



wwPDB EM Validation Summary Report ⓘ

Oct 20, 2024 – 02:32 AM EDT

PDB ID : 6UZV
EMDB ID : EMD-20963
Title : The structure of a red shifted photosystem I complex
Authors : Toporik, H.; Williams, D.; Chiu, P.L.; Mazor, Y.
Deposited on : 2019-11-15
Resolution : 3.10 Å(reported)
Based on initial models : 6KIG, 5OY0

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:

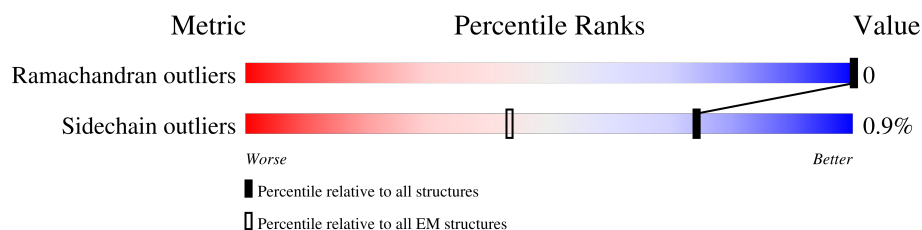
EMDB validation analysis : 0.0.1.dev113
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, 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 3.10 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	751	 98%
1	A	751	 98%
1	a	751	 98%
2	2	735	 99%
2	B	735	 99%
2	b	735	 99%
3	3	81	 98%
3	C	81	 98%
3	c	81	 98%

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Mol	Chain	Length	Quality of chain
4	4	141	13% 94% . .
4	D	141	15% 94% . .
4	d	141	14% 94% . .
5	5	74	16% 89% . 8%
5	E	74	18% 89% . 8%
5	e	74	16% 89% . 8%
6	6	165	13% 85% 15%
6	F	165	11% 85% 15%
6	f	165	13% 85% 15%
7	I	40	. 92% 8%
7	h	40	92% 8%
7	i	40	92% 8%
8	7	40	5% 98% .
8	J	40	8% 98% .
8	j	40	8% 98% .
9	0	157	8% 97% . .
9	L	157	9% 97% . .
9	l	157	9% 97% . .
10	9	31	10% 97% .
10	M	31	10% 97% .
10	m	31	10% 97% .
11	8	90	30% 86% . 12%
11	K	90	37% 86% . 12%
11	k	90	34% 86% . 12%

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
13	CL0	1	803	X	-	-	-
13	CL0	A	803	X	-	-	-
13	CL0	a	803	X	-	-	-
14	CLA	0	202	X	-	-	-
14	CLA	0	206	X	-	-	-
14	CLA	0	207	X	-	-	-
14	CLA	0	208	X	-	-	-
14	CLA	1	804	X	-	-	-
14	CLA	1	805	X	-	-	-
14	CLA	1	806	X	-	-	-
14	CLA	1	807	X	-	-	-
14	CLA	1	808	X	-	-	-
14	CLA	1	809	X	-	-	-
14	CLA	1	810	X	-	-	-
14	CLA	1	811	X	-	-	-
14	CLA	1	812	X	-	-	-
14	CLA	1	813	X	-	-	-
14	CLA	1	814	X	-	-	-
14	CLA	1	815	X	-	-	-
14	CLA	1	817	X	-	-	-
14	CLA	1	818	X	-	-	-
14	CLA	1	819	X	-	-	-
14	CLA	1	820	X	-	-	-
14	CLA	1	821	X	-	-	-
14	CLA	1	822	X	-	-	-
14	CLA	1	823	X	-	-	-
14	CLA	1	824	X	-	-	-
14	CLA	1	825	X	-	-	-
14	CLA	1	826	X	-	-	-
14	CLA	1	827	X	-	-	-
14	CLA	1	828	X	-	-	-
14	CLA	1	829	X	-	-	-
14	CLA	1	830	X	-	-	-
14	CLA	1	831	X	-	-	-
14	CLA	1	832	X	-	-	-
14	CLA	1	833	X	-	-	-
14	CLA	1	834	X	-	-	-
14	CLA	1	835	X	-	-	-
14	CLA	1	836	X	-	-	-
14	CLA	1	837	X	-	-	-
14	CLA	1	838	X	-	-	-
14	CLA	1	839	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	840	X	-	-	-
14	CLA	1	841	X	-	-	-
14	CLA	1	843	X	-	-	-
14	CLA	1	844	X	-	-	-
14	CLA	2	801	X	-	-	-
14	CLA	2	803	X	-	-	-
14	CLA	2	804	X	-	-	-
14	CLA	2	805	X	-	-	-
14	CLA	2	806	X	-	-	-
14	CLA	2	808	X	-	-	-
14	CLA	2	809	X	-	-	-
14	CLA	2	810	X	-	-	-
14	CLA	2	811	X	-	-	-
14	CLA	2	812	X	-	-	-
14	CLA	2	813	X	-	-	-
14	CLA	2	814	X	-	-	-
14	CLA	2	815	X	-	-	-
14	CLA	2	816	X	-	-	-
14	CLA	2	817	X	-	-	-
14	CLA	2	818	X	-	-	-
14	CLA	2	820	X	-	-	-
14	CLA	2	821	X	-	-	-
14	CLA	2	824	X	-	-	-
14	CLA	2	826	X	-	-	-
14	CLA	2	827	X	-	-	-
14	CLA	2	828	X	-	-	-
14	CLA	2	829	X	-	-	-
14	CLA	2	830	X	-	-	-
14	CLA	2	831	X	-	-	-
14	CLA	2	832	X	-	-	-
14	CLA	2	833	X	-	-	-
14	CLA	2	834	X	-	-	-
14	CLA	2	835	X	-	-	-
14	CLA	2	836	X	-	-	-
14	CLA	2	837	X	-	-	-
14	CLA	2	838	X	-	-	-
14	CLA	2	839	X	-	-	-
14	CLA	2	840	X	-	-	-
14	CLA	2	841	X	-	-	-
14	CLA	2	842	X	-	-	-
14	CLA	2	844	X	-	-	-
14	CLA	6	4403	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	6	4404	X	-	-	-
14	CLA	7	1101	X	-	-	-
14	CLA	7	1102	X	-	-	-
14	CLA	7	1103	X	-	-	-
14	CLA	8	4003	X	-	-	-
14	CLA	8	4004	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	841	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	B	801	X	-	-	-
14	CLA	B	802	X	-	-	-
14	CLA	B	804	X	-	-	-
14	CLA	B	805	X	-	-	-
14	CLA	B	806	X	-	-	-
14	CLA	B	807	X	-	-	-
14	CLA	B	809	X	-	-	-
14	CLA	B	810	X	-	-	-
14	CLA	B	811	X	-	-	-
14	CLA	B	812	X	-	-	-
14	CLA	B	813	X	-	-	-
14	CLA	B	814	X	-	-	-
14	CLA	B	815	X	-	-	-
14	CLA	B	816	X	-	-	-
14	CLA	B	817	X	-	-	-
14	CLA	B	818	X	-	-	-
14	CLA	B	819	X	-	-	-
14	CLA	B	821	X	-	-	-
14	CLA	B	822	X	-	-	-
14	CLA	B	825	X	-	-	-
14	CLA	B	827	X	-	-	-
14	CLA	B	828	X	-	-	-
14	CLA	B	829	X	-	-	-
14	CLA	B	830	X	-	-	-
14	CLA	B	831	X	-	-	-
14	CLA	B	832	X	-	-	-
14	CLA	B	833	X	-	-	-
14	CLA	B	834	X	-	-	-
14	CLA	B	835	X	-	-	-
14	CLA	B	836	X	-	-	-
14	CLA	B	837	X	-	-	-
14	CLA	B	838	X	-	-	-
14	CLA	B	839	X	-	-	-
14	CLA	B	840	X	-	-	-
14	CLA	B	841	X	-	-	-
14	CLA	B	842	X	-	-	-
14	CLA	B	843	X	-	-	-
14	CLA	B	845	X	-	-	-
14	CLA	F	201	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	F	204	X	-	-	-
14	CLA	F	205	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	4003	X	-	-	-
14	CLA	K	4004	X	-	-	-
14	CLA	L	1501	X	-	-	-
14	CLA	L	1502	X	-	-	-
14	CLA	L	1503	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	a	844	X	-	-	-
14	CLA	a	854	X	-	-	-
14	CLA	b	801	X	-	-	-
14	CLA	b	802	X	-	-	-
14	CLA	b	804	X	-	-	-
14	CLA	b	805	X	-	-	-
14	CLA	b	806	X	-	-	-
14	CLA	b	807	X	-	-	-
14	CLA	b	809	X	-	-	-
14	CLA	b	810	X	-	-	-
14	CLA	b	811	X	-	-	-
14	CLA	b	812	X	-	-	-
14	CLA	b	813	X	-	-	-
14	CLA	b	814	X	-	-	-
14	CLA	b	815	X	-	-	-
14	CLA	b	816	X	-	-	-
14	CLA	b	817	X	-	-	-
14	CLA	b	818	X	-	-	-
14	CLA	b	820	X	-	-	-
14	CLA	b	821	X	-	-	-
14	CLA	b	824	X	-	-	-
14	CLA	b	826	X	-	-	-
14	CLA	b	827	X	-	-	-
14	CLA	b	828	X	-	-	-
14	CLA	b	829	X	-	-	-
14	CLA	b	830	X	-	-	-
14	CLA	b	831	X	-	-	-
14	CLA	b	832	X	-	-	-
14	CLA	b	833	X	-	-	-
14	CLA	b	834	X	-	-	-
14	CLA	b	835	X	-	-	-
14	CLA	b	836	X	-	-	-
14	CLA	b	837	X	-	-	-
14	CLA	b	838	X	-	-	-
14	CLA	b	839	X	-	-	-
14	CLA	b	840	X	-	-	-
14	CLA	b	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	842	X	-	-	-
14	CLA	b	844	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	204	X	-	-	-
14	CLA	f	205	X	-	-	-
14	CLA	j	101	X	-	-	-
14	CLA	j	102	X	-	-	-
14	CLA	k	4003	X	-	-	-
14	CLA	l	4203	X	-	-	-
14	CLA	l	4204	X	-	-	-
14	CLA	l	4205	X	-	-	-
14	CLA	l	4206	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 72606 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	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	a	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		
1	1	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		
2	b	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		
2	2	733	Total	C	N	O	S	0	0
			5806	3824	973	994	15		

- 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
			600	369	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			600	369	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		
4	4	138	Total	C	N	O	S	0	0
			1078	683	187	205	3		

- 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
			537	337	95	105			
5	e	68	Total	C	N	O		0	0
			537	337	95	105			
5	5	68	Total	C	N	O		0	0
			537	337	95	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		
6	f	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		
6	6	141	Total	C	N	O	S	0	0
			1086	702	180	200	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	i	37	Total	C	N	O	S	0	0
			293	200	41	49	3		
7	h	37	Total	C	N	O	S	0	0
			293	200	41	49	3		

- 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	S	0	0
			311	210	46	52	3		
8	j	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	39	Total	C	N	O	S	0	0
			311	210	46	52	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	L	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		
9	1	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		
9	0	153	Total	C	N	O	S	0	0
			1138	745	186	205	2		

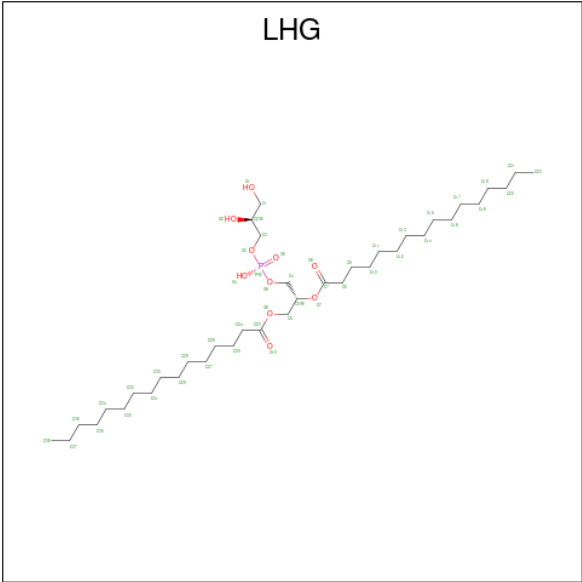
- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms				AltConf	Trace
10	M	30	Total	C	N	O	0	0
			230	154	35	41		
10	m	30	Total	C	N	O	0	0
			230	154	35	41		
10	9	30	Total	C	N	O	0	0
			230	154	35	41		

- Molecule 11 is a protein called Photosystem I reaction center subunit PsaK 2.

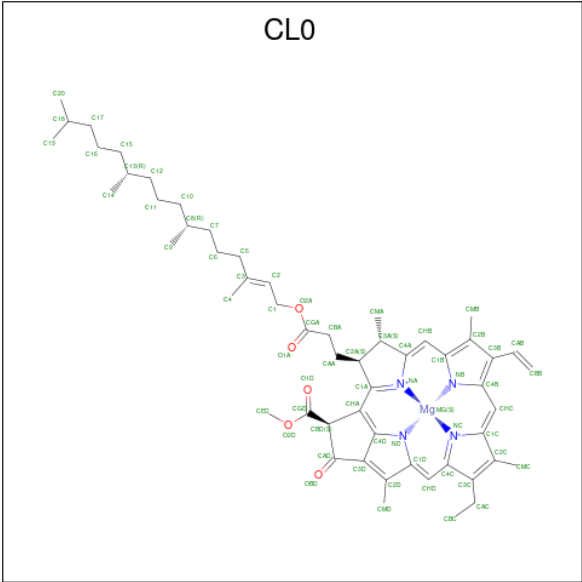
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	k	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	8	79	Total	C	N	O	S	0	0
			566	373	90	98	5		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



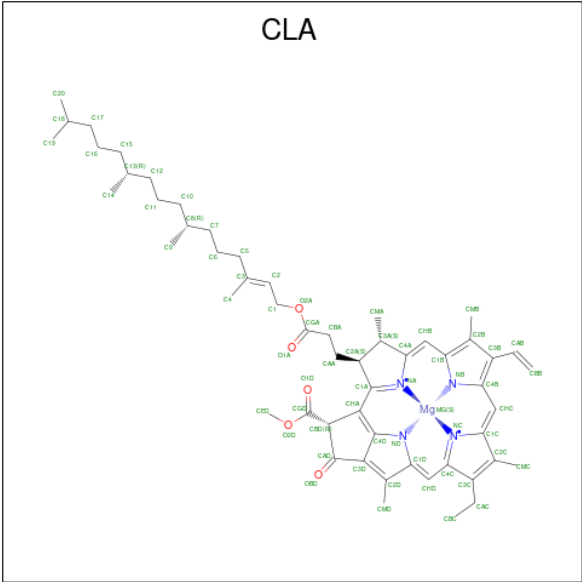
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	A	1	Total	C	O	P	0
			33	22	10	1	
12	B	1	Total	C	O	P	0
			39	28	10	1	
12	M	1	Total	C	O	P	0
			39	28	10	1	
12	a	1	Total	C	O	P	0
			49	38	10	1	
12	a	1	Total	C	O	P	0
			33	22	10	1	
12	1	1	Total	C	O	P	0
			49	38	10	1	
12	1	1	Total	C	O	P	0
			33	22	10	1	
12	b	1	Total	C	O	P	0
			39	28	10	1	
12	2	1	Total	C	O	P	0
			39	28	10	1	
12	m	1	Total	C	O	P	0
			39	28	10	1	
12	9	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



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
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	B	1	Total	C	Mg	N		0
			27	22	1	4		

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Mol	Chain	Residues	Atoms					AltConf
14	F	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	K	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 54	C 44	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 54	C 44	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	b	1	Total	C	Mg	N		0
			27	22	1	4		
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			61	51	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
14	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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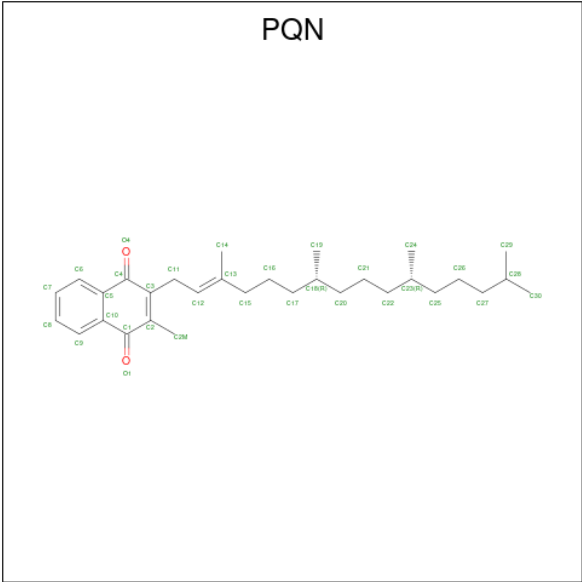
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	2	1	Total 62	C 52	Mg 1	N 4	O 5	0
14	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 27	C 22	Mg 1	N 4		0
14	f	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	7	1	Total 45	C 35	Mg 1	N 4	O 5	0

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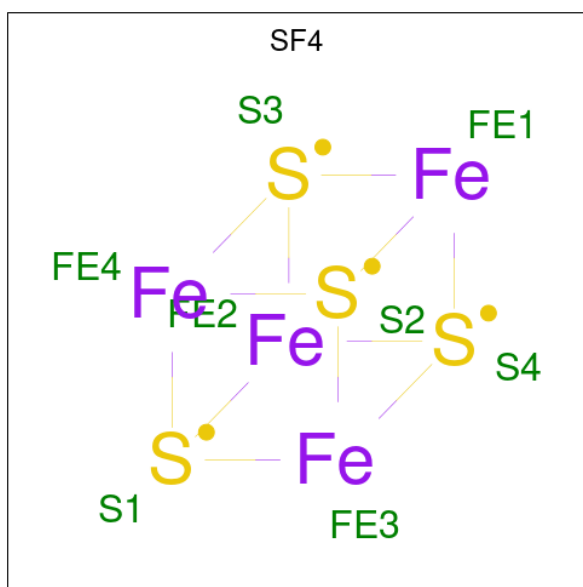
Mol	Chain	Residues	Atoms					AltConf
14	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
14	0	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



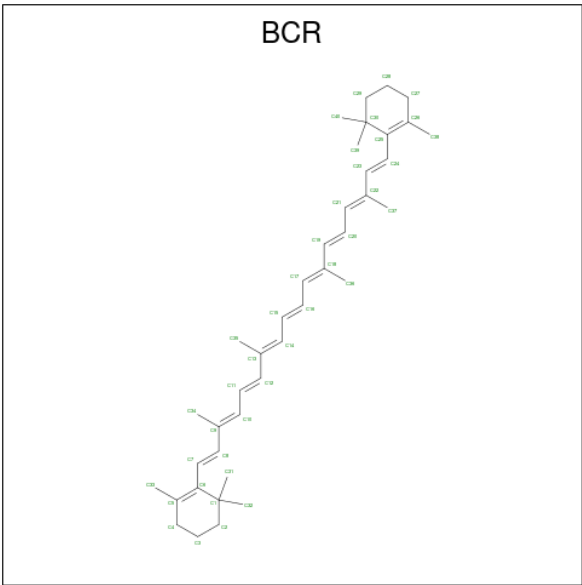
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



Mol	Chain	Residues	Atoms			AltConf
16	A	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	C	1	Total	Fe	S	0
			8	4	4	
16	a	1	Total	Fe	S	0
			8	4	4	
16	1	1	Total	Fe	S	0
			8	4	4	
16	c	1	Total	Fe	S	0
			8	4	4	
16	c	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	
16	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 17 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms		AltConf
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	A	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			25	25	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	B	1	Total	C	0
			40	40	
17	F	1	Total	C	0
			40	40	
17	F	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
17	I	1	Total C 40 40	0
17	I	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	J	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	L	1	Total C 40 40	0
17	M	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	K	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	a	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	1	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0

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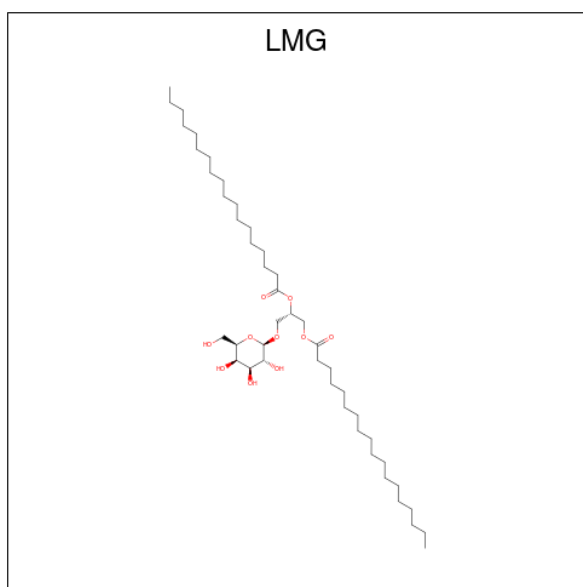
Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	f	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	6	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	i	1	Total C 40 40	0
17	h	1	Total C 40 40	0
17	h	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
17	j	1	Total C 40 40	0
17	j	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	7	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	k	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	8	1	Total C 40 40	0
17	l	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	0	1	Total C 40 40	0
17	9	1	Total C 40 40	0

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



Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			46	36	10	
18	A	1	Total	C	O	0
			32	22	10	
18	B	1	Total	C	O	0
			48	38	10	
18	L	1	Total	C	O	0
			38	28	10	
18	a	1	Total	C	O	0
			46	36	10	
18	a	1	Total	C	O	0
			32	22	10	
18	1	1	Total	C	O	0
			32	22	10	
18	b	1	Total	C	O	0
			48	38	10	
18	2	1	Total	C	O	0
			48	38	10	
18	1	1	Total	C	O	0
			38	28	10	
18	0	1	Total	C	O	0
			38	28	10	
18	0	1	Total	C	O	0
			46	36	10	

- Molecule 19 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
19	F	1	Total 35	C 24	O 11	0
19	I	1	Total 35	C 24	O 11	0
19	f	1	Total 35	C 24	O 11	0
19	6	1	Total 35	C 24	O 11	0
19	i	1	Total 35	C 24	O 11	0
19	h	1	Total 35	C 24	O 11	0

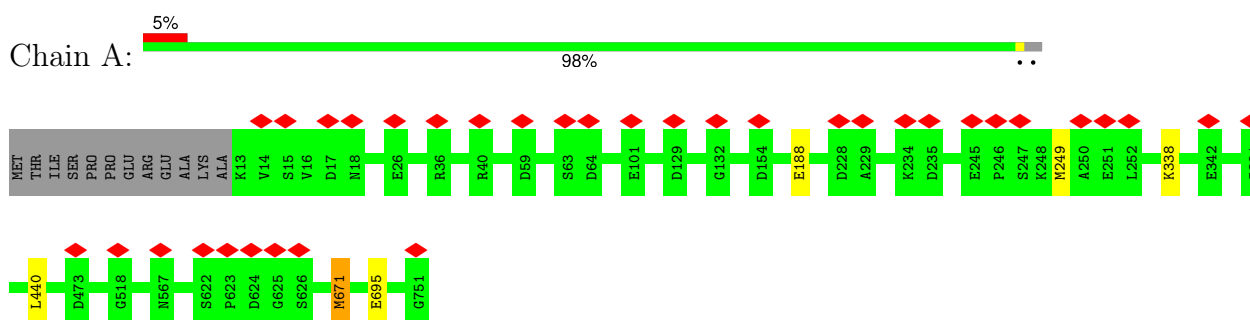
- Molecule 20 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
20	L	1	Total Ca 1 1	0
20	1	1	Total Ca 1 1	0
20	0	1	Total Ca 1 1	0

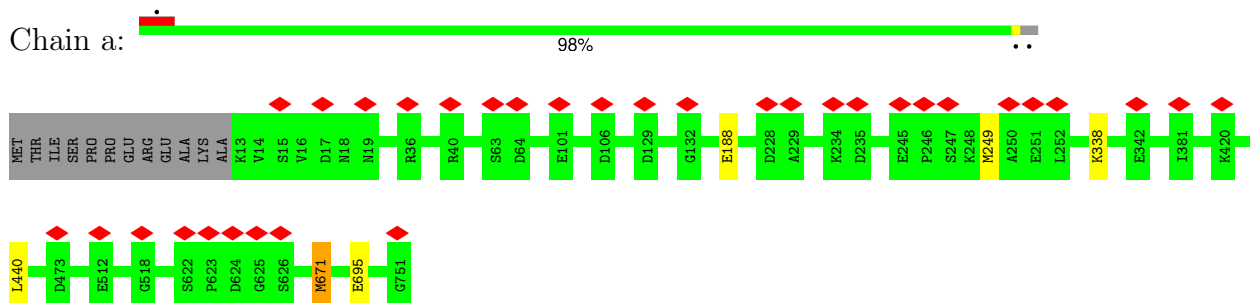
3 Residue-property plots [i](#)

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.

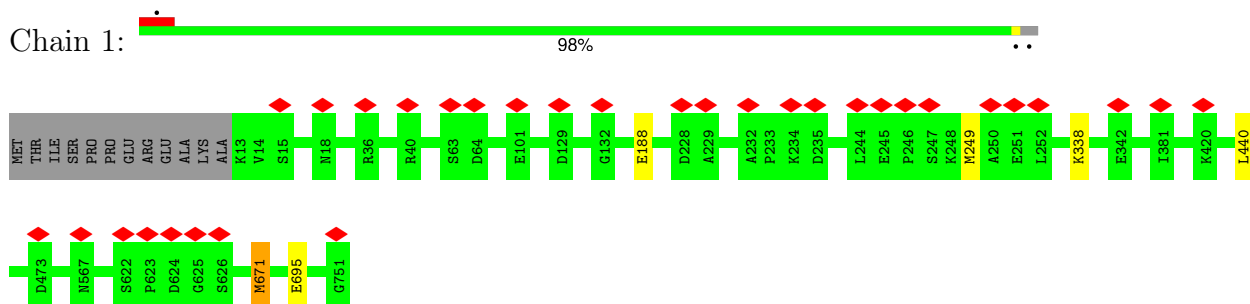
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

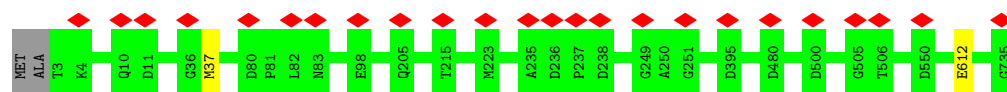


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

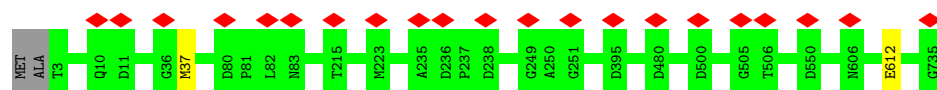


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

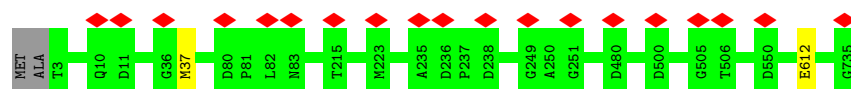




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



- Molecule 3: Photosystem I iron-sulfur center



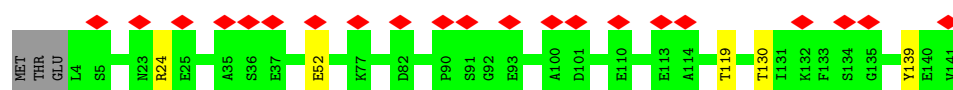
- Molecule 3: Photosystem I iron-sulfur center



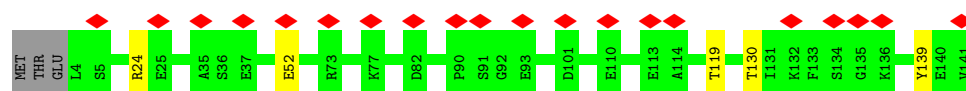
- Molecule 3: Photosystem I iron-sulfur center



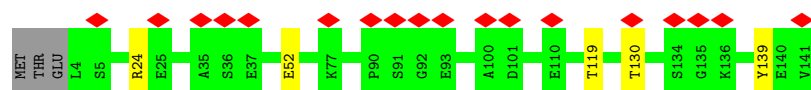
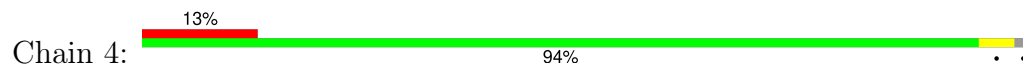
- Molecule 4: Photosystem I reaction center subunit II



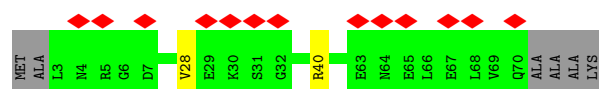
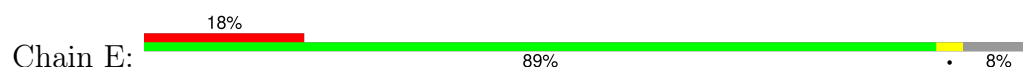
- Molecule 4: Photosystem I reaction center subunit II



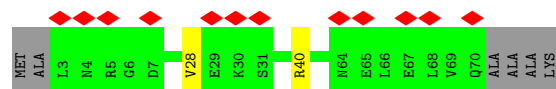
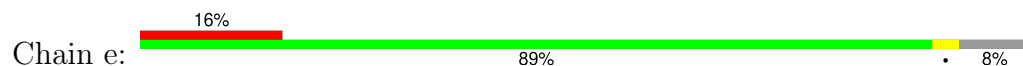
• Molecule 4: Photosystem I reaction center subunit II



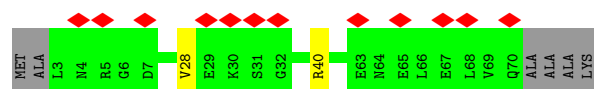
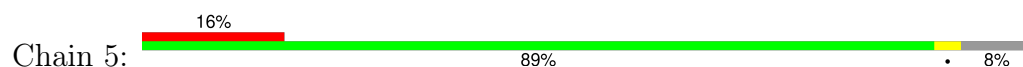
• Molecule 5: Photosystem I reaction center subunit IV



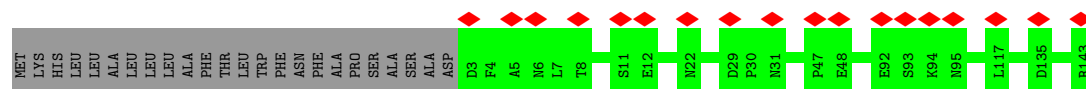
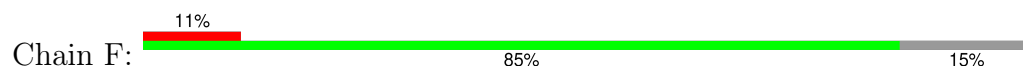
• Molecule 5: Photosystem I reaction center subunit IV



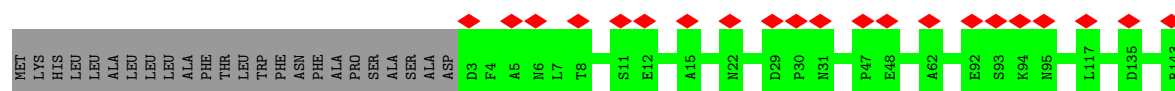
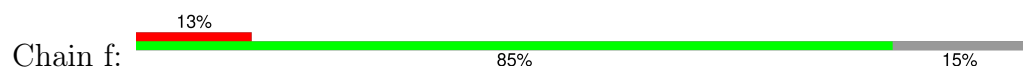
• Molecule 5: Photosystem I reaction center subunit IV



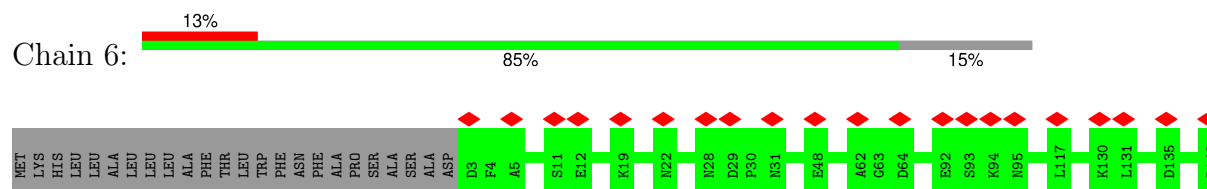
• Molecule 6: Photosystem I reaction center subunit III



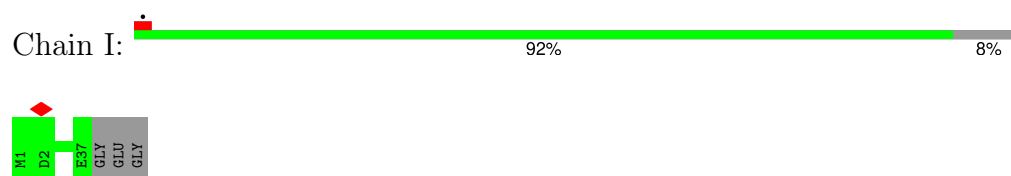
• Molecule 6: Photosystem I reaction center subunit III



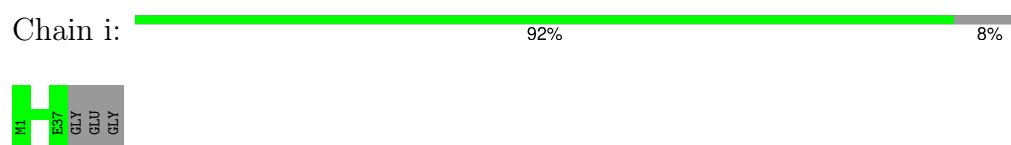
- Molecule 6: Photosystem I reaction center subunit III



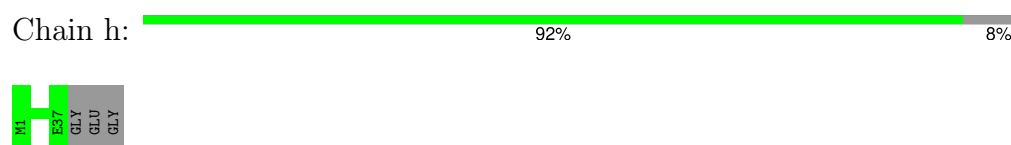
- Molecule 7: Photosystem I reaction center subunit VIII



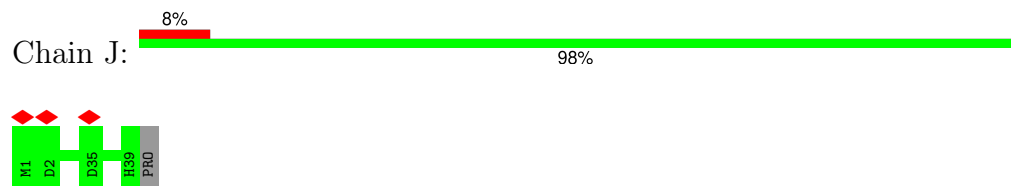
- Molecule 7: Photosystem I reaction center subunit VIII



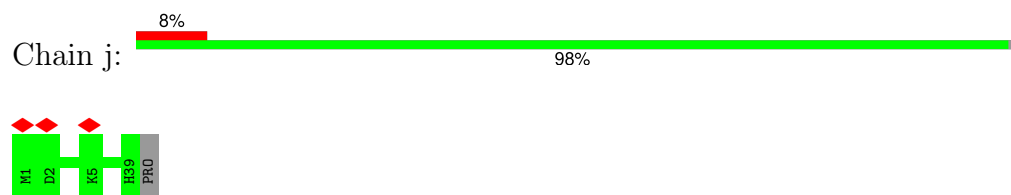
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX

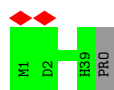


- Molecule 8: Photosystem I reaction center subunit IX

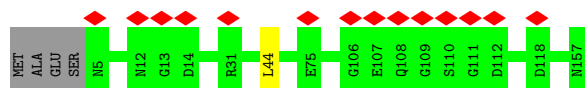


- Molecule 8: Photosystem I reaction center subunit IX

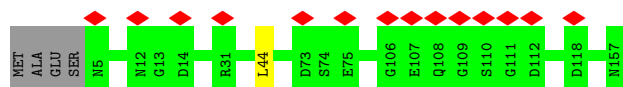




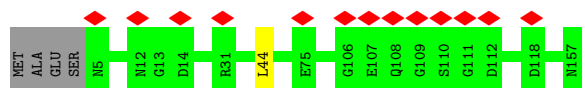
- Molecule 9: Photosystem I reaction center subunit XI



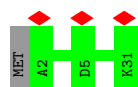
- Molecule 9: Photosystem I reaction center subunit XI



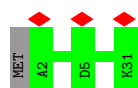
- Molecule 9: Photosystem I reaction center subunit XI



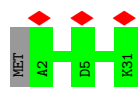
- Molecule 10: Photosystem I reaction center subunit XII



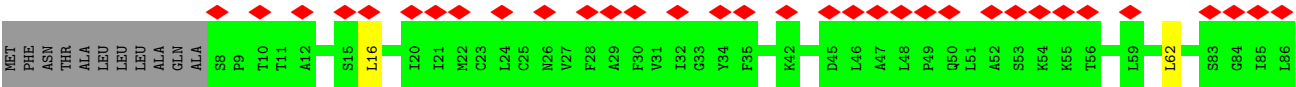
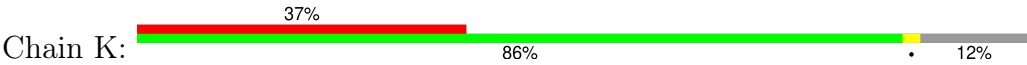
- Molecule 10: Photosystem I reaction center subunit XII



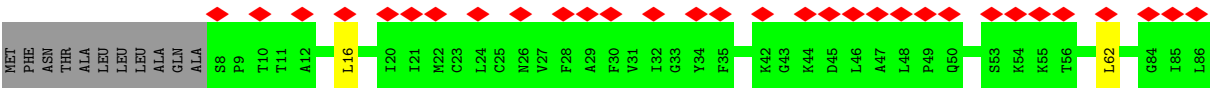
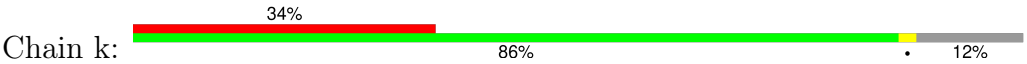
- Molecule 10: Photosystem I reaction center subunit XII



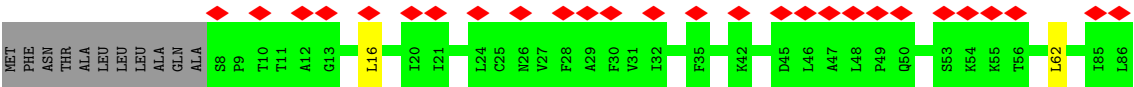
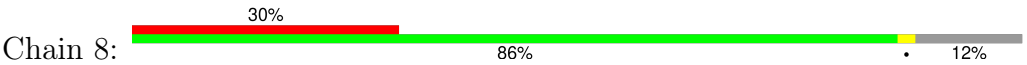
- Molecule 11: Photosystem I reaction center subunit PsaK 2



• Molecule 11: Photosystem I reaction center subunit PsaK 2



• Molecule 11: Photosystem I reaction center subunit PsaK 2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	196181	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.6	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	0.229	Depositor
Minimum map value	-0.131	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0187	Depositor
Map size (\AA)	325.5, 325.5, 325.5	wwPDB
Map dimensions	310, 310, 310	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.05, 1.05, 1.05	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, LMG, LHG, LMT, SF4, CLA, CA, BCR, 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	0.49	0/5985	0.56	3/8158 (0.0%)
1	A	0.49	0/5985	0.56	3/8158 (0.0%)
1	a	0.49	0/5985	0.56	3/8158 (0.0%)
2	2	0.51	0/6021	0.55	0/8237
2	B	0.51	0/6021	0.55	0/8237
2	b	0.51	0/6021	0.55	0/8237
3	3	0.50	0/610	0.54	0/826
3	C	0.50	0/610	0.54	0/826
3	c	0.50	0/610	0.54	0/826
4	4	0.41	0/1102	0.61	0/1485
4	D	0.41	0/1102	0.61	0/1485
4	d	0.41	0/1102	0.61	0/1485
5	5	0.45	0/546	0.51	0/738
5	E	0.45	0/546	0.51	0/738
5	e	0.45	0/546	0.52	0/738
6	6	0.33	0/1116	0.53	0/1520
6	F	0.33	0/1116	0.53	0/1520
6	f	0.33	0/1116	0.53	0/1520
7	I	0.43	0/304	0.57	0/416
7	h	0.43	0/304	0.58	0/416
7	i	0.43	0/304	0.58	0/416
8	7	0.35	0/319	0.58	0/431
8	J	0.35	0/319	0.58	0/431
8	j	0.35	0/319	0.58	0/431
9	0	0.43	0/1168	0.54	0/1588
9	L	0.43	0/1168	0.54	0/1588
9	l	0.43	0/1168	0.54	0/1588
10	9	0.31	0/233	0.55	0/316
10	M	0.31	0/233	0.55	0/316
10	m	0.31	0/233	0.55	0/316
11	8	0.31	0/577	0.61	1/778 (0.1%)
11	K	0.31	0/577	0.62	1/778 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	k	0.31	0/577	0.62	1/778 (0.1%)
All	All	0.47	0/53943	0.56	12/73479 (0.0%)

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	MET	CB-CG-SD	6.90	133.10	112.40
1	a	671	MET	CB-CG-SD	6.88	133.05	112.40
1	1	671	MET	CB-CG-SD	6.88	133.04	112.40
11	K	62	LEU	CA-CB-CG	6.45	130.13	115.30
1	a	671	MET	CG-SD-CE	6.43	110.49	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	A	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
1	a	737/751 (98%)	712 (97%)	25 (3%)	0	100	100
2	2	731/735 (100%)	700 (96%)	31 (4%)	0	100	100
2	B	731/735 (100%)	700 (96%)	31 (4%)	0	100	100
2	b	731/735 (100%)	700 (96%)	31 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	3	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	C	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
3	c	78/81 (96%)	74 (95%)	4 (5%)	0	100	100
4	4	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
4	D	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
4	d	136/141 (96%)	127 (93%)	9 (7%)	0	100	100
5	5	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
5	E	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
5	e	66/74 (89%)	63 (96%)	3 (4%)	0	100	100
6	6	139/165 (84%)	131 (94%)	8 (6%)	0	100	100
6	F	139/165 (84%)	131 (94%)	8 (6%)	0	100	100
6	f	139/165 (84%)	131 (94%)	8 (6%)	0	100	100
7	I	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
7	h	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
7	i	35/40 (88%)	33 (94%)	2 (6%)	0	100	100
8	7	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
8	J	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
8	j	37/40 (92%)	34 (92%)	3 (8%)	0	100	100
9	0	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
9	L	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
9	l	151/157 (96%)	148 (98%)	3 (2%)	0	100	100
10	9	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
10	M	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
10	m	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
11	8	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
11	K	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
11	k	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
All	All	6645/6915 (96%)	6366 (96%)	279 (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	593/603 (98%)	588 (99%)	5 (1%)	79	89
1	A	593/603 (98%)	588 (99%)	5 (1%)	79	89
1	a	593/603 (98%)	588 (99%)	5 (1%)	79	89
2	2	585/588 (100%)	583 (100%)	2 (0%)	91	95
2	B	585/588 (100%)	583 (100%)	2 (0%)	91	95
2	b	585/588 (100%)	583 (100%)	2 (0%)	91	95
3	3	68/69 (99%)	67 (98%)	1 (2%)	60	80
3	C	68/69 (99%)	67 (98%)	1 (2%)	60	80
3	c	68/69 (99%)	67 (98%)	1 (2%)	60	80
4	4	113/116 (97%)	108 (96%)	5 (4%)	24	54
4	D	113/116 (97%)	108 (96%)	5 (4%)	24	54
4	d	113/116 (97%)	108 (96%)	5 (4%)	24	54
5	5	58/60 (97%)	56 (97%)	2 (3%)	32	62
5	E	58/60 (97%)	56 (97%)	2 (3%)	32	62
5	e	58/60 (97%)	56 (97%)	2 (3%)	32	62
6	6	114/137 (83%)	114 (100%)	0	100	100
6	F	114/137 (83%)	114 (100%)	0	100	100
6	f	114/137 (83%)	114 (100%)	0	100	100
7	I	31/32 (97%)	31 (100%)	0	100	100
7	h	31/32 (97%)	31 (100%)	0	100	100
7	i	31/32 (97%)	31 (100%)	0	100	100
8	7	34/35 (97%)	34 (100%)	0	100	100
8	J	34/35 (97%)	34 (100%)	0	100	100
8	j	34/35 (97%)	34 (100%)	0	100	100
9	0	111/118 (94%)	110 (99%)	1 (1%)	75	88
9	L	111/118 (94%)	110 (99%)	1 (1%)	75	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	l	111/118 (94%)	110 (99%)	1 (1%)	75	88
10	9	24/25 (96%)	24 (100%)	0	100	100
10	M	24/25 (96%)	24 (100%)	0	100	100
10	m	24/25 (96%)	24 (100%)	0	100	100
11	8	59/68 (87%)	58 (98%)	1 (2%)	56	78
11	K	59/68 (87%)	58 (98%)	1 (2%)	56	78
11	k	59/68 (87%)	58 (98%)	1 (2%)	56	78
All	All	5370/5553 (97%)	5319 (99%)	51 (1%)	74	88

5 of 51 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	3	66	ARG
4	d	119	THR
9	l	44	LEU
2	b	37	MET
2	2	612	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
9	L	36	ASN
1	1	714	GLN
9	l	6	GLN
9	l	36	ASN
9	0	6	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 408 ligands modelled in this entry, 3 are monoatomic - leaving 405 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	a	834	-	48,58,73	1.47	8 (16%)	56,95,113	1.80	10 (17%)
14	CLA	L	1503	-	63,73,73	1.28	6 (9%)	74,113,113	1.36	8 (10%)
14	CLA	a	812	1	48,58,73	1.49	8 (16%)	56,95,113	1.68	9 (16%)
14	CLA	L	1502	-	63,73,73	1.30	8 (12%)	74,113,113	1.47	9 (12%)
14	CLA	1	813	-	52,62,73	1.45	9 (17%)	60,99,113	1.58	8 (13%)
14	CLA	a	824	-	63,73,73	1.34	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	1	812	-	63,73,73	1.29	8 (12%)	74,113,113	1.51	9 (12%)
17	BCR	7	1104	-	41,41,41	1.23	3 (7%)	56,56,56	1.32	5 (8%)
14	CLA	2	821	-	45,55,73	1.55	8 (17%)	52,91,113	1.55	6 (11%)
17	BCR	B	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	839	-	48,58,73	1.43	7 (14%)	56,95,113	1.72	10 (17%)
12	LHG	a	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	0	202	-	63,73,73	1.27	7 (11%)	74,113,113	1.38	7 (9%)
14	CLA	B	819	-	53,63,73	1.36	7 (13%)	62,101,113	1.63	7 (11%)
14	CLA	2	833	-	53,63,73	1.42	7 (13%)	62,101,113	1.52	7 (11%)
14	CLA	a	805	-	63,73,73	1.34	8 (12%)	74,113,113	1.20	6 (8%)
17	BCR	8	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
14	CLA	a	829	-	53,63,73	1.39	7 (13%)	62,101,113	1.42	6 (9%)
14	CLA	1	843	-	63,73,73	1.34	9 (14%)	74,113,113	1.39	7 (9%)
14	CLA	1	815	-	43,53,73	1.54	8 (18%)	50,89,113	1.70	6 (12%)
14	CLA	a	832	-	63,73,73	1.31	7 (11%)	74,113,113	1.51	9 (12%)
14	CLA	2	844	-	28,35,73	2.19	7 (25%)	28,60,113	1.78	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	F	201	-	49,59,73	1.47	8 (16%)	56,96,113	1.53	7 (12%)
14	CLA	A	825	-	49,59,73	1.48	7 (14%)	56,96,113	1.69	5 (8%)
14	CLA	b	837	-	43,53,73	1.58	8 (18%)	50,89,113	1.63	6 (12%)
14	CLA	b	806	-	63,73,73	1.29	8 (12%)	74,113,113	1.59	8 (10%)
14	CLA	b	804	-	63,73,73	1.32	8 (12%)	74,113,113	1.29	8 (10%)
14	CLA	8	4002	-	43,53,73	1.61	7 (16%)	50,89,113	1.62	8 (16%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
17	BCR	i	4102	-	41,41,41	1.23	2 (4%)	56,56,56	1.37	5 (8%)
17	BCR	a	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
14	CLA	a	839	-	49,59,73	1.44	9 (18%)	56,96,113	1.55	10 (17%)
14	CLA	a	821	-	52,62,73	1.44	8 (15%)	60,99,113	1.57	8 (13%)
14	CLA	k	4003	-	43,53,73	1.63	5 (11%)	50,89,113	1.70	7 (14%)
14	CLA	2	820	-	58,68,73	1.37	7 (12%)	68,107,113	1.53	9 (13%)
18	LMG	A	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	B	810	-	58,68,73	1.38	8 (13%)	68,107,113	1.38	9 (13%)
14	CLA	B	828	-	48,58,73	1.44	7 (14%)	56,95,113	1.49	9 (16%)
14	CLA	B	844	-	63,73,73	1.35	8 (12%)	74,113,113	1.46	9 (12%)
14	CLA	b	840	-	60,70,73	1.35	7 (11%)	70,109,113	1.34	7 (10%)
17	BCR	b	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.40	10 (17%)
18	LMG	A	852	-	46,46,55	0.86	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	B	834	-	53,63,73	1.42	6 (11%)	62,101,113	1.52	7 (11%)
14	CLA	A	810	1	63,73,73	1.30	7 (11%)	74,113,113	1.33	8 (10%)
17	BCR	j	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.31	6 (10%)
14	CLA	1	834	-	63,73,73	1.30	7 (11%)	74,113,113	1.54	12 (16%)
14	CLA	2	827	-	48,58,73	1.45	7 (14%)	56,95,113	1.49	9 (16%)
14	CLA	B	813	-	63,73,73	1.26	8 (12%)	74,113,113	1.50	9 (12%)
14	CLA	A	826	-	57,67,73	1.37	7 (12%)	66,105,113	1.57	9 (13%)
17	BCR	L	1505	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	1	825	-	57,67,73	1.36	7 (12%)	66,105,113	1.56	10 (15%)
14	CLA	a	854	-	53,63,73	1.42	7 (13%)	62,101,113	1.37	9 (14%)
12	LHG	A	802	14	32,32,48	0.87	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	A	804	-	63,73,73	1.35	8 (12%)	74,113,113	1.20	6 (8%)
14	CLA	1	817	-	44,54,73	1.57	7 (15%)	51,90,113	1.49	7 (13%)
14	CLA	A	842	-	63,73,73	1.31	8 (12%)	74,113,113	1.44	7 (9%)
17	BCR	h	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.36	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	814	-	43,53,73	1.57	8 (18%)	50,89,113	1.63	8 (16%)
14	CLA	B	823	-	43,53,73	1.57	6 (13%)	50,89,113	1.64	6 (12%)
14	CLA	a	819	-	44,54,73	1.57	7 (15%)	51,90,113	1.48	7 (13%)
19	LMT	i	4101	-	36,36,36	1.20	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	b	842	-	63,73,73	1.29	8 (12%)	74,113,113	1.26	7 (9%)
14	CLA	a	831	-	63,73,73	1.26	7 (11%)	74,113,113	1.60	11 (14%)
14	CLA	A	817	-	43,53,73	1.57	7 (16%)	50,89,113	1.59	6 (12%)
14	CLA	B	817	-	44,54,73	1.55	6 (13%)	51,90,113	1.66	5 (9%)
14	CLA	a	816	-	53,63,73	1.41	7 (13%)	62,101,113	1.51	8 (12%)
14	CLA	f	201	-	49,59,73	1.47	8 (16%)	56,96,113	1.54	7 (12%)
14	CLA	A	829	-	63,73,73	1.34	7 (11%)	74,113,113	1.60	7 (9%)
14	CLA	a	837	-	52,62,73	1.49	8 (15%)	60,99,113	1.51	6 (10%)
14	CLA	A	823	-	63,73,73	1.34	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	2	831	-	58,68,73	1.44	9 (15%)	68,107,113	1.74	8 (11%)
14	CLA	7	1101	-	63,73,73	1.33	8 (12%)	74,113,113	1.29	7 (9%)
18	LMG	0	201	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
14	CLA	b	822	-	43,53,73	1.57	6 (13%)	50,89,113	1.65	6 (12%)
14	CLA	7	1103	-	35,45,73	1.75	6 (17%)	42,78,113	1.55	5 (11%)
17	BCR	b	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	F	204	-	43,53,73	1.57	7 (16%)	50,89,113	1.77	7 (14%)
17	BCR	A	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
17	BCR	1	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
14	CLA	2	812	-	63,73,73	1.27	8 (12%)	74,113,113	1.50	9 (12%)
14	CLA	A	806	-	48,58,73	1.48	8 (16%)	56,95,113	1.69	9 (16%)
14	CLA	B	820	-	53,63,73	1.44	8 (15%)	62,101,113	1.69	7 (11%)
17	BCR	M	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
17	BCR	K	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
17	BCR	a	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
12	LHG	1	802	14	32,32,48	0.87	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	B	814	-	43,53,73	1.56	7 (16%)	50,89,113	1.56	7 (14%)
14	CLA	A	819	-	52,62,73	1.42	6 (11%)	60,99,113	1.56	7 (11%)
14	CLA	1	828	-	63,73,73	1.34	7 (11%)	74,113,113	1.59	7 (9%)
14	CLA	1	841	-	49,59,73	1.47	8 (16%)	56,96,113	1.53	7 (12%)
14	CLA	0	206	9	63,73,73	1.28	6 (9%)	74,113,113	1.48	9 (12%)
14	CLA	2	843	-	63,73,73	1.37	9 (14%)	74,113,113	1.46	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	836	-	43,53,73	1.54	7 (16%)	50,89,113	1.66	9 (18%)
14	CLA	A	836	-	52,62,73	1.50	8 (15%)	60,99,113	1.51	6 (10%)
14	CLA	a	828	-	63,73,73	1.29	8 (12%)	74,113,113	1.41	9 (12%)
14	CLA	A	812	-	43,53,73	1.56	7 (16%)	50,89,113	1.57	7 (14%)
14	CLA	1	814	-	53,63,73	1.41	7 (13%)	62,101,113	1.51	8 (12%)
16	SF4	c	102	3	0,12,12	-	-	-		
17	BCR	k	4004	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	5 (8%)
17	BCR	L	1504	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	1	816	-	43,53,73	1.56	7 (16%)	50,89,113	1.59	5 (10%)
14	CLA	a	820	-	52,62,73	1.42	7 (13%)	60,99,113	1.56	7 (11%)
14	CLA	B	840	-	48,58,73	1.43	7 (14%)	56,95,113	1.72	10 (17%)
14	CLA	b	809	-	63,73,73	1.32	8 (12%)	74,113,113	1.51	8 (10%)
12	LHG	A	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
17	BCR	b	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.35	7 (21%)
17	BCR	a	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	A	843	-	63,73,73	1.35	9 (14%)	74,113,113	1.39	7 (9%)
16	SF4	3	102	3	0,12,12	-	-	-		
14	CLA	2	816	-	44,54,73	1.56	6 (13%)	51,90,113	1.66	5 (9%)
14	CLA	2	809	-	58,68,73	1.37	7 (12%)	68,107,113	1.37	8 (11%)
14	CLA	A	841	-	63,73,73	1.27	8 (12%)	74,113,113	1.54	9 (12%)
14	CLA	f	204	-	43,53,73	1.56	7 (16%)	50,89,113	1.78	7 (14%)
14	CLA	B	841	-	60,70,73	1.34	7 (11%)	70,109,113	1.34	8 (11%)
17	BCR	A	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	10 (17%)
14	CLA	1	810	1	48,58,73	1.49	8 (16%)	56,95,113	1.68	9 (16%)
17	BCR	6	4402	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)
17	BCR	0	209	-	41,41,41	1.20	2 (4%)	56,56,56	1.41	9 (16%)
14	CLA	A	811	1	48,58,73	1.49	8 (16%)	56,95,113	1.67	9 (16%)
14	CLA	2	826	-	53,63,73	1.41	8 (15%)	62,101,113	1.63	10 (16%)
14	CLA	a	830	-	63,73,73	1.35	7 (11%)	74,113,113	1.59	7 (9%)
14	CLA	b	833	-	53,63,73	1.42	7 (13%)	62,101,113	1.52	7 (11%)
12	LHG	m	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	2	803	-	63,73,73	1.31	8 (12%)	74,113,113	1.29	8 (10%)
14	CLA	B	815	-	43,53,73	1.57	8 (18%)	50,89,113	1.64	8 (16%)
17	BCR	h	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)
19	LMT	I	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	809	-	63,73,73	1.33	9 (14%)	74,113,113	1.51	8 (10%)
14	CLA	2	805	-	63,73,73	1.28	8 (12%)	74,113,113	1.58	8 (10%)
17	BCR	A	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	2	832	-	43,53,73	1.58	8 (18%)	50,89,113	1.82	8 (16%)
14	CLA	2	815	-	63,73,73	1.33	8 (12%)	74,113,113	1.41	9 (12%)
14	CLA	1	842	-	63,73,73	1.30	8 (12%)	74,113,113	1.43	8 (10%)
17	BCR	6	4405	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	7 (12%)
14	CLA	2	838	-	44,54,73	1.58	6 (13%)	51,90,113	1.61	8 (15%)
14	CLA	K	4002	-	43,53,73	1.62	7 (16%)	50,89,113	1.62	8 (16%)
14	CLA	a	827	-	57,67,73	1.37	7 (12%)	66,105,113	1.57	10 (15%)
17	BCR	J	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	A	831	-	63,73,73	1.31	7 (11%)	74,113,113	1.50	9 (12%)
14	CLA	B	827	-	53,63,73	1.41	8 (15%)	62,101,113	1.62	10 (16%)
14	CLA	b	821	-	45,55,73	1.55	8 (17%)	52,91,113	1.56	7 (13%)
17	BCR	j	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	B	811	-	63,73,73	1.33	8 (12%)	74,113,113	1.42	8 (10%)
14	CLA	A	832	-	63,73,73	1.36	8 (12%)	74,113,113	1.56	7 (9%)
18	LMG	1	852	-	32,32,55	0.90	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	a	822	-	63,73,73	1.30	7 (11%)	74,113,113	1.48	8 (10%)
17	BCR	1	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
14	CLA	b	823	-	43,53,73	1.55	6 (13%)	50,89,113	1.69	7 (14%)
14	CLA	B	845	-	28,35,73	2.20	7 (25%)	28,60,113	1.77	5 (17%)
17	BCR	0	210	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
14	CLA	b	844	-	28,35,73	2.19	7 (25%)	28,60,113	1.77	5 (17%)
14	CLA	A	809	-	44,54,73	1.52	8 (18%)	51,90,113	1.61	7 (13%)
14	CLA	A	833	-	48,58,73	1.47	8 (16%)	56,95,113	1.79	10 (17%)
15	PQN	b	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
14	CLA	B	838	-	43,53,73	1.58	8 (18%)	50,89,113	1.63	6 (12%)
14	CLA	A	814	-	52,62,73	1.44	8 (15%)	60,99,113	1.58	8 (13%)
17	BCR	I	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)
14	CLA	1	838	-	63,73,73	1.33	7 (11%)	74,113,113	1.42	7 (9%)
14	CLA	a	804	-	58,68,73	1.36	8 (13%)	68,107,113	1.64	9 (13%)
14	CLA	B	830	-	58,68,73	1.36	8 (13%)	68,107,113	1.53	7 (10%)
14	CLA	l	4206	-	63,73,73	1.28	6 (9%)	74,113,113	1.36	8 (10%)
14	CLA	2	830	-	63,73,73	1.30	7 (11%)	74,113,113	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	821	-	58,68,73	1.37	7 (12%)	68,107,113	1.53	9 (13%)
14	CLA	b	824	-	43,53,73	1.58	8 (18%)	50,89,113	1.61	7 (14%)
14	CLA	b	820	-	58,68,73	1.37	7 (12%)	68,107,113	1.54	9 (13%)
14	CLA	a	809	-	63,73,73	1.29	8 (12%)	74,113,113	1.56	8 (10%)
14	CLA	A	844	12	43,53,73	1.60	8 (18%)	50,89,113	1.63	7 (14%)
14	CLA	a	835	-	63,73,73	1.26	7 (11%)	74,113,113	1.48	10 (13%)
14	CLA	k	4002	-	43,53,73	1.62	7 (16%)	50,89,113	1.63	8 (16%)
17	BCR	K	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.43	7 (12%)
15	PQN	A	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)
14	CLA	A	824	-	47,57,73	1.46	7 (14%)	53,93,113	1.70	8 (15%)
14	CLA	b	829	-	58,68,73	1.36	7 (12%)	68,107,113	1.52	7 (10%)
16	SF4	A	846	2,1	0,12,12	-	-	-	-	-
12	LHG	b	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	a	840	-	63,73,73	1.33	8 (12%)	74,113,113	1.42	7 (9%)
18	LMG	a	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
12	LHG	B	853	-	38,38,48	0.72	1 (2%)	41,44,54	1.22	3 (7%)
17	BCR	F	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
14	CLA	b	835	-	43,53,73	1.64	9 (20%)	50,89,113	1.68	7 (14%)
17	BCR	B	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	a	806	-	63,73,73	1.33	8 (12%)	74,113,113	1.30	7 (9%)
15	PQN	2	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
14	CLA	b	816	-	44,54,73	1.55	6 (13%)	51,90,113	1.66	5 (9%)
14	CLA	A	820	-	52,62,73	1.44	8 (15%)	60,99,113	1.57	8 (13%)
17	BCR	2	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	6 (10%)
17	BCR	k	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.42	7 (12%)
17	BCR	f	203	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	6	4403	-	43,53,73	1.56	7 (16%)	50,89,113	1.76	7 (14%)
14	CLA	a	825	-	47,57,73	1.45	6 (12%)	53,93,113	1.70	8 (15%)
14	CLA	L	1501	9	63,73,73	1.28	8 (12%)	74,113,113	1.48	9 (12%)
16	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	1	836	1	43,53,73	1.59	7 (16%)	50,89,113	1.71	8 (16%)
14	CLA	B	825	-	43,53,73	1.59	8 (18%)	50,89,113	1.61	7 (14%)
14	CLA	a	814	-	63,73,73	1.29	8 (12%)	74,113,113	1.51	8 (10%)
14	CLA	a	808	-	63,73,73	1.36	8 (12%)	74,113,113	1.39	7 (9%)
14	CLA	1	832	-	48,58,73	1.47	8 (16%)	56,95,113	1.80	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	824	-	43,53,73	1.58	8 (18%)	50,89,113	1.61	6 (12%)
17	BCR	F	203	-	41,41,41	1.26	2 (4%)	56,56,56	1.38	7 (12%)
17	BCR	A	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.21	5 (8%)
14	CLA	B	806	-	63,73,73	1.29	8 (12%)	74,113,113	1.58	8 (10%)
14	CLA	A	821	-	63,73,73	1.29	7 (11%)	74,113,113	1.48	8 (10%)
14	CLA	b	801	-	63,73,73	1.27	7 (11%)	74,113,113	1.39	7 (9%)
14	CLA	B	804	-	63,73,73	1.31	8 (12%)	74,113,113	1.29	9 (12%)
12	LHG	9	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	1	804	-	63,73,73	1.35	8 (12%)	74,113,113	1.20	6 (8%)
12	LHG	2	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	a	813	-	43,53,73	1.57	8 (18%)	50,89,113	1.57	7 (14%)
14	CLA	b	812	-	59,69,73	1.36	9 (15%)	69,108,113	1.67	9 (13%)
14	CLA	a	811	1	63,73,73	1.30	6 (9%)	74,113,113	1.33	7 (9%)
14	CLA	a	817	-	43,53,73	1.54	7 (16%)	50,89,113	1.69	6 (12%)
14	CLA	1	835	-	52,62,73	1.51	8 (15%)	60,99,113	1.51	6 (10%)
15	PQN	a	845	-	34,34,34	0.41	0	43,45,45	1.23	4 (9%)
17	BCR	6	4406	-	41,41,41	1.25	3 (7%)	56,56,56	1.39	8 (14%)
17	BCR	8	4001	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	7 (12%)
14	CLA	8	4004	-	53,63,73	1.43	7 (13%)	62,101,113	1.37	9 (14%)
14	CLA	A	834	-	63,73,73	1.27	7 (11%)	74,113,113	1.47	10 (13%)
14	CLA	b	826	-	53,63,73	1.41	8 (15%)	62,101,113	1.62	10 (16%)
17	BCR	b	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
17	BCR	b	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	8 (14%)
14	CLA	b	843	-	63,73,73	1.36	9 (14%)	74,113,113	1.46	9 (12%)
14	CLA	b	815	-	63,73,73	1.32	8 (12%)	74,113,113	1.42	9 (12%)
14	CLA	2	841	-	44,54,73	1.50	7 (15%)	51,90,113	1.77	9 (17%)
17	BCR	l	4207	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	807	-	52,62,73	1.39	6 (11%)	60,99,113	1.56	8 (13%)
14	CLA	1	831	-	63,73,73	1.36	8 (12%)	74,113,113	1.56	8 (10%)
14	CLA	b	836	-	43,53,73	1.54	7 (16%)	50,89,113	1.66	9 (18%)
19	LMT	F	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	2	814	-	43,53,73	1.58	8 (18%)	50,89,113	1.63	8 (16%)
17	BCR	B	849	-	25,25,41	1.17	2 (8%)	33,33,56	1.34	6 (18%)
14	CLA	B	802	-	63,73,73	1.27	7 (11%)	74,113,113	1.38	7 (9%)
15	PQN	B	846	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	818	-	43,53,73	1.55	7 (16%)	50,89,113	1.59	6 (12%)
14	CLA	2	840	-	60,70,73	1.34	7 (11%)	70,109,113	1.34	7 (10%)
14	CLA	A	835	-	63,73,73	1.30	7 (11%)	74,113,113	1.53	12 (16%)
14	CLA	J	101	-	43,53,73	1.57	6 (13%)	50,89,113	1.69	7 (14%)
14	CLA	B	816	-	63,73,73	1.32	8 (12%)	74,113,113	1.42	9 (12%)
14	CLA	F	205	-	43,53,73	1.59	7 (16%)	50,89,113	1.66	10 (20%)
17	BCR	a	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	8 (14%)
14	CLA	6	4404	-	43,53,73	1.58	7 (16%)	50,89,113	1.66	10 (20%)
14	CLA	8	4003	-	43,53,73	1.62	5 (11%)	50,89,113	1.70	7 (14%)
14	CLA	b	838	-	44,54,73	1.57	6 (13%)	51,90,113	1.62	8 (15%)
14	CLA	1	806	-	63,73,73	1.37	9 (14%)	74,113,113	1.38	7 (9%)
16	SF4	3	101	3	0,12,12	-	-	-	-	-
14	CLA	1	821	-	58,68,73	1.31	6 (10%)	68,107,113	1.38	7 (10%)
17	BCR	7	1105	-	41,41,41	1.18	3 (7%)	56,56,56	1.32	7 (12%)
14	CLA	2	819	-	53,63,73	1.43	8 (15%)	62,101,113	1.69	7 (11%)
14	CLA	A	805	-	63,73,73	1.33	8 (12%)	74,113,113	1.29	7 (9%)
14	CLA	2	835	-	43,53,73	1.64	8 (18%)	50,89,113	1.68	7 (14%)
14	CLA	1	822	-	63,73,73	1.35	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	B	805	-	63,73,73	1.36	7 (11%)	74,113,113	1.62	12 (16%)
17	BCR	J	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	2	811	-	59,69,73	1.35	8 (13%)	69,108,113	1.67	9 (13%)
16	SF4	a	846	2,1	0,12,12	-	-	-	-	-
14	CLA	1	829	-	63,73,73	1.27	7 (11%)	74,113,113	1.60	11 (14%)
14	CLA	1	823	-	47,57,73	1.46	6 (12%)	53,93,113	1.70	8 (15%)
14	CLA	A	827	-	63,73,73	1.29	8 (12%)	74,113,113	1.41	9 (12%)
17	BCR	2	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
14	CLA	a	833	-	63,73,73	1.36	8 (12%)	74,113,113	1.57	8 (10%)
13	CL0	A	803	-	63,73,73	1.35	7 (11%)	74,113,113	1.45	10 (13%)
14	CLA	1	805	-	48,58,73	1.48	8 (16%)	56,95,113	1.68	9 (16%)
14	CLA	A	839	-	63,73,73	1.33	8 (12%)	74,113,113	1.42	7 (9%)
14	CLA	2	829	-	58,68,73	1.35	7 (12%)	68,107,113	1.53	7 (10%)
14	CLA	B	842	-	44,54,73	1.51	7 (15%)	51,90,113	1.77	8 (15%)
17	BCR	b	854	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	a	841	-	45,55,73	1.49	8 (17%)	52,91,113	1.61	7 (13%)
14	CLA	2	828	-	63,73,73	1.32	7 (11%)	74,113,113	1.32	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	842	-	63,73,73	1.29	8 (12%)	74,113,113	1.26	7 (9%)
14	CLA	A	822	-	58,68,73	1.32	6 (10%)	68,107,113	1.37	7 (10%)
14	CLA	b	834	-	56,66,73	1.35	7 (12%)	65,104,113	1.46	9 (13%)
14	CLA	B	822	-	45,55,73	1.55	8 (17%)	52,91,113	1.56	7 (13%)
17	BCR	b	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	6 (10%)
17	BCR	2	846	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	1	811	-	43,53,73	1.57	8 (18%)	50,89,113	1.57	7 (14%)
14	CLA	b	830	-	63,73,73	1.30	7 (11%)	74,113,113	1.48	9 (12%)
14	CLA	b	813	-	43,53,73	1.56	8 (18%)	50,89,113	1.56	7 (14%)
14	CLA	B	812	-	59,69,73	1.36	9 (15%)	69,108,113	1.67	9 (13%)
19	LMT	h	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	B	836	-	43,53,73	1.64	9 (20%)	50,89,113	1.69	7 (14%)
14	CLA	1	819	-	52,62,73	1.44	8 (15%)	60,99,113	1.58	8 (13%)
14	CLA	1	824	-	49,59,73	1.48	7 (14%)	56,96,113	1.70	6 (10%)
14	CLA	A	828	-	53,63,73	1.38	7 (13%)	62,101,113	1.42	6 (9%)
14	CLA	B	833	-	43,53,73	1.59	8 (18%)	50,89,113	1.82	8 (16%)
14	CLA	1	826	-	63,73,73	1.28	8 (12%)	74,113,113	1.41	9 (12%)
14	CLA	2	822	-	43,53,73	1.57	6 (13%)	50,89,113	1.65	7 (14%)
17	BCR	1	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
12	LHG	M	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	1	807	-	63,73,73	1.30	8 (12%)	74,113,113	1.56	8 (10%)
14	CLA	A	838	-	49,59,73	1.44	9 (18%)	56,96,113	1.55	10 (17%)
14	CLA	b	832	-	43,53,73	1.59	8 (18%)	50,89,113	1.82	8 (16%)
14	CLA	B	826	-	43,53,73	1.55	8 (18%)	50,89,113	1.64	5 (10%)
14	CLA	l	4204	9	63,73,73	1.28	8 (12%)	74,113,113	1.48	9 (12%)
18	LMG	B	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
18	LMG	l	4202	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
17	BCR	2	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.34	5 (15%)
18	LMG	0	203	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	b	818	-	53,63,73	1.36	7 (13%)	62,101,113	1.62	7 (11%)
14	CLA	B	843	-	63,73,73	1.29	8 (12%)	74,113,113	1.26	6 (8%)
17	BCR	B	854	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	8 (14%)
18	LMG	L	1506	-	38,38,55	0.86	0	46,46,63	1.29	5 (10%)
17	BCR	2	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.33	8 (14%)
14	CLA	A	830	-	63,73,73	1.25	7 (11%)	74,113,113	1.60	11 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	809	1	63,73,73	1.30	6 (9%)	74,113,113	1.32	6 (8%)
14	CLA	f	205	-	43,53,73	1.59	7 (16%)	50,89,113	1.66	10 (20%)
14	CLA	b	817	-	43,53,73	1.56	6 (13%)	50,89,113	1.68	5 (10%)
14	CLA	2	801	-	58,68,73	1.36	8 (13%)	68,107,113	1.64	9 (13%)
14	CLA	j	102	-	35,45,73	1.75	6 (17%)	42,78,113	1.55	5 (11%)
17	BCR	B	851	-	41,41,41	1.25	5 (12%)	56,56,56	1.56	10 (17%)
14	CLA	1	830	-	63,73,73	1.31	7 (11%)	74,113,113	1.50	9 (12%)
14	CLA	2	837	-	43,53,73	1.58	8 (18%)	50,89,113	1.62	6 (12%)
14	CLA	A	815	-	53,63,73	1.42	7 (13%)	62,101,113	1.52	8 (12%)
14	CLA	2	834	-	56,66,73	1.35	7 (12%)	65,104,113	1.46	9 (13%)
13	CL0	a	803	-	63,73,73	1.36	7 (11%)	74,113,113	1.46	10 (13%)
14	CLA	b	808	-	63,73,73	1.32	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	0	207	-	63,73,73	1.29	8 (12%)	74,113,113	1.47	9 (12%)
17	BCR	1	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	5 (8%)
17	BCR	f	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
14	CLA	0	208	-	63,73,73	1.28	6 (9%)	74,113,113	1.36	8 (10%)
14	CLA	1	833	-	63,73,73	1.27	7 (11%)	74,113,113	1.48	10 (13%)
14	CLA	l	4205	-	63,73,73	1.30	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	a	823	-	58,68,73	1.32	6 (10%)	68,107,113	1.38	7 (10%)
14	CLA	B	837	-	43,53,73	1.54	7 (16%)	50,89,113	1.66	9 (18%)
14	CLA	2	823	-	43,53,73	1.55	6 (13%)	50,89,113	1.68	7 (14%)
14	CLA	b	802	-	63,73,73	1.27	8 (12%)	74,113,113	1.54	9 (12%)
14	CLA	b	831	-	58,68,73	1.44	9 (15%)	68,107,113	1.73	8 (11%)
14	CLA	A	808	-	63,73,73	1.30	8 (12%)	74,113,113	1.55	8 (10%)
17	BCR	b	853	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	8 (14%)
14	CLA	1	827	-	53,63,73	1.38	7 (13%)	62,101,113	1.42	6 (9%)
19	LMT	6	4401	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	2	804	-	63,73,73	1.36	7 (11%)	74,113,113	1.62	12 (16%)
14	CLA	A	807	-	63,73,73	1.37	8 (12%)	74,113,113	1.39	7 (9%)
14	CLA	K	4003	-	43,53,73	1.62	5 (11%)	50,89,113	1.71	7 (14%)
14	CLA	1	839	-	45,55,73	1.49	8 (17%)	52,91,113	1.61	7 (13%)
17	BCR	A	850	-	41,41,41	1.29	3 (7%)	56,56,56	1.41	9 (16%)
14	CLA	2	825	-	43,53,73	1.56	8 (18%)	50,89,113	1.66	5 (10%)
14	CLA	7	1102	-	43,53,73	1.57	6 (13%)	50,89,113	1.69	7 (14%)
14	CLA	B	808	-	63,73,73	1.32	7 (11%)	74,113,113	1.47	9 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	817	-	43,53,73	1.57	6 (13%)	50,89,113	1.68	6 (12%)
18	LMG	2	802	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	a	836	-	63,73,73	1.29	7 (11%)	74,113,113	1.54	12 (16%)
14	CLA	B	839	-	44,54,73	1.57	6 (13%)	51,90,113	1.61	8 (15%)
12	LHG	1	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	2	808	-	63,73,73	1.33	8 (12%)	74,113,113	1.51	8 (10%)
19	LMT	f	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	A	818	-	44,54,73	1.56	7 (15%)	51,90,113	1.49	7 (13%)
14	CLA	2	839	-	48,58,73	1.43	7 (14%)	56,95,113	1.71	10 (17%)
14	CLA	b	841	-	44,54,73	1.50	7 (15%)	51,90,113	1.78	9 (17%)
14	CLA	A	813	-	63,73,73	1.29	8 (12%)	74,113,113	1.51	8 (10%)
16	SF4	c	101	3	0,12,12	-	-	-	-	-
14	CLA	a	843	-	63,73,73	1.34	9 (14%)	74,113,113	1.39	7 (9%)
14	CLA	B	832	-	58,68,73	1.45	9 (15%)	68,107,113	1.74	8 (11%)
14	CLA	a	810	-	44,54,73	1.52	8 (18%)	51,90,113	1.62	7 (13%)
14	CLA	B	818	-	43,53,73	1.56	6 (13%)	50,89,113	1.67	5 (10%)
14	CLA	a	844	12	43,53,73	1.60	8 (18%)	50,89,113	1.63	7 (14%)
17	BCR	2	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	2	818	-	53,63,73	1.36	7 (13%)	62,101,113	1.63	7 (11%)
14	CLA	1	844	12	43,53,73	1.59	8 (18%)	50,89,113	1.63	7 (14%)
14	CLA	J	102	-	35,45,73	1.75	6 (17%)	42,78,113	1.55	5 (11%)
14	CLA	A	840	-	45,55,73	1.49	8 (17%)	52,91,113	1.60	7 (13%)
14	CLA	2	806	-	52,62,73	1.39	6 (11%)	60,99,113	1.54	8 (13%)
15	PQN	1	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)
14	CLA	1	808	-	44,54,73	1.52	8 (18%)	51,90,113	1.62	7 (13%)
17	BCR	i	4103	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	8 (14%)
14	CLA	A	816	-	43,53,73	1.54	7 (16%)	50,89,113	1.69	6 (12%)
17	BCR	B	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	B	824	-	43,53,73	1.55	6 (13%)	50,89,113	1.69	7 (14%)
13	CL0	1	803	-	63,73,73	1.35	7 (11%)	74,113,113	1.45	10 (13%)
14	CLA	A	837	1	43,53,73	1.58	7 (16%)	50,89,113	1.72	7 (14%)
14	CLA	b	827	-	48,58,73	1.45	7 (14%)	56,95,113	1.50	9 (16%)
14	CLA	b	825	-	43,53,73	1.56	8 (18%)	50,89,113	1.64	5 (10%)
14	CLA	b	819	-	53,63,73	1.44	8 (15%)	62,101,113	1.69	8 (12%)
14	CLA	b	811	-	63,73,73	1.32	8 (12%)	74,113,113	1.43	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	b	805	-	63,73,73	1.36	7 (11%)	74,113,113	1.62	12 (16%)
14	CLA	a	826	-	49,59,73	1.48	7 (14%)	56,96,113	1.68	5 (8%)
14	CLA	a	807	-	48,58,73	1.48	8 (16%)	56,95,113	1.69	9 (16%)
17	BCR	1	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	1	820	-	63,73,73	1.30	7 (11%)	74,113,113	1.47	8 (10%)
12	LHG	a	802	14	32,32,48	0.88	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	2	810	-	63,73,73	1.32	8 (12%)	74,113,113	1.43	7 (9%)
14	CLA	a	842	-	63,73,73	1.30	8 (12%)	74,113,113	1.43	8 (10%)
14	CLA	B	829	-	63,73,73	1.31	8 (12%)	74,113,113	1.32	7 (9%)
14	CLA	1	818	-	52,62,73	1.41	6 (11%)	60,99,113	1.56	7 (11%)
18	LMG	a	852	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	B	801	-	58,68,73	1.36	8 (13%)	68,107,113	1.65	9 (13%)
14	CLA	a	815	-	52,62,73	1.44	9 (17%)	60,99,113	1.59	8 (13%)
14	CLA	B	835	-	56,66,73	1.35	7 (12%)	65,104,113	1.46	9 (13%)
17	BCR	9	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	8 (14%)
18	LMG	b	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	B	831	-	63,73,73	1.30	7 (11%)	74,113,113	1.48	9 (12%)
14	CLA	j	101	-	43,53,73	1.56	6 (13%)	50,89,113	1.69	7 (14%)
14	CLA	a	838	1	43,53,73	1.59	7 (16%)	50,89,113	1.71	7 (14%)
14	CLA	l	4203	-	63,73,73	1.27	8 (12%)	74,113,113	1.49	9 (12%)
14	CLA	B	807	-	52,62,73	1.39	6 (11%)	60,99,113	1.56	9 (15%)
17	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
14	CLA	2	813	-	43,53,73	1.56	8 (18%)	50,89,113	1.56	7 (14%)
14	CLA	1	837	-	49,59,73	1.44	9 (18%)	56,96,113	1.54	10 (17%)
17	BCR	a	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	1	840	-	63,73,73	1.27	8 (12%)	74,113,113	1.54	9 (12%)
16	SF4	1	846	2,1	0,12,12	-	-	-	-	-
14	CLA	b	810	-	58,68,73	1.38	7 (12%)	68,107,113	1.37	8 (11%)
14	CLA	b	828	-	63,73,73	1.32	8 (12%)	74,113,113	1.32	7 (9%)
17	BCR	B	852	-	41,41,41	1.23	3 (7%)	56,56,56	1.33	8 (14%)
17	BCR	I	101	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	5 (8%)
14	CLA	2	807	-	63,73,73	1.32	7 (11%)	74,113,113	1.47	9 (12%)
14	CLA	K	4004	-	53,63,73	1.43	7 (13%)	62,101,113	1.38	9 (14%)

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
14	CLA	a	834	-	1/1/12/20	2/19/97/115	-
14	CLA	L	1503	-	1/1/15/20	13/37/115/115	-
14	CLA	a	812	1	1/1/12/20	7/19/97/115	-
14	CLA	L	1502	-	1/1/15/20	9/37/115/115	-
14	CLA	1	813	-	1/1/12/20	10/24/102/115	-
14	CLA	a	824	-	1/1/15/20	13/37/115/115	-
14	CLA	1	812	-	1/1/15/20	18/37/115/115	-
17	BCR	7	1104	-	-	13/29/63/63	0/2/2/2
14	CLA	2	821	-	1/1/11/20	4/16/94/115	-
17	BCR	B	850	-	-	15/29/63/63	0/2/2/2
14	CLA	b	839	-	1/1/12/20	7/19/97/115	-
14	CLA	0	202	-	1/1/15/20	10/37/115/115	-
12	LHG	a	801	-	-	22/53/53/53	-
14	CLA	B	819	-	1/1/13/20	10/25/103/115	-
14	CLA	2	833	-	1/1/13/20	12/25/103/115	-
14	CLA	a	805	-	1/1/15/20	9/37/115/115	-
17	BCR	8	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	a	829	-	1/1/13/20	6/25/103/115	-
14	CLA	1	843	-	1/1/15/20	17/37/115/115	-
14	CLA	1	815	-	1/1/11/20	4/13/91/115	-
14	CLA	a	832	-	1/1/15/20	7/37/115/115	-
14	CLA	2	844	-	1/1/5/20	-	-
14	CLA	F	201	-	1/1/12/20	10/21/99/115	-
14	CLA	A	825	-	1/1/12/20	9/21/99/115	-
14	CLA	b	837	-	1/1/11/20	2/13/91/115	-
14	CLA	b	806	-	1/1/15/20	14/37/115/115	-
14	CLA	b	804	-	1/1/15/20	11/37/115/115	-
14	CLA	8	4002	-	-	6/13/91/115	-
16	SF4	C	101	3	-	-	0/6/5/5
17	BCR	i	4102	-	-	16/29/63/63	0/2/2/2
17	BCR	a	847	-	-	11/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/12/20	7/21/99/115	-
14	CLA	a	821	-	1/1/12/20	4/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	k	4003	-	1/1/11/20	8/13/91/115	-
14	CLA	2	820	-	1/1/14/20	15/31/109/115	-
18	LMG	A	853	-	-	8/27/47/70	0/1/1/1
14	CLA	B	810	-	1/1/14/20	7/31/109/115	-
14	CLA	B	828	-	1/1/12/20	2/19/97/115	-
14	CLA	B	844	-	-	18/37/115/115	-
14	CLA	b	840	-	1/1/14/20	6/34/112/115	-
17	BCR	b	849	-	-	15/29/63/63	0/2/2/2
18	LMG	A	852	-	-	21/41/61/70	0/1/1/1
14	CLA	B	834	-	1/1/13/20	12/25/103/115	-
14	CLA	A	810	1	1/1/15/20	23/37/115/115	-
17	BCR	j	104	-	-	10/29/63/63	0/2/2/2
14	CLA	1	834	-	1/1/15/20	5/37/115/115	-
14	CLA	2	827	-	1/1/12/20	2/19/97/115	-
14	CLA	B	813	-	1/1/15/20	7/37/115/115	-
14	CLA	A	826	-	1/1/13/20	13/30/108/115	-
17	BCR	L	1505	-	-	13/29/63/63	0/2/2/2
14	CLA	1	825	-	1/1/13/20	13/30/108/115	-
14	CLA	a	854	-	1/1/13/20	5/25/103/115	-
14	CLA	A	804	-	1/1/15/20	9/37/115/115	-
14	CLA	1	817	-	1/1/11/20	5/15/93/115	-
12	LHG	A	802	14	-	13/37/37/53	-
14	CLA	A	842	-	-	11/37/115/115	-
17	BCR	h	101	-	-	16/29/63/63	0/2/2/2
14	CLA	b	814	-	1/1/11/20	9/13/91/115	-
14	CLA	B	823	-	-	5/13/91/115	-
14	CLA	a	819	-	1/1/11/20	5/15/93/115	-
19	LMT	i	4101	-	-	8/21/61/61	0/2/2/2
14	CLA	b	842	-	1/1/15/20	11/37/115/115	-
14	CLA	a	831	-	1/1/15/20	10/37/115/115	-
14	CLA	A	817	-	-	2/13/91/115	-
14	CLA	B	817	-	1/1/11/20	7/15/93/115	-
14	CLA	a	816	-	1/1/13/20	9/25/103/115	-
14	CLA	f	201	-	1/1/12/20	10/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	829	-	1/1/15/20	11/37/115/115	-
14	CLA	a	837	-	1/1/12/20	9/24/102/115	-
14	CLA	A	823	-	1/1/15/20	13/37/115/115	-
14	CLA	2	831	-	1/1/14/20	11/31/109/115	-
14	CLA	7	1101	-	1/1/15/20	14/37/115/115	-
18	LMG	0	201	-	-	20/33/53/70	0/1/1/1
14	CLA	b	822	-	-	5/13/91/115	-
14	CLA	7	1103	-	1/1/8/20	1/2/76/115	-
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	F	204	-	1/1/11/20	5/13/91/115	-
17	BCR	A	849	-	-	7/29/63/63	0/2/2/2
17	BCR	1	847	-	-	11/29/63/63	0/2/2/2
14	CLA	2	812	-	1/1/15/20	7/37/115/115	-
14	CLA	A	806	-	1/1/12/20	3/19/97/115	-
14	CLA	B	820	-	-	7/25/103/115	-
17	BCR	M	102	-	-	15/29/63/63	0/2/2/2
17	BCR	K	4005	-	-	10/29/63/63	0/2/2/2
17	BCR	a	850	-	-	19/29/63/63	0/2/2/2
14	CLA	B	814	-	1/1/11/20	3/13/91/115	-
12	LHG	1	802	14	-	13/37/37/53	-
14	CLA	A	819	-	1/1/12/20	6/24/102/115	-
14	CLA	1	828	-	1/1/15/20	11/37/115/115	-
14	CLA	1	841	-	1/1/12/20	10/21/99/115	-
14	CLA	0	206	9	1/1/15/20	14/37/115/115	-
14	CLA	2	843	-	-	18/37/115/115	-
14	CLA	2	836	-	1/1/11/20	4/13/91/115	-
14	CLA	A	836	-	1/1/12/20	9/24/102/115	-
14	CLA	a	828	-	1/1/15/20	13/37/115/115	-
14	CLA	A	812	-	1/1/11/20	7/13/91/115	-
14	CLA	1	814	-	1/1/13/20	9/25/103/115	-
16	SF4	c	102	3	-	-	0/6/5/5
17	BCR	k	4004	-	-	10/29/63/63	0/2/2/2
17	BCR	L	1504	-	-	14/29/63/63	0/2/2/2
14	CLA	1	816	-	-	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	820	-	1/1/12/20	6/24/102/115	-
14	CLA	B	840	-	1/1/12/20	7/19/97/115	-
14	CLA	b	809	-	1/1/15/20	22/37/115/115	-
12	LHG	A	801	-	-	22/53/53/53	-
17	BCR	b	848	-	-	4/18/35/63	0/1/1/2
17	BCR	a	848	-	-	10/29/63/63	0/2/2/2
14	CLA	A	843	-	1/1/15/20	17/37/115/115	-
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	2	816	-	1/1/11/20	7/15/93/115	-
14	CLA	2	809	-	1/1/14/20	7/31/109/115	-
14	CLA	A	841	-	1/1/15/20	8/37/115/115	-
14	CLA	f	204	-	1/1/11/20	6/13/91/115	-
14	CLA	B	841	-	1/1/14/20	6/34/112/115	-
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
14	CLA	1	810	1	1/1/12/20	7/19/97/115	-
17	BCR	6	4402	-	-	13/29/63/63	0/2/2/2
17	BCR	0	209	-	-	14/29/63/63	0/2/2/2
14	CLA	A	811	1	1/1/12/20	7/19/97/115	-
14	CLA	2	826	-	1/1/13/20	3/25/103/115	-
14	CLA	a	830	-	1/1/15/20	11/37/115/115	-
14	CLA	b	833	-	1/1/13/20	12/25/103/115	-
12	LHG	m	101	-	-	20/43/43/53	-
14	CLA	2	803	-	1/1/15/20	11/37/115/115	-
14	CLA	B	815	-	1/1/11/20	9/13/91/115	-
17	BCR	h	102	-	-	20/29/63/63	0/2/2/2
19	LMT	I	103	-	-	8/21/61/61	0/2/2/2
14	CLA	B	809	-	1/1/15/20	22/37/115/115	-
14	CLA	2	805	-	1/1/15/20	14/37/115/115	-
17	BCR	A	851	-	-	21/29/63/63	0/2/2/2
14	CLA	2	832	-	1/1/11/20	5/13/91/115	-
14	CLA	2	815	-	1/1/15/20	21/37/115/115	-
14	CLA	1	842	-	-	11/37/115/115	-
17	BCR	6	4405	-	-	13/29/63/63	0/2/2/2
14	CLA	2	838	-	1/1/11/20	4/15/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	K	4002	-	-	6/13/91/115	-
14	CLA	a	827	-	1/1/13/20	13/30/108/115	-
17	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	A	831	-	1/1/15/20	7/37/115/115	-
14	CLA	B	827	-	1/1/13/20	3/25/103/115	-
14	CLA	b	821	-	1/1/11/20	4/16/94/115	-
17	BCR	j	103	-	-	13/29/63/63	0/2/2/2
14	CLA	B	811	-	1/1/15/20	14/37/115/115	-
14	CLA	A	832	-	1/1/15/20	19/37/115/115	-
18	LMG	l	852	-	-	8/27/47/70	0/1/1/1
14	CLA	a	822	-	1/1/15/20	19/37/115/115	-
17	BCR	l	850	-	-	19/29/63/63	0/2/2/2
14	CLA	b	823	-	-	6/13/91/115	-
14	CLA	B	845	-	1/1/5/20	-	-
17	BCR	0	210	-	-	13/29/63/63	0/2/2/2
14	CLA	b	844	-	1/1/5/20	-	-
14	CLA	A	809	-	1/1/11/20	5/15/93/115	-
14	CLA	A	833	-	1/1/12/20	2/19/97/115	-
15	PQN	b	845	-	-	10/23/43/43	0/2/2/2
14	CLA	B	838	-	1/1/11/20	2/13/91/115	-
14	CLA	A	814	-	1/1/12/20	10/24/102/115	-
17	BCR	I	102	-	-	20/29/63/63	0/2/2/2
14	CLA	l	838	-	1/1/15/20	10/37/115/115	-
14	CLA	a	804	-	1/1/14/20	11/31/109/115	-
14	CLA	B	830	-	1/1/14/20	7/31/109/115	-
14	CLA	l	4206	-	1/1/15/20	13/37/115/115	-
14	CLA	2	830	-	1/1/15/20	8/37/115/115	-
14	CLA	B	821	-	1/1/14/20	15/31/109/115	-
14	CLA	b	824	-	1/1/11/20	5/13/91/115	-
14	CLA	b	820	-	1/1/14/20	15/31/109/115	-
14	CLA	a	809	-	1/1/15/20	13/37/115/115	-
14	CLA	A	844	12	1/1/11/20	4/13/91/115	-
14	CLA	a	835	-	1/1/15/20	14/37/115/115	-
14	CLA	k	4002	-	-	6/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
15	PQN	A	845	-	-	4/23/43/43	0/2/2/2
14	CLA	A	824	-	1/1/11/20	13/18/96/115	-
14	CLA	b	829	-	1/1/14/20	7/31/109/115	-
16	SF4	A	846	2,1	-	-	0/6/5/5
14	CLA	a	840	-	1/1/15/20	10/37/115/115	-
12	LHG	b	852	-	-	22/43/43/53	-
18	LMG	a	853	-	-	8/27/47/70	0/1/1/1
12	LHG	B	853	-	-	22/43/43/53	-
17	BCR	F	206	-	-	14/29/63/63	0/2/2/2
14	CLA	b	835	-	1/1/11/20	2/13/91/115	-
17	BCR	B	847	-	-	12/29/63/63	0/2/2/2
14	CLA	a	806	-	1/1/15/20	14/37/115/115	-
15	PQN	2	845	-	-	10/23/43/43	0/2/2/2
14	CLA	b	816	-	1/1/11/20	7/15/93/115	-
14	CLA	A	820	-	1/1/12/20	4/24/102/115	-
17	BCR	2	847	-	-	7/29/63/63	0/2/2/2
17	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
17	BCR	f	203	-	-	13/29/63/63	0/2/2/2
14	CLA	6	4403	-	1/1/11/20	5/13/91/115	-
14	CLA	a	825	-	1/1/11/20	13/18/96/115	-
14	CLA	L	1501	9	1/1/15/20	14/37/115/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	1	836	1	1/1/11/20	5/13/91/115	-
14	CLA	B	825	-	1/1/11/20	5/13/91/115	-
14	CLA	a	814	-	1/1/15/20	18/37/115/115	-
14	CLA	a	808	-	1/1/15/20	15/37/115/115	-
14	CLA	1	832	-	1/1/12/20	2/19/97/115	-
14	CLA	2	824	-	1/1/11/20	5/13/91/115	-
17	BCR	F	203	-	-	13/29/63/63	0/2/2/2
17	BCR	A	848	-	-	11/29/63/63	0/2/2/2
14	CLA	B	806	-	1/1/15/20	14/37/115/115	-
14	CLA	A	821	-	1/1/15/20	19/37/115/115	-
14	CLA	b	801	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	804	-	1/1/15/20	11/37/115/115	-
14	CLA	1	804	-	1/1/15/20	9/37/115/115	-
12	LHG	9	101	-	-	20/43/43/53	-
12	LHG	2	852	-	-	22/43/43/53	-
14	CLA	a	813	-	1/1/11/20	7/13/91/115	-
14	CLA	b	812	-	1/1/14/20	13/33/111/115	-
14	CLA	a	811	1	1/1/15/20	23/37/115/115	-
14	CLA	a	817	-	1/1/11/20	4/13/91/115	-
14	CLA	1	835	-	1/1/12/20	9/24/102/115	-
15	PQN	a	845	-	-	4/23/43/43	0/2/2/2
17	BCR	6	4406	-	-	13/29/63/63	0/2/2/2
17	BCR	8	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	8	4004	-	1/1/13/20	5/25/103/115	-
14	CLA	A	834	-	1/1/15/20	14/37/115/115	-
14	CLA	b	826	-	1/1/13/20	3/25/103/115	-
17	BCR	b	850	-	-	19/29/63/63	0/2/2/2
17	BCR	b	851	-	-	10/29/63/63	0/2/2/2
14	CLA	b	843	-	-	18/37/115/115	-
14	CLA	b	815	-	1/1/15/20	21/37/115/115	-
14	CLA	2	841	-	1/1/11/20	4/15/93/115	-
17	BCR	l	4207	-	-	14/29/63/63	0/2/2/2
14	CLA	b	807	-	1/1/12/20	9/24/102/115	-
14	CLA	1	831	-	1/1/15/20	19/37/115/115	-
14	CLA	b	836	-	1/1/11/20	4/13/91/115	-
19	LMT	F	202	-	-	3/21/61/61	0/2/2/2
14	CLA	2	814	-	1/1/11/20	9/13/91/115	-
17	BCR	B	849	-	-	4/18/35/63	0/1/1/2
14	CLA	B	802	-	1/1/15/20	10/37/115/115	-
15	PQN	B	846	-	-	10/23/43/43	0/2/2/2
14	CLA	2	840	-	1/1/14/20	6/34/112/115	-
14	CLA	a	818	-	-	2/13/91/115	-
14	CLA	A	835	-	1/1/15/20	5/37/115/115	-
14	CLA	J	101	-	1/1/11/20	6/13/91/115	-
14	CLA	B	816	-	1/1/15/20	21/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	F	205	-	1/1/11/20	6/13/91/115	-
17	BCR	a	849	-	-	7/29/63/63	0/2/2/2
14	CLA	6	4404	-	1/1/11/20	6/13/91/115	-
14	CLA	8	4003	-	1/1/11/20	8/13/91/115	-
14	CLA	b	838	-	1/1/11/20	4/15/93/115	-
14	CLA	1	806	-	1/1/15/20	15/37/115/115	-
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	1	821	-	1/1/14/20	7/31/109/115	-
17	BCR	7	1105	-	-	10/29/63/63	0/2/2/2
14	CLA	2	819	-	-	7/25/103/115	-
14	CLA	A	805	-	1/1/15/20	14/37/115/115	-
14	CLA	2	835	-	1/1/11/20	2/13/91/115	-
14	CLA	1	822	-	1/1/15/20	13/37/115/115	-
14	CLA	B	805	-	1/1/15/20	13/37/115/115	-
17	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	2	811	-	1/1/14/20	13/33/111/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5
14	CLA	1	829	-	1/1/15/20	10/37/115/115	-
14	CLA	1	823	-	1/1/11/20	13/18/96/115	-
14	CLA	A	827	-	1/1/15/20	13/37/115/115	-
17	BCR	2	850	-	-	19/29/63/63	0/2/2/2
14	CLA	a	833	-	1/1/15/20	19/37/115/115	-
13	CL0	A	803	-	3/3/20/25	13/37/135/135	-
14	CLA	1	805	-	1/1/12/20	3/19/97/115	-
14	CLA	A	839	-	1/1/15/20	10/37/115/115	-
14	CLA	2	829	-	1/1/14/20	7/31/109/115	-
14	CLA	B	842	-	1/1/11/20	4/15/93/115	-
17	BCR	b	854	-	-	15/29/63/63	0/2/2/2
14	CLA	a	841	-	1/1/11/20	2/16/94/115	-
14	CLA	2	828	-	1/1/15/20	8/37/115/115	-
14	CLA	2	842	-	1/1/15/20	11/37/115/115	-
14	CLA	A	822	-	1/1/14/20	7/31/109/115	-
14	CLA	b	834	-	1/1/13/20	14/29/107/115	-
14	CLA	B	822	-	1/1/11/20	4/16/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	b	847	-	-	7/29/63/63	0/2/2/2
17	BCR	2	846	-	-	12/29/63/63	0/2/2/2
14	CLA	1	811	-	1/1/11/20	7/13/91/115	-
14	CLA	b	830	-	1/1/15/20	8/37/115/115	-
14	CLA	b	813	-	1/1/11/20	3/13/91/115	-
14	CLA	B	812	-	1/1/14/20	13/33/111/115	-
19	LMT	h	103	-	-	8/21/61/61	0/2/2/2
14	CLA	B	836	-	1/1/11/20	2/13/91/115	-
14	CLA	1	819	-	1/1/12/20	4/24/102/115	-
14	CLA	1	824	-	1/1/12/20	9/21/99/115	-
14	CLA	A	828	-	1/1/13/20	6/25/103/115	-
14	CLA	B	833	-	1/1/11/20	5/13/91/115	-
14	CLA	1	826	-	1/1/15/20	13/37/115/115	-
14	CLA	2	822	-	-	5/13/91/115	-
17	BCR	1	851	-	-	21/29/63/63	0/2/2/2
12	LHG	M	101	-	-	20/43/43/53	-
14	CLA	1	807	-	1/1/15/20	13/37/115/115	-
14	CLA	A	838	-	1/1/12/20	7/21/99/115	-
14	CLA	b	832	-	1/1/11/20	5/13/91/115	-
14	CLA	B	826	-	-	5/13/91/115	-
14	CLA	l	4204	9	1/1/15/20	14/37/115/115	-
18	LMG	B	803	-	-	20/43/63/70	0/1/1/1
18	LMG	l	4202	-	-	20/33/53/70	0/1/1/1
17	BCR	2	848	-	-	4/18/35/63	0/1/1/2
18	LMG	0	203	-	-	21/41/61/70	0/1/1/1
14	CLA	b	818	-	1/1/13/20	10/25/103/115	-
14	CLA	B	843	-	1/1/15/20	11/37/115/115	-
17	BCR	B	854	-	-	13/29/63/63	0/2/2/2
18	LMG	L	1506	-	-	20/33/53/70	0/1/1/1
17	BCR	2	851	-	-	10/29/63/63	0/2/2/2
14	CLA	A	830	-	1/1/15/20	10/37/115/115	-
14	CLA	1	809	1	1/1/15/20	23/37/115/115	-
14	CLA	f	205	-	1/1/11/20	6/13/91/115	-
14	CLA	b	817	-	1/1/11/20	2/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	801	-	1/1/14/20	11/31/109/115	-
14	CLA	j	102	-	1/1/8/20	1/2/76/115	-
17	BCR	B	851	-	-	19/29/63/63	0/2/2/2
14	CLA	1	830	-	1/1/15/20	7/37/115/115	-
14	CLA	2	837	-	1/1/11/20	2/13/91/115	-
14	CLA	A	815	-	1/1/13/20	9/25/103/115	-
14	CLA	2	834	-	1/1/13/20	14/29/107/115	-
13	CL0	a	803	-	3/3/20/25	13/37/135/135	-
14	CLA	0	207	-	1/1/15/20	9/37/115/115	-
14	CLA	b	808	-	-	10/37/115/115	-
17	BCR	1	848	-	-	11/29/63/63	0/2/2/2
17	BCR	f	206	-	-	13/29/63/63	0/2/2/2
14	CLA	0	208	-	1/1/15/20	13/37/115/115	-
14	CLA	1	833	-	1/1/15/20	14/37/115/115	-
14	CLA	l	4205	-	1/1/15/20	9/37/115/115	-
14	CLA	a	823	-	1/1/14/20	7/31/109/115	-
14	CLA	B	837	-	1/1/11/20	4/13/91/115	-
14	CLA	2	823	-	-	6/13/91/115	-
14	CLA	b	802	-	1/1/15/20	8/37/115/115	-
14	CLA	b	831	-	1/1/14/20	11/31/109/115	-
14	CLA	A	808	-	1/1/15/20	13/37/115/115	-
17	BCR	b	853	-	-	13/29/63/63	0/2/2/2
14	CLA	1	827	-	1/1/13/20	6/25/103/115	-
19	LMT	6	4401	-	-	3/21/61/61	0/2/2/2
14	CLA	2	804	-	1/1/15/20	13/37/115/115	-
14	CLA	A	807	-	1/1/15/20	15/37/115/115	-
14	CLA	K	4003	-	1/1/11/20	8/13/91/115	-
14	CLA	1	839	-	1/1/11/20	2/16/94/115	-
17	BCR	A	850	-	-	19/29/63/63	0/2/2/2
14	CLA	2	825	-	-	5/13/91/115	-
14	CLA	7	1102	-	1/1/11/20	6/13/91/115	-
14	CLA	B	808	-	-	10/37/115/115	-
14	CLA	2	817	-	1/1/11/20	2/13/91/115	-
18	LMG	2	802	-	-	20/43/63/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	836	-	1/1/15/20	5/37/115/115	-
14	CLA	B	839	-	1/1/11/20	4/15/93/115	-
14	CLA	2	808	-	1/1/15/20	22/37/115/115	-
12	LHG	1	801	-	-	22/53/53/53	-
19	LMT	f	202	-	-	3/21/61/61	0/2/2/2
14	CLA	A	818	-	1/1/11/20	5/15/93/115	-
14	CLA	2	839	-	1/1/12/20	7/19/97/115	-
14	CLA	b	841	-	1/1/11/20	4/15/93/115	-
14	CLA	A	813	-	1/1/15/20	18/37/115/115	-
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	a	843	-	1/1/15/20	17/37/115/115	-
14	CLA	B	832	-	1/1/14/20	11/31/109/115	-
14	CLA	a	810	-	1/1/11/20	5/15/93/115	-
14	CLA	B	818	-	1/1/11/20	2/13/91/115	-
14	CLA	a	844	12	1/1/11/20	4/13/91/115	-
17	BCR	2	849	-	-	15/29/63/63	0/2/2/2
14	CLA	2	818	-	1/1/13/20	10/25/103/115	-
14	CLA	1	844	12	1/1/11/20	4/13/91/115	-
14	CLA	J	102	-	1/1/8/20	1/2/76/115	-
14	CLA	A	840	-	1/1/11/20	2/16/94/115	-
14	CLA	2	806	-	1/1/12/20	9/24/102/115	-
15	PQN	1	845	-	-	4/23/43/43	0/2/2/2
14	CLA	1	808	-	1/1/11/20	5/15/93/115	-
17	BCR	i	4103	-	-	20/29/63/63	0/2/2/2
14	CLA	A	816	-	1/1/11/20	4/13/91/115	-
17	BCR	B	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	824	-	-	6/13/91/115	-
13	CL0	1	803	-	3/3/20/25	13/37/135/135	-
14	CLA	A	837	1	1/1/11/20	5/13/91/115	-
14	CLA	b	827	-	1/1/12/20	2/19/97/115	-
14	CLA	b	825	-	-	5/13/91/115	-
14	CLA	b	819	-	-	7/25/103/115	-
14	CLA	b	811	-	1/1/15/20	14/37/115/115	-
14	CLA	b	805	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	826	-	1/1/12/20	9/21/99/115	-
14	CLA	a	807	-	1/1/12/20	3/19/97/115	-
17	BCR	1	849	-	-	7/29/63/63	0/2/2/2
14	CLA	1	820	-	1/1/15/20	19/37/115/115	-
14	CLA	2	810	-	1/1/15/20	15/37/115/115	-
12	LHG	a	802	14	-	13/37/37/53	-
14	CLA	a	842	-	-	11/37/115/115	-
14	CLA	B	829	-	1/1/15/20	8/37/115/115	-
14	CLA	1	818	-	1/1/12/20	6/24/102/115	-
18	LMG	a	852	-	-	21/41/61/70	0/1/1/1
14	CLA	B	801	-	1/1/14/20	11/31/109/115	-
14	CLA	a	815	-	1/1/12/20	10/24/102/115	-
14	CLA	B	835	-	1/1/13/20	14/29/107/115	-
17	BCR	9	102	-	-	15/29/63/63	0/2/2/2
18	LMG	b	803	-	-	20/43/63/70	0/1/1/1
14	CLA	B	831	-	1/1/15/20	8/37/115/115	-
14	CLA	j	101	-	1/1/11/20	6/13/91/115	-
14	CLA	a	838	1	1/1/11/20	5/13/91/115	-
14	CLA	l	4203	-	1/1/15/20	7/37/115/115	-
14	CLA	B	807	-	1/1/12/20	9/24/102/115	-
17	BCR	0	204	-	-	13/29/63/63	0/2/2/2
14	CLA	2	813	-	1/1/11/20	3/13/91/115	-
14	CLA	1	837	-	1/1/12/20	7/21/99/115	-
17	BCR	a	851	-	-	21/29/63/63	0/2/2/2
14	CLA	1	840	-	1/1/15/20	8/37/115/115	-
16	SF4	1	846	2,1	-	-	0/6/5/5
14	CLA	b	810	-	1/1/14/20	7/31/109/115	-
14	CLA	b	828	-	1/1/15/20	8/37/115/115	-
17	BCR	B	852	-	-	10/29/63/63	0/2/2/2
17	BCR	I	101	-	-	16/29/63/63	0/2/2/2
14	CLA	2	807	-	-	10/37/115/115	-
14	CLA	K	4004	-	1/1/13/20	5/25/103/115	-

The worst 5 of 2386 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	804	CLA	CHB-C4A	6.22	1.38	1.33
14	1	806	CLA	CHB-C4A	6.21	1.38	1.33
14	b	805	CLA	CHB-C4A	6.16	1.38	1.33
14	A	807	CLA	CHB-C4A	6.16	1.38	1.33
14	a	808	CLA	CHB-C4A	6.14	1.38	1.33

The worst 5 of 2952 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	829	CLA	C4A-NA-C1A	8.22	110.43	106.68
14	a	830	CLA	C4A-NA-C1A	8.19	110.42	106.68
14	1	828	CLA	C4A-NA-C1A	8.17	110.41	106.68
14	A	825	CLA	C4A-NA-C1A	7.96	110.31	106.68
14	1	824	CLA	C4A-NA-C1A	7.94	110.30	106.68

5 of 270 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	803	CL0	NC
13	A	803	CL0	ND
13	A	803	CL0	NA
13	a	803	CL0	NC
13	a	803	CL0	ND

5 of 3965 torsion outliers are listed below:

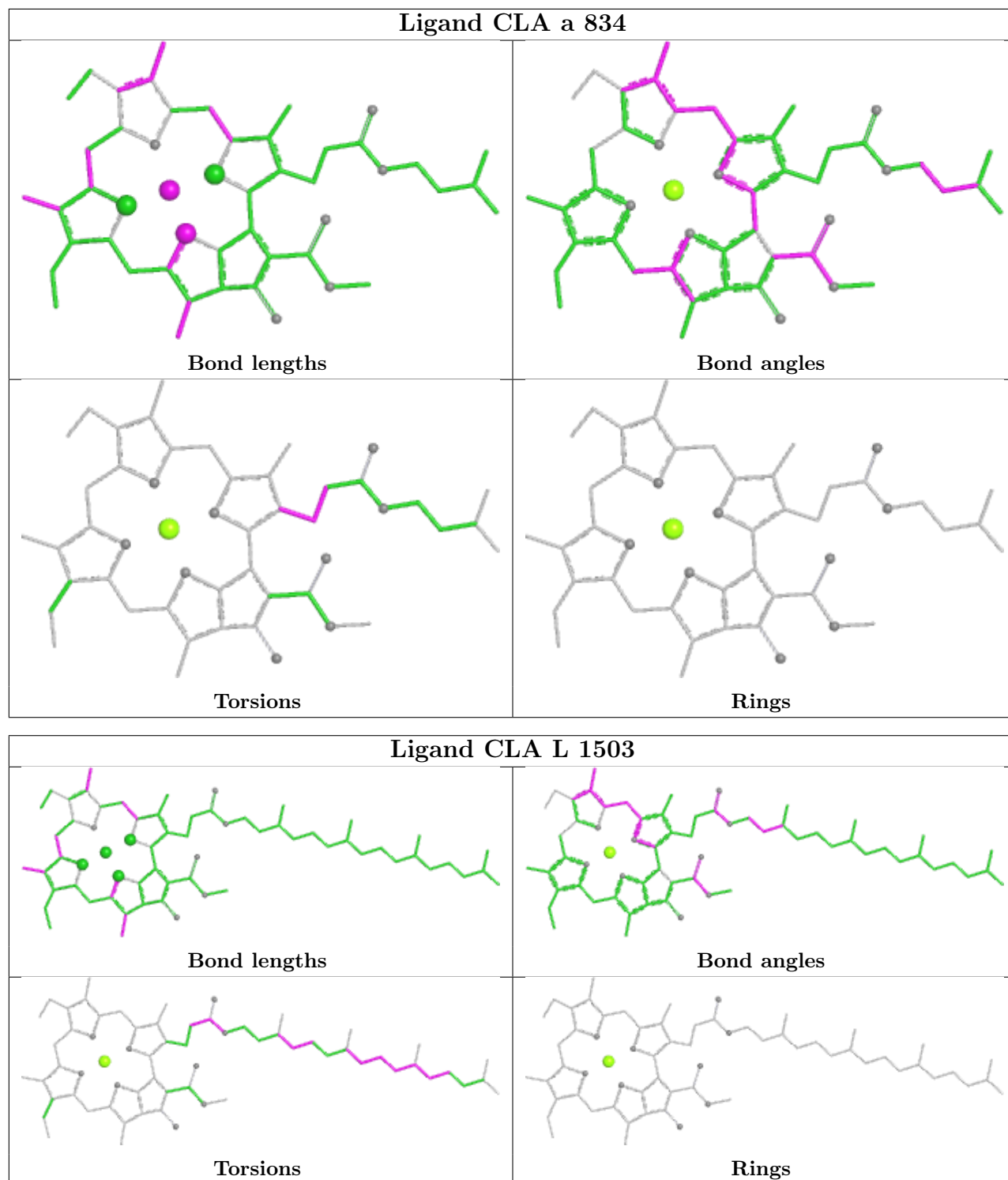
Mol	Chain	Res	Type	Atoms
12	A	801	LHG	C3-O3-P-O4
12	A	801	LHG	O10-C23-O8-C6
12	A	802	LHG	O1-C1-C2-C3
12	A	802	LHG	C3-O3-P-O4
12	A	802	LHG	C3-O3-P-O5

There are no ring outliers.

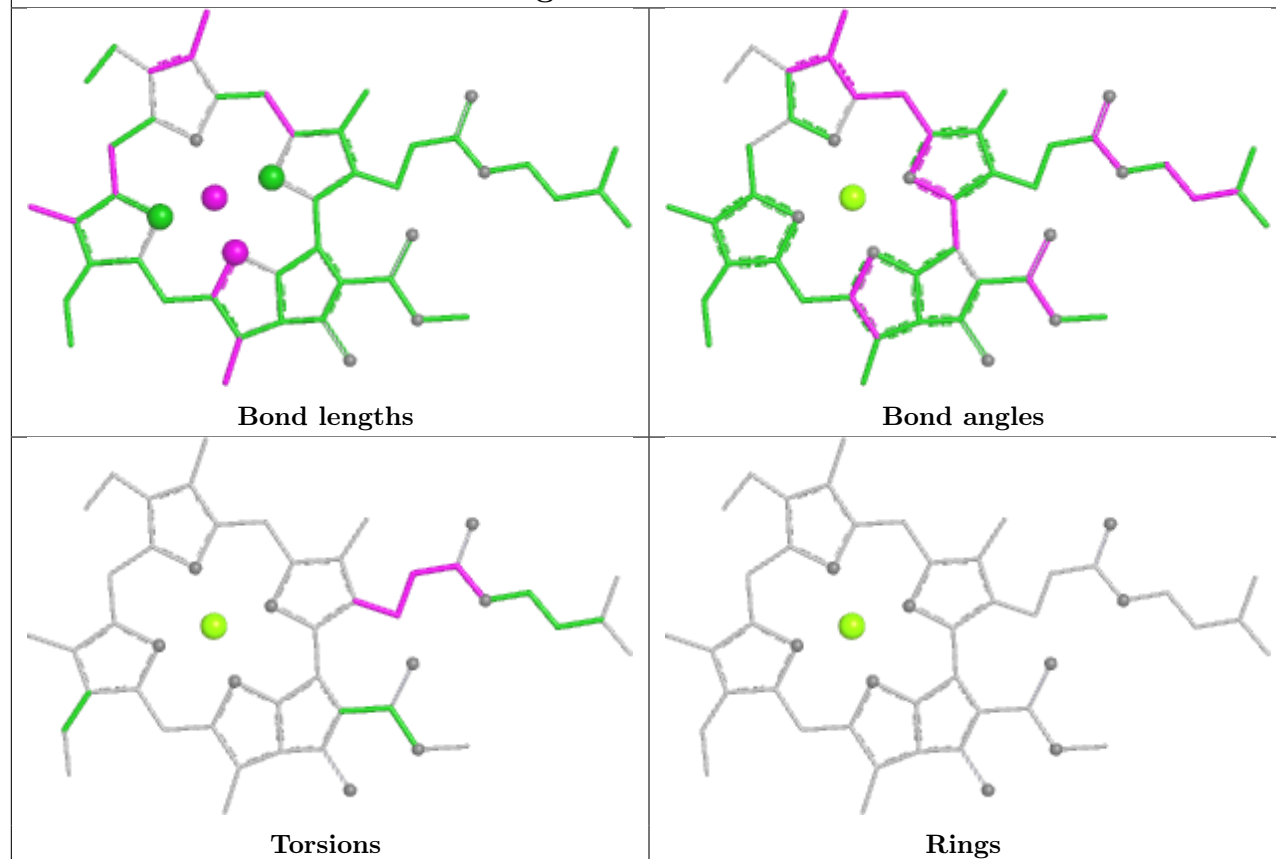
No monomer is involved in short contacts.

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

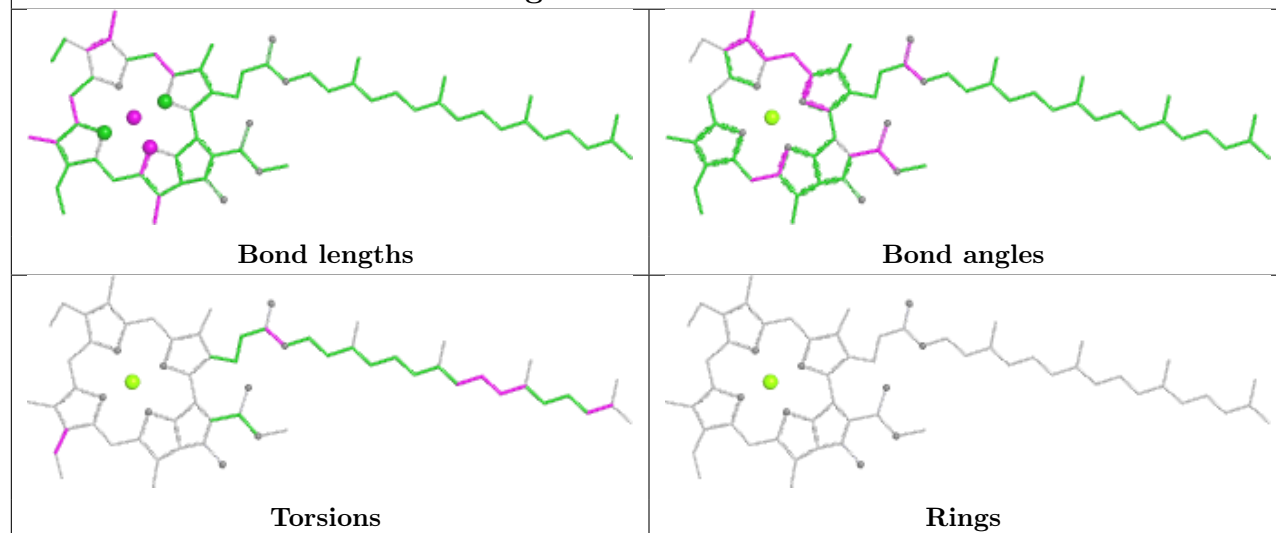
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers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

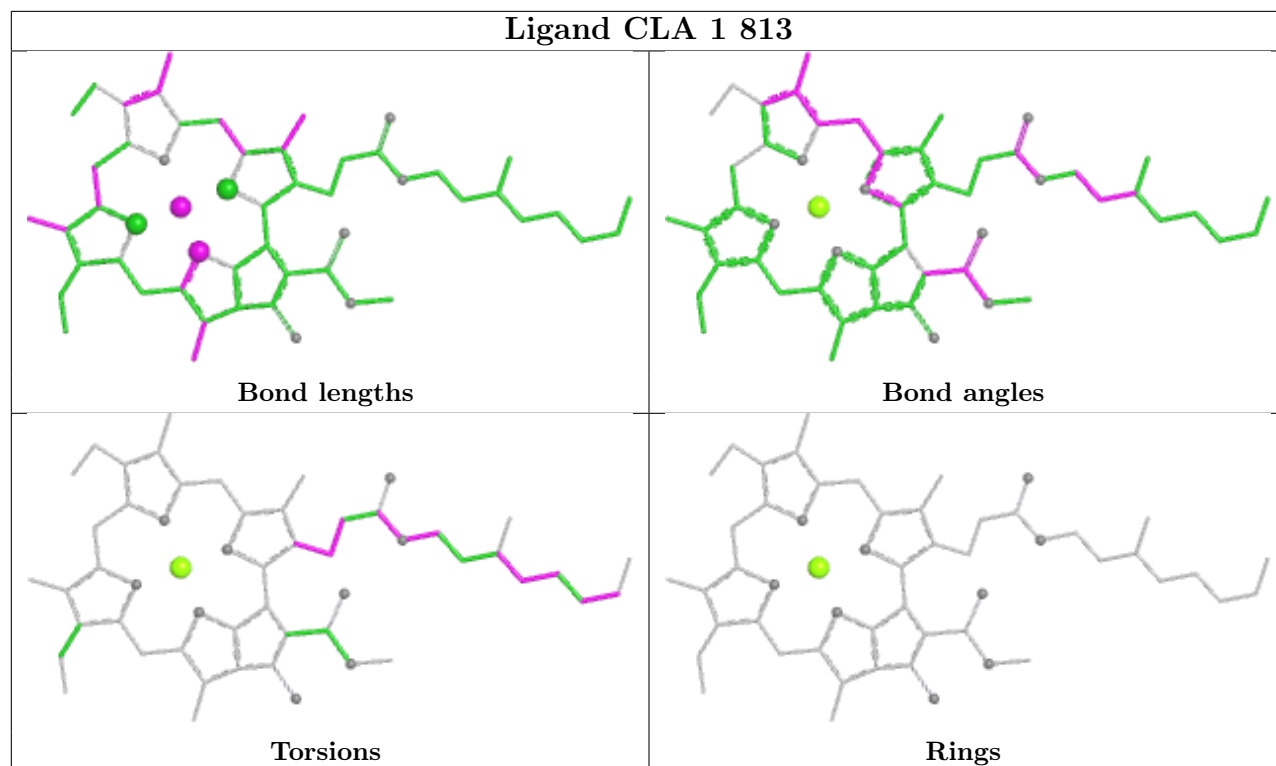
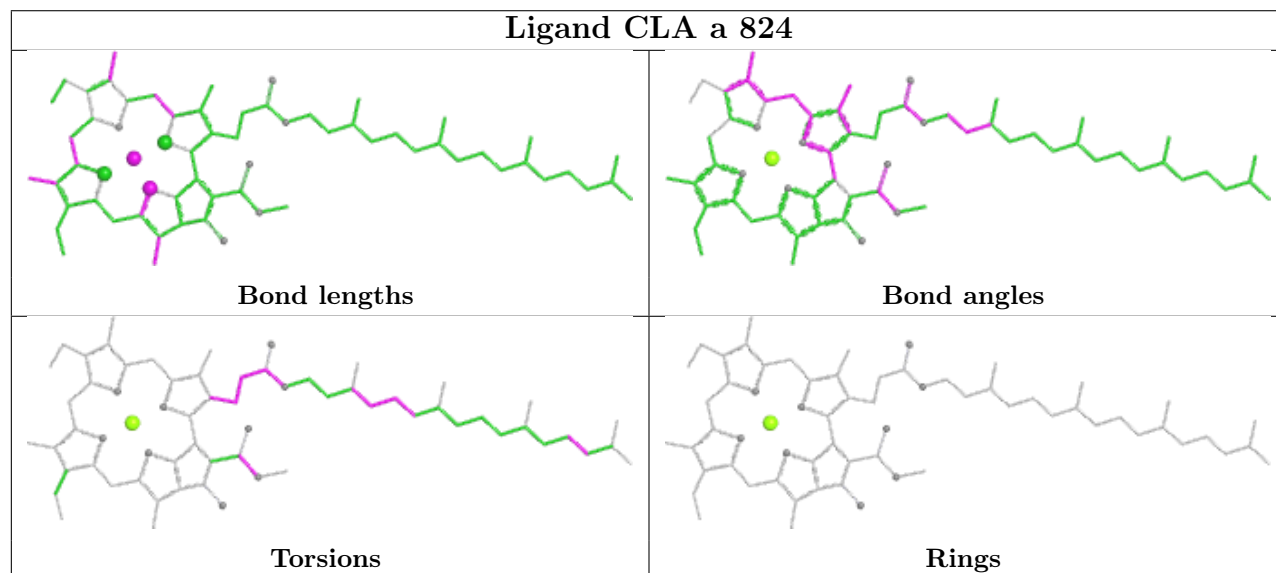


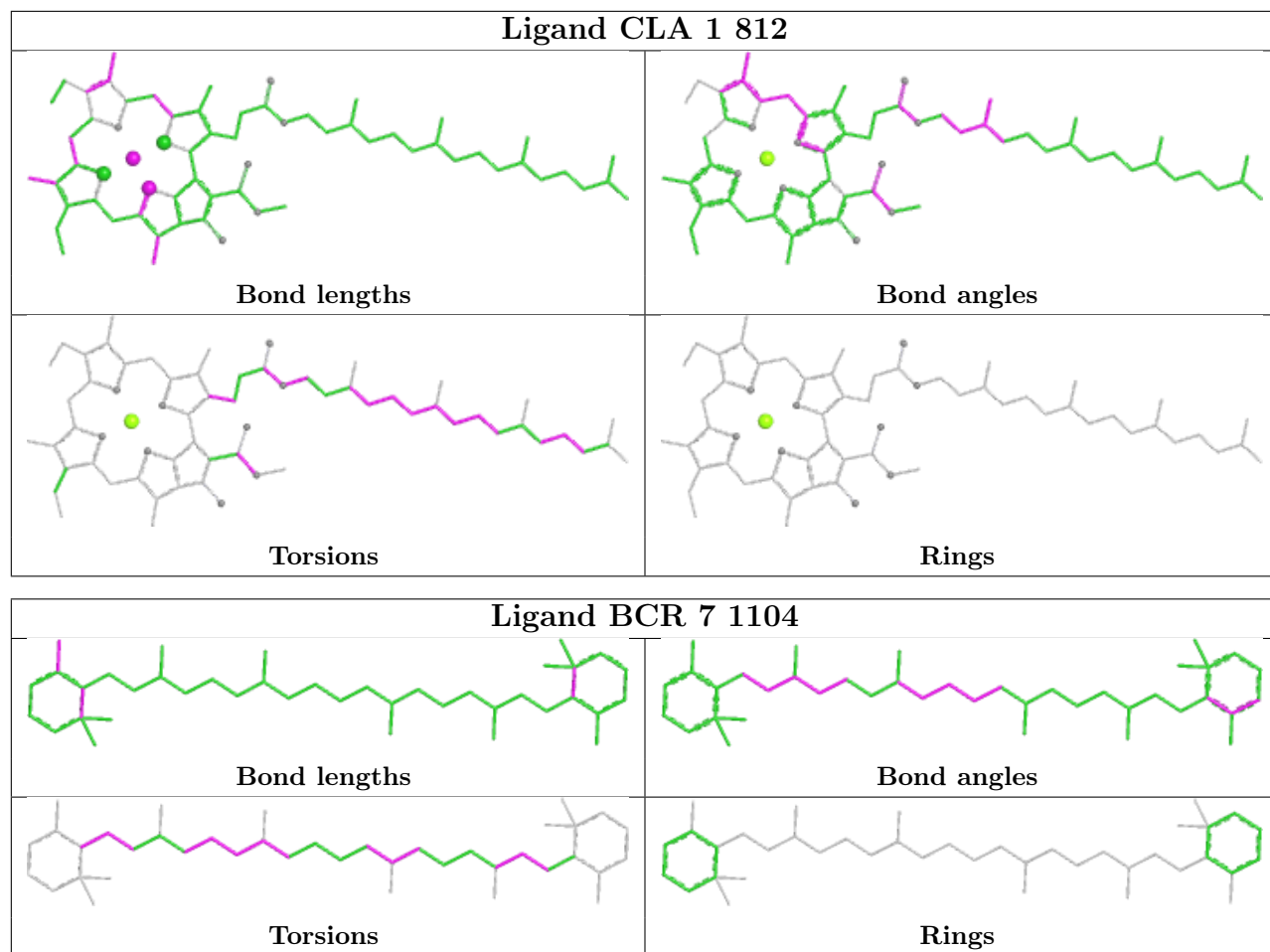
Ligand CLA a 812



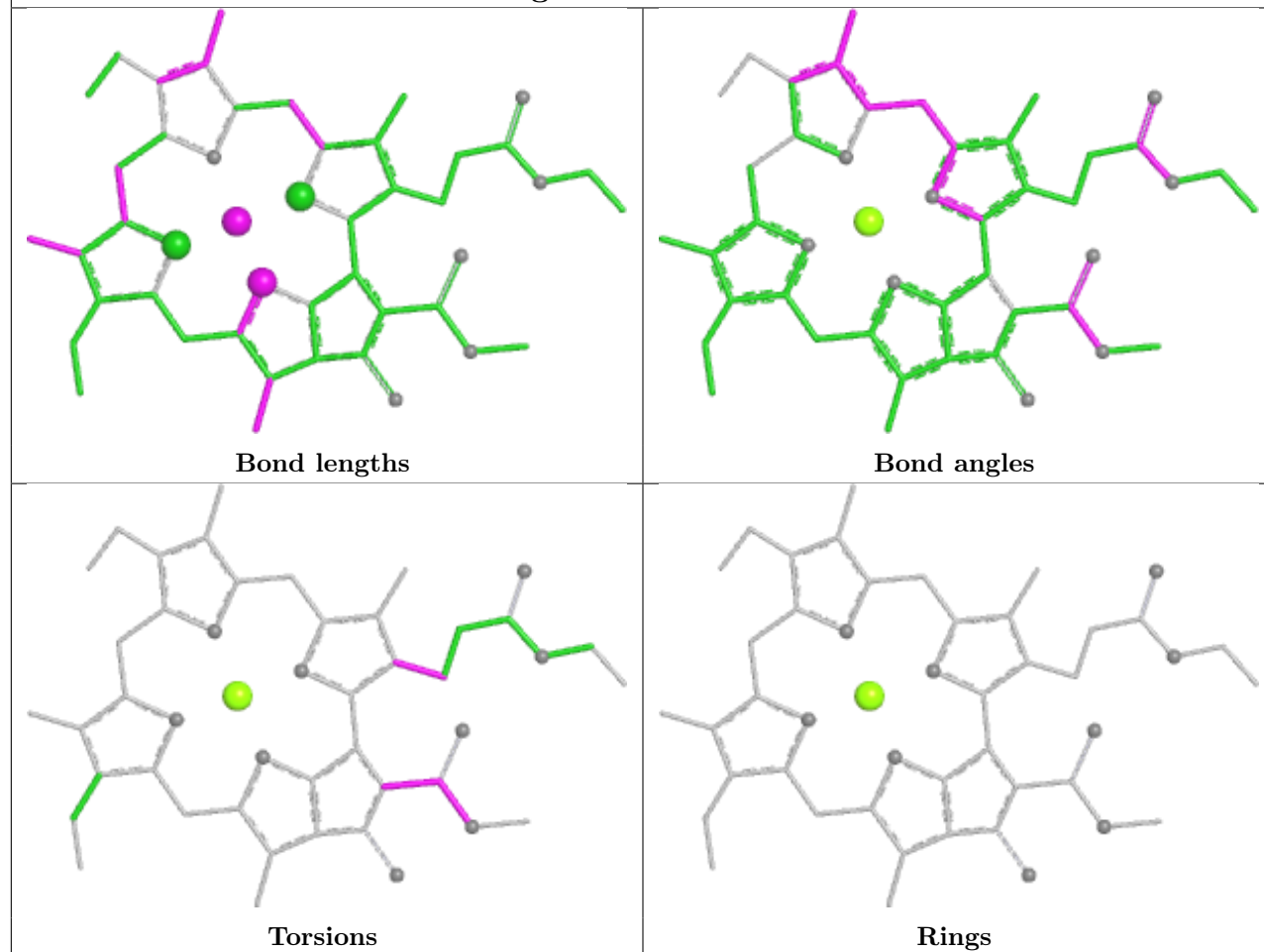
Ligand CLA L 1502



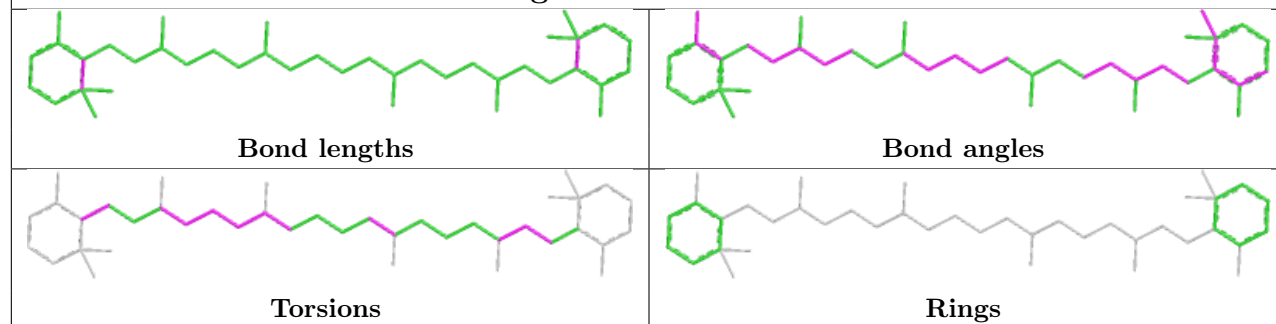
Ligand CLA 1 813**Ligand CLA a 824**

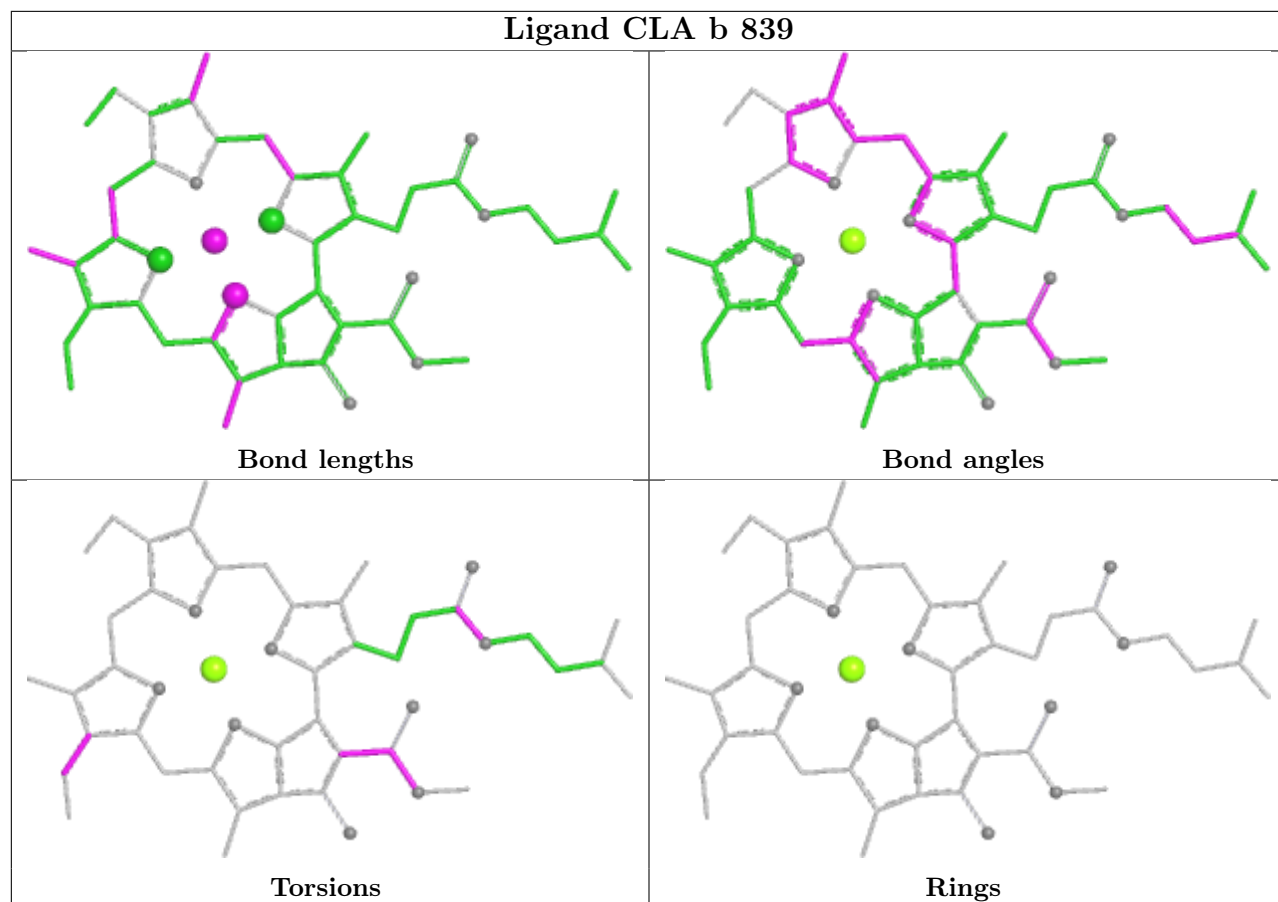


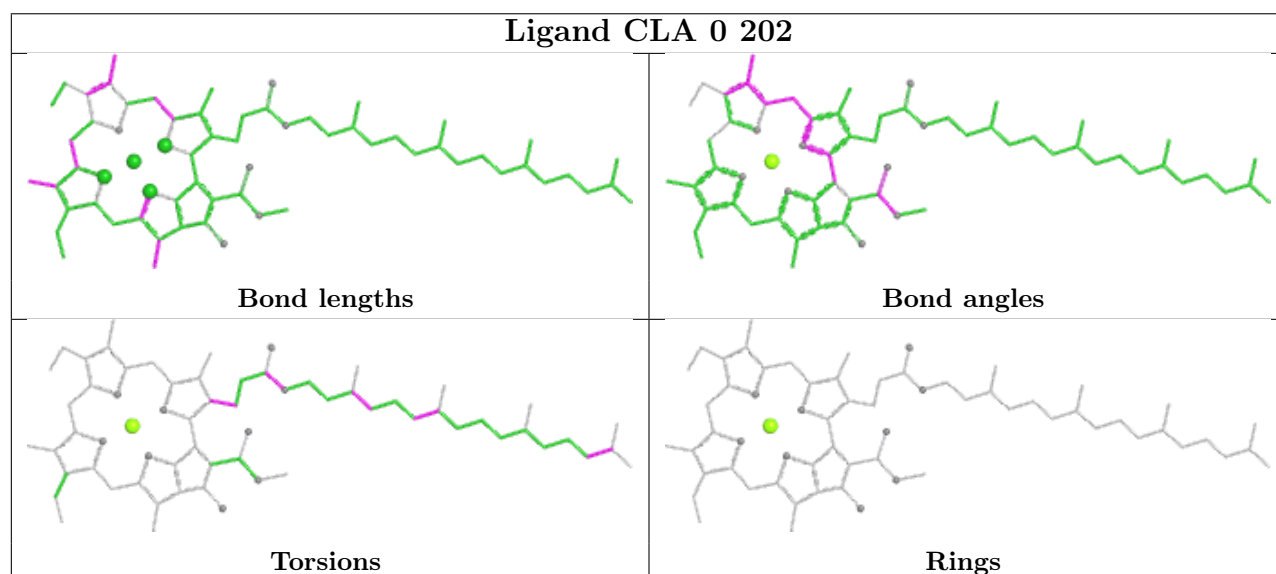
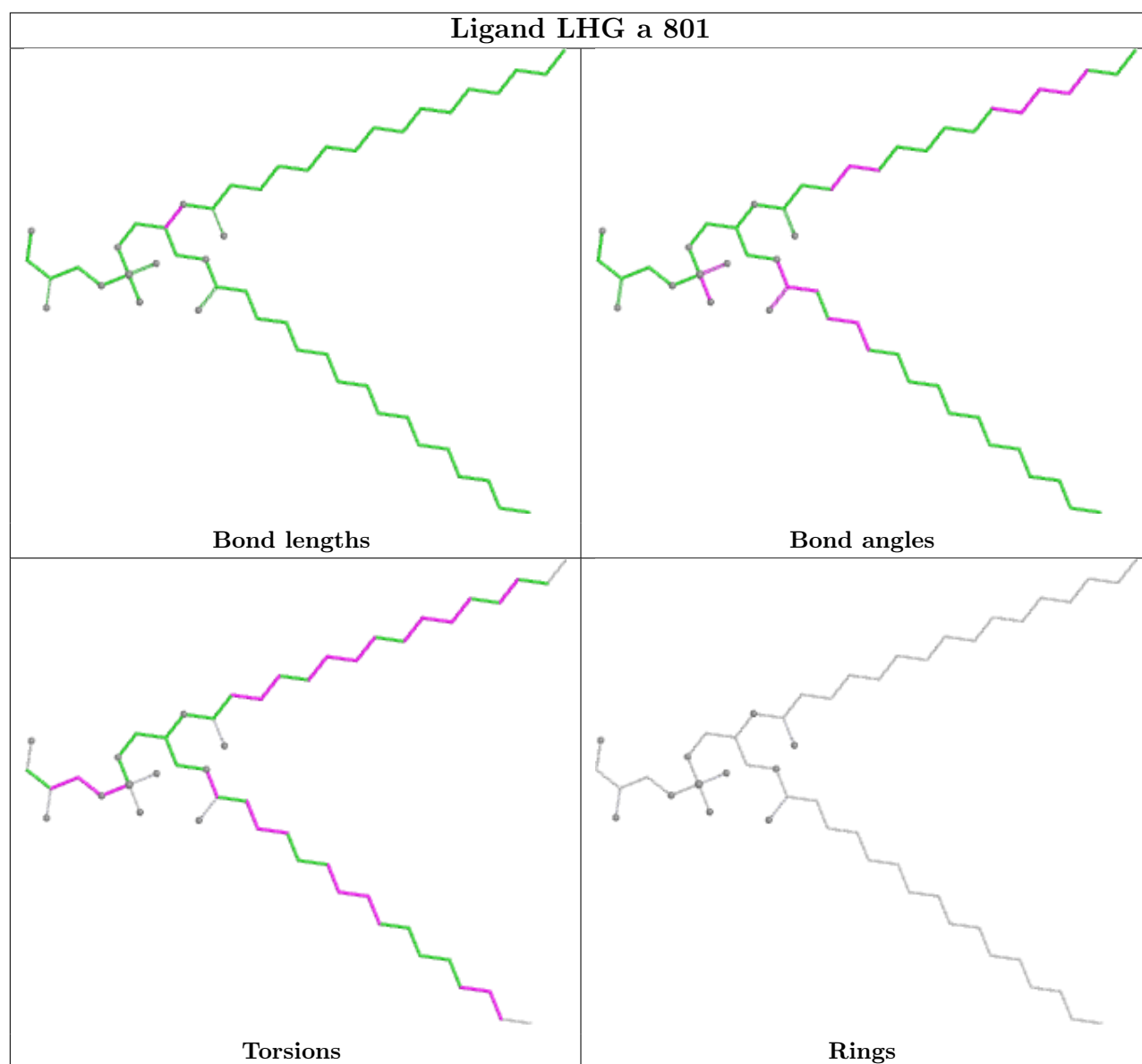
Ligand CLA 2 821



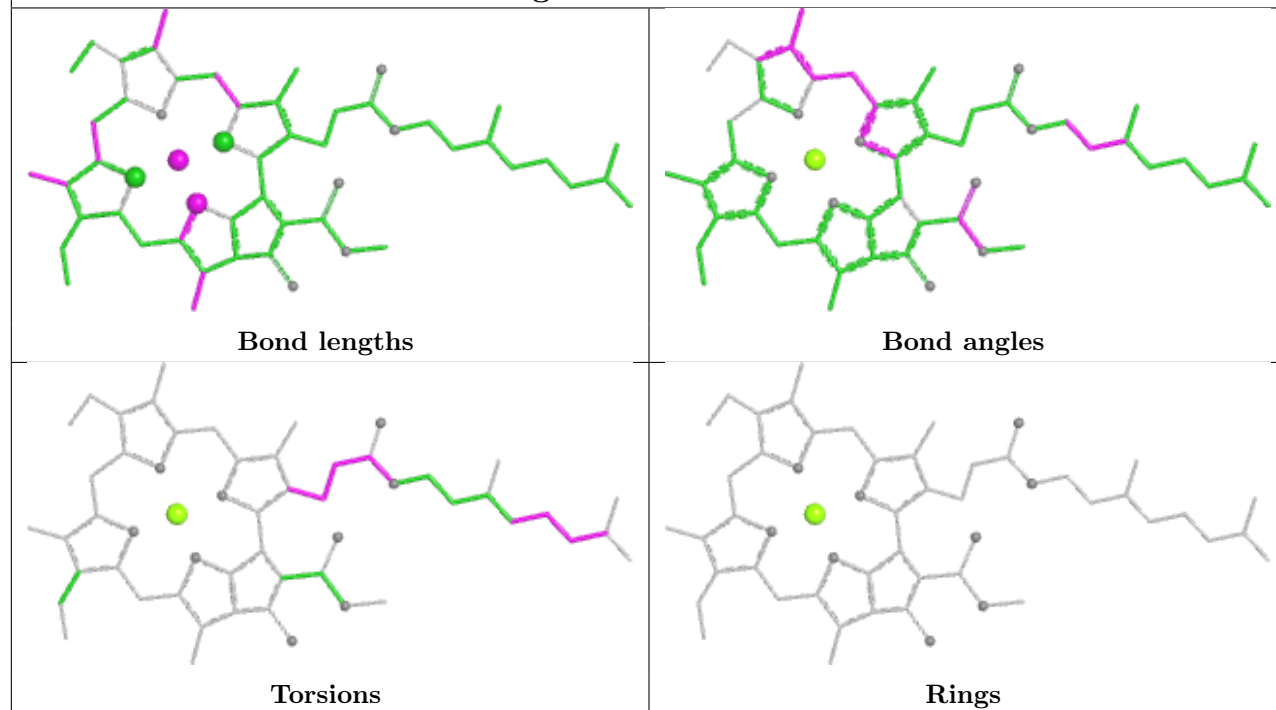
Ligand BCR B 850



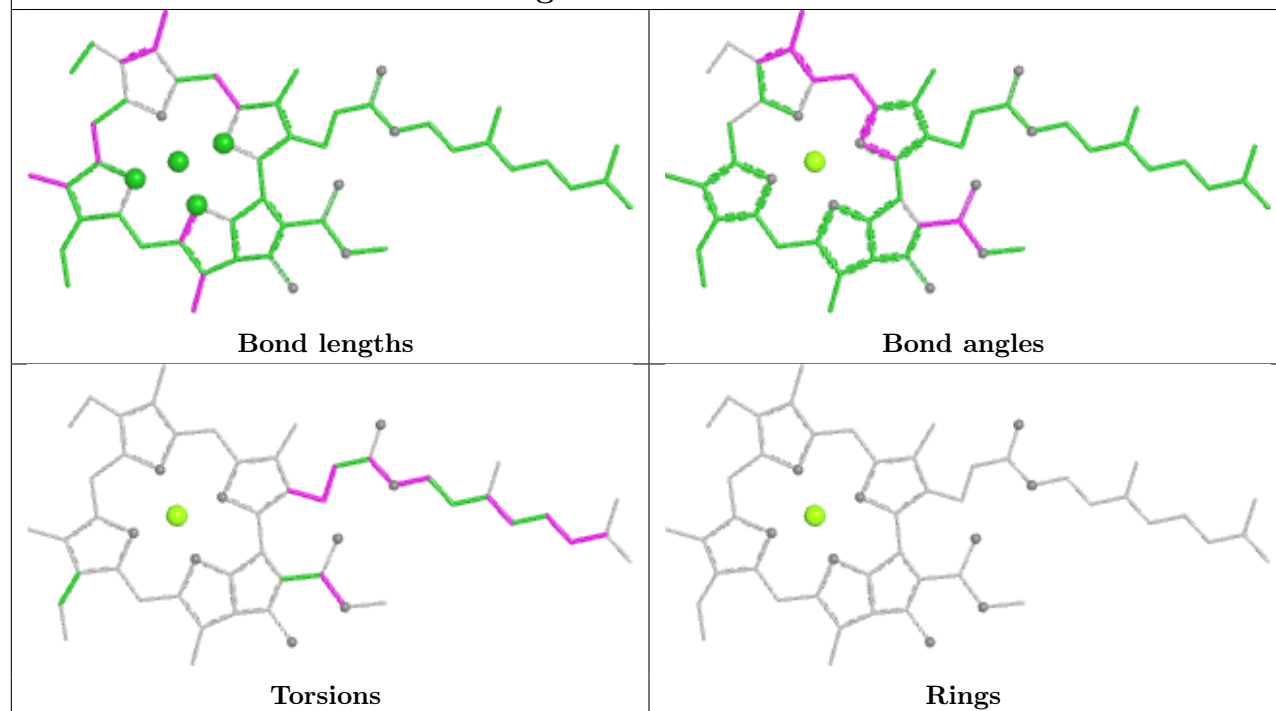


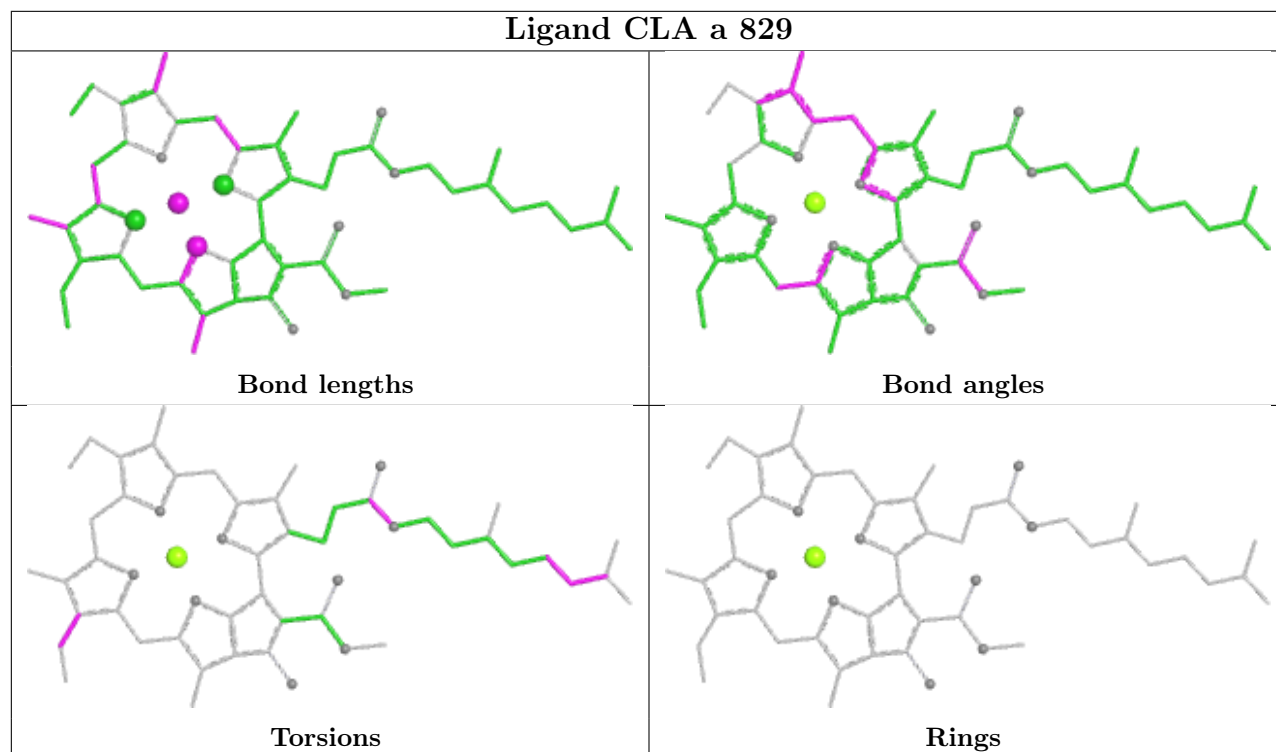
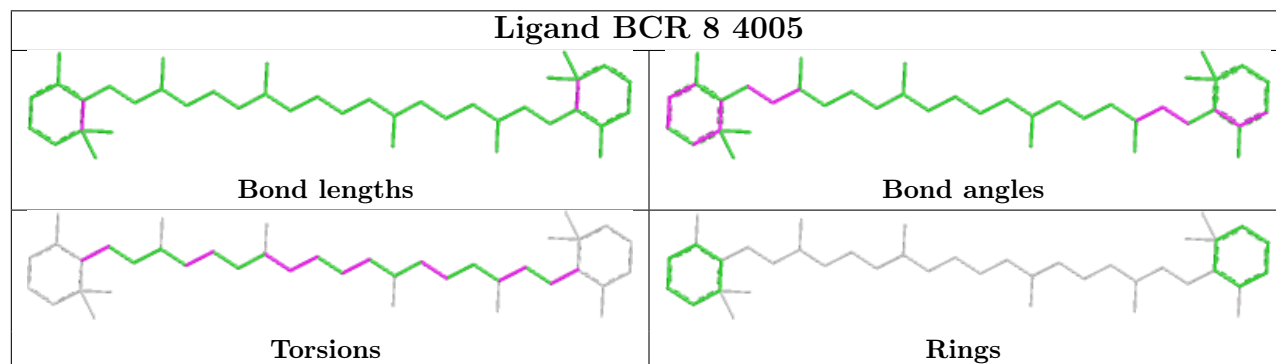
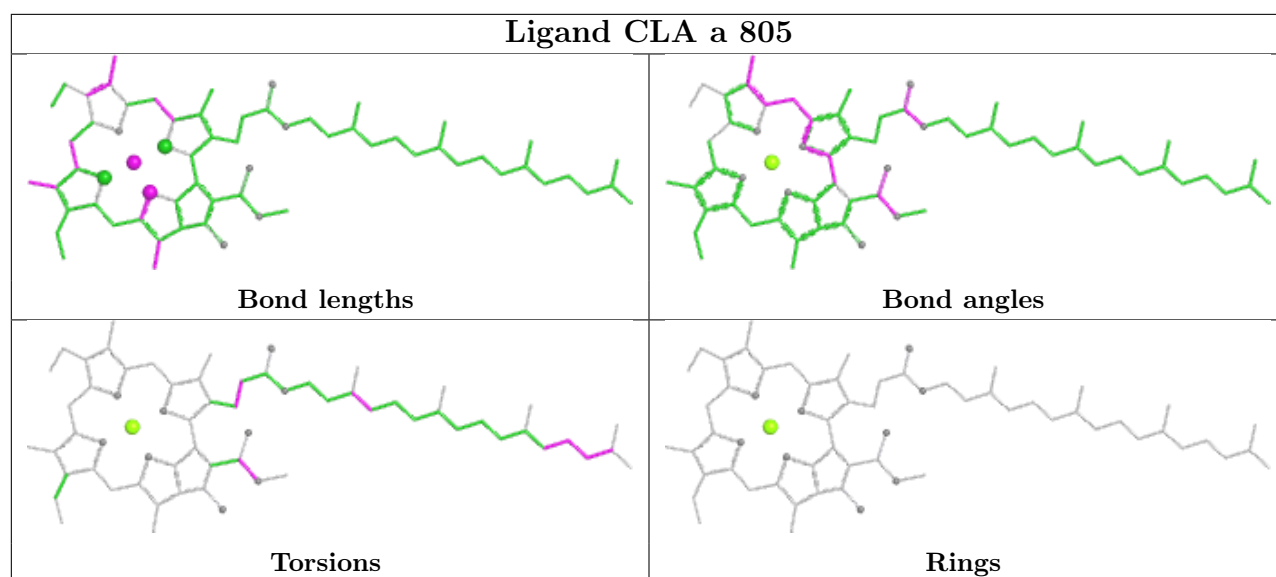


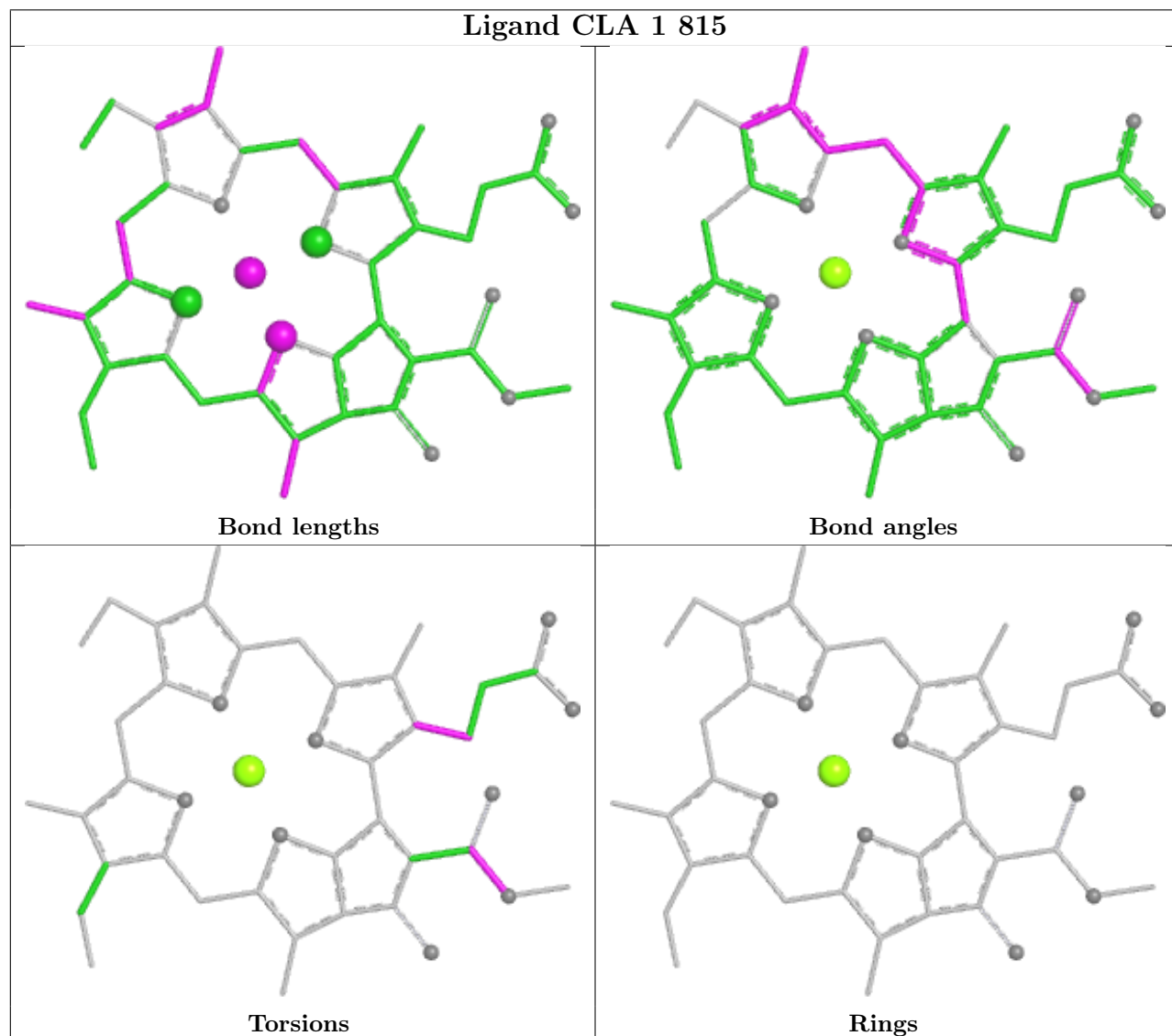
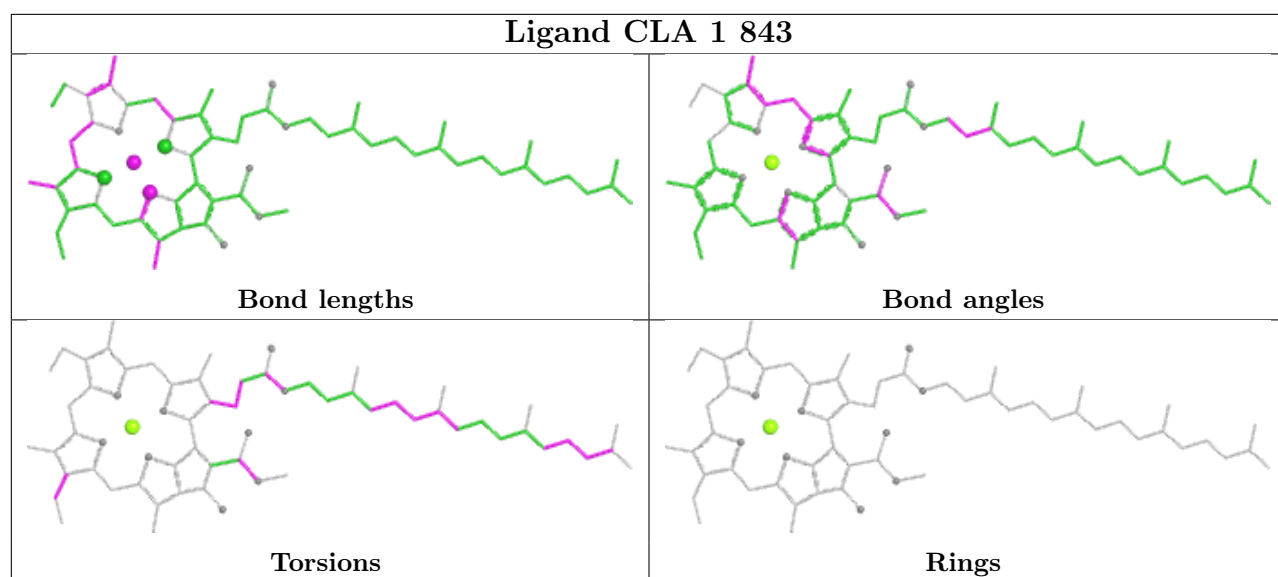
Ligand CLA B 819

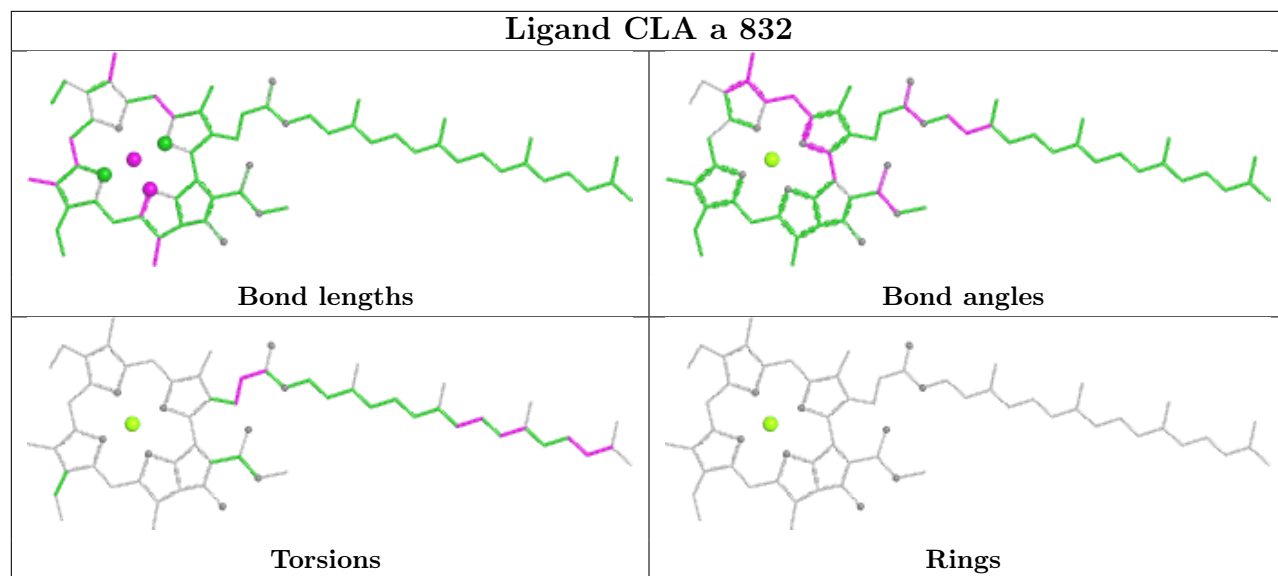


Ligand CLA 2 833

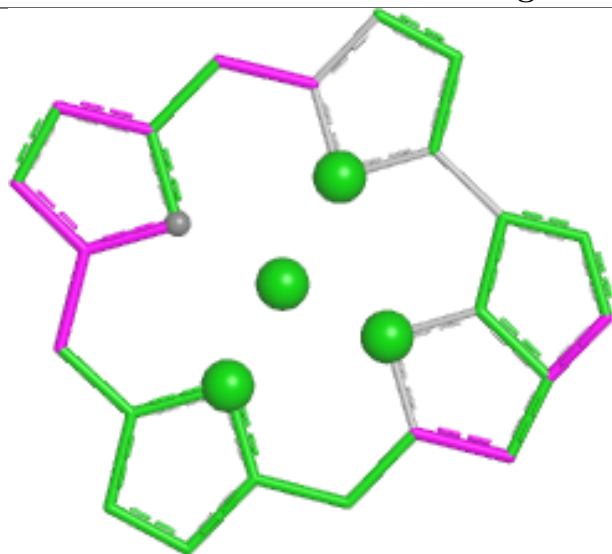




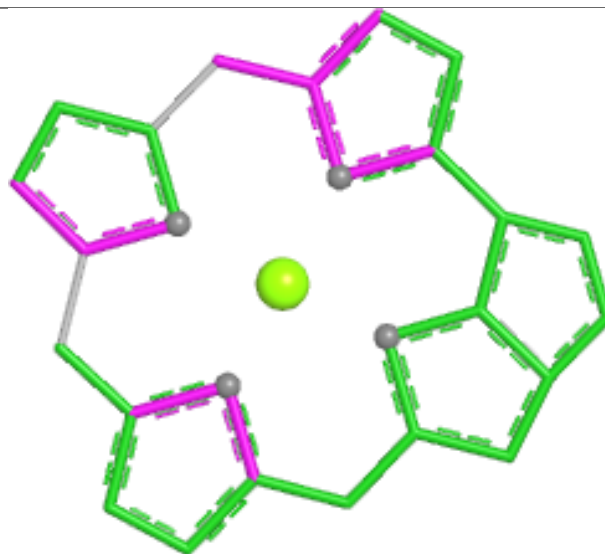




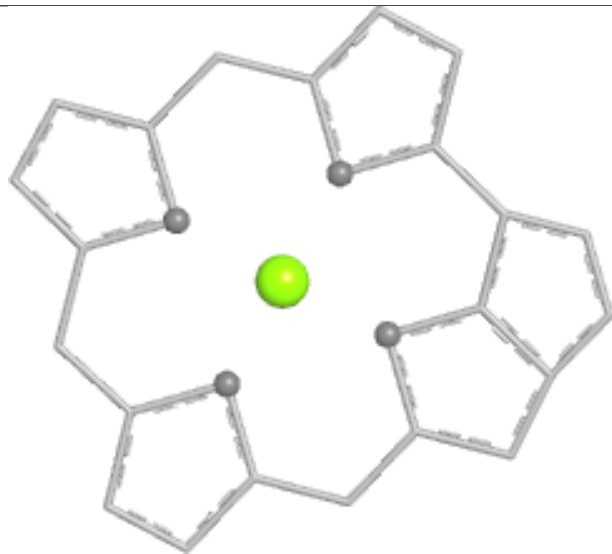
Ligand CLA 2 844



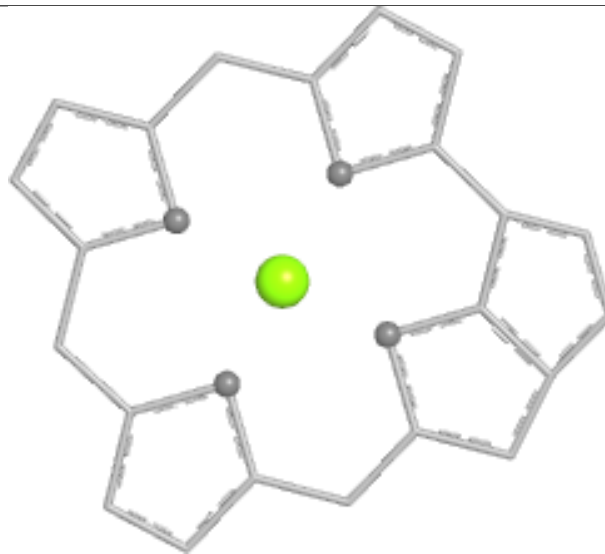
Bond lengths



Bond angles

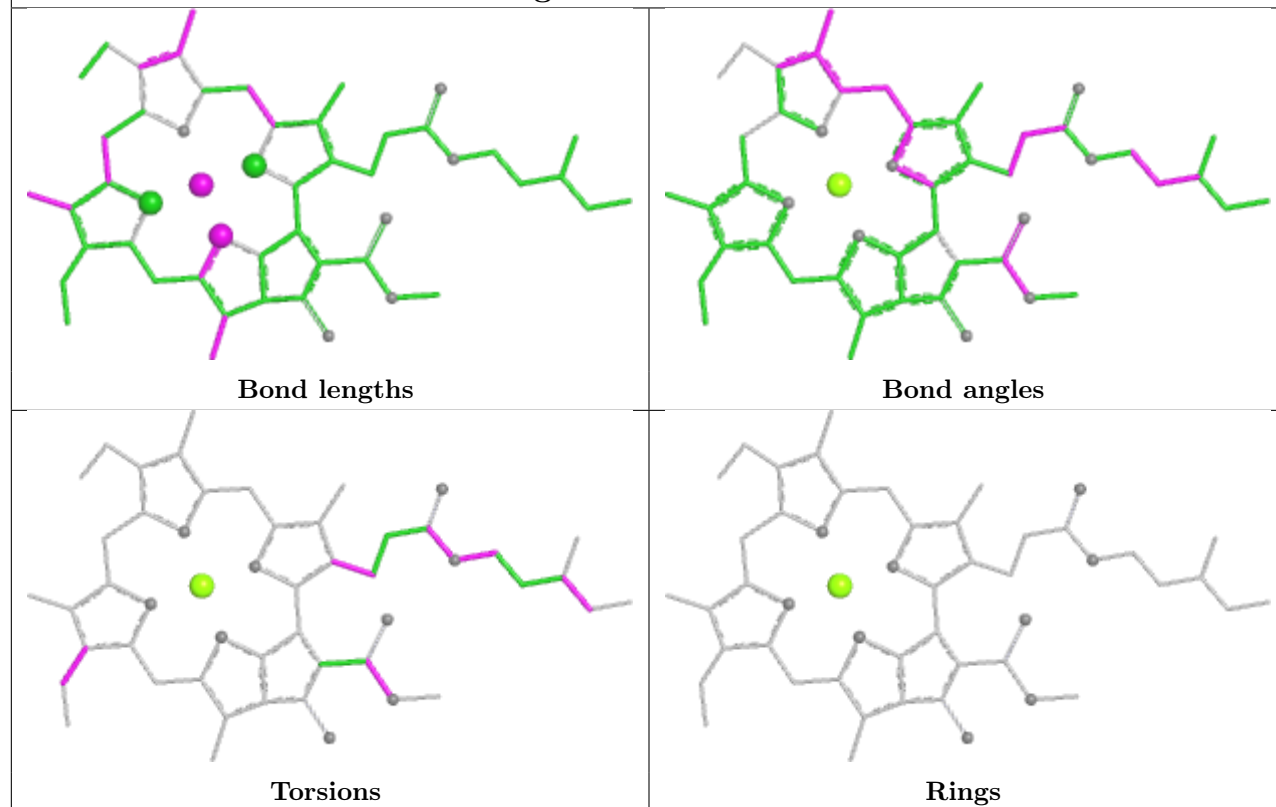


Torsions

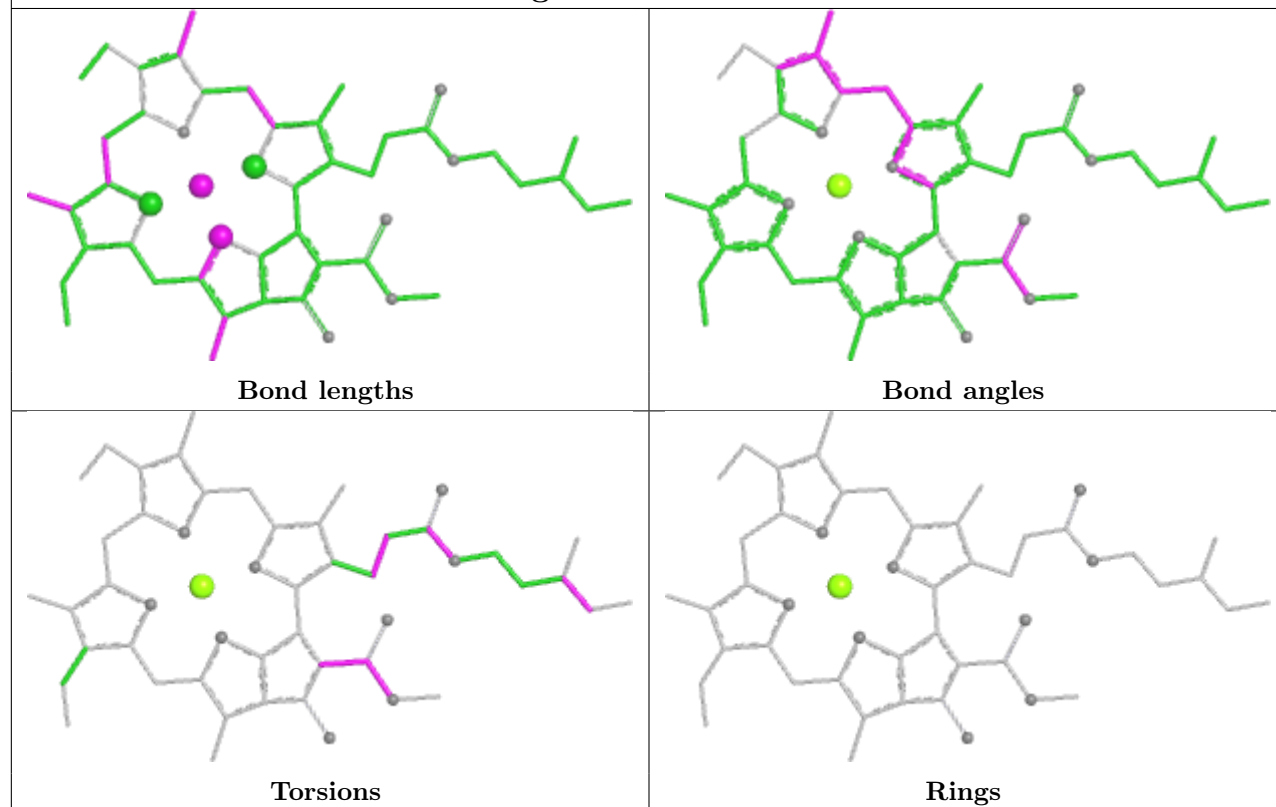


Rings

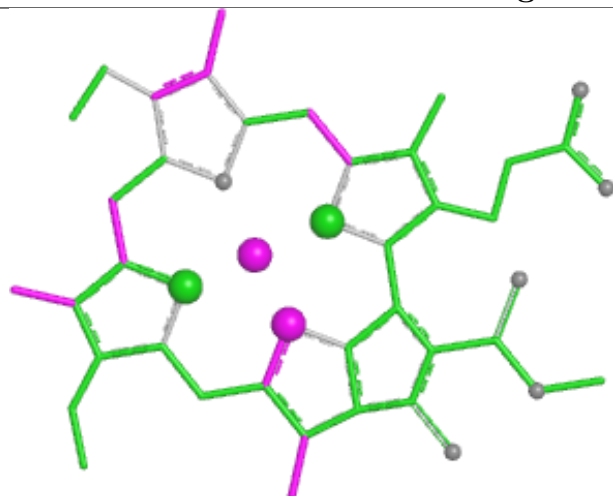
Ligand CLA F 201



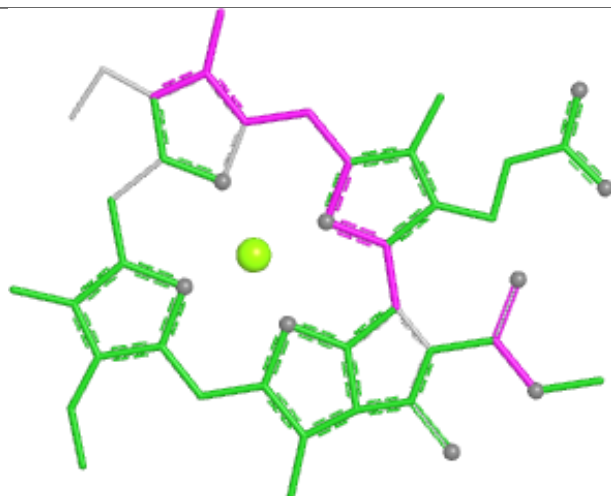
Ligand CLA A 825



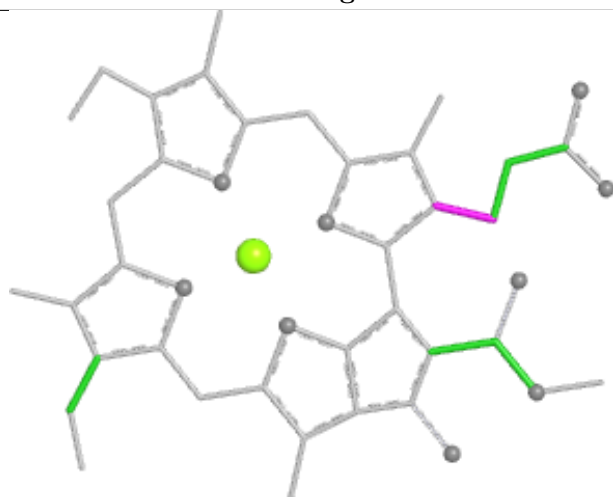
Ligand CLA b 837



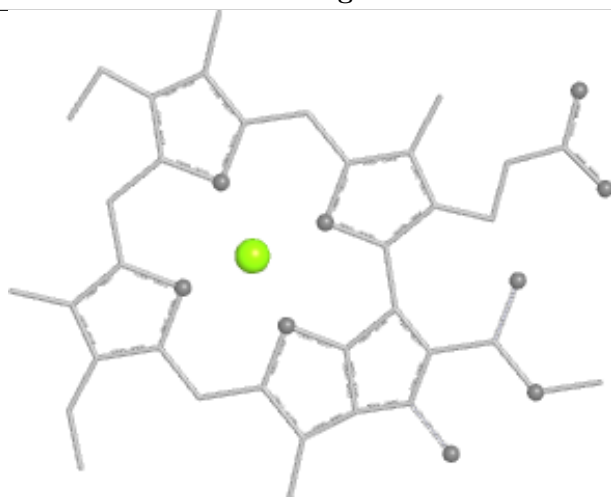
Bond lengths



Bond angles

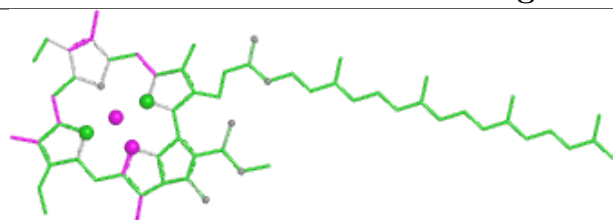


Torsions

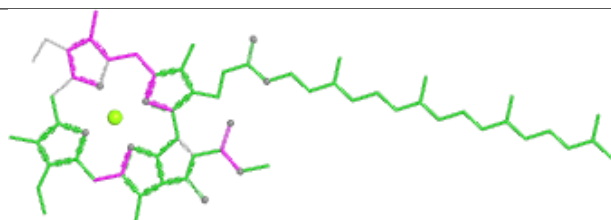


Rings

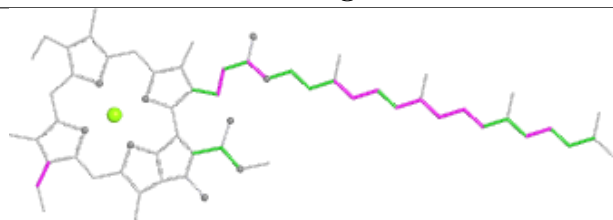
Ligand CLA b 806



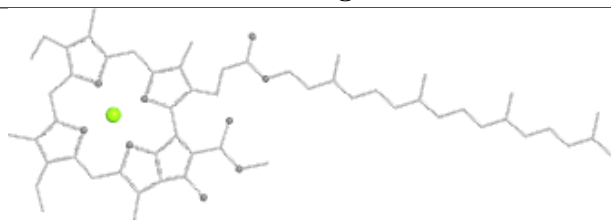
Bond lengths



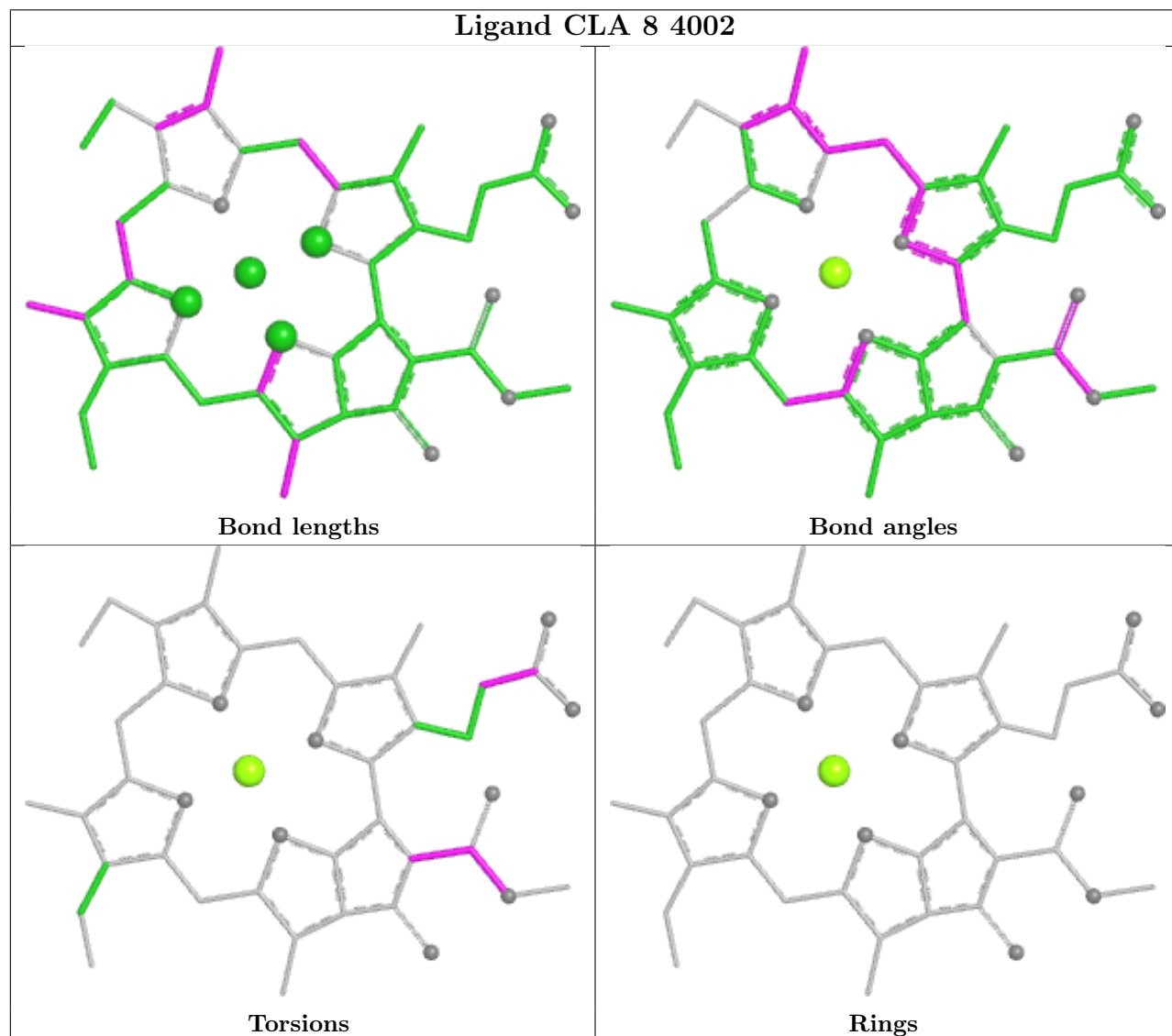
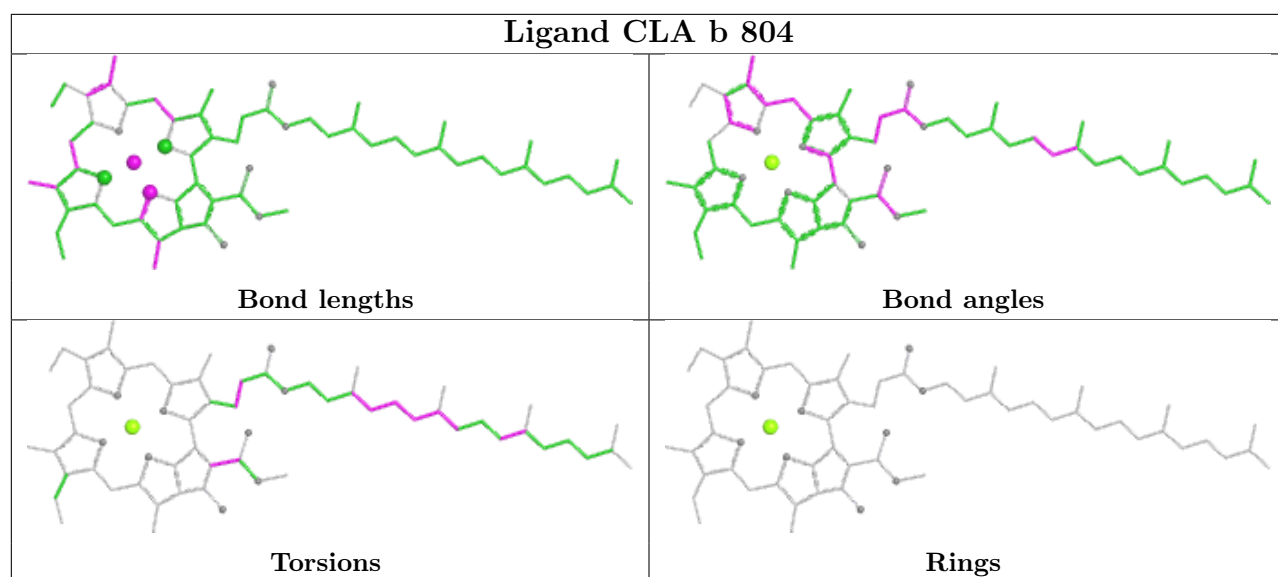
Bond angles

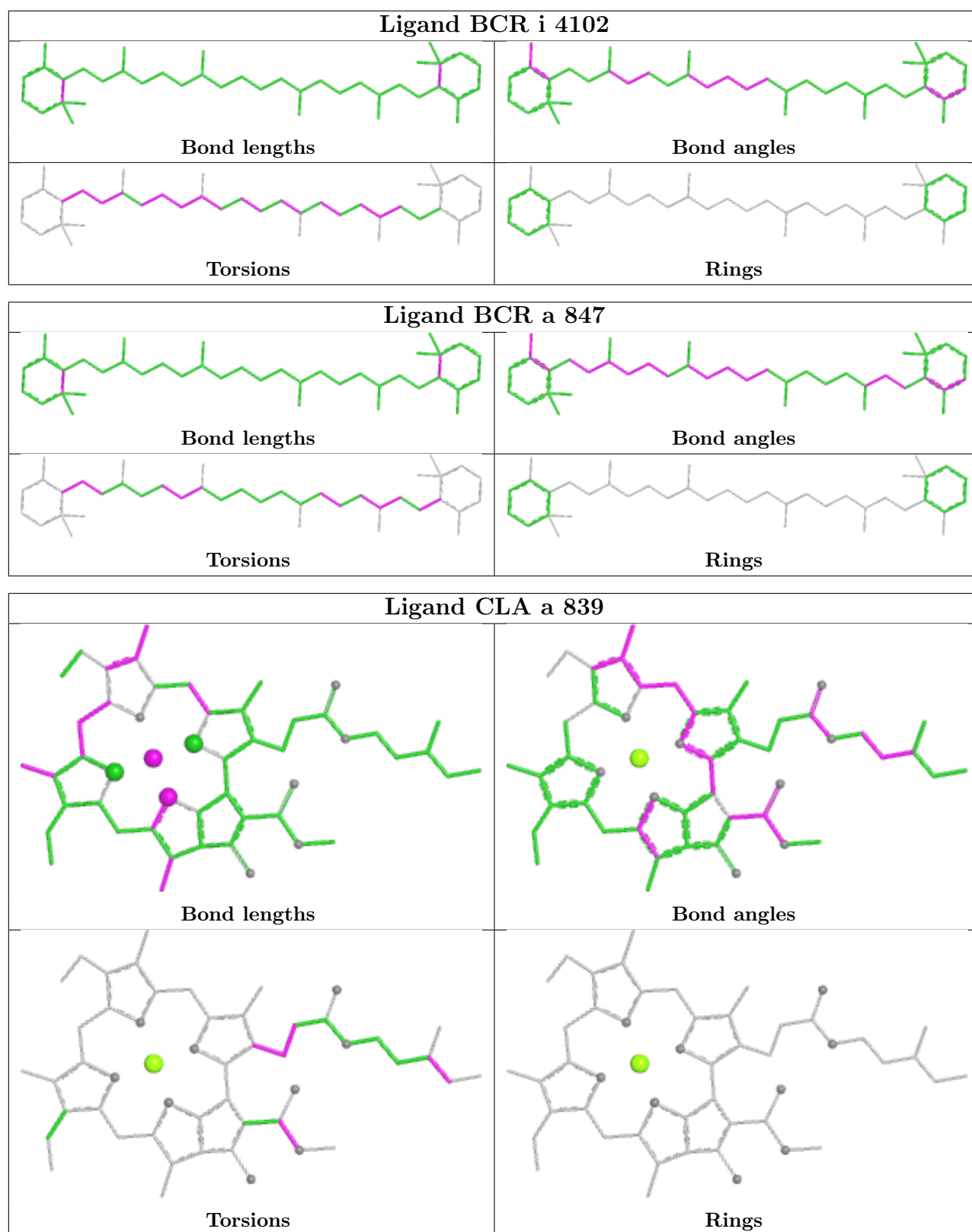


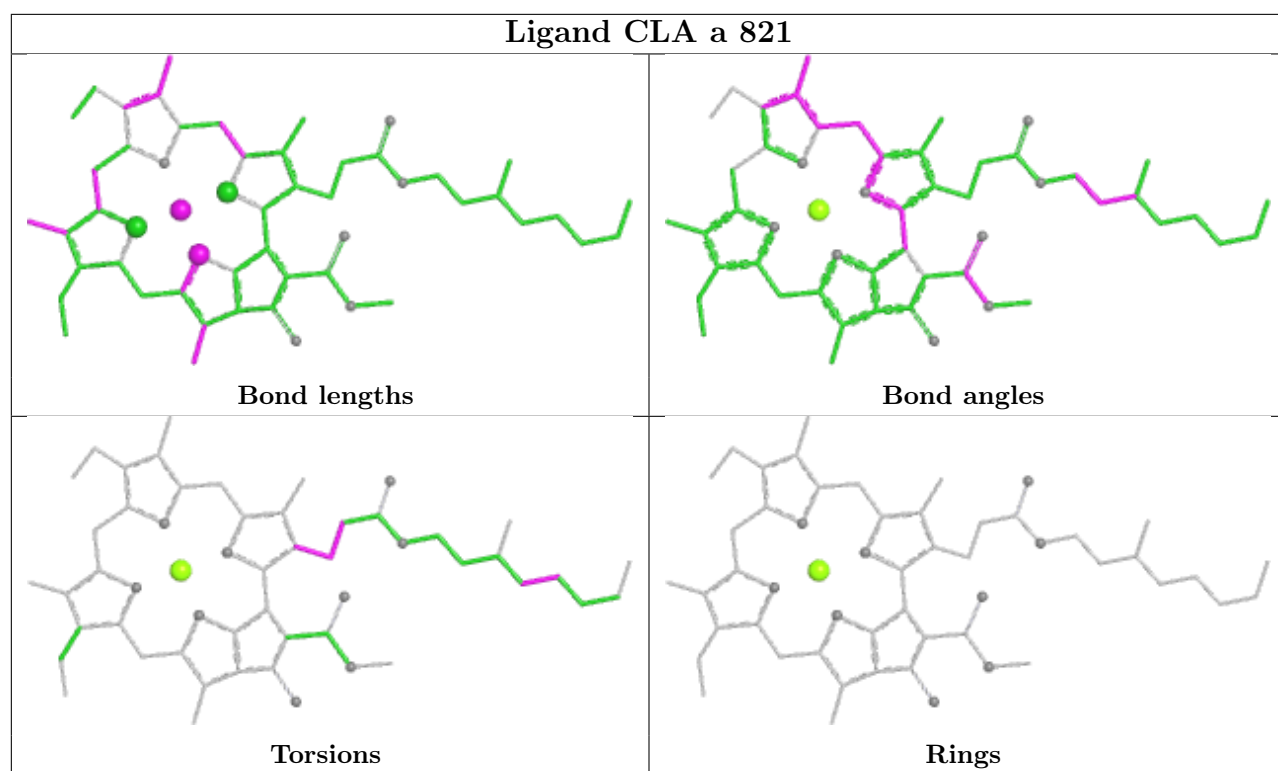
Torsions

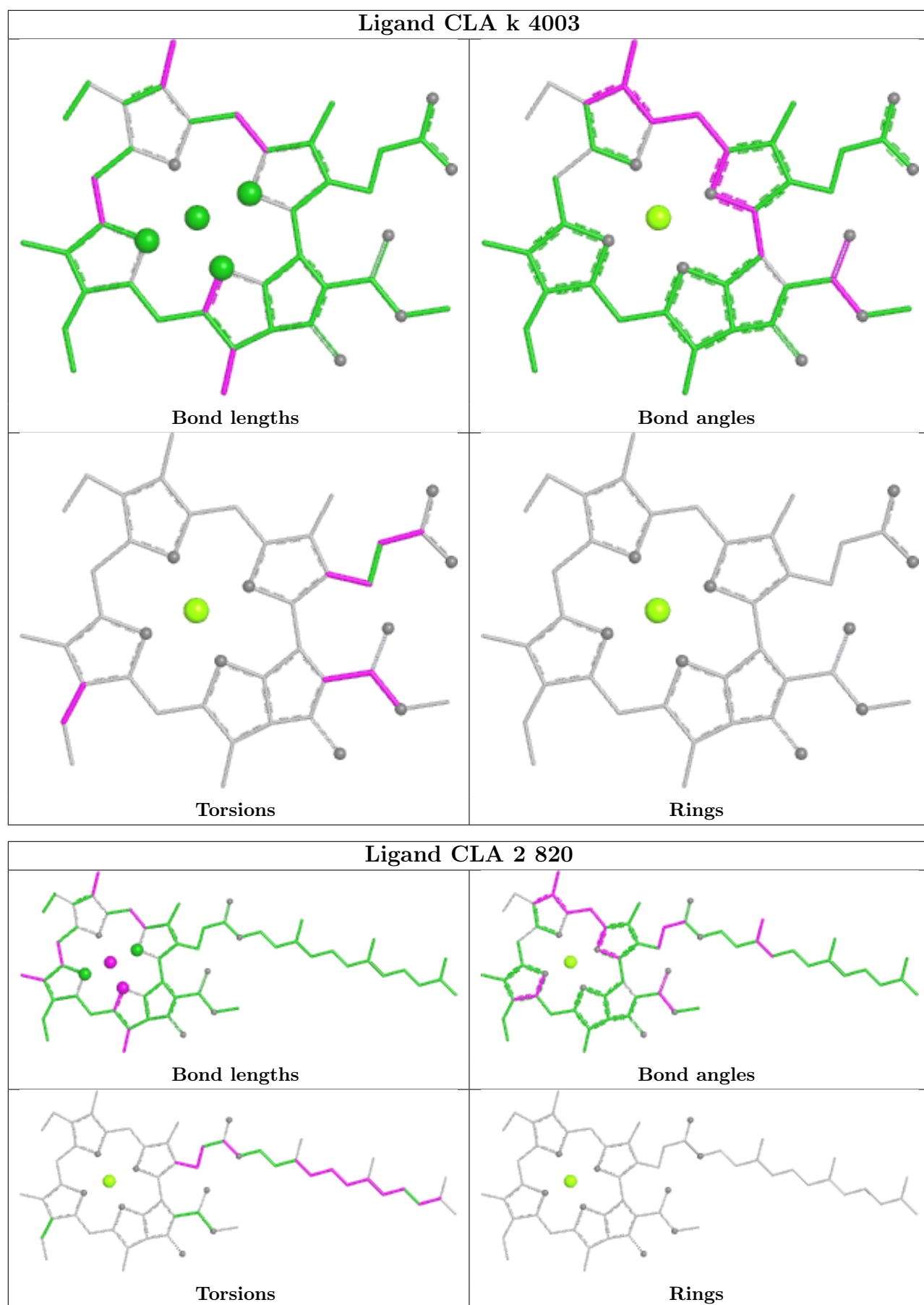


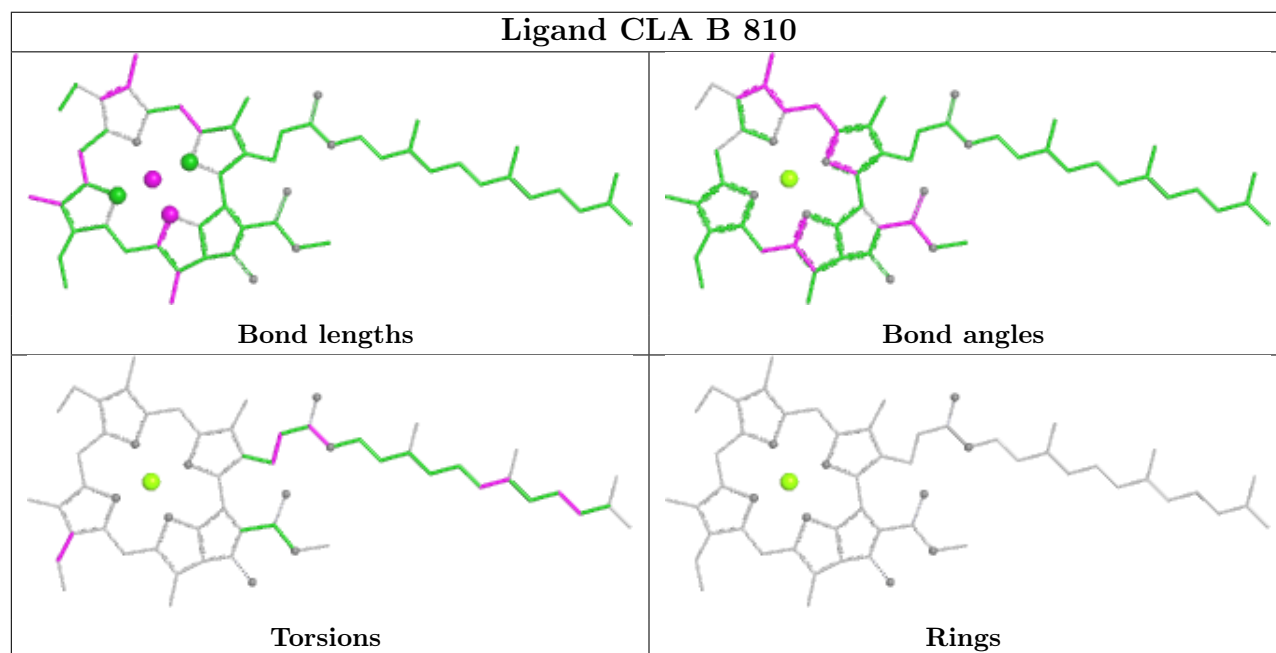
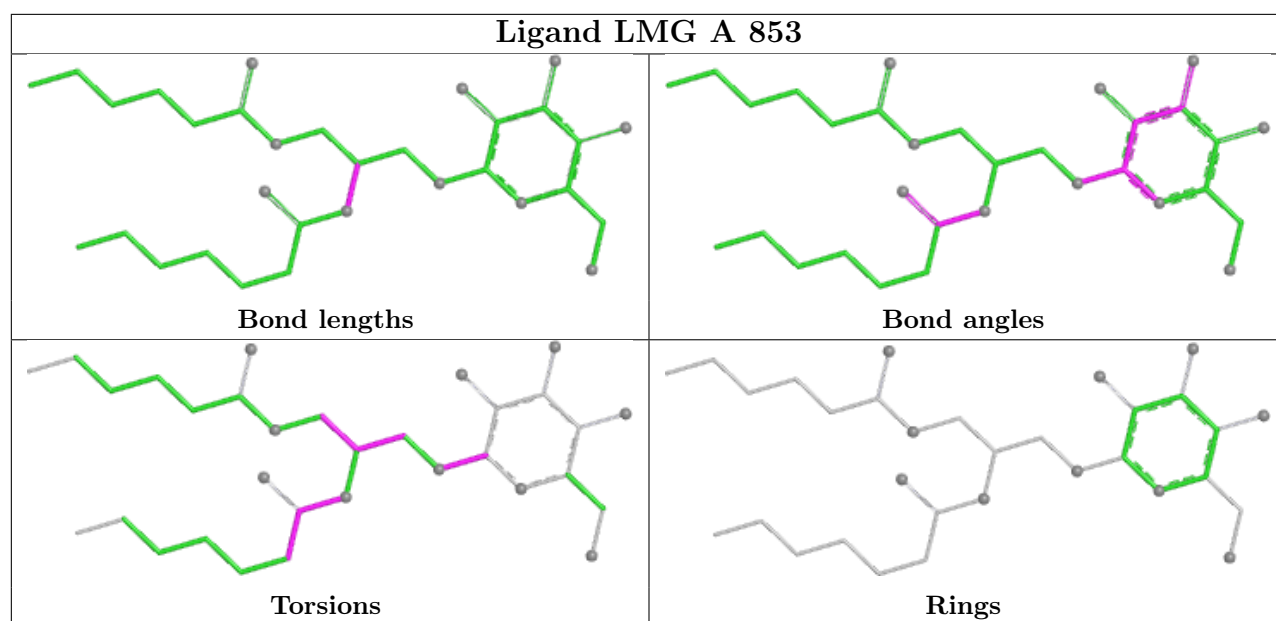
Rings



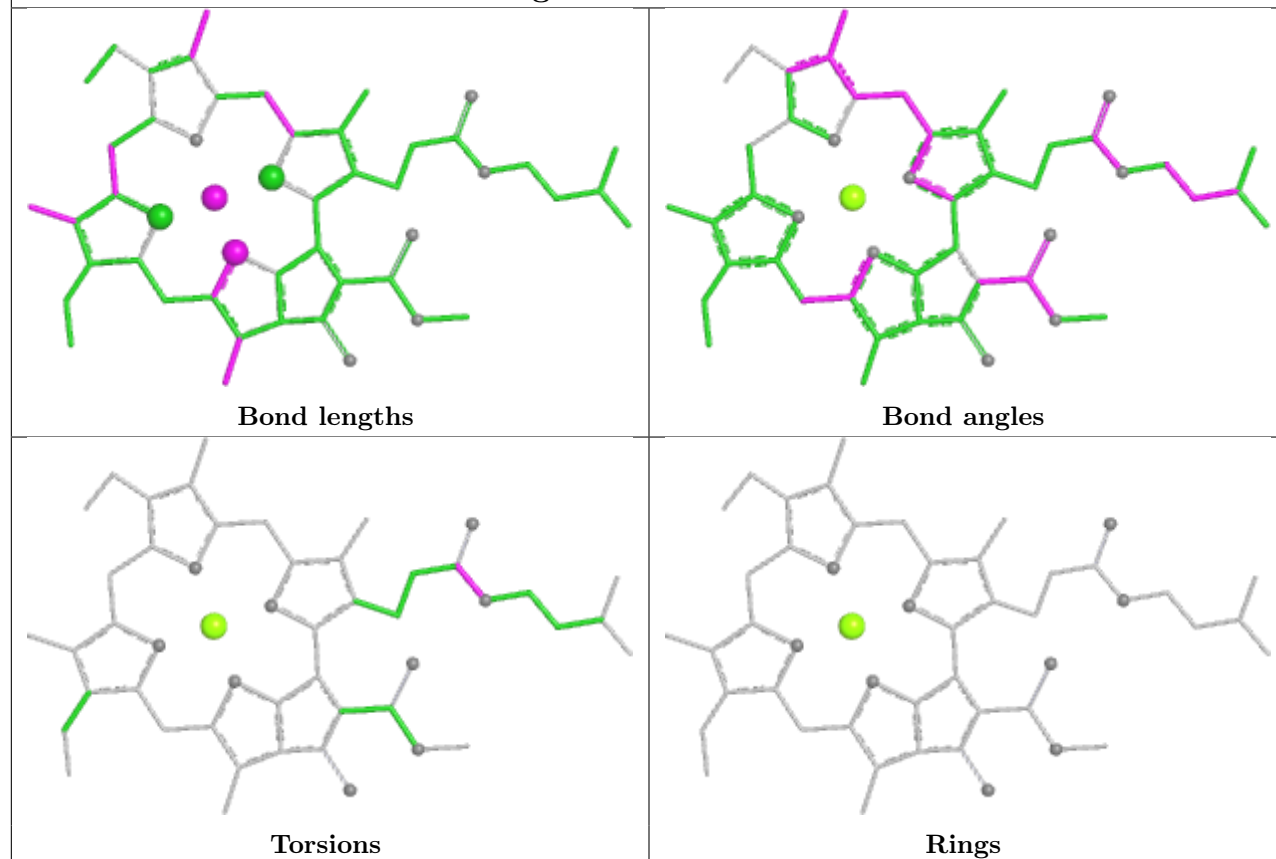




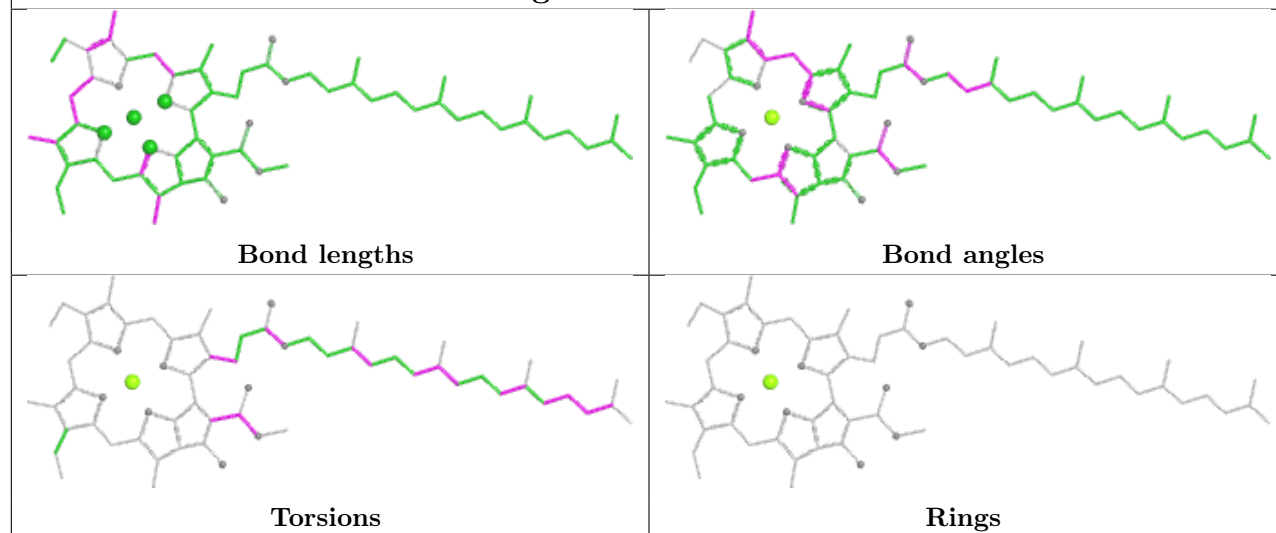


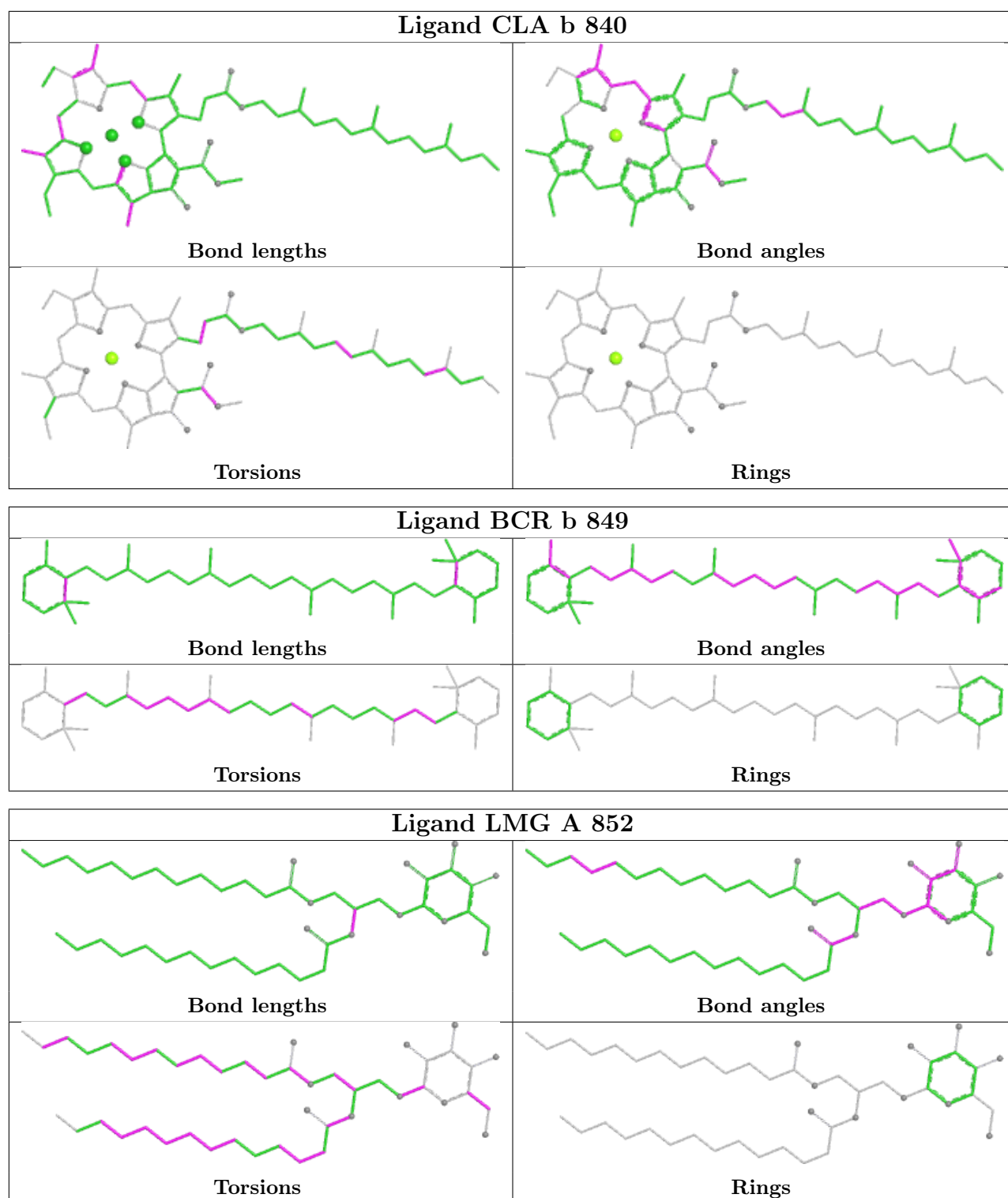


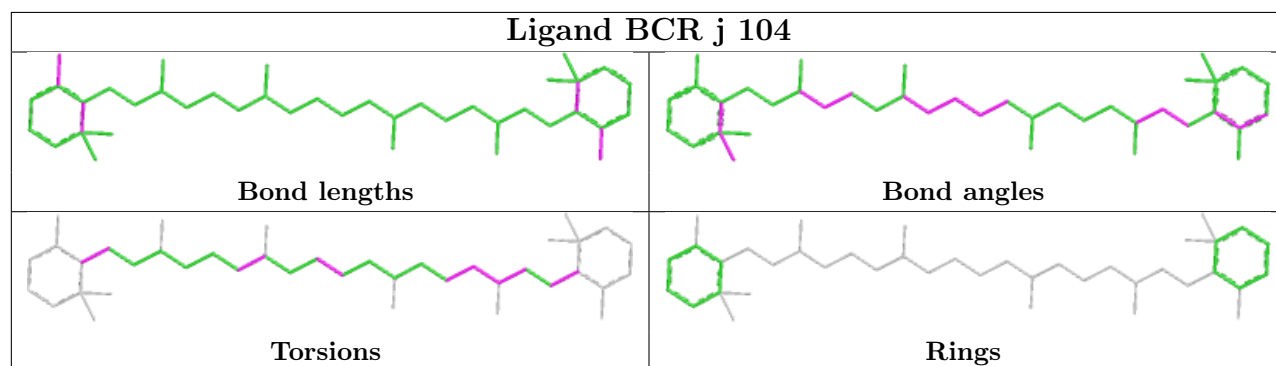
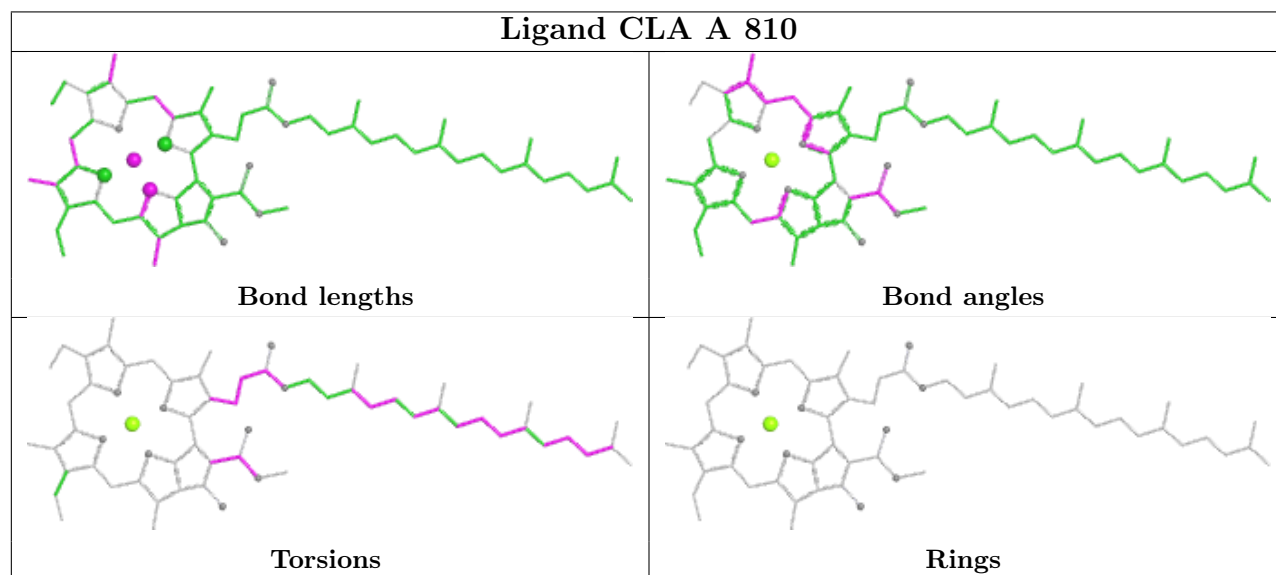
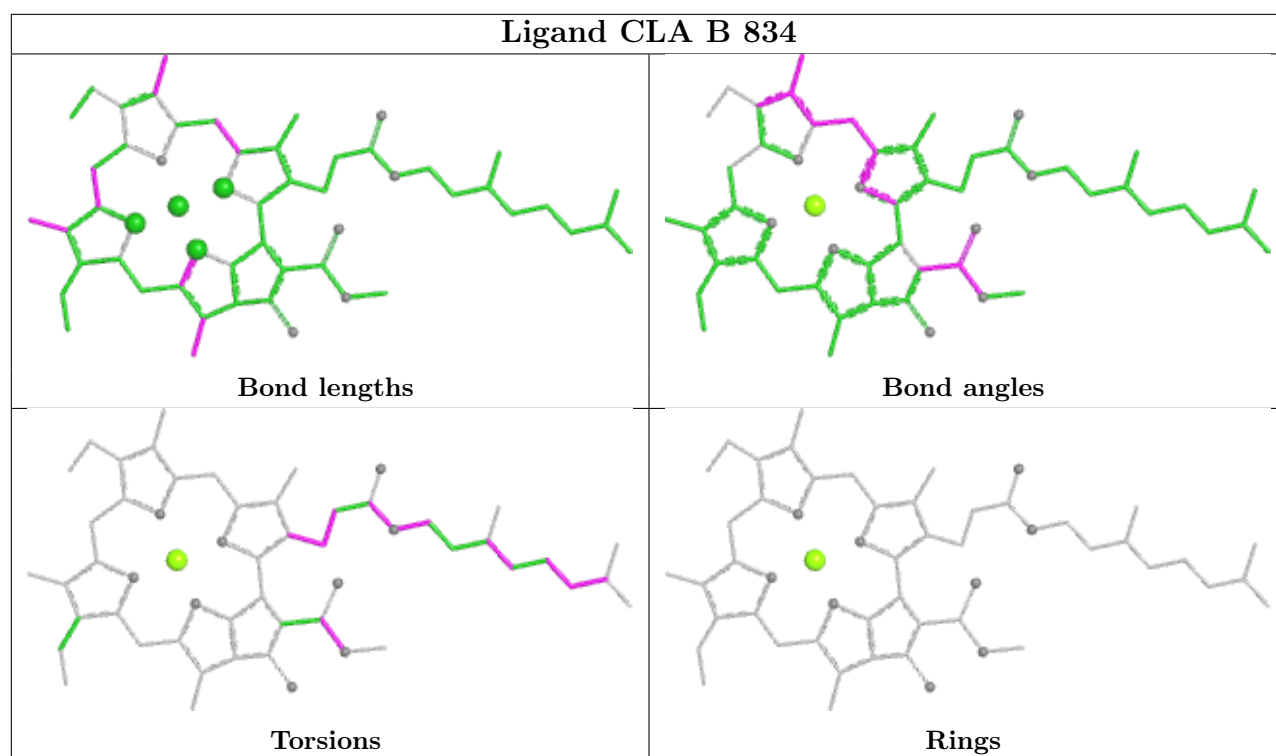
Ligand CLA B 828



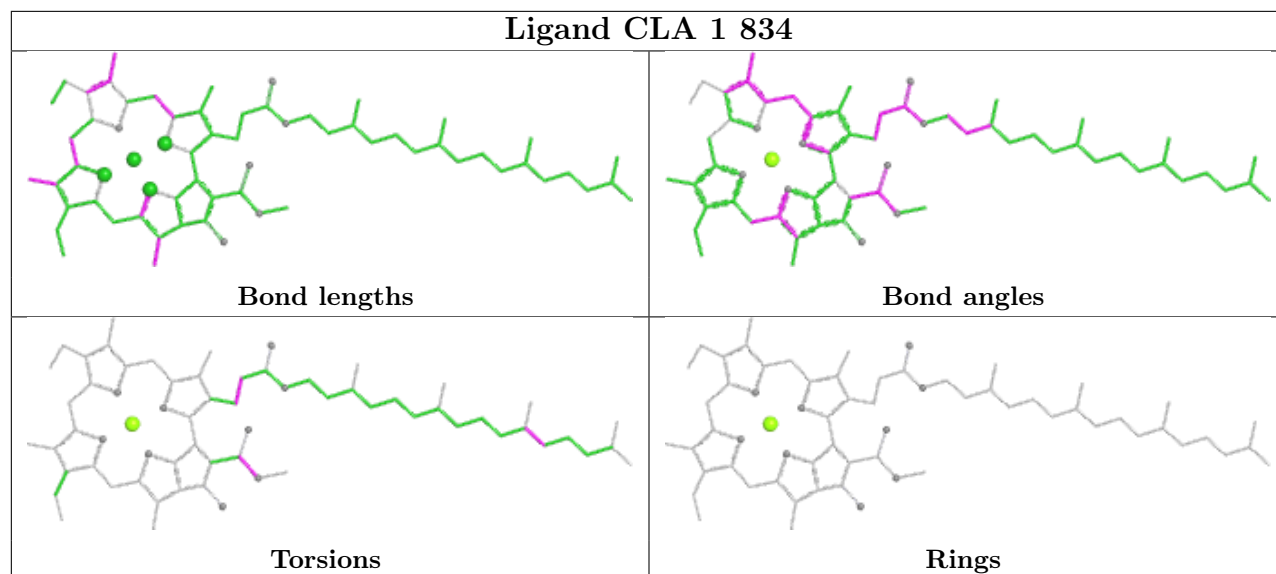
Ligand CLA B 844



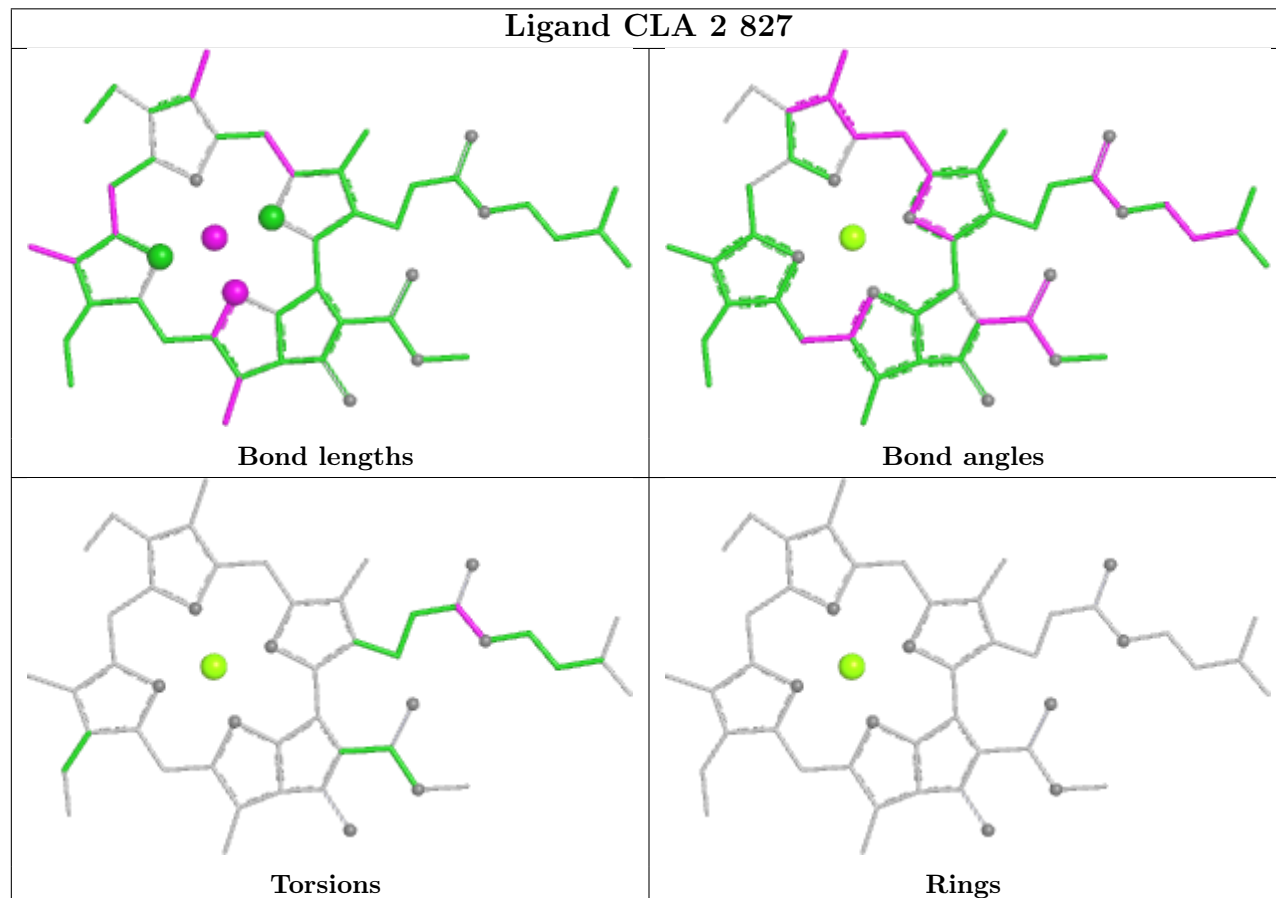


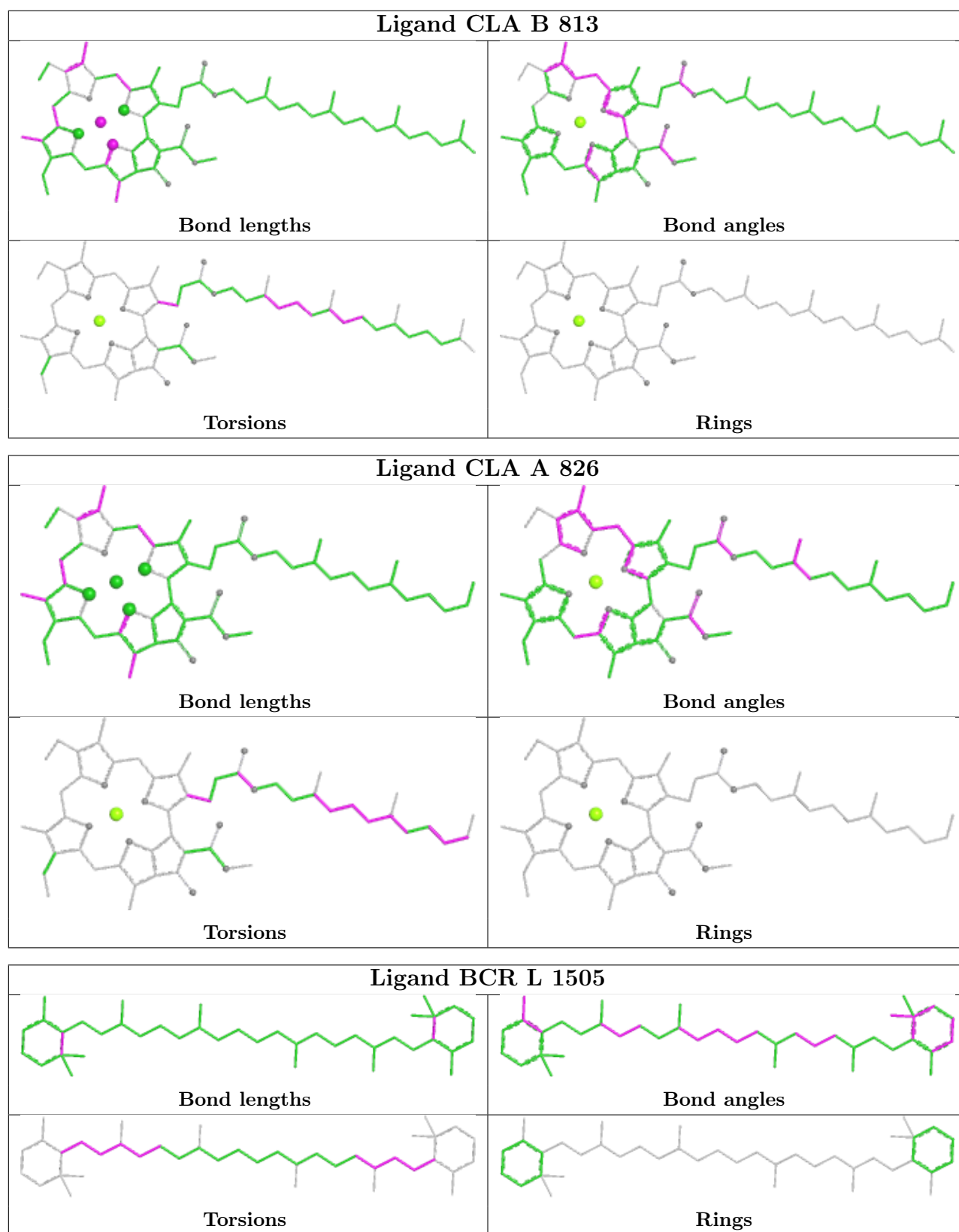


Ligand CLA 1 834

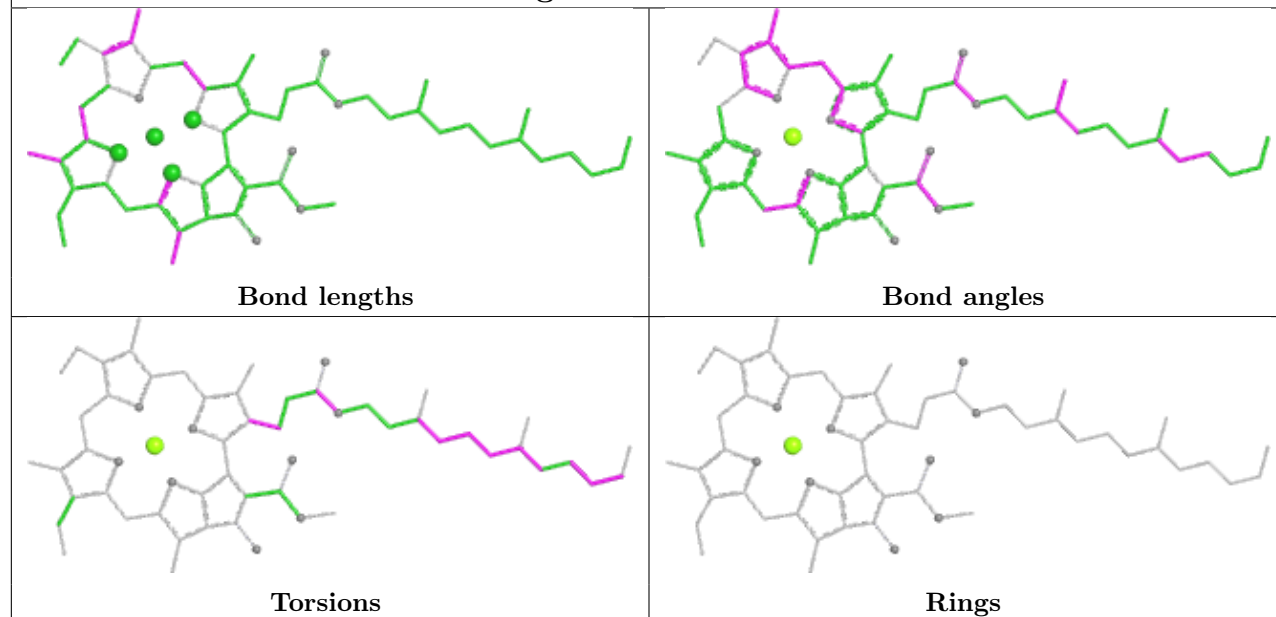


Ligand CLA 2 827

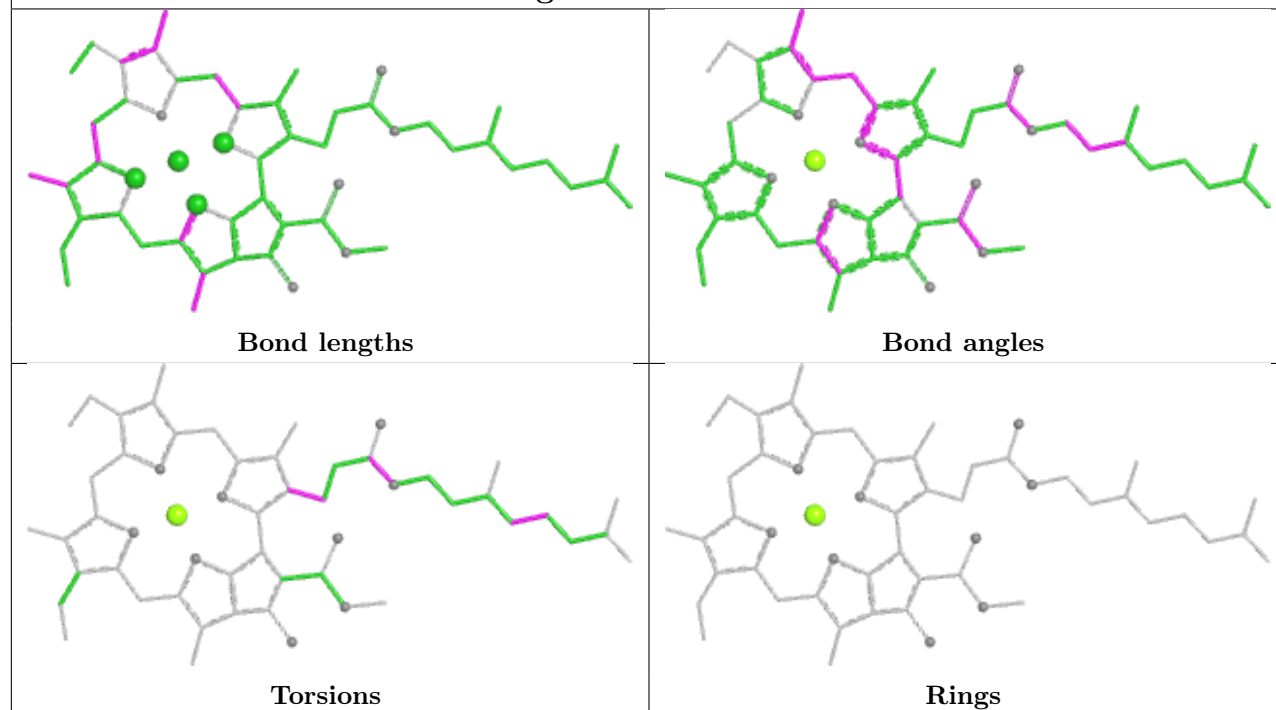


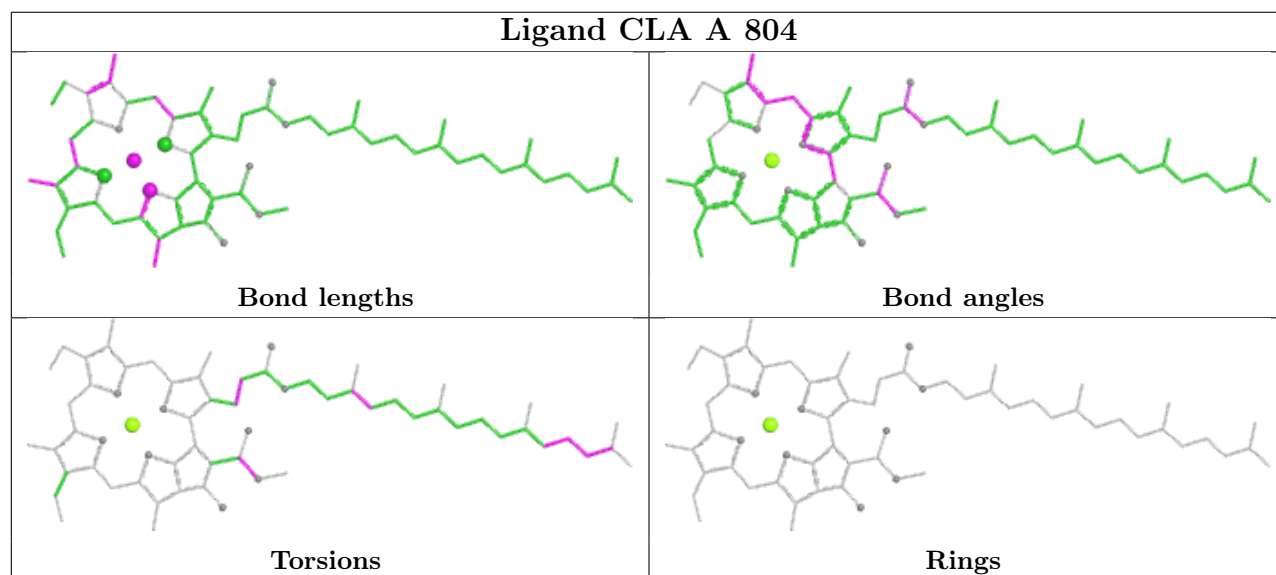
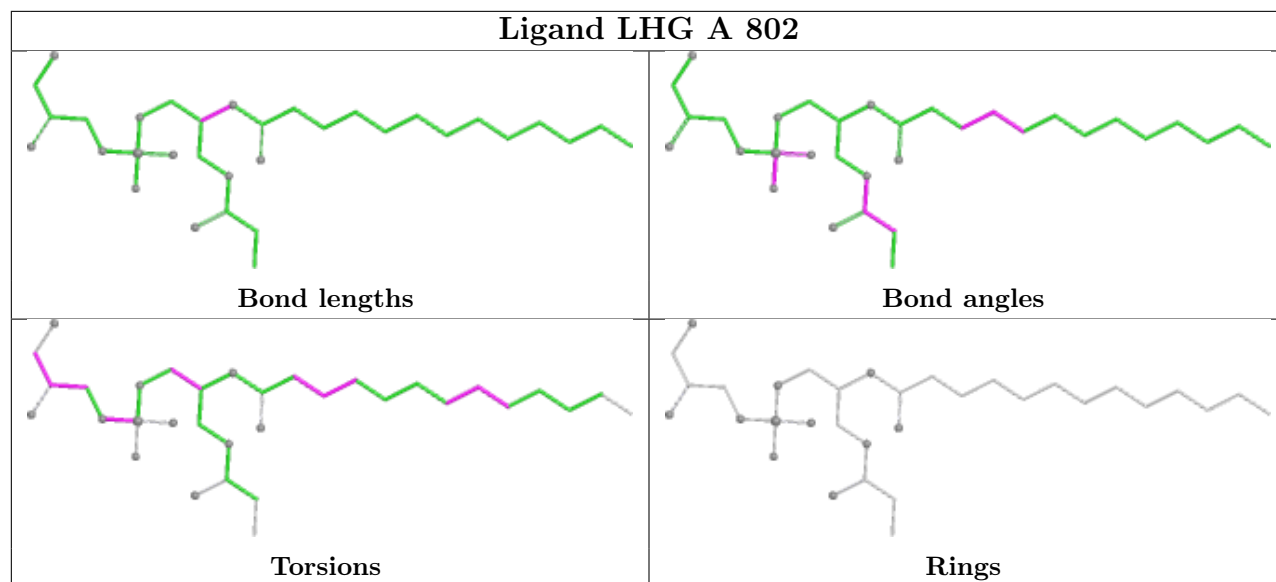


Ligand CLA 1 825

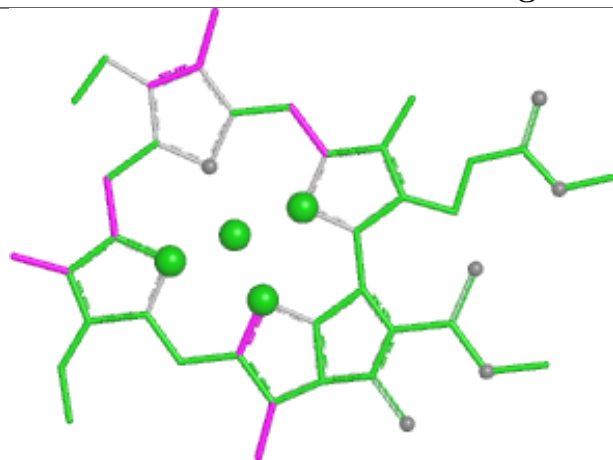


Ligand CLA a 854

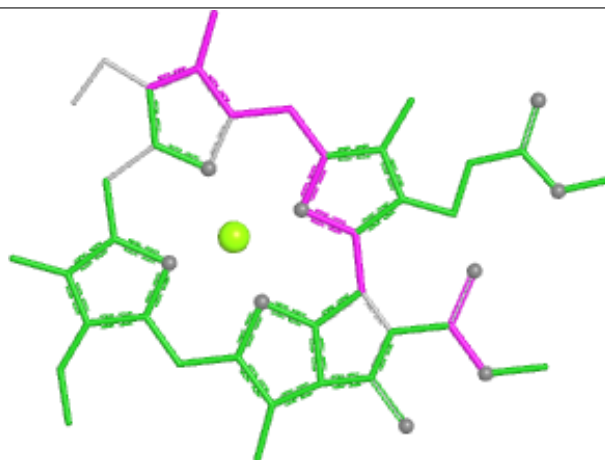




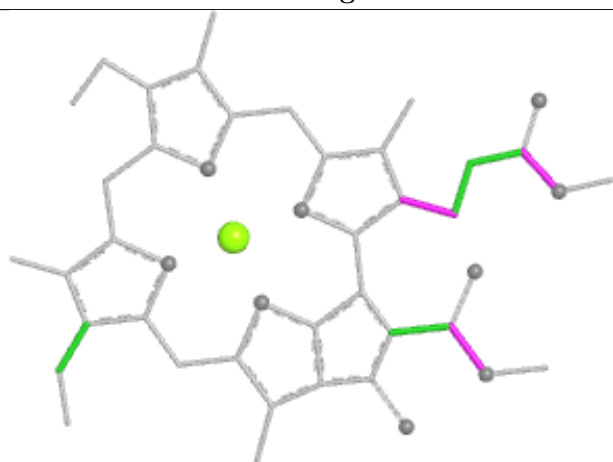
Ligand CLA 1 817



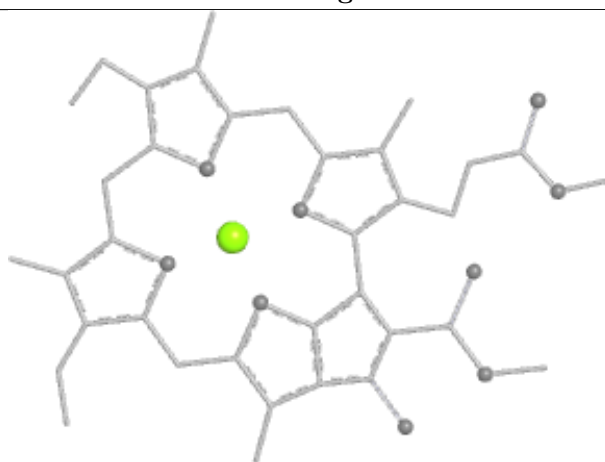
Bond lengths



Bond angles

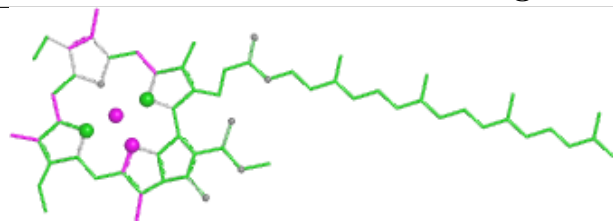


Torsions

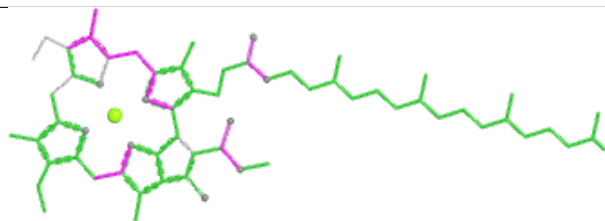


Rings

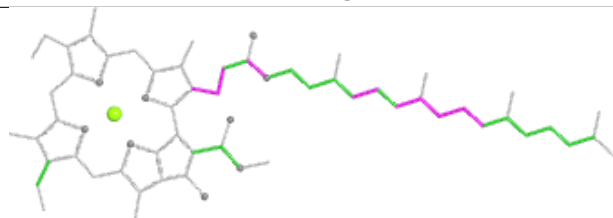
Ligand CLA A 842



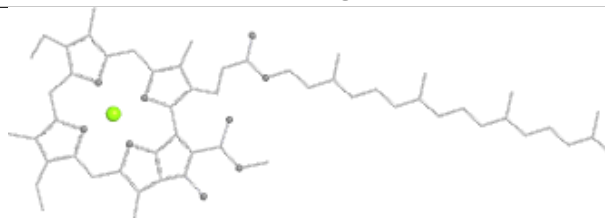
Bond lengths



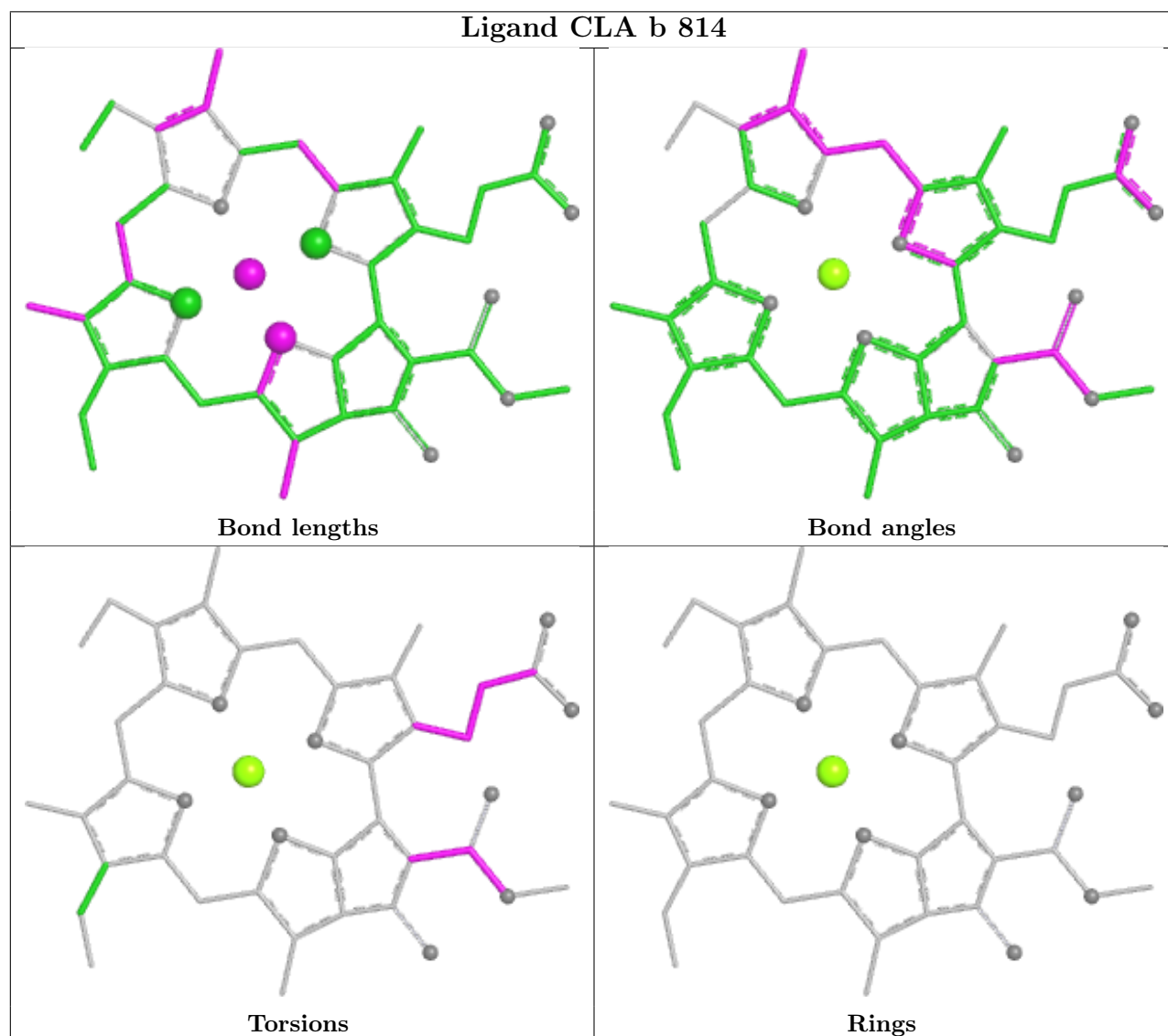
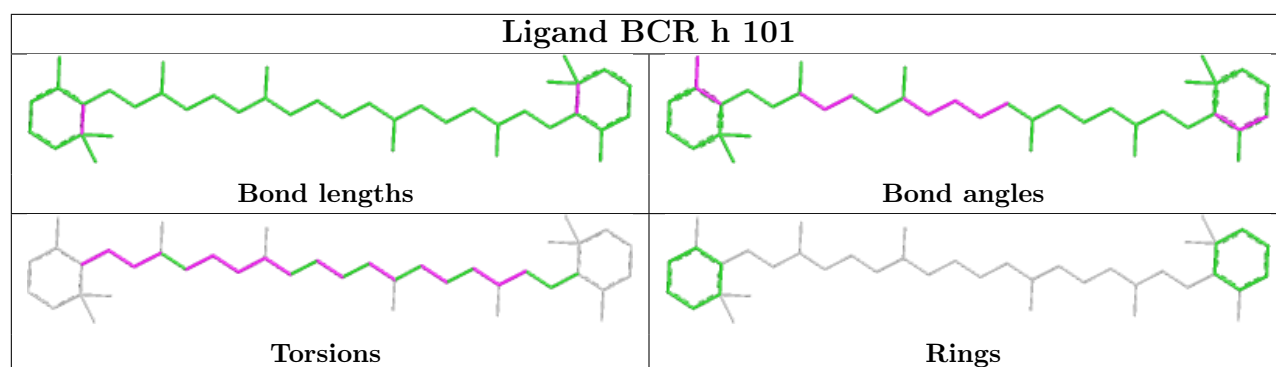
Bond angles



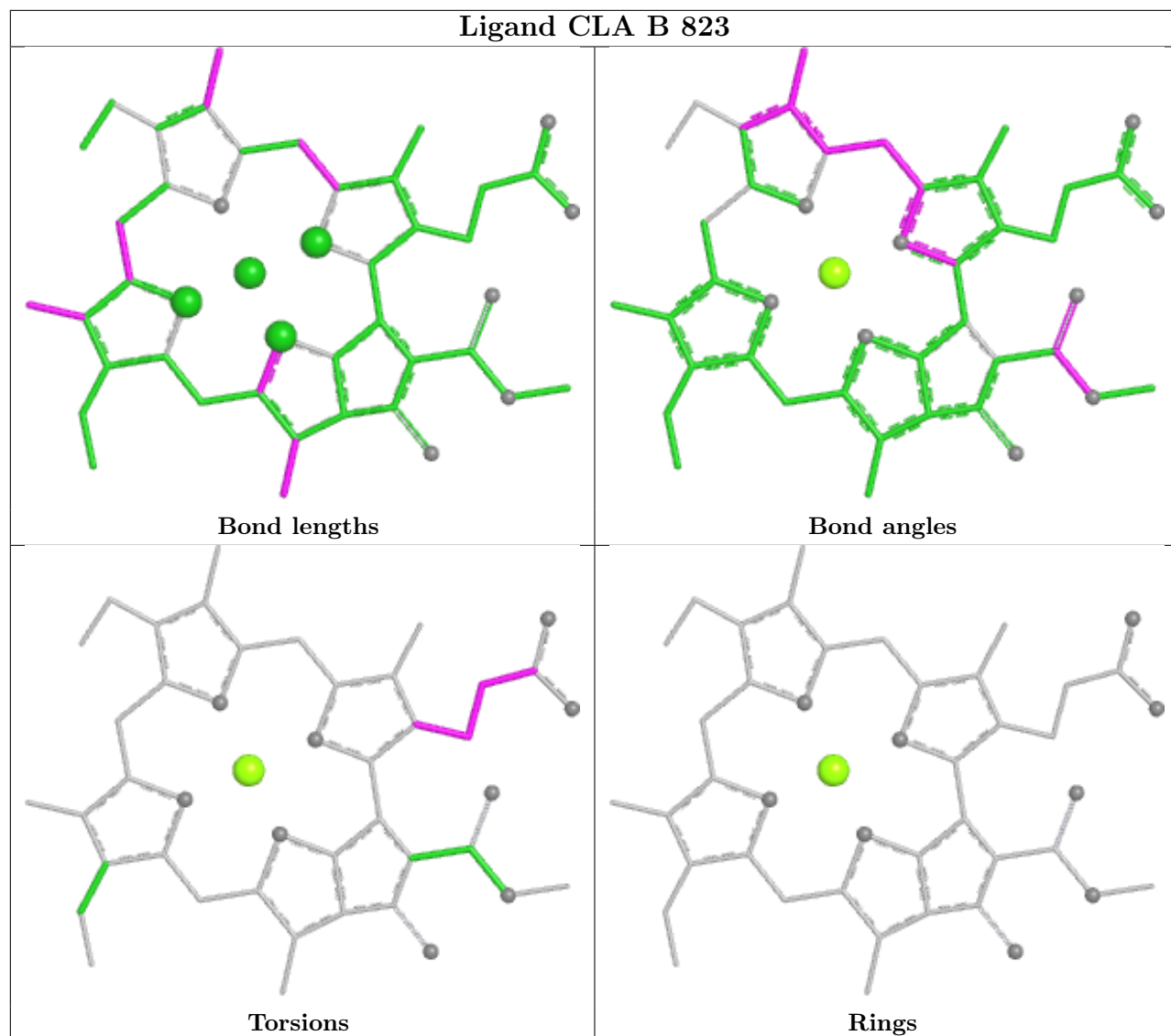
Torsions



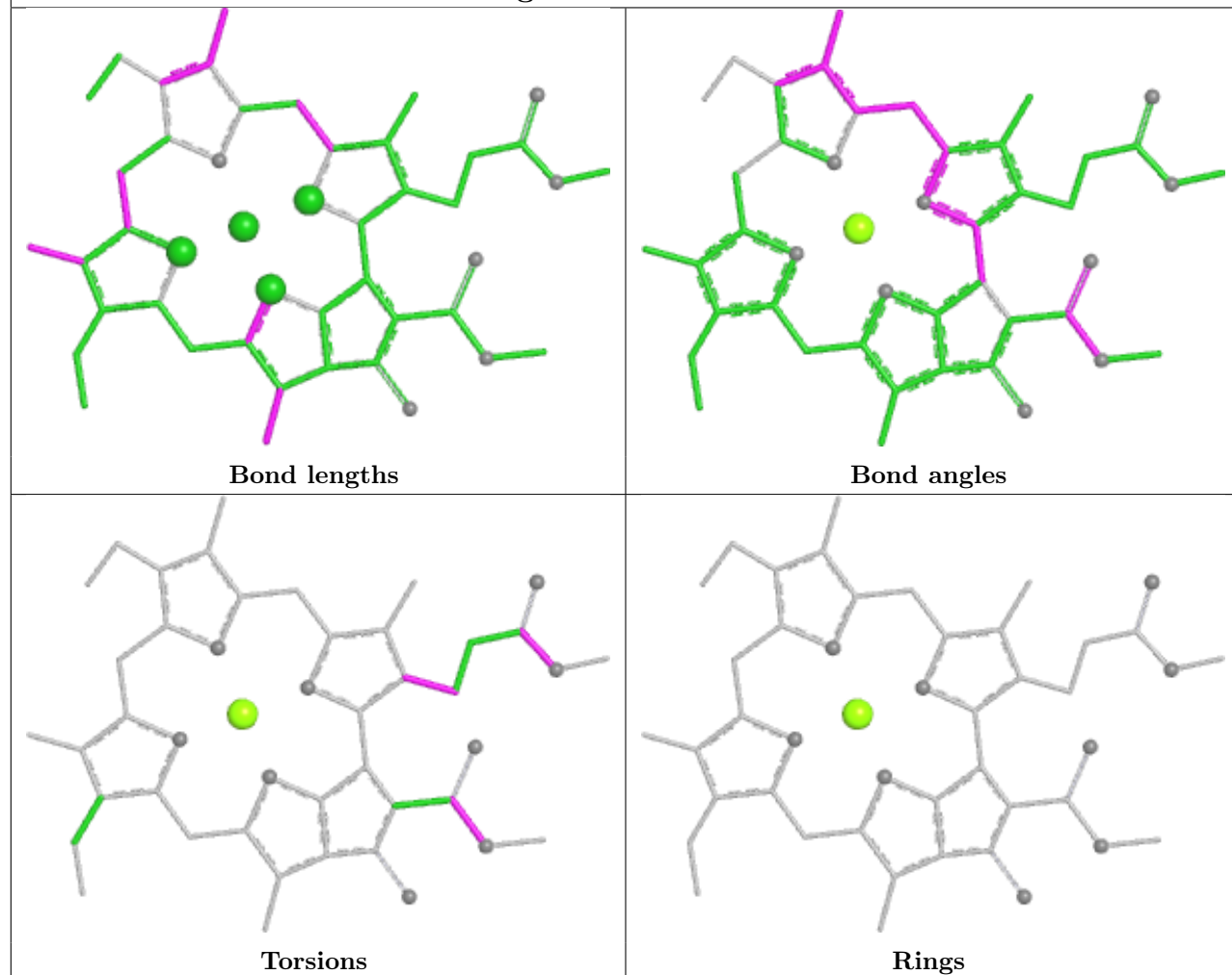
Rings



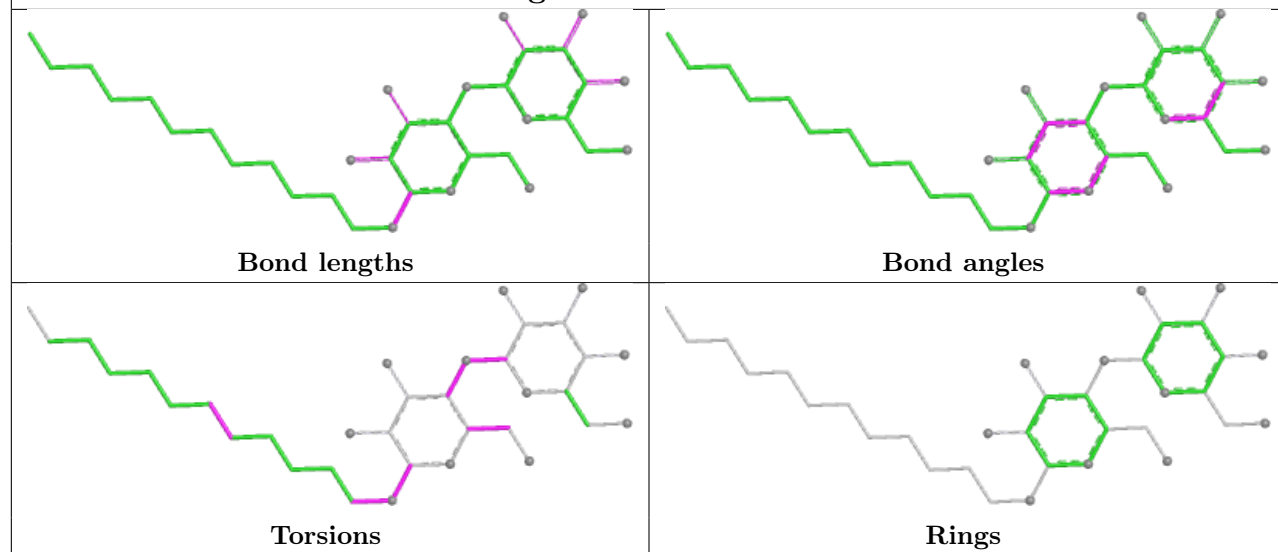
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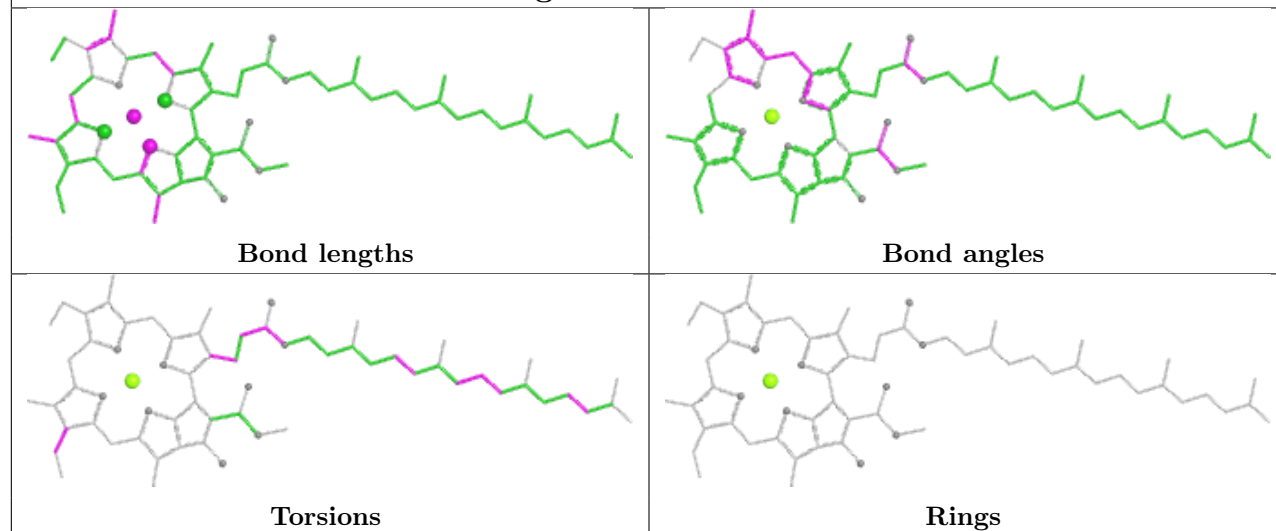
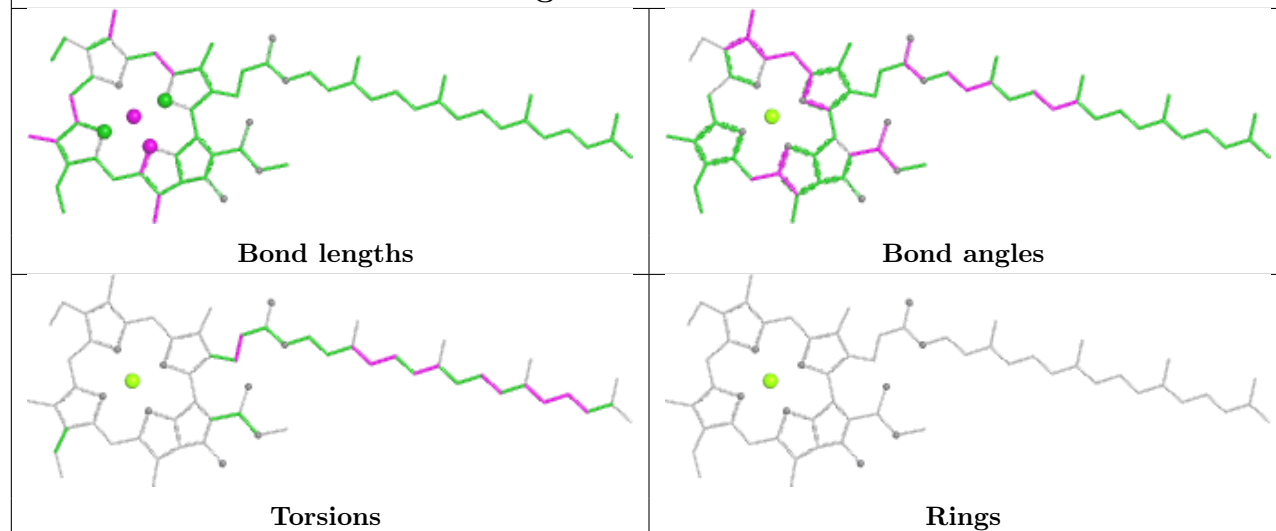


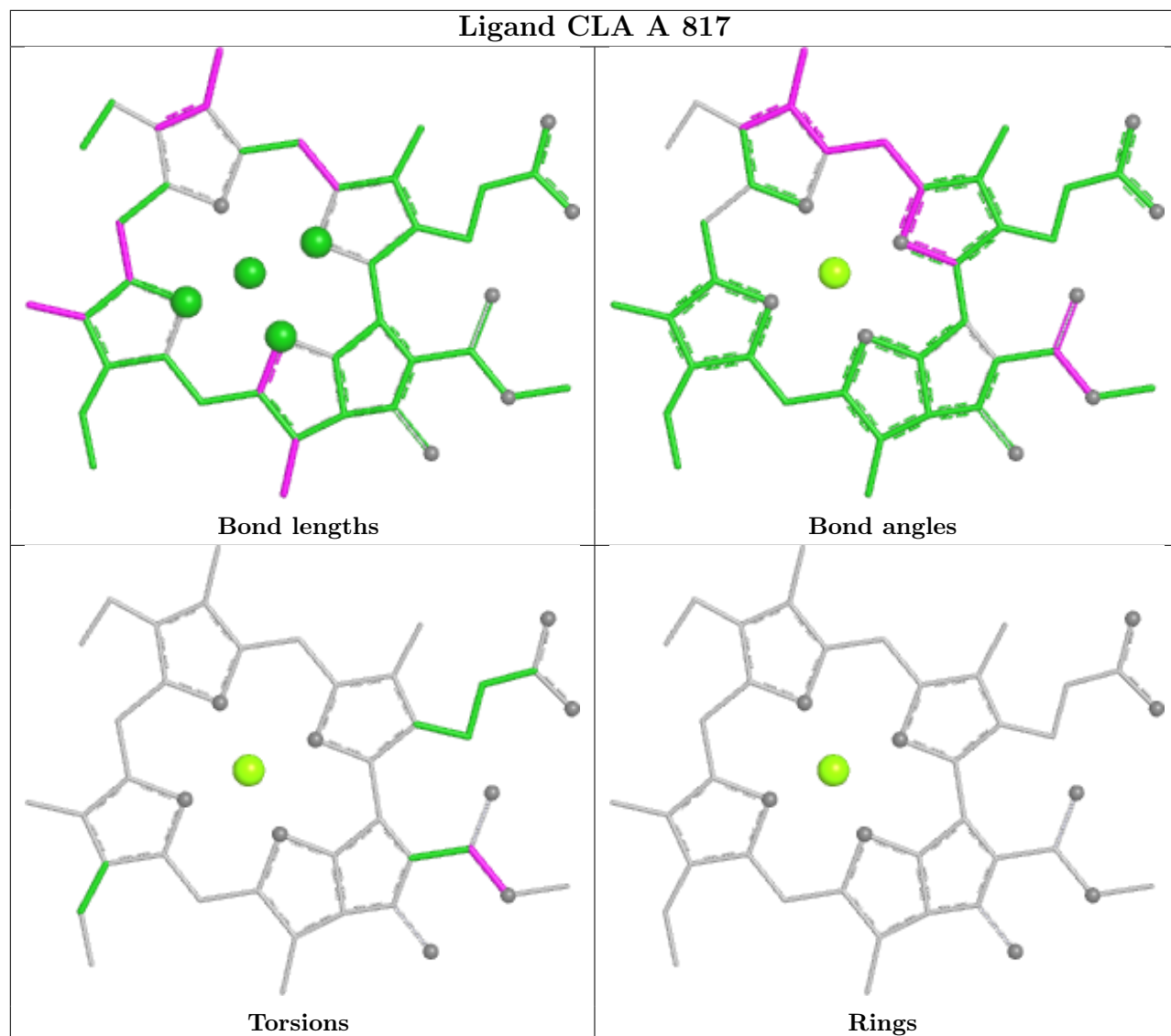
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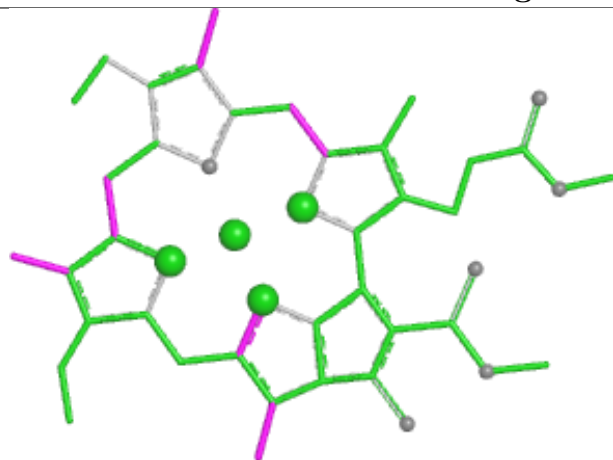
Ligand LMT i 4101



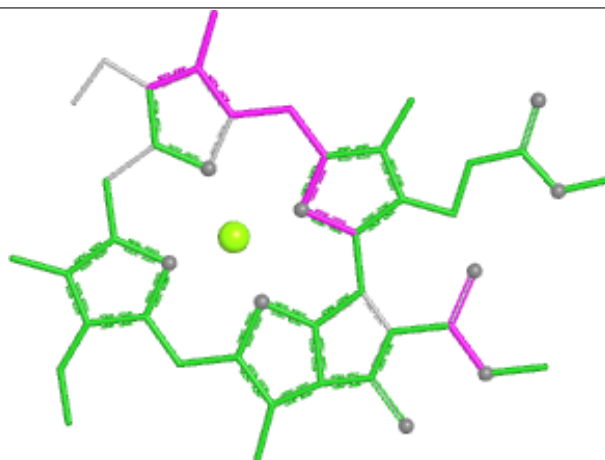
Ligand CLA b 842**Ligand CLA a 831**



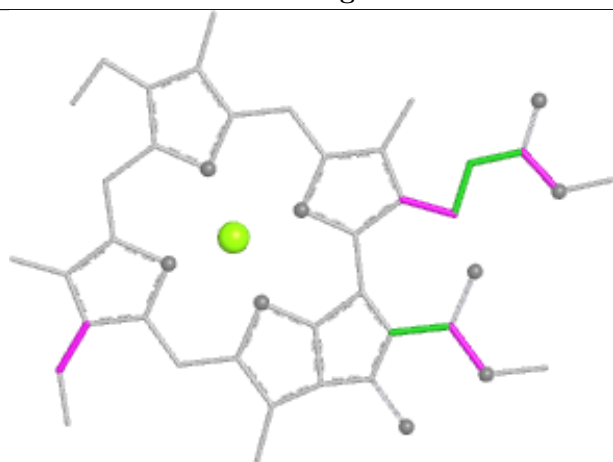
Ligand CLA B 817



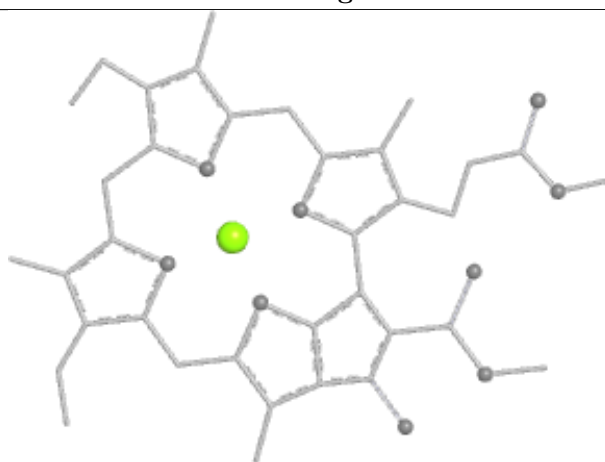
Bond lengths



Bond angles

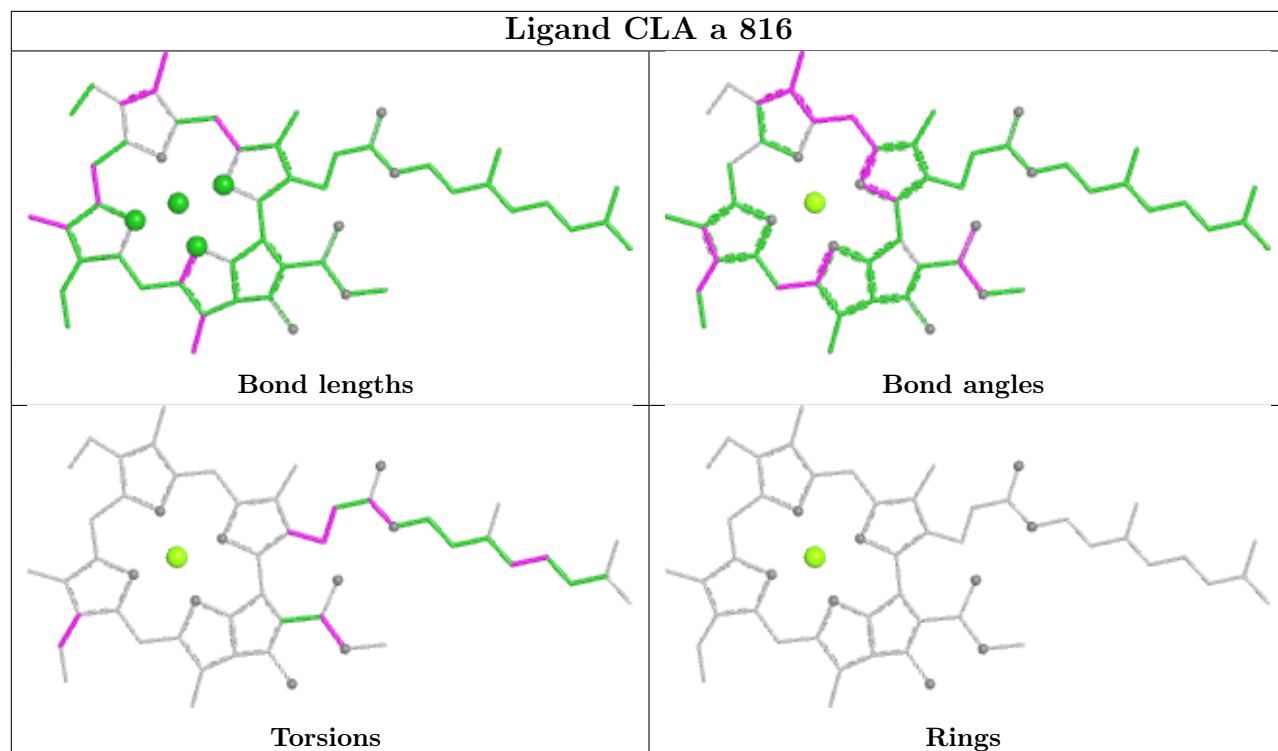


Torsions

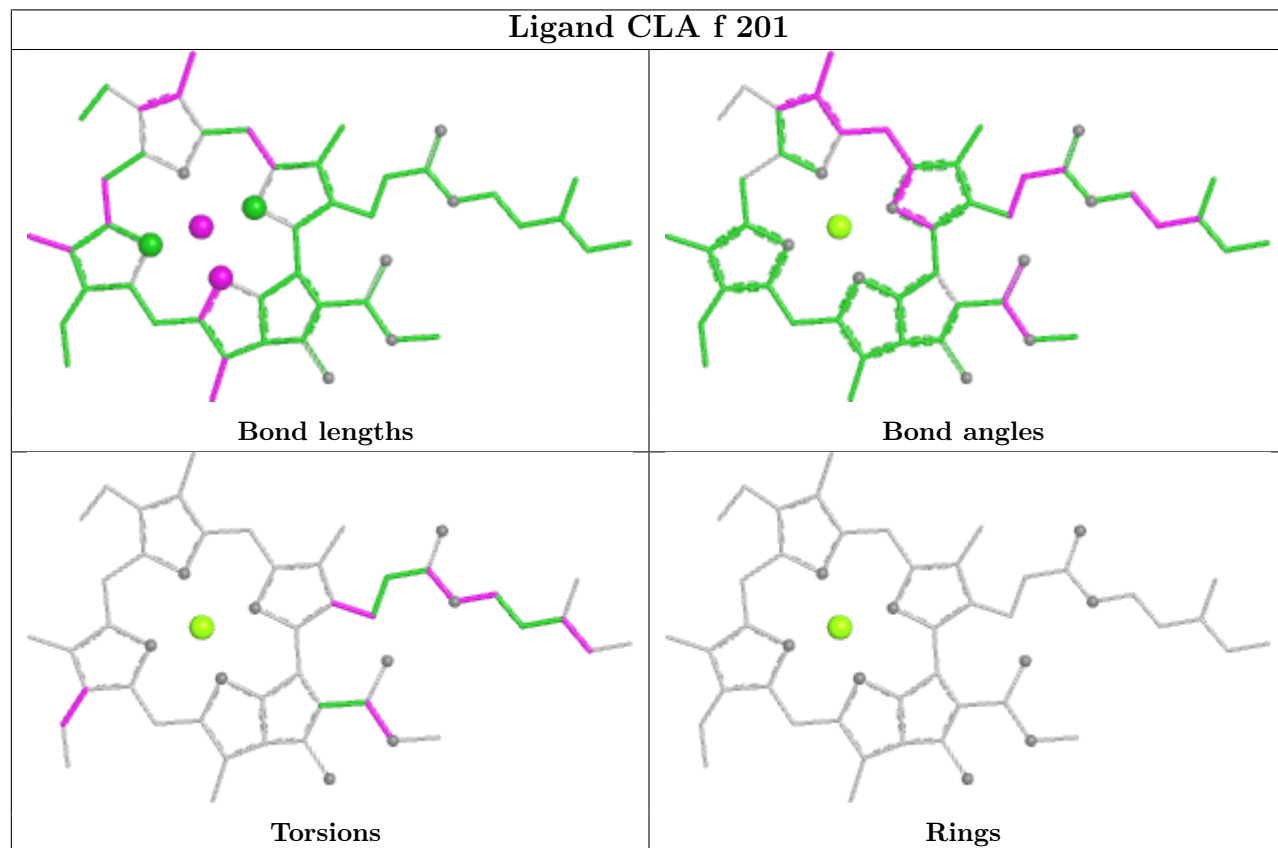


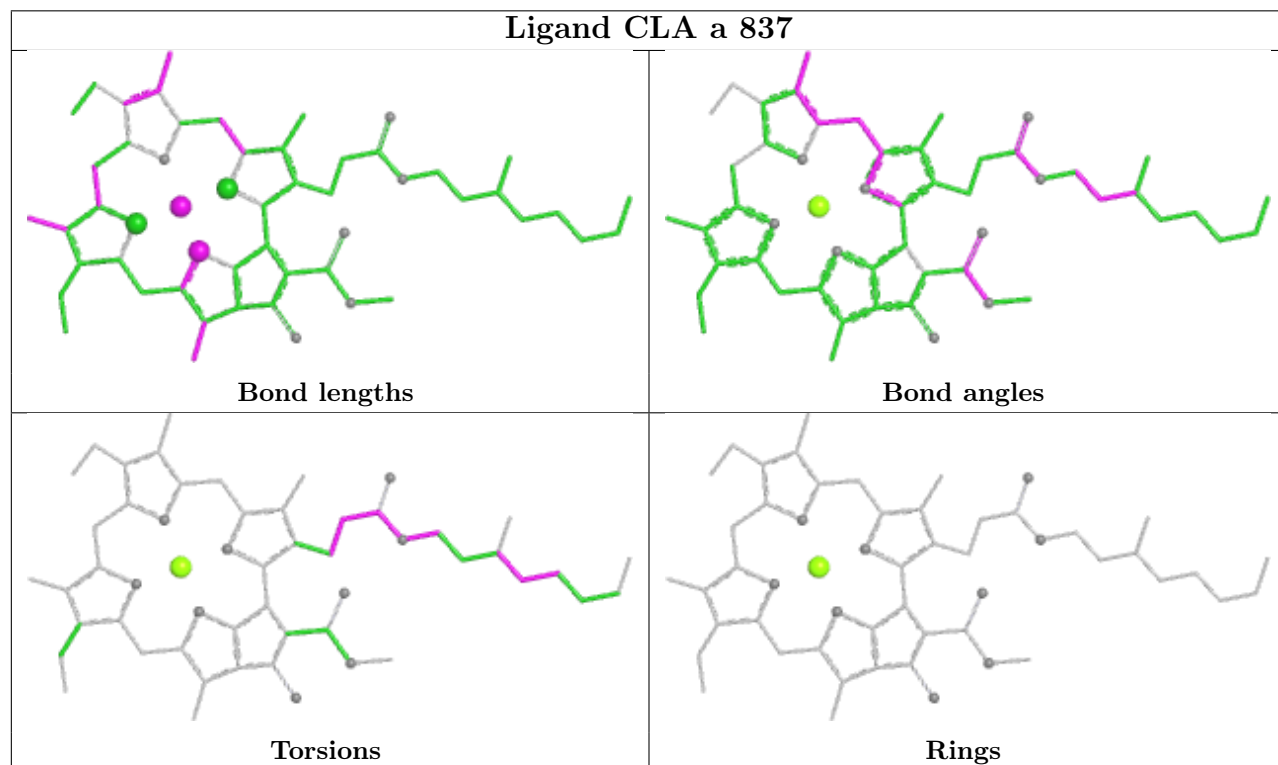
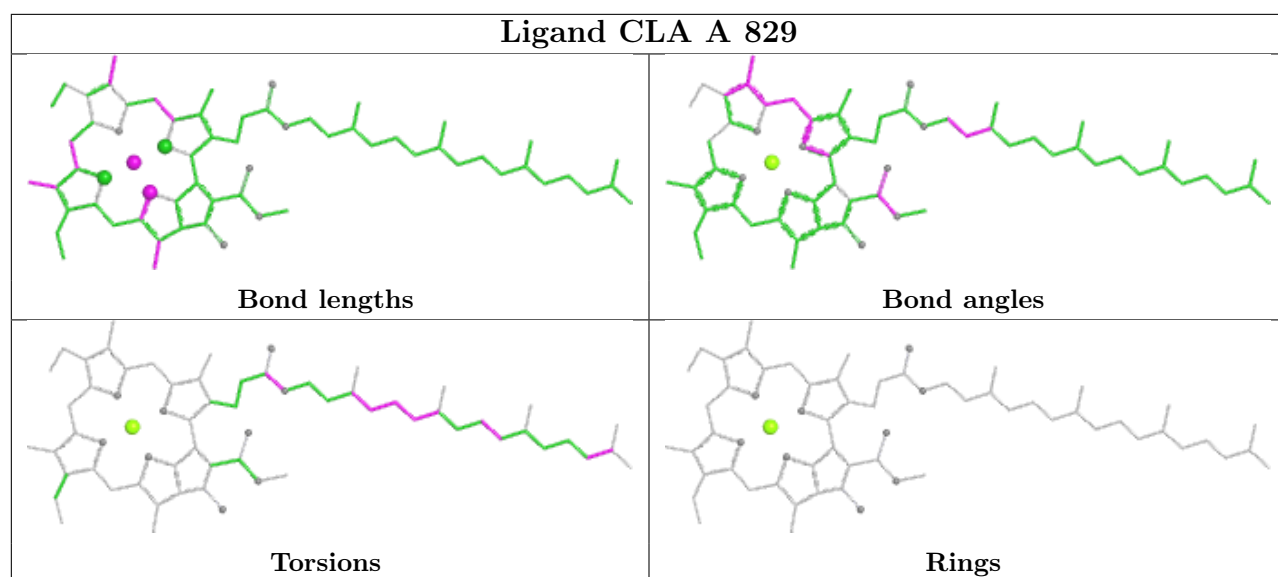
Rings

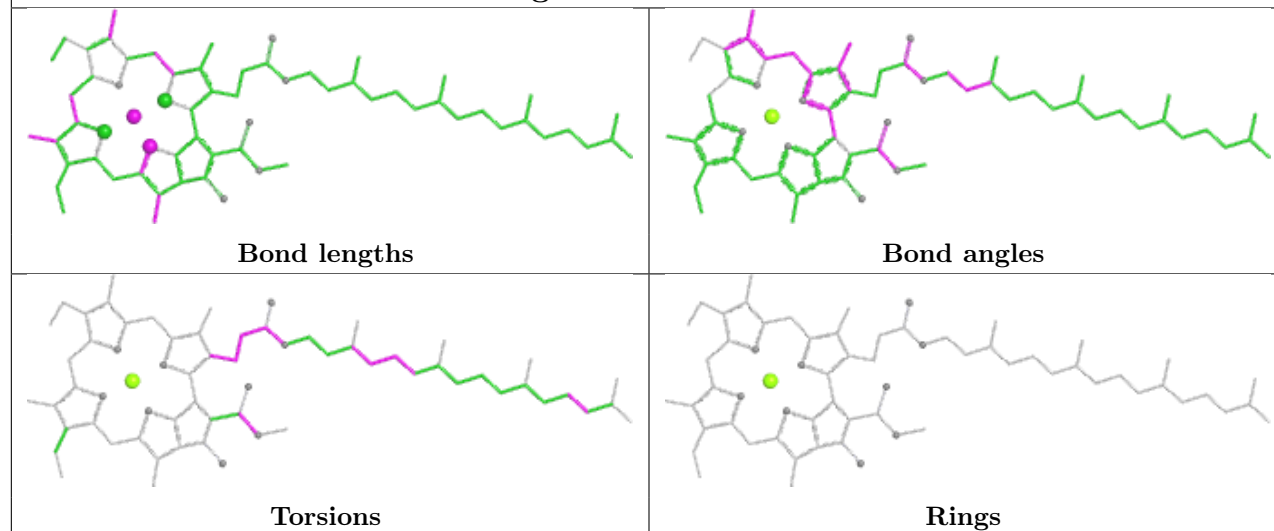
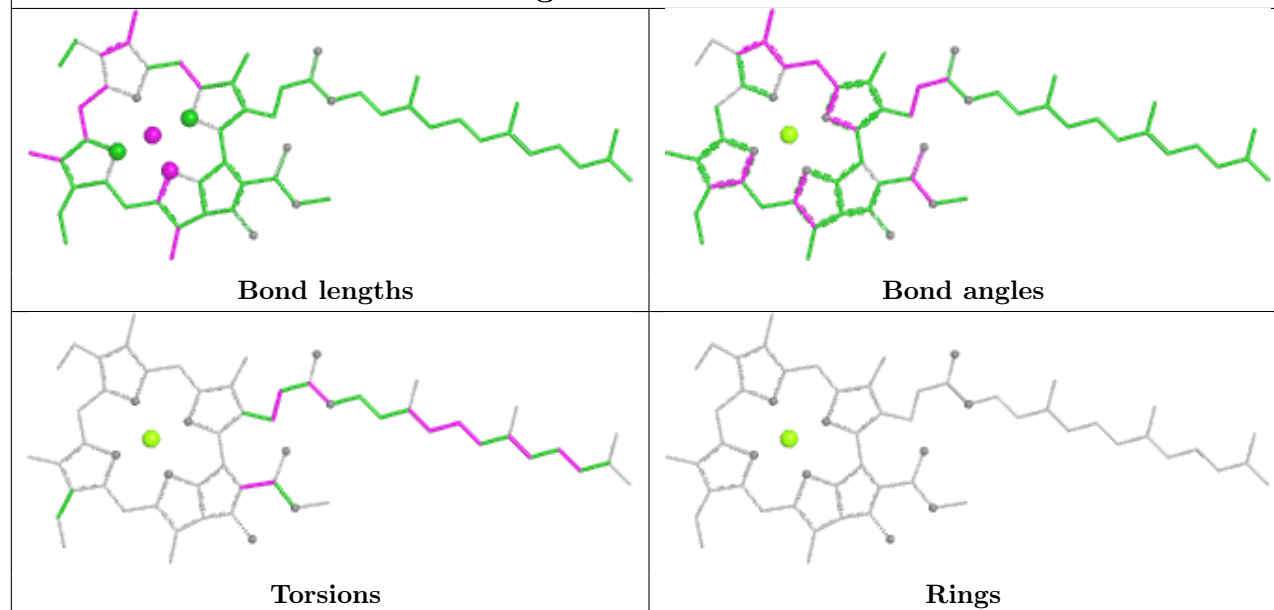
Ligand CLA a 816

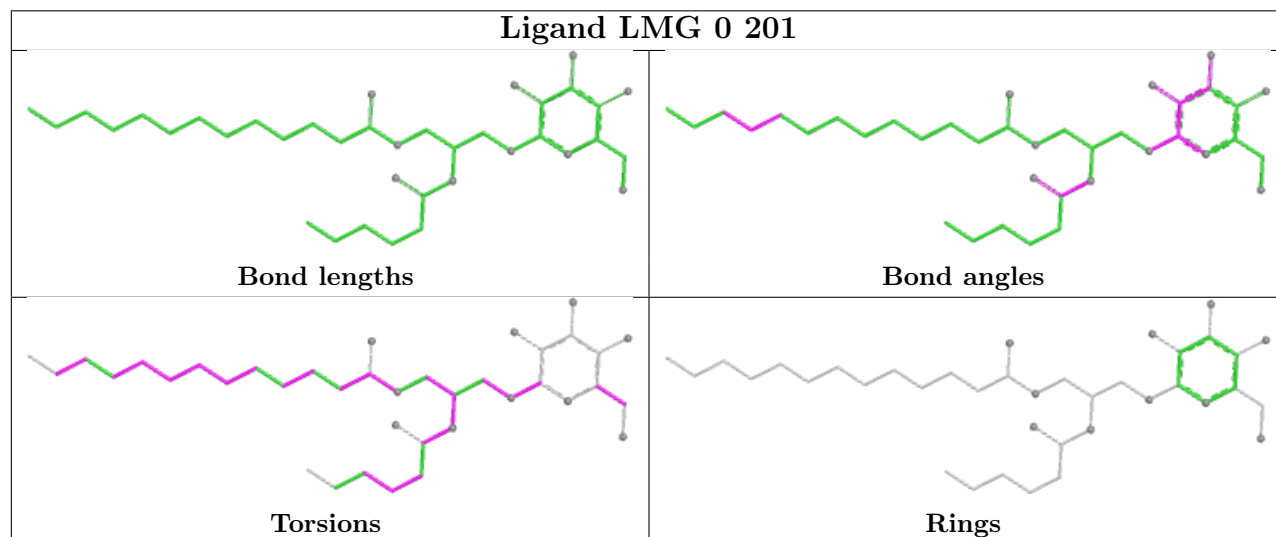
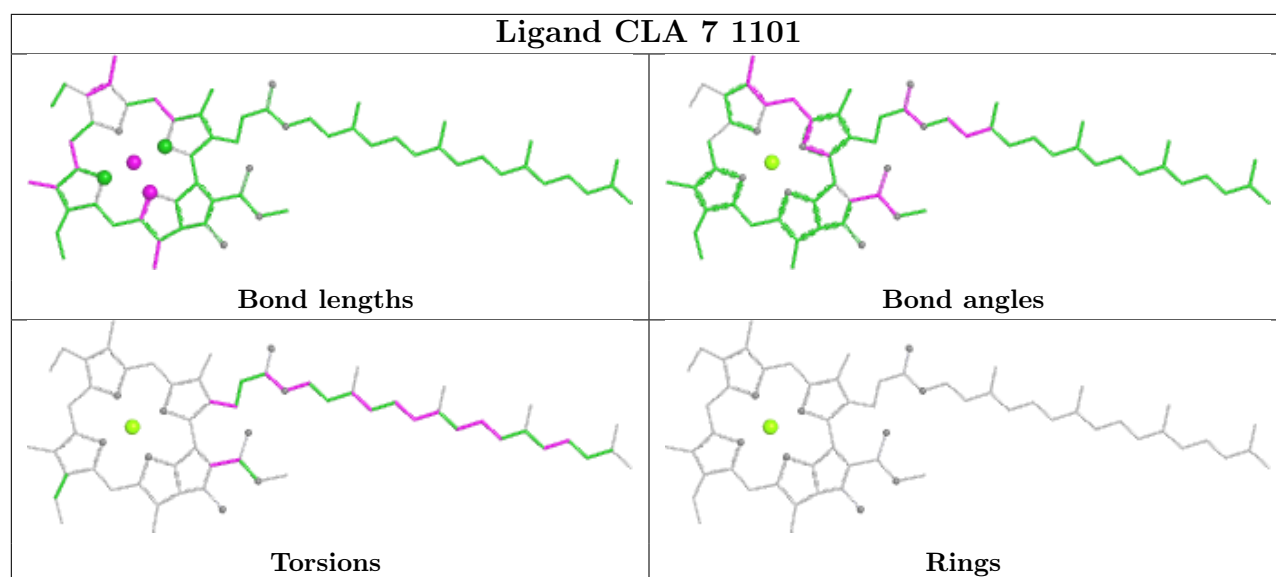


Ligand CLA f 201

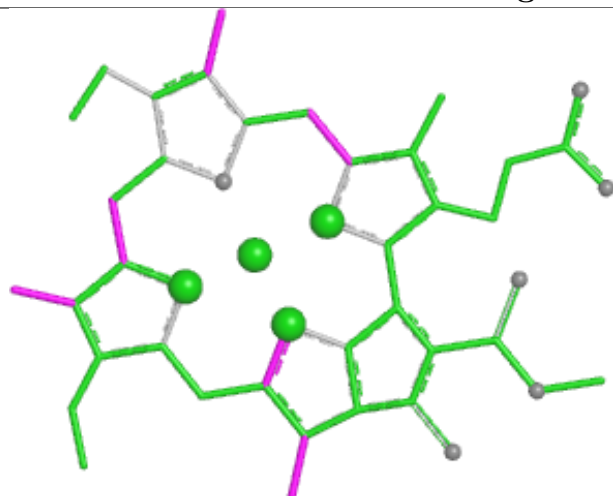




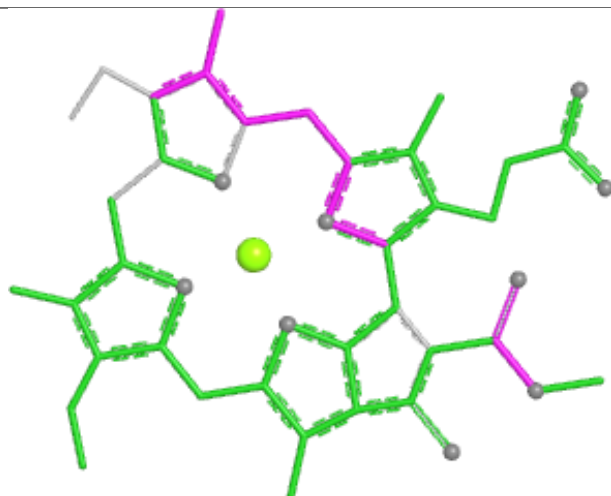
Ligand CLA A 823**Ligand CLA 2 831**



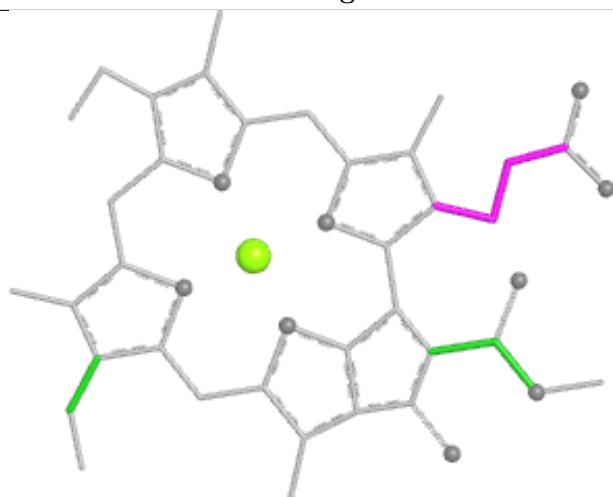
Ligand CLA b 822



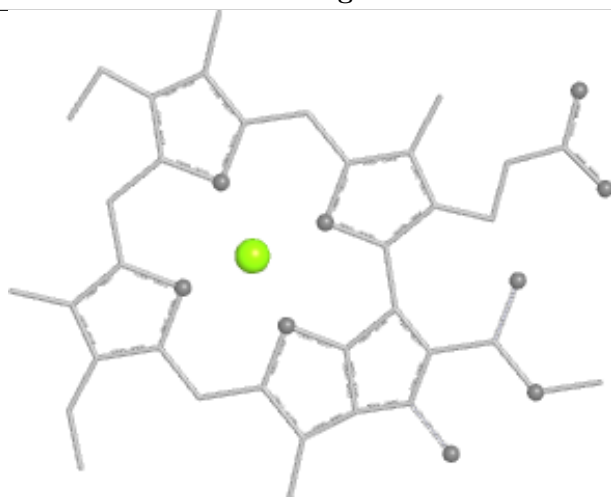
Bond lengths



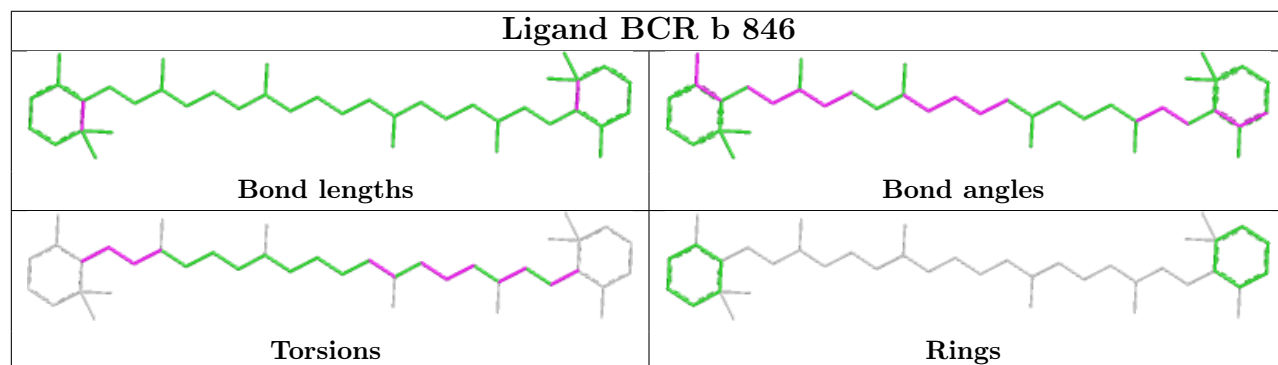
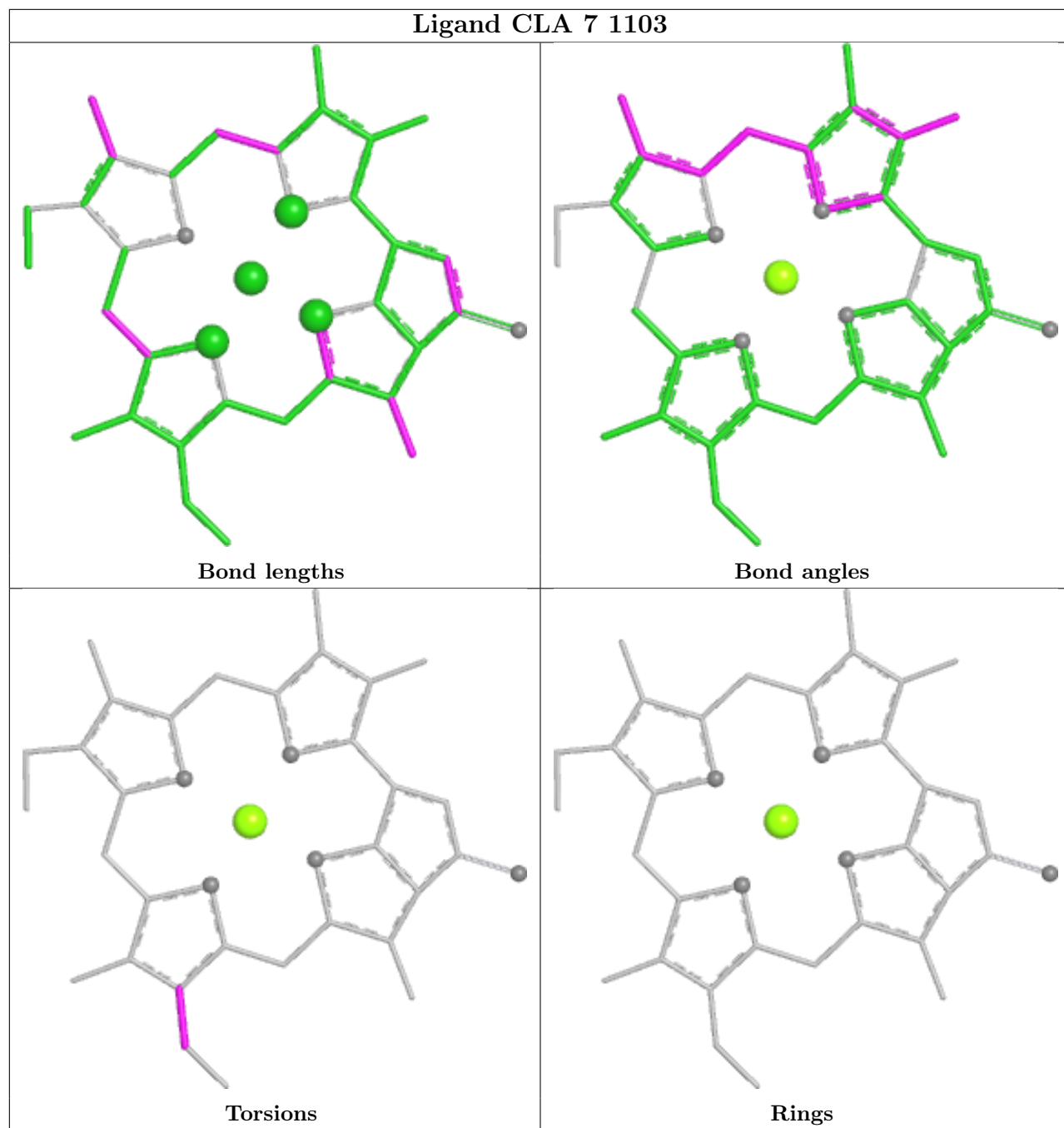
Bond angles



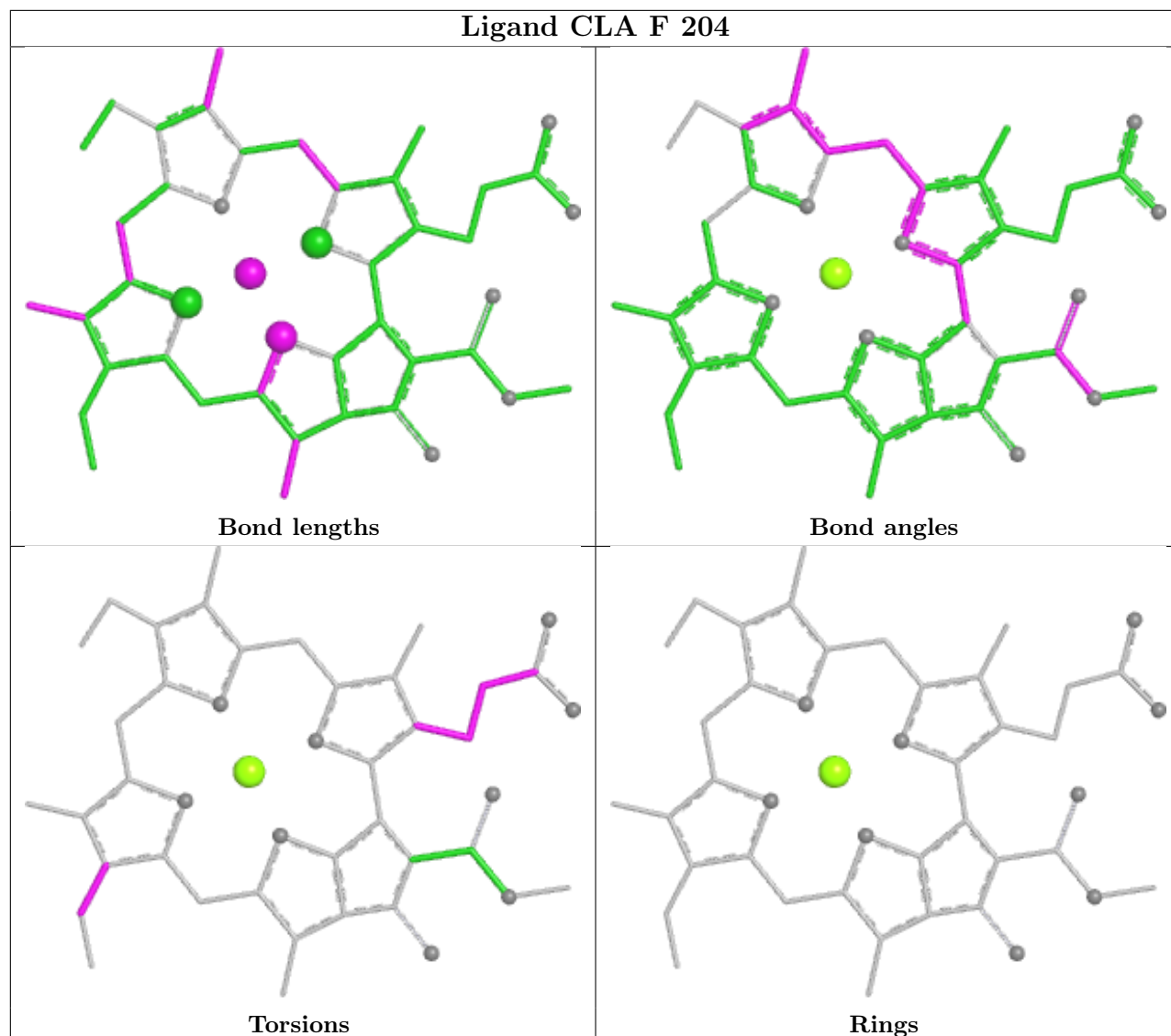
Torsions



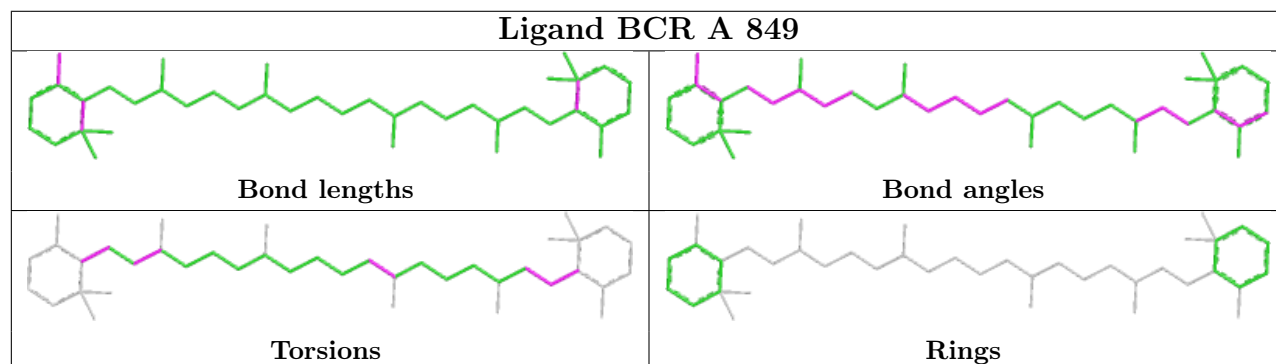
Rings

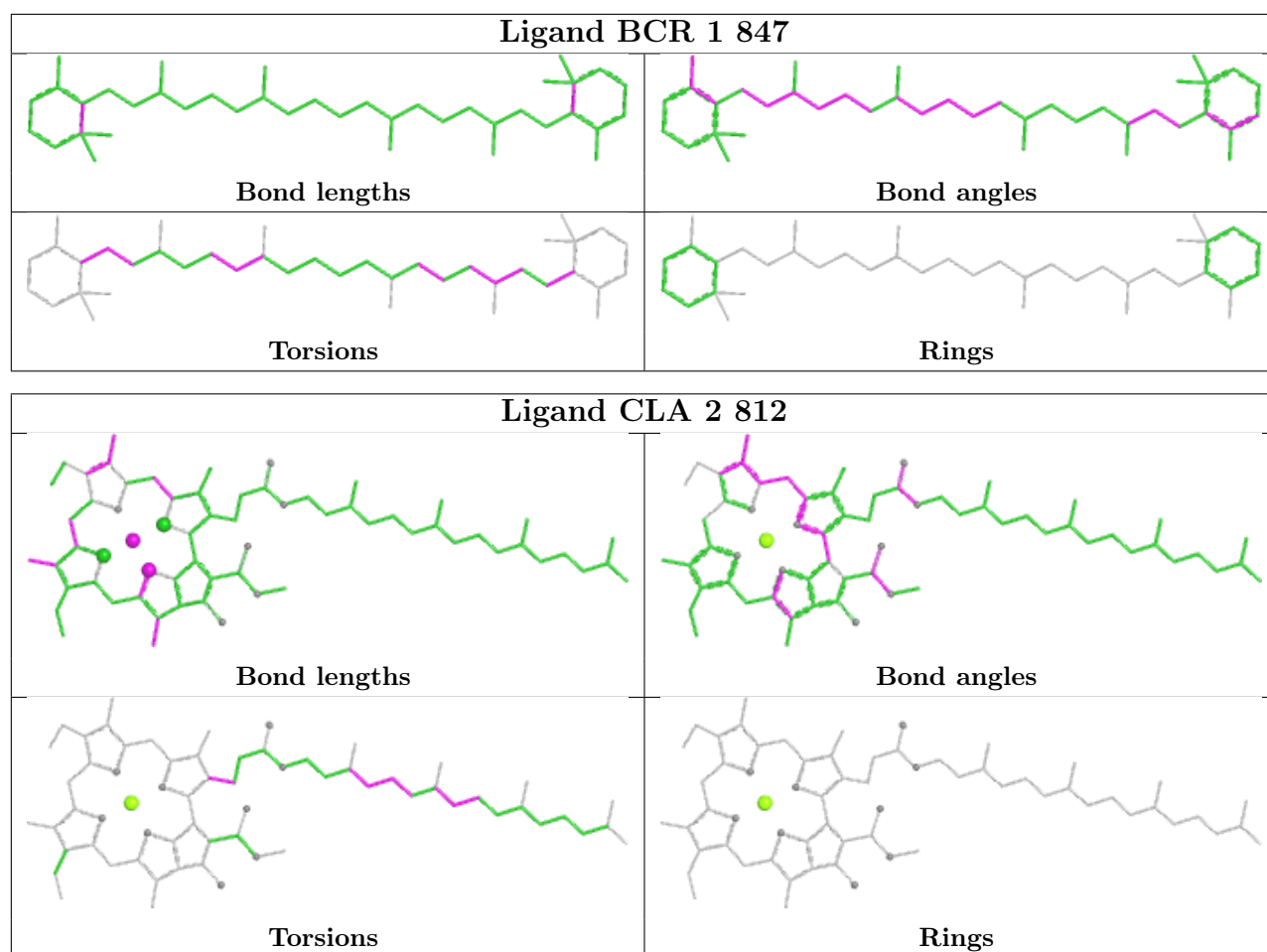


Ligand CLA F 204

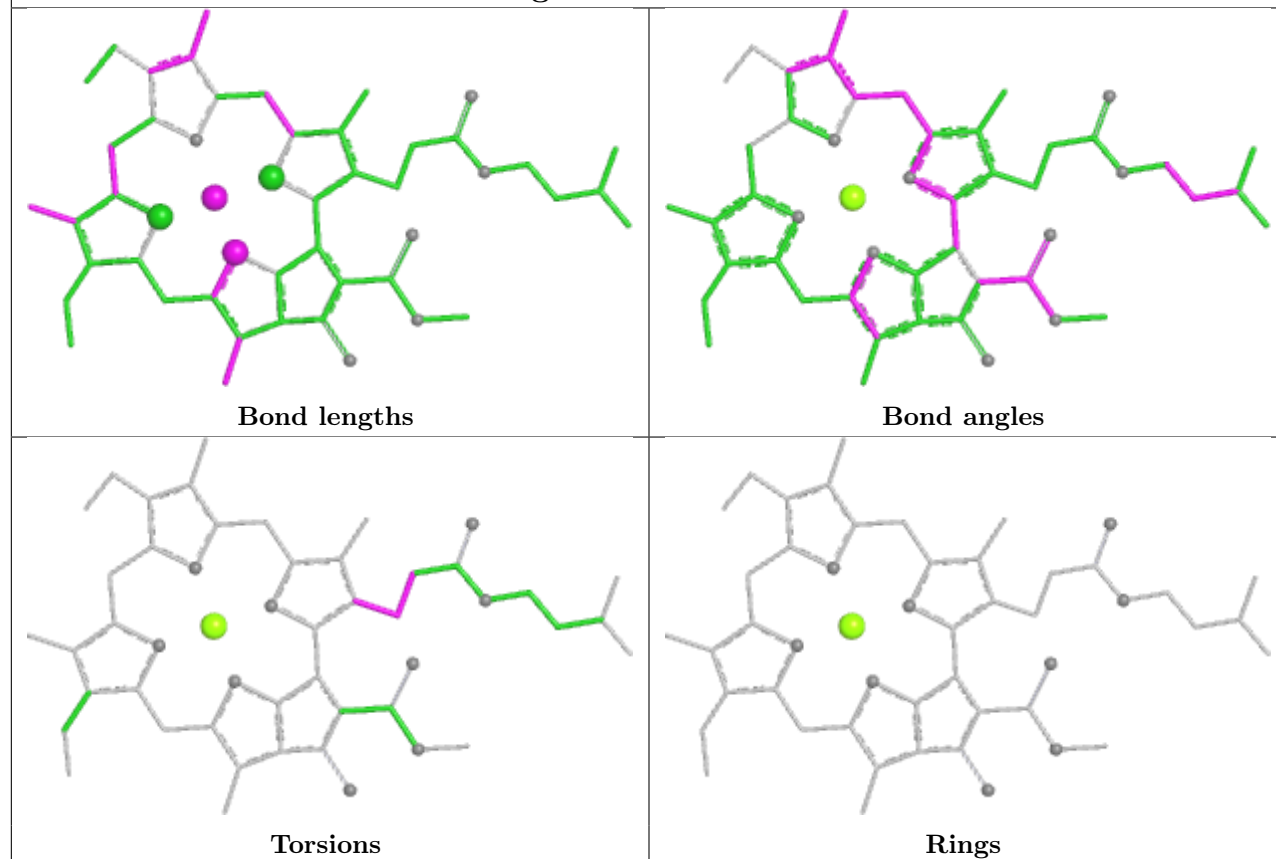


Ligand BCR A 849

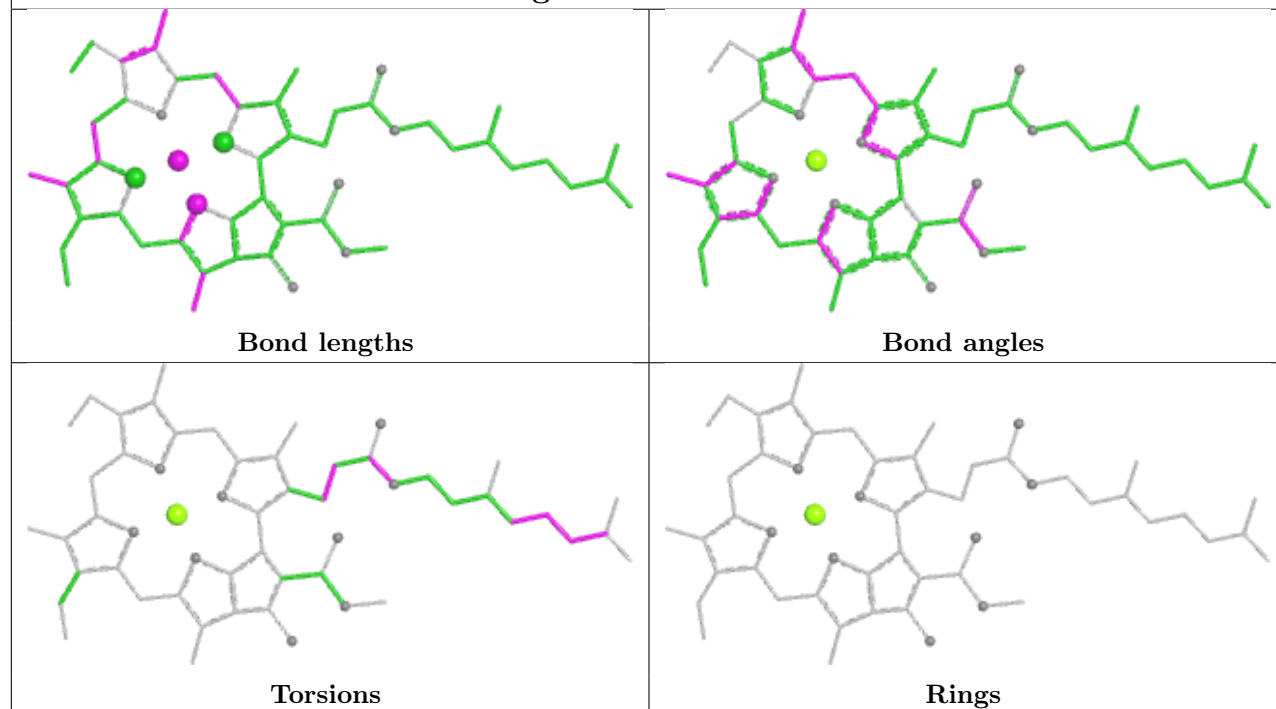


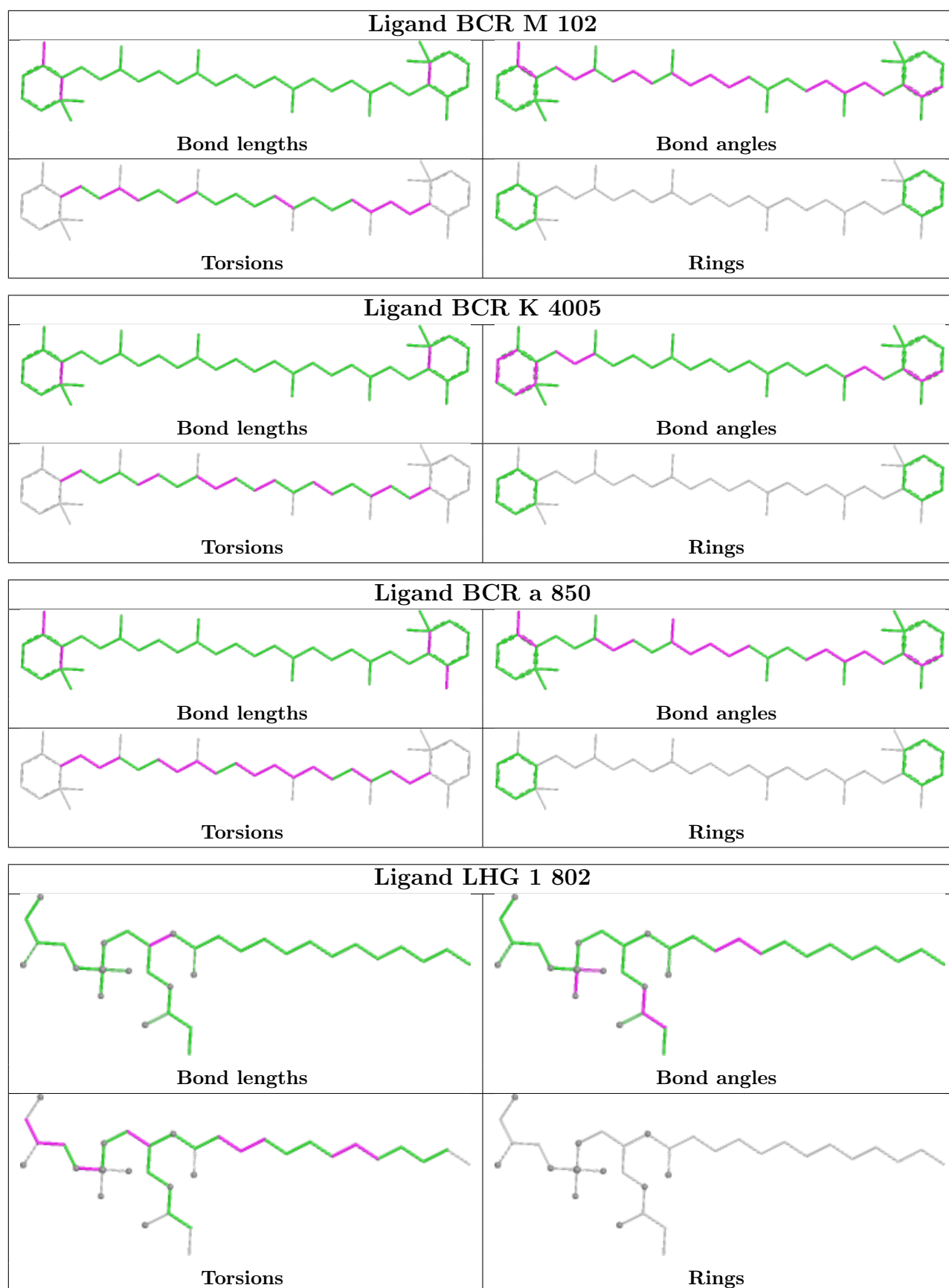


Ligand CLA A 806

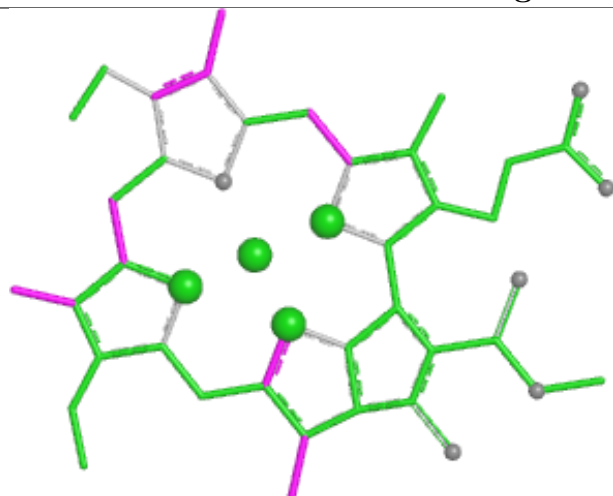


Ligand CLA B 820

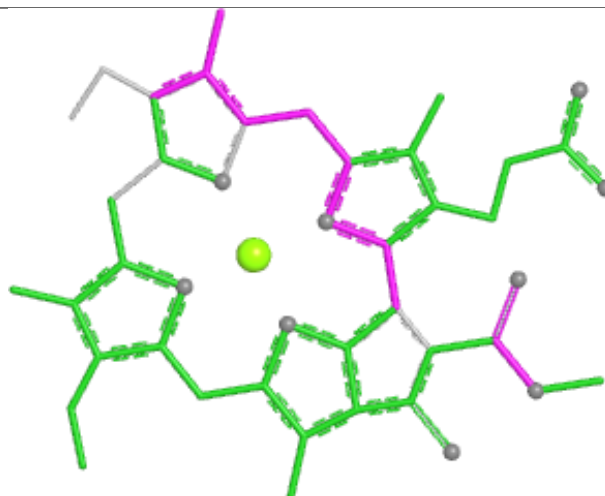




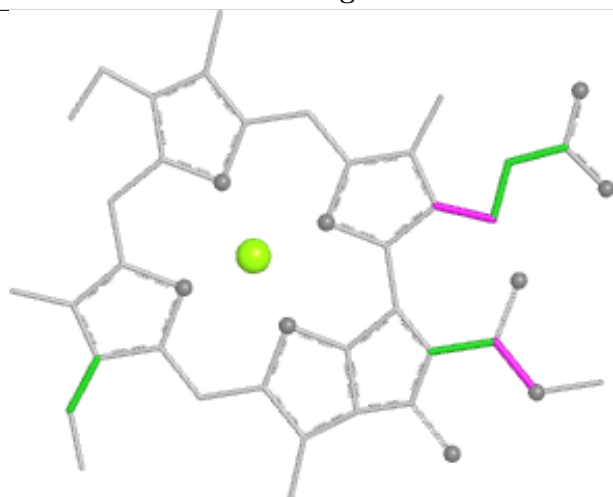
Ligand CLA B 814



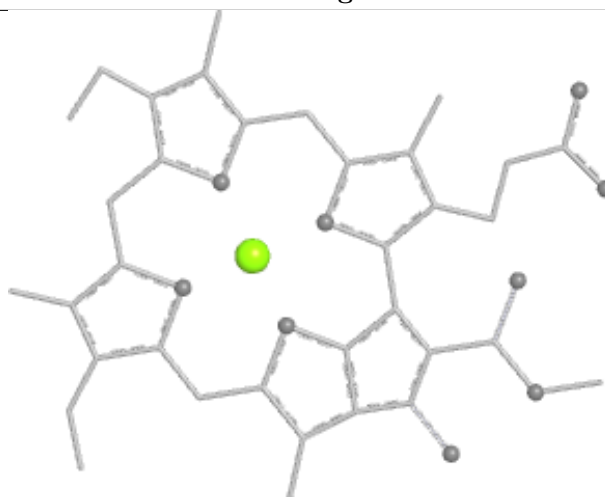
Bond lengths



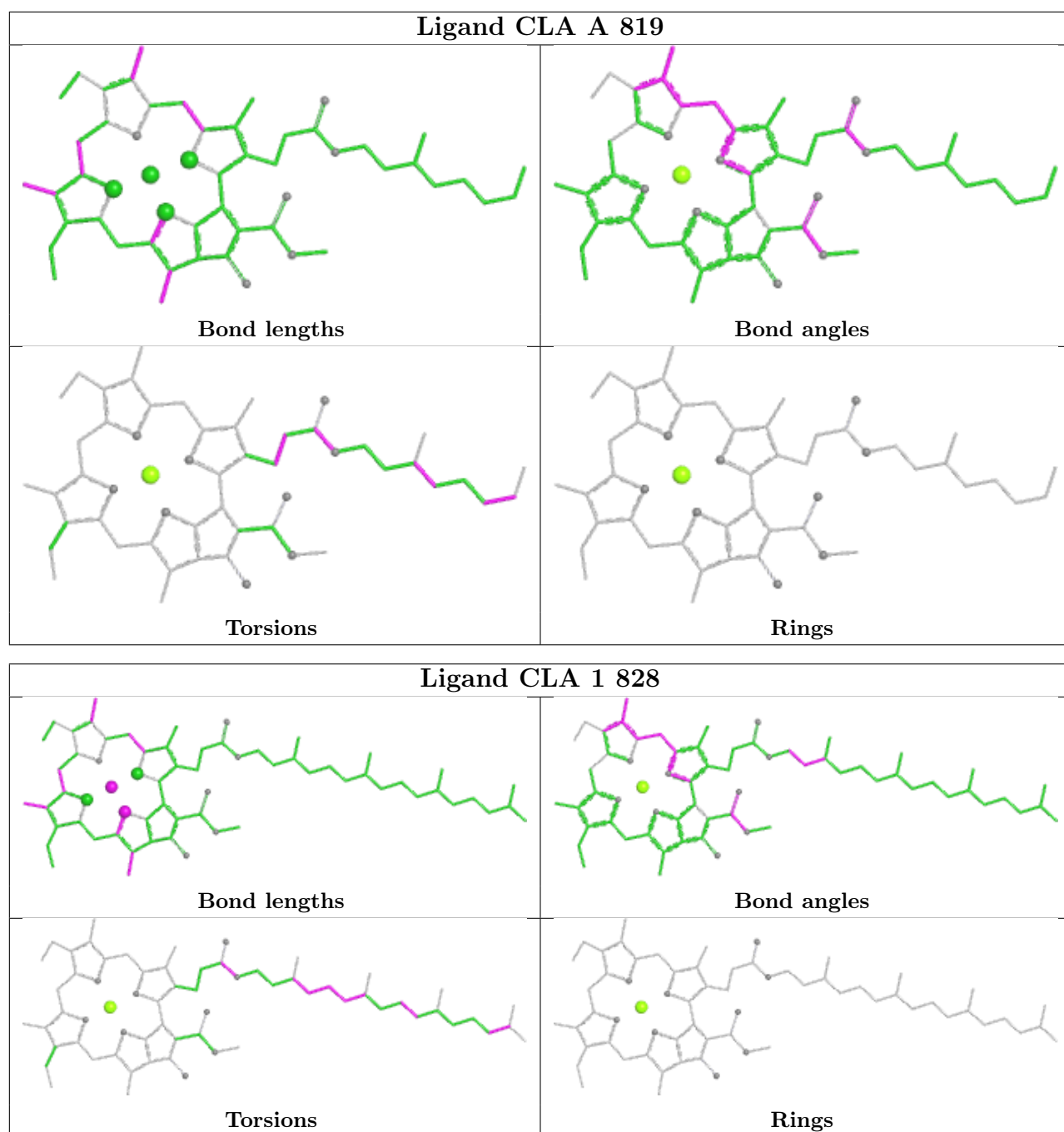
Bond angles

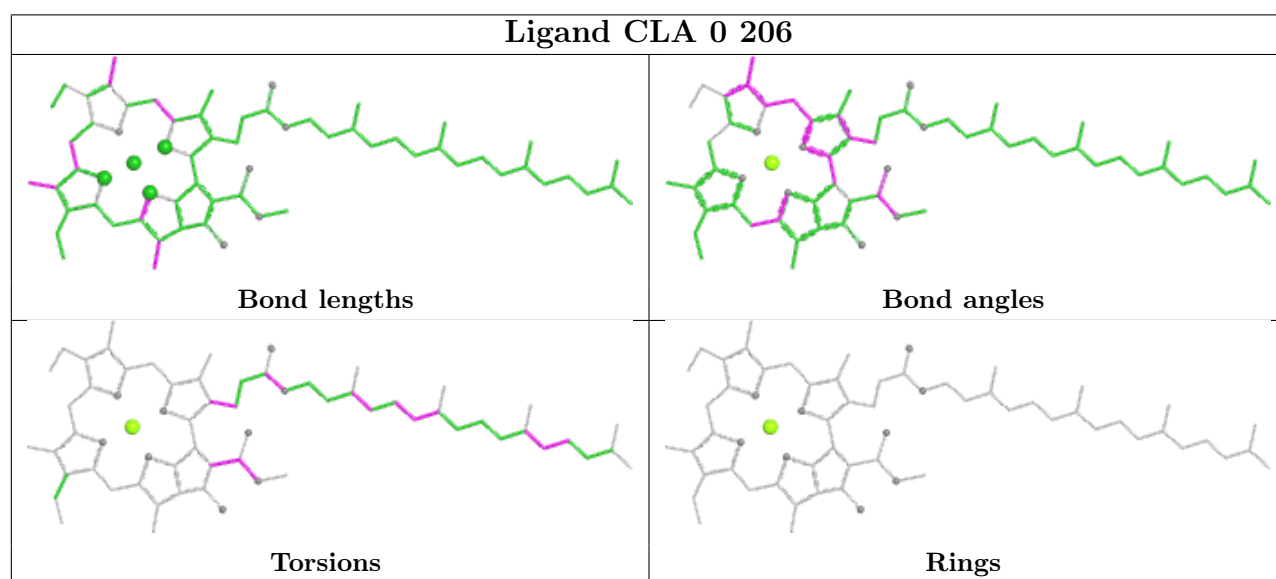
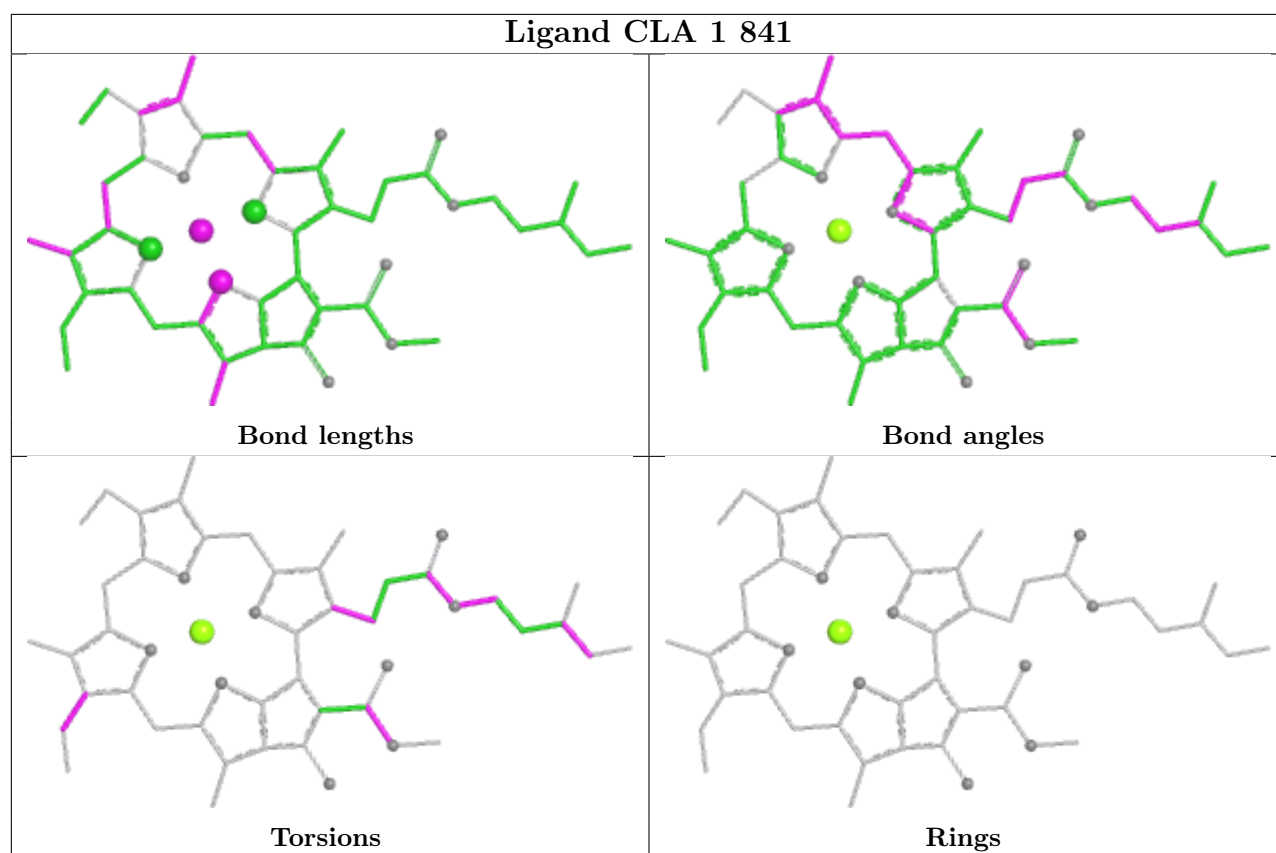


Torsions

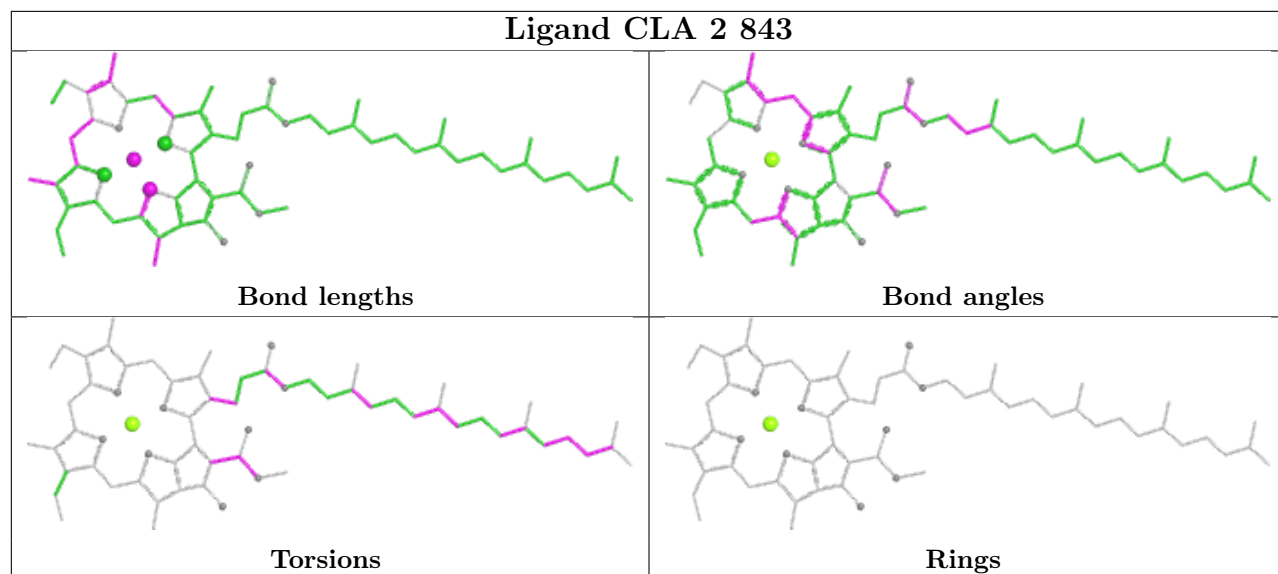


Rings

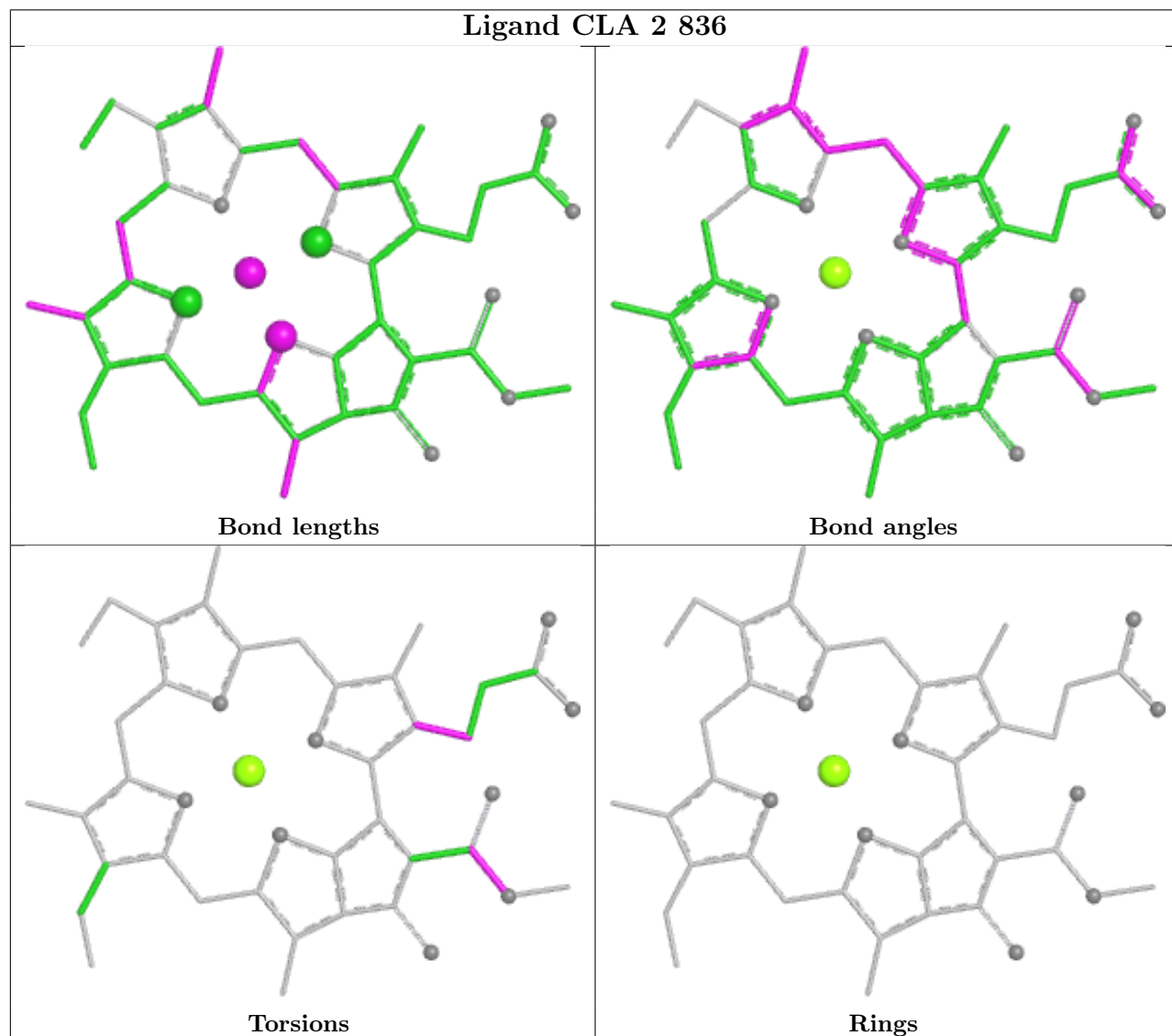


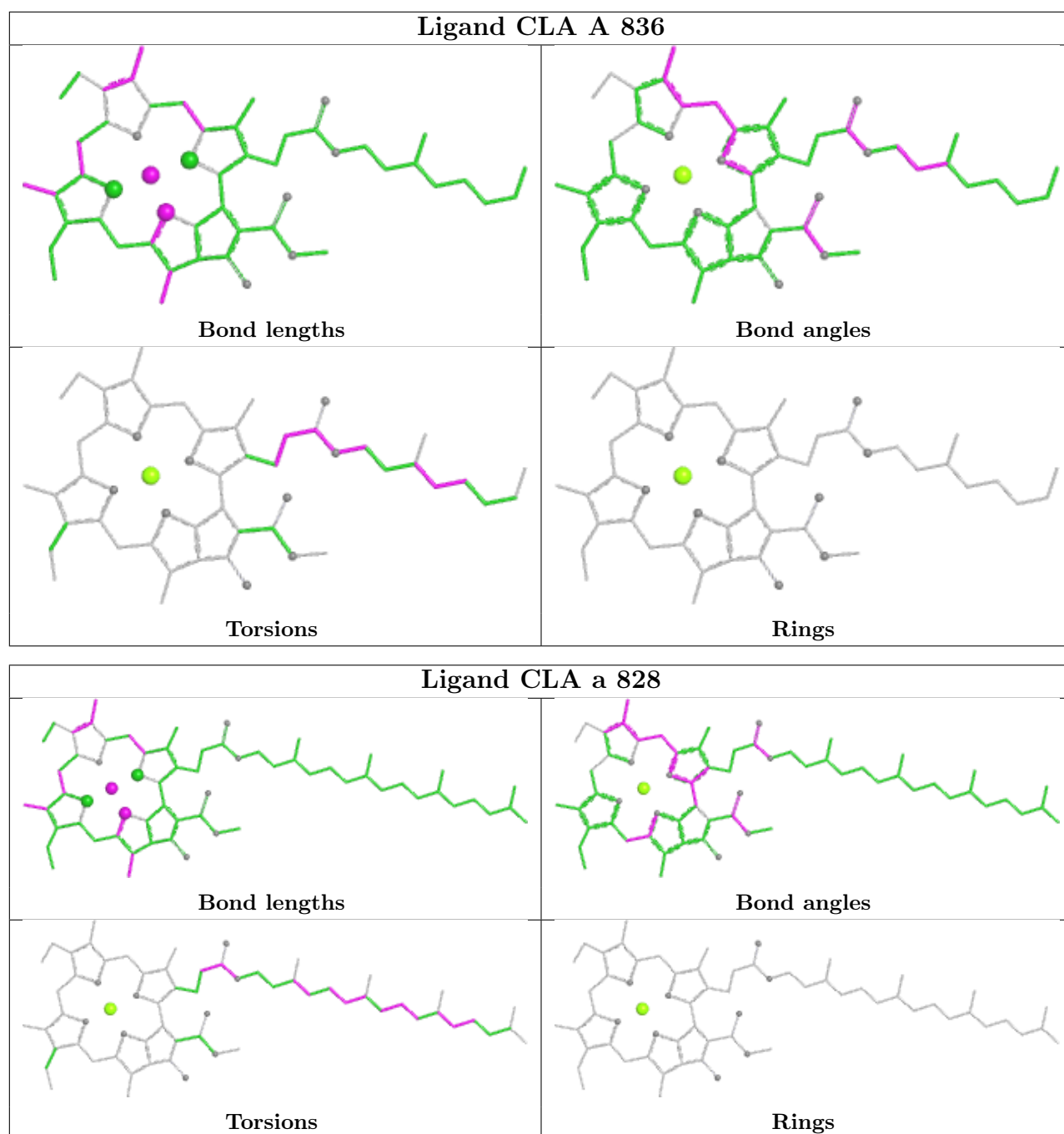


Ligand CLA 2 843

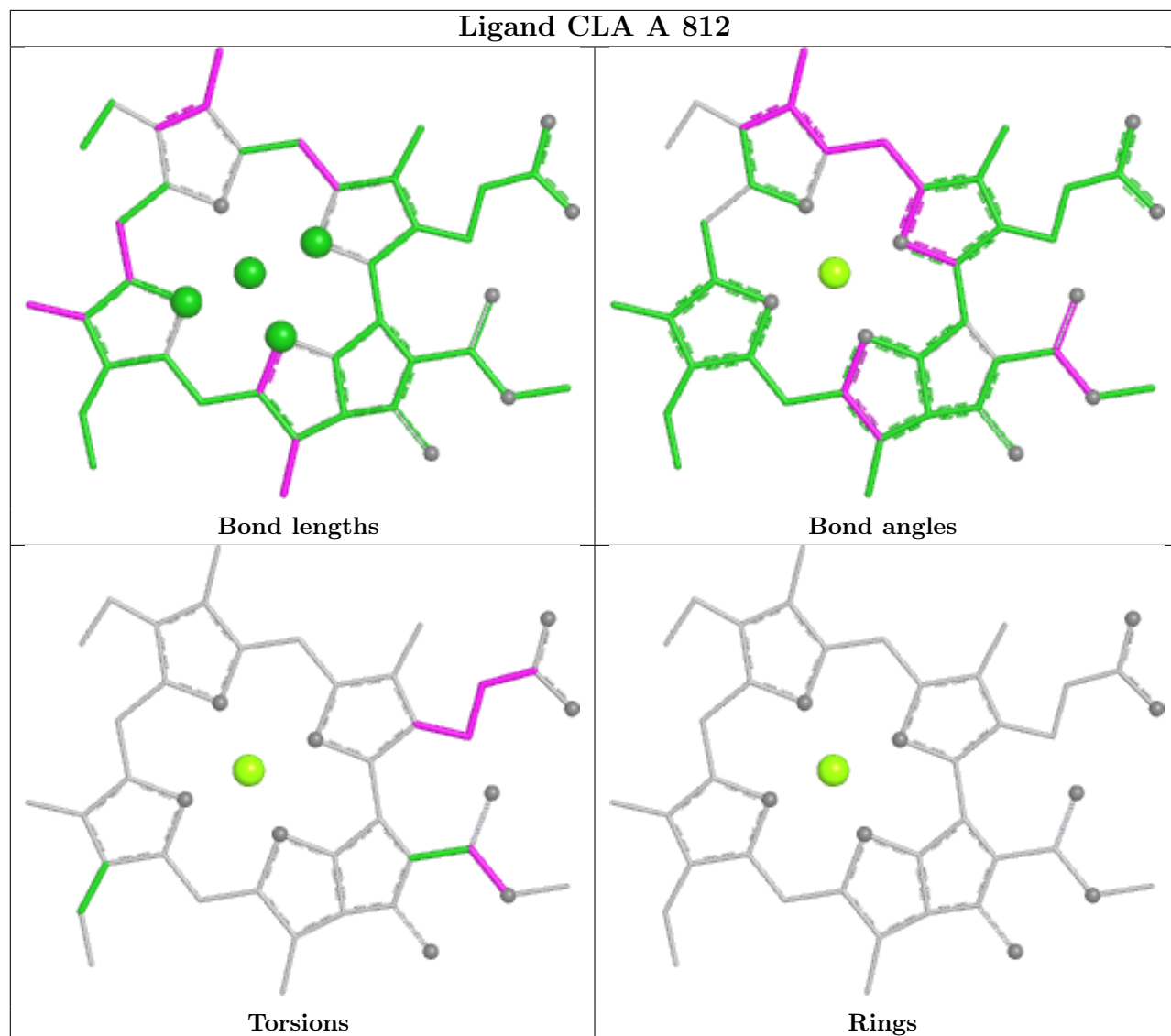


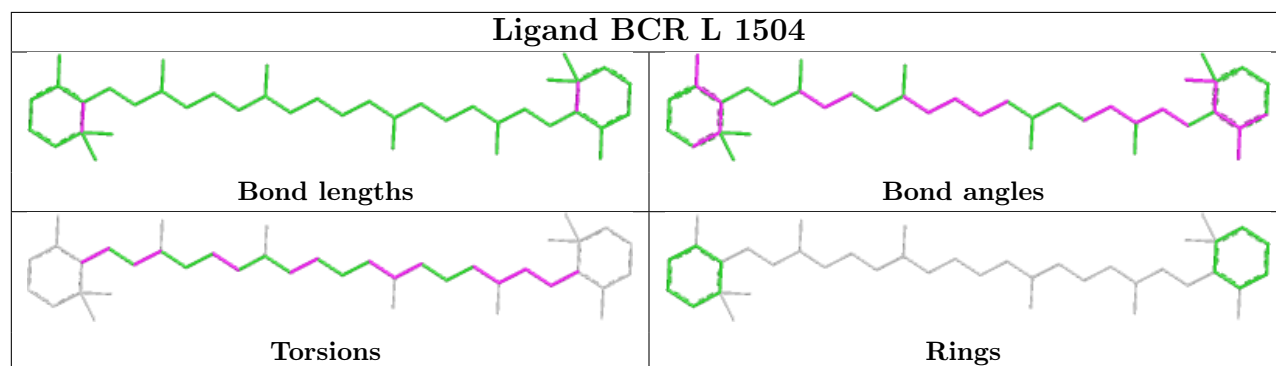
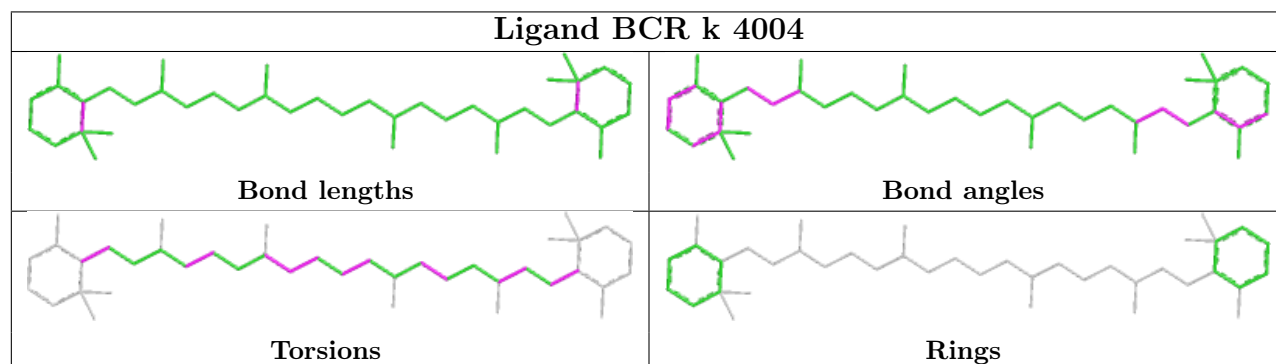
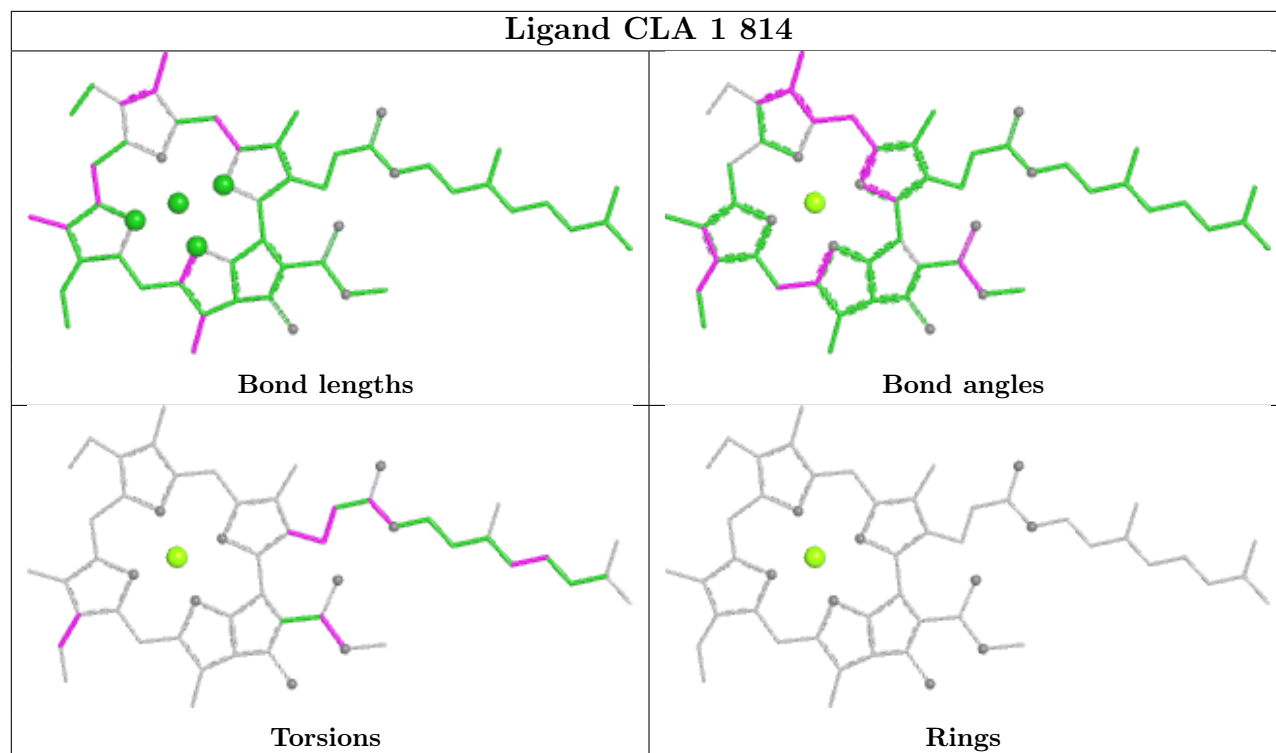
Ligand CLA 2 836



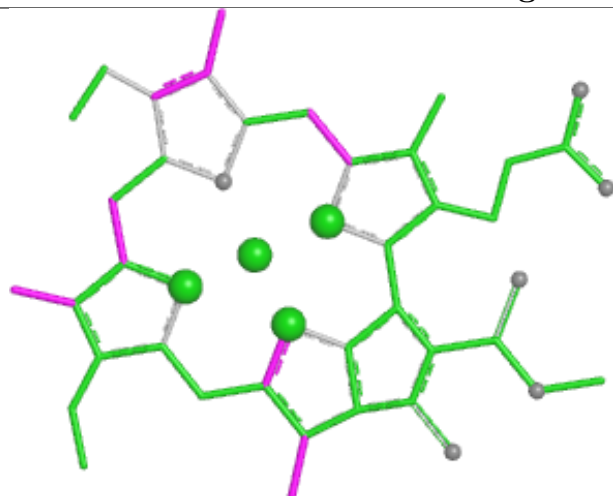


Ligand CLA A 812

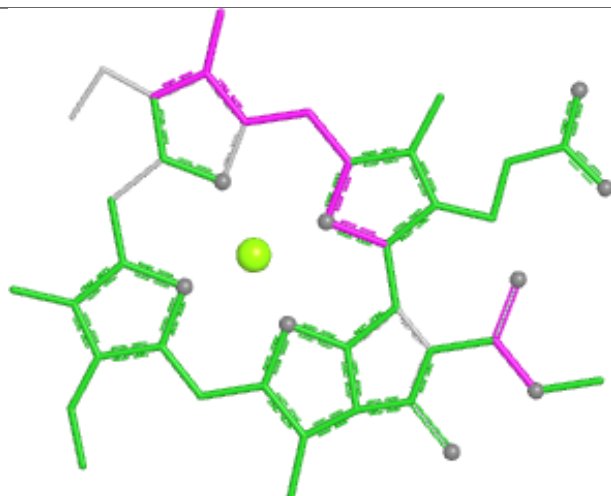




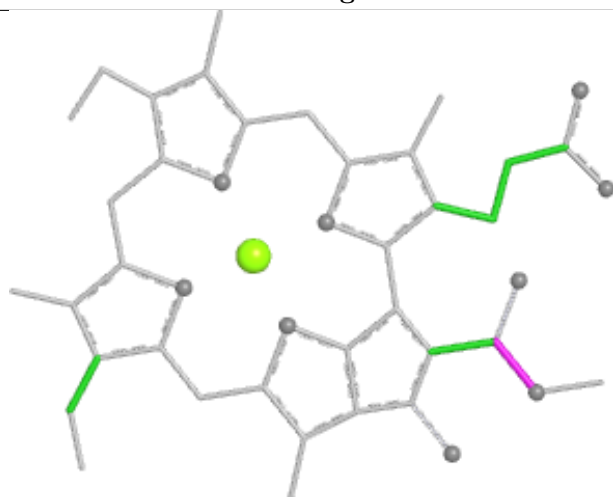
Ligand CLA 1 816



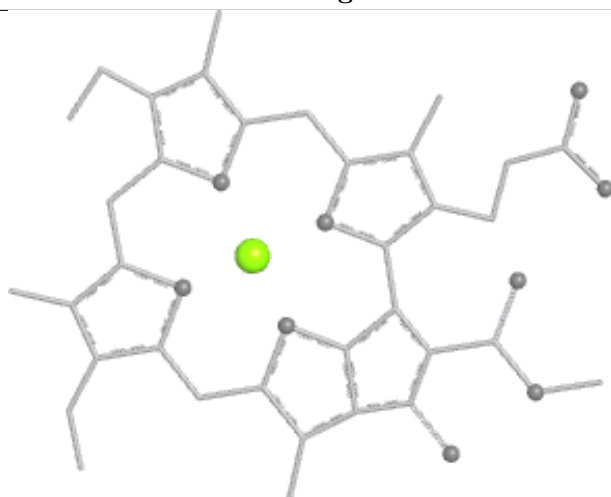
Bond lengths



Bond angles

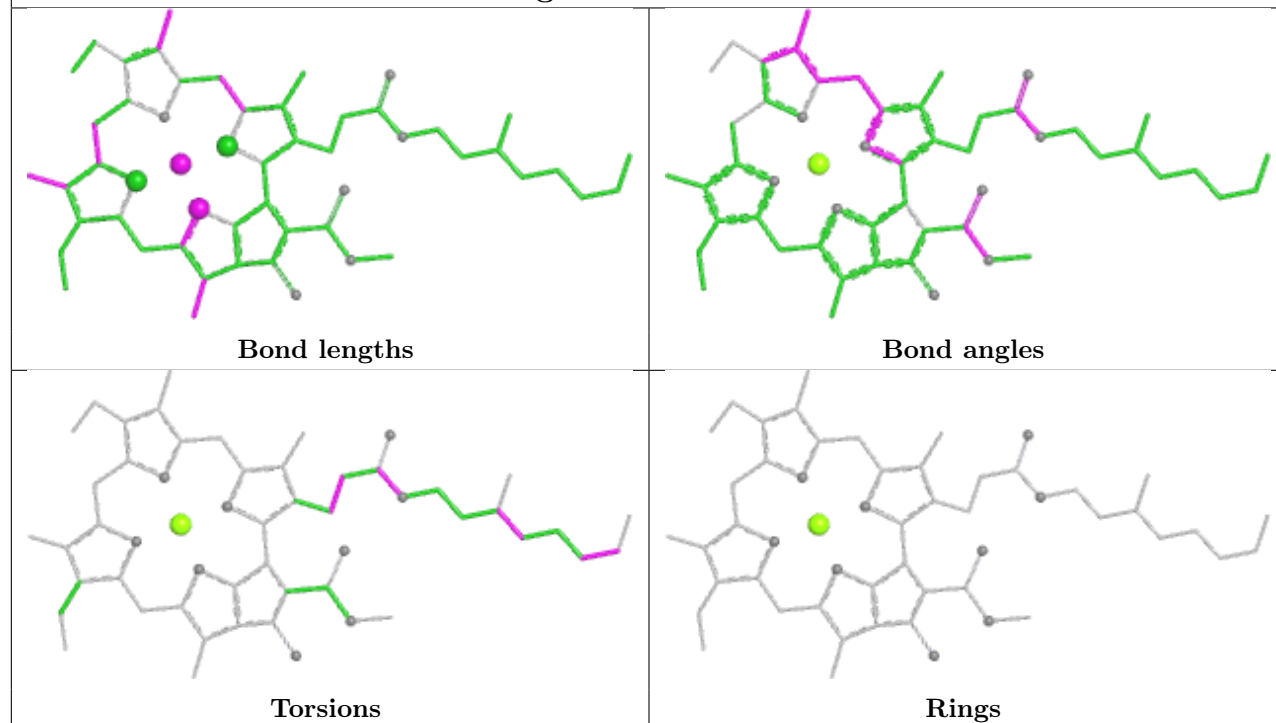


Torsions

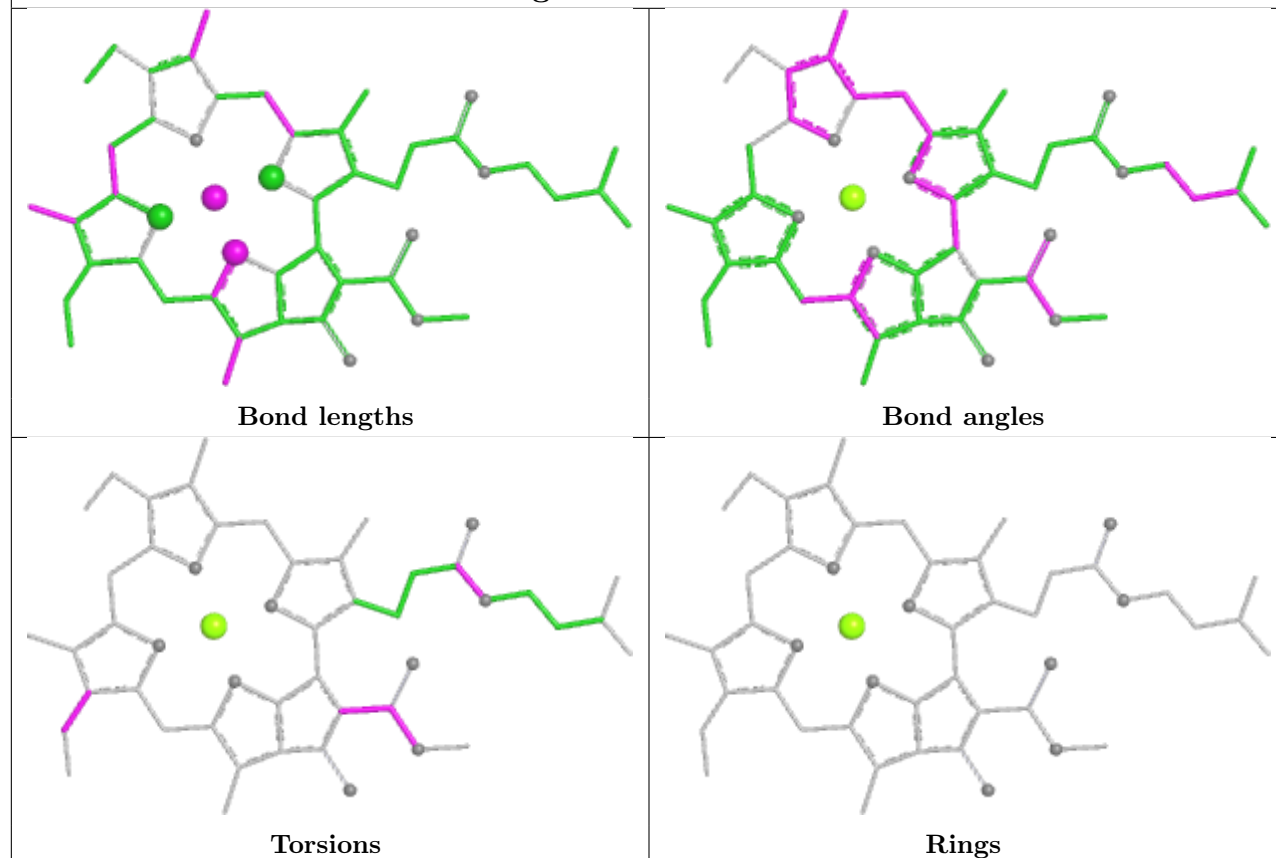


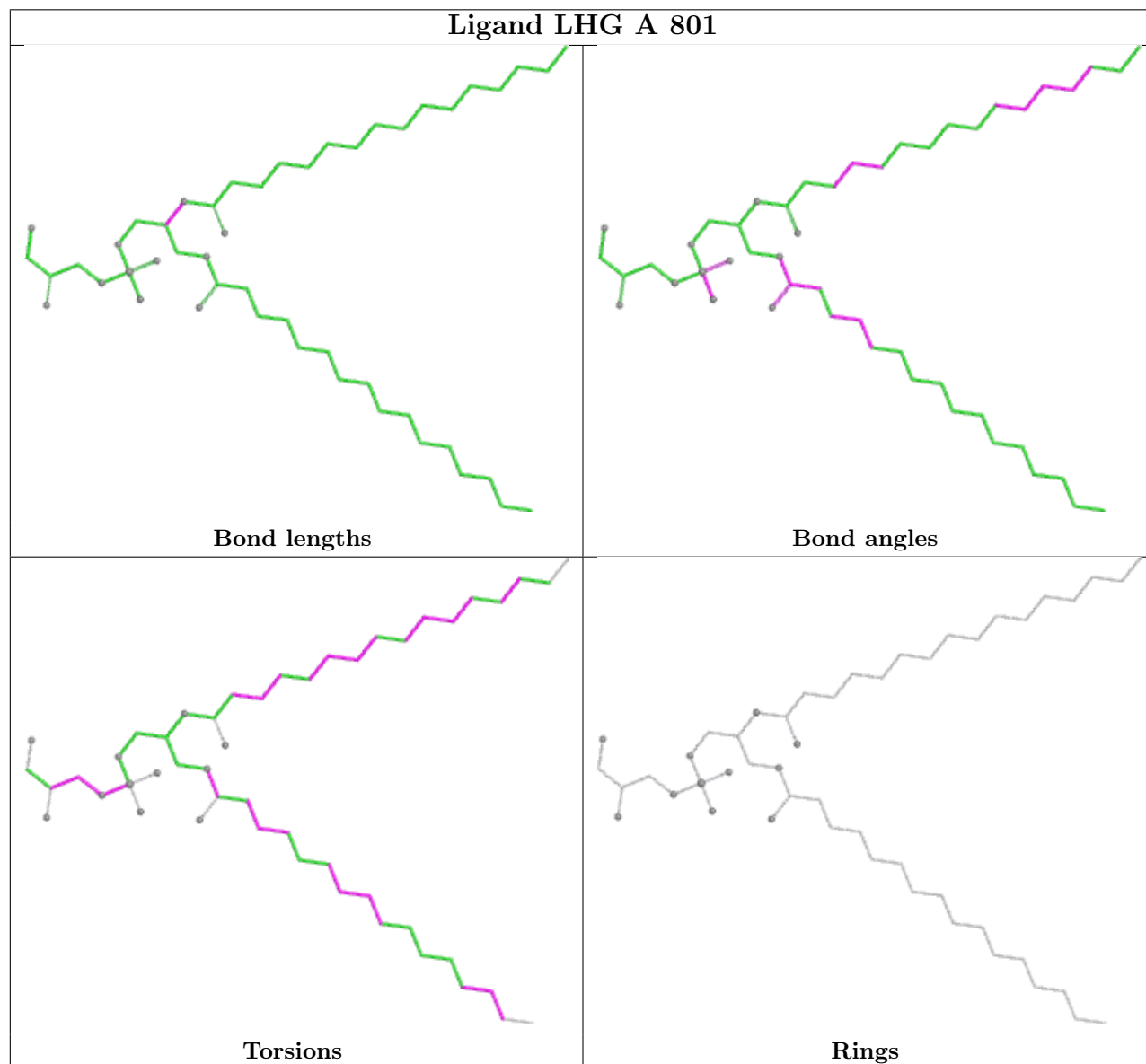
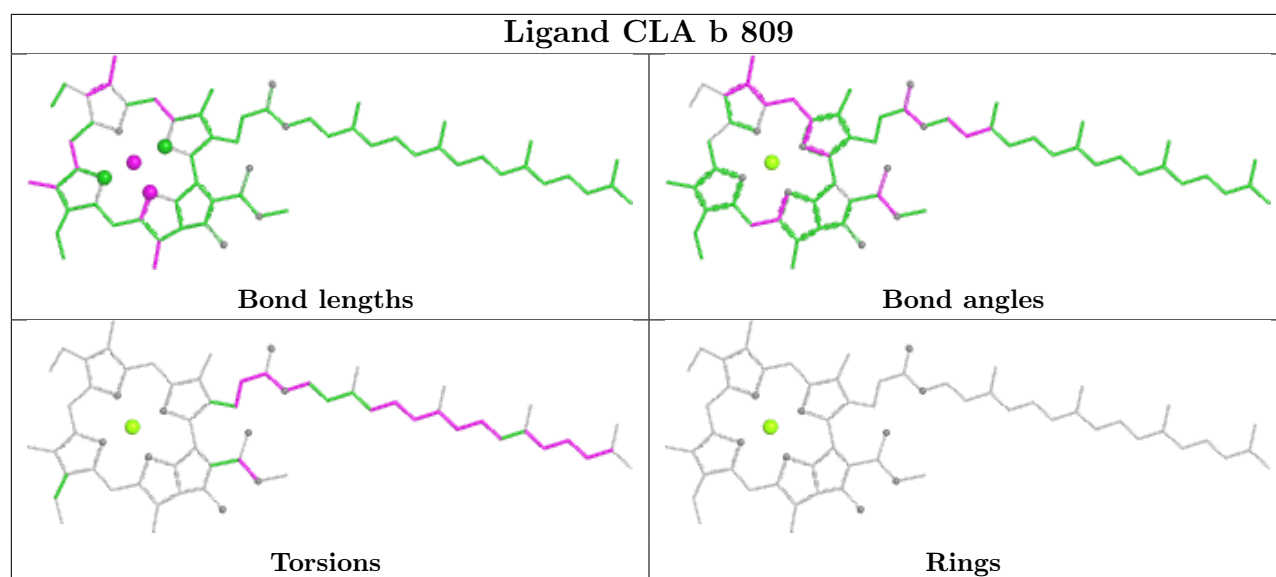
Rings

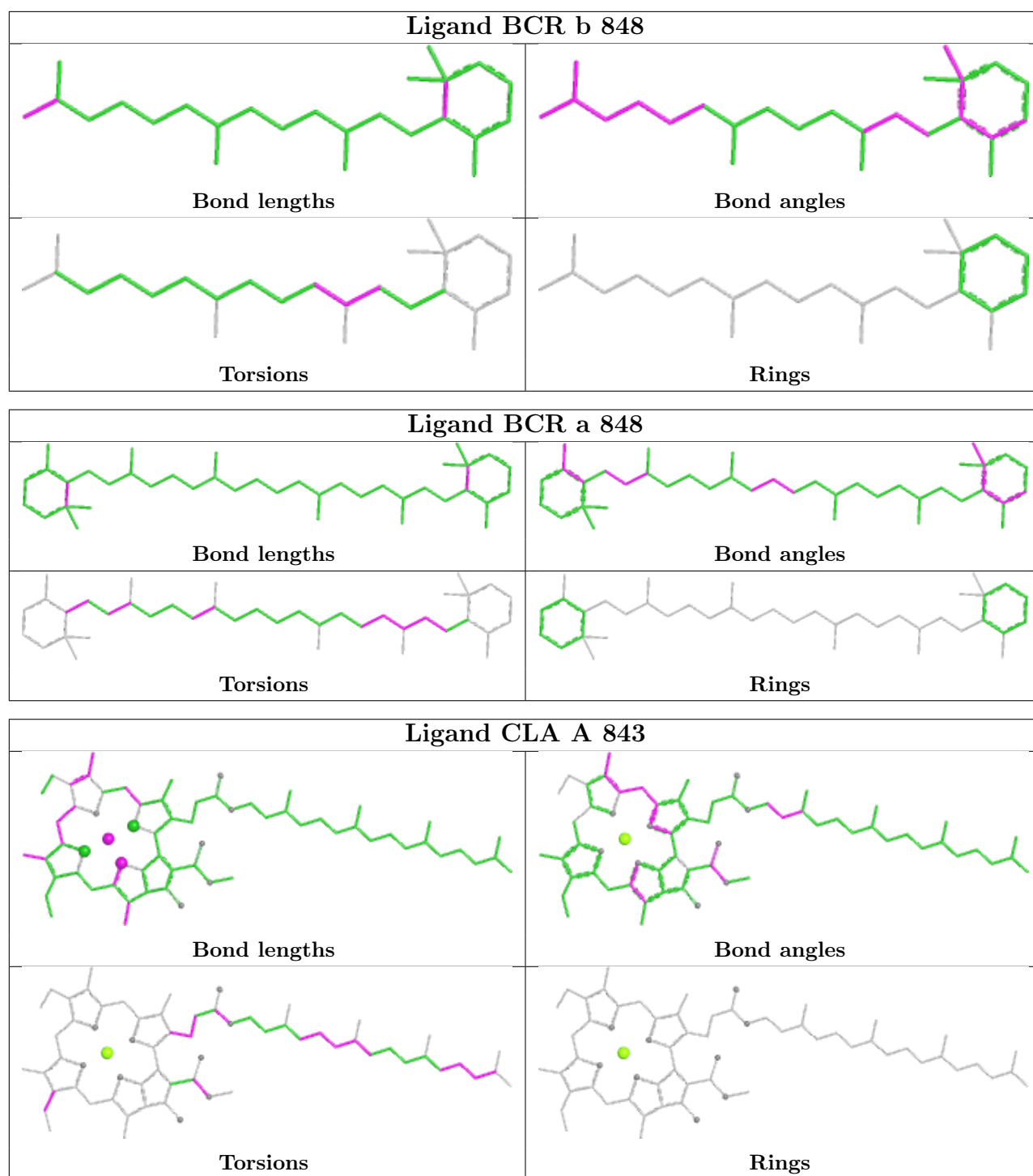
Ligand CLA a 820



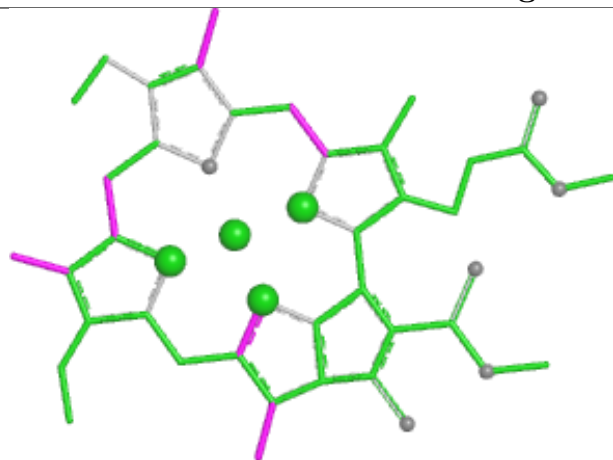
Ligand CLA B 840



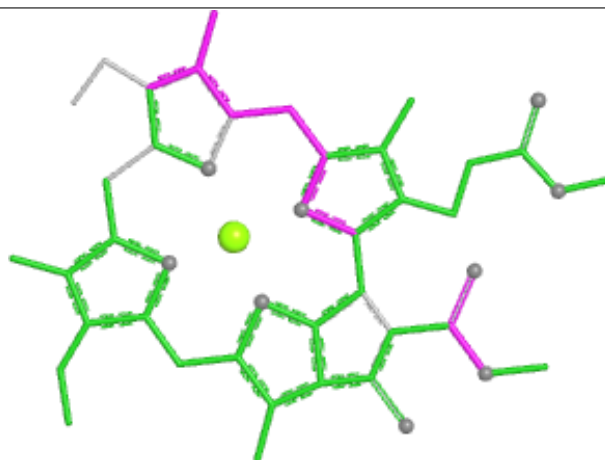




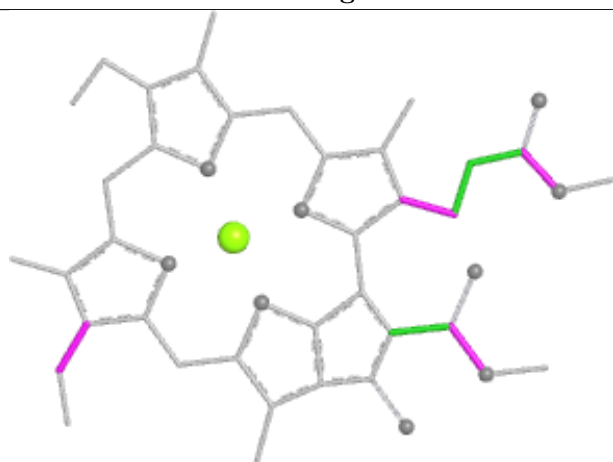
Ligand CLA 2 816



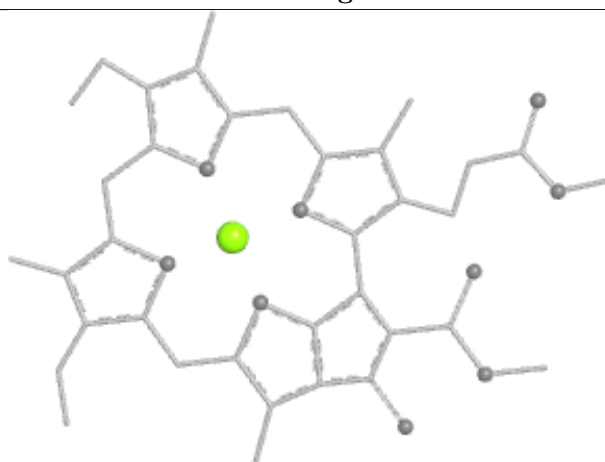
Bond lengths



Bond angles

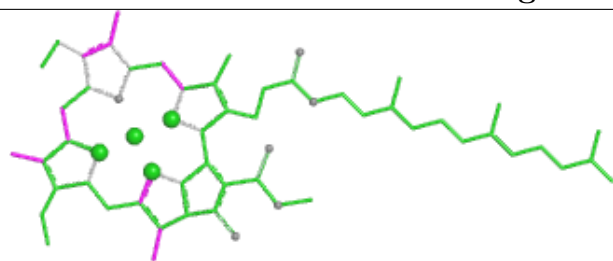


Torsions

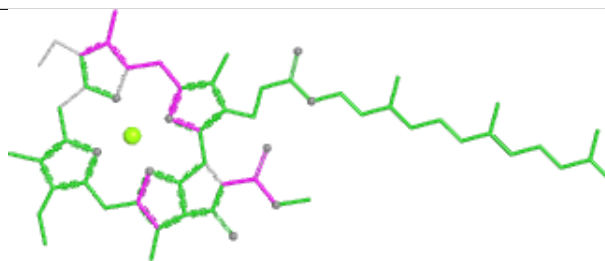


Rings

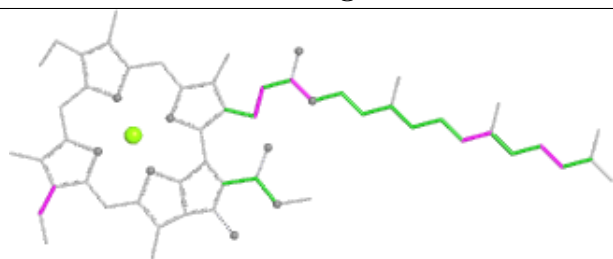
Ligand CLA 2 809



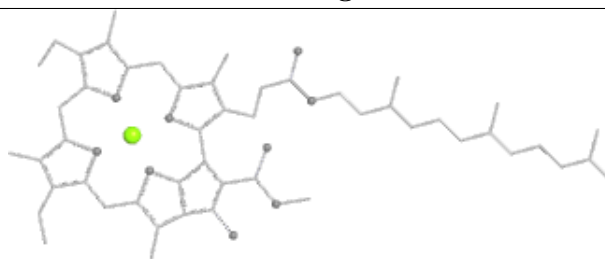
Bond lengths



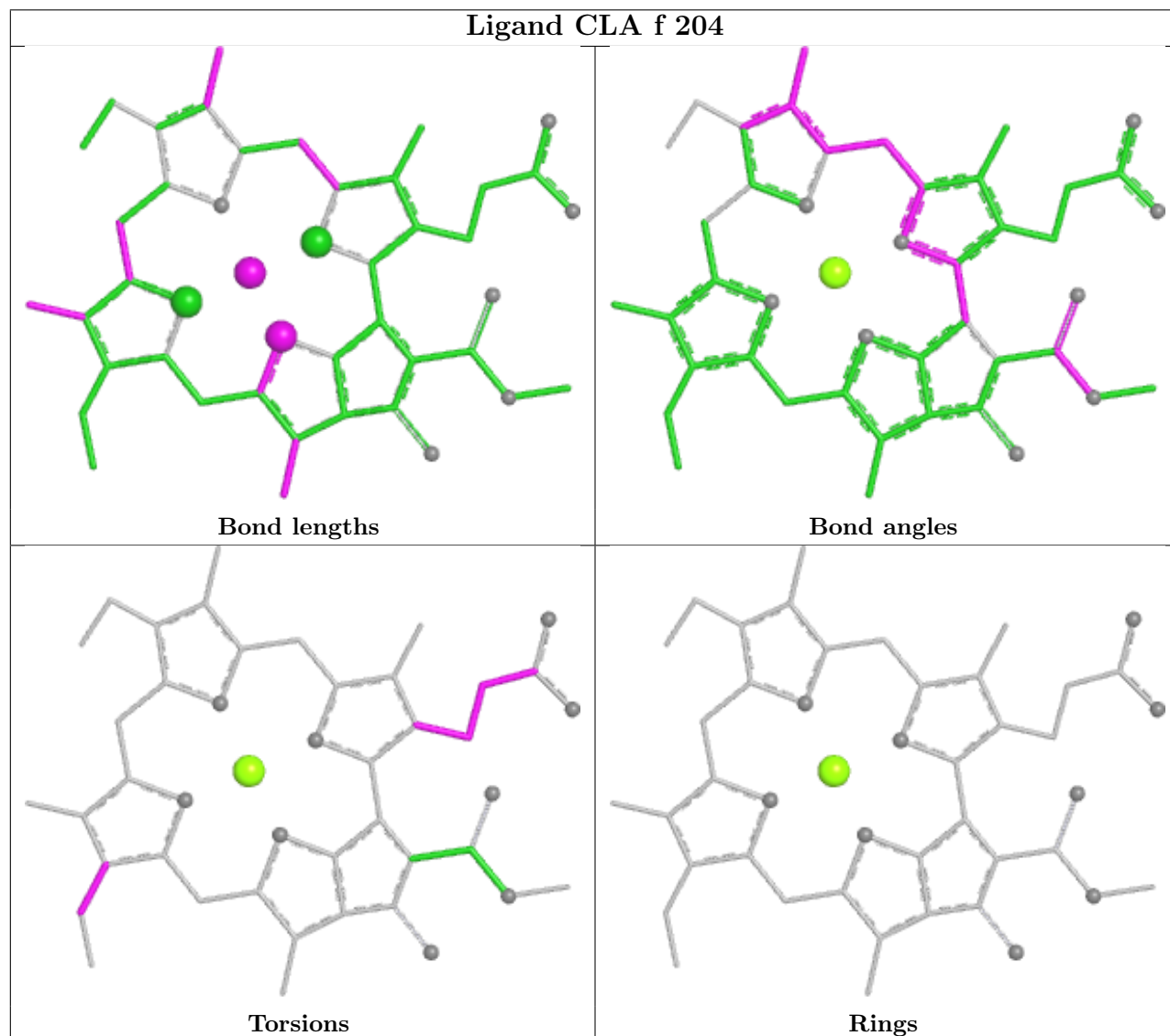
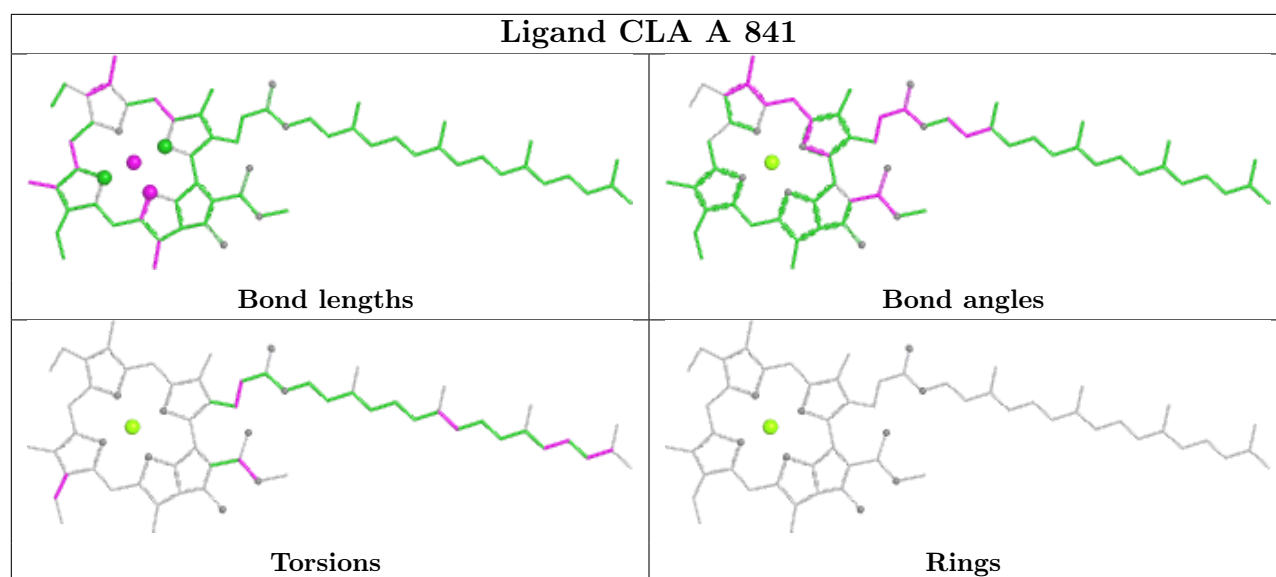
Bond angles

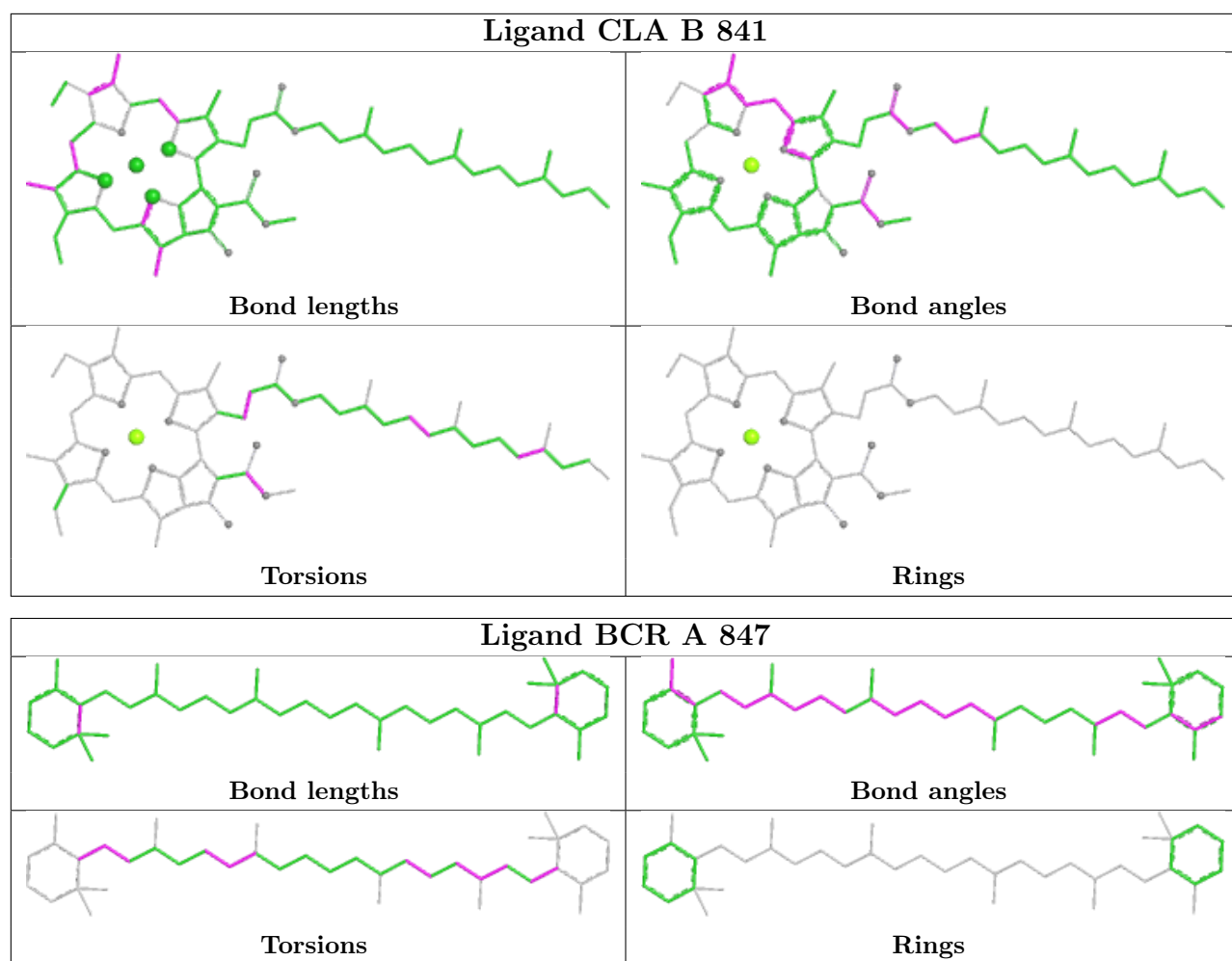


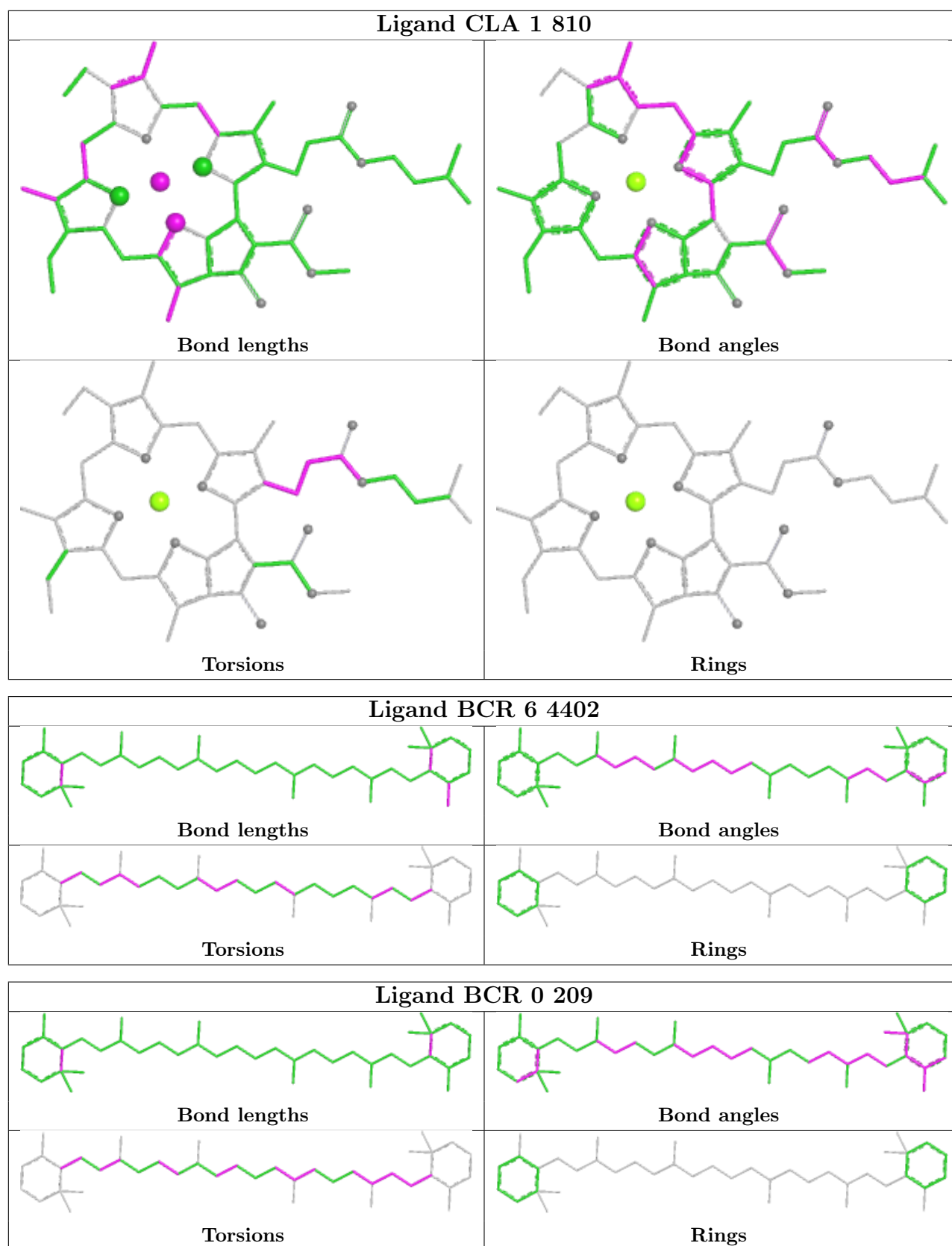
Torsions



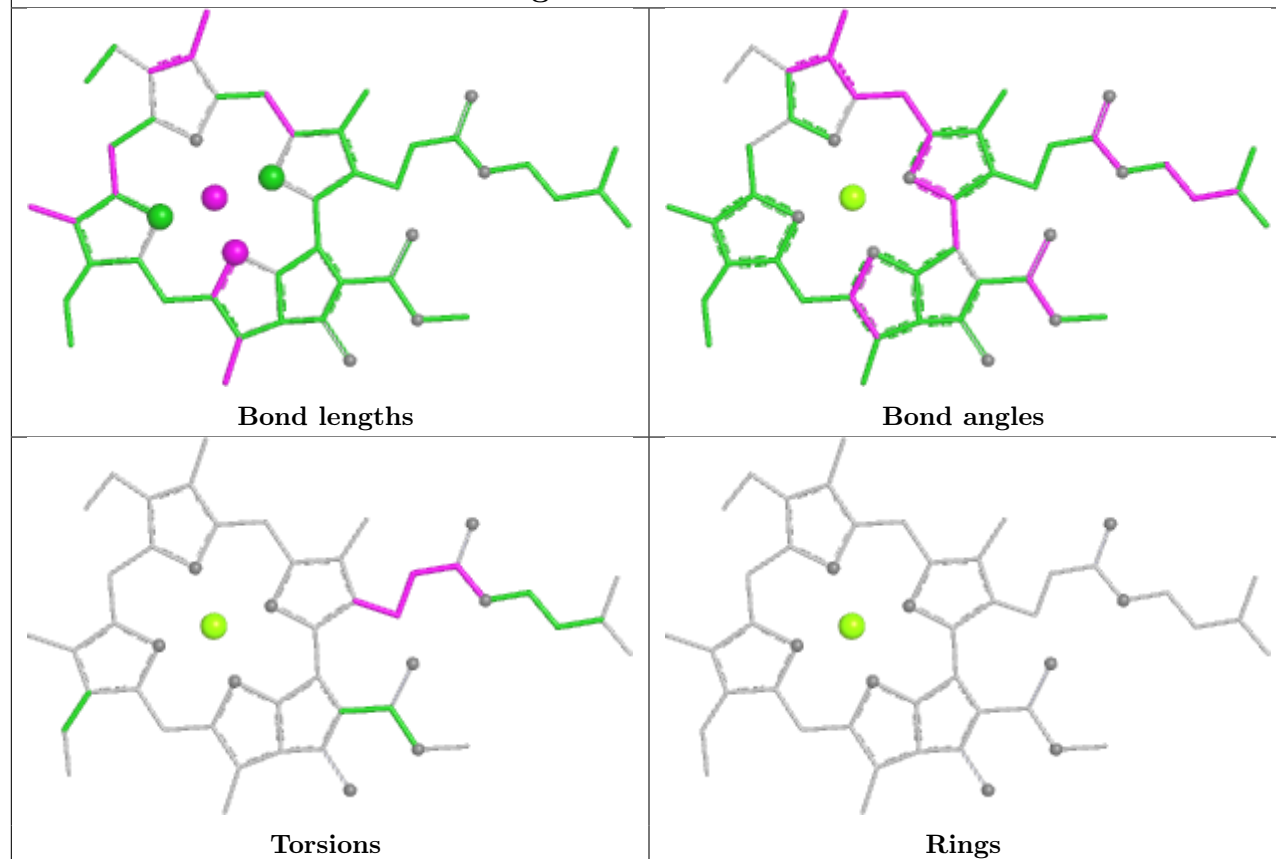
Rings



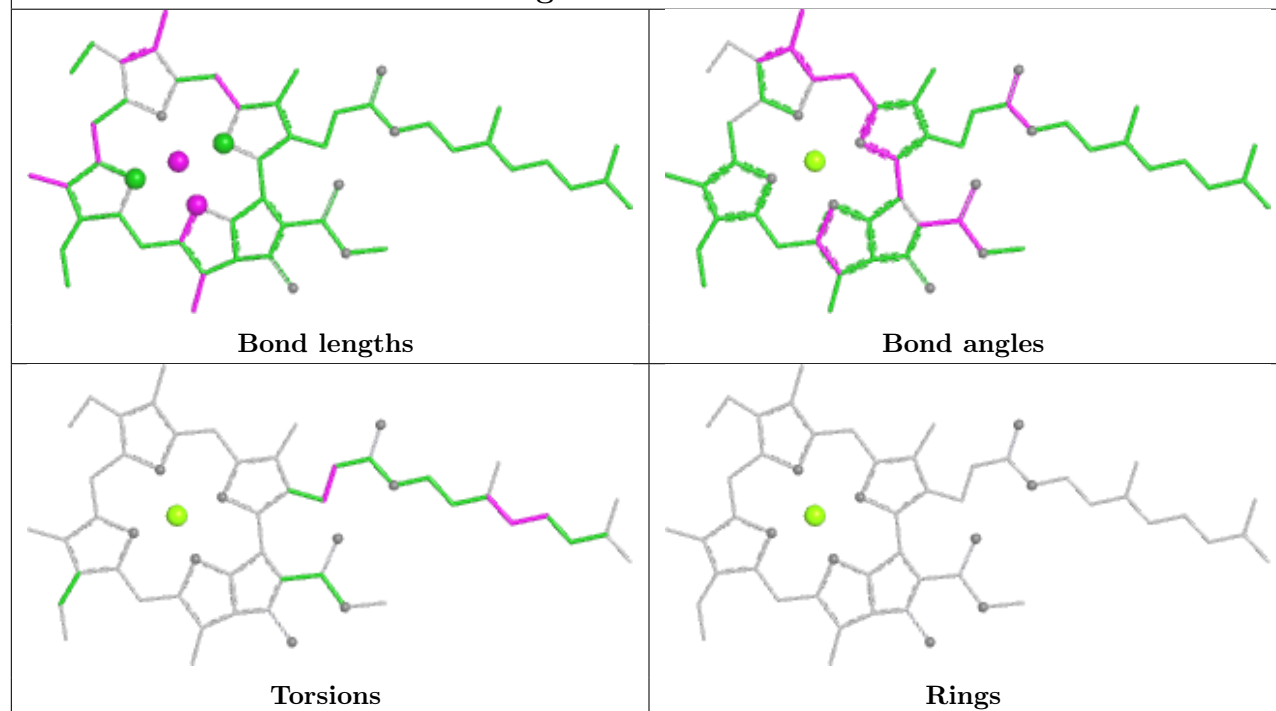


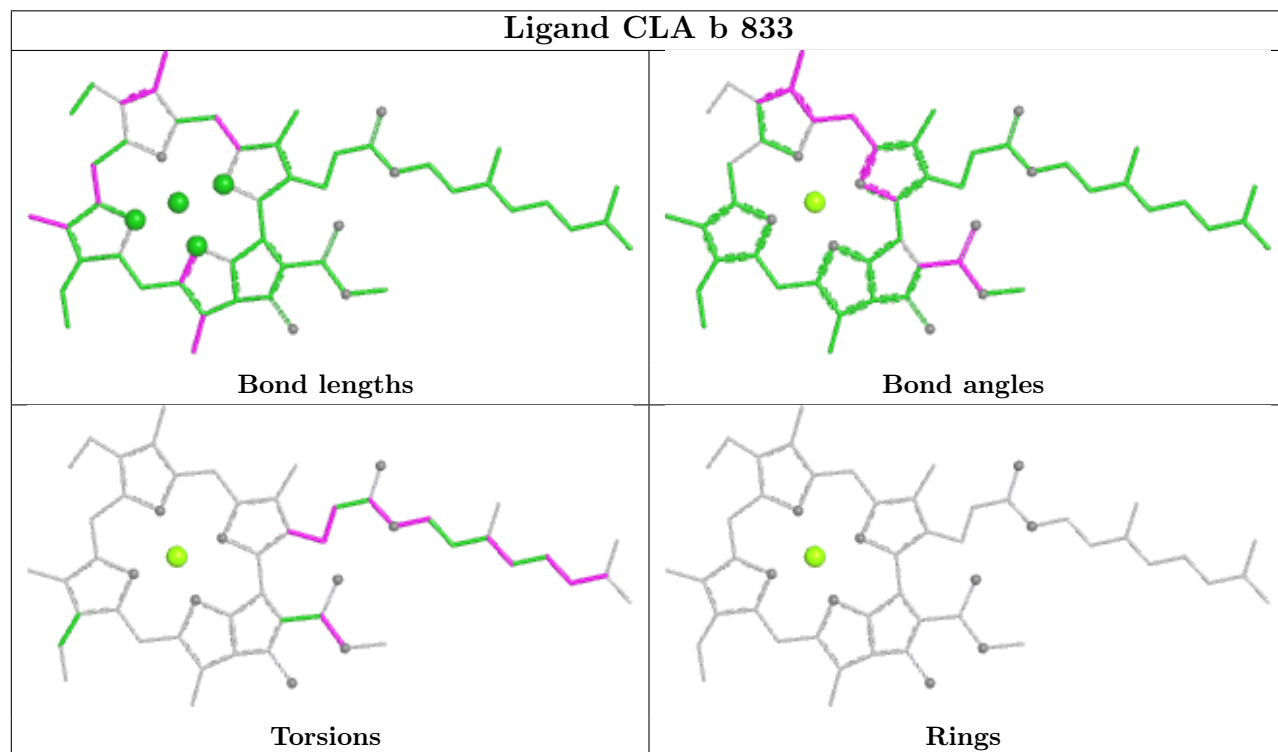
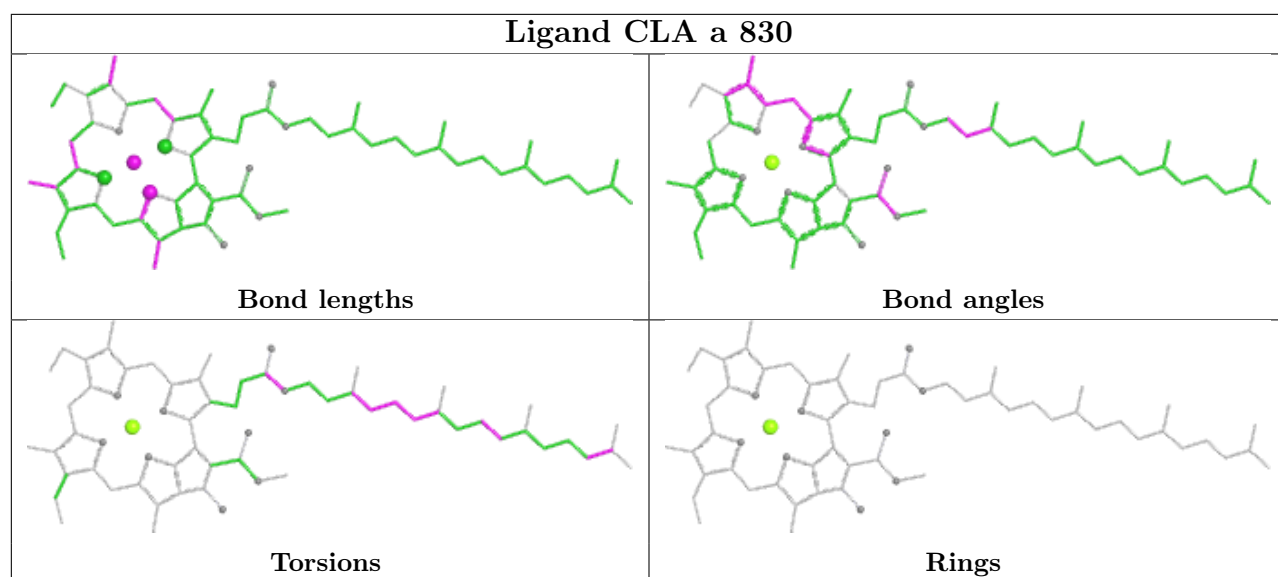


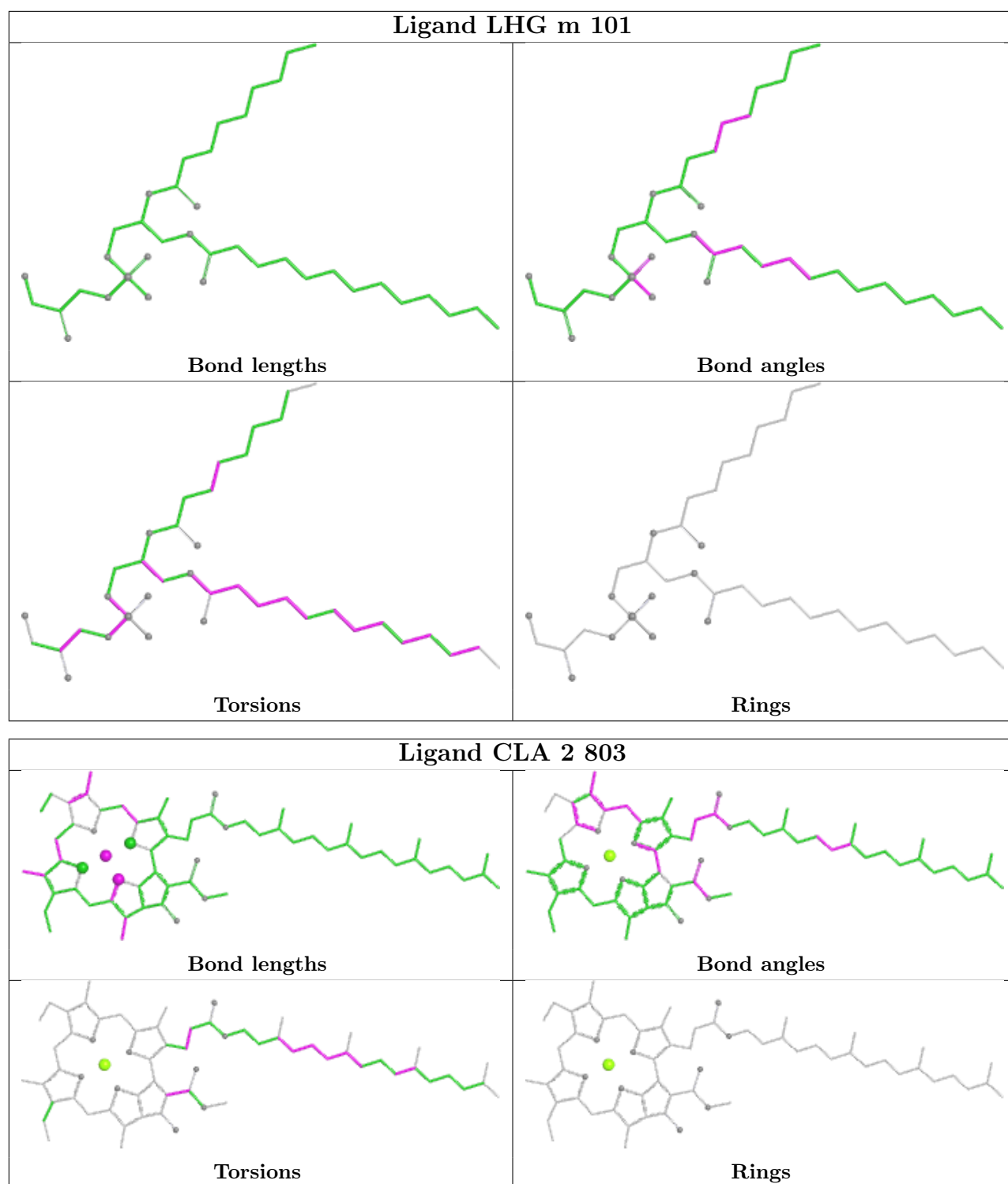
Ligand CLA A 811

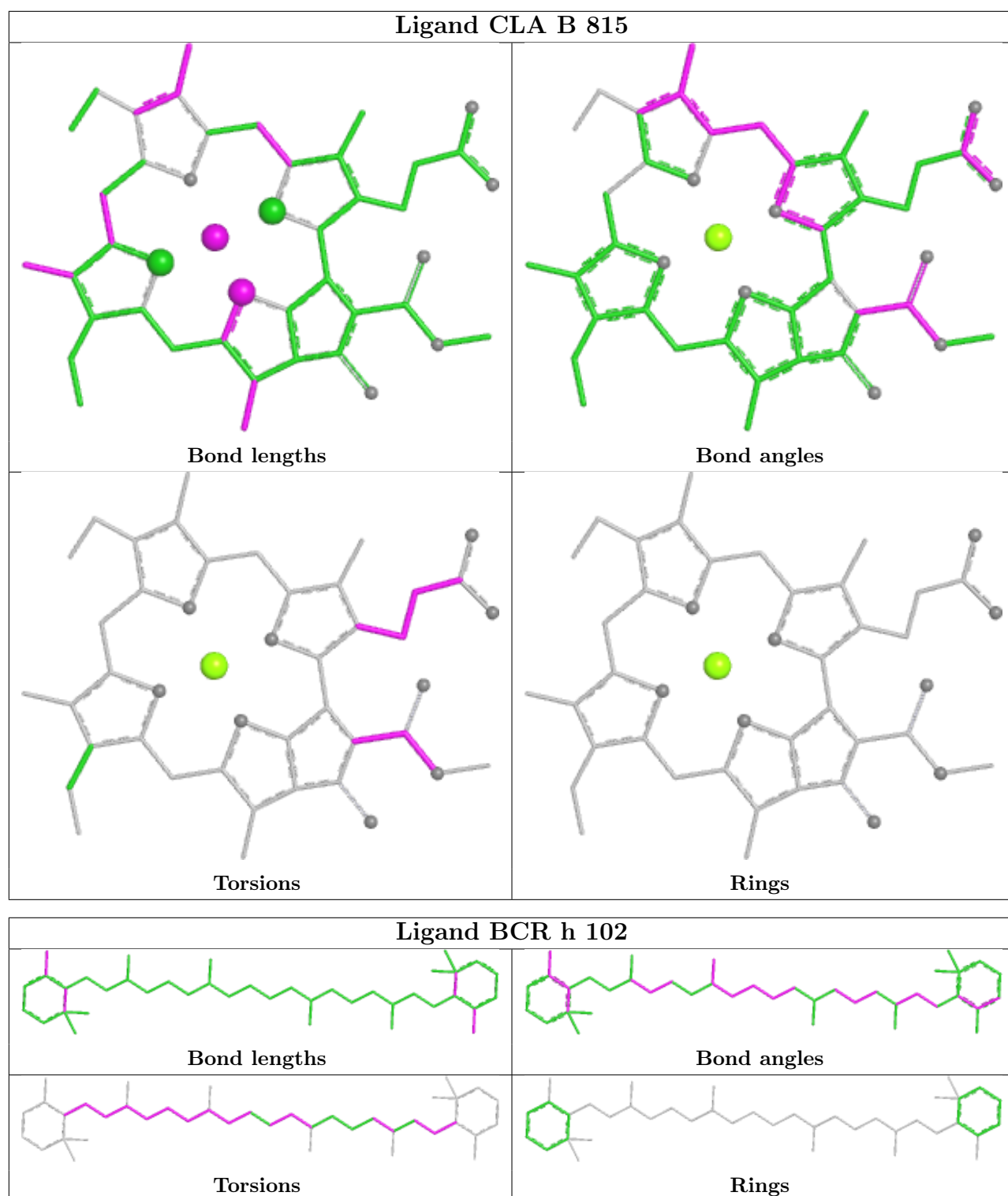


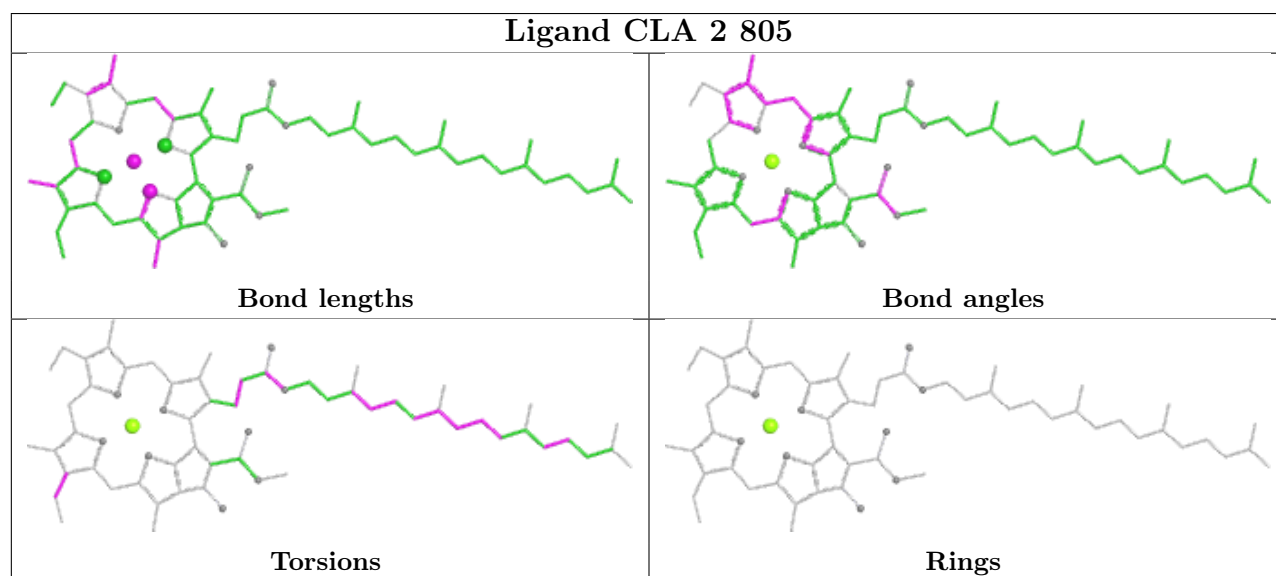
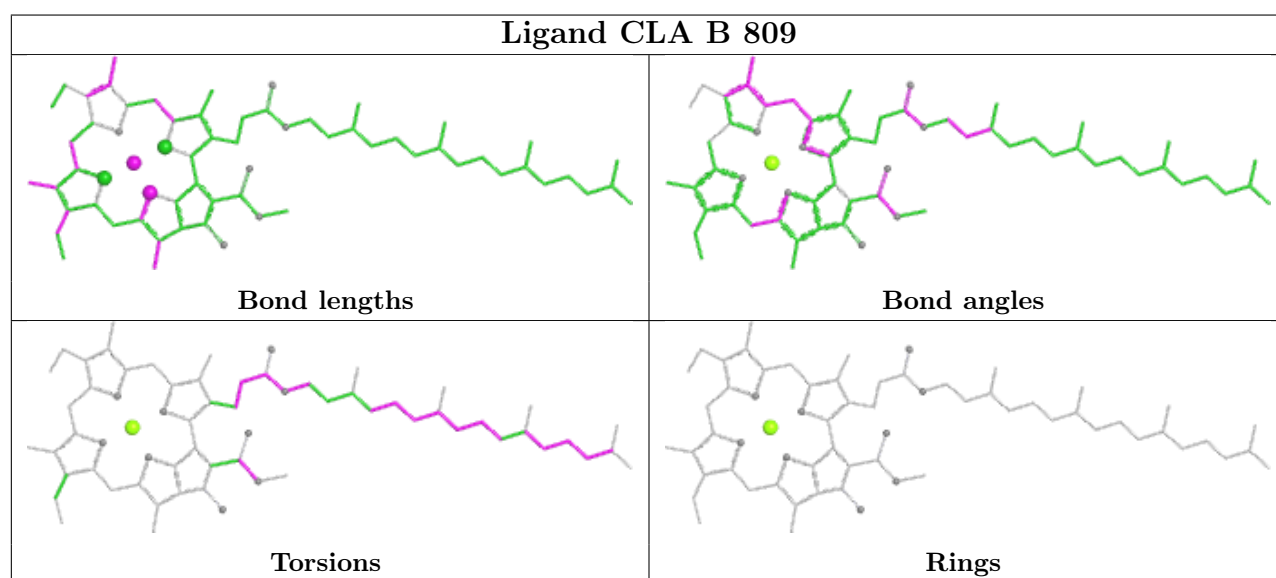
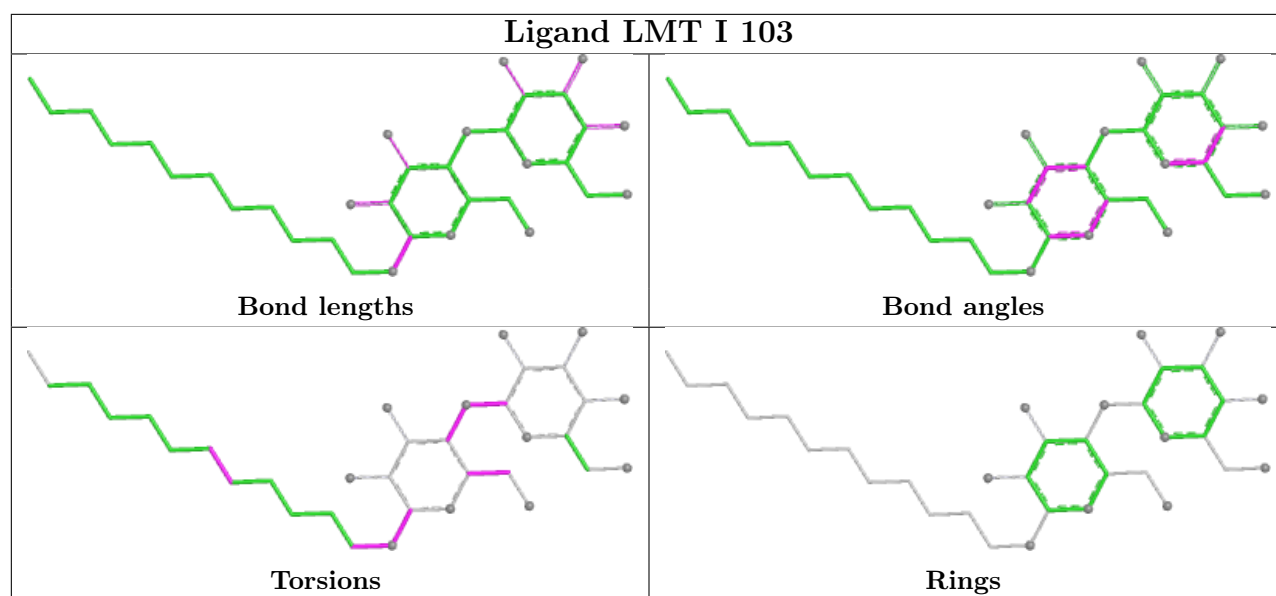
Ligand CLA 2 826

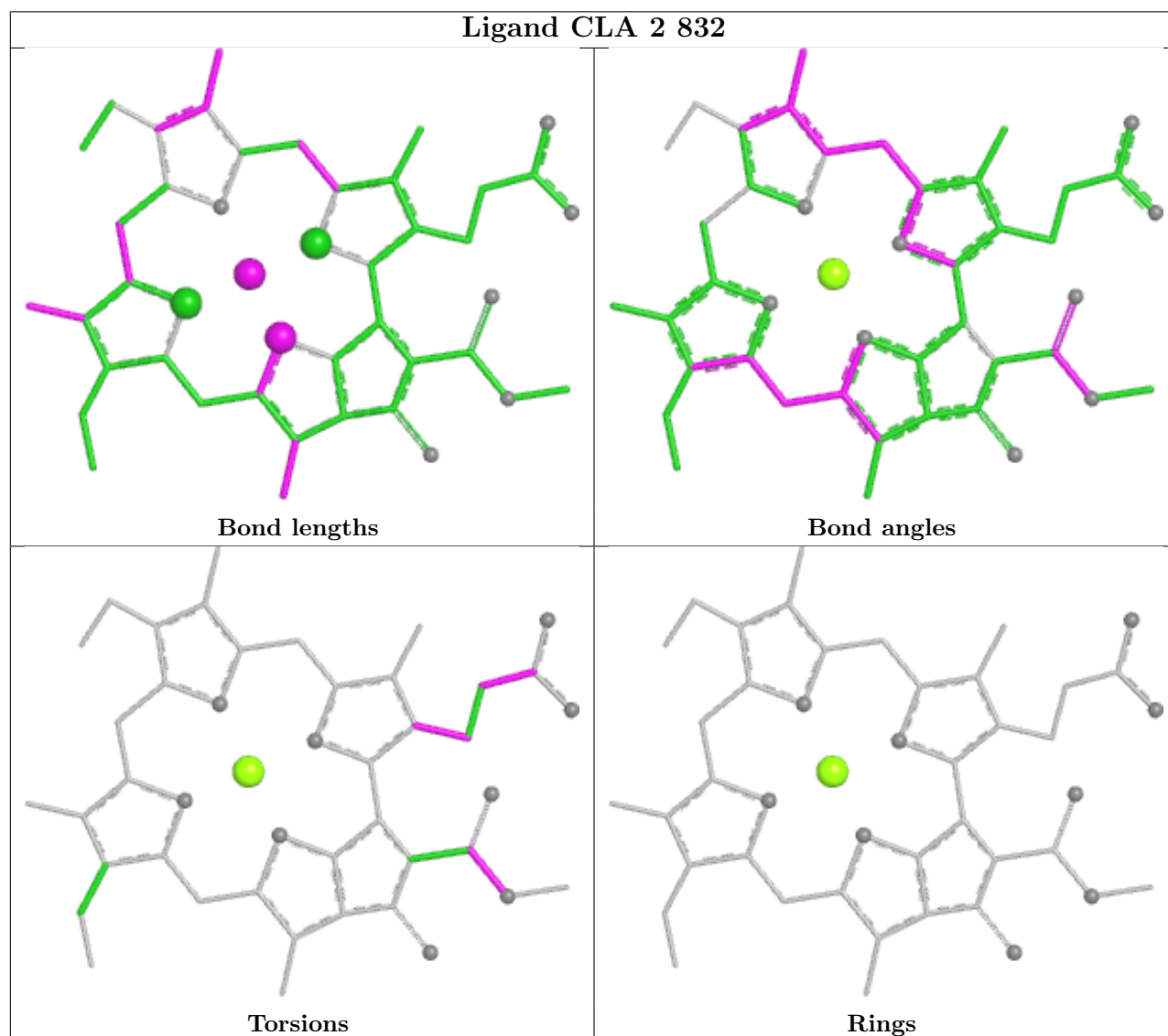
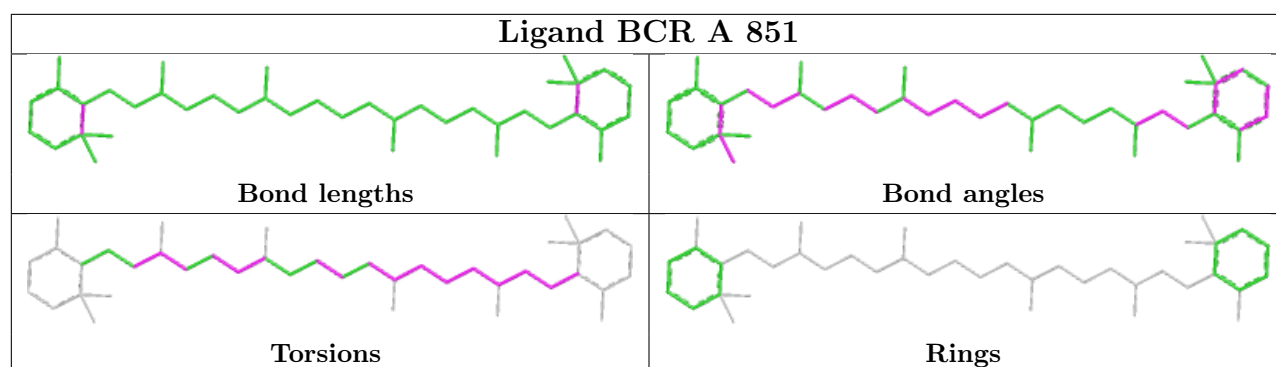


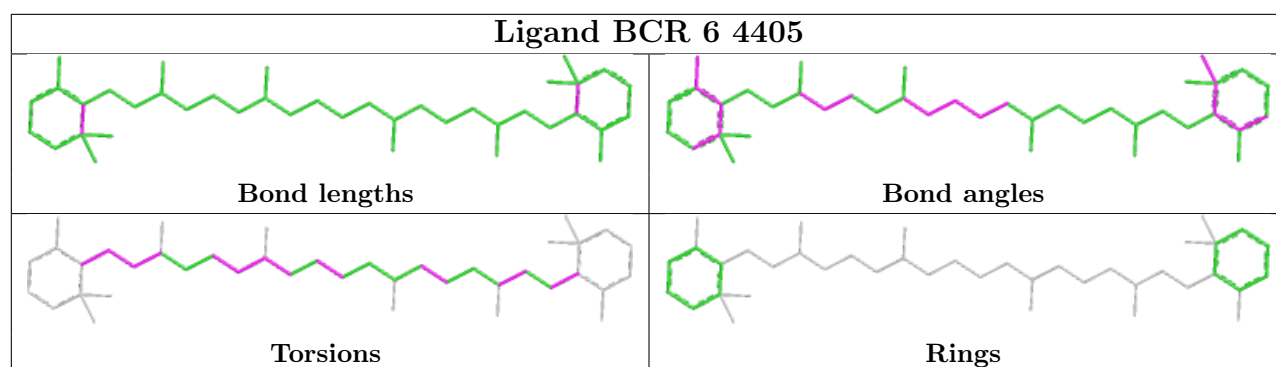
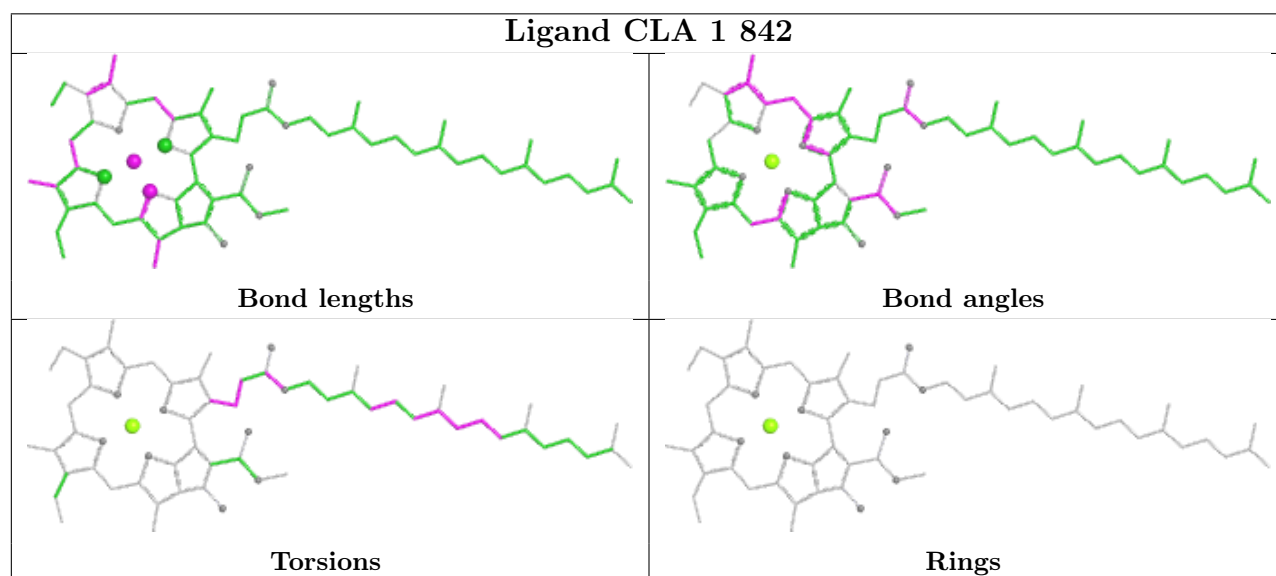
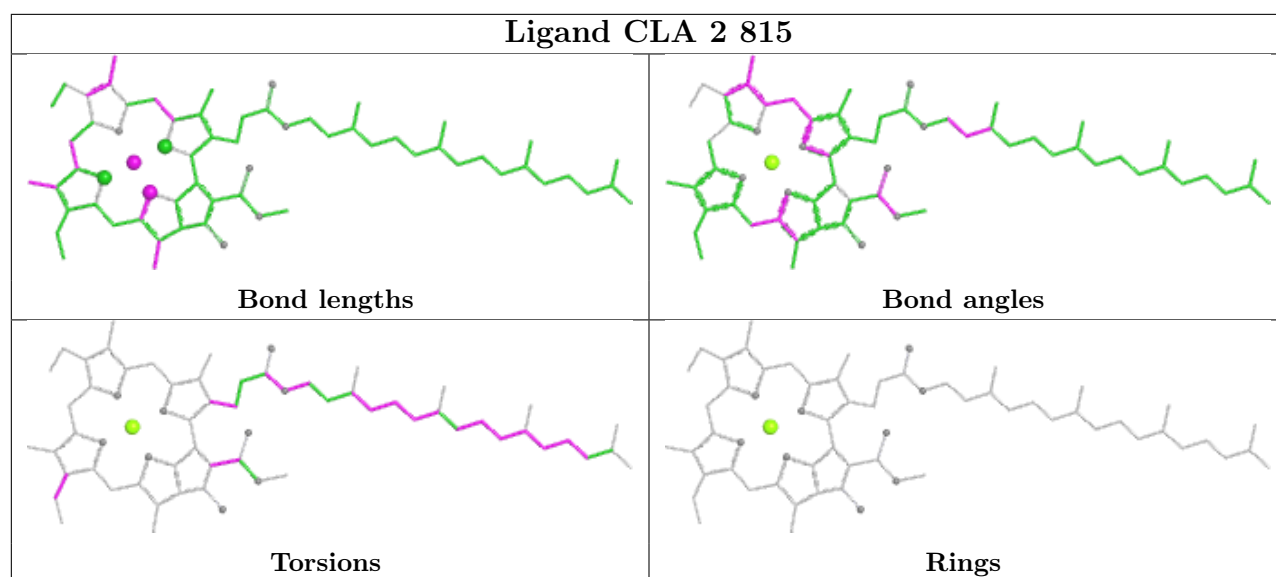




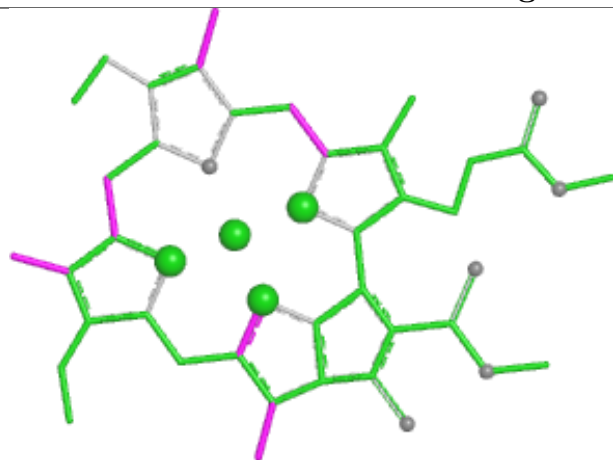




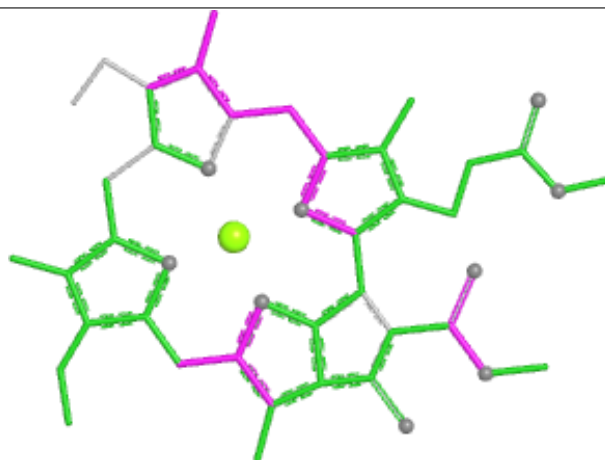




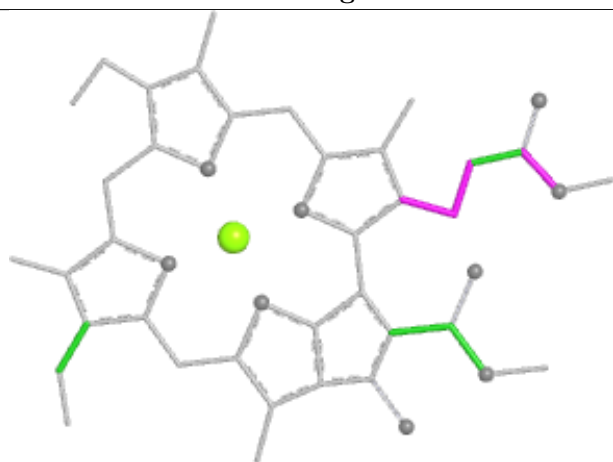
Ligand CLA 2 838



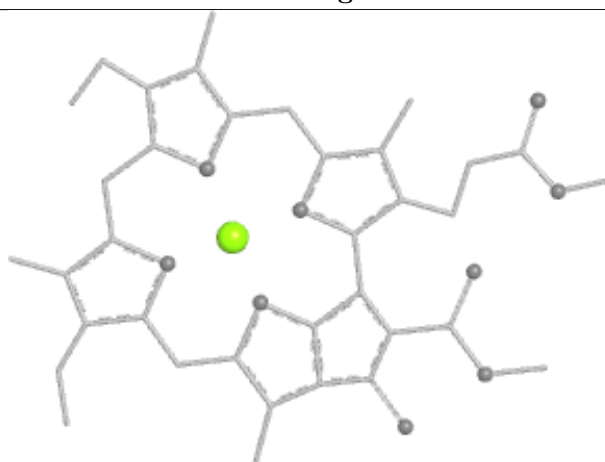
Bond lengths



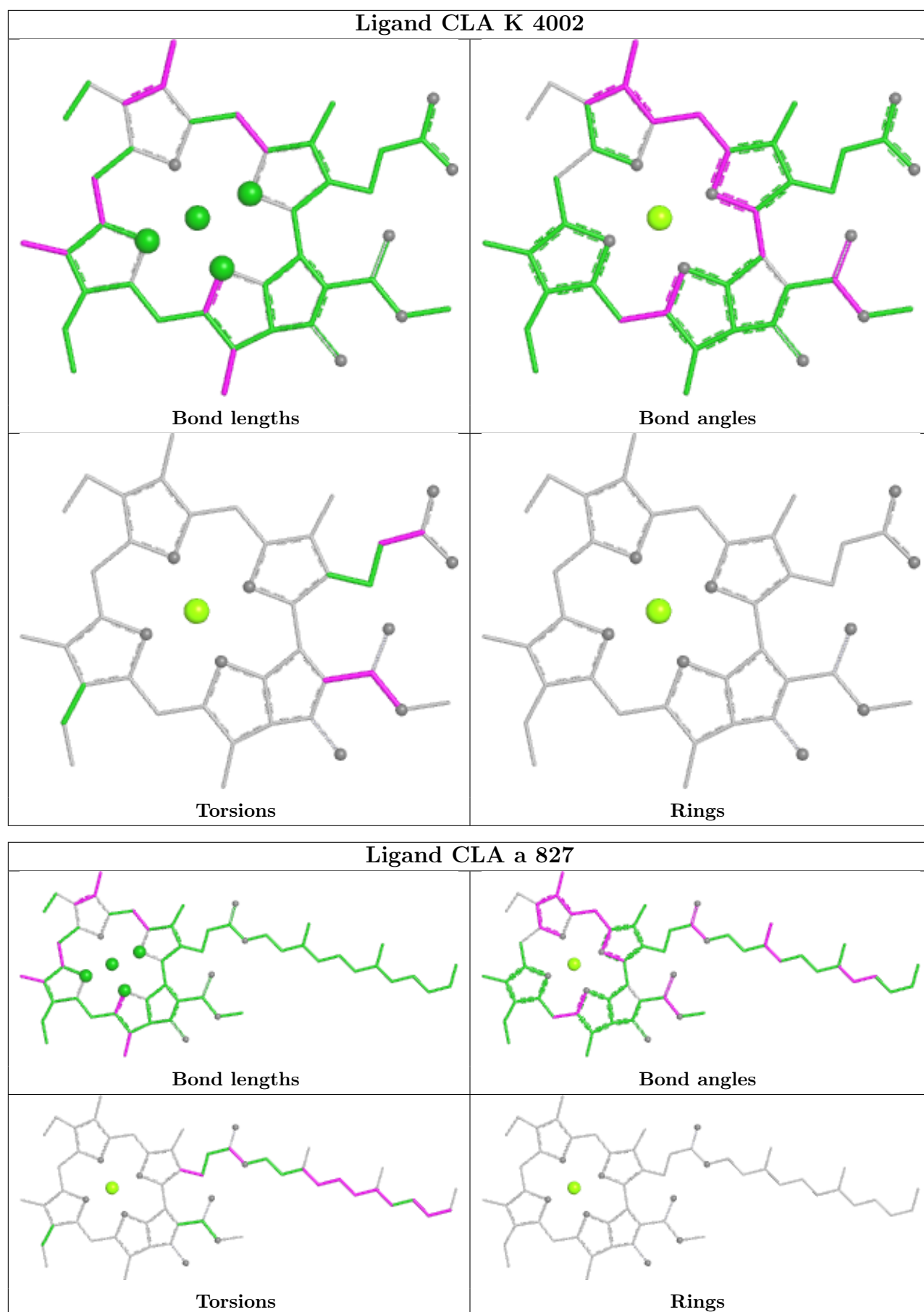
Bond angles

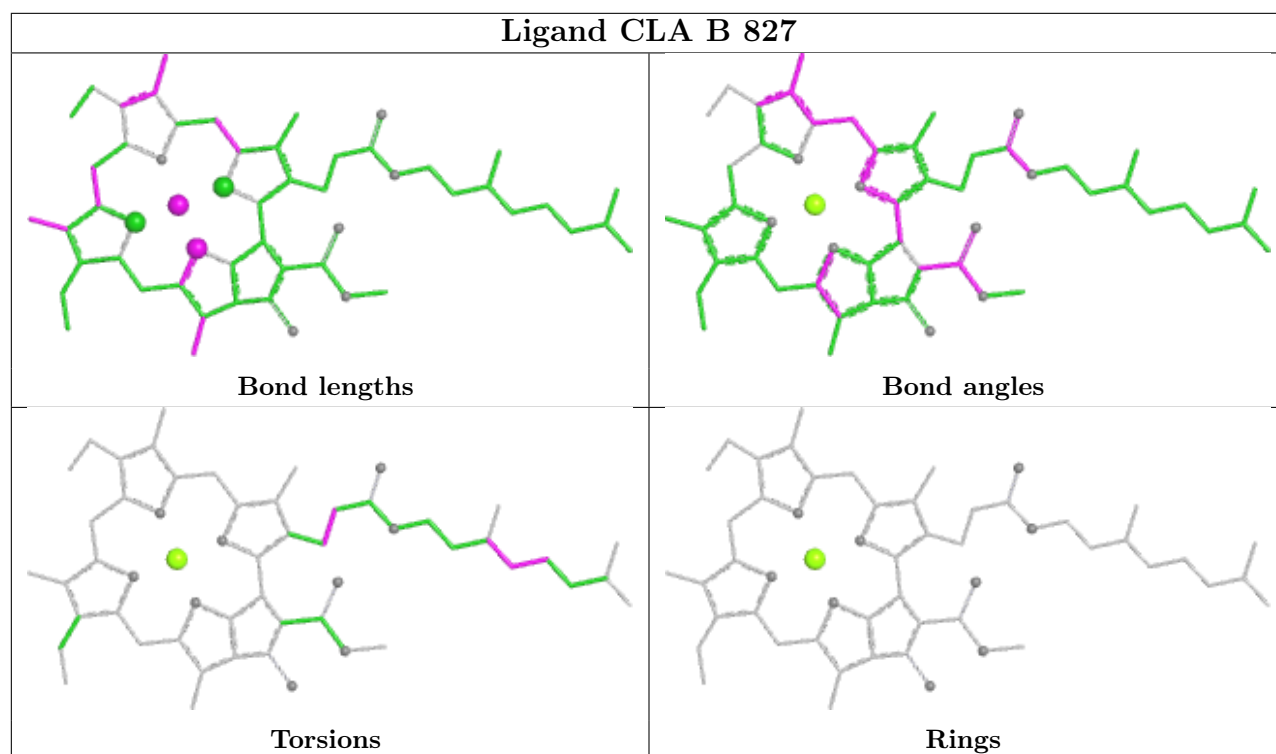
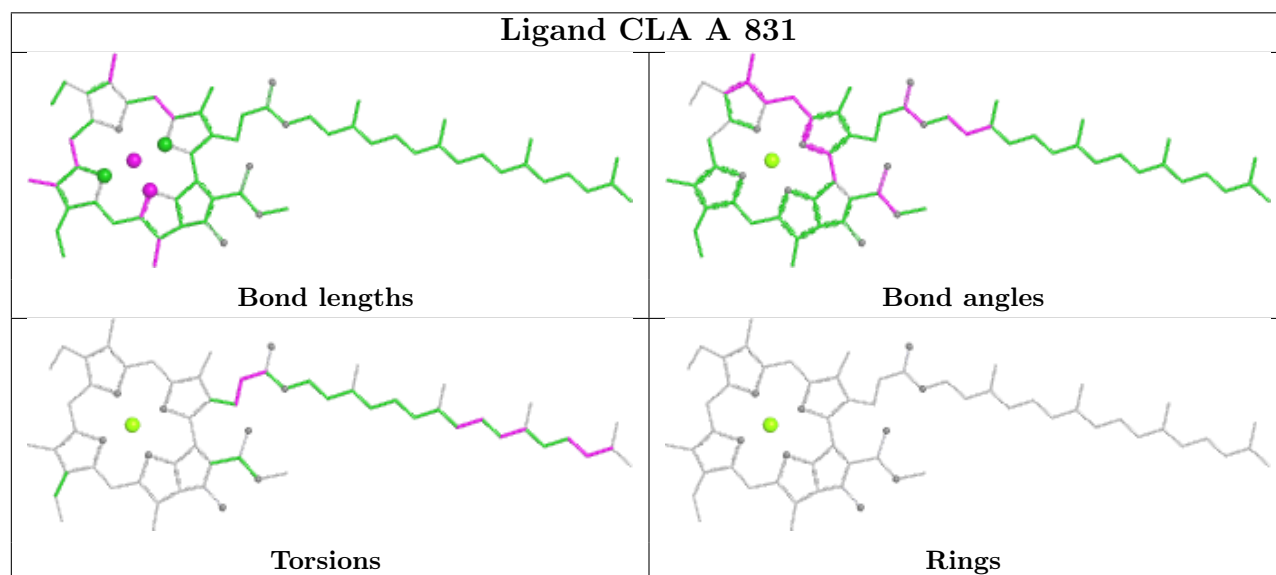
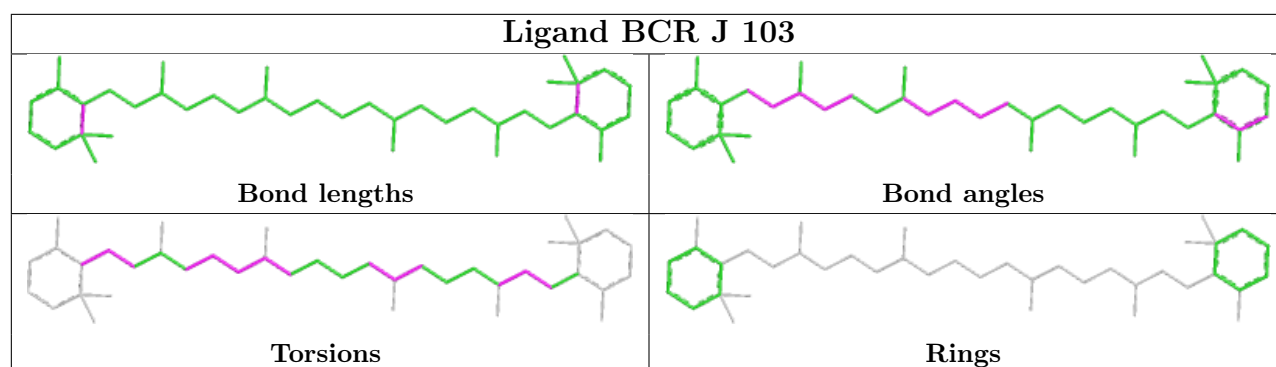


Torsions

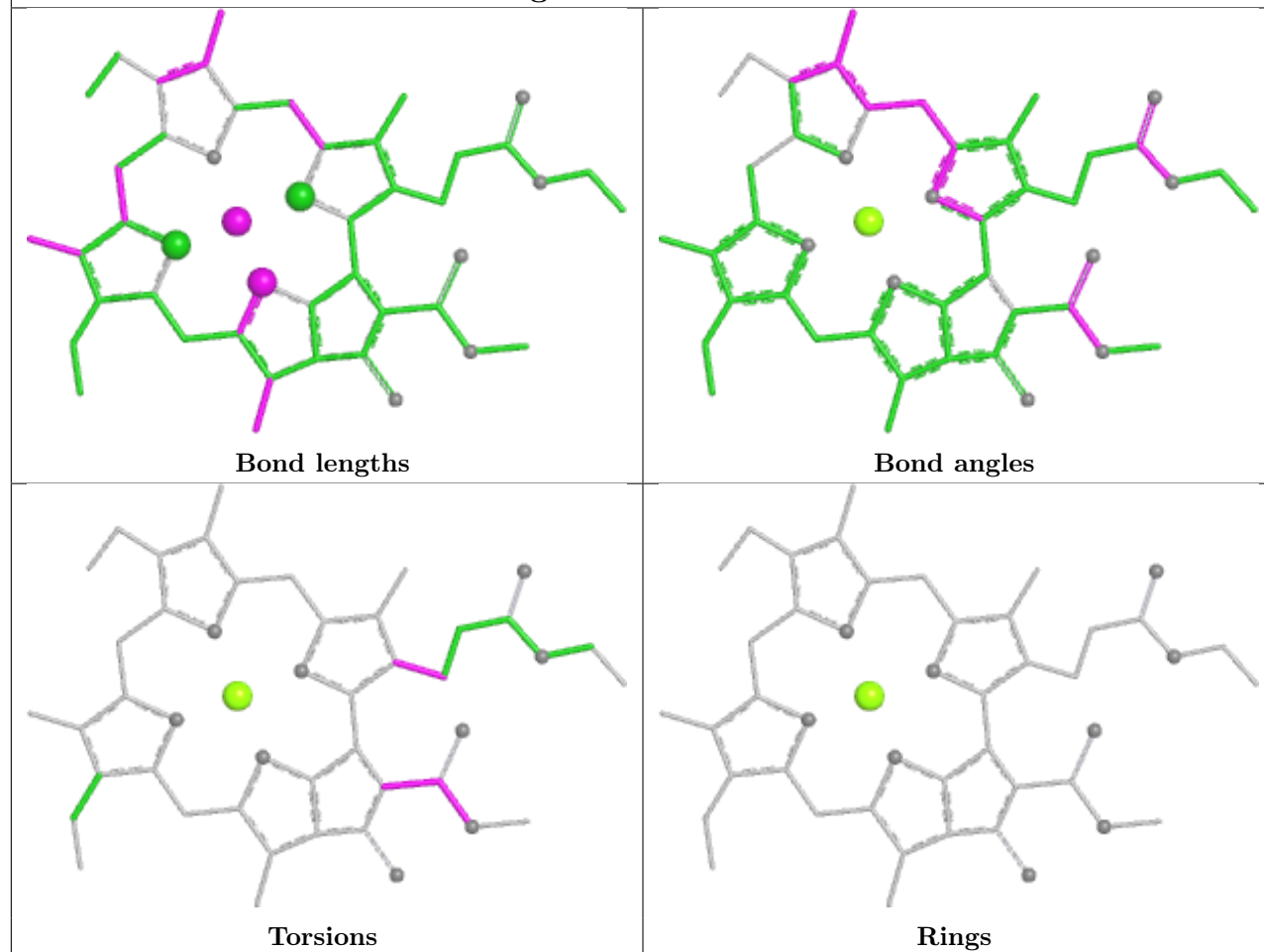


Rings

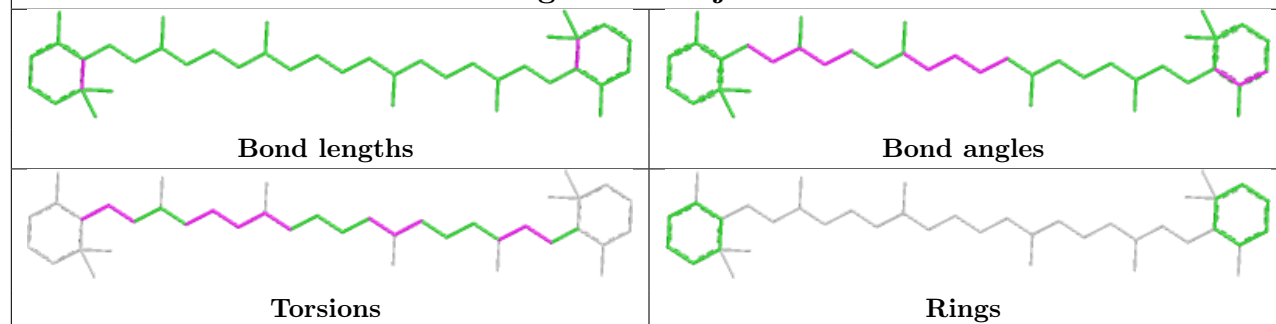


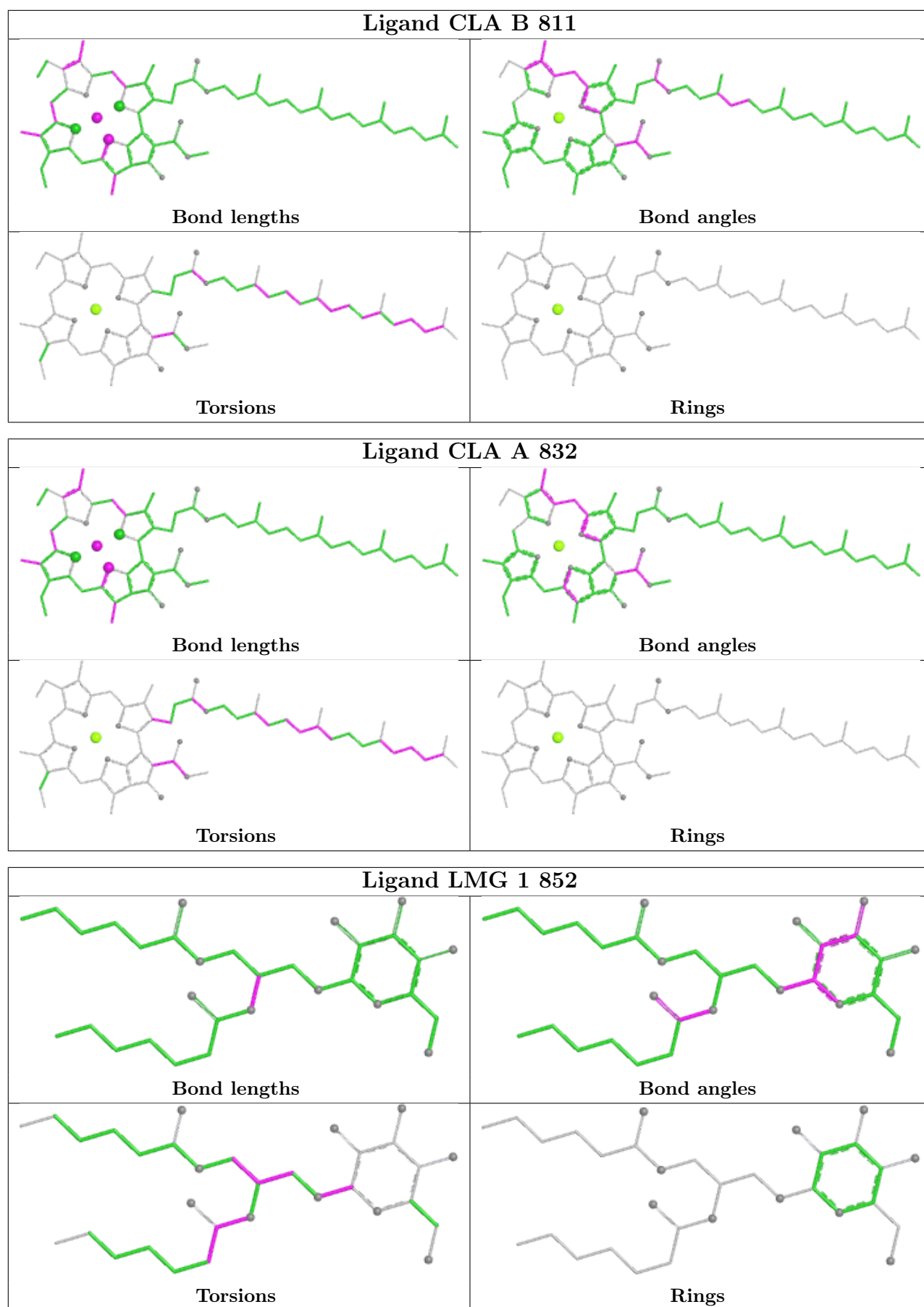


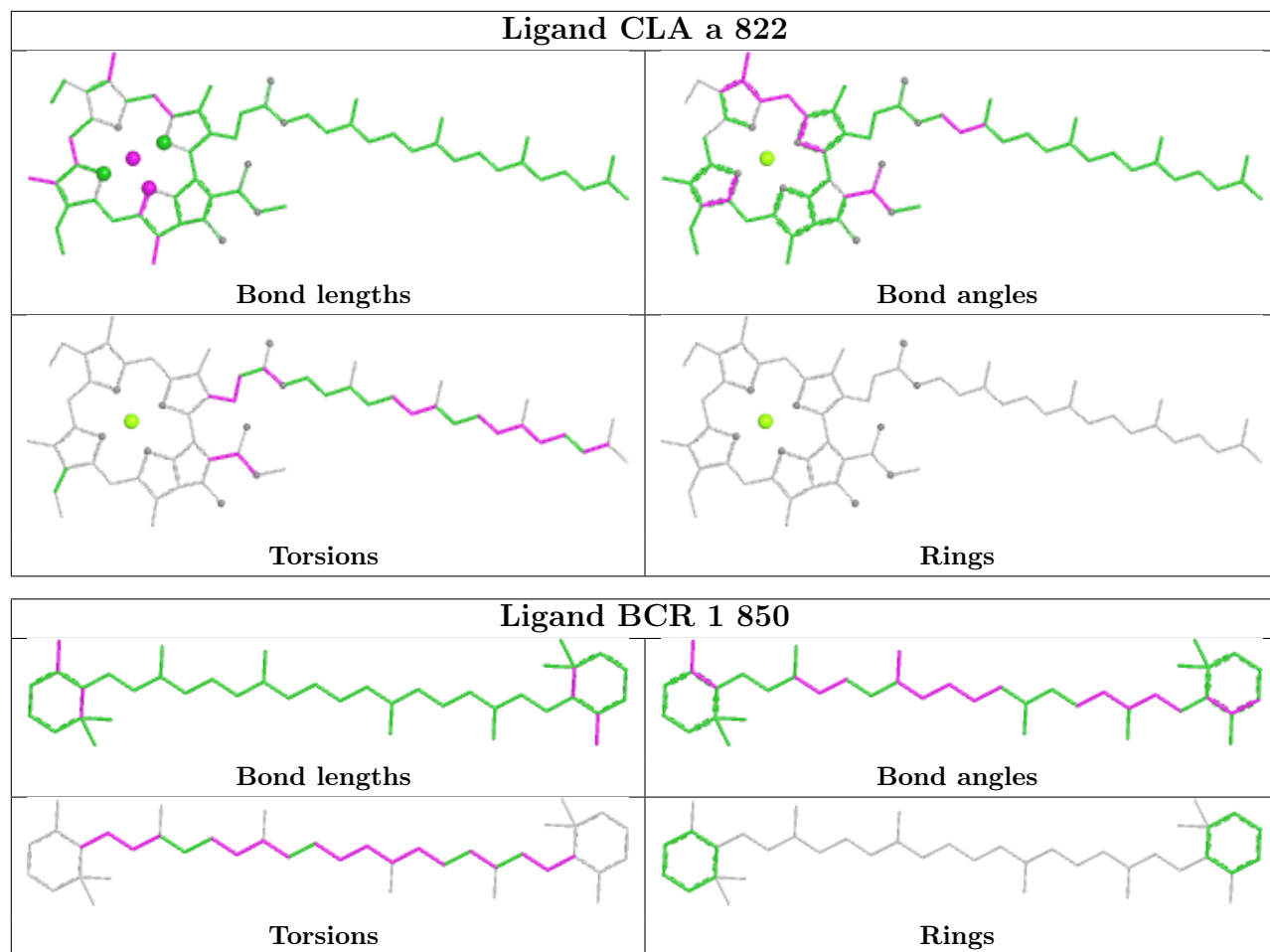
Ligand CLA b 821



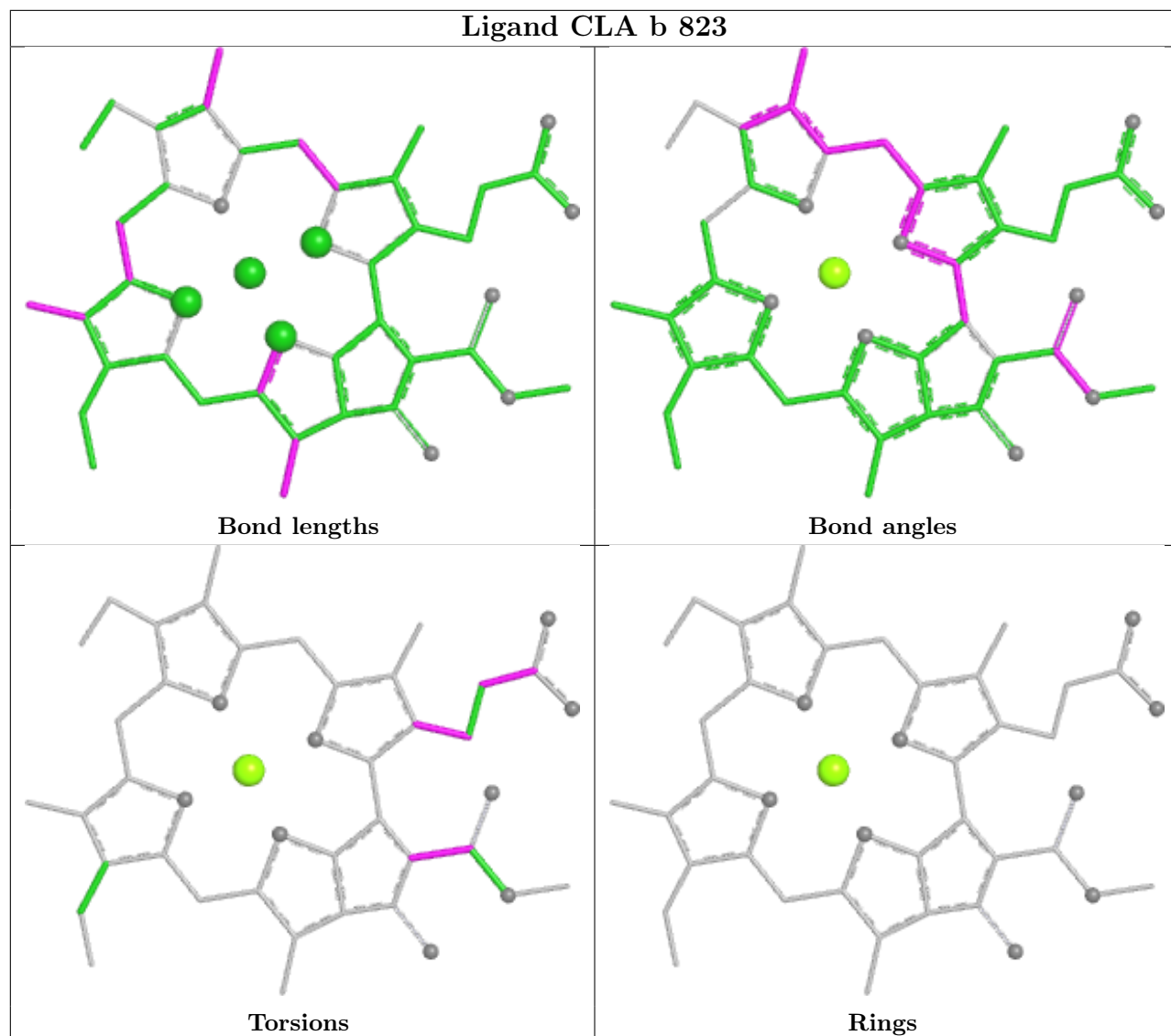
Ligand BCR j 103

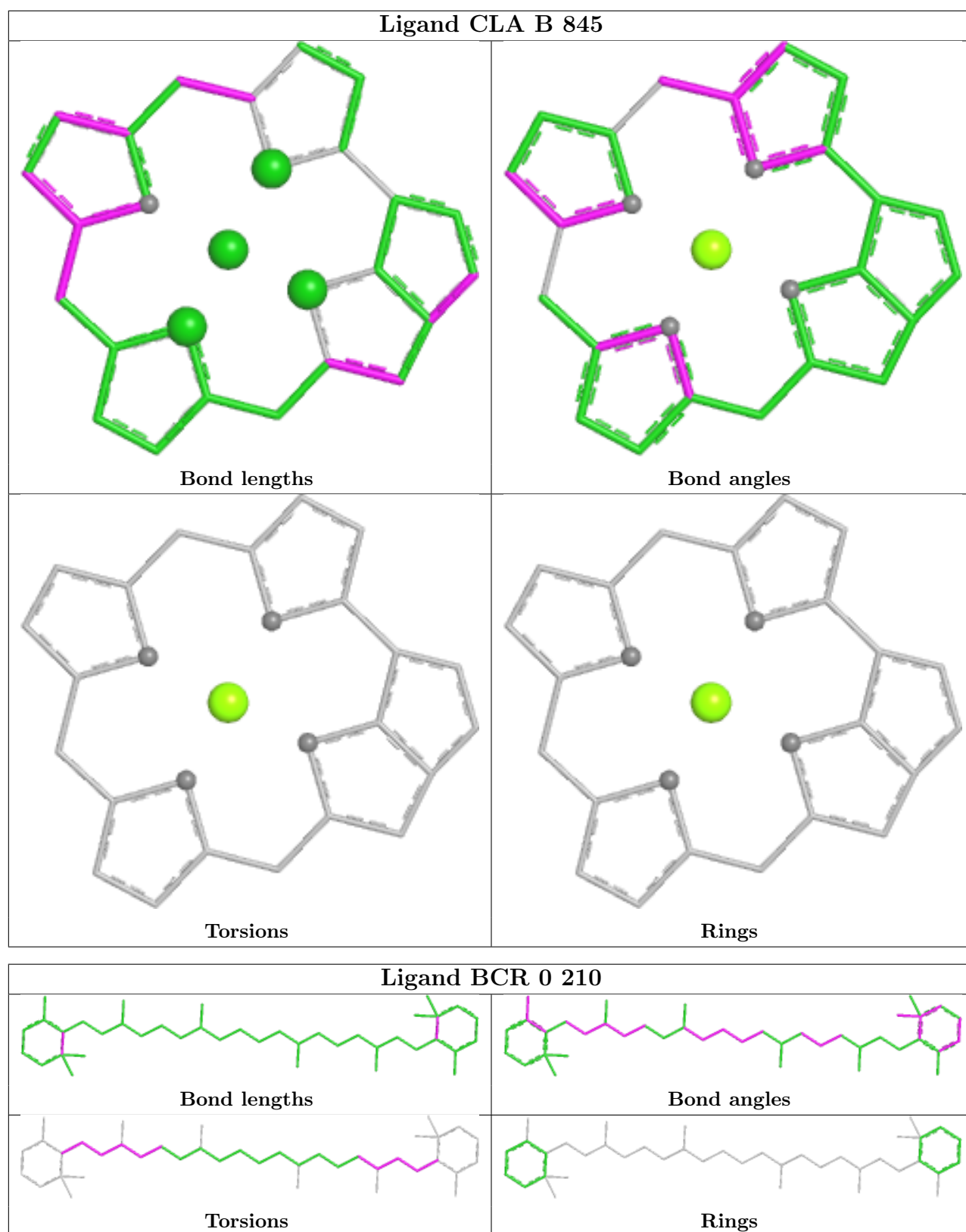




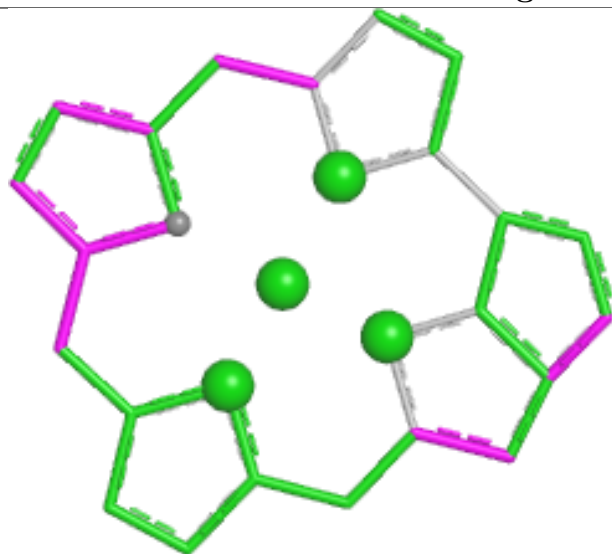


Ligand CLA b 823

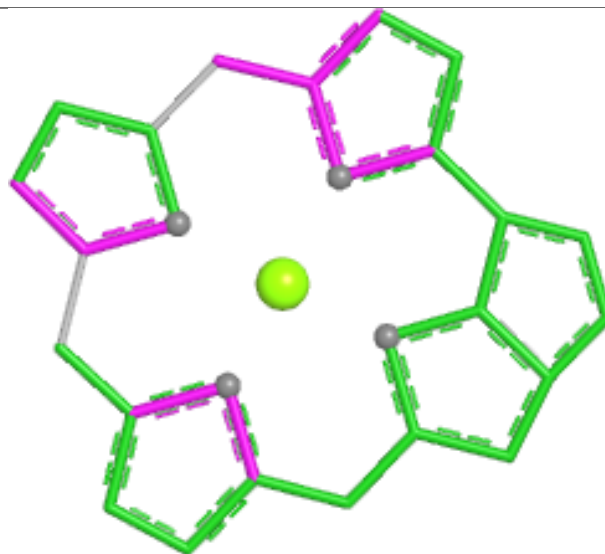




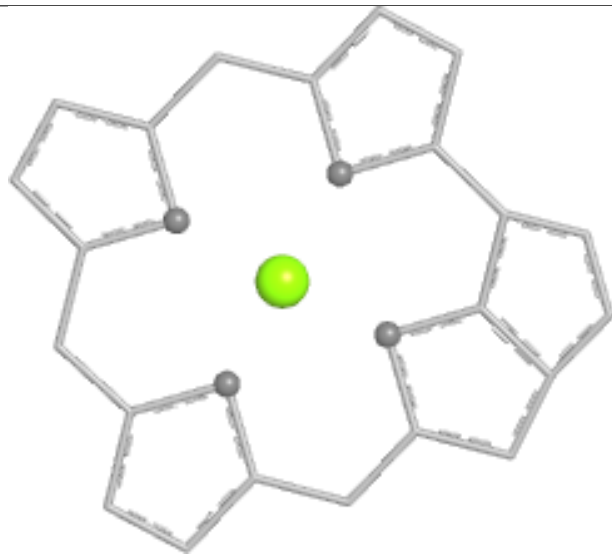
Ligand CLA b 844



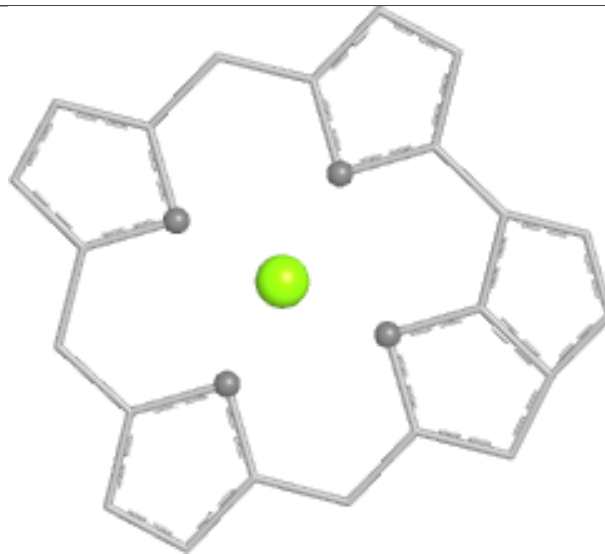
Bond lengths



Bond angles

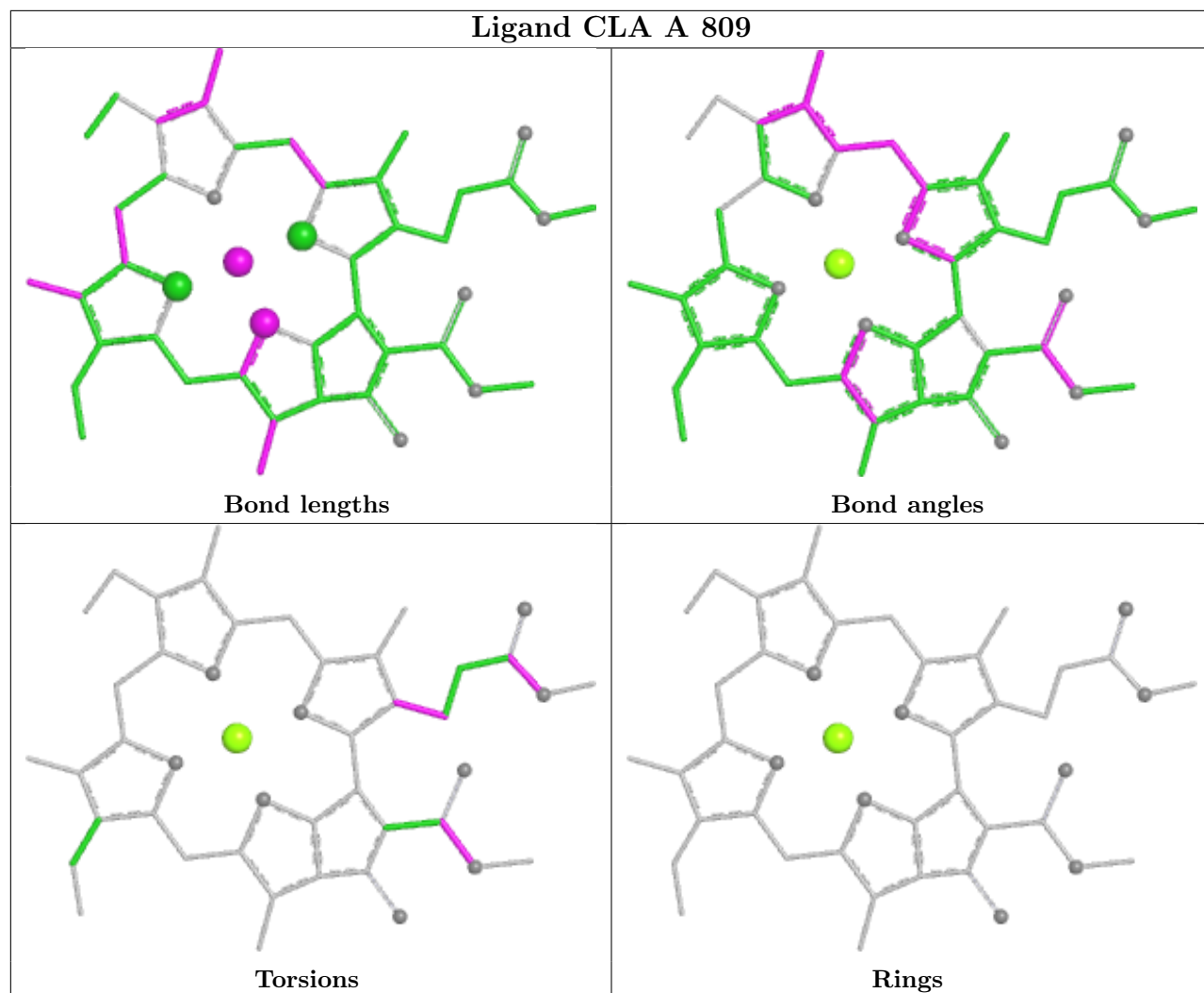


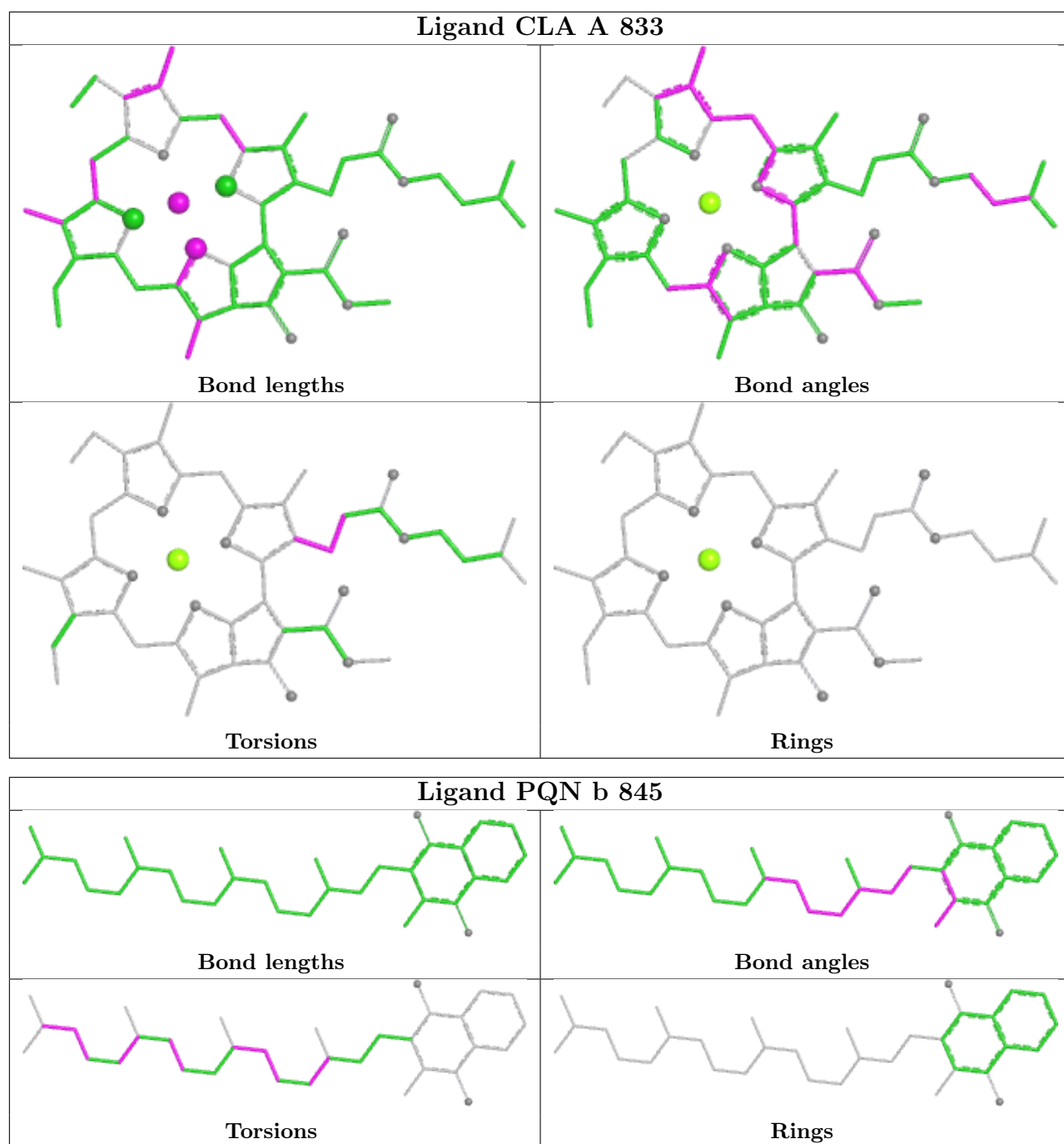
Torsions



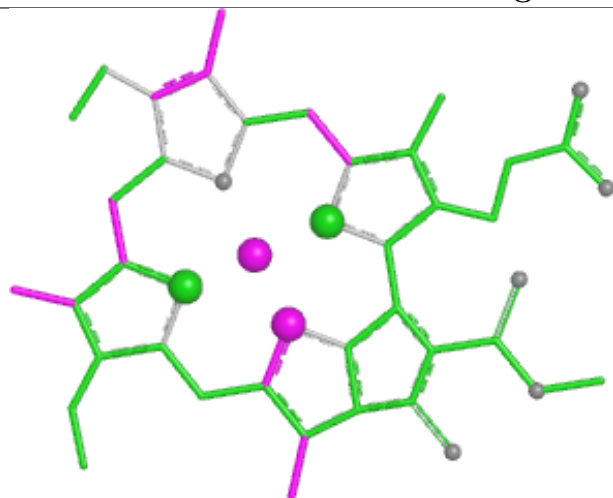
Rings

Ligand CLA A 809

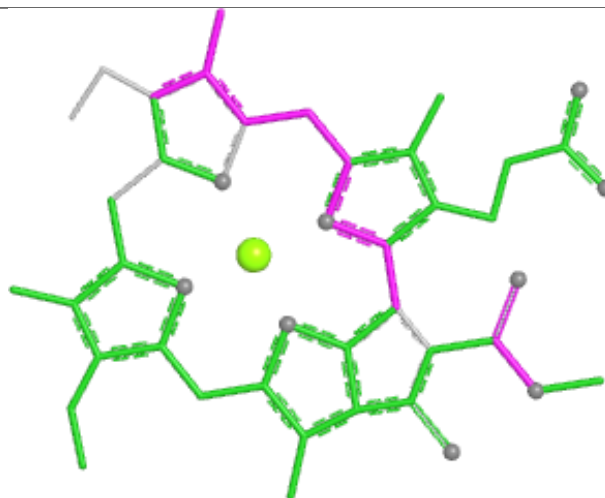




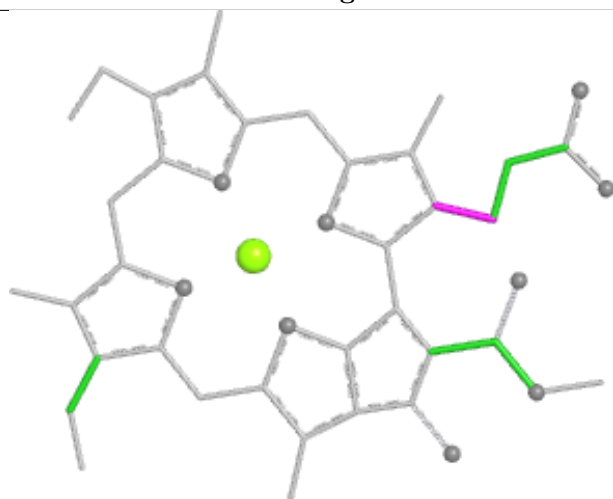
Ligand CLA B 838



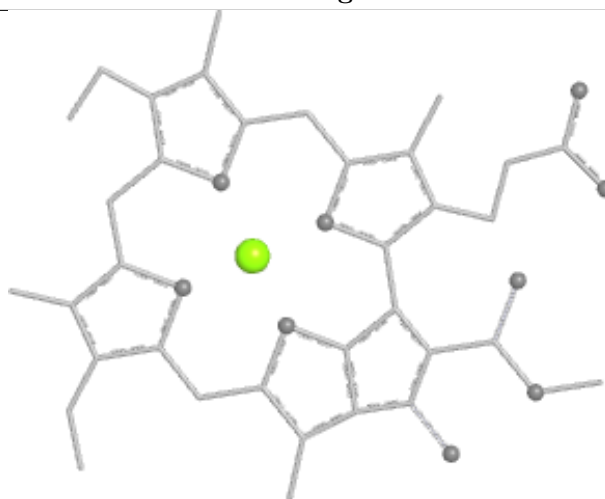
Bond lengths



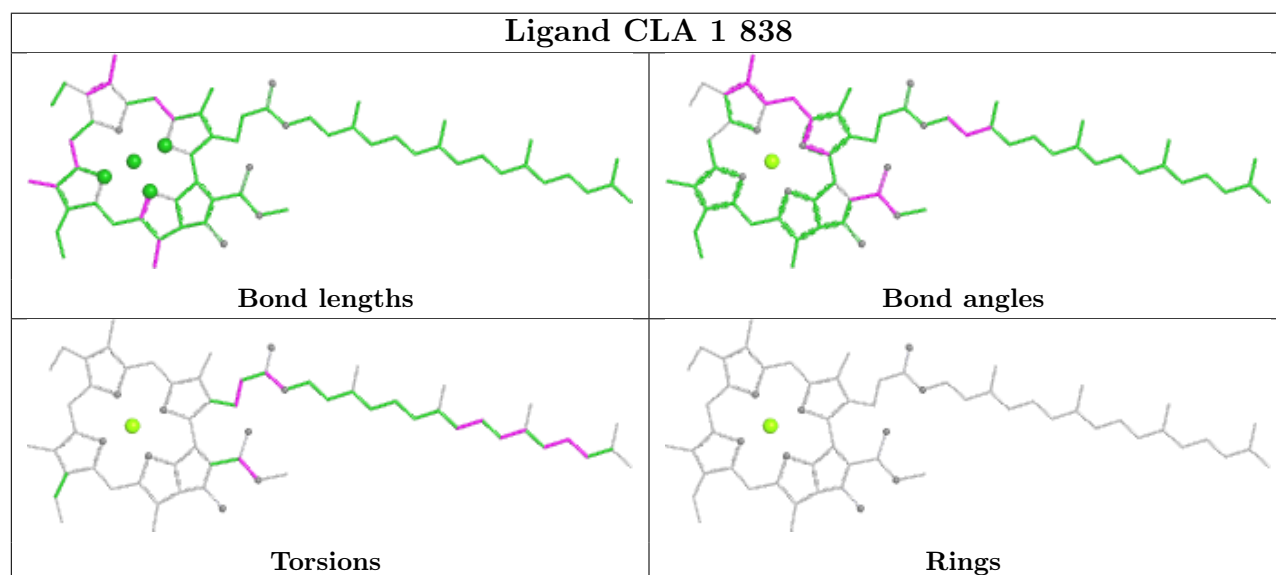
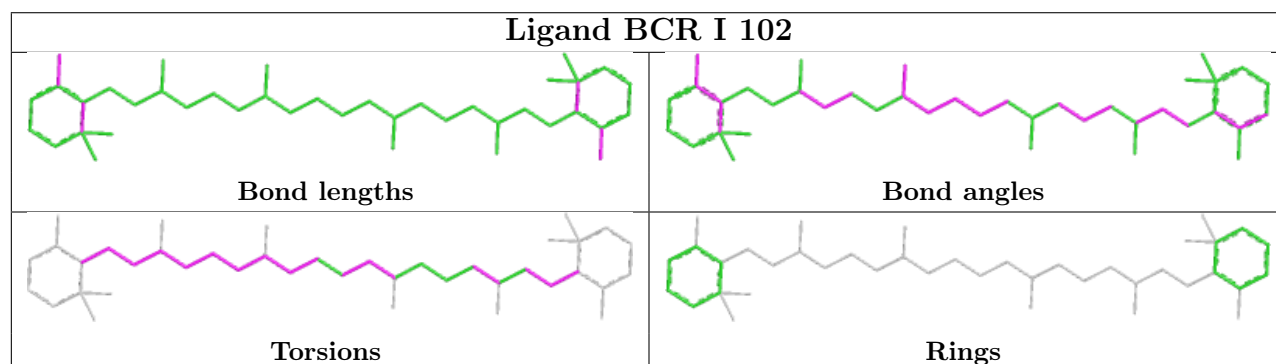
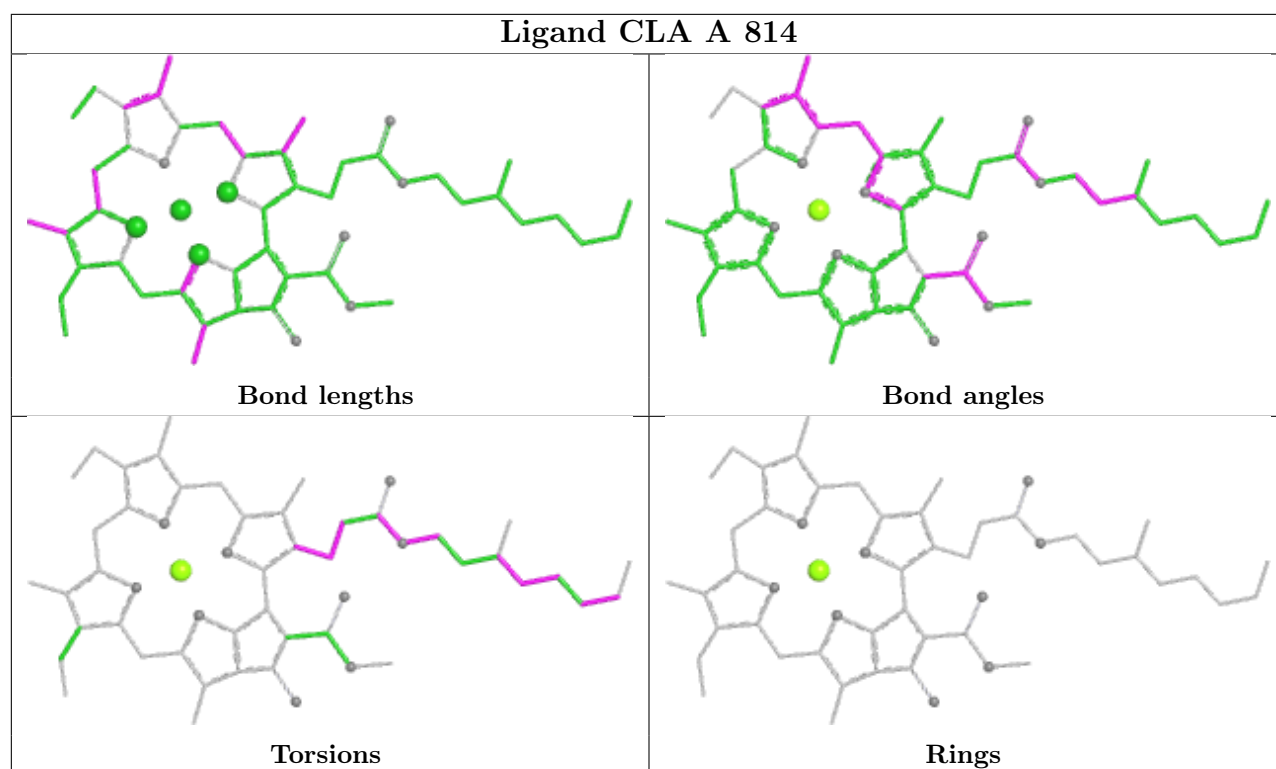
Bond angles

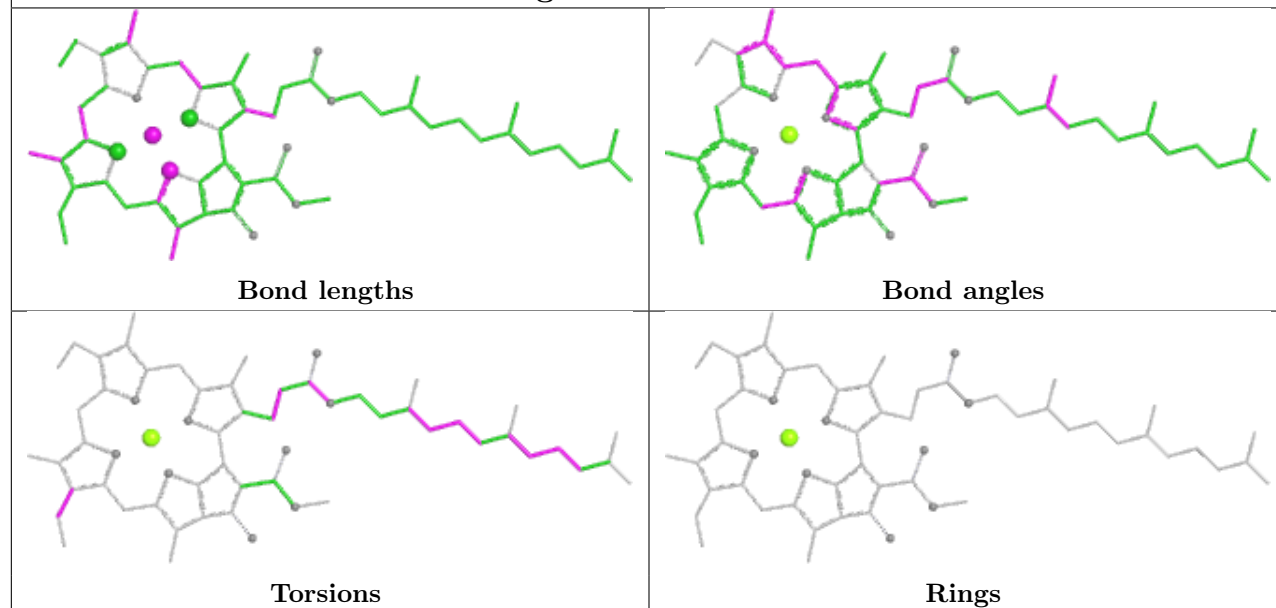
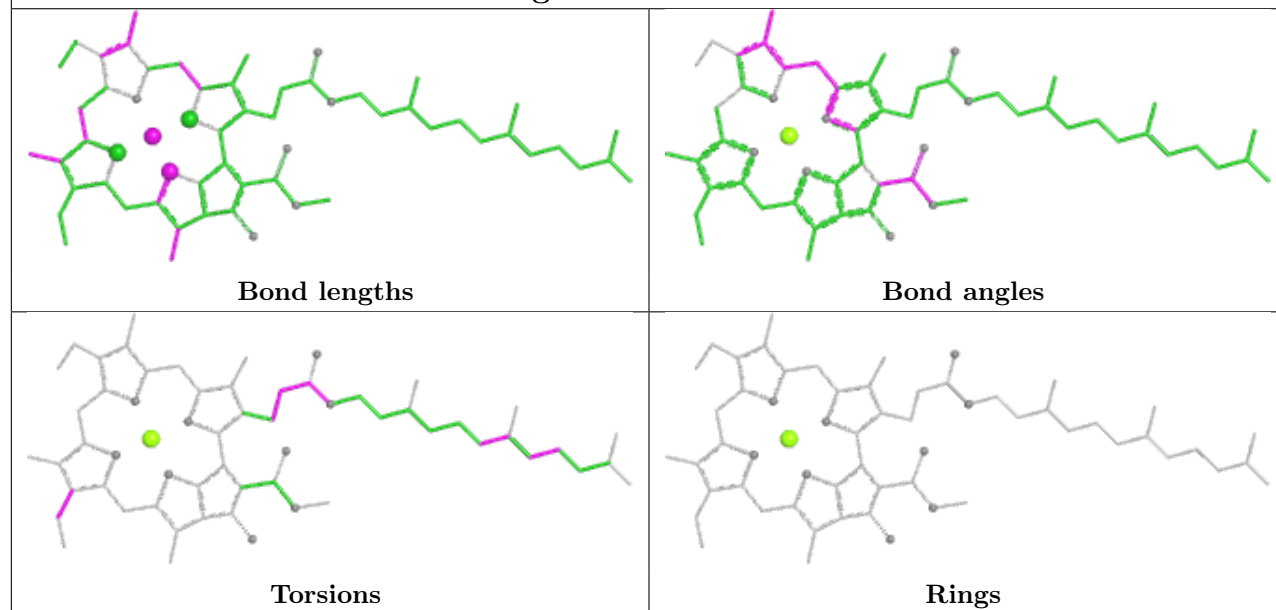


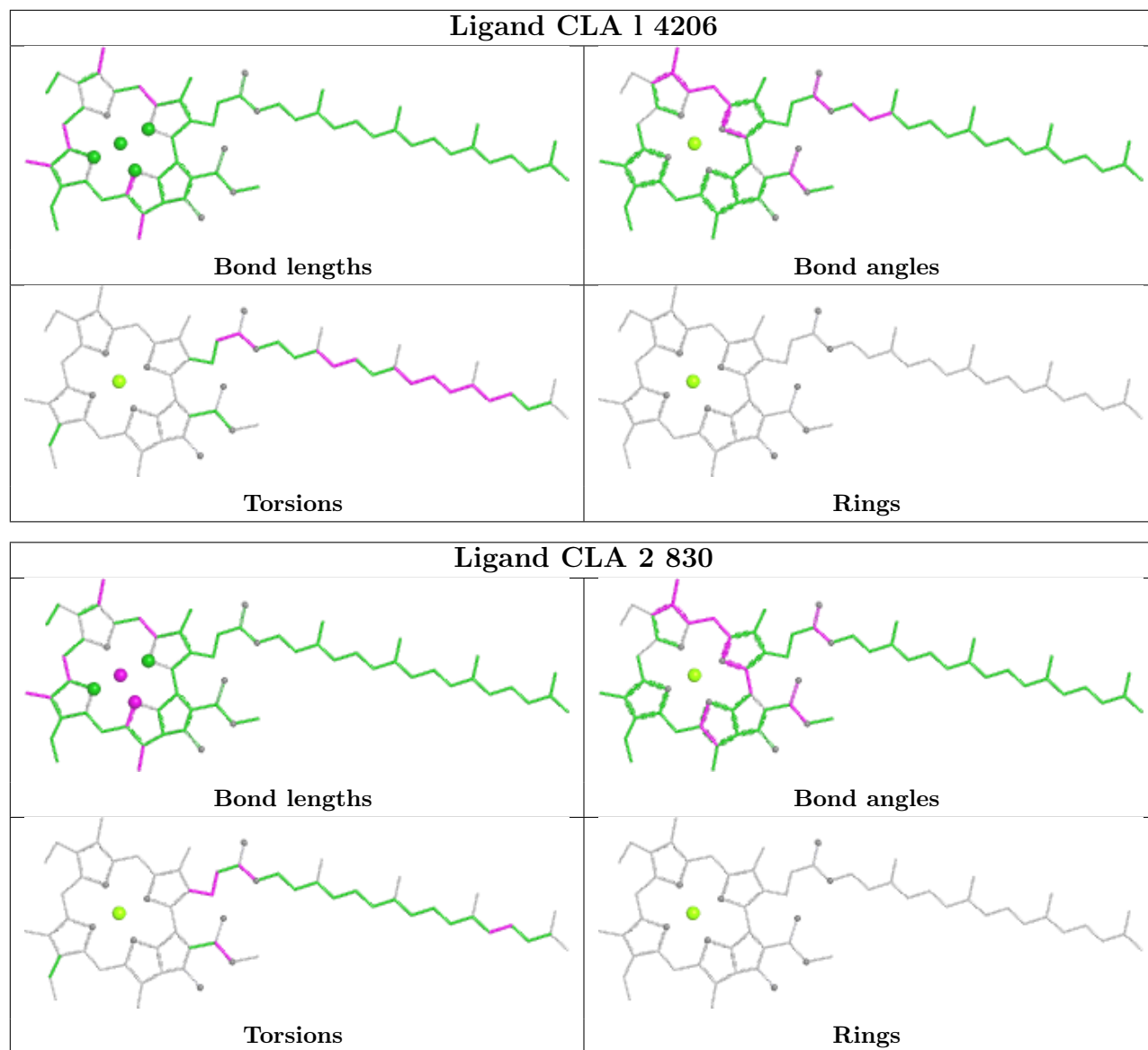
Torsions

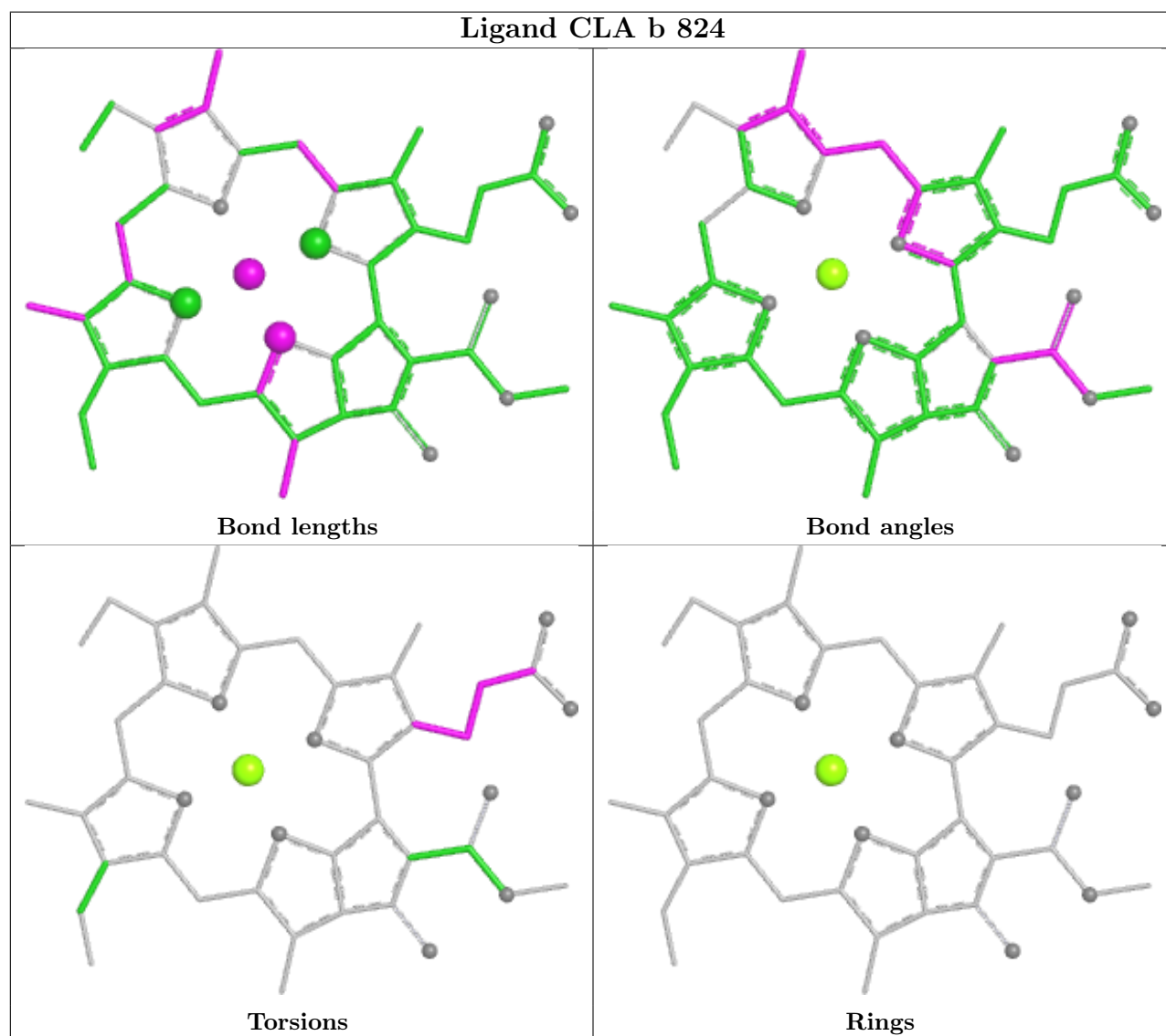
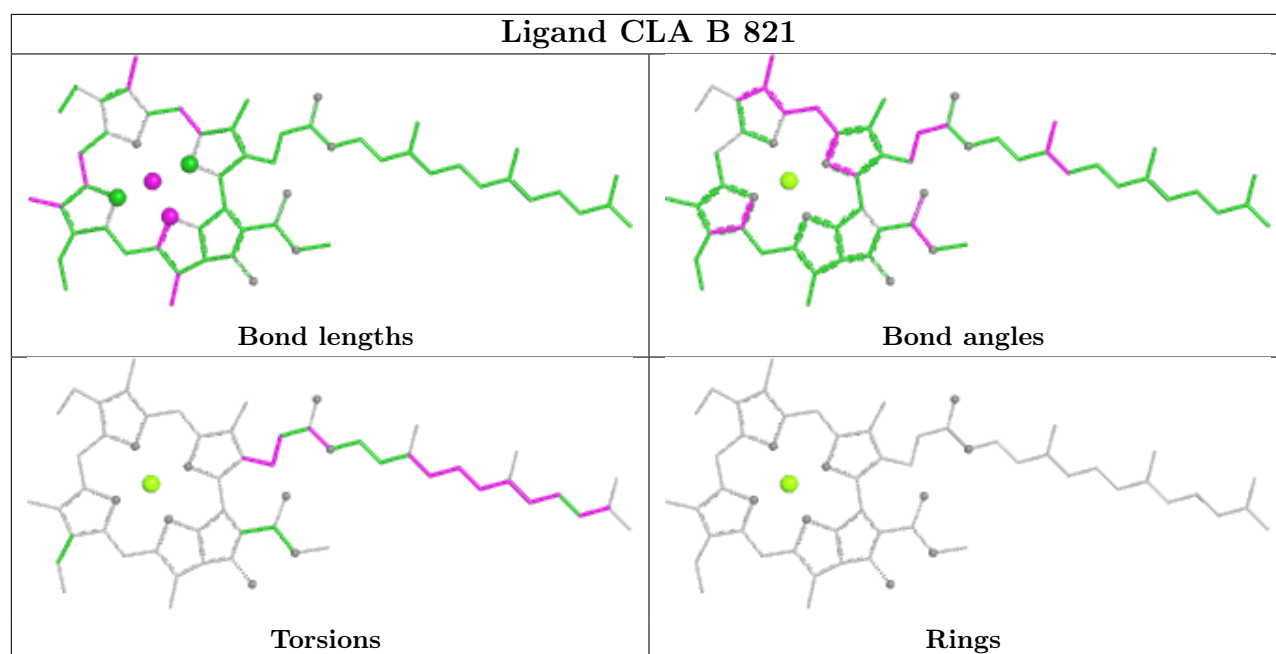


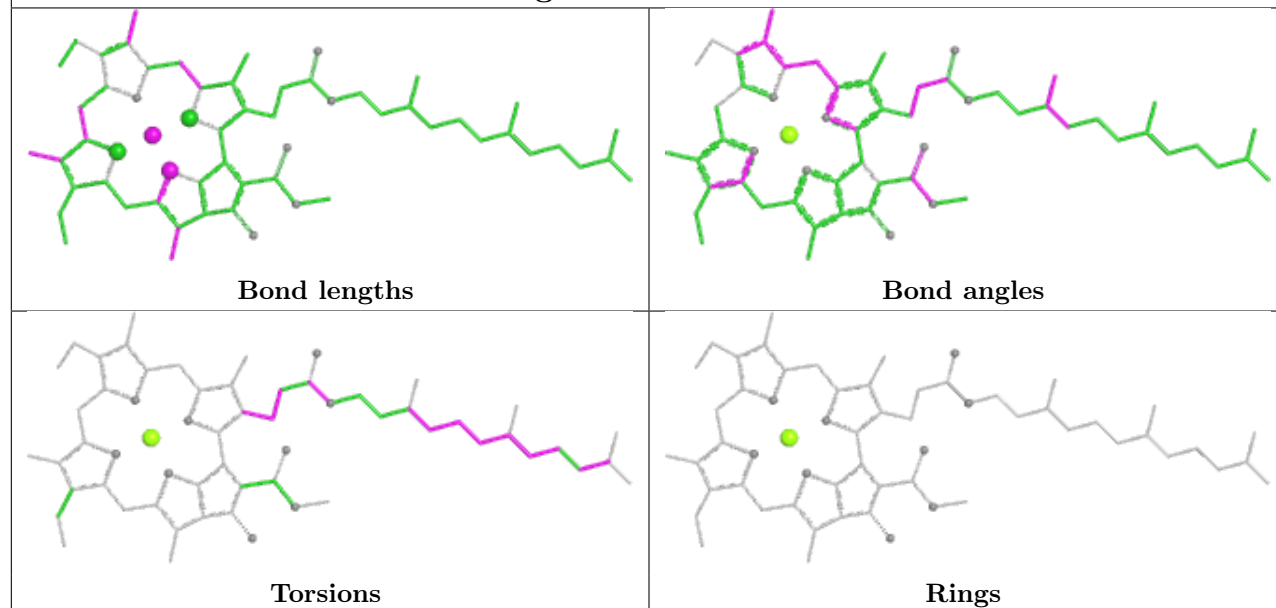
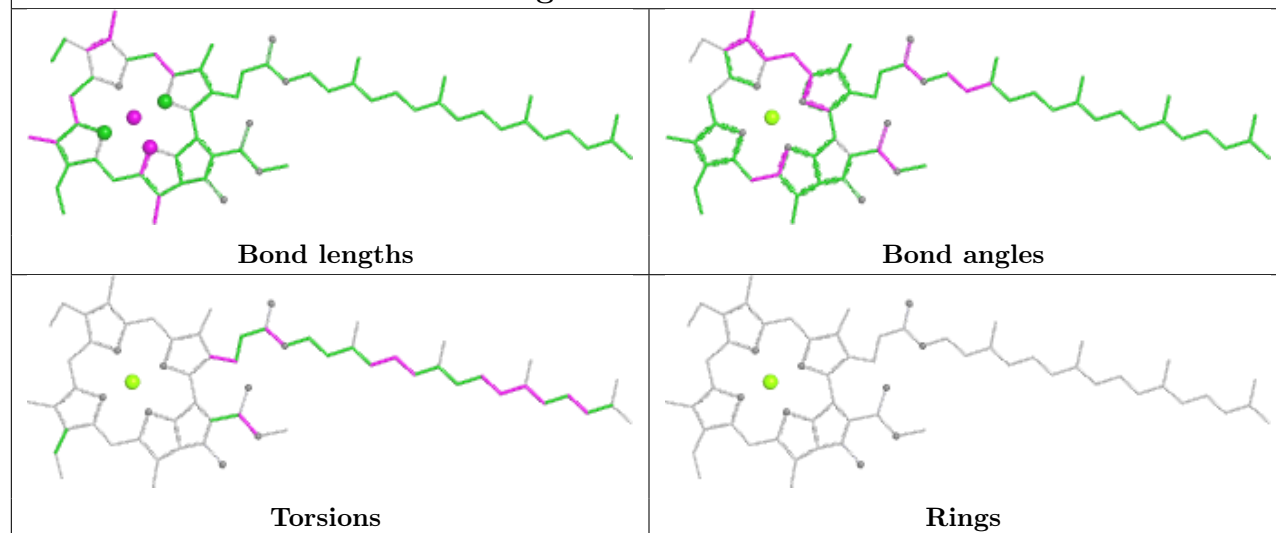
Rings

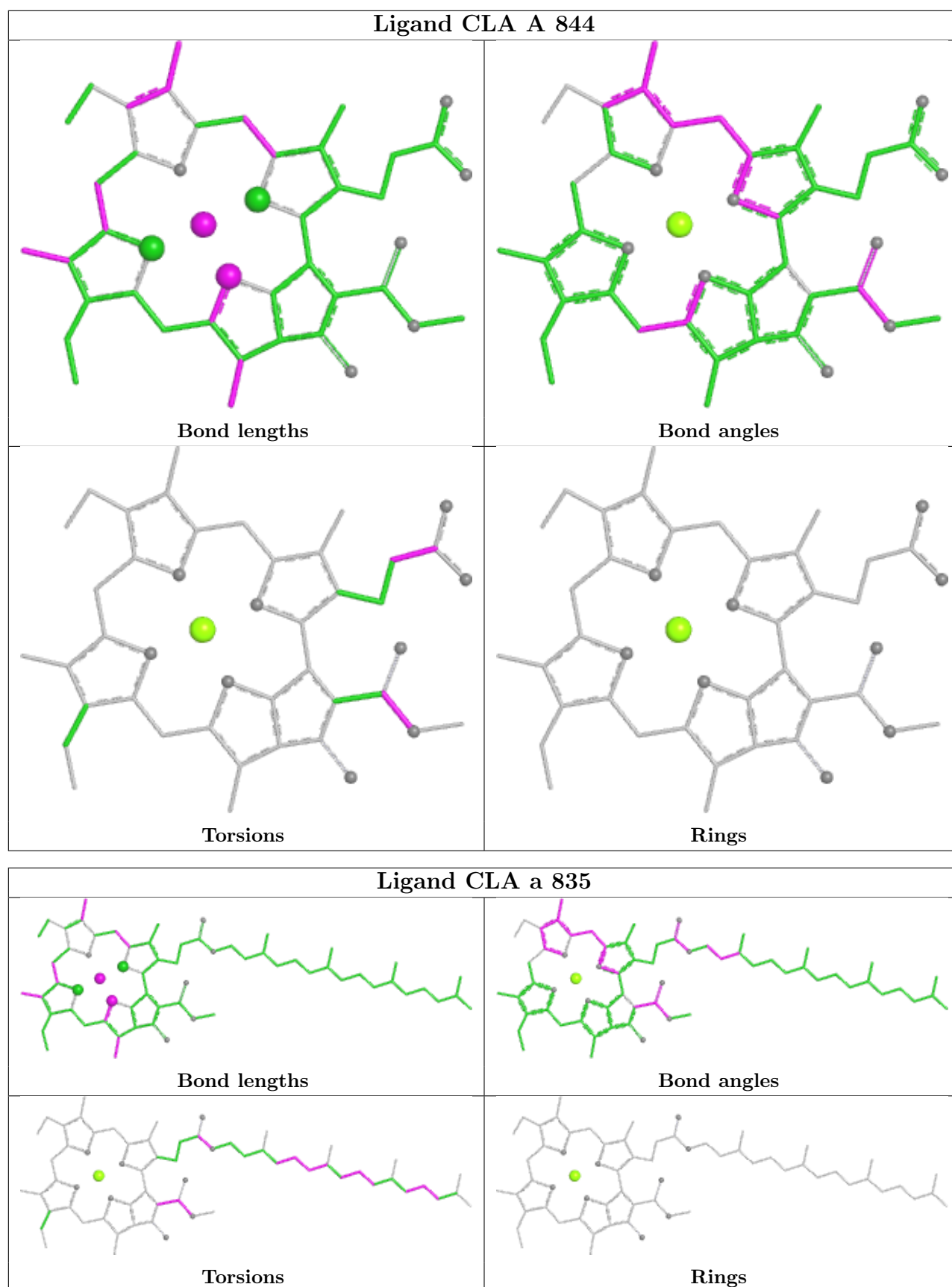


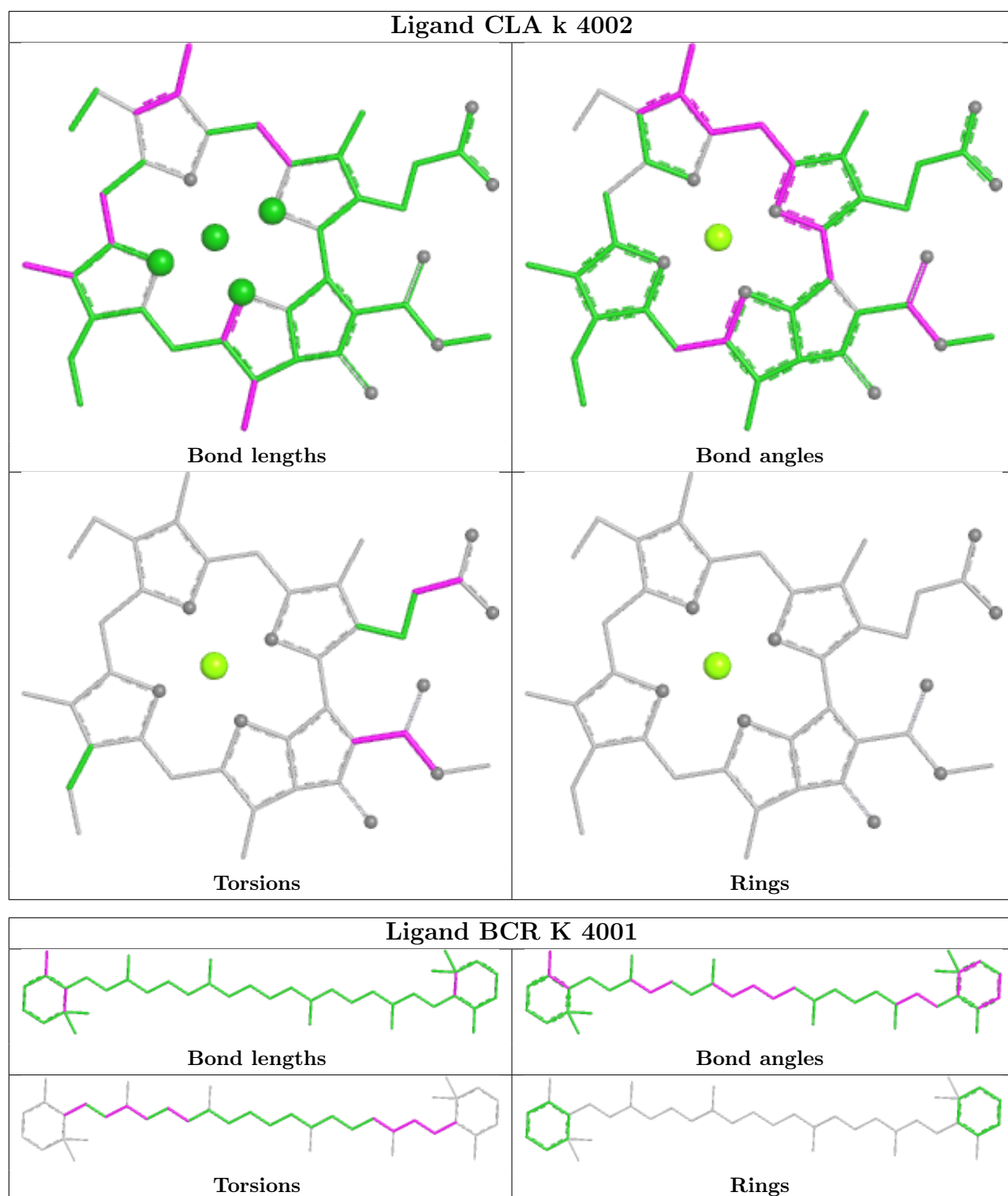
Ligand CLA a 804**Ligand CLA B 830**

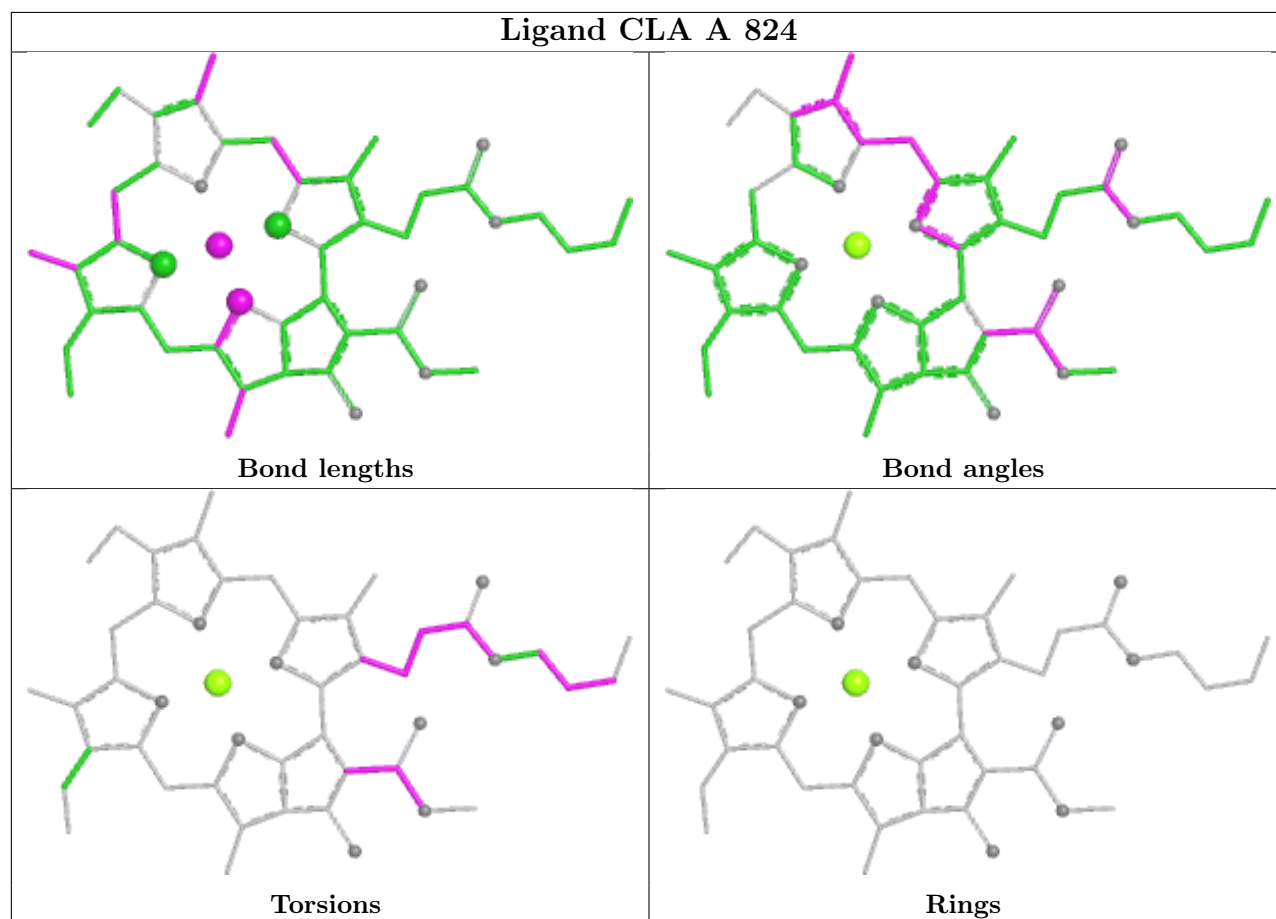
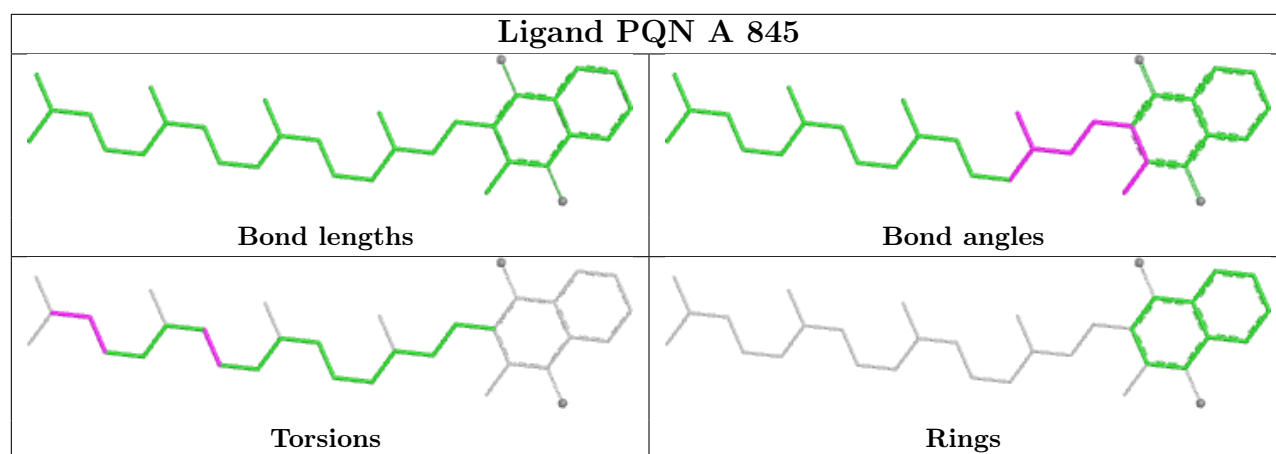


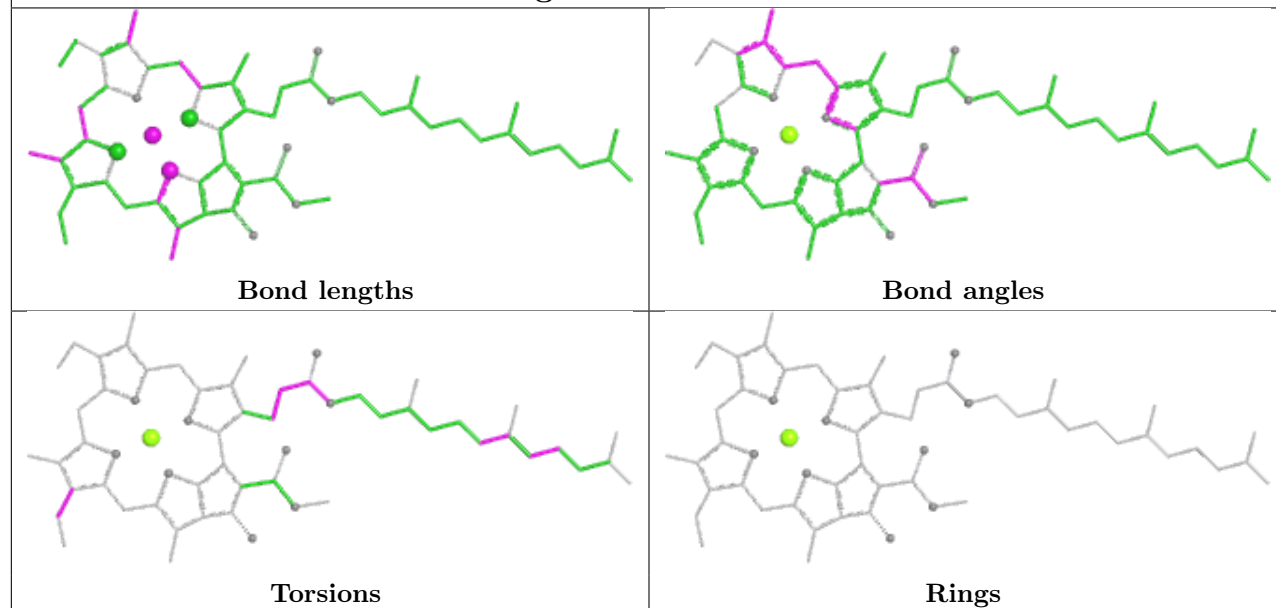
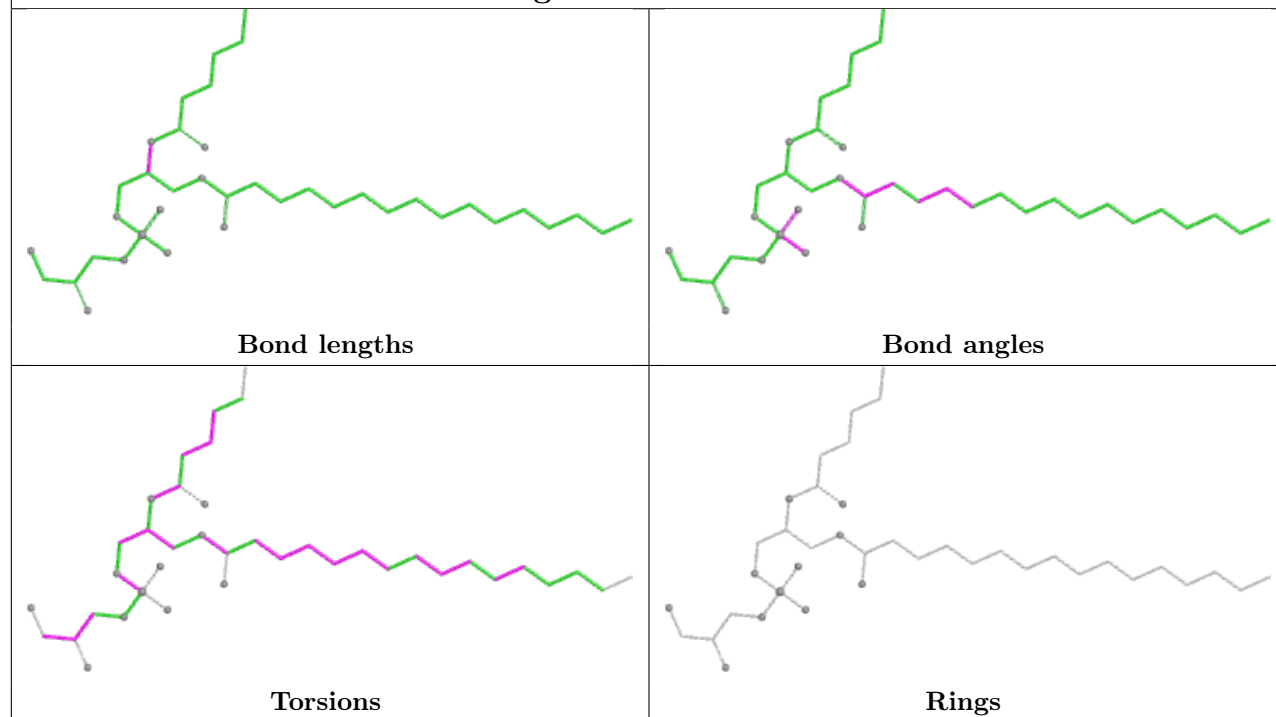


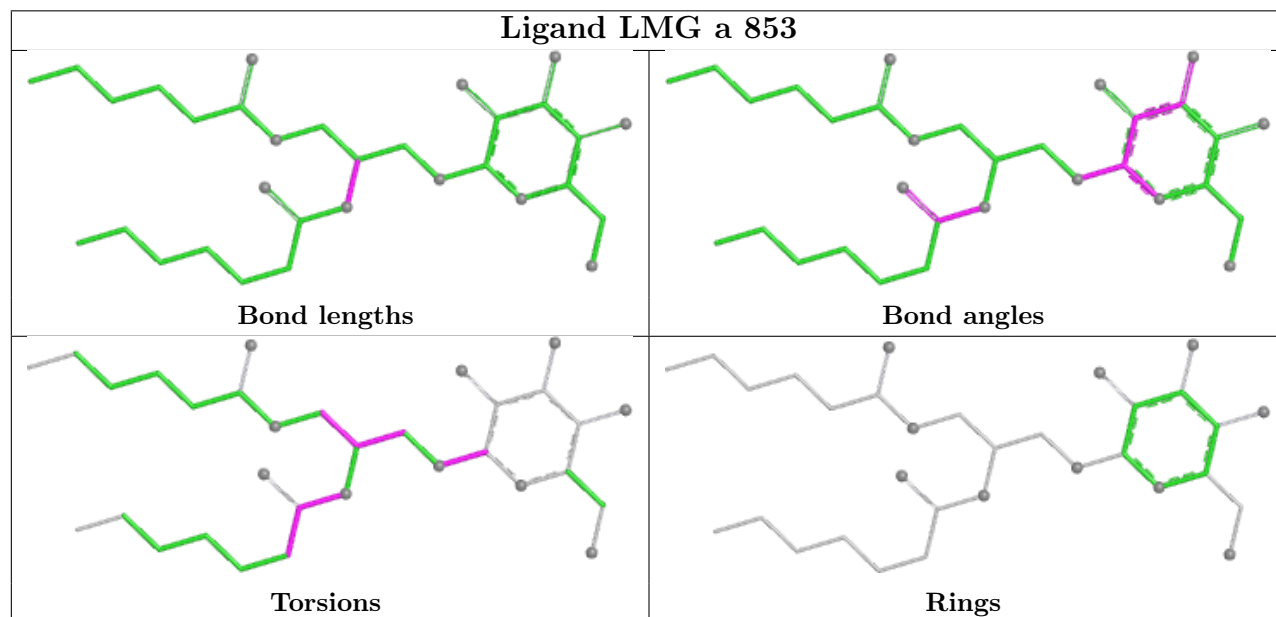
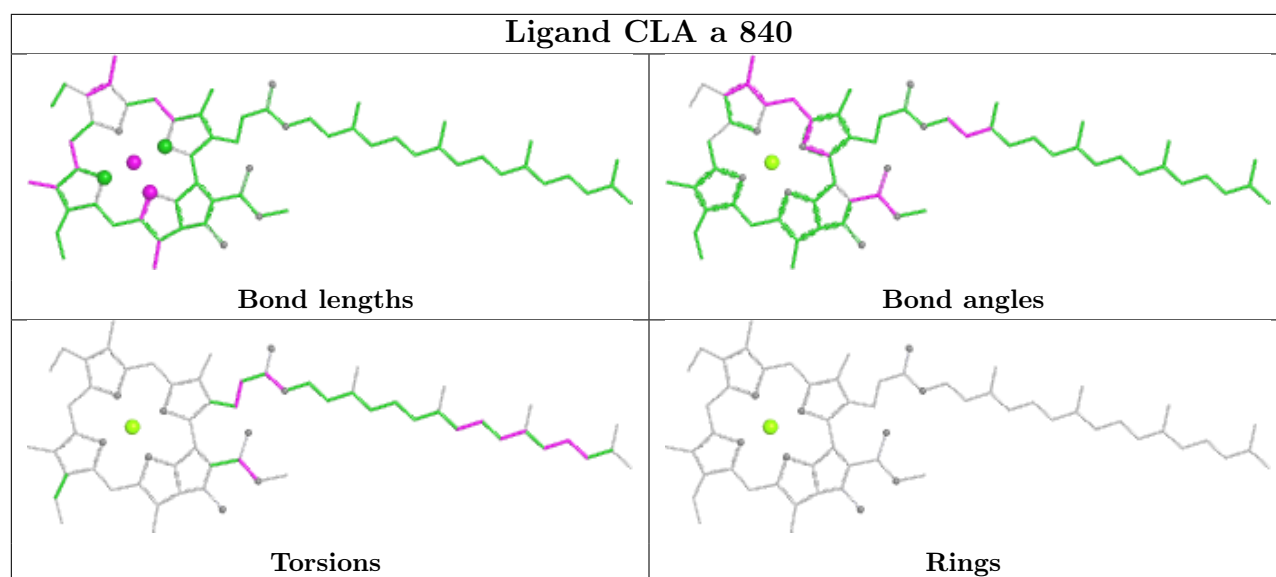
Ligand CLA b 820**Ligand CLA a 809**

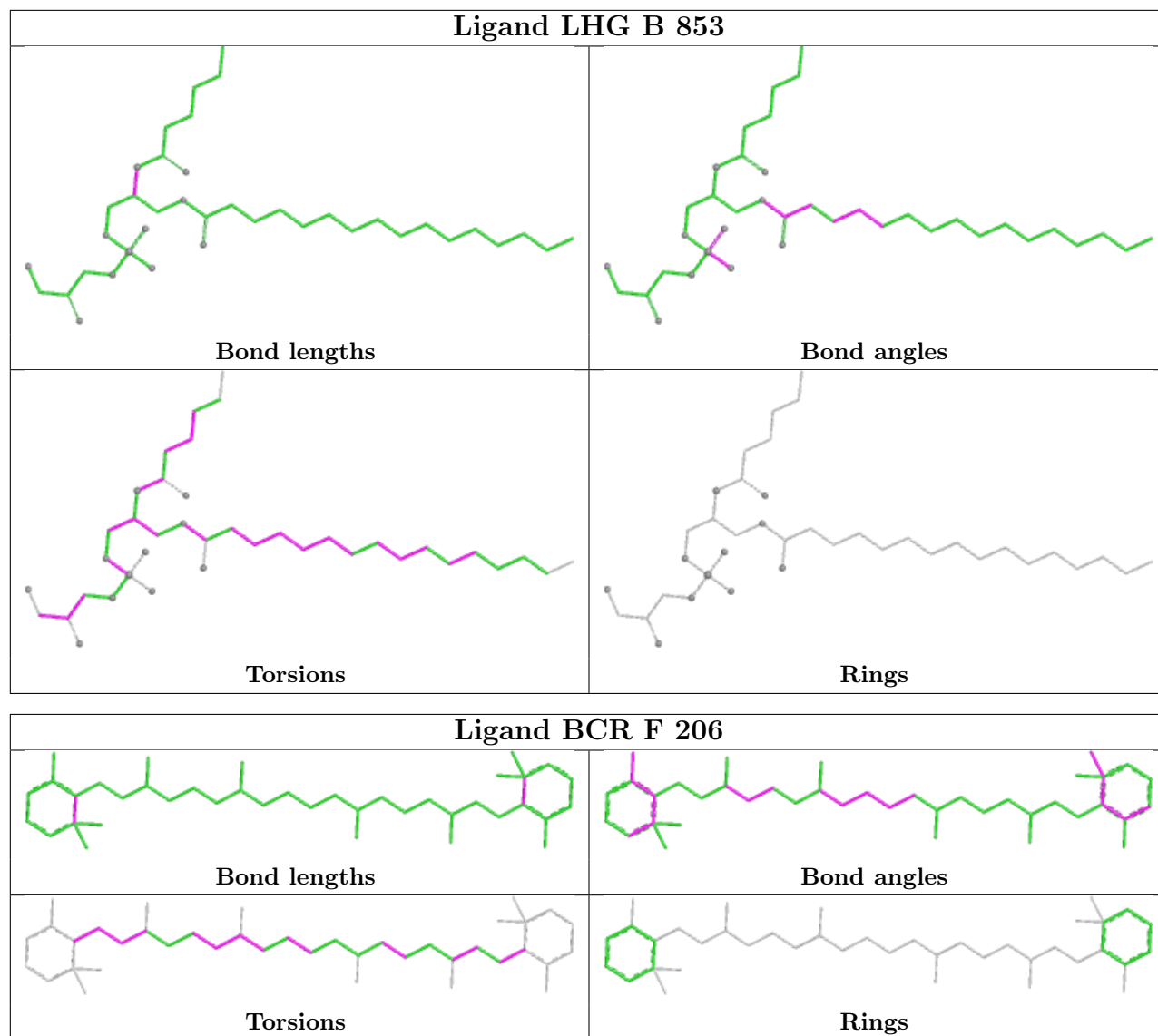




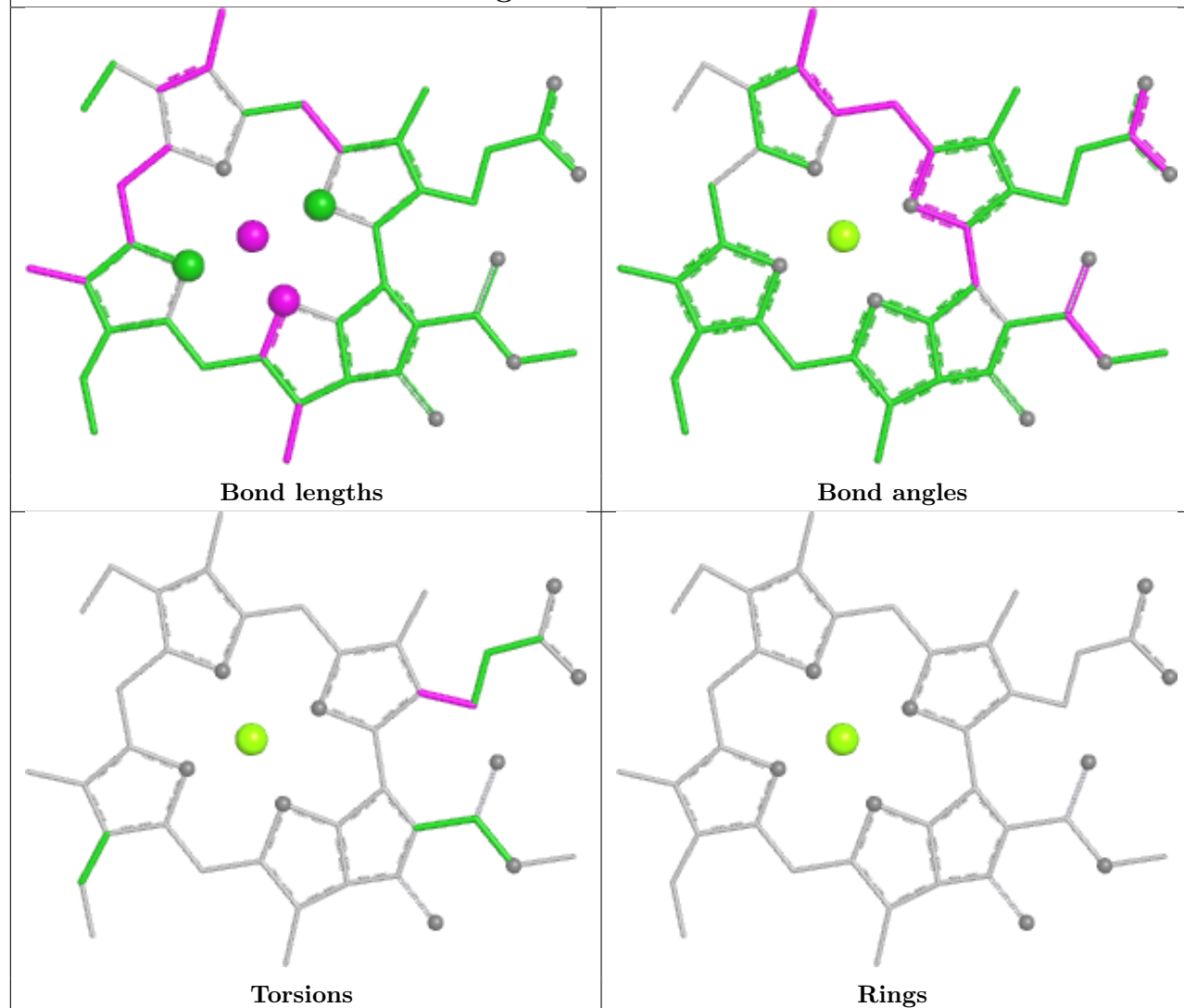


Ligand CLA b 829**Ligand LHG b 852**

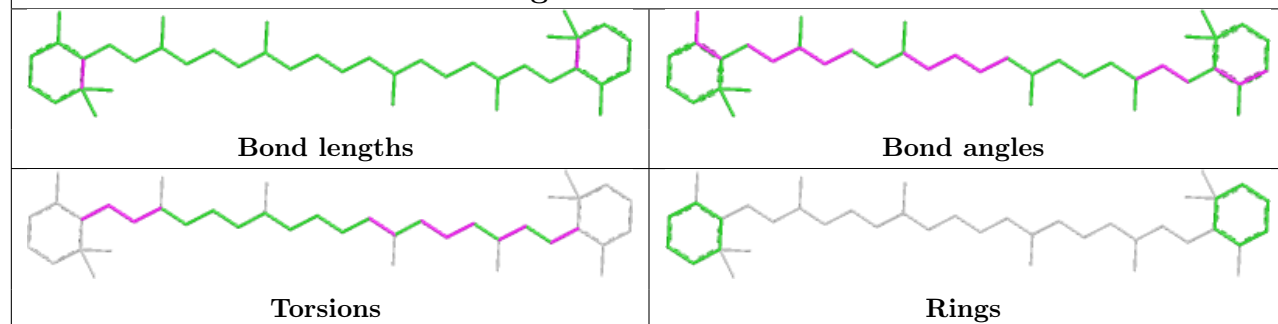


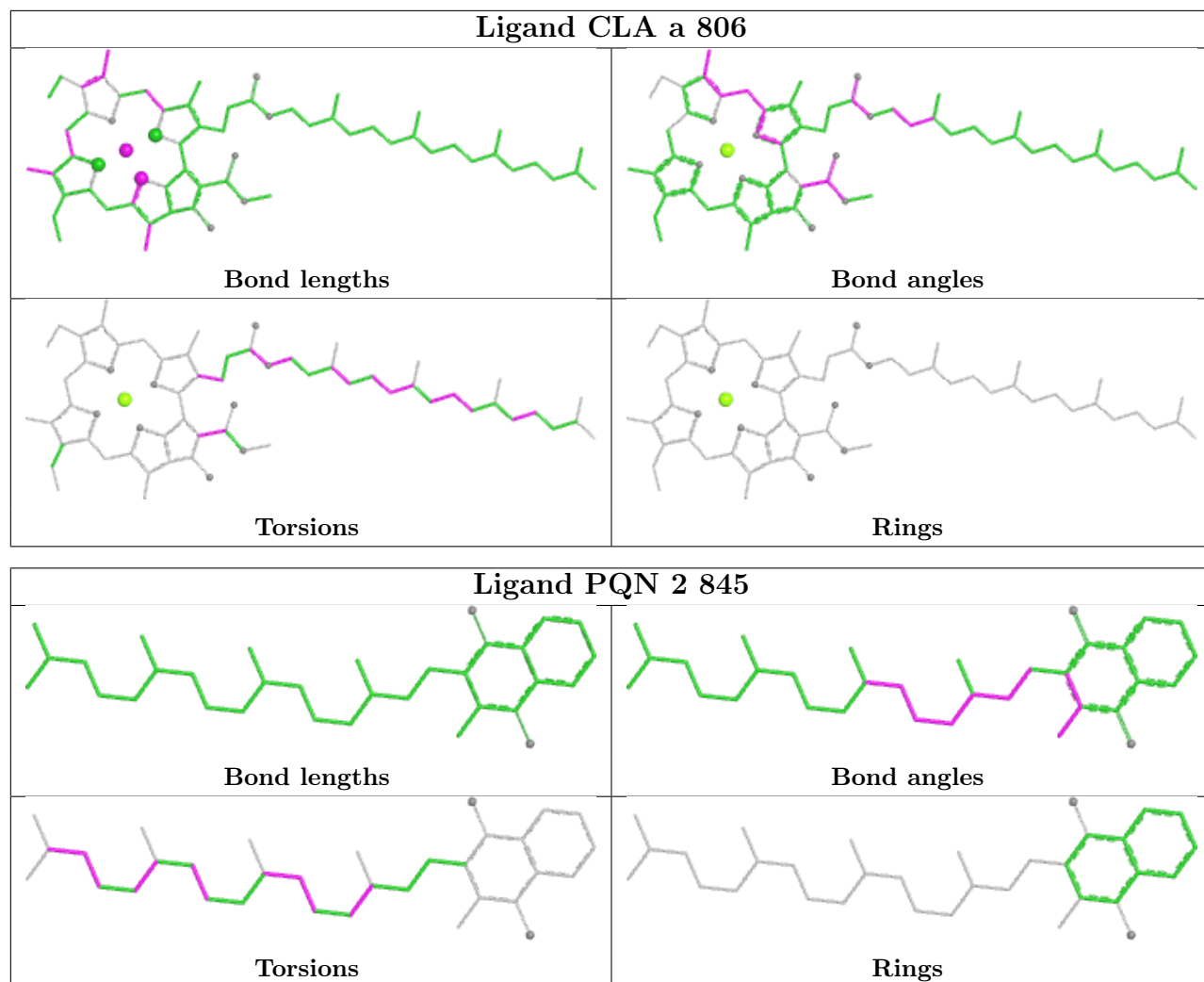


Ligand CLA b 835

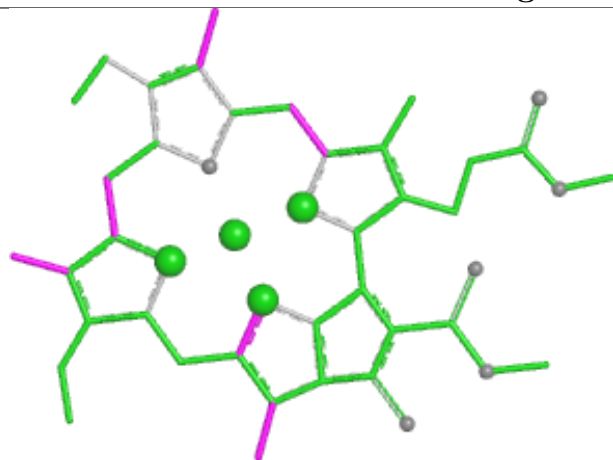


Ligand BCR B 847

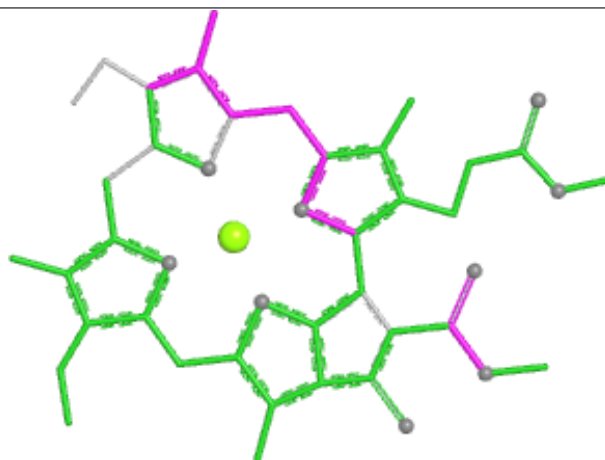




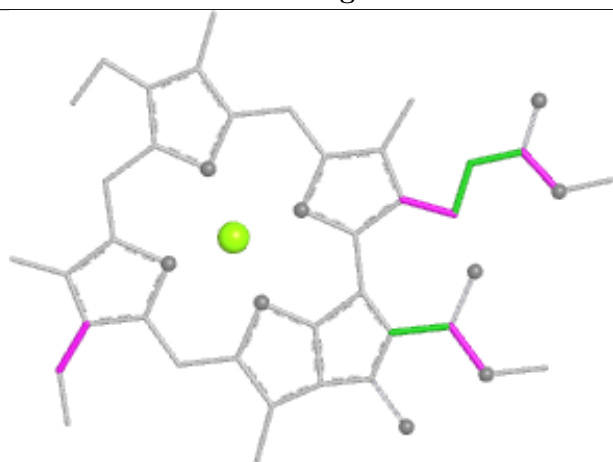
Ligand CLA b 816



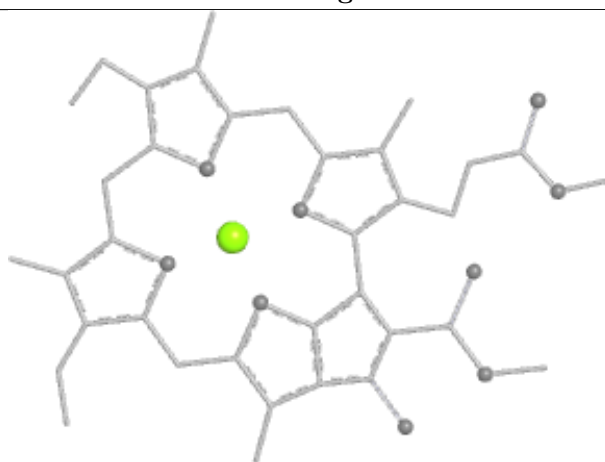
Bond lengths



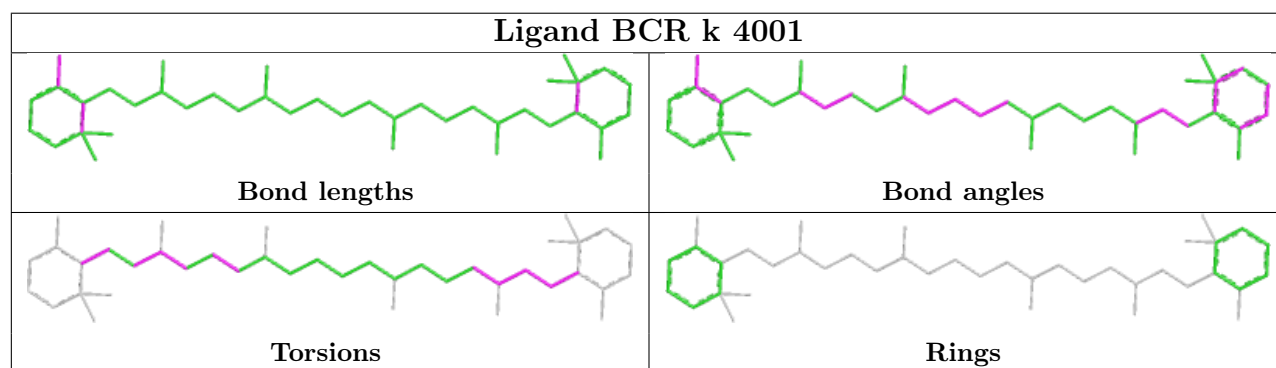
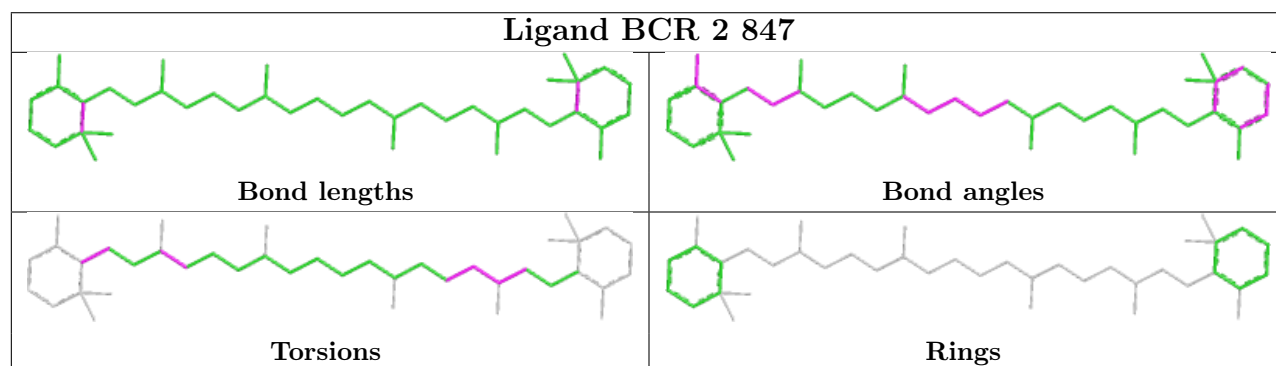
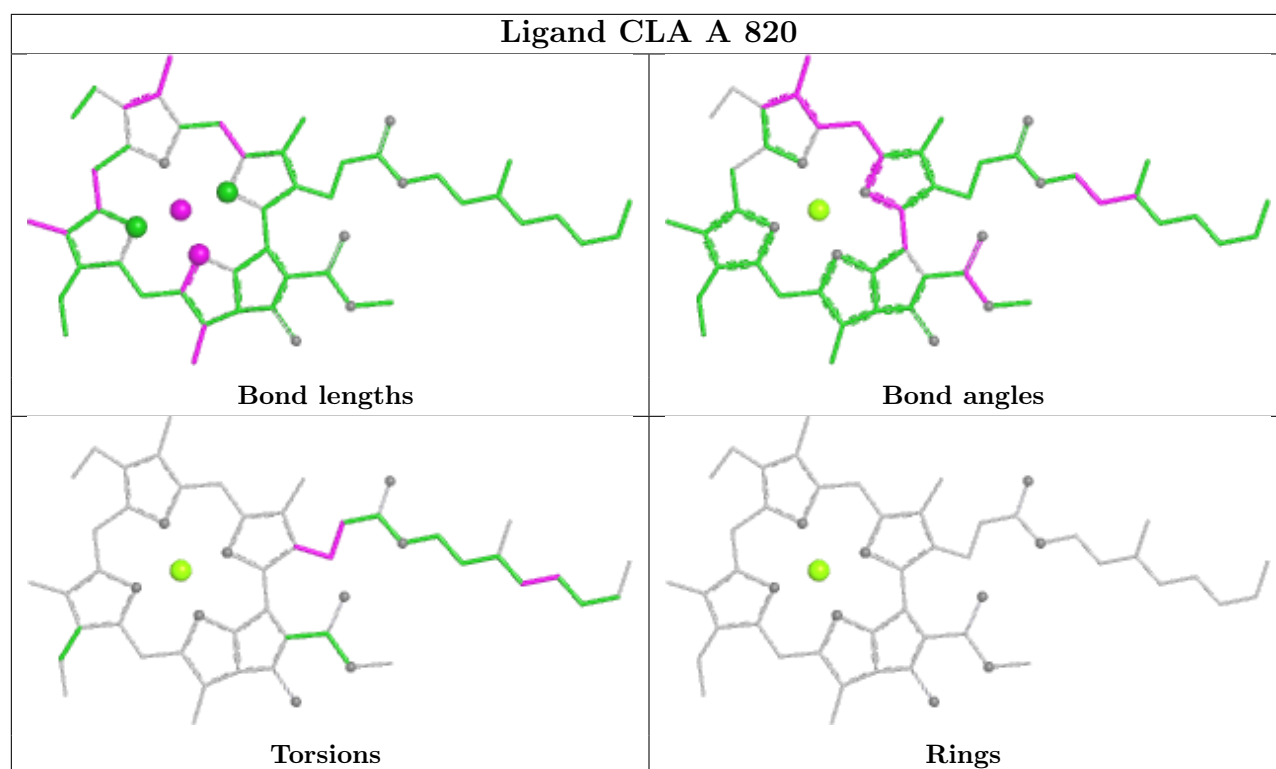
Bond angles

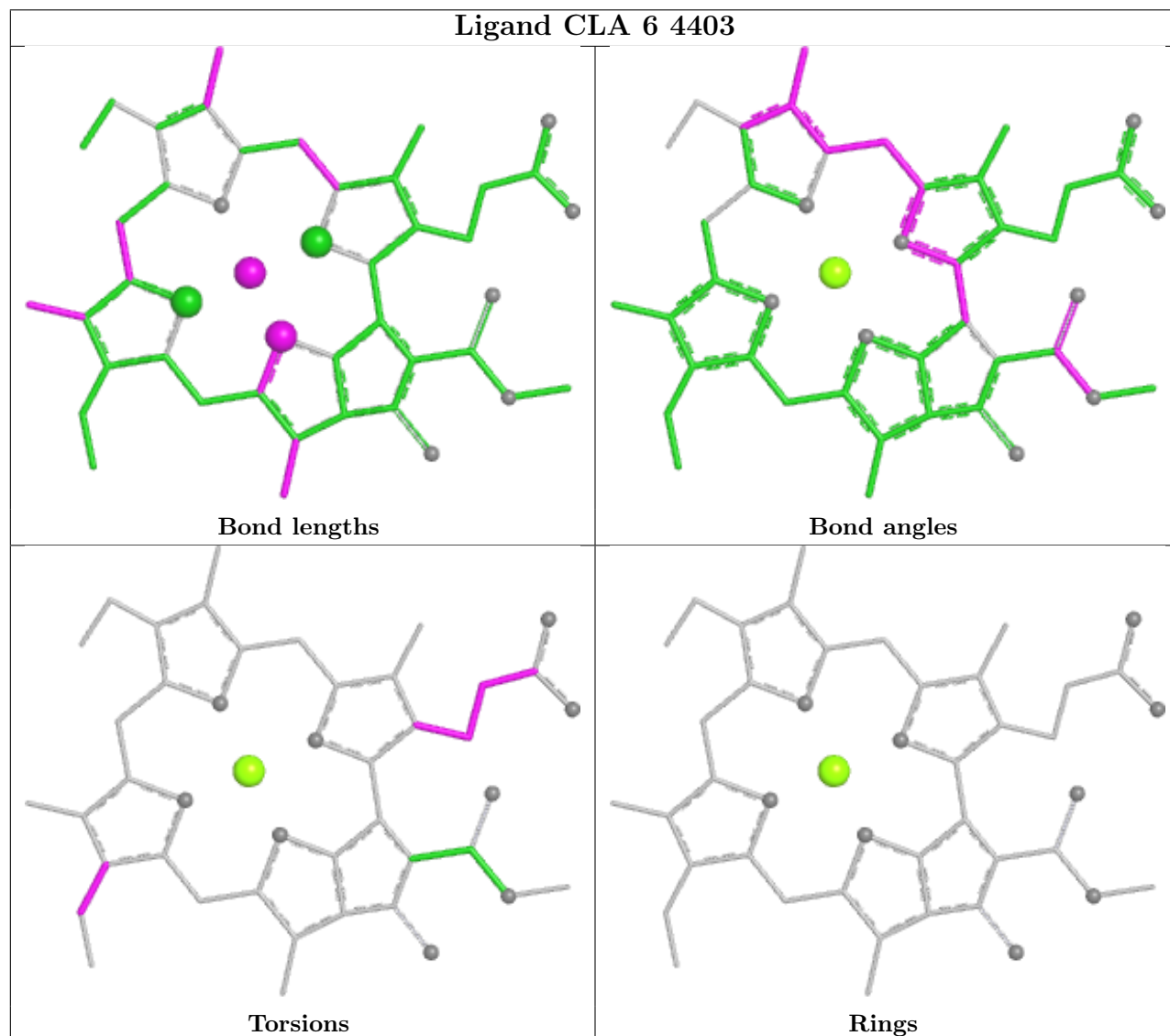
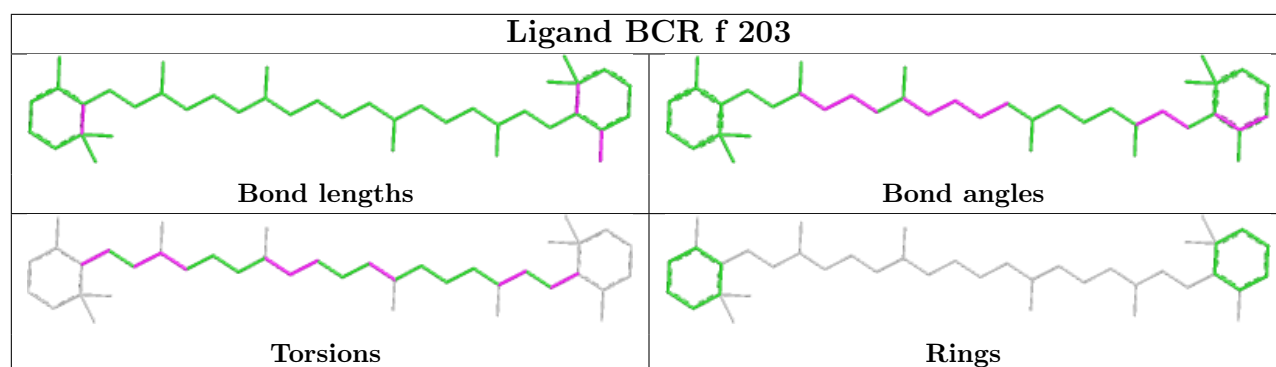


Torsions

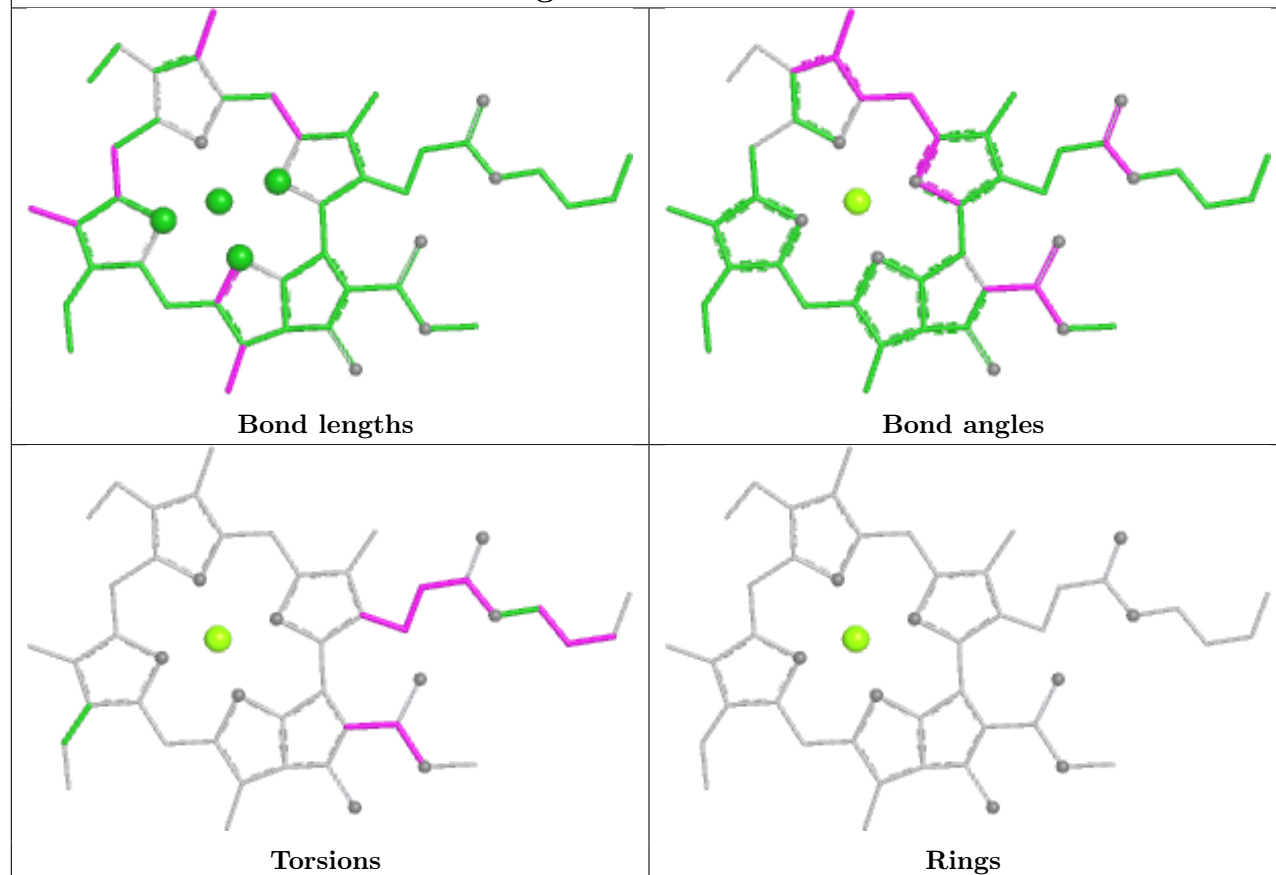


Rings

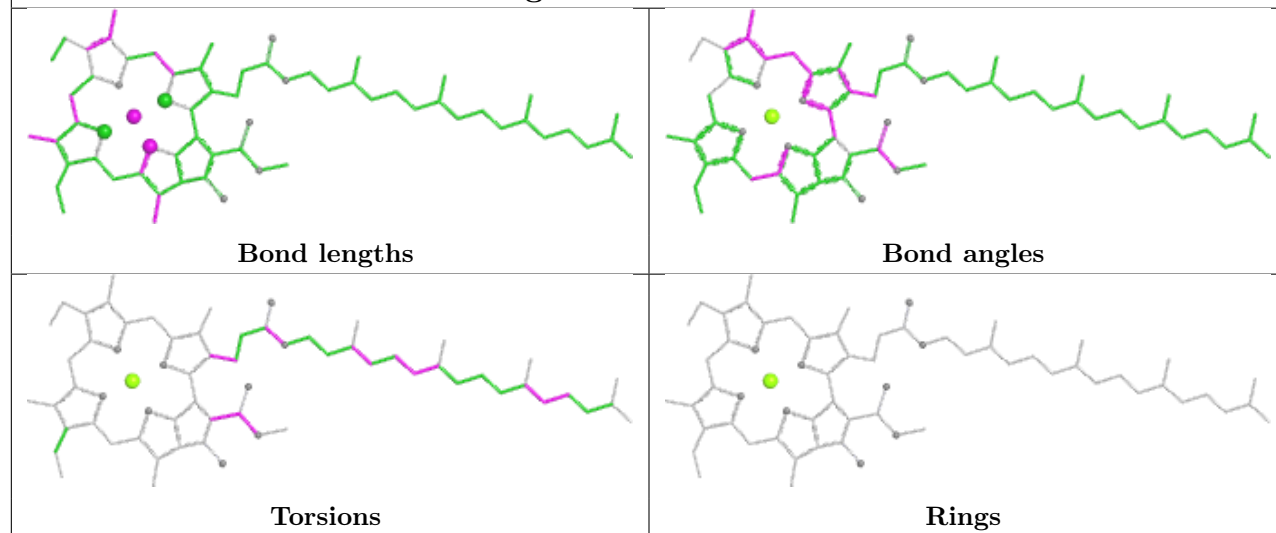




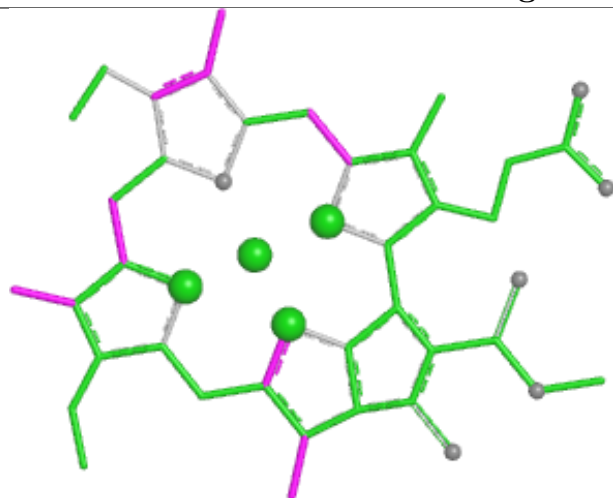
Ligand CLA a 825



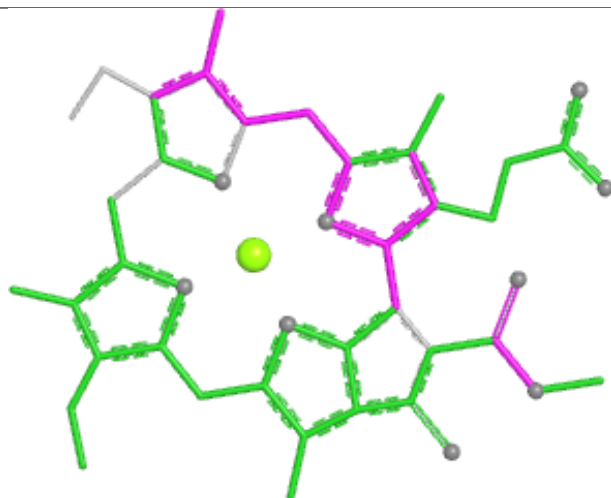
Ligand CLA L 1501



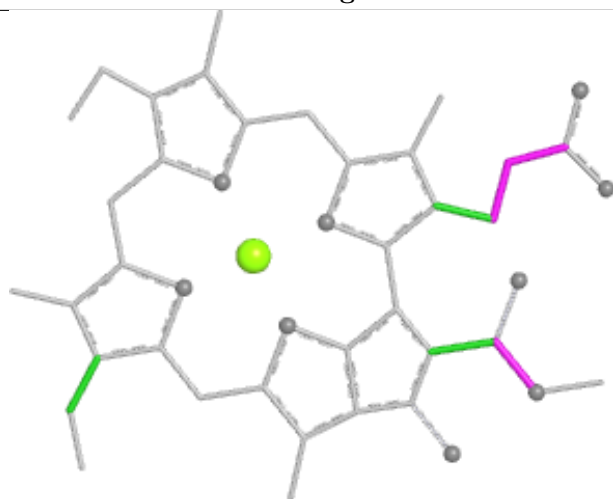
Ligand CLA 1 836



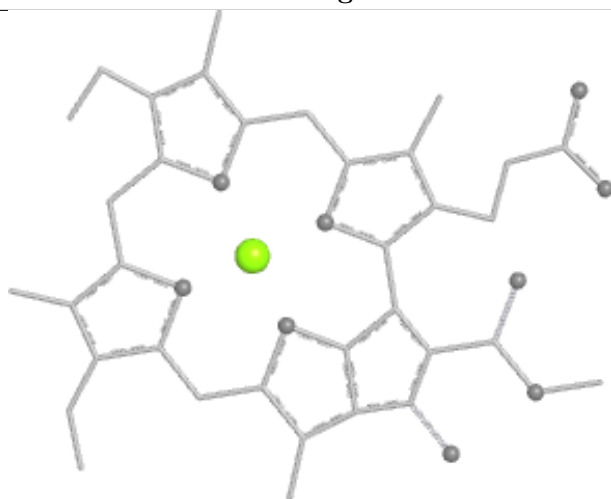
Bond lengths



Bond angles

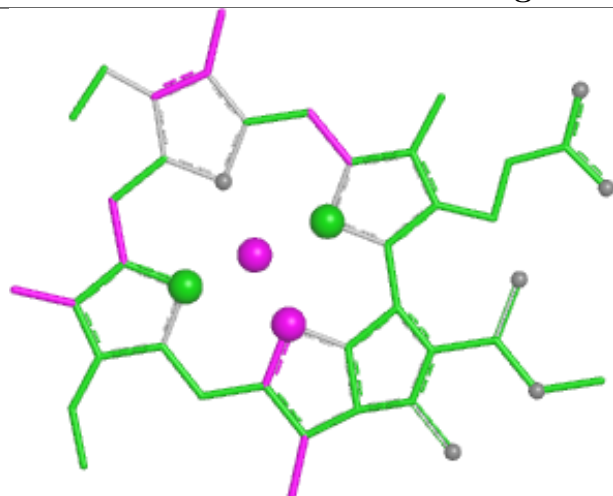


Torsions

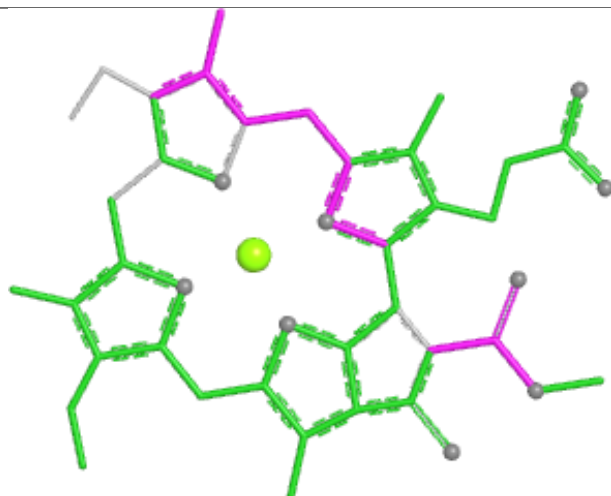


Rings

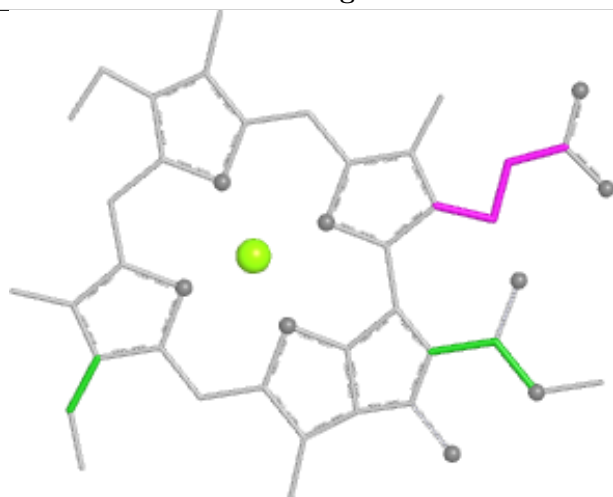
Ligand CLA B 825



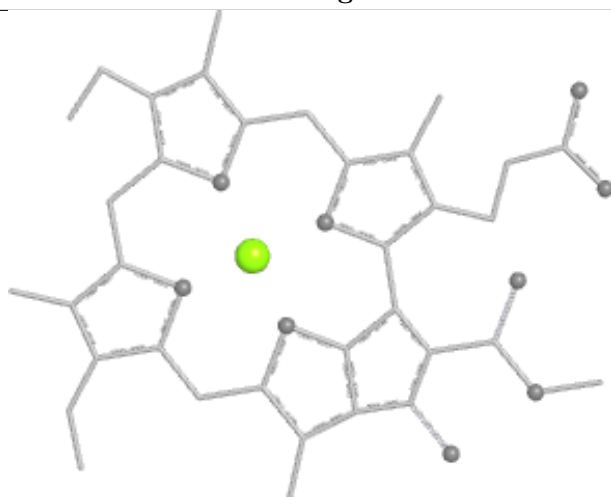
Bond lengths



Bond angles

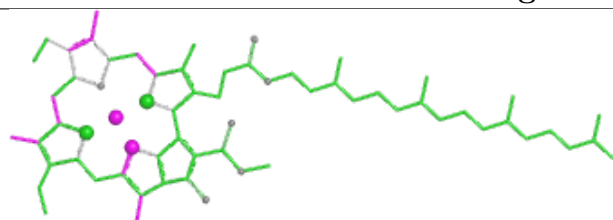


Torsions

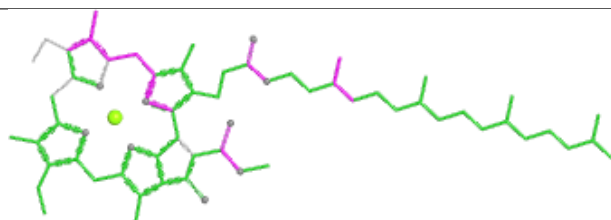


Rings

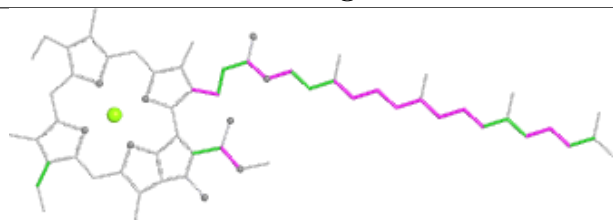
Ligand CLA a 814



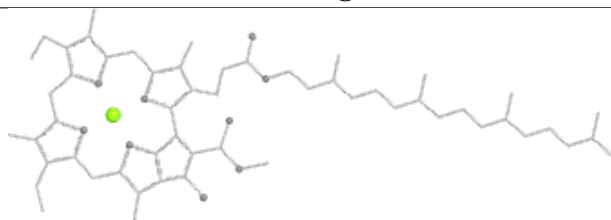
Bond lengths



Bond angles

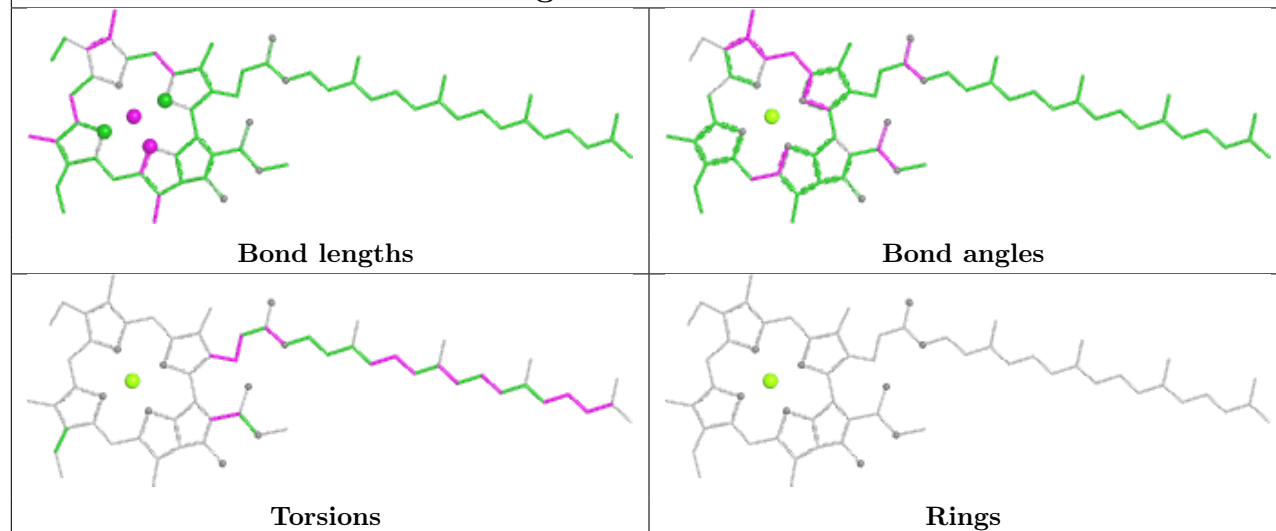


Torsions

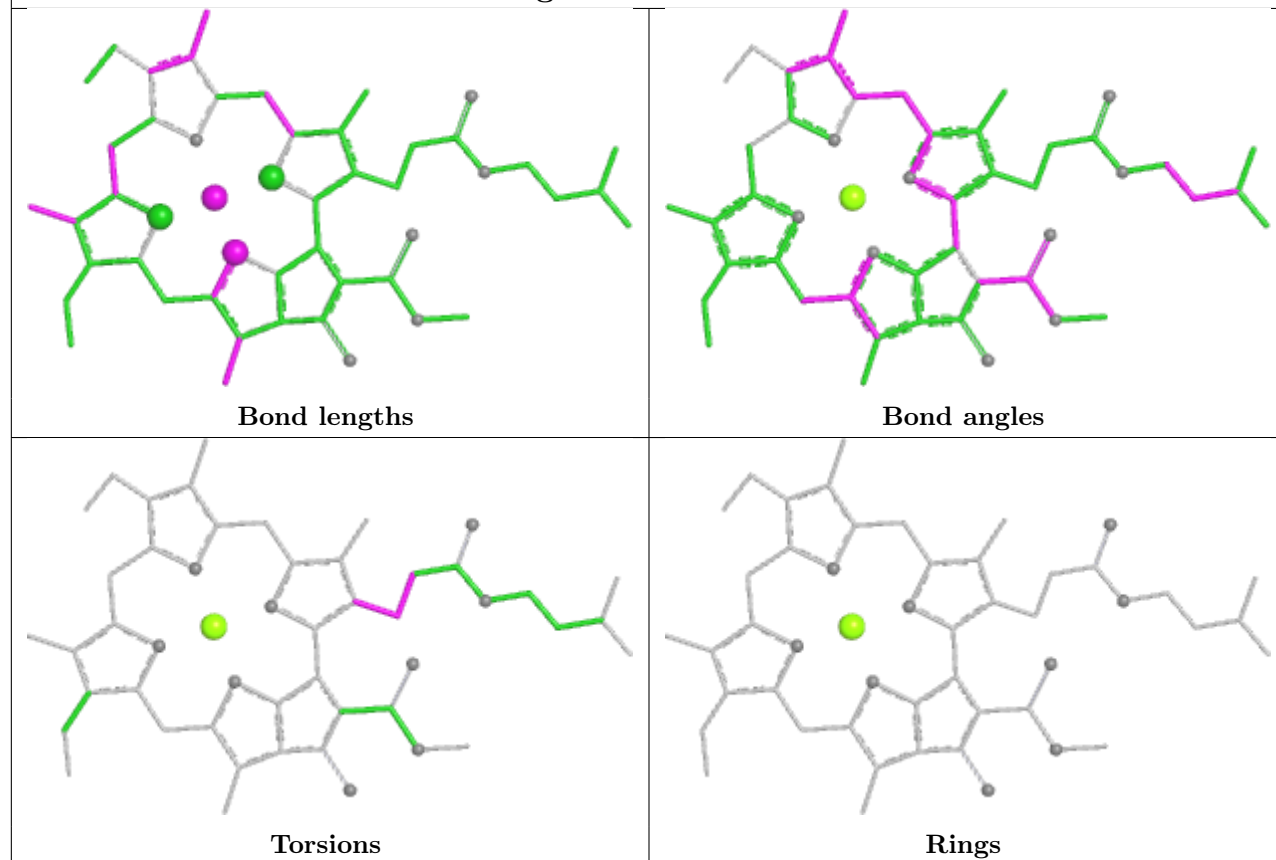


Rings

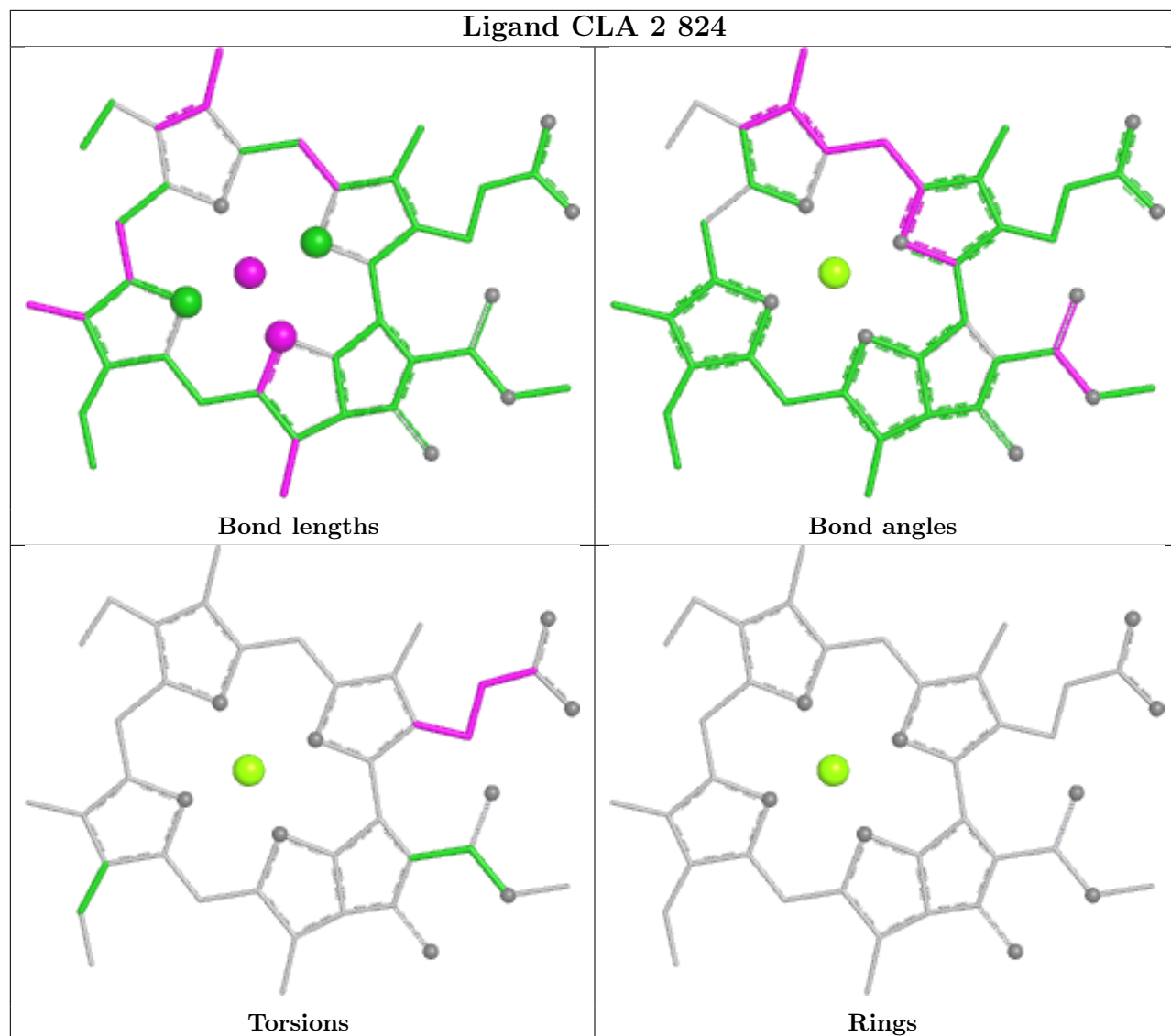
Ligand CLA a 808



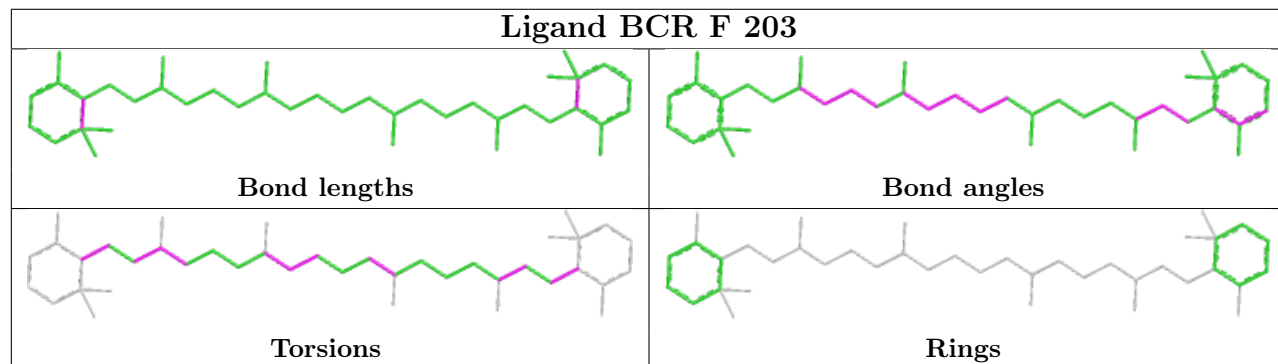
Ligand CLA 1 832

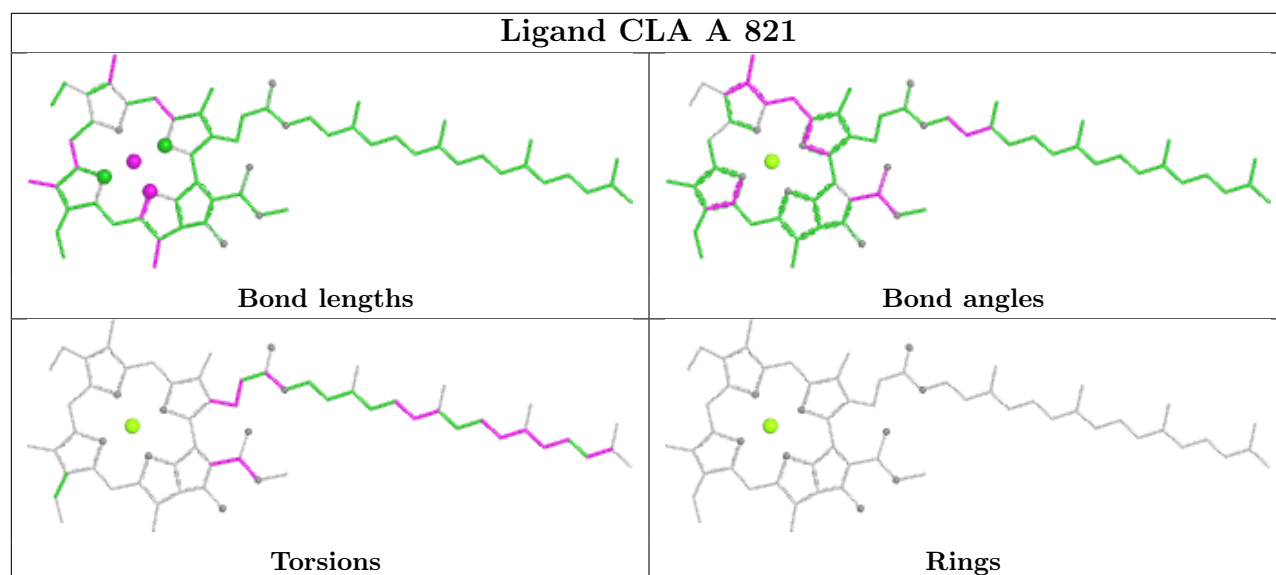
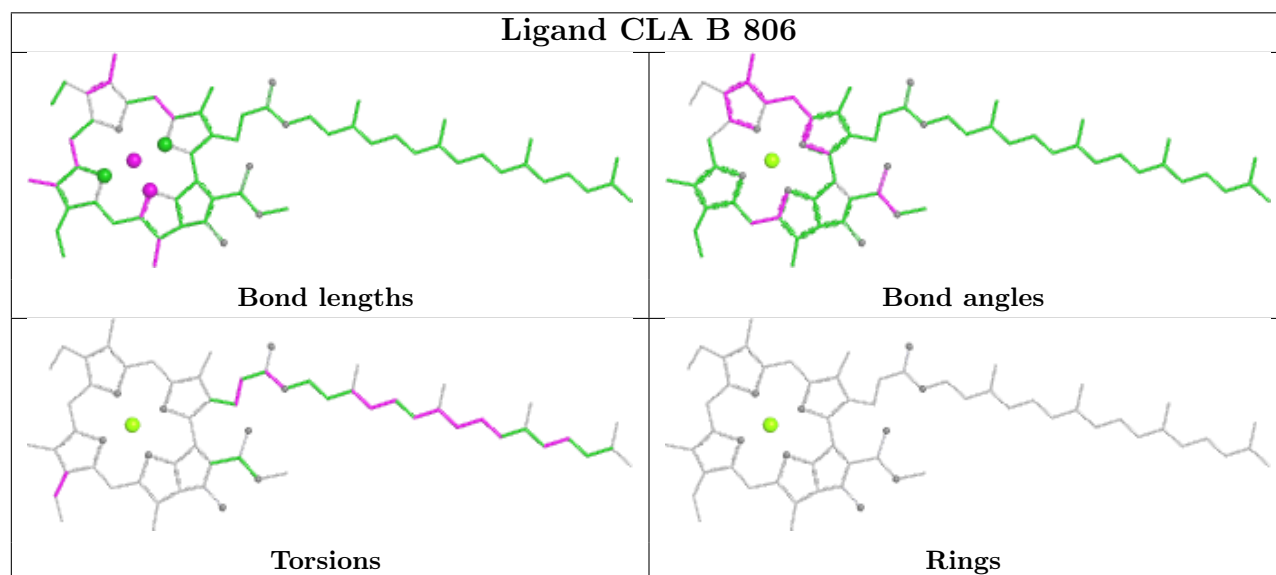
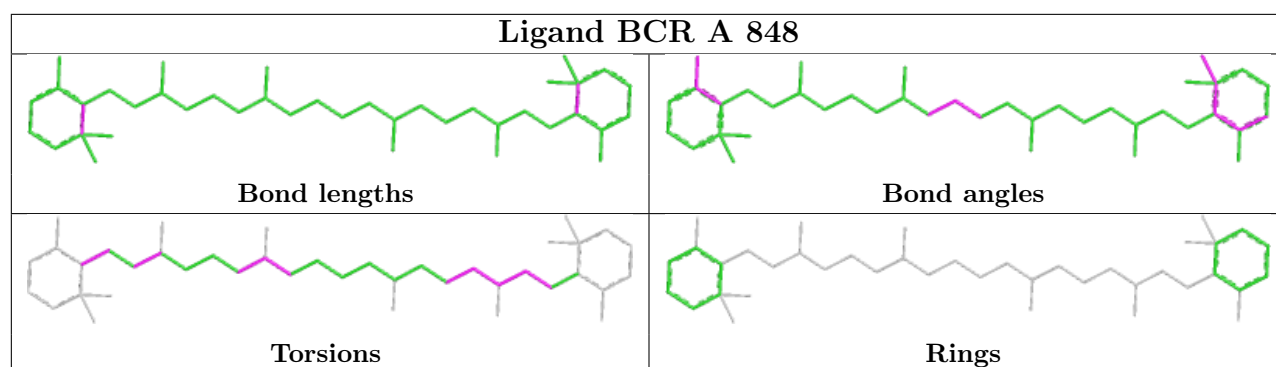


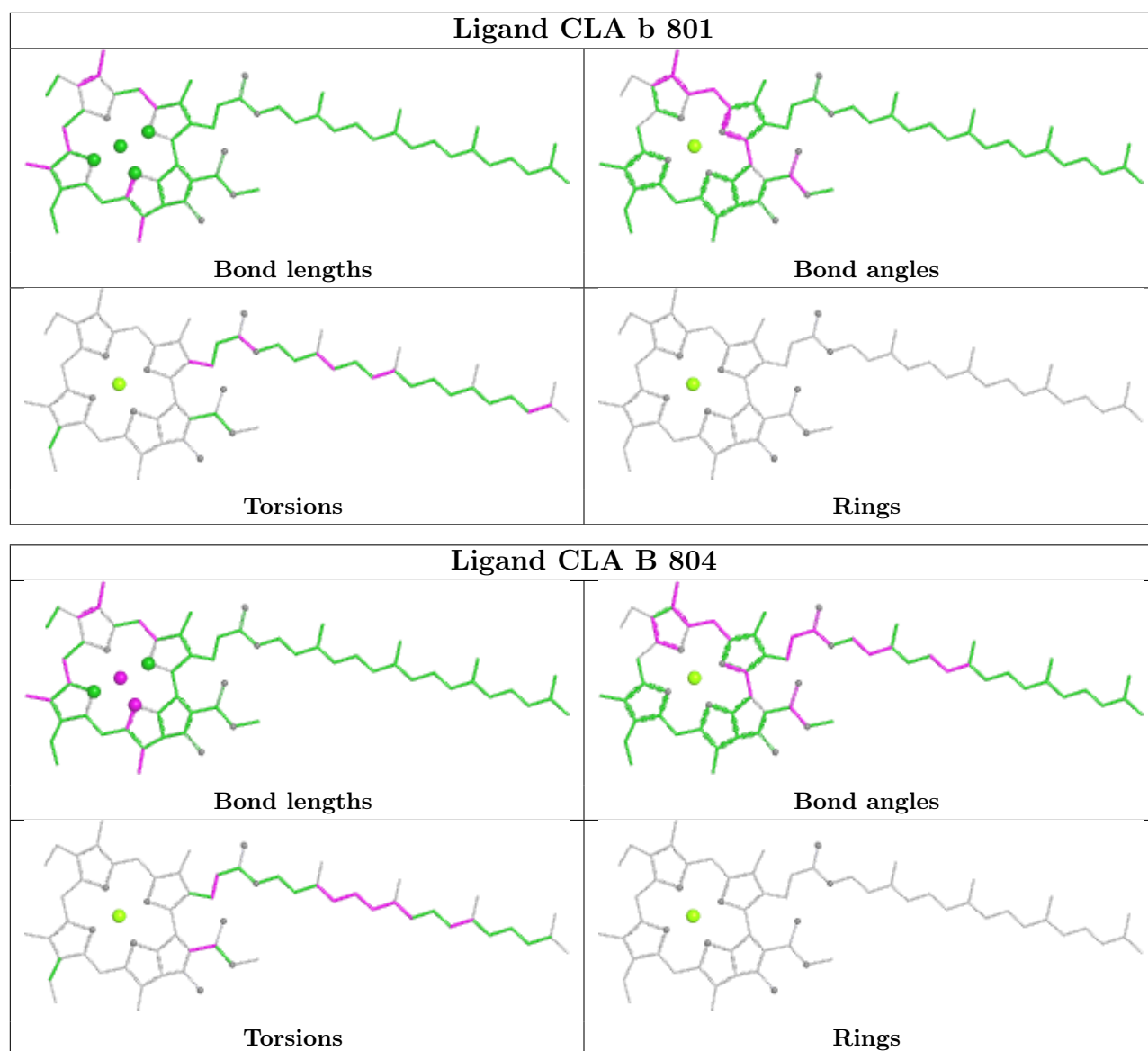
Ligand CLA 2 824



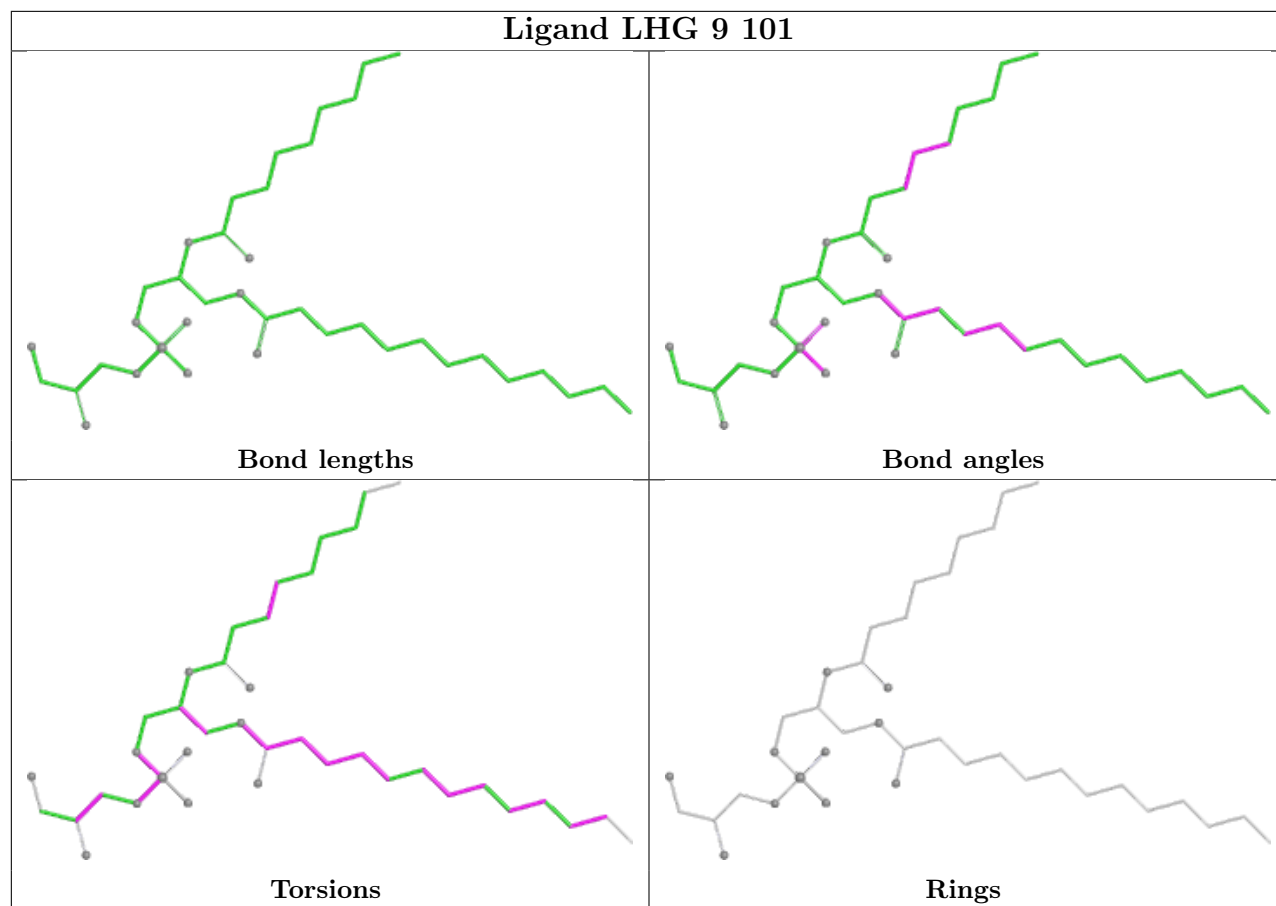
Ligand BCR F 203



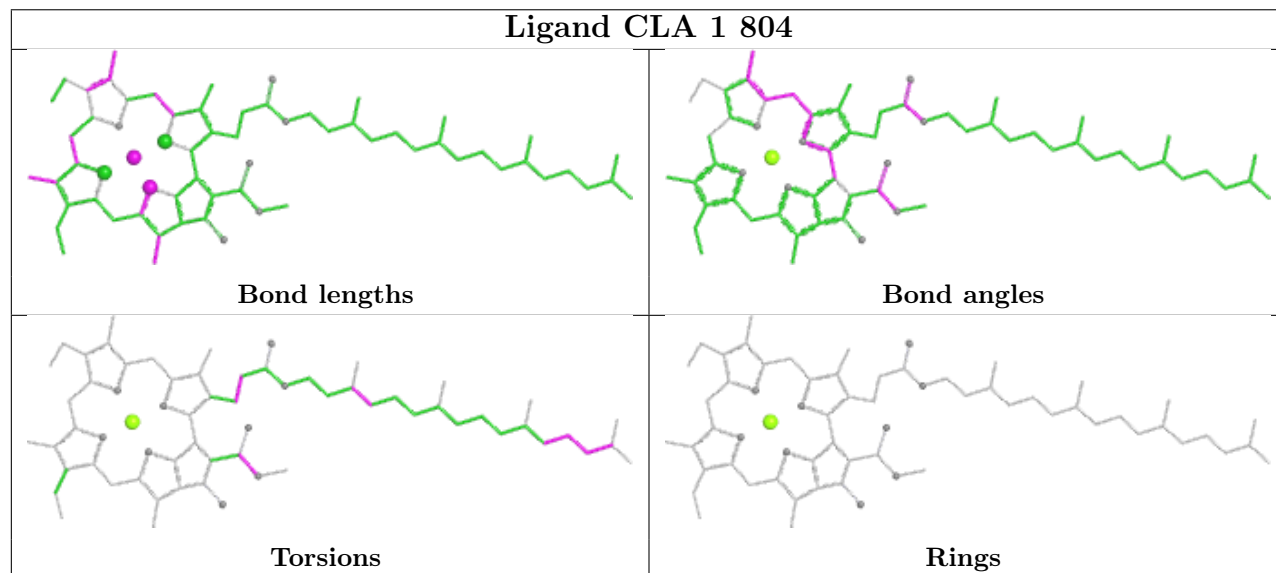


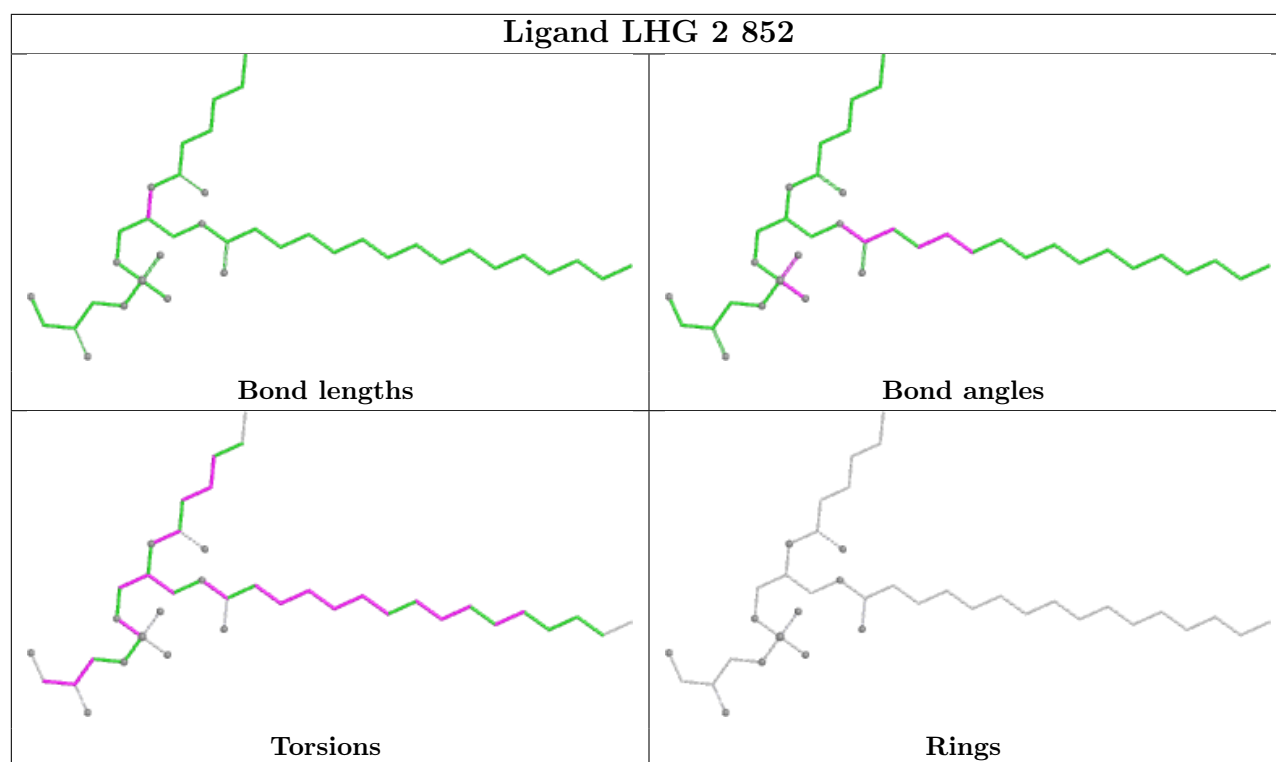


Ligand LHG 9 101

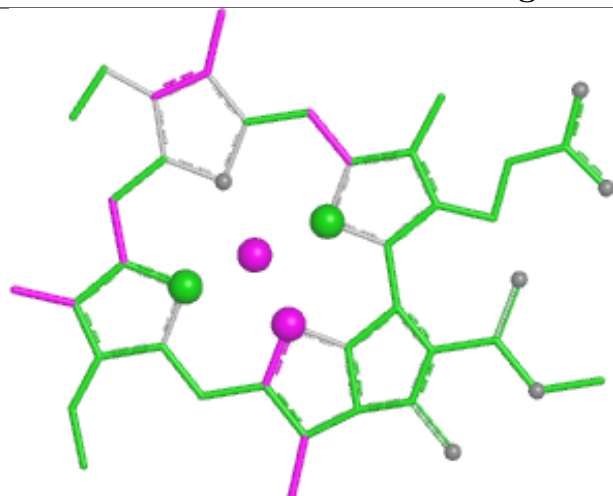


Ligand CLA 1 804

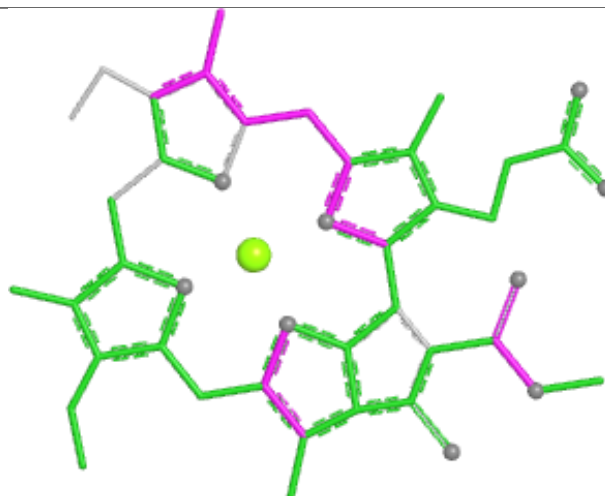




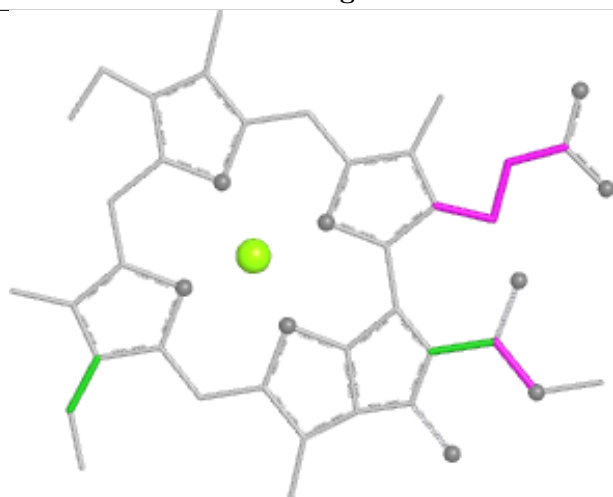
Ligand CLA a 813



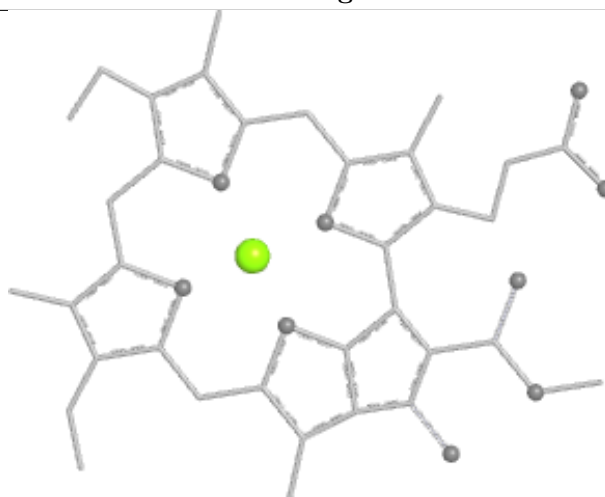
Bond lengths



Bond angles

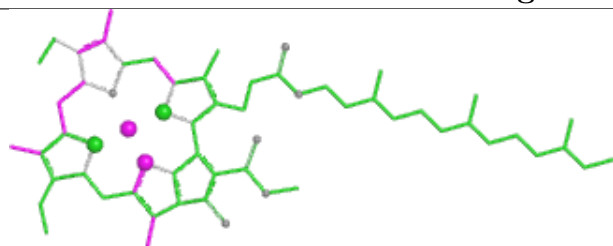


Torsions

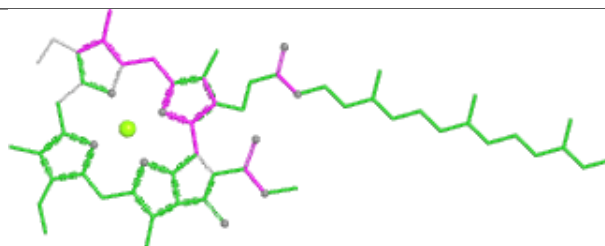


Rings

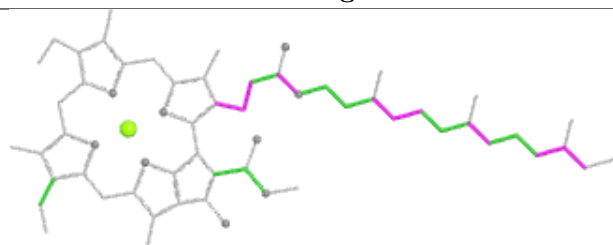
Ligand CLA b 812



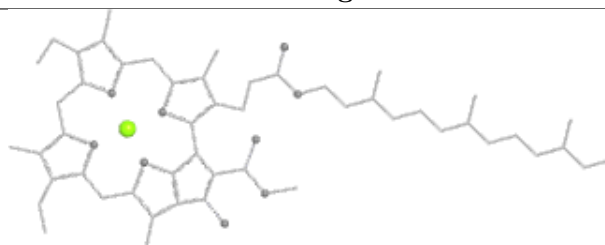
Bond lengths



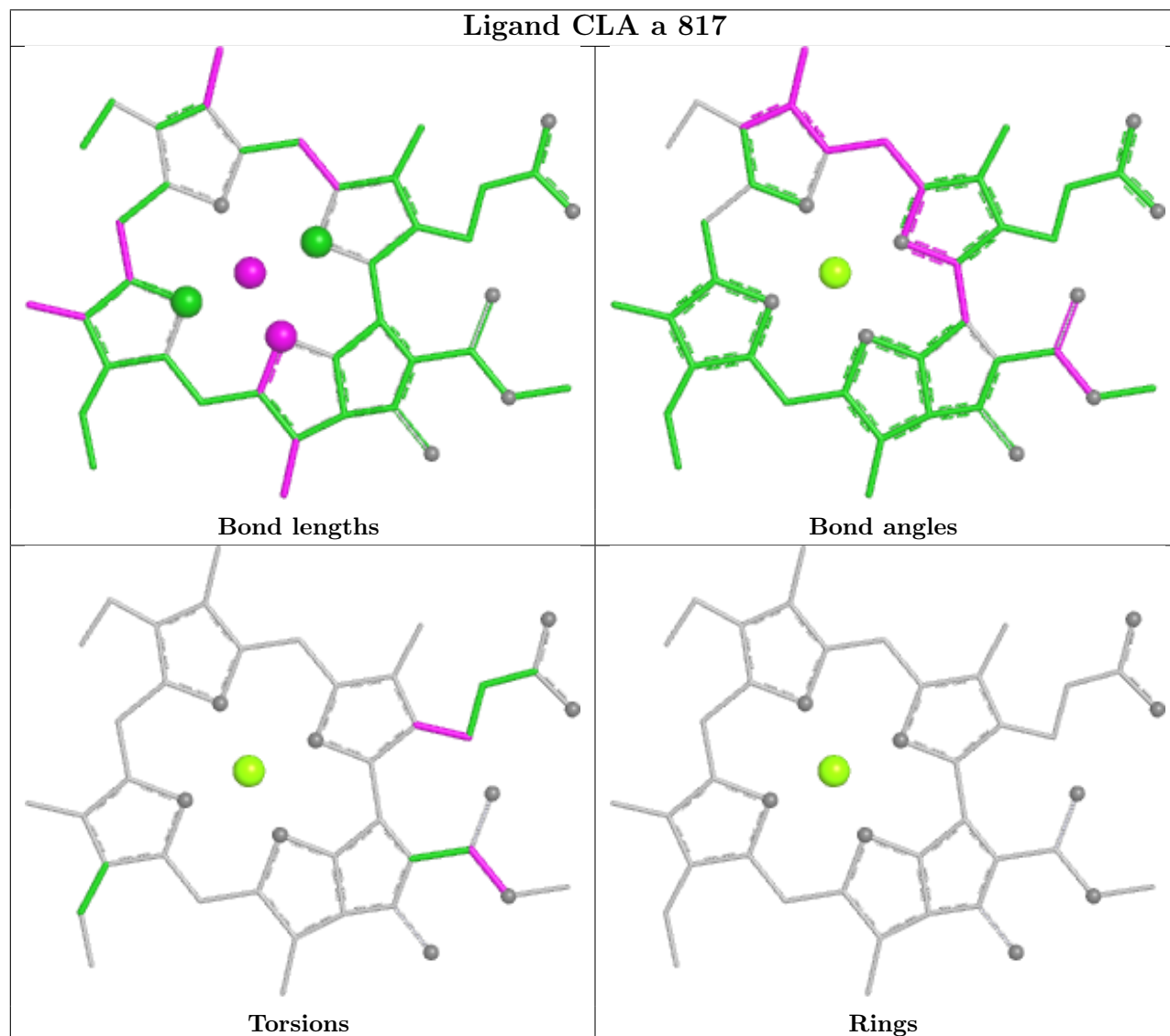
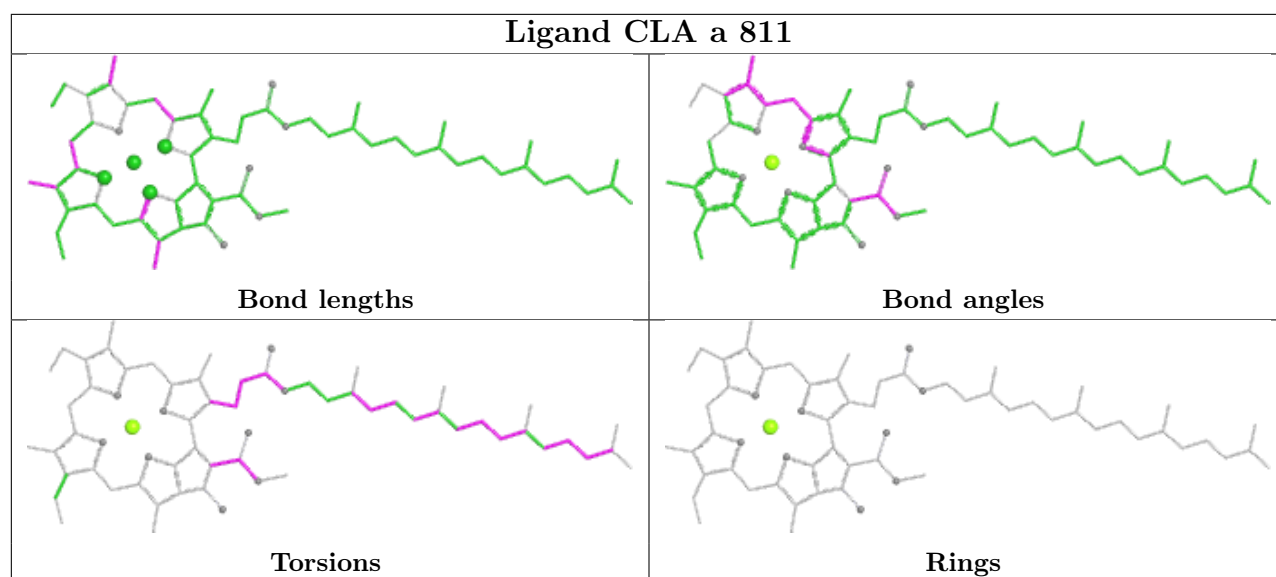
Bond angles

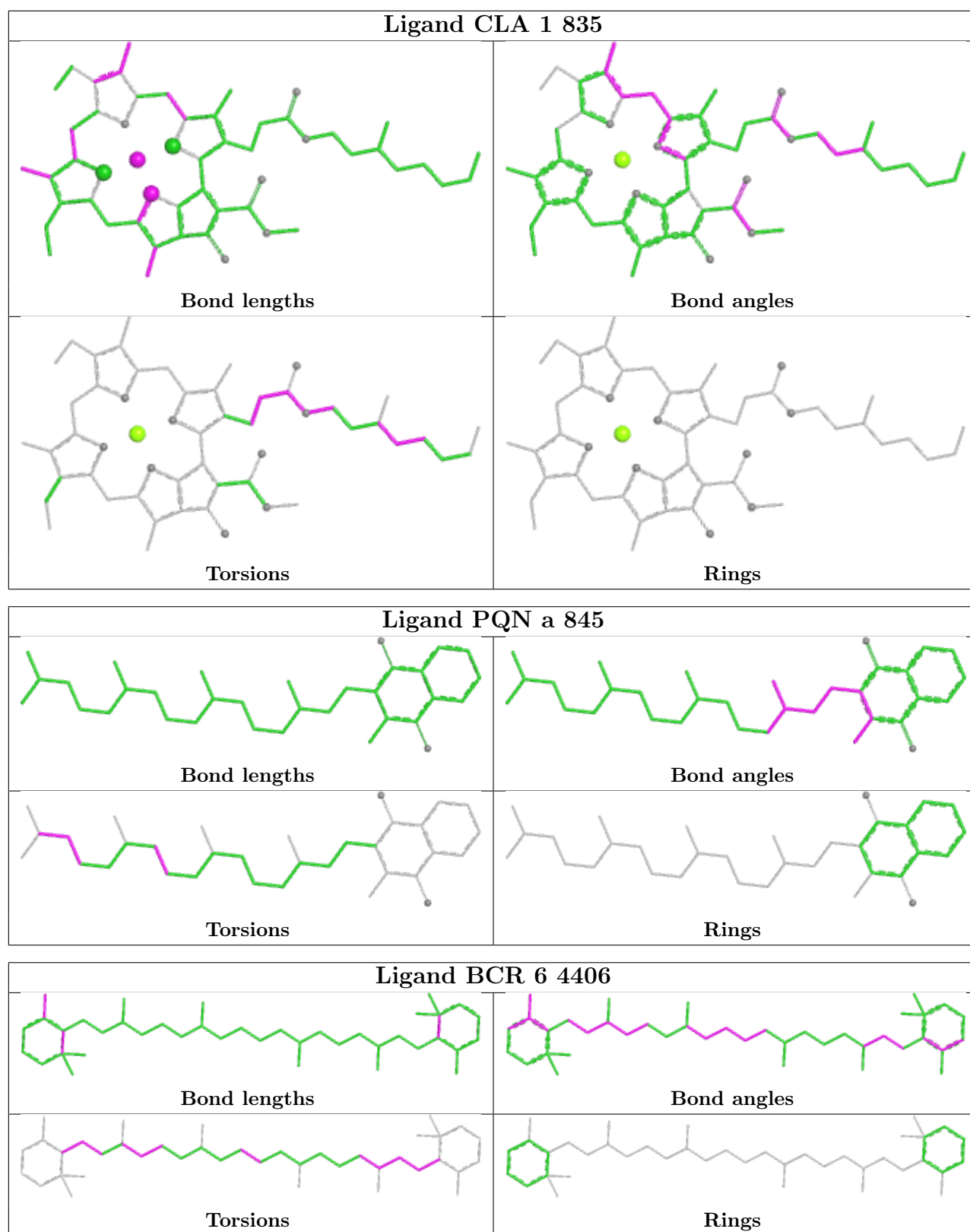


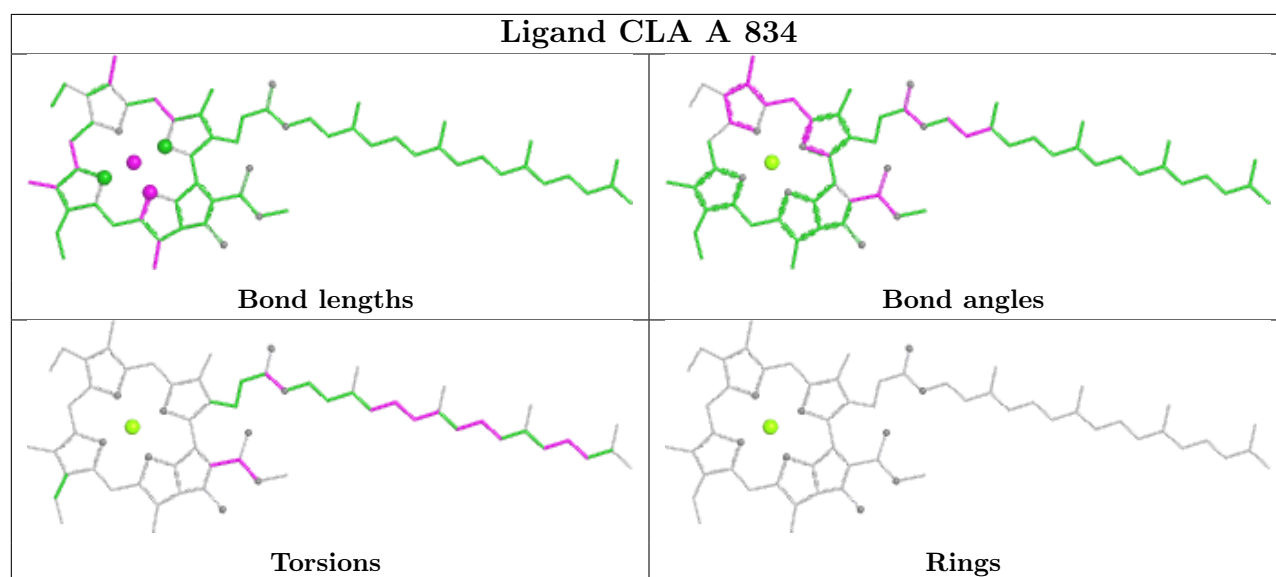
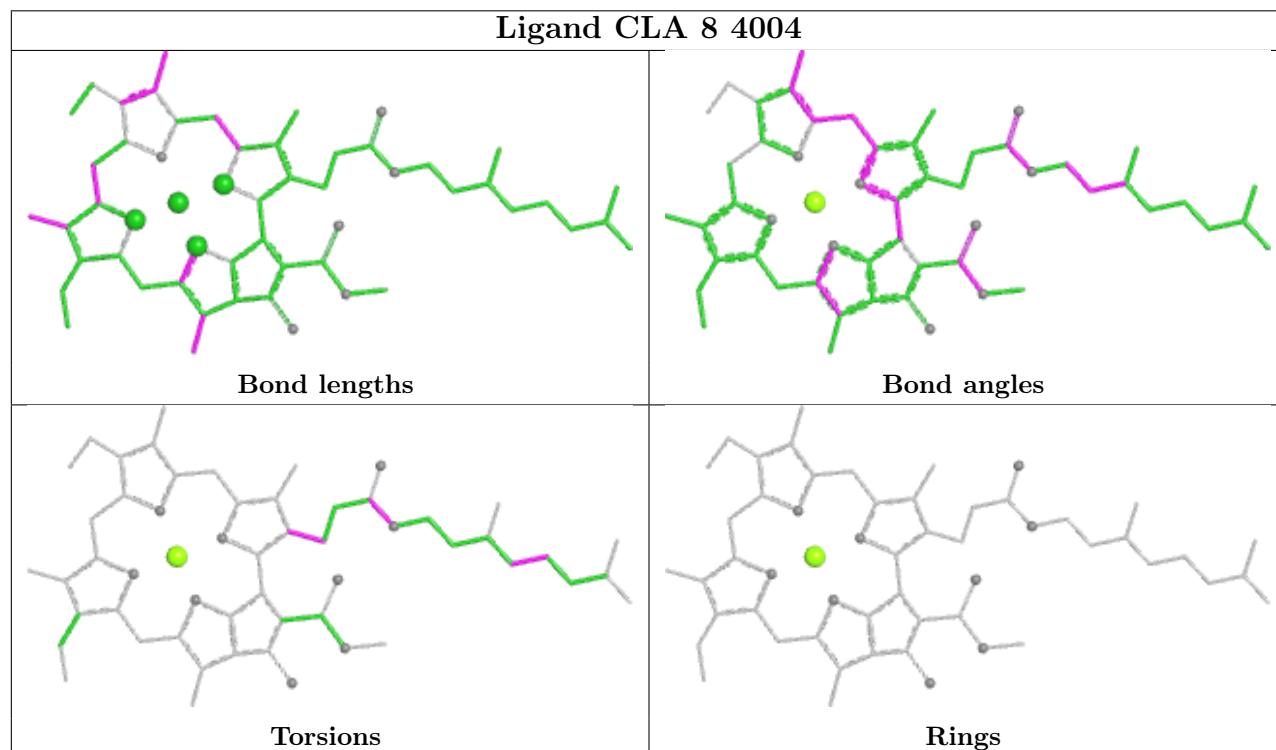
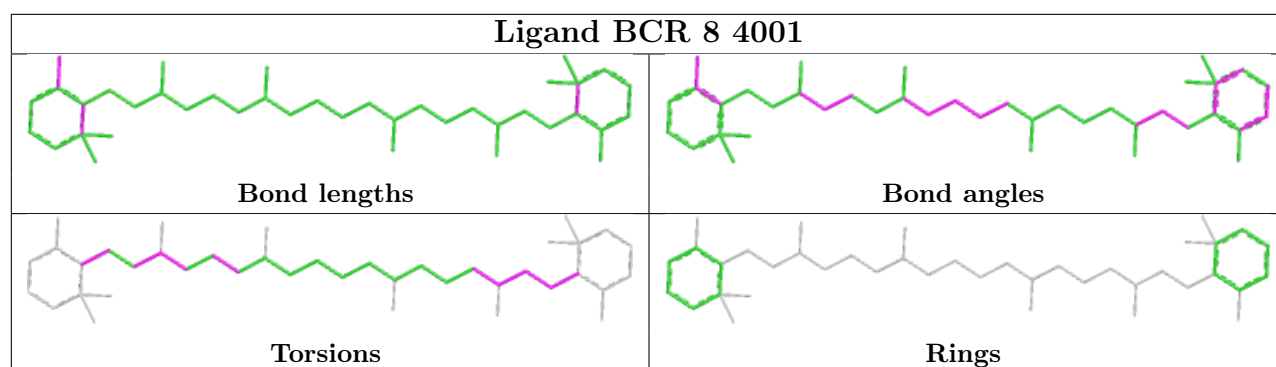
Torsions

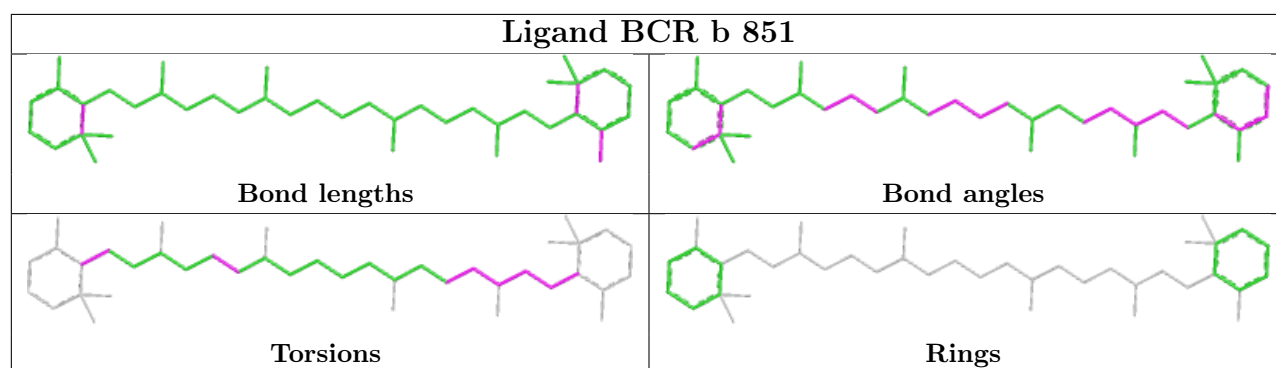
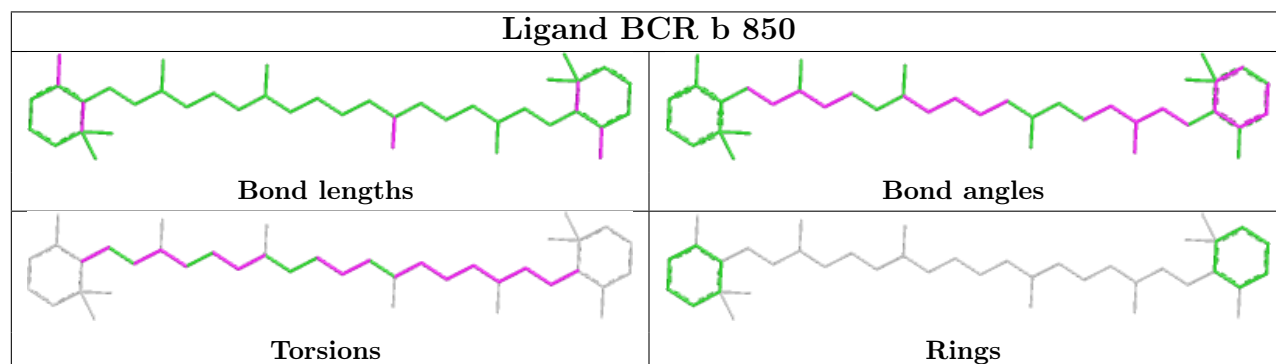
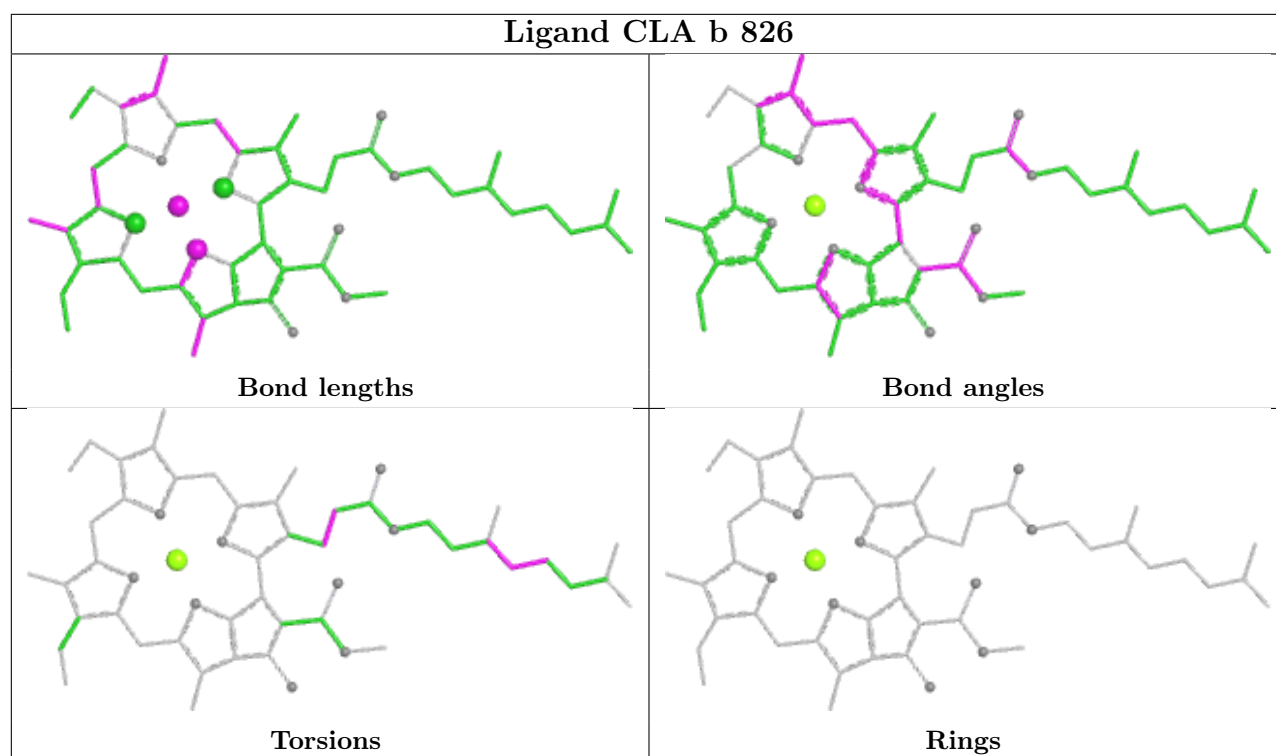


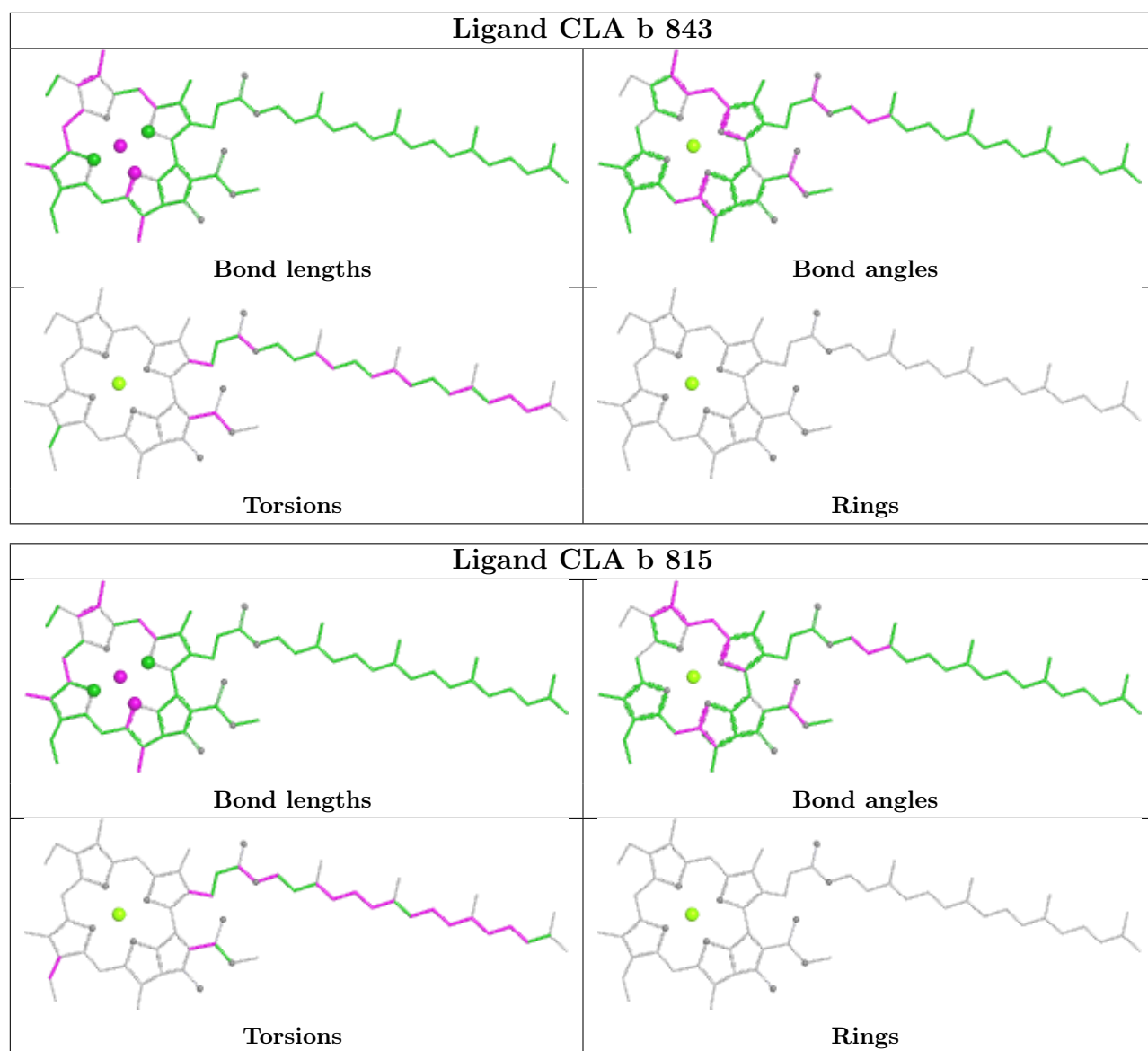
Rings

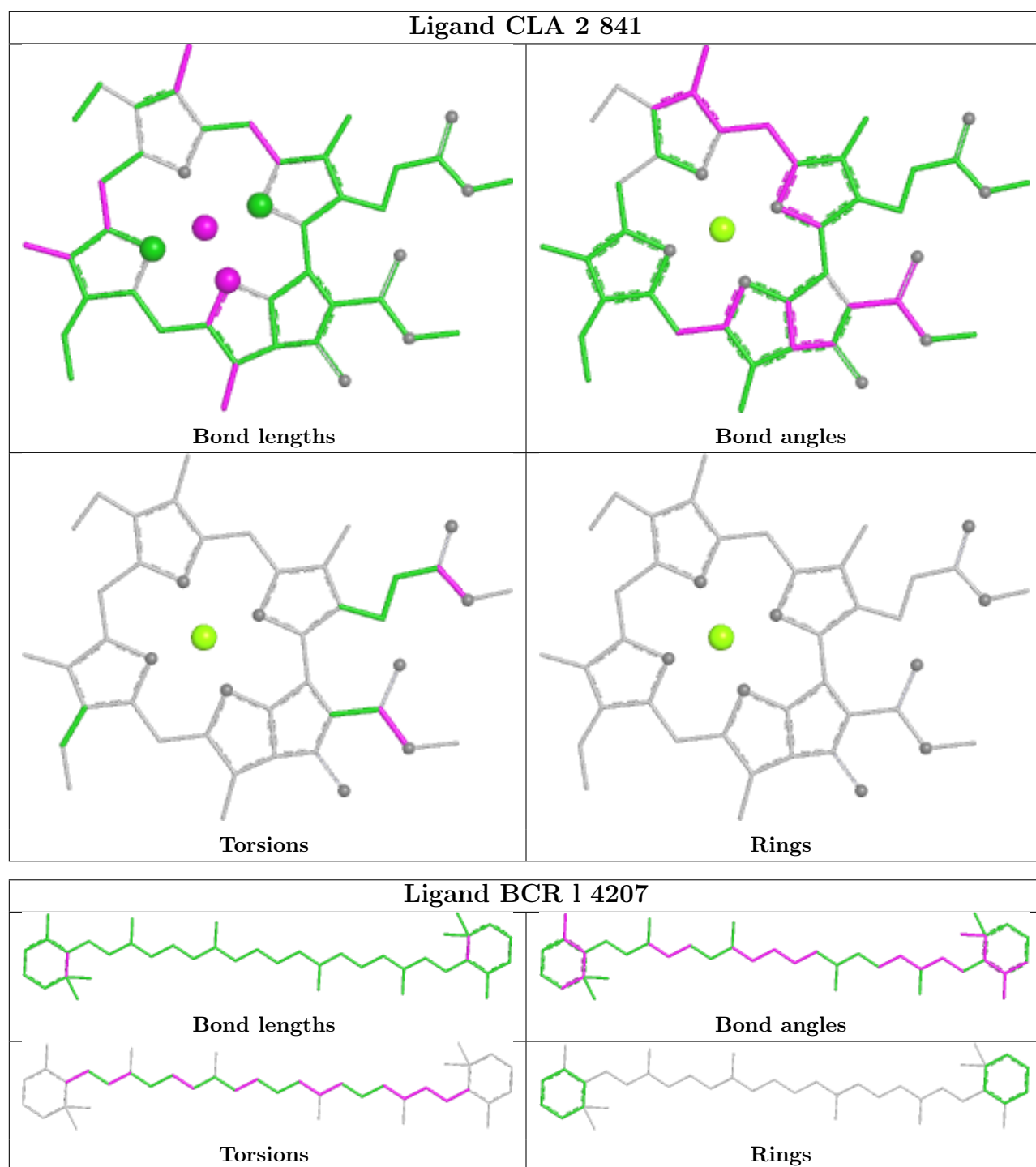


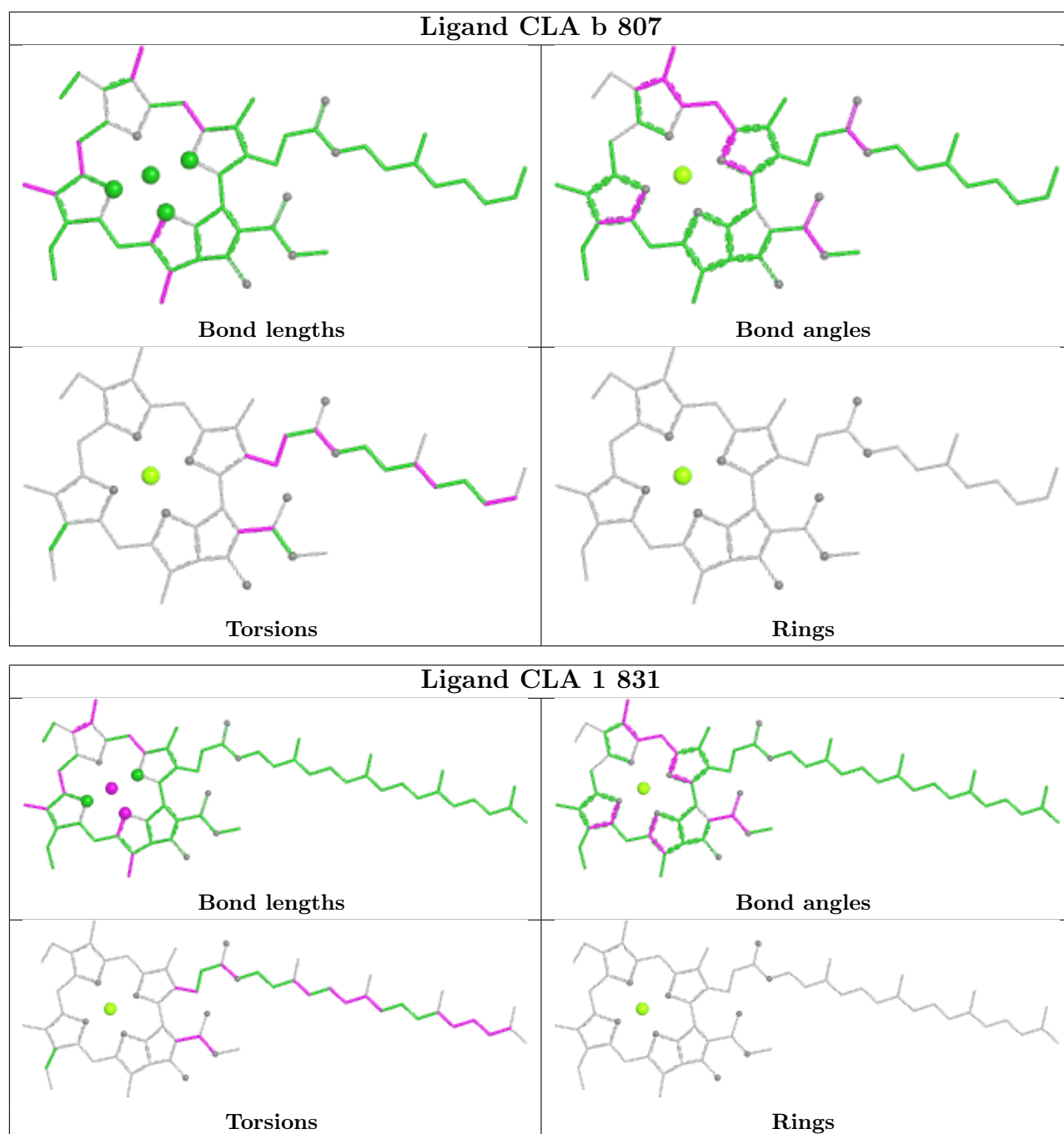




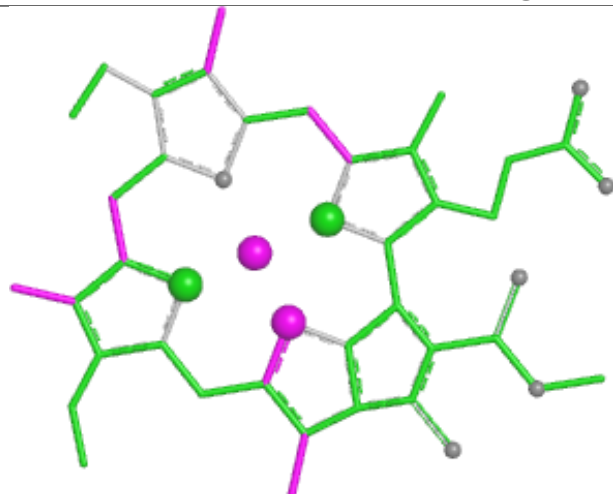




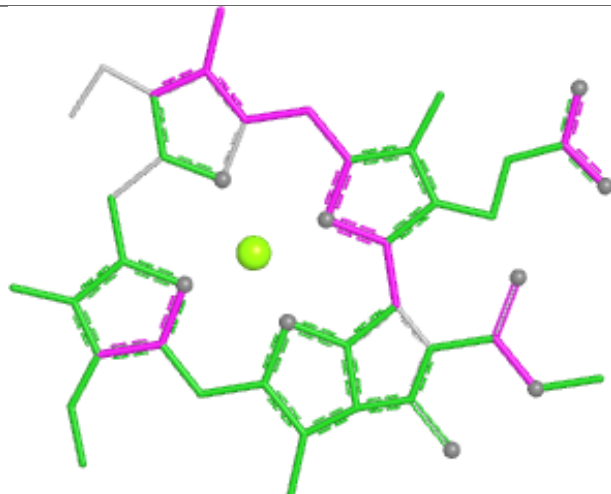




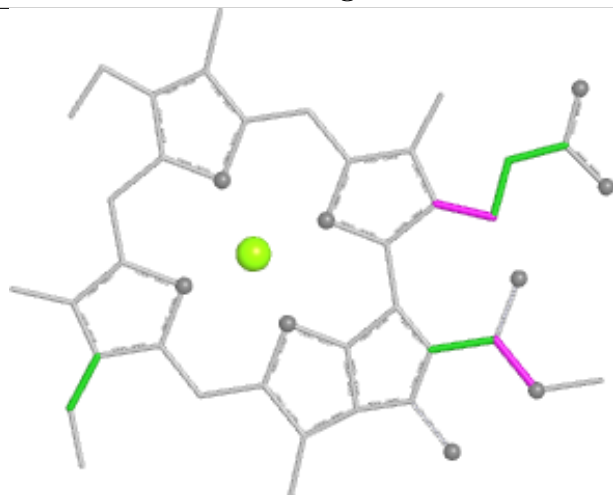
Ligand CLA b 836



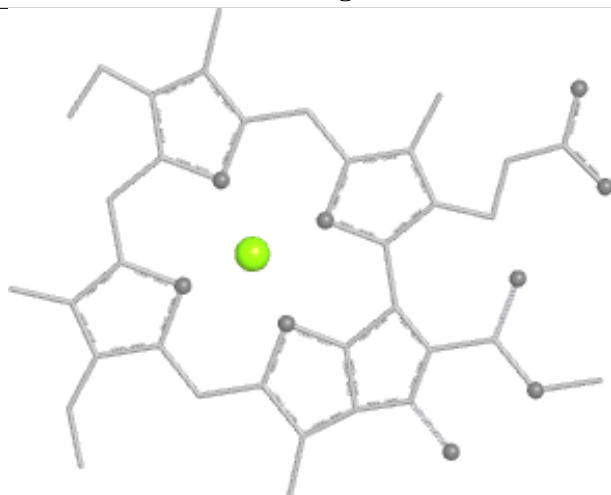
Bond lengths



Bond angles

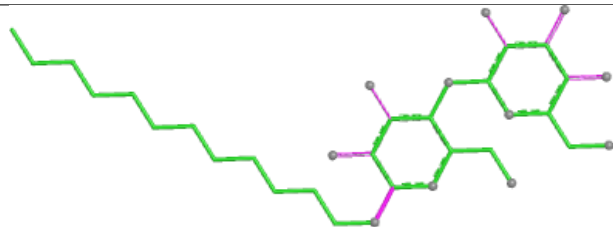


Torsions

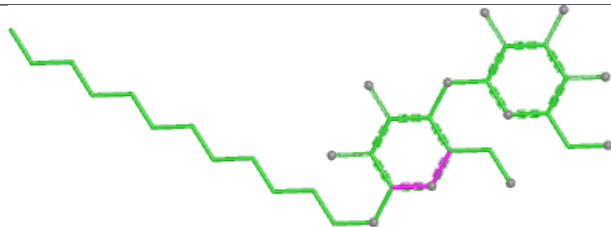


Rings

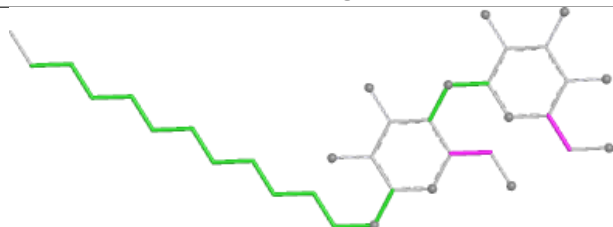
Ligand LMT F 202



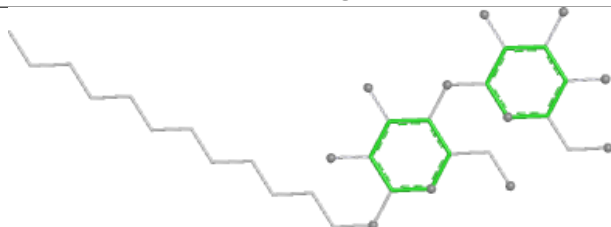
Bond lengths



Bond angles

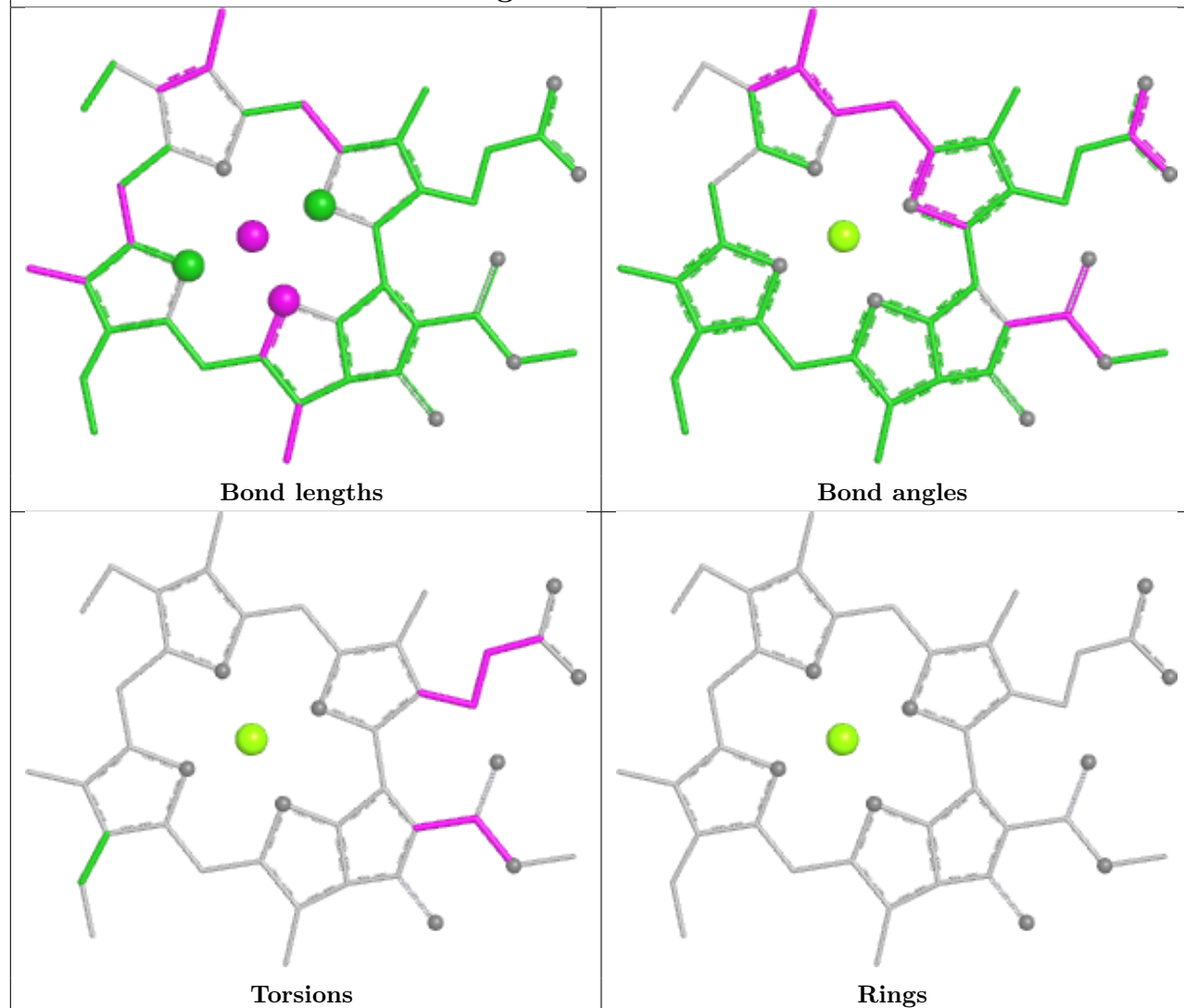


Torsions

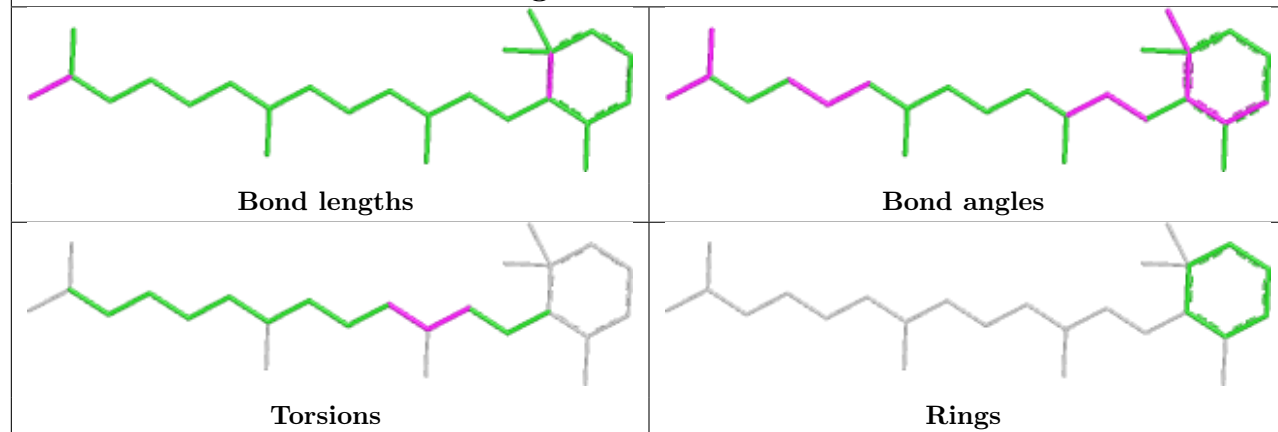


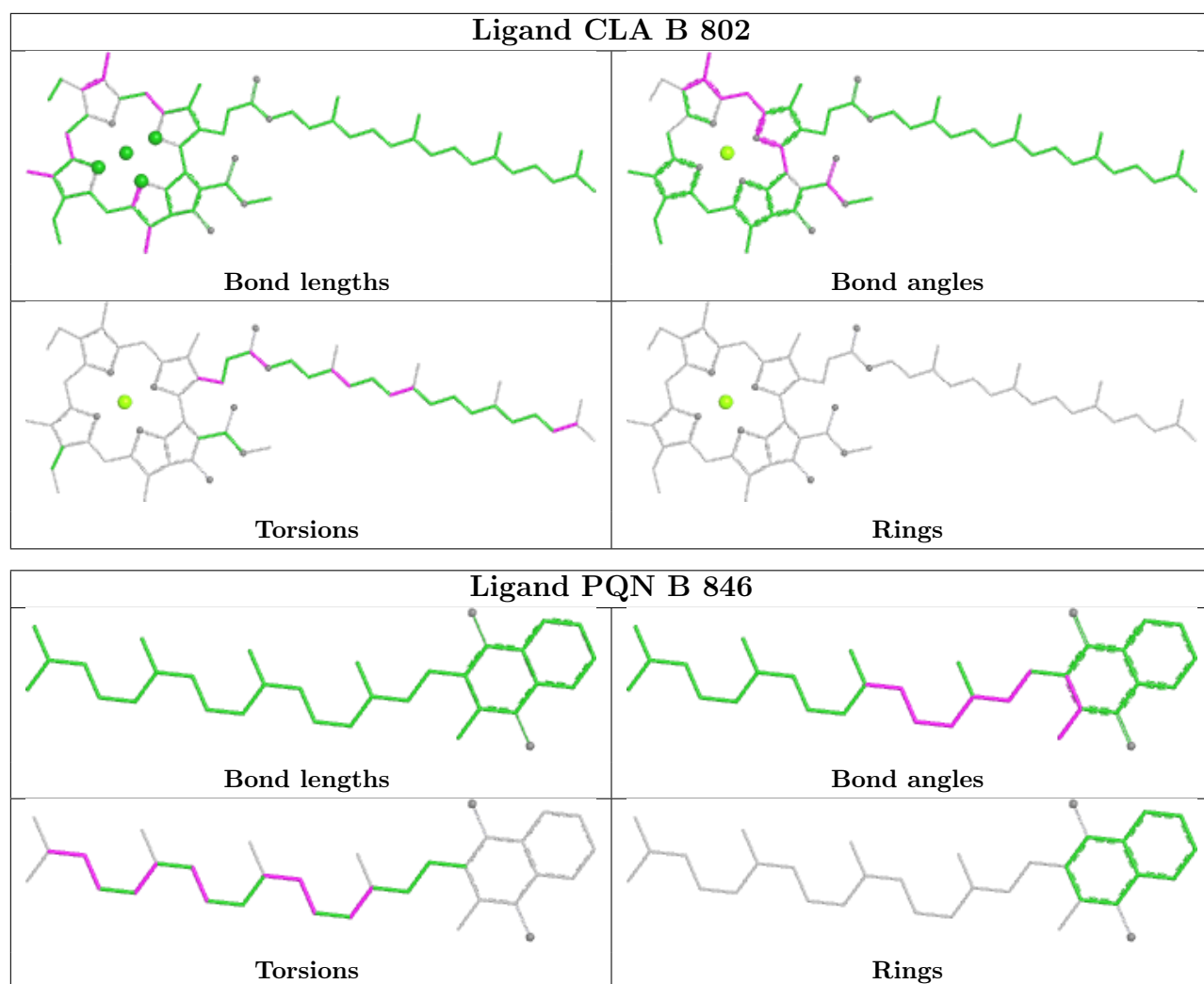
Rings

Ligand CLA 2 814

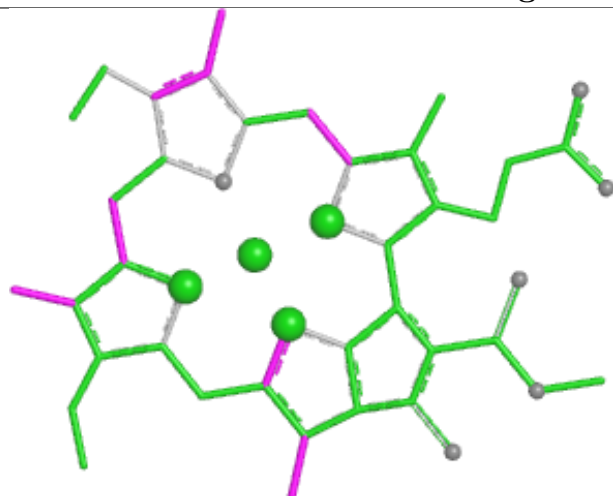


Ligand BCR B 849

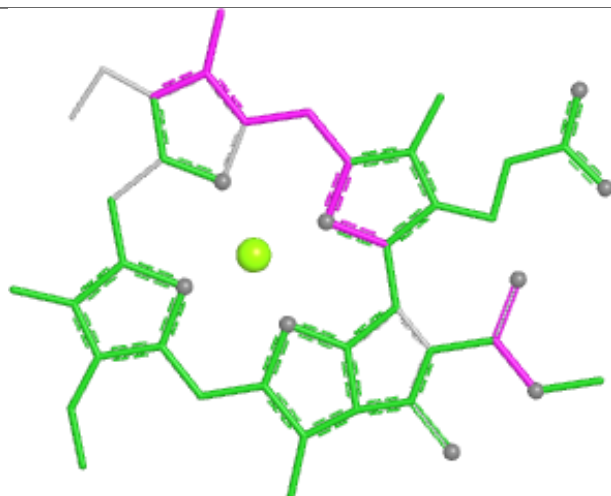




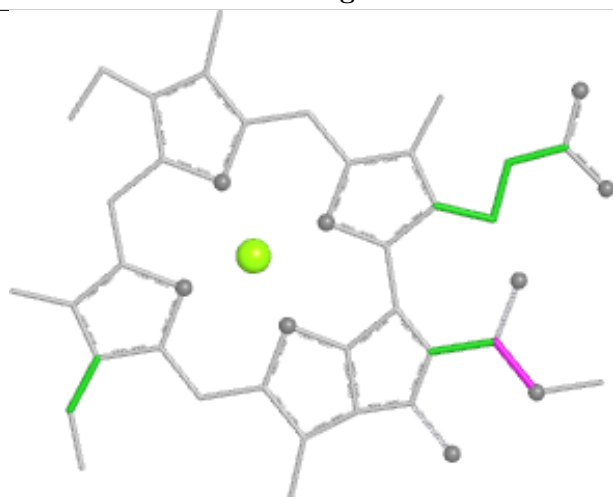
Ligand CLA a 818



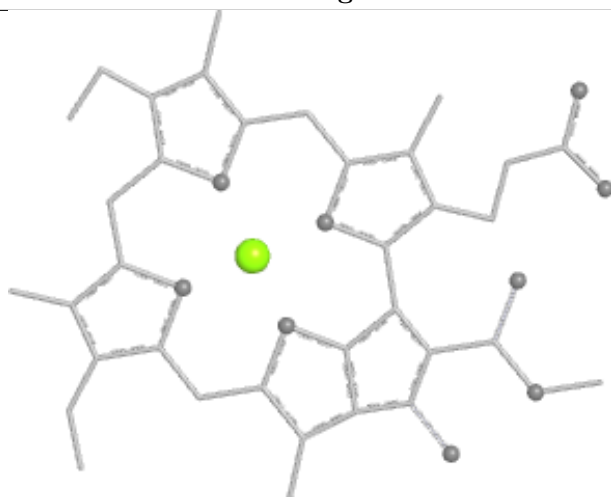
Bond lengths



Bond angles

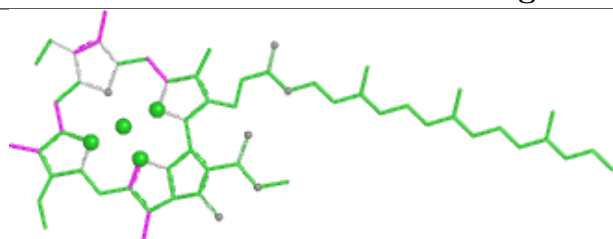


Torsions

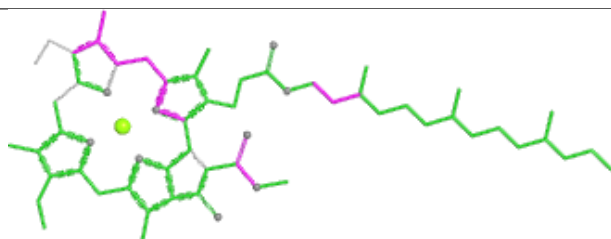


Rings

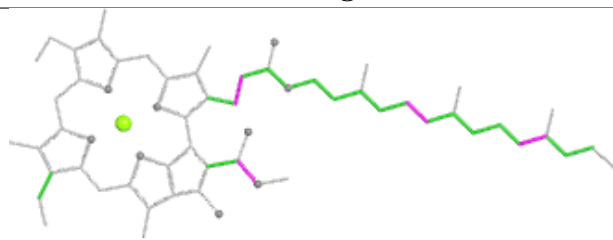
Ligand CLA 2 840



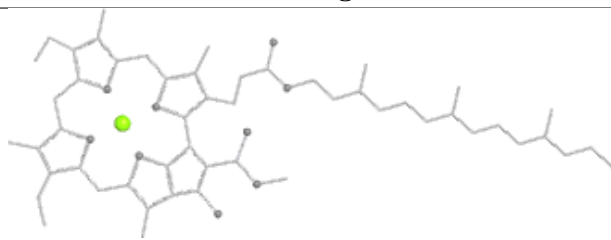
Bond lengths



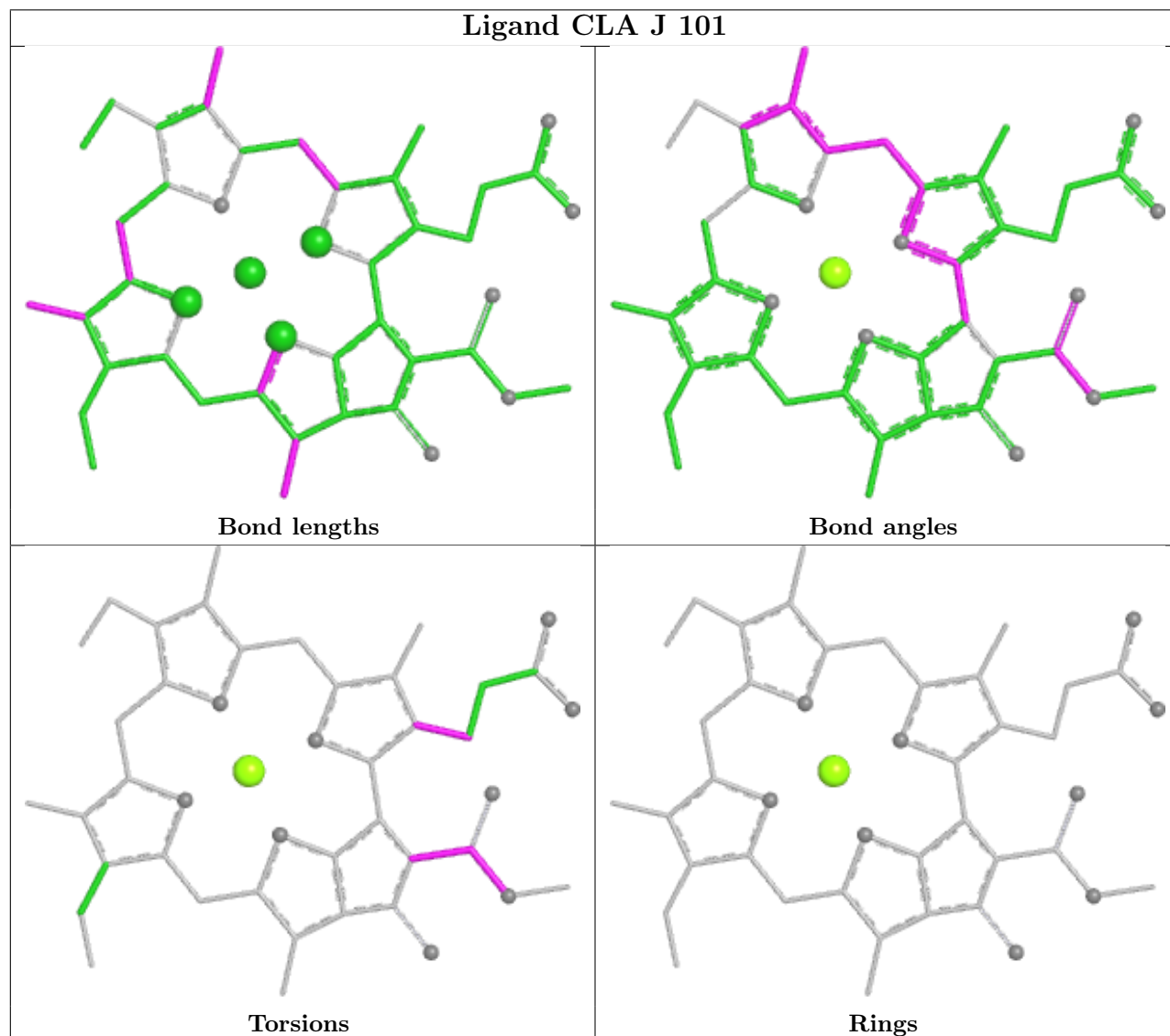
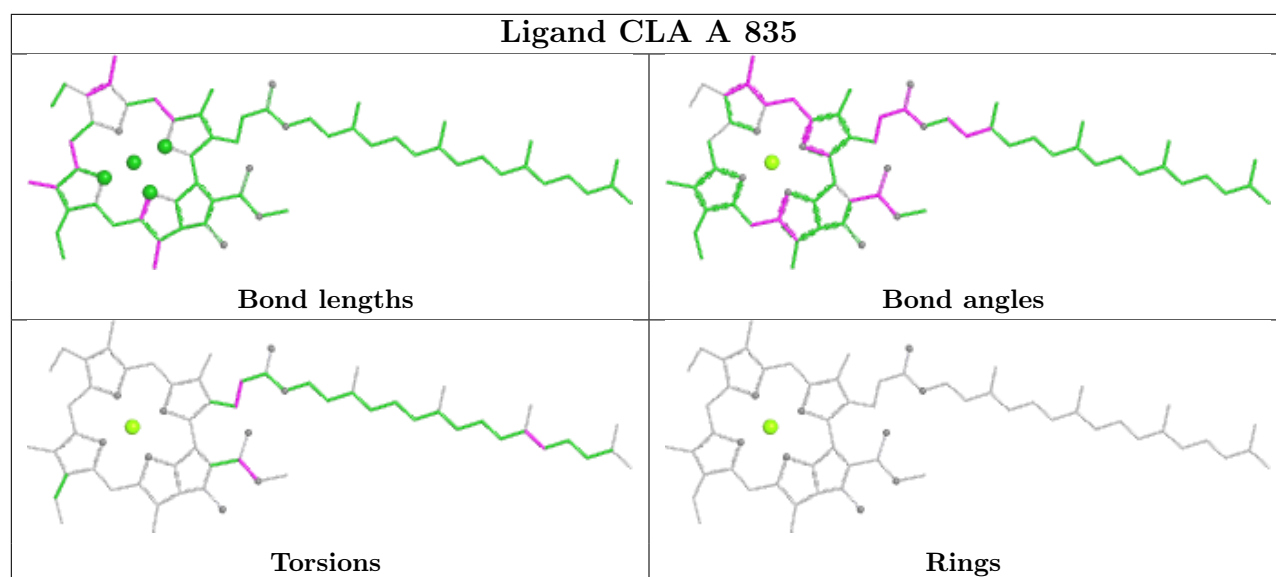
Bond angles

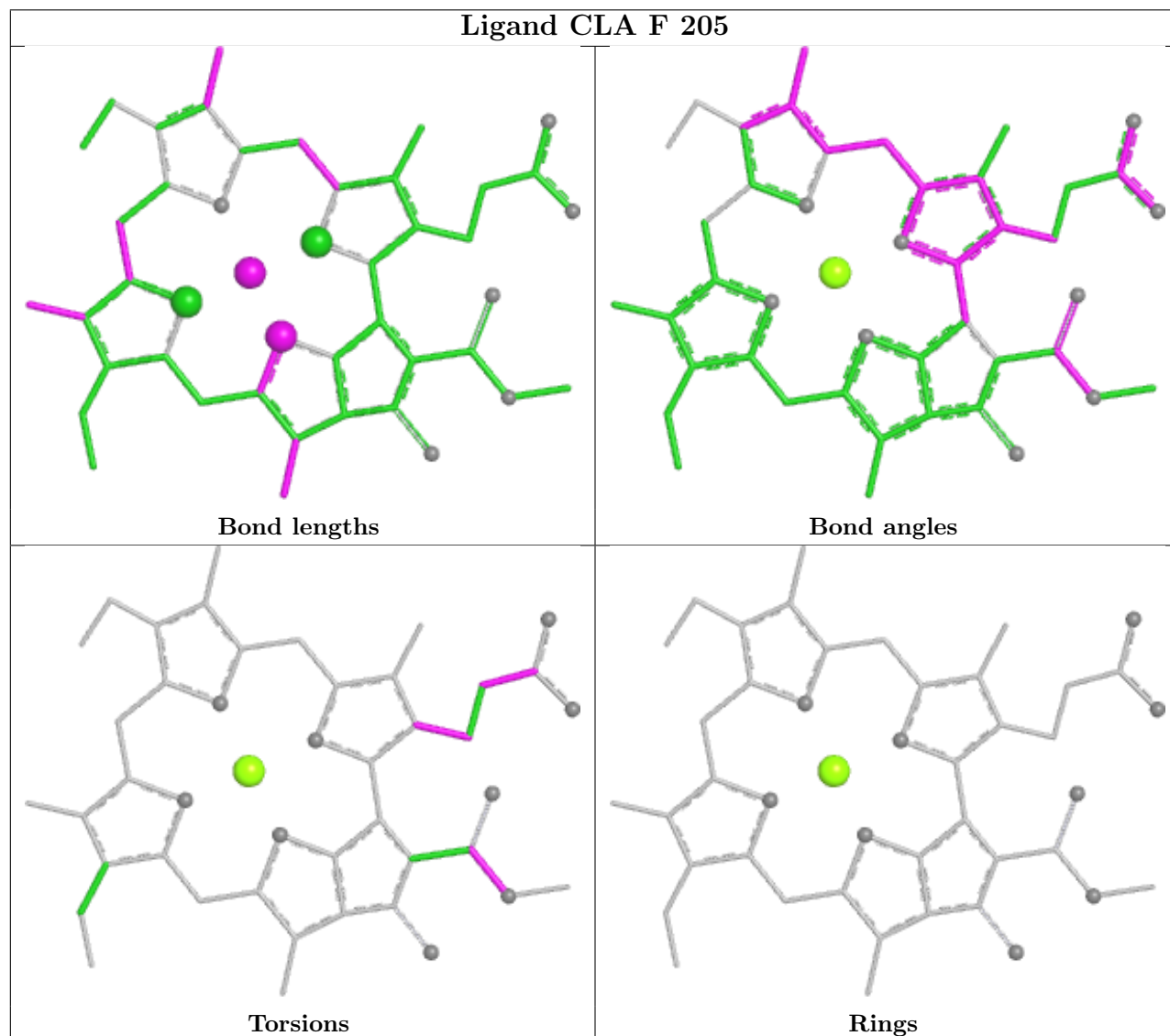
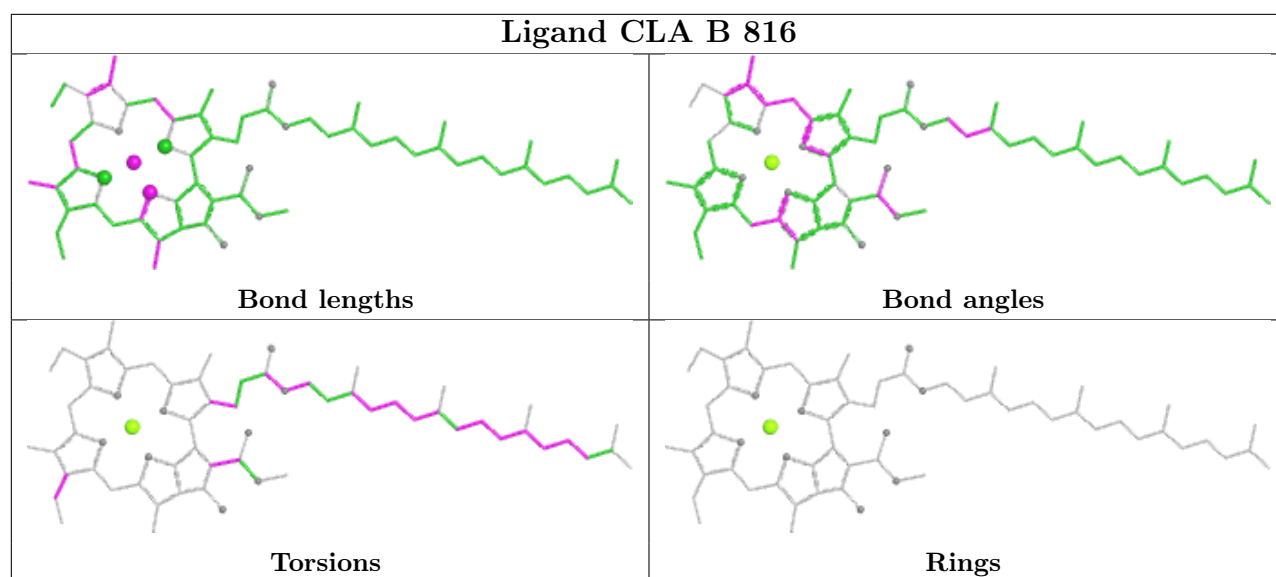


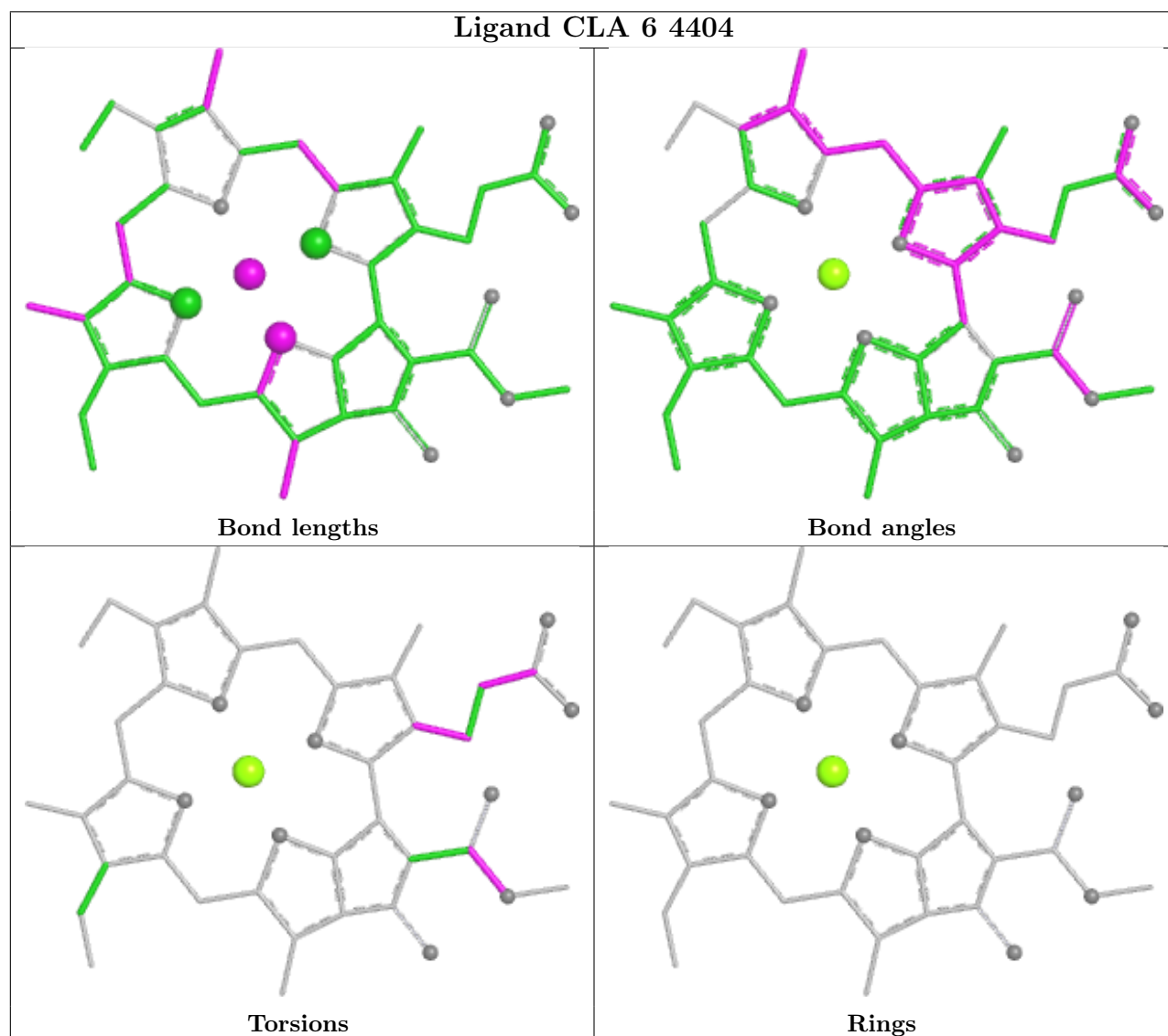
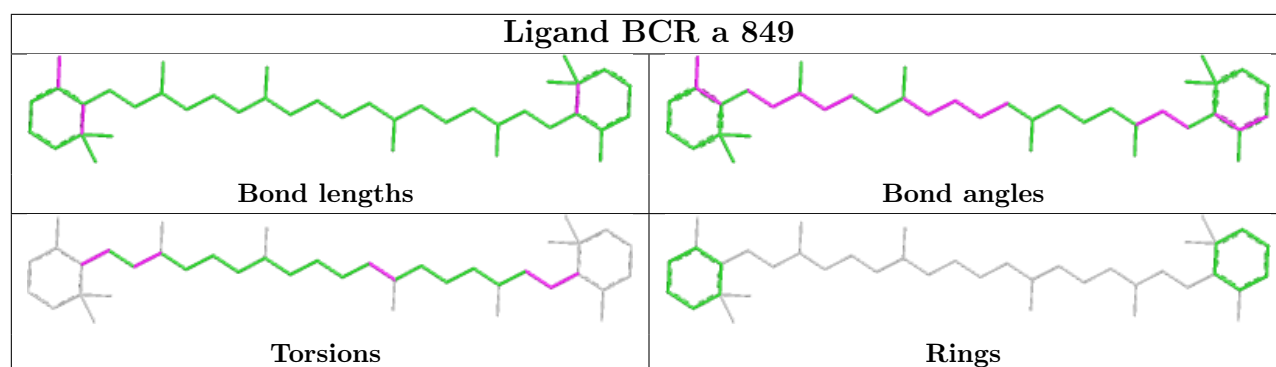
Torsions

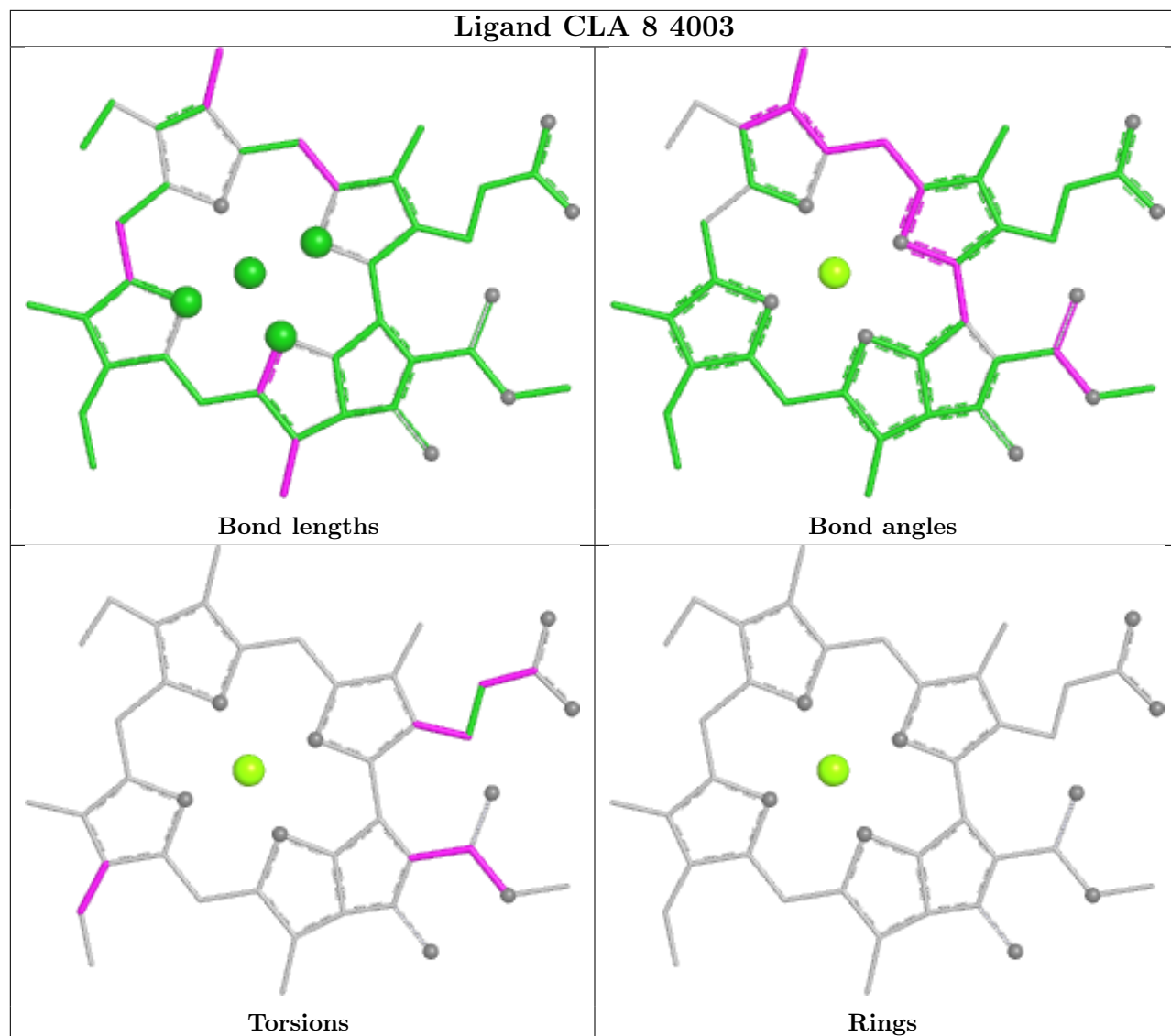


Rings

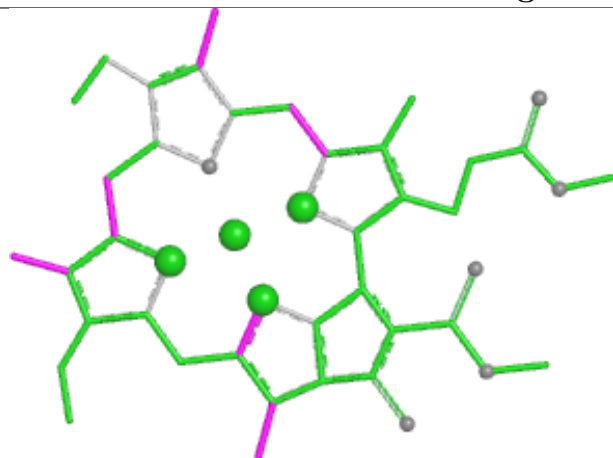




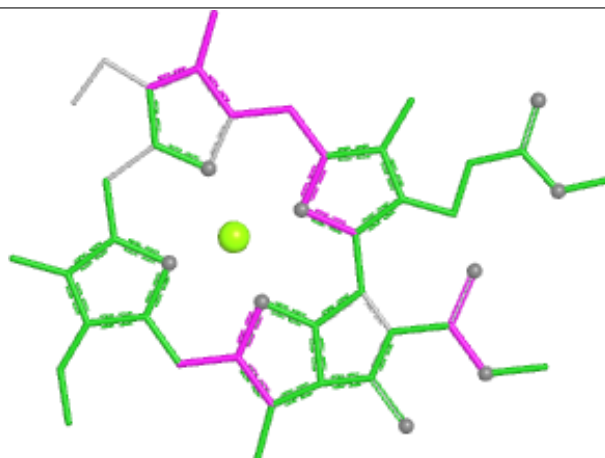




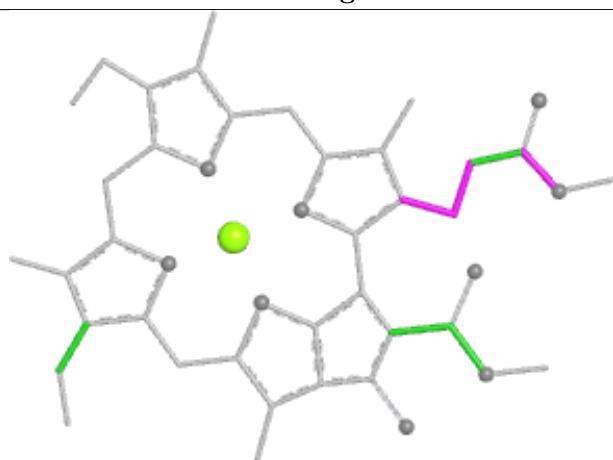
Ligand CLA b 838



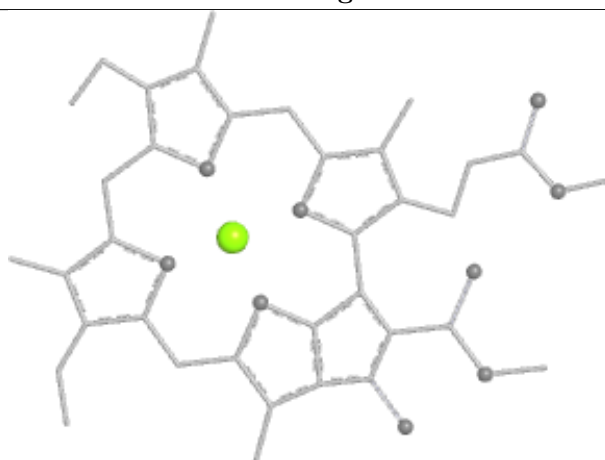
Bond lengths



Bond angles

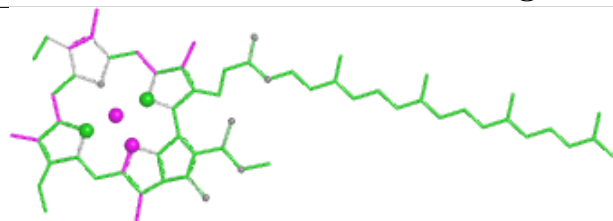


Torsions

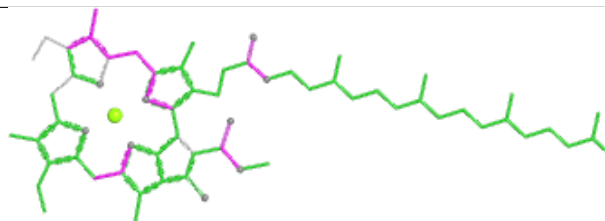


Rings

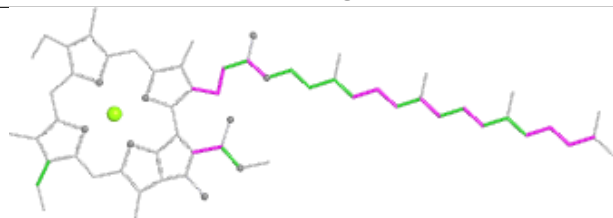
Ligand CLA 1 806



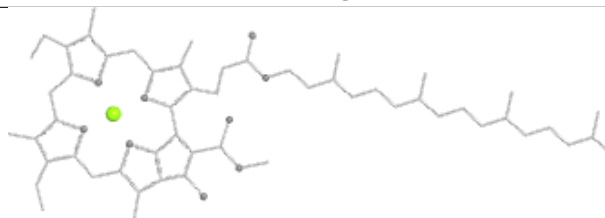
Bond lengths



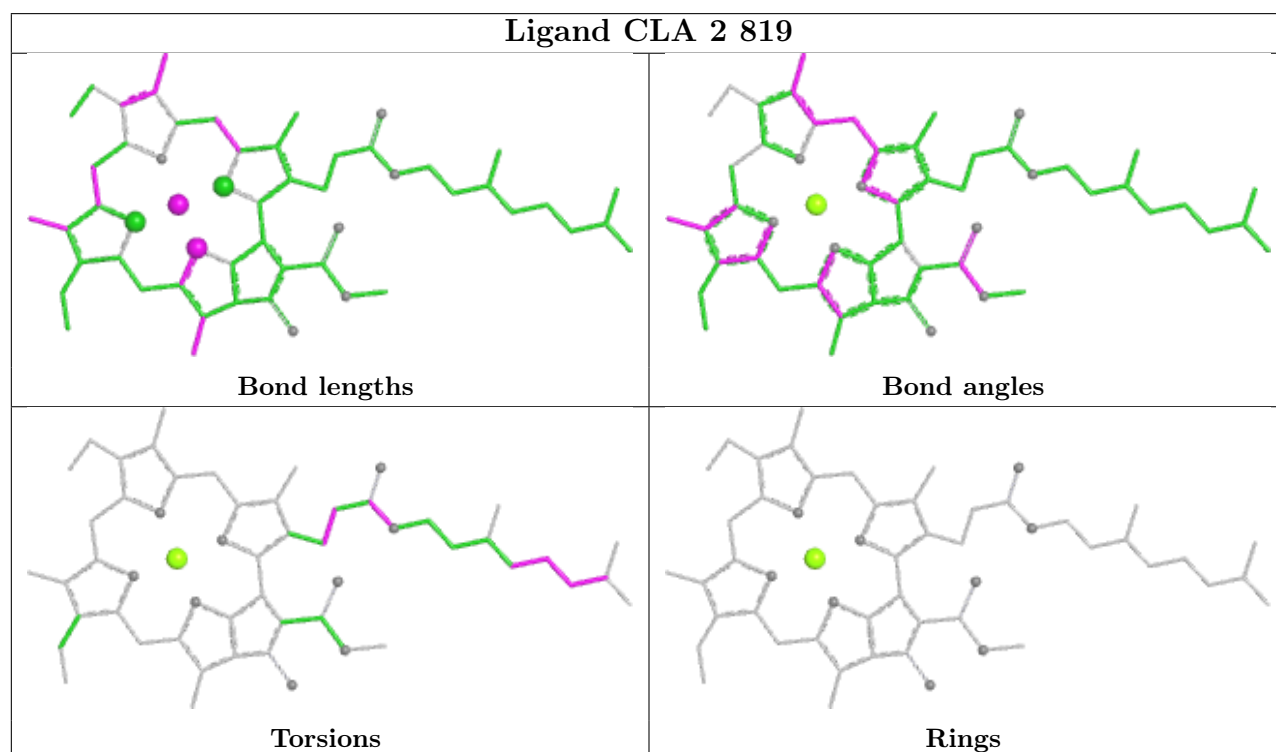
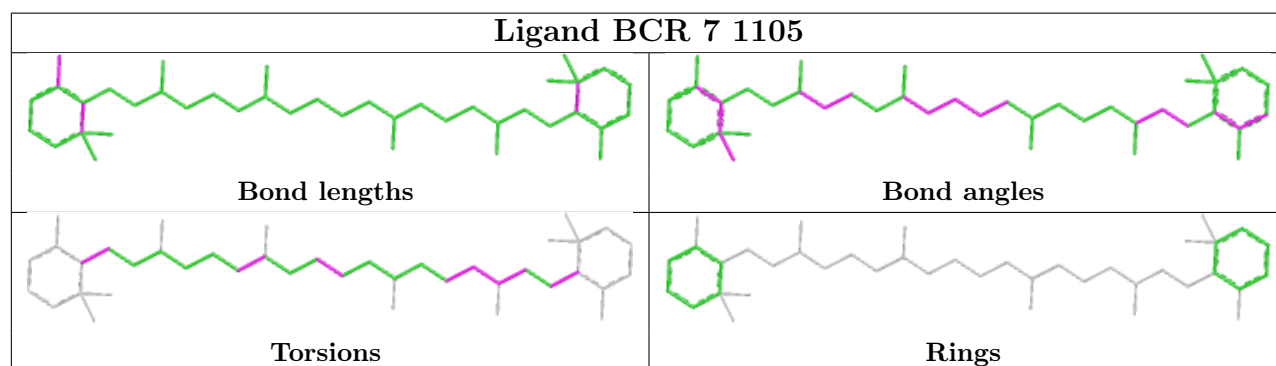
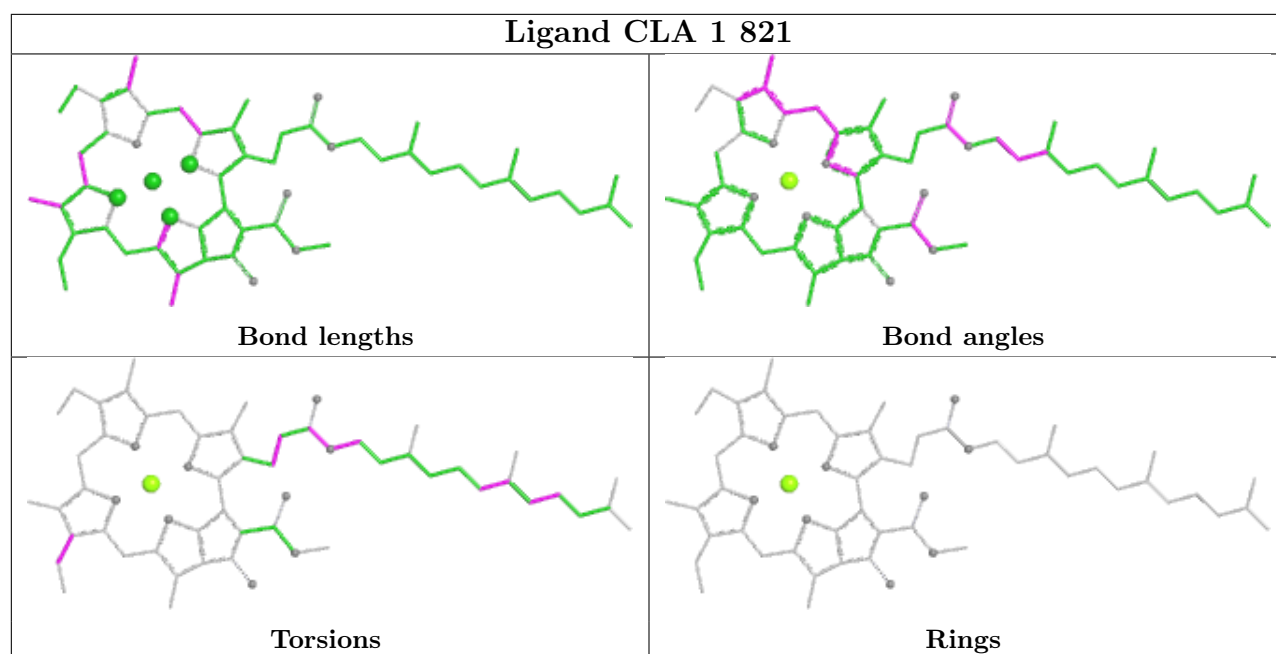
Bond angles

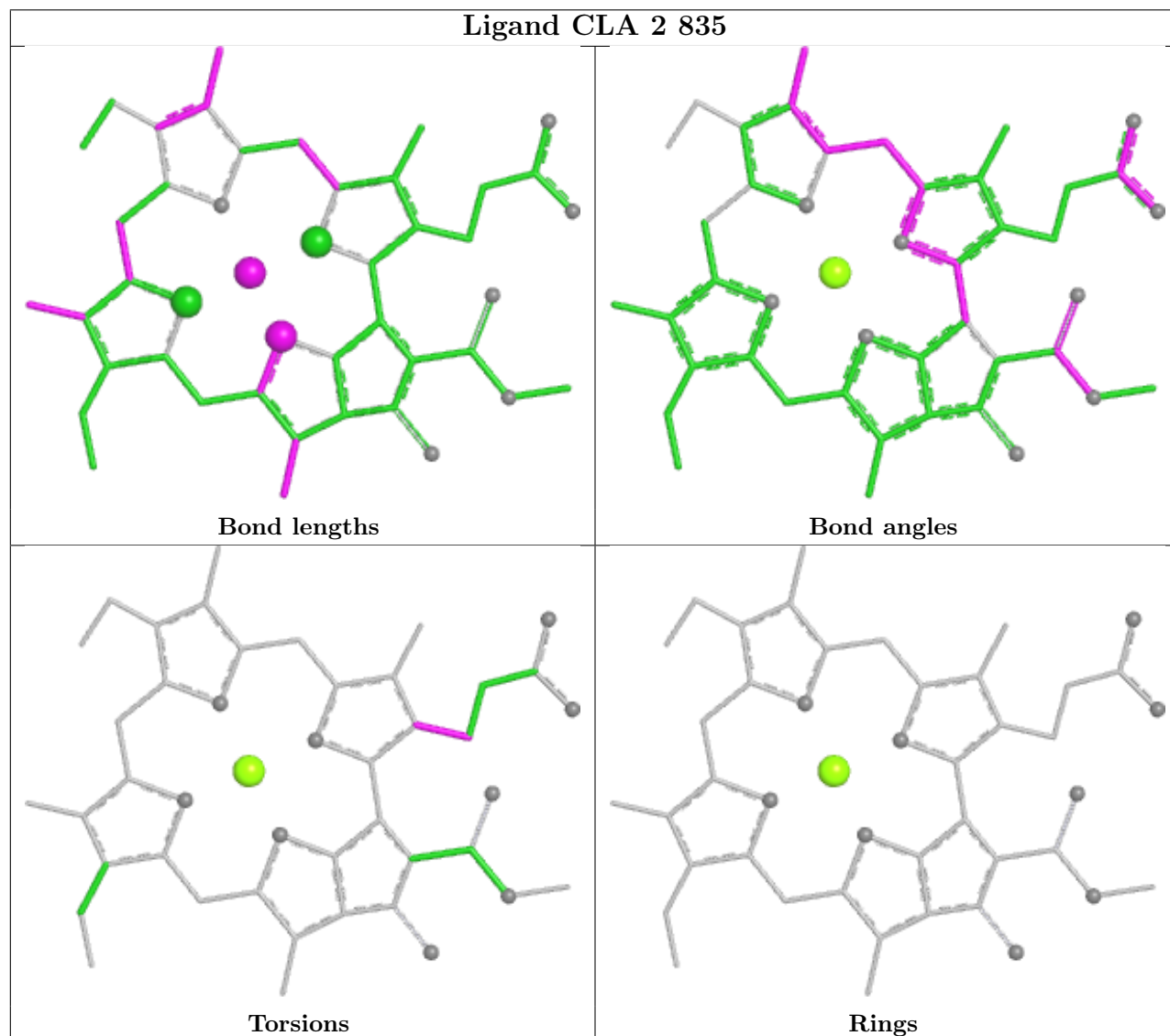
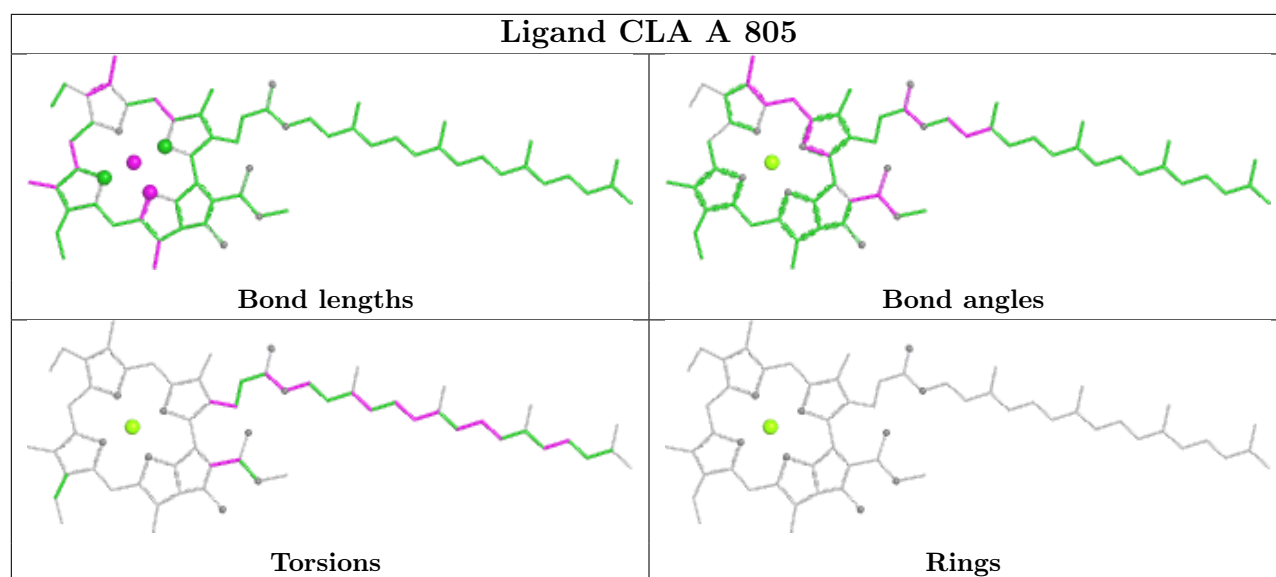


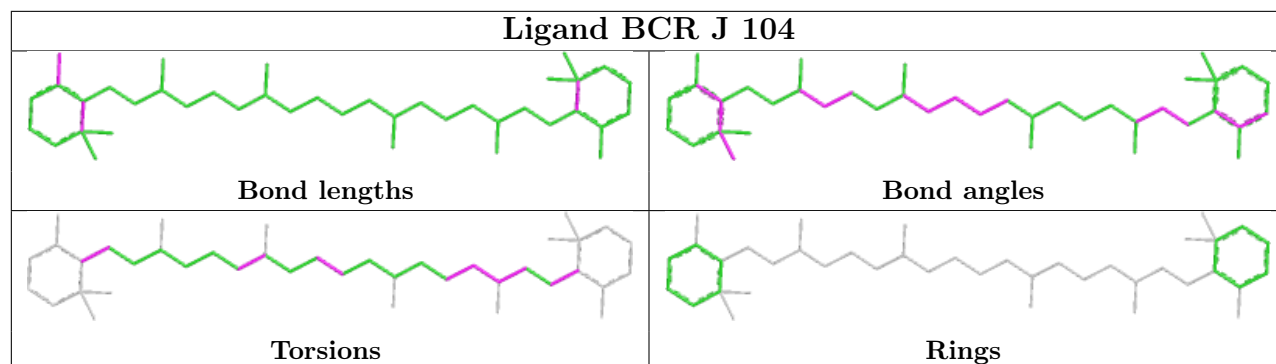
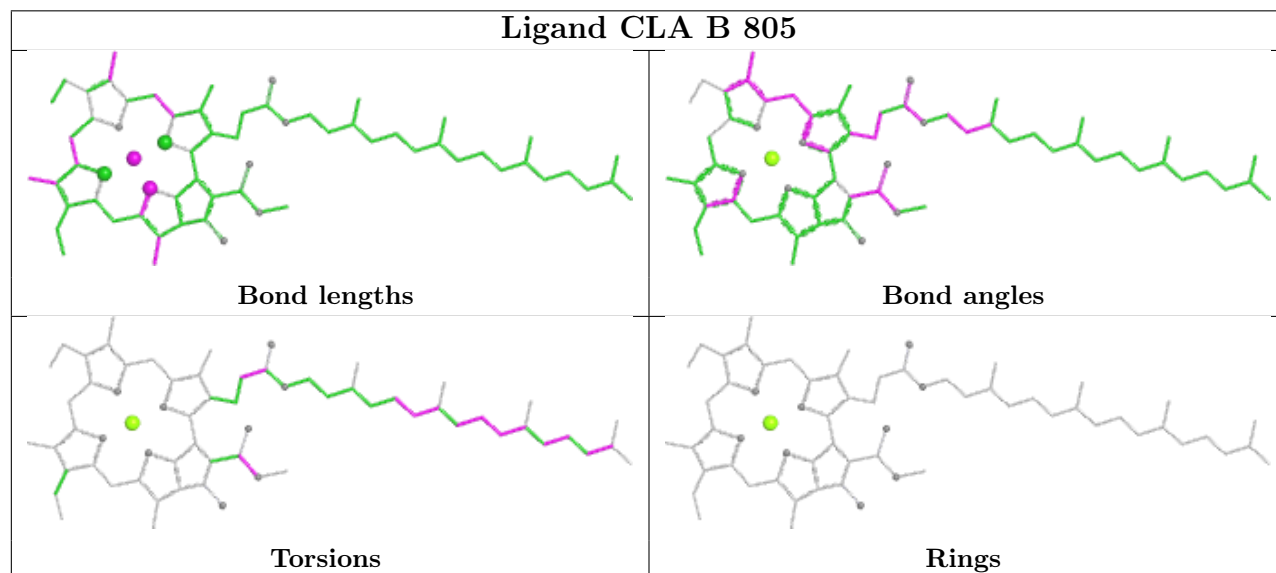
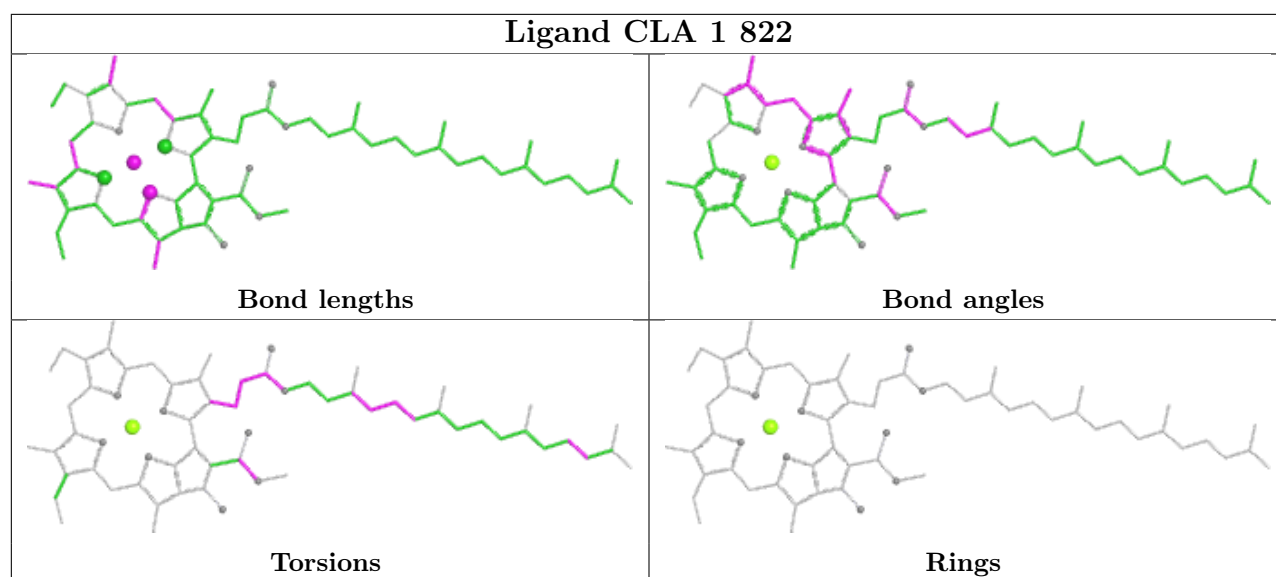
Torsions

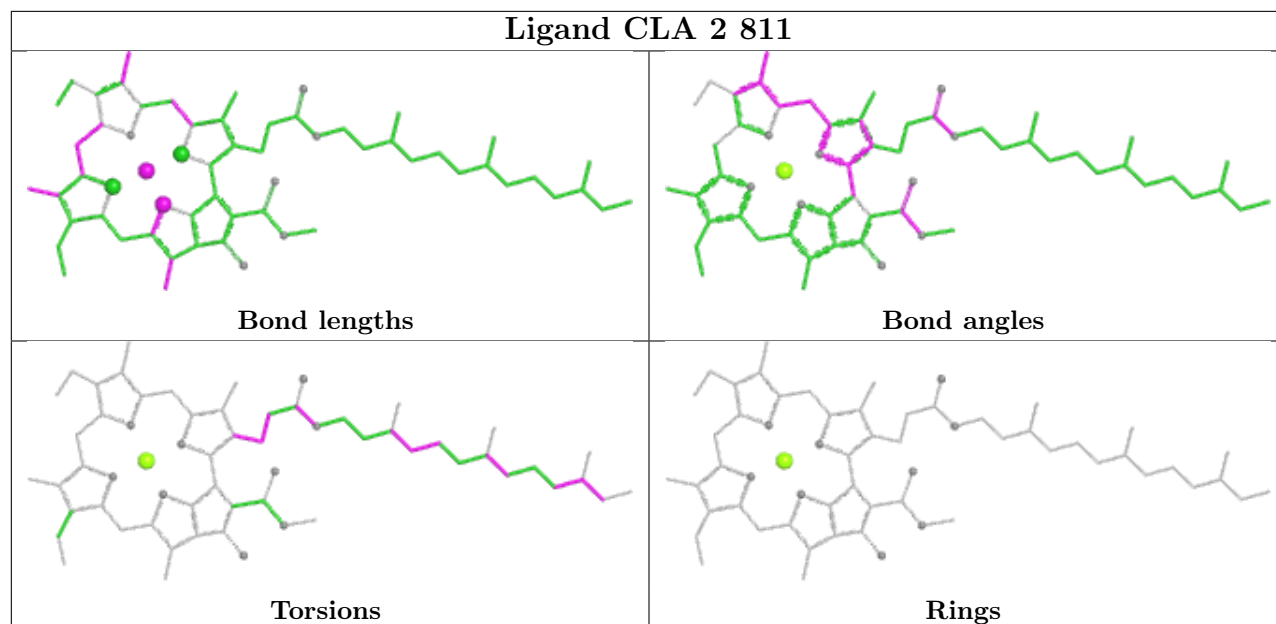
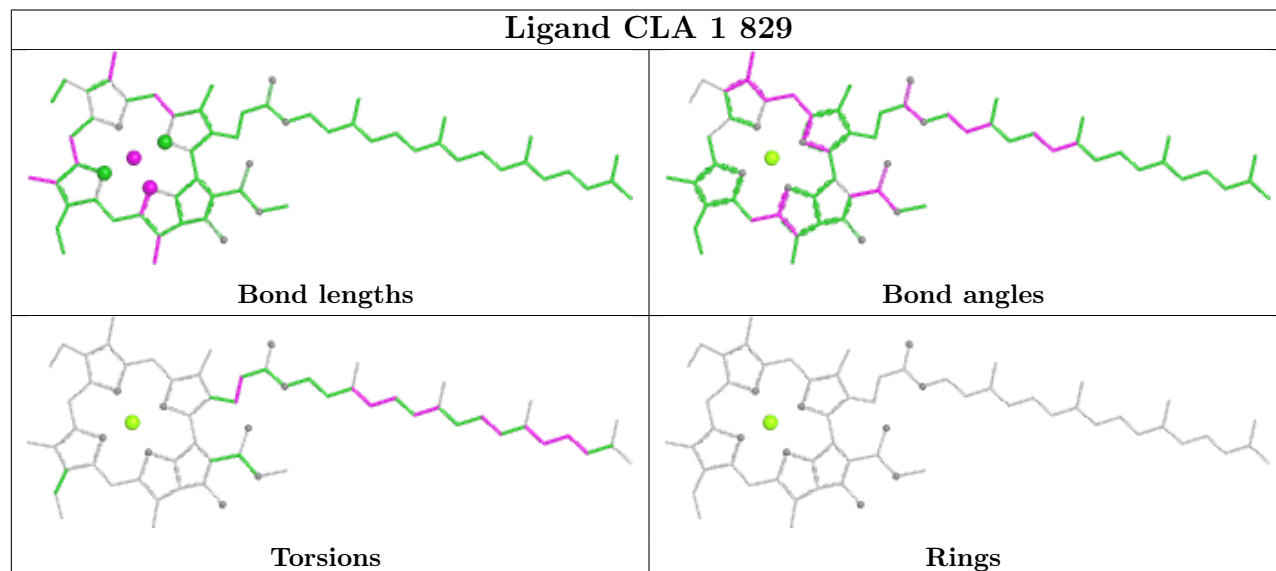


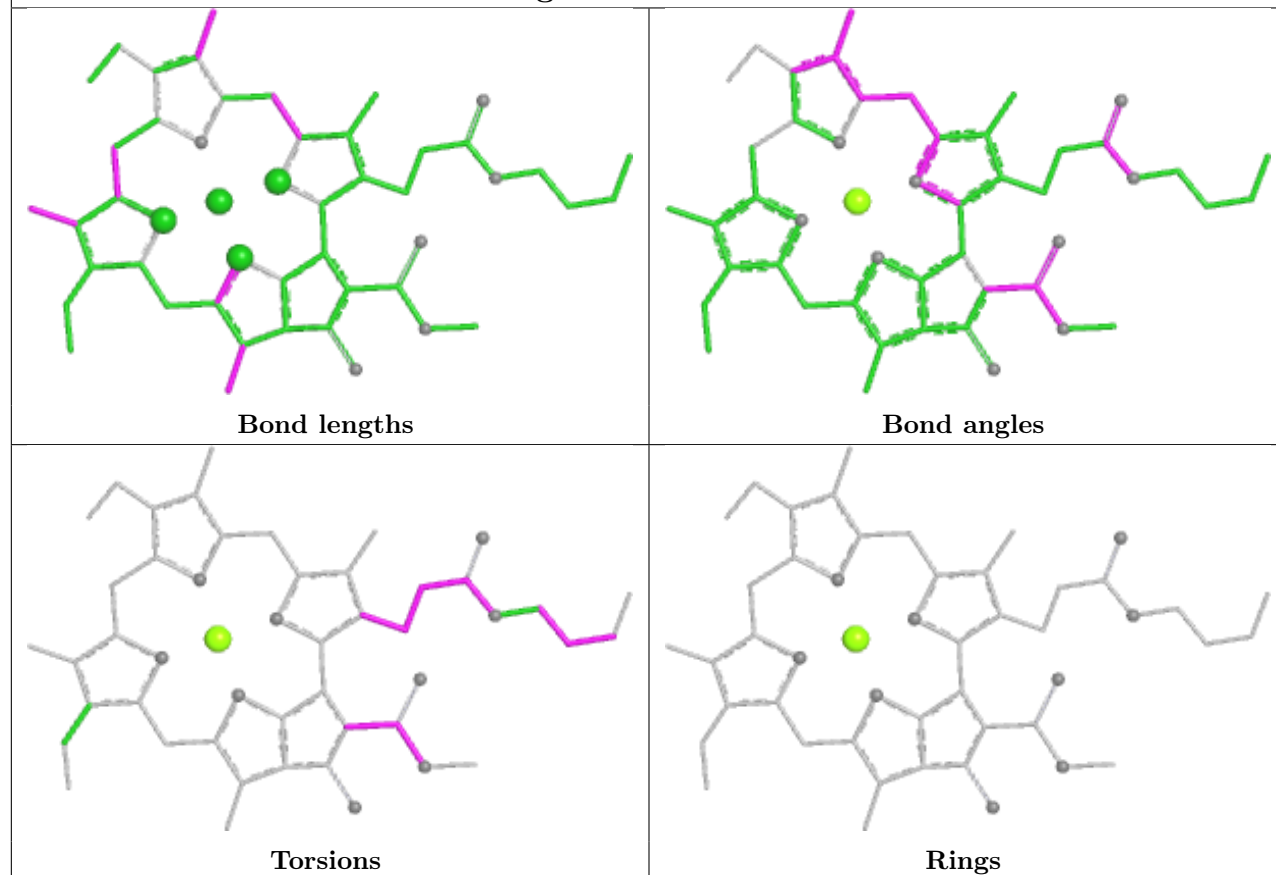
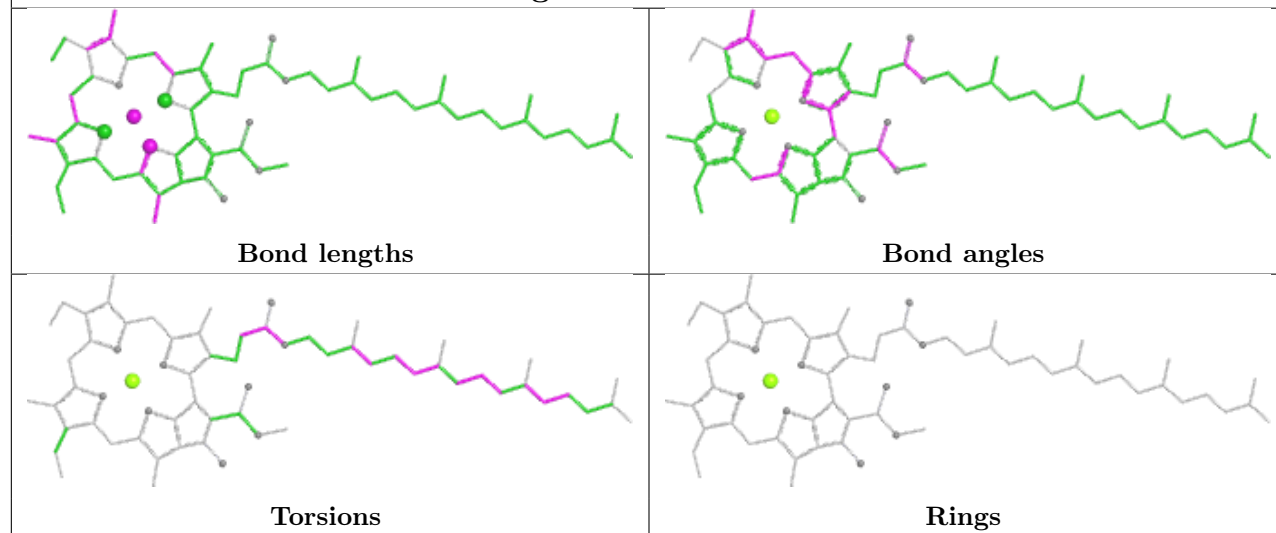
Rings

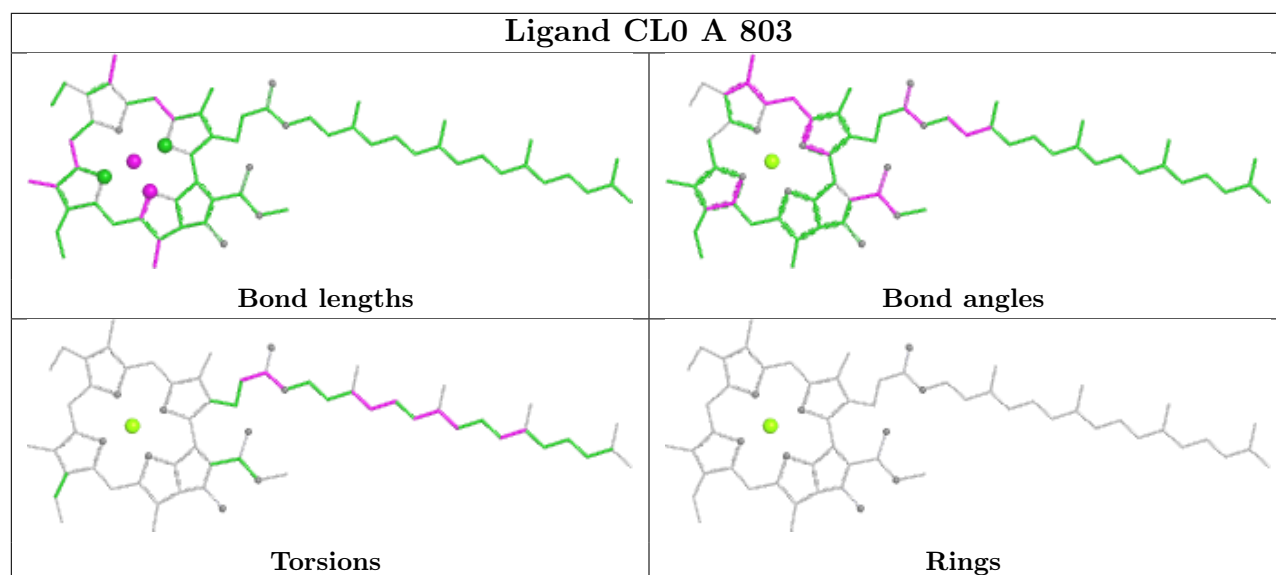
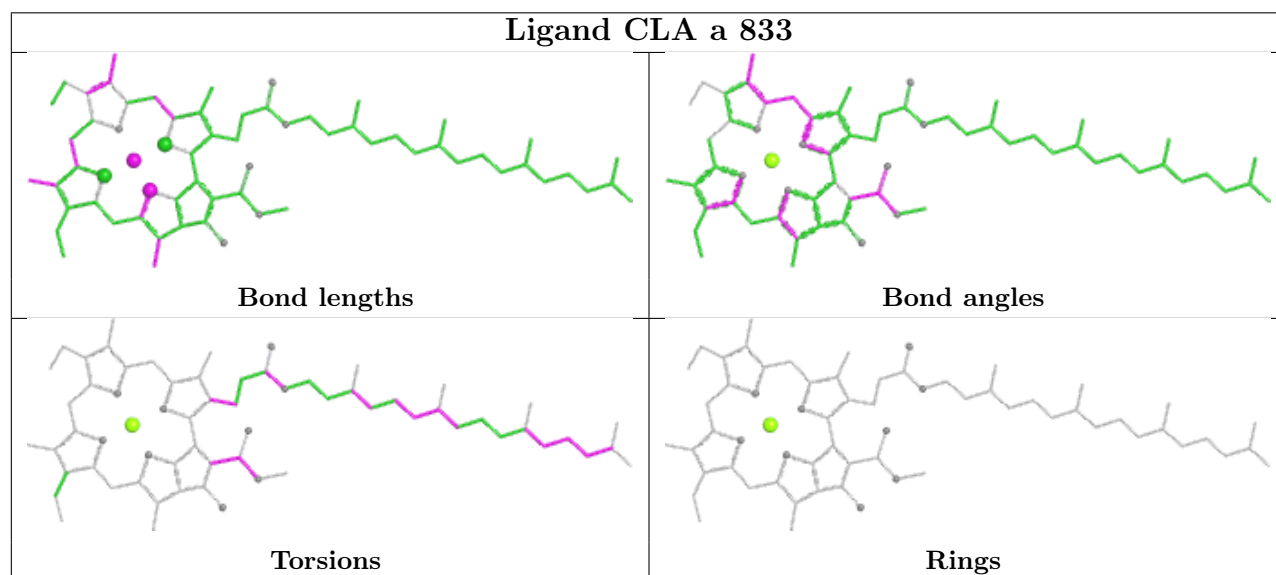
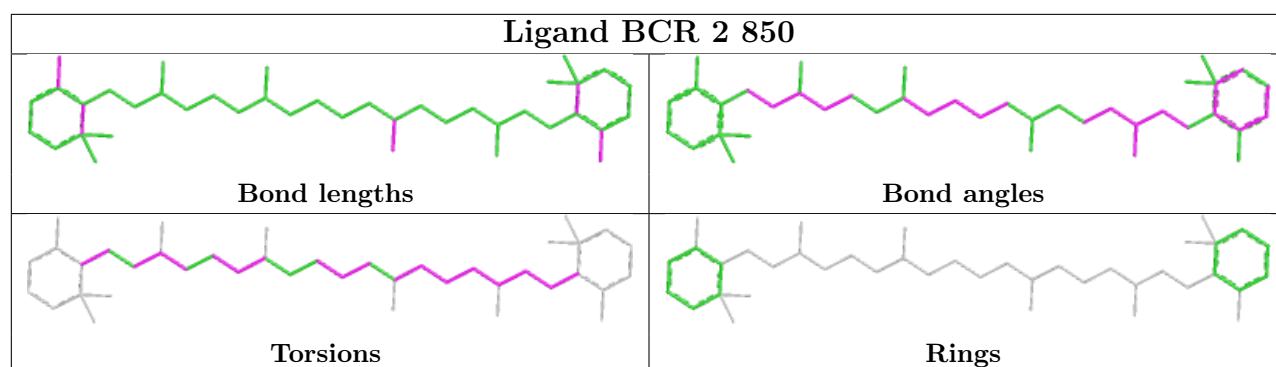




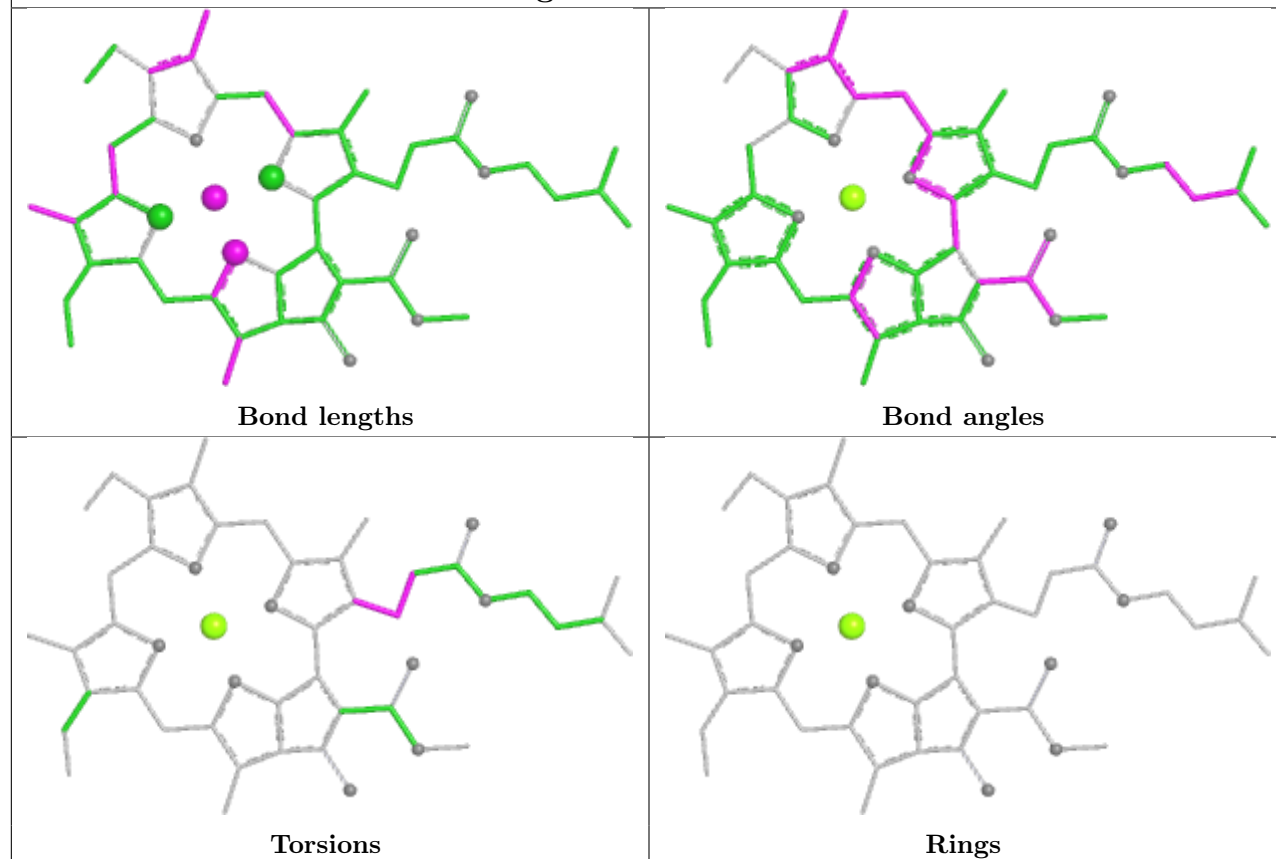


Ligand CLA 2 811**Ligand CLA 1 829**

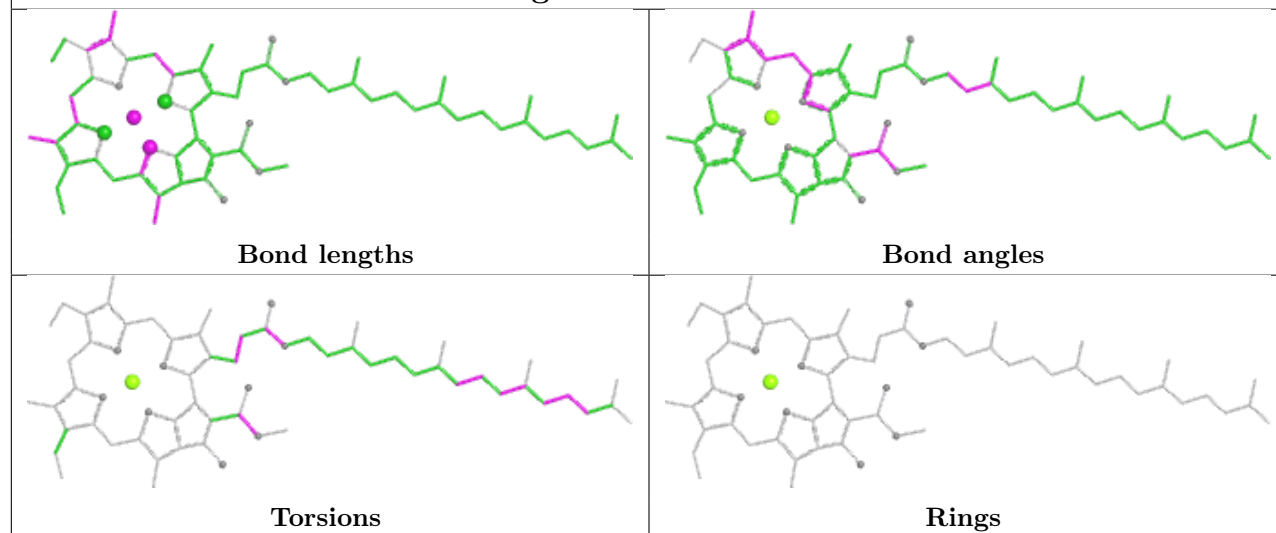
Ligand CLA 1 823**Ligand CLA A 827**



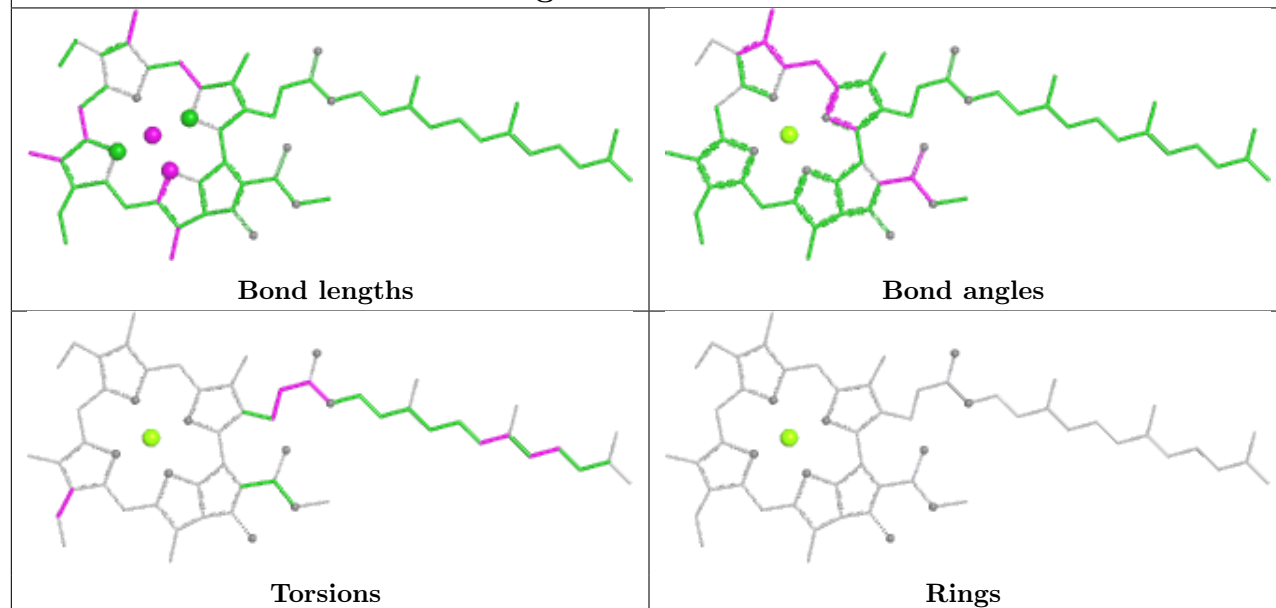
Ligand CLA 1 805



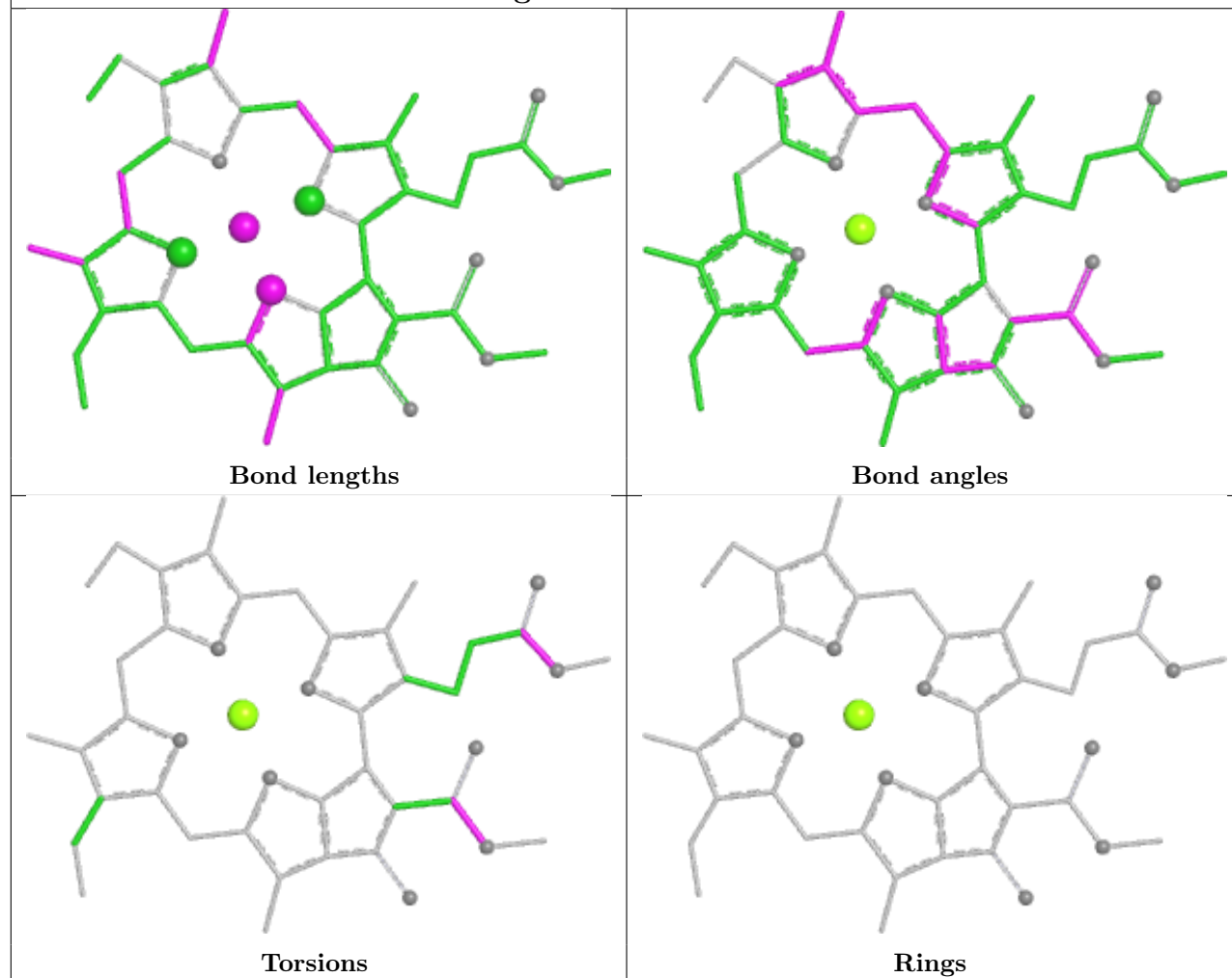
Ligand CLA A 839

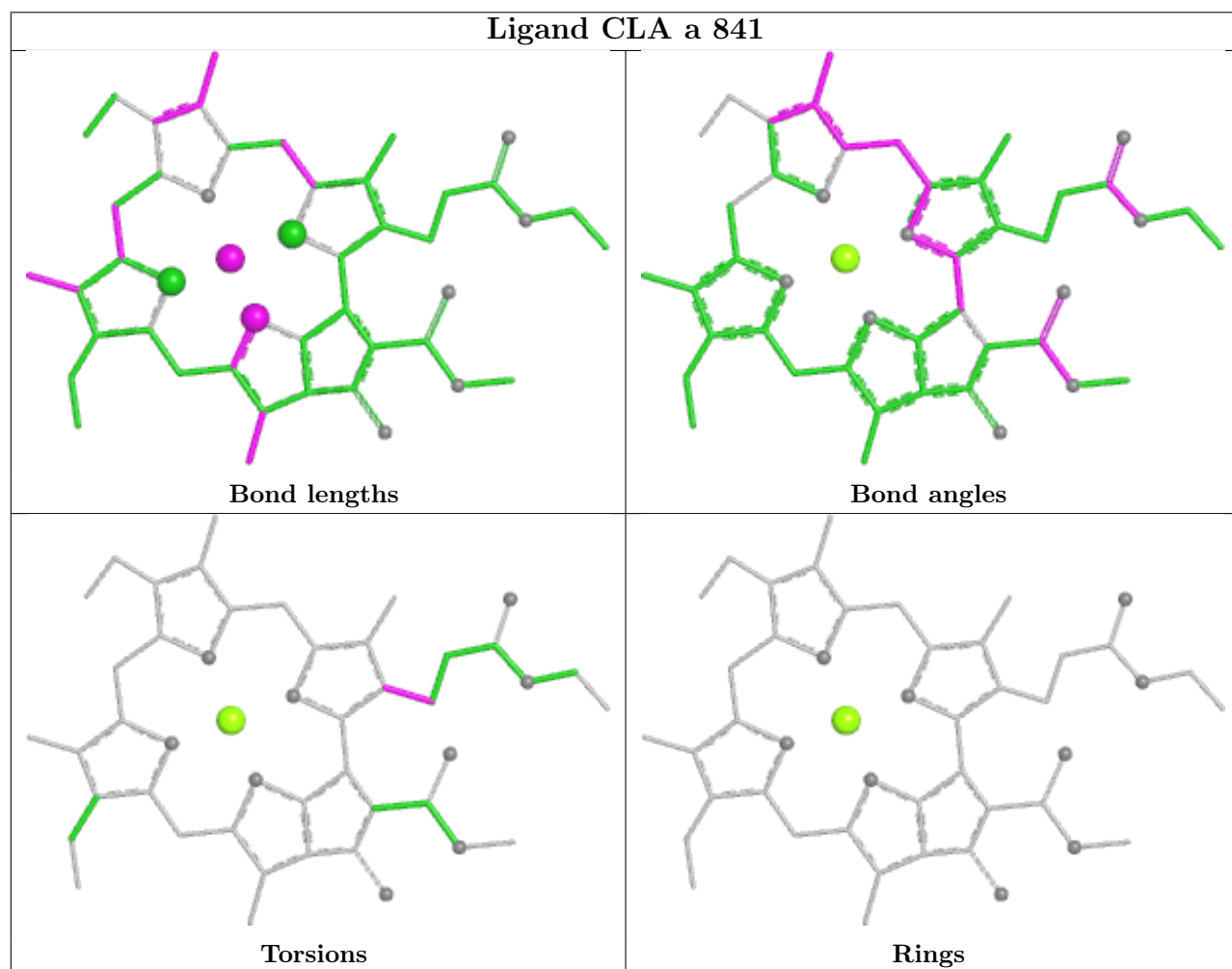
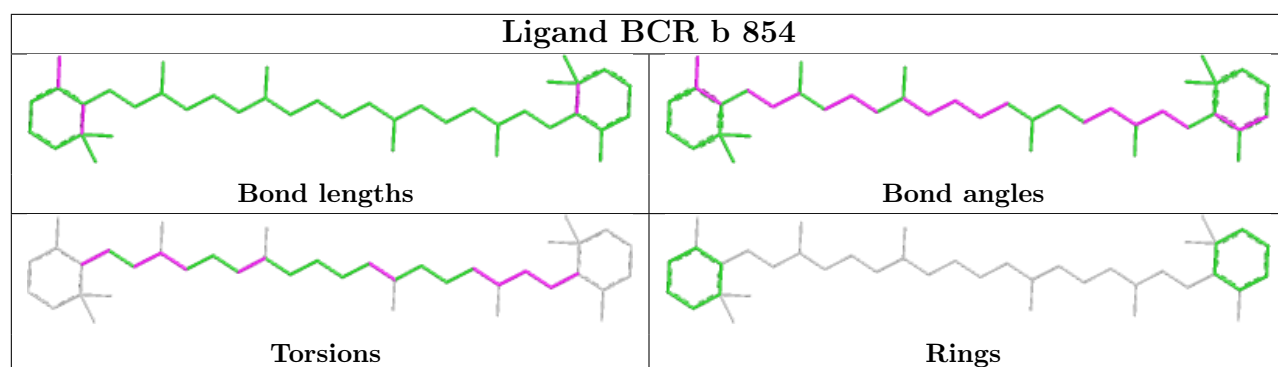


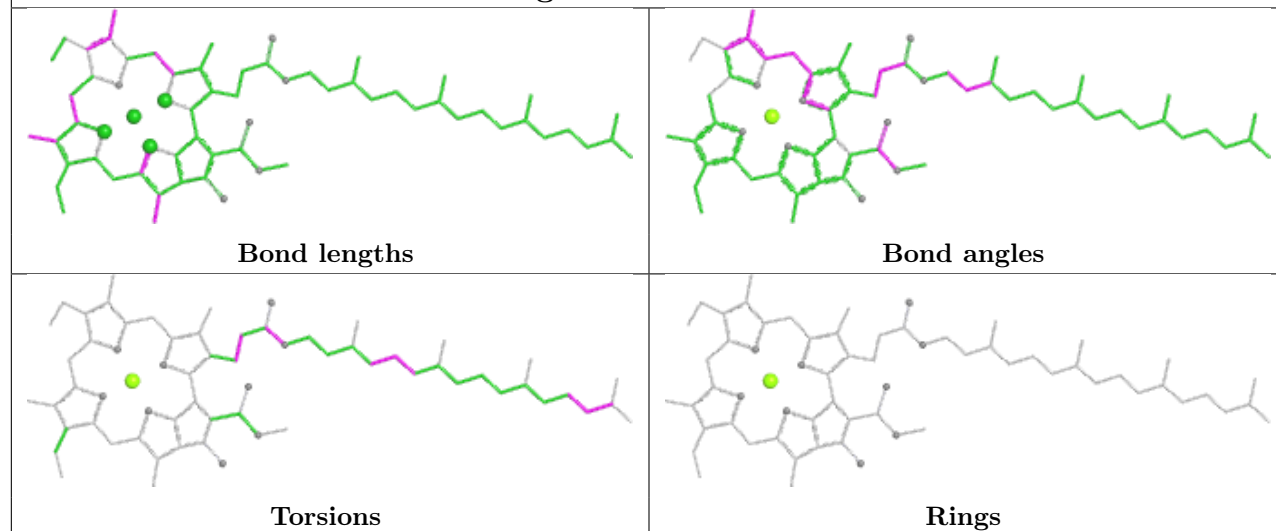
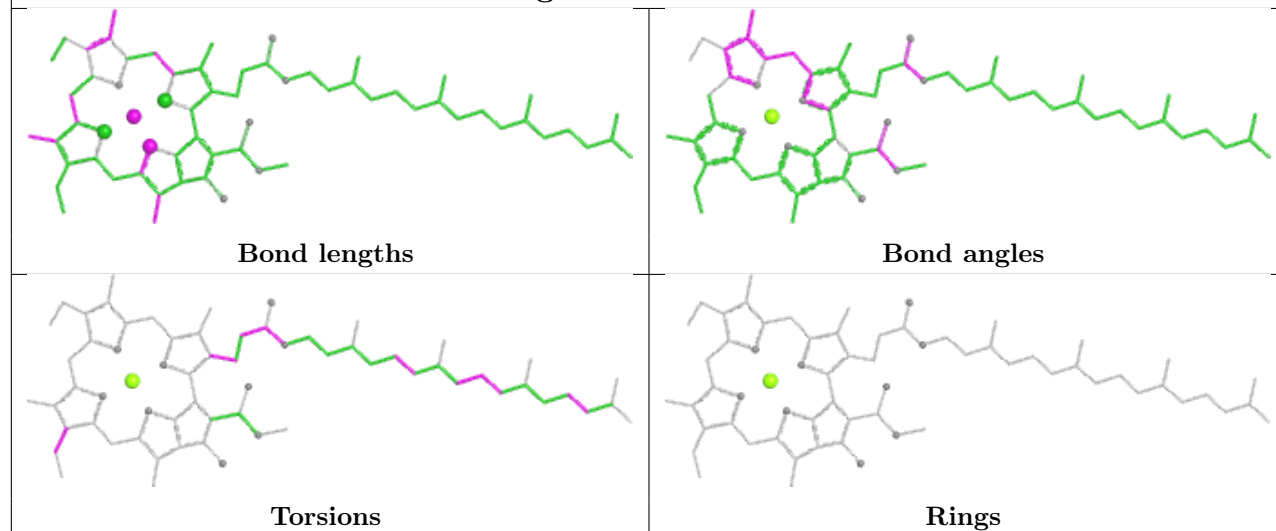
Ligand CLA 2 829

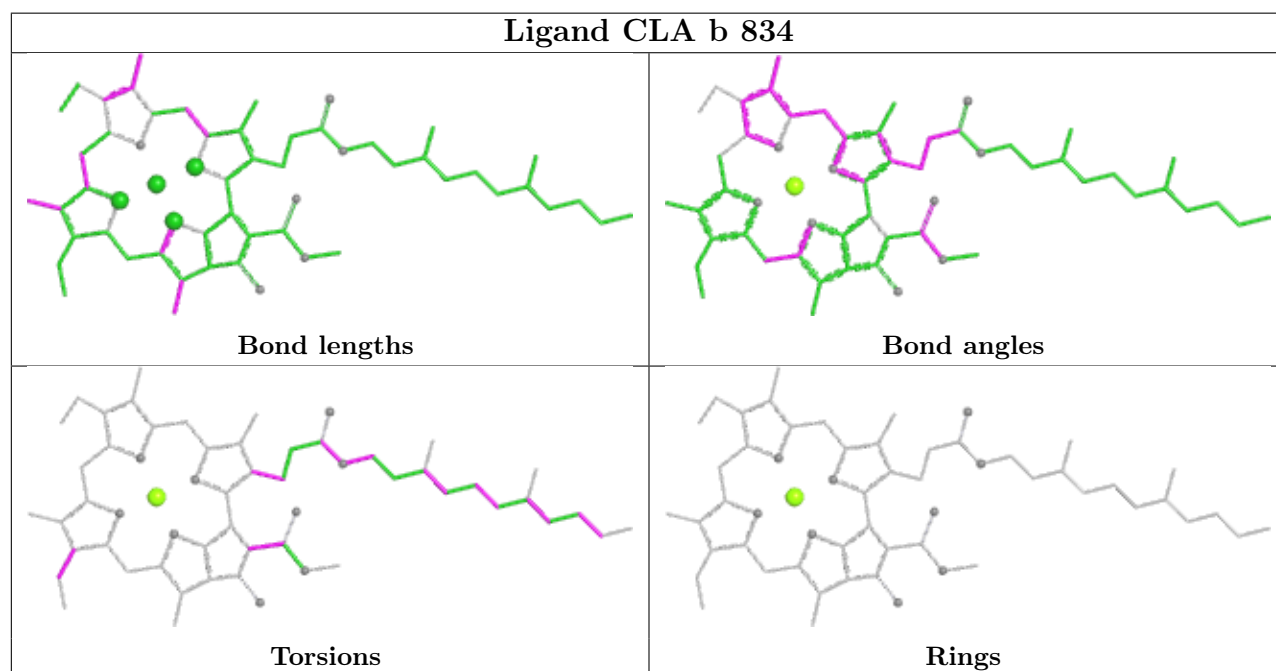
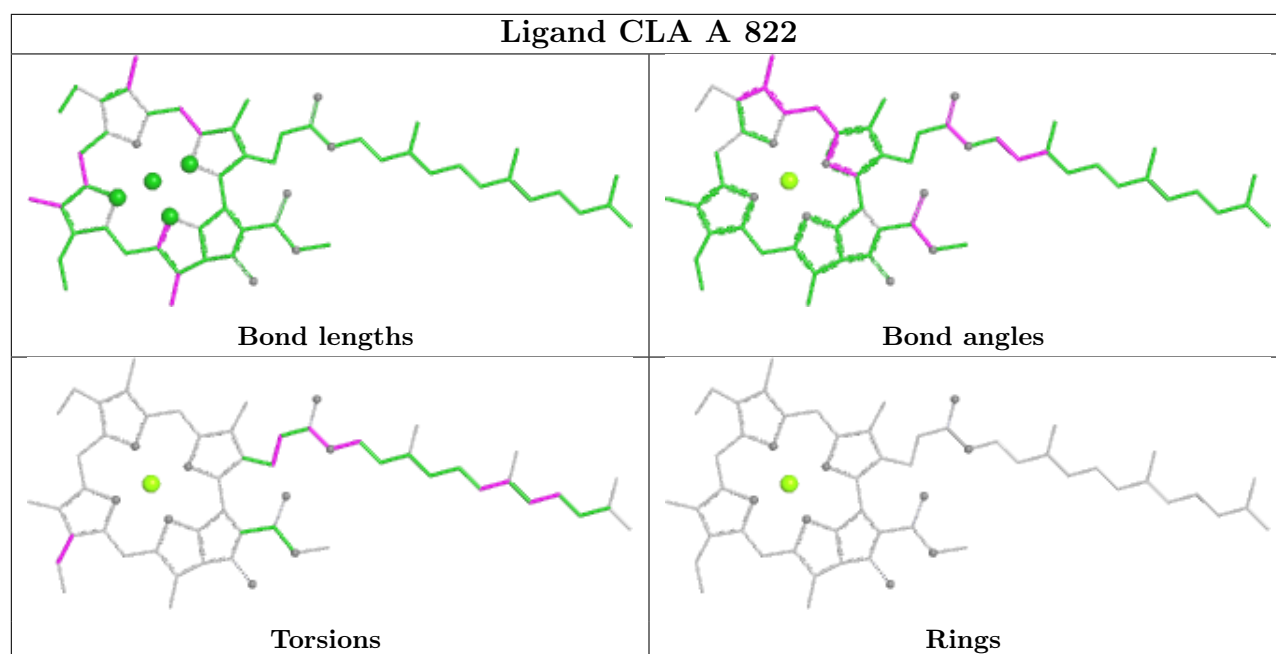


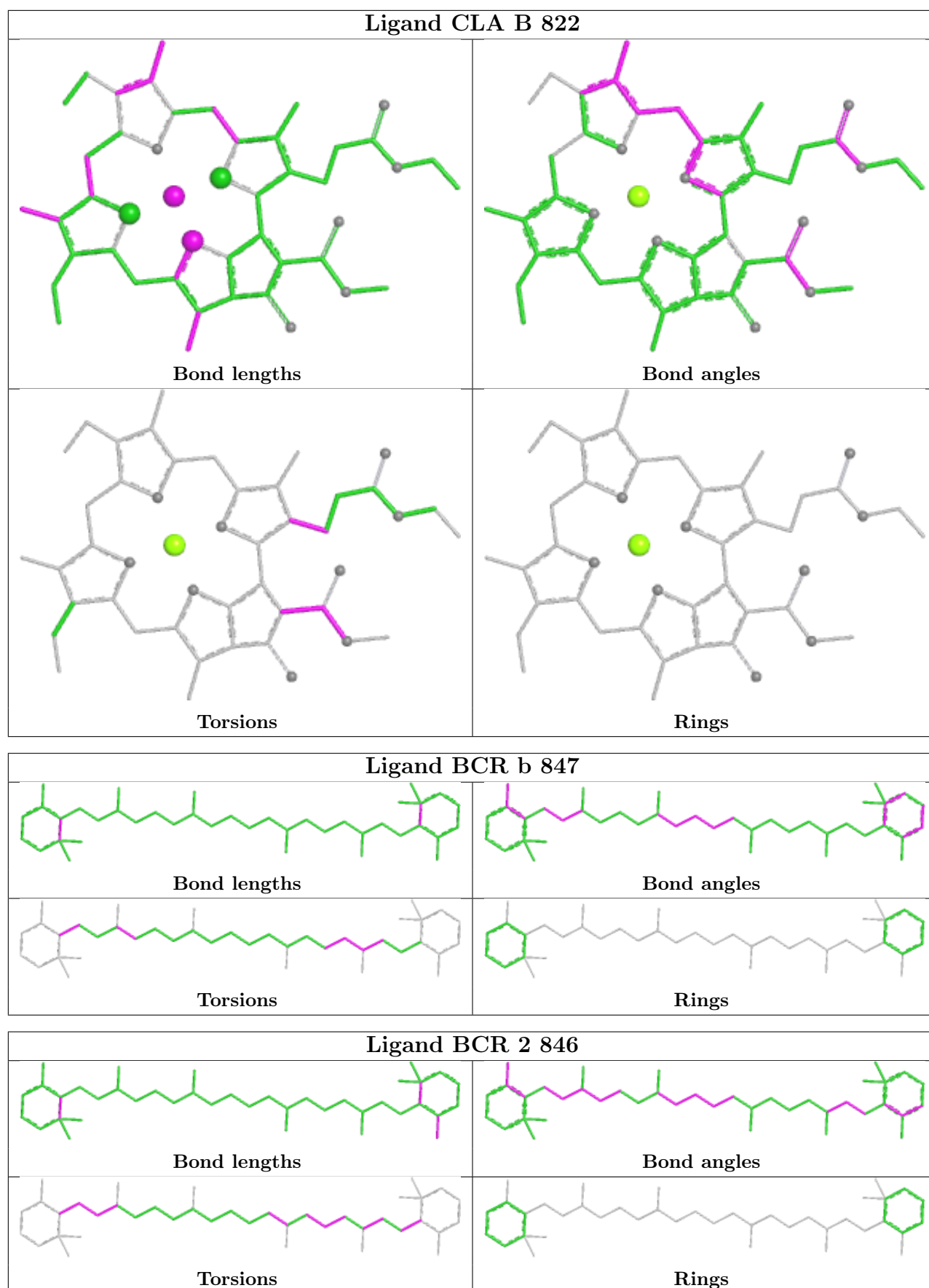
Ligand CLA B 842



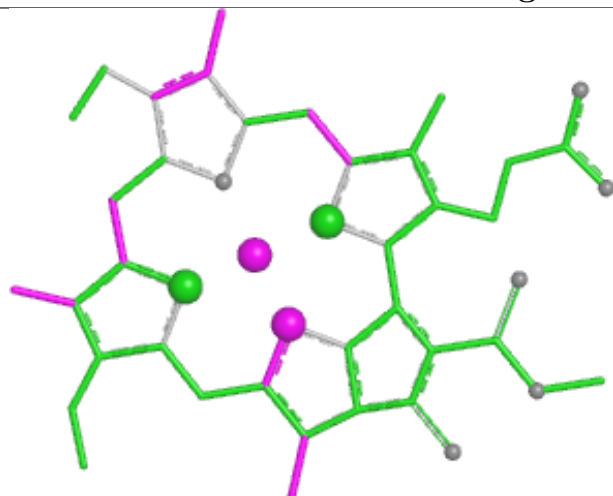


Ligand CLA 2 828**Ligand CLA 2 842**

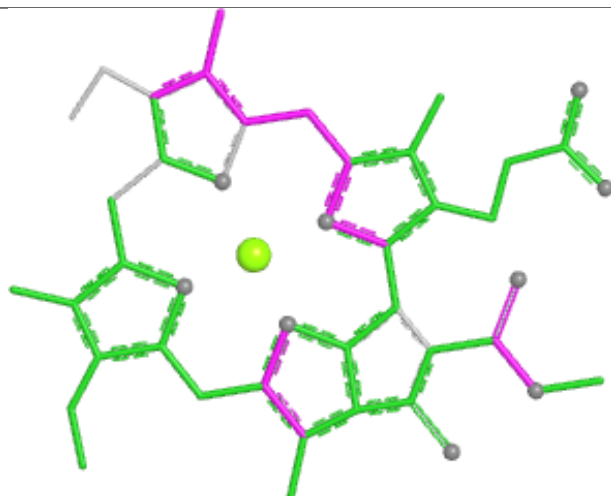




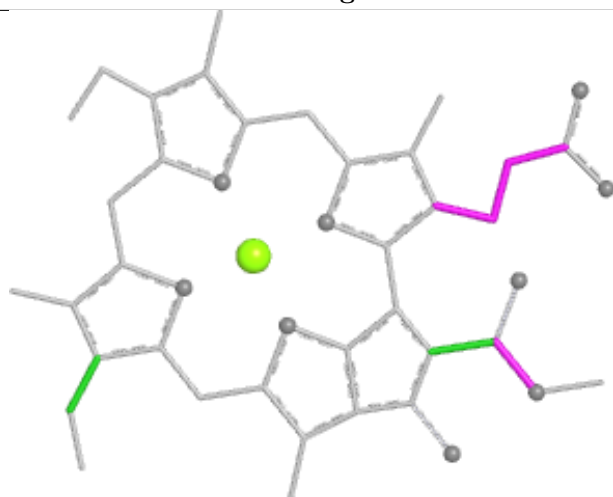
Ligand CLA 1 811



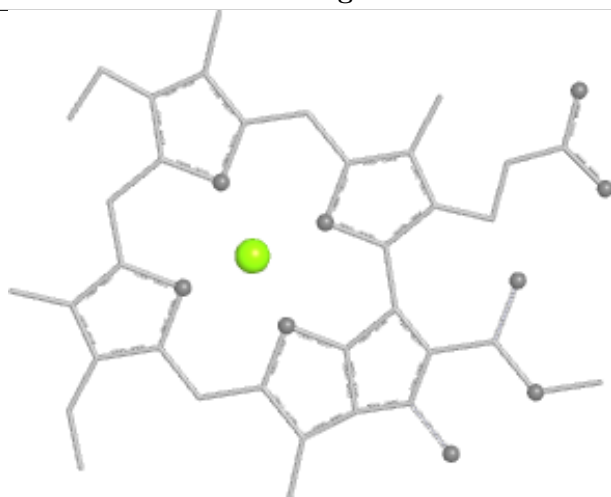
Bond lengths



Bond angles

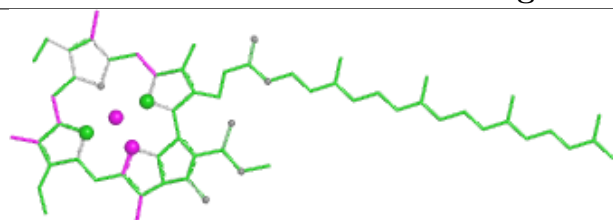


Torsions

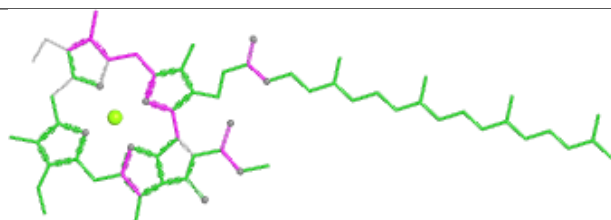


Rings

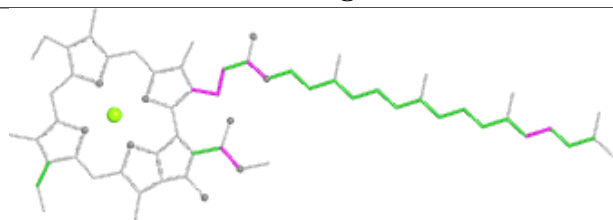
Ligand CLA b 830



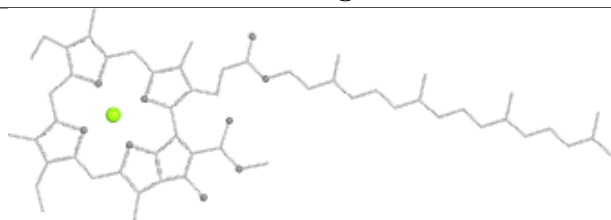
Bond lengths



Bond angles

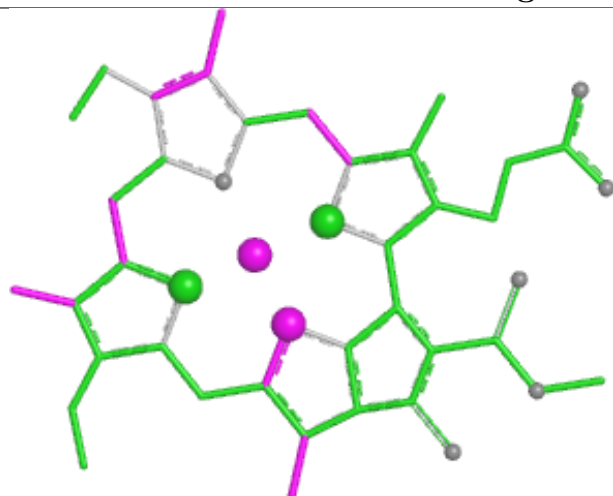


Torsions

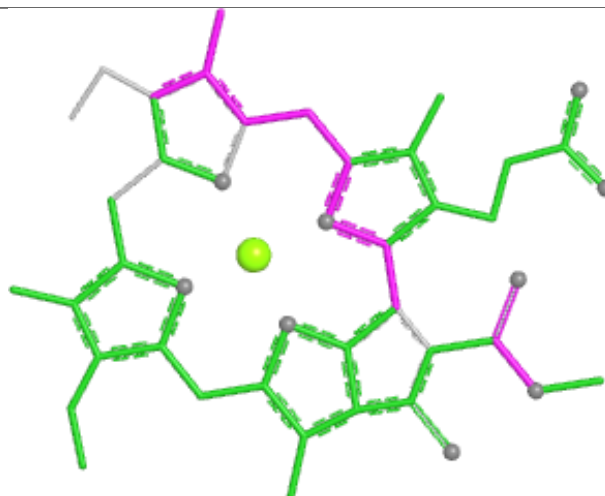


Rings

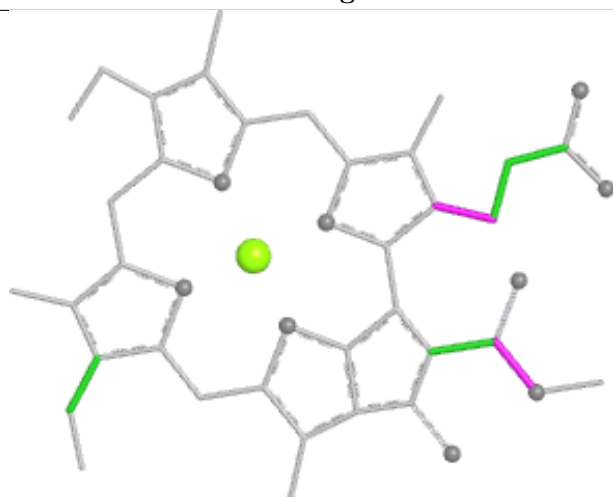
Ligand CLA b 813



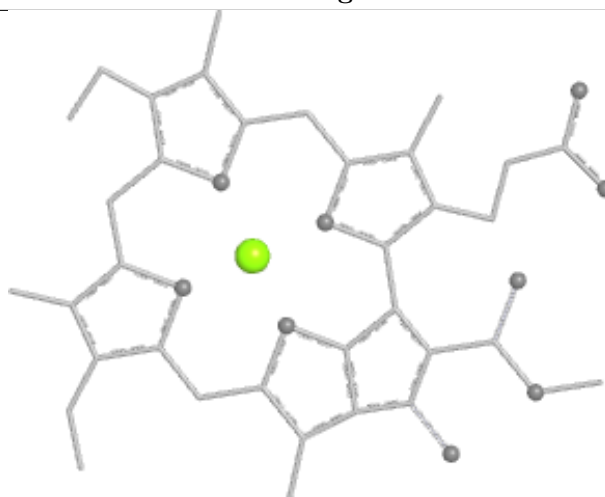
Bond lengths



Bond angles

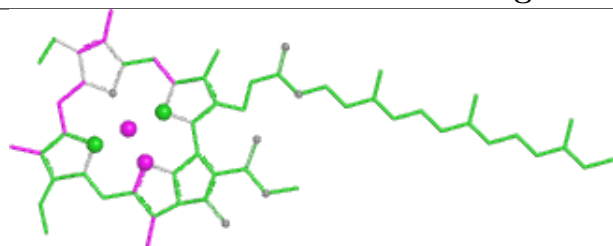


Torsions

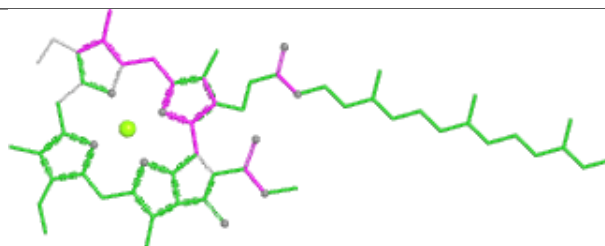


Rings

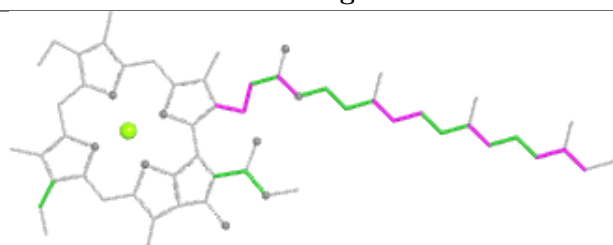
Ligand CLA B 812



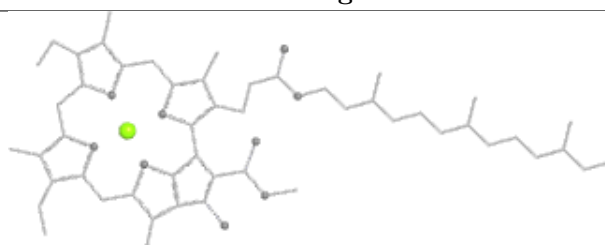
Bond lengths



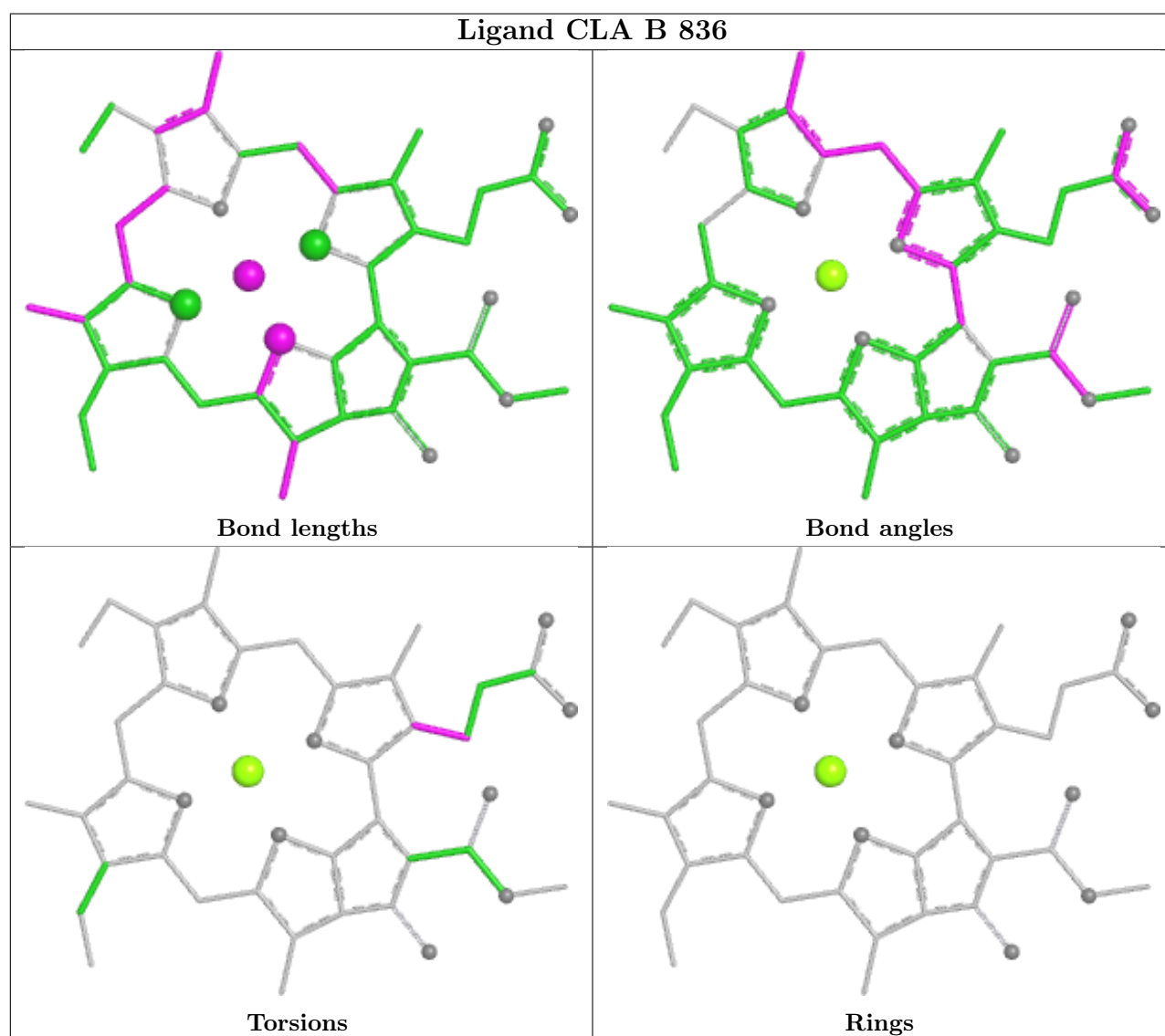
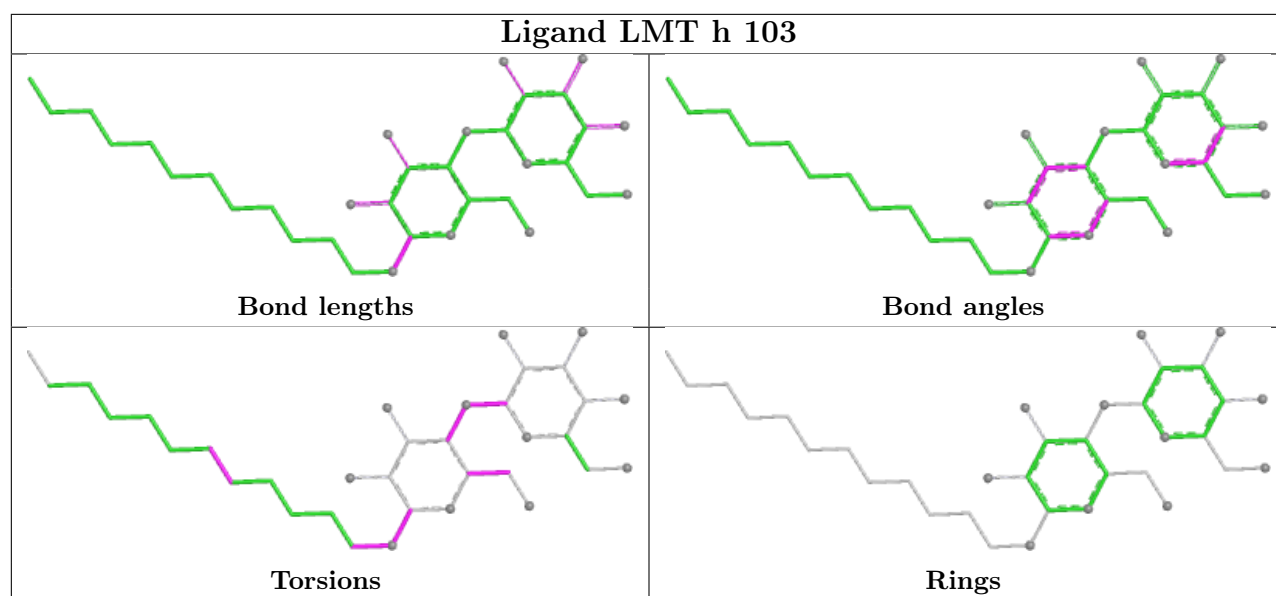
Bond angles



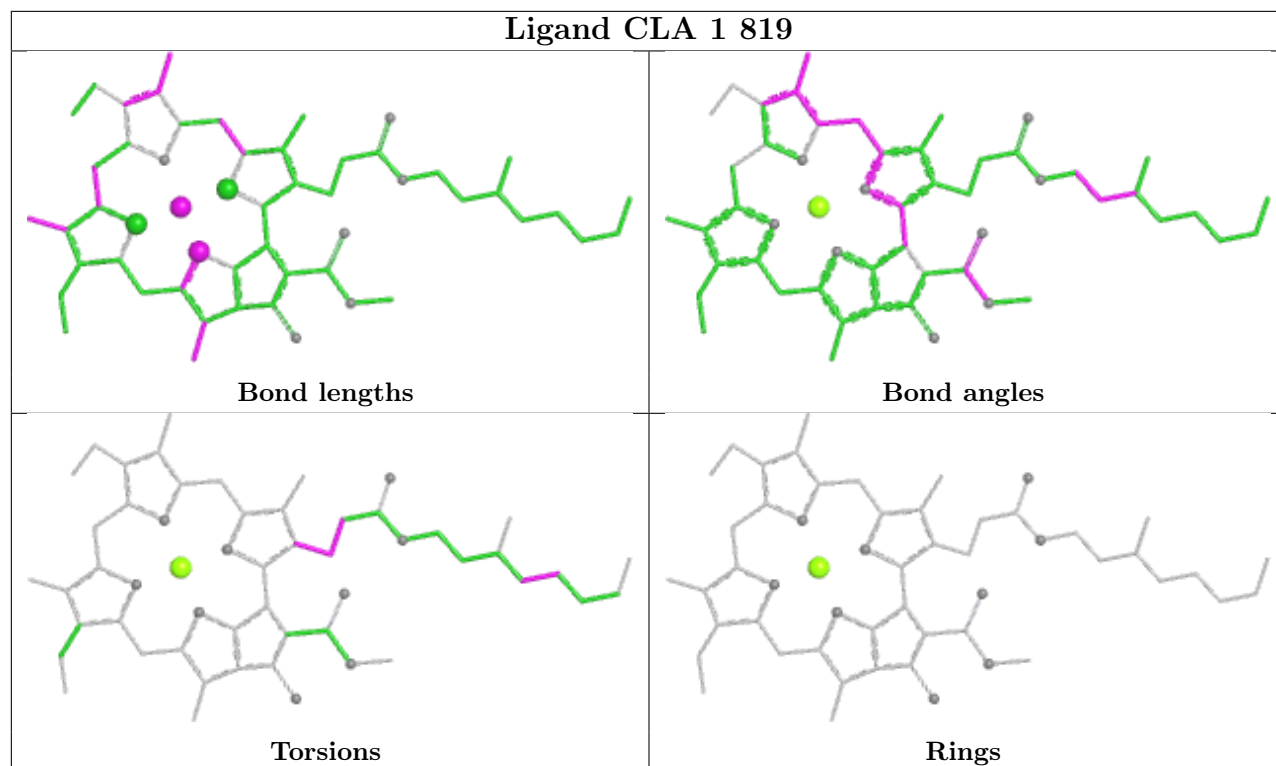
Torsions



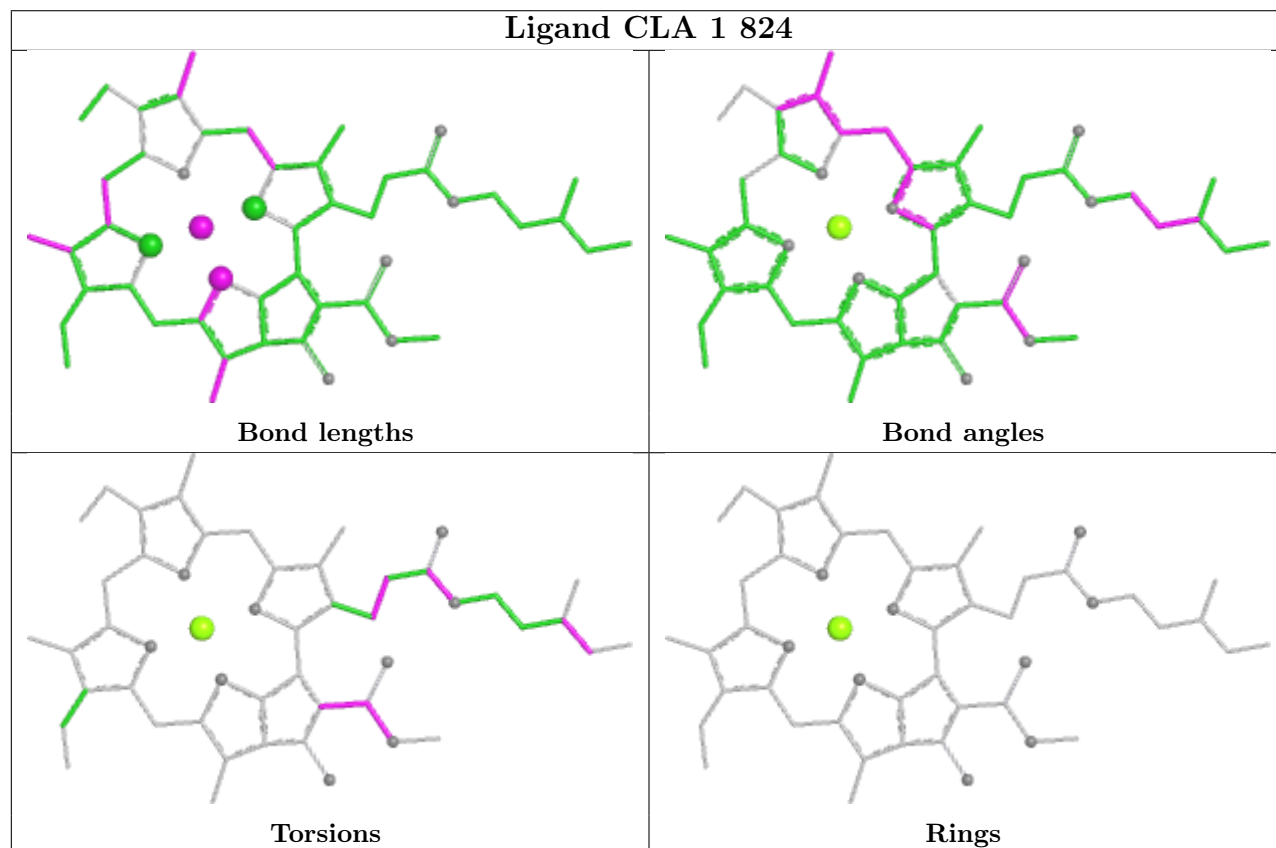
Rings

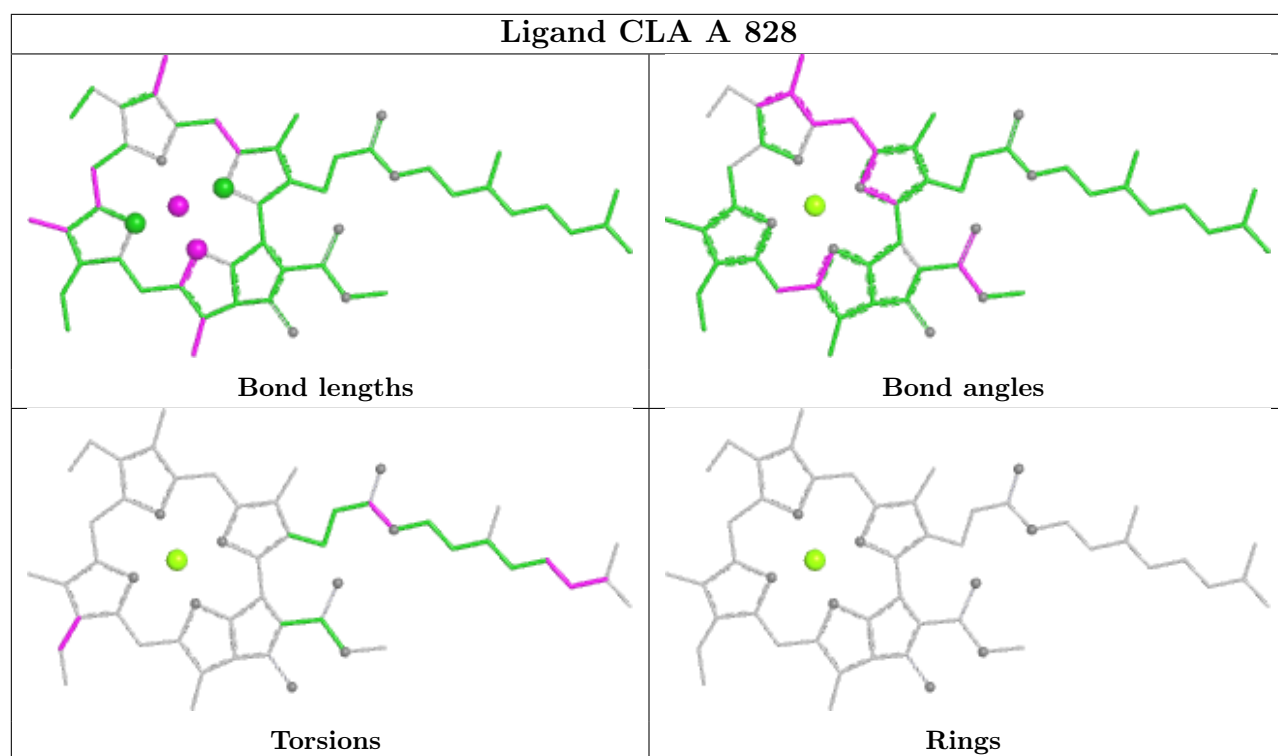


Ligand CLA 1 819

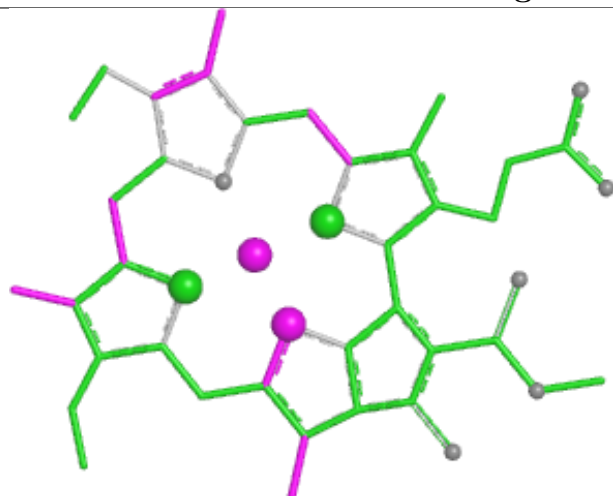


Ligand CLA 1 824

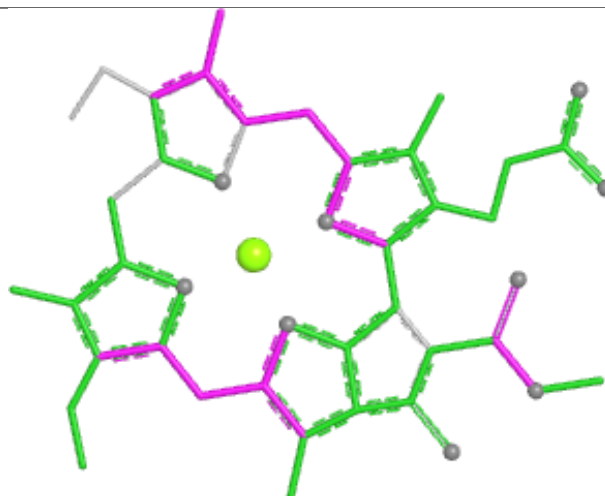




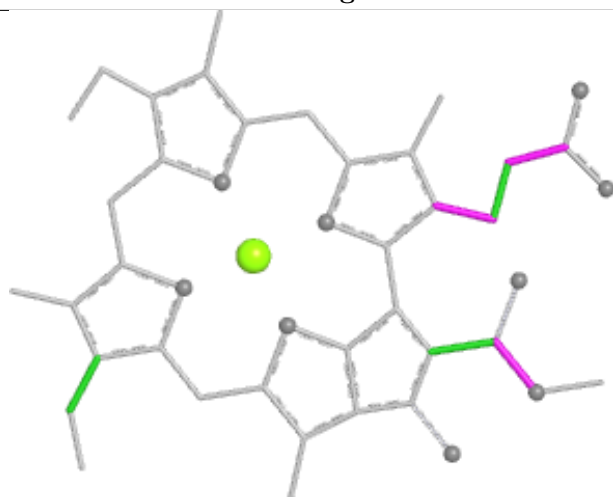
Ligand CLA B 833



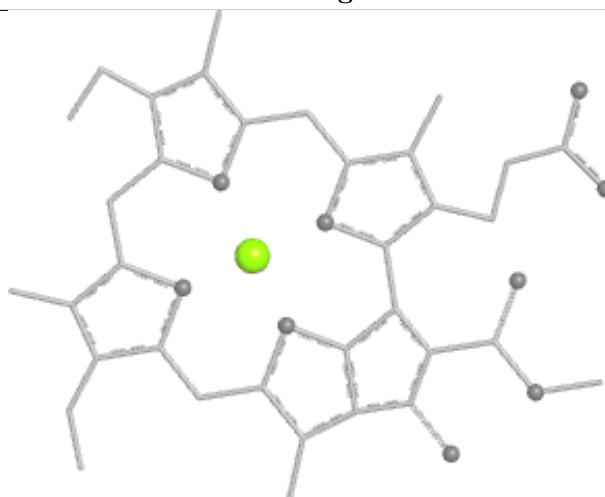
Bond lengths



Bond angles

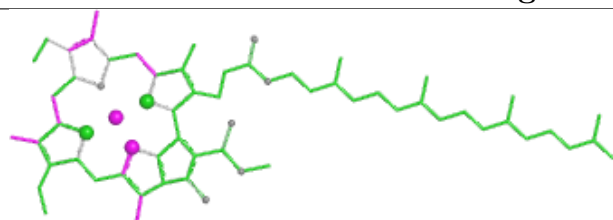


Torsions

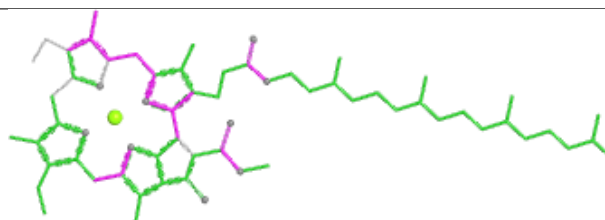


Rings

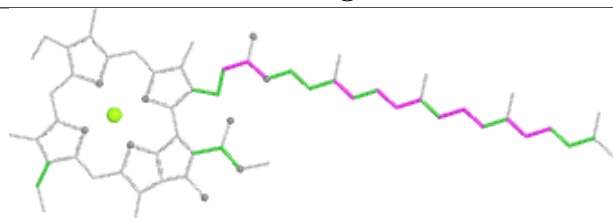
Ligand CLA 1 826



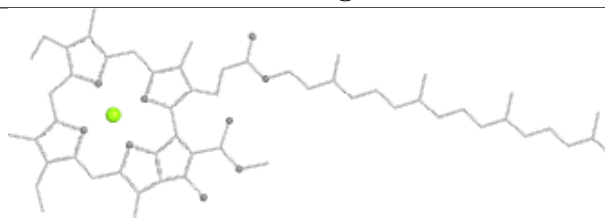
Bond lengths



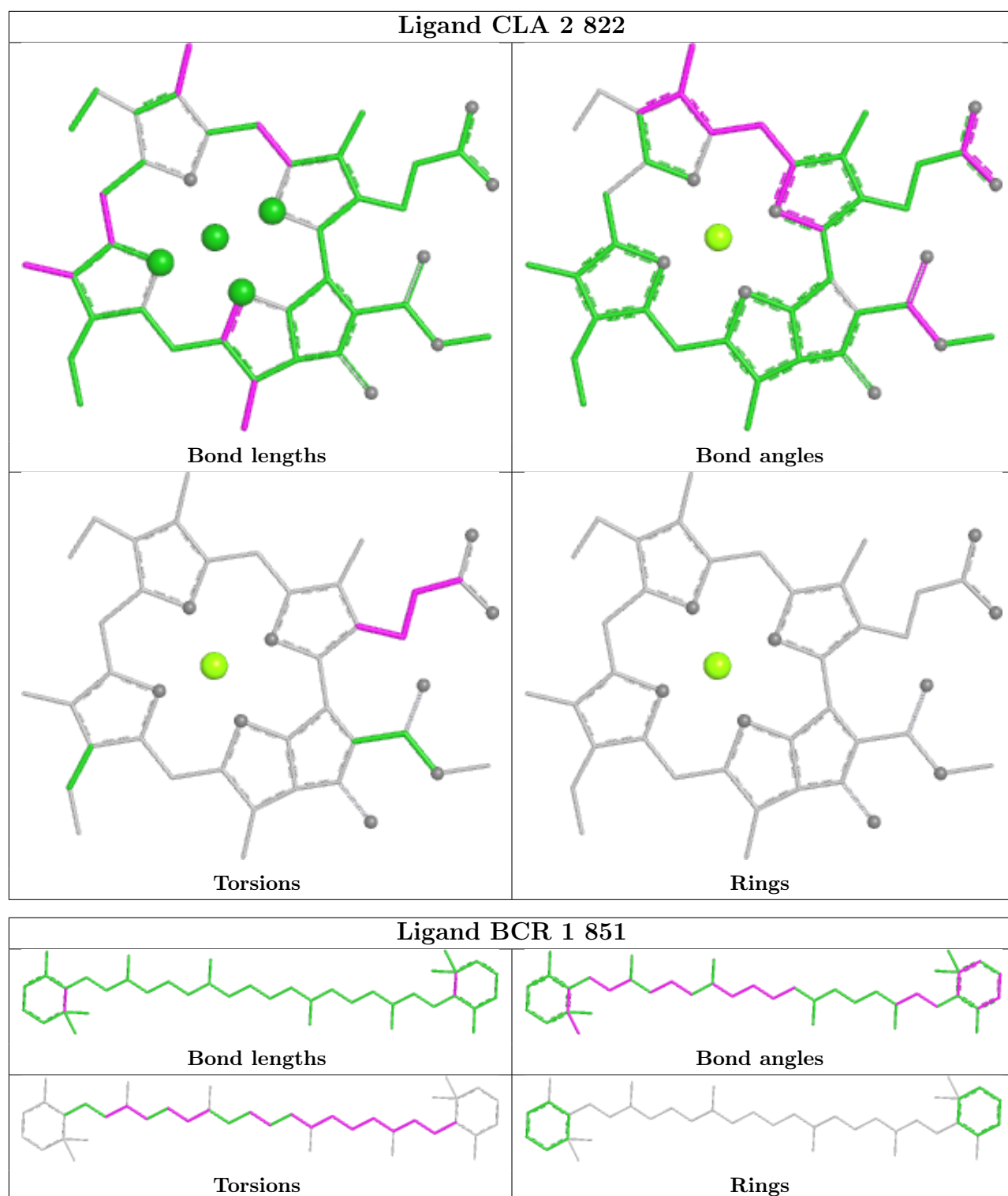
Bond angles

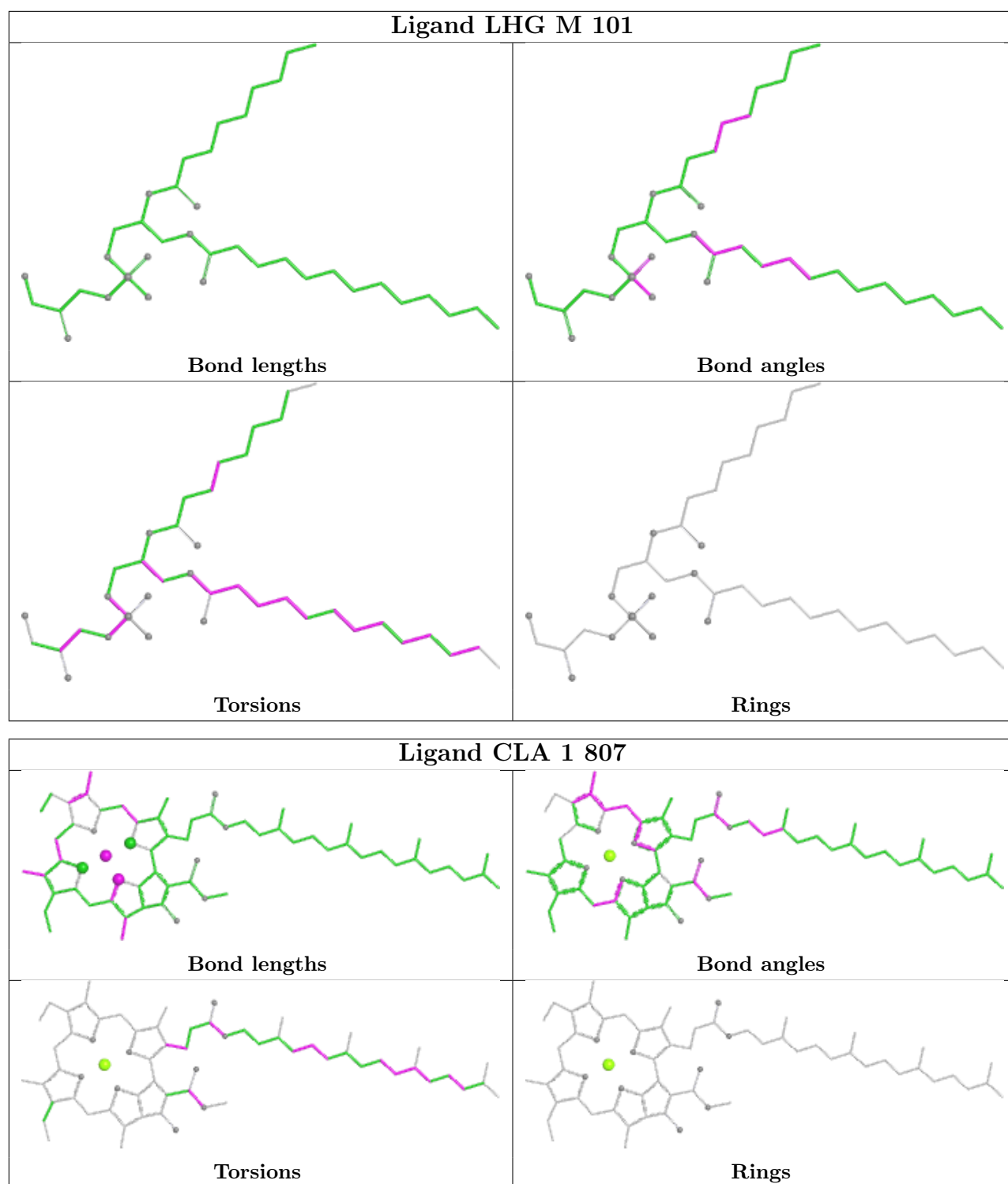


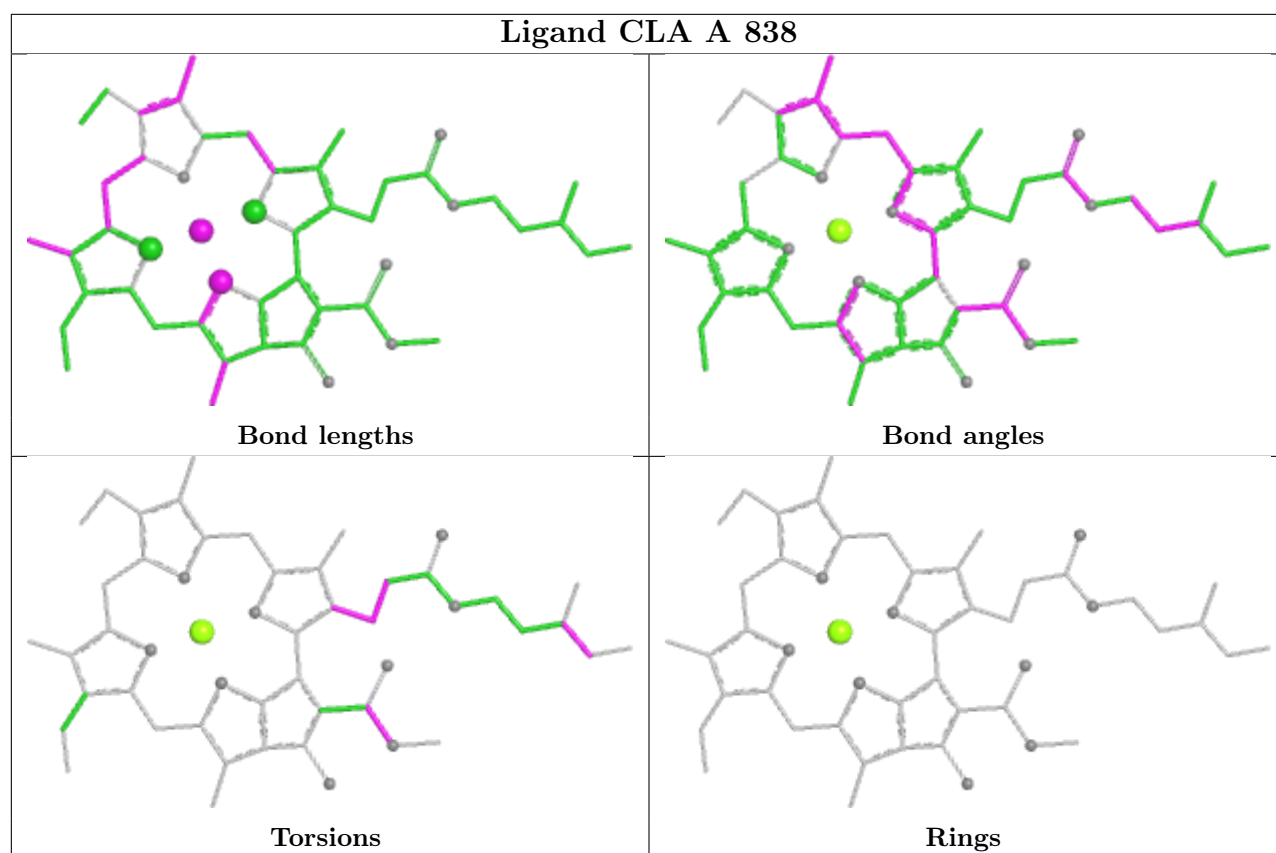
Torsions



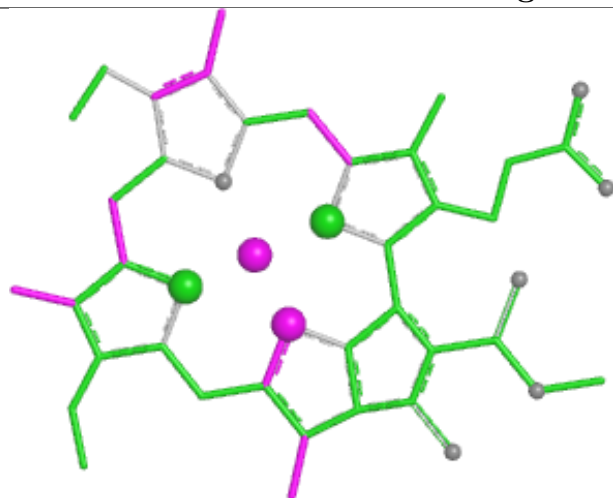
Rings



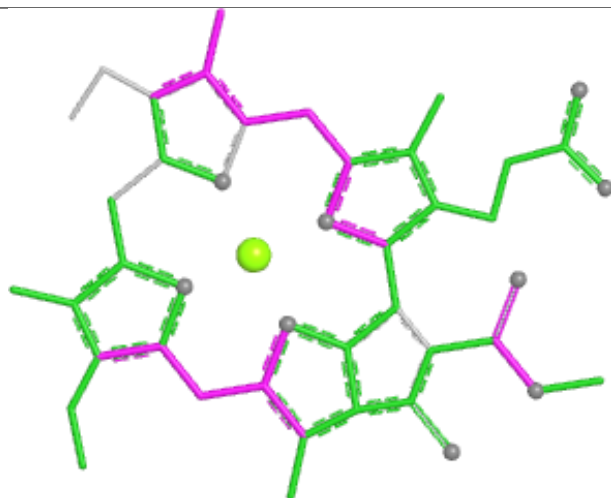




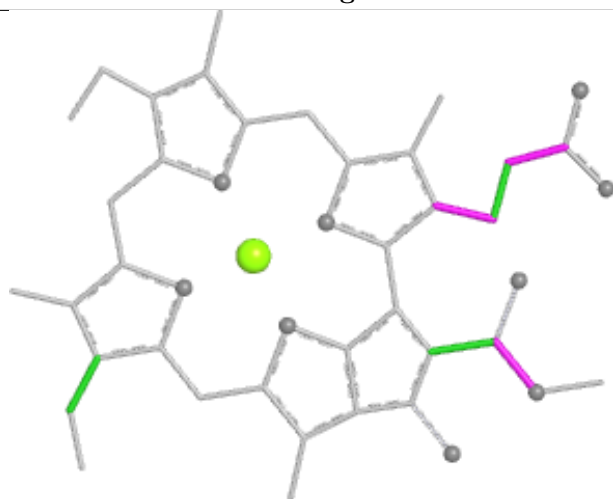
Ligand CLA b 832



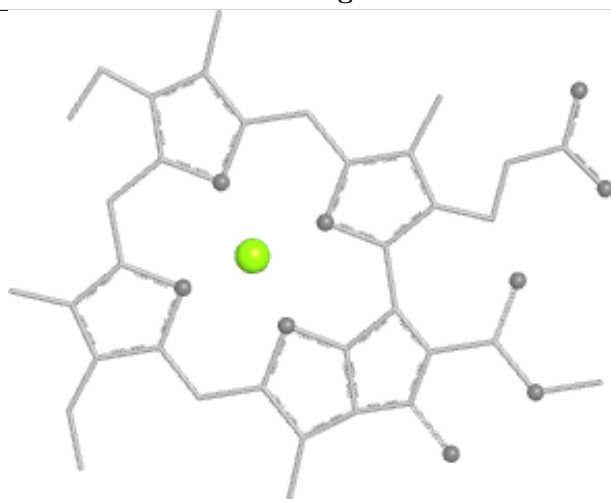
Bond lengths



Bond angles

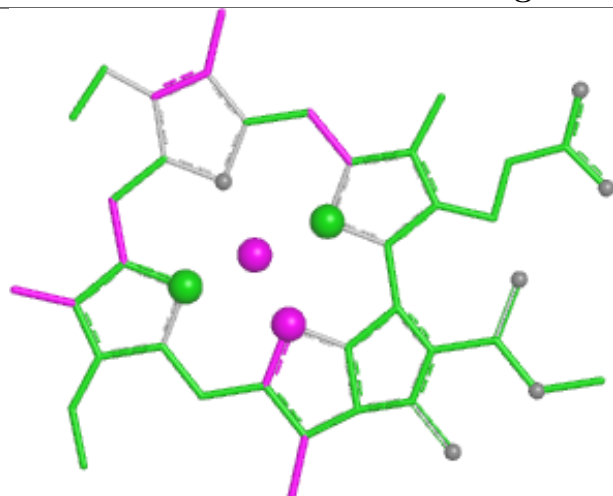


Torsions

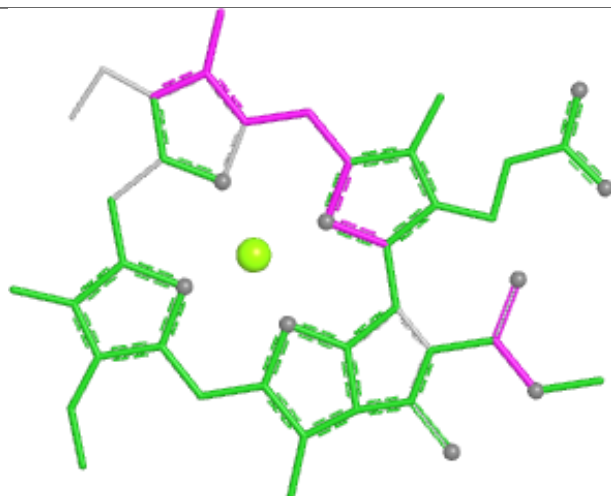


Rings

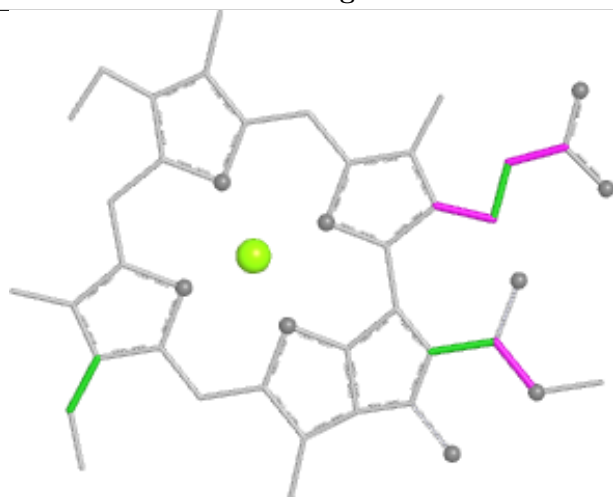
Ligand CLA B 826



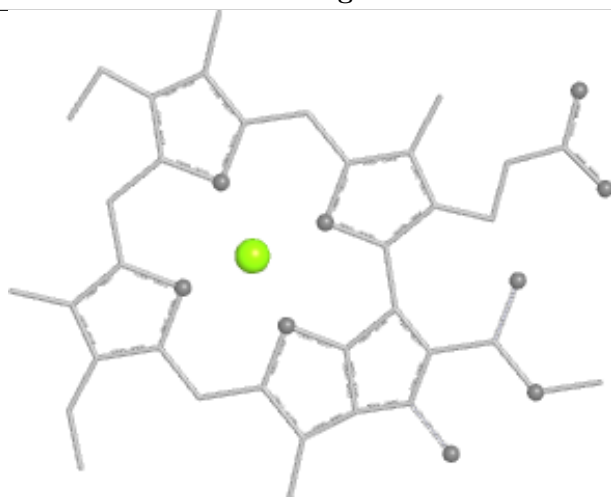
Bond lengths



Bond angles

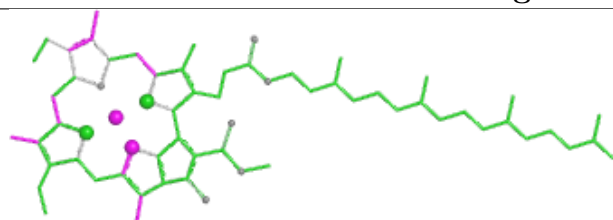


Torsions

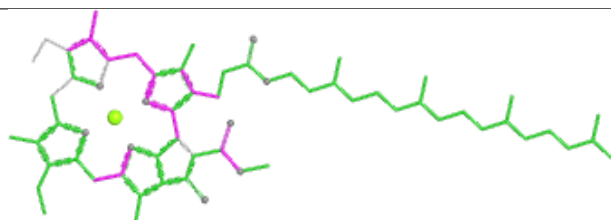


Rings

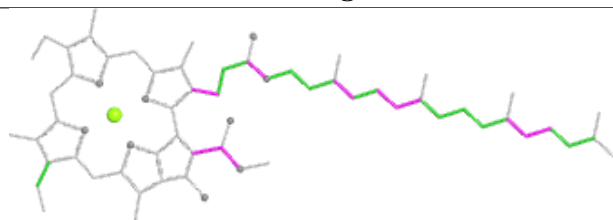
Ligand CLA I 4204



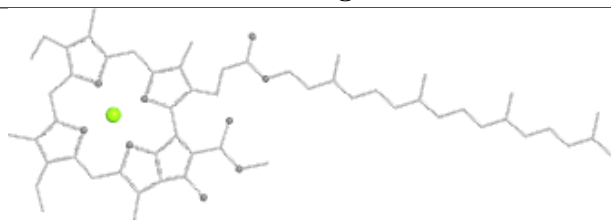
Bond lengths



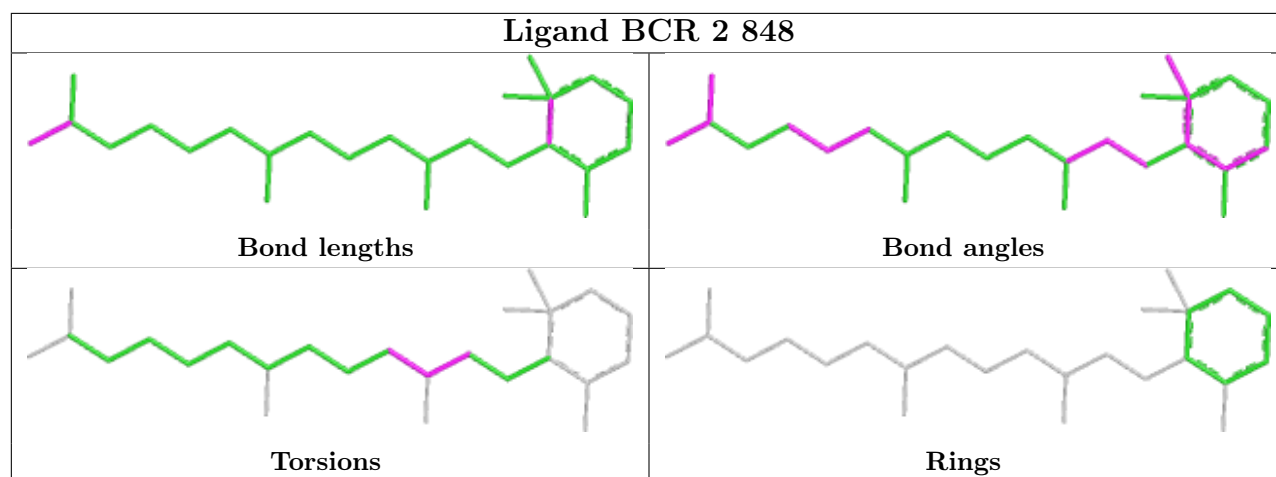
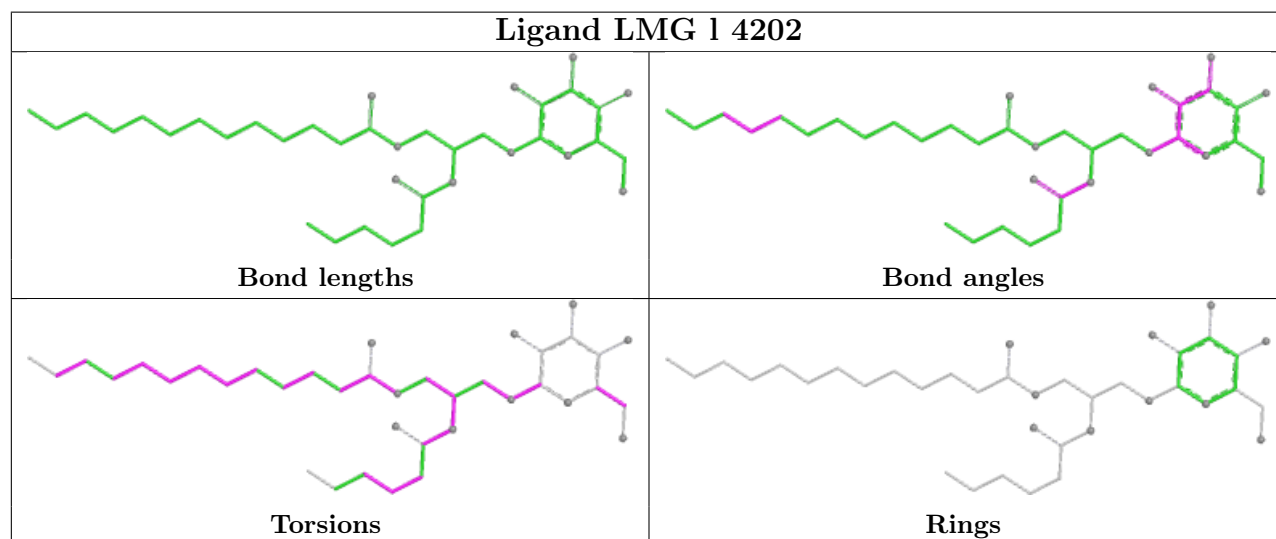
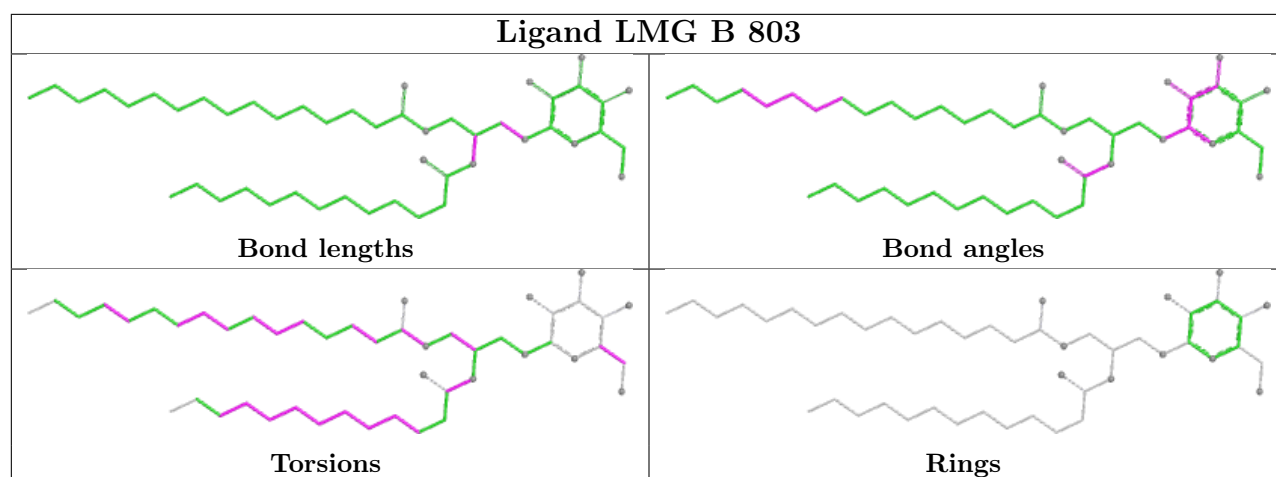
Bond angles

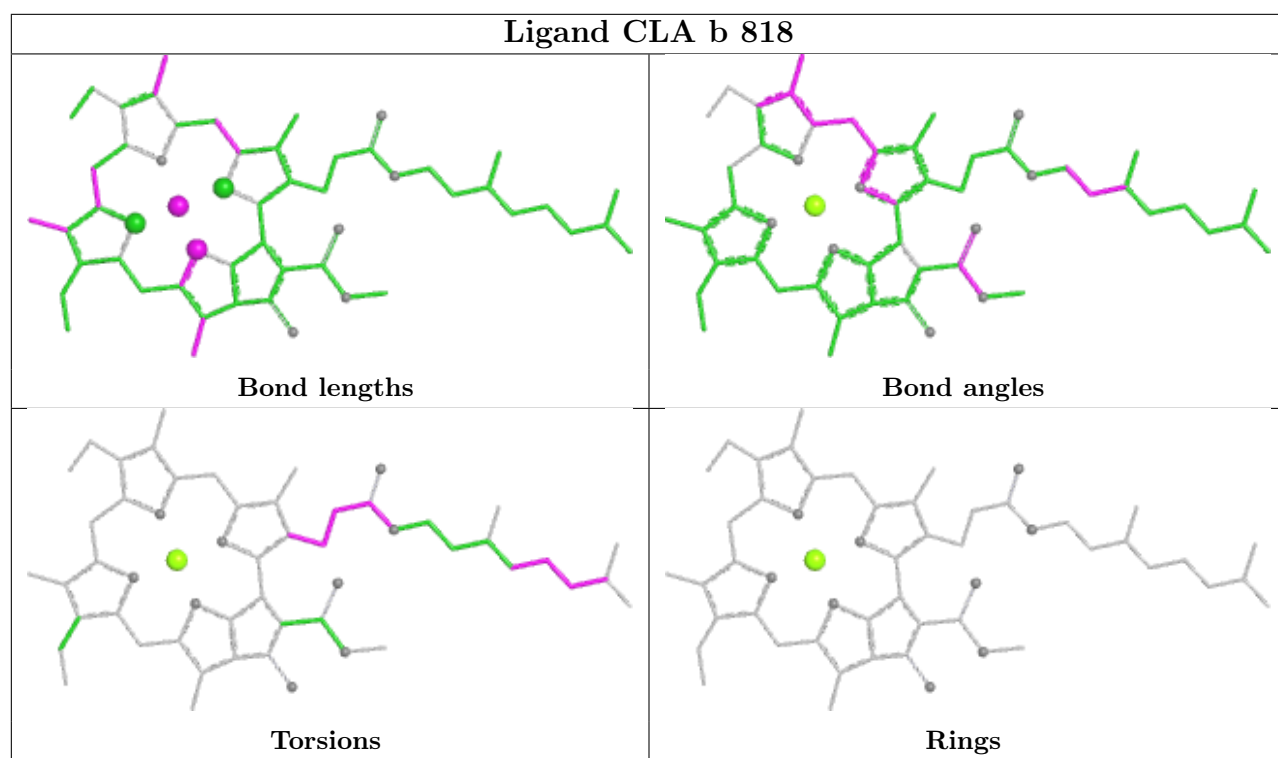
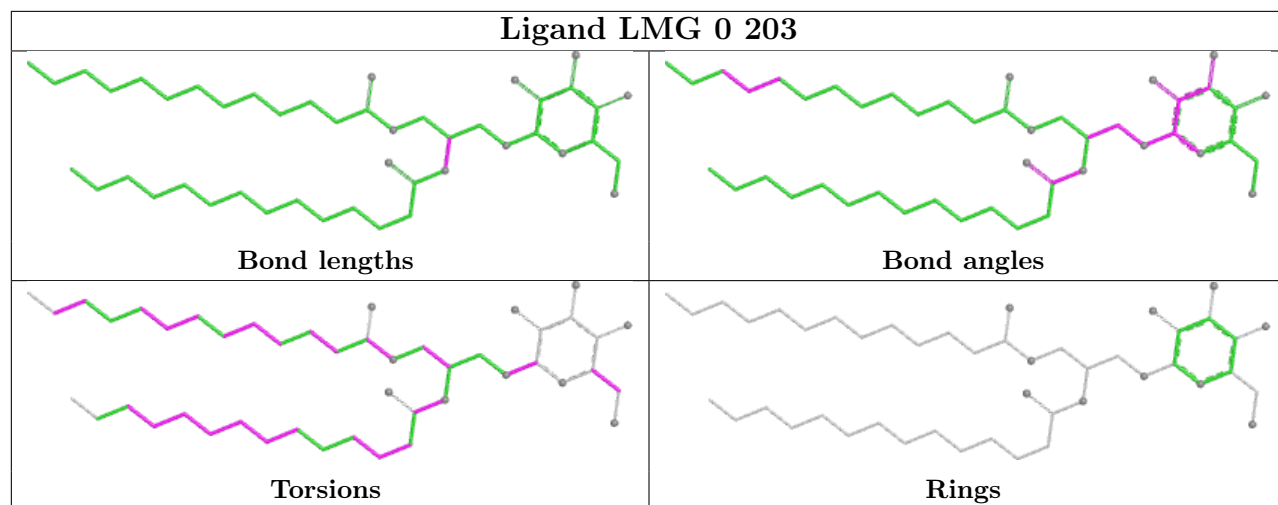


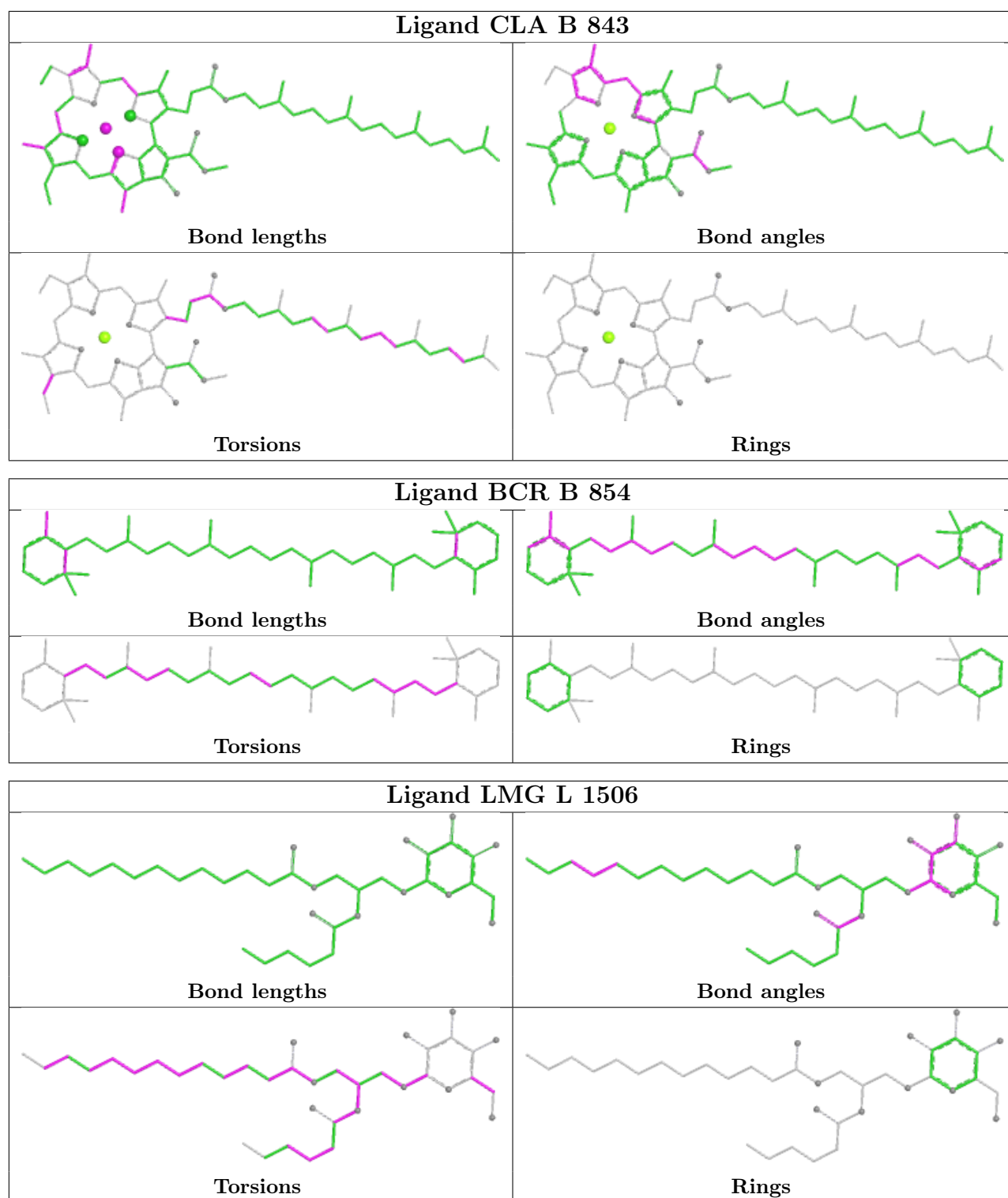
Torsions

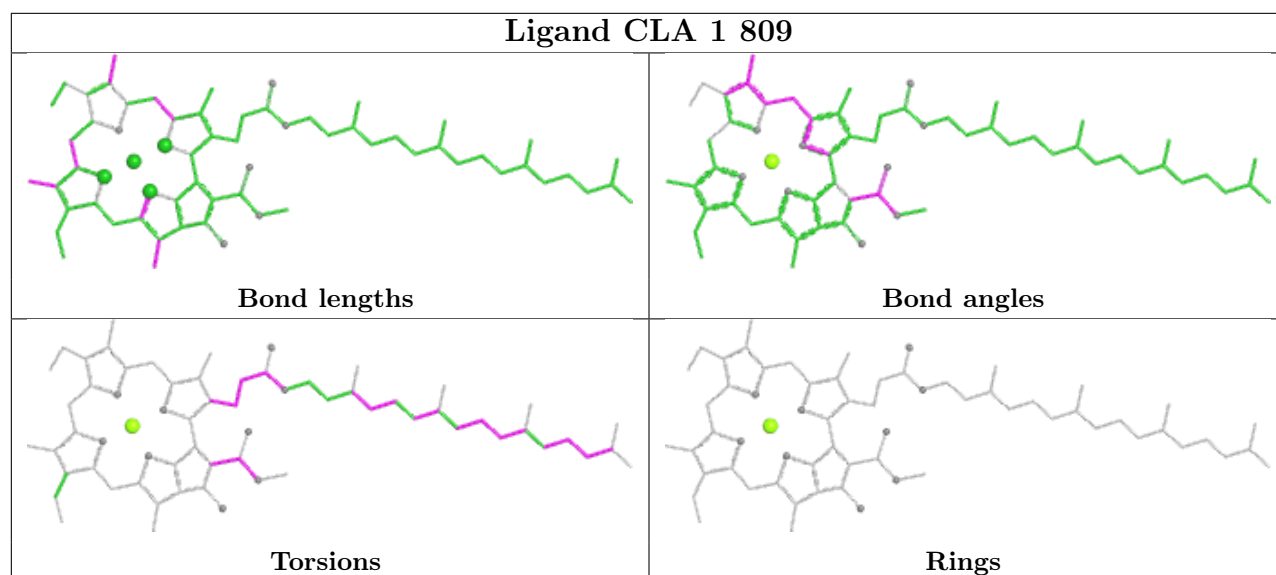
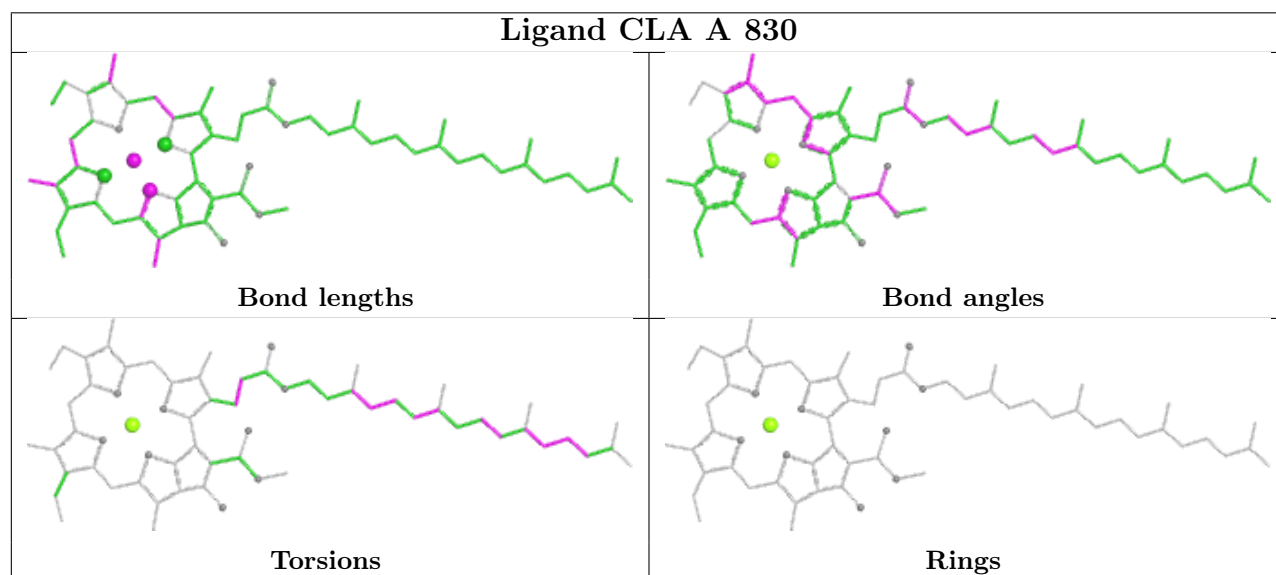
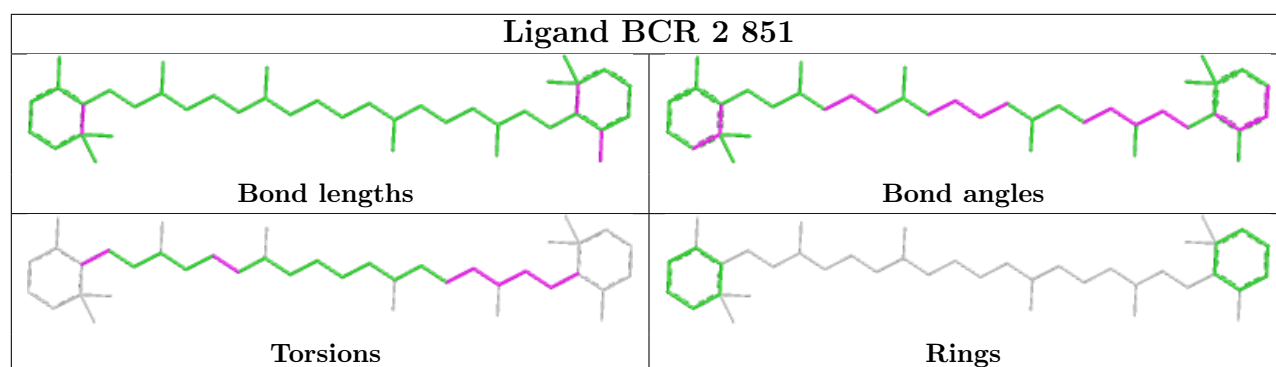


Rings

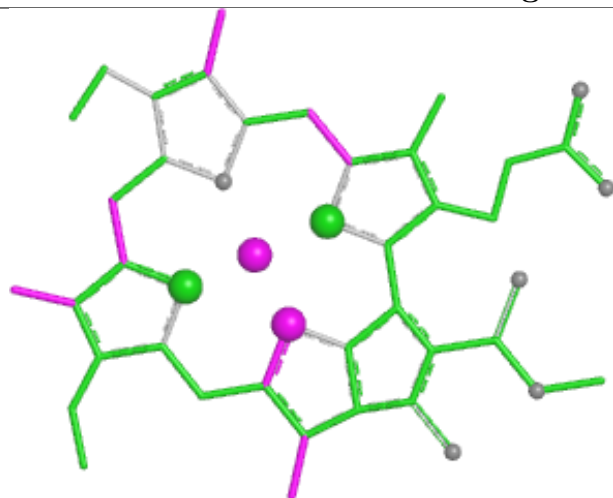




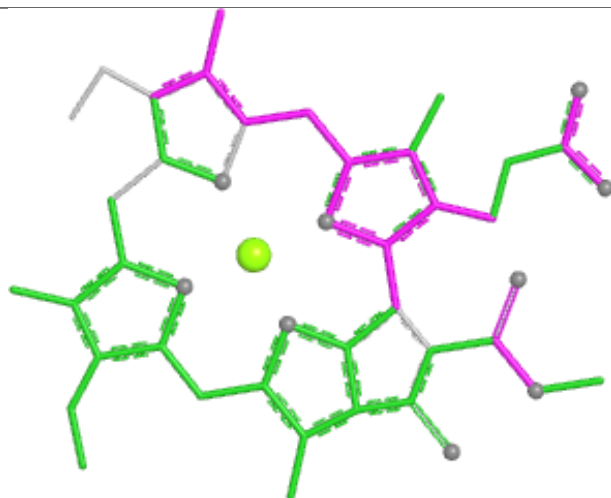




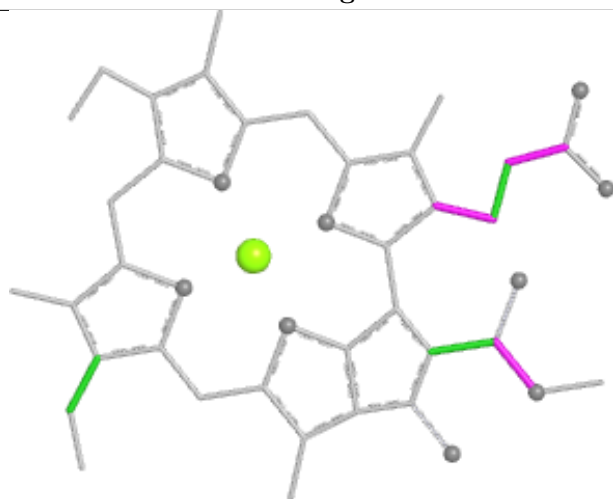
Ligand CLA f 205



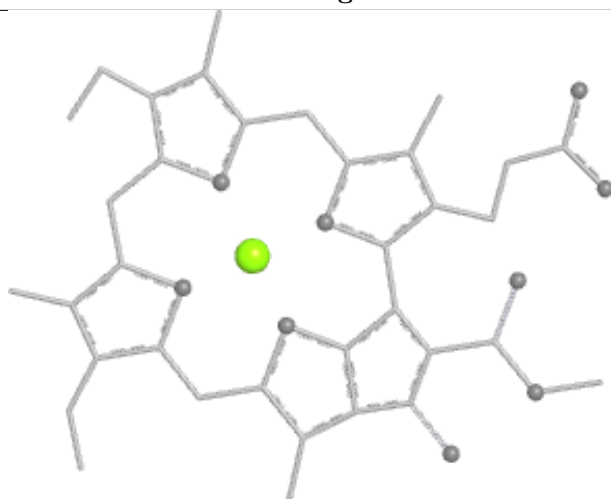
Bond lengths



Bond angles

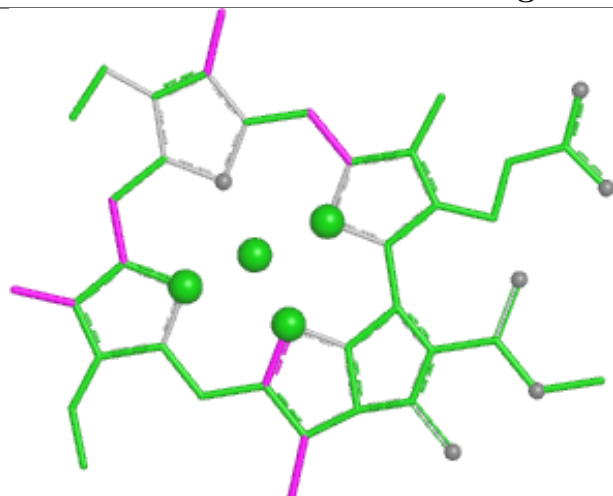


Torsions

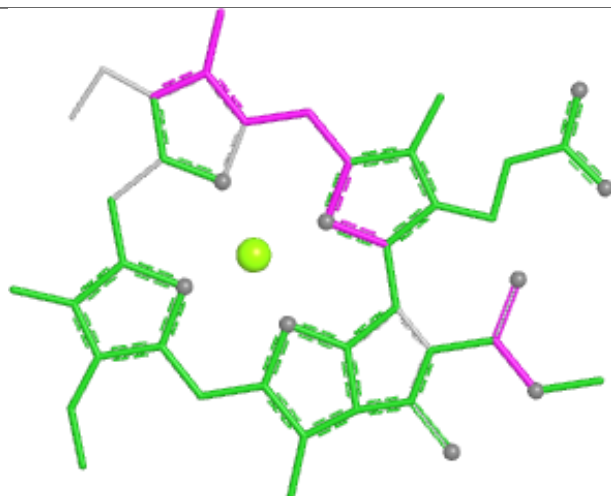


Rings

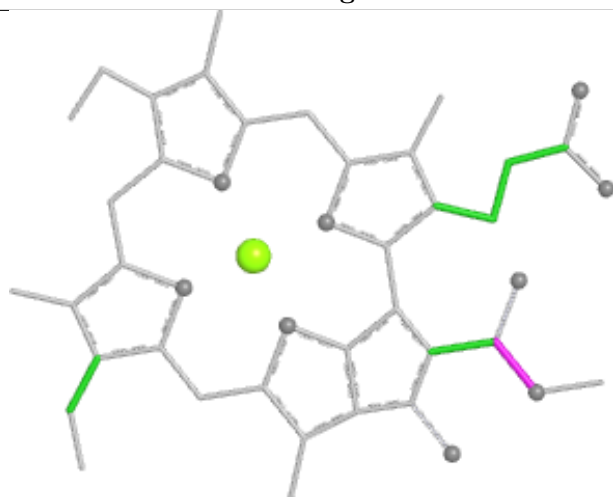
Ligand CLA b 817



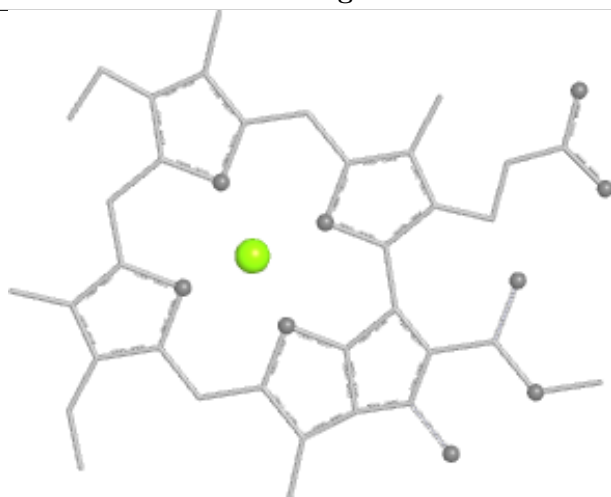
Bond lengths



Bond angles

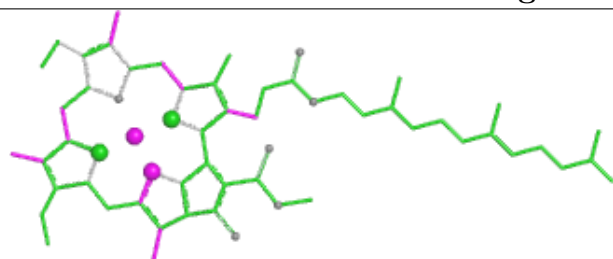


Torsions

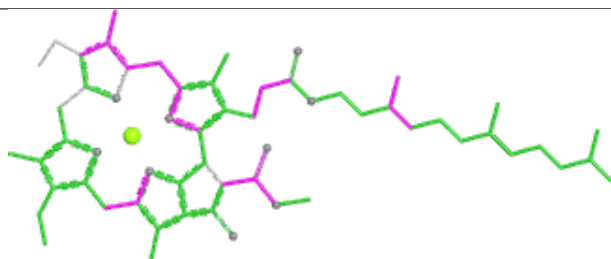


Rings

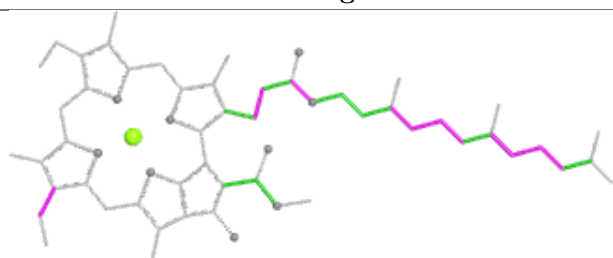
Ligand CLA 2 801



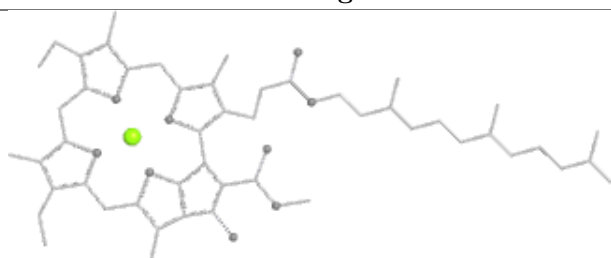
Bond lengths



Bond angles

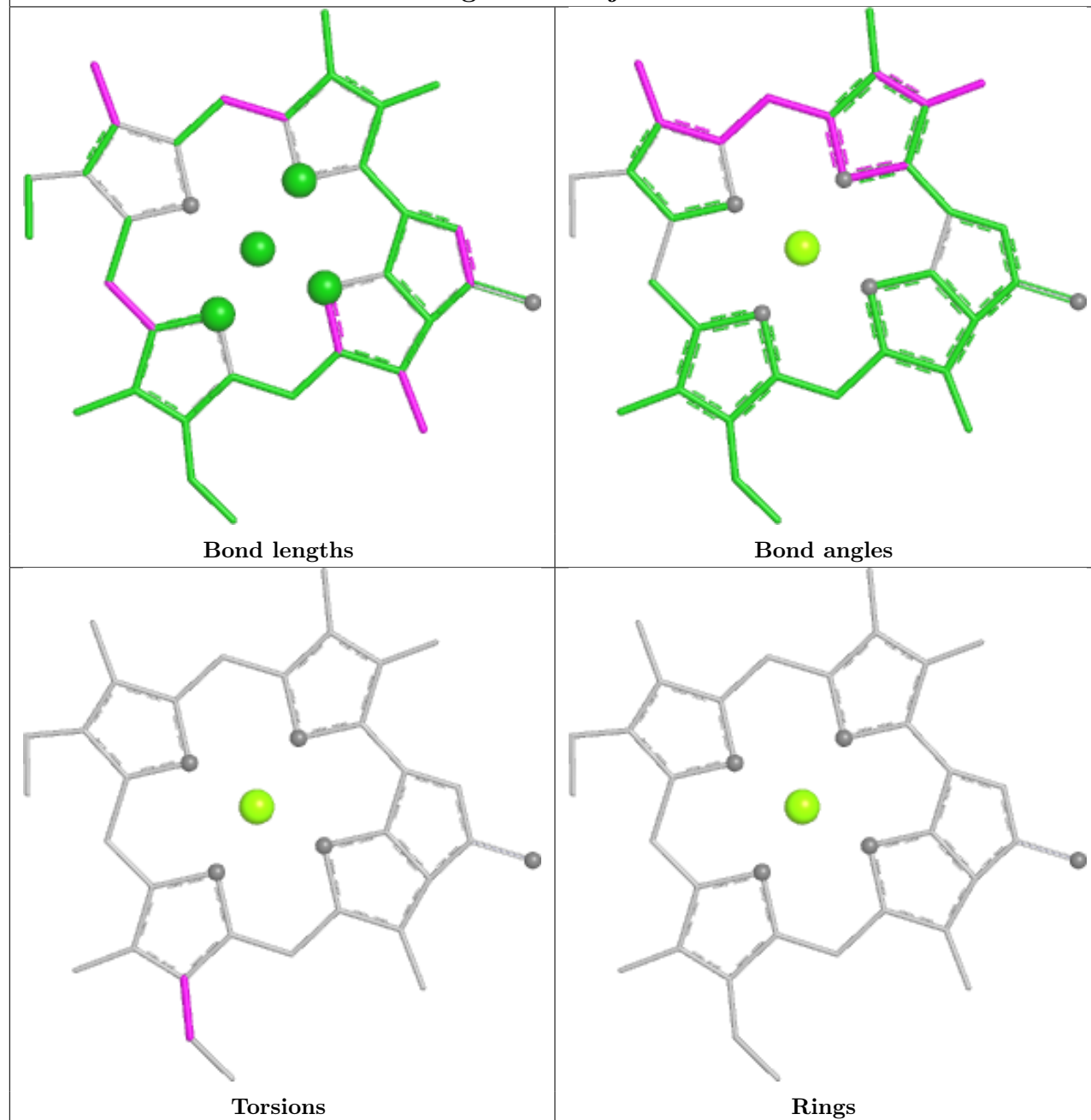


Torsions

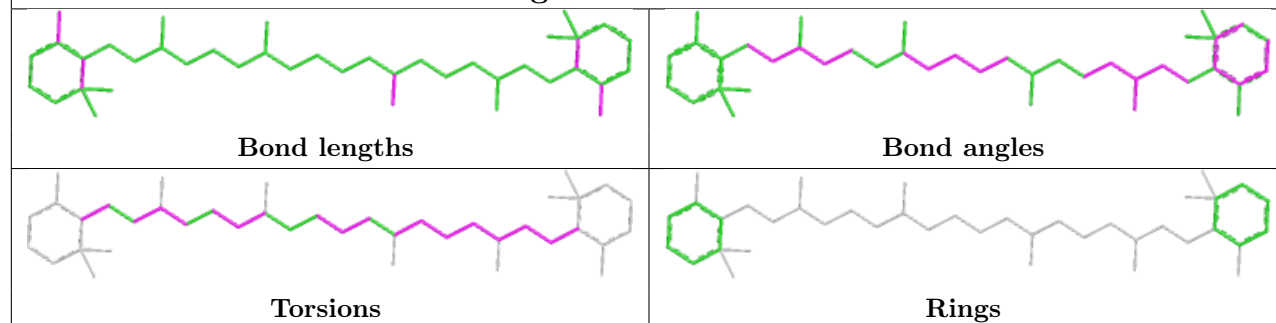


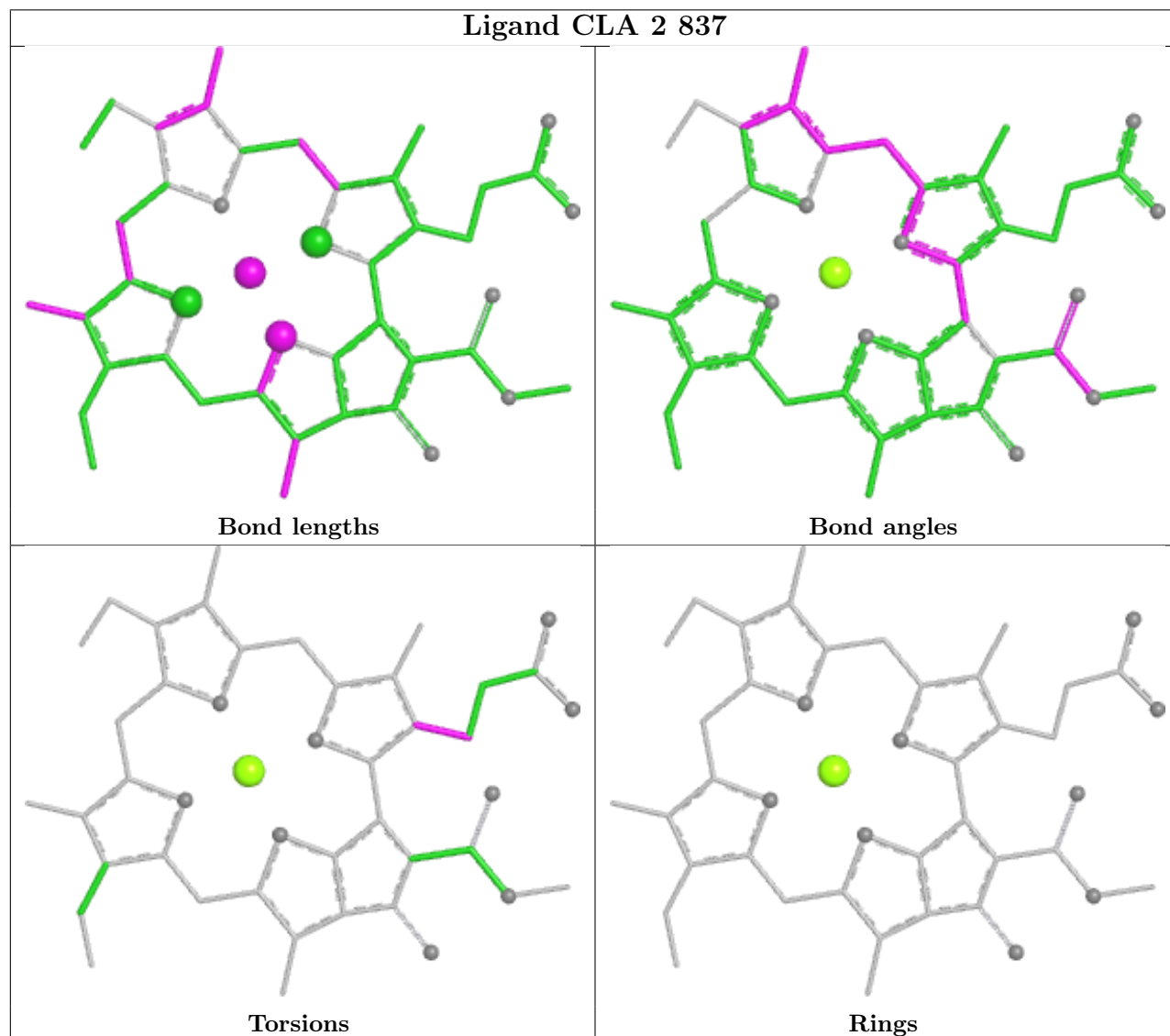
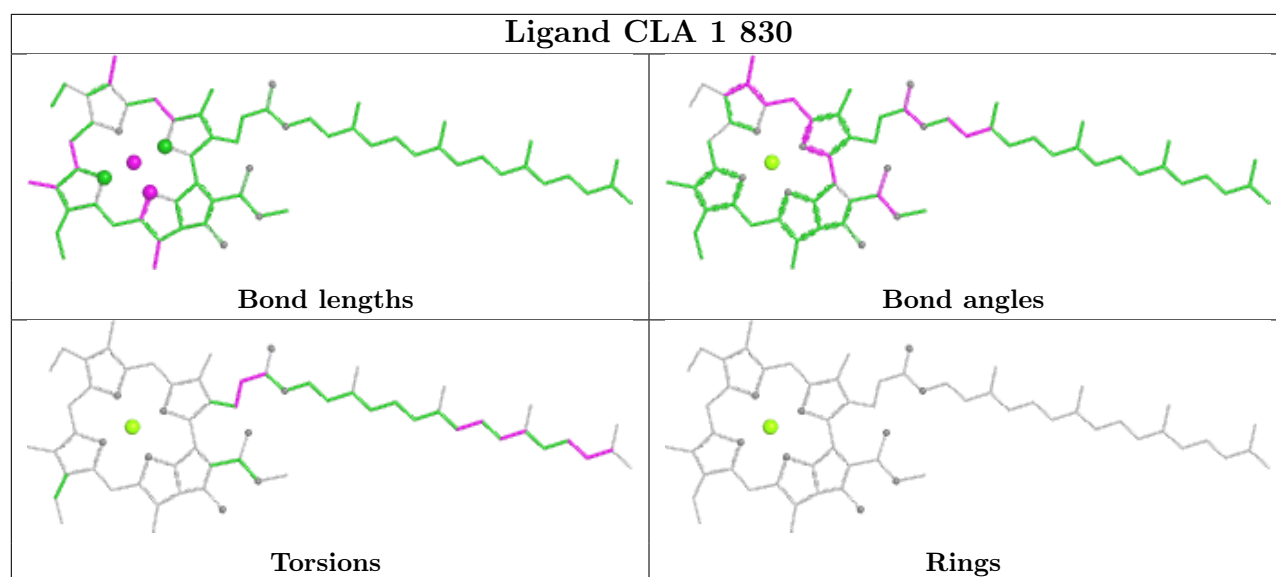
Rings

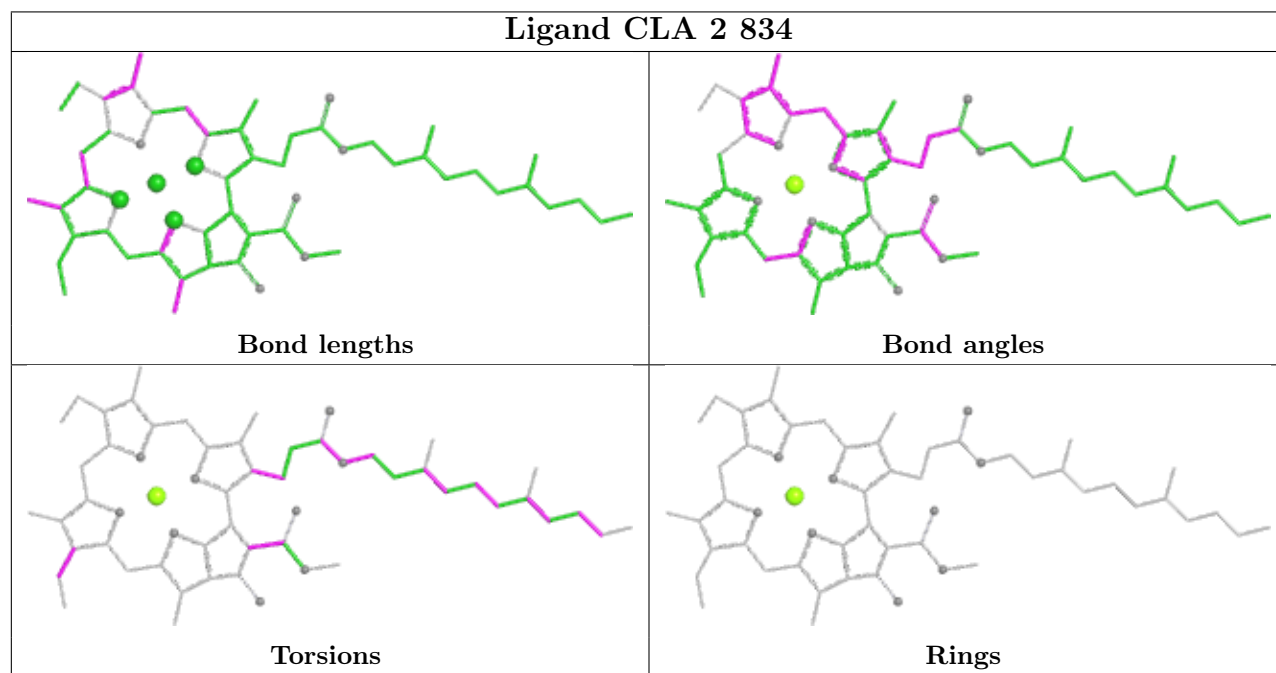
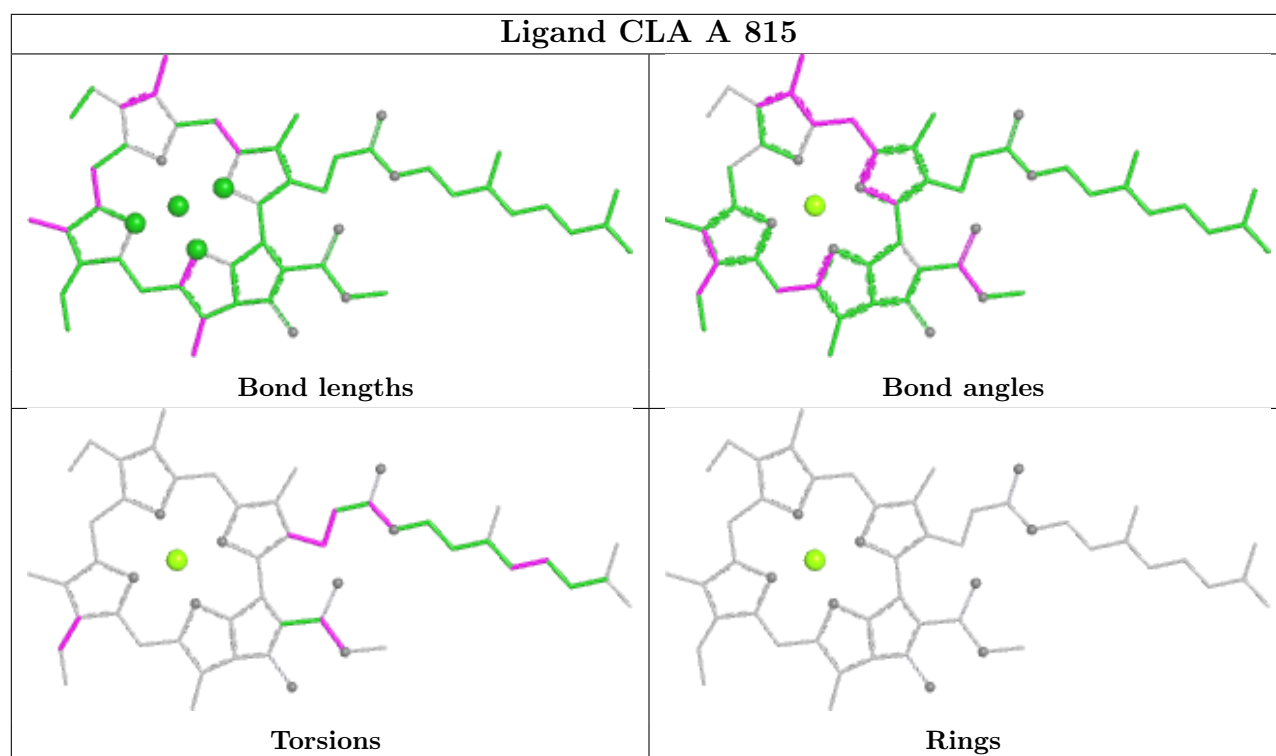
Ligand CLA j 102

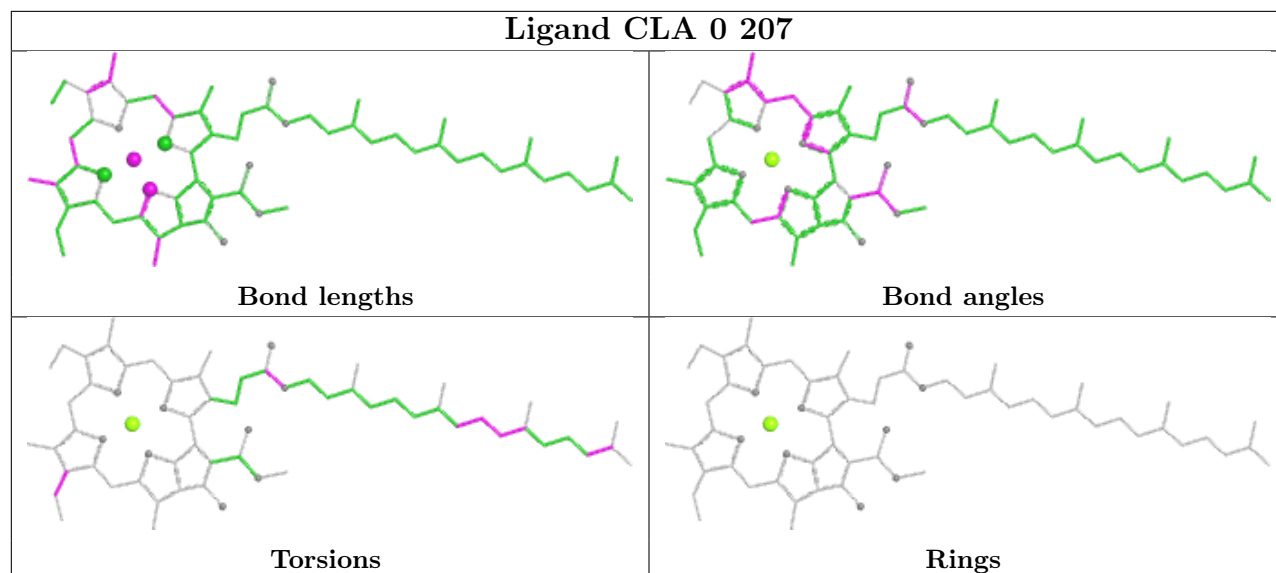
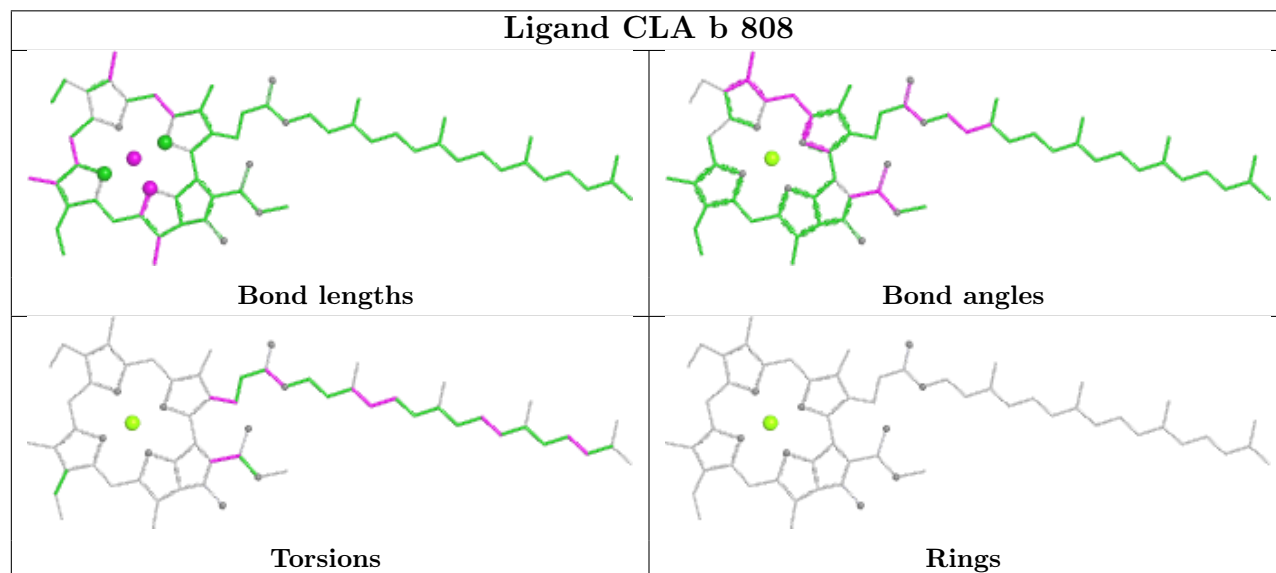
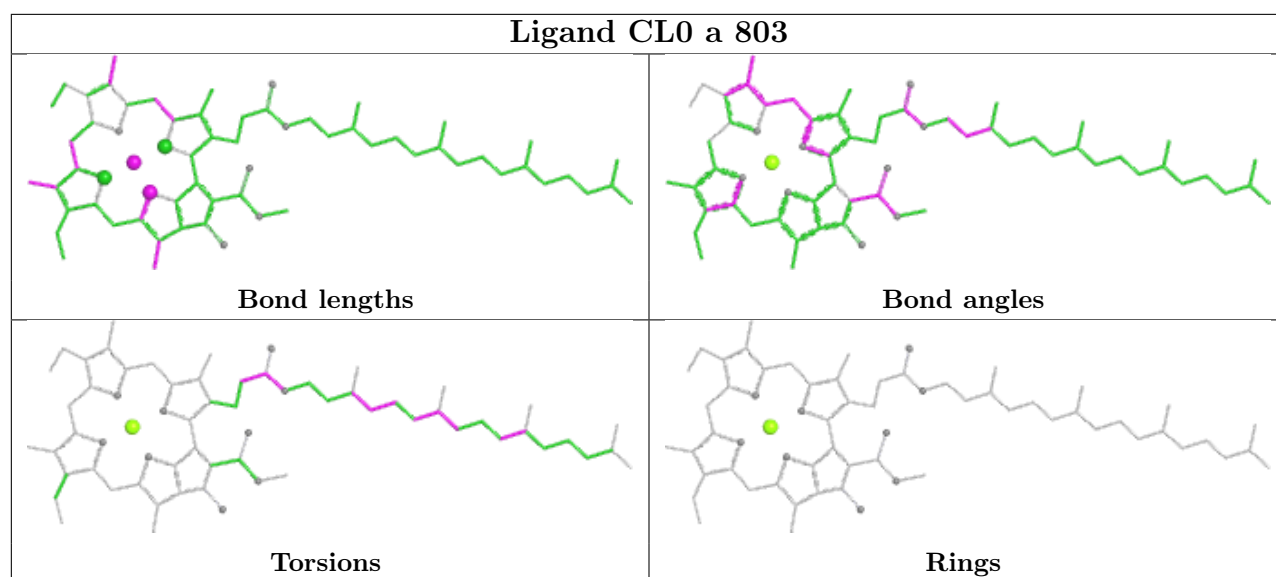


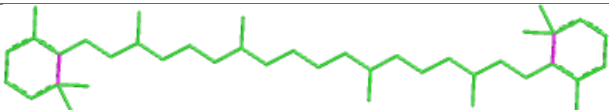
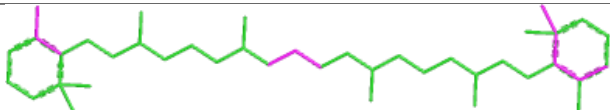
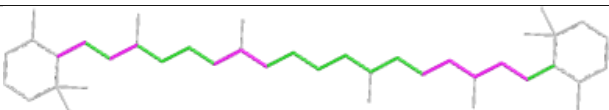
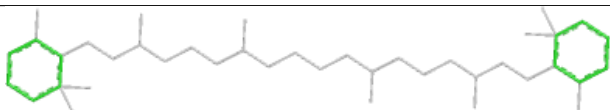
Ligand BCR B 851


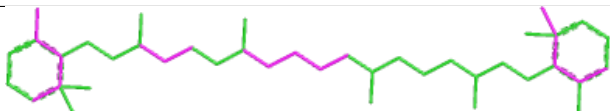
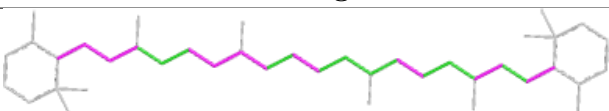
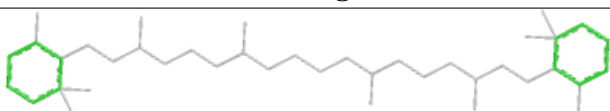


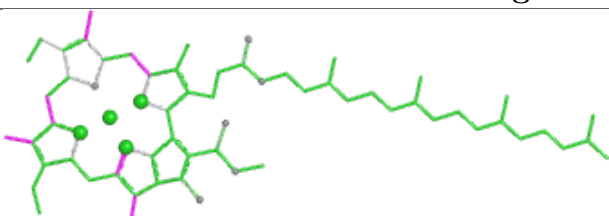
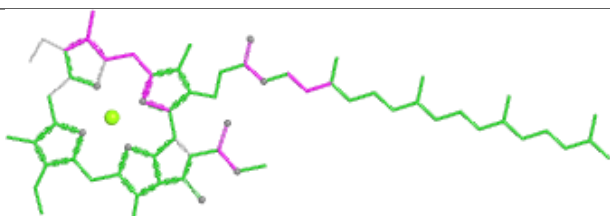
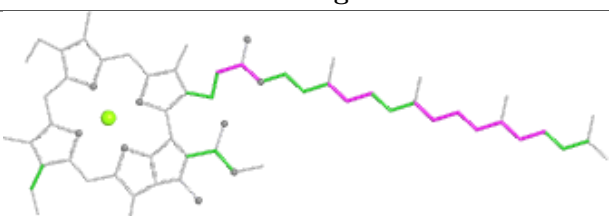
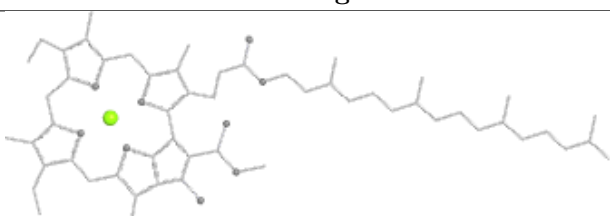


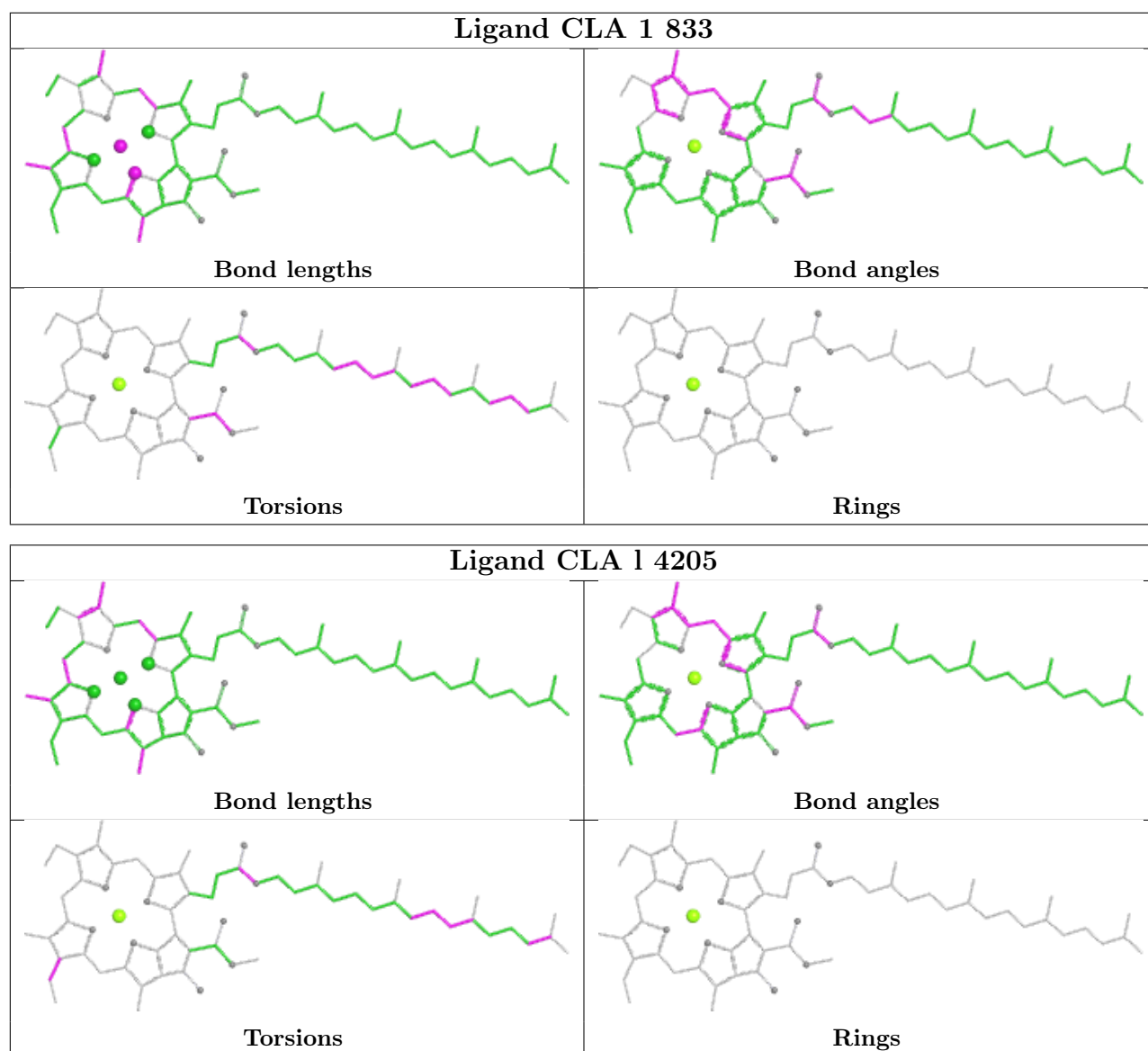


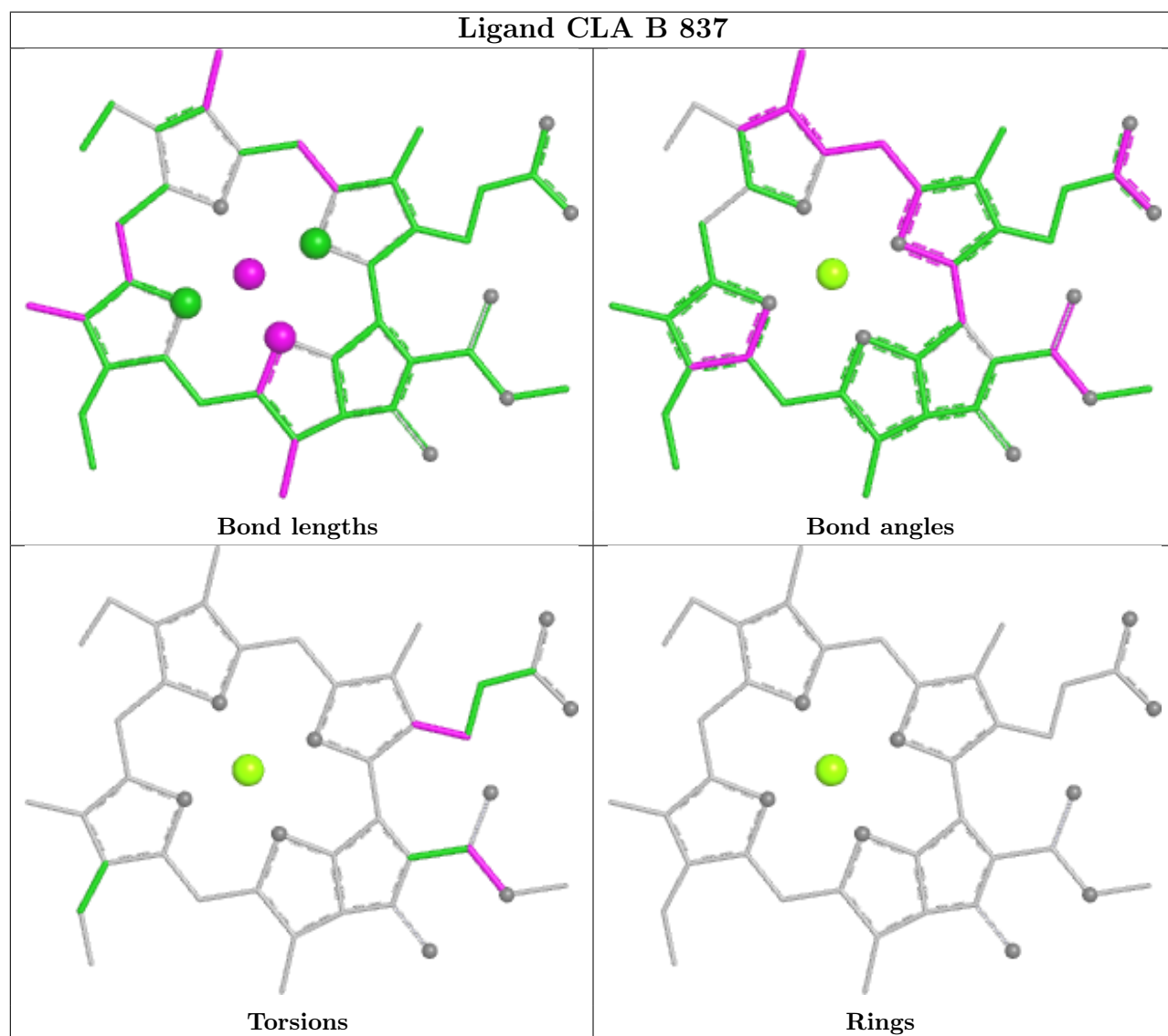
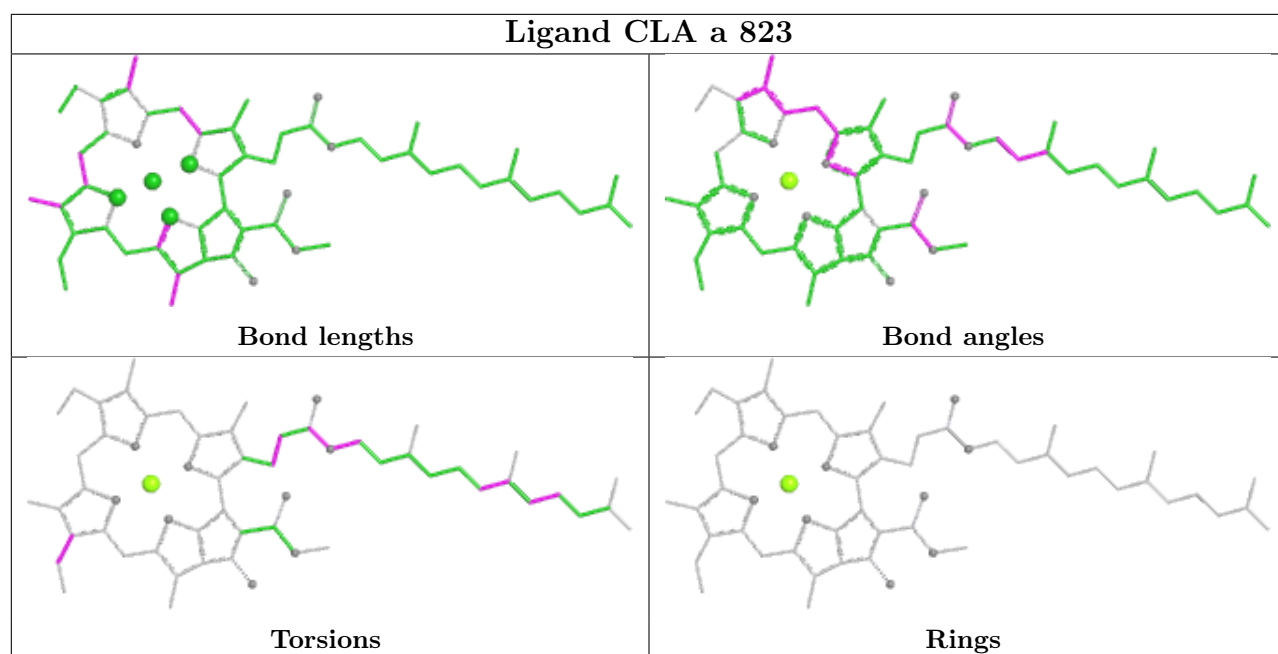


Ligand BCR 1 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

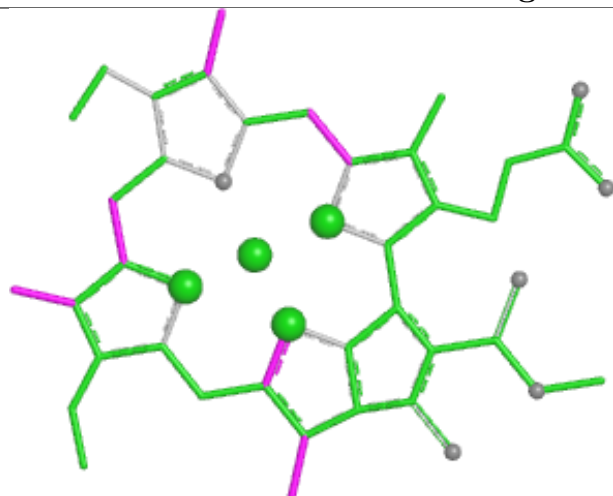
Ligand BCR f 206	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 0 208	
	
Bond lengths	Bond angles
	
Torsions	Rings

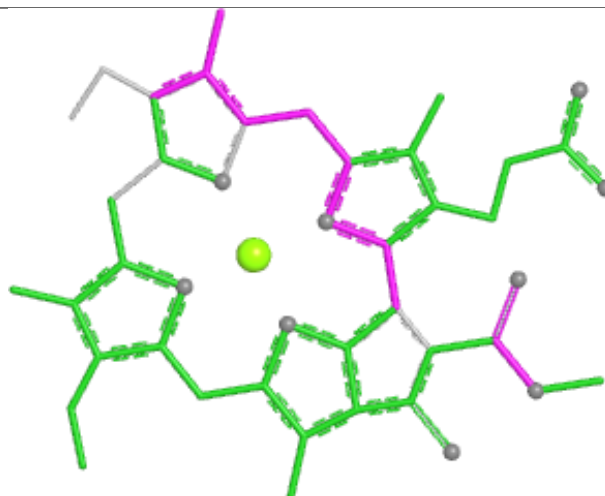




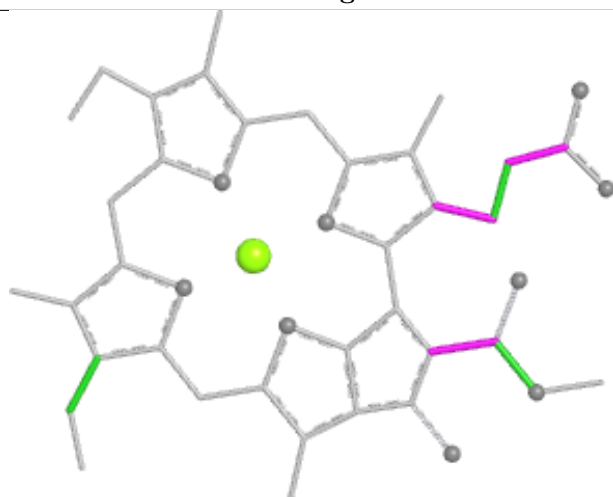
Ligand CLA 2 823



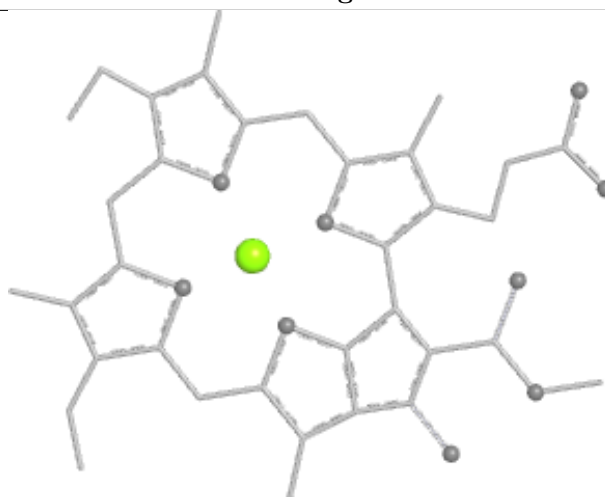
Bond lengths



Bond angles

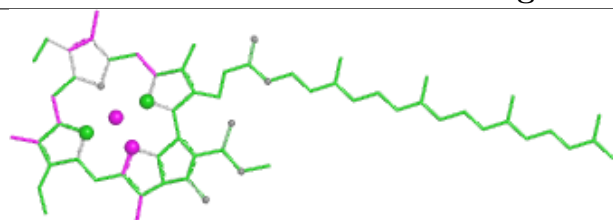


Torsions

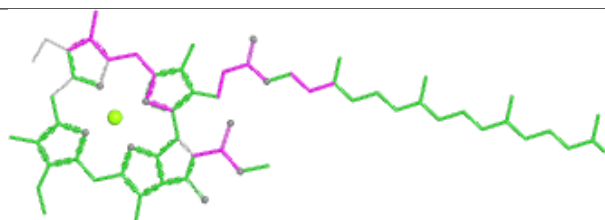


Rings

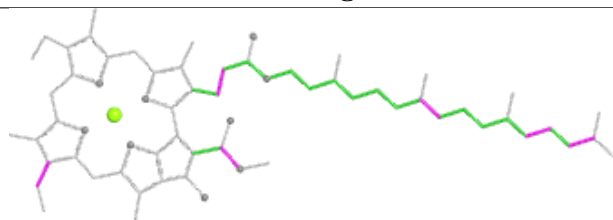
Ligand CLA b 802



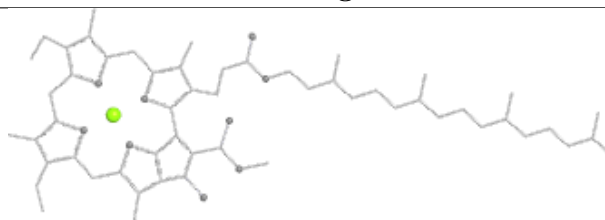
Bond lengths



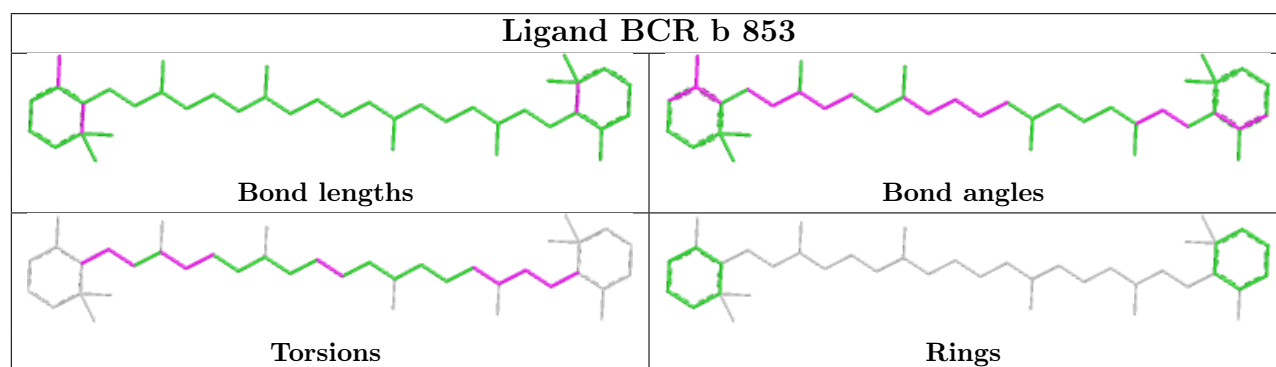
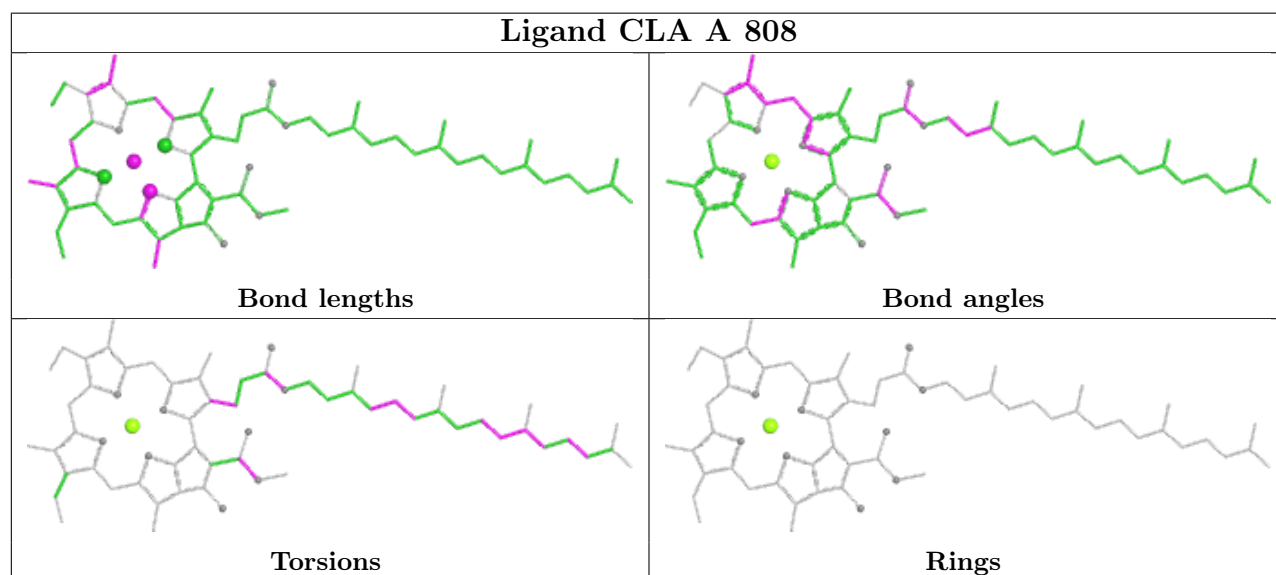
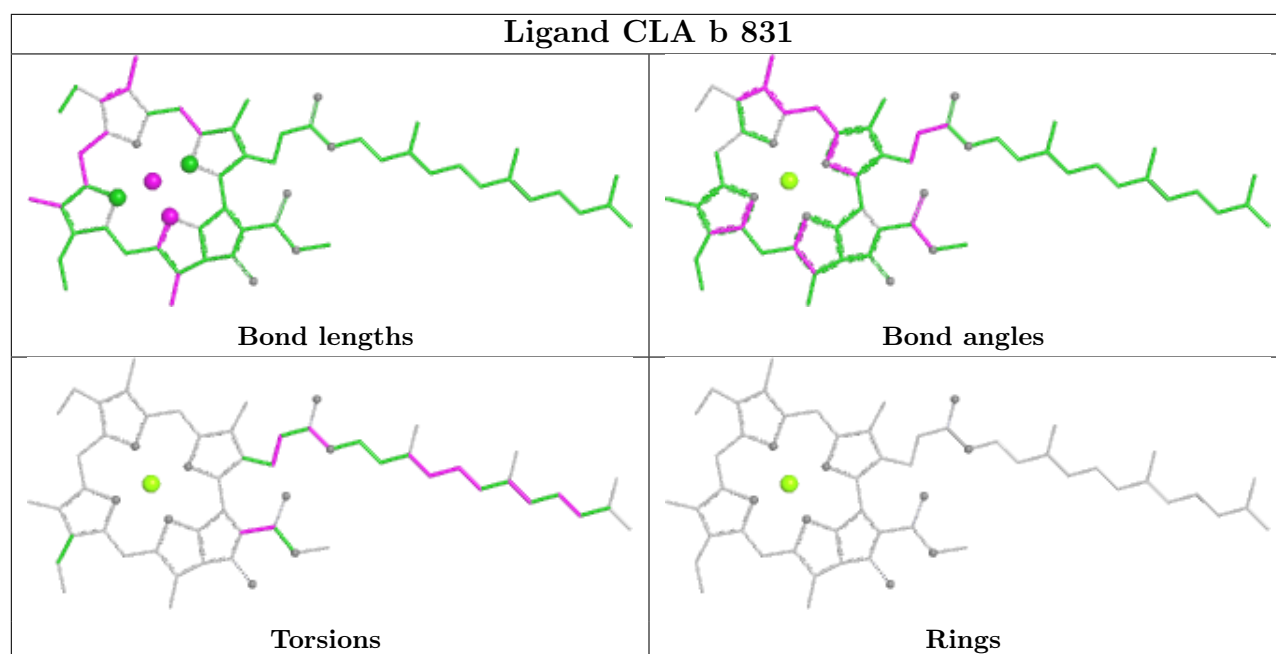
Bond angles

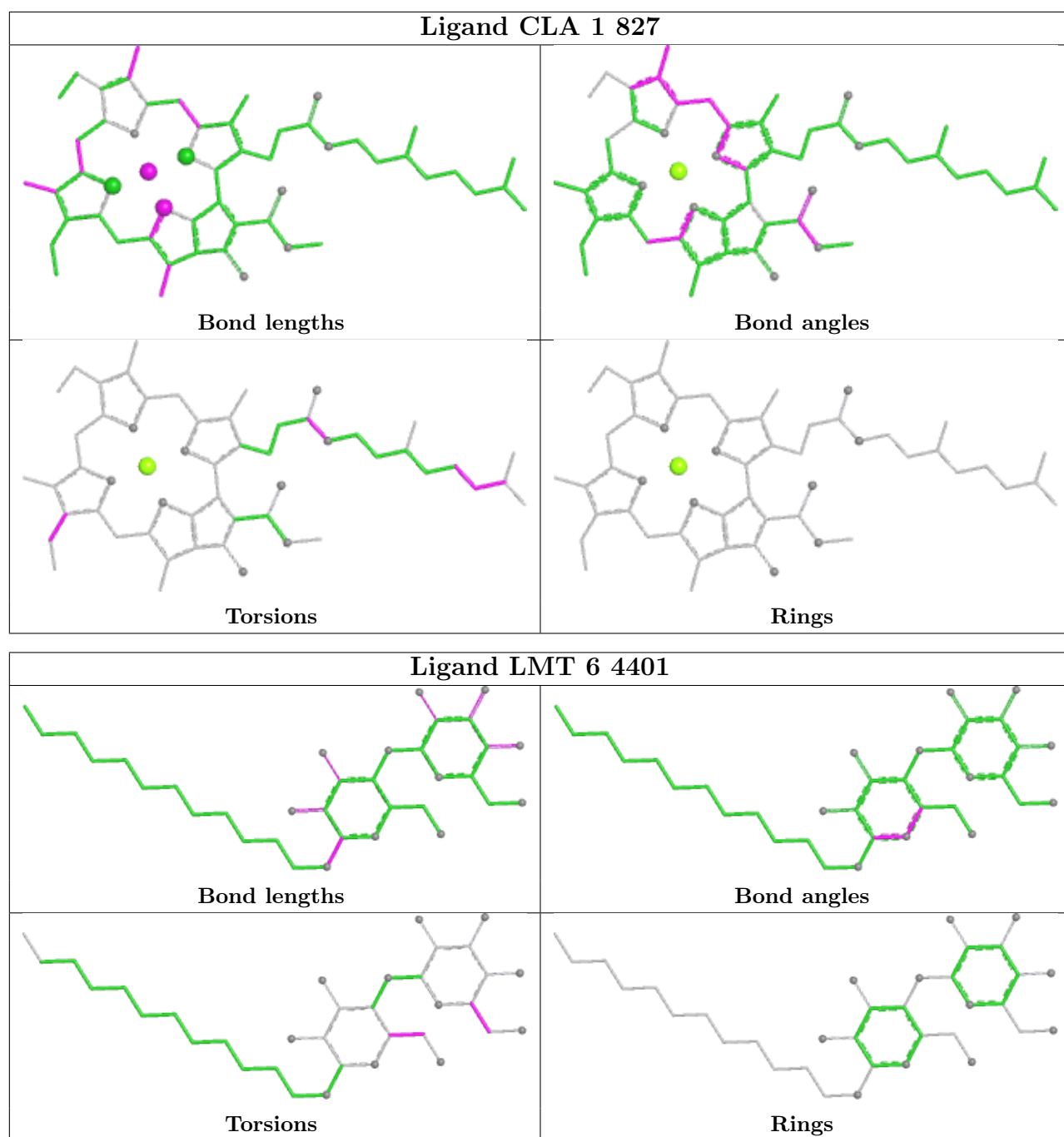


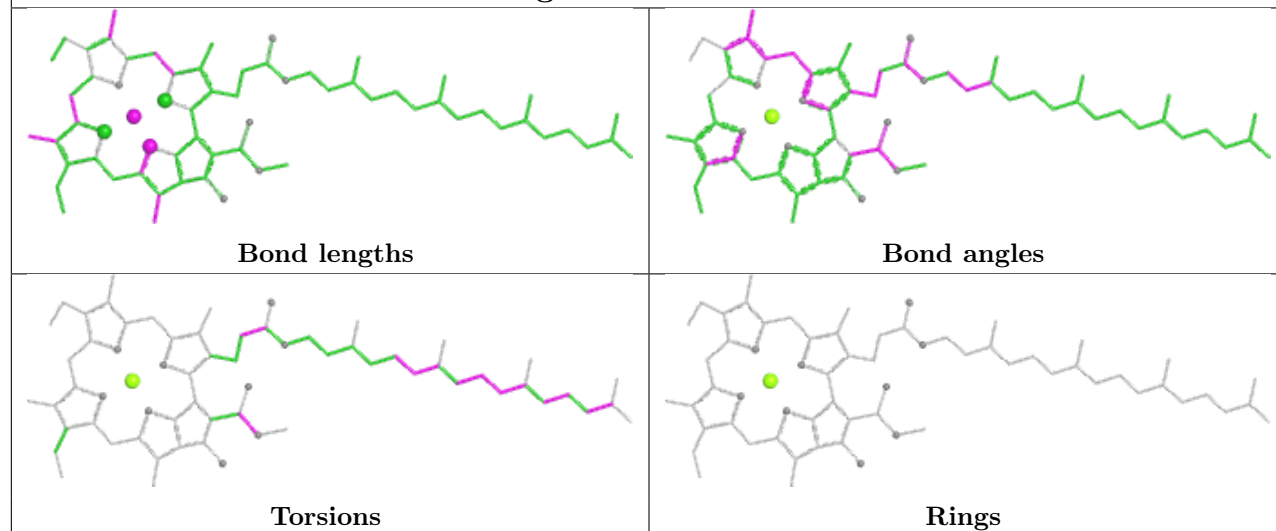
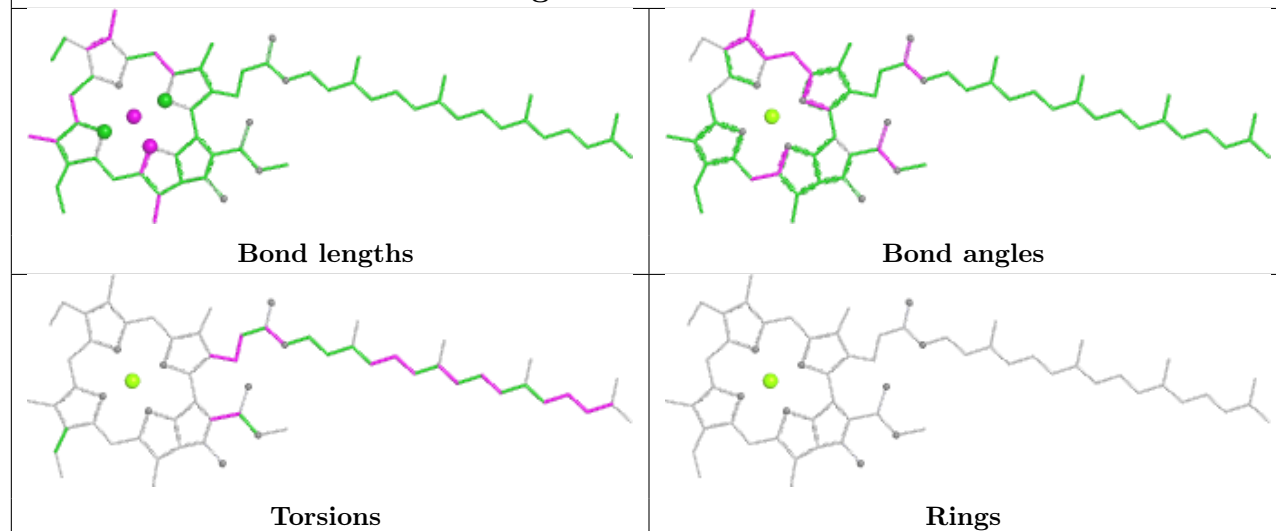
Torsions



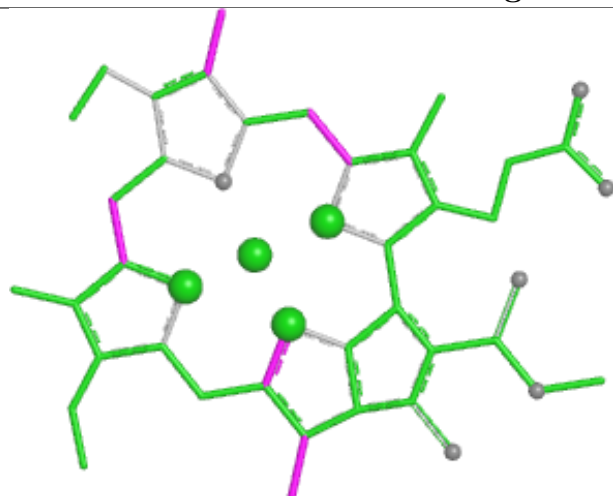
Rings



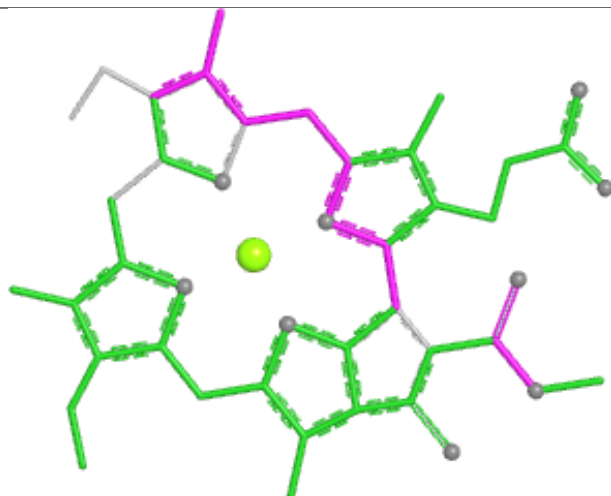


Ligand CLA 2 804**Ligand CLA A 807**

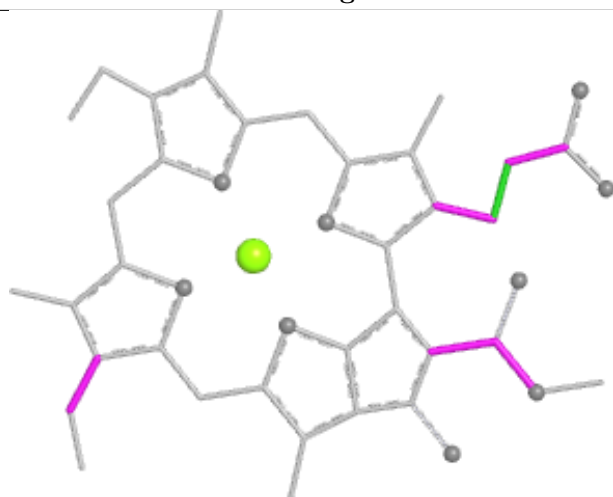
Ligand CLA K 4003



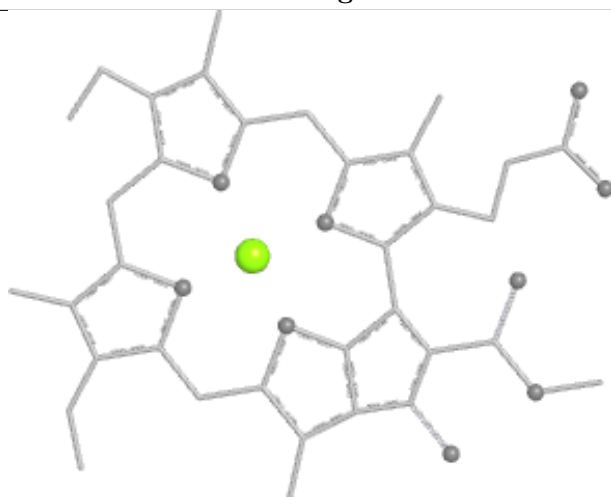
Bond lengths



Bond angles

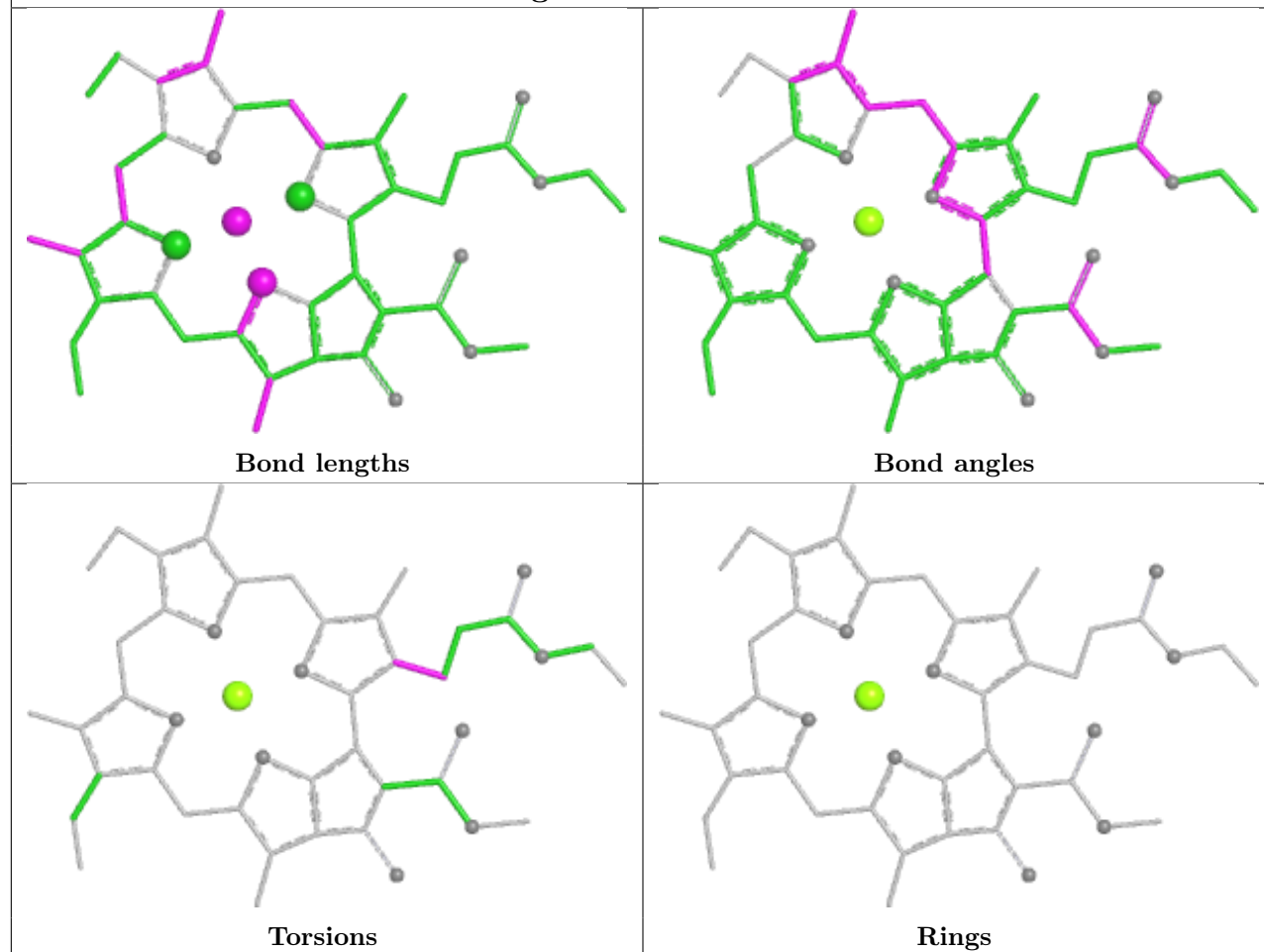


Torsions

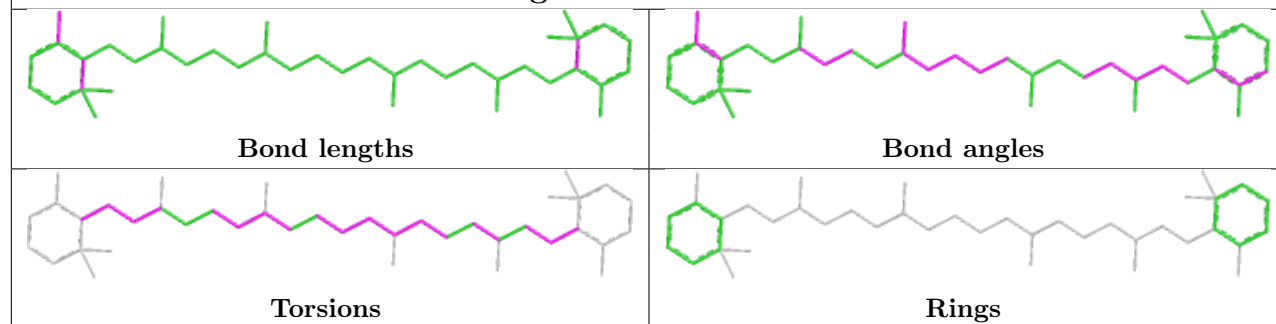


Rings

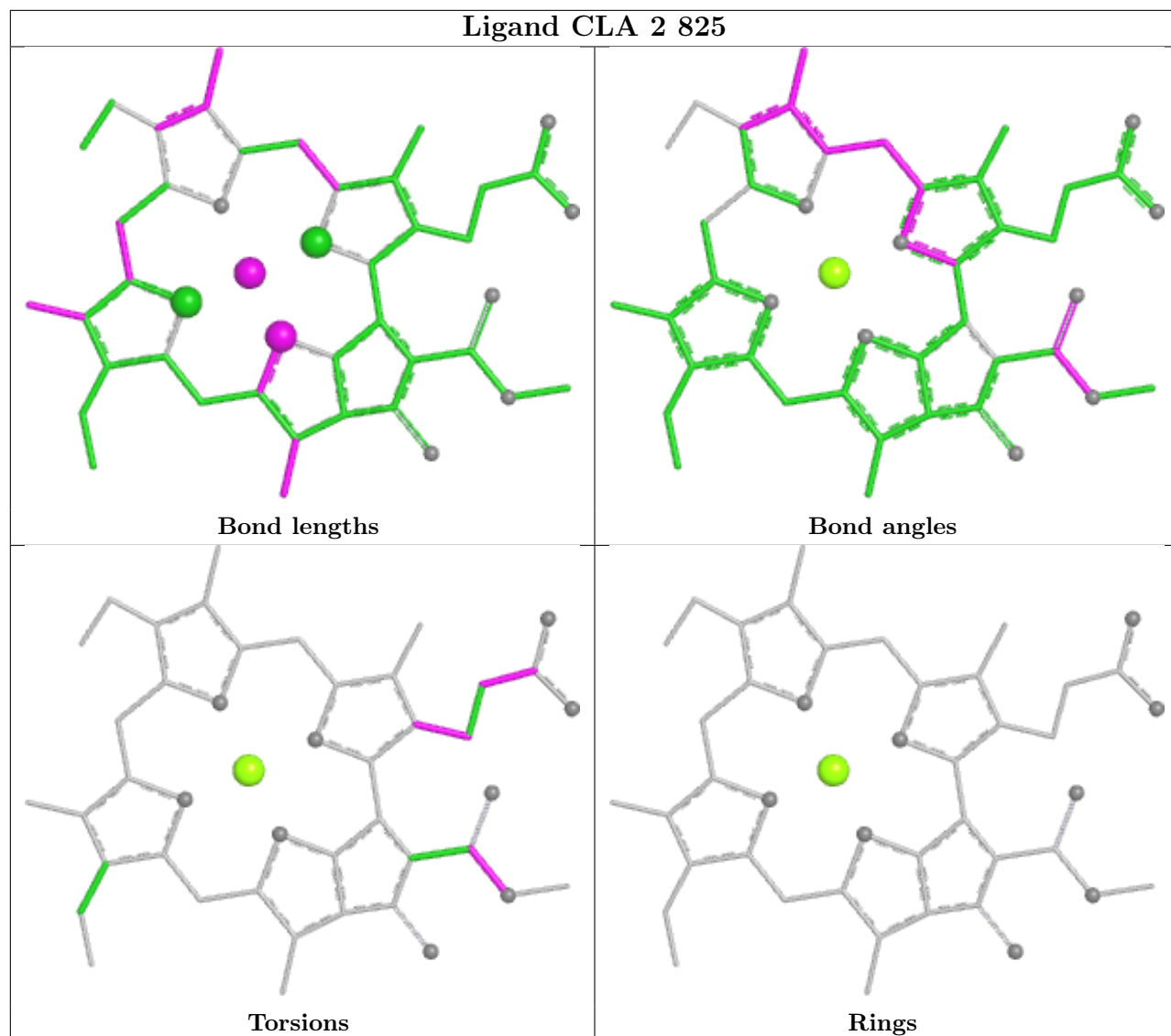
Ligand CLA 1 839

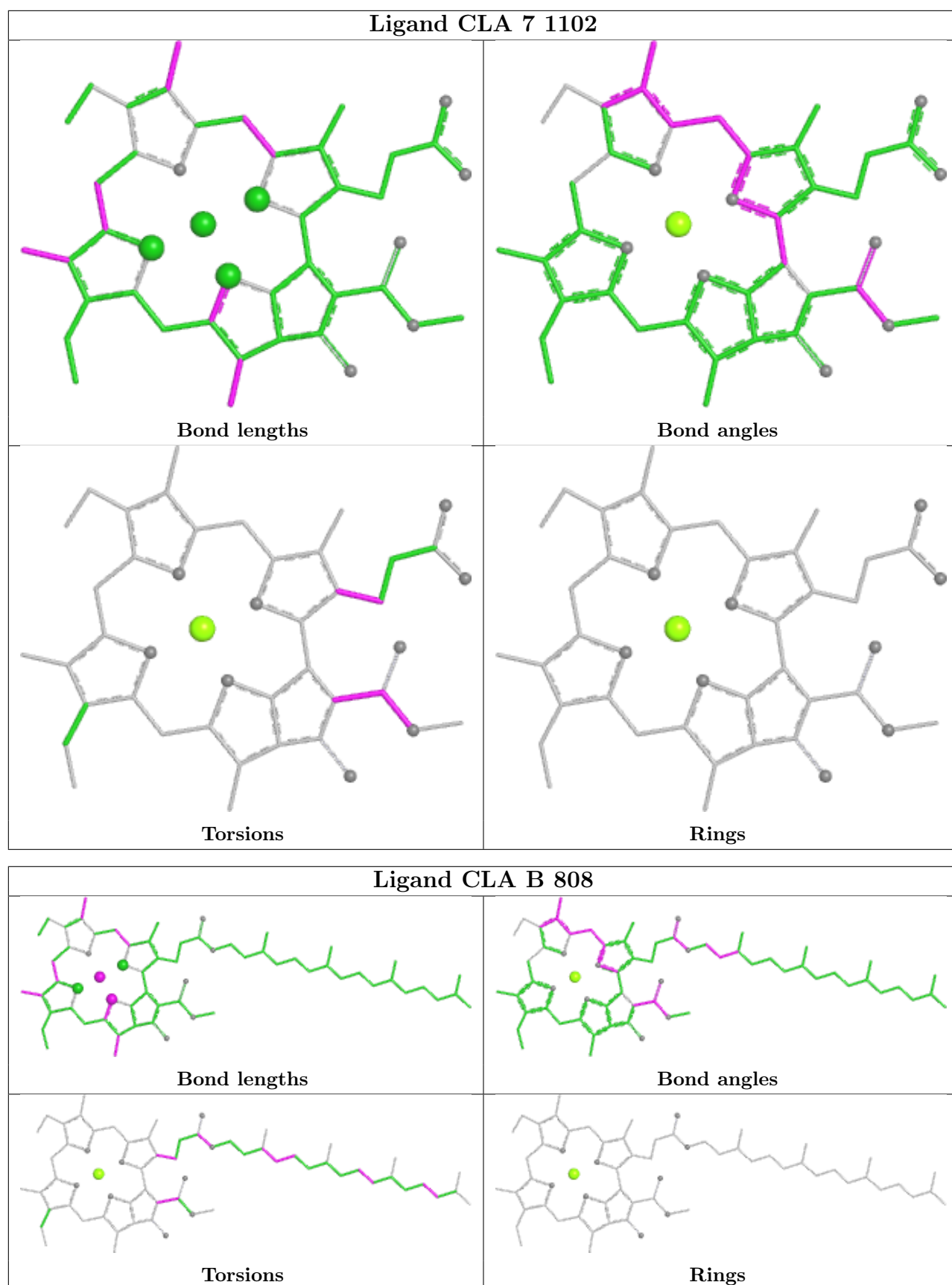


Ligand BCR A 850

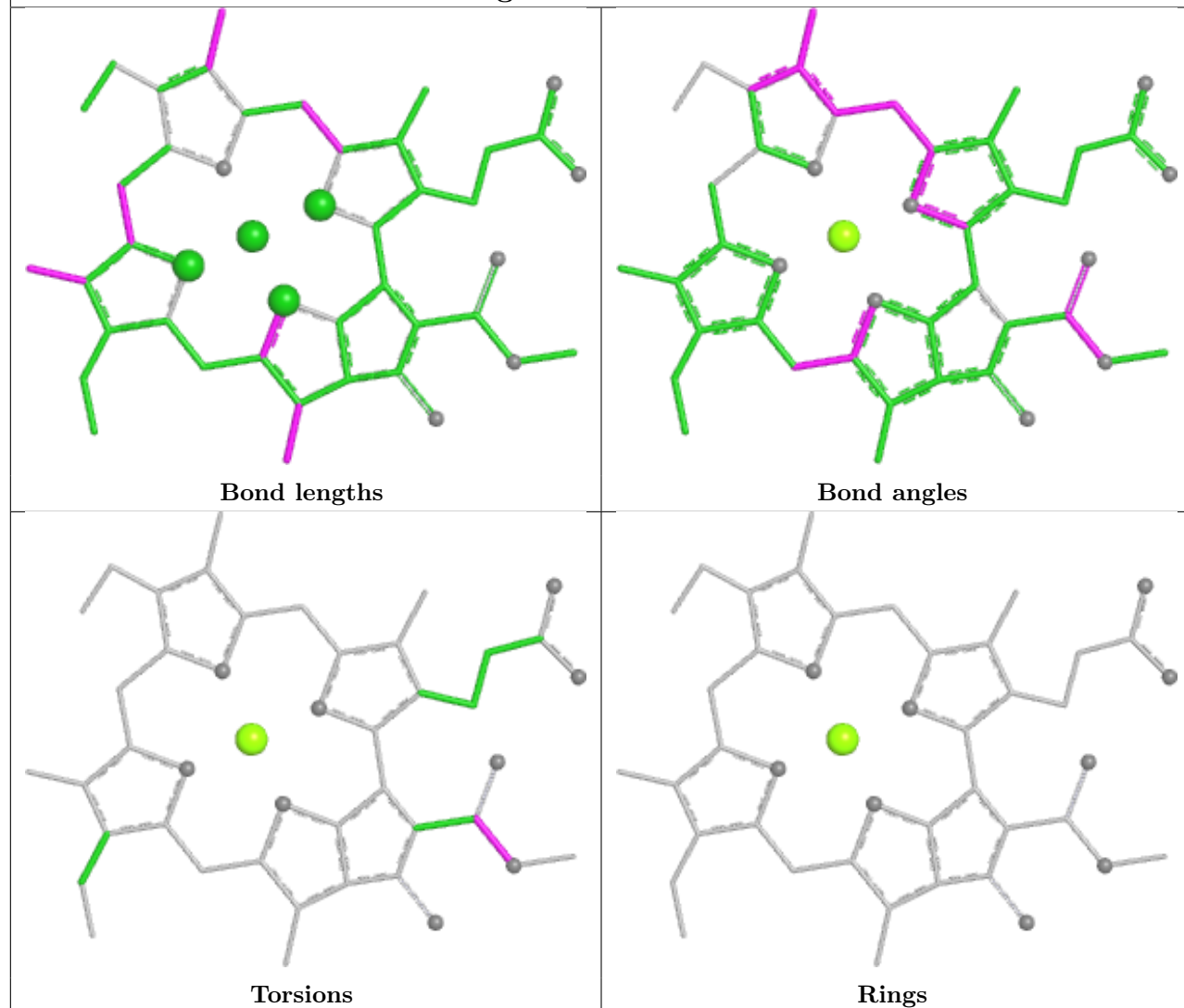


Ligand CLA 2 825

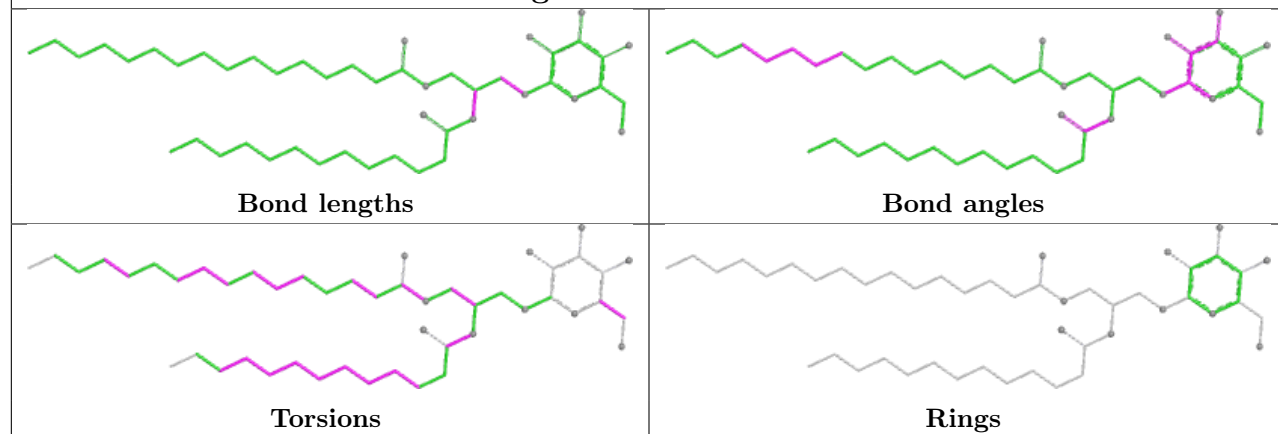


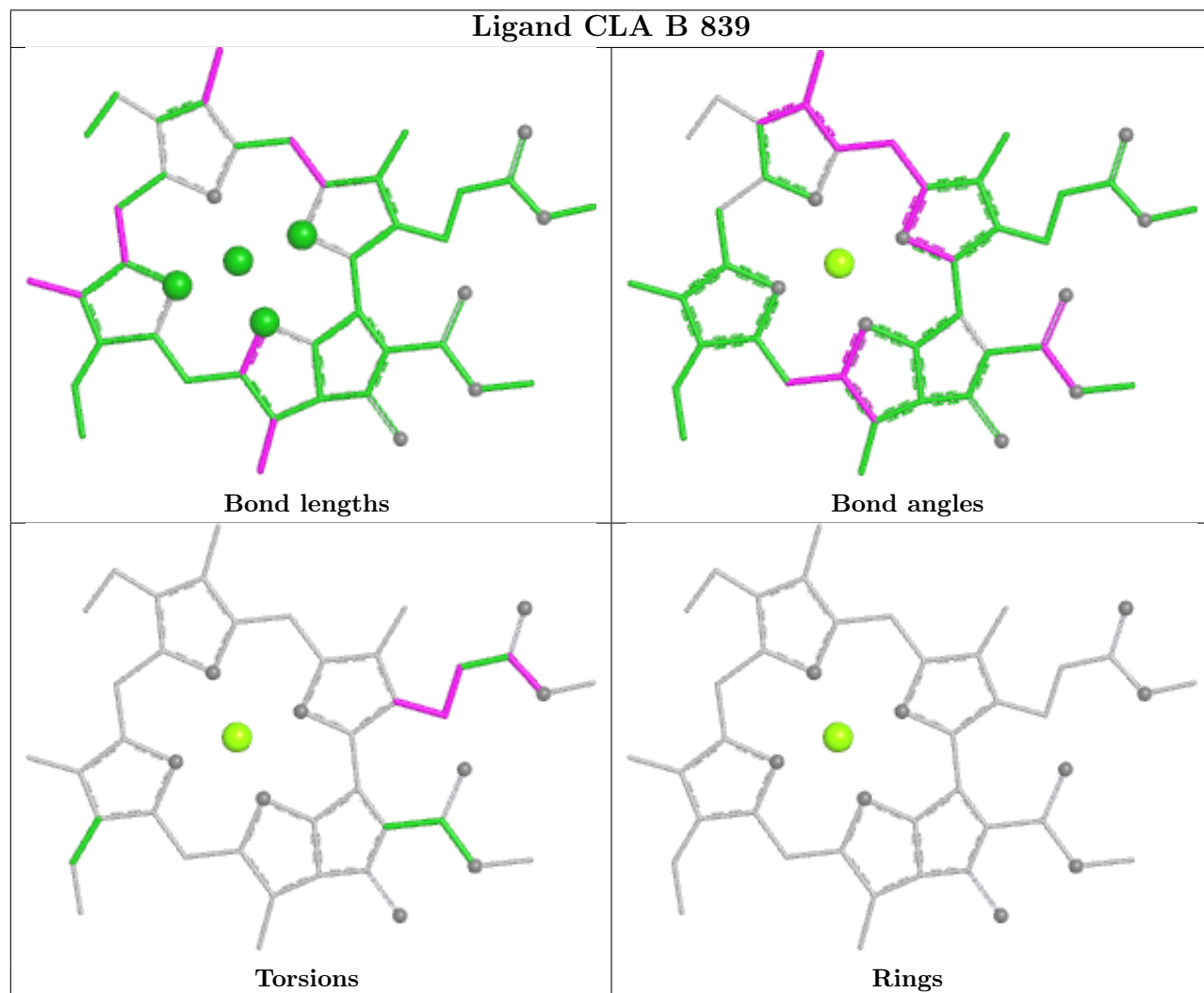
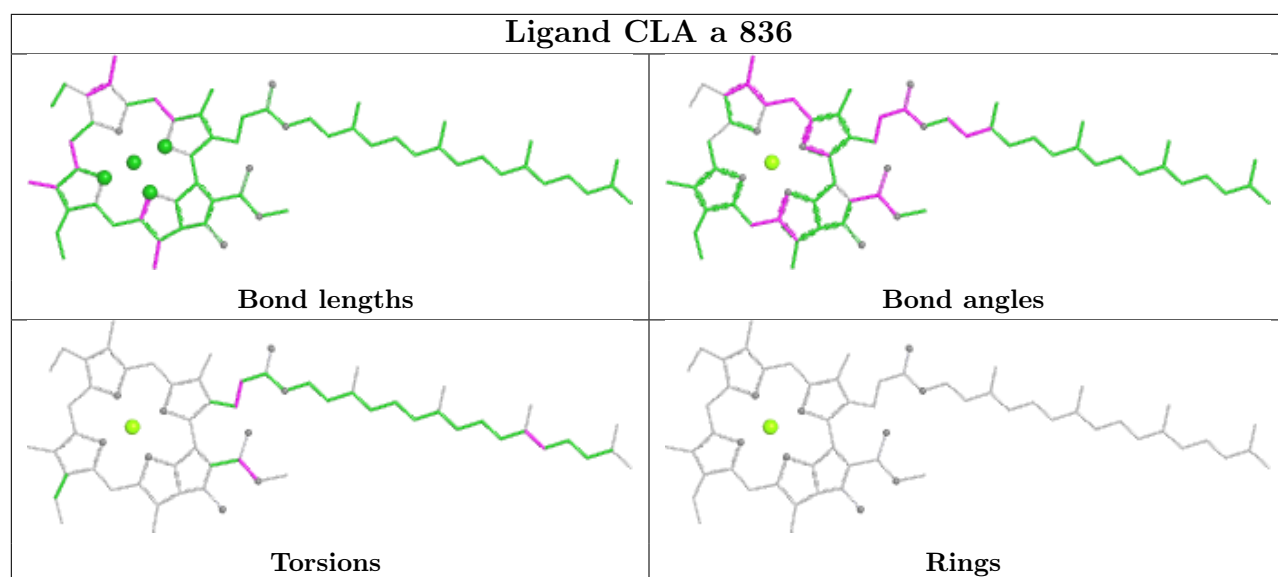


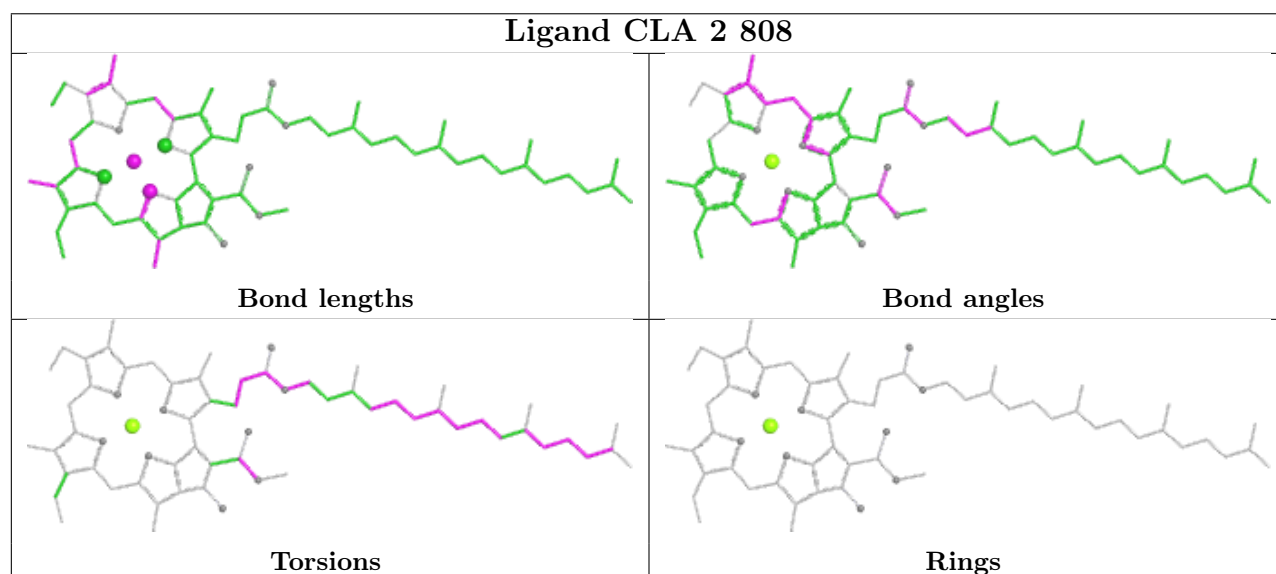
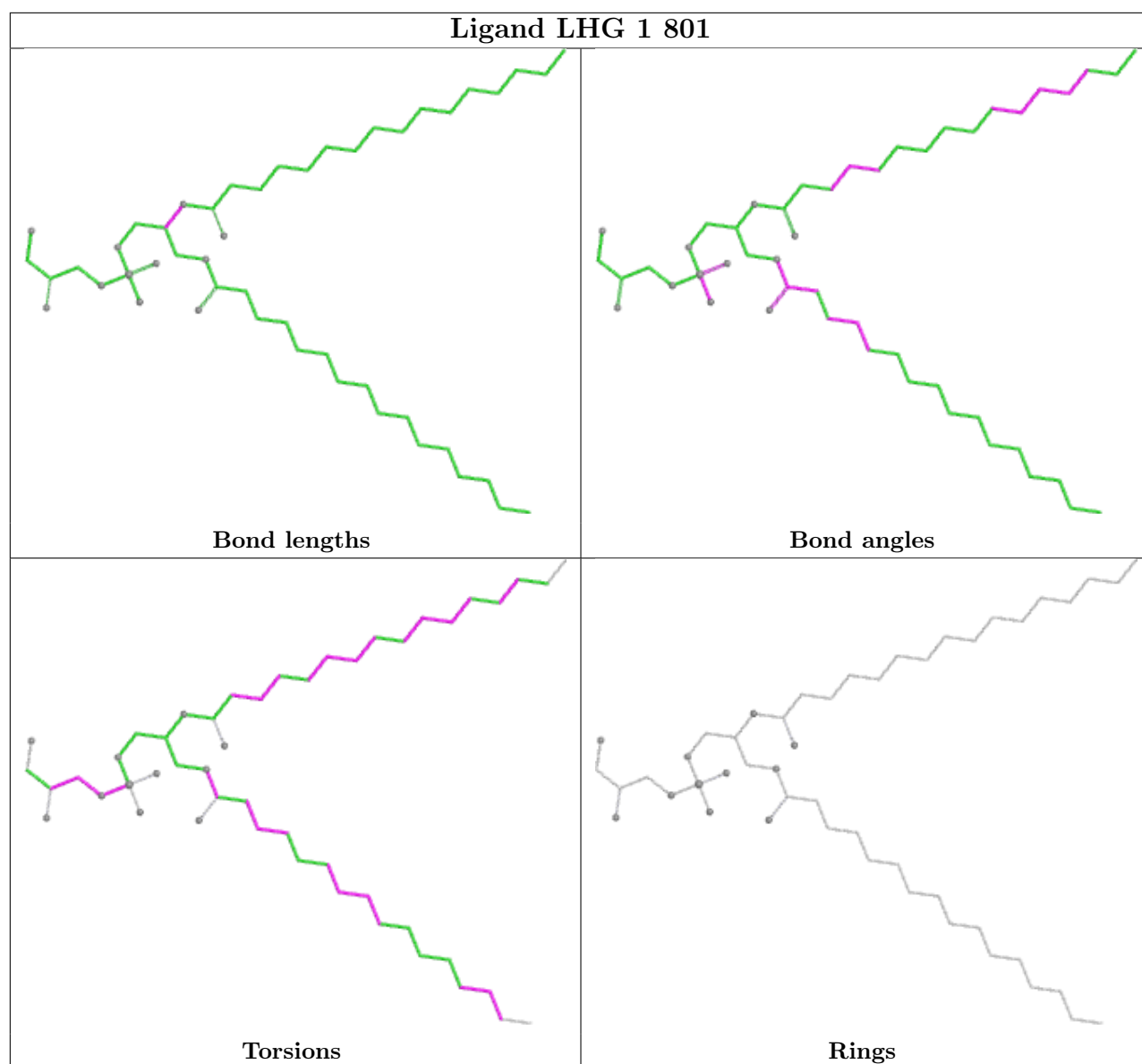
Ligand CLA 2 817

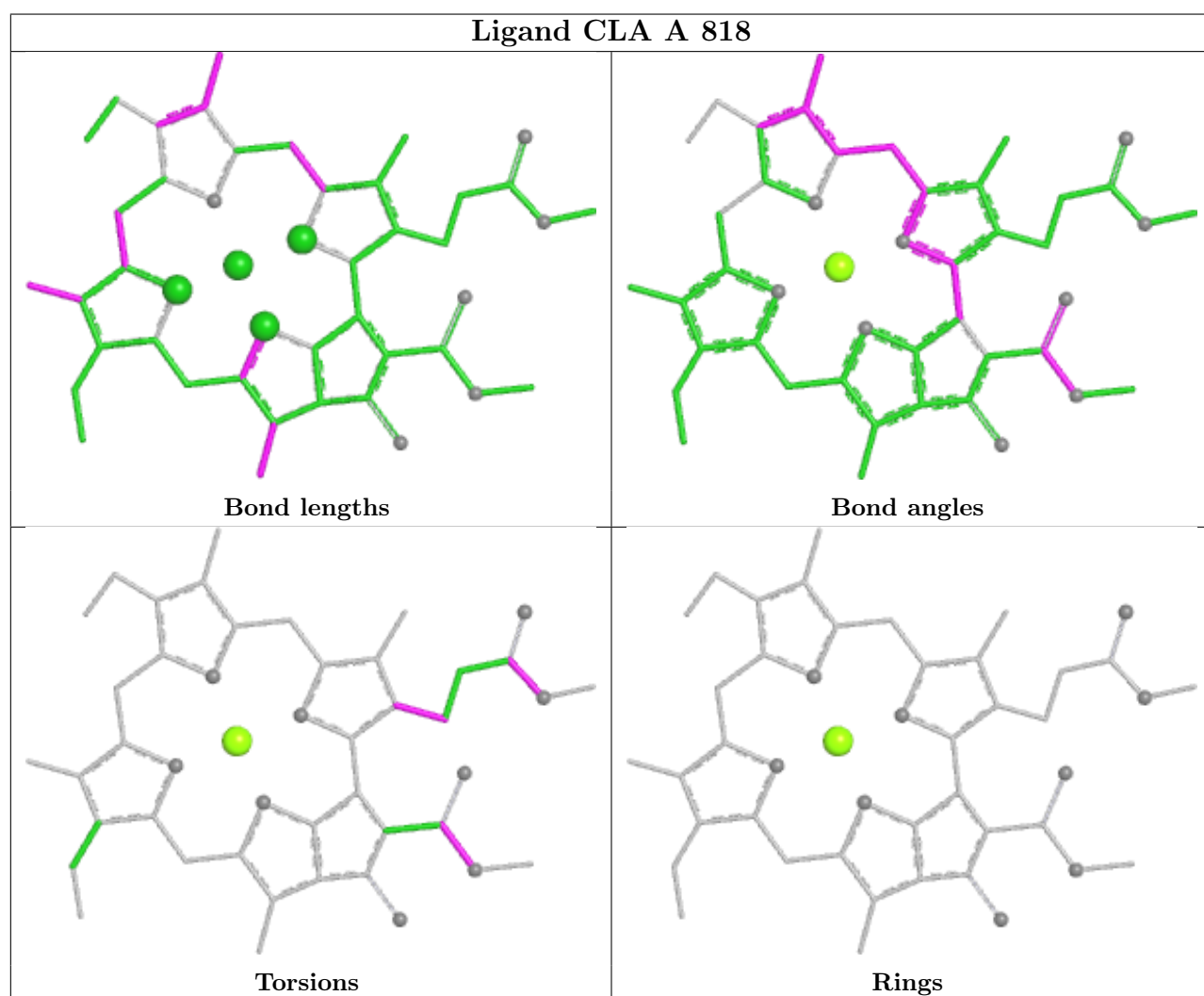
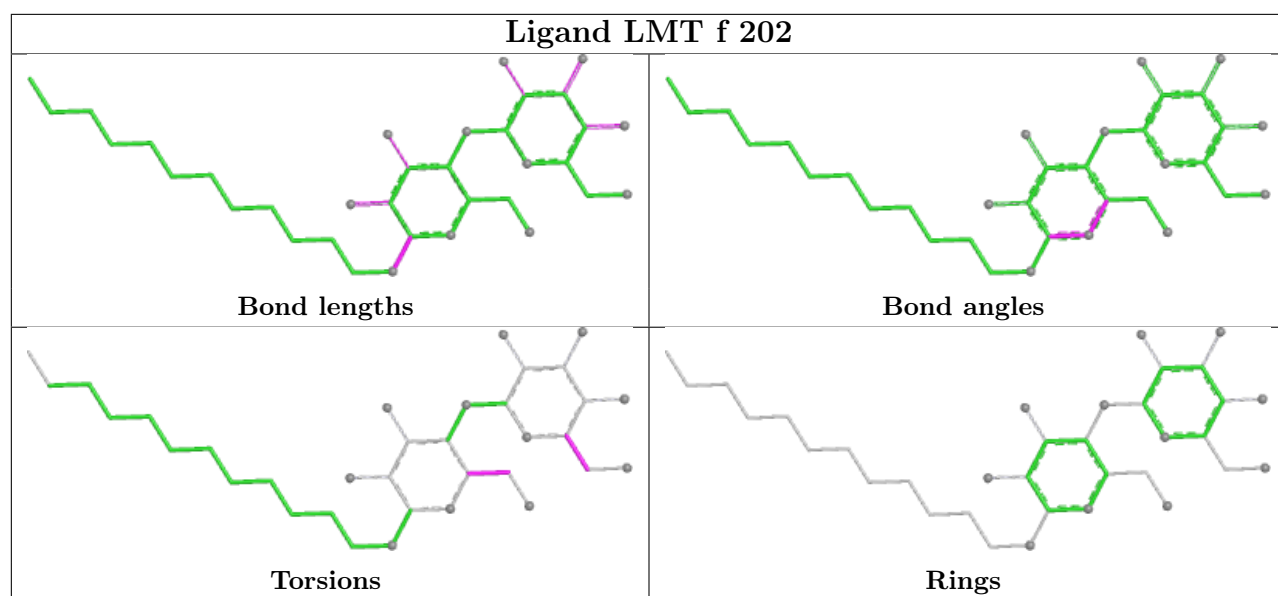


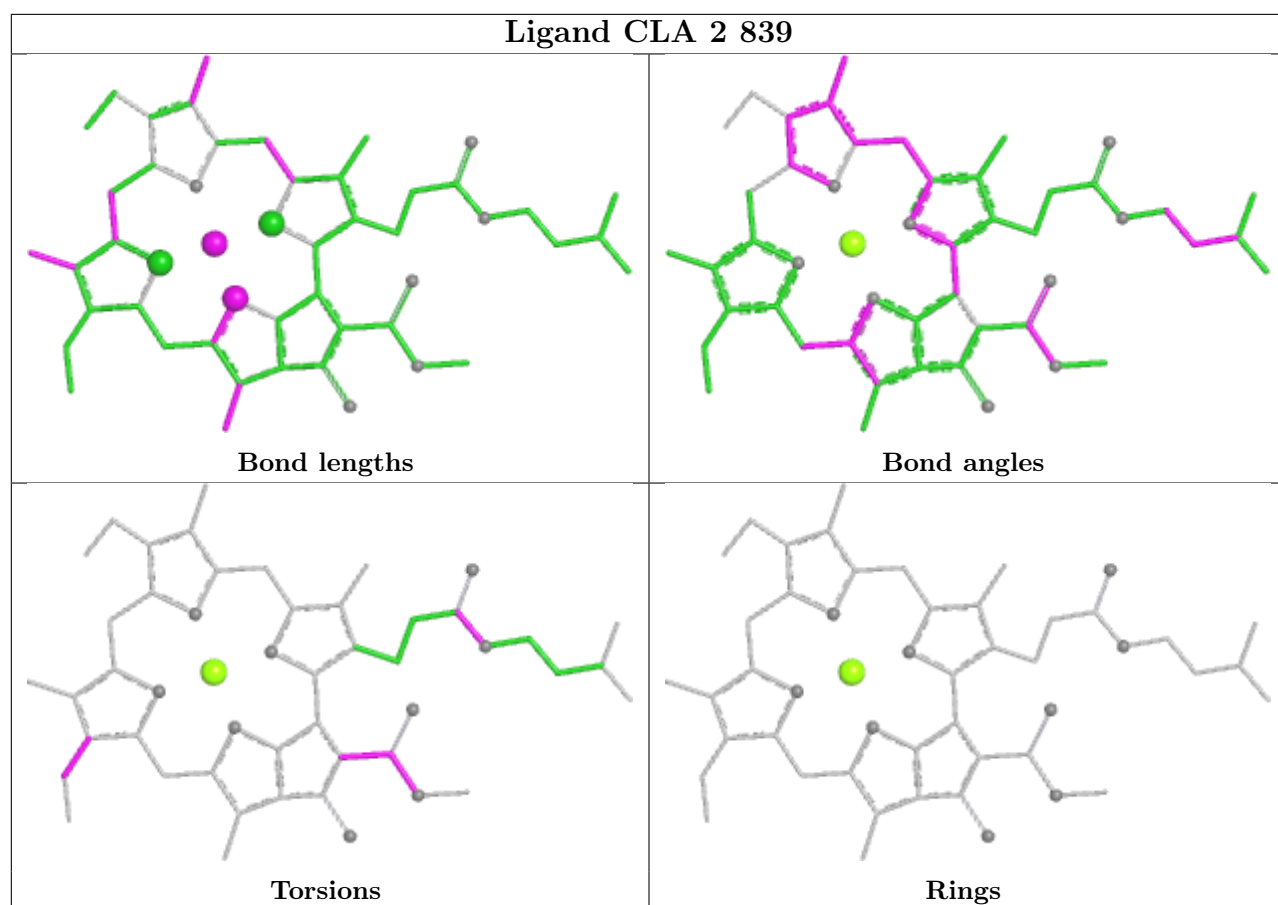
Ligand LMG 2 802



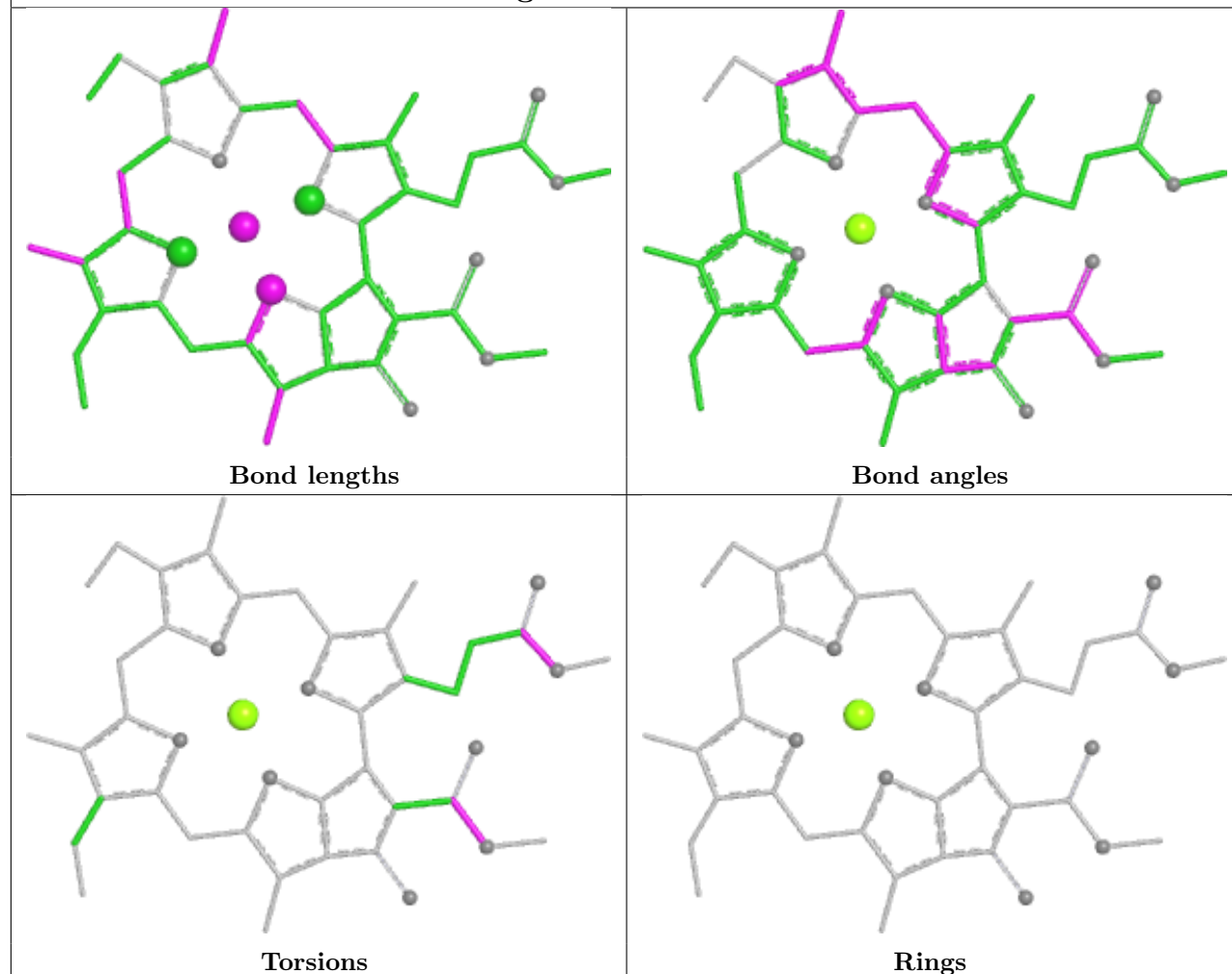




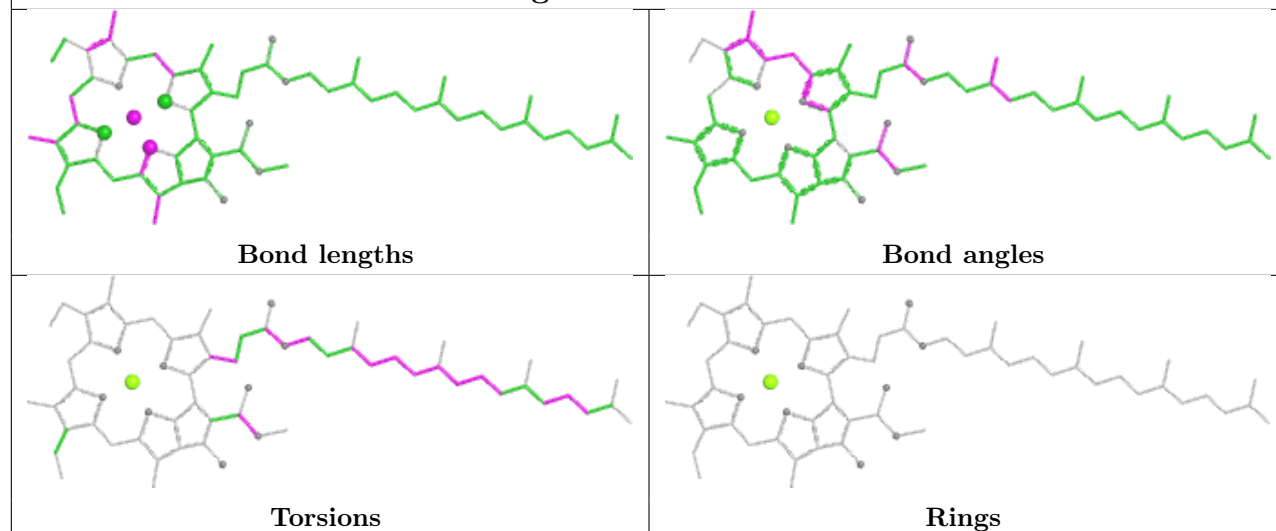


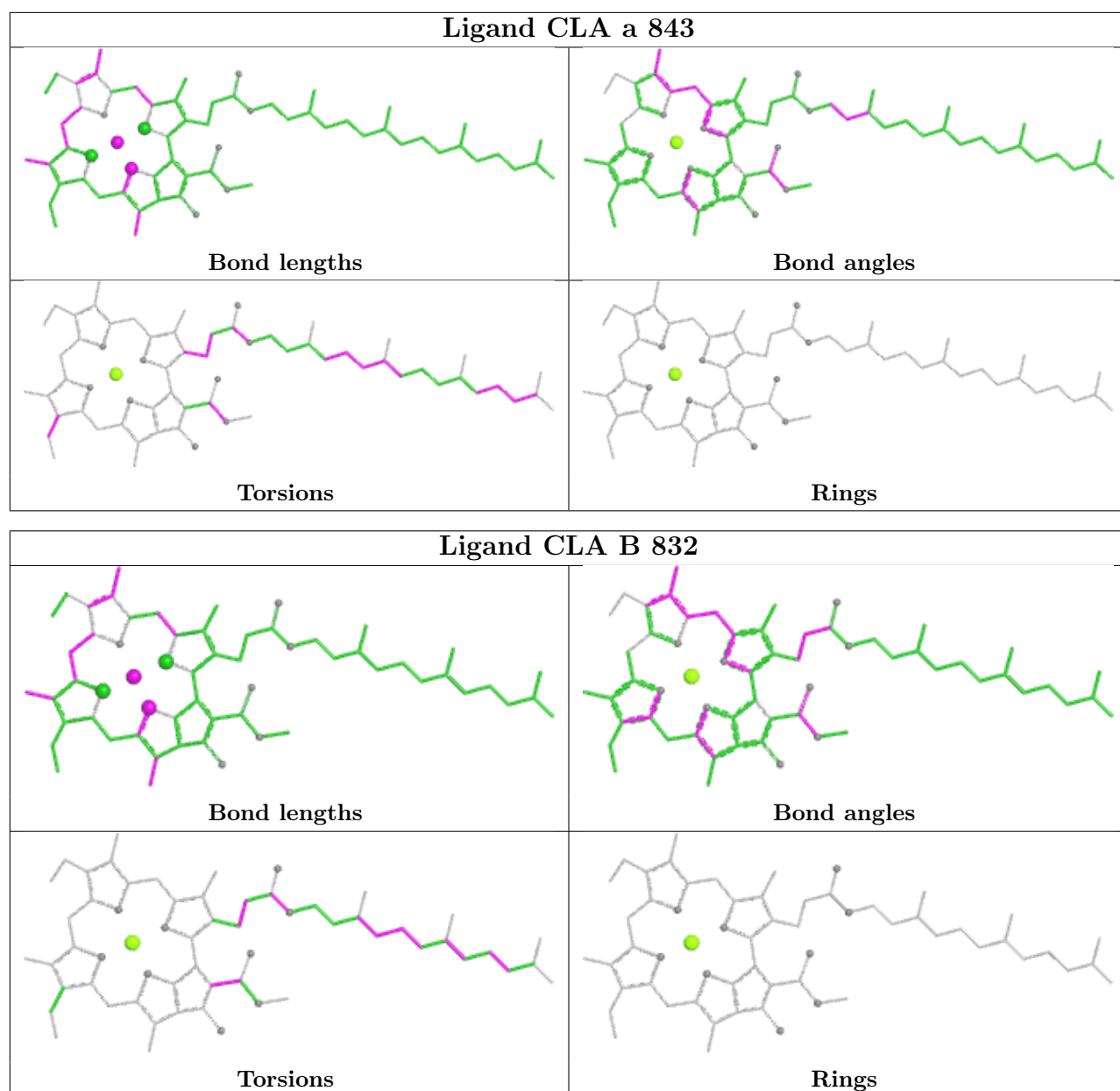


Ligand CLA b 841

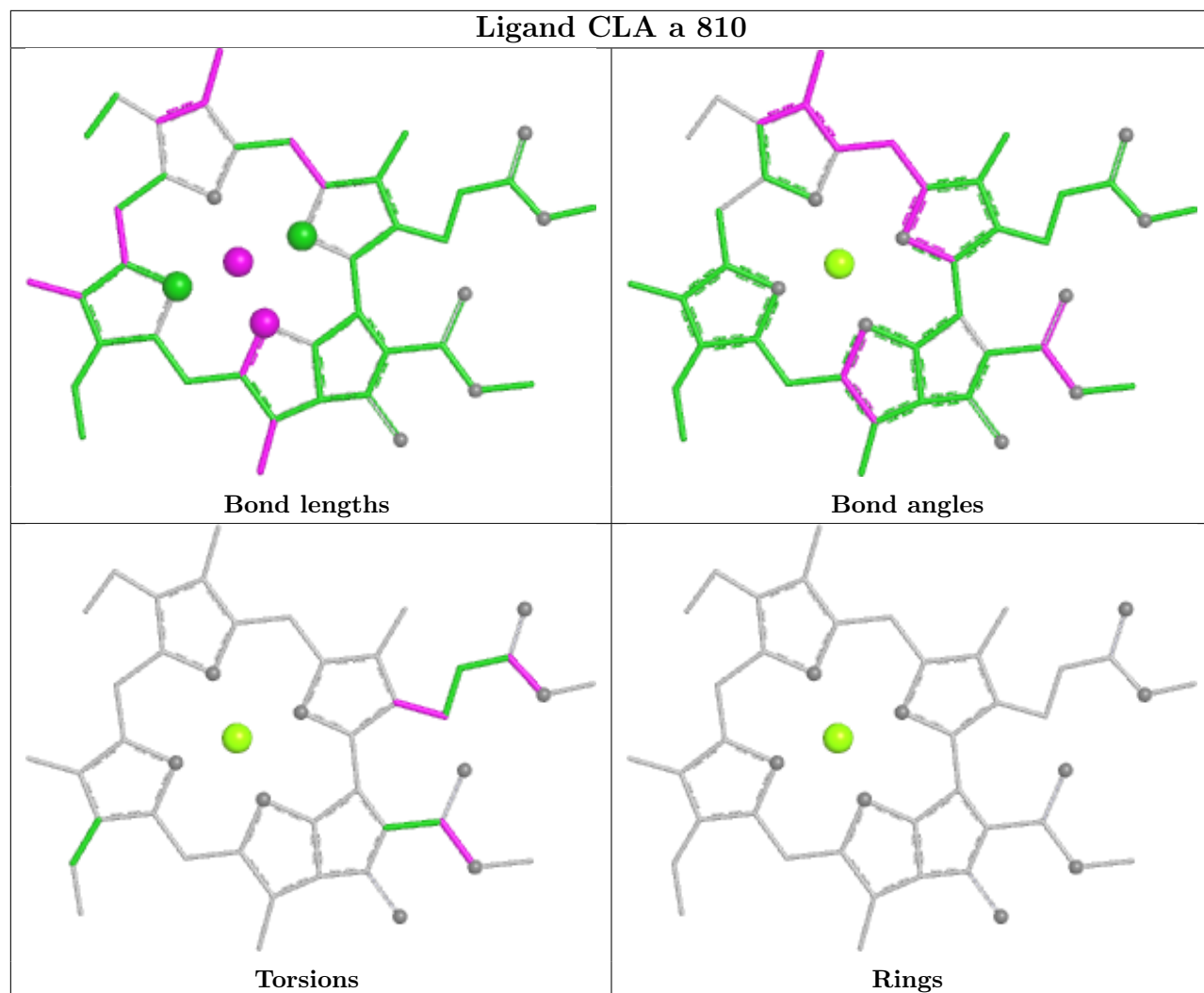


Ligand CLA A 813

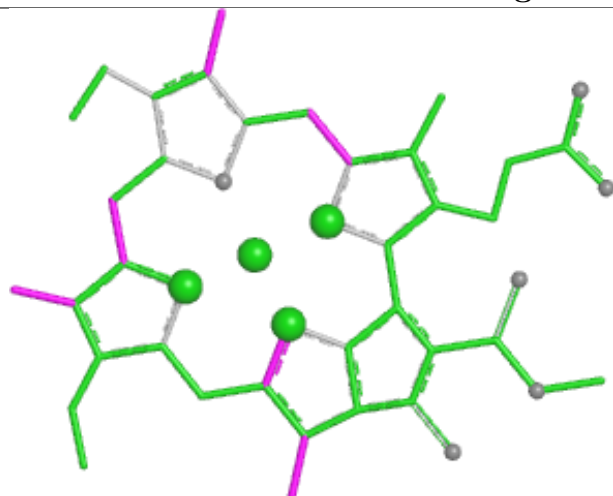




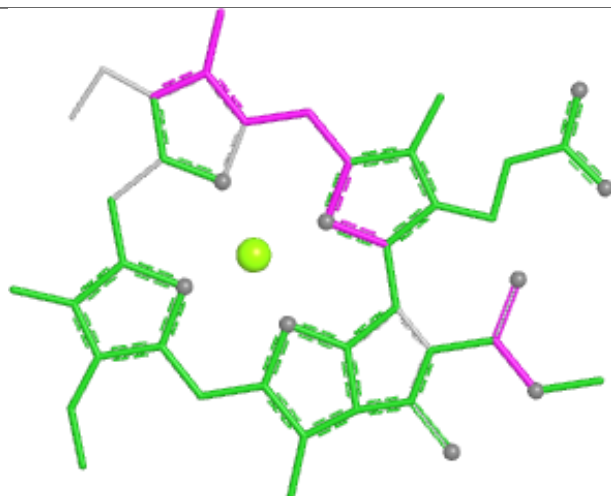
Ligand CLA a 810



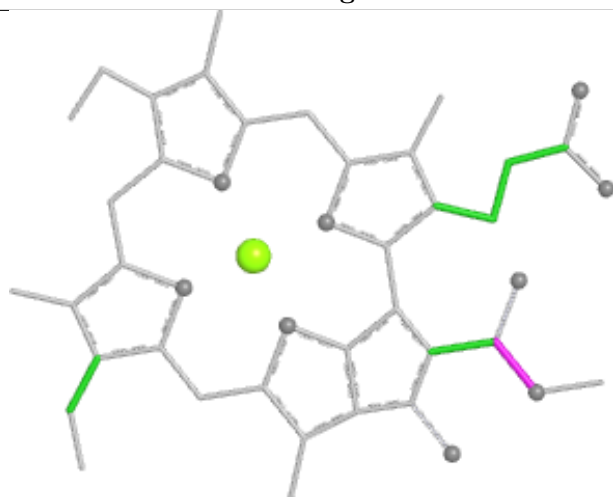
Ligand CLA B 818



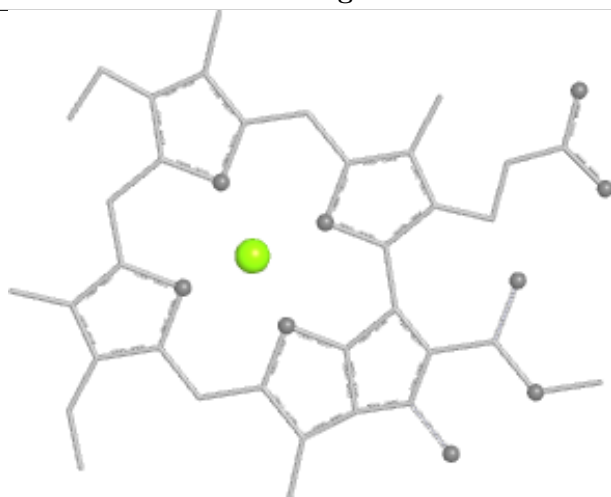
Bond lengths



Bond angles

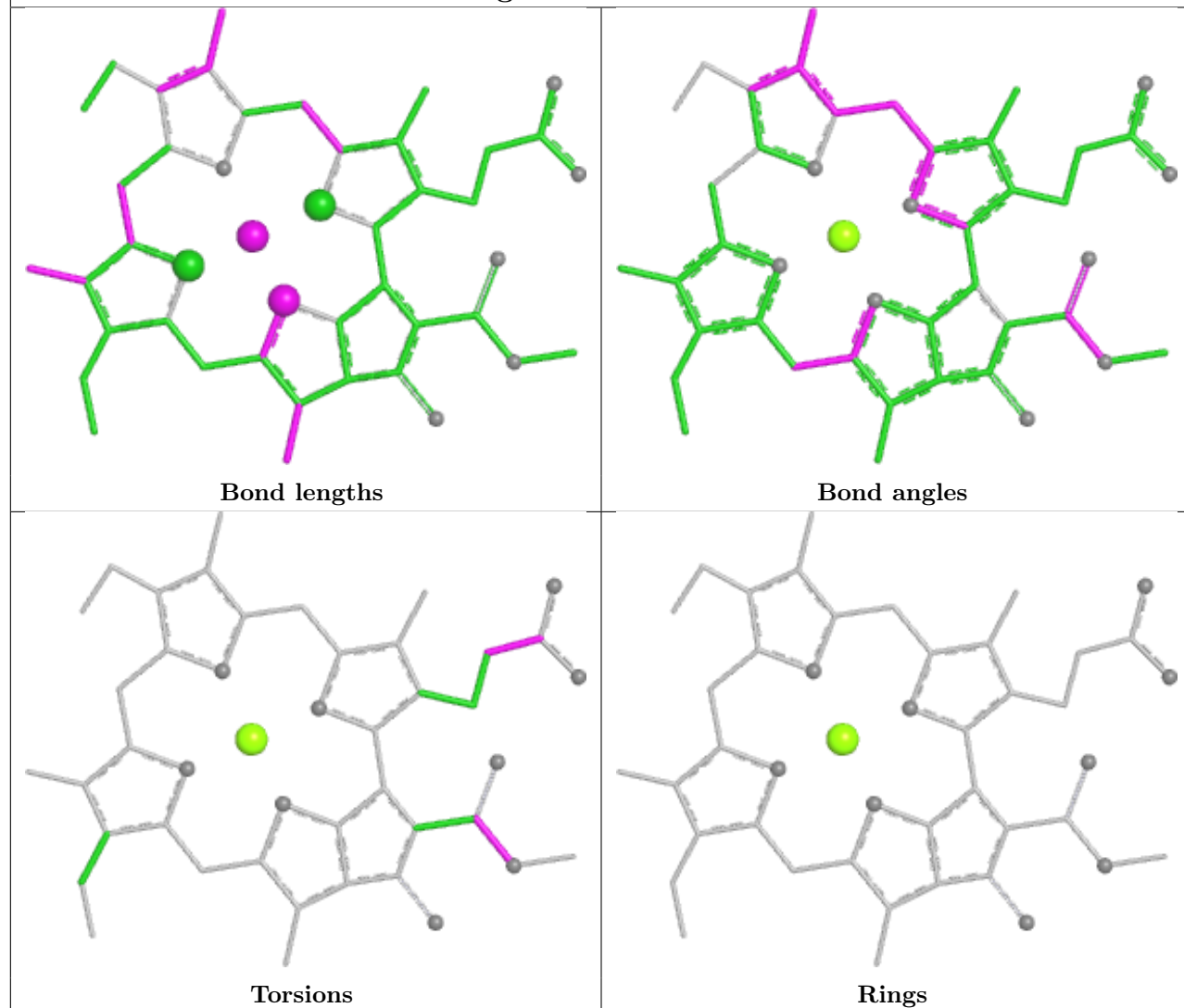


Torsions

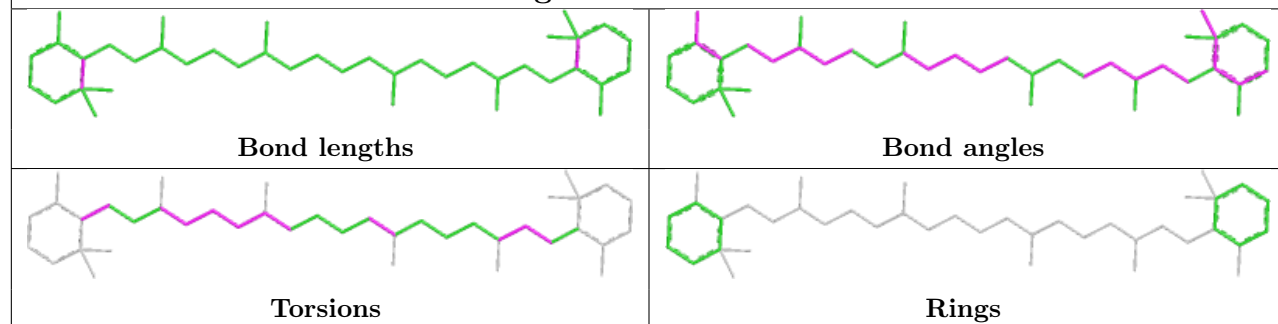


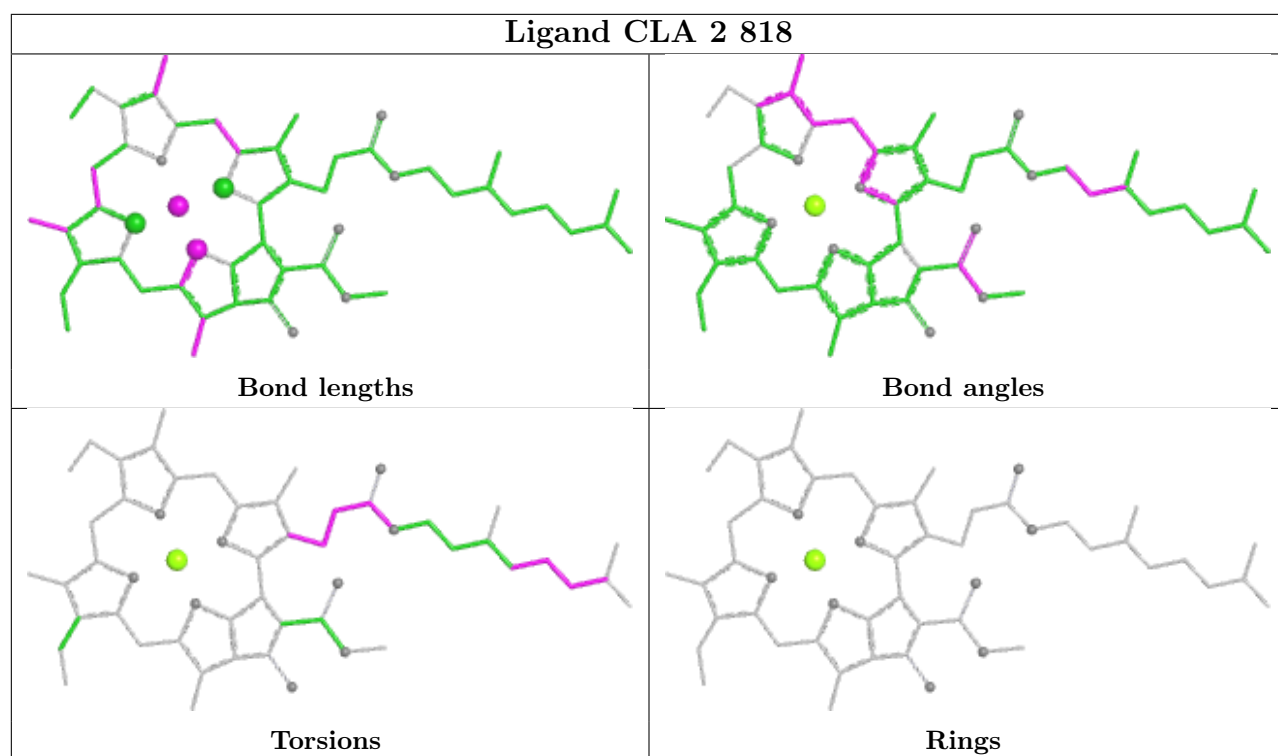
Rings

Ligand CLA a 844

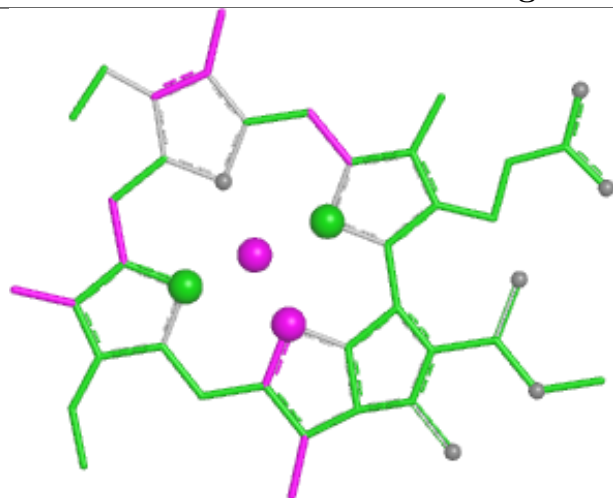


Ligand BCR 2 849

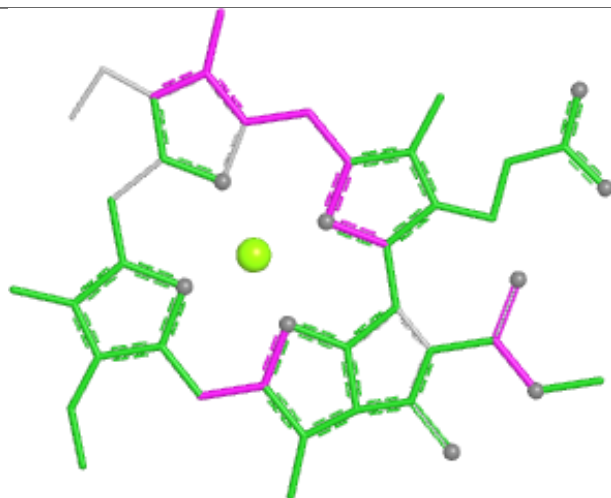




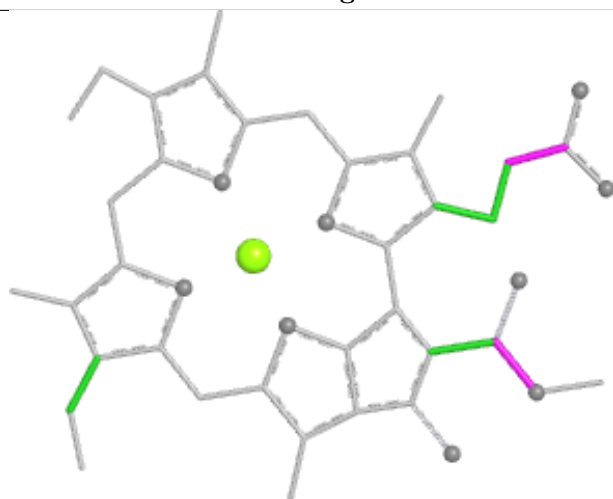
Ligand CLA 1 844



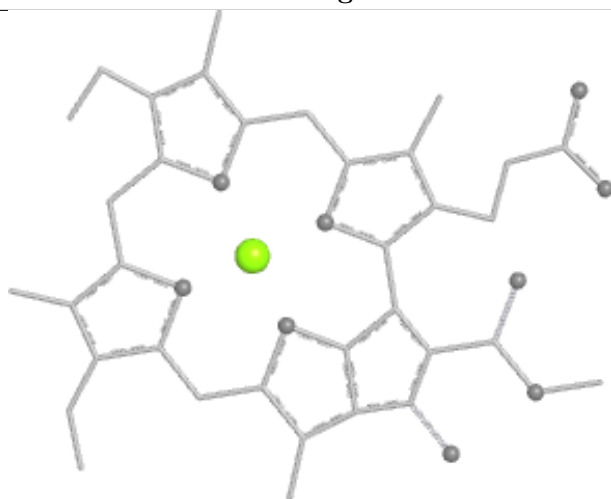
Bond lengths



Bond angles

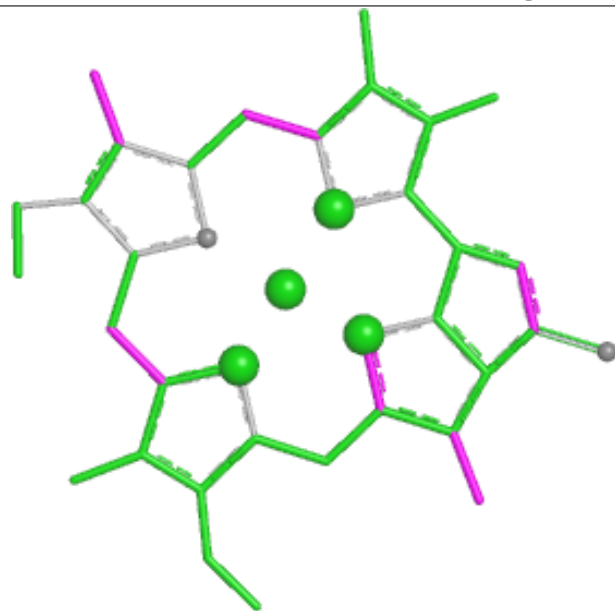


Torsions

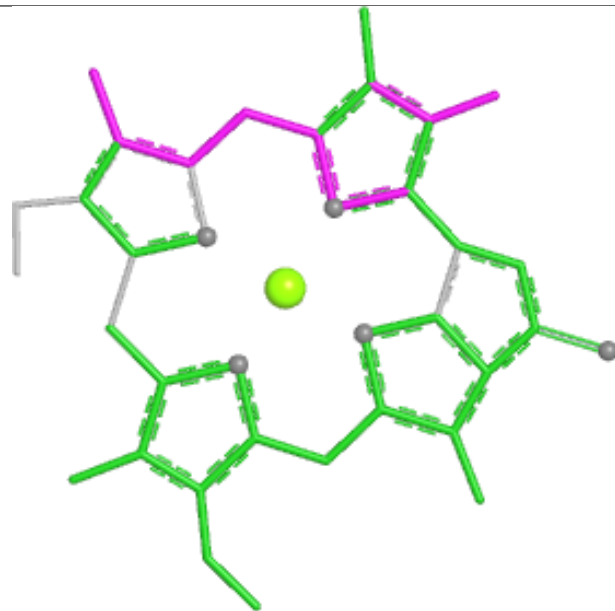


Rings

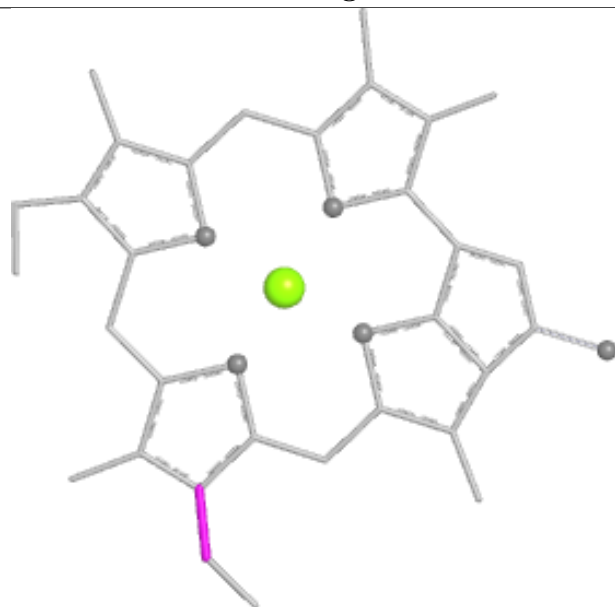
Ligand CLA J 102



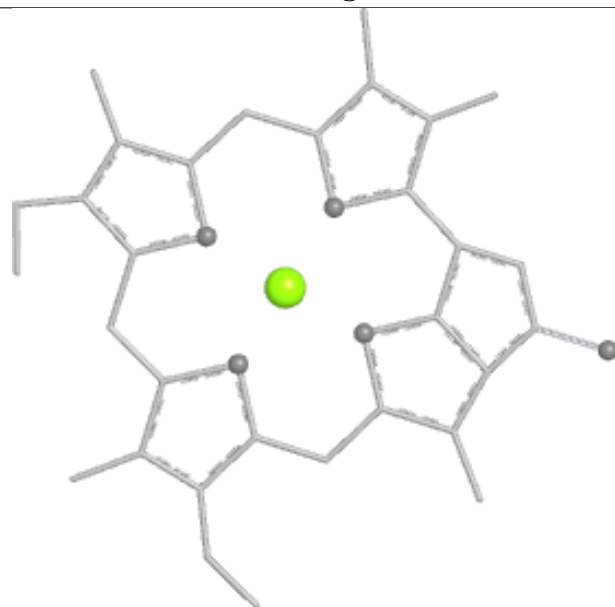
Bond lengths



Bond angles

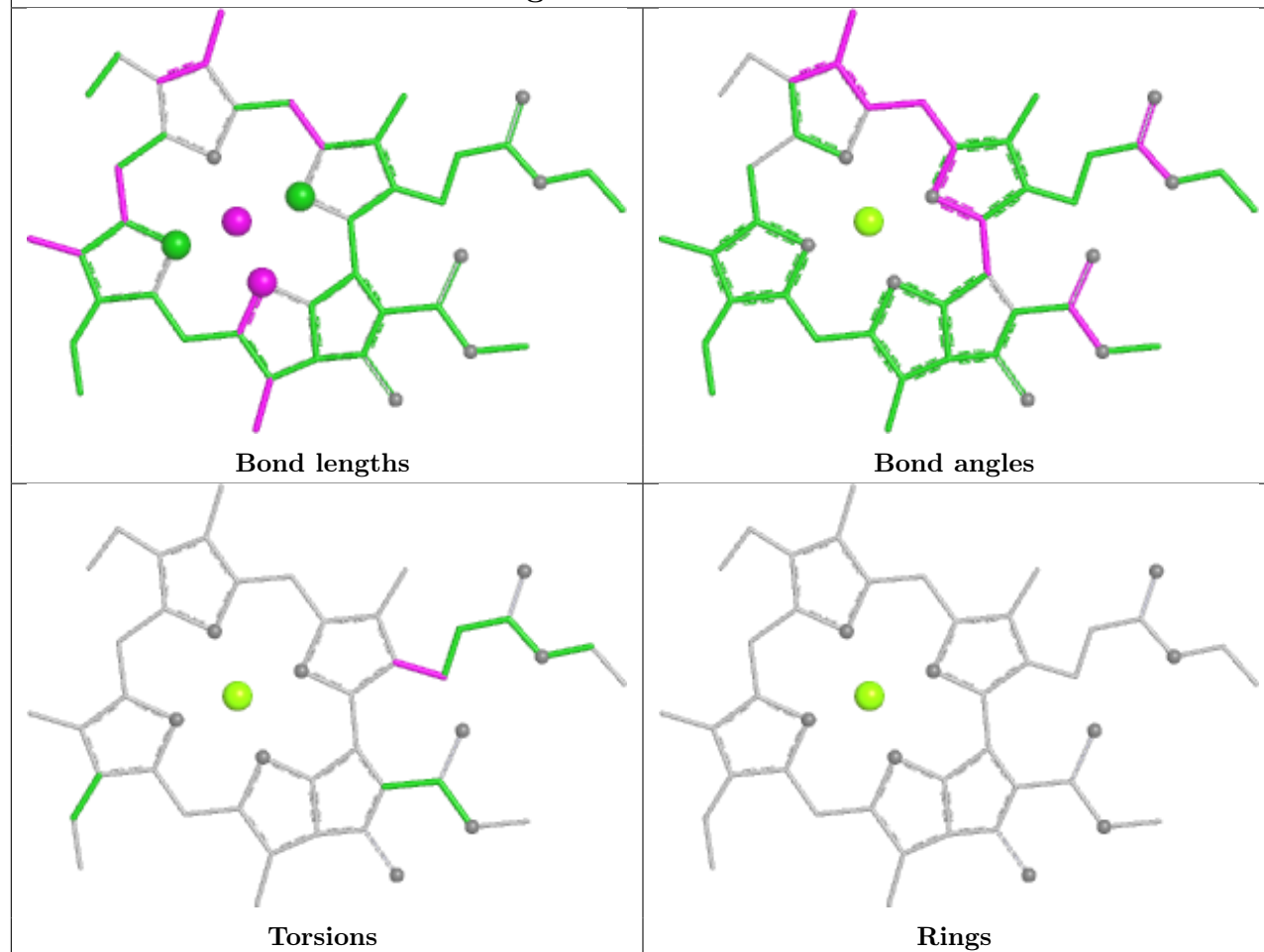


Torsions

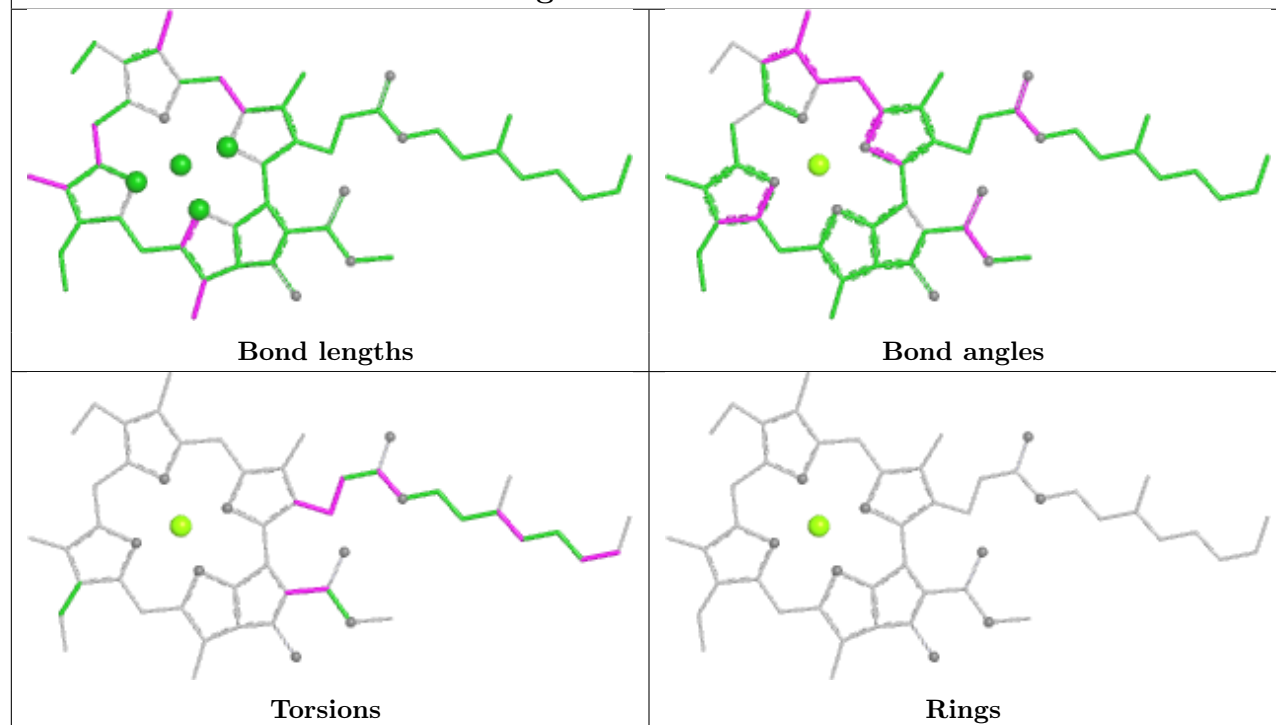


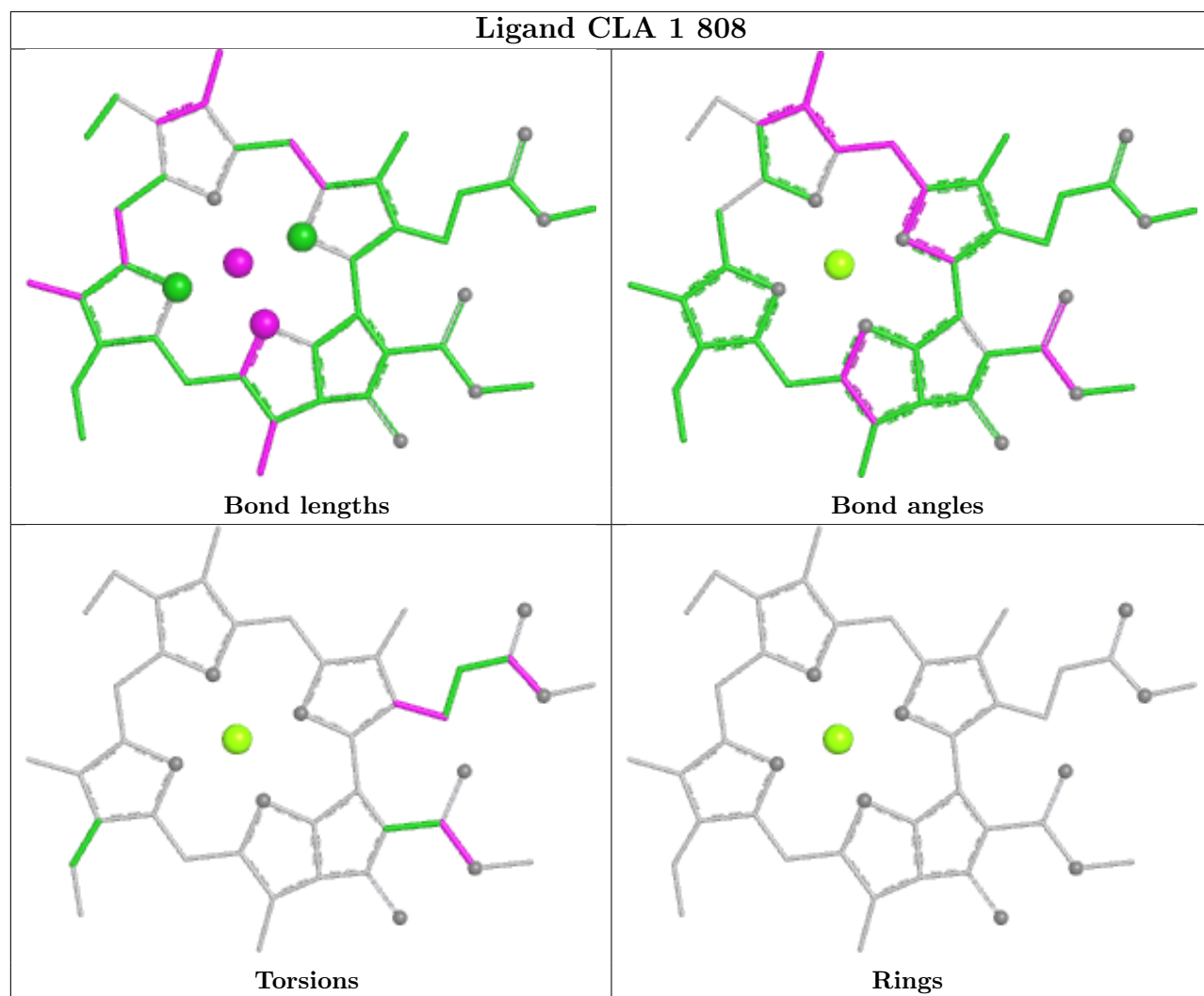
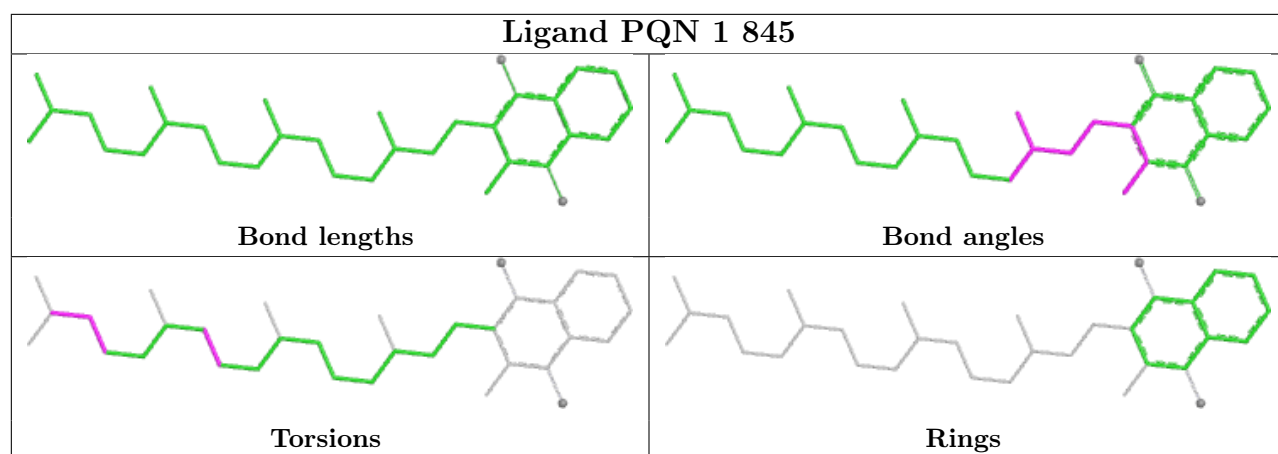
Rings

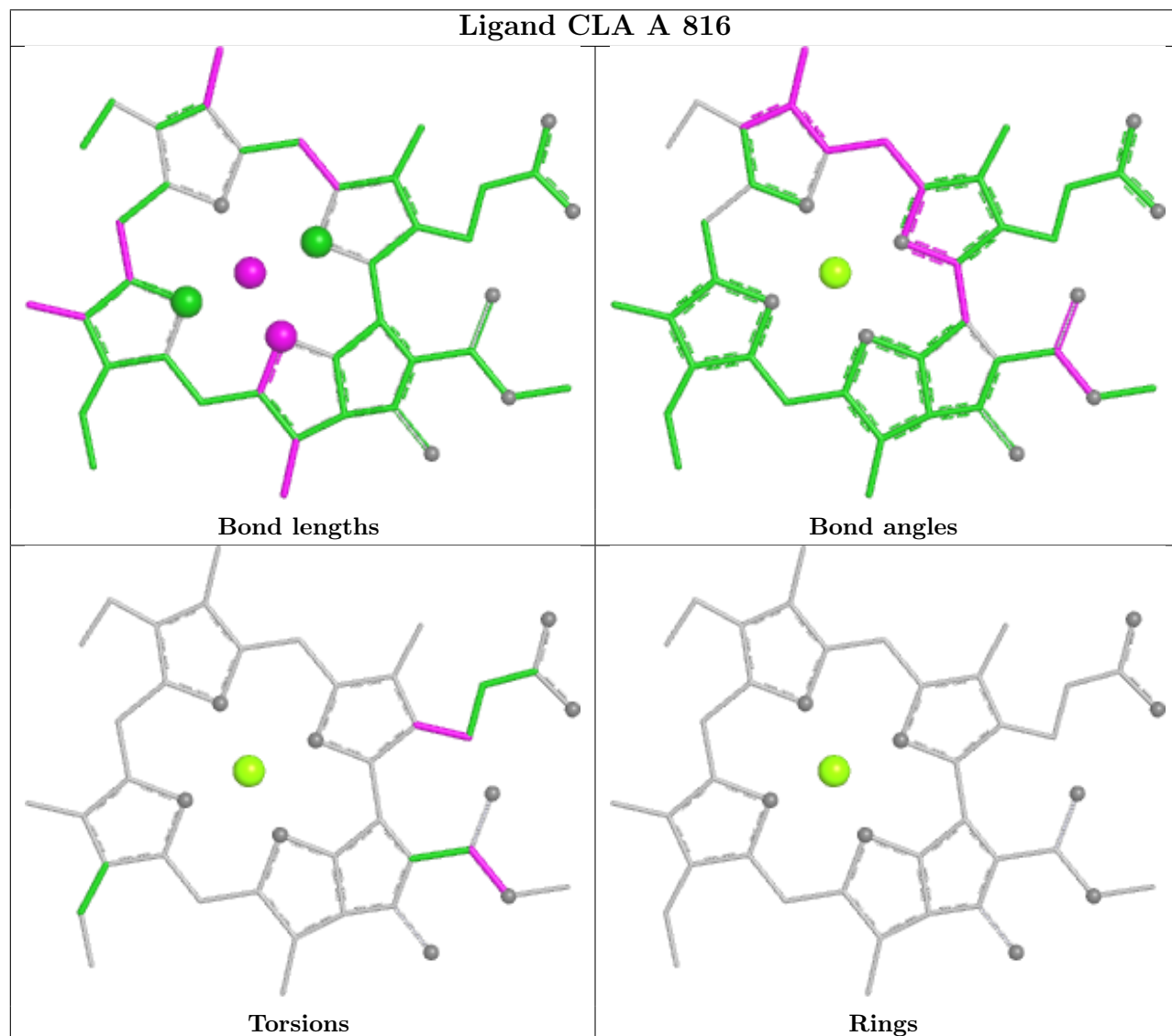
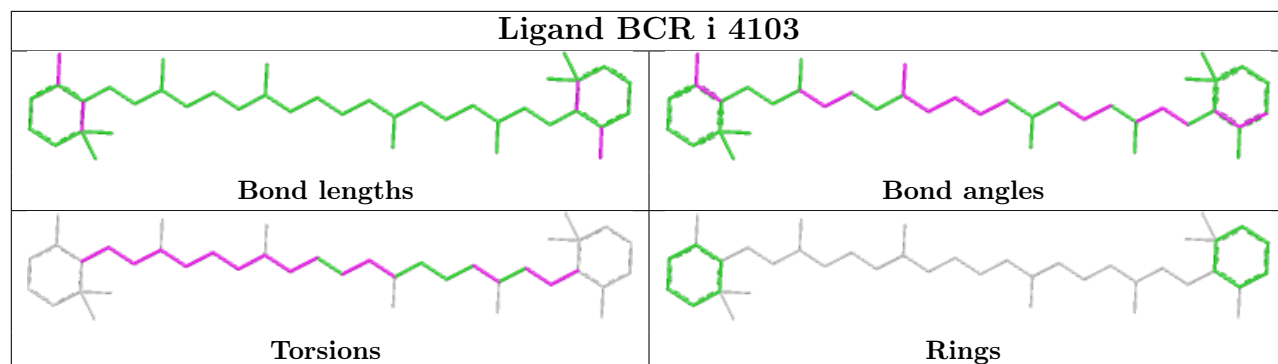
Ligand CLA A 840

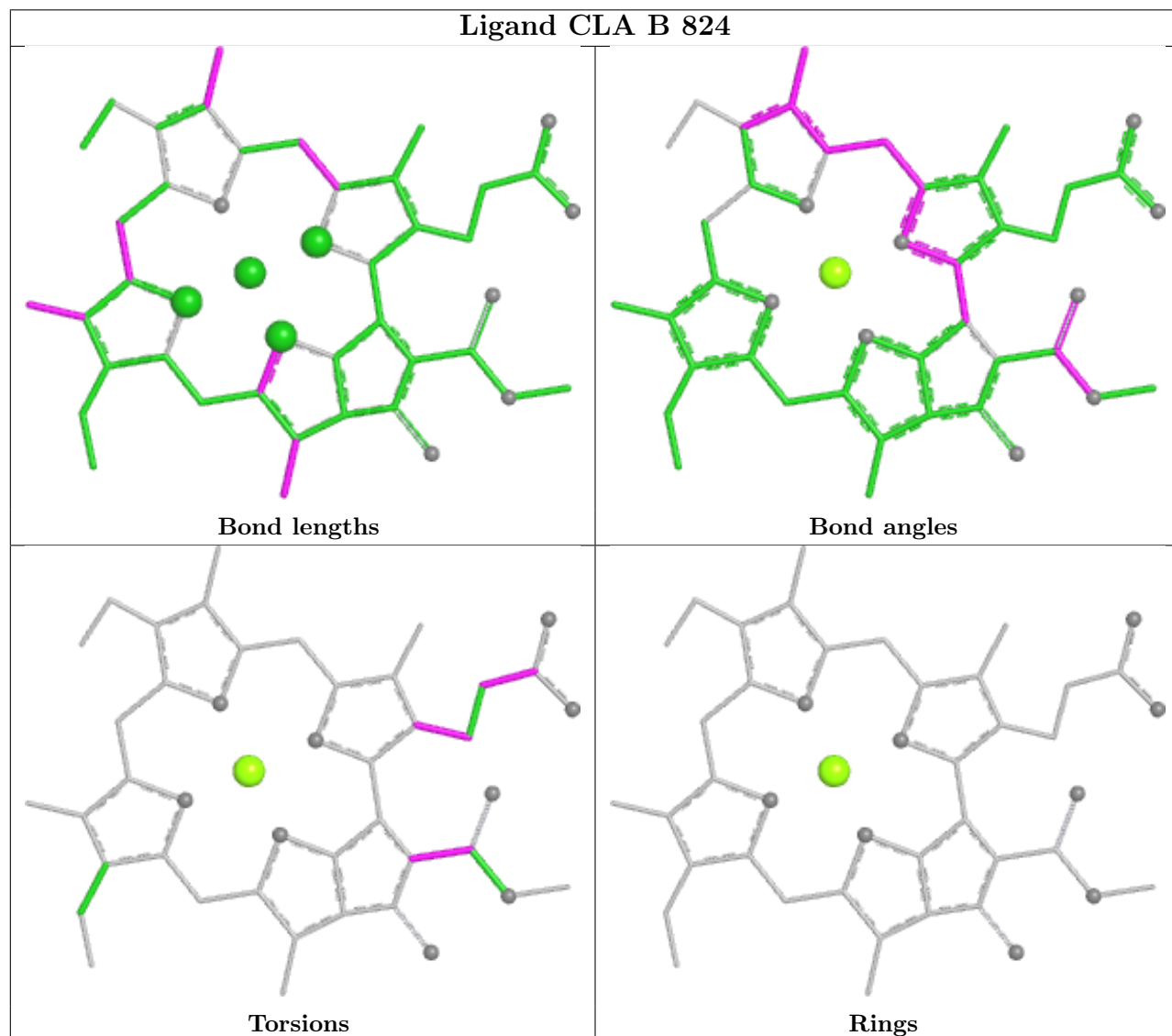
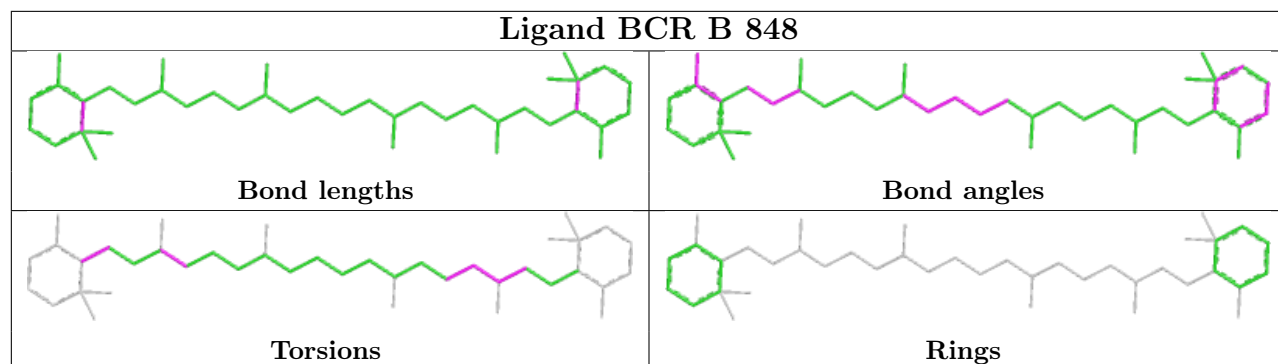


Ligand CLA 2 806

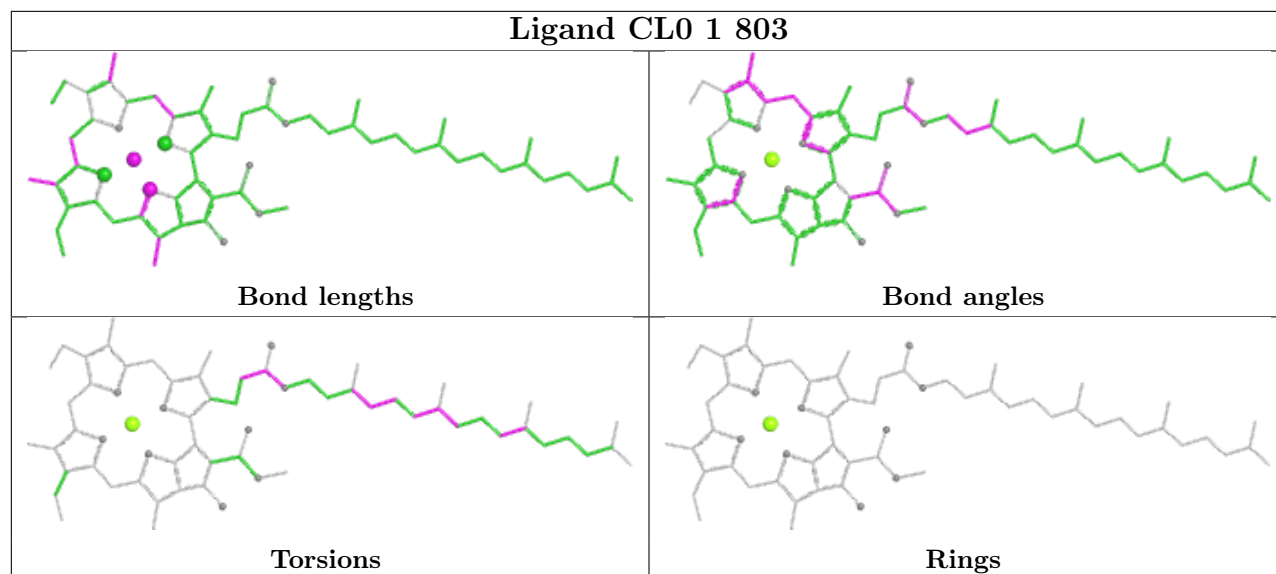




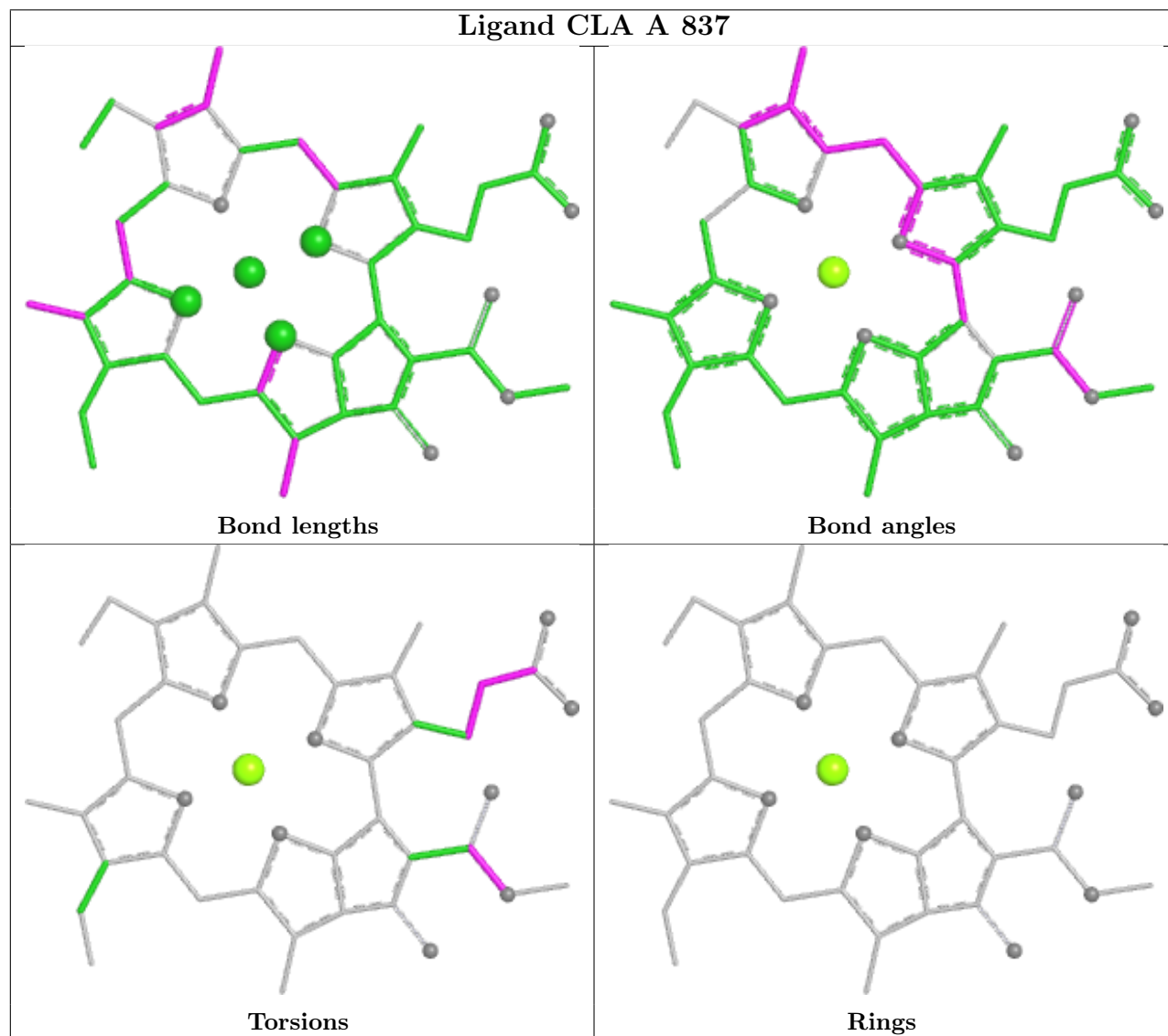


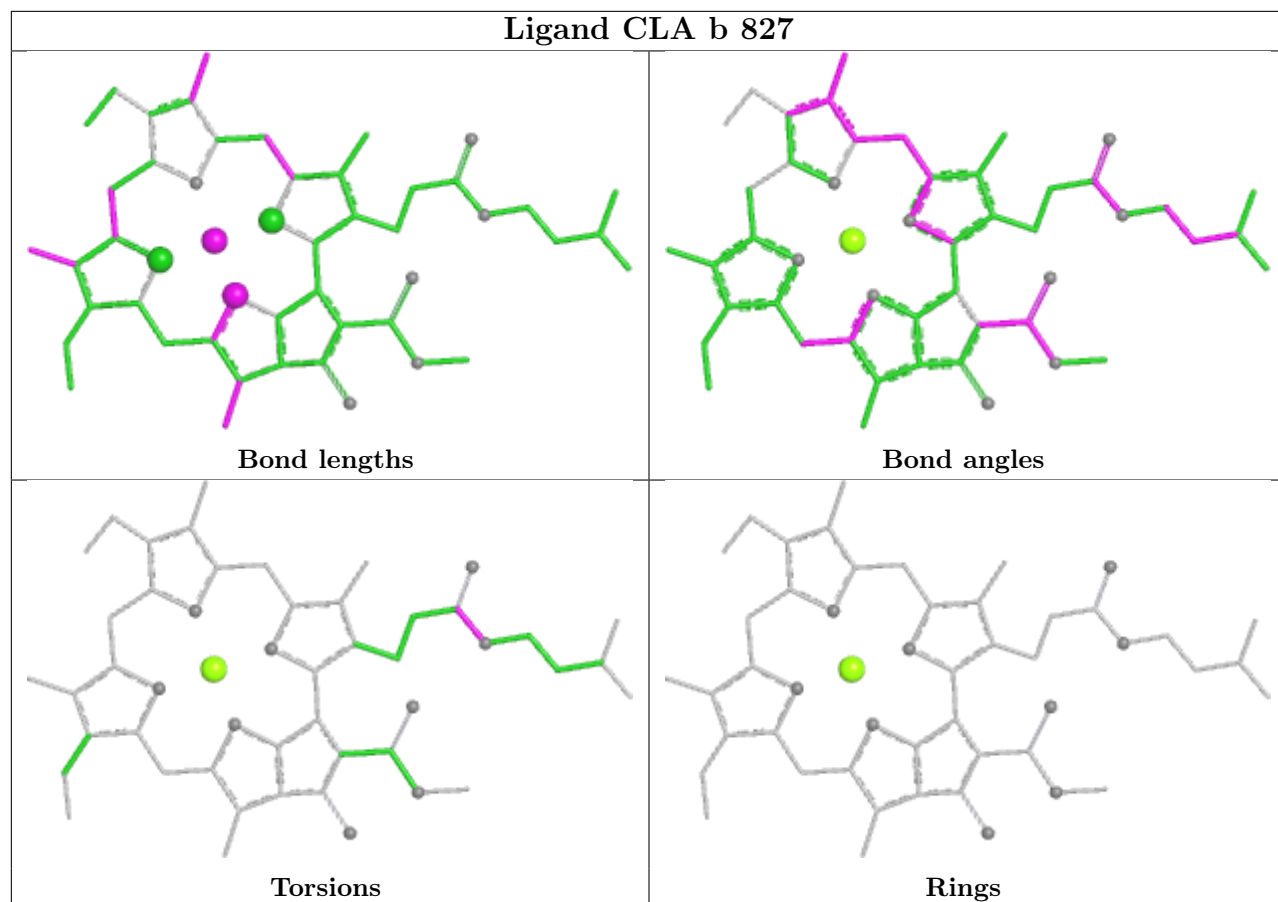


Ligand CL0 1 803

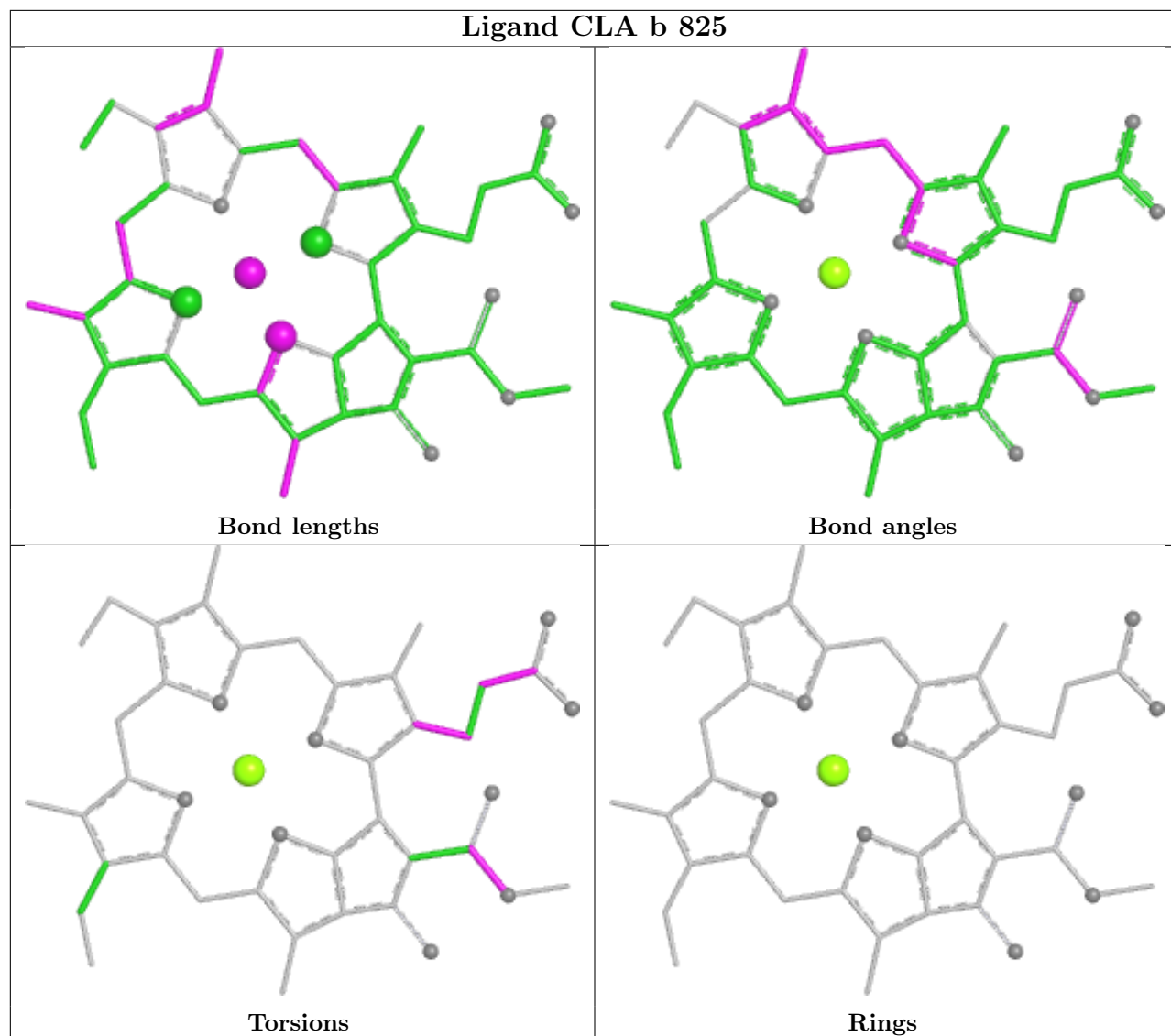


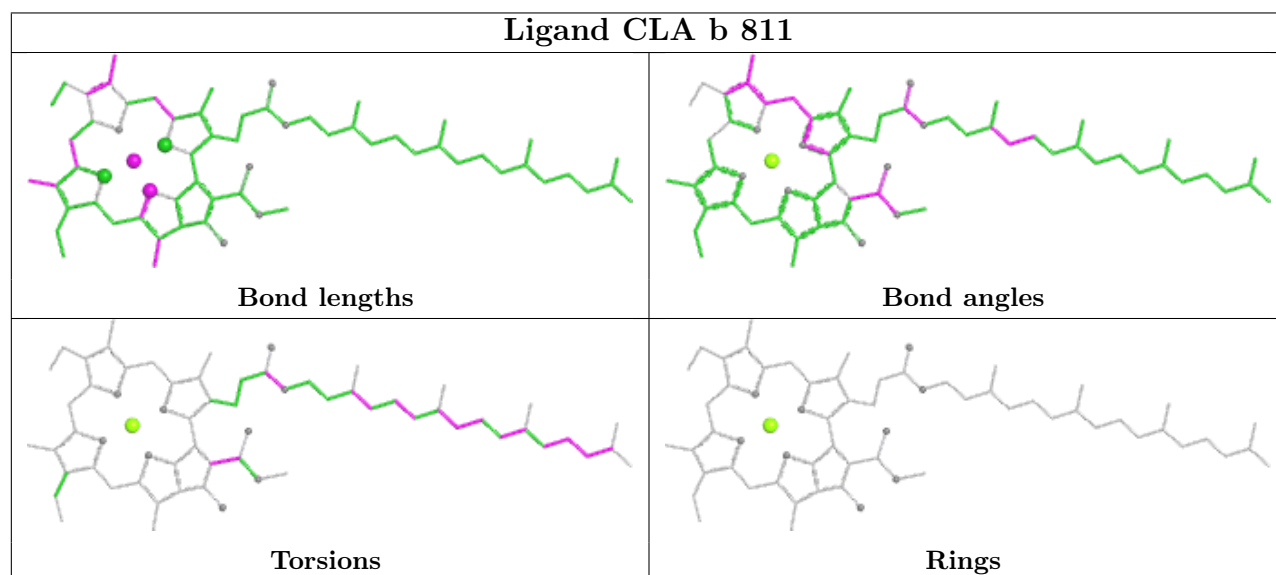
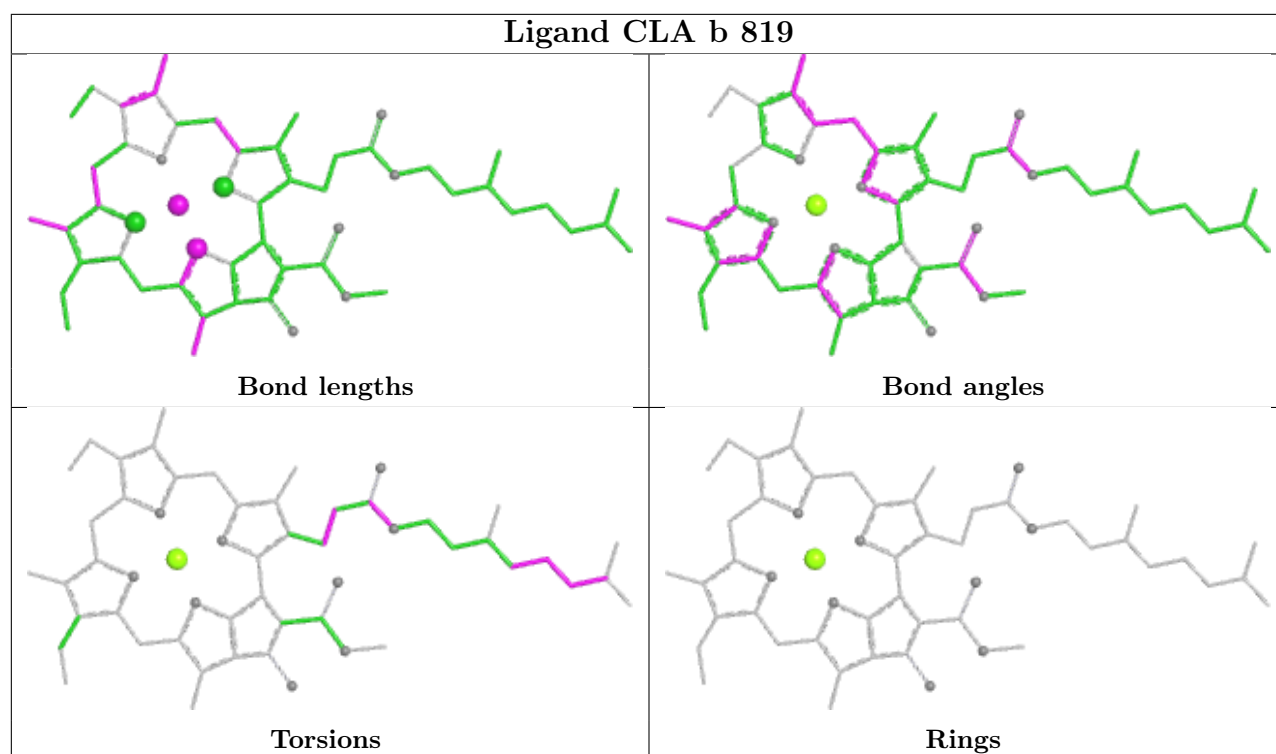
Ligand CLA A 837

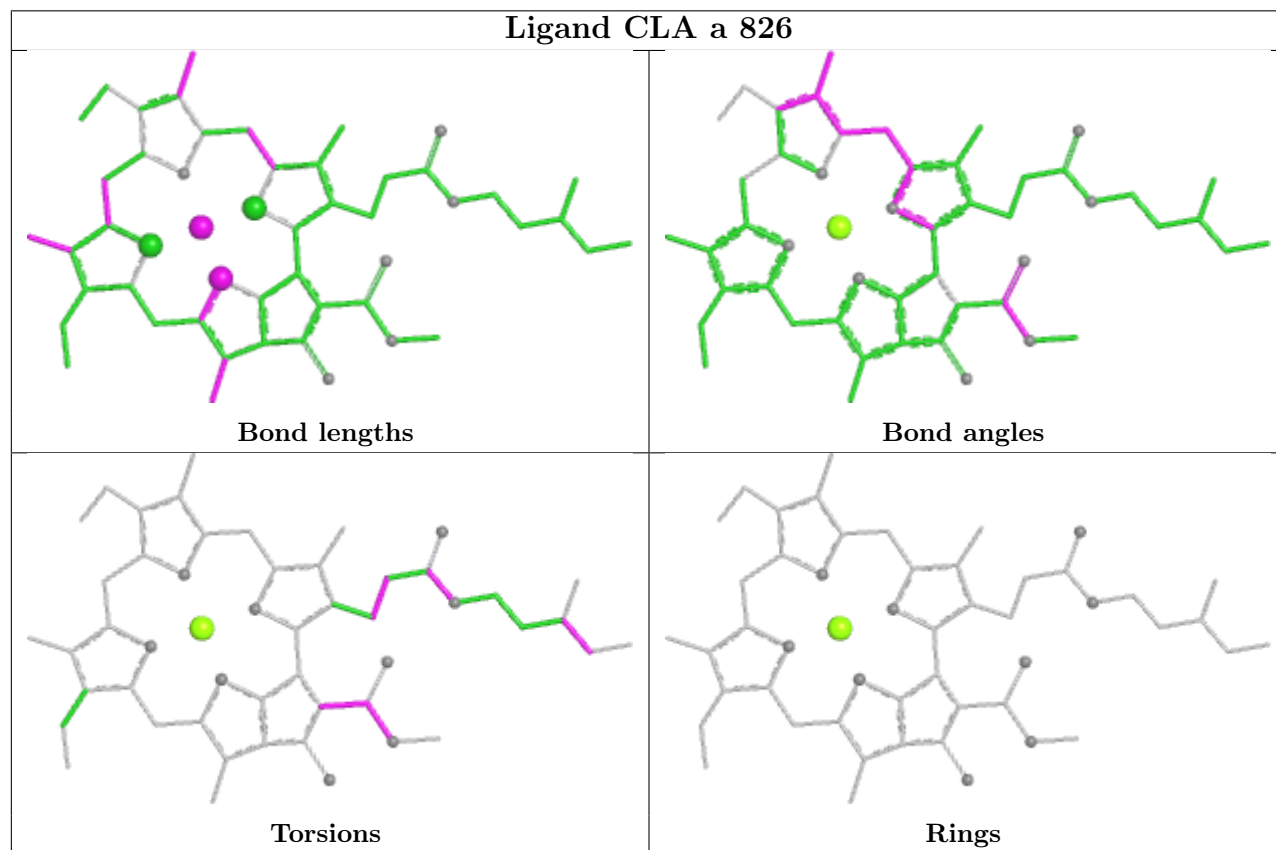
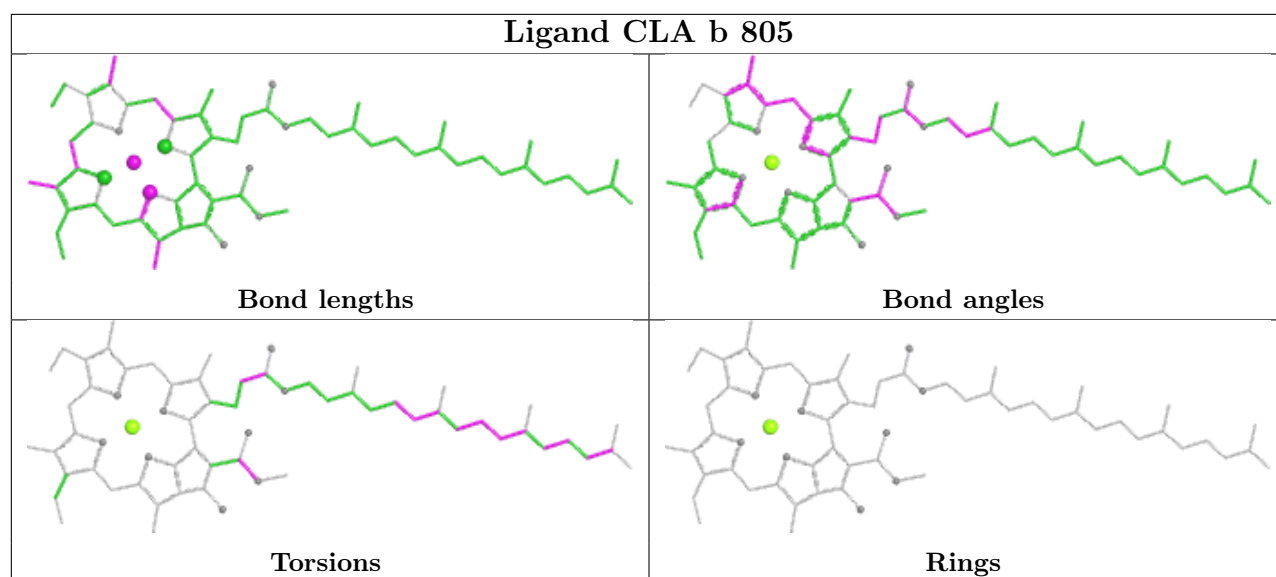




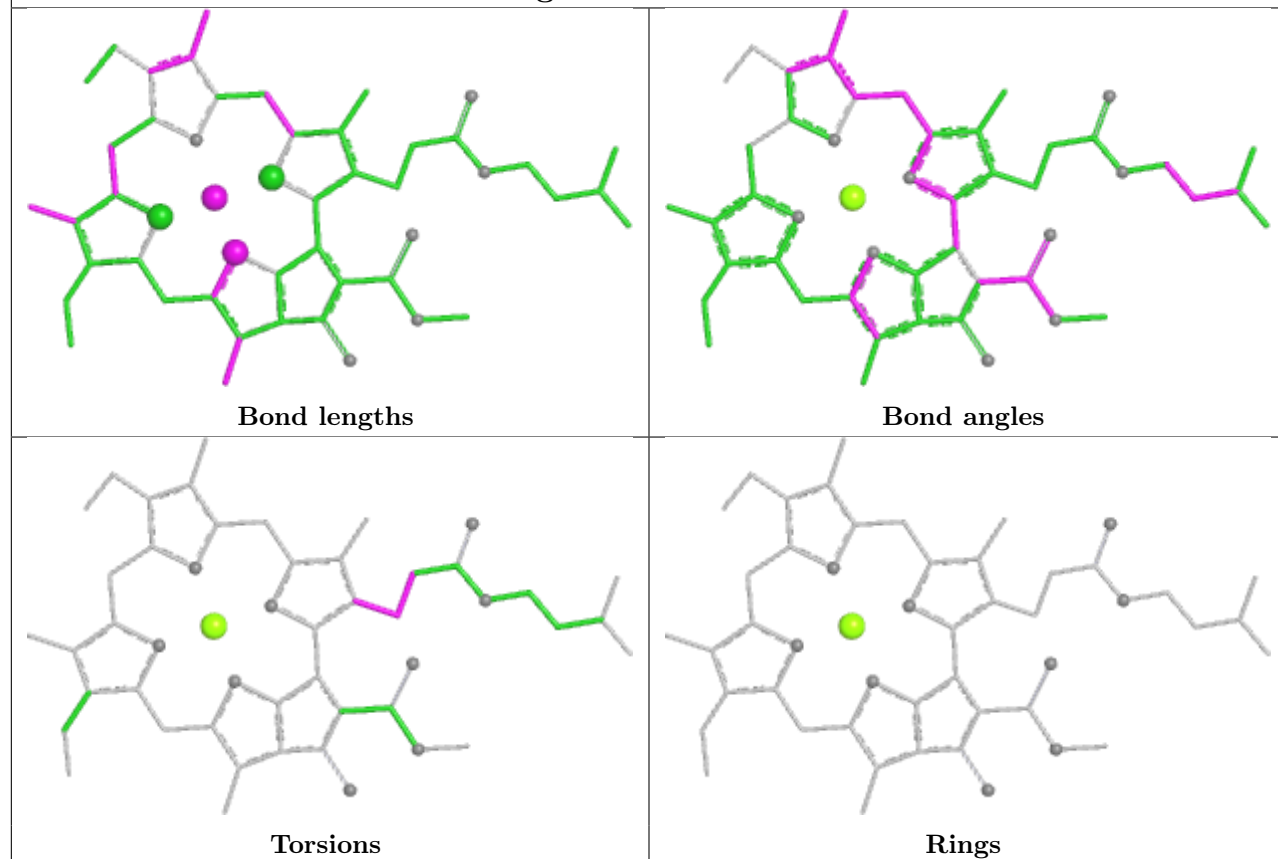
Ligand CLA b 825



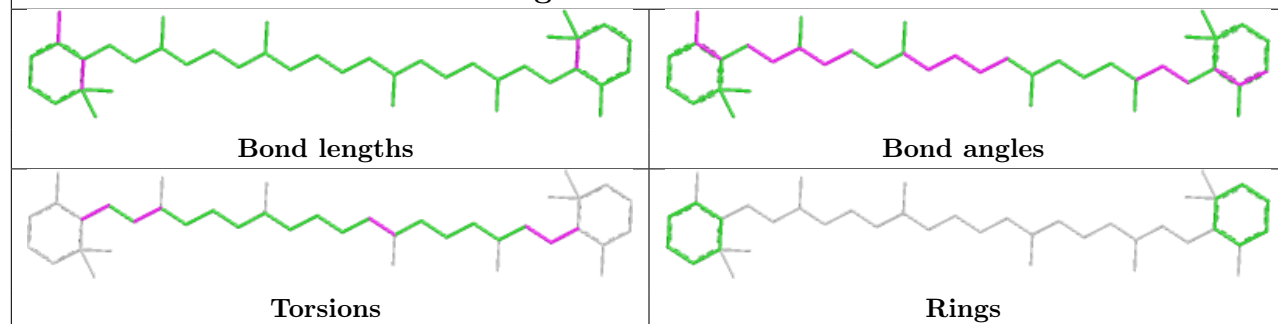




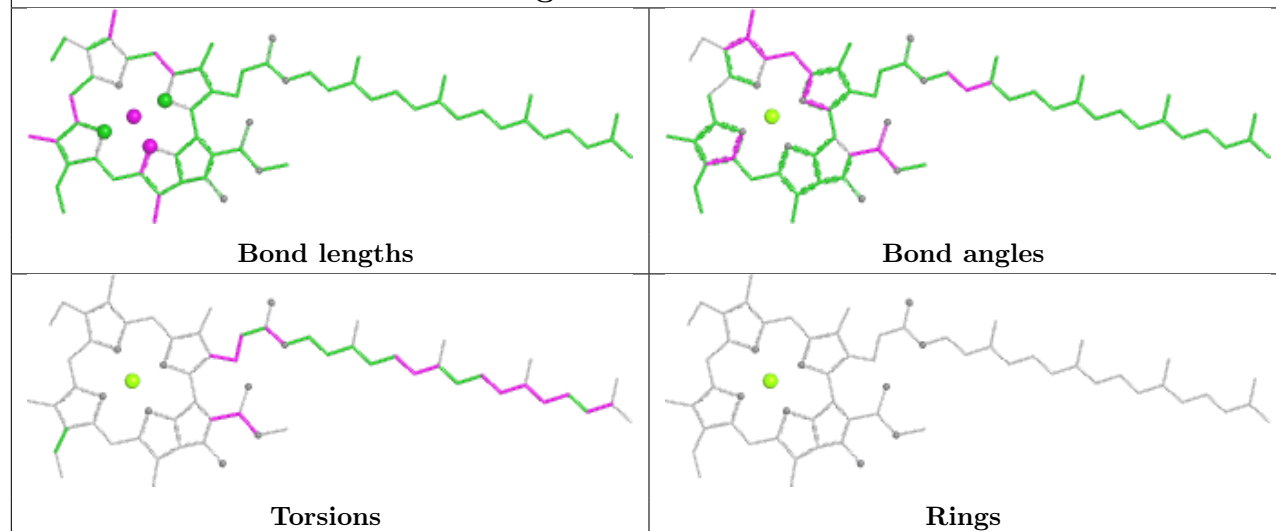
Ligand CLA a 807



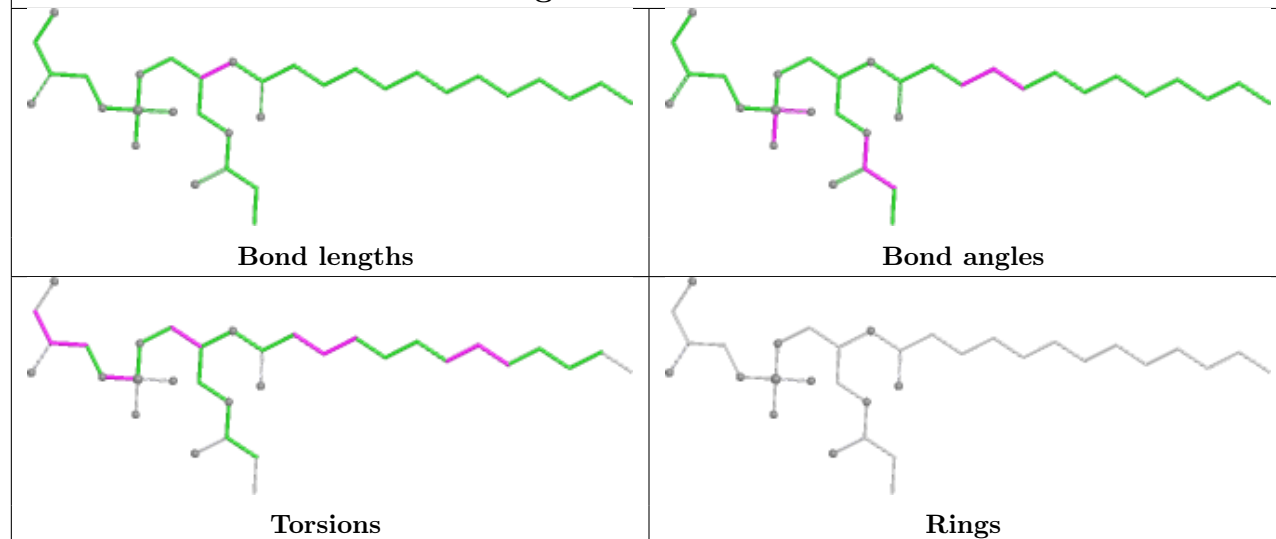
Ligand BCR 1 849



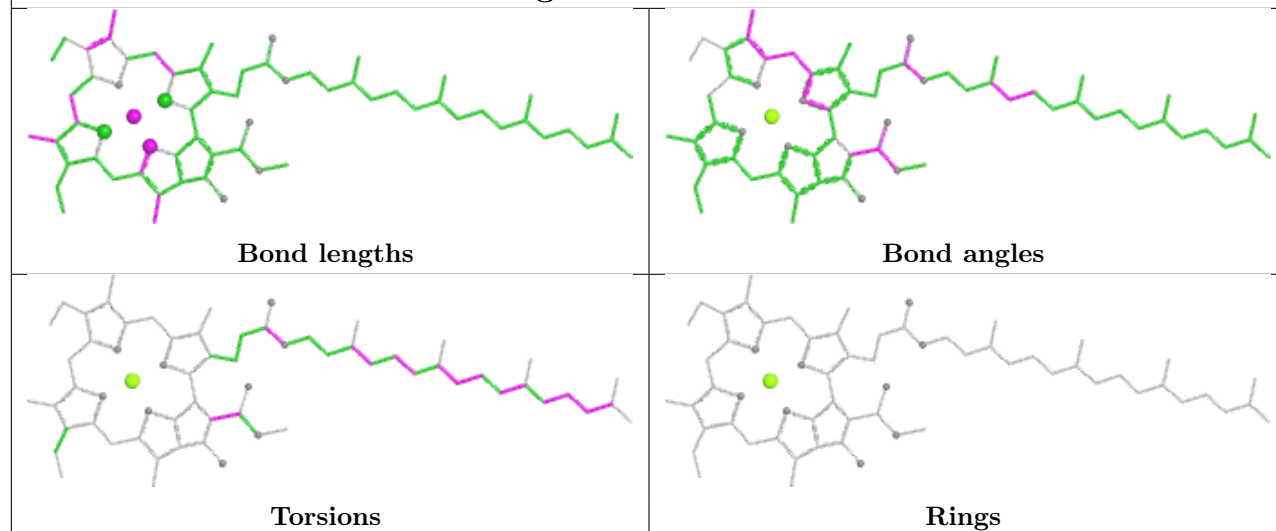
Ligand CLA 1 820

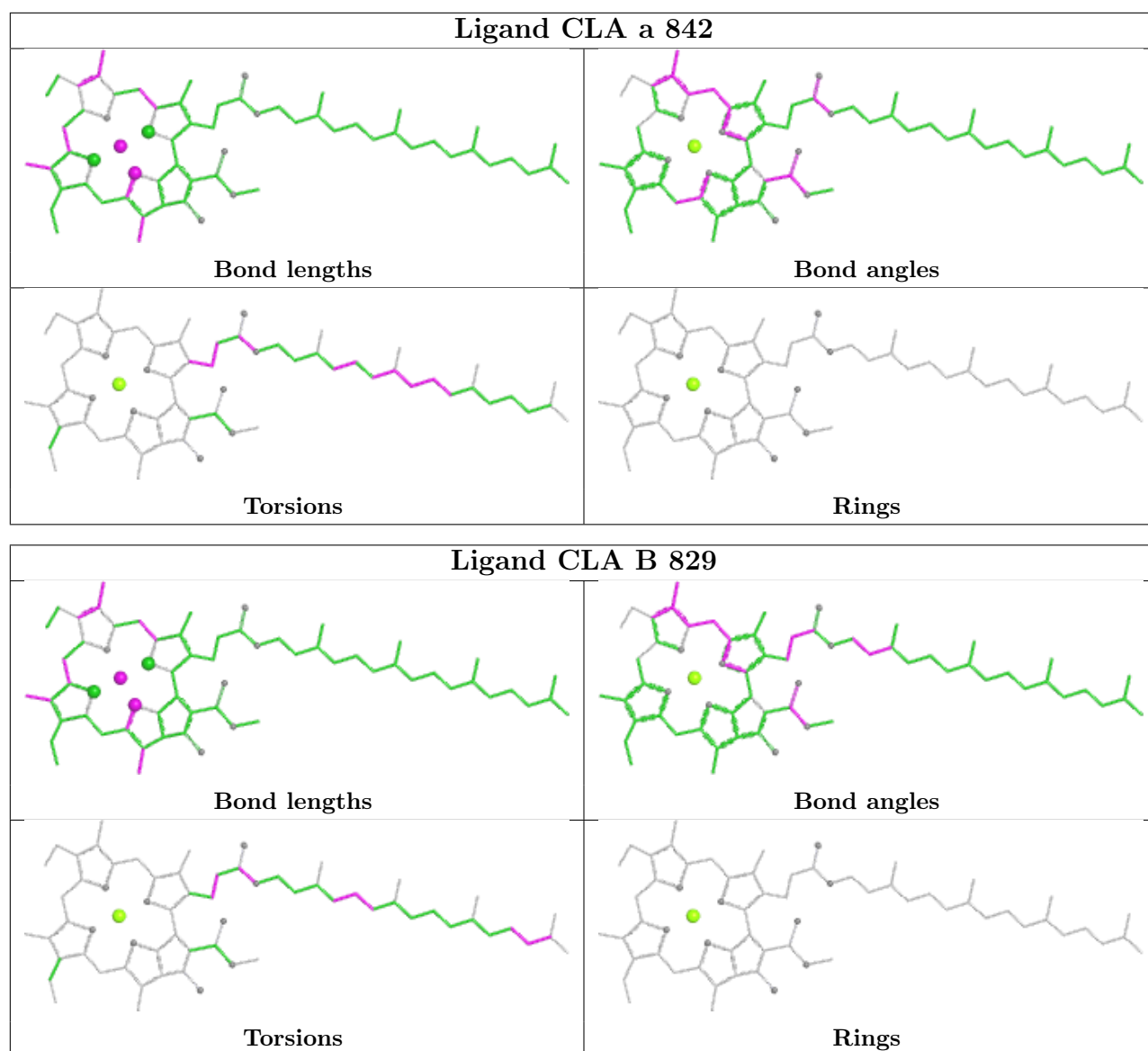


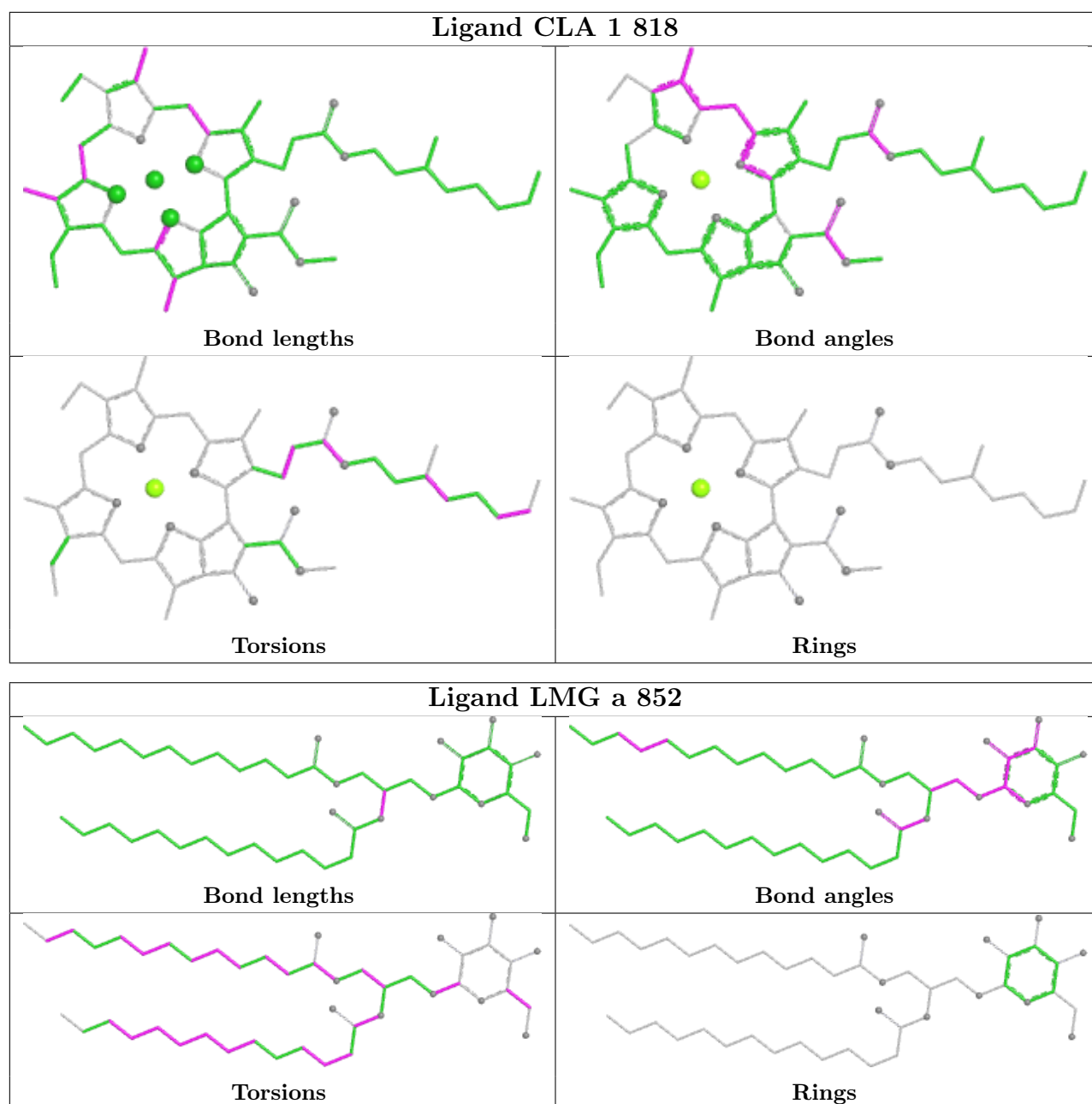
Ligand LHG a 802

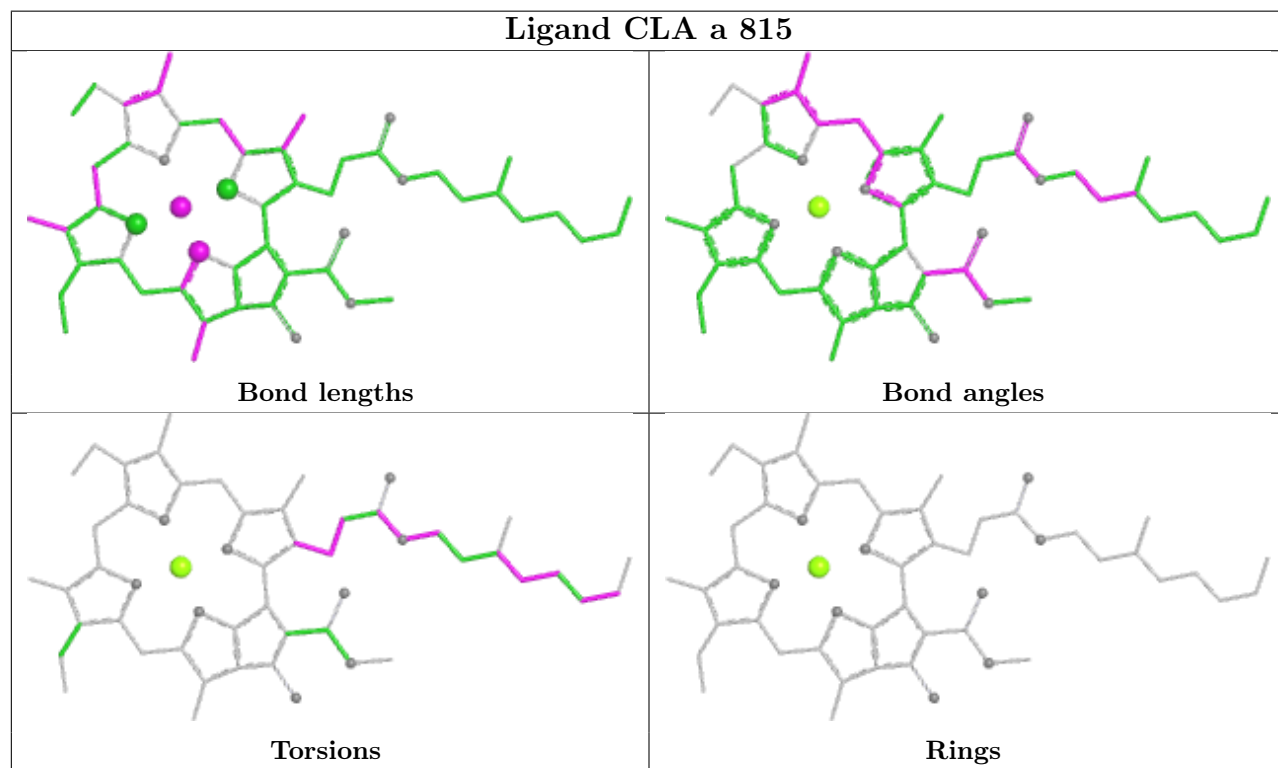
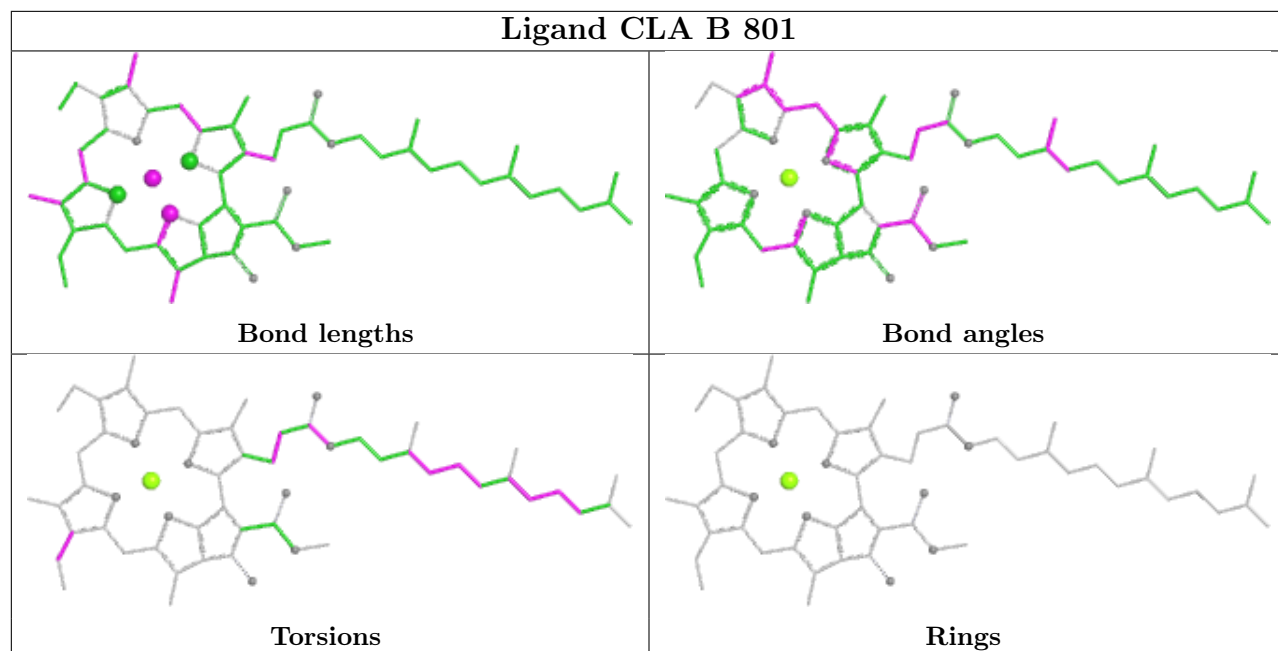


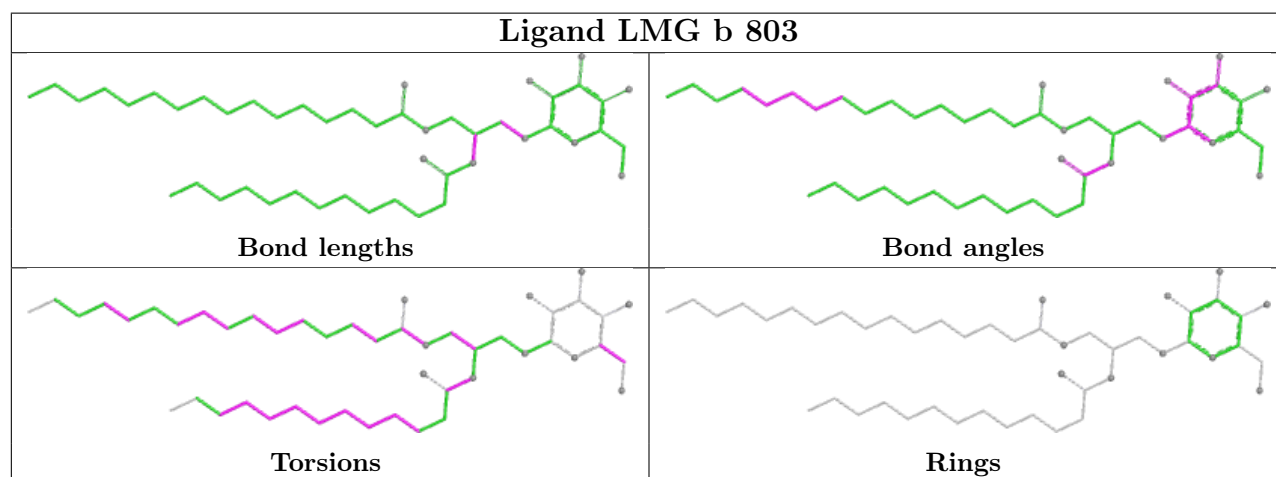
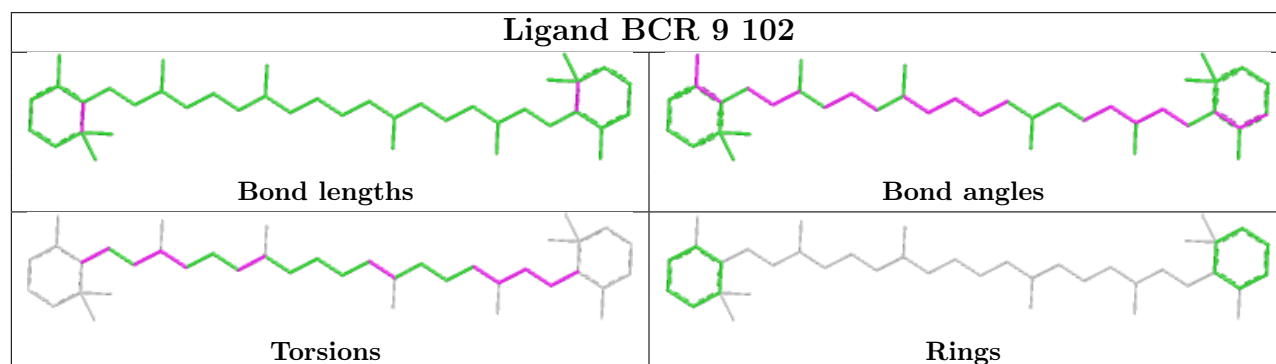
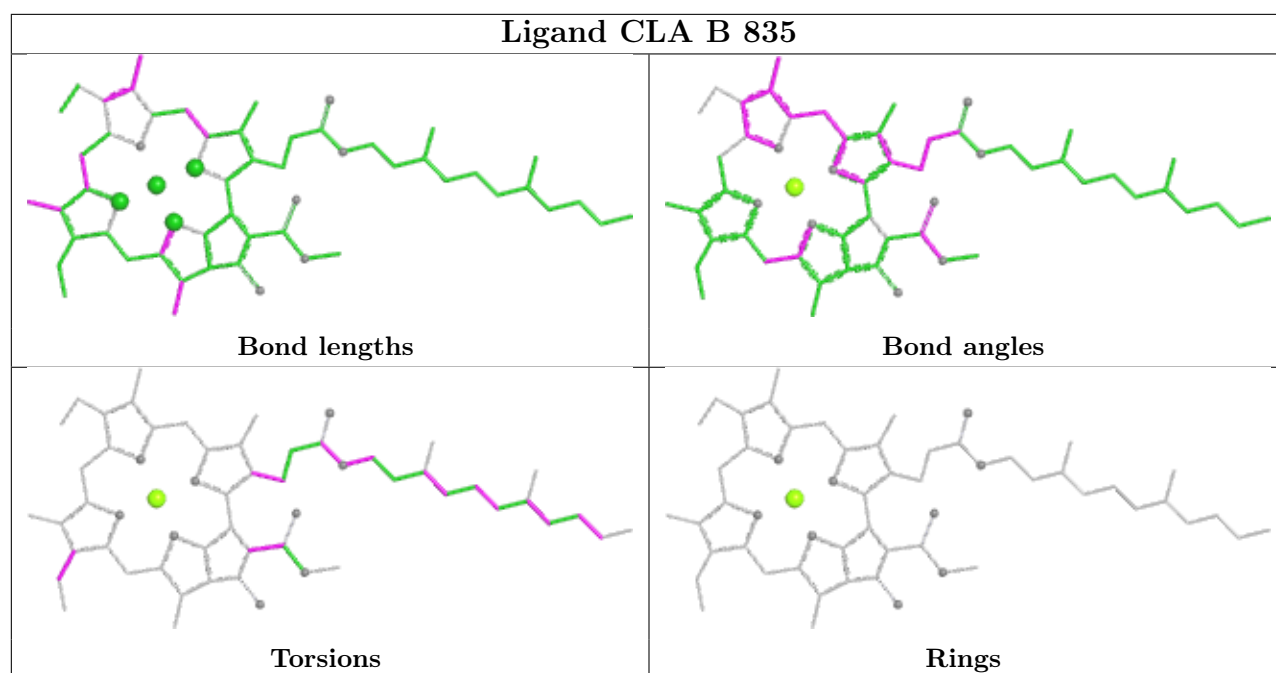
Ligand CLA 2 810

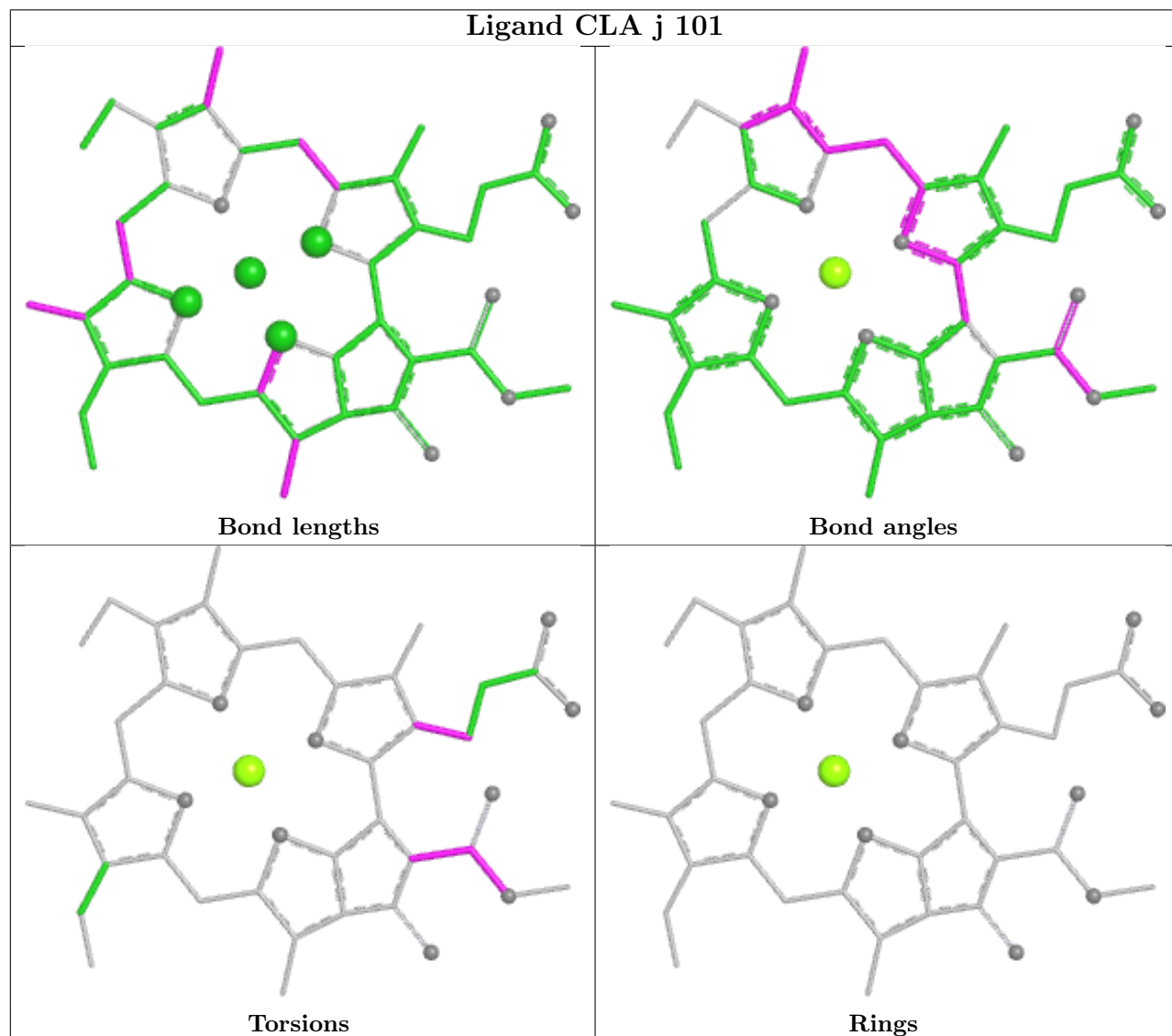
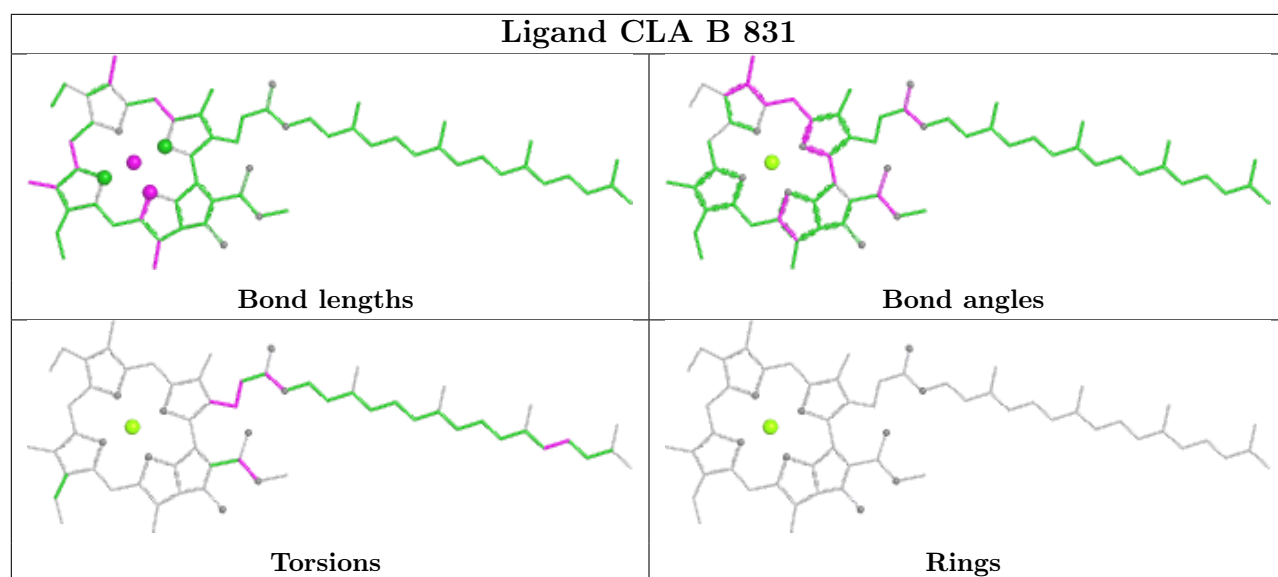




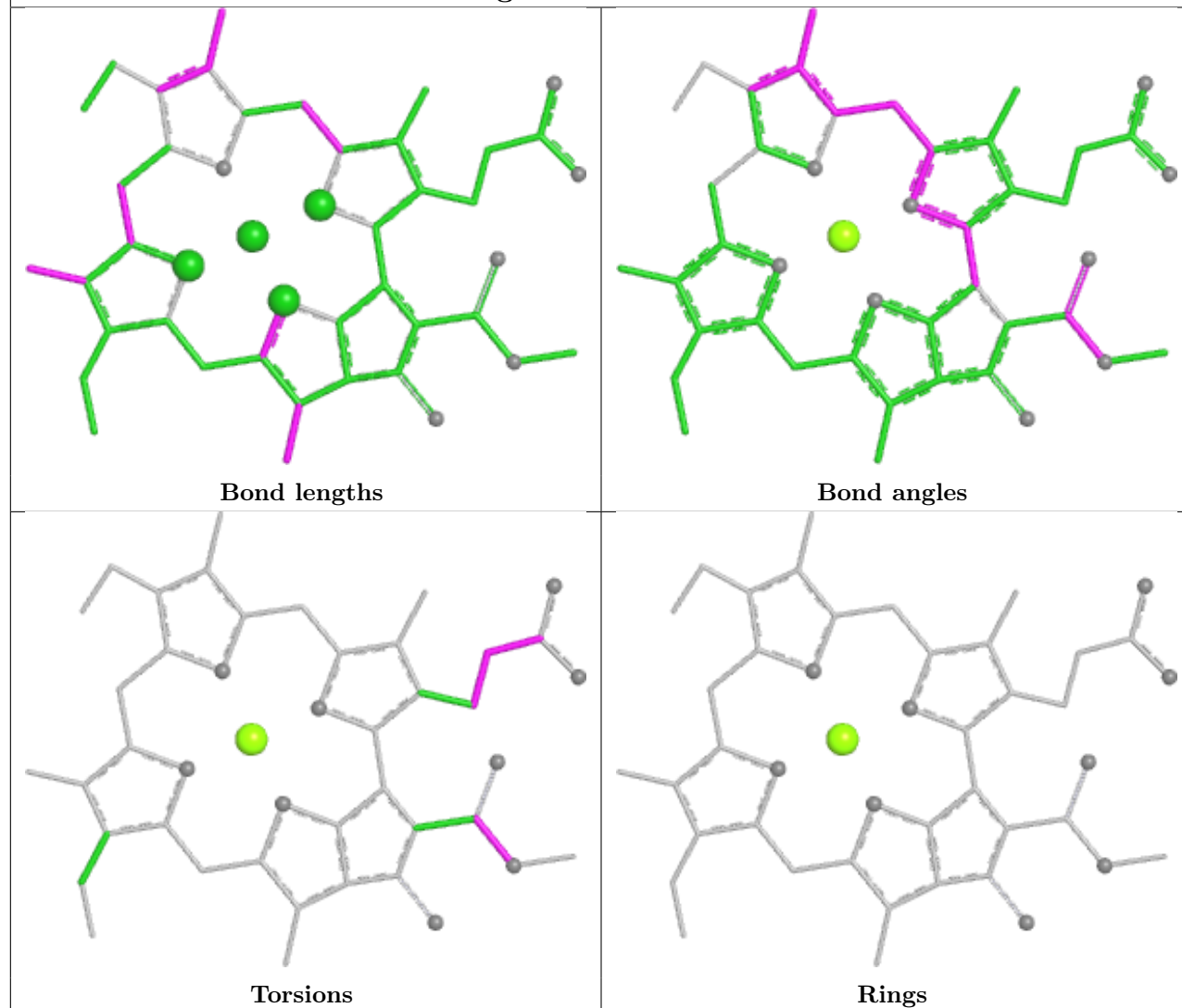




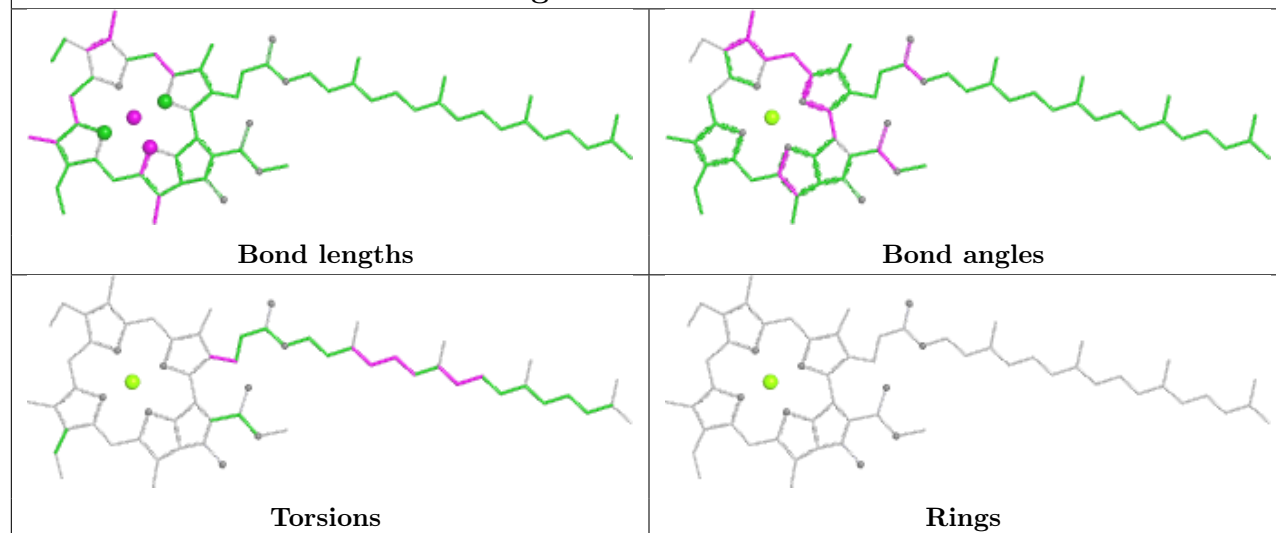


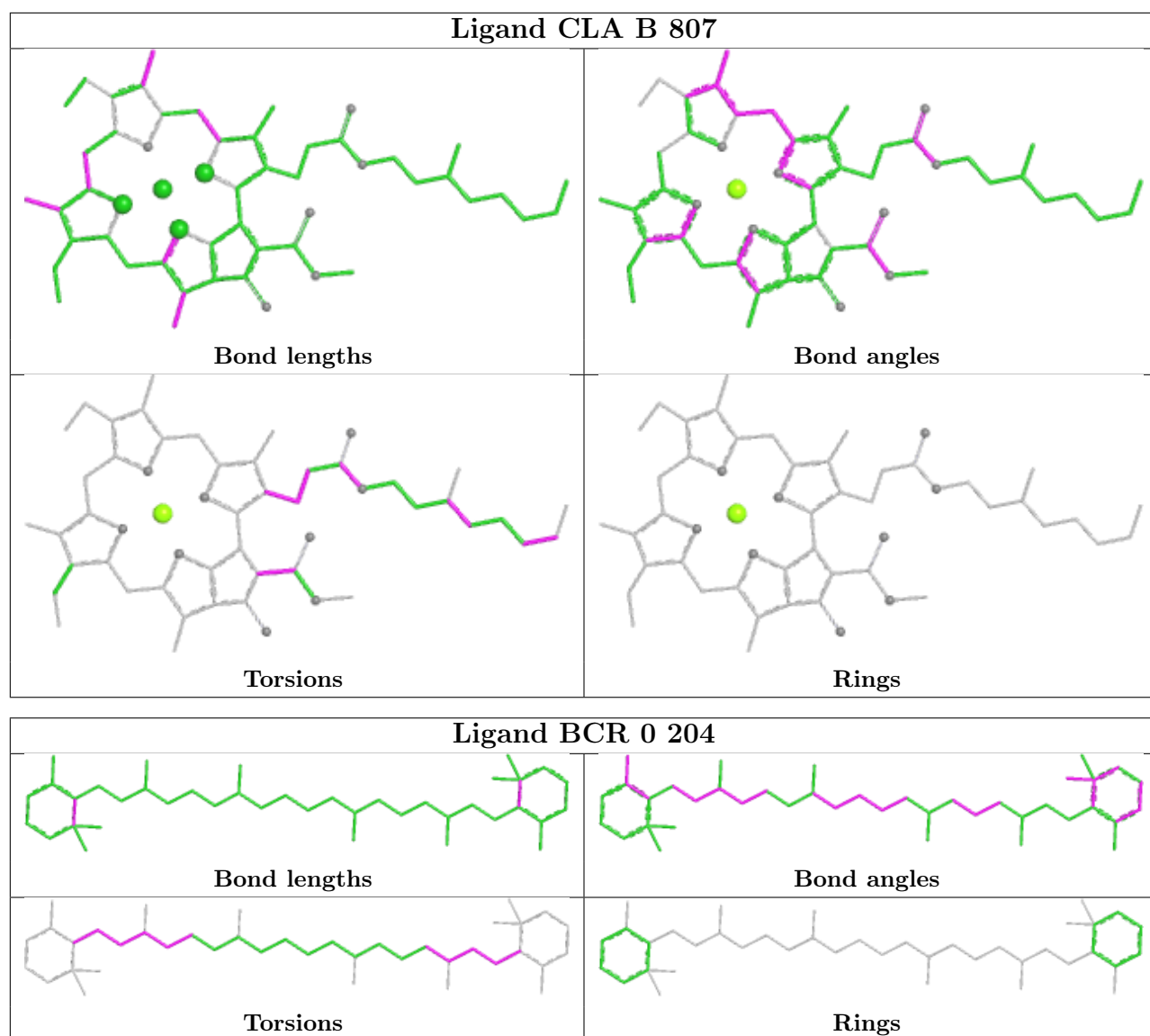


Ligand CLA a 838

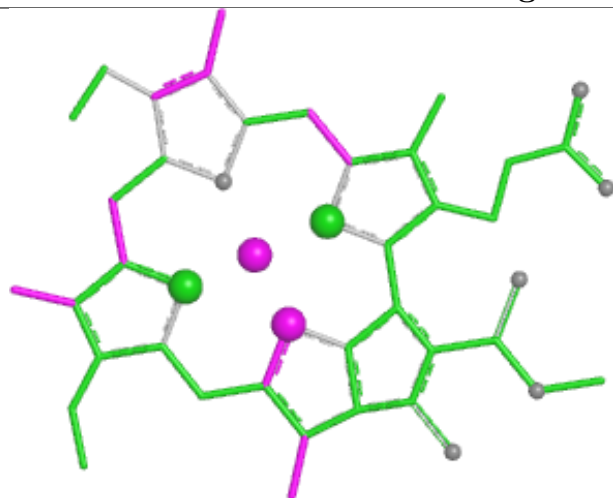


Ligand CLA l 4203

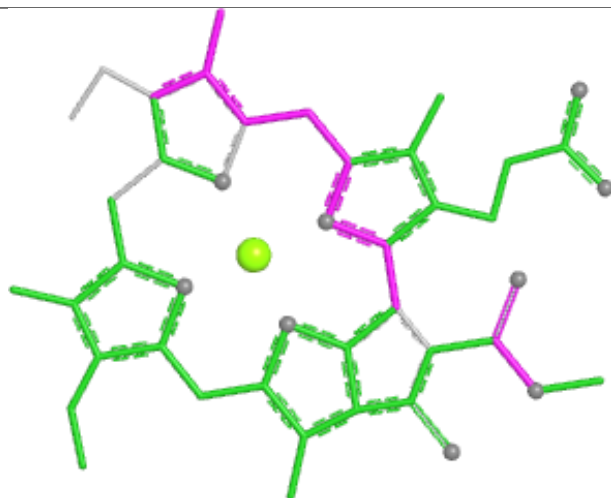




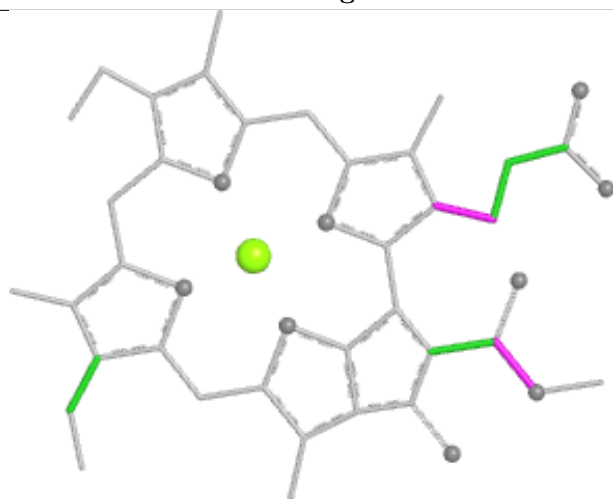
Ligand CLA 2 813



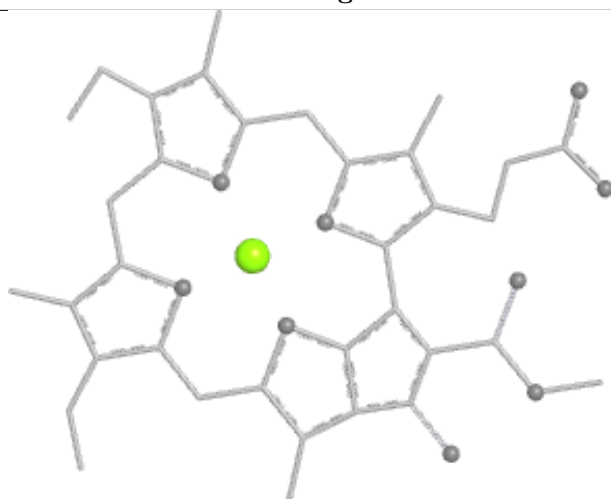
Bond lengths



Bond angles

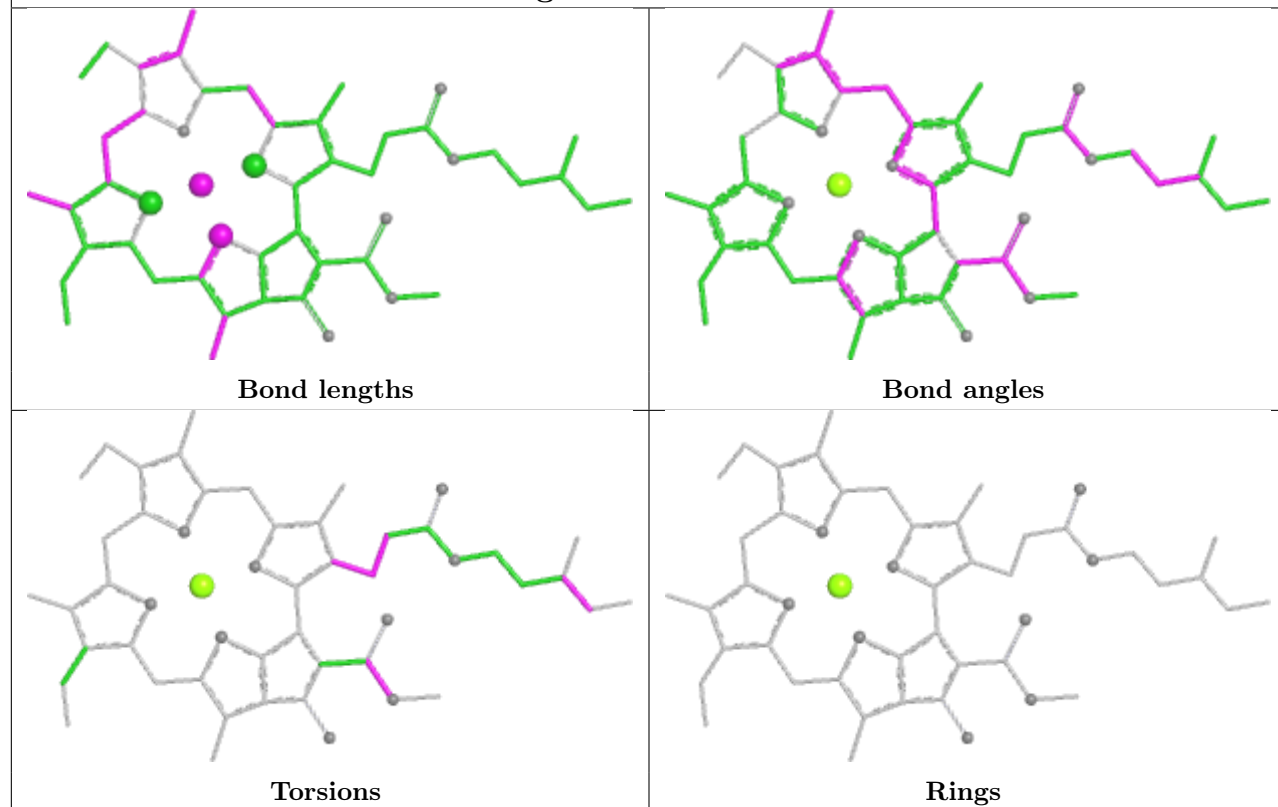


Torsions

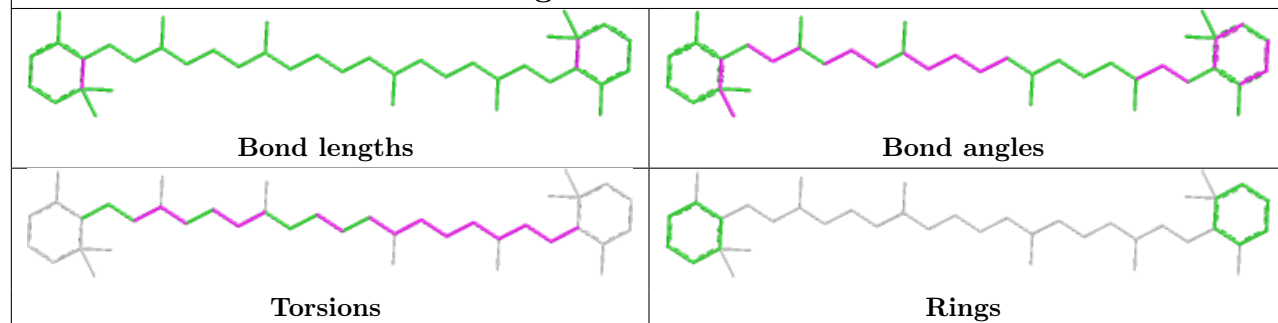


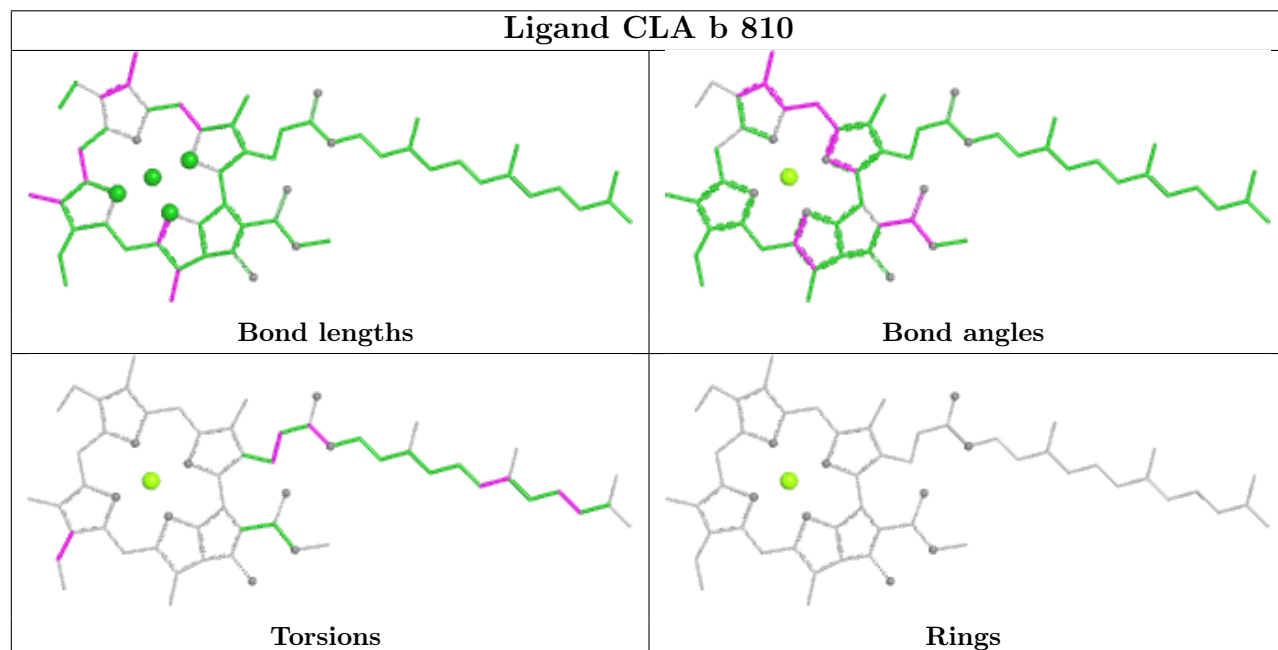
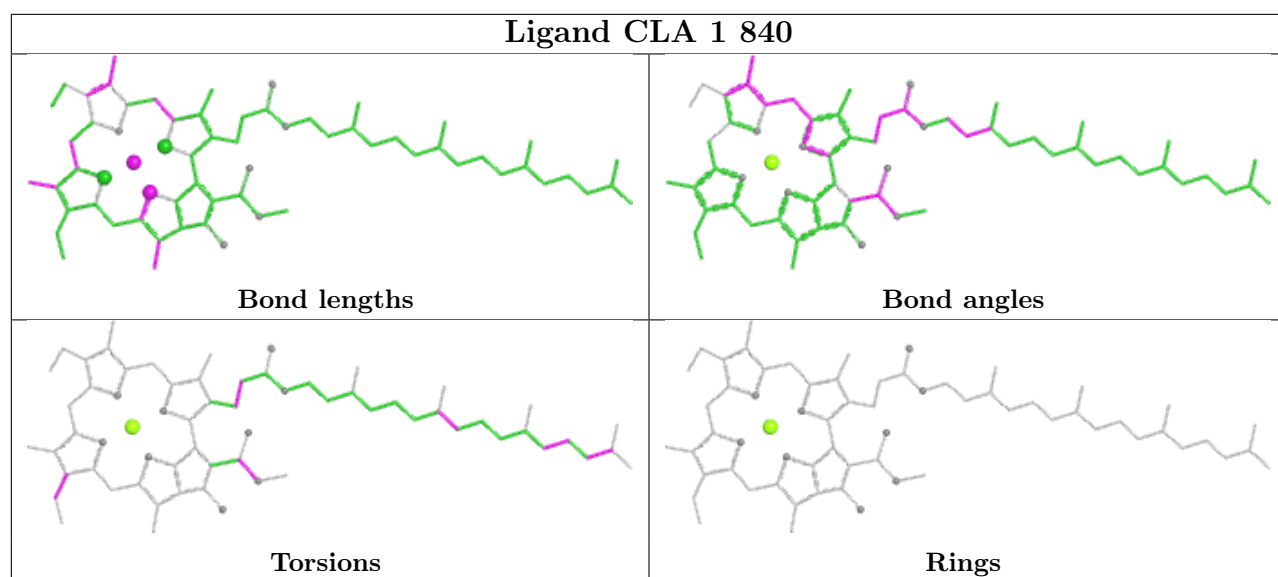
Rings

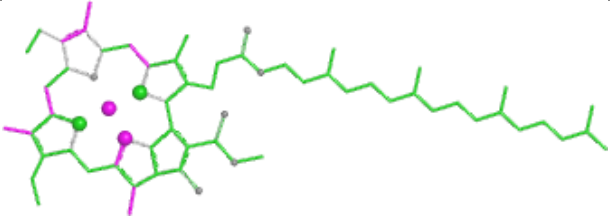
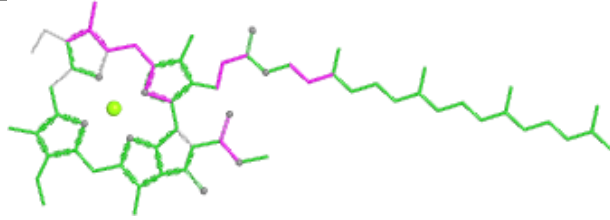
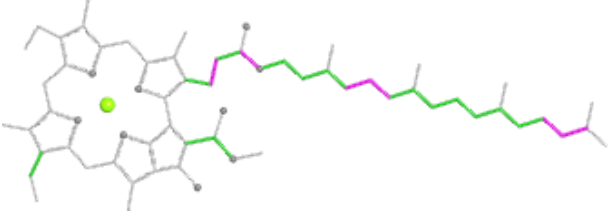
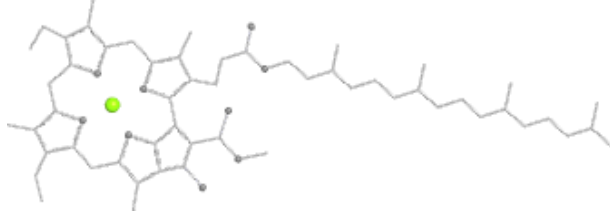
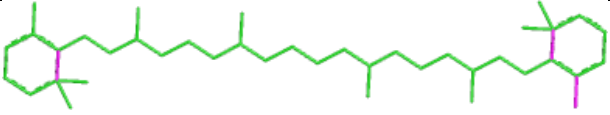
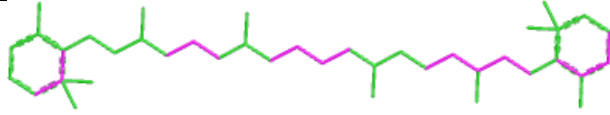
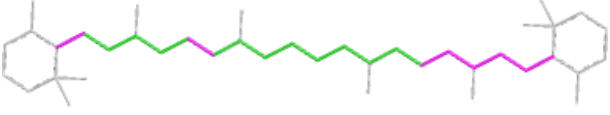
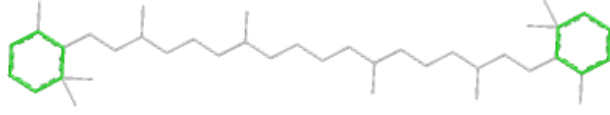
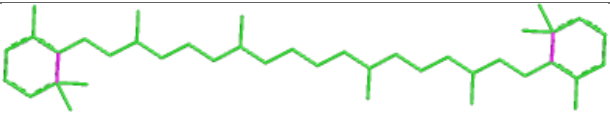
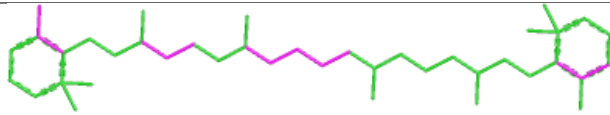
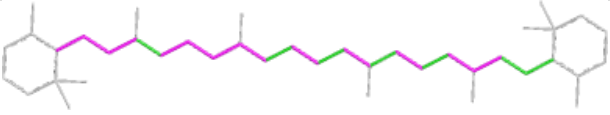
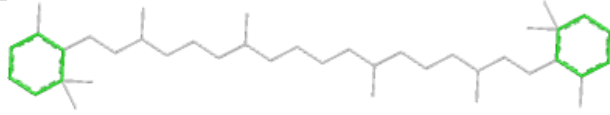
Ligand CLA 1 837

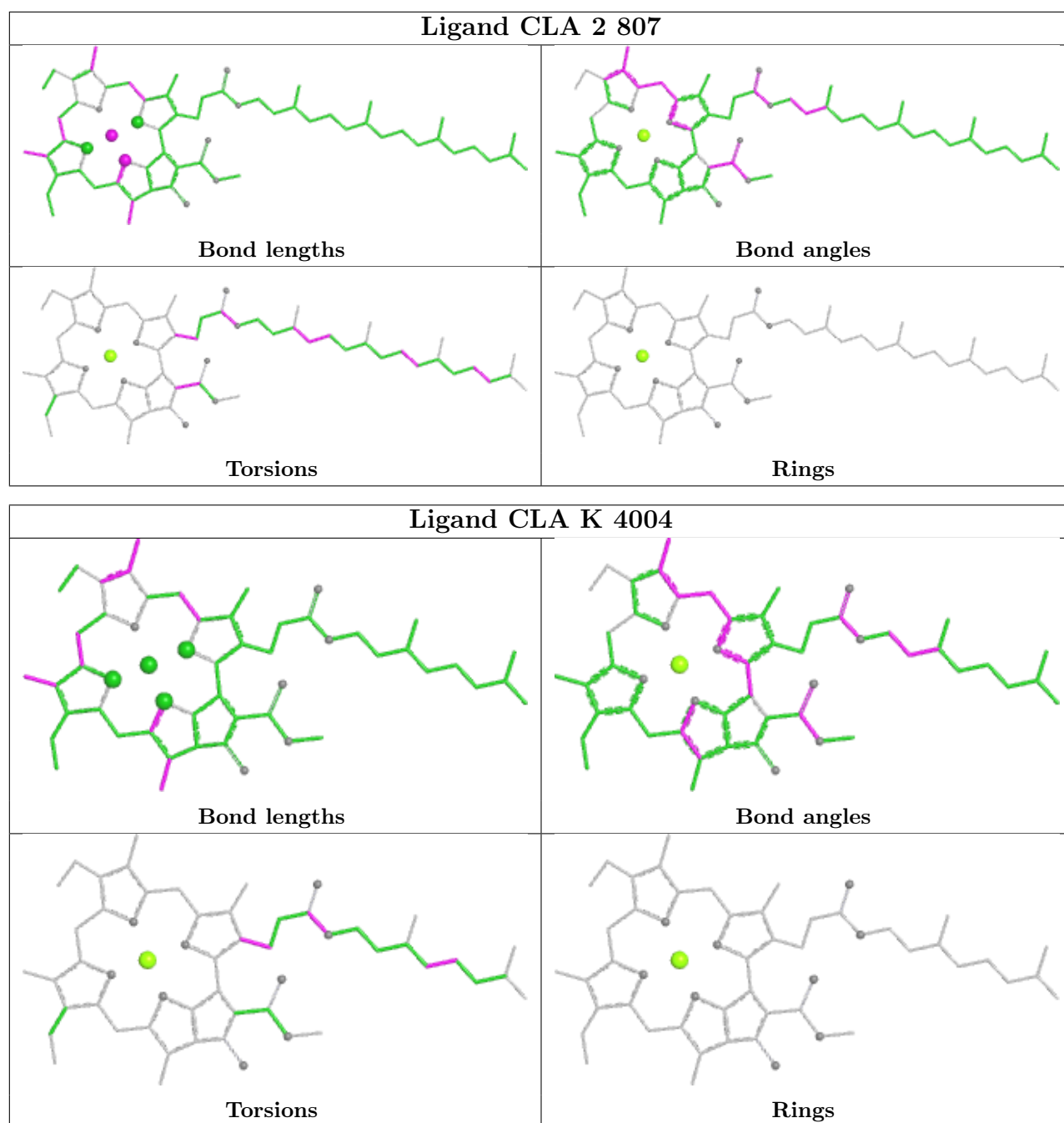


Ligand BCR a 851





Ligand CLA b 828	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B 852	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR I 101	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



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.

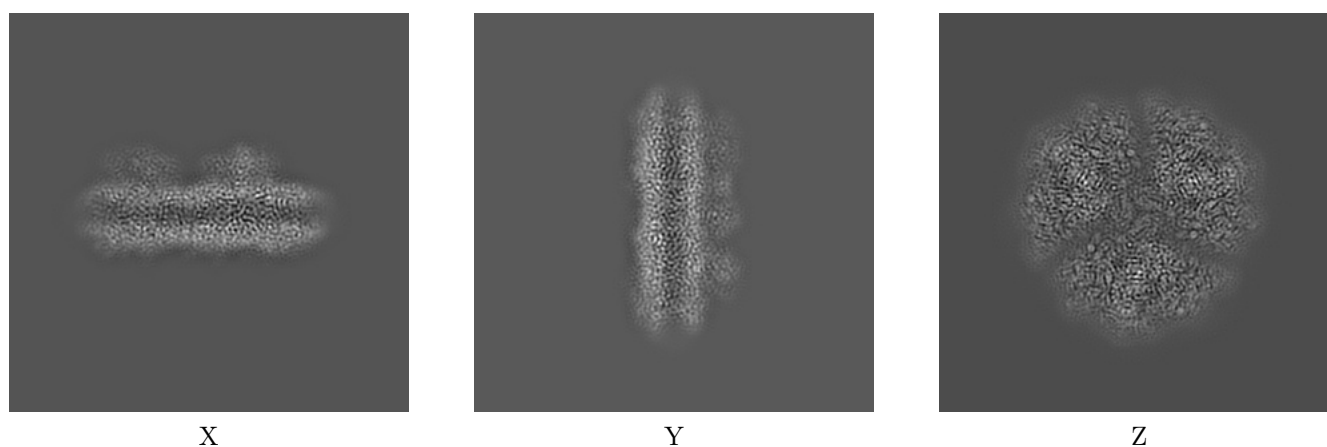
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20963. 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](#)

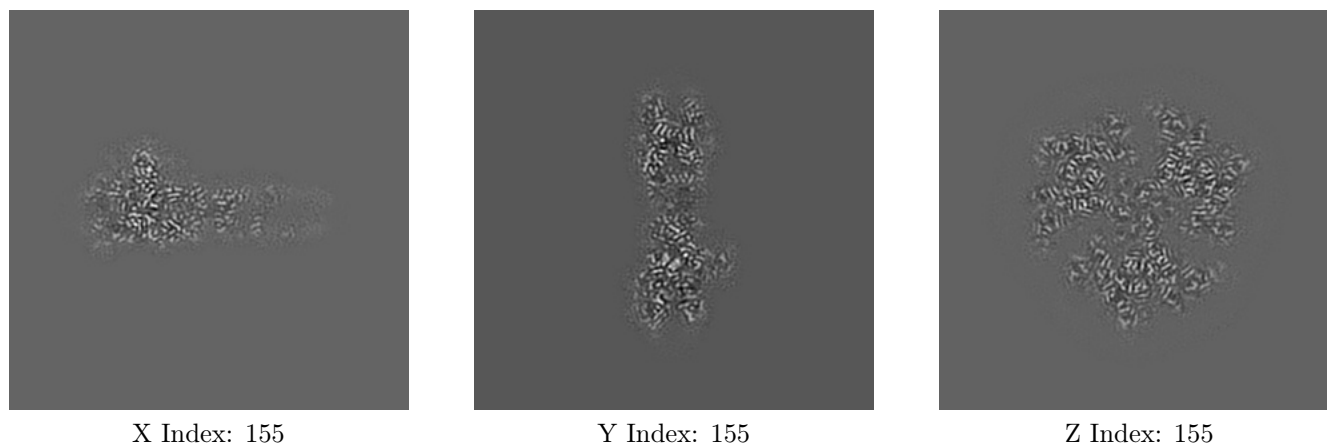
6.1.1 Primary map



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

6.2 Central slices [i](#)

6.2.1 Primary map



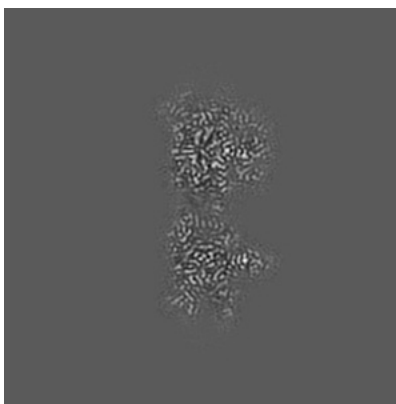
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

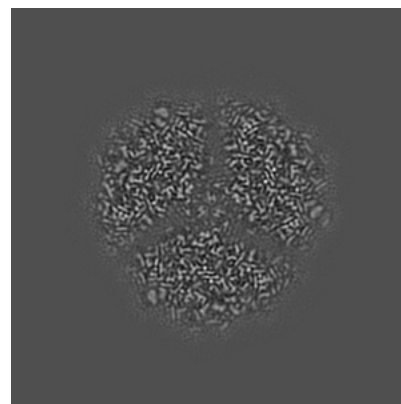
6.3.1 Primary map



X Index: 113



Y Index: 179

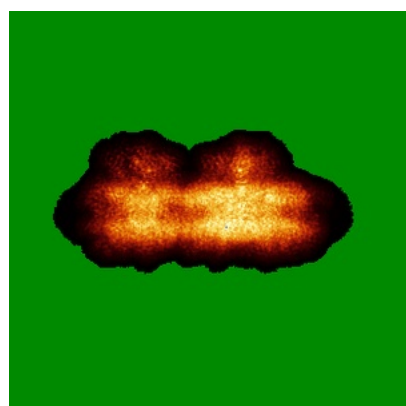


Z Index: 143

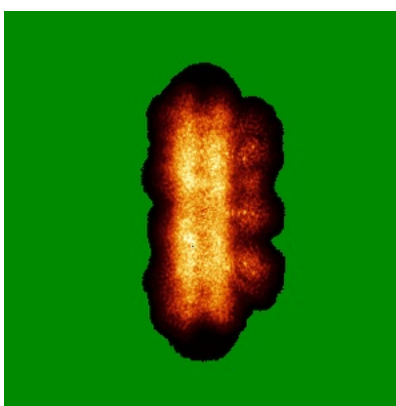
The images above show the largest variance slices of the map in three orthogonal directions.

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

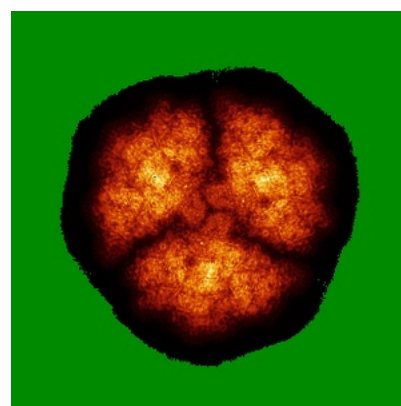
6.4.1 Primary map



X



Y

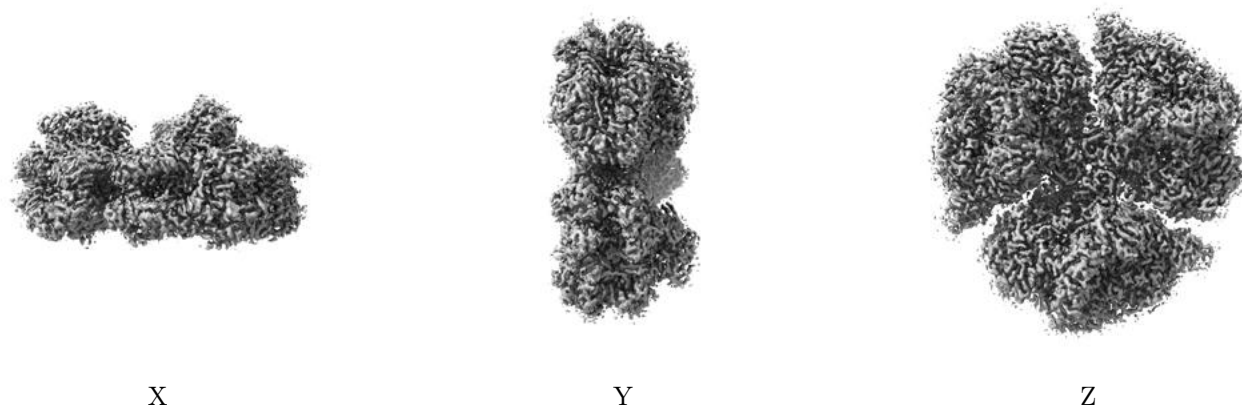


Z

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 0.0187. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

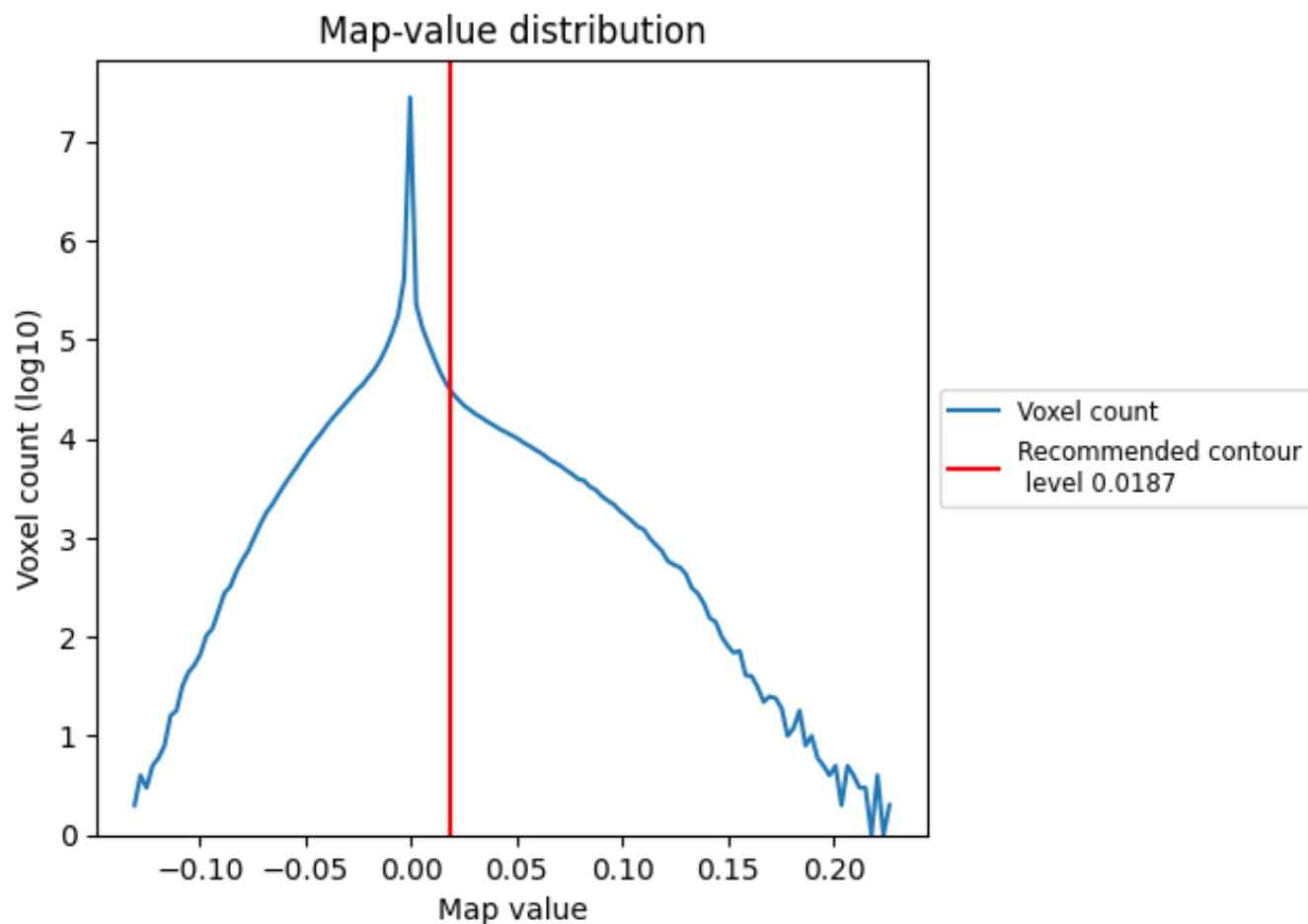
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

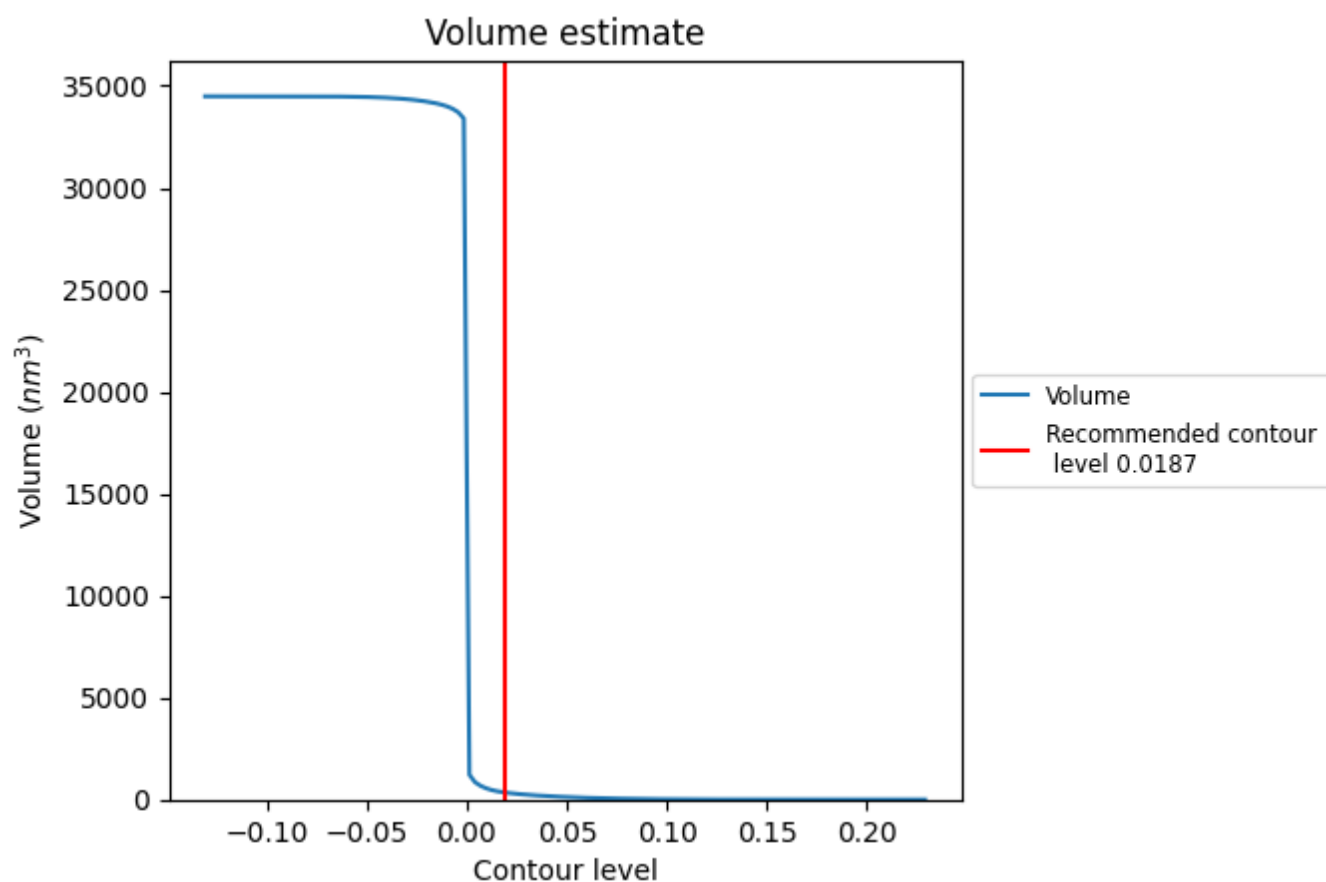
This section contains the results of statistical analysis of the map.

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.

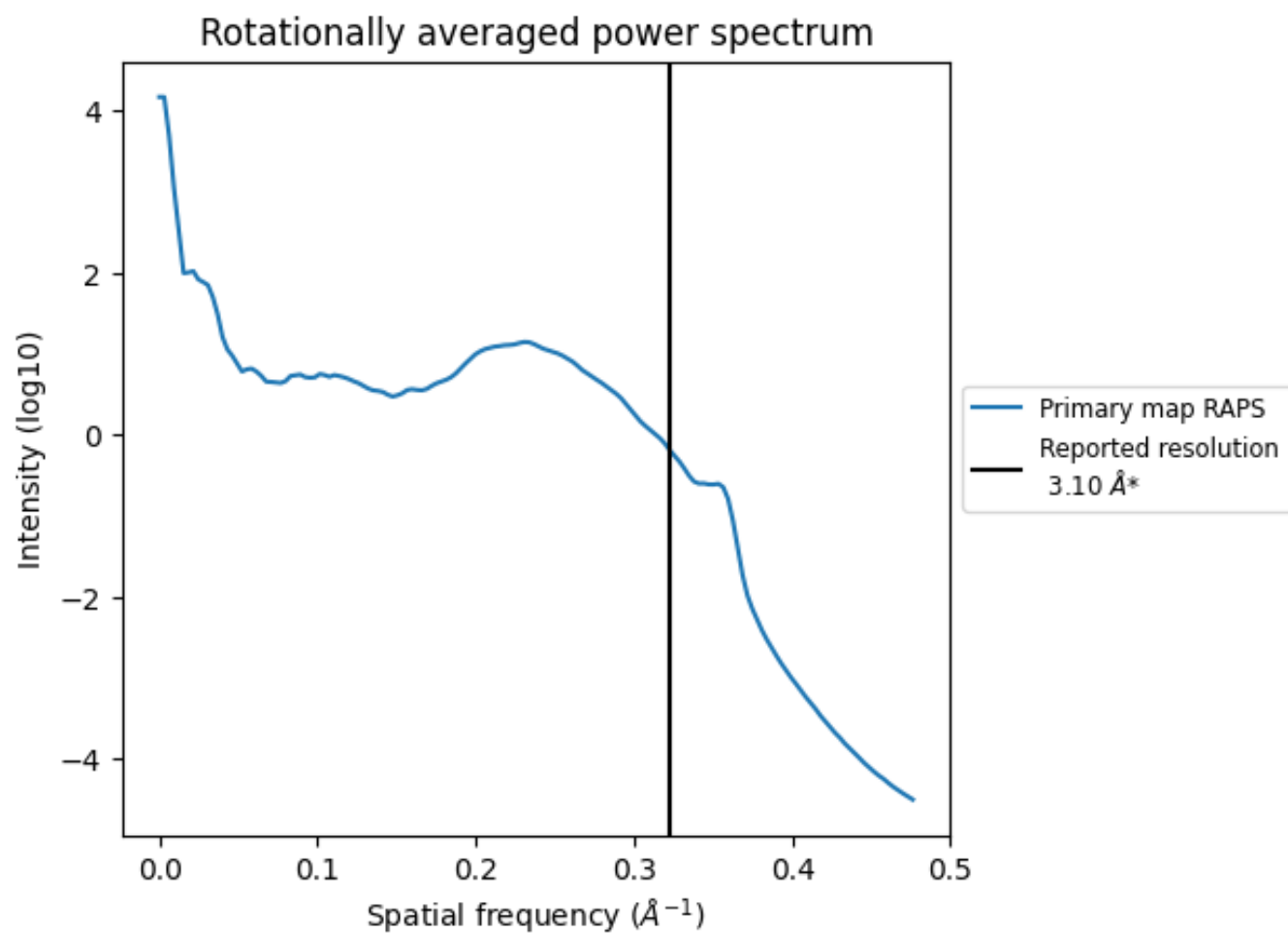
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 351 nm³; this corresponds to an approximate mass of 317 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 0.323 Å⁻¹

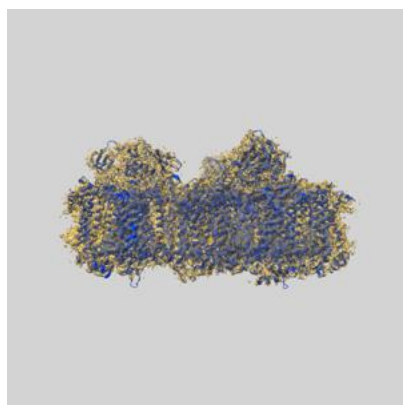
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

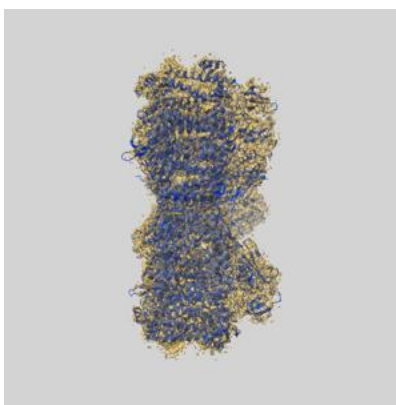
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-20963 and PDB model 6UZV. Per-residue inclusion information can be found in section [3](#) on page [38](#).

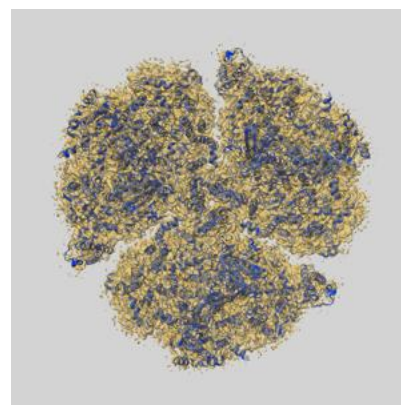
9.1 Map-model overlay [i](#)



X



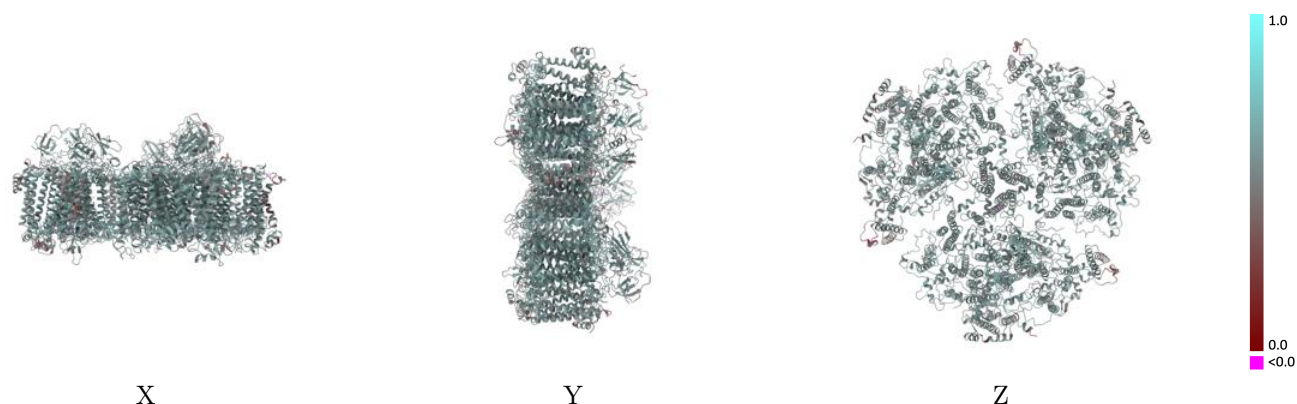
Y



Z

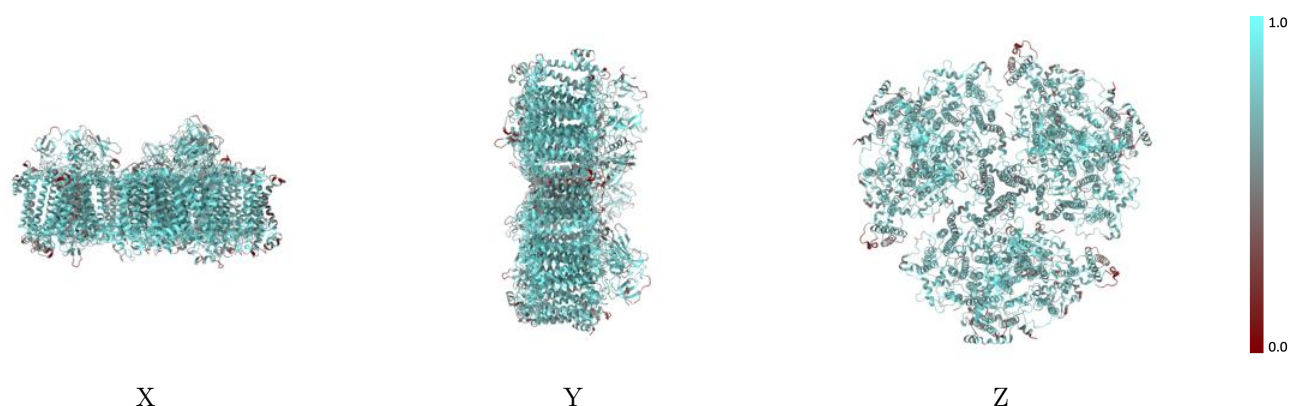
The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



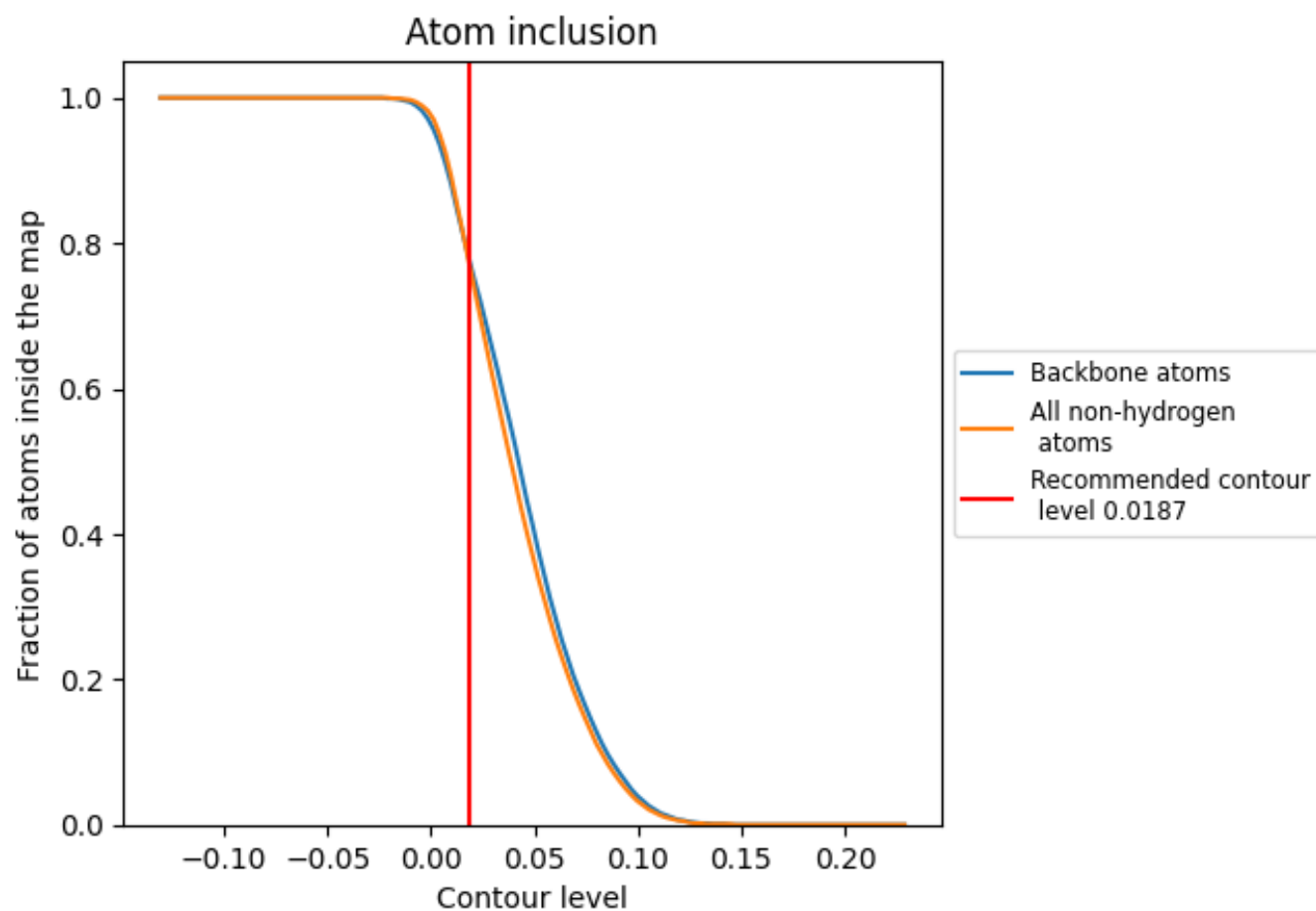
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0187).





































































9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 77% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.0187) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7690	 0.5660
0	 0.7080	 0.5640
1	 0.8110	 0.5790
2	 0.8170	 0.5800
3	 0.8340	 0.5710
4	 0.6650	 0.5280
5	 0.6550	 0.5010
6	 0.6370	 0.5200
7	 0.6540	 0.5280
8	 0.5150	 0.4620
9	 0.6180	 0.5450
A	 0.8030	 0.5800
B	 0.8120	 0.5820
C	 0.8340	 0.5710
D	 0.6460	 0.5280
E	 0.6380	 0.5110
F	 0.6510	 0.5260
I	 0.7450	 0.5690
J	 0.6320	 0.5210
K	 0.5010	 0.4640
L	 0.7020	 0.5600
M	 0.6240	 0.5470
a	 0.8060	 0.5790
b	 0.8200	 0.5820
c	 0.8340	 0.5710
d	 0.6520	 0.5240
e	 0.6420	 0.5020
f	 0.6420	 0.5220
h	 0.7480	 0.5690
i	 0.7450	 0.5670
j	 0.6450	 0.5260
k	 0.4900	 0.4500
l	 0.7160	 0.5640
m	 0.6170	 0.5450

