



wwPDB EM Validation Summary Report ⓘ

Nov 10, 2024 – 10:19 AM EST

PDB ID : 6VPV
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.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

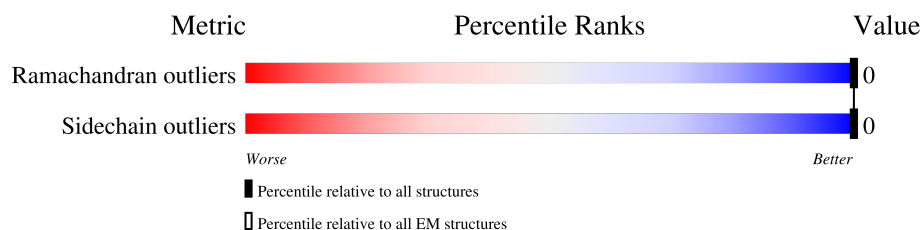
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

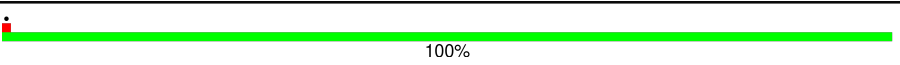
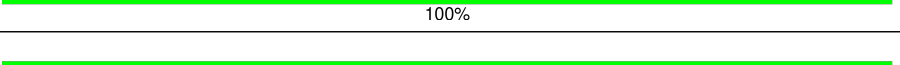
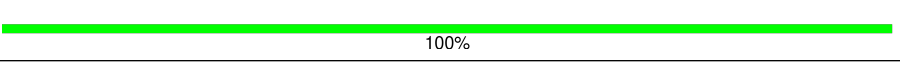
The reported resolution of this entry is 2.70 Å.

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.




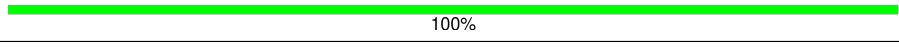
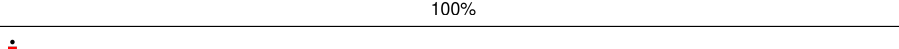
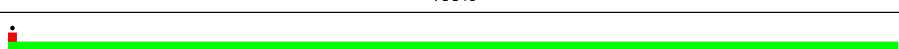

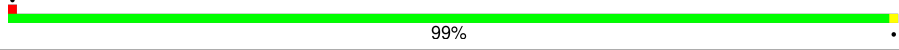
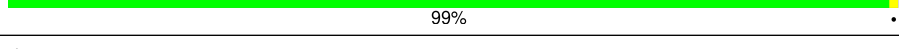
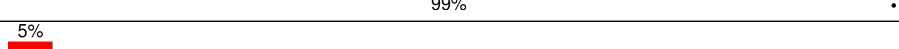
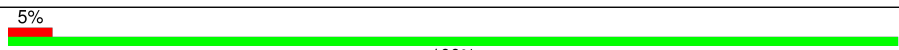

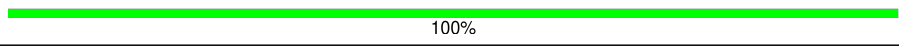
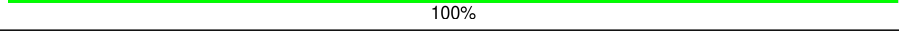
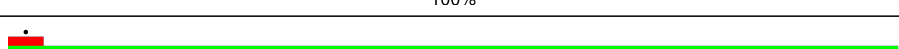


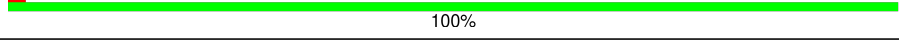
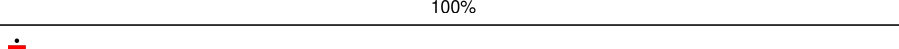


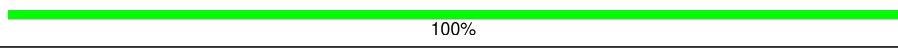




Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	1	741	 100%
1	A	741	 100%
1	a	741	 100%
2	2	737	 100%
2	B	737	 100%
2	b	737	 100%
3	3	80	 100%
3	C	80	 100%
3	c	80	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	4	139	 100%
4	D	139	 100%
4	d	139	 100%
5	5	68	 100%
5	E	68	 100%
5	e	68	 100%
6	6	141	 99%
6	F	141	 99%
6	f	141	 99%
7	7	38	 5%100%
7	I	38	 5%100%
7	i	38	 5%100%
8	8	39	 100%
8	J	39	 100%
8	j	39	 100%
9	9	78	 100%
9	K	78	 100%
9	k	78	 100%
10	0	160	 100%
10	L	160	 100%
10	l	160	 99%
11	M	30	 100%
11	m	30	 100%
11	z	30	 100%

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 crite-

ria:

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	-	-	-
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	-	-	-

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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		

Continued on next page...

Continued from previous page...

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		

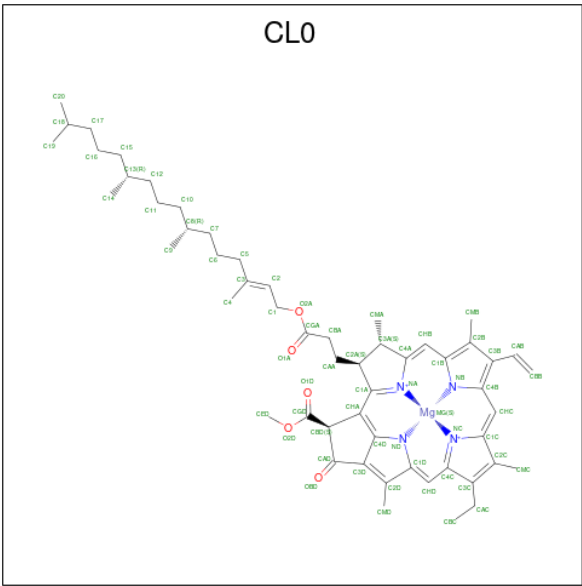
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

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.

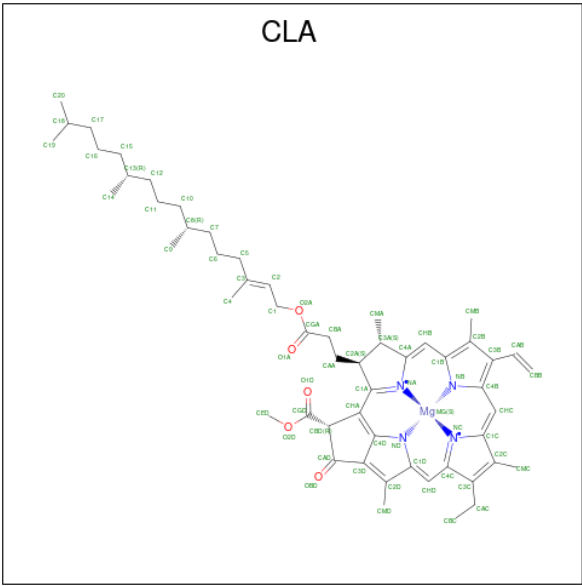
Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	30	Total	C	N	O		0	0
			232	156	35	41			
11	m	30	Total	C	N	O		0	0
			232	156	35	41			
11	z	30	Total	C	N	O		0	0
			232	156	35	41			

- Molecule 12 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



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 (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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	

Continued on next page...

Continued from previous page...

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 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			65	55	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
			51	41	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
			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
			60	50	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
			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
			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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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	

Continued on next page...

Continued from previous page...

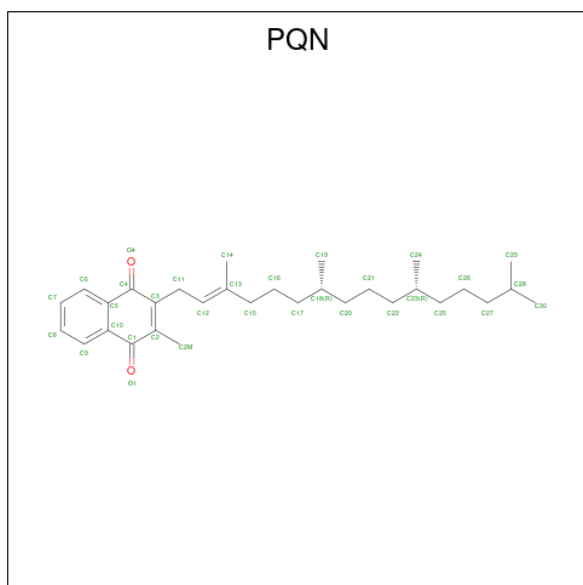
Mol	Chain	Residues	Atoms					AltConf
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
13	2	1	Total 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

Continued on next page...

Continued from previous page...

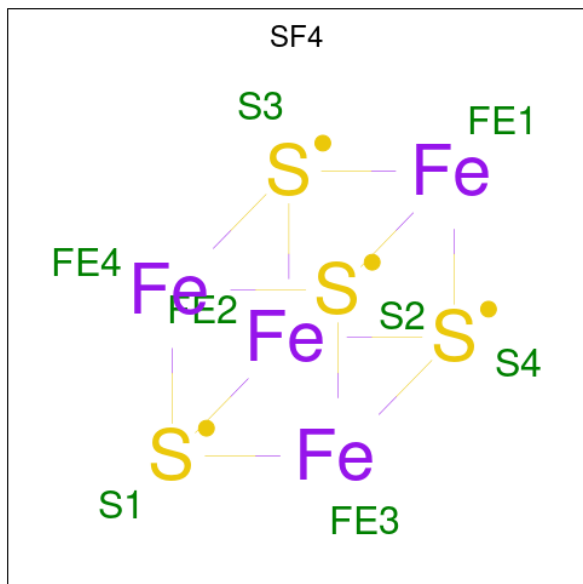
Mol	Chain	Residues	Atoms					AltConf
13	8	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	8	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
13	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
13	9	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
13	0	1	Total	C	Mg	N	O	0
			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 (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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 (three-letter code: SF4) (formula: Fe₄S₄).



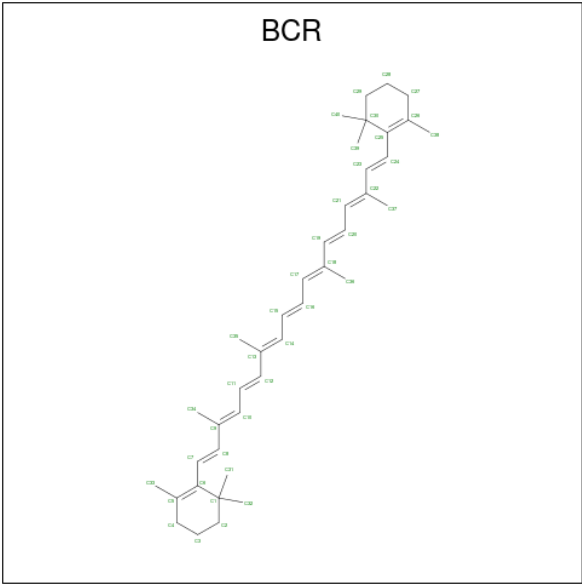
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	C	1	Total	Fe	S	0
			8	4	4	
15	a	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	
15	c	1	Total	Fe	S	0
			8	4	4	

Continued on next page...

Continued from previous page...

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 (three-letter code: 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	

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

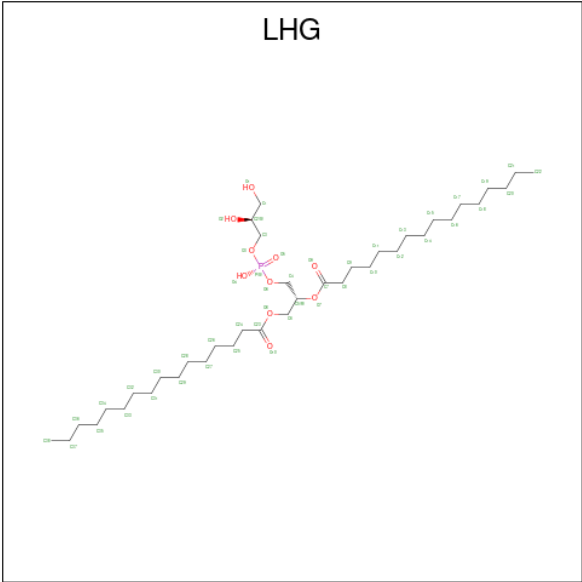
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C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

Continued on next page...

Continued from previous page...

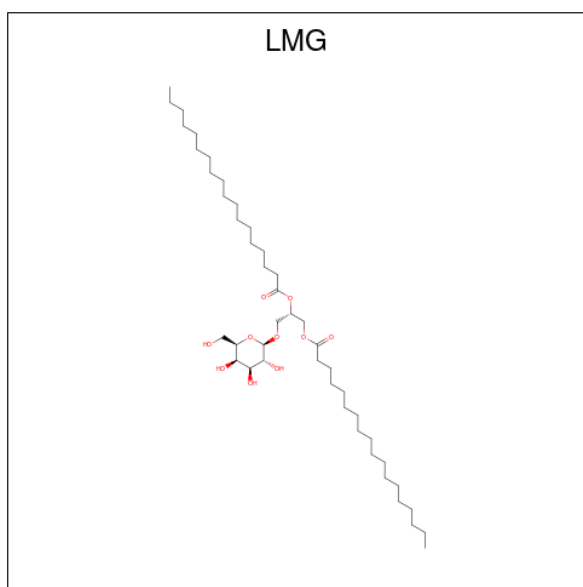
Mol	Chain	Residues	Atoms	AltConf
16	1	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 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 (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



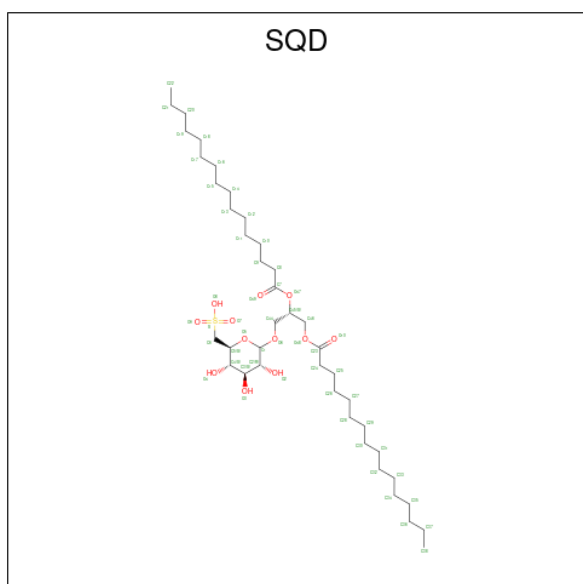
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			36	25	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	a	1	Total	C	O	P	0
			36	25	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	1	1	Total	C	O	P	0
			36	25	10	1	
17	1	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 18 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



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

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

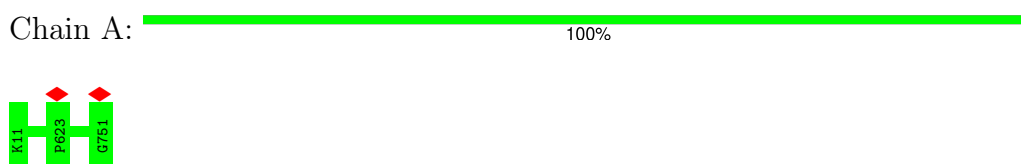


Mol	Chain	Residues	Atoms				AltConf
19	I	1	Total 50	C 37	O 12	S 1	0
19	i	1	Total 50	C 37	O 12	S 1	0
19	7	1	Total 50	C 37	O 12	S 1	0

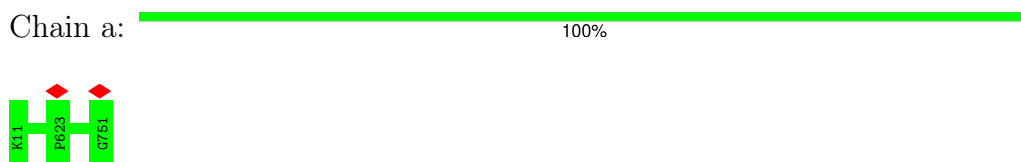
3 Residue-property plots [i](#)

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

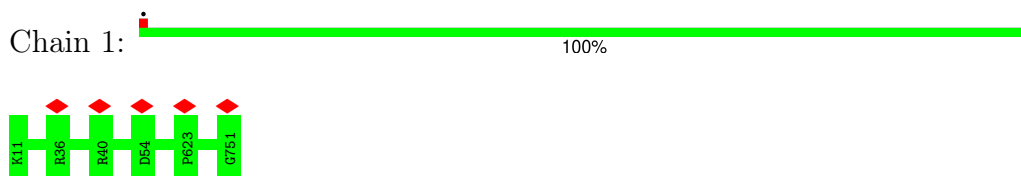
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



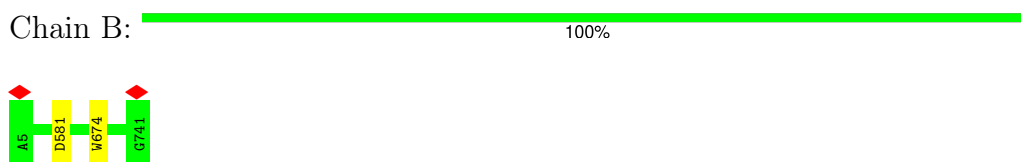
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



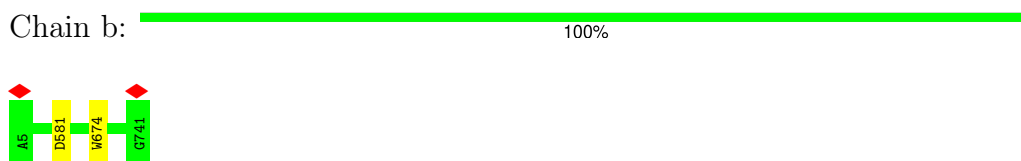
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



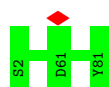
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain 2:  100%



- Molecule 3: Photosystem I iron-sulfur center

Chain C:  100%



- Molecule 3: Photosystem I iron-sulfur center

Chain c:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Photosystem I iron-sulfur center

Chain 3:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I reaction center subunit II

Chain D:  100%

There are no outlier residues recorded for this chain.

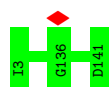
- Molecule 4: Photosystem I reaction center subunit II

Chain d:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: Photosystem I reaction center subunit II

Chain 4:  100%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E:  100%



- Molecule 5: Photosystem I reaction center subunit IV

Chain e: 100%



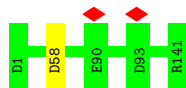
- Molecule 5: Photosystem I reaction center subunit IV

Chain 5: 100%



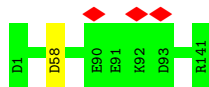
- Molecule 6: PSI-F

Chain F: 99%



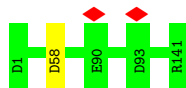
- Molecule 6: PSI-F

Chain f: 99%



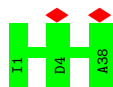
- Molecule 6: PSI-F

Chain 6: 99%

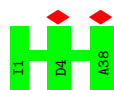


- Molecule 7: Photosystem I reaction center subunit VIII

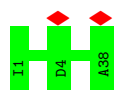
Chain I: 5% 100%



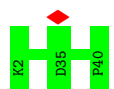
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



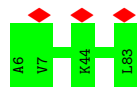
There are no outlier residues recorded for this chain.

- Molecule 8: Photosystem I reaction center subunit IX

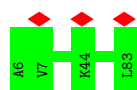


There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem I reaction center subunit PsaK

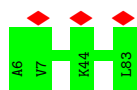


- Molecule 9: Photosystem I reaction center subunit PsaK



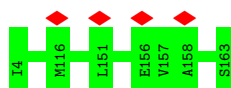
- Molecule 9: Photosystem I reaction center subunit PsaK





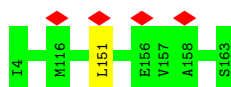
- Molecule 10: Photosystem I reaction center subunit XI

Chain L: 100%



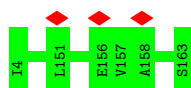
- Molecule 10: Photosystem I reaction center subunit XI

Chain l: 99%



- Molecule 10: Photosystem I reaction center subunit XI

Chain 0: 100%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I reaction center subunit XII

Chain m: 100%

There are no outlier residues recorded for this chain.

- Molecule 11: Photosystem I reaction center subunit XII

Chain z: 100%

There are no outlier residues recorded for this chain.

4 Experimental information

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	1	0.32	0/5986	0.49	0/8157
1	A	0.32	0/5986	0.49	0/8157
1	a	0.32	0/5986	0.49	0/8157
2	2	0.33	0/6026	0.52	1/8237 (0.0%)
2	B	0.33	0/6026	0.52	1/8237 (0.0%)
2	b	0.33	0/6026	0.52	1/8237 (0.0%)
3	3	0.35	0/609	0.58	0/824
3	C	0.35	0/609	0.57	0/824
3	c	0.35	0/609	0.57	0/824
4	4	0.30	0/1123	0.57	0/1514
4	D	0.30	0/1123	0.57	0/1514
4	d	0.30	0/1123	0.57	0/1514
5	5	0.33	0/549	0.52	0/741
5	E	0.33	0/549	0.52	0/741
5	e	0.33	0/549	0.52	0/741
6	6	0.30	0/1130	0.57	1/1533 (0.1%)
6	F	0.30	0/1130	0.57	1/1533 (0.1%)
6	f	0.31	0/1130	0.57	1/1533 (0.1%)
7	7	0.30	0/280	0.66	0/381
7	I	0.30	0/280	0.66	0/381
7	i	0.30	0/280	0.66	0/381
8	8	0.30	0/318	0.46	0/435
8	J	0.30	0/318	0.46	0/435
8	j	0.30	0/318	0.46	0/435
9	9	0.33	0/556	0.67	0/759
9	K	0.33	0/556	0.67	0/759
9	k	0.33	0/556	0.67	0/759
10	0	0.31	0/1215	0.60	0/1659
10	L	0.31	0/1215	0.60	0/1659
10	l	0.31	0/1215	0.60	1/1659 (0.1%)
11	M	0.26	0/235	0.41	0/318
11	m	0.26	0/235	0.41	0/318

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	z	0.26	0/235	0.41	0/318
All	All	0.32	0/54081	0.53	7/73674 (0.0%)

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.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	f	58	ASP	CB-CG-OD1	7.08	124.67	118.30
6	6	58	ASP	CB-CG-OD1	7.08	124.67	118.30
6	F	58	ASP	CB-CG-OD1	7.06	124.65	118.30
2	2	581	ASP	CB-CG-OD1	5.87	123.58	118.30
2	B	581	ASP	CB-CG-OD1	5.85	123.56	118.30

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
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 14 such sidechains are listed below:

Mol	Chain	Res	Type
10	l	45	ASN
10	l	150	HIS
10	0	150	HIS
2	2	135	ASN
10	0	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	812	-	43,53,73	1.61	6 (13%)	50,89,113	1.54	7 (14%)
13	CLA	i	102	-	63,73,73	1.30	5 (7%)	74,113,113	1.42	7 (9%)
13	CLA	A	819	-	58,68,73	1.38	6 (10%)	68,107,113	1.63	8 (11%)
13	CLA	2	808	-	43,53,73	1.60	5 (11%)	50,89,113	1.58	7 (14%)
13	CLA	9	4005	-	41,52,73	1.67	6 (14%)	47,88,113	1.64	8 (17%)
16	BCR	k	4001	-	41,41,41	1.09	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	1	807	-	53,63,73	1.42	6 (11%)	62,101,113	1.56	7 (11%)
13	CLA	k	4005	-	41,52,73	1.66	6 (14%)	47,88,113	1.64	8 (17%)
13	CLA	a	804	-	53,63,73	1.41	6 (11%)	62,101,113	1.49	7 (11%)
13	CLA	2	810	-	44,54,73	1.54	6 (13%)	51,90,113	1.72	7 (13%)
13	CLA	A	816	-	44,54,73	1.58	5 (11%)	51,90,113	1.43	5 (9%)
13	CLA	8	1103	-	43,53,73	1.62	5 (11%)	50,89,113	1.48	7 (14%)
13	CLA	B	833	-	48,58,73	1.47	6 (12%)	56,95,113	1.69	10 (17%)
13	CLA	B	834	-	58,68,73	1.37	6 (10%)	68,107,113	1.33	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	A	814	-	48,58,73	1.51	6 (12%)	56,95,113	1.65	10 (17%)
13	CLA	1	842	-	43,53,73	1.62	6 (13%)	50,89,113	1.80	6 (12%)
13	CLA	B	823	-	63,73,73	1.35	6 (9%)	74,113,113	1.29	7 (9%)
16	BCR	1	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	B	817	-	39,49,73	1.62	5 (12%)	46,84,113	1.35	6 (13%)
16	BCR	b	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	2	820	-	63,73,73	1.33	6 (9%)	74,113,113	1.45	8 (10%)
13	CLA	l	202	-	58,68,73	1.35	6 (10%)	68,107,113	1.47	8 (11%)
17	LHG	1	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
16	BCR	b	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
16	BCR	2	844	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
13	CLA	a	821	-	63,73,73	1.35	6 (9%)	74,113,113	1.32	6 (8%)
13	CLA	2	805	-	63,73,73	1.33	6 (9%)	74,113,113	1.37	7 (9%)
13	CLA	1	816	-	44,54,73	1.59	5 (11%)	51,90,113	1.43	5 (9%)
13	CLA	b	801	-	63,73,73	1.37	7 (11%)	74,113,113	1.69	11 (14%)
16	BCR	7	103	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
12	CL0	A	801	-	63,73,73	1.33	6 (9%)	74,113,113	1.23	7 (9%)
13	CLA	6	201	-	53,63,73	1.46	5 (9%)	62,101,113	1.45	7 (11%)
16	BCR	F	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	1	819	-	58,68,73	1.37	6 (10%)	68,107,113	1.64	8 (11%)
13	CLA	9	4003	-	44,54,73	1.60	6 (13%)	51,90,113	1.51	7 (13%)
14	PQN	a	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	A	828	-	63,73,73	1.31	6 (9%)	74,113,113	1.49	6 (8%)
13	CLA	b	819	-	44,54,73	1.58	6 (13%)	51,90,113	1.53	5 (9%)
13	CLA	a	822	-	48,58,73	1.51	6 (12%)	56,95,113	1.68	9 (16%)
13	CLA	a	816	-	44,54,73	1.58	5 (11%)	51,90,113	1.43	5 (9%)
13	CLA	a	813	-	53,63,73	1.46	6 (11%)	62,101,113	1.43	9 (14%)
13	CLA	1	827	-	63,73,73	1.32	7 (11%)	74,113,113	1.34	7 (9%)
13	CLA	B	801	-	63,73,73	1.37	7 (11%)	74,113,113	1.68	11 (14%)
13	CLA	a	803	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	9 (12%)
13	CLA	A	825	-	60,70,73	1.36	6 (10%)	70,109,113	1.53	8 (11%)
13	CLA	2	802	-	63,73,73	1.33	7 (11%)	74,113,113	1.51	7 (9%)
16	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.27	9 (16%)
13	CLA	A	812	-	44,54,73	1.55	5 (11%)	51,90,113	1.46	6 (11%)
13	CLA	a	852	-	58,68,73	1.39	7 (12%)	68,107,113	1.32	7 (10%)

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%)
16	BCR	1	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.26	7 (12%)
19	SQD	7	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.46	10 (17%)
17	LHG	A	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	b	806	-	63,73,73	1.36	6 (9%)	74,113,113	1.37	6 (8%)
13	CLA	A	823	-	48,58,73	1.53	5 (10%)	56,95,113	1.56	6 (10%)
13	CLA	b	802	-	63,73,73	1.33	7 (11%)	74,113,113	1.51	7 (9%)
13	CLA	A	813	-	53,63,73	1.46	6 (11%)	62,101,113	1.43	8 (12%)
16	BCR	1	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
16	BCR	a	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
17	LHG	A	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	B	819	-	44,54,73	1.58	6 (13%)	51,90,113	1.53	5 (9%)
13	CLA	2	812	-	63,73,73	1.32	5 (7%)	74,113,113	1.41	9 (12%)
13	CLA	b	832	-	38,48,73	1.69	5 (13%)	43,82,113	1.65	6 (13%)
13	CLA	b	814	-	48,58,73	1.49	6 (12%)	56,95,113	1.56	7 (12%)
13	CLA	k	4002	-	43,53,73	1.66	5 (11%)	50,89,113	1.52	6 (12%)
13	CLA	a	836	-	49,59,73	1.49	7 (14%)	56,96,113	1.52	9 (16%)
13	CLA	A	838	-	63,73,73	1.32	6 (9%)	74,113,113	1.43	8 (10%)
13	CLA	A	810	-	43,53,73	1.60	6 (13%)	50,89,113	1.57	6 (12%)
13	CLA	1	818	-	52,62,73	1.45	6 (11%)	60,99,113	1.59	8 (13%)
13	CLA	2	822	-	63,73,73	1.34	6 (9%)	74,113,113	1.29	7 (9%)
13	CLA	A	831	-	48,58,73	1.48	6 (12%)	56,95,113	1.55	9 (16%)
13	CLA	B	826	-	58,68,73	1.42	8 (13%)	68,107,113	1.63	9 (13%)
17	LHG	1	850	-	40,40,48	0.69	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	B	806	-	63,73,73	1.36	6 (9%)	74,113,113	1.37	6 (8%)
13	CLA	F	203	-	43,53,73	1.61	5 (11%)	50,89,113	1.51	8 (16%)
16	BCR	a	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.43	9 (16%)
13	CLA	1	829	-	63,73,73	1.32	7 (11%)	74,113,113	1.55	8 (10%)
13	CLA	2	801	-	63,73,73	1.37	7 (11%)	74,113,113	1.68	12 (16%)
15	SF4	a	844	1,2	0,12,12	-	-	-	-	-
13	CLA	l	207	-	63,73,73	1.33	5 (7%)	74,113,113	1.46	7 (9%)
13	CLA	b	827	-	43,53,73	1.61	7 (16%)	50,89,113	1.42	8 (16%)
13	CLA	B	809	-	43,53,73	1.61	5 (11%)	50,89,113	1.57	6 (12%)
13	CLA	A	806	-	63,73,73	1.33	7 (11%)	74,113,113	1.46	8 (10%)
13	CLA	1	812	-	44,54,73	1.55	5 (11%)	51,90,113	1.47	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	B	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
16	BCR	0	207	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	a	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
13	CLA	b	807	-	63,73,73	1.33	6 (9%)	74,113,113	1.36	7 (9%)
14	PQN	1	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
16	BCR	2	843	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	B	802	-	63,73,73	1.33	7 (11%)	74,113,113	1.51	8 (10%)
13	CLA	2	834	-	48,58,73	1.50	5 (10%)	56,95,113	1.54	8 (14%)
13	CLA	A	835	-	54,64,73	1.44	5 (9%)	63,102,113	1.38	7 (11%)
13	CLA	2	824	-	63,73,73	1.32	7 (11%)	74,113,113	1.46	7 (9%)
13	CLA	A	824	-	58,68,73	1.38	6 (10%)	68,107,113	1.50	7 (10%)
13	CLA	B	810	-	63,73,73	1.33	7 (11%)	74,113,113	1.45	7 (9%)
13	CLA	1	808	-	48,58,73	1.50	6 (12%)	56,95,113	1.90	7 (12%)
13	CLA	B	807	-	63,73,73	1.33	6 (9%)	74,113,113	1.36	8 (10%)
16	BCR	A	846	-	41,41,41	1.15	3 (7%)	56,56,56	1.28	6 (10%)
16	BCR	m	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	b	834	-	58,68,73	1.37	7 (12%)	68,107,113	1.34	7 (10%)
13	CLA	1	834	-	63,73,73	1.34	7 (11%)	74,113,113	1.40	4 (5%)
13	CLA	A	818	-	52,62,73	1.46	7 (13%)	60,99,113	1.59	8 (13%)
13	CLA	1	806	-	63,73,73	1.33	6 (9%)	74,113,113	1.46	8 (10%)
13	CLA	2	821	-	48,58,73	1.52	6 (12%)	56,95,113	1.52	8 (14%)
13	CLA	b	830	-	56,66,73	1.44	7 (12%)	65,104,113	1.52	7 (10%)
13	CLA	1	817	-	53,63,73	1.42	6 (11%)	62,101,113	1.56	9 (14%)
13	CLA	1	839	-	63,73,73	1.28	7 (11%)	74,113,113	1.55	10 (13%)
13	CLA	a	842	-	43,53,73	1.62	6 (13%)	50,89,113	1.79	6 (12%)
16	BCR	A	845	-	41,41,41	1.10	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	K	4003	-	44,54,73	1.60	6 (13%)	51,90,113	1.51	7 (13%)
13	CLA	B	813	-	63,73,73	1.32	6 (9%)	74,113,113	1.41	9 (12%)
13	CLA	b	825	-	63,73,73	1.33	7 (11%)	74,113,113	1.45	7 (9%)
16	BCR	l	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	6 (10%)
13	CLA	J	1101	-	48,58,73	1.52	6 (12%)	56,95,113	1.44	9 (16%)
13	CLA	b	823	-	63,73,73	1.35	6 (9%)	74,113,113	1.29	7 (9%)
13	CLA	2	813	-	48,58,73	1.49	6 (12%)	56,95,113	1.56	7 (12%)
13	CLA	2	836	-	63,73,73	1.35	6 (9%)	74,113,113	1.30	7 (9%)
13	CLA	2	803	-	58,68,73	1.35	6 (10%)	68,107,113	1.56	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	808	-	63,73,73	1.31	6 (9%)	74,113,113	1.46	6 (8%)
13	CLA	L	203	-	48,58,73	1.51	6 (12%)	56,95,113	1.66	9 (16%)
13	CLA	A	815	-	43,53,73	1.62	6 (13%)	50,89,113	1.60	6 (12%)
13	CLA	B	830	-	56,66,73	1.44	7 (12%)	65,104,113	1.51	7 (10%)
13	CLA	1	836	-	49,59,73	1.49	7 (14%)	56,96,113	1.53	9 (16%)
13	CLA	B	825	-	63,73,73	1.32	6 (9%)	74,113,113	1.45	7 (9%)
13	CLA	b	805	-	63,73,73	1.33	6 (9%)	74,113,113	1.37	7 (9%)
13	CLA	2	829	-	56,66,73	1.43	7 (12%)	65,104,113	1.51	7 (10%)
15	SF4	c	102	3	0,12,12	-	-	-	-	-
16	BCR	B	843	-	41,41,41	1.10	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	2	831	-	38,48,73	1.69	5 (13%)	43,82,113	1.65	6 (13%)
13	CLA	a	828	-	63,73,73	1.32	6 (9%)	74,113,113	1.50	6 (8%)
13	CLA	a	809	-	48,58,73	1.52	6 (12%)	56,95,113	1.46	8 (14%)
13	CLA	b	817	-	39,49,73	1.62	6 (15%)	46,84,113	1.34	6 (13%)
13	CLA	A	808	-	48,58,73	1.50	6 (12%)	56,95,113	1.89	8 (14%)
13	CLA	1	821	-	63,73,73	1.34	6 (9%)	74,113,113	1.33	6 (8%)
16	BCR	1	847	-	41,41,41	1.13	3 (7%)	56,56,56	1.42	9 (16%)
13	CLA	b	824	-	53,63,73	1.47	7 (13%)	62,101,113	1.75	10 (16%)
13	CLA	A	830	-	63,73,73	1.35	6 (9%)	74,113,113	1.57	6 (8%)
13	CLA	B	816	-	58,68,73	1.41	6 (10%)	68,107,113	1.49	6 (8%)
16	BCR	6	205	-	41,41,41	1.06	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	2	811	-	43,53,73	1.60	6 (13%)	50,89,113	1.54	7 (14%)
13	CLA	B	805	-	63,73,73	1.33	6 (9%)	74,113,113	1.37	7 (9%)
13	CLA	B	804	-	63,73,73	1.32	6 (9%)	74,113,113	1.33	8 (10%)
13	CLA	2	809	-	63,73,73	1.32	7 (11%)	74,113,113	1.45	7 (9%)
13	CLA	A	802	-	58,68,73	1.36	7 (12%)	68,107,113	1.66	10 (14%)
13	CLA	A	827	-	63,73,73	1.32	7 (11%)	74,113,113	1.34	6 (8%)
13	CLA	1	838	-	63,73,73	1.32	6 (9%)	74,113,113	1.43	8 (10%)
16	BCR	K	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	K	4005	-	41,52,73	1.66	6 (14%)	47,88,113	1.64	8 (17%)
13	CLA	2	804	-	63,73,73	1.32	6 (9%)	74,113,113	1.33	8 (10%)
13	CLA	2	835	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	7 (9%)
13	CLA	l	204	-	48,58,73	1.52	6 (12%)	56,95,113	1.66	10 (17%)
13	CLA	A	822	-	48,58,73	1.50	6 (12%)	56,95,113	1.68	9 (16%)
13	CLA	B	835	-	48,58,73	1.51	5 (10%)	56,95,113	1.53	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	BCR	b	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.26	6 (10%)
16	BCR	I	102	-	41,41,41	1.07	2 (4%)	56,56,56	1.38	10 (17%)
15	SF4	C	102	3	0,12,12	-	-	-	-	-
13	CLA	1	823	-	48,58,73	1.54	5 (10%)	56,95,113	1.56	6 (10%)
13	CLA	a	812	-	44,54,73	1.55	6 (13%)	51,90,113	1.46	6 (11%)
13	CLA	1	837	-	58,68,73	1.37	7 (12%)	68,107,113	1.36	7 (10%)
13	CLA	B	827	-	43,53,73	1.61	7 (16%)	50,89,113	1.42	8 (16%)
13	CLA	b	821	-	63,73,73	1.32	6 (9%)	74,113,113	1.45	8 (10%)
16	BCR	A	851	-	41,41,41	1.13	3 (7%)	56,56,56	1.29	7 (12%)
13	CLA	B	818	-	44,54,73	1.58	6 (13%)	51,90,113	1.56	7 (13%)
16	BCR	8	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	B	803	-	58,68,73	1.35	6 (10%)	68,107,113	1.55	9 (13%)
13	CLA	B	829	-	60,70,73	1.36	6 (10%)	70,109,113	1.54	9 (12%)
13	CLA	a	819	-	58,68,73	1.39	6 (10%)	68,107,113	1.62	8 (11%)
16	BCR	B	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	A	821	-	63,73,73	1.34	6 (9%)	74,113,113	1.32	6 (8%)
16	BCR	b	841	-	41,41,41	1.07	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	l	205	-	44,54,73	1.57	6 (13%)	51,90,113	1.51	5 (9%)
13	CLA	a	833	-	63,73,73	1.33	6 (9%)	74,113,113	1.51	8 (10%)
13	CLA	B	831	-	63,73,73	1.34	5 (7%)	74,113,113	1.49	9 (12%)
13	CLA	a	838	-	63,73,73	1.33	6 (9%)	74,113,113	1.42	8 (10%)
14	PQN	A	843	-	34,34,34	0.39	0	43,45,45	1.08	2 (4%)
13	CLA	A	807	-	53,63,73	1.43	6 (11%)	62,101,113	1.56	7 (11%)
12	CL0	a	801	-	63,73,73	1.33	6 (9%)	74,113,113	1.23	7 (9%)
13	CLA	a	810	-	43,53,73	1.60	6 (13%)	50,89,113	1.56	6 (12%)
13	CLA	a	832	-	63,73,73	1.33	6 (9%)	74,113,113	1.39	8 (10%)
14	PQN	b	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	2	830	-	63,73,73	1.34	6 (9%)	74,113,113	1.49	9 (12%)
16	BCR	2	840	-	41,41,41	1.08	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	B	824	-	53,63,73	1.47	7 (13%)	62,101,113	1.74	11 (17%)
16	BCR	f	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	2	823	-	53,63,73	1.48	7 (13%)	62,101,113	1.75	11 (17%)
13	CLA	A	834	-	63,73,73	1.34	7 (11%)	74,113,113	1.39	4 (5%)
13	CLA	b	820	-	53,63,73	1.48	6 (11%)	62,101,113	1.41	6 (9%)
15	SF4	A	844	1,2	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	F	204	-	44,54,73	1.59	5 (11%)	51,90,113	1.42	5 (9%)
13	CLA	8	1102	-	38,48,73	1.71	5 (13%)	43,82,113	1.67	7 (16%)
13	CLA	B	808	-	63,73,73	1.31	6 (9%)	74,113,113	1.46	6 (8%)
13	CLA	A	826	-	53,63,73	1.42	6 (11%)	62,101,113	1.38	7 (11%)
13	CLA	B	821	-	63,73,73	1.32	6 (9%)	74,113,113	1.45	8 (10%)
13	CLA	2	816	-	39,49,73	1.62	5 (12%)	46,84,113	1.35	6 (13%)
13	CLA	a	837	-	58,68,73	1.38	7 (12%)	68,107,113	1.35	7 (10%)
13	CLA	B	811	-	44,54,73	1.55	6 (13%)	51,90,113	1.72	7 (13%)
16	BCR	a	845	-	41,41,41	1.09	2 (4%)	56,56,56	1.17	3 (5%)
13	CLA	A	811	-	54,64,73	1.45	6 (11%)	63,102,113	1.46	7 (11%)
13	CLA	a	826	-	53,63,73	1.43	6 (11%)	62,101,113	1.38	7 (11%)
13	CLA	1	813	-	53,63,73	1.46	6 (11%)	62,101,113	1.43	9 (14%)
13	CLA	B	832	-	38,48,73	1.69	5 (13%)	43,82,113	1.65	6 (13%)
13	CLA	L	206	-	63,73,73	1.33	6 (9%)	74,113,113	1.47	7 (9%)
13	CLA	j	1101	-	48,58,73	1.52	6 (12%)	56,95,113	1.44	8 (14%)
15	SF4	3	101	3	0,12,12	-	-	-	-	-
16	BCR	9	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	1	828	-	63,73,73	1.31	6 (9%)	74,113,113	1.49	6 (8%)
15	SF4	3	102	3	0,12,12	-	-	-	-	-
13	CLA	B	820	-	53,63,73	1.47	6 (11%)	62,101,113	1.40	6 (9%)
15	SF4	1	844	1,2	0,12,12	-	-	-	-	-
13	CLA	a	818	-	52,62,73	1.45	7 (13%)	60,99,113	1.59	8 (13%)
16	BCR	b	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.33	6 (10%)
16	BCR	6	202	-	41,41,41	1.07	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	1	804	-	53,63,73	1.41	6 (11%)	62,101,113	1.50	7 (11%)
13	CLA	k	4003	-	44,54,73	1.59	6 (13%)	51,90,113	1.51	7 (13%)
13	CLA	1	831	-	48,58,73	1.48	6 (12%)	56,95,113	1.54	9 (16%)
13	CLA	1	815	-	43,53,73	1.61	6 (13%)	50,89,113	1.59	6 (12%)
13	CLA	A	805	-	53,63,73	1.45	6 (11%)	62,101,113	1.43	7 (11%)
16	BCR	l	203	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	9 (16%)
13	CLA	J	1103	-	43,53,73	1.62	5 (11%)	50,89,113	1.48	7 (14%)
13	CLA	1	803	-	63,73,73	1.33	6 (9%)	74,113,113	1.37	9 (12%)
16	BCR	J	1104	-	41,41,41	1.05	2 (4%)	56,56,56	1.35	9 (16%)
13	CLA	0	202	-	58,68,73	1.35	6 (10%)	68,107,113	1.47	8 (11%)
16	BCR	2	841	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	825	-	60,70,73	1.36	6 (10%)	70,109,113	1.53	8 (11%)
13	CLA	A	842	-	43,53,73	1.62	6 (13%)	50,89,113	1.79	6 (12%)
13	CLA	A	817	-	53,63,73	1.42	6 (11%)	62,101,113	1.56	9 (14%)
13	CLA	2	837	-	63,73,73	1.35	5 (7%)	74,113,113	1.33	6 (8%)
16	BCR	b	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
16	BCR	j	1104	-	41,41,41	1.06	2 (4%)	56,56,56	1.34	9 (16%)
13	CLA	a	839	-	63,73,73	1.27	6 (9%)	74,113,113	1.56	9 (12%)
13	CLA	f	203	-	43,53,73	1.61	5 (11%)	50,89,113	1.51	8 (16%)
13	CLA	b	847	-	63,73,73	1.33	6 (9%)	74,113,113	1.49	8 (10%)
13	CLA	a	806	-	63,73,73	1.33	7 (11%)	74,113,113	1.47	8 (10%)
16	BCR	F	205	-	41,41,41	1.07	2 (4%)	56,56,56	1.31	7 (12%)
13	CLA	1	805	-	53,63,73	1.45	6 (11%)	62,101,113	1.43	6 (9%)
13	CLA	7	102	-	63,73,73	1.30	5 (7%)	74,113,113	1.40	7 (9%)
16	BCR	L	205	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
16	BCR	2	847	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
16	BCR	z	101	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	A	841	-	58,68,73	1.41	7 (12%)	68,107,113	1.36	8 (11%)
13	CLA	2	826	-	43,53,73	1.61	7 (16%)	50,89,113	1.43	8 (16%)
13	CLA	a	814	-	48,58,73	1.51	6 (12%)	56,95,113	1.66	11 (19%)
13	CLA	2	819	-	53,63,73	1.47	6 (11%)	62,101,113	1.40	6 (9%)
19	SQD	i	101	-	48,50,54	0.99	3 (6%)	58,61,65	1.45	10 (17%)
13	CLA	b	822	-	48,58,73	1.51	6 (12%)	56,95,113	1.52	8 (14%)
13	CLA	1	811	-	54,64,73	1.44	6 (11%)	63,102,113	1.46	6 (9%)
13	CLA	a	808	-	48,58,73	1.50	6 (12%)	56,95,113	1.89	8 (14%)
13	CLA	b	813	-	63,73,73	1.32	6 (9%)	74,113,113	1.42	9 (12%)
13	CLA	b	815	-	63,73,73	1.31	6 (9%)	74,113,113	1.41	8 (10%)
16	BCR	B	844	-	41,41,41	1.13	2 (4%)	56,56,56	1.43	6 (10%)
13	CLA	b	836	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	7 (9%)
13	CLA	f	204	-	44,54,73	1.58	5 (11%)	51,90,113	1.43	5 (9%)
16	BCR	8	1105	-	41,41,41	1.11	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	b	803	-	58,68,73	1.35	6 (10%)	68,107,113	1.55	9 (13%)
13	CLA	0	208	-	63,73,73	1.33	6 (9%)	74,113,113	1.47	7 (9%)
13	CLA	1	809	-	48,58,73	1.52	6 (12%)	56,95,113	1.47	8 (14%)
13	CLA	2	806	-	63,73,73	1.37	6 (9%)	74,113,113	1.37	6 (8%)
13	CLA	A	804	-	53,63,73	1.41	6 (11%)	62,101,113	1.49	7 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	0	206	-	44,54,73	1.56	6 (13%)	51,90,113	1.51	5 (9%)
13	CLA	a	805	-	53,63,73	1.44	6 (11%)	62,101,113	1.43	7 (11%)
13	CLA	J	1102	-	38,48,73	1.72	5 (13%)	43,82,113	1.68	7 (16%)
16	BCR	B	842	-	41,41,41	1.10	2 (4%)	56,56,56	1.32	6 (10%)
16	BCR	M	101	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	8 (14%)
13	CLA	6	203	-	43,53,73	1.61	5 (11%)	50,89,113	1.51	8 (16%)
13	CLA	6	204	-	44,54,73	1.58	4 (9%)	51,90,113	1.43	5 (9%)
13	CLA	2	814	-	63,73,73	1.32	6 (9%)	74,113,113	1.41	8 (10%)
18	LMG	2	845	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	B	836	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	7 (9%)
13	CLA	1	802	-	58,68,73	1.36	7 (12%)	68,107,113	1.66	10 (14%)
16	BCR	b	848	-	41,41,41	1.16	3 (7%)	56,56,56	1.31	8 (14%)
13	CLA	B	822	-	48,58,73	1.52	6 (12%)	56,95,113	1.51	8 (14%)
13	CLA	b	804	-	63,73,73	1.33	6 (9%)	74,113,113	1.32	8 (10%)
16	BCR	a	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	1	835	-	54,64,73	1.44	5 (9%)	63,102,113	1.37	6 (9%)
13	CLA	a	827	-	63,73,73	1.33	7 (11%)	74,113,113	1.34	6 (8%)
13	CLA	b	835	-	48,58,73	1.50	5 (10%)	56,95,113	1.53	8 (14%)
13	CLA	2	846	-	63,73,73	1.33	6 (9%)	74,113,113	1.48	8 (10%)
13	CLA	A	840	-	63,73,73	1.32	6 (9%)	74,113,113	1.34	7 (9%)
13	CLA	2	832	-	48,58,73	1.47	6 (12%)	56,95,113	1.69	10 (17%)
13	CLA	1	824	-	58,68,73	1.38	6 (10%)	68,107,113	1.51	7 (10%)
13	CLA	0	205	-	48,58,73	1.52	6 (12%)	56,95,113	1.66	9 (16%)
16	BCR	9	4001	-	41,41,41	1.10	3 (7%)	56,56,56	1.33	6 (10%)
13	CLA	B	847	-	63,73,73	1.32	6 (9%)	74,113,113	1.48	8 (10%)
12	CL0	1	801	-	63,73,73	1.33	6 (9%)	74,113,113	1.22	7 (9%)
13	CLA	A	832	-	63,73,73	1.33	6 (9%)	74,113,113	1.39	9 (12%)
13	CLA	b	818	-	44,54,73	1.58	5 (11%)	51,90,113	1.55	7 (13%)
13	CLA	1	820	-	44,54,73	1.54	6 (13%)	51,90,113	1.41	6 (11%)
13	CLA	1	833	-	63,73,73	1.32	6 (9%)	74,113,113	1.50	8 (10%)
13	CLA	L	201	-	58,68,73	1.35	6 (10%)	68,107,113	1.47	8 (11%)
17	LHG	a	850	-	40,40,48	0.68	1 (2%)	43,46,54	1.29	6 (13%)
13	CLA	b	837	-	63,73,73	1.34	6 (9%)	74,113,113	1.30	7 (9%)
13	CLA	9	4002	-	43,53,73	1.66	5 (11%)	50,89,113	1.52	6 (12%)
13	CLA	b	829	-	60,70,73	1.36	6 (10%)	70,109,113	1.53	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	b	831	-	63,73,73	1.34	5 (7%)	74,113,113	1.49	9 (12%)
13	CLA	2	807	-	63,73,73	1.31	6 (9%)	74,113,113	1.45	6 (8%)
13	CLA	0	203	-	63,73,73	1.32	6 (9%)	74,113,113	1.37	7 (9%)
13	CLA	A	820	-	44,54,73	1.54	6 (13%)	51,90,113	1.41	6 (11%)
16	BCR	K	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
13	CLA	1	841	-	58,68,73	1.41	7 (12%)	68,107,113	1.36	8 (11%)
13	CLA	a	830	-	63,73,73	1.35	6 (9%)	74,113,113	1.57	6 (8%)
13	CLA	1	830	-	63,73,73	1.34	6 (9%)	74,113,113	1.56	6 (8%)
13	CLA	a	807	-	53,63,73	1.43	6 (11%)	62,101,113	1.56	7 (11%)
13	CLA	B	837	-	63,73,73	1.35	6 (9%)	74,113,113	1.30	7 (9%)
16	BCR	i	103	-	41,41,41	1.08	2 (4%)	56,56,56	1.38	10 (17%)
16	BCR	L	207	-	41,41,41	1.06	2 (4%)	56,56,56	1.26	7 (12%)
16	BCR	l	206	-	41,41,41	1.11	2 (4%)	56,56,56	1.30	6 (10%)
13	CLA	a	825	-	60,70,73	1.36	6 (10%)	70,109,113	1.53	8 (11%)
13	CLA	a	823	-	48,58,73	1.53	5 (10%)	56,95,113	1.57	6 (10%)
13	CLA	b	816	-	58,68,73	1.41	6 (10%)	68,107,113	1.49	6 (8%)
13	CLA	a	802	-	58,68,73	1.36	7 (12%)	68,107,113	1.66	10 (14%)
13	CLA	2	828	-	60,70,73	1.35	6 (10%)	70,109,113	1.54	10 (14%)
13	CLA	A	833	-	63,73,73	1.32	6 (9%)	74,113,113	1.51	8 (10%)
13	CLA	1	822	-	48,58,73	1.51	5 (10%)	56,95,113	1.68	9 (16%)
13	CLA	8	1101	-	48,58,73	1.52	6 (12%)	56,95,113	1.44	9 (16%)
16	BCR	2	839	-	41,41,41	1.09	2 (4%)	56,56,56	1.25	6 (10%)
13	CLA	1	852	-	58,68,73	1.38	7 (12%)	68,107,113	1.32	7 (10%)
13	CLA	2	825	-	58,68,73	1.42	8 (13%)	68,107,113	1.64	9 (13%)
13	CLA	A	836	-	49,59,73	1.49	7 (14%)	56,96,113	1.52	9 (16%)
13	CLA	j	1103	-	43,53,73	1.63	5 (11%)	50,89,113	1.48	7 (14%)
13	CLA	a	817	-	53,63,73	1.42	6 (11%)	62,101,113	1.55	9 (14%)
16	BCR	2	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.24	6 (10%)
13	CLA	b	811	-	44,54,73	1.55	6 (13%)	51,90,113	1.72	7 (13%)
18	LMG	b	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
17	LHG	a	849	-	35,35,48	0.76	1 (2%)	38,41,54	1.28	4 (10%)
13	CLA	B	838	-	63,73,73	1.34	5 (7%)	74,113,113	1.33	6 (8%)
13	CLA	A	839	-	63,73,73	1.27	6 (9%)	74,113,113	1.55	10 (13%)
13	CLA	I	101	-	63,73,73	1.30	6 (9%)	74,113,113	1.41	7 (9%)
13	CLA	B	814	-	48,58,73	1.49	6 (12%)	56,95,113	1.56	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	PQN	B	839	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	841	-	58,68,73	1.41	7 (12%)	68,107,113	1.36	9 (13%)
13	CLA	f	201	-	53,63,73	1.46	6 (11%)	62,101,113	1.46	7 (11%)
13	CLA	2	817	-	44,54,73	1.58	6 (13%)	51,90,113	1.56	7 (13%)
13	CLA	a	834	-	63,73,73	1.34	7 (11%)	74,113,113	1.39	5 (6%)
13	CLA	L	204	-	44,54,73	1.56	6 (13%)	51,90,113	1.51	5 (9%)
16	BCR	L	202	-	41,41,41	1.11	2 (4%)	56,56,56	1.28	9 (16%)
16	BCR	0	201	-	41,41,41	1.06	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	b	828	-	53,63,73	1.44	6 (11%)	62,101,113	1.51	6 (9%)
13	CLA	b	809	-	43,53,73	1.61	5 (11%)	50,89,113	1.57	6 (12%)
13	CLA	2	833	-	58,68,73	1.37	6 (10%)	68,107,113	1.33	6 (8%)
13	CLA	2	827	-	53,63,73	1.44	5 (9%)	62,101,113	1.50	6 (9%)
18	LMG	B	846	-	41,41,55	0.94	3 (7%)	49,49,63	1.19	3 (6%)
13	CLA	A	803	-	63,73,73	1.32	6 (9%)	74,113,113	1.38	9 (12%)
13	CLA	b	826	-	58,68,73	1.42	8 (13%)	68,107,113	1.64	9 (13%)
13	CLA	1	826	-	53,63,73	1.42	6 (11%)	62,101,113	1.38	7 (11%)
13	CLA	a	815	-	43,53,73	1.61	6 (13%)	50,89,113	1.60	7 (14%)
13	CLA	A	852	-	58,68,73	1.38	7 (12%)	68,107,113	1.31	7 (10%)
13	CLA	a	811	-	54,64,73	1.44	6 (11%)	63,102,113	1.47	7 (11%)
13	CLA	j	1102	-	38,48,73	1.71	5 (13%)	43,82,113	1.67	7 (16%)
13	CLA	2	818	-	44,54,73	1.59	6 (13%)	51,90,113	1.52	5 (9%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.42	9 (16%)
15	SF4	C	101	3	0,12,12	-	-	-	-	-
16	BCR	A	848	-	41,41,41	1.04	2 (4%)	56,56,56	1.27	7 (12%)
13	CLA	F	201	-	53,63,73	1.46	6 (11%)	62,101,113	1.45	7 (11%)
13	CLA	K	4002	-	43,53,73	1.66	5 (11%)	50,89,113	1.52	6 (12%)
16	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.25	6 (10%)
15	SF4	c	101	3	0,12,12	-	-	-	-	-
13	CLA	a	829	-	63,73,73	1.32	7 (11%)	74,113,113	1.55	8 (10%)
13	CLA	b	838	-	63,73,73	1.34	5 (7%)	74,113,113	1.32	6 (8%)
13	CLA	a	840	-	63,73,73	1.32	6 (9%)	74,113,113	1.33	7 (9%)
13	CLA	2	815	-	58,68,73	1.41	6 (10%)	68,107,113	1.49	6 (8%)
16	BCR	f	202	-	41,41,41	1.08	2 (4%)	56,56,56	1.27	6 (10%)
13	CLA	b	810	-	63,73,73	1.32	7 (11%)	74,113,113	1.45	7 (9%)
13	CLA	1	810	-	43,53,73	1.61	6 (13%)	50,89,113	1.56	6 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	1	814	-	48,58,73	1.52	6 (12%)	56,95,113	1.65	11 (19%)
16	BCR	J	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	b	812	-	43,53,73	1.62	6 (13%)	50,89,113	1.54	7 (14%)
13	CLA	a	835	-	54,64,73	1.45	5 (9%)	63,102,113	1.37	7 (11%)
13	CLA	a	831	-	48,58,73	1.49	6 (12%)	56,95,113	1.55	9 (16%)
16	BCR	1	851	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	7 (12%)
13	CLA	A	809	-	48,58,73	1.52	6 (12%)	56,95,113	1.47	8 (14%)
13	CLA	a	824	-	58,68,73	1.37	6 (10%)	68,107,113	1.50	7 (10%)
16	BCR	B	845	-	41,41,41	1.16	2 (4%)	56,56,56	1.19	6 (10%)
16	BCR	j	1105	-	41,41,41	1.12	2 (4%)	56,56,56	1.32	7 (12%)
13	CLA	B	828	-	53,63,73	1.44	6 (11%)	62,101,113	1.50	6 (9%)
13	CLA	1	832	-	63,73,73	1.33	6 (9%)	74,113,113	1.39	9 (12%)
13	CLA	1	840	-	63,73,73	1.31	6 (9%)	74,113,113	1.34	7 (9%)
13	CLA	A	837	-	58,68,73	1.37	7 (12%)	68,107,113	1.35	7 (10%)
16	BCR	k	4004	-	41,41,41	1.11	2 (4%)	56,56,56	1.22	6 (10%)
14	PQN	2	838	-	34,34,34	0.36	0	43,45,45	1.15	3 (6%)
13	CLA	a	820	-	44,54,73	1.55	6 (13%)	51,90,113	1.41	6 (11%)
13	CLA	A	829	-	63,73,73	1.33	7 (11%)	74,113,113	1.55	8 (10%)
13	CLA	b	833	-	48,58,73	1.48	6 (12%)	56,95,113	1.68	10 (17%)
13	CLA	B	815	-	63,73,73	1.31	6 (9%)	74,113,113	1.41	8 (10%)

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	812	-	1/1/11/20	2/13/91/115	-
13	CLA	i	102	-	1/1/15/20	13/37/115/115	-
13	CLA	A	819	-	1/1/14/20	11/31/109/115	-
13	CLA	2	808	-	-	4/13/91/115	-
13	CLA	9	4005	-	1/1/11/20	4/11/89/115	-
16	BCR	k	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	1	807	-	1/1/13/20	3/25/103/115	-
13	CLA	k	4005	-	1/1/11/20	4/11/89/115	-
13	CLA	a	804	-	1/1/13/20	2/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	810	-	1/1/11/20	7/15/93/115	-
13	CLA	A	816	-	1/1/11/20	6/15/93/115	-
13	CLA	8	1103	-	1/1/11/20	7/13/91/115	-
13	CLA	B	833	-	1/1/12/20	5/19/97/115	-
13	CLA	B	834	-	1/1/14/20	4/31/109/115	-
13	CLA	A	814	-	1/1/12/20	2/19/97/115	-
13	CLA	1	842	-	1/1/11/20	6/13/91/115	-
13	CLA	B	823	-	1/1/15/20	10/37/115/115	-
16	BCR	1	846	-	-	6/29/63/63	0/2/2/2
13	CLA	B	817	-	-	0/8/86/115	-
16	BCR	b	843	-	-	9/29/63/63	0/2/2/2
13	CLA	2	820	-	-	18/37/115/115	-
13	CLA	1	202	-	-	10/31/109/115	-
17	LHG	1	849	-	-	16/40/40/53	-
16	BCR	b	845	-	-	15/29/63/63	0/2/2/2
16	BCR	2	844	-	-	15/29/63/63	0/2/2/2
13	CLA	a	821	-	1/1/15/20	11/37/115/115	-
13	CLA	2	805	-	1/1/15/20	11/37/115/115	-
13	CLA	1	816	-	1/1/11/20	6/15/93/115	-
13	CLA	b	801	-	1/1/15/20	6/37/115/115	-
16	BCR	7	103	-	-	8/29/63/63	0/2/2/2
12	CL0	A	801	-	2/2/20/25	13/37/135/135	-
13	CLA	6	201	-	1/1/13/20	4/25/103/115	-
16	BCR	F	202	-	-	12/29/63/63	0/2/2/2
13	CLA	1	819	-	1/1/14/20	11/31/109/115	-
13	CLA	9	4003	-	1/1/11/20	6/15/93/115	-
14	PQN	a	843	-	-	10/23/43/43	0/2/2/2
13	CLA	A	828	-	1/1/15/20	9/37/115/115	-
13	CLA	b	819	-	-	6/15/93/115	-
13	CLA	a	822	-	-	7/19/97/115	-
13	CLA	a	816	-	1/1/11/20	6/15/93/115	-
13	CLA	a	813	-	1/1/13/20	10/25/103/115	-
13	CLA	1	827	-	1/1/15/20	12/37/115/115	-
13	CLA	B	801	-	1/1/15/20	6/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	803	-	1/1/15/20	11/37/115/115	-
13	CLA	A	825	-	-	14/34/112/115	-
13	CLA	2	802	-	-	9/37/115/115	-
16	BCR	0	204	-	-	10/29/63/63	0/2/2/2
13	CLA	A	812	-	-	4/15/93/115	-
13	CLA	a	852	-	1/1/14/20	11/31/109/115	-
19	SQD	I	103	-	-	19/45/65/69	0/1/1/1
16	BCR	1	848	-	-	15/29/63/63	0/2/2/2
19	SQD	7	101	-	-	19/45/65/69	0/1/1/1
17	LHG	A	849	-	-	16/40/40/53	-
13	CLA	b	806	-	1/1/15/20	15/37/115/115	-
13	CLA	A	823	-	1/1/12/20	5/19/97/115	-
13	CLA	b	802	-	-	9/37/115/115	-
13	CLA	A	813	-	1/1/13/20	10/25/103/115	-
16	BCR	1	845	-	-	8/29/63/63	0/2/2/2
16	BCR	a	848	-	-	15/29/63/63	0/2/2/2
17	LHG	A	850	-	-	19/45/45/53	-
13	CLA	B	819	-	-	6/15/93/115	-
13	CLA	2	812	-	1/1/15/20	15/37/115/115	-
13	CLA	b	832	-	1/1/9/20	2/8/82/115	-
13	CLA	b	814	-	-	6/19/97/115	-
13	CLA	k	4002	-	1/1/11/20	5/13/91/115	-
13	CLA	a	836	-	1/1/12/20	5/21/99/115	-
13	CLA	A	838	-	1/1/15/20	9/37/115/115	-
13	CLA	A	810	-	-	6/13/91/115	-
13	CLA	1	818	-	1/1/12/20	7/24/102/115	-
13	CLA	2	822	-	1/1/15/20	10/37/115/115	-
13	CLA	A	831	-	-	7/19/97/115	-
13	CLA	B	826	-	-	13/31/109/115	-
17	LHG	1	850	-	-	20/45/45/53	-
13	CLA	B	806	-	1/1/15/20	15/37/115/115	-
13	CLA	F	203	-	1/1/11/20	0/13/91/115	-
16	BCR	a	847	-	-	15/29/63/63	0/2/2/2
13	CLA	1	829	-	1/1/15/20	10/37/115/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	801	-	1/1/15/20	6/37/115/115	-
15	SF4	a	844	1,2	-	-	0/6/5/5
13	CLA	l	207	-	1/1/15/20	8/37/115/115	-
13	CLA	b	827	-	-	6/13/91/115	-
13	CLA	B	809	-	-	4/13/91/115	-
13	CLA	A	806	-	1/1/15/20	11/37/115/115	-
13	CLA	1	812	-	-	4/15/93/115	-
16	BCR	B	841	-	-	8/29/63/63	0/2/2/2
16	BCR	0	207	-	-	11/29/63/63	0/2/2/2
16	BCR	a	846	-	-	6/29/63/63	0/2/2/2
13	CLA	b	807	-	1/1/15/20	14/37/115/115	-
14	PQN	1	843	-	-	10/23/43/43	0/2/2/2
16	BCR	2	843	-	-	6/29/63/63	0/2/2/2
13	CLA	B	802	-	-	9/37/115/115	-
13	CLA	2	834	-	1/1/12/20	1/19/97/115	-
13	CLA	2	824	-	1/1/15/20	8/37/115/115	-
13	CLA	A	835	-	-	13/27/105/115	-
13	CLA	A	824	-	1/1/14/20	14/31/109/115	-
13	CLA	B	810	-	1/1/15/20	13/37/115/115	-
13	CLA	1	808	-	1/1/12/20	3/19/97/115	-
13	CLA	B	807	-	1/1/15/20	14/37/115/115	-
16	BCR	A	846	-	-	6/29/63/63	0/2/2/2
16	BCR	m	101	-	-	7/29/63/63	0/2/2/2
13	CLA	b	834	-	1/1/14/20	4/31/109/115	-
13	CLA	1	834	-	-	10/37/115/115	-
13	CLA	A	818	-	1/1/12/20	7/24/102/115	-
13	CLA	1	806	-	1/1/15/20	11/37/115/115	-
13	CLA	2	821	-	1/1/12/20	2/19/97/115	-
13	CLA	b	830	-	1/1/13/20	9/29/107/115	-
13	CLA	1	817	-	-	7/25/103/115	-
13	CLA	1	839	-	1/1/15/20	9/37/115/115	-
13	CLA	a	842	-	1/1/11/20	6/13/91/115	-
16	BCR	A	845	-	-	8/29/63/63	0/2/2/2
13	CLA	K	4003	-	1/1/11/20	6/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	813	-	1/1/15/20	14/37/115/115	-
13	CLA	b	825	-	1/1/15/20	8/37/115/115	-
16	BCR	l	201	-	-	7/29/63/63	0/2/2/2
13	CLA	J	1101	-	1/1/12/20	8/19/97/115	-
13	CLA	b	823	-	1/1/15/20	10/37/115/115	-
13	CLA	2	813	-	-	6/19/97/115	-
13	CLA	2	836	-	-	12/37/115/115	-
13	CLA	2	803	-	1/1/14/20	11/31/109/115	-
13	CLA	b	808	-	-	13/37/115/115	-
13	CLA	L	203	-	1/1/12/20	6/19/97/115	-
13	CLA	A	815	-	1/1/11/20	2/13/91/115	-
13	CLA	B	830	-	1/1/13/20	9/29/107/115	-
13	CLA	1	836	-	1/1/12/20	5/21/99/115	-
13	CLA	B	825	-	1/1/15/20	8/37/115/115	-
13	CLA	b	805	-	1/1/15/20	11/37/115/115	-
13	CLA	2	829	-	1/1/13/20	9/29/107/115	-
15	SF4	c	102	3	-	-	0/6/5/5
16	BCR	B	843	-	-	9/29/63/63	0/2/2/2
13	CLA	2	831	-	1/1/9/20	2/8/82/115	-
13	CLA	a	828	-	1/1/15/20	9/37/115/115	-
13	CLA	a	809	-	-	7/19/97/115	-
13	CLA	b	817	-	-	0/8/86/115	-
13	CLA	A	808	-	1/1/12/20	3/19/97/115	-
13	CLA	1	821	-	1/1/15/20	11/37/115/115	-
16	BCR	1	847	-	-	15/29/63/63	0/2/2/2
13	CLA	b	824	-	1/1/13/20	7/25/103/115	-
13	CLA	A	830	-	-	13/37/115/115	-
13	CLA	B	816	-	1/1/14/20	5/31/109/115	-
16	BCR	6	205	-	-	12/29/63/63	0/2/2/2
13	CLA	2	811	-	1/1/11/20	2/13/91/115	-
13	CLA	B	805	-	1/1/15/20	11/37/115/115	-
13	CLA	B	804	-	1/1/15/20	15/37/115/115	-
13	CLA	2	809	-	1/1/15/20	13/37/115/115	-
13	CLA	A	802	-	1/1/14/20	10/31/109/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	827	-	1/1/15/20	12/37/115/115	-
13	CLA	1	838	-	1/1/15/20	9/37/115/115	-
16	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
13	CLA	K	4005	-	1/1/11/20	4/11/89/115	-
13	CLA	2	804	-	1/1/15/20	15/37/115/115	-
13	CLA	2	835	-	1/1/15/20	5/37/115/115	-
13	CLA	l	204	-	1/1/12/20	6/19/97/115	-
13	CLA	B	835	-	1/1/12/20	1/19/97/115	-
13	CLA	A	822	-	-	7/19/97/115	-
16	BCR	b	840	-	-	11/29/63/63	0/2/2/2
16	BCR	I	102	-	-	8/29/63/63	0/2/2/2
15	SF4	C	102	3	-	-	0/6/5/5
13	CLA	1	823	-	1/1/12/20	5/19/97/115	-
13	CLA	a	812	-	-	4/15/93/115	-
13	CLA	1	837	-	1/1/14/20	7/31/109/115	-
13	CLA	B	827	-	-	6/13/91/115	-
13	CLA	b	821	-	-	18/37/115/115	-
16	BCR	A	851	-	-	13/29/63/63	0/2/2/2
13	CLA	B	818	-	-	9/15/93/115	-
16	BCR	8	1104	-	-	9/29/63/63	0/2/2/2
13	CLA	B	803	-	1/1/14/20	11/31/109/115	-
13	CLA	B	829	-	1/1/14/20	17/34/112/115	-
13	CLA	a	819	-	1/1/14/20	11/31/109/115	-
16	BCR	B	848	-	-	10/29/63/63	0/2/2/2
13	CLA	A	821	-	1/1/15/20	11/37/115/115	-
16	BCR	b	841	-	-	8/29/63/63	0/2/2/2
13	CLA	l	205	-	1/1/11/20	3/15/93/115	-
13	CLA	a	833	-	1/1/15/20	11/37/115/115	-
13	CLA	B	831	-	1/1/15/20	5/37/115/115	-
13	CLA	a	838	-	1/1/15/20	9/37/115/115	-
14	PQN	A	843	-	-	10/23/43/43	0/2/2/2
13	CLA	A	807	-	1/1/13/20	3/25/103/115	-
12	CL0	a	801	-	2/2/20/25	13/37/135/135	-
13	CLA	a	810	-	-	6/13/91/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	a	832	-	-	7/37/115/115	-
14	PQN	b	839	-	-	10/23/43/43	0/2/2/2
13	CLA	2	830	-	1/1/15/20	5/37/115/115	-
16	BCR	2	840	-	-	8/29/63/63	0/2/2/2
13	CLA	B	824	-	1/1/13/20	7/25/103/115	-
16	BCR	f	205	-	-	12/29/63/63	0/2/2/2
13	CLA	2	823	-	1/1/13/20	7/25/103/115	-
13	CLA	A	834	-	-	10/37/115/115	-
13	CLA	b	820	-	1/1/13/20	6/25/103/115	-
15	SF4	A	844	1,2	-	-	0/6/5/5
13	CLA	F	204	-	1/1/11/20	6/15/93/115	-
13	CLA	8	1102	-	1/1/9/20	4/8/82/115	-
13	CLA	B	808	-	-	13/37/115/115	-
13	CLA	A	826	-	1/1/13/20	6/25/103/115	-
13	CLA	B	821	-	-	18/37/115/115	-
13	CLA	2	816	-	-	0/8/86/115	-
13	CLA	a	837	-	1/1/14/20	7/31/109/115	-
13	CLA	B	811	-	1/1/11/20	7/15/93/115	-
16	BCR	a	845	-	-	8/29/63/63	0/2/2/2
13	CLA	A	811	-	1/1/13/20	8/27/105/115	-
13	CLA	a	826	-	1/1/13/20	6/25/103/115	-
13	CLA	1	813	-	1/1/13/20	10/25/103/115	-
13	CLA	B	832	-	1/1/9/20	2/8/82/115	-
13	CLA	L	206	-	1/1/15/20	8/37/115/115	-
13	CLA	j	1101	-	1/1/12/20	8/19/97/115	-
15	SF4	3	101	3	-	-	0/6/5/5
16	BCR	9	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	1	828	-	1/1/15/20	9/37/115/115	-
15	SF4	3	102	3	-	-	0/6/5/5
13	CLA	B	820	-	1/1/13/20	6/25/103/115	-
15	SF4	1	844	1,2	-	-	0/6/5/5
13	CLA	a	818	-	1/1/12/20	7/24/102/115	-
16	BCR	b	842	-	-	14/29/63/63	0/2/2/2
16	BCR	6	202	-	-	12/29/63/63	0/2/2/2
13	CLA	1	804	-	1/1/13/20	2/25/103/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	k	4003	-	1/1/11/20	6/15/93/115	-
13	CLA	1	831	-	-	7/19/97/115	-
13	CLA	1	815	-	1/1/11/20	2/13/91/115	-
13	CLA	A	805	-	1/1/13/20	10/25/103/115	-
16	BCR	l	203	-	-	10/29/63/63	0/2/2/2
13	CLA	J	1103	-	1/1/11/20	7/13/91/115	-
13	CLA	1	803	-	1/1/15/20	11/37/115/115	-
16	BCR	J	1104	-	-	8/29/63/63	0/2/2/2
13	CLA	0	202	-	-	10/31/109/115	-
16	BCR	2	841	-	-	14/29/63/63	0/2/2/2
13	CLA	1	825	-	-	14/34/112/115	-
13	CLA	A	842	-	1/1/11/20	6/13/91/115	-
13	CLA	A	817	-	-	7/25/103/115	-
13	CLA	2	837	-	-	7/37/115/115	-
16	BCR	b	844	-	-	6/29/63/63	0/2/2/2
16	BCR	j	1104	-	-	8/29/63/63	0/2/2/2
13	CLA	a	839	-	1/1/15/20	9/37/115/115	-
13	CLA	f	203	-	1/1/11/20	0/13/91/115	-
13	CLA	b	847	-	1/1/15/20	9/37/115/115	-
13	CLA	a	806	-	1/1/15/20	11/37/115/115	-
16	BCR	F	205	-	-	12/29/63/63	0/2/2/2
13	CLA	1	805	-	1/1/13/20	10/25/103/115	-
13	CLA	7	102	-	1/1/15/20	13/37/115/115	-
16	BCR	L	205	-	-	11/29/63/63	0/2/2/2
16	BCR	2	847	-	-	10/29/63/63	0/2/2/2
16	BCR	z	101	-	-	7/29/63/63	0/2/2/2
13	CLA	A	841	-	1/1/14/20	10/31/109/115	-
13	CLA	2	826	-	-	6/13/91/115	-
13	CLA	a	814	-	1/1/12/20	2/19/97/115	-
13	CLA	2	819	-	1/1/13/20	6/25/103/115	-
19	SQD	i	101	-	-	19/45/65/69	0/1/1/1
13	CLA	b	822	-	1/1/12/20	2/19/97/115	-
13	CLA	1	811	-	1/1/13/20	8/27/105/115	-
13	CLA	a	808	-	1/1/12/20	3/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	b	813	-	1/1/15/20	14/37/115/115	-
13	CLA	b	815	-	1/1/15/20	12/37/115/115	-
16	BCR	B	844	-	-	6/29/63/63	0/2/2/2
13	CLA	b	836	-	1/1/15/20	5/37/115/115	-
13	CLA	f	204	-	1/1/11/20	6/15/93/115	-
16	BCR	8	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	b	803	-	1/1/14/20	11/31/109/115	-
13	CLA	0	208	-	1/1/15/20	8/37/115/115	-
13	CLA	1	809	-	-	7/19/97/115	-
13	CLA	2	806	-	1/1/15/20	16/37/115/115	-
13	CLA	A	804	-	1/1/13/20	2/25/103/115	-
13	CLA	0	206	-	1/1/11/20	3/15/93/115	-
13	CLA	a	805	-	1/1/13/20	10/25/103/115	-
13	CLA	J	1102	-	1/1/9/20	4/8/82/115	-
16	BCR	B	842	-	-	14/29/63/63	0/2/2/2
16	BCR	M	101	-	-	7/29/63/63	0/2/2/2
13	CLA	6	203	-	1/1/11/20	0/13/91/115	-
13	CLA	6	204	-	1/1/11/20	6/15/93/115	-
13	CLA	2	814	-	1/1/15/20	12/37/115/115	-
18	LMG	2	845	-	-	17/36/56/70	0/1/1/1
13	CLA	B	836	-	1/1/15/20	5/37/115/115	-
13	CLA	1	802	-	1/1/14/20	10/31/109/115	-
16	BCR	b	848	-	-	10/29/63/63	0/2/2/2
13	CLA	B	822	-	1/1/12/20	2/19/97/115	-
13	CLA	b	804	-	1/1/15/20	15/37/115/115	-
16	BCR	a	851	-	-	13/29/63/63	0/2/2/2
13	CLA	1	835	-	-	13/27/105/115	-
13	CLA	a	827	-	1/1/15/20	12/37/115/115	-
13	CLA	b	835	-	1/1/12/20	1/19/97/115	-
13	CLA	2	846	-	1/1/15/20	9/37/115/115	-
13	CLA	A	840	-	-	11/37/115/115	-
13	CLA	2	832	-	1/1/12/20	5/19/97/115	-
13	CLA	1	824	-	1/1/14/20	14/31/109/115	-
13	CLA	0	205	-	1/1/12/20	6/19/97/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	9	4001	-	-	9/29/63/63	0/2/2/2
13	CLA	B	847	-	1/1/15/20	9/37/115/115	-
12	CL0	1	801	-	2/2/20/25	13/37/135/135	-
13	CLA	A	832	-	-	7/37/115/115	-
13	CLA	b	818	-	-	9/15/93/115	-
13	CLA	1	820	-	-	3/15/93/115	-
13	CLA	1	833	-	1/1/15/20	11/37/115/115	-
13	CLA	L	201	-	-	10/31/109/115	-
17	LHG	a	850	-	-	19/45/45/53	-
13	CLA	b	837	-	-	12/37/115/115	-
13	CLA	9	4002	-	1/1/11/20	5/13/91/115	-
13	CLA	b	829	-	1/1/14/20	17/34/112/115	-
13	CLA	b	831	-	1/1/15/20	5/37/115/115	-
13	CLA	2	807	-	-	13/37/115/115	-
13	CLA	0	203	-	1/1/15/20	14/37/115/115	-
13	CLA	A	820	-	-	3/15/93/115	-
16	BCR	K	4004	-	-	11/29/63/63	0/2/2/2
13	CLA	1	841	-	1/1/14/20	10/31/109/115	-
13	CLA	a	830	-	-	13/37/115/115	-
13	CLA	1	830	-	-	13/37/115/115	-
13	CLA	a	807	-	1/1/13/20	3/25/103/115	-
13	CLA	B	837	-	-	12/37/115/115	-
16	BCR	i	103	-	-	8/29/63/63	0/2/2/2
16	BCR	L	207	-	-	7/29/63/63	0/2/2/2
16	BCR	l	206	-	-	11/29/63/63	0/2/2/2
13	CLA	a	825	-	-	14/34/112/115	-
13	CLA	a	823	-	1/1/12/20	5/19/97/115	-
13	CLA	b	816	-	1/1/14/20	5/31/109/115	-
13	CLA	a	802	-	1/1/14/20	10/31/109/115	-
13	CLA	2	828	-	1/1/14/20	17/34/112/115	-
13	CLA	A	833	-	1/1/15/20	11/37/115/115	-
13	CLA	1	822	-	-	7/19/97/115	-
13	CLA	8	1101	-	1/1/12/20	8/19/97/115	-
16	BCR	2	839	-	-	11/29/63/63	0/2/2/2

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	1	852	-	1/1/14/20	11/31/109/115	-
13	CLA	2	825	-	-	13/31/109/115	-
13	CLA	A	836	-	1/1/12/20	5/21/99/115	-
13	CLA	j	1103	-	1/1/11/20	7/13/91/115	-
13	CLA	a	817	-	-	7/25/103/115	-
16	BCR	2	842	-	-	9/29/63/63	0/2/2/2
13	CLA	b	811	-	1/1/11/20	7/15/93/115	-
18	LMG	b	846	-	-	17/36/56/70	0/1/1/1
17	LHG	a	849	-	-	16/40/40/53	-
13	CLA	B	838	-	-	7/37/115/115	-
13	CLA	A	839	-	1/1/15/20	9/37/115/115	-
13	CLA	I	101	-	1/1/15/20	13/37/115/115	-
13	CLA	B	814	-	-	6/19/97/115	-
14	PQN	B	839	-	-	10/23/43/43	0/2/2/2
13	CLA	a	841	-	1/1/14/20	10/31/109/115	-
13	CLA	f	201	-	1/1/13/20	4/25/103/115	-
13	CLA	2	817	-	-	9/15/93/115	-
13	CLA	a	834	-	-	10/37/115/115	-
13	CLA	L	204	-	1/1/11/20	3/15/93/115	-
16	BCR	L	202	-	-	10/29/63/63	0/2/2/2
16	BCR	0	201	-	-	7/29/63/63	0/2/2/2
13	CLA	b	828	-	-	8/25/103/115	-
13	CLA	b	809	-	-	4/13/91/115	-
13	CLA	2	833	-	1/1/14/20	4/31/109/115	-
13	CLA	2	827	-	-	8/25/103/115	-
18	LMG	B	846	-	-	17/36/56/70	0/1/1/1
13	CLA	A	803	-	1/1/15/20	11/37/115/115	-
13	CLA	b	826	-	-	13/31/109/115	-
13	CLA	1	826	-	1/1/13/20	6/25/103/115	-
13	CLA	a	815	-	1/1/11/20	2/13/91/115	-
13	CLA	A	852	-	1/1/14/20	11/31/109/115	-
13	CLA	a	811	-	1/1/13/20	8/27/105/115	-
13	CLA	j	1102	-	1/1/9/20	4/8/82/115	-
13	CLA	2	818	-	-	6/15/93/115	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	A	847	-	-	15/29/63/63	0/2/2/2
15	SF4	C	101	3	-	-	0/6/5/5
16	BCR	A	848	-	-	15/29/63/63	0/2/2/2
13	CLA	F	201	-	1/1/13/20	4/25/103/115	-
13	CLA	K	4002	-	1/1/11/20	5/13/91/115	-
16	BCR	B	840	-	-	11/29/63/63	0/2/2/2
15	SF4	c	101	3	-	-	0/6/5/5
13	CLA	a	829	-	1/1/15/20	10/37/115/115	-
13	CLA	b	838	-	-	7/37/115/115	-
13	CLA	2	815	-	1/1/14/20	5/31/109/115	-
13	CLA	a	840	-	-	11/37/115/115	-
16	BCR	f	202	-	-	12/29/63/63	0/2/2/2
13	CLA	b	810	-	1/1/15/20	13/37/115/115	-
13	CLA	1	810	-	-	6/13/91/115	-
13	CLA	1	814	-	1/1/12/20	2/19/97/115	-
16	BCR	J	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	b	812	-	1/1/11/20	2/13/91/115	-
13	CLA	a	835	-	-	13/27/105/115	-
13	CLA	a	831	-	-	7/19/97/115	-
16	BCR	1	851	-	-	13/29/63/63	0/2/2/2
13	CLA	A	809	-	-	7/19/97/115	-
13	CLA	a	824	-	1/1/14/20	14/31/109/115	-
16	BCR	B	845	-	-	15/29/63/63	0/2/2/2
16	BCR	j	1105	-	-	11/29/63/63	0/2/2/2
13	CLA	B	828	-	-	8/25/103/115	-
13	CLA	1	832	-	-	8/37/115/115	-
13	CLA	1	840	-	-	11/37/115/115	-
13	CLA	A	837	-	1/1/14/20	7/31/109/115	-
16	BCR	k	4004	-	-	11/29/63/63	0/2/2/2
14	PQN	2	838	-	-	10/23/43/43	0/2/2/2
13	CLA	a	820	-	-	3/15/93/115	-
13	CLA	A	829	-	1/1/15/20	10/37/115/115	-
13	CLA	b	833	-	1/1/12/20	5/19/97/115	-
13	CLA	B	815	-	1/1/15/20	12/37/115/115	-

The worst 5 of 1908 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	801	CLA	CHB-C4A	6.62	1.39	1.33
13	B	801	CLA	CHB-C4A	6.59	1.39	1.33
13	b	801	CLA	CHB-C4A	6.50	1.39	1.33
13	2	806	CLA	CHB-C4A	6.49	1.39	1.33
13	B	806	CLA	CHB-C4A	6.39	1.39	1.33

The worst 5 of 2682 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
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 3273 torsion outliers are listed below:

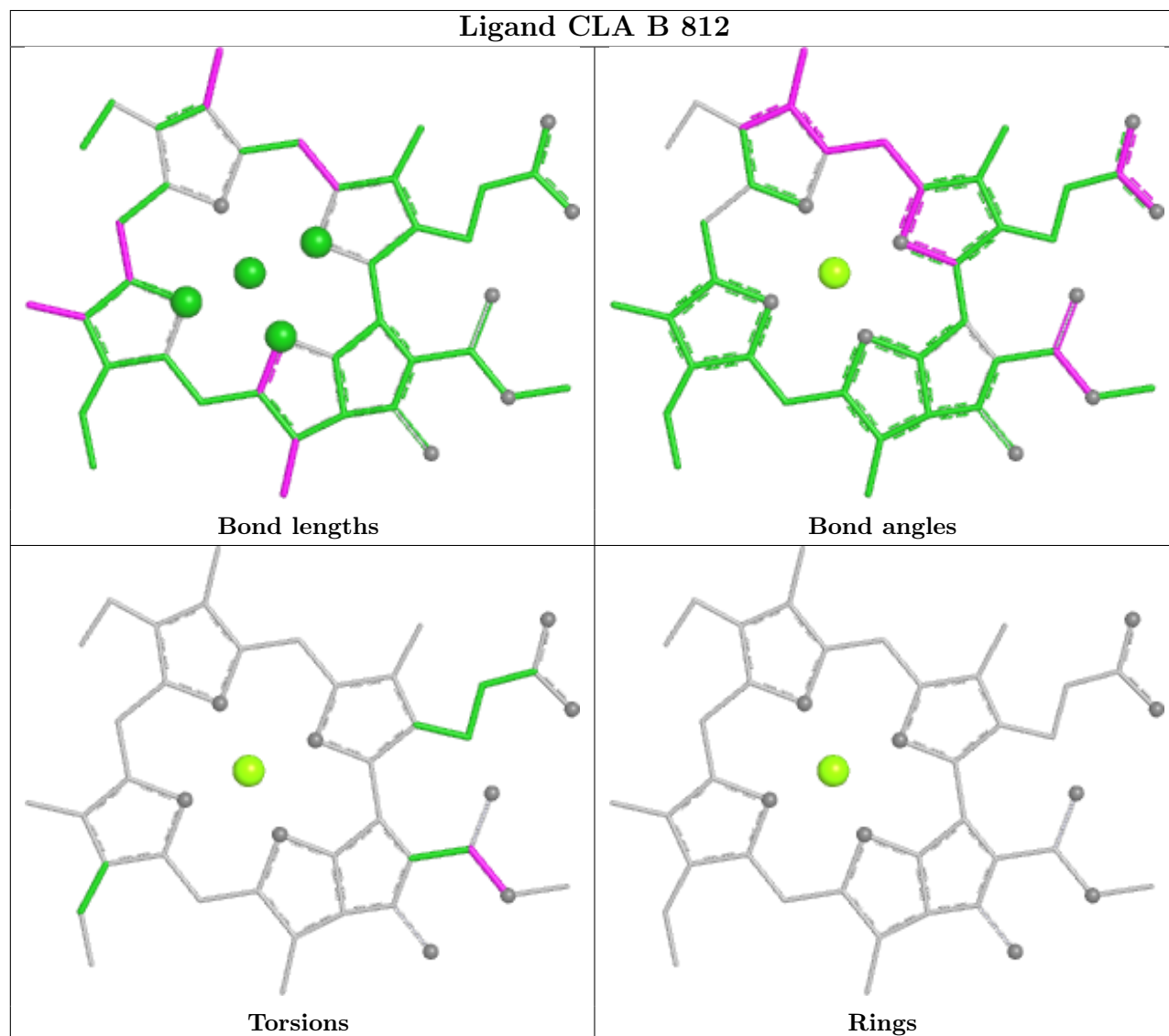
Mol	Chain	Res	Type	Atoms
13	A	805	CLA	CBA-CGA-O2A-C1
13	A	805	CLA	O1A-CGA-O2A-C1
13	A	806	CLA	C1A-C2A-CAA-CBA
13	A	807	CLA	CBD-CGD-O2D-CED
13	A	808	CLA	CHA-CBD-CGD-O1D

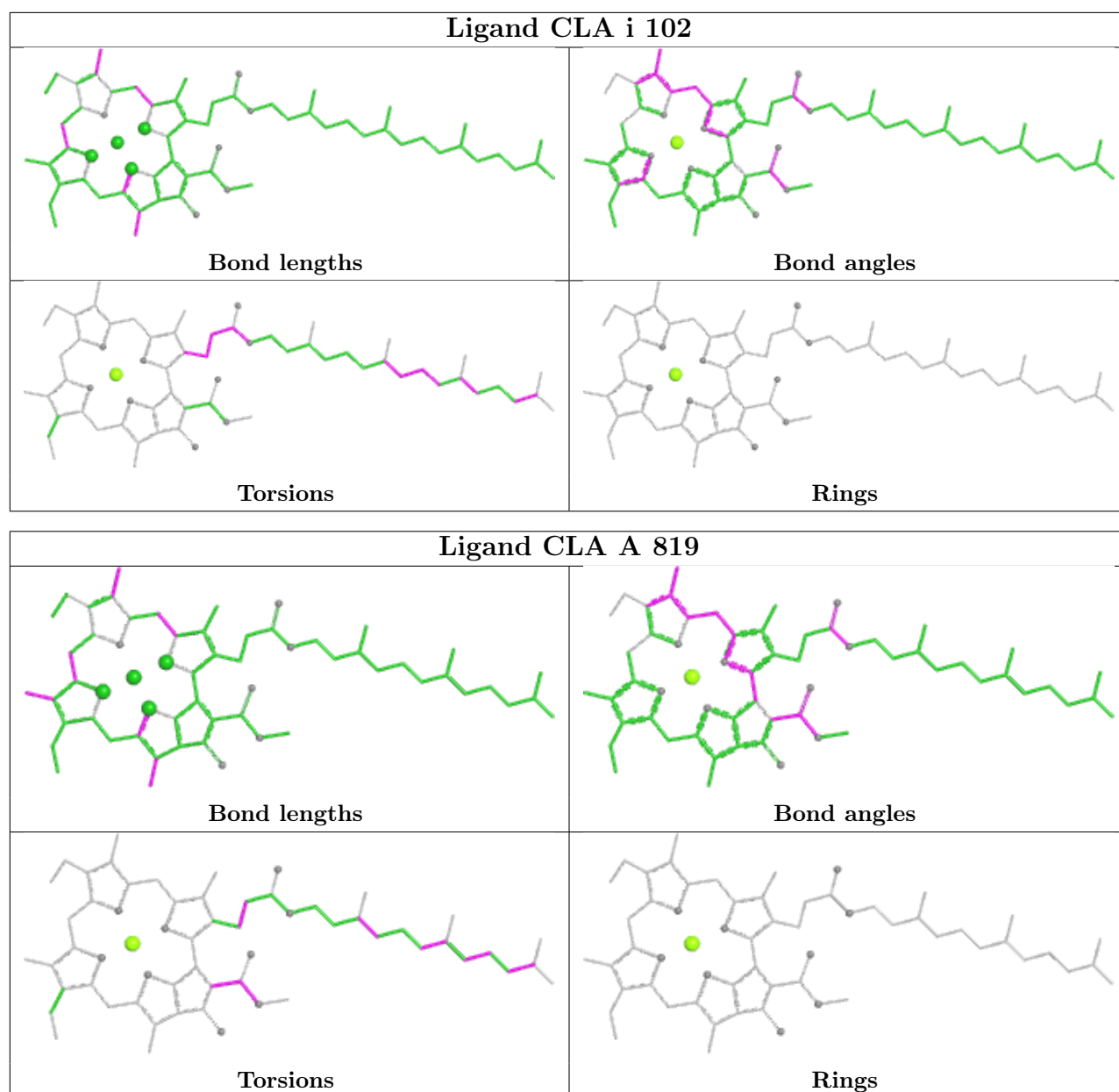
There are no ring outliers.

No monomer is involved in short contacts.

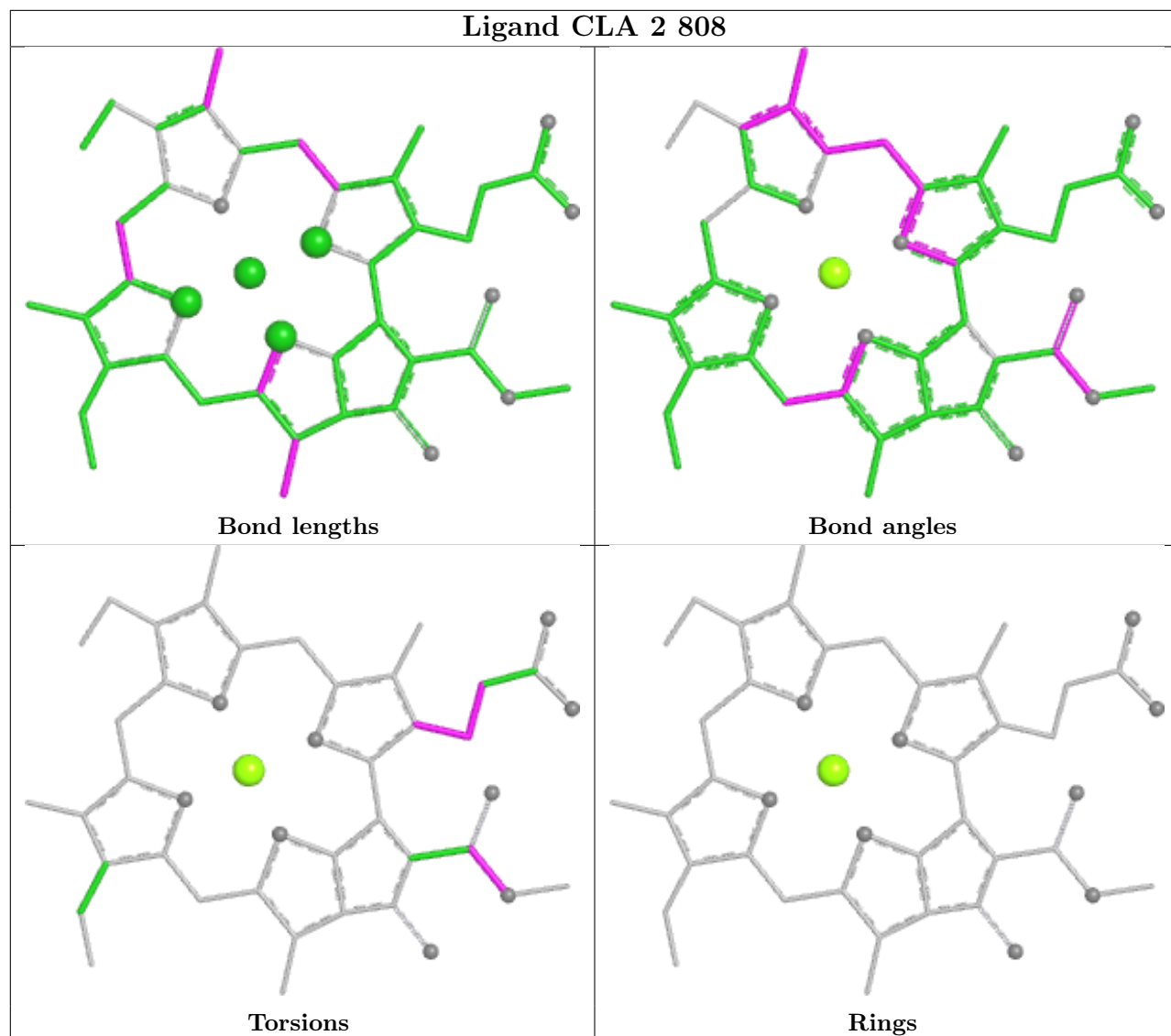
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

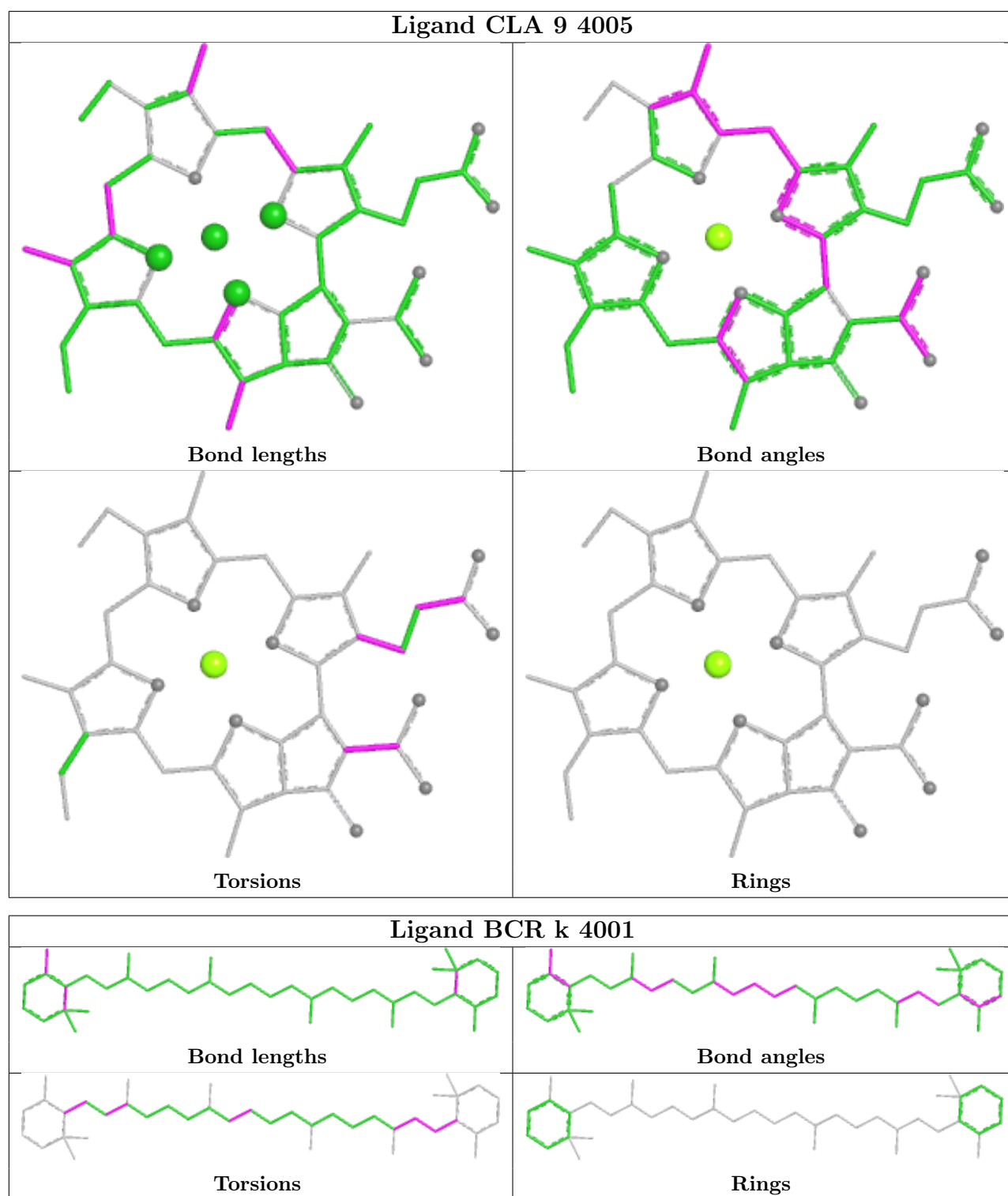
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

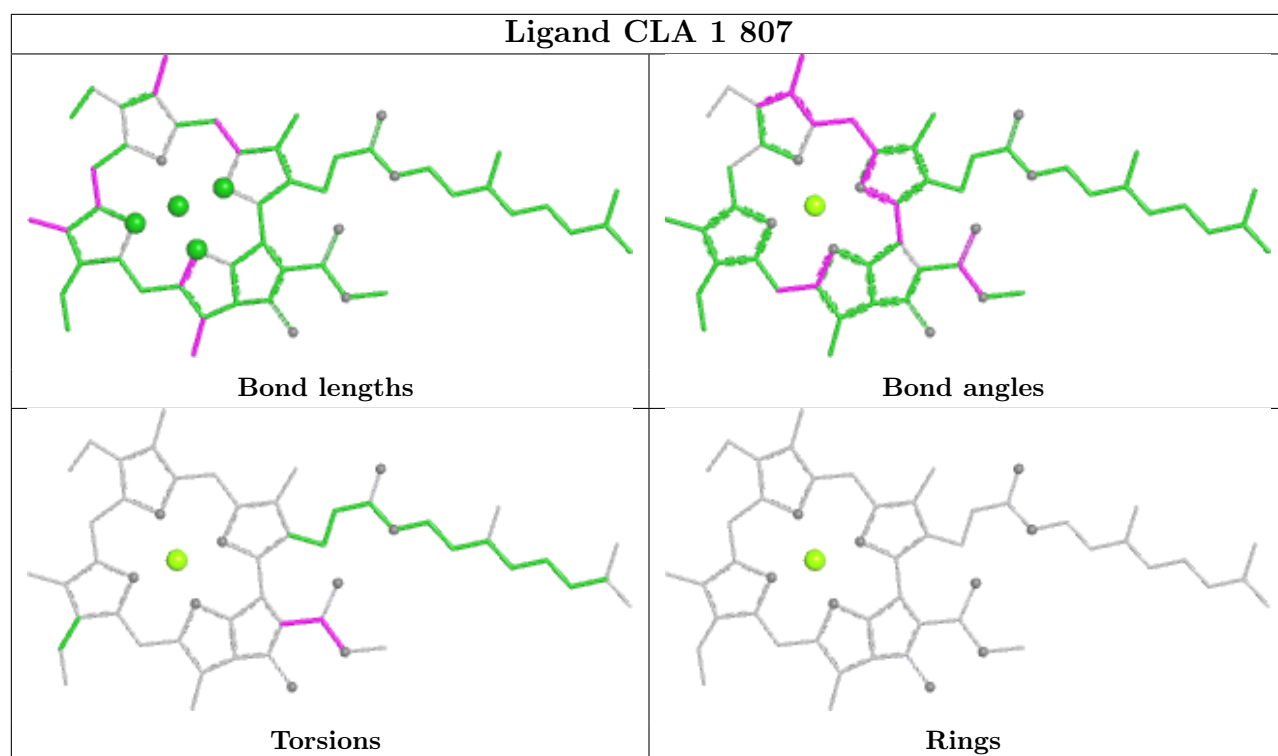


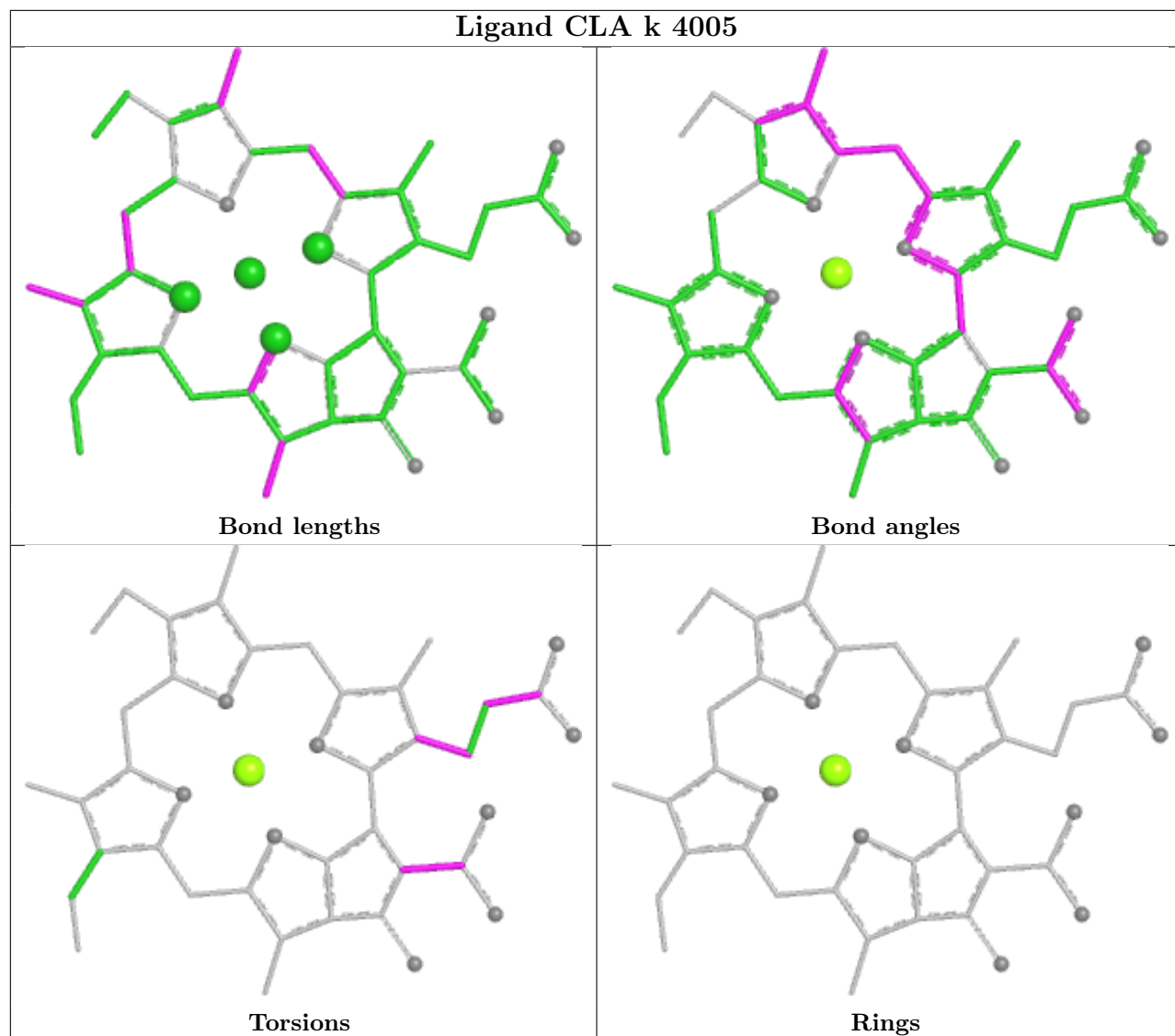


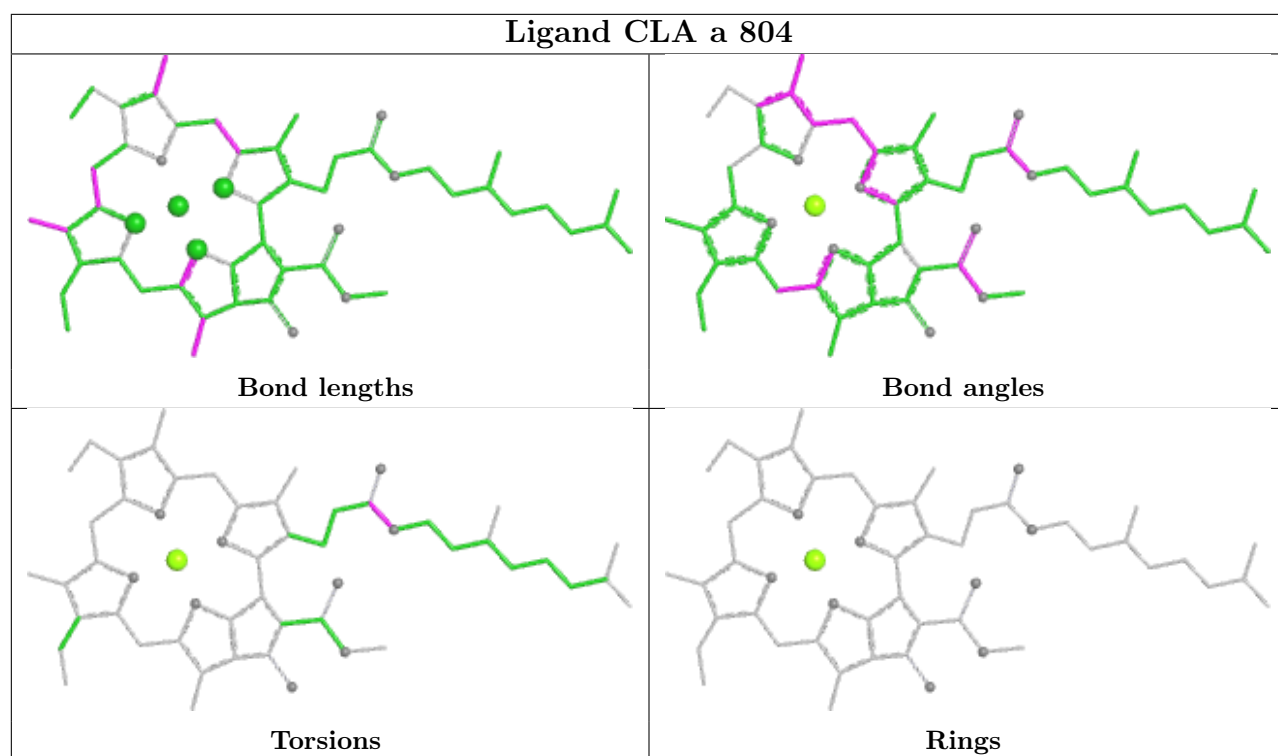
Ligand CLA 2 808



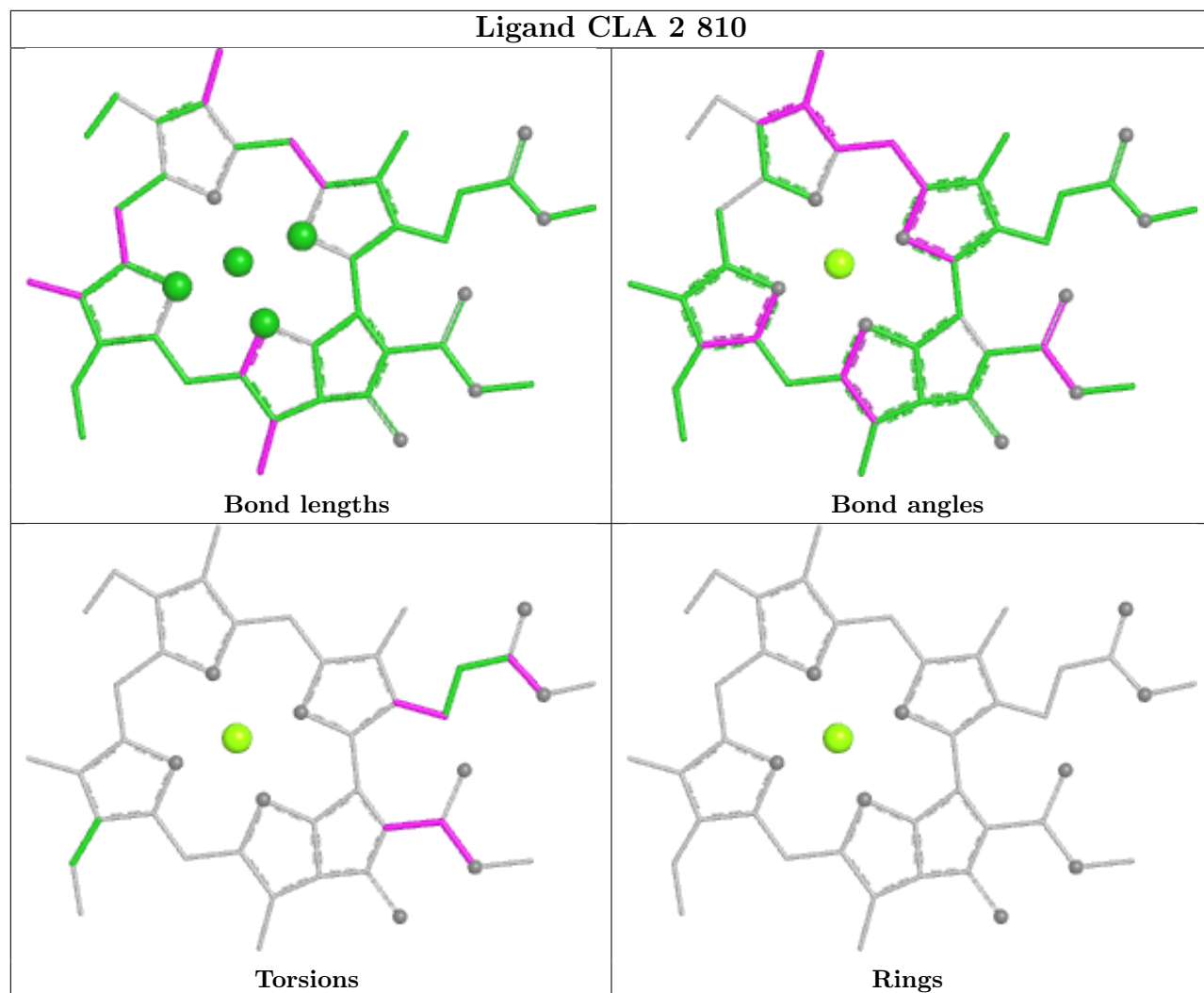




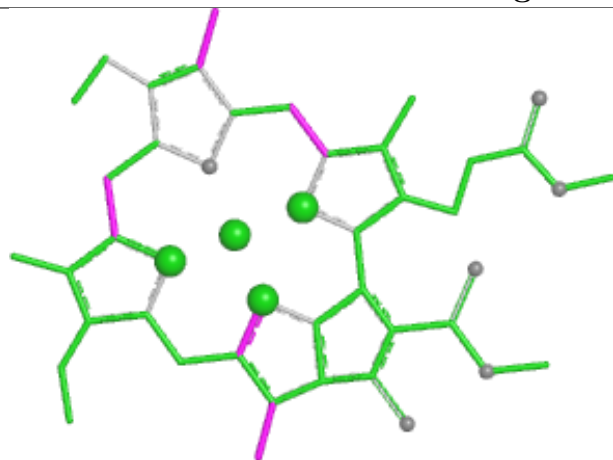




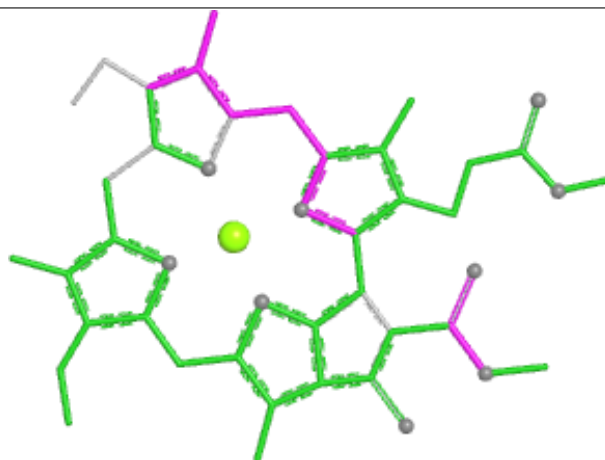
Ligand CLA 2 810



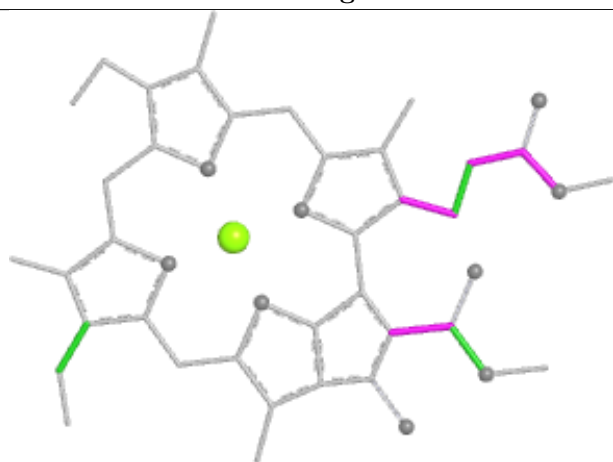
Ligand CLA A 816



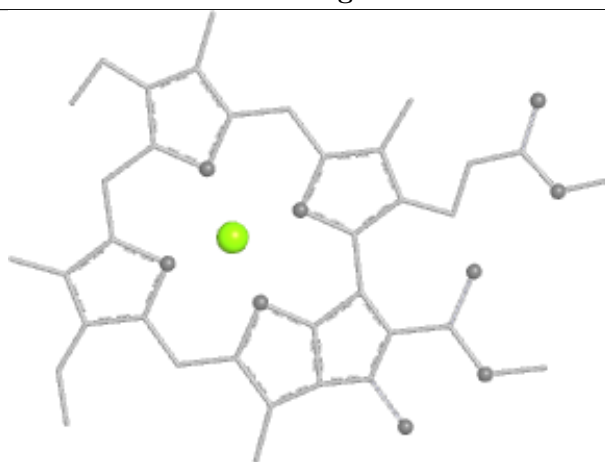
Bond lengths



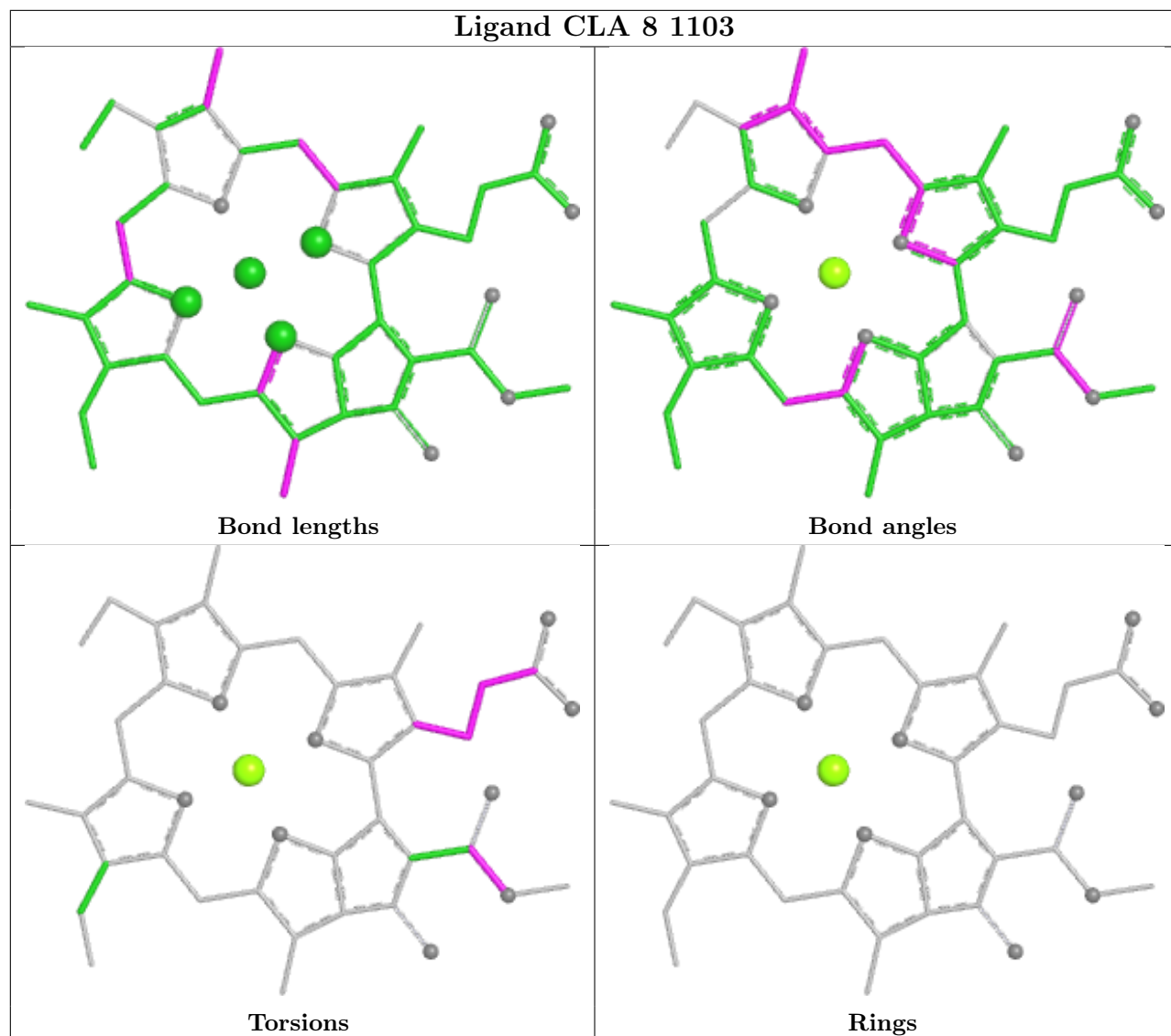
Bond angles

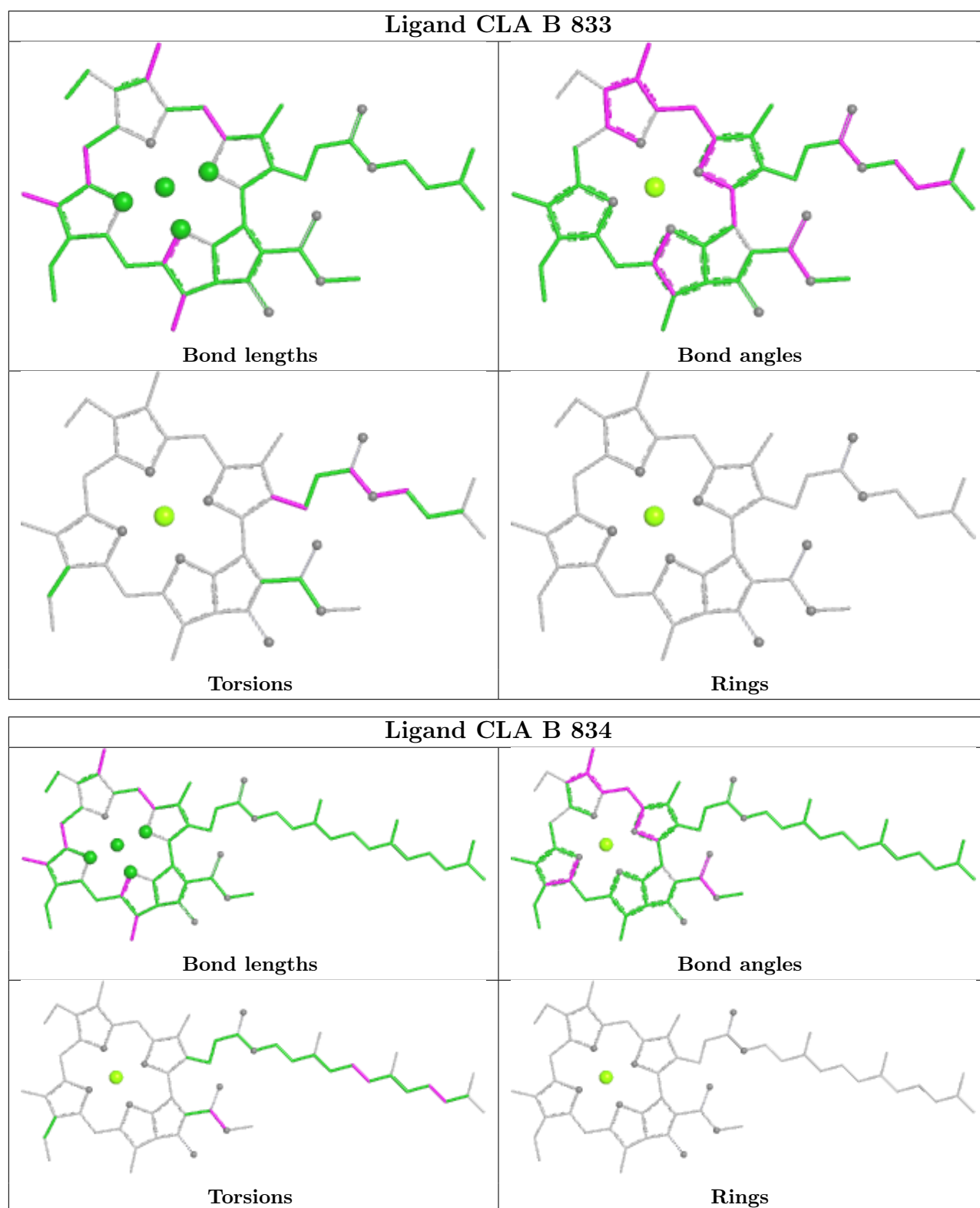


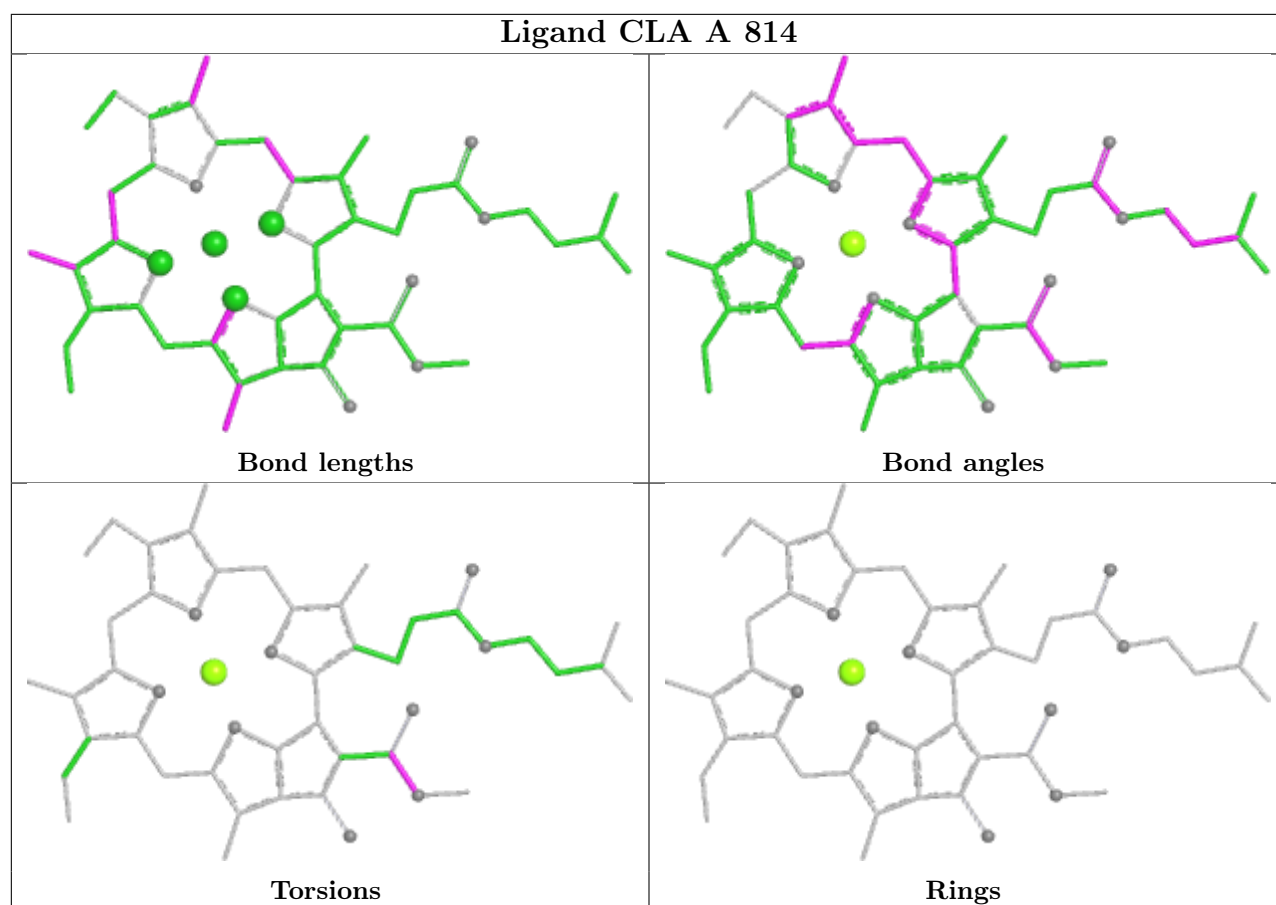
Torsions



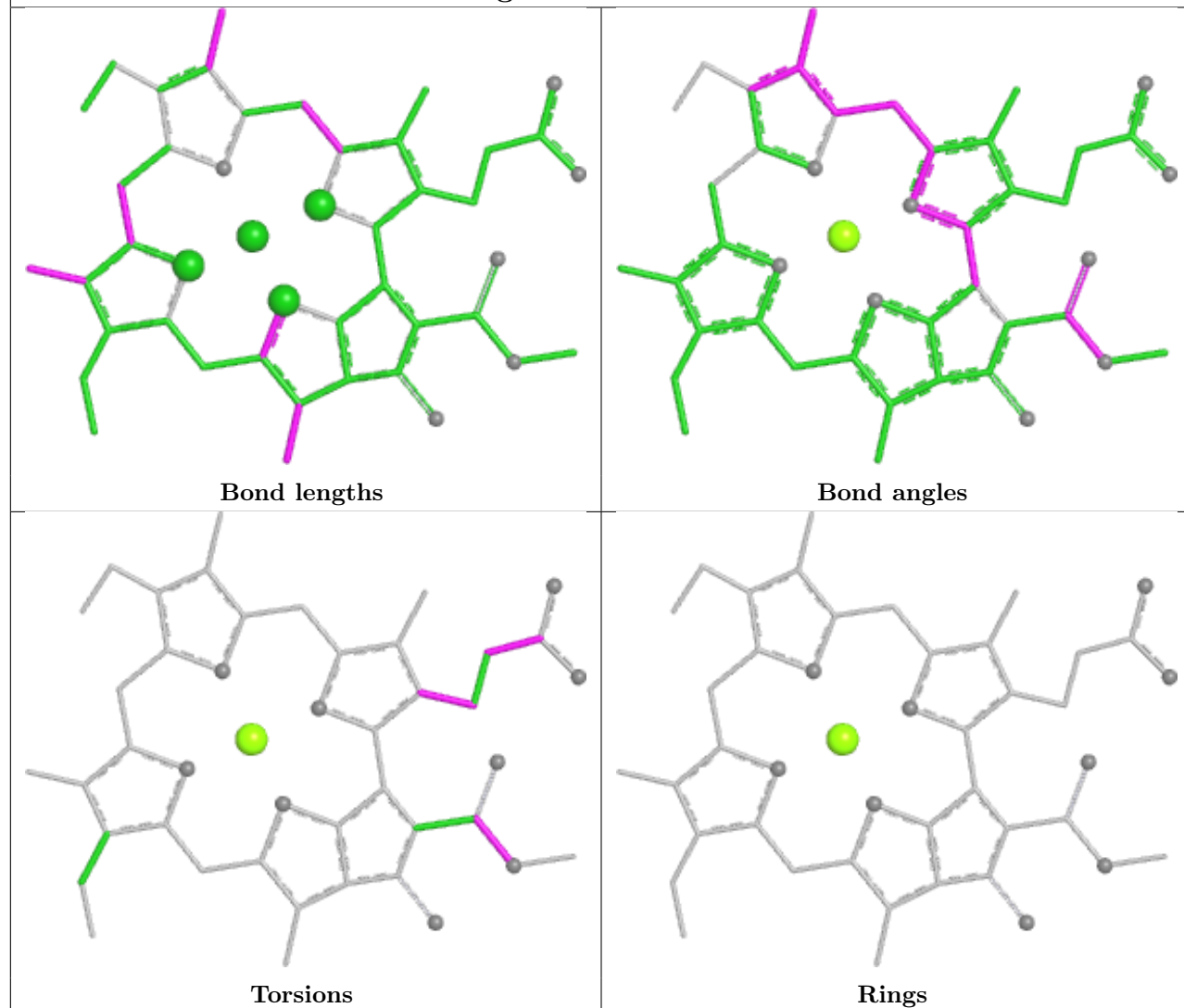
Rings



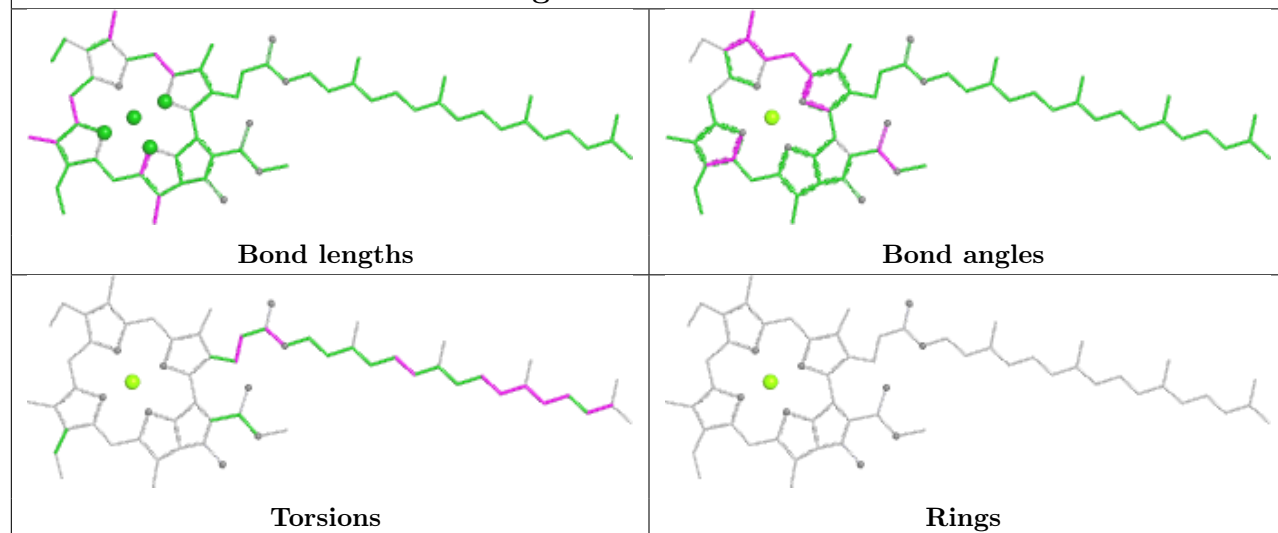


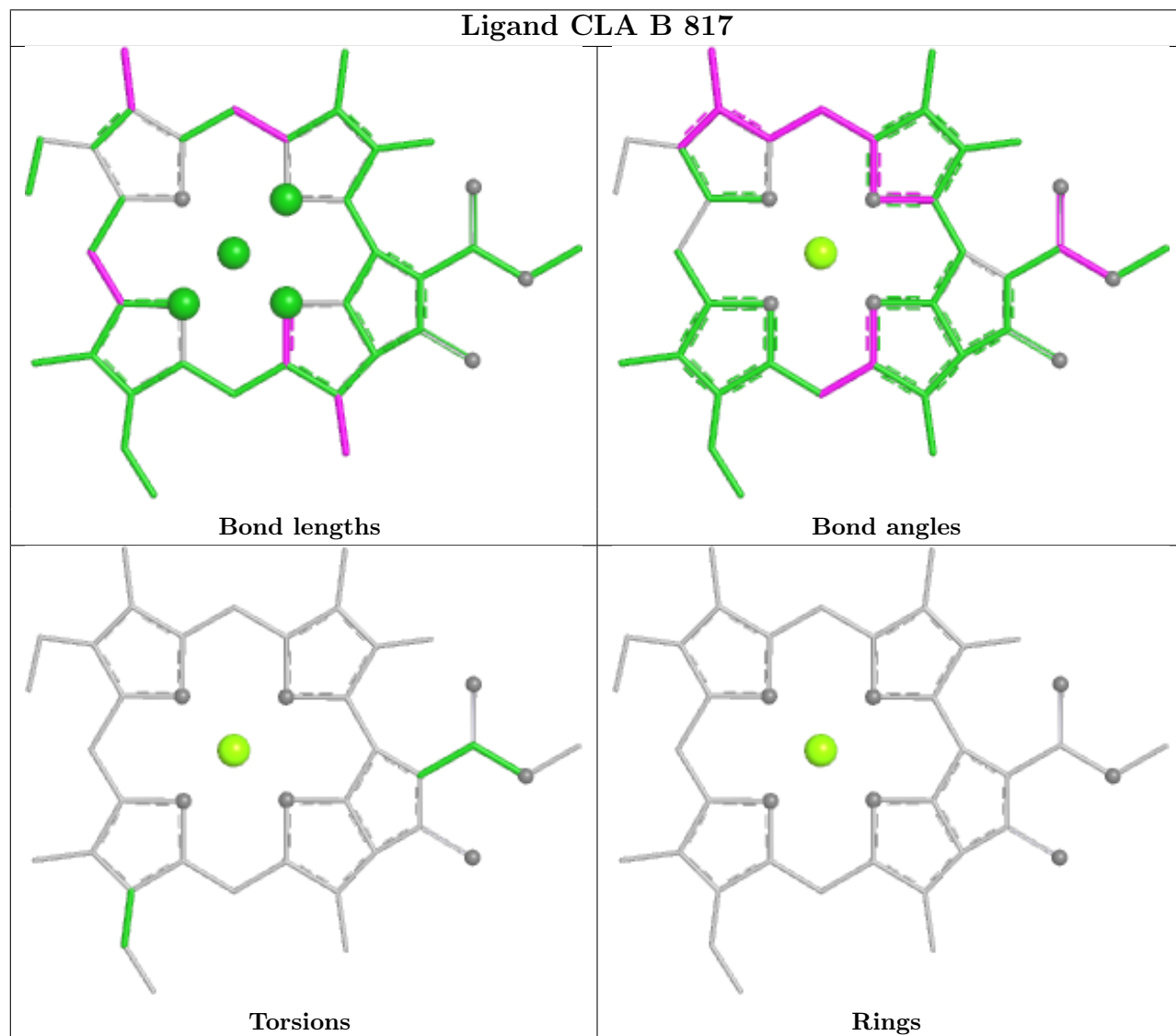
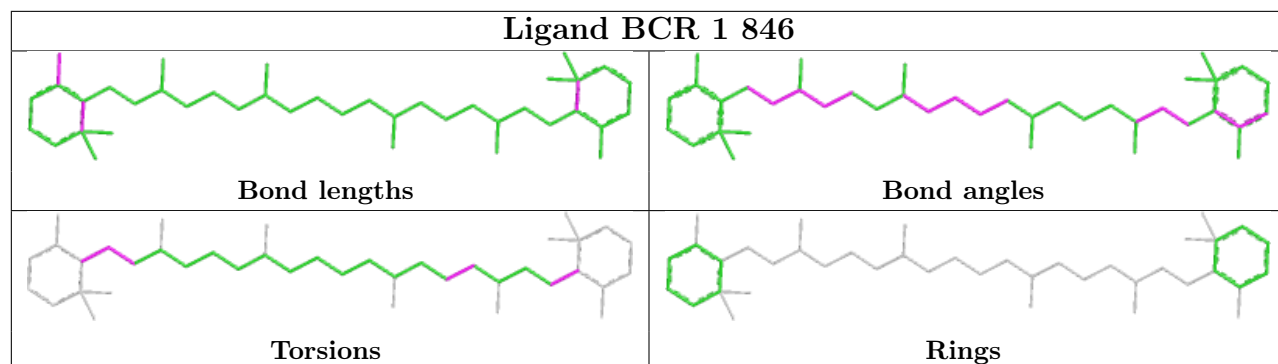


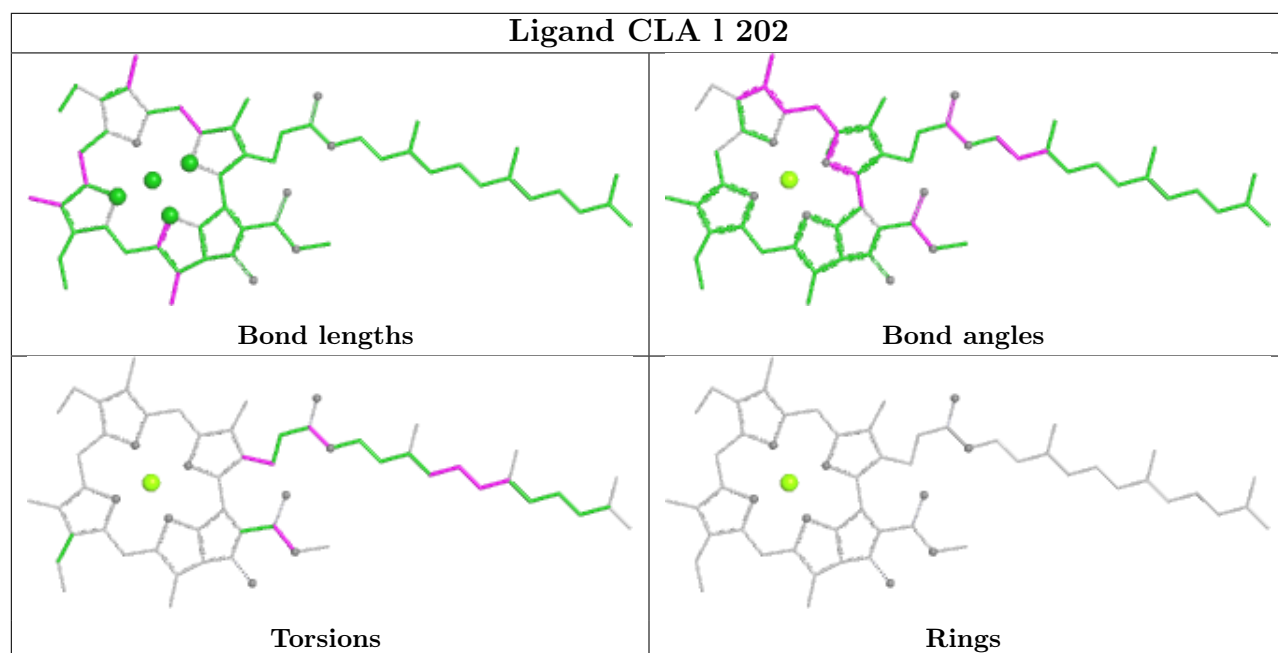
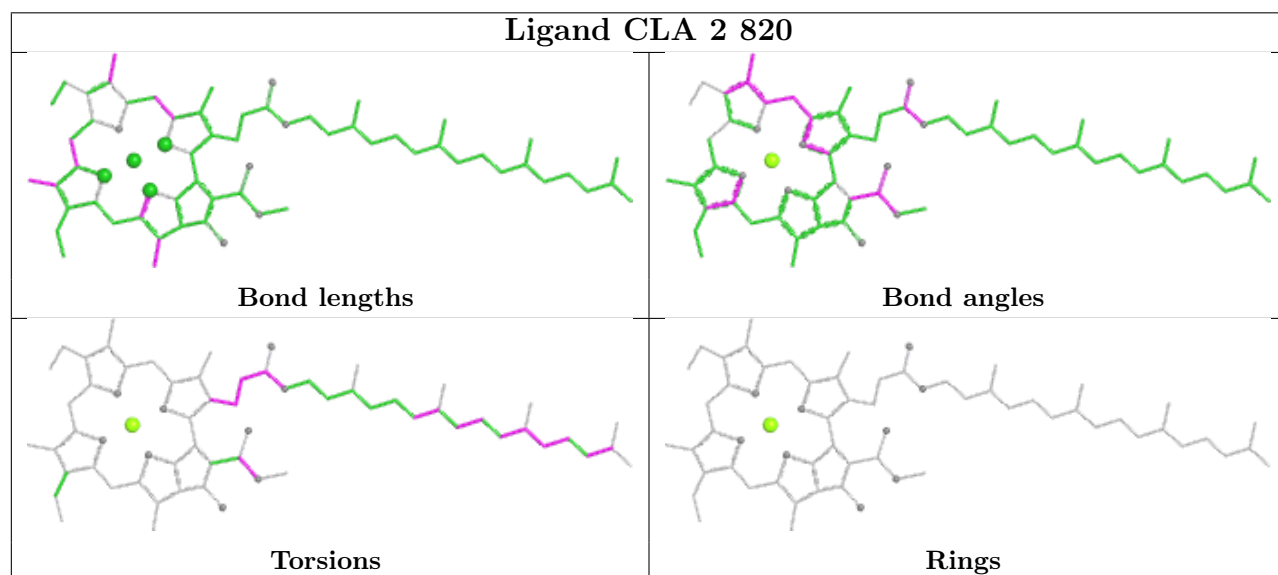
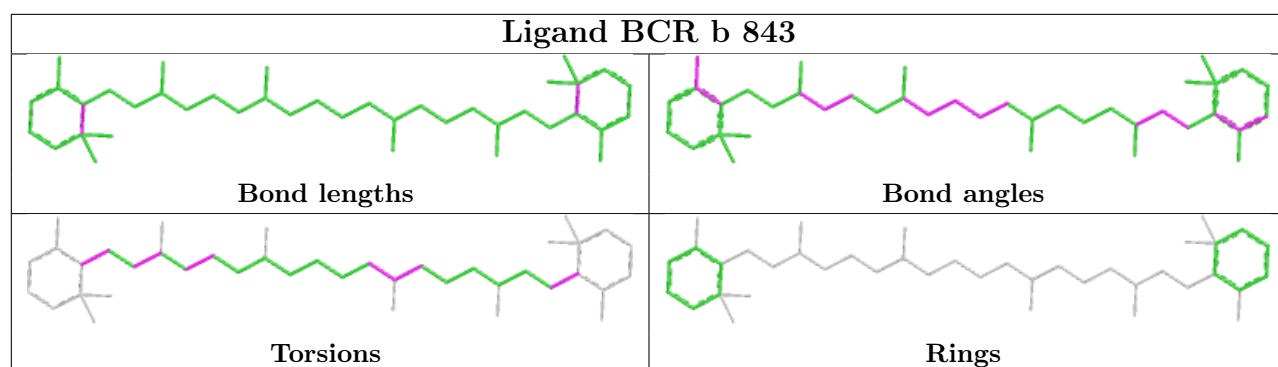
Ligand CLA 1 842

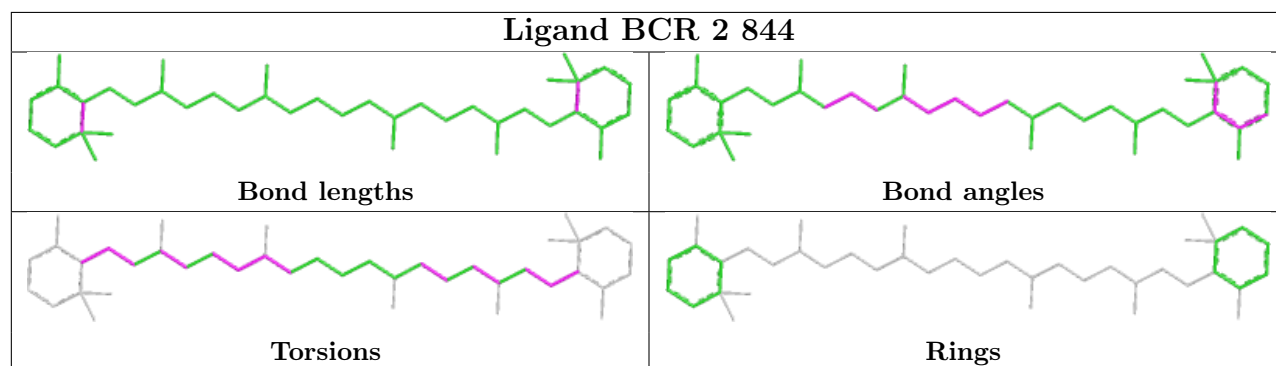
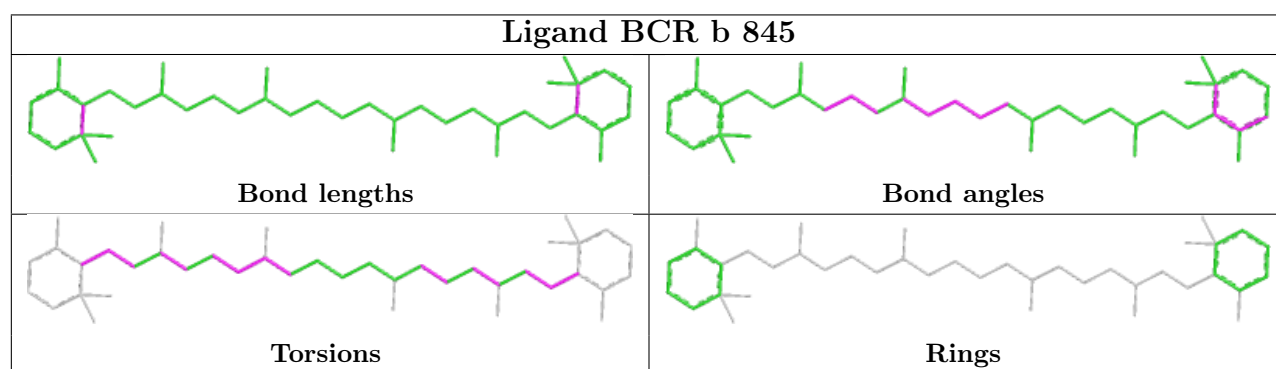
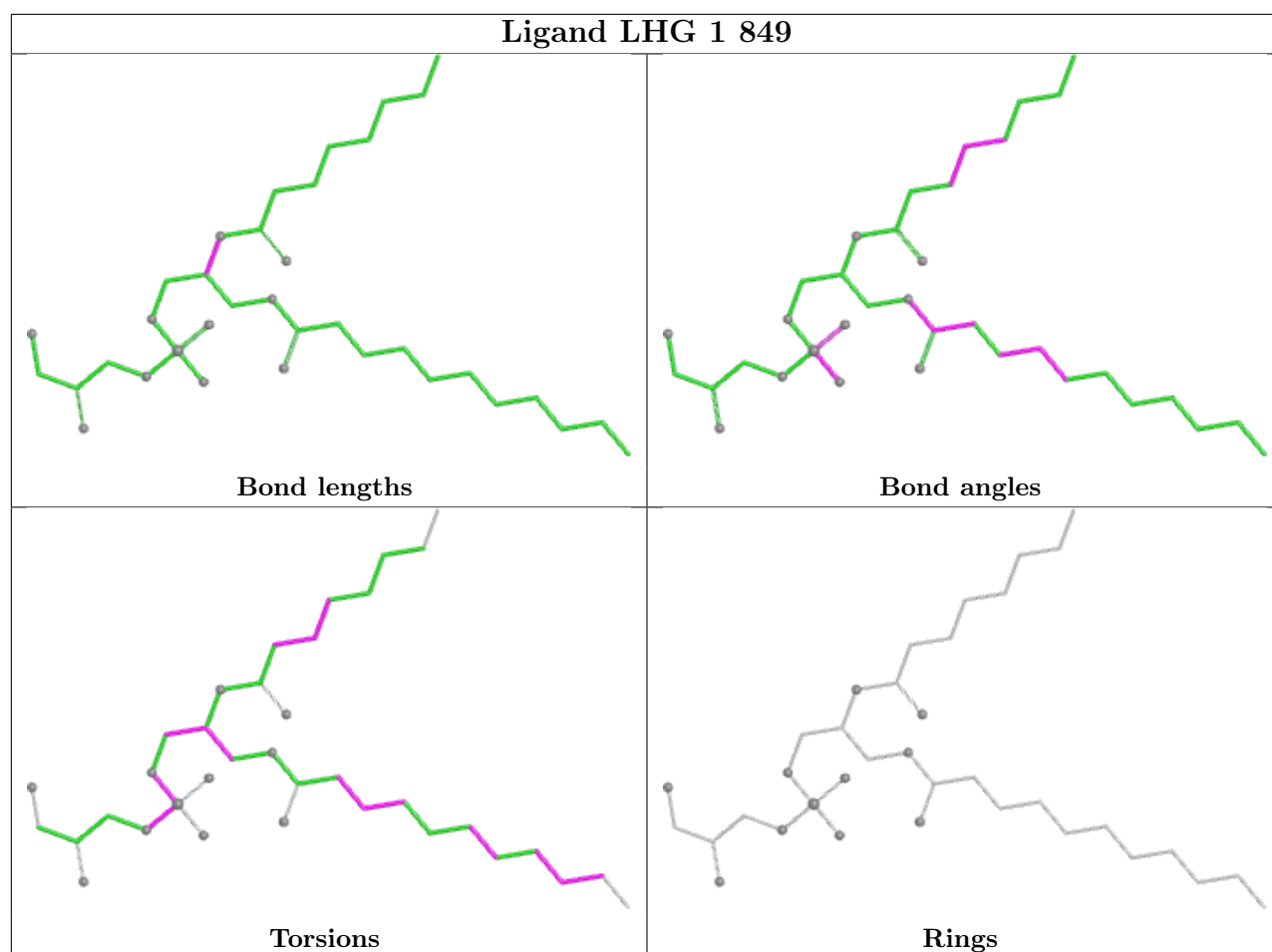


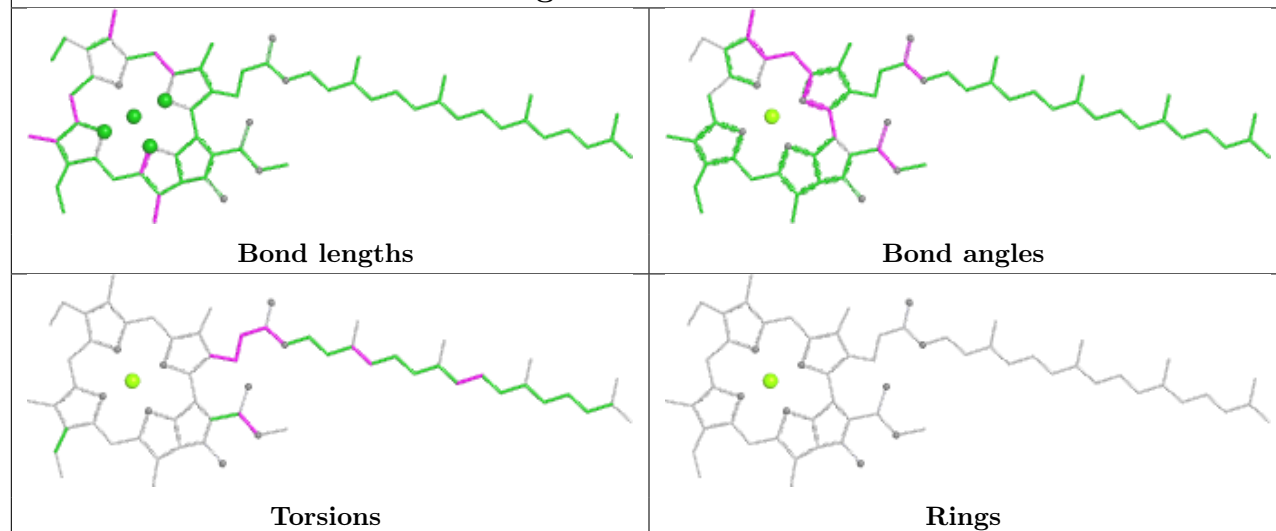
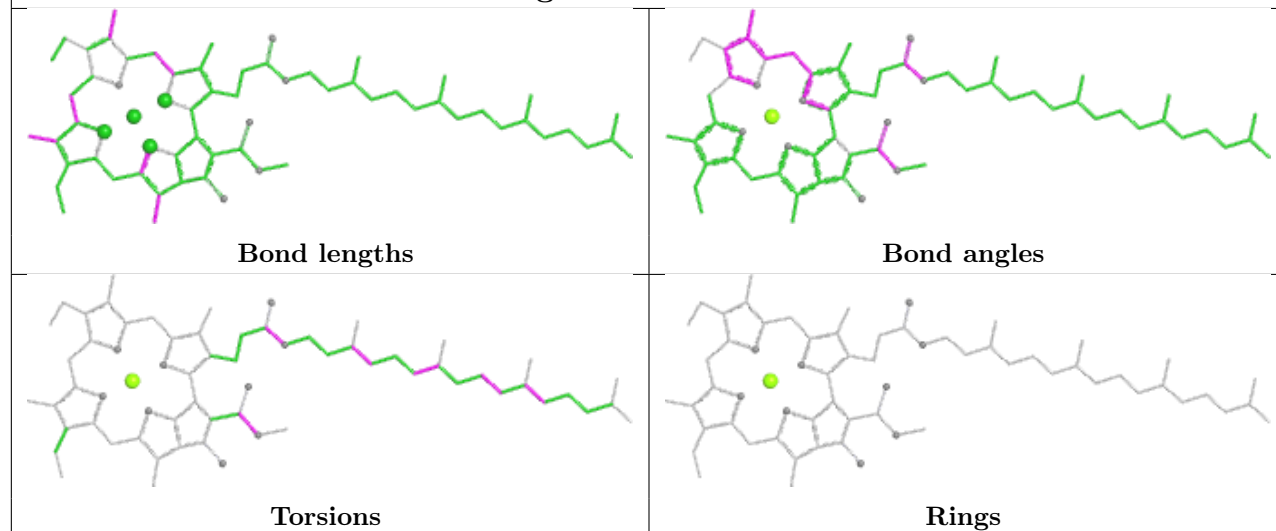
Ligand CLA B 823



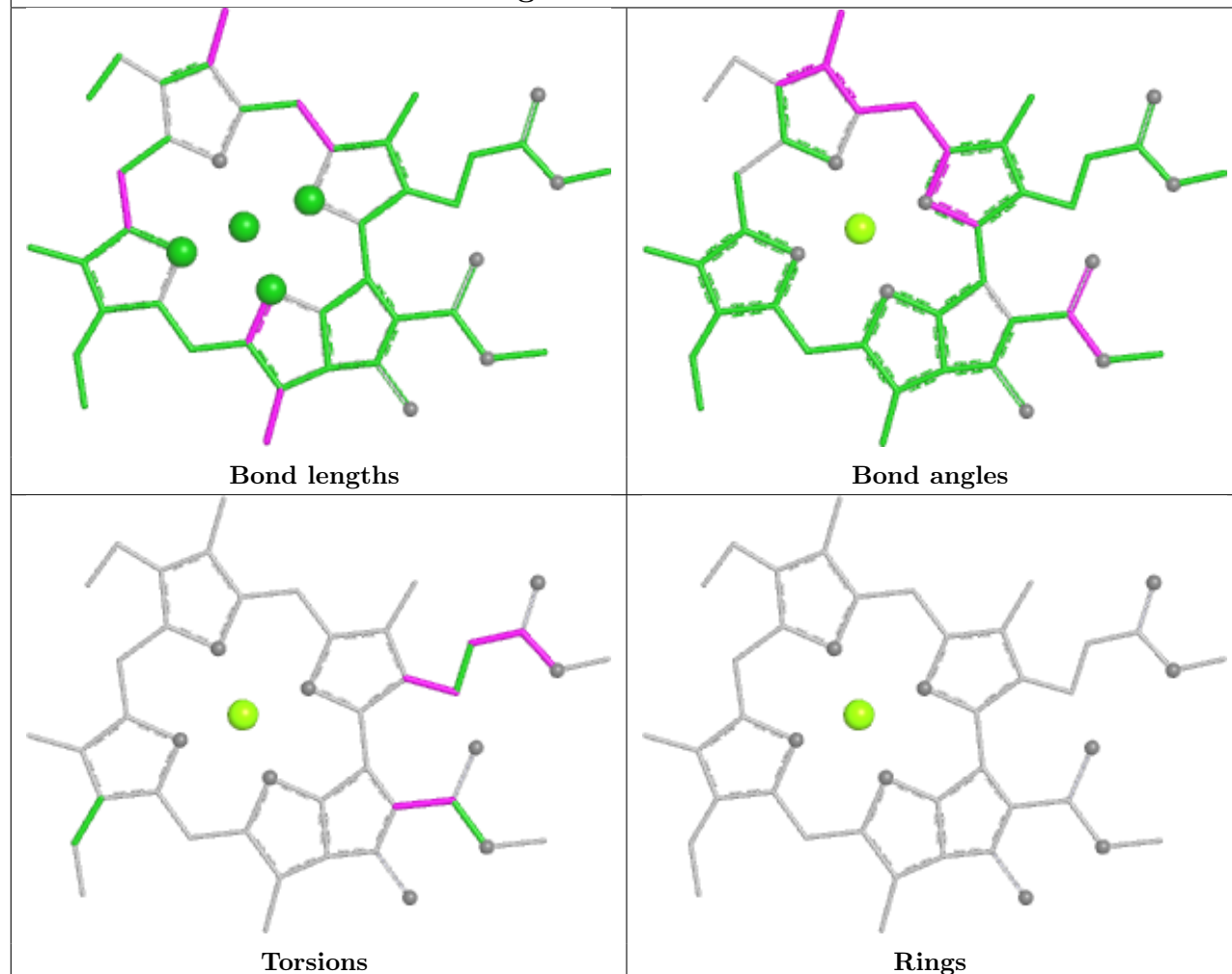




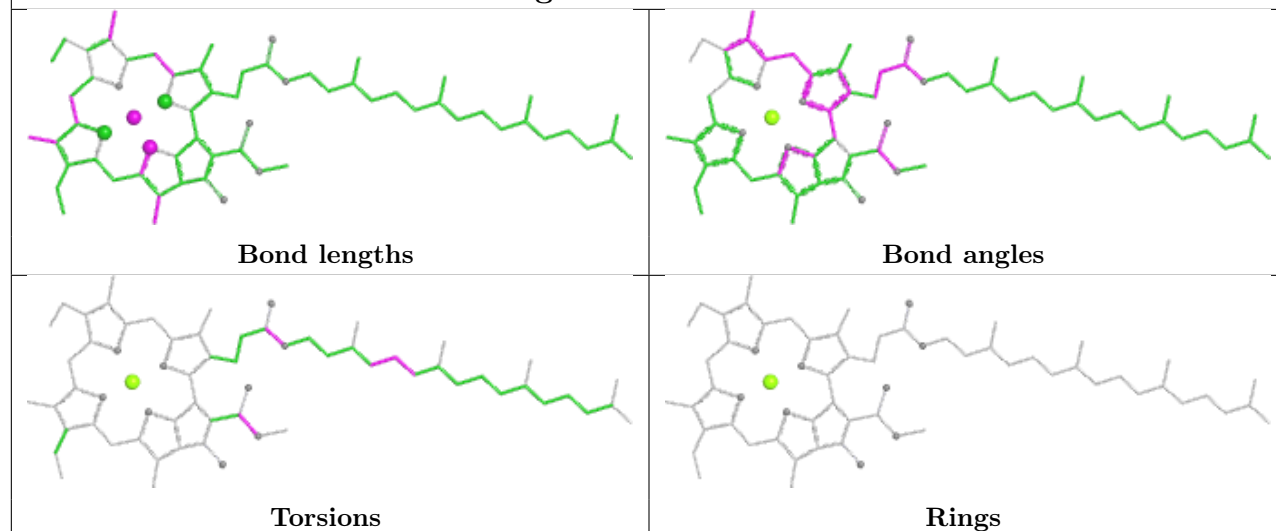


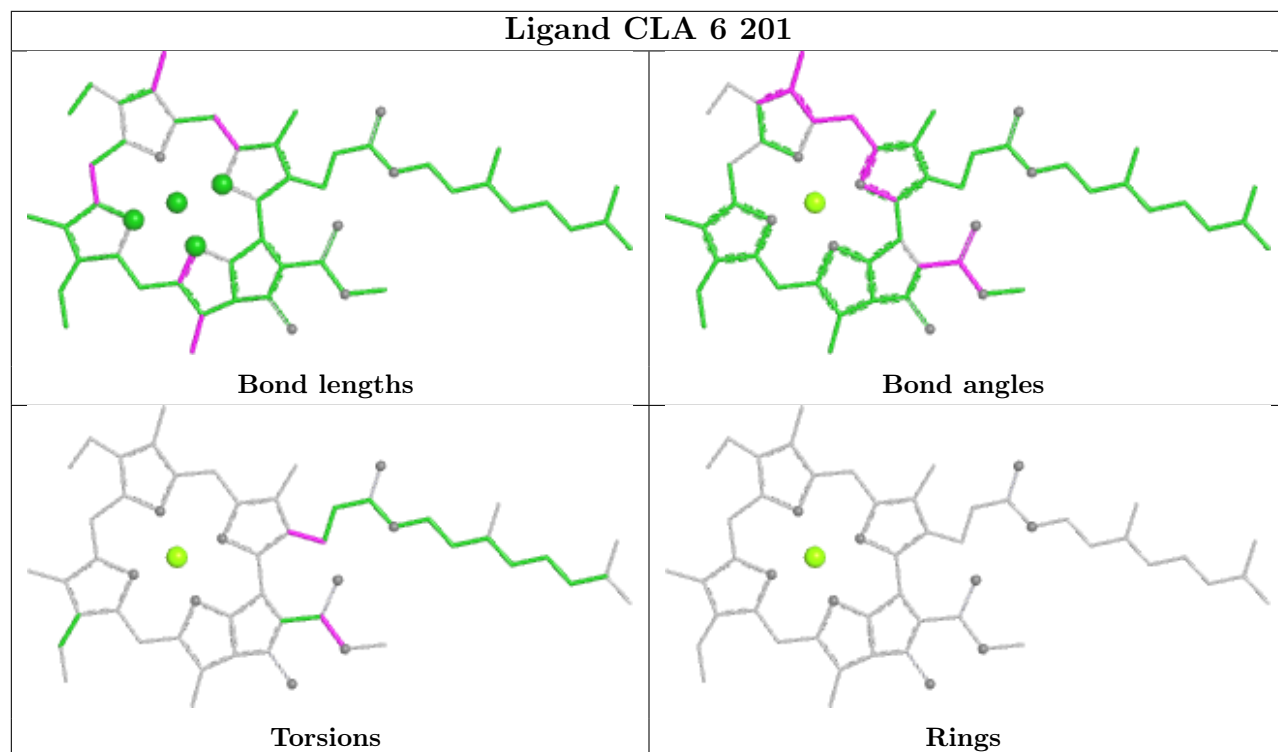
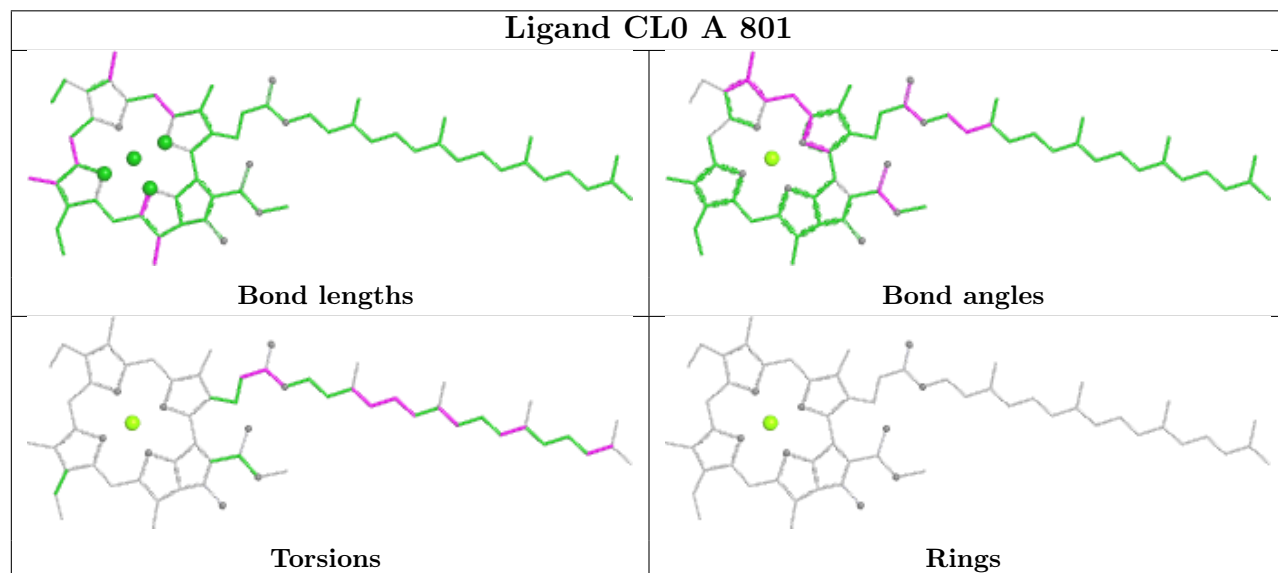
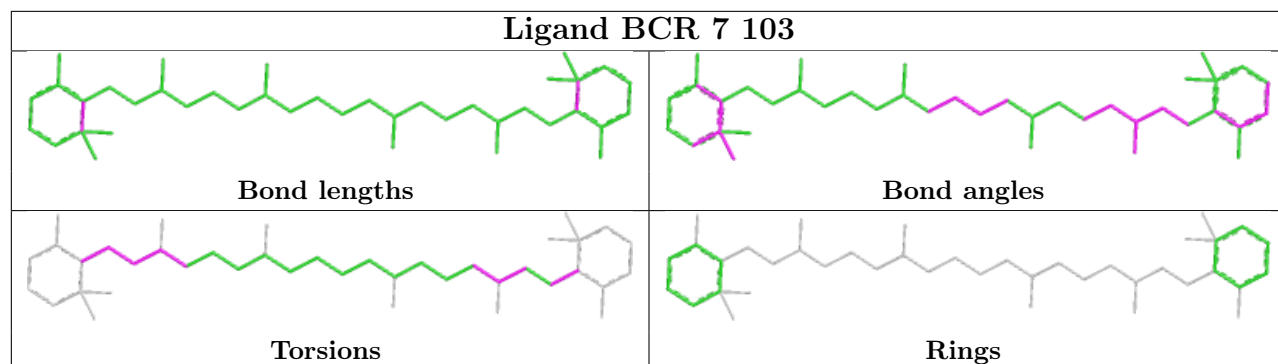
Ligand CLA a 821**Ligand CLA 2 805**

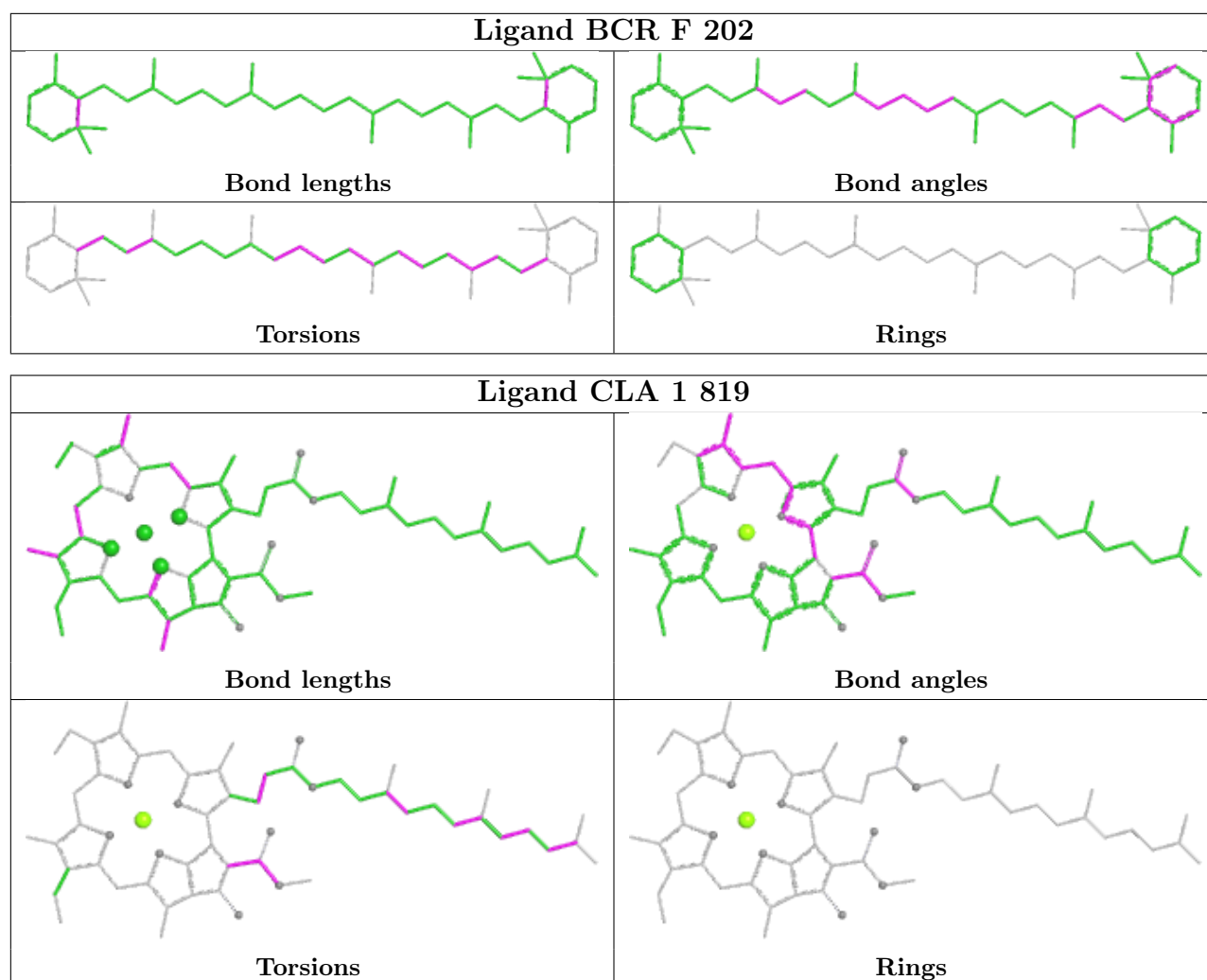
Ligand CLA 1 816

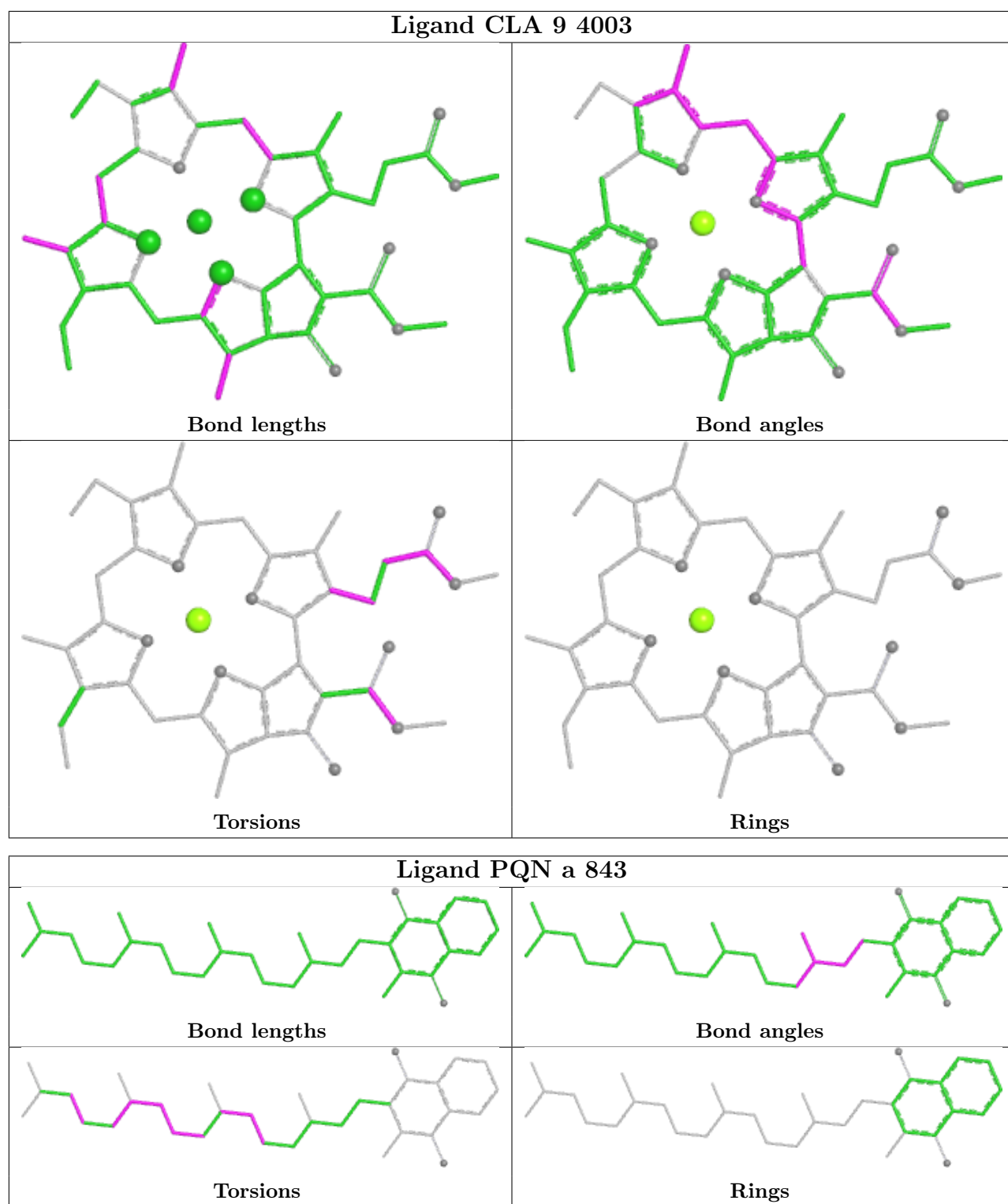


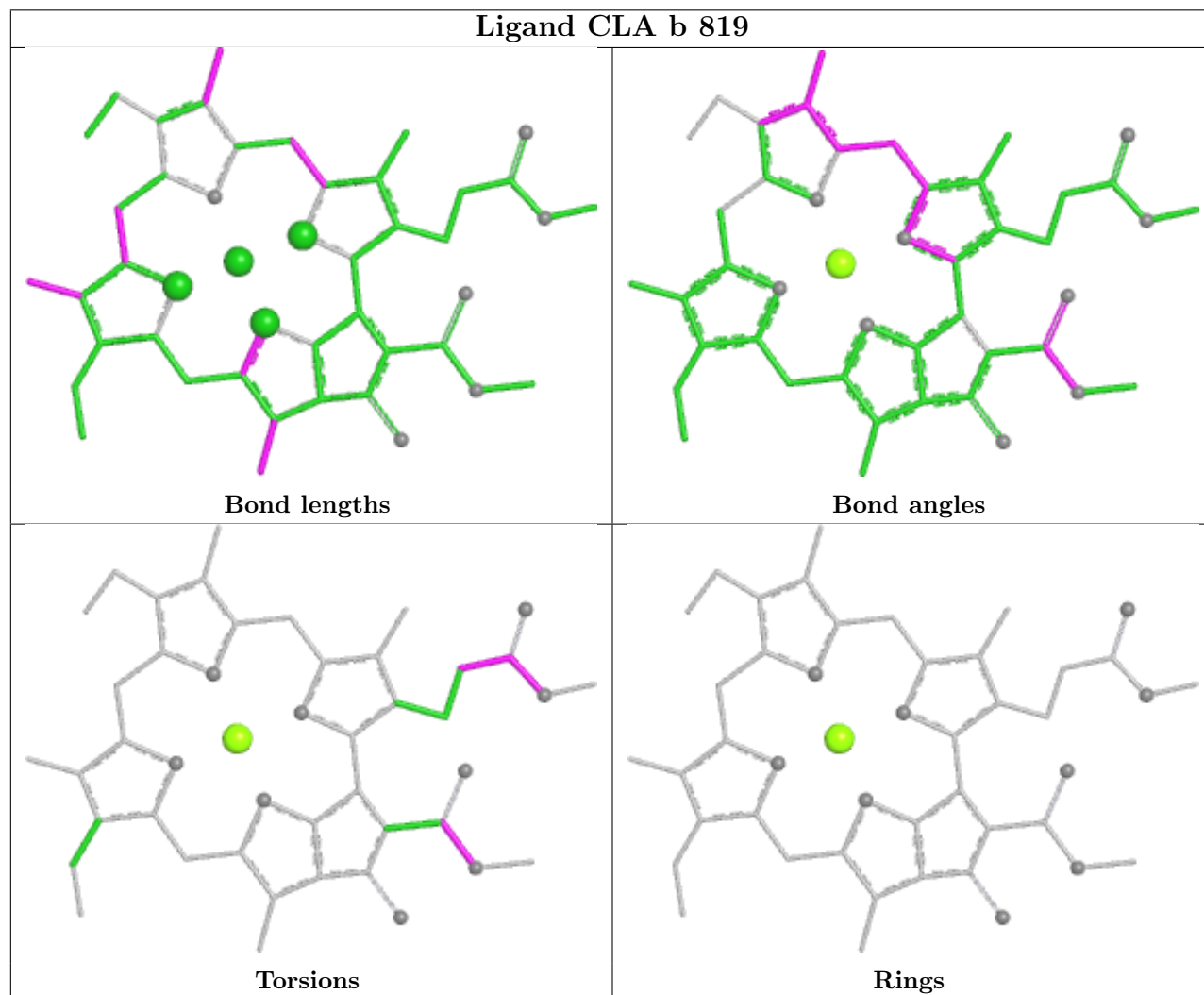
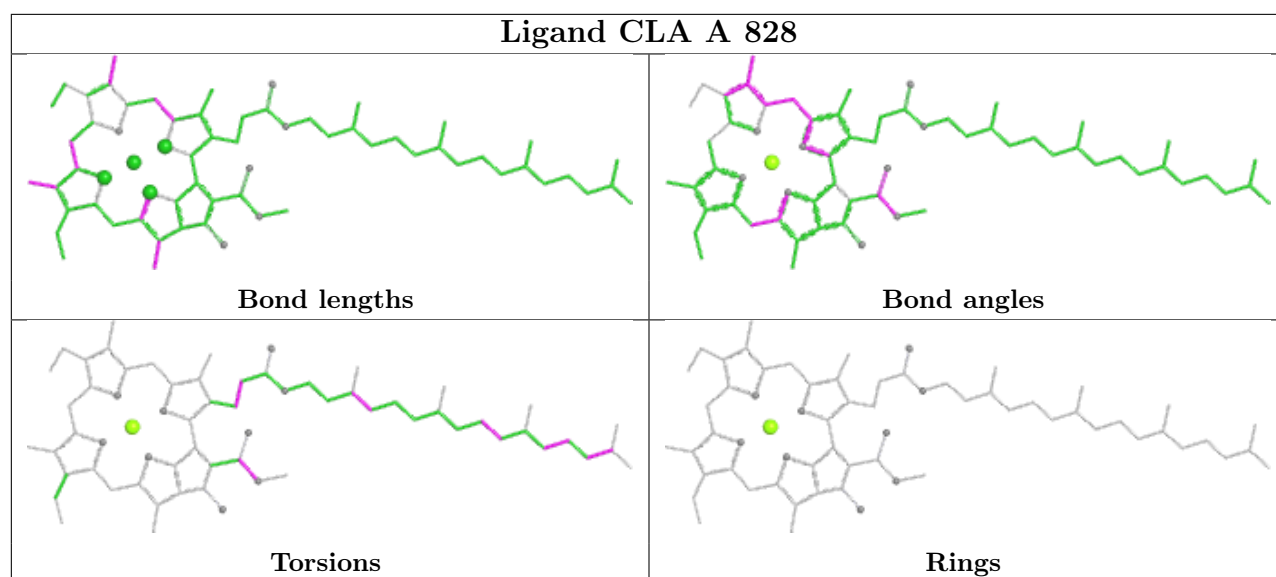
Ligand CLA b 801

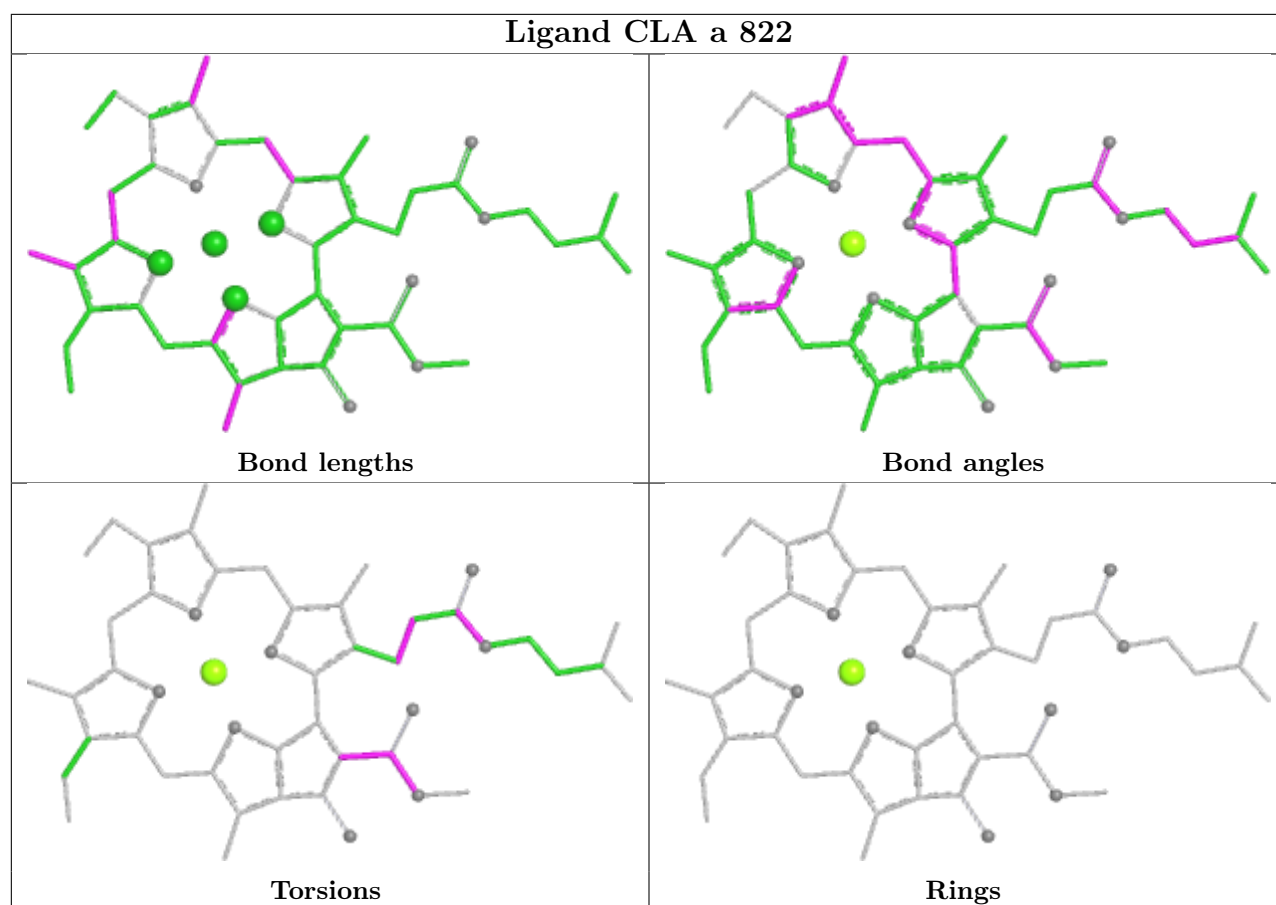




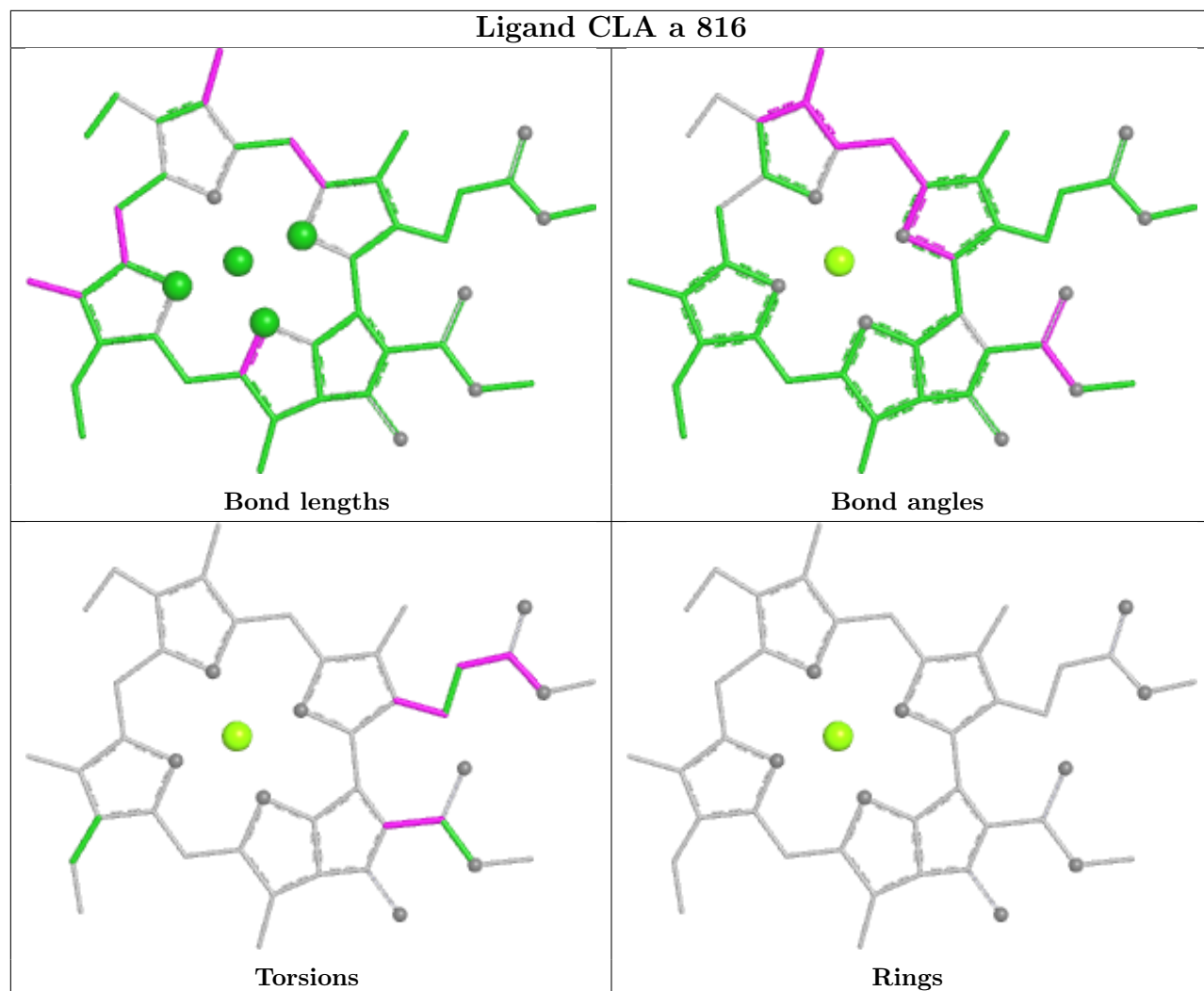


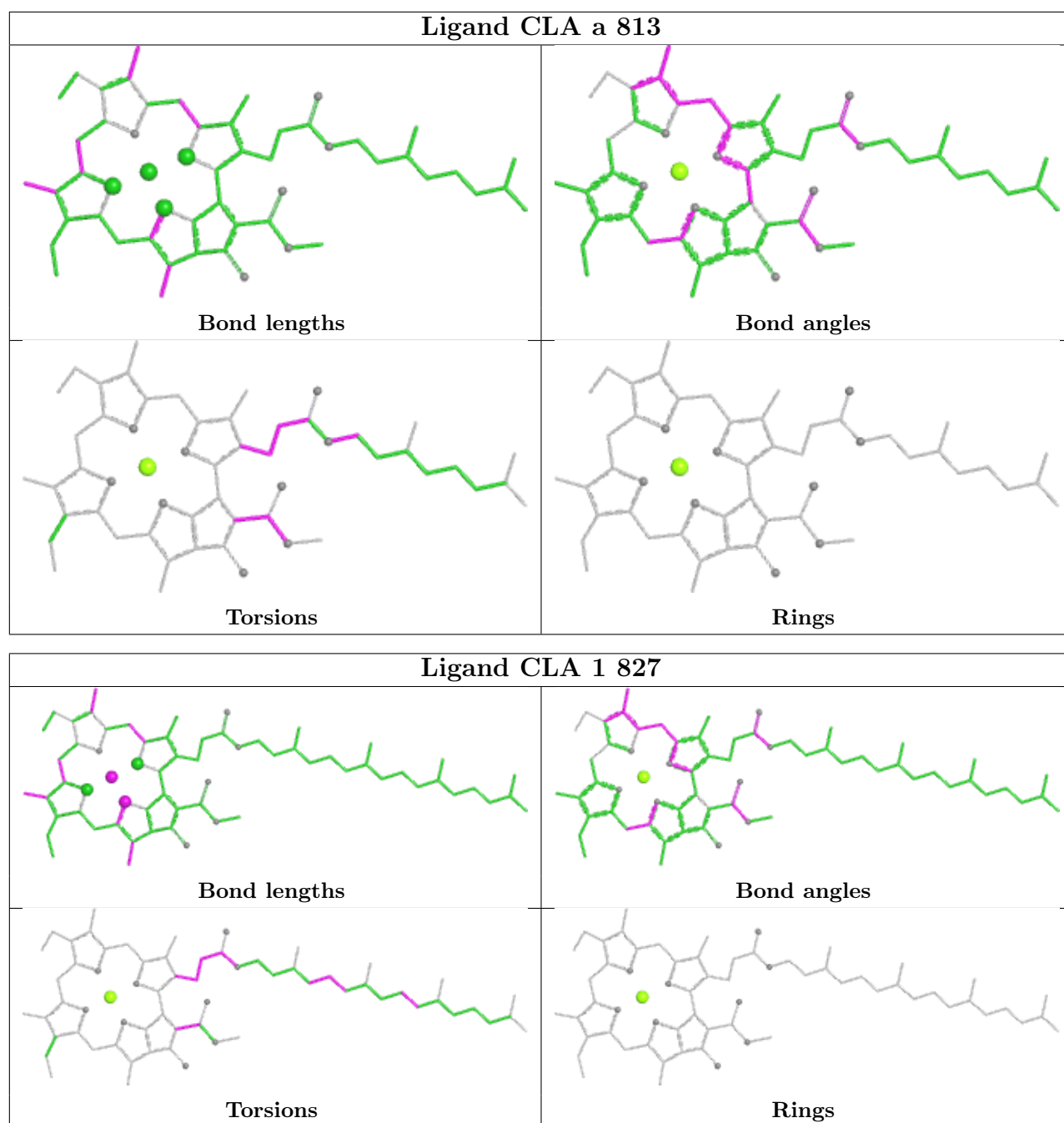


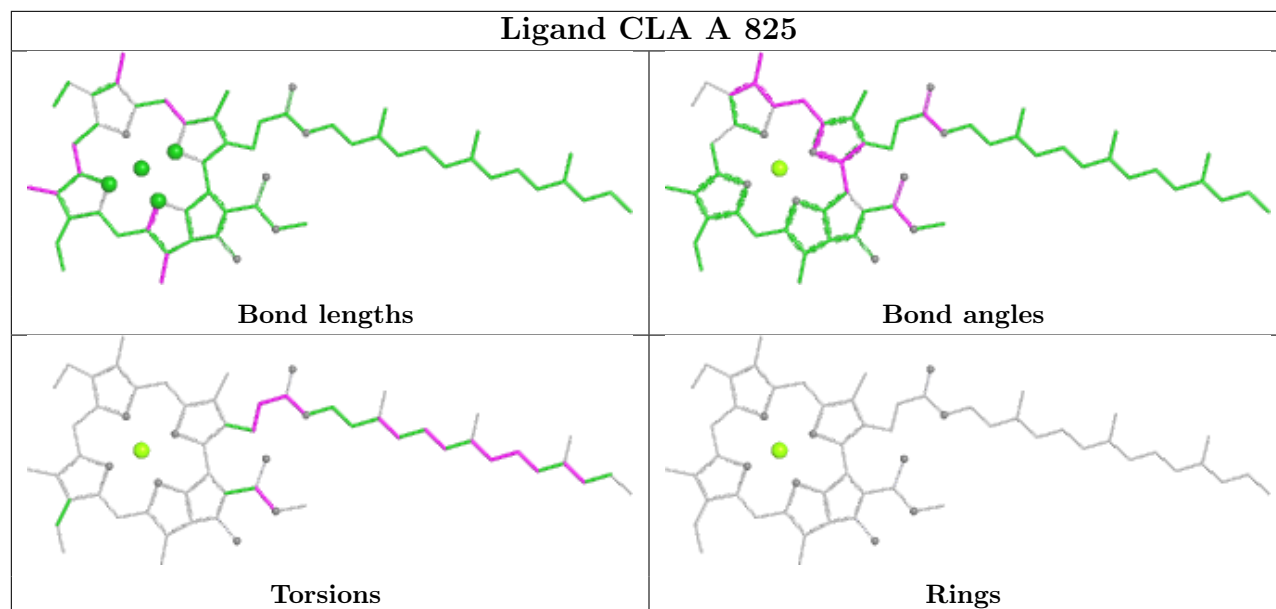
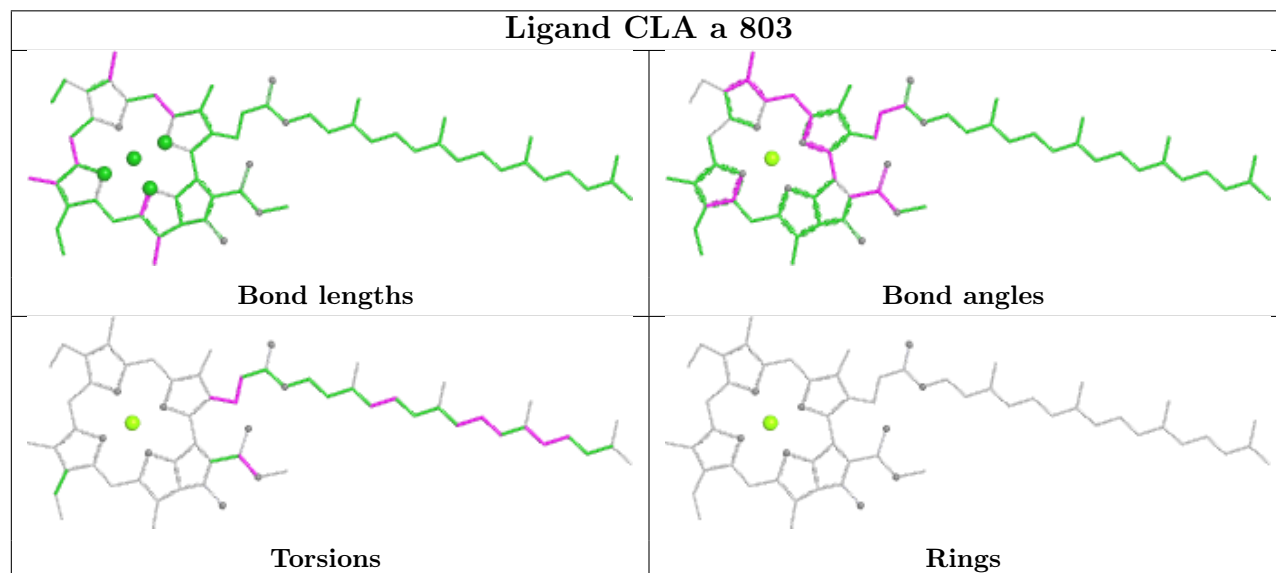
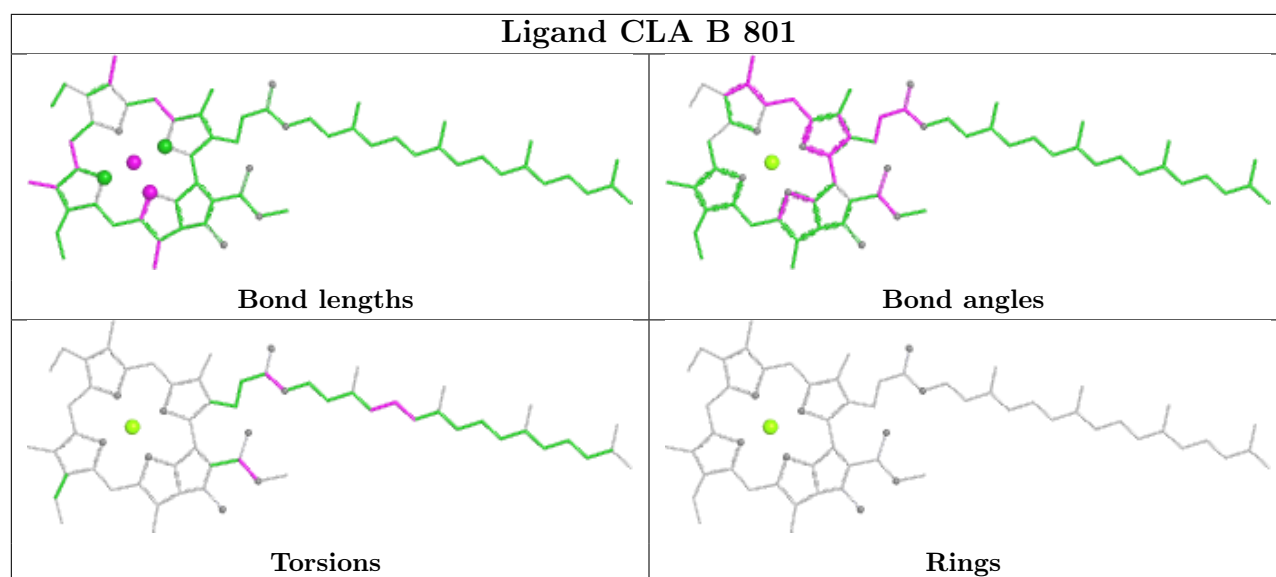


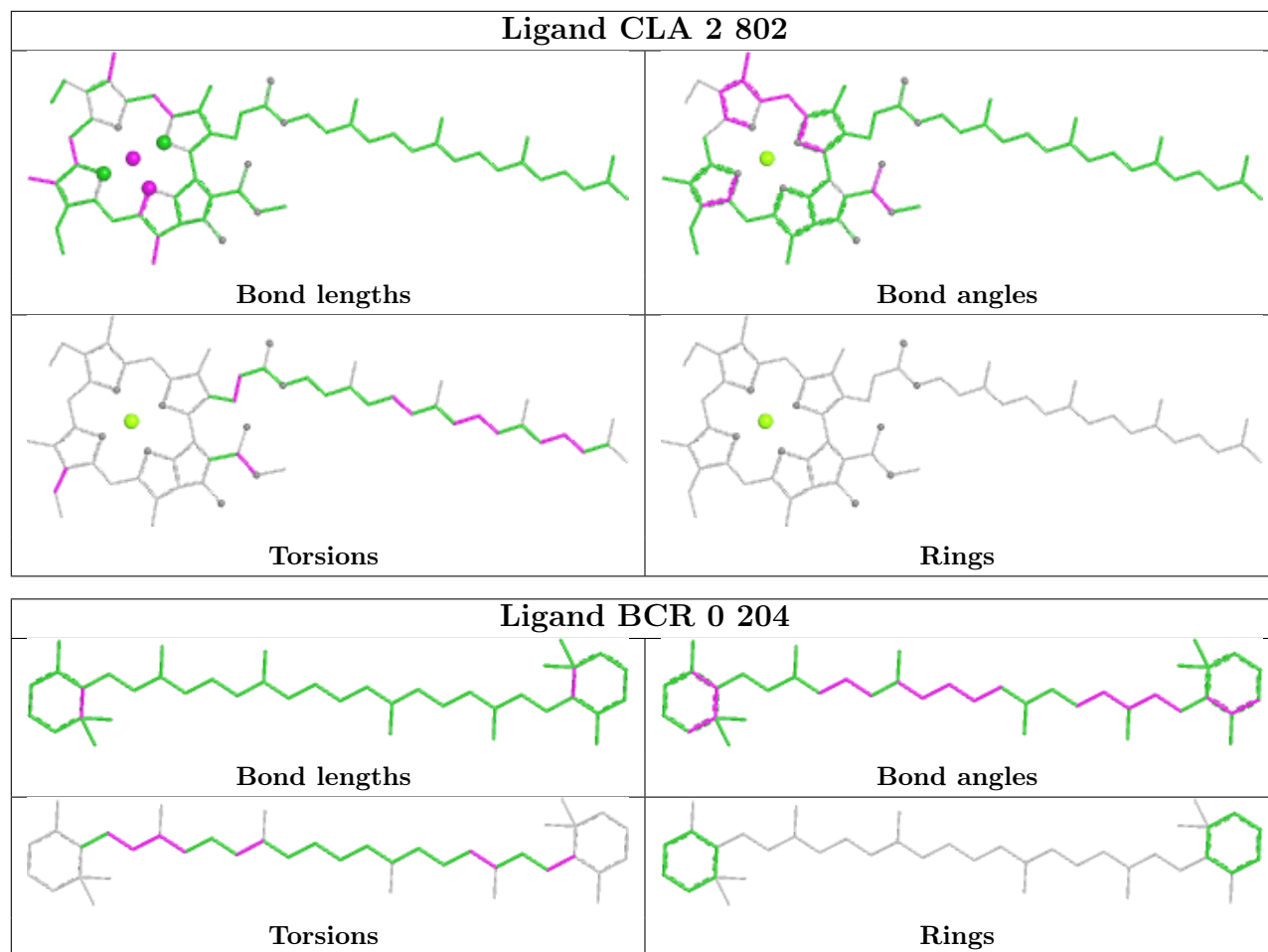


Ligand CLA a 816

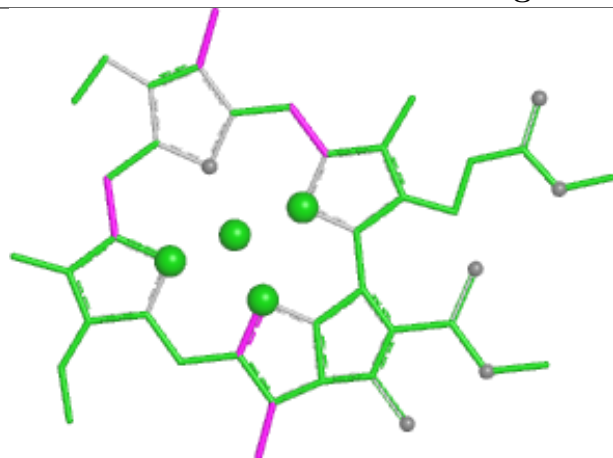




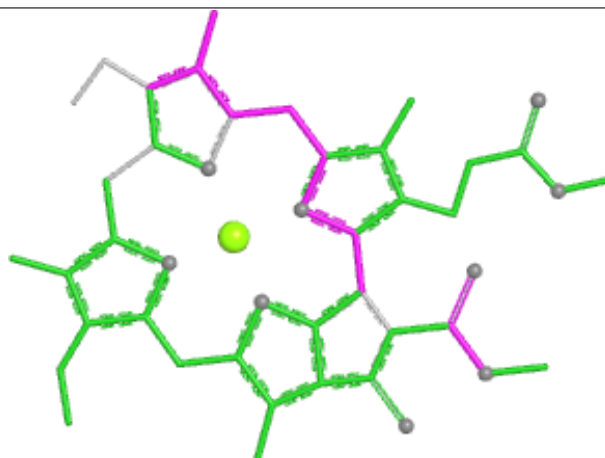




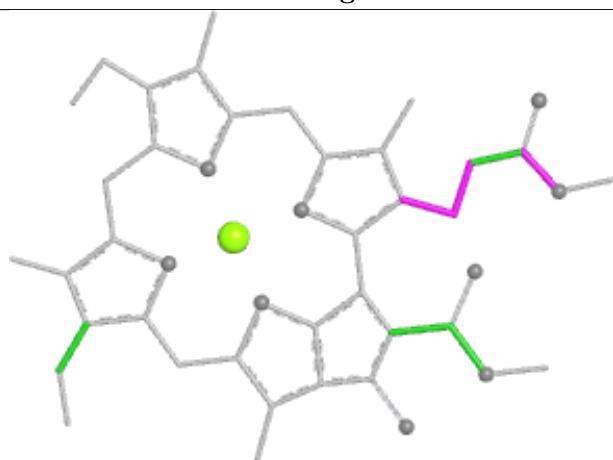
Ligand CLA A 812



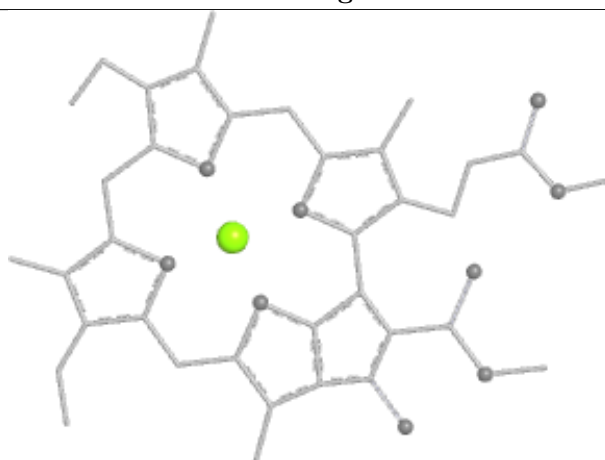
Bond lengths



Bond angles

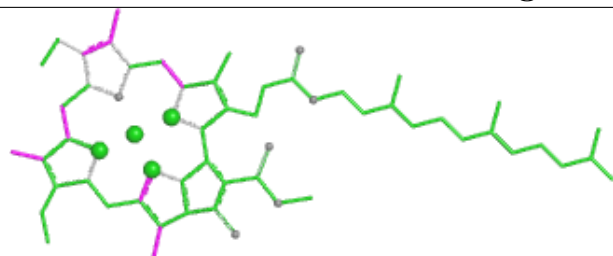


Torsions

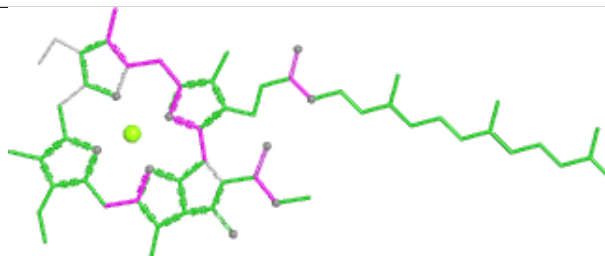


Rings

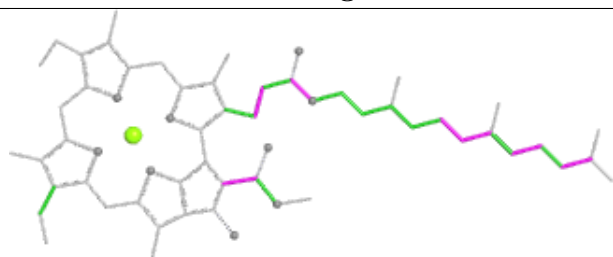
Ligand CLA a 852



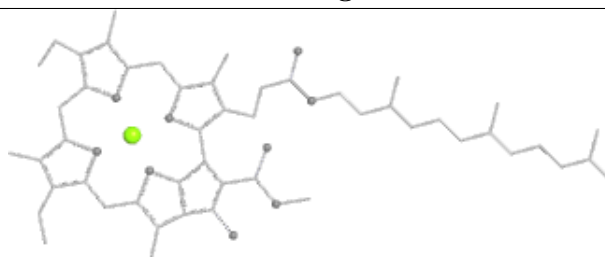
Bond lengths



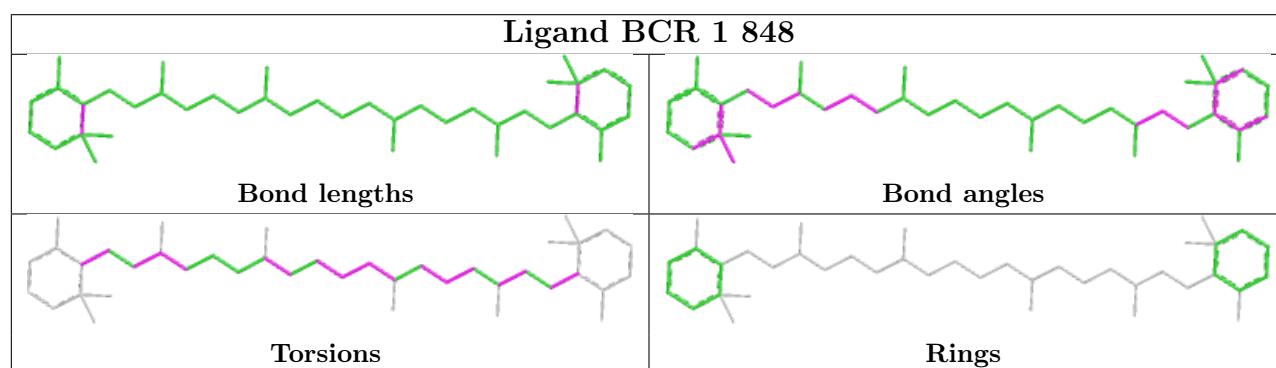
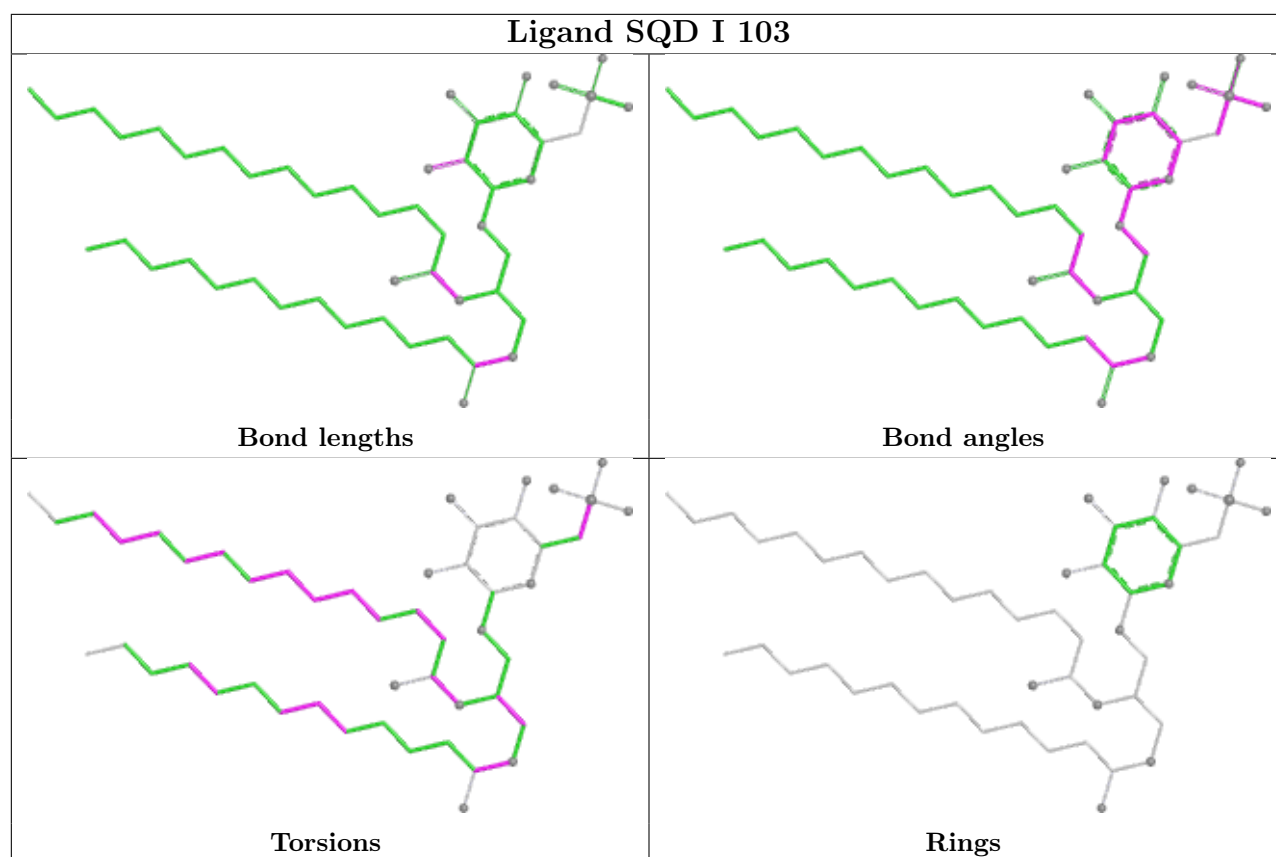
Bond angles

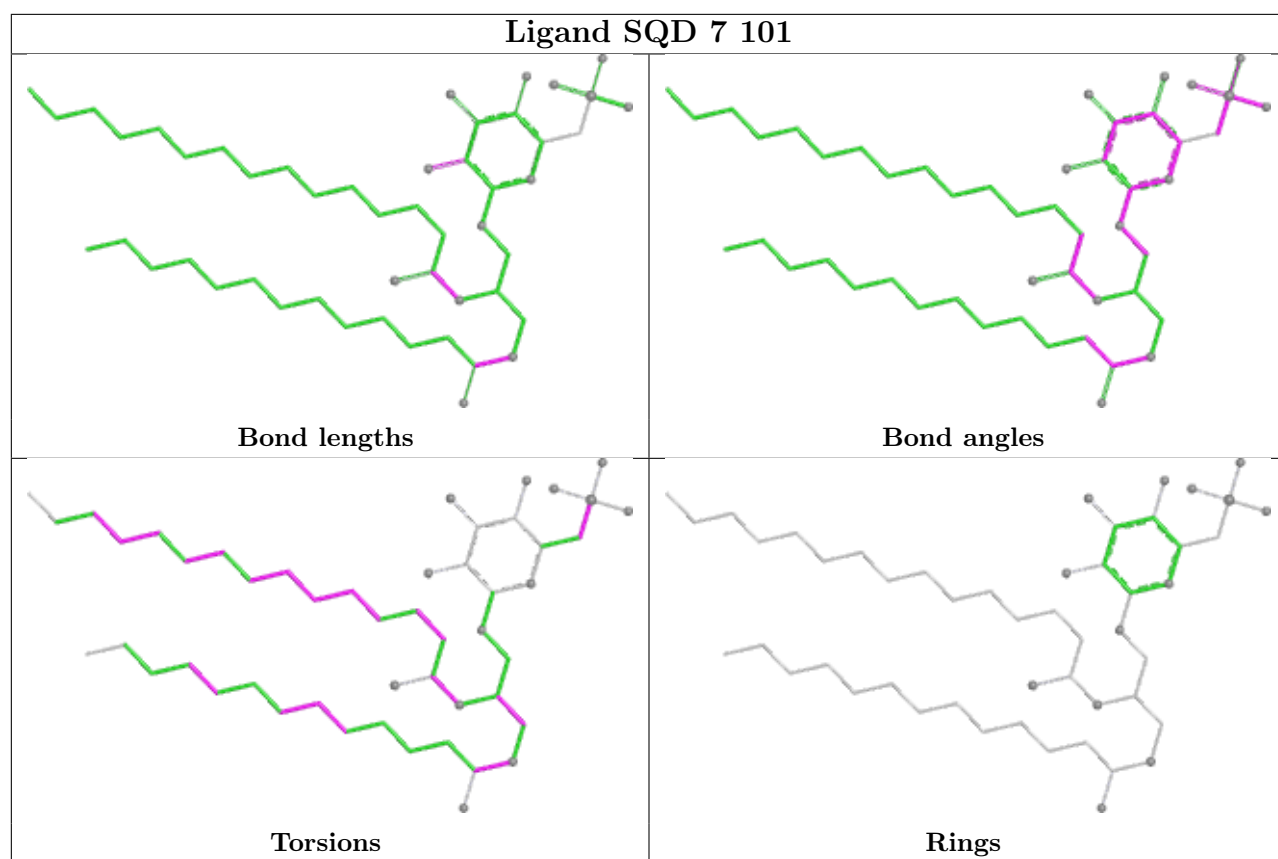


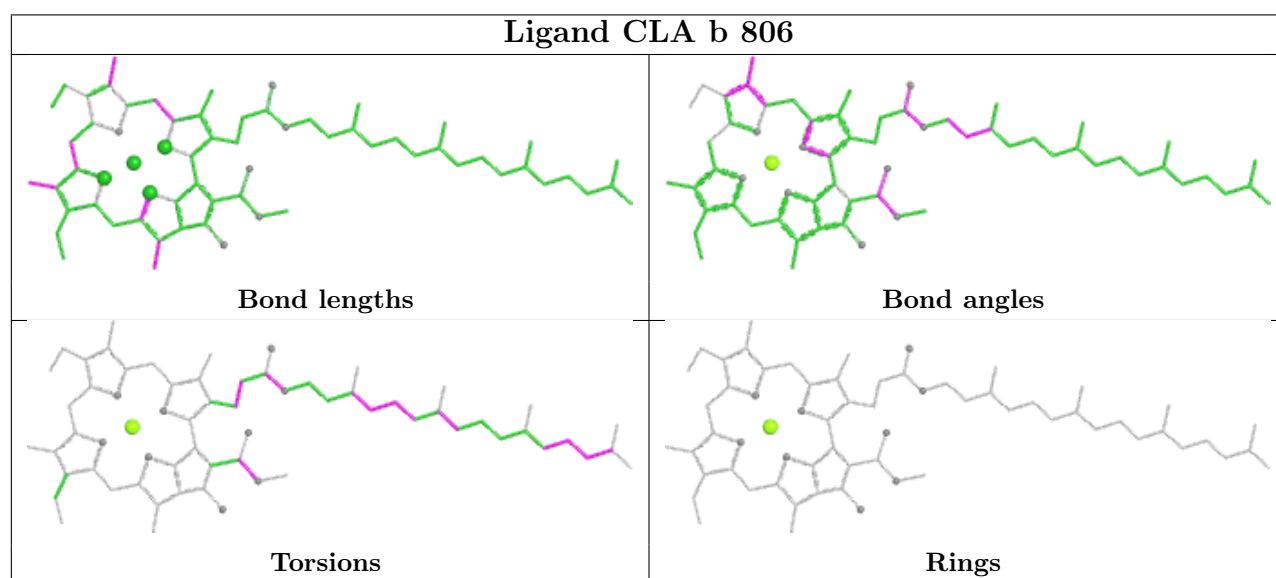
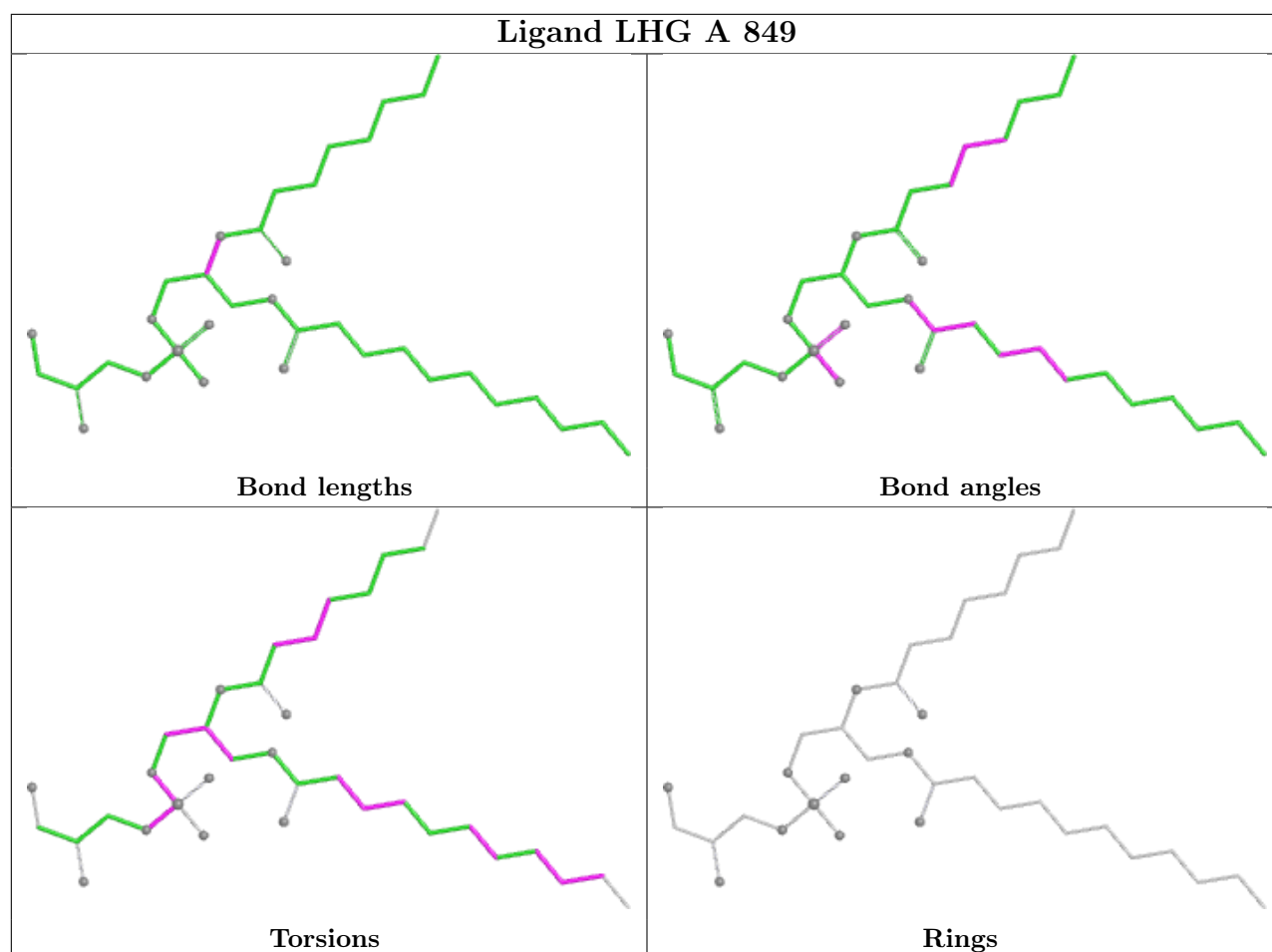
Torsions



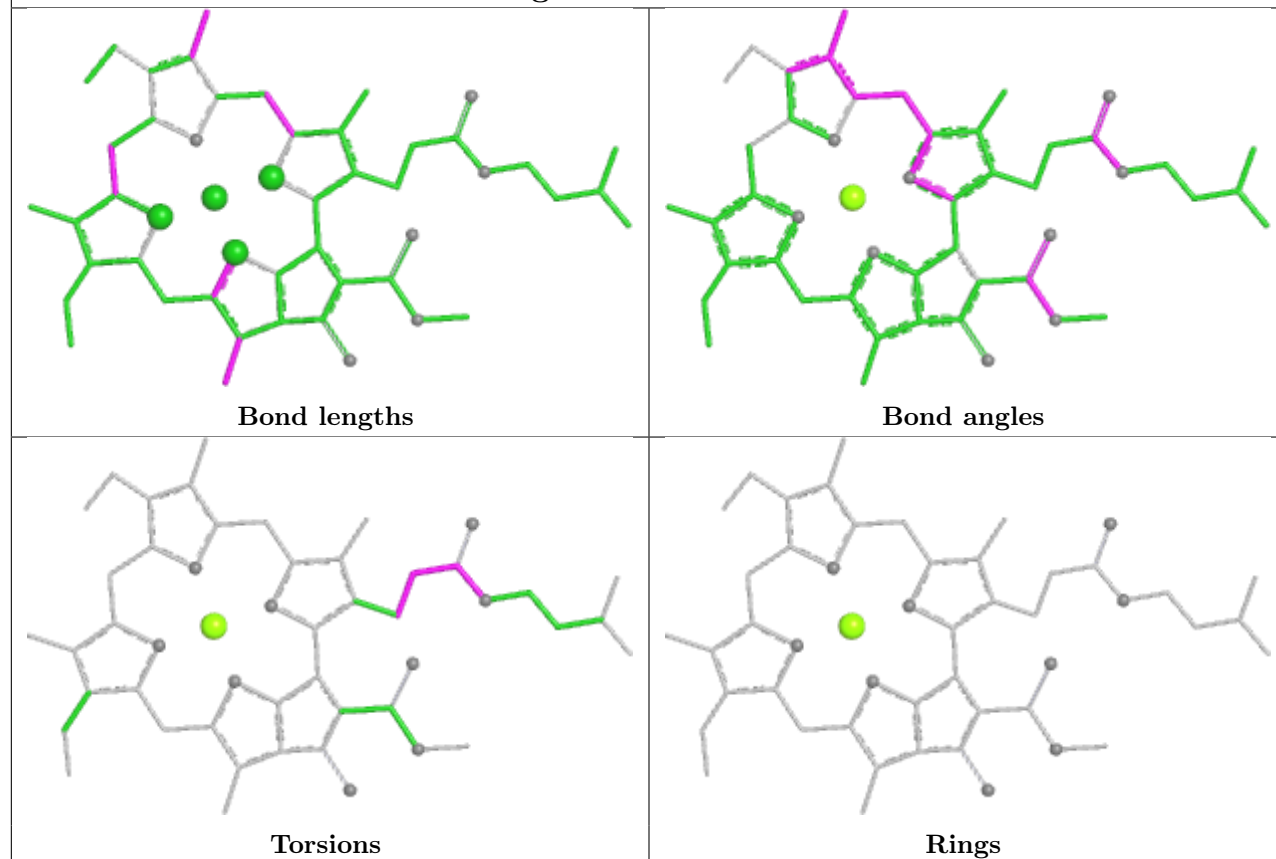
Rings



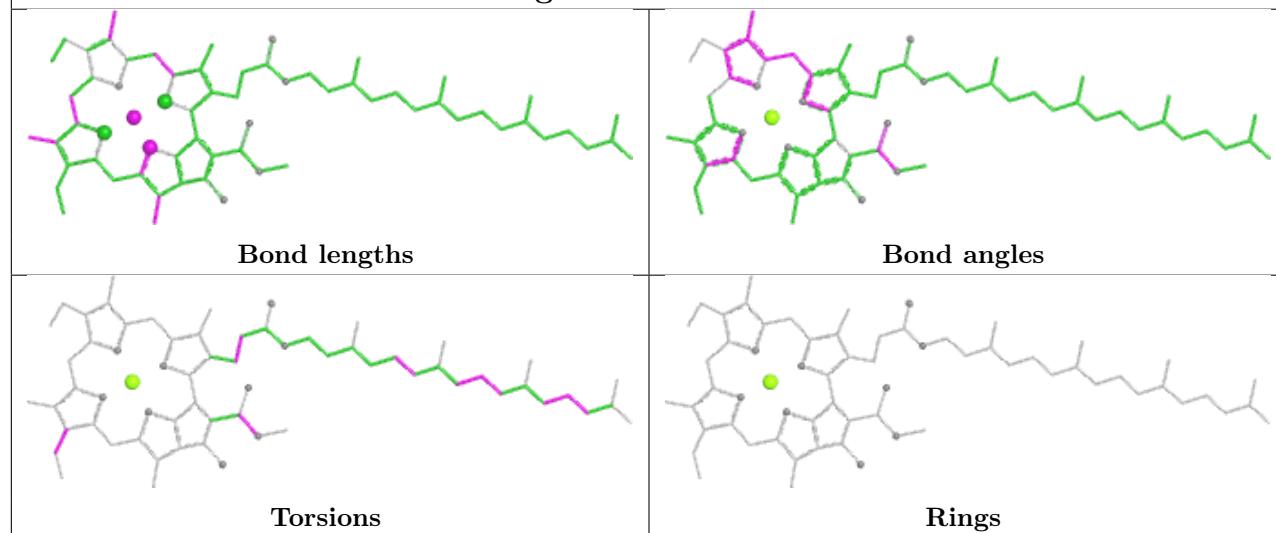


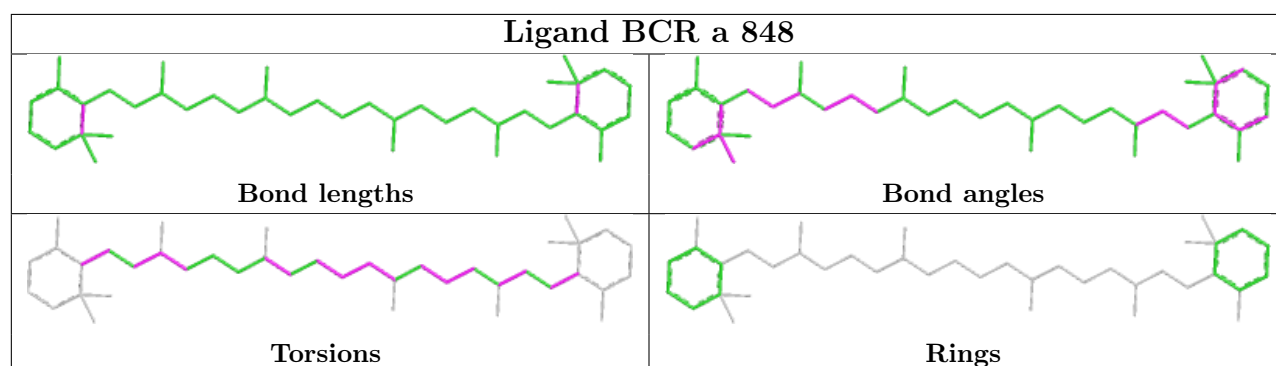
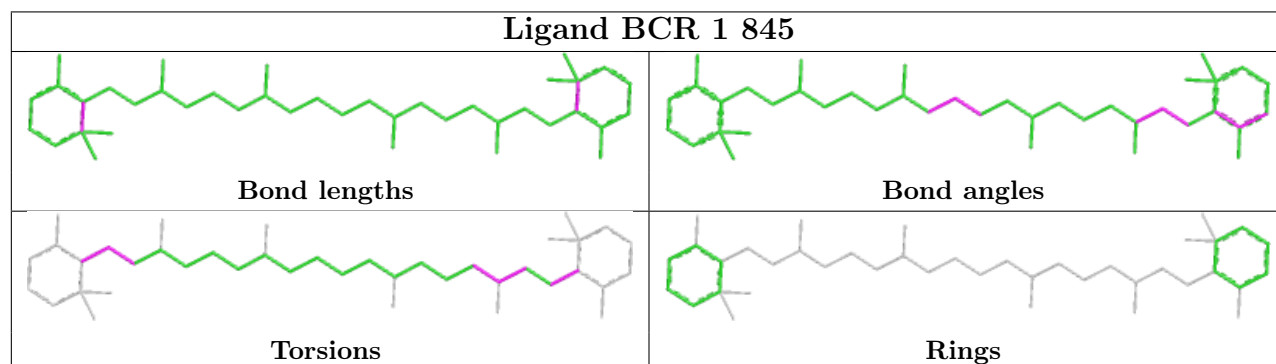
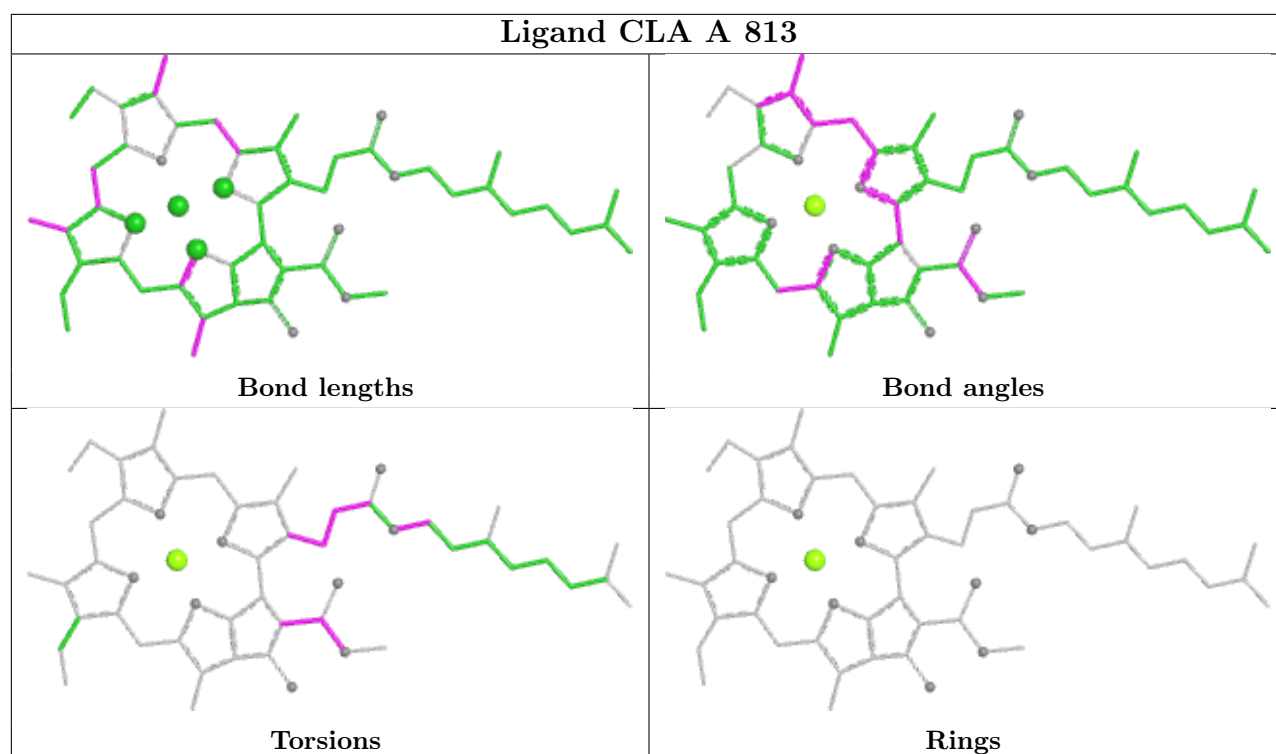


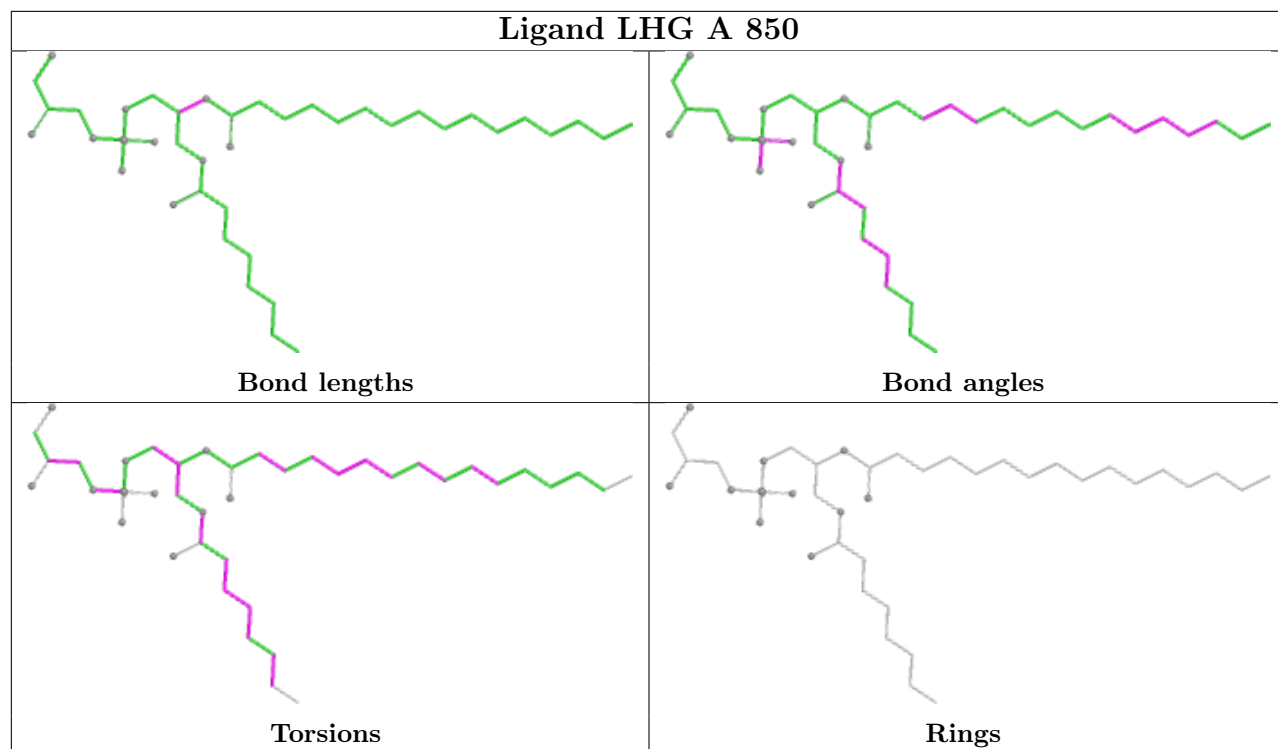
Ligand CLA A 823



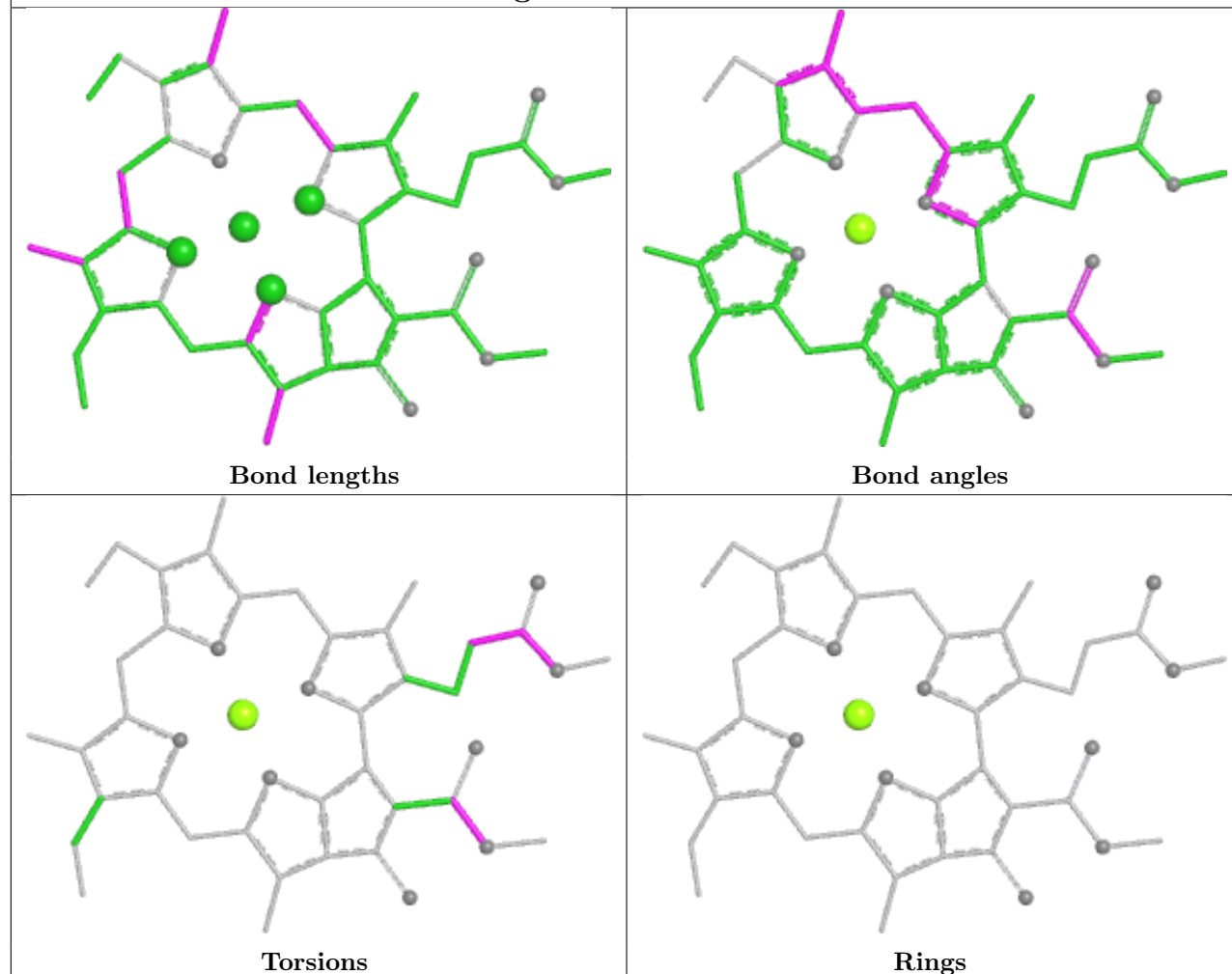
Ligand CLA b 802



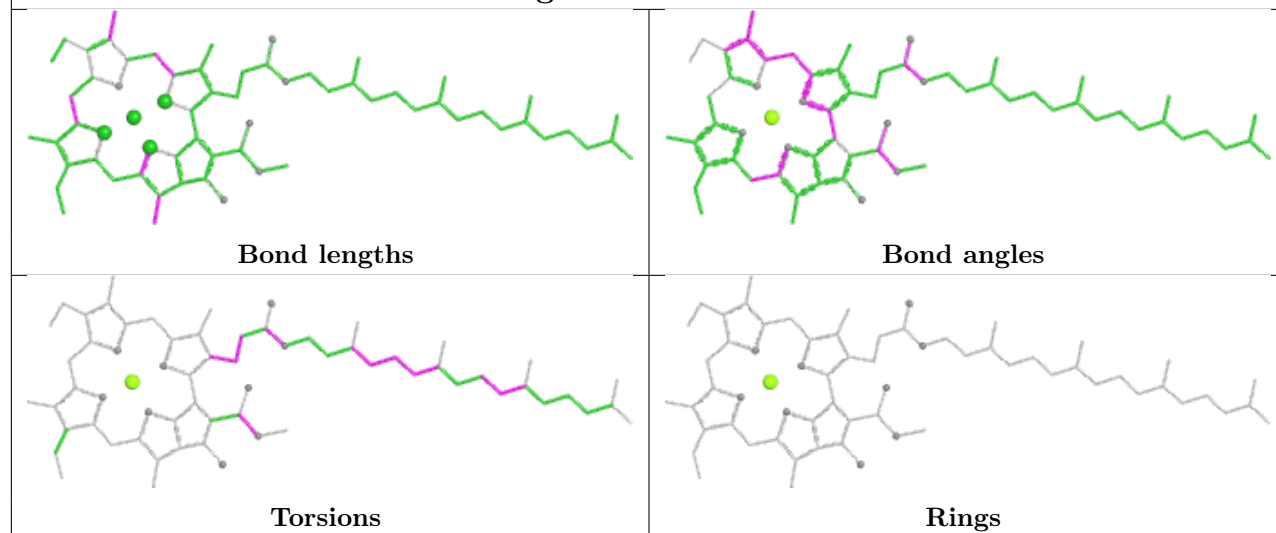




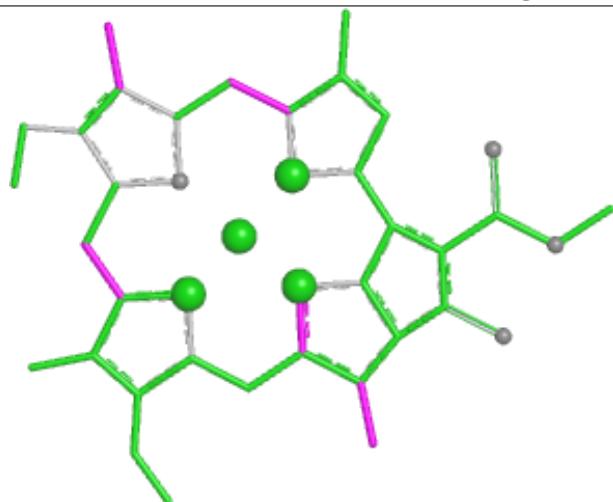
Ligand CLA B 819



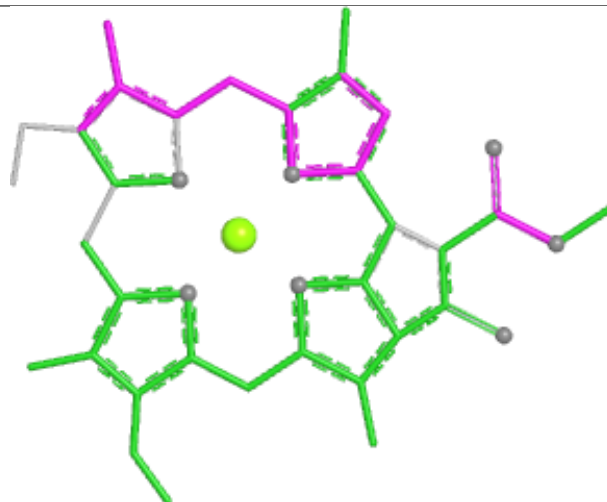
Ligand CLA 2 812



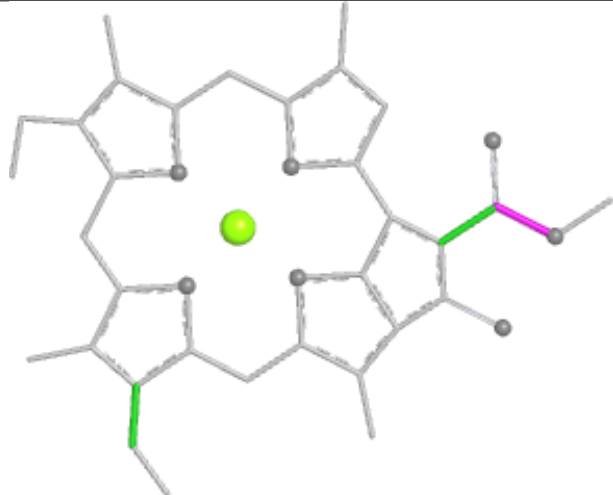
Ligand CLA b 832



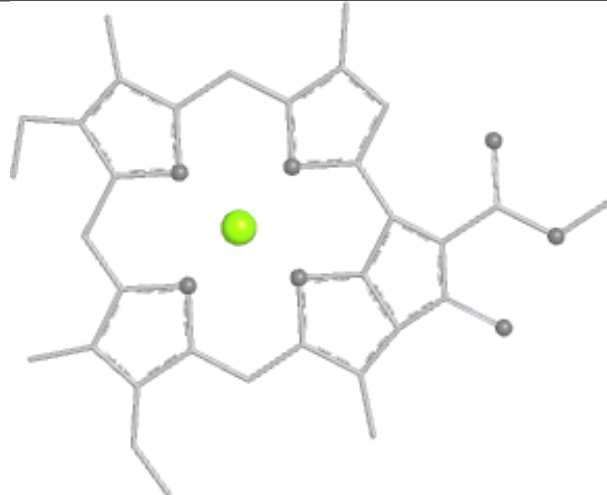
Bond lengths



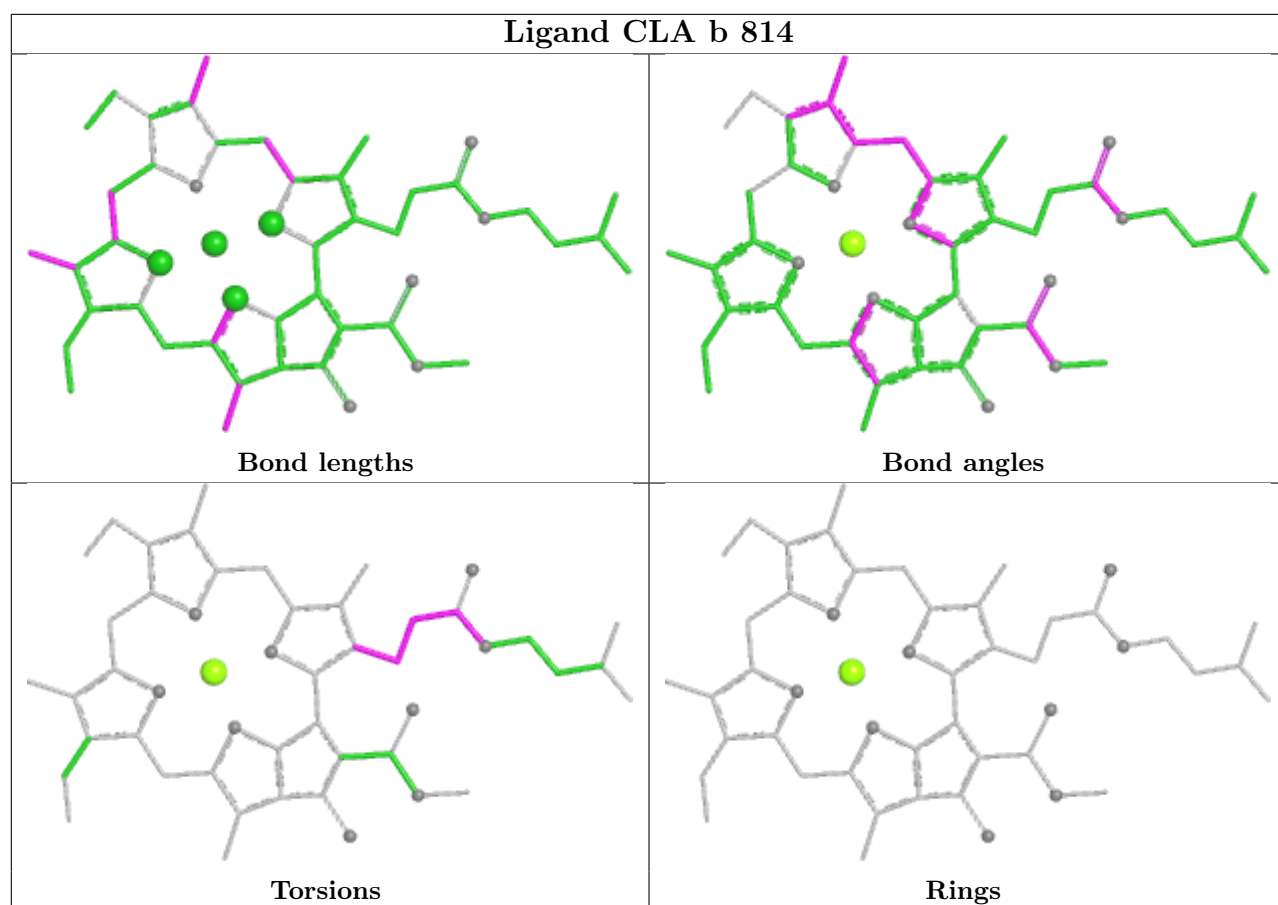
Bond angles

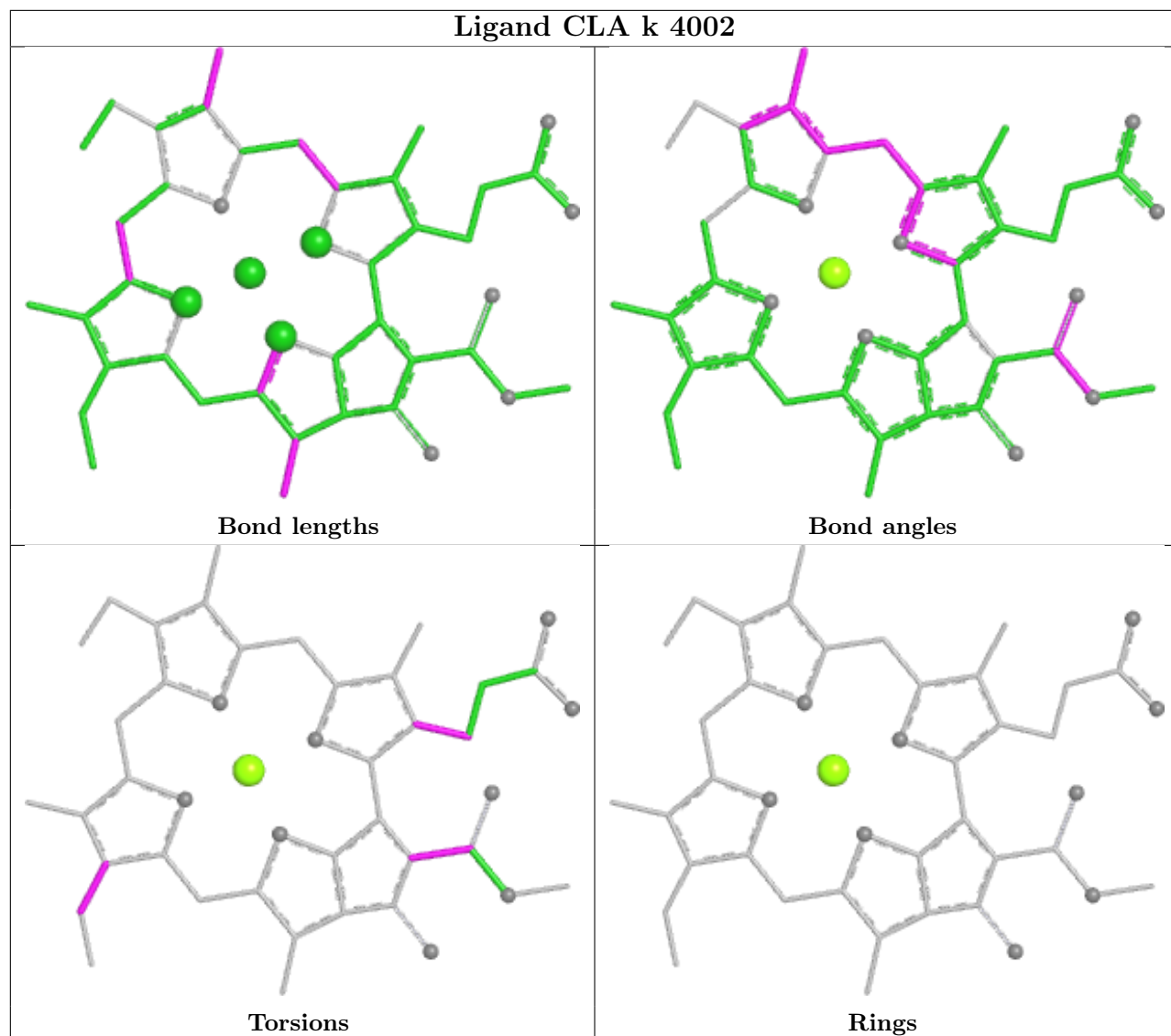


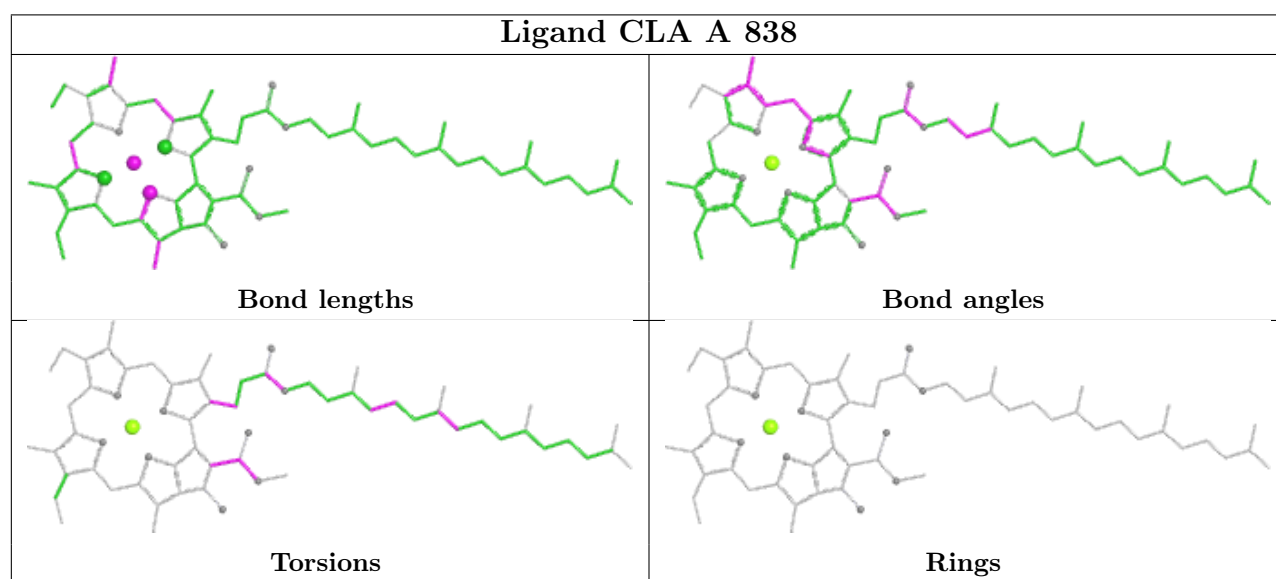
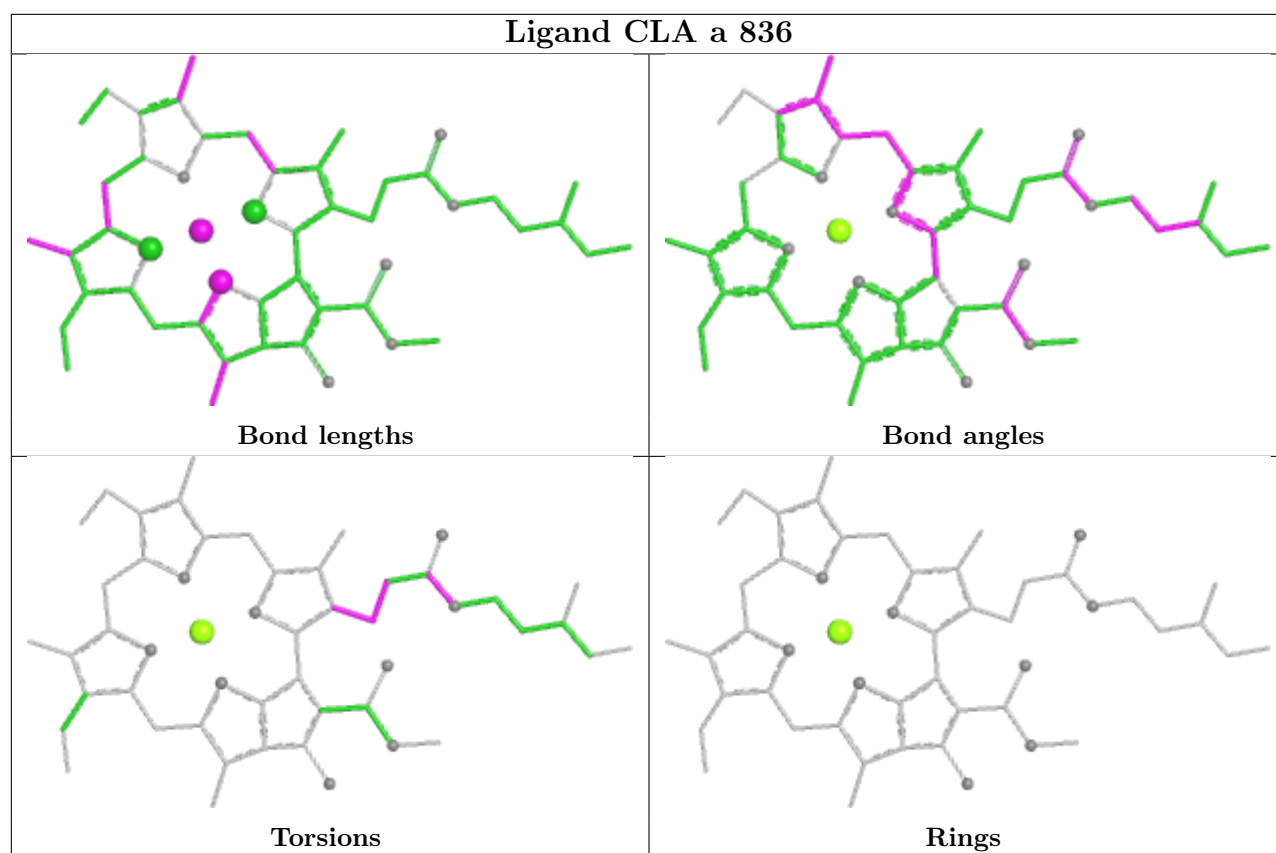
Torsions



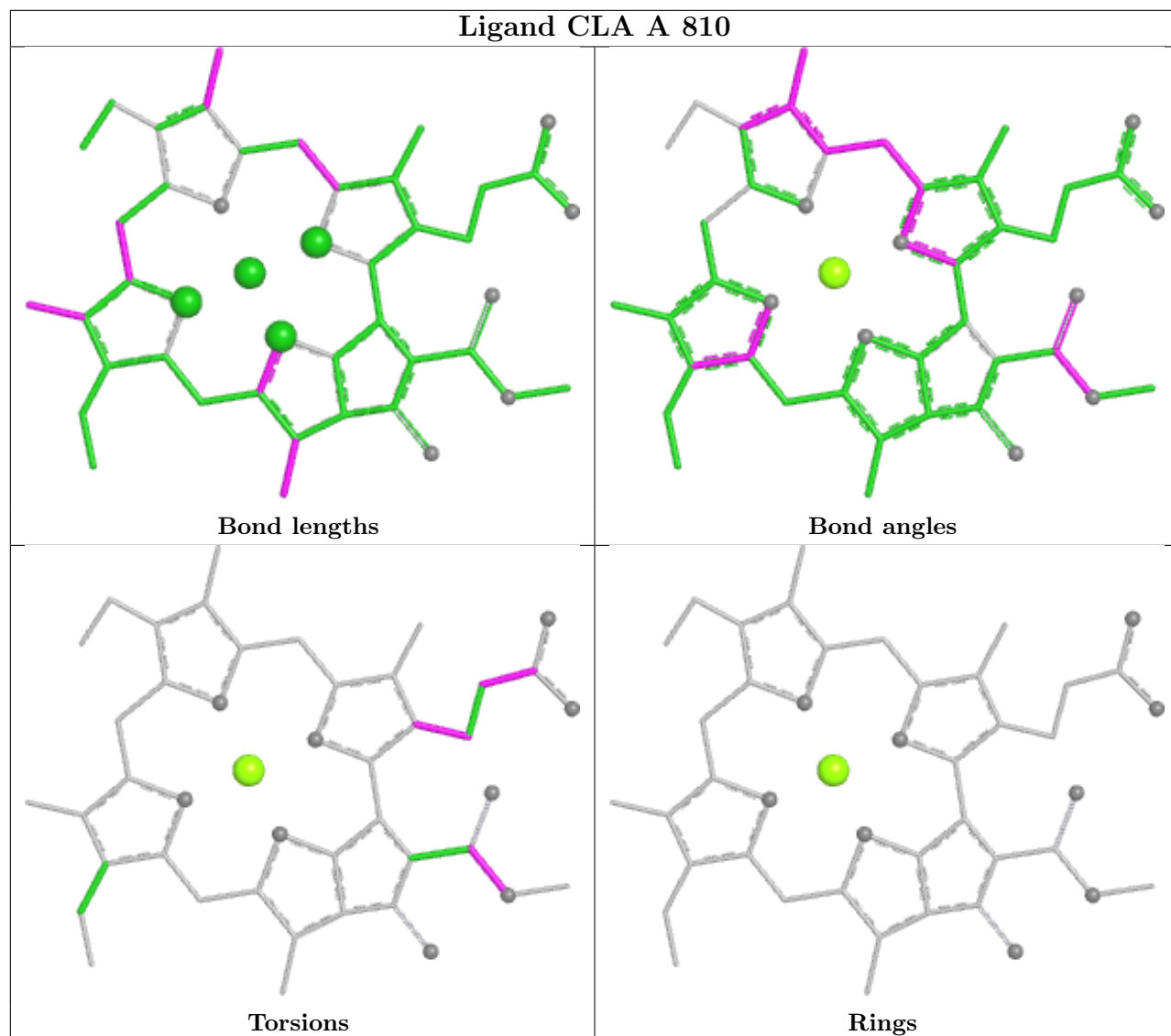
Rings



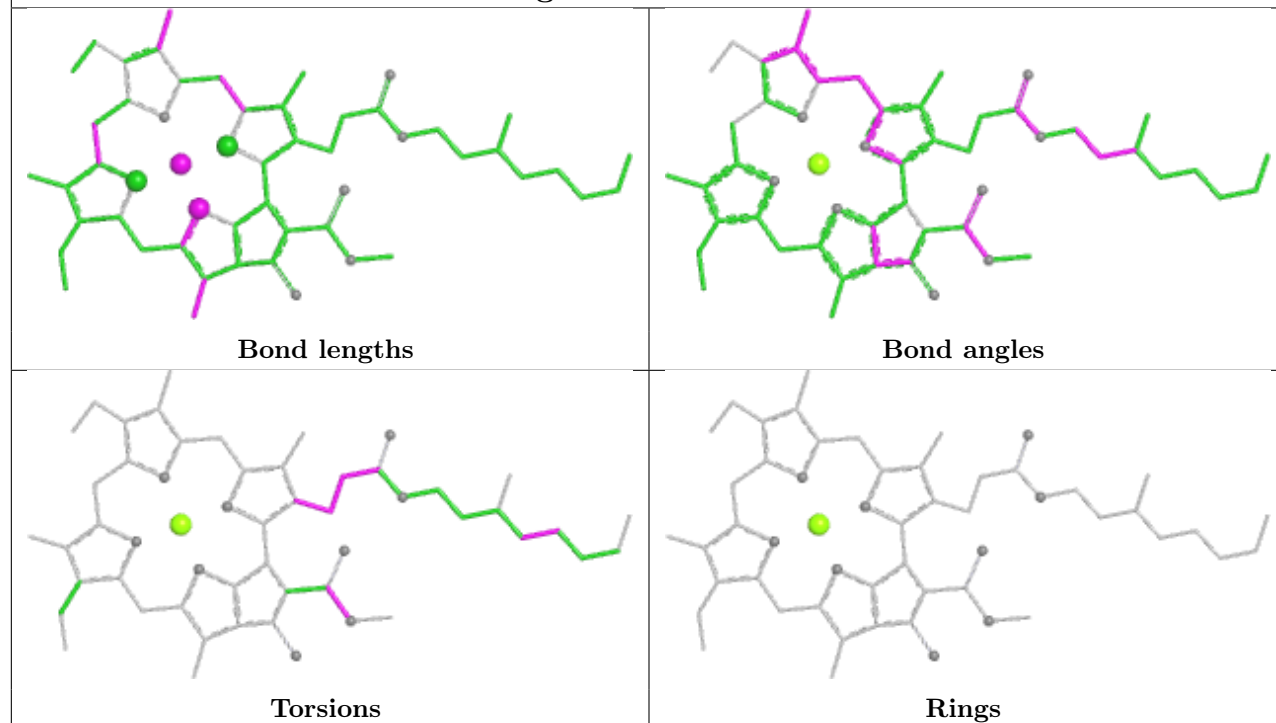




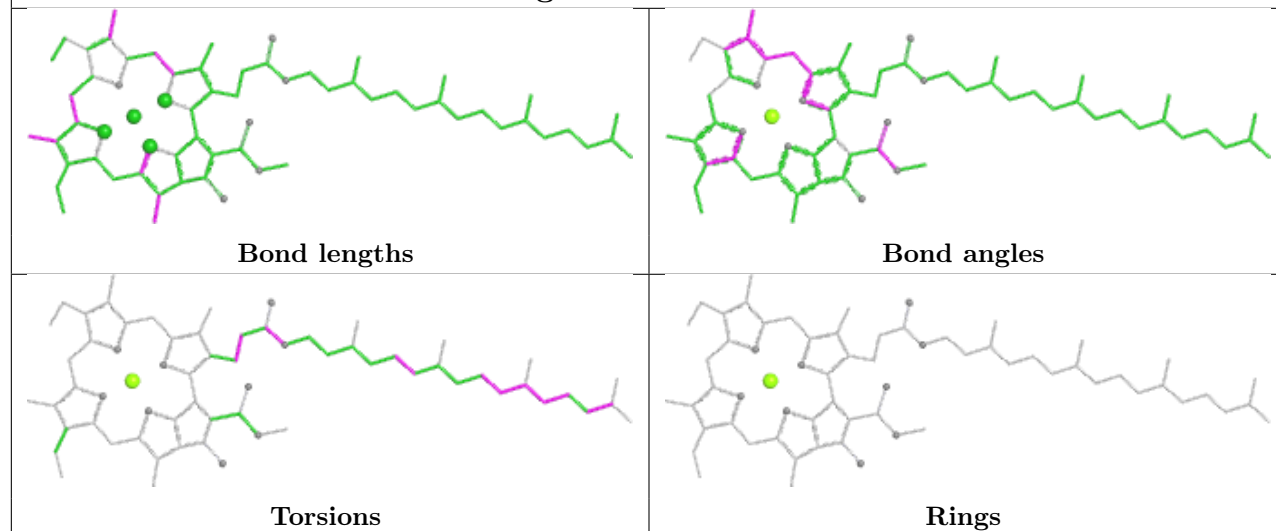
Ligand CLA A 810



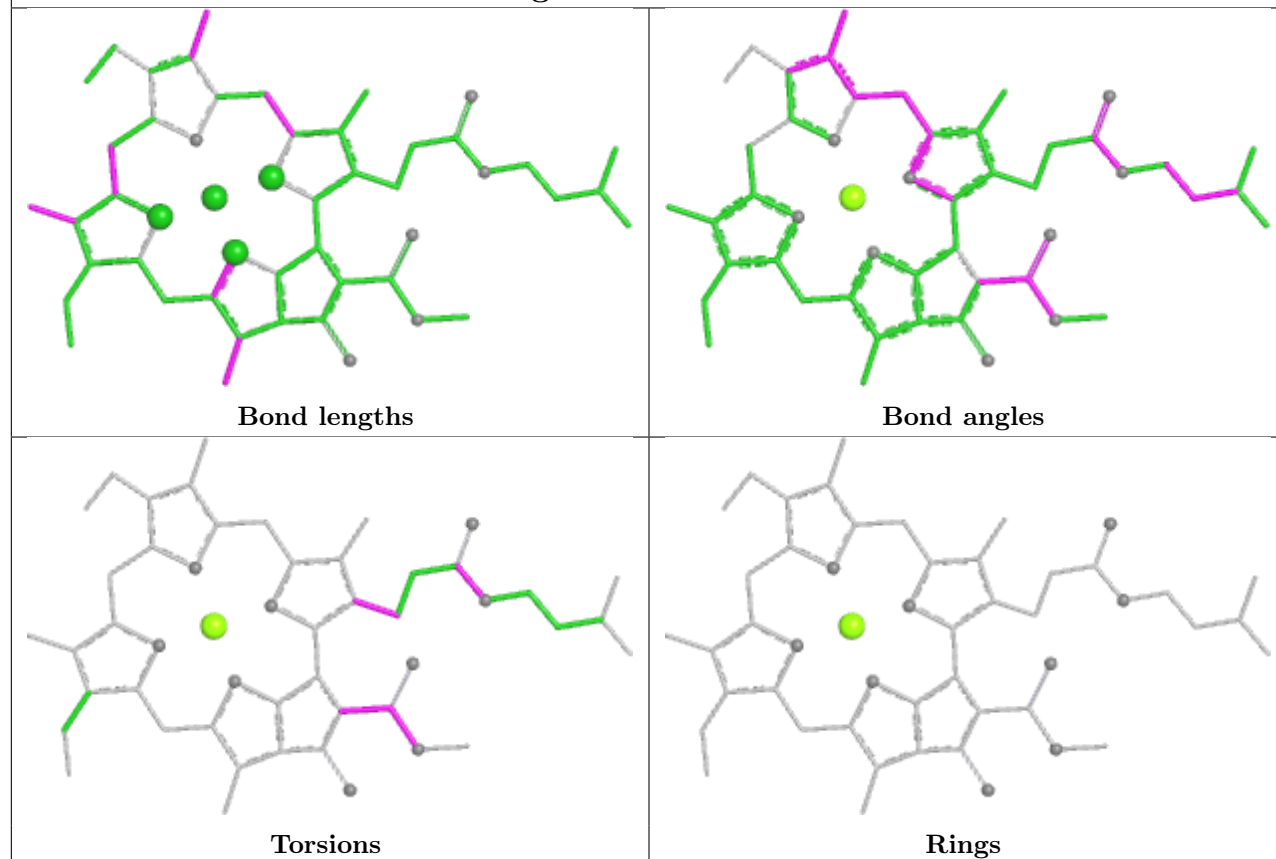
Ligand CLA 1 818



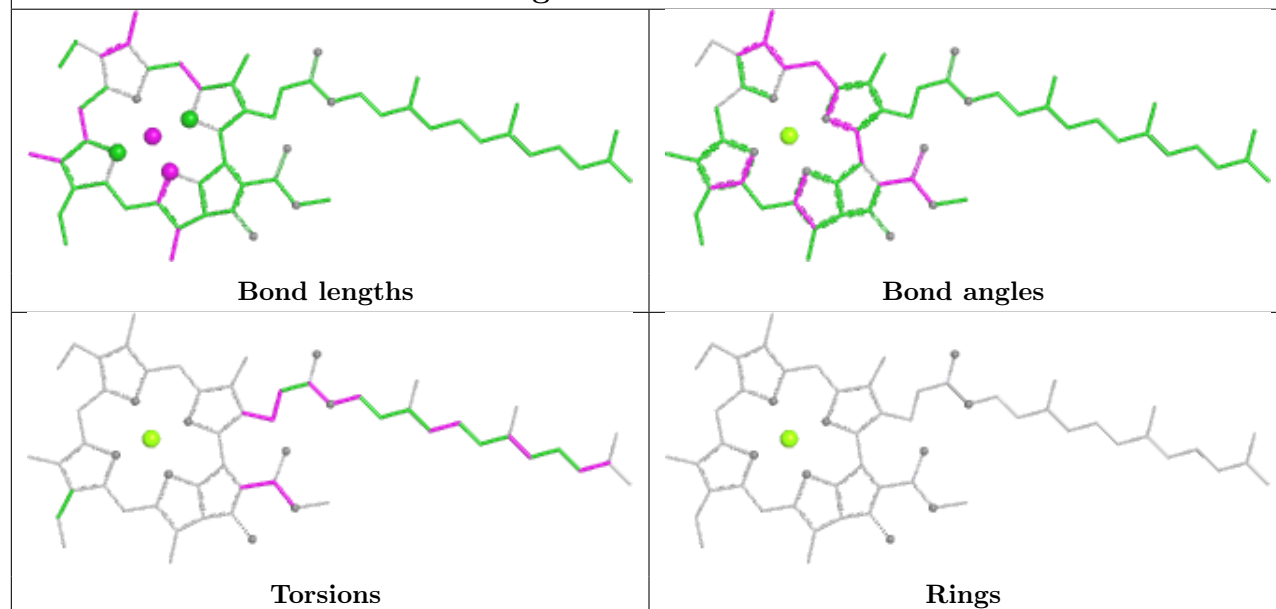
Ligand CLA 2 822

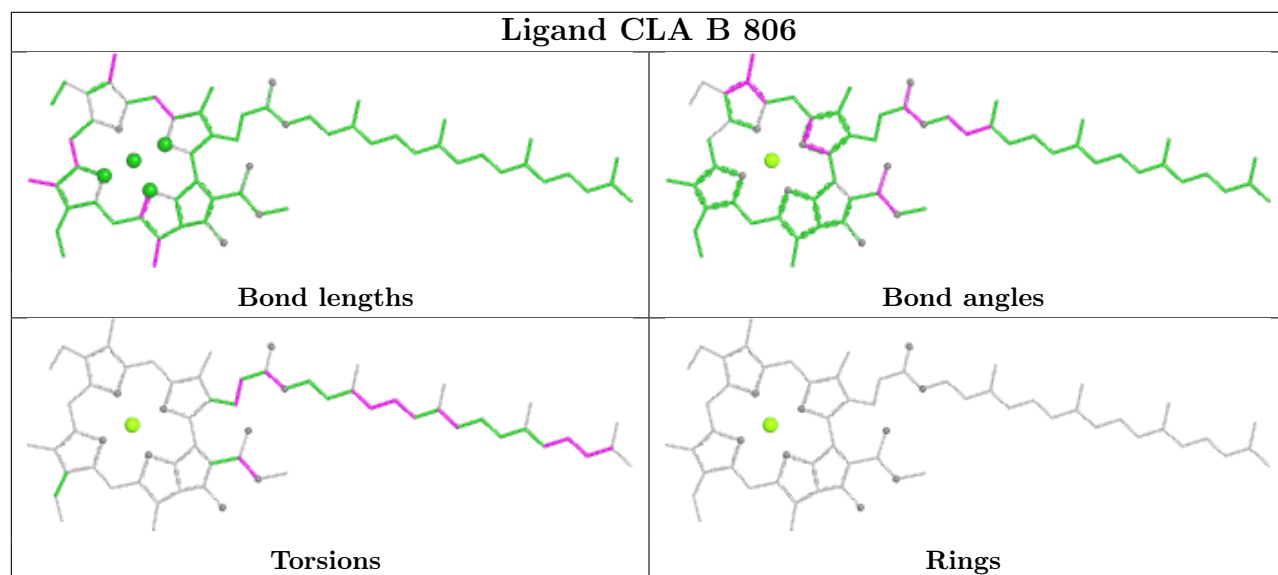
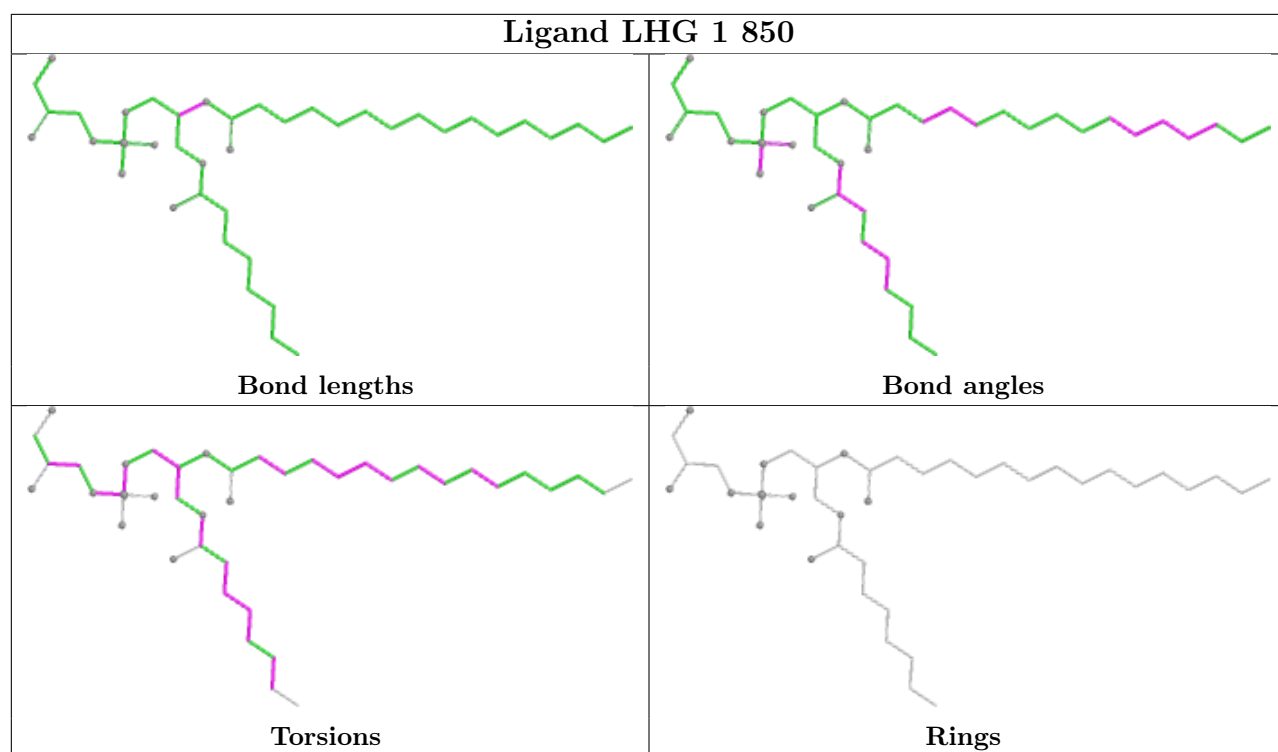


Ligand CLA A 831

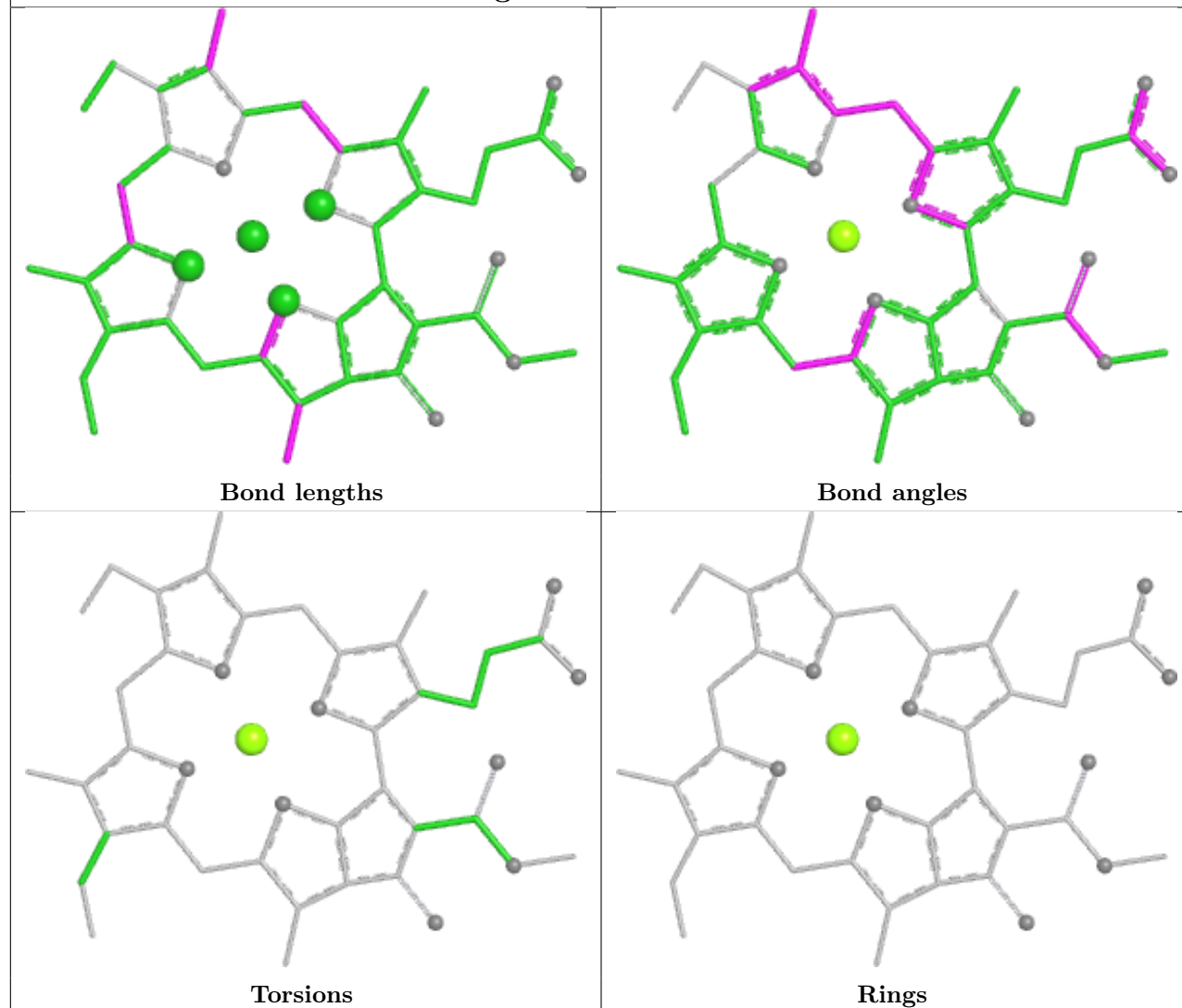


Ligand CLA B 826

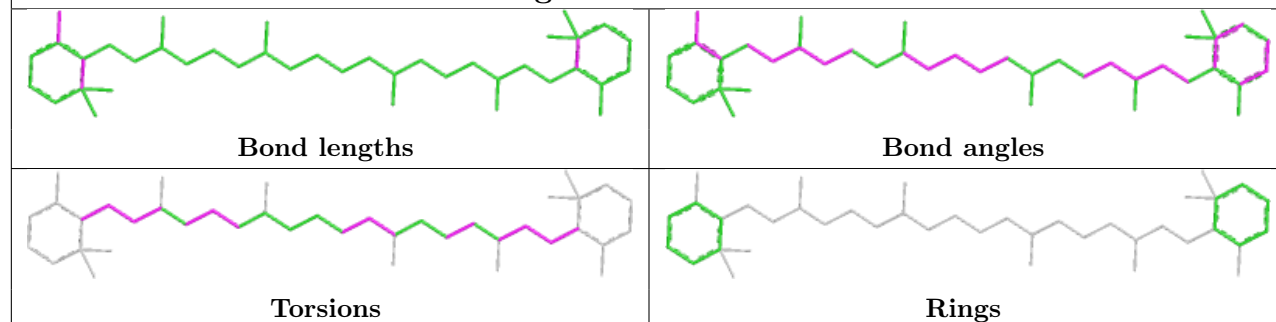


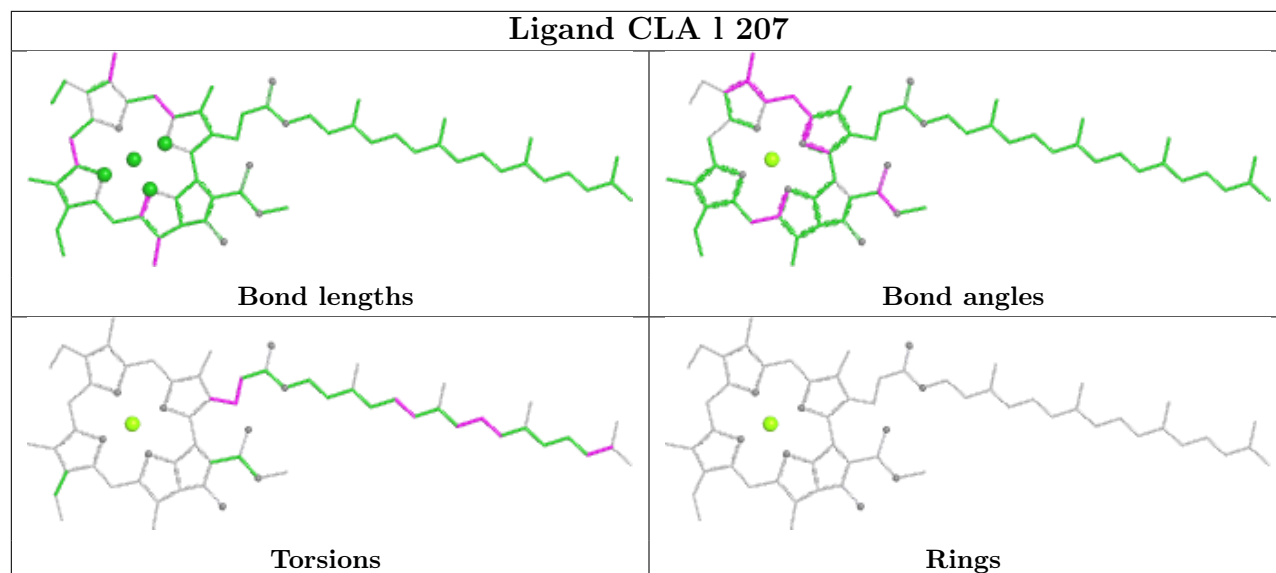
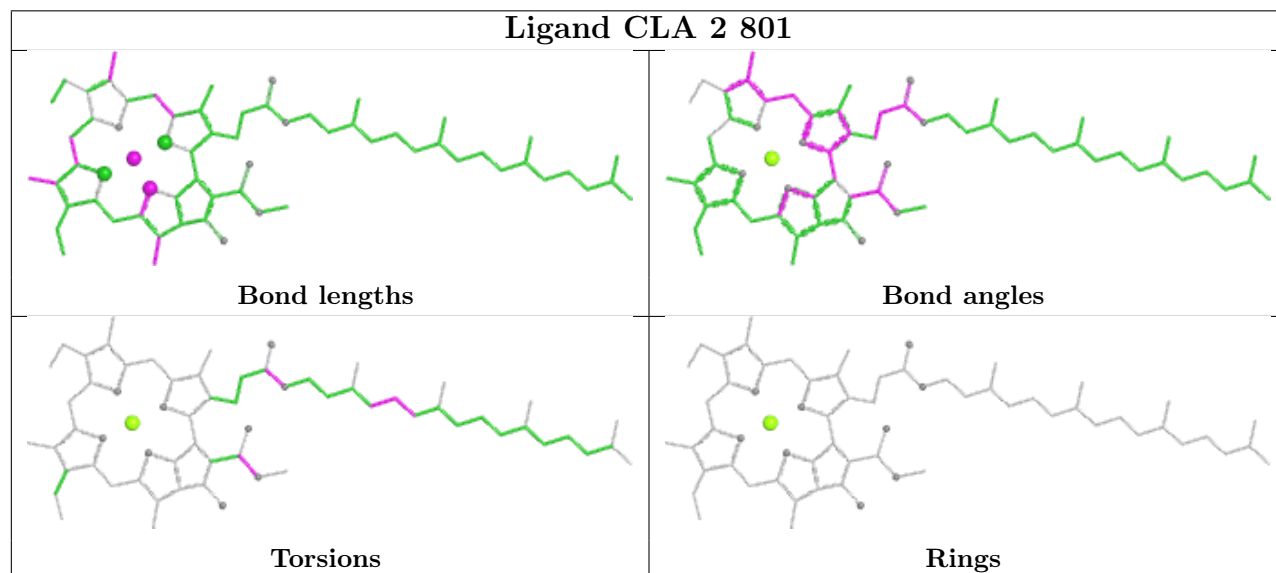
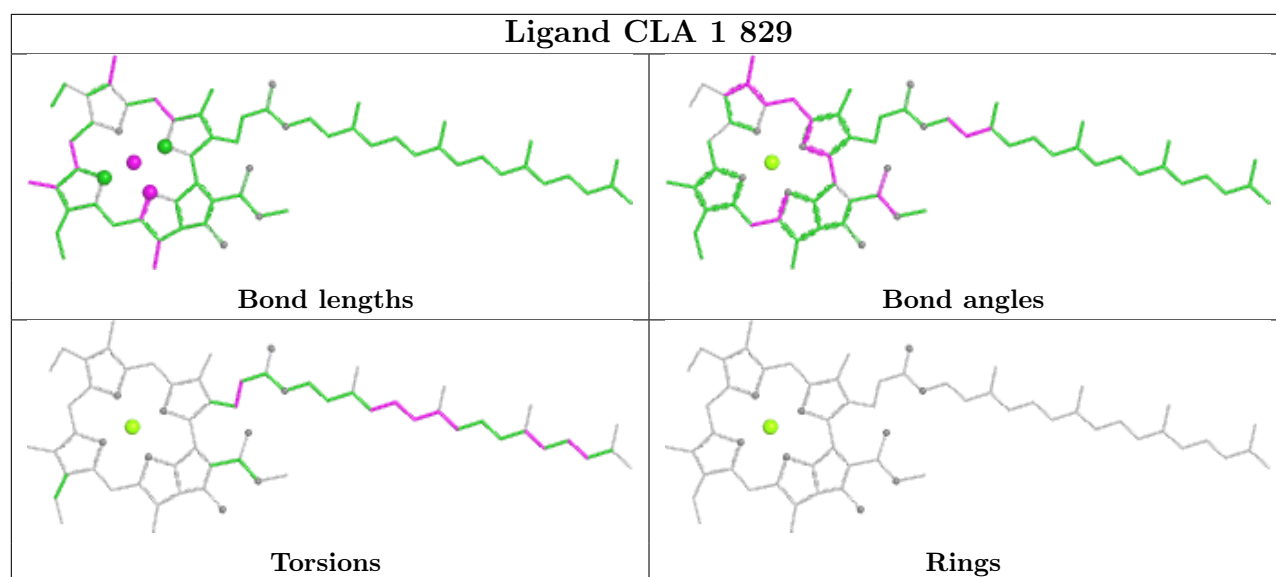


Ligand CLA F 203

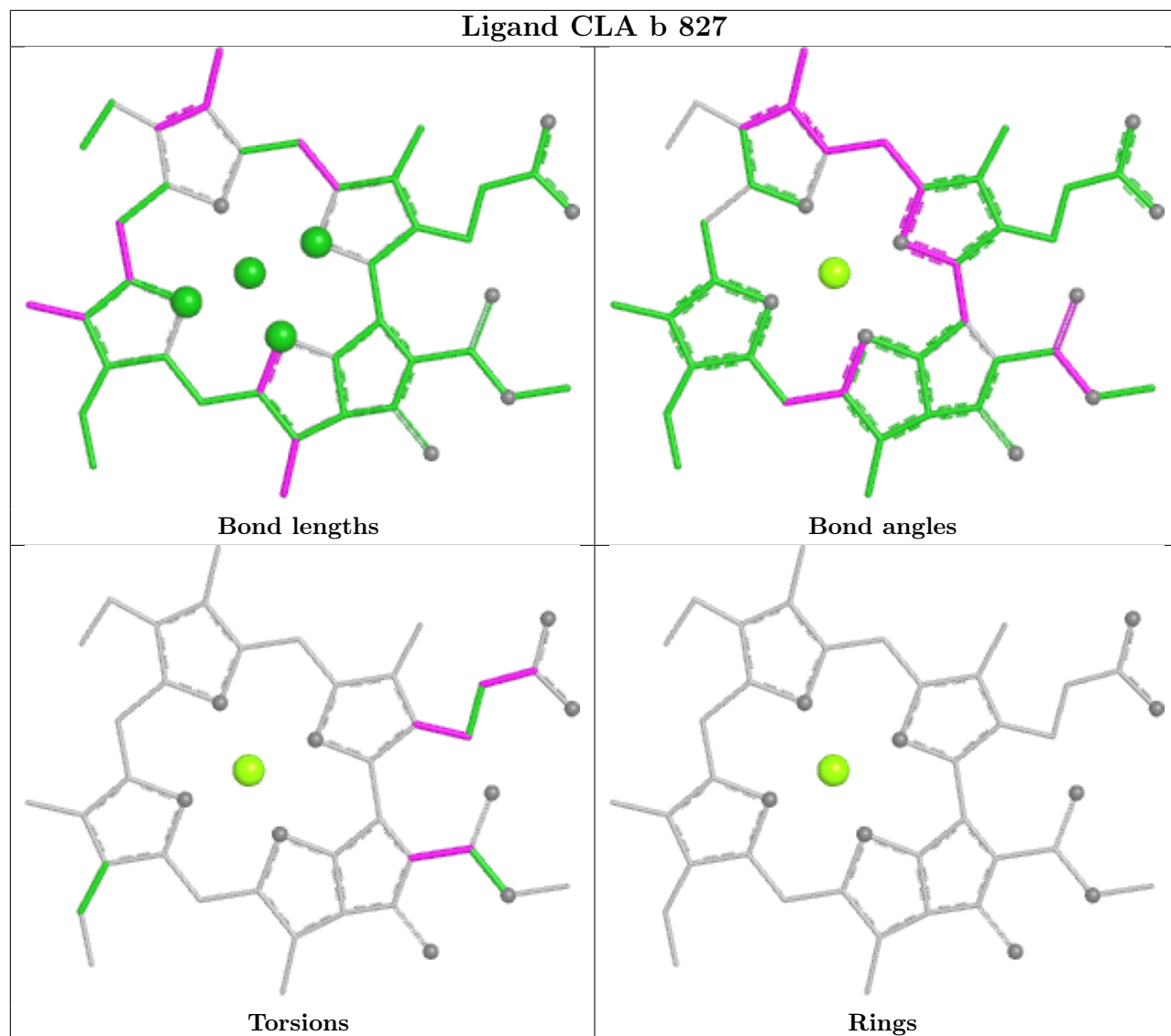


Ligand BCR a 847

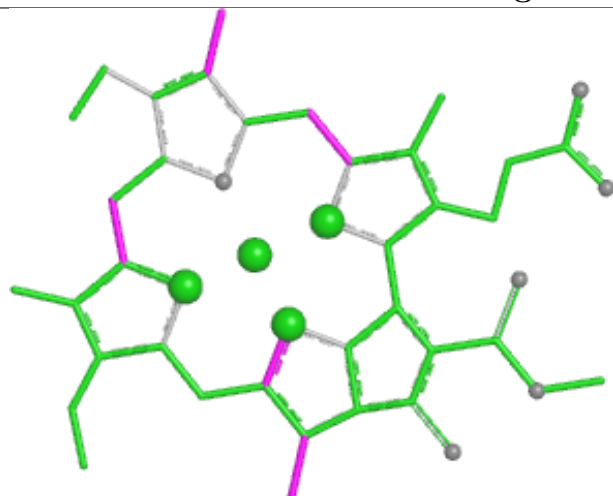




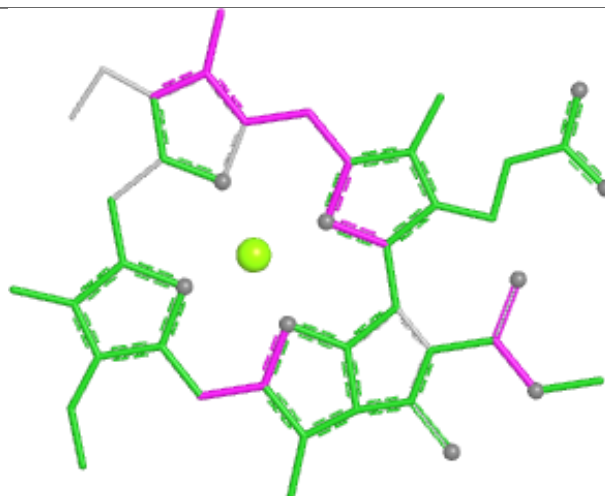
Ligand CLA b 827



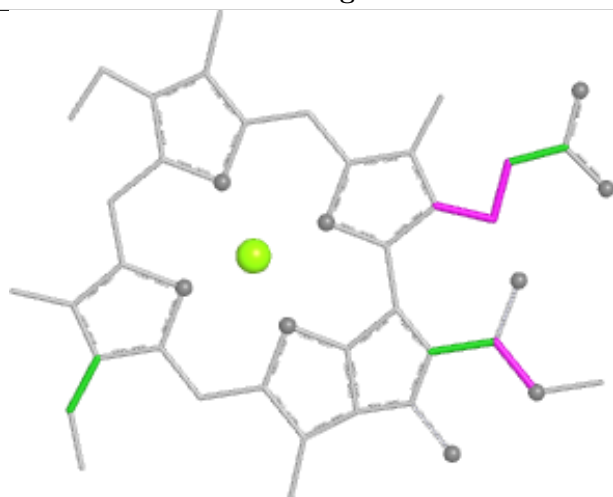
Ligand CLA B 809



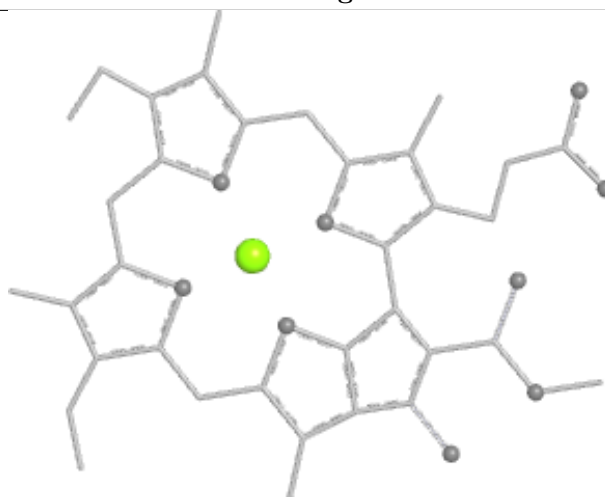
Bond lengths



Bond angles

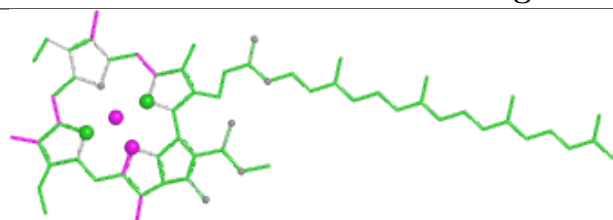


Torsions

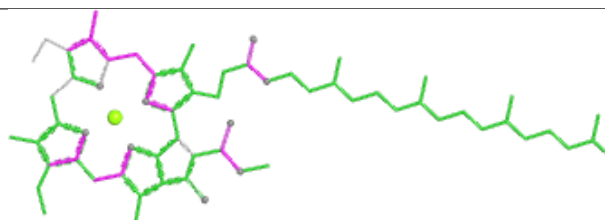


Rings

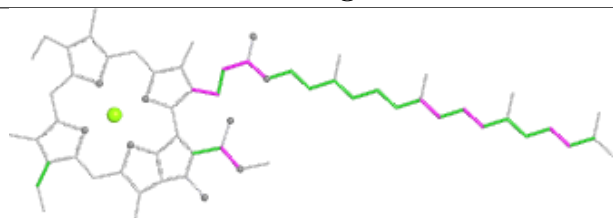
Ligand CLA A 806



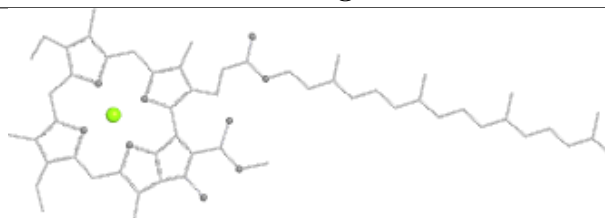
Bond lengths



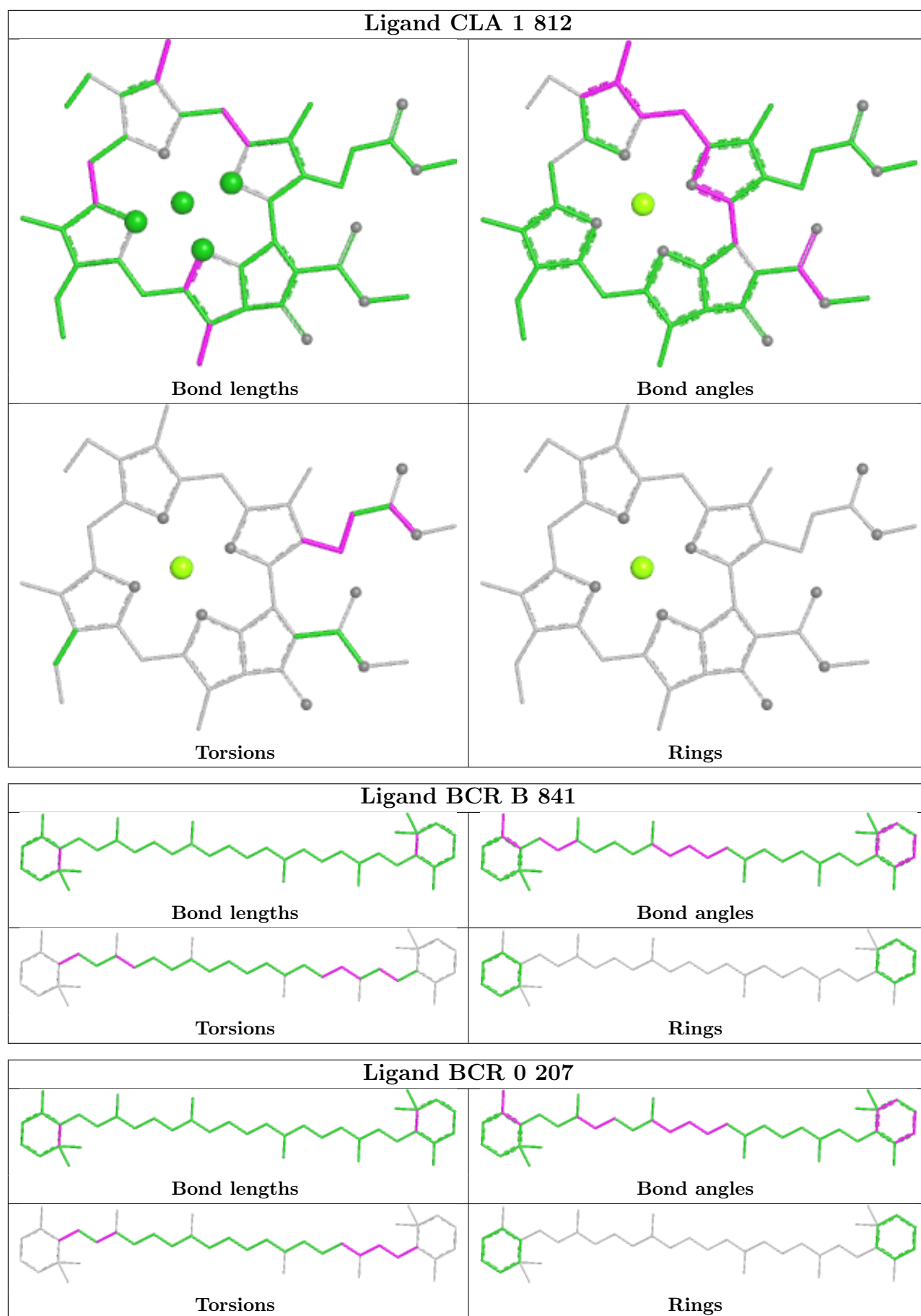
Bond angles

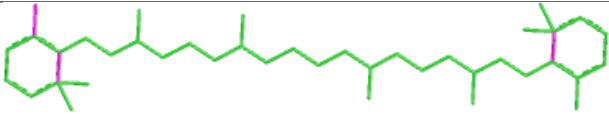
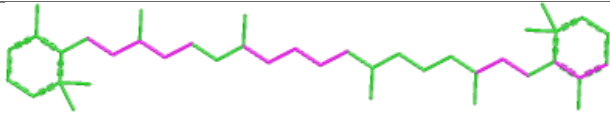
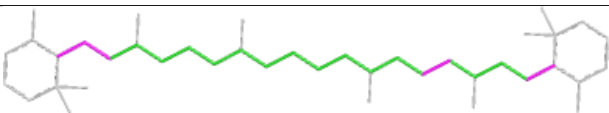
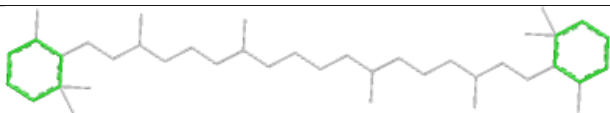


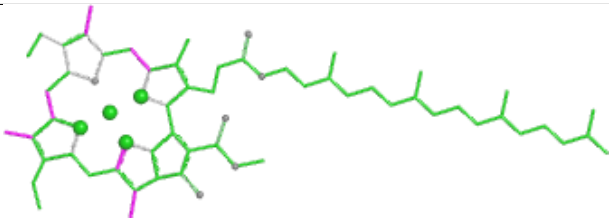
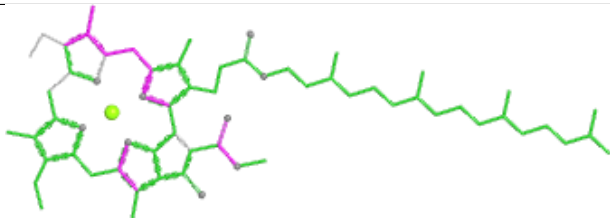
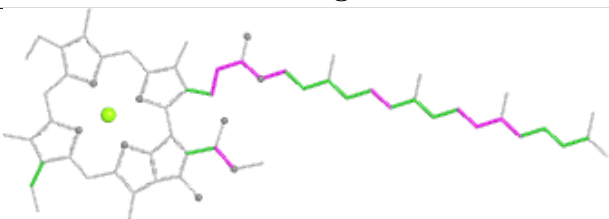
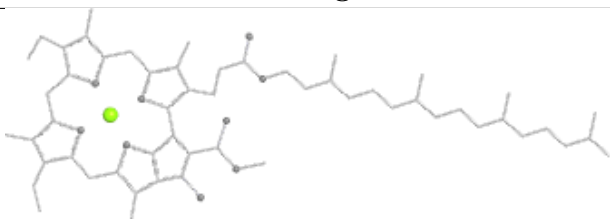
Torsions

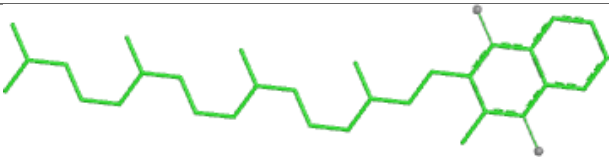
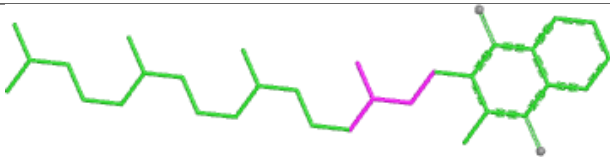
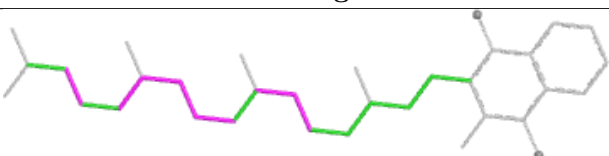
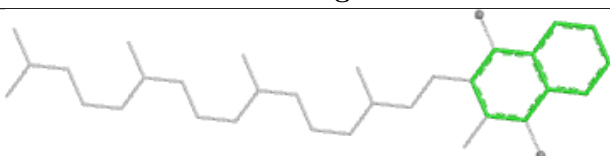


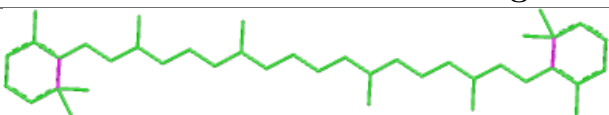
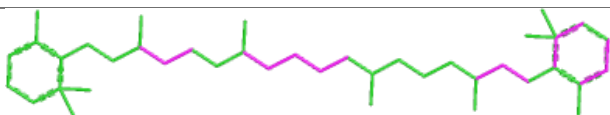
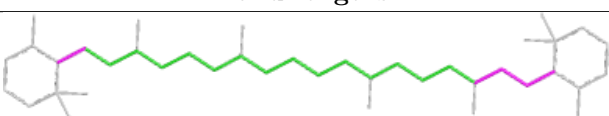
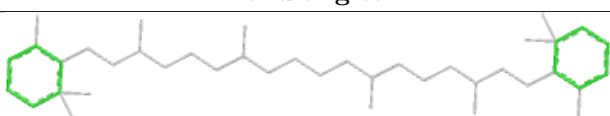
Rings



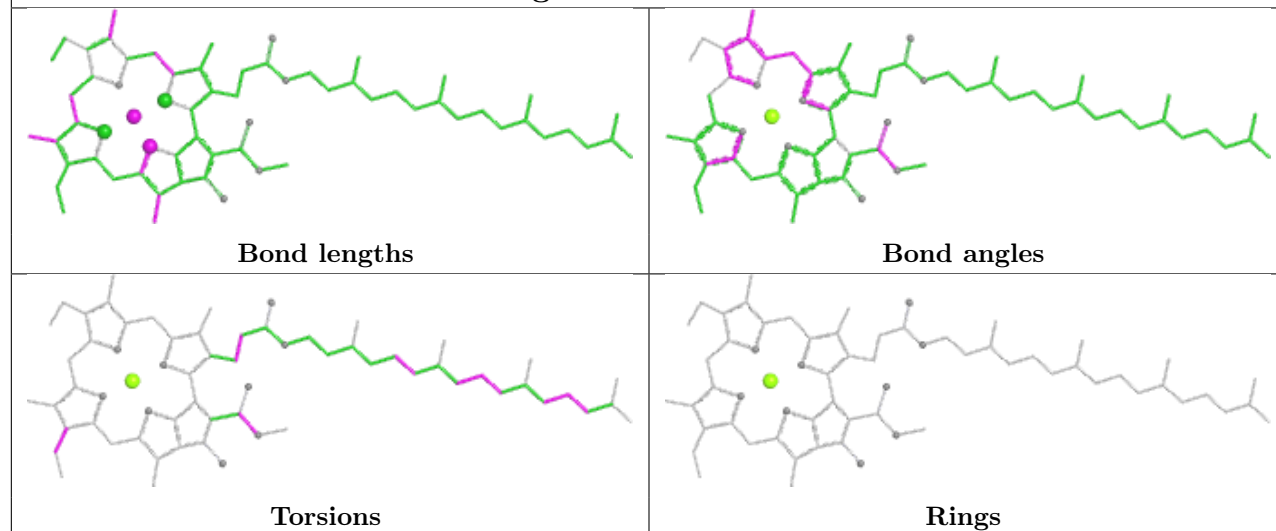
Ligand BCR a 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b 807	
	
Bond lengths	Bond angles
	
Torsions	Rings

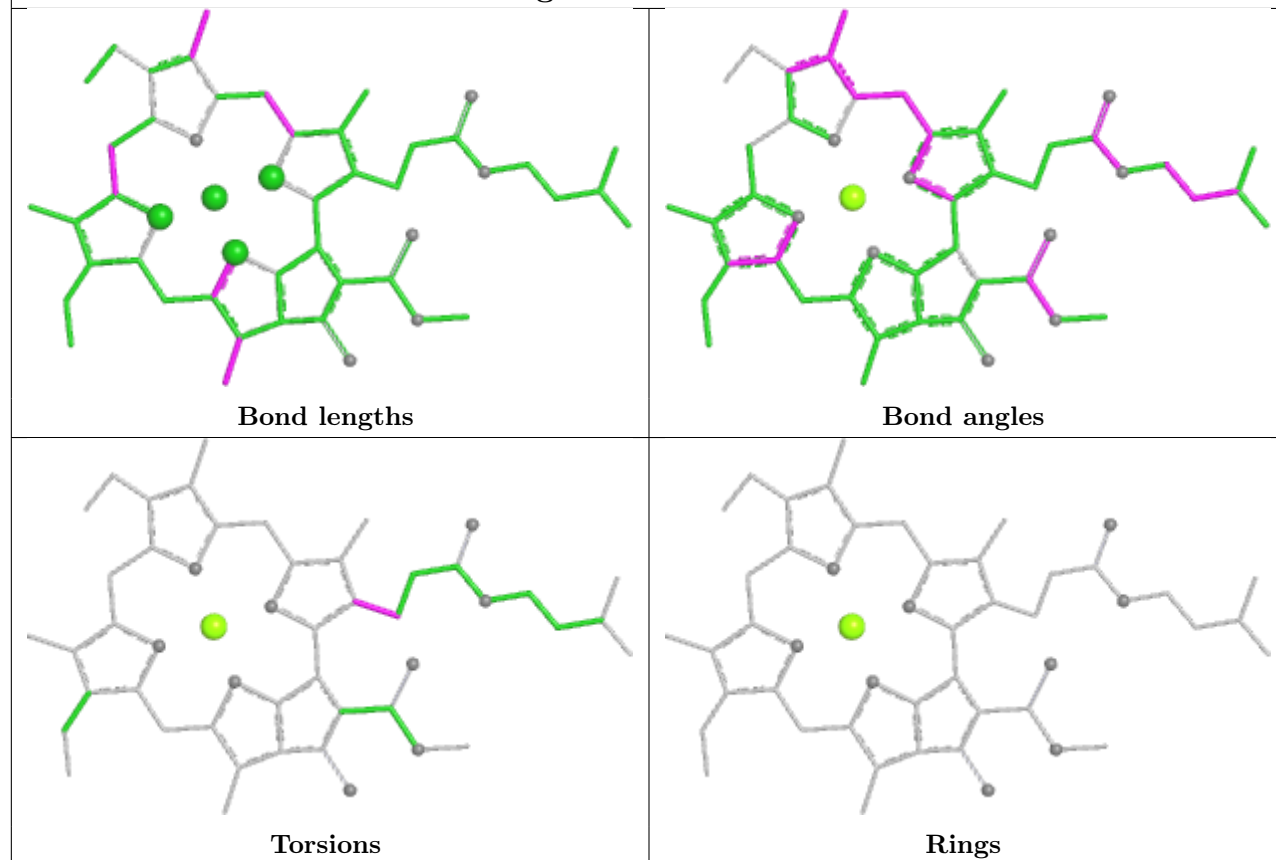
Ligand PQN 1 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

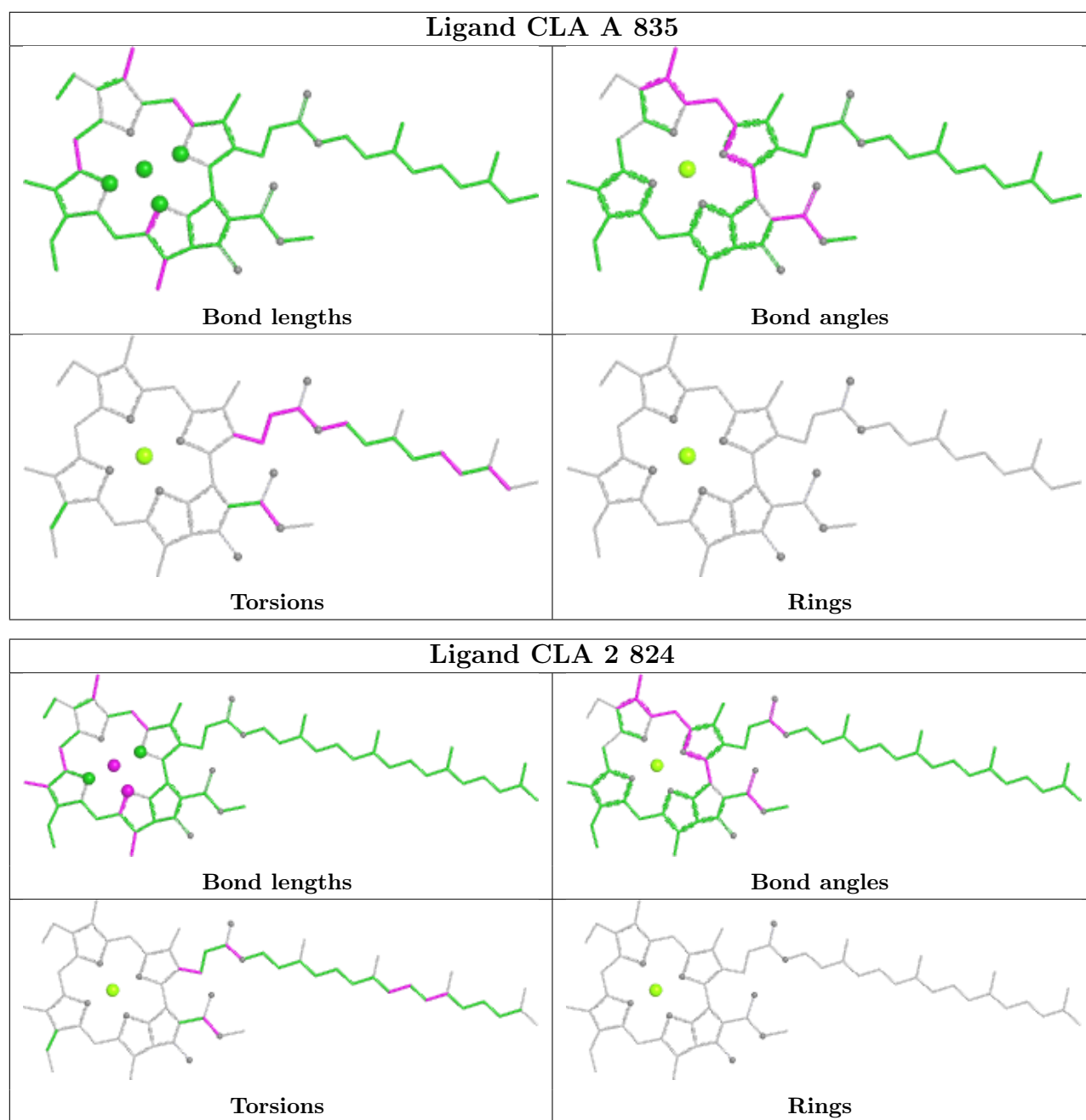
Ligand BCR 2 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

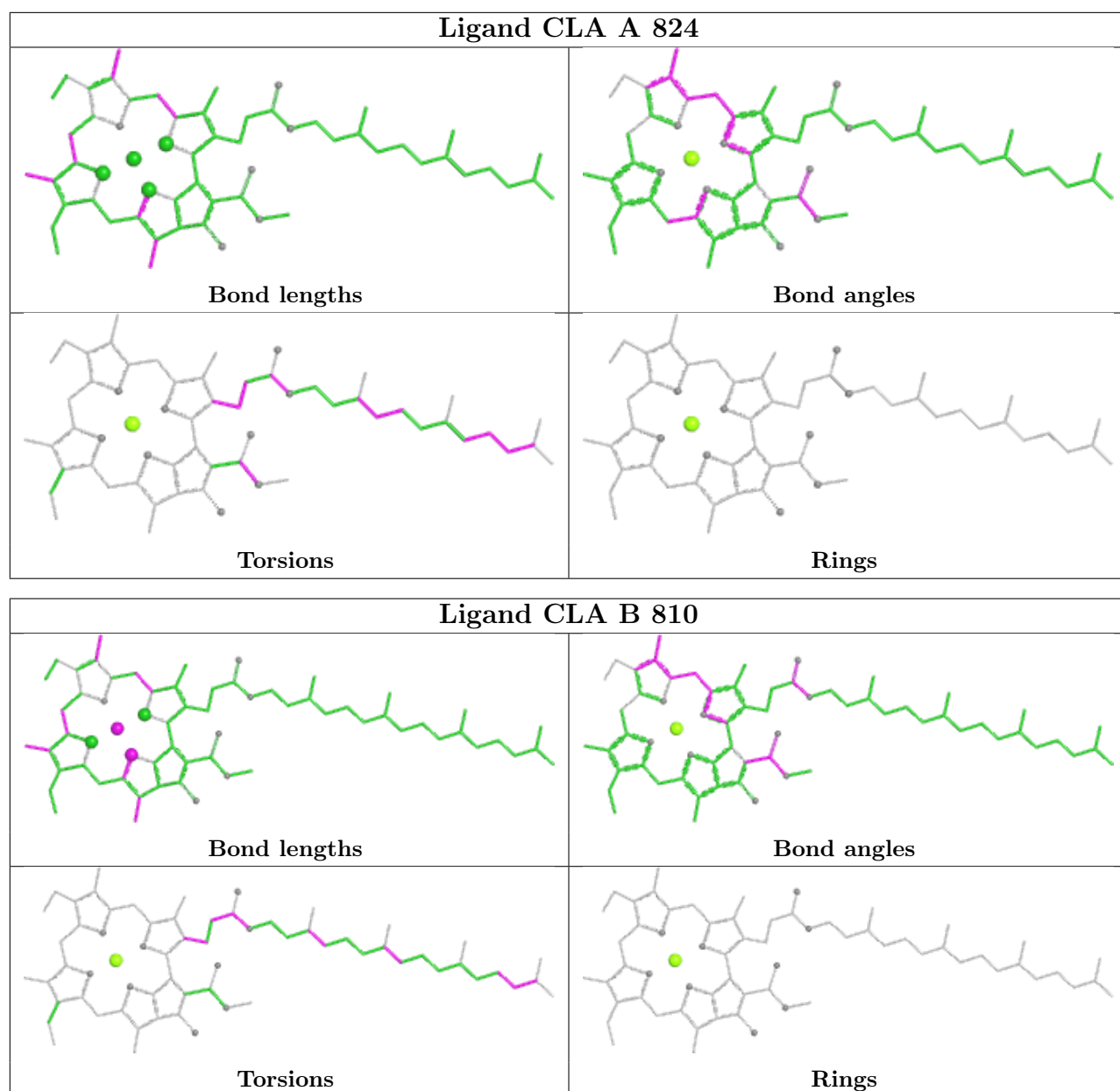
Ligand CLA B 802



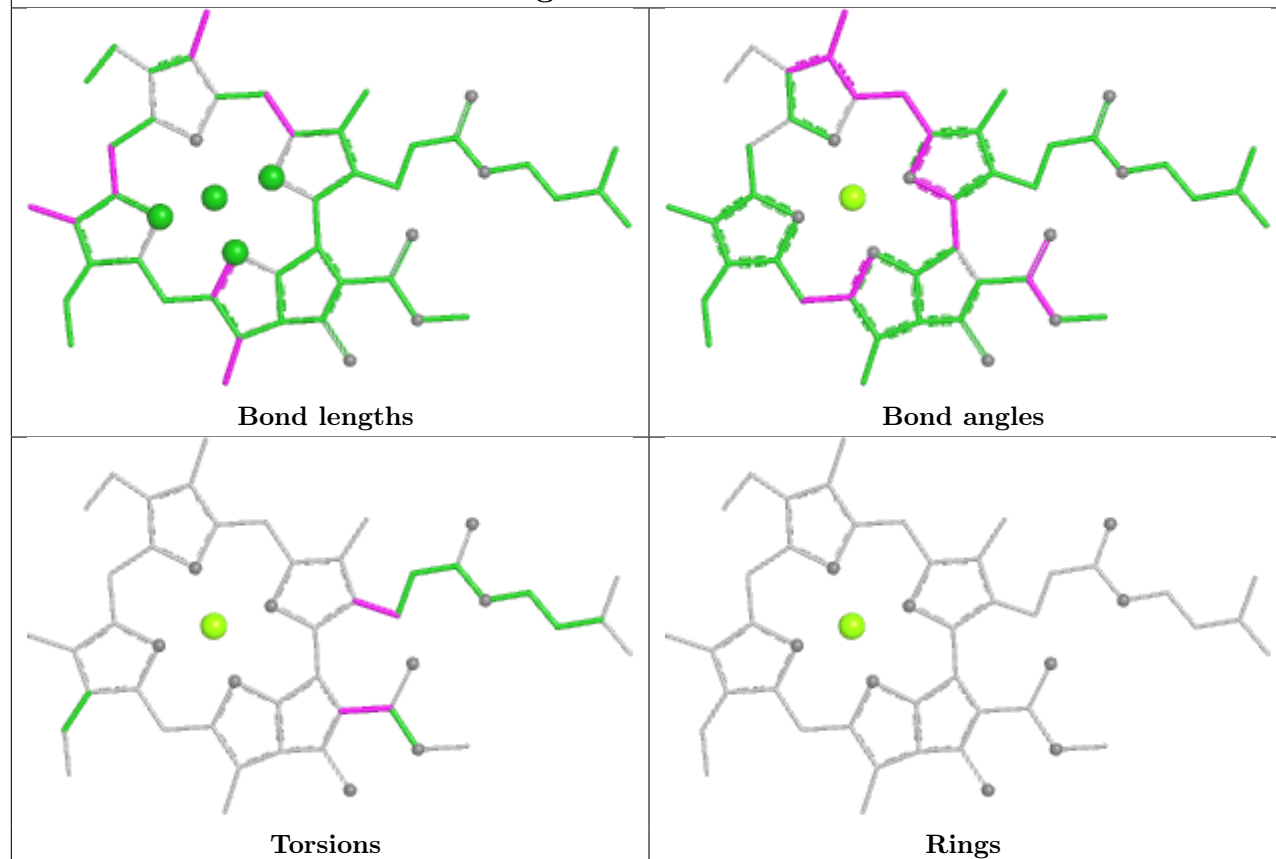
Ligand CLA 2 834



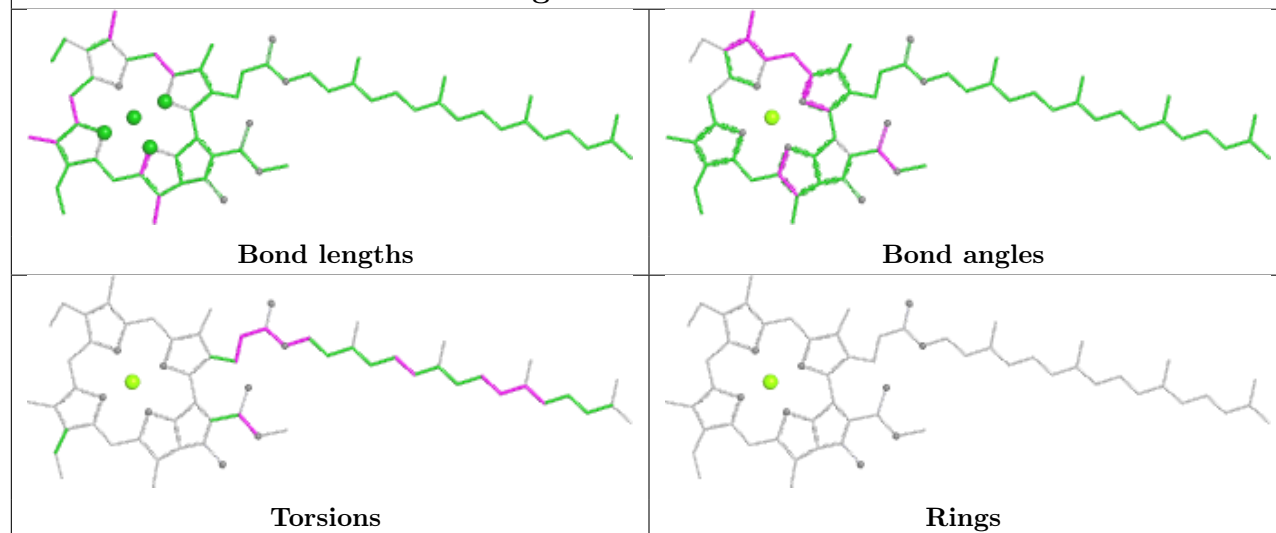


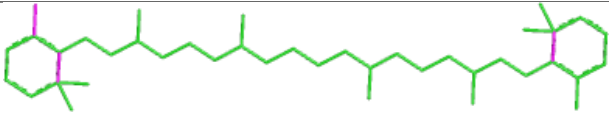
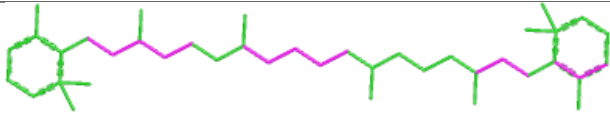
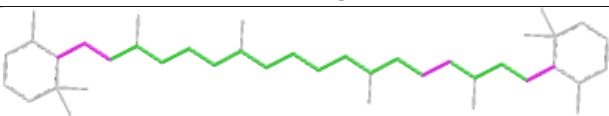
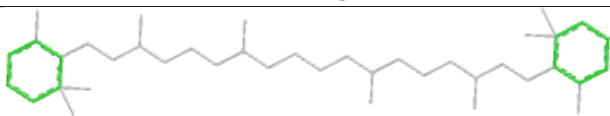



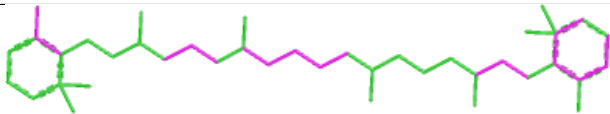
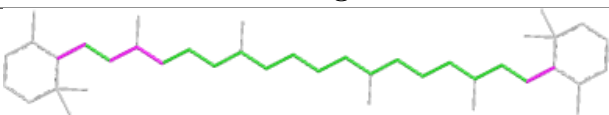
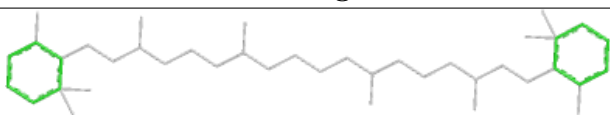
Ligand CLA 1 808

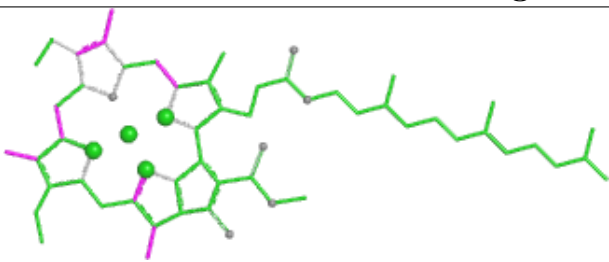
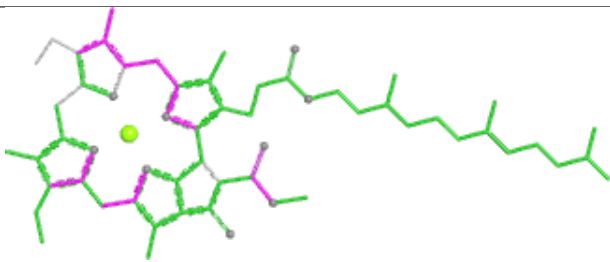
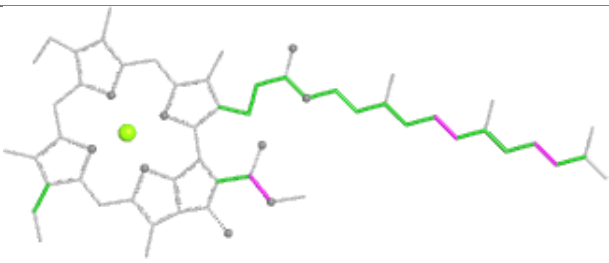
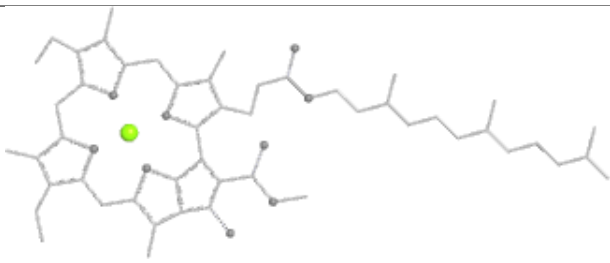


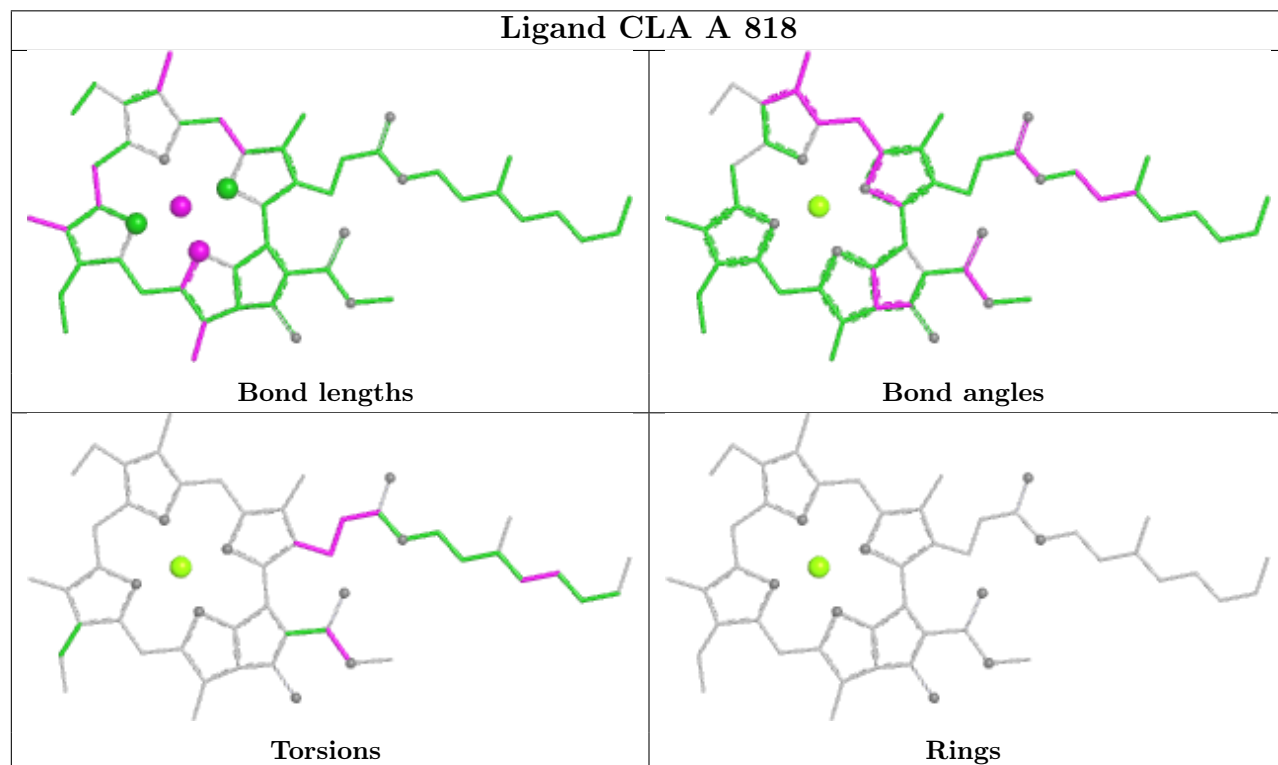
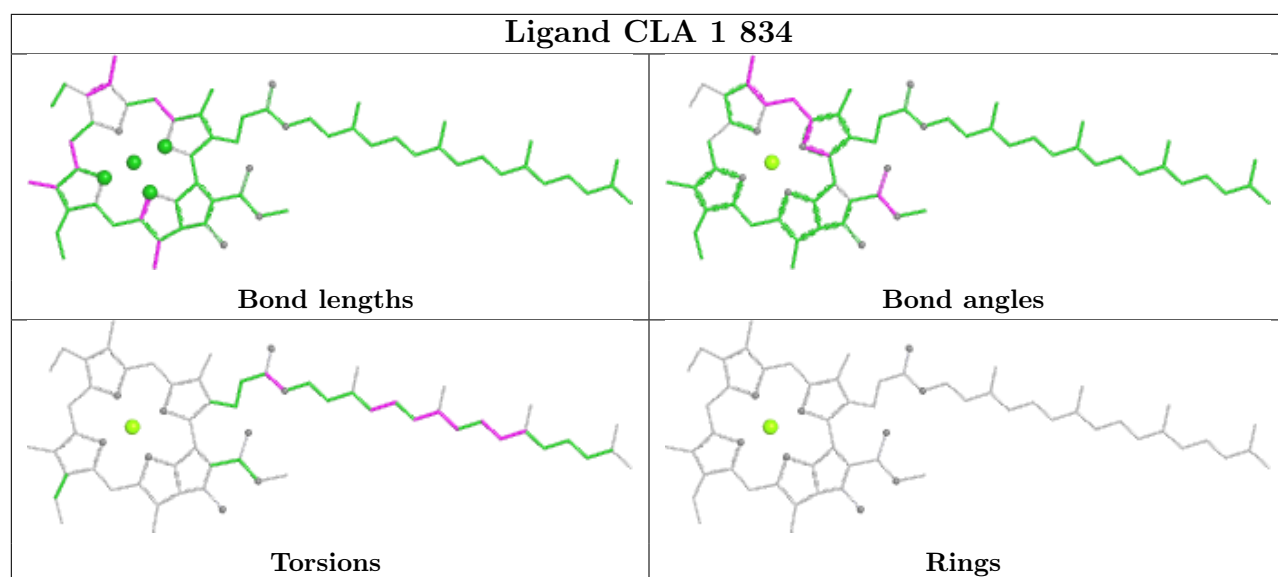
Ligand CLA B 807



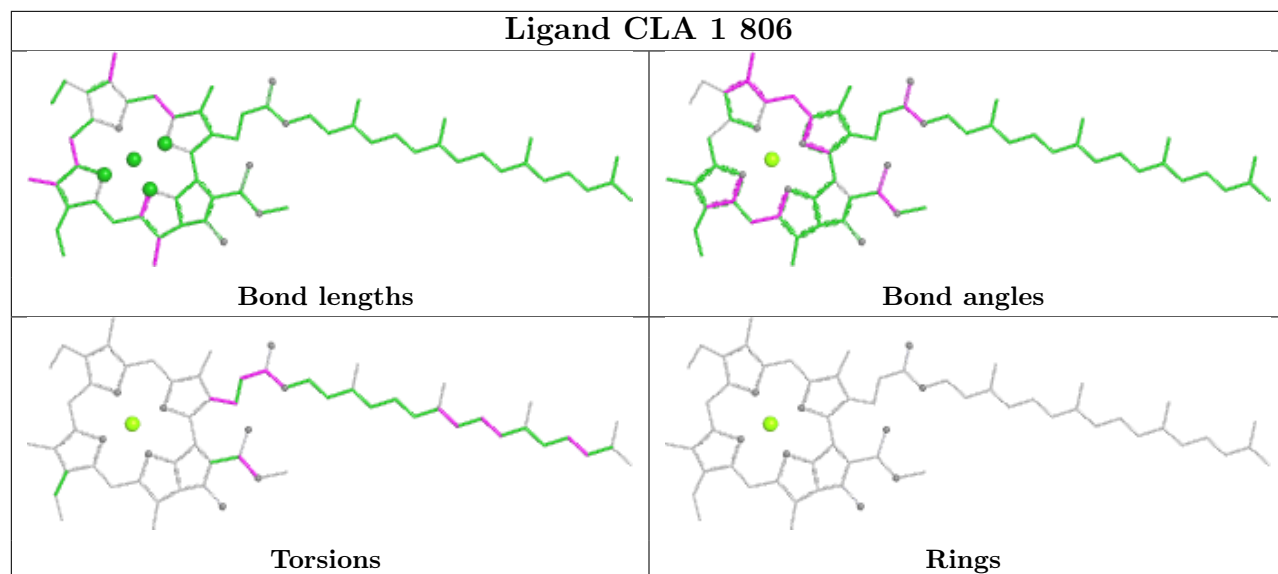
Ligand BCR A 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR m 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

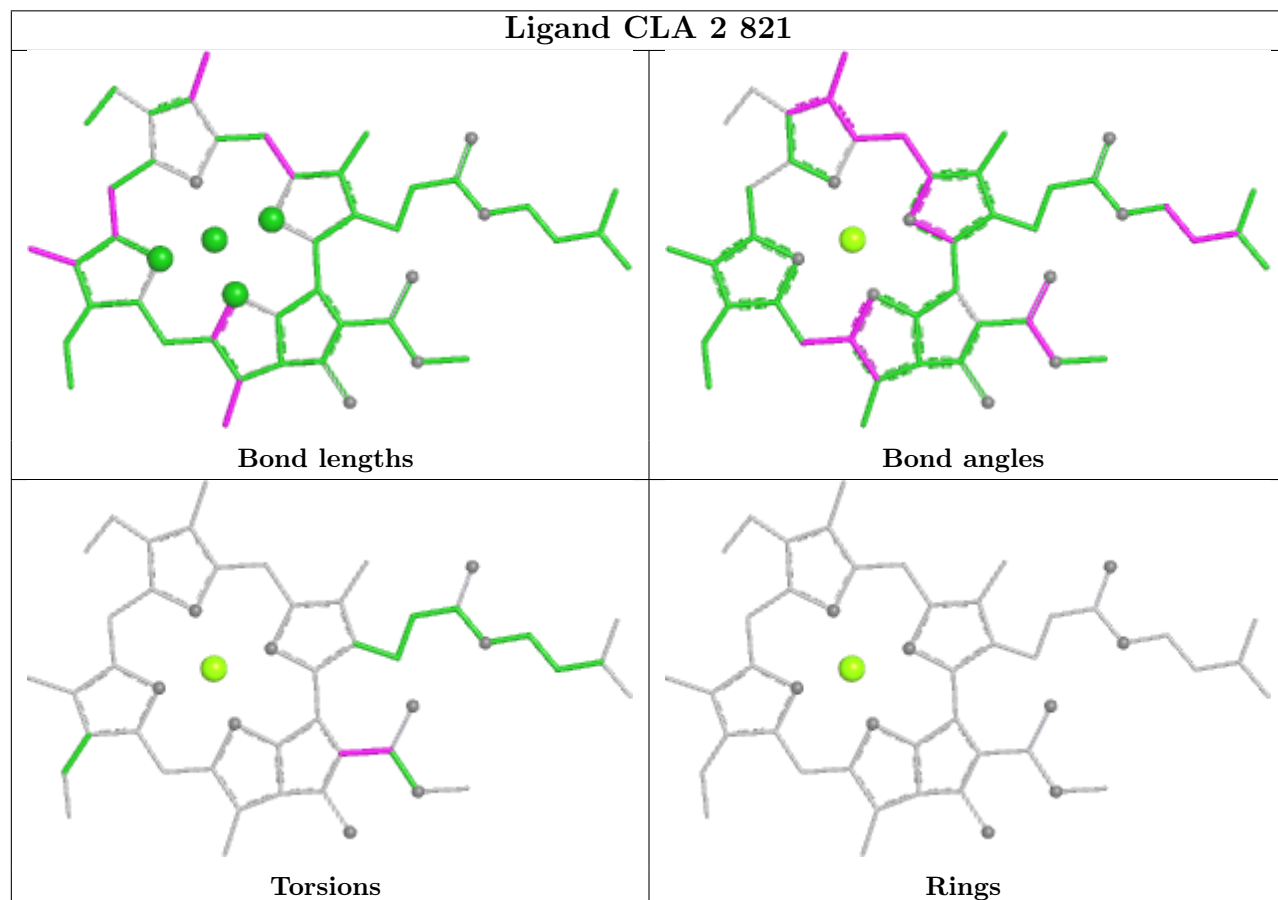
Ligand CLA b 834	
	
Bond lengths	Bond angles
	
Torsions	Rings



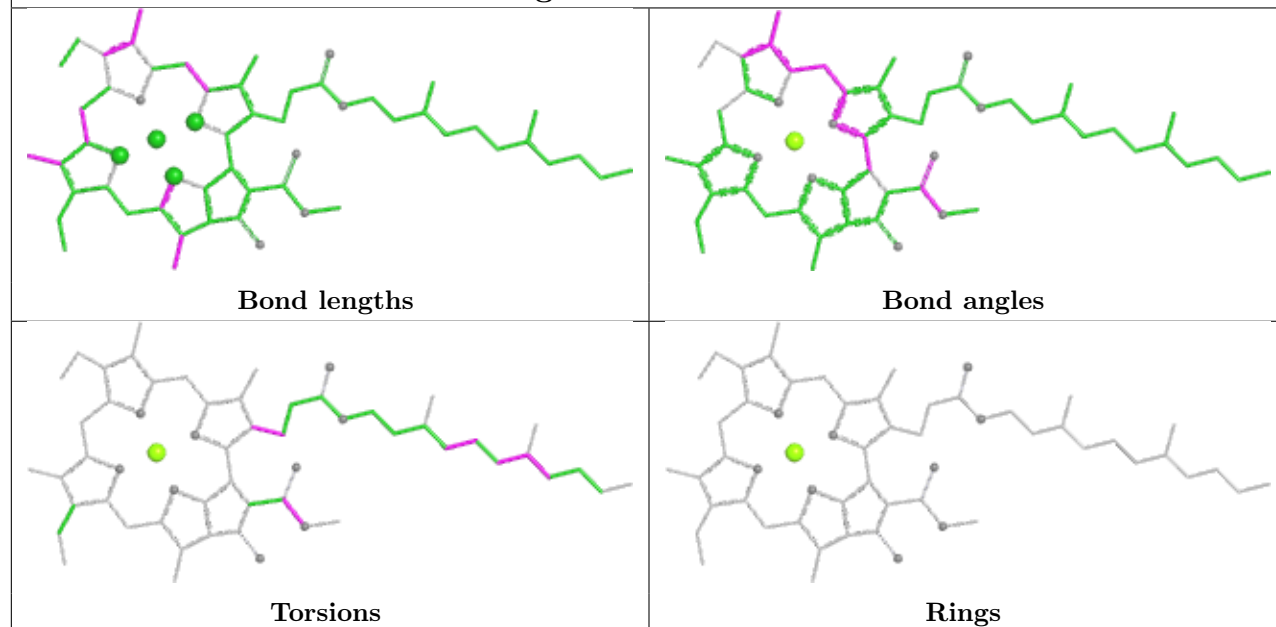
Ligand CLA 1 806



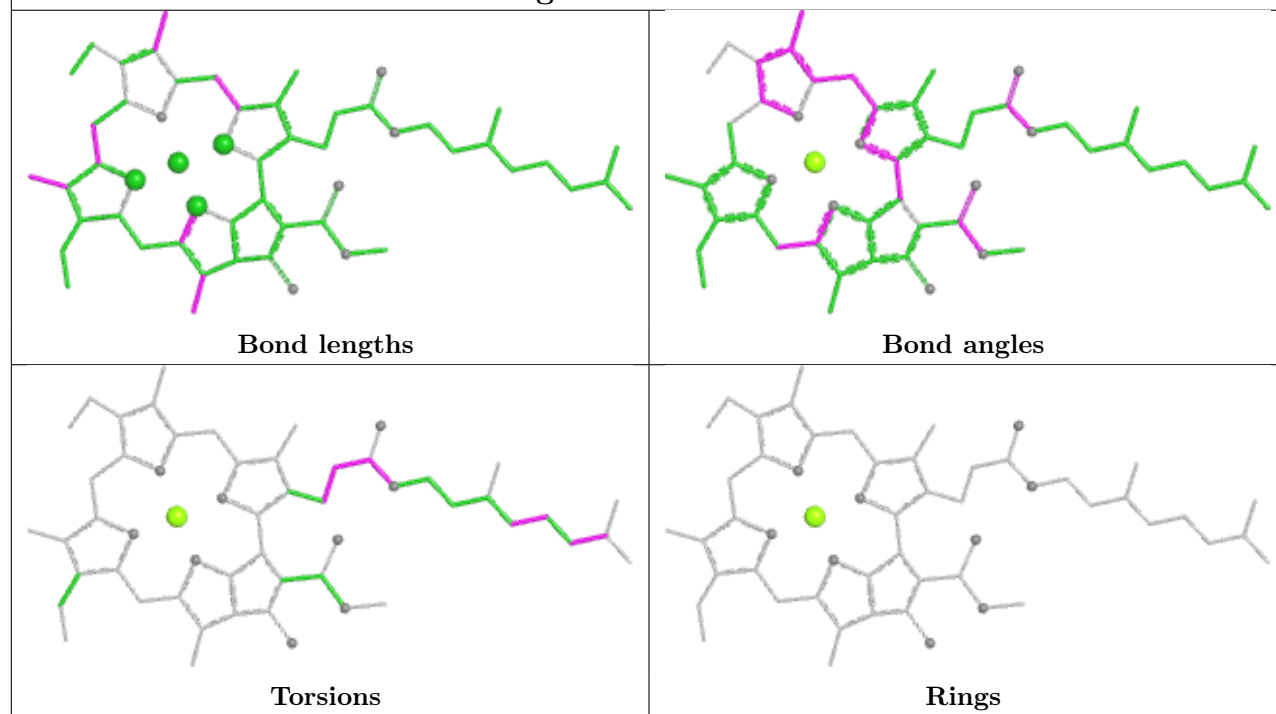
Ligand CLA 2 821

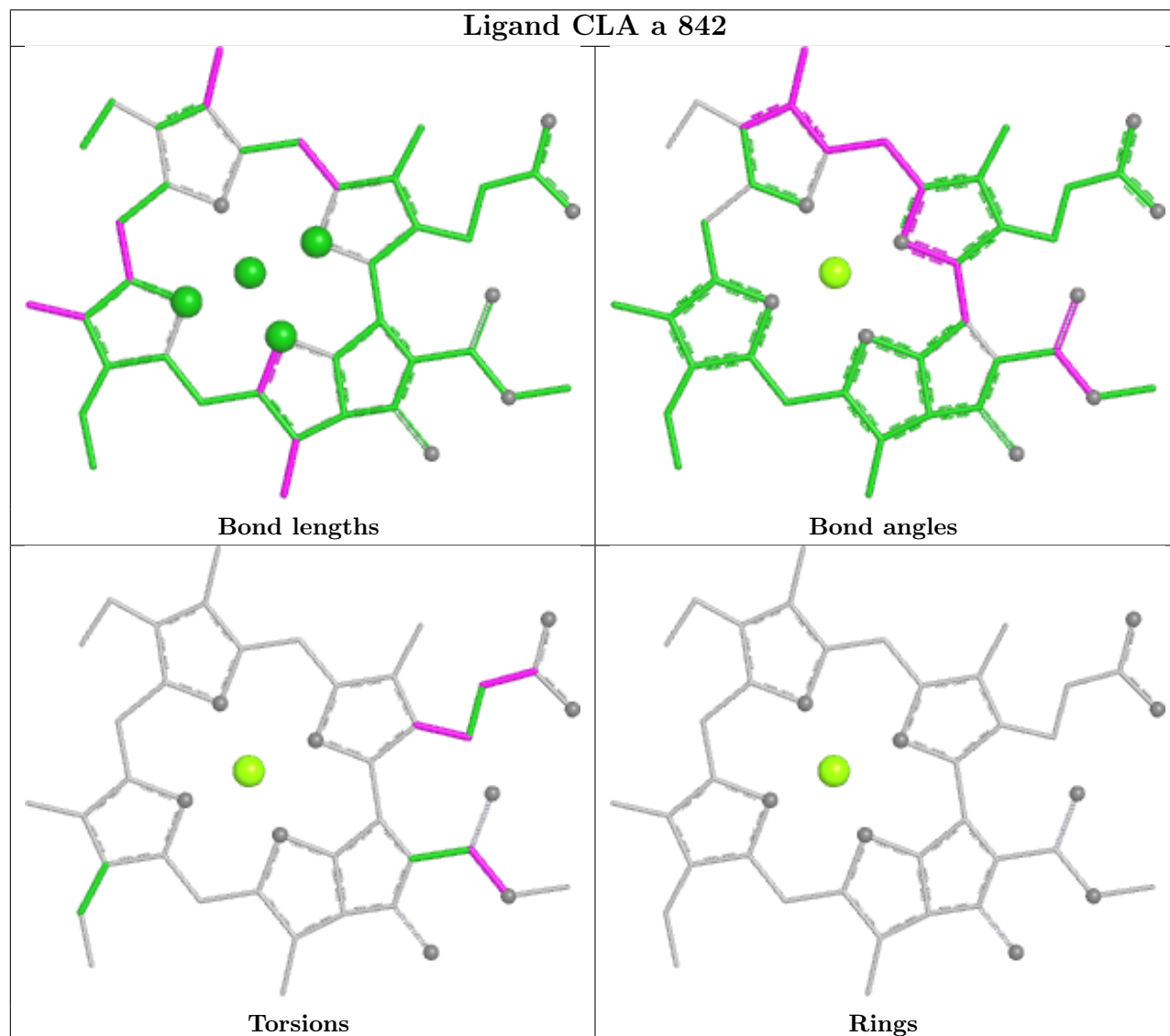
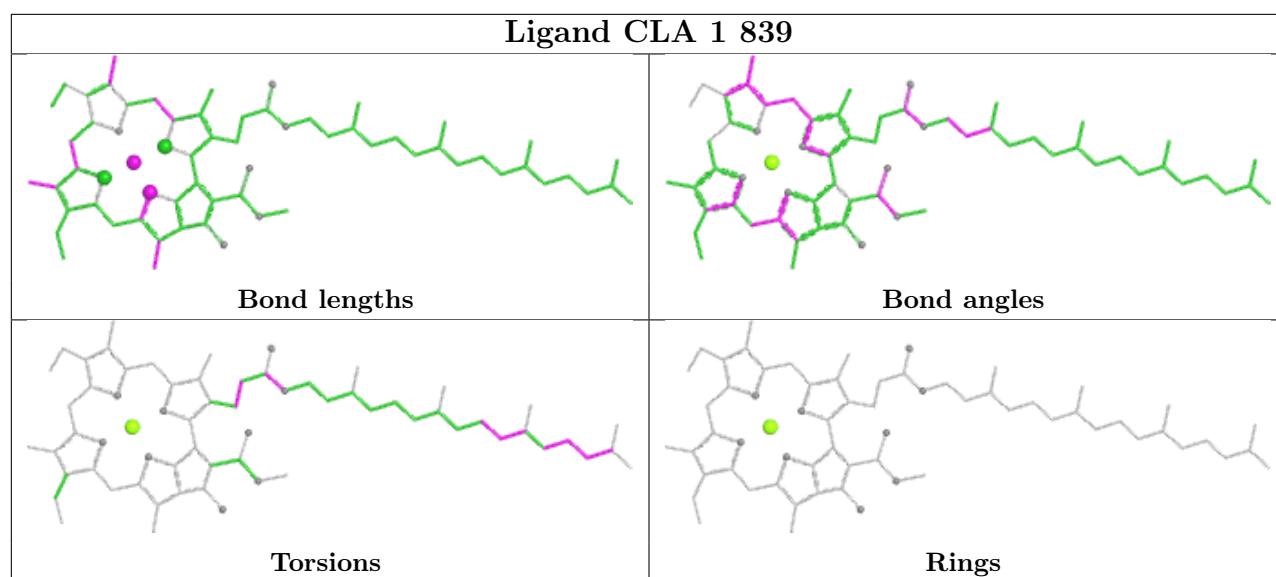


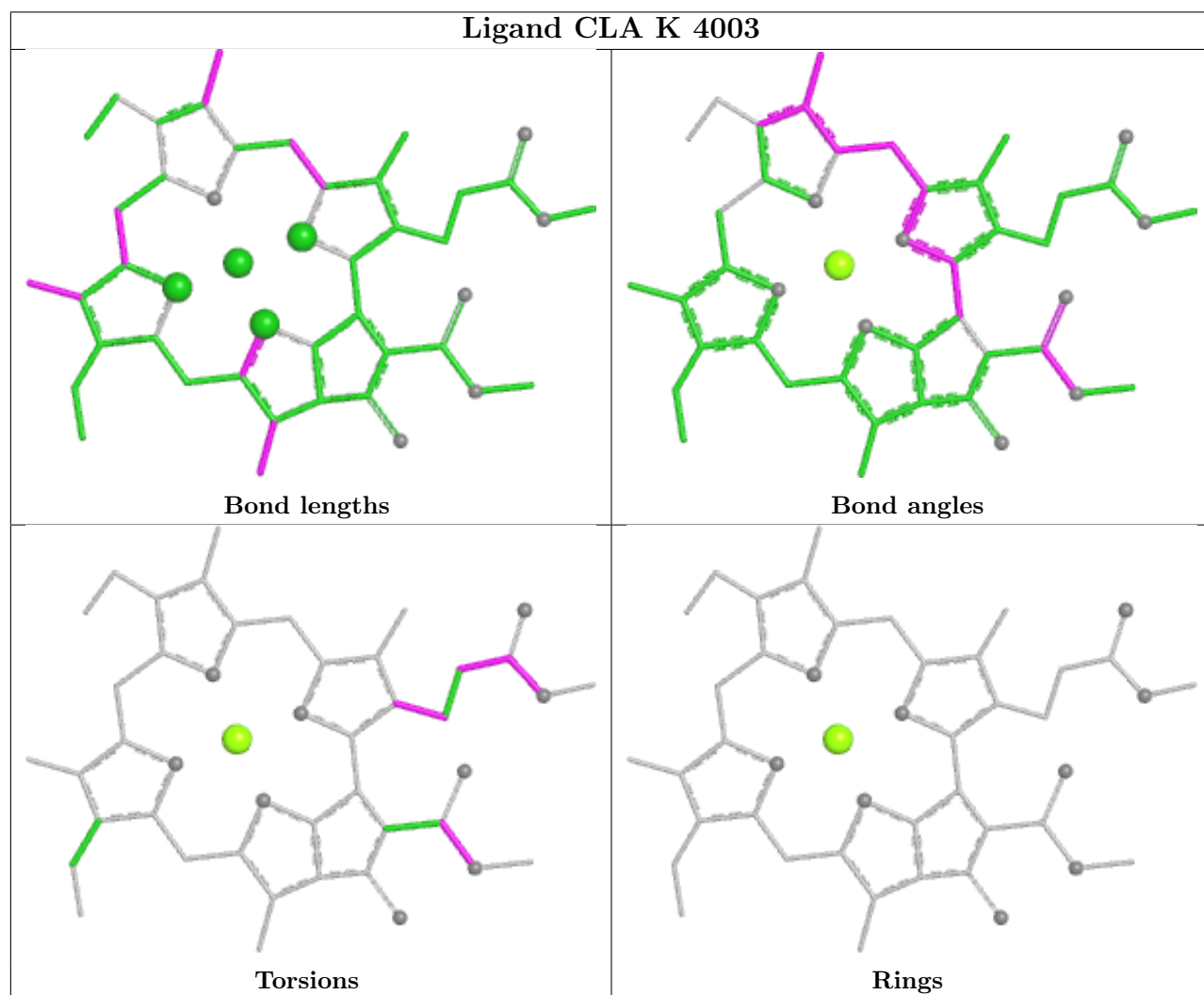
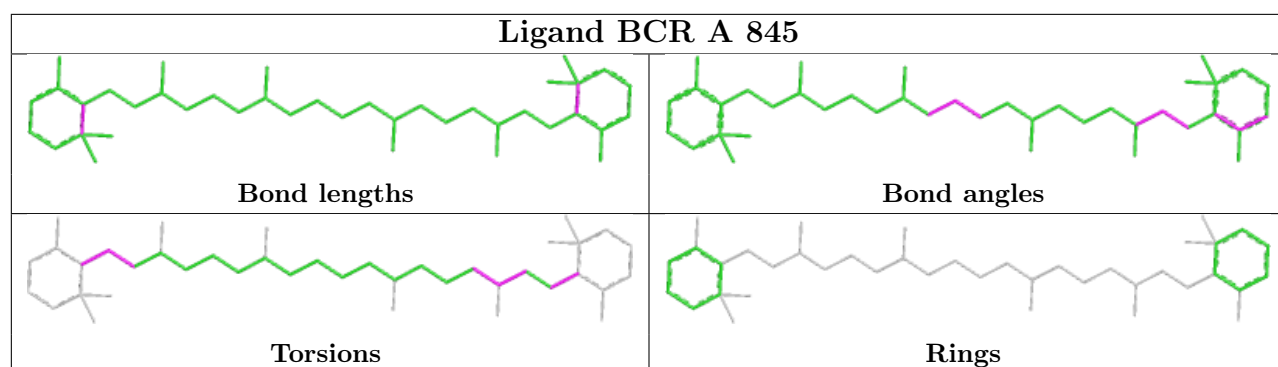
Ligand CLA b 830

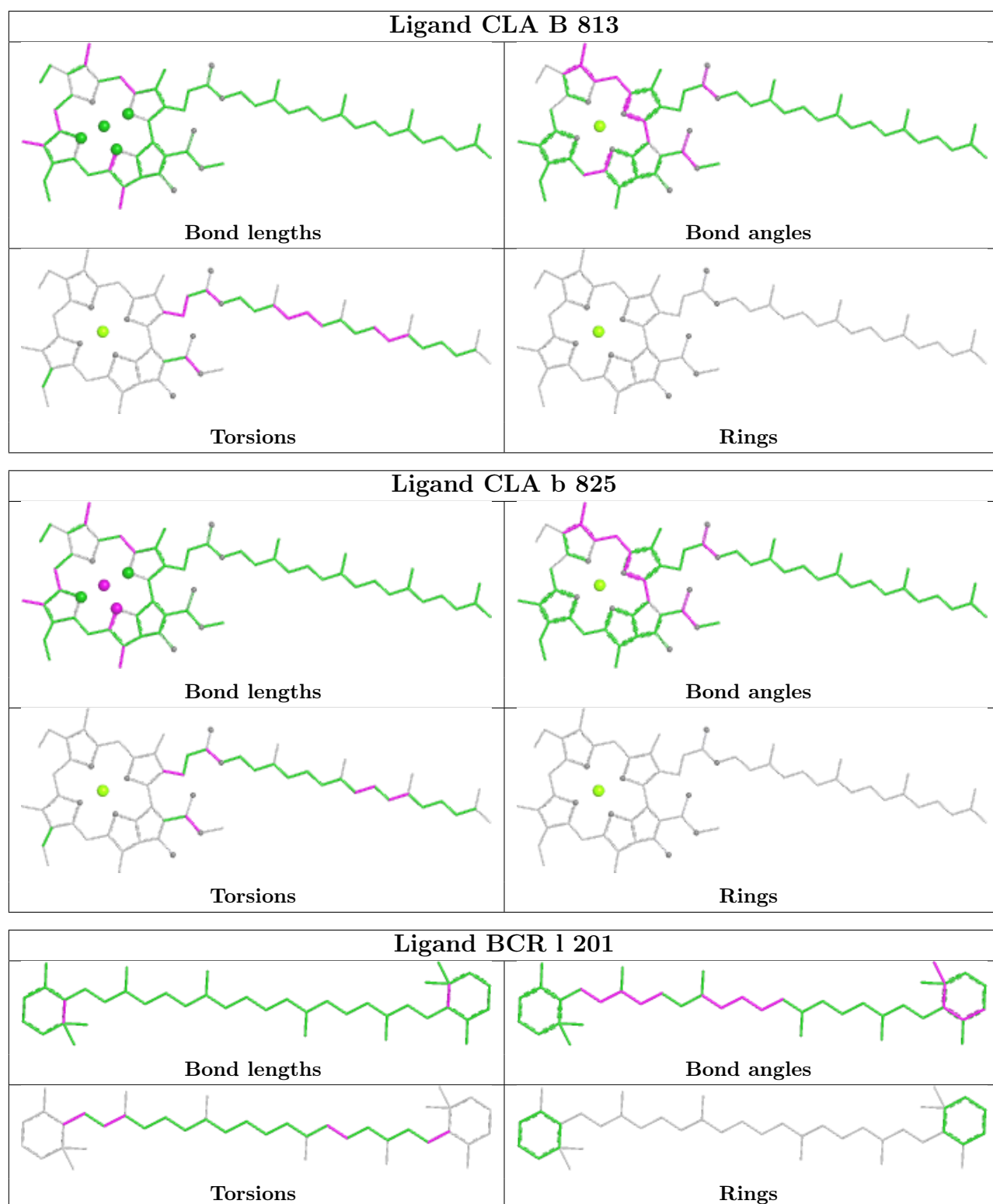


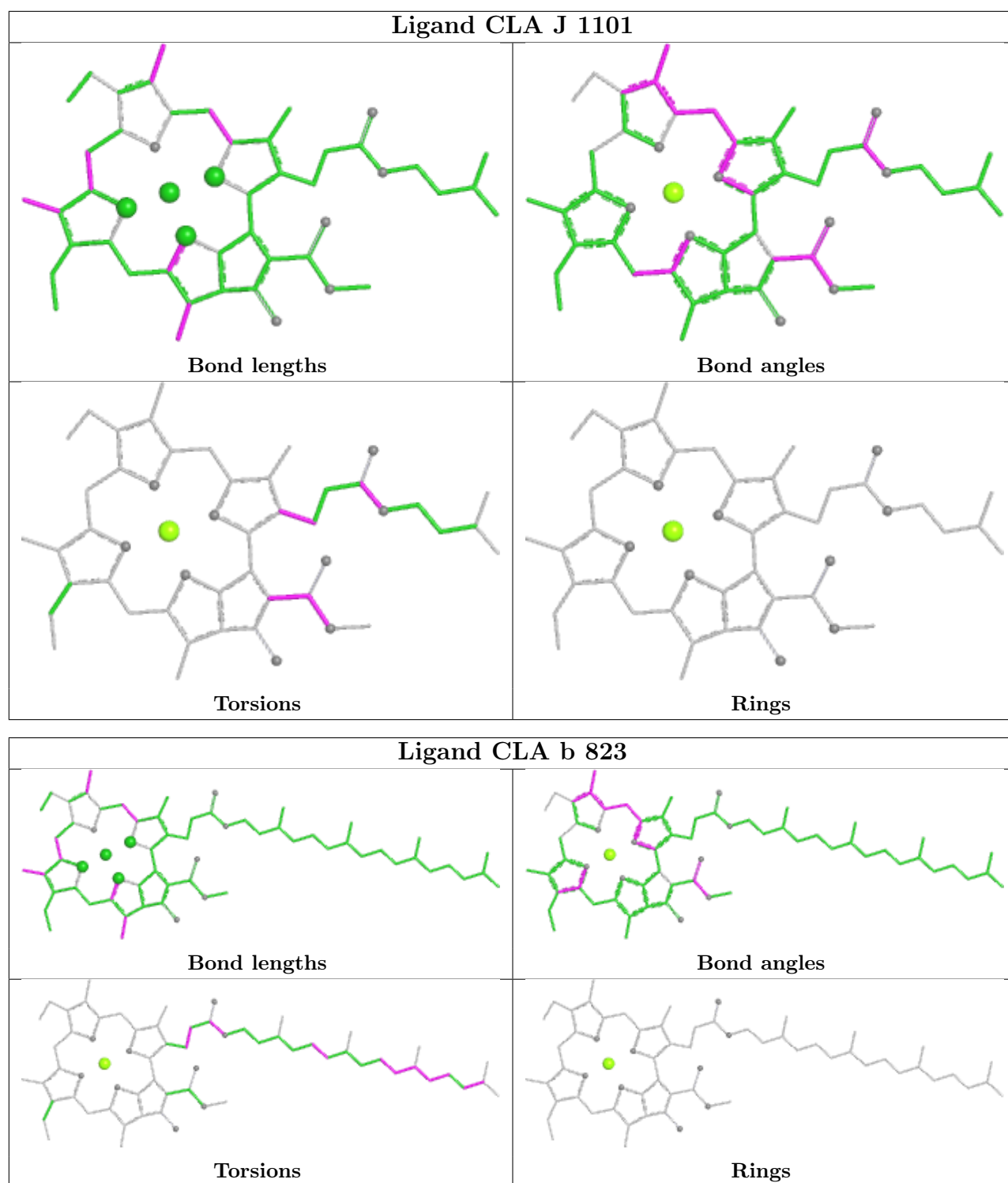
Ligand CLA 1 817



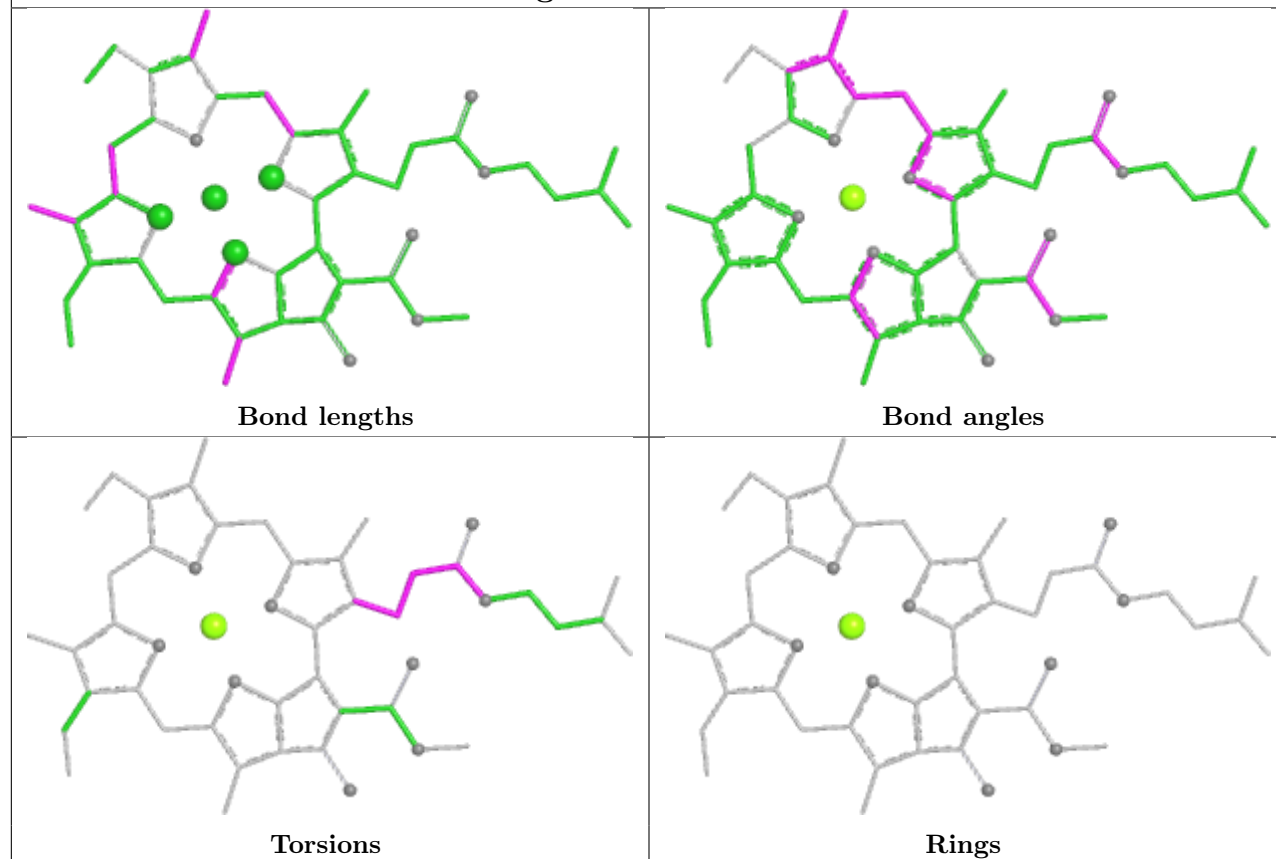




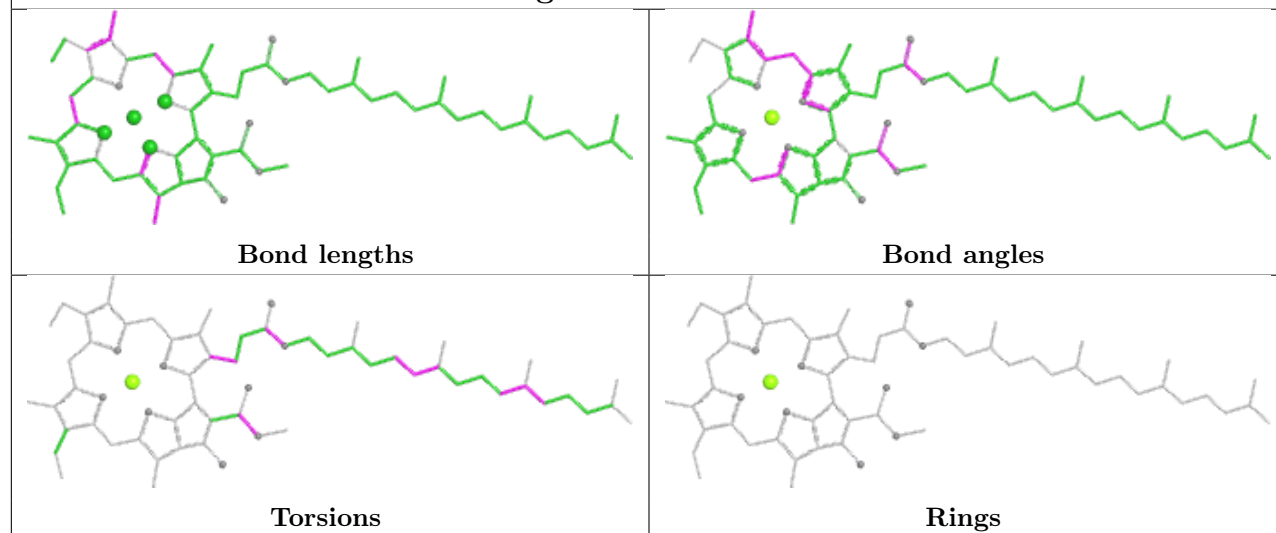


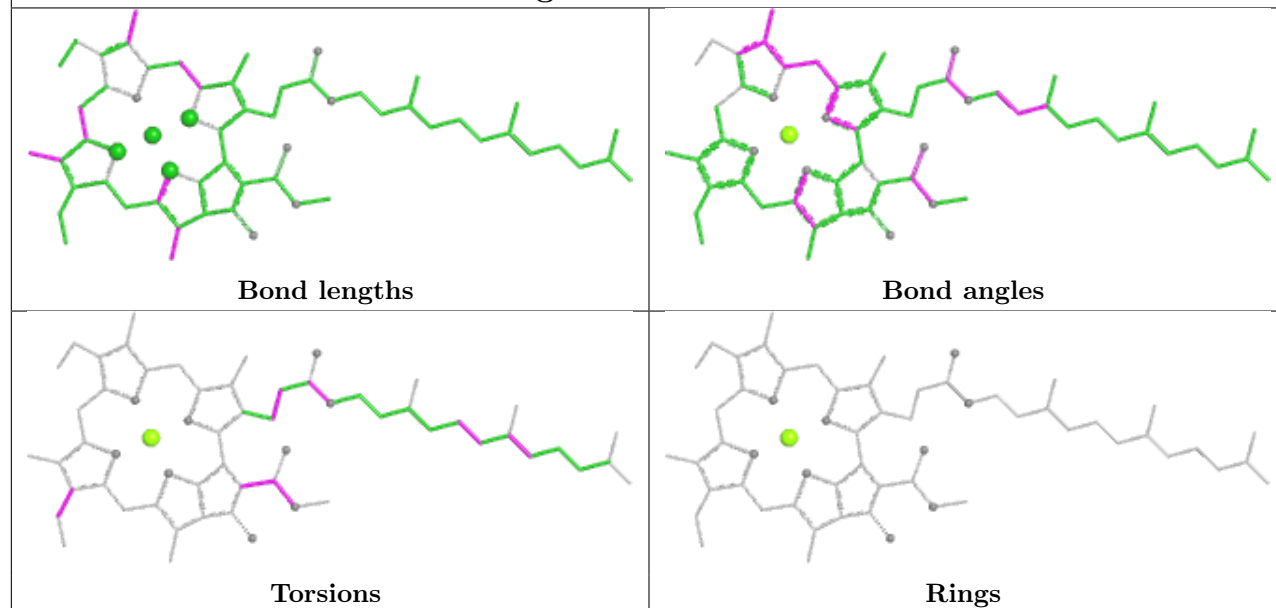
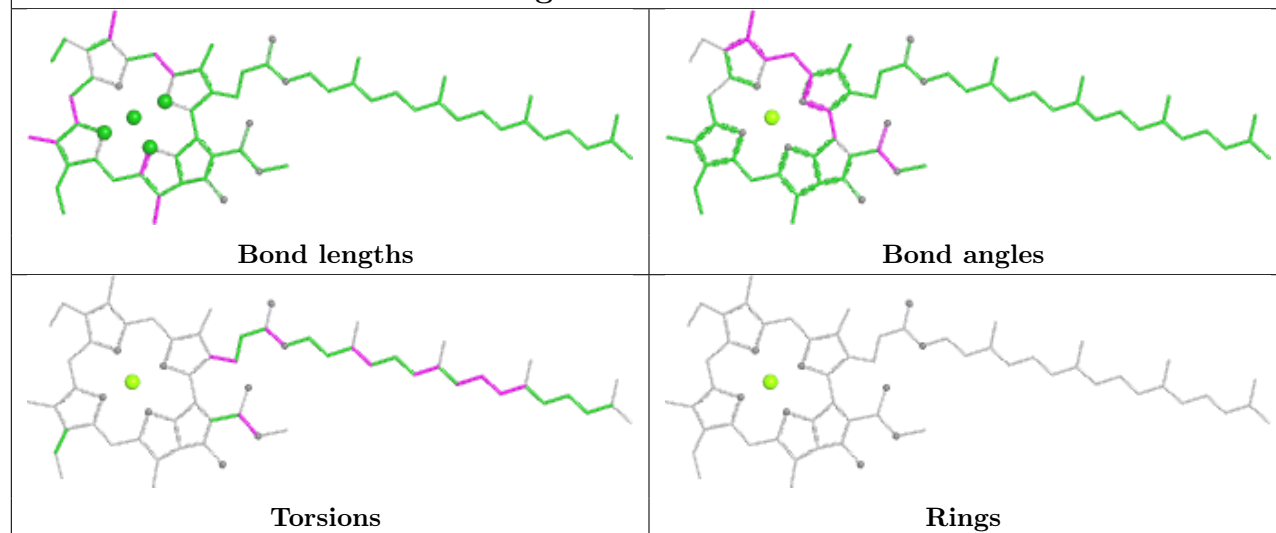


Ligand CLA 2 813

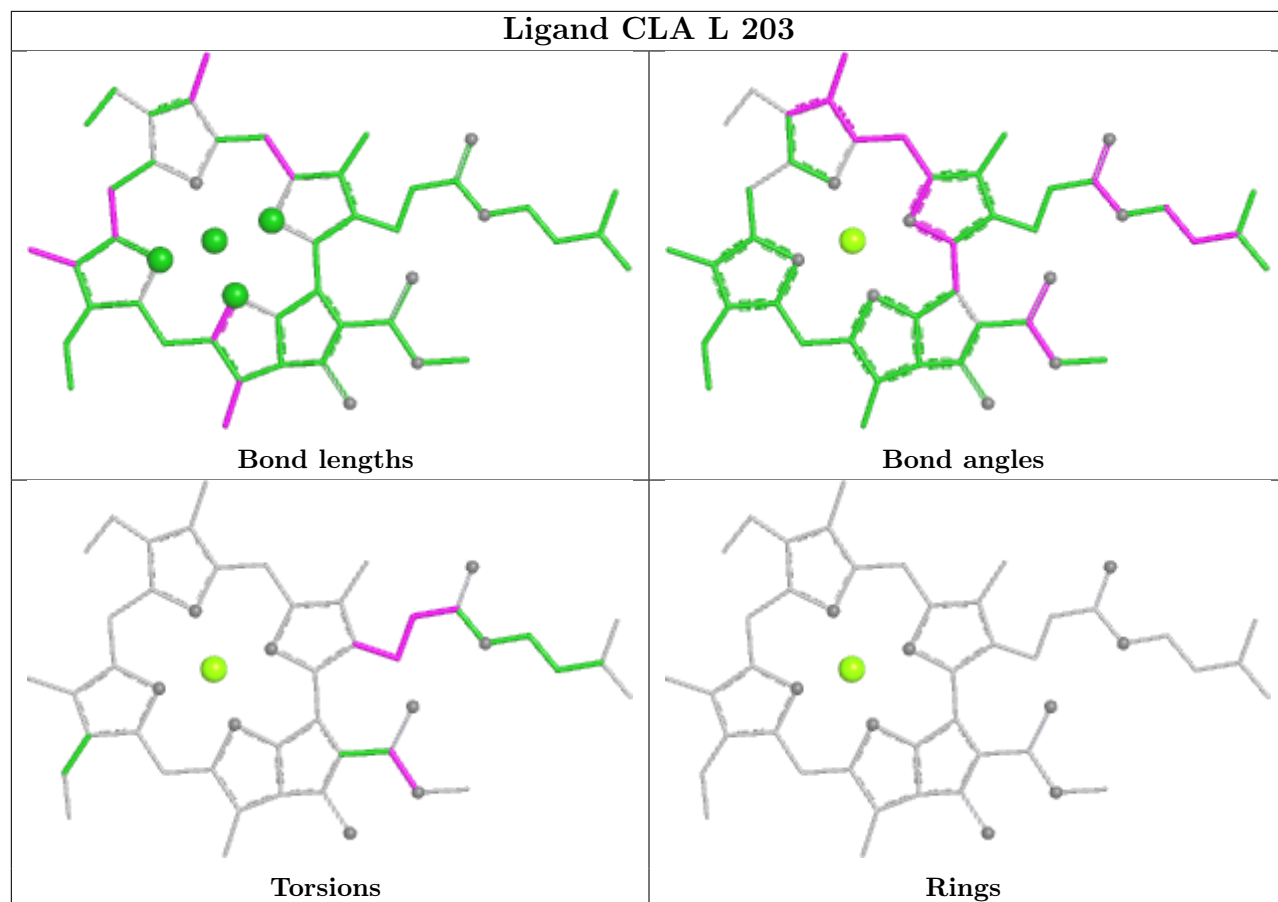


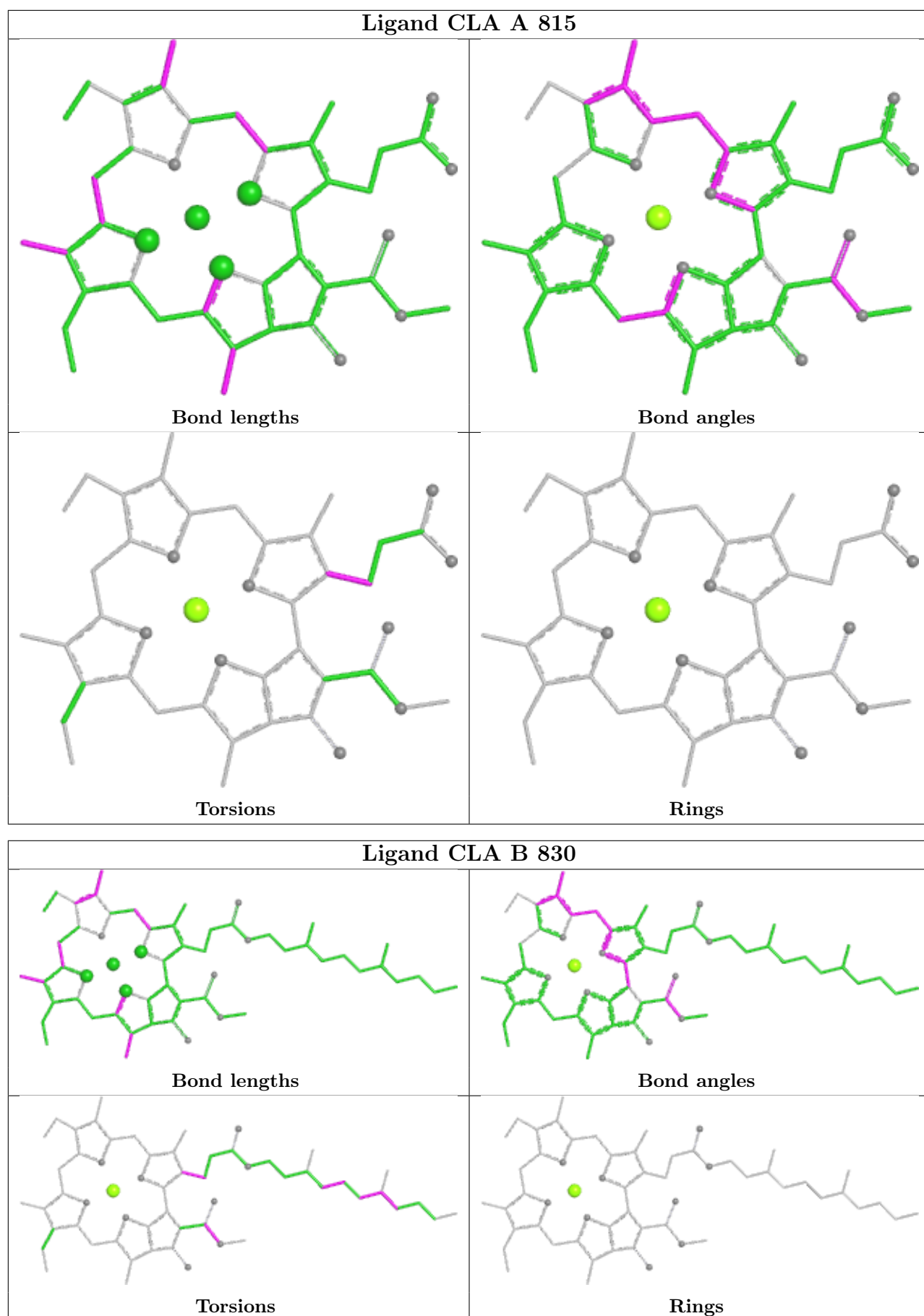
Ligand CLA 2 836

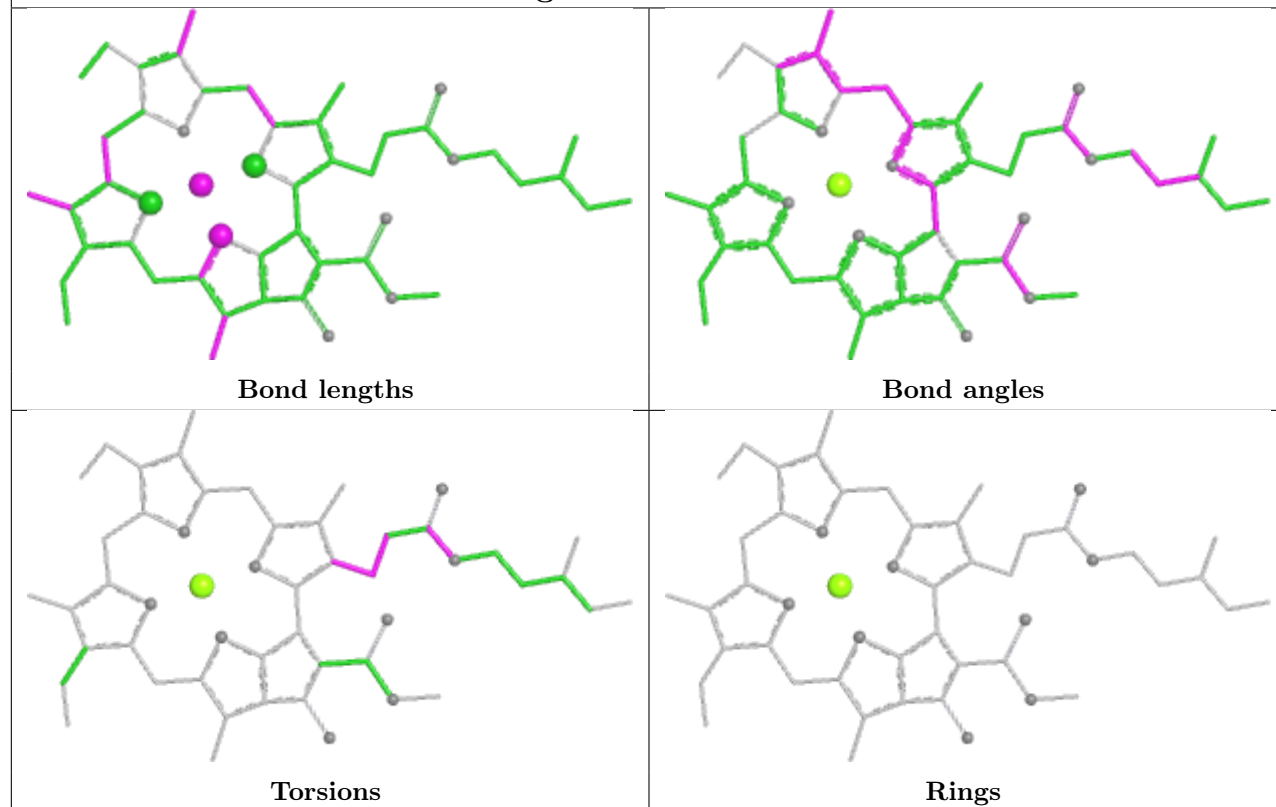
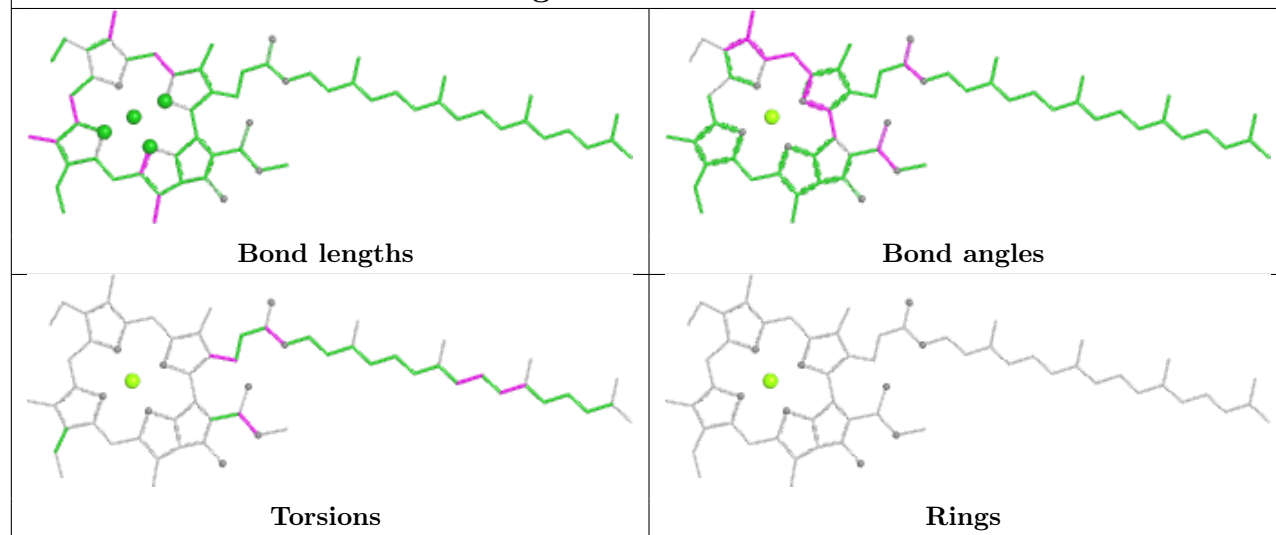


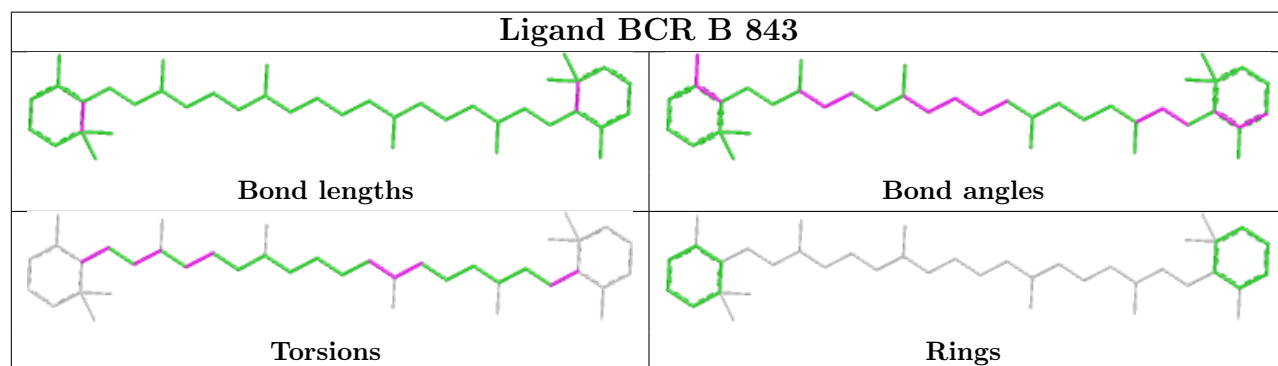
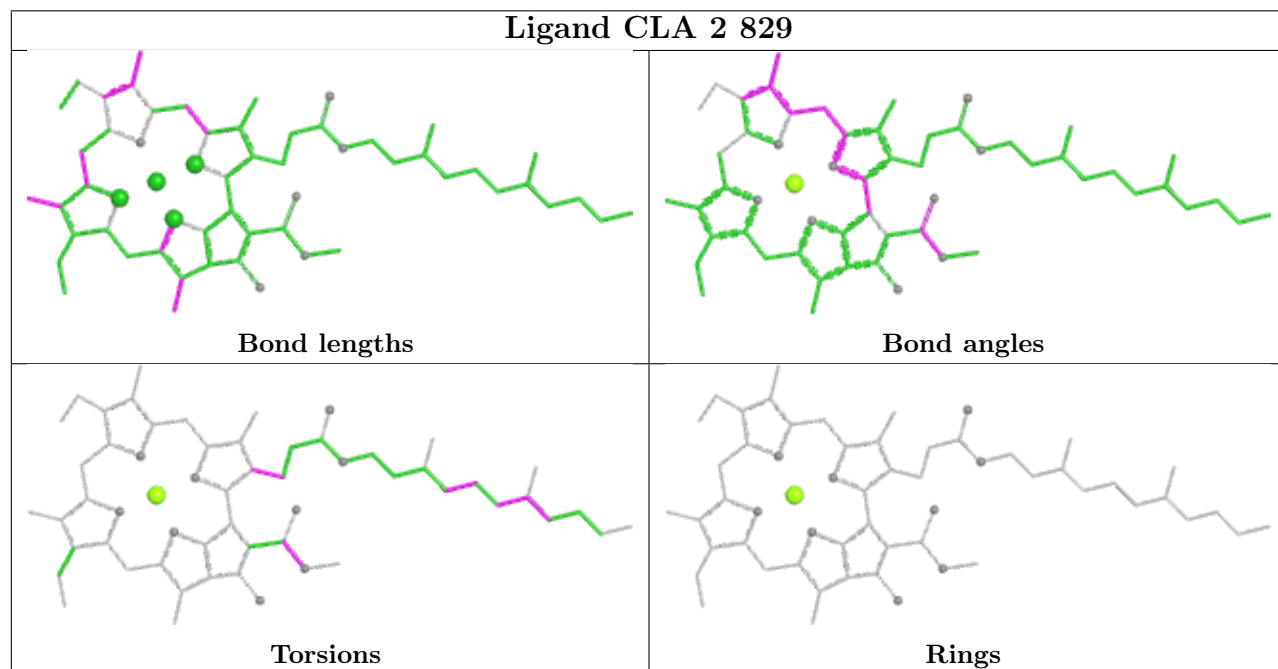
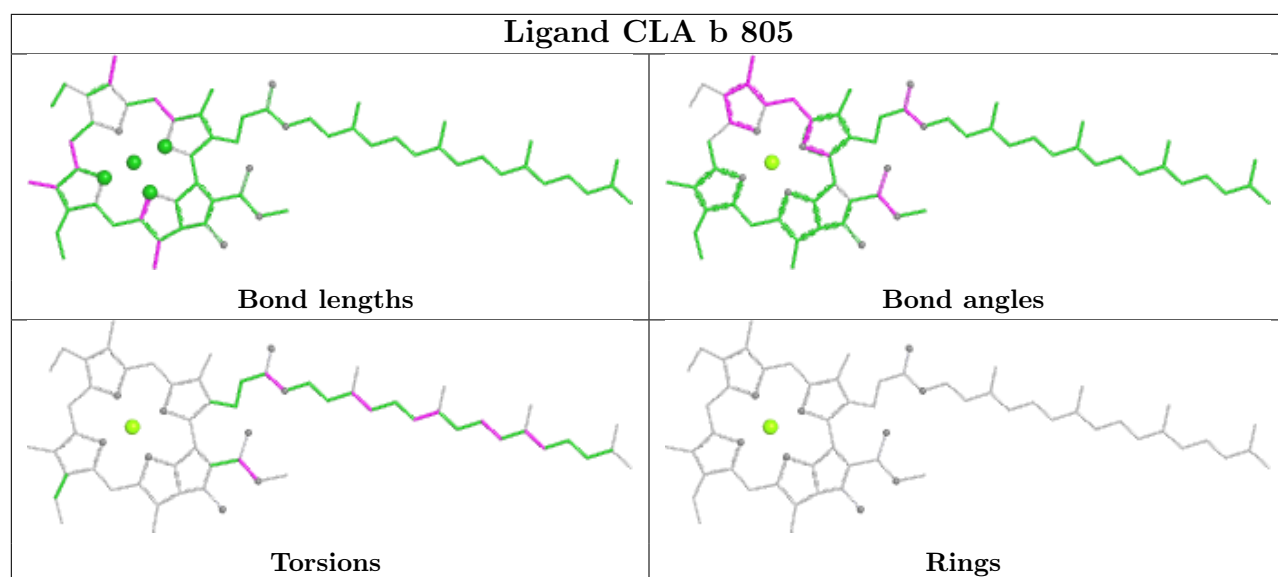
Ligand CLA 2 803**Ligand CLA b 808**

Ligand CLA L 203

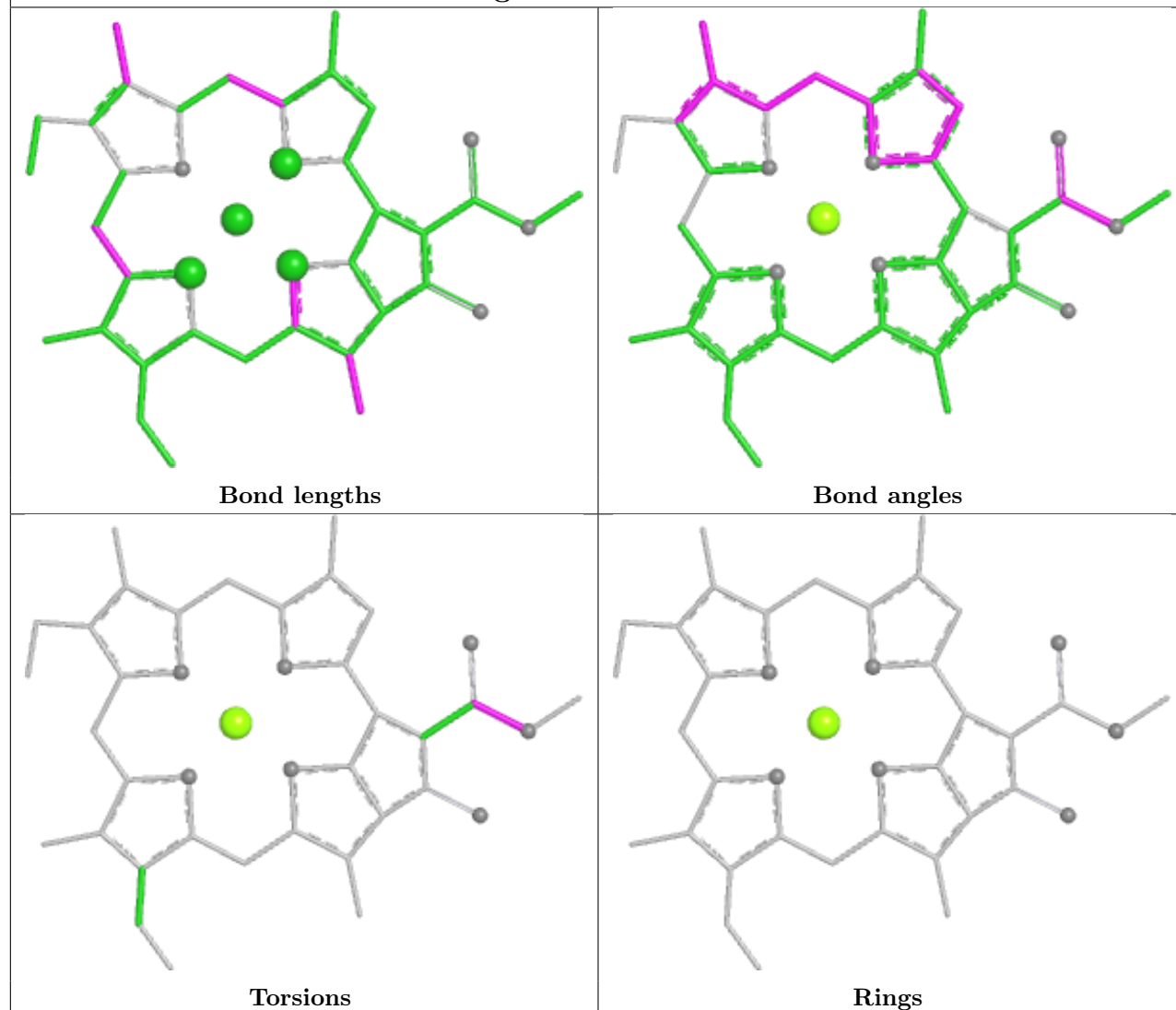




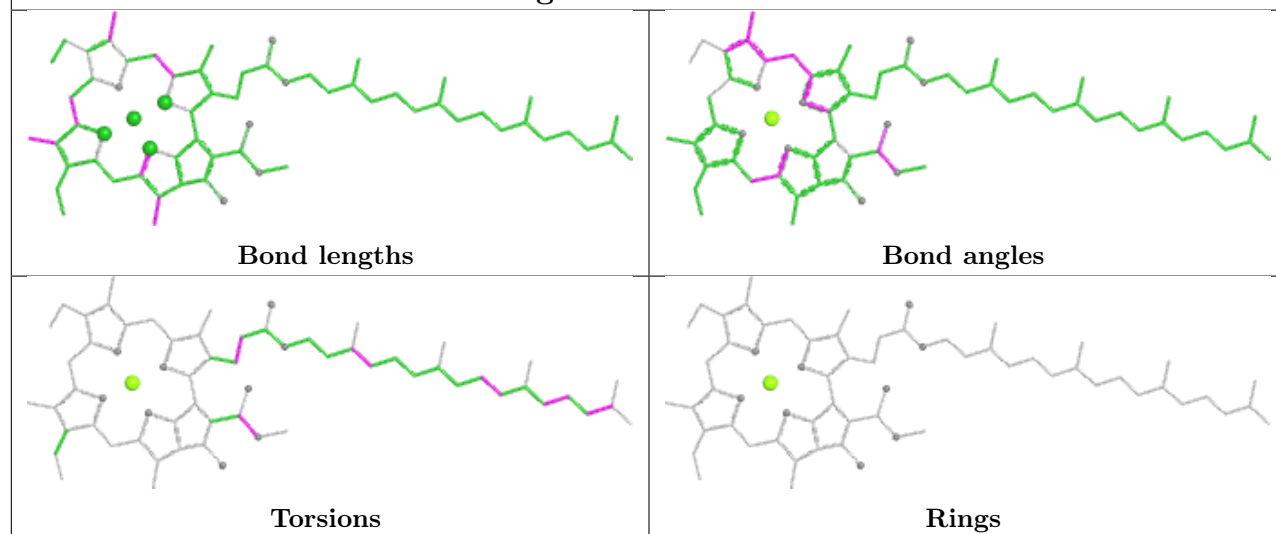
Ligand CLA 1 836**Ligand CLA B 825**

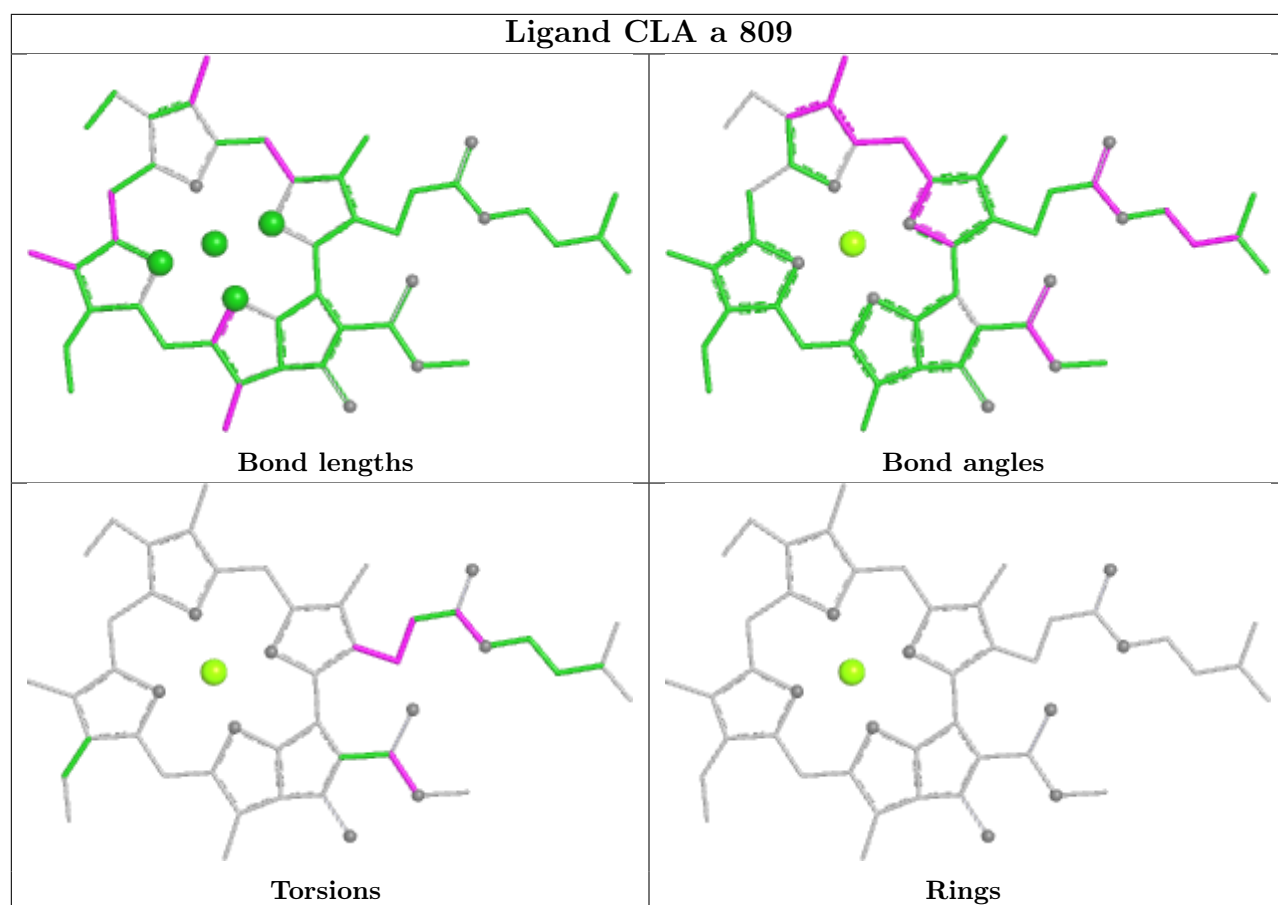


Ligand CLA 2 831

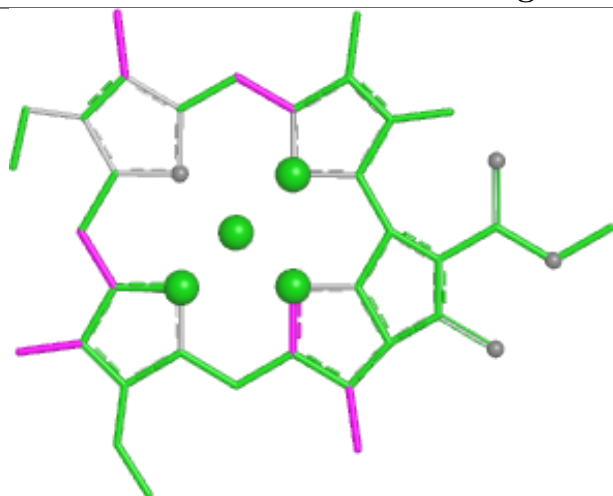


Ligand CLA a 828

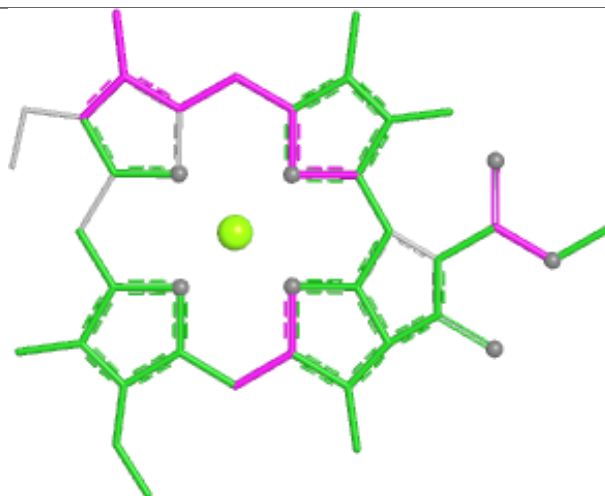




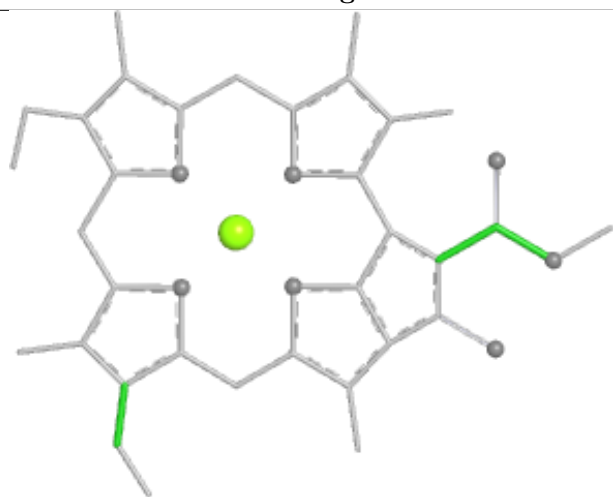
Ligand CLA b 817



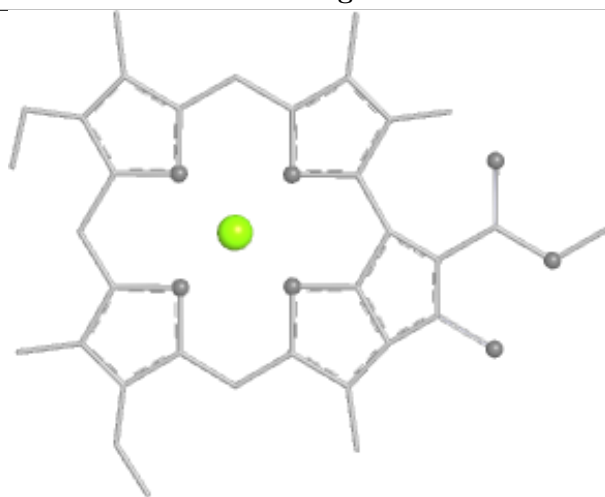
Bond lengths



Bond angles

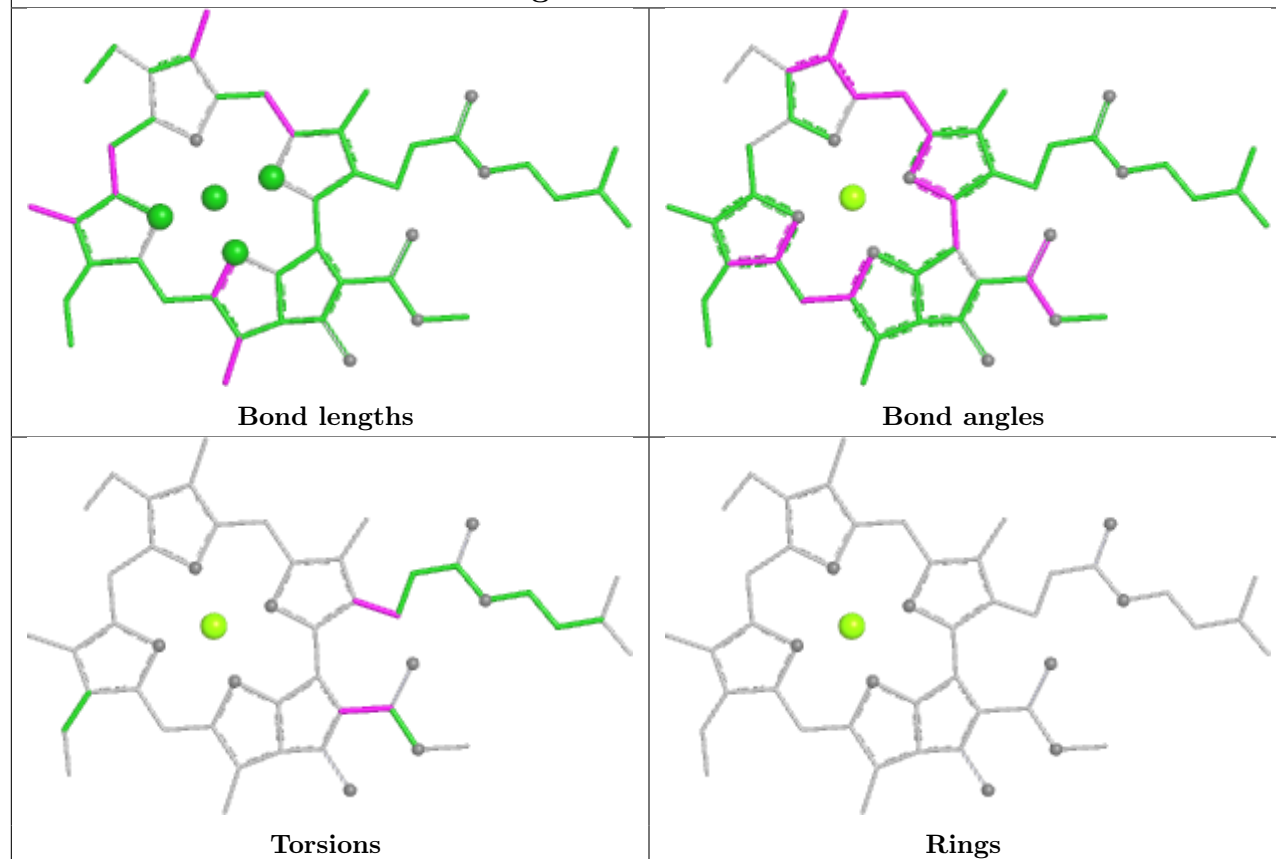


Torsions

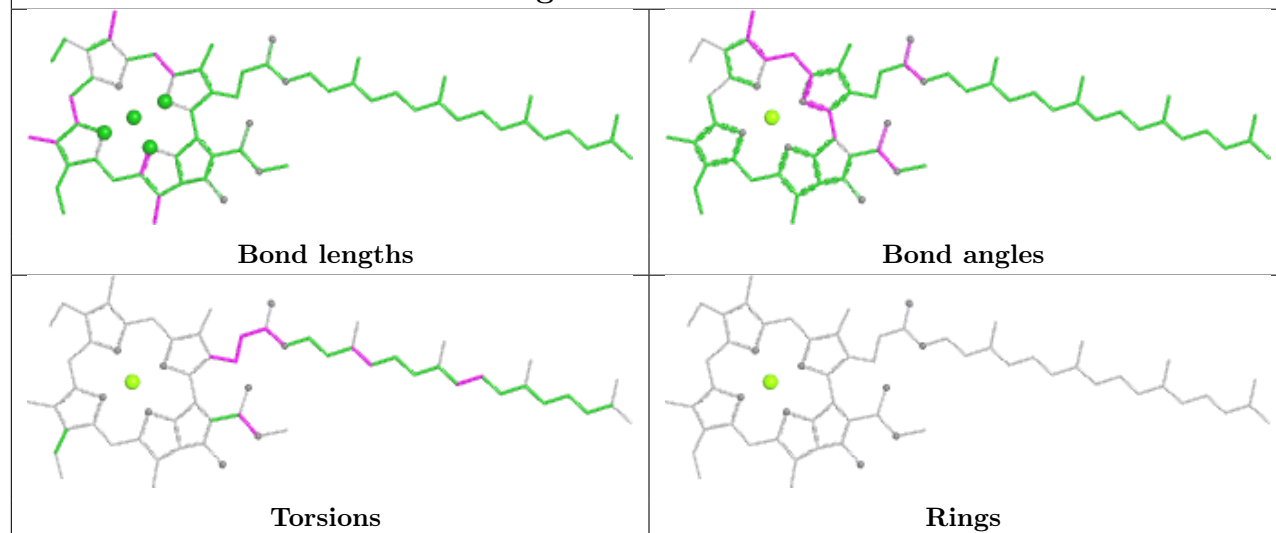


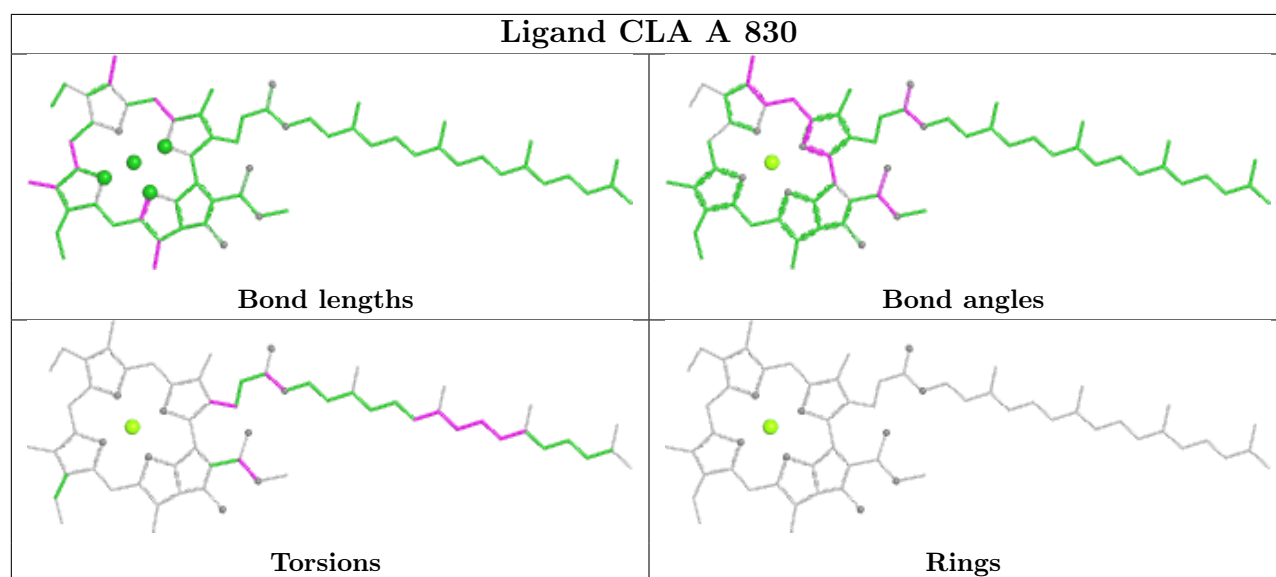
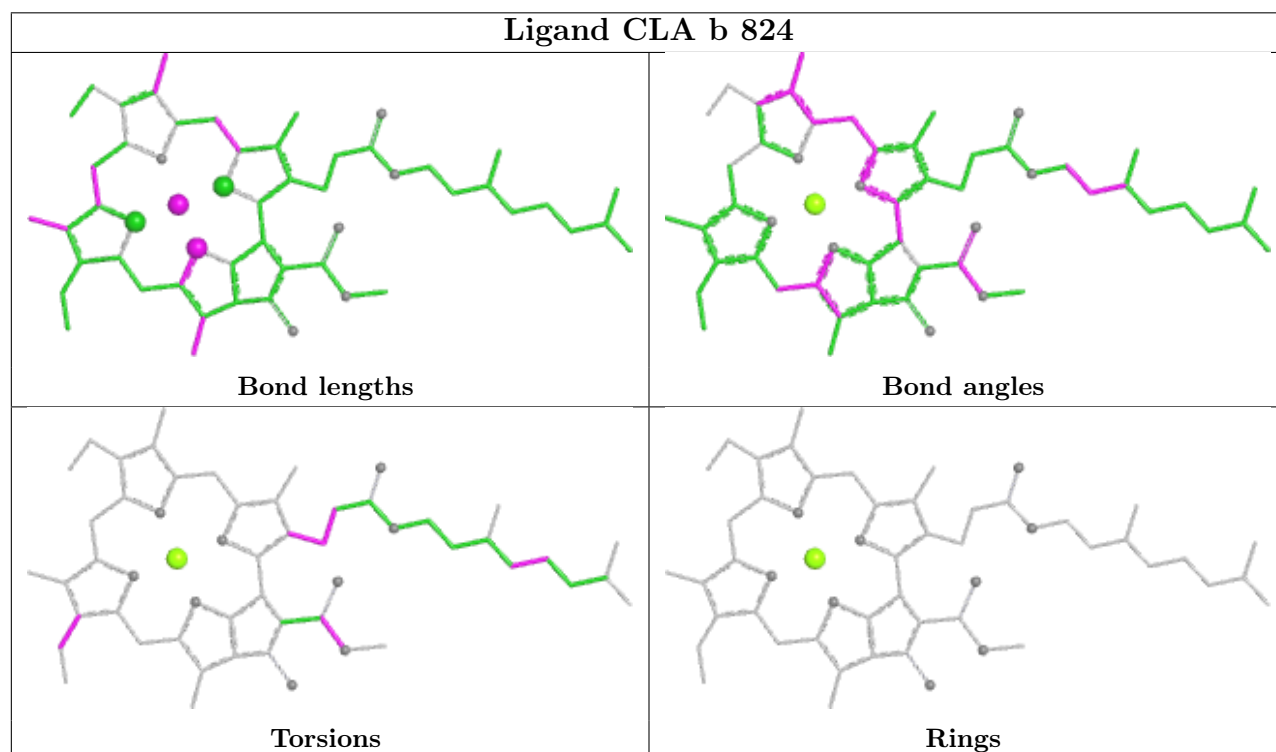
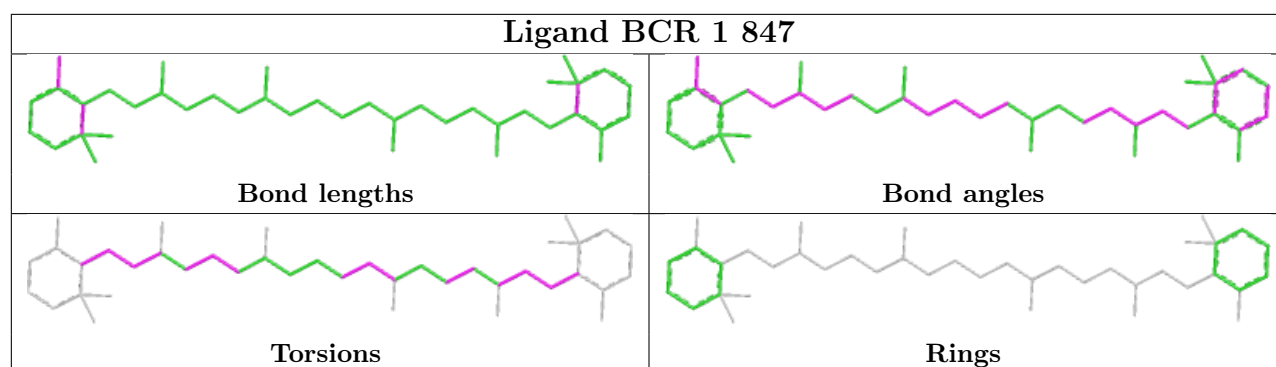
Rings

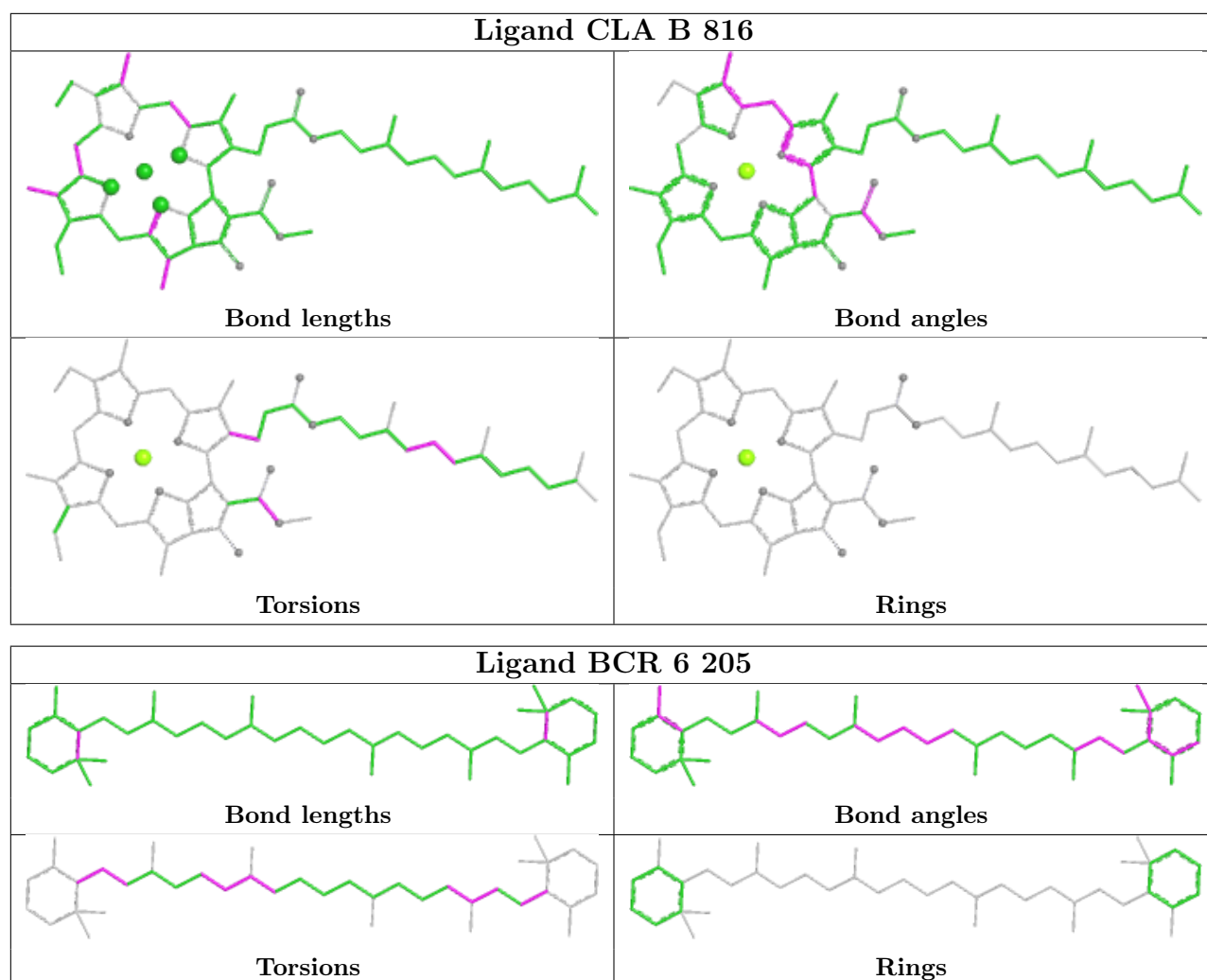
Ligand CLA A 808



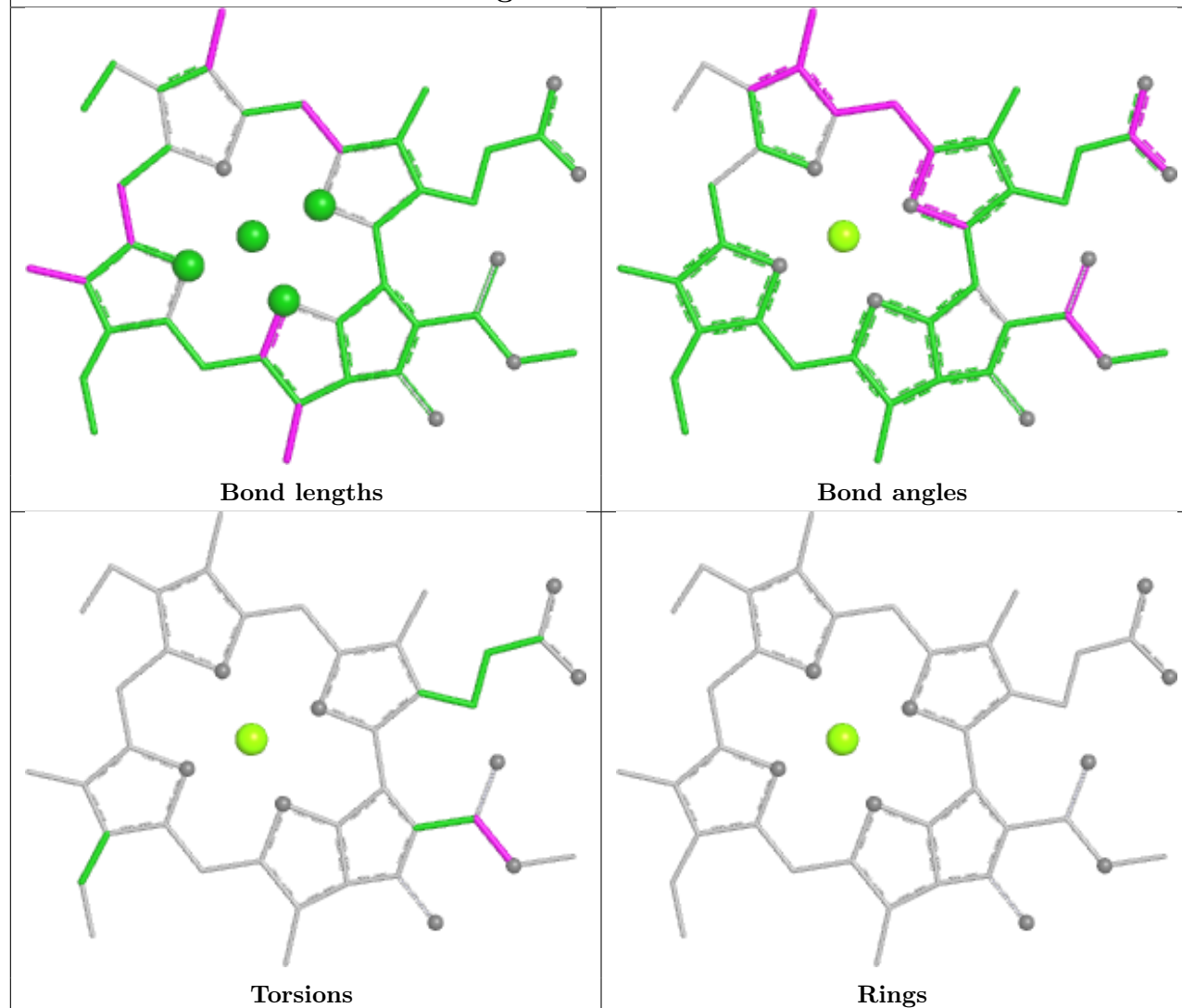
Ligand CLA 1 821



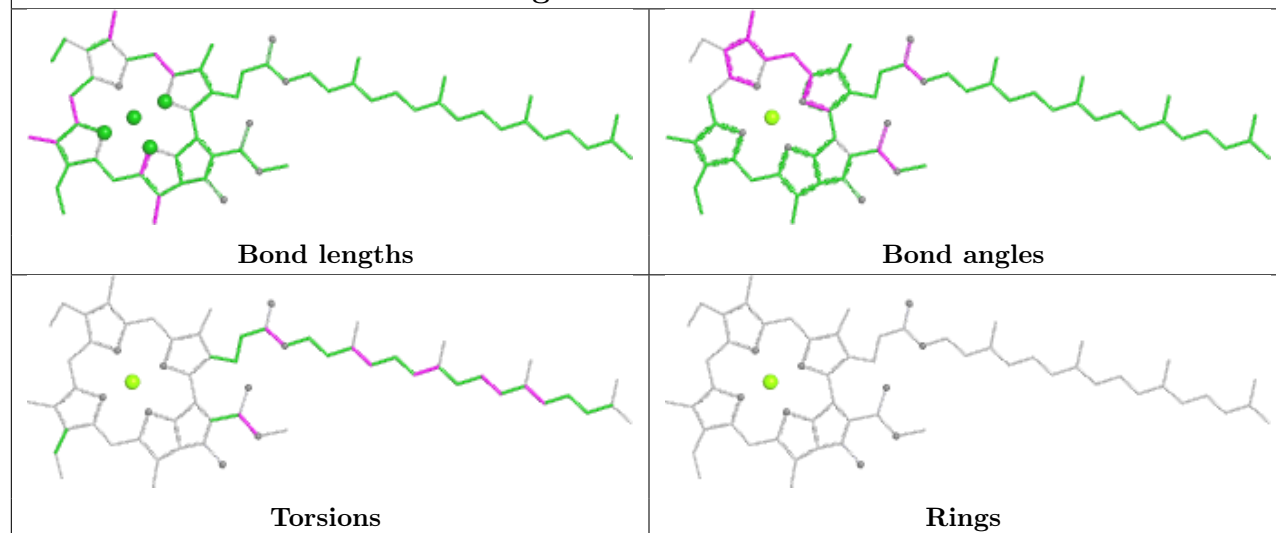


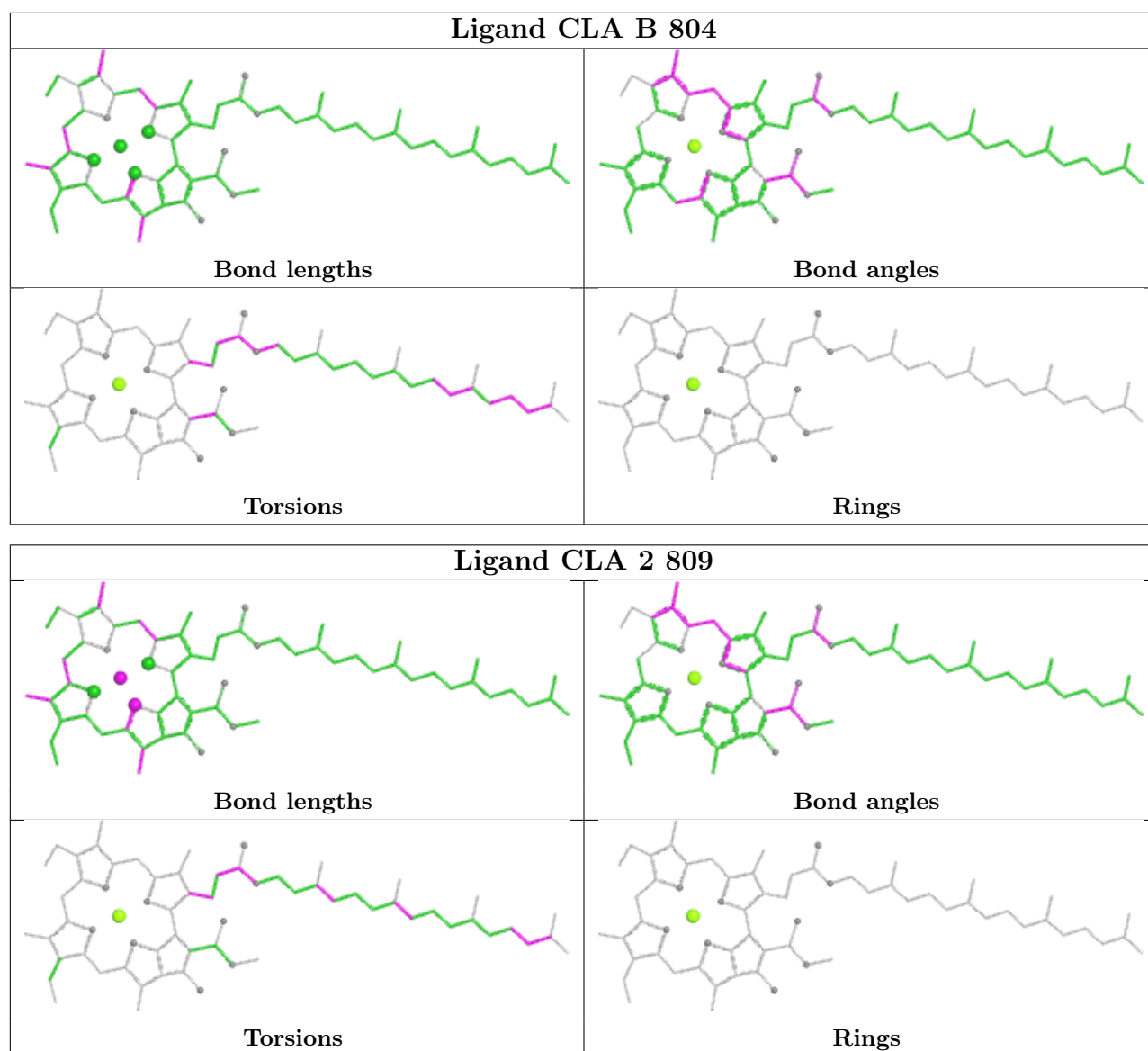


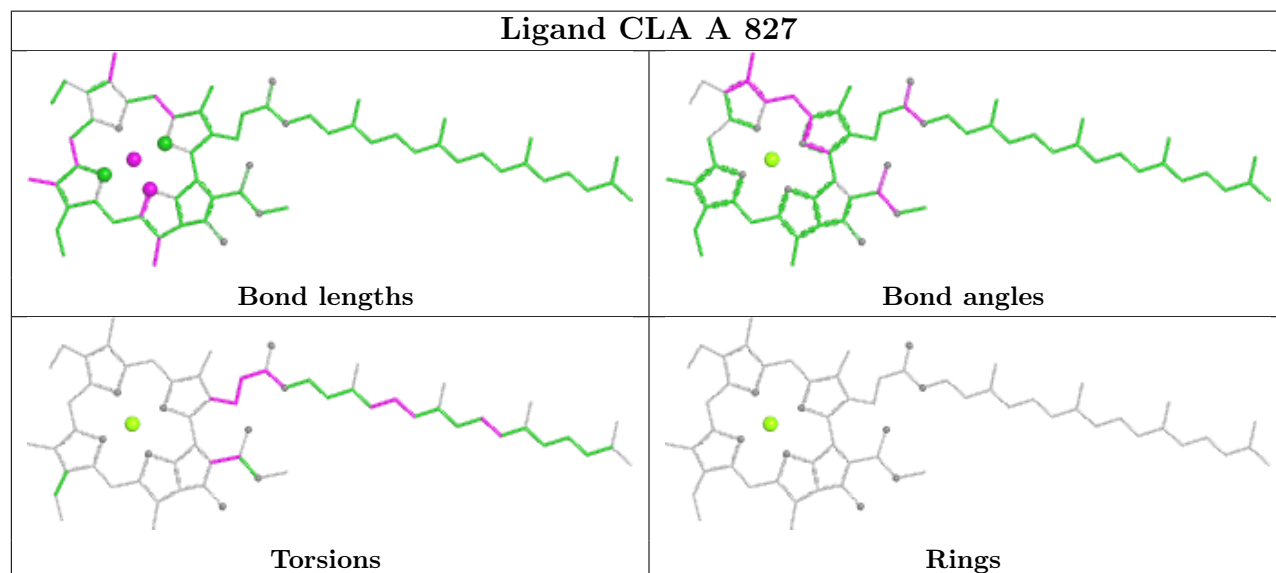
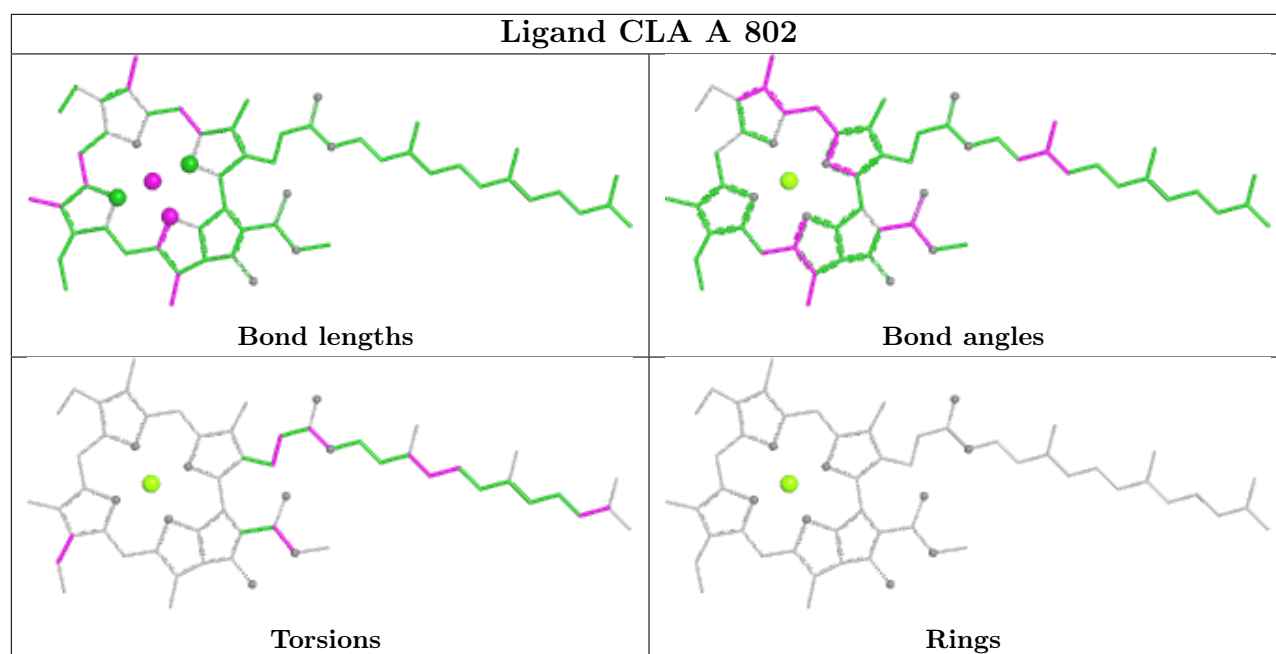
Ligand CLA 2 811

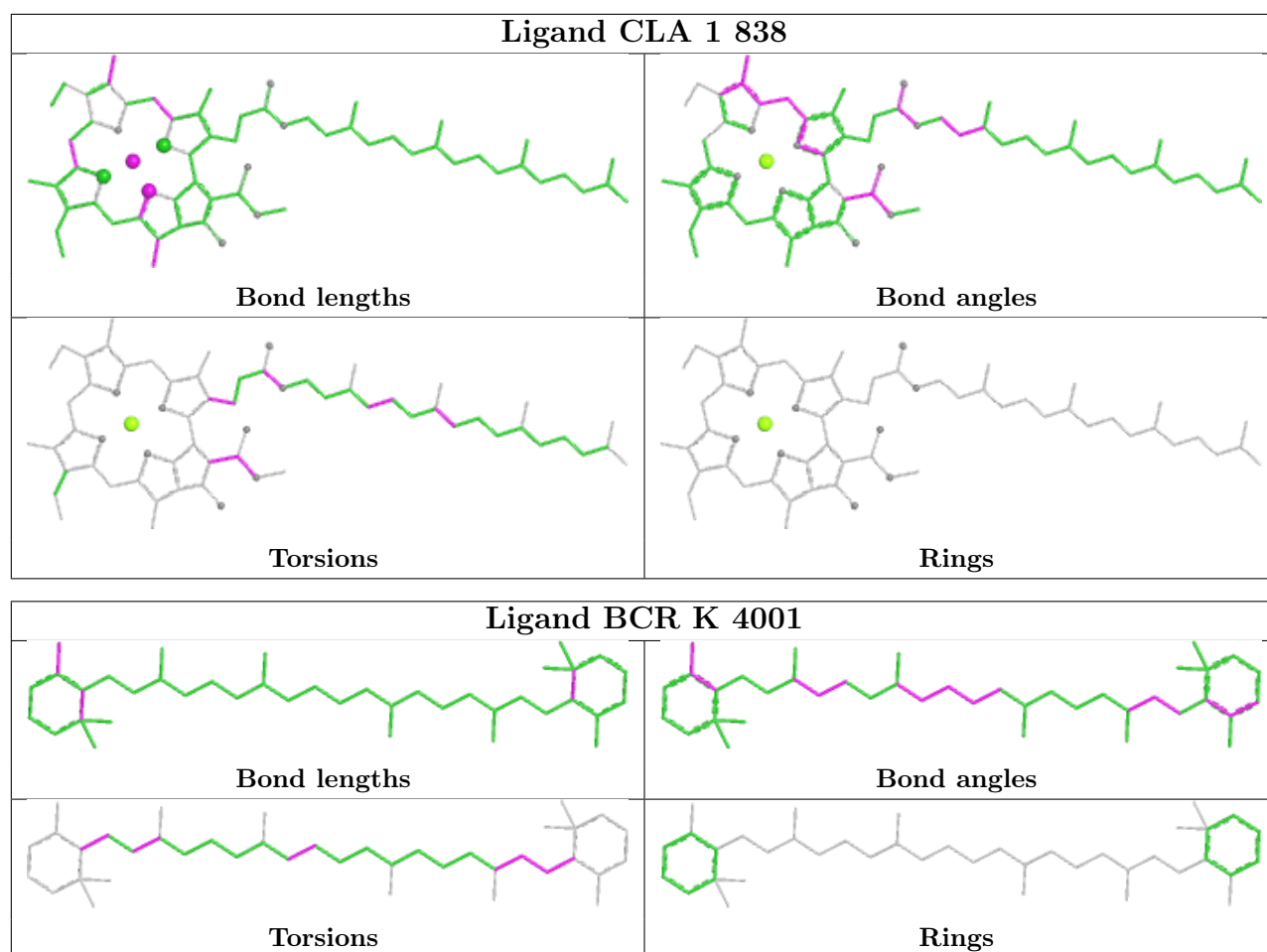


Ligand CLA B 805

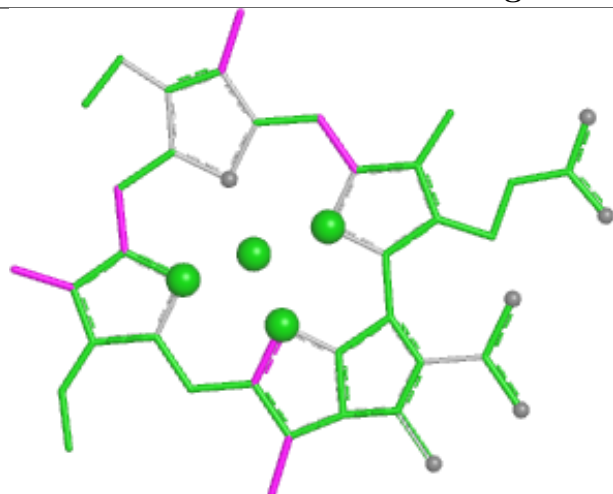




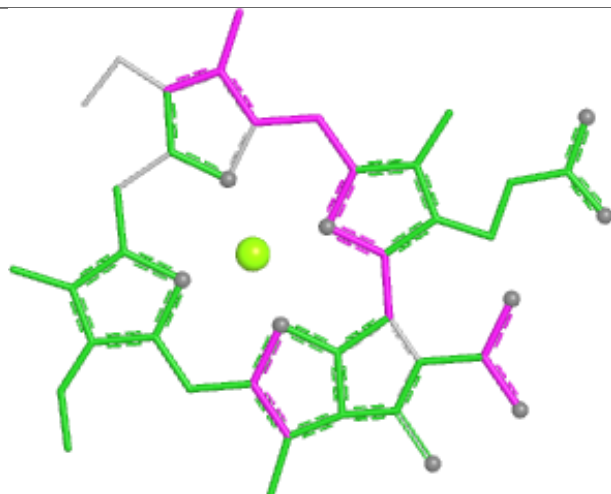




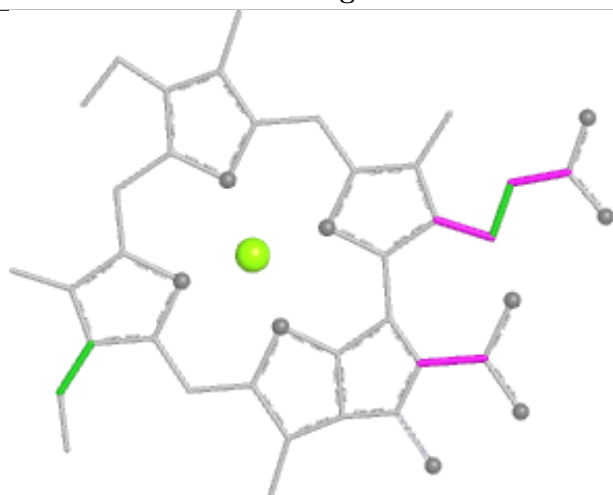
Ligand CLA K 4005



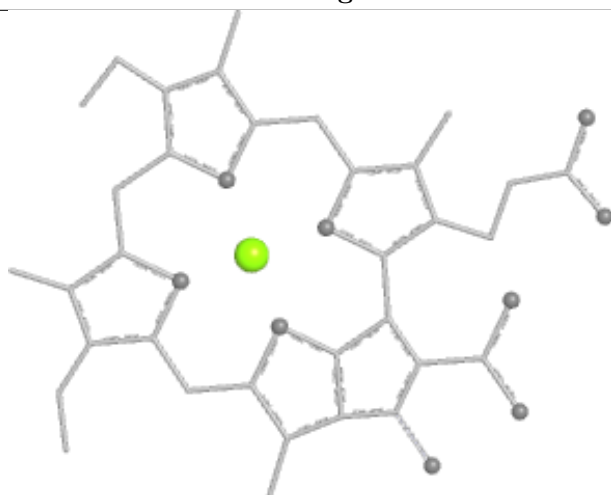
Bond lengths



Bond angles

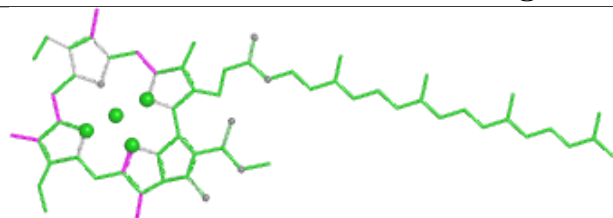


Torsions

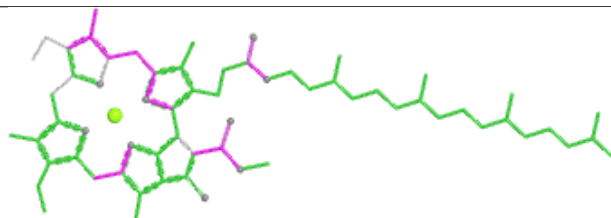


Rings

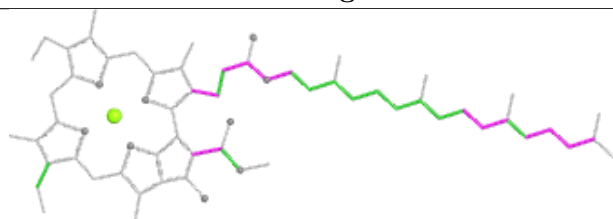
Ligand CLA 2 804



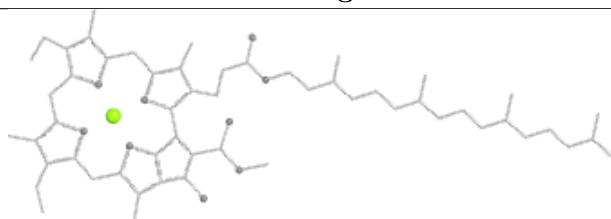
Bond lengths



Bond angles

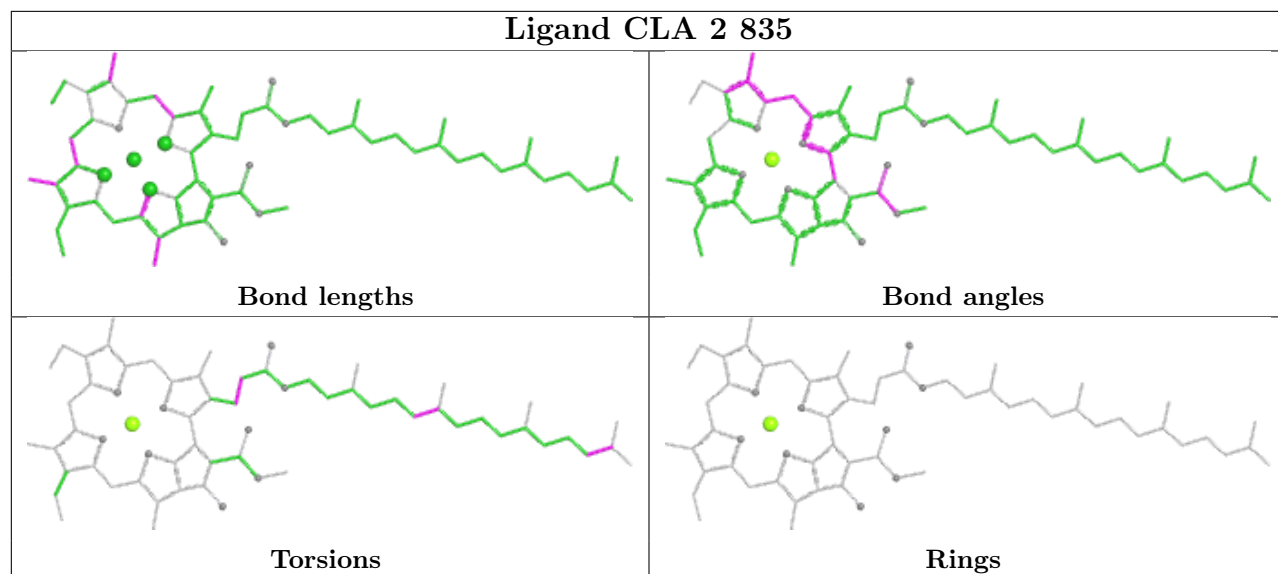


Torsions

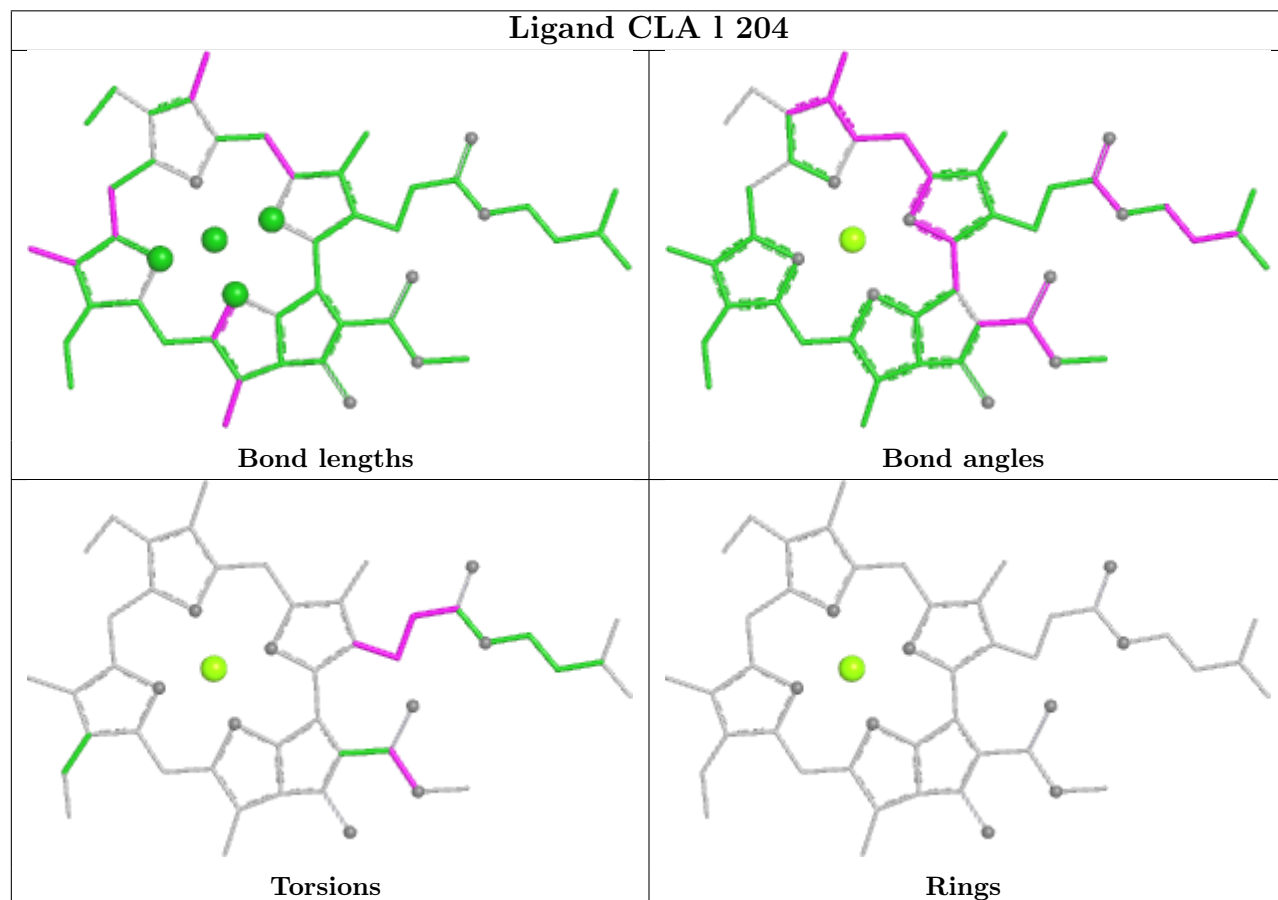


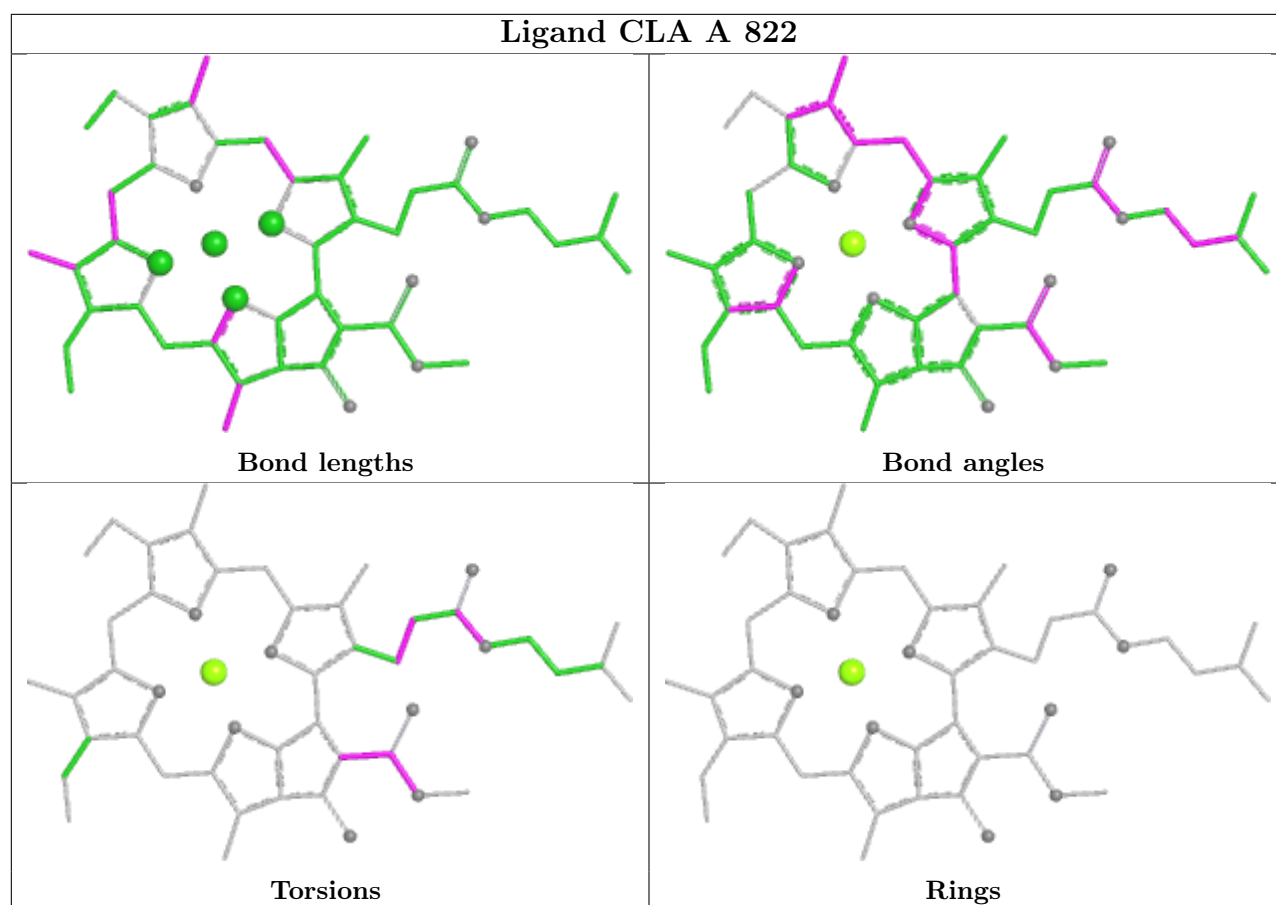
Rings

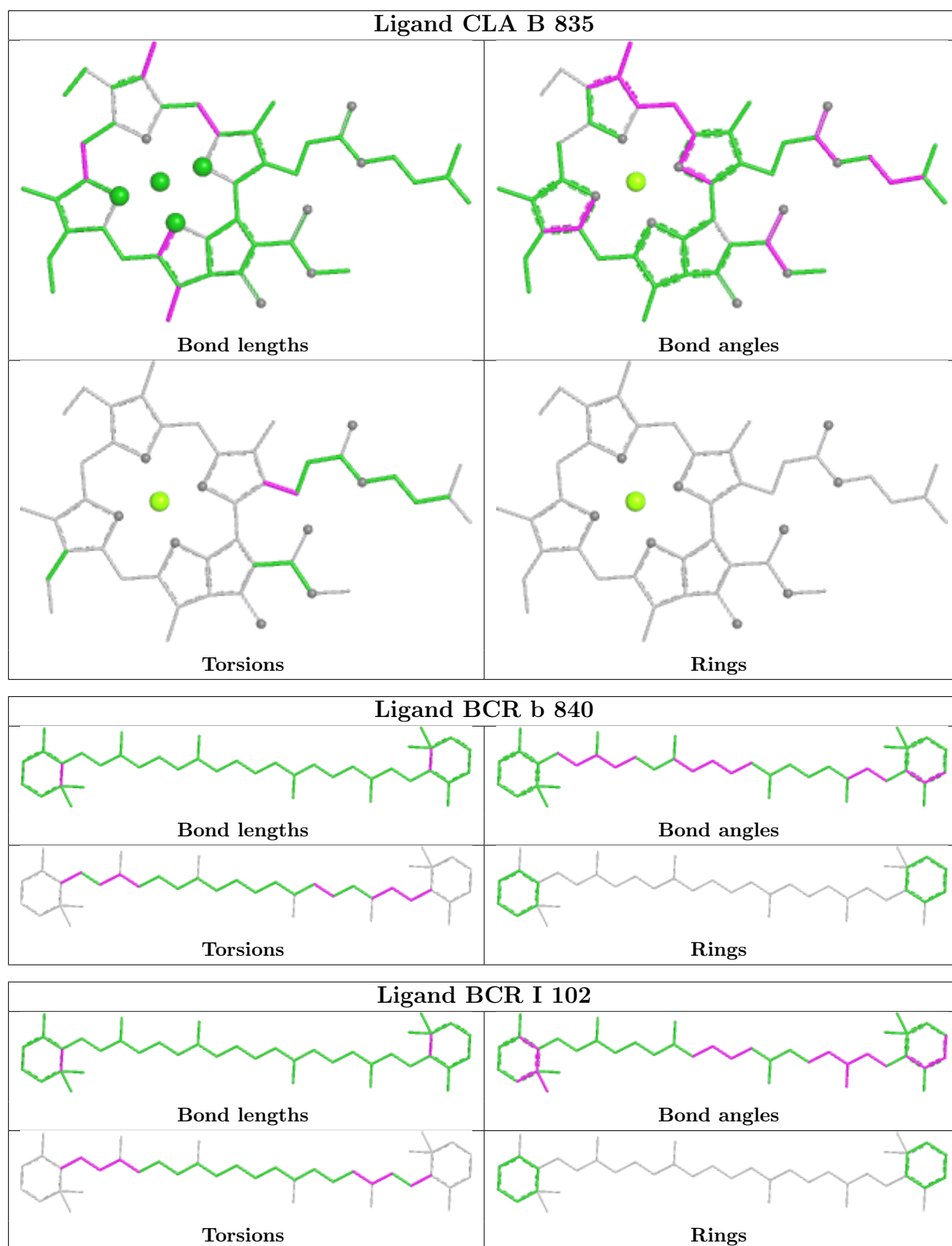
Ligand CLA 2 835



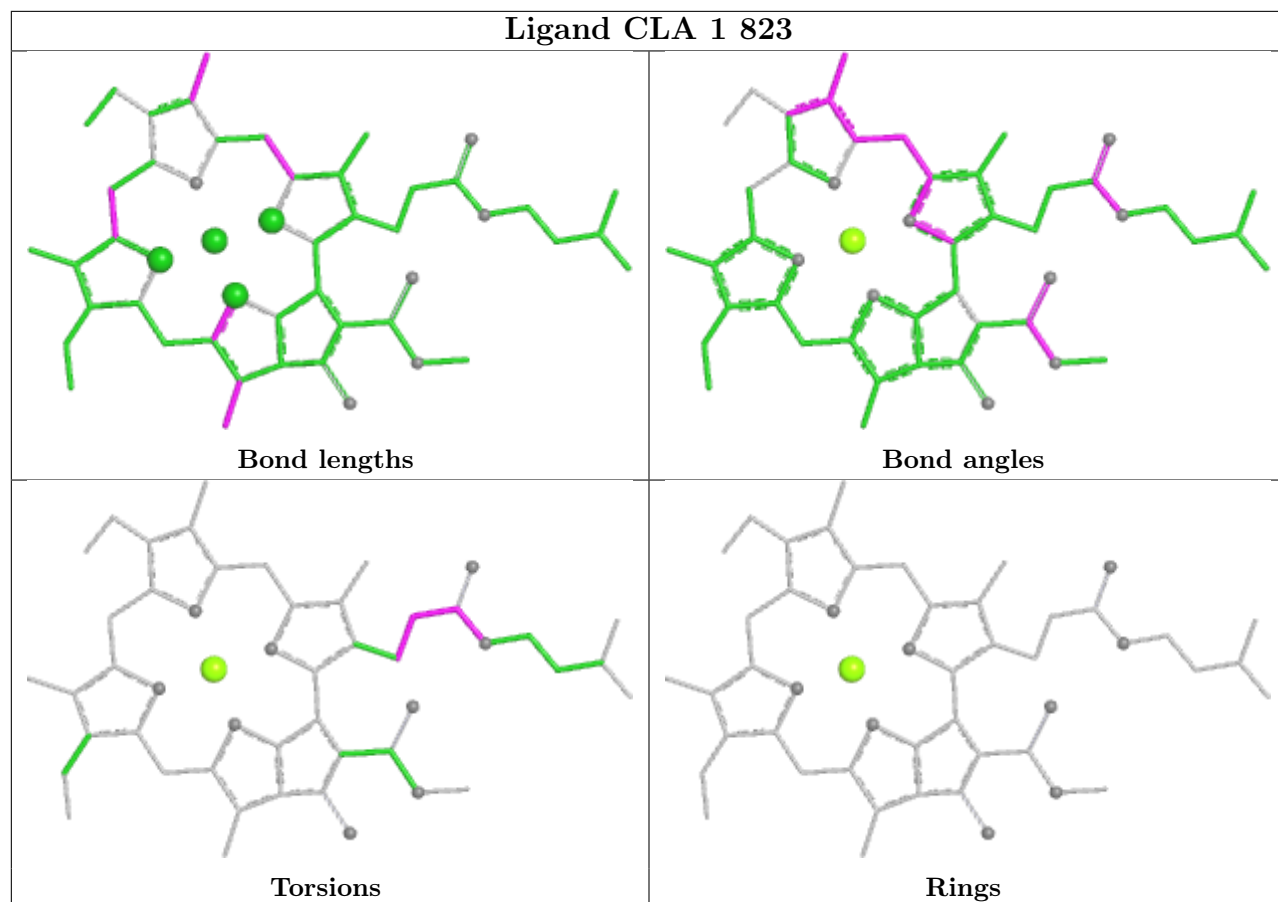
Ligand CLA 1 204



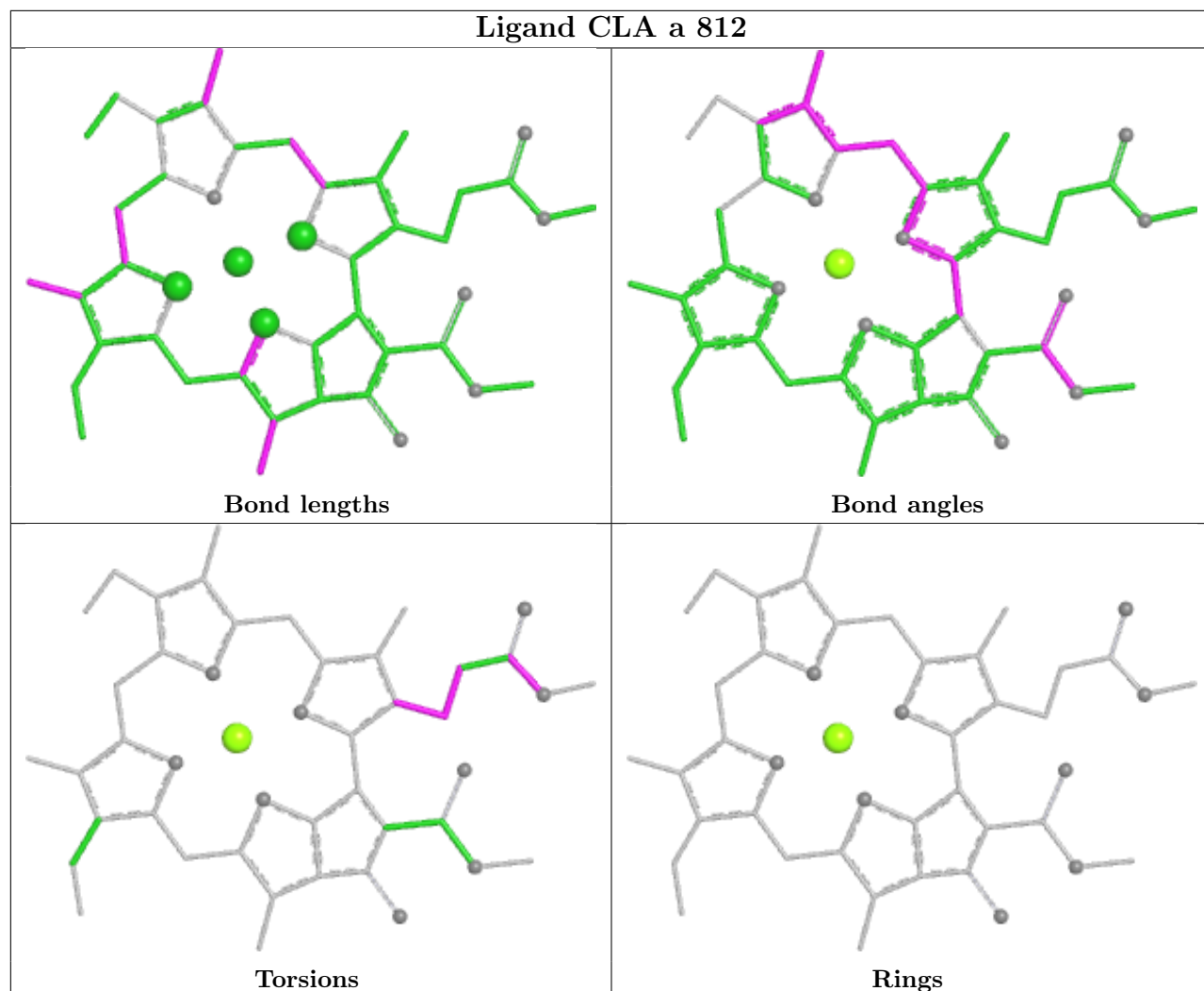




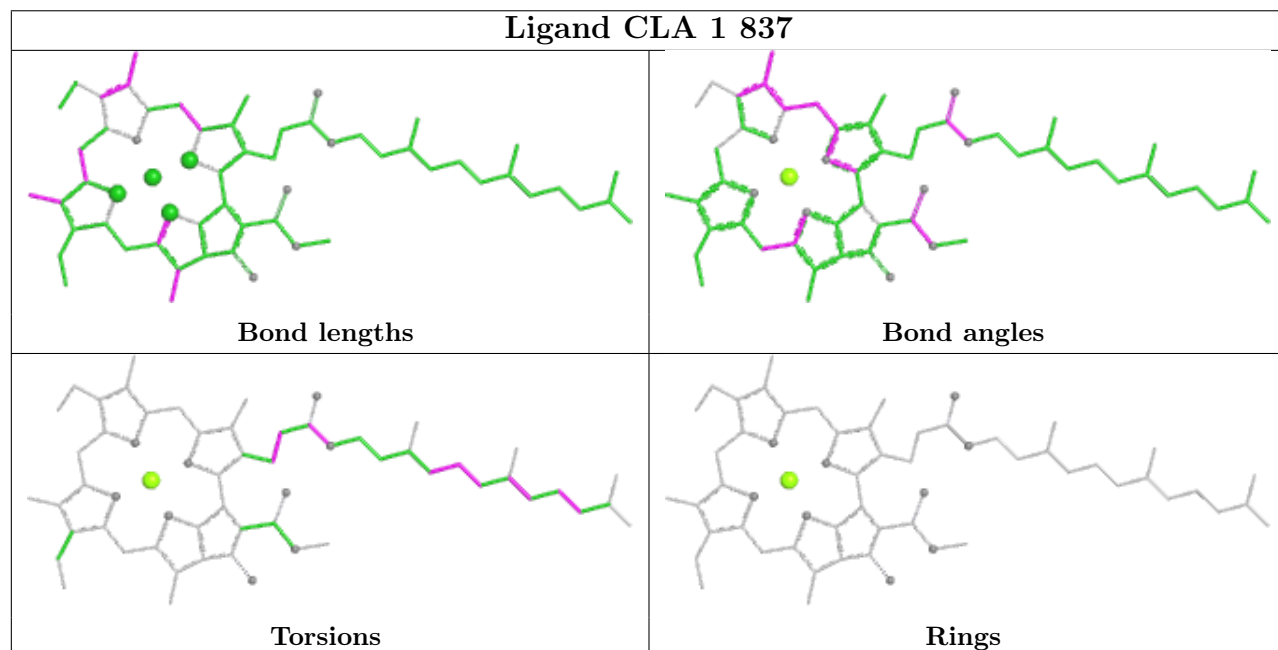
Ligand CLA 1 823

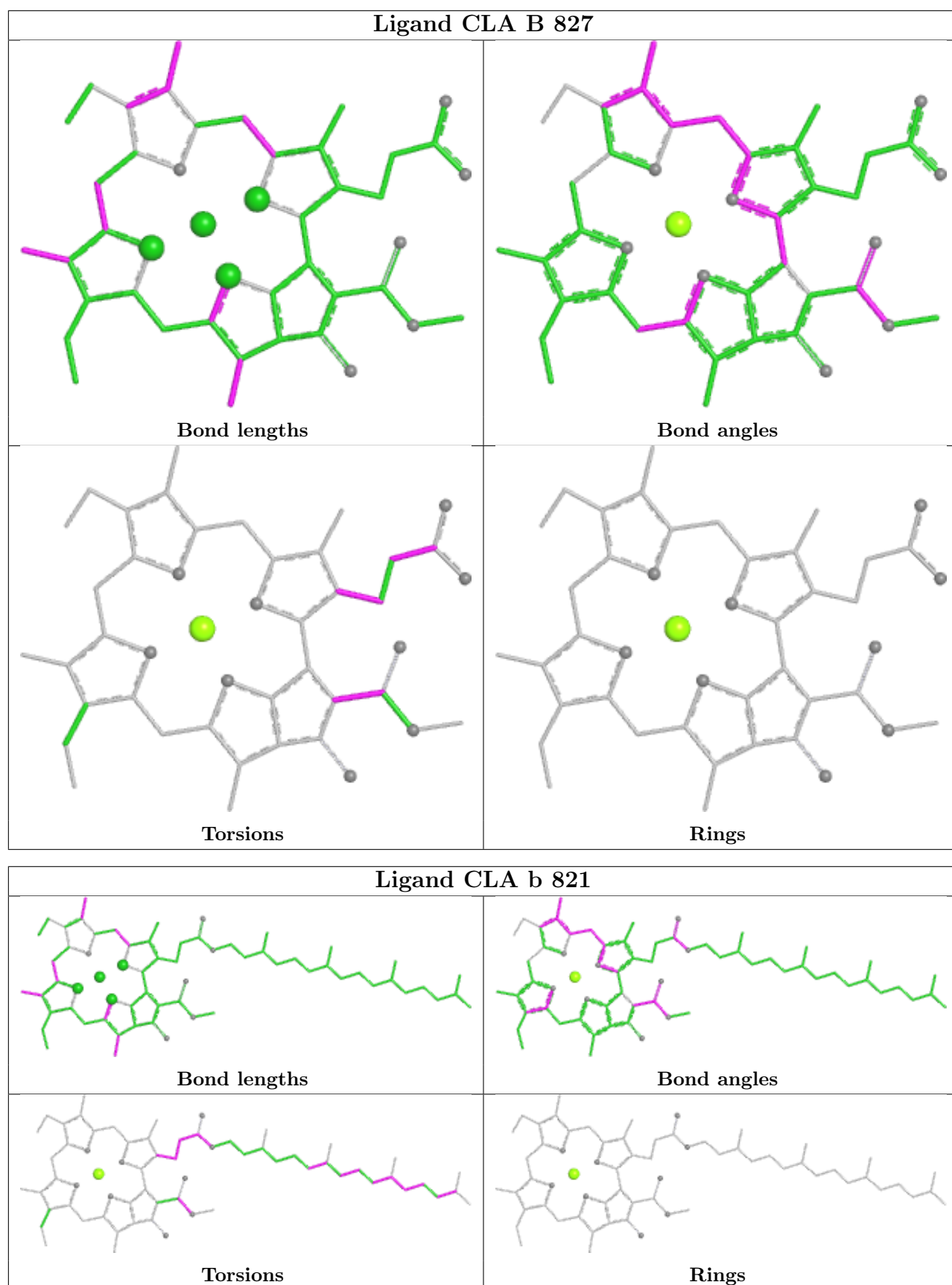


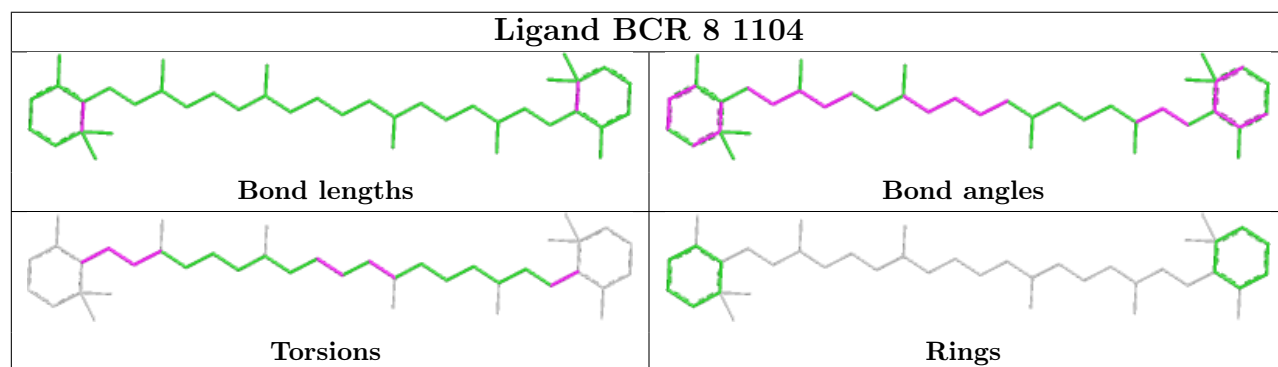
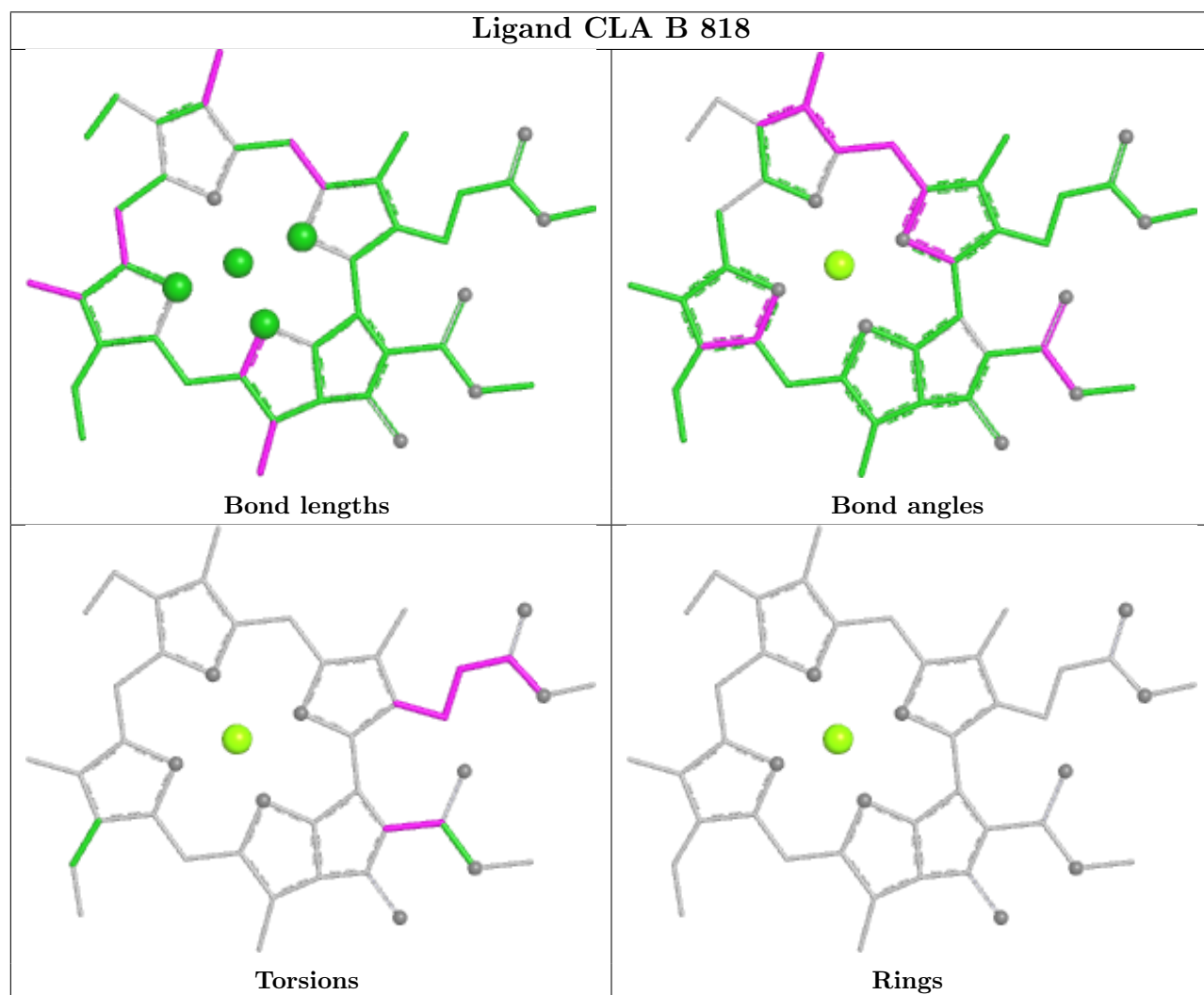
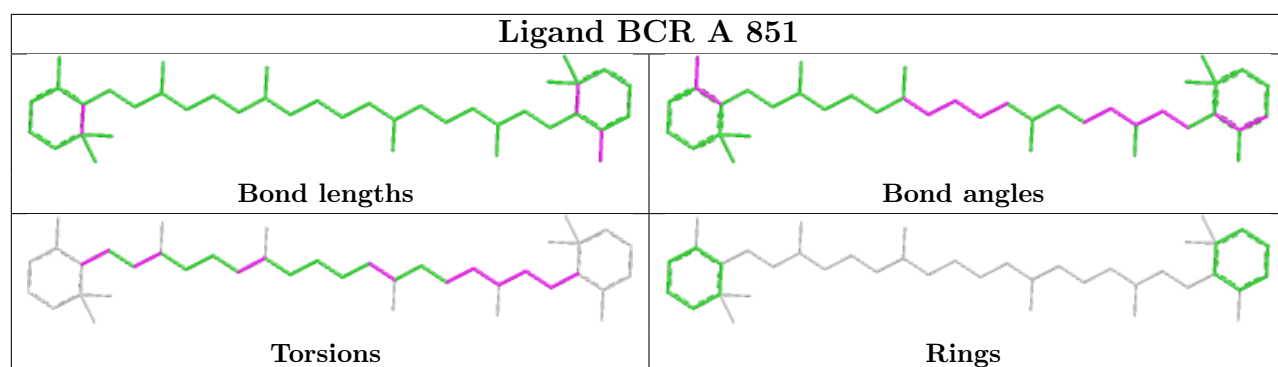
Ligand CLA a 812

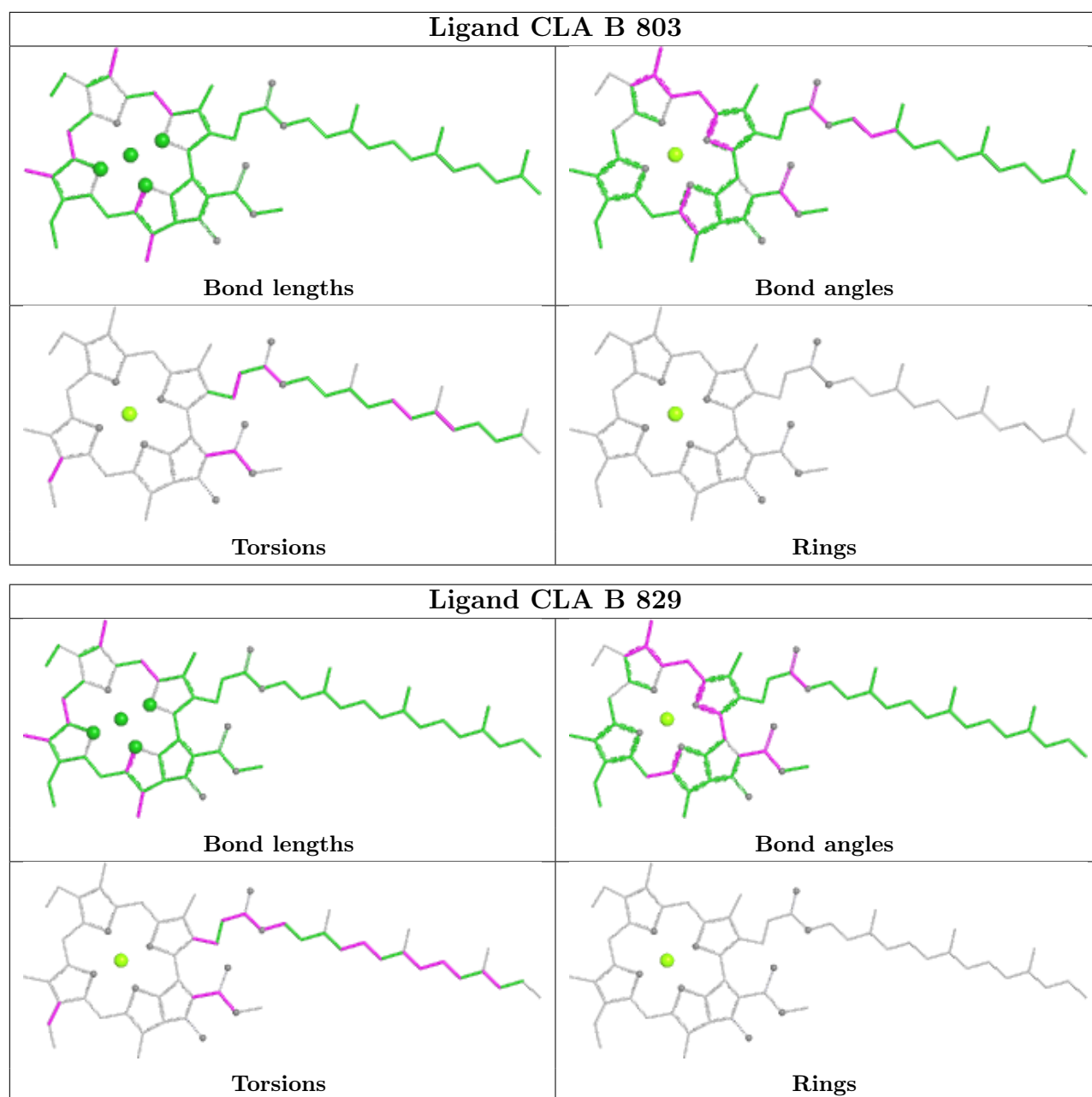


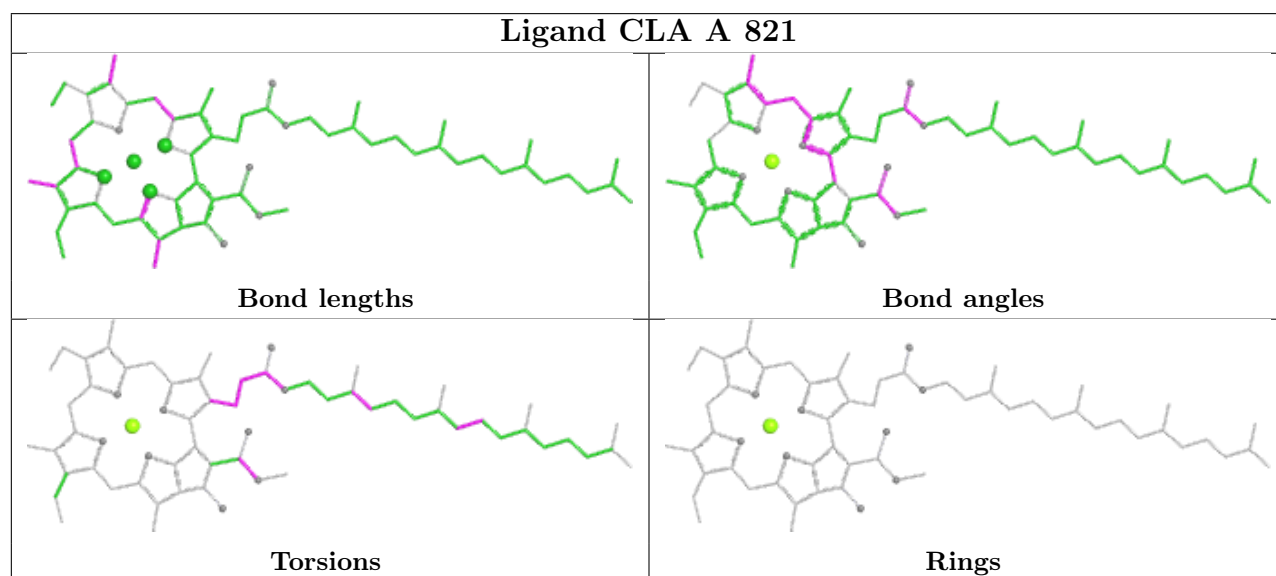
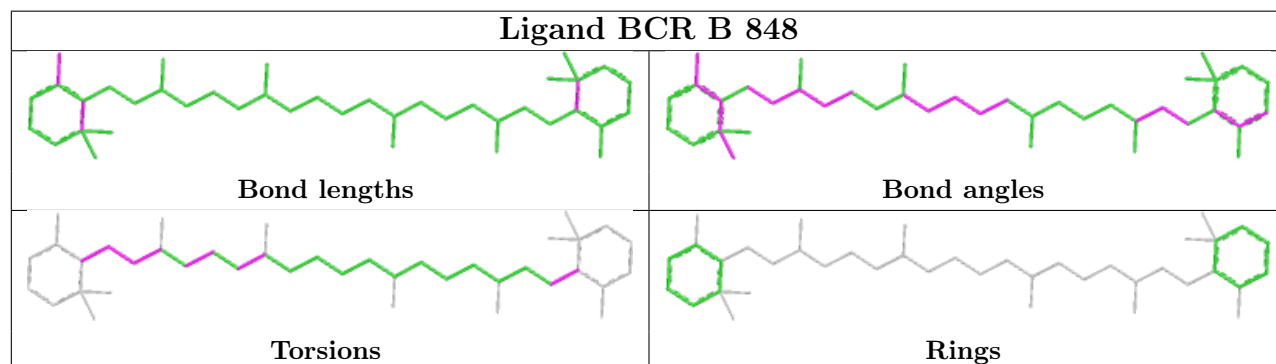
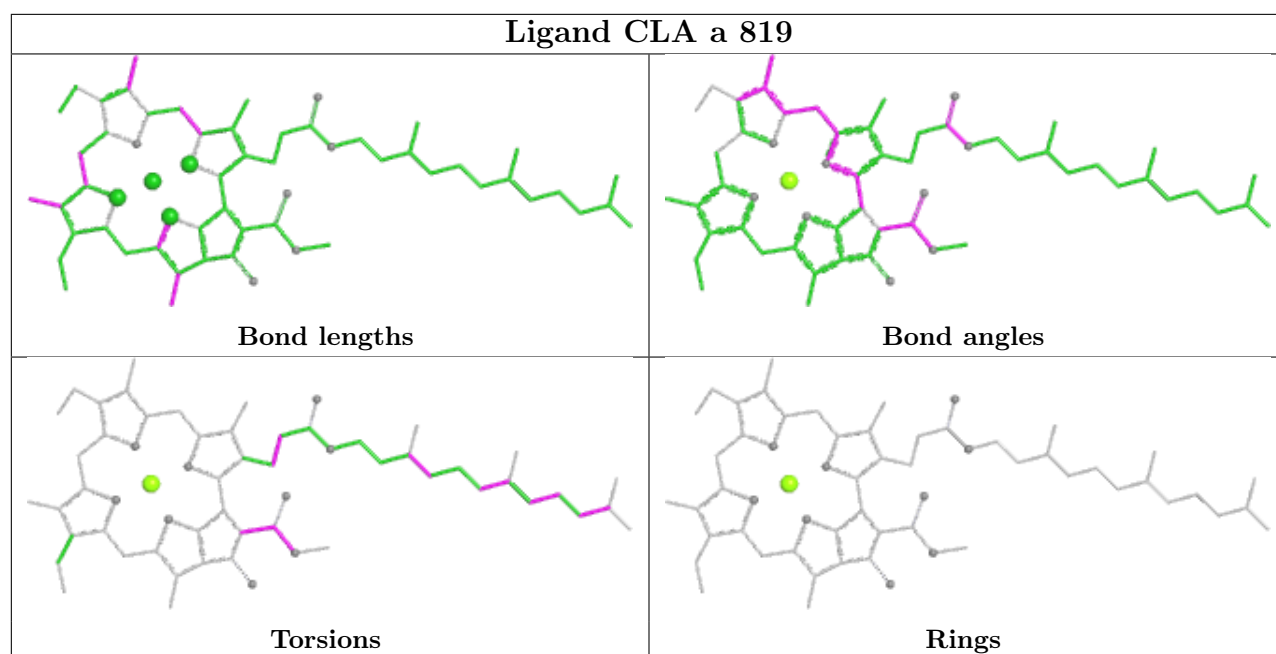
Ligand CLA 1 837

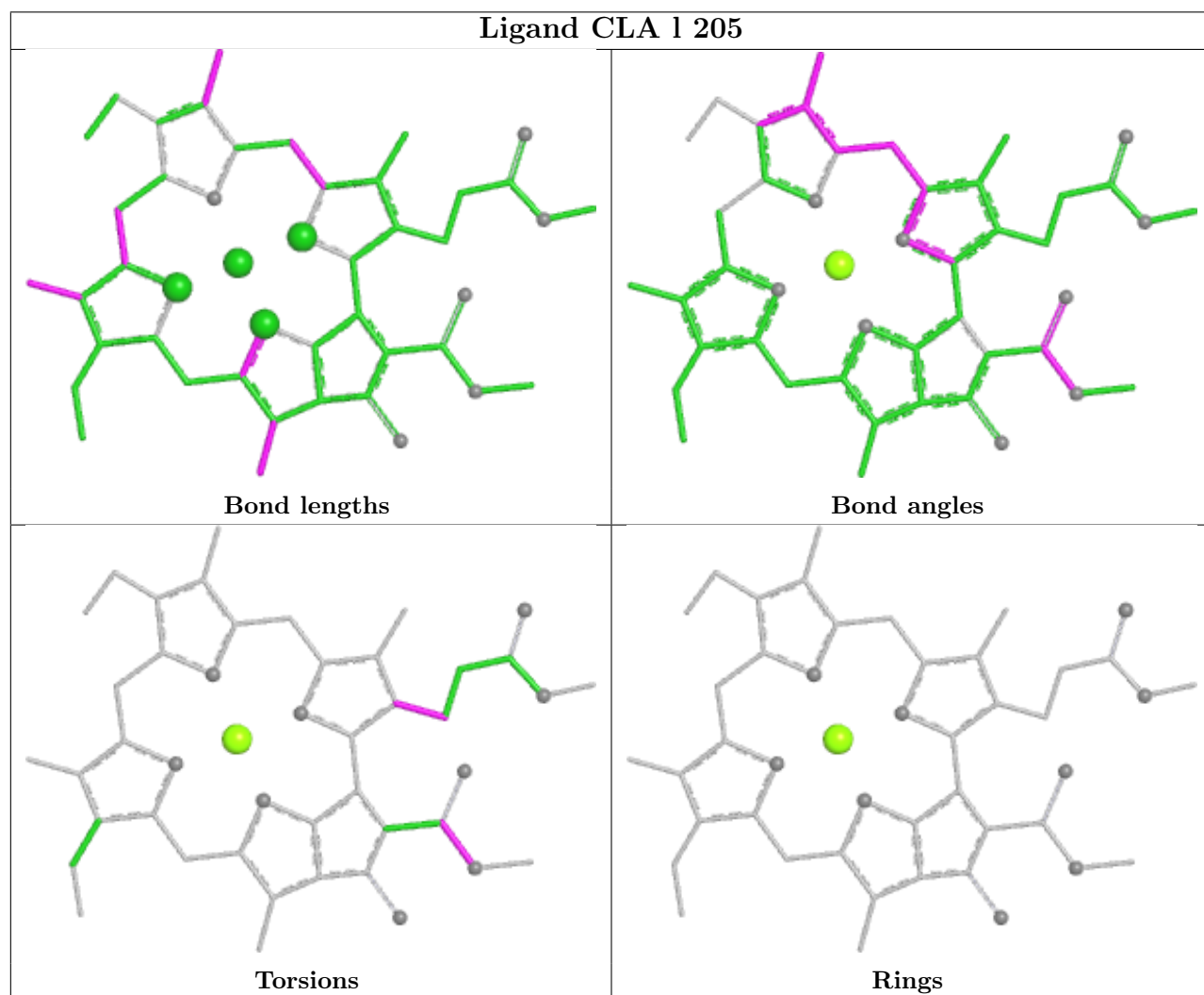
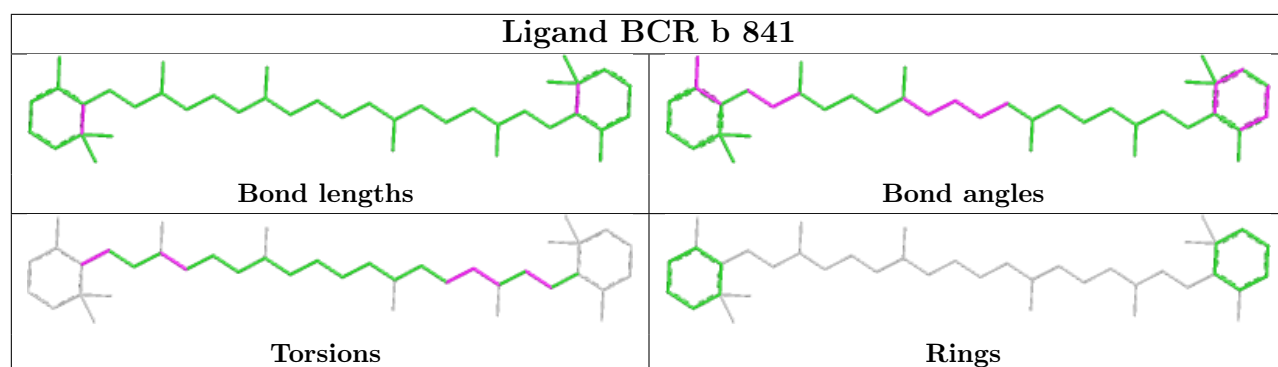


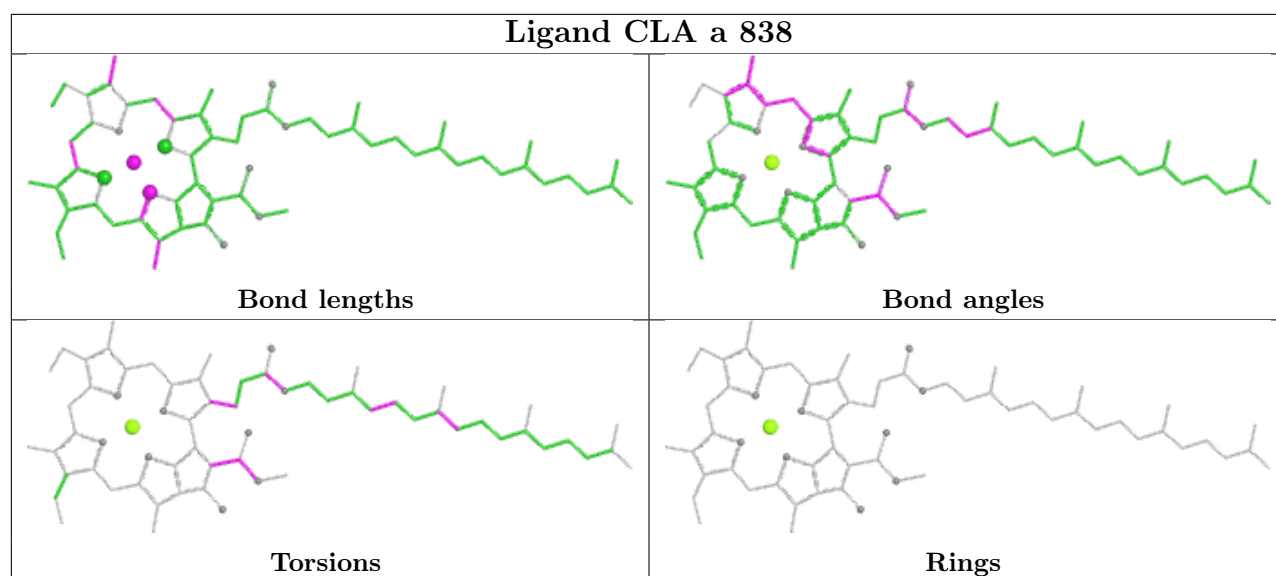
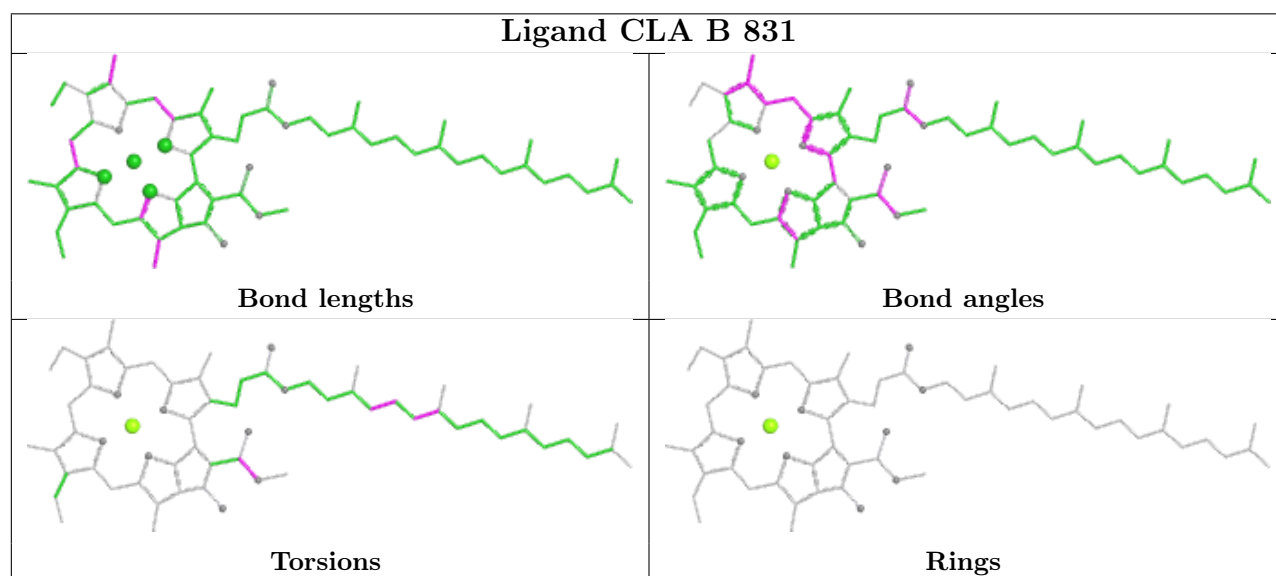
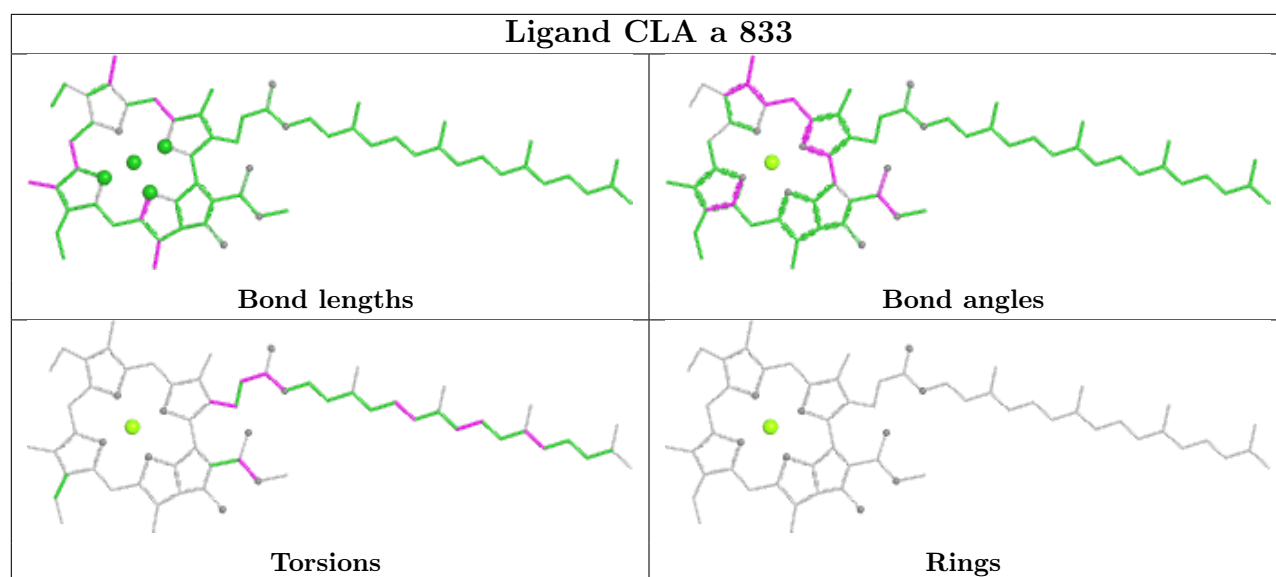


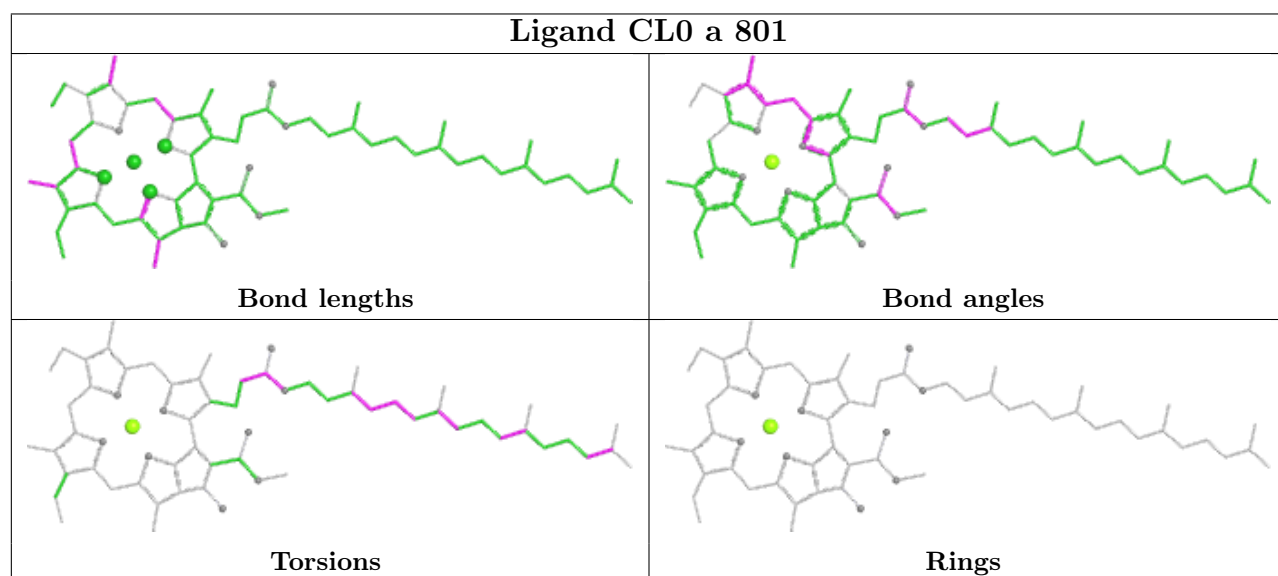
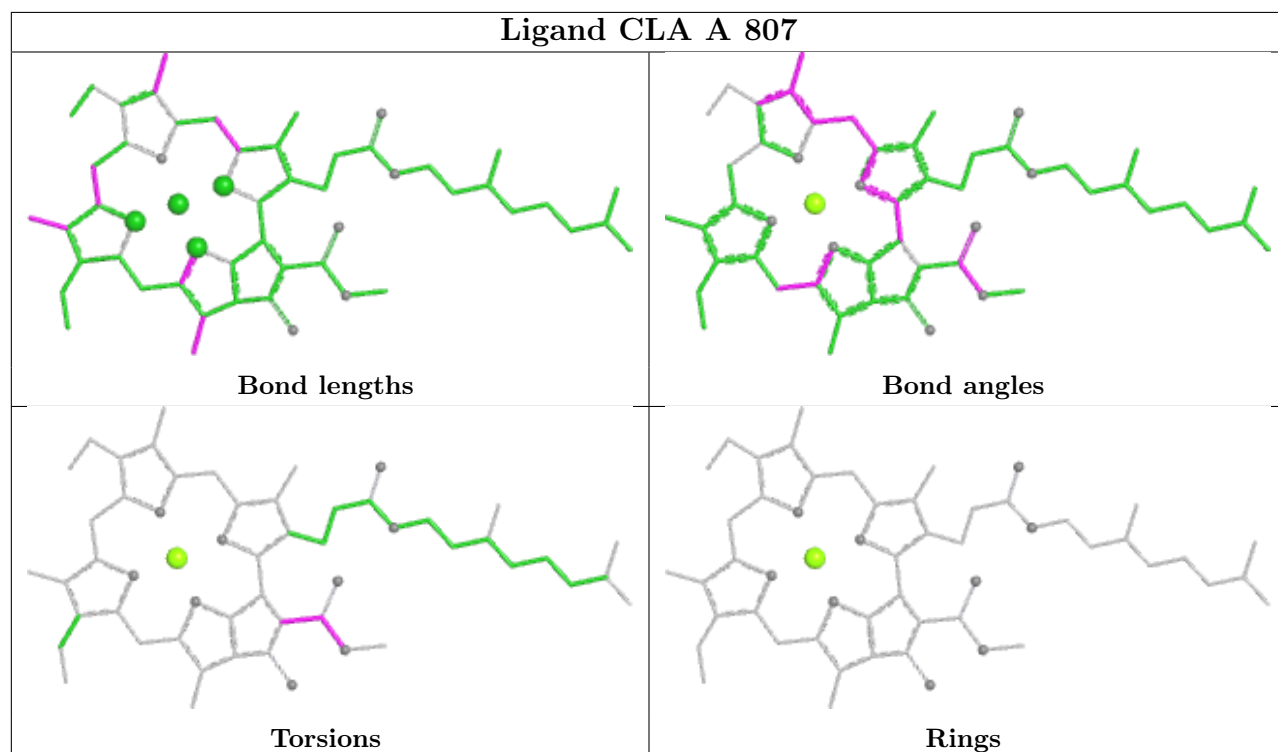
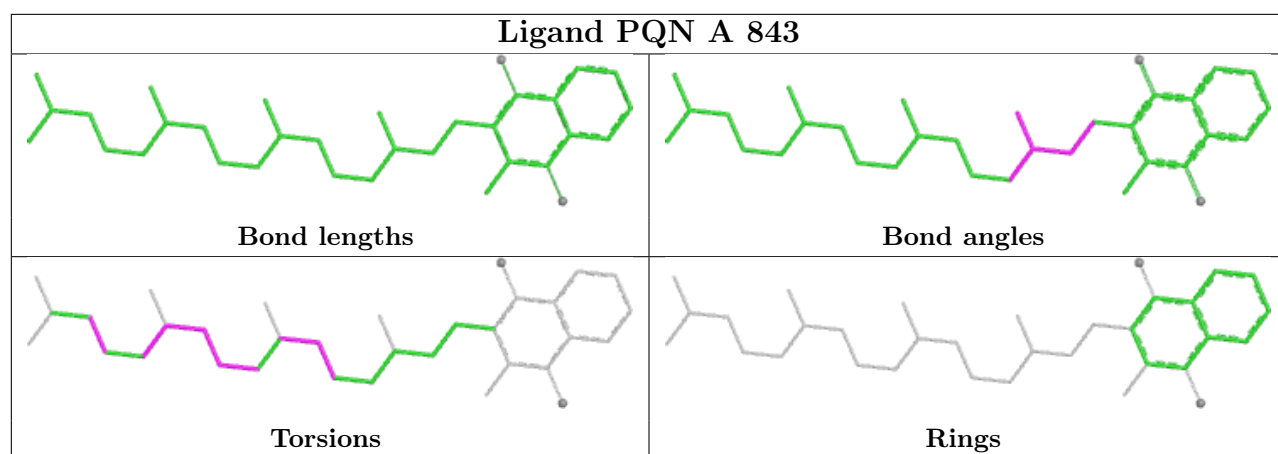




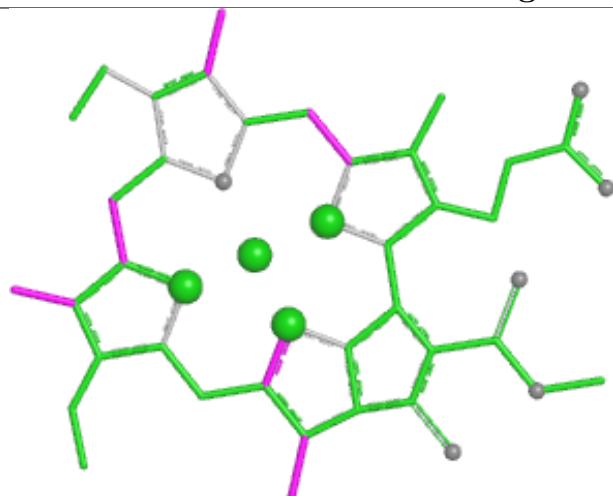




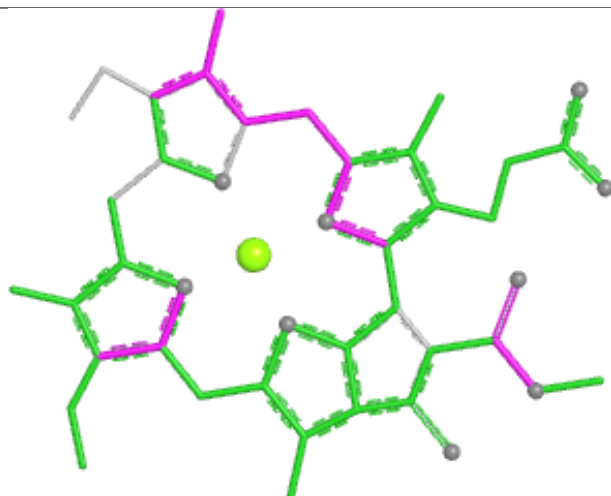




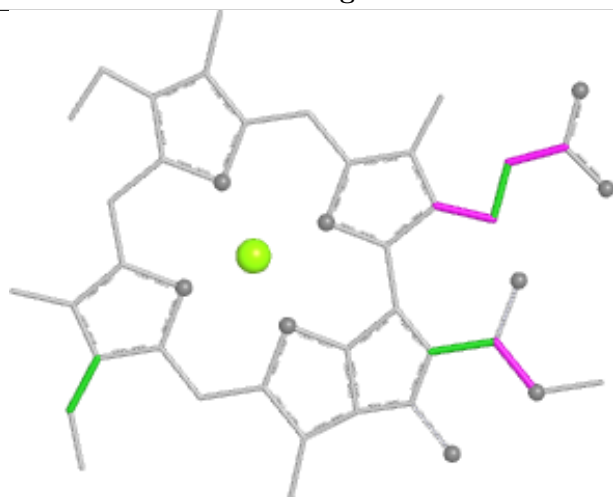
Ligand CLA a 810



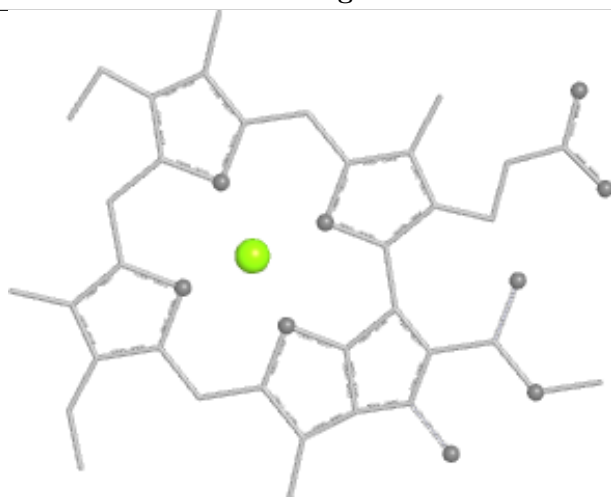
Bond lengths



Bond angles

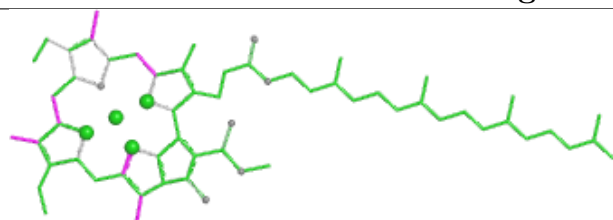


Torsions

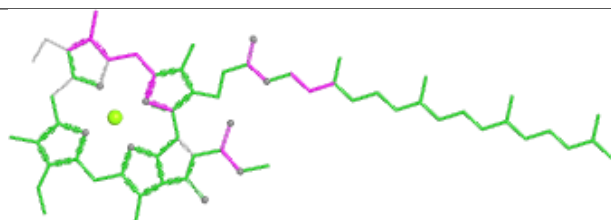


Rings

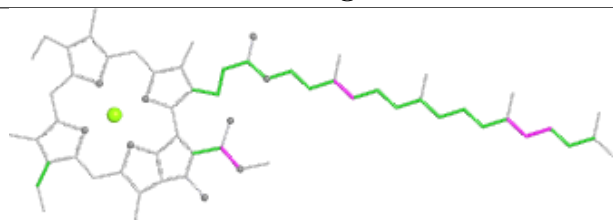
Ligand CLA a 832



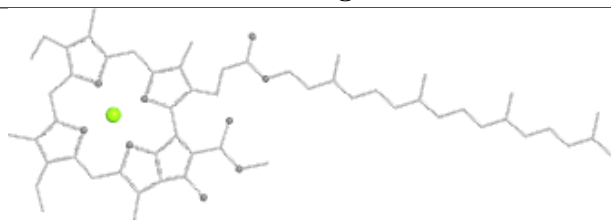
Bond lengths



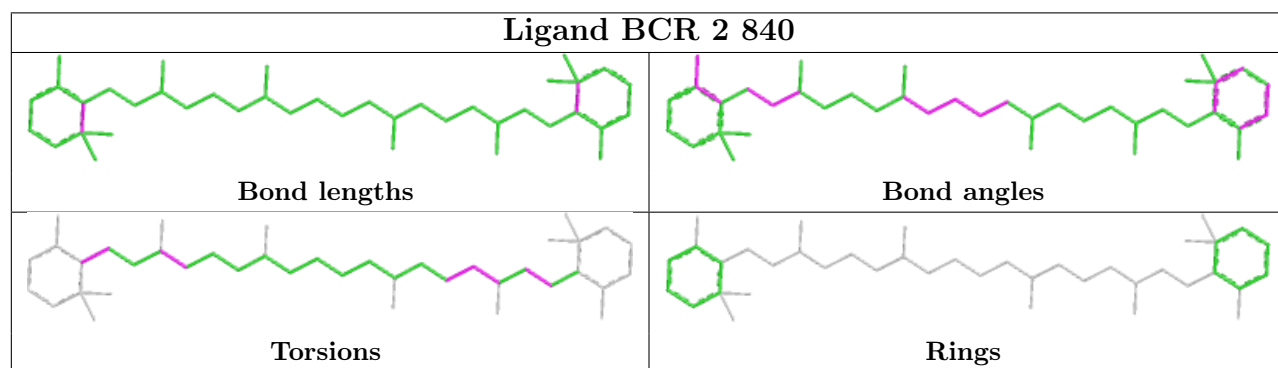
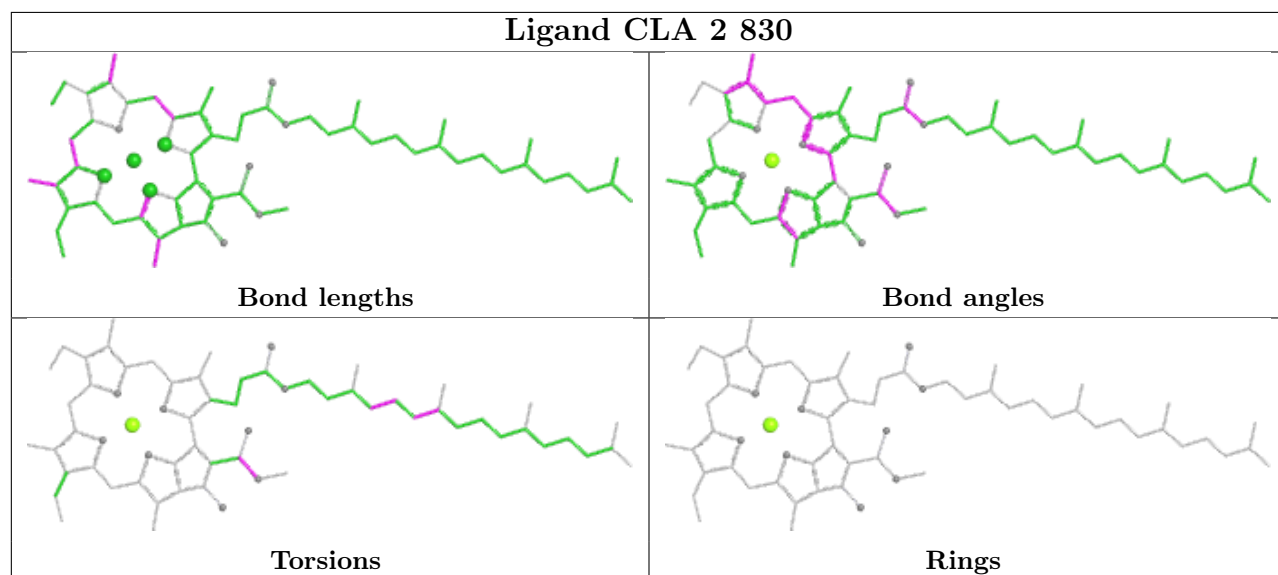
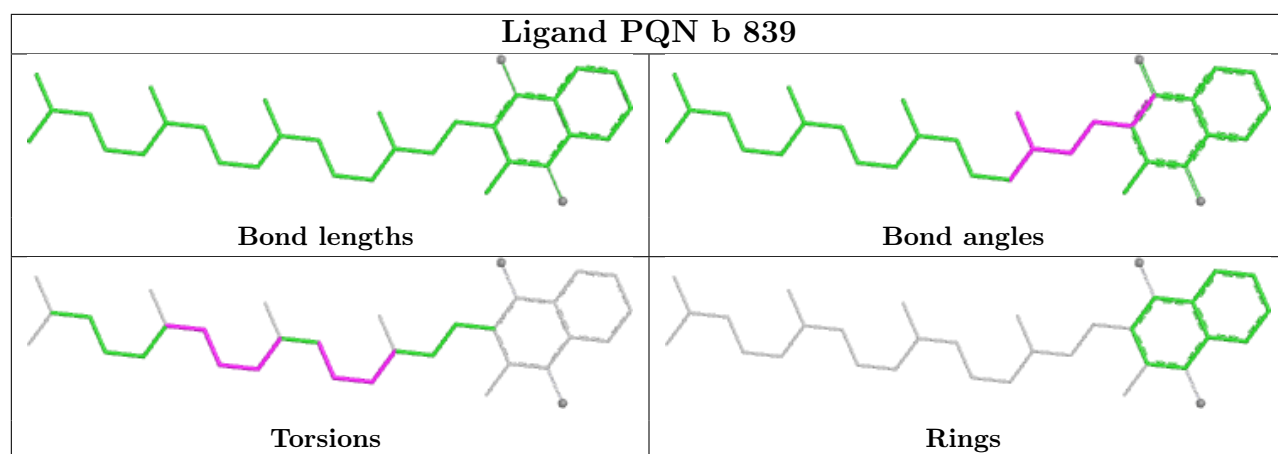
Bond angles

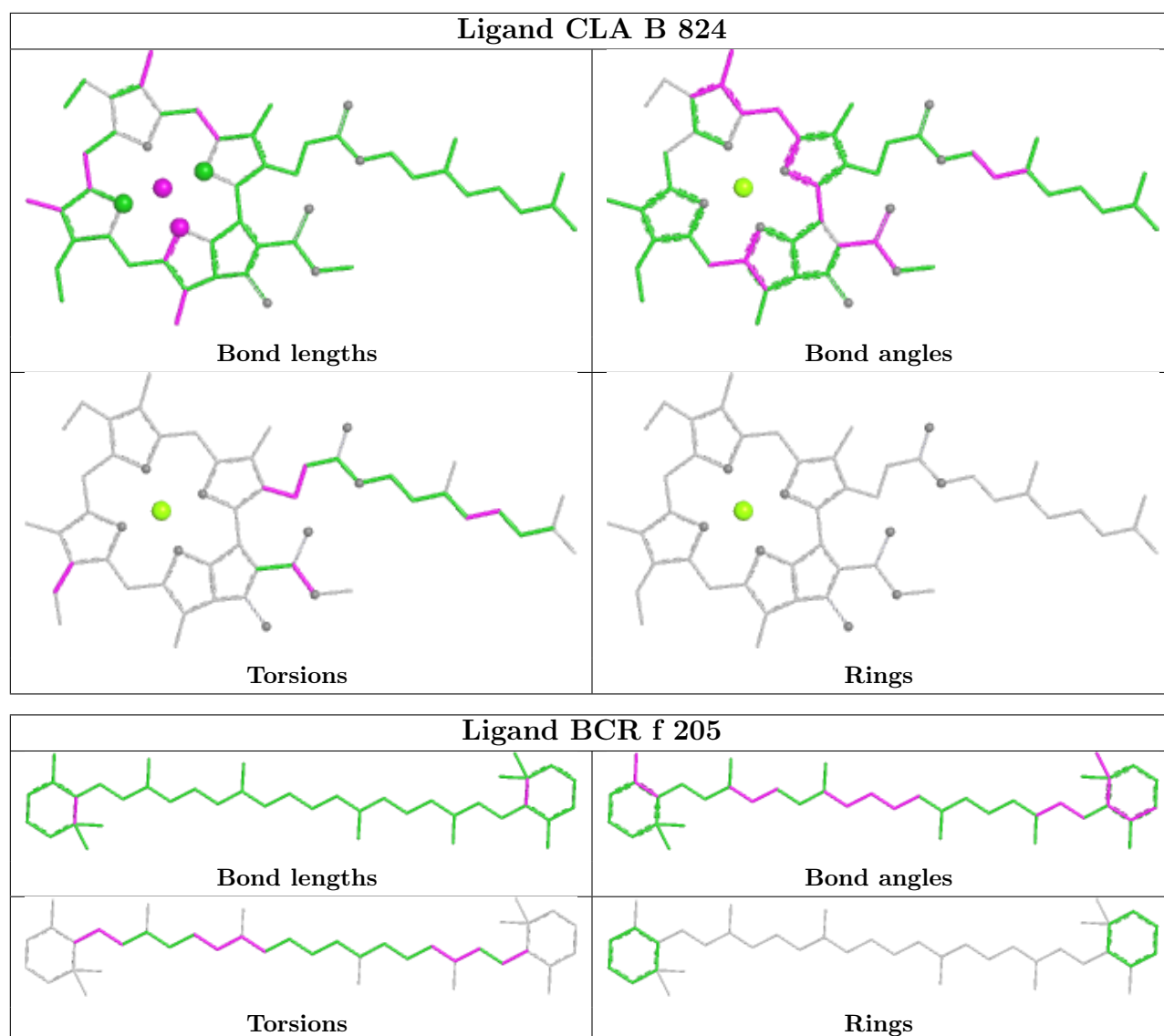


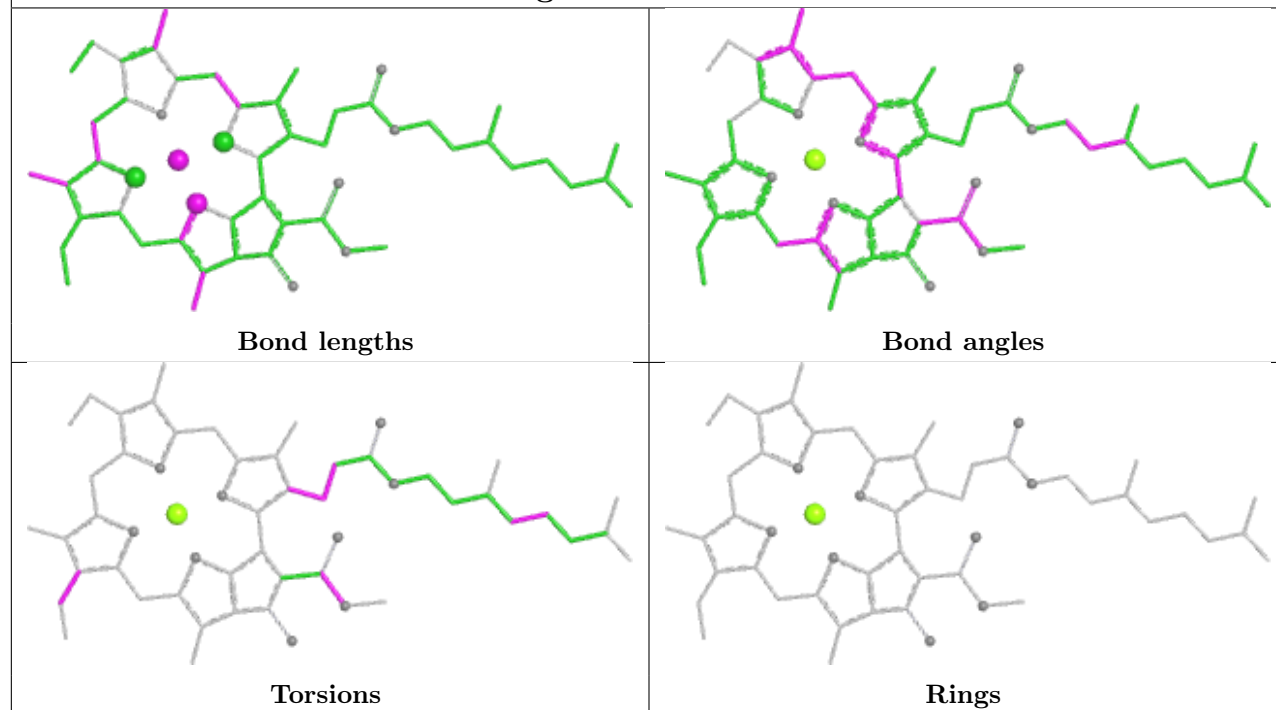
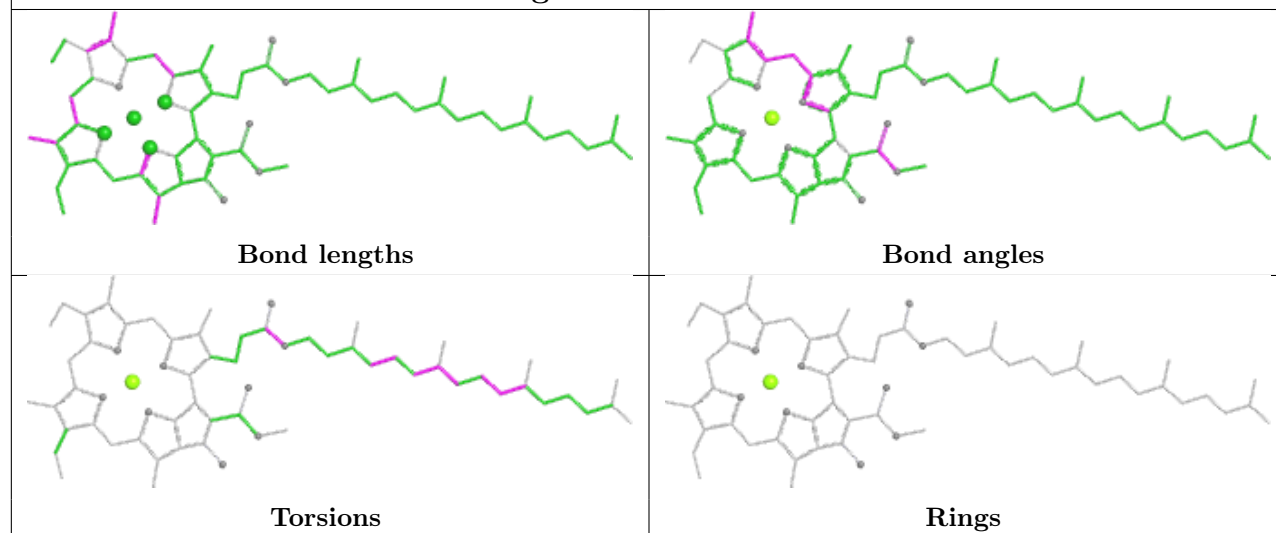
Torsions

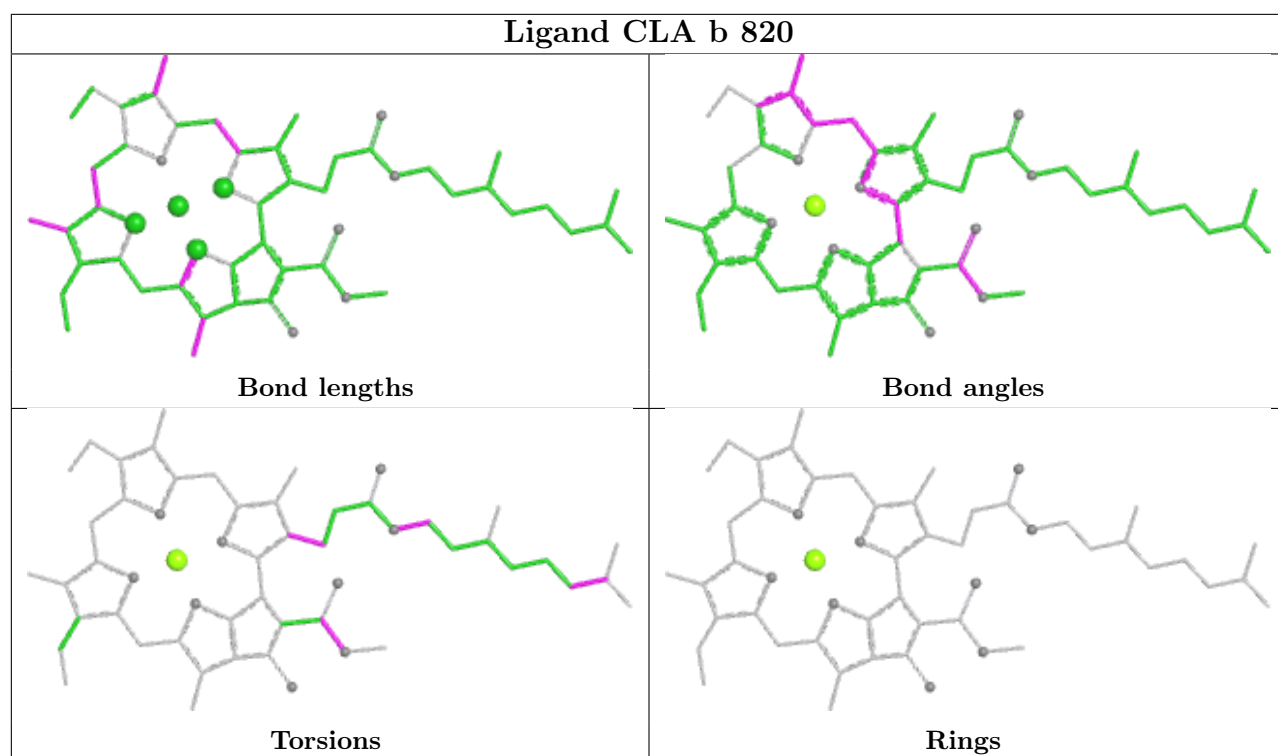


Rings

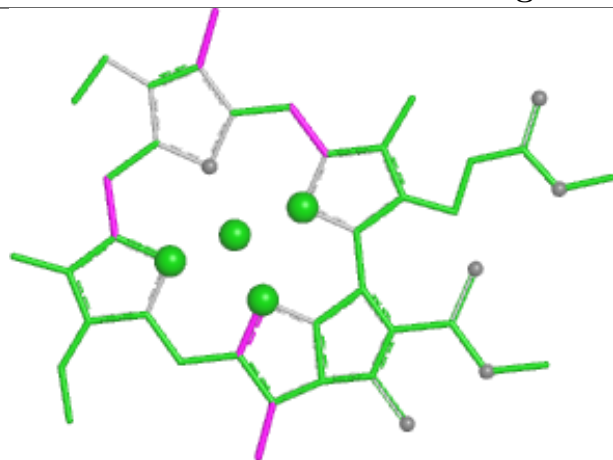




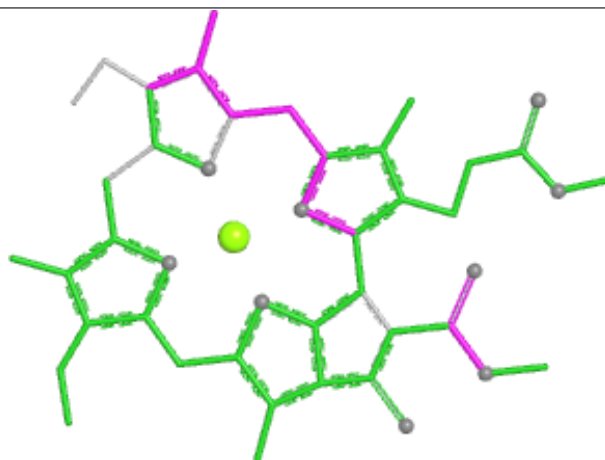
Ligand CLA 2 823**Ligand CLA A 834**



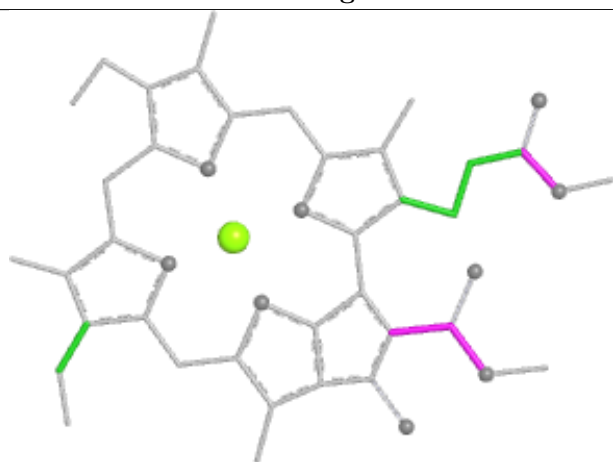
Ligand CLA F 204



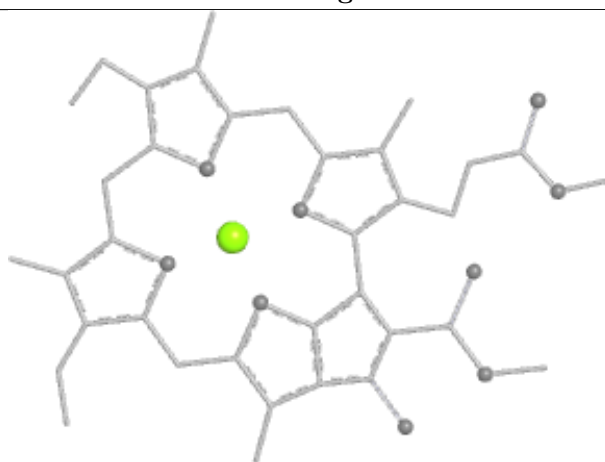
Bond lengths



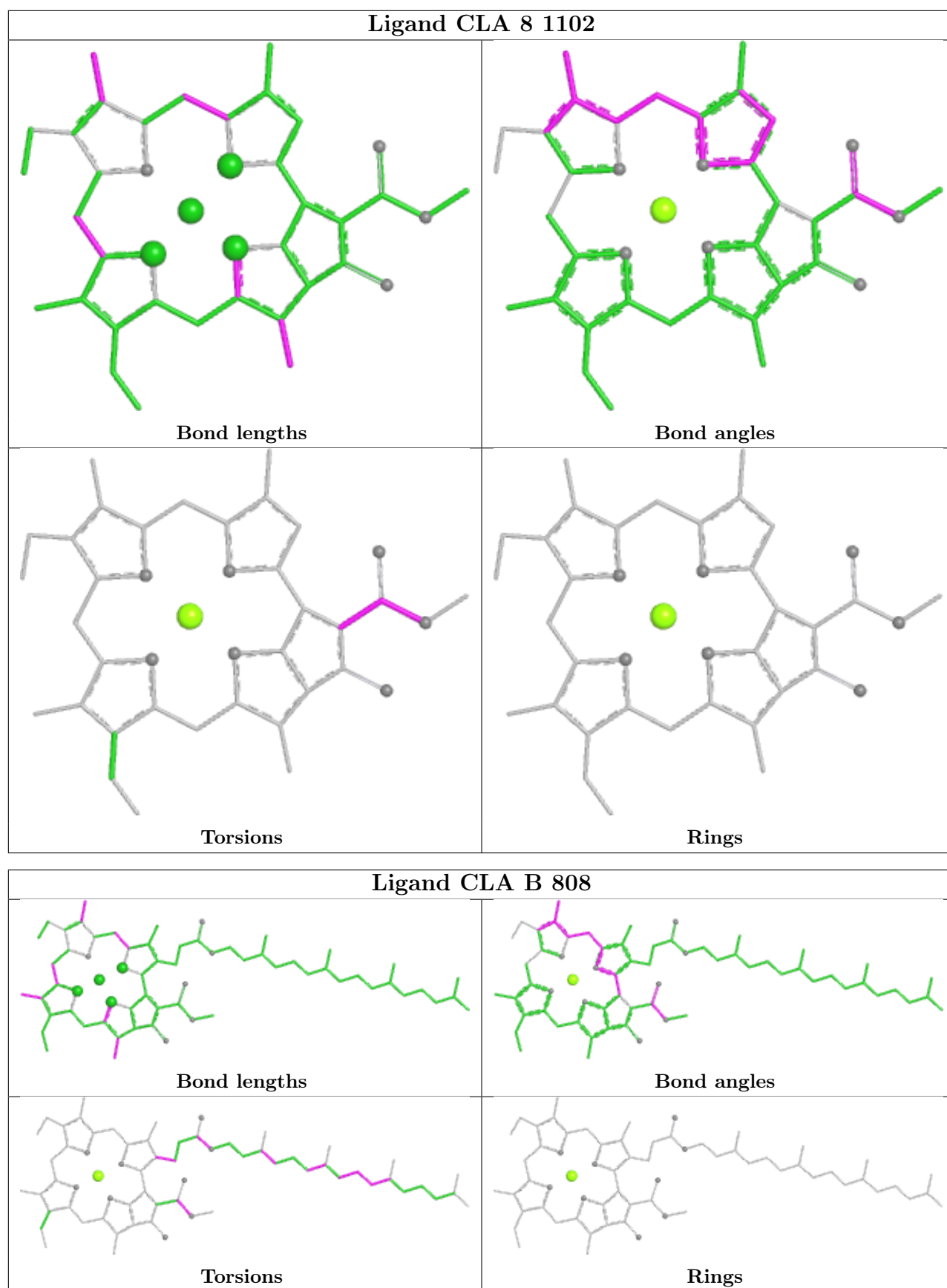
Bond angles



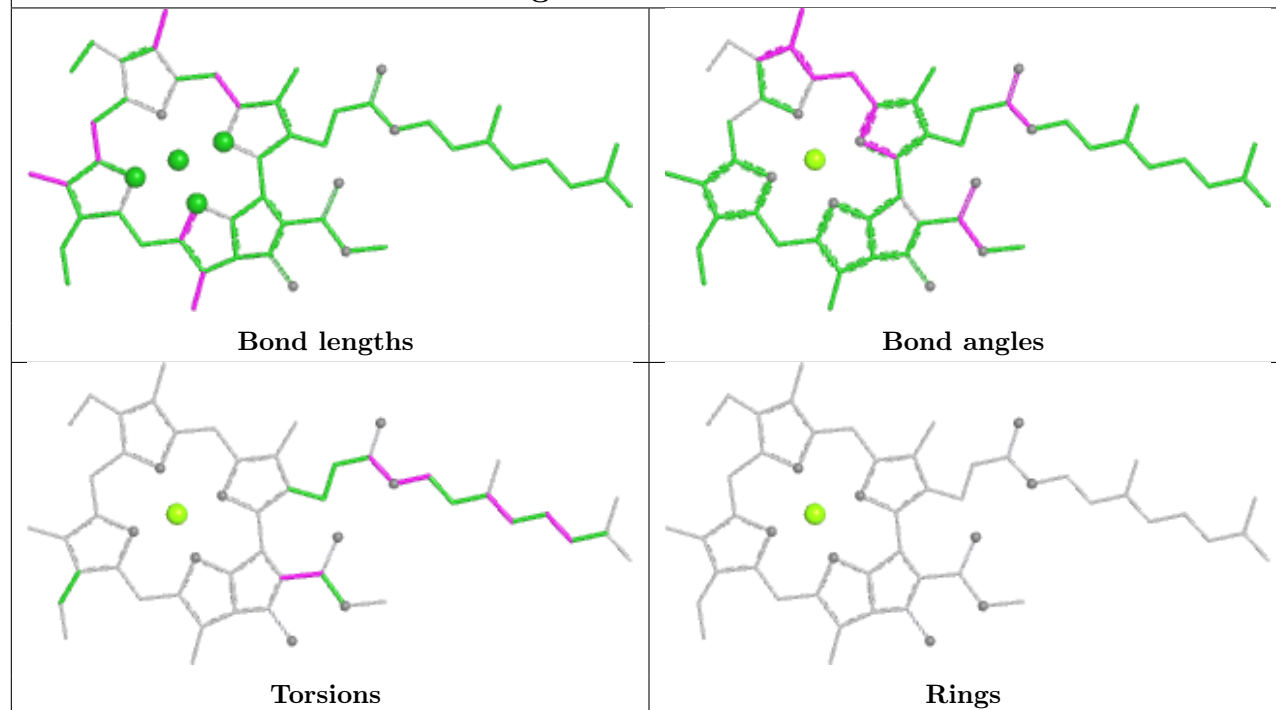
Torsions



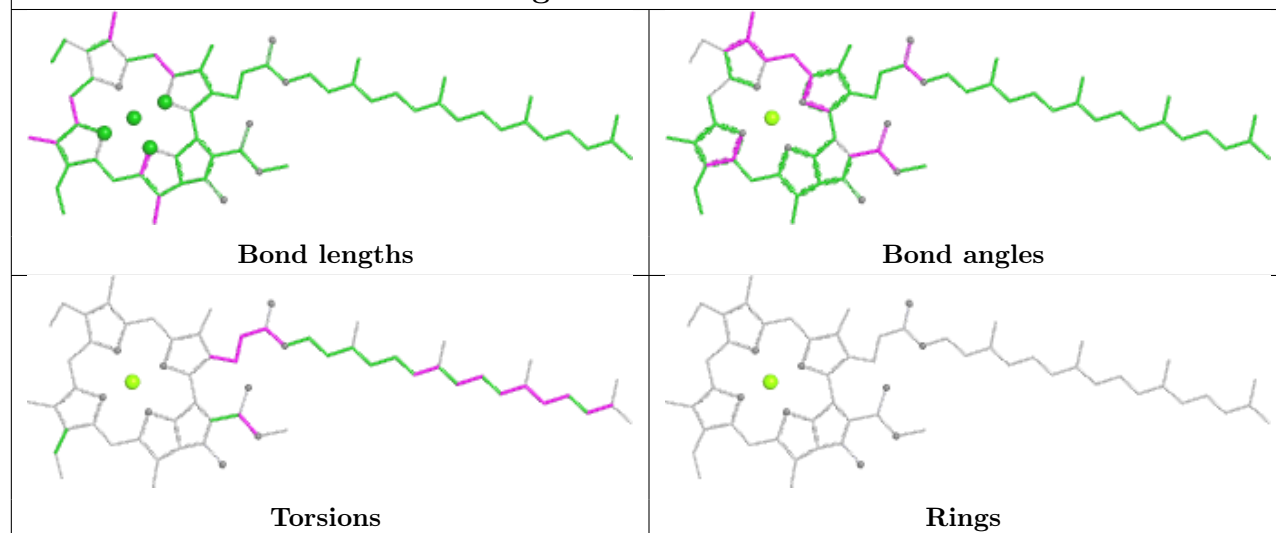
Rings



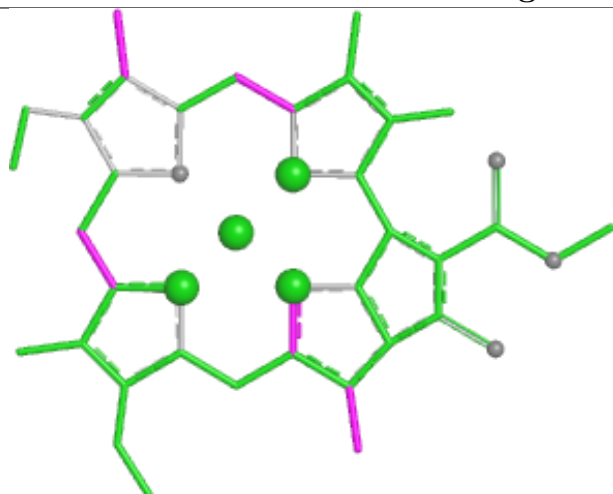
Ligand CLA A 826



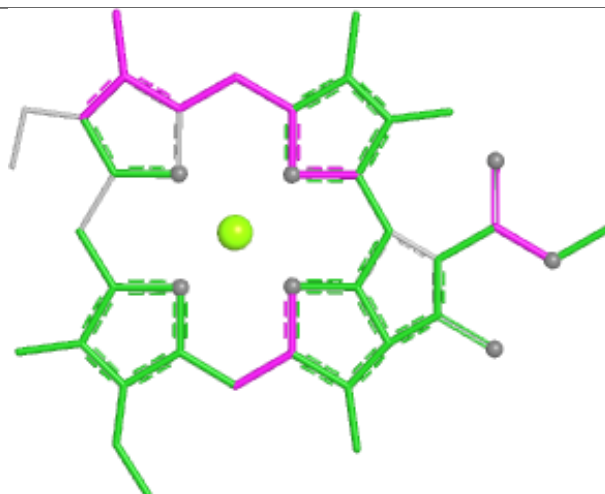
Ligand CLA B 821



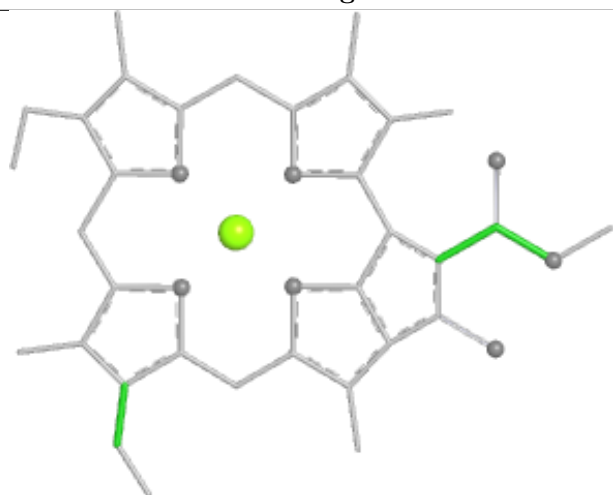
Ligand CLA 2 816



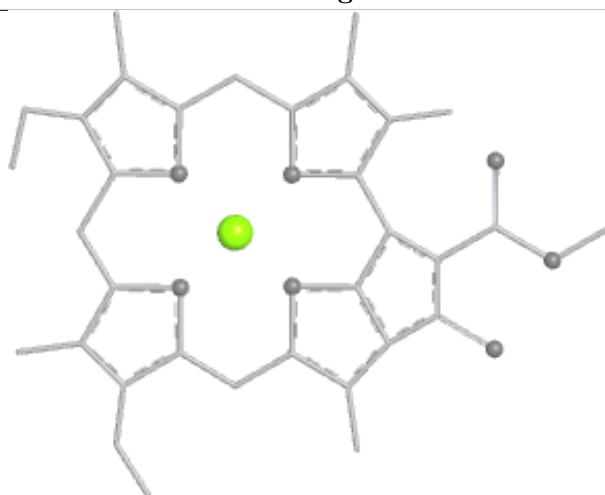
Bond lengths



Bond angles

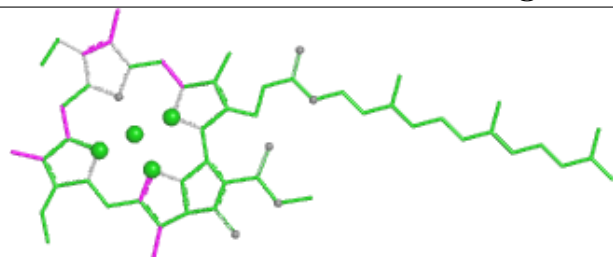


Torsions

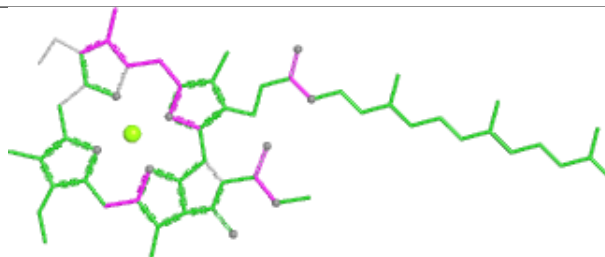


Rings

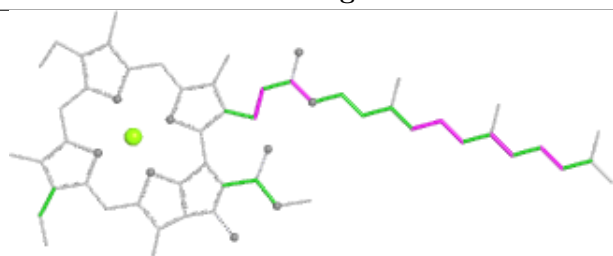
Ligand CLA a 837



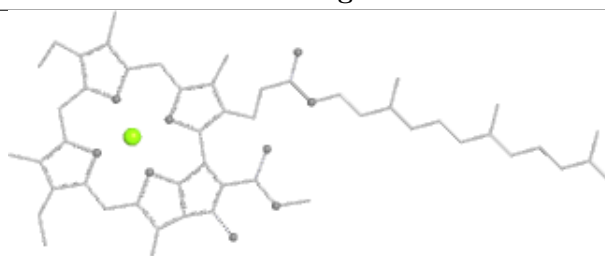
Bond lengths



Bond angles

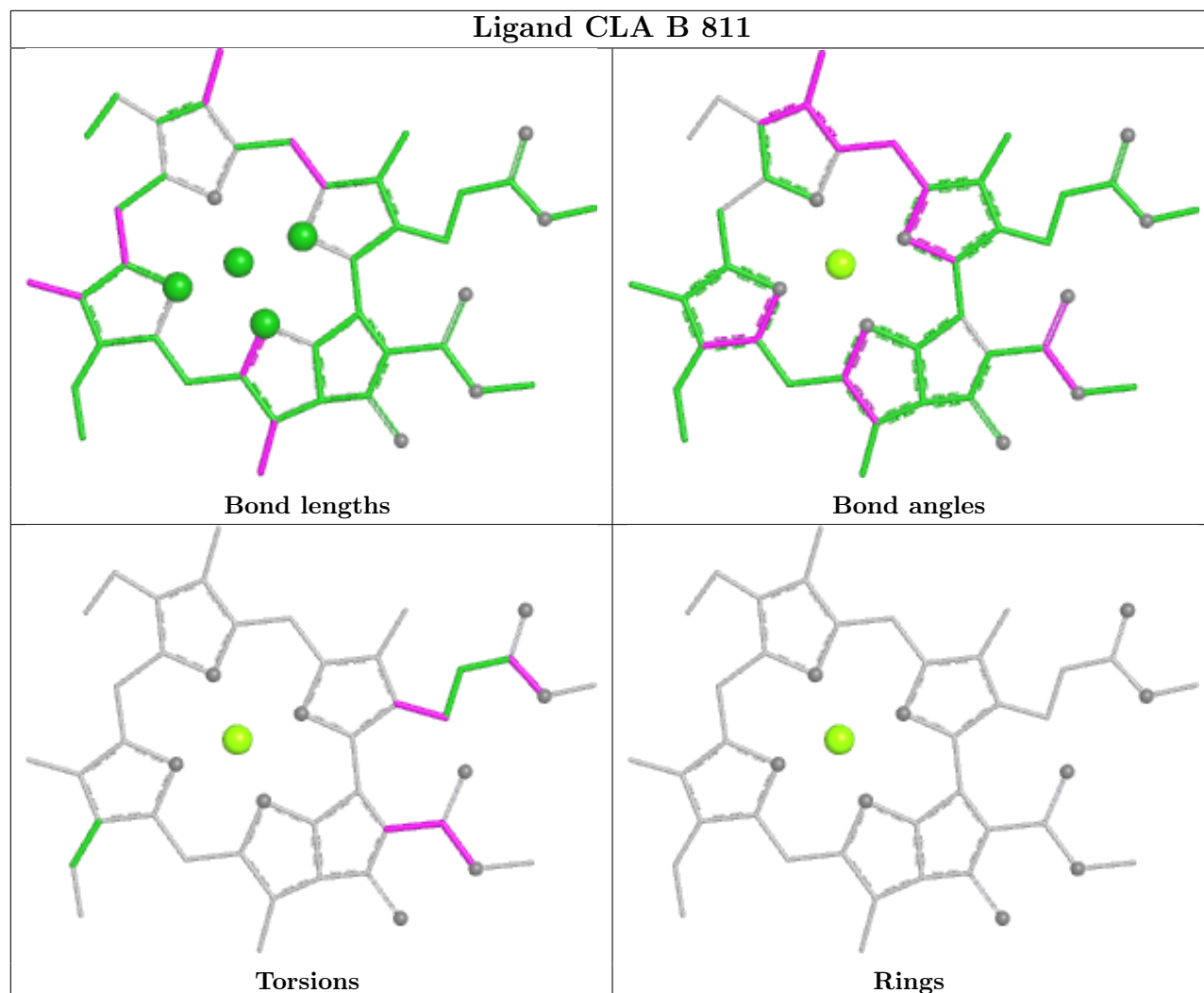


Torsions

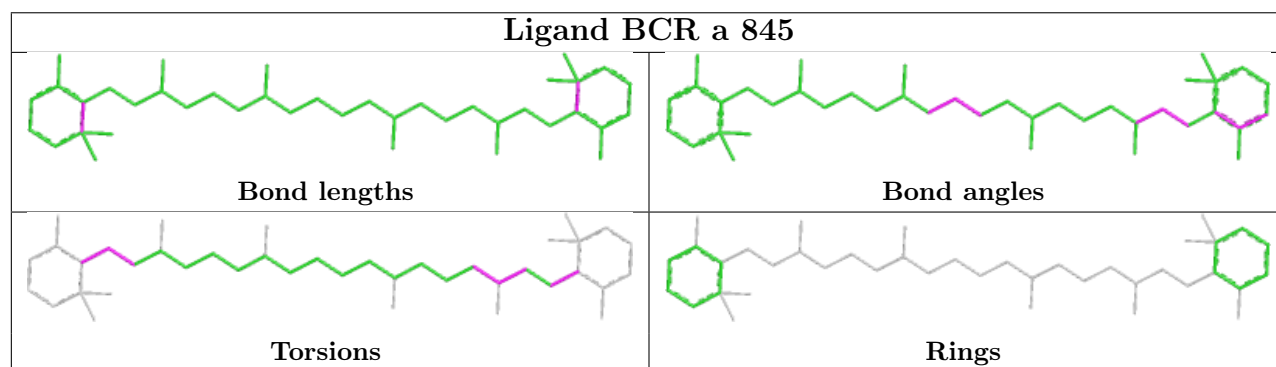


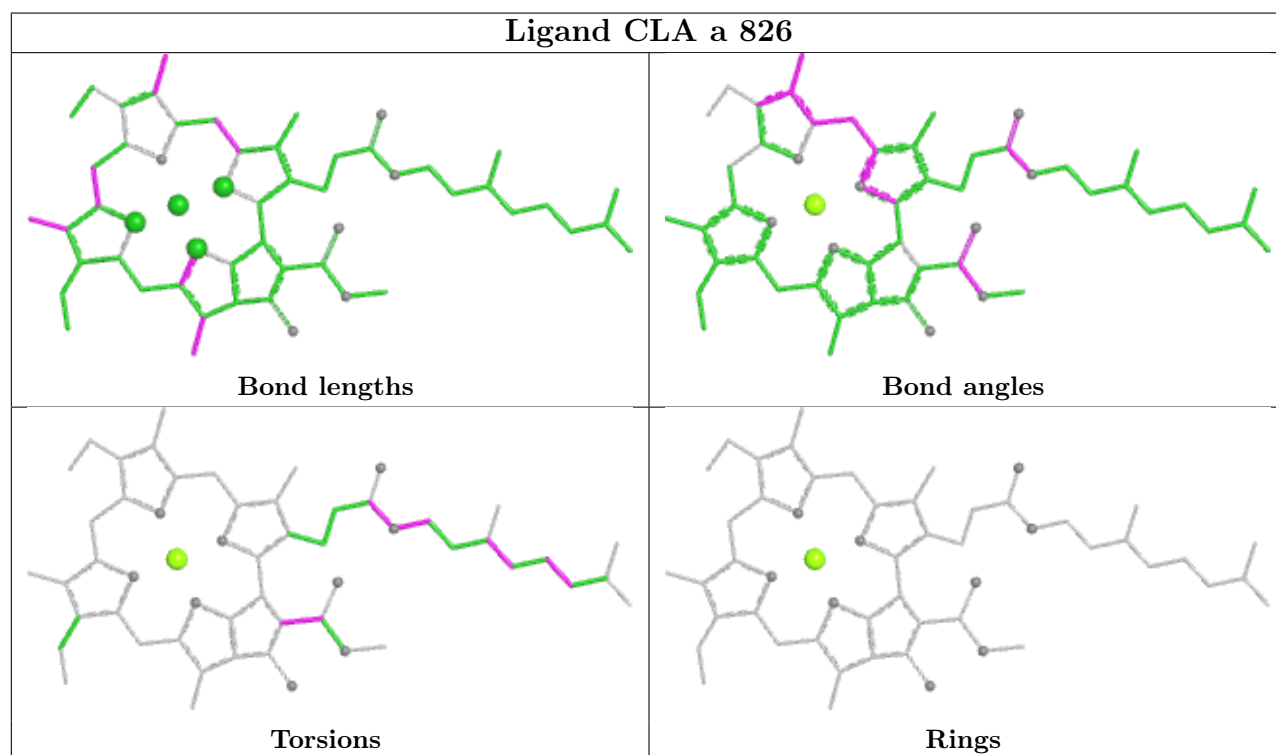
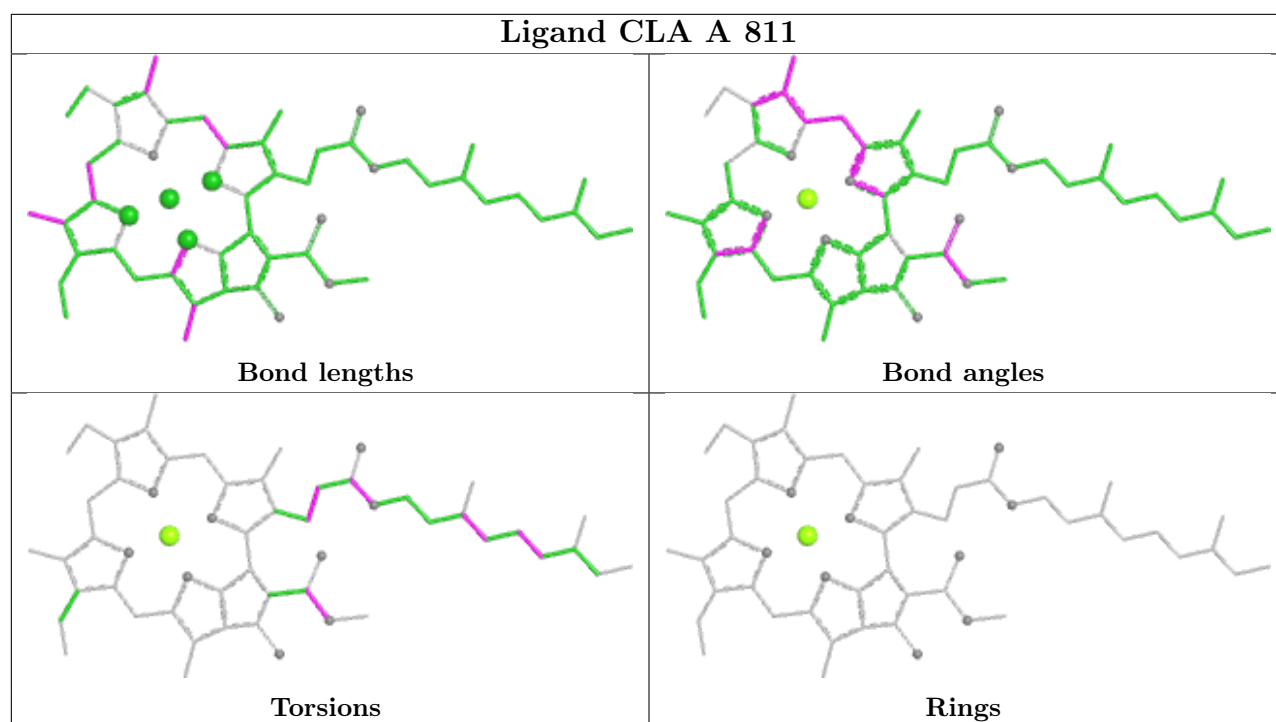
Rings

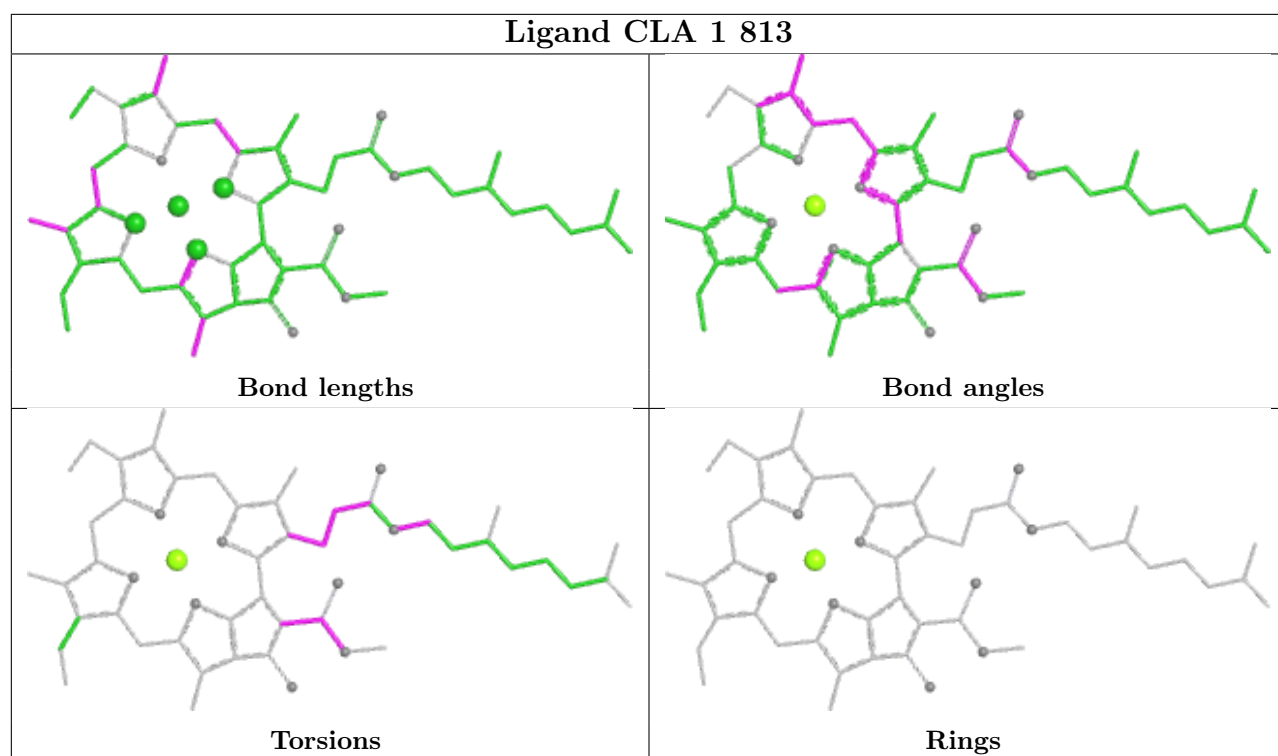
Ligand CLA B 811



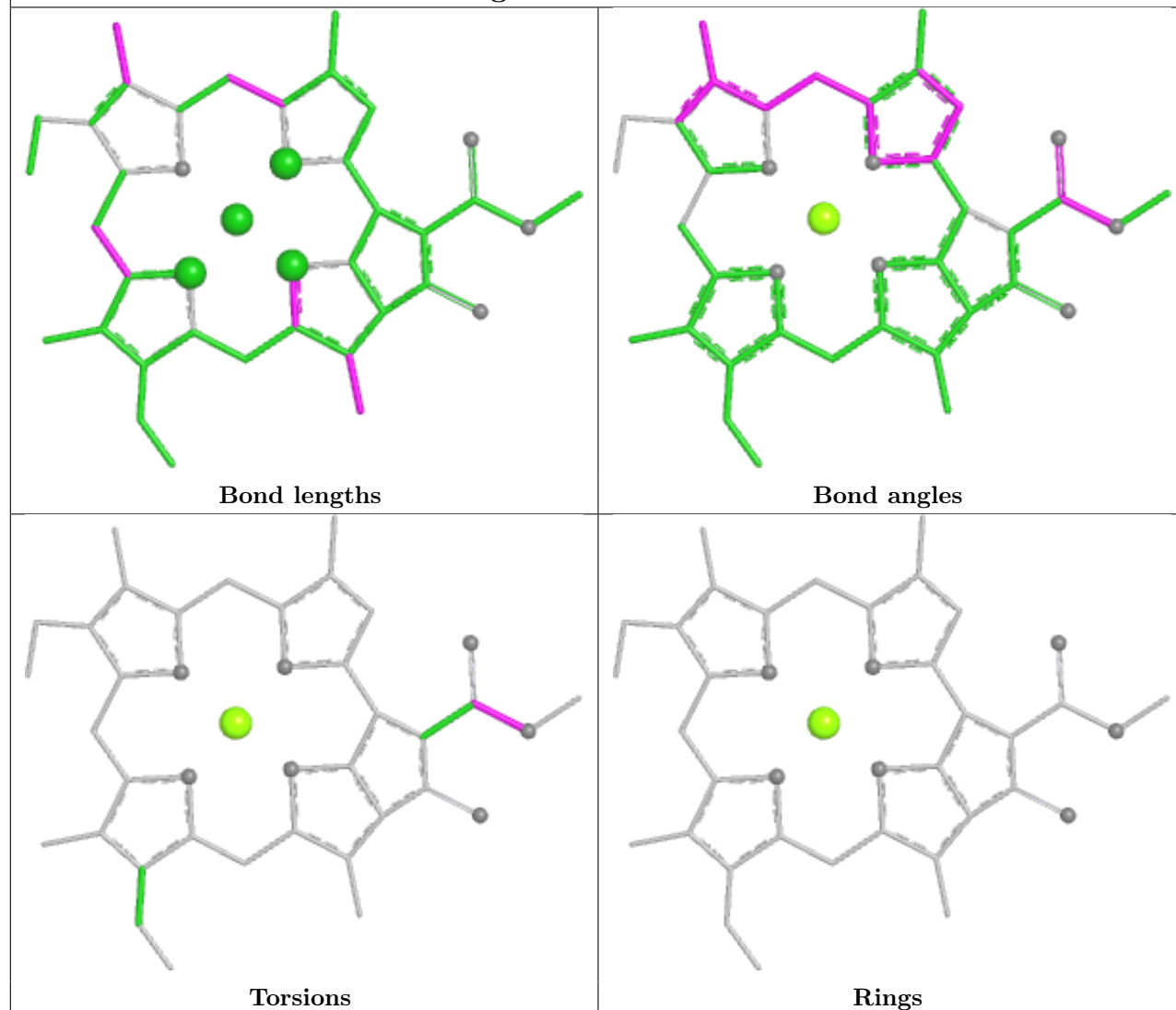
Ligand BCR a 845



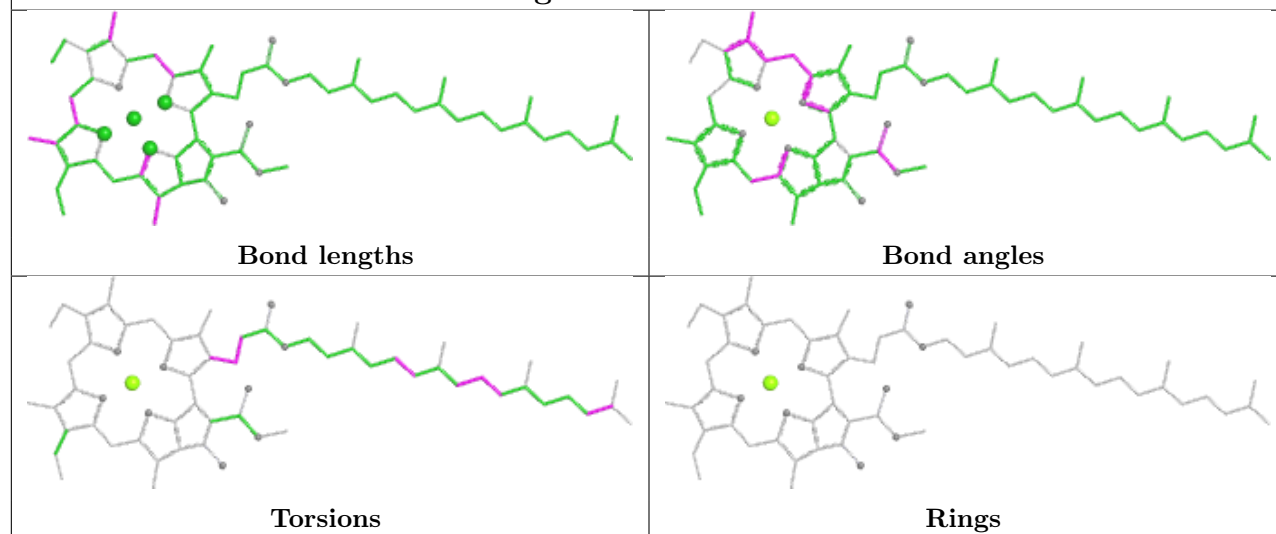


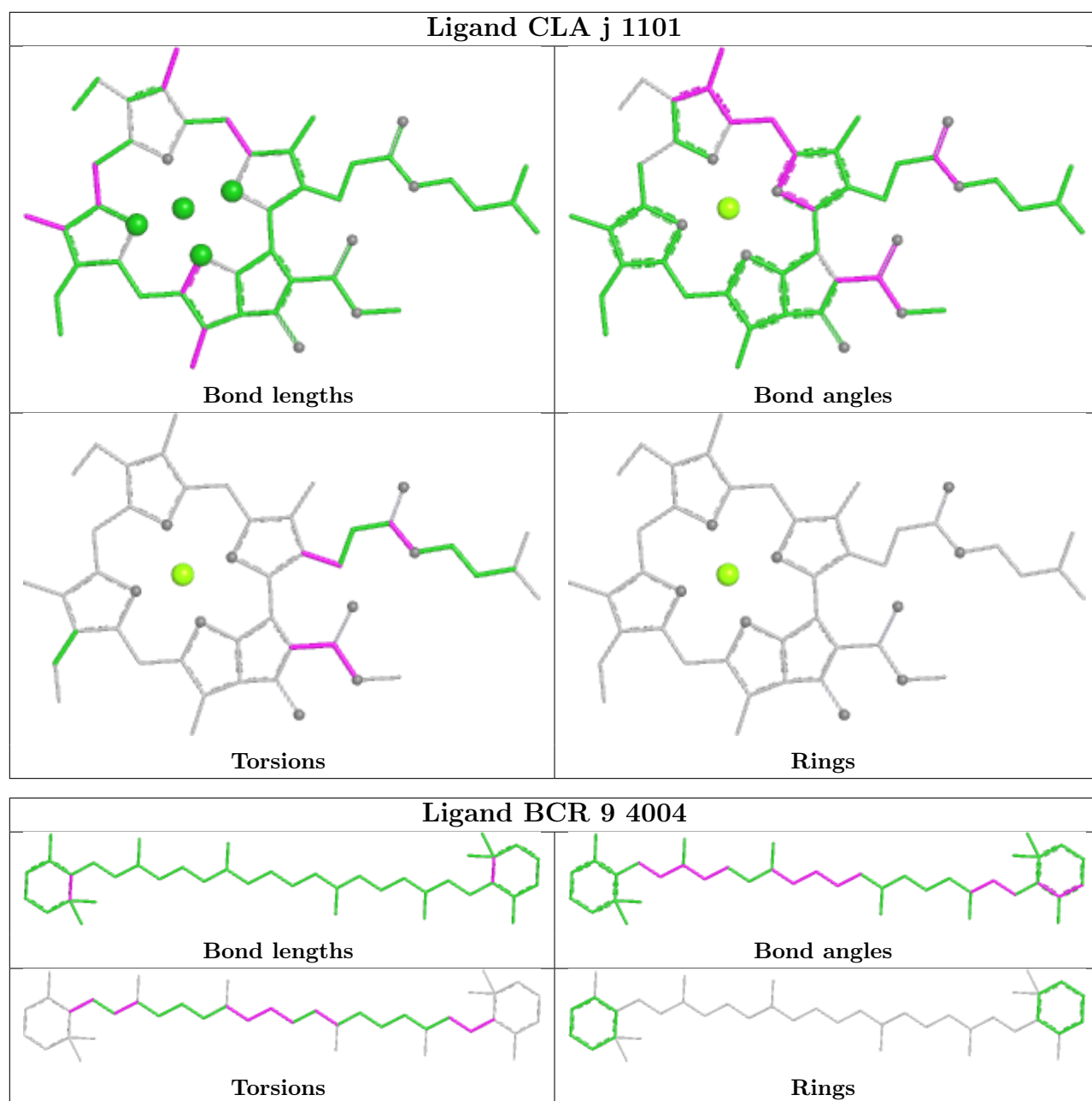


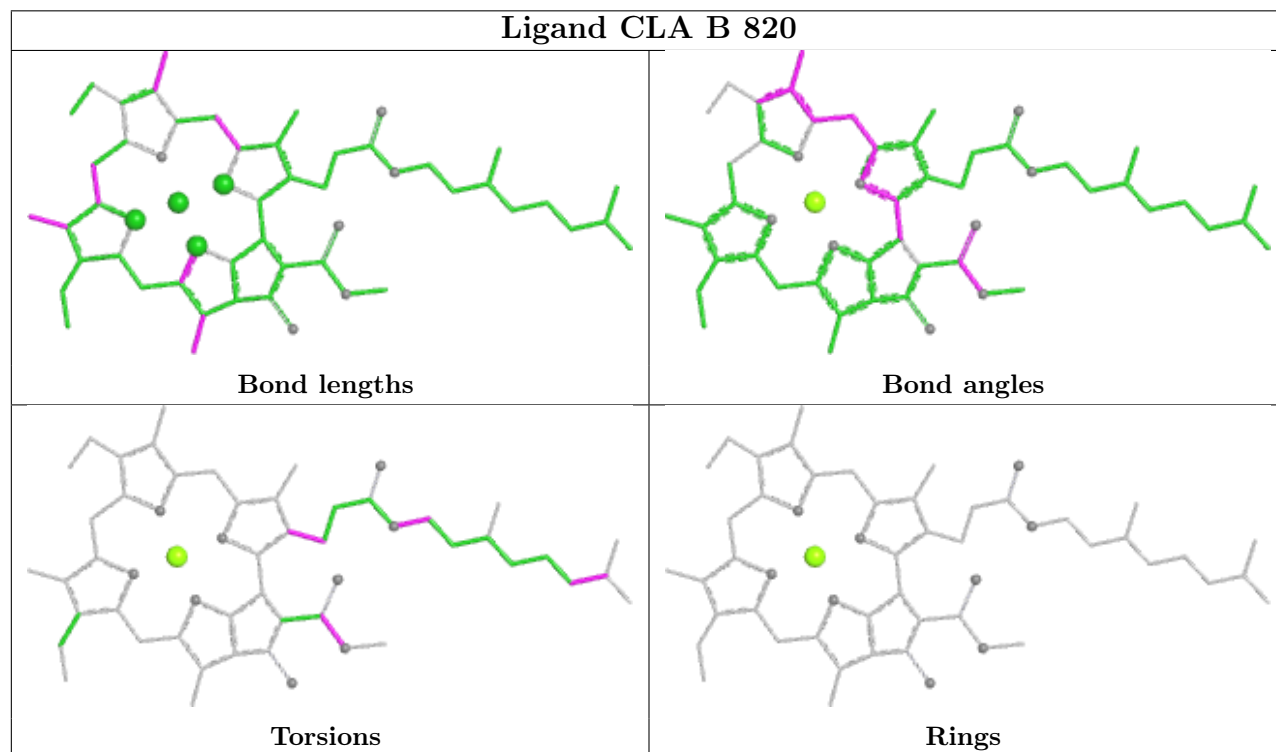
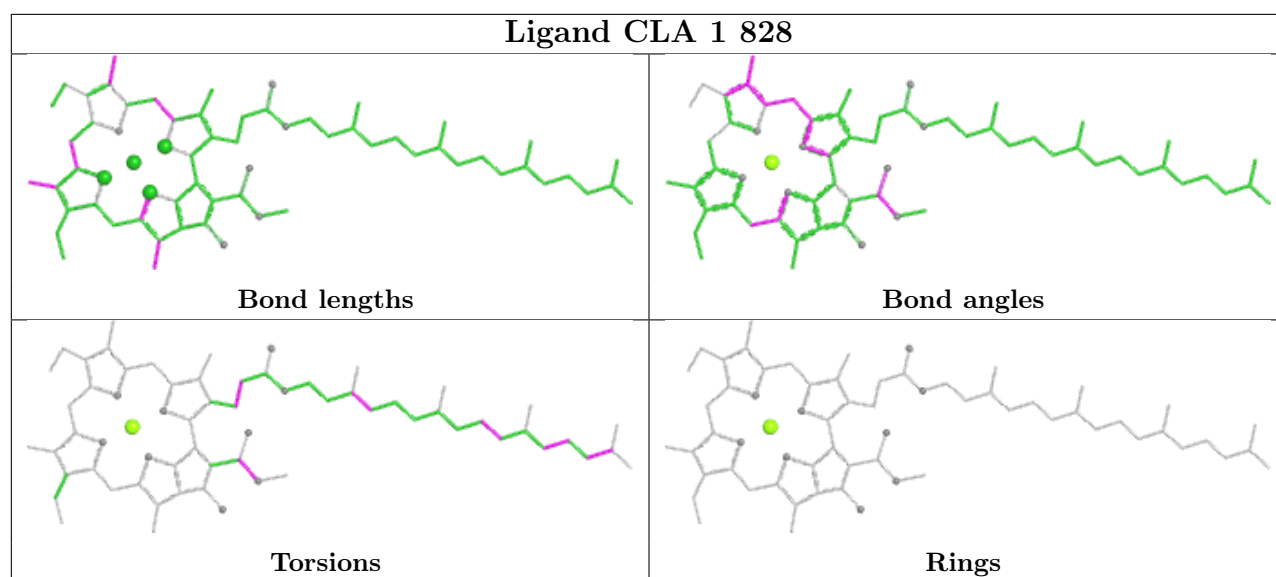
Ligand CLA B 832

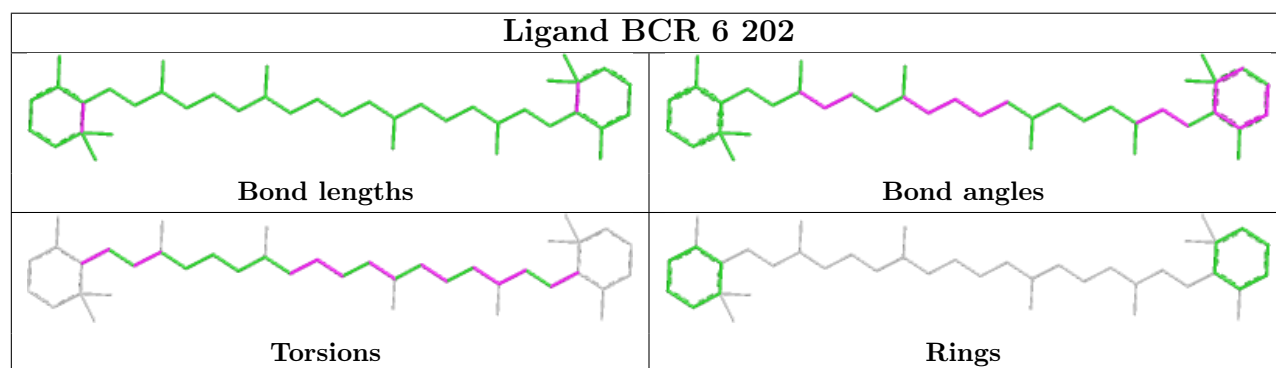
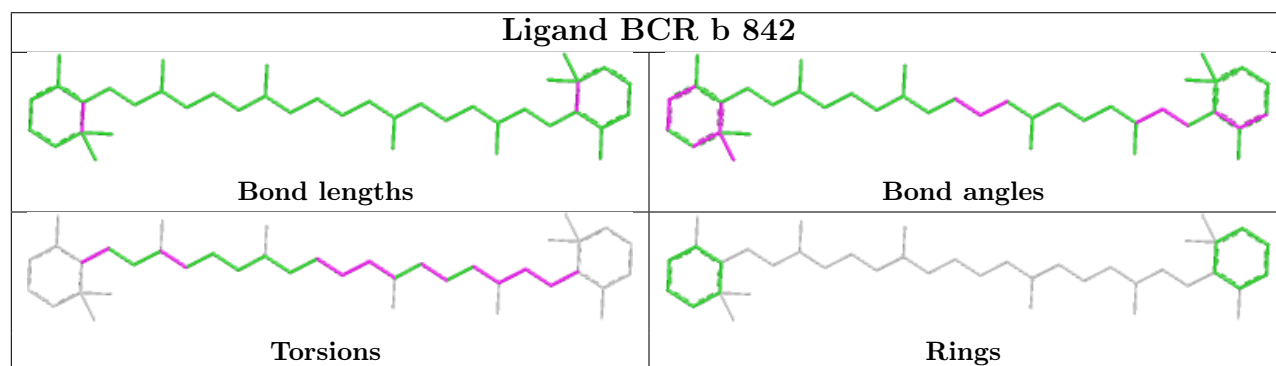
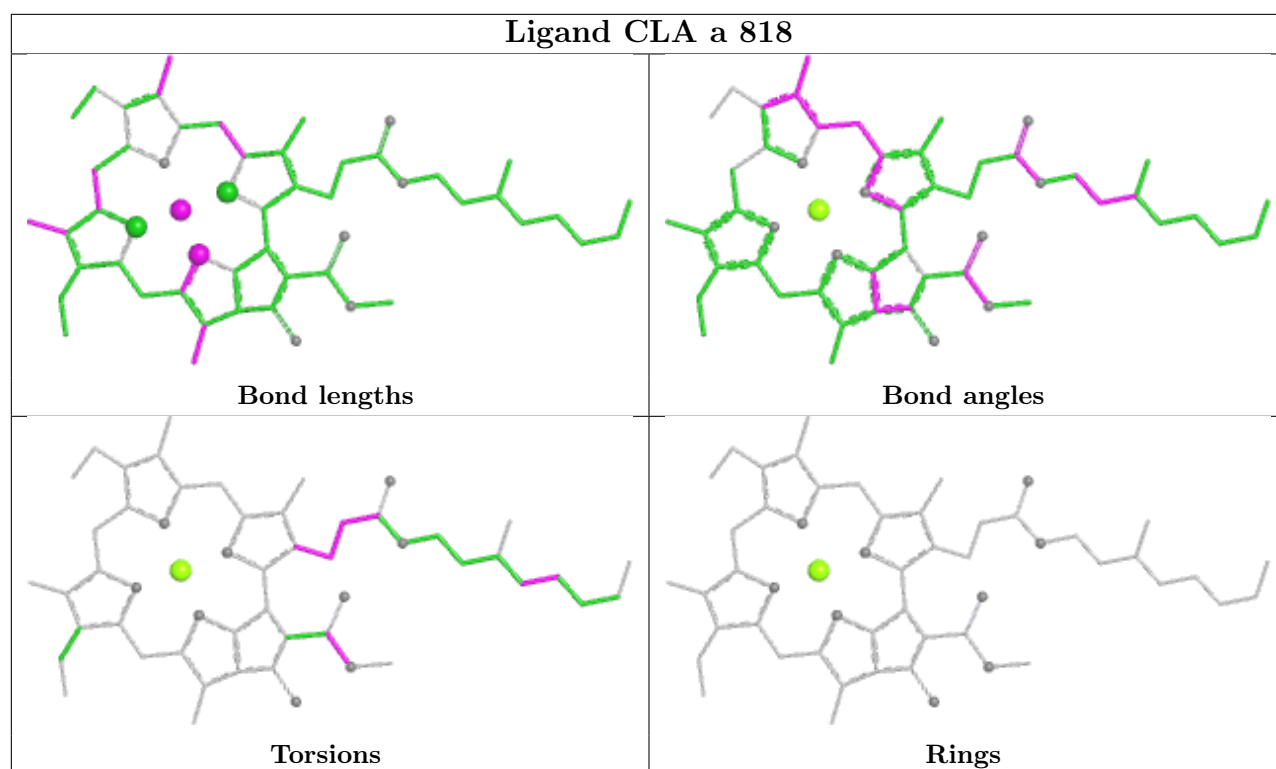


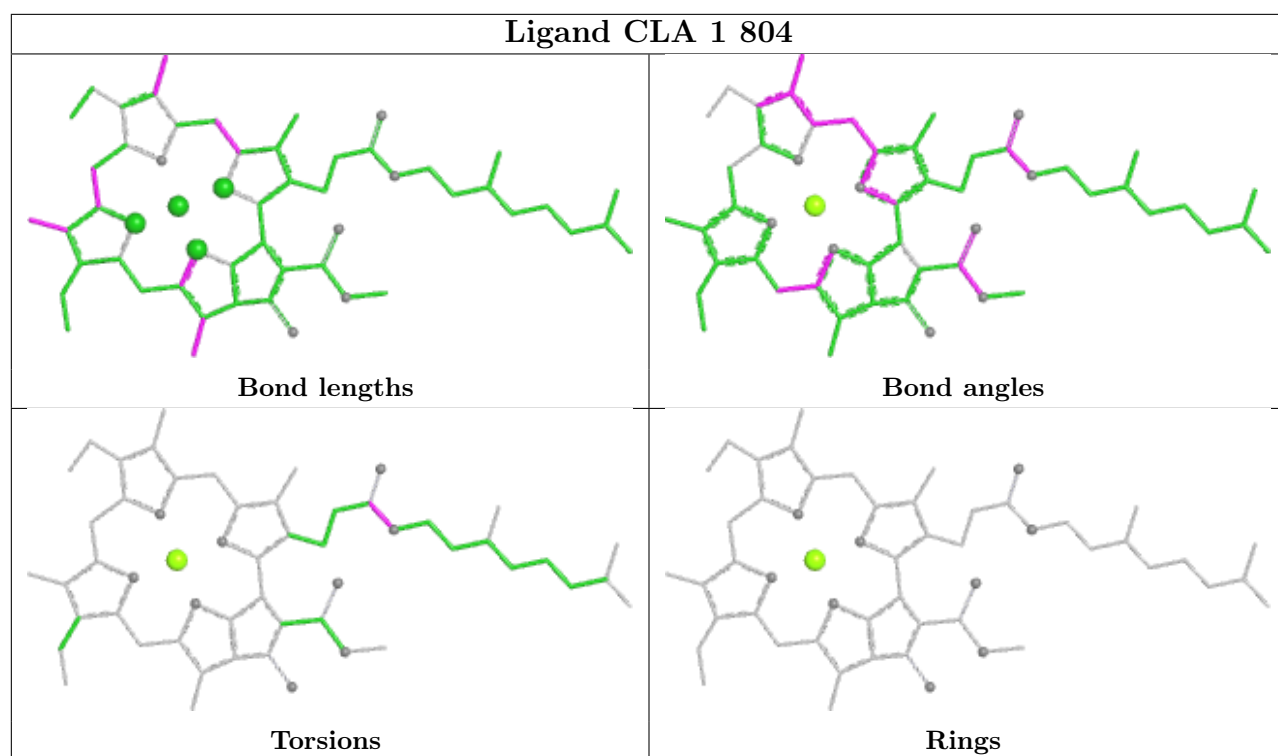
Ligand CLA L 206

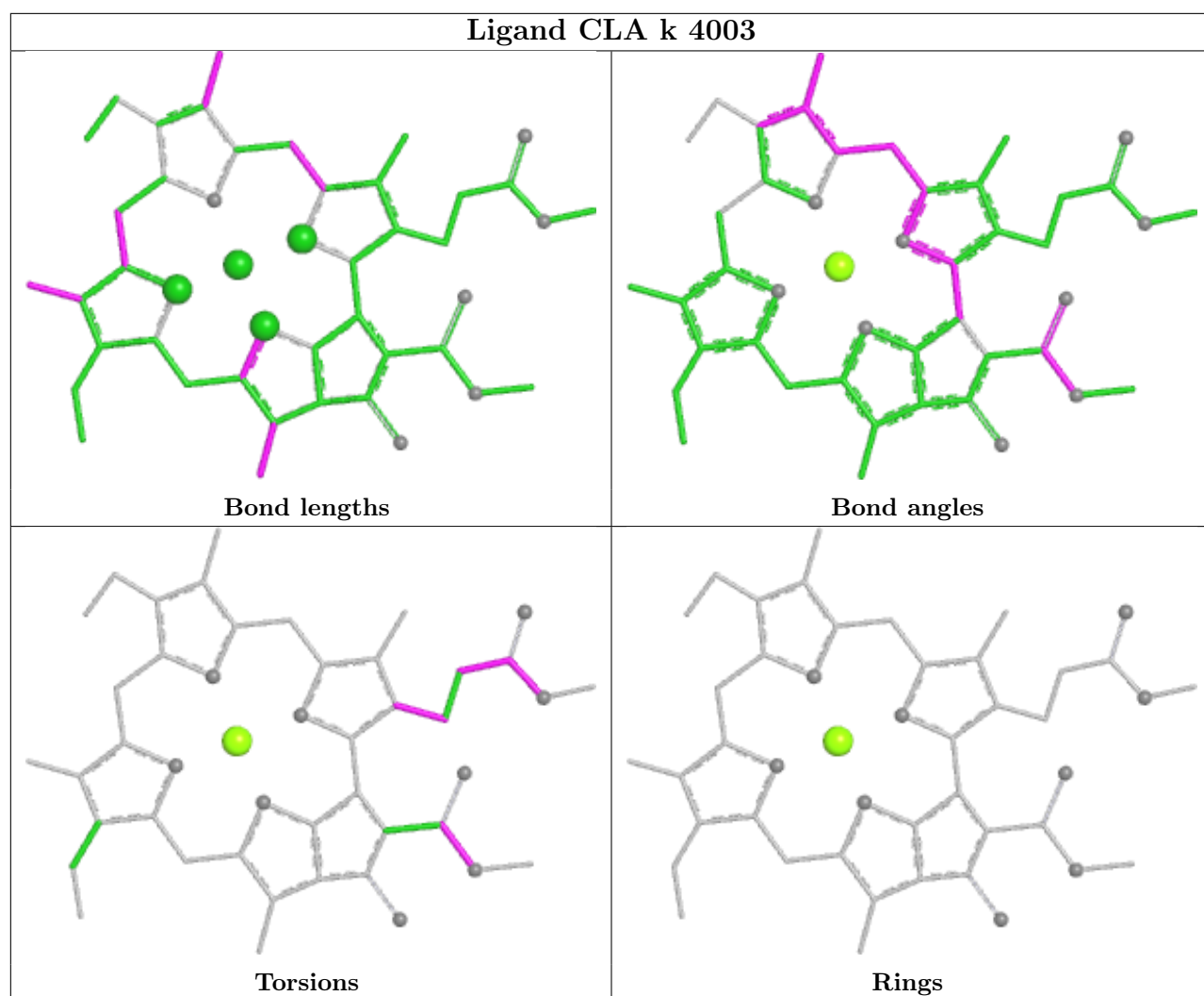




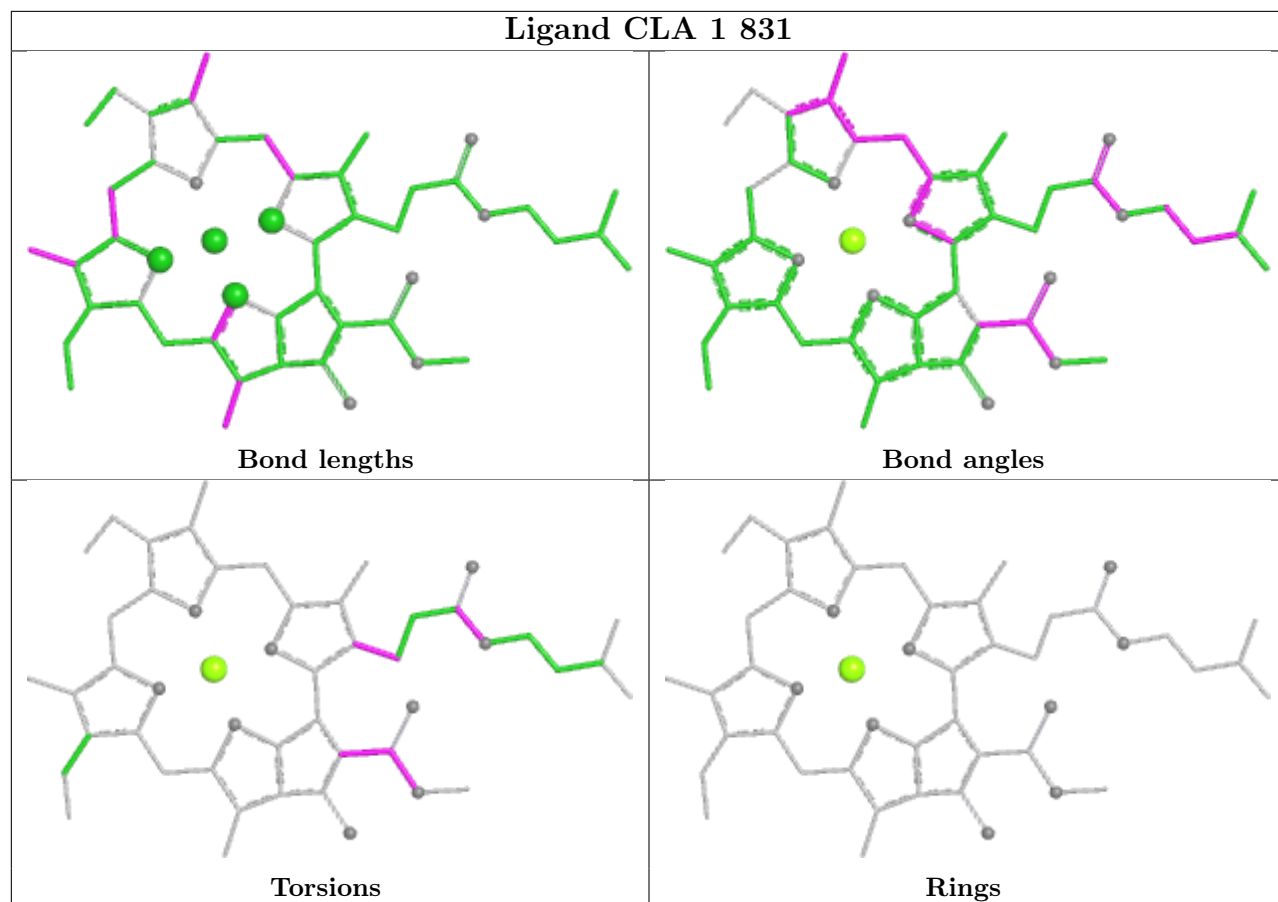




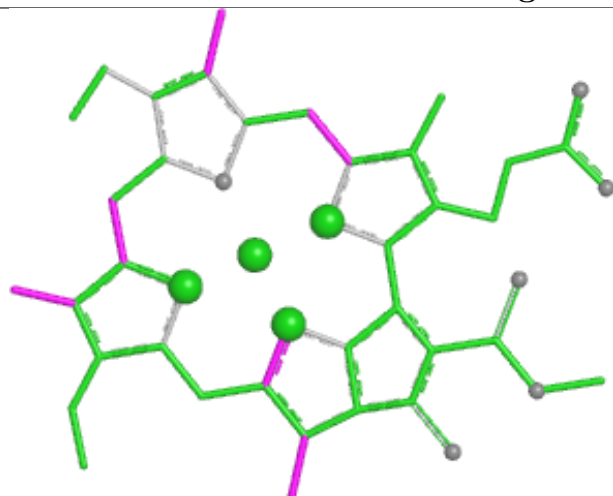




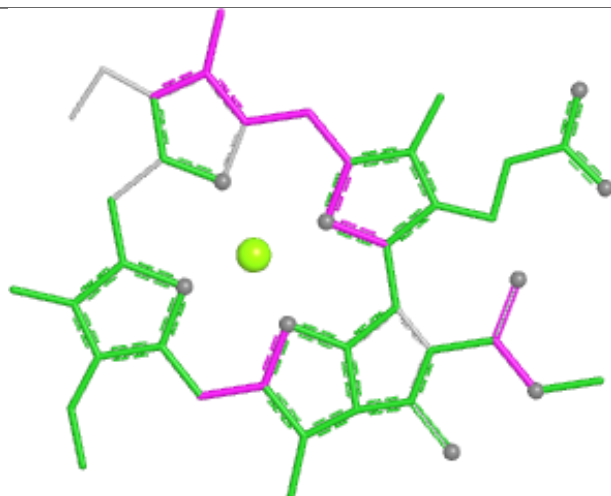
Ligand CLA 1 831



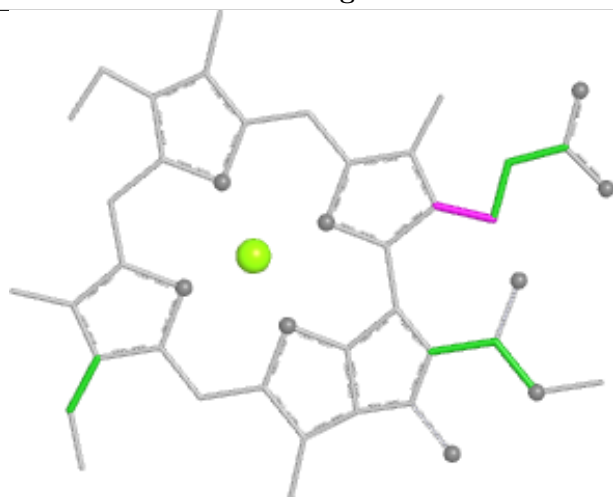
Ligand CLA 1 815



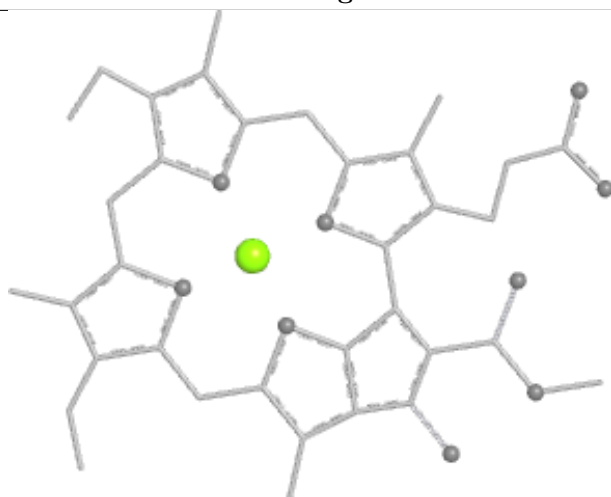
Bond lengths



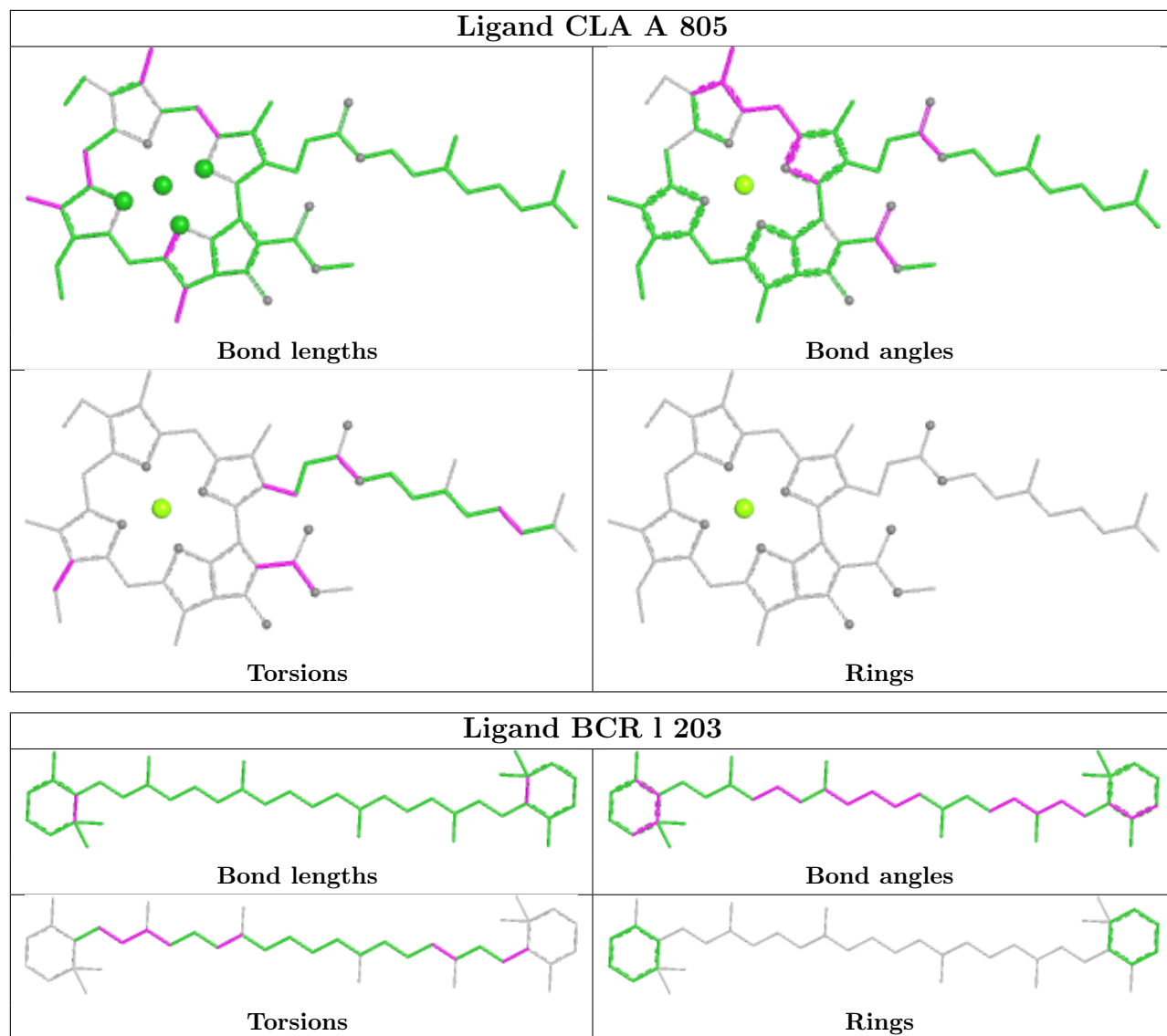
Bond angles

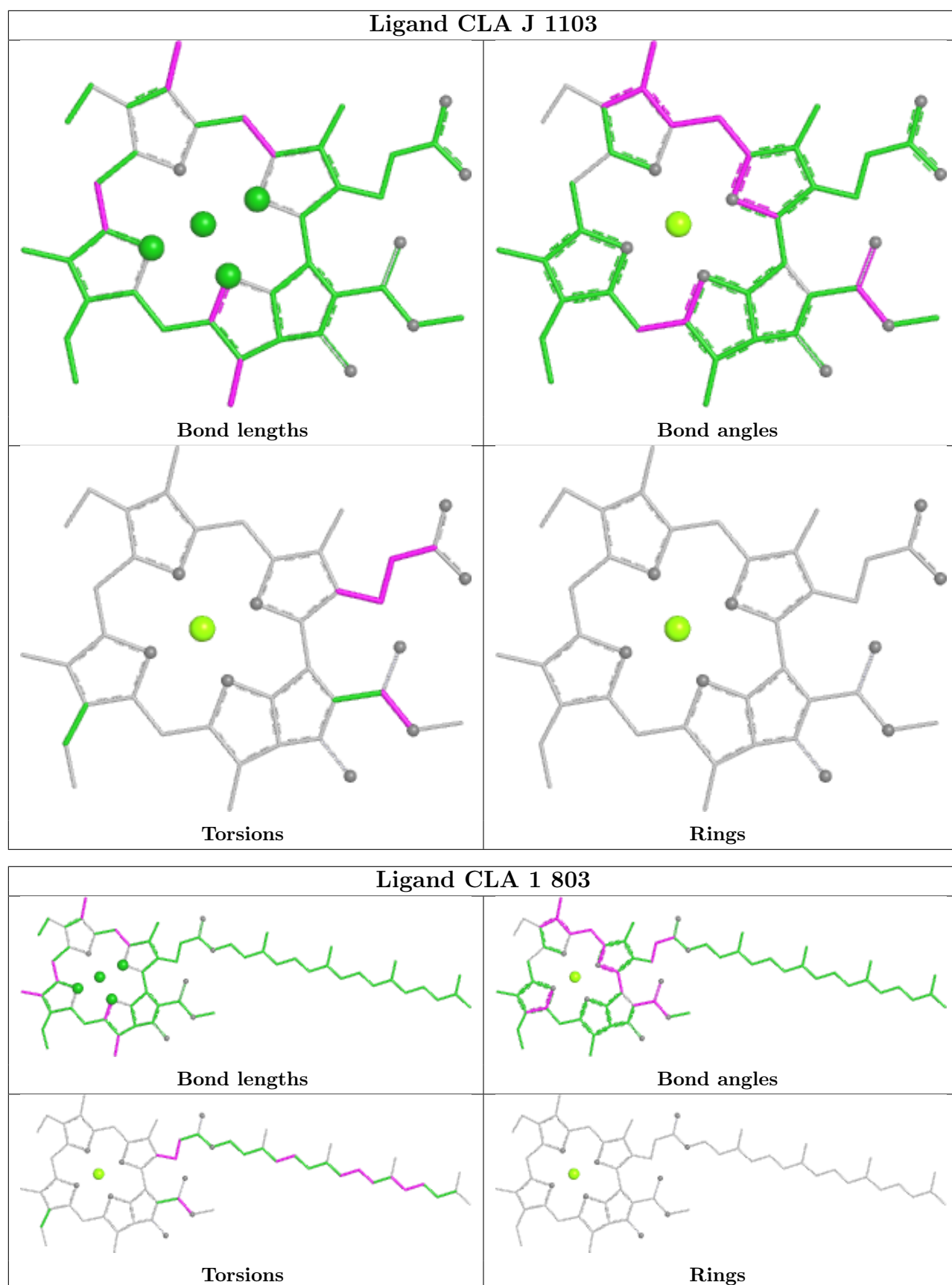


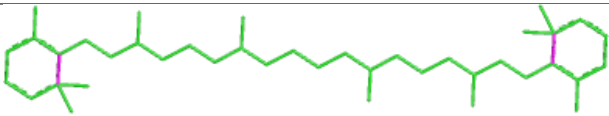
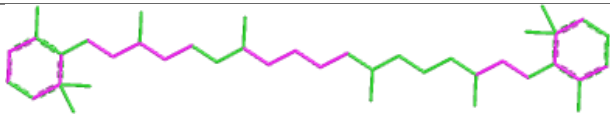
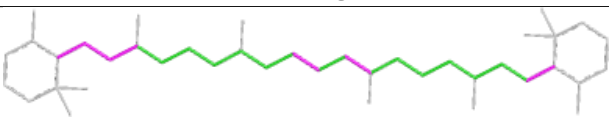
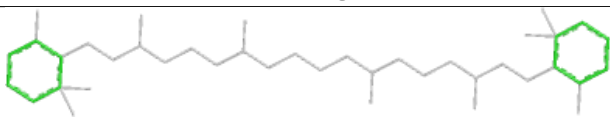
Torsions

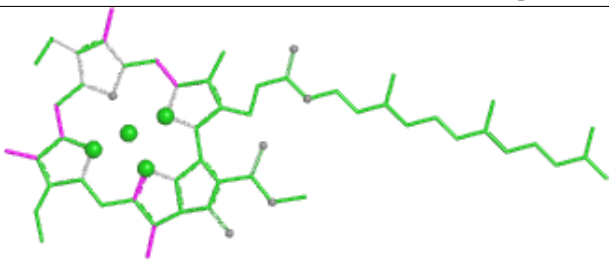
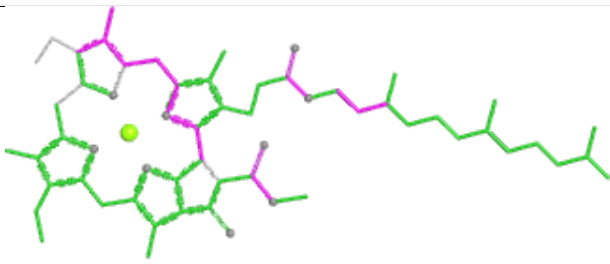
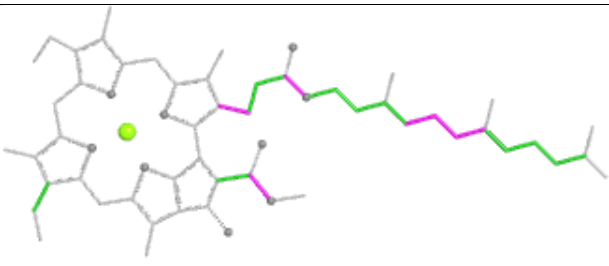
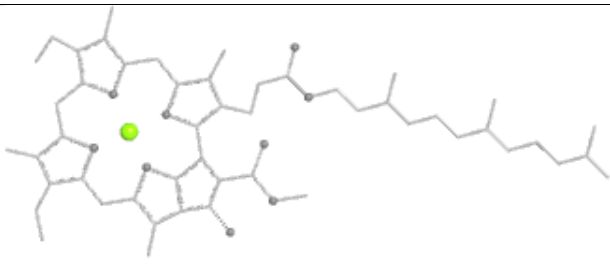


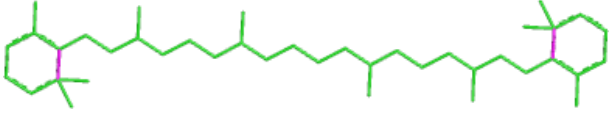
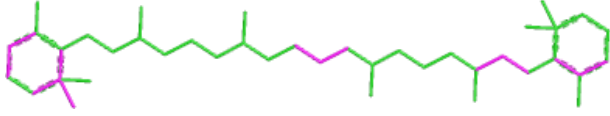
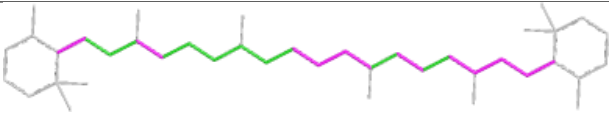
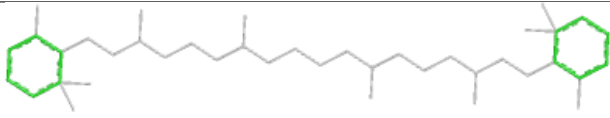
Rings



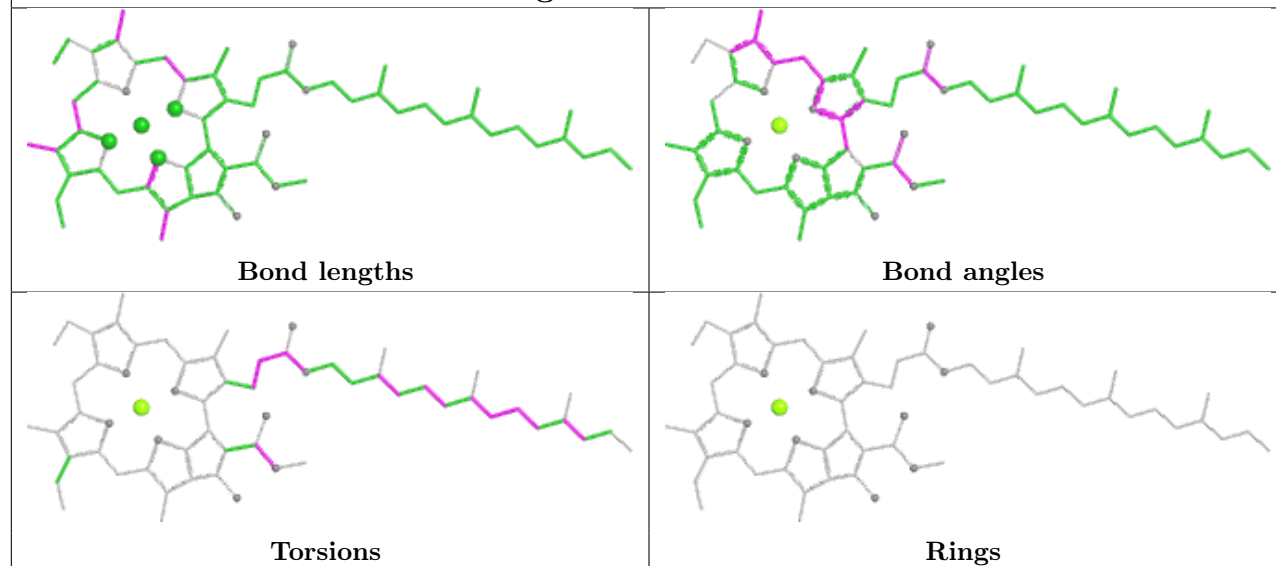


Ligand BCR J 1104	
	
Bond lengths	Bond angles
	
Torsions	Rings

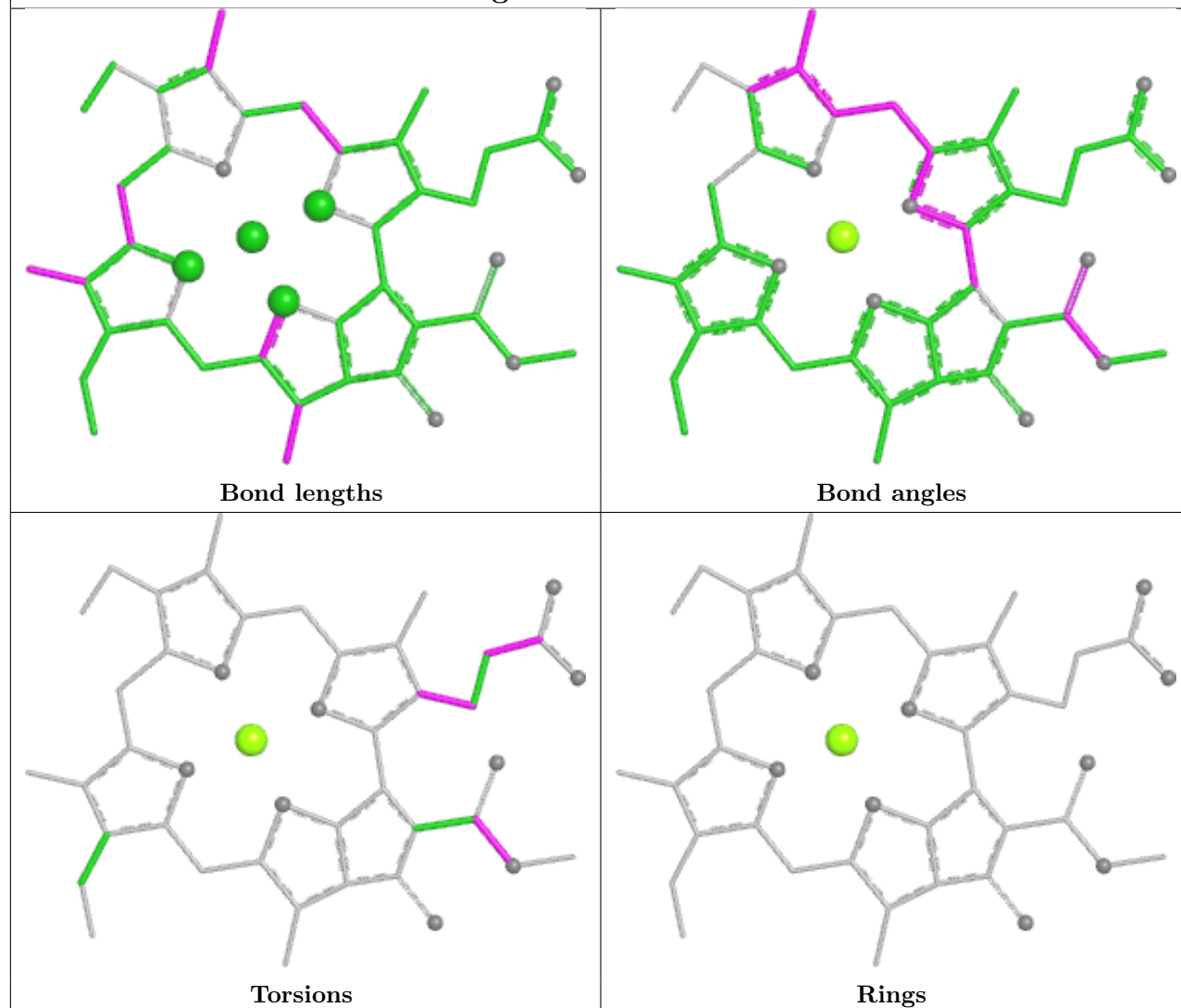
Ligand CLA 0 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

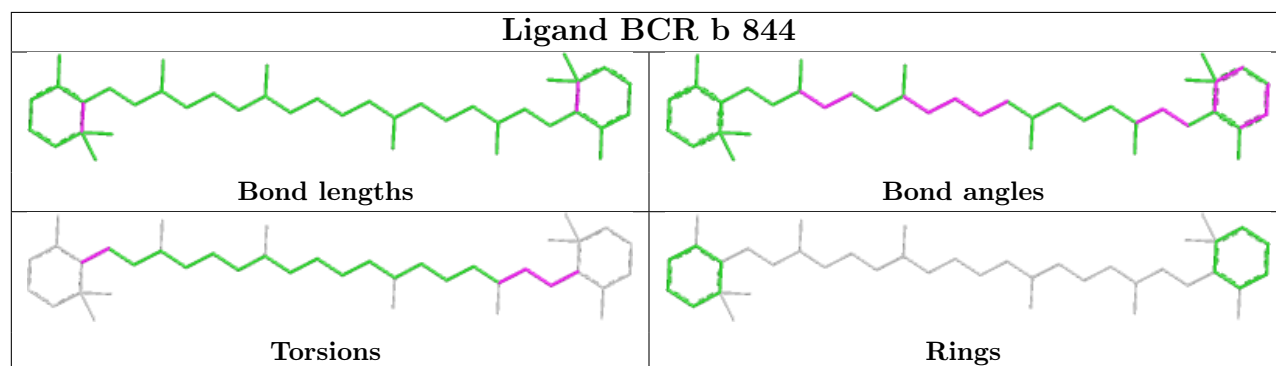
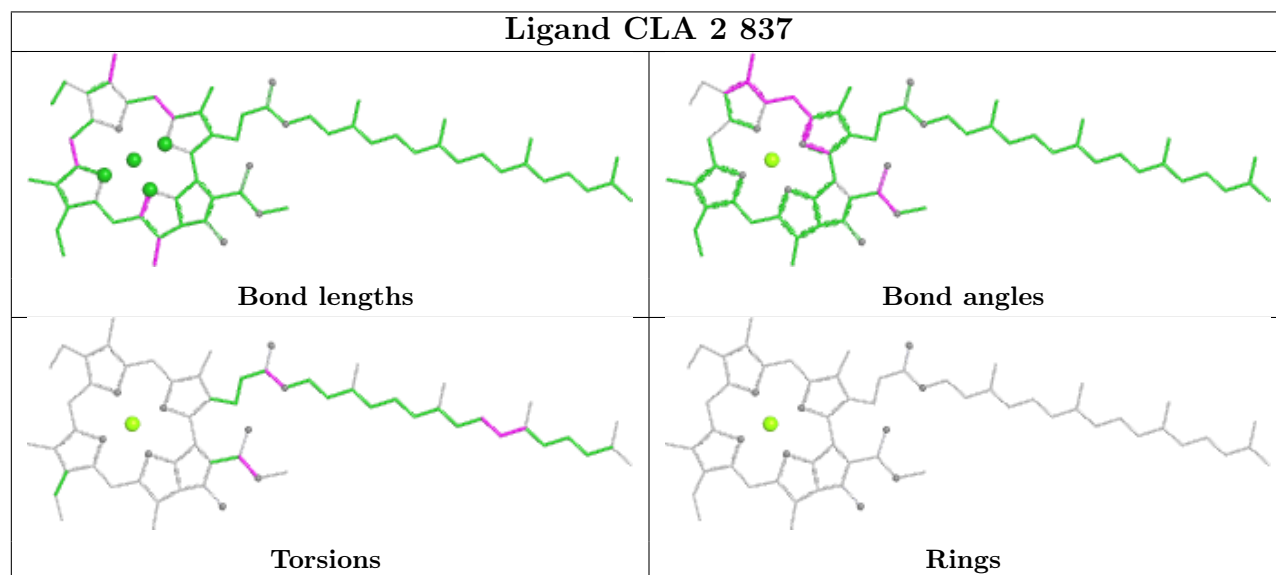
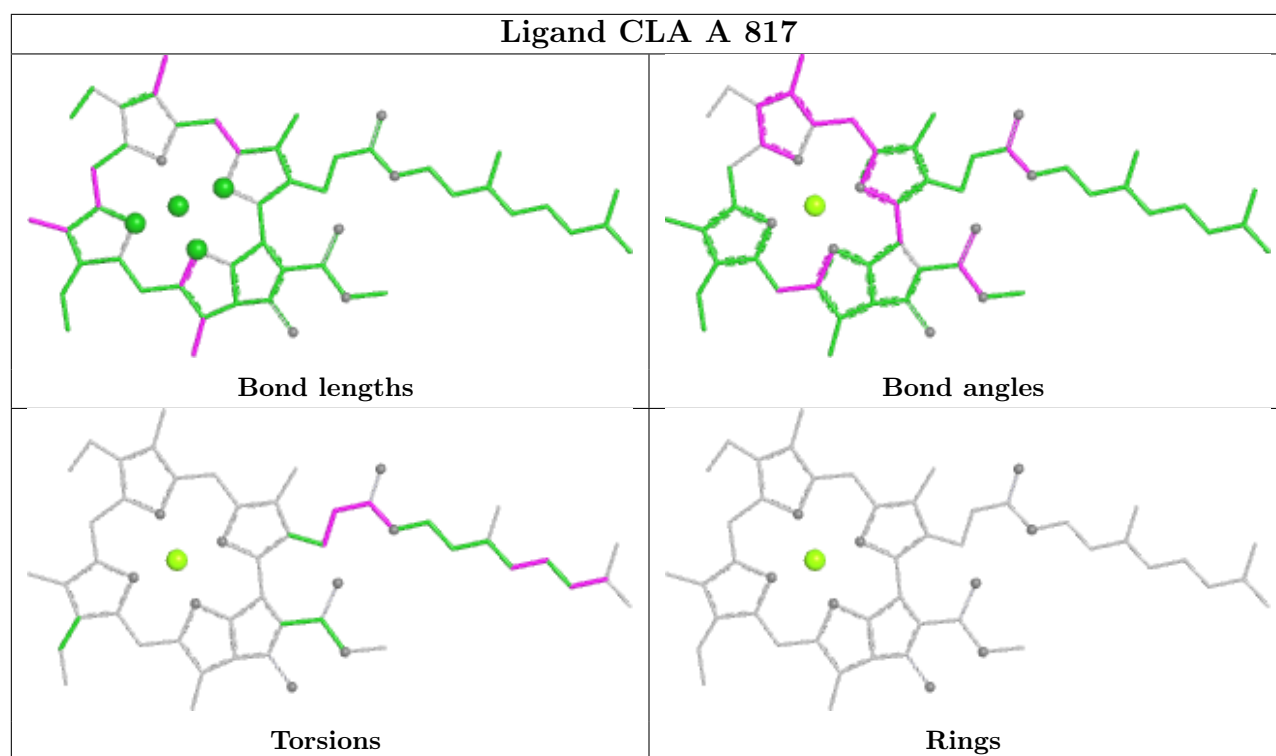
Ligand BCR 2 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

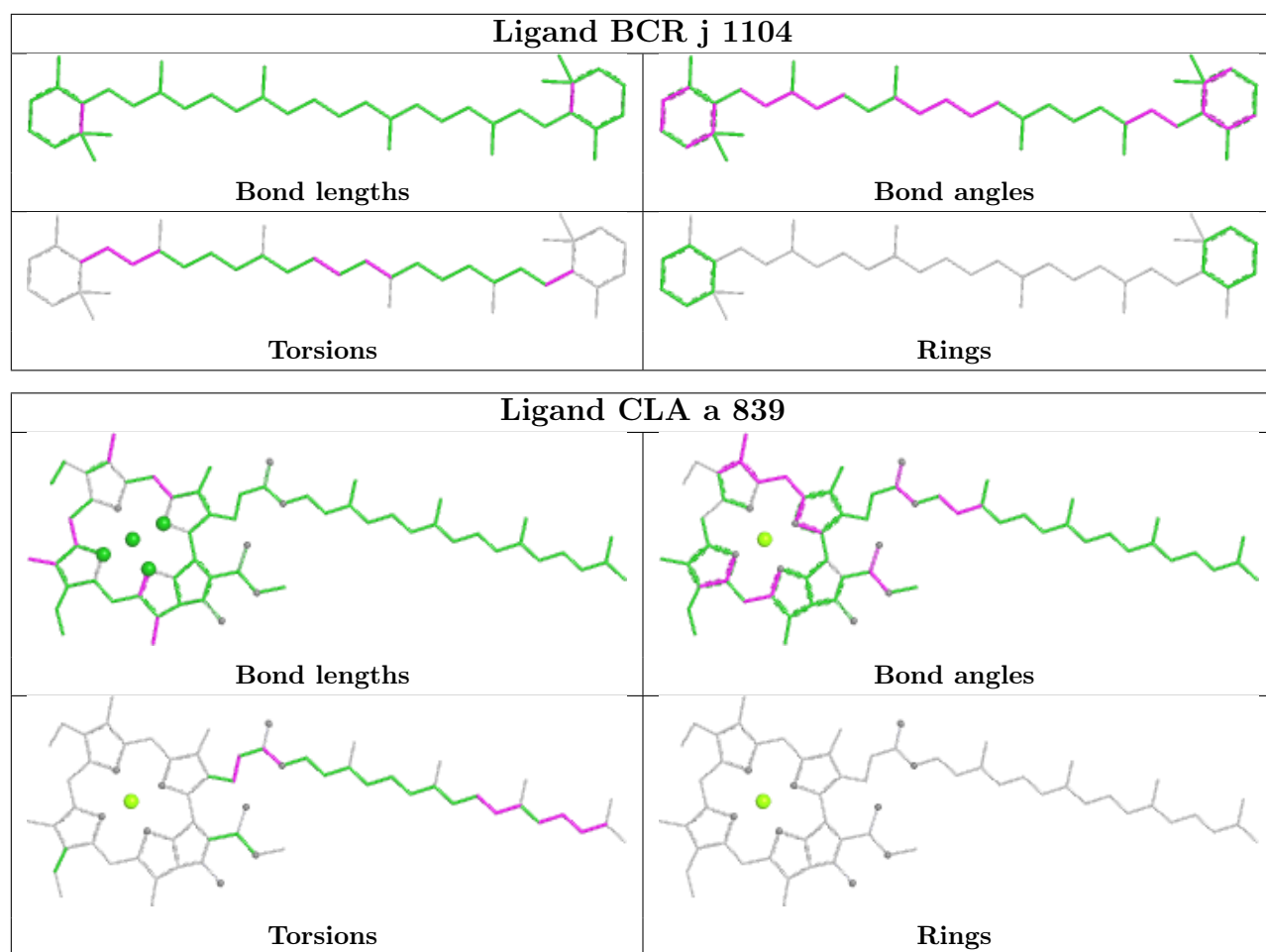
Ligand CLA 1 825



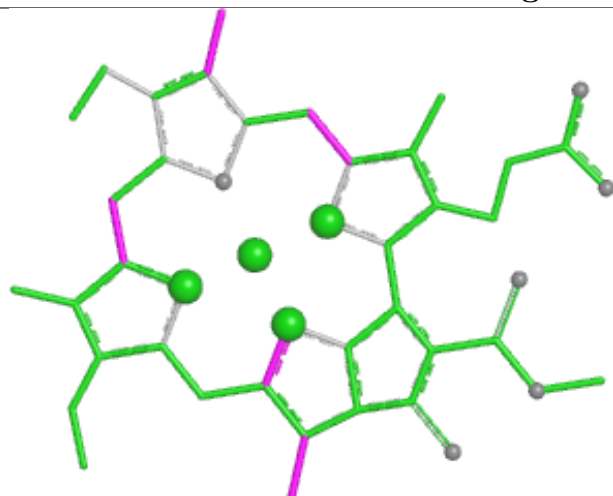
Ligand CLA A 842



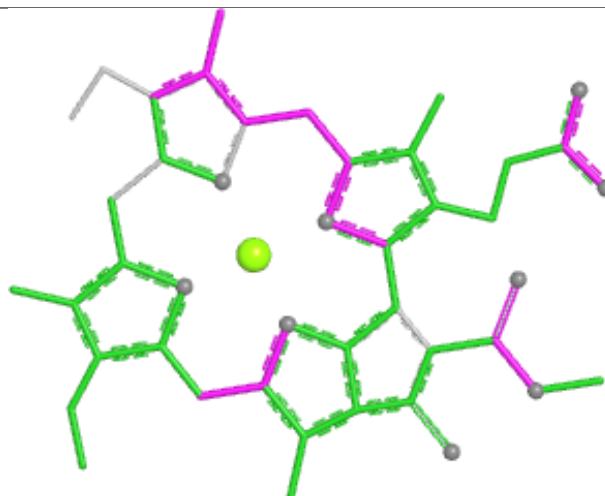




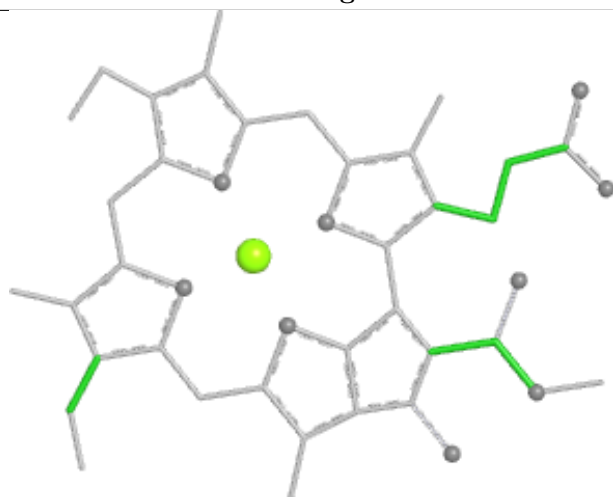
Ligand CLA f 203



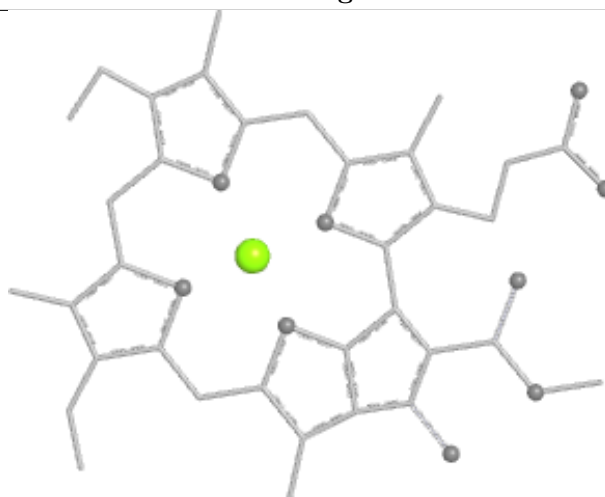
Bond lengths



Bond angles

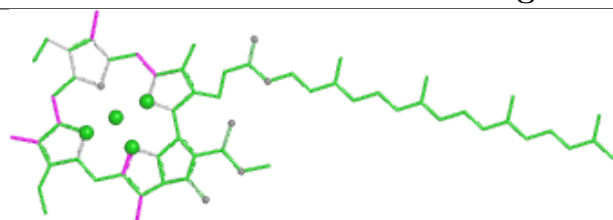


Torsions

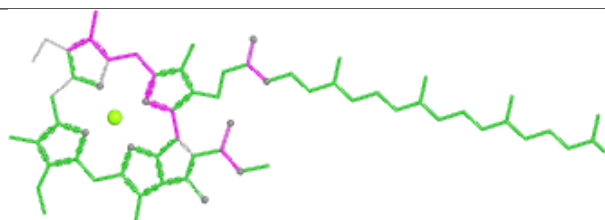


Rings

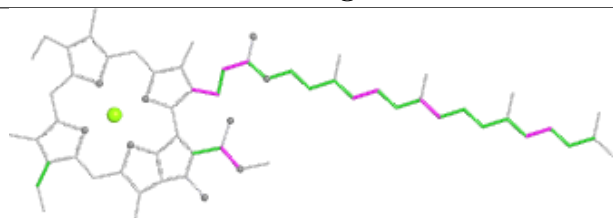
Ligand CLA b 847



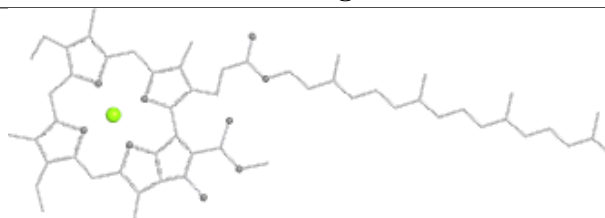
Bond lengths



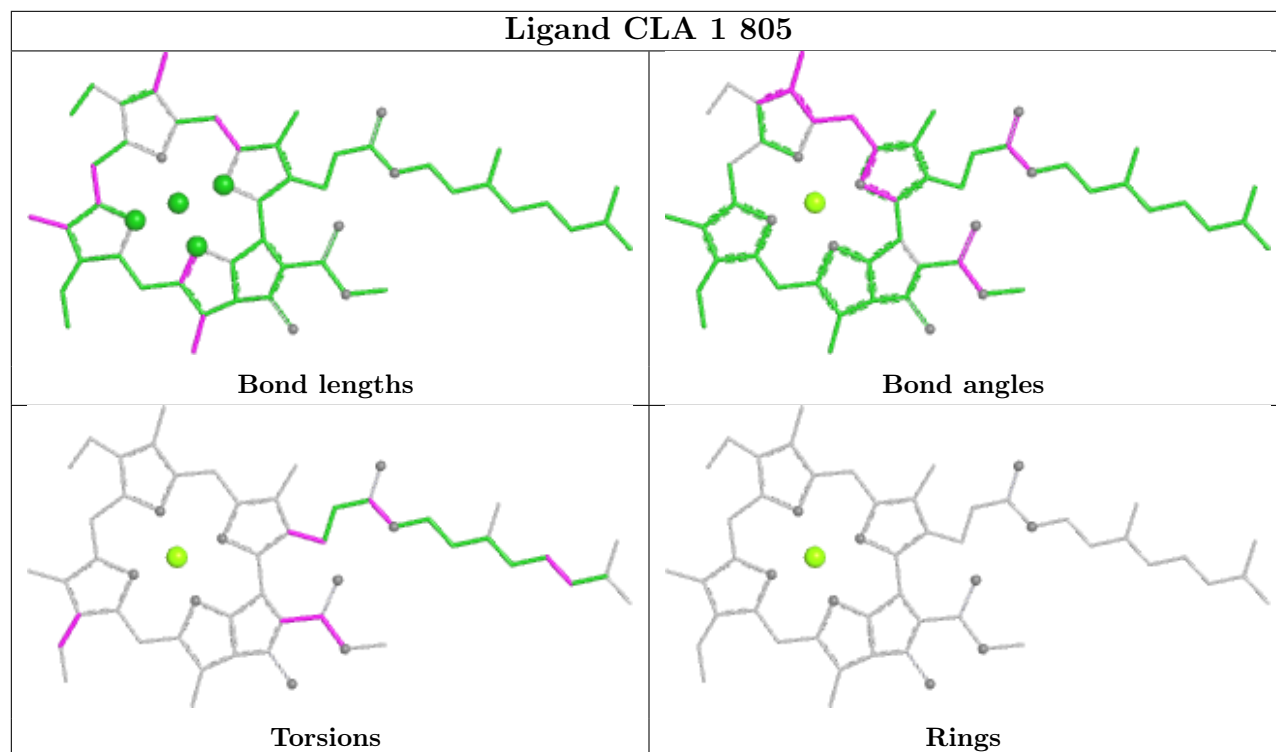
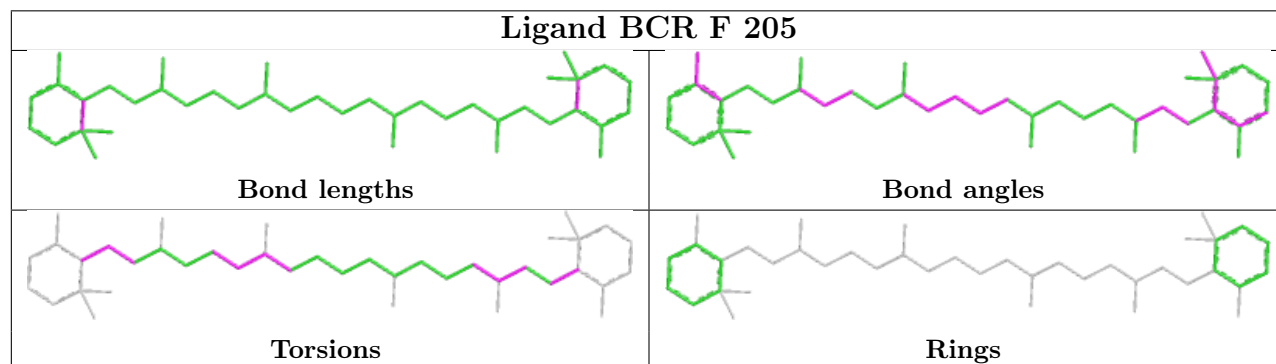
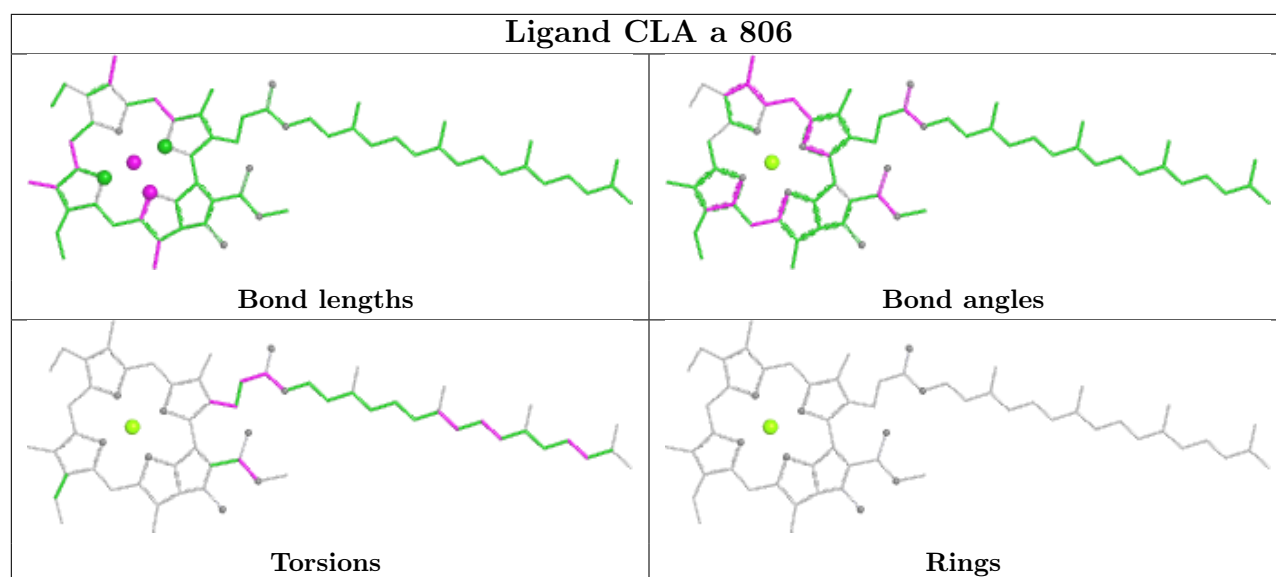
Bond angles

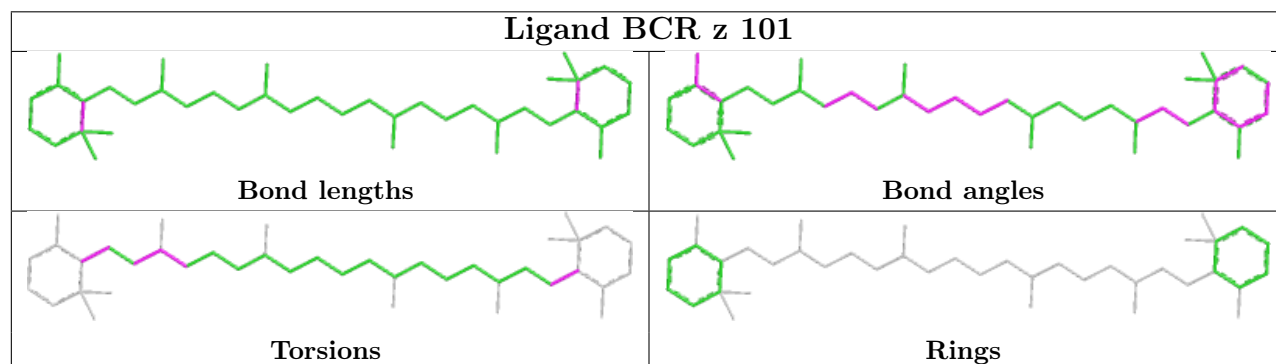
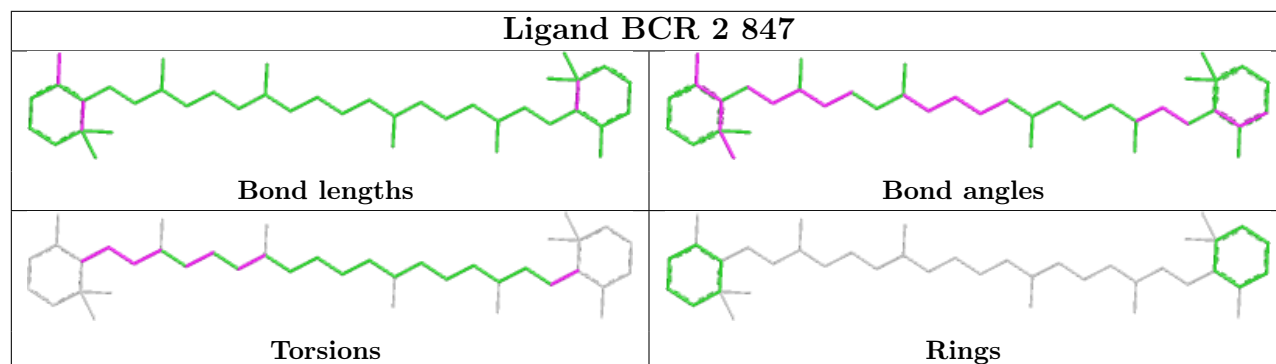
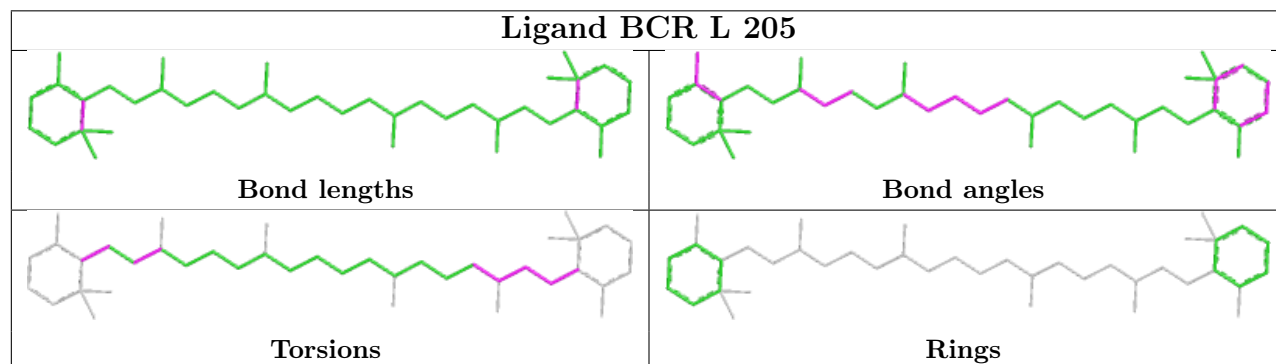
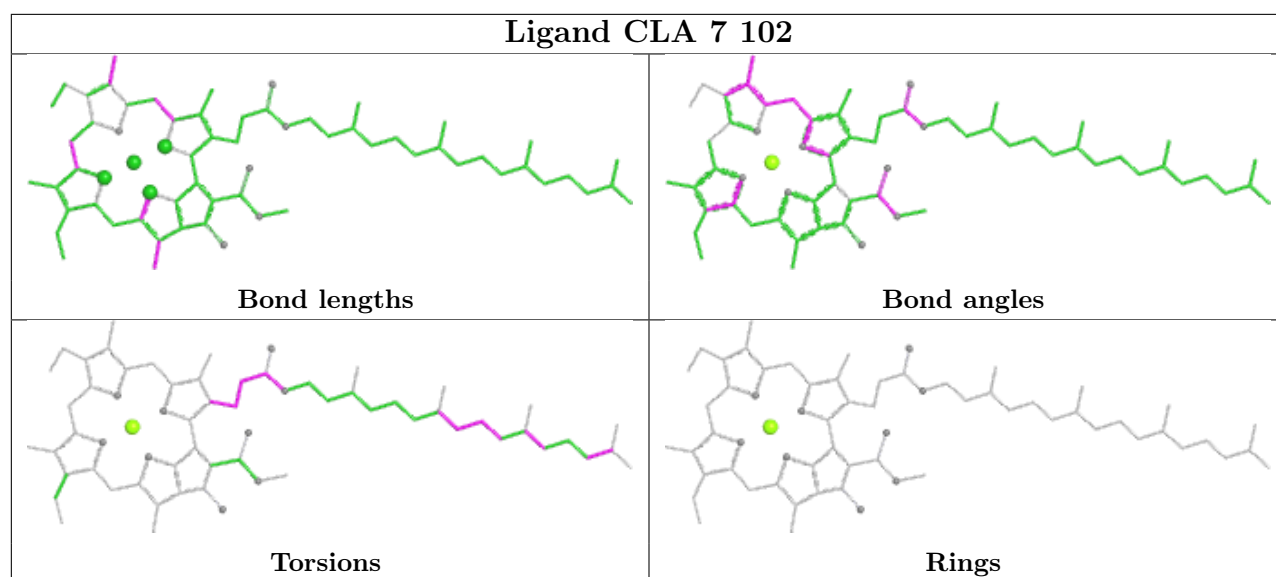


Torsions

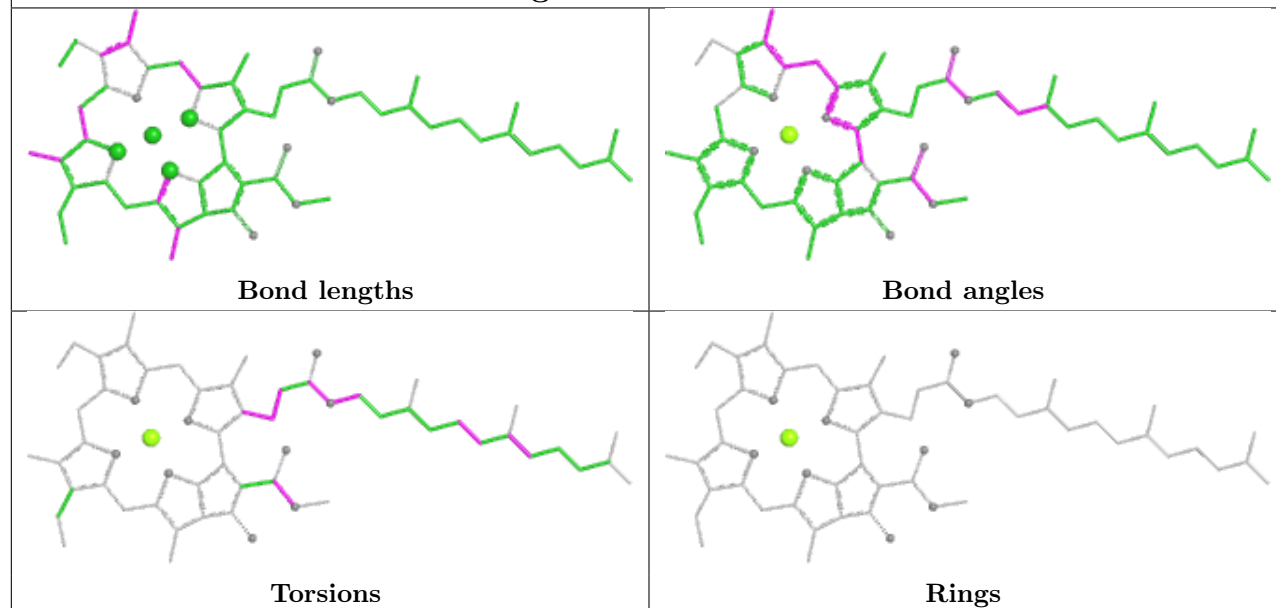


Rings

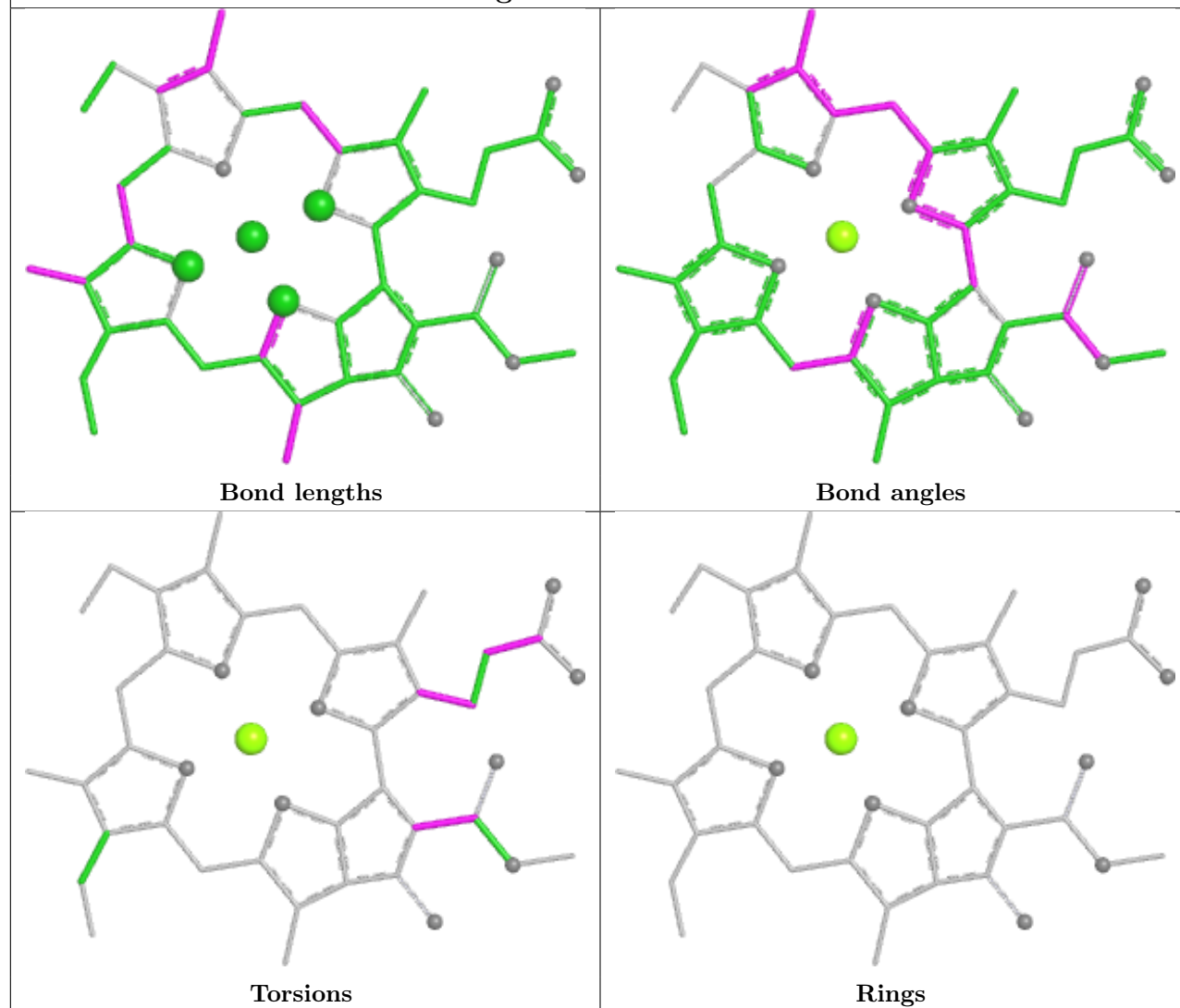




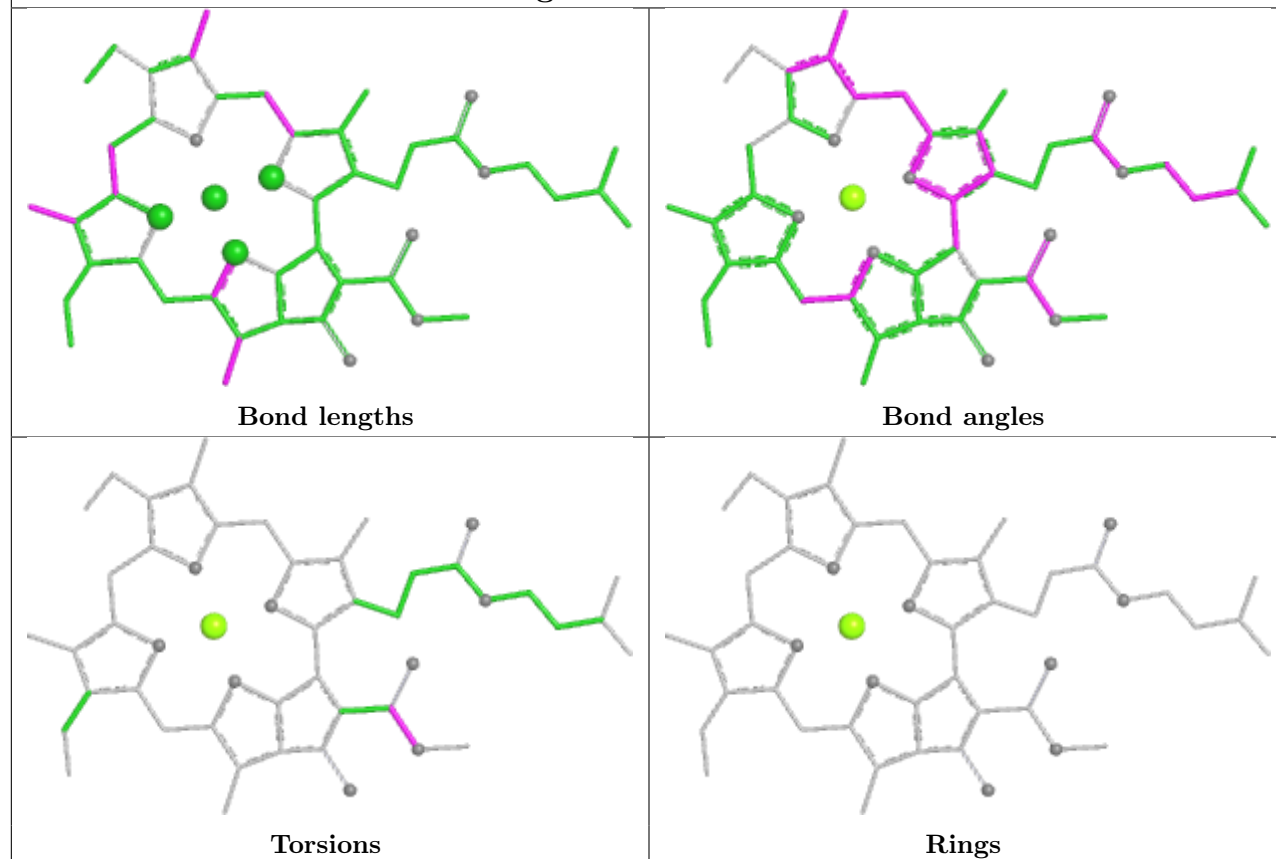
Ligand CLA A 841



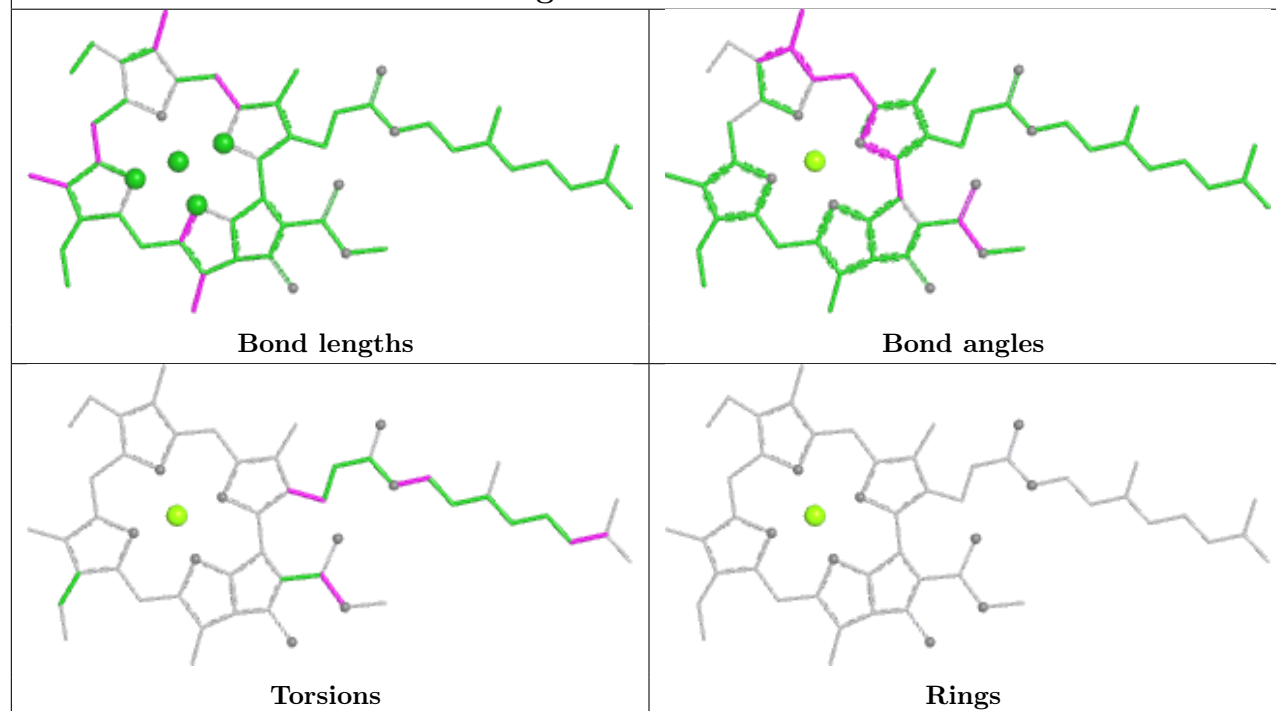
Ligand CLA 2 826

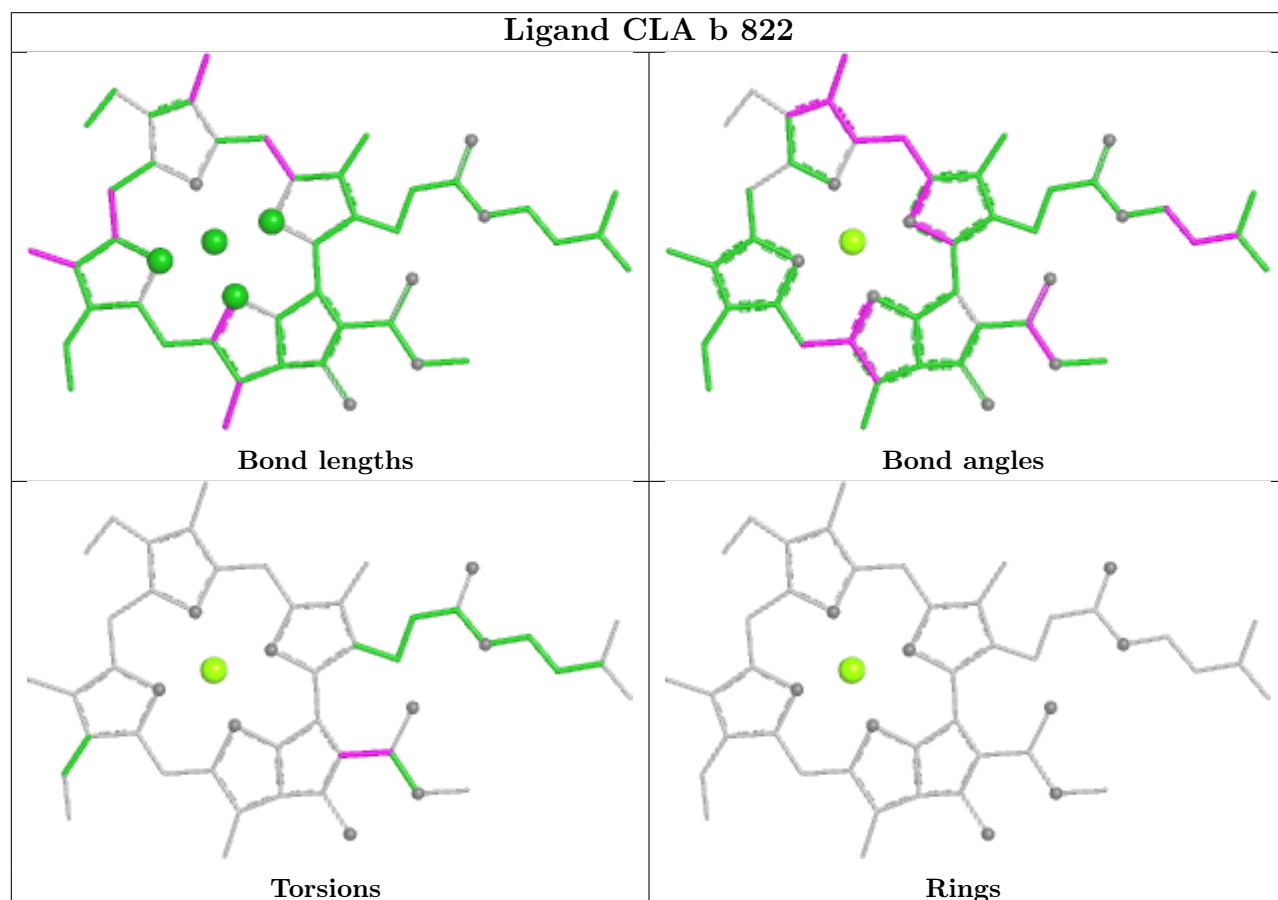
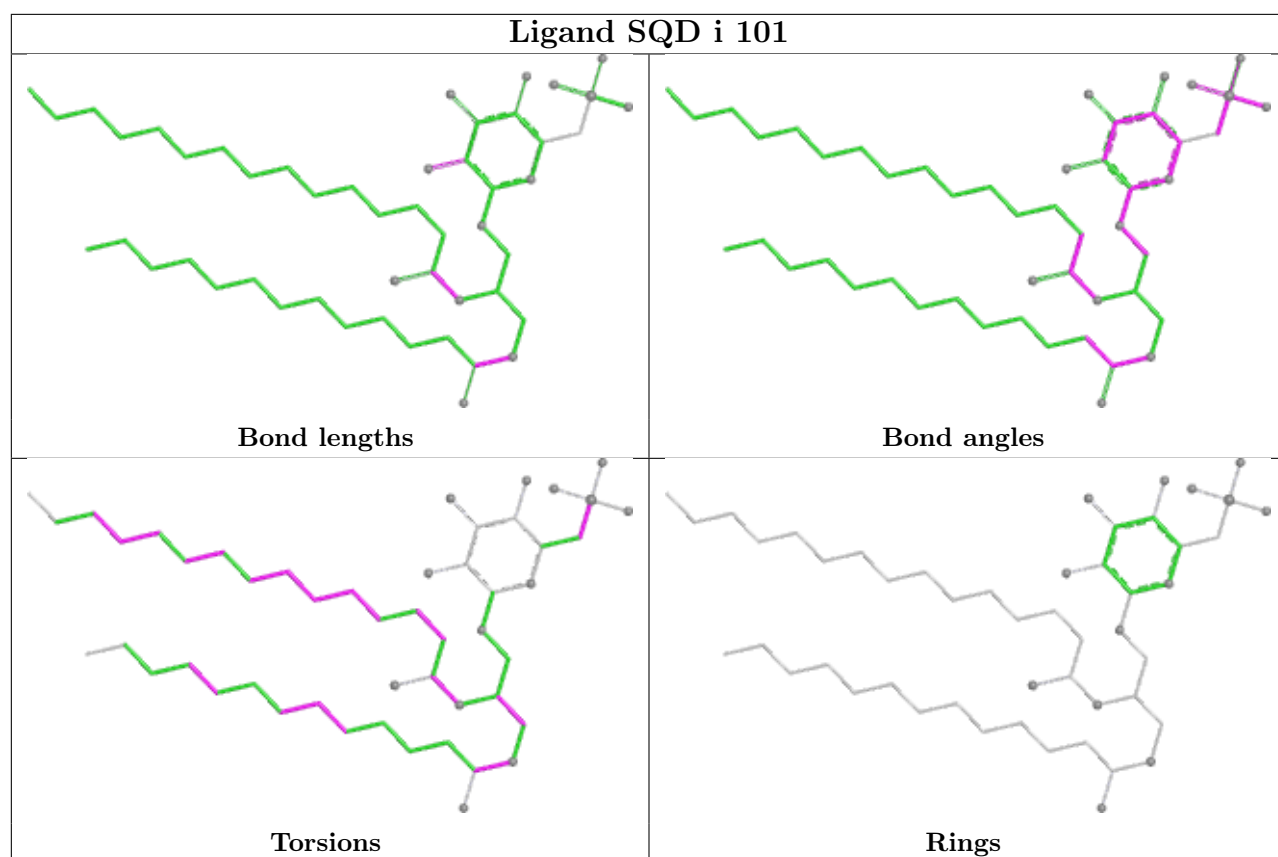


Ligand CLA a 814

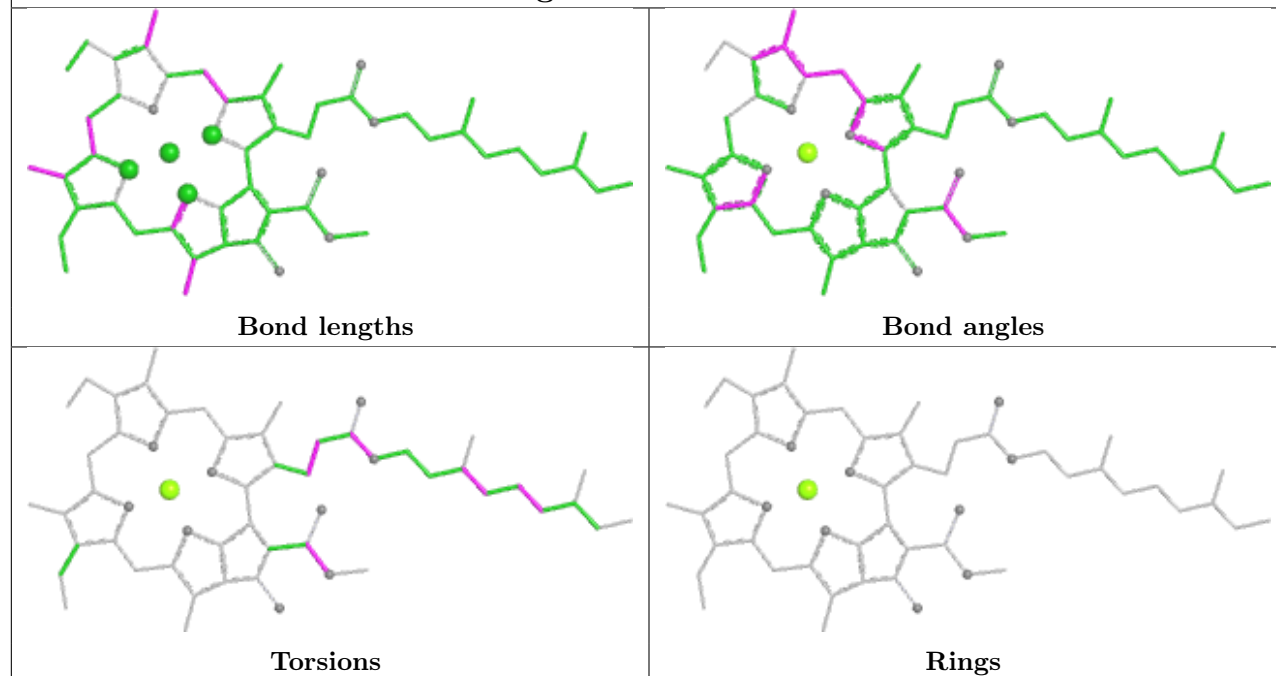


Ligand CLA 2 819

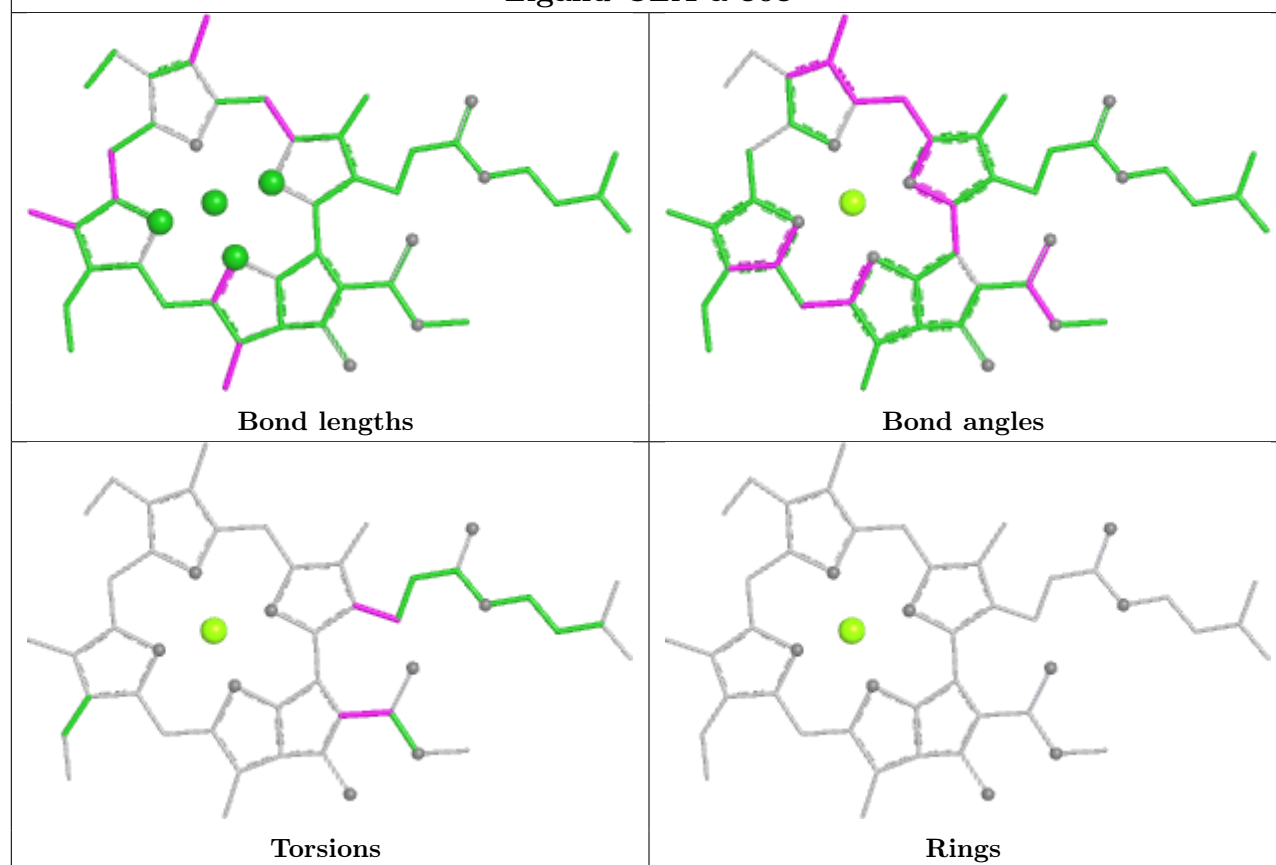


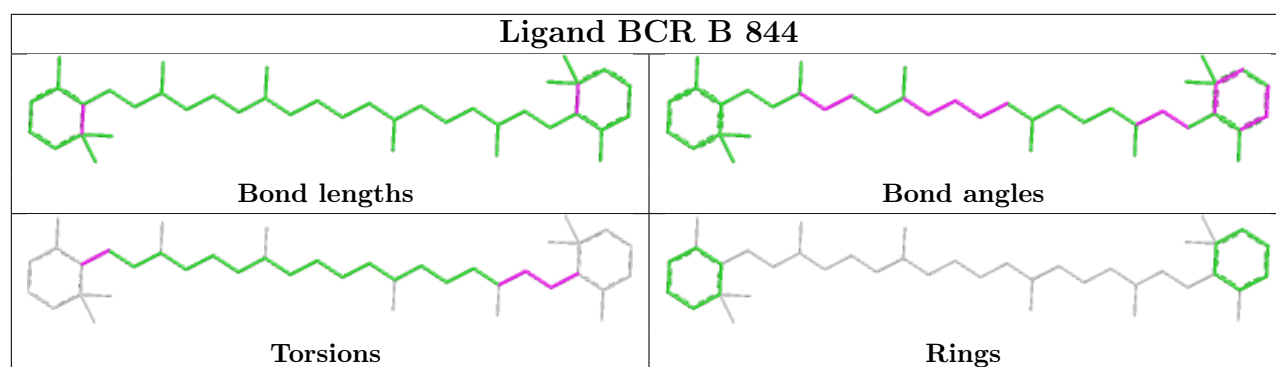
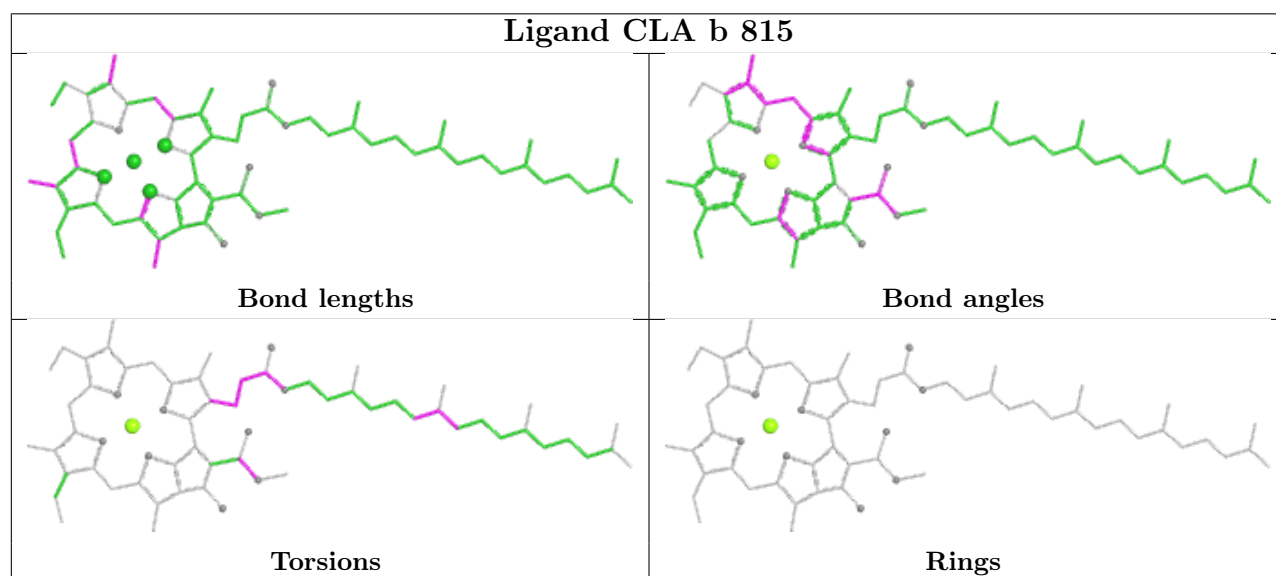
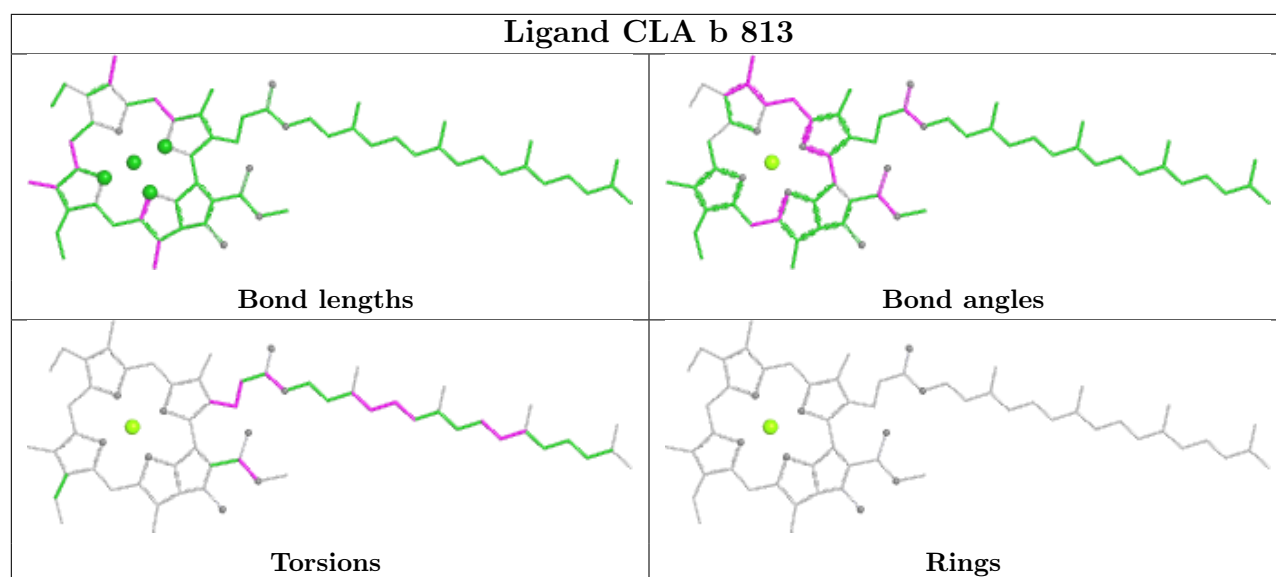


Ligand CLA 1 811

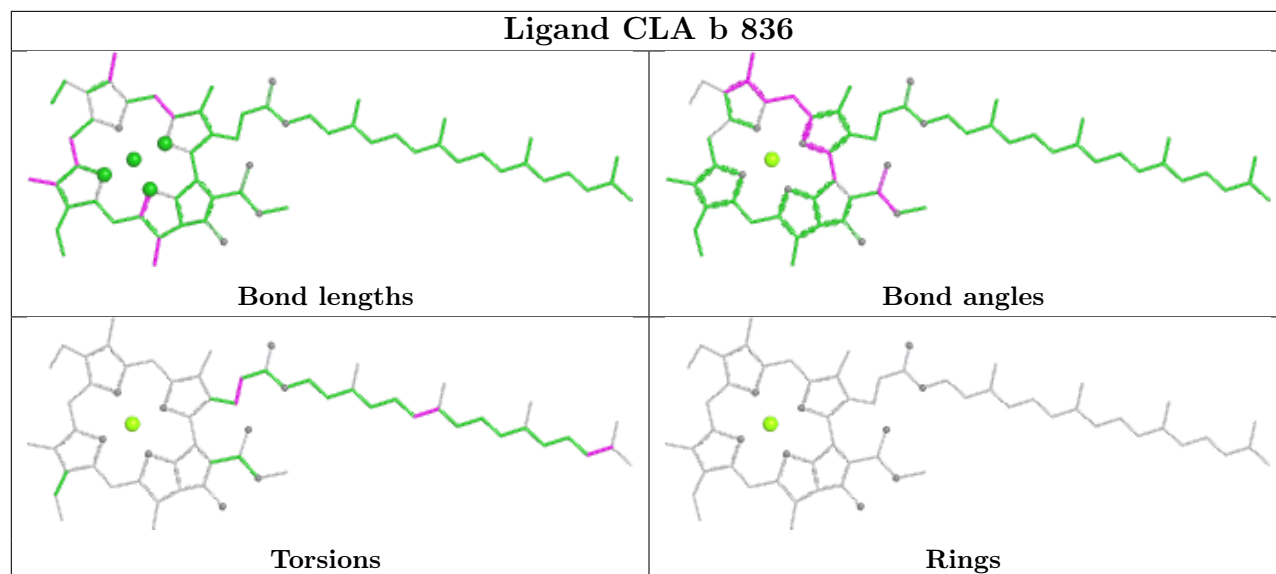


Ligand CLA a 808

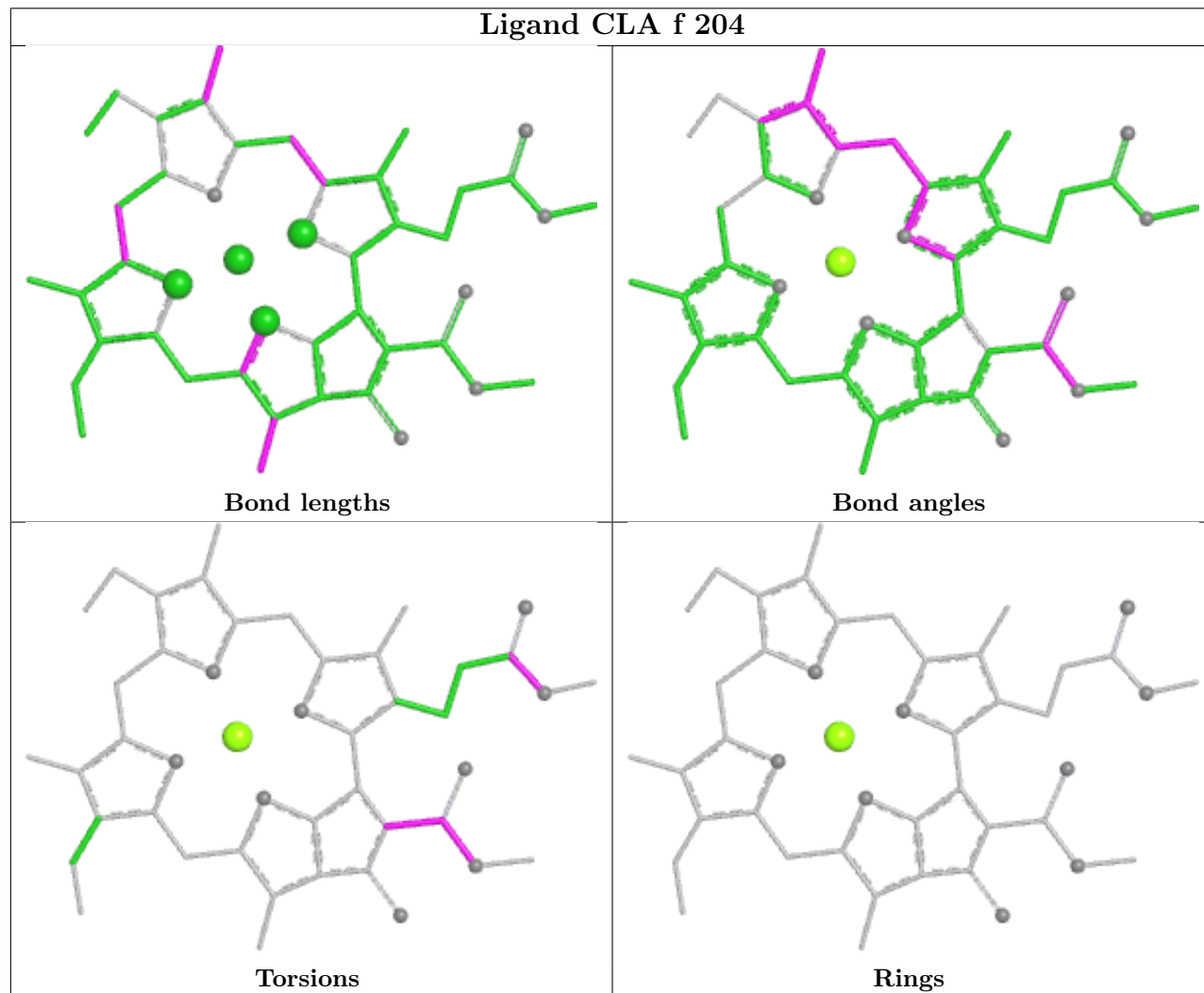


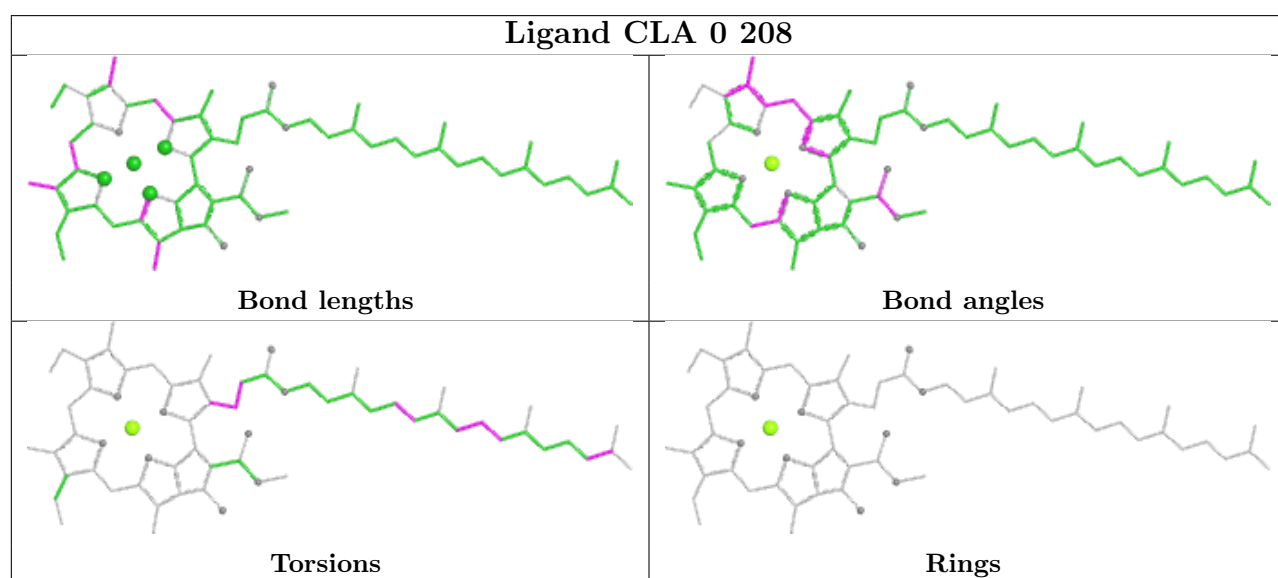
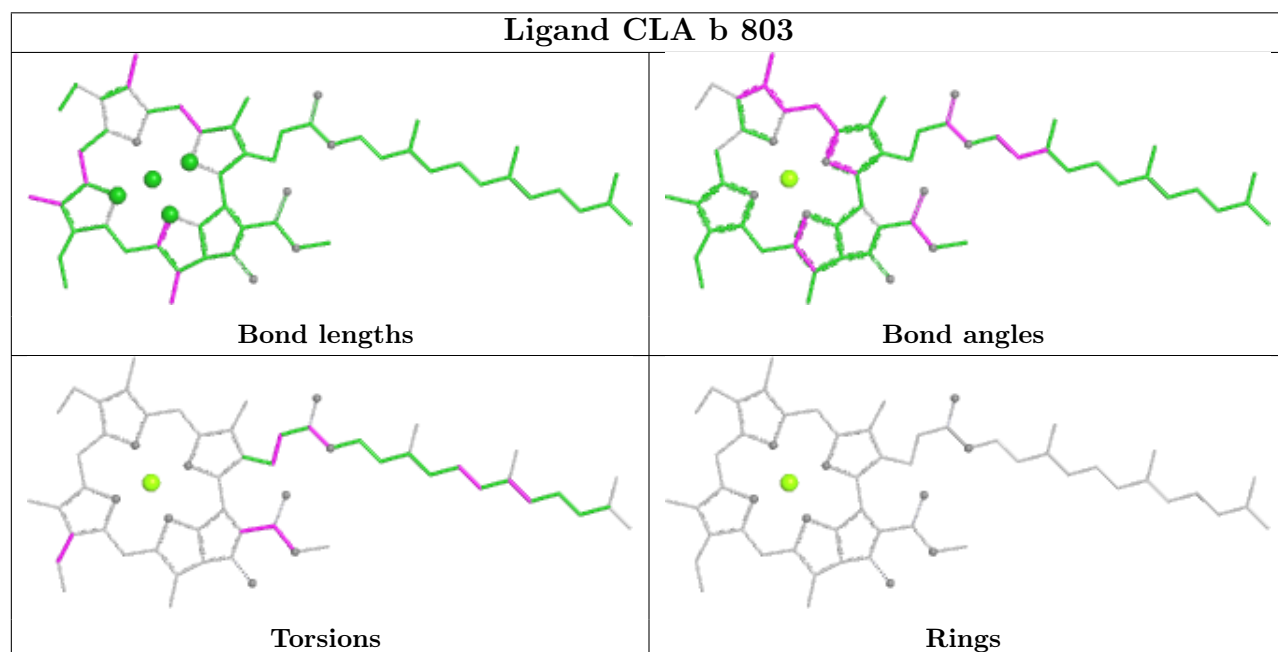
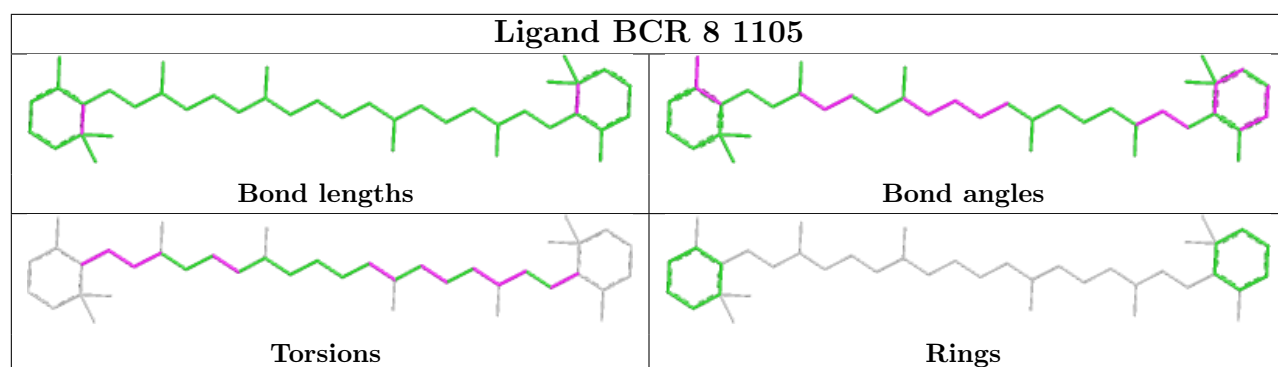


Ligand CLA b 836

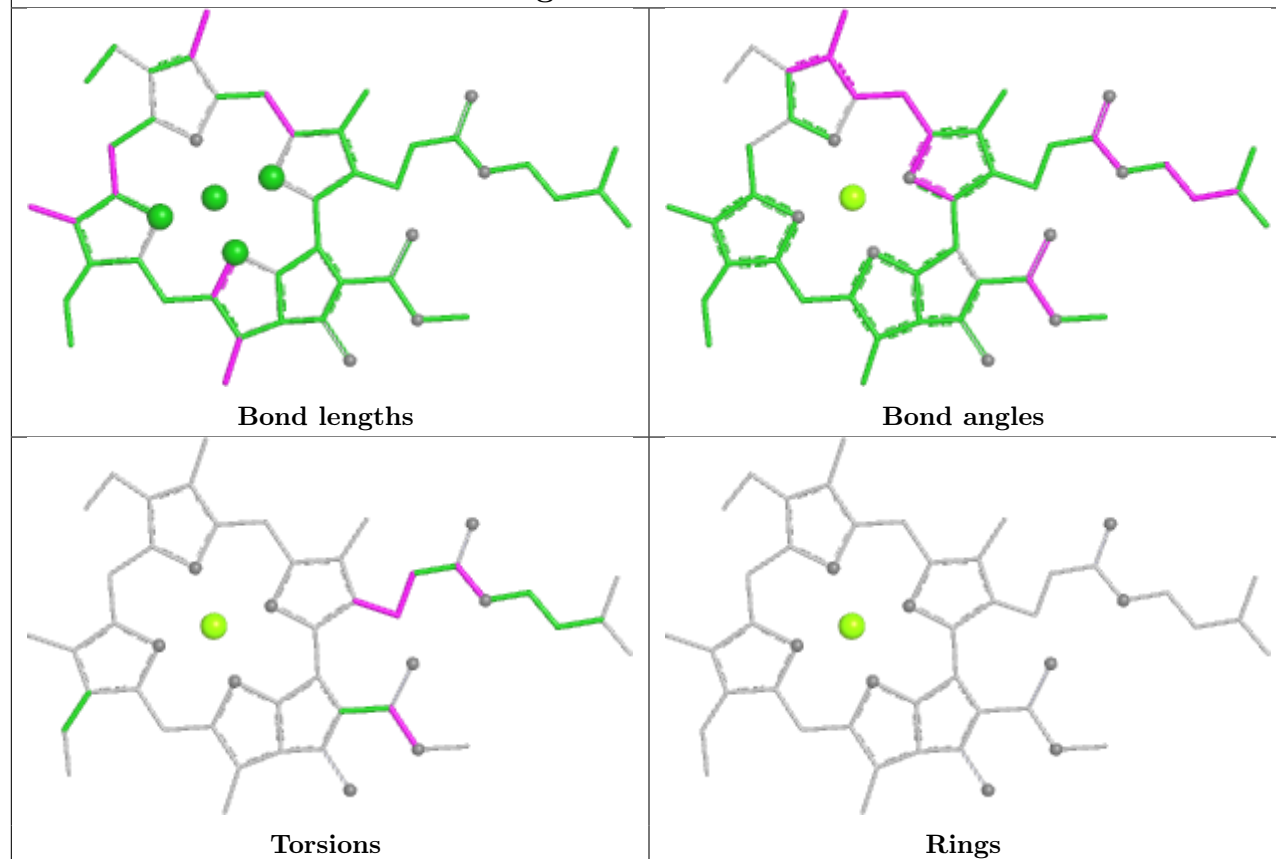


Ligand CLA f 204

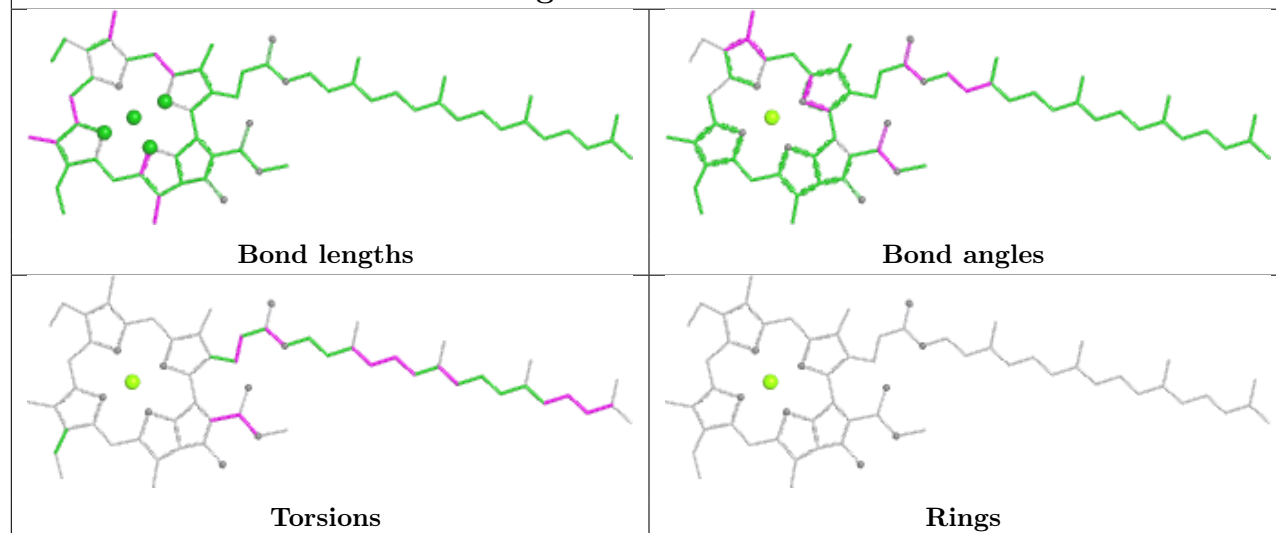


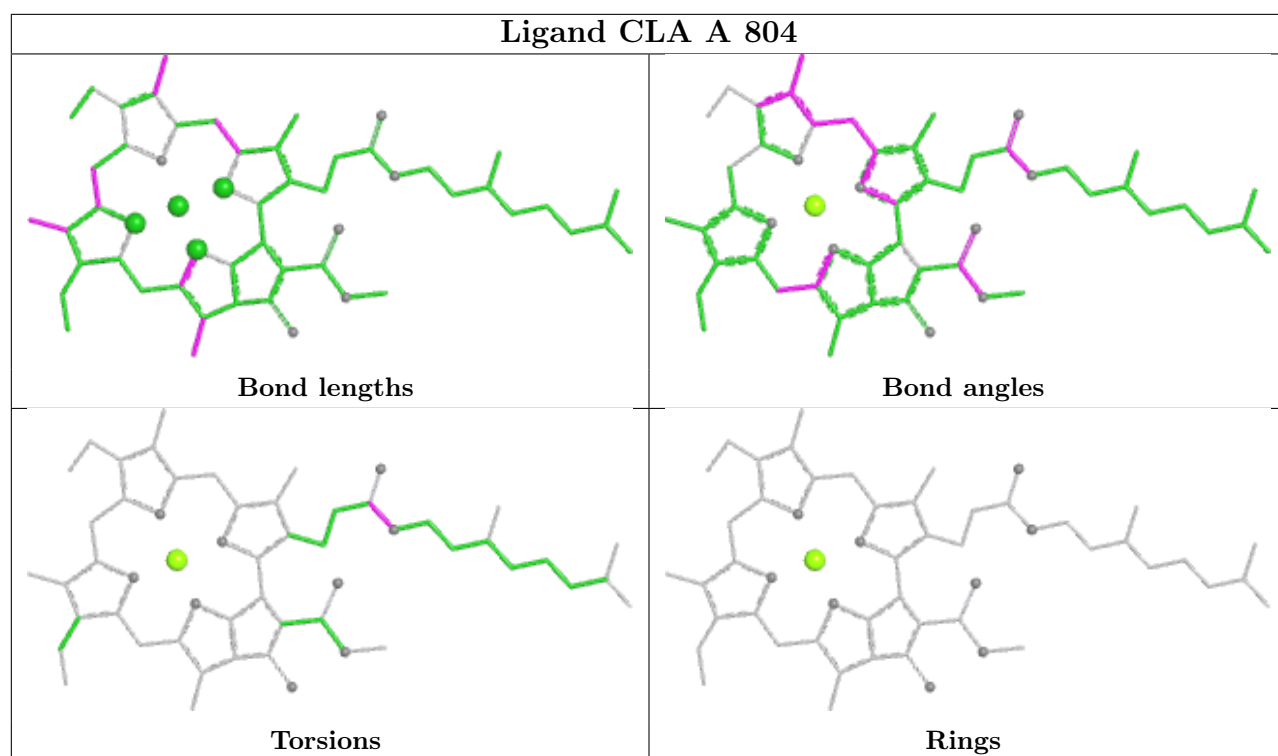


Ligand CLA 1 809

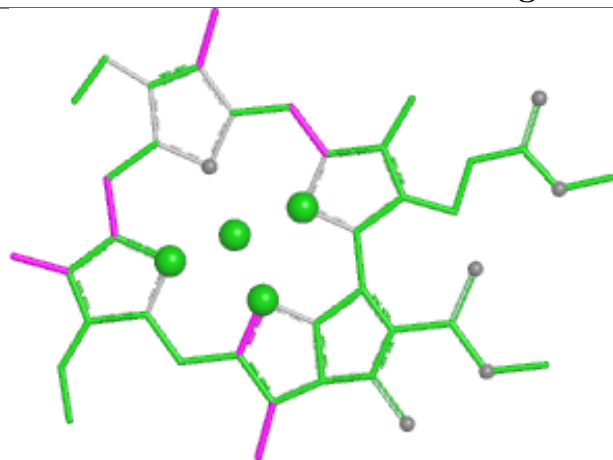


Ligand CLA 2 806

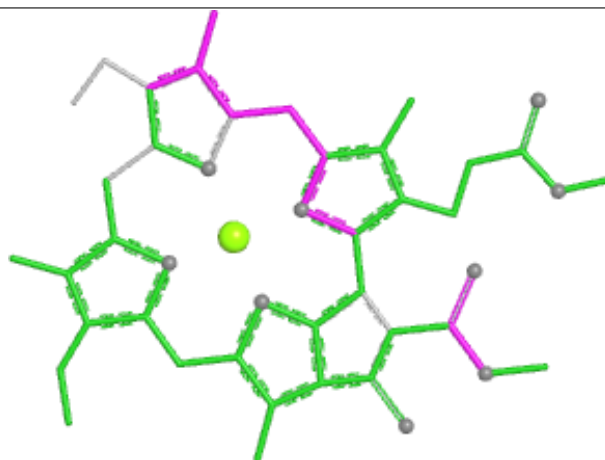




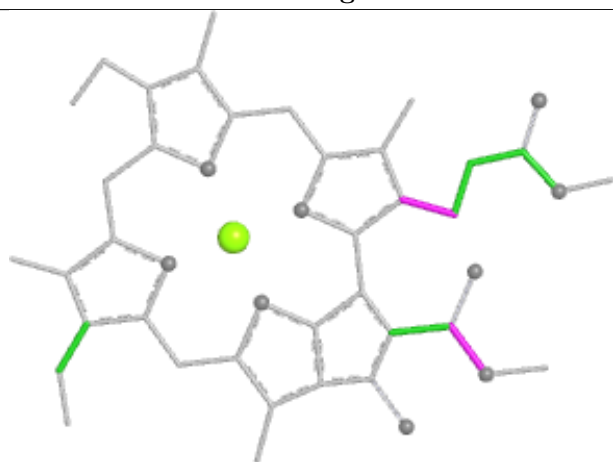
Ligand CLA 0 206



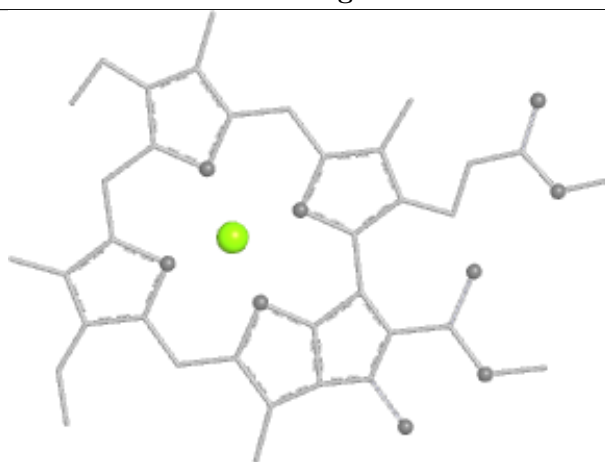
Bond lengths



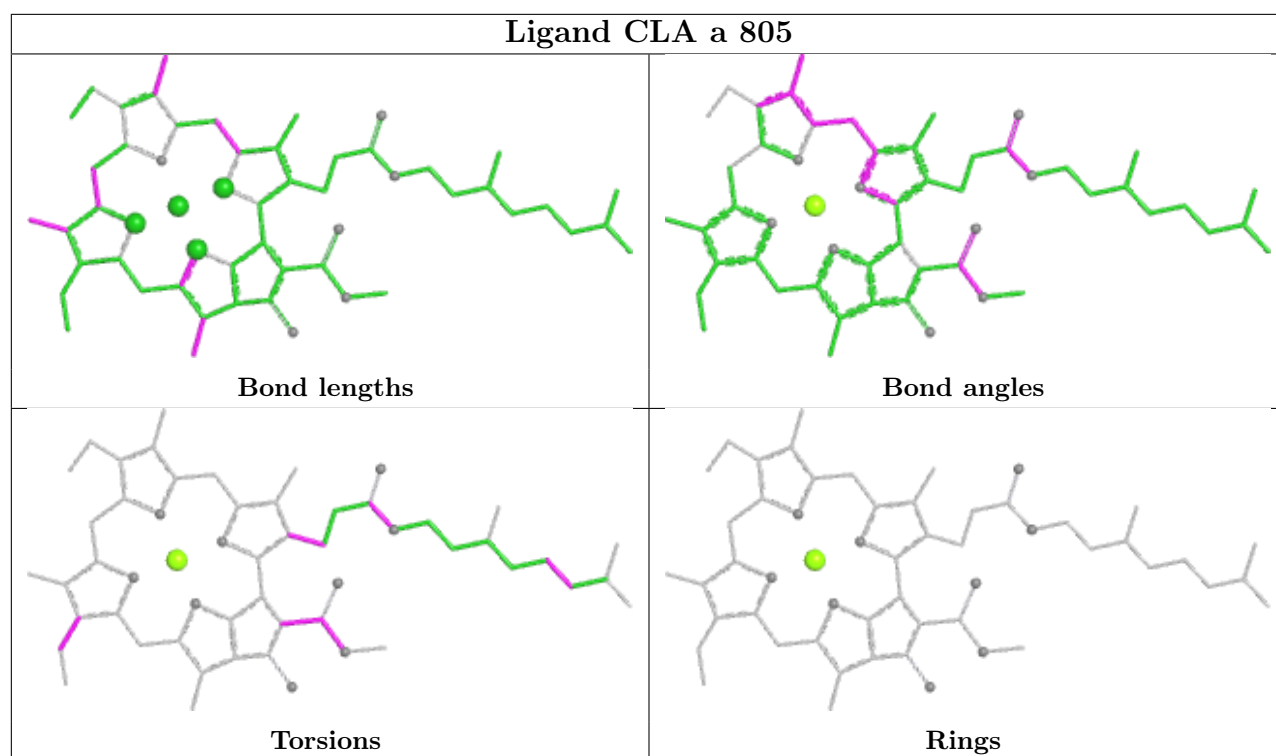
Bond angles

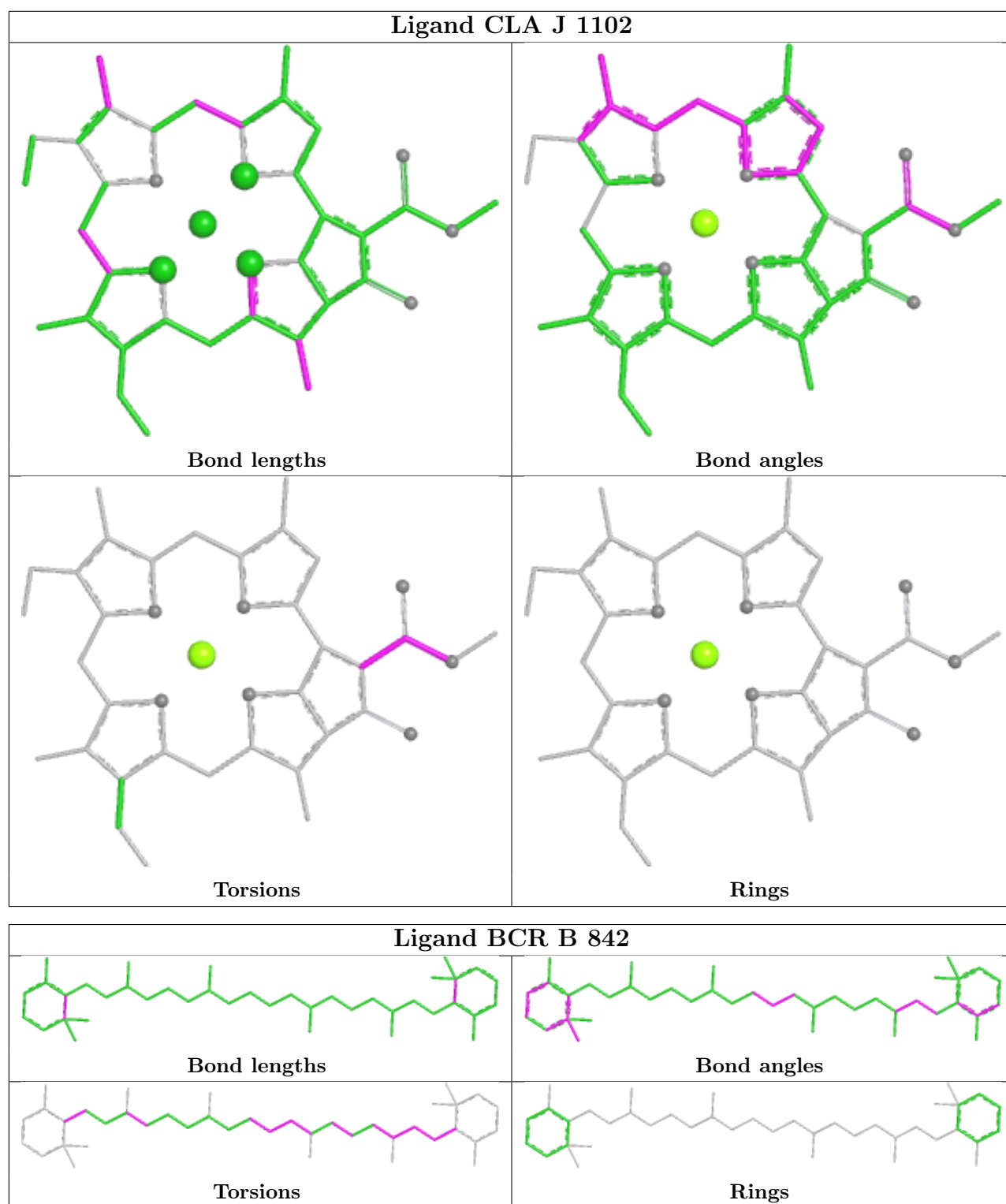


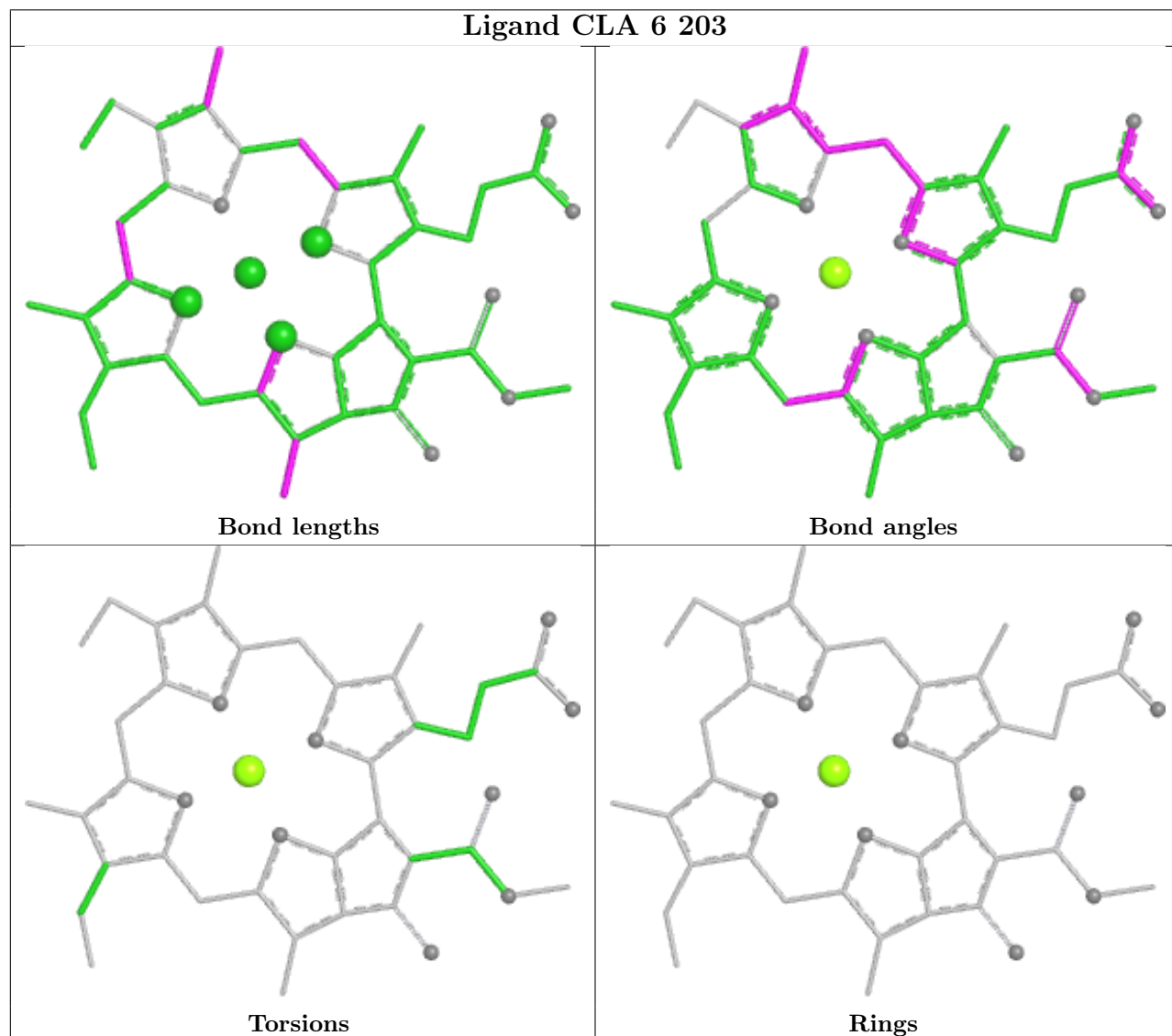
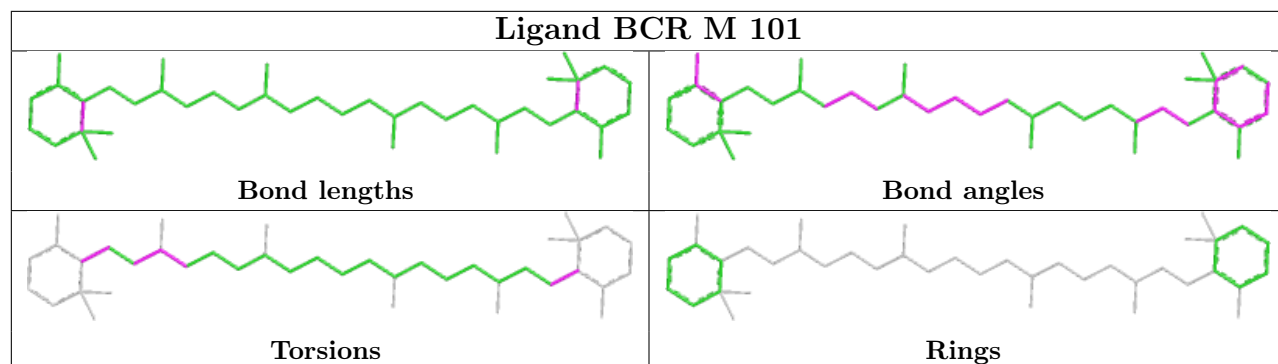
Torsions



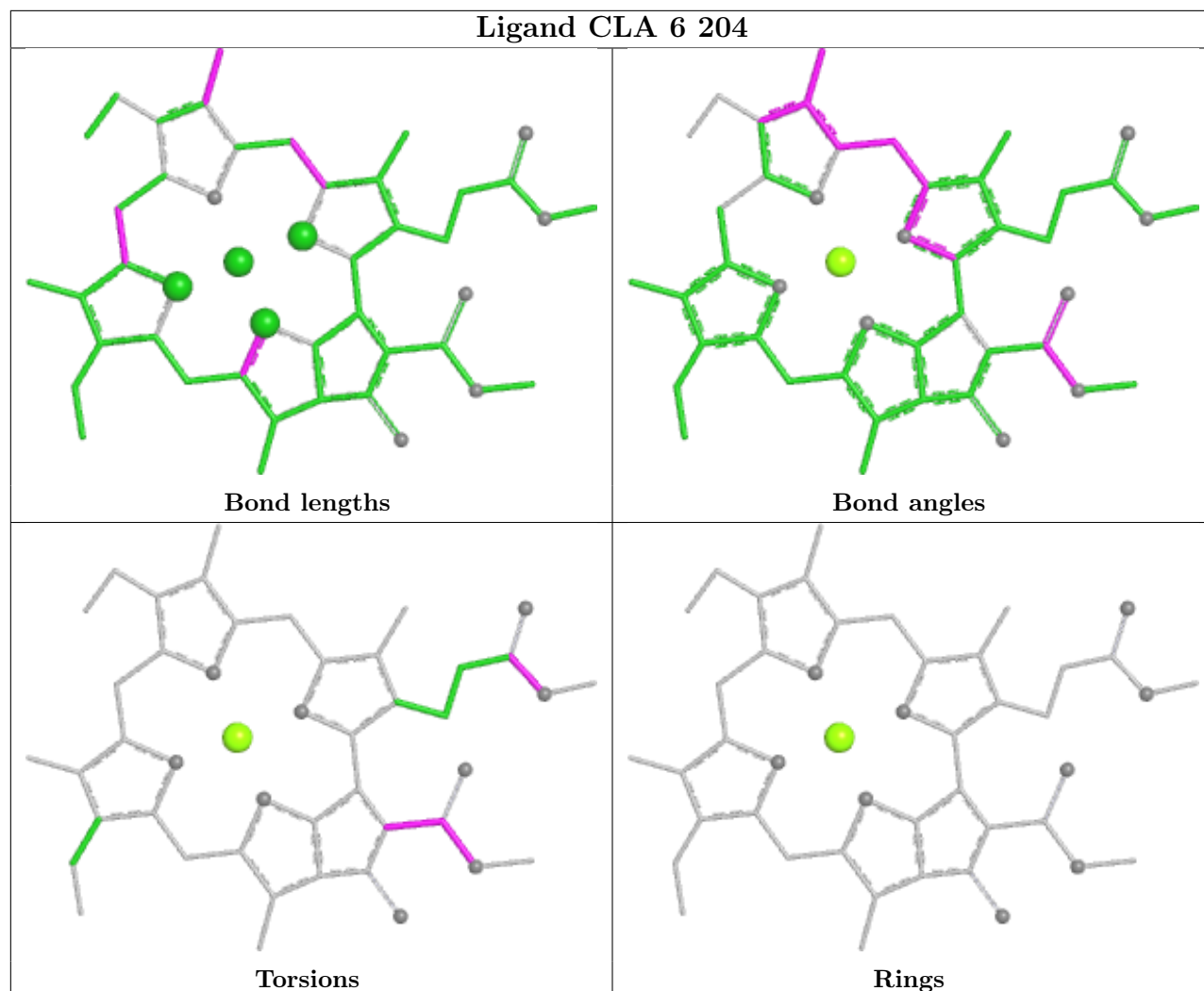
Rings



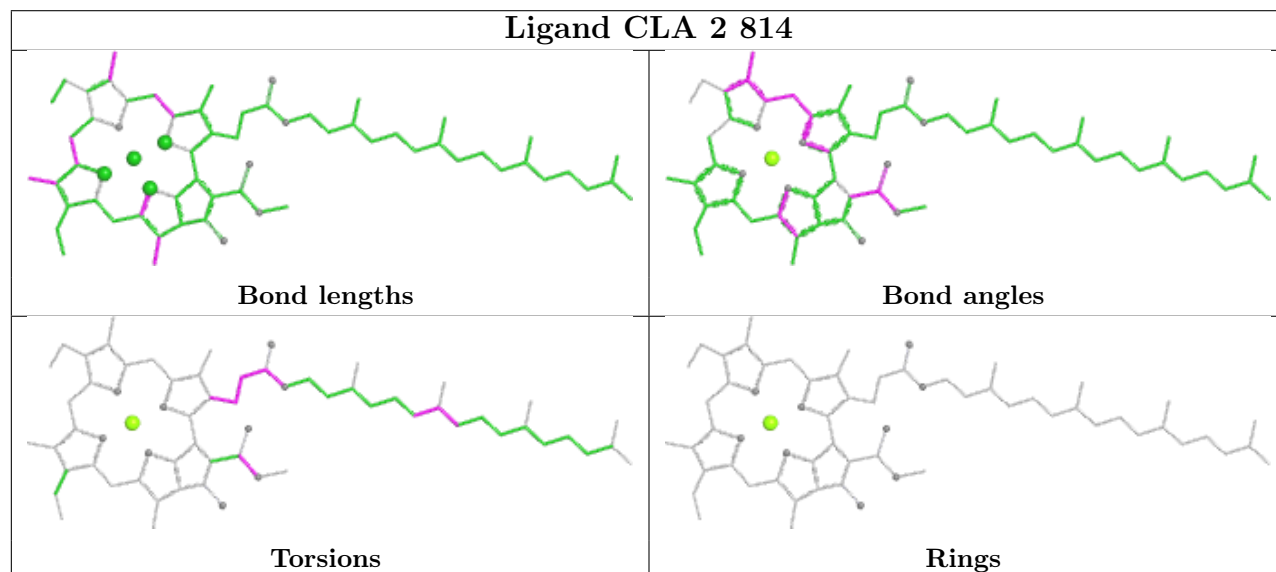


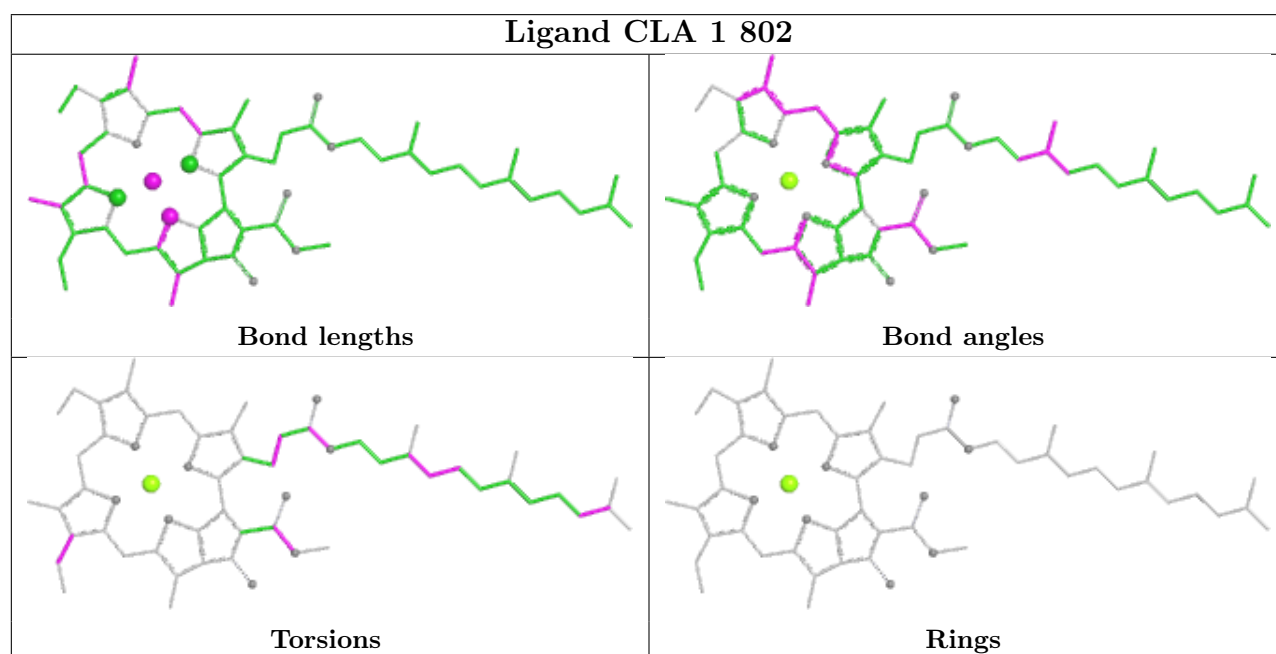
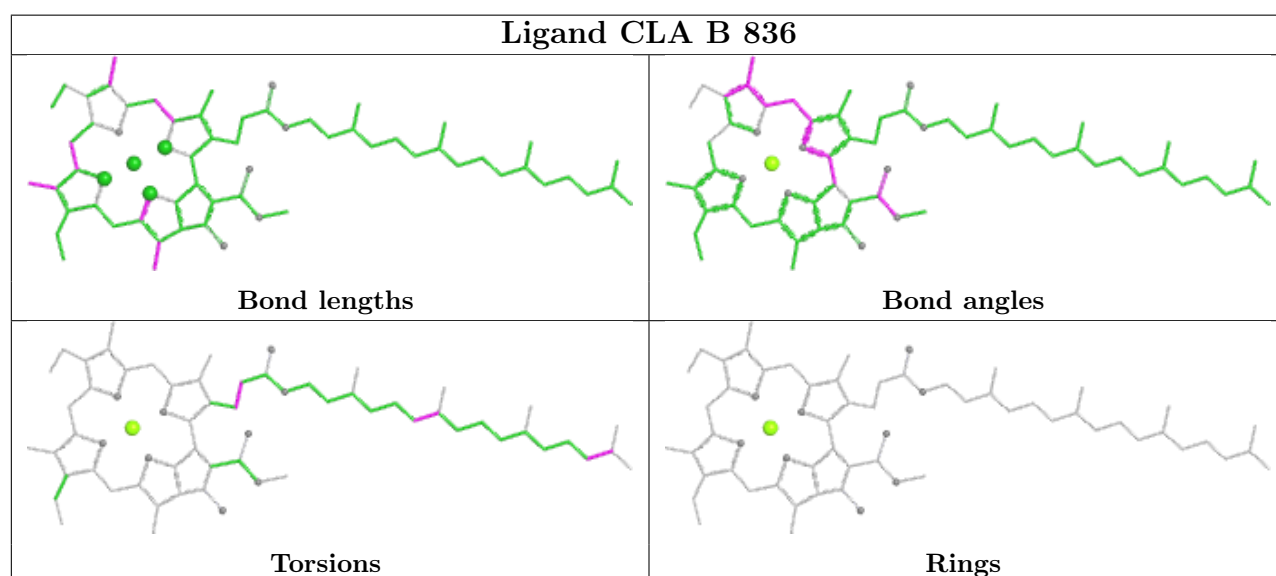
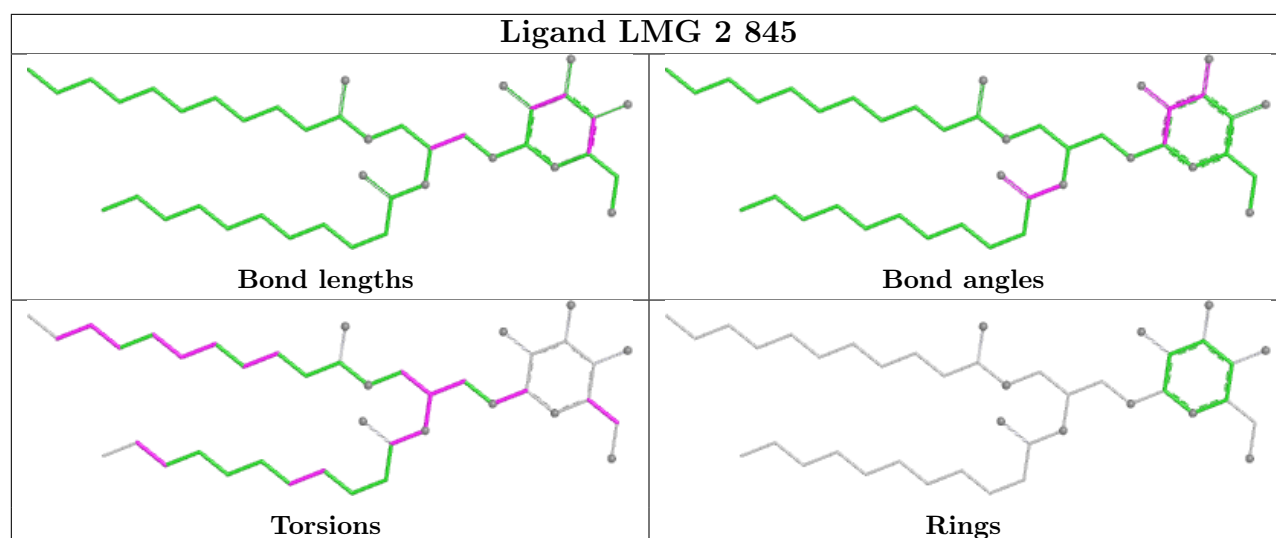


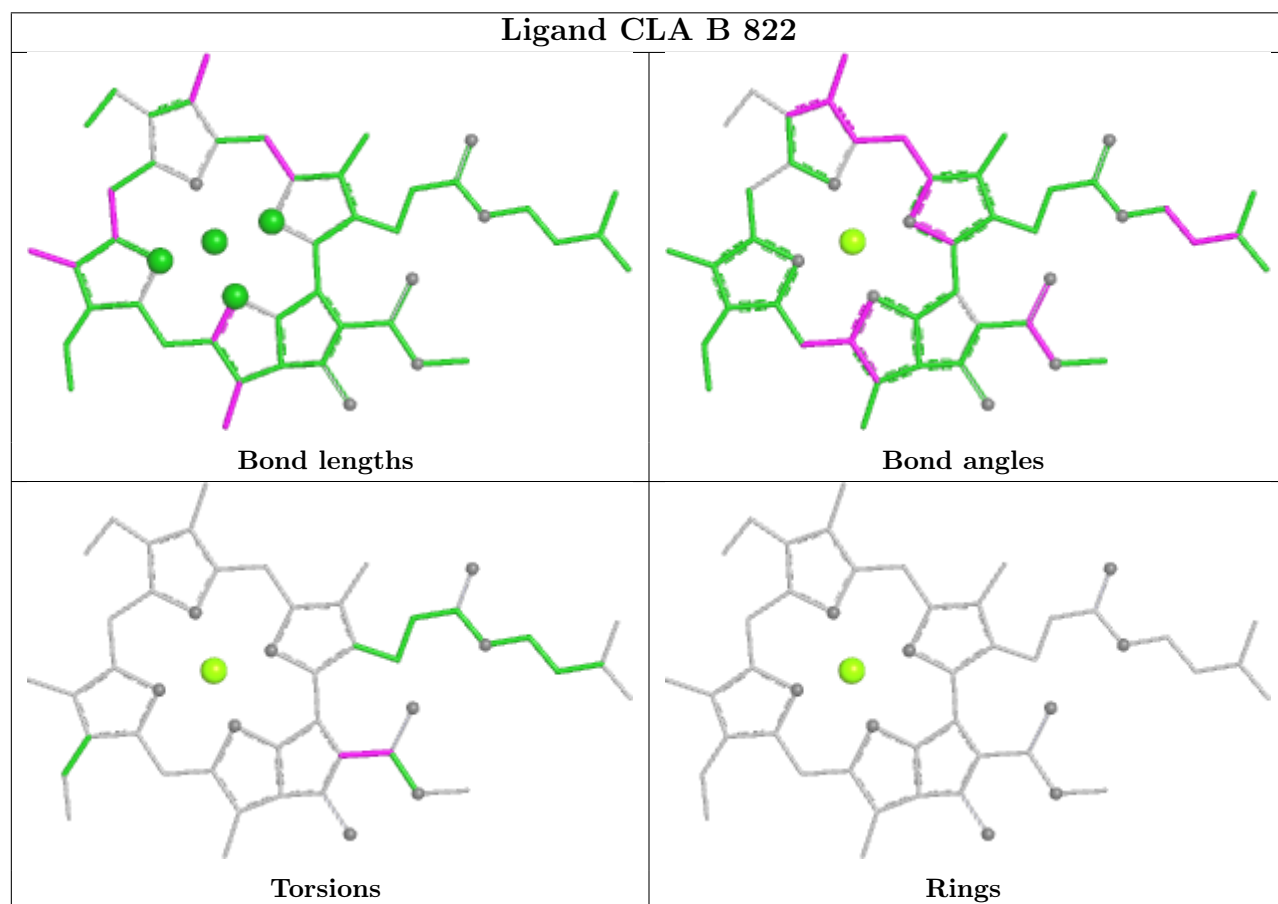
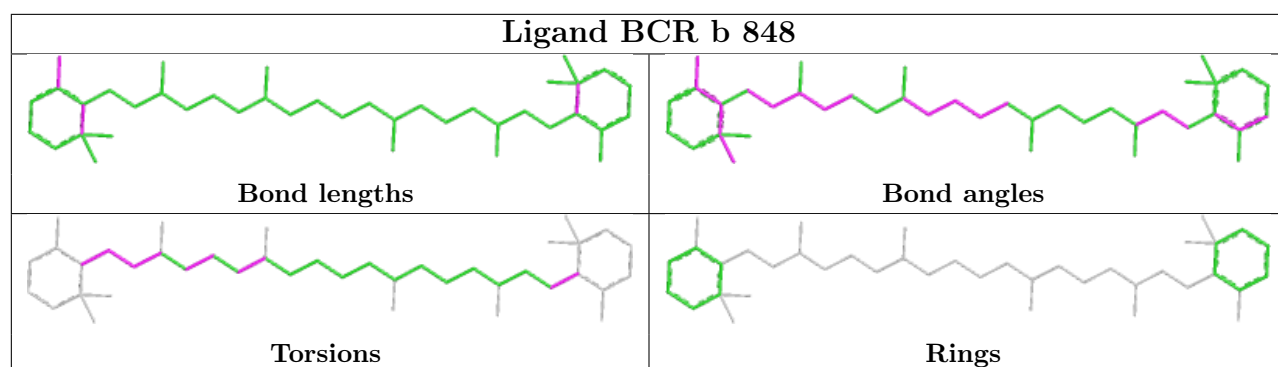
Ligand CLA 6 204

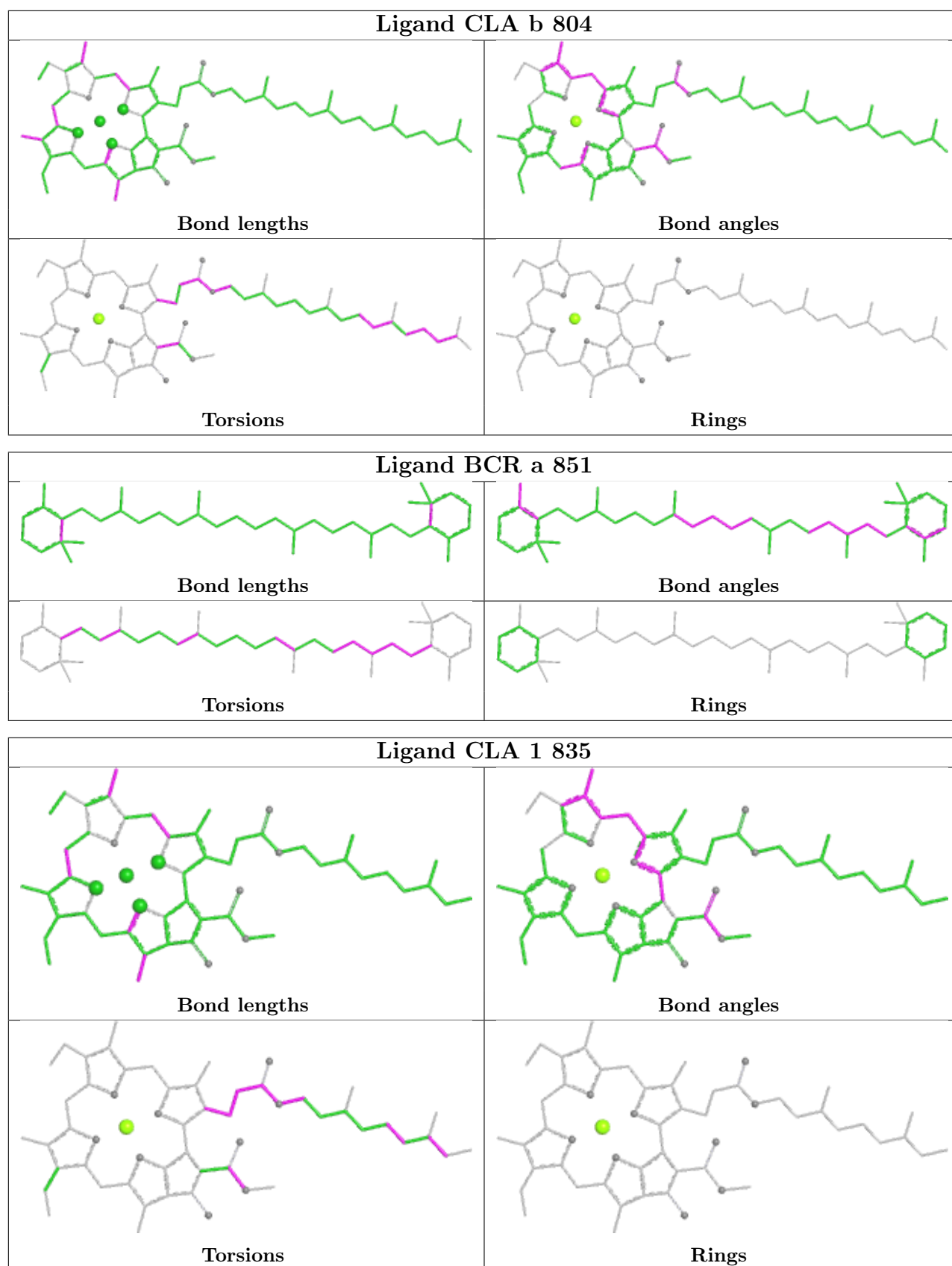


Ligand CLA 2 814

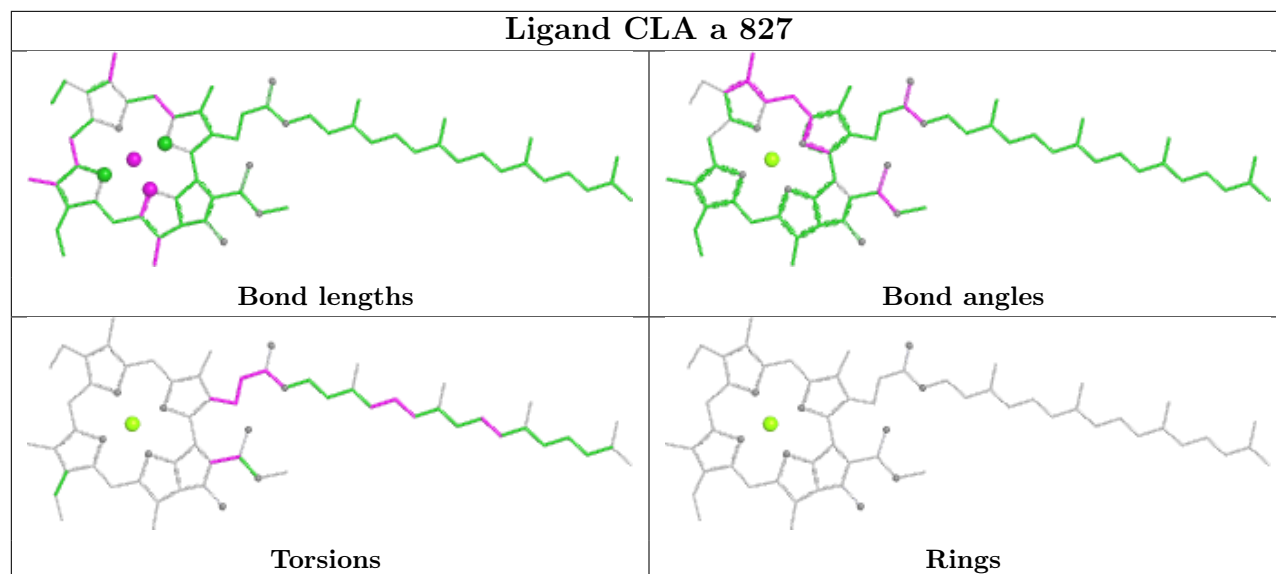




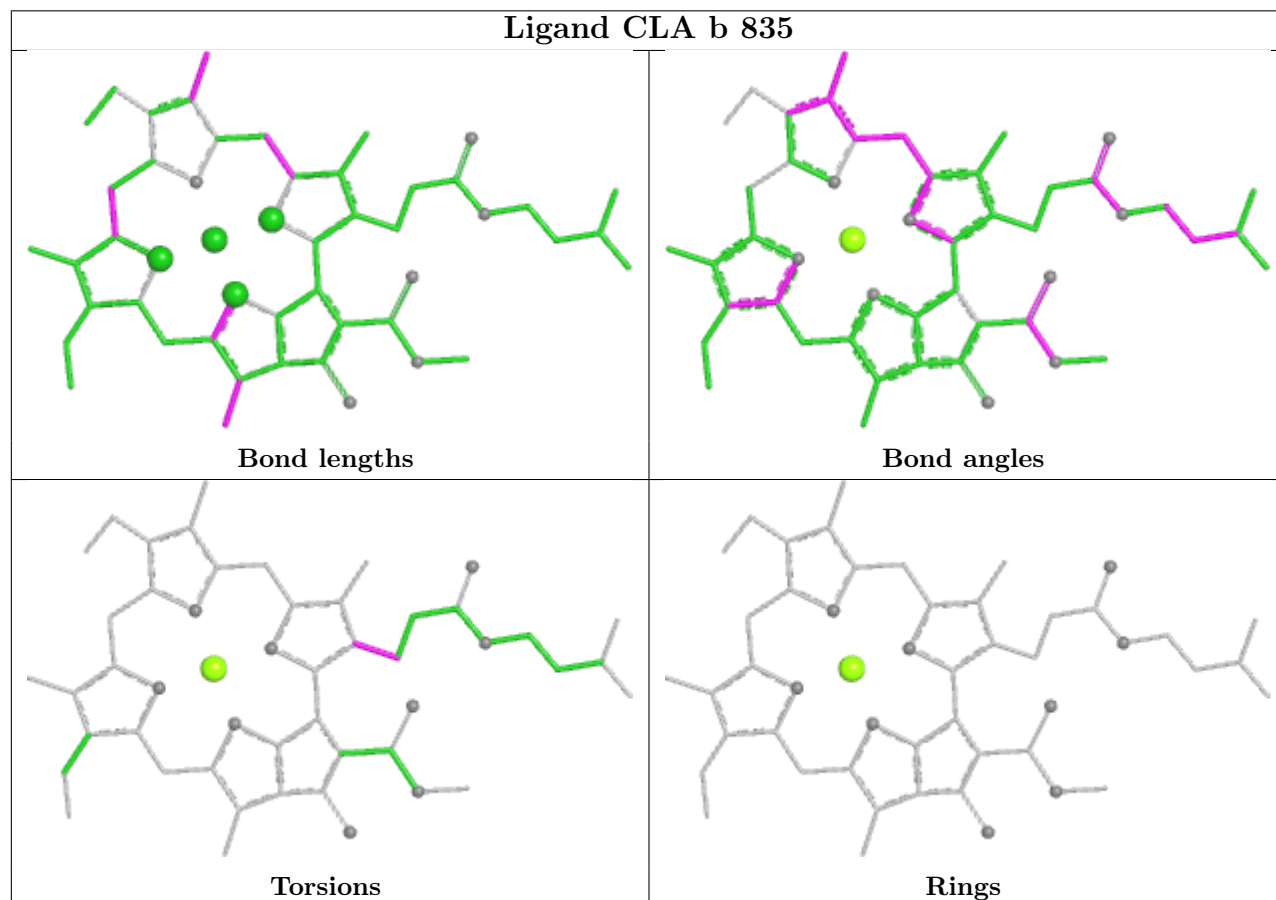


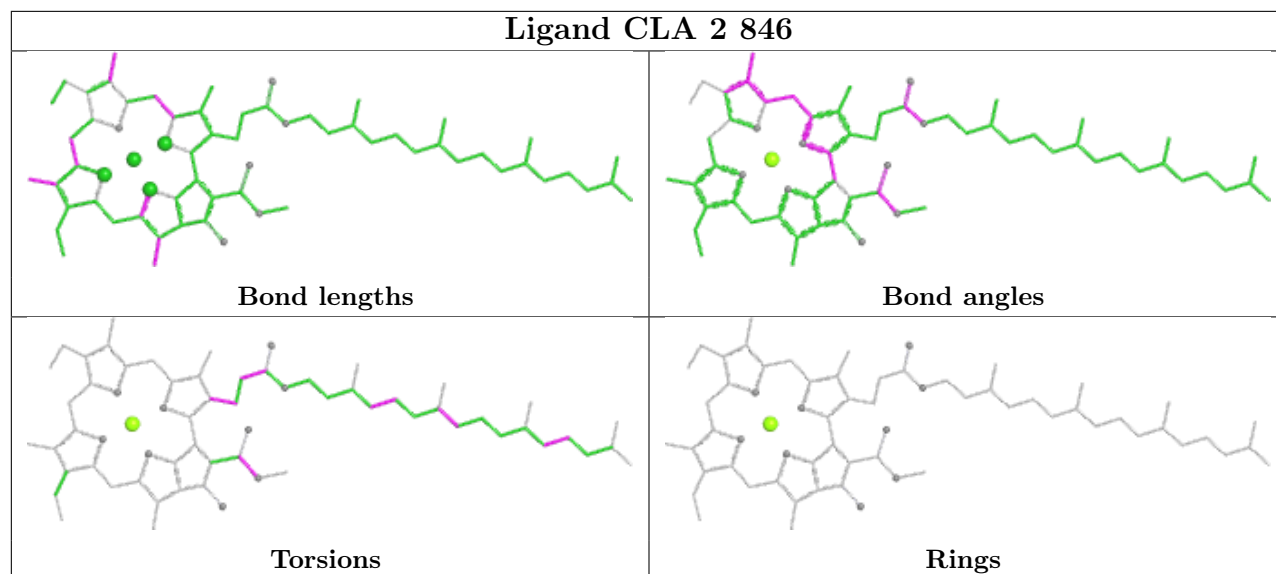
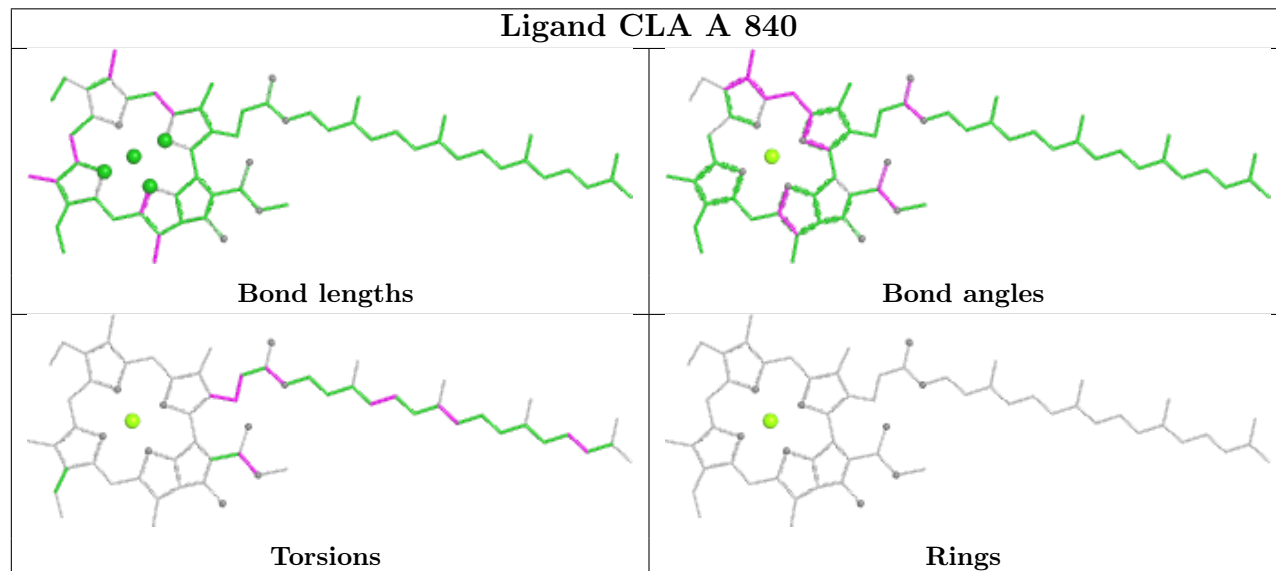


Ligand CLA a 827

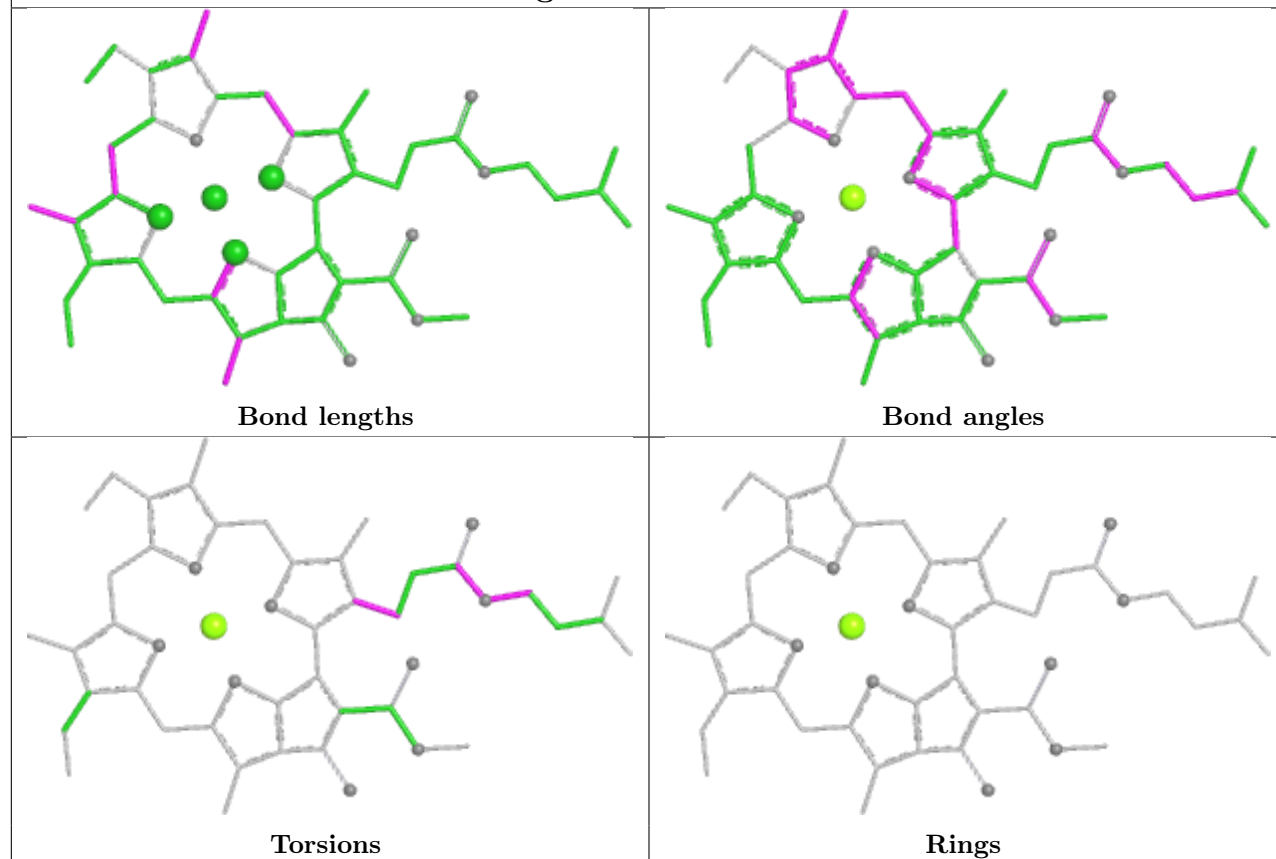


Ligand CLA b 835

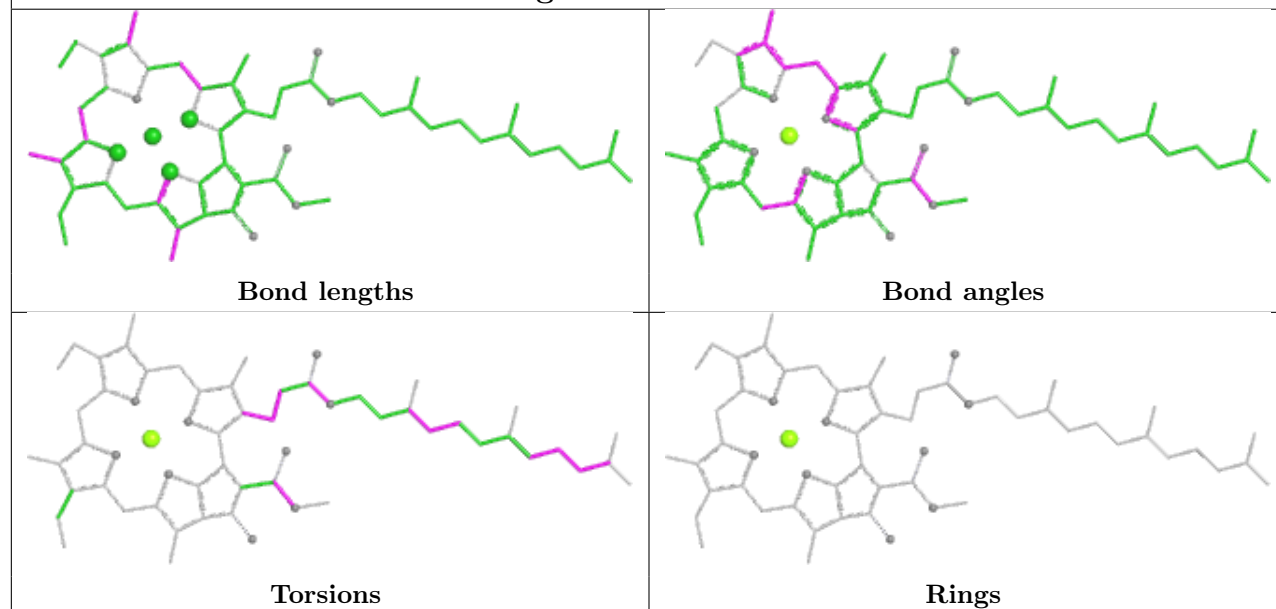


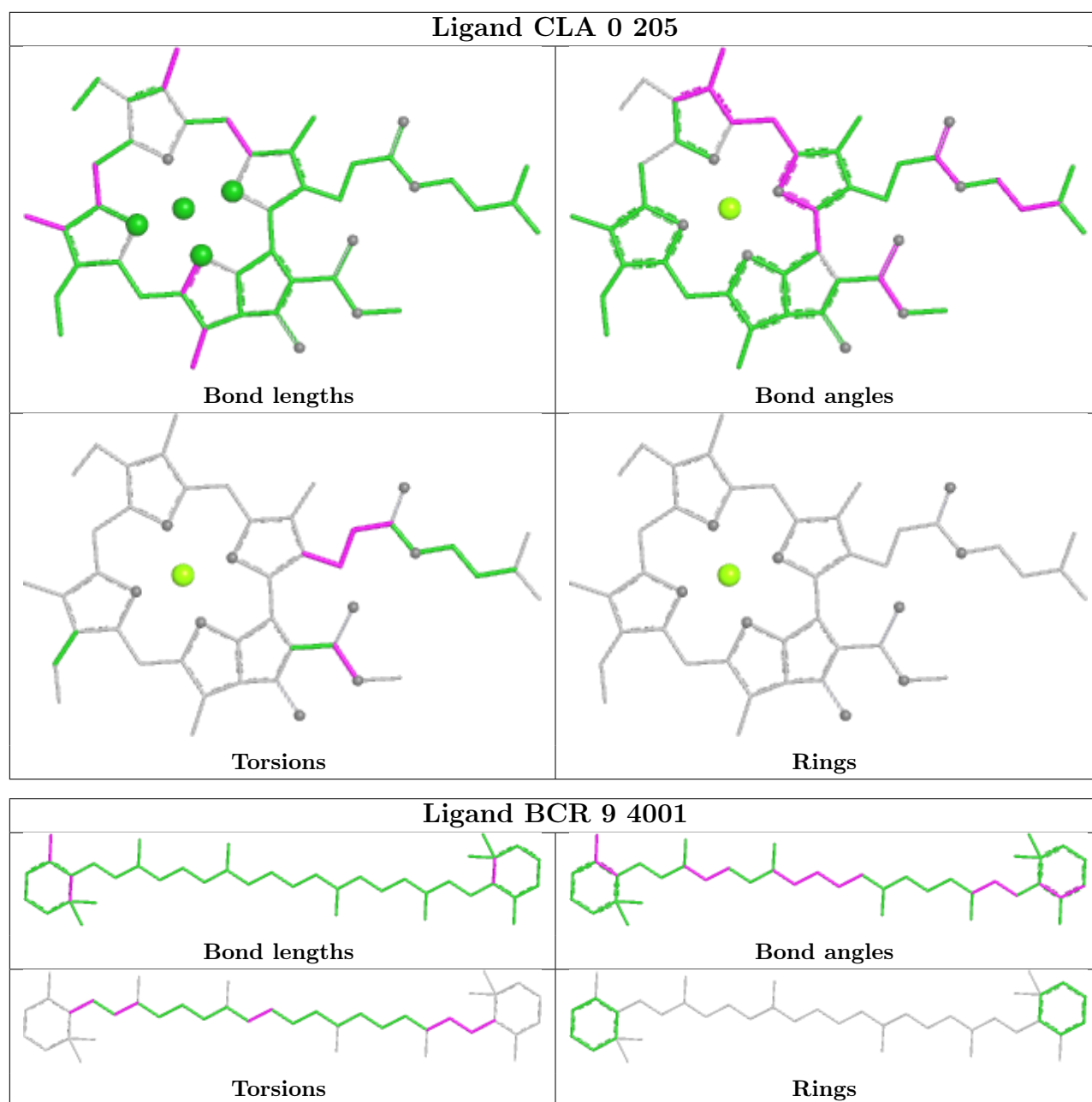
Ligand CLA 2 846**Ligand CLA A 840**

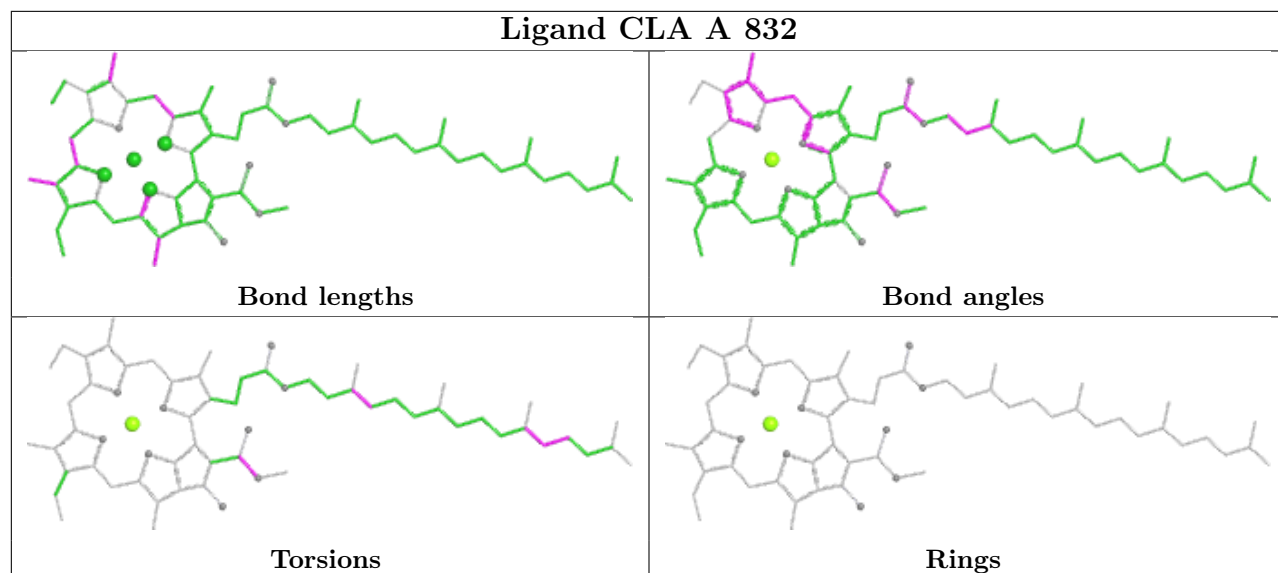
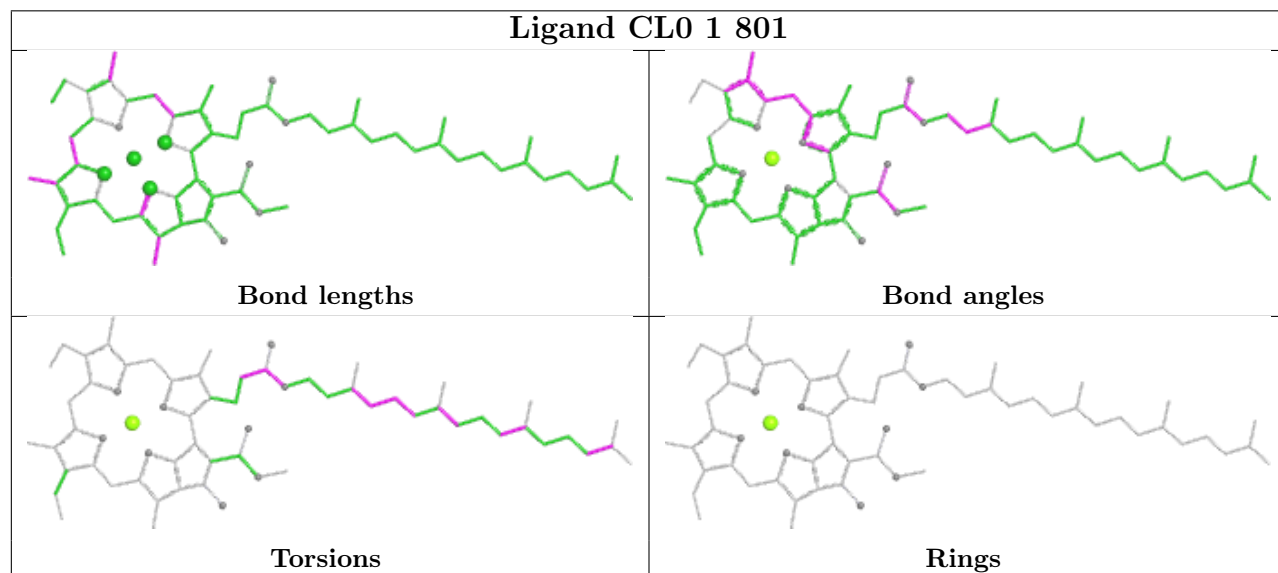
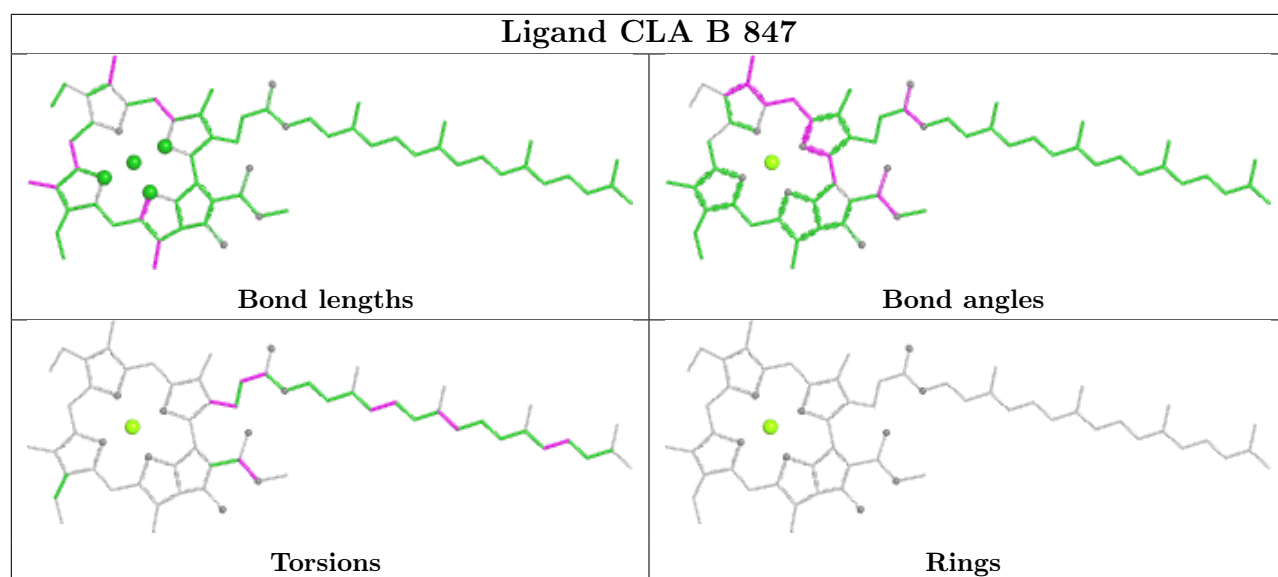
Ligand CLA 2 832



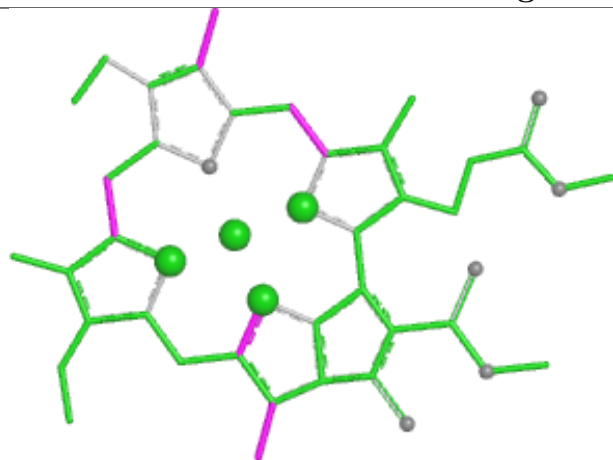
Ligand CLA 1 824



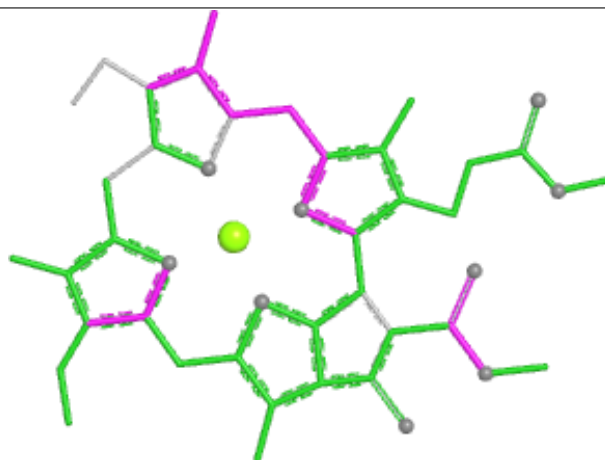




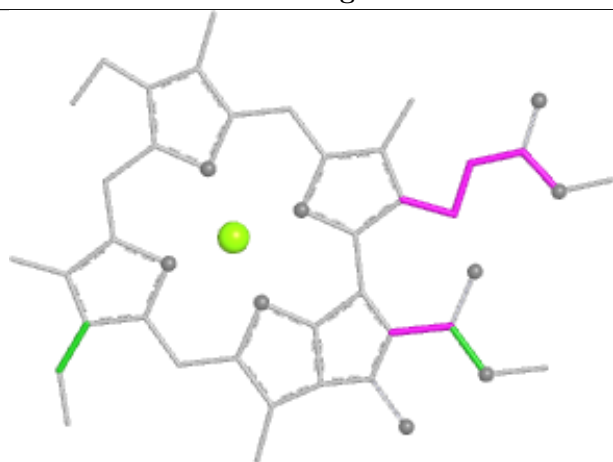
Ligand CLA b 818



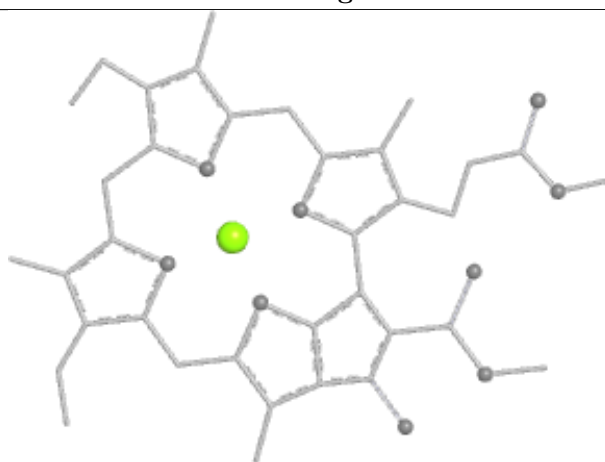
Bond lengths



Bond angles

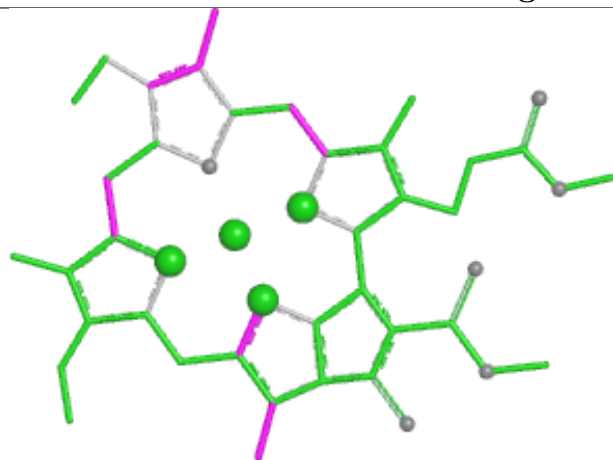


Torsions

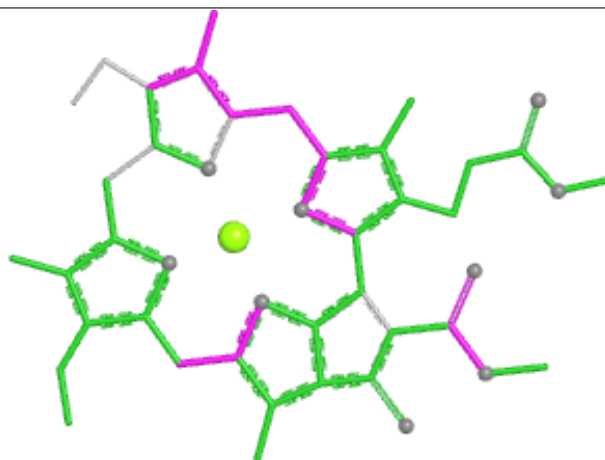


Rings

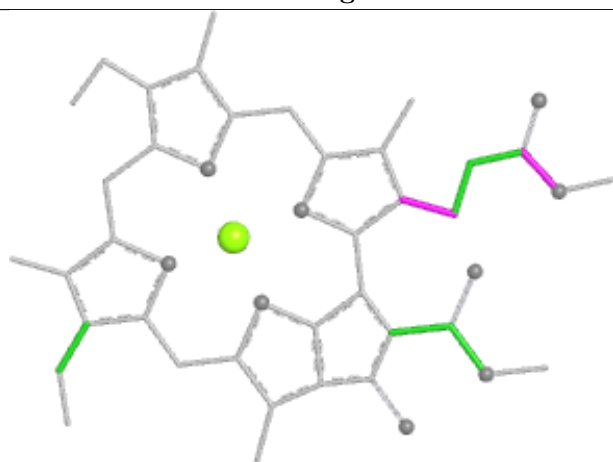
Ligand CLA 1 820



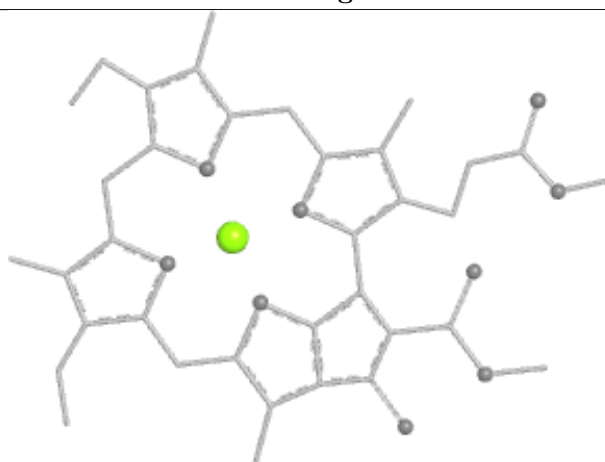
Bond lengths



Bond angles

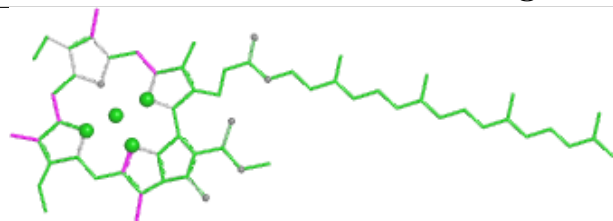


Torsions

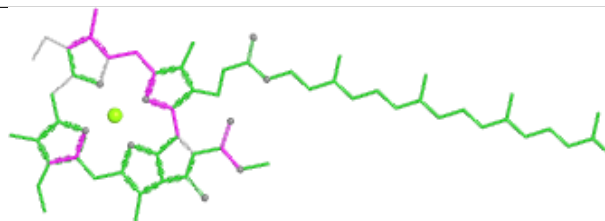


Rings

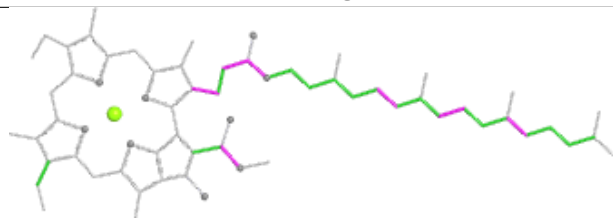
Ligand CLA 1 833



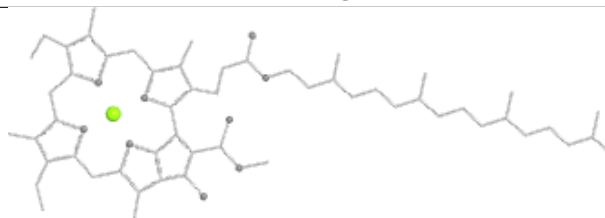
Bond lengths



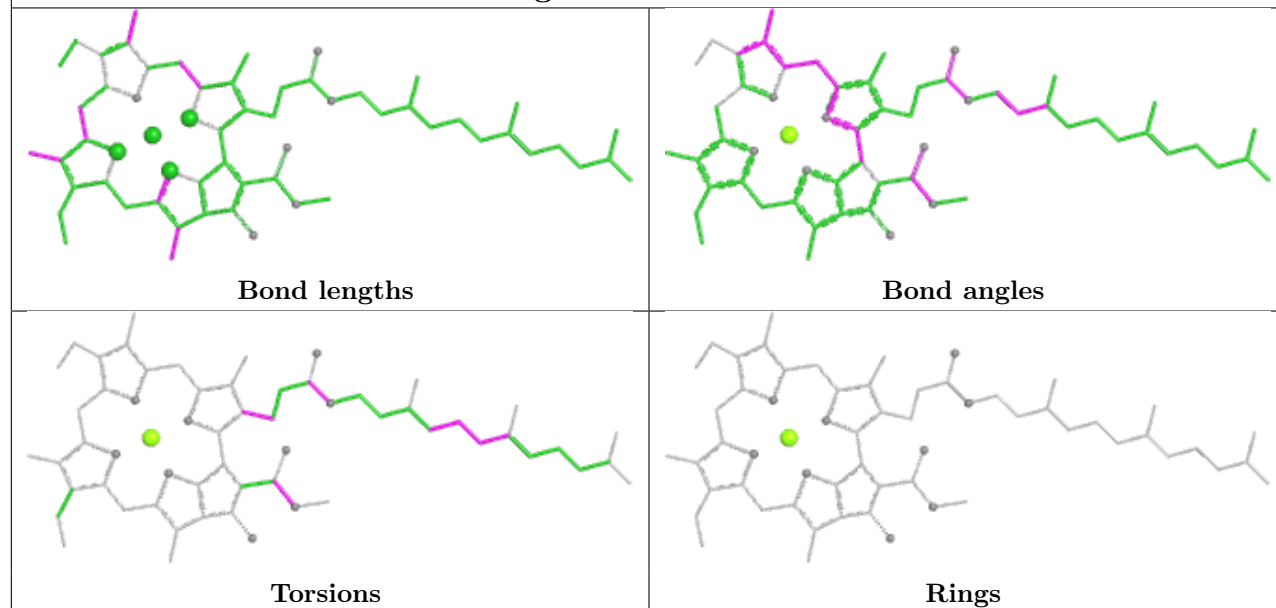
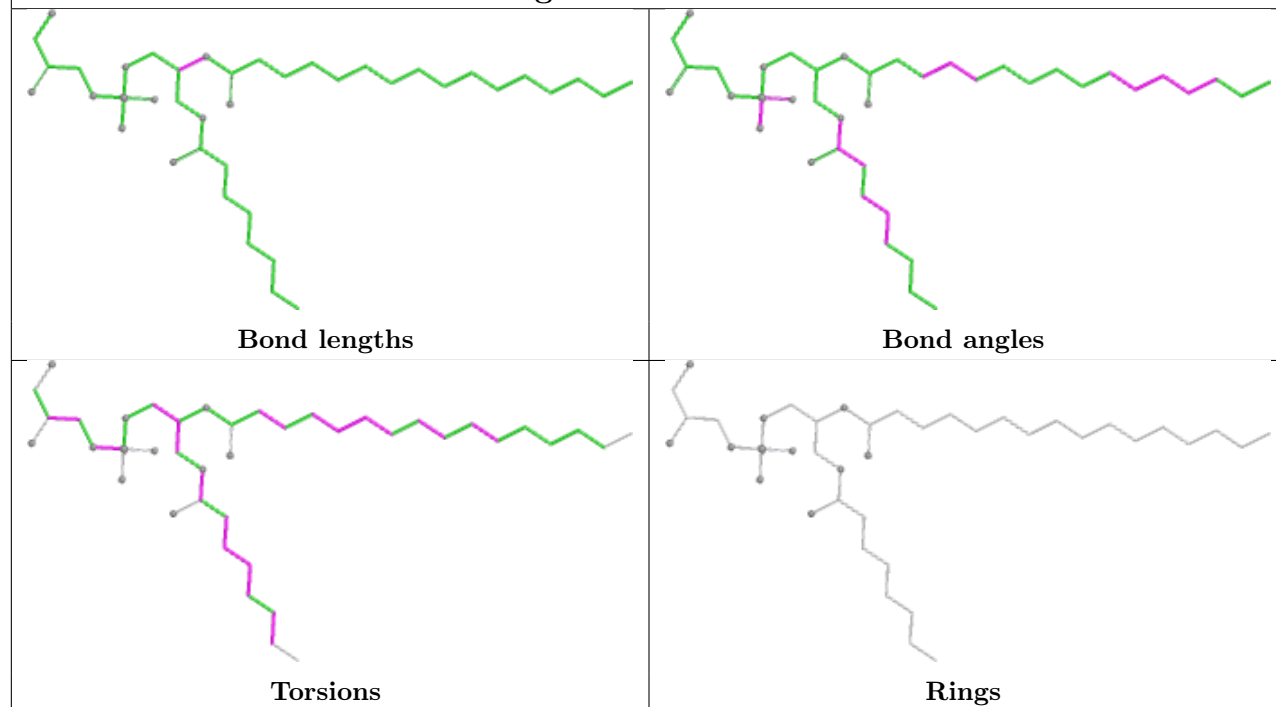
Bond angles



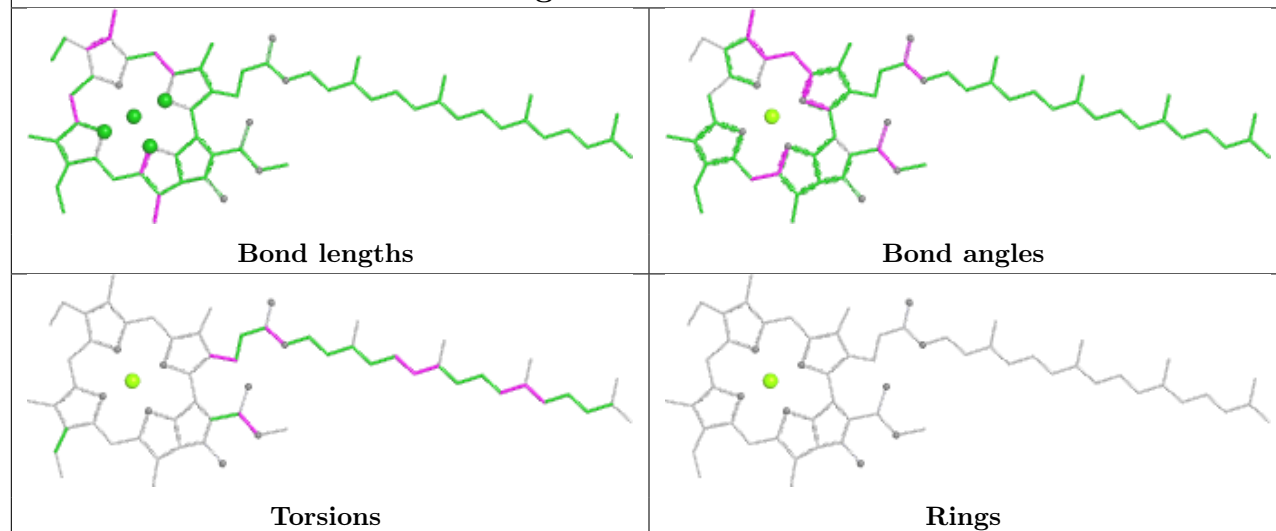
Torsions



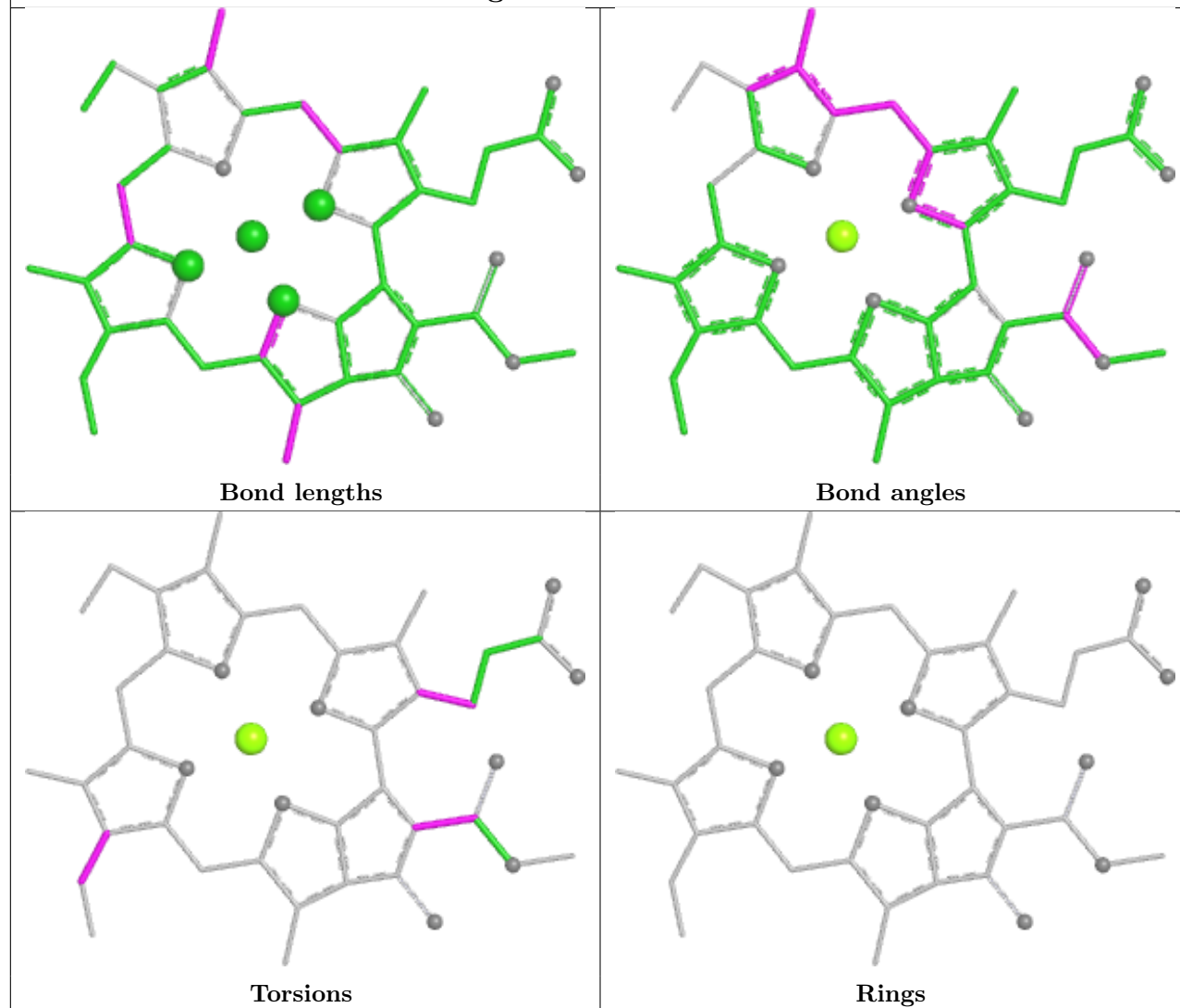
Rings

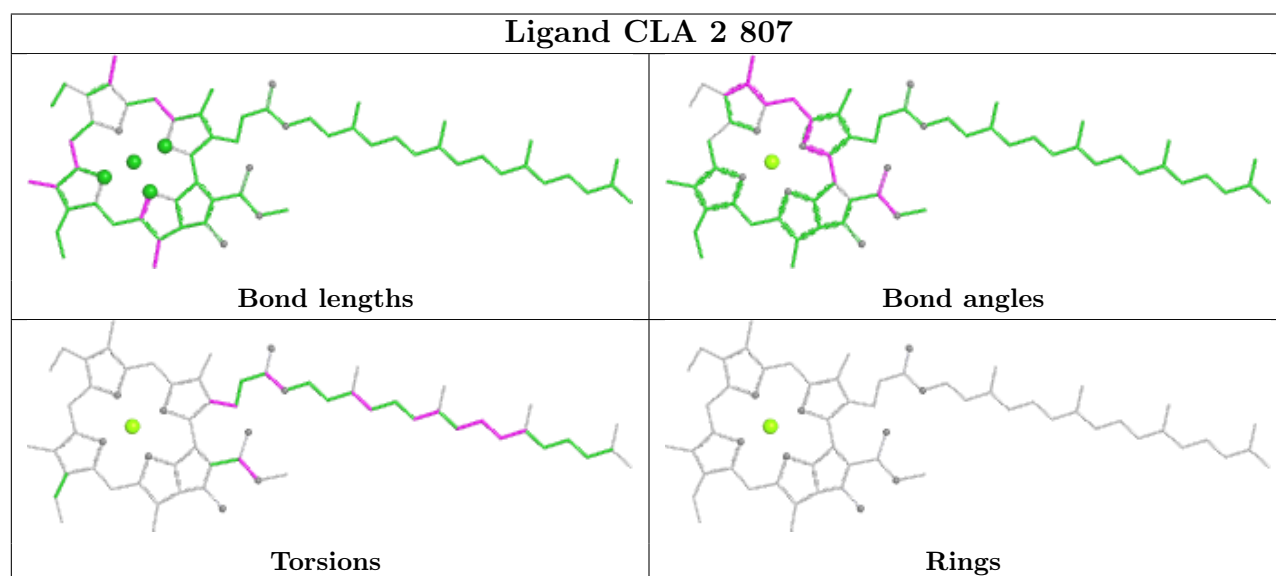
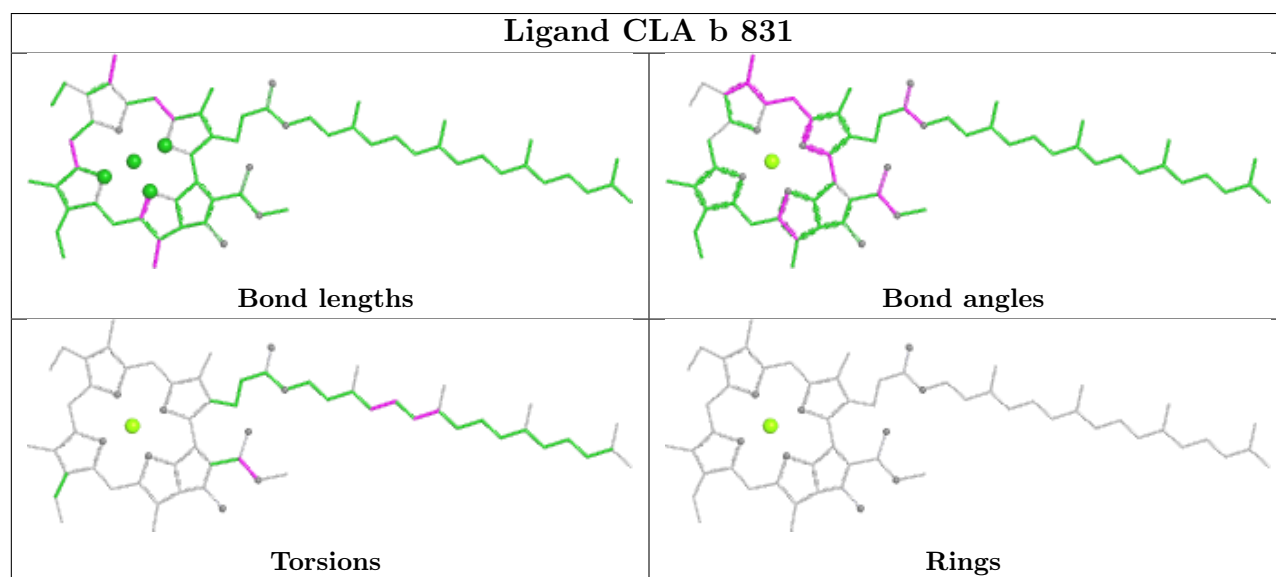
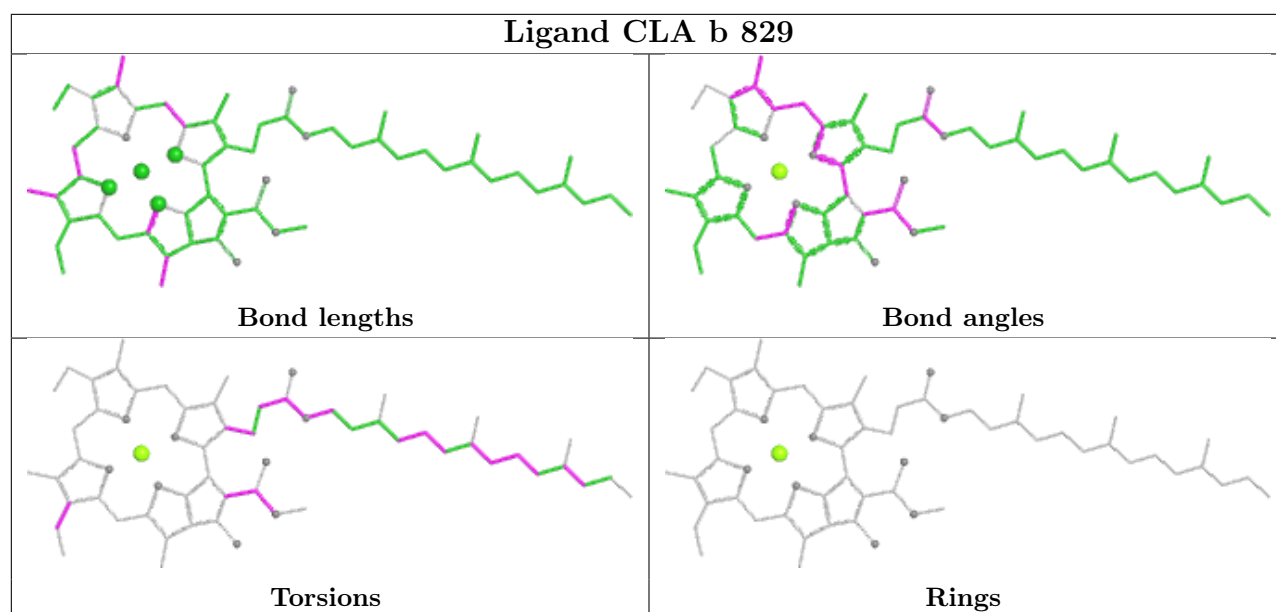
Ligand CLA L 201**Ligand LHG a 850**

Ligand CLA b 837

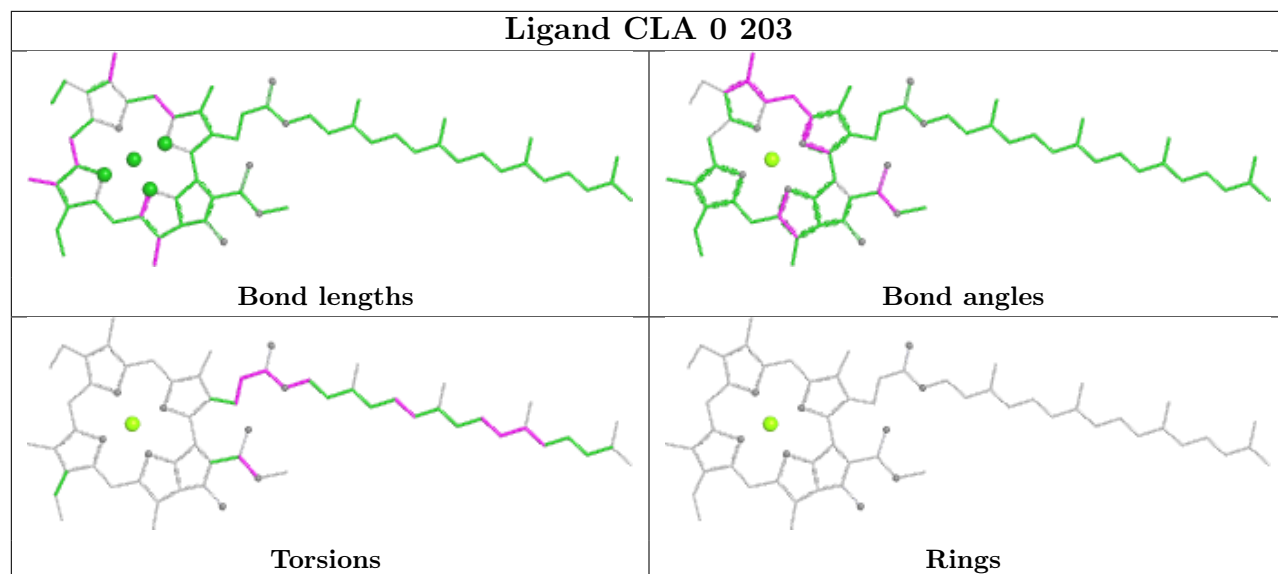


Ligand CLA 9 4002

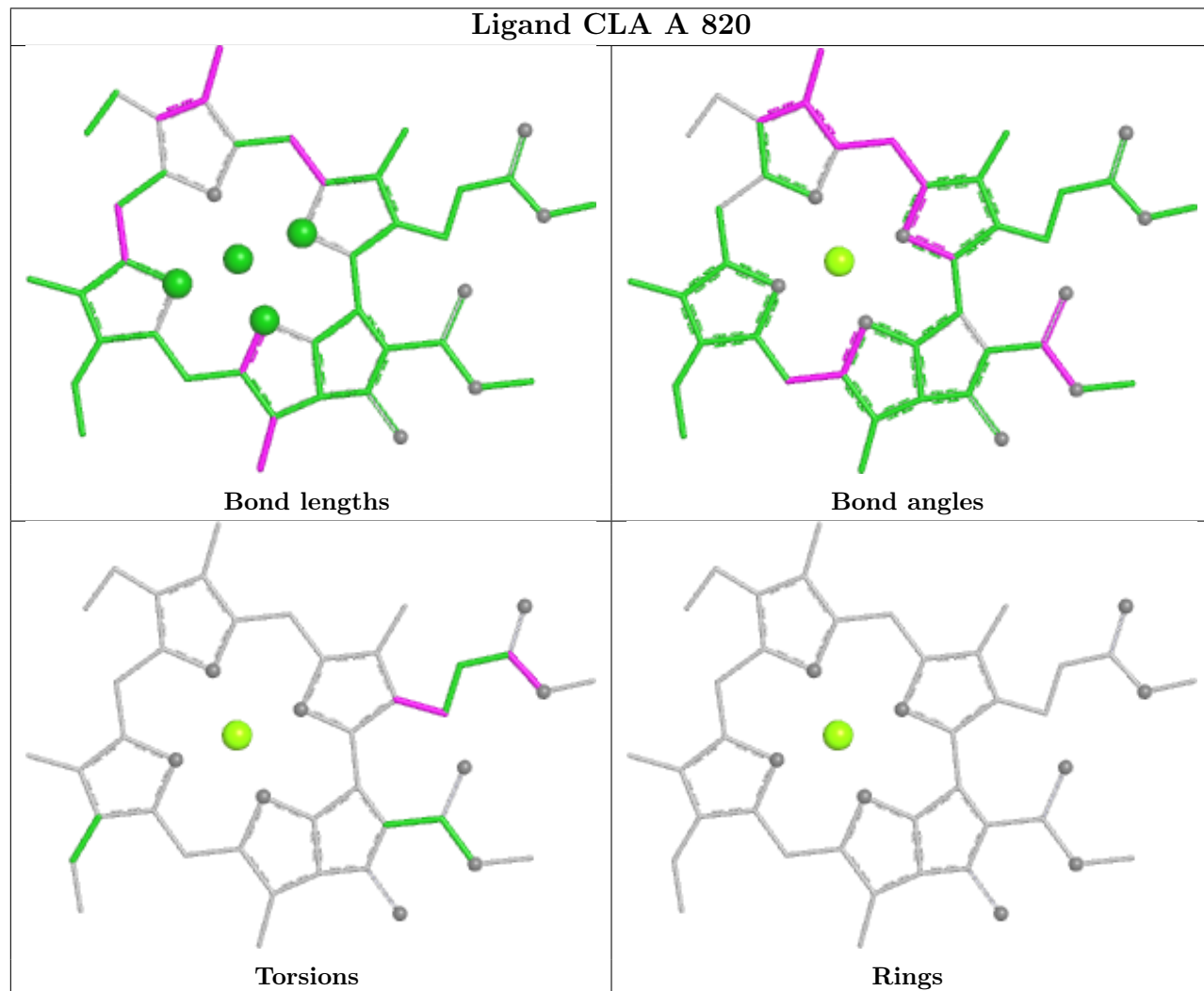


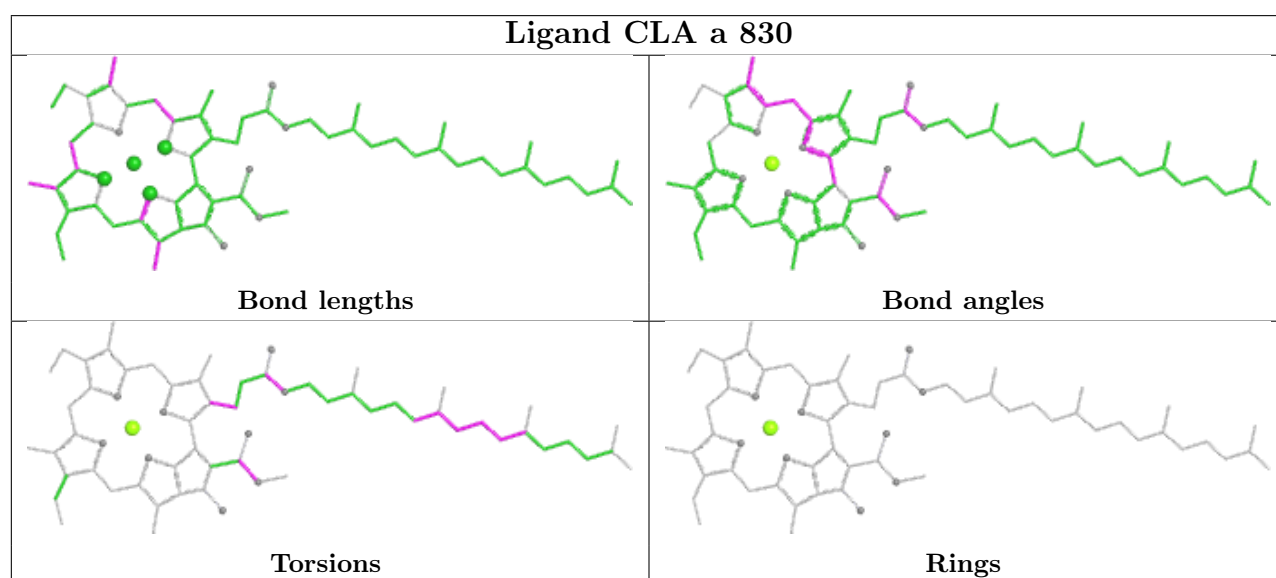
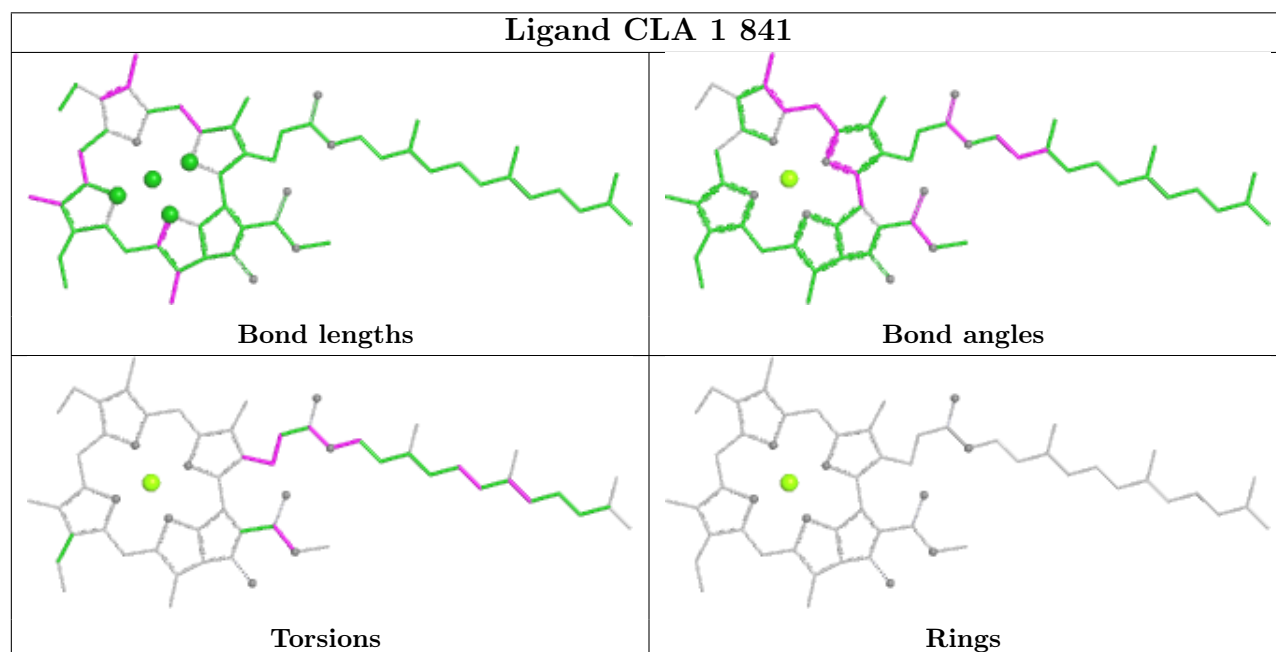
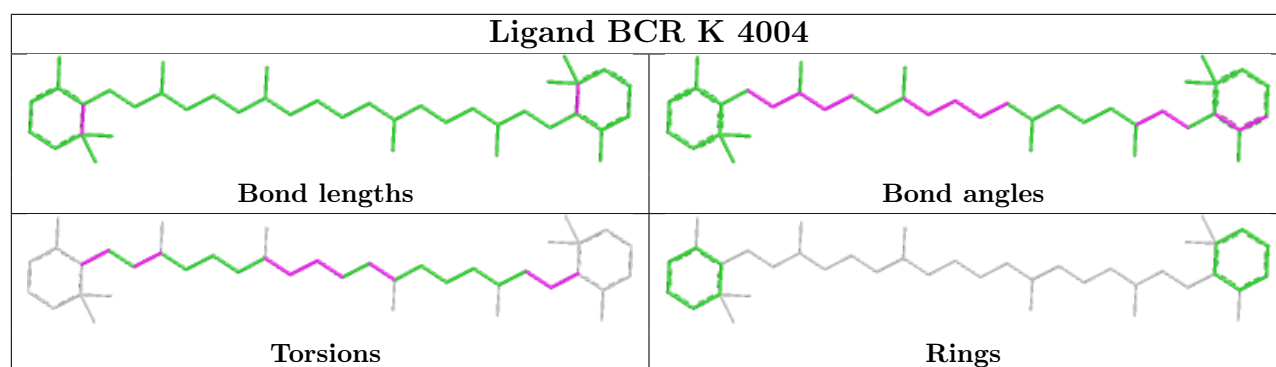


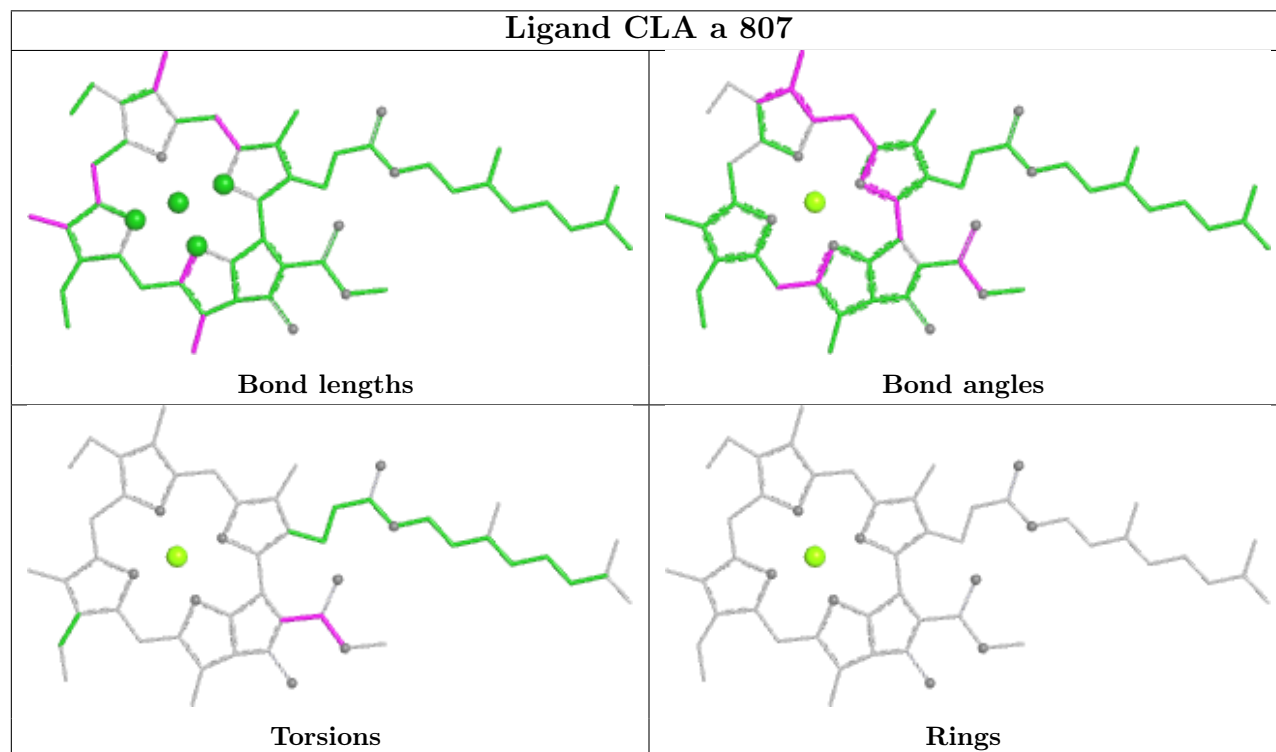
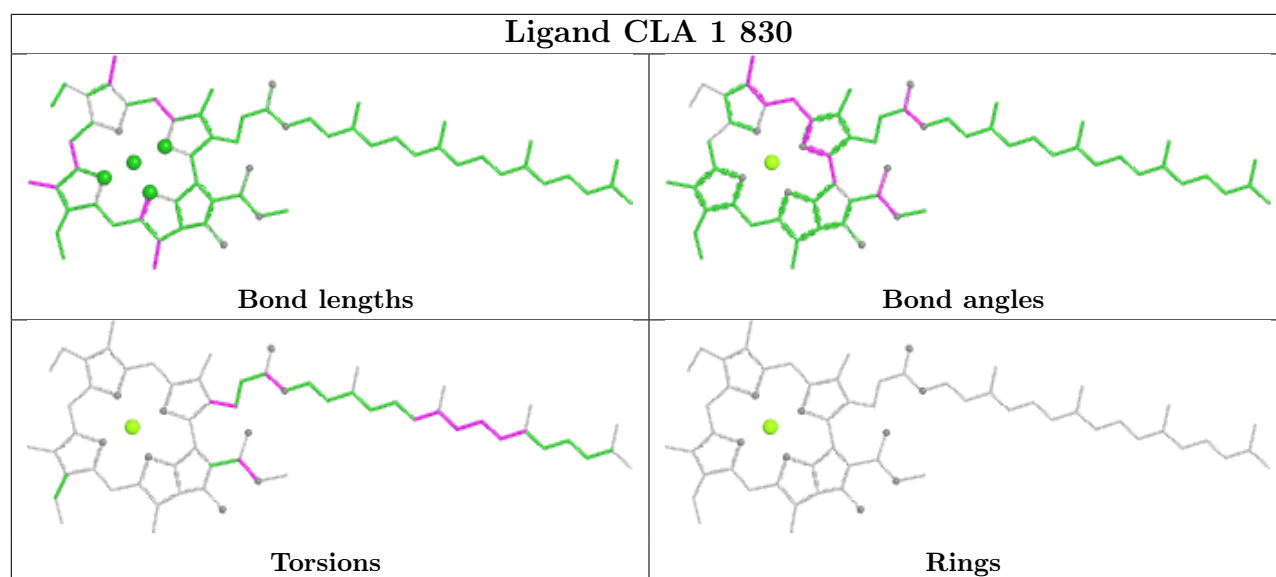
Ligand CLA 0 203

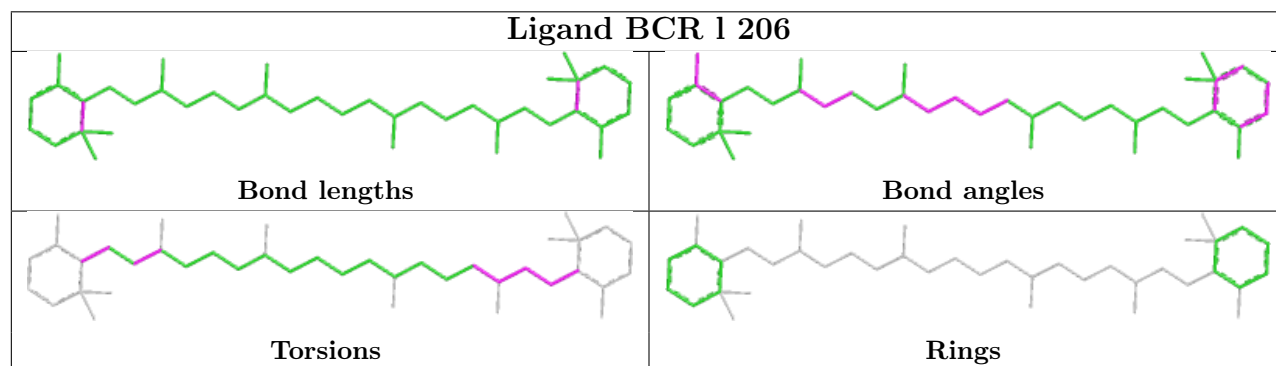
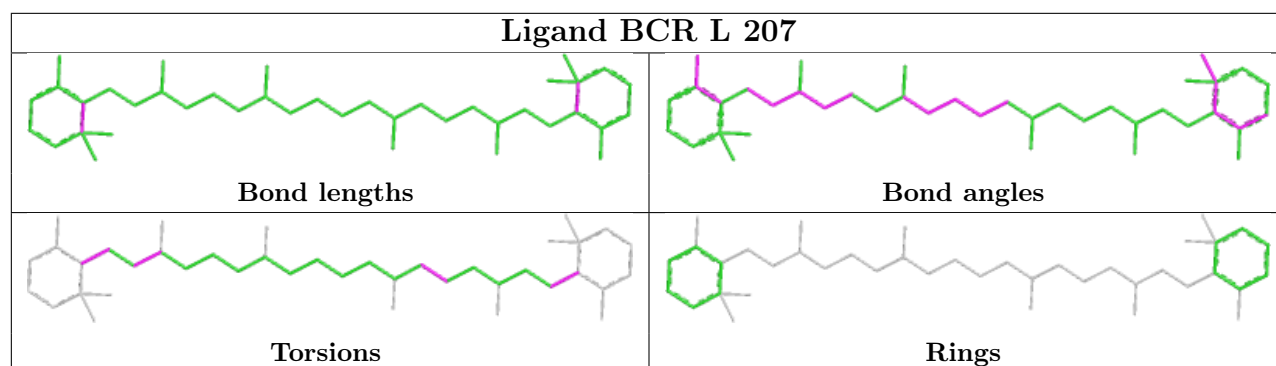
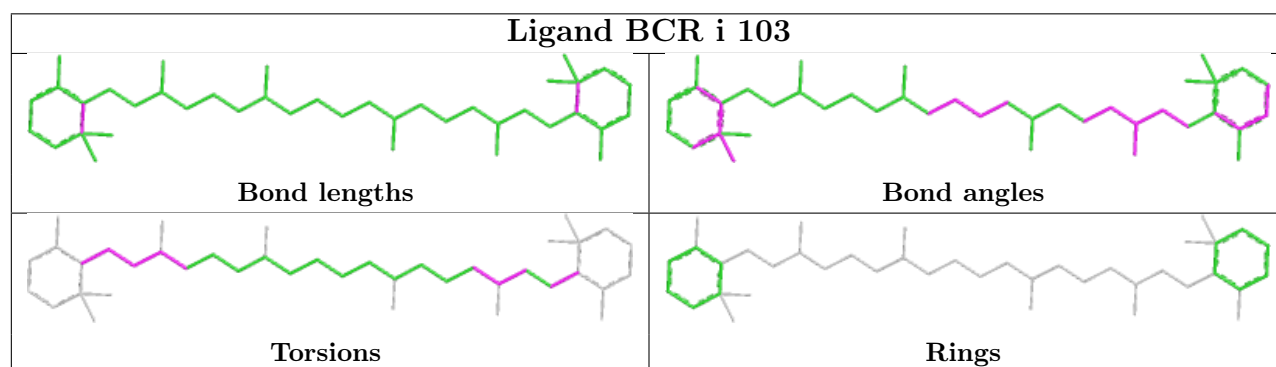
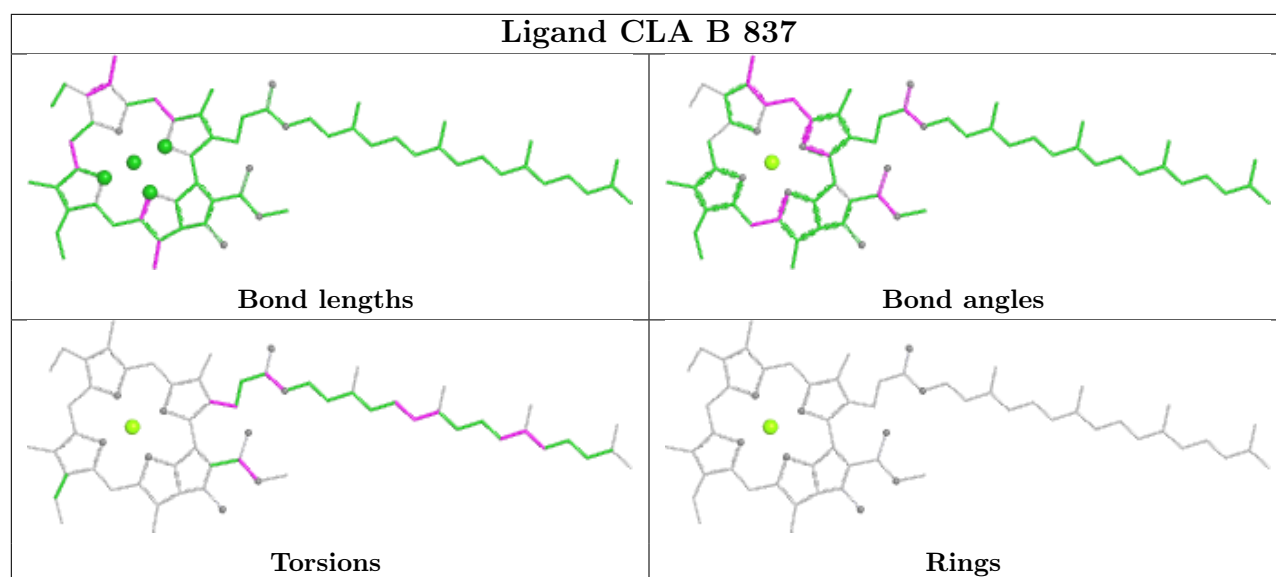


Ligand CLA A 820

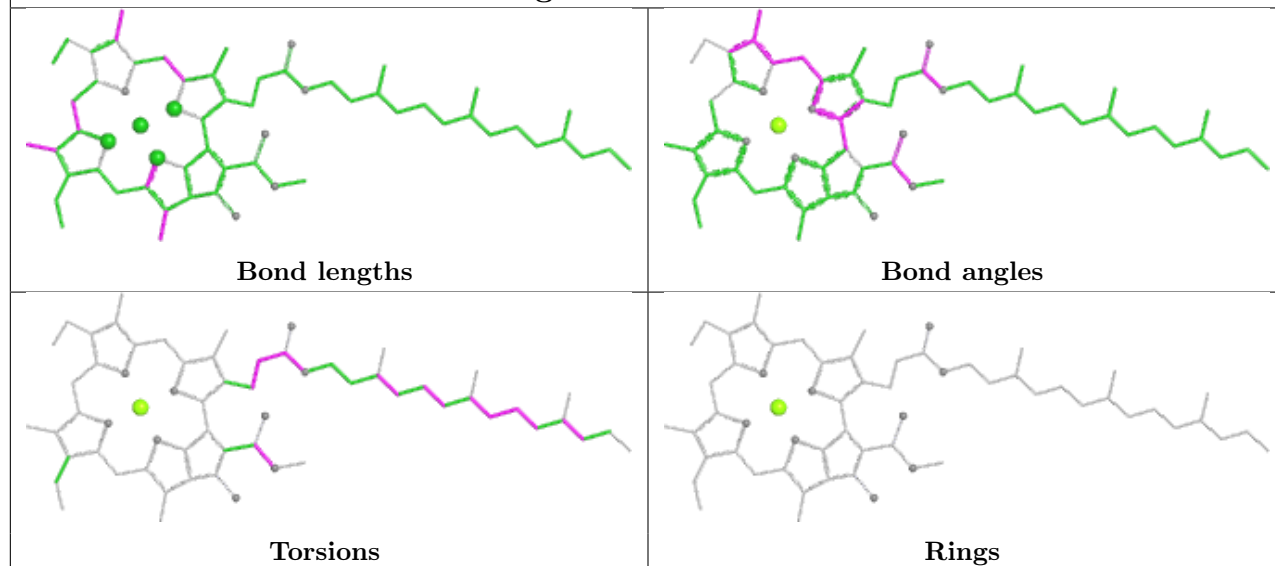




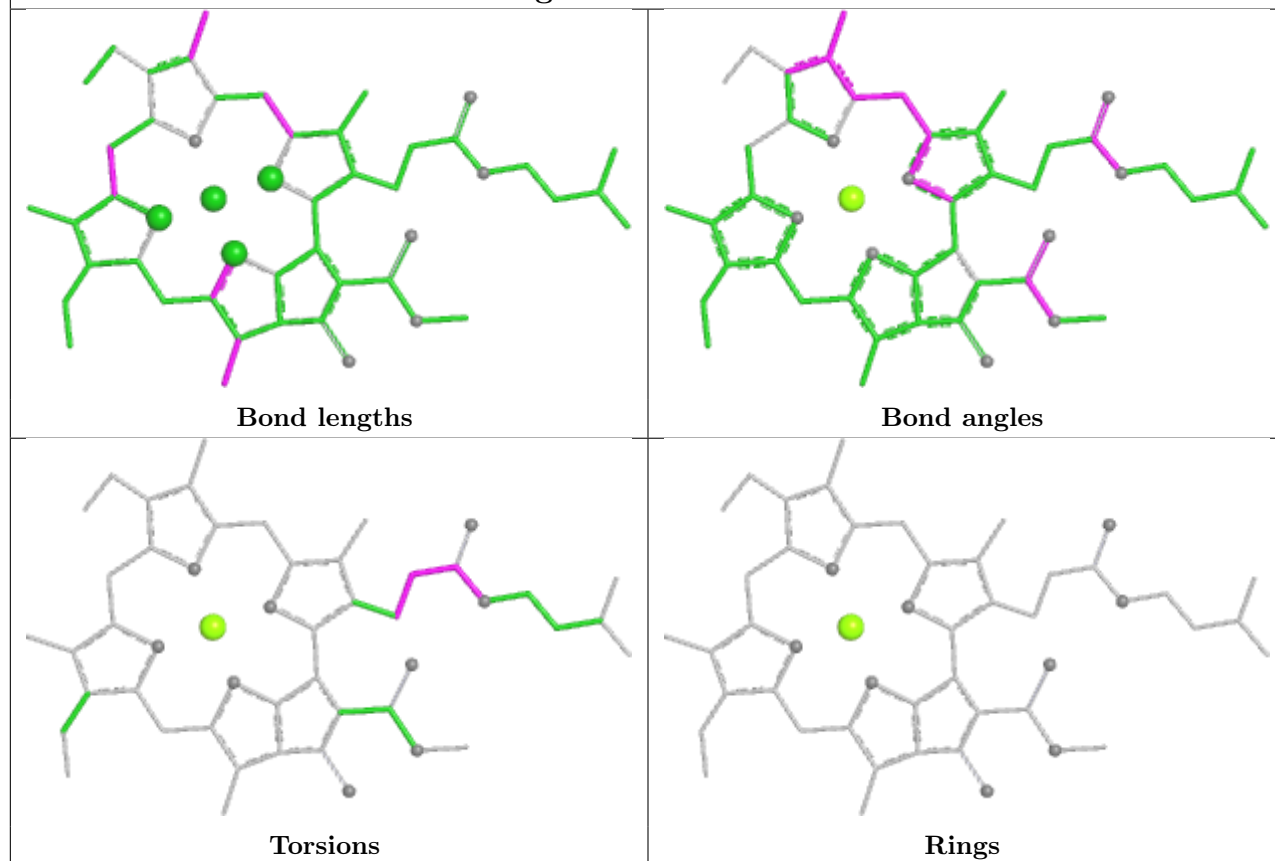


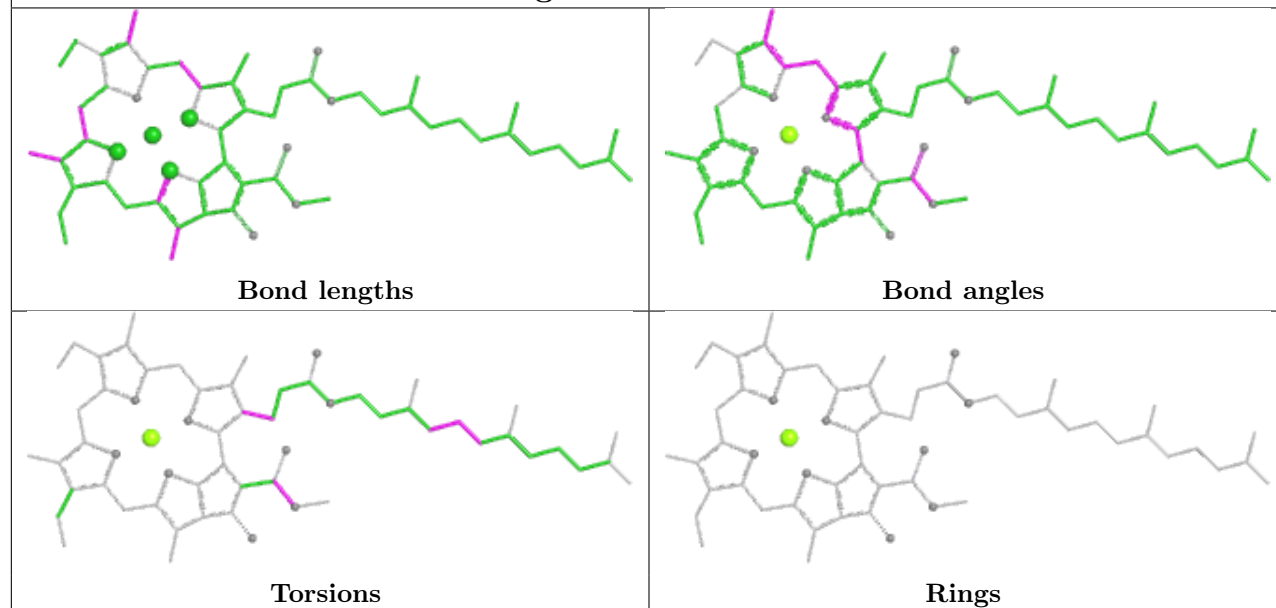
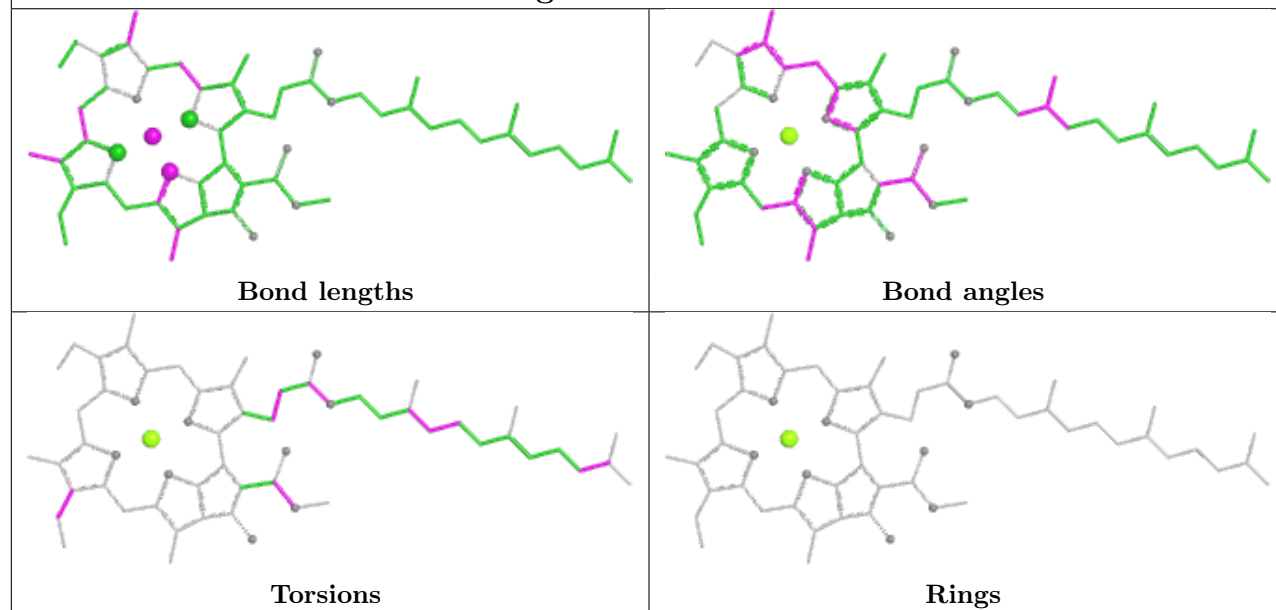


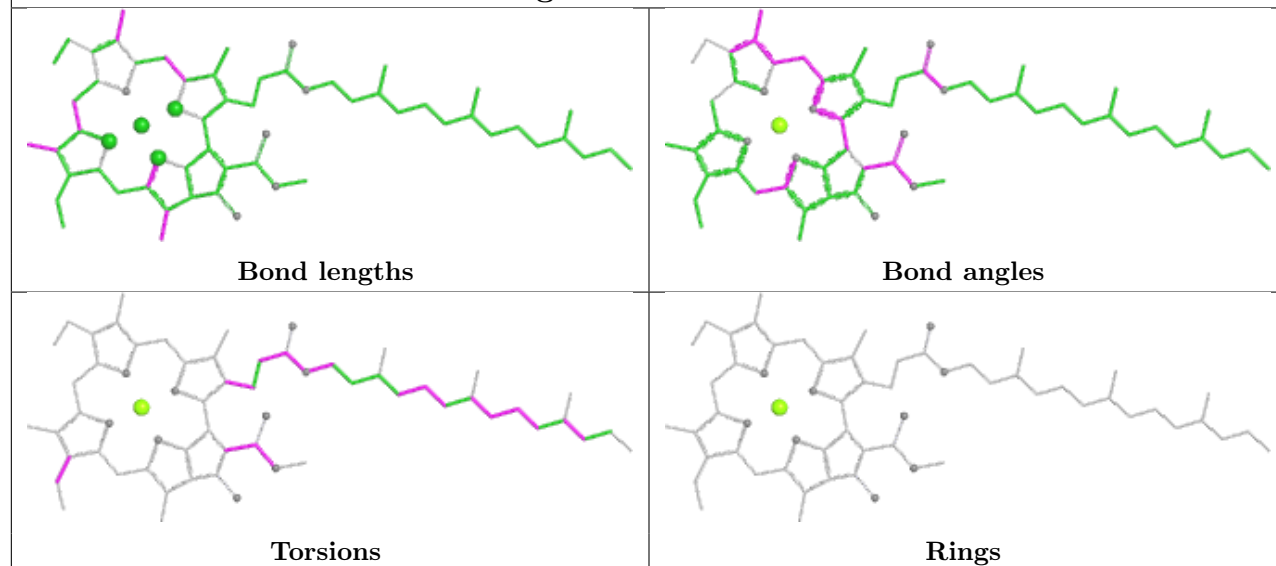
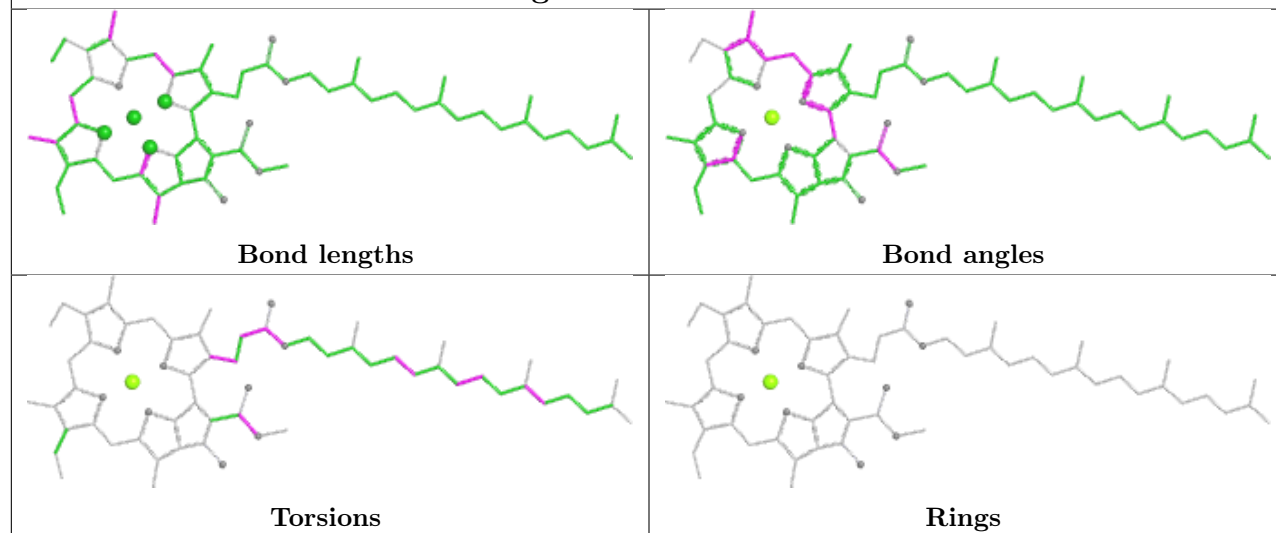
Ligand CLA a 825



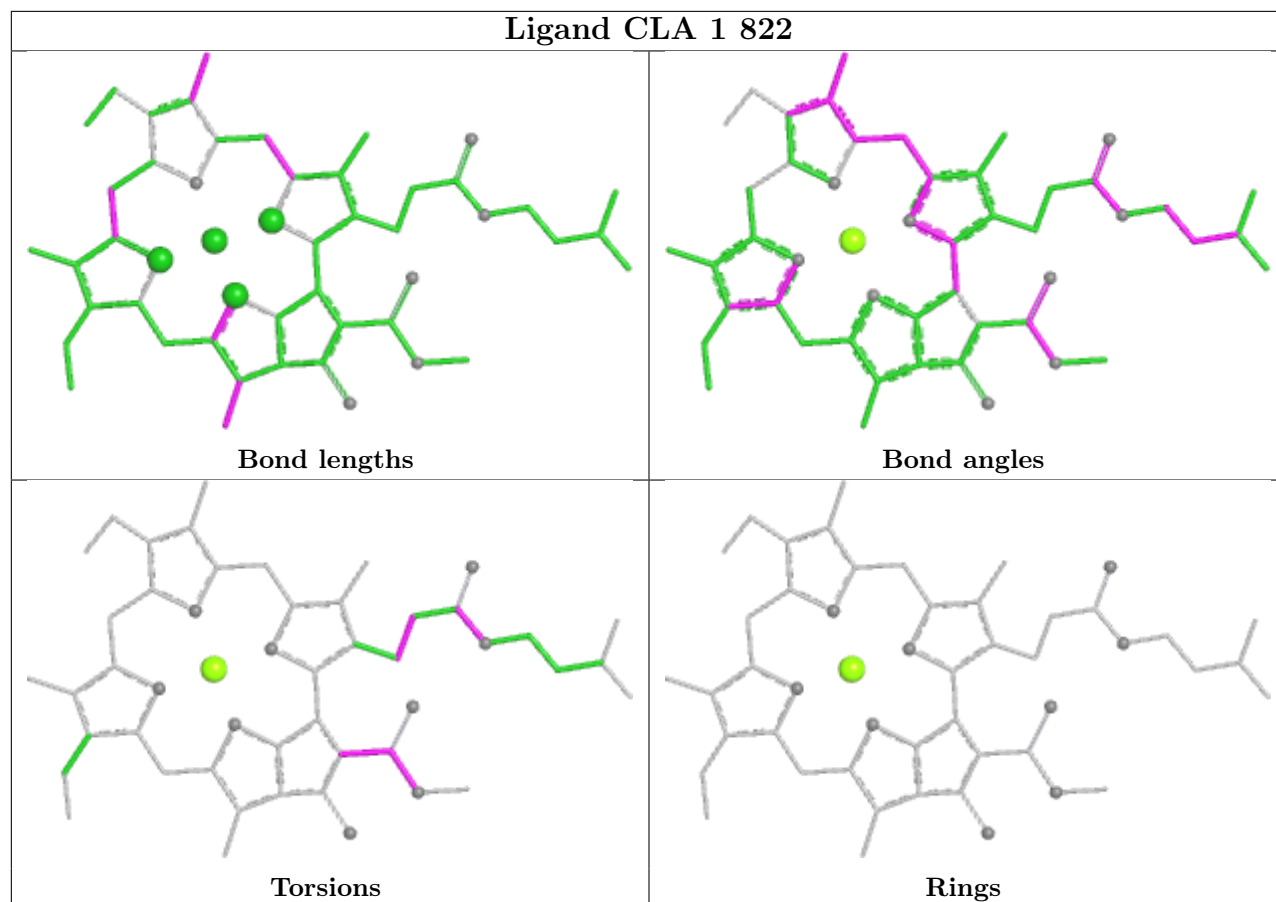
Ligand CLA a 823

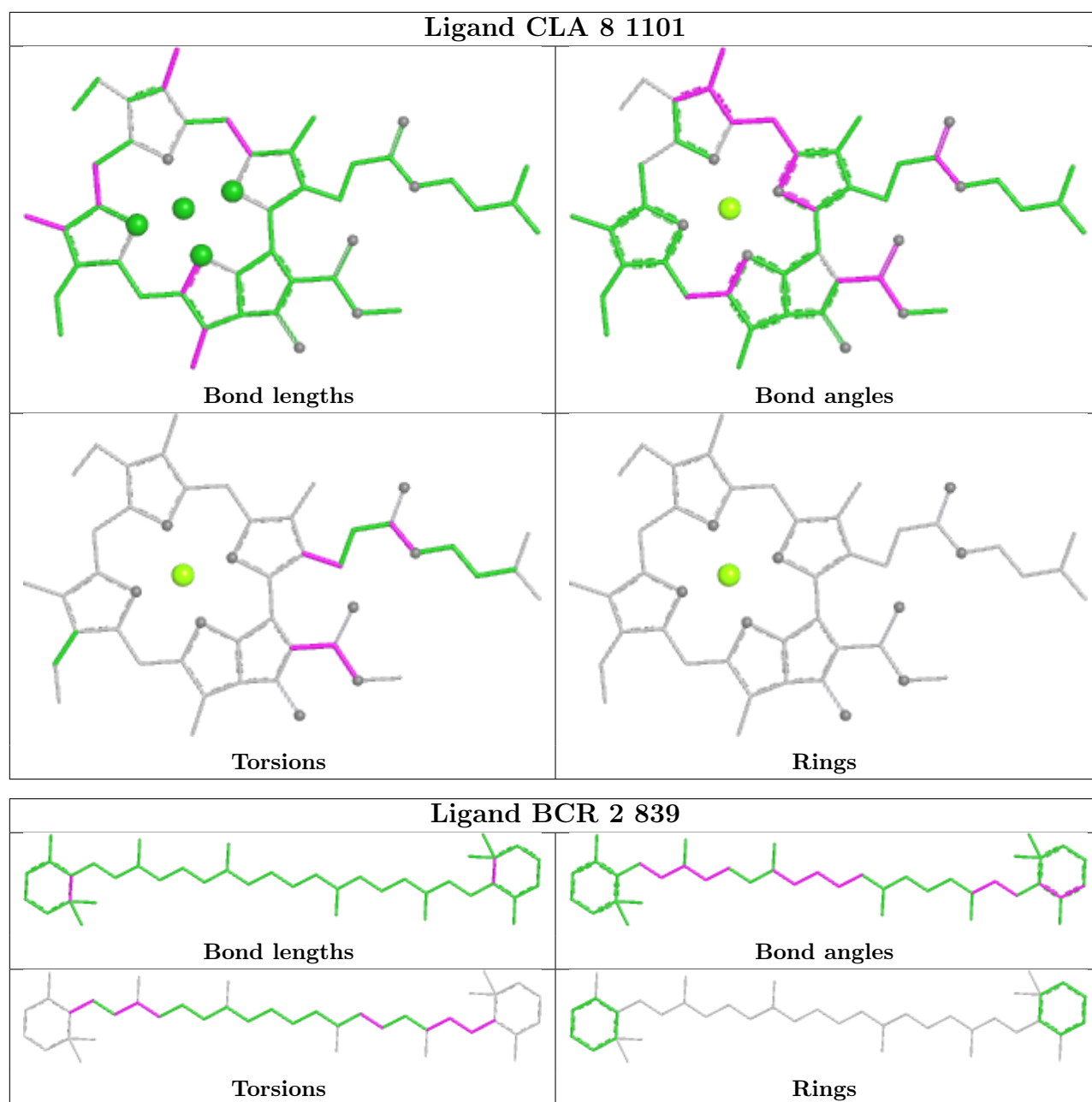


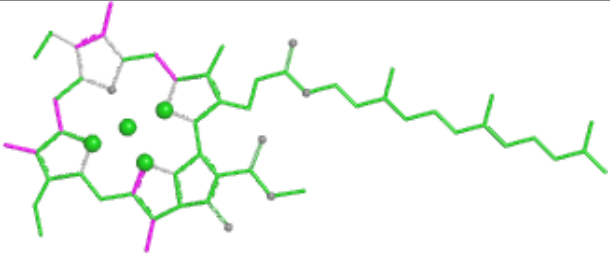
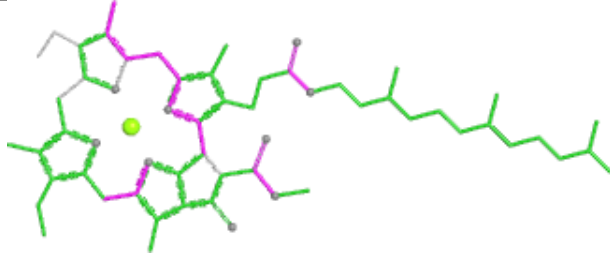
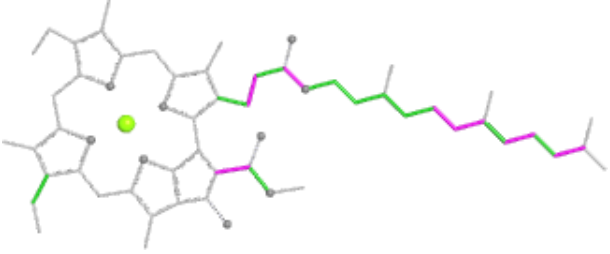
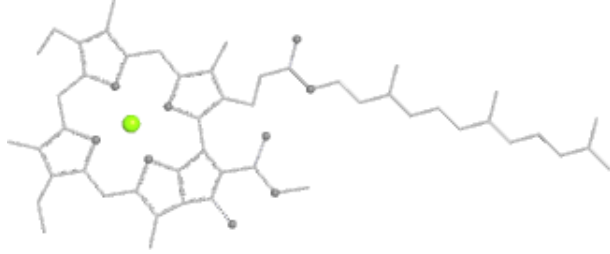
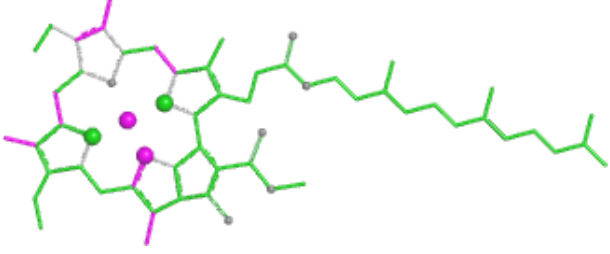
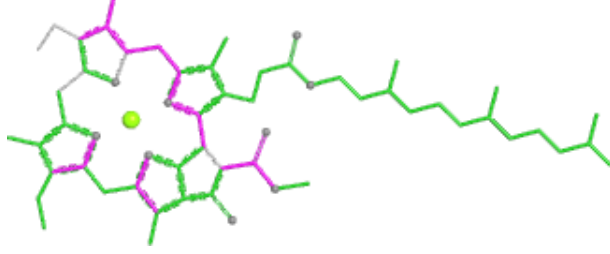
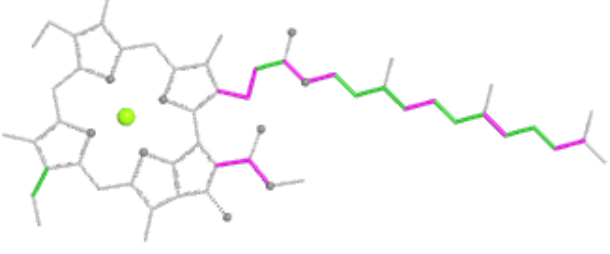
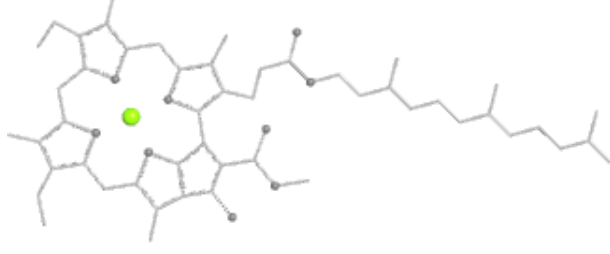
Ligand CLA b 816**Ligand CLA a 802**

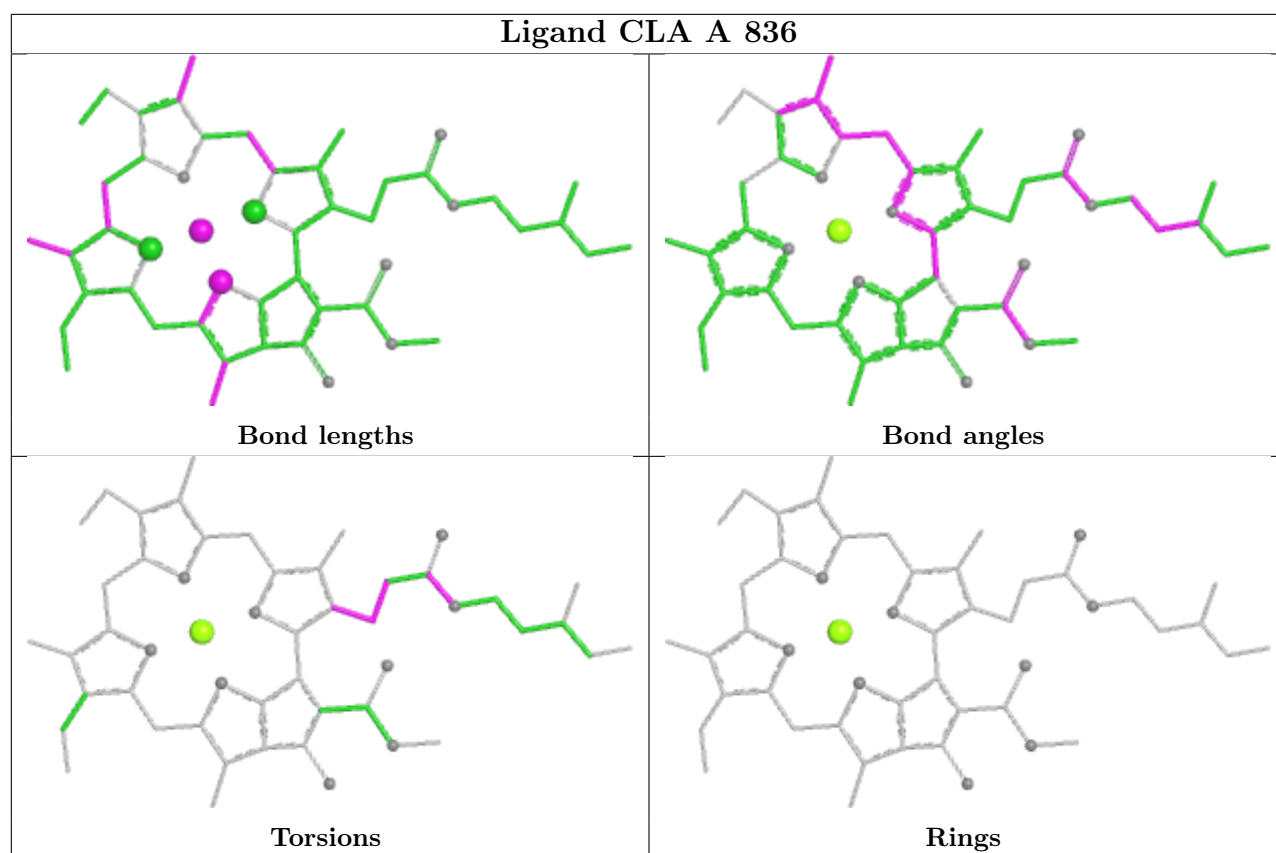
Ligand CLA 2 828**Ligand CLA A 833**

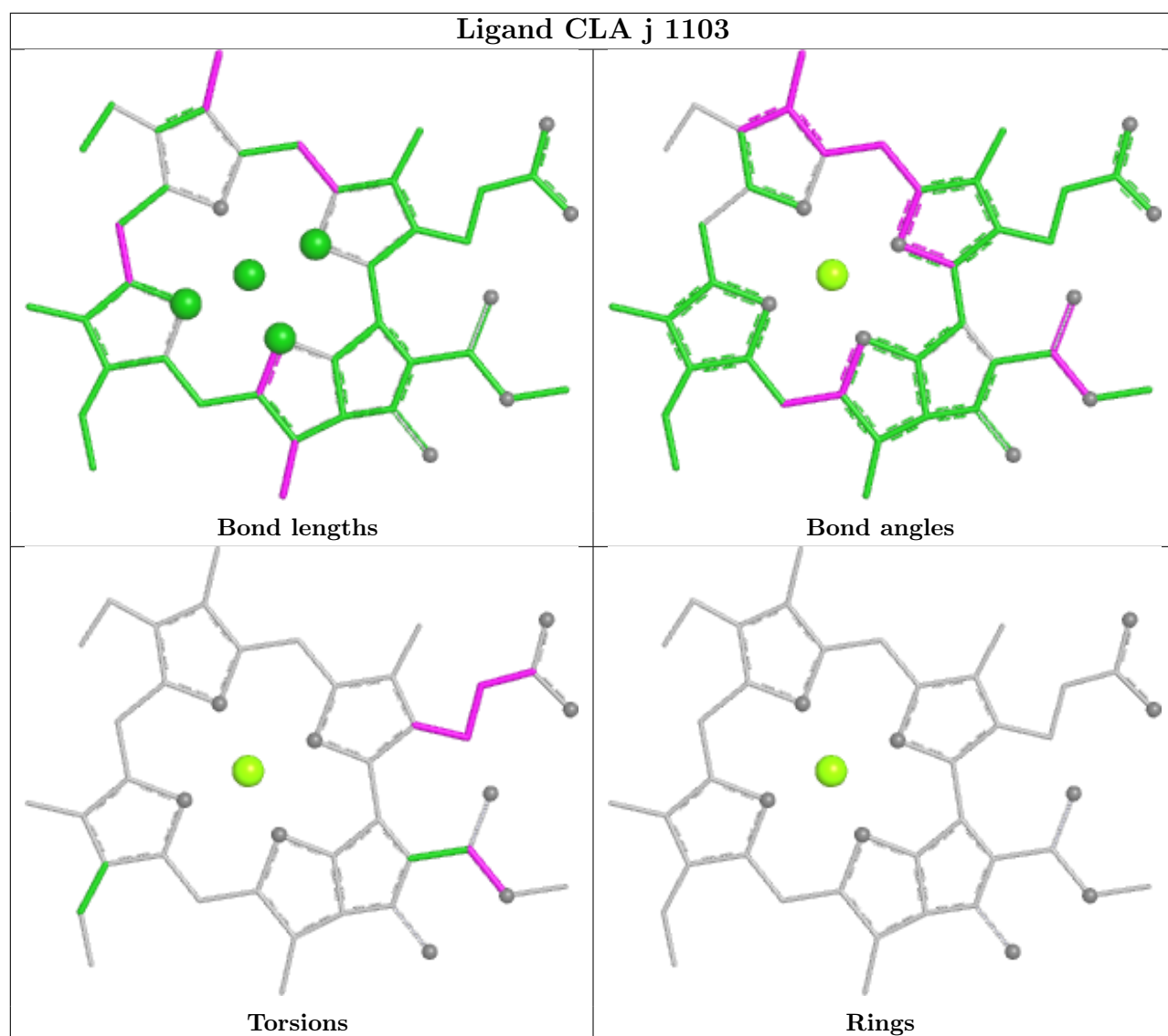
Ligand CLA 1 822

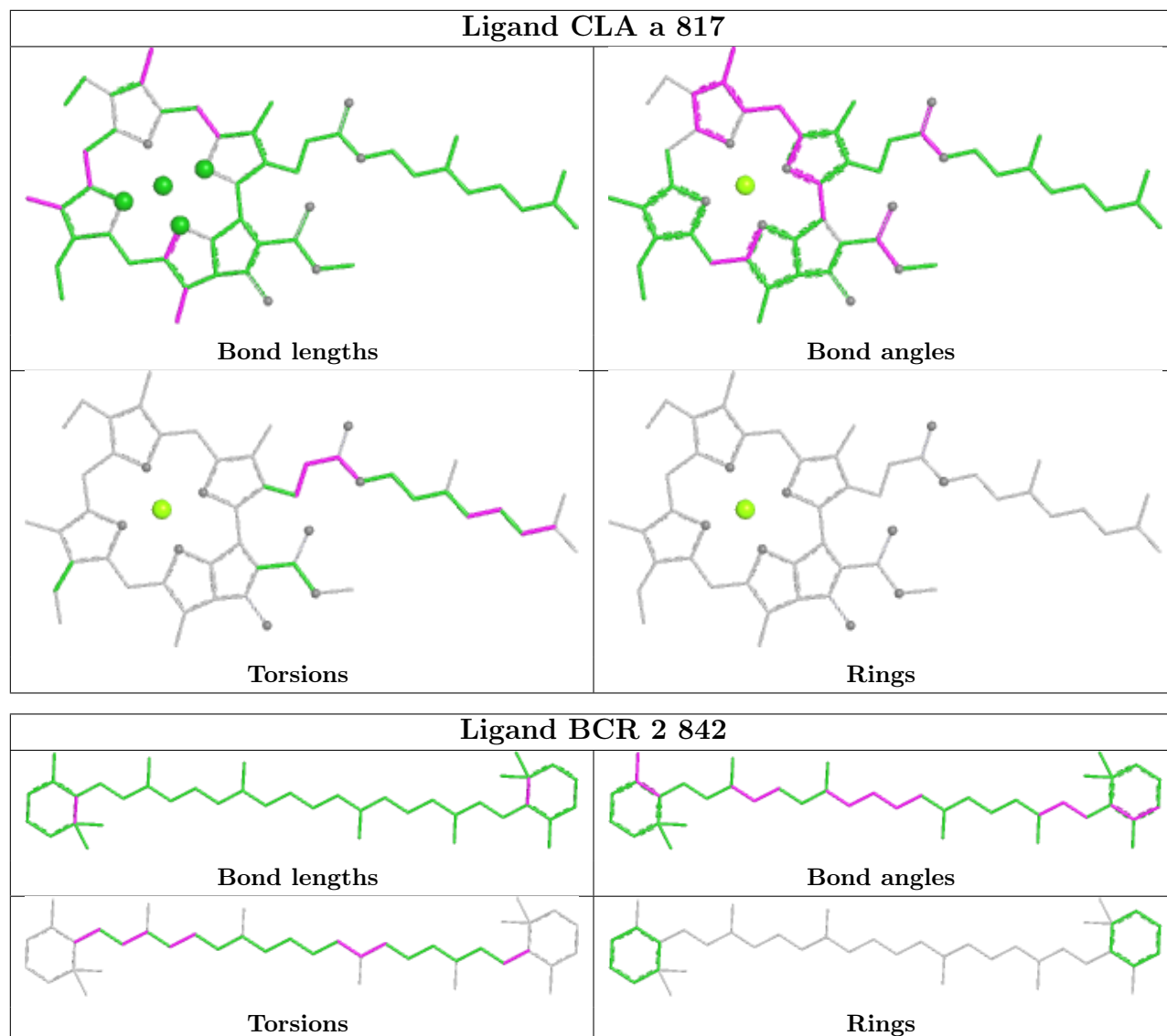




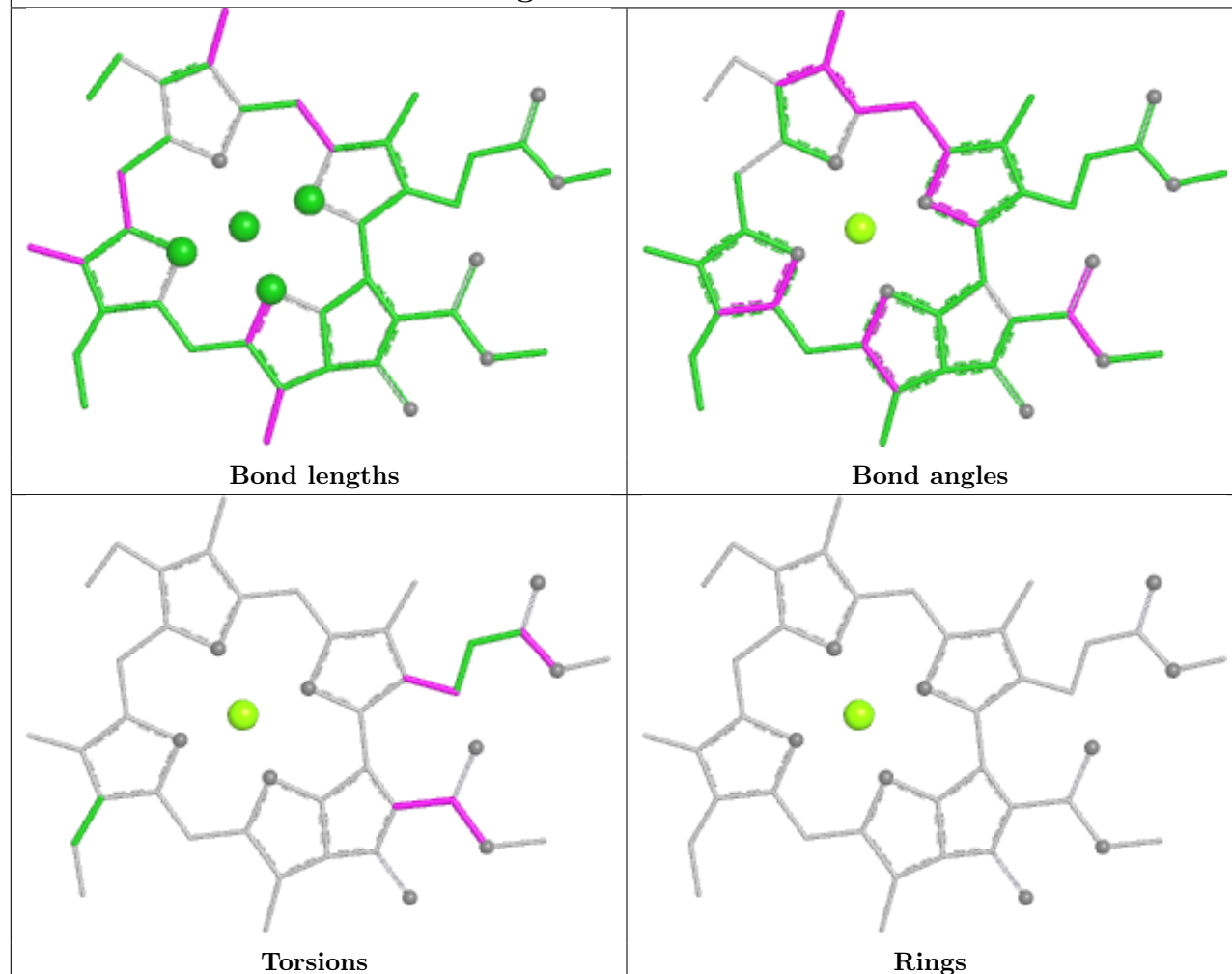
Ligand CLA 1 852	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA 2 825	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



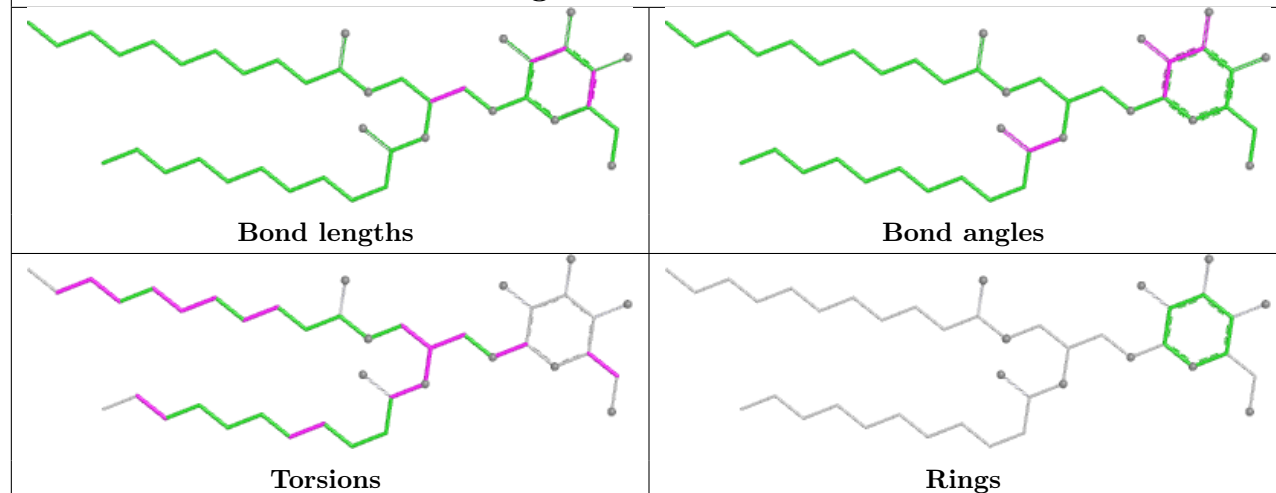


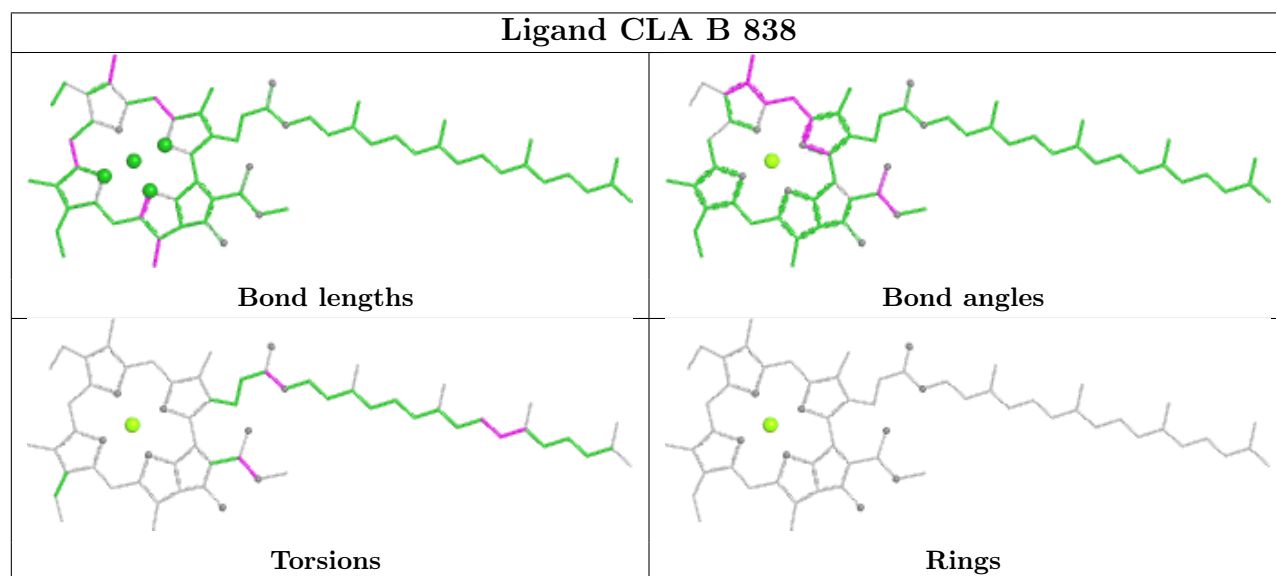
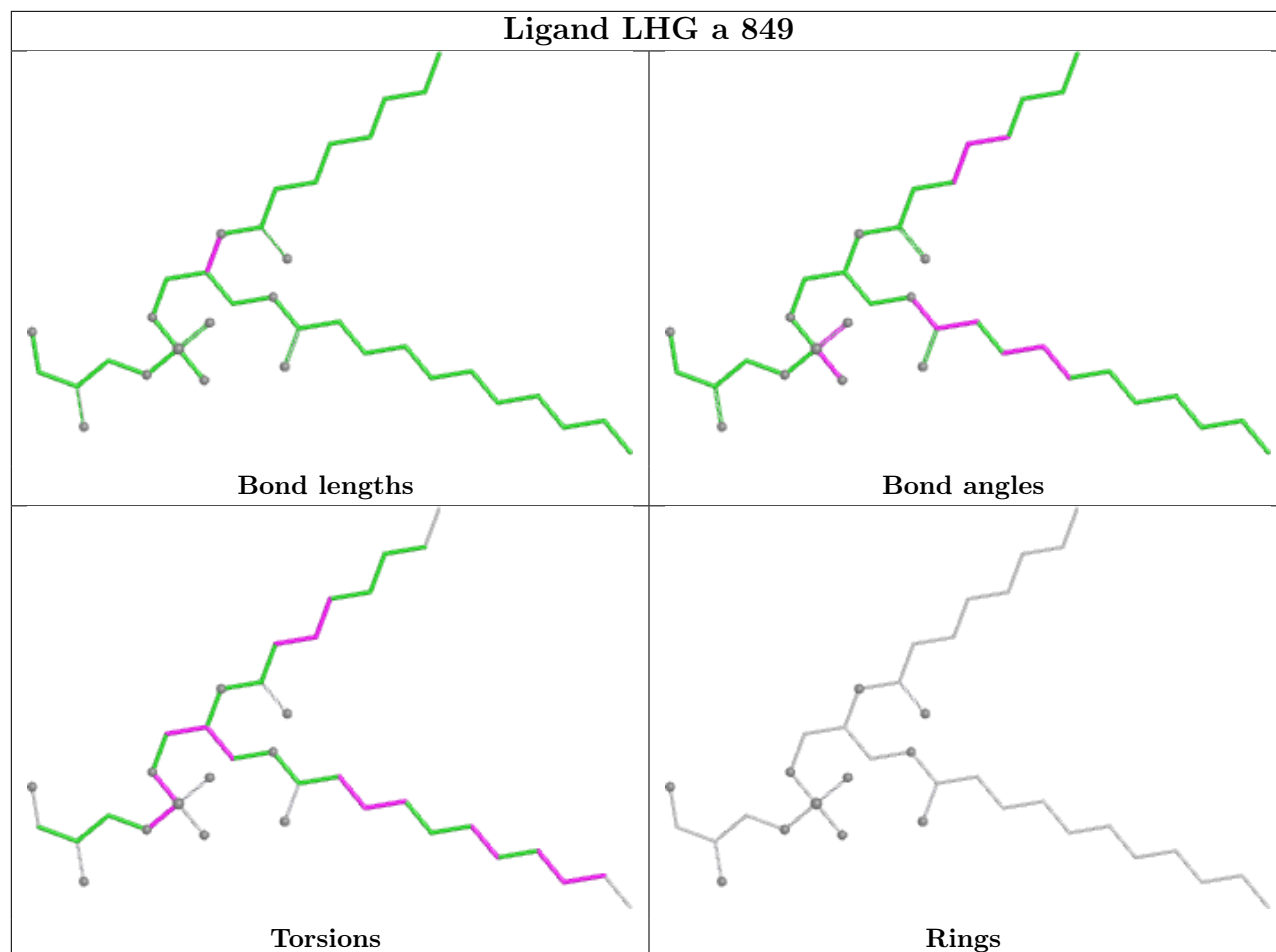


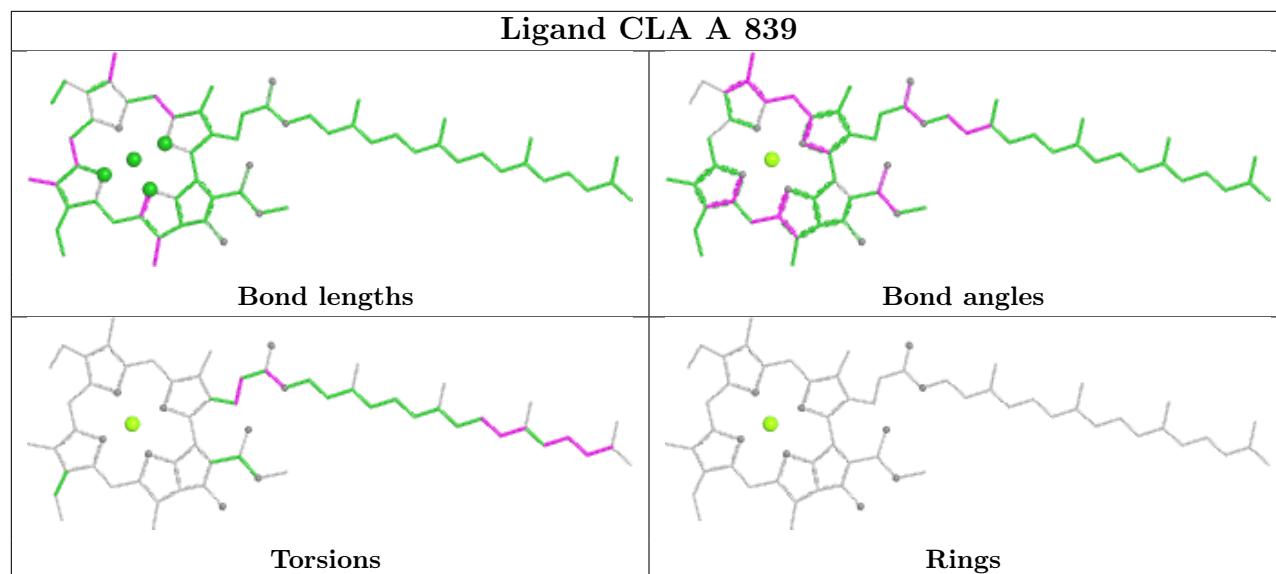
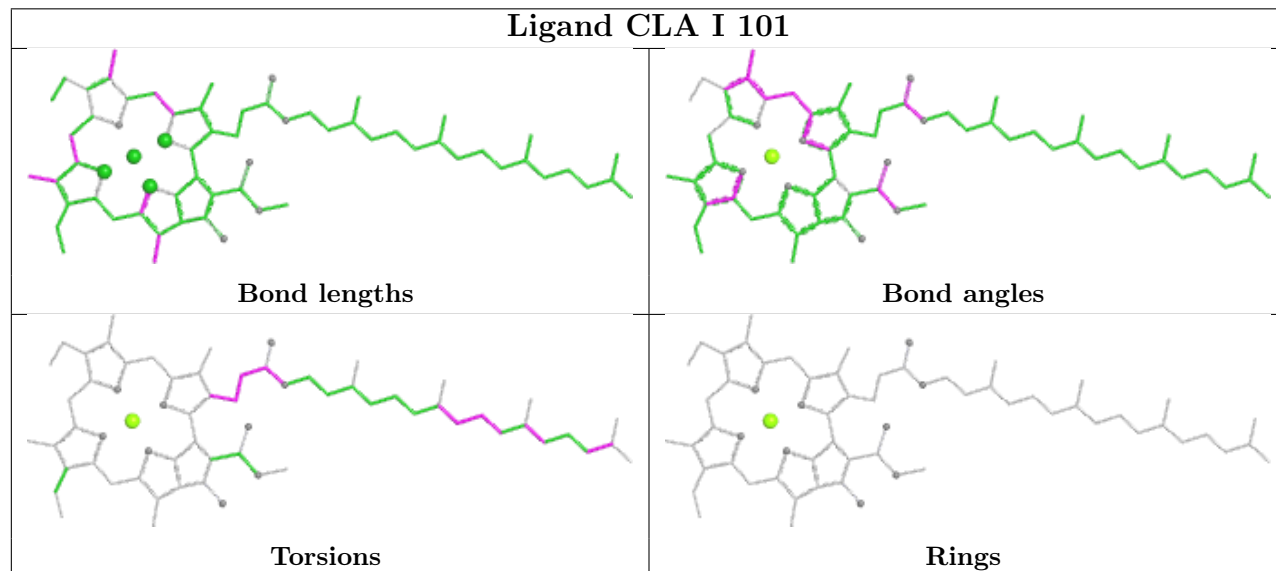
Ligand CLA b 811

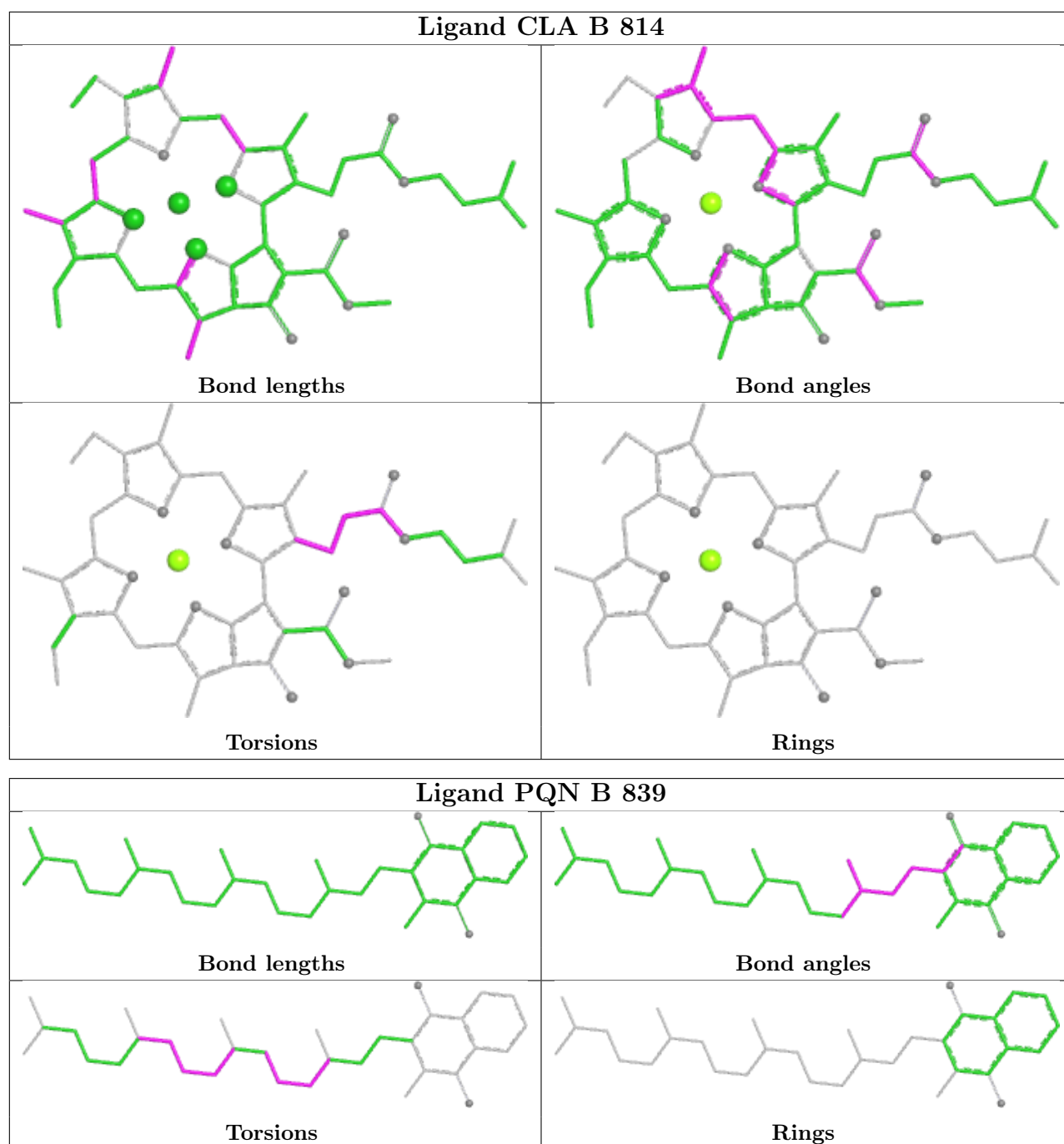


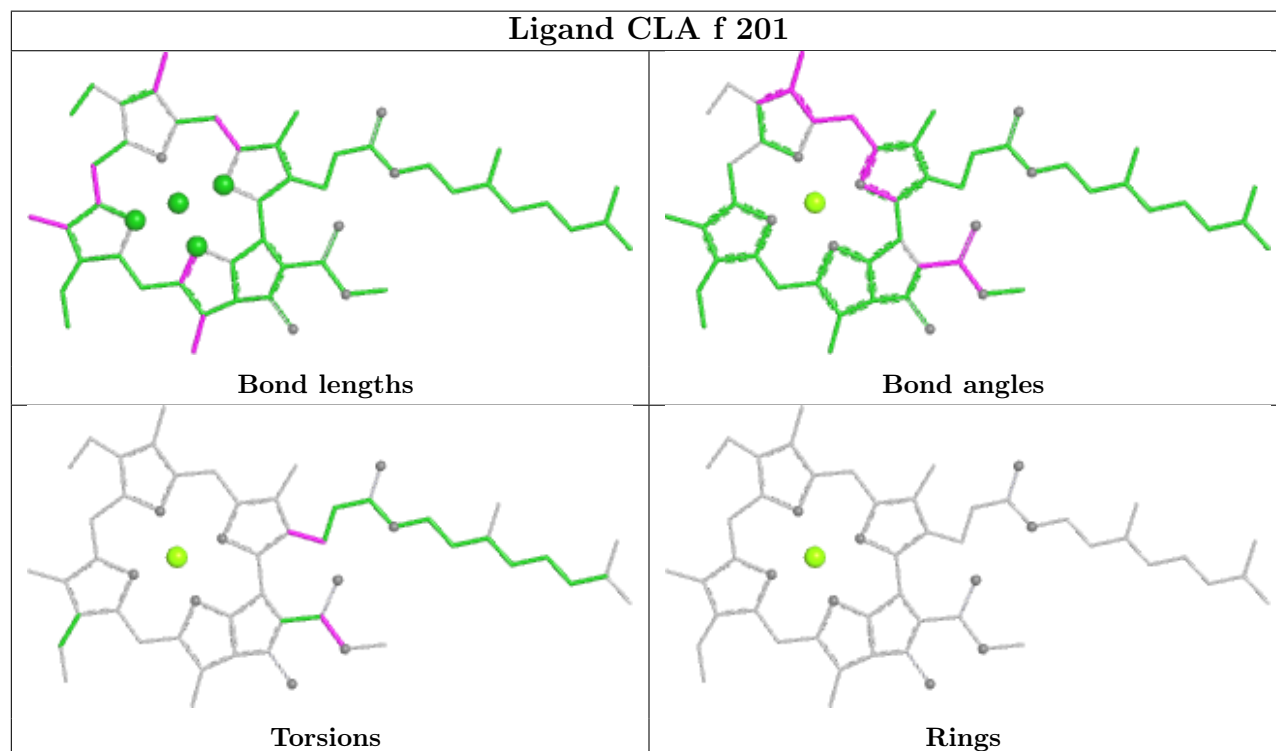
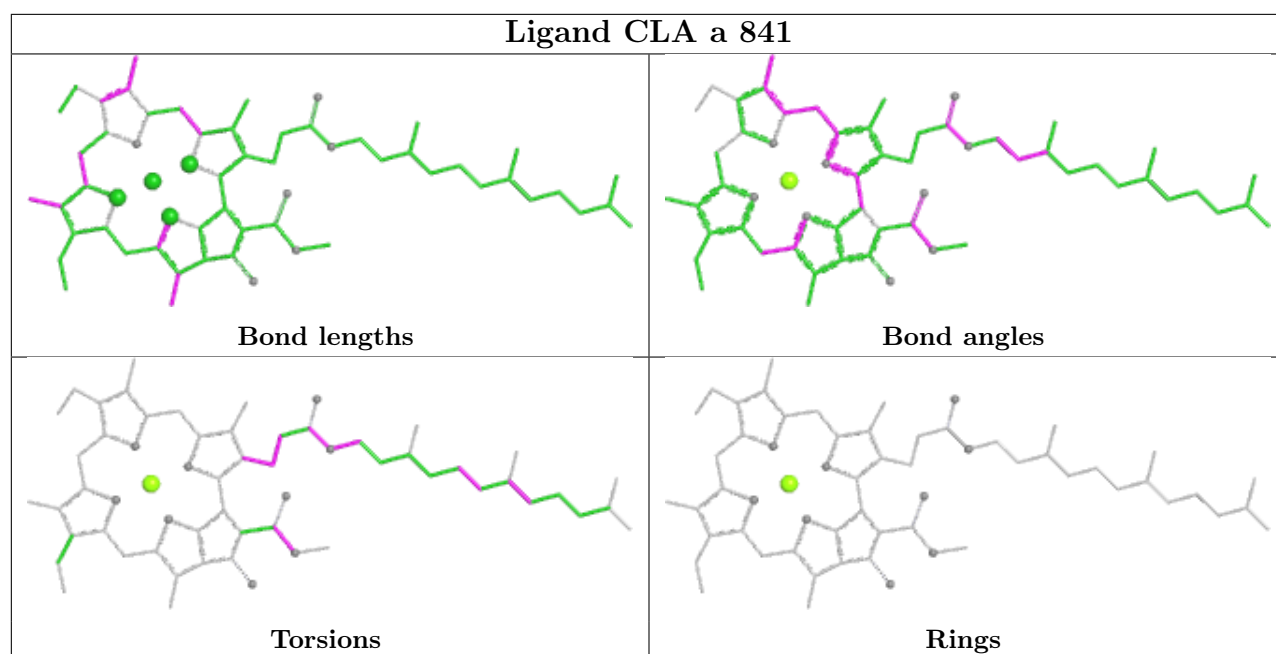
Ligand LMG b 846



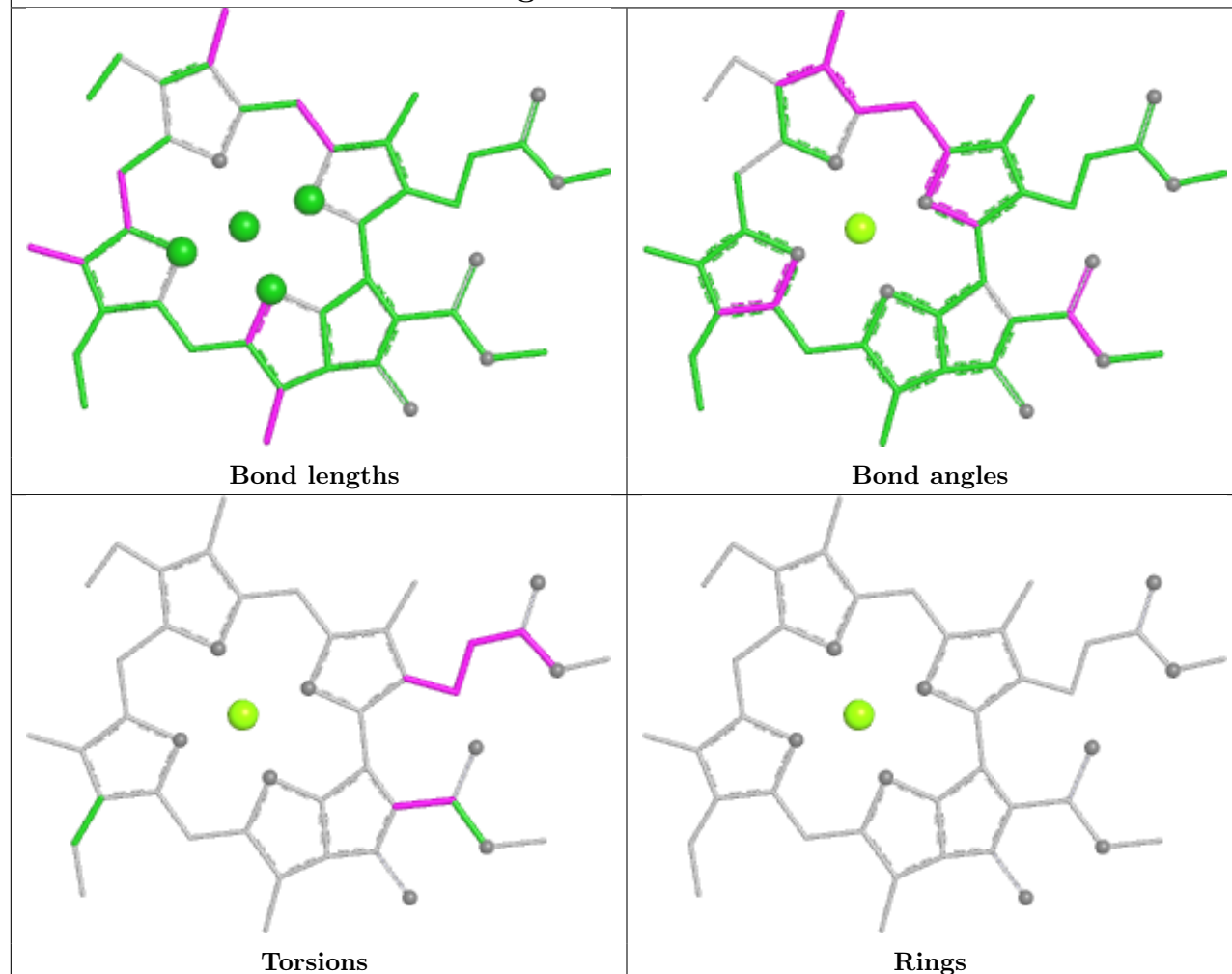


Ligand CLA A 839**Ligand CLA I 101**

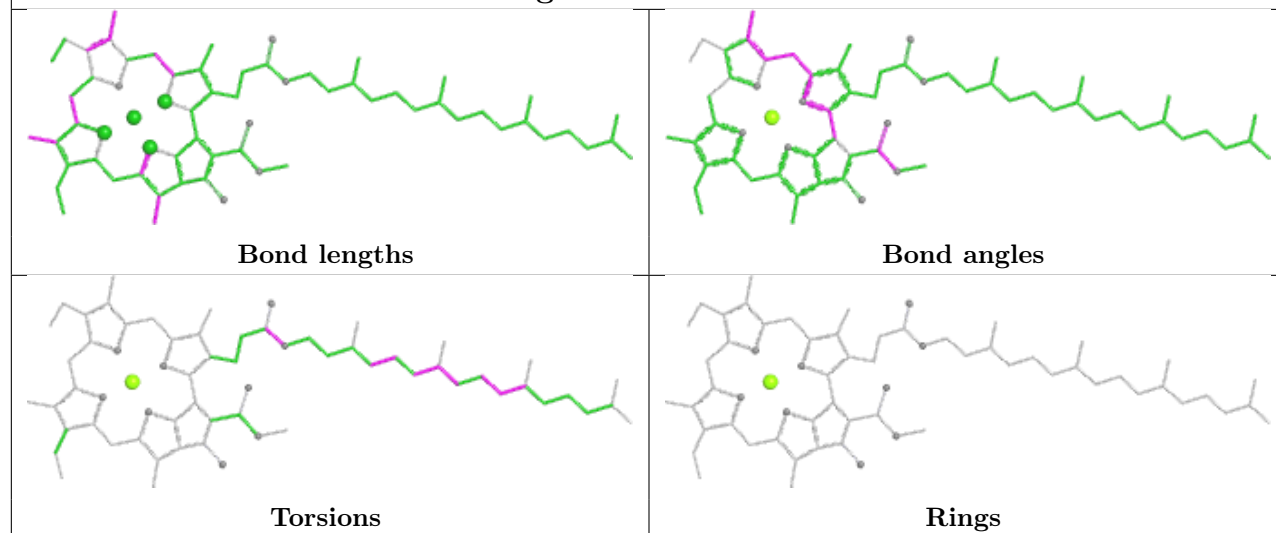




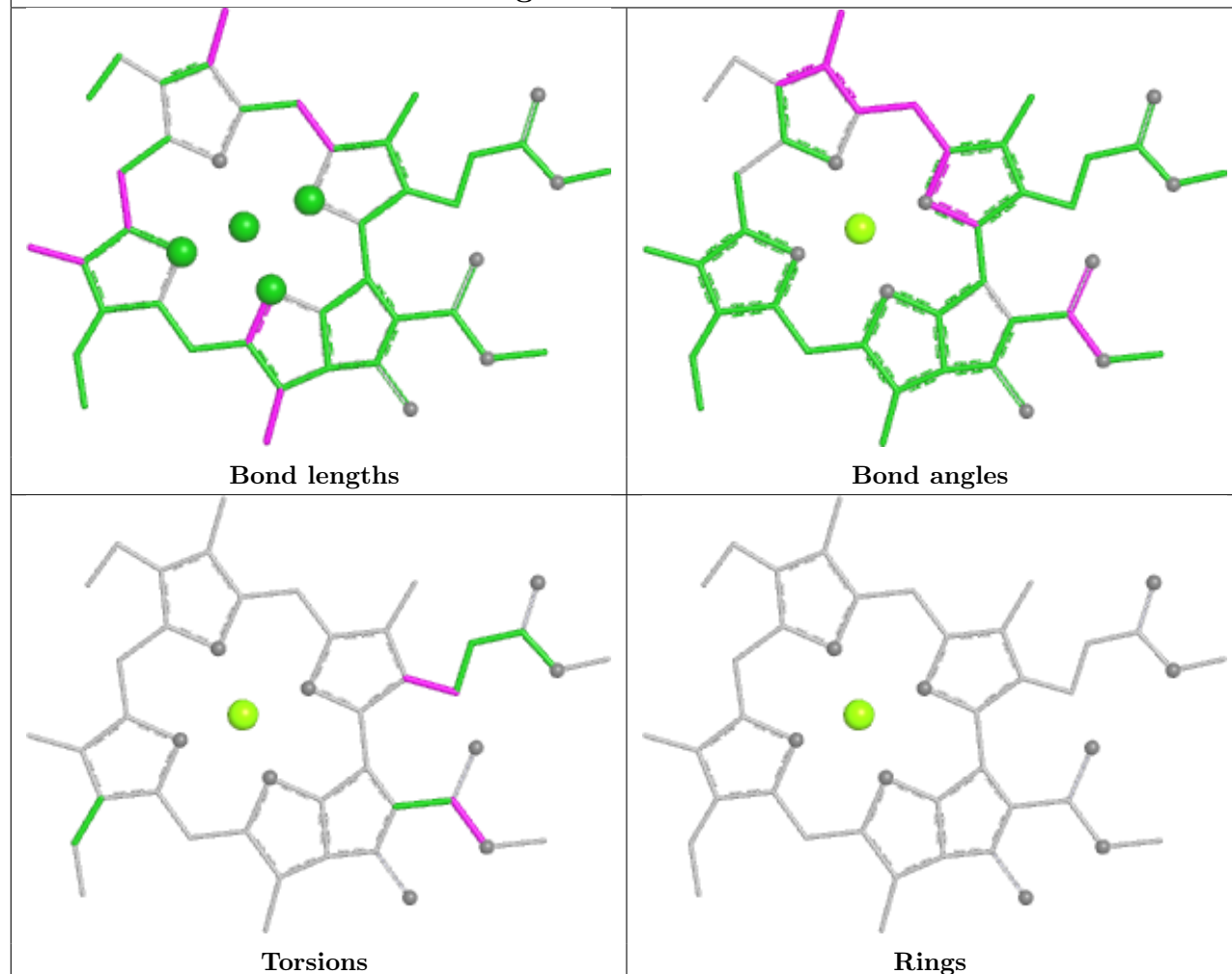
Ligand CLA 2 817



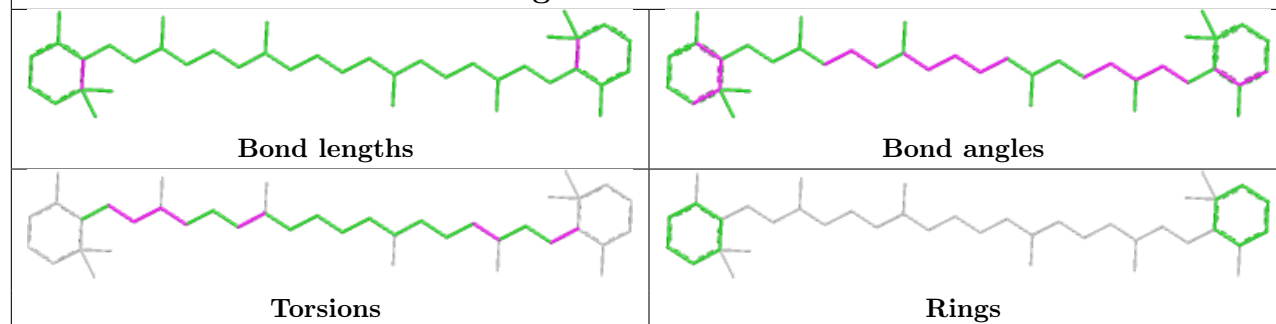
Ligand CLA a 834



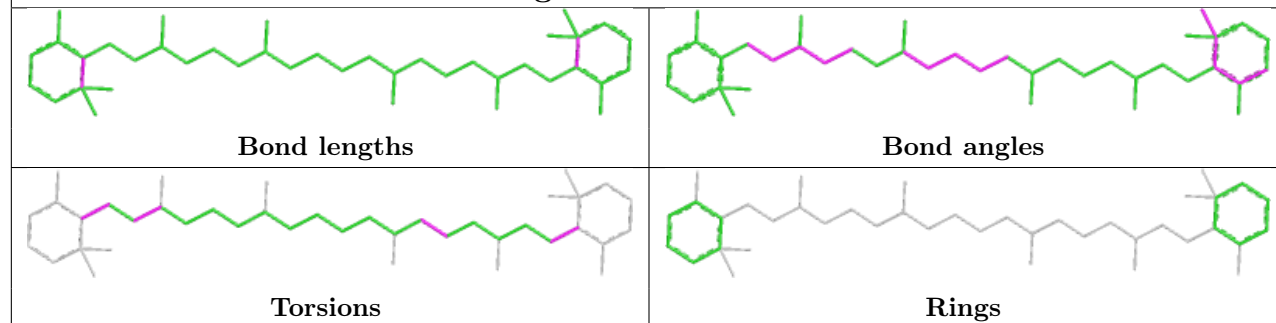
Ligand CLA L 204

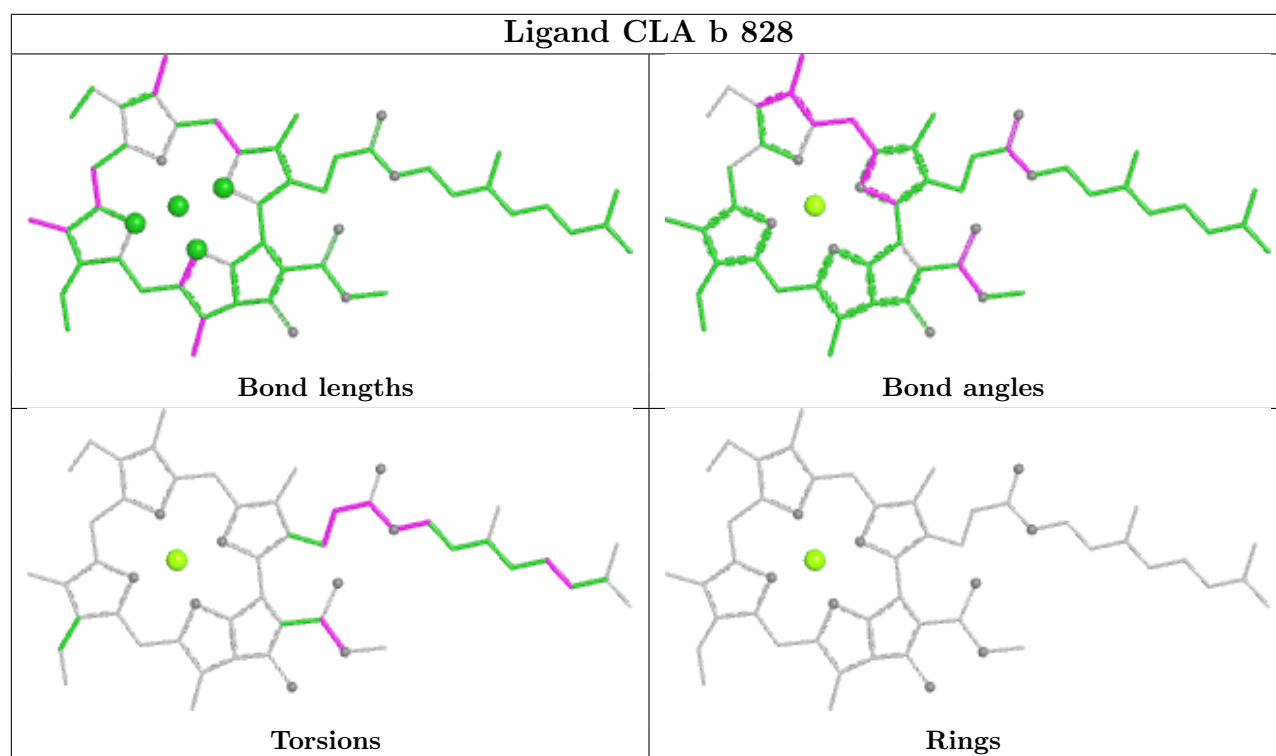


Ligand BCR L 202

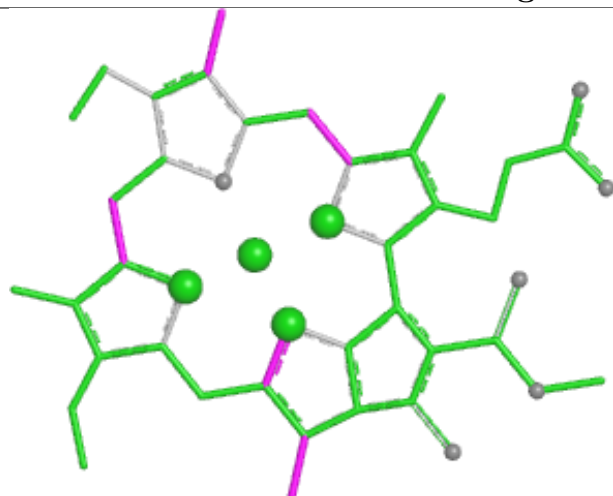


Ligand BCR 0 201

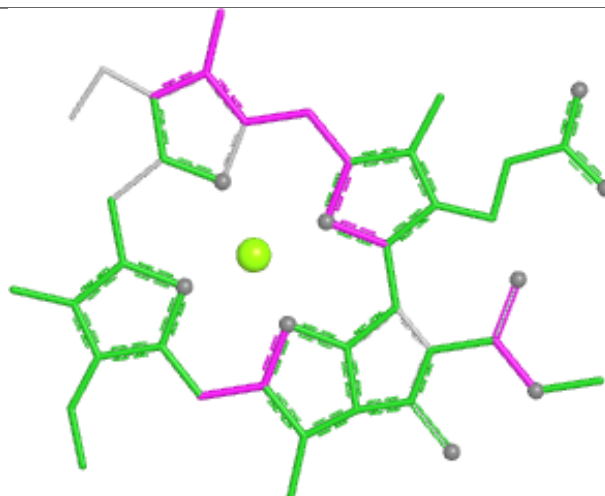




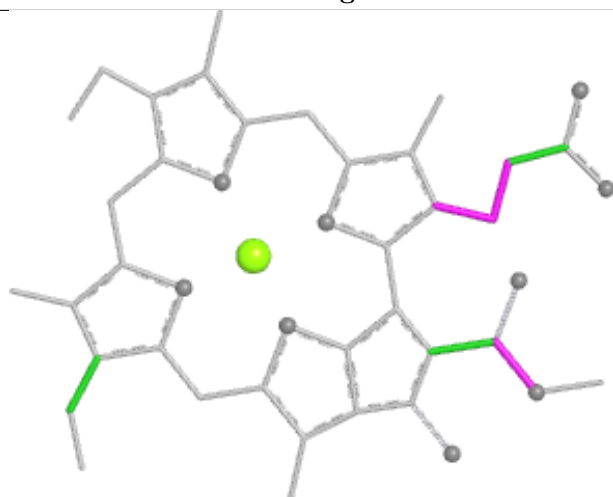
Ligand CLA b 809



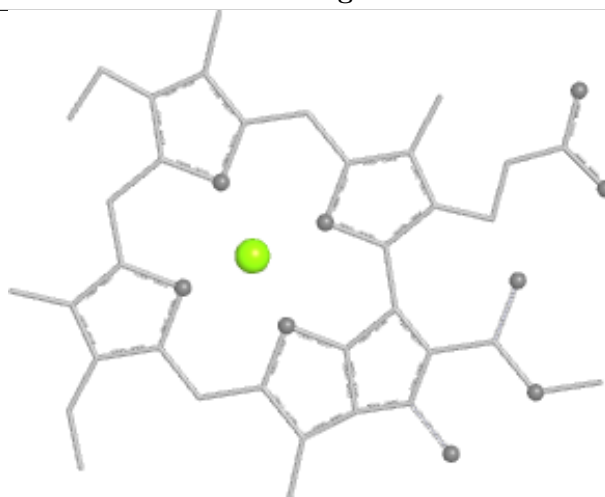
Bond lengths



Bond angles

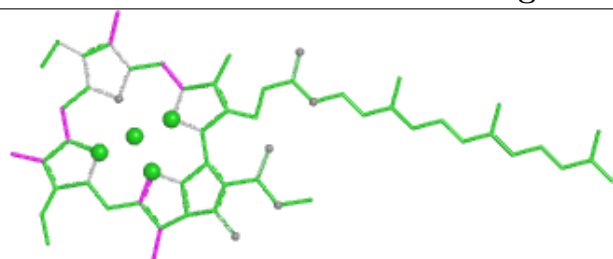


Torsions

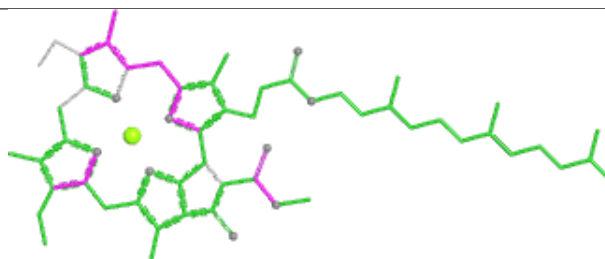


Rings

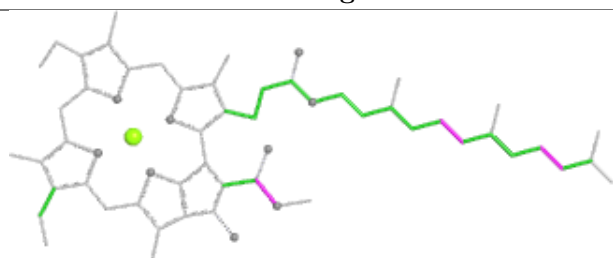
Ligand CLA 2 833



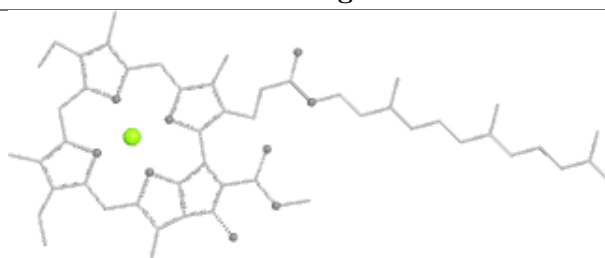
Bond lengths



Bond angles

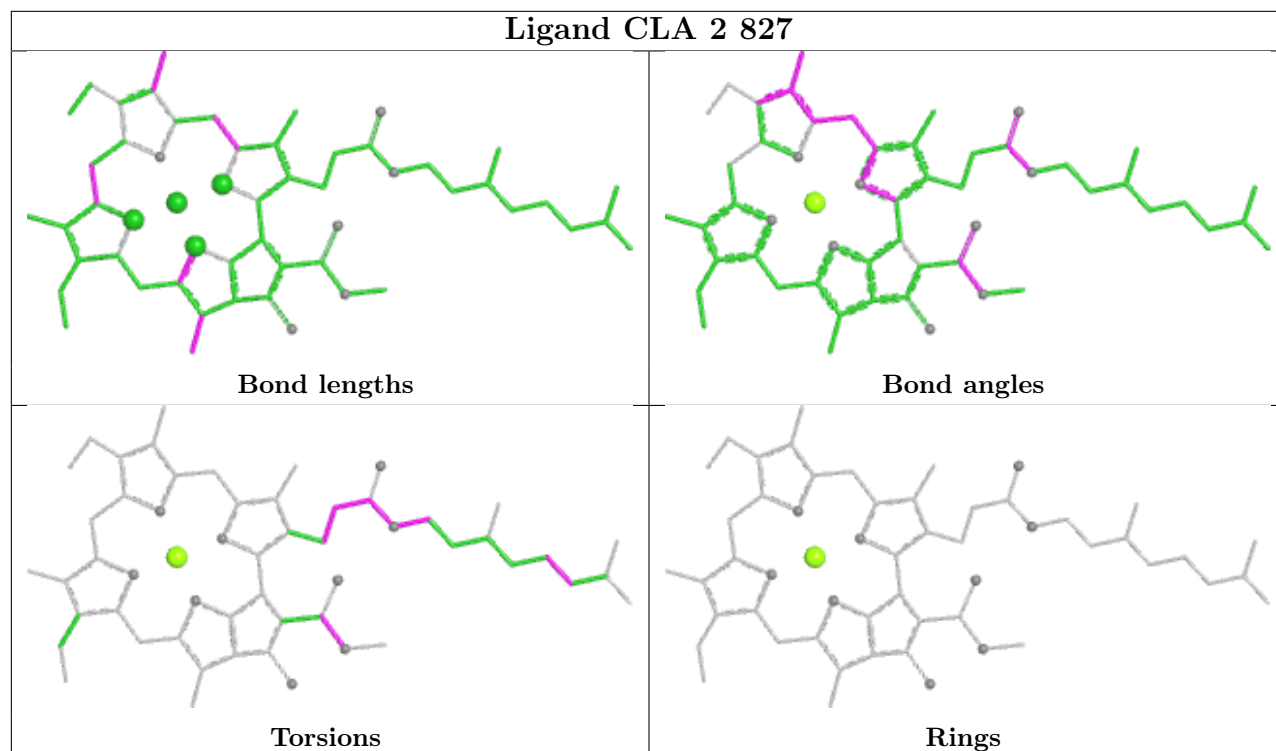


Torsions

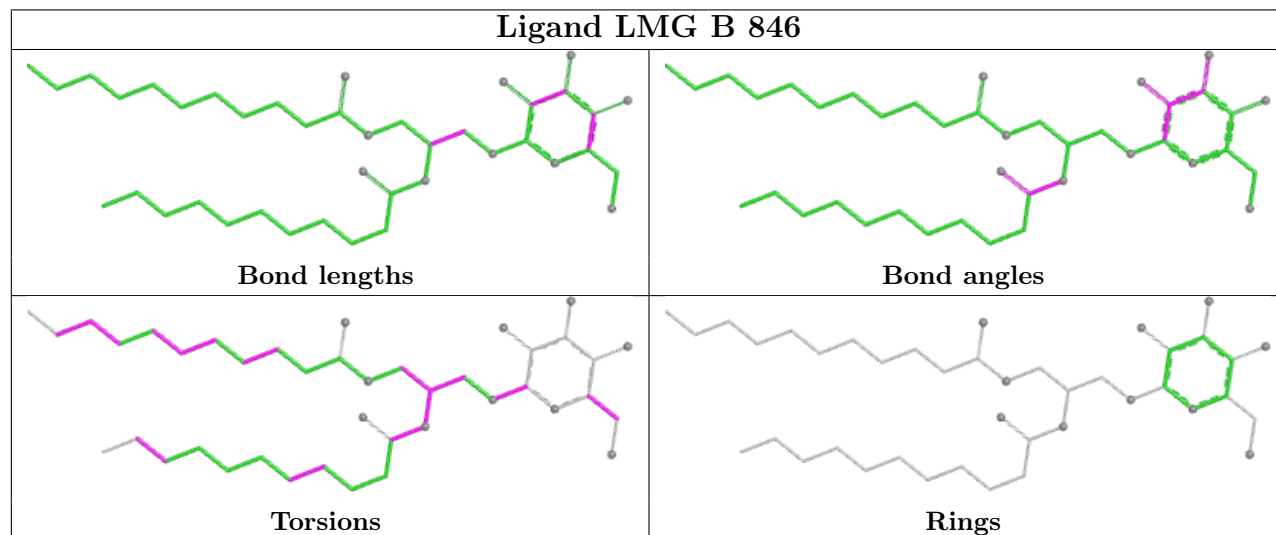


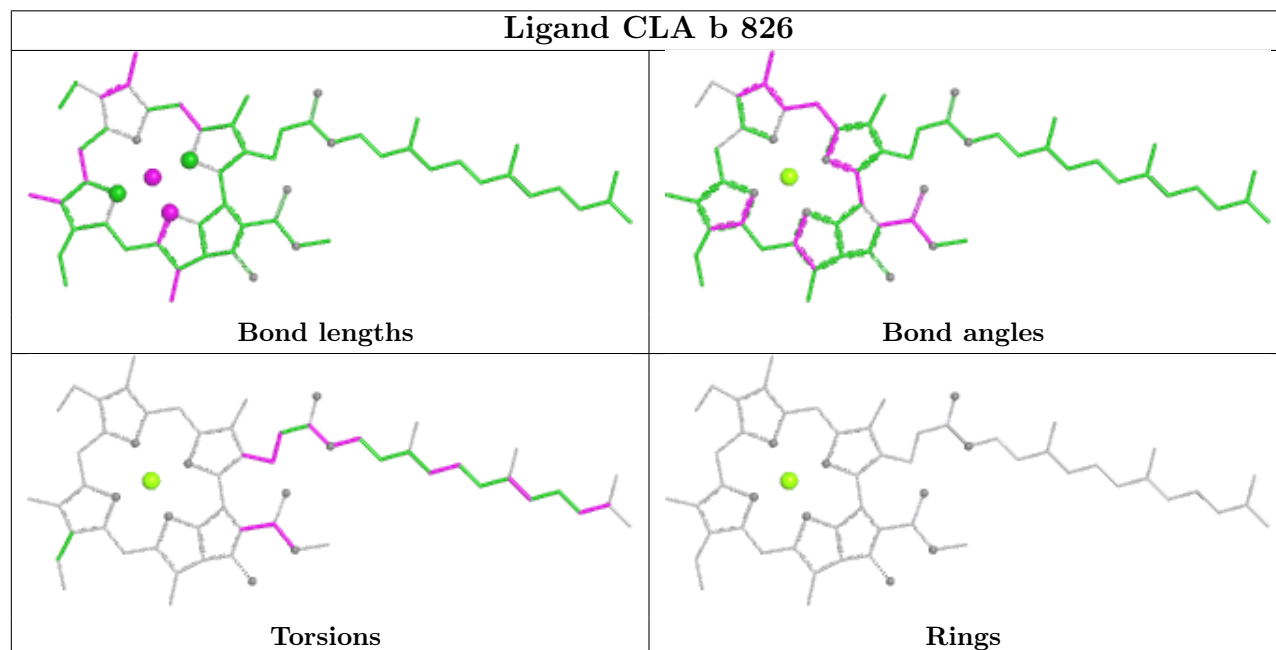
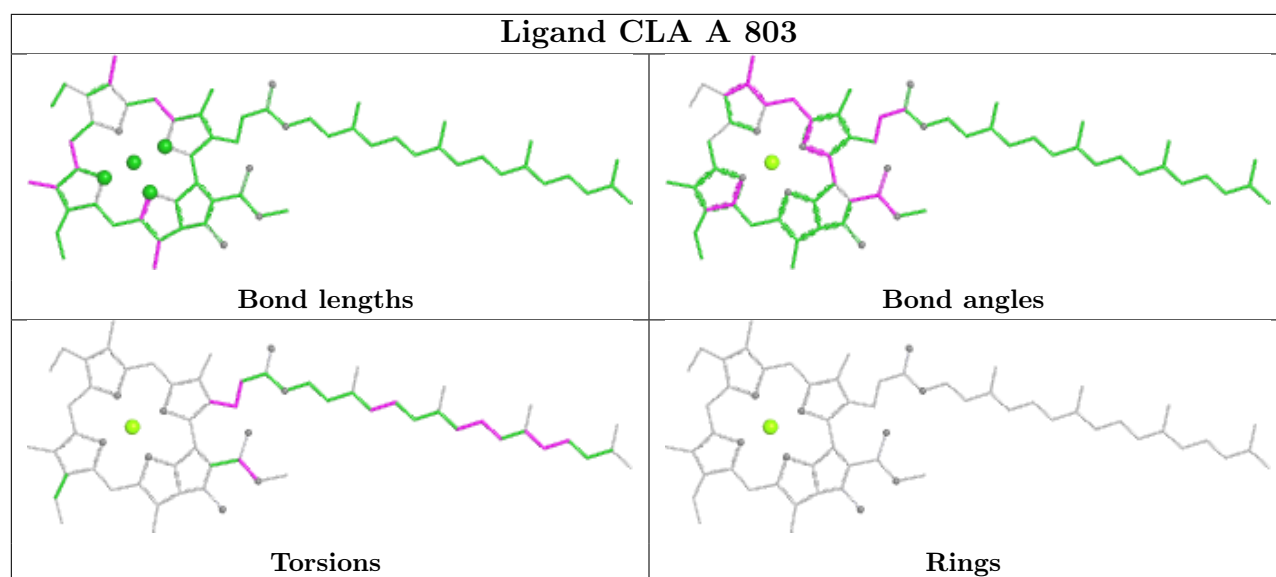
Rings

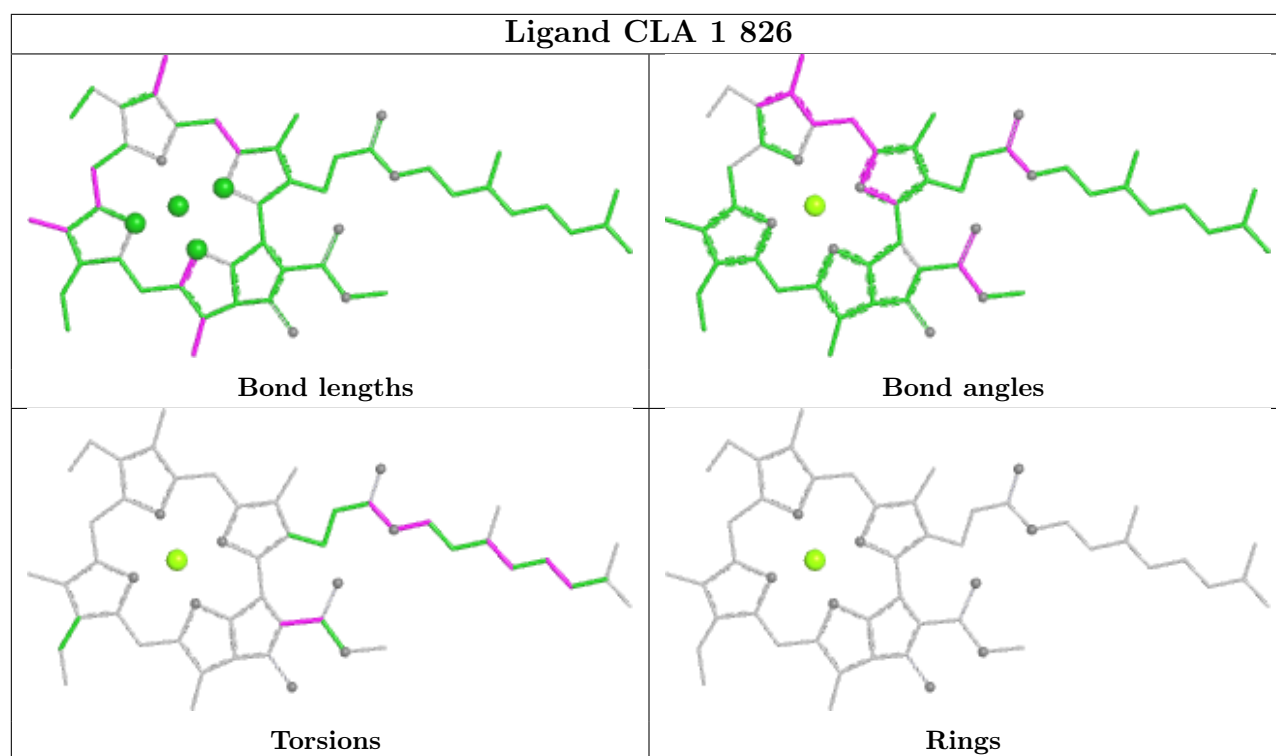
Ligand CLA 2 827



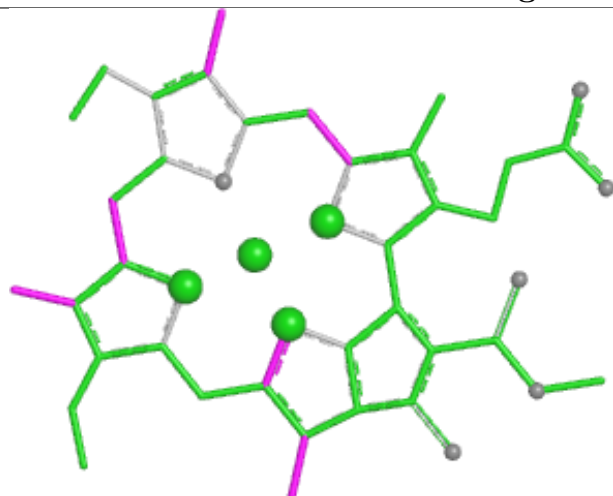
Ligand LMG B 846



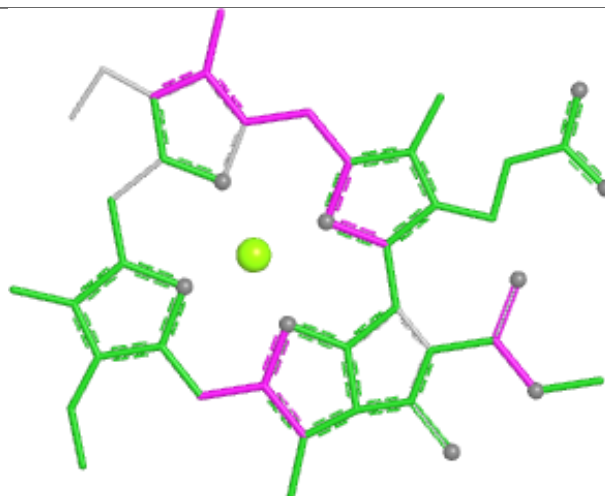




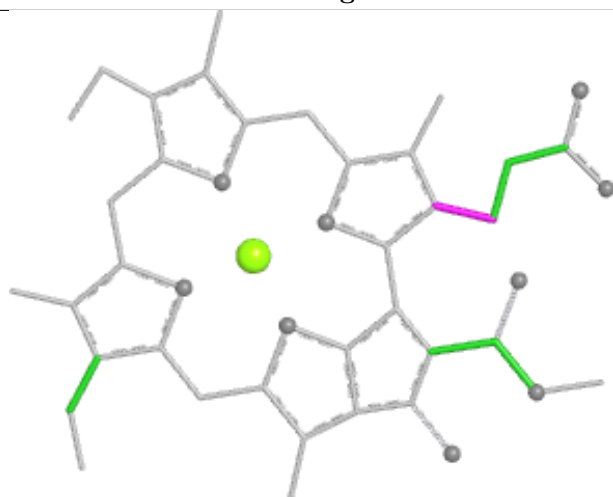
Ligand CLA a 815



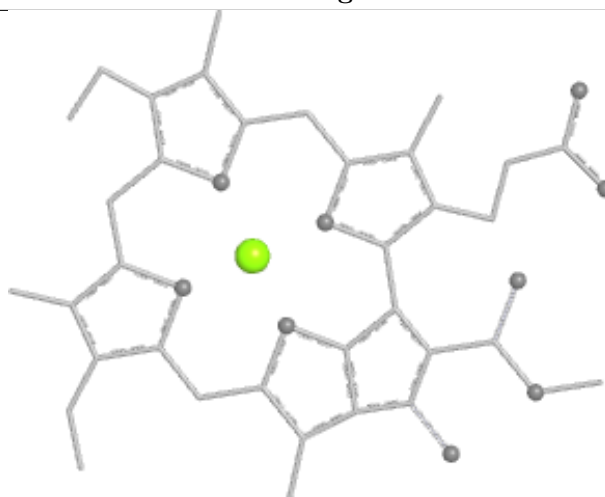
Bond lengths



Bond angles

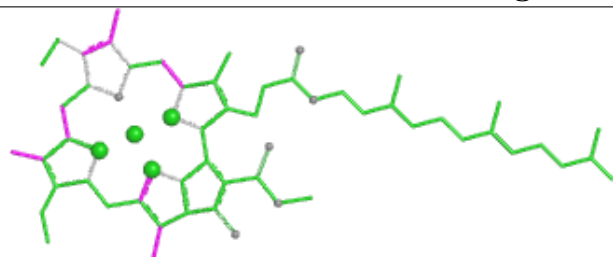


Torsions

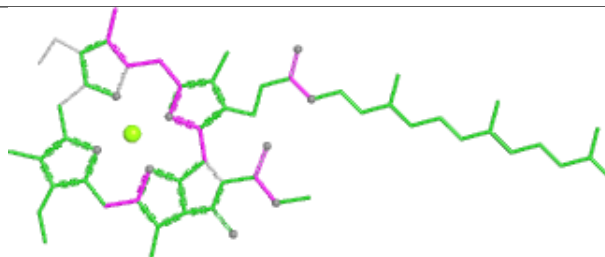


Rings

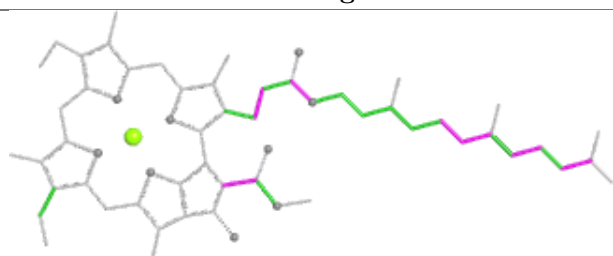
Ligand CLA A 852



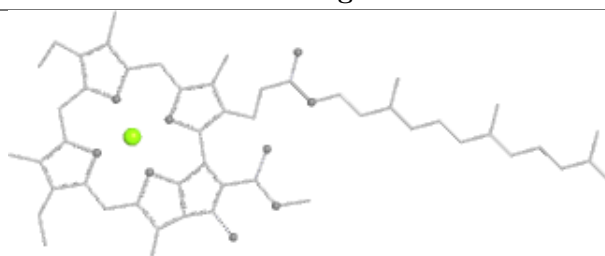
Bond lengths



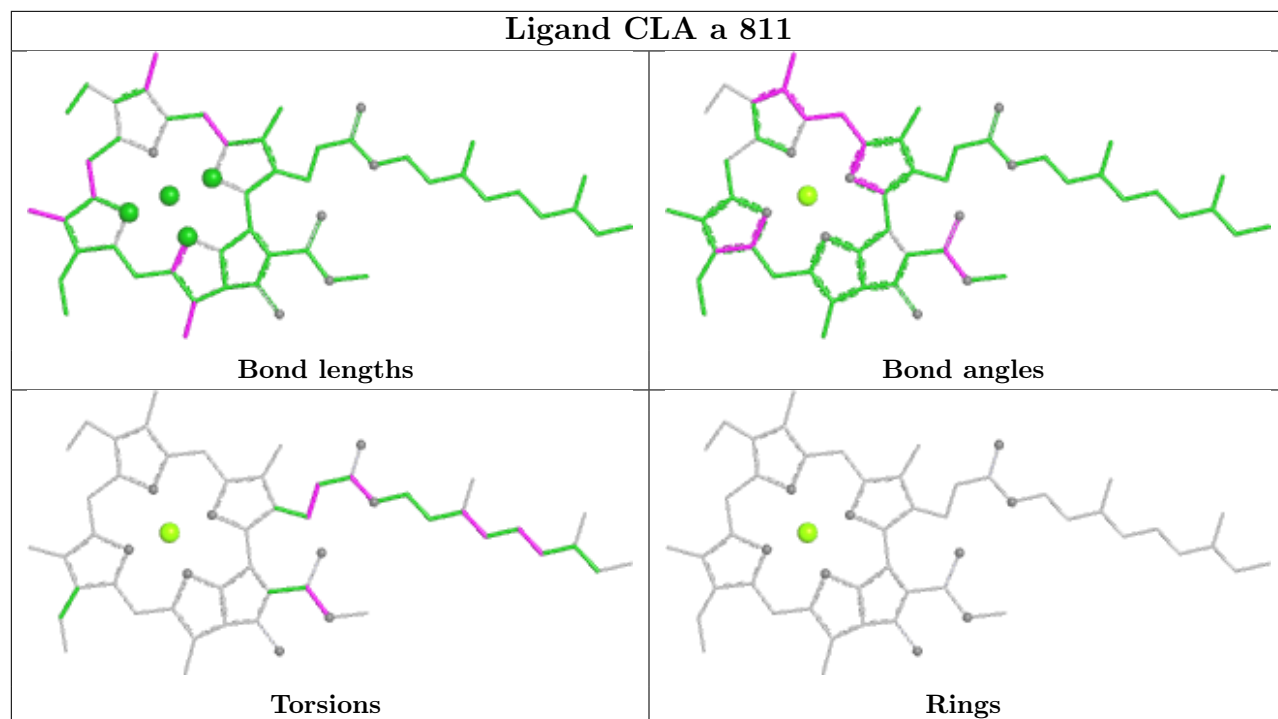
Bond angles

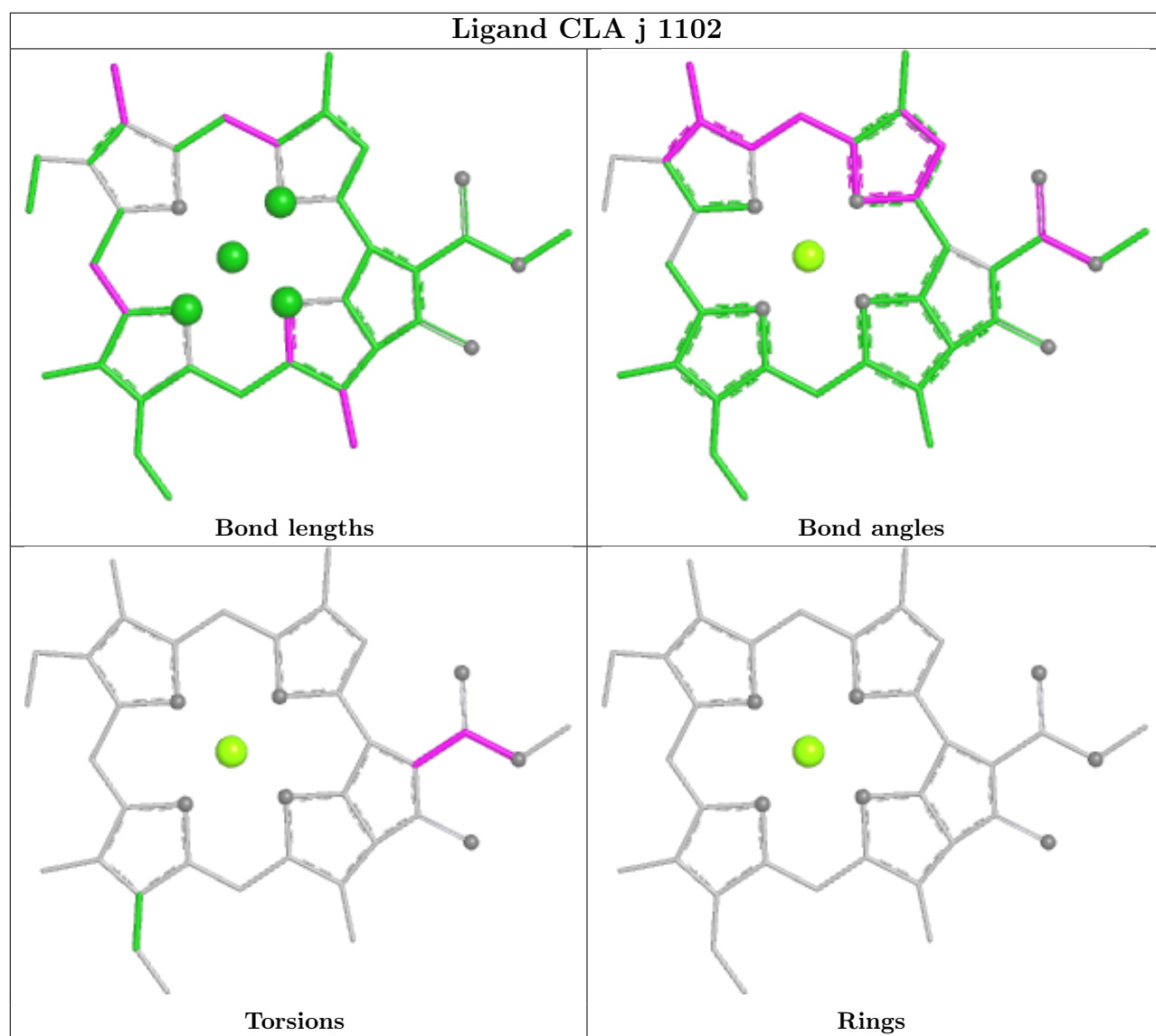


Torsions

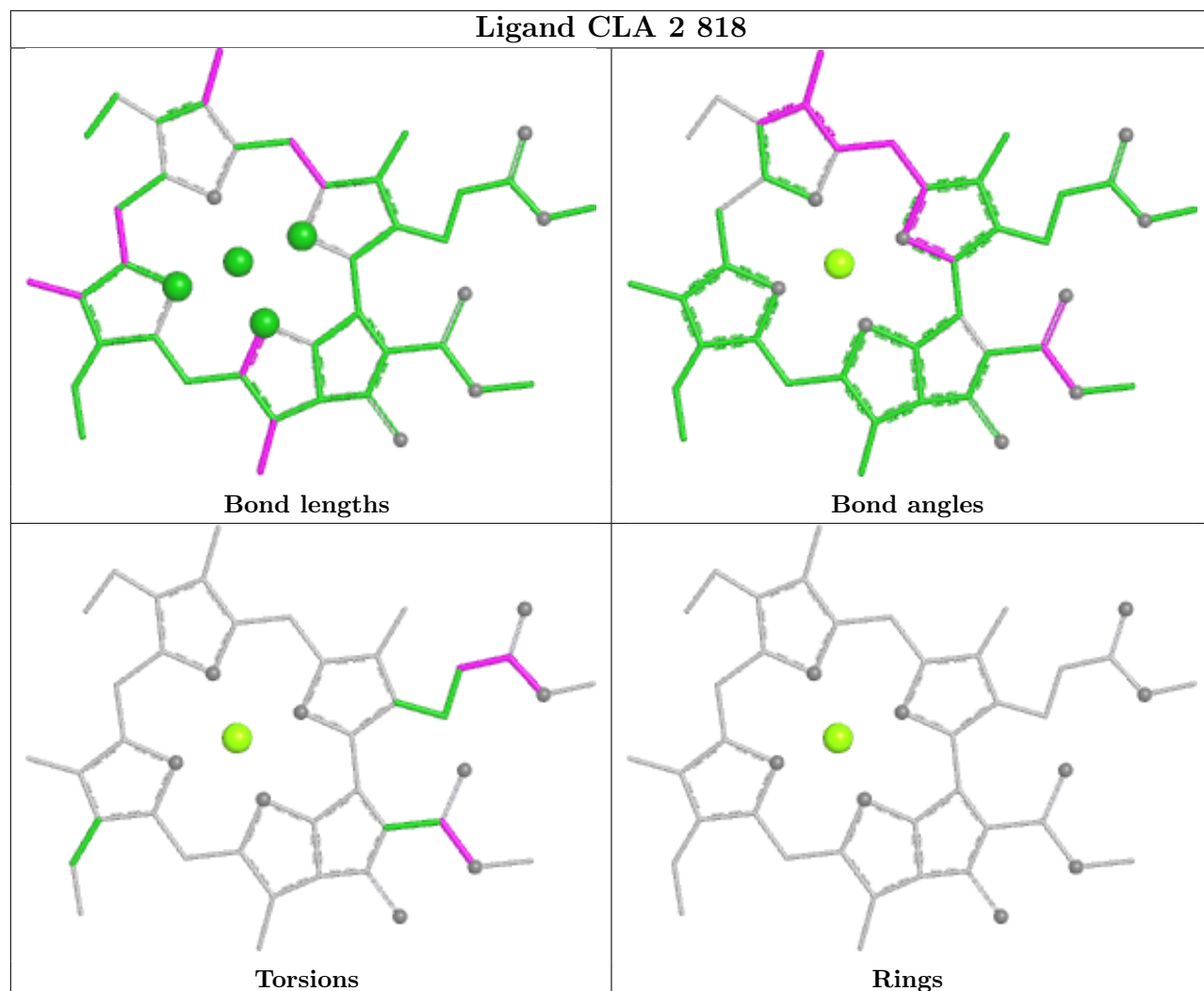


Rings

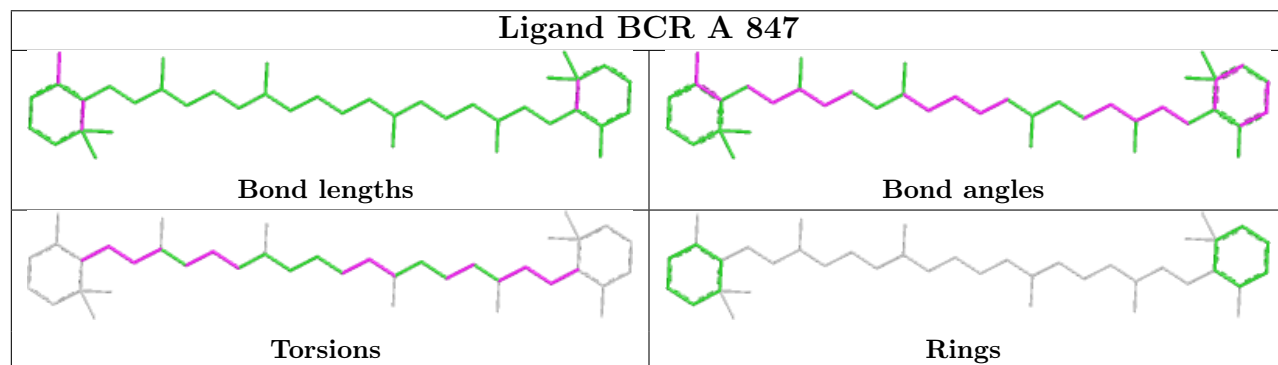




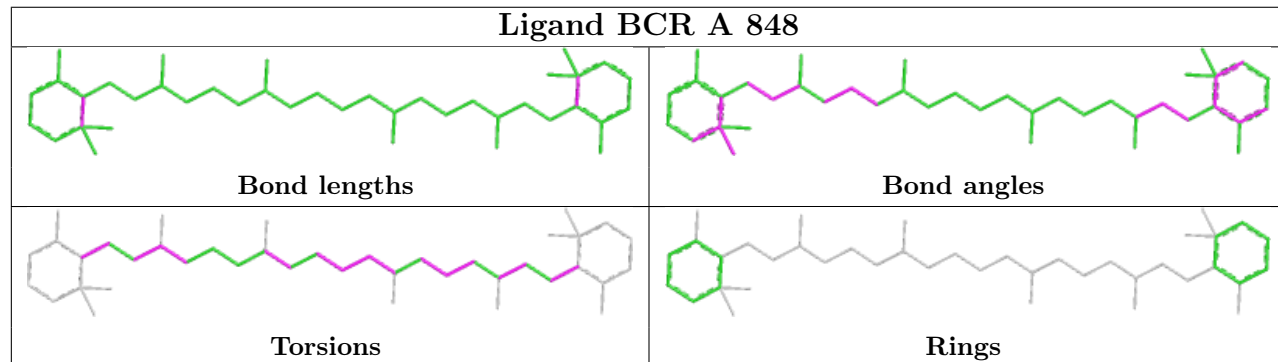
Ligand CLA 2 818

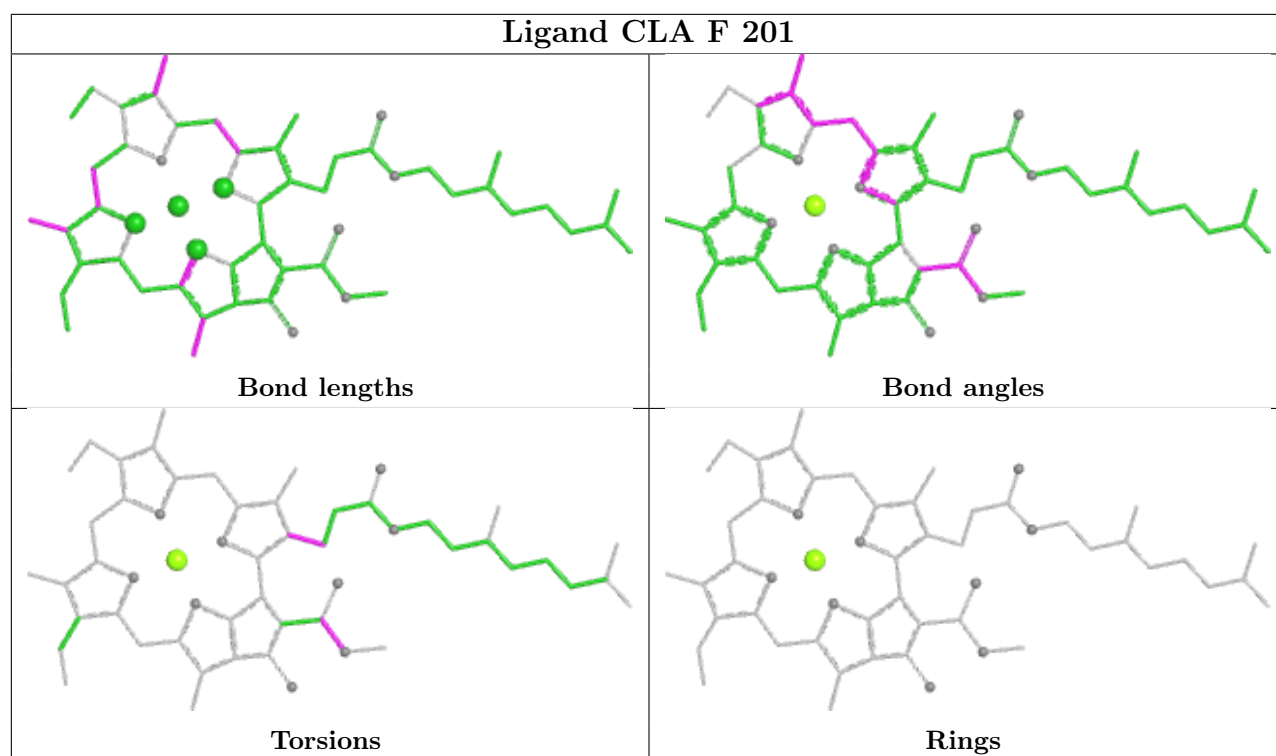


Ligand BCR A 847

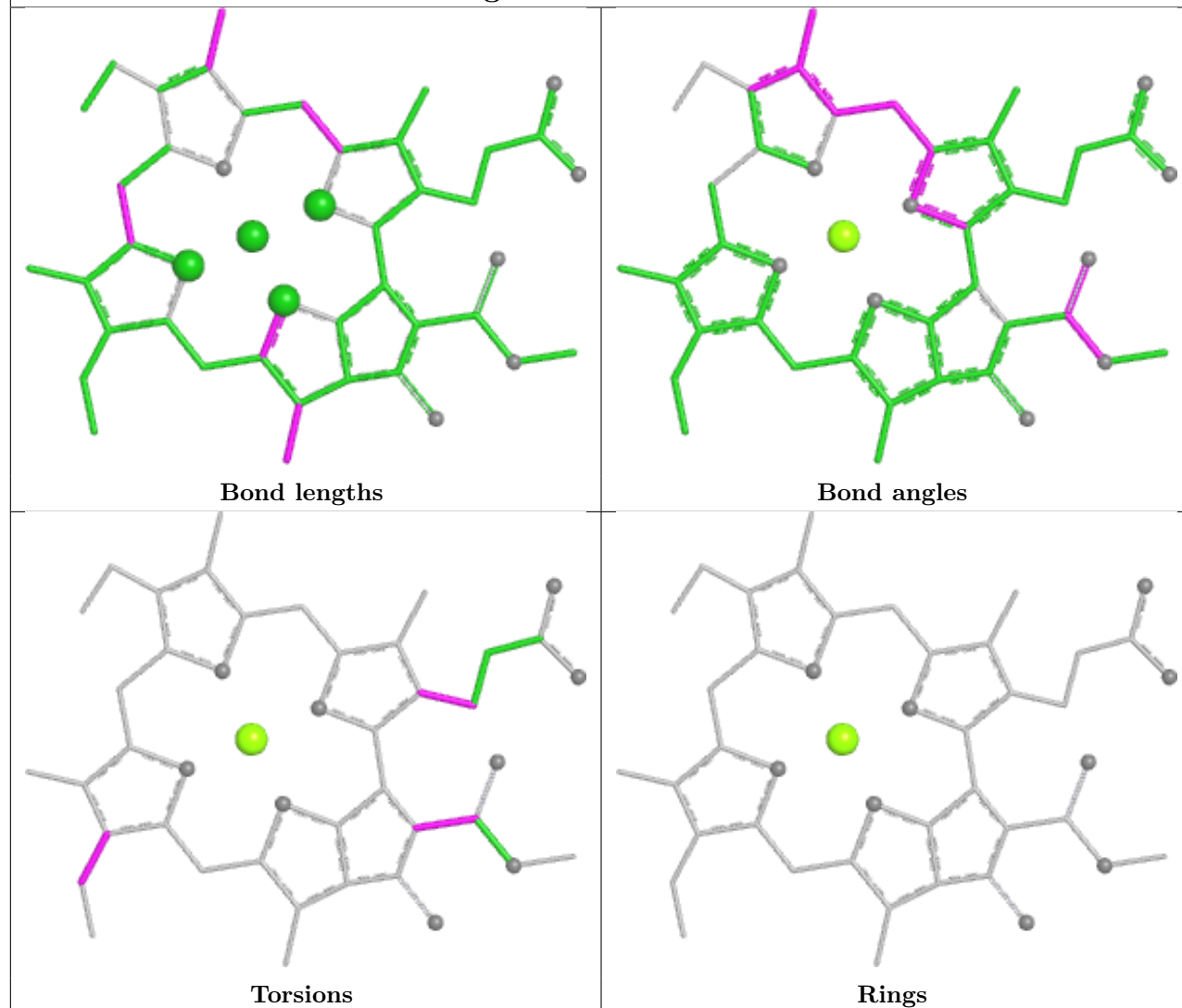


Ligand BCR A 848

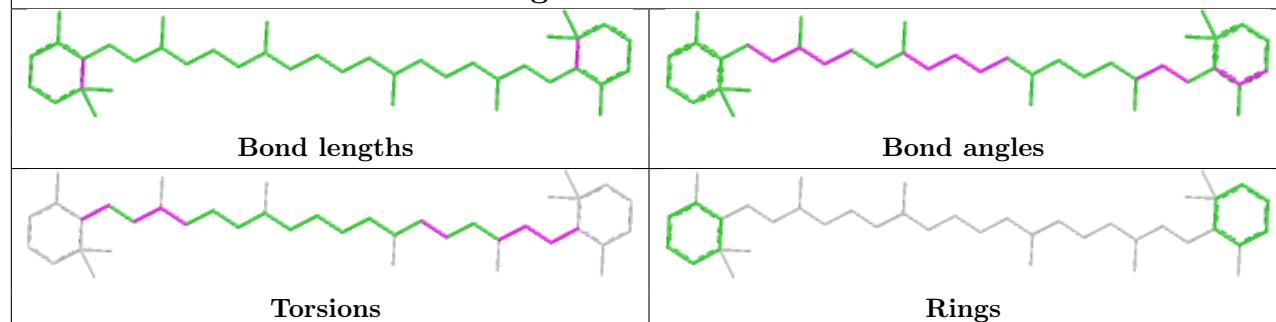


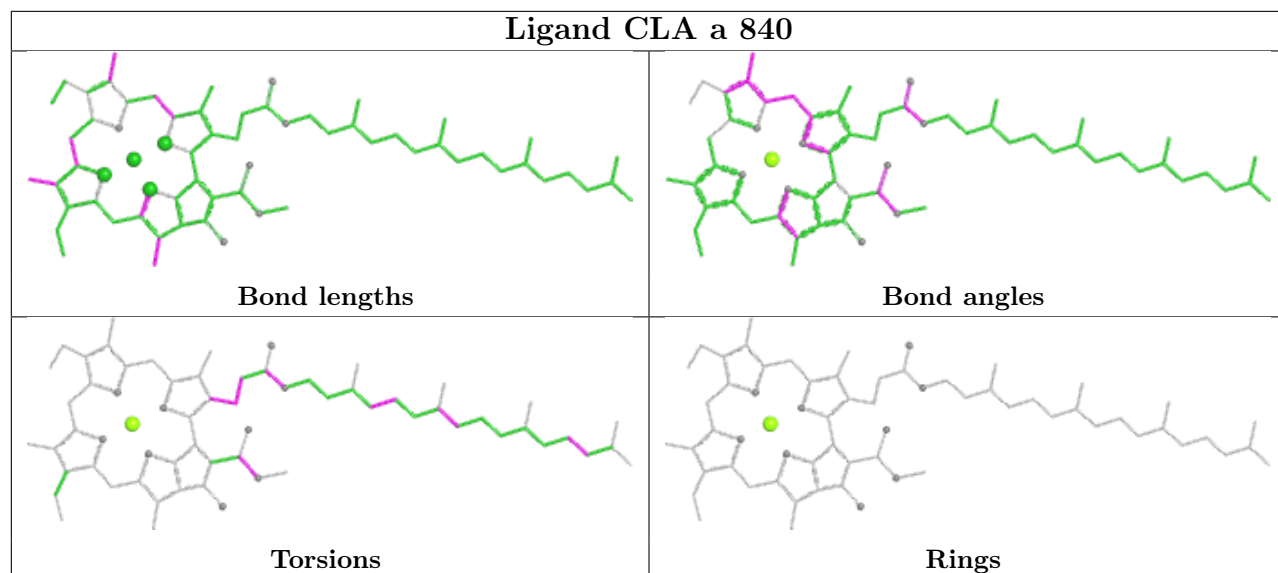
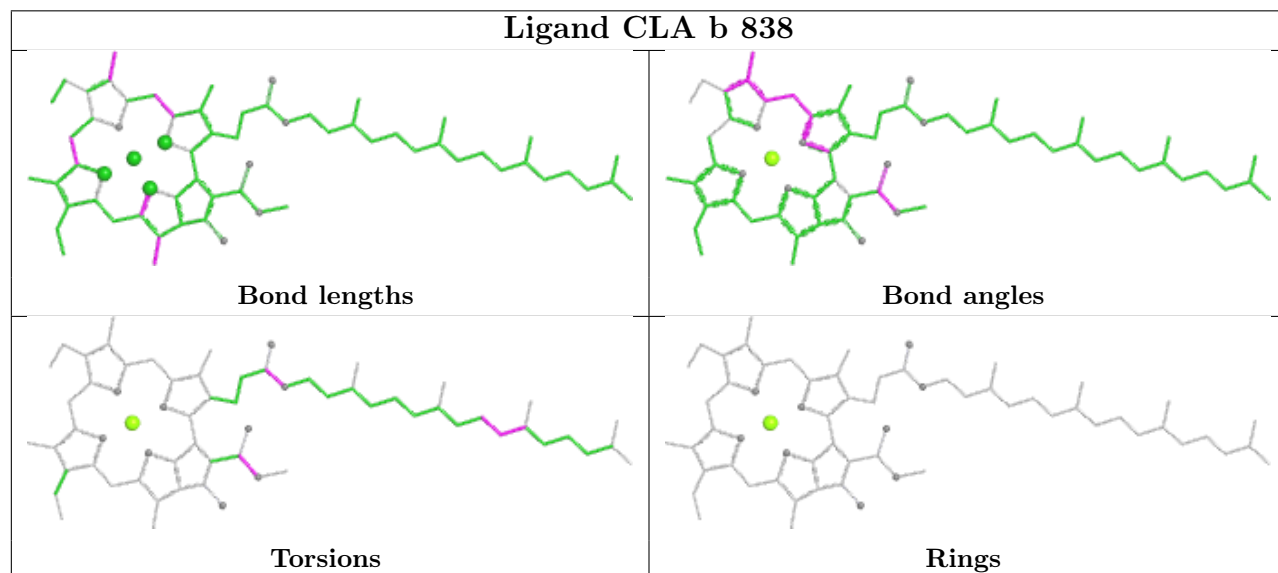
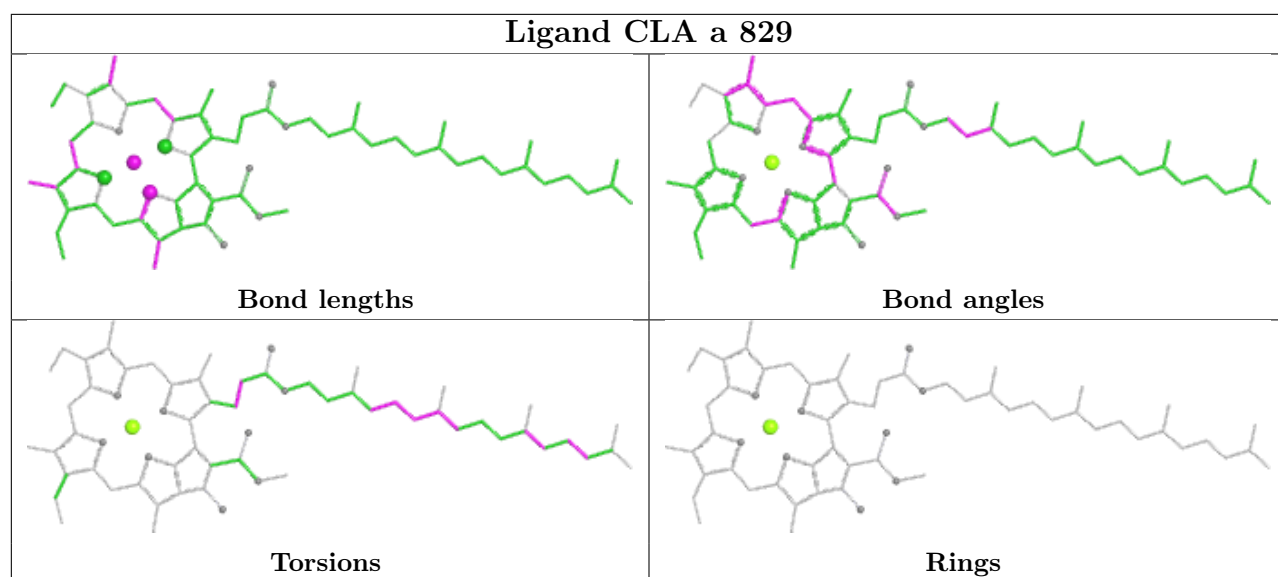


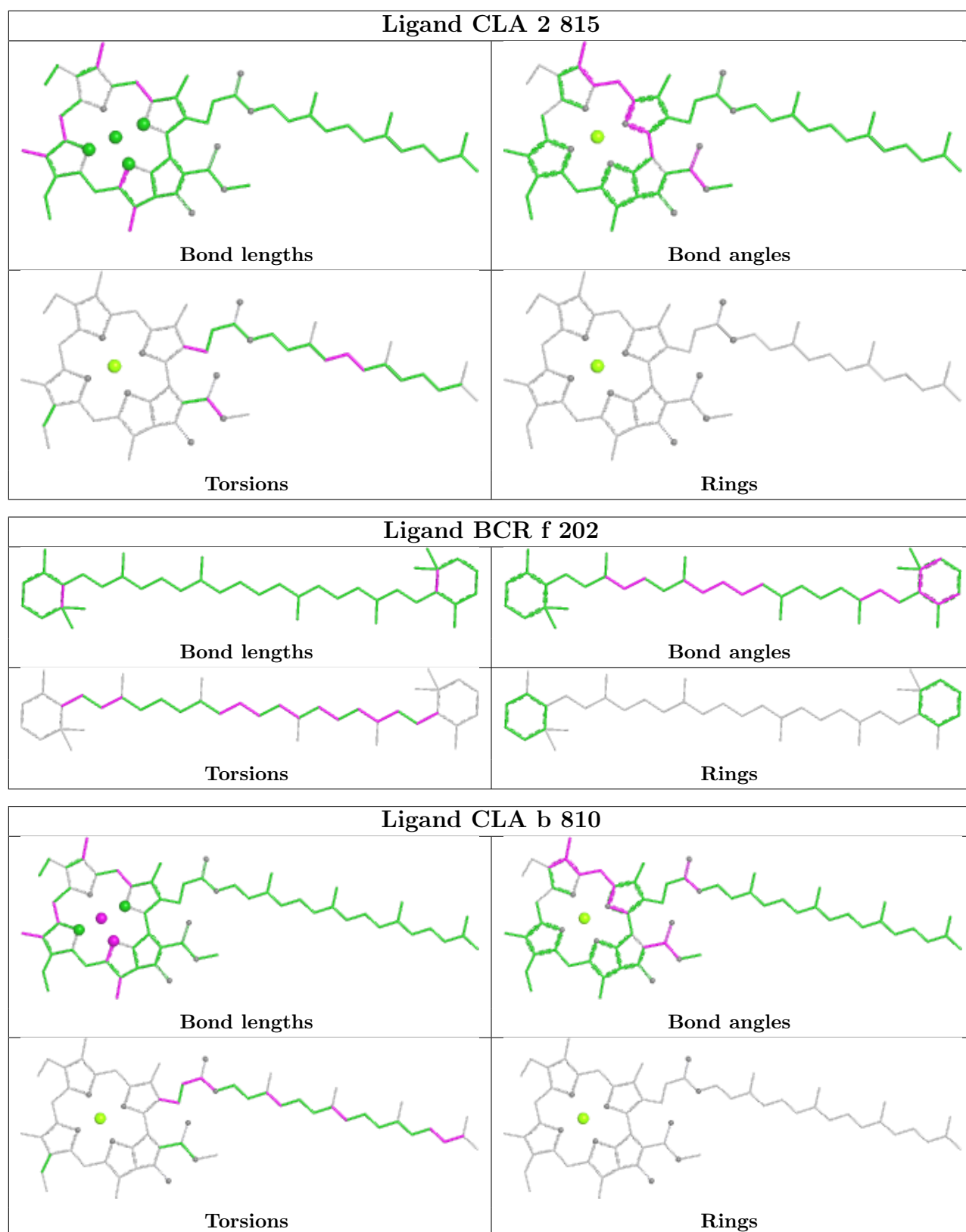
Ligand CLA K 4002



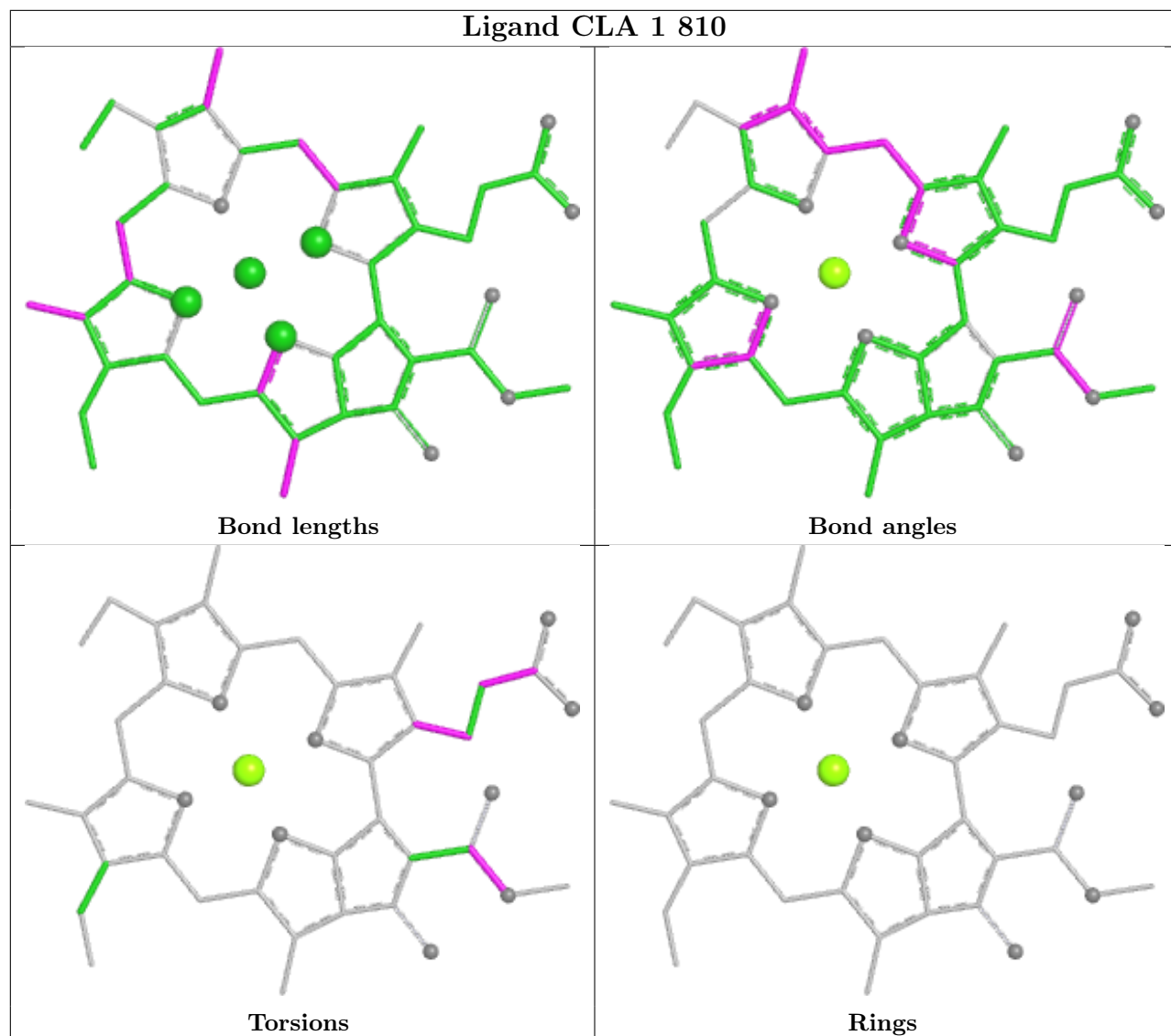
Ligand BCR B 840

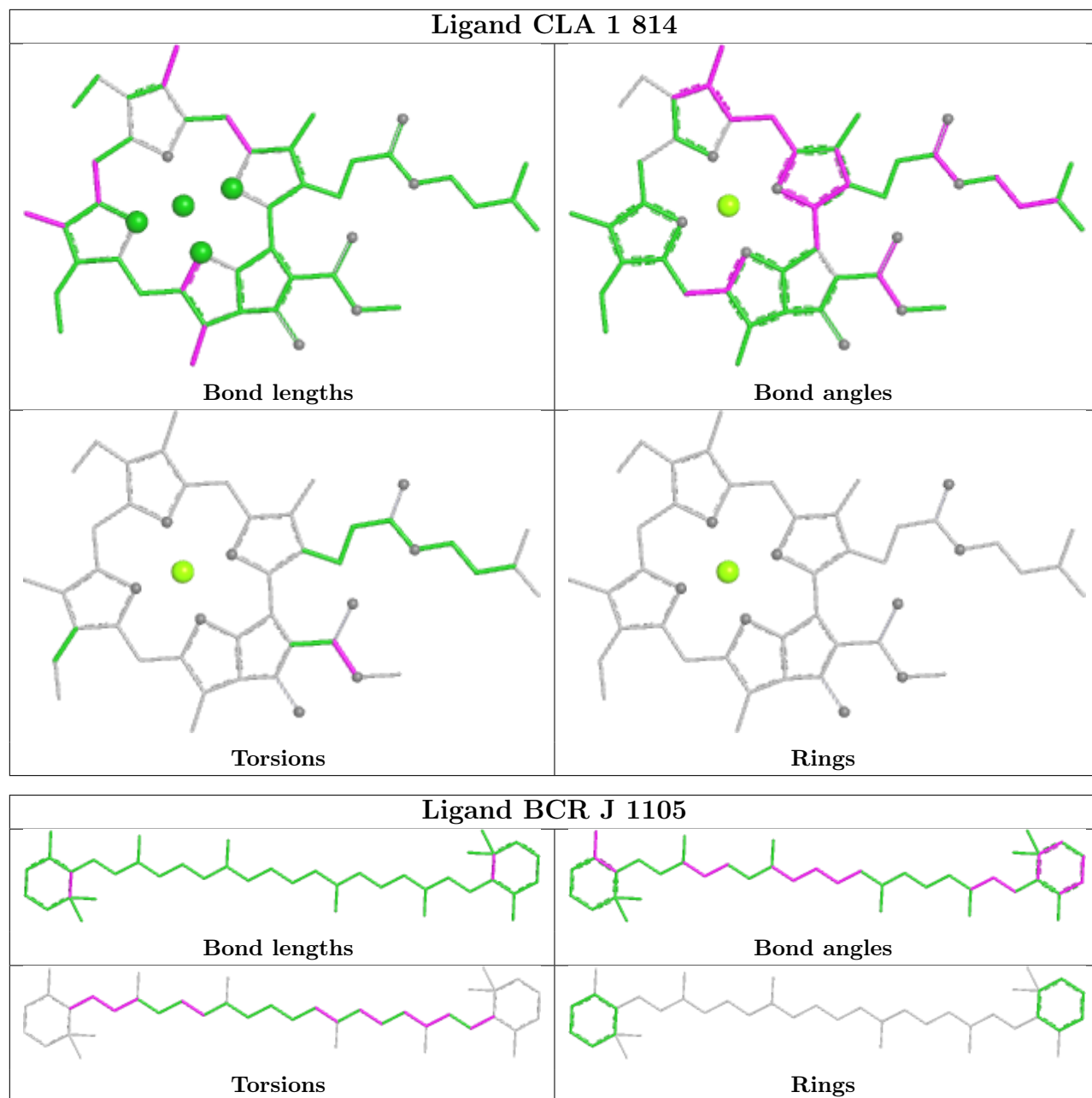




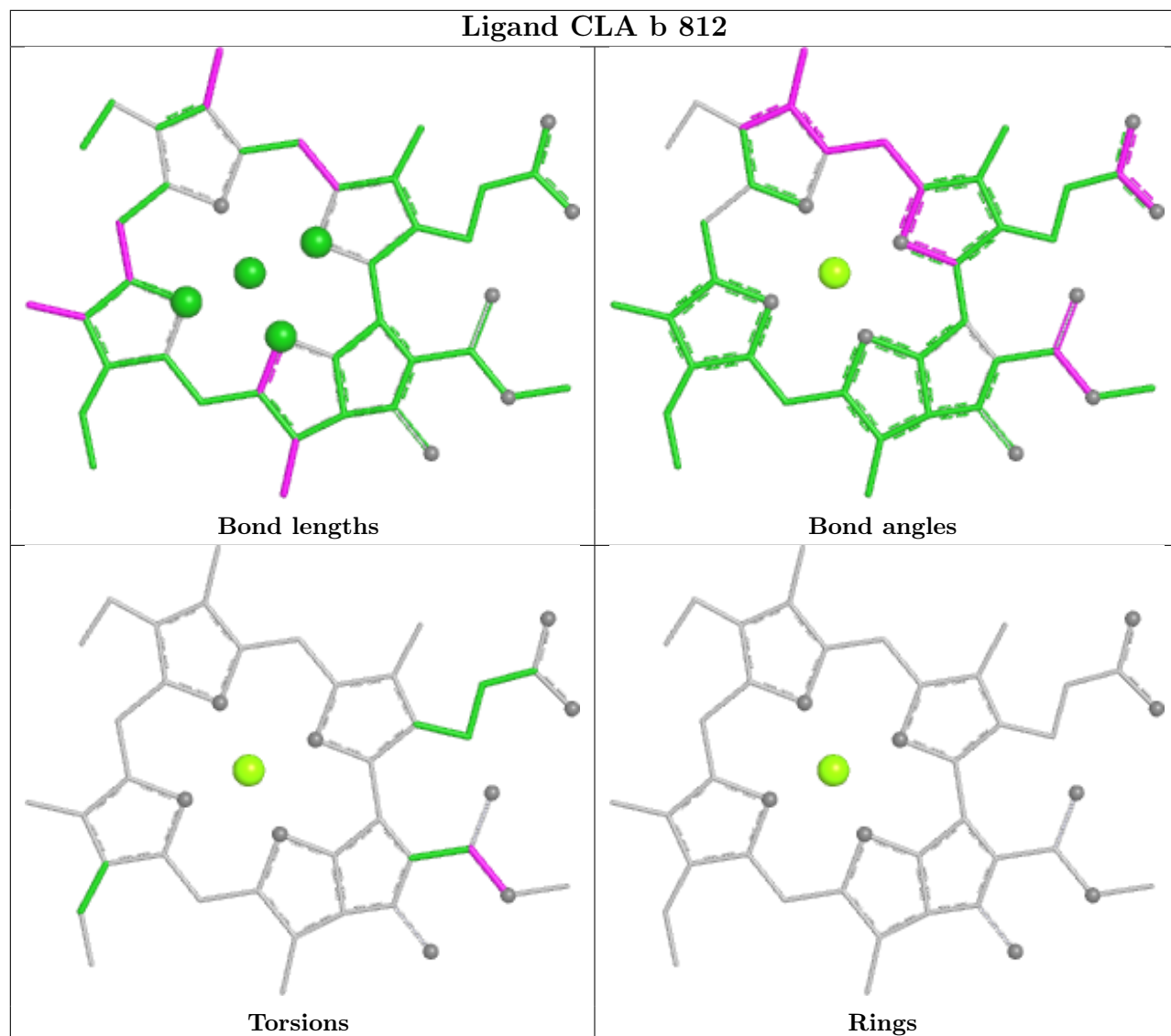


Ligand CLA 1 810

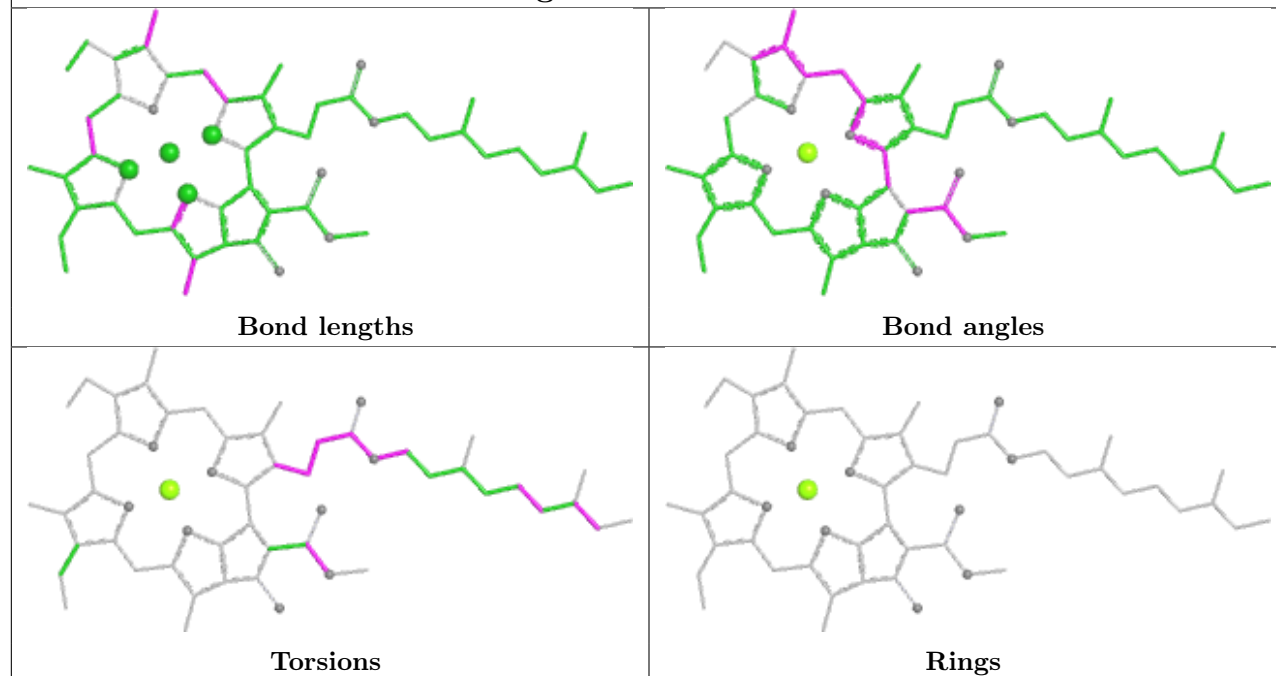




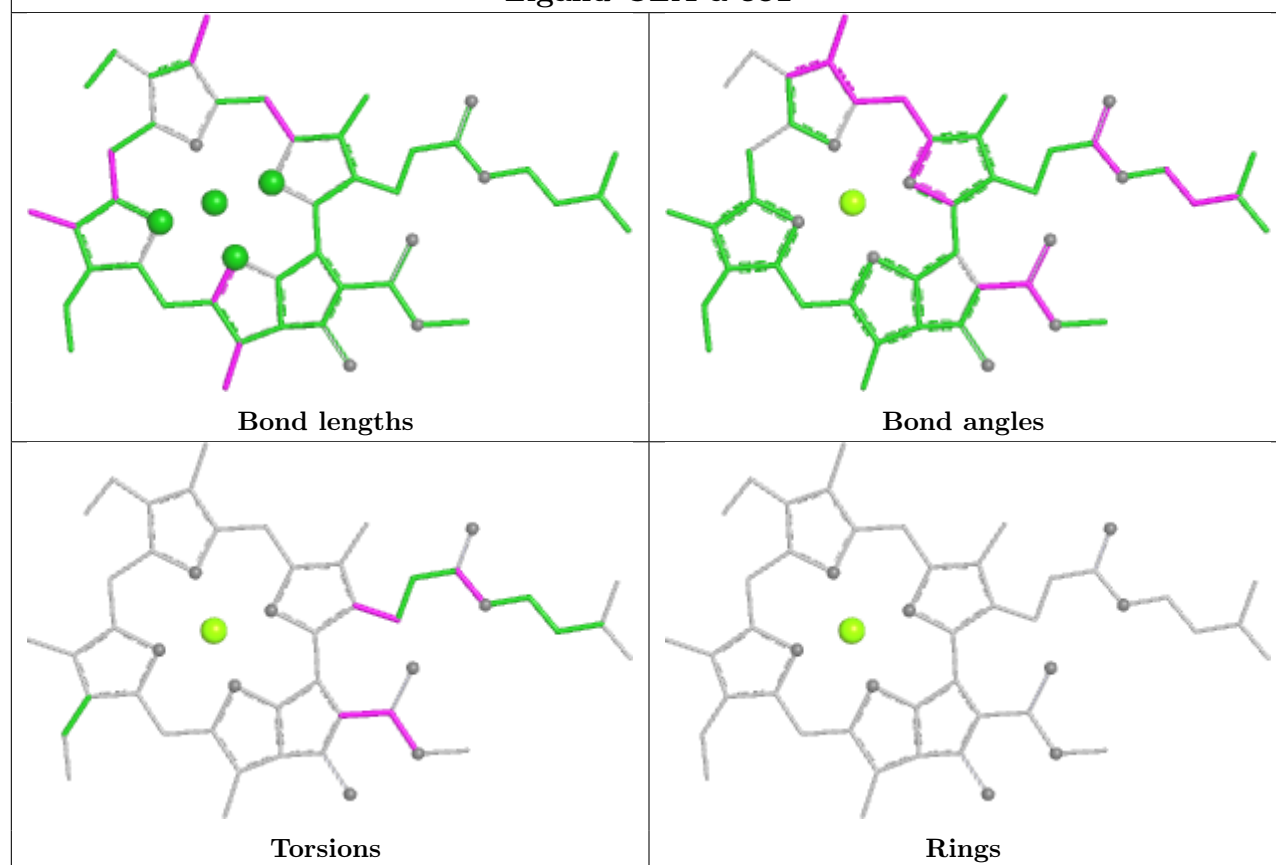
Ligand CLA b 812

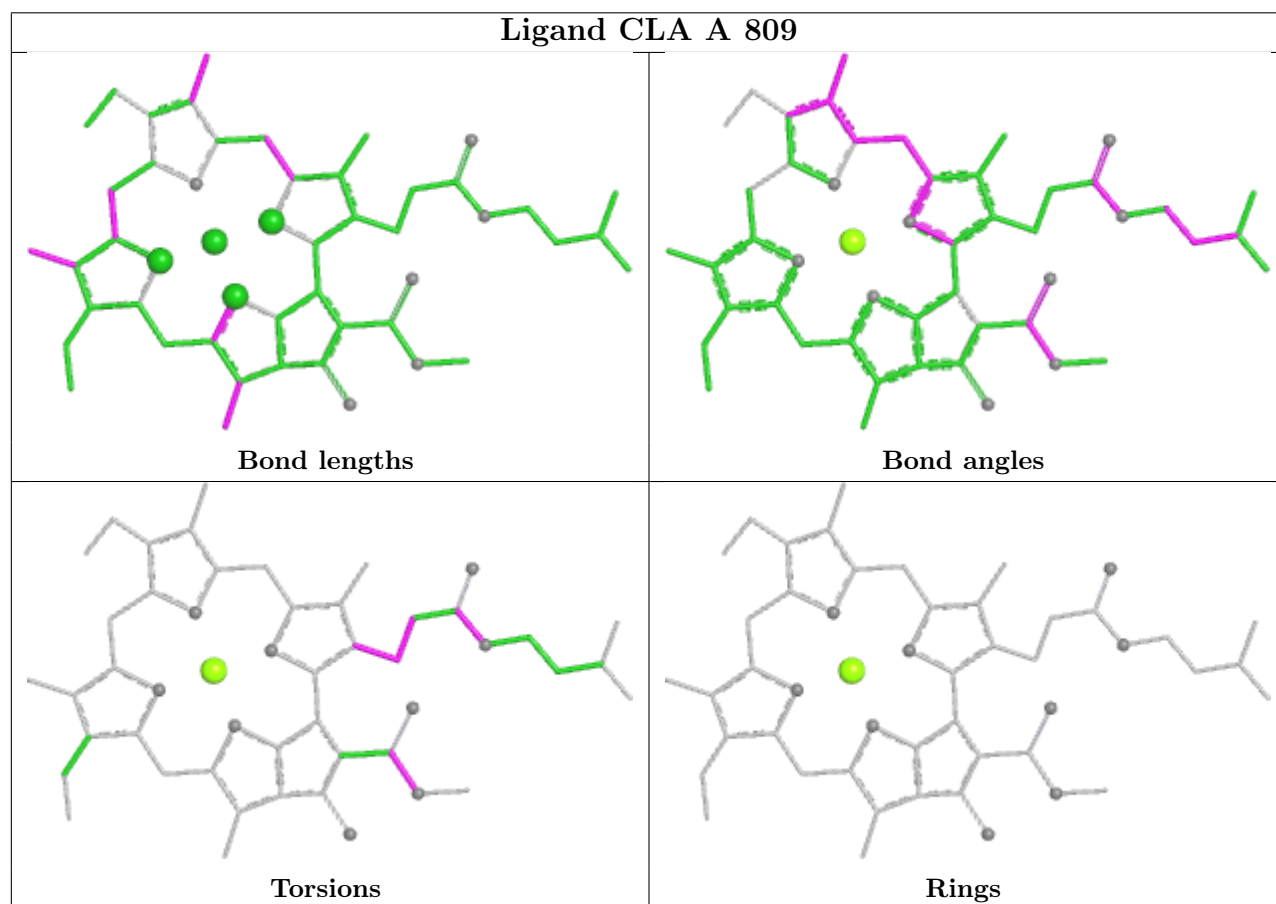
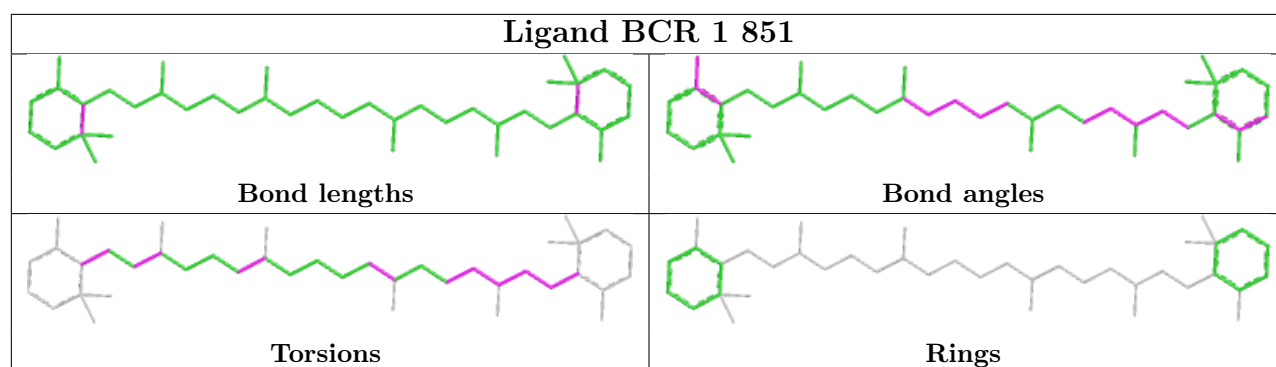


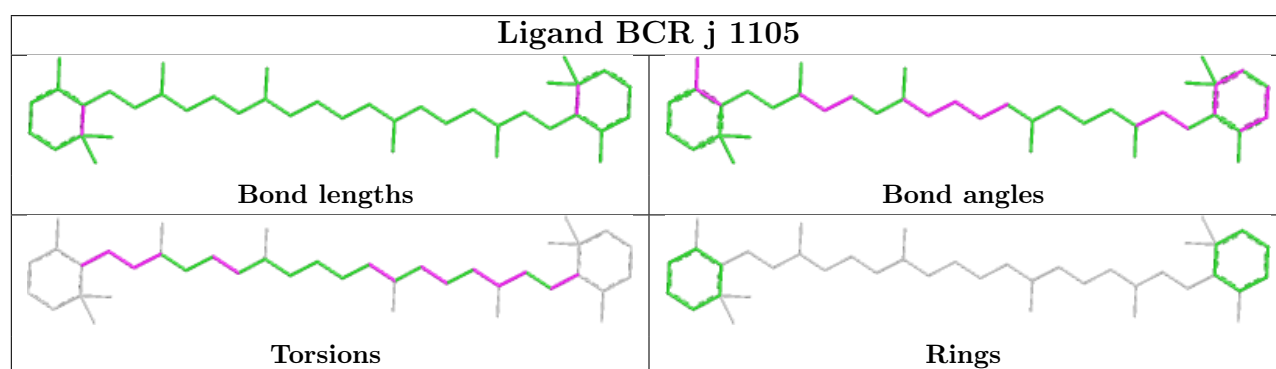
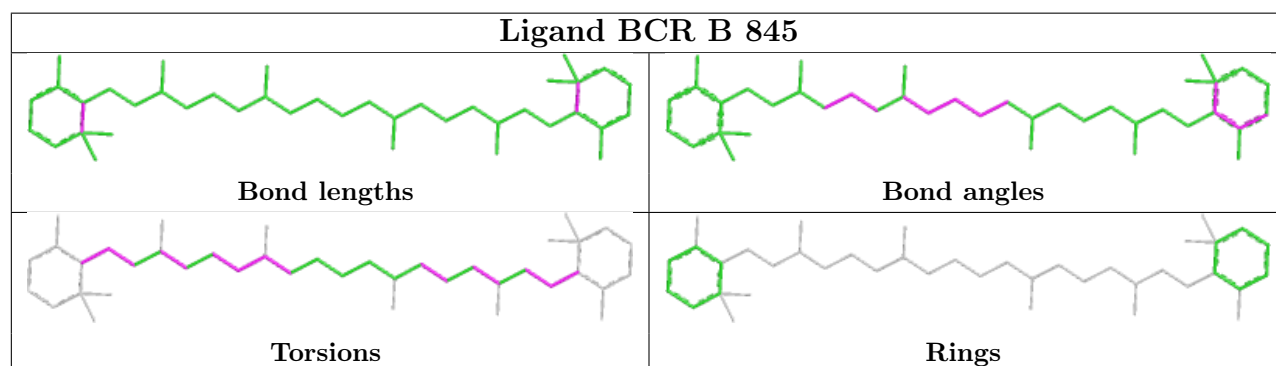
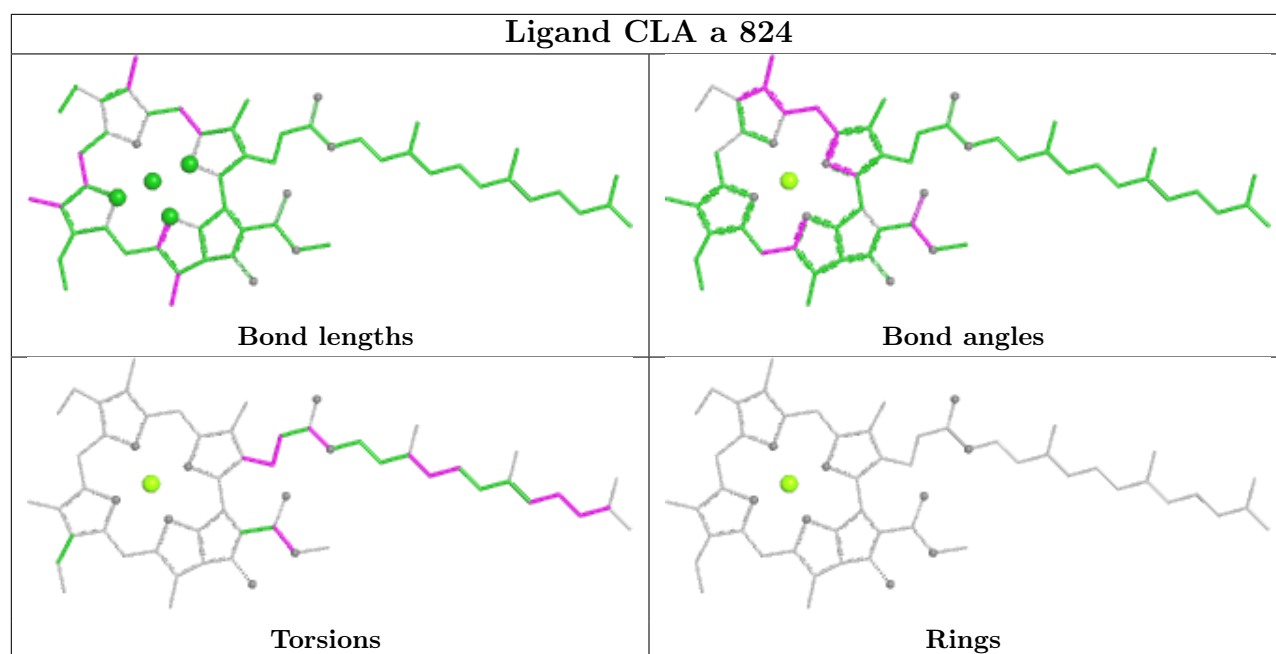
Ligand CLA a 835



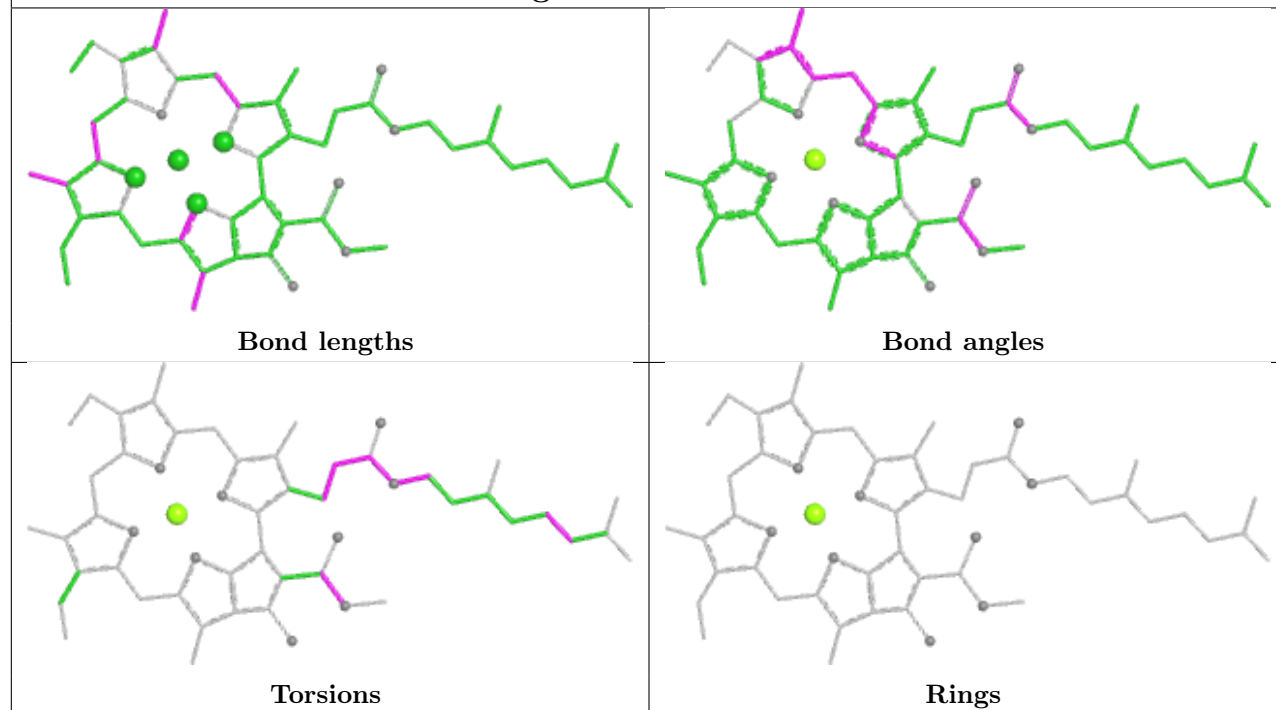
Ligand CLA a 831



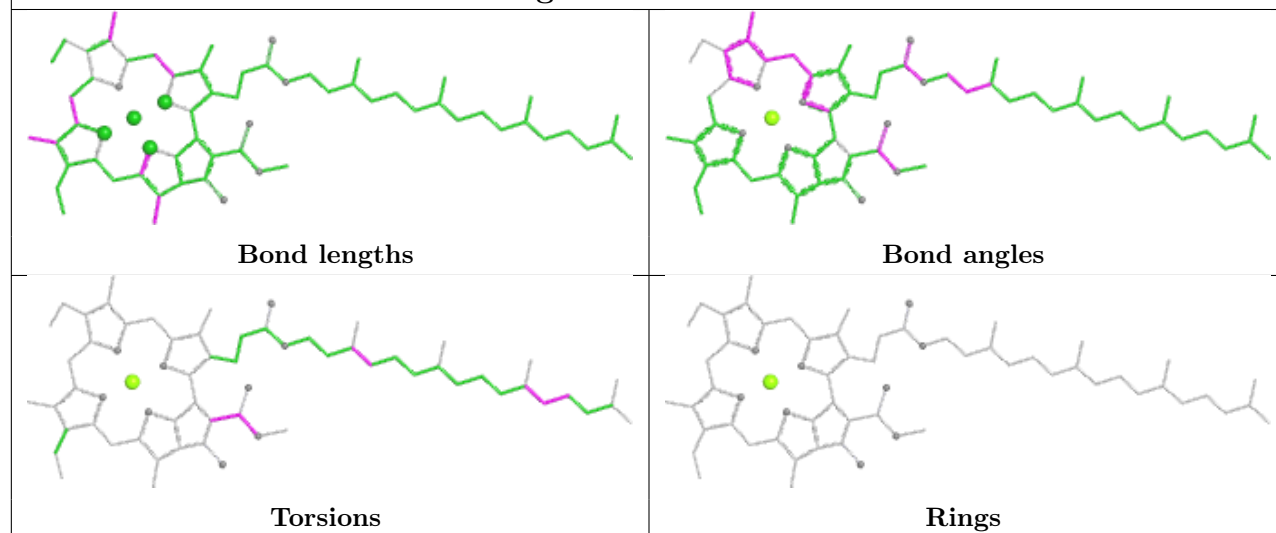


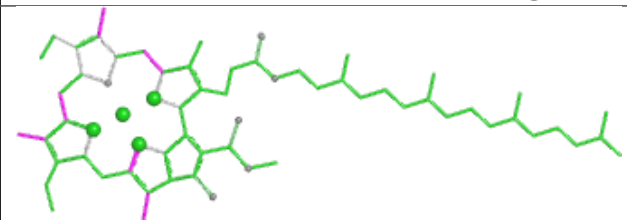
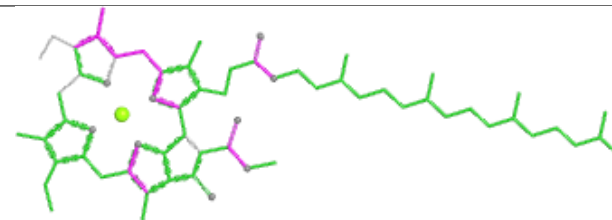
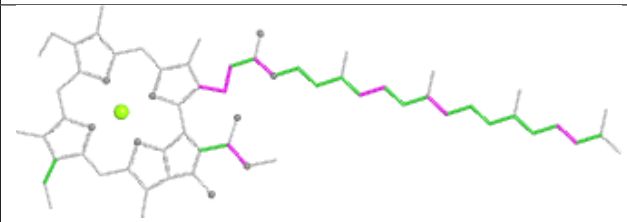
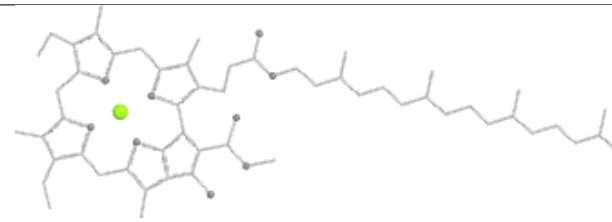


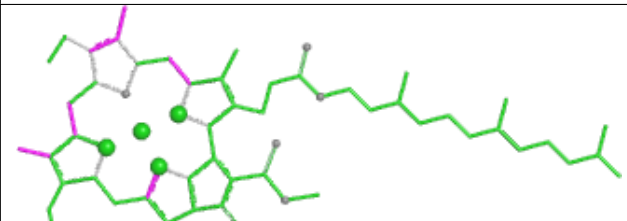
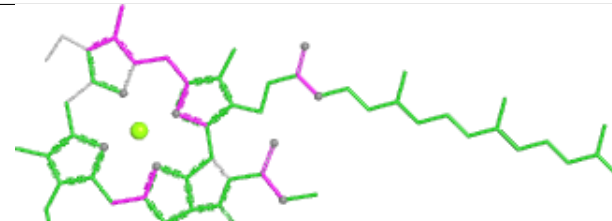
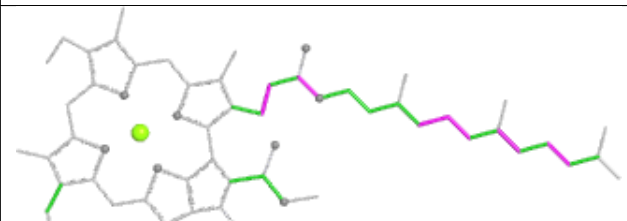
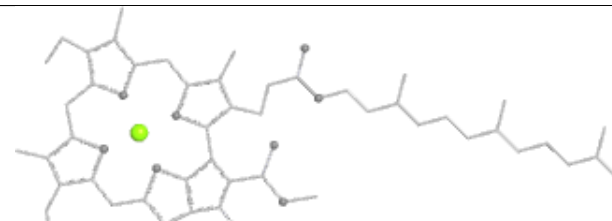
Ligand CLA B 828


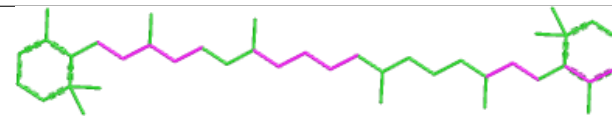
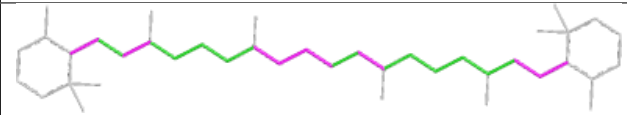
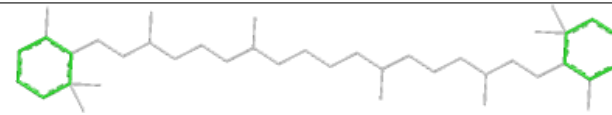


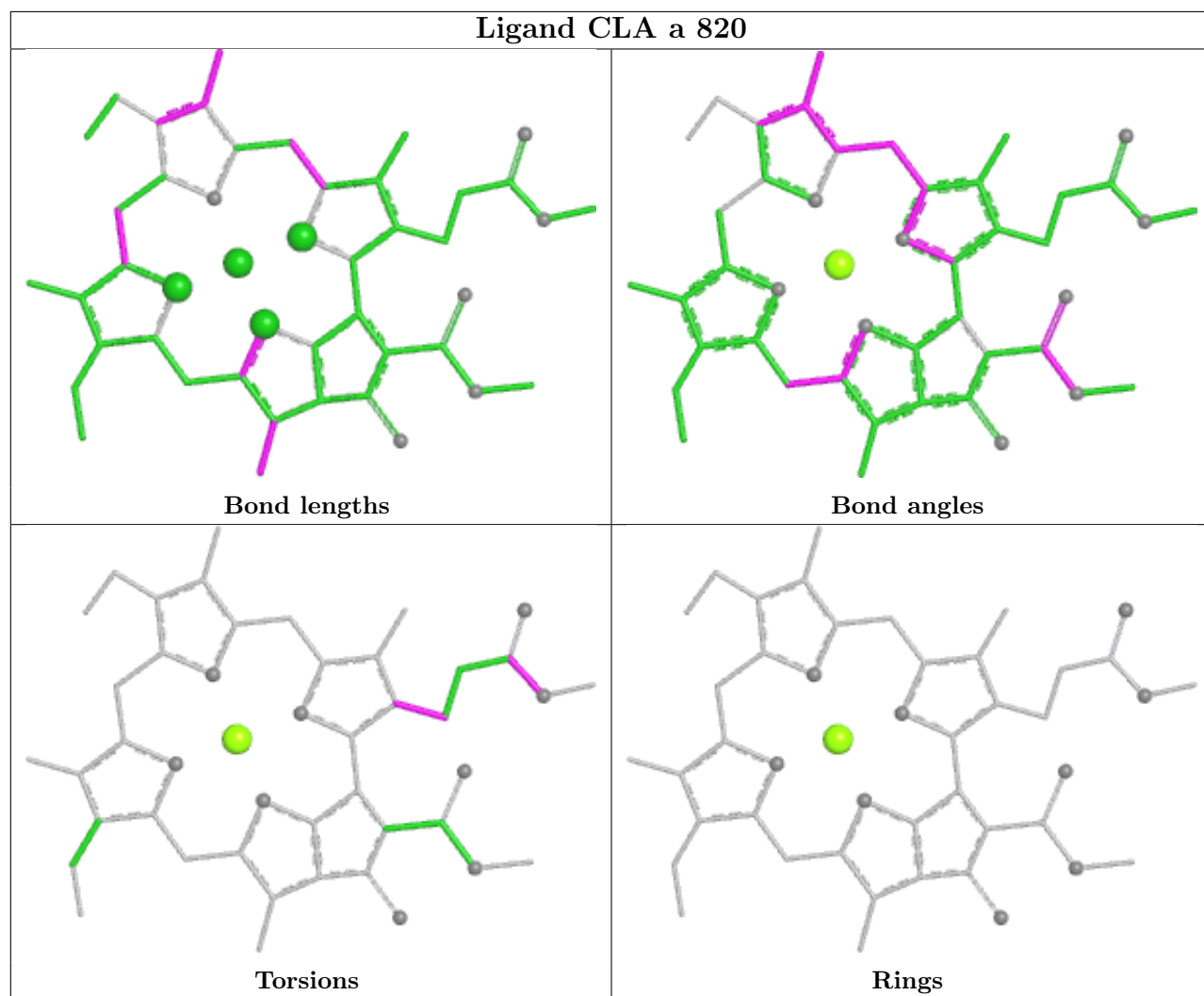
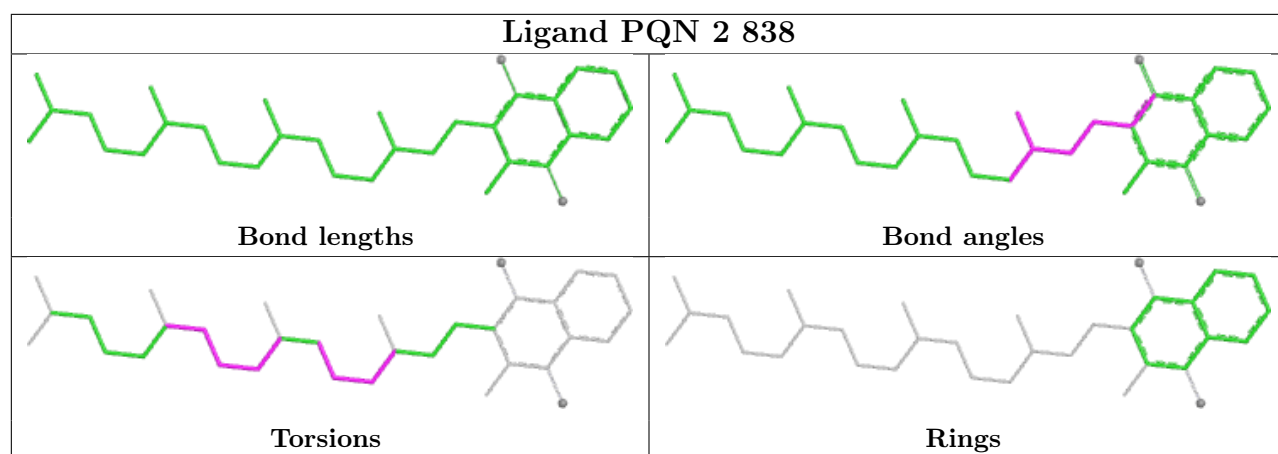
Ligand CLA 1 832



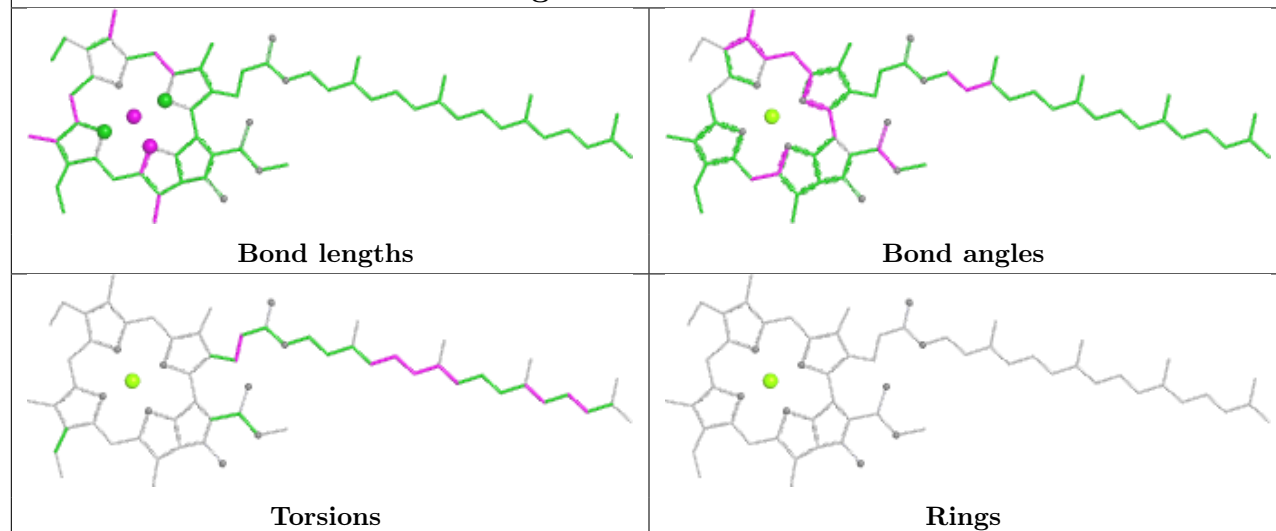
Ligand CLA 1 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 837	
	
Bond lengths	Bond angles
	
Torsions	Rings

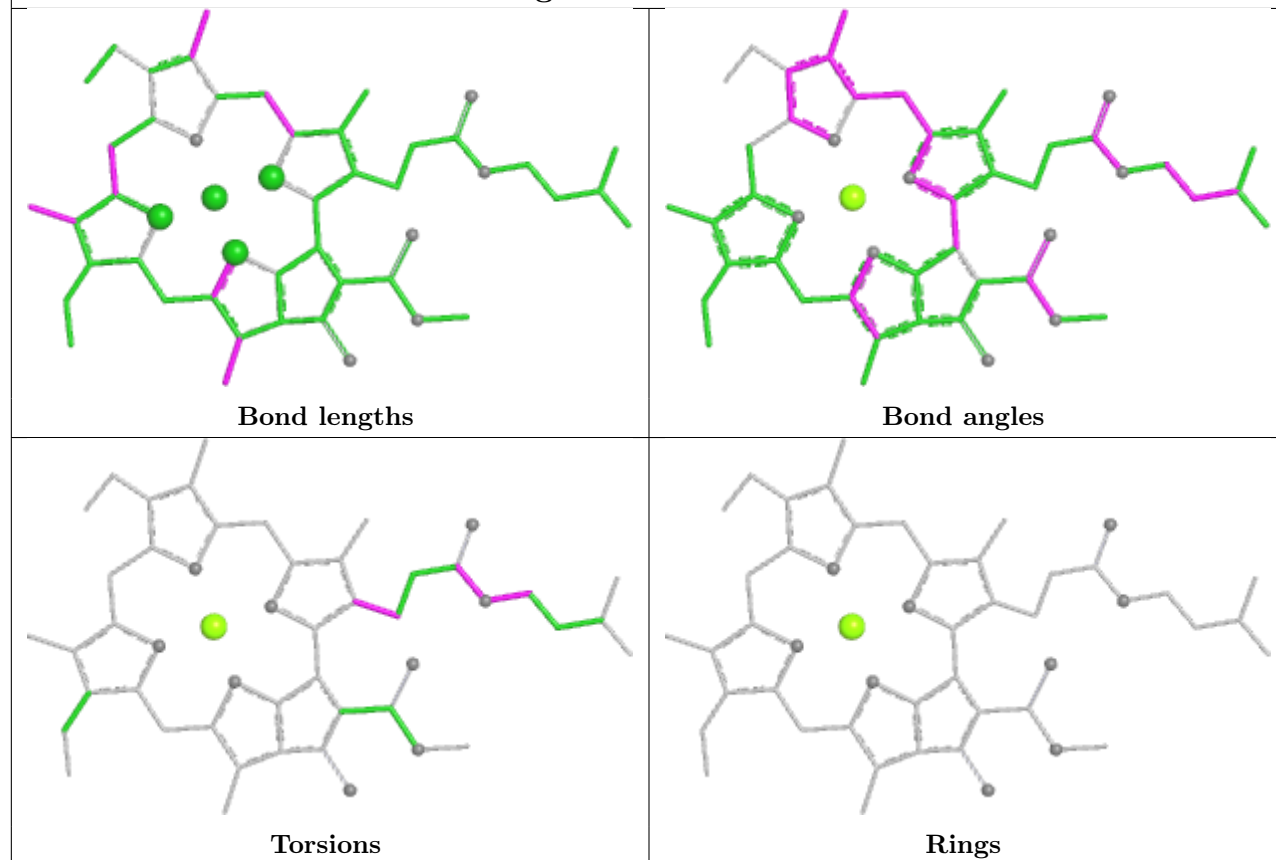
Ligand BCR k 4004	
	
Bond lengths	Bond angles
	
Torsions	Rings

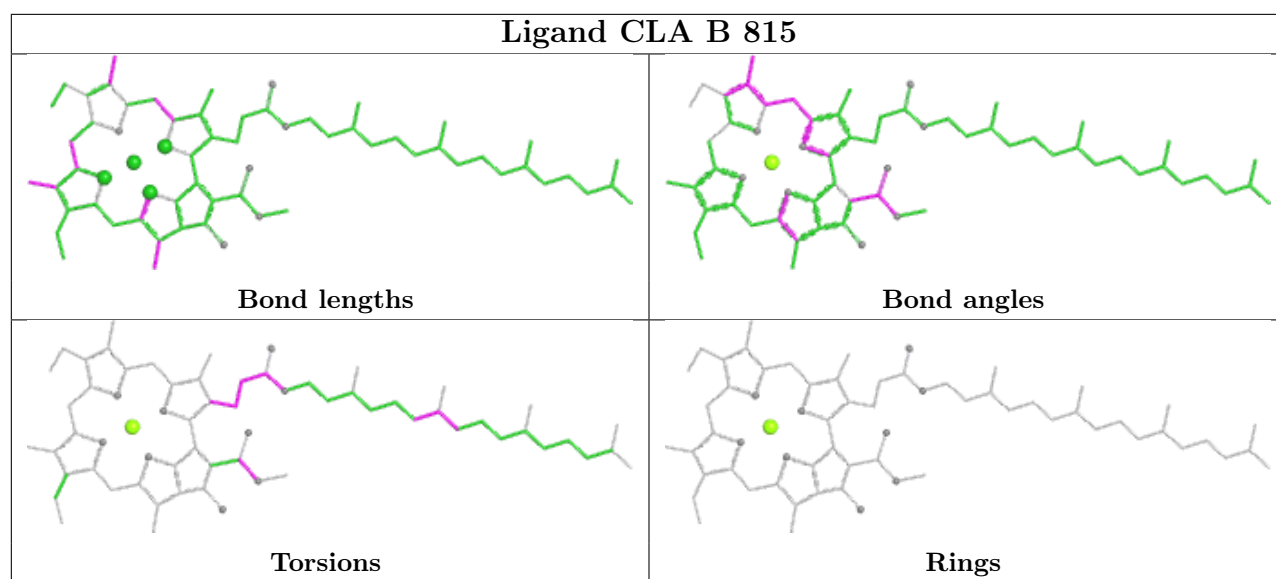


Ligand CLA A 829



Ligand CLA b 833





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.

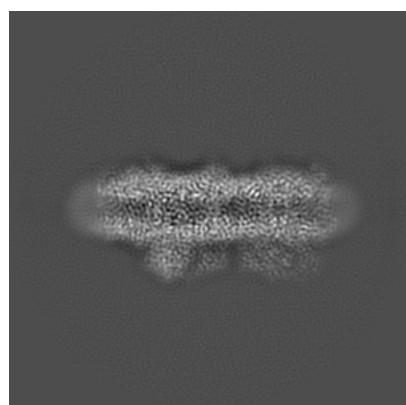
6 Map visualisation [i](#)

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.

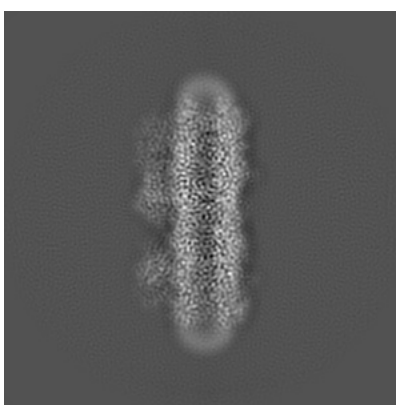
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

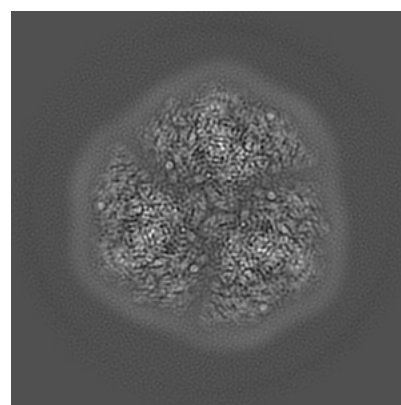
6.1.1 Primary map



X



Y

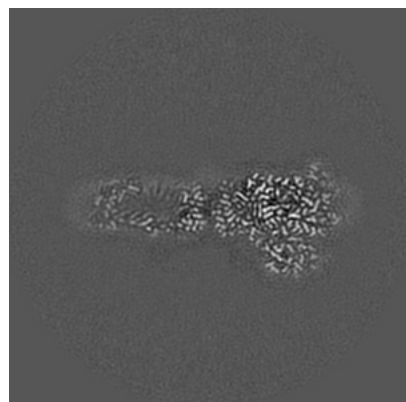


Z

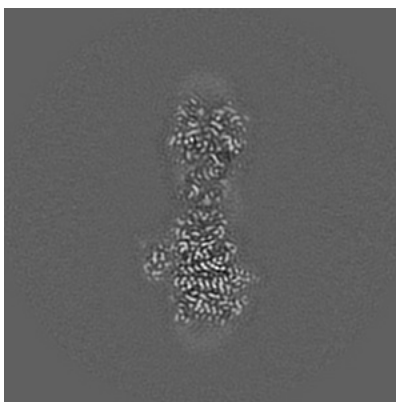
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

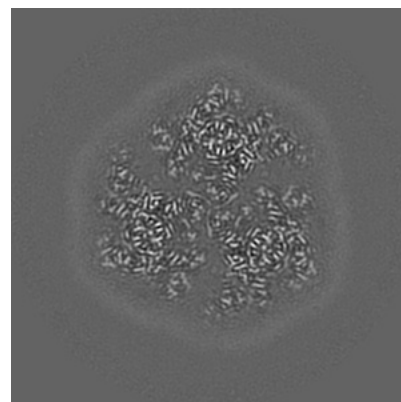
6.2.1 Primary map



X Index: 150



Y Index: 150

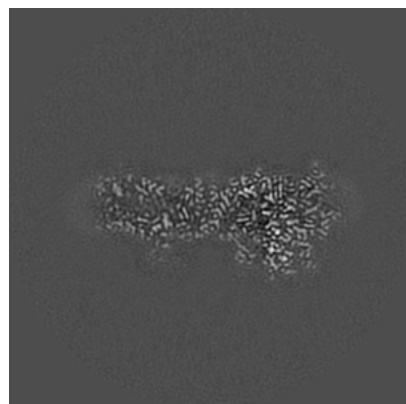


Z Index: 150

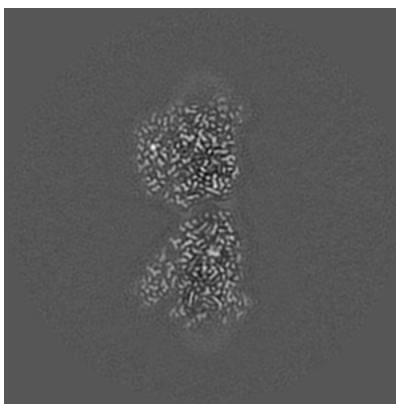
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

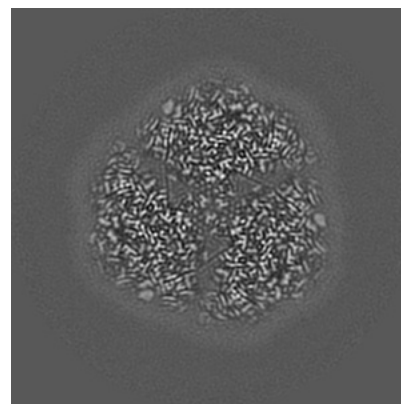
6.3.1 Primary map



X Index: 158



Y Index: 116

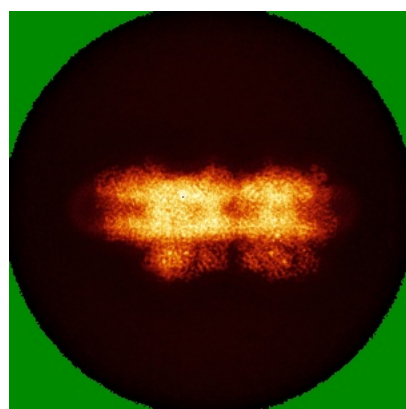


Z Index: 161

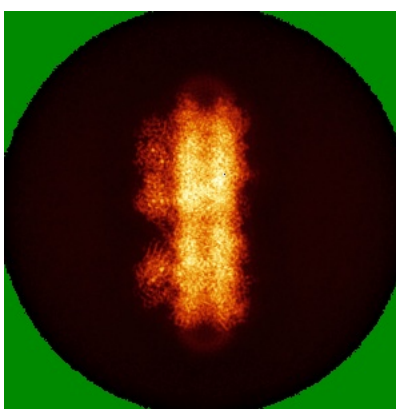
The images above show the largest variance slices of the map in three orthogonal directions.

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

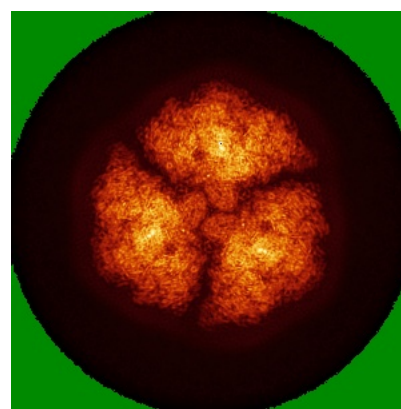
6.4.1 Primary map



X



Y

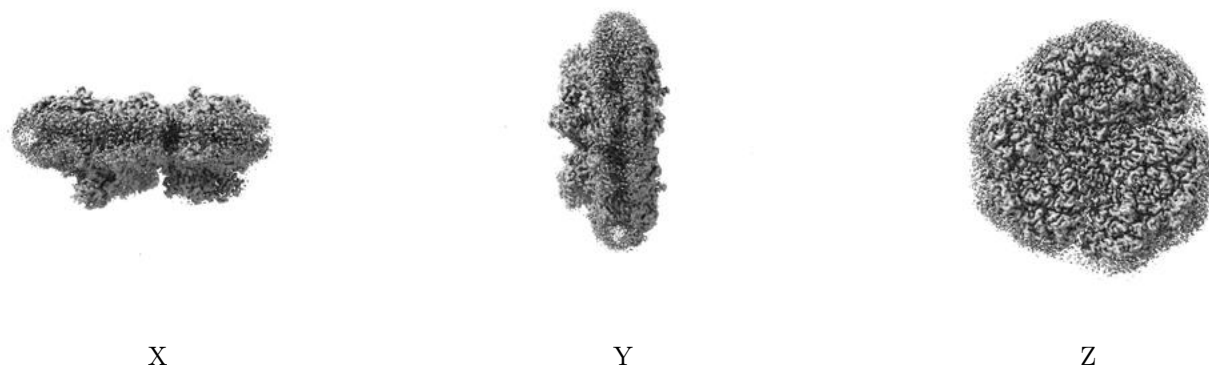


Z

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.

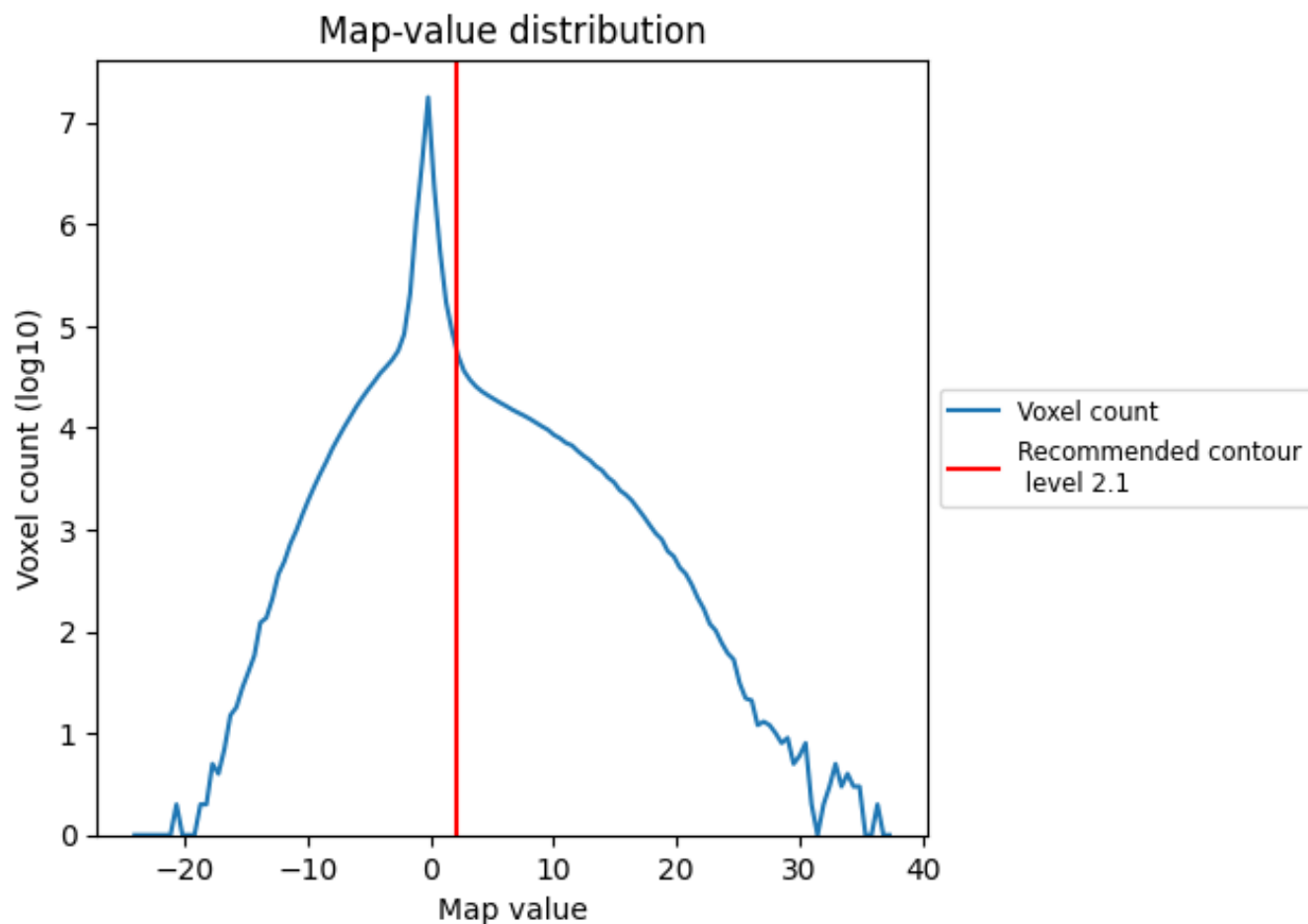
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

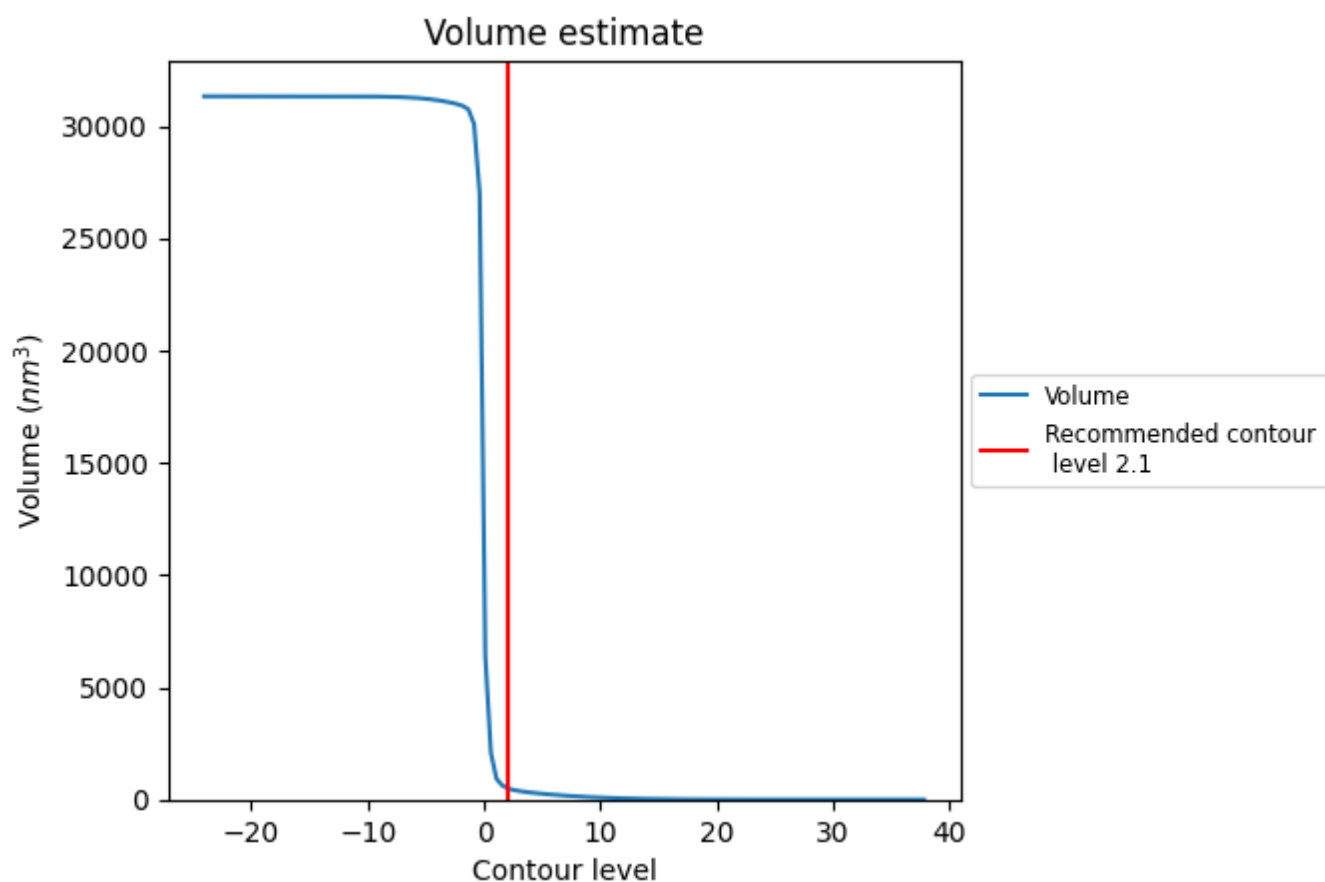
This section contains the results of statistical analysis of the map.

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.

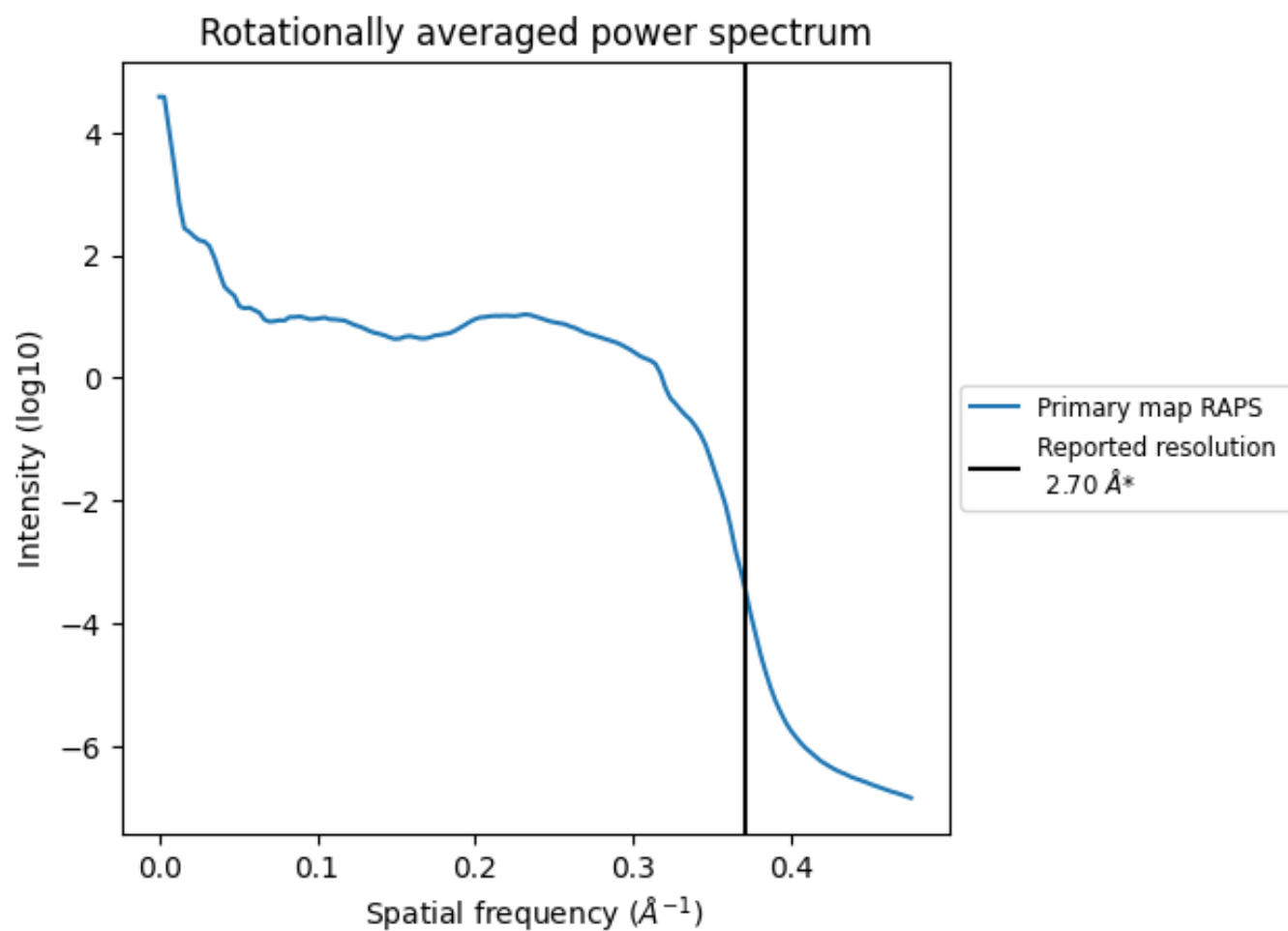
7.2 Volume estimate [i](#)



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 ⓘ

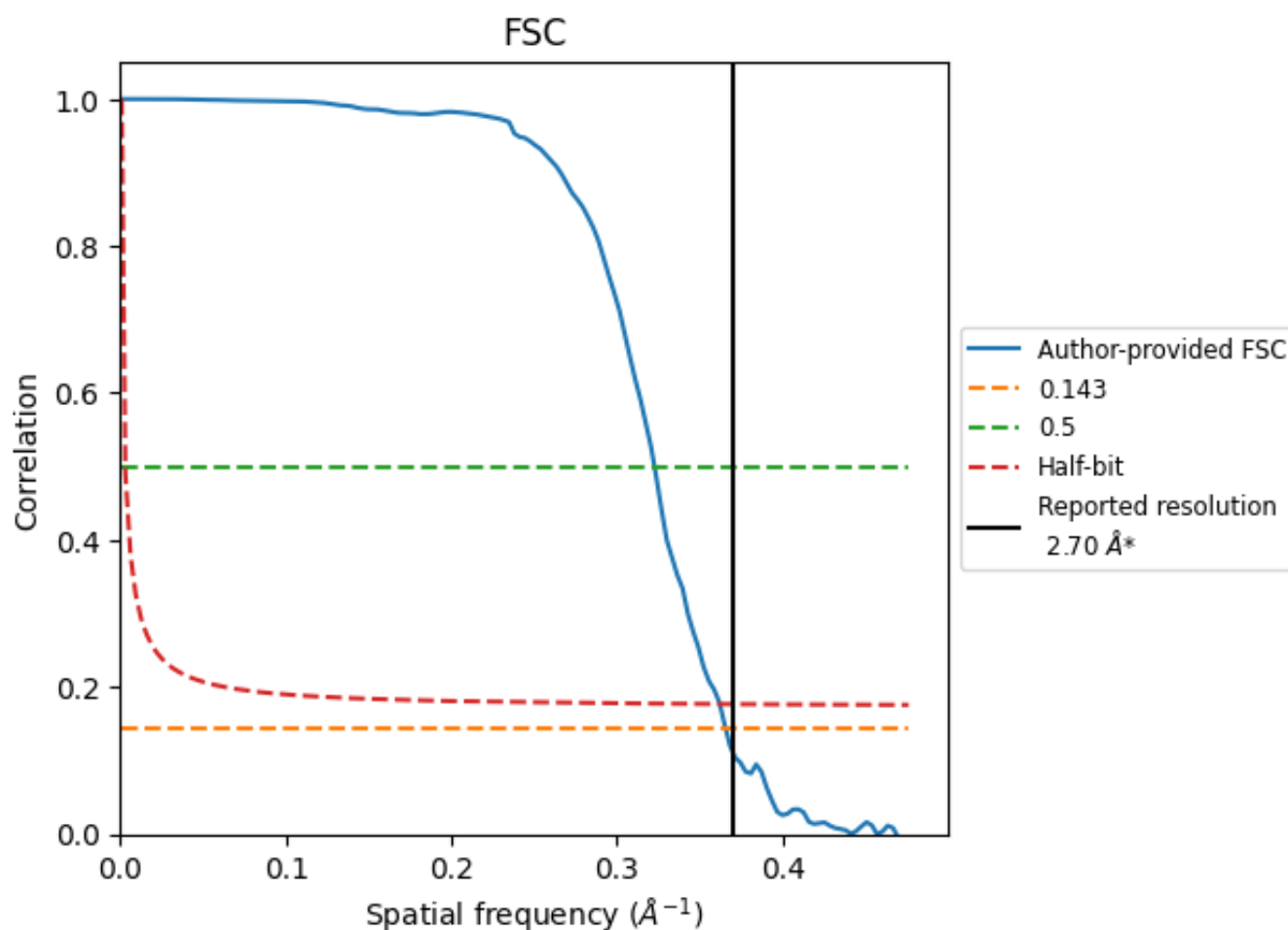


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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](#)

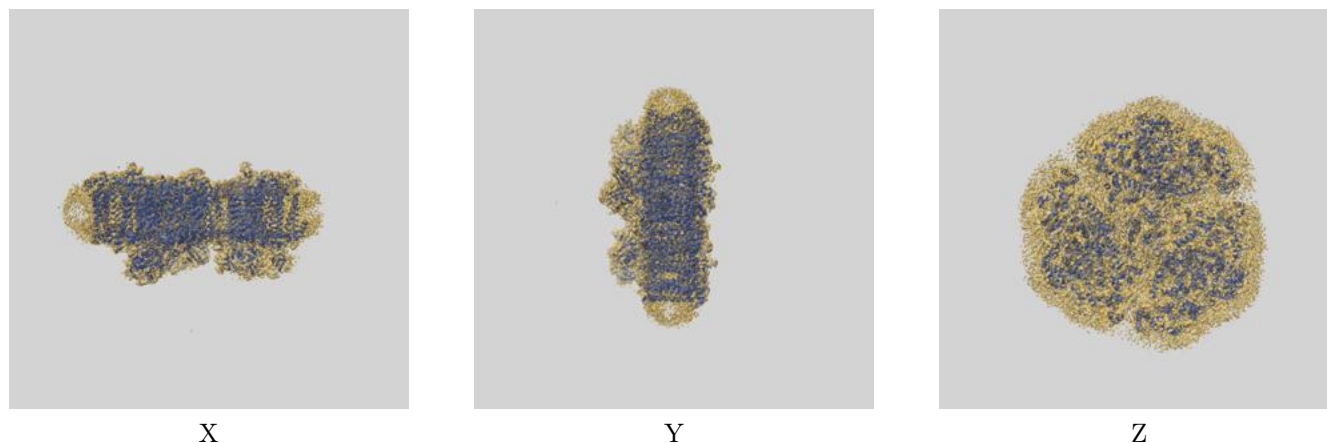
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.73	3.10	2.76
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

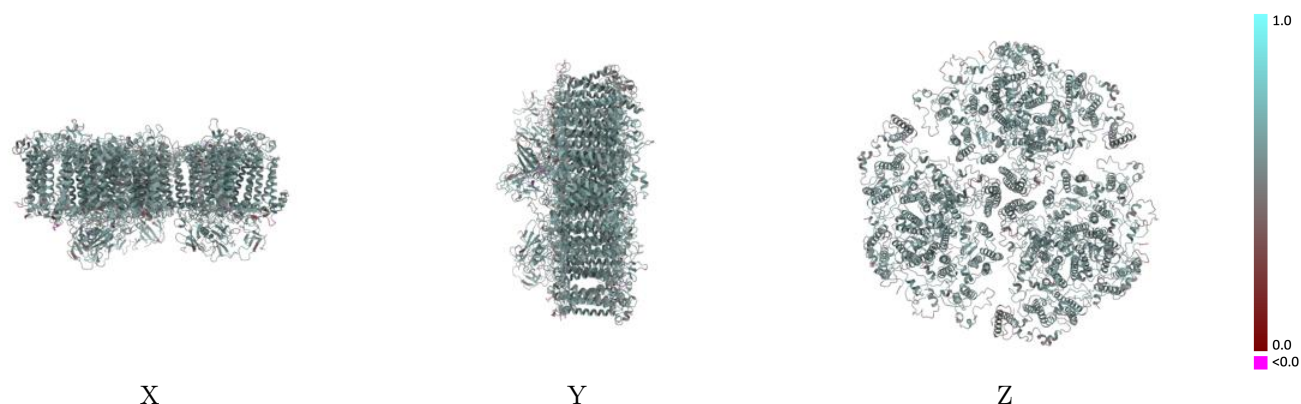
This section contains information regarding the fit between EMDB map EMD-21320 and PDB model 6VPV. Per-residue inclusion information can be found in section [3](#) on page [35](#).

9.1 Map-model overlay [i](#)



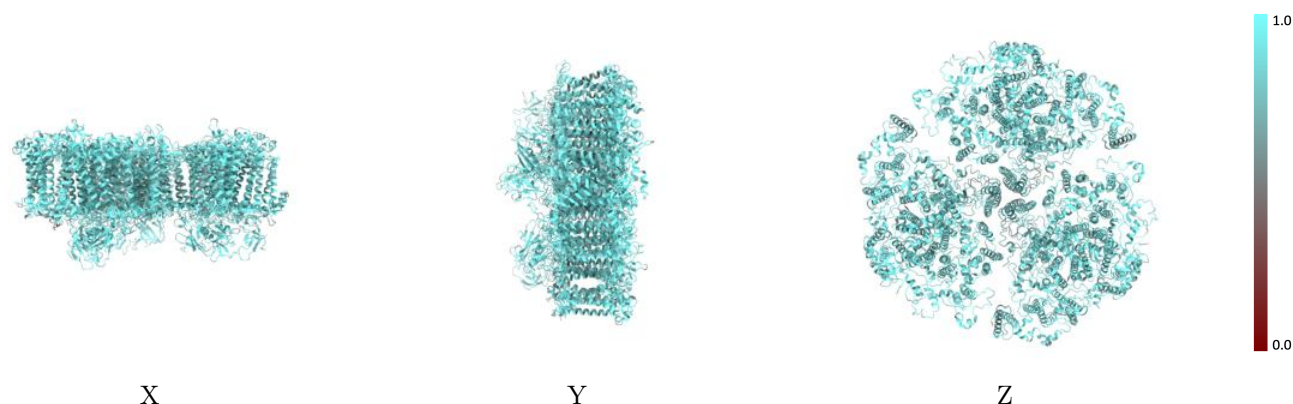
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



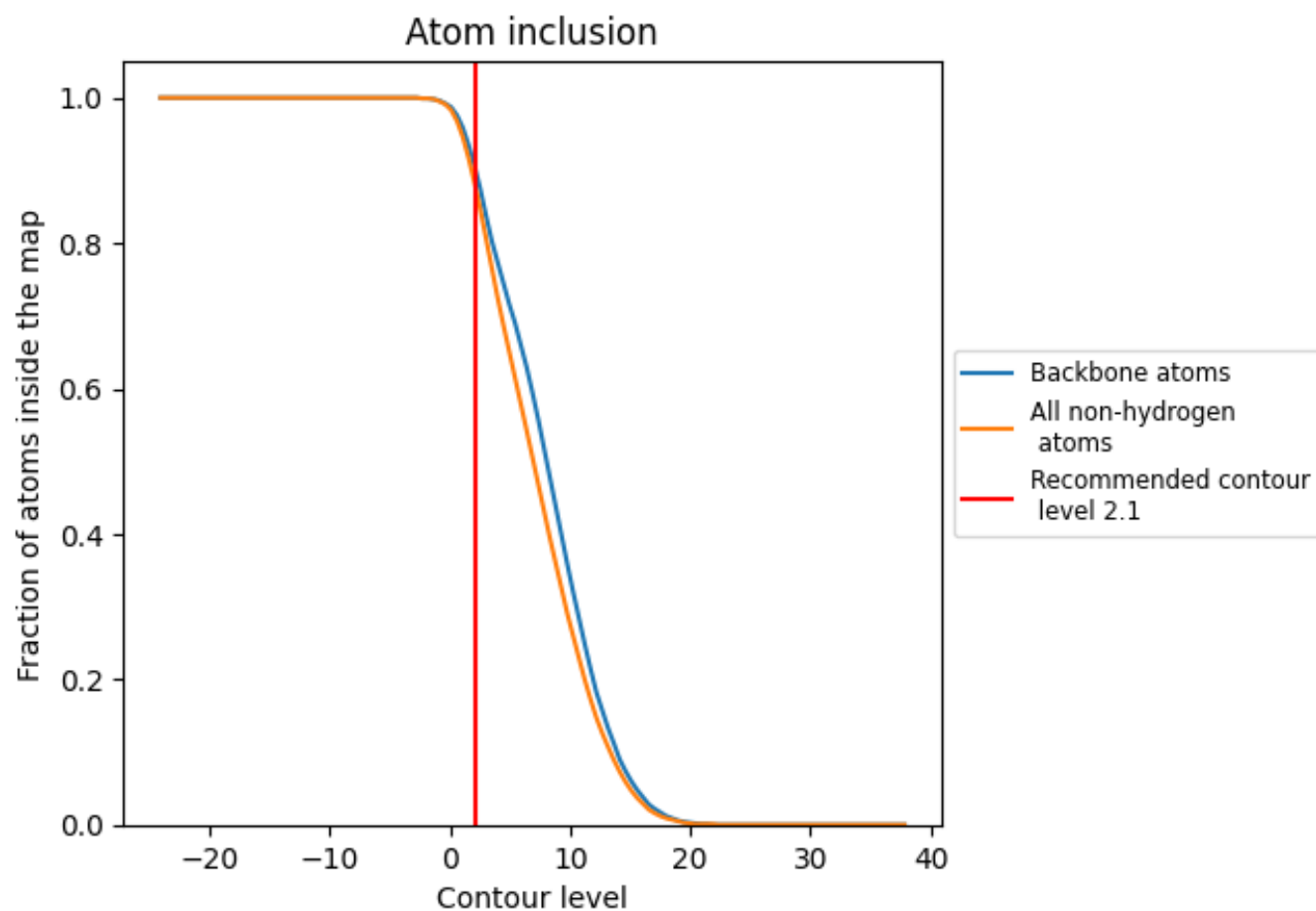
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

