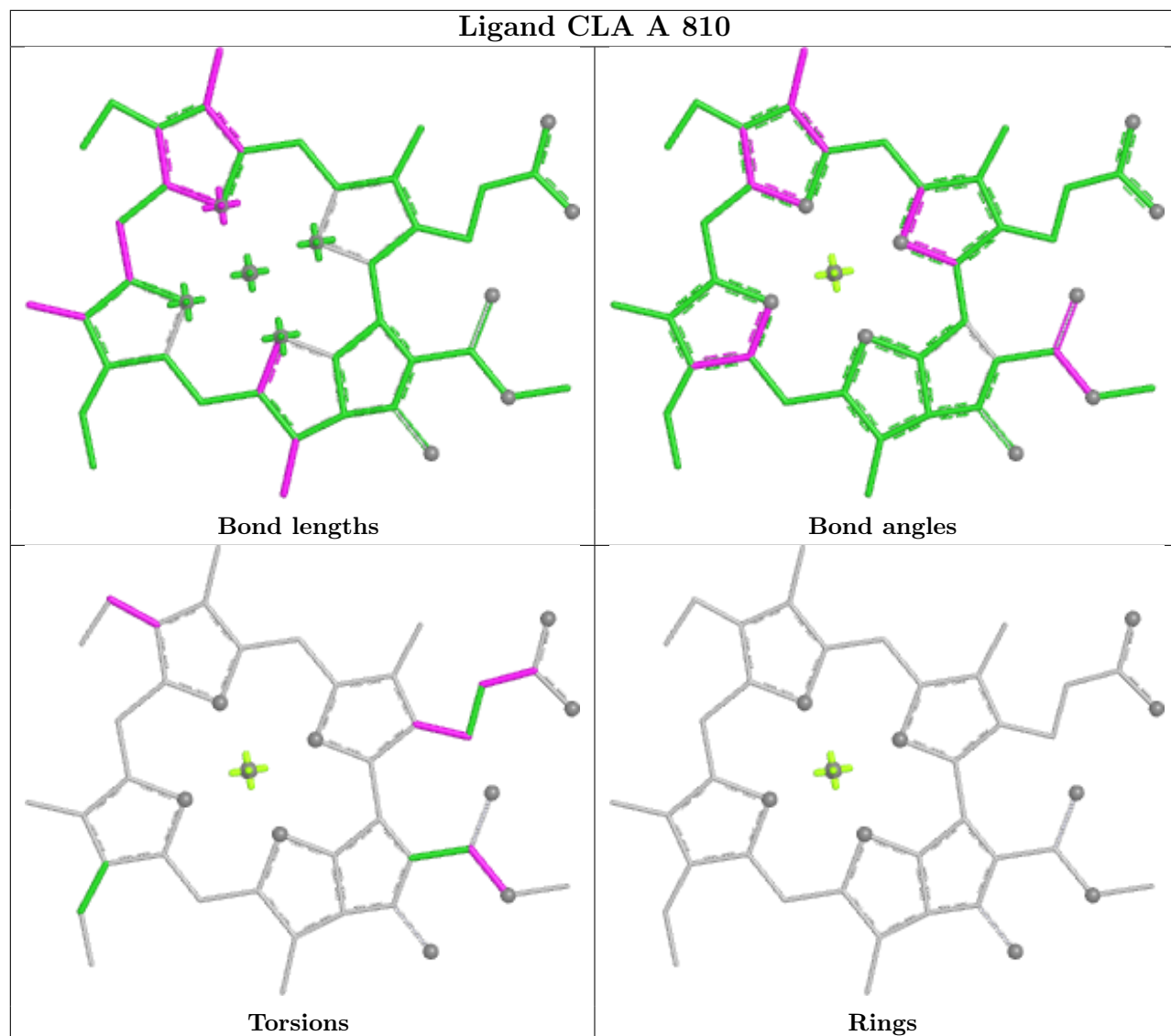


Ligand CLA b 820

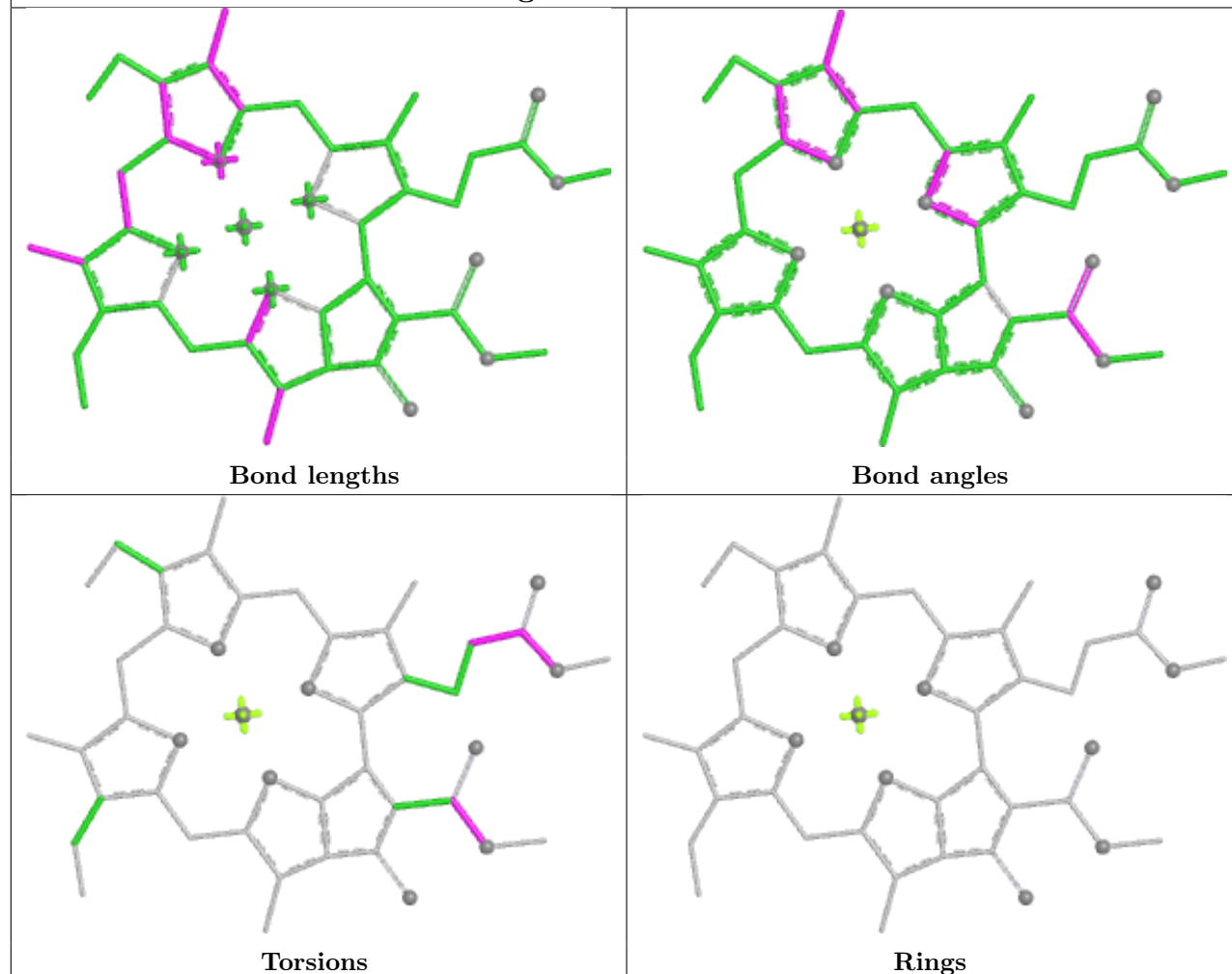


Ligand CLA a 824	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 809	
 Bond lengths	 Bond angles
 Torsions	 Rings

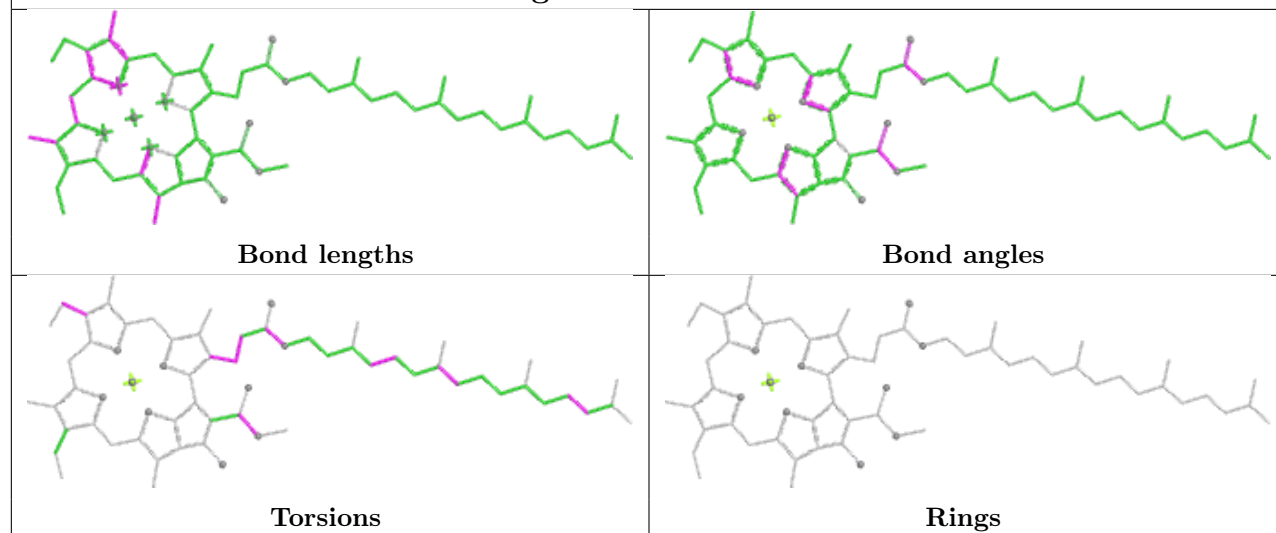
Ligand CLA A 810



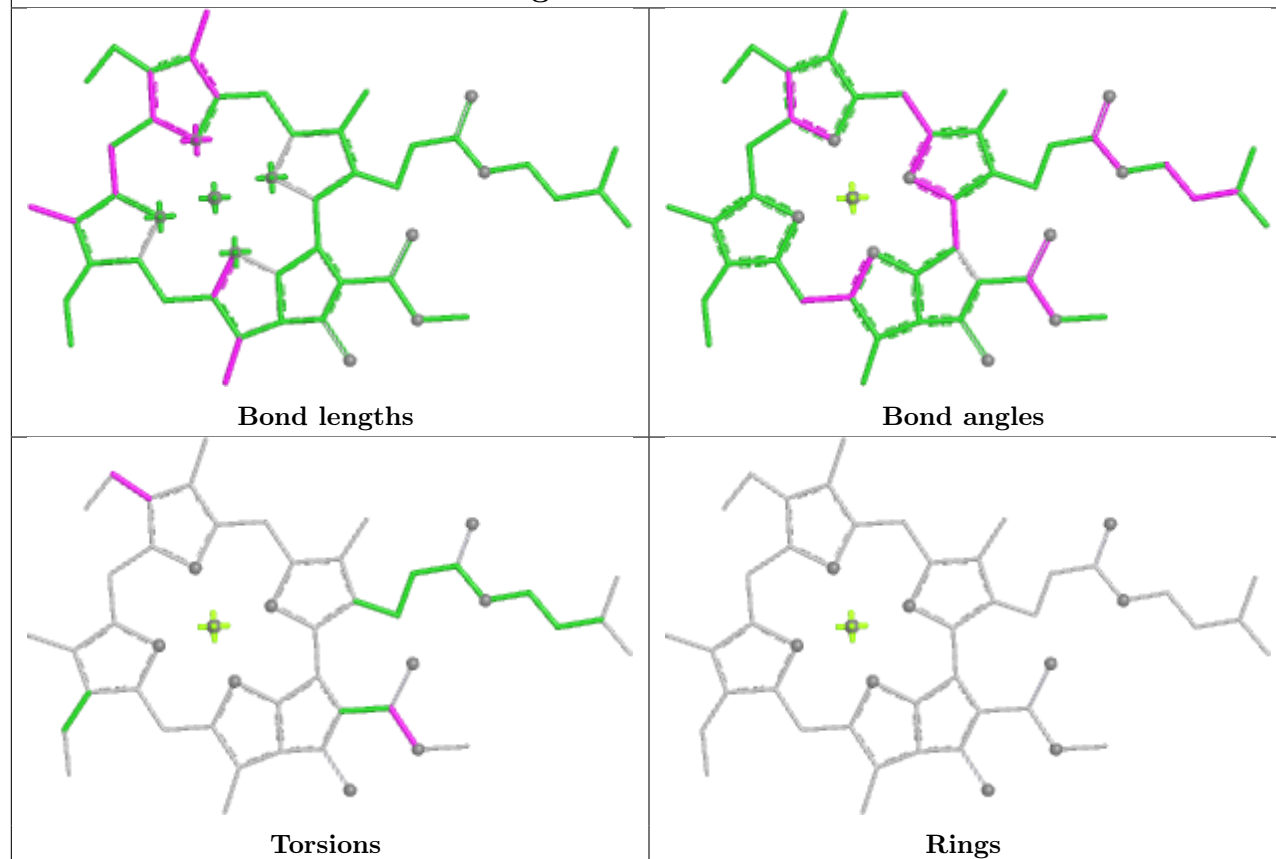
Ligand CLA 2 818



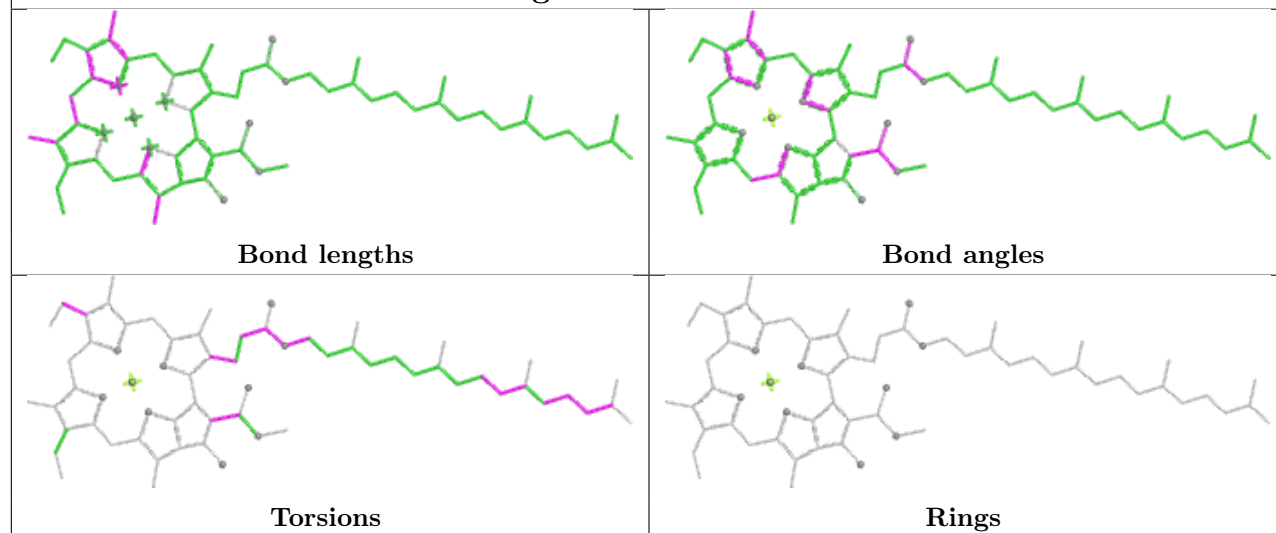
Ligand CLA A 840



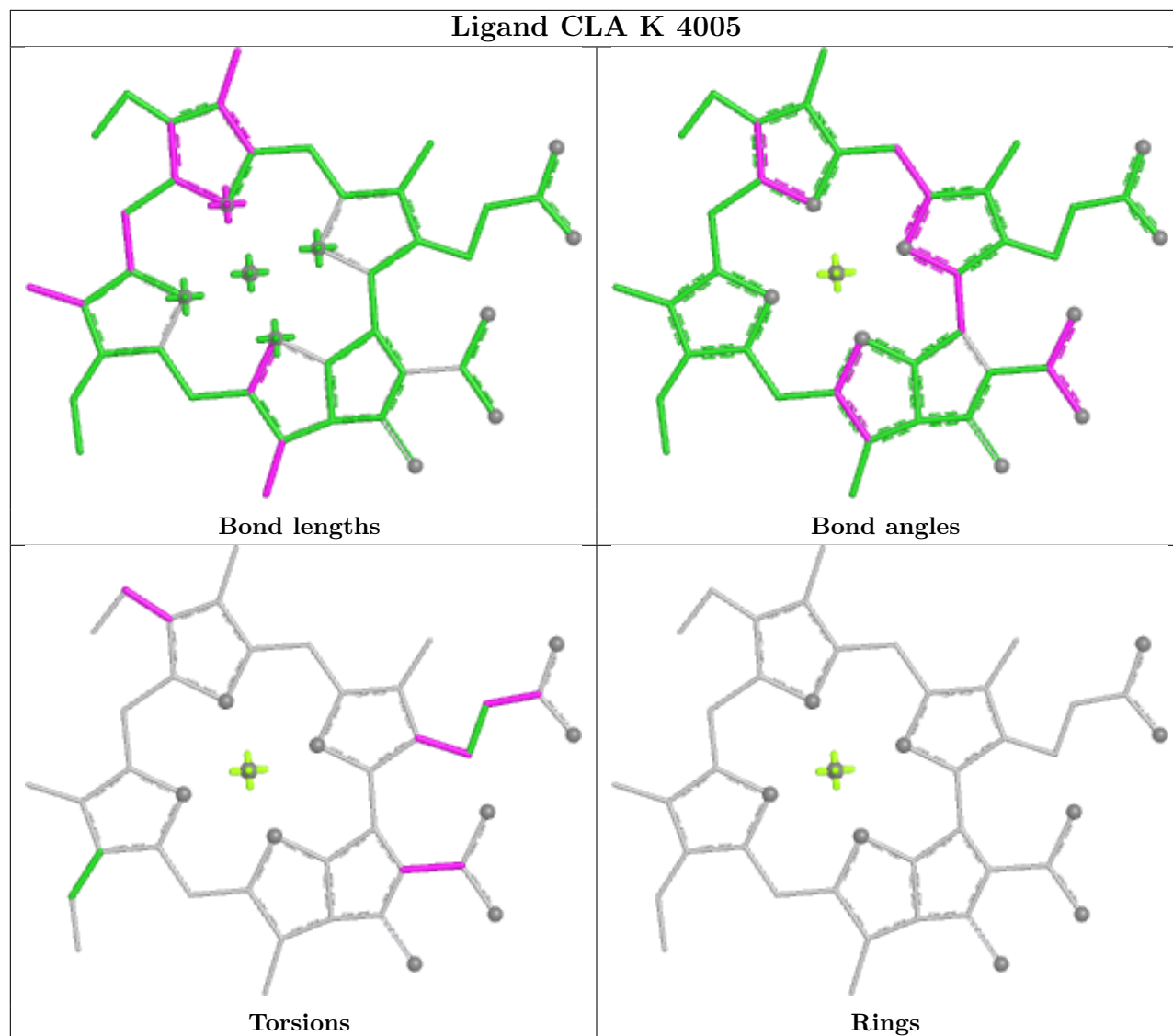
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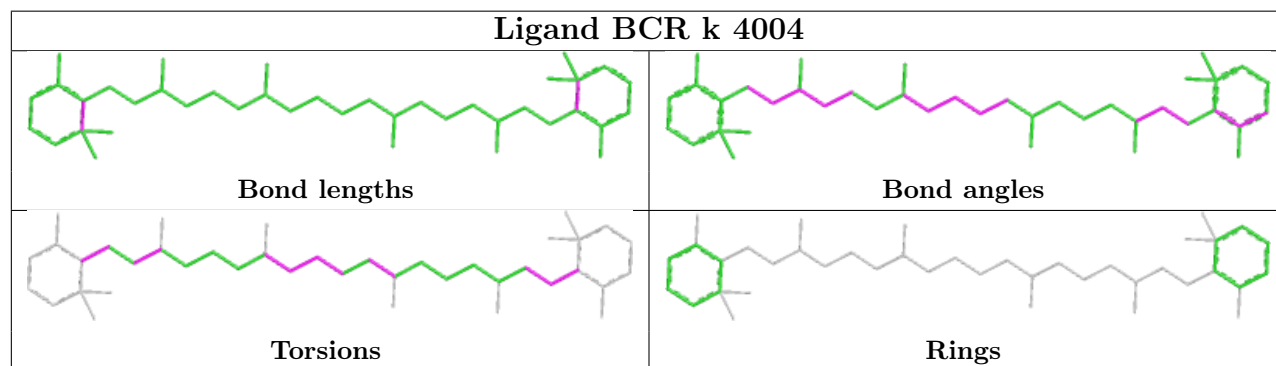
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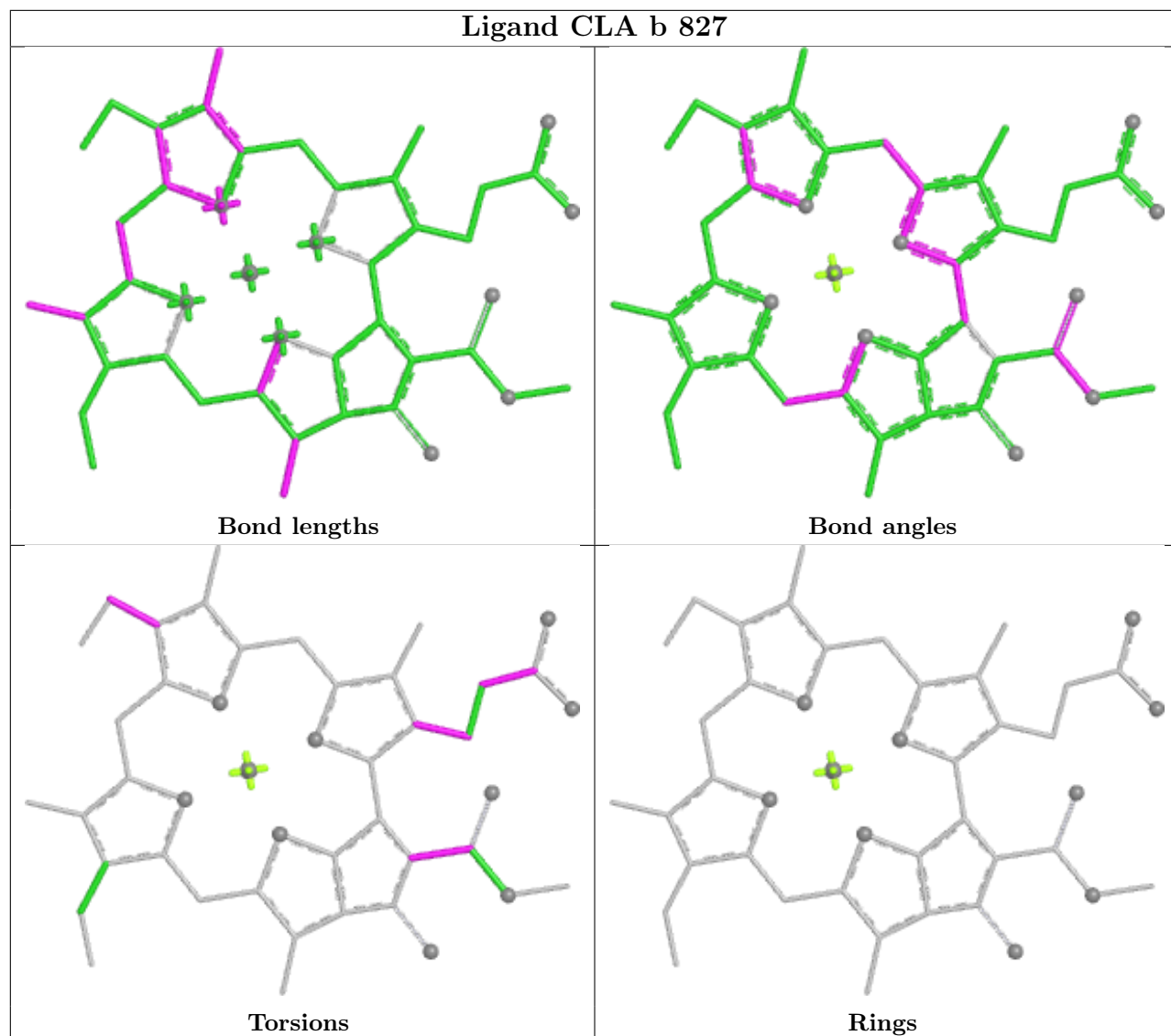
Ligand CLA K 4005

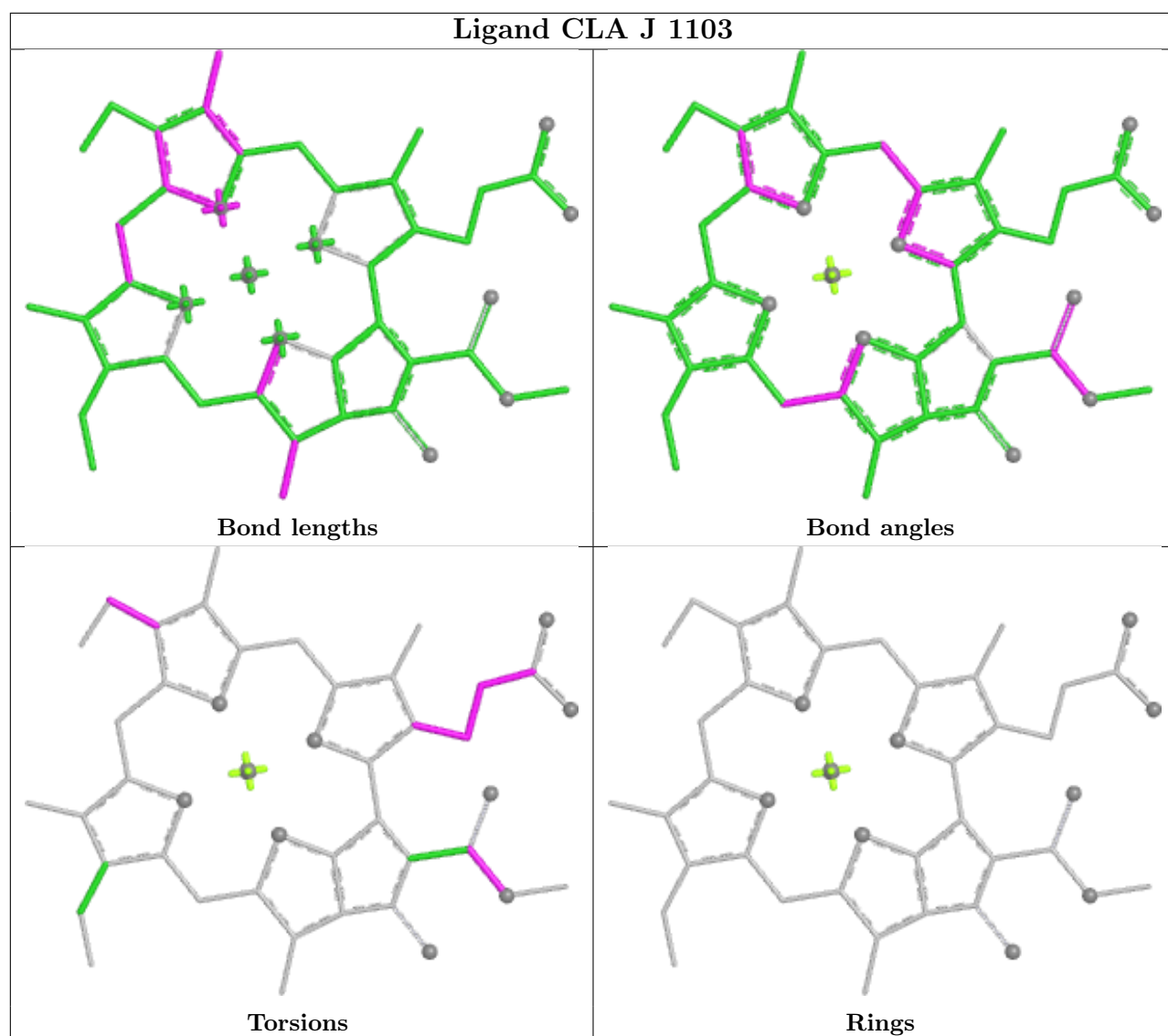


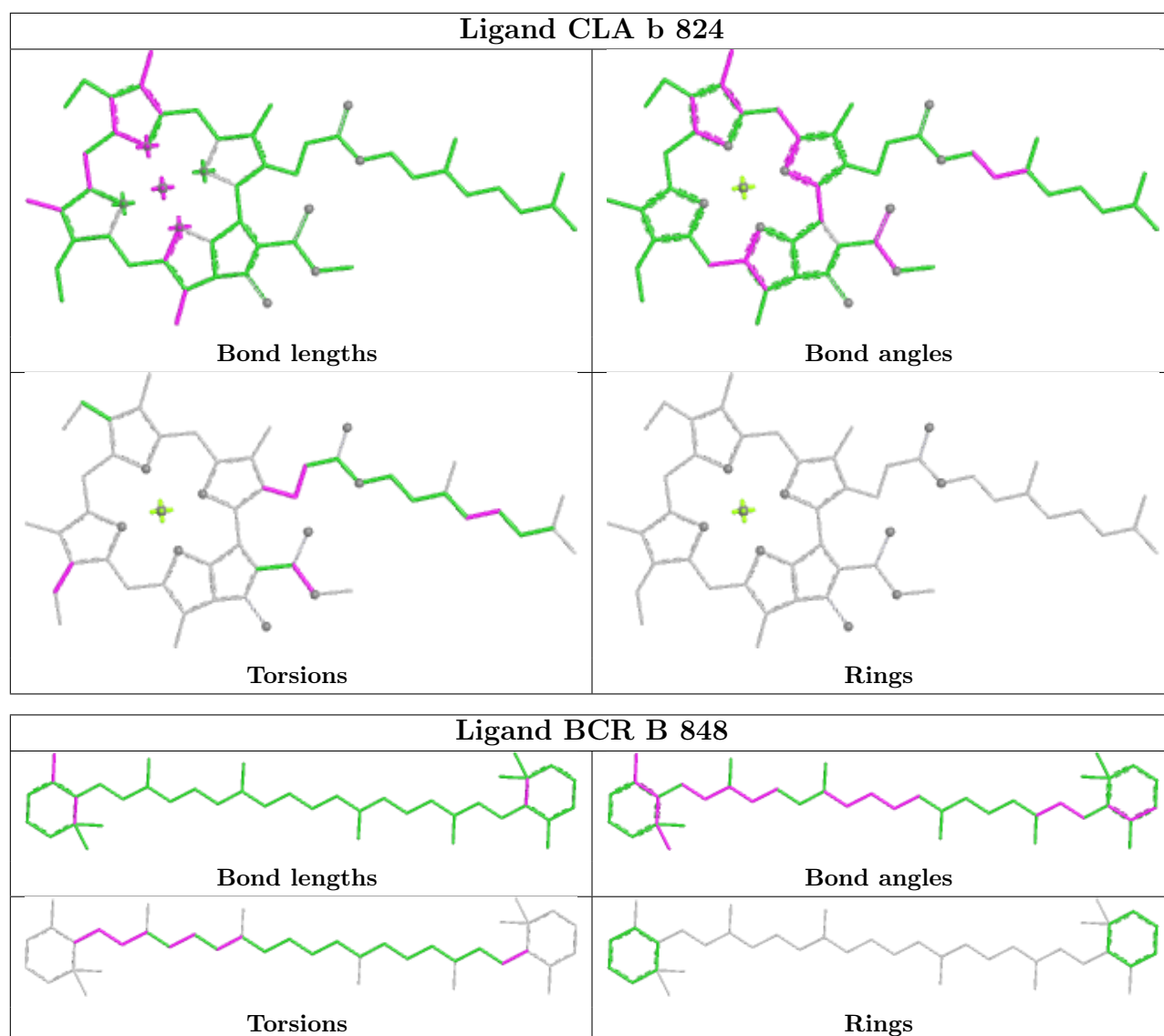
Ligand BCR k 4004



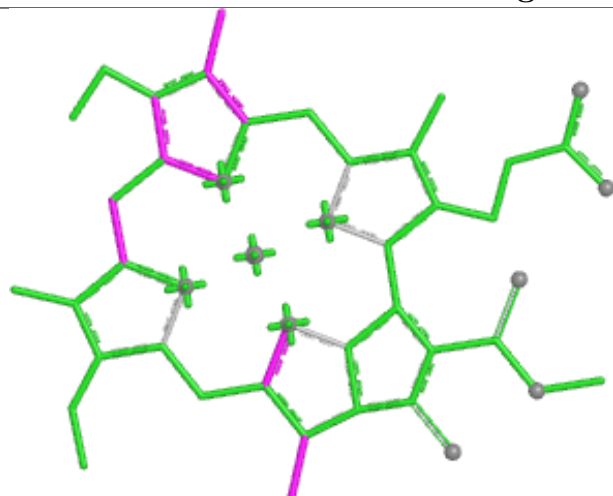
Ligand CLA b 827



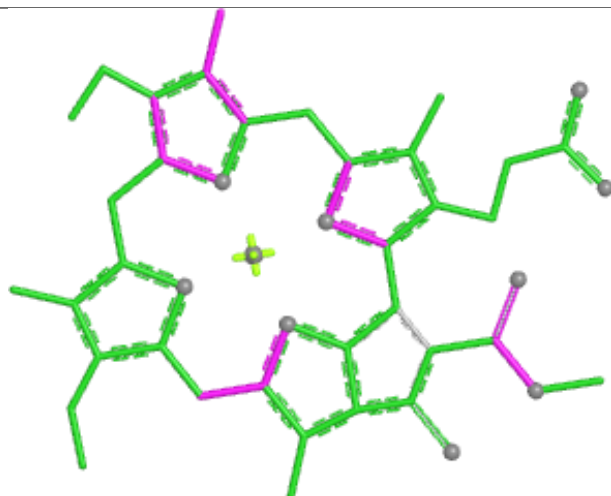




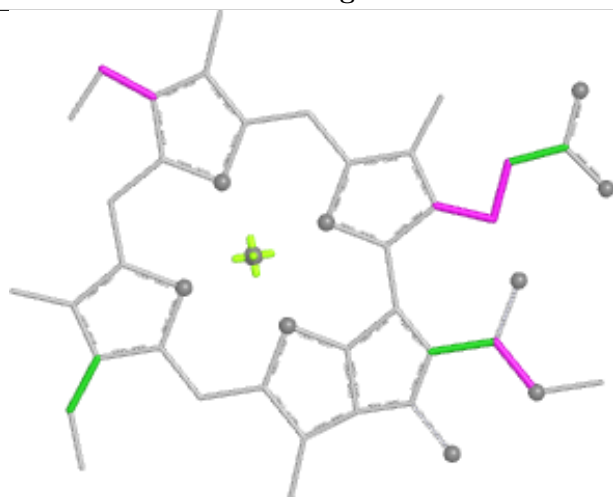
Ligand CLA b 809



Bond lengths



Bond angles

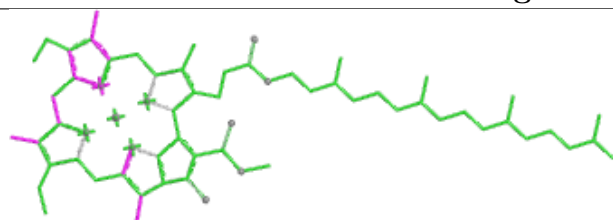


Torsions

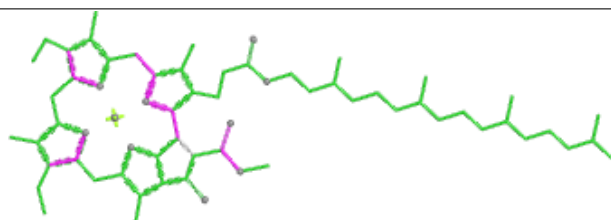


Rings

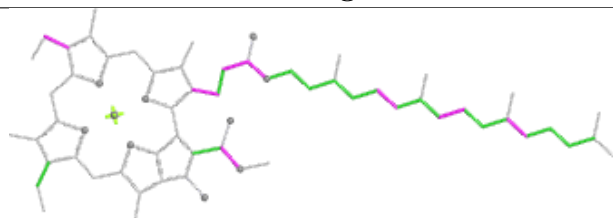
Ligand CLA A 833



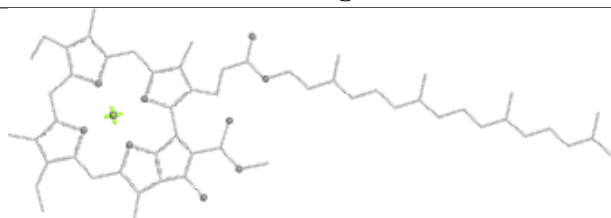
Bond lengths



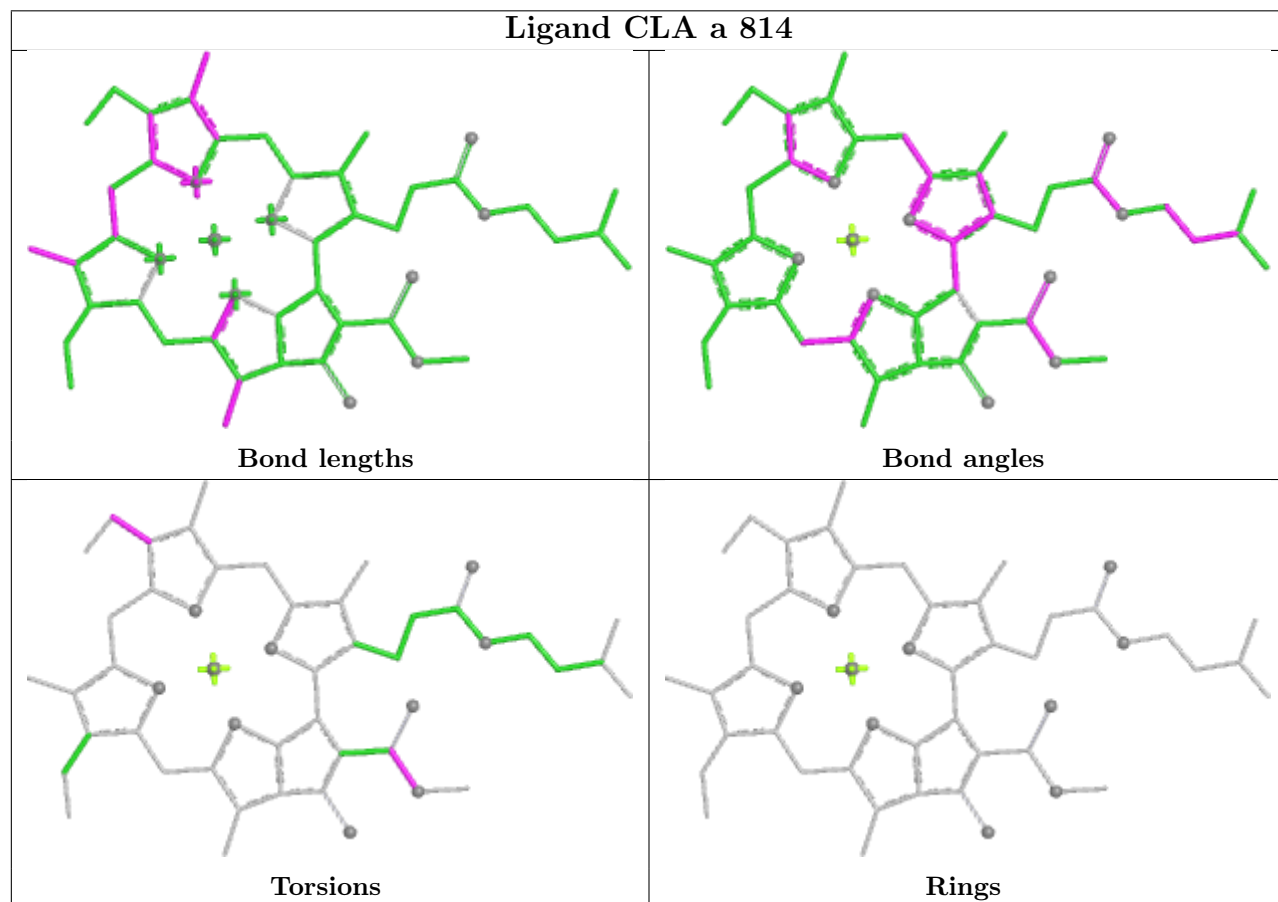
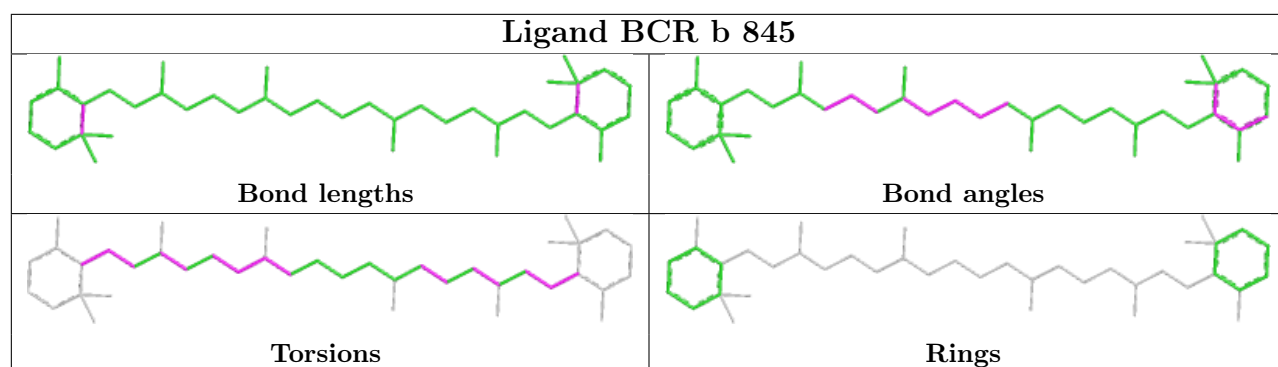
Bond angles

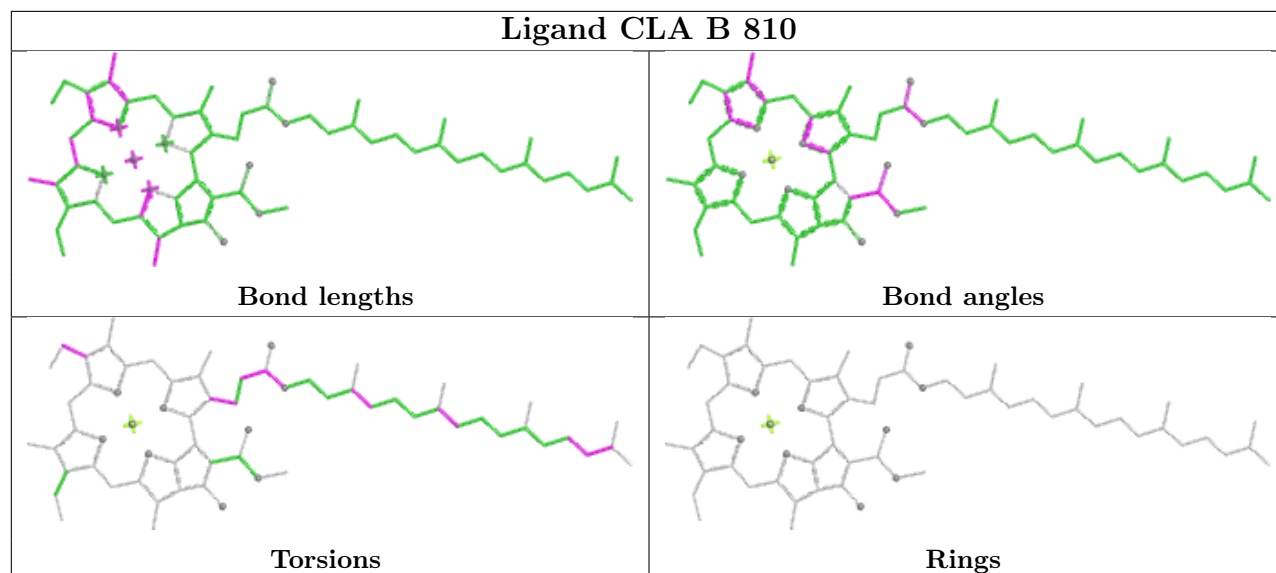
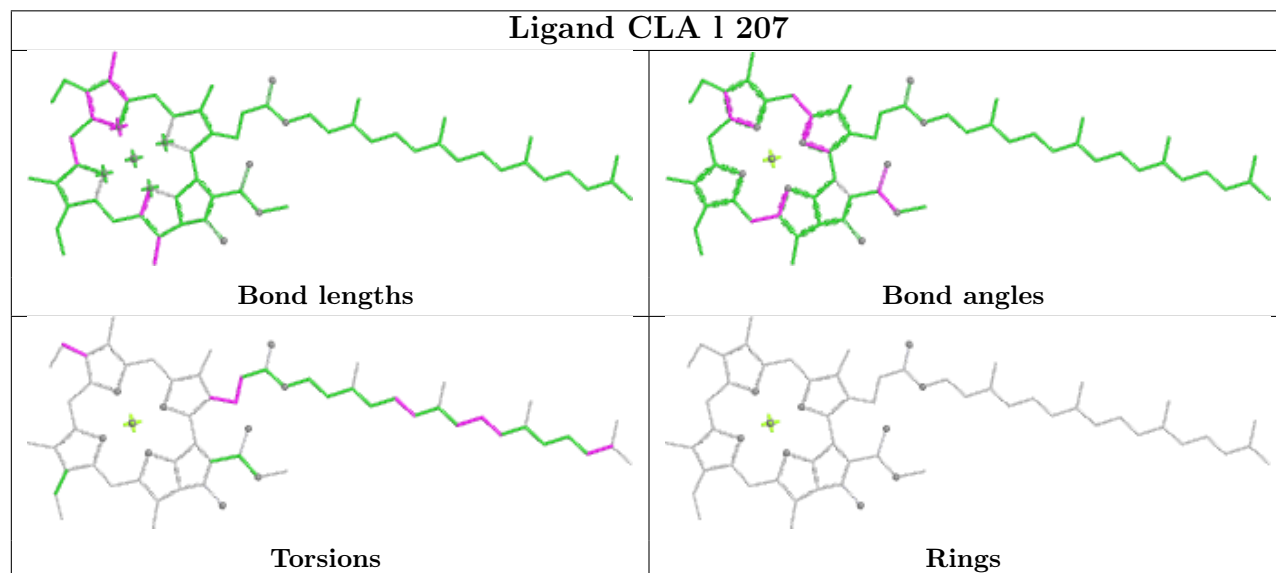
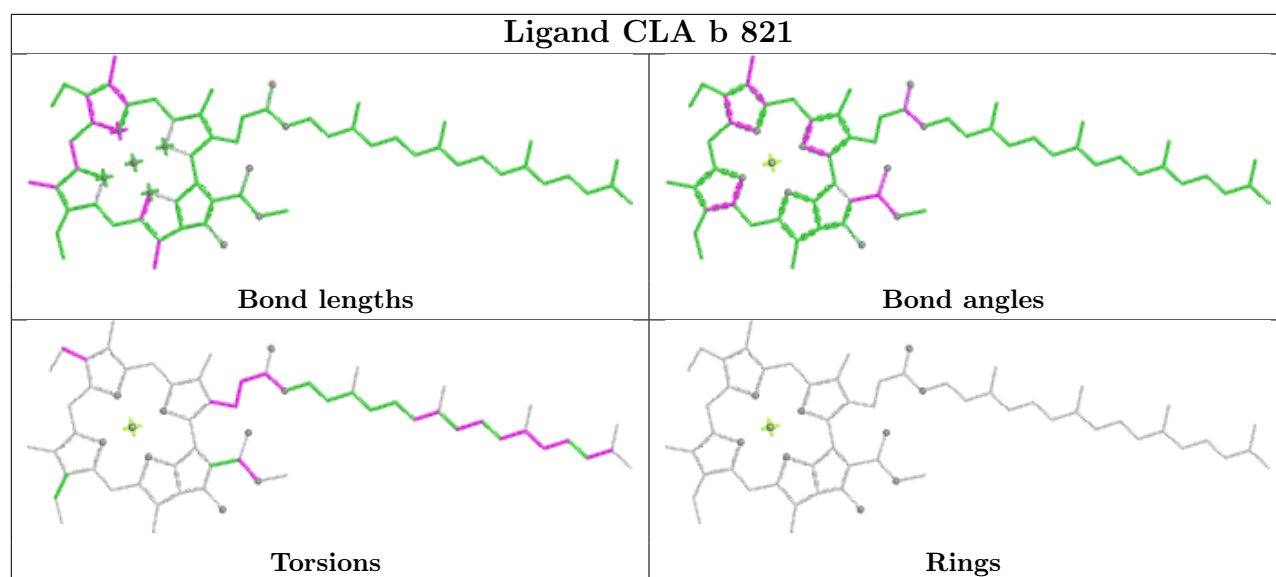


Torsions

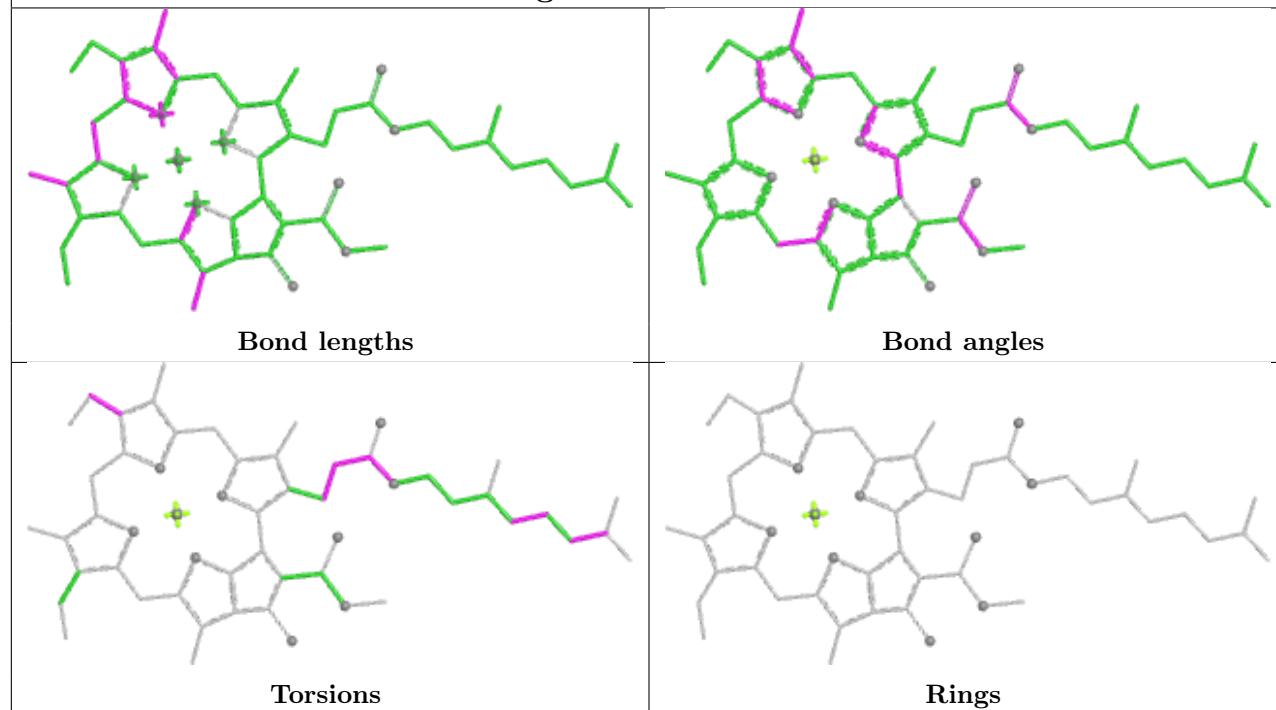


Rings

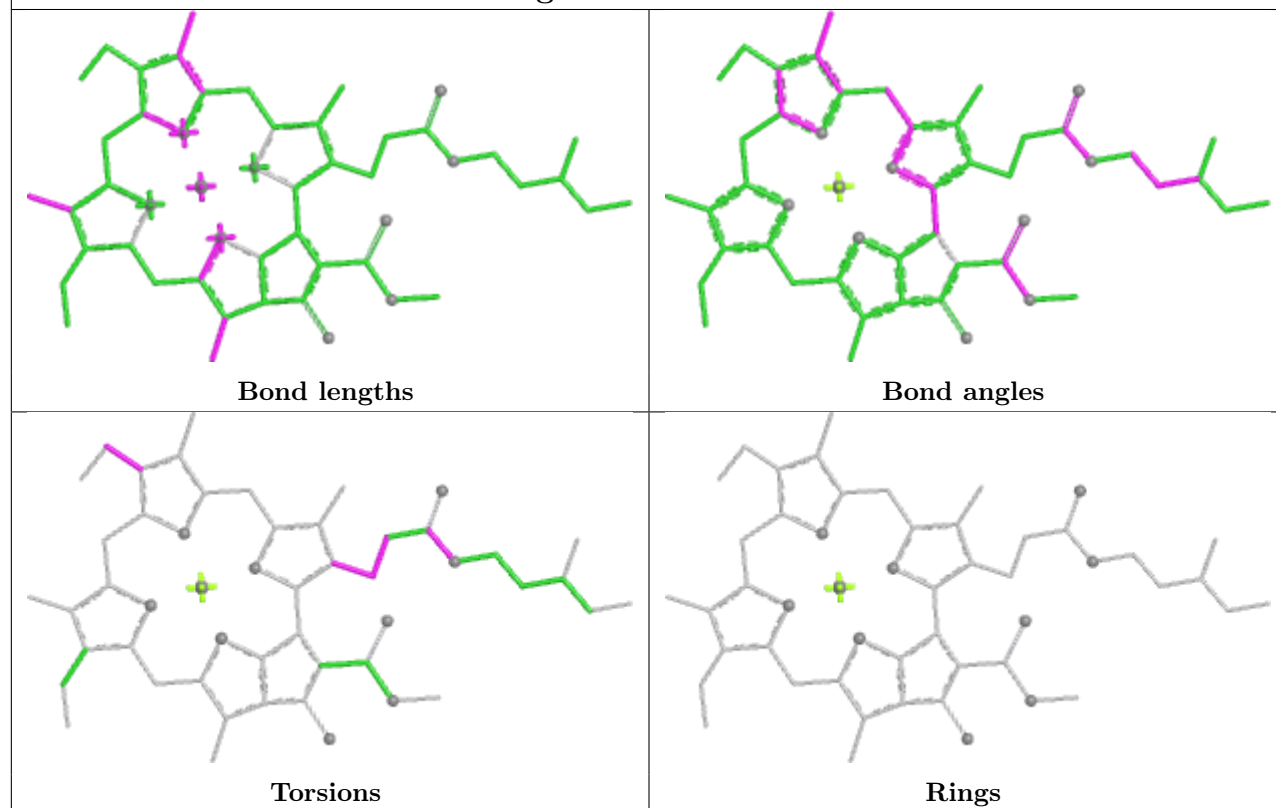


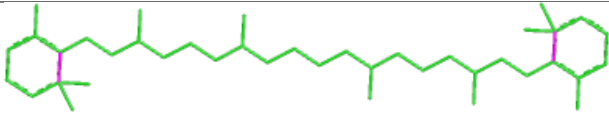
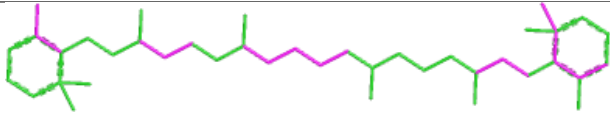
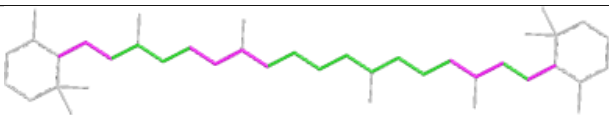
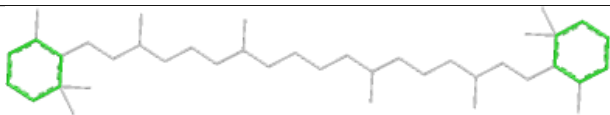


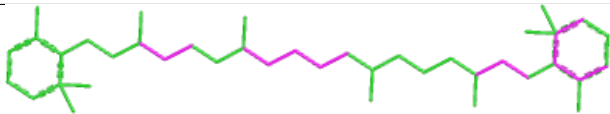
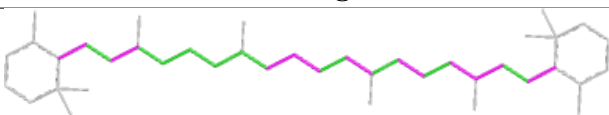
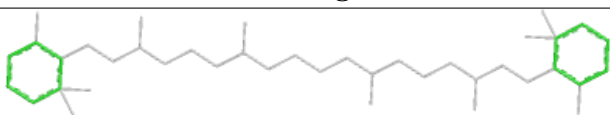
Ligand CLA a 817

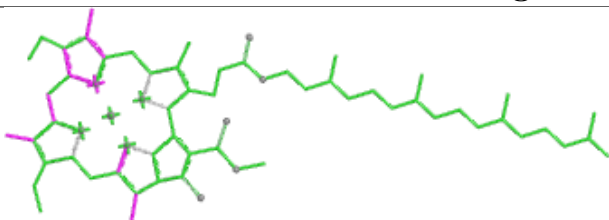
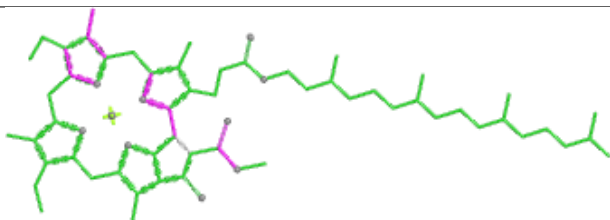
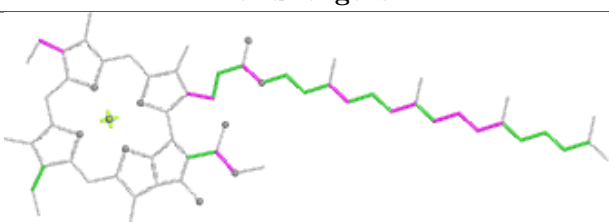
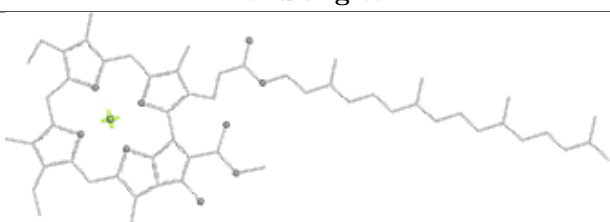


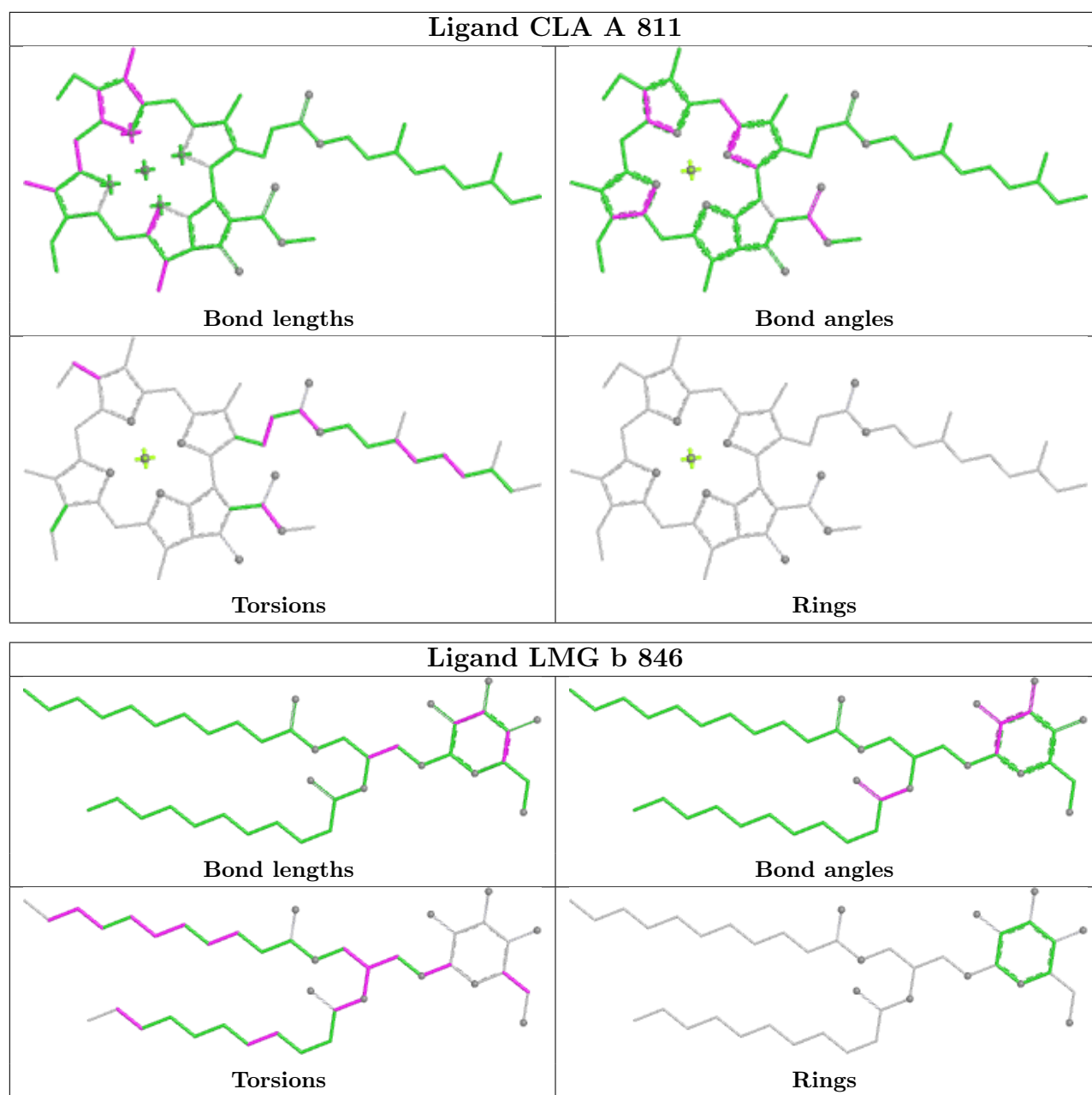
Ligand CLA a 836



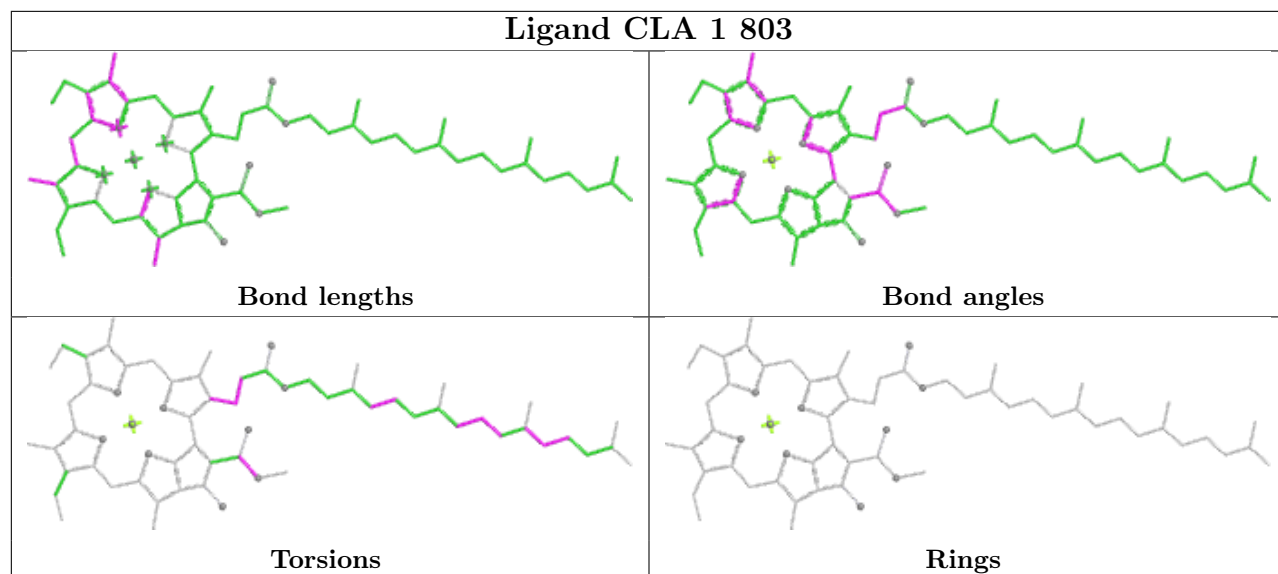
Ligand BCR f 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR f 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

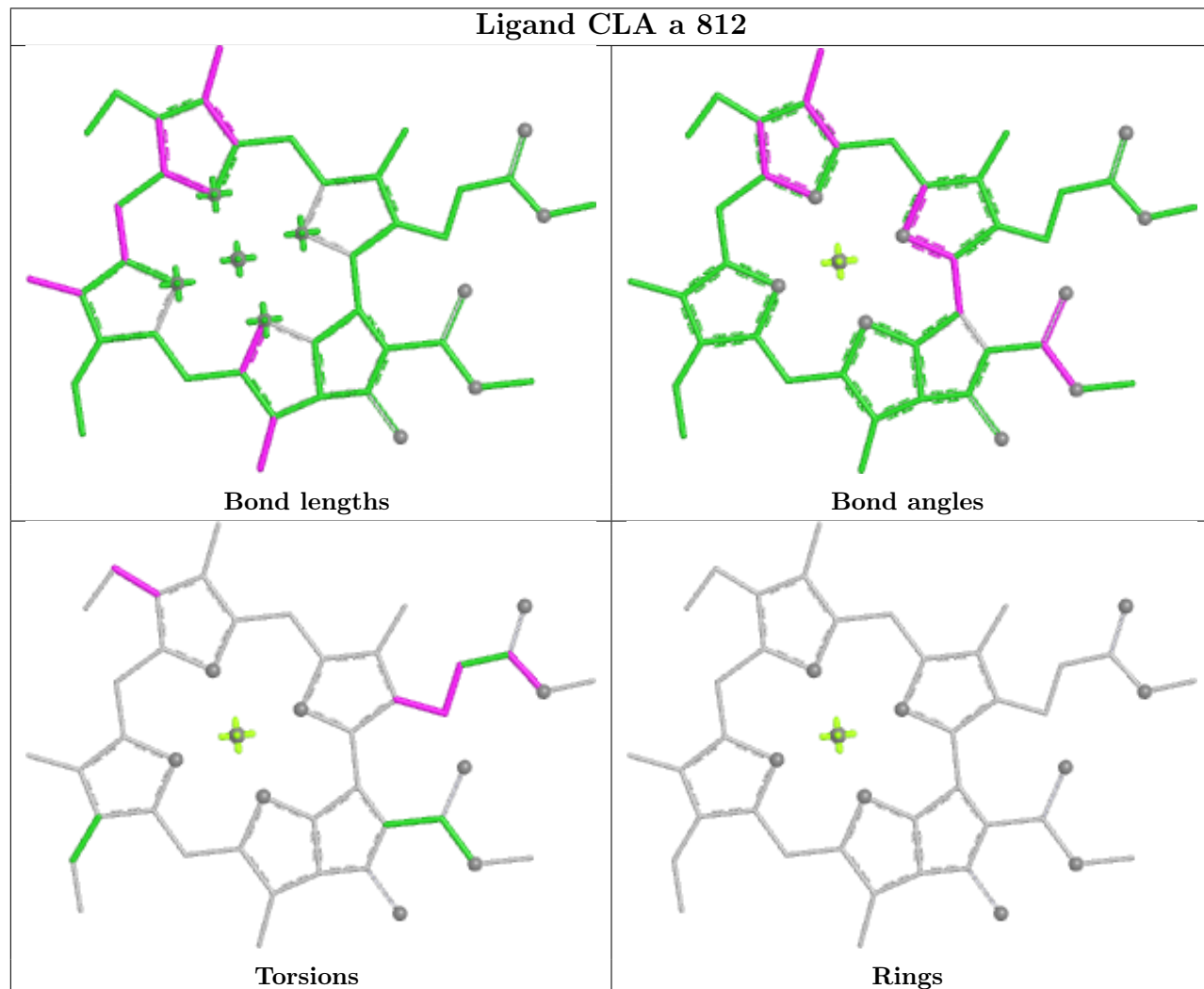
Ligand CLA b 808	
	
Bond lengths	Bond angles
	
Torsions	Rings

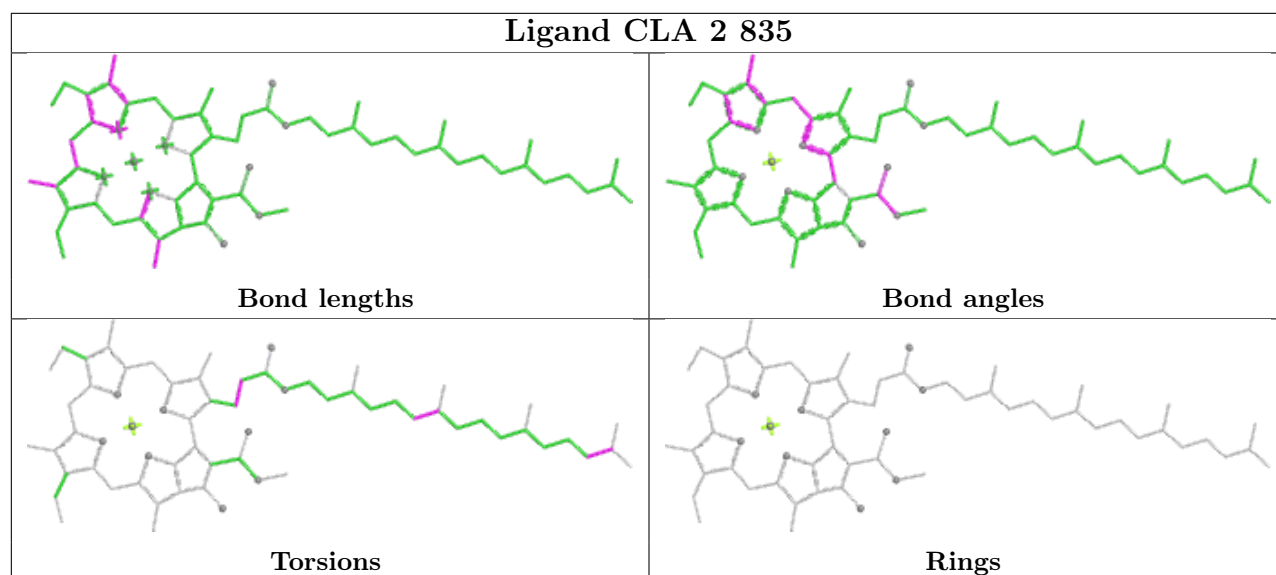
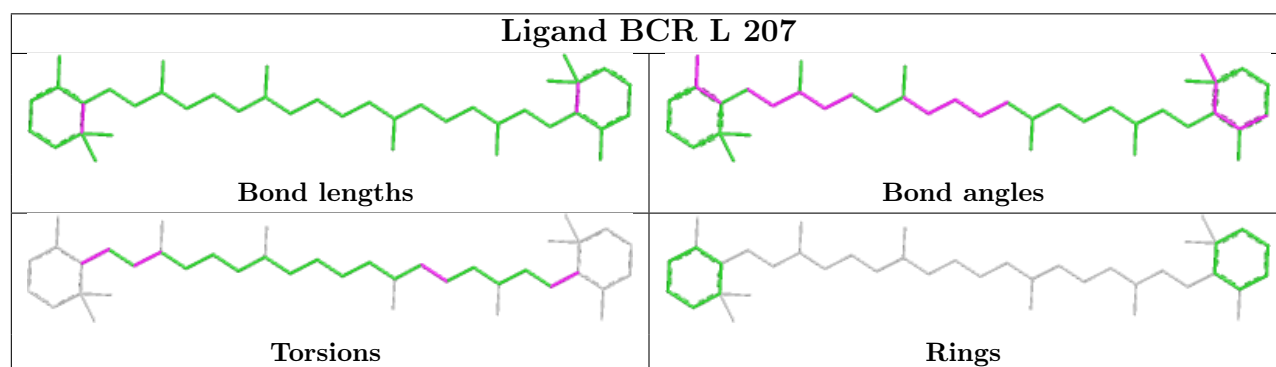
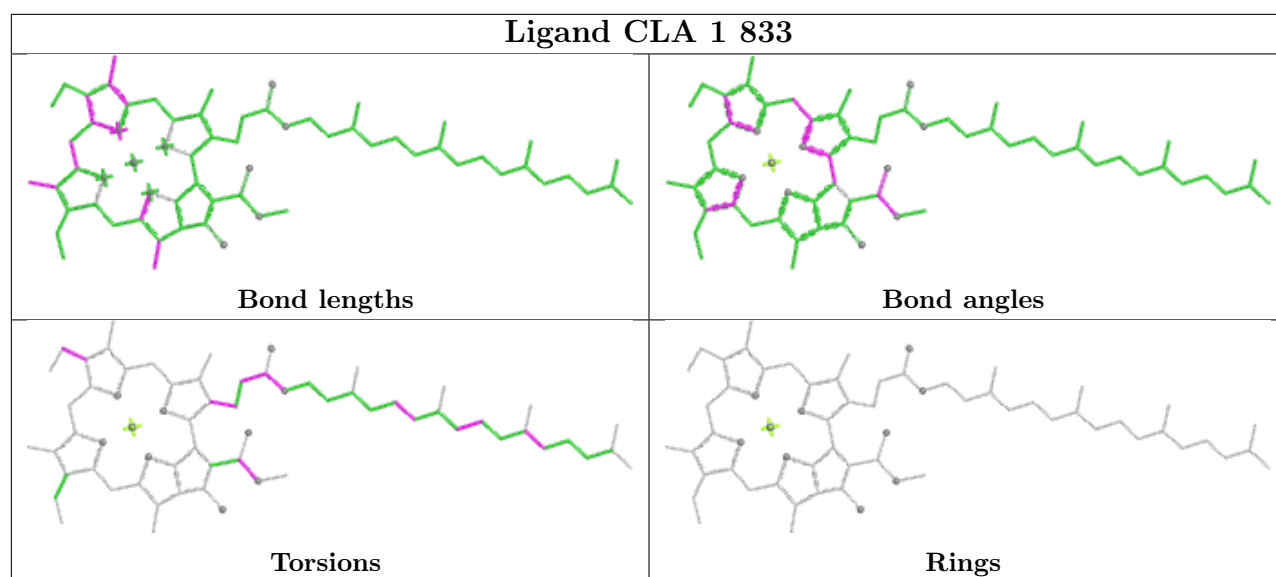


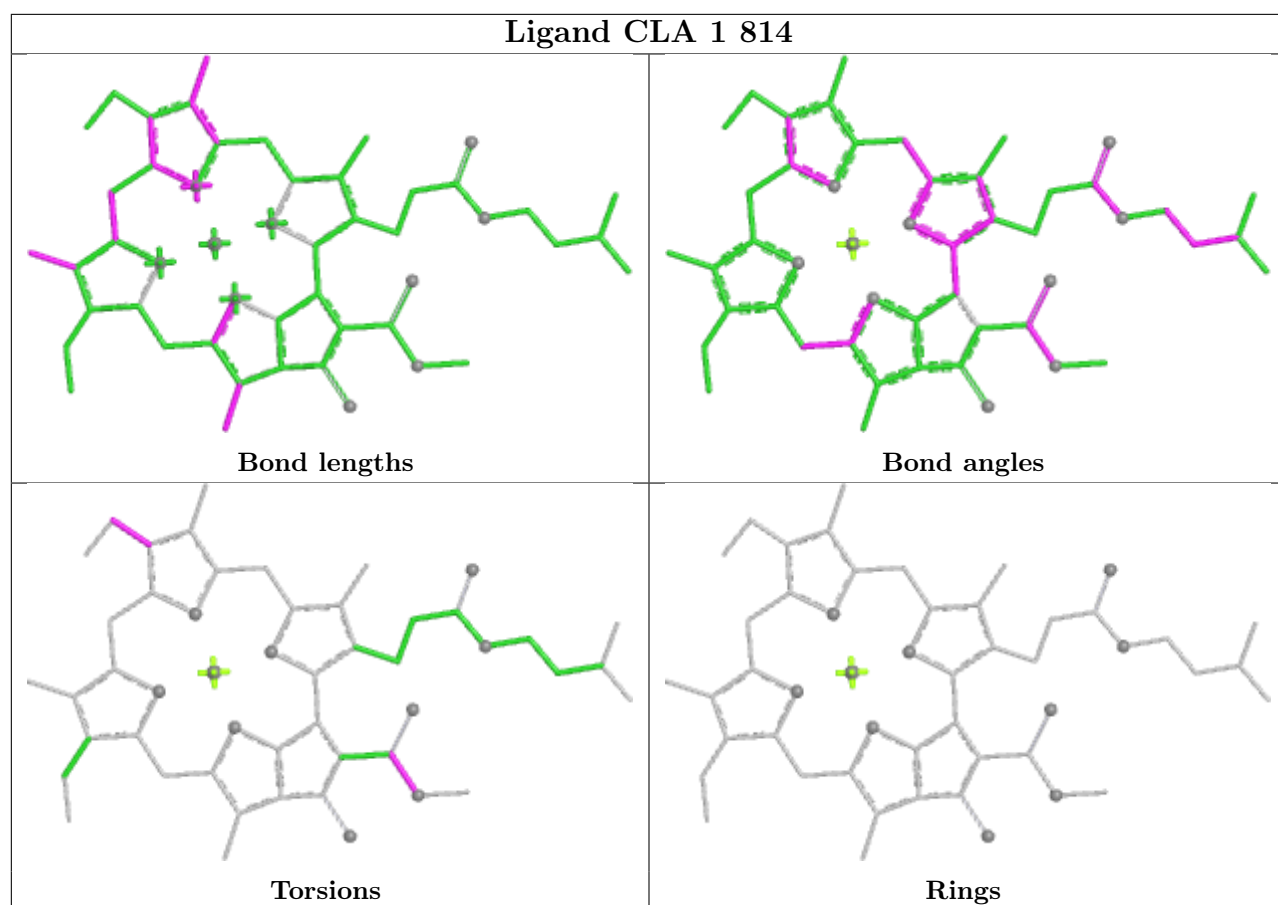
Ligand CLA 1 803



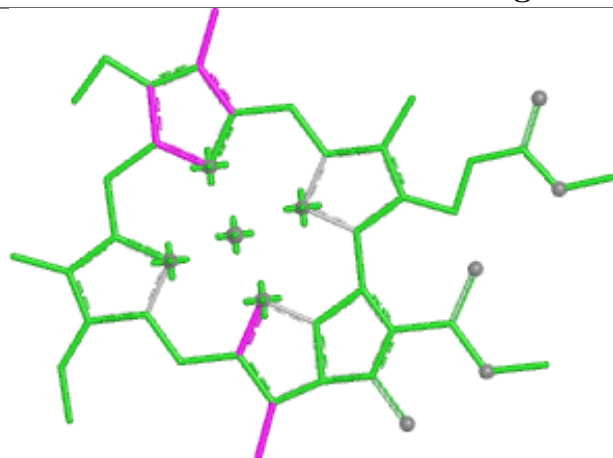
Ligand CLA a 812



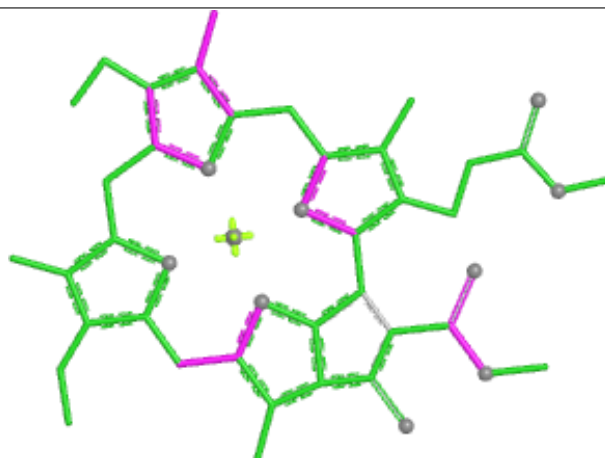




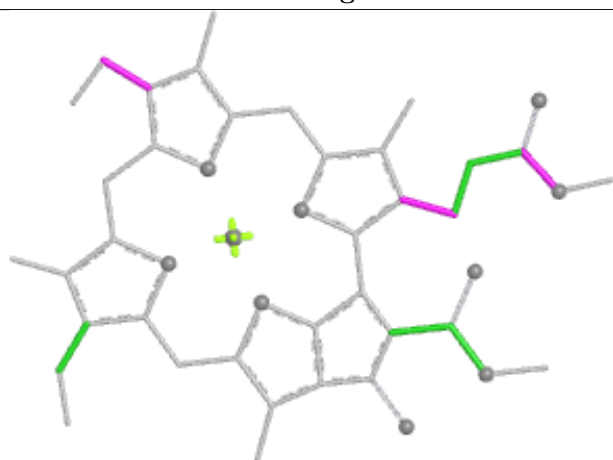
Ligand CLA A 820



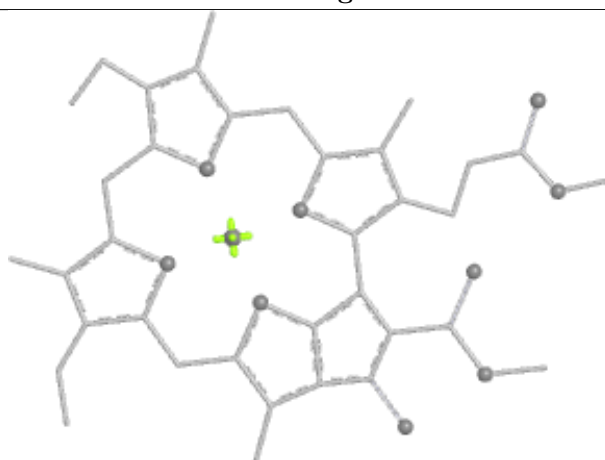
Bond lengths



Bond angles

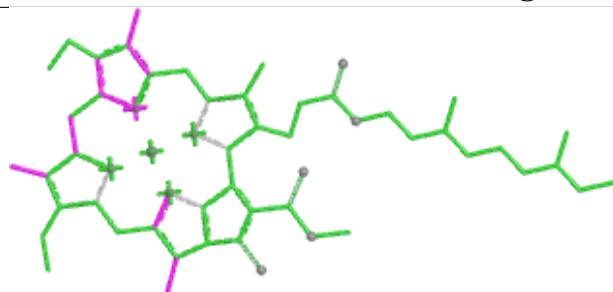


Torsions

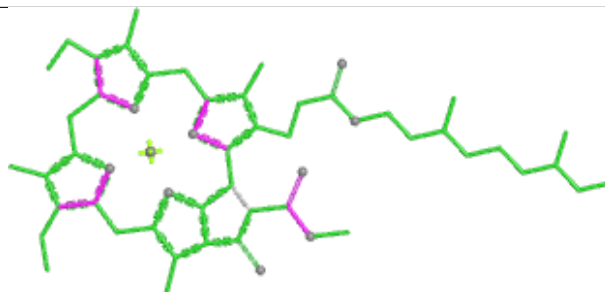


Rings

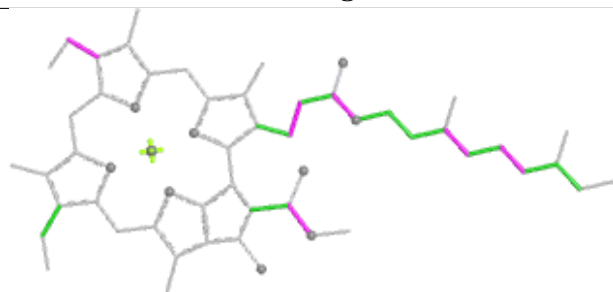
Ligand CLA 1 811



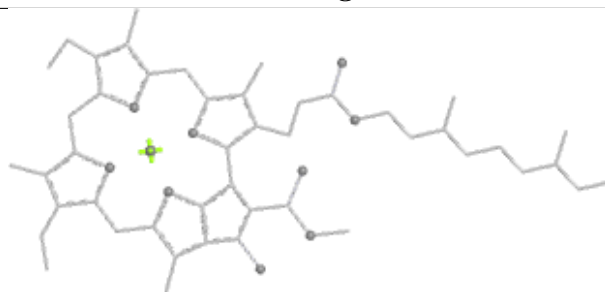
Bond lengths



Bond angles

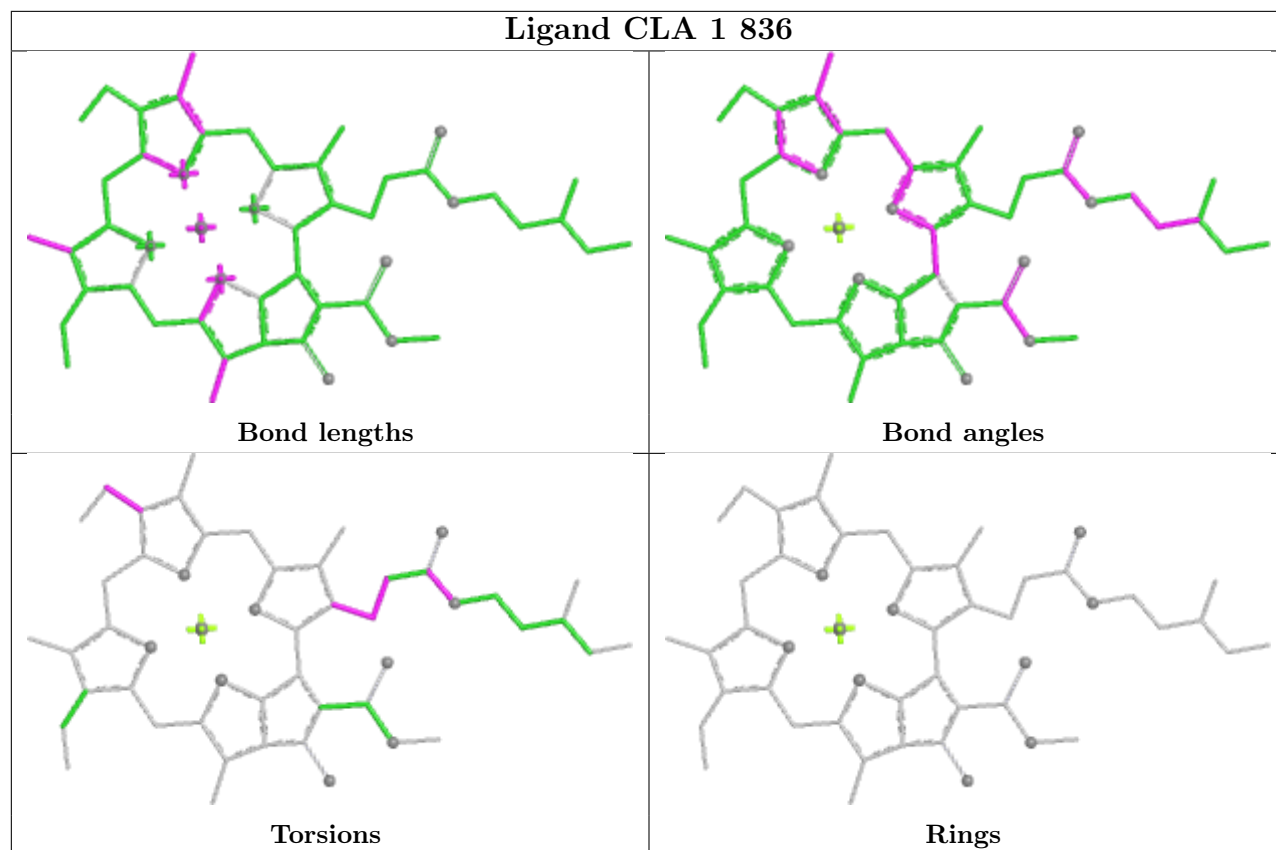


Torsions

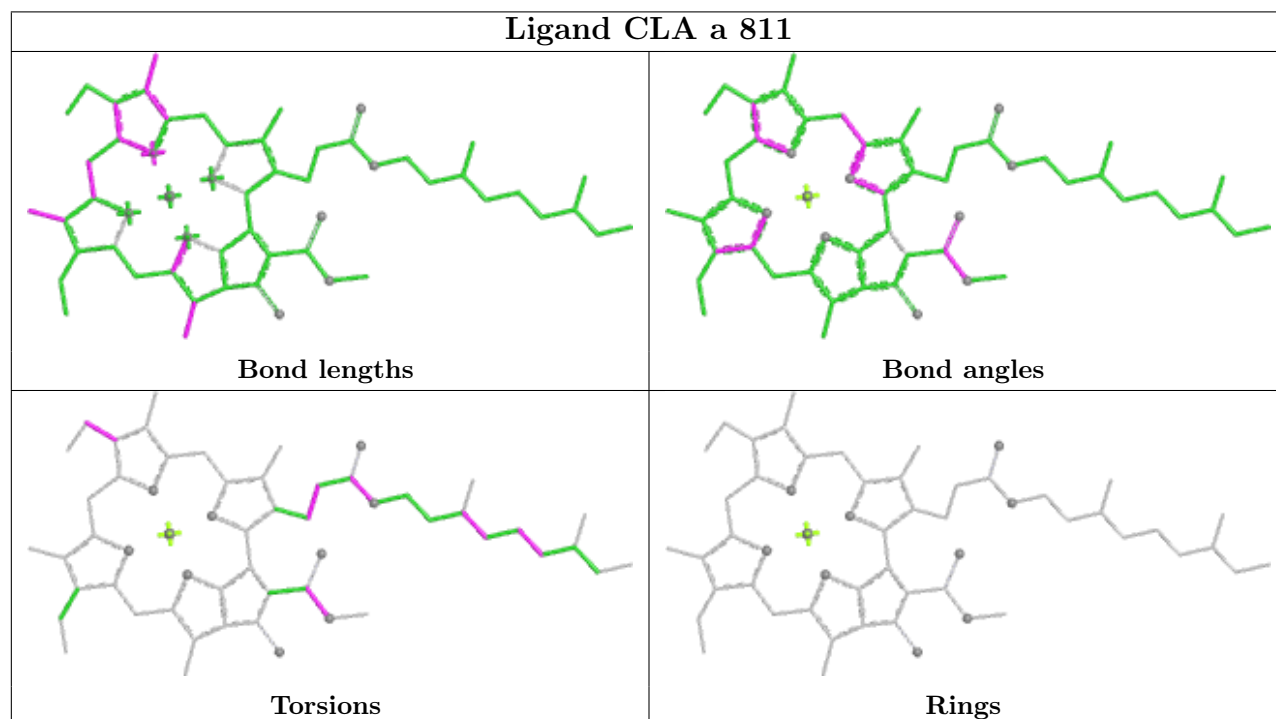


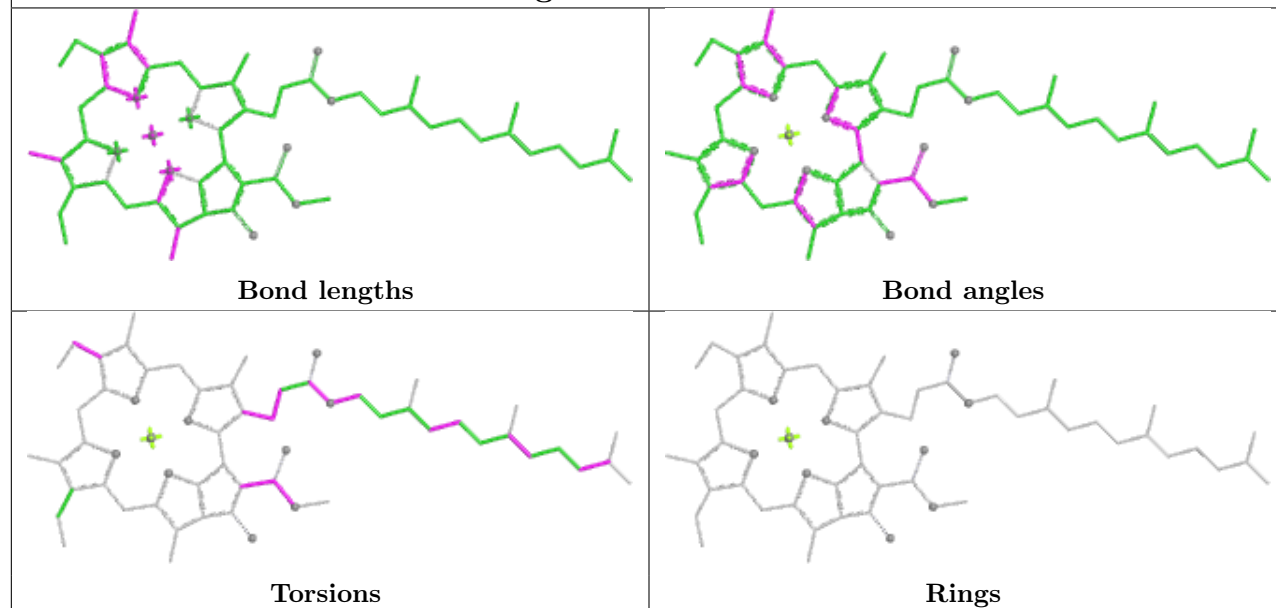
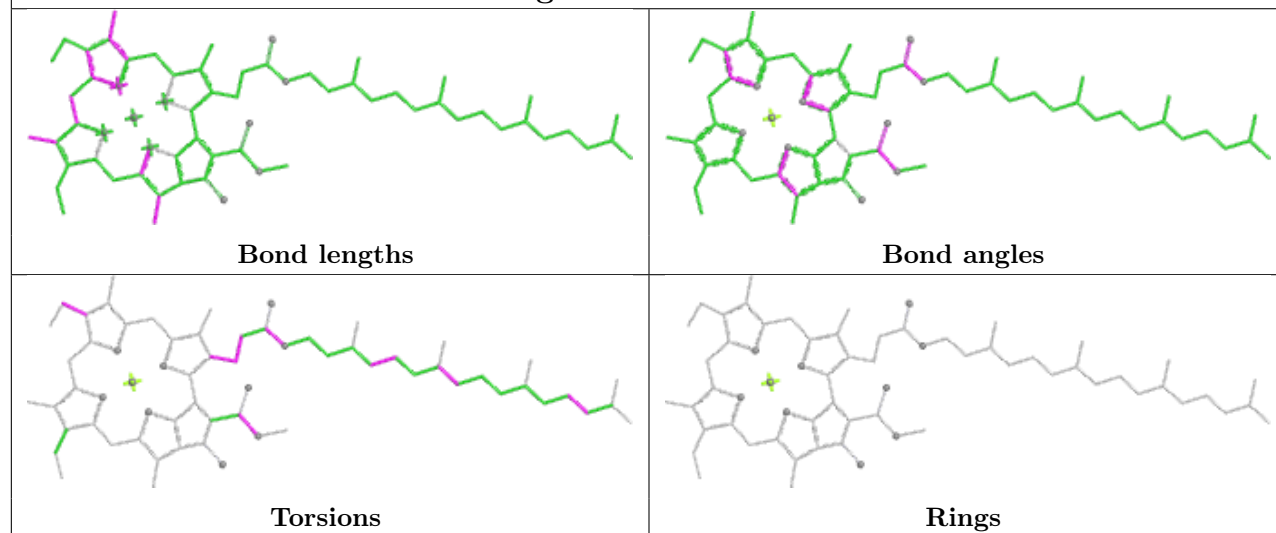
Rings

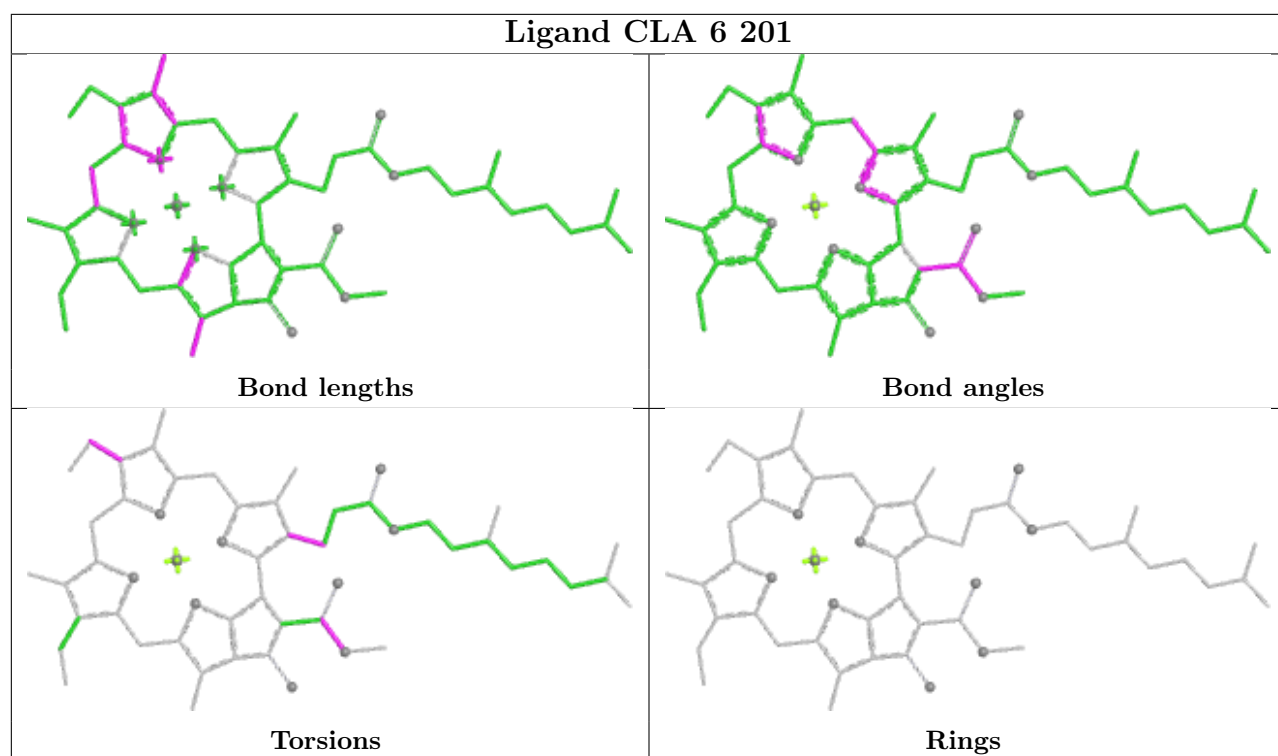
Ligand CLA 1 836



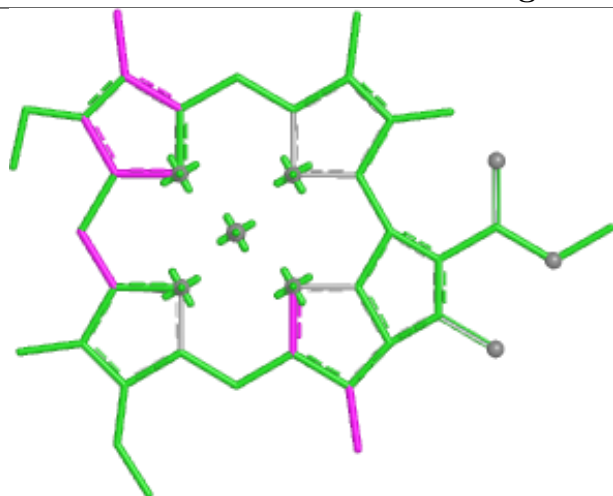
Ligand CLA a 811



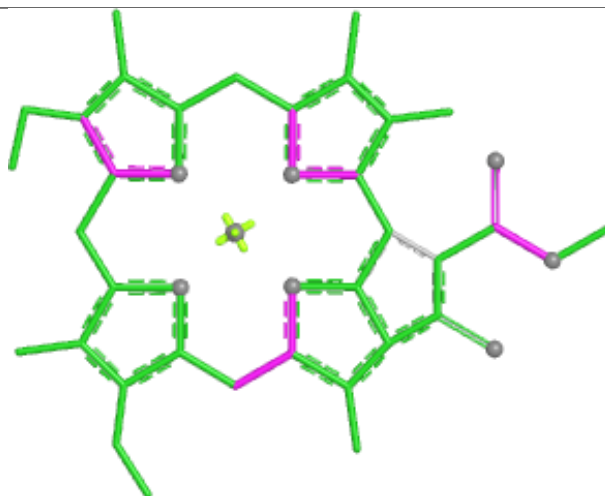
Ligand CLA b 826**Ligand CLA a 840**



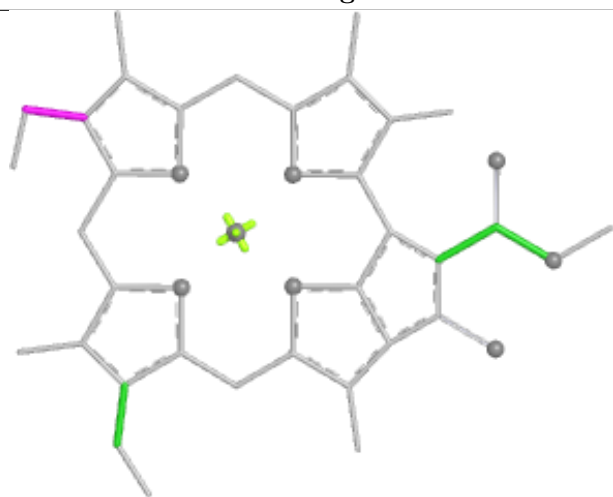
Ligand CLA 2 816



Bond lengths



Bond angles

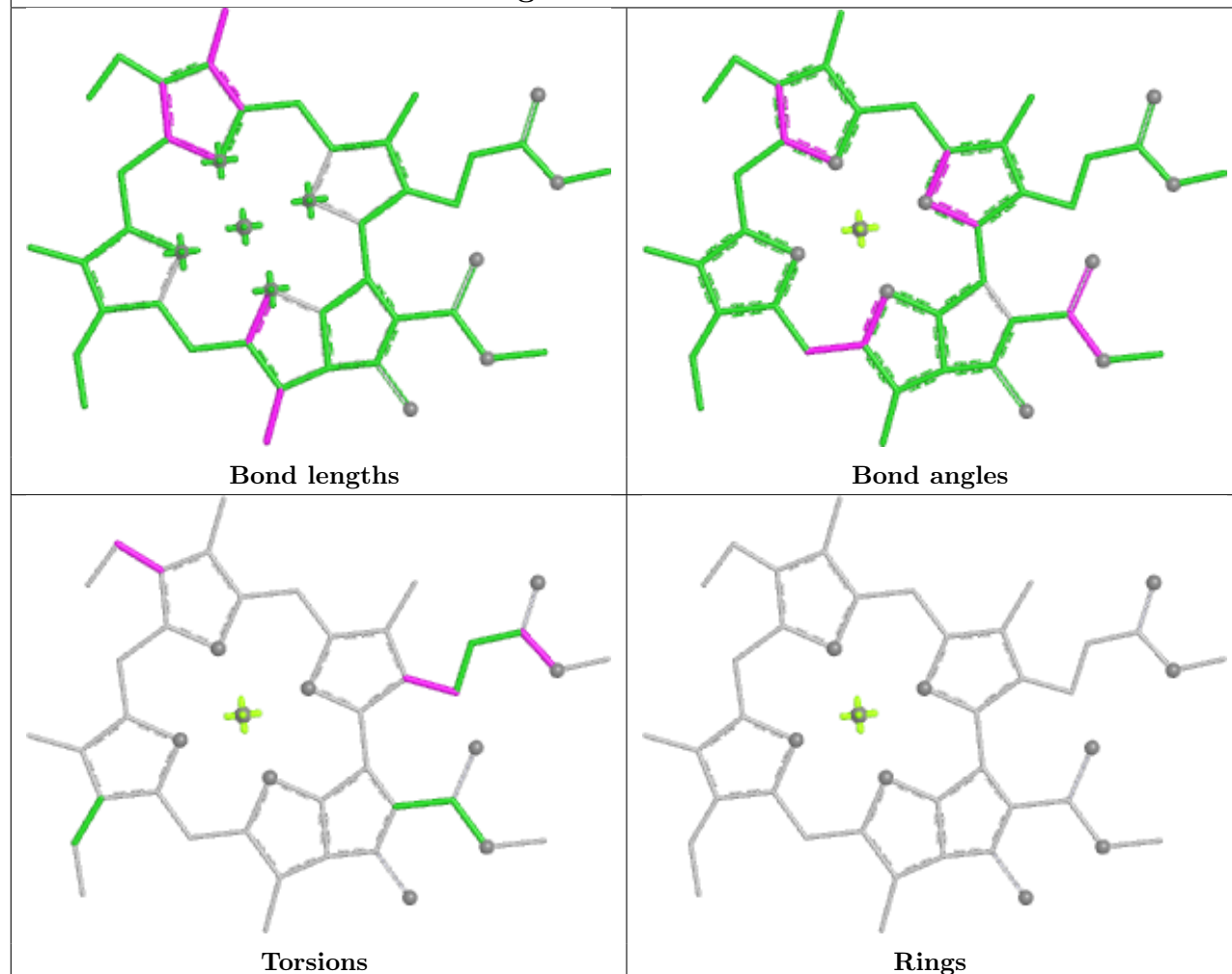


Torsions

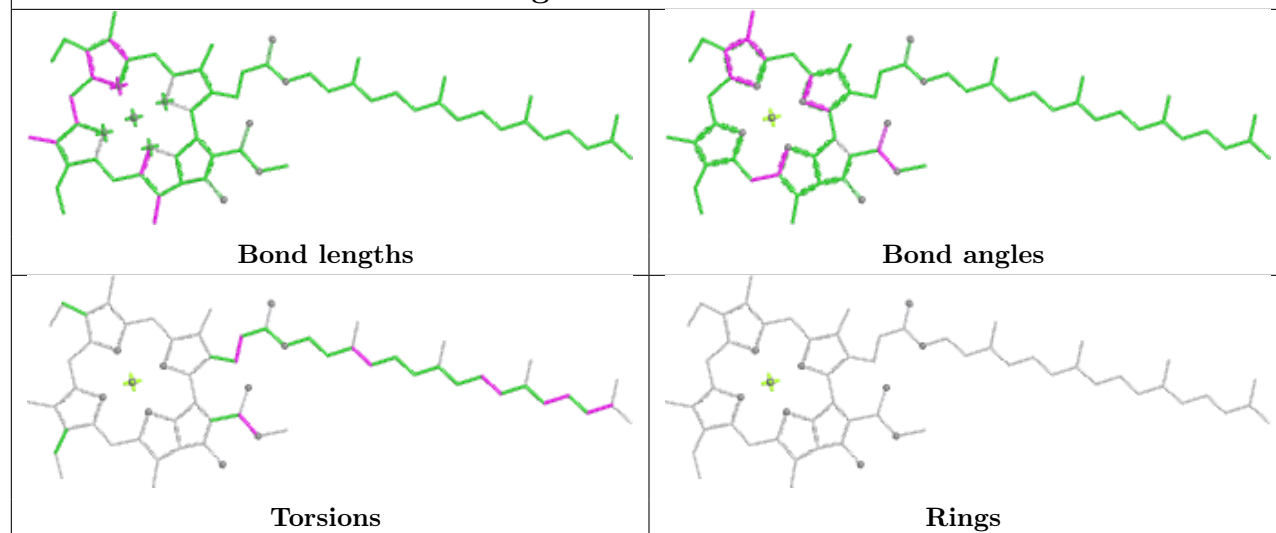


Rings

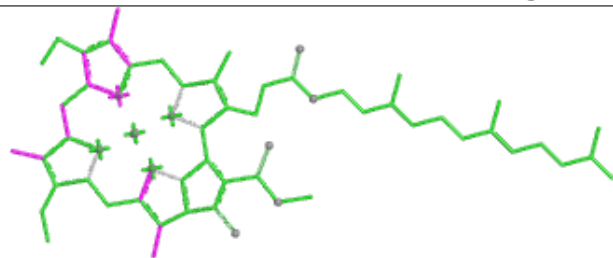
Ligand CLA 1 820



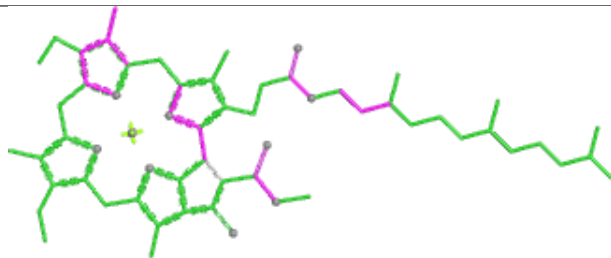
Ligand CLA A 828



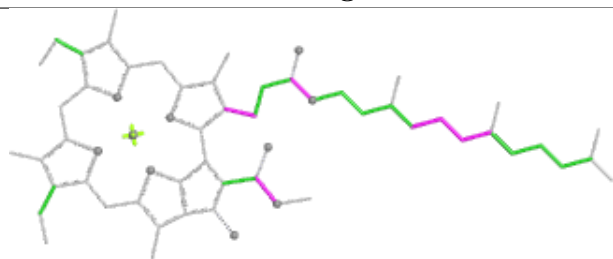
Ligand CLA I 202



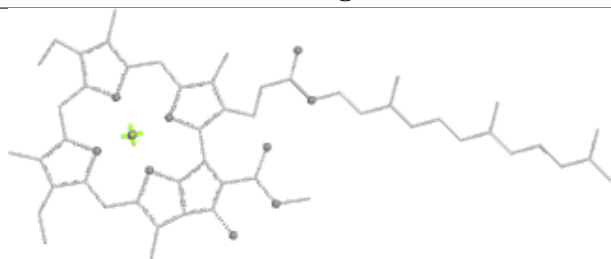
Bond lengths



Bond angles

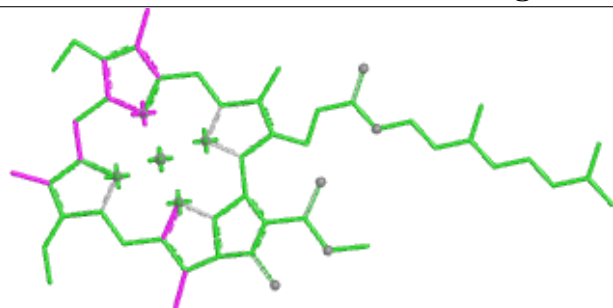


Torsions

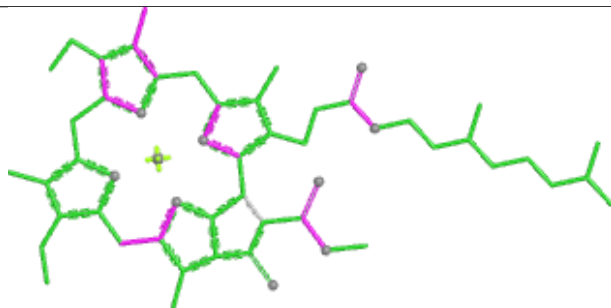


Rings

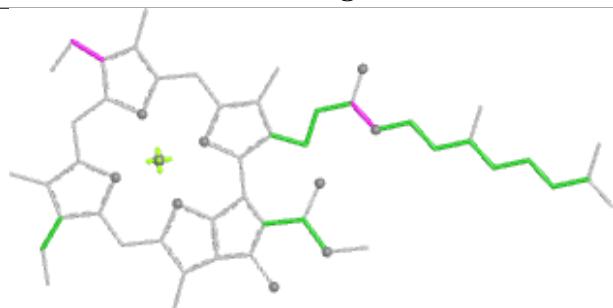
Ligand CLA A 804



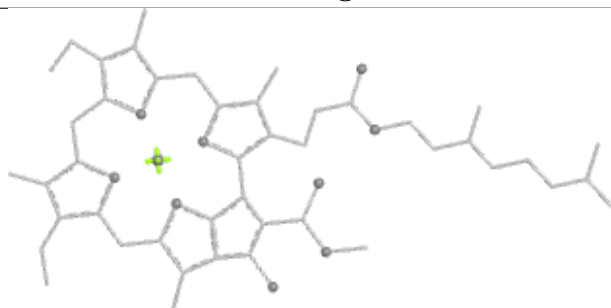
Bond lengths



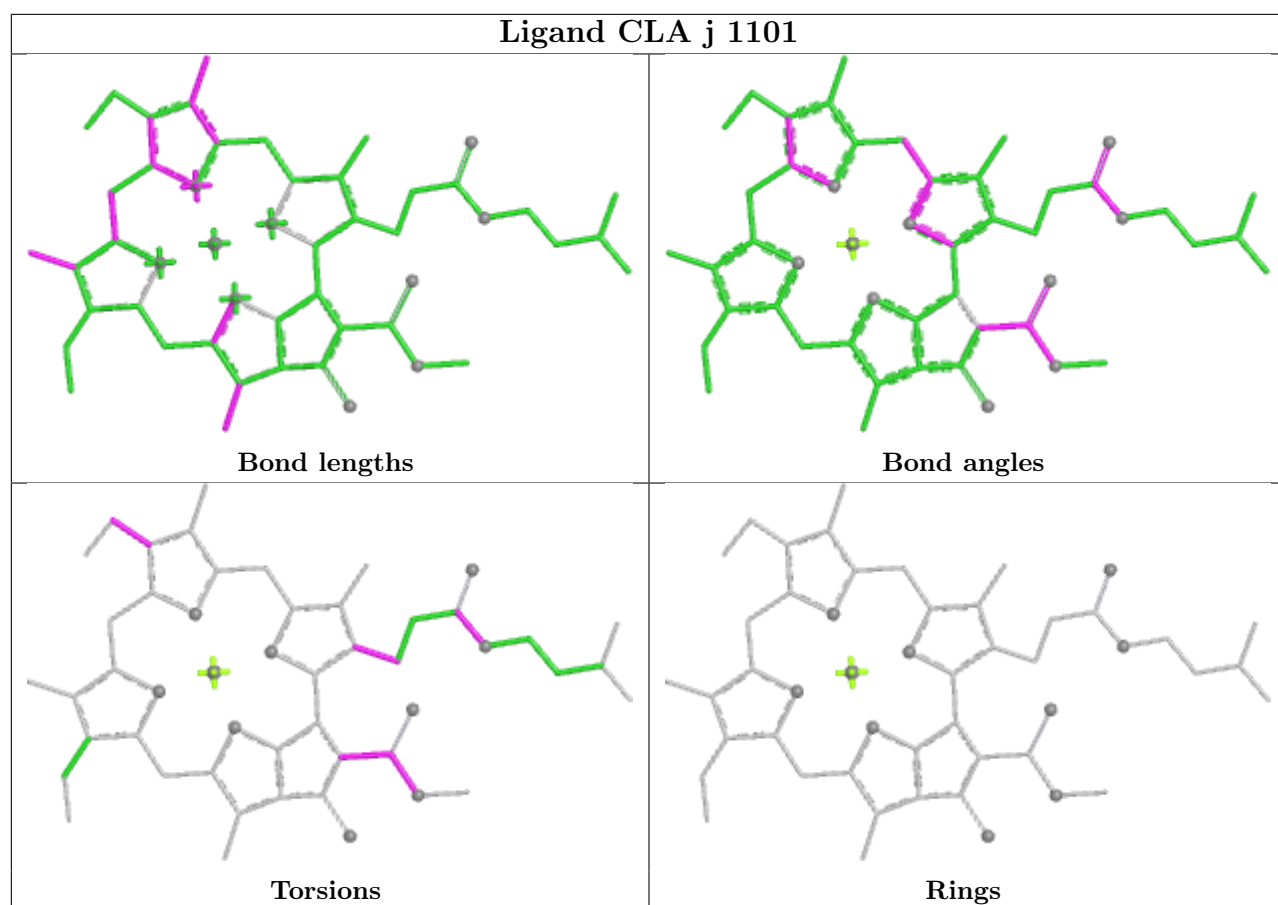
Bond angles



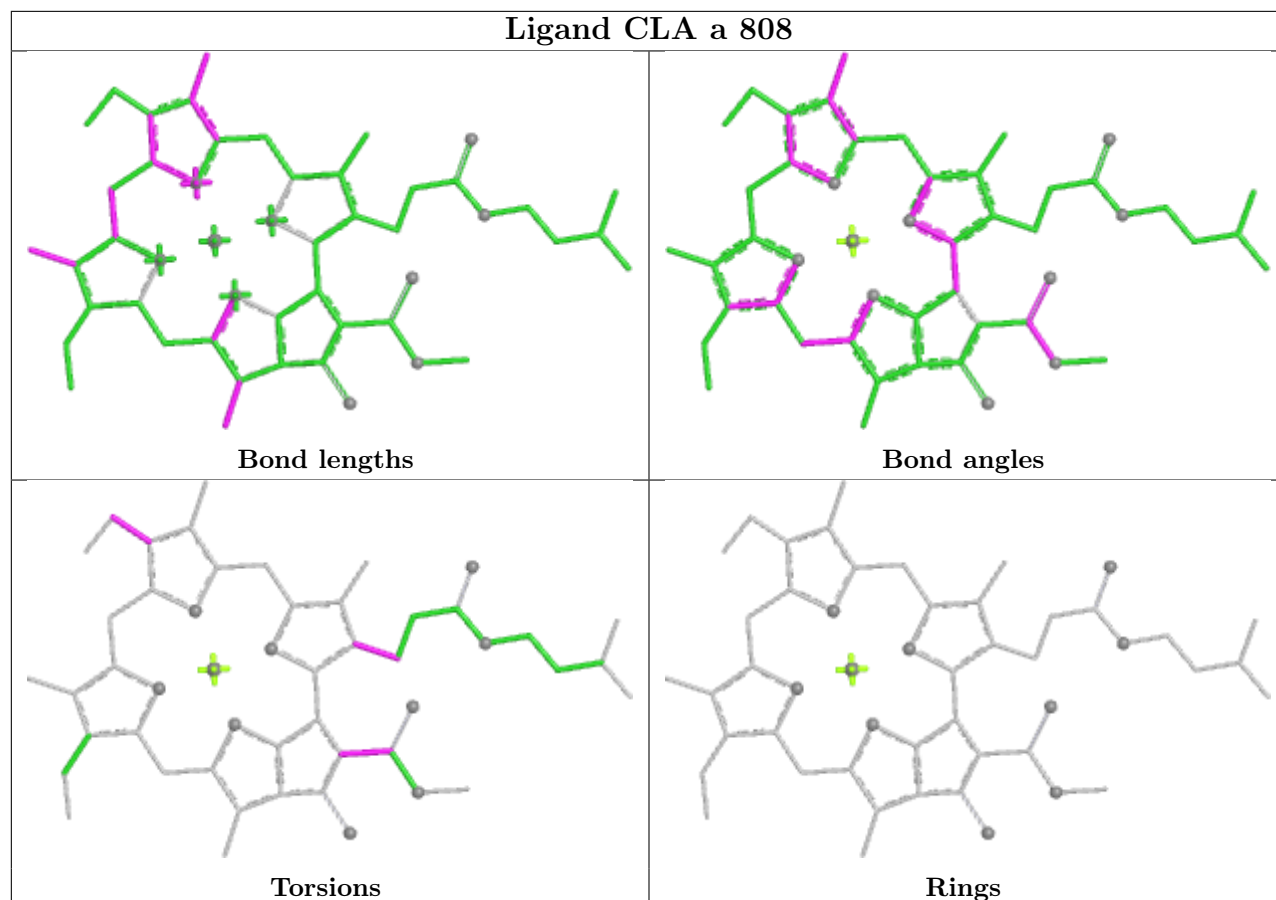
Torsions



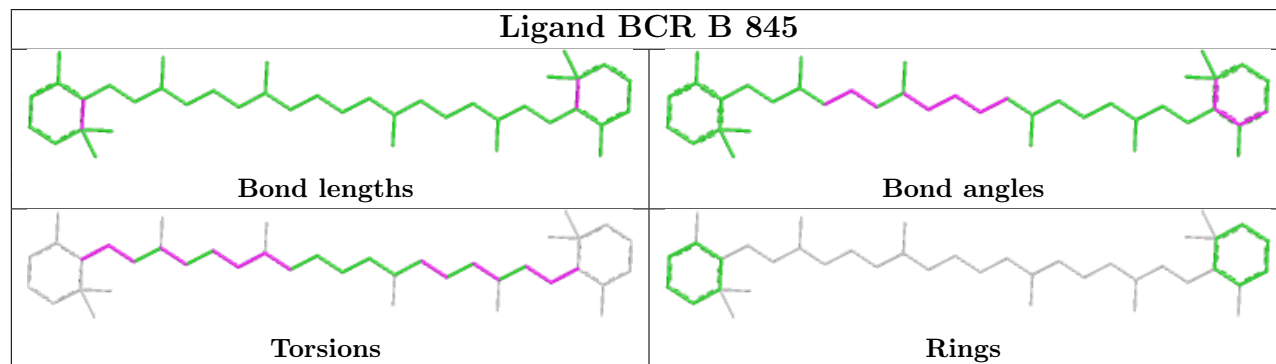
Rings

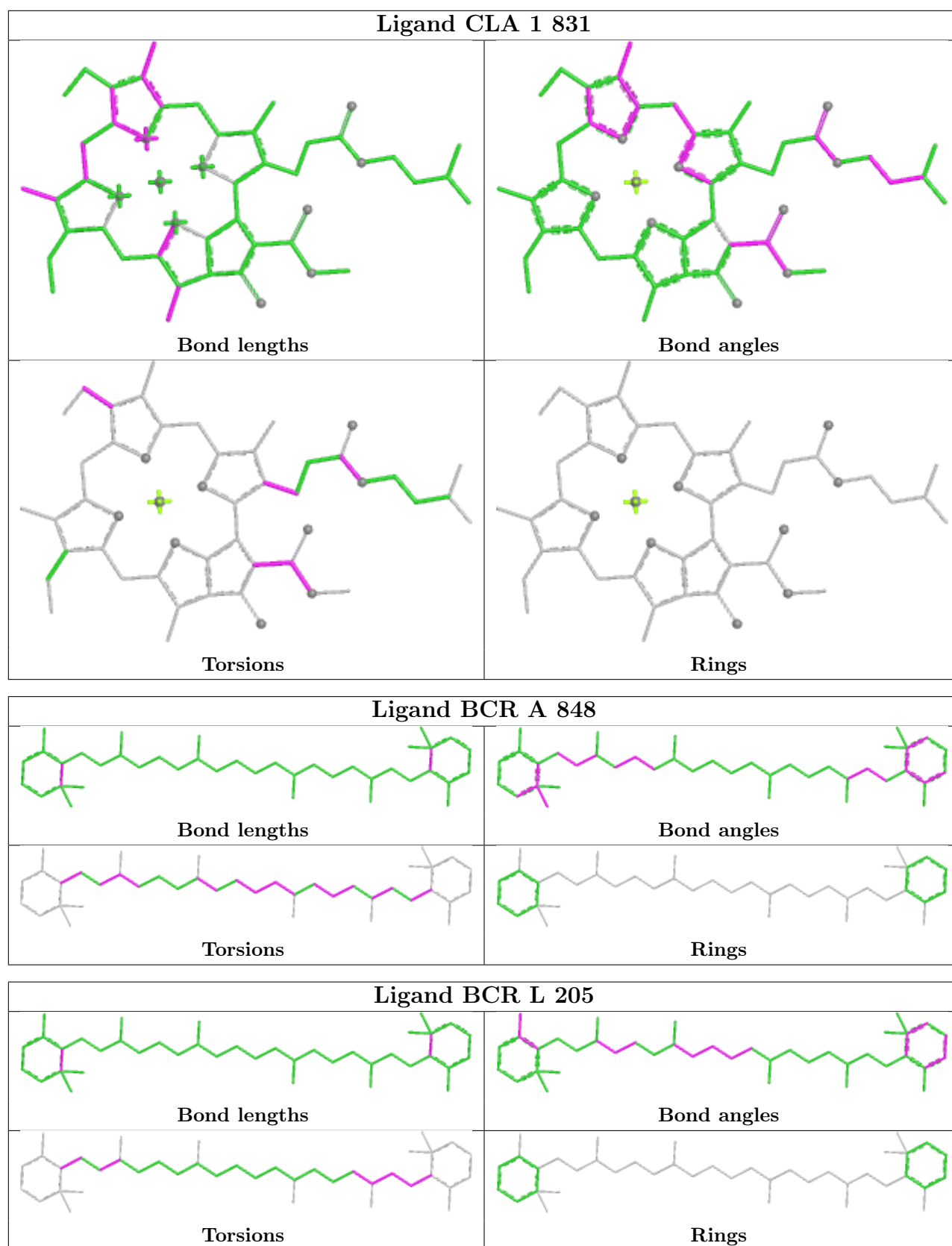


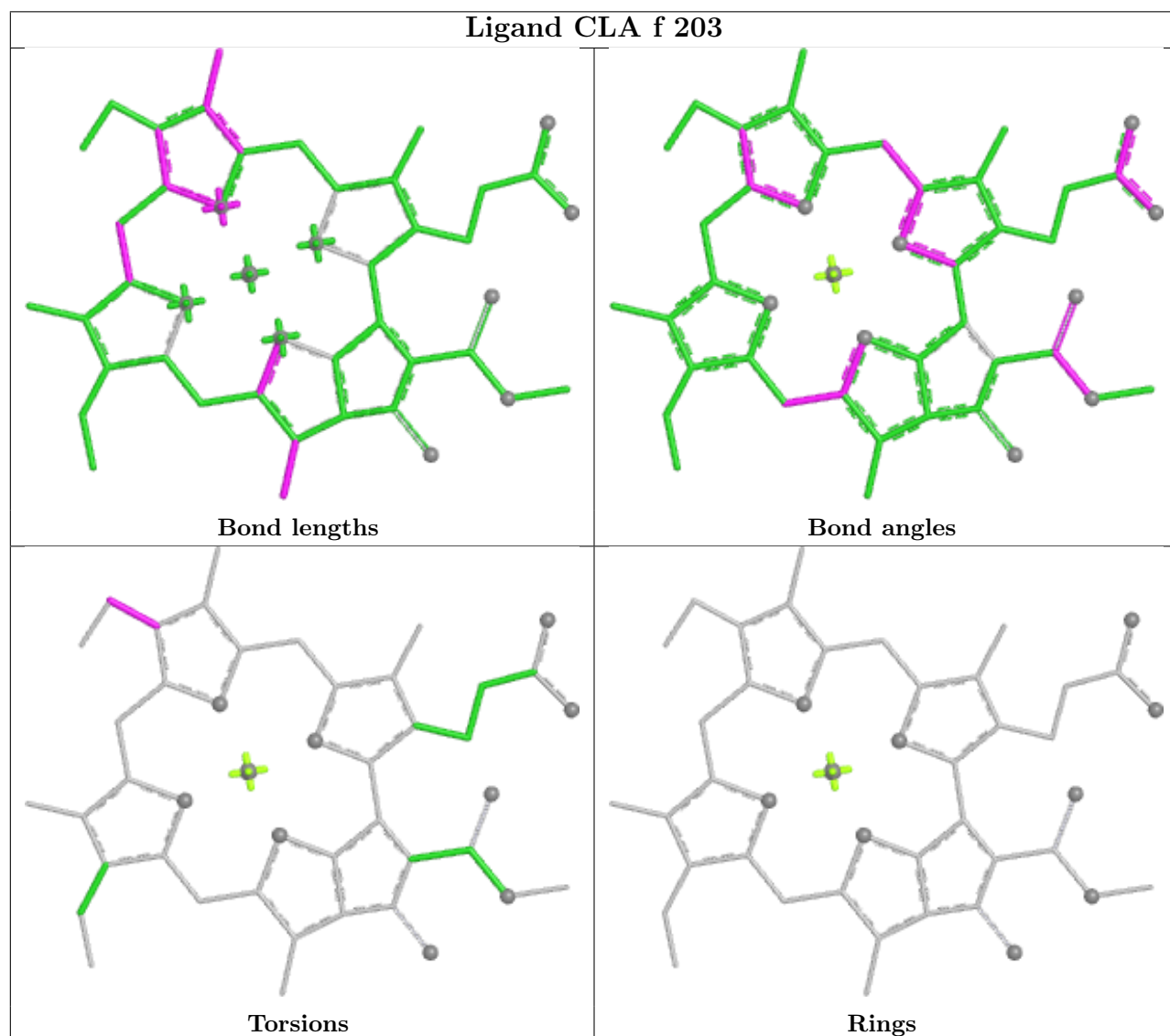
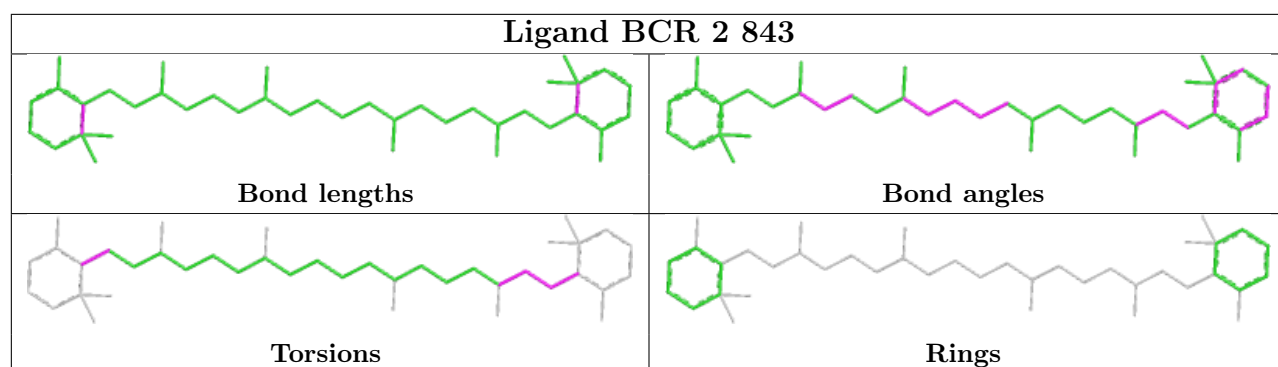
Ligand CLA a 808

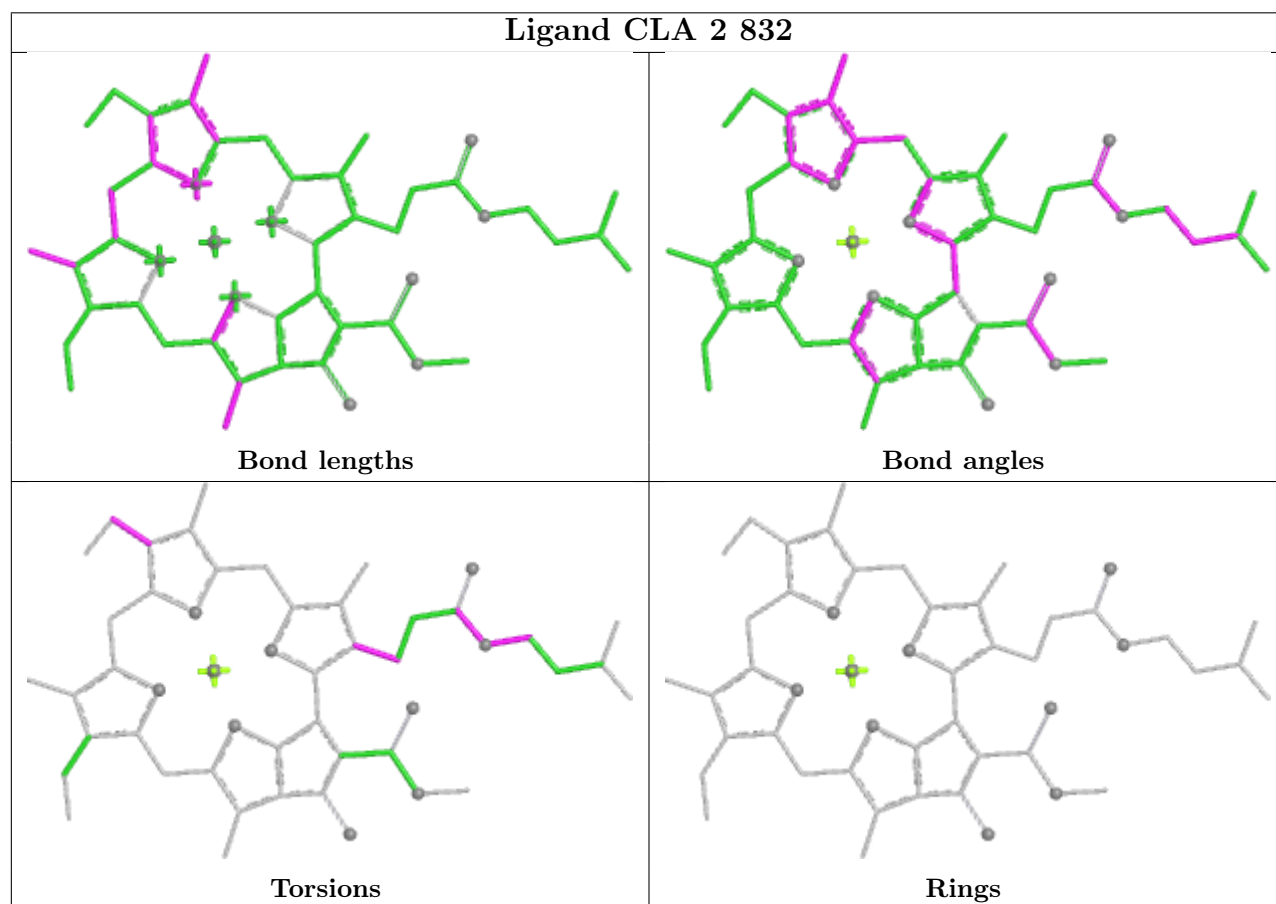
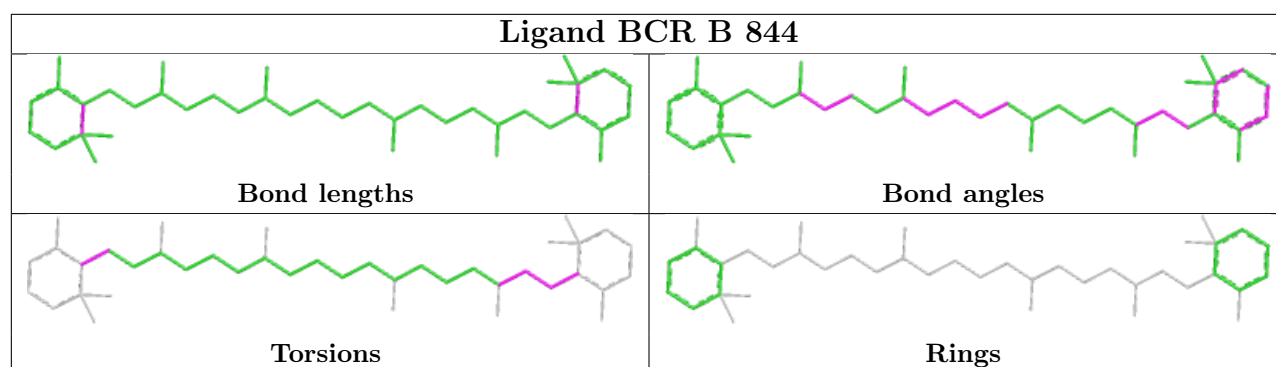


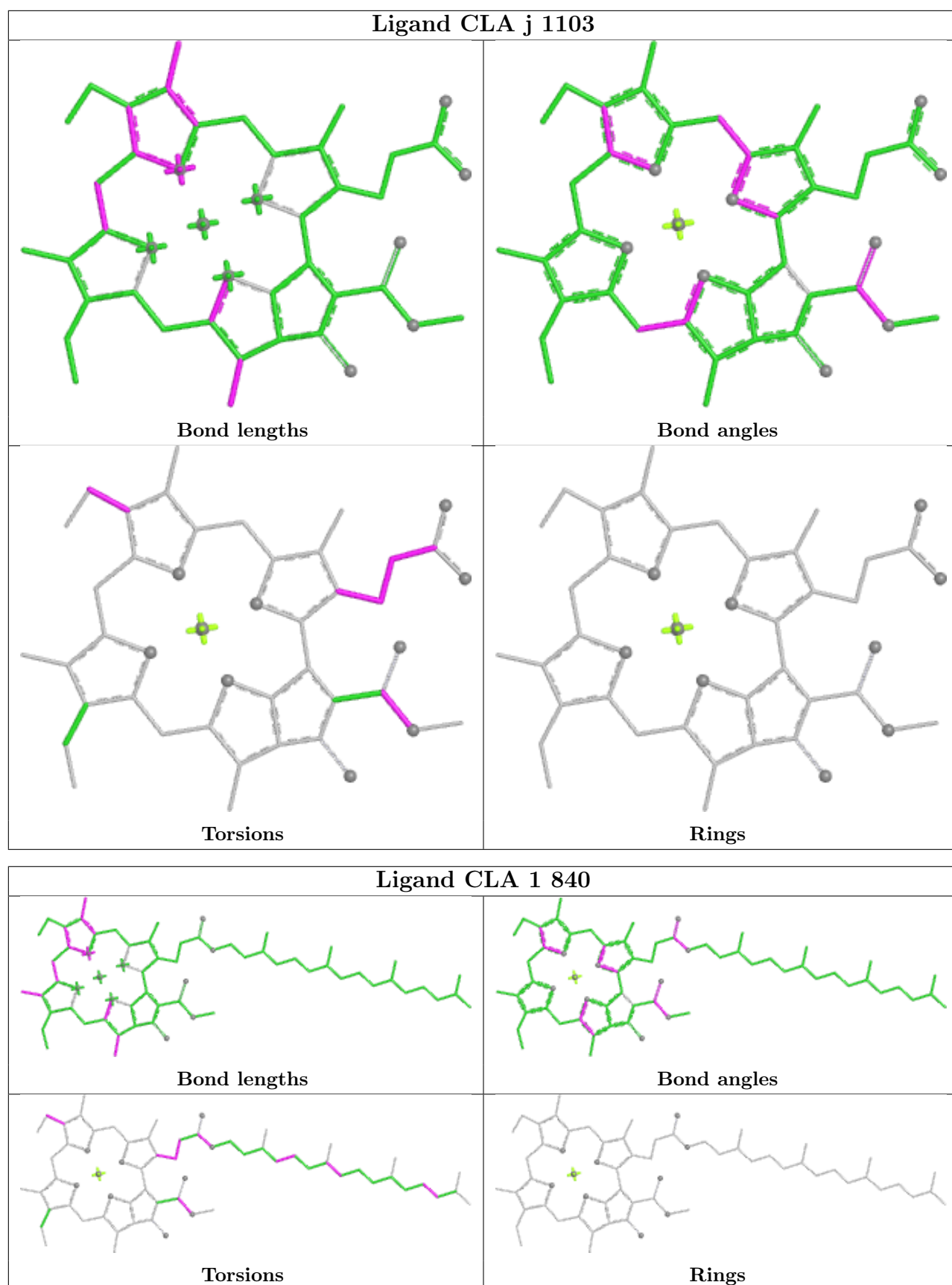
Ligand BCR B 845

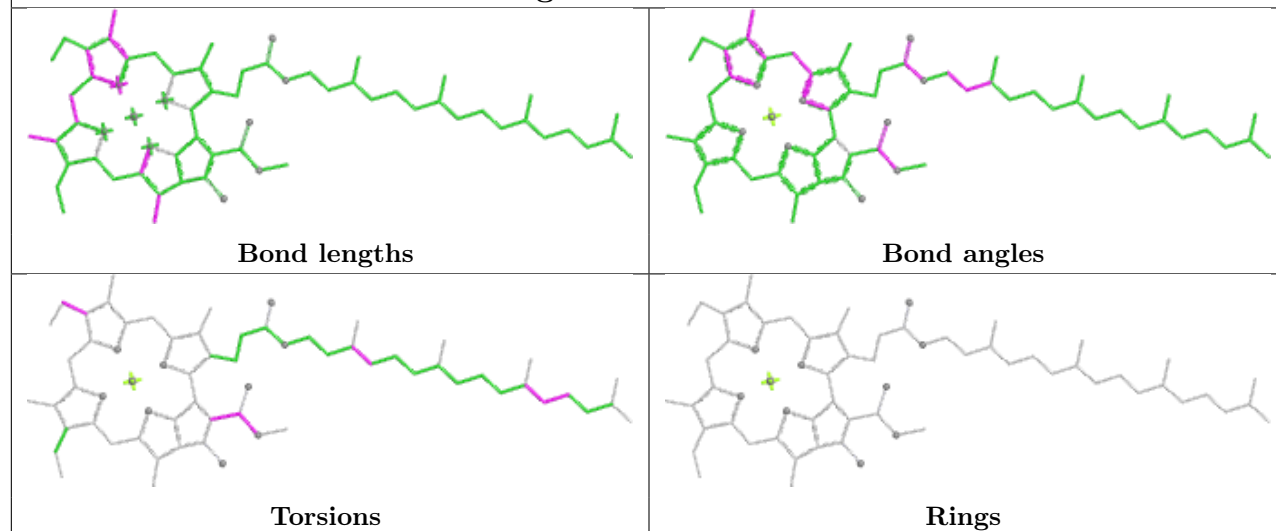
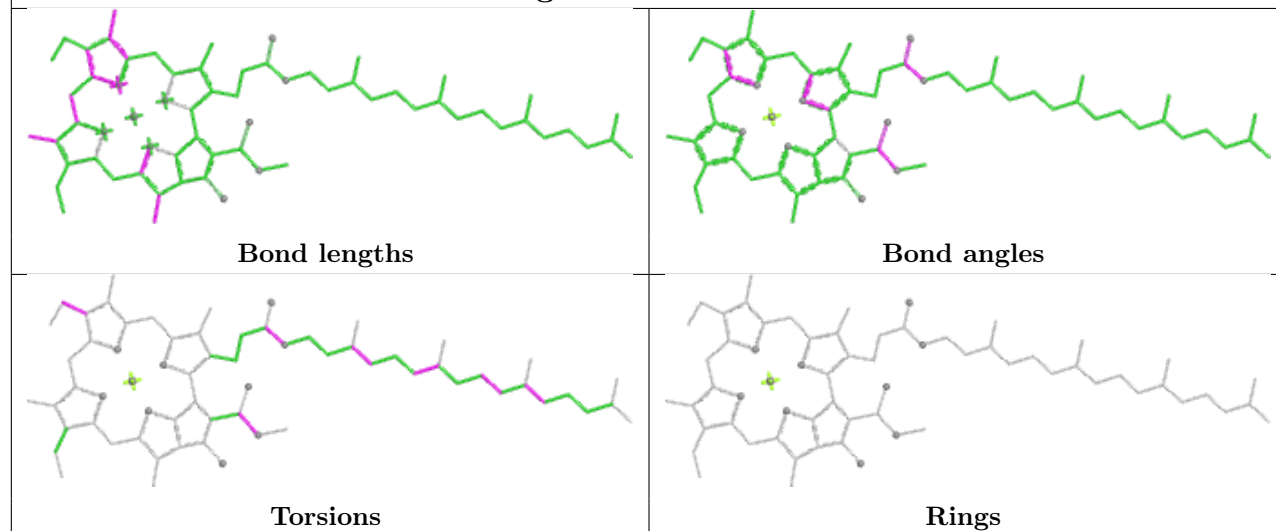


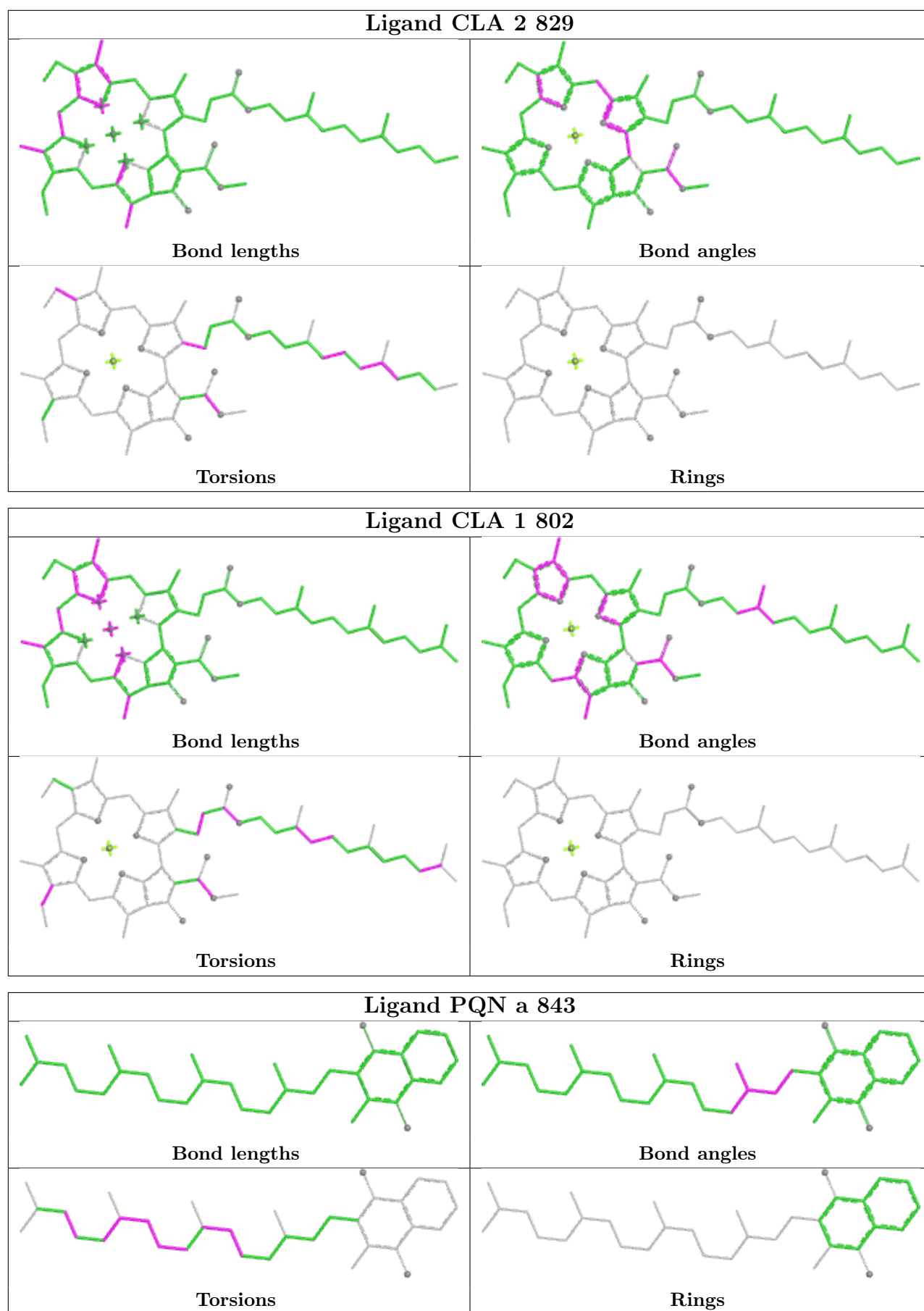


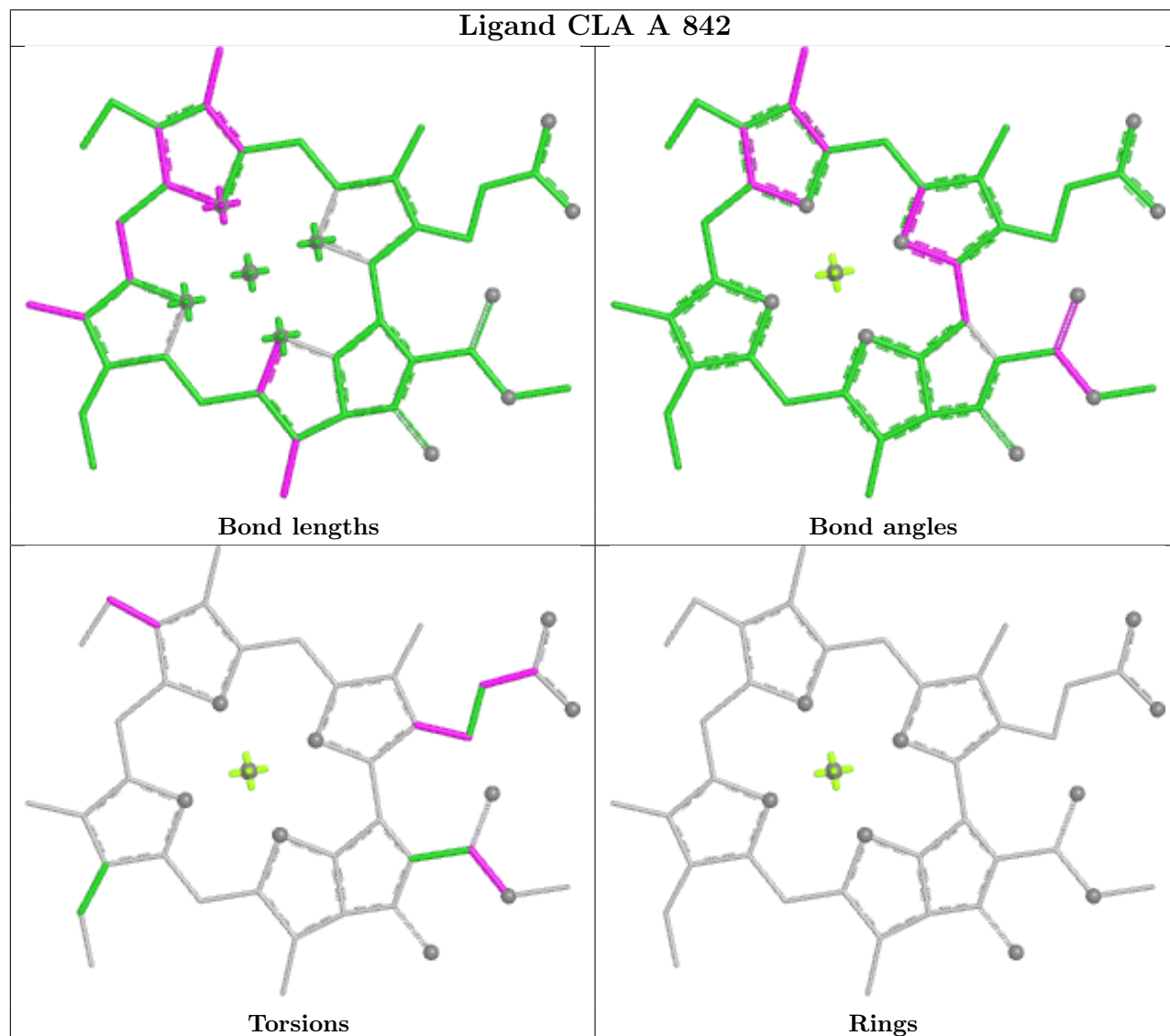
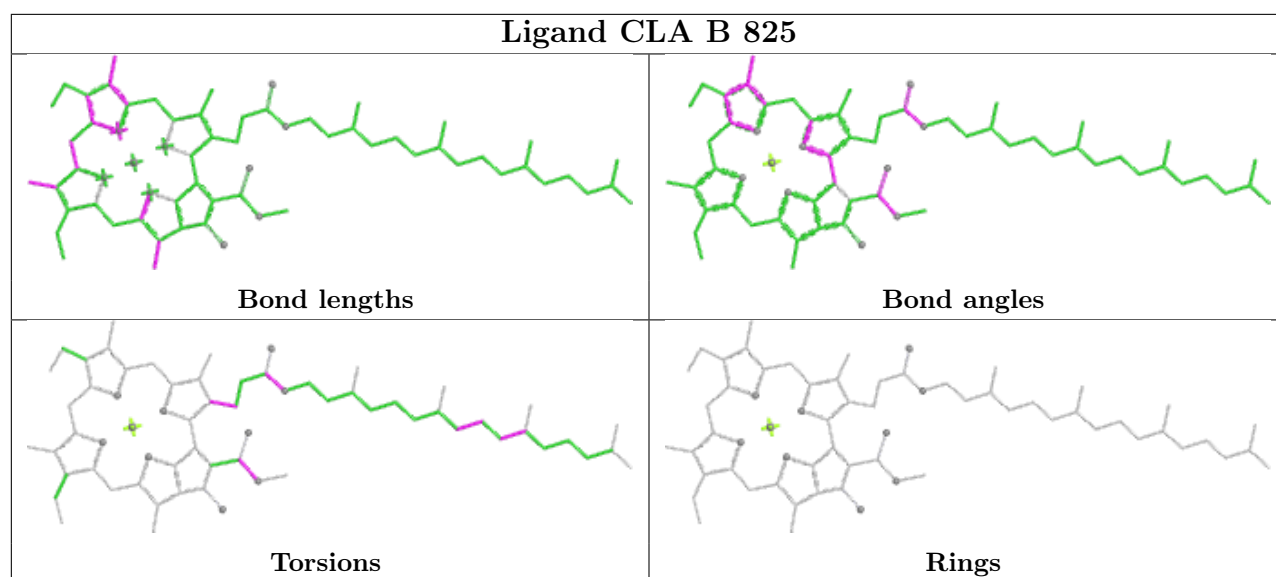




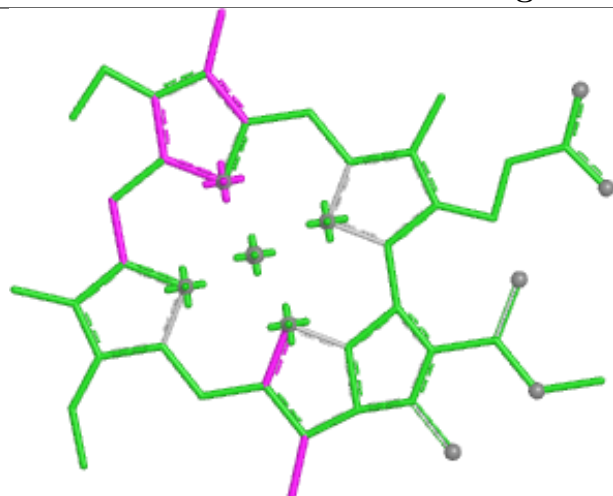


Ligand CLA 1 832**Ligand CLA 2 805**

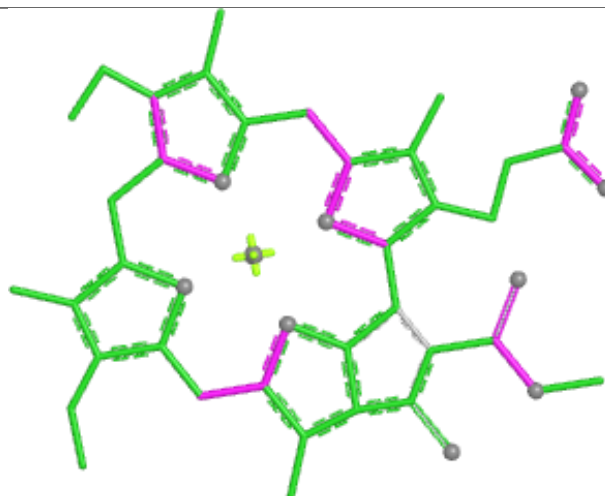




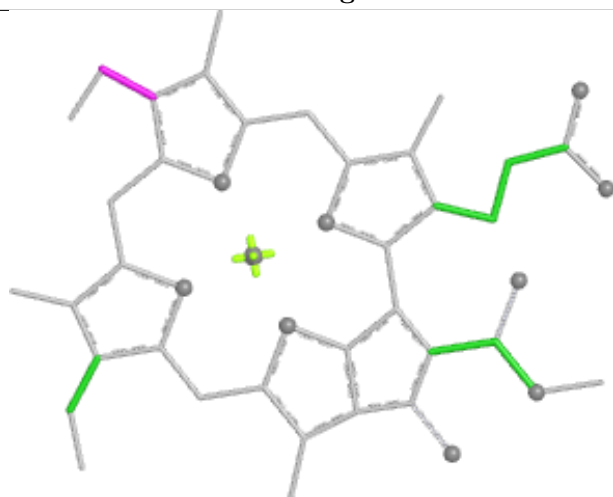
Ligand CLA F 203



Bond lengths



Bond angles

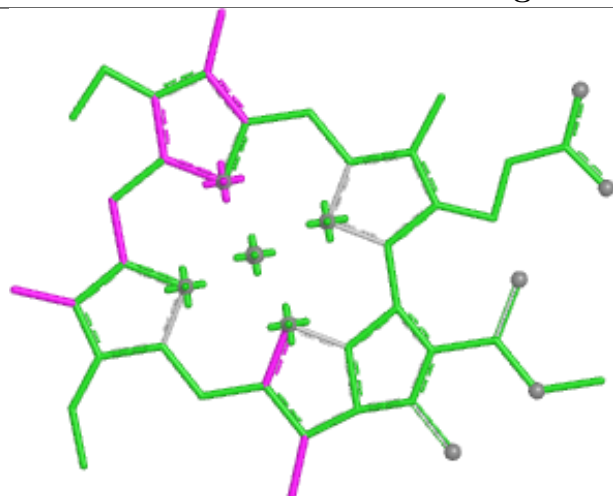


Torsions

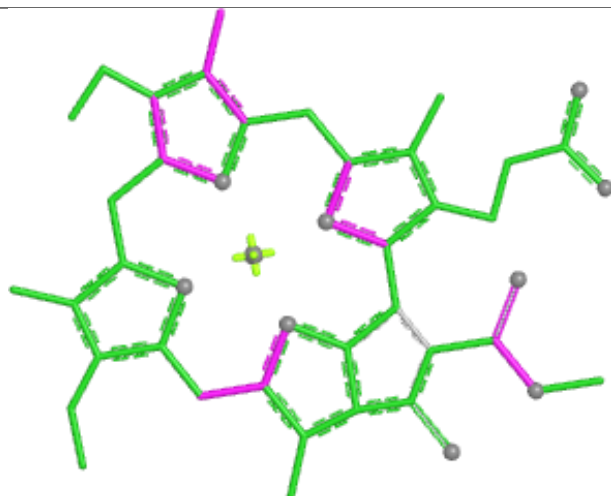


Rings

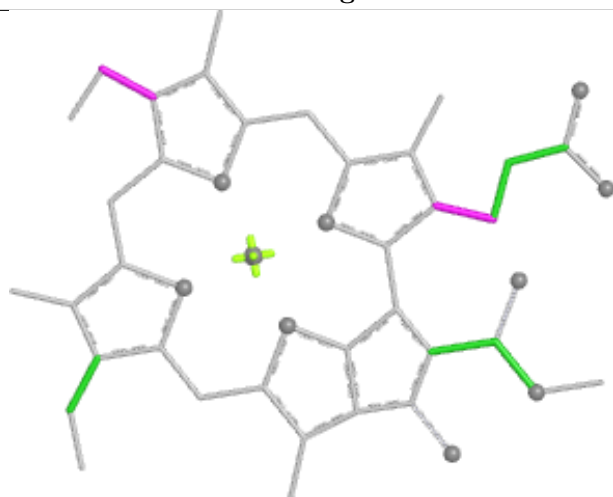
Ligand CLA A 815



Bond lengths



Bond angles

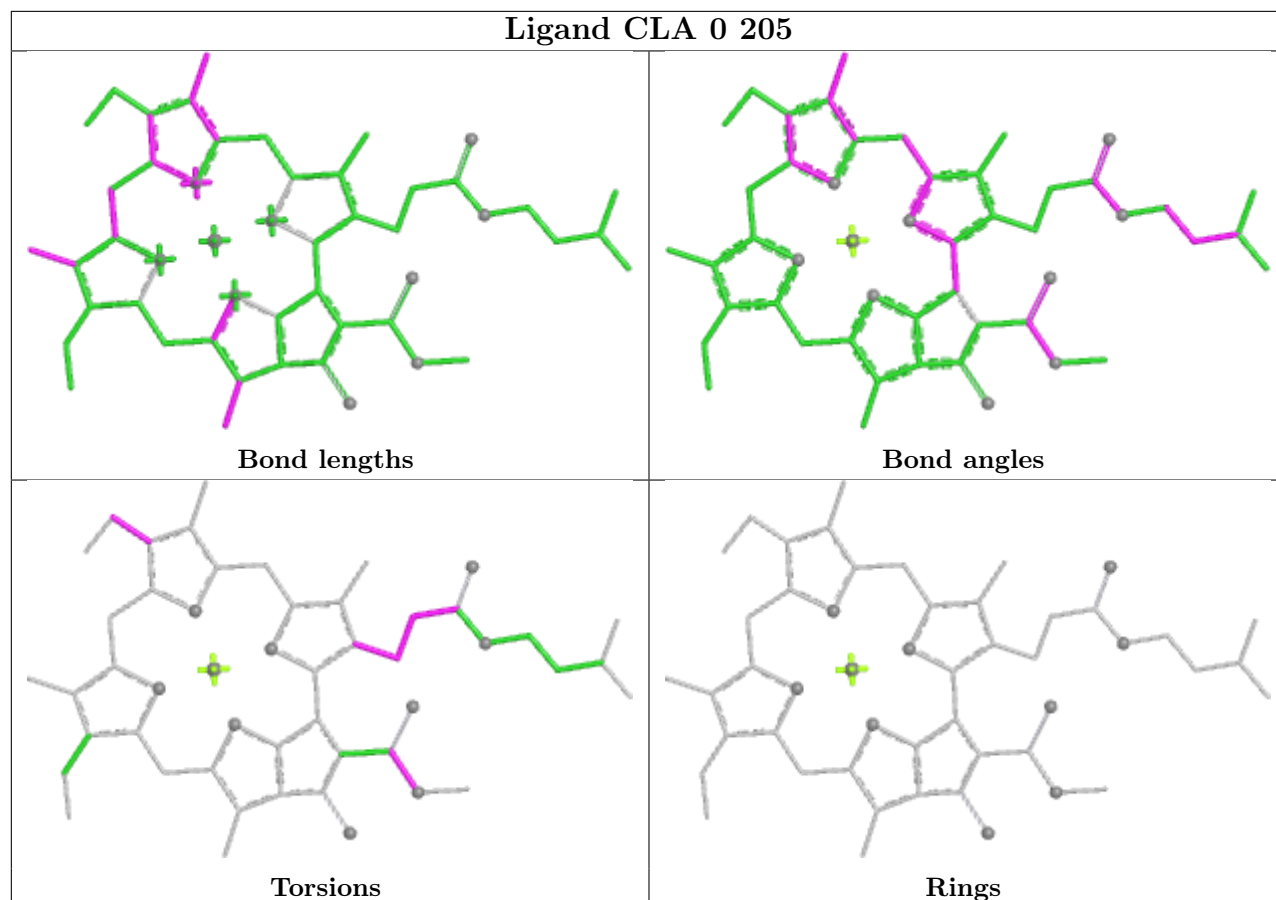


Torsions

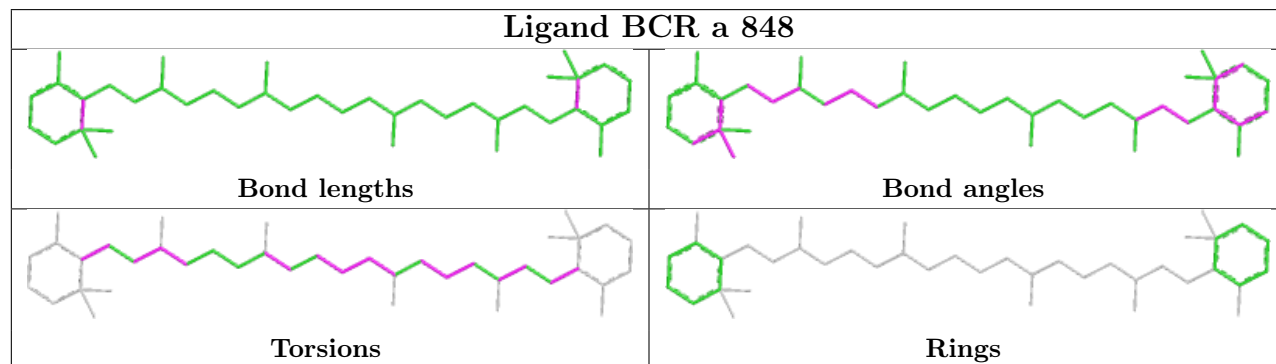


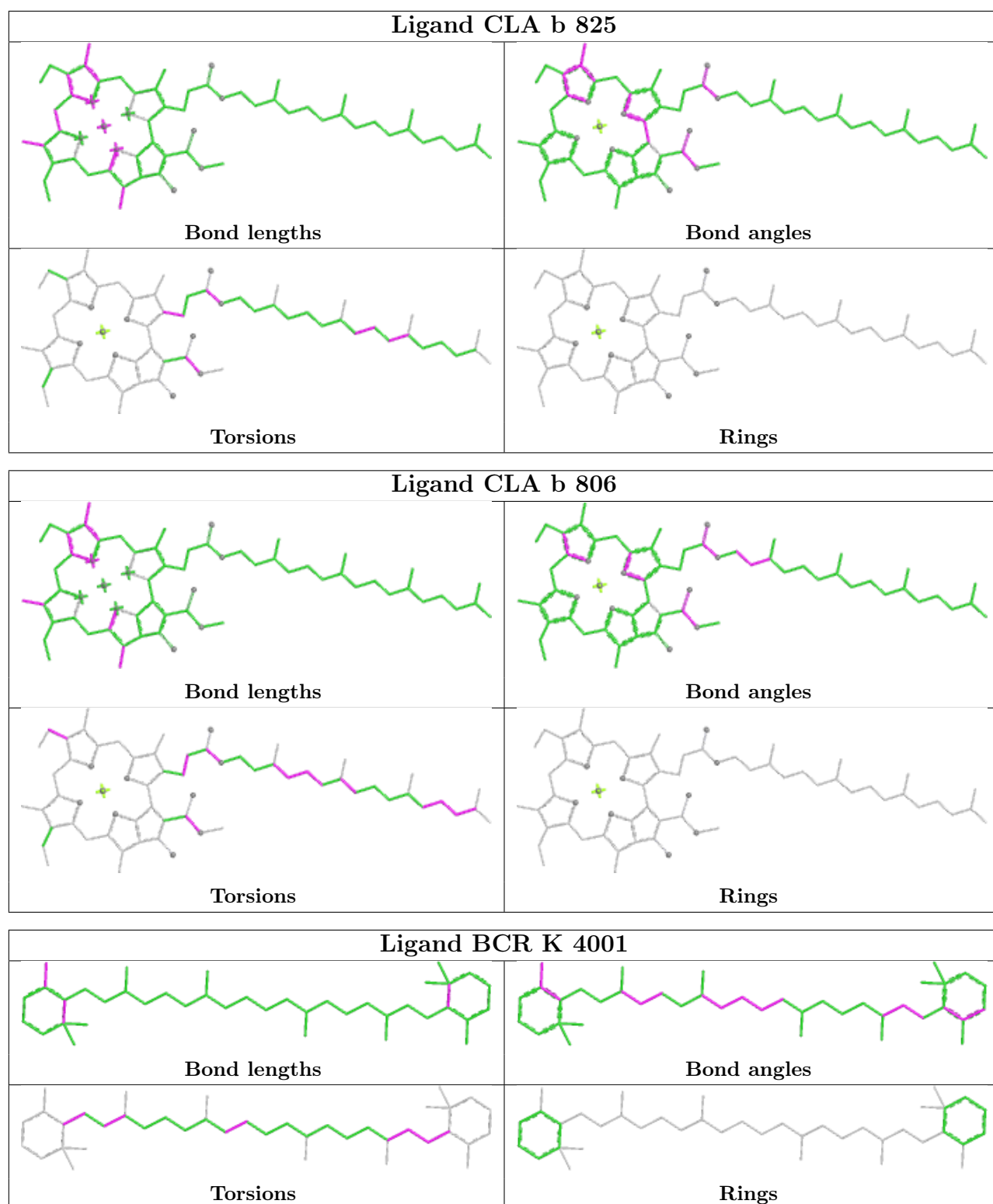
Rings

Ligand CLA 0 205

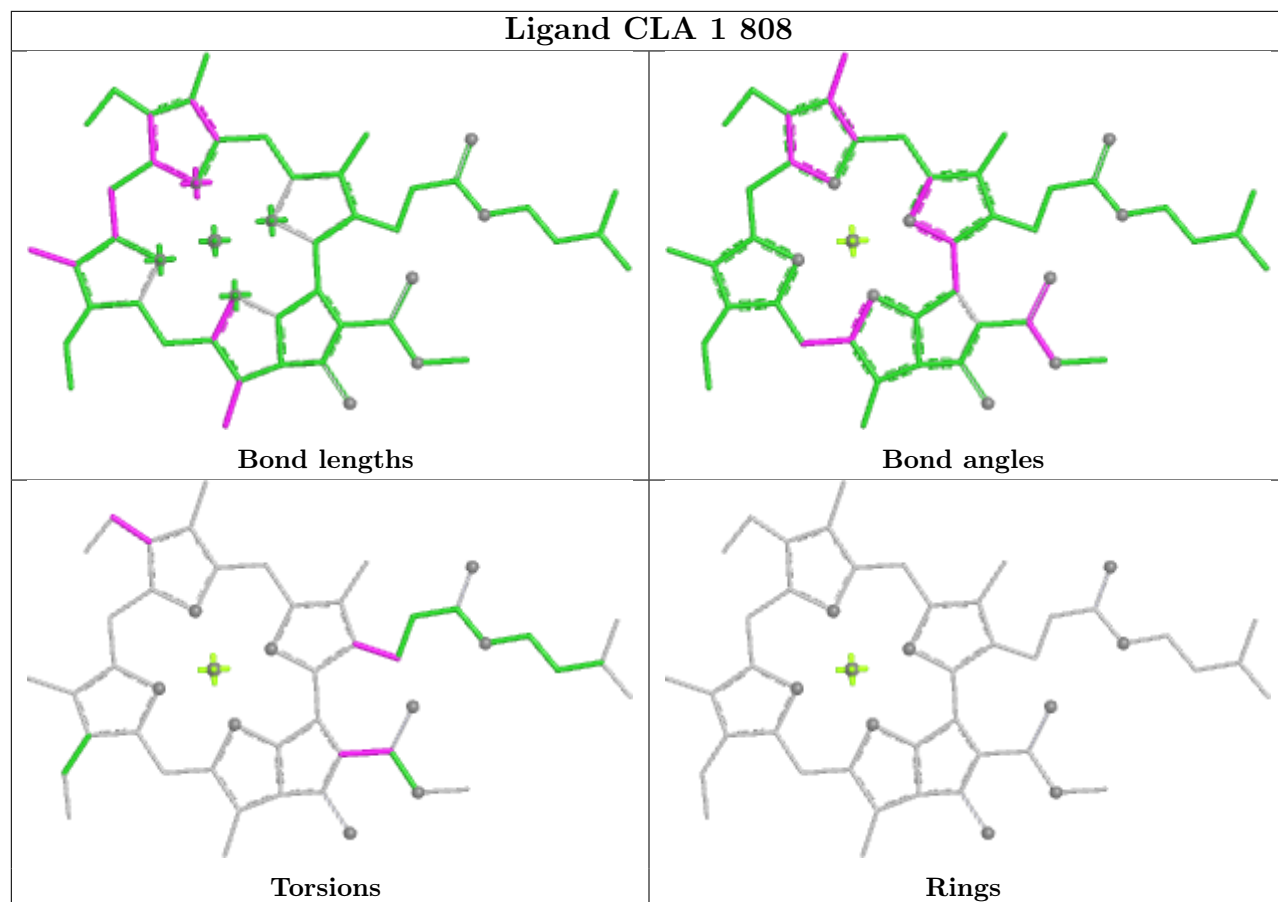


Ligand BCR a 848

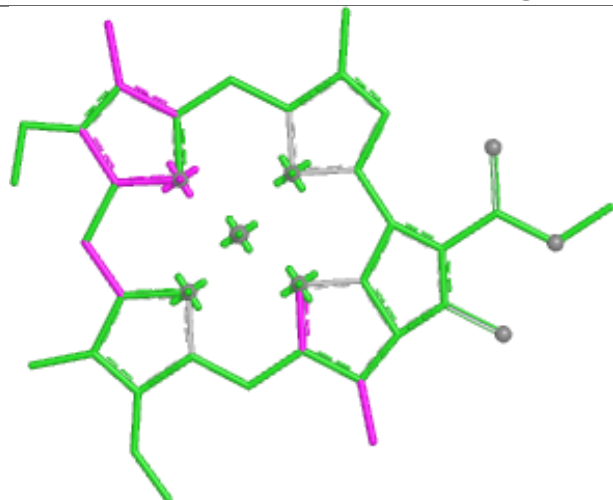




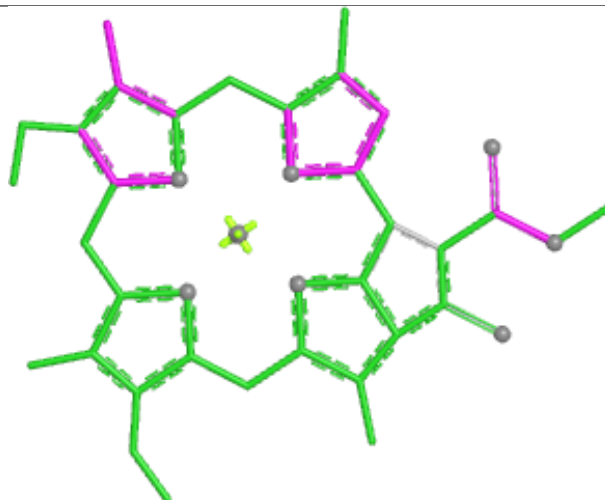
Ligand CLA 1 808



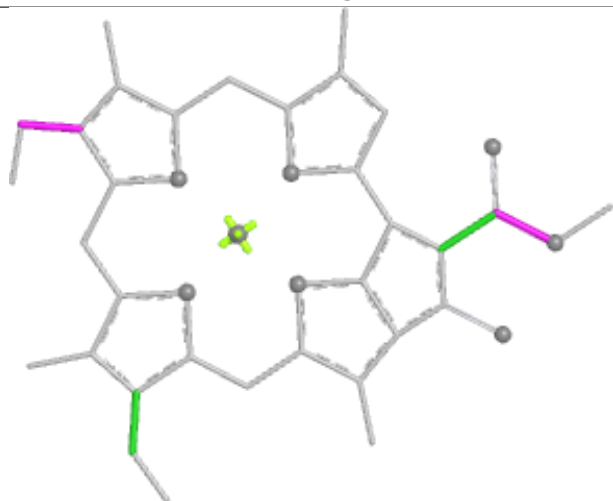
Ligand CLA b 832



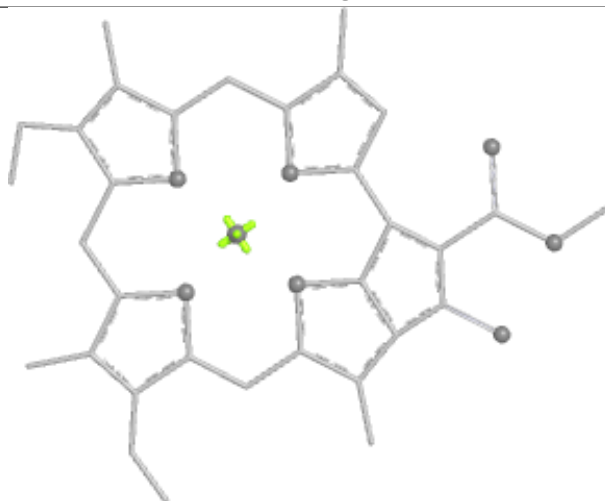
Bond lengths



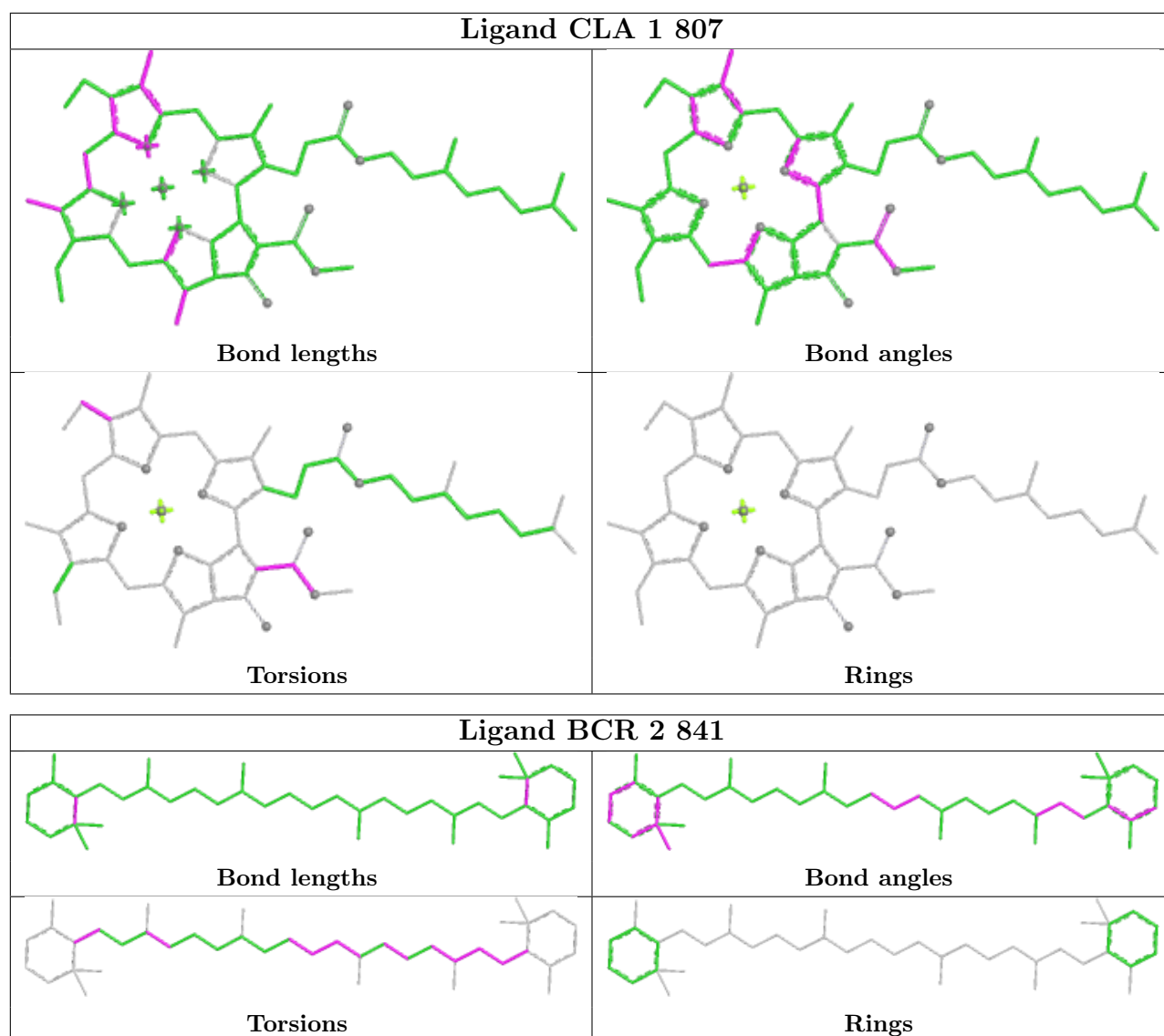
Bond angles



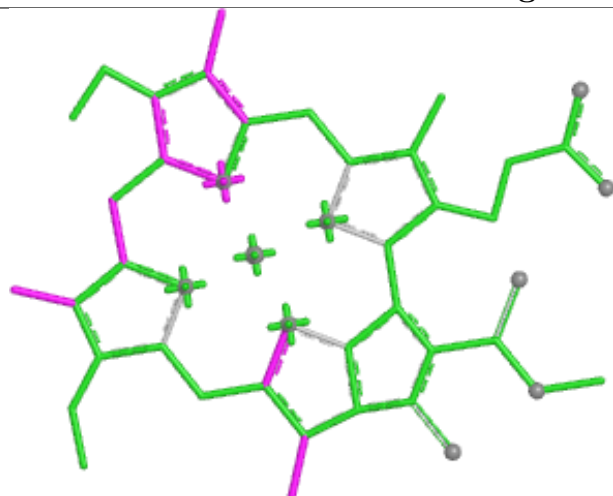
Torsions



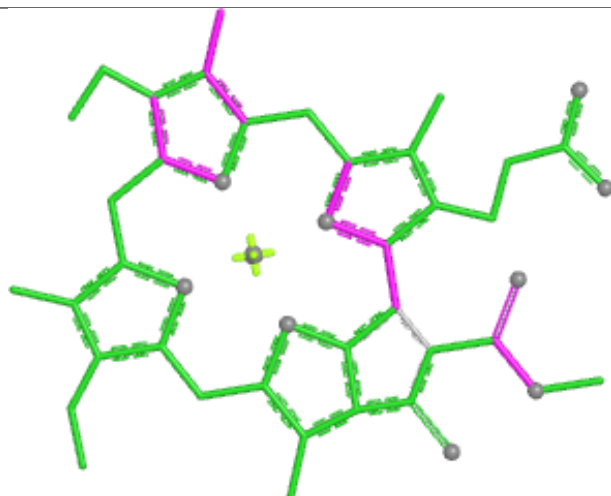
Rings



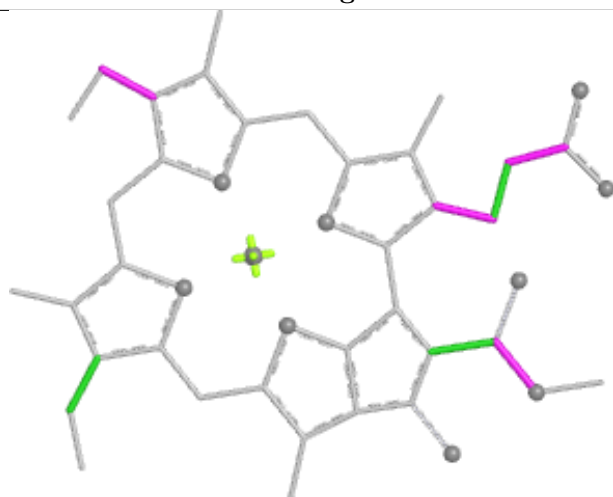
Ligand CLA a 842



Bond lengths



Bond angles

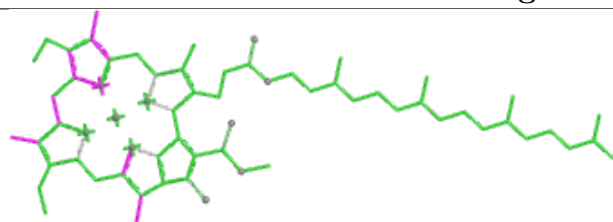


Torsions

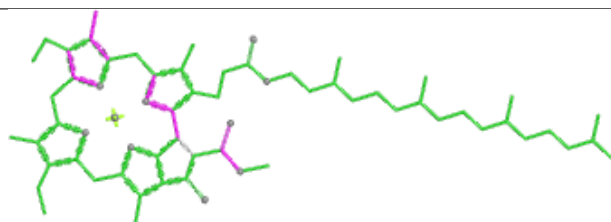


Rings

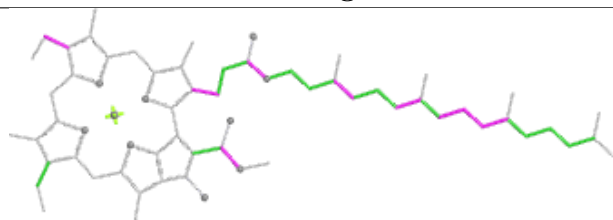
Ligand CLA 2 807



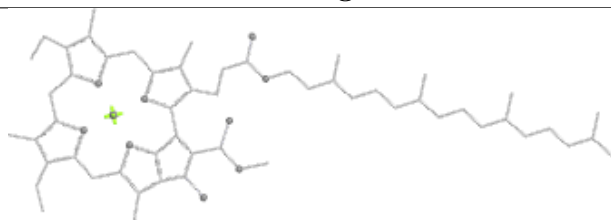
Bond lengths



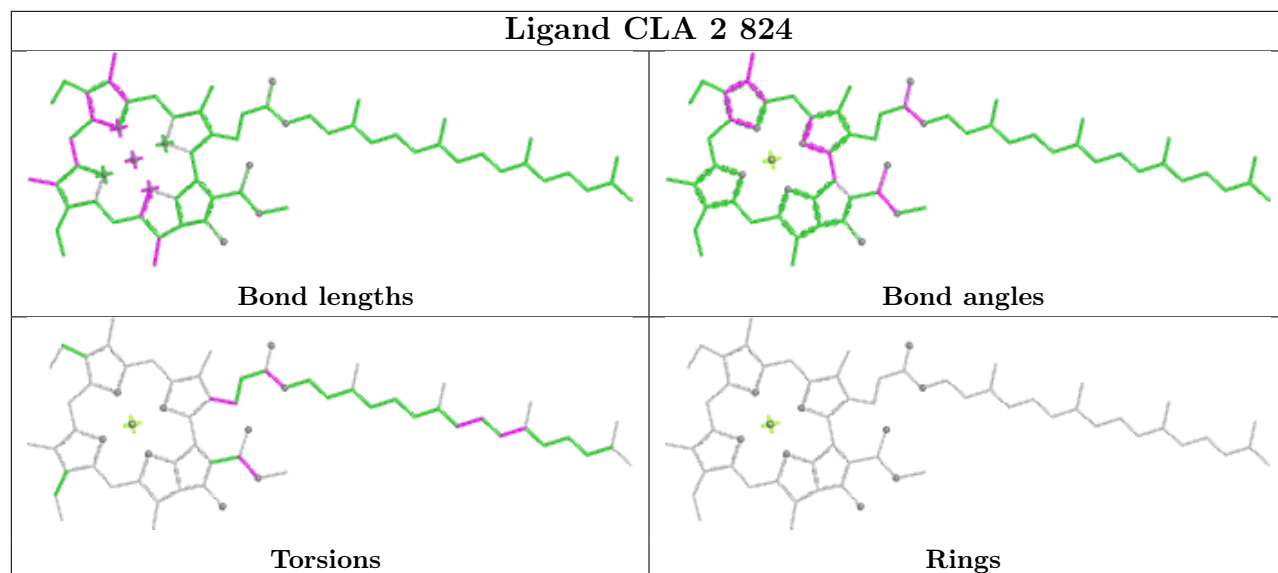
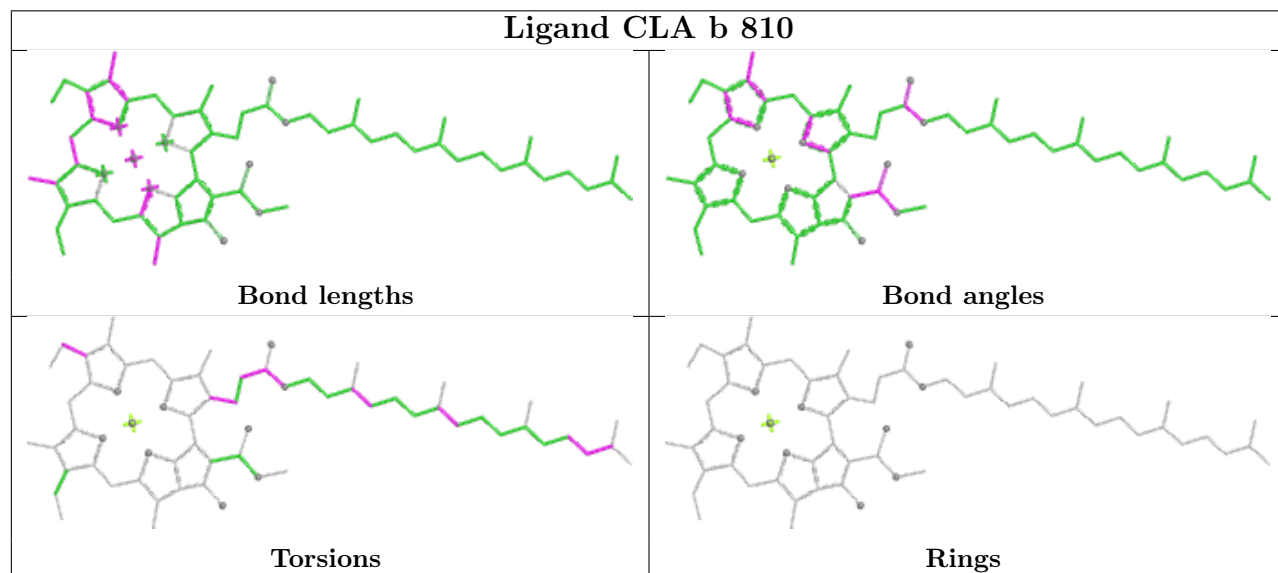
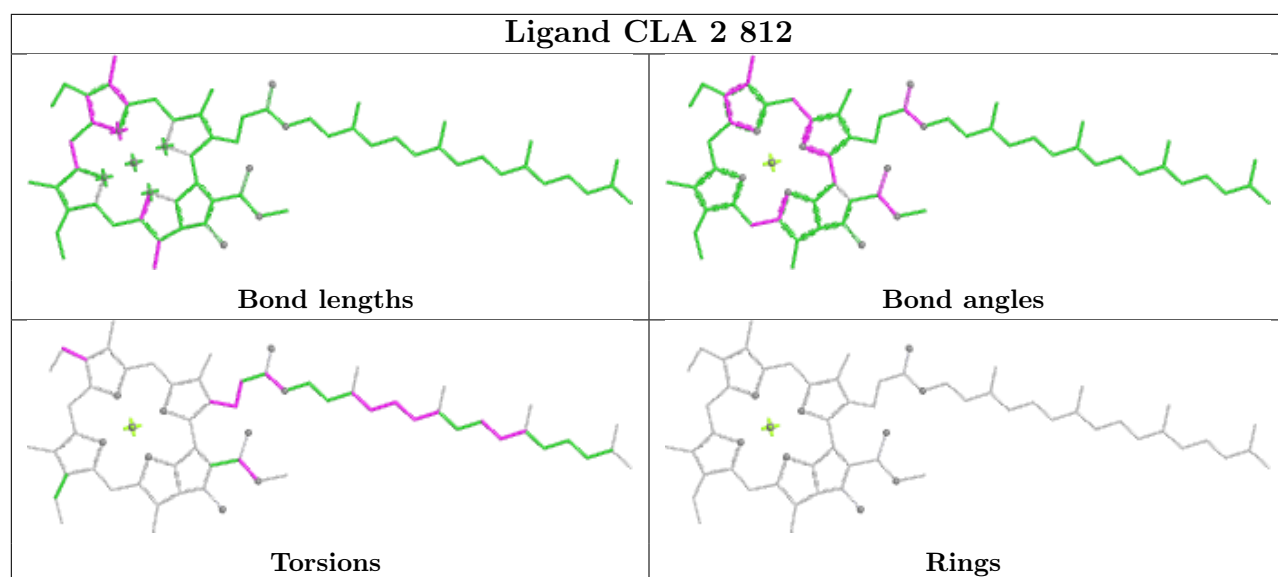
Bond angles

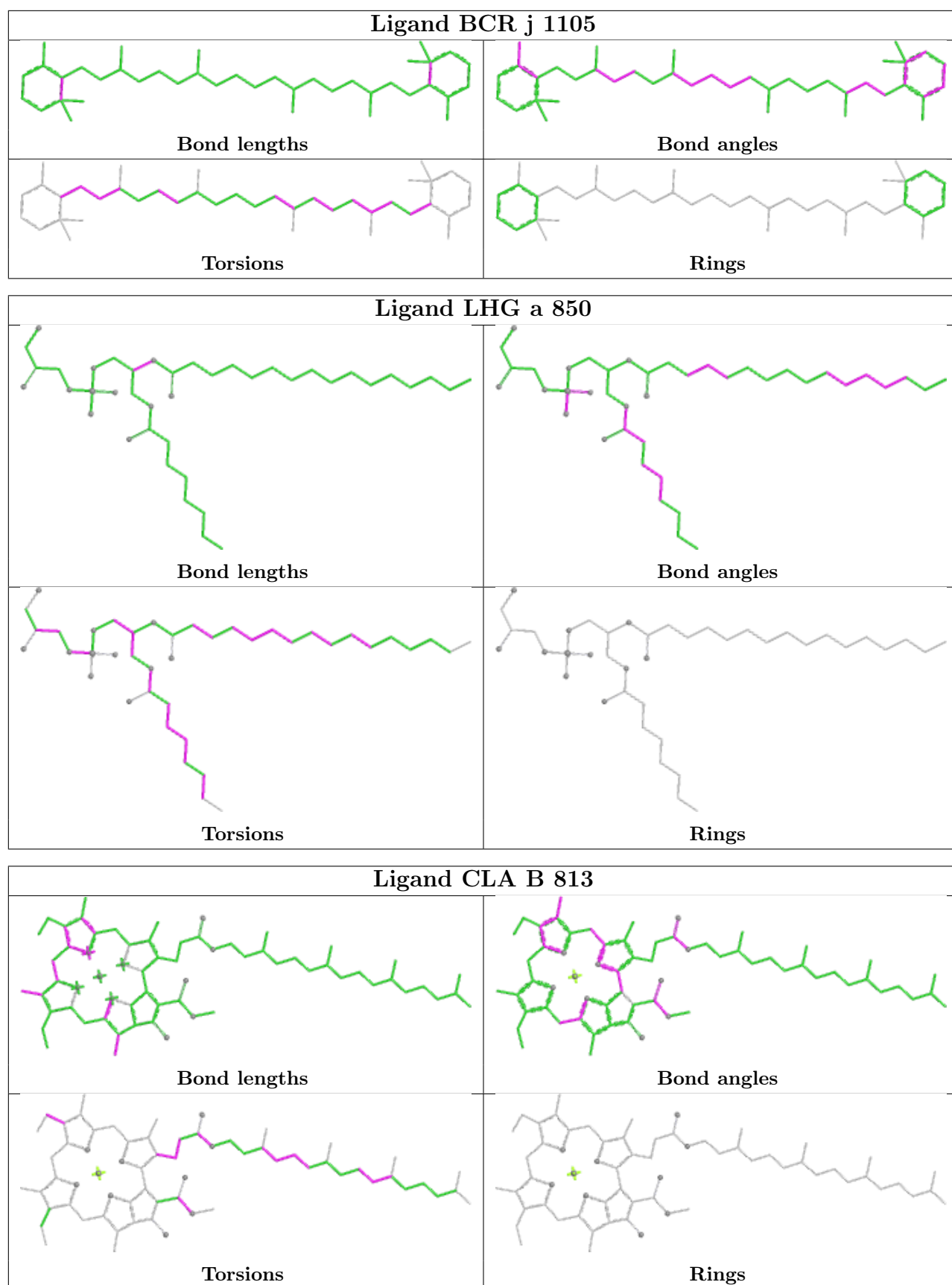


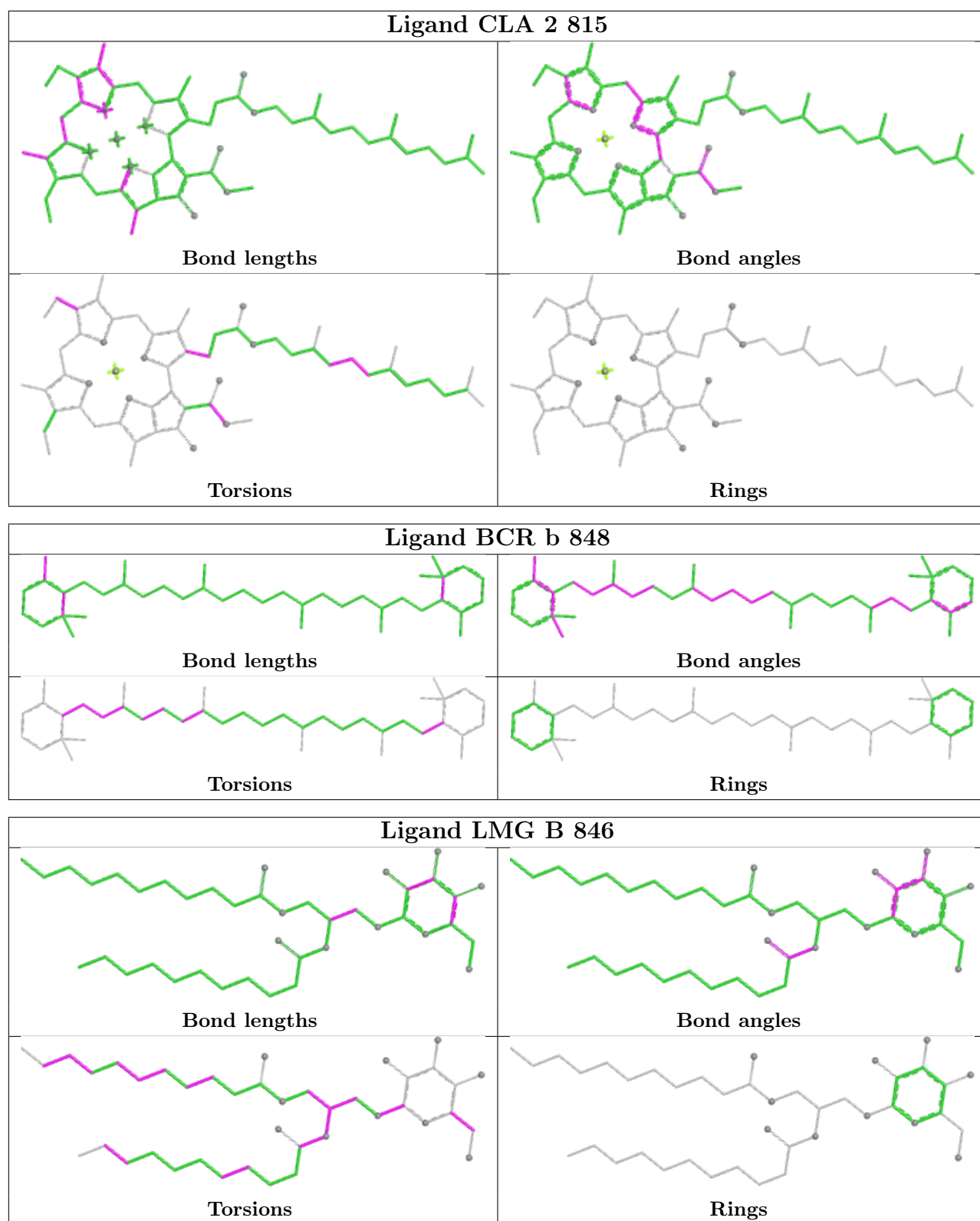
Torsions

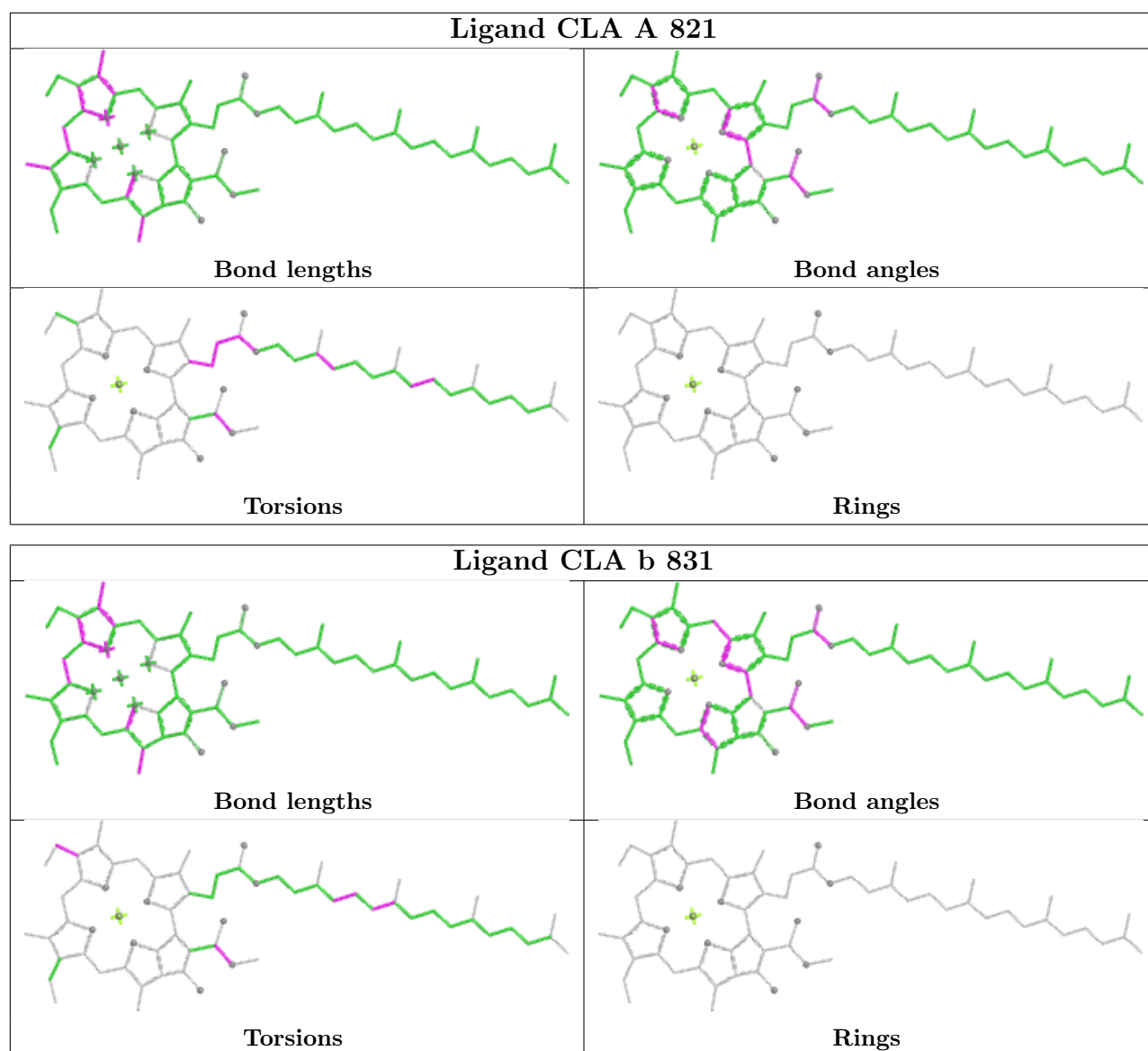


Rings

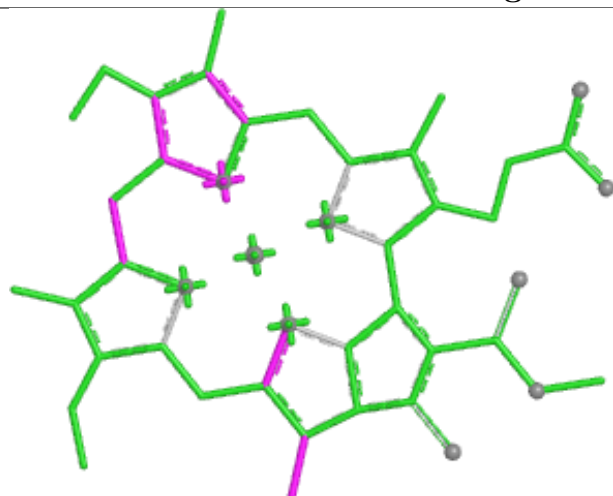




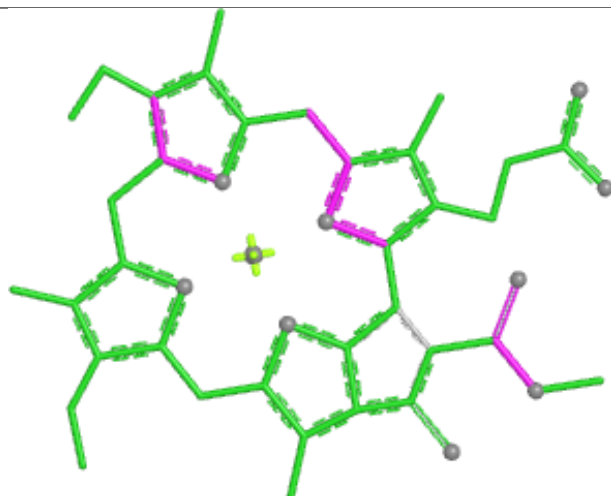




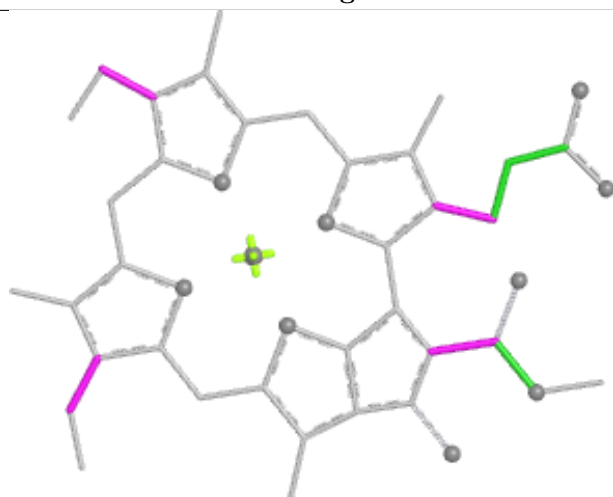
Ligand CLA K 4002



Bond lengths



Bond angles

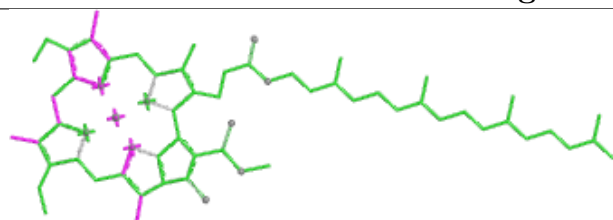


Torsions

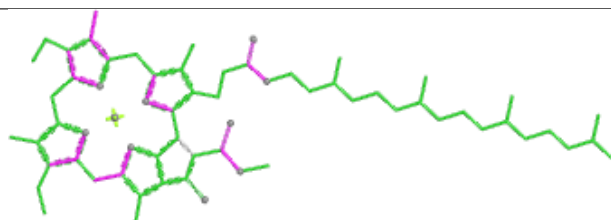


Rings

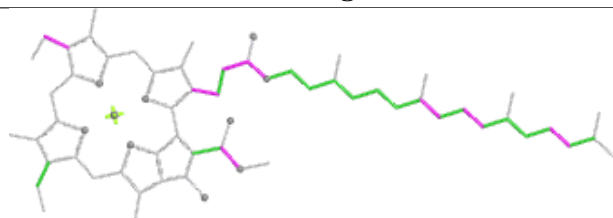
Ligand CLA a 806



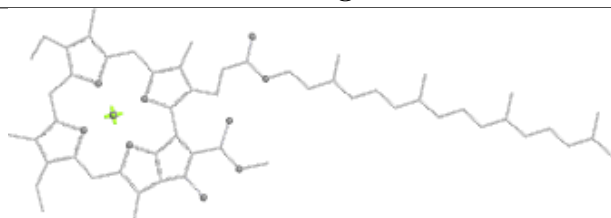
Bond lengths



Bond angles

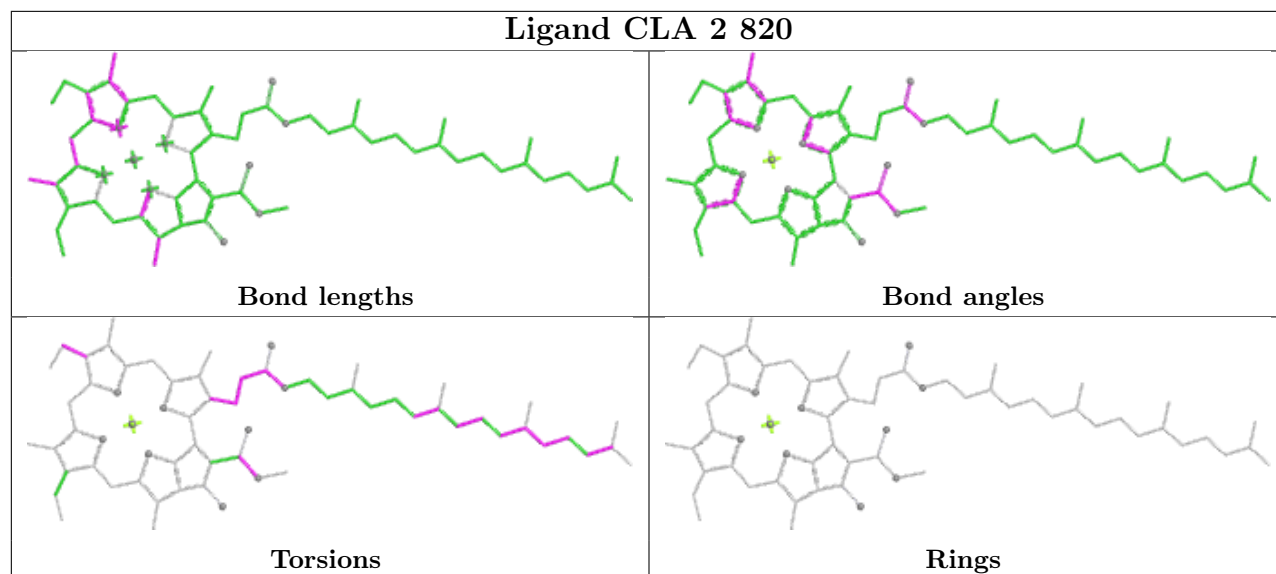


Torsions

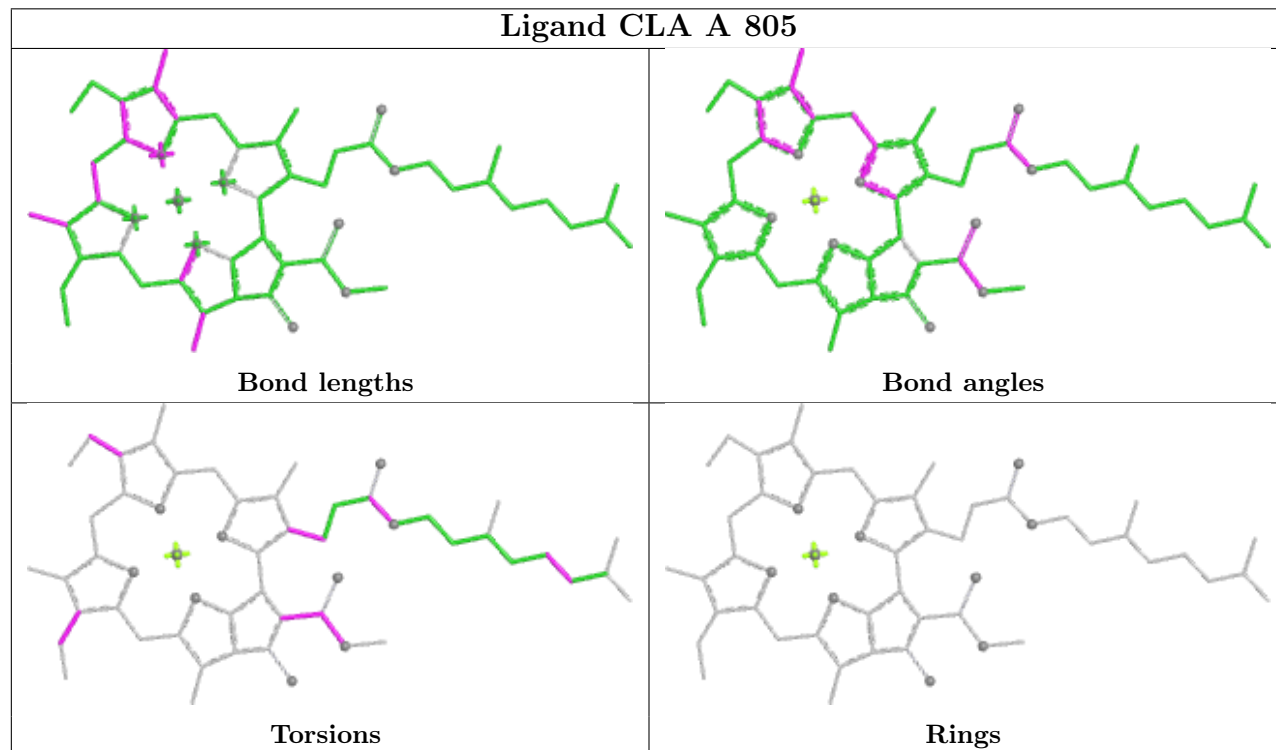


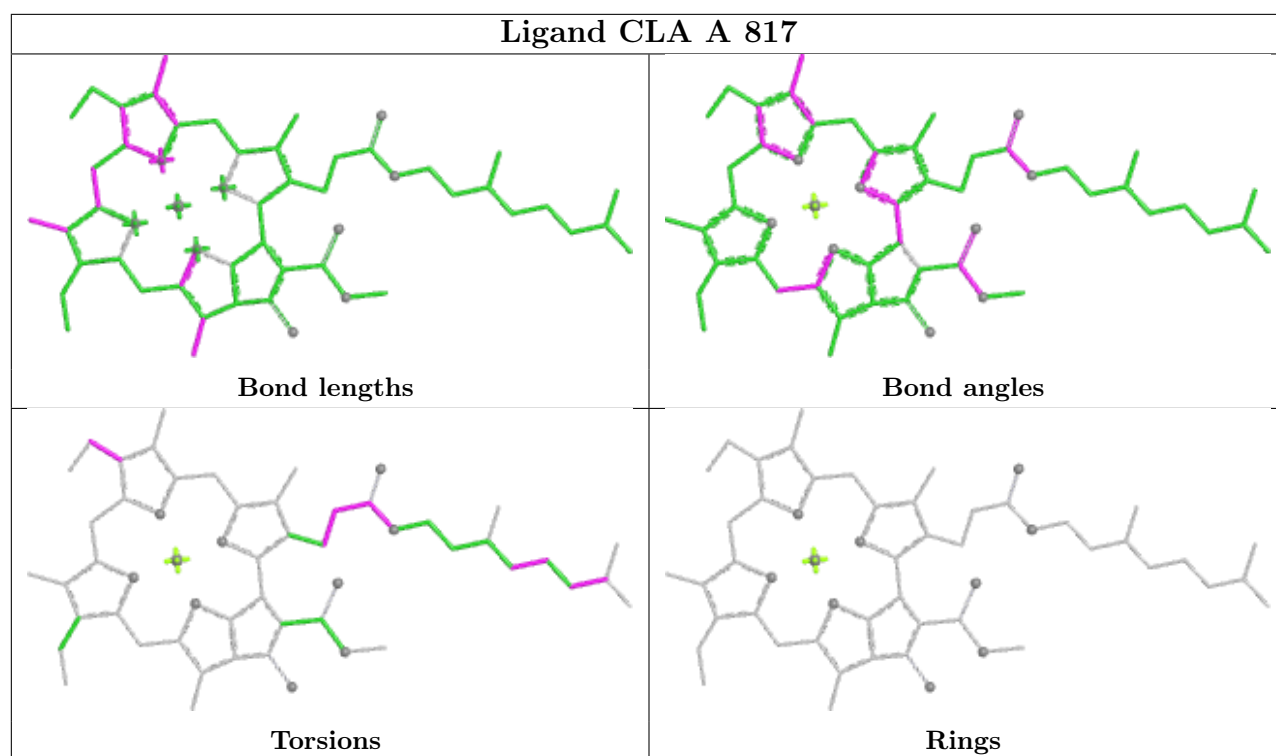
Rings

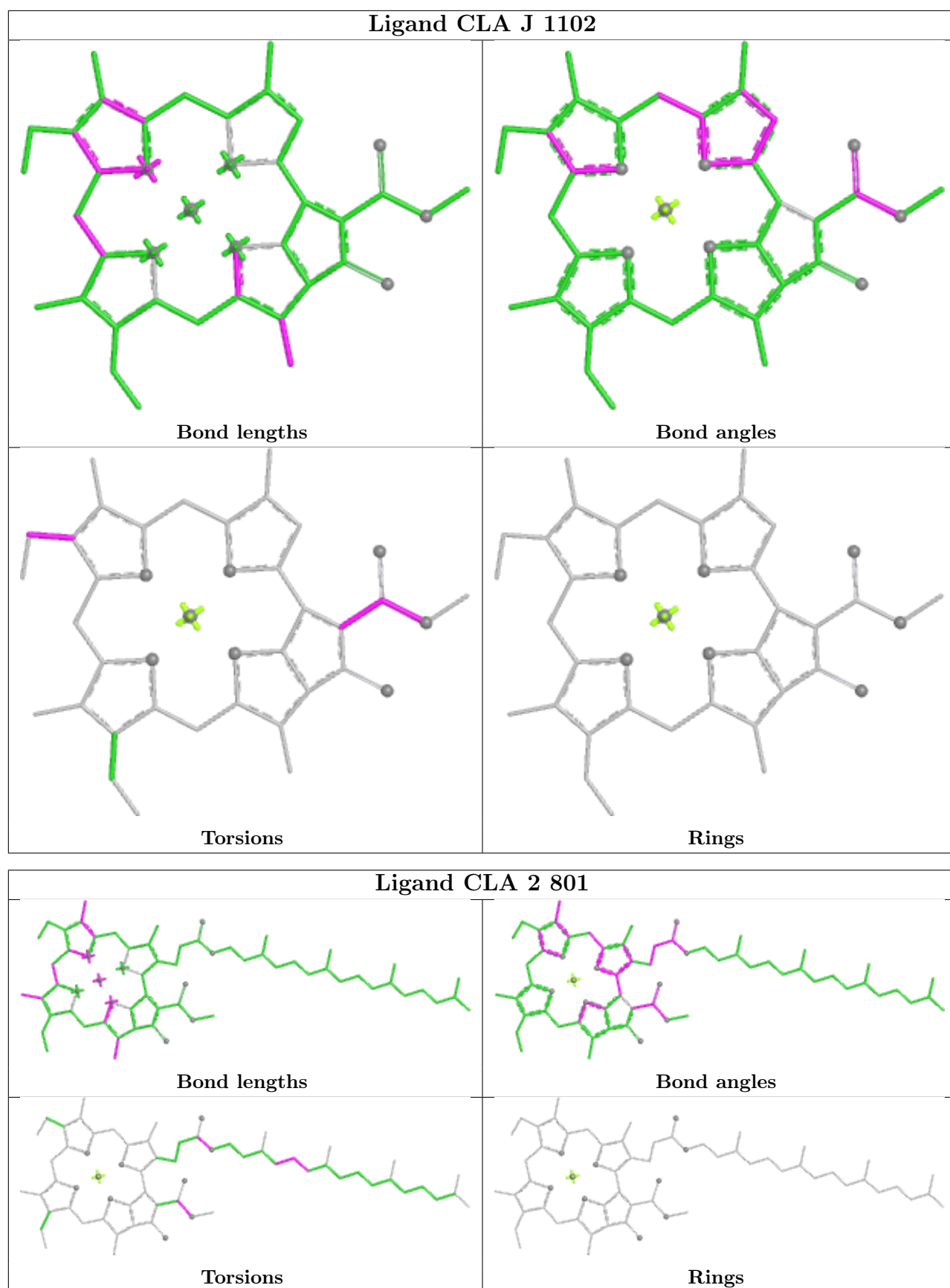
Ligand CLA 2 820

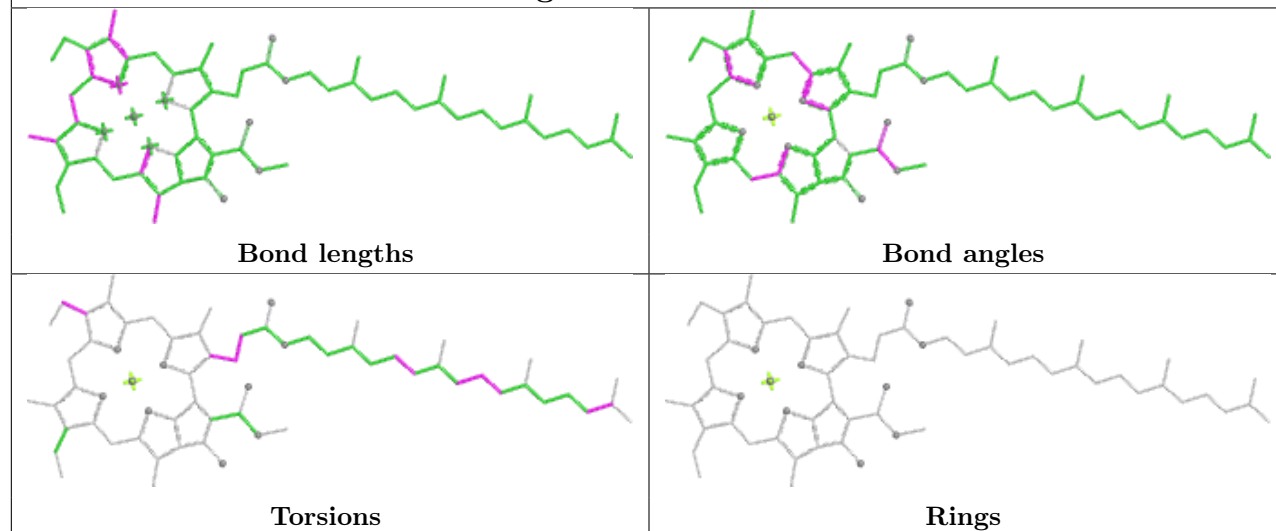
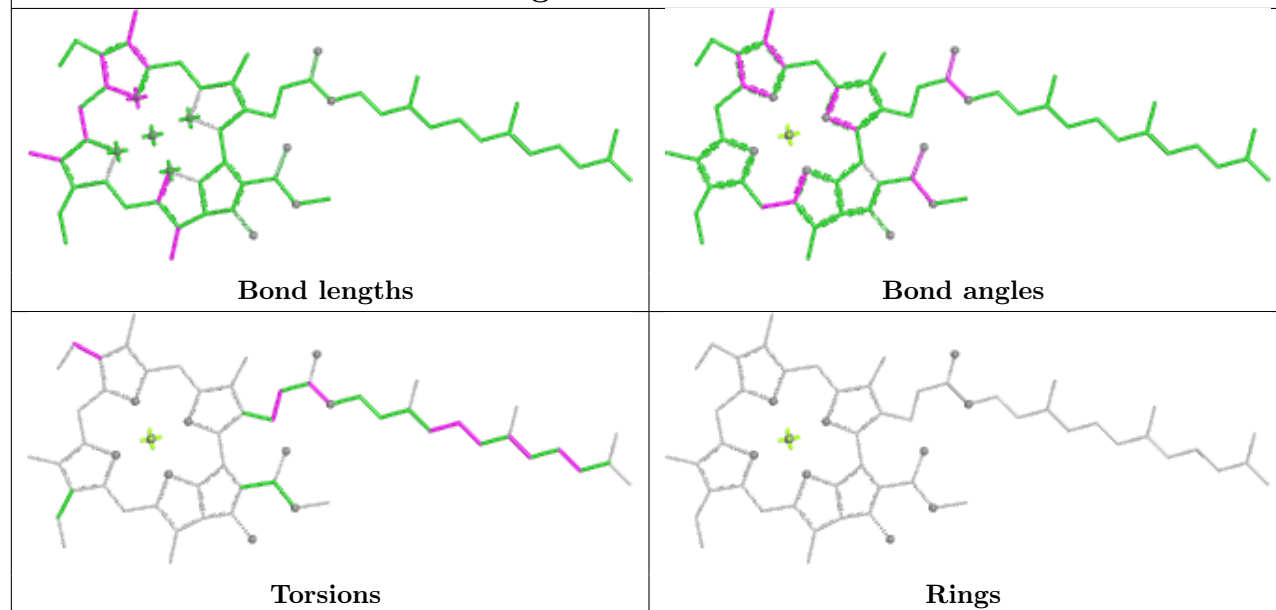


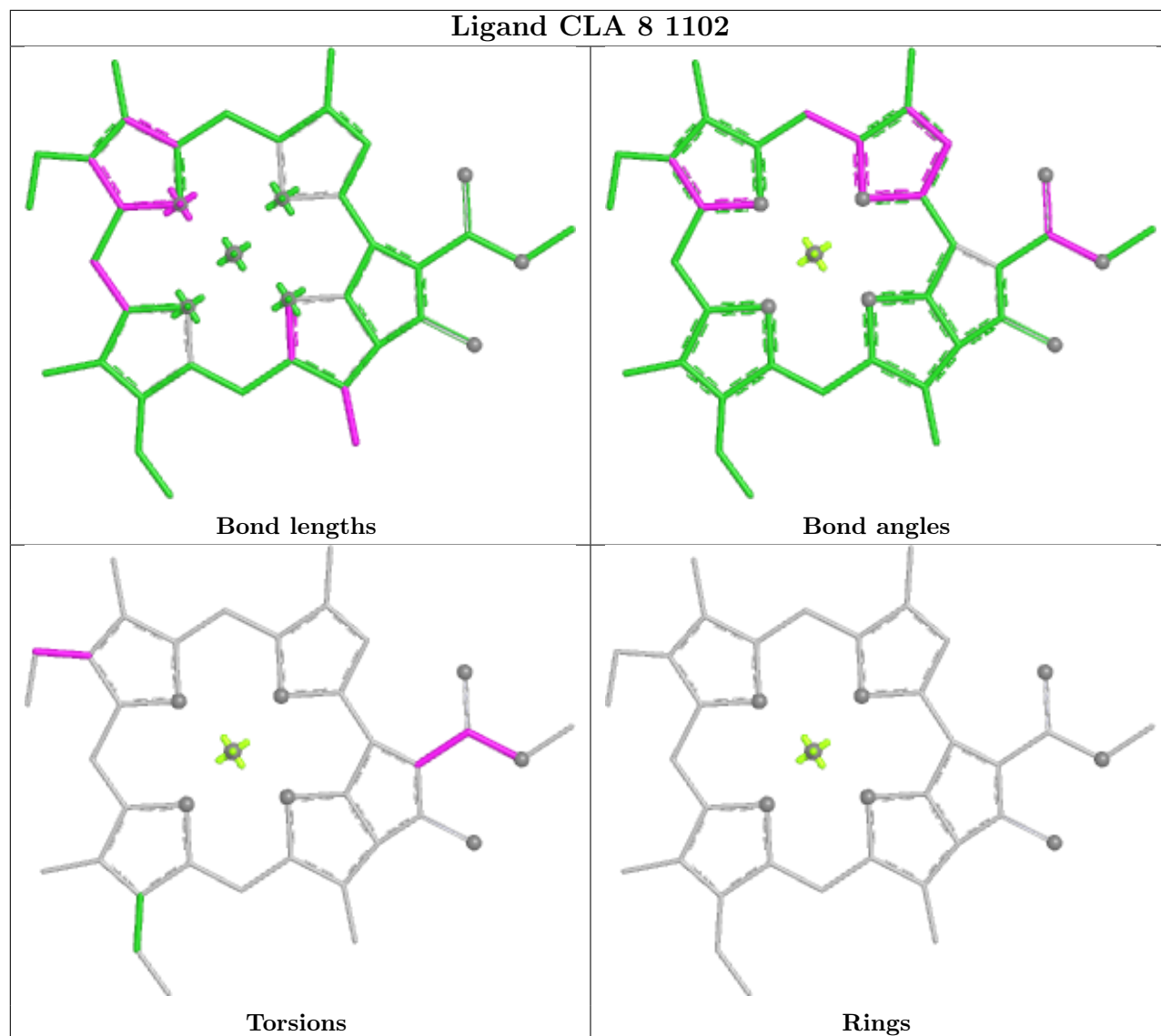
Ligand CLA A 805

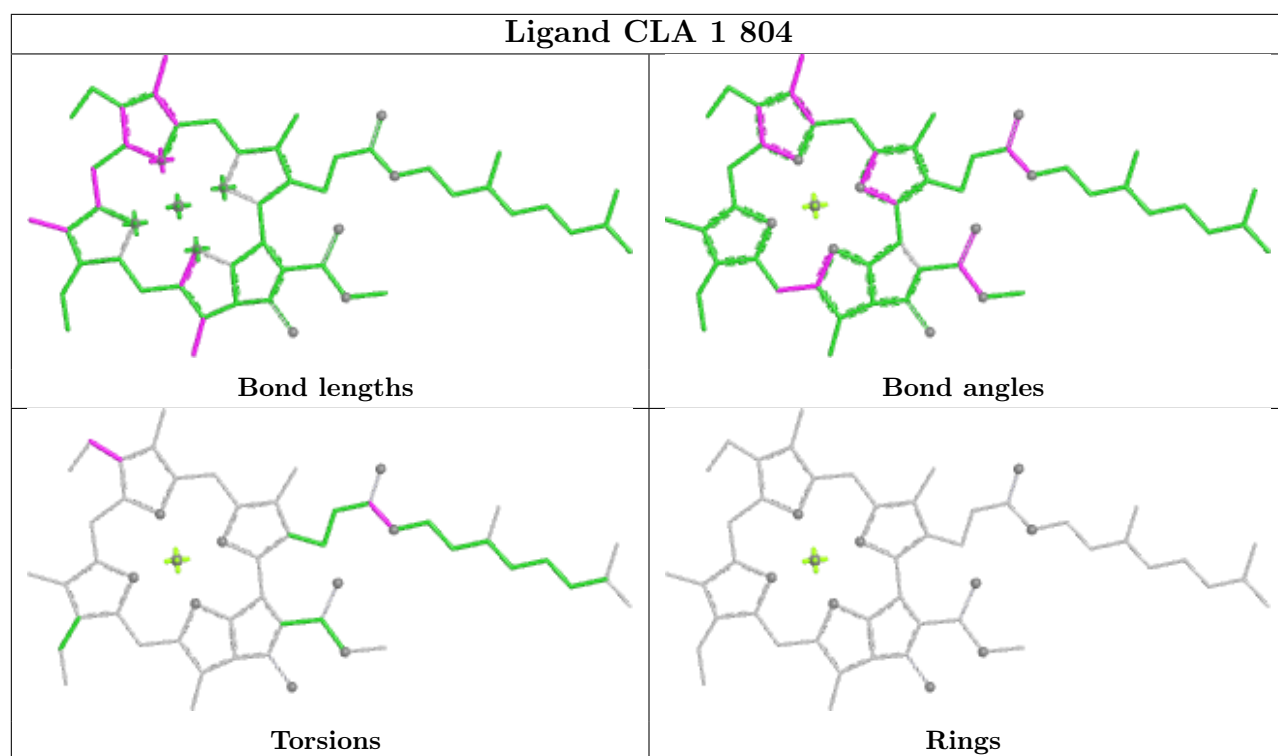


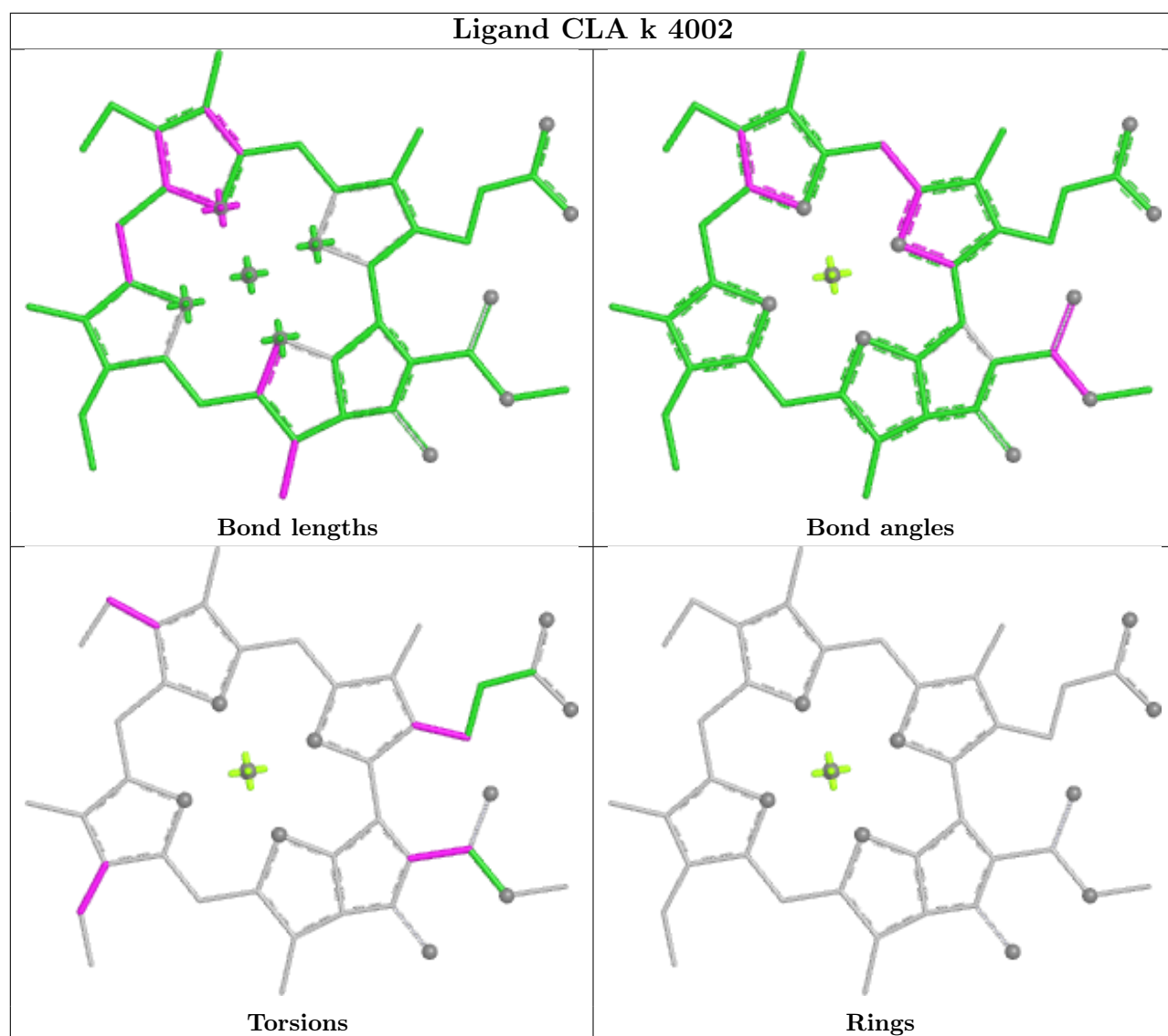


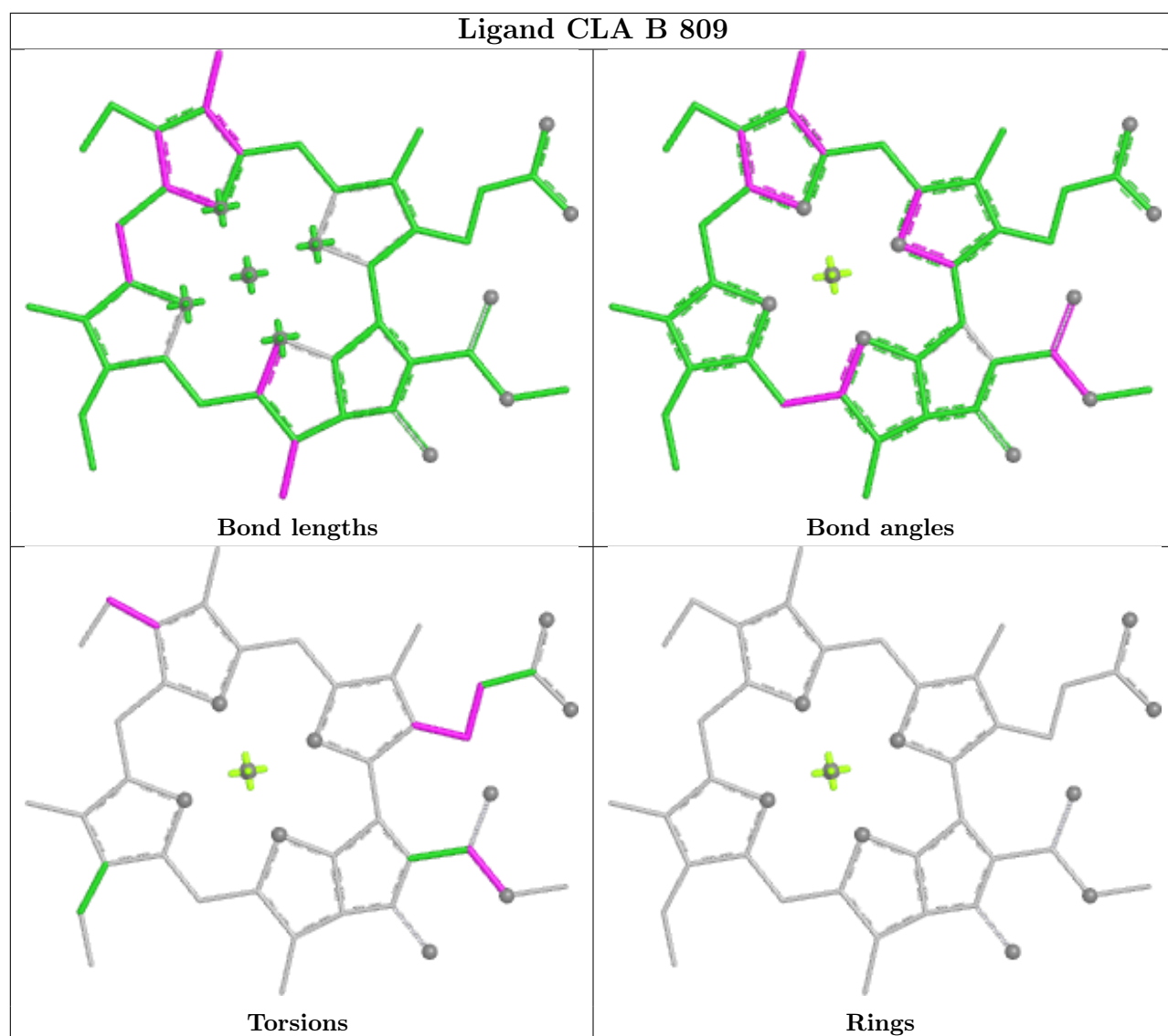


Ligand CLA 0 208**Ligand CLA A 837**









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

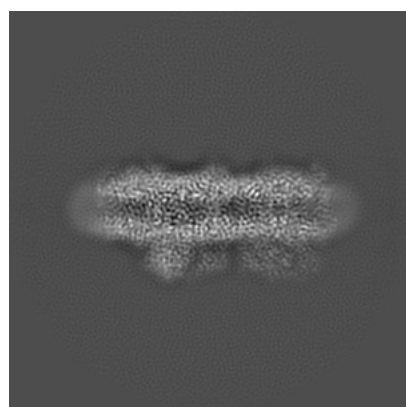
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21320. These allow visual inspection of the internal detail of the map and identification of artifacts.

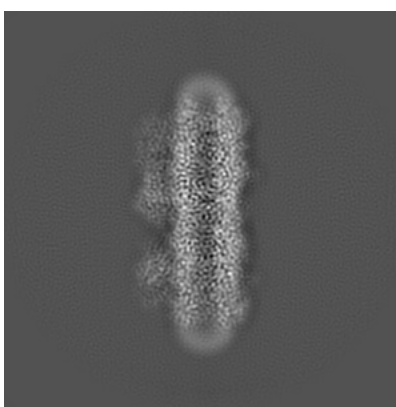
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

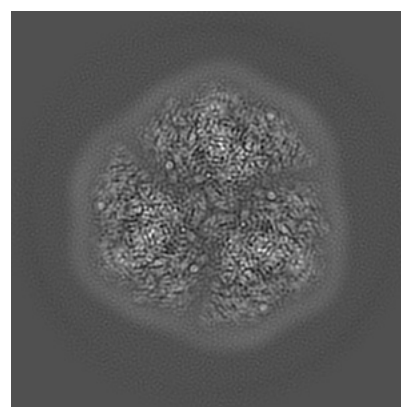
6.1.1 Primary map



X



Y

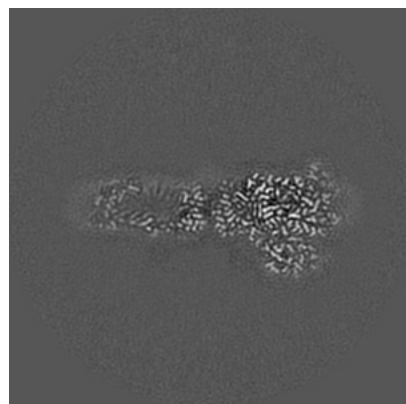


Z

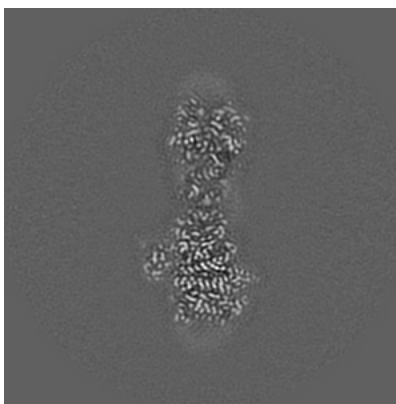
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

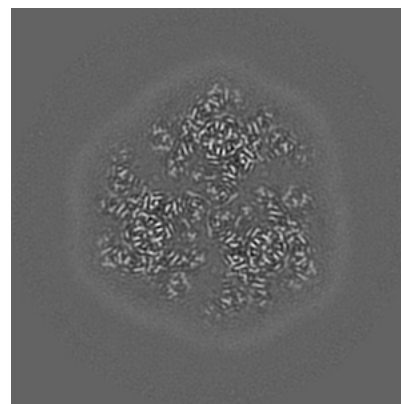
6.2.1 Primary map



X Index: 150



Y Index: 150

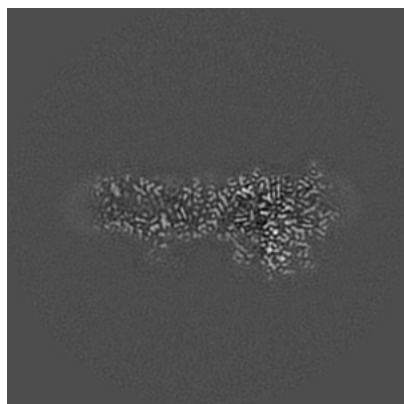


Z Index: 150

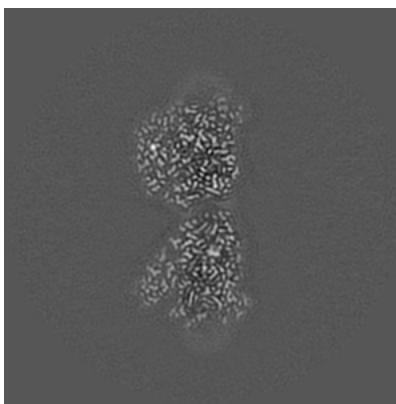
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

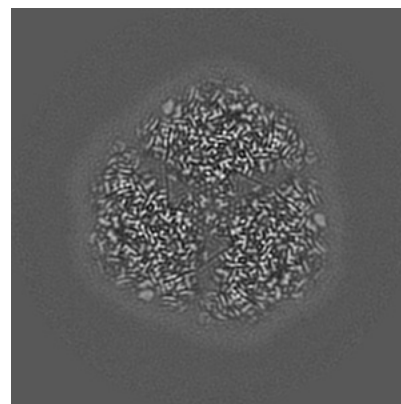
6.3.1 Primary map



X Index: 158



Y Index: 116

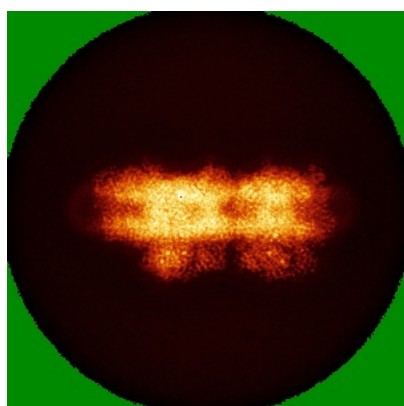


Z Index: 161

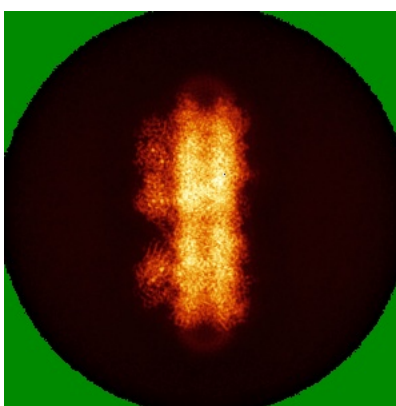
The images above show the largest variance slices of the map in three orthogonal directions.

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

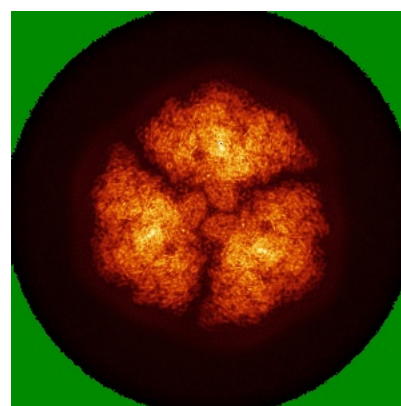
6.4.1 Primary map



X



Y

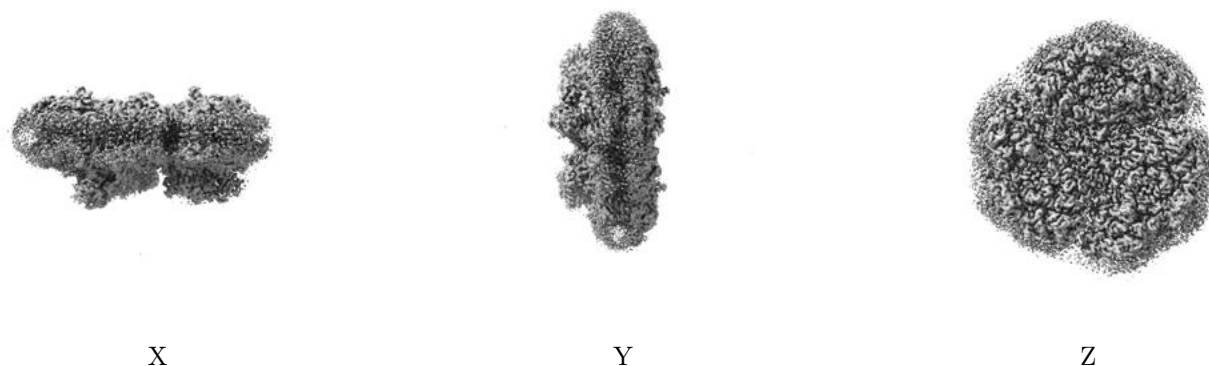


Z

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 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

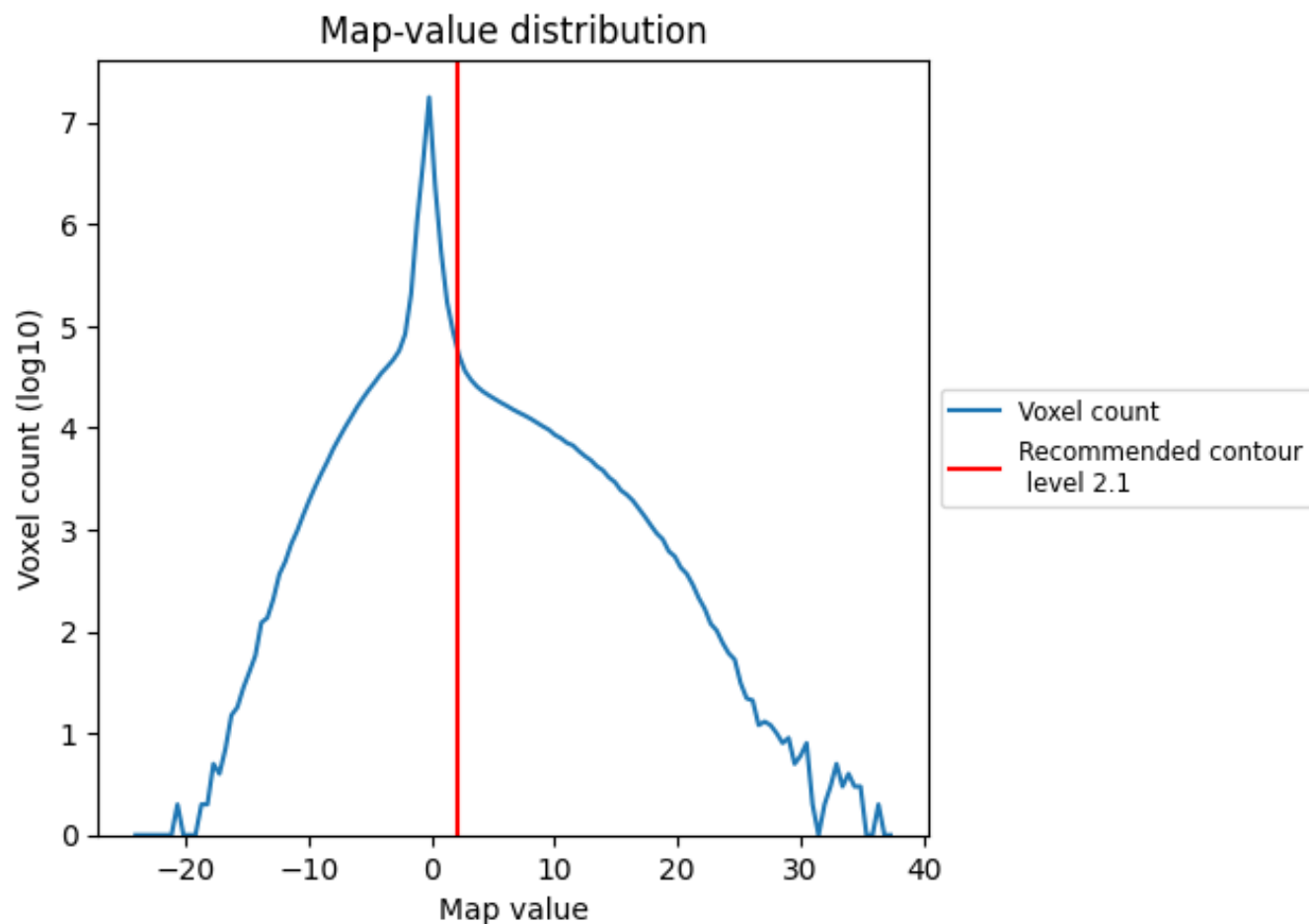
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

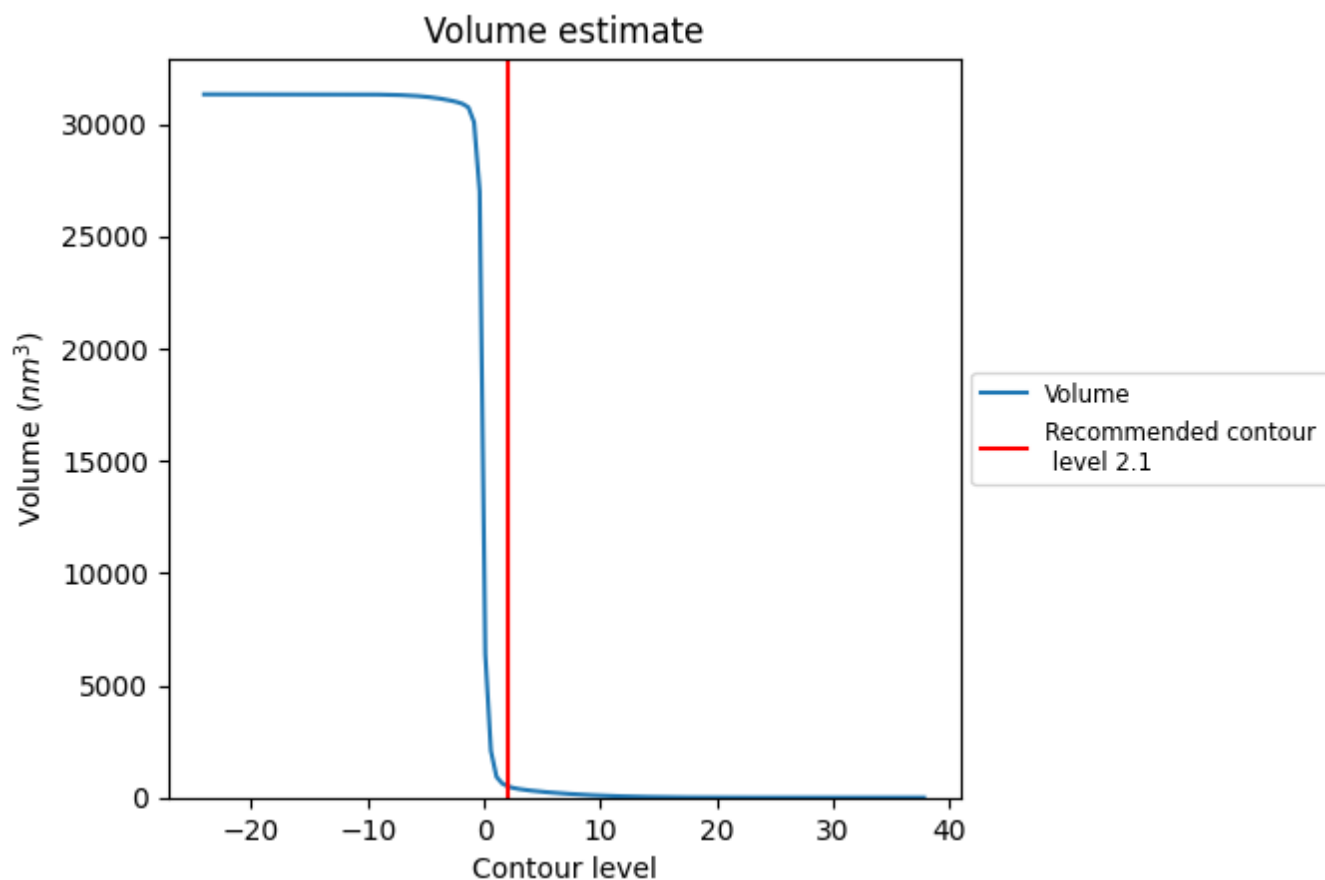
This section contains the results of statistical analysis of the map.

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.

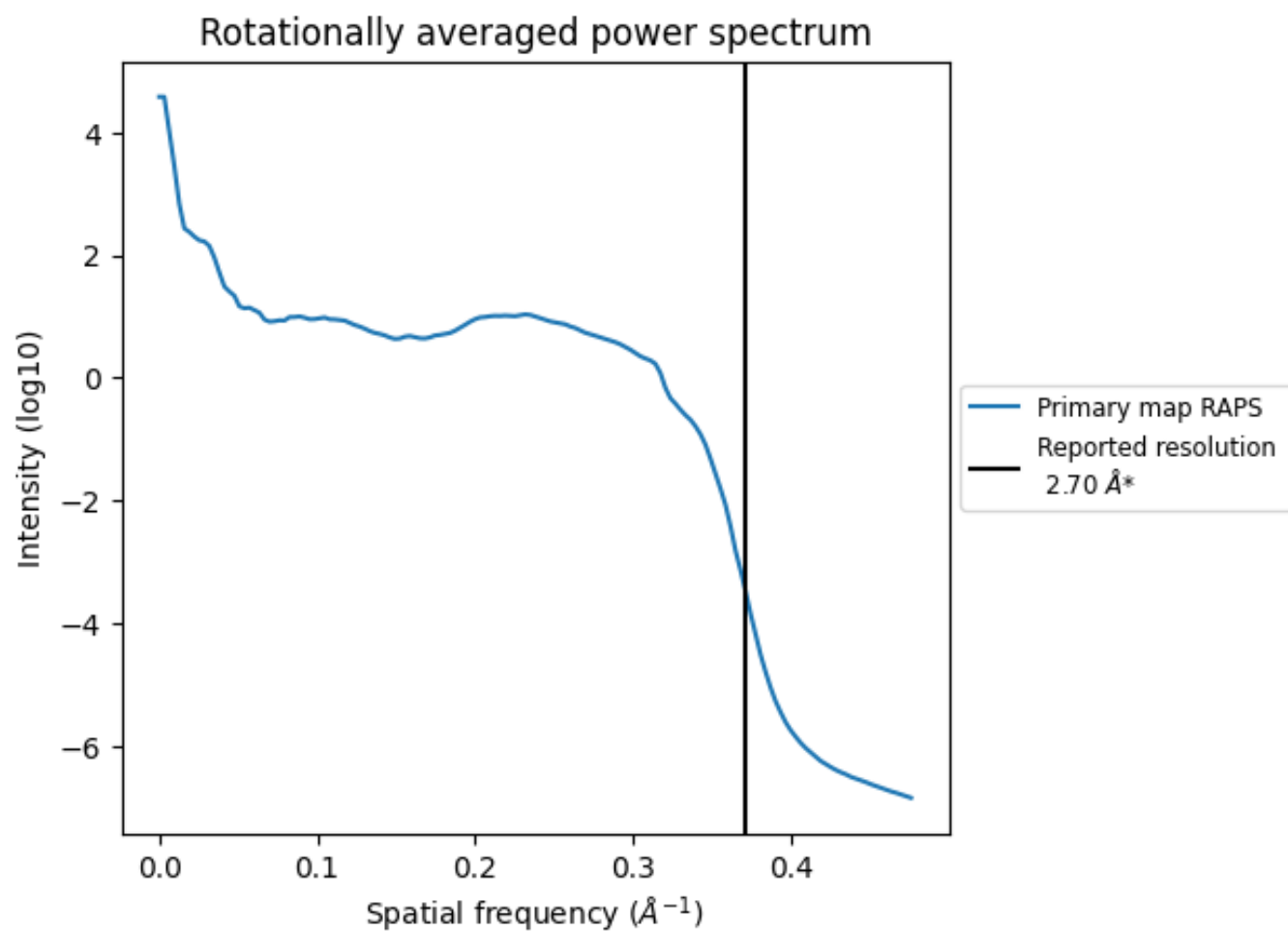
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 492 nm^3 ; this corresponds to an approximate mass of 445 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 ⓘ

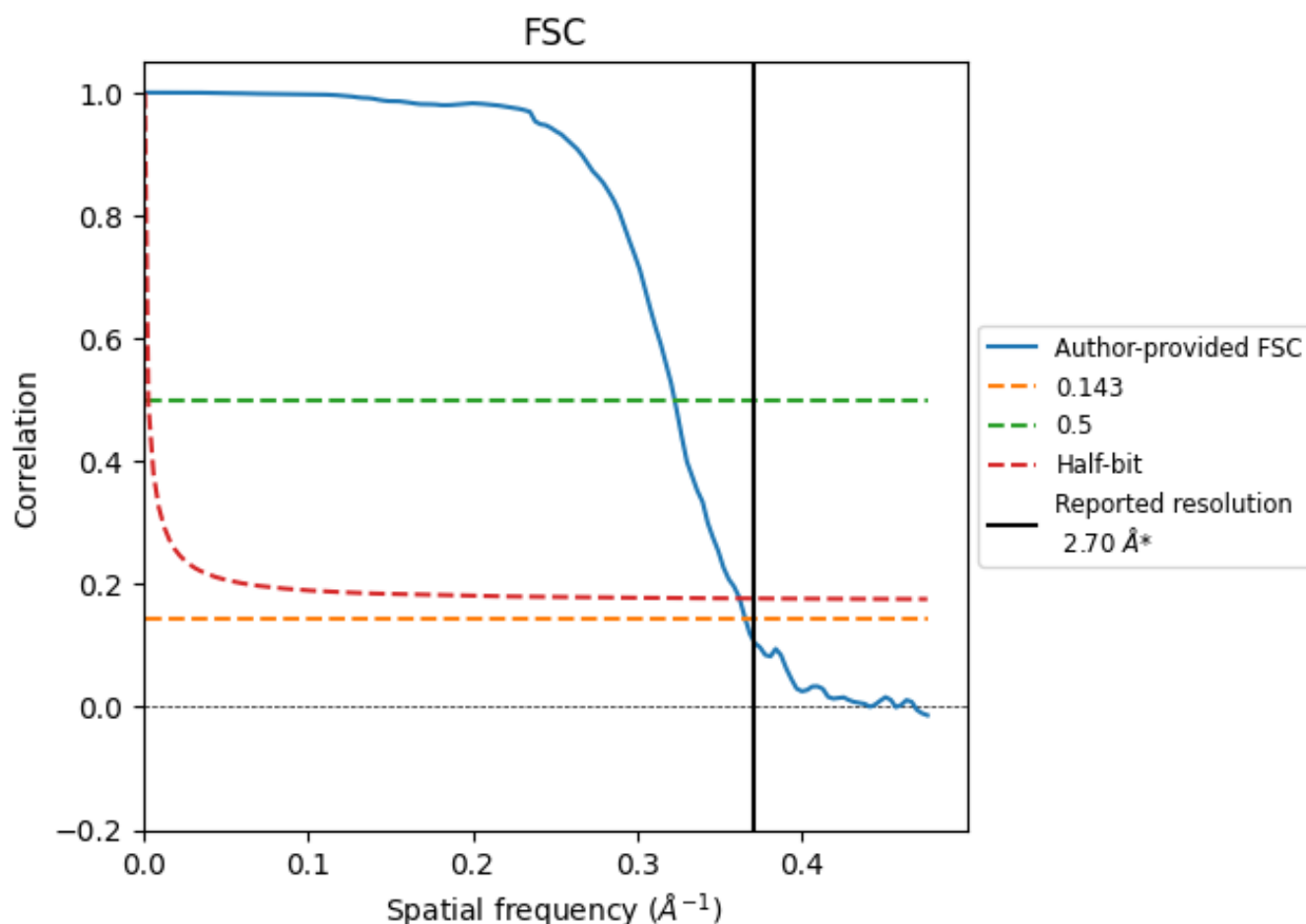


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 Å⁻¹

8.2 Resolution estimates [i](#)

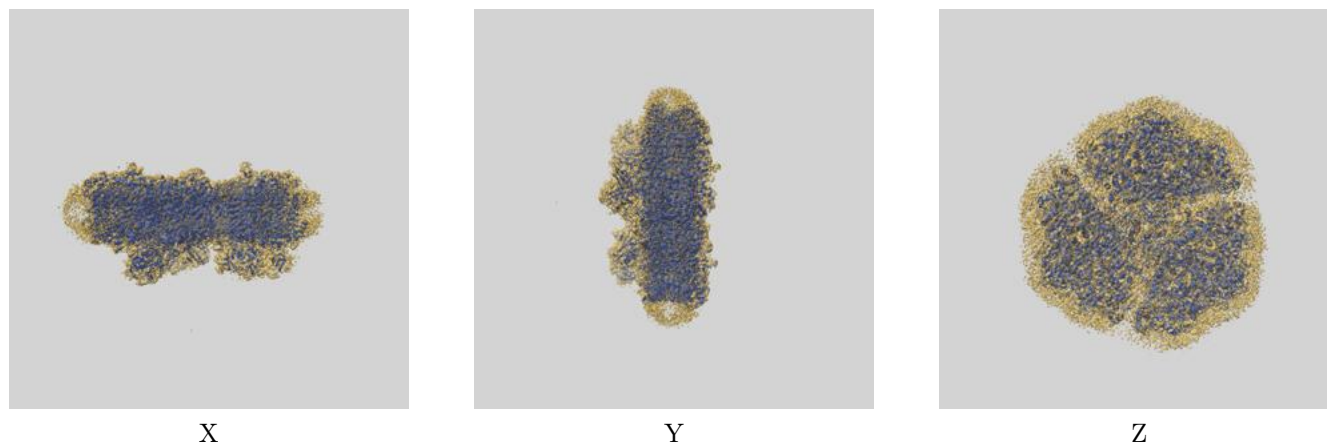
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.10	2.76
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

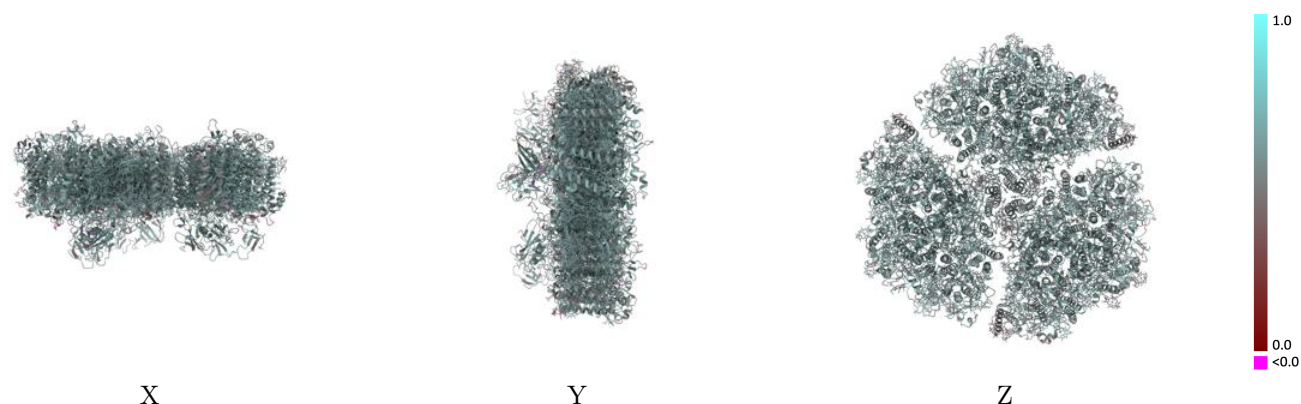
This section contains information regarding the fit between EMDB map EMD-21320 and PDB model 6VPV. Per-residue inclusion information can be found in section [3](#) on page [31](#).

9.1 Map-model overlay [i](#)



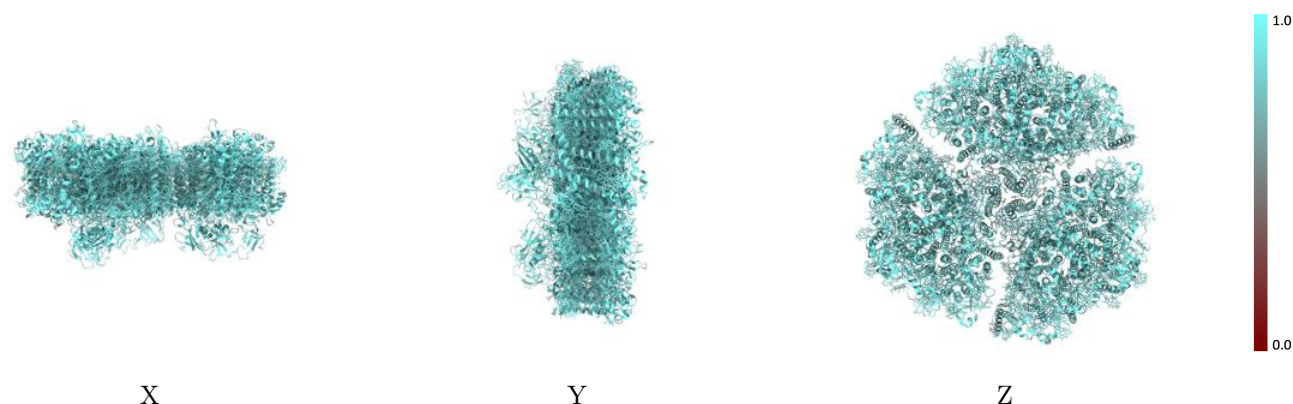
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



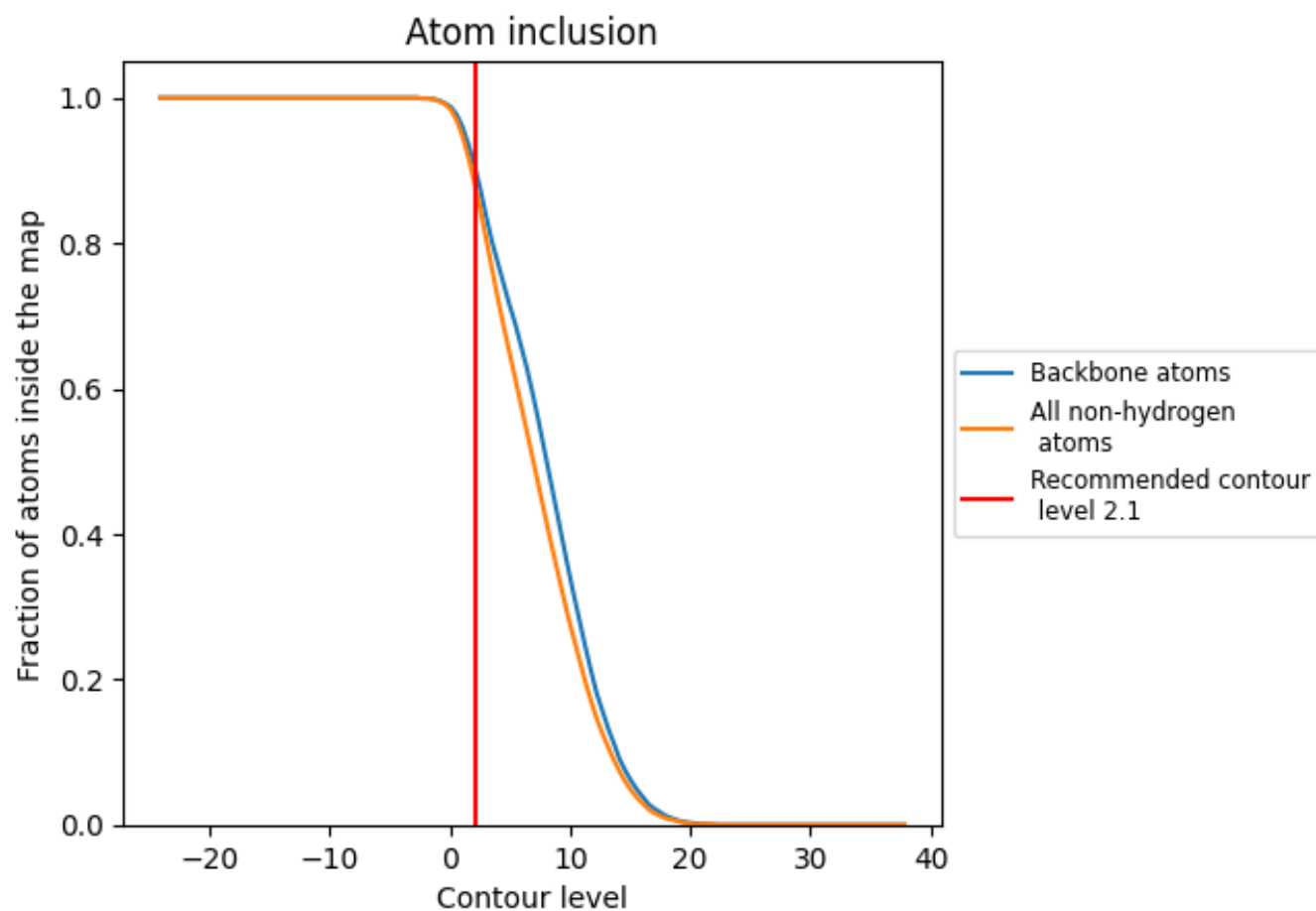
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (2.1).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 88% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8800	 0.5690
0	 0.8310	 0.5540
1	 0.8910	 0.5810
2	 0.8870	 0.5730
3	 0.9220	 0.5680
4	 0.8620	 0.5350
5	 0.8590	 0.5340
6	 0.8340	 0.5290
7	 0.8120	 0.5610
8	 0.8270	 0.5480
9	 0.7340	 0.4740
A	 0.8990	 0.5850
B	 0.8970	 0.5800
C	 0.9430	 0.5710
D	 0.8730	 0.5410
E	 0.8750	 0.5440
F	 0.8380	 0.5340
I	 0.8290	 0.5630
J	 0.8370	 0.5650
K	 0.7620	 0.4920
L	 0.8420	 0.5560
M	 0.8220	 0.5660
a	 0.9020	 0.5830
b	 0.9020	 0.5810
c	 0.9430	 0.5770
d	 0.8700	 0.5410
e	 0.8710	 0.5430
f	 0.8410	 0.5370
i	 0.8290	 0.5690
j	 0.8410	 0.5610
k	 0.7600	 0.4880
l	 0.8410	 0.5560
m	 0.8250	 0.5650
z	 0.7880	 0.5480

