



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 04:21 AM UTC

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

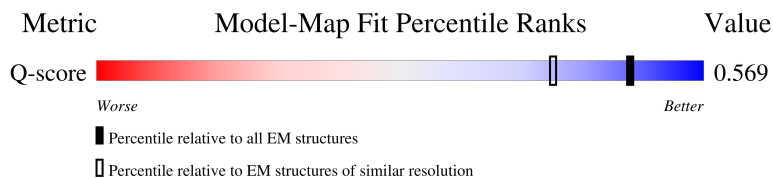
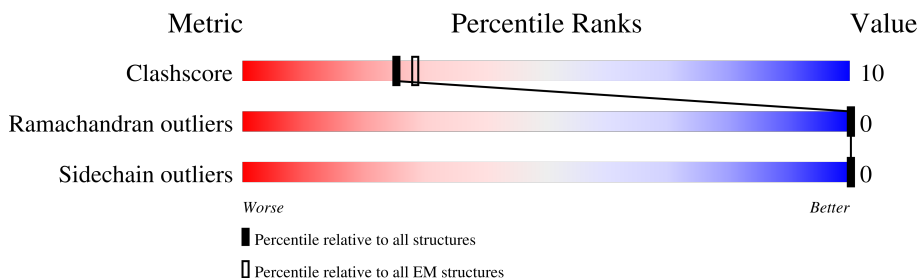
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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.



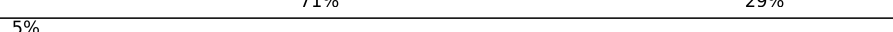
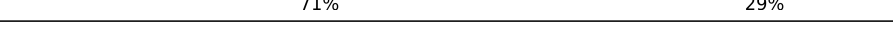
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10327 (2.20 - 3.20)

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	 83% 17%
1	A	741	 83% 17%
1	a	741	 83% 17%
2	2	737	 82% 18%

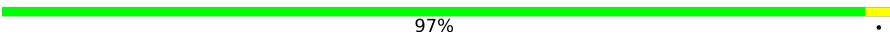
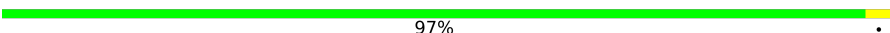
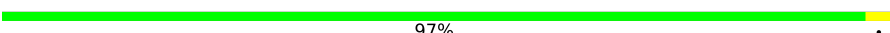
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Mol	Chain	Length	Quality of chain
2	B	737	 83%17%
2	b	737	 82%18%
3	3	80	 79%21%
3	C	80	 80%20%
3	c	80	 80%20%
4	4	139	 88%12%
4	D	139	 87%13%
4	d	139	 87%13%
5	5	68	 84%16%
5	E	68	 87%13%
5	e	68	 88%12%
6	6	141	 91%9%
6	F	141	 89%11%
6	f	141	 90%10%
7	7	38	 5%74%26%
7	I	38	 5%71%29%
7	i	38	 5%71%29%
8	8	39	 82%18%
8	J	39	 82%18%
8	j	39	 82%18%
9	9	78	 90%10%
9	K	78	 87%13%
9	k	78	 90%10%
10	0	160	 74%26%
10	L	160	 71%29%

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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%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CL0	1	801	X	-	-	-
12	CL0	A	801	X	-	-	-
12	CL0	a	801	X	-	-	-
13	CLA	0	203	X	-	-	-
13	CLA	0	205	X	-	-	-
13	CLA	0	206	X	-	-	-
13	CLA	0	208	X	-	-	-
13	CLA	1	802	X	-	-	-
13	CLA	1	803	X	-	-	-
13	CLA	1	804	X	-	-	-
13	CLA	1	805	X	-	-	-
13	CLA	1	806	X	-	-	-
13	CLA	1	807	X	-	-	-
13	CLA	1	808	X	-	-	-
13	CLA	1	811	X	-	-	-
13	CLA	1	813	X	-	-	-
13	CLA	1	814	X	-	-	-
13	CLA	1	815	X	-	-	-
13	CLA	1	816	X	-	-	-
13	CLA	1	818	X	-	-	-
13	CLA	1	819	X	-	-	-
13	CLA	1	821	X	-	-	-
13	CLA	1	823	X	-	-	-
13	CLA	1	824	X	-	-	-
13	CLA	1	826	X	-	-	-
13	CLA	1	827	X	-	-	-
13	CLA	1	828	X	-	-	-
13	CLA	1	829	X	-	-	-
13	CLA	1	833	X	-	-	-
13	CLA	1	836	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	837	X	-	-	-
13	CLA	1	838	X	-	-	-
13	CLA	1	839	X	-	-	-
13	CLA	1	841	X	-	-	-
13	CLA	1	842	X	-	-	-
13	CLA	1	852	X	-	-	-
13	CLA	2	801	X	-	-	-
13	CLA	2	803	X	-	-	-
13	CLA	2	804	X	-	-	-
13	CLA	2	805	X	-	-	-
13	CLA	2	806	X	-	-	-
13	CLA	2	809	X	-	-	-
13	CLA	2	810	X	-	-	-
13	CLA	2	811	X	-	-	-
13	CLA	2	812	X	-	-	-
13	CLA	2	814	X	-	-	-
13	CLA	2	815	X	-	-	-
13	CLA	2	819	X	-	-	-
13	CLA	2	821	X	-	-	-
13	CLA	2	822	X	-	-	-
13	CLA	2	823	X	-	-	-
13	CLA	2	824	X	-	-	-
13	CLA	2	828	X	-	-	-
13	CLA	2	829	X	-	-	-
13	CLA	2	830	X	-	-	-
13	CLA	2	831	X	-	-	-
13	CLA	2	832	X	-	-	-
13	CLA	2	833	X	-	-	-
13	CLA	2	834	X	-	-	-
13	CLA	2	835	X	-	-	-
13	CLA	2	846	X	-	-	-
13	CLA	6	201	X	-	-	-
13	CLA	6	203	X	-	-	-
13	CLA	6	204	X	-	-	-
13	CLA	7	102	X	-	-	-
13	CLA	8	1101	X	-	-	-
13	CLA	8	1102	X	-	-	-
13	CLA	8	1103	X	-	-	-
13	CLA	9	4002	X	-	-	-
13	CLA	9	4003	X	-	-	-
13	CLA	9	4005	X	-	-	-
13	CLA	A	802	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	803	X	-	-	-
13	CLA	A	804	X	-	-	-
13	CLA	A	805	X	-	-	-
13	CLA	A	806	X	-	-	-
13	CLA	A	807	X	-	-	-
13	CLA	A	808	X	-	-	-
13	CLA	A	811	X	-	-	-
13	CLA	A	813	X	-	-	-
13	CLA	A	814	X	-	-	-
13	CLA	A	815	X	-	-	-
13	CLA	A	816	X	-	-	-
13	CLA	A	818	X	-	-	-
13	CLA	A	819	X	-	-	-
13	CLA	A	821	X	-	-	-
13	CLA	A	823	X	-	-	-
13	CLA	A	824	X	-	-	-
13	CLA	A	826	X	-	-	-
13	CLA	A	827	X	-	-	-
13	CLA	A	828	X	-	-	-
13	CLA	A	829	X	-	-	-
13	CLA	A	833	X	-	-	-
13	CLA	A	836	X	-	-	-
13	CLA	A	837	X	-	-	-
13	CLA	A	838	X	-	-	-
13	CLA	A	839	X	-	-	-
13	CLA	A	841	X	-	-	-
13	CLA	A	842	X	-	-	-
13	CLA	A	852	X	-	-	-
13	CLA	B	801	X	-	-	-
13	CLA	B	803	X	-	-	-
13	CLA	B	804	X	-	-	-
13	CLA	B	805	X	-	-	-
13	CLA	B	806	X	-	-	-
13	CLA	B	807	X	-	-	-
13	CLA	B	810	X	-	-	-
13	CLA	B	811	X	-	-	-
13	CLA	B	812	X	-	-	-
13	CLA	B	813	X	-	-	-
13	CLA	B	815	X	-	-	-
13	CLA	B	816	X	-	-	-
13	CLA	B	820	X	-	-	-
13	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	823	X	-	-	-
13	CLA	B	824	X	-	-	-
13	CLA	B	825	X	-	-	-
13	CLA	B	829	X	-	-	-
13	CLA	B	830	X	-	-	-
13	CLA	B	831	X	-	-	-
13	CLA	B	832	X	-	-	-
13	CLA	B	833	X	-	-	-
13	CLA	B	834	X	-	-	-
13	CLA	B	835	X	-	-	-
13	CLA	B	836	X	-	-	-
13	CLA	B	847	X	-	-	-
13	CLA	F	201	X	-	-	-
13	CLA	F	203	X	-	-	-
13	CLA	F	204	X	-	-	-
13	CLA	I	101	X	-	-	-
13	CLA	J	1101	X	-	-	-
13	CLA	J	1102	X	-	-	-
13	CLA	J	1103	X	-	-	-
13	CLA	K	4002	X	-	-	-
13	CLA	K	4003	X	-	-	-
13	CLA	K	4005	X	-	-	-
13	CLA	L	203	X	-	-	-
13	CLA	L	204	X	-	-	-
13	CLA	L	206	X	-	-	-
13	CLA	a	802	X	-	-	-
13	CLA	a	803	X	-	-	-
13	CLA	a	804	X	-	-	-
13	CLA	a	805	X	-	-	-
13	CLA	a	806	X	-	-	-
13	CLA	a	807	X	-	-	-
13	CLA	a	808	X	-	-	-
13	CLA	a	811	X	-	-	-
13	CLA	a	813	X	-	-	-
13	CLA	a	814	X	-	-	-
13	CLA	a	815	X	-	-	-
13	CLA	a	816	X	-	-	-
13	CLA	a	818	X	-	-	-
13	CLA	a	819	X	-	-	-
13	CLA	a	821	X	-	-	-
13	CLA	a	823	X	-	-	-
13	CLA	a	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	a	826	X	-	-	-
13	CLA	a	827	X	-	-	-
13	CLA	a	828	X	-	-	-
13	CLA	a	829	X	-	-	-
13	CLA	a	833	X	-	-	-
13	CLA	a	836	X	-	-	-
13	CLA	a	837	X	-	-	-
13	CLA	a	838	X	-	-	-
13	CLA	a	839	X	-	-	-
13	CLA	a	841	X	-	-	-
13	CLA	a	842	X	-	-	-
13	CLA	a	852	X	-	-	-
13	CLA	b	801	X	-	-	-
13	CLA	b	803	X	-	-	-
13	CLA	b	804	X	-	-	-
13	CLA	b	805	X	-	-	-
13	CLA	b	806	X	-	-	-
13	CLA	b	807	X	-	-	-
13	CLA	b	810	X	-	-	-
13	CLA	b	811	X	-	-	-
13	CLA	b	812	X	-	-	-
13	CLA	b	813	X	-	-	-
13	CLA	b	815	X	-	-	-
13	CLA	b	816	X	-	-	-
13	CLA	b	820	X	-	-	-
13	CLA	b	822	X	-	-	-
13	CLA	b	823	X	-	-	-
13	CLA	b	824	X	-	-	-
13	CLA	b	825	X	-	-	-
13	CLA	b	829	X	-	-	-
13	CLA	b	830	X	-	-	-
13	CLA	b	831	X	-	-	-
13	CLA	b	832	X	-	-	-
13	CLA	b	833	X	-	-	-
13	CLA	b	834	X	-	-	-
13	CLA	b	835	X	-	-	-
13	CLA	b	836	X	-	-	-
13	CLA	b	847	X	-	-	-
13	CLA	f	201	X	-	-	-
13	CLA	f	203	X	-	-	-
13	CLA	f	204	X	-	-	-
13	CLA	i	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	j	1101	X	-	-	-
13	CLA	j	1102	X	-	-	-
13	CLA	j	1103	X	-	-	-
13	CLA	k	4002	X	-	-	-
13	CLA	k	4003	X	-	-	-
13	CLA	k	4005	X	-	-	-
13	CLA	l	204	X	-	-	-
13	CLA	l	205	X	-	-	-
13	CLA	l	207	X	-	-	-

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		

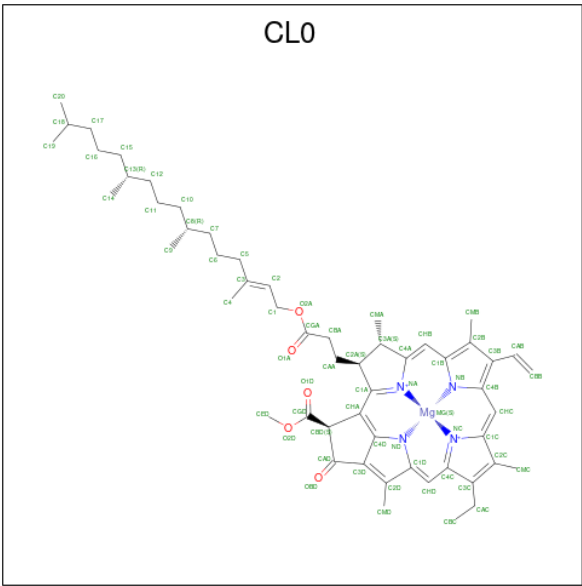
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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.

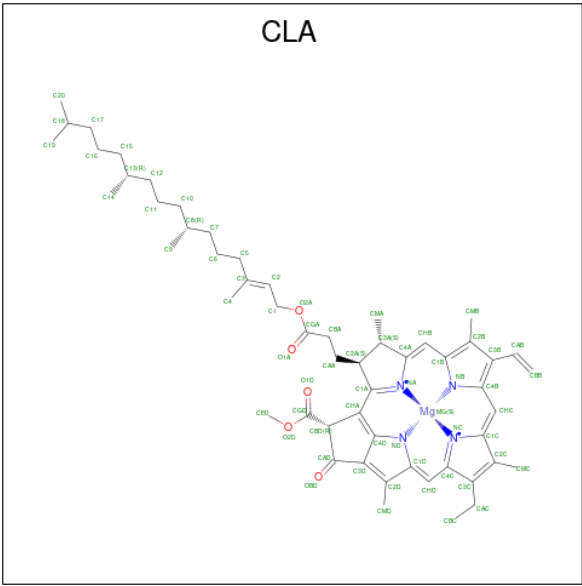
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	30	Total	C	N	O		0	0
			232	156	35	41			
11	m	30	Total	C	N	O		0	0
			232	156	35	41			
11	z	30	Total	C	N	O		0	0
			232	156	35	41			

- 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	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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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	C	Mg	N	O	0
			50	40	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	K	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	L	1	Total	C	Mg	N	O	0
			65	55	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
			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	

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Mol	Chain	Residues	Atoms					AltConf
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	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			62	52	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
			65	55	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
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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

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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
			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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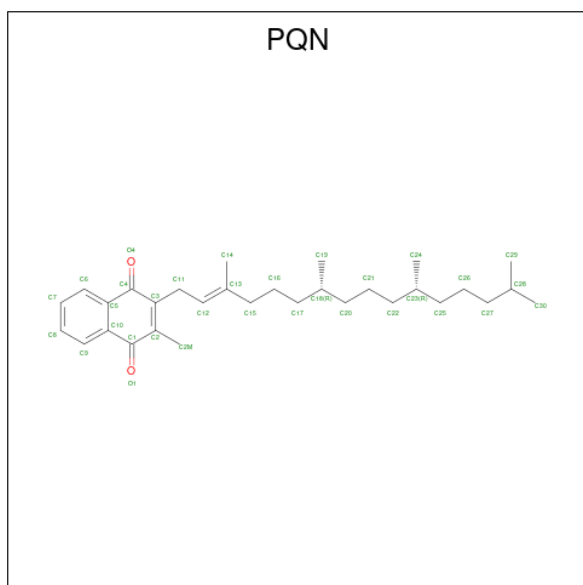
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	2	1	Total 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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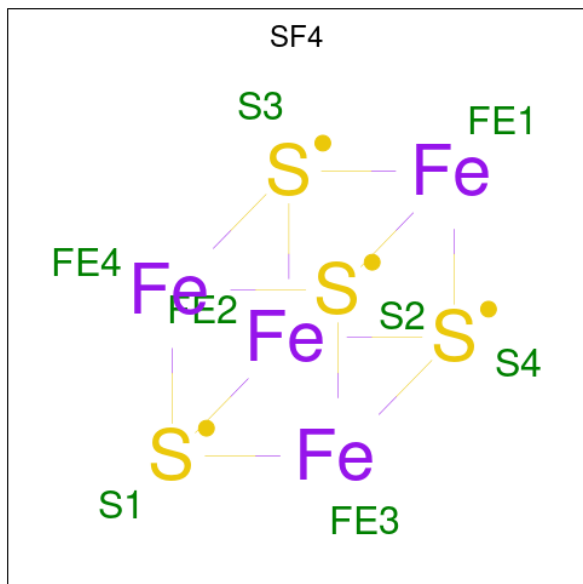
Mol	Chain	Residues	Atoms					AltConf
13	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			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).



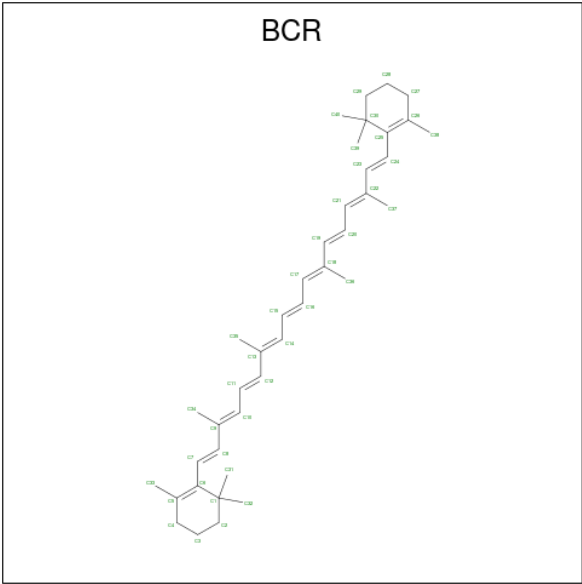
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	a	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	

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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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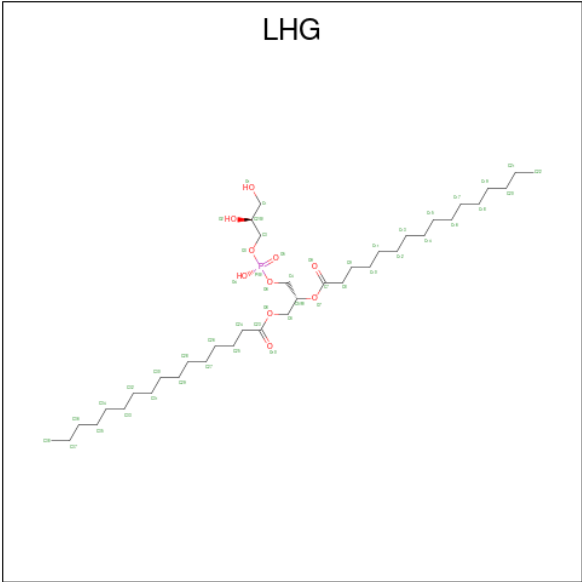
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 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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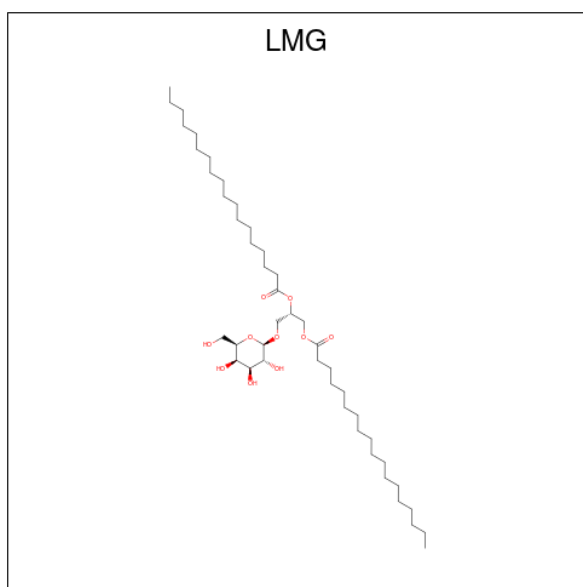
Mol	Chain	Residues	Atoms	AltConf
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 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: $C_{38}H_{75}O_{10}P$).



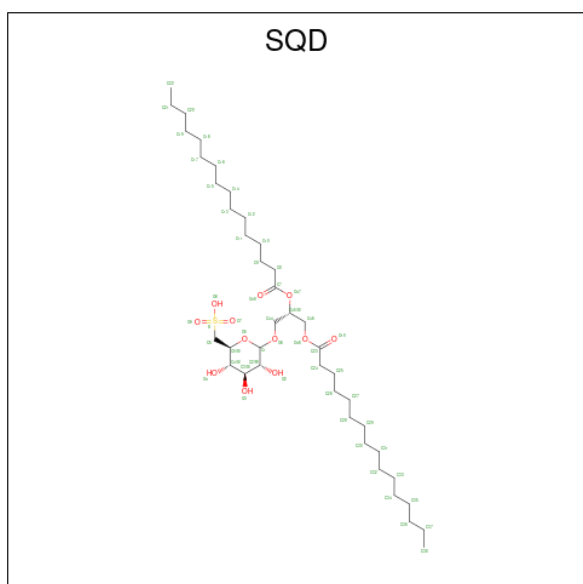
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	a	1	Total	C	O	P	0
			36	25	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	1	1	Total	C	O	P	0
			36	25	10	1	
17	1	1	Total	C	O	P	0
			41	30	10	1	

- 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: $C_{41}H_{78}O_{12}S$).

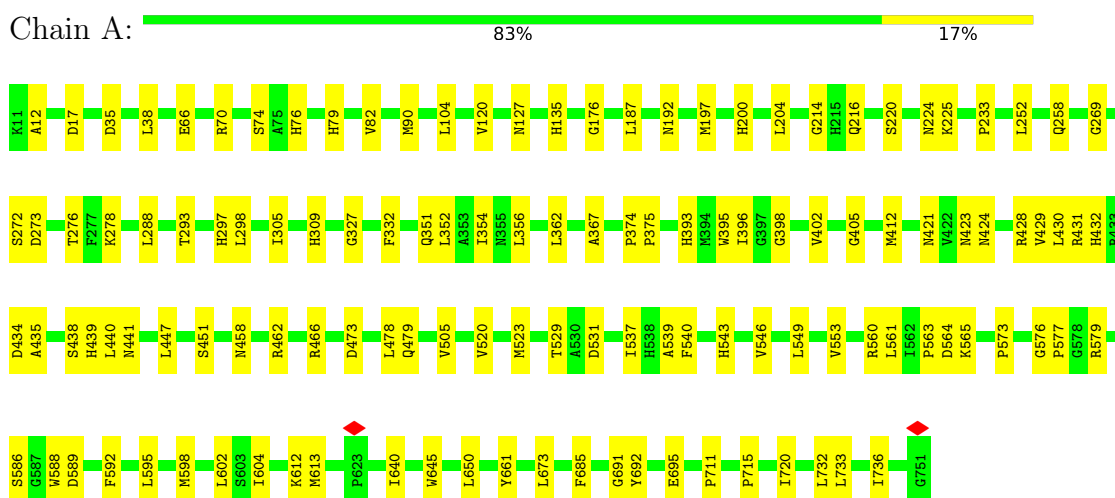


Mol	Chain	Residues	Atoms				AltConf
19	I	1	Total	C	O	S	0
			50	37	12	1	
19	i	1	Total	C	O	S	0
			50	37	12	1	
19	7	1	Total	C	O	S	0
			50	37	12	1	

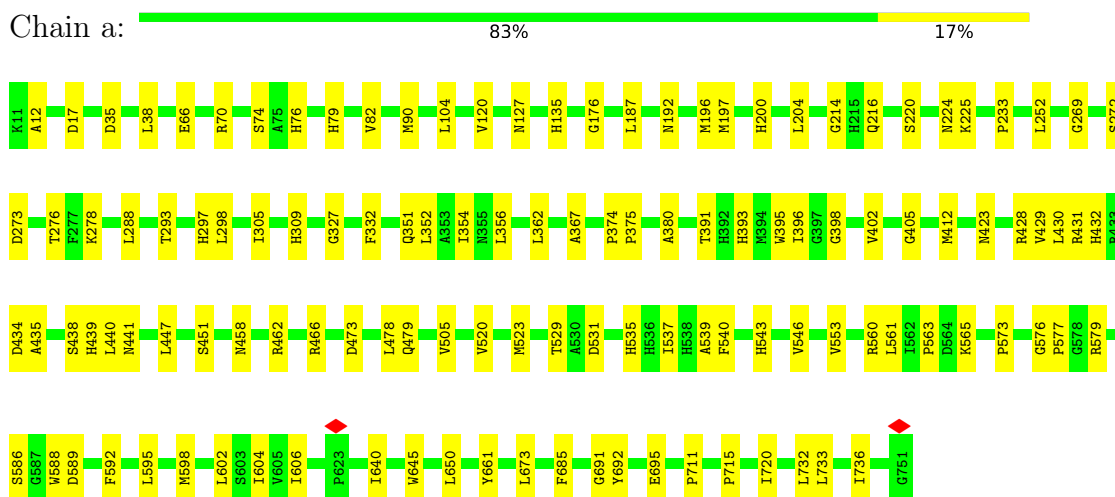
3 Residue-property plots

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.

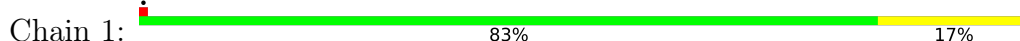
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

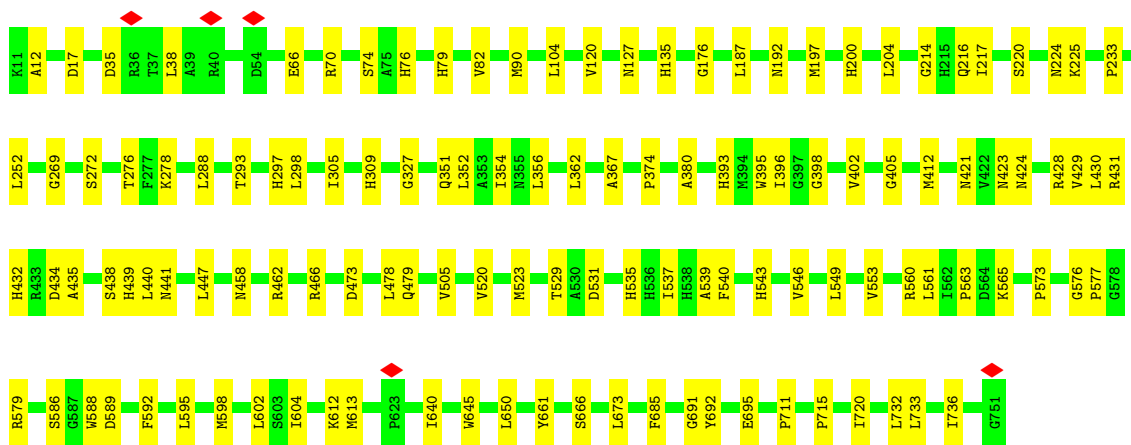


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



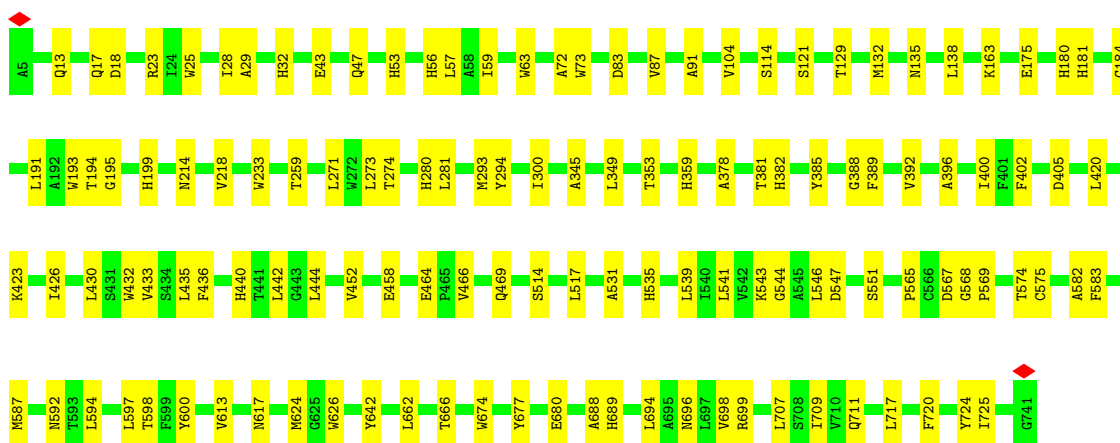
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





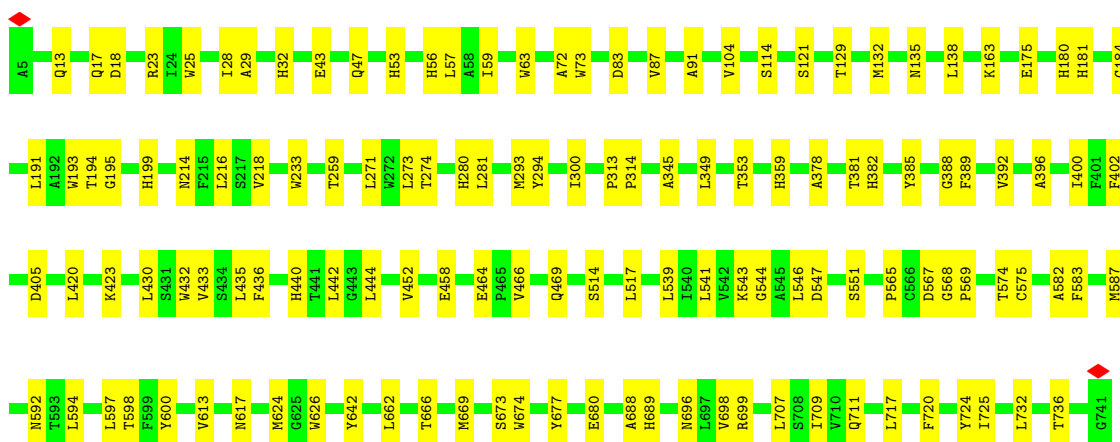
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 83% 17%



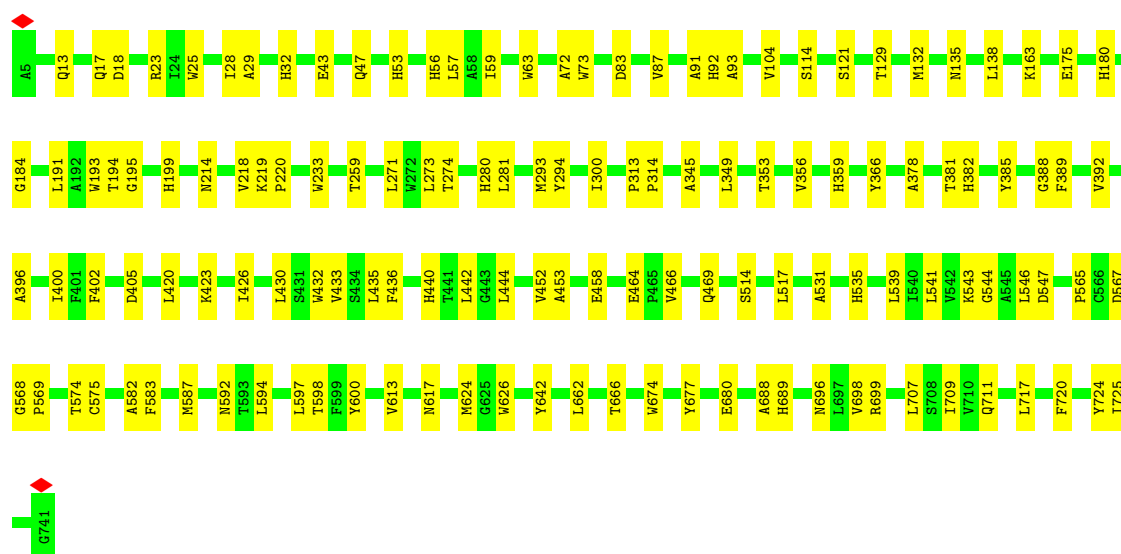
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain b: 82% 18%



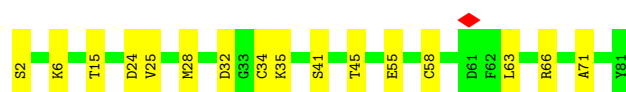
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  82% 18%



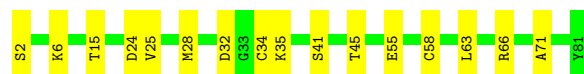
- Molecule 3: Photosystem I iron-sulfur center

Chain C:  80% 20%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  80% 20%



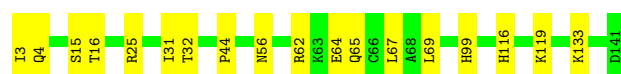
- Molecule 3: Photosystem I iron-sulfur center

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%



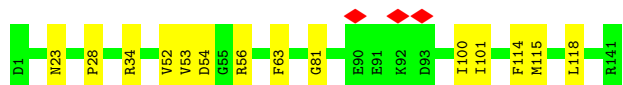
- Molecule 6: PSI-F

Chain F:  89% 11%

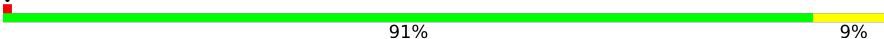


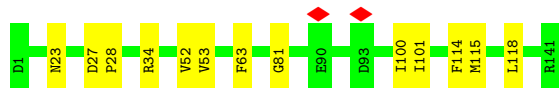
- Molecule 6: PSI-F

Chain f:  90% 10%



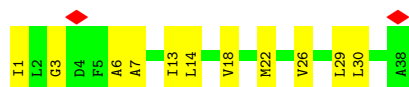
- Molecule 6: PSI-F

Chain 6:  91% 9%



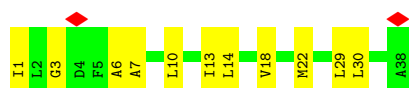
- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  5% 71% 29%



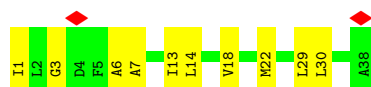
- Molecule 7: Photosystem I reaction center subunit VIII

Chain i:  5% 71% 29%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain 7:  5% 74% 26%



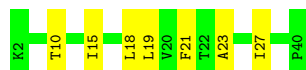
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  82% 18%



- Molecule 8: Photosystem I reaction center subunit IX

Chain j:  82% 18%

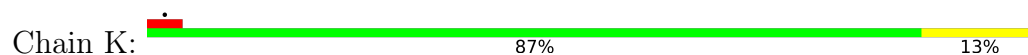


- Molecule 8: Photosystem I reaction center subunit IX

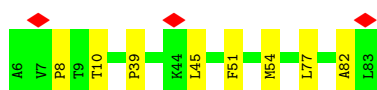
Chain 8:  82% 18%



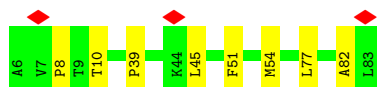
- Molecule 9: Photosystem I reaction center subunit PsaK



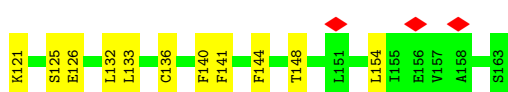
- Molecule 9: Photosystem I reaction center subunit PsaK



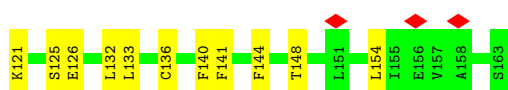
- Molecule 9: Photosystem I reaction center subunit PsaK



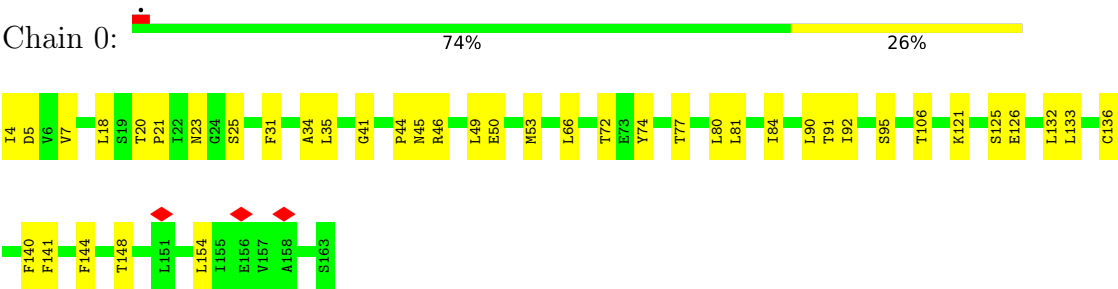
- Molecule 10: Photosystem I reaction center subunit XI



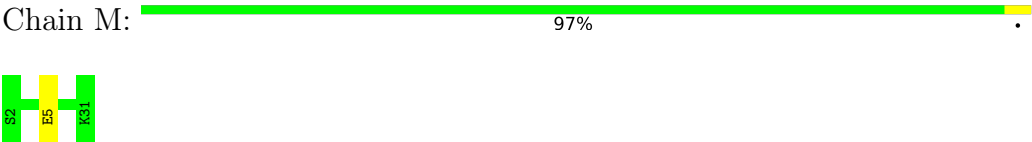
- Molecule 10: Photosystem I reaction center subunit XI



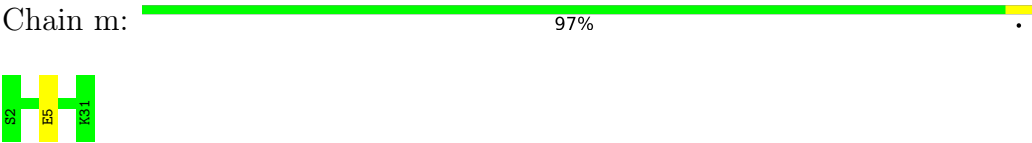
- Molecule 10: Photosystem I reaction center subunit XI



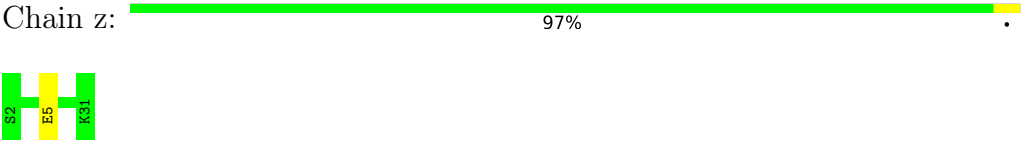
• Molecule 11: Photosystem I reaction center subunit XII



• 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: CL0, BCR, LHG, PQN, SF4, CLA, LMG, SQD

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

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	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
13	CLA	2	827	-	59,63,73	1.26	8 (13%)	70,101,113	1.37	5 (7%)
13	CLA	b	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
17	LHG	1	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	B	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.30	4 (5%)
16	BCR	a	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	f	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	8	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	0	205	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
13	CLA	I	101	-	69,73,73	1.14	9 (13%)	82,113,113	1.27	6 (7%)
13	CLA	a	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
13	CLA	6	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
16	BCR	1	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	1	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
18	LMG	2	845	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	A	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
13	CLA	F	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.33	6 (10%)
16	BCR	6	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	B	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	10 (14%)
13	CLA	a	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
14	PQN	A	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	a	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	8 (11%)
16	BCR	z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)
16	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	K	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	k	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	830	-	62,66,73	1.25	9 (14%)	73,104,113	1.41	5 (6%)
13	CLA	A	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.35	5 (7%)
17	LHG	1	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
16	BCR	2	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	2	801	-	69,73,73	1.17	9 (13%)	82,113,113	1.56	11 (13%)
19	SQD	7	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.46	10 (17%)
13	CLA	B	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.30	6 (10%)
13	CLA	A	807	-	59,63,73	1.25	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	a	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
15	SF4	c	101	3	0,12,12	-	-	-	-	-
13	CLA	b	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
13	CLA	1	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	5 (7%)
13	CLA	2	815	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
17	LHG	a	850	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	A	819	-	64,68,73	1.19	9 (14%)	76,107,113	1.52	7 (9%)
13	CLA	7	102	-	69,73,73	1.14	8 (11%)	82,113,113	1.27	6 (7%)
13	CLA	b	813	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	A	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
13	CLA	1	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	2	826	-	49,53,73	1.40	9 (18%)	58,89,113	1.30	6 (10%)
13	CLA	A	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	A	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.25	6 (7%)
16	BCR	a	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	2	823	-	59,63,73	1.26	10 (16%)	70,101,113	1.57	10 (14%)
16	BCR	1	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
16	BCR	L	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
16	BCR	L	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	9 (16%)
13	CLA	B	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	B	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	2	812	-	69,73,73	1.17	8 (11%)	82,113,113	1.31	8 (9%)
16	BCR	J	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	B	833	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	b	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	7 (8%)
13	CLA	A	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.33	6 (8%)

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	1.23	8 (9%)
13	CLA	B	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	9 (16%)
13	CLA	J	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	2	809	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	A	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	k	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.37	4 (6%)
13	CLA	a	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	7 (8%)
13	CLA	A	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	a	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	5 (7%)
16	BCR	9	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
14	PQN	1	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	B	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)
13	CLA	a	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	B	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
16	BCR	b	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
16	BCR	L	205	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
13	CLA	b	830	-	62,66,73	1.26	9 (14%)	73,104,113	1.43	5 (6%)
13	CLA	0	203	-	69,73,73	1.16	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	1	825	-	66,70,73	1.20	9 (13%)	78,109,113	1.38	7 (8%)
16	BCR	8	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	b	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	1	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
16	BCR	j	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	1	808	-	54,58,73	1.29	8 (14%)	64,95,113	1.73	6 (9%)
13	CLA	1	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.25	4 (6%)
16	BCR	B	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	a	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	B	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
13	CLA	a	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	1	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
16	BCR	A	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	2	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.29	4 (5%)
15	SF4	3	101	3	0,12,12	-	-	-	-	-
13	CLA	a	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	7 (8%)
13	CLA	b	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
13	CLA	j	1103	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	5 (8%)
13	CLA	1	837	-	64,68,73	1.20	9 (14%)	76,107,113	1.26	6 (7%)
13	CLA	A	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
13	CLA	b	836	-	69,73,73	1.17	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	2	817	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)
13	CLA	0	208	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	2	831	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	B	817	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
16	BCR	K	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	1	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	9 (14%)
13	CLA	l	205	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	A	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	9	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
15	SF4	1	844	1,2	0,12,12	-	-	-	-	-
13	CLA	b	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	j	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	6 (9%)
16	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	b	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	b	818	-	50,54,73	1.35	7 (14%)	59,90,113	1.41	6 (10%)
16	BCR	F	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	2	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	1	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	6	204	-	50,54,73	1.36	7 (14%)	59,90,113	1.27	3 (5%)
13	CLA	b	847	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	7 (8%)
13	CLA	B	831	-	69,73,73	1.16	8 (11%)	82,113,113	1.41	7 (8%)
13	CLA	F	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.26	3 (5%)
13	CLA	a	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.53	8 (12%)
13	CLA	B	816	-	64,68,73	1.22	9 (14%)	76,107,113	1.38	5 (6%)
16	BCR	1	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	B	804	-	69,73,73	1.15	9 (13%)	82,113,113	1.22	7 (8%)
13	CLA	1	807	-	59,63,73	1.24	9 (15%)	70,101,113	1.42	6 (8%)
13	CLA	1	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	B	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	b	809	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	5 (8%)
16	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	6	201	-	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
13	CLA	A	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	2	821	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	A	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)
16	BCR	b	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	1	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	l	207	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	5 (6%)
16	BCR	l	206	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
15	SF4	c	102	3	0,12,12	-	-	-	-	-
13	CLA	F	201	-	59,63,73	1.26	9 (15%)	70,101,113	1.34	5 (7%)
13	CLA	a	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	f	203	-	49,53,73	1.39	8 (16%)	58,89,113	1.34	6 (10%)
13	CLA	L	206	-	69,73,73	1.15	9 (13%)	82,113,113	1.36	5 (6%)
13	CLA	2	836	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	a	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)
16	BCR	b	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	B	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	7 (8%)
13	CLA	1	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
13	CLA	B	834	-	64,68,73	1.20	9 (14%)	76,107,113	1.22	5 (6%)
13	CLA	b	817	-	45,49,73	1.40	8 (17%)	54,84,113	1.16	4 (7%)
13	CLA	K	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
16	BCR	B	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
16	BCR	f	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
16	BCR	F	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
16	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	2	828	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	9 (11%)
13	CLA	B	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	2	818	-	50,54,73	1.36	9 (18%)	59,90,113	1.38	4 (6%)
16	BCR	9	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	2	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	2	824	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	SQD	I	103	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
13	CLA	2	816	-	45,49,73	1.40	7 (15%)	54,84,113	1.16	4 (7%)
16	BCR	K	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	A	840	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	A	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.24	6 (7%)
13	CLA	2	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
19	SQD	i	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
13	CLA	A	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	9 (10%)
13	CLA	A	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
13	CLA	2	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	6 (7%)
13	CLA	B	828	-	59,63,73	1.26	9 (15%)	70,101,113	1.37	5 (7%)
16	BCR	b	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	2	835	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
16	BCR	8	1105	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	B	822	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
13	CLA	b	838	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
13	CLA	1	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	A	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	7 (9%)
13	CLA	B	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
13	CLA	B	836	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	6 (7%)
13	CLA	A	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.23	6 (8%)
13	CLA	i	102	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
15	SF4	3	102	3	0,12,12	-	-	-	-	-
13	CLA	1	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
14	PQN	b	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	B	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
16	BCR	0	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
14	PQN	B	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	0	202	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	1	830	-	69,73,73	1.17	9 (13%)	82,113,113	1.43	7 (8%)
13	CLA	1	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.32	7 (8%)
16	BCR	A	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	1	827	-	69,73,73	1.14	10 (14%)	82,113,113	1.20	6 (7%)
13	CLA	a	836	-	55,59,73	1.28	8 (14%)	64,96,113	1.39	8 (12%)
13	CLA	B	818	-	50,54,73	1.35	9 (18%)	59,90,113	1.42	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PQN	2	838	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	1	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.53	7 (9%)
16	BCR	7	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	A	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)
16	BCR	I	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
16	BCR	l	203	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	9 (16%)
13	CLA	b	834	-	64,68,73	1.21	9 (14%)	76,107,113	1.22	6 (7%)
13	CLA	B	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)
12	CL0	a	801	-	58,73,73	2.24	10 (17%)	60,113,113	1.61	14 (23%)
13	CLA	9	4003	-	50,54,73	1.37	9 (18%)	59,90,113	1.35	5 (8%)
16	BCR	i	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	10 (17%)
13	CLA	a	827	-	69,73,73	1.15	10 (14%)	82,113,113	1.20	5 (6%)
16	BCR	k	4001	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)
16	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	2	808	-	49,53,73	1.37	7 (14%)	58,89,113	1.41	6 (10%)
13	CLA	1	822	-	54,58,73	1.30	8 (14%)	64,95,113	1.53	8 (12%)
13	CLA	1	839	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
16	BCR	2	839	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
16	BCR	b	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
16	BCR	6	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	A	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
18	LMG	B	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	B	826	-	64,68,73	1.25	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	1	829	-	69,73,73	1.15	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	B	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	5 (6%)
13	CLA	J	1101	-	54,58,73	1.32	9 (16%)	64,95,113	1.31	7 (10%)
13	CLA	2	813	-	54,58,73	1.32	9 (16%)	64,95,113	1.42	7 (10%)
13	CLA	1	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.40	6 (7%)
16	BCR	2	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	a	824	-	64,68,73	1.20	9 (14%)	76,107,113	1.37	5 (6%)
13	CLA	1	826	-	59,63,73	1.24	9 (15%)	70,101,113	1.22	6 (8%)
13	CLA	a	808	-	54,58,73	1.29	9 (16%)	64,95,113	1.72	7 (10%)
13	CLA	b	837	-	69,73,73	1.16	6 (8%)	82,113,113	1.21	6 (7%)
16	BCR	J	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
16	BCR	1	847	-	41,41,41	1.13	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	K	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
13	CLA	a	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	b	829	-	66,70,73	1.18	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	a	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	2	825	-	64,68,73	1.24	9 (14%)	76,107,113	1.48	8 (10%)
13	CLA	a	809	-	54,58,73	1.30	9 (16%)	64,95,113	1.34	7 (10%)
13	CLA	a	823	-	54,58,73	1.31	8 (14%)	64,95,113	1.43	4 (6%)
13	CLA	b	835	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	b	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.39	4 (6%)
16	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	a	838	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	6 (7%)
13	CLA	b	808	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	8	1102	-	44,48,73	1.45	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	b	814	-	54,58,73	1.32	9 (16%)	64,95,113	1.41	7 (10%)
13	CLA	a	819	-	64,68,73	1.20	9 (14%)	76,107,113	1.51	7 (9%)
13	CLA	B	819	-	50,54,73	1.35	9 (18%)	59,90,113	1.38	4 (6%)
16	BCR	j	1104	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	9 (16%)
15	SF4	a	844	1,2	0,12,12	-	-	-	-	-
13	CLA	A	834	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	4 (4%)
13	CLA	a	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	6 (10%)
13	CLA	0	206	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
13	CLA	b	812	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
13	CLA	B	813	-	69,73,73	1.16	8 (11%)	82,113,113	1.31	8 (9%)
13	CLA	A	836	-	55,59,73	1.29	8 (14%)	64,96,113	1.39	8 (12%)
12	CL0	A	801	-	58,73,73	2.24	10 (17%)	60,113,113	1.61	14 (23%)
13	CLA	a	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
13	CLA	L	203	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	8 (12%)
16	BCR	A	851	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	7 (12%)
13	CLA	9	4002	-	49,53,73	1.41	7 (14%)	58,89,113	1.36	4 (6%)
13	CLA	a	826	-	59,63,73	1.25	9 (15%)	70,101,113	1.23	6 (8%)
13	CLA	b	823	-	69,73,73	1.16	9 (13%)	82,113,113	1.18	6 (7%)
17	LHG	A	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	1	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
13	CLA	2	810	-	50,54,73	1.33	9 (18%)	59,90,113	1.55	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	b	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
16	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	B	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
13	CLA	2	830	-	69,73,73	1.15	9 (13%)	82,113,113	1.41	7 (8%)
13	CLA	f	204	-	50,54,73	1.36	8 (16%)	59,90,113	1.27	3 (5%)
13	CLA	1	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
13	CLA	2	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.43	8 (10%)
13	CLA	A	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)
13	CLA	A	813	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	7 (10%)
13	CLA	B	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.55	10 (12%)
13	CLA	1	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	5 (7%)
13	CLA	b	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	a	829	-	69,73,73	1.16	10 (14%)	82,113,113	1.46	7 (8%)
13	CLA	b	832	-	44,48,73	1.45	8 (18%)	51,82,113	1.41	5 (9%)
13	CLA	8	1103	-	49,53,73	1.38	8 (16%)	58,89,113	1.35	5 (8%)
16	BCR	2	841	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
13	CLA	a	831	-	54,58,73	1.30	9 (16%)	64,95,113	1.44	9 (14%)
13	CLA	l	202	-	64,68,73	1.19	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	1	804	-	59,63,73	1.23	9 (15%)	70,101,113	1.34	6 (8%)
13	CLA	A	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.41	6 (7%)
17	LHG	a	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	1	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
12	CL0	1	801	-	58,73,73	2.23	10 (17%)	60,113,113	1.61	14 (23%)
13	CLA	2	811	-	49,53,73	1.37	9 (18%)	58,89,113	1.35	6 (10%)
16	BCR	2	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	2	837	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	5 (6%)
13	CLA	A	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.50	8 (12%)
13	CLA	A	824	-	64,68,73	1.21	9 (14%)	76,107,113	1.38	5 (6%)
13	CLA	2	820	-	69,73,73	1.20	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	L	204	-	50,54,73	1.34	9 (18%)	59,90,113	1.33	4 (6%)
16	BCR	1	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
13	CLA	a	840	-	69,73,73	1.15	9 (13%)	82,113,113	1.23	5 (6%)
13	CLA	A	842	-	49,53,73	1.37	9 (18%)	58,89,113	1.61	5 (8%)
13	CLA	A	805	-	59,63,73	1.26	9 (15%)	70,101,113	1.29	6 (8%)
13	CLA	A	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	803	-	64,68,73	1.18	8 (12%)	76,107,113	1.42	8 (10%)
13	CLA	2	807	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	5 (6%)
13	CLA	2	832	-	54,58,73	1.29	9 (16%)	64,95,113	1.50	11 (17%)
13	CLA	A	809	-	54,58,73	1.31	8 (14%)	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%)
13	CLA	l	204	-	54,58,73	1.30	9 (16%)	64,95,113	1.52	9 (14%)
13	CLA	a	834	-	69,73,73	1.17	9 (13%)	82,113,113	1.26	5 (6%)
13	CLA	1	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.54	11 (14%)
13	CLA	B	811	-	50,54,73	1.34	9 (18%)	59,90,113	1.55	7 (11%)
13	CLA	a	841	-	64,68,73	1.21	8 (12%)	76,107,113	1.26	8 (10%)
13	CLA	A	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
13	CLA	A	803	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
13	CLA	B	823	-	69,73,73	1.17	9 (13%)	82,113,113	1.18	6 (7%)
13	CLA	a	804	-	59,63,73	1.24	9 (15%)	70,101,113	1.32	6 (8%)
16	BCR	a	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.43	9 (16%)
14	PQN	a	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
15	SF4	A	844	1,2	0,12,12	-	-	-	-	-
13	CLA	2	829	-	62,66,73	1.25	9 (14%)	73,104,113	1.42	5 (6%)
13	CLA	a	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.26	6 (8%)
13	CLA	2	822	-	69,73,73	1.17	9 (13%)	82,113,113	1.17	6 (7%)
13	CLA	b	821	-	69,73,73	1.19	9 (13%)	82,113,113	1.32	7 (8%)
13	CLA	J	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.48	5 (9%)
13	CLA	1	811	-	60,64,73	1.25	9 (15%)	71,102,113	1.36	4 (5%)
13	CLA	b	801	-	69,73,73	1.17	10 (14%)	82,113,113	1.56	10 (12%)
17	LHG	A	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	A	812	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
13	CLA	A	817	-	59,63,73	1.25	9 (15%)	70,101,113	1.45	7 (10%)
16	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	1	831	-	54,58,73	1.29	9 (16%)	64,95,113	1.44	9 (14%)
13	CLA	b	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	7 (8%)
13	CLA	A	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.42	5 (8%)
13	CLA	1	852	-	64,68,73	1.23	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	A	810	-	49,53,73	1.37	9 (18%)	58,89,113	1.43	5 (8%)
13	CLA	a	802	-	64,68,73	1.20	11 (17%)	76,107,113	1.55	11 (14%)
16	BCR	a	845	-	41,41,41	1.09	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
18	LMG	b	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	1	818	-	58,62,73	1.26	9 (15%)	68,99,113	1.45	7 (10%)
13	CLA	L	201	-	64,68,73	1.18	9 (14%)	76,107,113	1.31	8 (10%)
13	CLA	b	824	-	59,63,73	1.26	10 (16%)	70,101,113	1.56	9 (12%)
13	CLA	a	814	-	54,58,73	1.31	9 (16%)	64,95,113	1.51	9 (14%)
13	CLA	a	816	-	50,54,73	1.36	8 (16%)	59,90,113	1.28	3 (5%)
16	BCR	l	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	a	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
16	BCR	f	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	b	803	-	64,68,73	1.18	9 (14%)	76,107,113	1.42	8 (10%)
13	CLA	b	828	-	59,63,73	1.27	9 (15%)	70,101,113	1.38	4 (5%)
13	CLA	1	823	-	54,58,73	1.30	8 (14%)	64,95,113	1.42	4 (6%)
13	CLA	A	828	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	6 (7%)
13	CLA	b	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	6 (7%)
16	BCR	2	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	B	802	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	7 (8%)
16	BCR	b	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
16	BCR	0	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	A	820	-	50,54,73	1.35	6 (12%)	59,90,113	1.26	5 (8%)
13	CLA	a	818	-	58,62,73	1.27	10 (17%)	68,99,113	1.45	7 (10%)
13	CLA	b	827	-	49,53,73	1.39	9 (18%)	58,89,113	1.29	6 (10%)
16	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	9 (16%)
13	CLA	B	829	-	66,70,73	1.17	9 (13%)	78,109,113	1.40	8 (10%)
13	CLA	a	837	-	64,68,73	1.21	9 (14%)	76,107,113	1.25	6 (7%)
13	CLA	k	4005	-	47,52,73	1.41	9 (19%)	55,88,113	1.48	6 (10%)
13	CLA	1	821	-	69,73,73	1.15	9 (13%)	82,113,113	1.21	5 (6%)
13	CLA	1	815	-	49,53,73	1.37	9 (18%)	58,89,113	1.41	5 (8%)
13	CLA	b	825	-	69,73,73	1.16	10 (14%)	82,113,113	1.29	7 (8%)
13	CLA	1	813	-	59,63,73	1.25	9 (15%)	70,101,113	1.29	8 (11%)
16	BCR	k	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	2	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.29	5 (6%)
13	CLA	a	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.42	6 (7%)
16	BCR	m	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	B	847	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	A	835	-	60,64,73	1.25	8 (13%)	71,102,113	1.27	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	822	-	54,58,73	1.31	9 (16%)	64,95,113	1.35	7 (10%)
13	CLA	1	809	-	54,58,73	1.30	8 (14%)	64,95,113	1.35	7 (10%)
13	CLA	j	1102	-	44,48,73	1.46	7 (15%)	51,82,113	1.47	5 (9%)
13	CLA	2	846	-	69,73,73	1.17	9 (13%)	82,113,113	1.33	7 (8%)
13	CLA	a	839	-	69,73,73	1.15	9 (13%)	82,113,113	1.40	8 (9%)
13	CLA	2	834	-	54,58,73	1.29	8 (14%)	64,95,113	1.42	6 (9%)
13	CLA	1	838	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	6 (7%)
13	CLA	b	805	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	4 (4%)

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	820	-	1/1/13/20	8/27/103/115	-
13	CLA	2	827	-	-	9/27/103/115	-
13	CLA	b	833	-	1/1/12/20	6/21/97/115	-
17	LHG	1	849	-	-	16/40/40/53	-
13	CLA	B	820	-	1/1/13/20	8/27/103/115	-
16	BCR	a	848	-	-	15/29/63/63	0/2/2/2
13	CLA	f	201	-	1/1/13/20	6/27/103/115	-
13	CLA	8	1101	-	1/1/12/20	9/21/97/115	-
13	CLA	0	205	-	1/1/12/20	7/21/97/115	-
13	CLA	I	101	-	1/1/15/20	14/39/115/115	-
13	CLA	a	825	-	-	15/36/112/115	-
13	CLA	6	203	-	1/1/11/20	1/15/91/115	-
16	BCR	1	851	-	-	13/29/63/63	0/2/2/2
13	CLA	1	828	-	1/1/15/20	9/39/115/115	-
18	LMG	2	845	-	-	17/36/56/70	0/1/1/1
13	CLA	F	203	-	1/1/11/20	1/15/91/115	-
13	CLA	A	825	-	-	15/36/112/115	-
16	BCR	6	202	-	-	12/29/63/63	0/2/2/2
13	CLA	B	824	-	1/1/13/20	7/27/103/115	-
13	CLA	a	812	-	-	6/17/93/115	-
14	PQN	A	843	-	-	10/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	813	-	1/1/13/20	10/27/103/115	-
16	BCR	z	101	-	-	7/29/63/63	0/2/2/2
16	BCR	B	841	-	-	8/29/63/63	0/2/2/2
13	CLA	K	4002	-	1/1/11/20	7/15/91/115	-
13	CLA	k	4003	-	1/1/11/20	8/17/93/115	-
13	CLA	B	830	-	1/1/13/20	10/31/107/115	-
13	CLA	A	811	-	1/1/13/20	10/29/105/115	-
17	LHG	1	850	-	-	20/45/45/53	-
16	BCR	2	840	-	-	8/29/63/63	0/2/2/2
13	CLA	2	801	-	1/1/15/20	6/39/115/115	-
19	SQD	7	101	-	-	19/45/65/69	0/1/1/1
13	CLA	B	827	-	-	8/15/91/115	-
13	CLA	A	807	-	1/1/13/20	4/27/103/115	-
13	CLA	a	852	-	1/1/14/20	13/33/109/115	-
15	SF4	c	101	3	-	-	0/6/5/5
13	CLA	b	806	-	1/1/15/20	16/39/115/115	-
13	CLA	1	805	-	1/1/13/20	12/27/103/115	-
13	CLA	2	815	-	1/1/14/20	7/33/109/115	-
17	LHG	a	850	-	-	19/45/45/53	-
13	CLA	A	819	-	1/1/14/20	12/33/109/115	-
13	CLA	7	102	-	1/1/15/20	14/39/115/115	-
13	CLA	b	813	-	1/1/15/20	15/39/115/115	-
13	CLA	A	818	-	1/1/12/20	7/26/102/115	-
13	CLA	1	806	-	1/1/15/20	12/39/115/115	-
13	CLA	2	826	-	-	8/15/91/115	-
13	CLA	A	822	-	-	8/21/97/115	-
13	CLA	A	837	-	1/1/14/20	8/33/109/115	-
16	BCR	a	851	-	-	13/29/63/63	0/2/2/2
13	CLA	2	823	-	1/1/13/20	7/27/103/115	-
16	BCR	1	846	-	-	6/29/63/63	0/2/2/2
16	BCR	L	207	-	-	7/29/63/63	0/2/2/2
15	SF4	C	101	3	-	-	0/6/5/5
16	BCR	L	202	-	-	10/29/63/63	0/2/2/2
13	CLA	B	832	-	1/1/9/20	4/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	835	-	1/1/12/20	3/21/97/115	-
13	CLA	2	812	-	1/1/15/20	16/39/115/115	-
16	BCR	J	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	B	833	-	1/1/12/20	6/21/97/115	-
13	CLA	b	804	-	1/1/15/20	17/39/115/115	-
13	CLA	A	804	-	1/1/13/20	3/27/103/115	-
13	CLA	a	803	-	1/1/15/20	11/39/115/115	-
13	CLA	B	814	-	-	8/21/97/115	-
16	BCR	A	847	-	-	15/29/63/63	0/2/2/2
13	CLA	J	1103	-	1/1/11/20	8/15/91/115	-
13	CLA	2	809	-	1/1/15/20	15/39/115/115	-
13	CLA	A	830	-	-	13/39/115/115	-
13	CLA	k	4002	-	1/1/11/20	7/15/91/115	-
13	CLA	a	830	-	-	13/39/115/115	-
13	CLA	A	829	-	1/1/15/20	12/39/115/115	-
13	CLA	a	811	-	1/1/13/20	10/29/105/115	-
16	BCR	9	4001	-	-	9/29/63/63	0/2/2/2
14	PQN	1	843	-	-	10/23/43/43	0/2/2/2
13	CLA	B	809	-	-	5/15/91/115	-
13	CLA	a	820	-	-	5/17/93/115	-
13	CLA	B	812	-	1/1/11/20	4/15/91/115	-
16	BCR	b	841	-	-	8/29/63/63	0/2/2/2
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
13	CLA	b	830	-	1/1/13/20	10/31/107/115	-
13	CLA	0	203	-	1/1/15/20	15/39/115/115	-
13	CLA	1	825	-	-	15/36/112/115	-
16	BCR	8	1104	-	-	9/29/63/63	0/2/2/2
13	CLA	b	816	-	1/1/14/20	7/33/109/115	-
13	CLA	1	816	-	1/1/11/20	8/17/93/115	-
16	BCR	j	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	1	808	-	1/1/12/20	5/21/97/115	-
13	CLA	1	820	-	-	5/17/93/115	-
16	BCR	B	848	-	-	10/29/63/63	0/2/2/2
13	CLA	a	807	-	1/1/13/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	838	-	-	7/39/115/115	-
13	CLA	a	810	-	-	8/15/91/115	-
13	CLA	1	842	-	1/1/11/20	7/15/91/115	-
16	BCR	A	845	-	-	8/29/63/63	0/2/2/2
13	CLA	2	819	-	1/1/13/20	8/27/103/115	-
15	SF4	3	101	3	-	-	0/6/5/5
13	CLA	a	832	-	-	9/39/115/115	-
13	CLA	B	825	-	1/1/15/20	8/39/115/115	-
13	CLA	b	802	-	-	9/39/115/115	-
13	CLA	j	1103	-	1/1/11/20	8/15/91/115	-
13	CLA	1	837	-	1/1/14/20	8/33/109/115	-
13	CLA	A	808	-	1/1/12/20	5/21/97/115	-
13	CLA	b	836	-	1/1/15/20	5/39/115/115	-
13	CLA	2	817	-	-	10/17/93/115	-
13	CLA	0	208	-	1/1/15/20	9/39/115/115	-
13	CLA	2	831	-	1/1/9/20	4/10/82/115	-
13	CLA	B	817	-	-	2/10/86/115	-
16	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	1	814	-	1/1/12/20	4/21/97/115	-
13	CLA	l	205	-	1/1/11/20	4/17/93/115	-
13	CLA	A	823	-	1/1/12/20	7/21/97/115	-
13	CLA	9	4005	-	1/1/11/20	6/13/89/115	-
15	SF4	1	844	1,2	-	-	0/6/5/5
13	CLA	b	811	-	1/1/11/20	8/17/93/115	-
13	CLA	j	1101	-	1/1/12/20	9/21/97/115	-
16	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	b	831	-	1/1/15/20	7/39/115/115	-
13	CLA	b	818	-	-	10/17/93/115	-
16	BCR	F	202	-	-	12/29/63/63	0/2/2/2
13	CLA	2	804	-	1/1/15/20	17/39/115/115	-
13	CLA	1	836	-	1/1/12/20	6/23/99/115	-
13	CLA	6	204	-	1/1/11/20	8/17/93/115	-
13	CLA	b	847	-	1/1/15/20	9/39/115/115	-
13	CLA	B	831	-	1/1/15/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	F	204	-	1/1/11/20	8/17/93/115	-
13	CLA	a	822	-	-	8/21/97/115	-
13	CLA	B	816	-	1/1/14/20	7/33/109/115	-
16	BCR	1	845	-	-	8/29/63/63	0/2/2/2
13	CLA	B	804	-	1/1/15/20	17/39/115/115	-
13	CLA	1	807	-	1/1/13/20	4/27/103/115	-
13	CLA	1	810	-	-	8/15/91/115	-
13	CLA	B	815	-	1/1/15/20	12/39/115/115	-
13	CLA	b	826	-	-	14/33/109/115	-
13	CLA	b	809	-	-	5/15/91/115	-
16	BCR	B	845	-	-	15/29/63/63	0/2/2/2
13	CLA	6	201	-	1/1/13/20	6/27/103/115	-
13	CLA	A	832	-	-	9/39/115/115	-
13	CLA	2	821	-	1/1/12/20	2/21/97/115	-
13	CLA	A	827	-	1/1/15/20	13/39/115/115	-
16	BCR	b	848	-	-	10/29/63/63	0/2/2/2
13	CLA	1	803	-	1/1/15/20	11/39/115/115	-
13	CLA	l	207	-	1/1/15/20	9/39/115/115	-
16	BCR	l	206	-	-	11/29/63/63	0/2/2/2
15	SF4	c	102	3	-	-	0/6/5/5
13	CLA	F	201	-	1/1/13/20	6/27/103/115	-
13	CLA	a	806	-	1/1/15/20	12/39/115/115	-
13	CLA	f	203	-	1/1/11/20	1/15/91/115	-
13	CLA	L	206	-	1/1/15/20	9/39/115/115	-
13	CLA	2	836	-	-	14/39/115/115	-
13	CLA	a	821	-	1/1/15/20	11/39/115/115	-
16	BCR	b	844	-	-	6/29/63/63	0/2/2/2
13	CLA	B	821	-	-	19/39/115/115	-
13	CLA	1	841	-	1/1/14/20	12/33/109/115	-
13	CLA	B	834	-	1/1/14/20	6/33/109/115	-
13	CLA	b	817	-	-	2/10/86/115	-
13	CLA	K	4003	-	1/1/11/20	8/17/93/115	-
16	BCR	B	842	-	-	14/29/63/63	0/2/2/2
16	BCR	f	202	-	-	12/29/63/63	0/2/2/2
15	SF4	C	102	3	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	F	205	-	-	12/29/63/63	0/2/2/2
16	BCR	B	840	-	-	11/29/63/63	0/2/2/2
13	CLA	2	828	-	1/1/14/20	17/36/112/115	-
13	CLA	B	807	-	1/1/15/20	15/39/115/115	-
13	CLA	2	818	-	-	6/17/93/115	-
16	BCR	9	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	2	814	-	1/1/15/20	12/39/115/115	-
13	CLA	2	824	-	1/1/15/20	8/39/115/115	-
19	SQD	I	103	-	-	19/45/65/69	0/1/1/1
13	CLA	2	816	-	-	2/10/86/115	-
16	BCR	K	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	A	840	-	-	13/39/115/115	-
13	CLA	A	852	-	1/1/14/20	13/33/109/115	-
13	CLA	2	805	-	1/1/15/20	13/39/115/115	-
19	SQD	i	101	-	-	19/45/65/69	0/1/1/1
13	CLA	A	839	-	1/1/15/20	9/39/115/115	-
13	CLA	A	806	-	1/1/15/20	12/39/115/115	-
13	CLA	2	802	-	-	9/39/115/115	-
13	CLA	B	828	-	-	9/27/103/115	-
16	BCR	b	843	-	-	9/29/63/63	0/2/2/2
13	CLA	2	835	-	1/1/15/20	5/39/115/115	-
16	BCR	8	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	B	822	-	1/1/12/20	2/21/97/115	-
13	CLA	b	838	-	-	7/39/115/115	-
13	CLA	1	824	-	1/1/14/20	16/33/109/115	-
13	CLA	A	841	-	1/1/14/20	12/33/109/115	-
13	CLA	B	837	-	-	14/39/115/115	-
13	CLA	B	836	-	1/1/15/20	5/39/115/115	-
13	CLA	A	826	-	1/1/13/20	7/27/103/115	-
13	CLA	i	102	-	1/1/15/20	14/39/115/115	-
15	SF4	3	102	3	-	-	0/6/5/5
13	CLA	1	817	-	-	8/27/103/115	-
14	PQN	b	839	-	-	10/23/43/43	0/2/2/2
13	CLA	B	808	-	-	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	0	207	-	-	11/29/63/63	0/2/2/2
14	PQN	B	839	-	-	10/23/43/43	0/2/2/2
13	CLA	0	202	-	-	10/33/109/115	-
13	CLA	1	830	-	-	13/39/115/115	-
13	CLA	1	832	-	-	10/39/115/115	-
16	BCR	A	846	-	-	6/29/63/63	0/2/2/2
13	CLA	1	827	-	1/1/15/20	13/39/115/115	-
13	CLA	a	836	-	1/1/12/20	6/23/99/115	-
13	CLA	B	818	-	-	10/17/93/115	-
14	PQN	2	838	-	-	10/23/43/43	0/2/2/2
13	CLA	1	819	-	1/1/14/20	12/33/109/115	-
16	BCR	7	103	-	-	8/29/63/63	0/2/2/2
13	CLA	A	802	-	1/1/14/20	10/33/109/115	-
16	BCR	I	102	-	-	8/29/63/63	0/2/2/2
16	BCR	l	203	-	-	10/29/63/63	0/2/2/2
13	CLA	b	834	-	1/1/14/20	6/33/109/115	-
13	CLA	B	805	-	1/1/15/20	13/39/115/115	-
12	CL0	a	801	-	2/2/20/25	15/37/135/135	-
13	CLA	9	4003	-	1/1/11/20	8/17/93/115	-
16	BCR	i	103	-	-	8/29/63/63	0/2/2/2
13	CLA	a	827	-	1/1/15/20	13/39/115/115	-
16	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	2	808	-	-	5/15/91/115	-
13	CLA	1	839	-	1/1/15/20	9/39/115/115	-
13	CLA	1	822	-	-	8/21/97/115	-
16	BCR	2	839	-	-	11/29/63/63	0/2/2/2
16	BCR	b	840	-	-	11/29/63/63	0/2/2/2
16	BCR	6	205	-	-	12/29/63/63	0/2/2/2
13	CLA	A	816	-	1/1/11/20	8/17/93/115	-
18	LMG	B	846	-	-	17/36/56/70	0/1/1/1
13	CLA	B	826	-	-	14/33/109/115	-
13	CLA	1	829	-	1/1/15/20	12/39/115/115	-
13	CLA	B	806	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	J	1101	-	1/1/12/20	9/21/97/115	-
13	CLA	2	813	-	-	8/21/97/115	-
13	CLA	1	833	-	1/1/15/20	13/39/115/115	-
16	BCR	2	842	-	-	9/29/63/63	0/2/2/2
13	CLA	a	824	-	1/1/14/20	16/33/109/115	-
13	CLA	1	826	-	1/1/13/20	7/27/103/115	-
13	CLA	a	808	-	1/1/12/20	5/21/97/115	-
13	CLA	b	837	-	-	14/39/115/115	-
16	BCR	J	1104	-	-	8/29/63/63	0/2/2/2
16	BCR	1	847	-	-	15/29/63/63	0/2/2/2
16	BCR	M	101	-	-	7/29/63/63	0/2/2/2
13	CLA	K	4005	-	1/1/11/20	6/13/89/115	-
13	CLA	a	842	-	1/1/11/20	7/15/91/115	-
13	CLA	b	829	-	1/1/14/20	17/36/112/115	-
13	CLA	a	805	-	1/1/13/20	12/27/103/115	-
13	CLA	2	825	-	-	14/33/109/115	-
13	CLA	a	809	-	-	9/21/97/115	-
13	CLA	a	823	-	1/1/12/20	7/21/97/115	-
13	CLA	b	835	-	1/1/12/20	3/21/97/115	-
13	CLA	b	819	-	-	6/17/93/115	-
16	BCR	A	848	-	-	15/29/63/63	0/2/2/2
13	CLA	a	838	-	1/1/15/20	10/39/115/115	-
13	CLA	8	1102	-	1/1/9/20	6/10/82/115	-
13	CLA	b	808	-	-	14/39/115/115	-
13	CLA	b	814	-	-	8/21/97/115	-
13	CLA	a	819	-	1/1/14/20	12/33/109/115	-
13	CLA	B	819	-	-	6/17/93/115	-
16	BCR	j	1104	-	-	8/29/63/63	0/2/2/2
15	SF4	a	844	1,2	-	-	0/6/5/5
13	CLA	A	834	-	-	12/39/115/115	-
13	CLA	a	815	-	1/1/11/20	3/15/91/115	-
13	CLA	0	206	-	1/1/11/20	4/17/93/115	-
13	CLA	b	812	-	1/1/11/20	4/15/91/115	-
13	CLA	B	813	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	836	-	1/1/12/20	6/23/99/115	-
12	CL0	A	801	-	2/2/20/25	15/37/135/135	-
13	CLA	a	817	-	-	8/27/103/115	-
13	CLA	L	203	-	1/1/12/20	7/21/97/115	-
16	BCR	A	851	-	-	13/29/63/63	0/2/2/2
13	CLA	9	4002	-	1/1/11/20	7/15/91/115	-
13	CLA	a	826	-	1/1/13/20	7/27/103/115	-
13	CLA	b	823	-	1/1/15/20	12/39/115/115	-
17	LHG	A	850	-	-	19/45/45/53	-
13	CLA	1	840	-	-	13/39/115/115	-
13	CLA	2	810	-	1/1/11/20	8/17/93/115	-
16	BCR	b	845	-	-	15/29/63/63	0/2/2/2
16	BCR	2	847	-	-	10/29/63/63	0/2/2/2
13	CLA	B	810	-	1/1/15/20	15/39/115/115	-
13	CLA	2	830	-	1/1/15/20	7/39/115/115	-
13	CLA	f	204	-	1/1/11/20	8/17/93/115	-
13	CLA	1	834	-	-	12/39/115/115	-
13	CLA	2	803	-	1/1/14/20	11/33/109/115	-
13	CLA	A	831	-	-	8/21/97/115	-
13	CLA	A	813	-	1/1/13/20	10/27/103/115	-
13	CLA	B	801	-	1/1/15/20	6/39/115/115	-
13	CLA	1	835	-	-	14/29/105/115	-
13	CLA	b	807	-	1/1/15/20	15/39/115/115	-
13	CLA	a	829	-	1/1/15/20	12/39/115/115	-
13	CLA	b	832	-	1/1/9/20	4/10/82/115	-
13	CLA	8	1103	-	1/1/11/20	8/15/91/115	-
16	BCR	2	841	-	-	14/29/63/63	0/2/2/2
13	CLA	a	831	-	-	8/21/97/115	-
13	CLA	l	202	-	-	10/33/109/115	-
13	CLA	1	804	-	1/1/13/20	3/27/103/115	-
13	CLA	A	833	-	1/1/15/20	13/39/115/115	-
17	LHG	a	849	-	-	16/40/40/53	-
13	CLA	1	812	-	-	6/17/93/115	-
12	CL0	1	801	-	2/2/20/25	15/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	811	-	1/1/11/20	4/15/91/115	-
16	BCR	2	843	-	-	6/29/63/63	0/2/2/2
13	CLA	2	837	-	-	7/39/115/115	-
13	CLA	A	814	-	1/1/12/20	4/21/97/115	-
13	CLA	A	824	-	1/1/14/20	16/33/109/115	-
13	CLA	2	820	-	-	19/39/115/115	-
13	CLA	L	204	-	1/1/11/20	4/17/93/115	-
16	BCR	1	848	-	-	15/29/63/63	0/2/2/2
13	CLA	a	840	-	-	13/39/115/115	-
13	CLA	A	842	-	1/1/11/20	7/15/91/115	-
13	CLA	A	805	-	1/1/13/20	12/27/103/115	-
13	CLA	A	821	-	1/1/15/20	11/39/115/115	-
13	CLA	B	803	-	1/1/14/20	11/33/109/115	-
13	CLA	2	807	-	-	14/39/115/115	-
13	CLA	2	832	-	1/1/12/20	6/21/97/115	-
13	CLA	A	809	-	-	9/21/97/115	-
13	CLA	2	833	-	1/1/14/20	6/33/109/115	-
13	CLA	l	204	-	1/1/12/20	7/21/97/115	-
13	CLA	a	834	-	-	12/39/115/115	-
13	CLA	1	802	-	1/1/14/20	10/33/109/115	-
13	CLA	B	811	-	1/1/11/20	8/17/93/115	-
13	CLA	a	841	-	1/1/14/20	12/33/109/115	-
13	CLA	A	838	-	1/1/15/20	10/39/115/115	-
13	CLA	A	803	-	1/1/15/20	11/39/115/115	-
13	CLA	B	823	-	1/1/15/20	12/39/115/115	-
13	CLA	a	804	-	1/1/13/20	3/27/103/115	-
16	BCR	a	847	-	-	15/29/63/63	0/2/2/2
14	PQN	a	843	-	-	10/23/43/43	0/2/2/2
15	SF4	A	844	1,2	-	-	0/6/5/5
13	CLA	2	829	-	1/1/13/20	10/31/107/115	-
13	CLA	a	835	-	-	14/29/105/115	-
13	CLA	2	822	-	1/1/15/20	12/39/115/115	-
13	CLA	b	821	-	-	19/39/115/115	-
13	CLA	J	1102	-	1/1/9/20	6/10/82/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	811	-	1/1/13/20	10/29/105/115	-
13	CLA	b	801	-	1/1/15/20	6/39/115/115	-
17	LHG	A	849	-	-	16/40/40/53	-
13	CLA	A	812	-	-	6/17/93/115	-
13	CLA	A	817	-	-	8/27/103/115	-
16	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	1	831	-	-	8/21/97/115	-
13	CLA	b	815	-	1/1/15/20	12/39/115/115	-
13	CLA	A	815	-	1/1/11/20	3/15/91/115	-
13	CLA	1	852	-	1/1/14/20	13/33/109/115	-
13	CLA	A	810	-	-	8/15/91/115	-
13	CLA	a	802	-	1/1/14/20	10/33/109/115	-
16	BCR	a	845	-	-	8/29/63/63	0/2/2/2
18	LMG	b	846	-	-	17/36/56/70	0/1/1/1
13	CLA	1	818	-	1/1/12/20	7/26/102/115	-
13	CLA	L	201	-	-	10/33/109/115	-
13	CLA	b	824	-	1/1/13/20	7/27/103/115	-
13	CLA	a	814	-	1/1/12/20	4/21/97/115	-
13	CLA	a	816	-	1/1/11/20	8/17/93/115	-
16	BCR	l	201	-	-	7/29/63/63	0/2/2/2
13	CLA	a	828	-	1/1/15/20	9/39/115/115	-
16	BCR	f	205	-	-	12/29/63/63	0/2/2/2
13	CLA	b	803	-	1/1/14/20	11/33/109/115	-
13	CLA	b	828	-	-	9/27/103/115	-
13	CLA	1	823	-	1/1/12/20	7/21/97/115	-
13	CLA	A	828	-	1/1/15/20	9/39/115/115	-
13	CLA	b	810	-	1/1/15/20	15/39/115/115	-
16	BCR	2	844	-	-	15/29/63/63	0/2/2/2
13	CLA	B	802	-	-	9/39/115/115	-
16	BCR	b	842	-	-	14/29/63/63	0/2/2/2
16	BCR	0	201	-	-	7/29/63/63	0/2/2/2
13	CLA	A	820	-	-	5/17/93/115	-
13	CLA	a	818	-	1/1/12/20	7/26/102/115	-
13	CLA	b	827	-	-	8/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	0	204	-	-	10/29/63/63	0/2/2/2
13	CLA	B	829	-	1/1/14/20	17/36/112/115	-
13	CLA	a	837	-	1/1/14/20	8/33/109/115	-
13	CLA	k	4005	-	1/1/11/20	6/13/89/115	-
13	CLA	1	821	-	1/1/15/20	11/39/115/115	-
13	CLA	1	815	-	1/1/11/20	3/15/91/115	-
13	CLA	b	825	-	1/1/15/20	8/39/115/115	-
13	CLA	1	813	-	1/1/13/20	10/27/103/115	-
16	BCR	k	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	2	806	-	1/1/15/20	17/39/115/115	-
13	CLA	a	833	-	1/1/15/20	13/39/115/115	-
16	BCR	m	101	-	-	7/29/63/63	0/2/2/2
13	CLA	B	847	-	1/1/15/20	9/39/115/115	-
13	CLA	A	835	-	-	14/29/105/115	-
13	CLA	b	822	-	1/1/12/20	2/21/97/115	-
13	CLA	1	809	-	-	9/21/97/115	-
13	CLA	j	1102	-	1/1/9/20	6/10/82/115	-
13	CLA	2	846	-	1/1/15/20	9/39/115/115	-
13	CLA	a	839	-	1/1/15/20	9/39/115/115	-
13	CLA	2	834	-	1/1/12/20	3/21/97/115	-
13	CLA	1	838	-	1/1/15/20	10/39/115/115	-
13	CLA	b	805	-	1/1/15/20	13/39/115/115	-

The worst 5 of 2699 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	a	801	CL0	C3B-C4B	8.78	1.49	1.41
12	A	801	CL0	C3B-C4B	8.77	1.49	1.41
12	1	801	CL0	C3B-C4B	8.69	1.49	1.41
12	A	801	CL0	C1B-C2B	8.14	1.48	1.39
12	1	801	CL0	C1B-C2B	8.12	1.48	1.39

The worst 5 of 2369 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

5 of 210 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	A	801	CL0	NA
12	A	801	CL0	NC
12	a	801	CL0	NA
12	a	801	CL0	NC
12	1	801	CL0	NA

5 of 3618 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	820	CLA	3	0
13	2	827	CLA	2	0
13	b	833	CLA	2	0
13	B	820	CLA	2	0
16	a	848	BCR	6	0
13	f	201	CLA	5	0
13	8	1101	CLA	1	0
13	0	205	CLA	8	0
13	I	101	CLA	9	0
13	a	825	CLA	4	0
16	1	851	BCR	2	0
13	1	828	CLA	9	0
18	2	845	LMG	3	0
13	A	825	CLA	4	0
13	F	203	CLA	1	0
16	6	202	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	824	CLA	6	0
14	A	843	PQN	4	0
13	a	813	CLA	4	0
16	z	101	BCR	3	0
16	B	841	BCR	5	0
13	B	830	CLA	2	0
13	A	811	CLA	2	0
17	1	850	LHG	2	0
16	2	840	BCR	5	0
13	2	801	CLA	1	0
19	7	101	SQD	12	0
13	B	827	CLA	2	0
13	A	807	CLA	1	0
13	a	852	CLA	9	0
13	b	806	CLA	8	0
13	1	805	CLA	4	0
13	2	815	CLA	1	0
17	a	850	LHG	1	0
13	A	819	CLA	5	0
13	7	102	CLA	8	0
13	b	813	CLA	2	0
13	A	818	CLA	4	0
13	1	806	CLA	7	0
13	2	826	CLA	1	0
13	A	822	CLA	1	0
13	A	837	CLA	4	0
16	a	851	BCR	2	0
13	2	823	CLA	7	0
16	1	846	BCR	3	0
16	L	207	BCR	10	0
16	L	202	BCR	2	0
13	B	832	CLA	1	0
13	B	835	CLA	3	0
13	2	812	CLA	2	0
16	J	1105	BCR	1	0
13	B	833	CLA	2	0
13	b	804	CLA	7	0
13	A	804	CLA	3	0
13	a	803	CLA	2	0
13	B	814	CLA	2	0
16	A	847	BCR	4	0
13	J	1103	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	809	CLA	7	0
13	A	830	CLA	4	0
13	a	830	CLA	4	0
13	A	829	CLA	3	0
13	a	811	CLA	2	0
16	9	4001	BCR	4	0
14	1	843	PQN	2	0
13	B	809	CLA	1	0
13	a	820	CLA	1	0
13	B	812	CLA	1	0
16	b	841	BCR	4	0
16	L	205	BCR	4	0
13	b	830	CLA	2	0
13	0	203	CLA	1	0
13	1	825	CLA	5	0
16	8	1104	BCR	3	0
13	b	816	CLA	1	0
16	j	1105	BCR	2	0
13	1	808	CLA	4	0
13	1	820	CLA	1	0
16	B	848	BCR	2	0
13	B	838	CLA	1	0
13	a	810	CLA	1	0
13	1	842	CLA	1	0
16	A	845	BCR	3	0
13	2	819	CLA	2	0
13	a	832	CLA	3	0
13	B	825	CLA	2	0
13	b	802	CLA	3	0
13	j	1103	CLA	2	0
13	1	837	CLA	3	0
13	A	808	CLA	4	0
13	b	836	CLA	3	0
13	2	817	CLA	1	0
13	0	208	CLA	5	0
13	2	831	CLA	1	0
13	B	817	CLA	1	0
16	K	4001	BCR	1	0
13	l	205	CLA	1	0
13	A	823	CLA	2	0
13	b	811	CLA	2	0
13	j	1101	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	843	BCR	1	0
13	b	831	CLA	2	0
13	b	818	CLA	1	0
16	F	202	BCR	2	0
13	2	804	CLA	5	0
13	1	836	CLA	1	0
13	b	847	CLA	2	0
13	B	831	CLA	2	0
13	a	822	CLA	1	0
13	B	816	CLA	1	0
16	1	845	BCR	2	0
13	B	804	CLA	6	0
13	1	807	CLA	1	0
13	1	810	CLA	1	0
13	B	815	CLA	5	0
13	b	826	CLA	4	0
13	b	809	CLA	1	0
16	B	845	BCR	3	0
13	6	201	CLA	3	0
13	A	832	CLA	3	0
13	A	827	CLA	2	0
16	b	848	BCR	4	0
13	1	803	CLA	3	0
13	l	207	CLA	5	0
16	l	206	BCR	3	0
13	F	201	CLA	5	0
13	a	806	CLA	5	0
13	f	203	CLA	1	0
13	L	206	CLA	7	0
13	2	836	CLA	3	0
13	a	821	CLA	6	0
16	b	844	BCR	4	0
13	B	821	CLA	6	0
13	1	841	CLA	5	0
13	b	817	CLA	1	0
16	B	842	BCR	1	0
16	f	202	BCR	2	0
16	F	205	BCR	3	0
16	B	840	BCR	4	0
13	2	828	CLA	4	0
16	9	4004	BCR	1	0
13	2	814	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	824	CLA	4	0
19	I	103	SQD	13	0
13	2	816	CLA	1	0
16	K	4004	BCR	1	0
13	A	840	CLA	3	0
13	A	852	CLA	8	0
13	2	805	CLA	5	0
19	i	101	SQD	12	0
13	A	839	CLA	3	0
13	A	806	CLA	6	0
13	2	802	CLA	4	0
13	B	828	CLA	2	0
16	b	843	BCR	2	0
13	2	835	CLA	4	0
16	8	1105	BCR	2	0
13	b	838	CLA	1	0
13	1	824	CLA	3	0
13	A	841	CLA	5	0
13	B	837	CLA	3	0
13	B	836	CLA	4	0
13	A	826	CLA	3	0
13	i	102	CLA	9	0
15	3	102	SF4	1	0
13	1	817	CLA	3	0
14	b	839	PQN	6	0
13	B	808	CLA	3	0
16	0	207	BCR	1	0
14	B	839	PQN	7	0
13	0	202	CLA	2	0
13	1	830	CLA	4	0
13	1	832	CLA	3	0
16	A	846	BCR	5	0
13	1	827	CLA	3	0
13	a	836	CLA	1	0
13	B	818	CLA	1	0
14	2	838	PQN	7	0
13	1	819	CLA	5	0
16	7	103	BCR	3	0
13	A	802	CLA	5	0
16	I	102	BCR	5	0
16	l	203	BCR	2	0
13	B	805	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	a	801	CL0	5	0
13	9	4003	CLA	1	0
16	i	103	BCR	5	0
13	a	827	CLA	2	0
16	k	4001	BCR	1	0
16	B	844	BCR	4	0
13	2	808	CLA	1	0
13	1	822	CLA	1	0
13	1	839	CLA	3	0
16	2	839	BCR	4	0
16	b	840	BCR	4	0
16	6	205	BCR	3	0
18	B	846	LMG	3	0
13	B	826	CLA	3	0
13	1	829	CLA	3	0
13	B	806	CLA	8	0
13	J	1101	CLA	1	0
13	2	813	CLA	2	0
13	1	833	CLA	3	0
16	2	842	BCR	2	0
13	a	824	CLA	4	0
13	1	826	CLA	4	0
13	a	808	CLA	4	0
13	b	837	CLA	3	0
16	J	1104	BCR	2	0
16	1	847	BCR	5	0
16	M	101	BCR	2	0
13	a	842	CLA	1	0
13	b	829	CLA	4	0
13	a	805	CLA	2	0
13	2	825	CLA	3	0
13	a	809	CLA	1	0
13	a	823	CLA	2	0
13	b	835	CLA	2	0
16	A	848	BCR	6	0
13	a	838	CLA	5	0
13	b	808	CLA	3	0
13	b	814	CLA	3	0
13	a	819	CLA	5	0
16	j	1104	BCR	2	0
13	A	834	CLA	4	0
13	a	815	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	813	CLA	1	0
13	A	836	CLA	1	0
12	A	801	CL0	5	0
13	a	817	CLA	3	0
13	L	203	CLA	9	0
16	A	851	BCR	2	0
13	a	826	CLA	4	0
13	b	823	CLA	3	0
17	A	850	LHG	2	0
13	1	840	CLA	5	0
13	2	810	CLA	2	0
16	b	845	BCR	3	0
16	2	847	BCR	4	0
13	B	810	CLA	7	0
13	2	830	CLA	2	0
13	1	834	CLA	4	0
13	2	803	CLA	1	0
13	A	831	CLA	4	0
13	A	813	CLA	3	0
13	B	801	CLA	1	0
13	1	835	CLA	1	0
13	b	807	CLA	1	0
13	a	829	CLA	3	0
13	b	832	CLA	1	0
13	8	1103	CLA	2	0
16	2	841	BCR	1	0
13	a	831	CLA	4	0
13	l	202	CLA	2	0
13	1	804	CLA	3	0
13	A	833	CLA	2	0
12	1	801	CL0	5	0
13	2	811	CLA	1	0
16	2	843	BCR	5	0
13	2	837	CLA	1	0
13	A	824	CLA	3	0
13	2	820	CLA	7	0
13	L	204	CLA	1	0
16	1	848	BCR	6	0
13	a	840	CLA	3	0
13	A	842	CLA	1	0
13	A	805	CLA	2	0
13	A	821	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	803	CLA	2	0
13	2	807	CLA	3	0
13	2	832	CLA	2	0
13	A	809	CLA	2	0
13	l	204	CLA	7	0
13	a	834	CLA	4	0
13	1	802	CLA	5	0
13	B	811	CLA	2	0
13	a	841	CLA	5	0
13	A	838	CLA	5	0
13	A	803	CLA	2	0
13	B	823	CLA	4	0
13	a	804	CLA	3	0
16	a	847	BCR	3	0
14	a	843	PQN	4	0
13	2	829	CLA	2	0
13	a	835	CLA	1	0
13	2	822	CLA	3	0
13	b	821	CLA	6	0
13	1	811	CLA	2	0
13	b	801	CLA	1	0
13	A	817	CLA	3	0
16	a	846	BCR	4	0
13	1	831	CLA	4	0
13	b	815	CLA	4	0
13	A	815	CLA	2	0
13	1	852	CLA	8	0
13	A	810	CLA	2	0
13	a	802	CLA	5	0
16	a	845	BCR	2	0
18	b	846	LMG	3	0
13	1	818	CLA	4	0
13	L	201	CLA	2	0
13	b	824	CLA	7	0
16	l	201	BCR	7	0
13	a	828	CLA	9	0
16	f	205	BCR	2	0
13	b	803	CLA	2	0
13	b	828	CLA	2	0
13	1	823	CLA	2	0
13	A	828	CLA	10	0
13	b	810	CLA	7	0

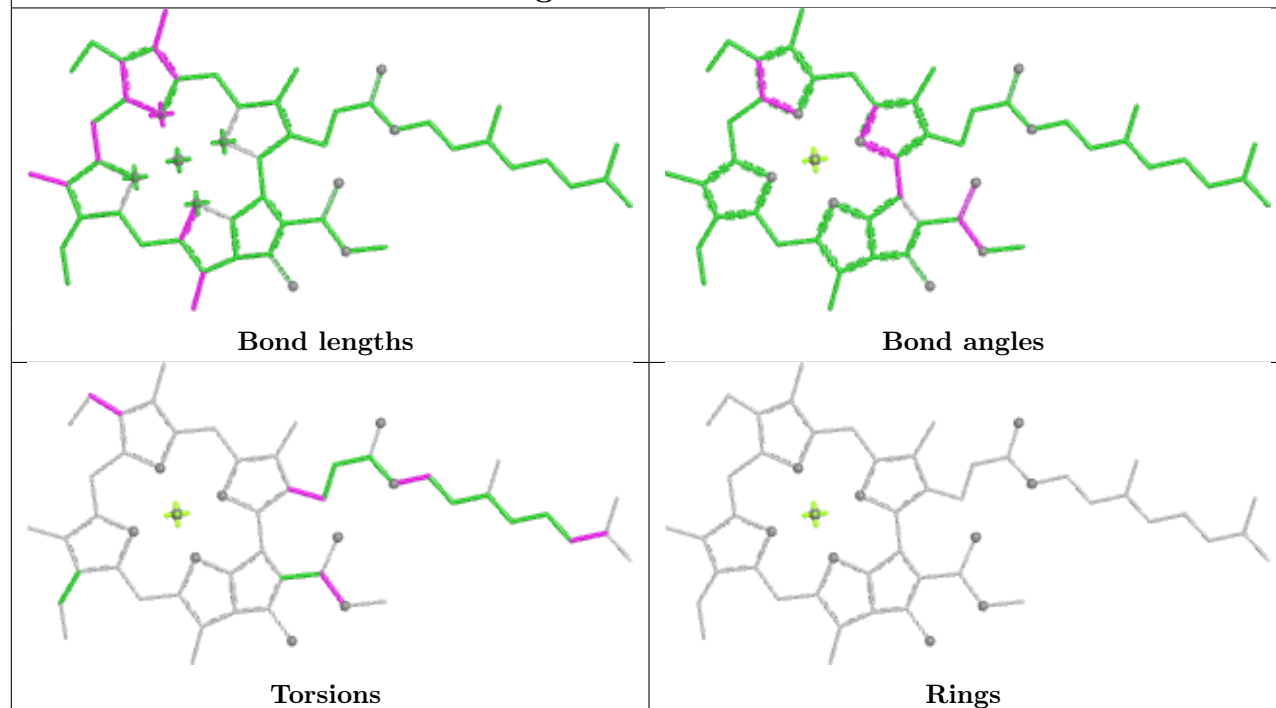
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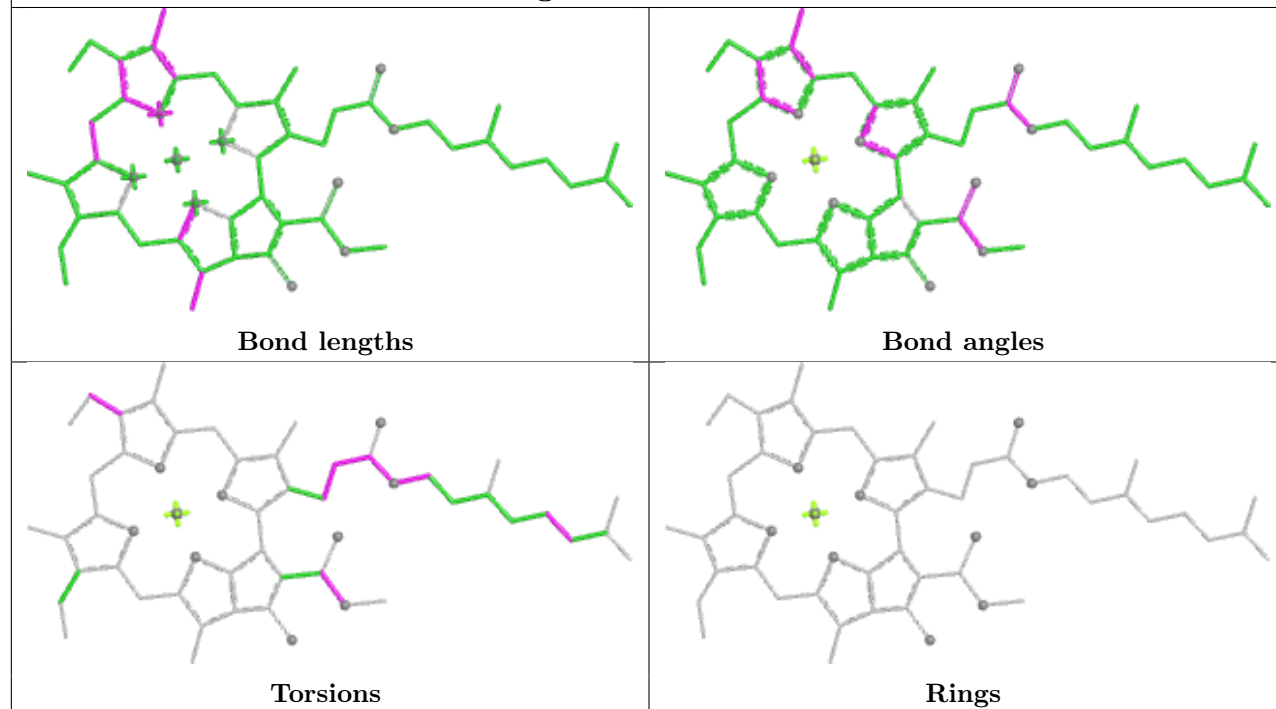
Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	2	844	BCR	3	0
13	B	802	CLA	5	0
16	b	842	BCR	1	0
16	0	201	BCR	6	0
13	A	820	CLA	1	0
13	a	818	CLA	4	0
13	b	827	CLA	2	0
16	0	204	BCR	3	0
13	B	829	CLA	4	0
13	a	837	CLA	4	0
13	1	821	CLA	6	0
13	1	815	CLA	2	0
13	b	825	CLA	4	0
13	1	813	CLA	3	0
16	k	4004	BCR	1	0
13	2	806	CLA	9	0
13	a	833	CLA	3	0
16	m	101	BCR	2	0
13	B	847	CLA	2	0
13	A	835	CLA	1	0
13	1	809	CLA	2	0
13	2	846	CLA	2	0
13	a	839	CLA	4	0
13	2	834	CLA	3	0
13	1	838	CLA	5	0
13	b	805	CLA	6	0

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

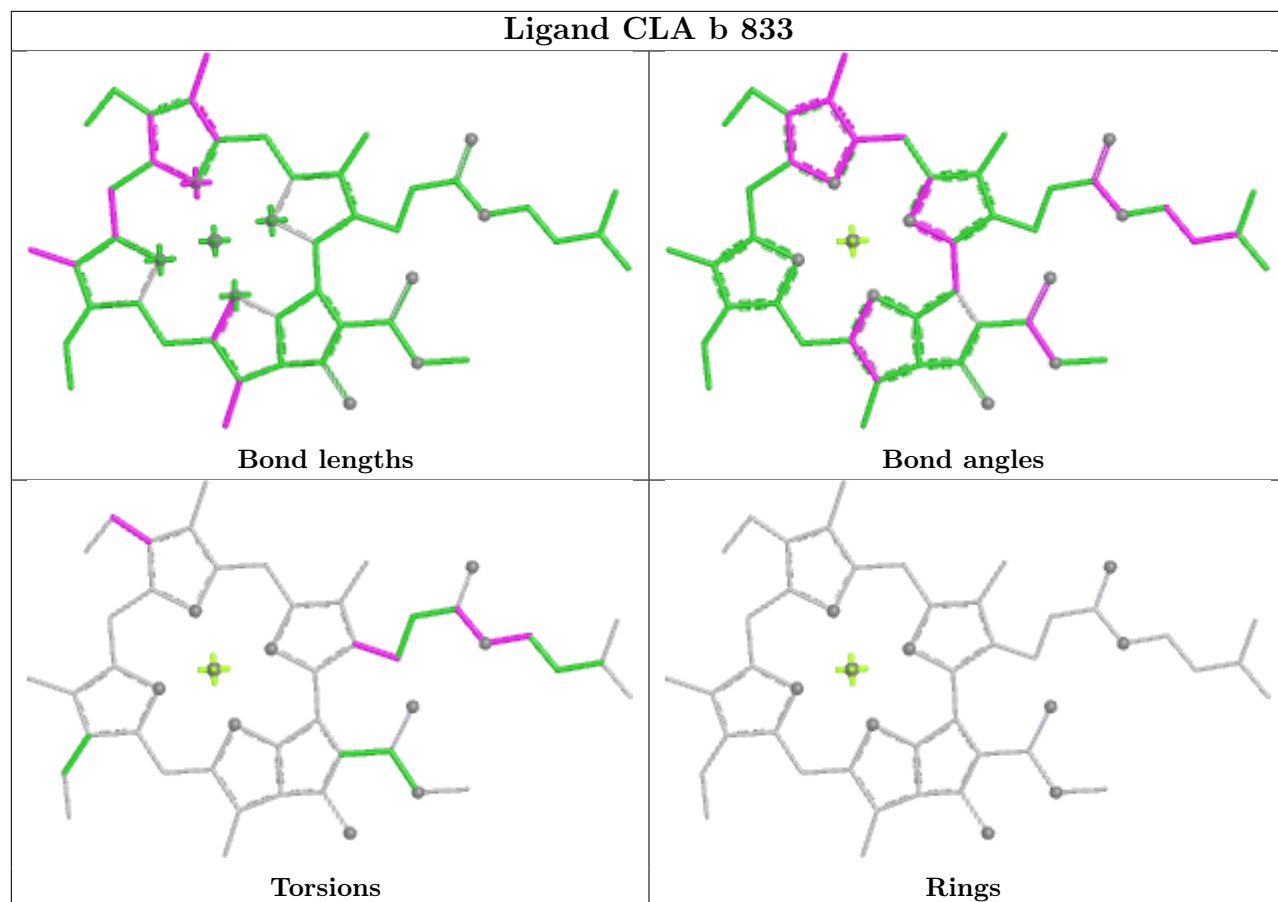
Ligand CLA b 820

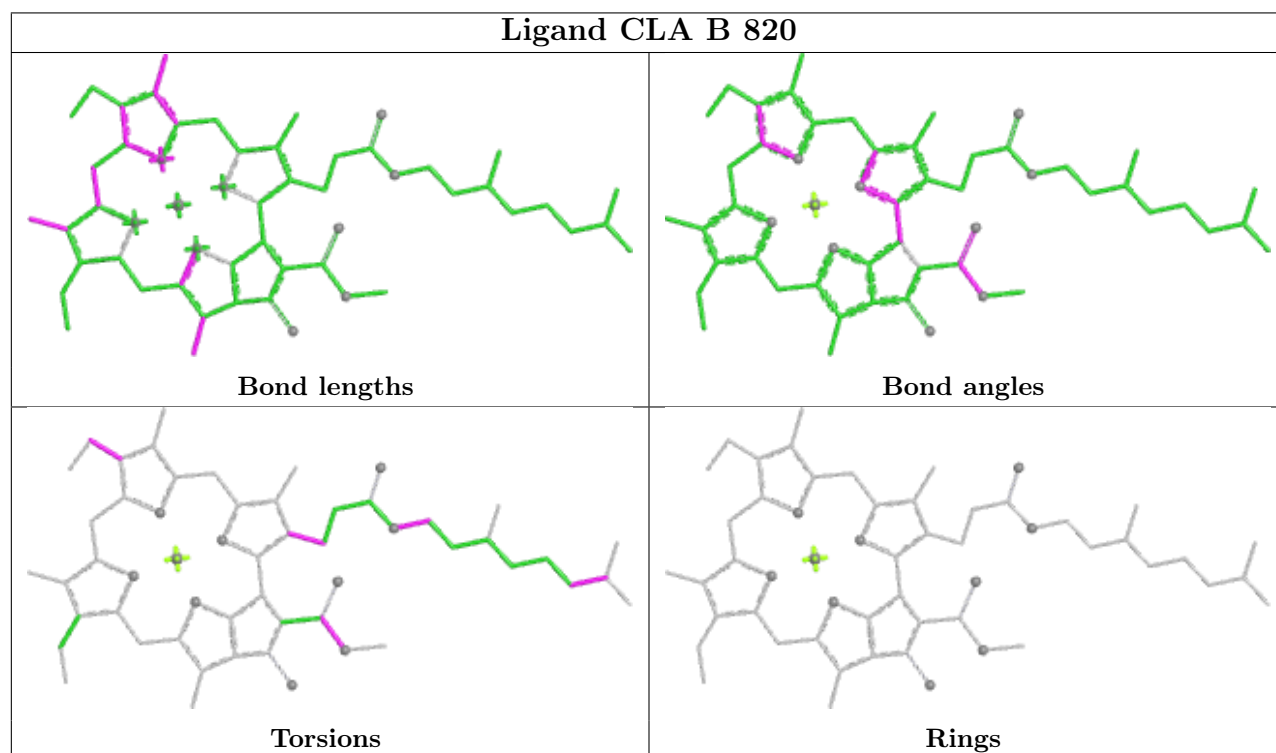
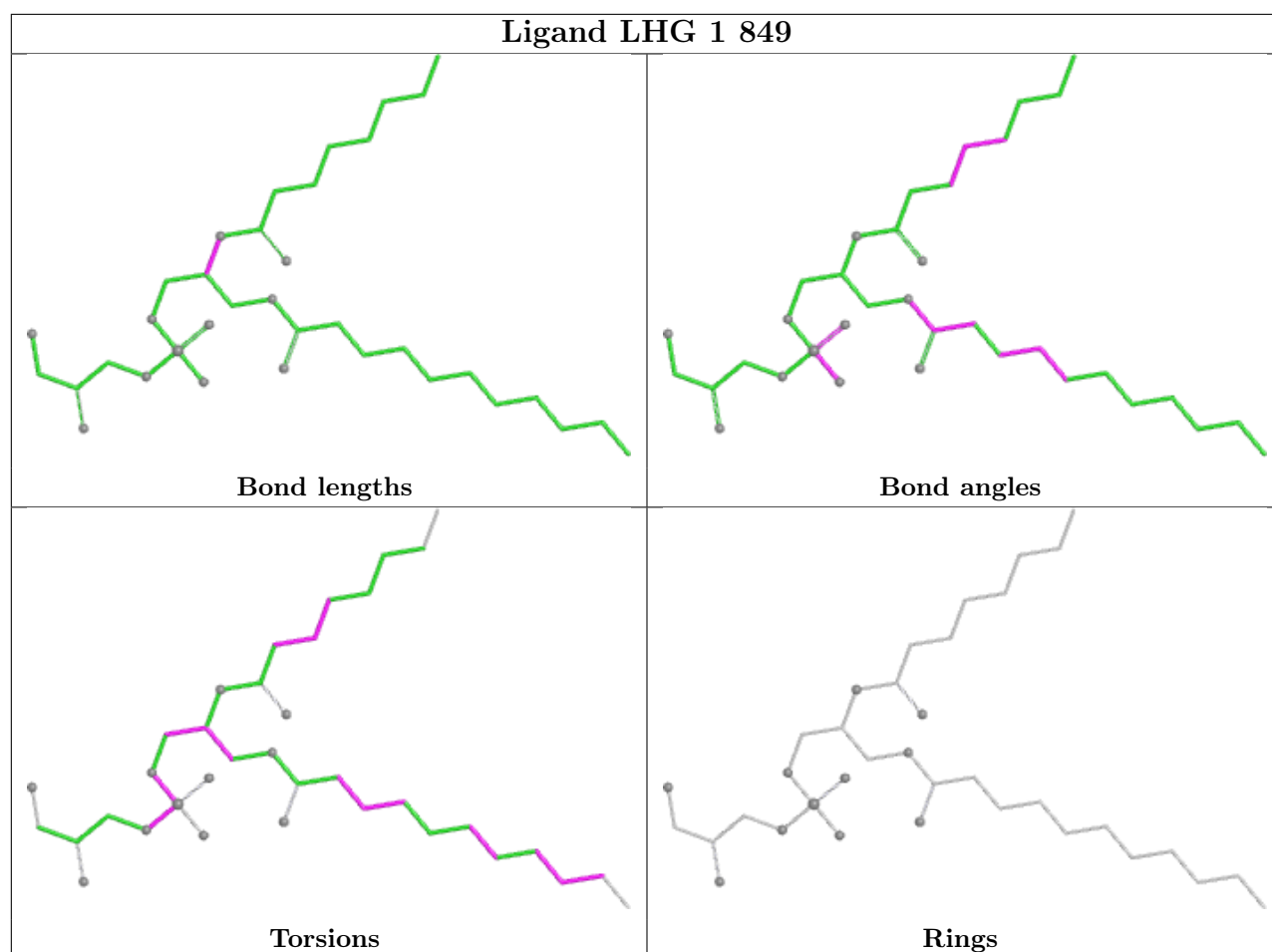


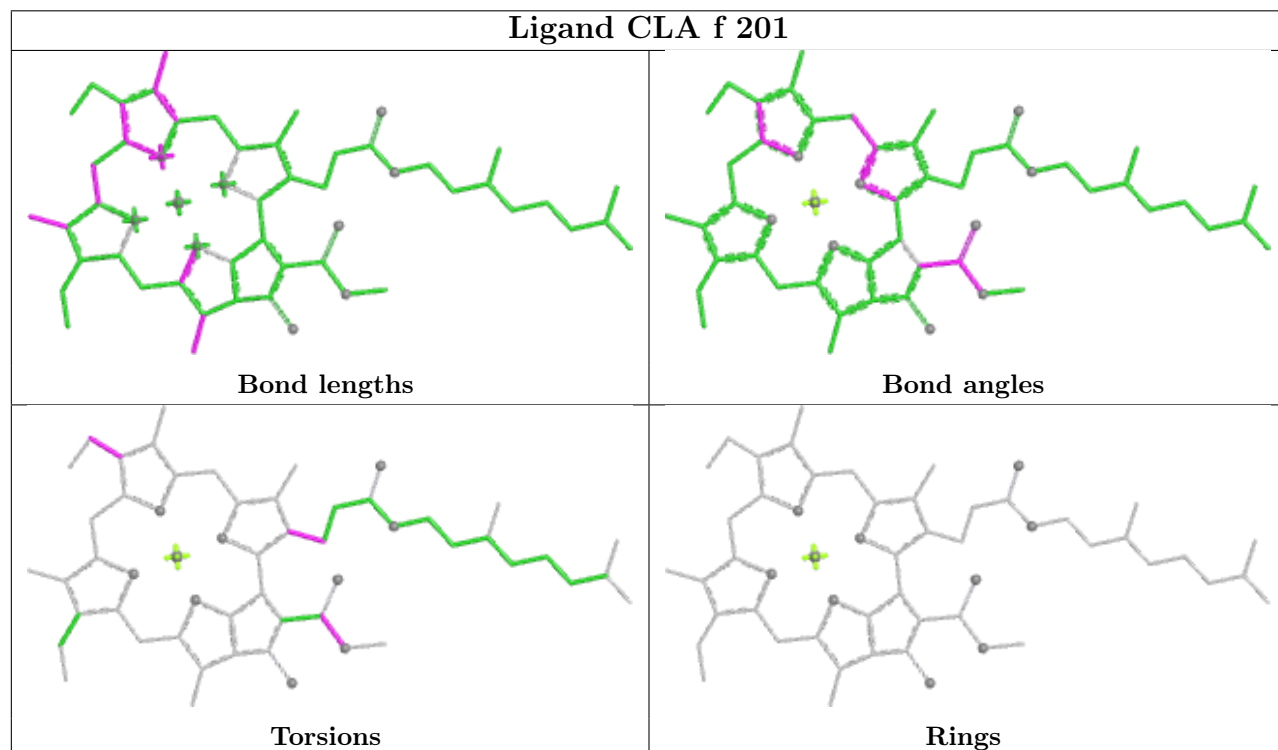
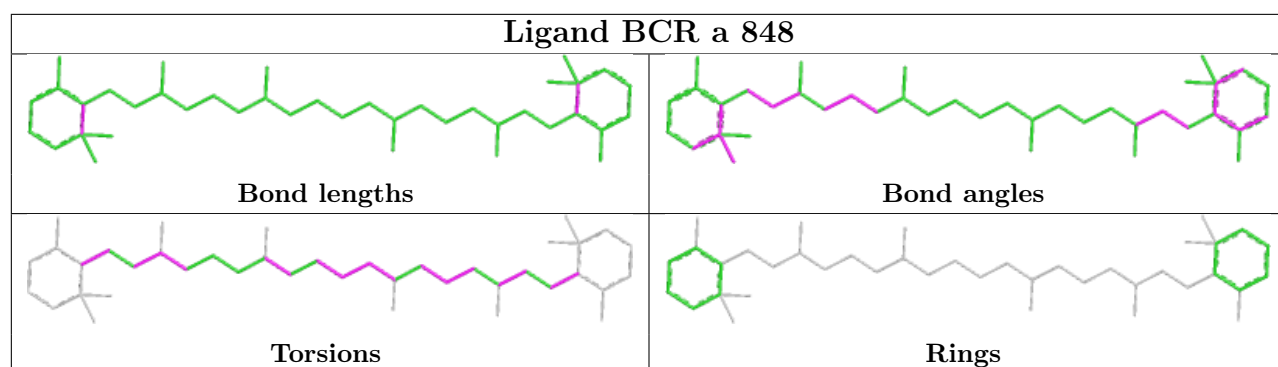
Ligand CLA 2 827

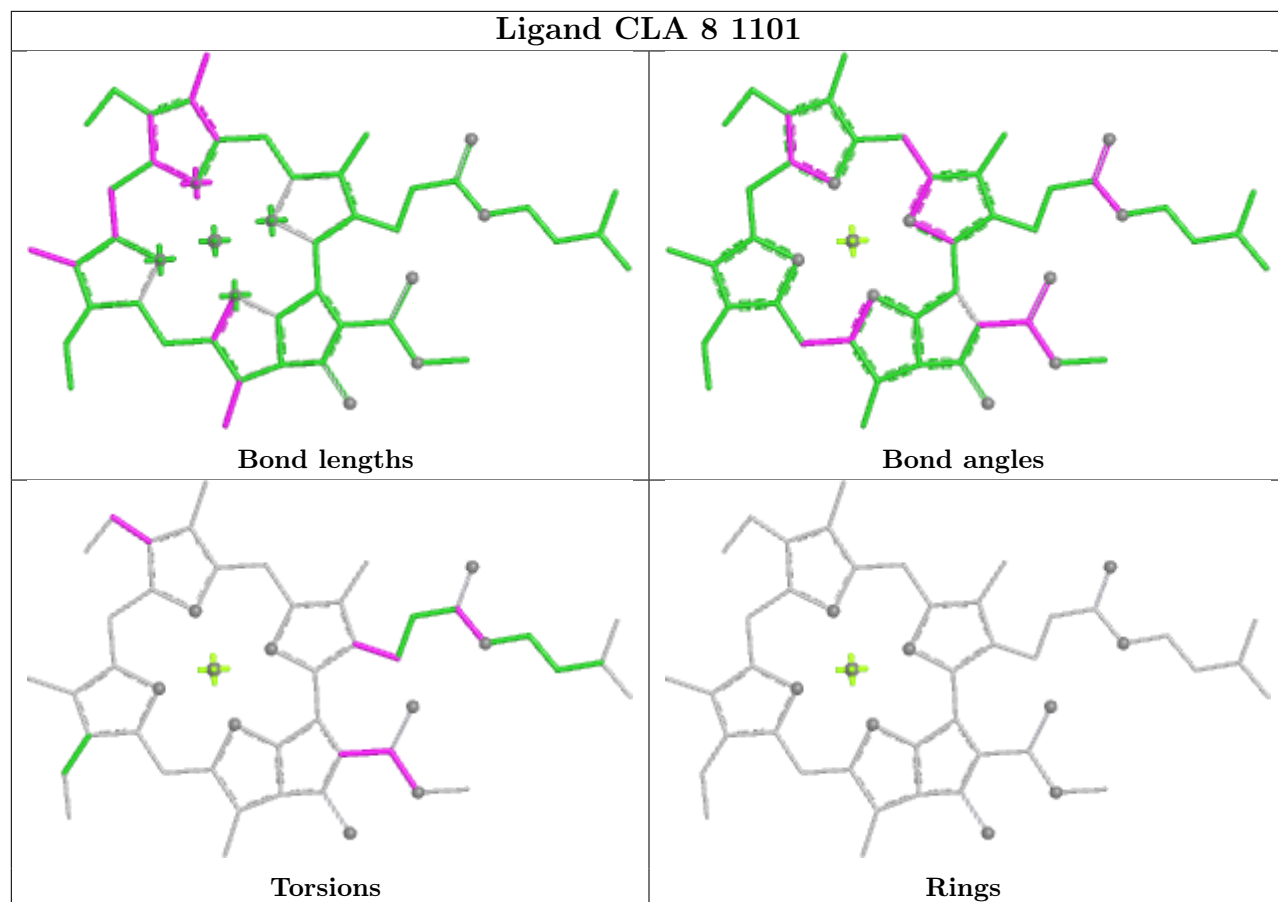


Ligand CLA b 833

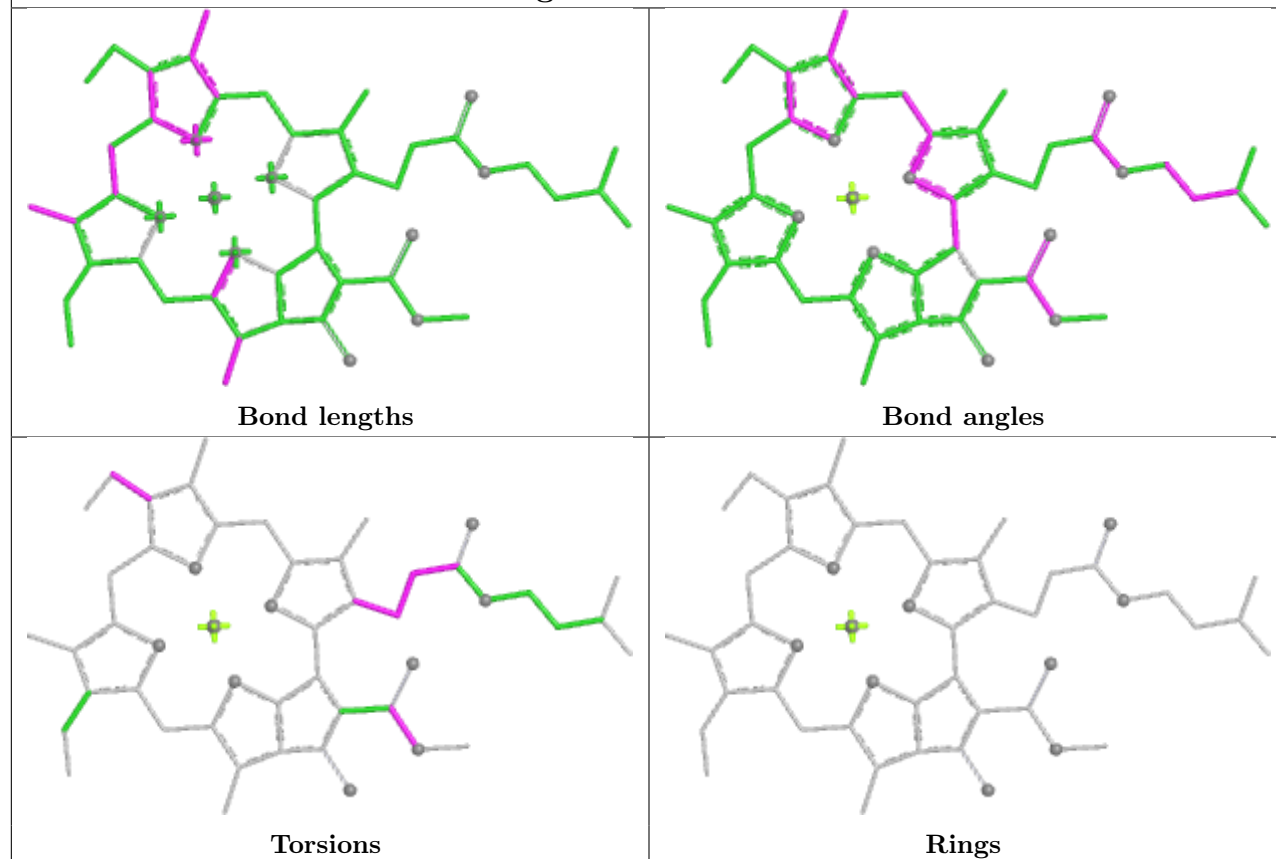




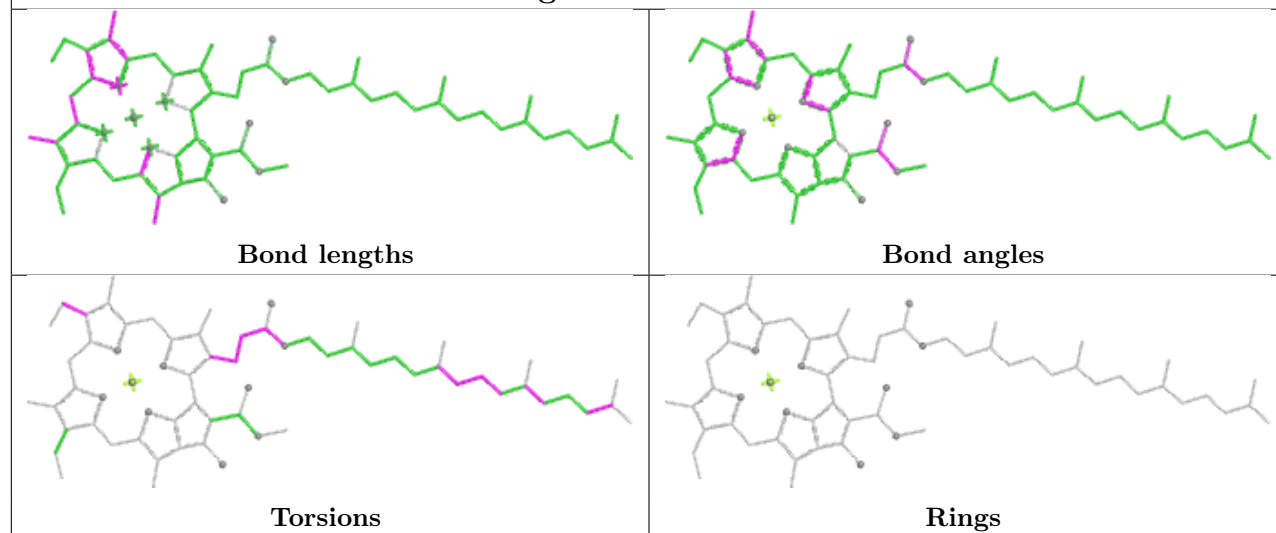


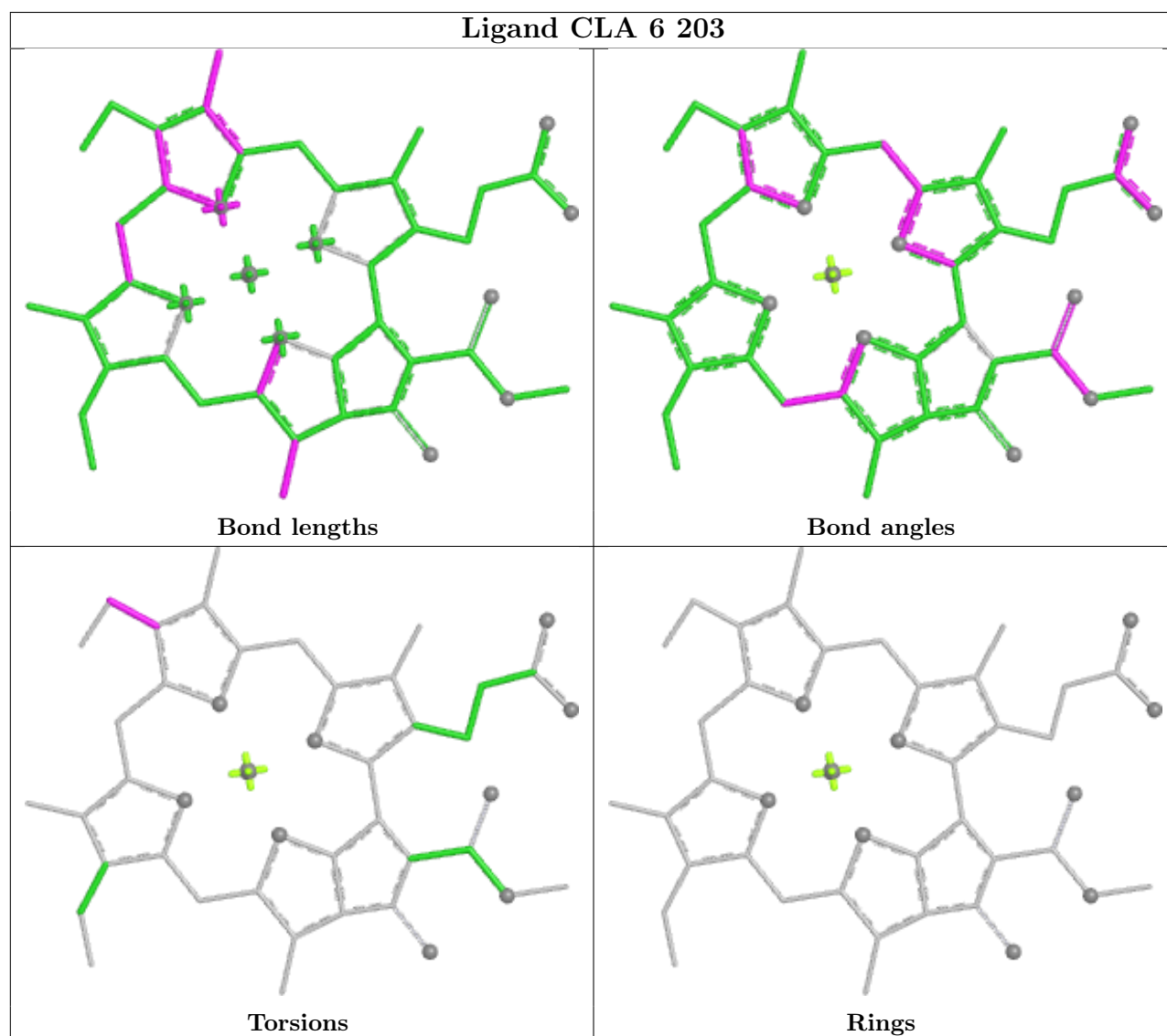
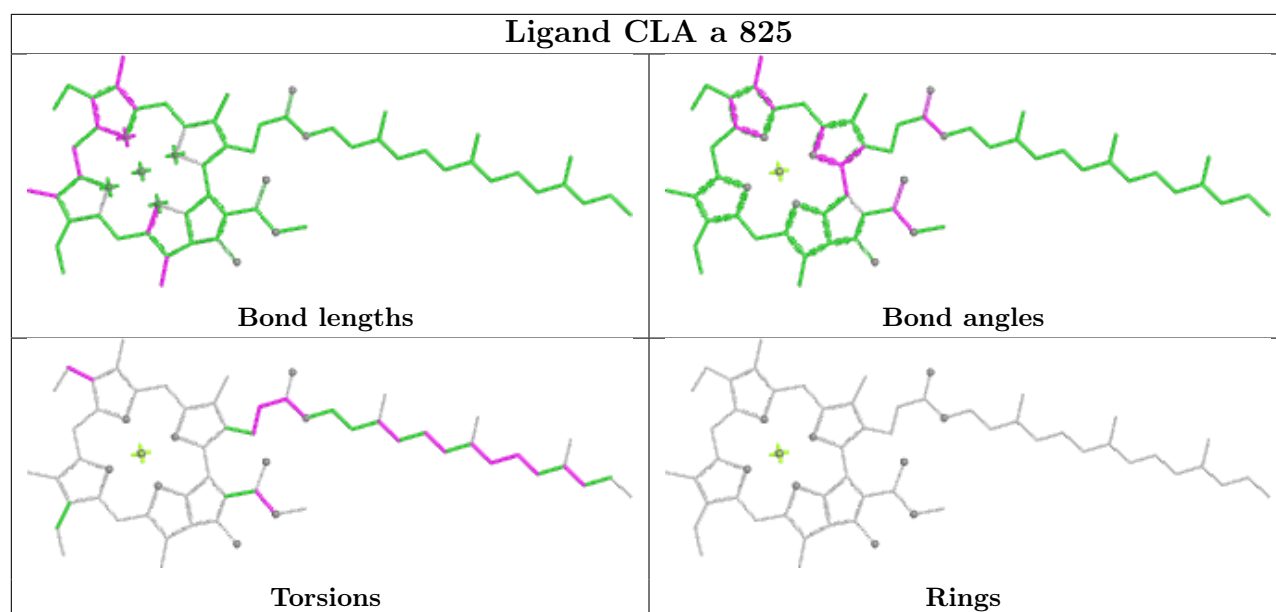


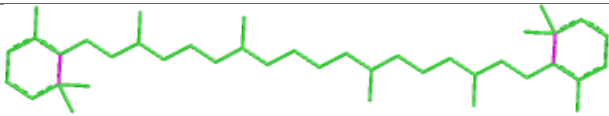
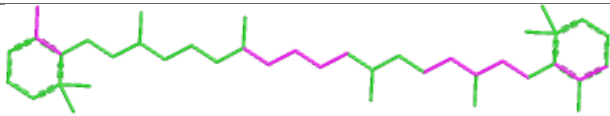
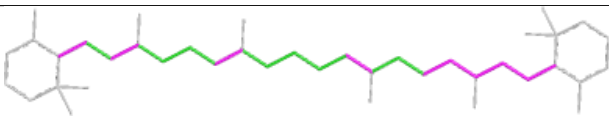
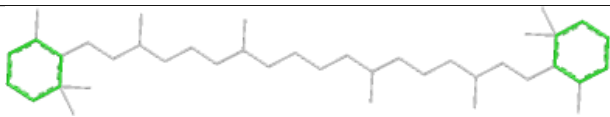
Ligand CLA 0 205

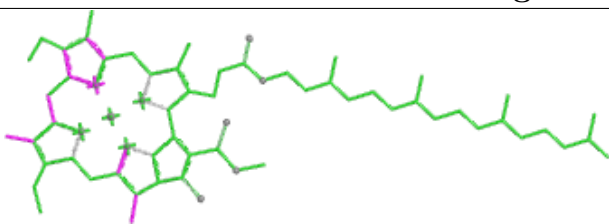
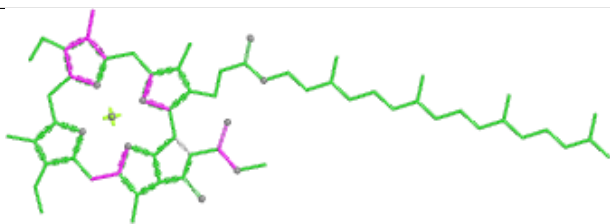
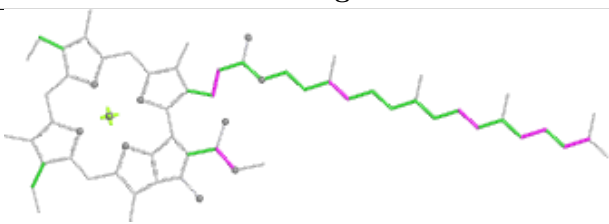
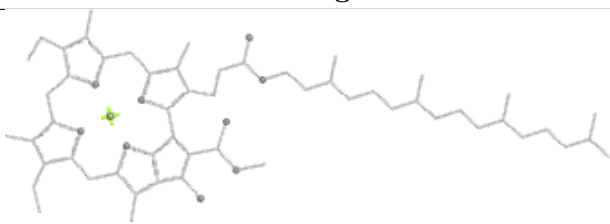


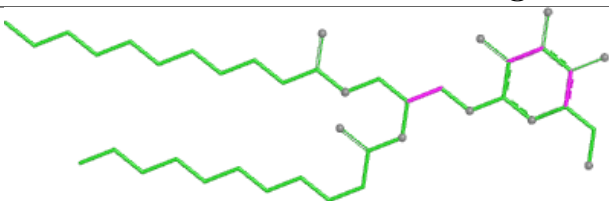
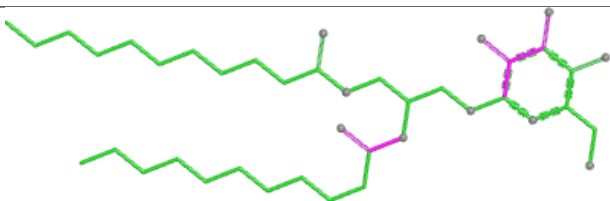
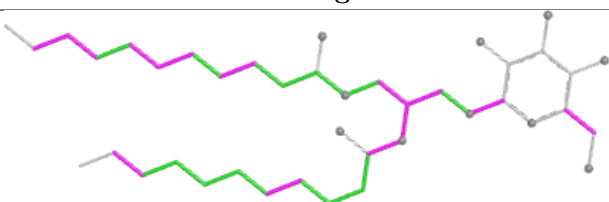
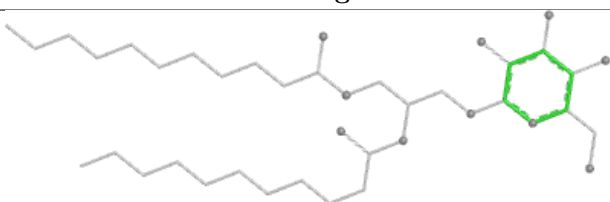
Ligand CLA I 101



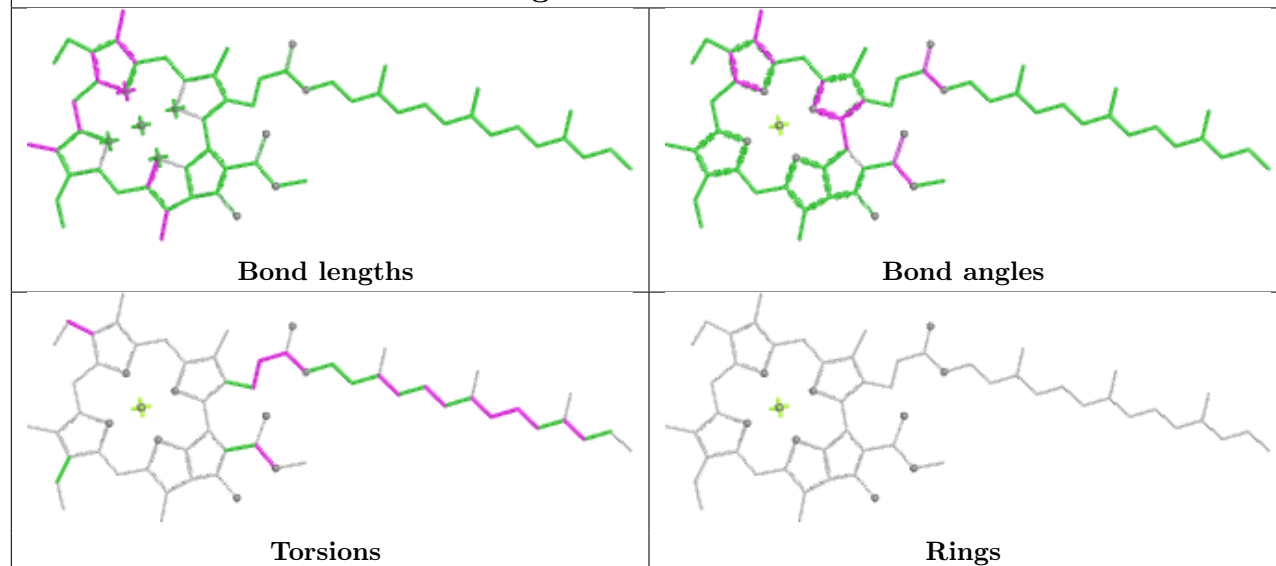


Ligand BCR 1 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

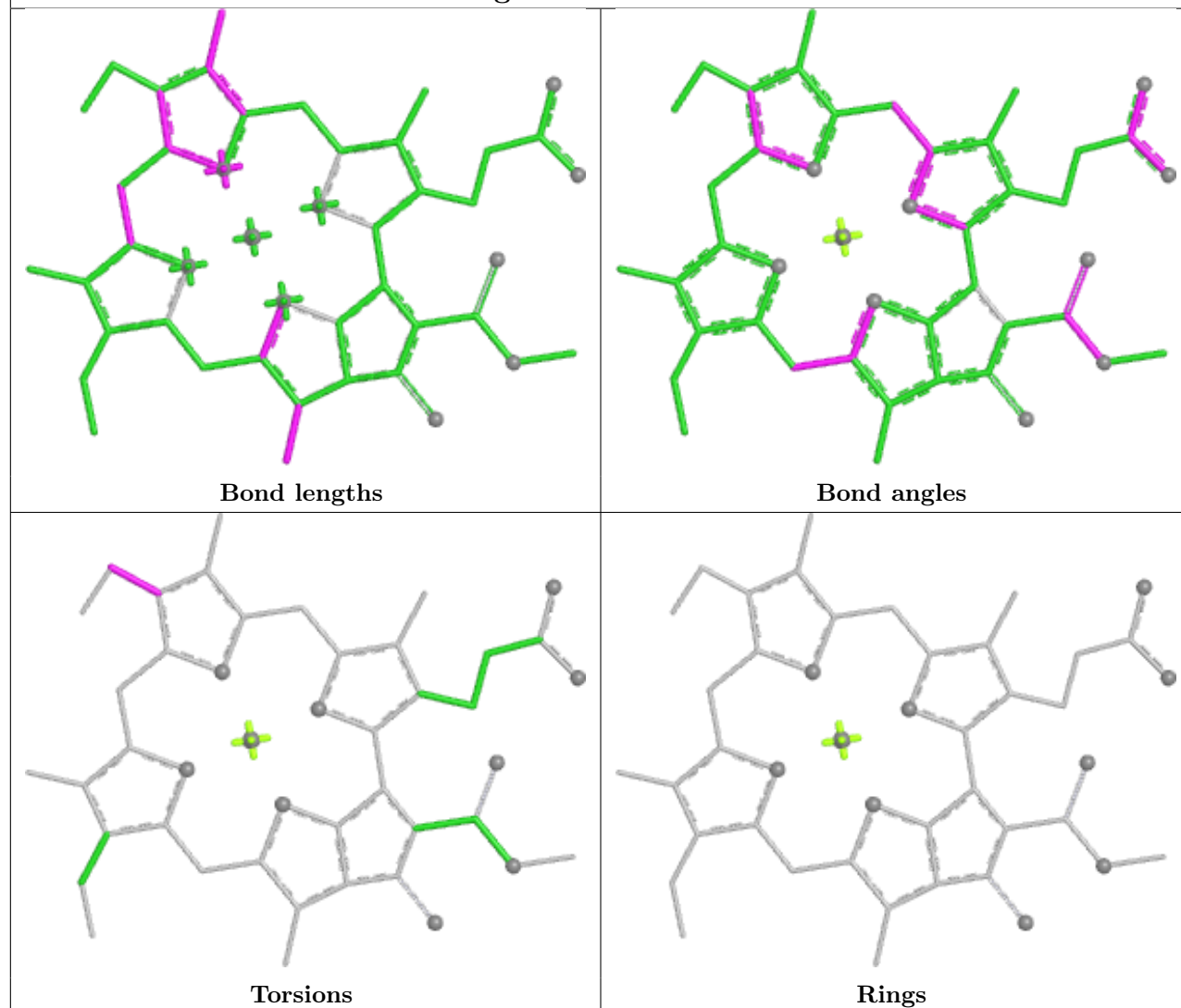
Ligand CLA 1 828	
	
Bond lengths	Bond angles
	
Torsions	Rings

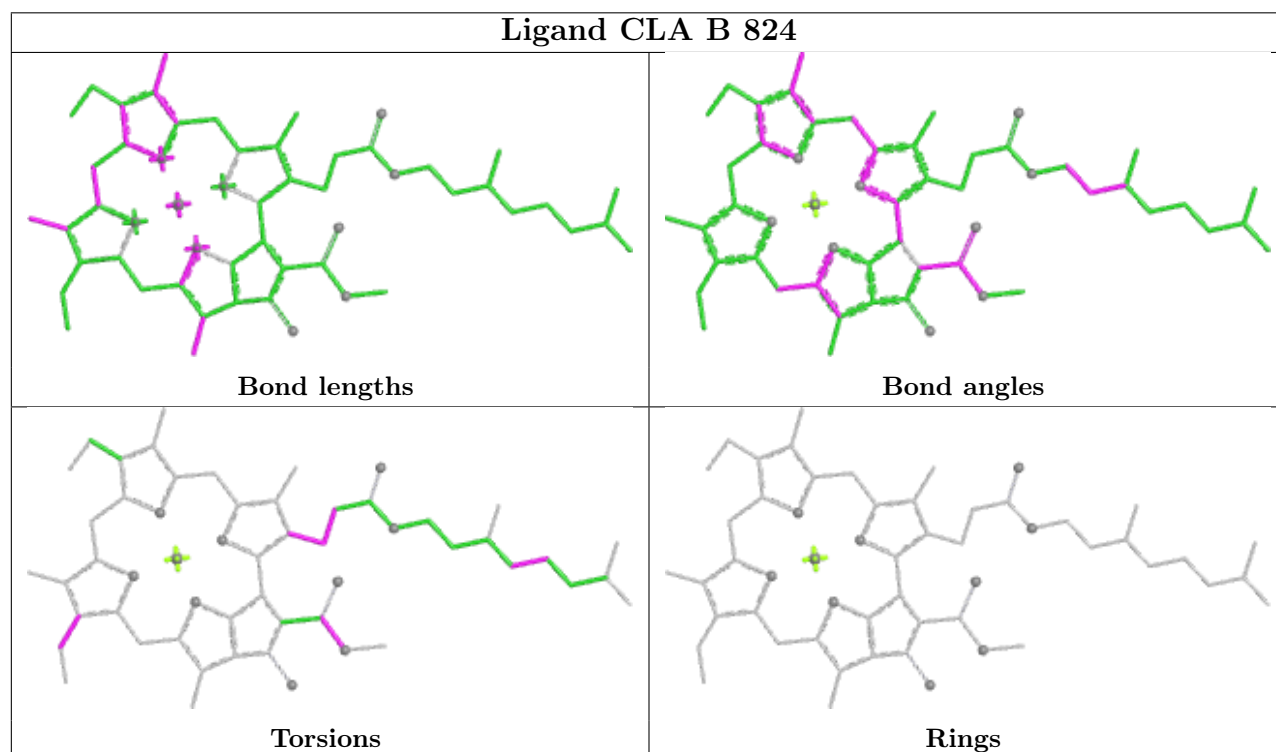
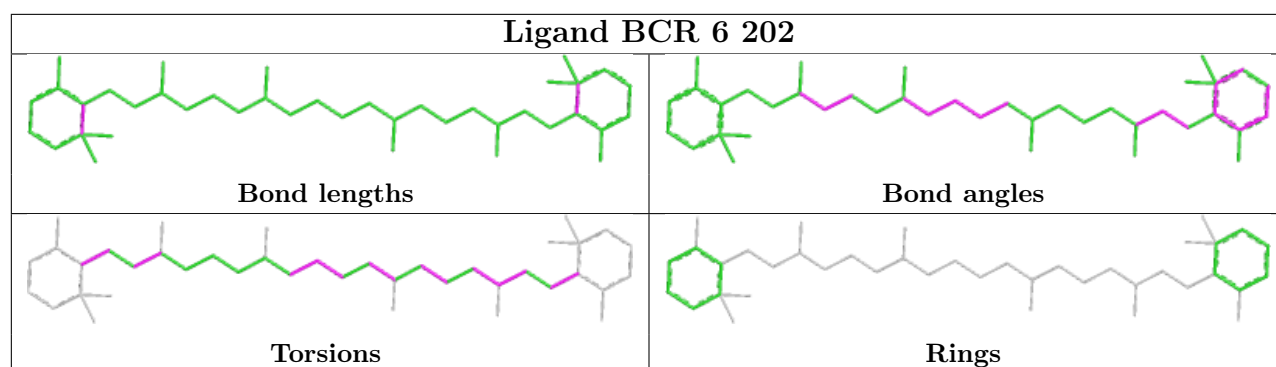
Ligand LMG 2 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 825

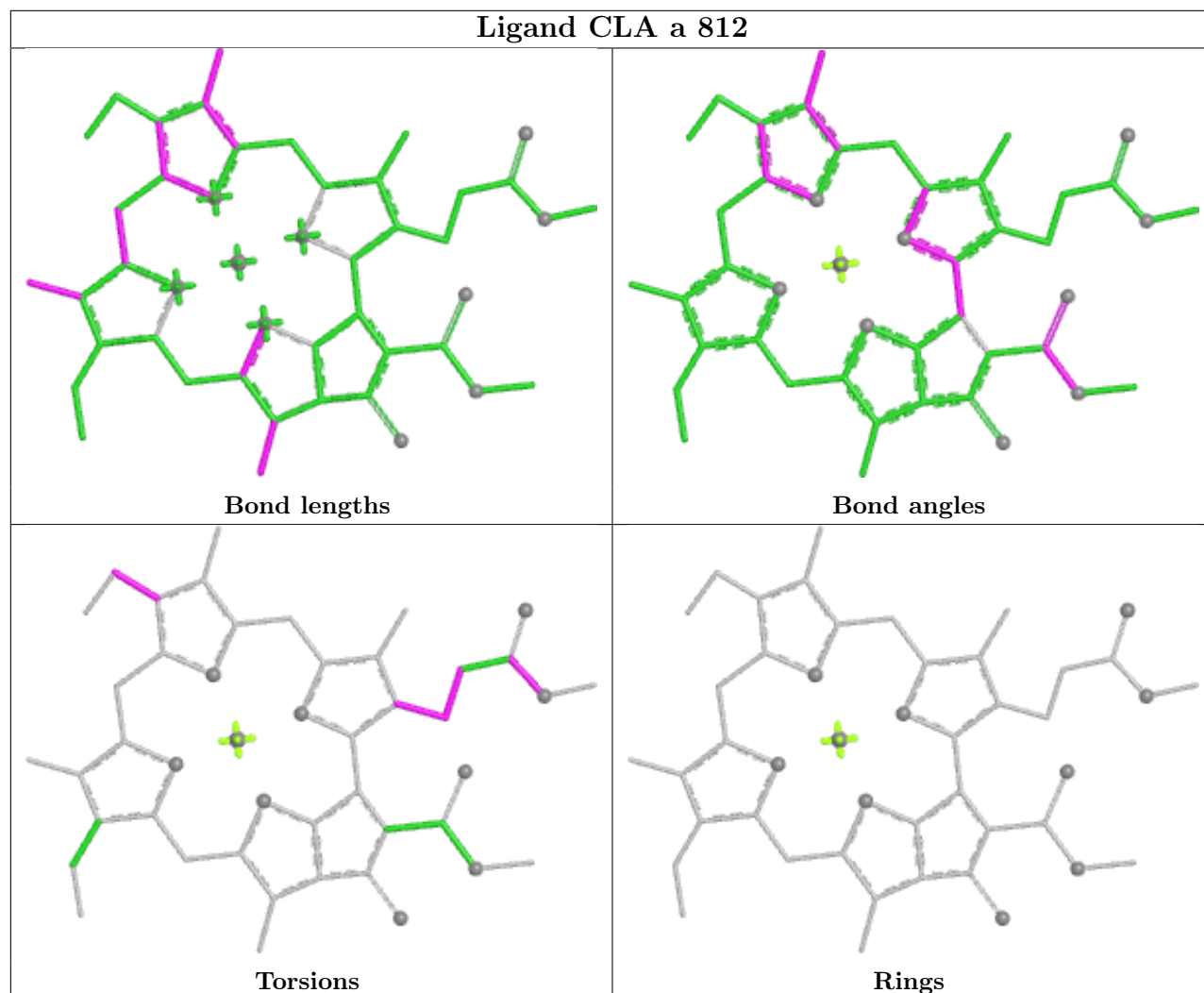


Ligand CLA F 203

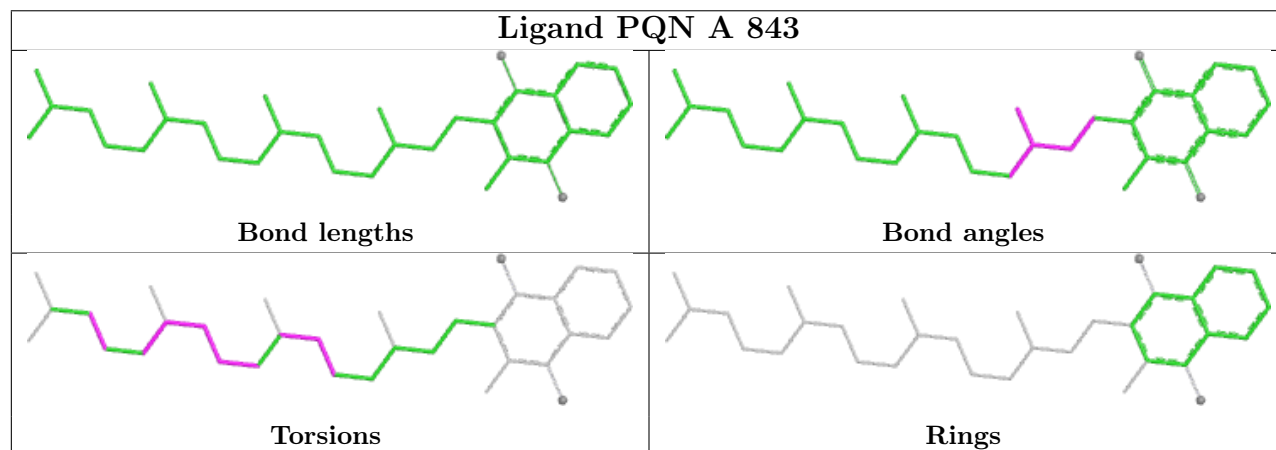


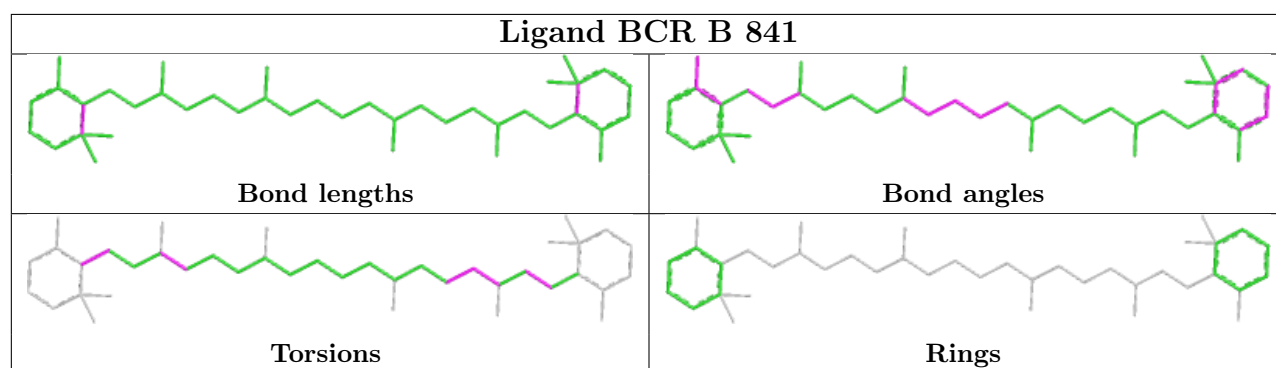
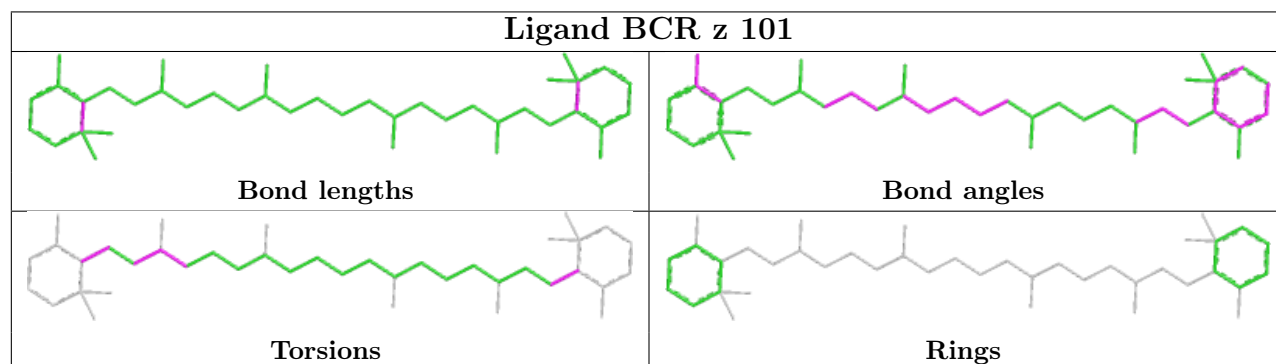
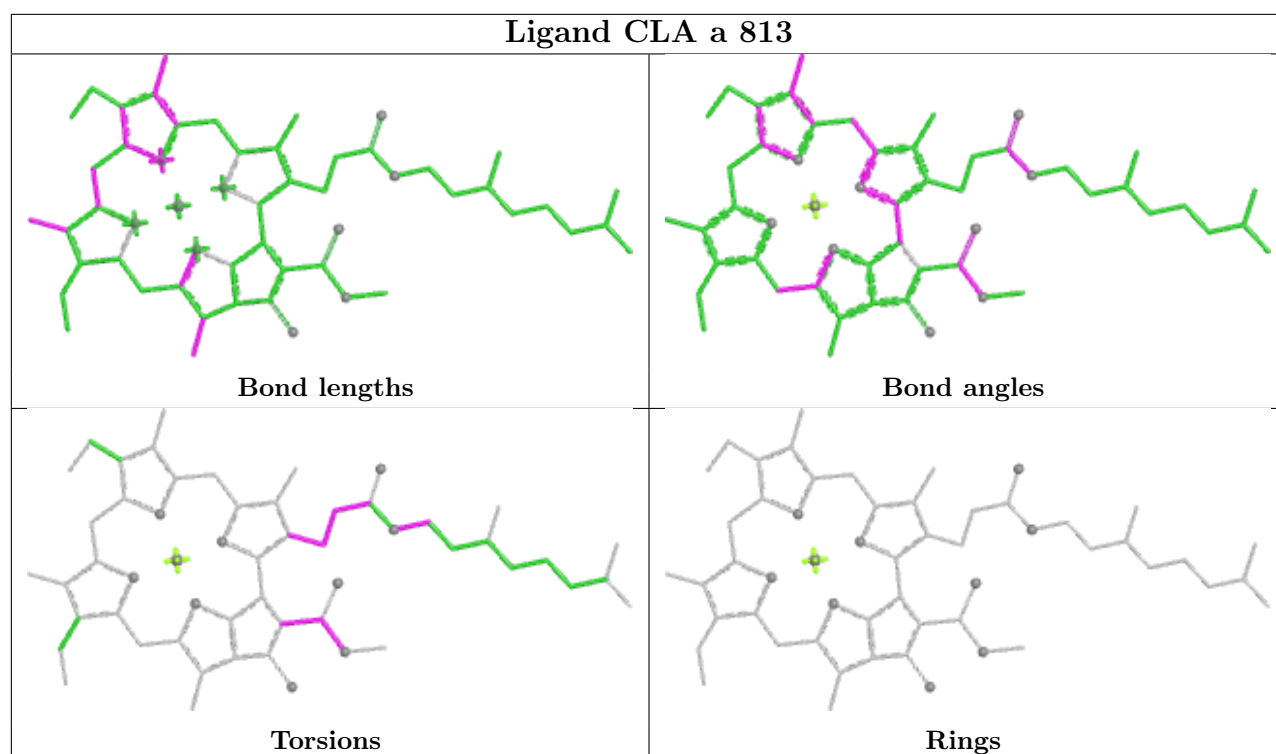


Ligand CLA a 812

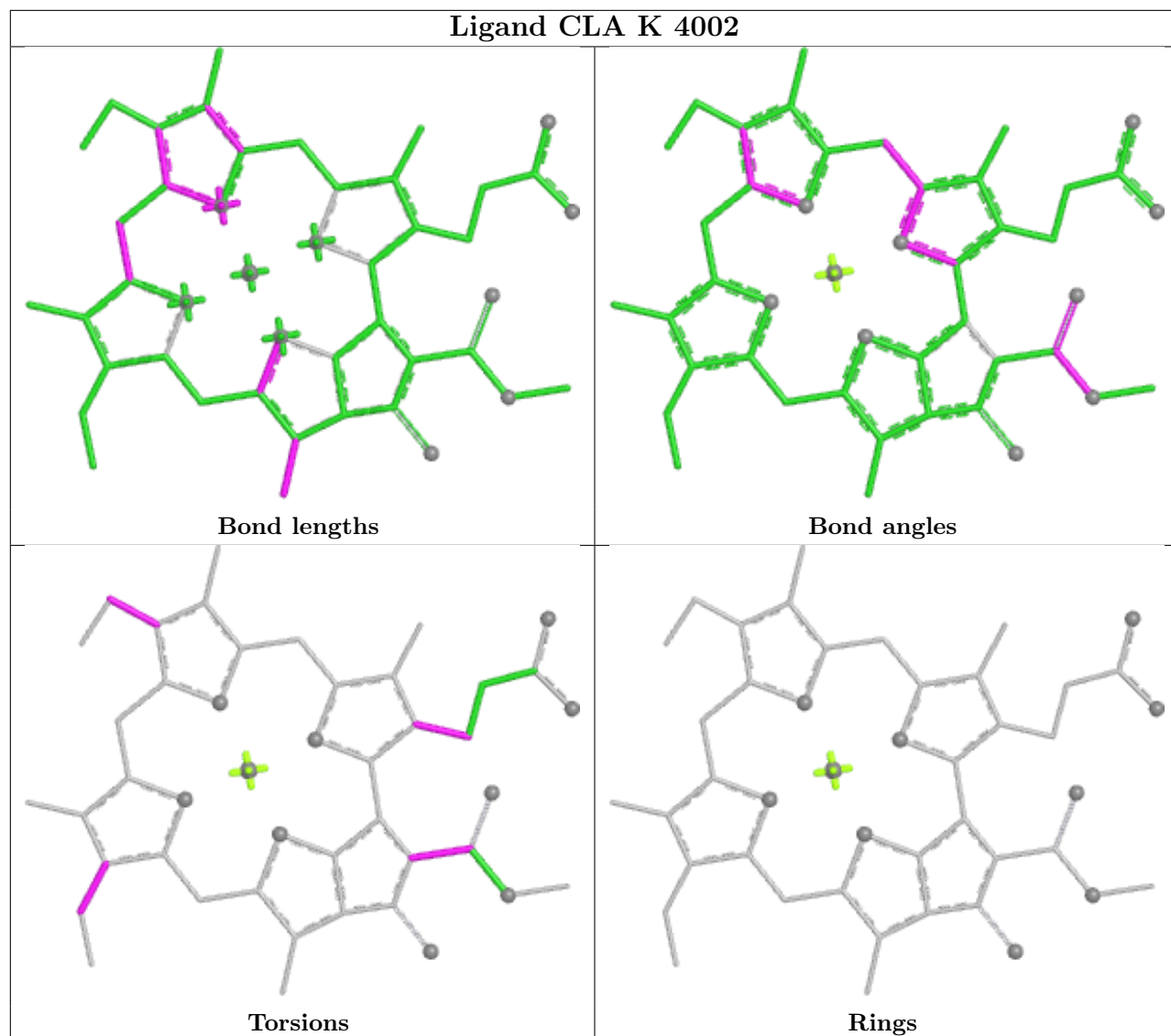


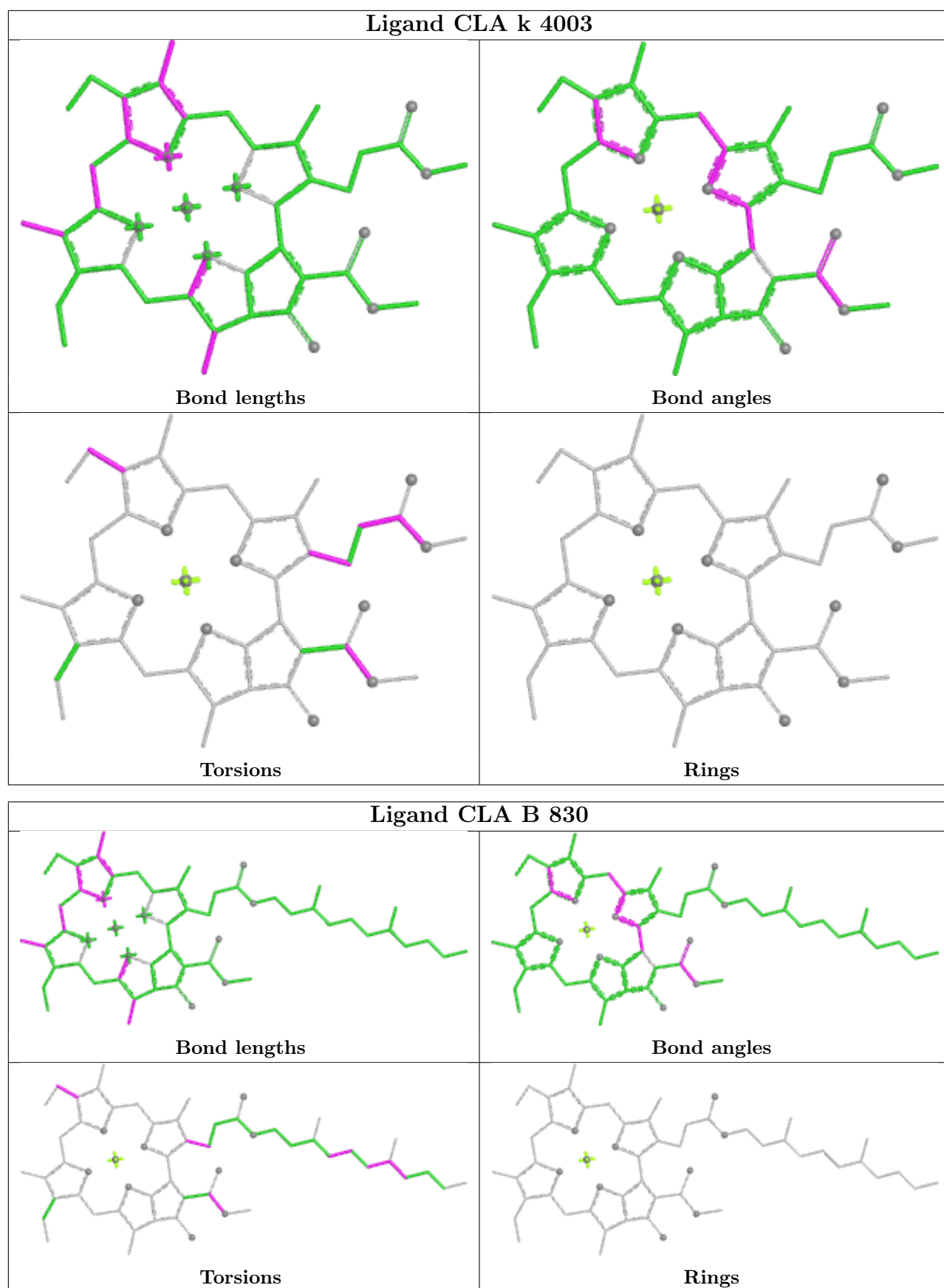
Ligand PQN A 843

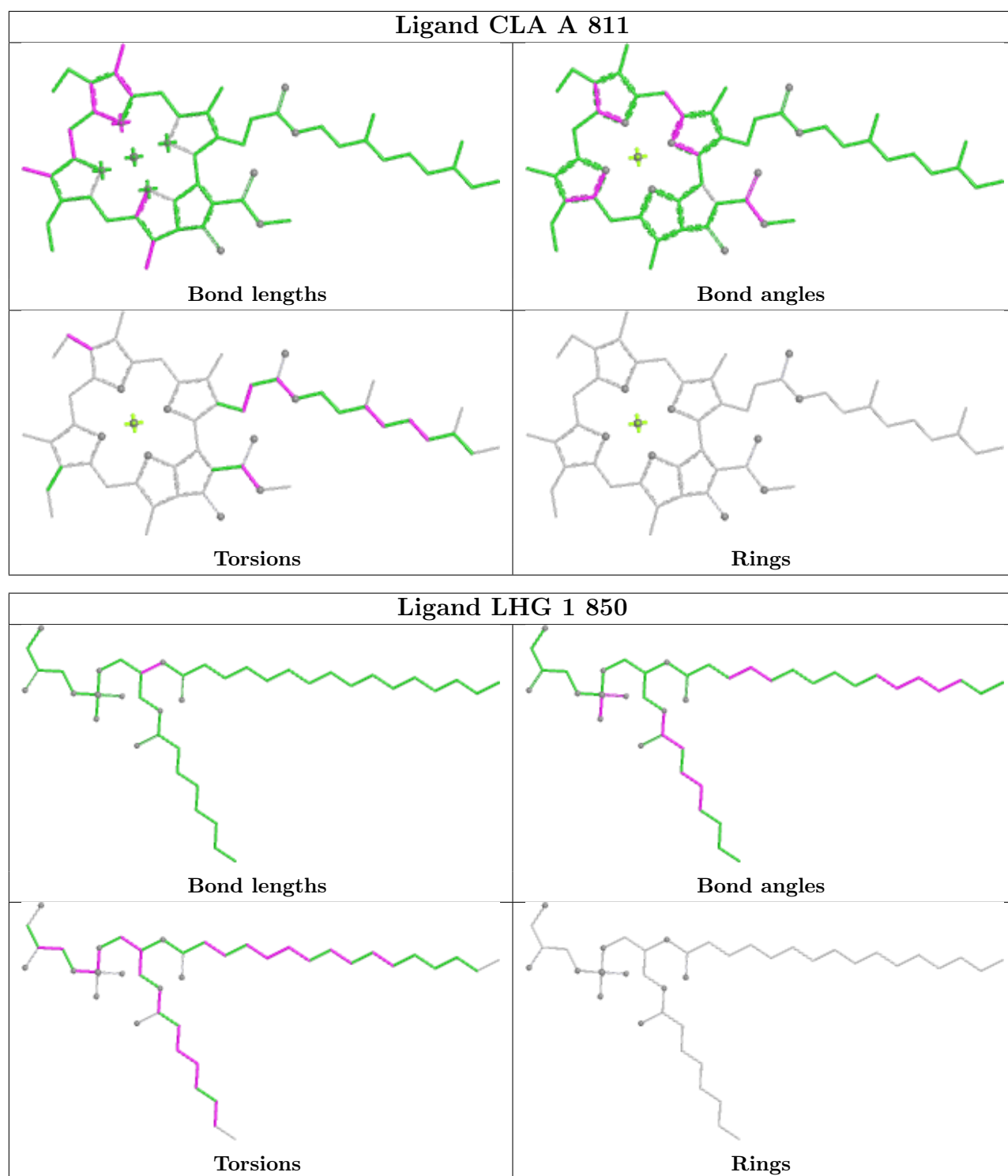


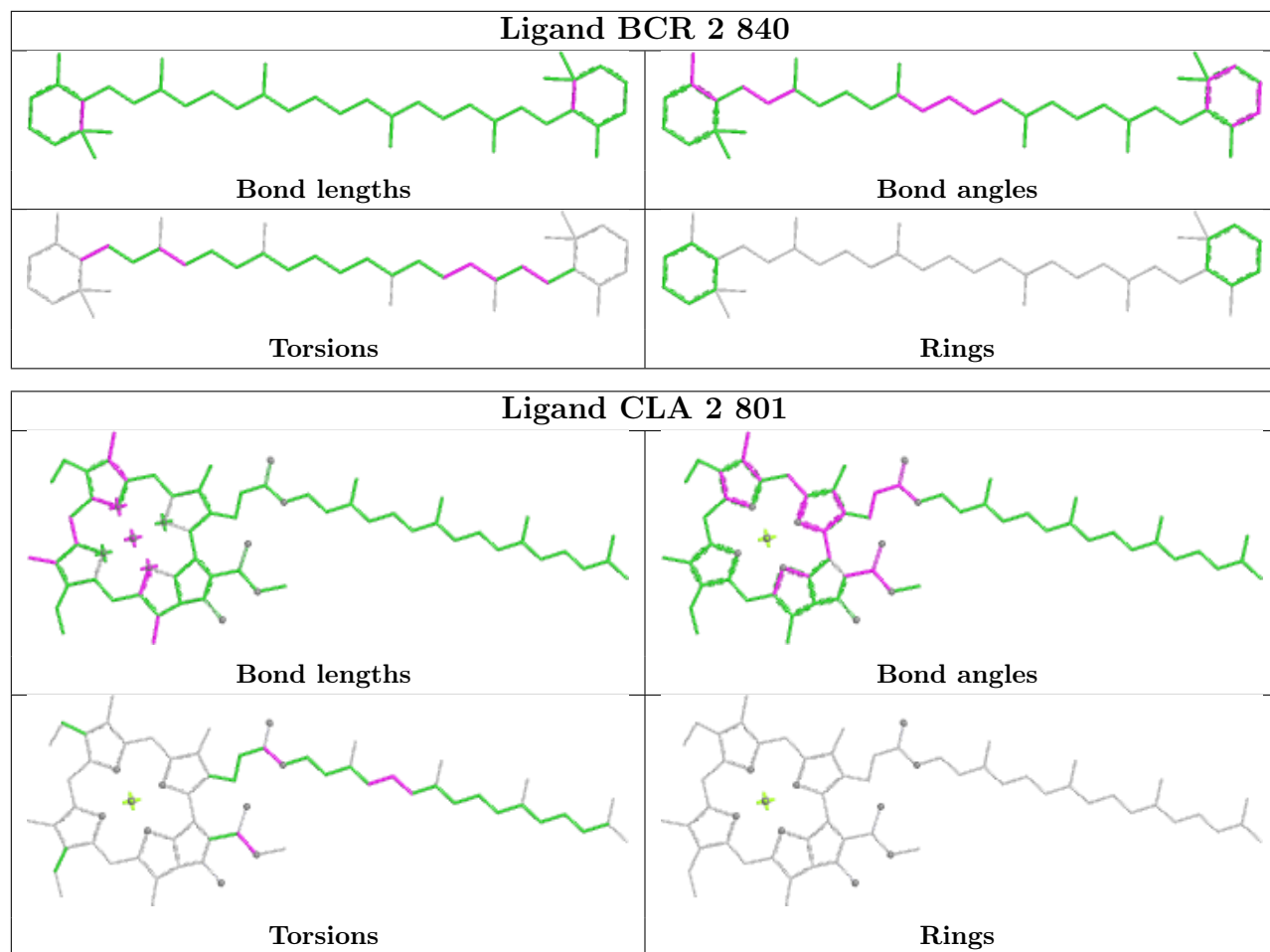


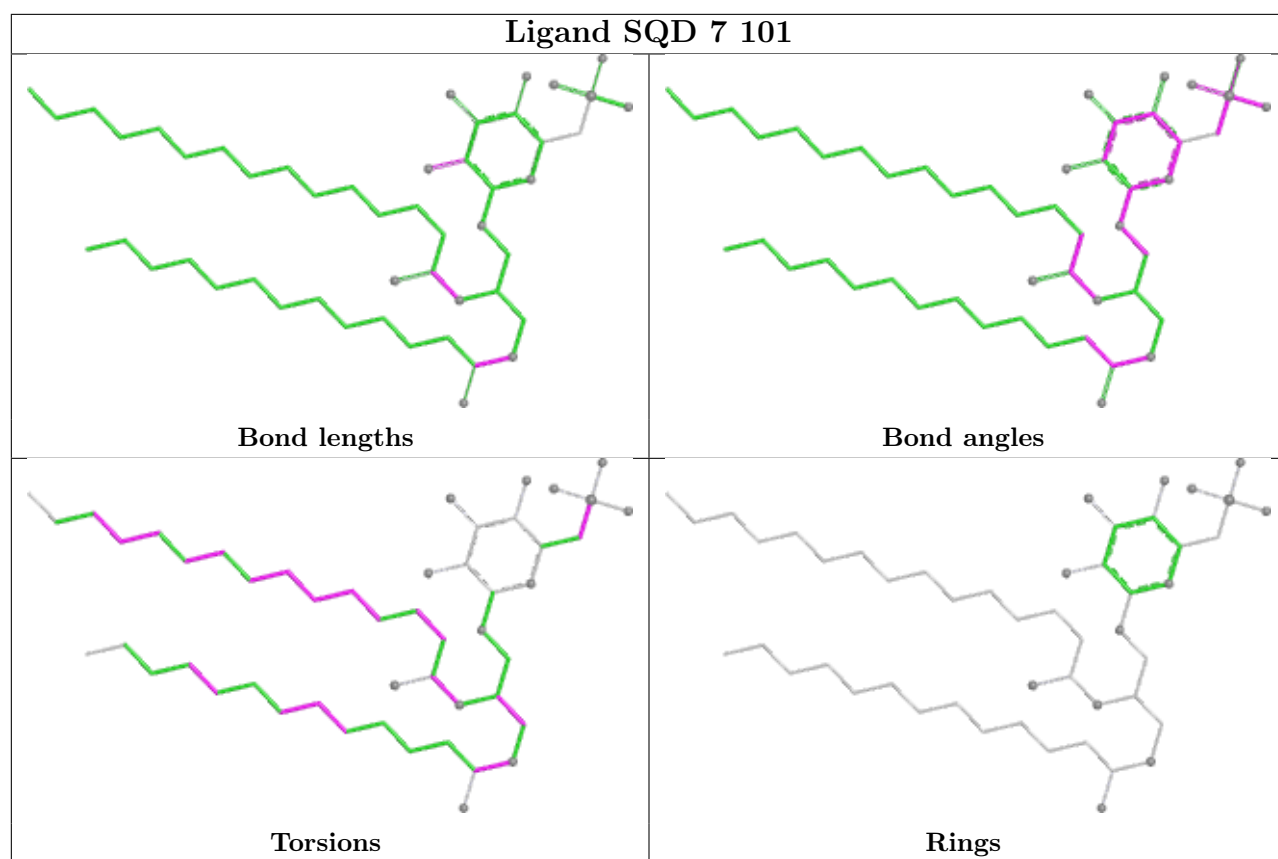
Ligand CLA K 4002



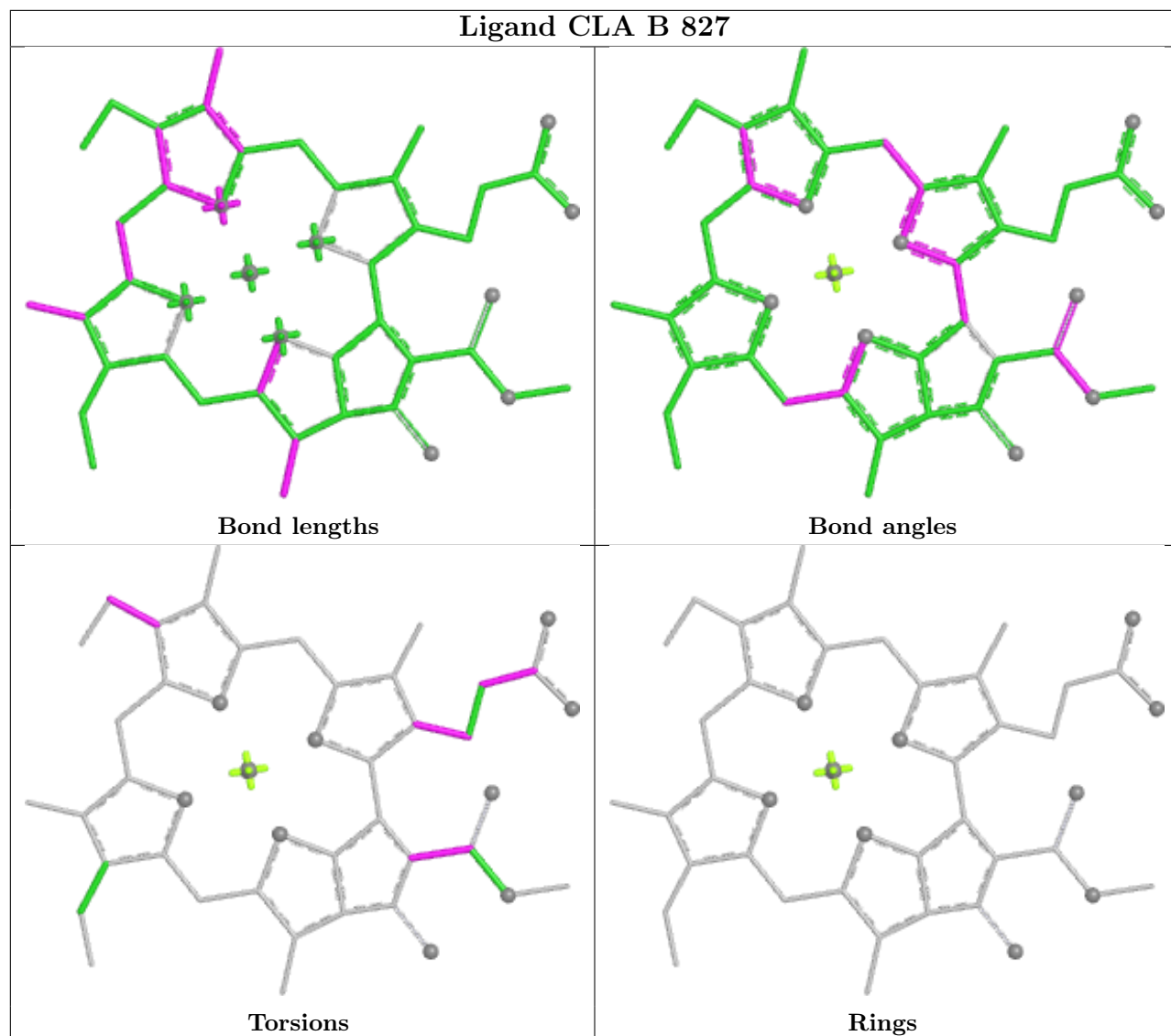




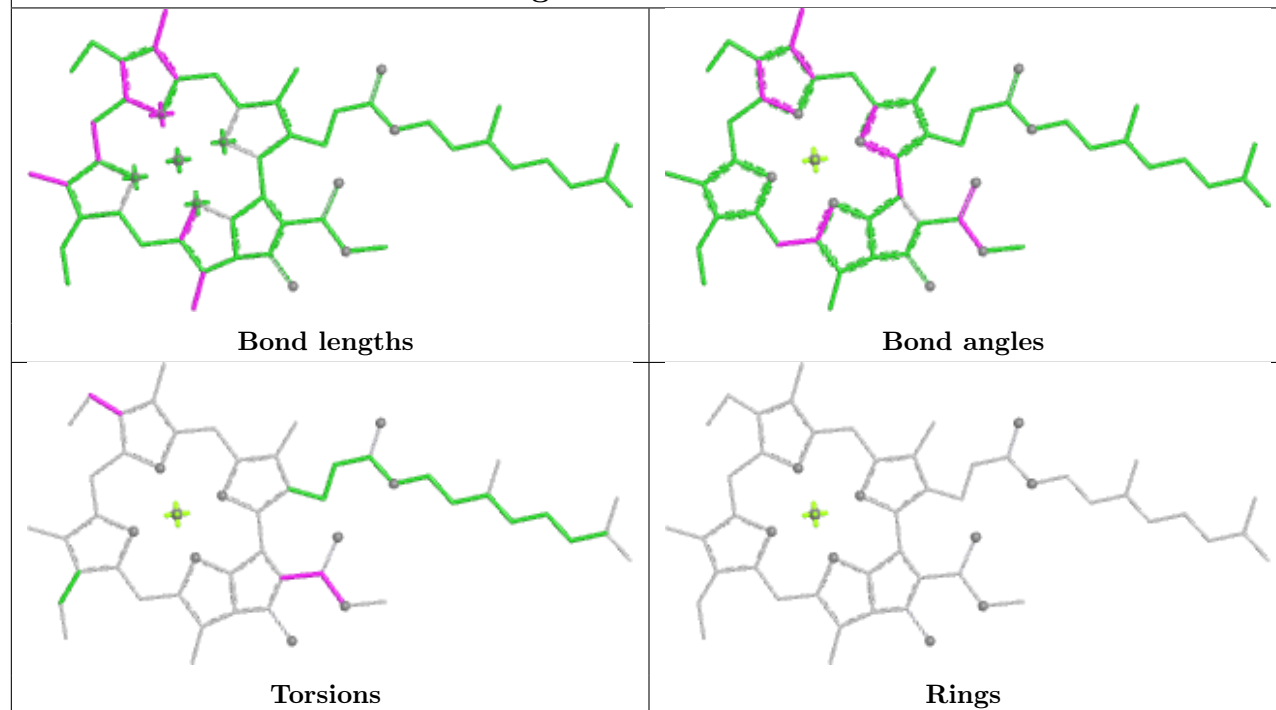




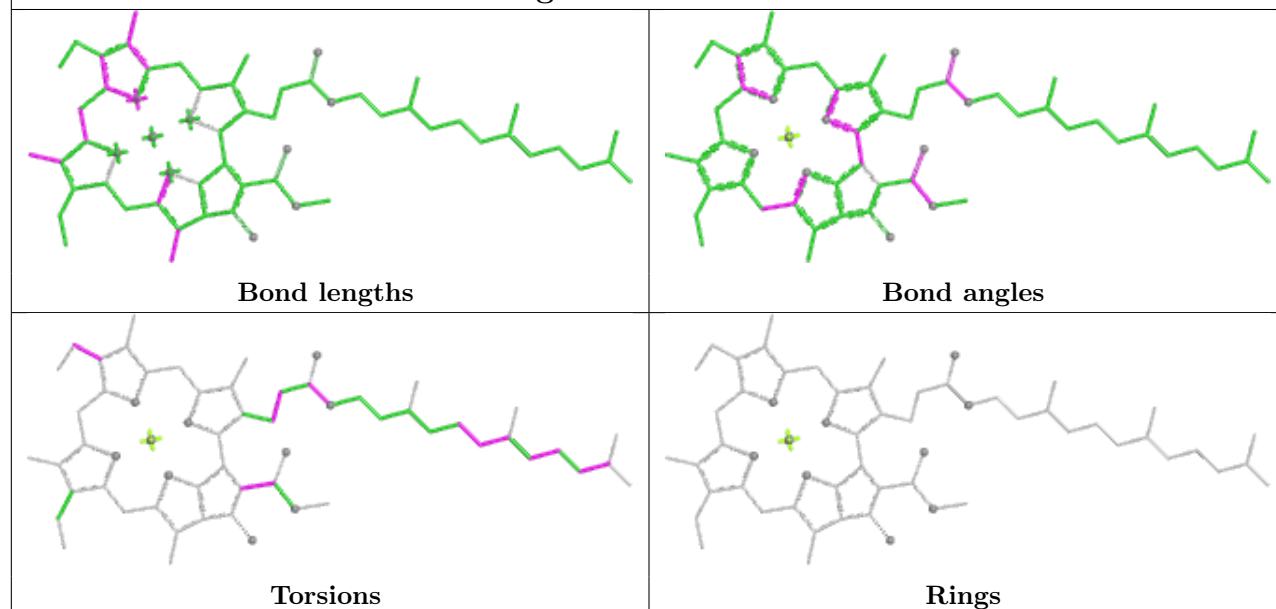
Ligand CLA B 827

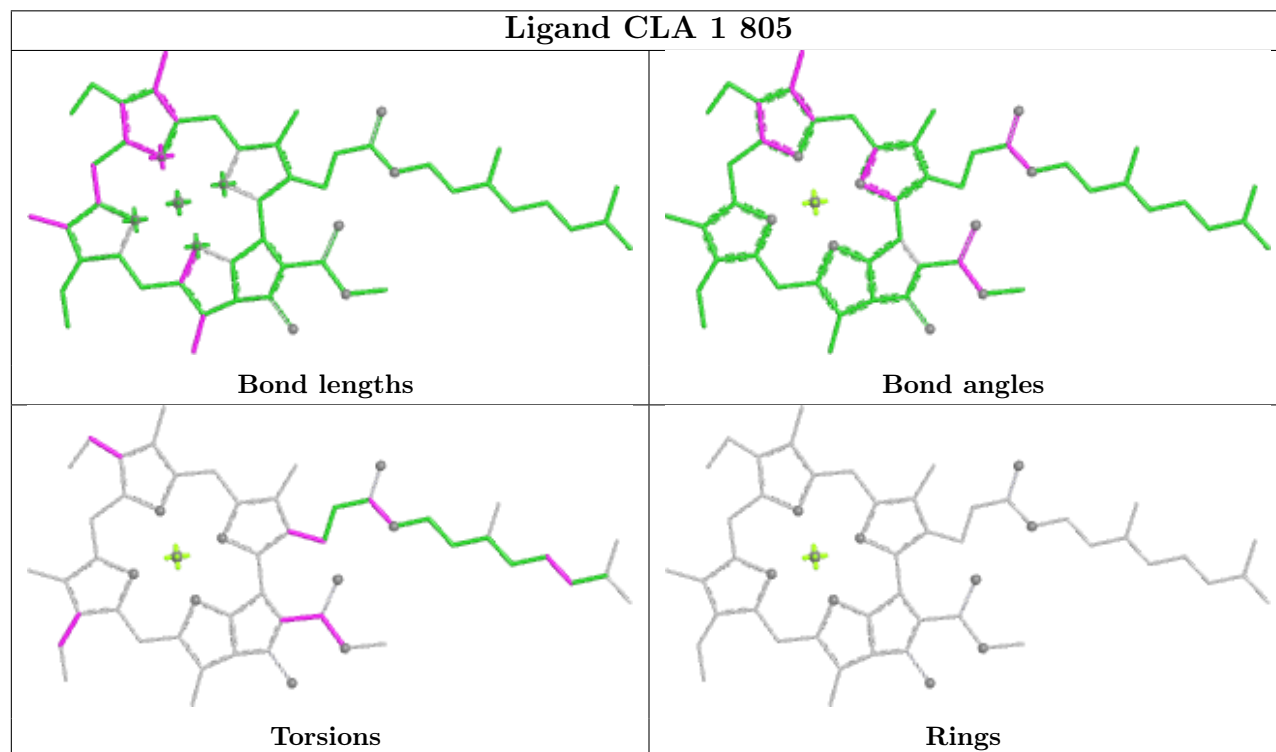
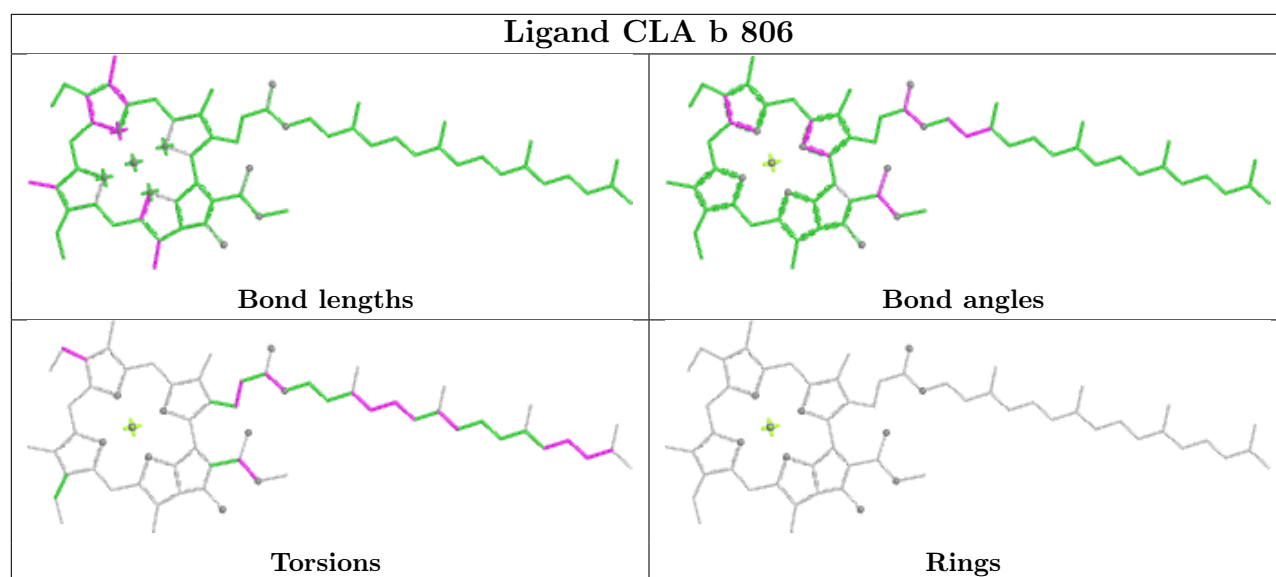


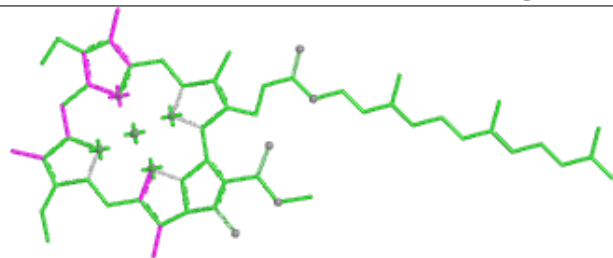
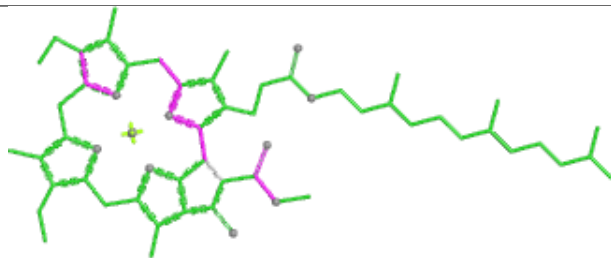
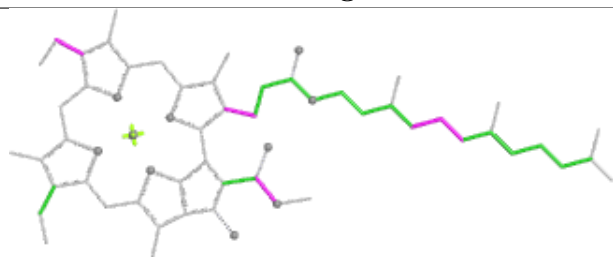
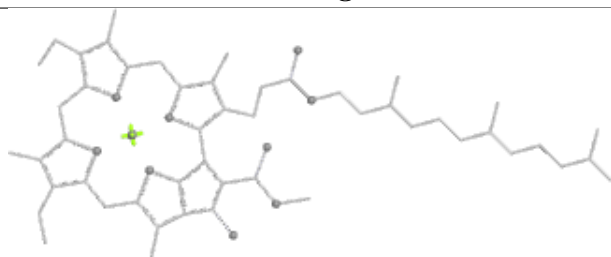
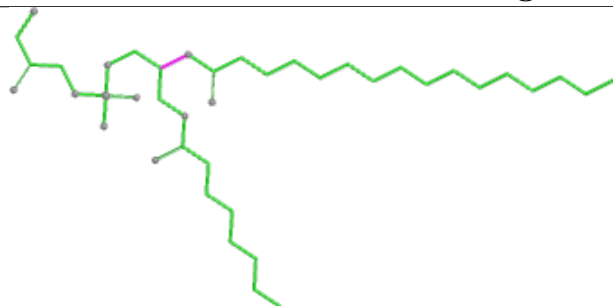
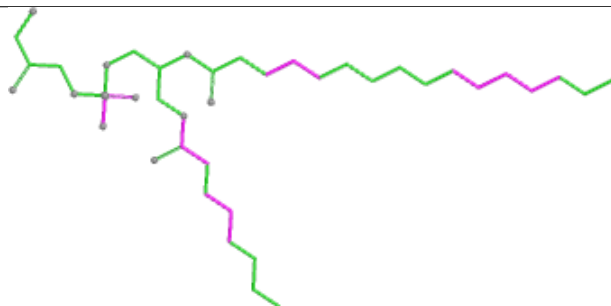
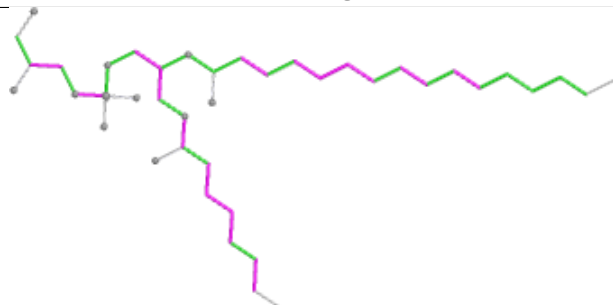
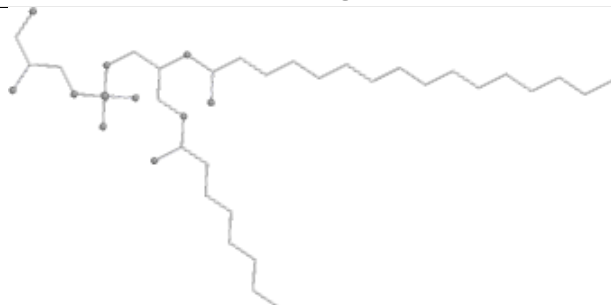
Ligand CLA A 807

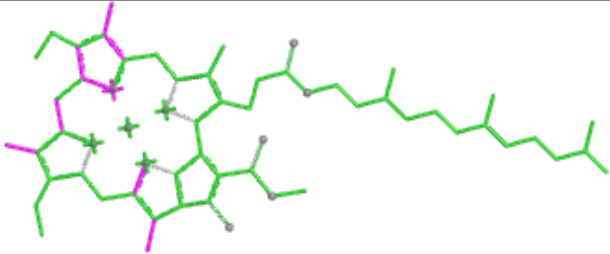
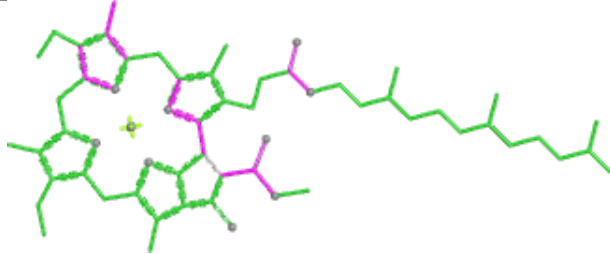
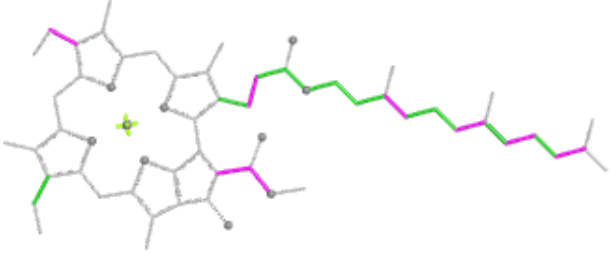
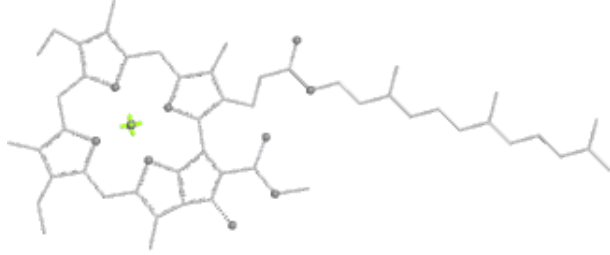
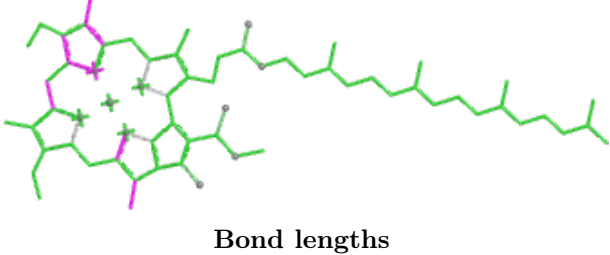
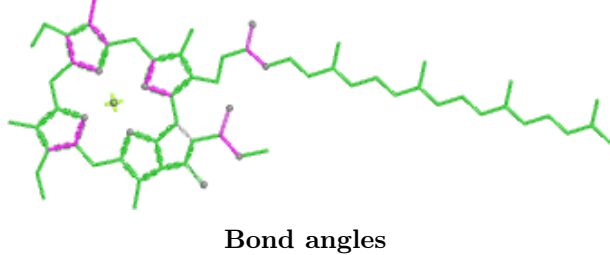
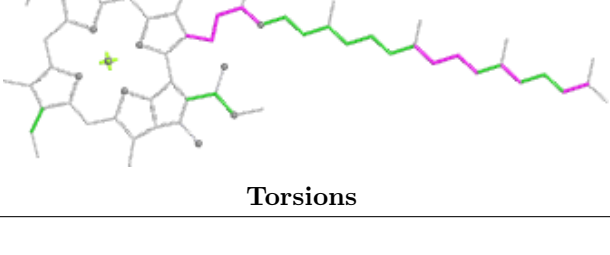
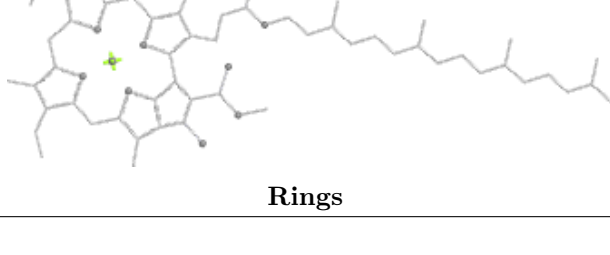


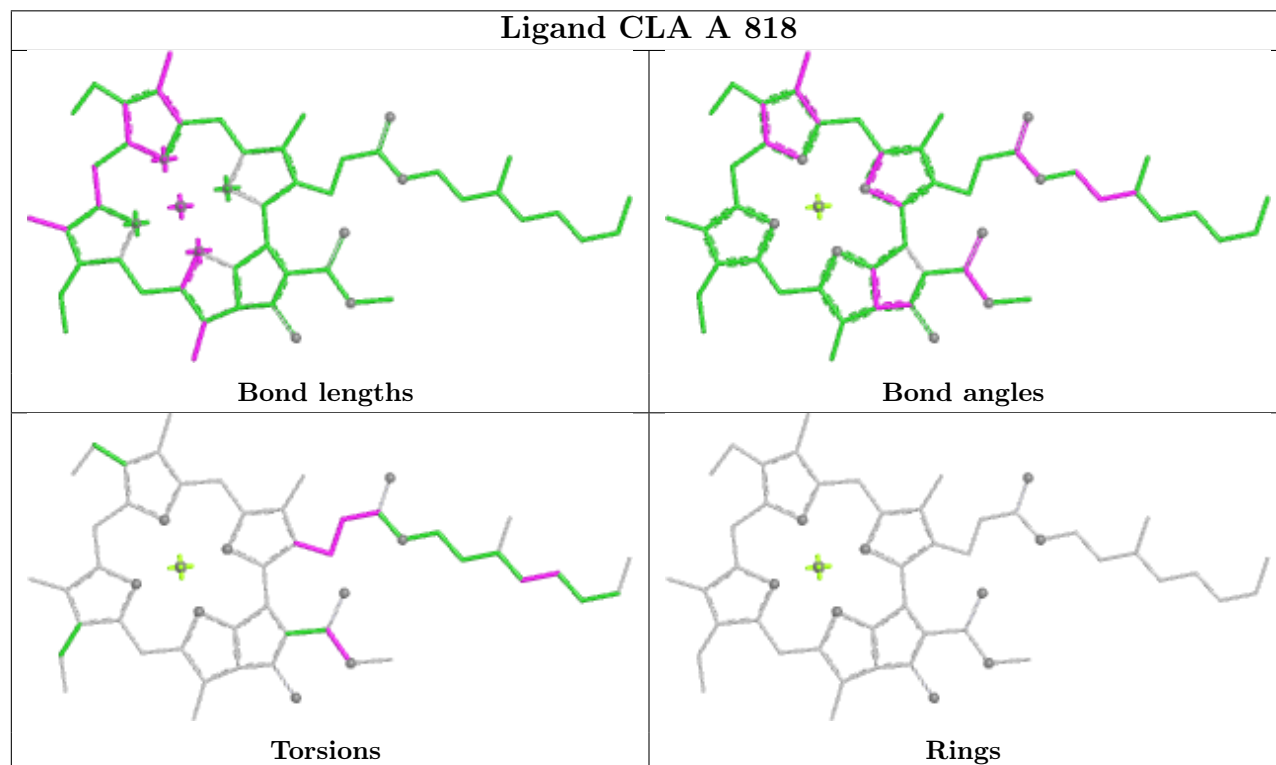
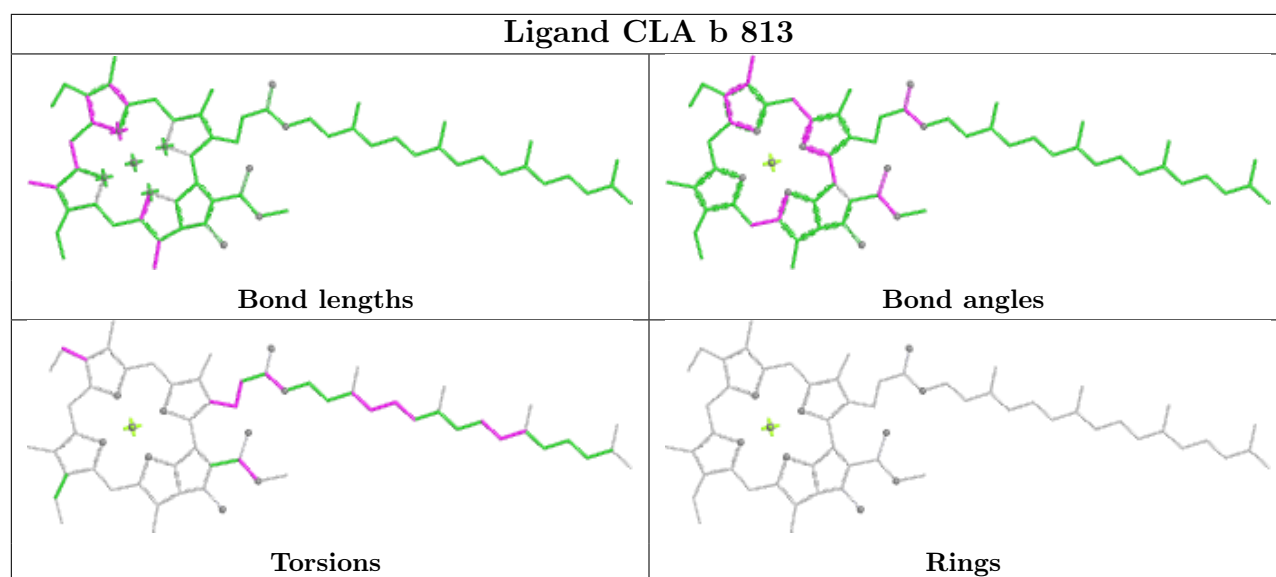
Ligand CLA a 852



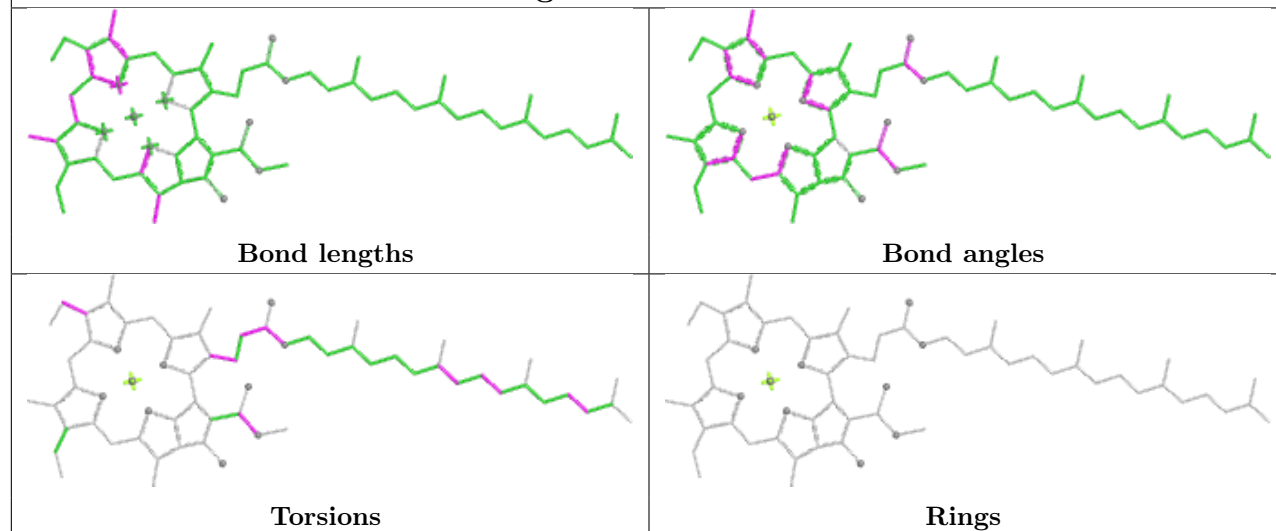


Ligand CLA 2 815**Bond lengths****Bond angles****Torsions****Rings****Ligand LHG a 850****Bond lengths****Bond angles****Torsions****Rings**

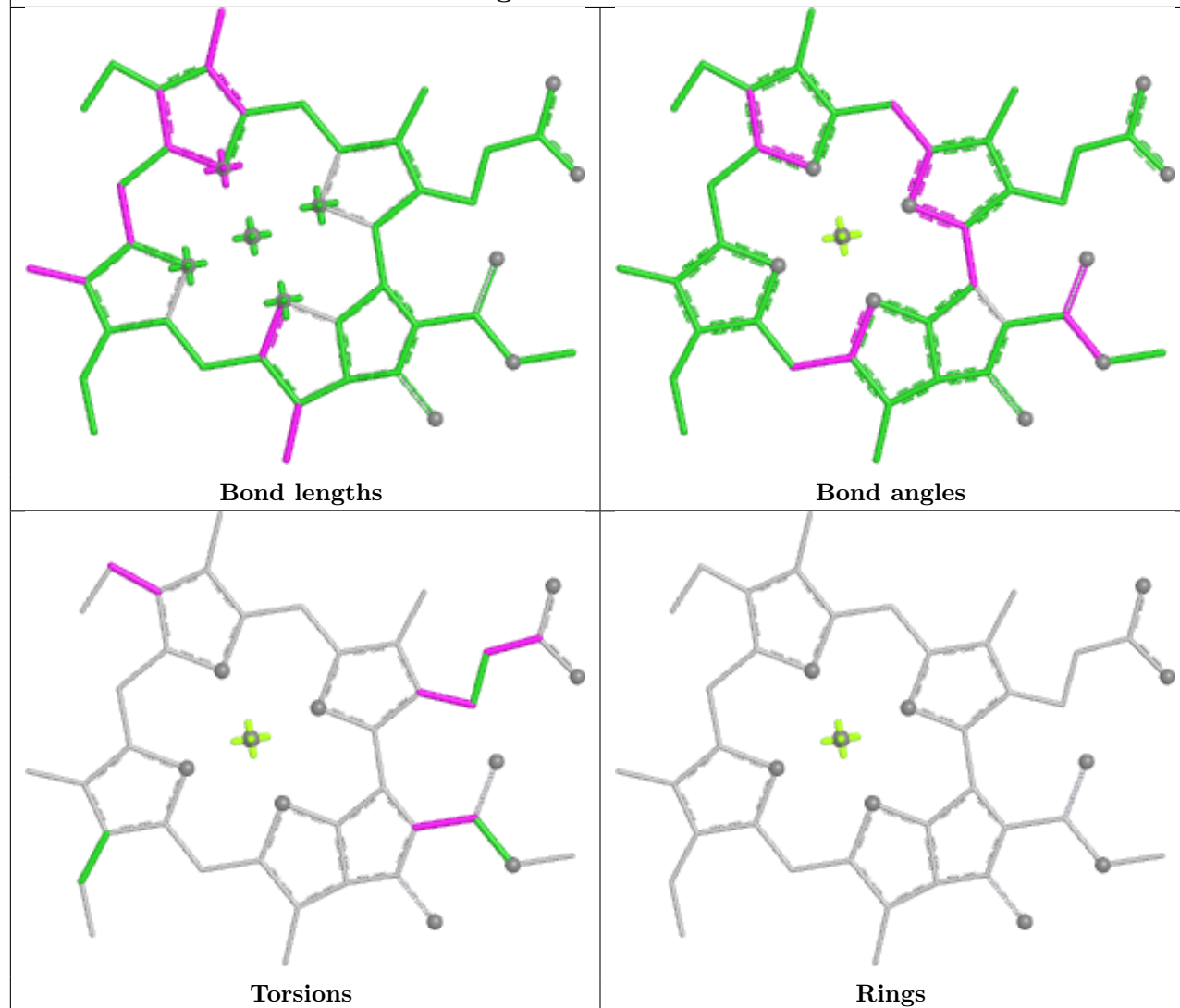
Ligand CLA A 819	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 7 102	
 Bond lengths	 Bond angles
 Torsions	 Rings



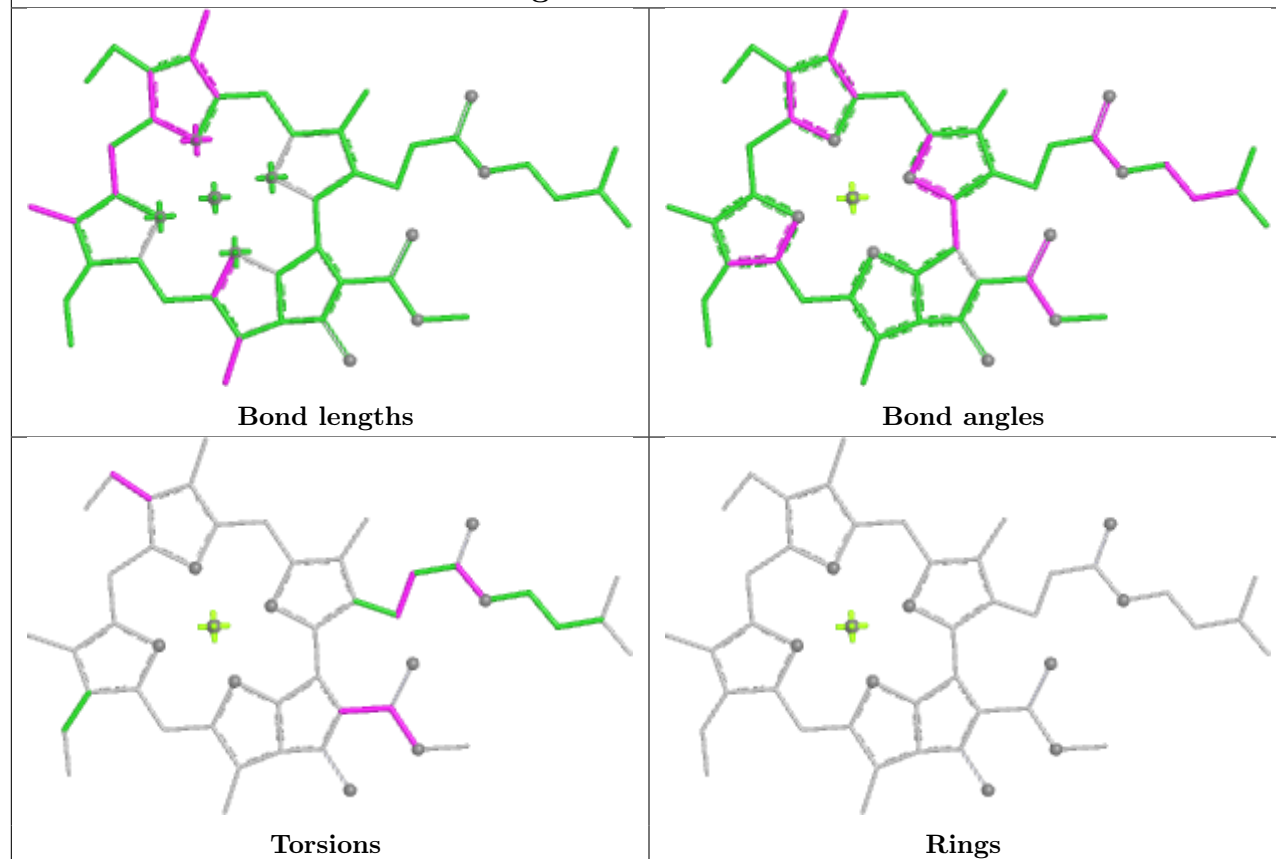
Ligand CLA 1 806



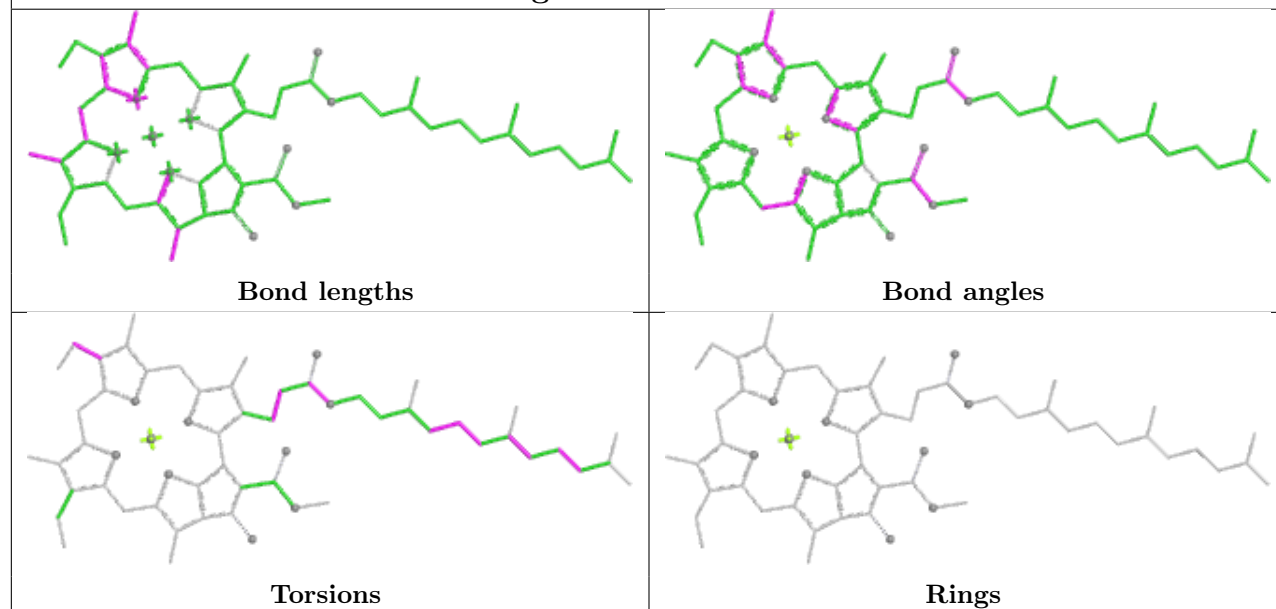
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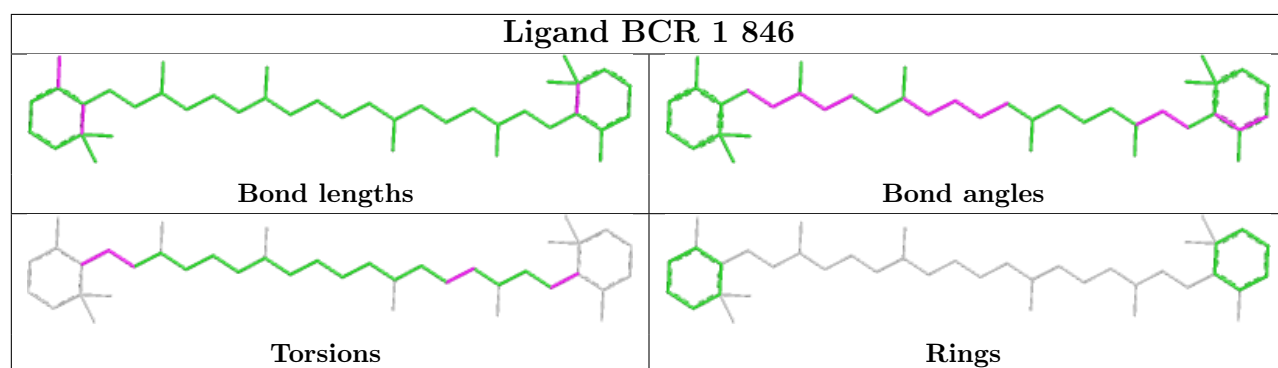
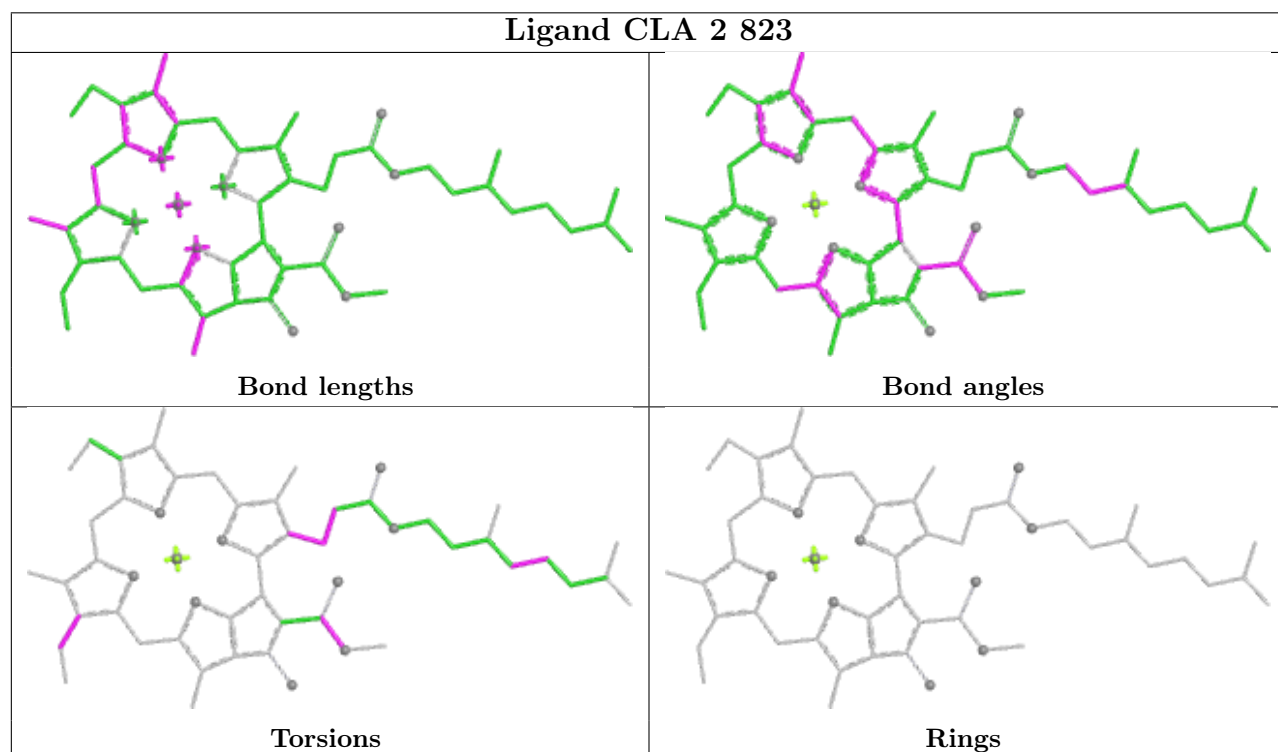
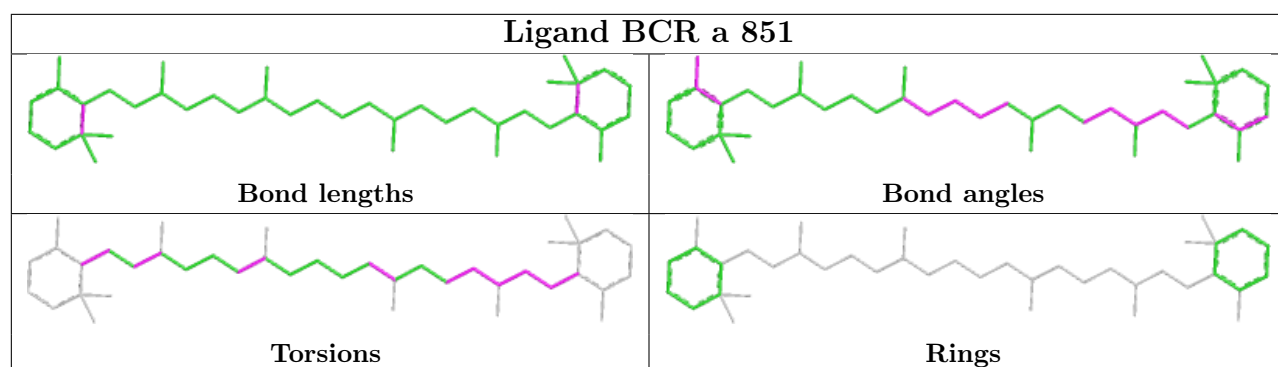


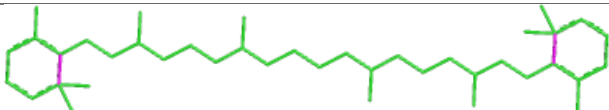
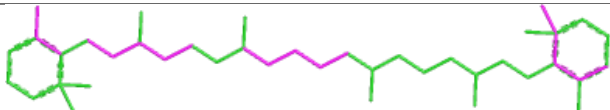
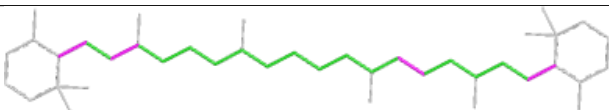
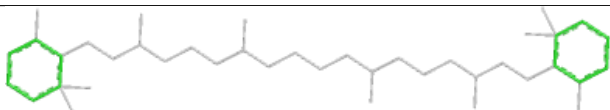
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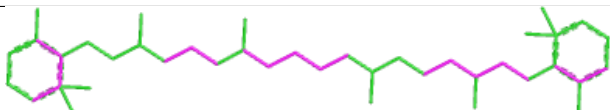
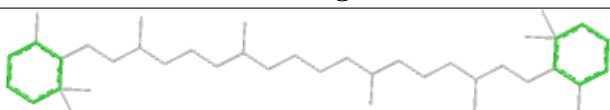


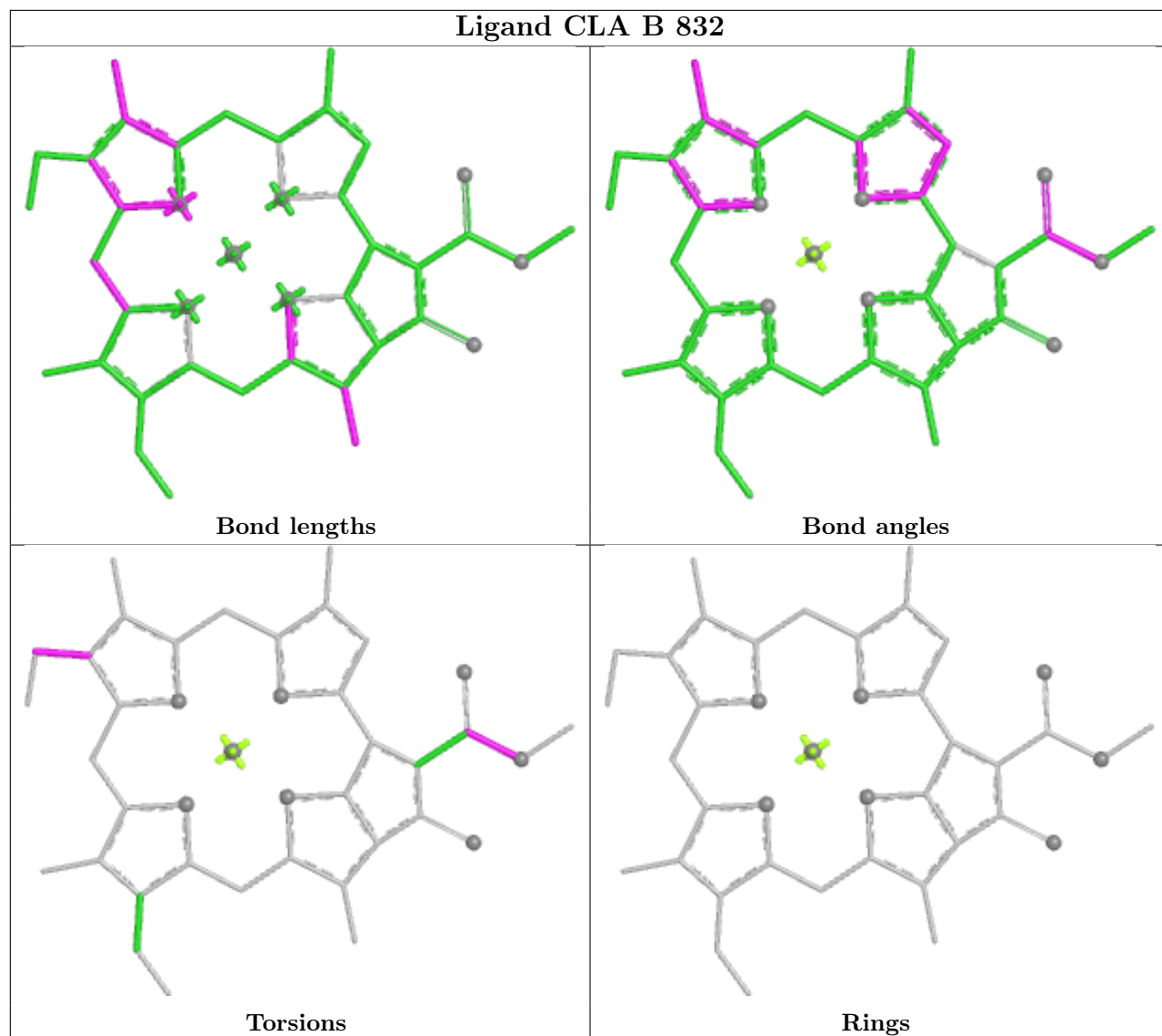
Ligand CLA A 837



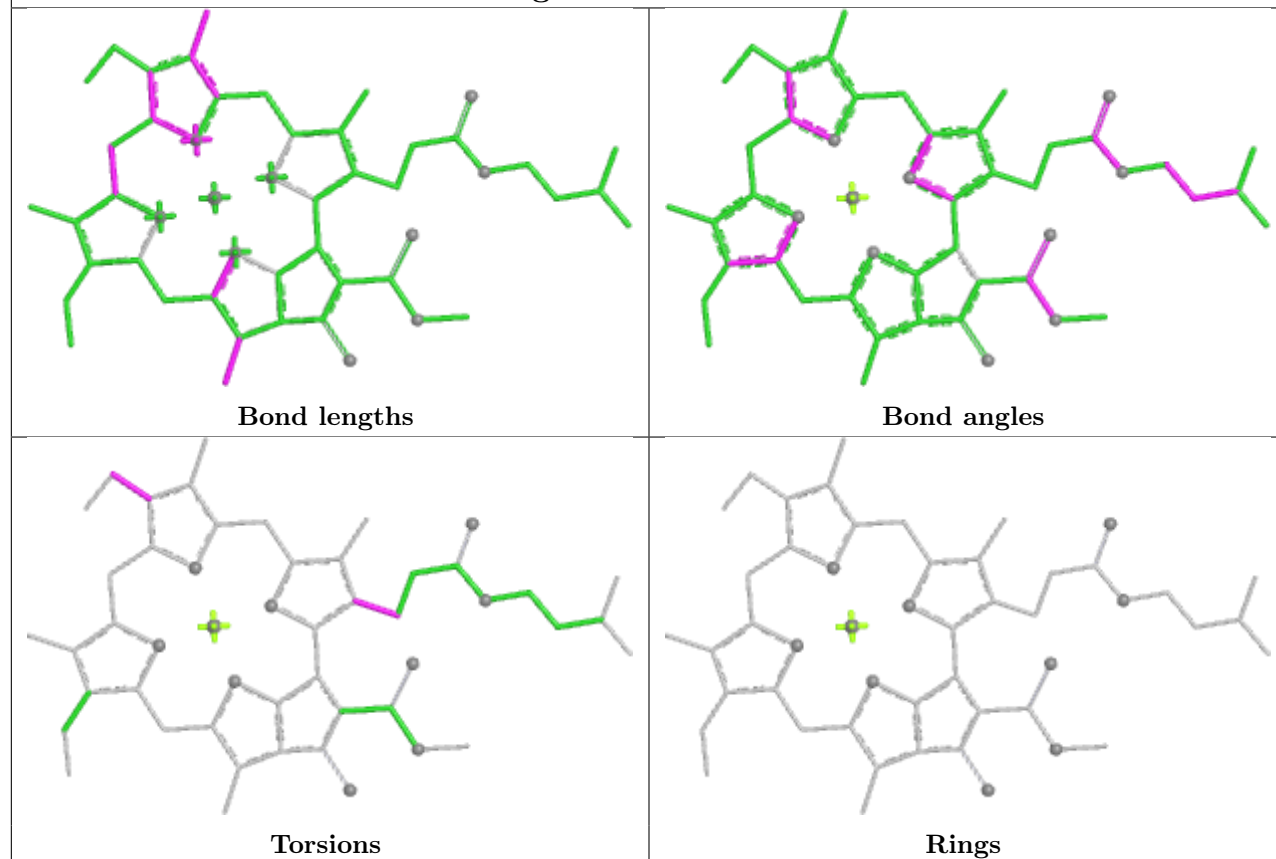


Ligand BCR L 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

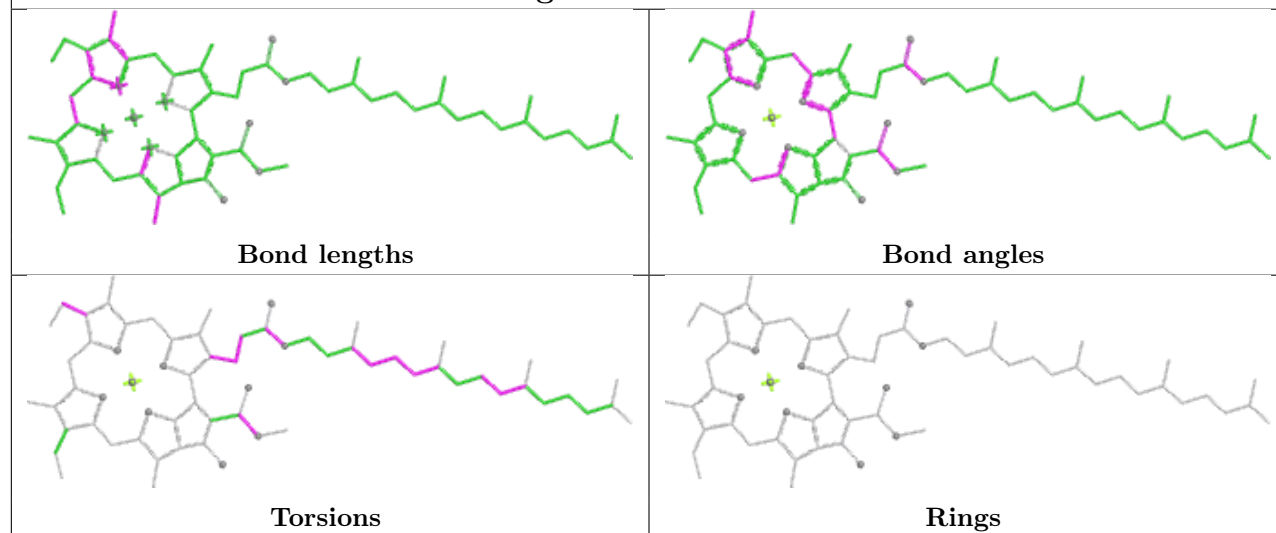
Ligand BCR L 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

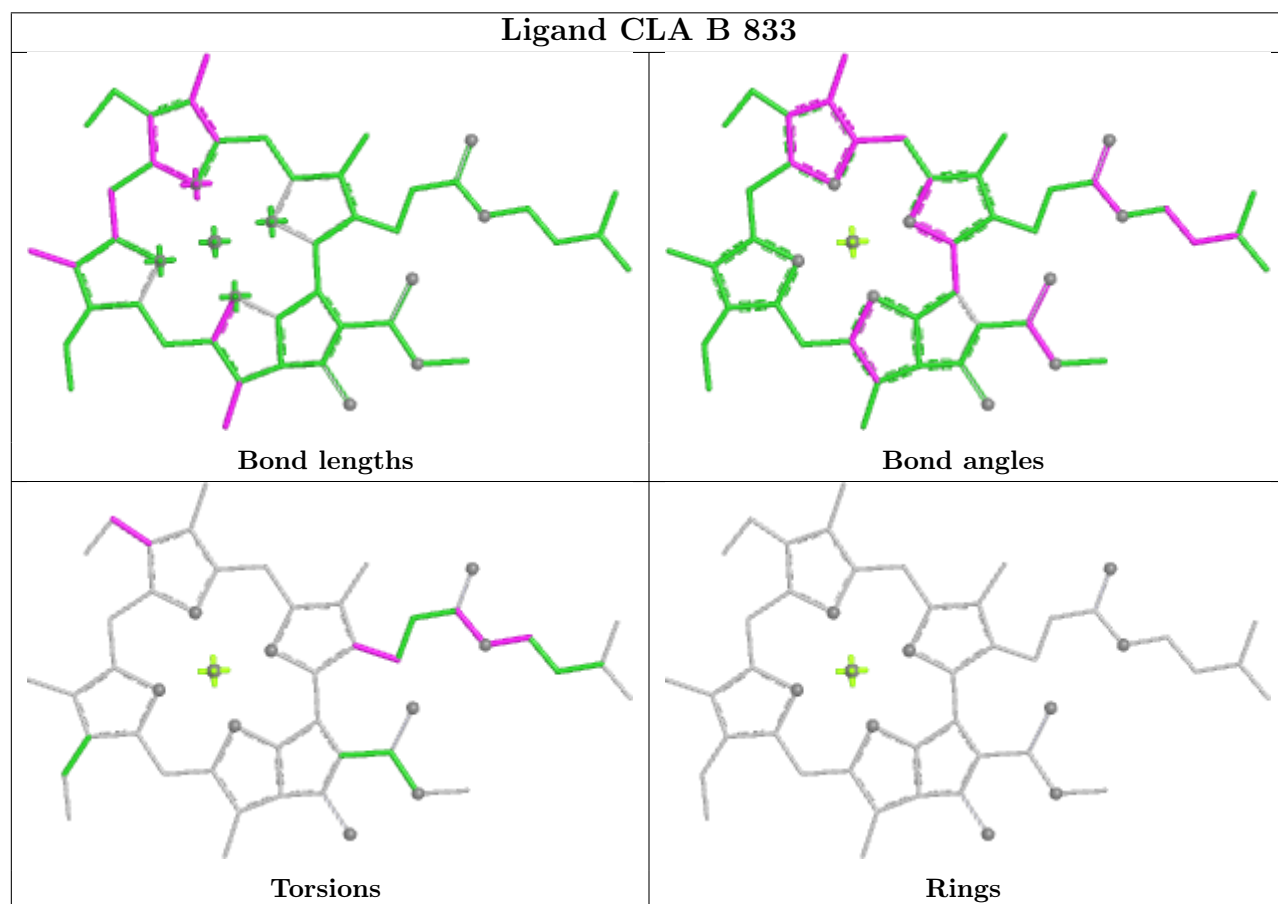
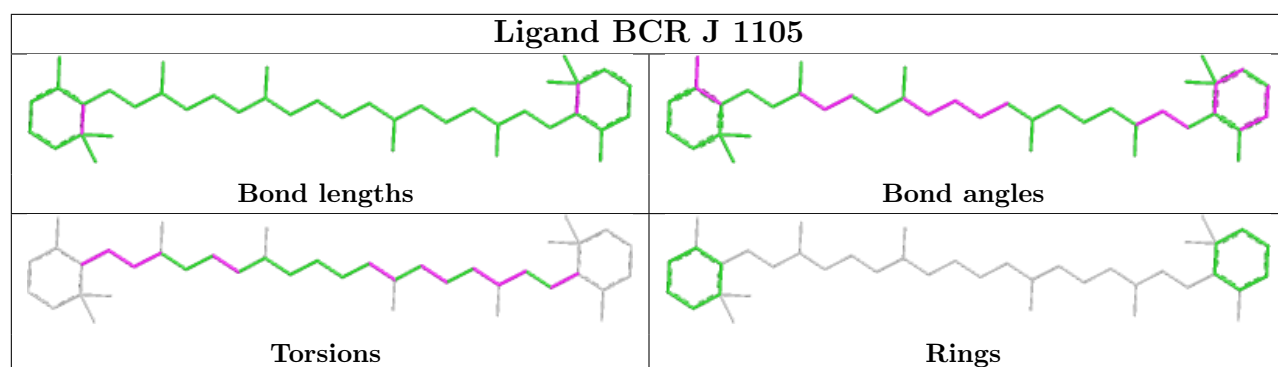


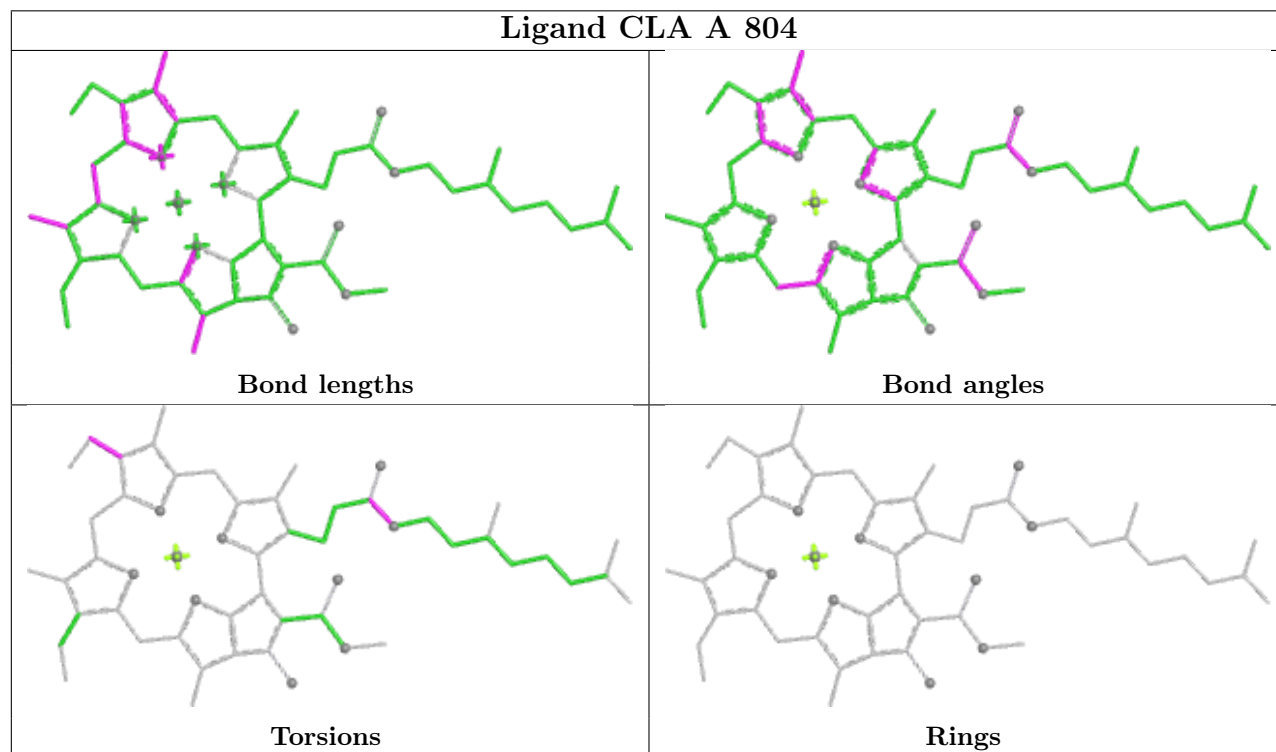
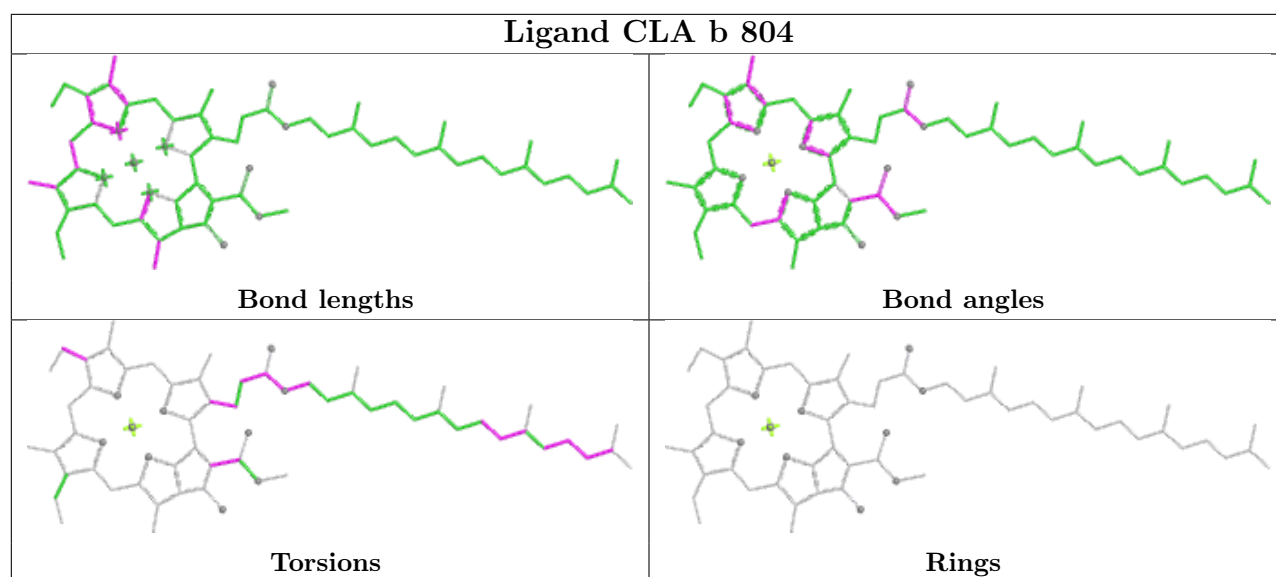
Ligand CLA B 835



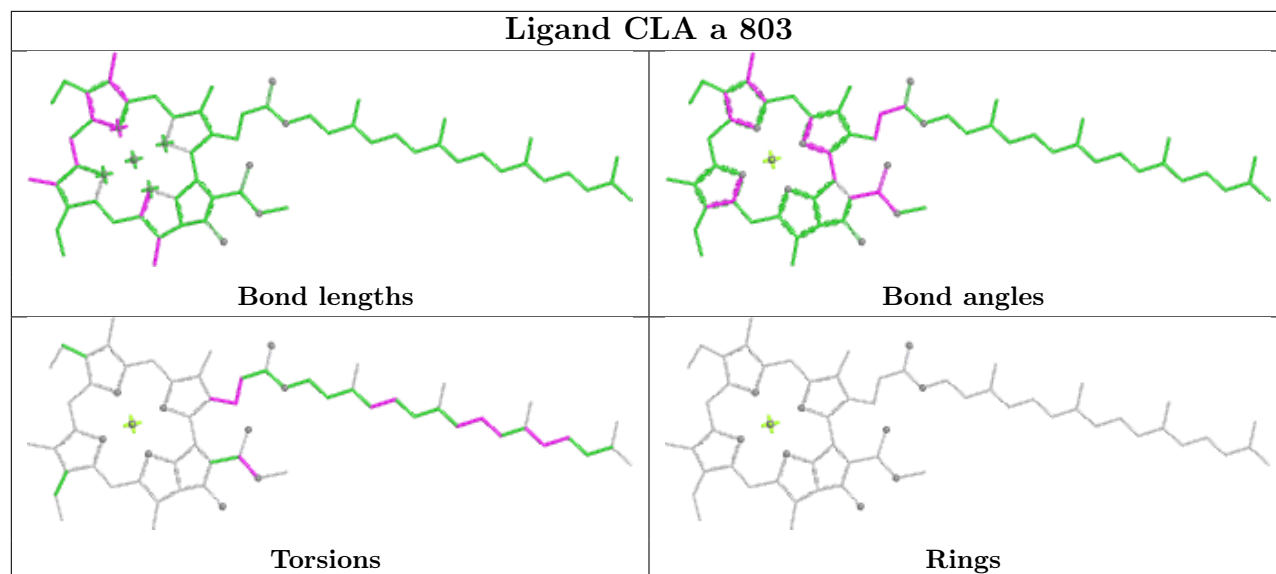
Ligand CLA 2 812



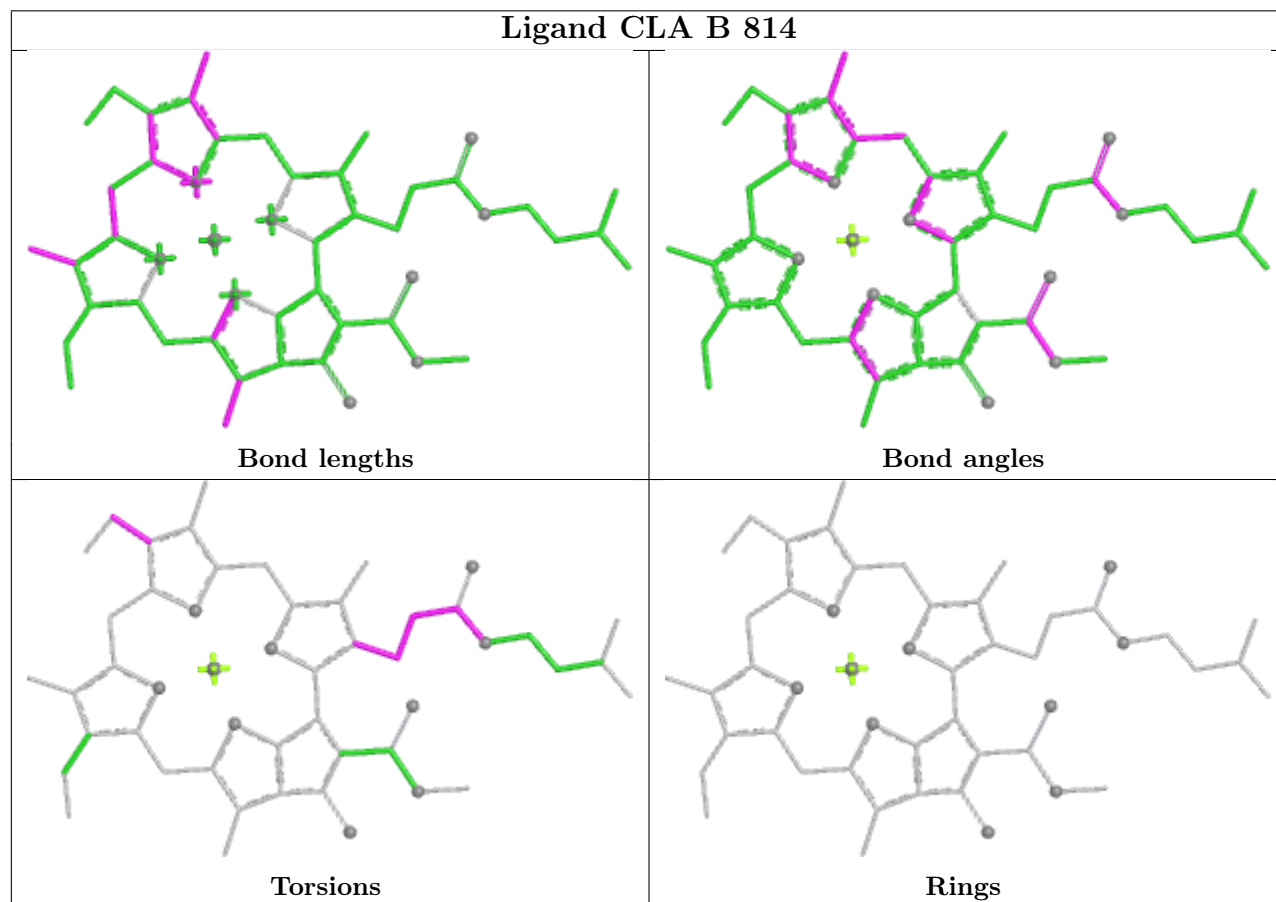


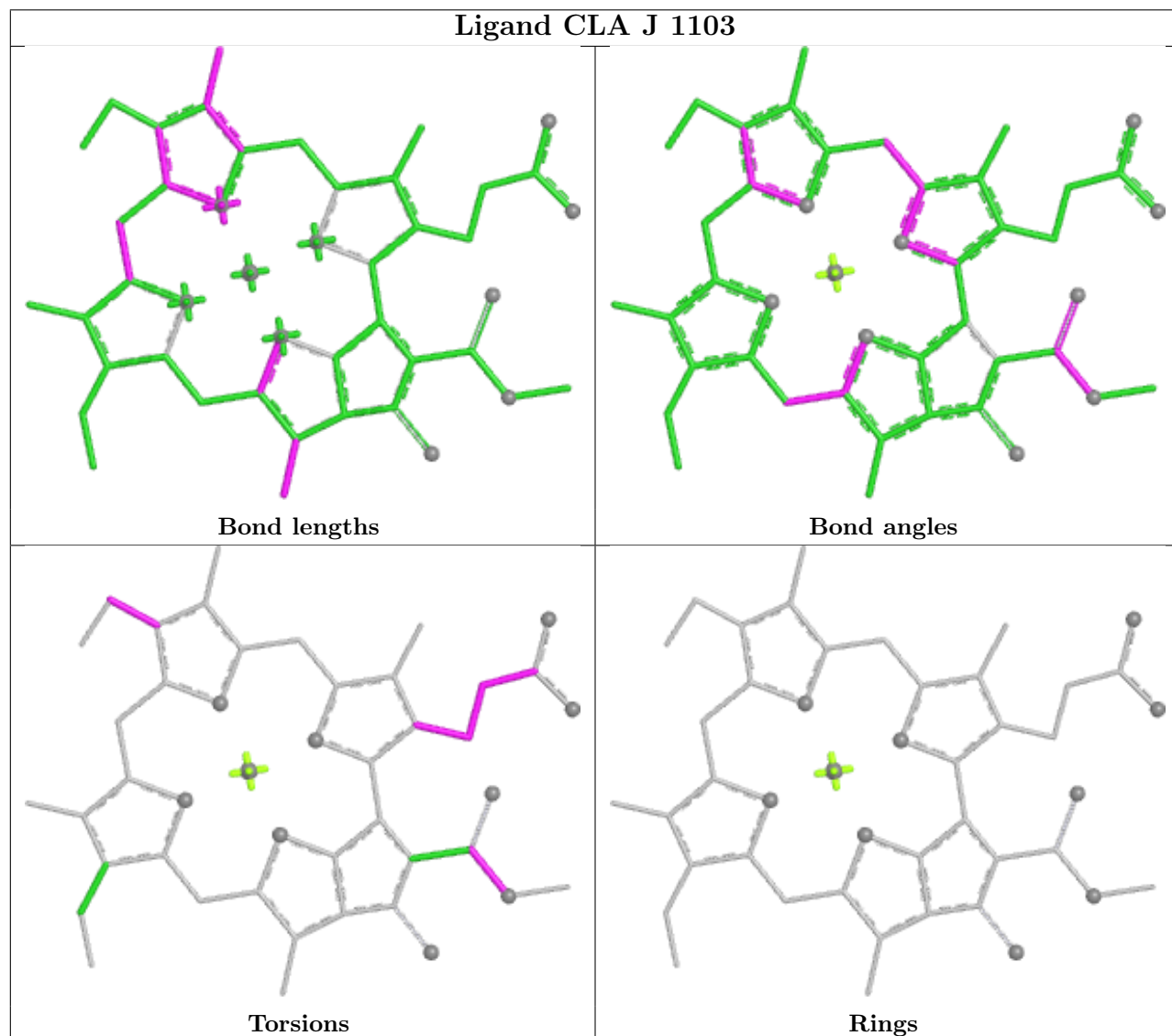
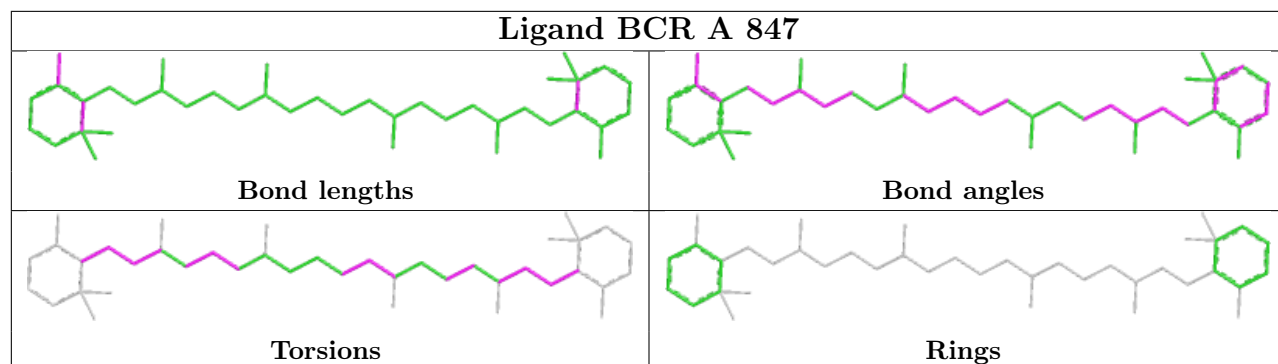


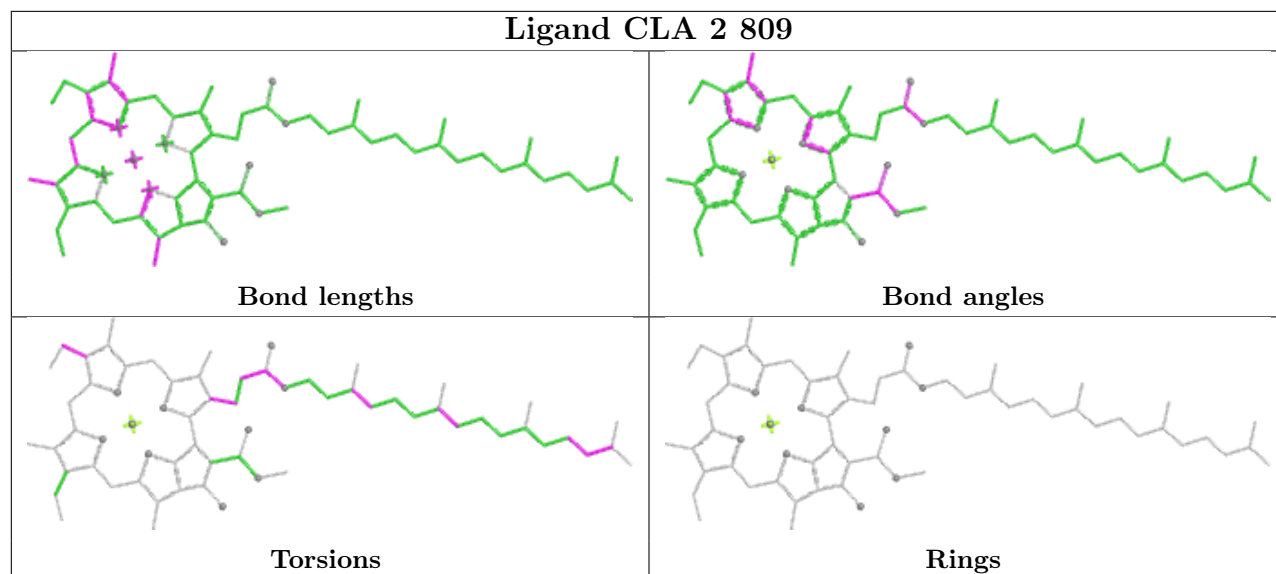
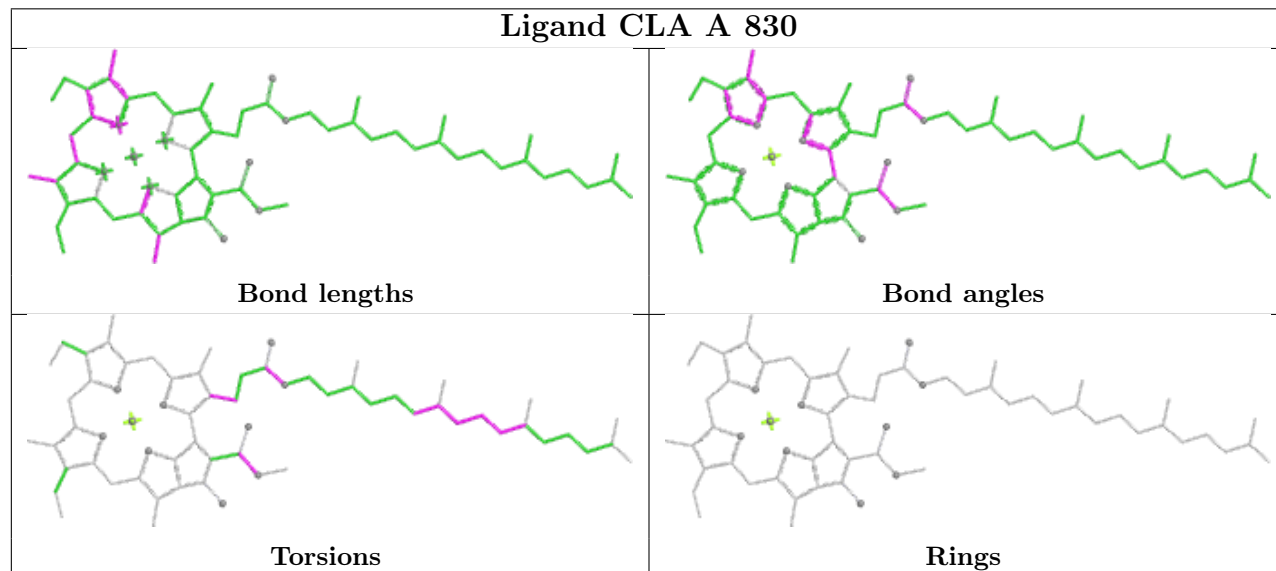
Ligand CLA a 803

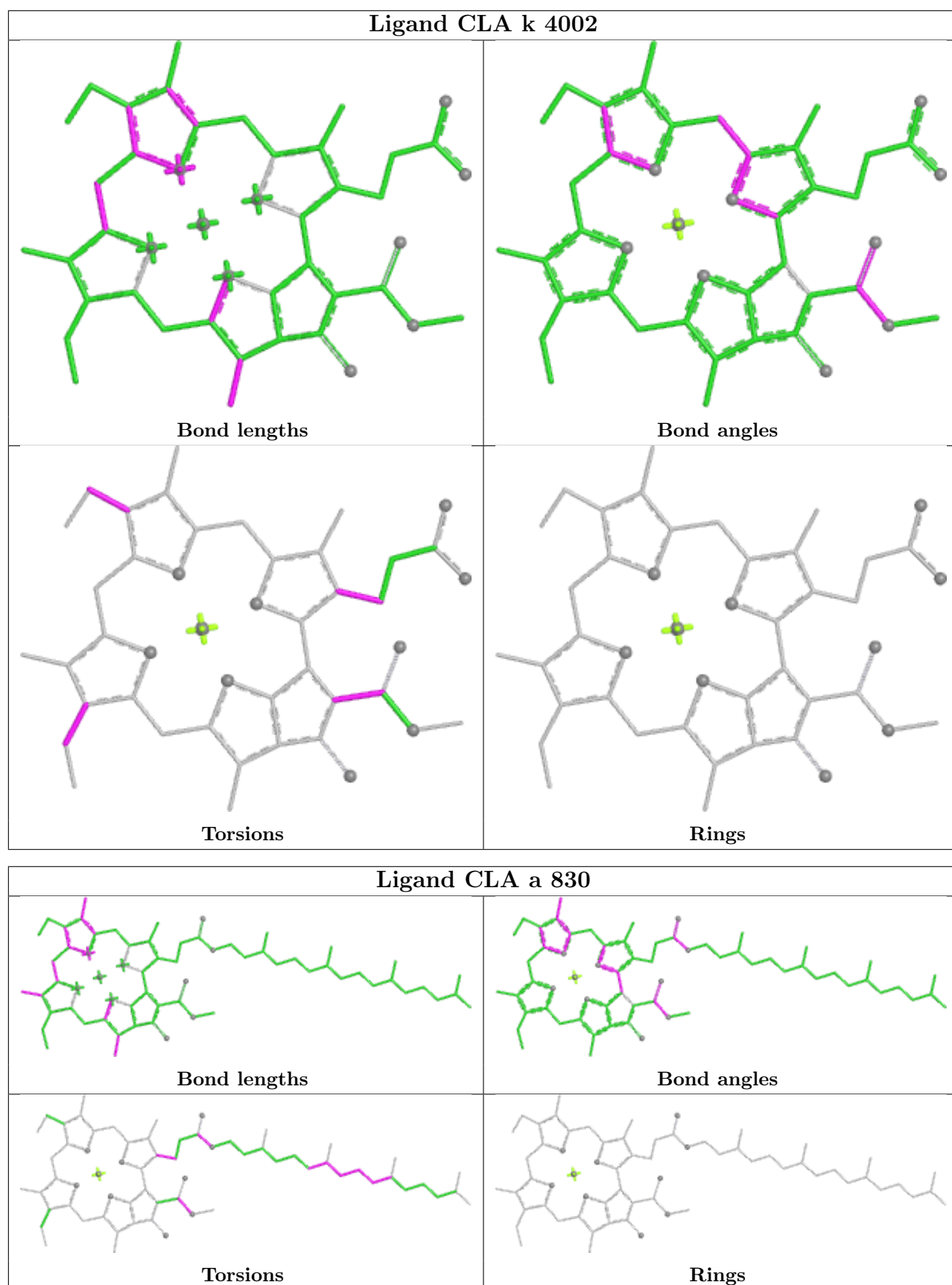


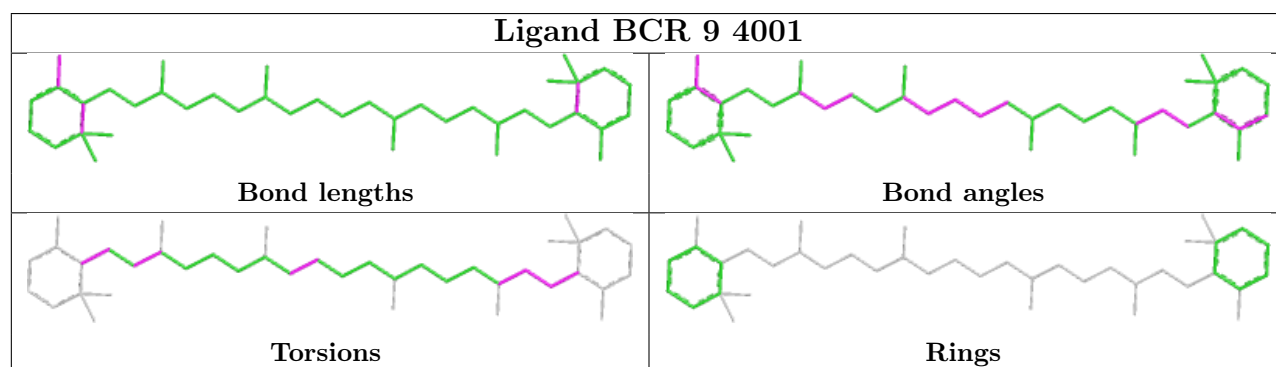
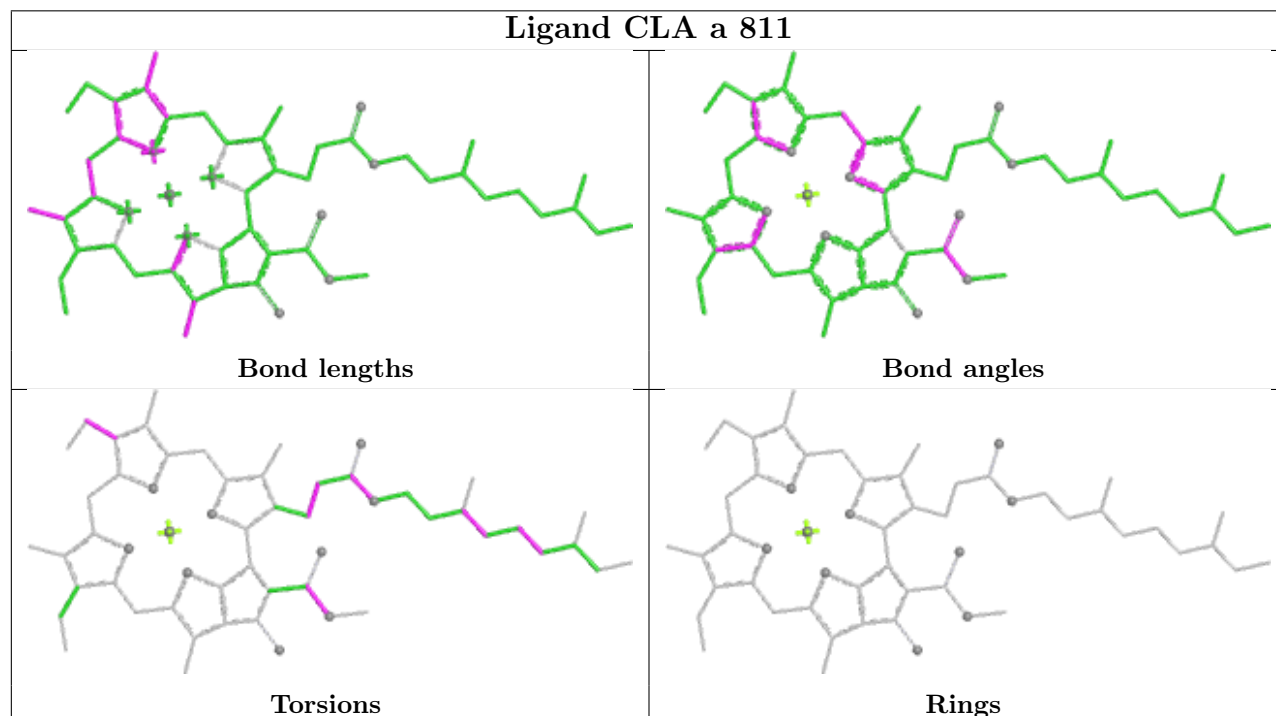
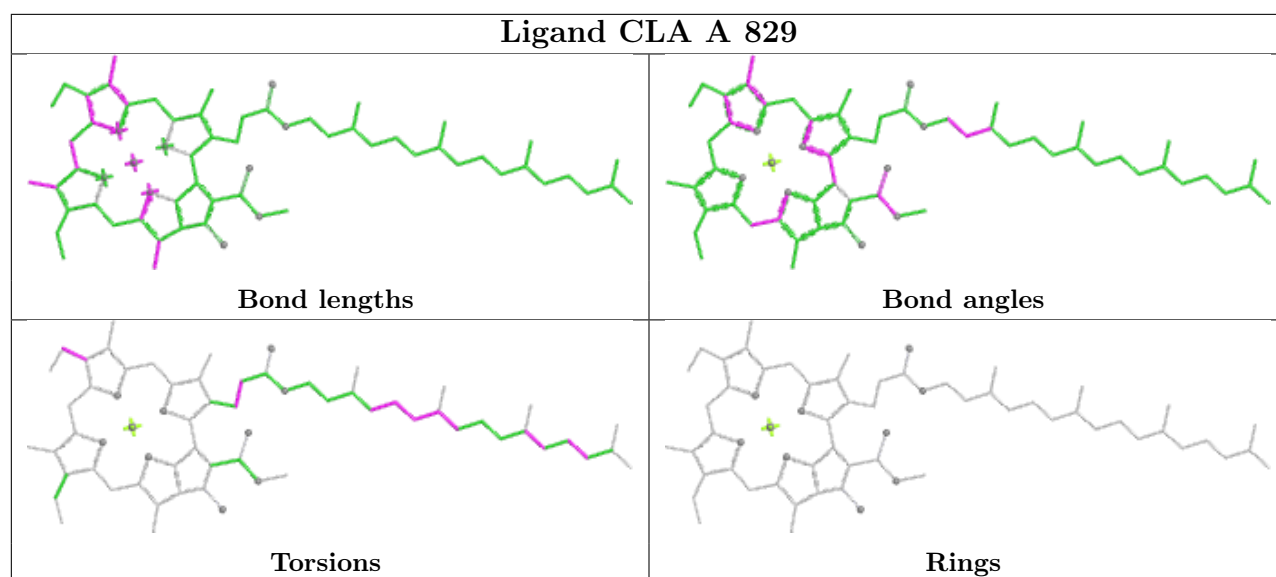
Ligand CLA B 814

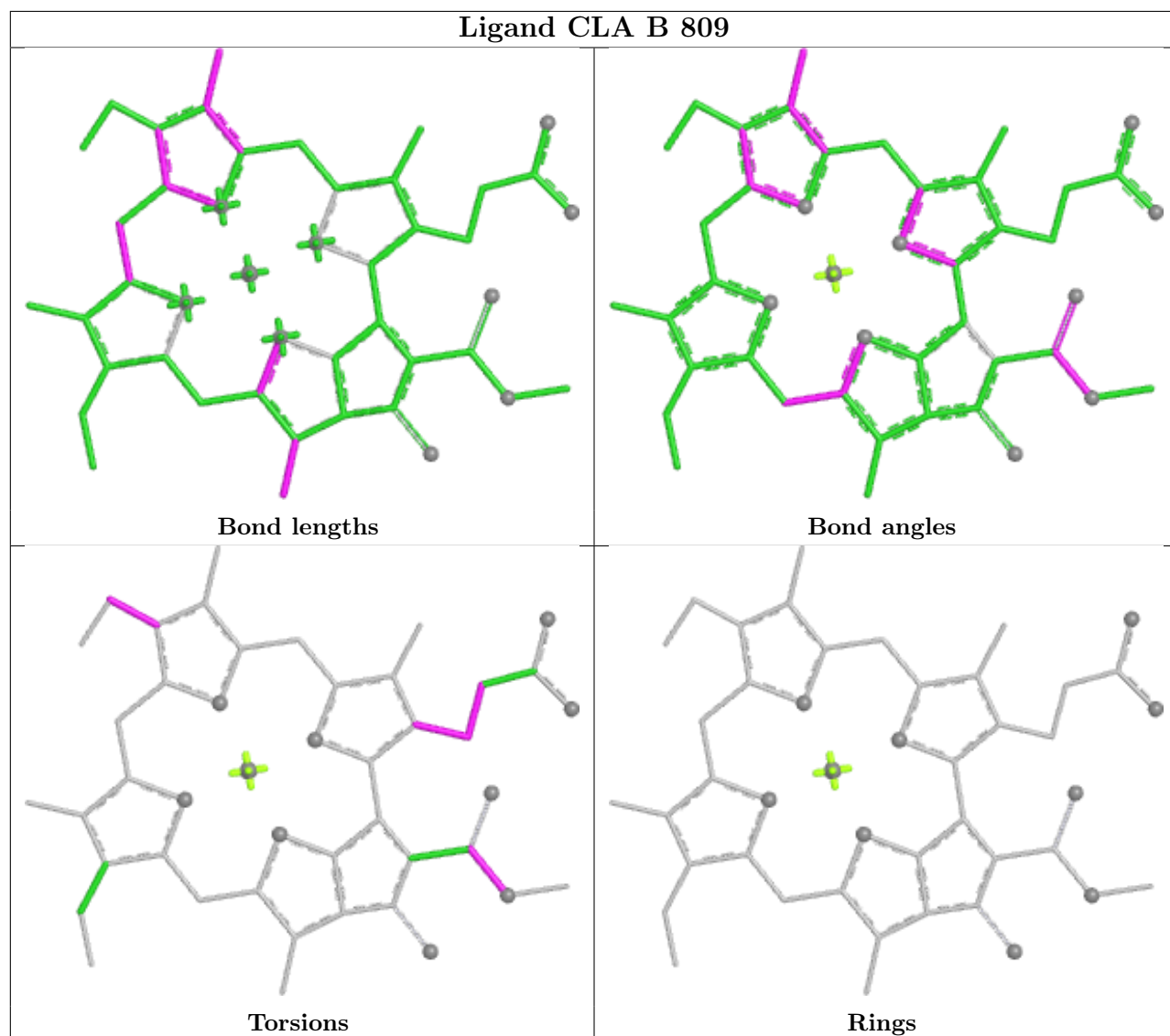
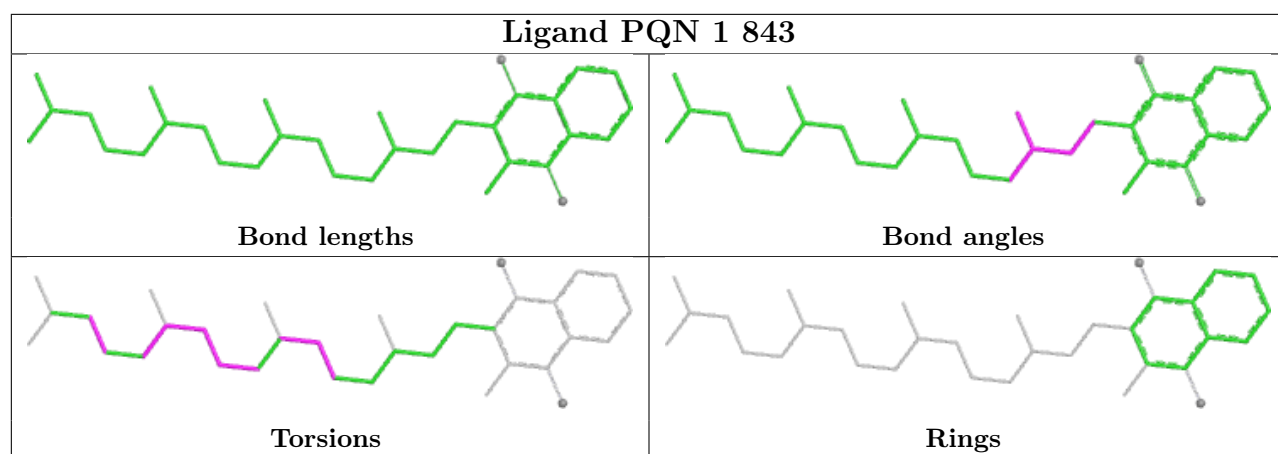




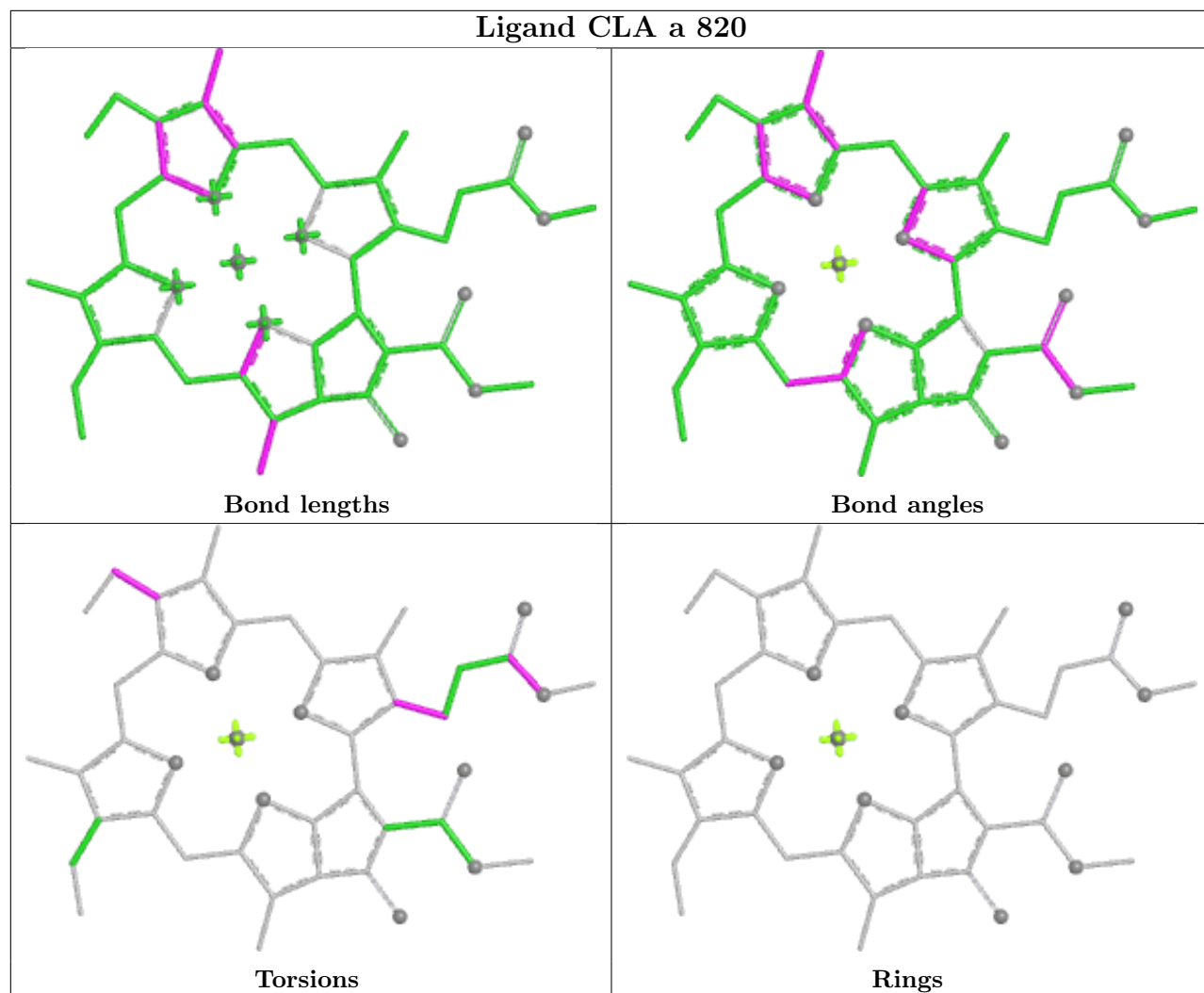
Ligand CLA 2 809**Ligand CLA A 830**



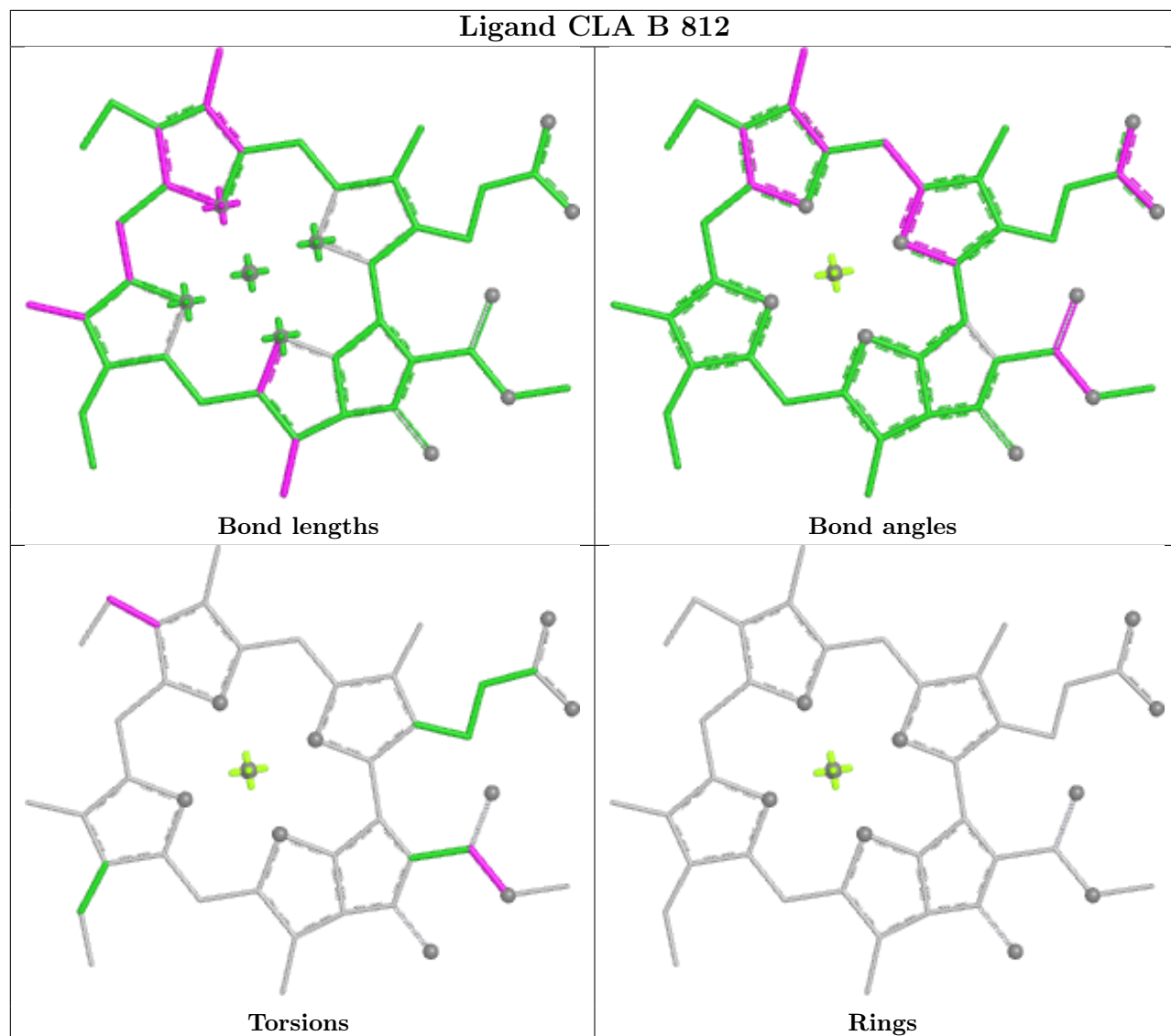




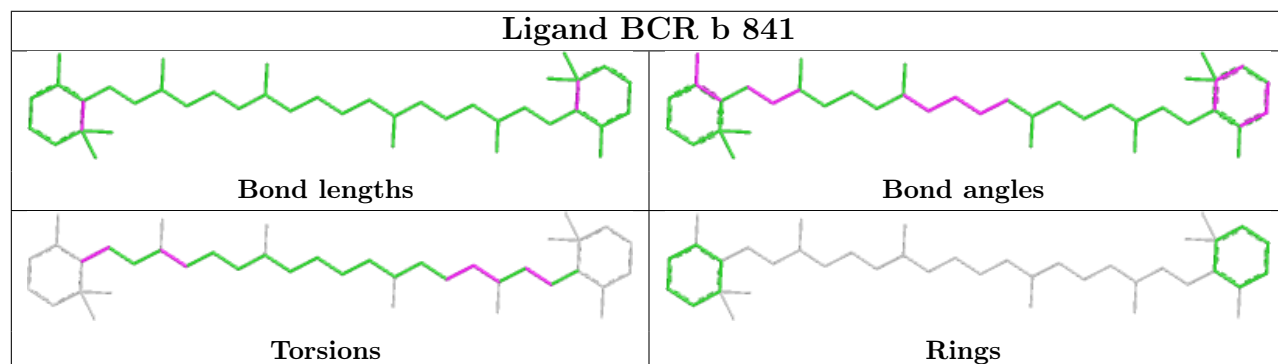
Ligand CLA a 820

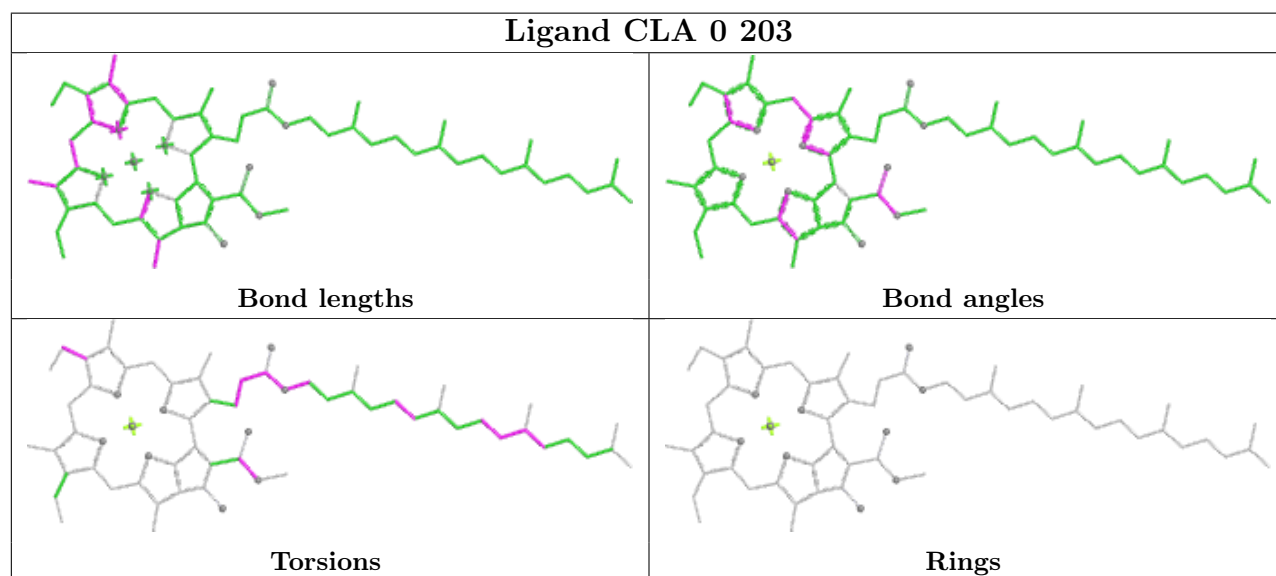
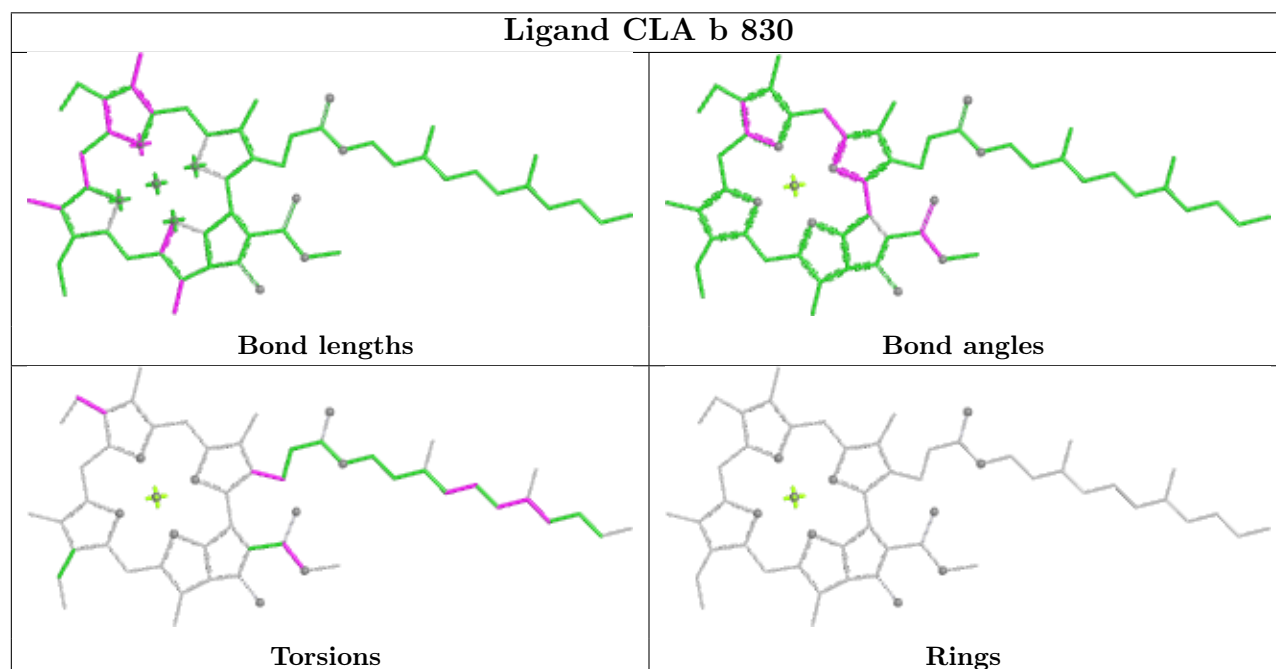
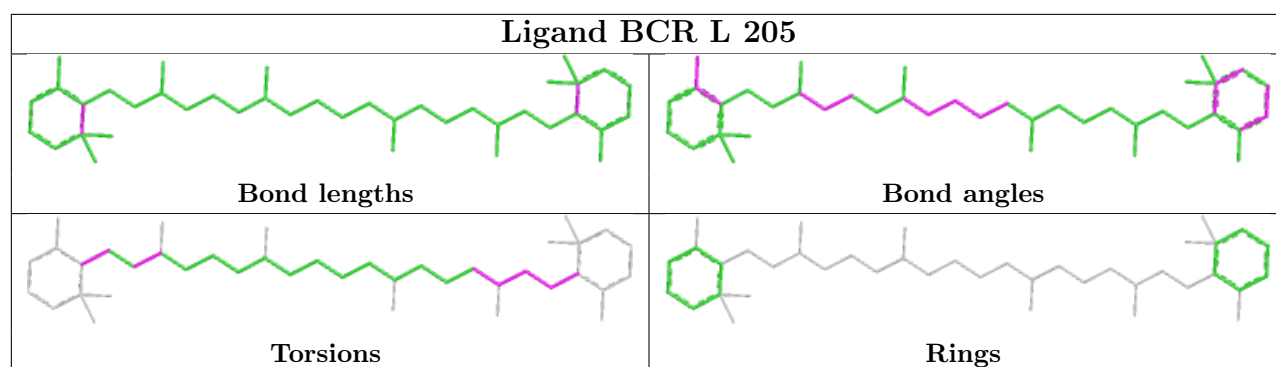


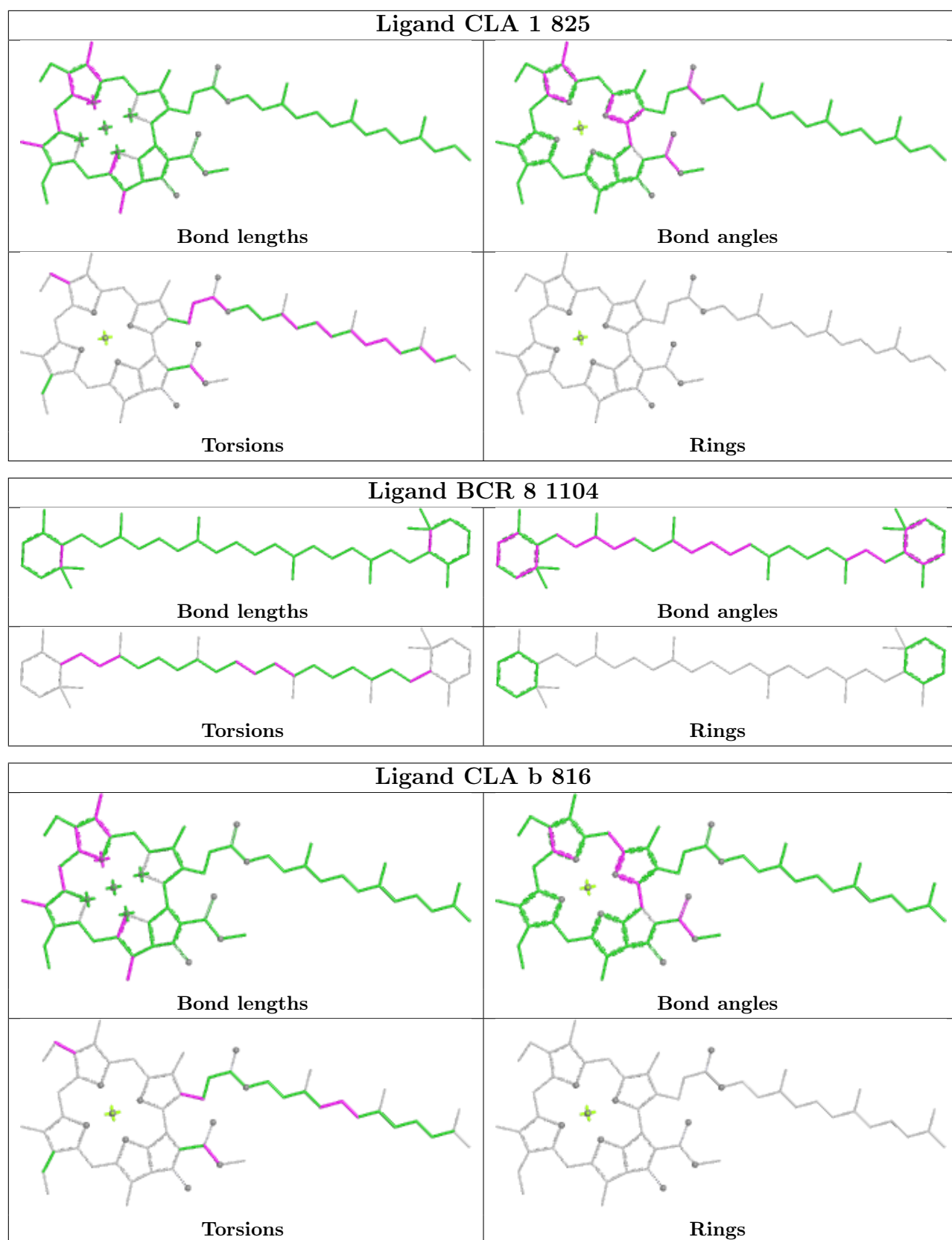
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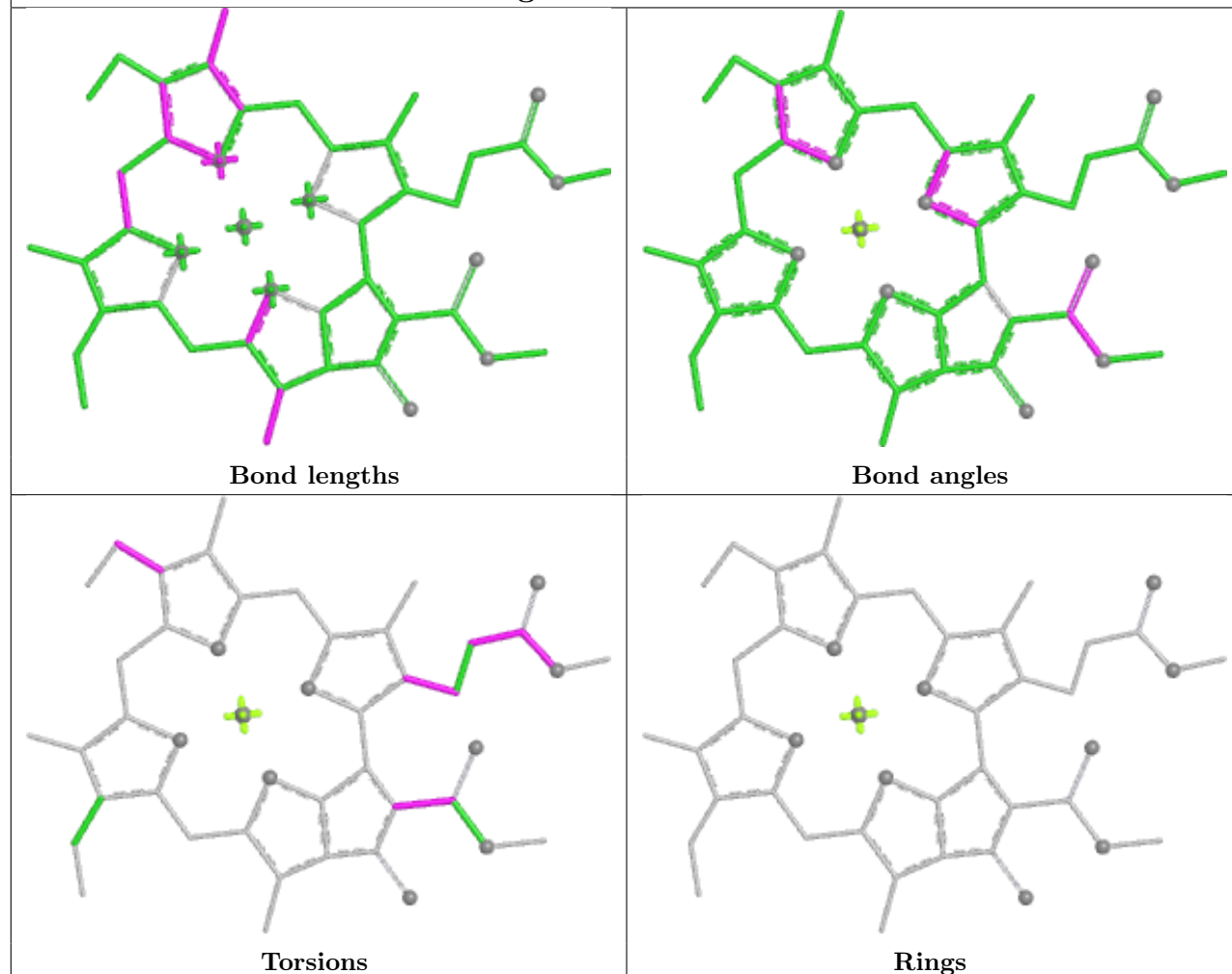
Ligand BCR b 841



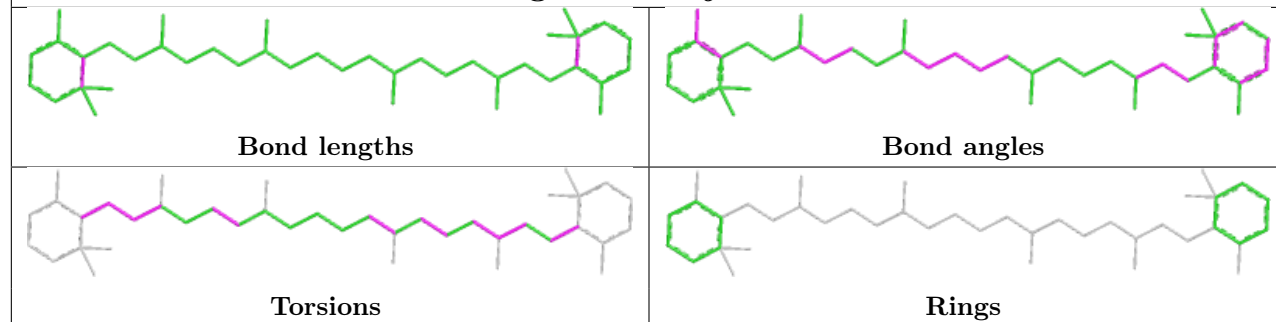




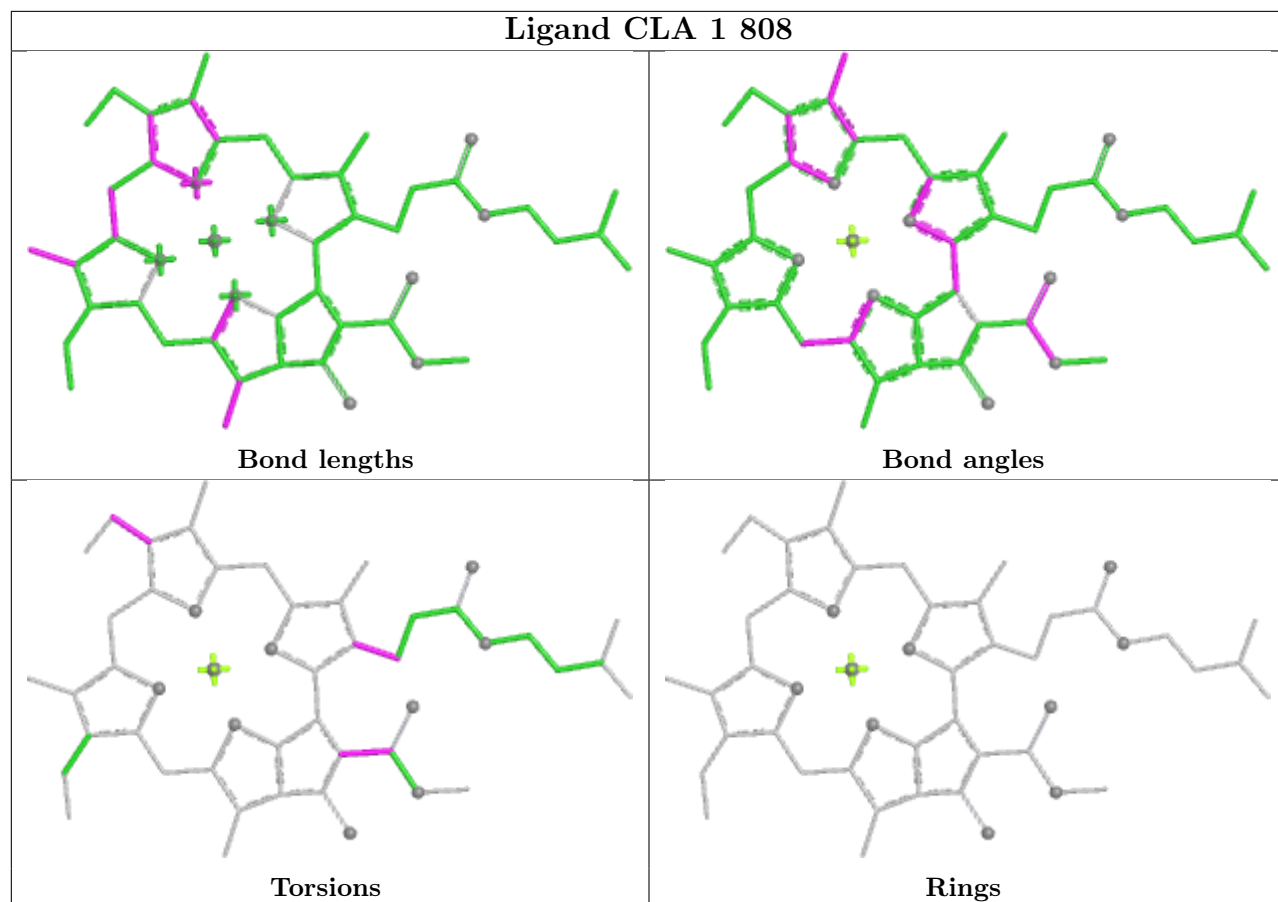
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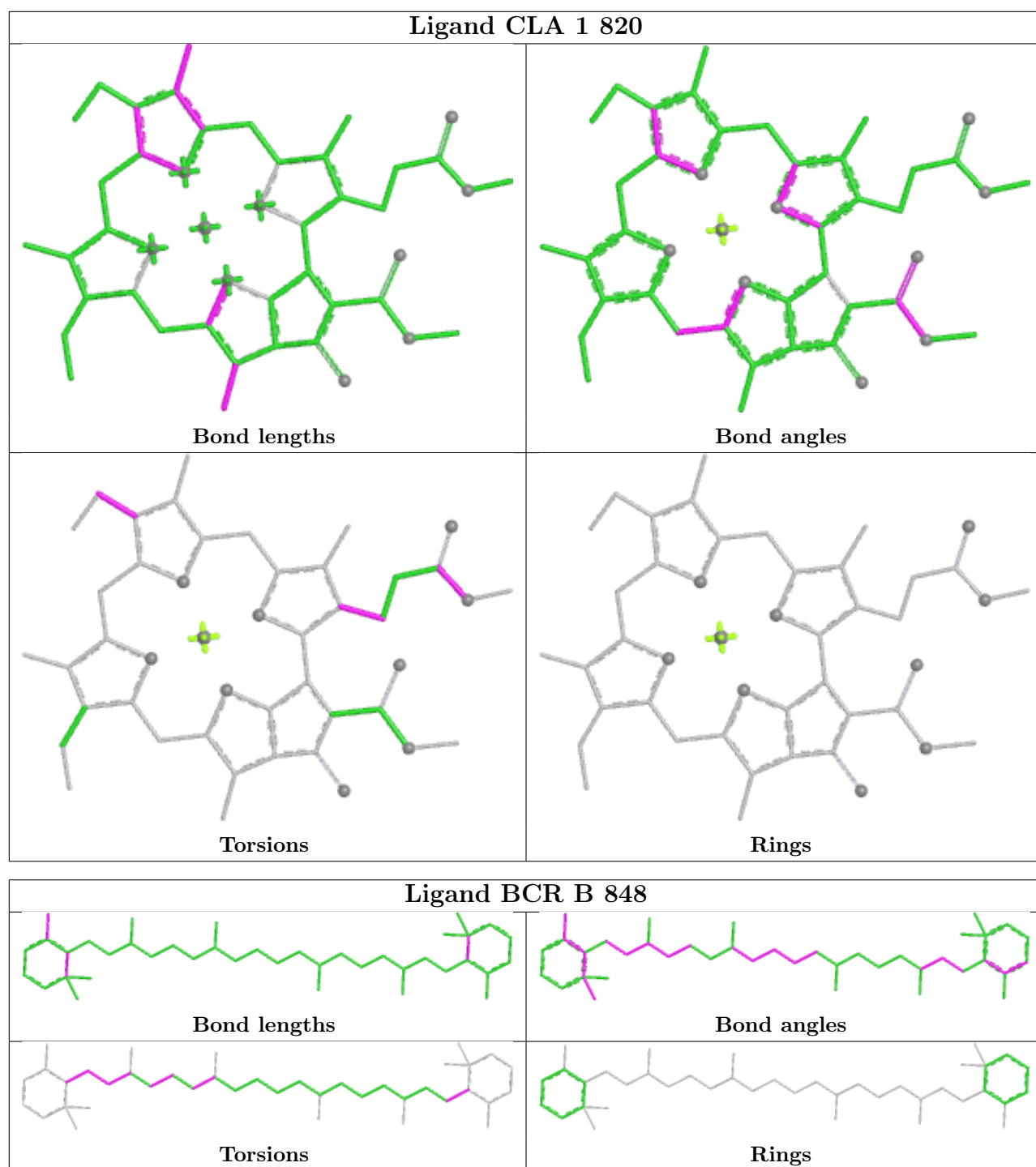


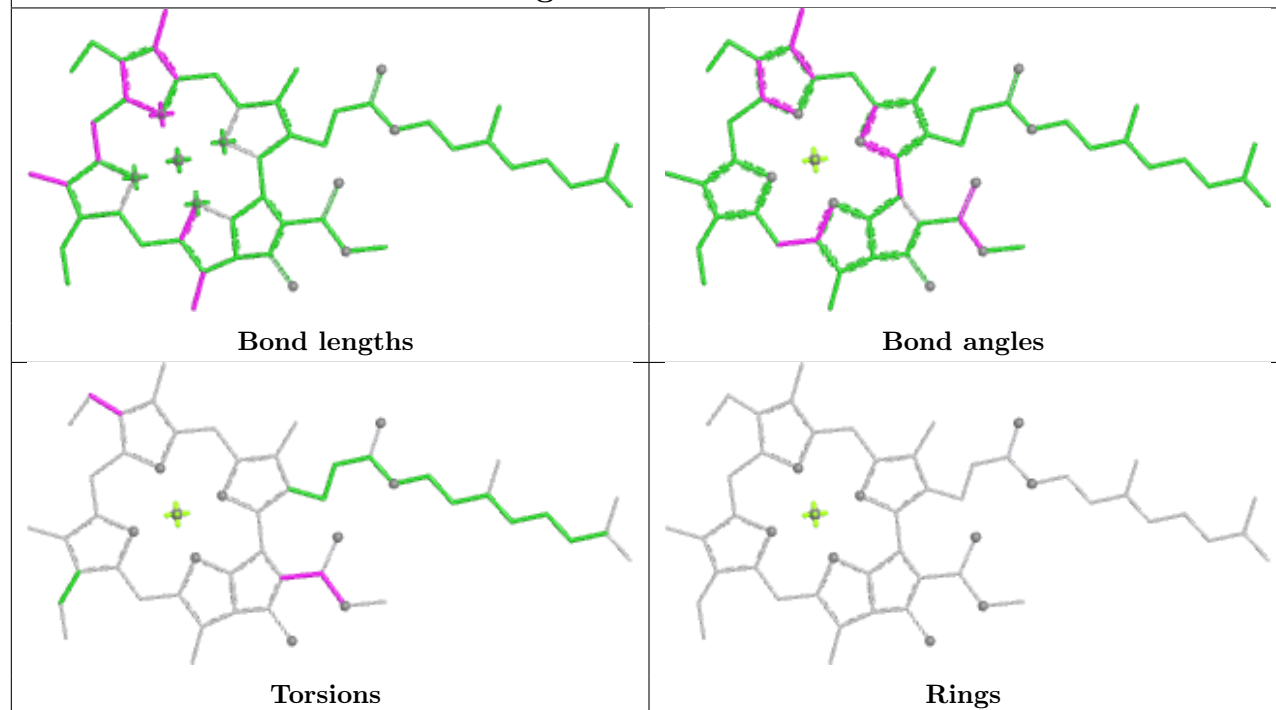
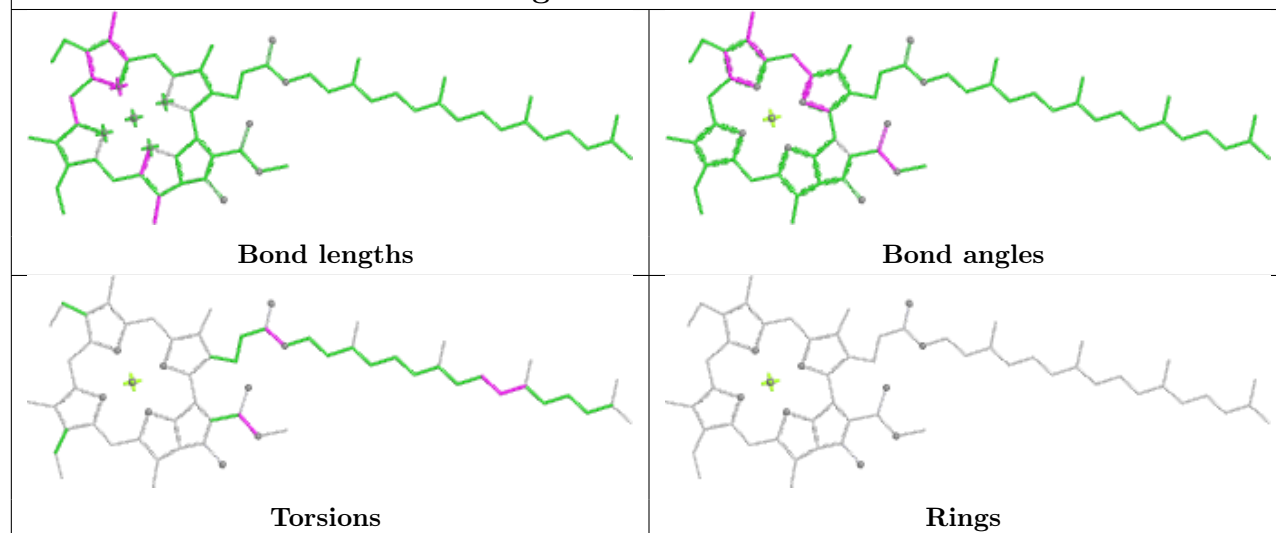
Ligand BCR j 1105



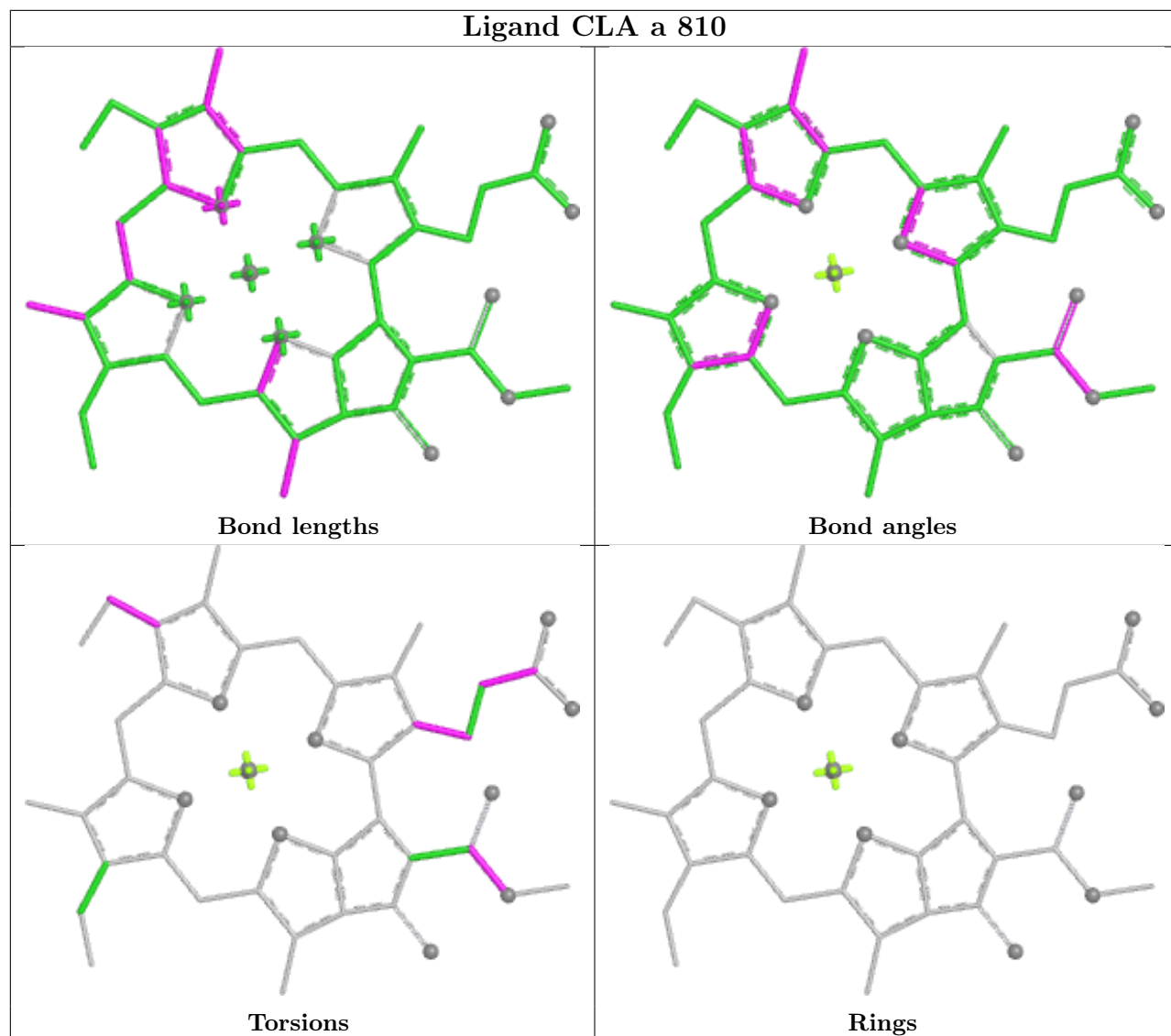
Ligand CLA 1 808



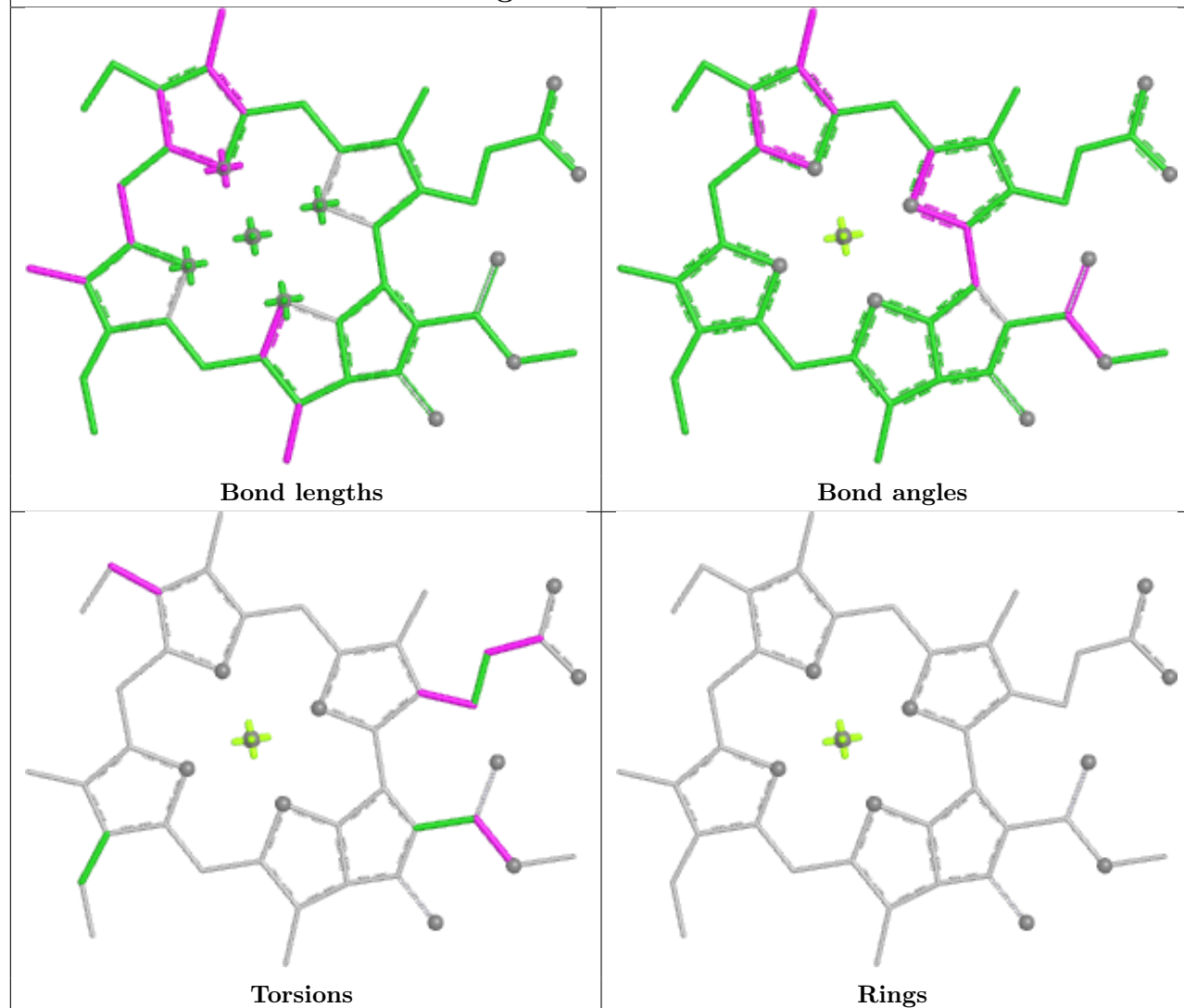


Ligand CLA a 807**Ligand CLA B 838**

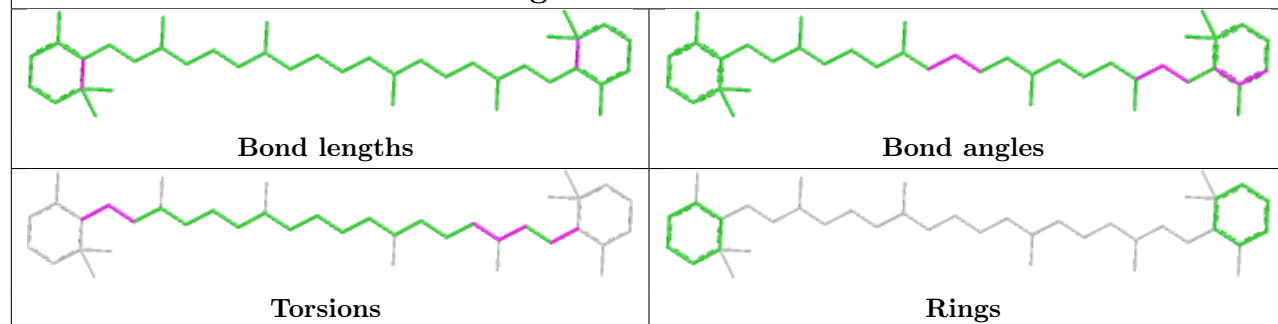
Ligand CLA a 810

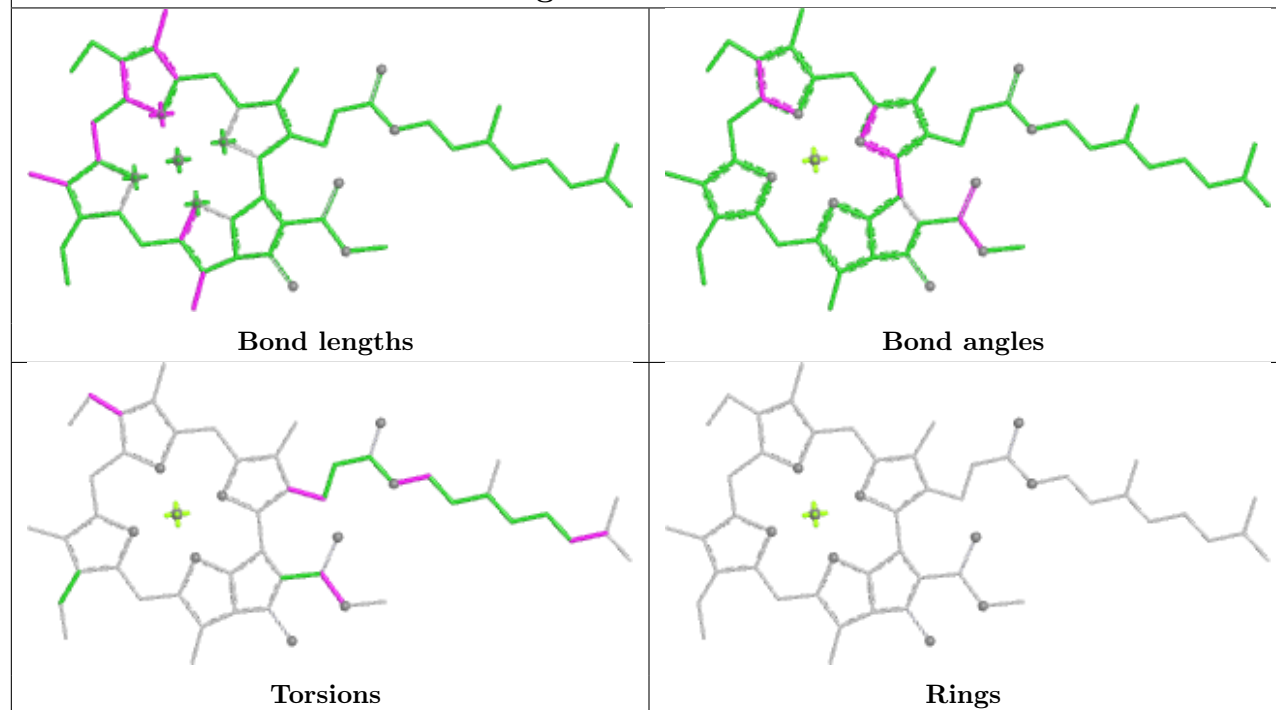
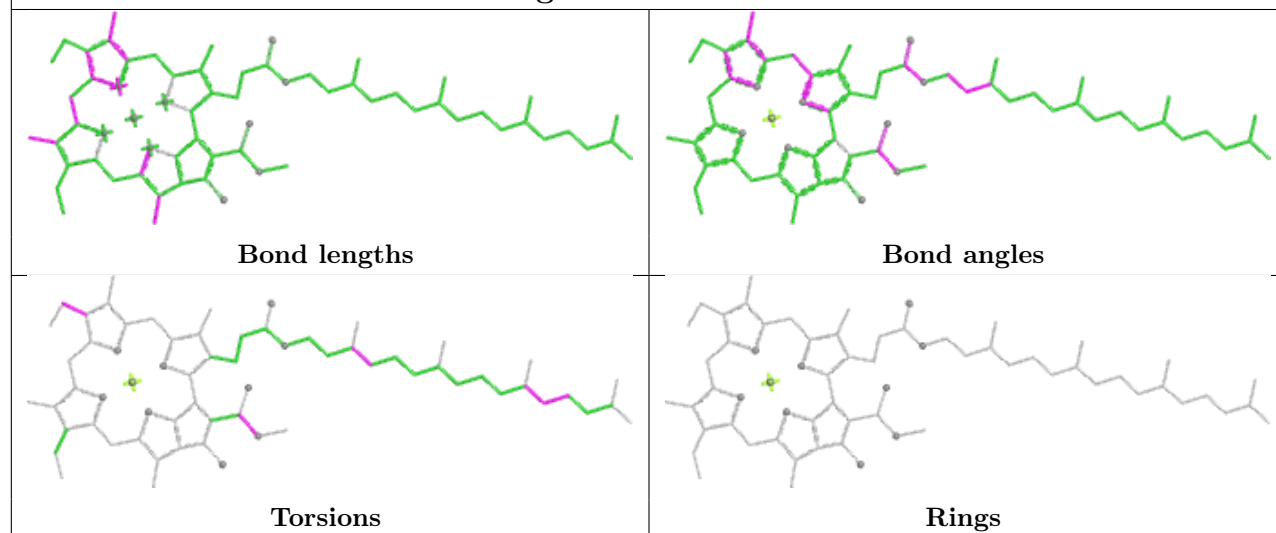


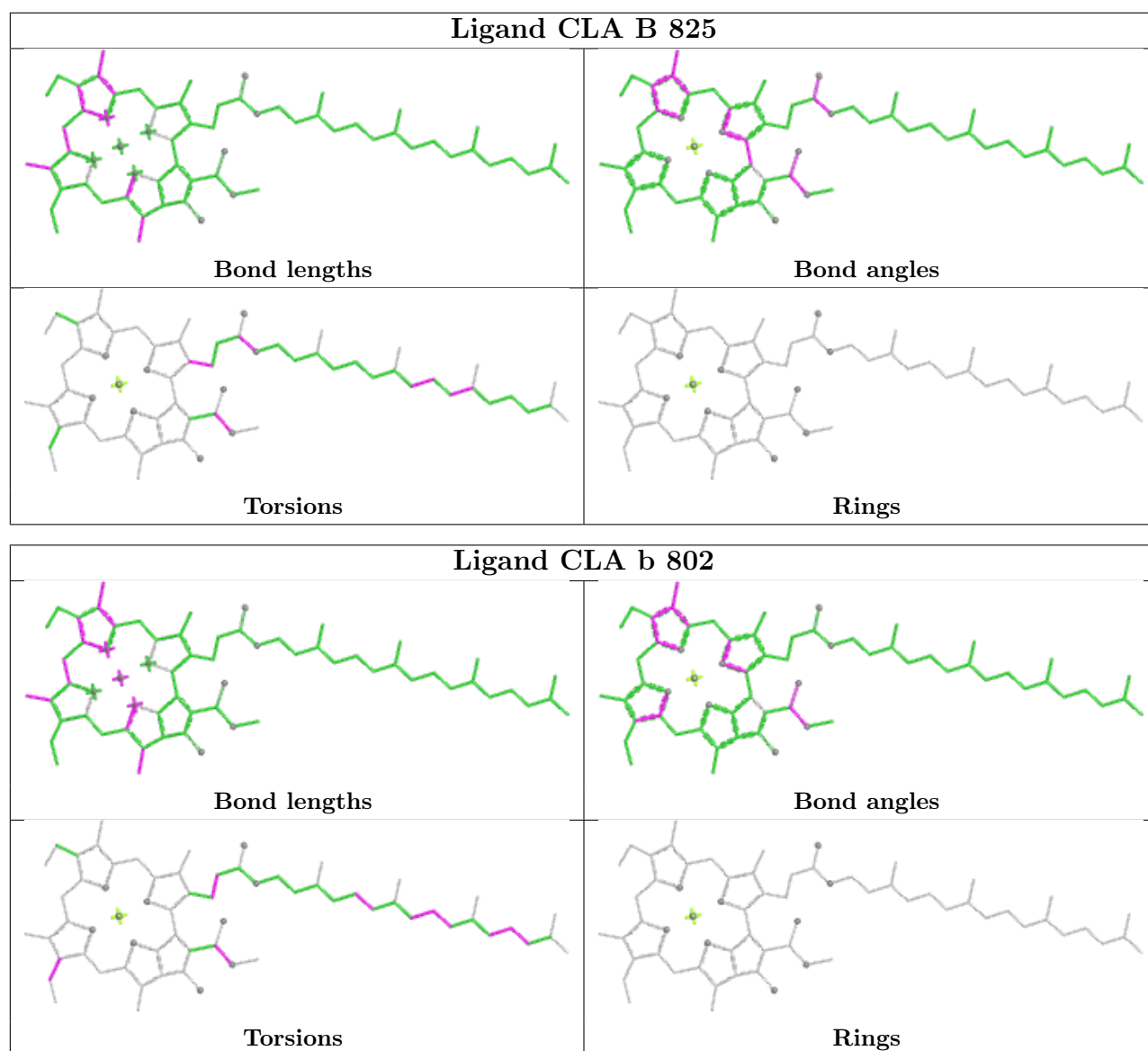
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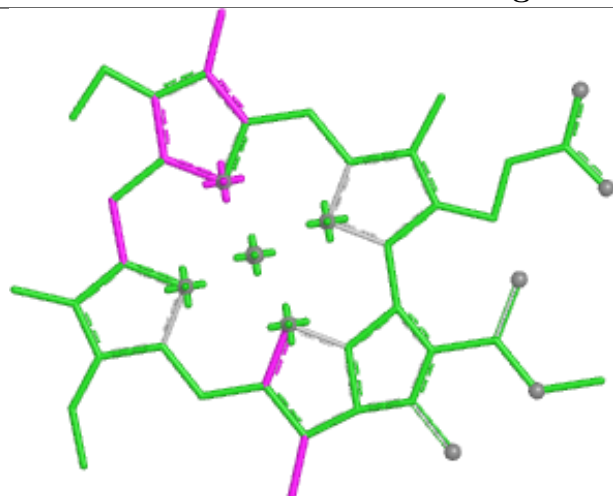
Ligand BCR A 845



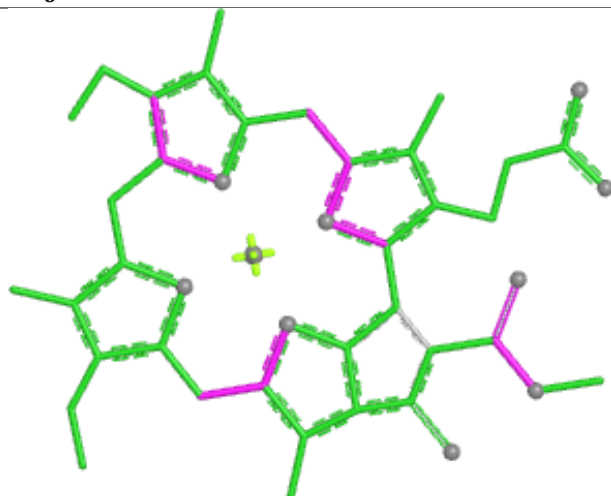
Ligand CLA 2 819**Ligand CLA a 832**



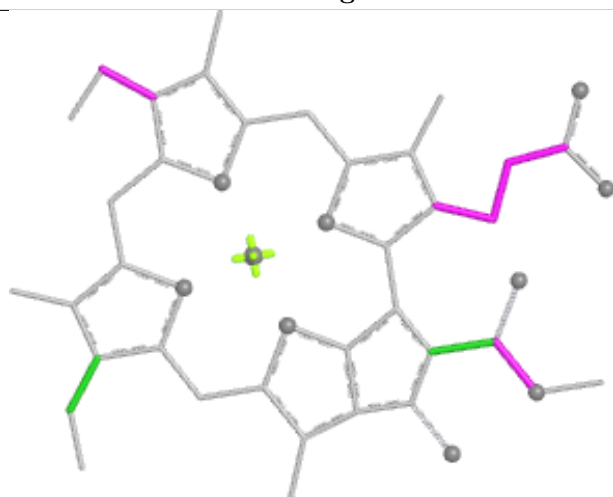
Ligand CLA j 1103



Bond lengths



Bond angles

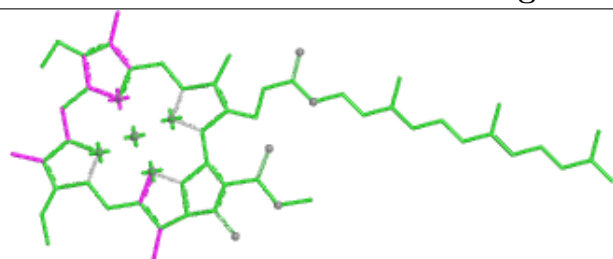


Torsions

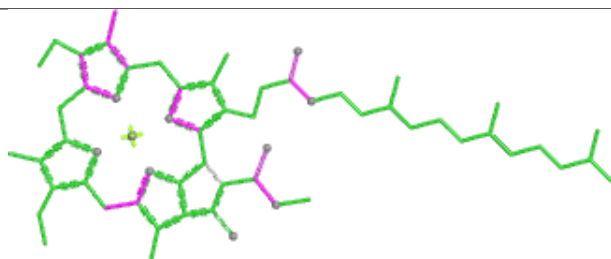


Rings

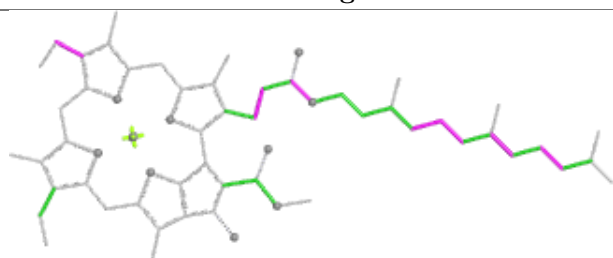
Ligand CLA 1 837



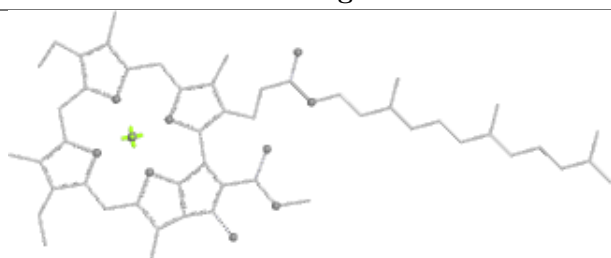
Bond lengths



Bond angles

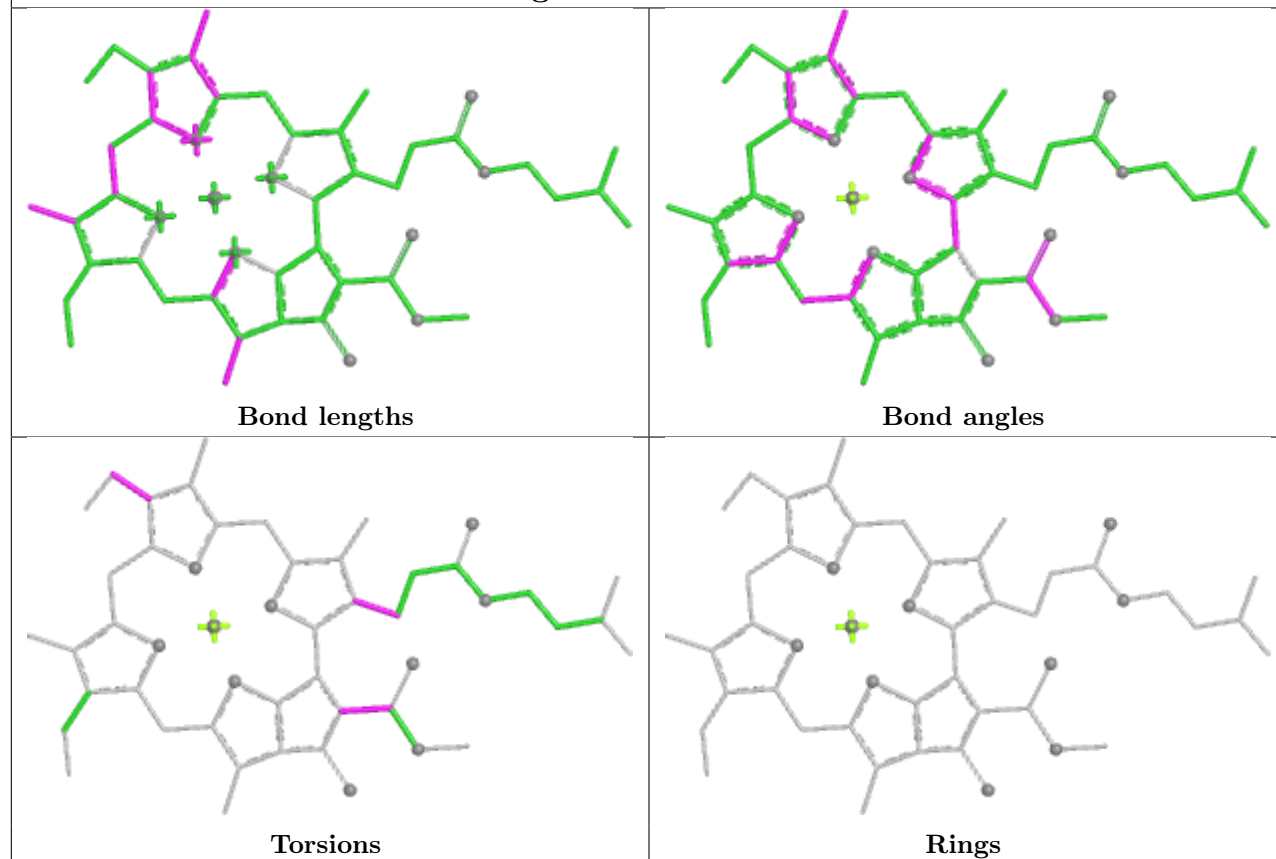


Torsions

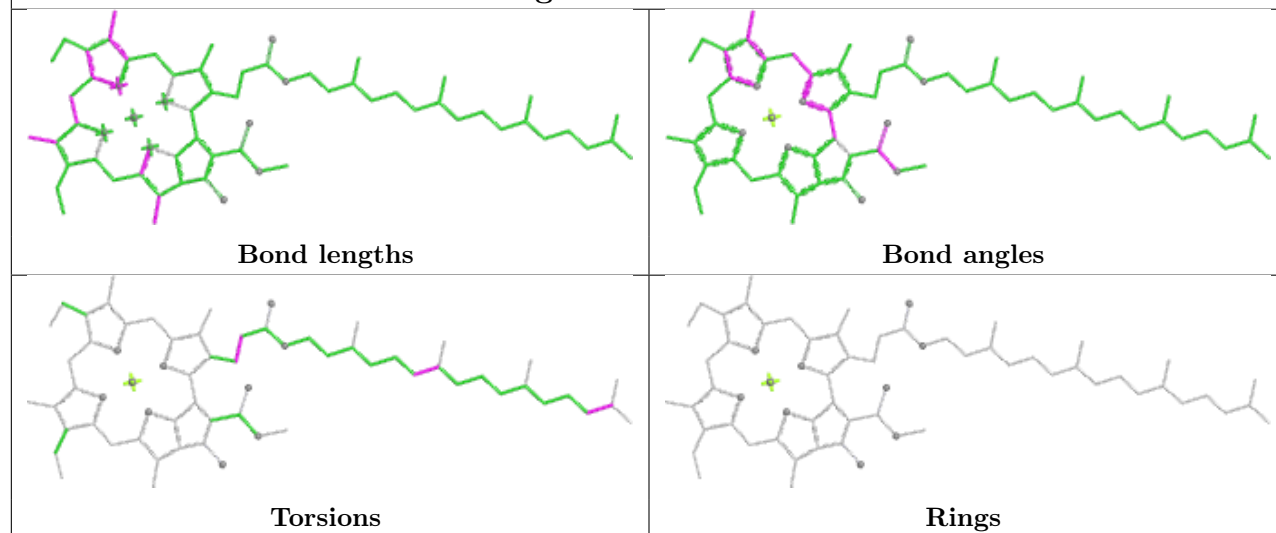


Rings

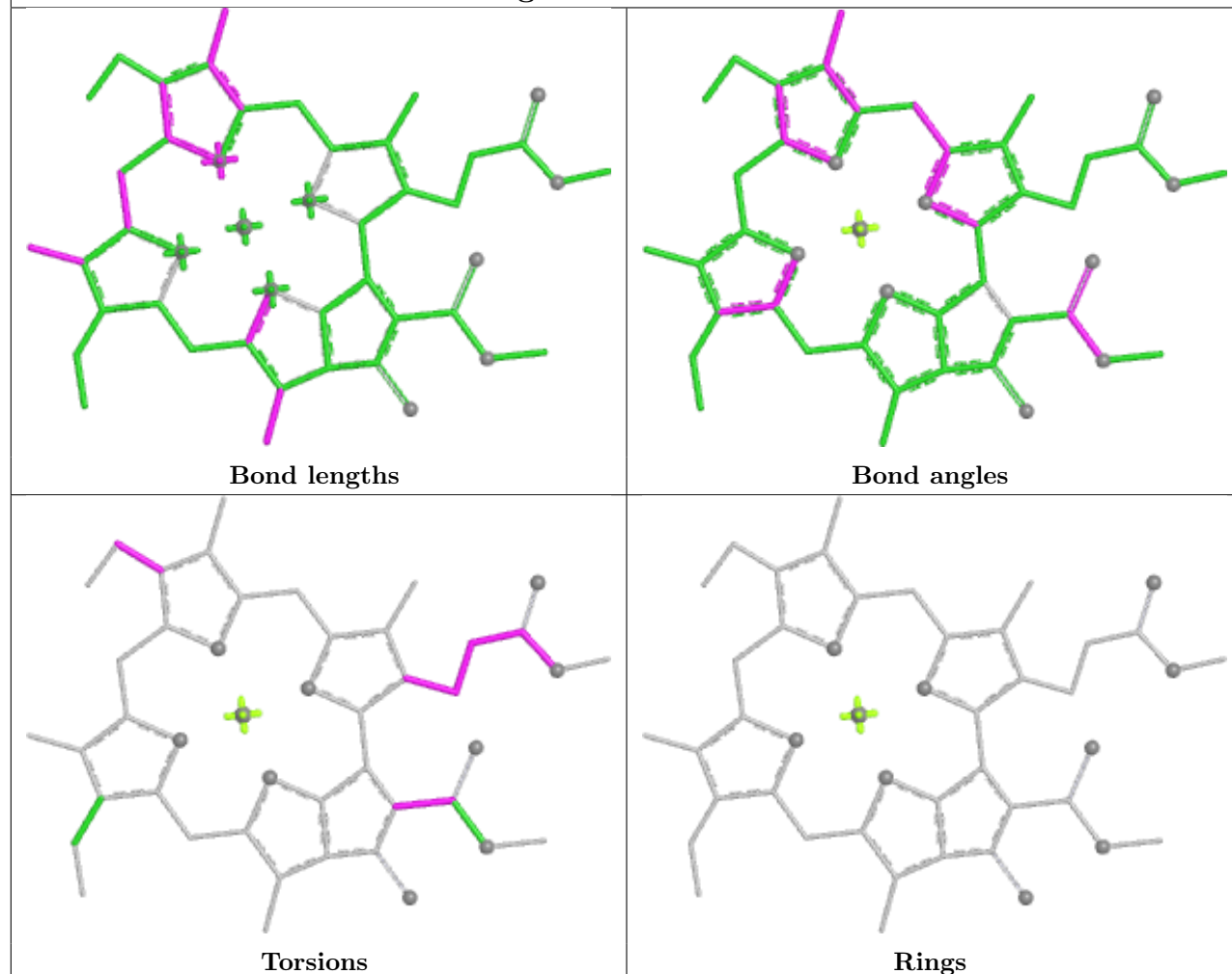
Ligand CLA A 808



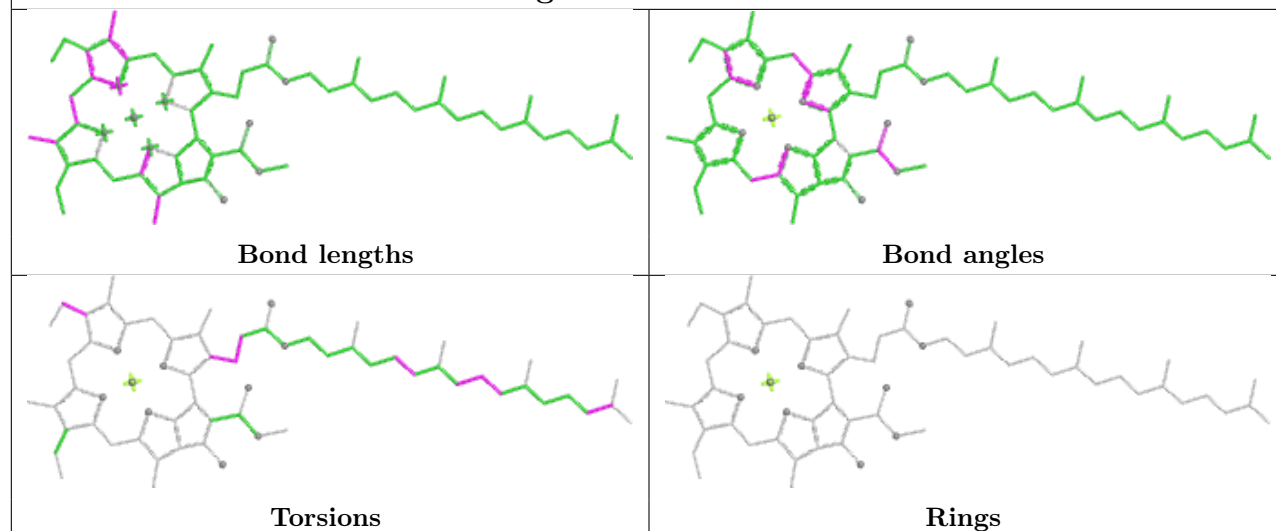
Ligand CLA b 836



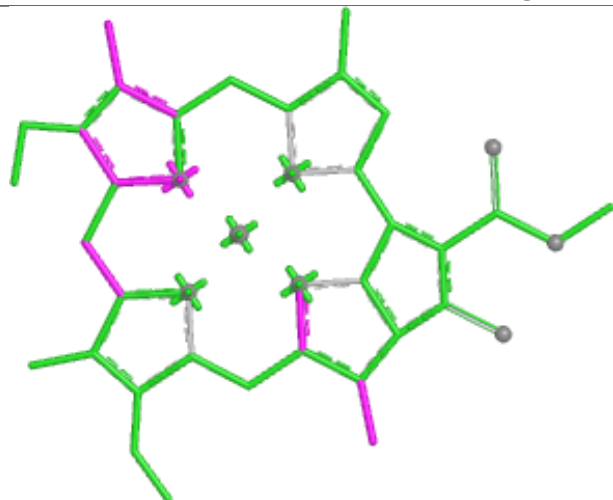
Ligand CLA 2 817



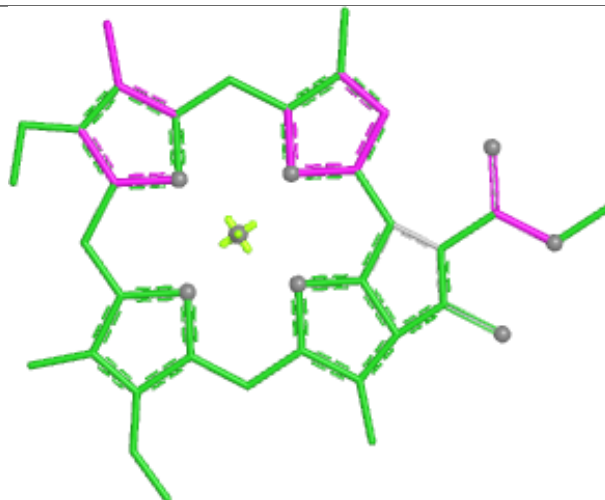
Ligand CLA 0 208



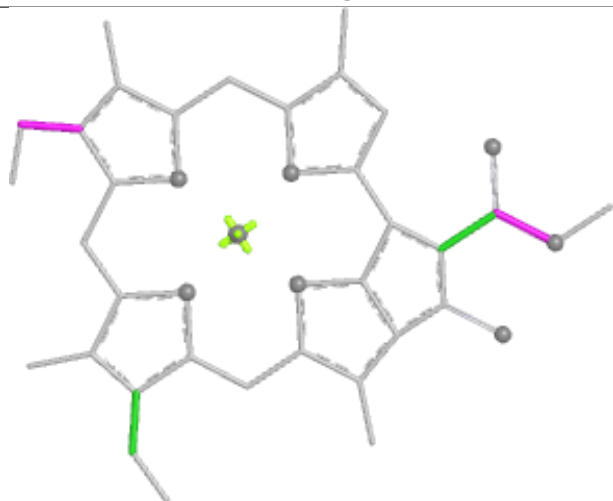
Ligand CLA 2 831



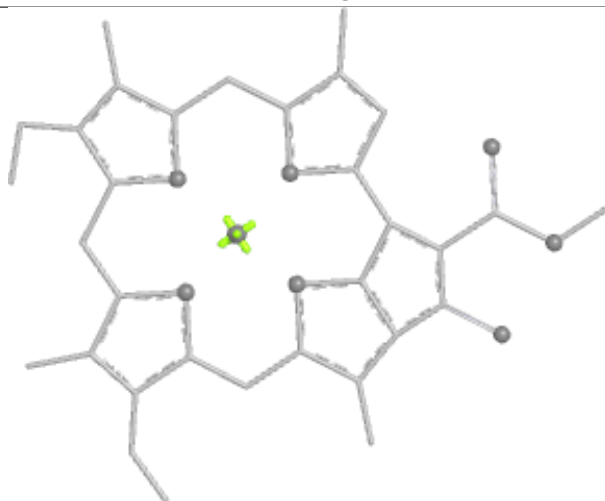
Bond lengths



Bond angles

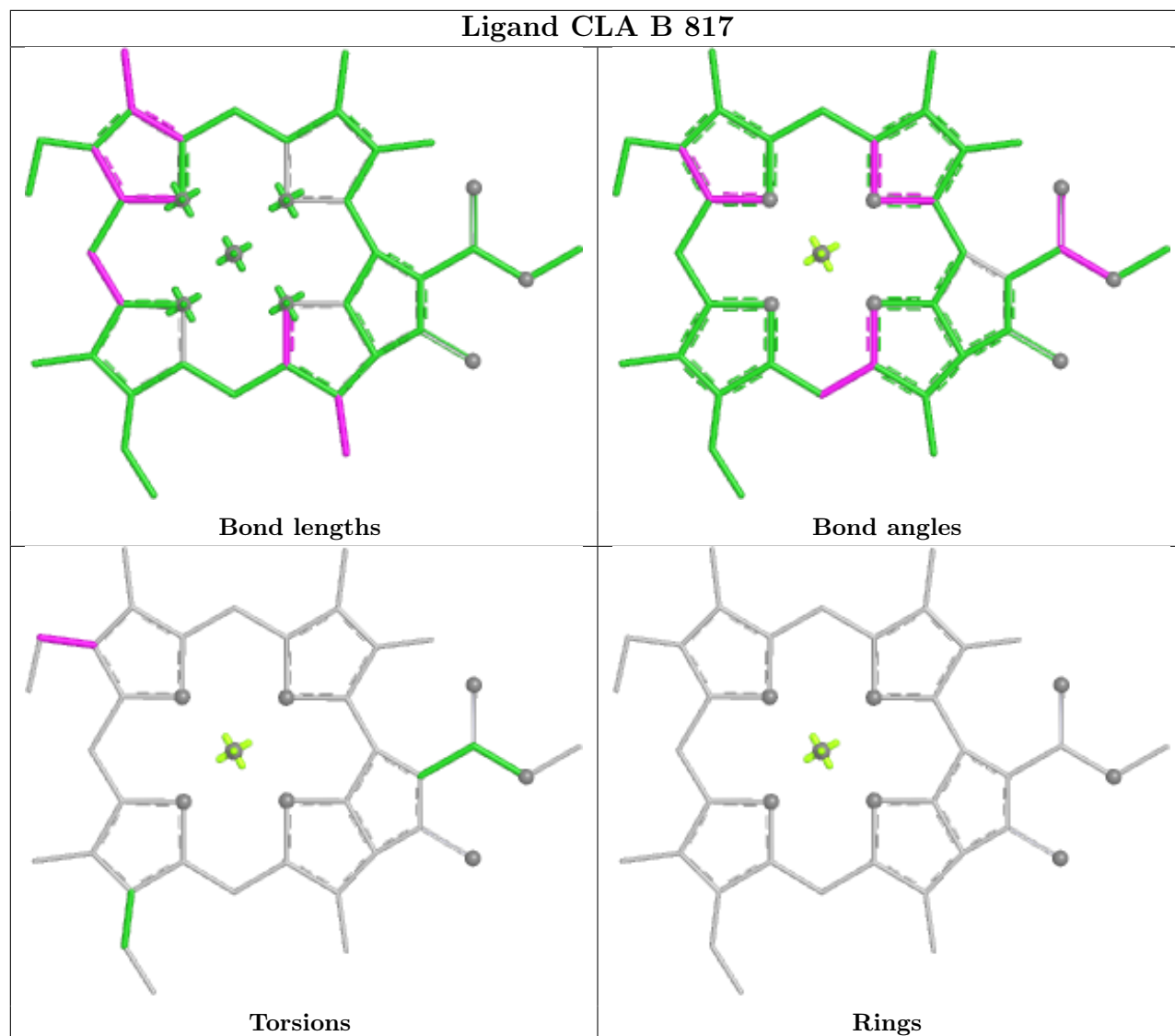


Torsions

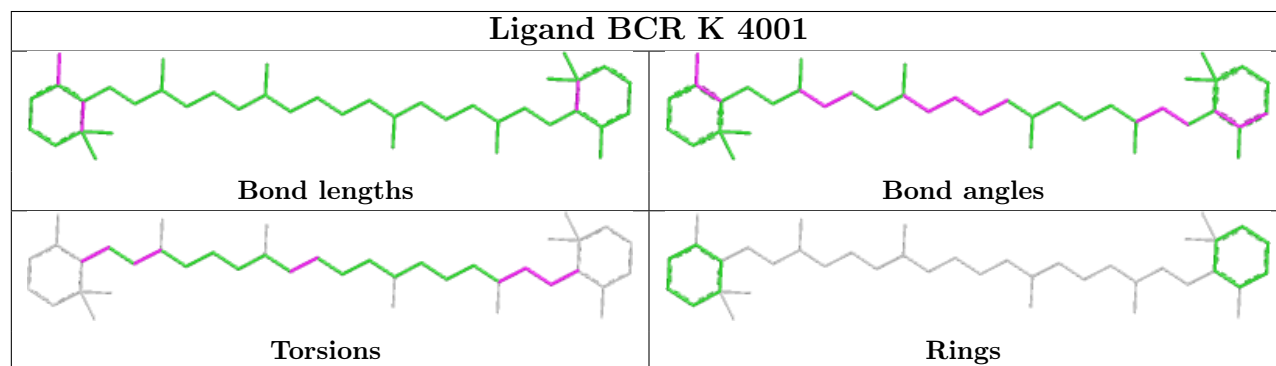


Rings

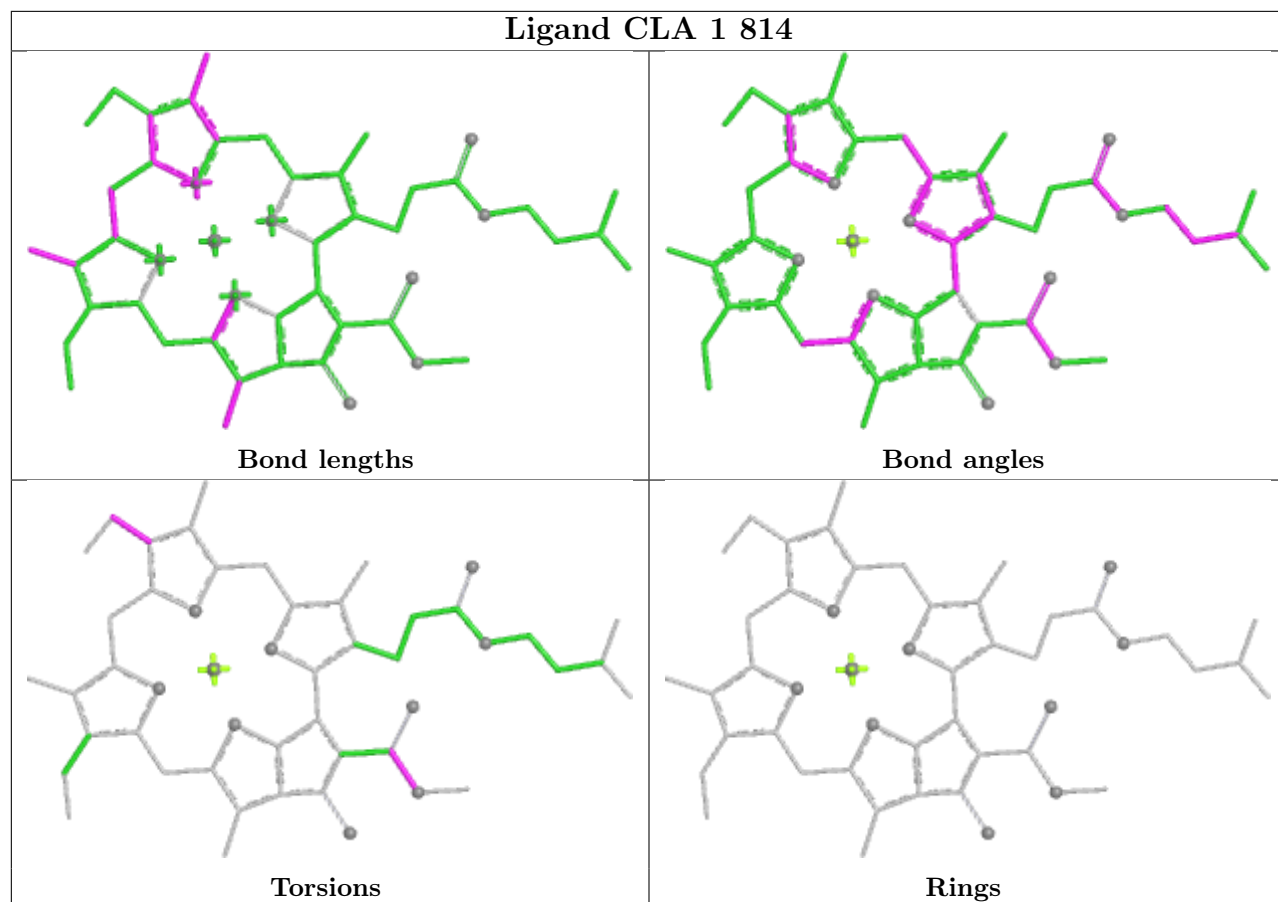
Ligand CLA B 817



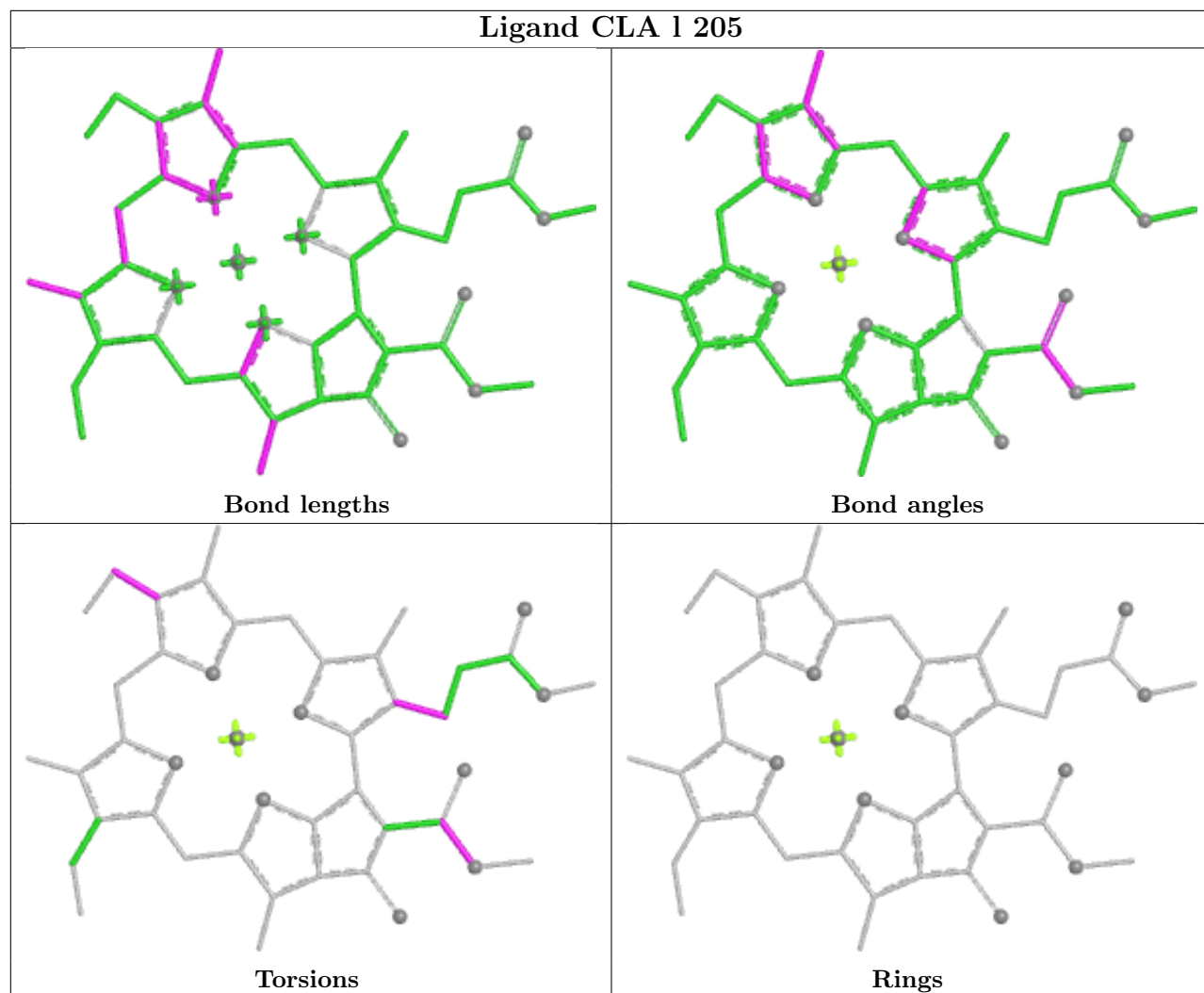
Ligand BCR K 4001



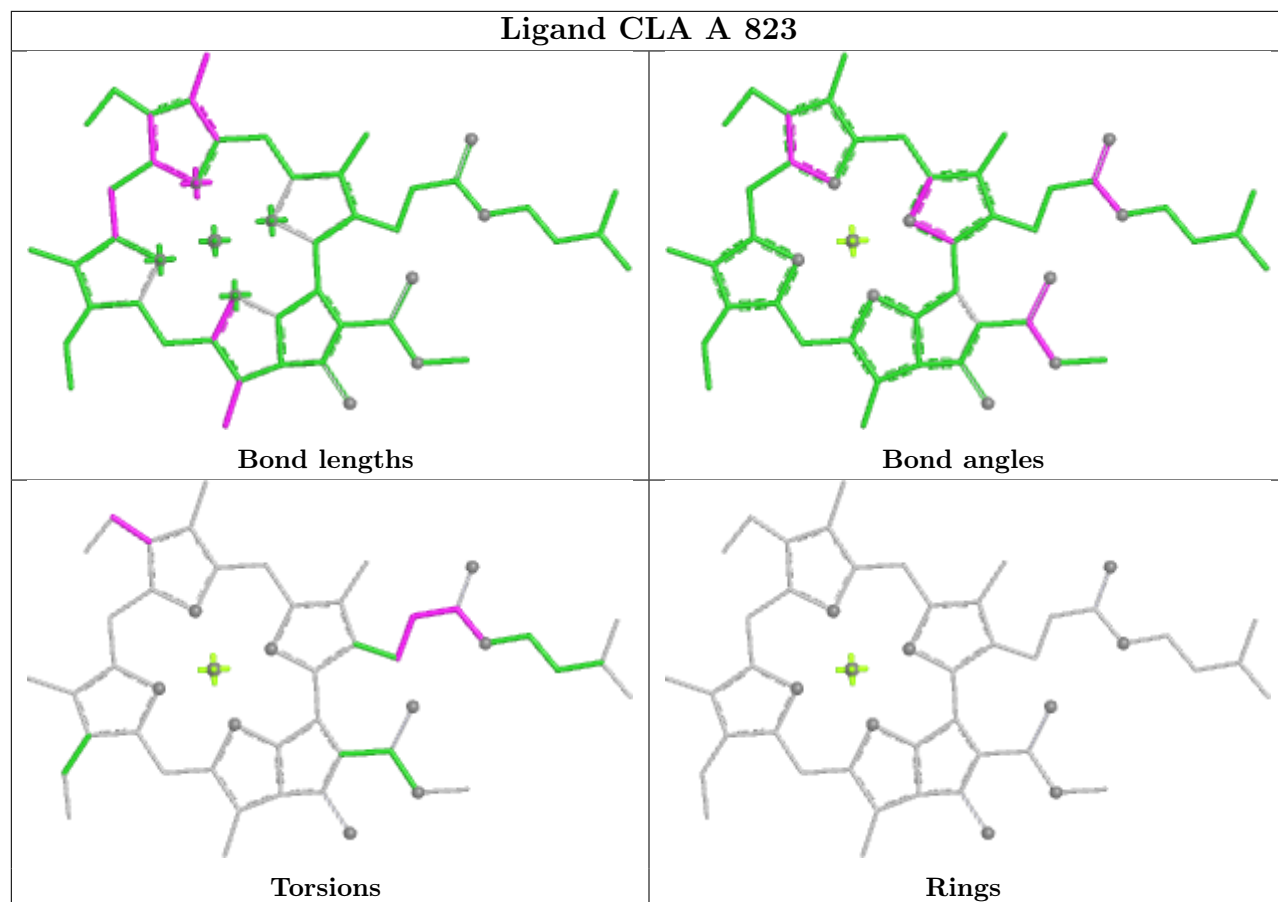
Ligand CLA 1 814

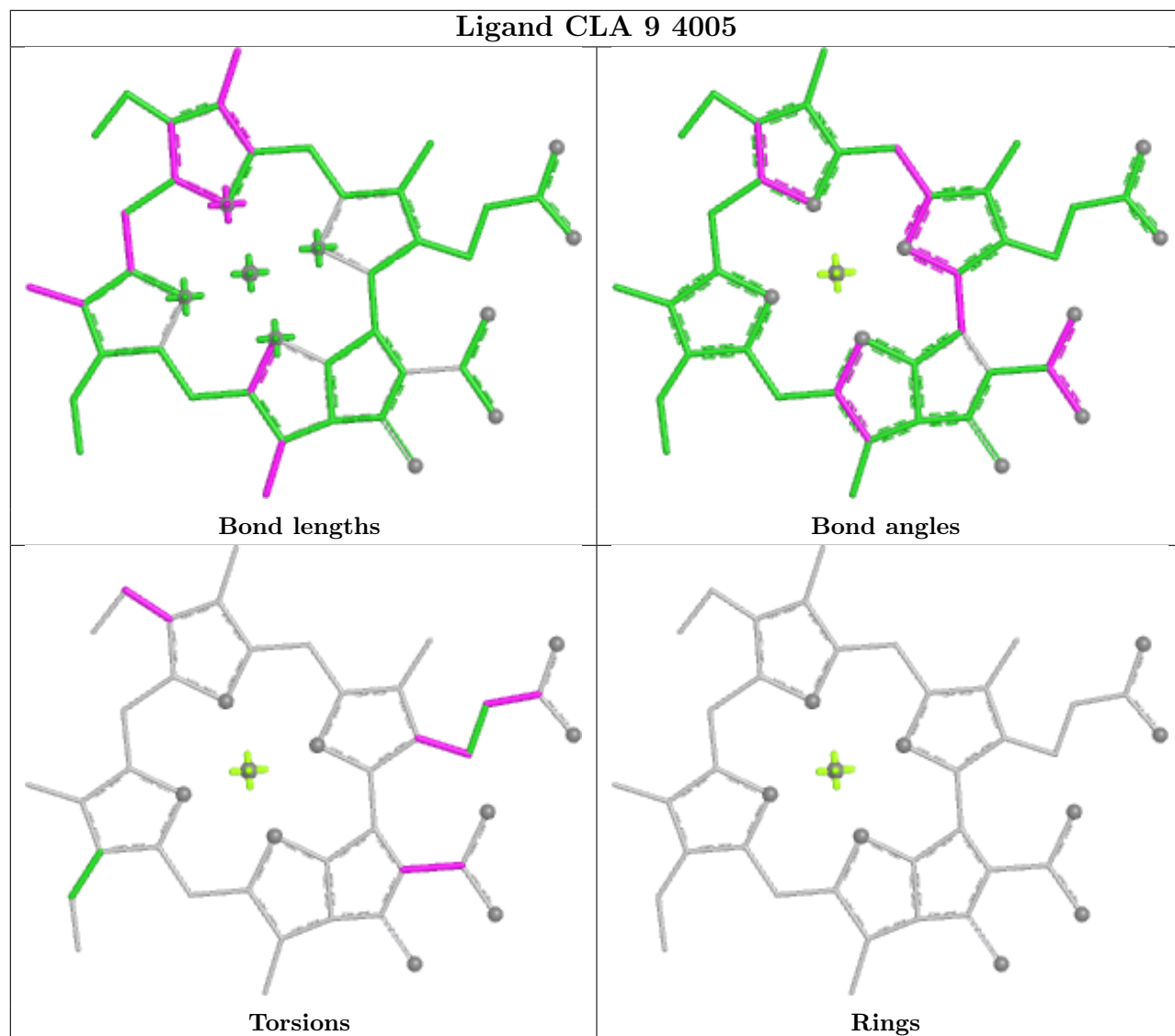


Ligand CLA 1 205

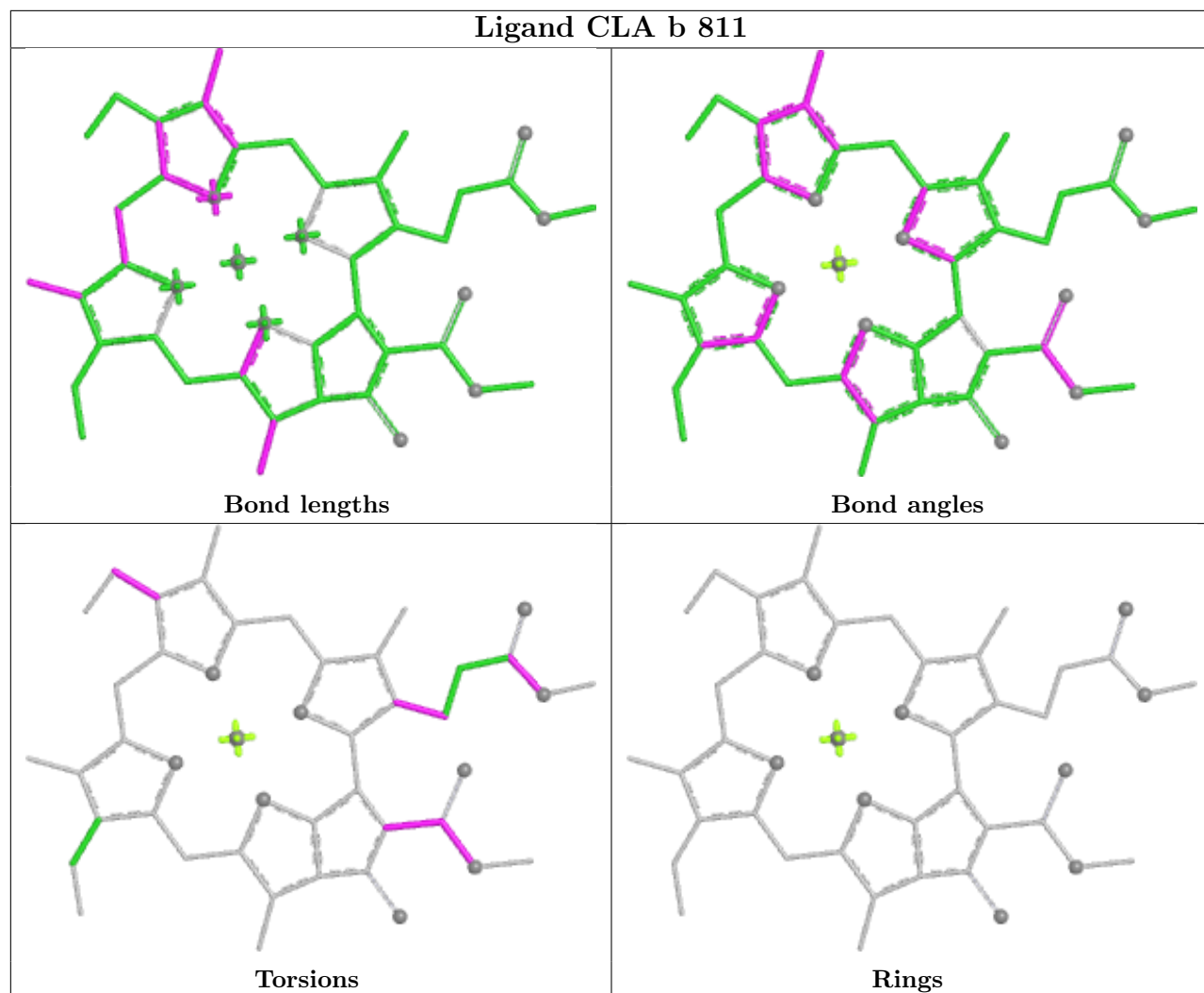


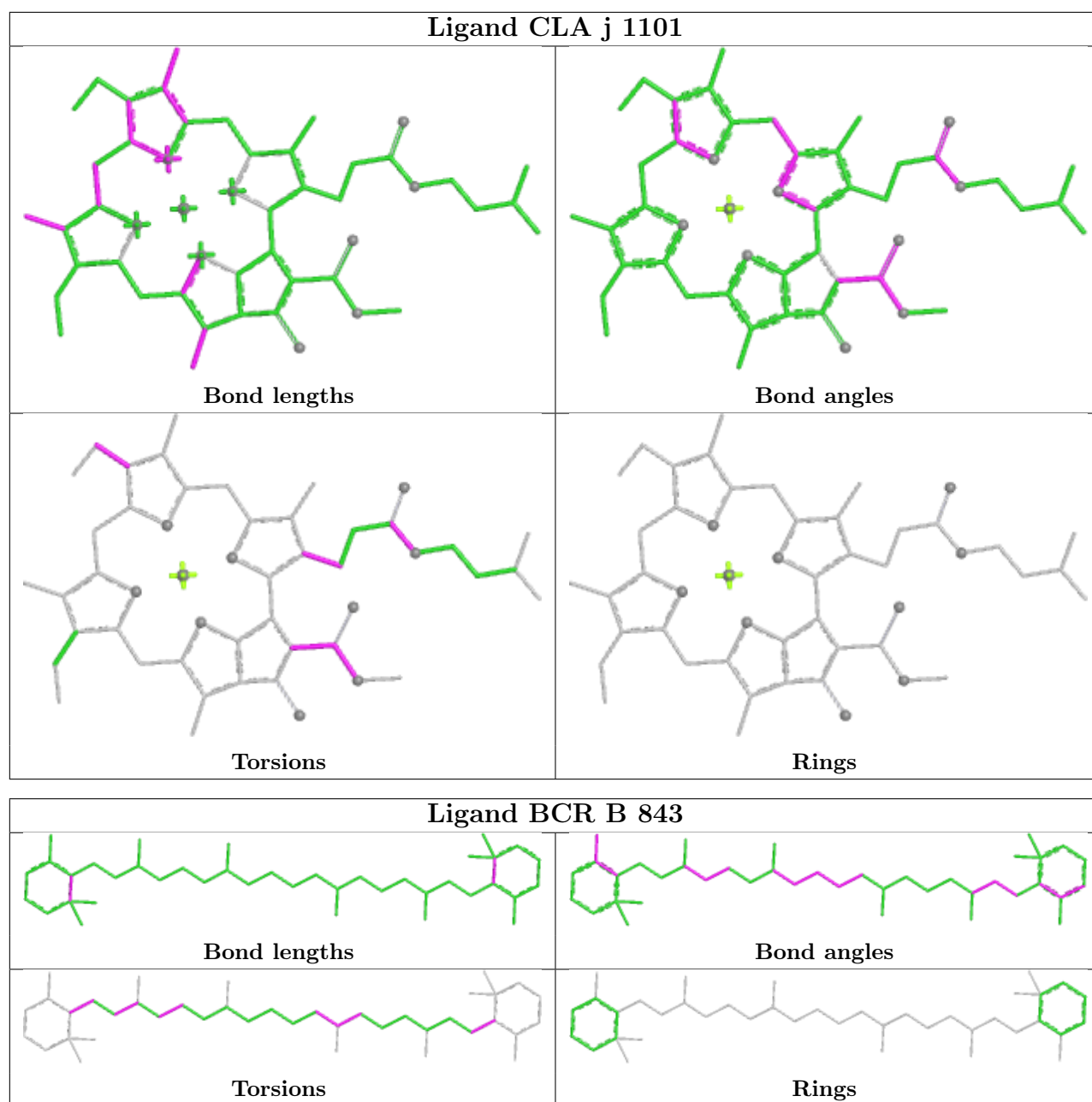
Ligand CLA A 823



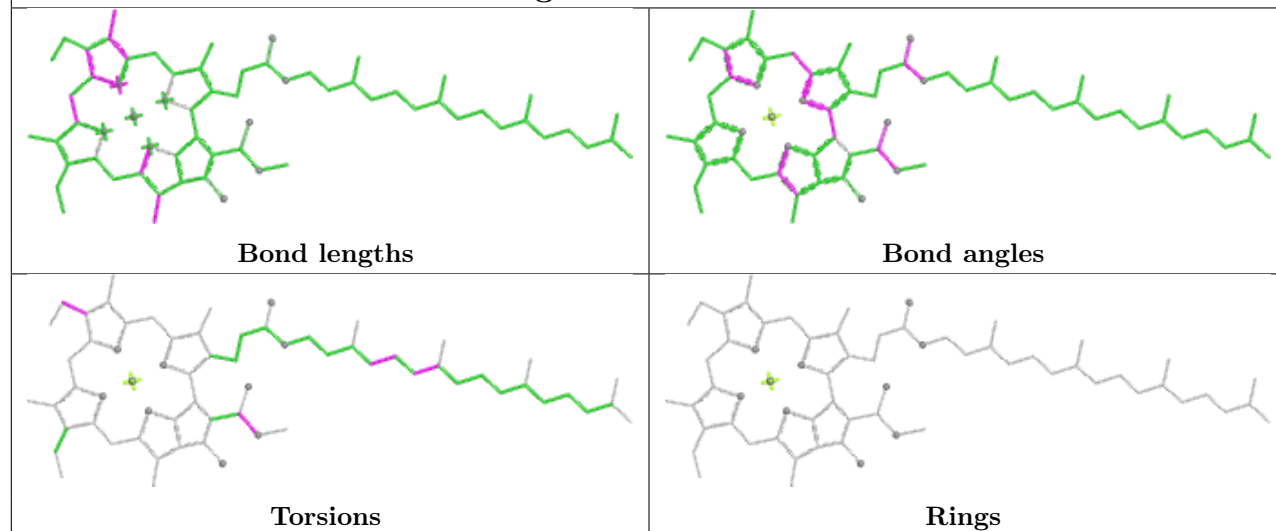


Ligand CLA b 811

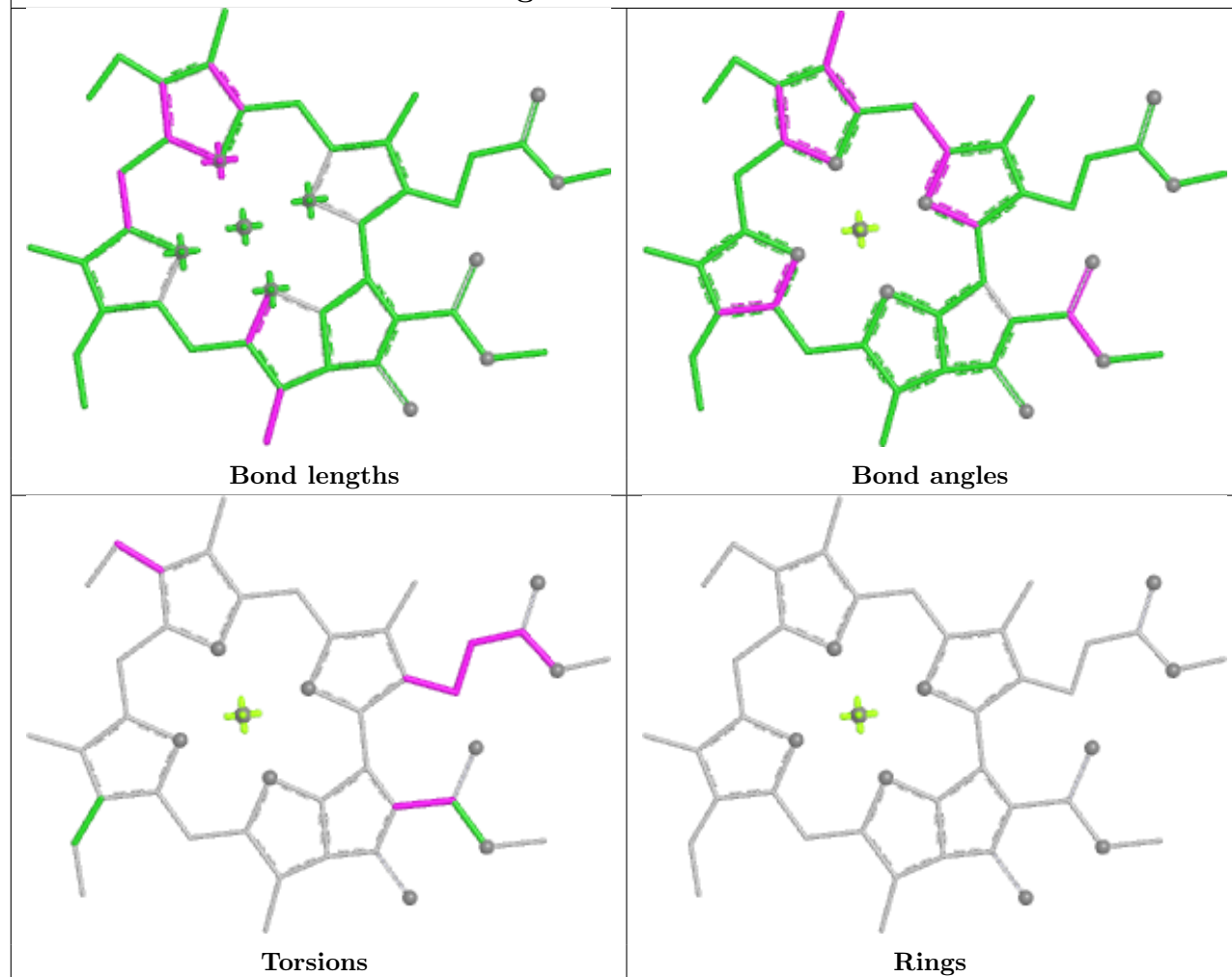


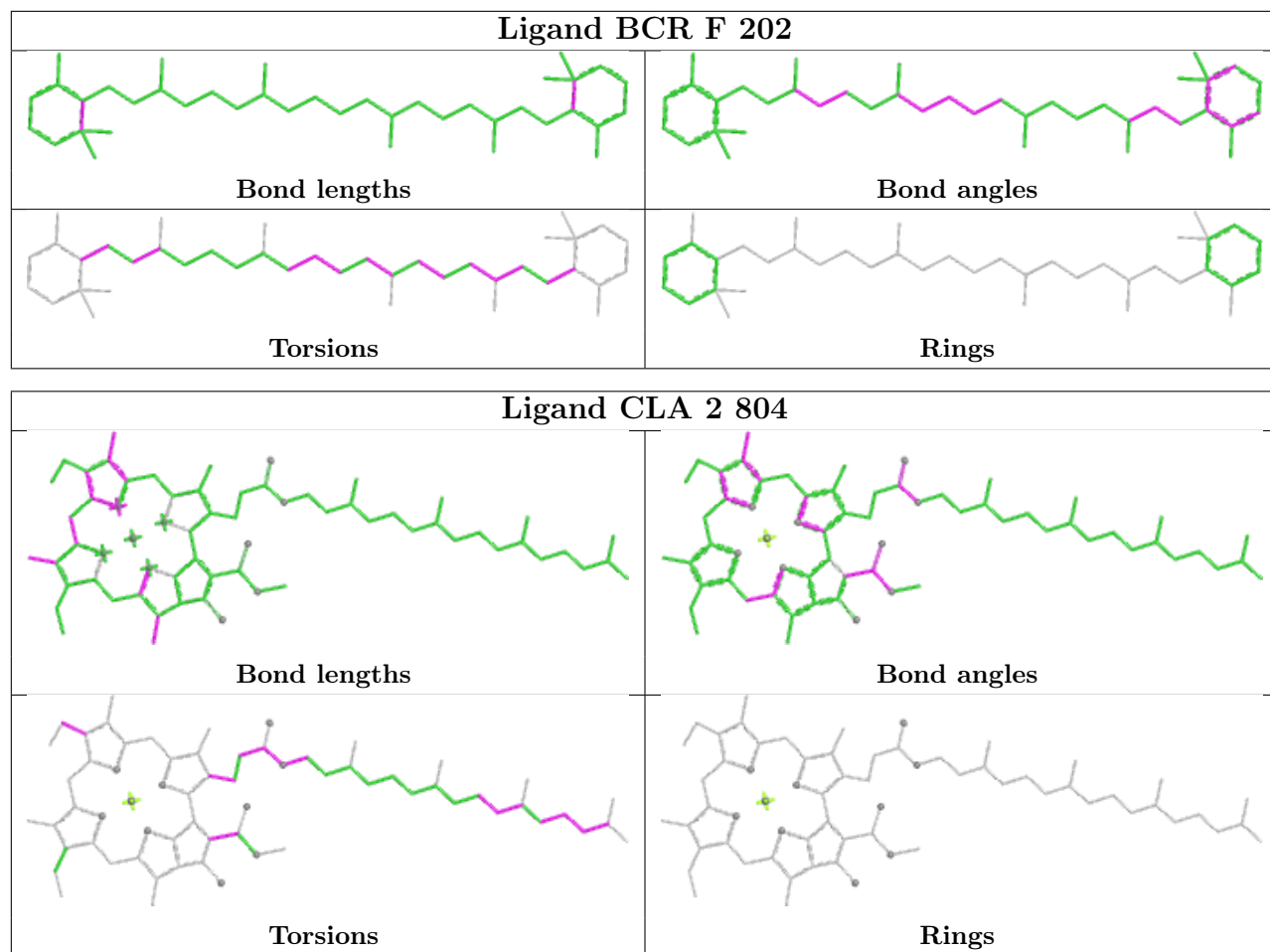


Ligand CLA b 831

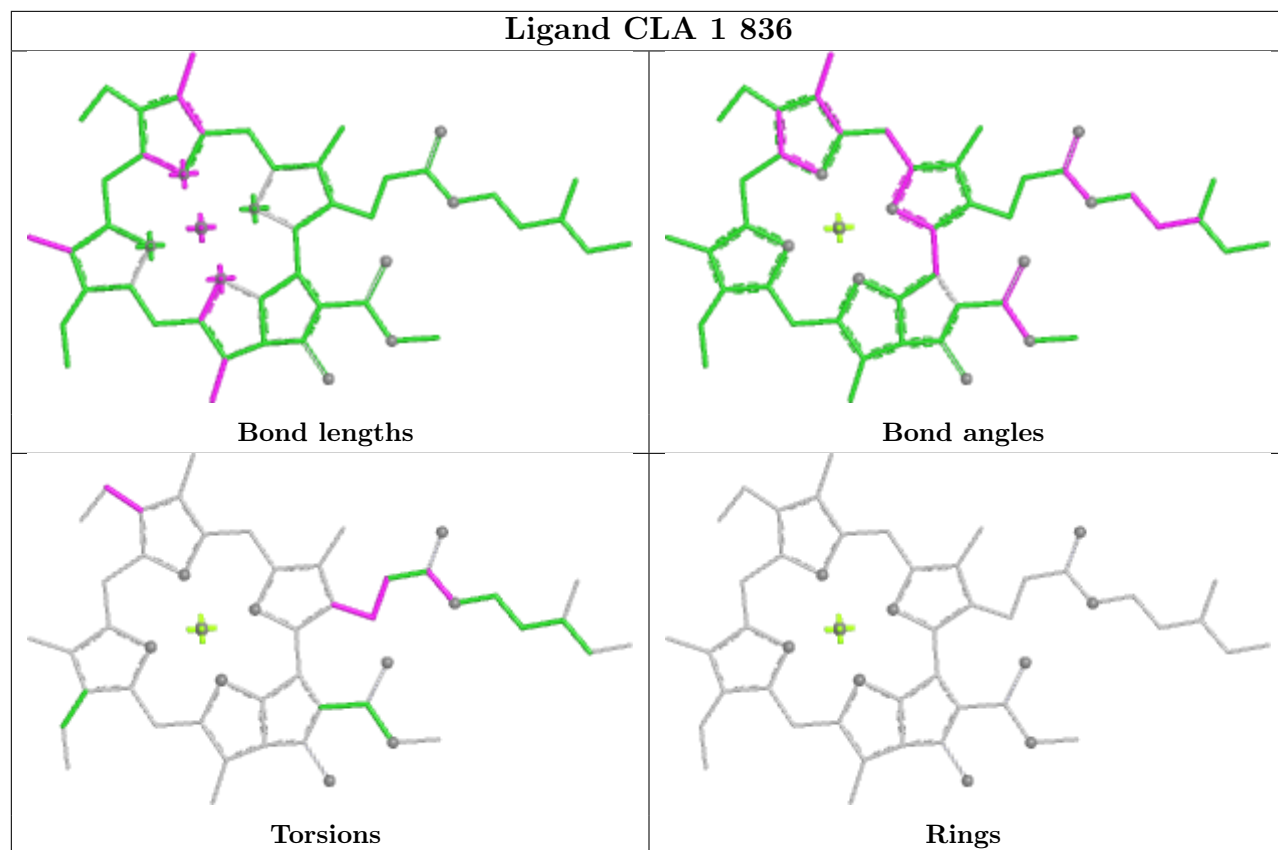


Ligand CLA b 818

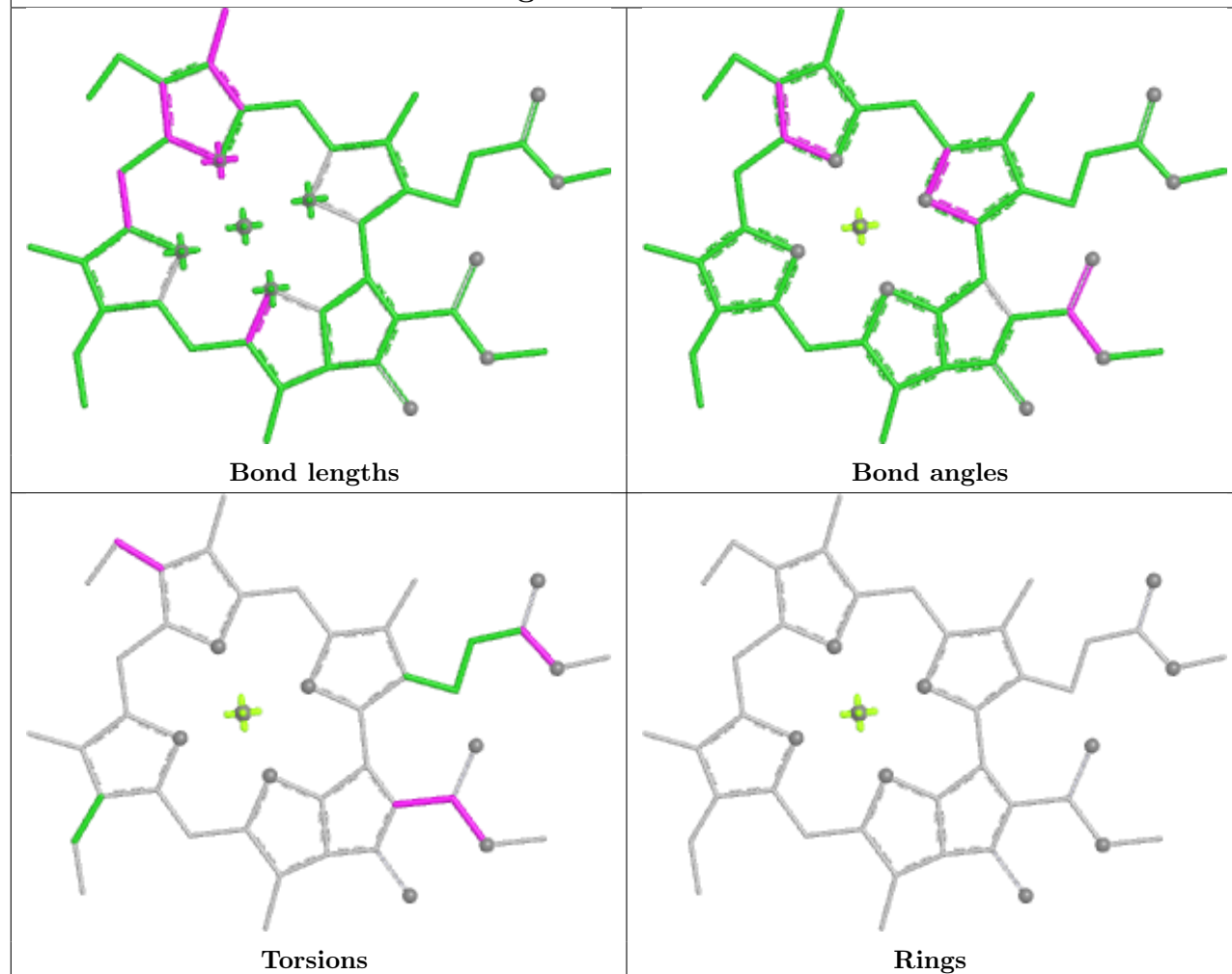




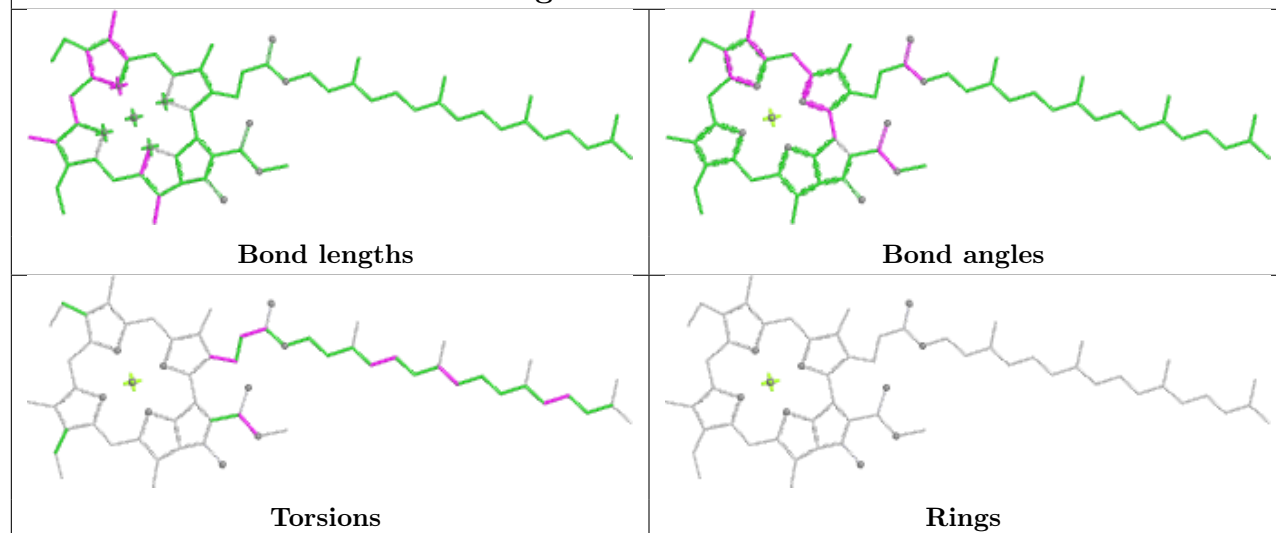
Ligand CLA 1 836



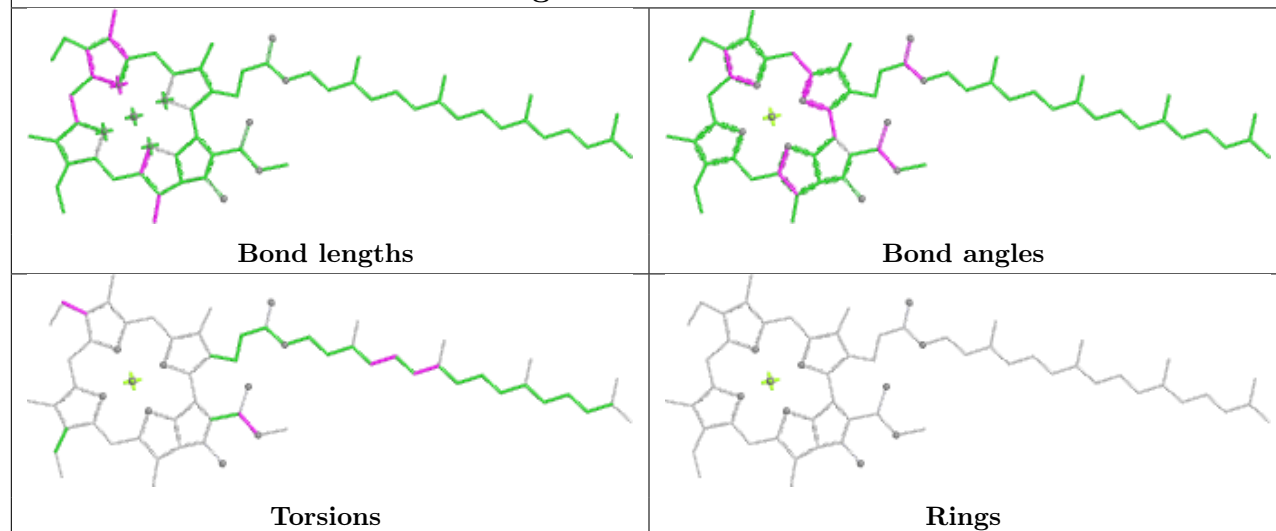
Ligand CLA 6 204



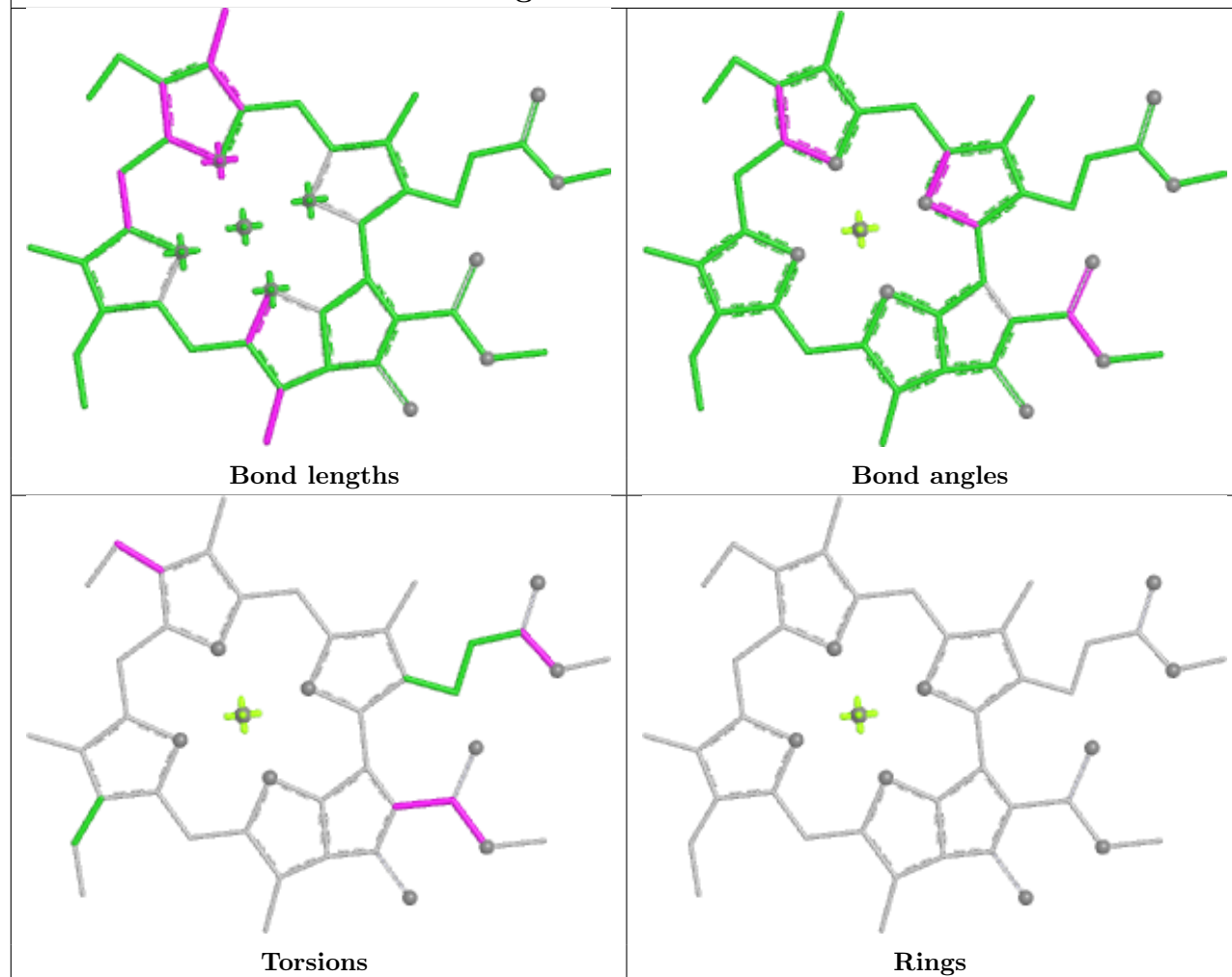
Ligand CLA b 847



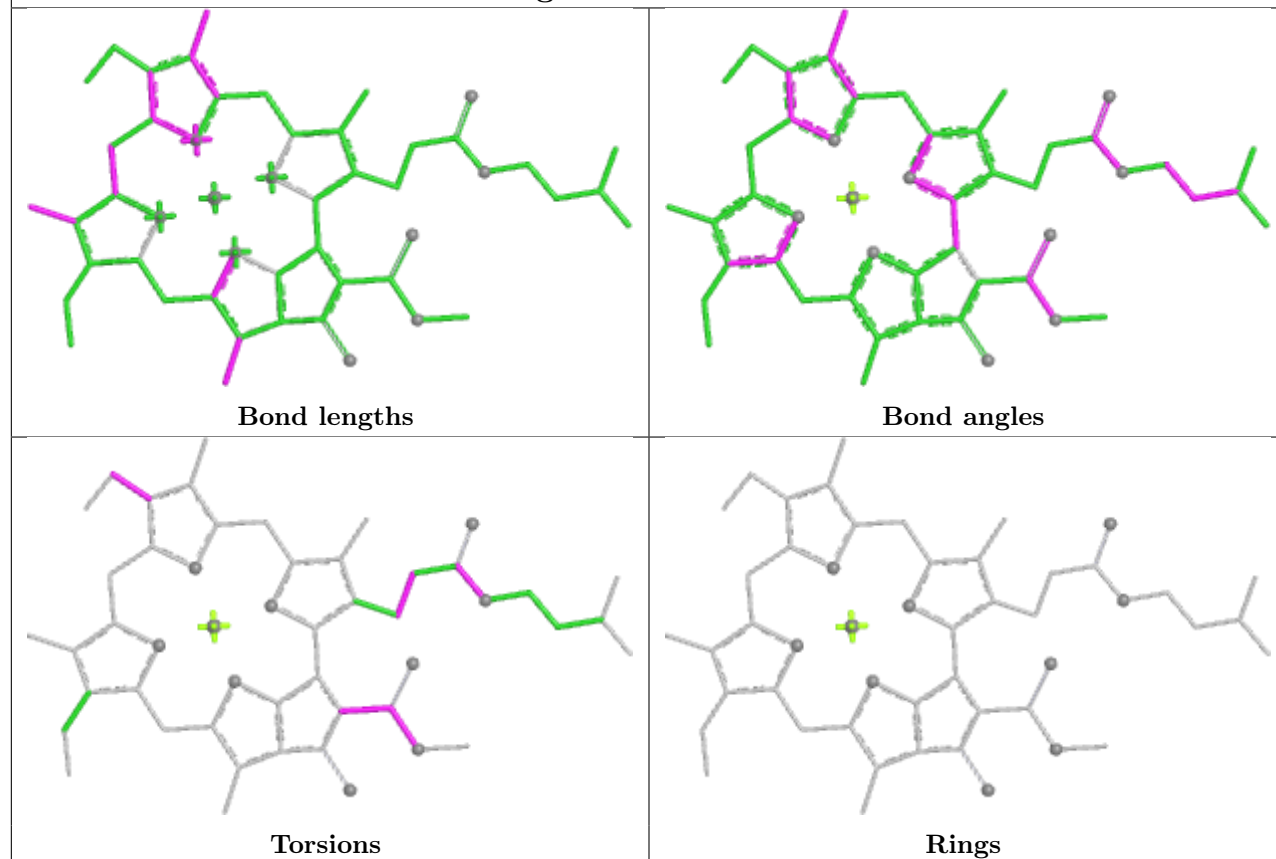
Ligand CLA B 831



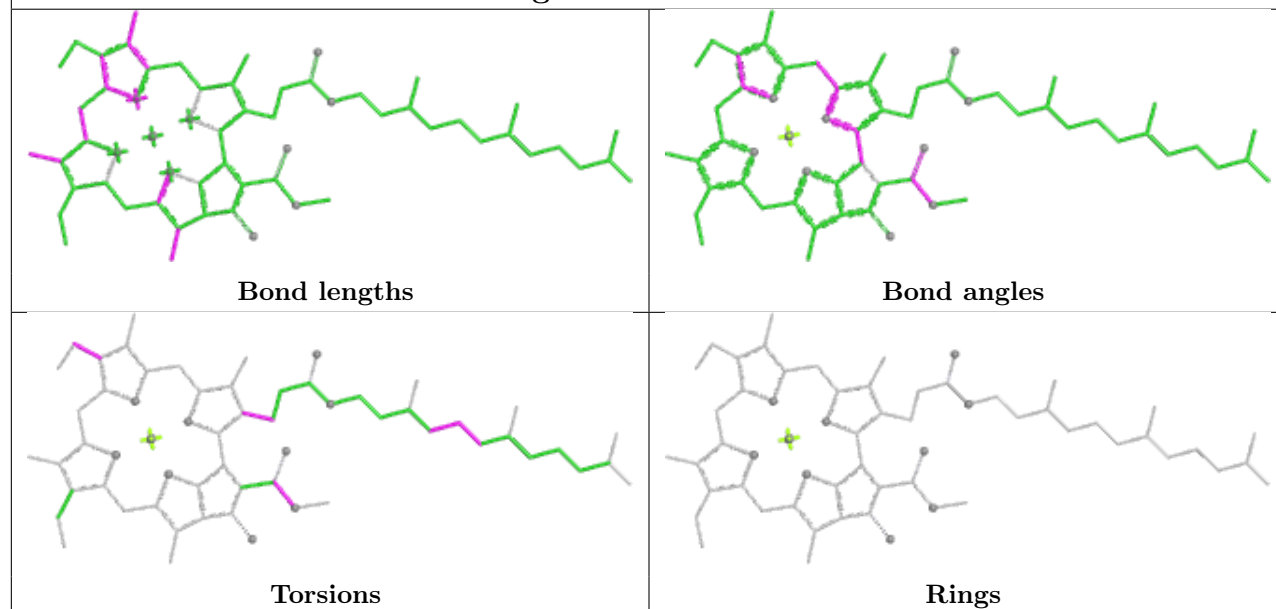
Ligand CLA F 204

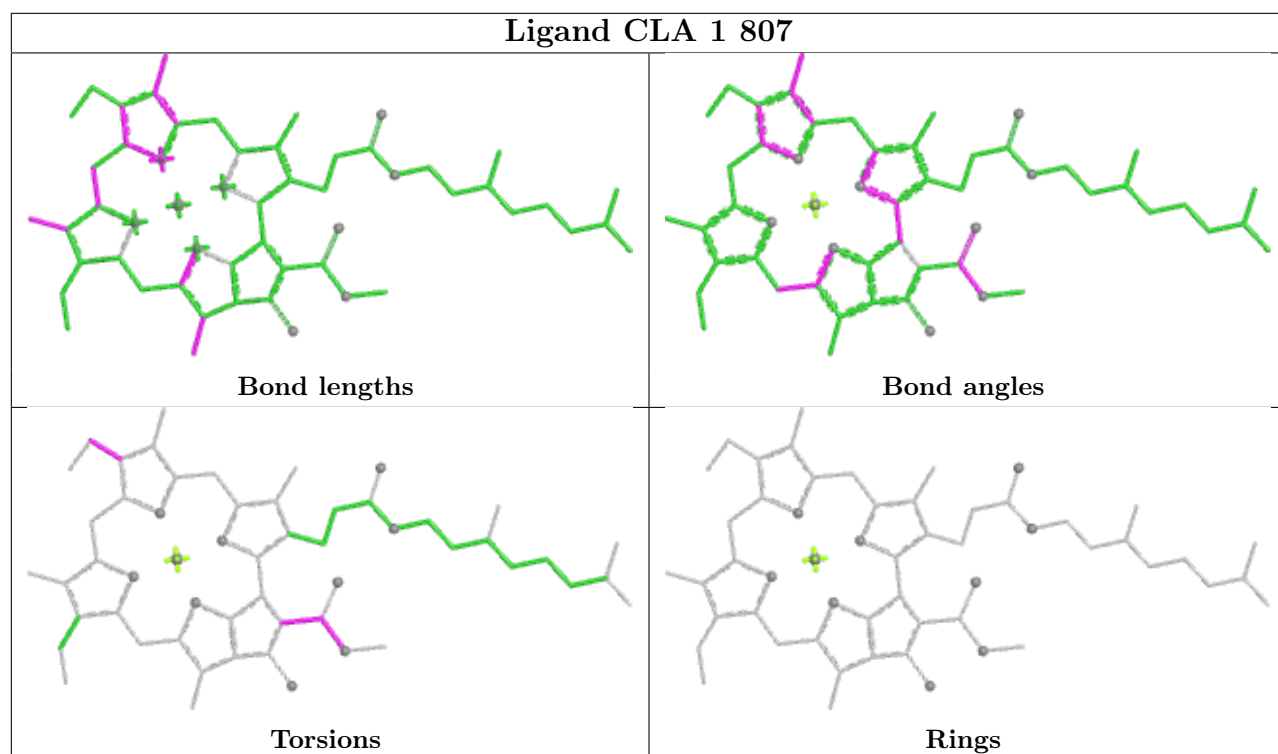
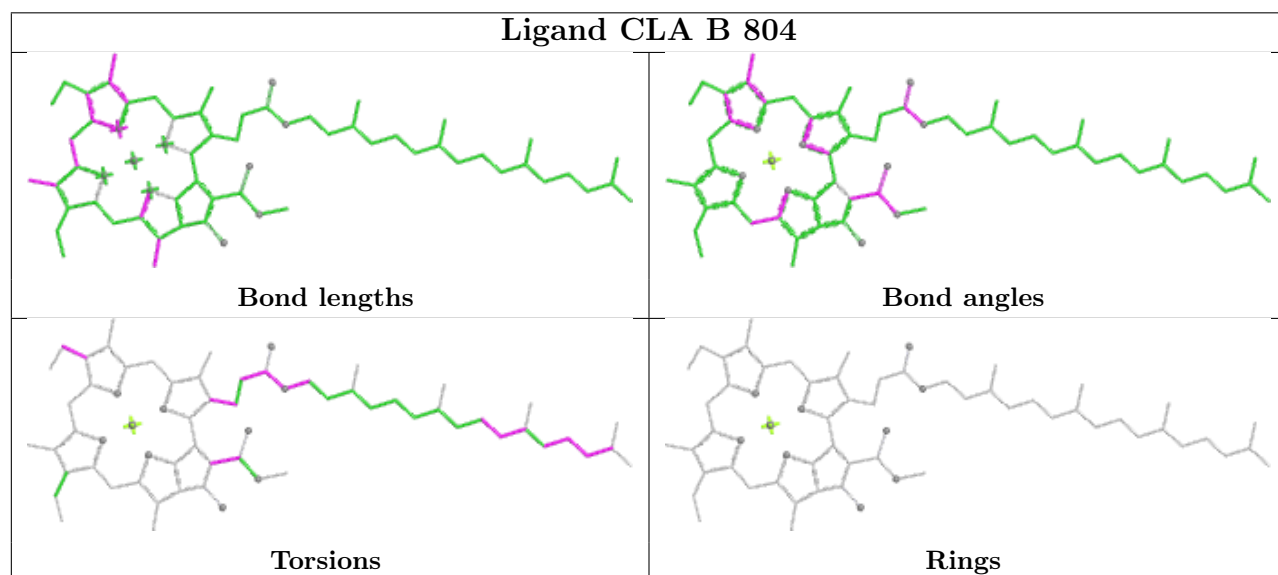
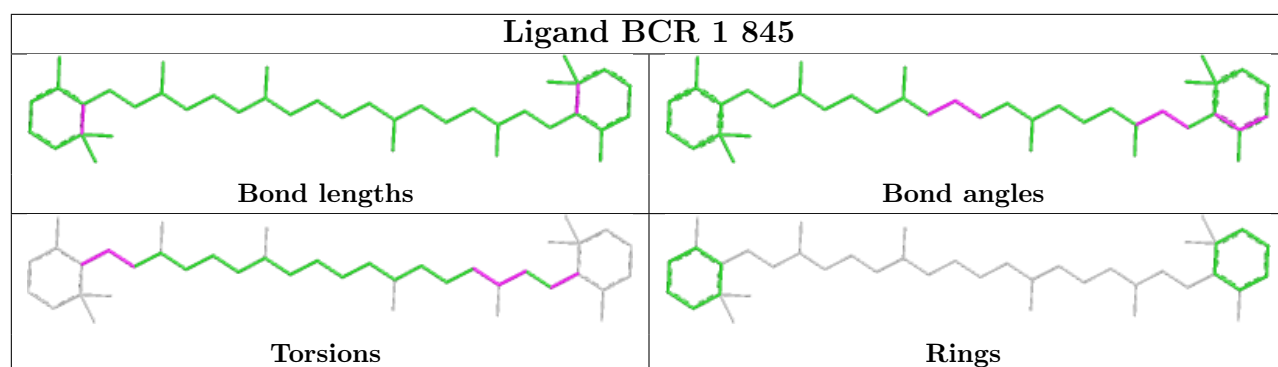


Ligand CLA a 822

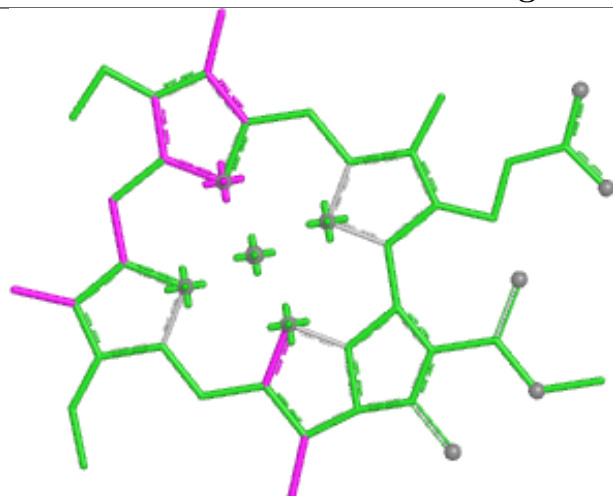


Ligand CLA B 816

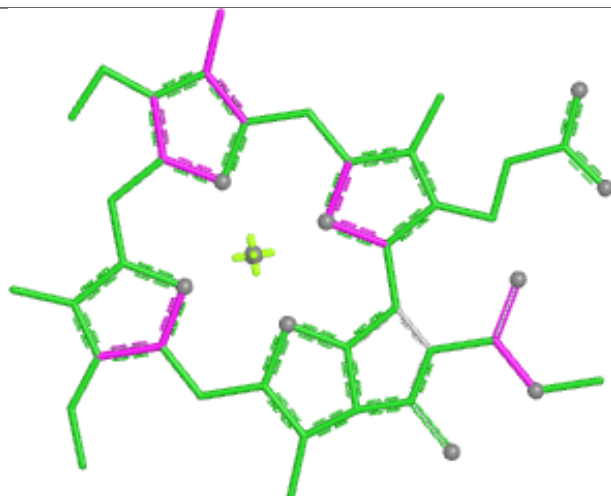




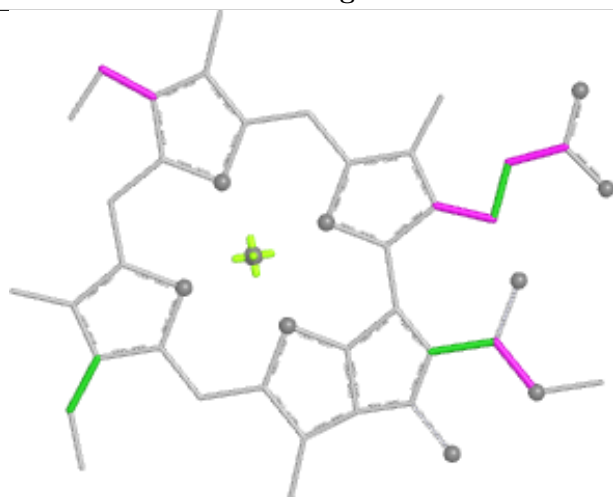
Ligand CLA 1 810



Bond lengths



Bond angles

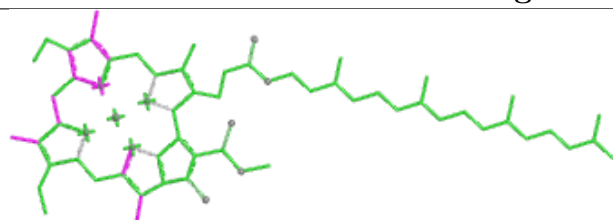


Torsions

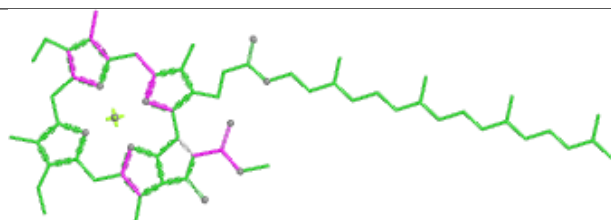


Rings

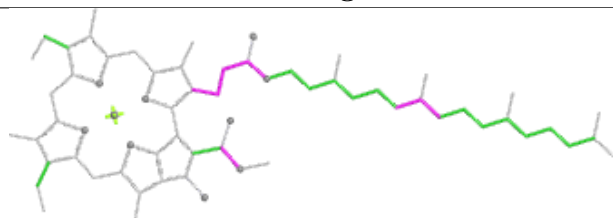
Ligand CLA B 815



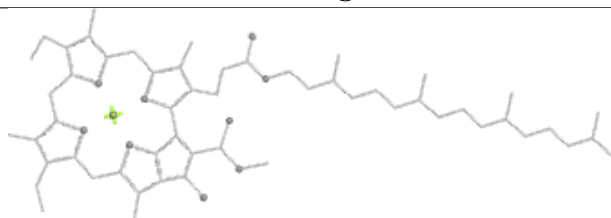
Bond lengths



Bond angles

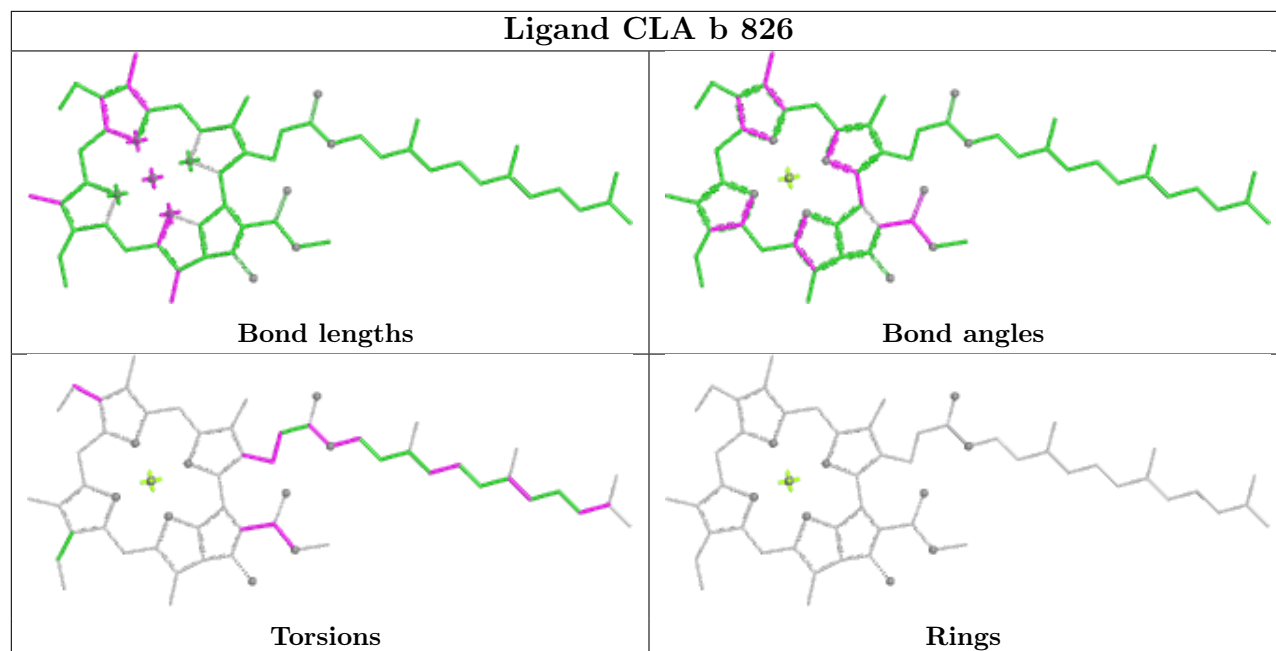


Torsions

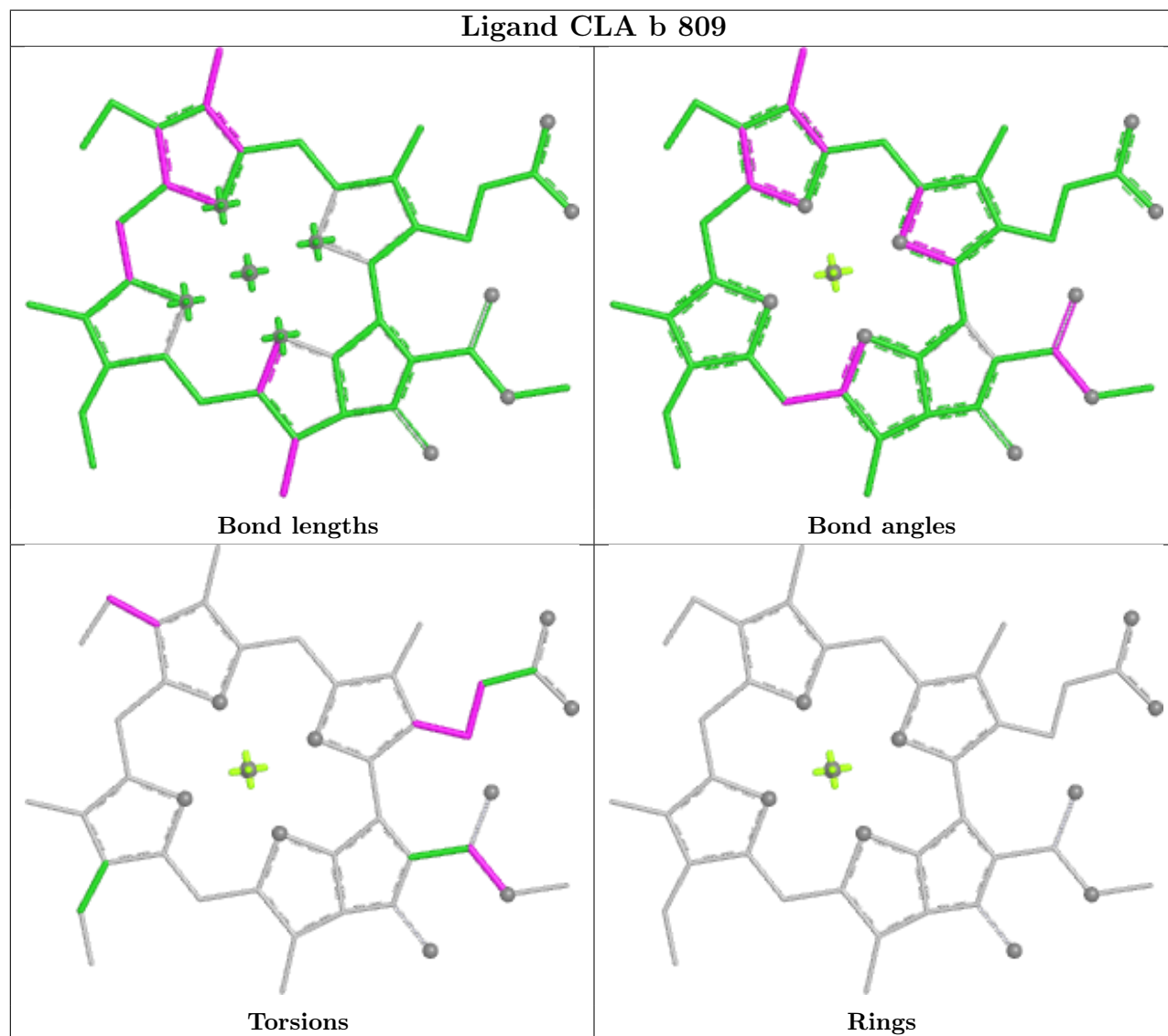


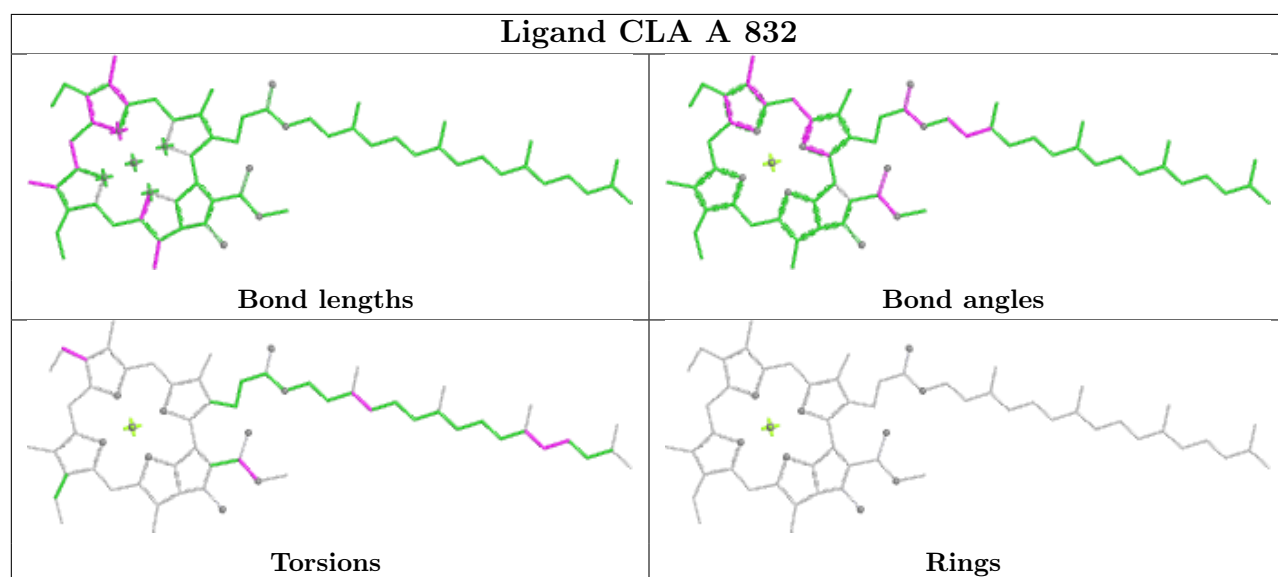
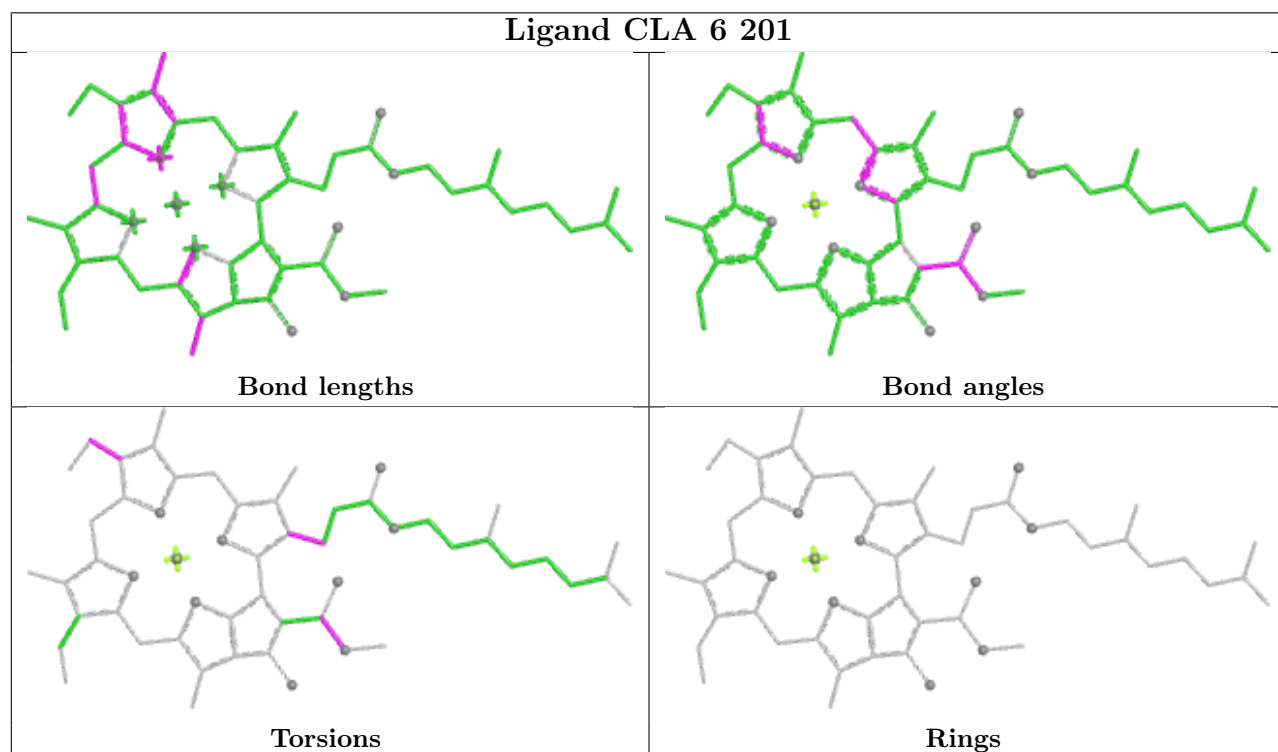
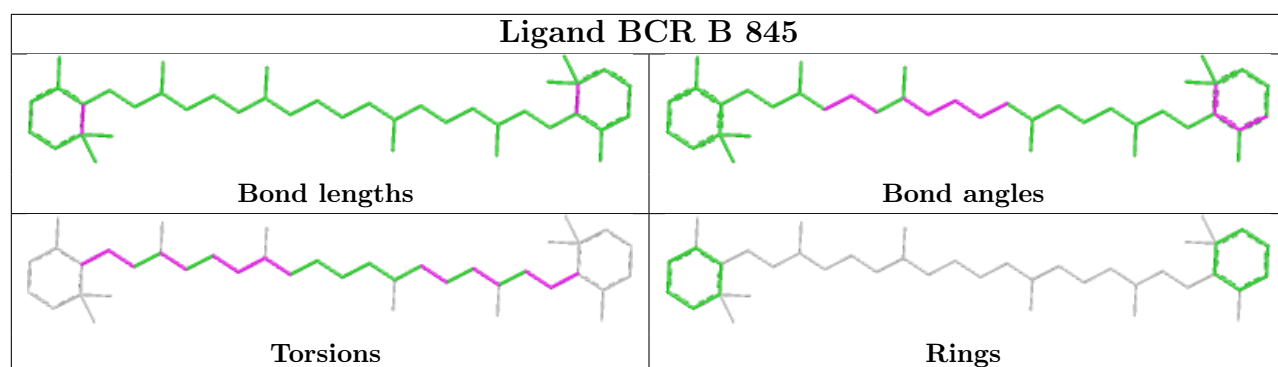
Rings

Ligand CLA b 826

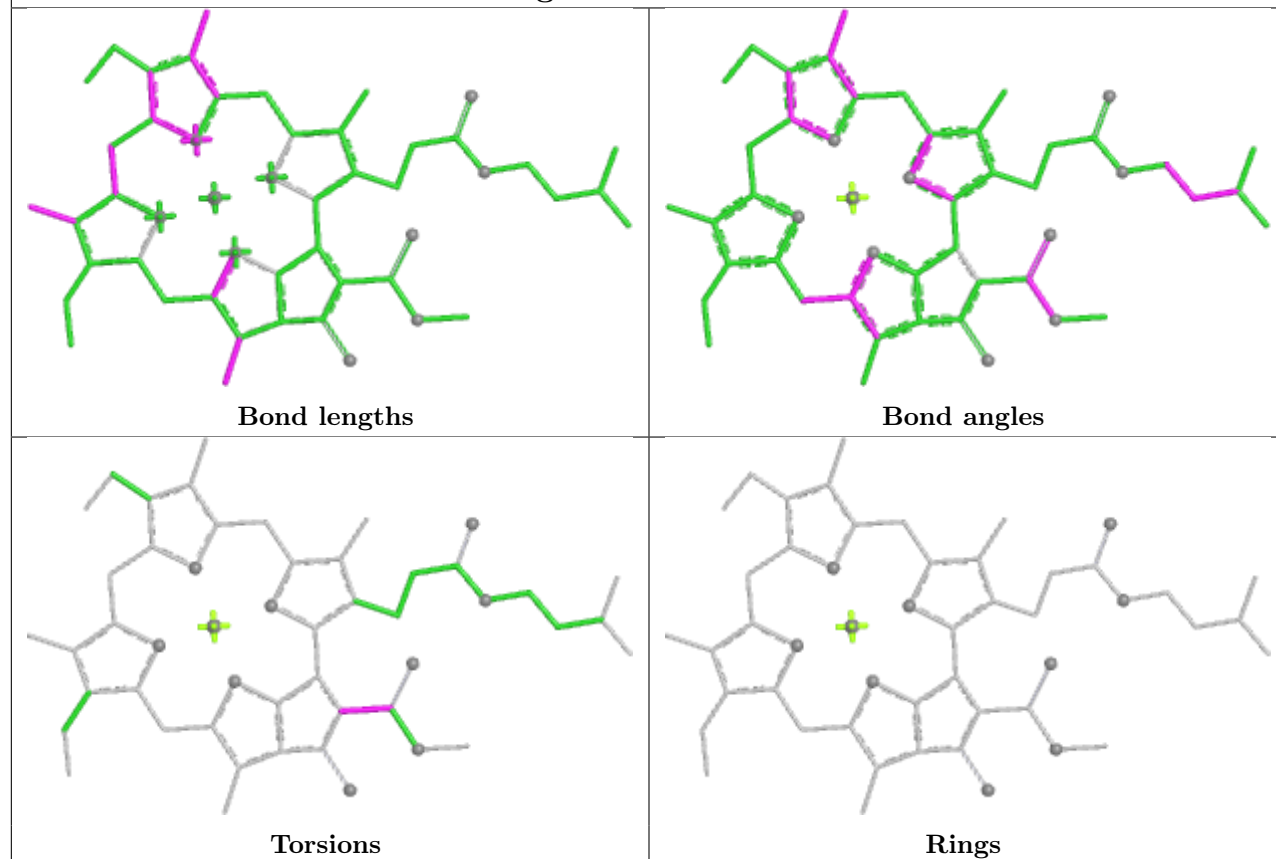


Ligand CLA b 809

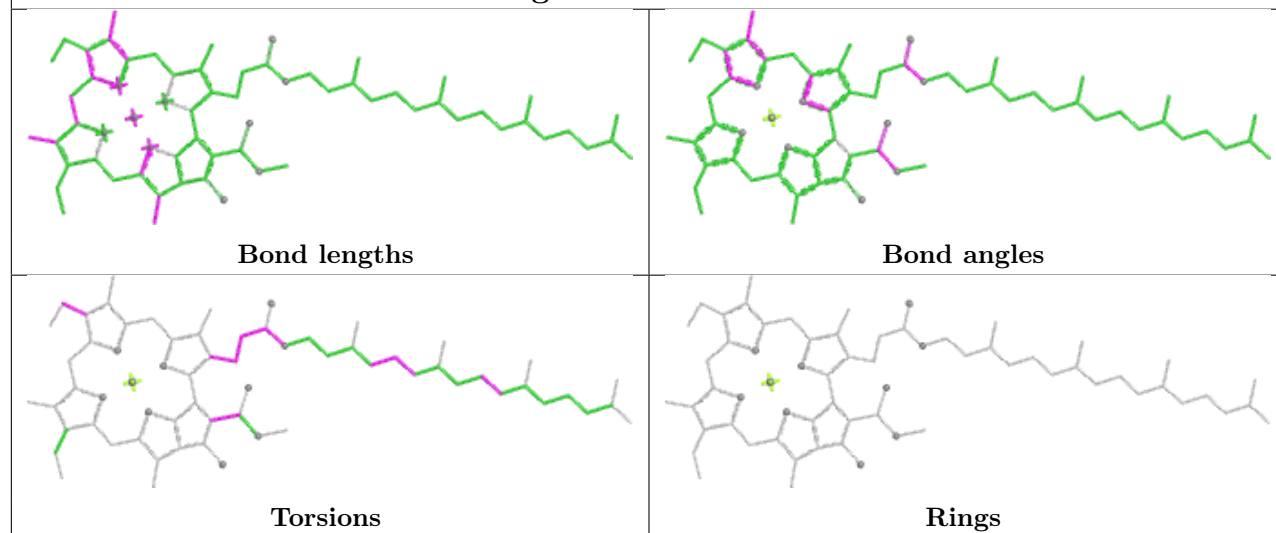


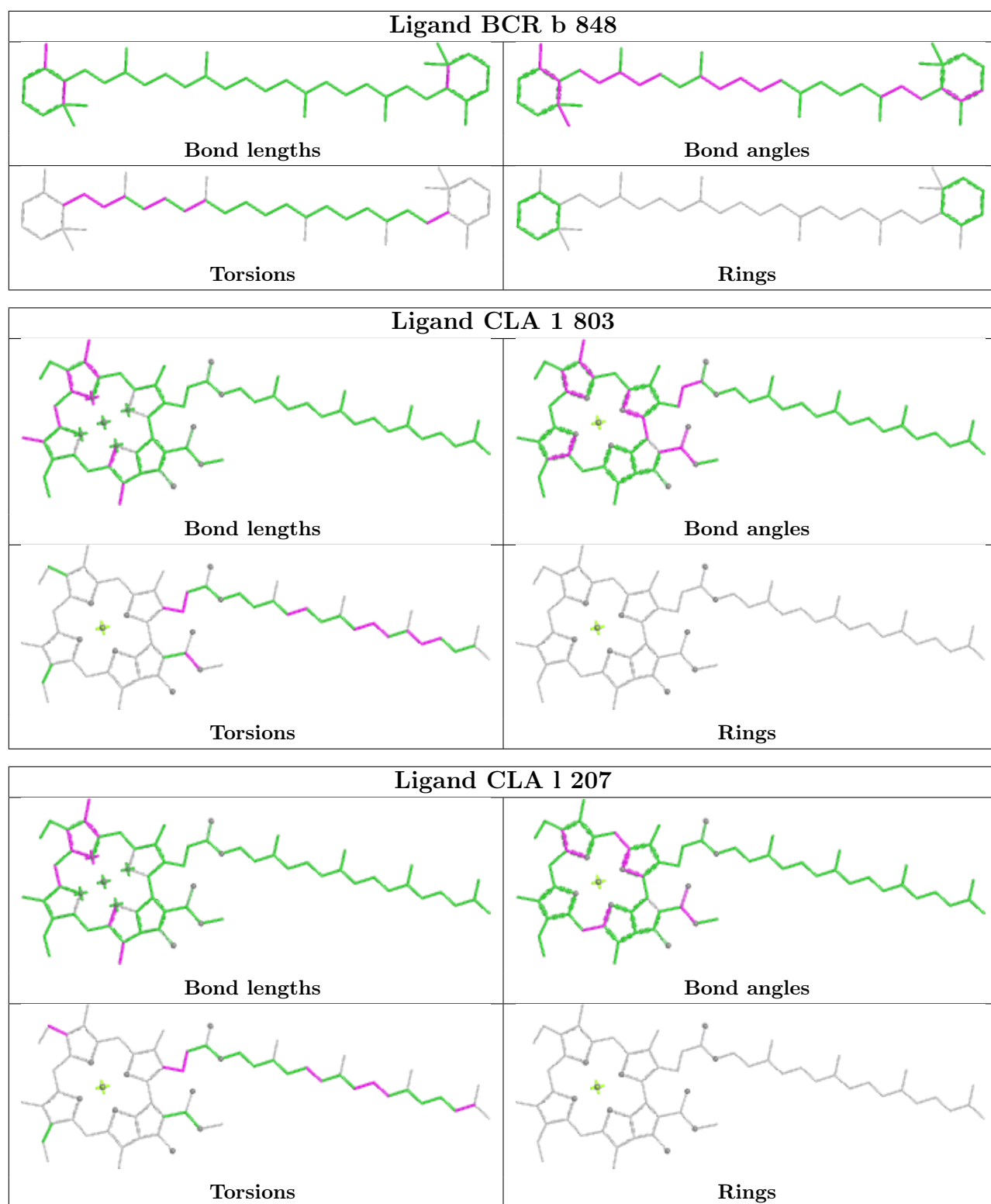


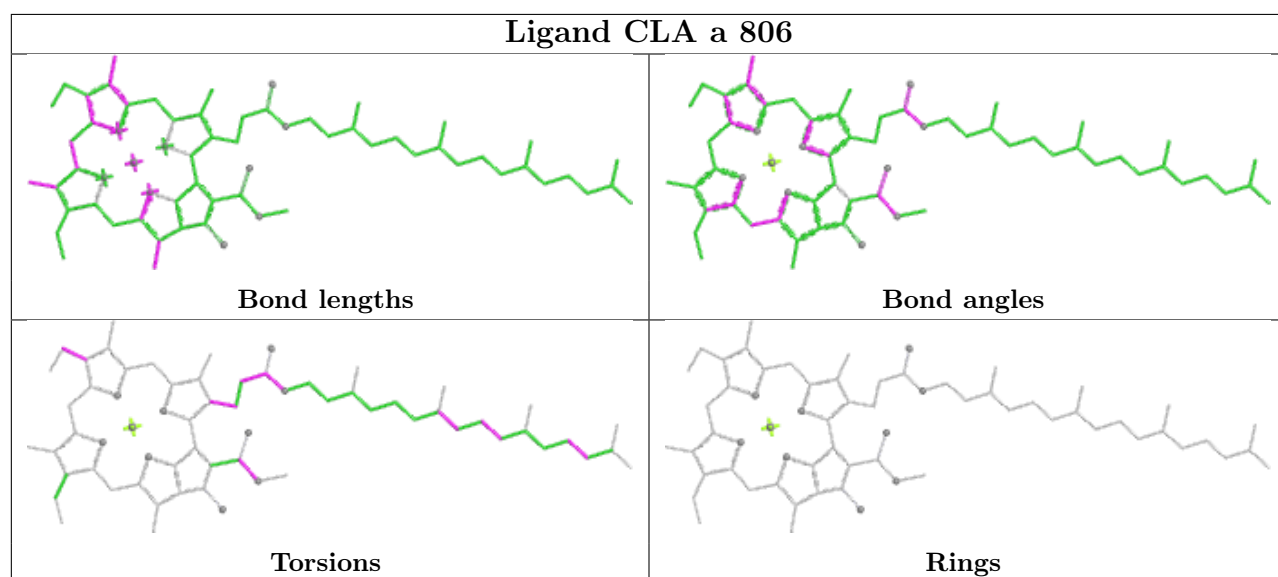
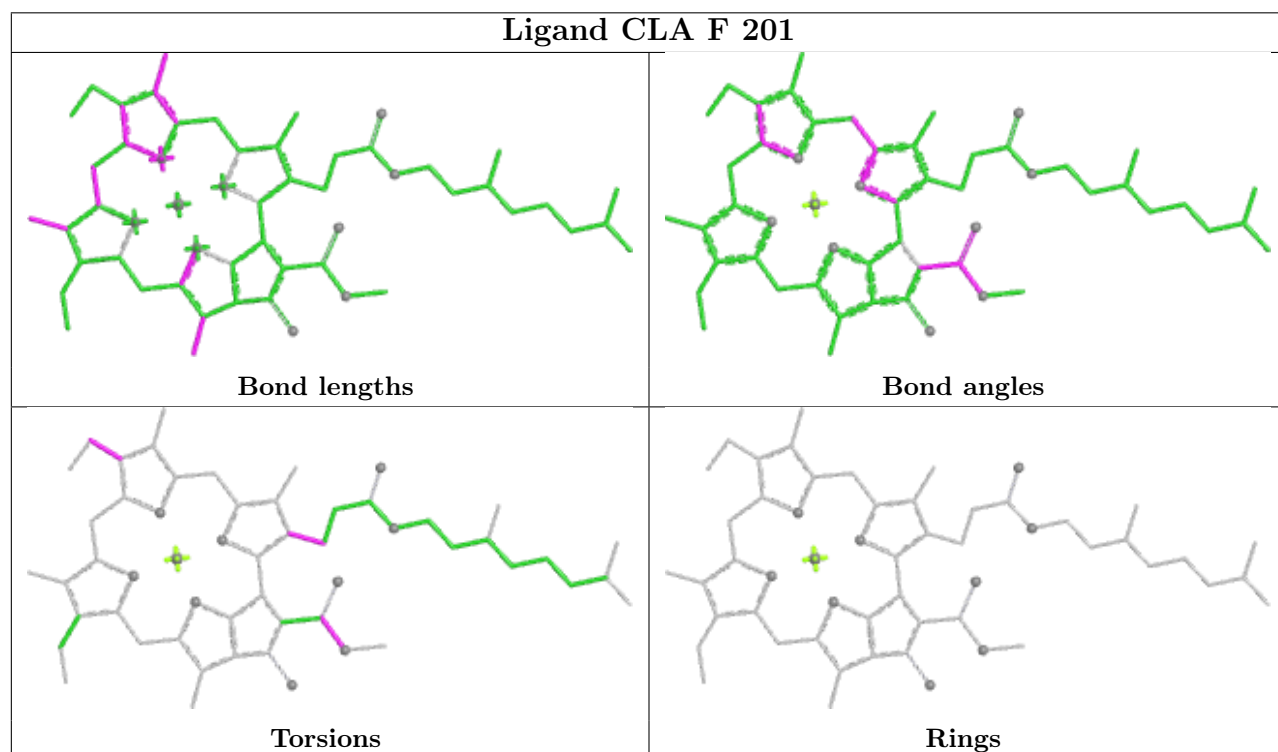
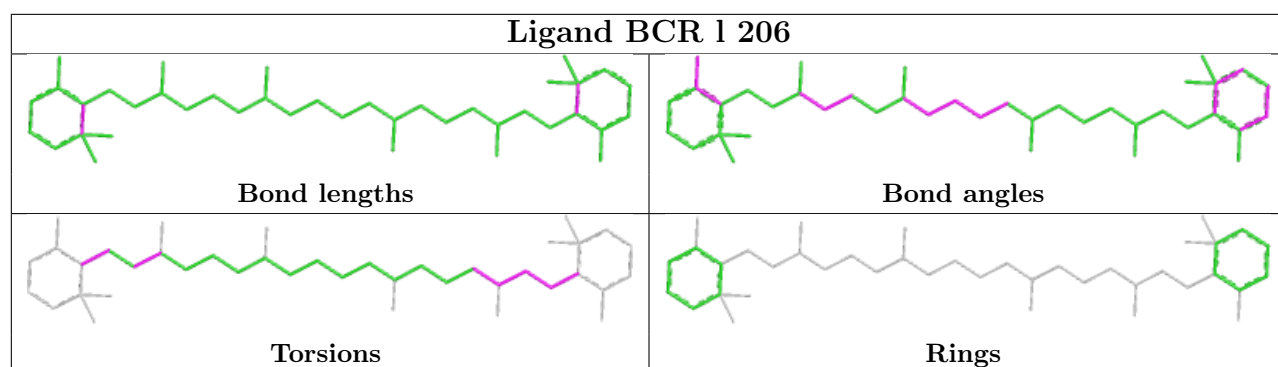
Ligand CLA 2 821



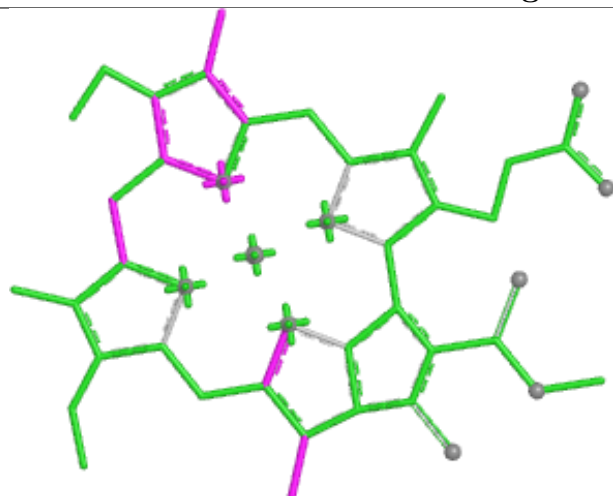
Ligand CLA A 827



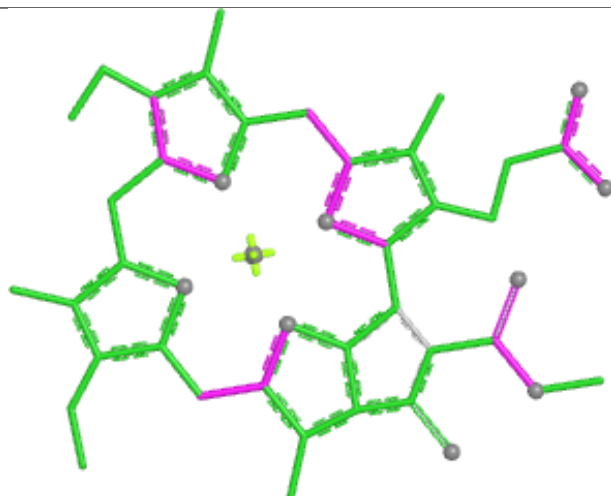




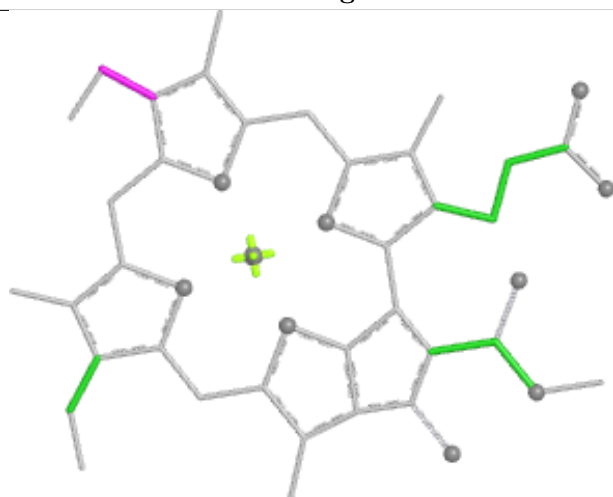
Ligand CLA f 203



Bond lengths



Bond angles

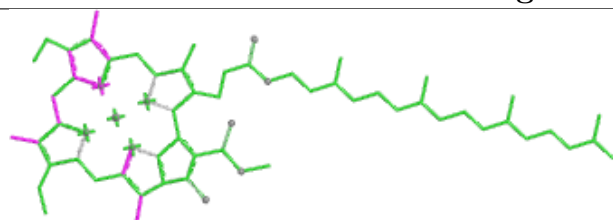


Torsions

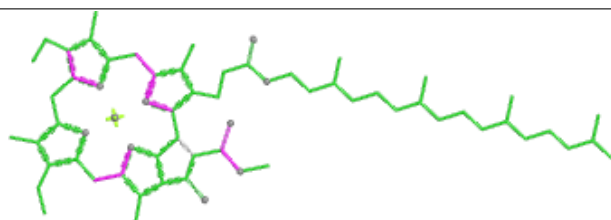


Rings

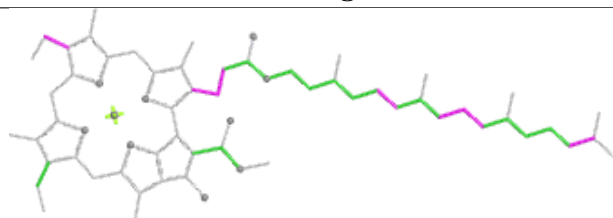
Ligand CLA L 206



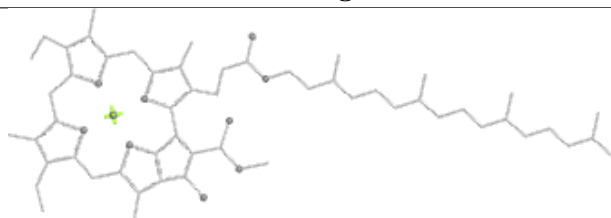
Bond lengths



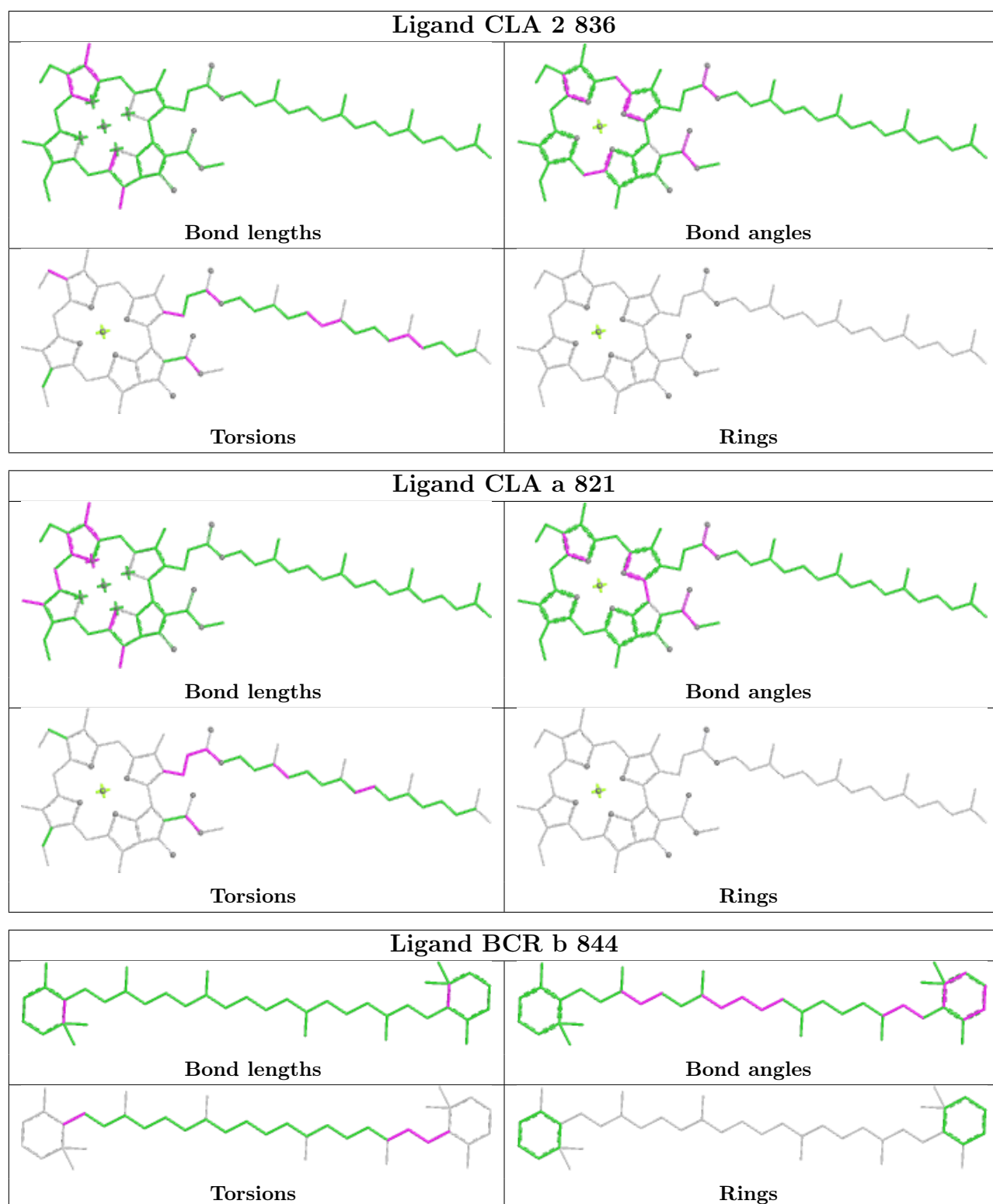
Bond angles

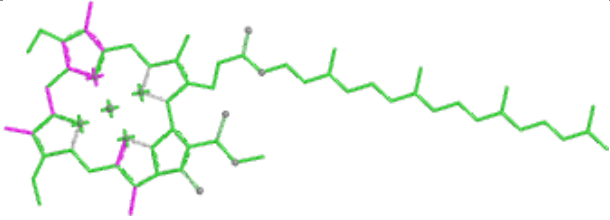
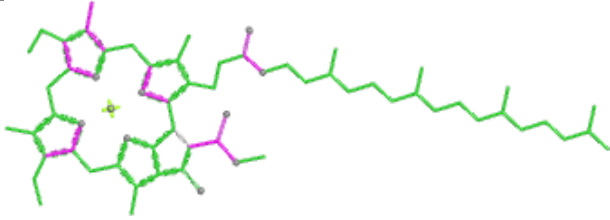
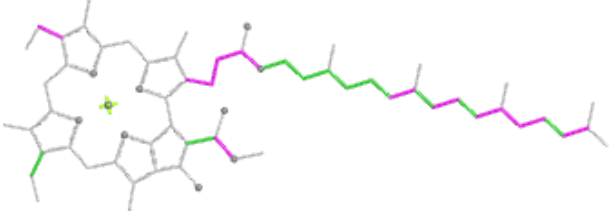
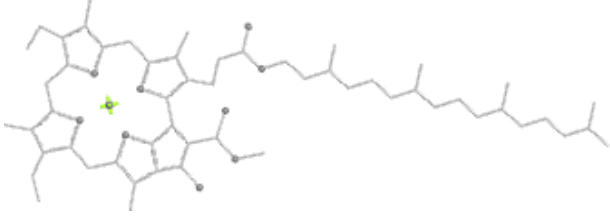
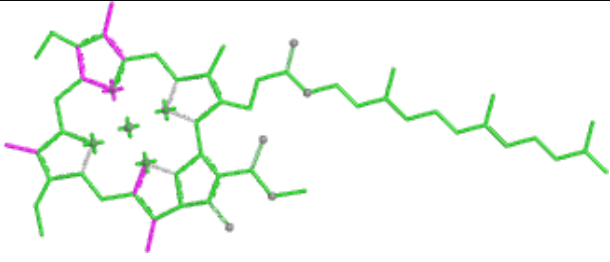
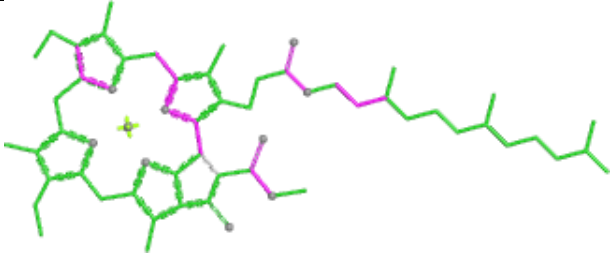
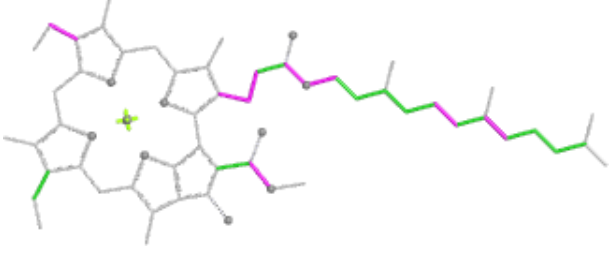
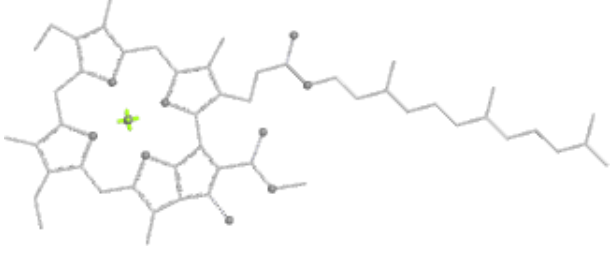


Torsions

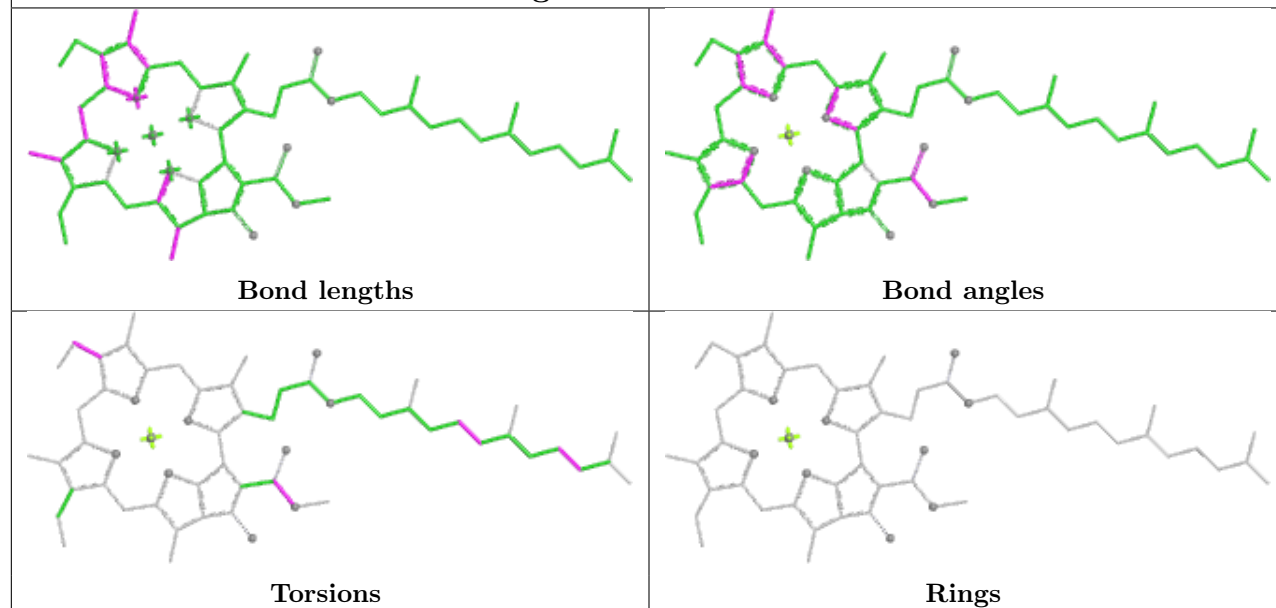


Rings

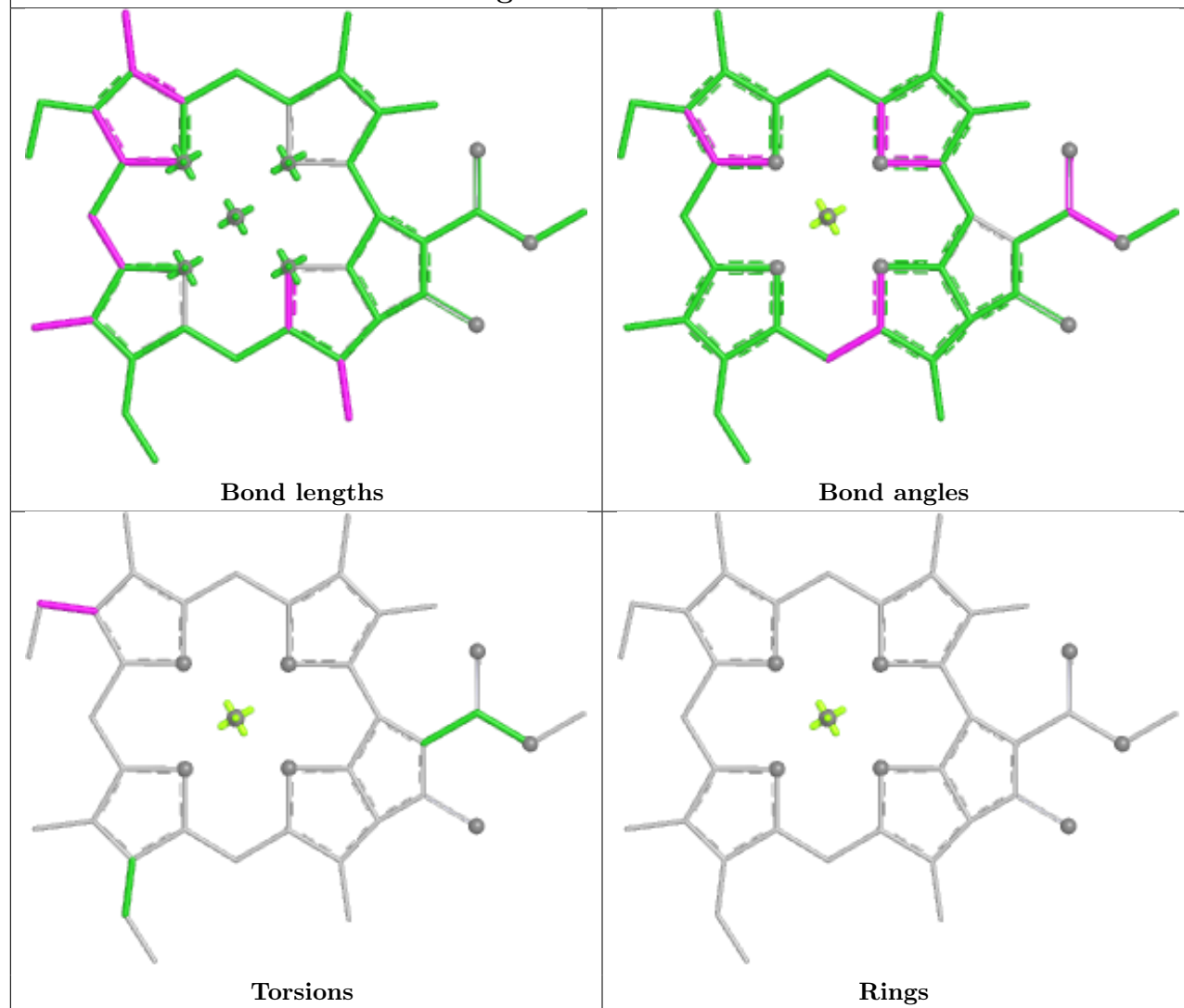


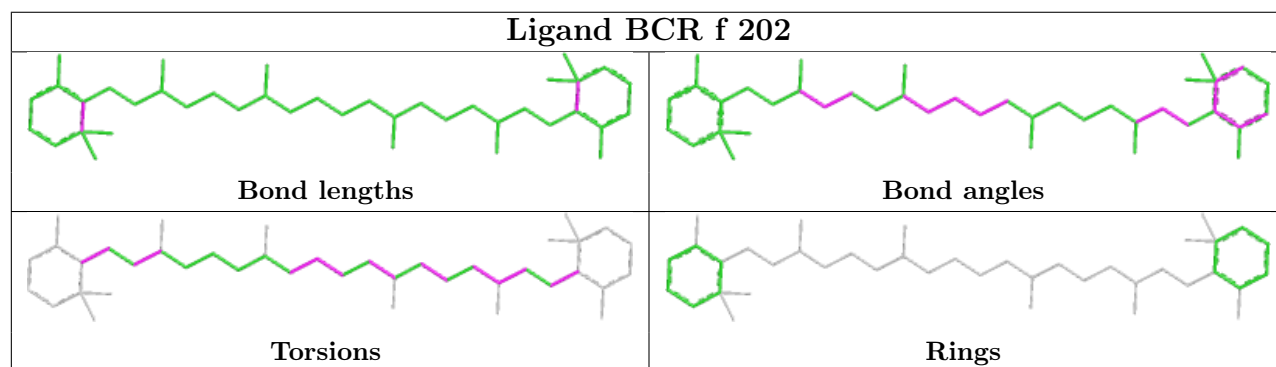
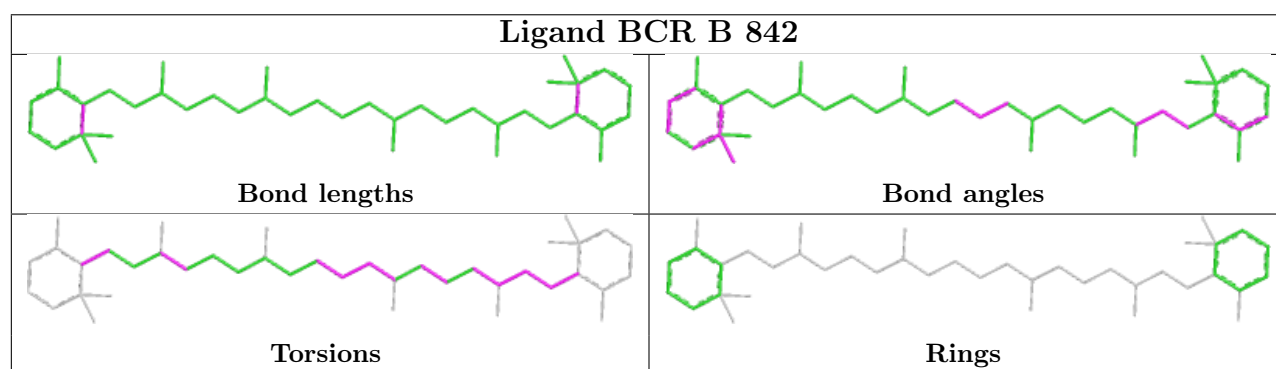
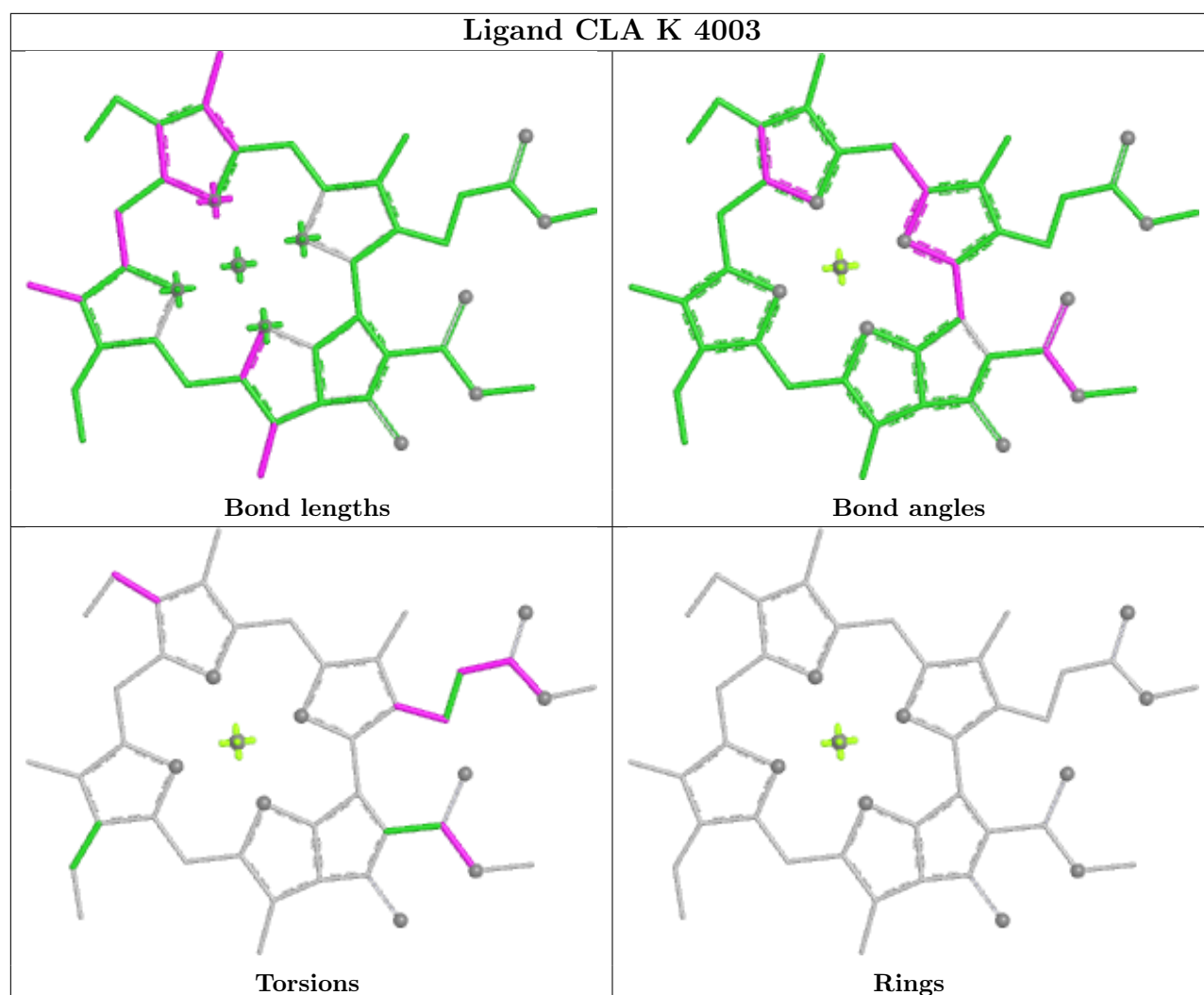
Ligand CLA B 821	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1 841	
 Bond lengths	 Bond angles
 Torsions	 Rings

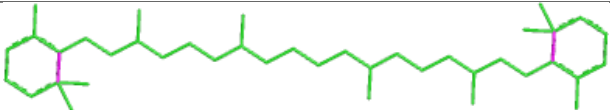
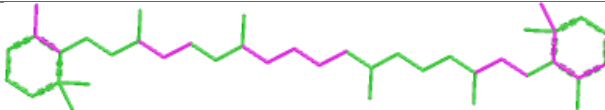
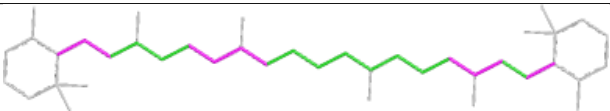
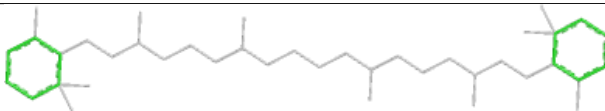
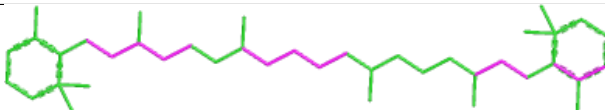
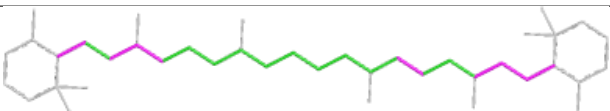
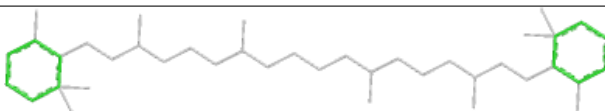
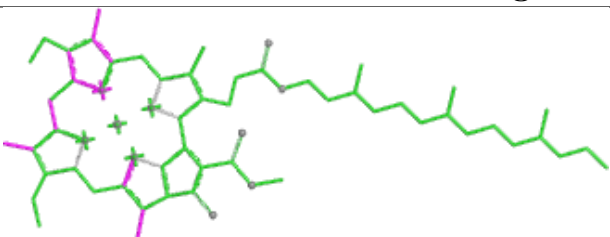
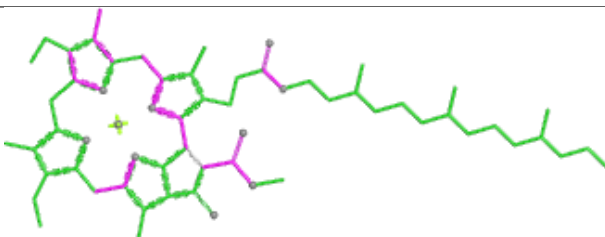
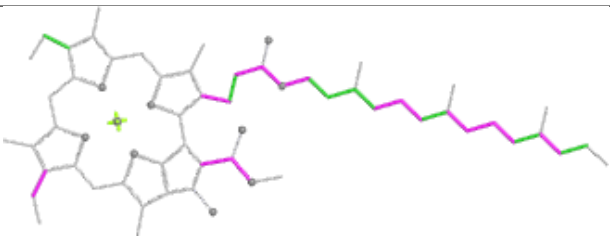
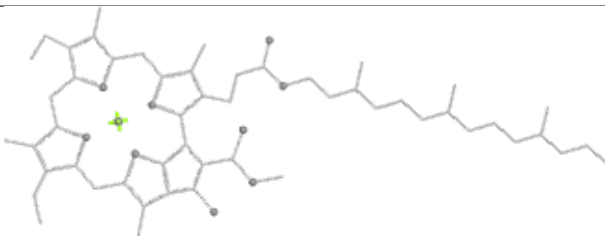
Ligand CLA B 834

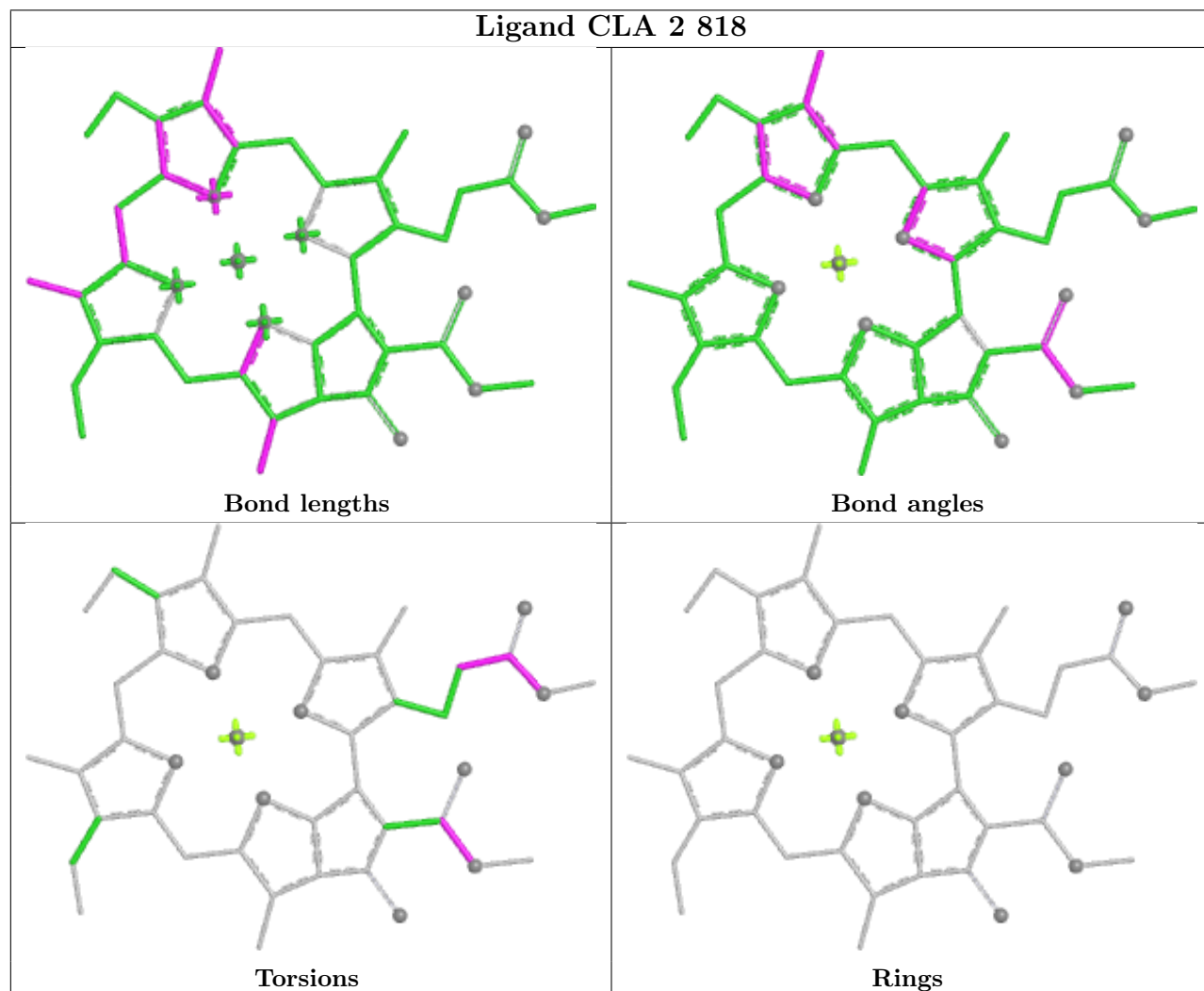
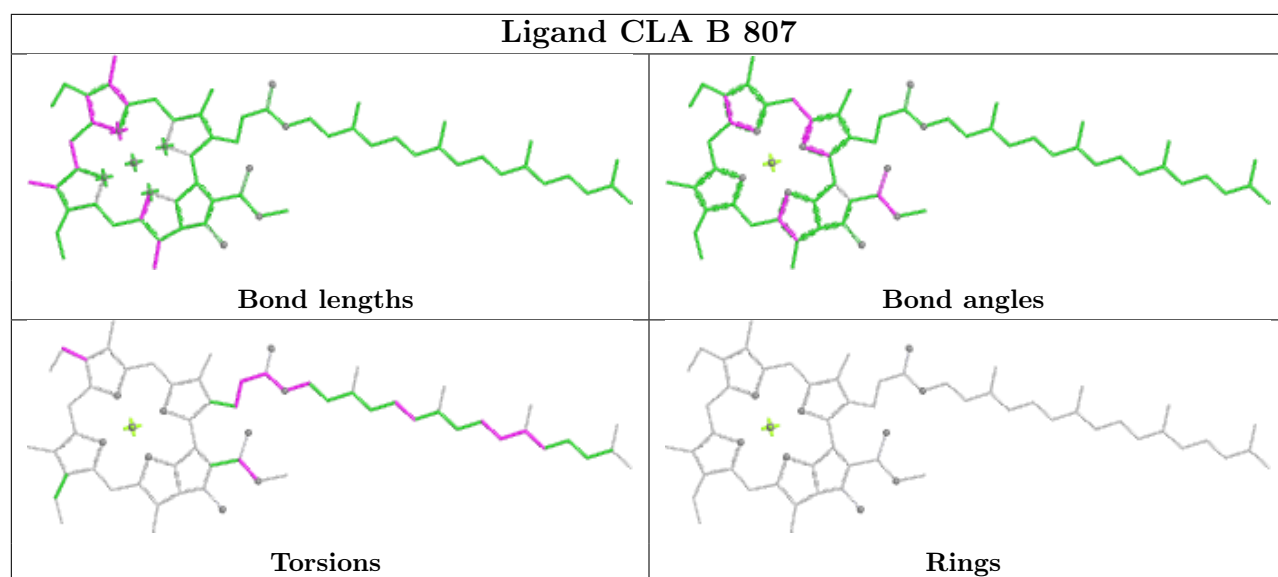


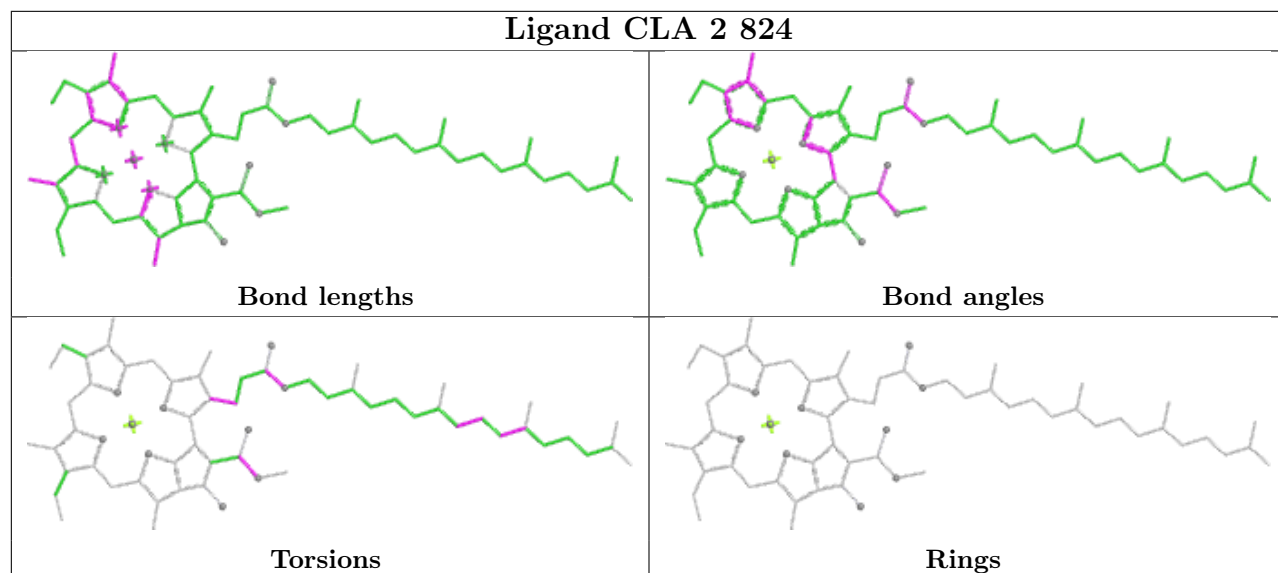
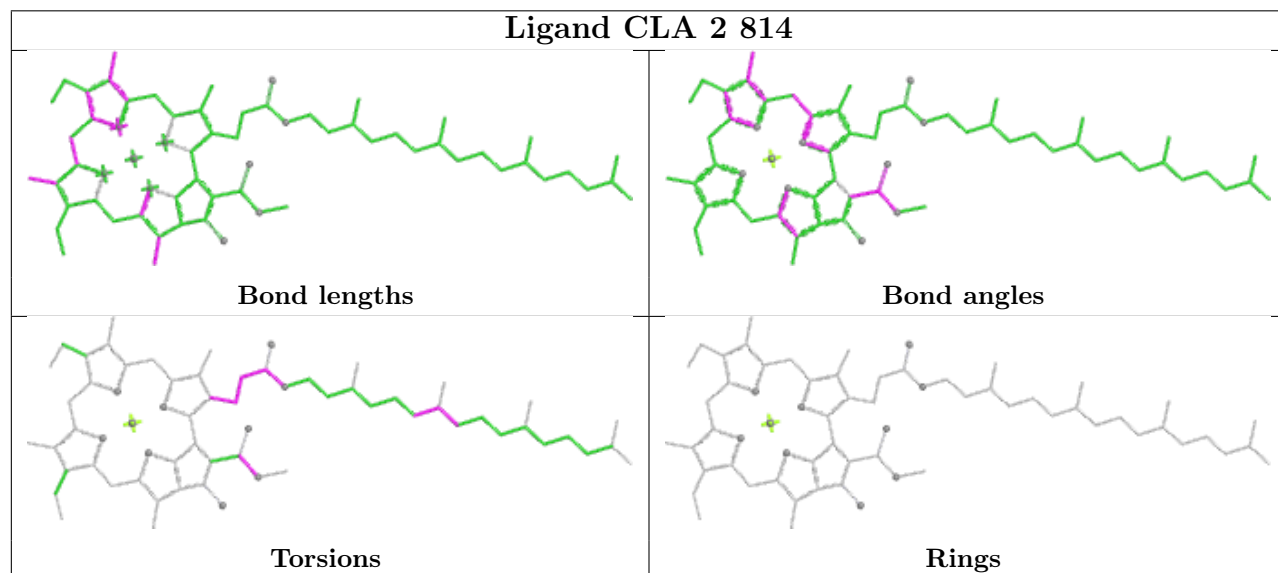
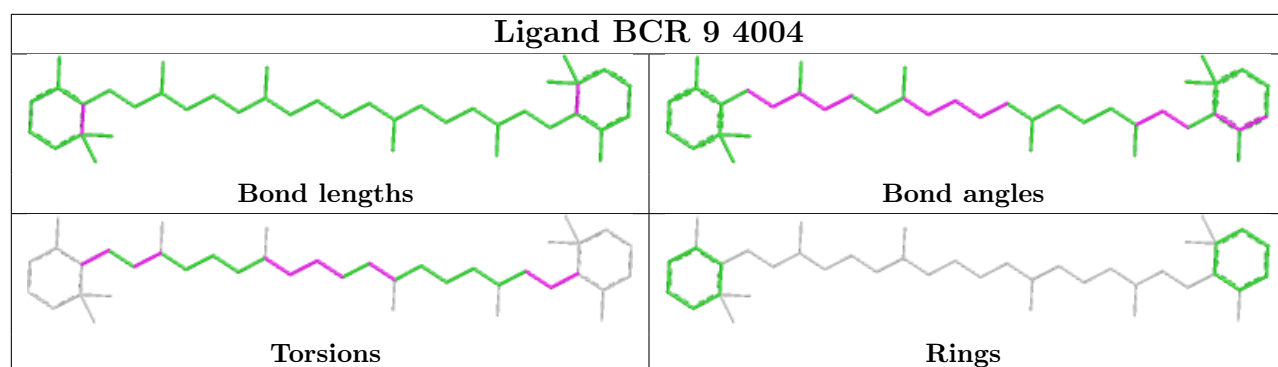
Ligand CLA b 817

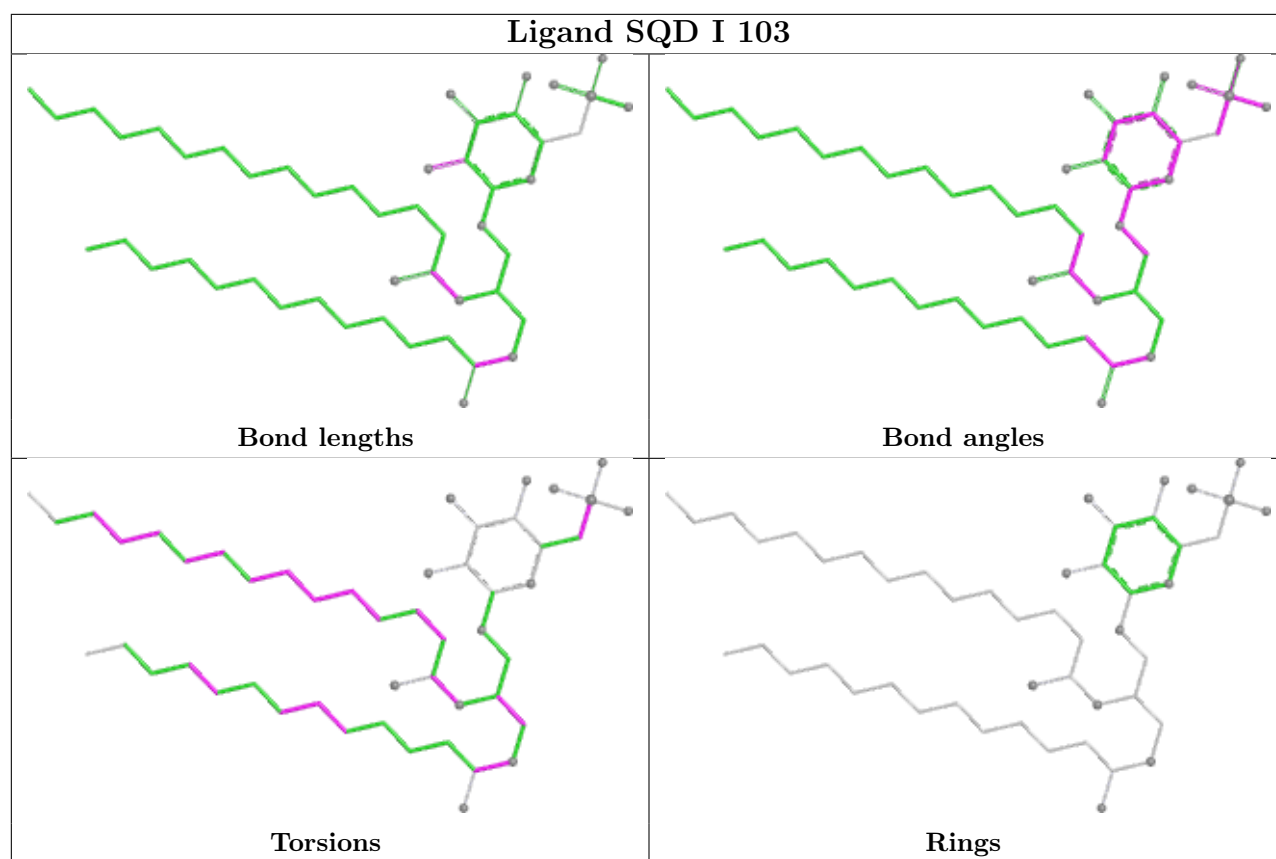




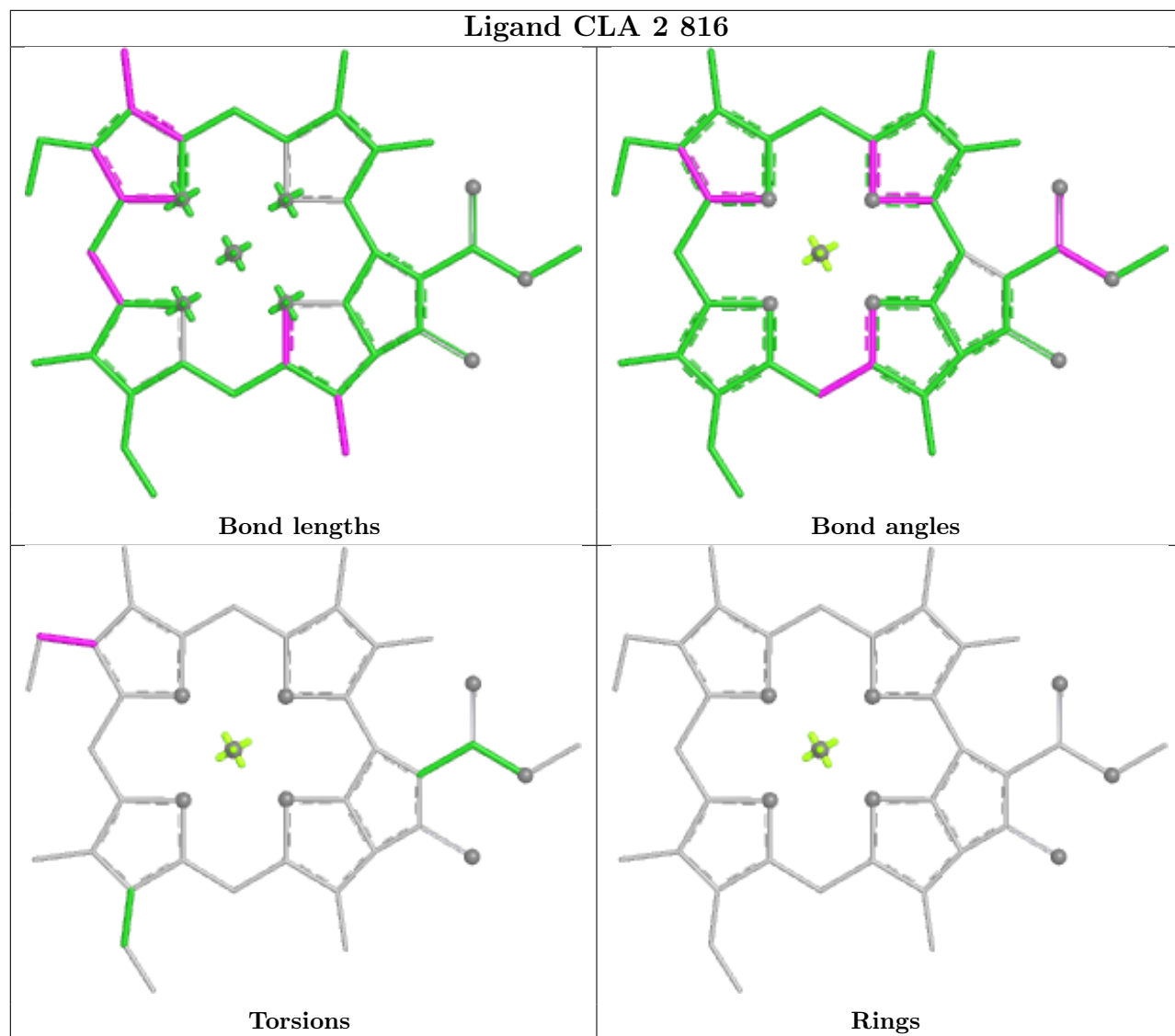
Ligand BCR F 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 840	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 828	
 Bond lengths	 Bond angles
 Torsions	 Rings



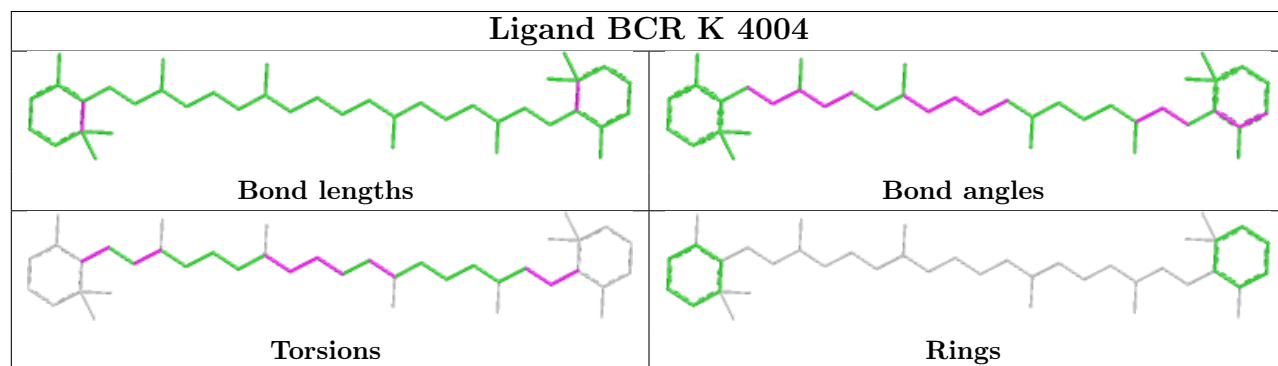


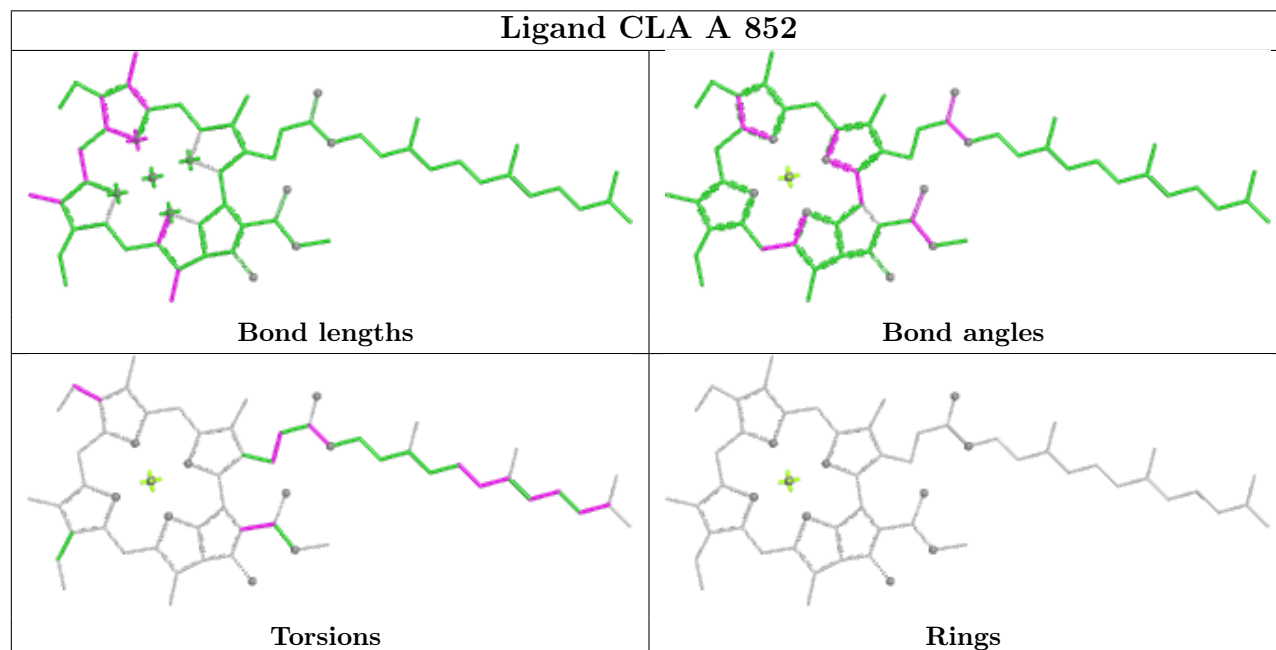
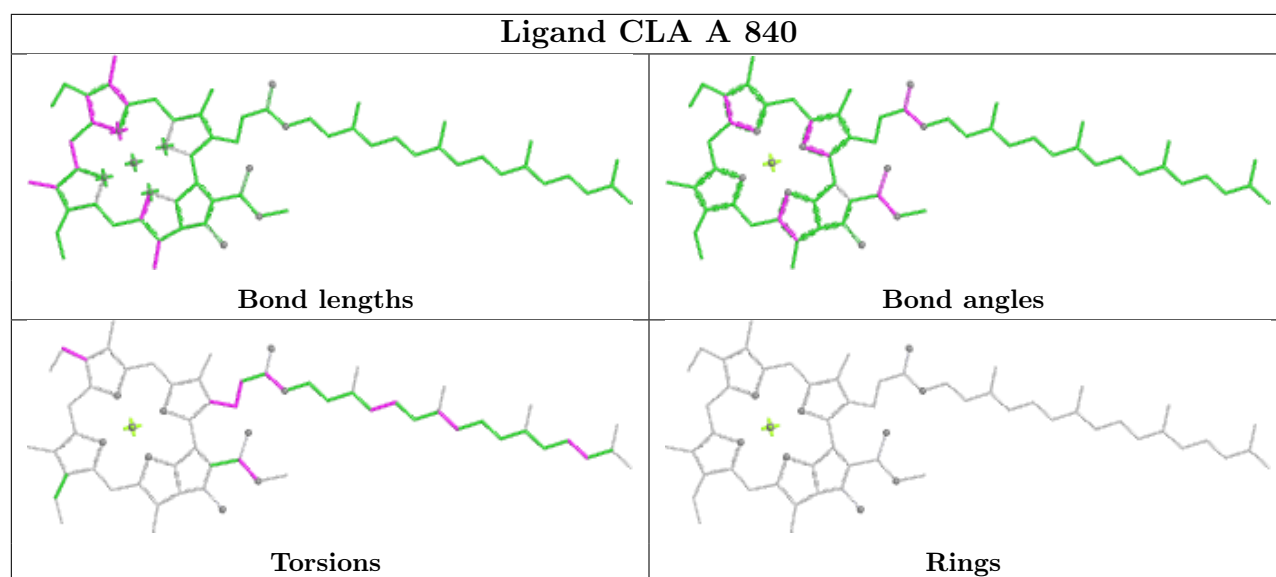


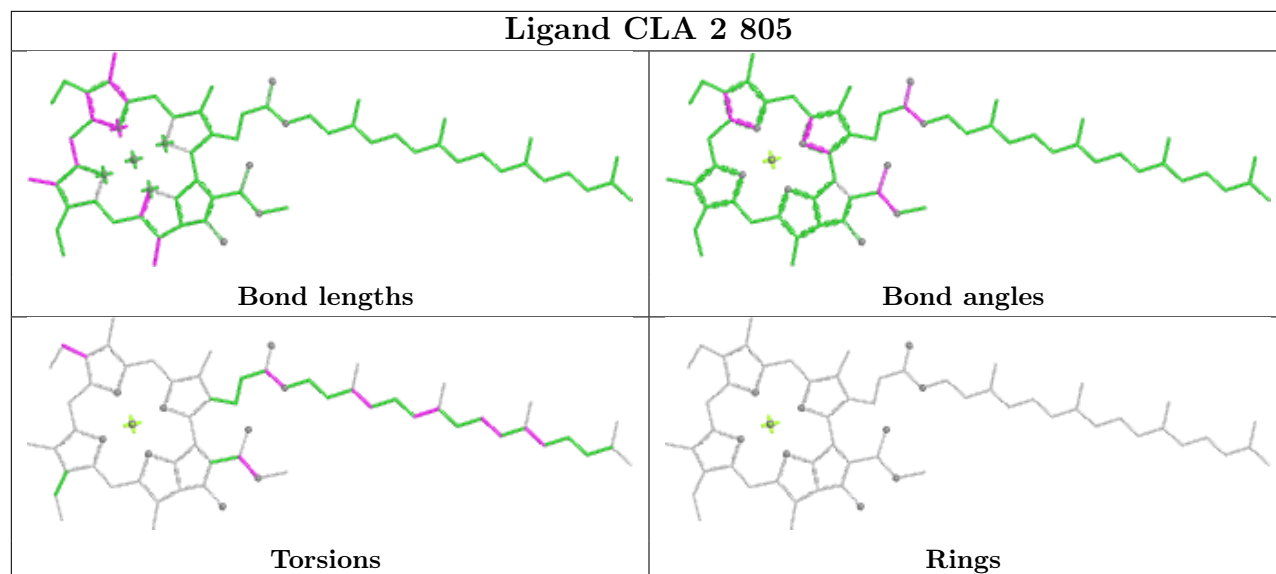
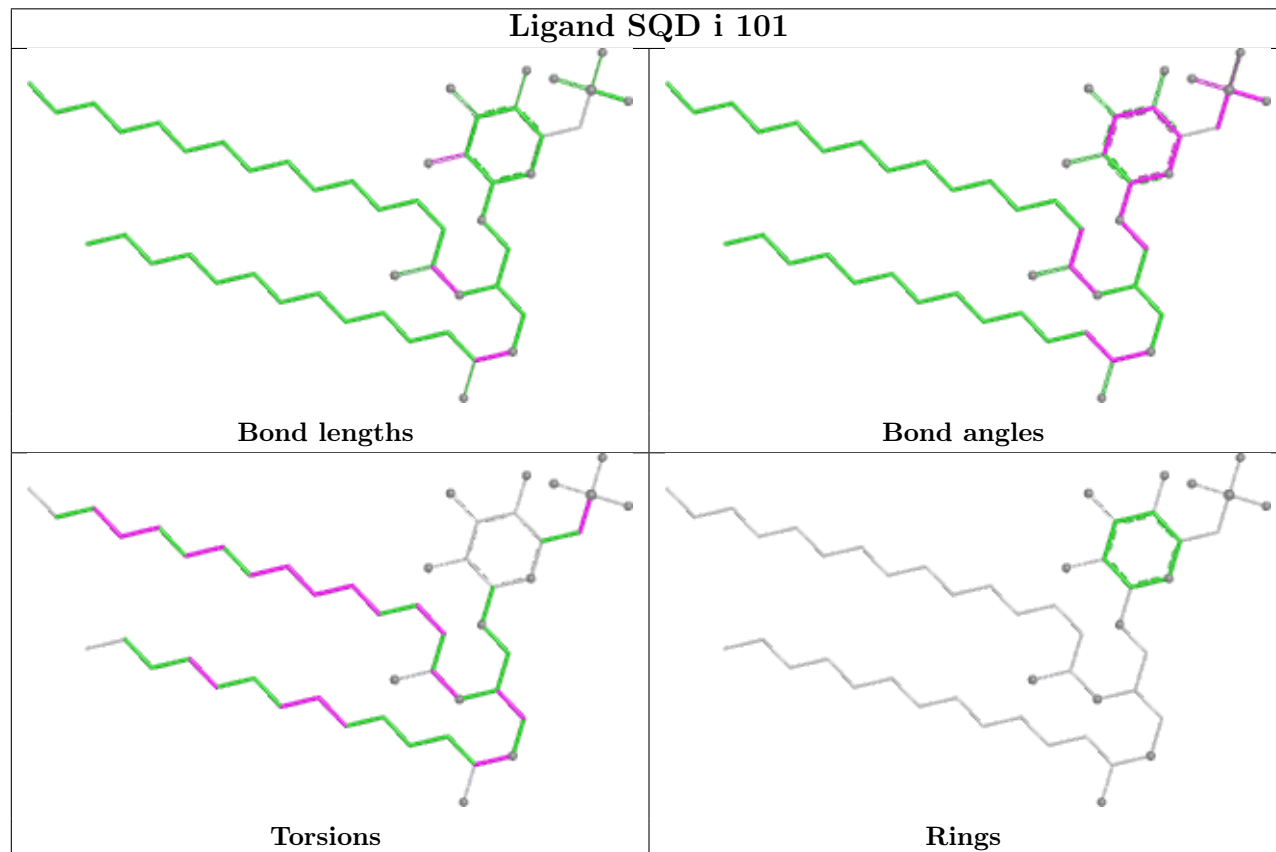
Ligand CLA 2 816

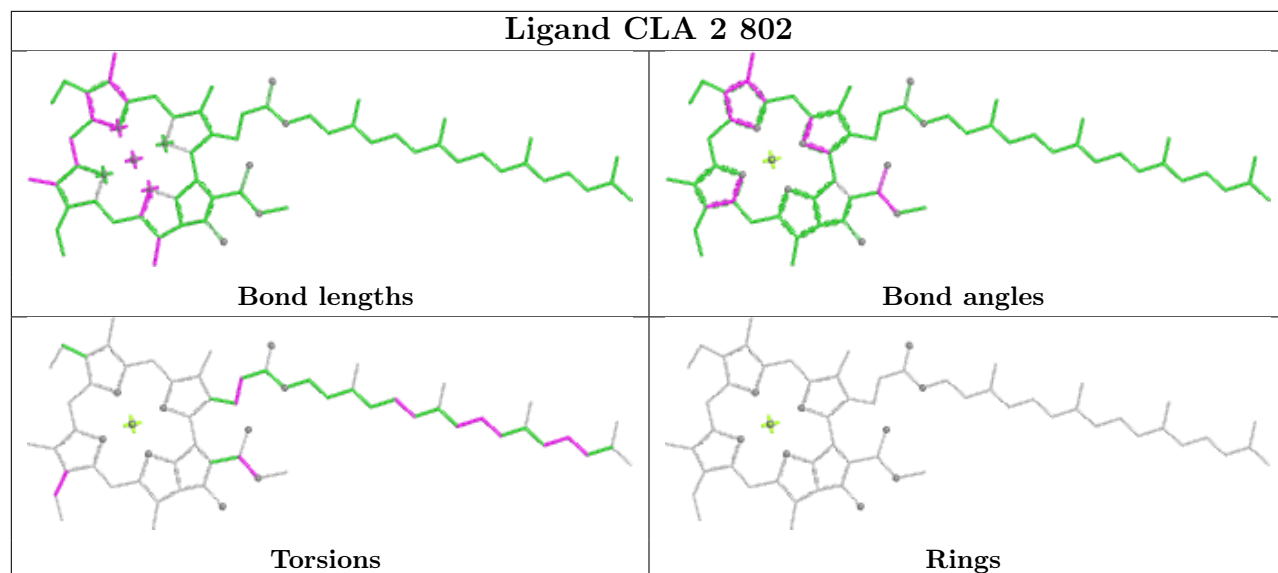
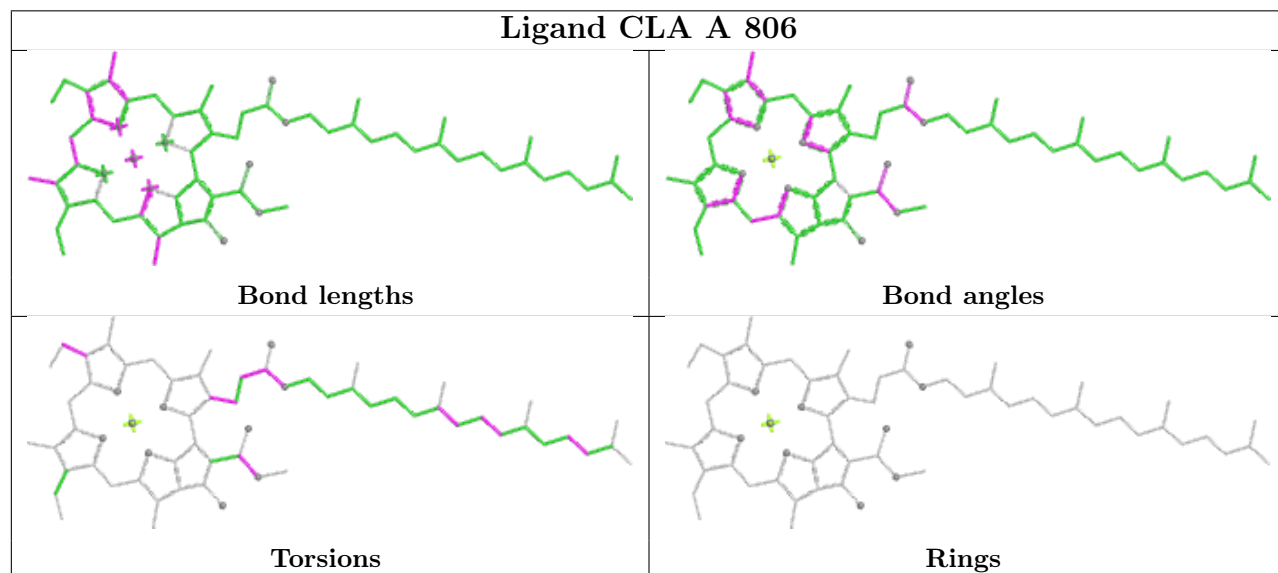
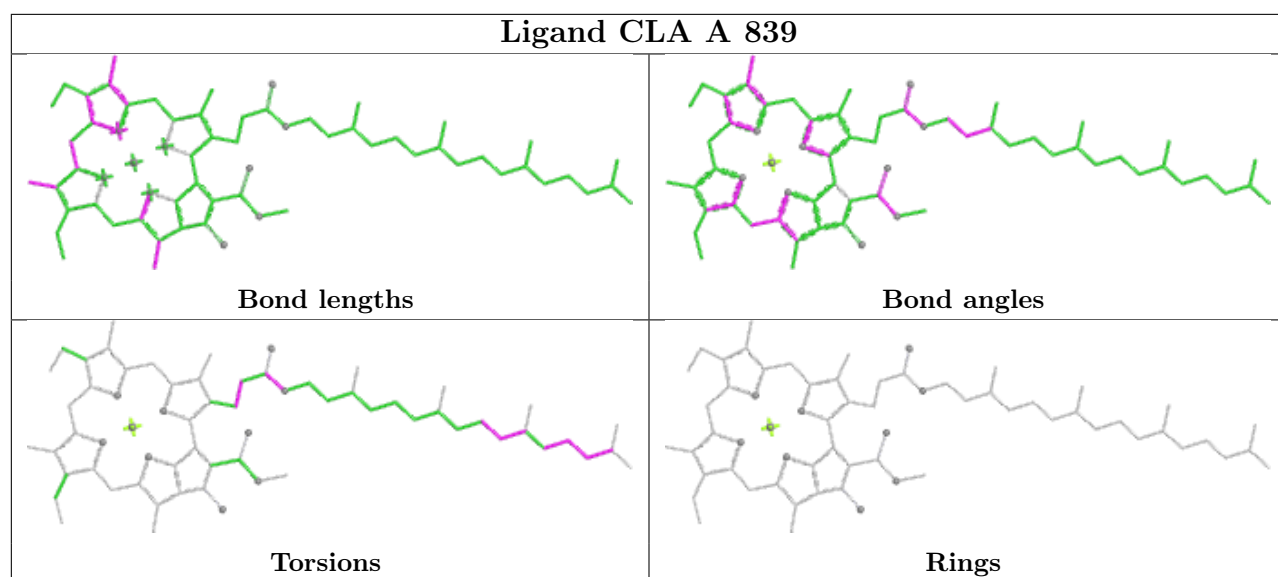


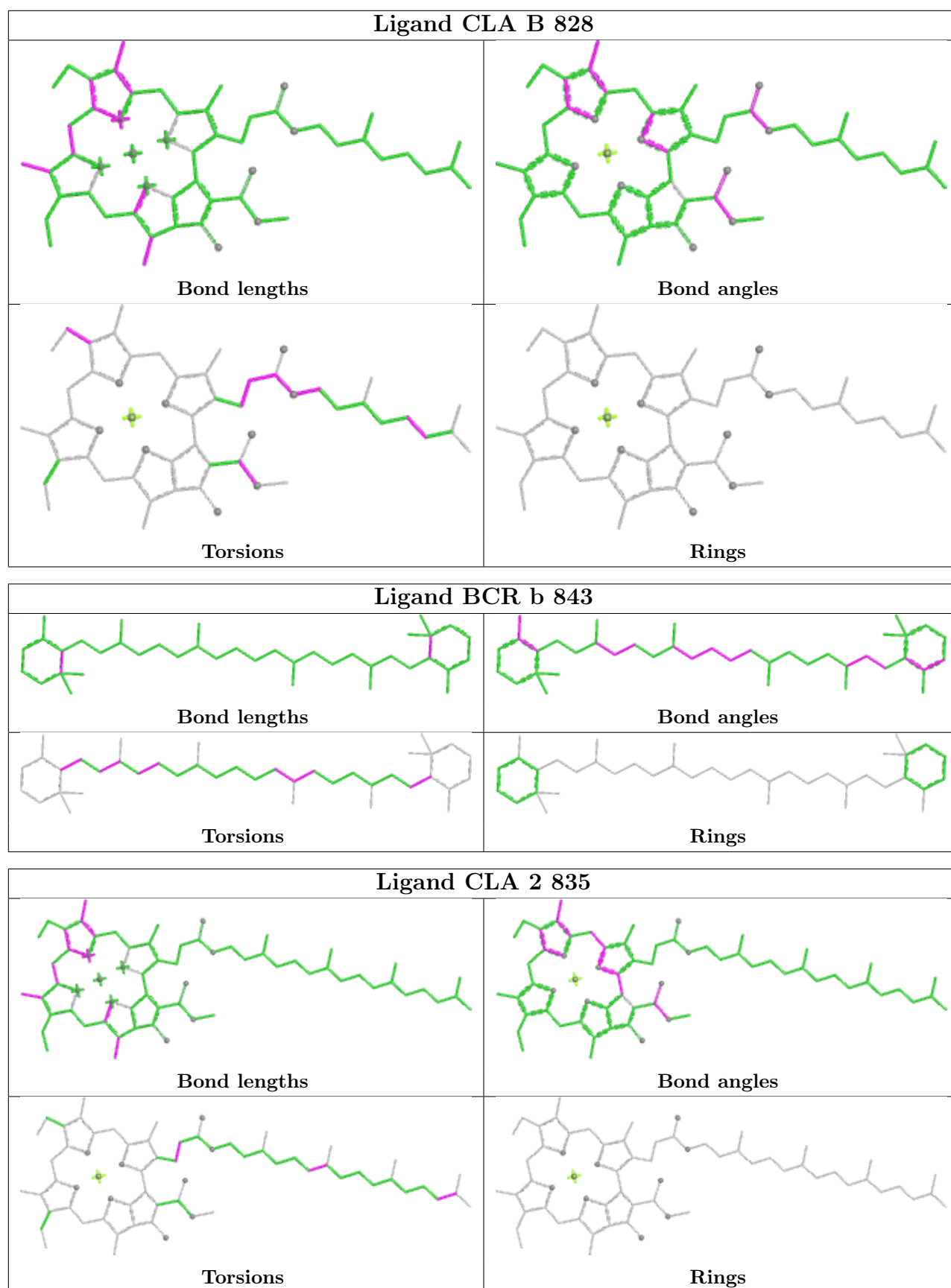
Ligand BCR K 4004

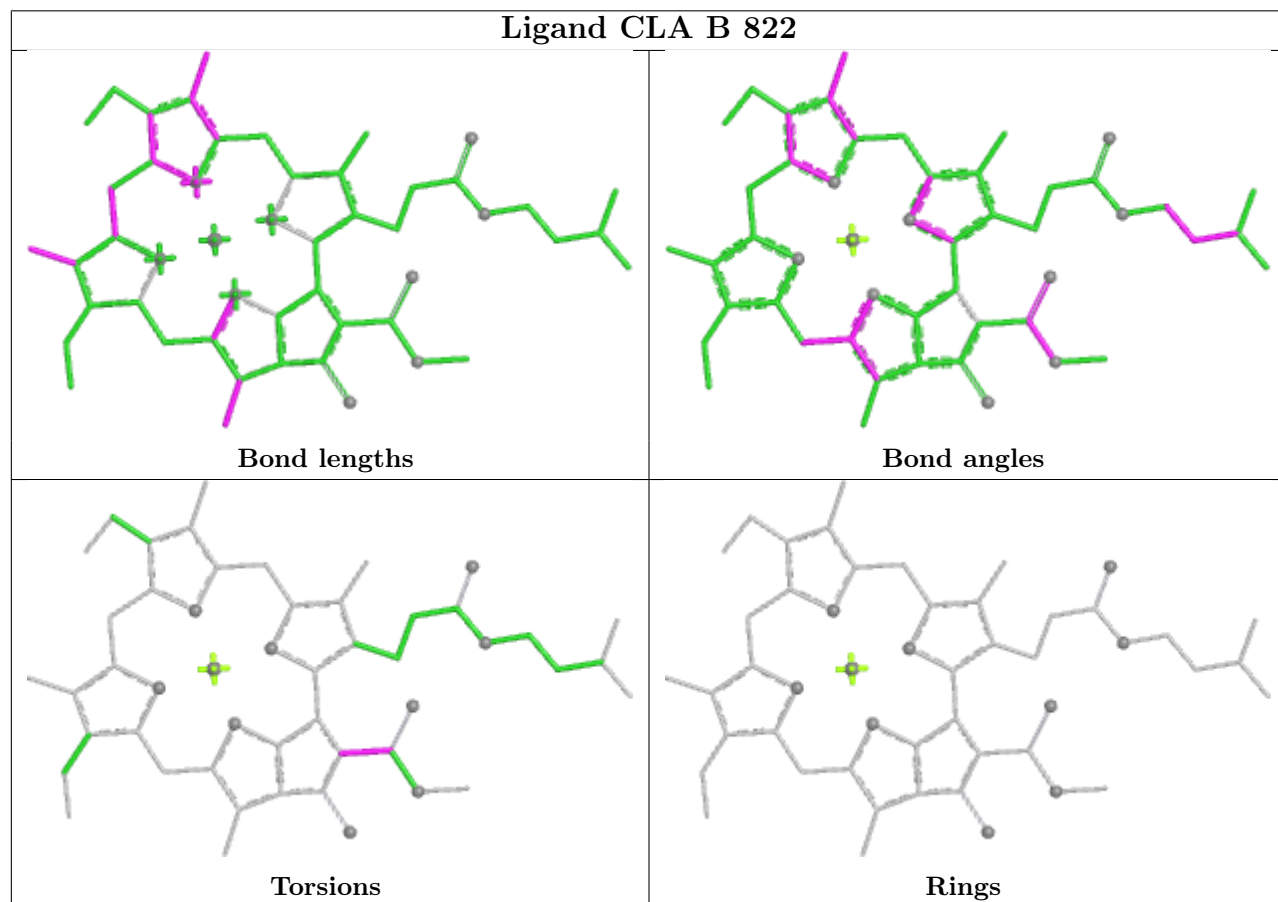
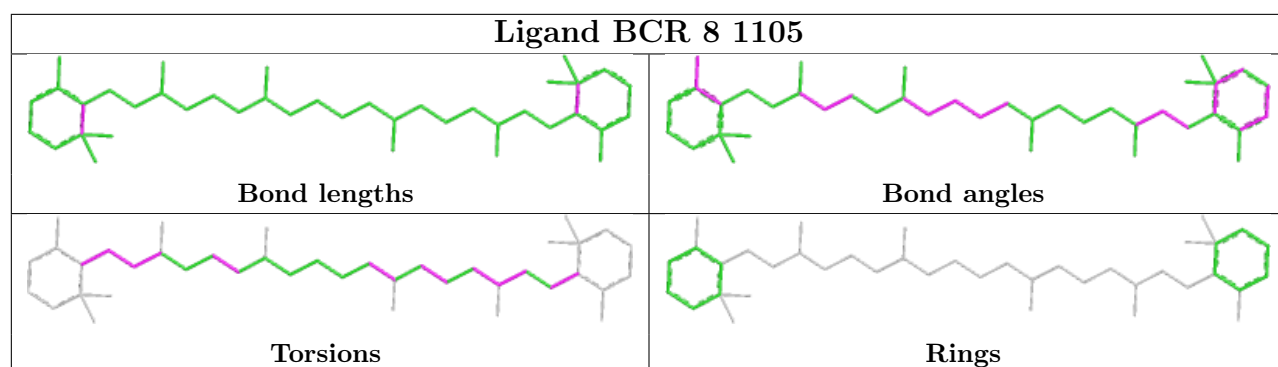


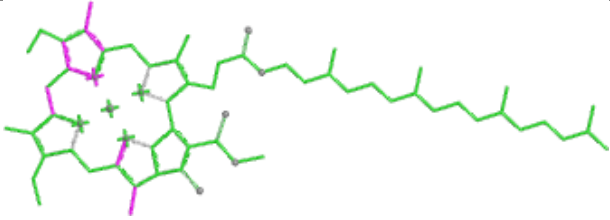
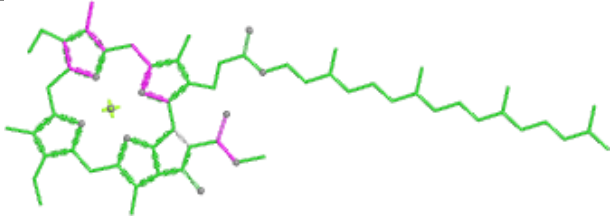
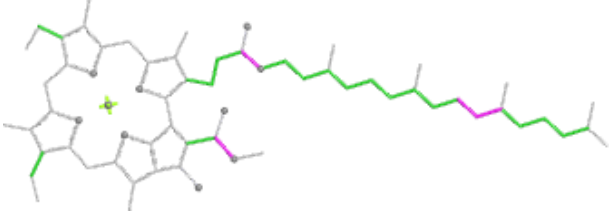
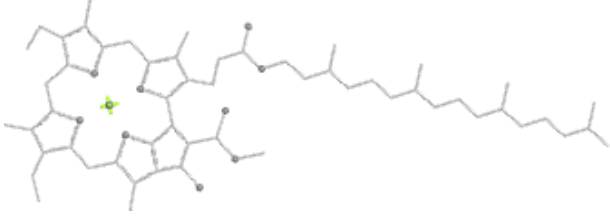
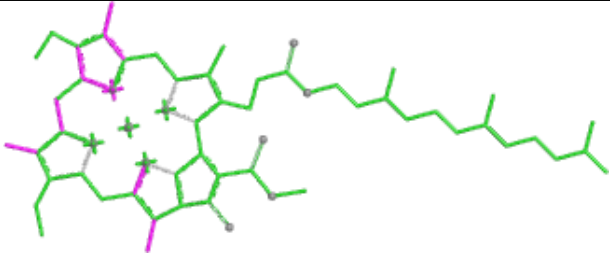
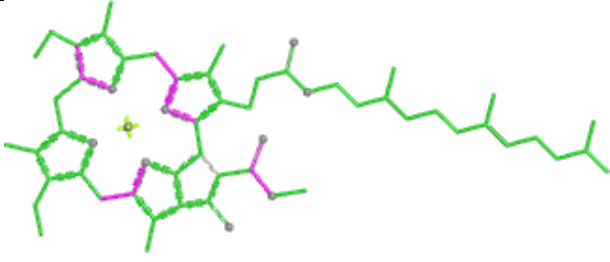
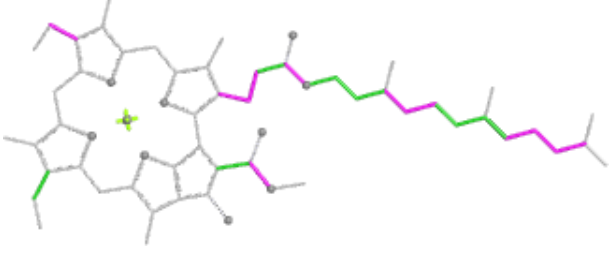
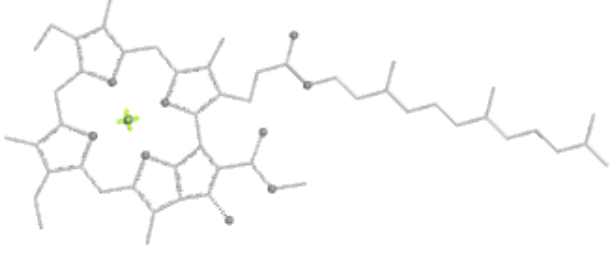


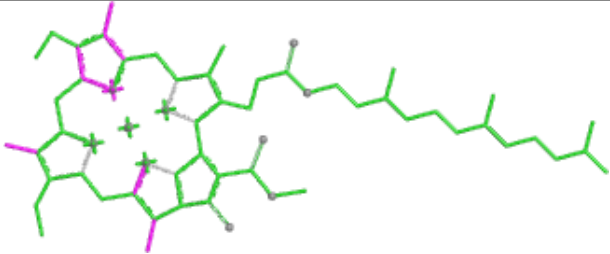
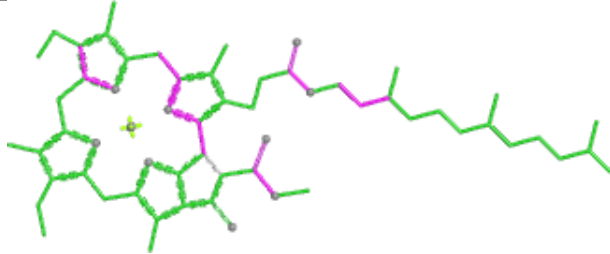
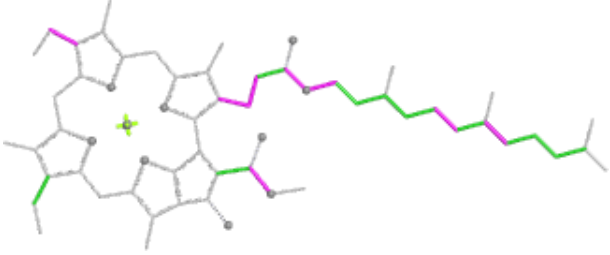
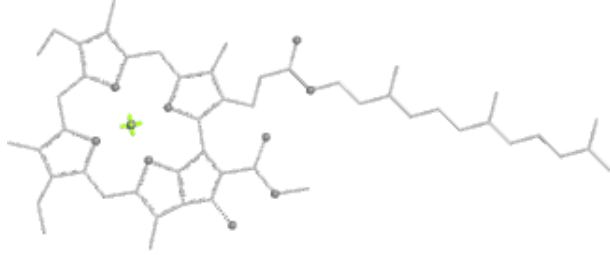
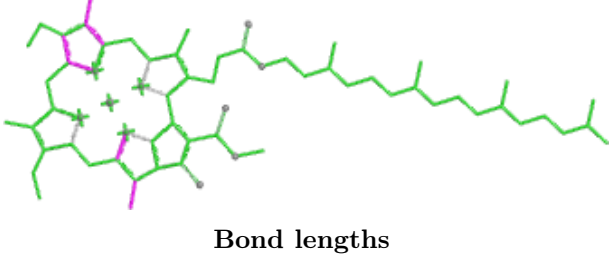
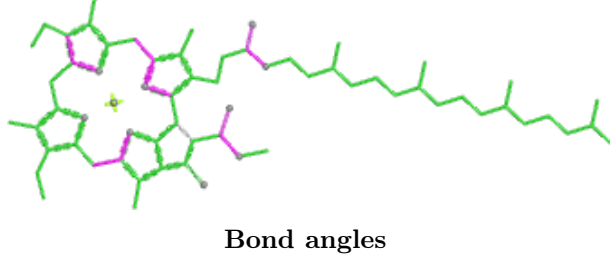
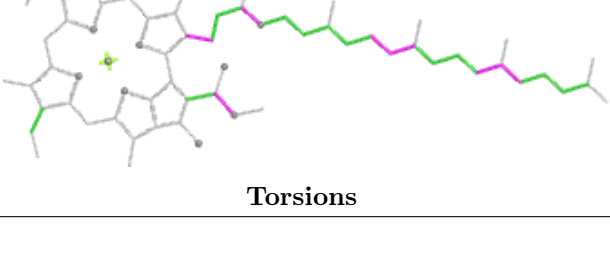
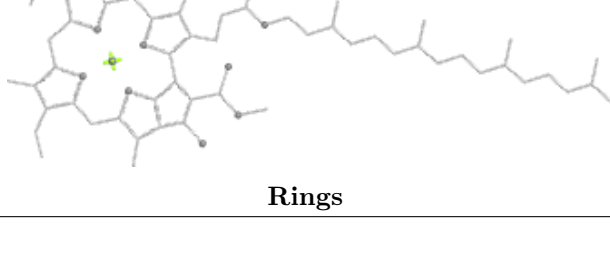
Ligand CLA 2 805**Ligand SQD i 101**

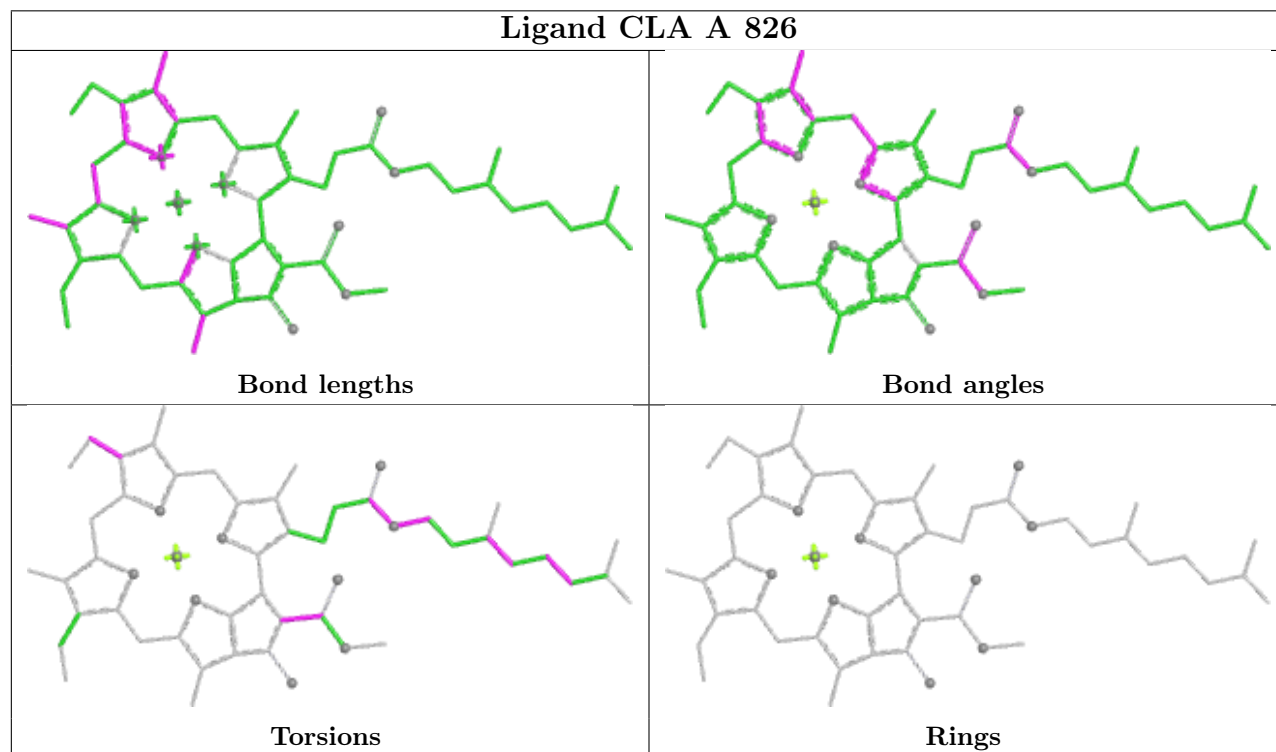
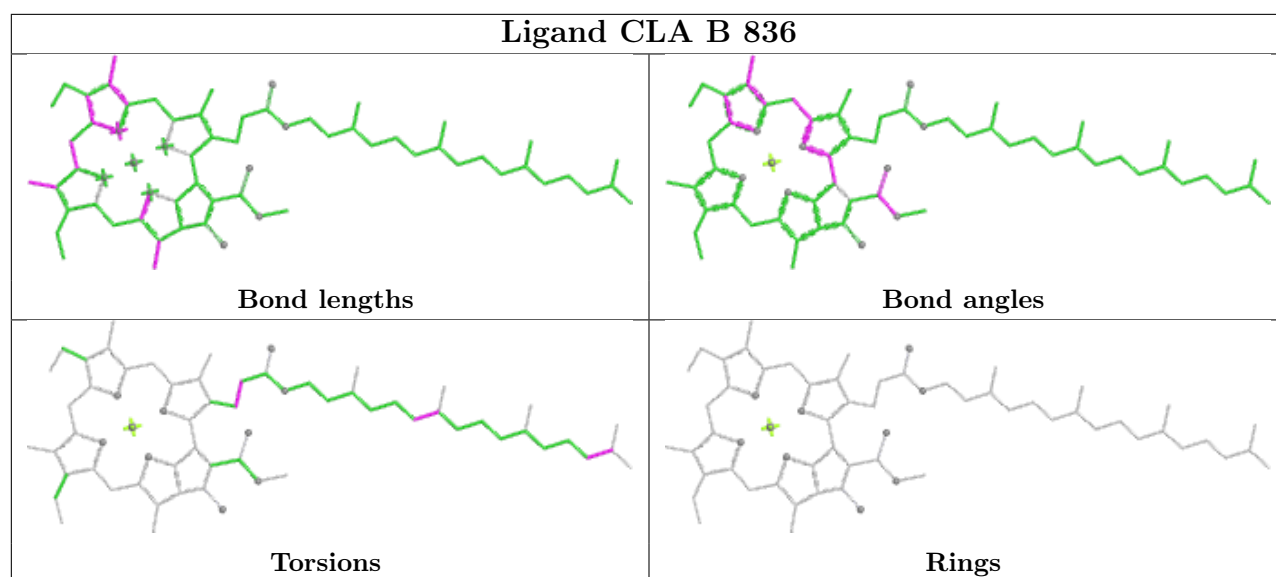


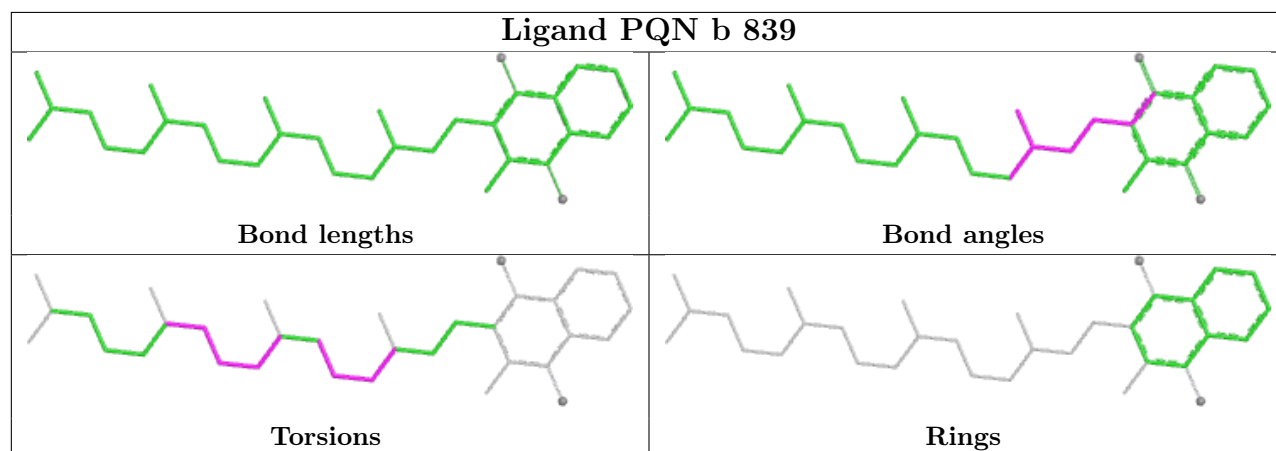
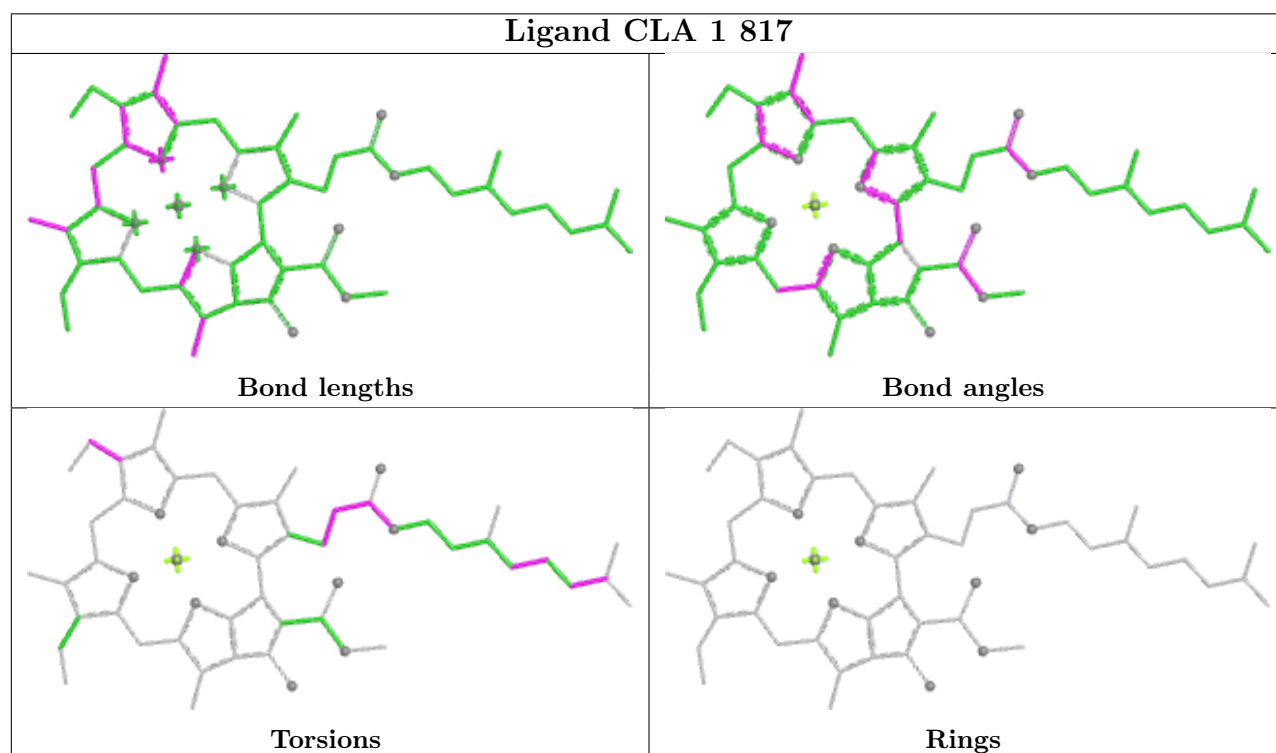
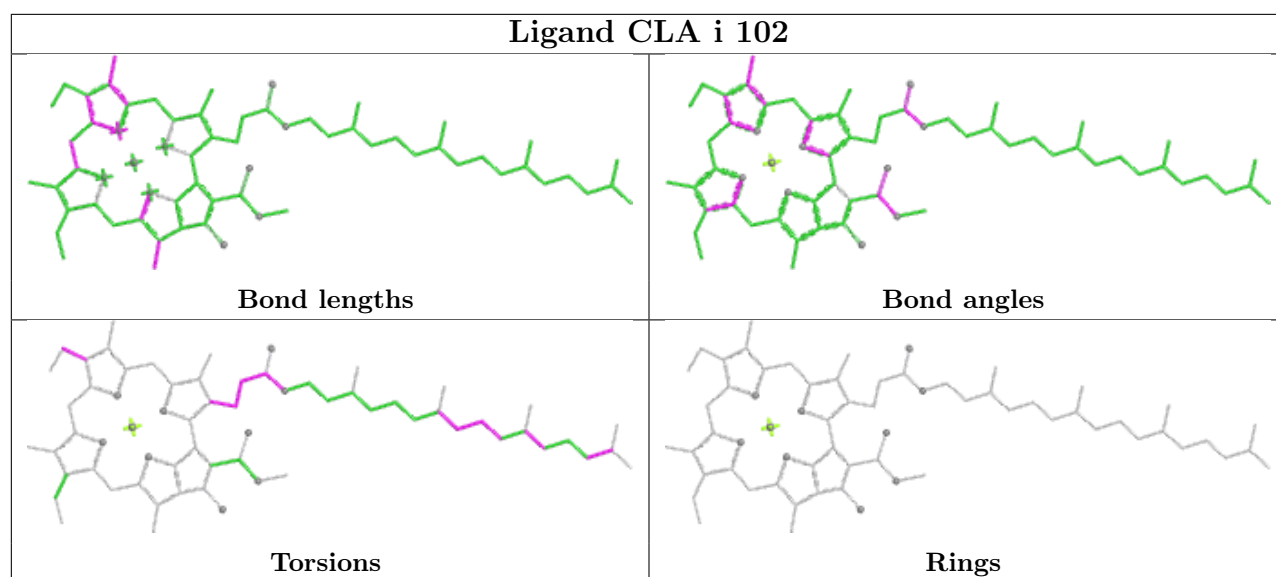


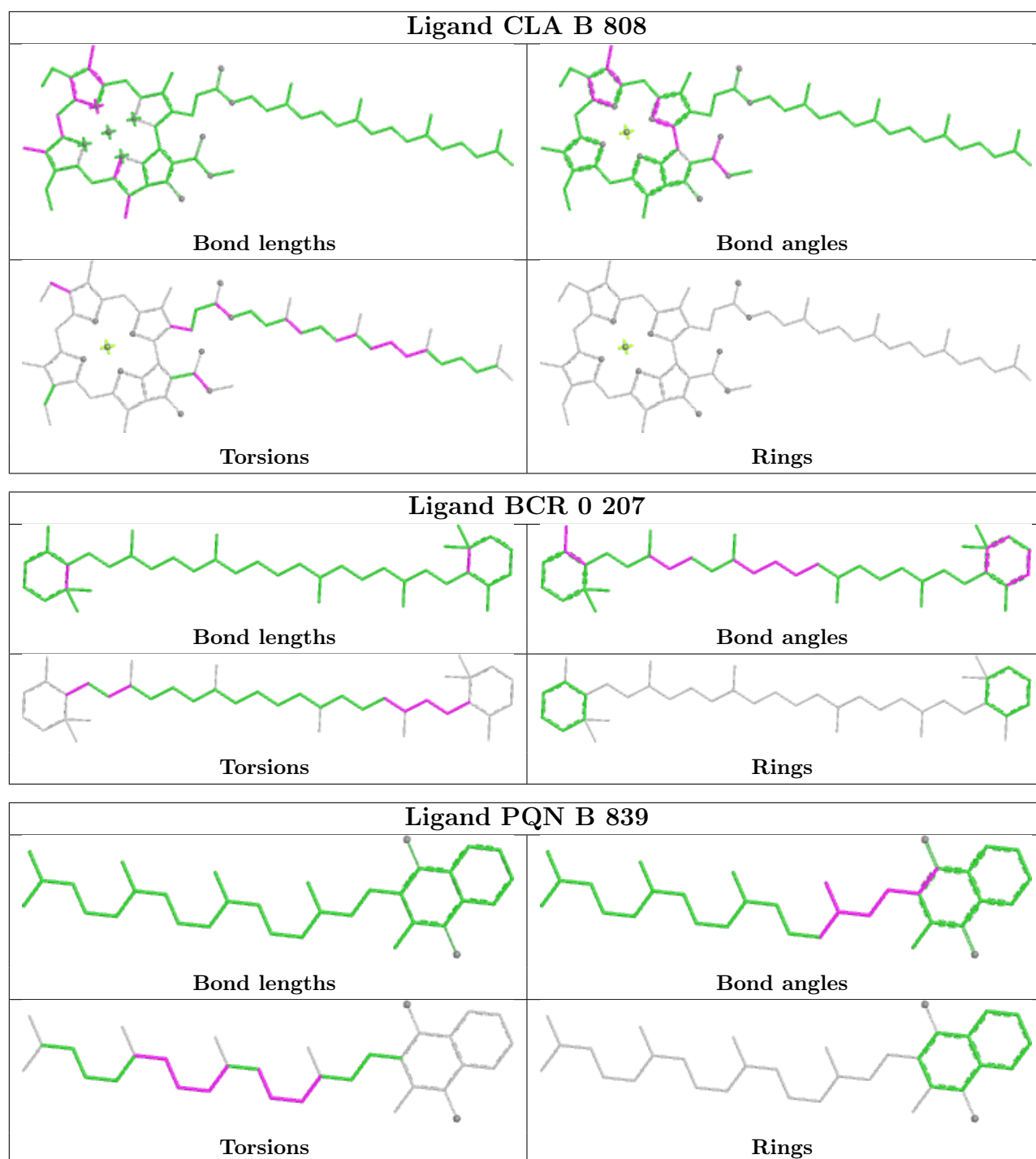


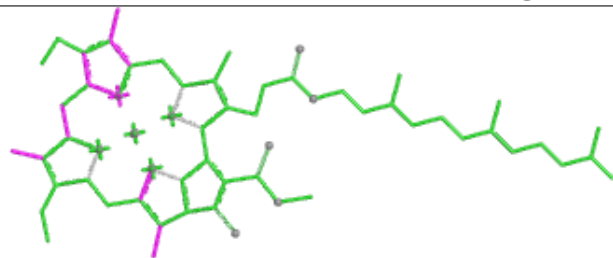
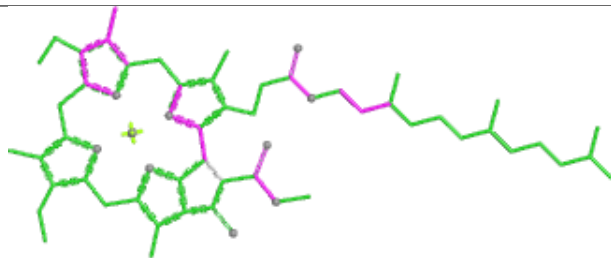
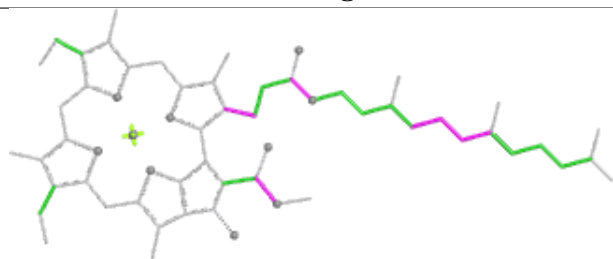
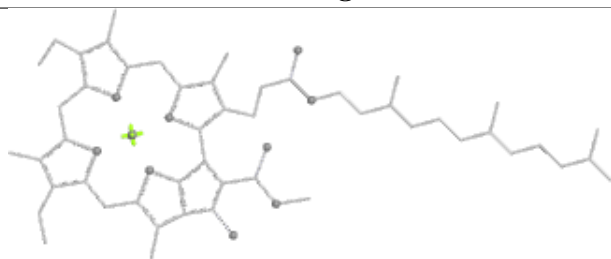
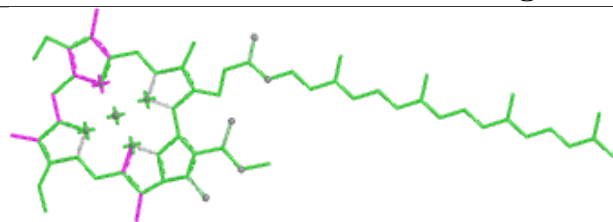
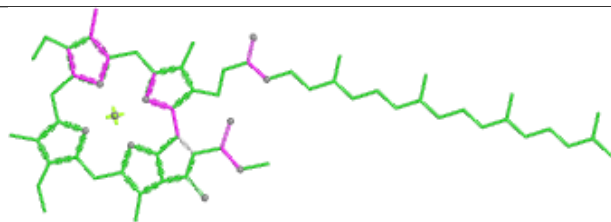
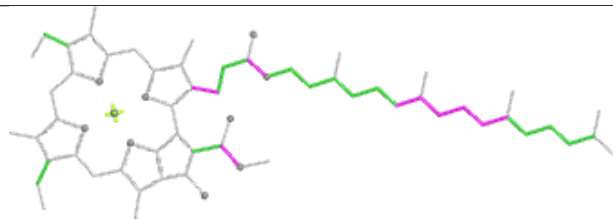
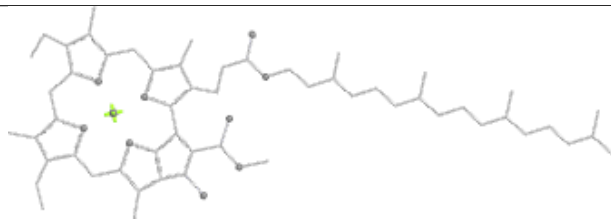
Ligand CLA b 838	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 1 824	
 Bond lengths	 Bond angles
 Torsions	 Rings

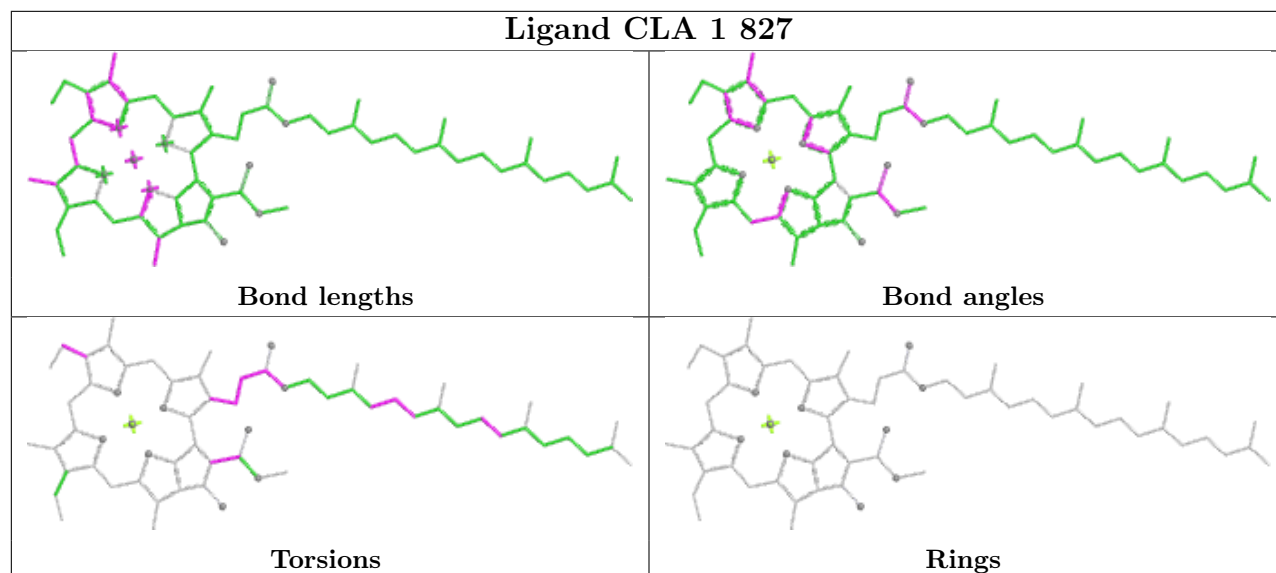
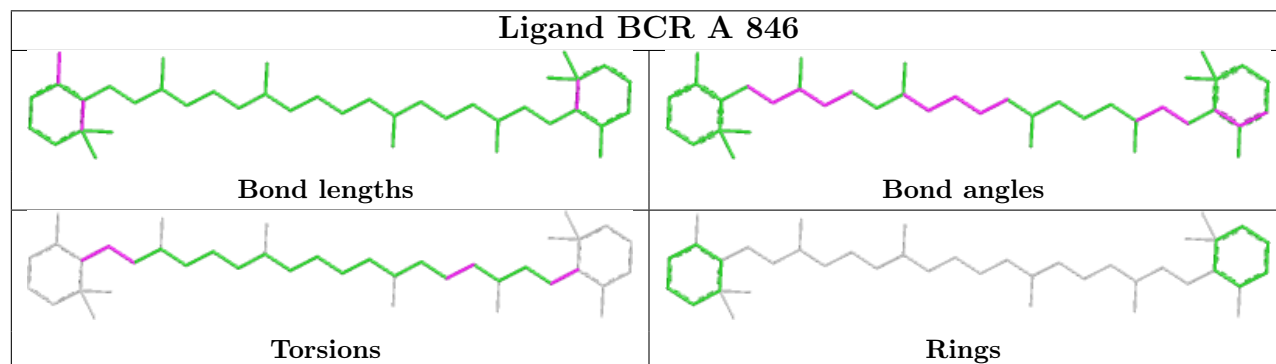
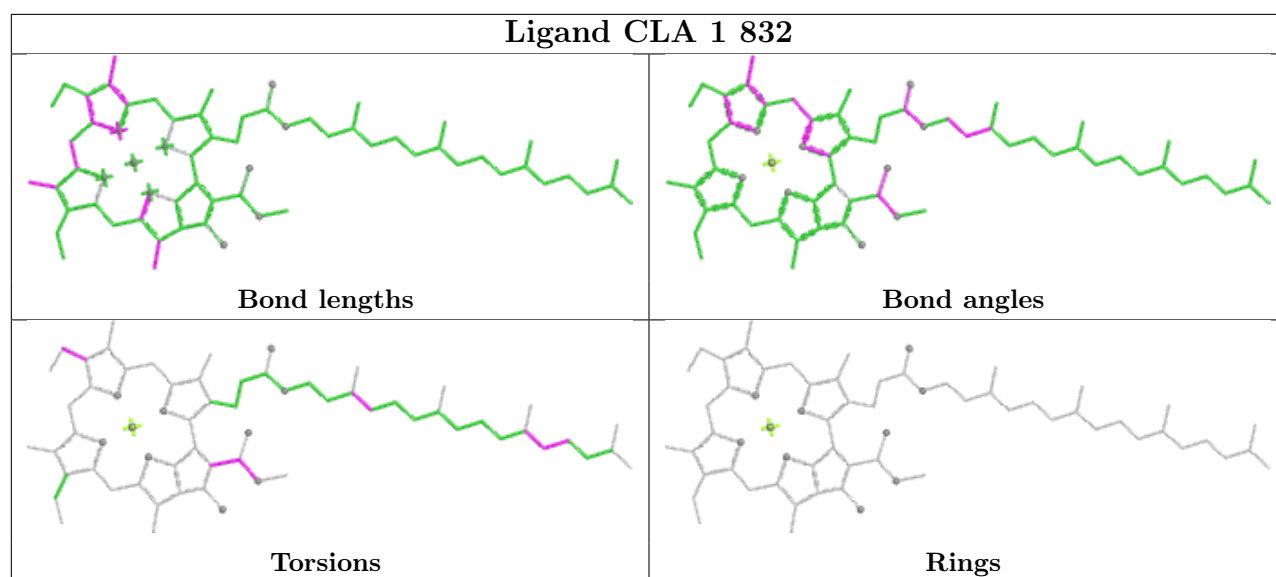
Ligand CLA A 841	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 837	
 Bond lengths	 Bond angles
 Torsions	 Rings



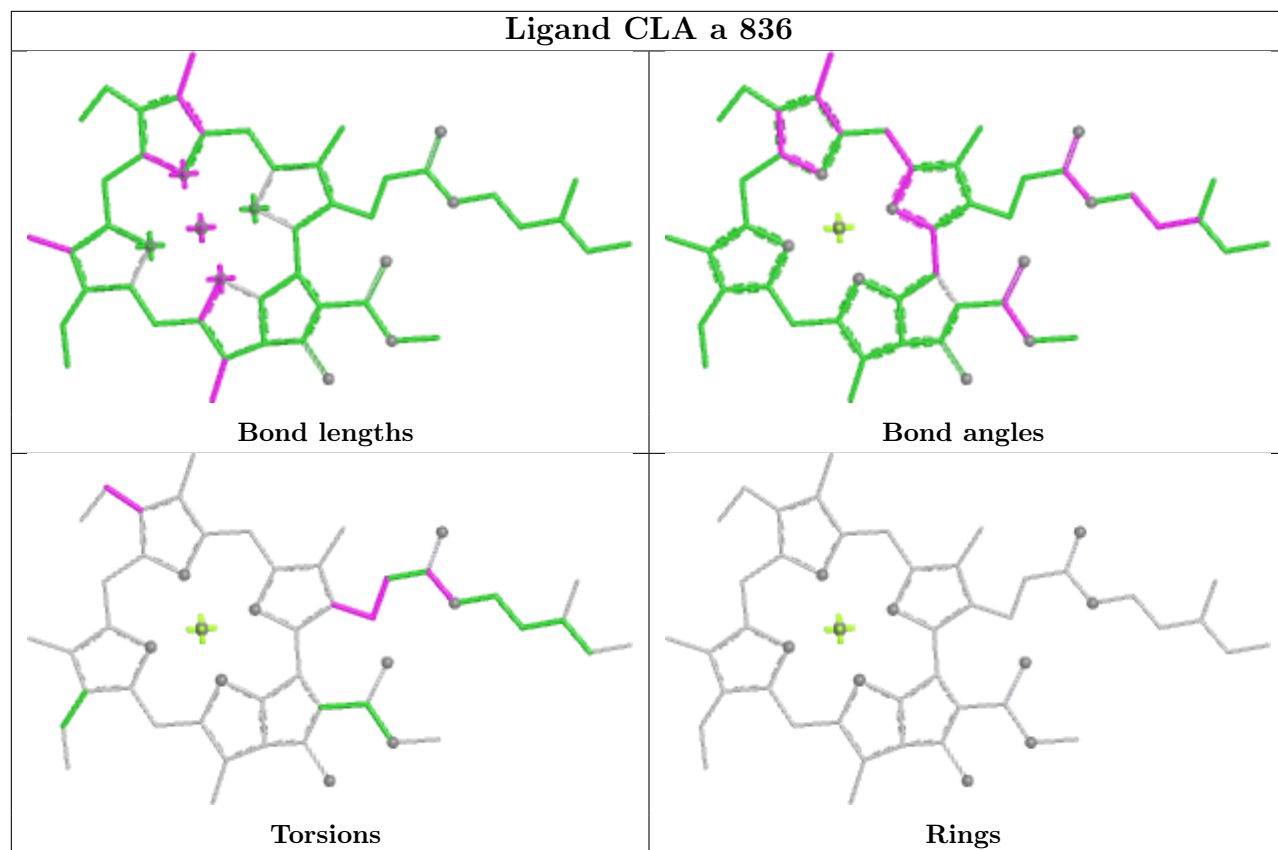




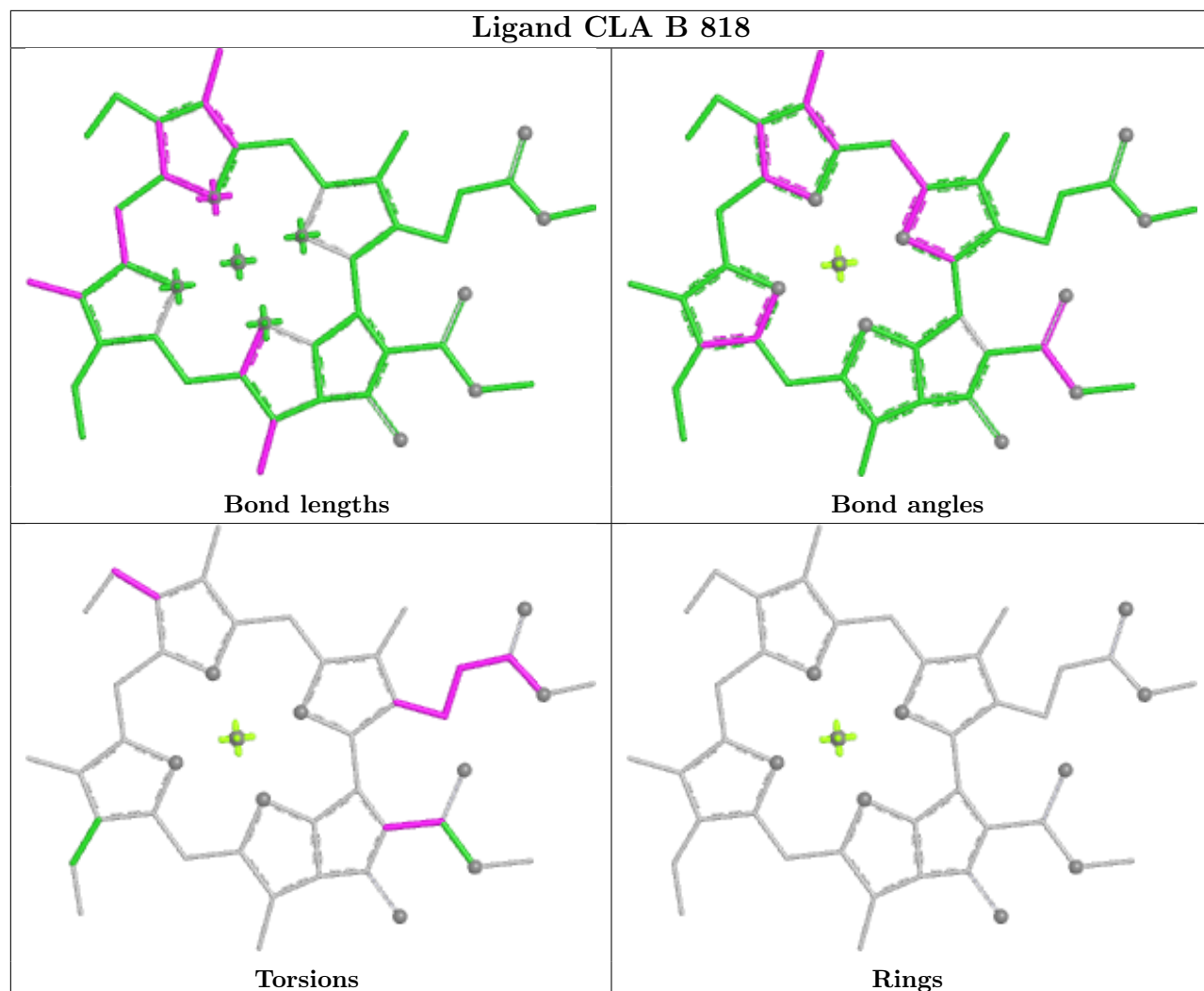
Ligand CLA 0 202**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 1 830****Bond lengths****Bond angles****Torsions****Rings**



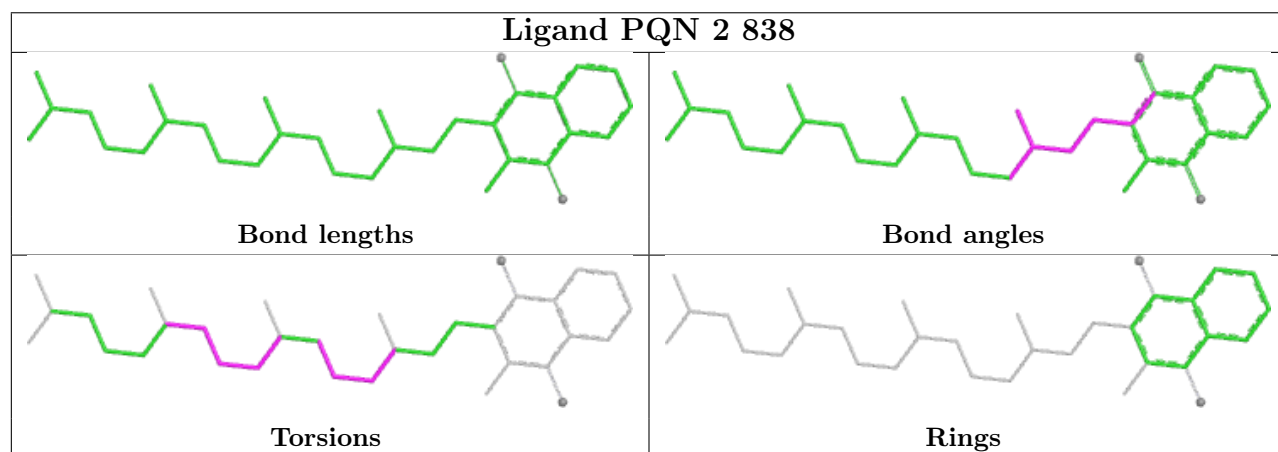
Ligand CLA a 836



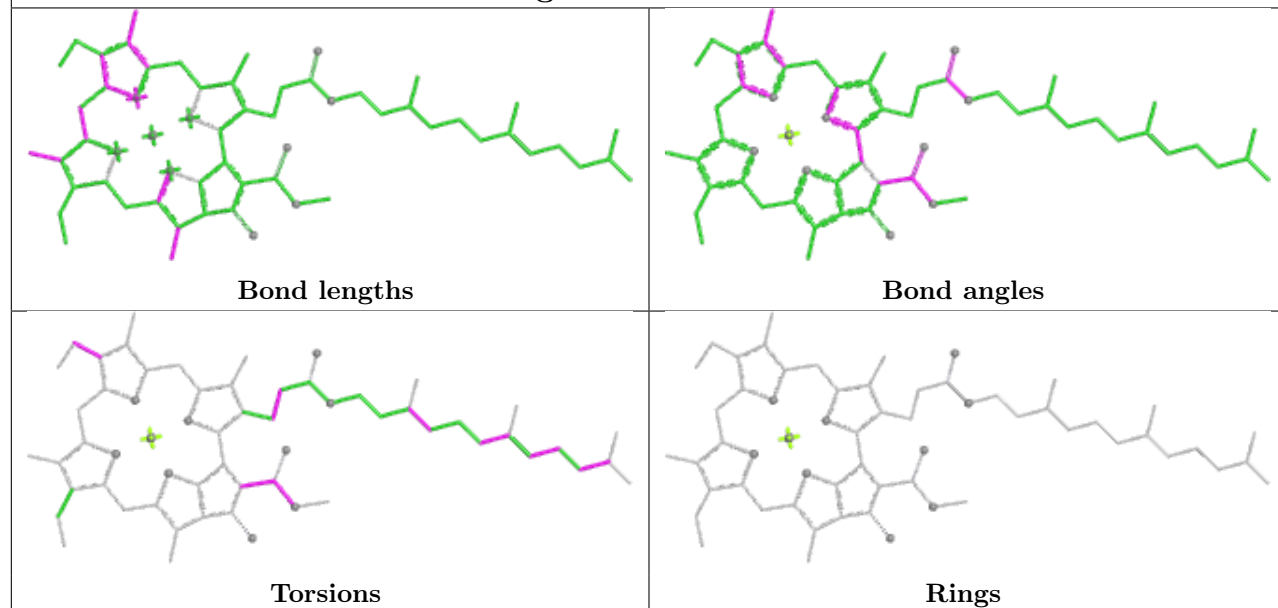
Ligand CLA B 818



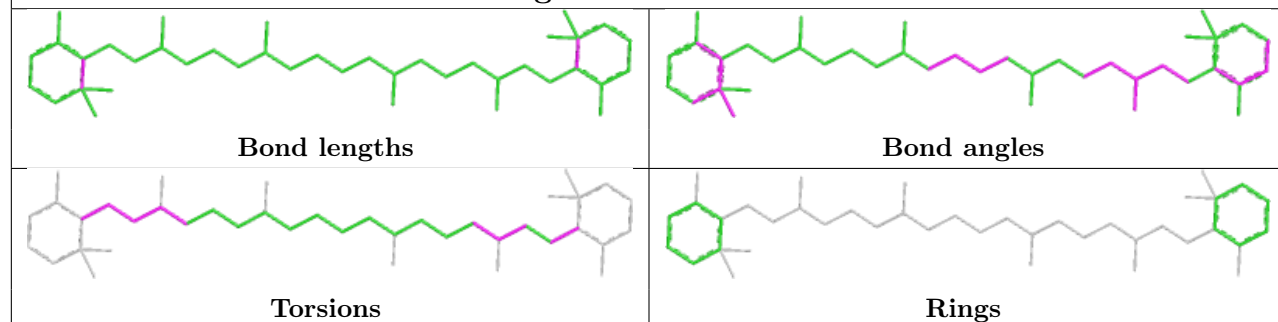
Ligand PQN 2 838



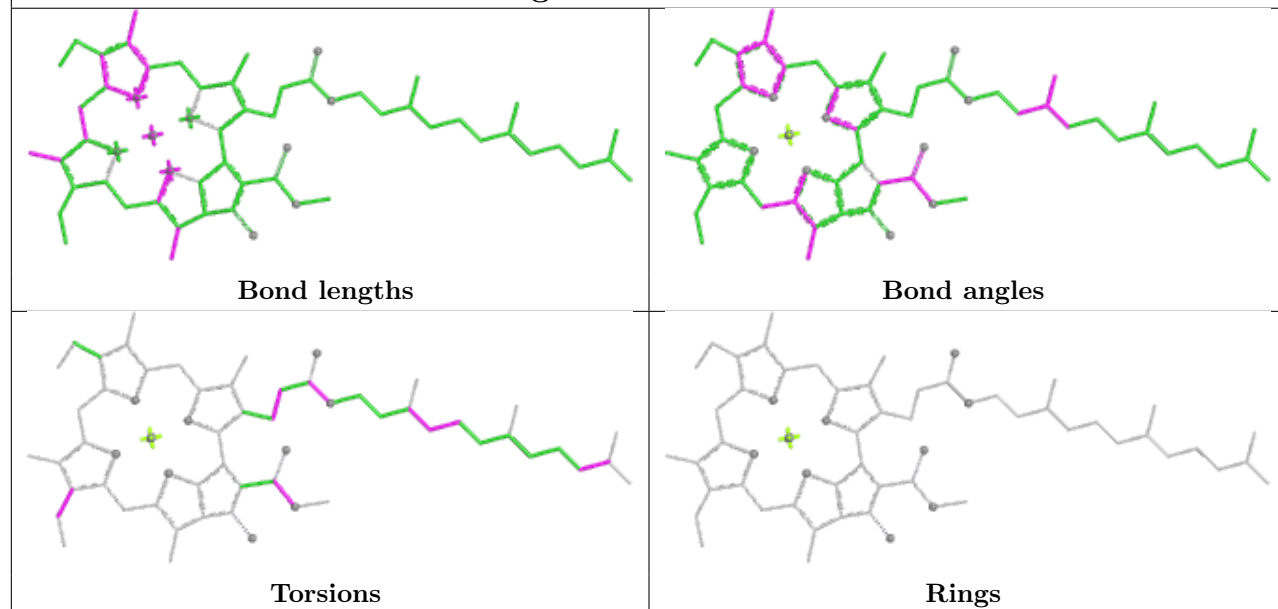
Ligand CLA 1 819

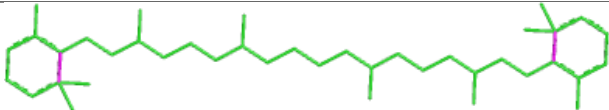
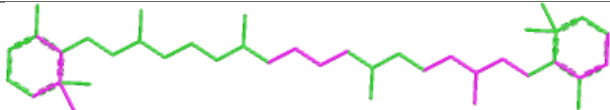
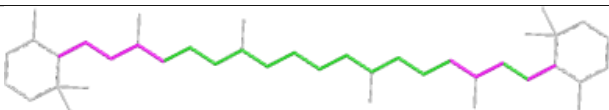
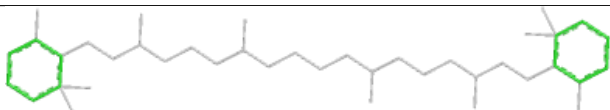


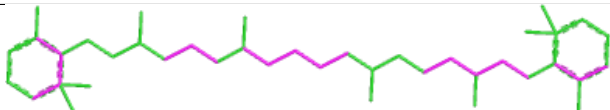
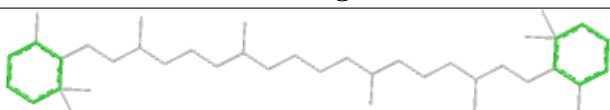
Ligand BCR 7 103

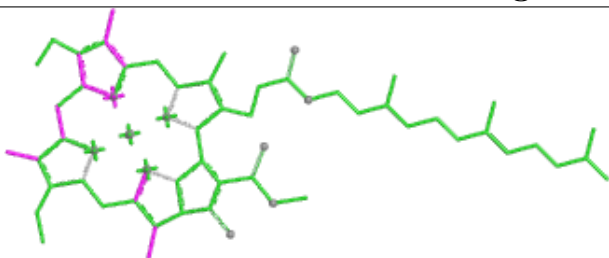
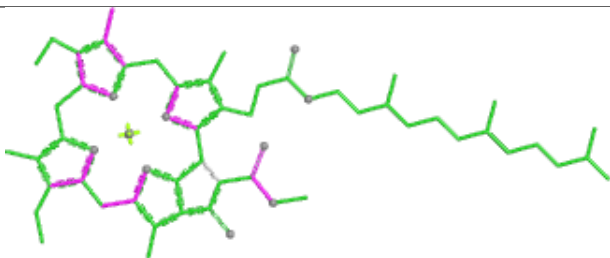
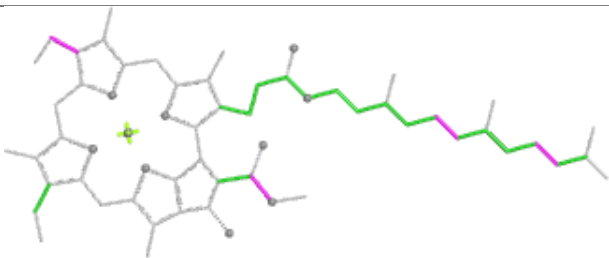
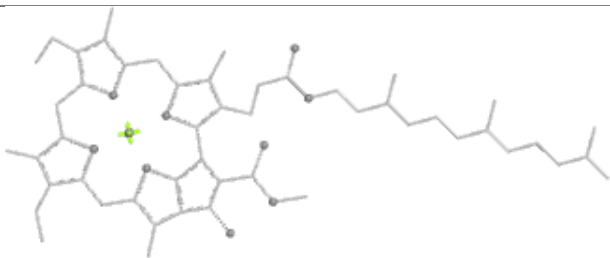


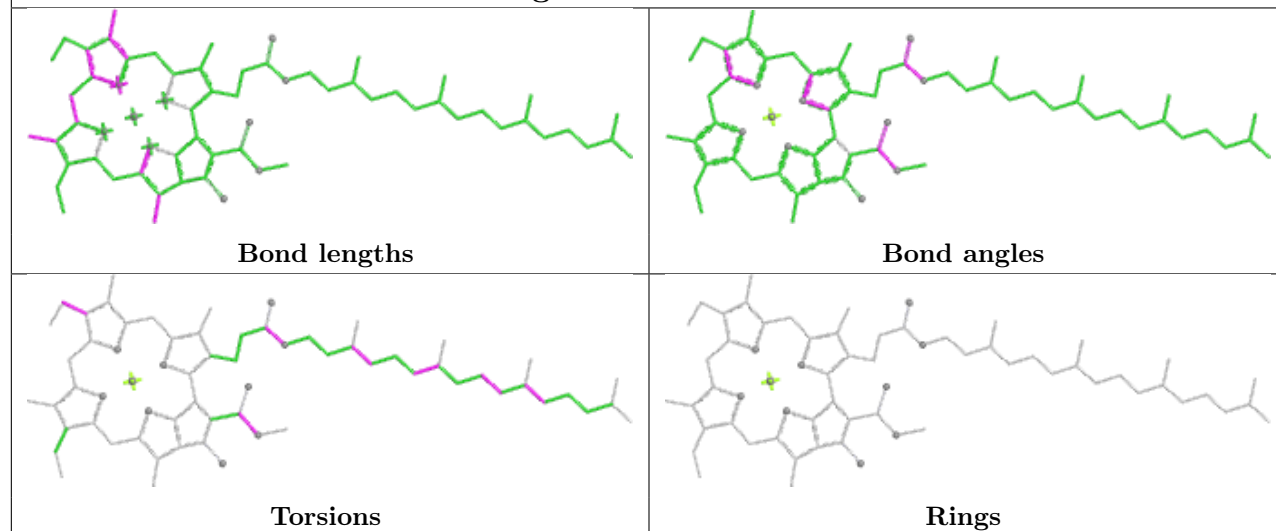
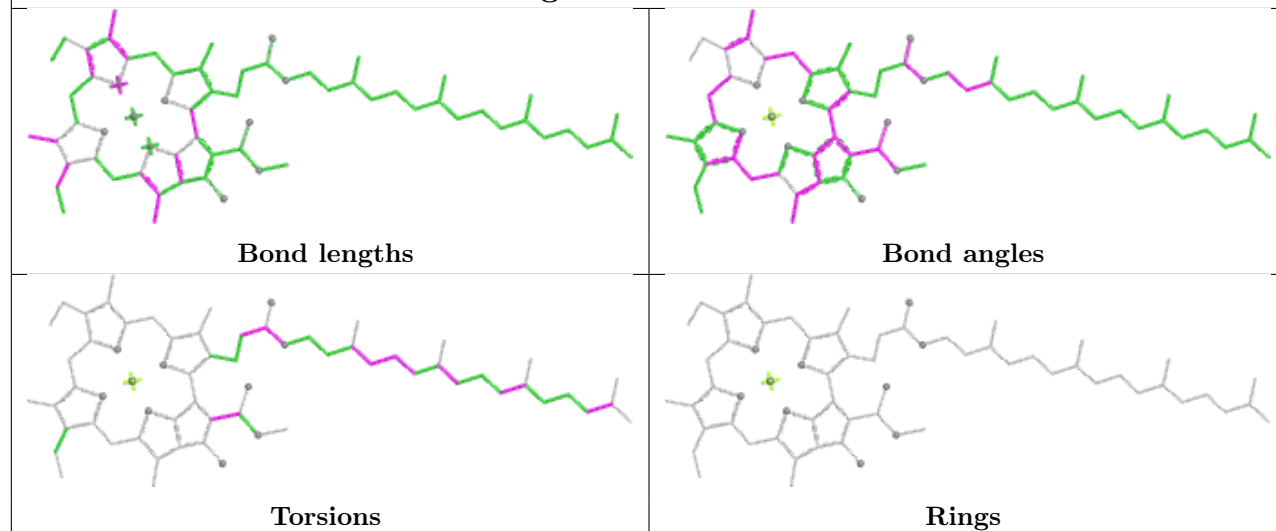
Ligand CLA A 802

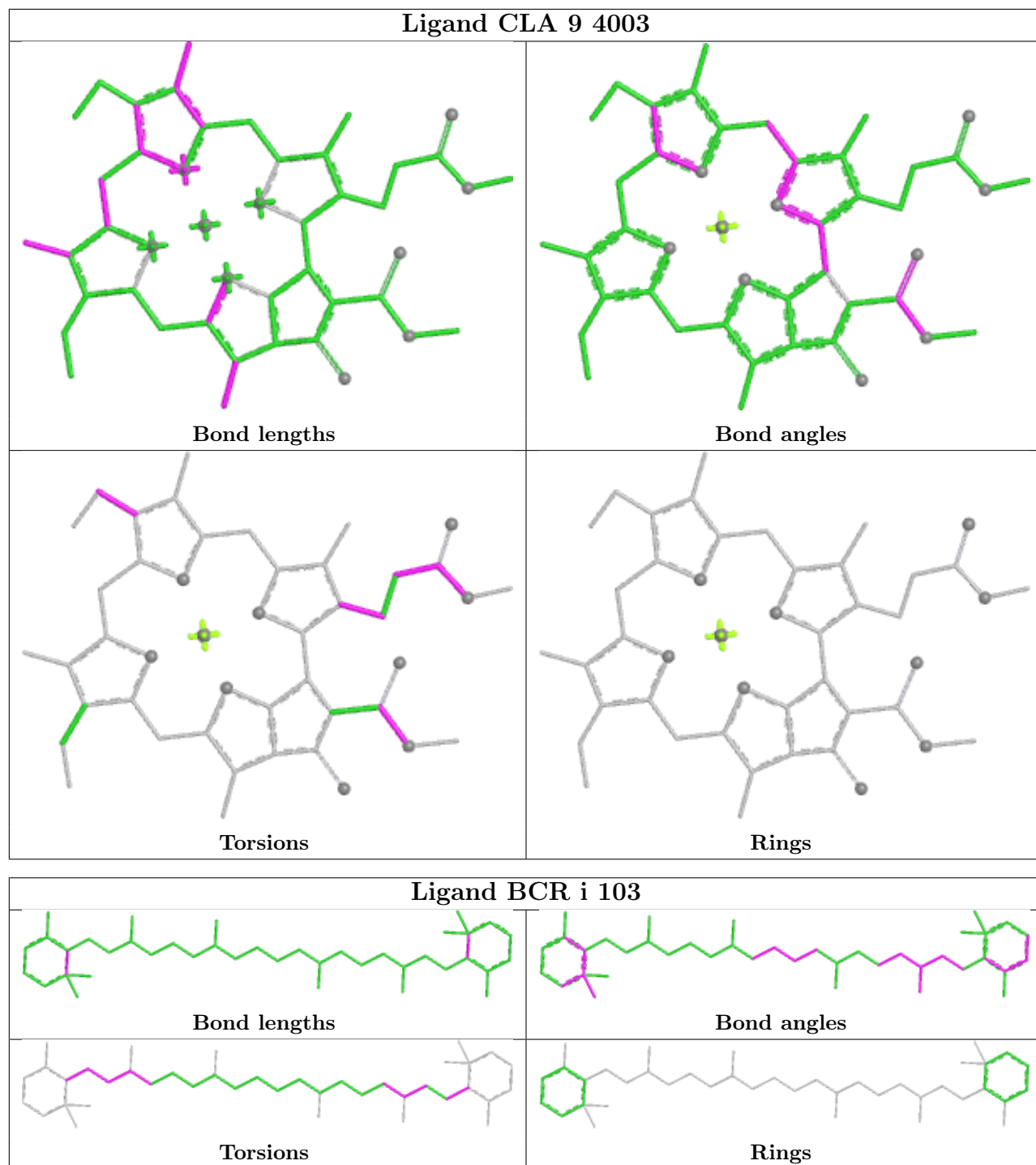


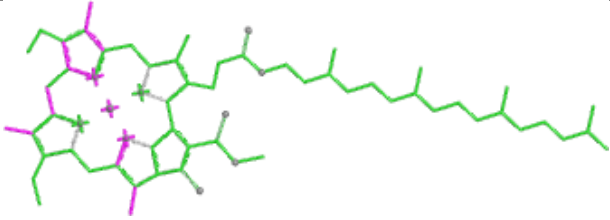
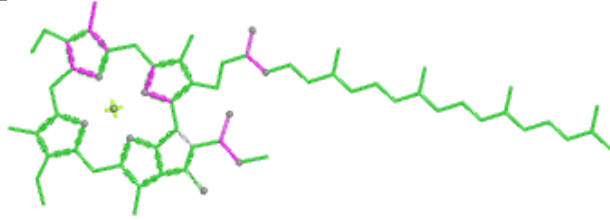
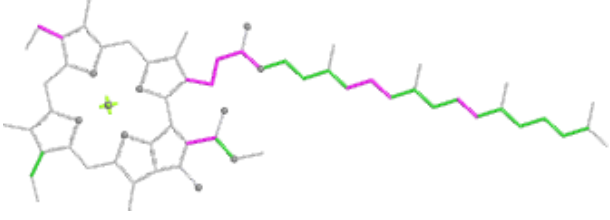
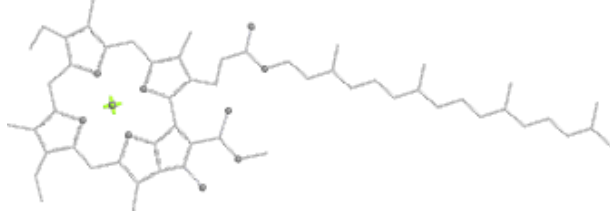
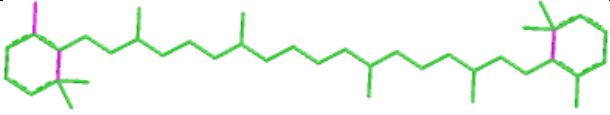
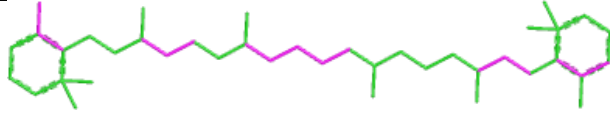
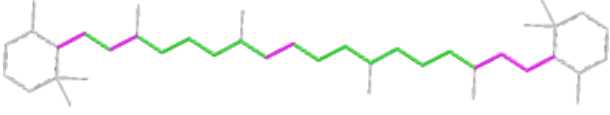
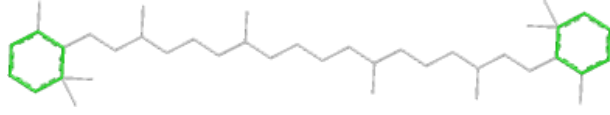
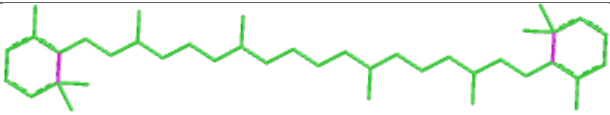
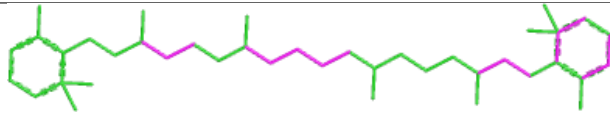
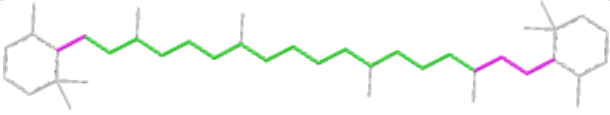
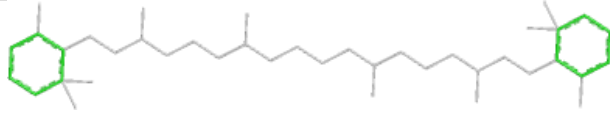
Ligand BCR I 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR I 203	
	
Bond lengths	Bond angles
	
Torsions	Rings

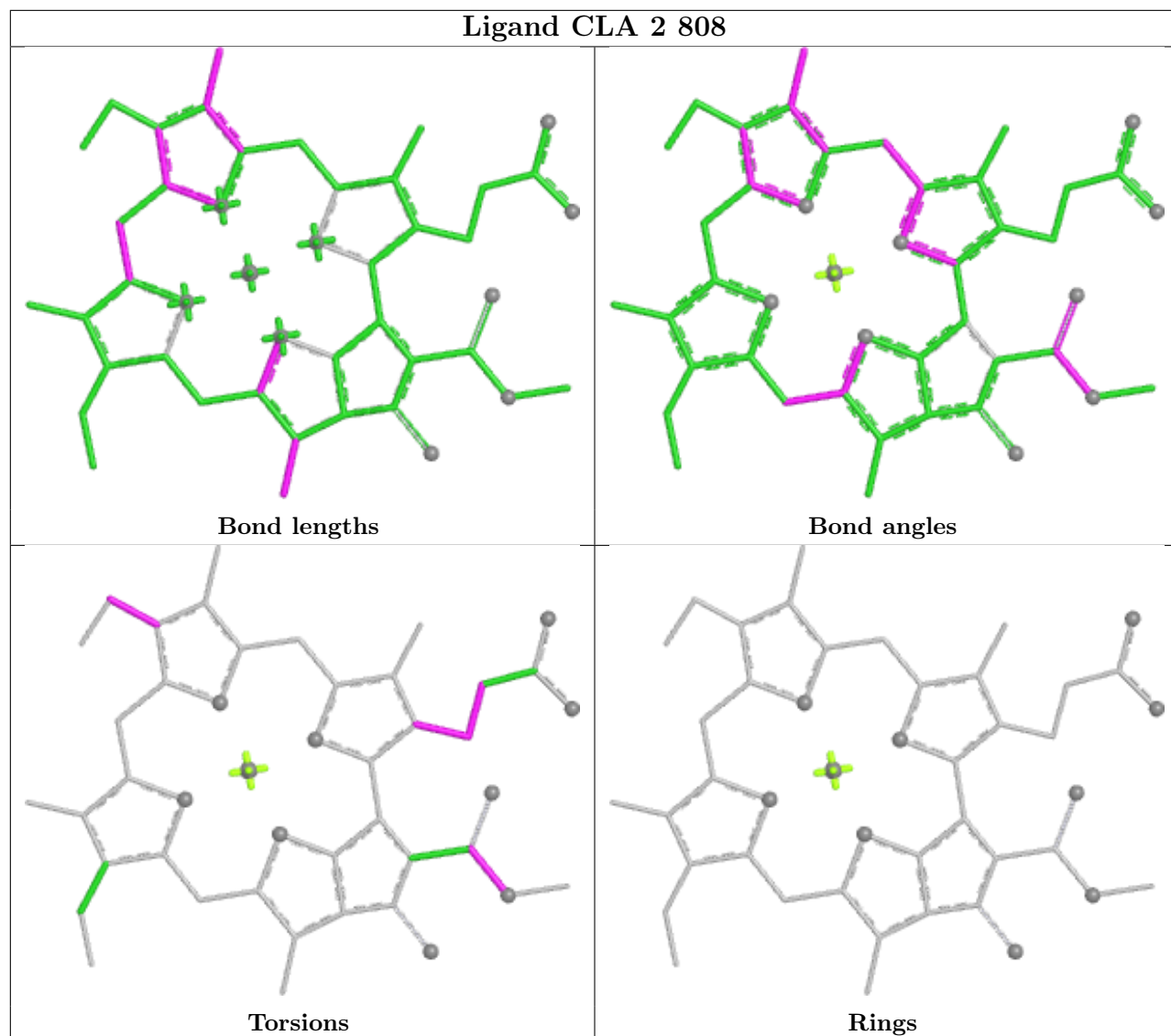
Ligand CLA b 834	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 805**Ligand CL0 a 801**

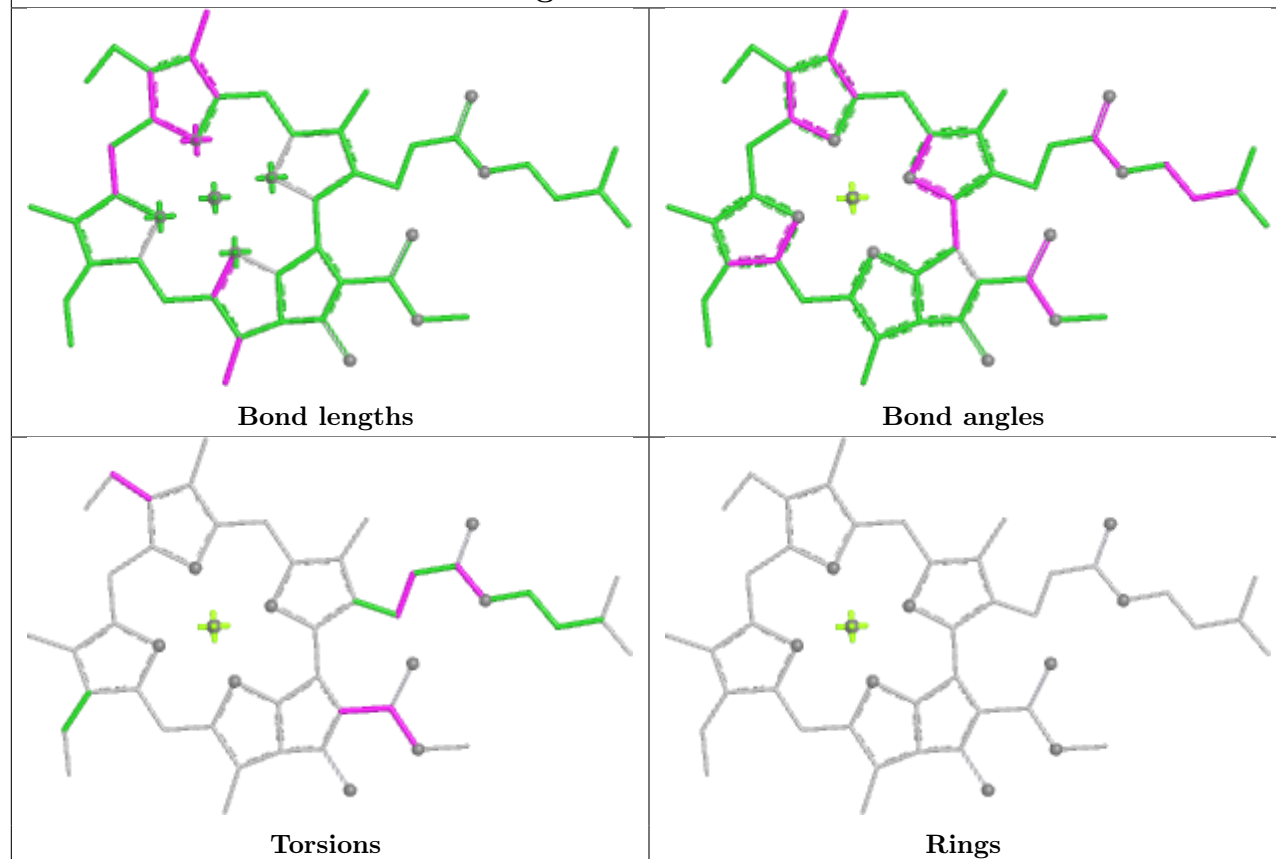


Ligand CLA a 827	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR k 4001	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 844	
 Bond lengths	 Bond angles
 Torsions	 Rings

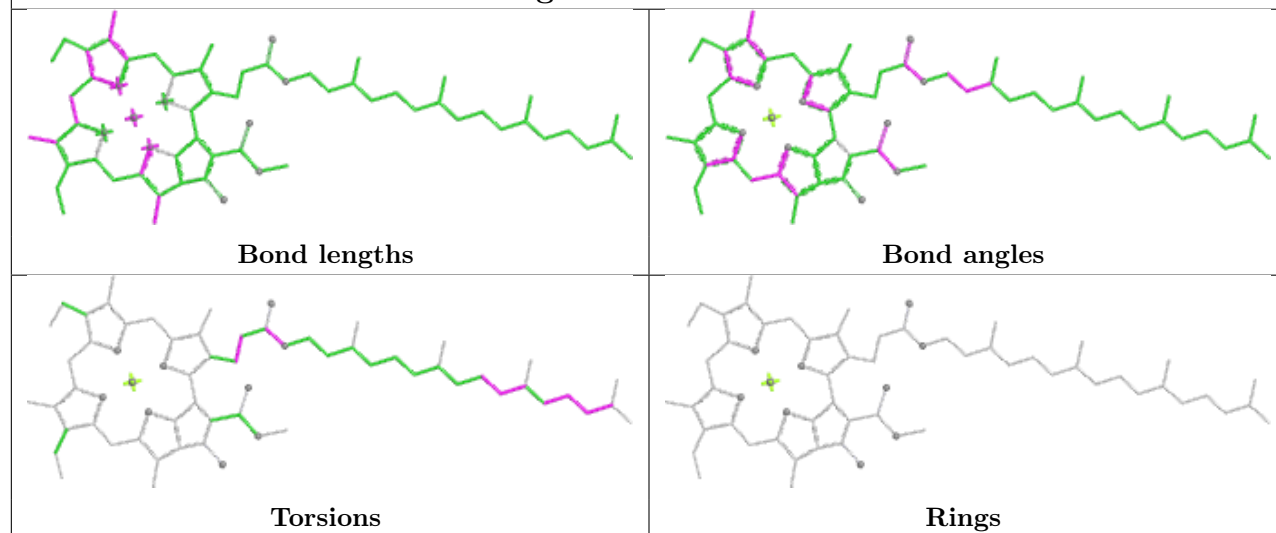
Ligand CLA 2 808

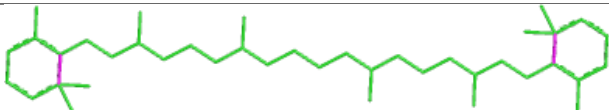
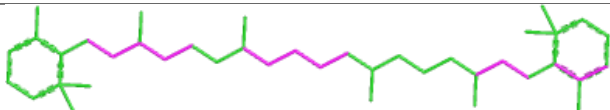
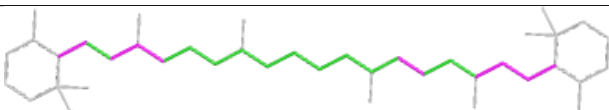
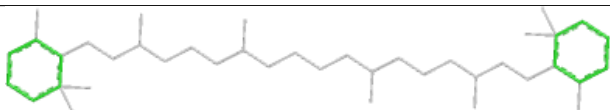


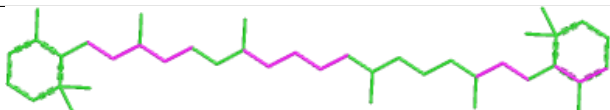
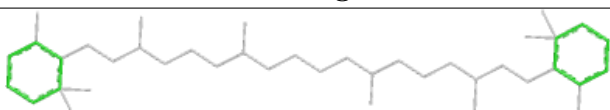
Ligand CLA 1 822

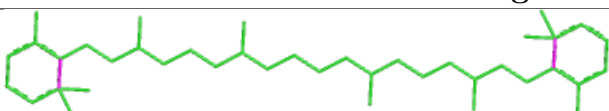
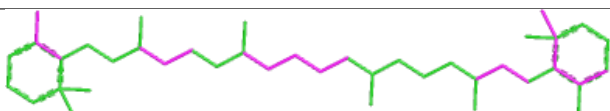
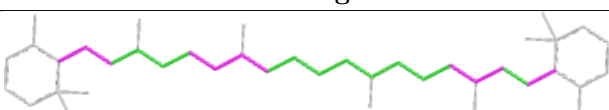
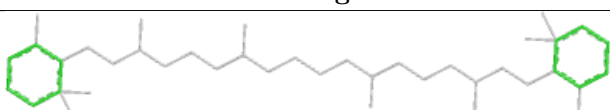


Ligand CLA 1 839

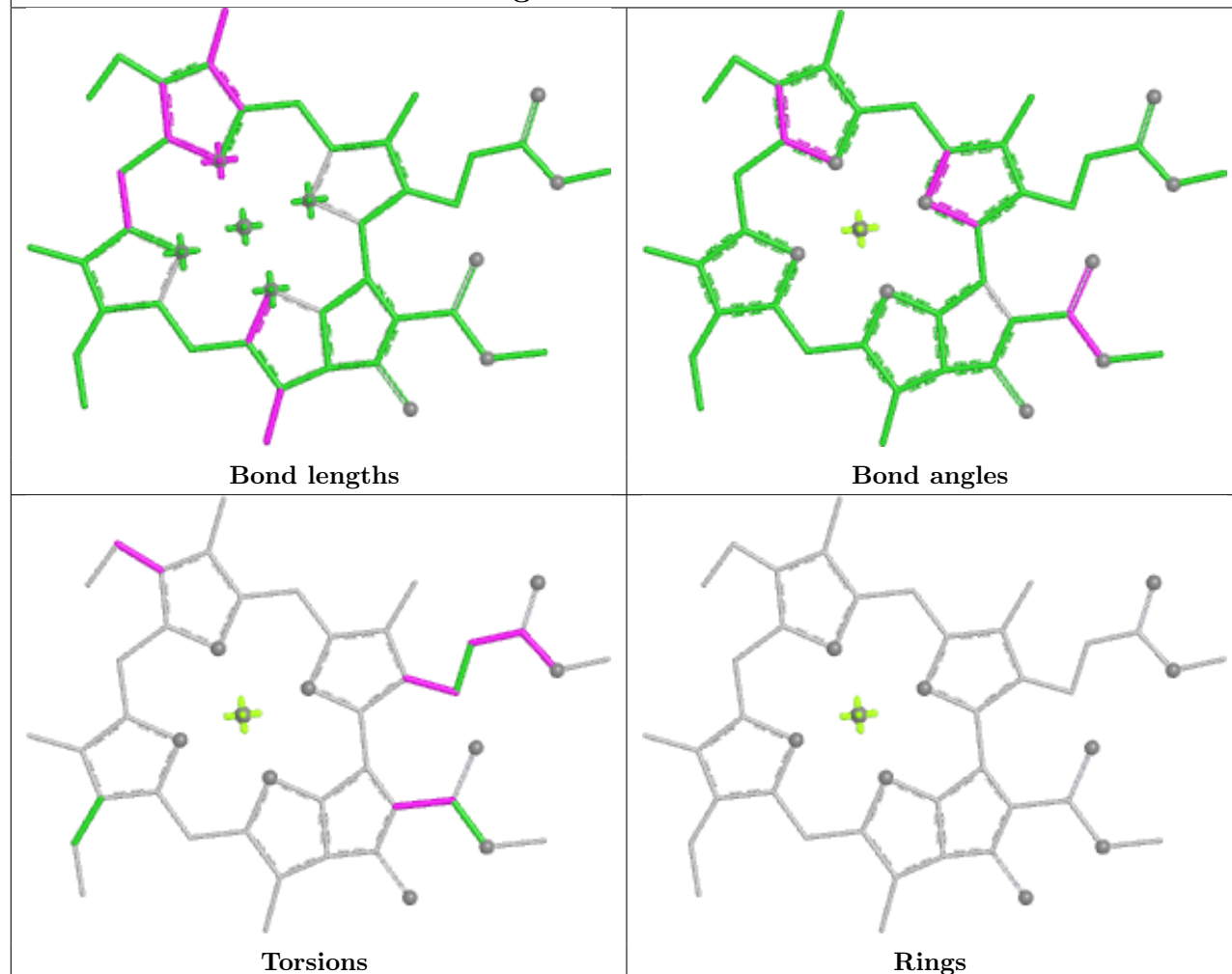


Ligand BCR 2 839	
 Bond lengths	 Bond angles
 Torsions	 Rings

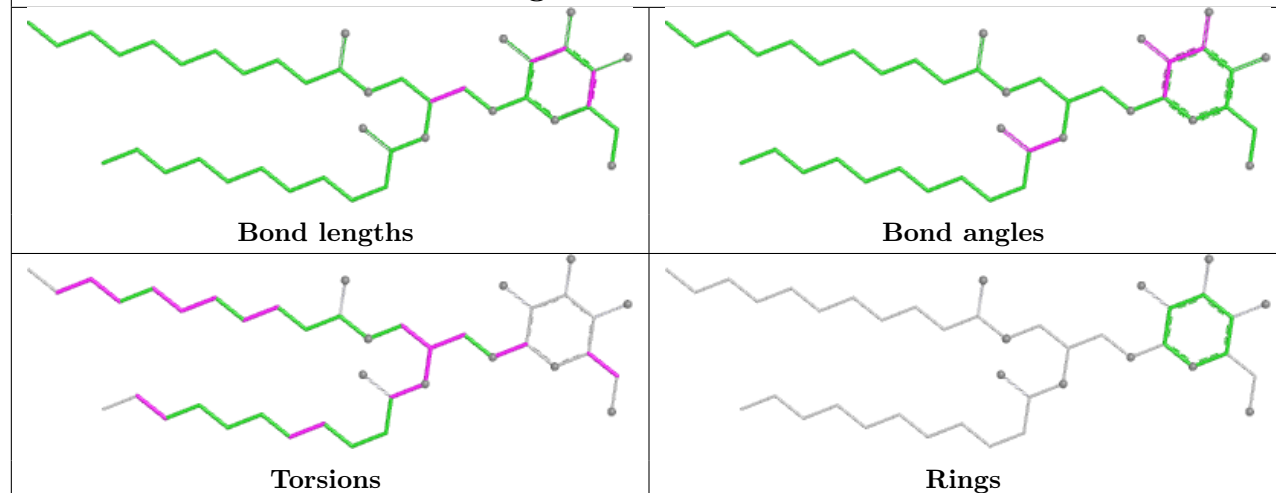
Ligand BCR b 840	
 Bond lengths	 Bond angles
 Torsions	 Rings

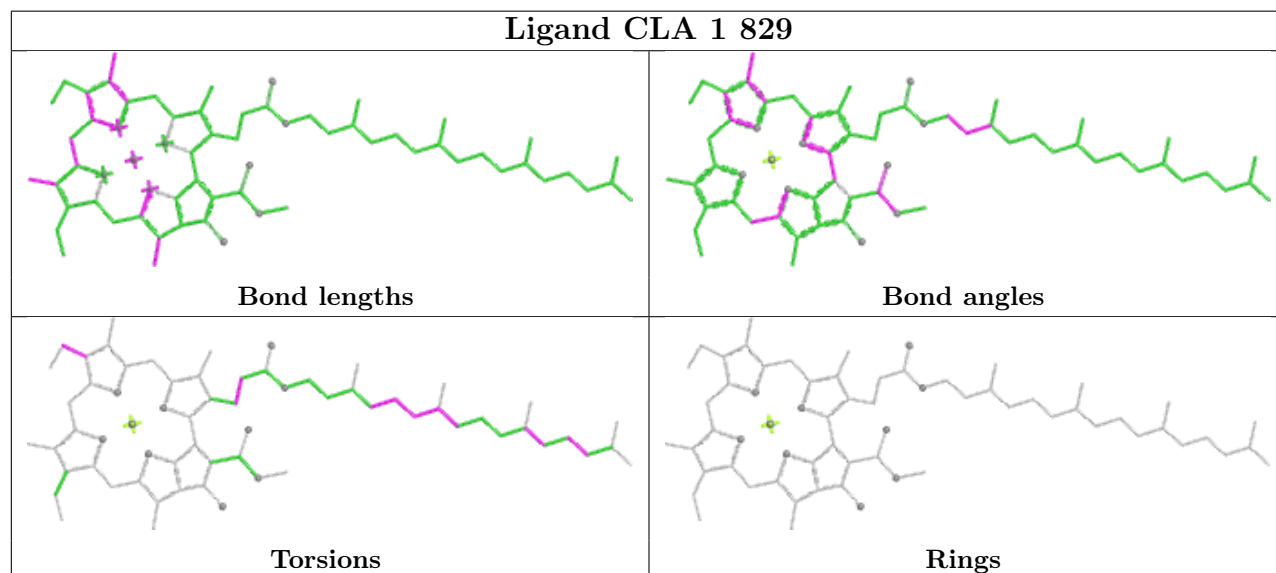
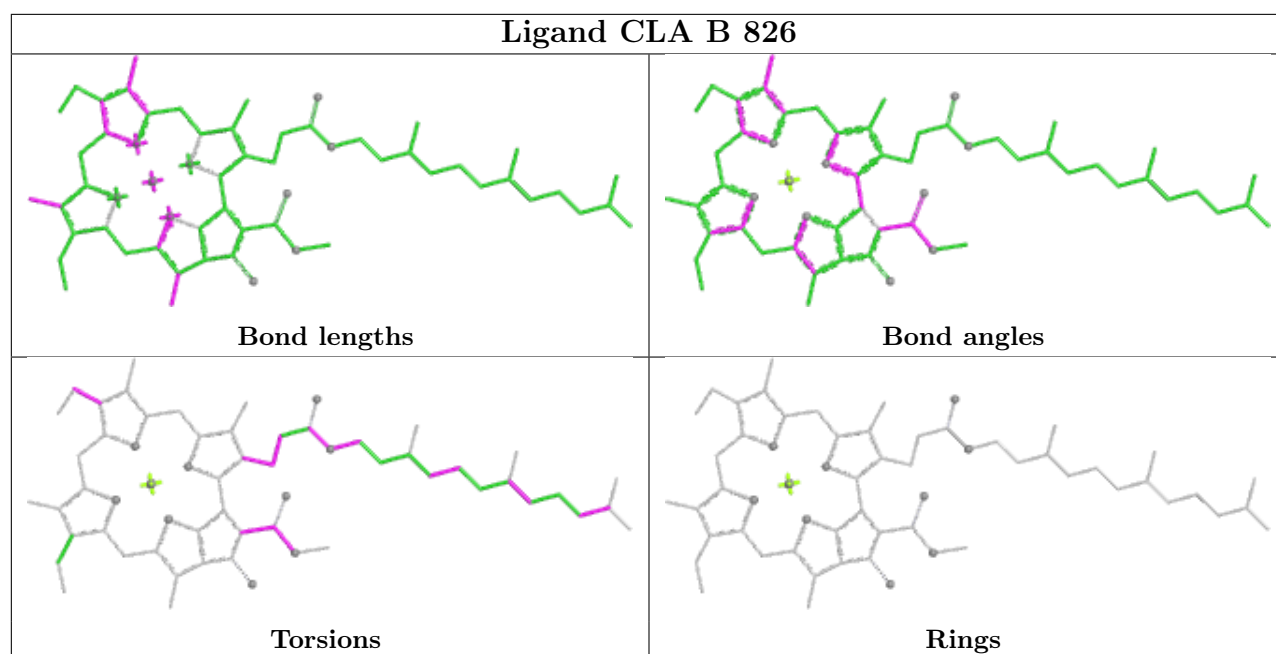
Ligand BCR 6 205	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A 816

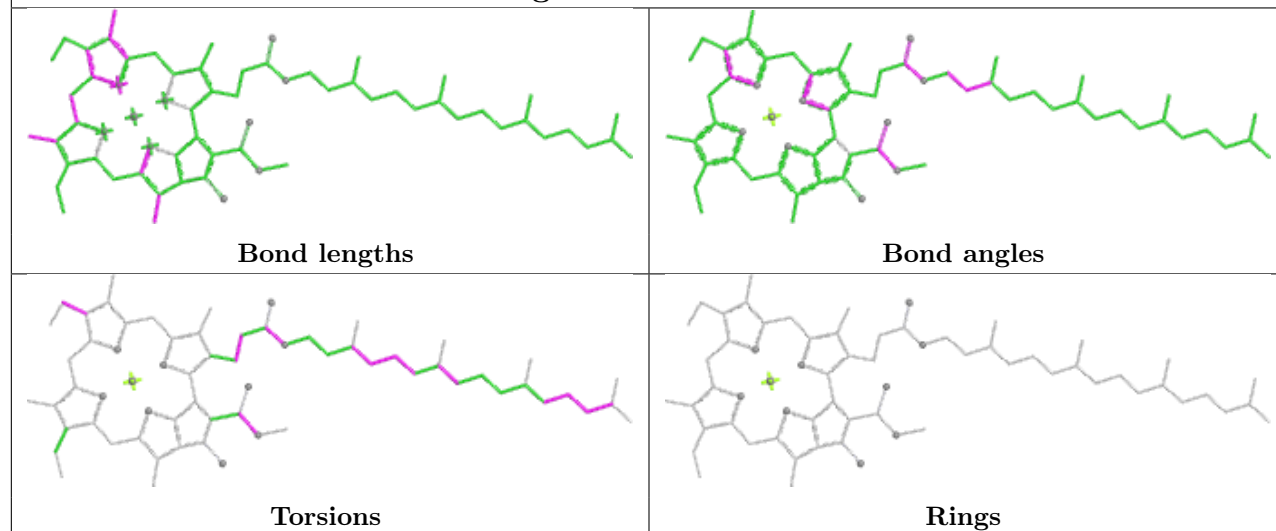


Ligand LMG B 846

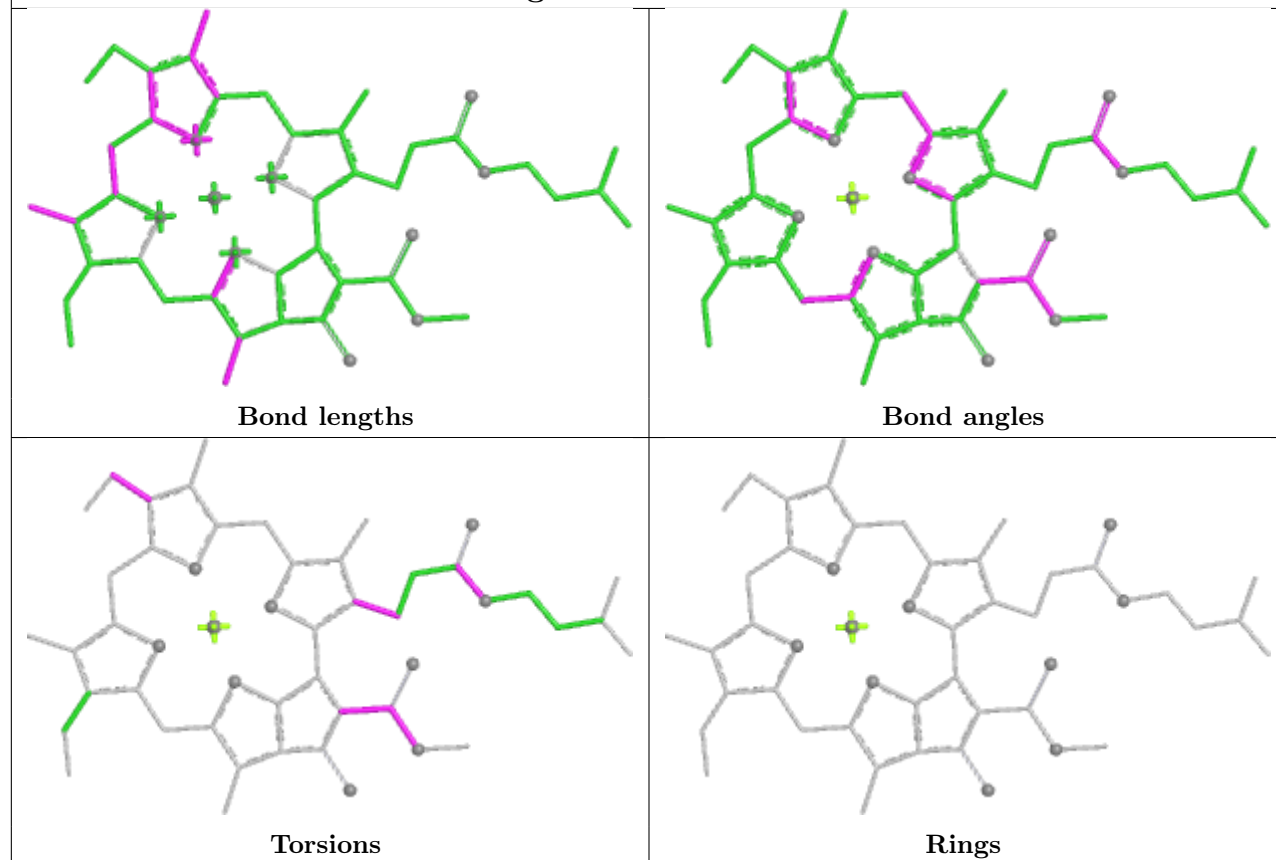




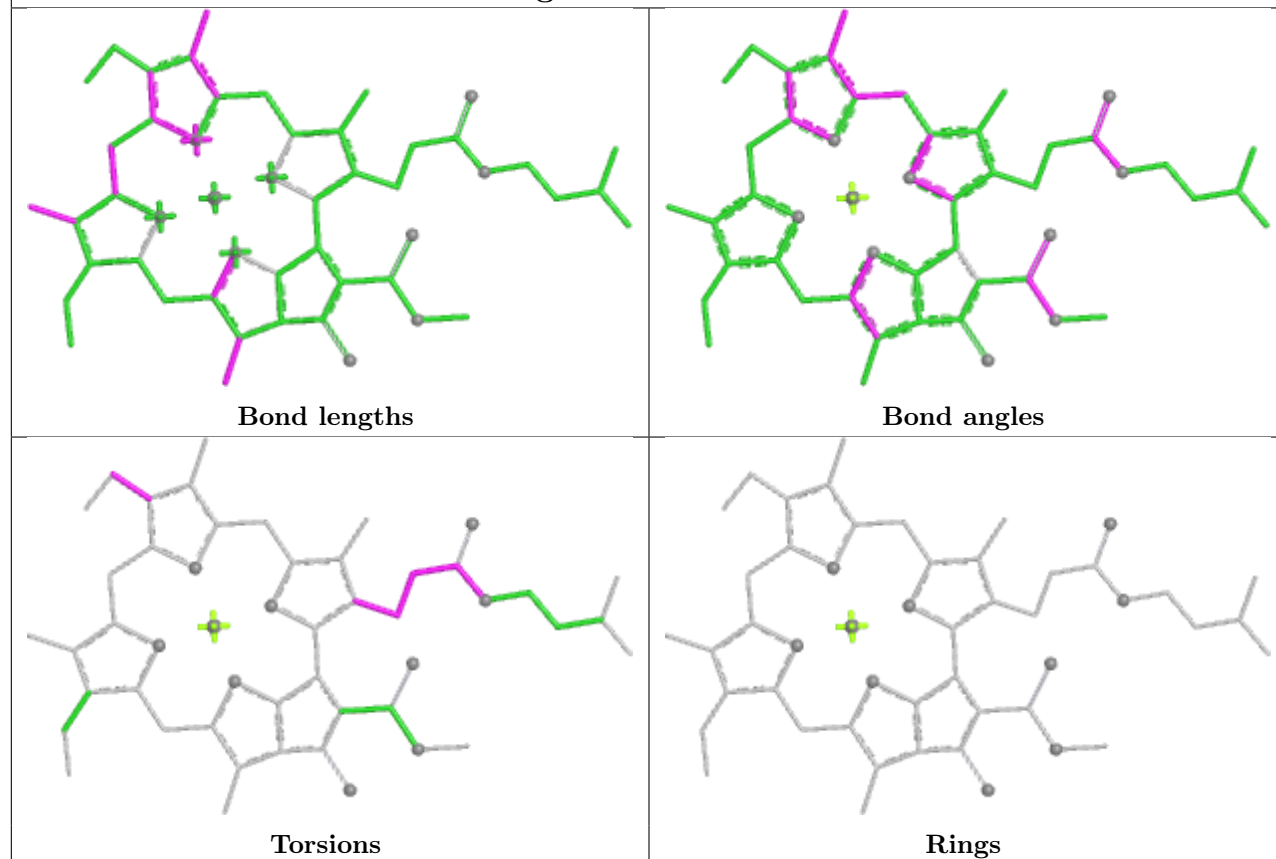
Ligand CLA B 806



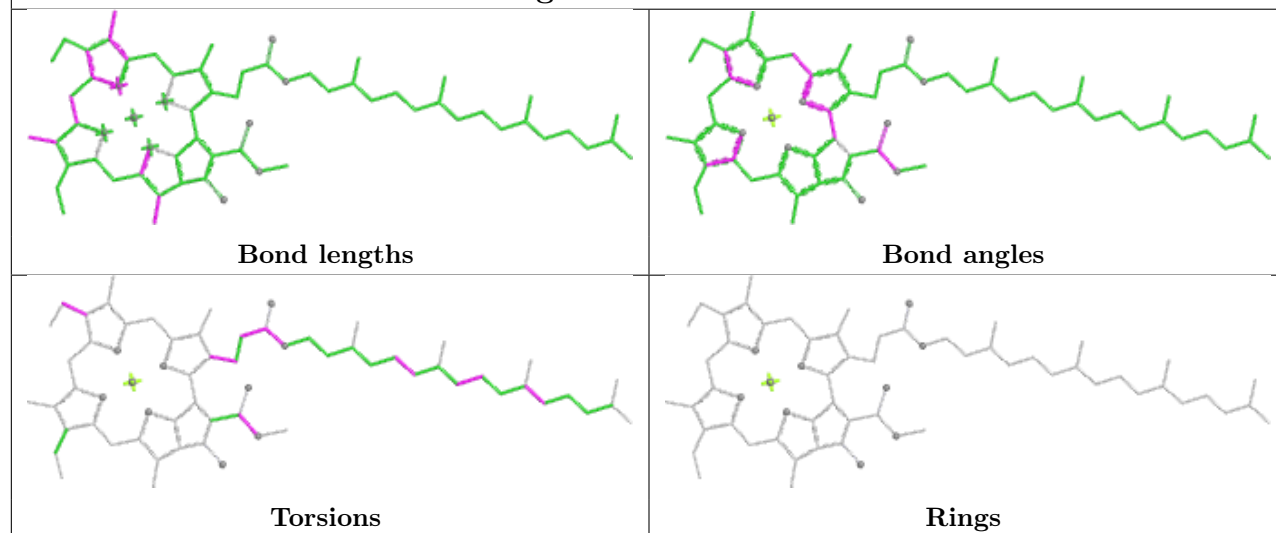
Ligand CLA J 1101

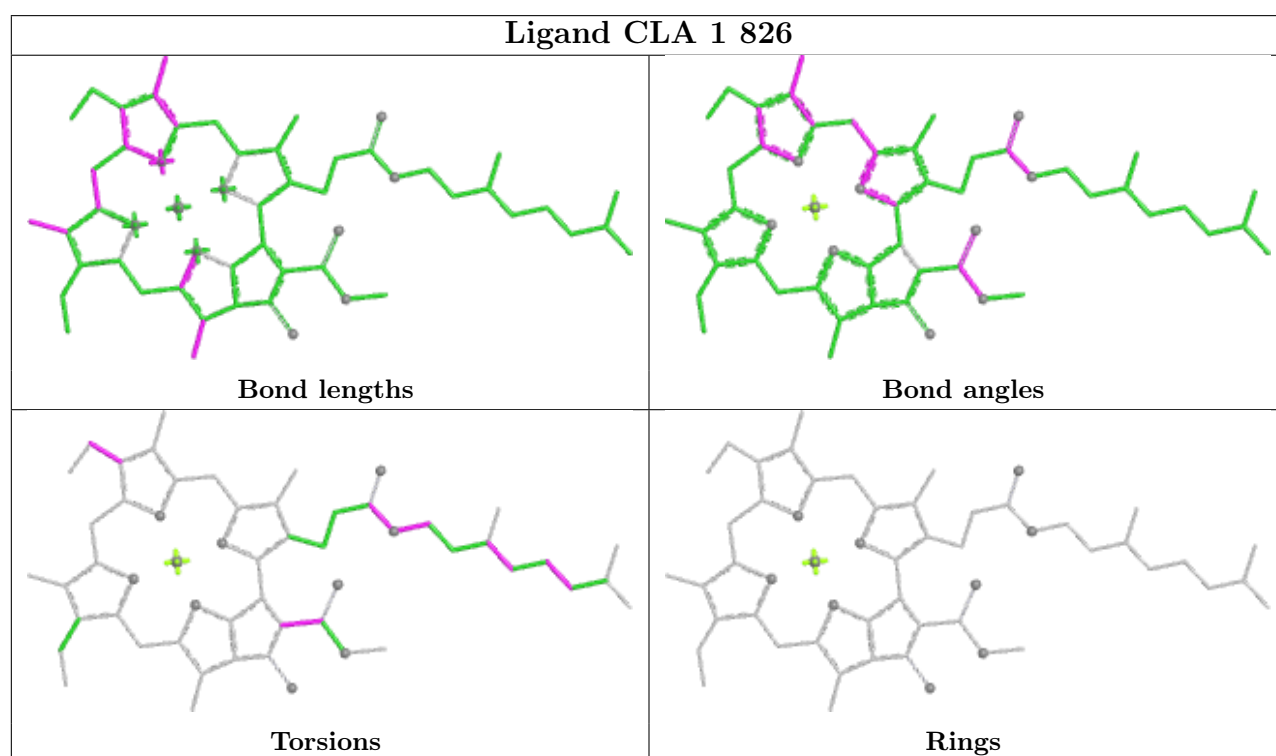
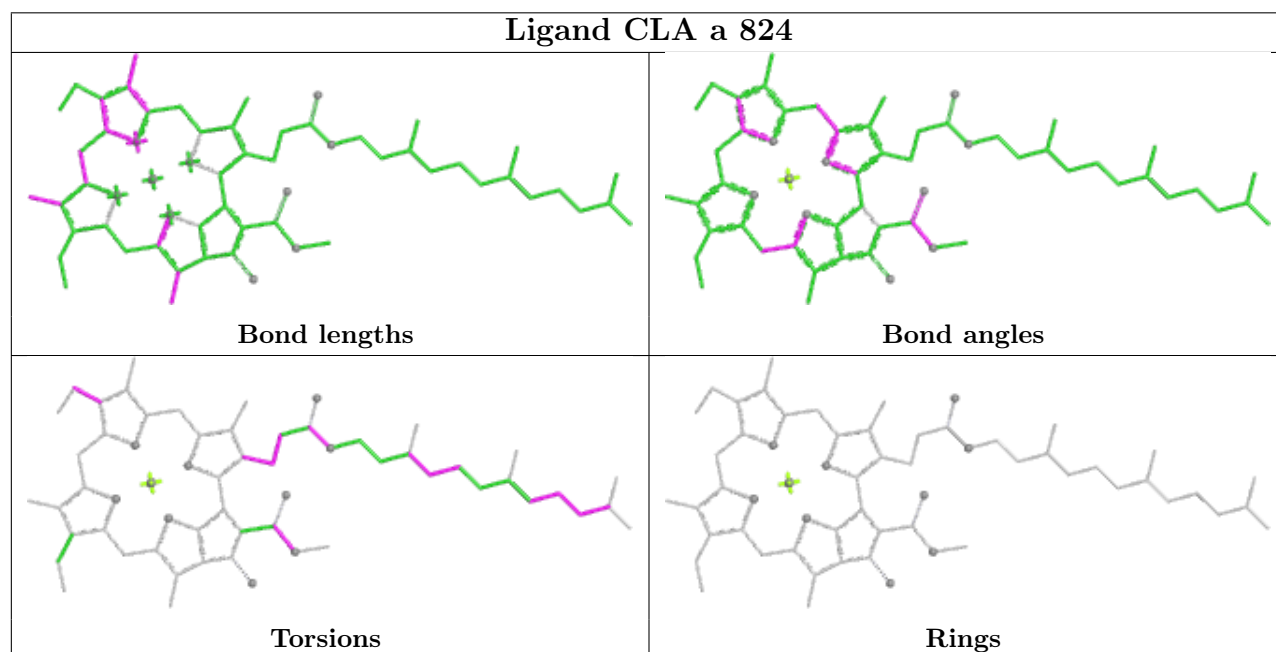
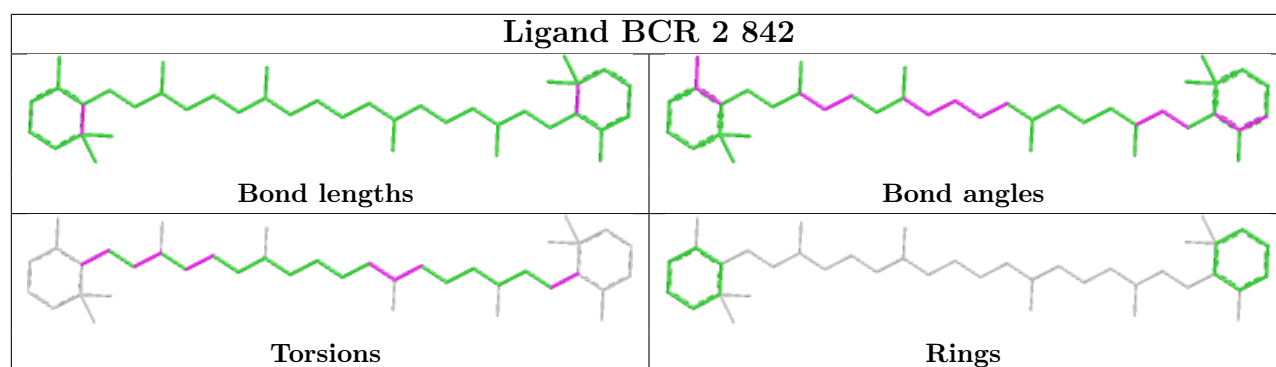


Ligand CLA 2 813

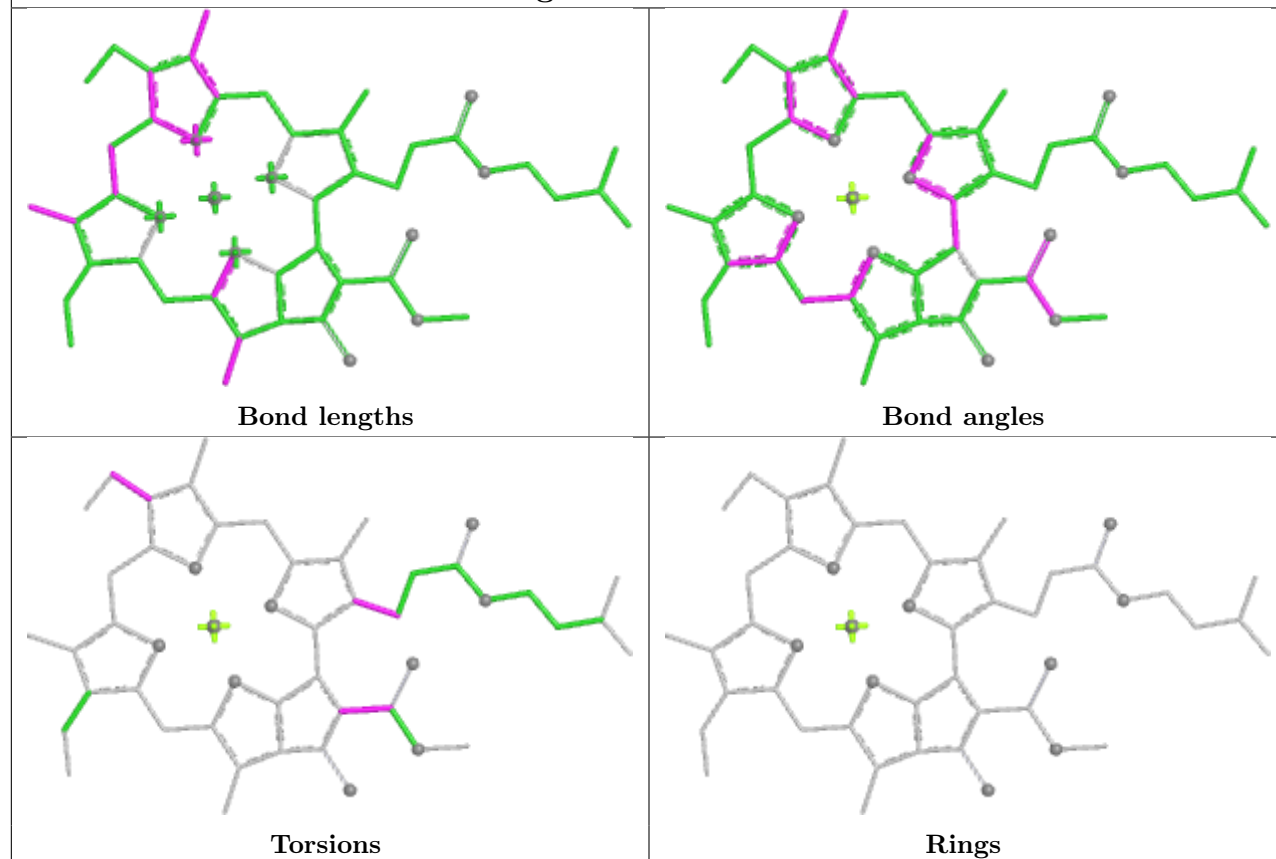


Ligand CLA 1 833

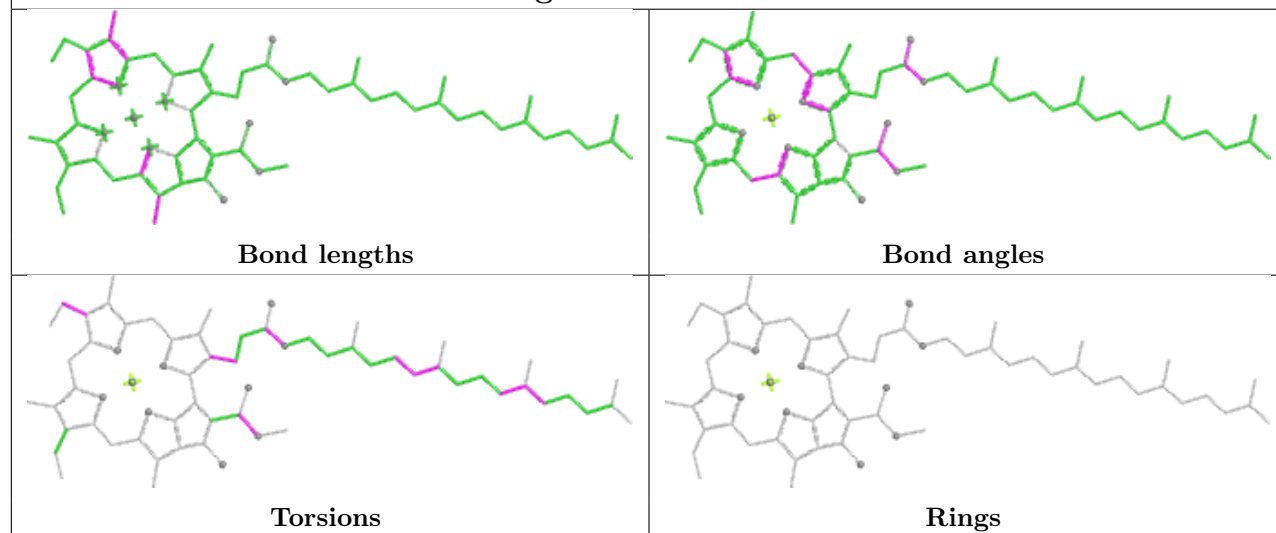


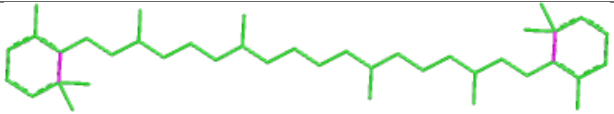
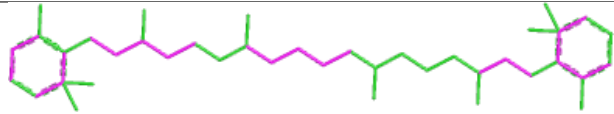
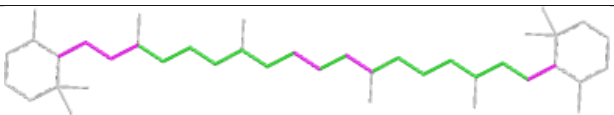
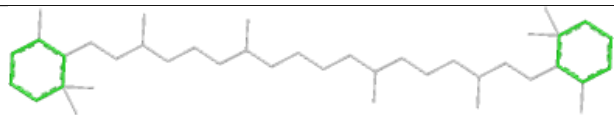


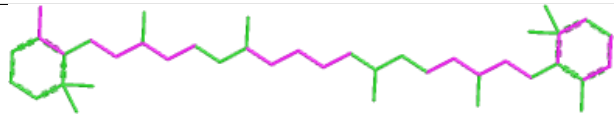
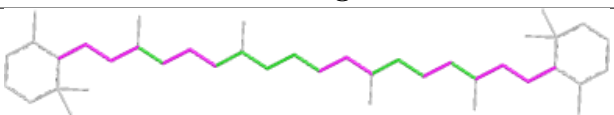
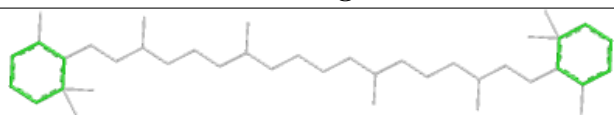
Ligand CLA a 808

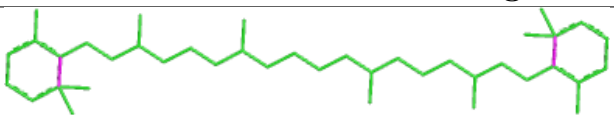
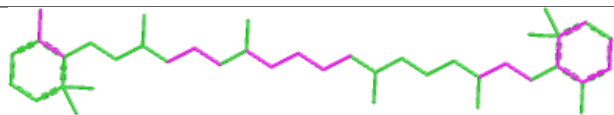
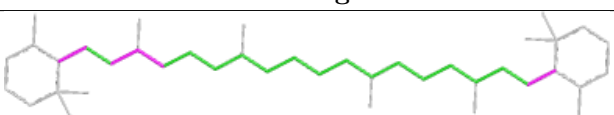
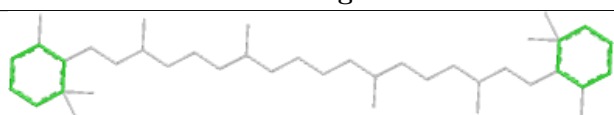


Ligand CLA b 837

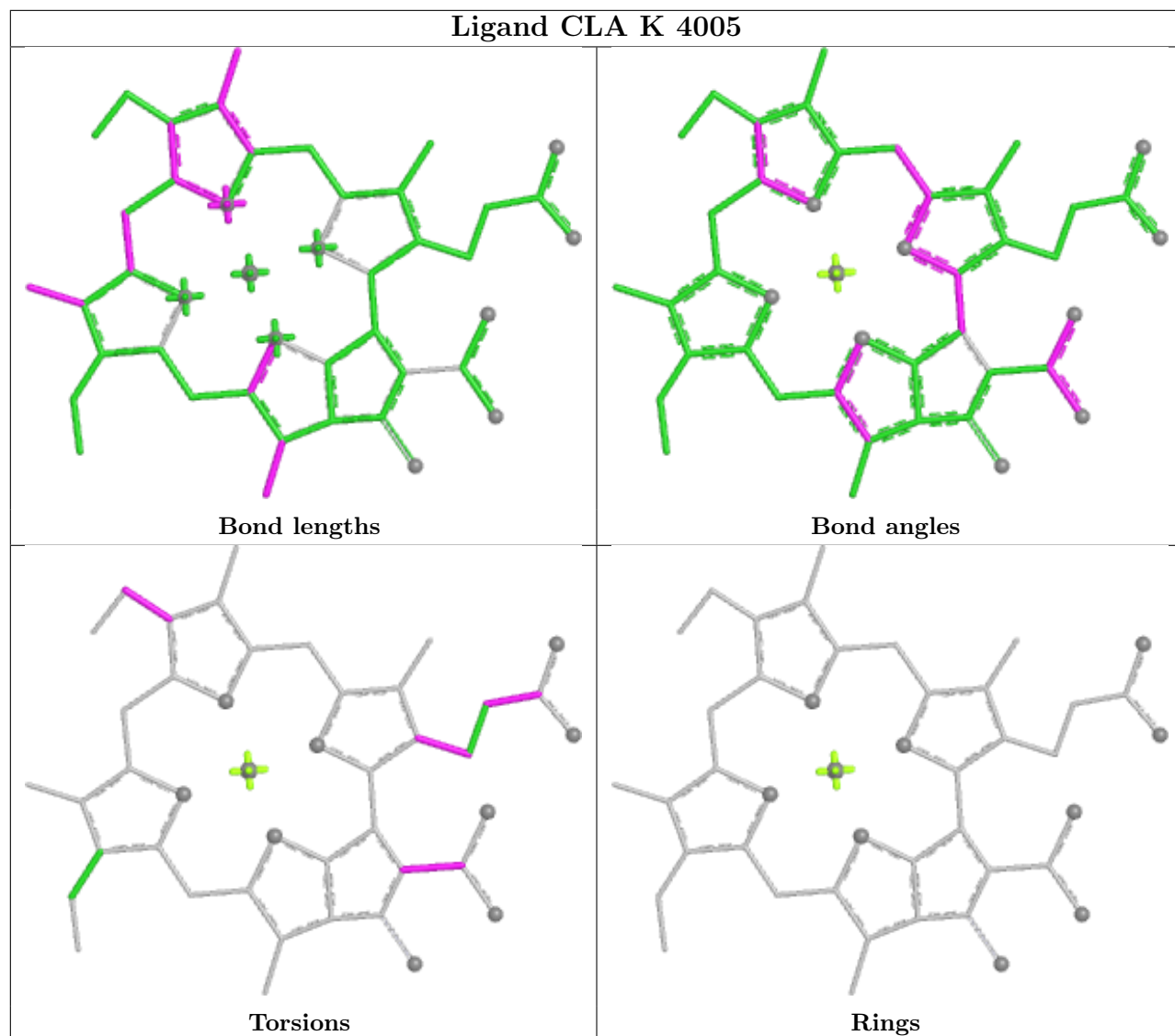


Ligand BCR J 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

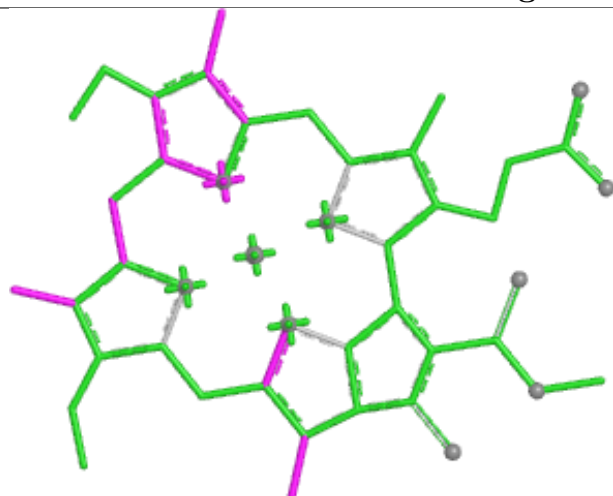
Ligand BCR 1 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR M 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

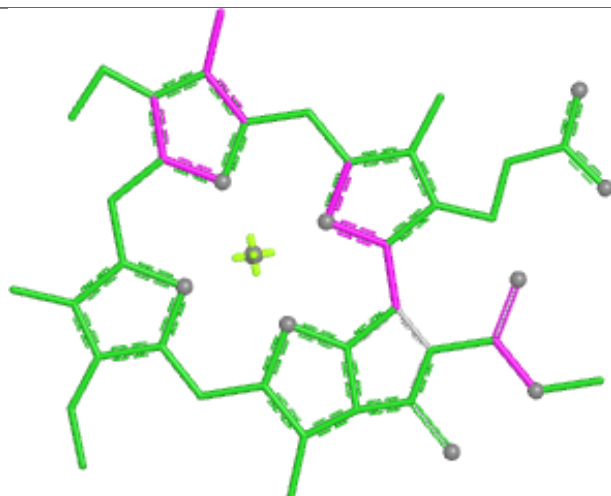
Ligand CLA K 4005



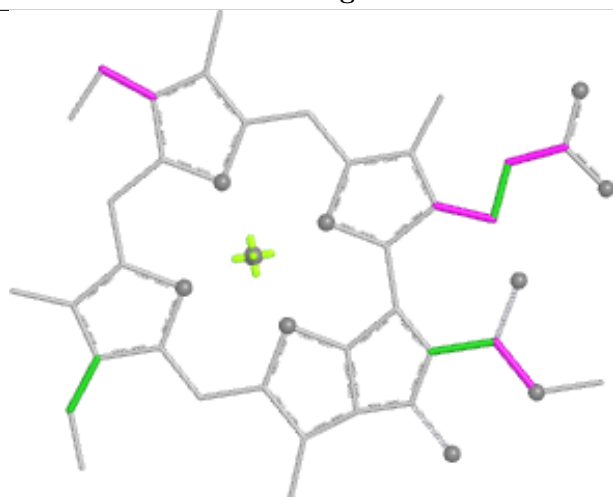
Ligand CLA a 842



Bond lengths



Bond angles

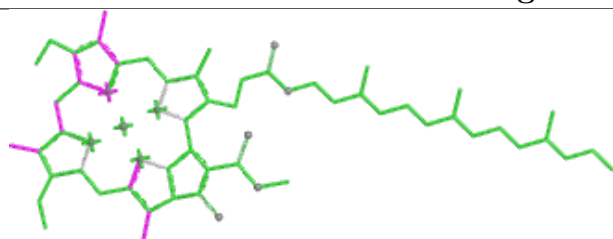


Torsions

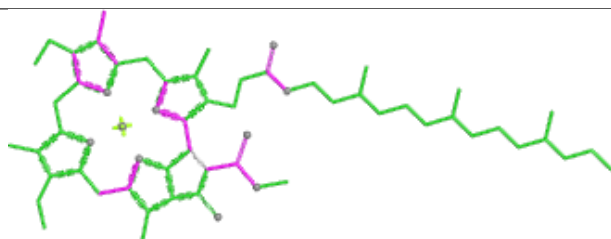


Rings

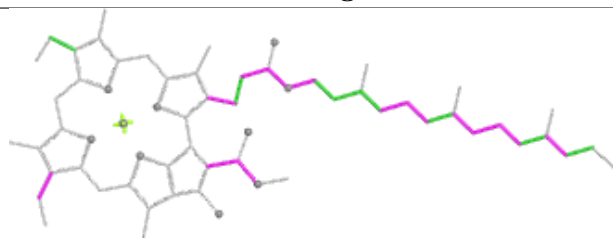
Ligand CLA b 829



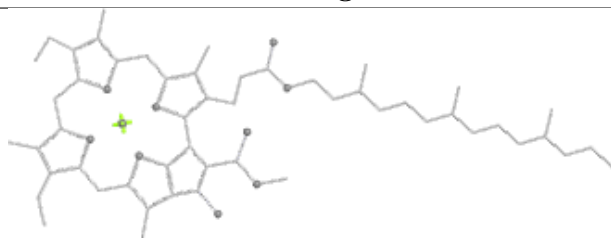
Bond lengths



Bond angles

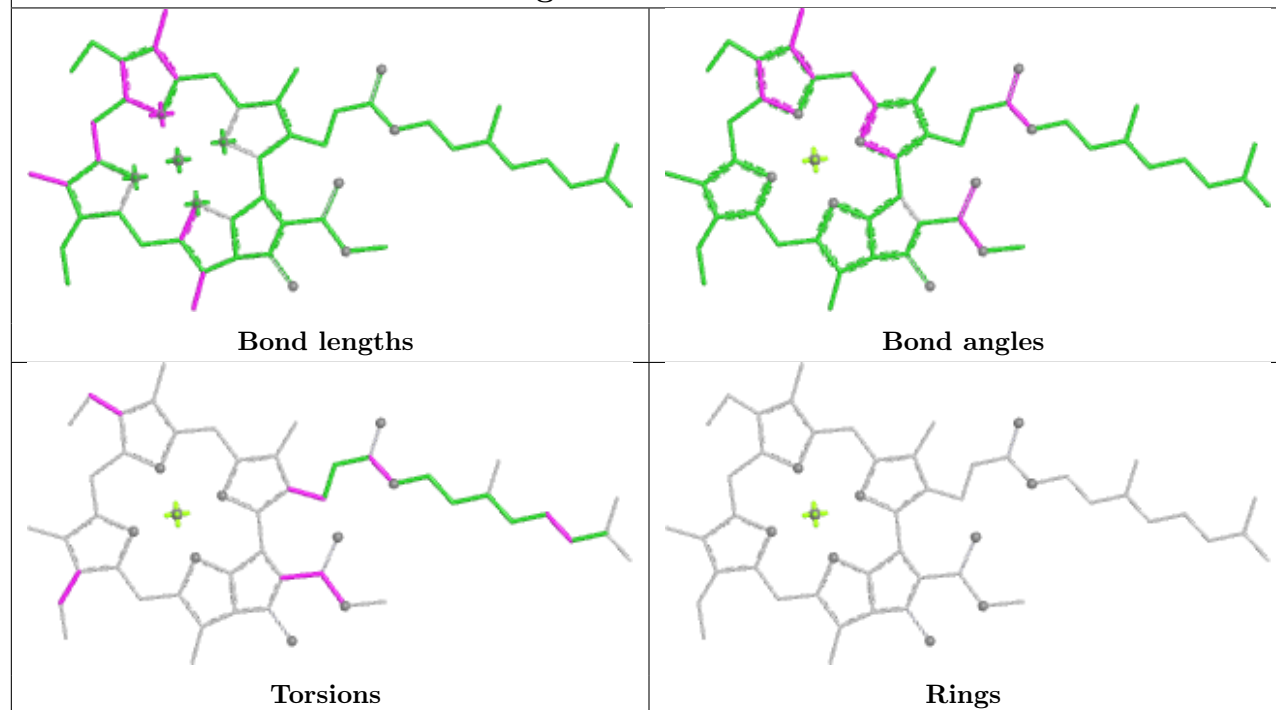


Torsions

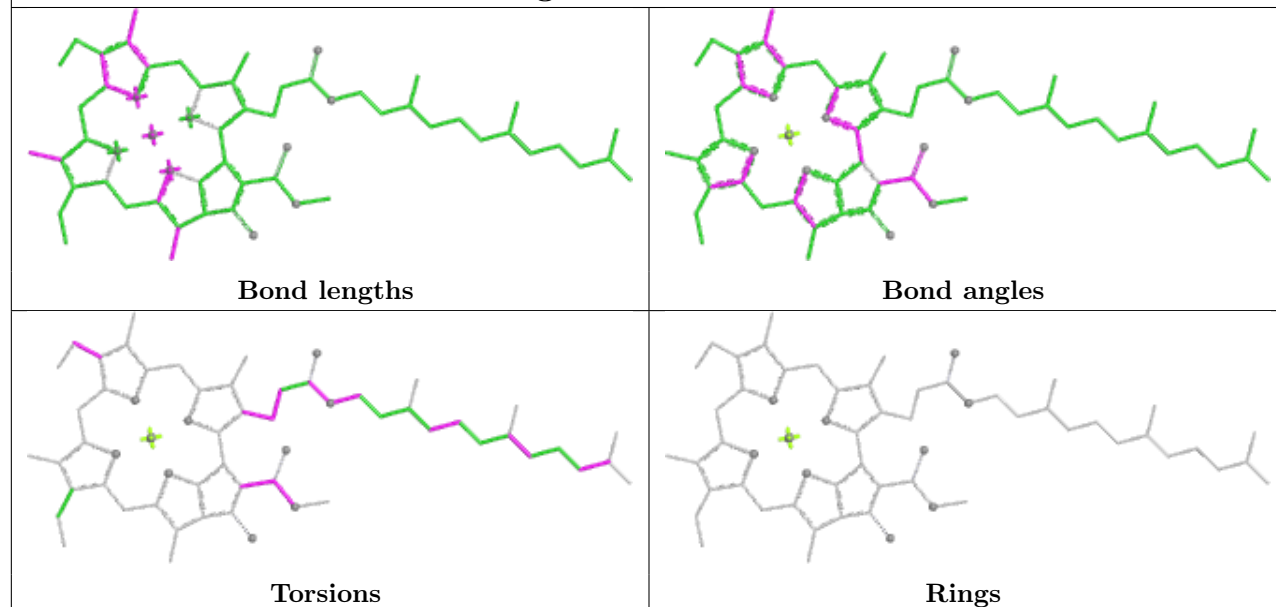


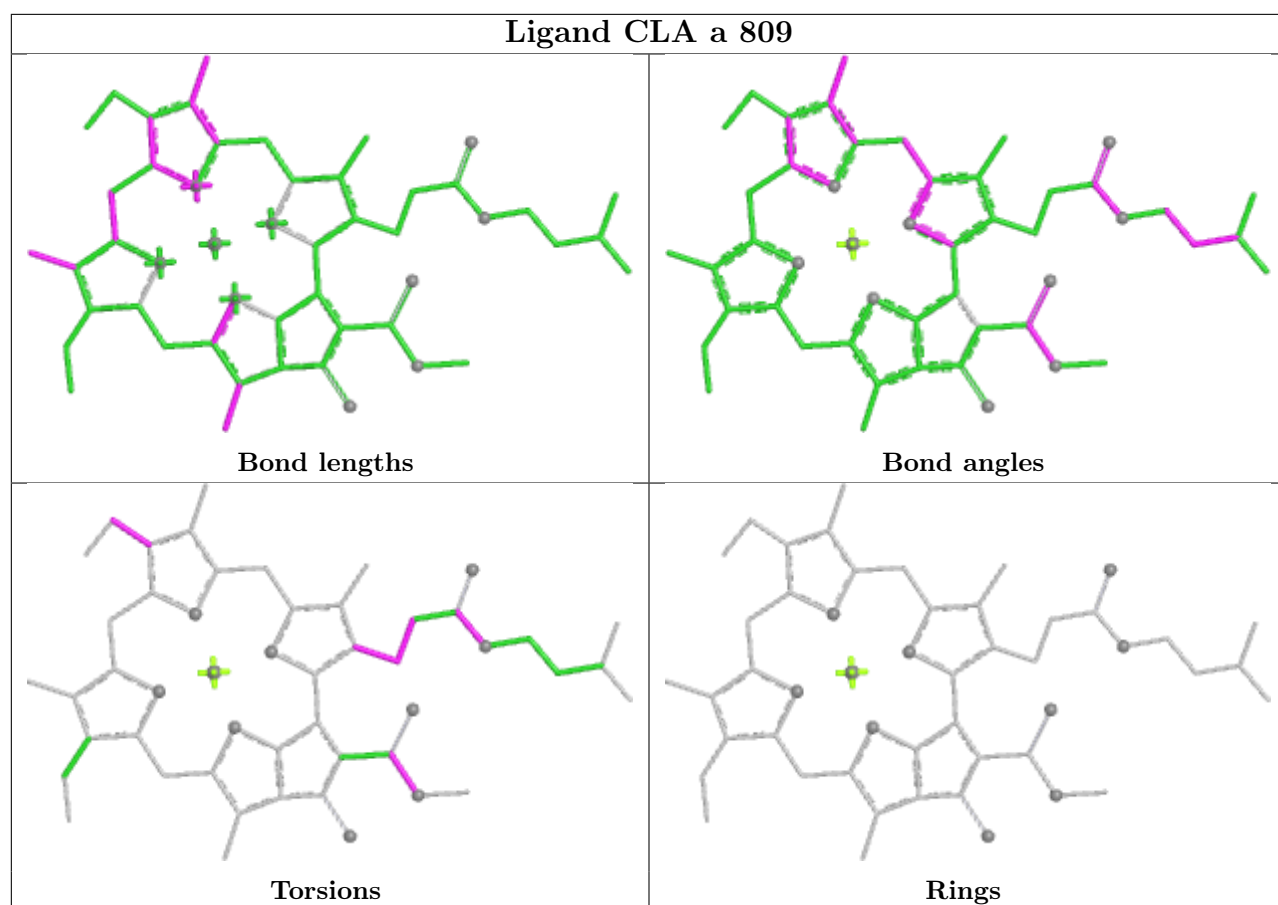
Rings

Ligand CLA a 805

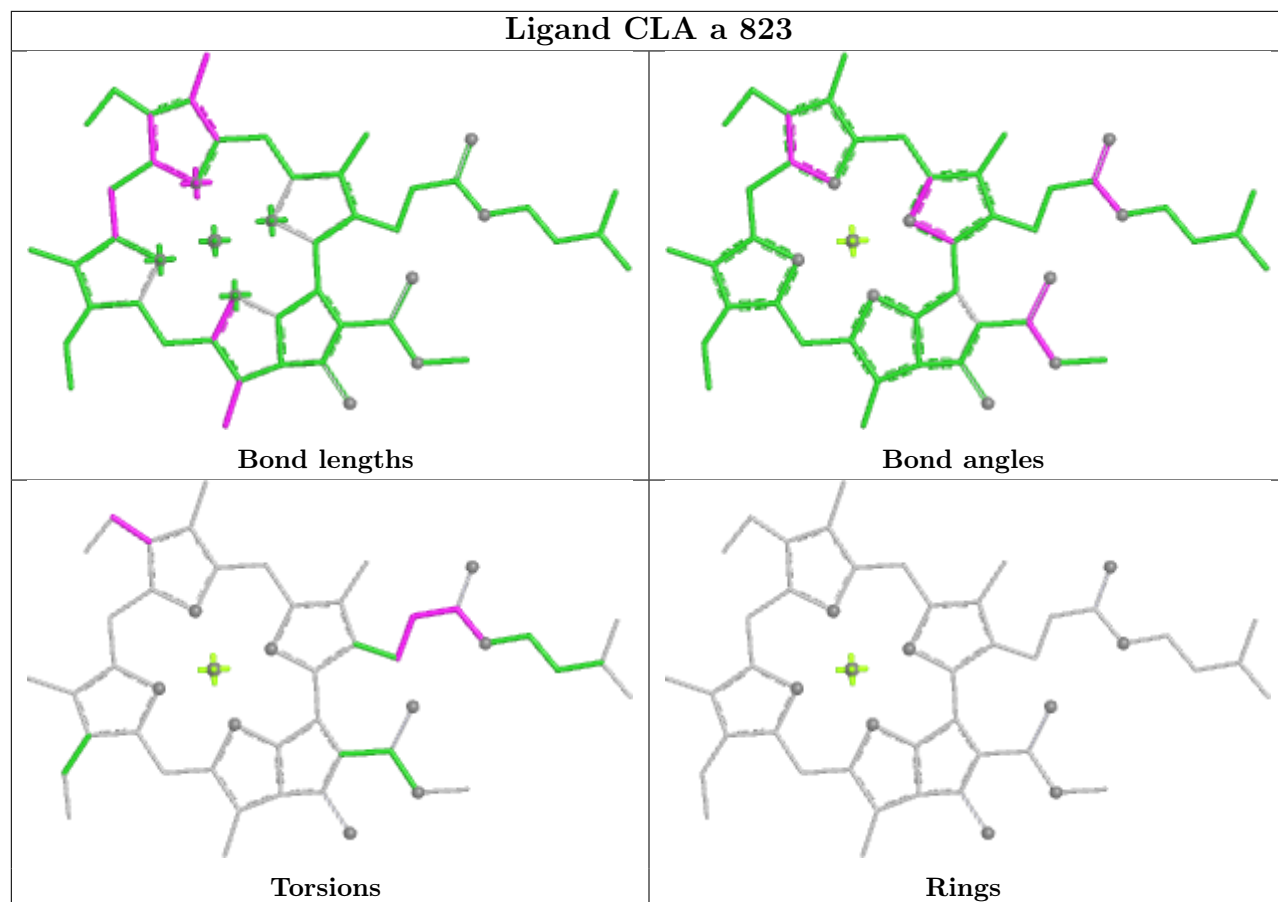


Ligand CLA 2 825

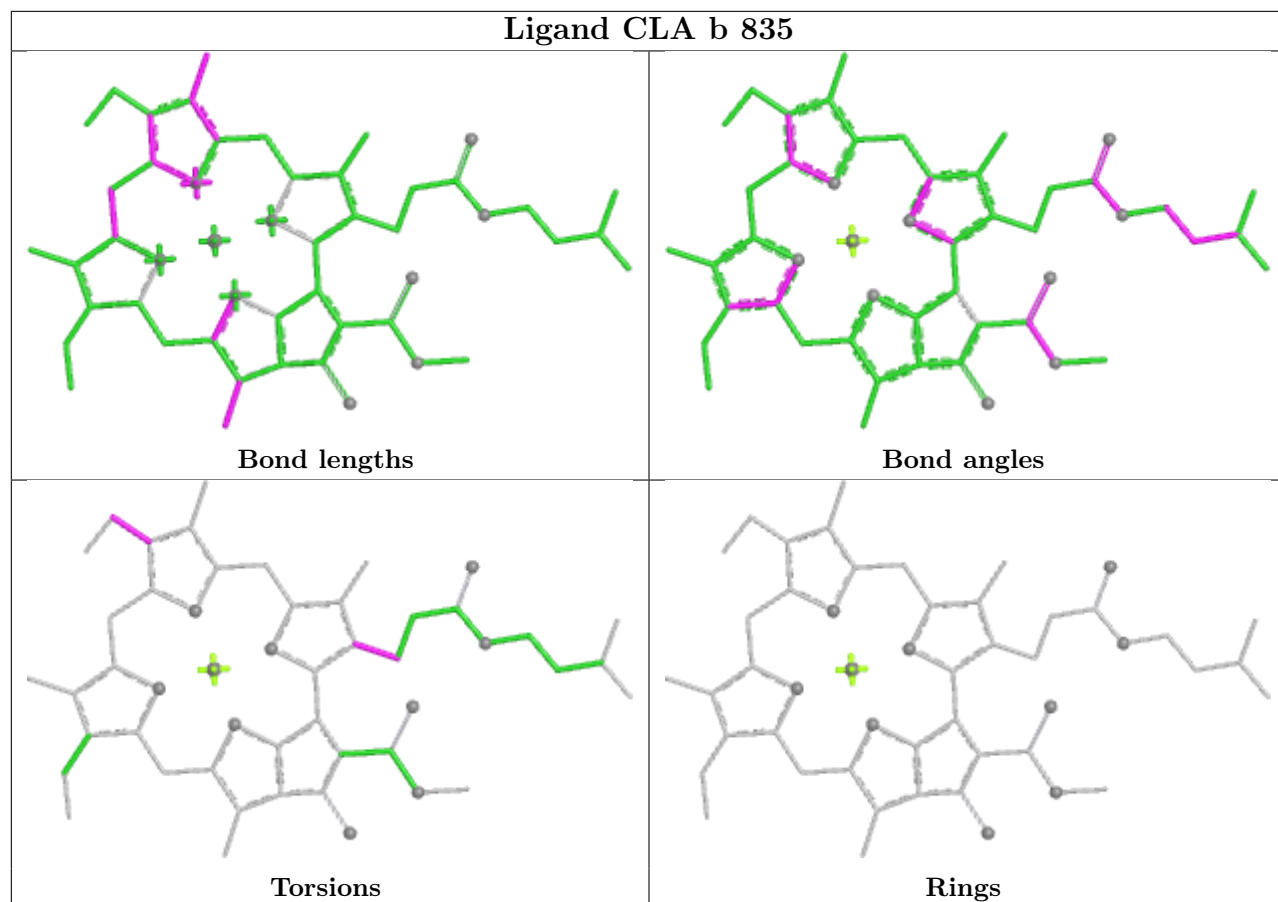




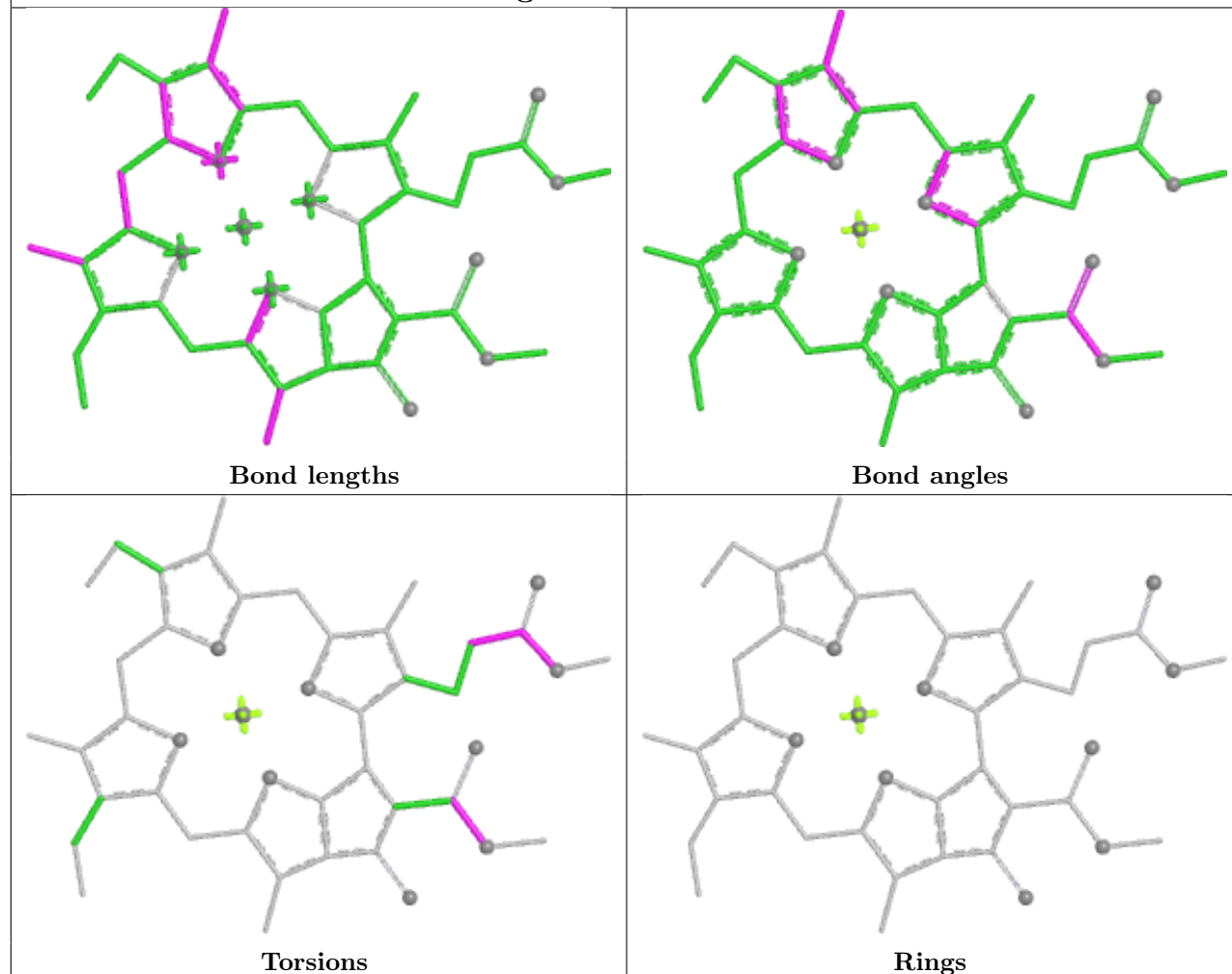
Ligand CLA a 823



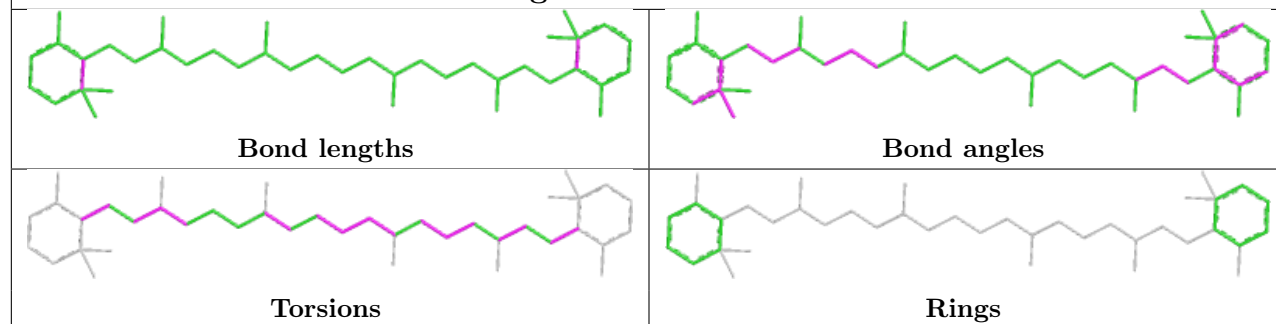
Ligand CLA b 835

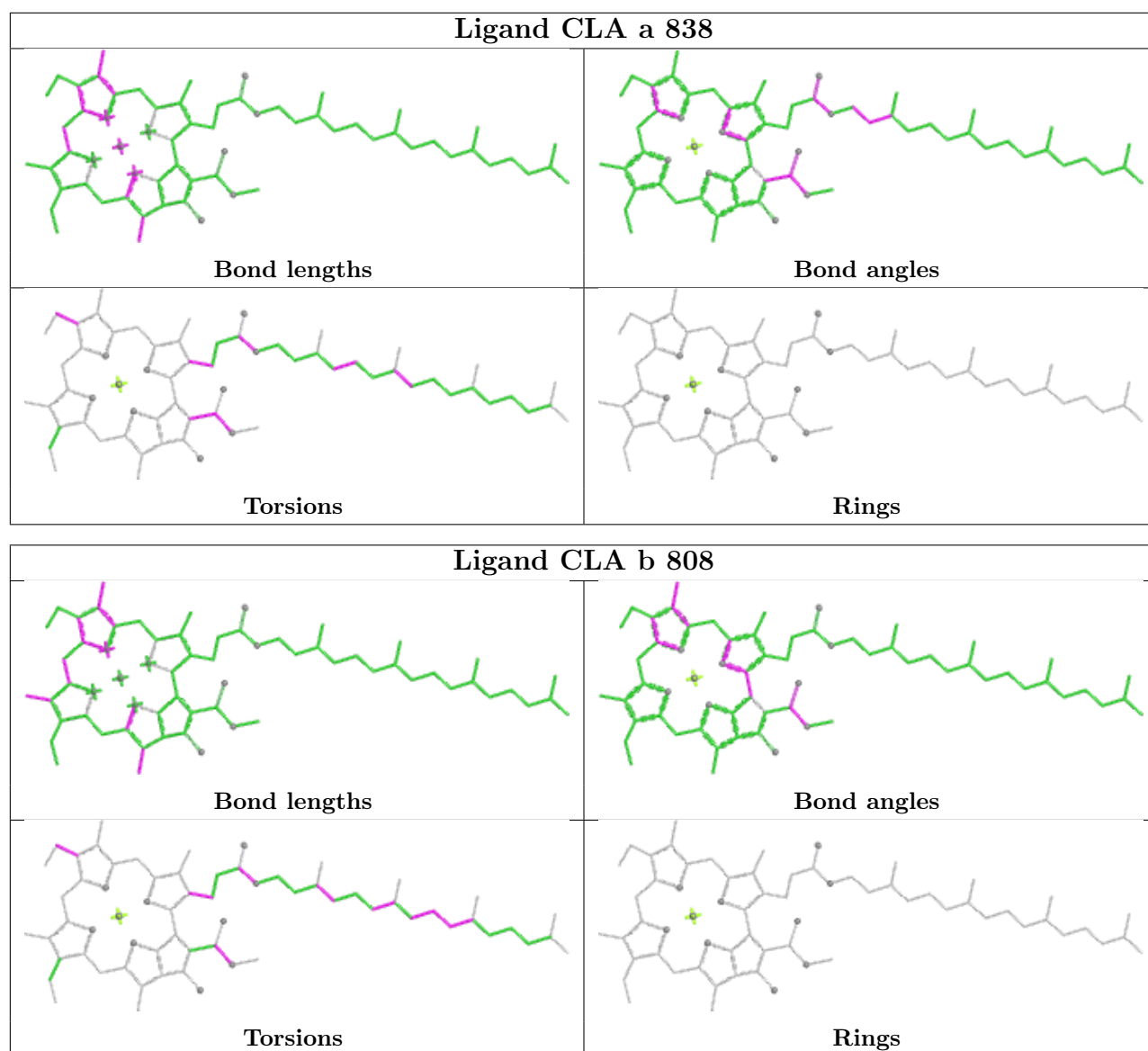


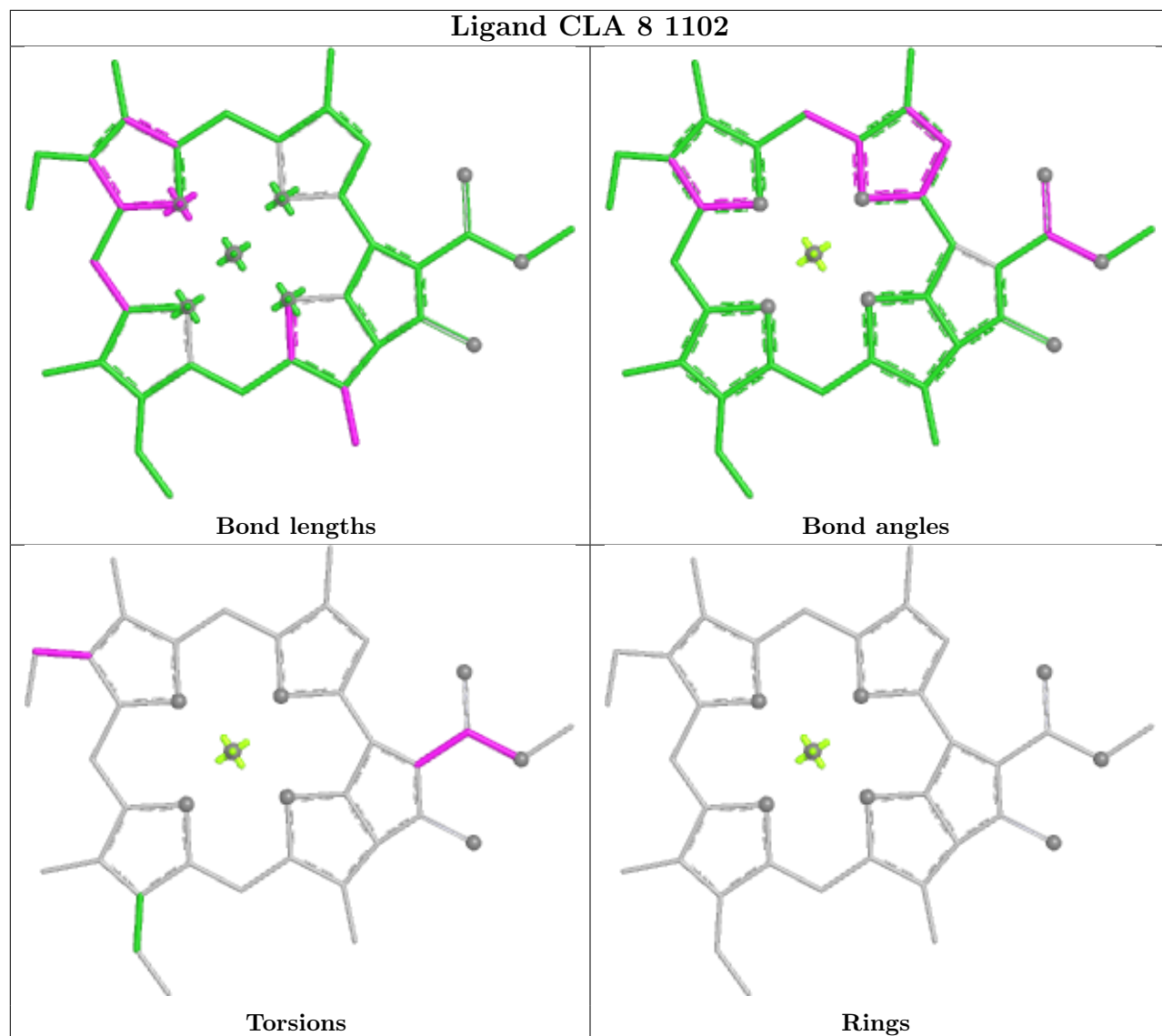
Ligand CLA b 819



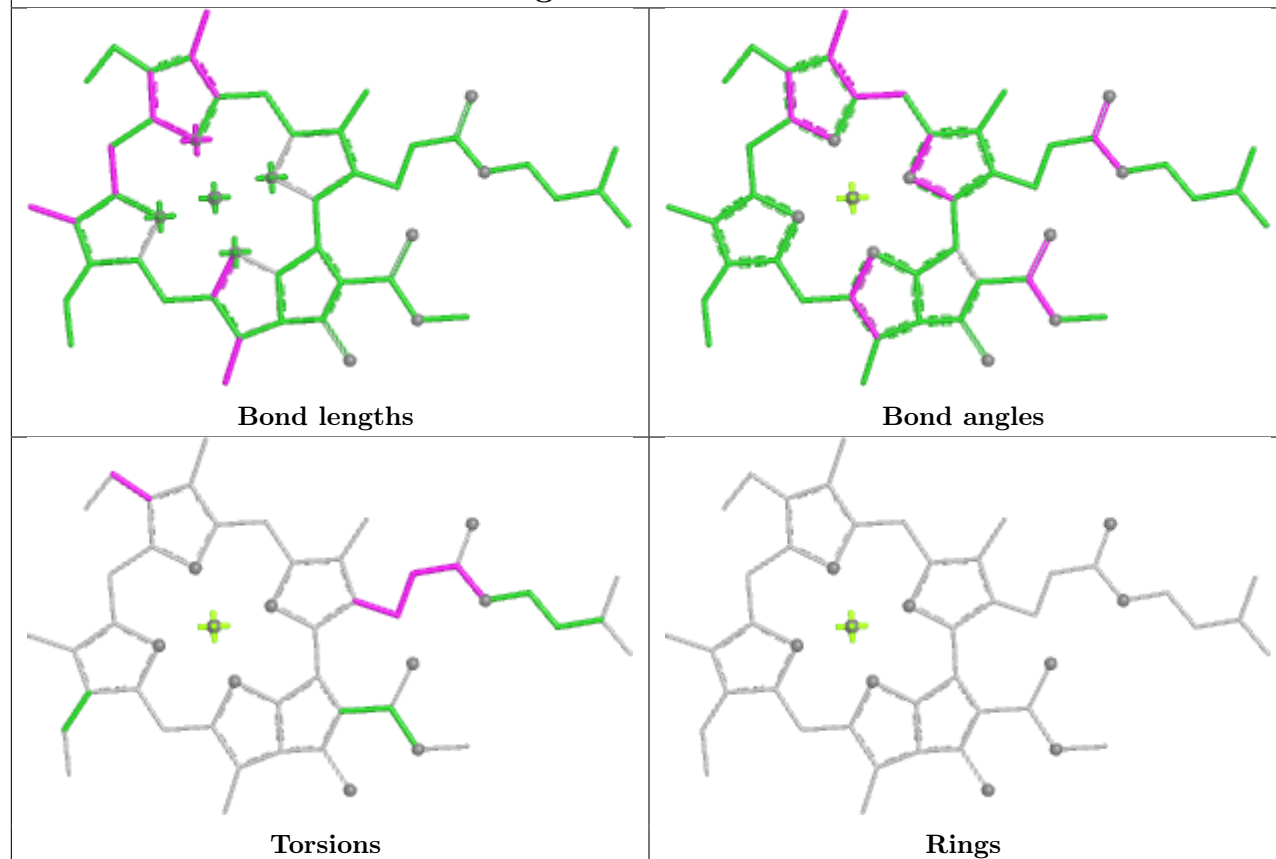
Ligand BCR A 848



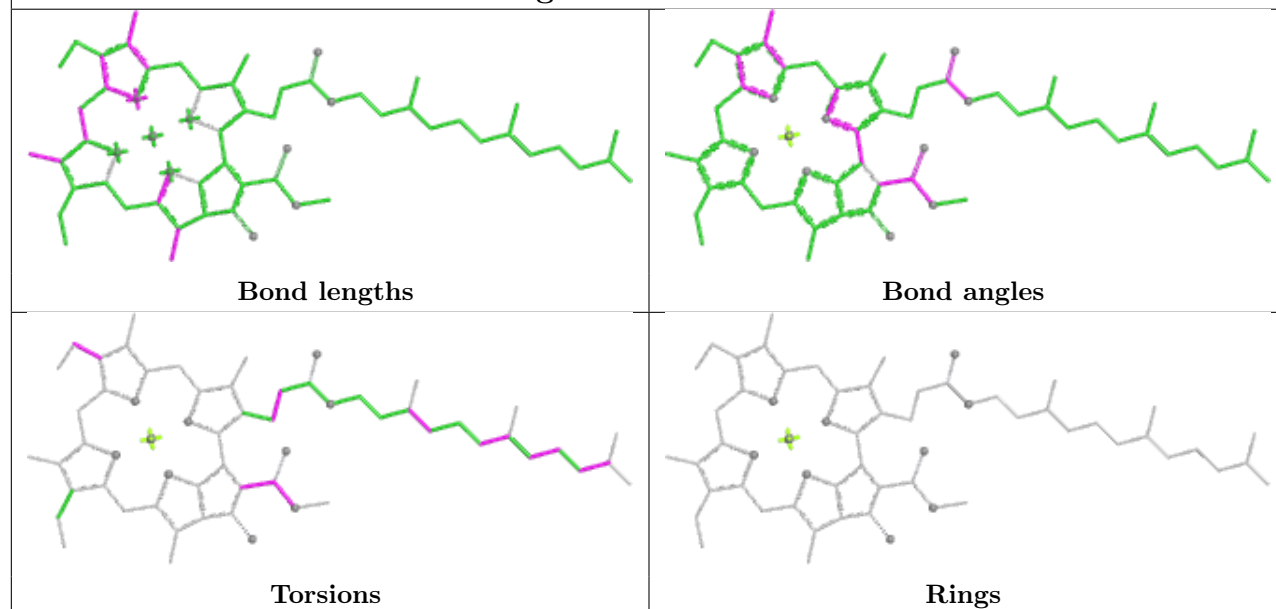


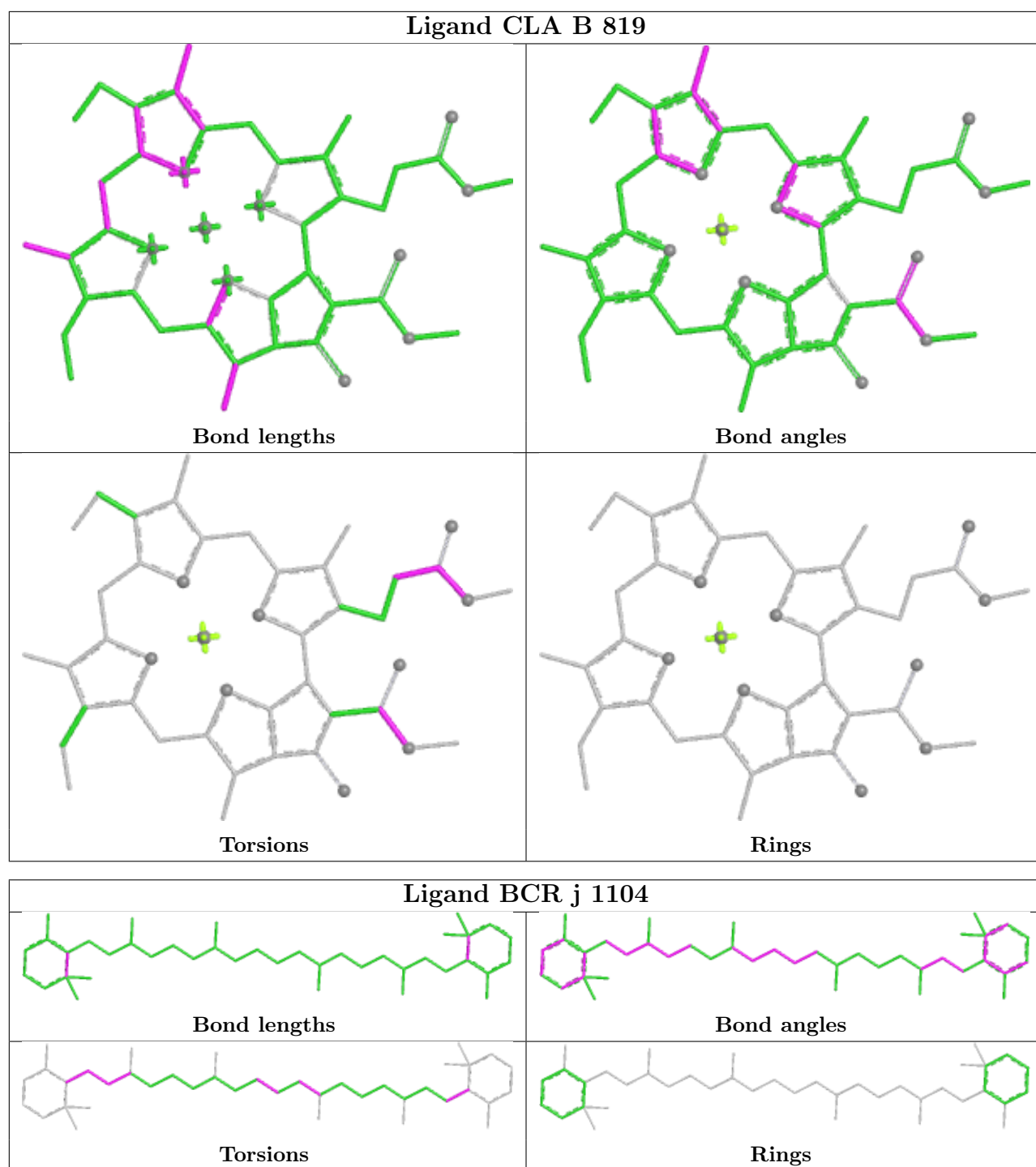


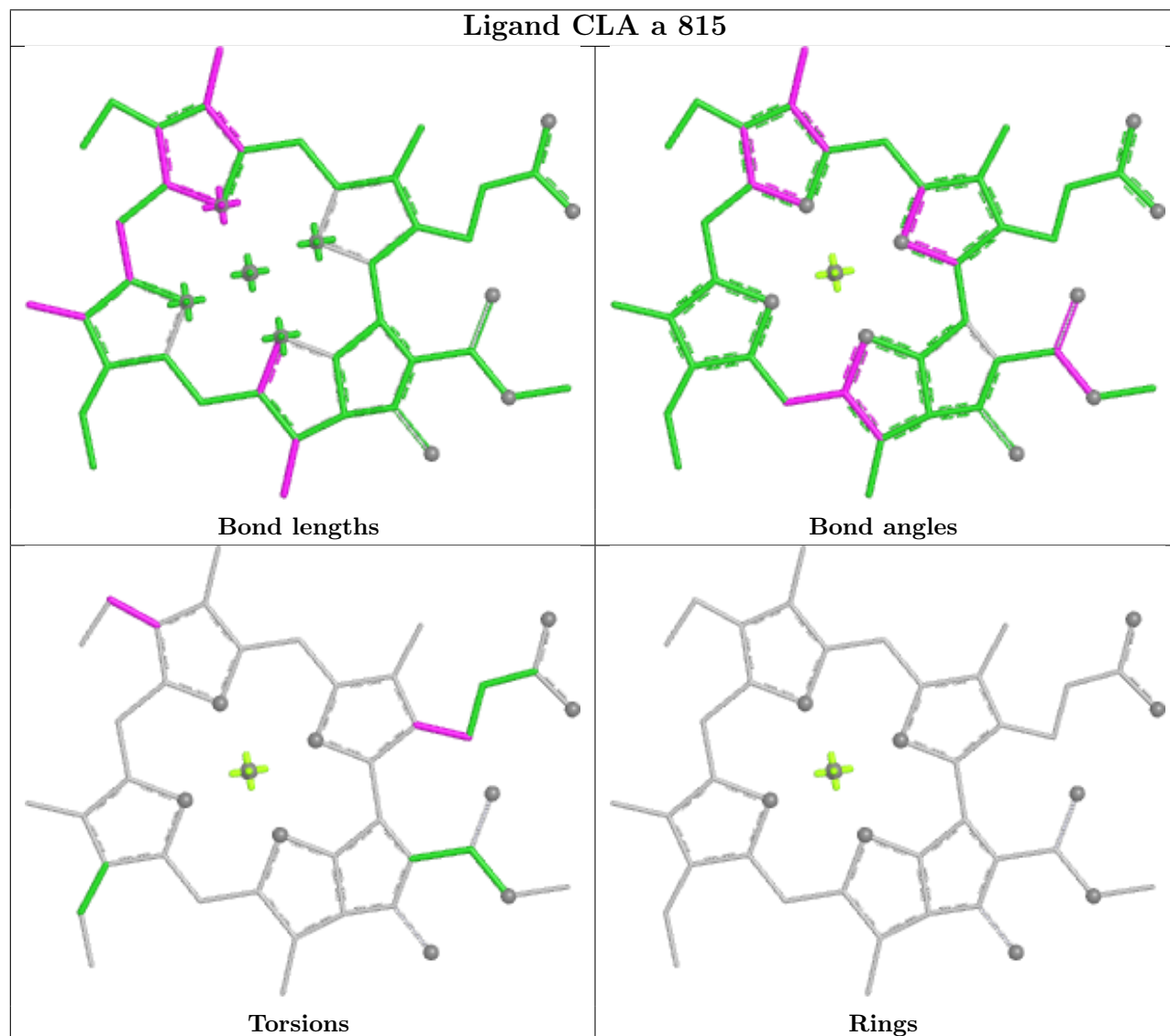
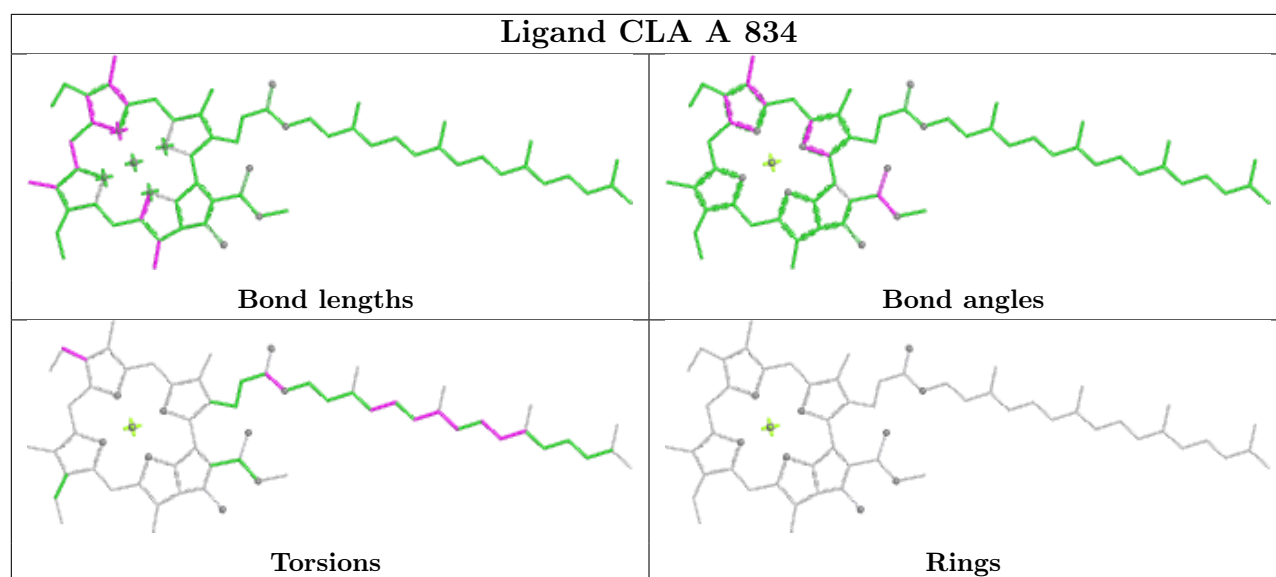
Ligand CLA b 814



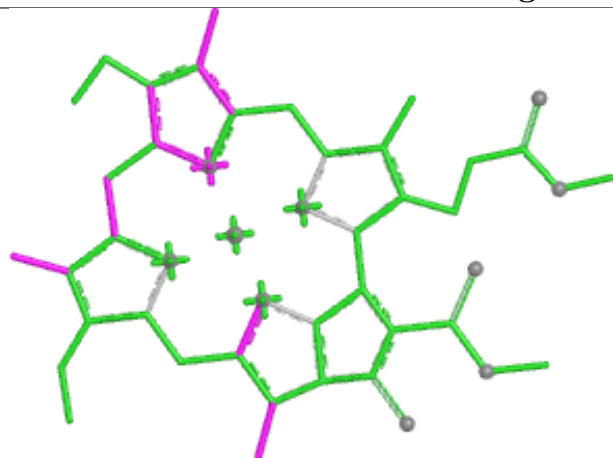
Ligand CLA a 819



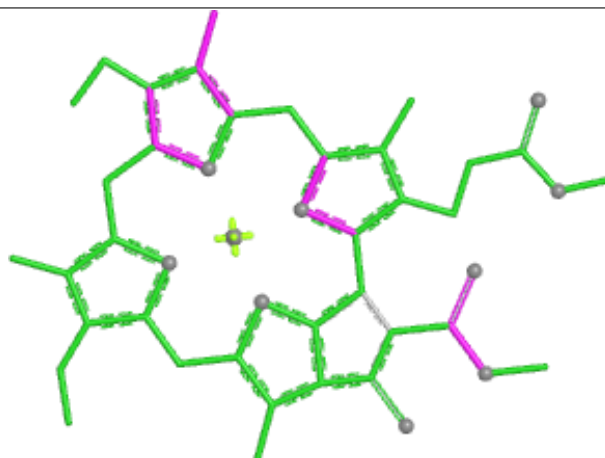




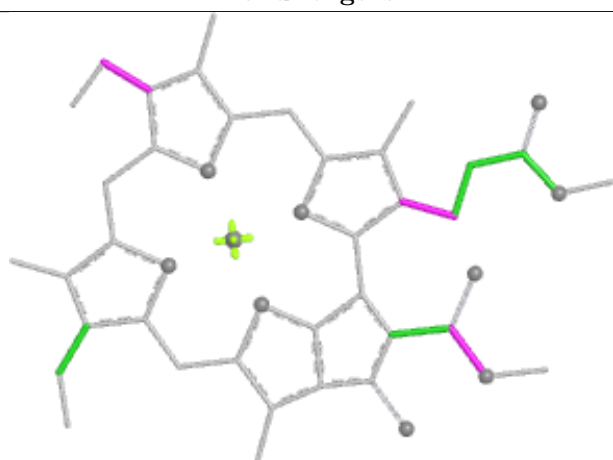
Ligand CLA 0 206



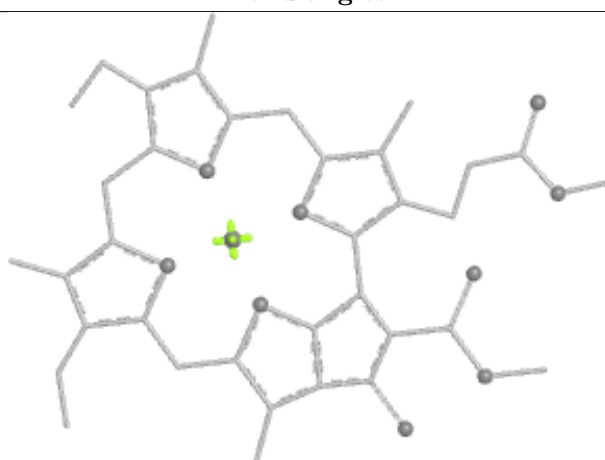
Bond lengths



Bond angles

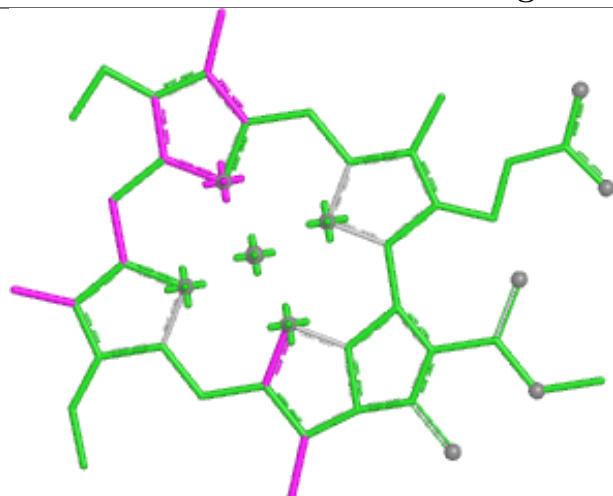


Torsions

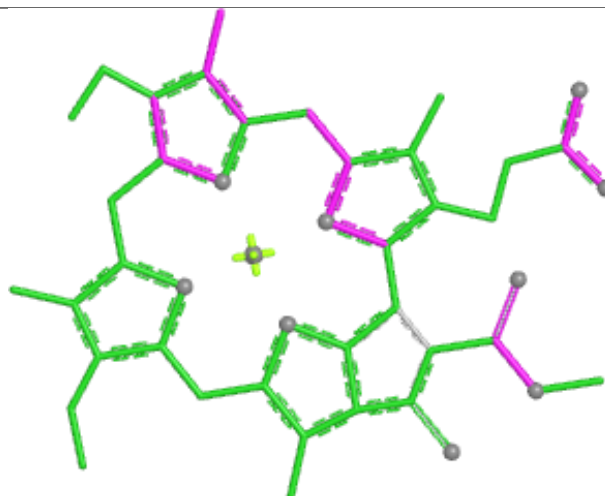


Rings

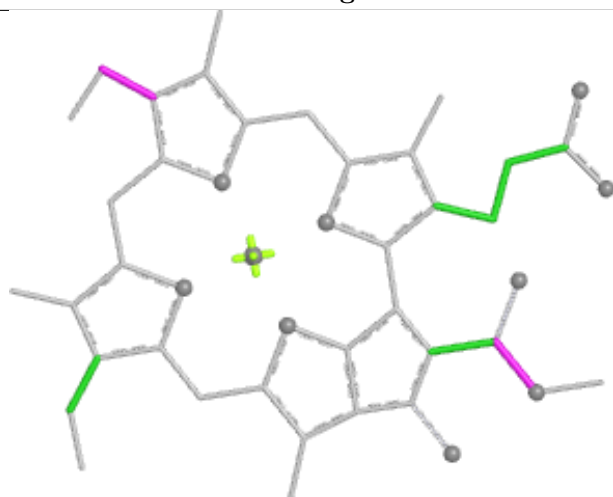
Ligand CLA b 812



Bond lengths



Bond angles

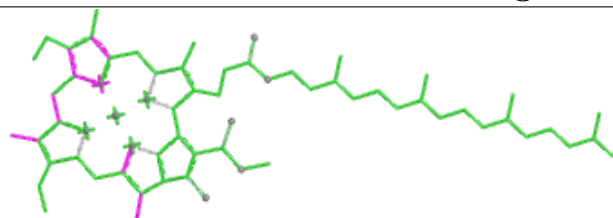


Torsions

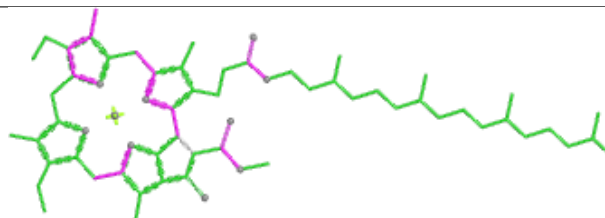


Rings

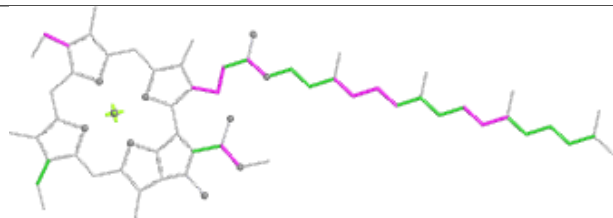
Ligand CLA B 813



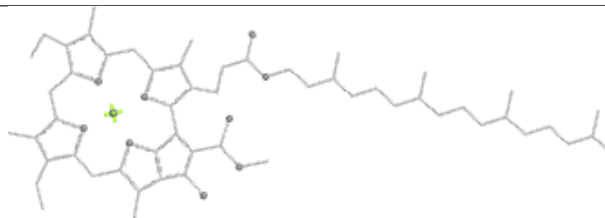
Bond lengths



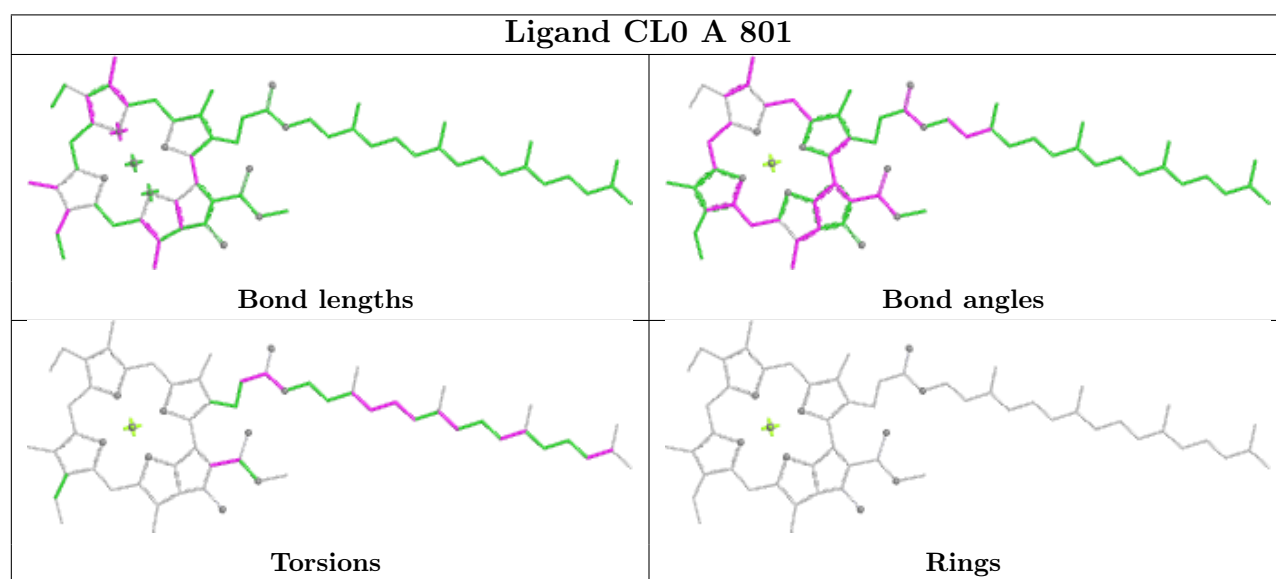
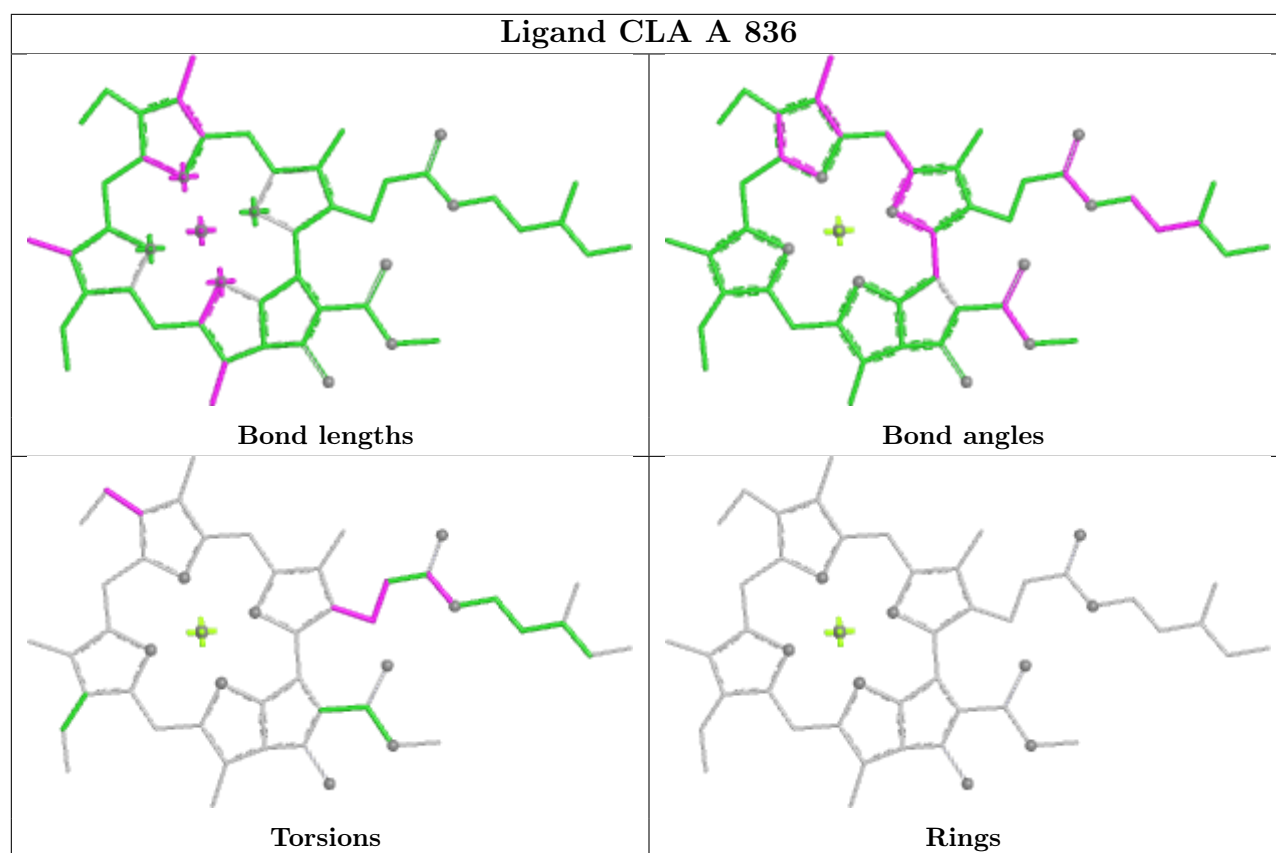
Bond angles



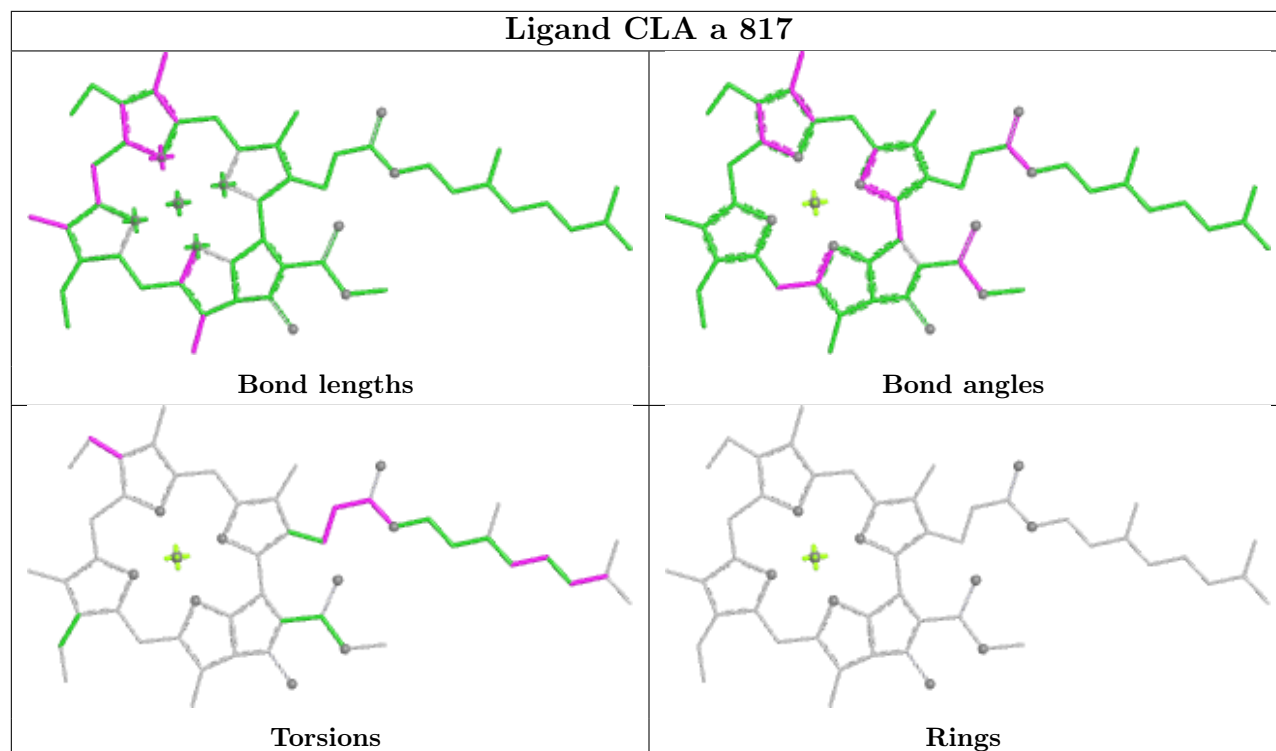
Torsions



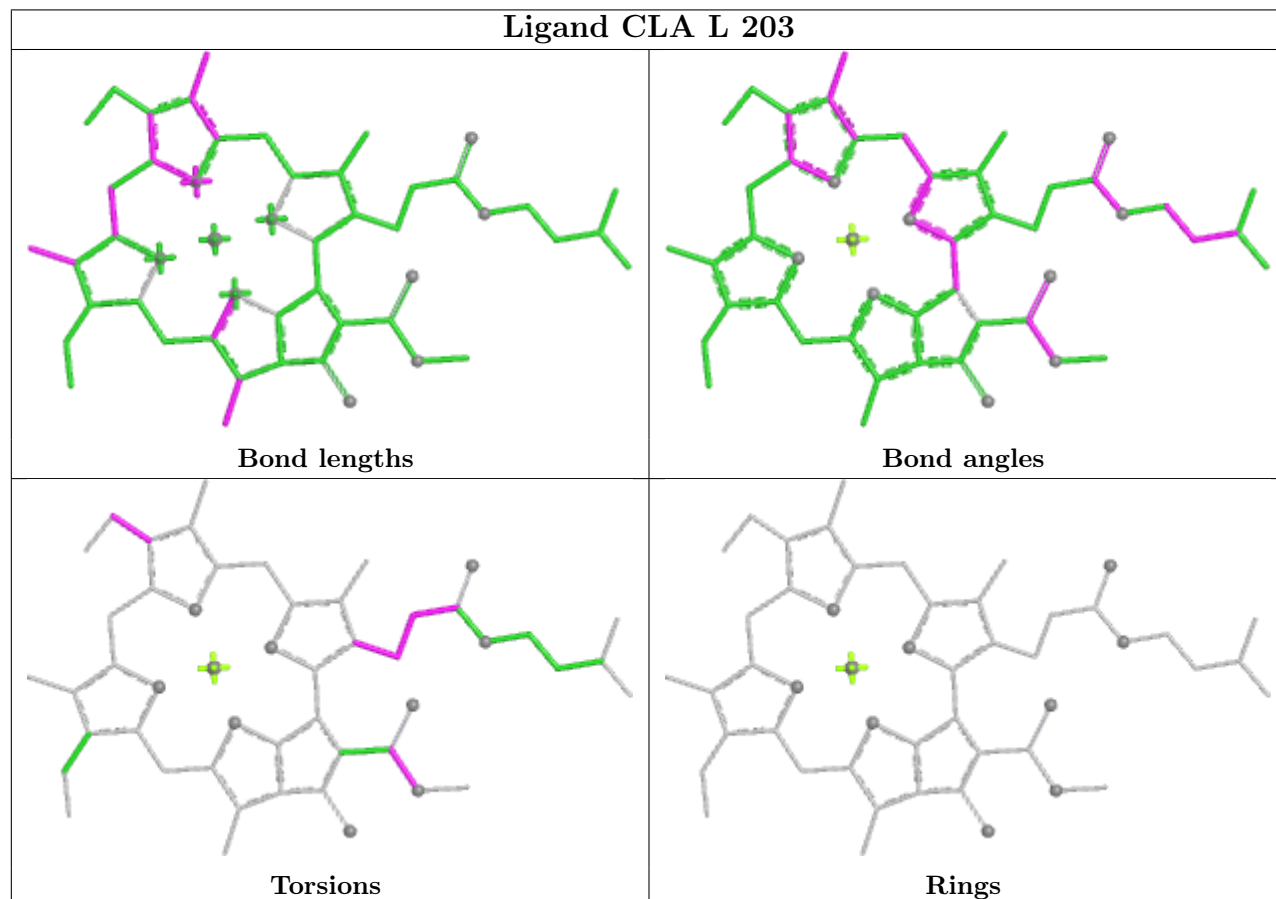
Rings

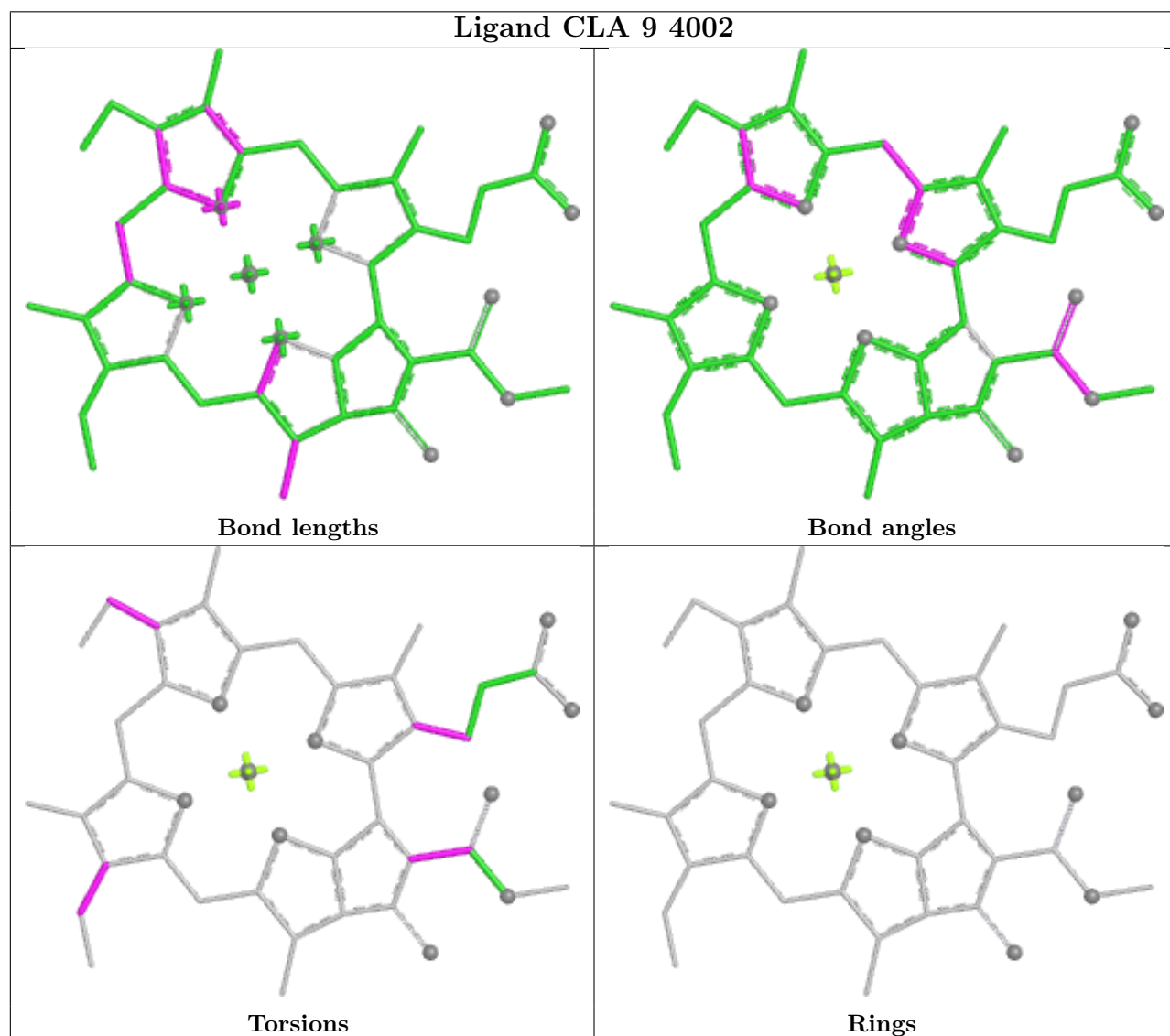
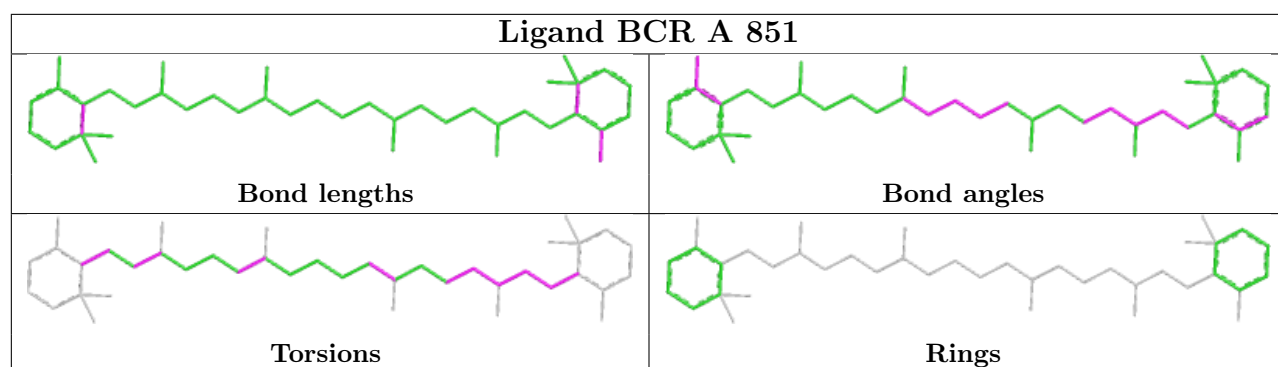


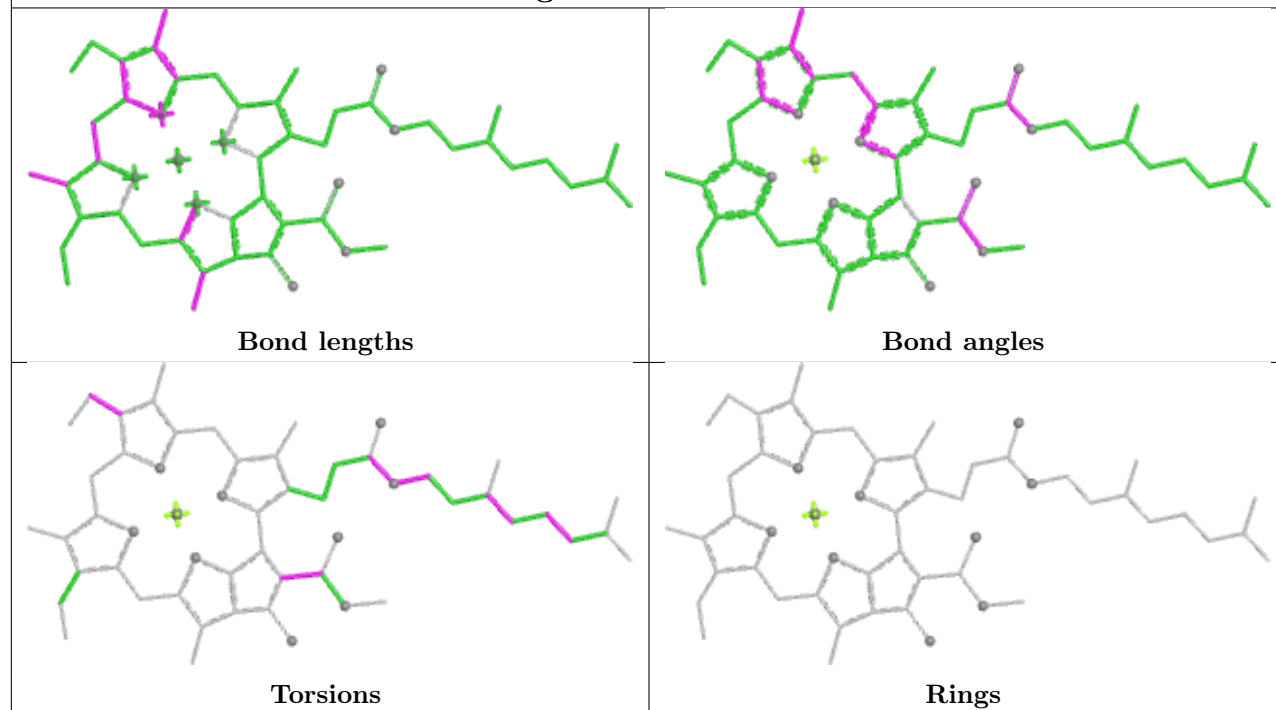
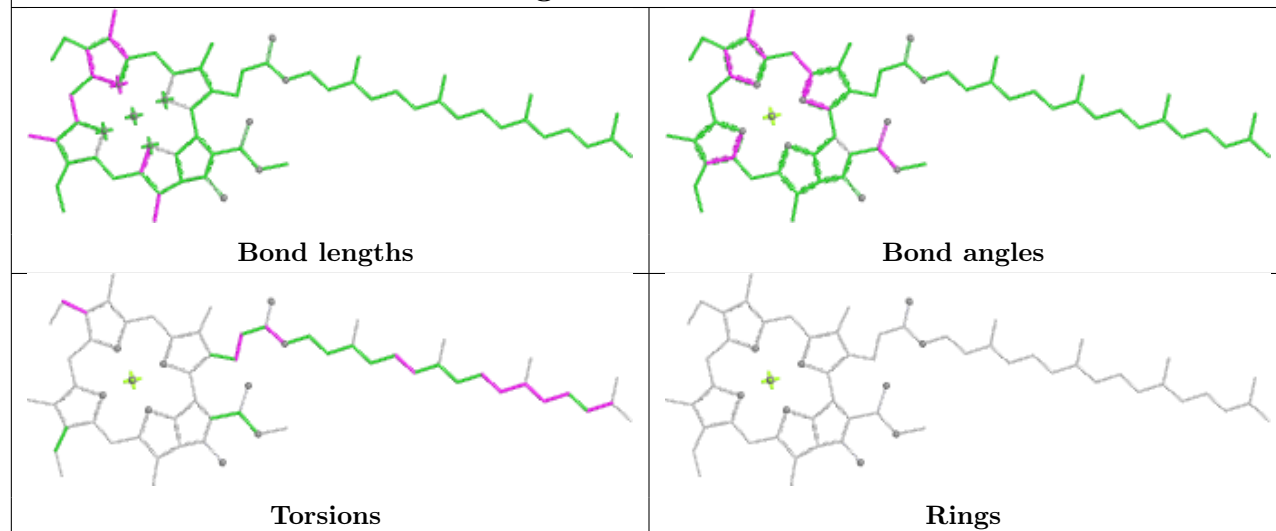
Ligand CLA a 817

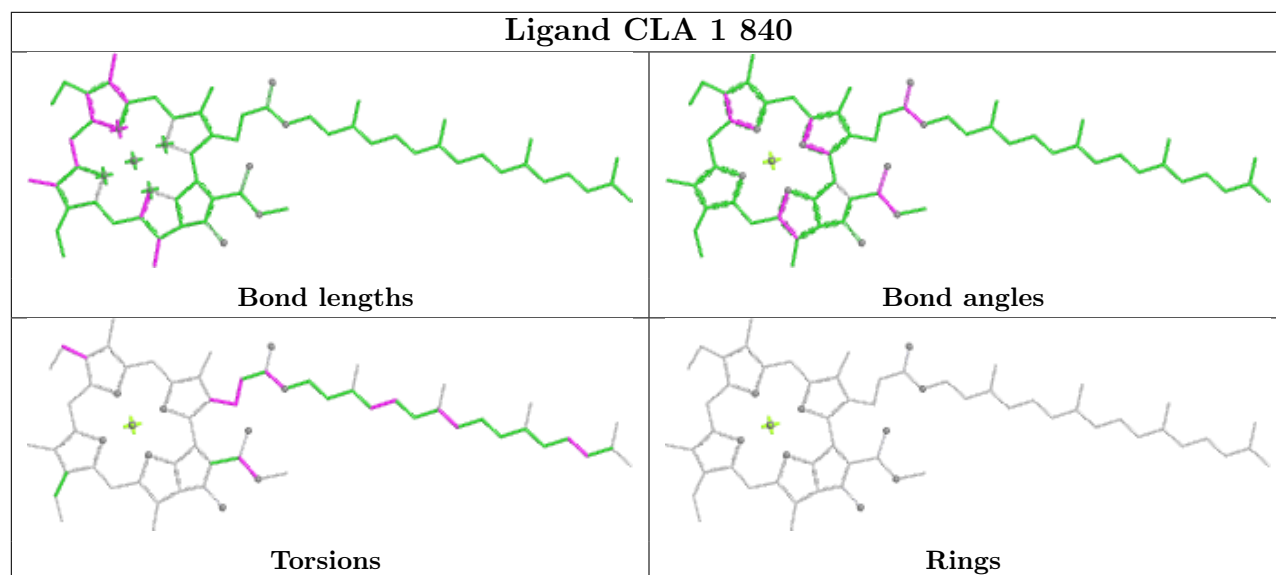
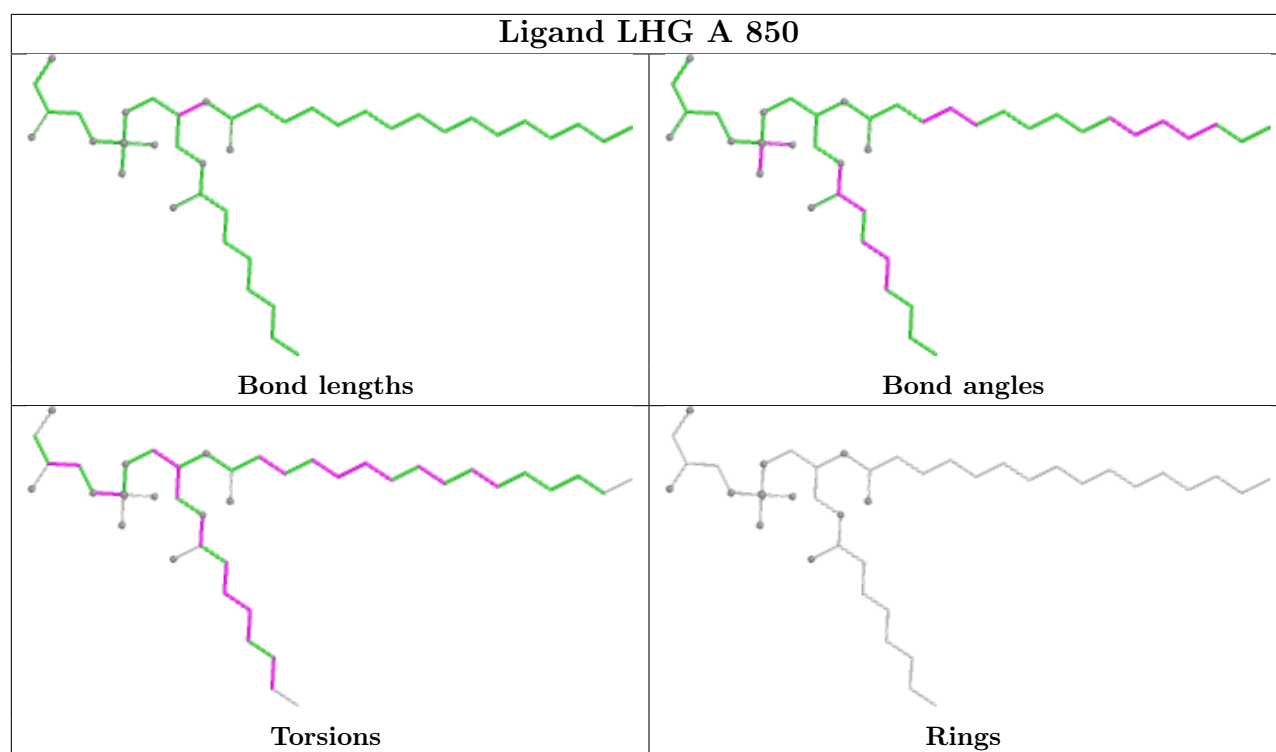


Ligand CLA L 203

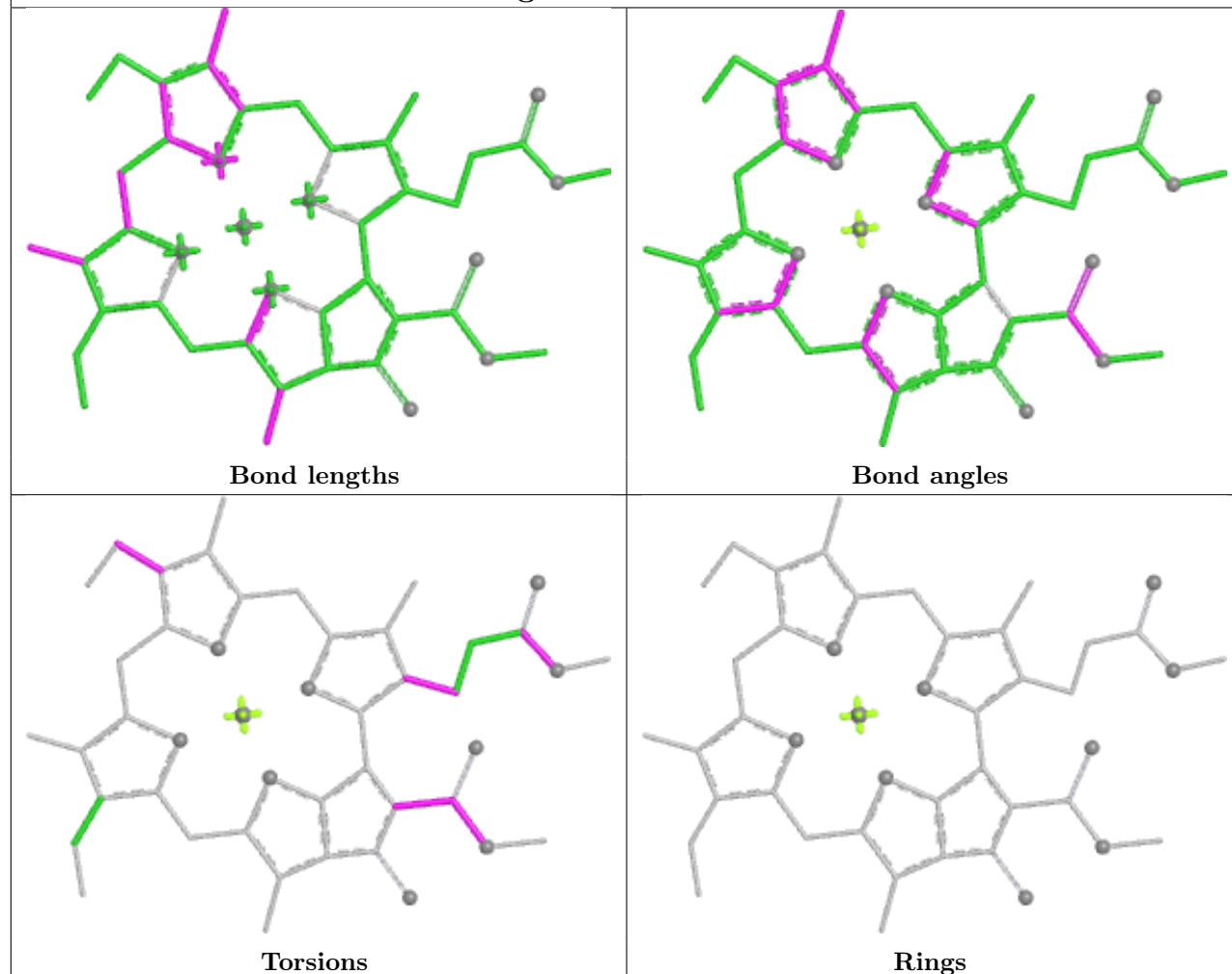




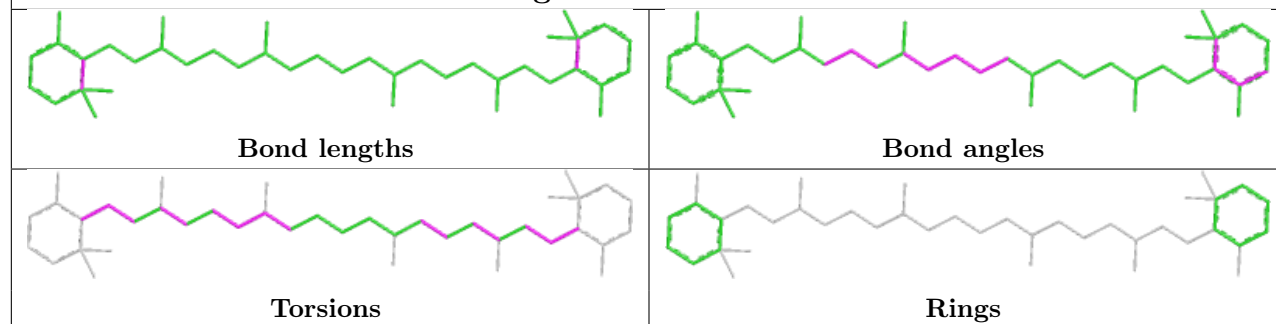
Ligand CLA a 826**Ligand CLA b 823**



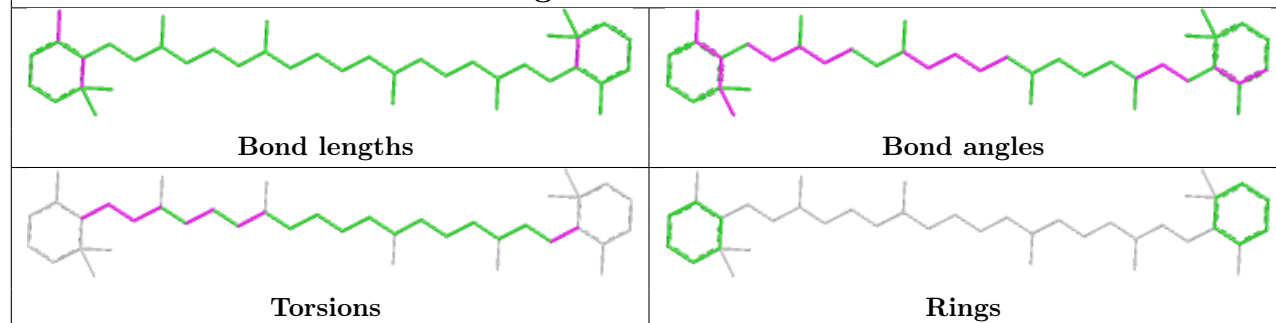
Ligand CLA 2 810

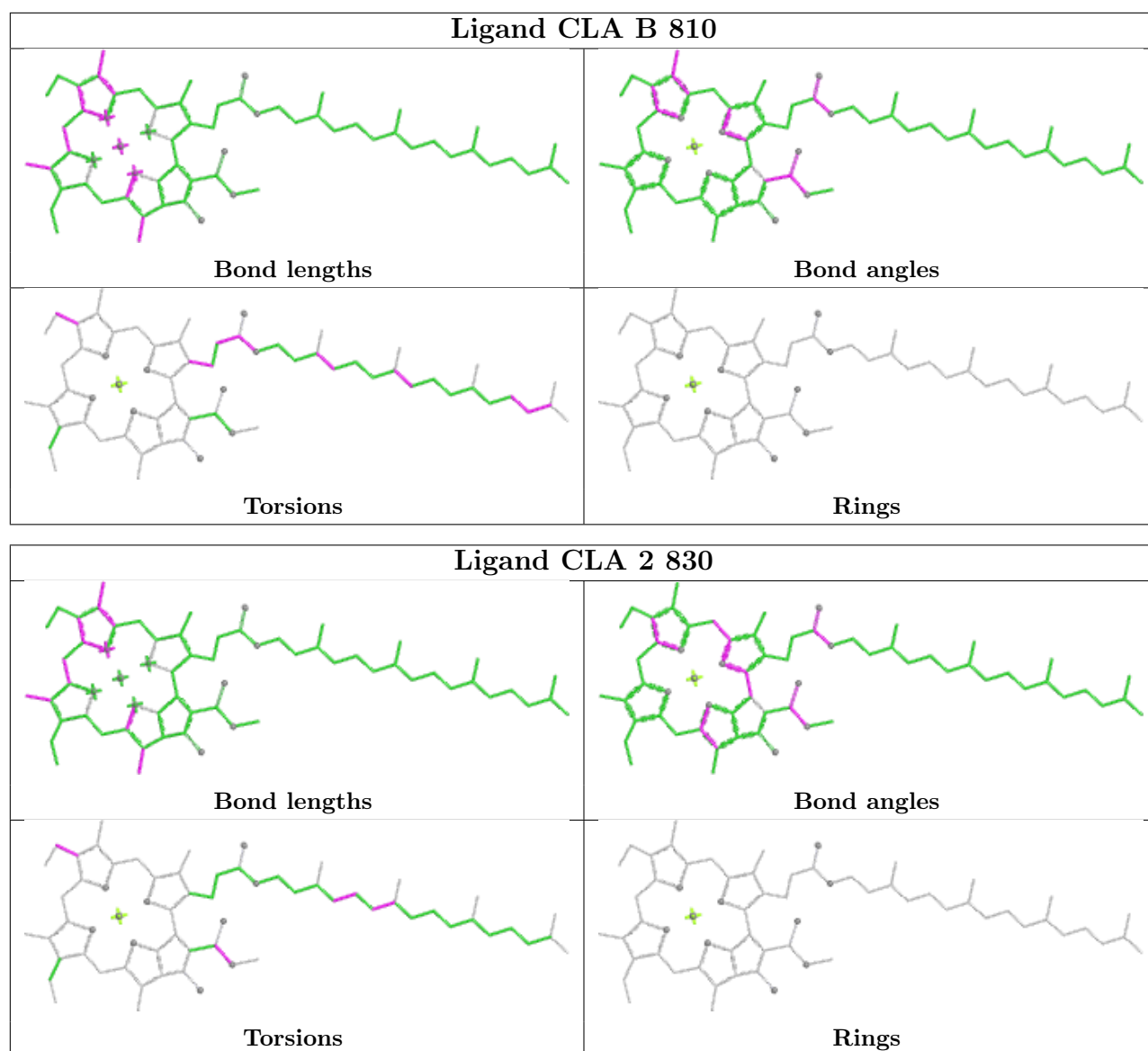


Ligand BCR b 845

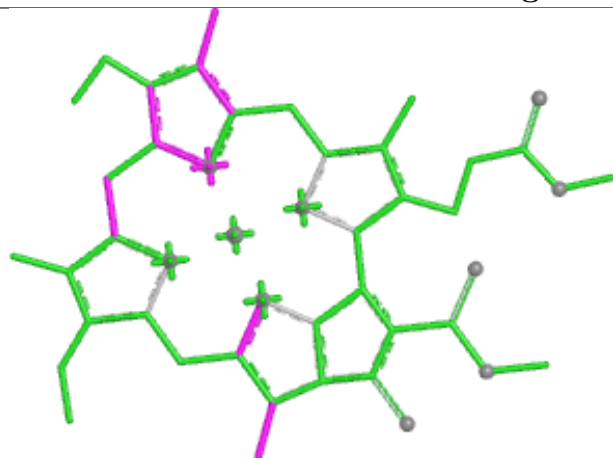


Ligand BCR 2 847

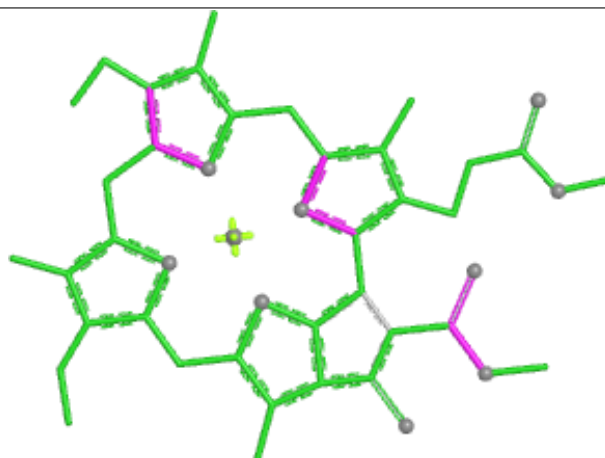




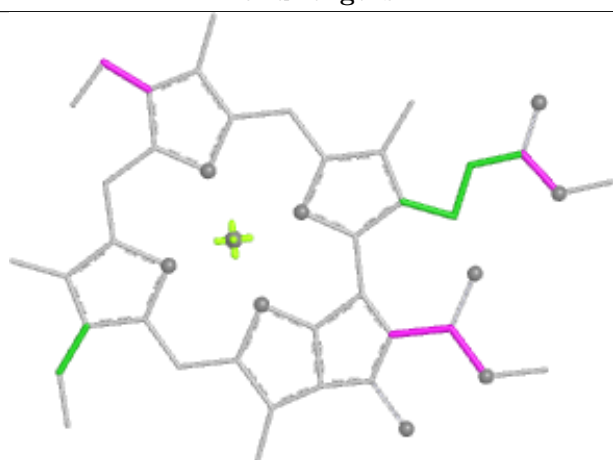
Ligand CLA f 204



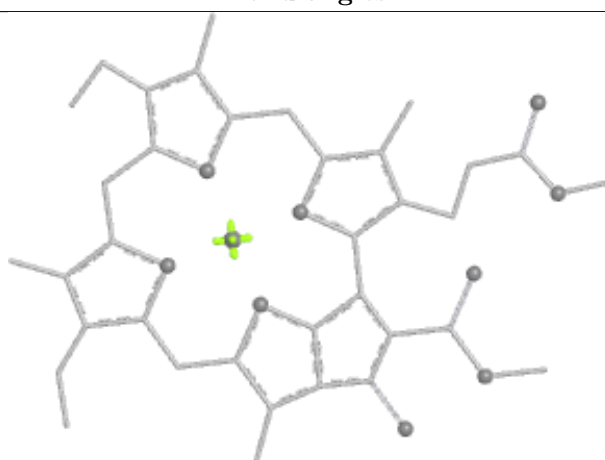
Bond lengths



Bond angles

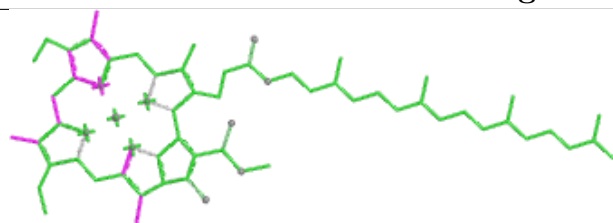


Torsions

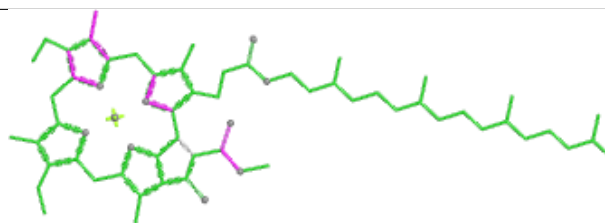


Rings

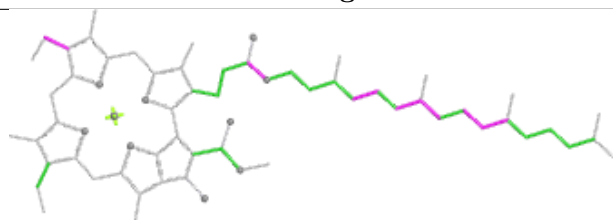
Ligand CLA 1 834



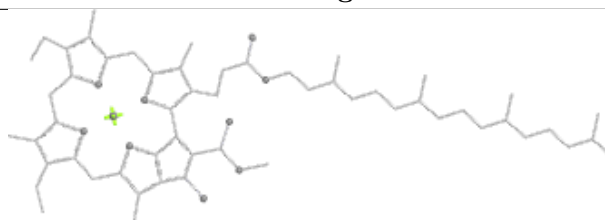
Bond lengths



Bond angles

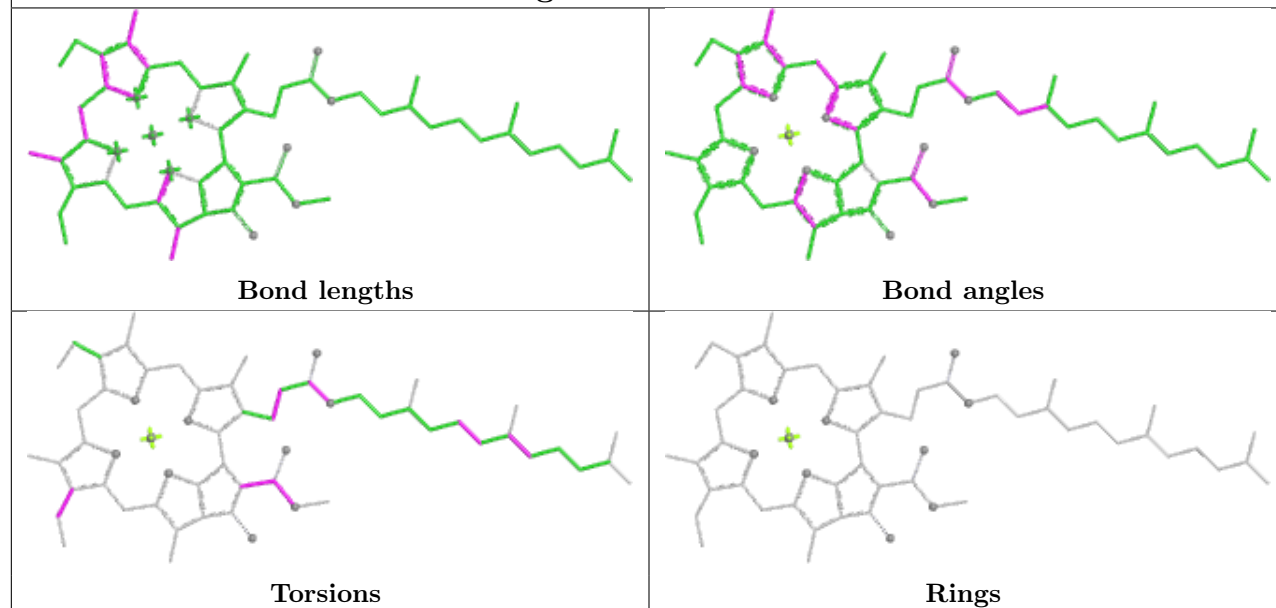


Torsions

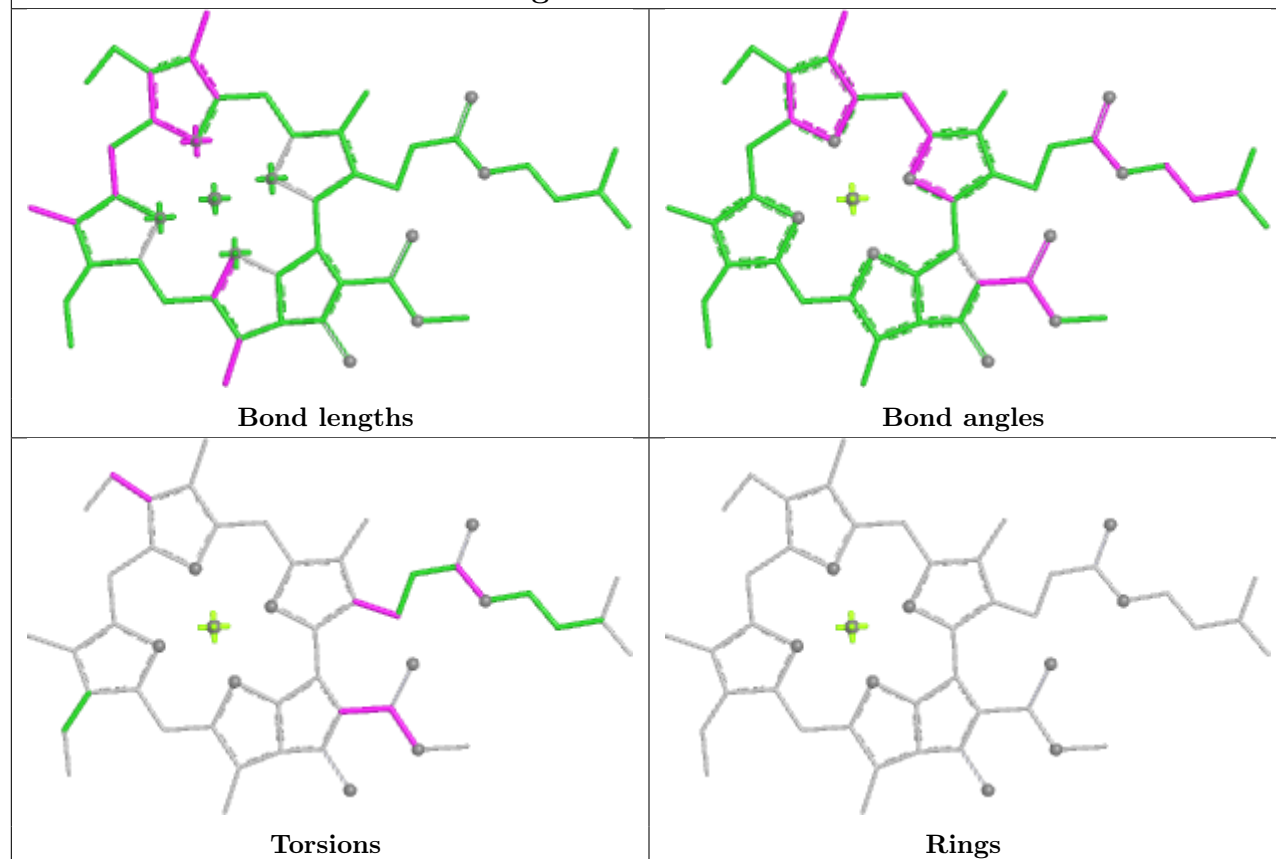


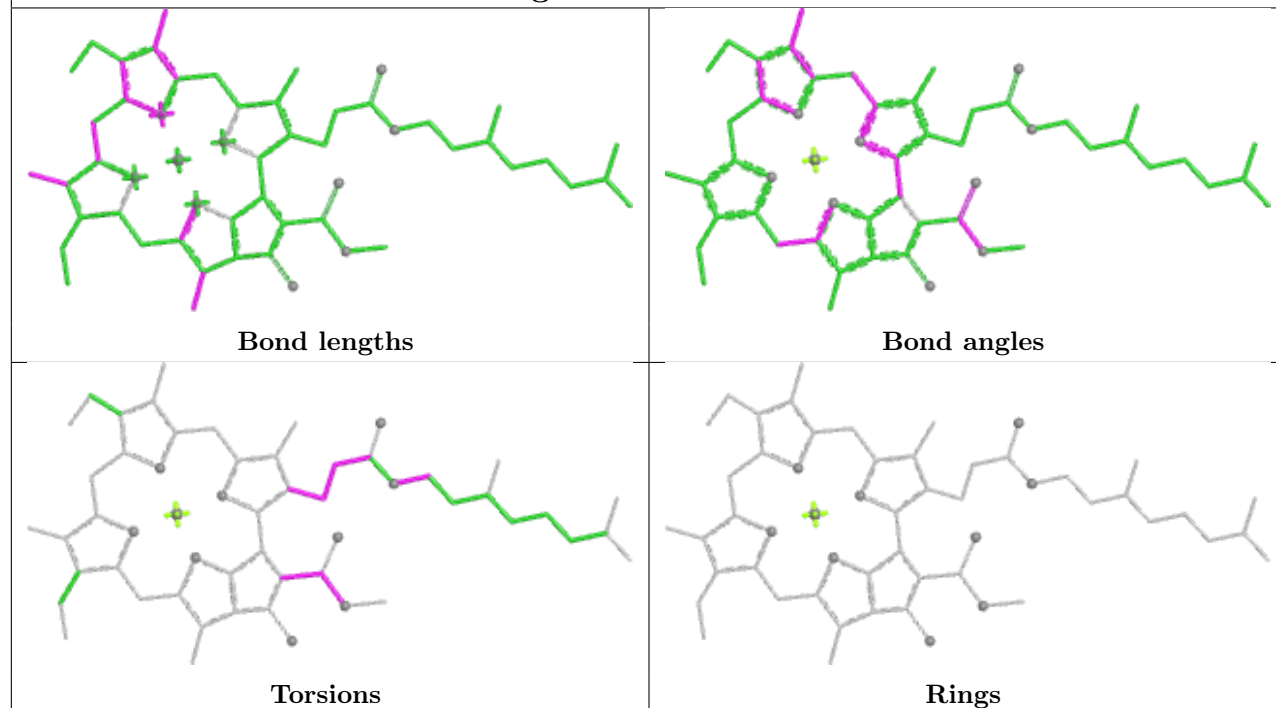
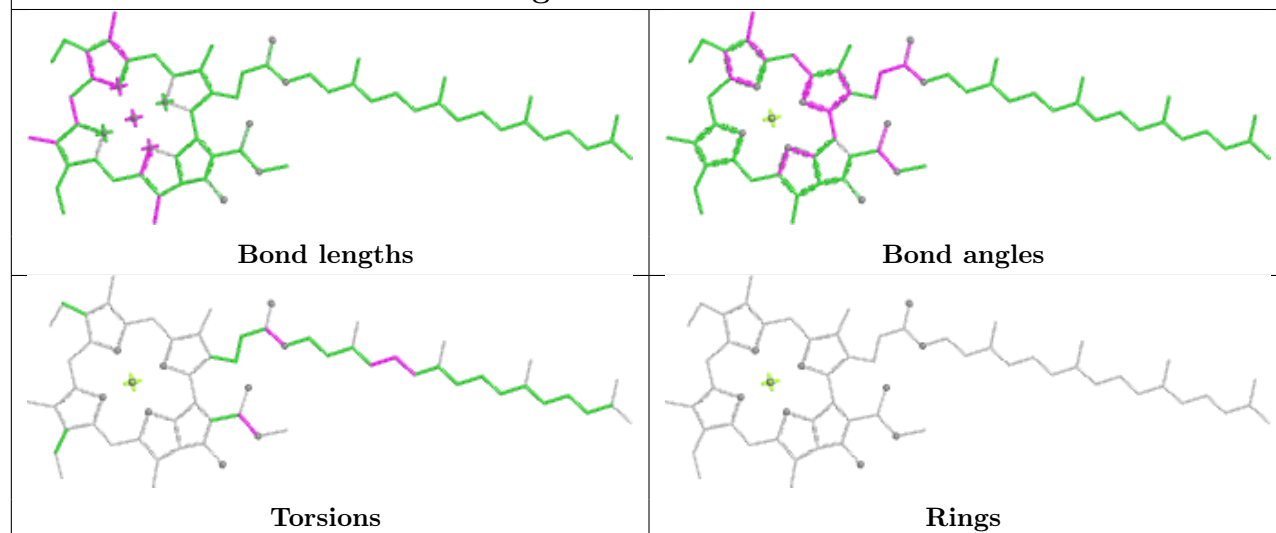
Rings

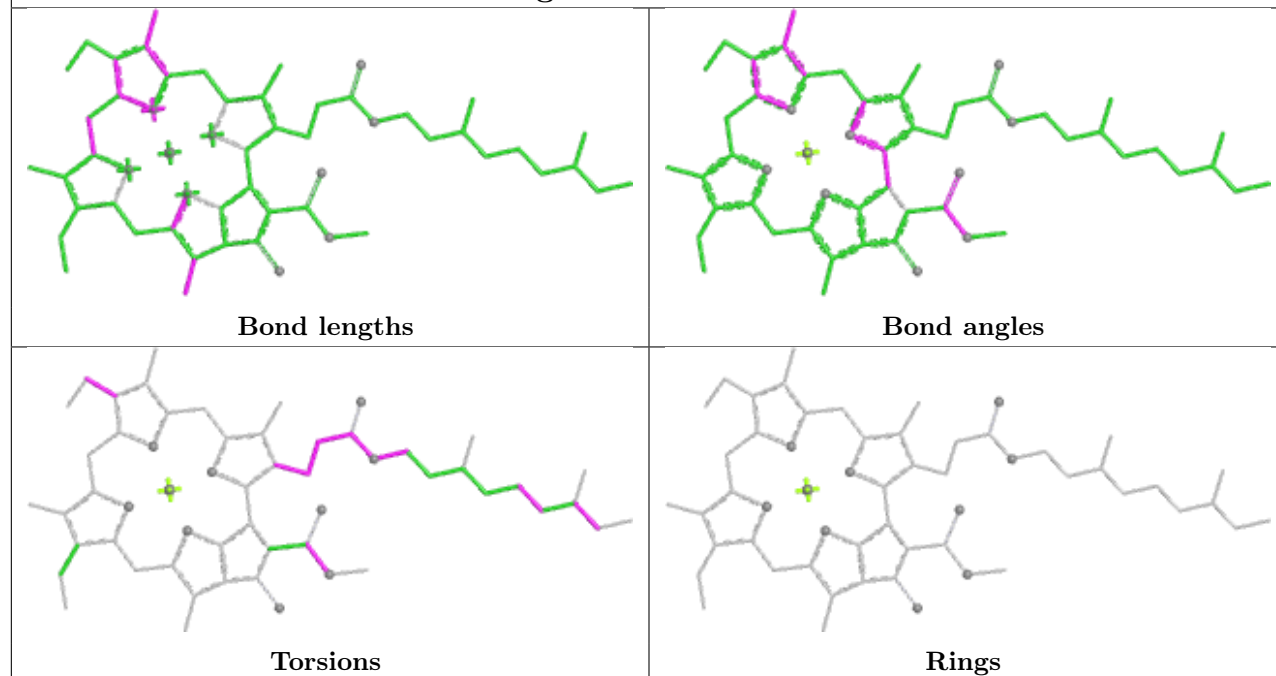
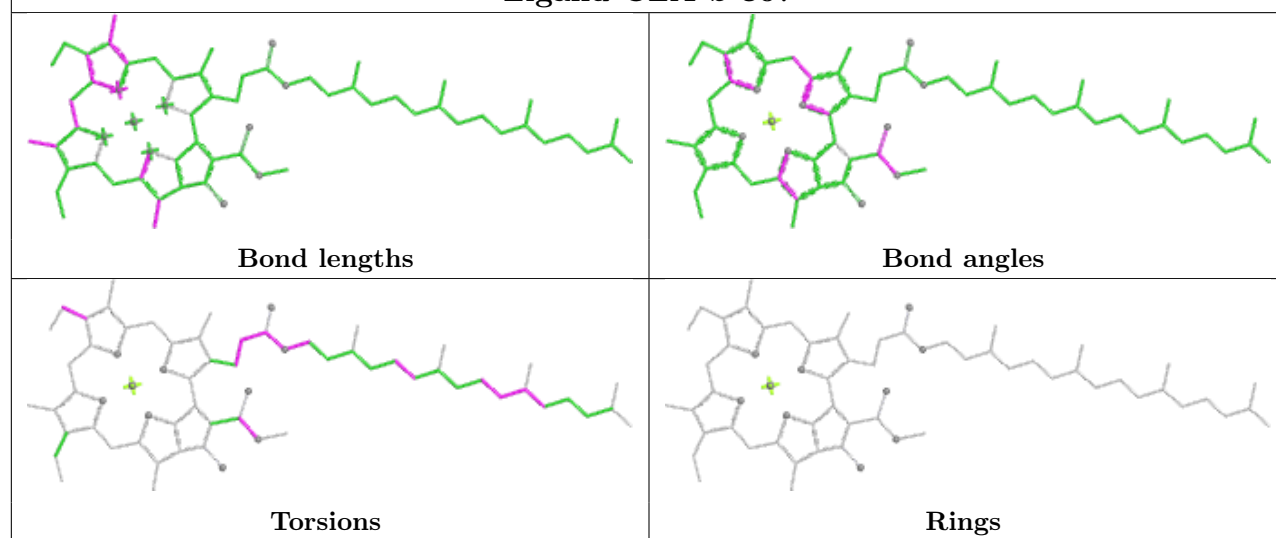
Ligand CLA 2 803



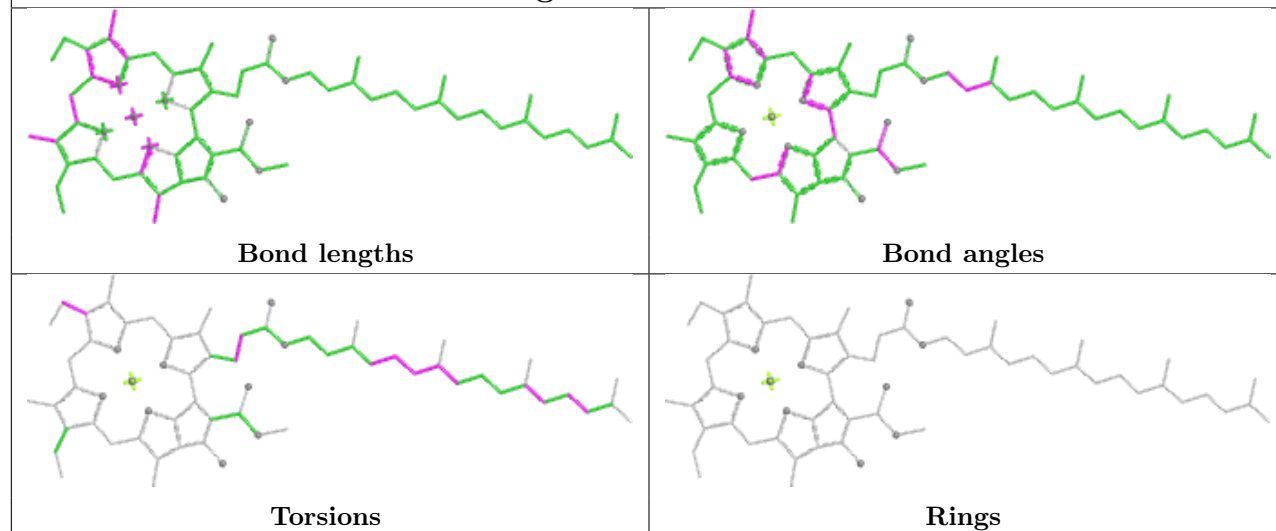
Ligand CLA A 831



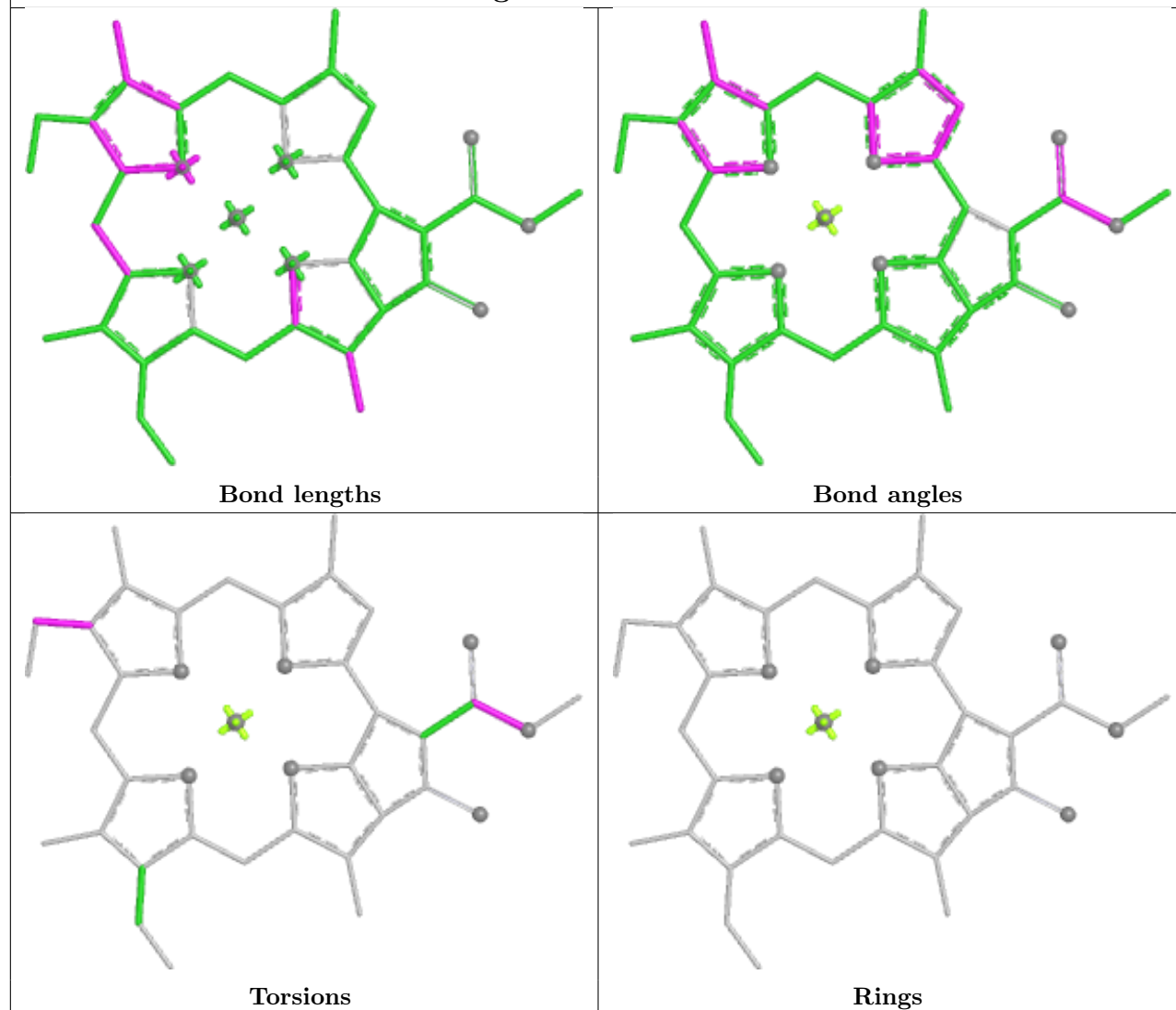
Ligand CLA A 813**Ligand CLA B 801**

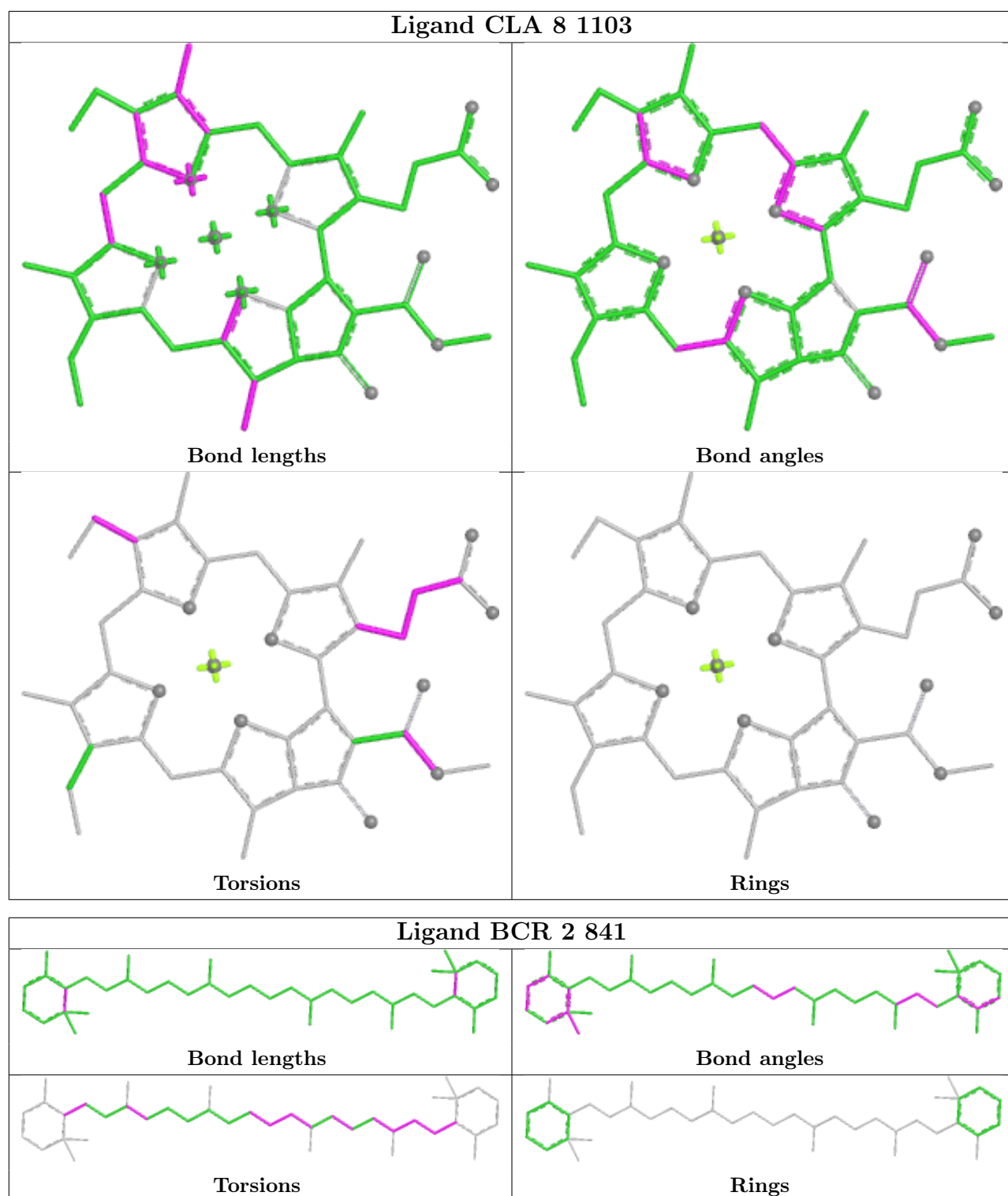
Ligand CLA 1 835**Ligand CLA b 807**

Ligand CLA a 829

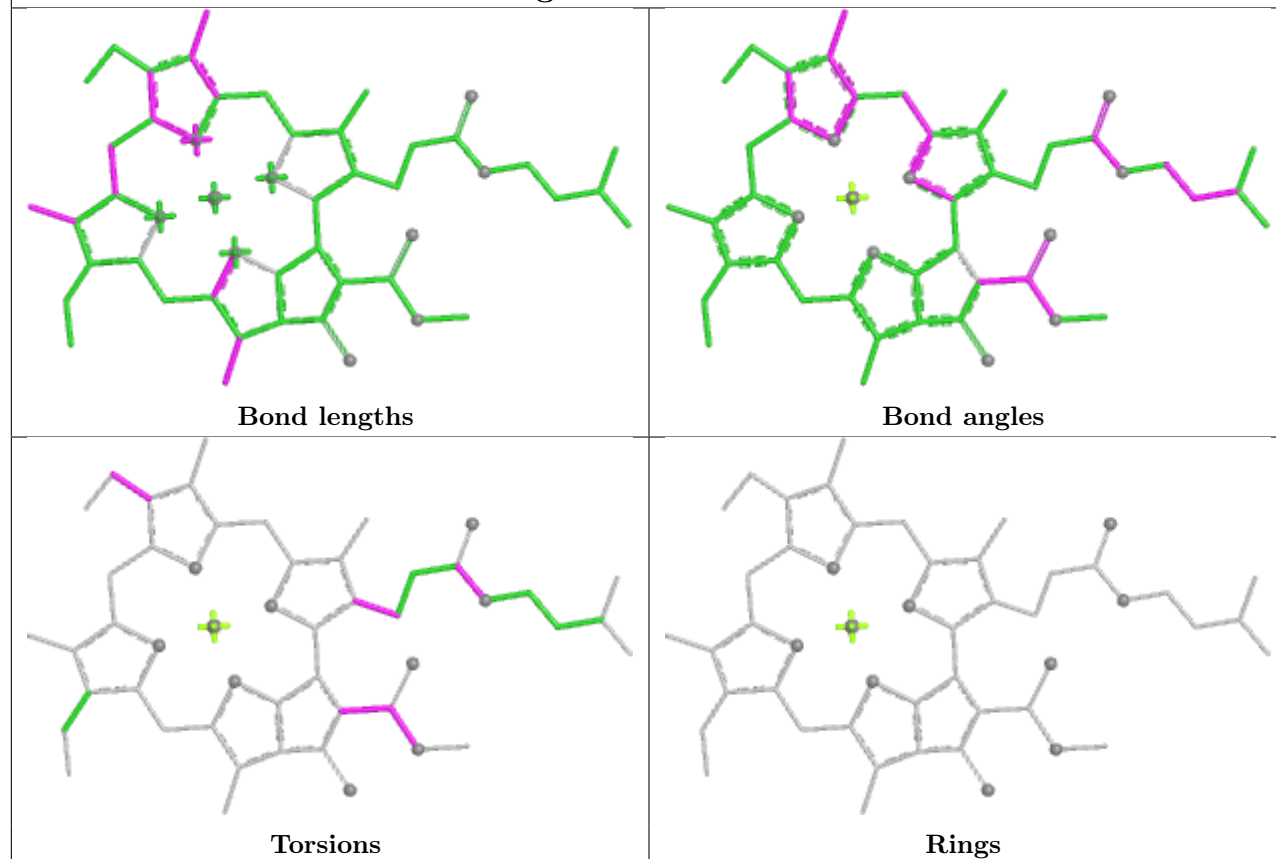


Ligand CLA b 832

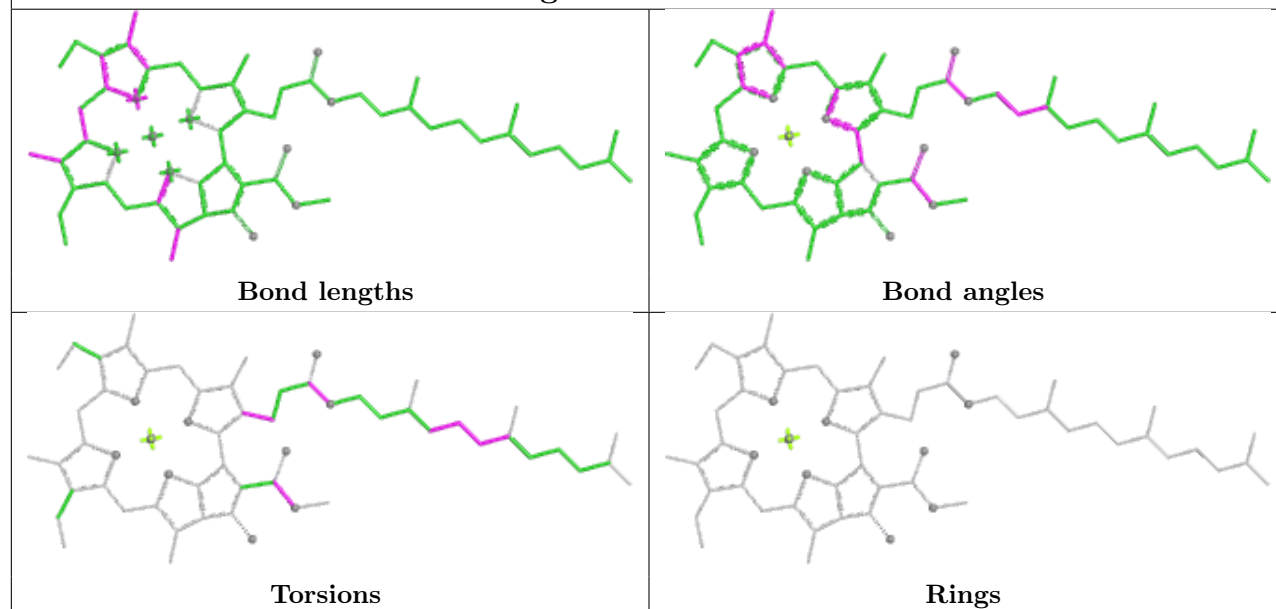


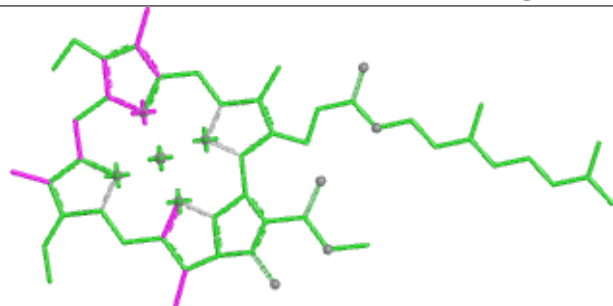


Ligand CLA a 831

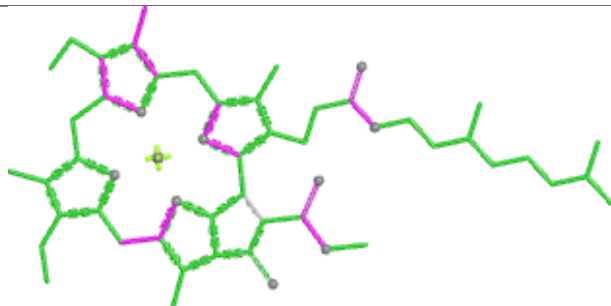


Ligand CLA l 202

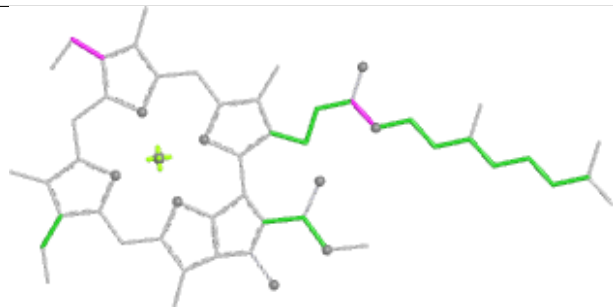


Ligand CLA 1 804

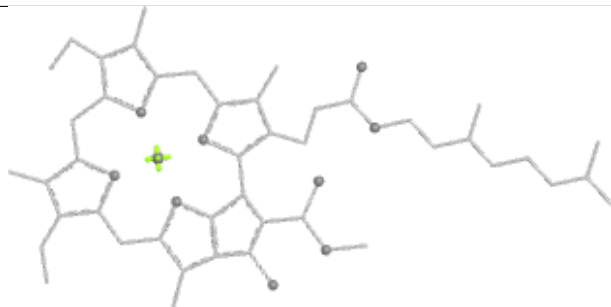
Bond lengths



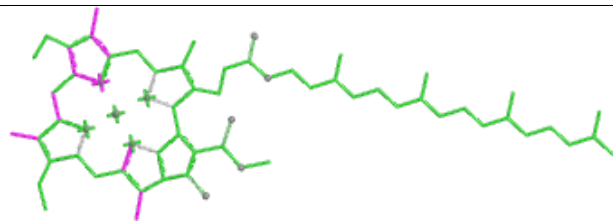
Bond angles



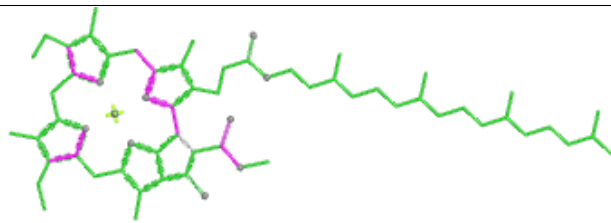
Torsions



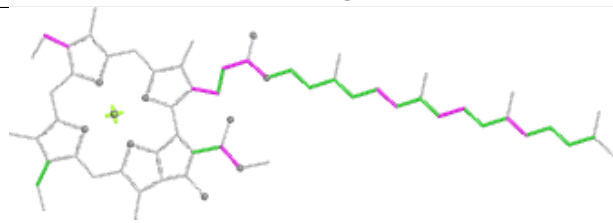
Rings

Ligand CLA A 833

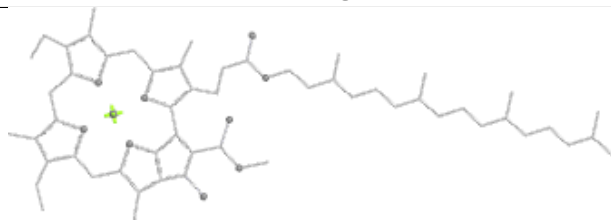
Bond lengths



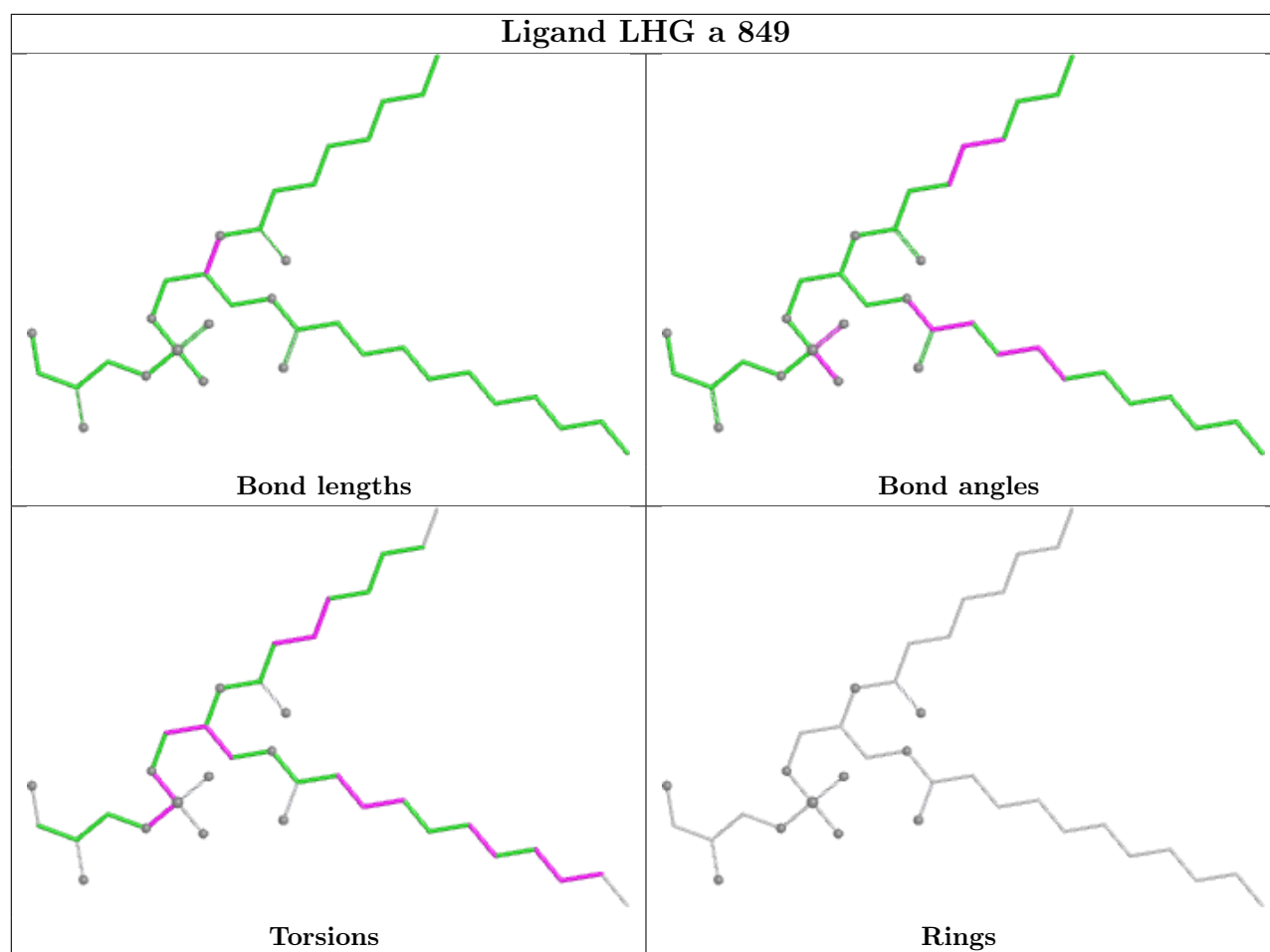
Bond angles



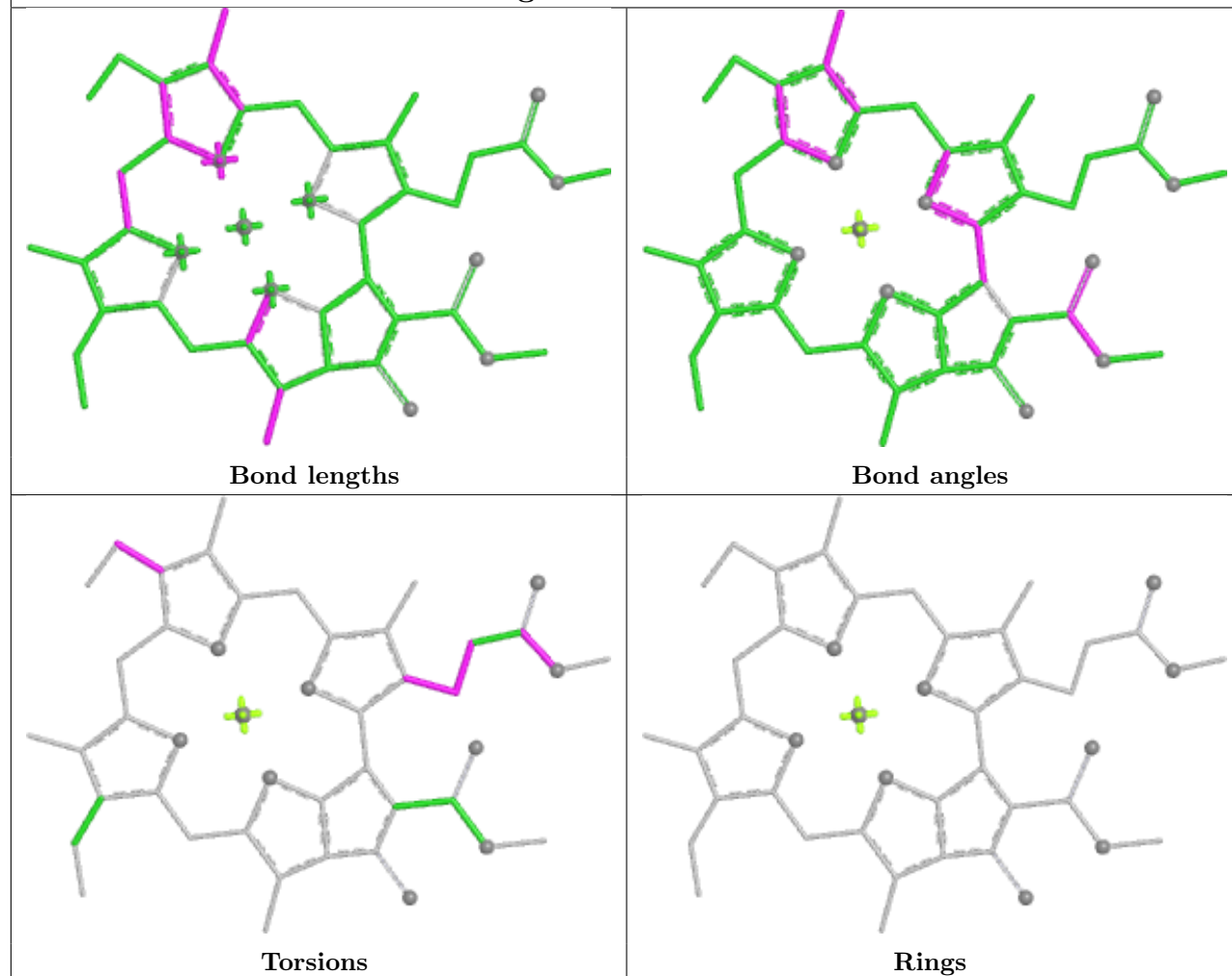
Torsions



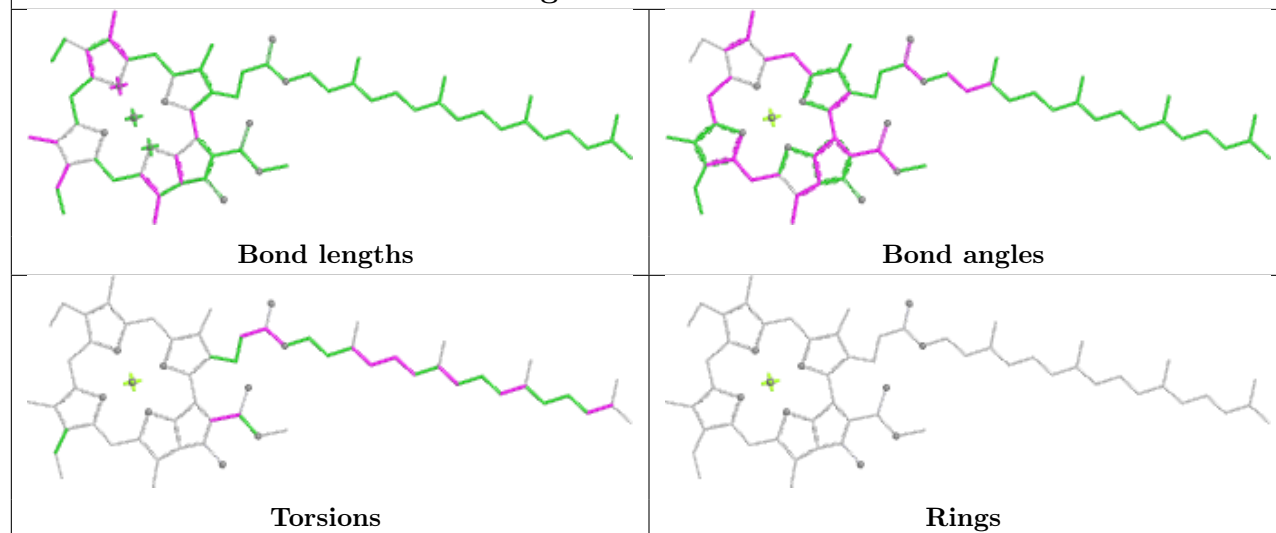
Rings



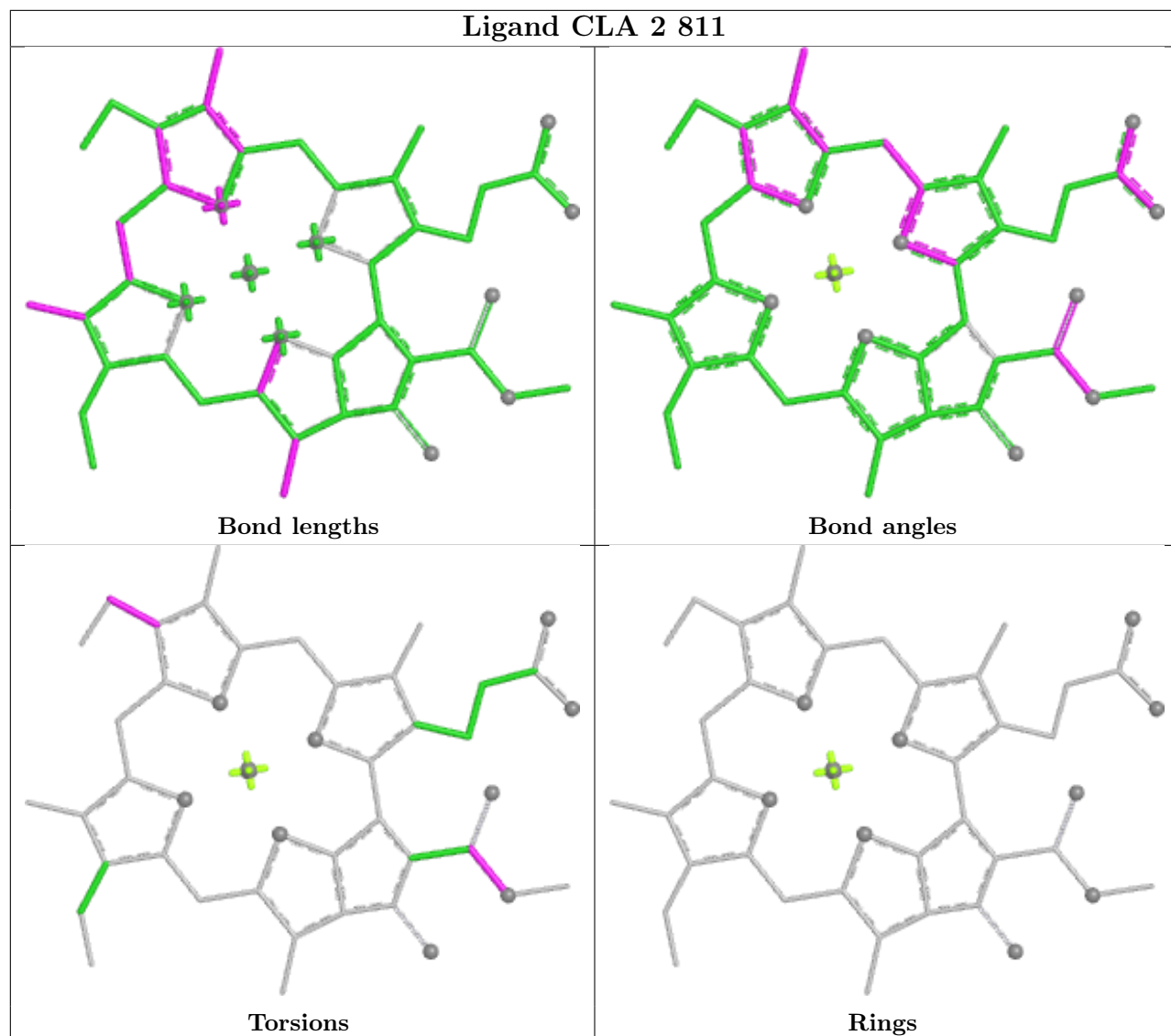
Ligand CLA 1 812



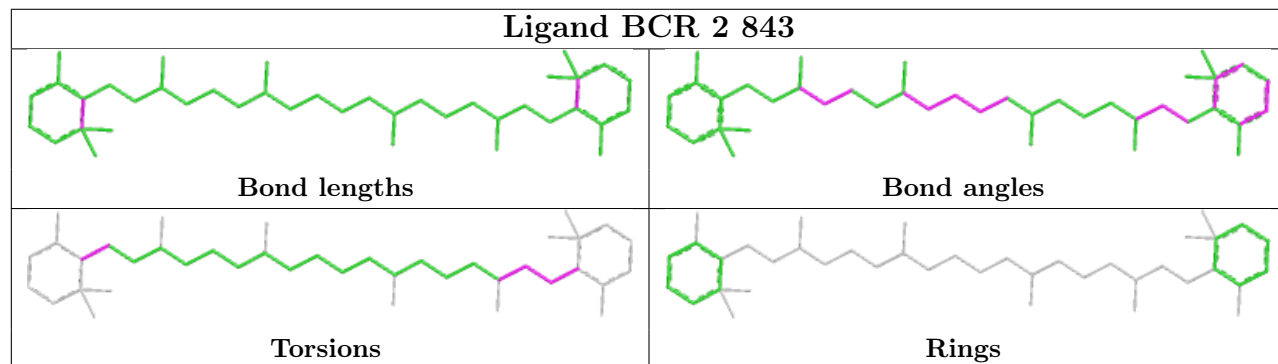
Ligand CL0 1 801



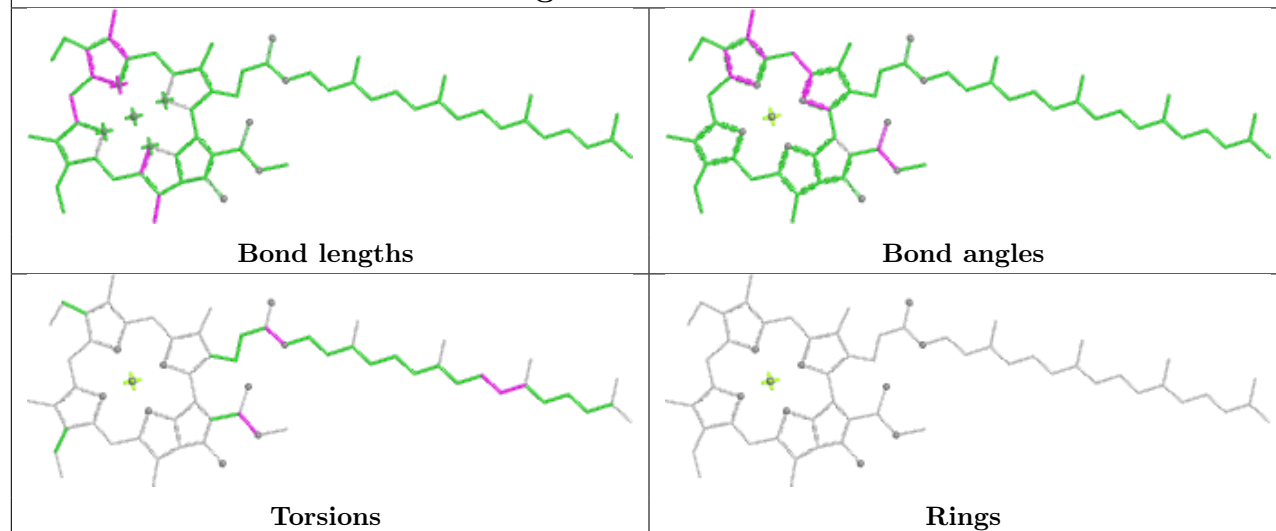
Ligand CLA 2 811



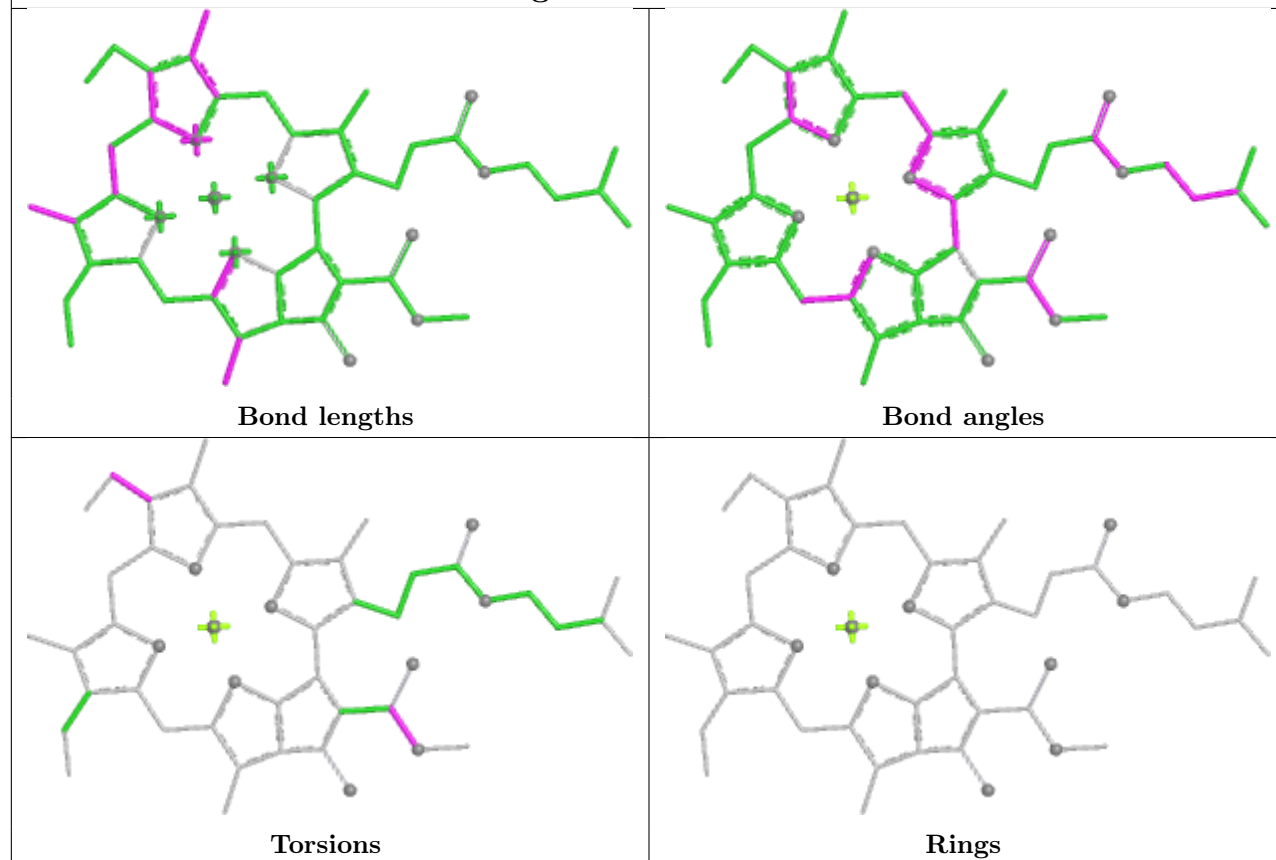
Ligand BCR 2 843

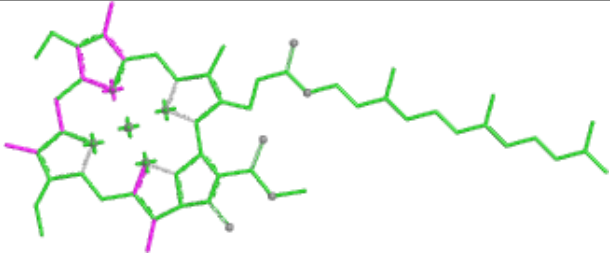
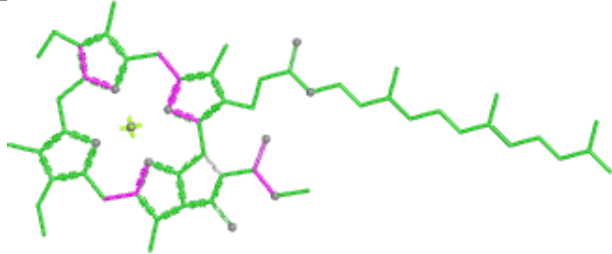
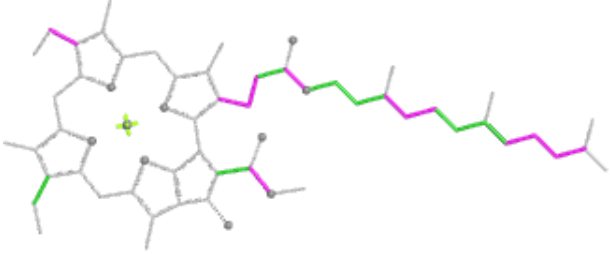
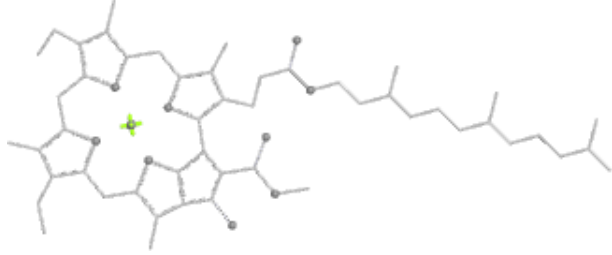
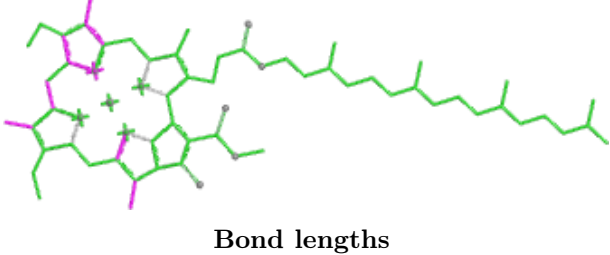
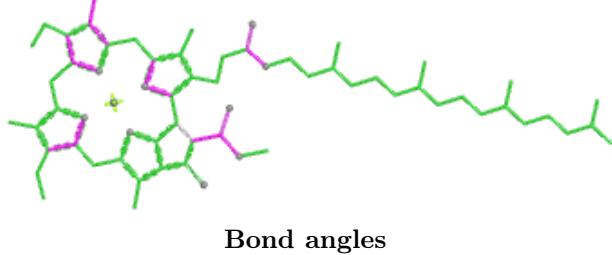
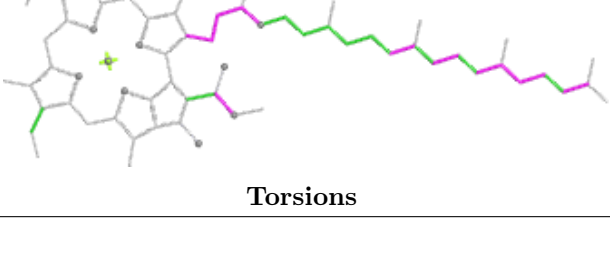
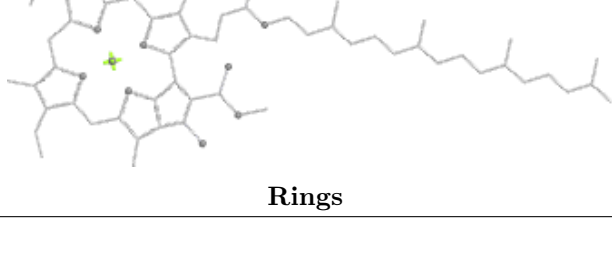


Ligand CLA 2 837

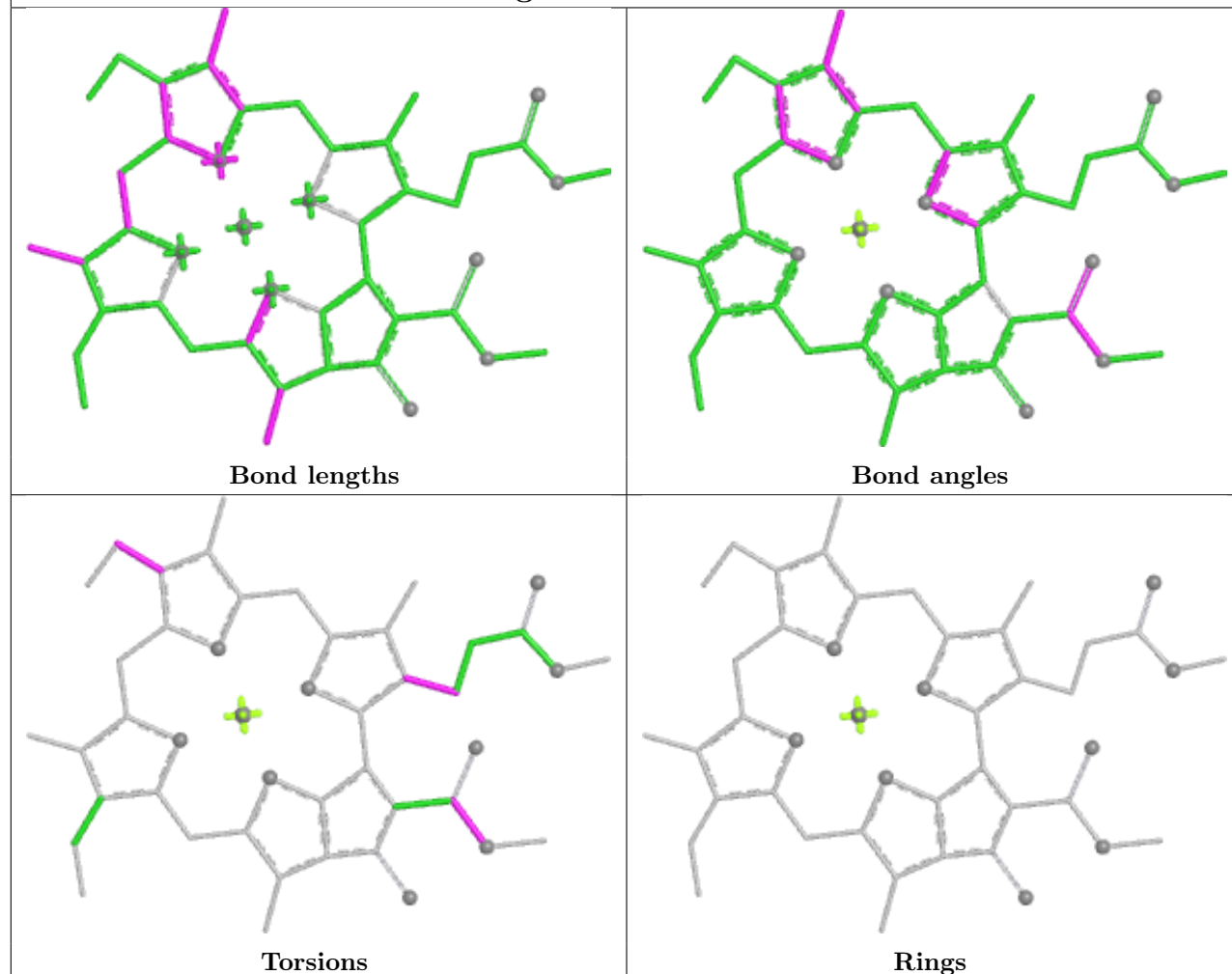


Ligand CLA A 814

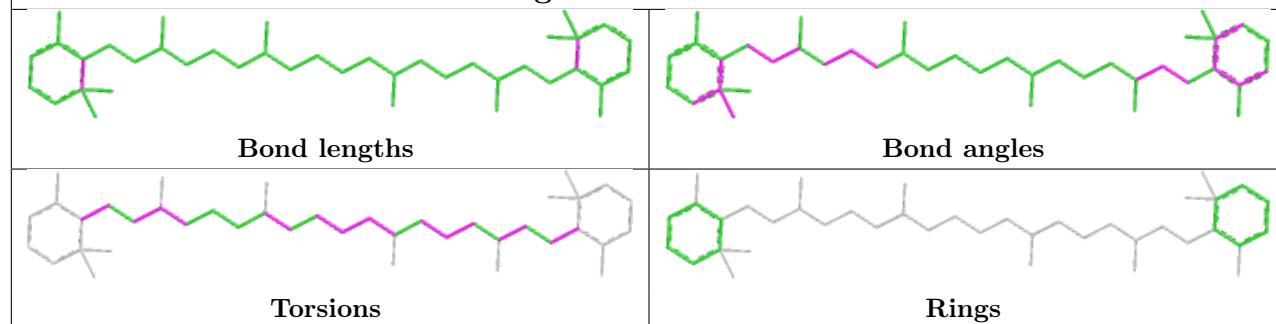


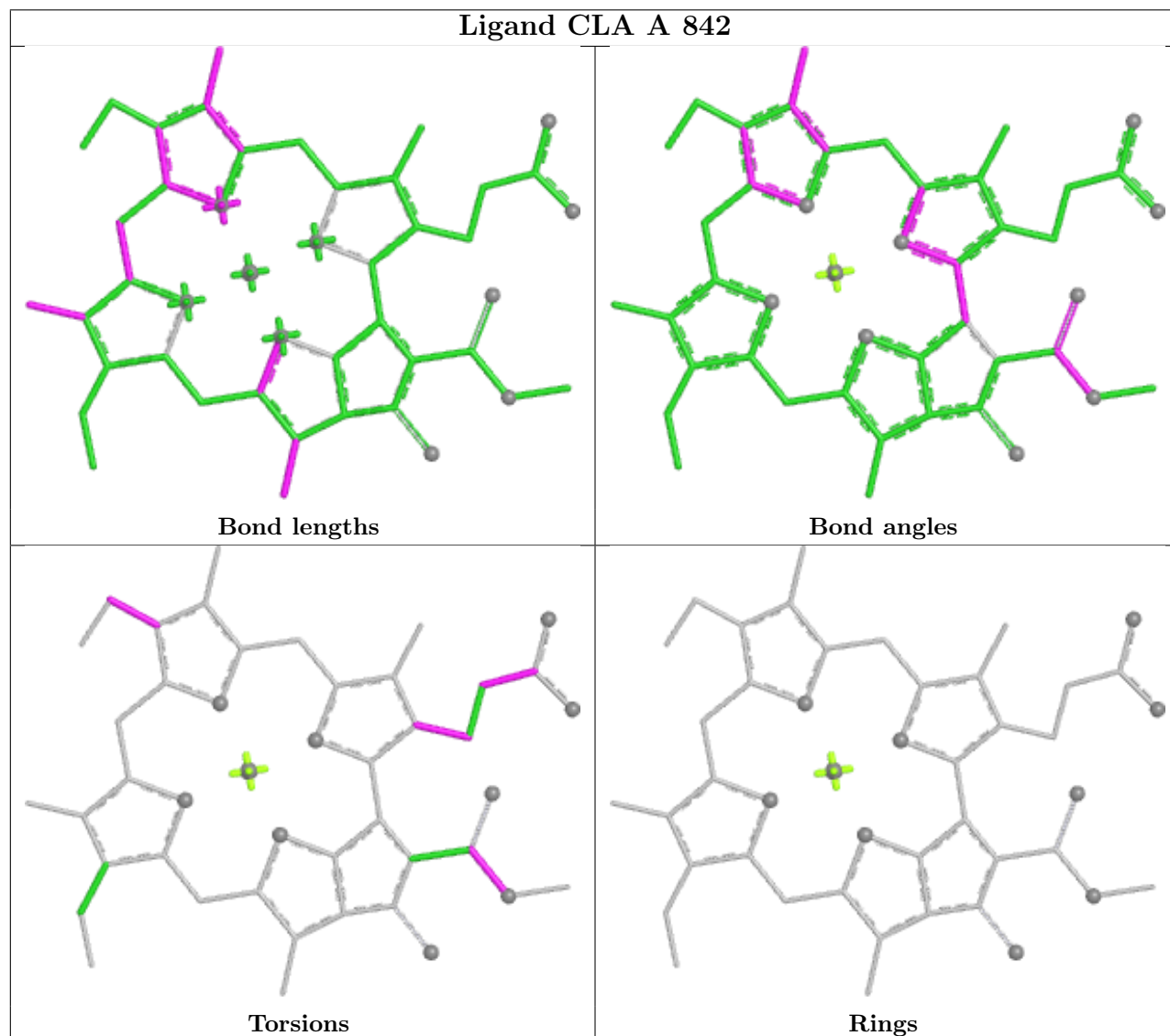
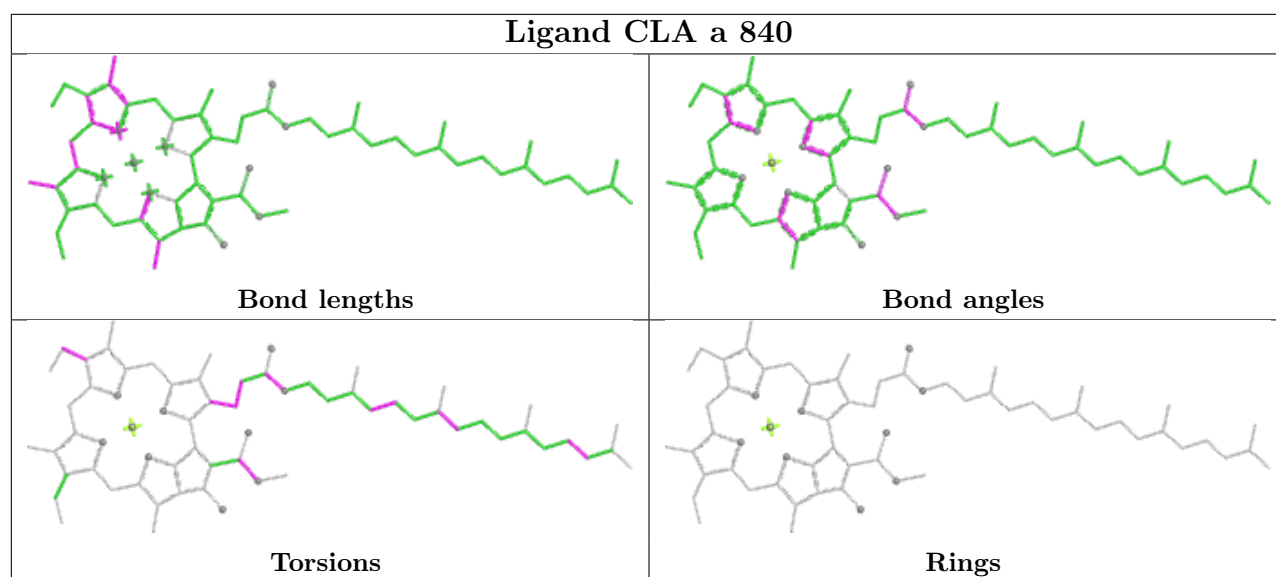
Ligand CLA A 824	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 820	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA L 204

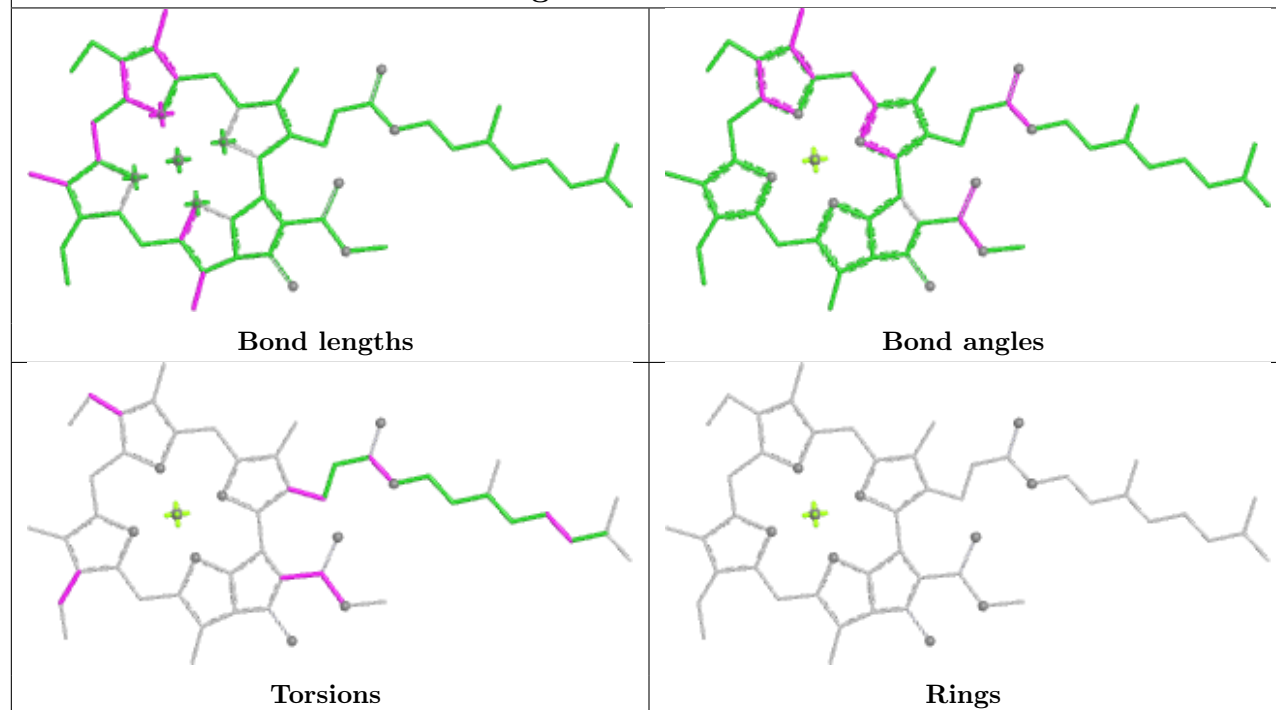


Ligand BCR 1 848

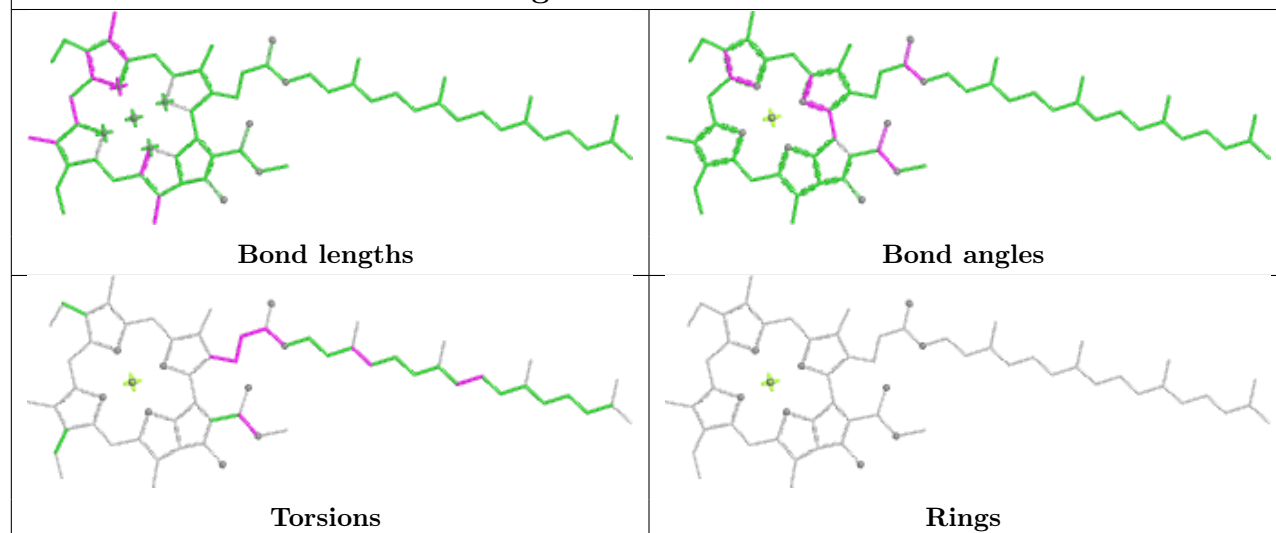


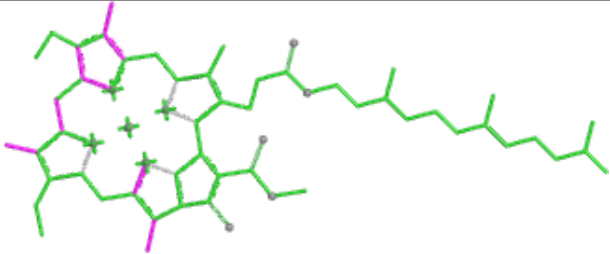
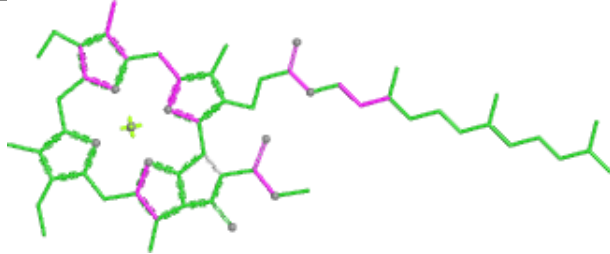
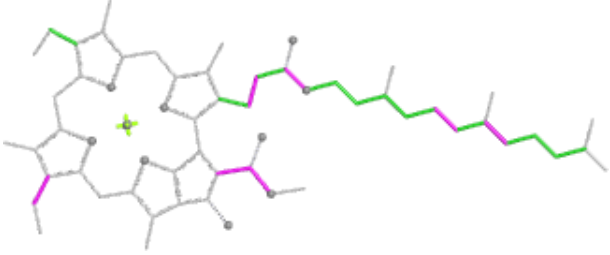
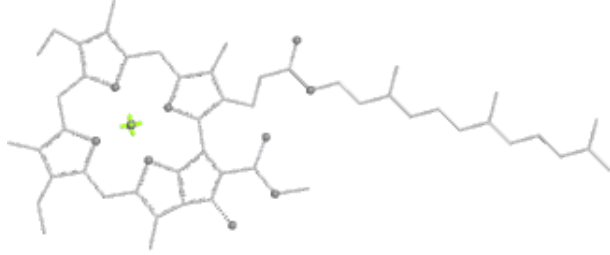
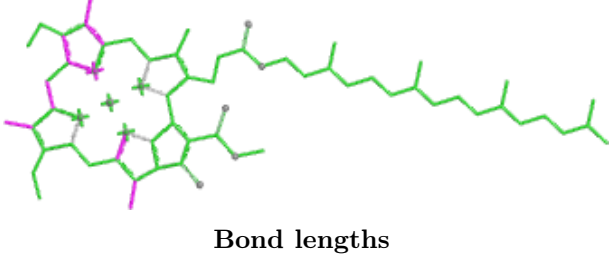
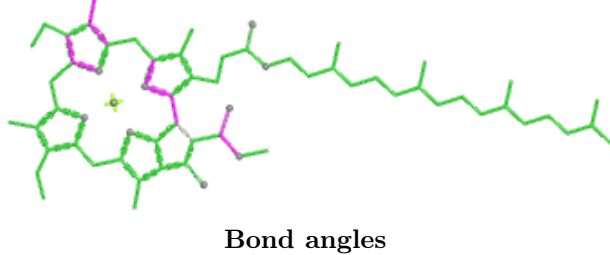
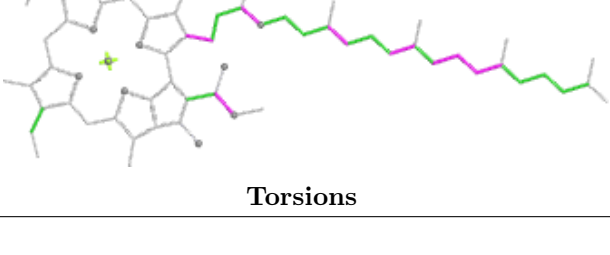
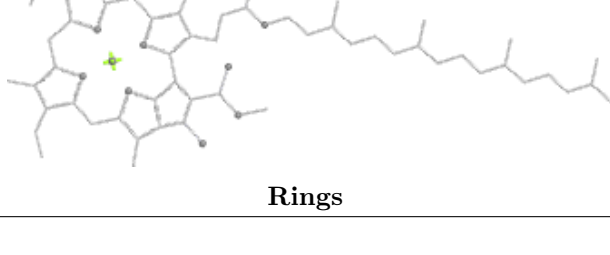


Ligand CLA A 805

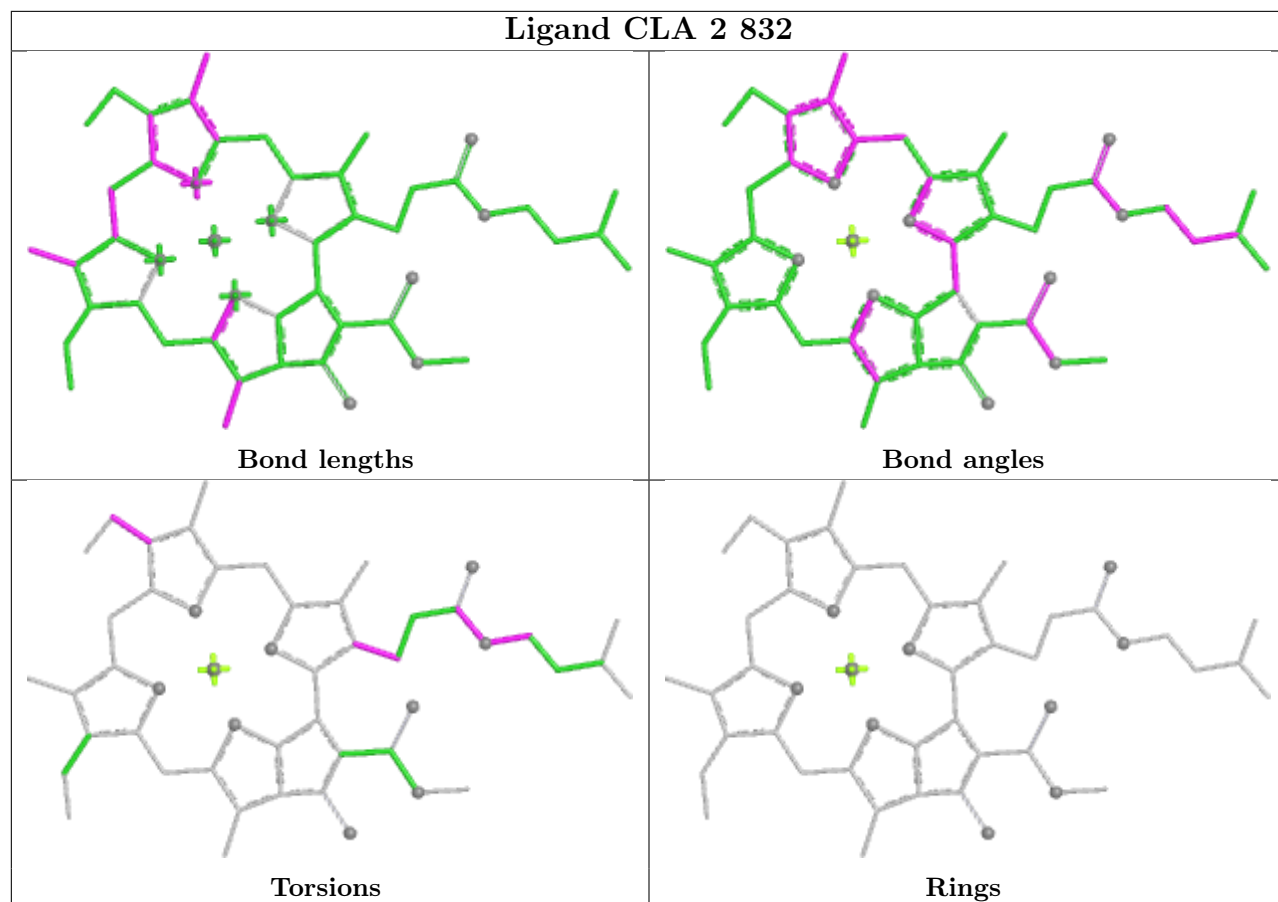


Ligand CLA A 821

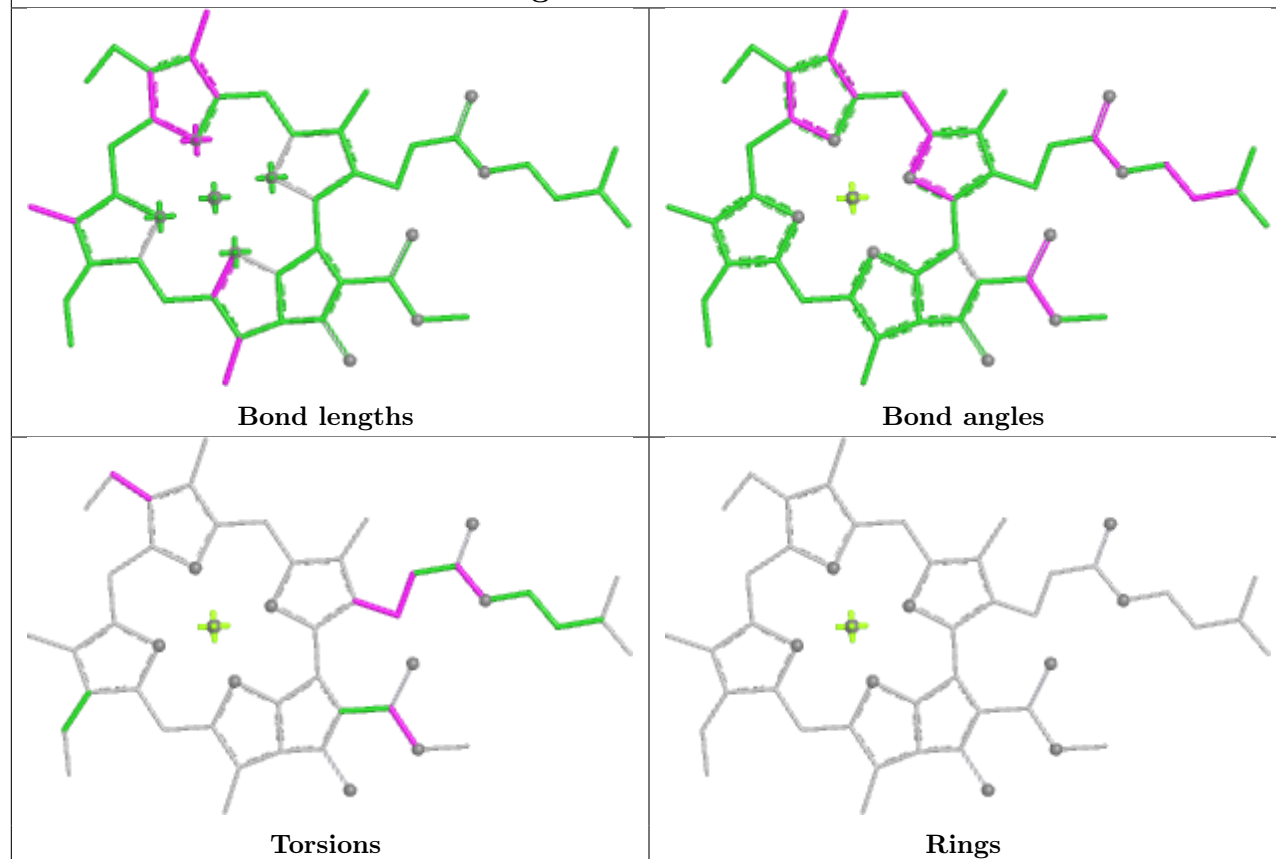


Ligand CLA B 803	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 2 807	
 Bond lengths	 Bond angles
 Torsions	 Rings

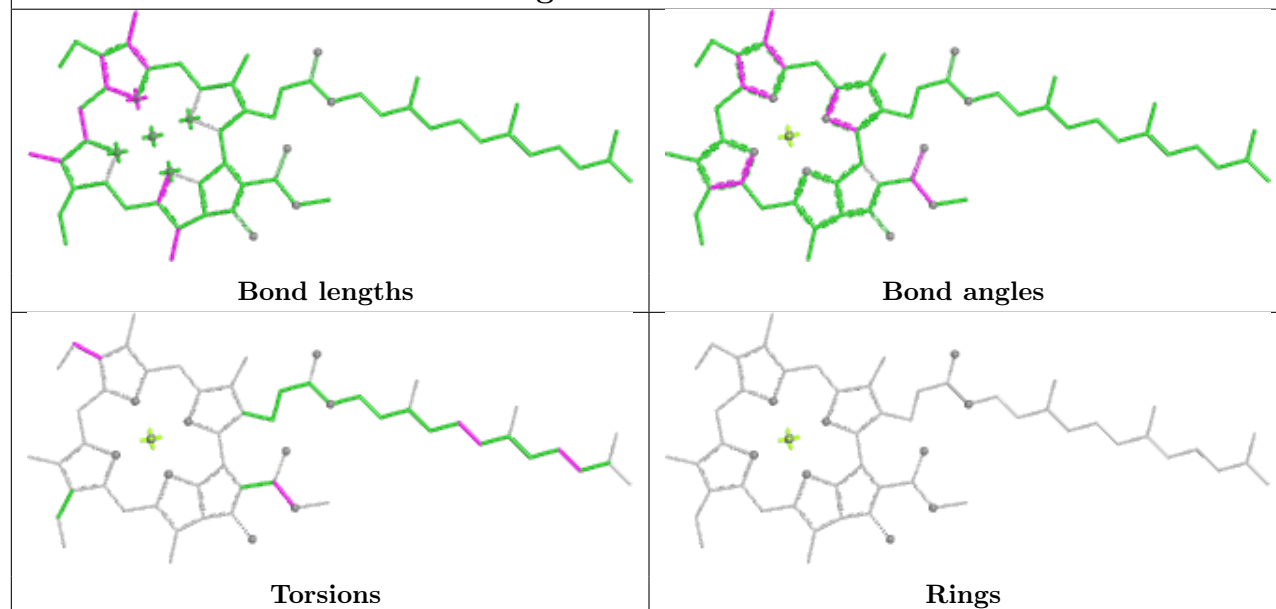
Ligand CLA 2 832



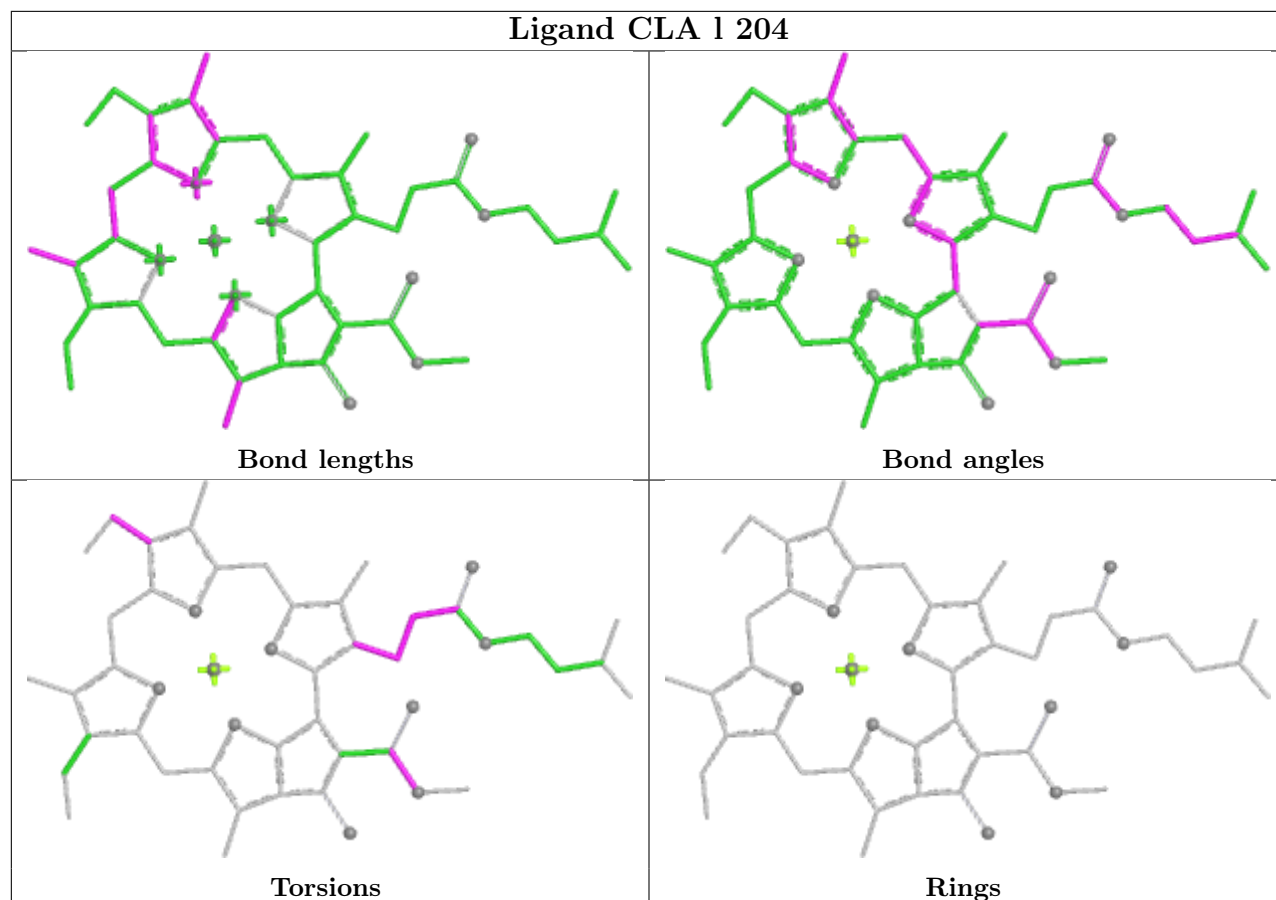
Ligand CLA A 809



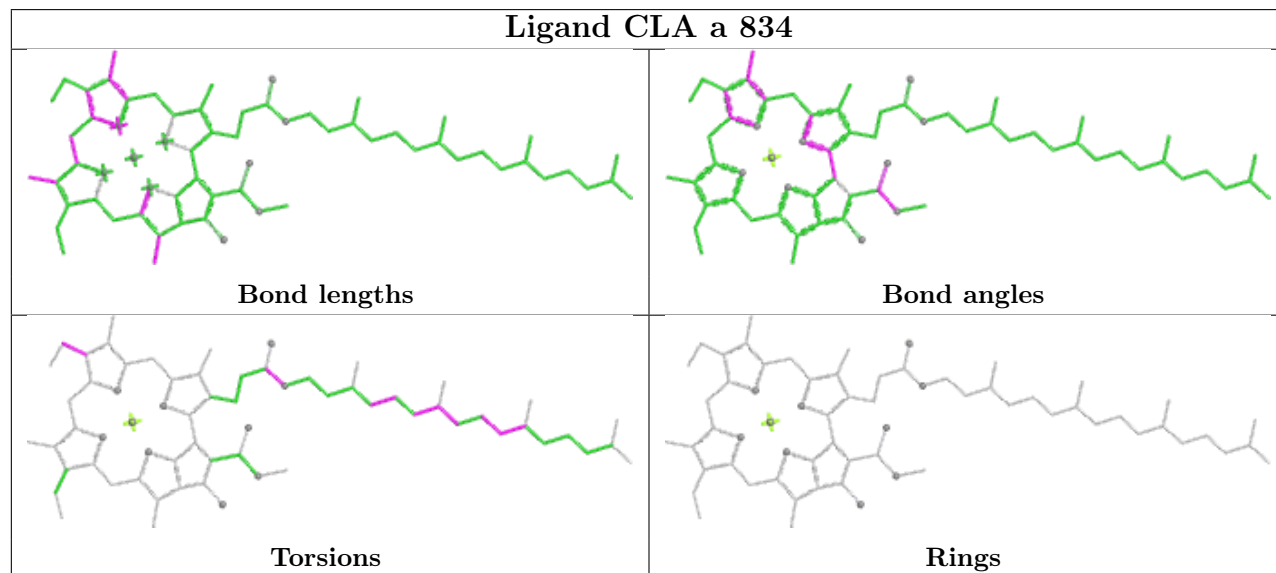
Ligand CLA 2 833



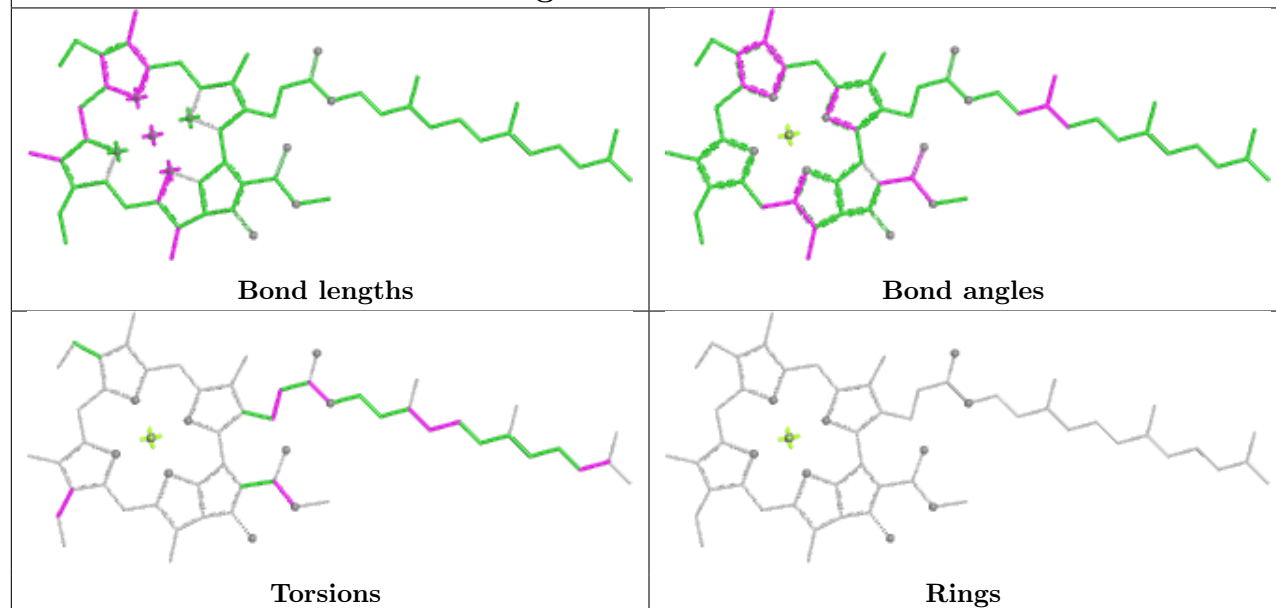
Ligand CLA 1 204



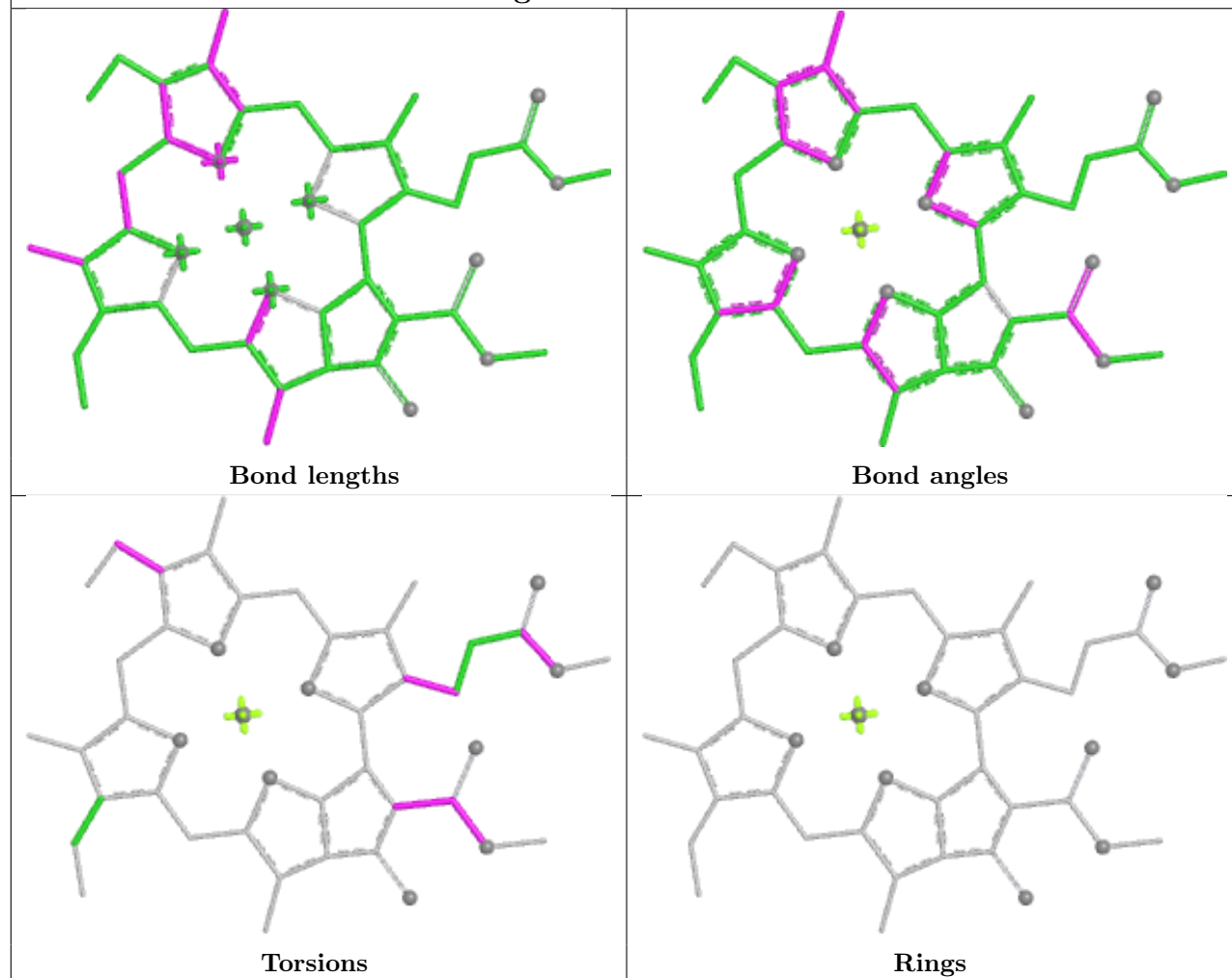
Ligand CLA a 834

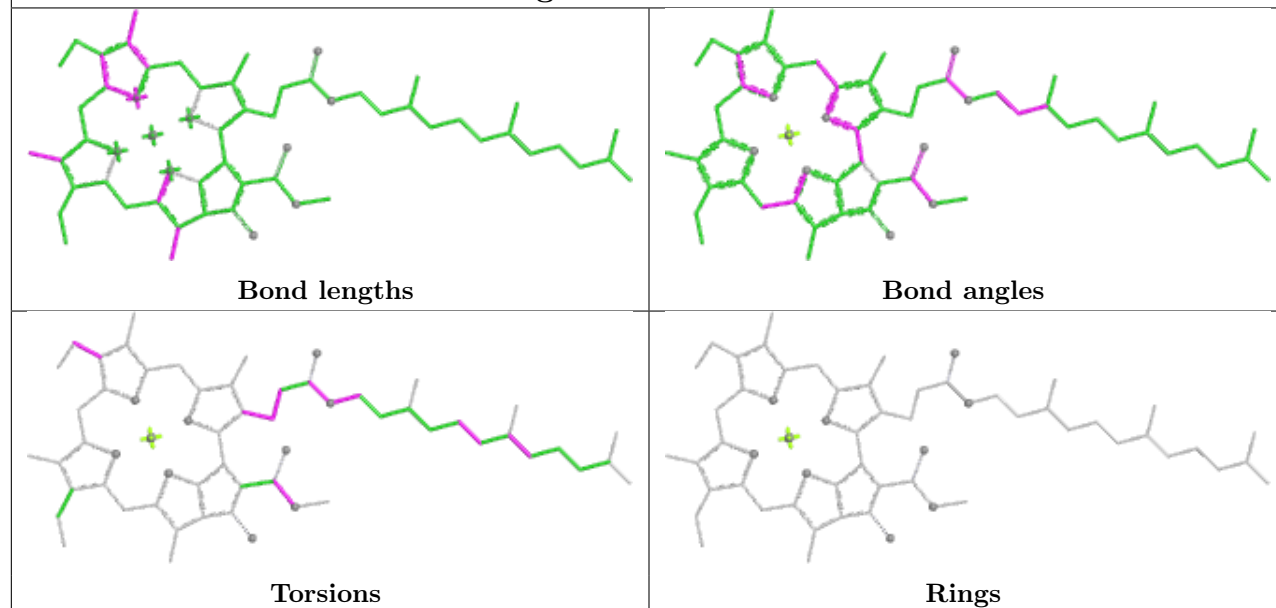
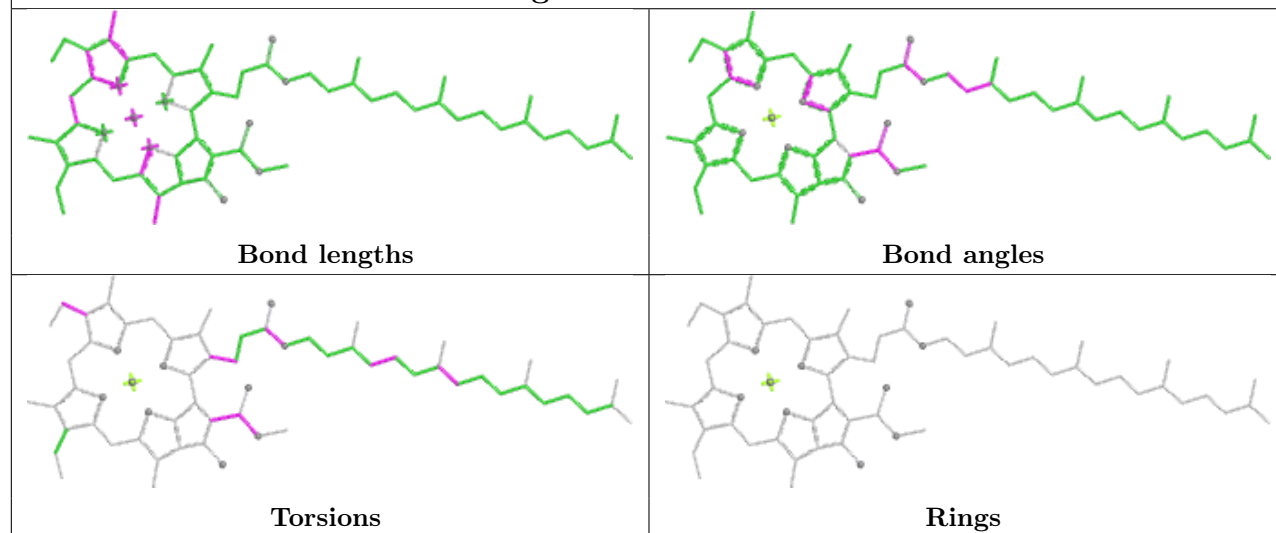


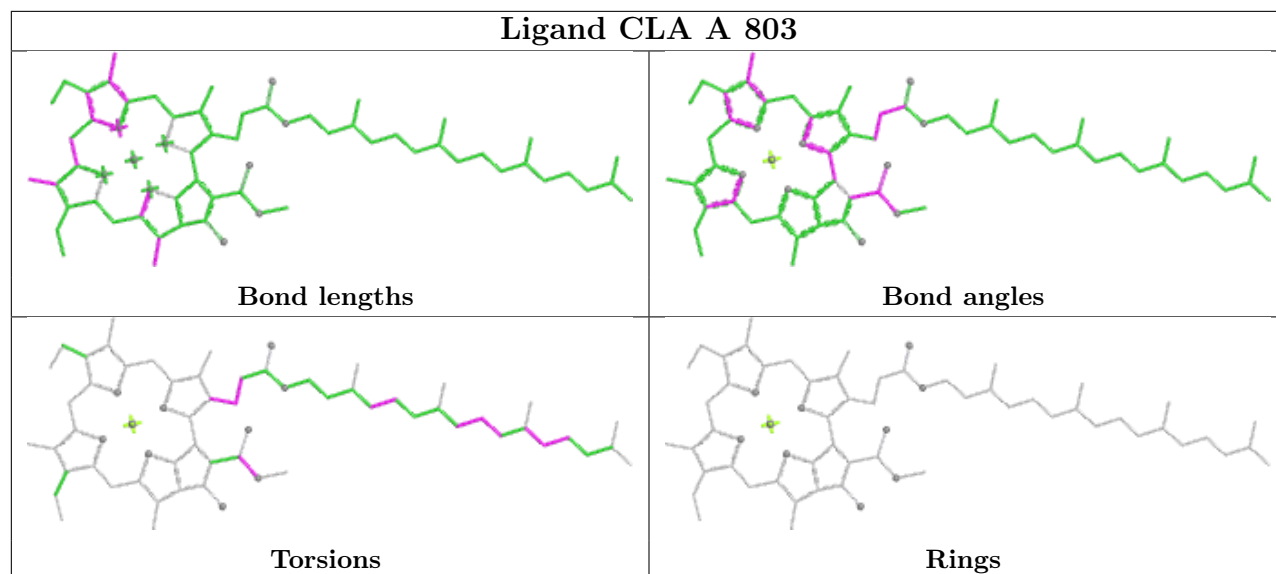
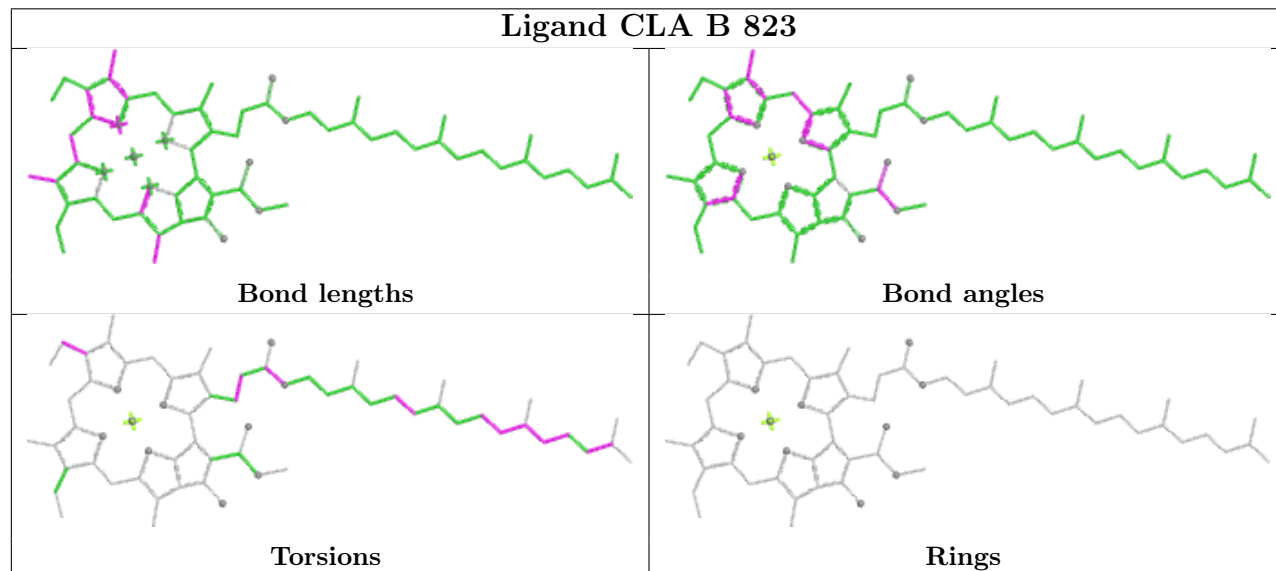
Ligand CLA 1 802

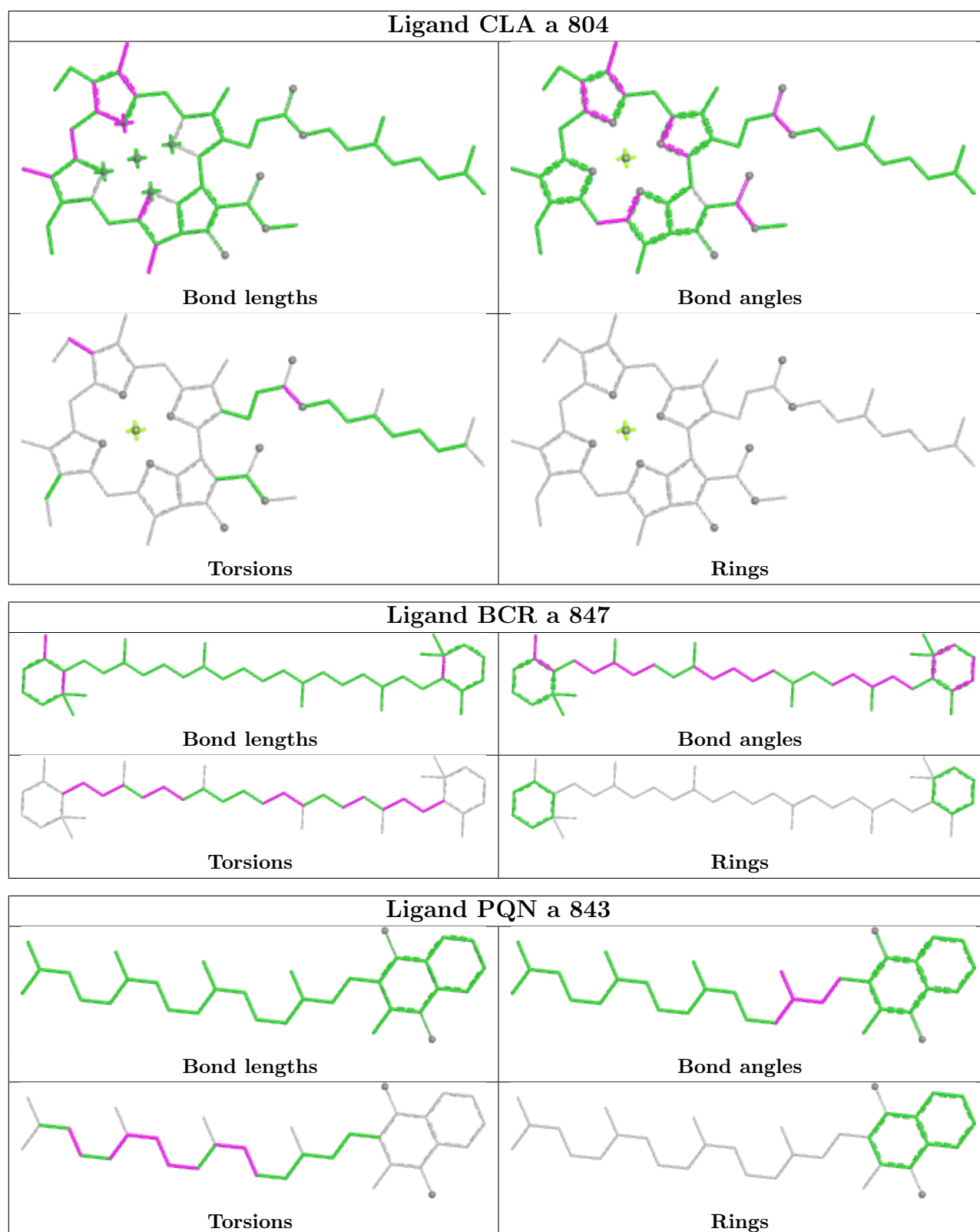


Ligand CLA B 811

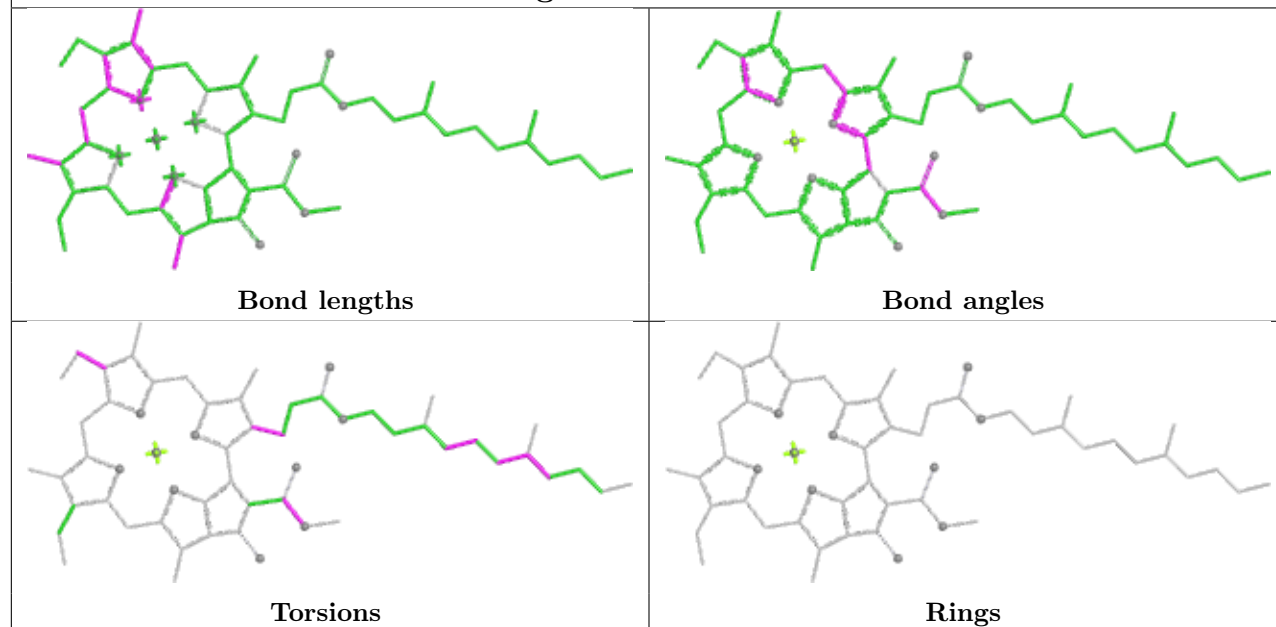


Ligand CLA a 841**Ligand CLA A 838**

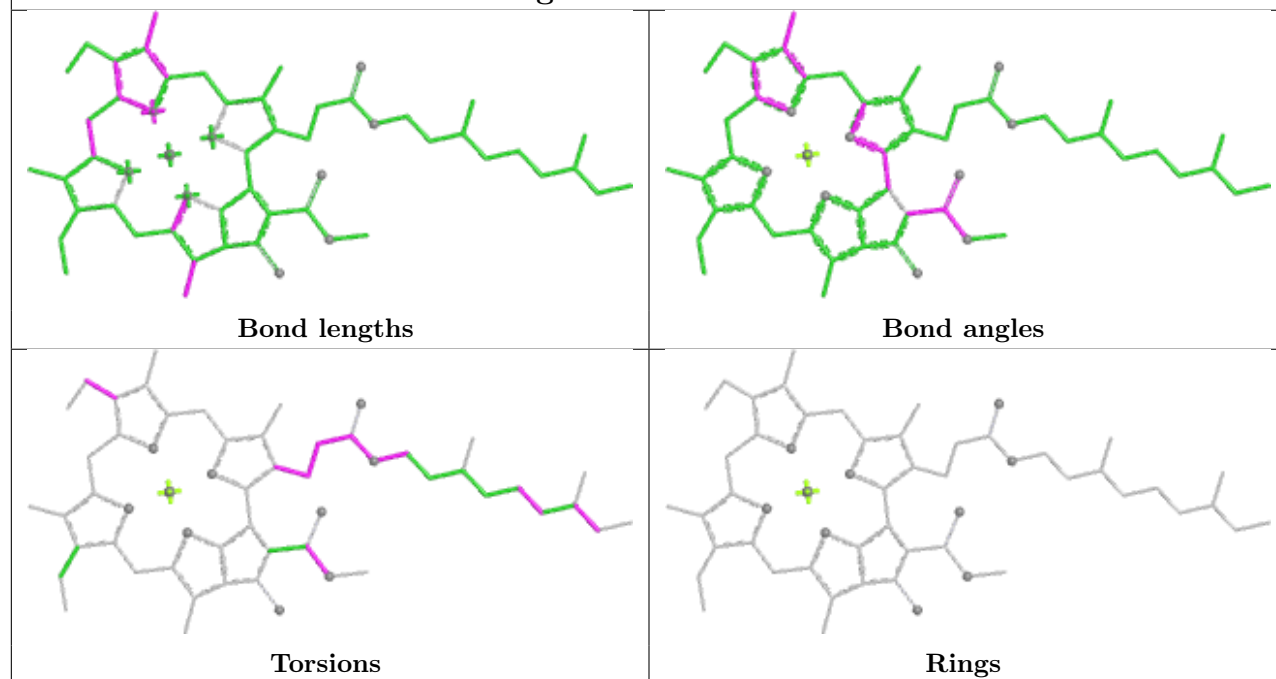
Ligand CLA A 803**Ligand CLA B 823**

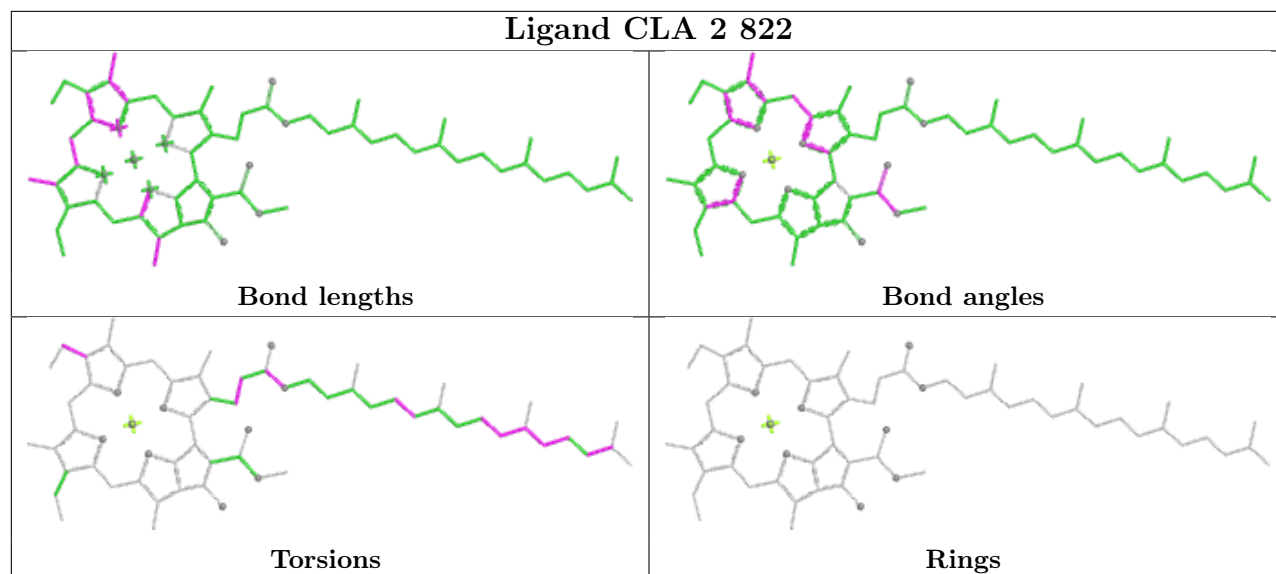
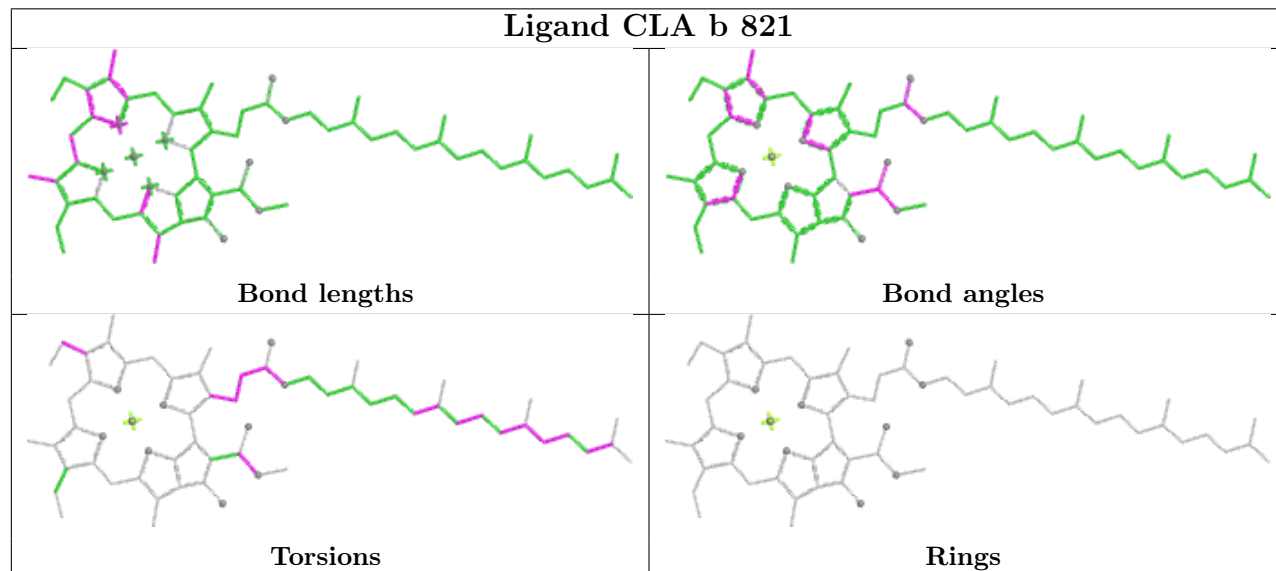


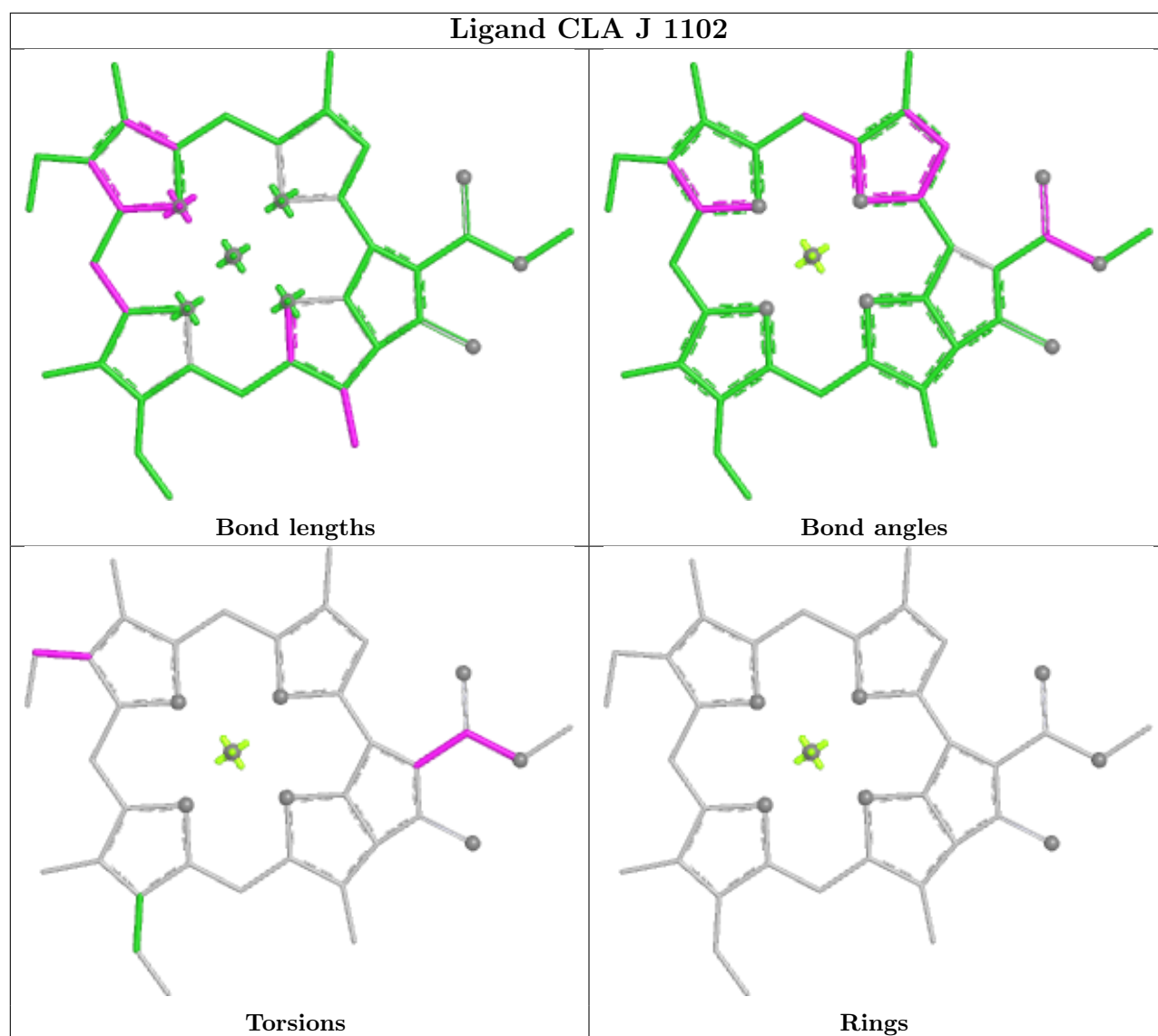
Ligand CLA 2 829

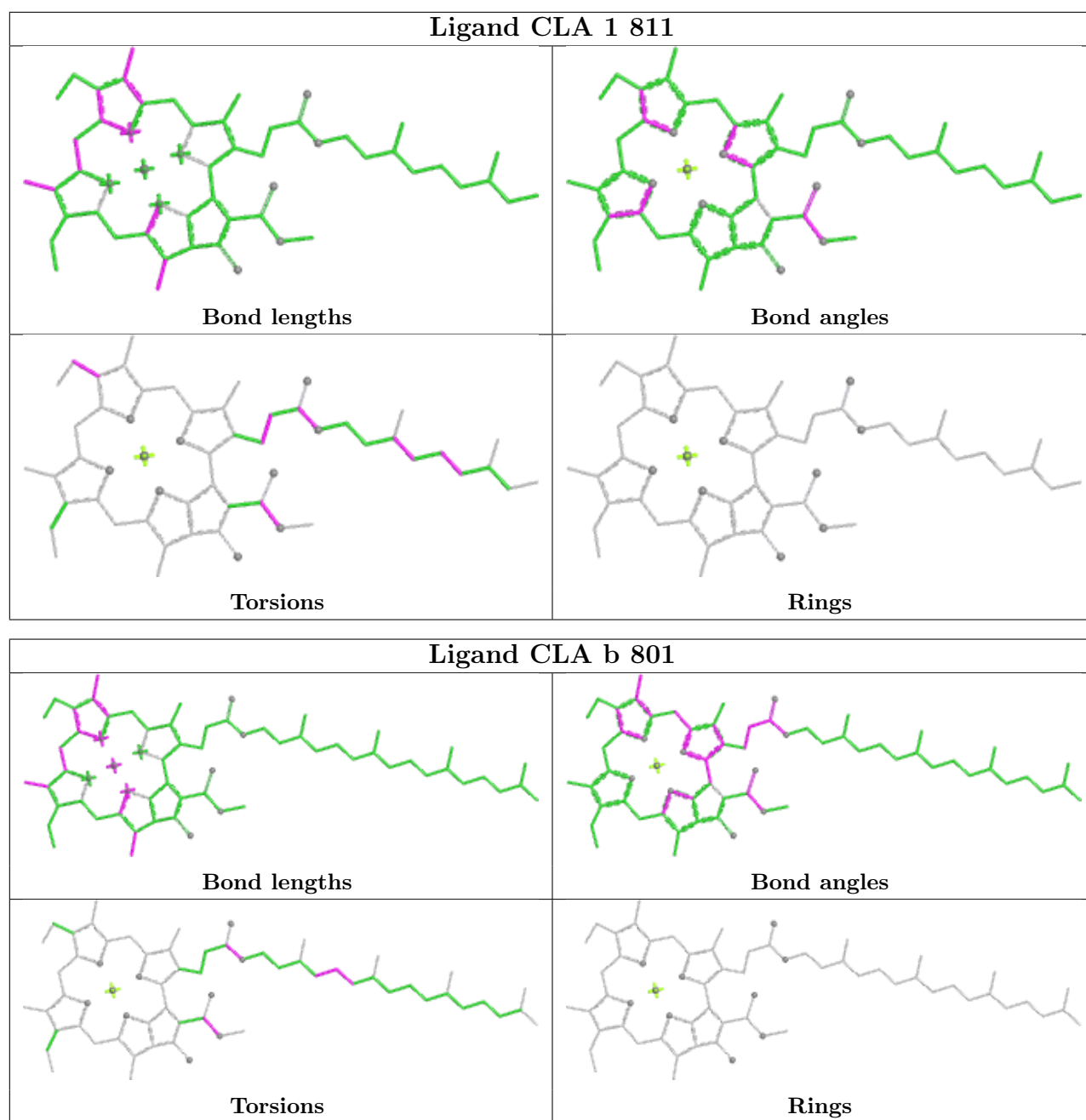


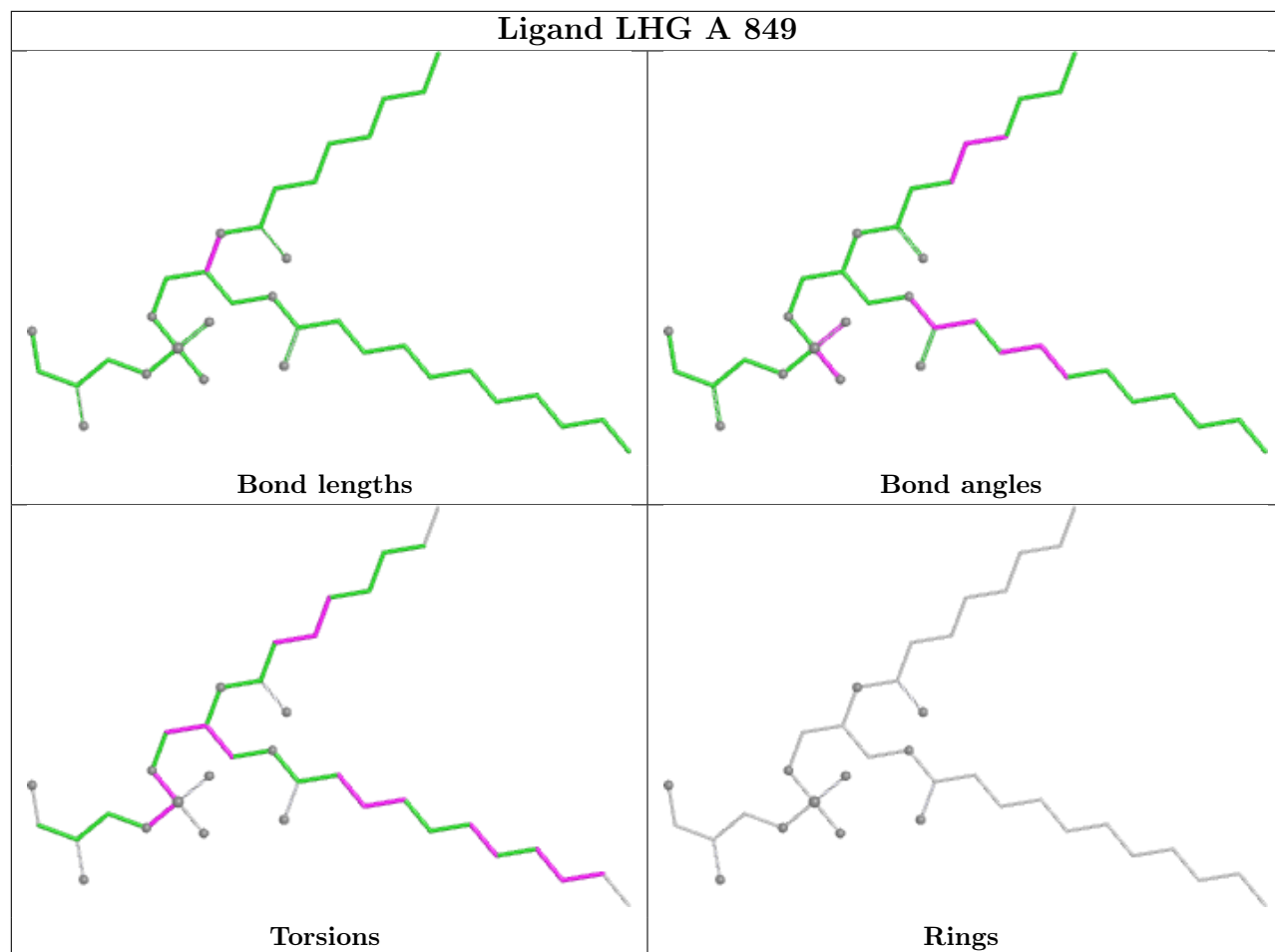
Ligand CLA a 835



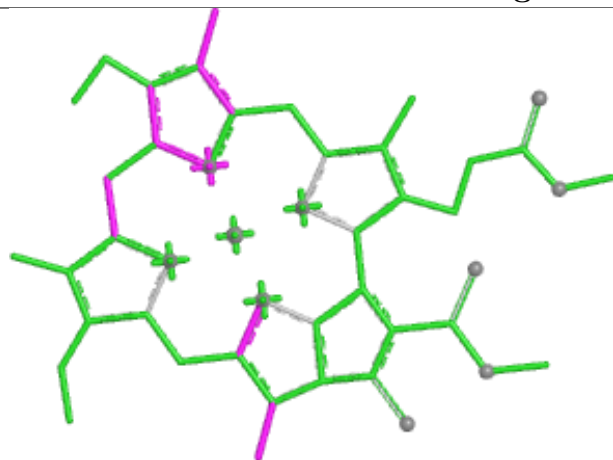
Ligand CLA 2 822**Ligand CLA b 821**



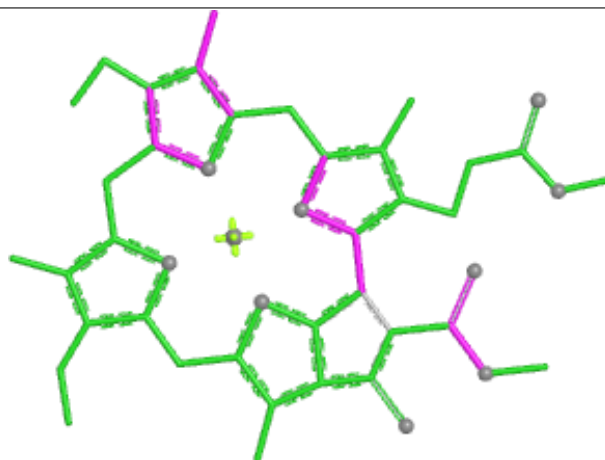




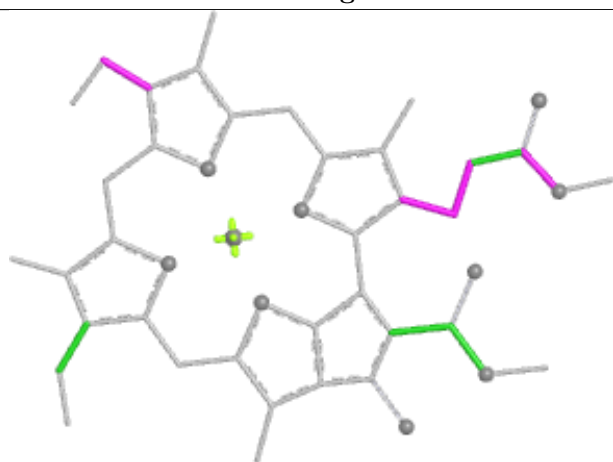
Ligand CLA A 812



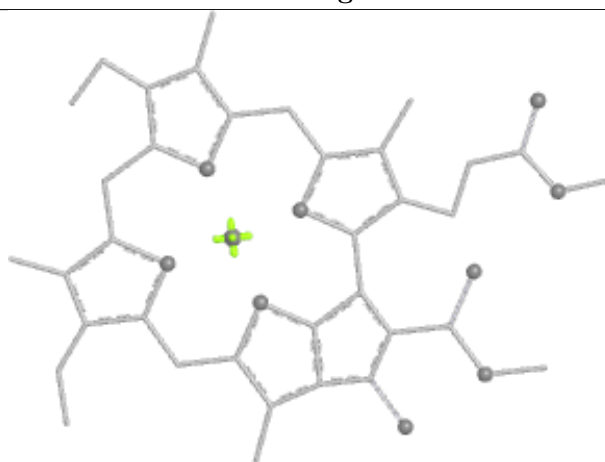
Bond lengths



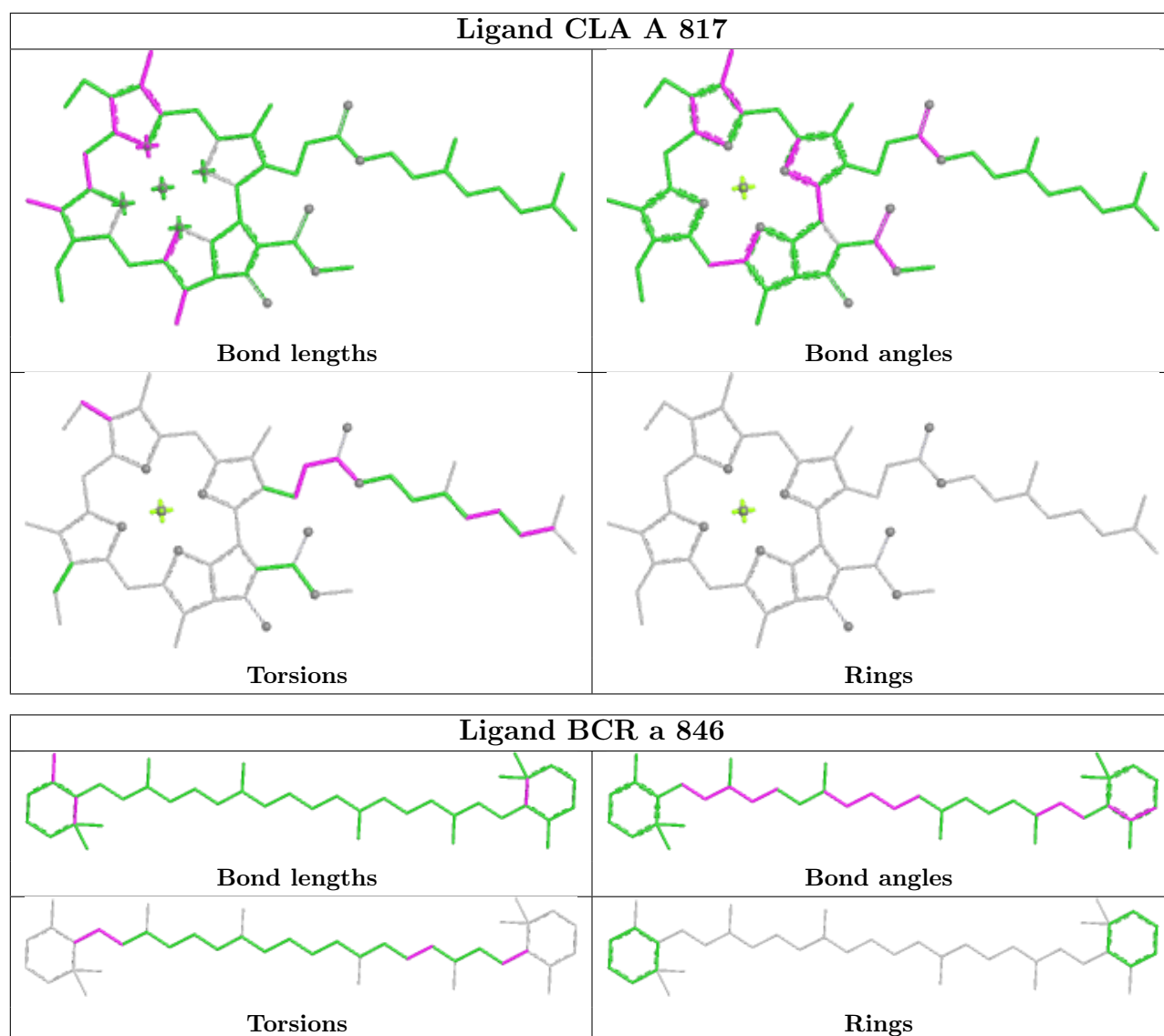
Bond angles



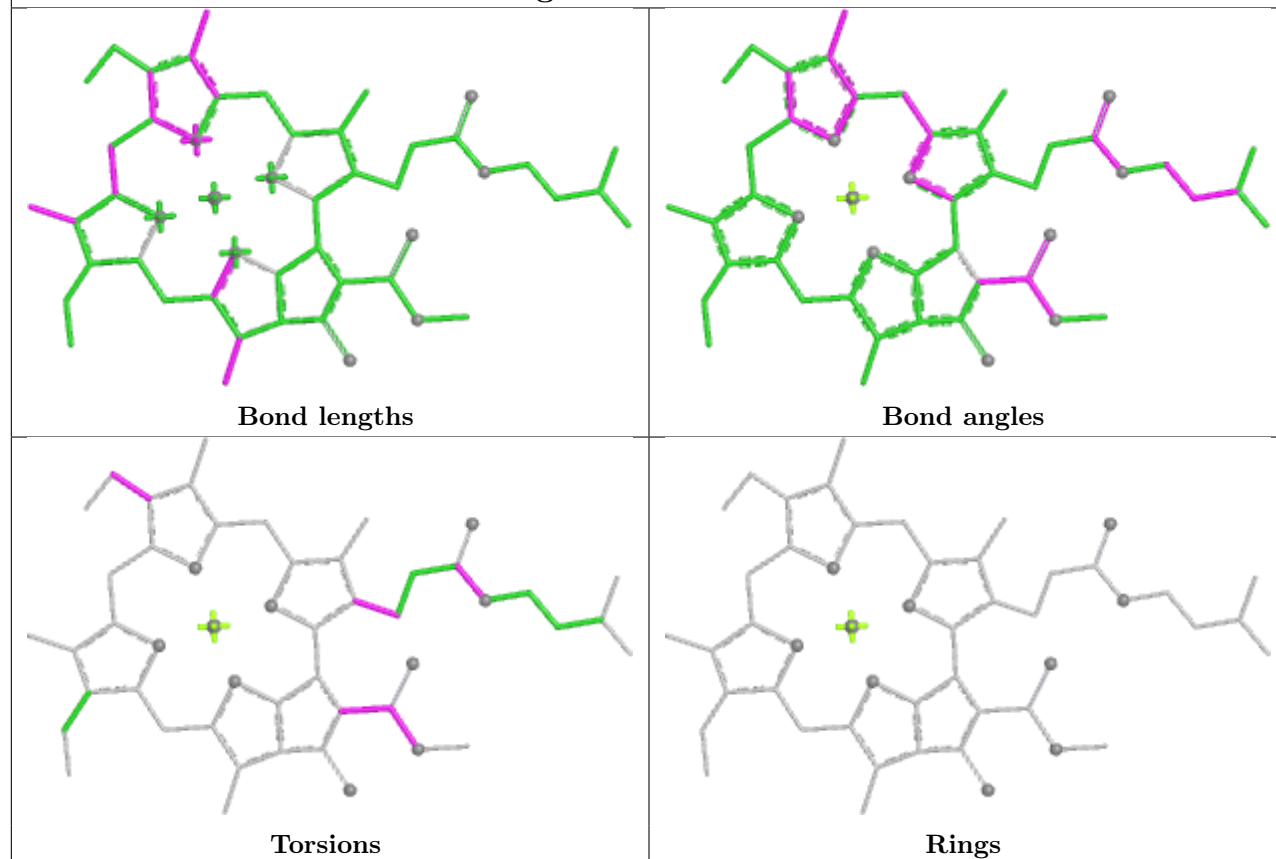
Torsions



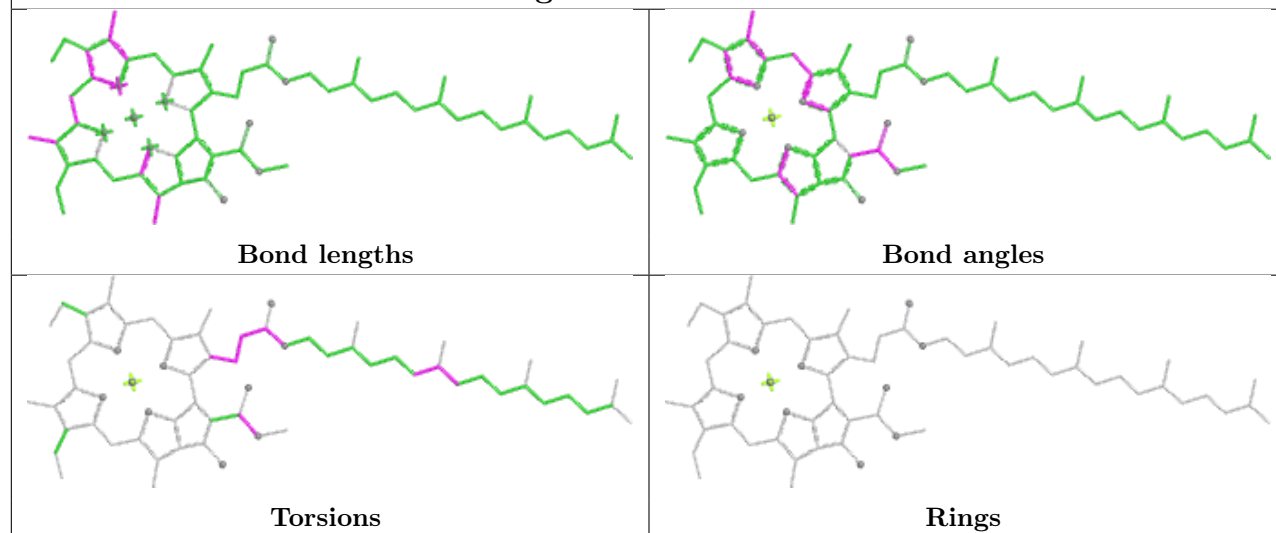
Rings



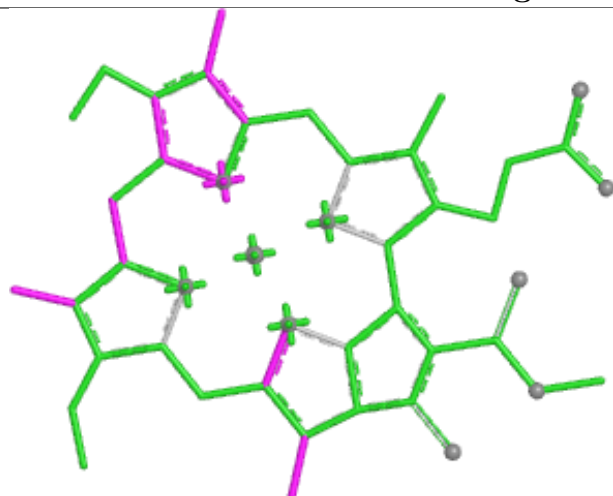
Ligand CLA 1 831



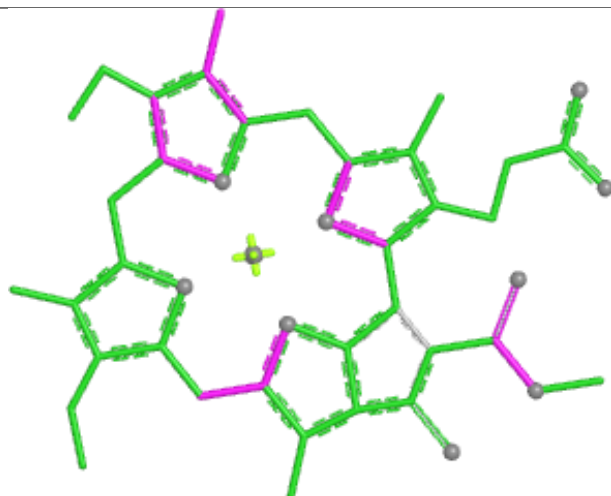
Ligand CLA b 815



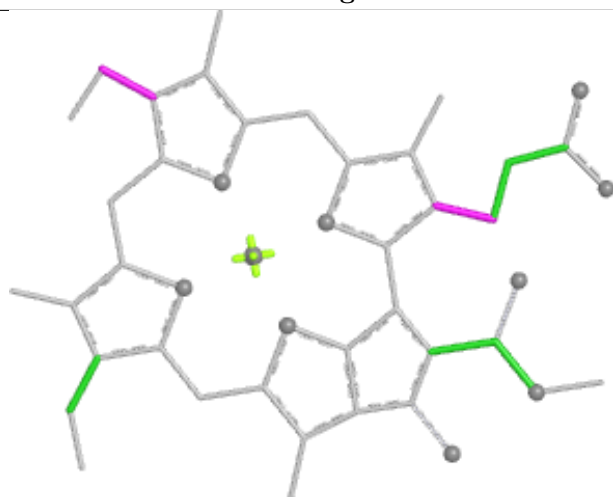
Ligand CLA A 815



Bond lengths



Bond angles

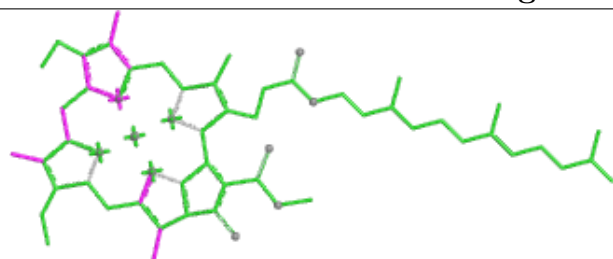


Torsions

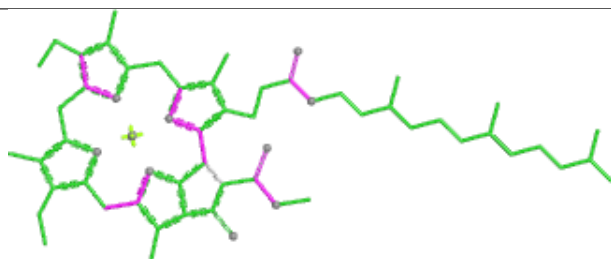


Rings

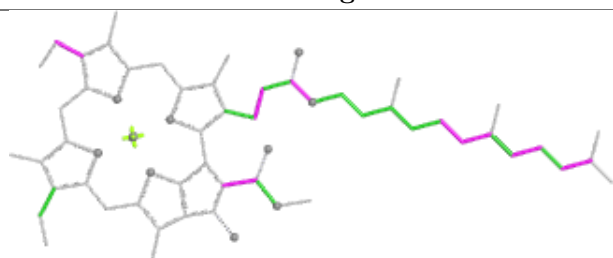
Ligand CLA 1 852



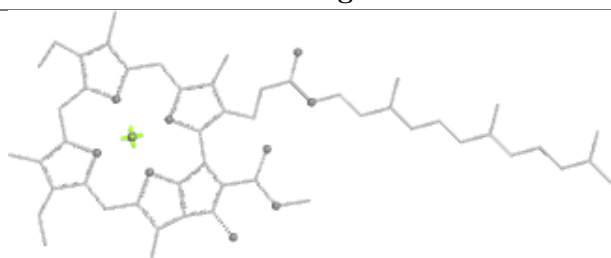
Bond lengths



Bond angles

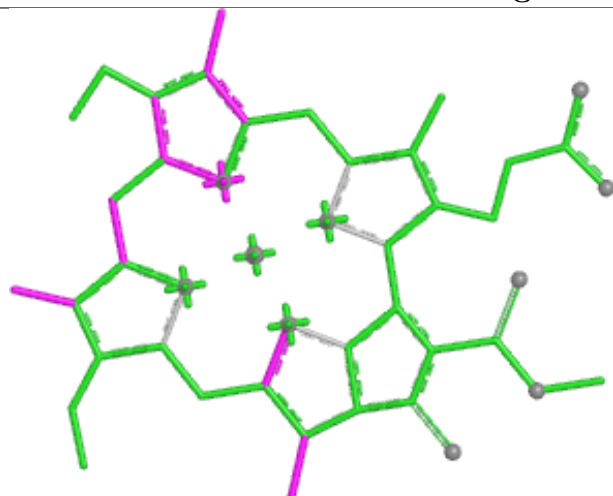


Torsions

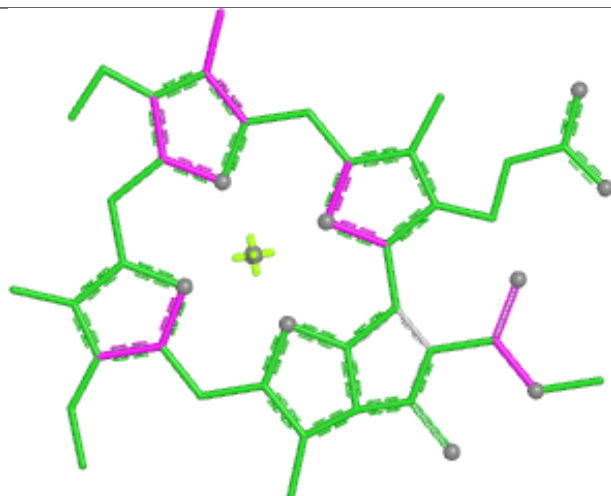


Rings

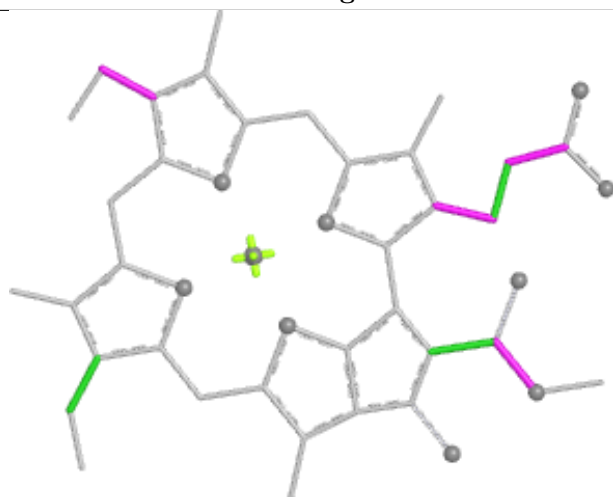
Ligand CLA A 810



Bond lengths



Bond angles

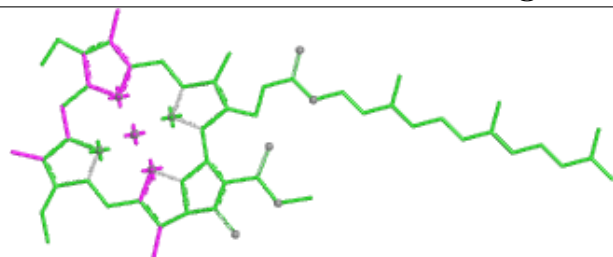


Torsions

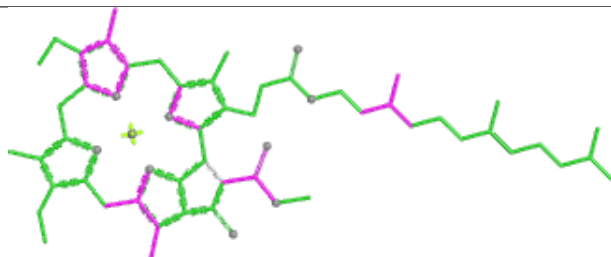


Rings

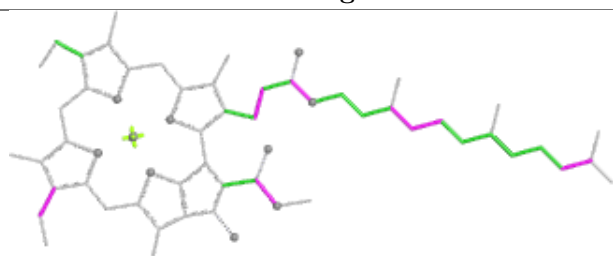
Ligand CLA a 802



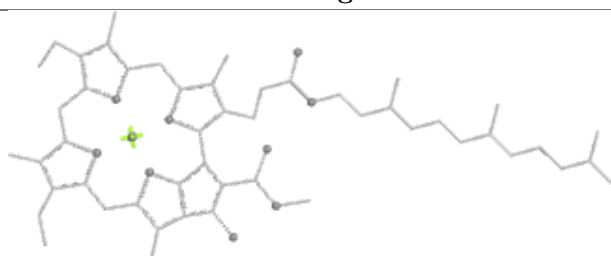
Bond lengths



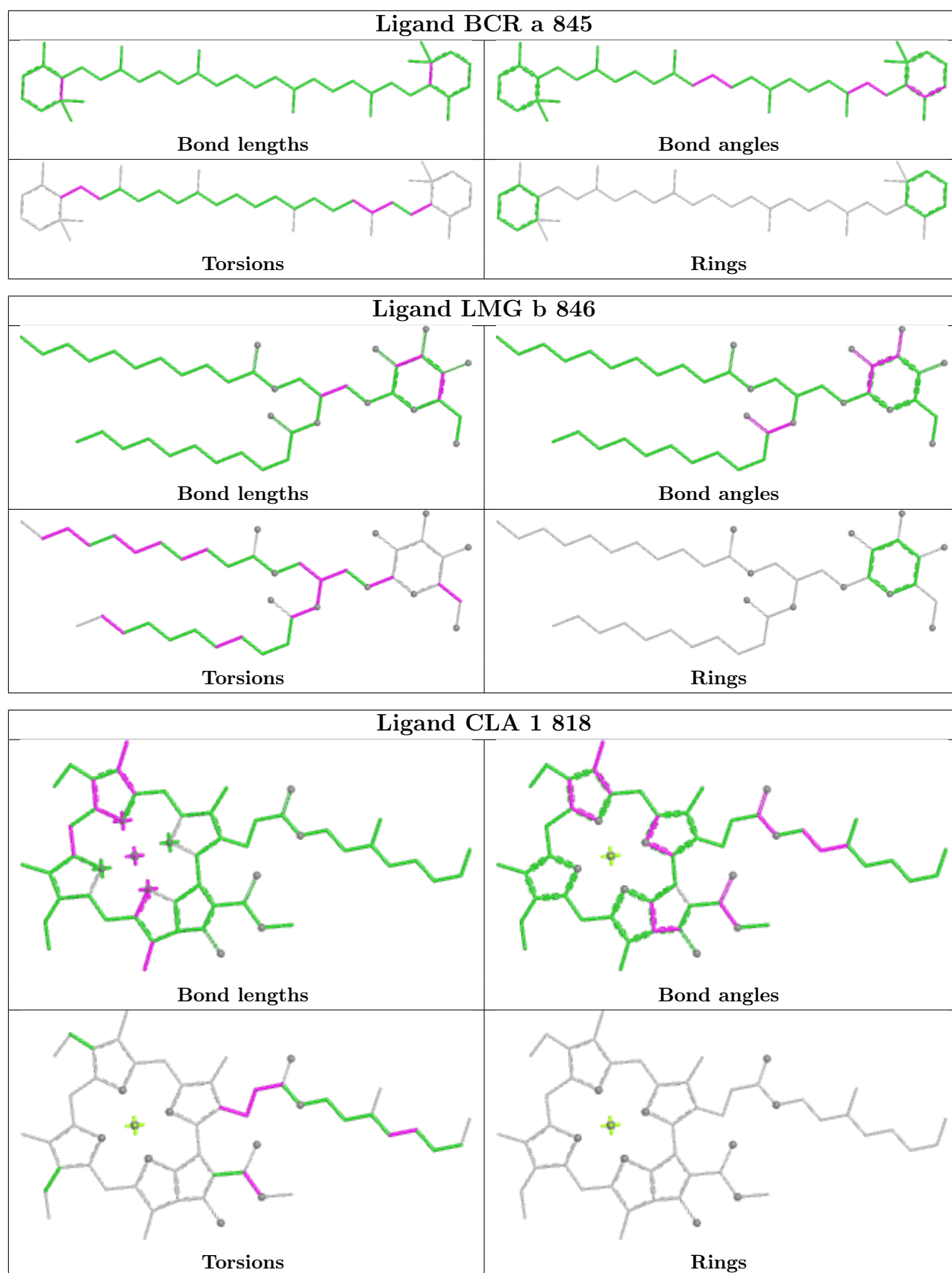
Bond angles



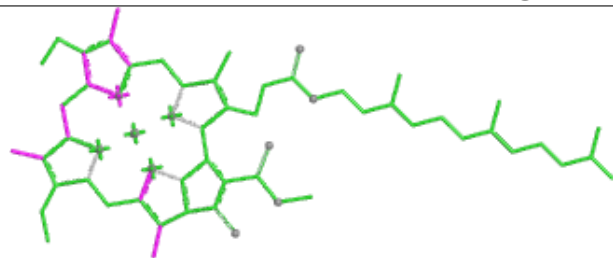
Torsions



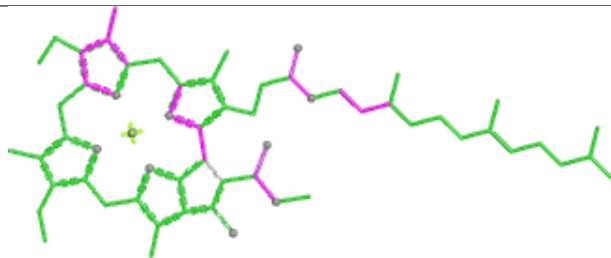
Rings



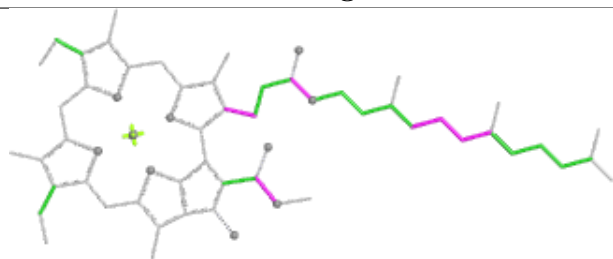
Ligand CLA L 201



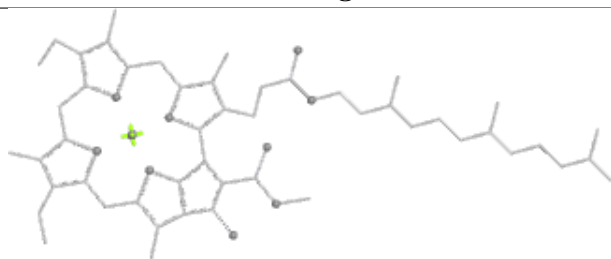
Bond lengths



Bond angles

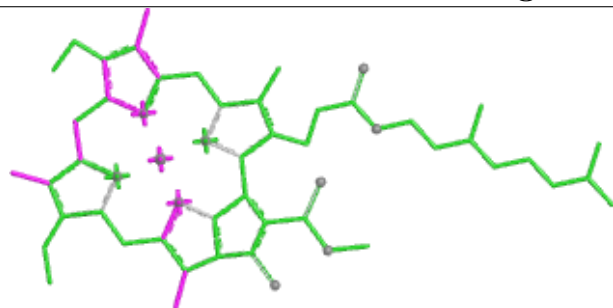


Torsions

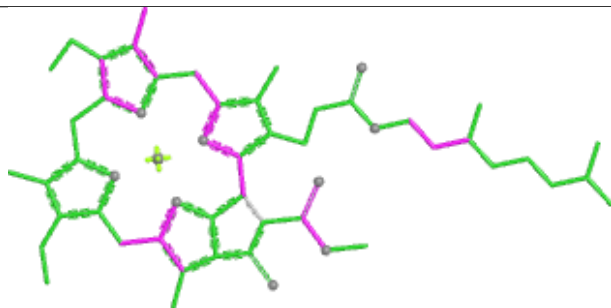


Rings

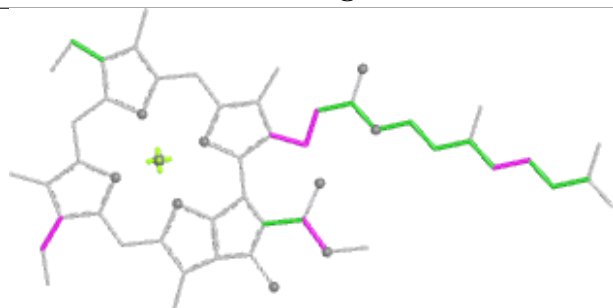
Ligand CLA b 824



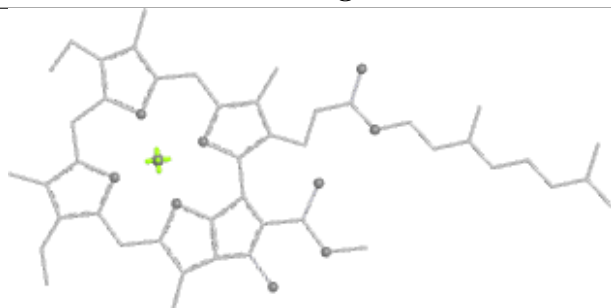
Bond lengths



Bond angles

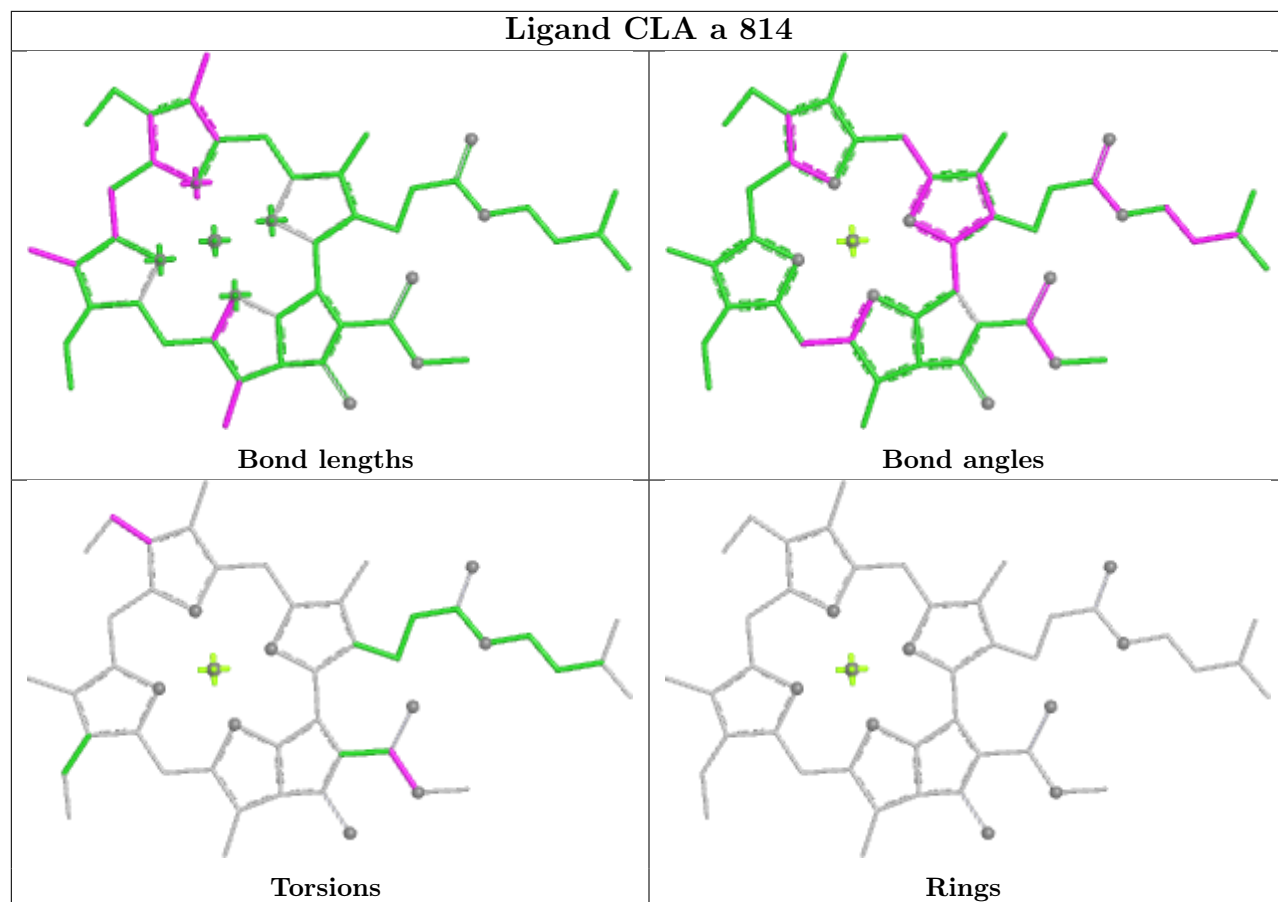


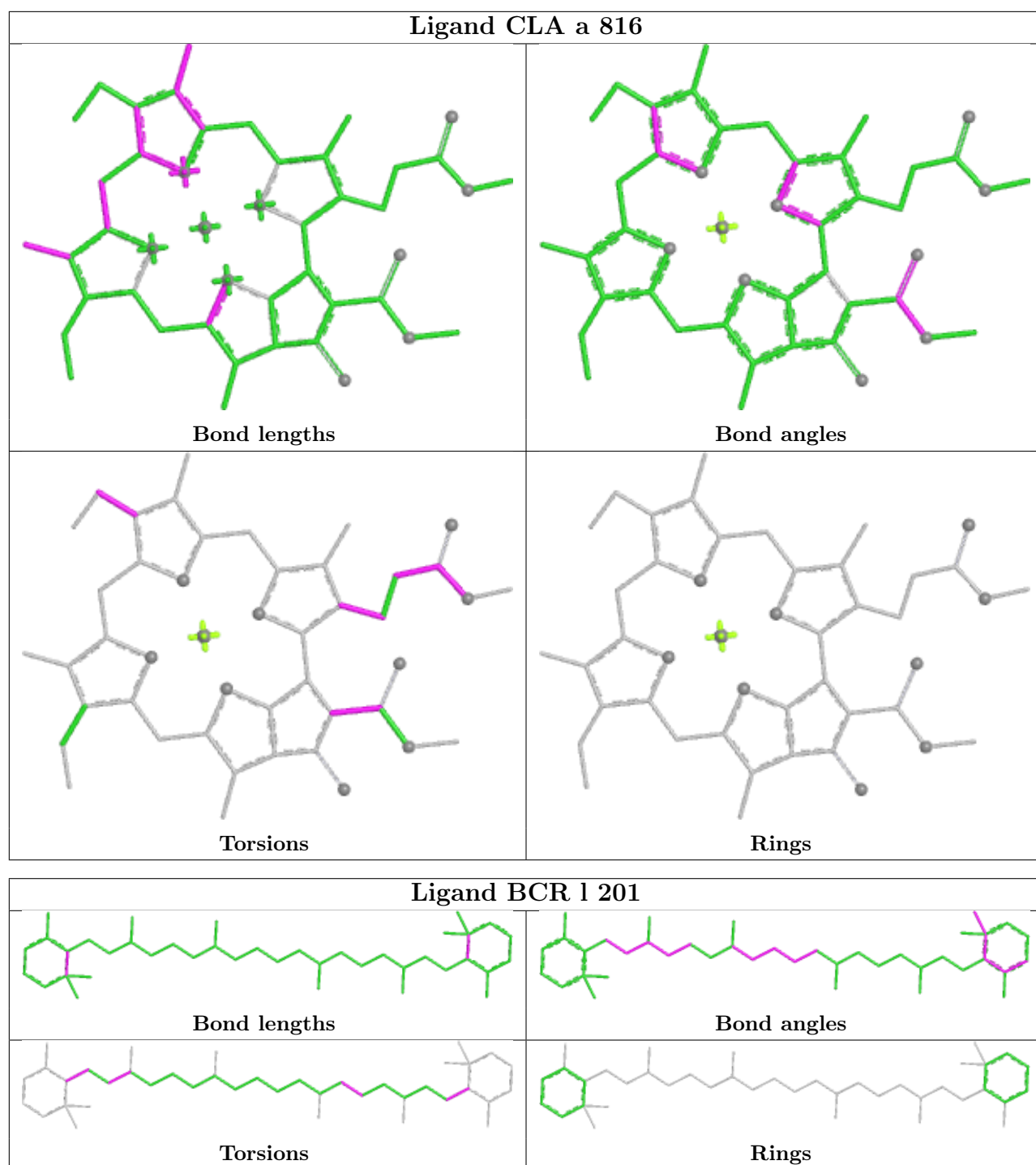
Torsions

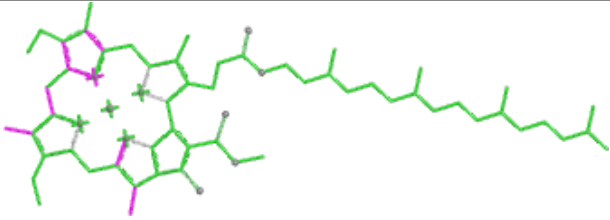
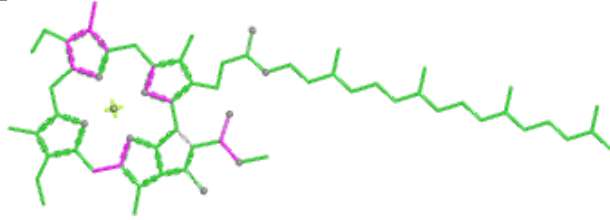
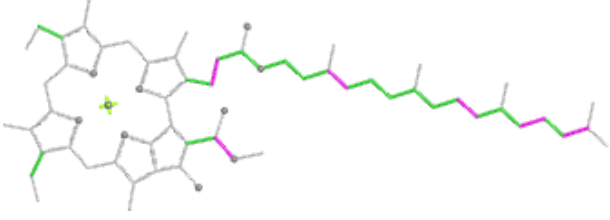
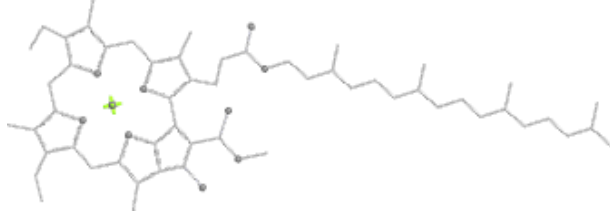
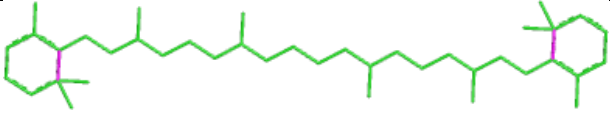
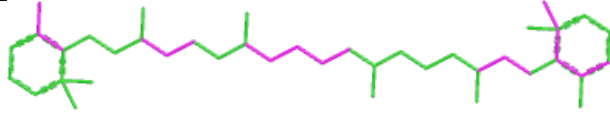
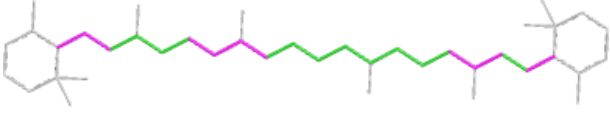
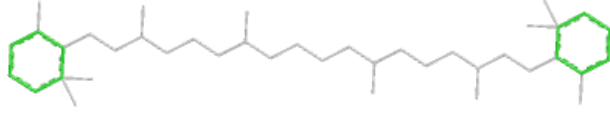
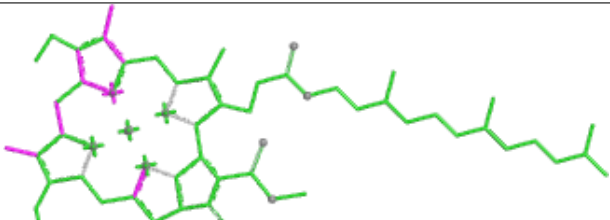
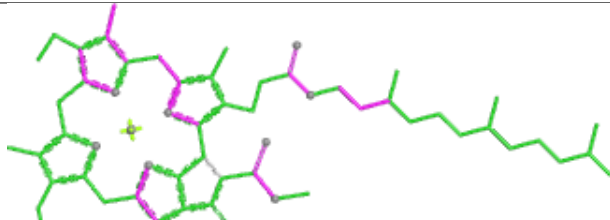
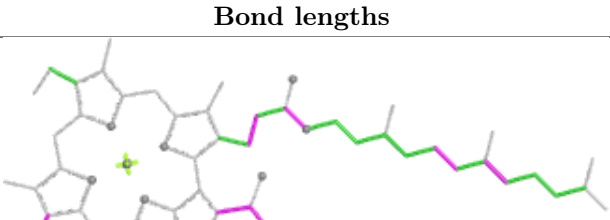
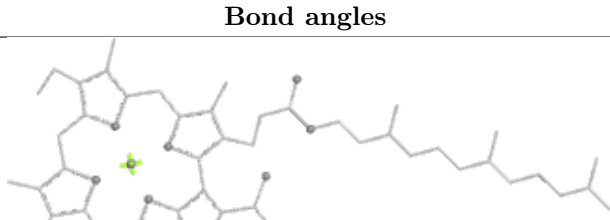


Rings

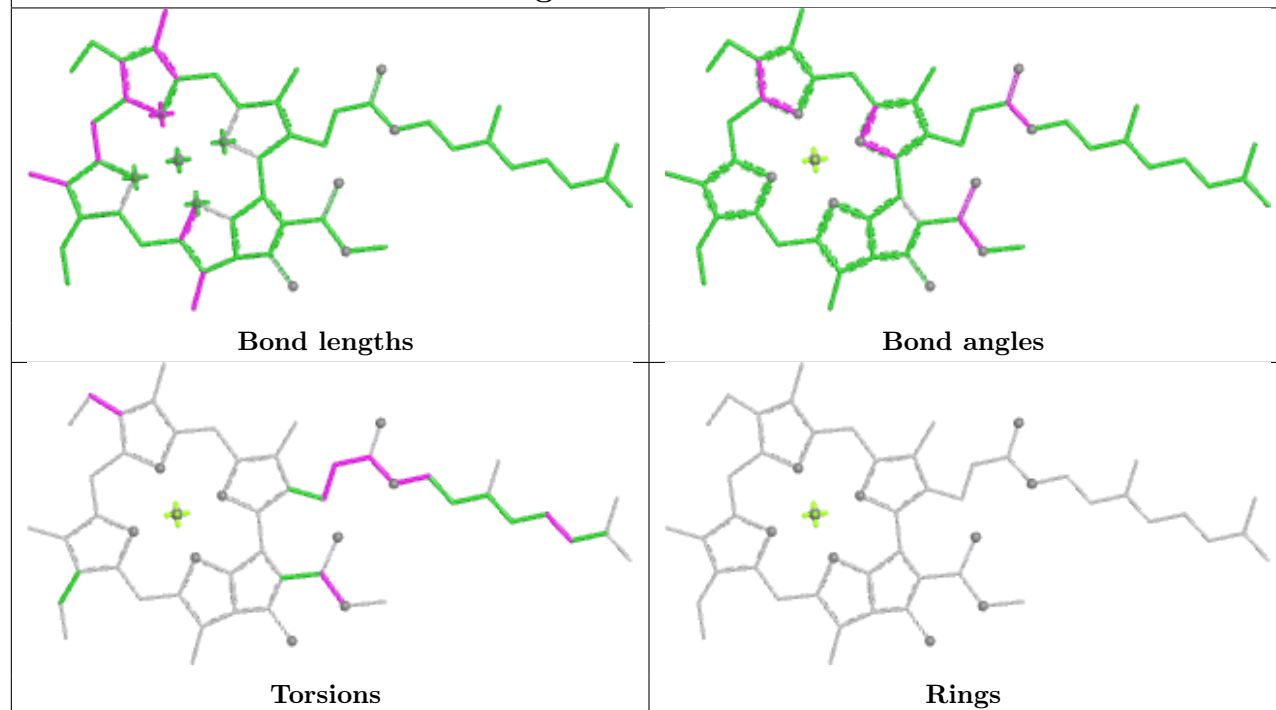
Ligand CLA a 814



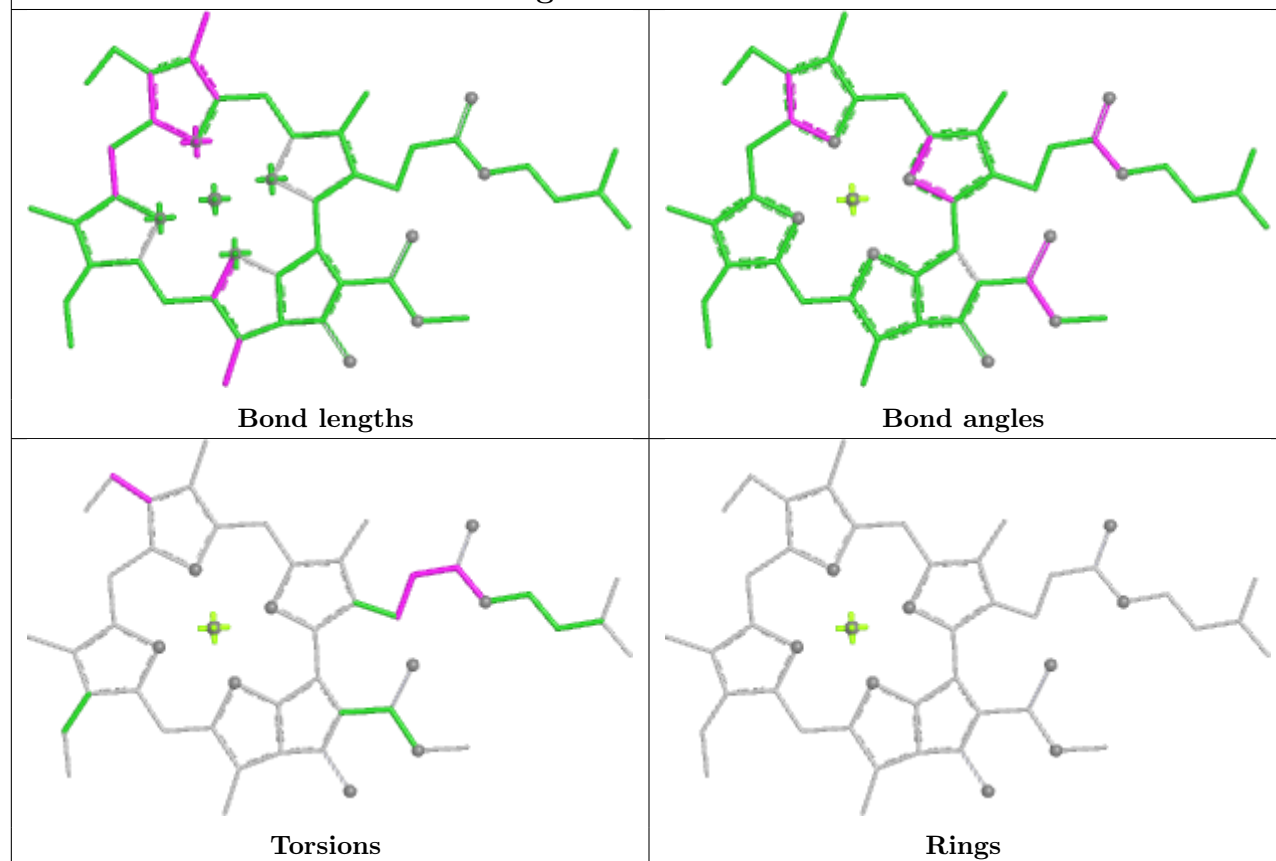


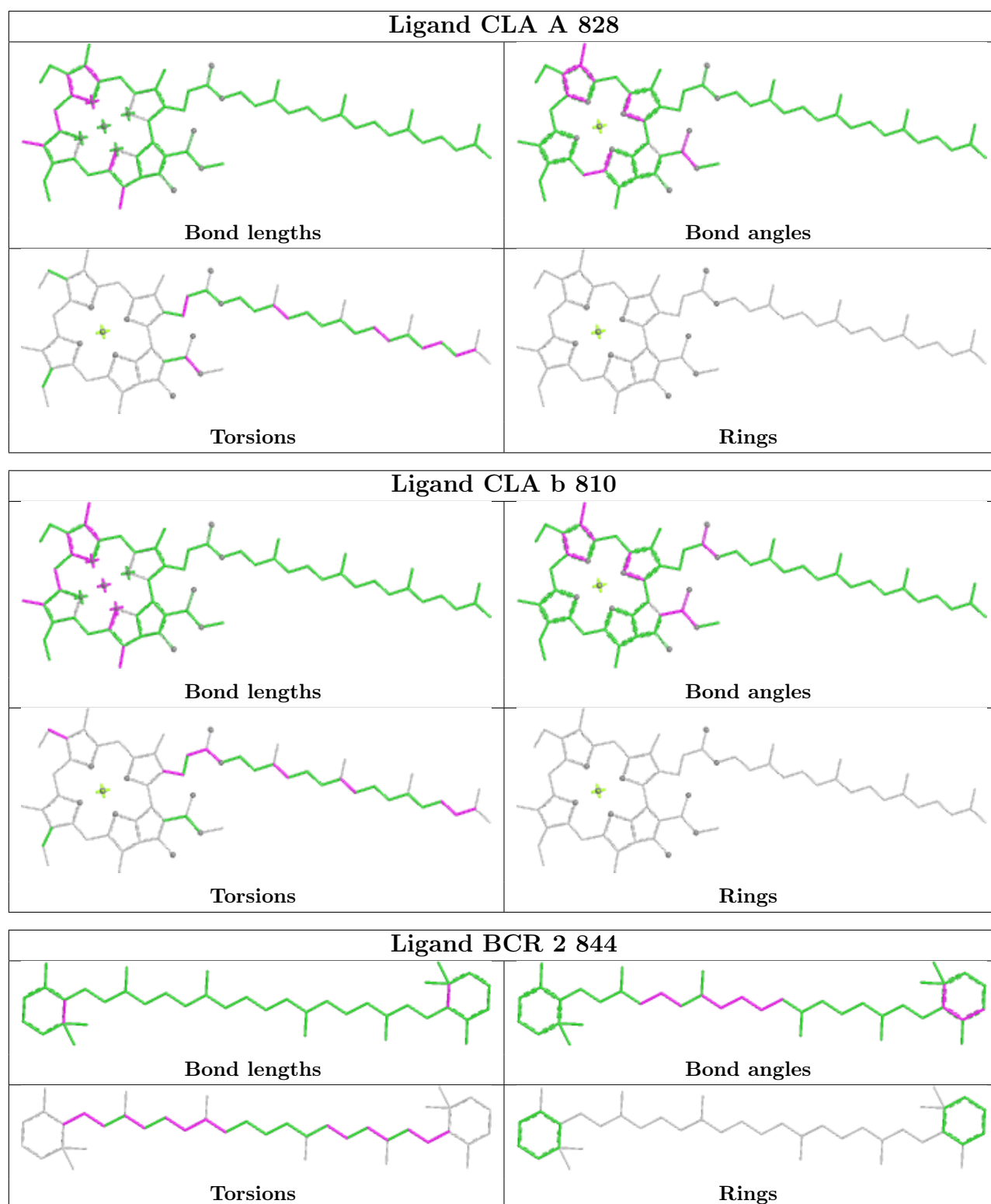
Ligand CLA a 828	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR f 205	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA b 803	
 Bond lengths	 Bond angles
 Torsions	 Rings

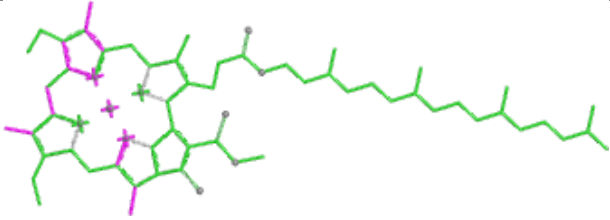
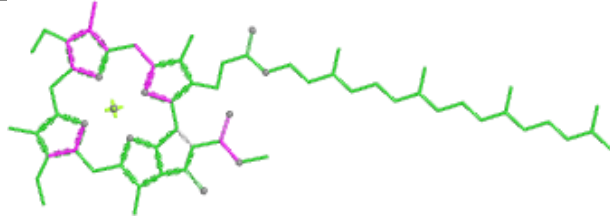
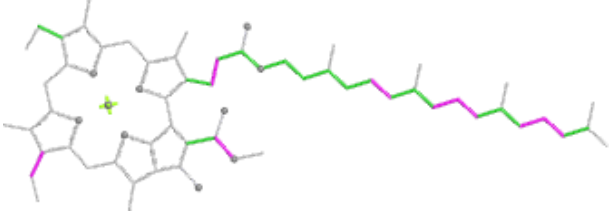
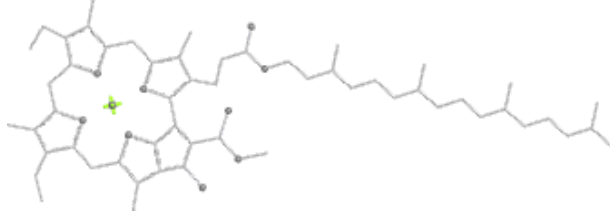
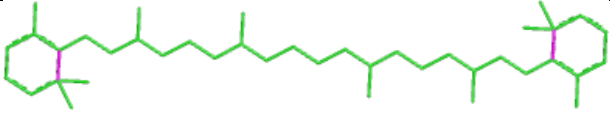
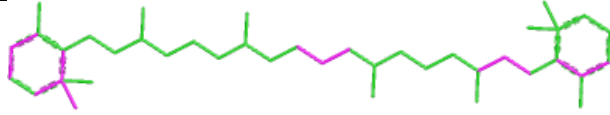
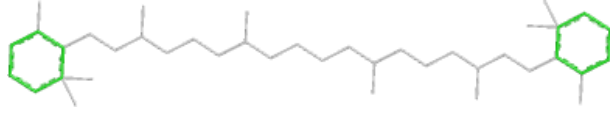
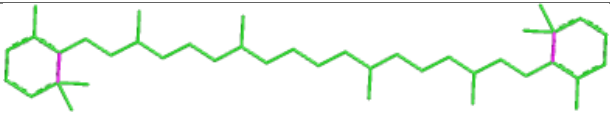
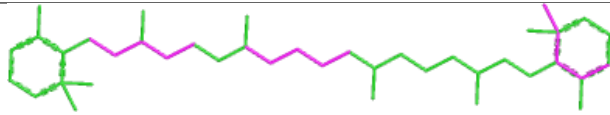
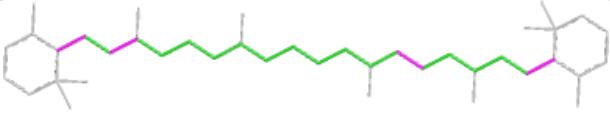
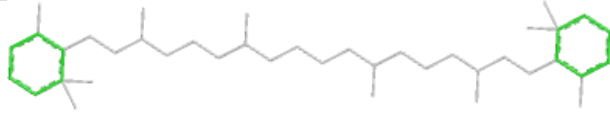
Ligand CLA b 828



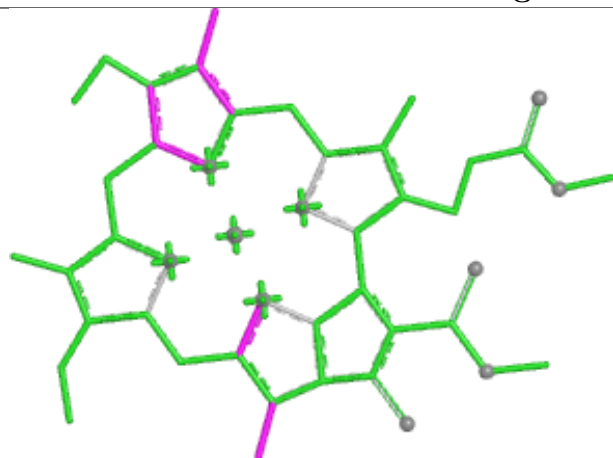
Ligand CLA 1 823



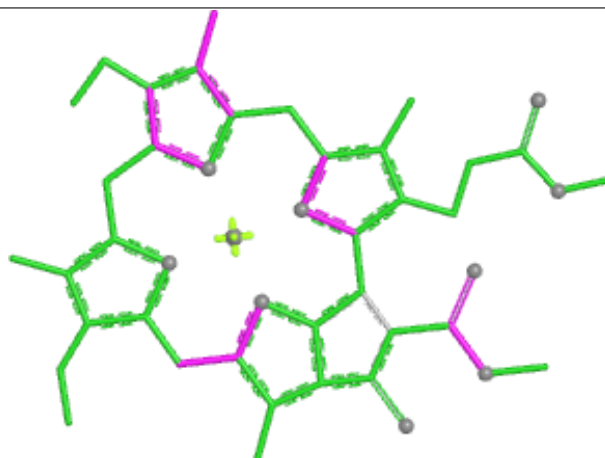


Ligand CLA B 802	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR b 842	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 0 201	
 Bond lengths	 Bond angles
 Torsions	 Rings

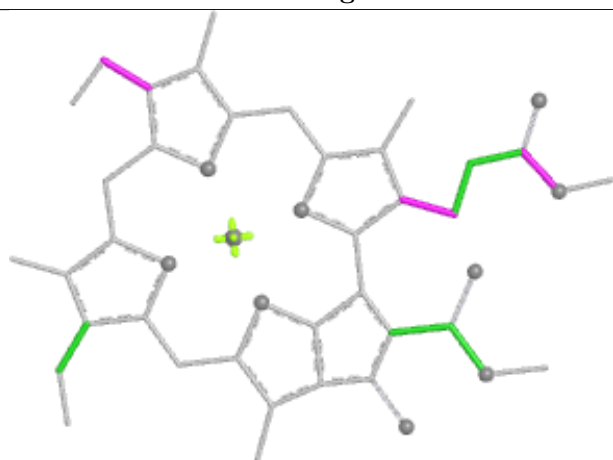
Ligand CLA A 820



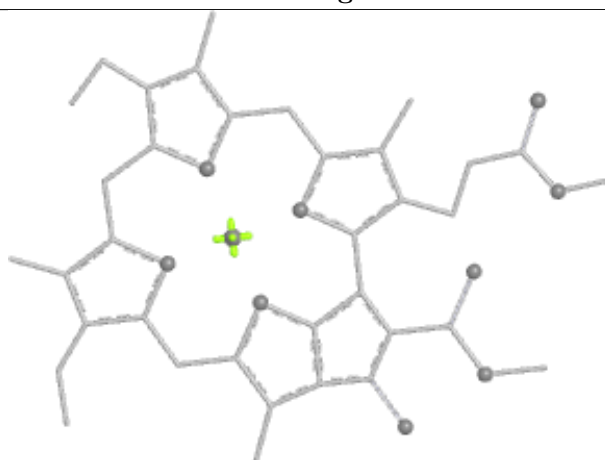
Bond lengths



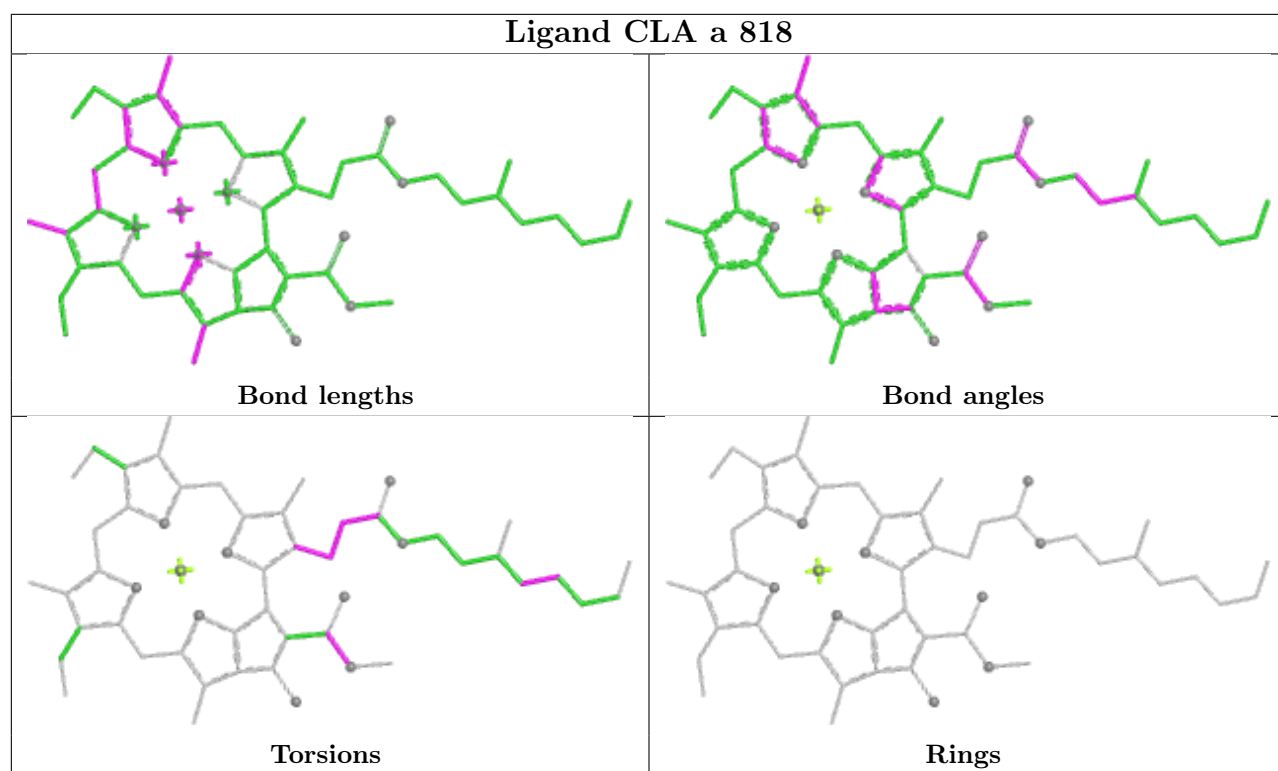
Bond angles



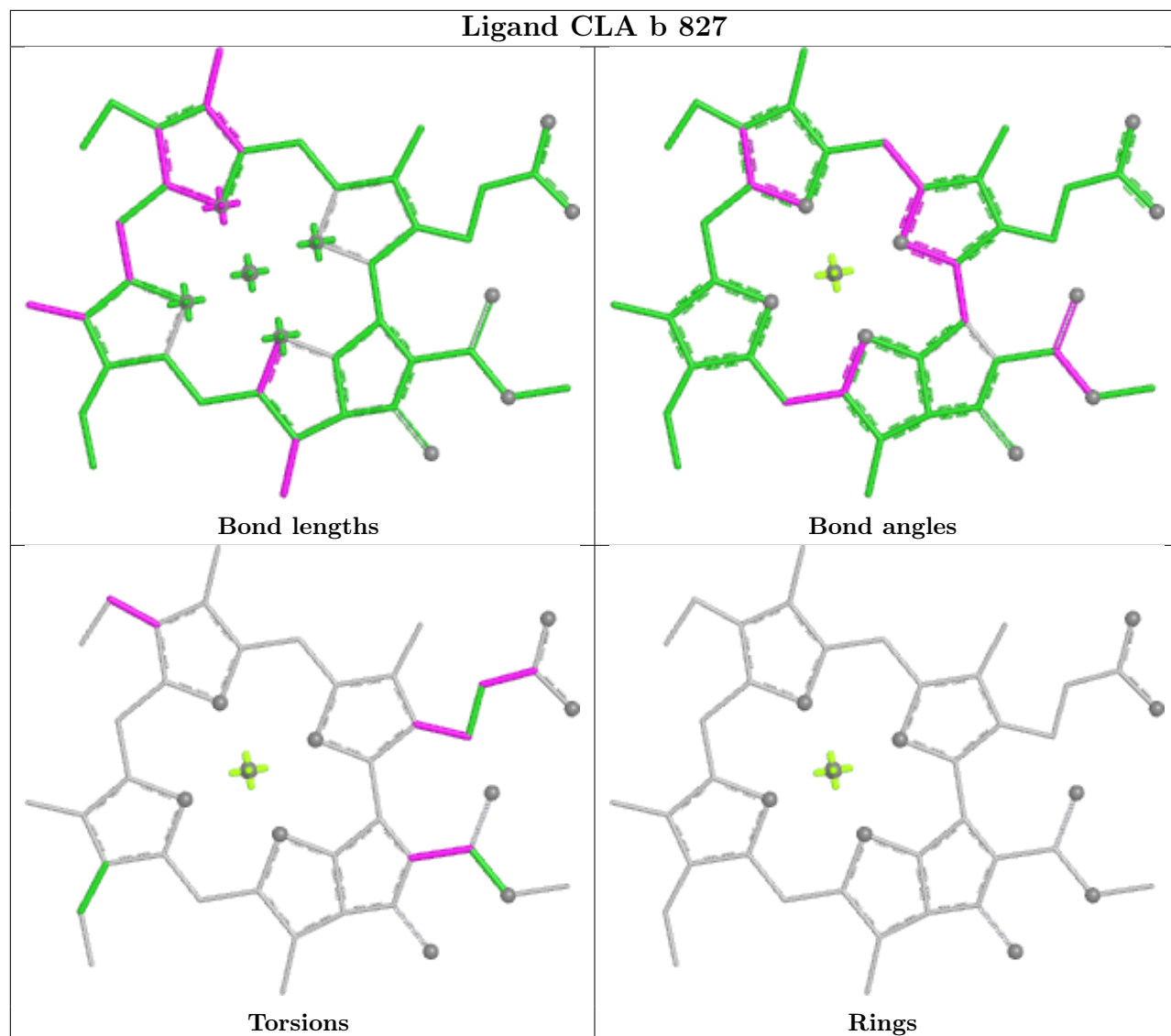
Torsions



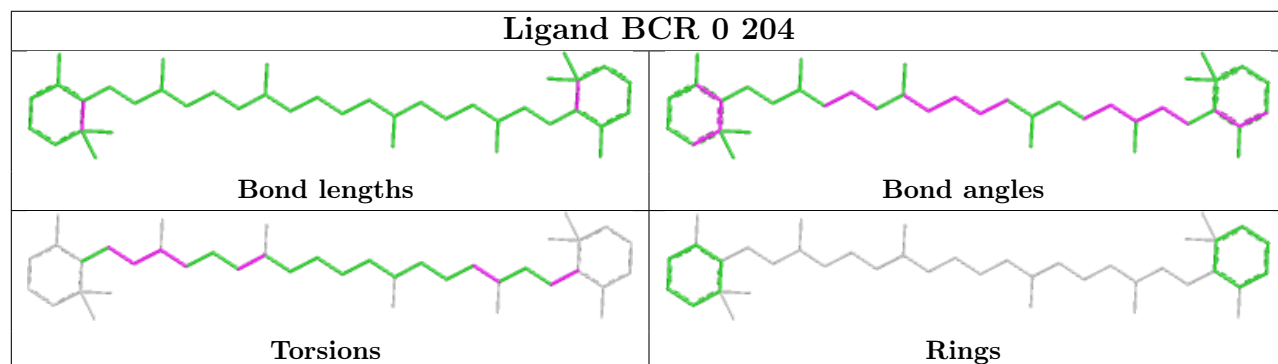
Rings

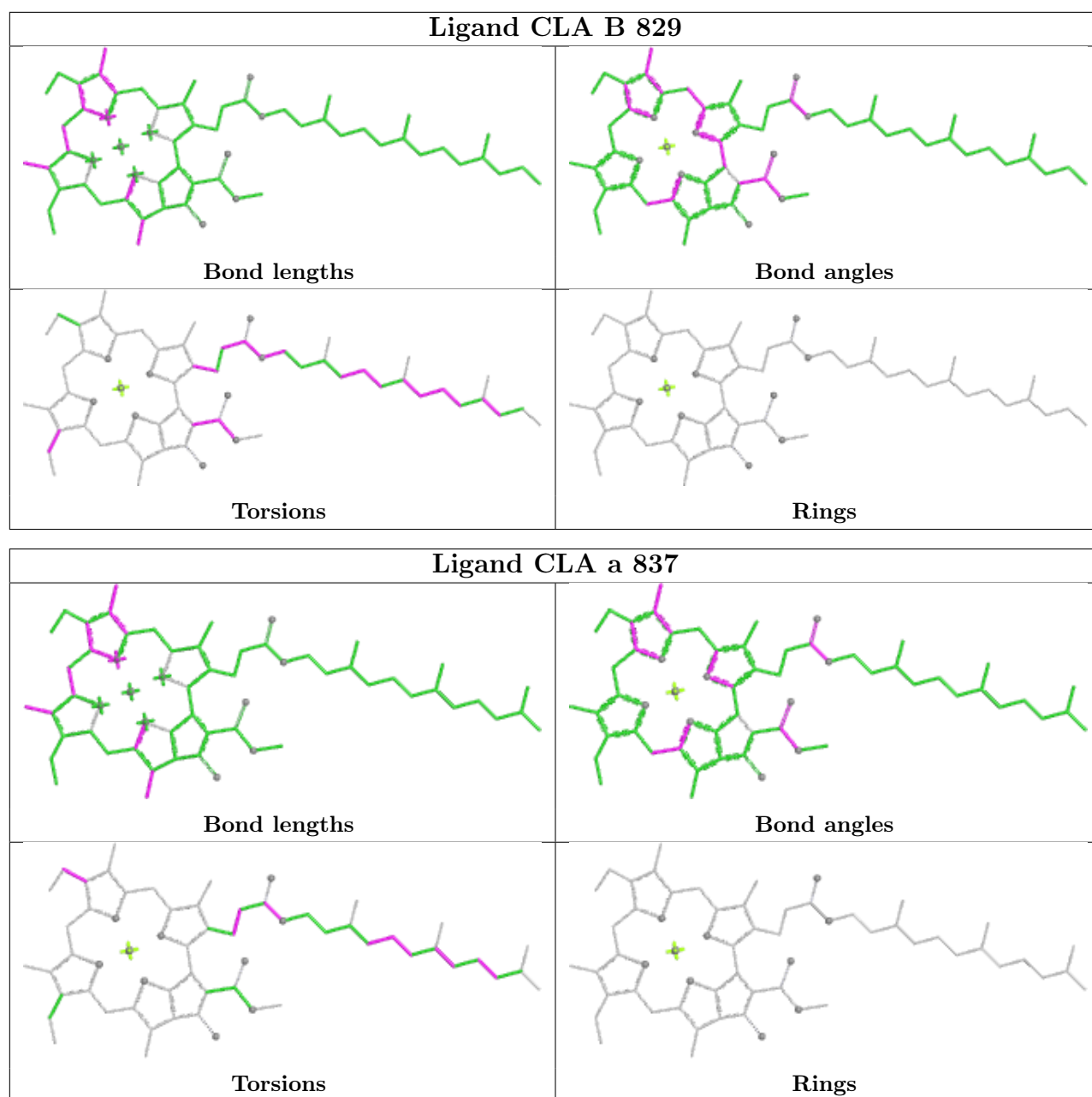


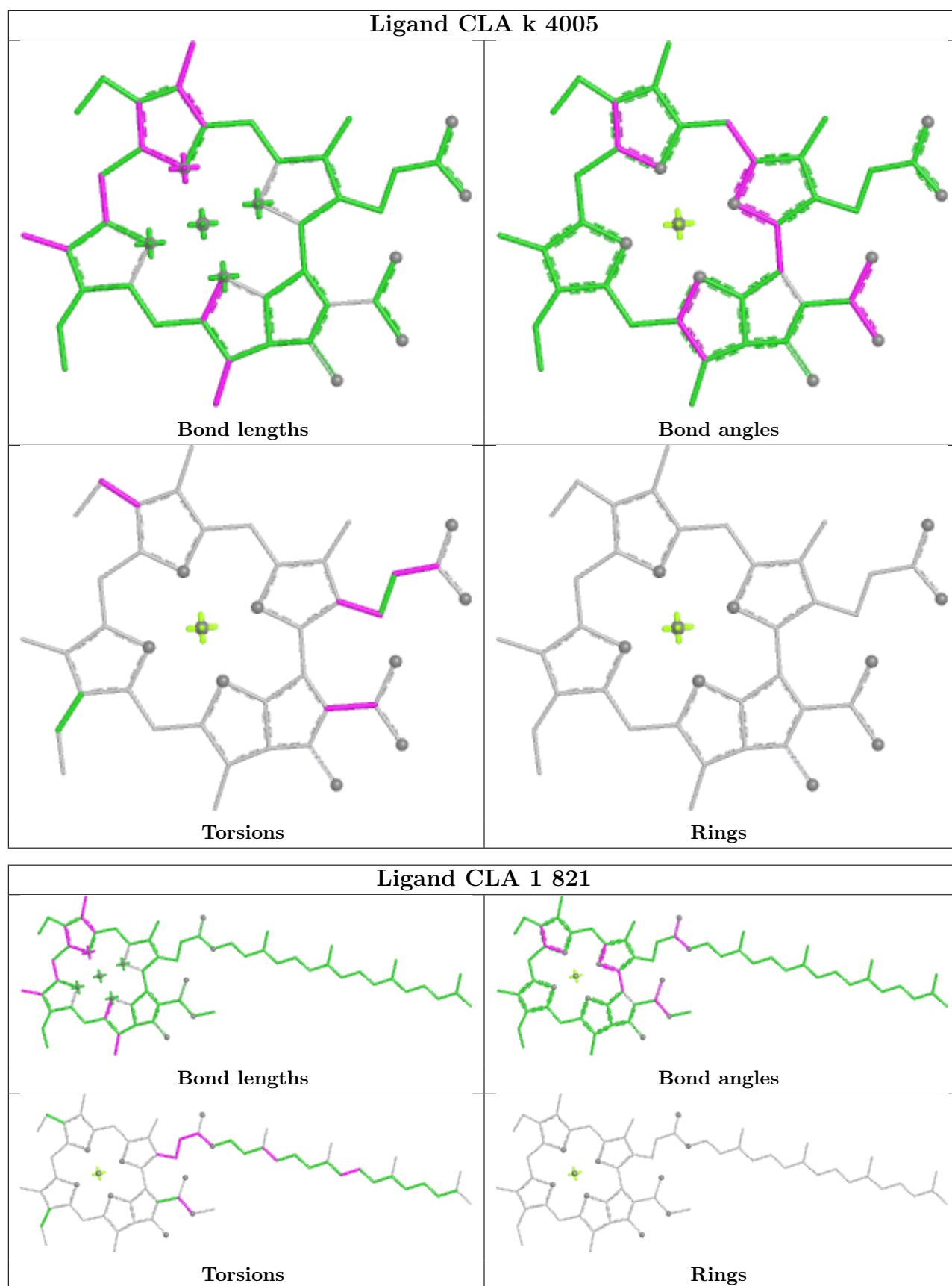
Ligand CLA b 827



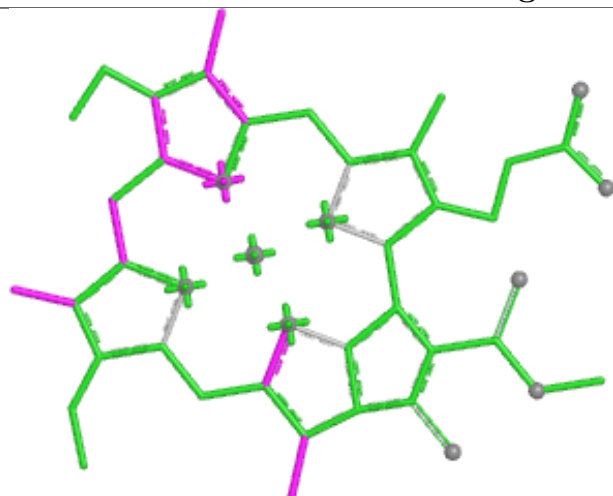
Ligand BCR 0 204



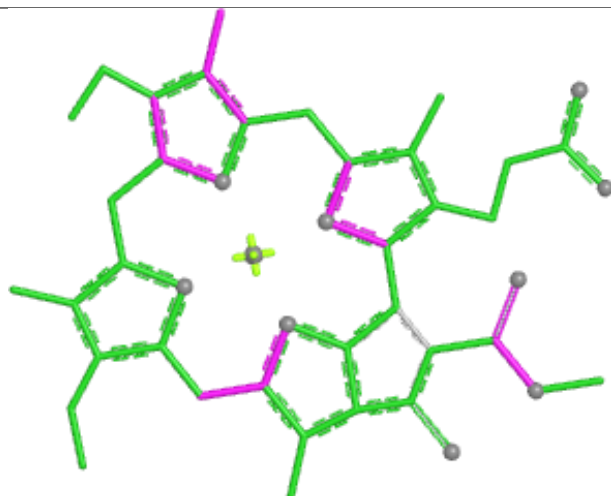




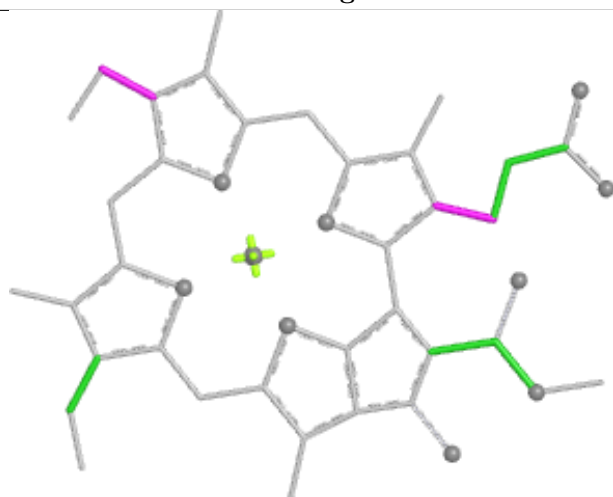
Ligand CLA 1 815



Bond lengths



Bond angles

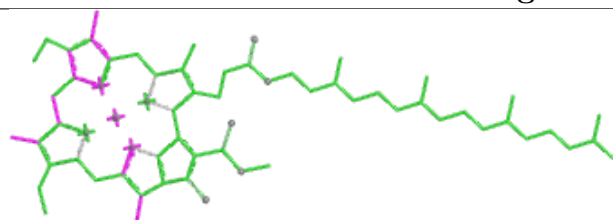


Torsions

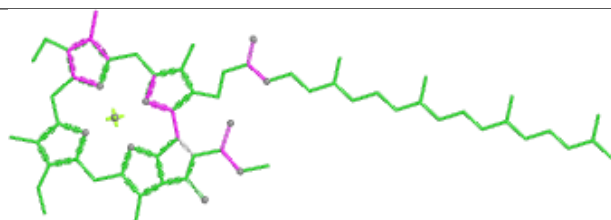


Rings

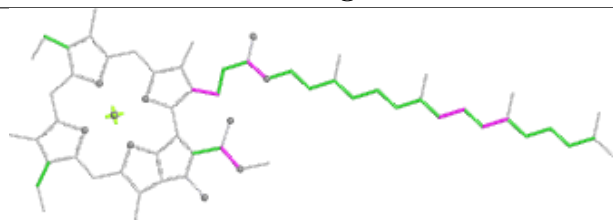
Ligand CLA b 825



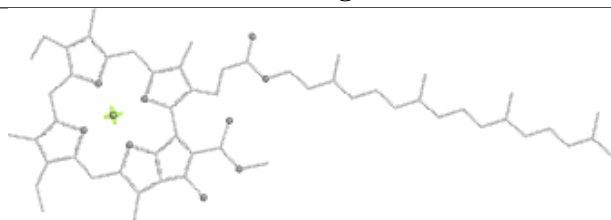
Bond lengths



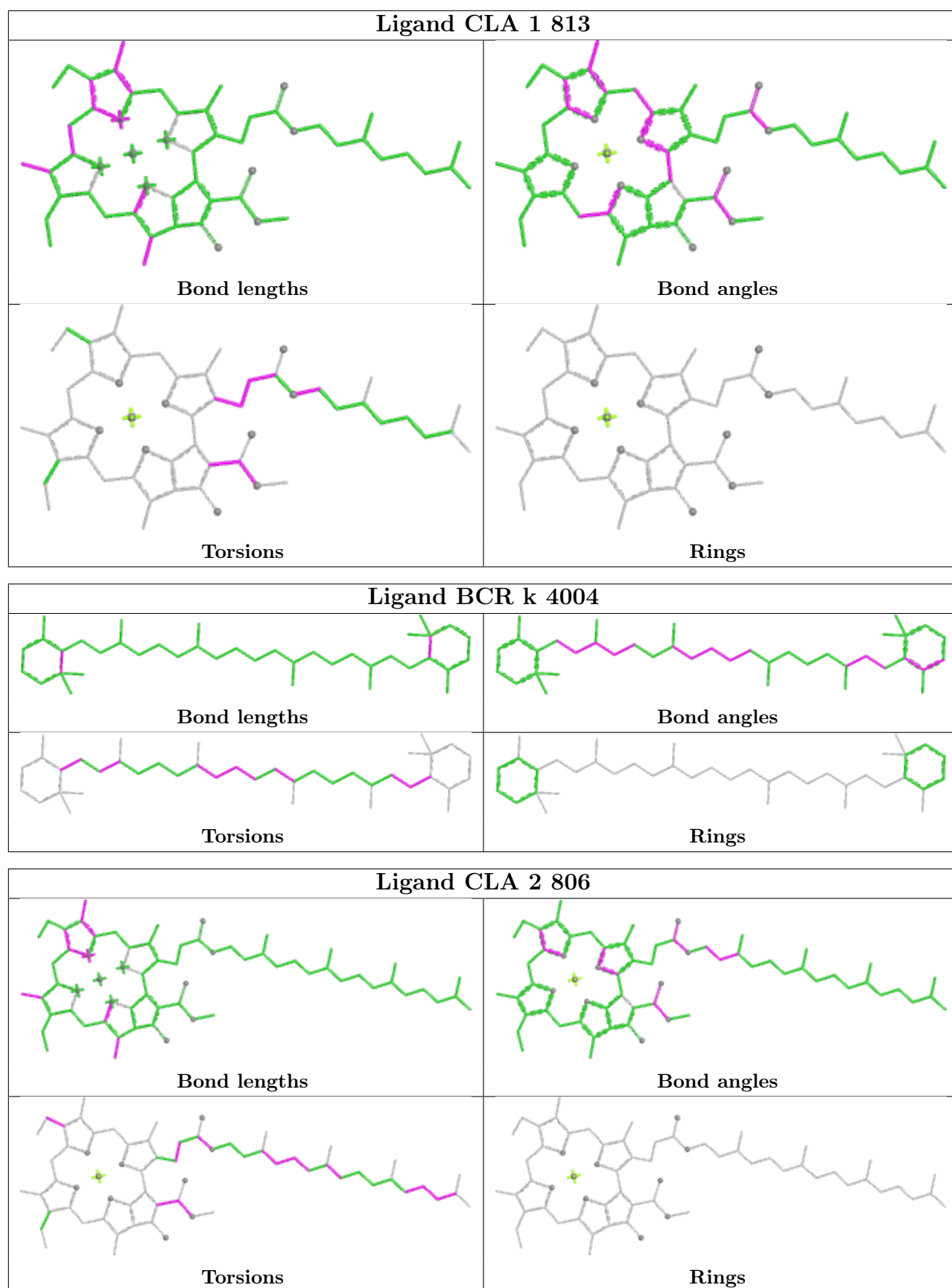
Bond angles

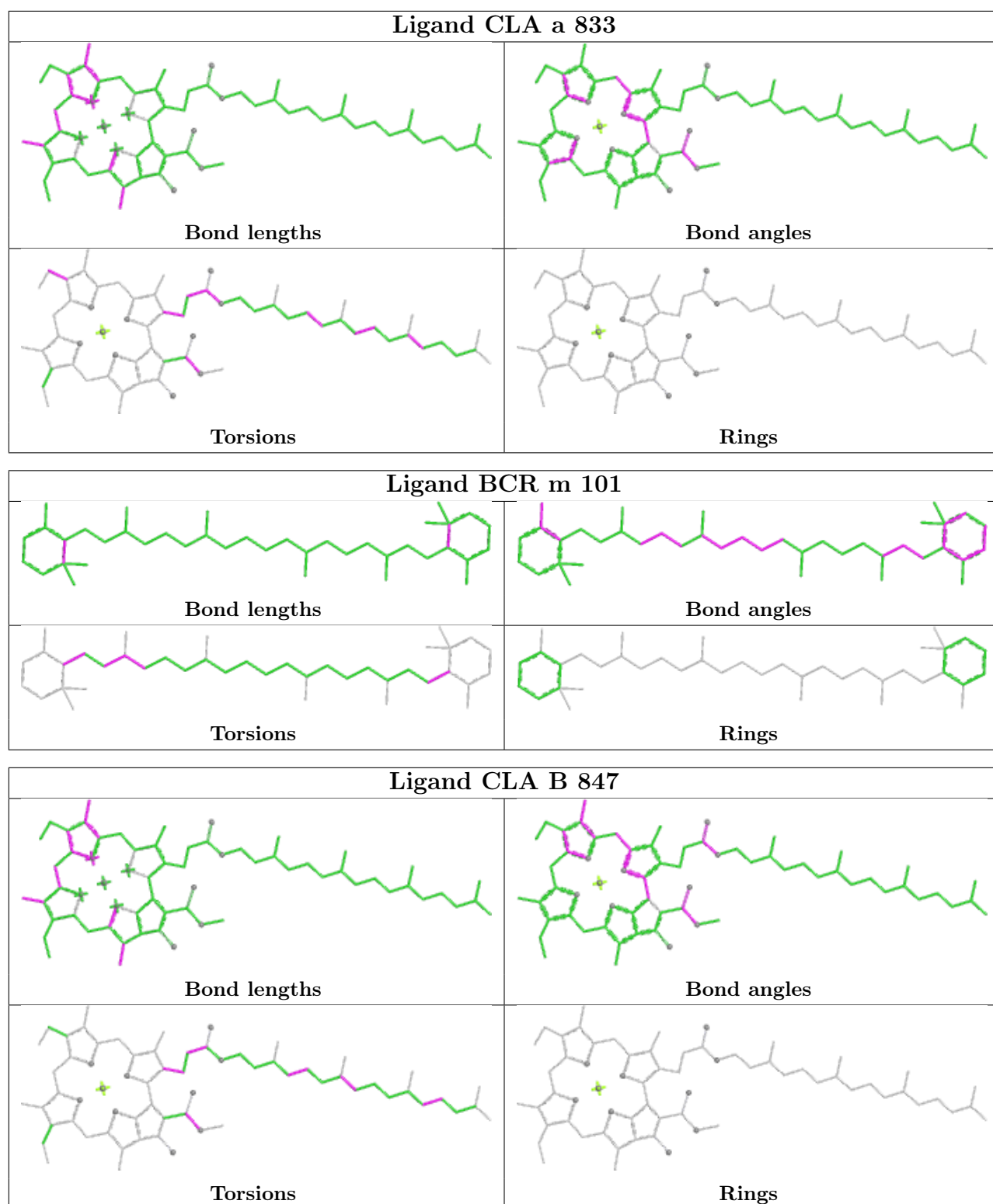


Torsions

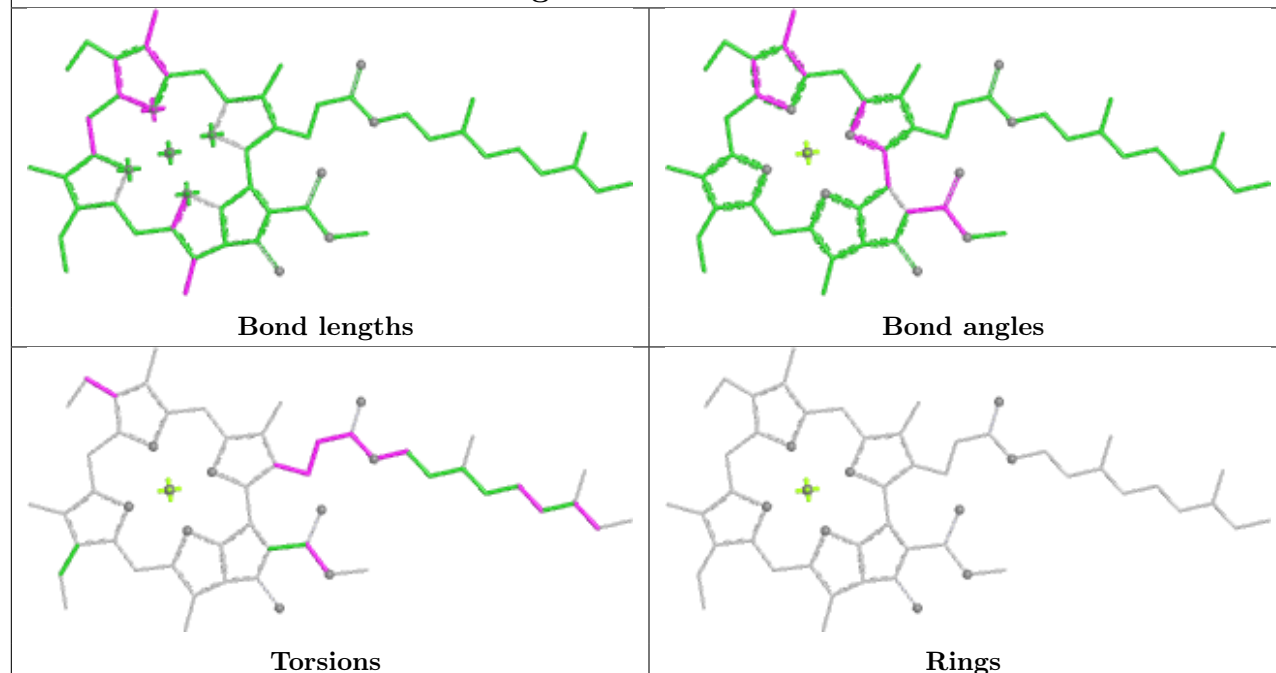


Rings

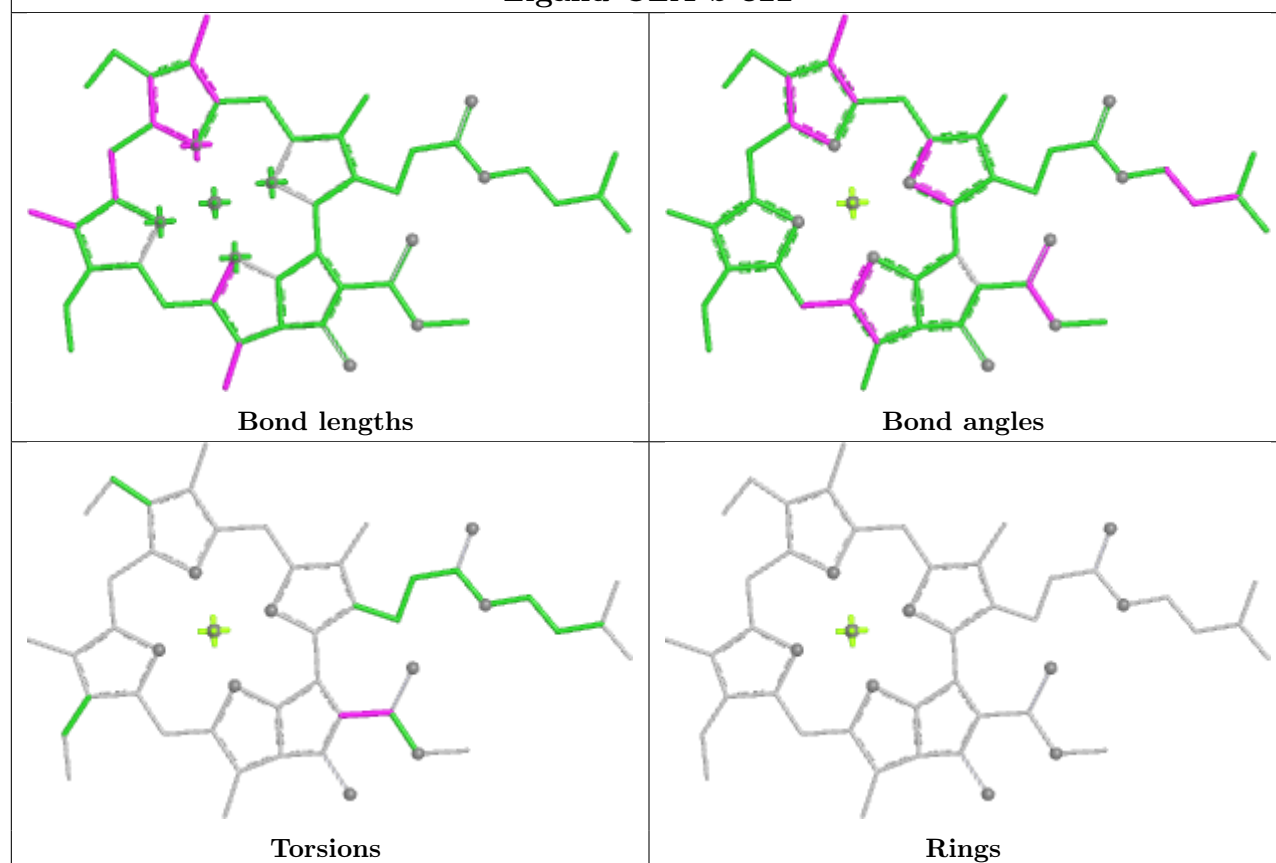




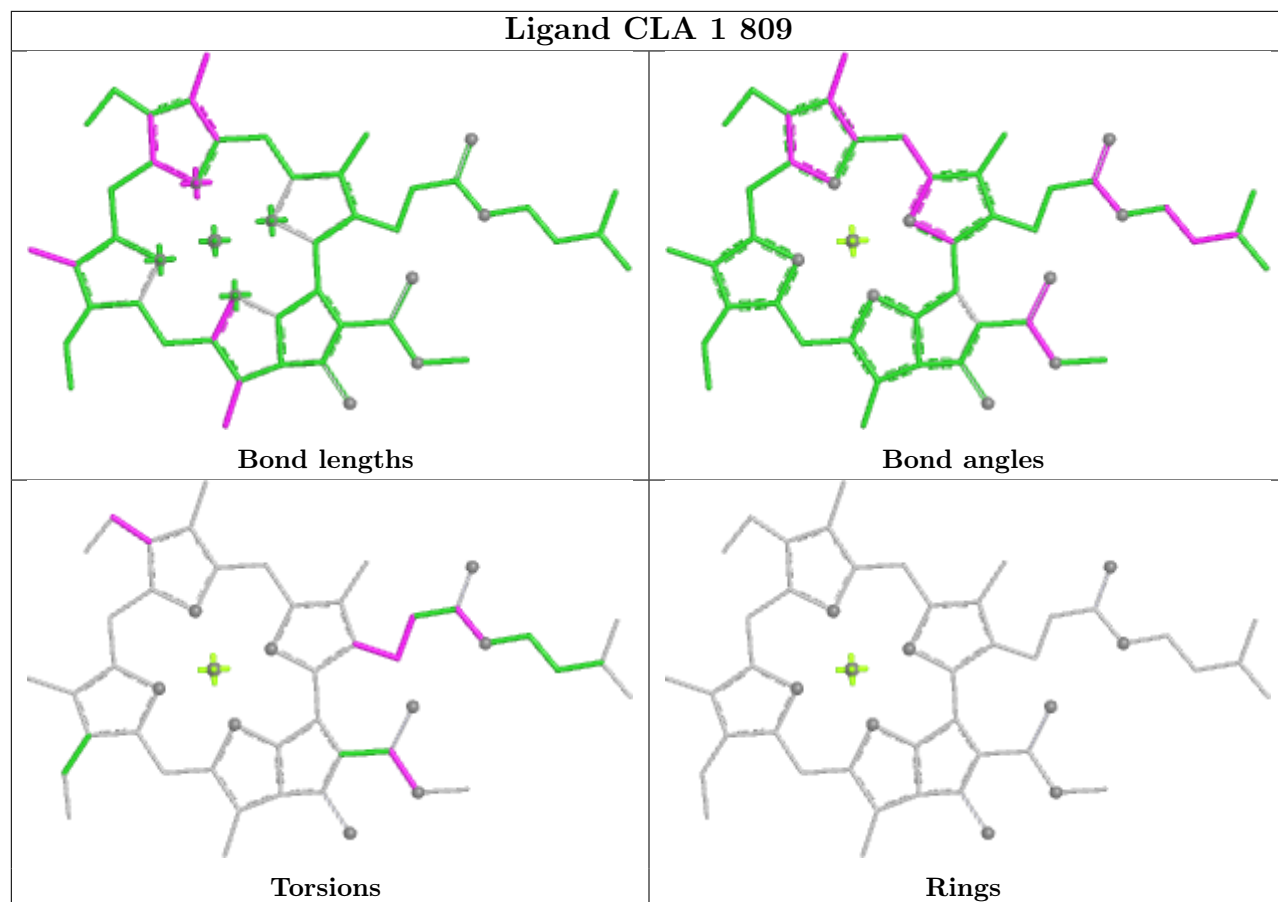
Ligand CLA A 835



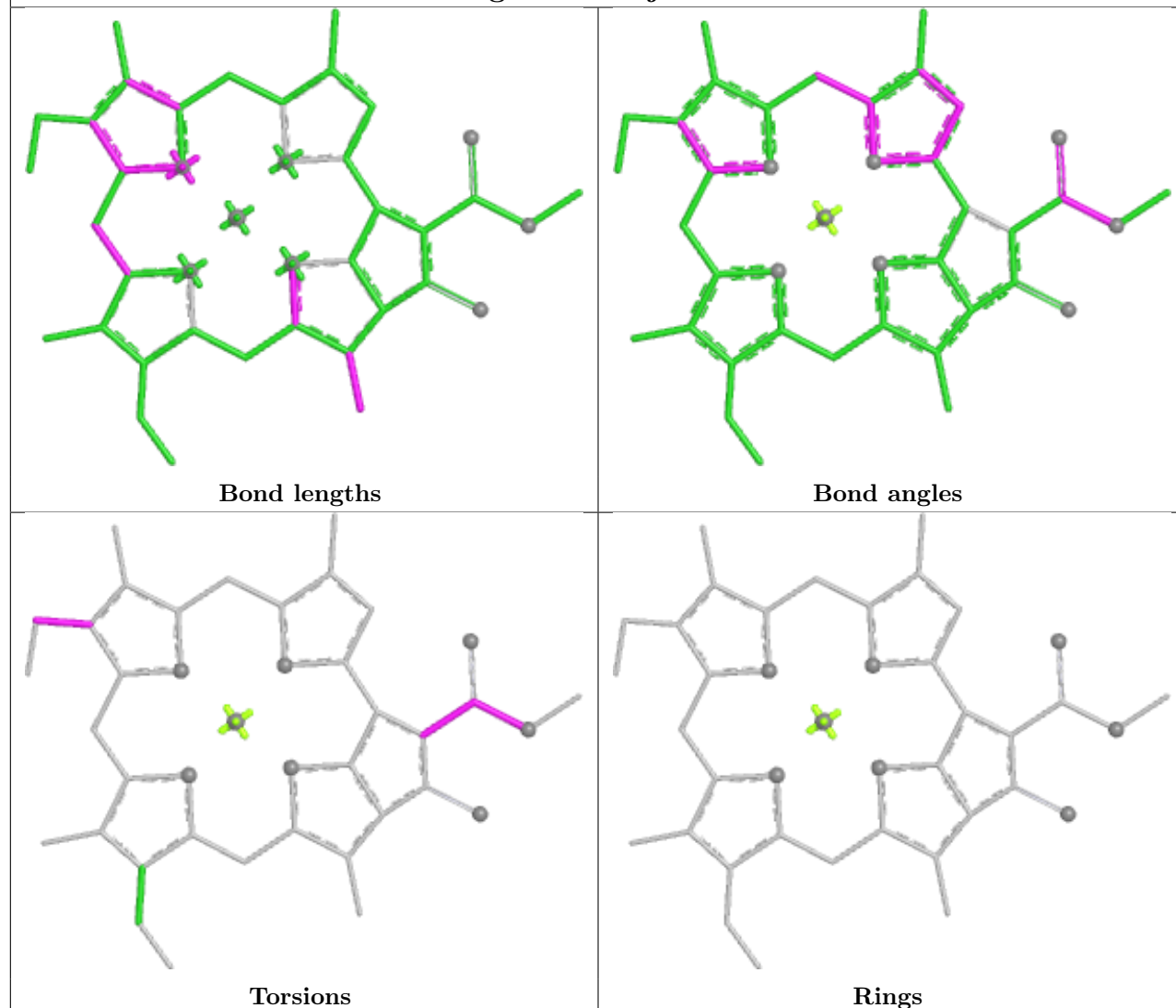
Ligand CLA b 822



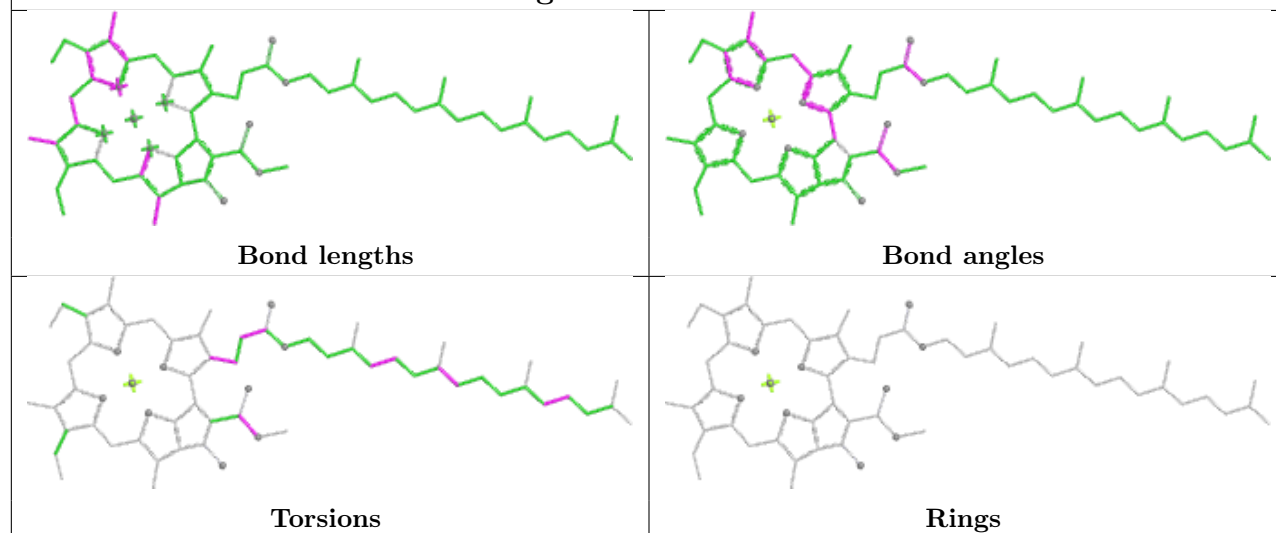
Ligand CLA 1 809



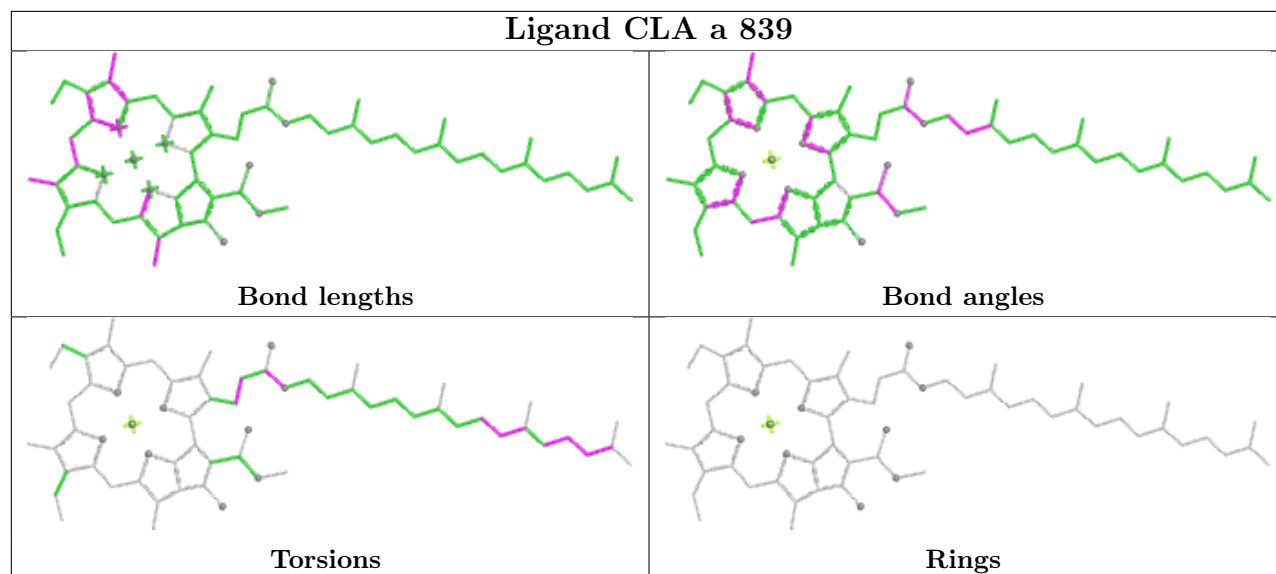
Ligand CLA j 1102



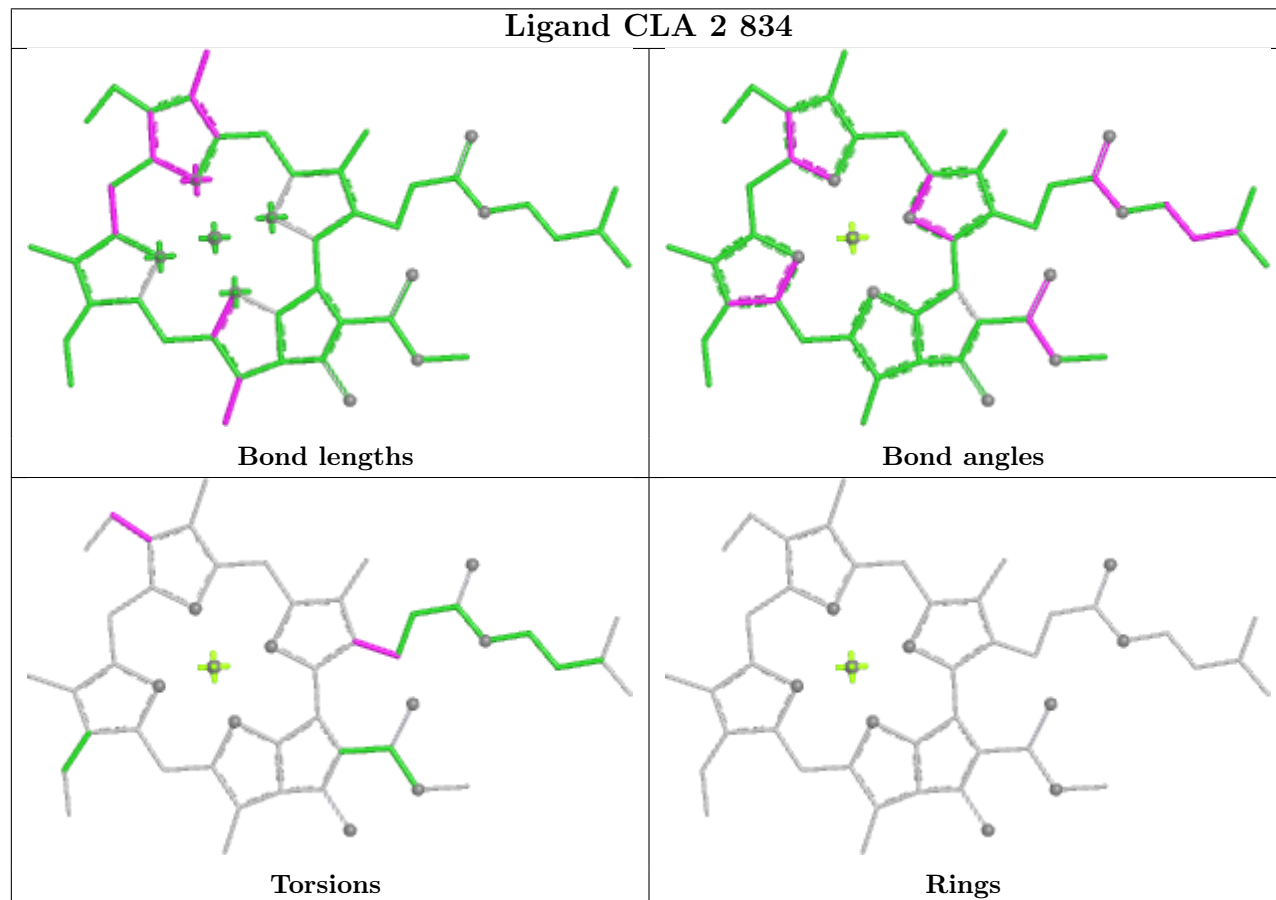
Ligand CLA 2 846

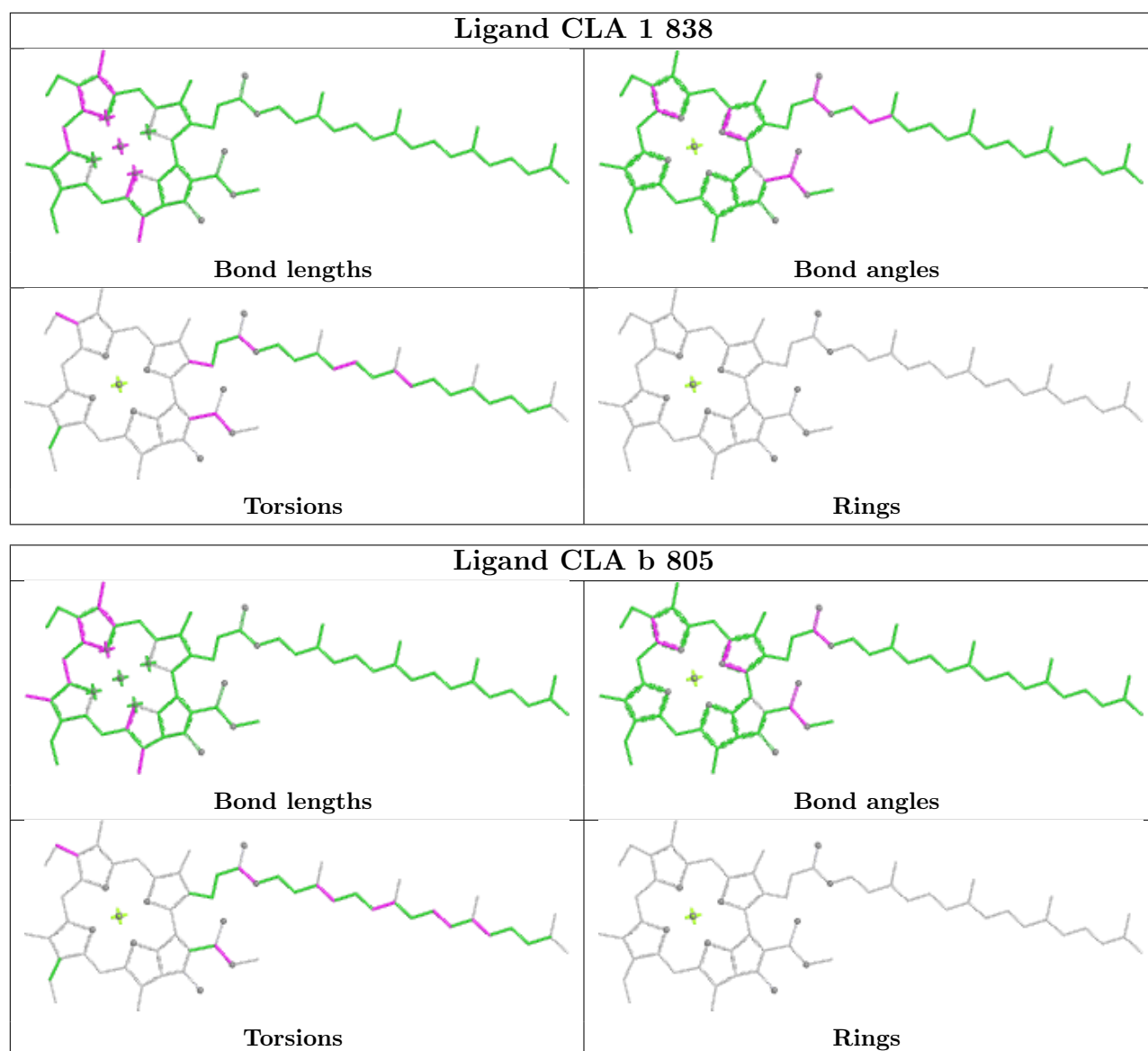


Ligand CLA a 839



Ligand CLA 2 834





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.

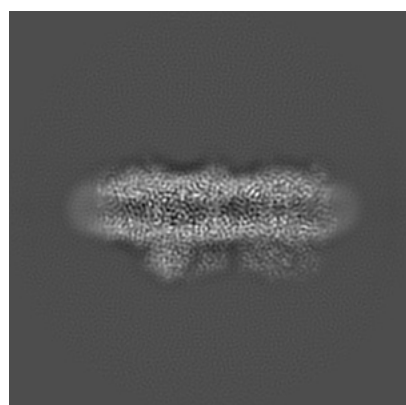
6 Map visualisation [i](#)

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.

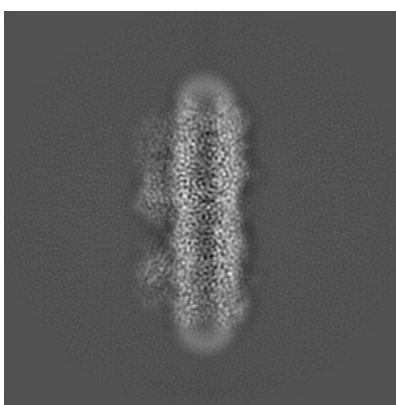
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

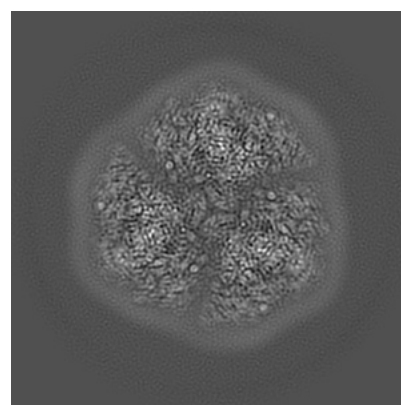
6.1.1 Primary map



X



Y

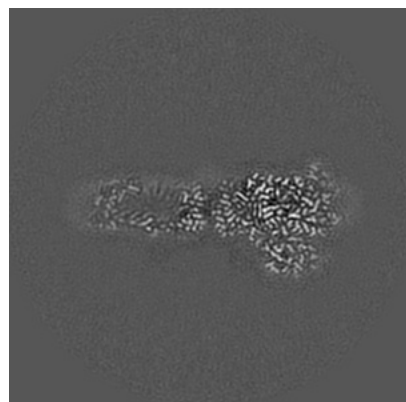


Z

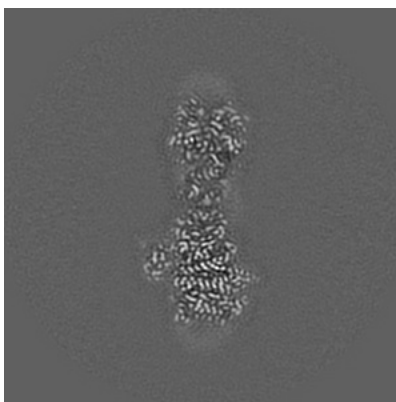
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

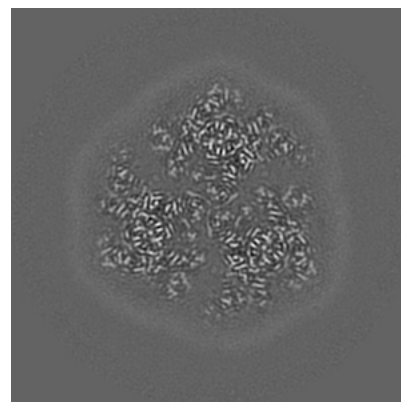
6.2.1 Primary map



X Index: 150



Y Index: 150

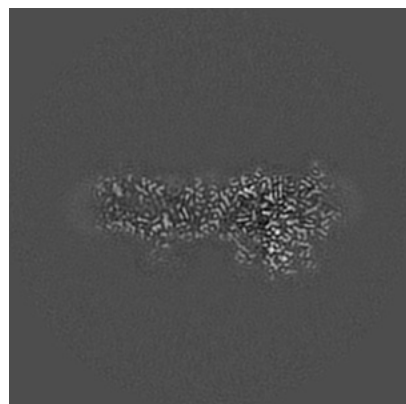


Z Index: 150

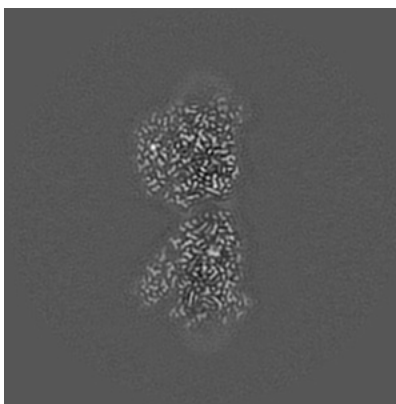
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

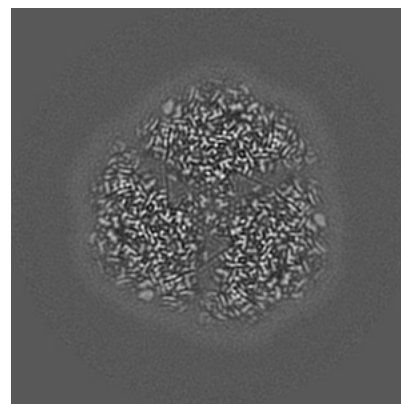
6.3.1 Primary map



X Index: 158



Y Index: 116

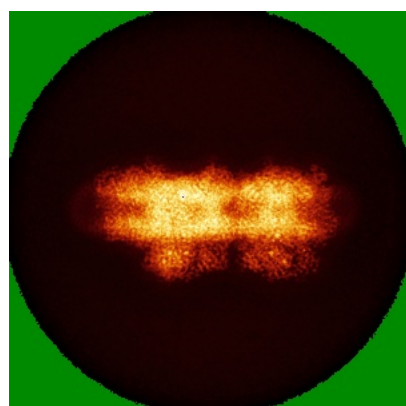


Z Index: 161

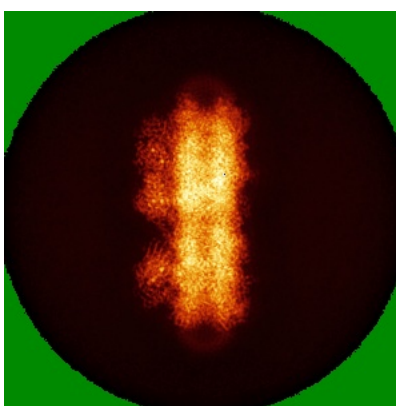
The images above show the largest variance slices of the map in three orthogonal directions.

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

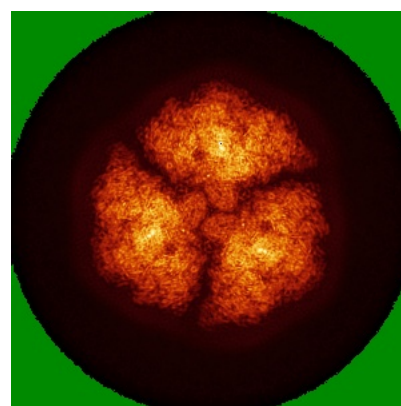
6.4.1 Primary map



X



Y

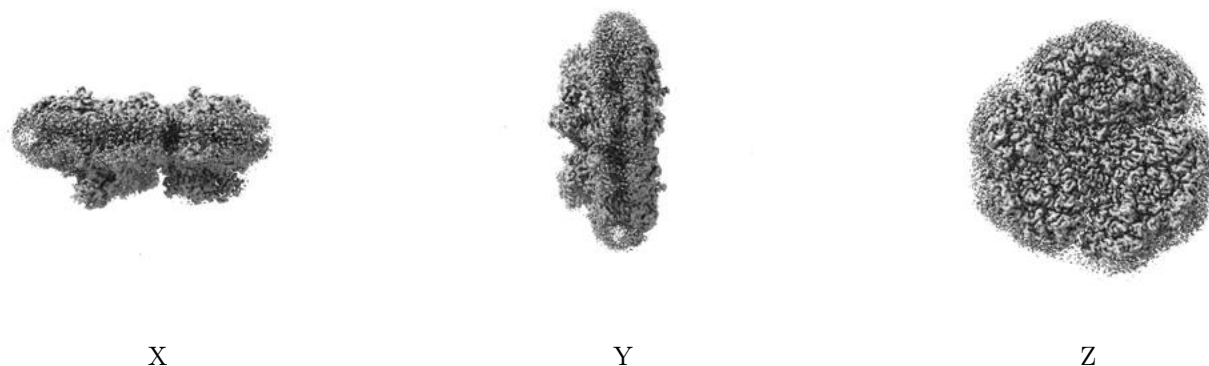


Z

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.

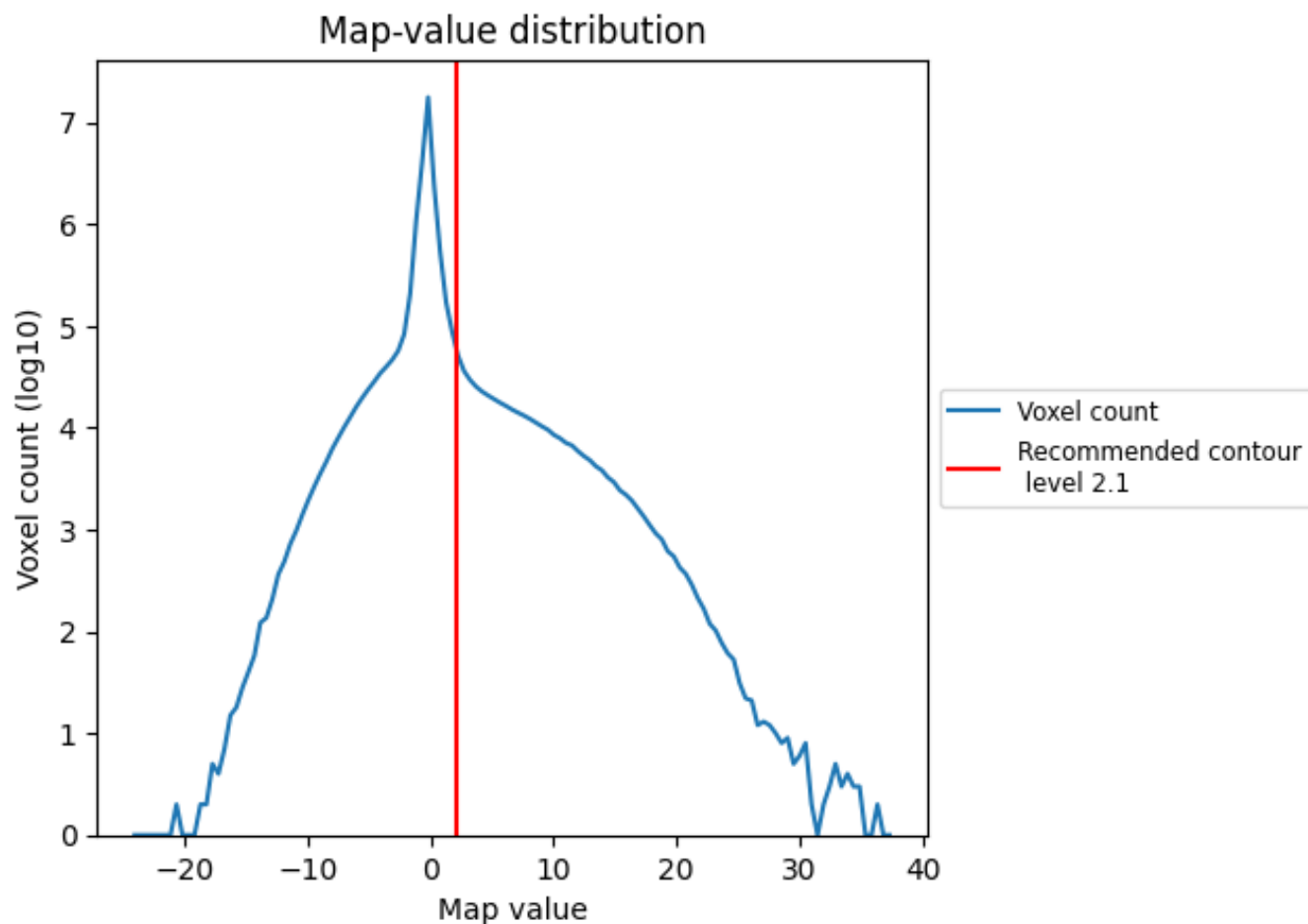
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

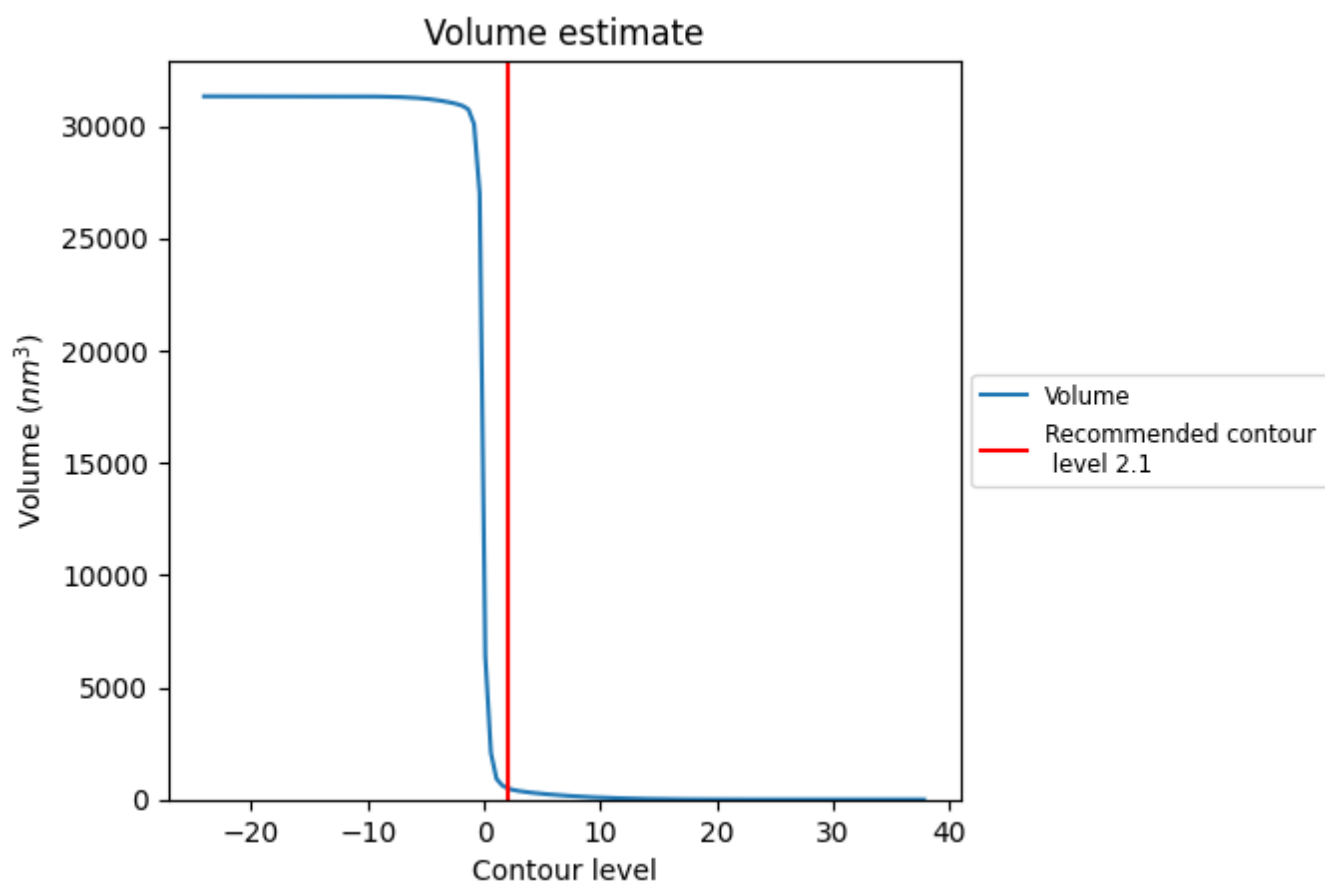
This section contains the results of statistical analysis of the map.

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.

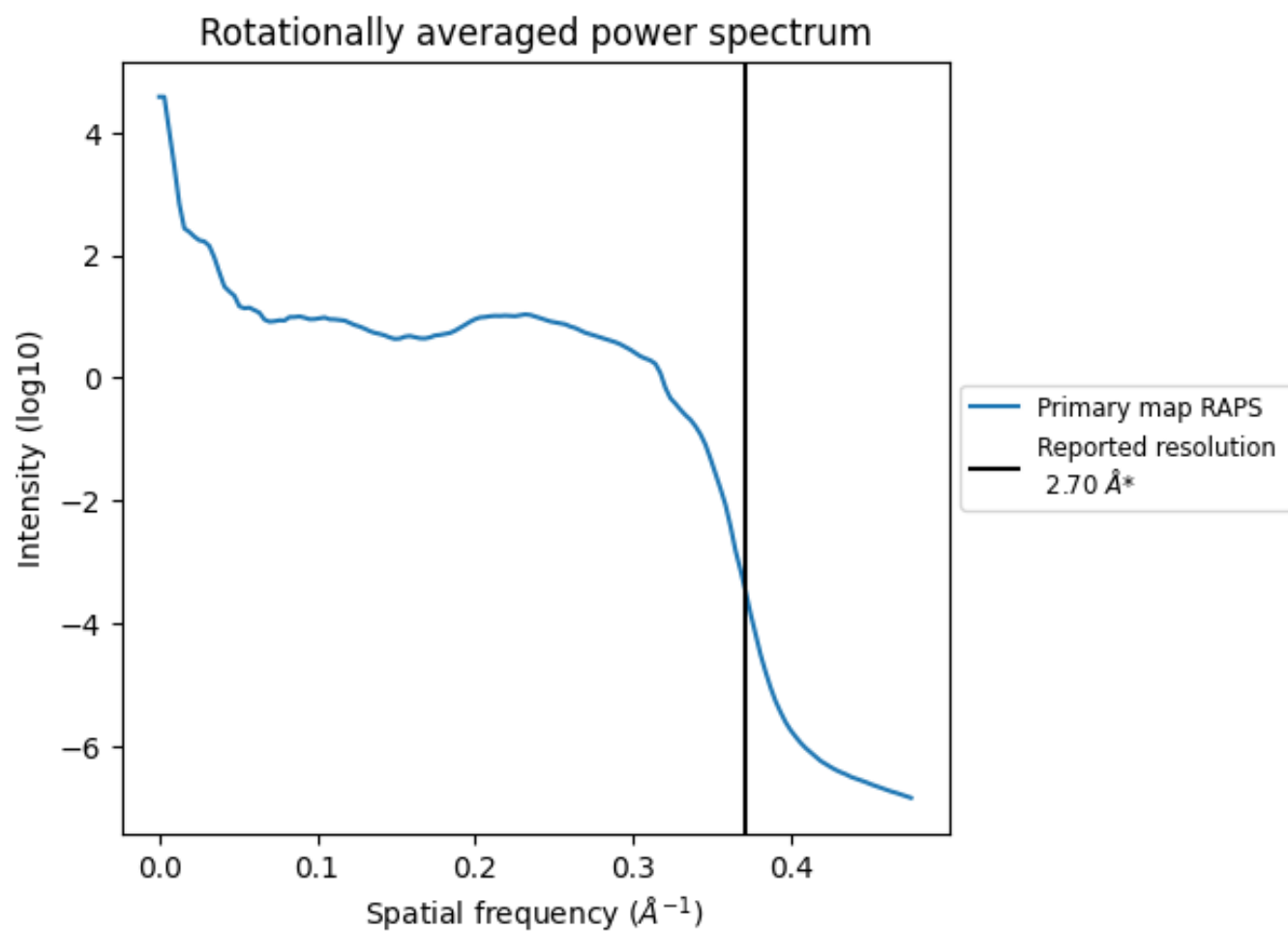
7.2 Volume estimate [i](#)



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 ⓘ

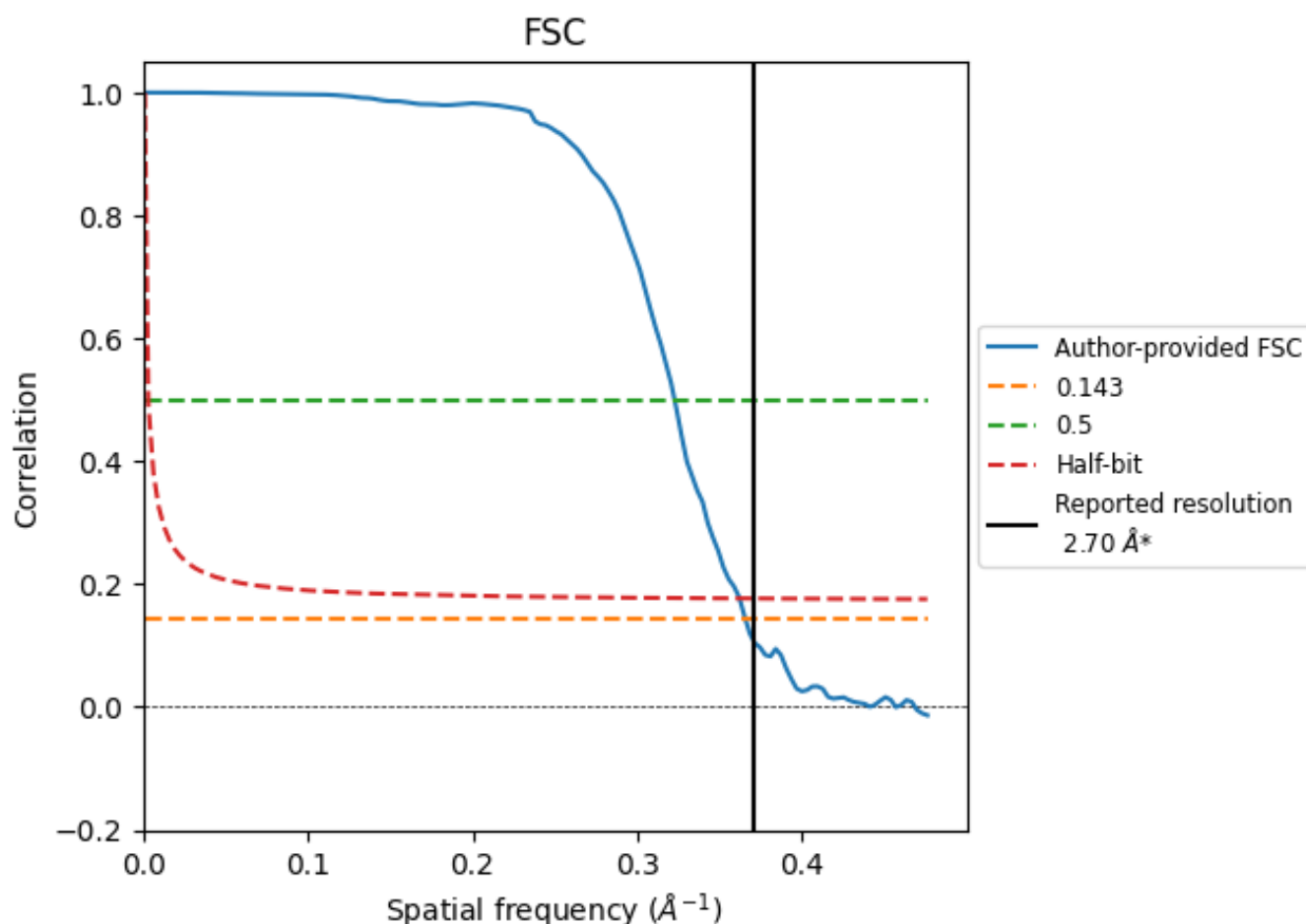


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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](#)

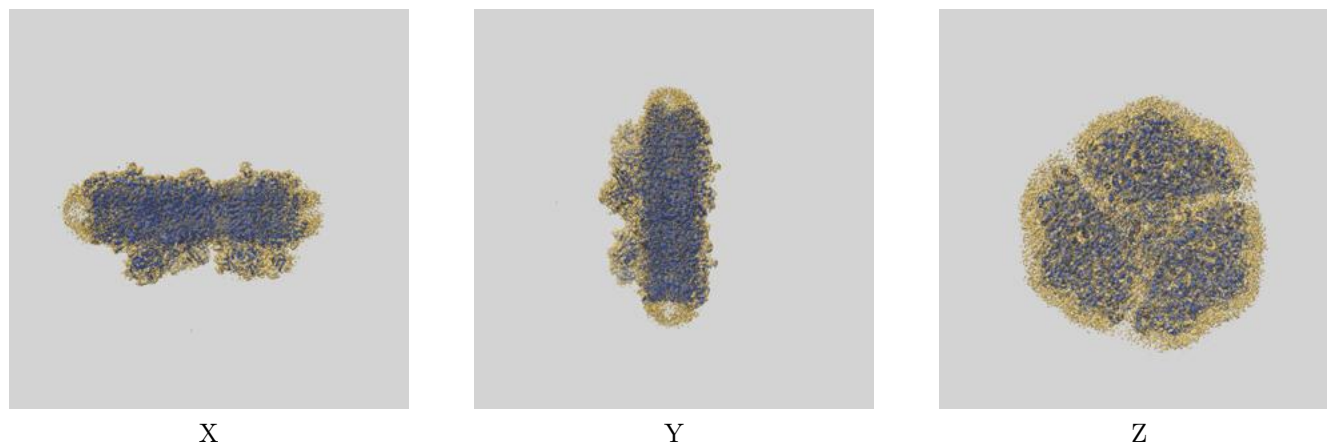
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.10	2.76
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

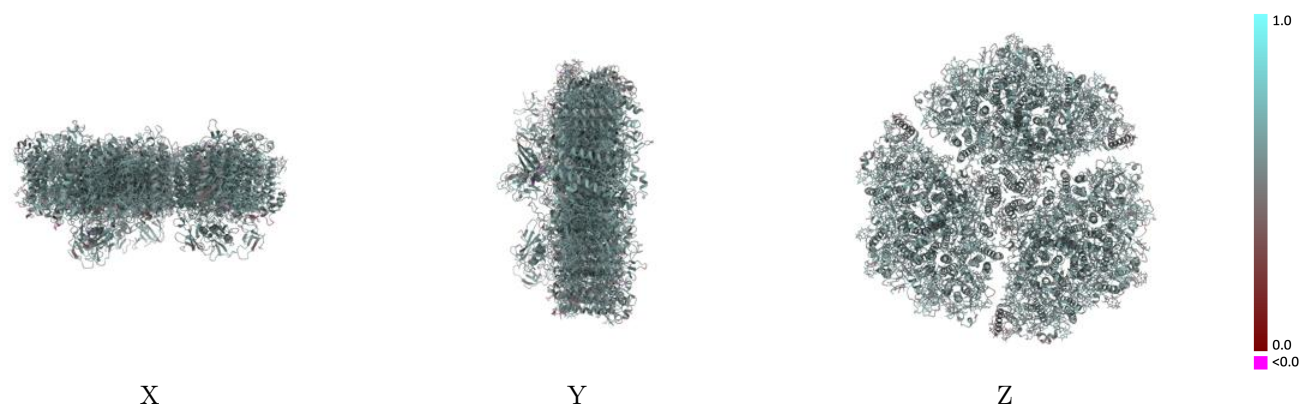
This section contains information regarding the fit between EMDB map EMD-21320 and PDB model 6VPV. Per-residue inclusion information can be found in section [3](#) on page [36](#).

9.1 Map-model overlay [i](#)



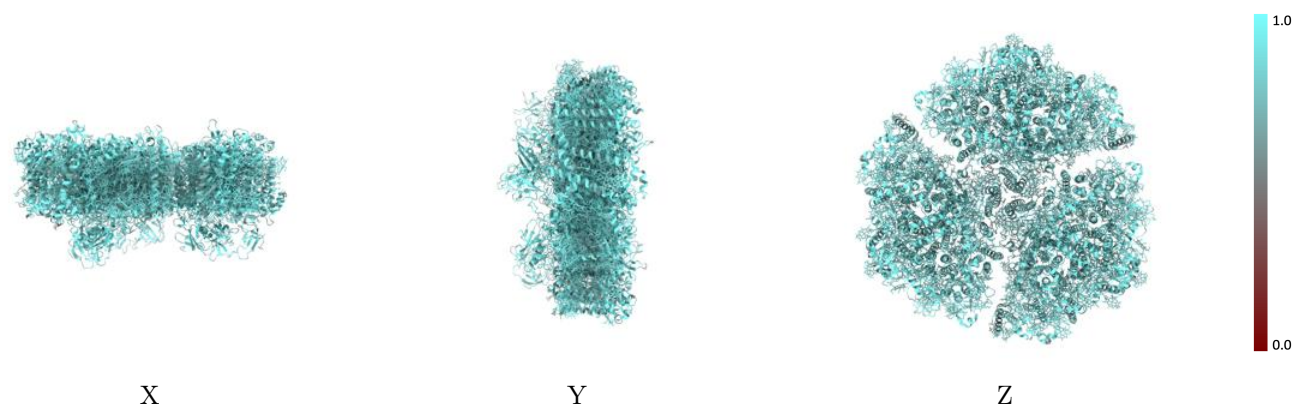
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



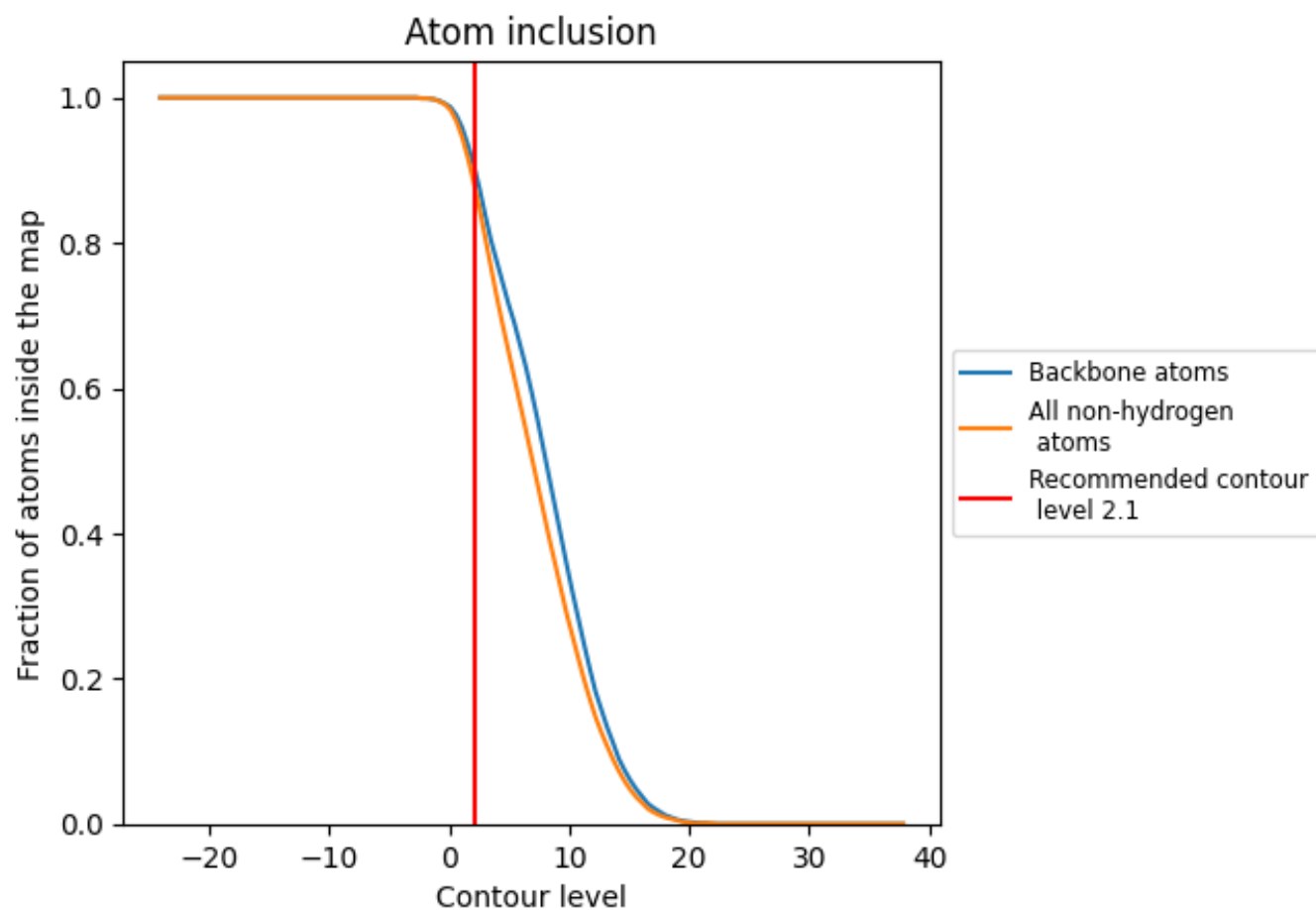
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

