



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 12:13 AM UTC

PDB ID : 6UZV / pdb_00006uzv
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 : 5OY0, 6KIG

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

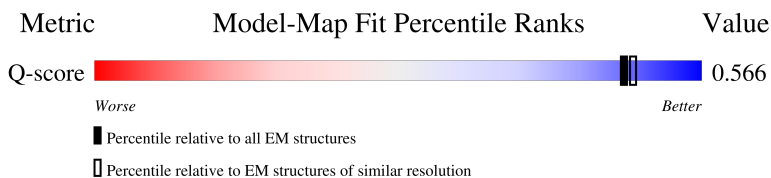
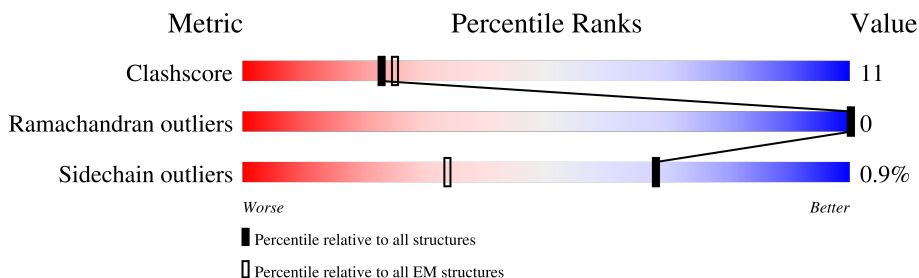
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

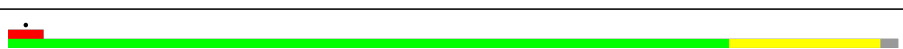
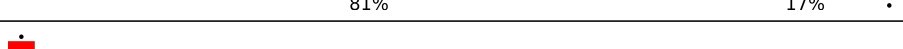
The reported resolution of this entry is 3.10 Å.

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.



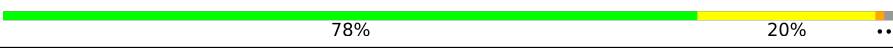
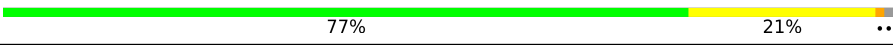
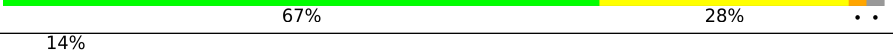
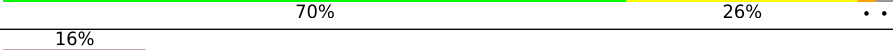
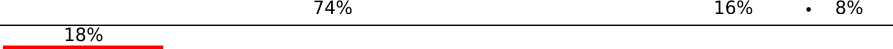
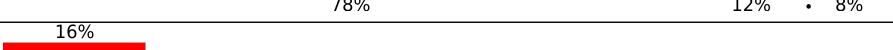
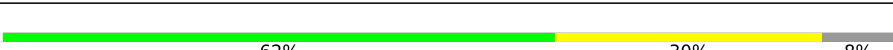
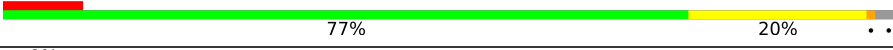
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	
1	A	751	
1	a	751	
2	2	735	

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Mol	Chain	Length	Quality of chain
2	B	735	
2	b	735	
3	3	81	
3	C	81	
3	c	81	
4	4	141	
4	D	141	
4	d	141	
5	5	74	
5	E	74	
5	e	74	
6	6	165	
6	F	165	
6	f	165	
7	I	40	
7	h	40	
7	i	40	
8	7	40	
8	J	40	
8	j	40	
9	0	157	
9	L	157	
9	l	157	
10	9	31	
10	M	31	

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Mol	Chain	Length	Quality of chain
10	m	31	
11	8	90	
11	K	90	
11	k	90	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	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	-	-	-

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	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		

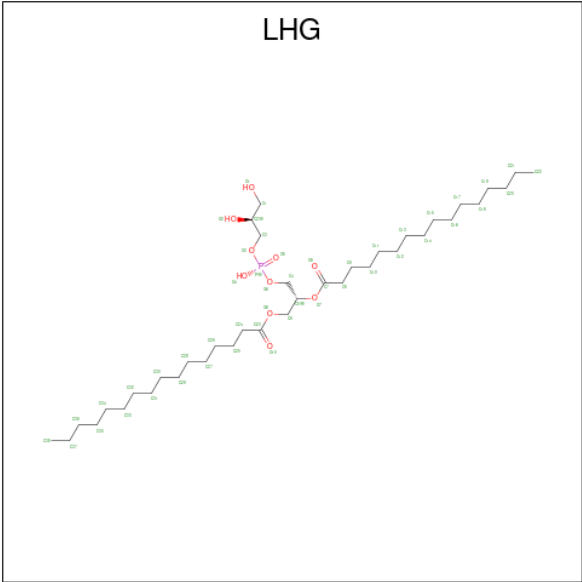
- Molecule 10 is a protein called Photosystem I reaction center subunit XII.

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.

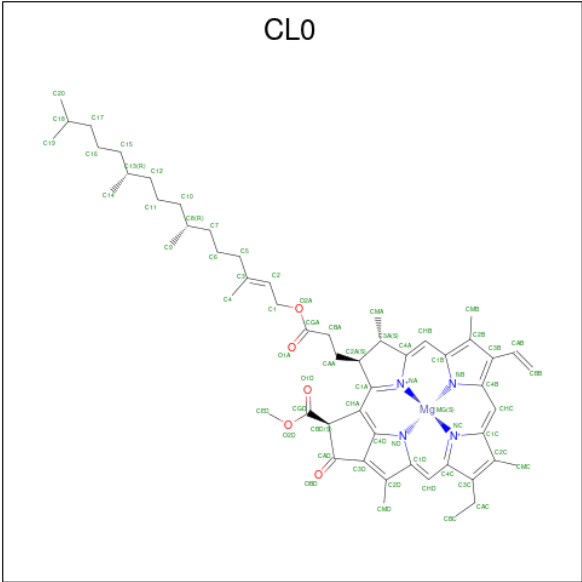
Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	k	79	Total	C	N	O	S	0	0
			566	373	90	98	5		
11	8	79	Total	C	N	O	S	0	0
			566	373	90	98	5		

- Molecule 12 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



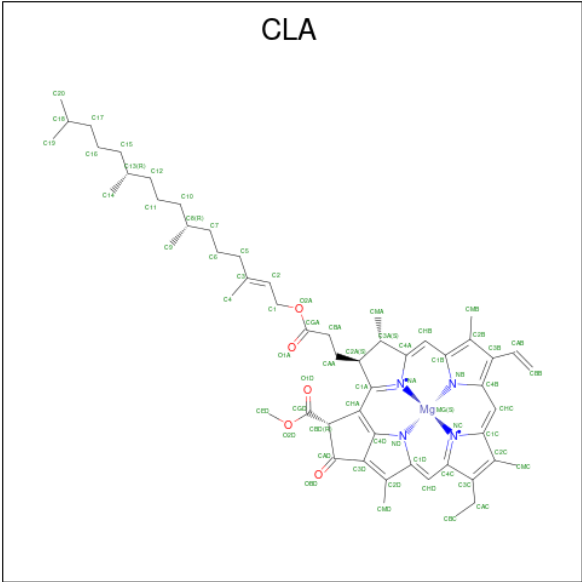
Mol	Chain	Residues	Atoms				AltConf
12	A	1	Total	C	O	P	0
			49	38	10	1	
12	A	1	Total	C	O	P	0
			33	22	10	1	
12	B	1	Total	C	O	P	0
			39	28	10	1	
12	M	1	Total	C	O	P	0
			39	28	10	1	
12	a	1	Total	C	O	P	0
			49	38	10	1	
12	a	1	Total	C	O	P	0
			33	22	10	1	
12	1	1	Total	C	O	P	0
			49	38	10	1	
12	1	1	Total	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 (CCD ID: 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 (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (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	C	Mg	N	O	0
			51	41	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	J	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
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	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	K	1	Total	C	Mg	N	O	0
			55	45	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
			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
			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	

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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
			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 54	C 44	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 51	C 41	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 47	C 37	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 51	C 41	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 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 65	C 55	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 65	C 55	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 54	C 44	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 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 61	C 51	Mg 1	N 4	O 5	0

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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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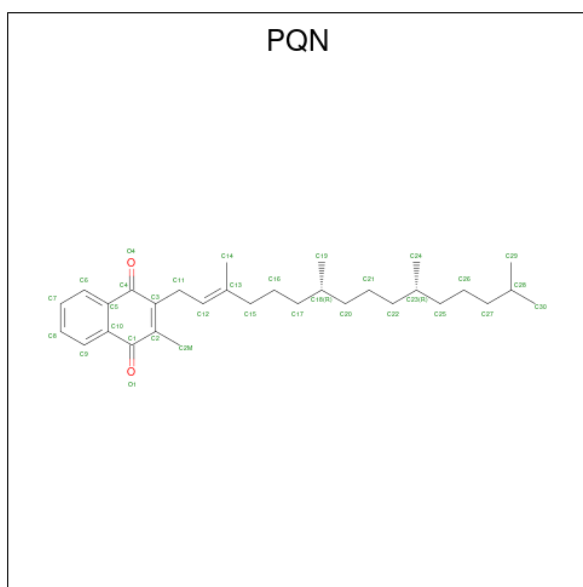
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	2	1	Total 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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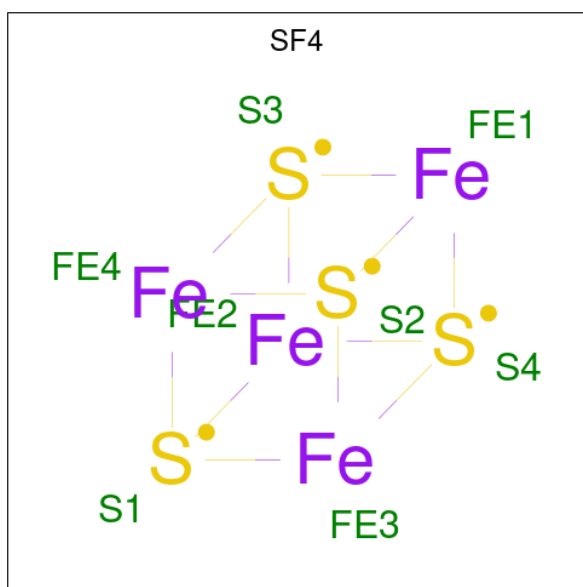
Mol	Chain	Residues	Atoms					AltConf
14	7	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	k	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
14	8	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
14	l	1	Total	C	Mg	N	O	0
			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 (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



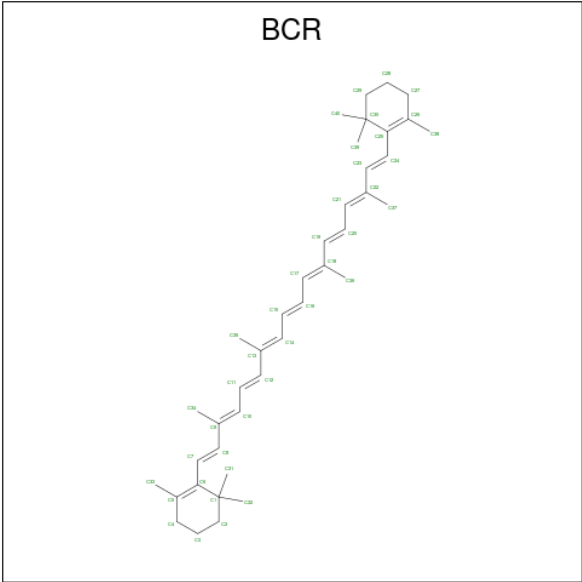
Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	C	O	0
			33	31	2	
15	B	1	Total	C	O	0
			33	31	2	
15	a	1	Total	C	O	0
			33	31	2	
15	1	1	Total	C	O	0
			33	31	2	
15	b	1	Total	C	O	0
			33	31	2	
15	2	1	Total	C	O	0
			33	31	2	

- Molecule 16 is IRON/SULFUR CLUSTER (CCD ID: 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 (CCD ID: BCR) (formula: C₄₀H₅₆).



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

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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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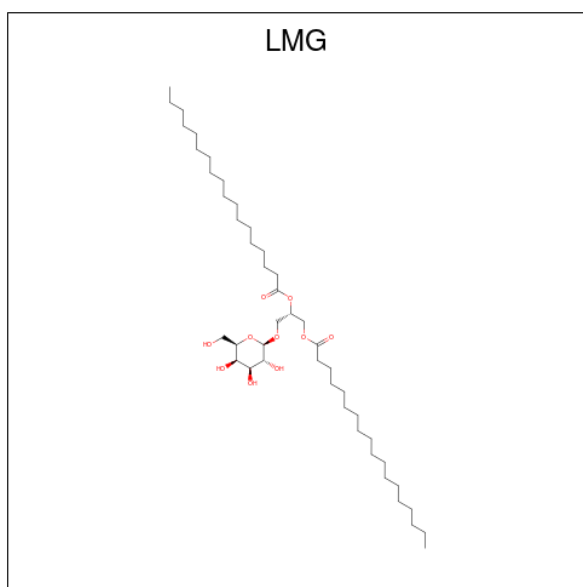
Mol	Chain	Residues	Atoms	AltConf
17	b	1	Total C 25 25	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	b	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 25 25	0
17	2	1	Total C 40 40	0
17	2	1	Total C 40 40	0
17	2	1	Total C 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	o	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	o	1	Total C 40 40	0
17	9	1	Total C 40 40	0

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



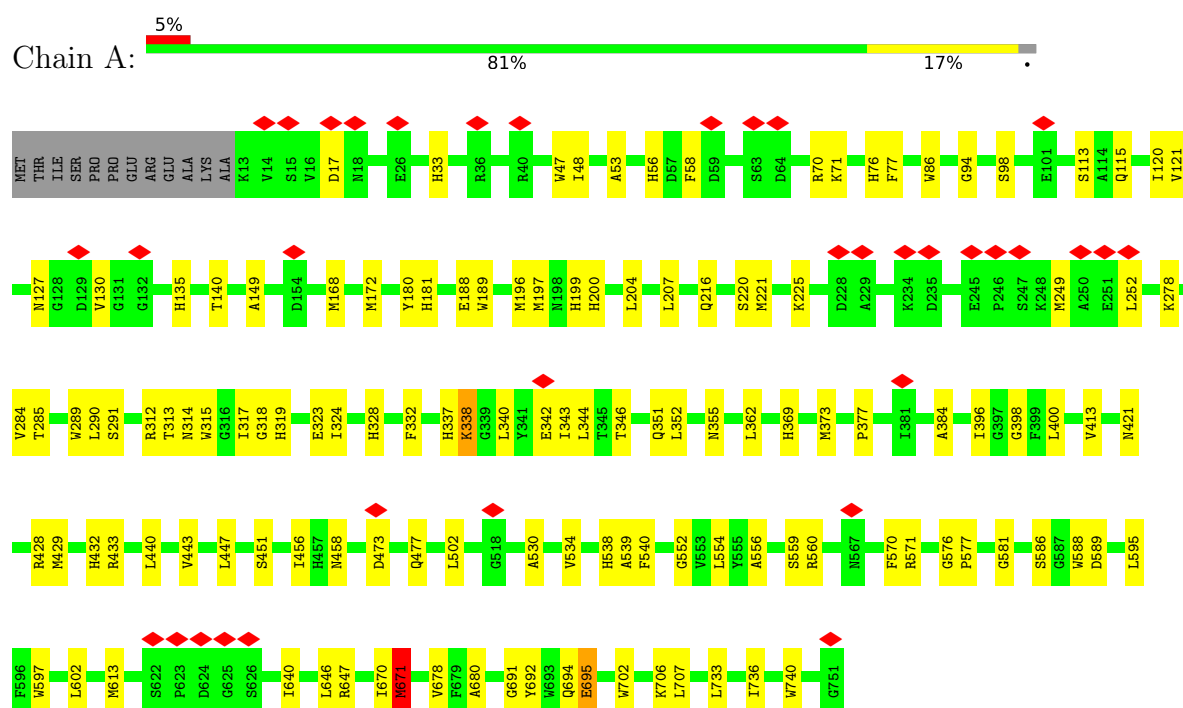
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			46	36	10	
18	A	1	Total	C	O	0
			32	22	10	
18	B	1	Total	C	O	0
			48	38	10	
18	L	1	Total	C	O	0
			38	28	10	
18	a	1	Total	C	O	0
			46	36	10	
18	a	1	Total	C	O	0
			32	22	10	
18	1	1	Total	C	O	0
			32	22	10	
18	b	1	Total	C	O	0
			48	38	10	
18	2	1	Total	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 (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).

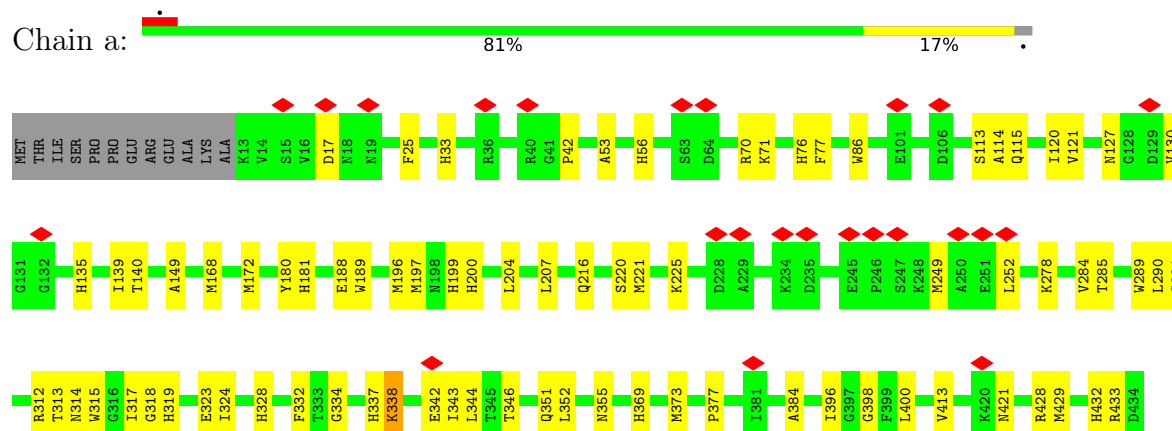
3 Residue-property plots

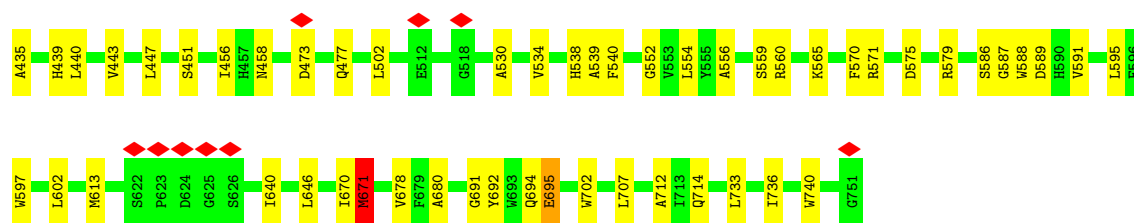
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



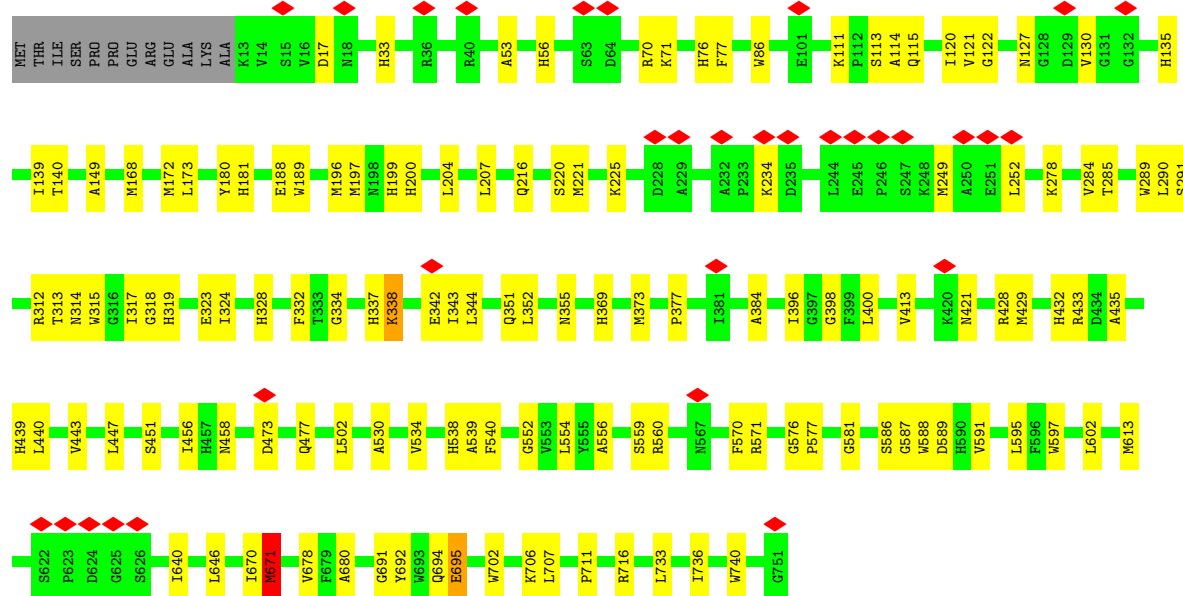
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





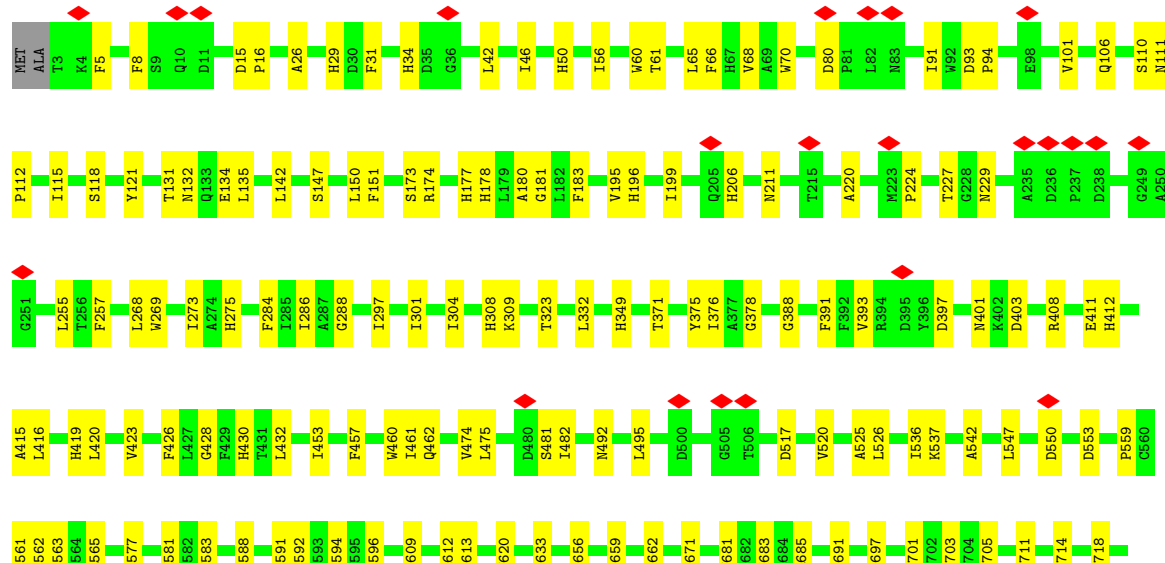
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain 1: 81% 17%



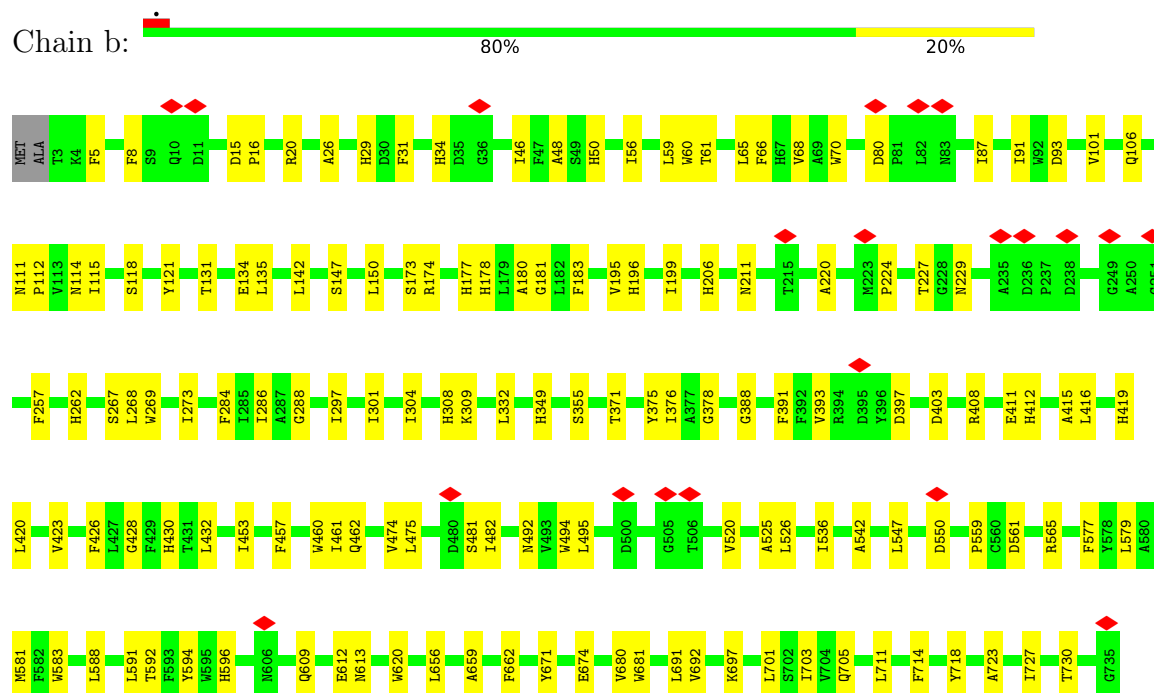
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 79% 20%

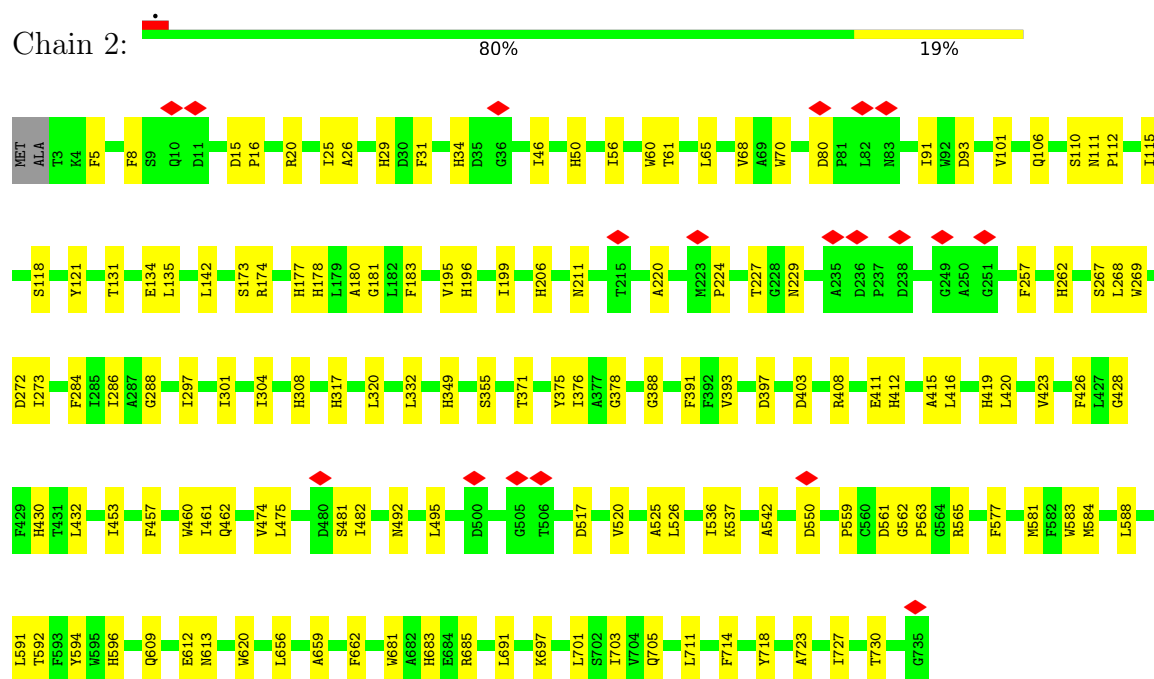




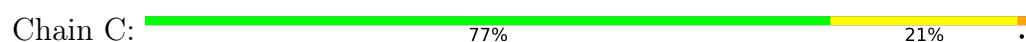
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

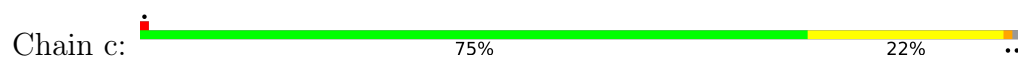


• Molecule 3: Photosystem I iron-sulfur center

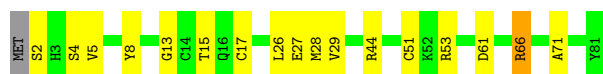
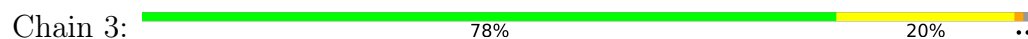




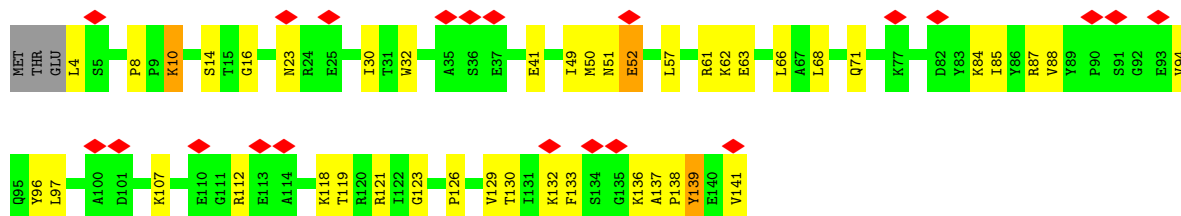
- Molecule 3: Photosystem I iron-sulfur center



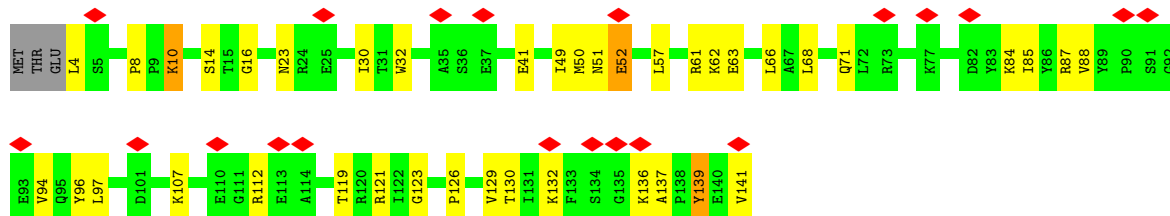
- Molecule 3: Photosystem I iron-sulfur center



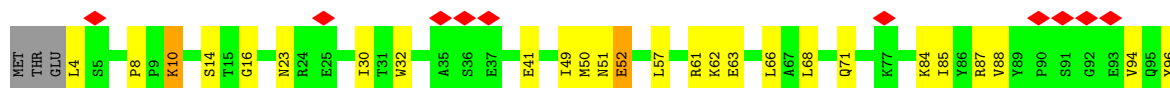
- Molecule 4: Photosystem I reaction center subunit II

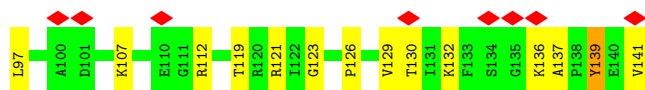


- Molecule 4: Photosystem I reaction center subunit II

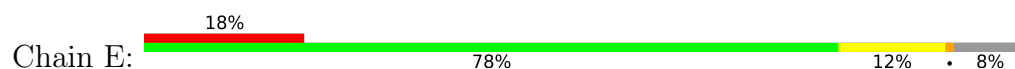


- Molecule 4: Photosystem I reaction center subunit II





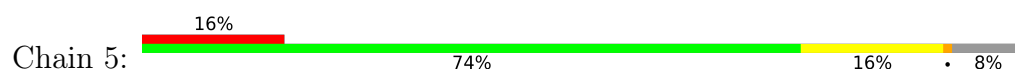
- Molecule 5: Photosystem I reaction center subunit IV



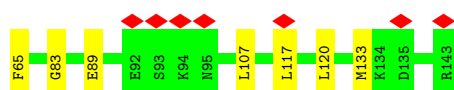
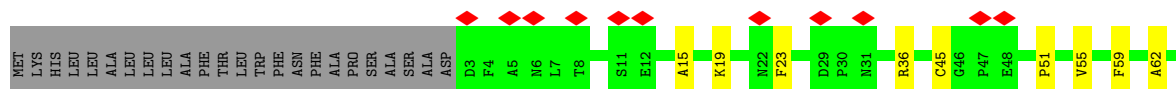
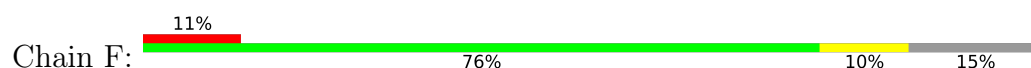
- Molecule 5: Photosystem I reaction center subunit IV



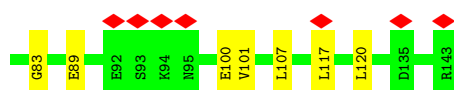
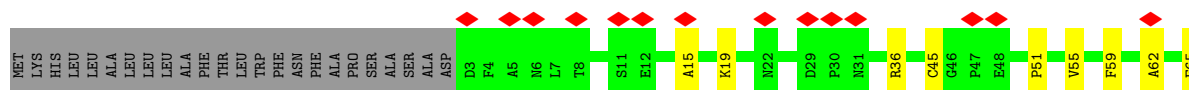
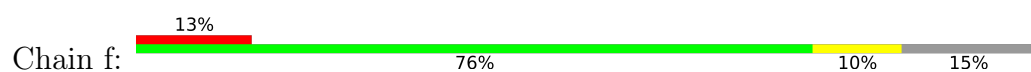
- Molecule 5: Photosystem I reaction center subunit IV



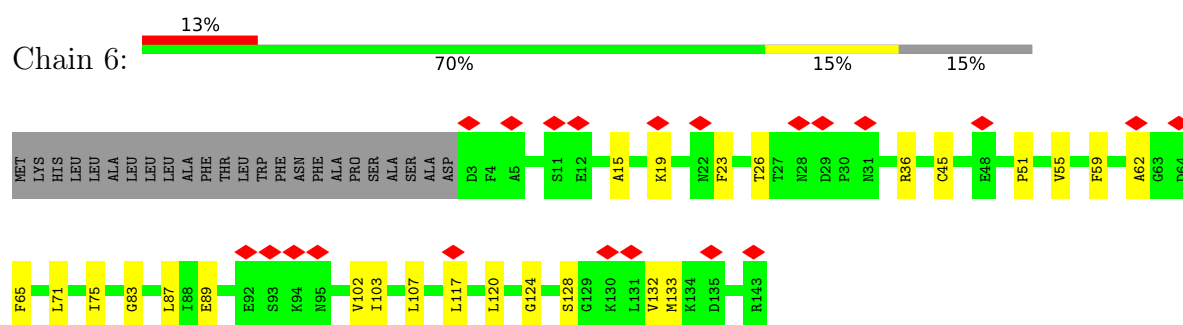
- Molecule 6: Photosystem I reaction center subunit III



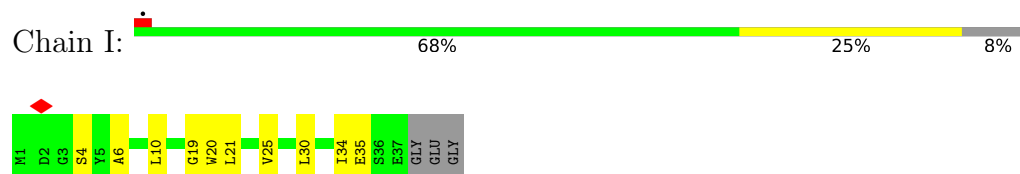
- Molecule 6: Photosystem I reaction center subunit III



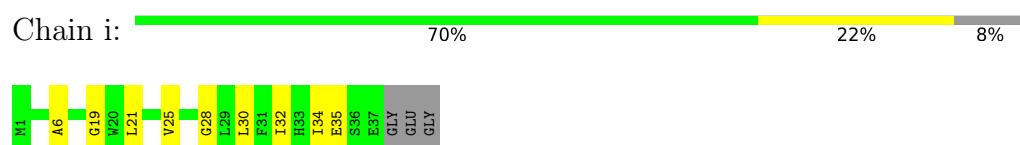
- Molecule 6: Photosystem I reaction center subunit III



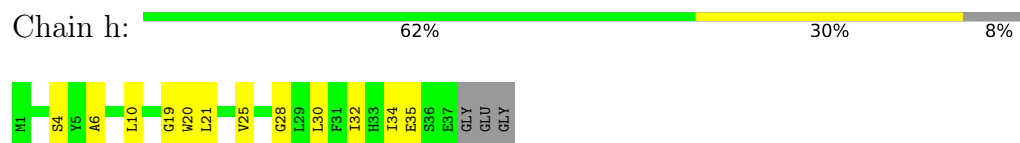
• Molecule 7: Photosystem I reaction center subunit VIII



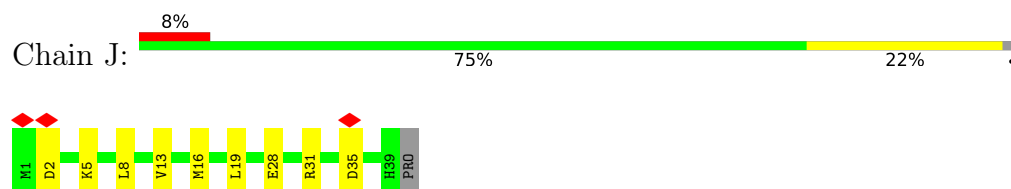
• Molecule 7: Photosystem I reaction center subunit VIII



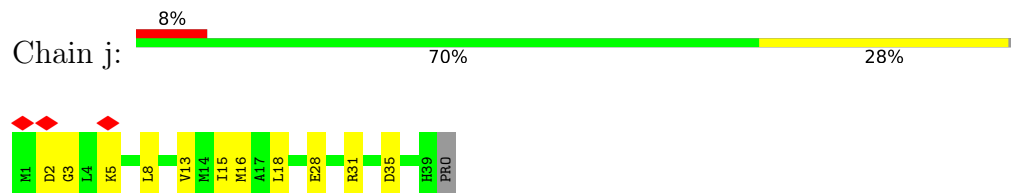
• Molecule 7: Photosystem I reaction center subunit VIII



• Molecule 8: Photosystem I reaction center subunit IX



• Molecule 8: Photosystem I reaction center subunit IX

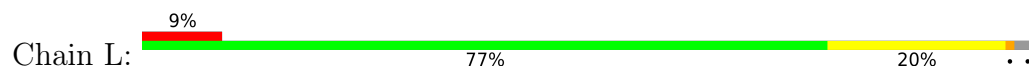


• Molecule 8: Photosystem I reaction center subunit IX

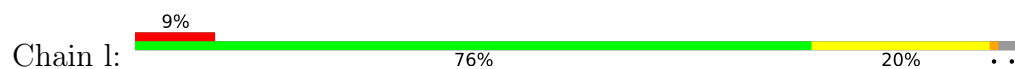




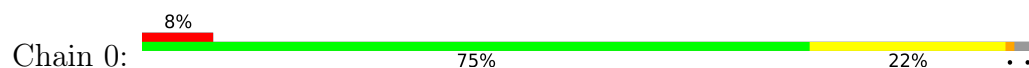
• Molecule 9: Photosystem I reaction center subunit XI



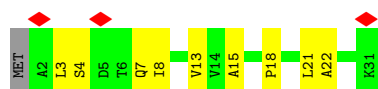
• Molecule 9: Photosystem I reaction center subunit XI



• Molecule 9: Photosystem I reaction center subunit XI



• Molecule 10: Photosystem I reaction center subunit XII

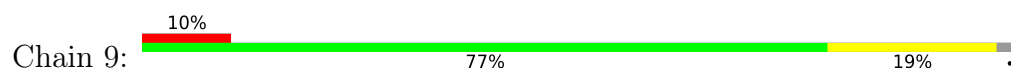


• Molecule 10: Photosystem I reaction center subunit XII

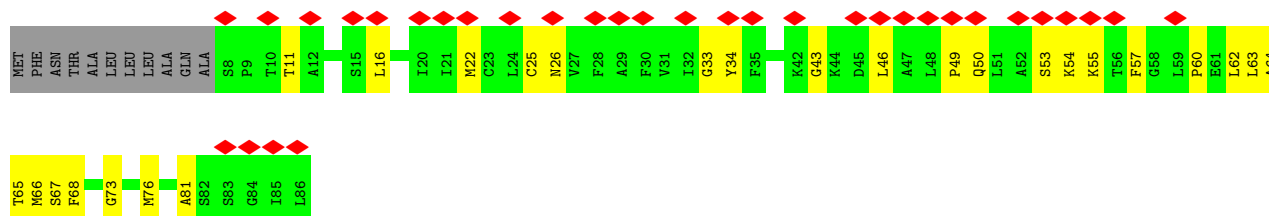




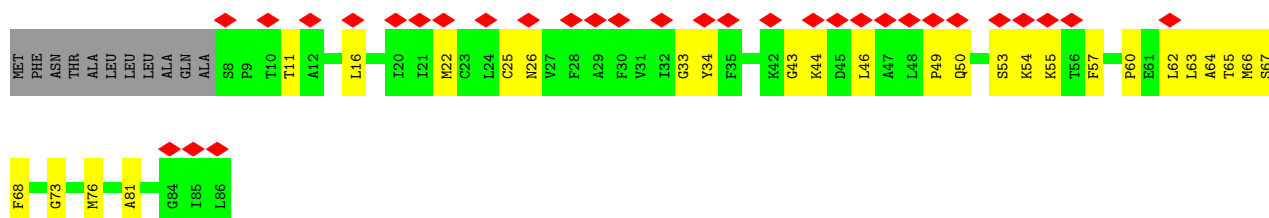
- Molecule 10: Photosystem I reaction center subunit XII



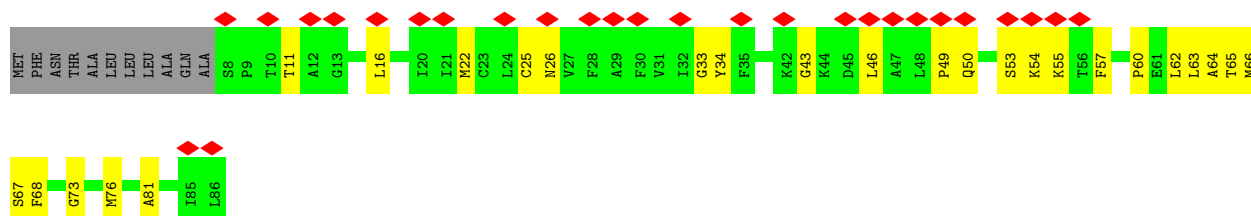
- Molecule 11: Photosystem I reaction center subunit PsaK 2



- 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 ($\text{\AA}$)	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 ($\text{\AA}$)	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: BCR, LMG, CLA, CA, LHG, PQN, SF4, CL0, LMT

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	0.43	0/5985	0.53	1/8158 (0.0%)
1	A	0.43	0/5985	0.53	1/8158 (0.0%)
1	a	0.43	0/5985	0.53	1/8158 (0.0%)
2	2	0.44	0/6021	0.51	0/8237
2	B	0.44	0/6021	0.51	0/8237
2	b	0.44	0/6021	0.51	0/8237
3	3	0.40	0/610	0.54	0/826
3	C	0.40	0/610	0.54	0/826
3	c	0.40	0/610	0.54	0/826
4	4	0.30	0/1102	0.57	0/1485
4	D	0.30	0/1102	0.57	0/1485
4	d	0.31	0/1102	0.57	0/1485
5	5	0.30	0/546	0.48	0/738
5	E	0.30	0/546	0.48	0/738
5	e	0.30	0/546	0.48	0/738
6	6	0.26	0/1116	0.54	0/1520
6	F	0.26	0/1116	0.54	0/1520
6	f	0.26	0/1116	0.54	0/1520
7	I	0.38	0/304	0.56	0/416
7	h	0.38	0/304	0.56	0/416
7	i	0.38	0/304	0.56	0/416
8	7	0.30	0/319	0.61	0/431
8	J	0.30	0/319	0.62	0/431
8	j	0.30	0/319	0.61	0/431
9	0	0.35	0/1168	0.47	0/1588
9	L	0.35	0/1168	0.47	0/1588
9	l	0.35	0/1168	0.47	0/1588
10	9	0.28	0/233	0.44	0/316
10	M	0.28	0/233	0.44	0/316
10	m	0.28	0/233	0.44	0/316
11	8	0.24	0/577	0.56	0/778
11	K	0.24	0/577	0.56	0/778

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	k	0.24	0/577	0.56	0/778
All	All	0.40	0/53943	0.52	3/73479 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	MET	CB-CG-SD	6.80	133.10	112.70
1	a	671	MET	CB-CG-SD	6.79	133.05	112.70
1	1	671	MET	CB-CG-SD	6.78	133.04	112.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5787	0	5646	108	0
1	A	5787	0	5646	101	0
1	a	5787	0	5646	108	0
2	2	5806	0	5567	116	0
2	B	5806	0	5567	125	0
2	b	5806	0	5567	120	0
3	3	600	0	581	12	0
3	C	600	0	581	13	0
3	c	600	0	581	16	0
4	4	1078	0	1076	29	0
4	D	1078	0	1076	31	0
4	d	1078	0	1076	29	0
5	5	537	0	520	9	0
5	E	537	0	520	8	0
5	e	537	0	520	10	0
6	6	1086	0	1063	18	0
6	F	1086	0	1063	11	0
6	f	1086	0	1063	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	I	293	0	292	10	0
7	h	293	0	292	12	0
7	i	293	0	292	8	0
8	7	311	0	321	13	0
8	J	311	0	321	7	0
8	j	311	0	321	8	0
9	0	1138	0	1107	32	0
9	L	1138	0	1107	27	0
9	l	1138	0	1107	29	0
10	9	230	0	248	4	0
10	M	230	0	248	9	0
10	m	230	0	248	8	0
11	8	566	0	598	22	0
11	K	566	0	598	23	0
11	k	566	0	598	25	0
12	1	82	0	110	5	0
12	2	39	0	51	2	0
12	9	39	0	48	0	0
12	A	82	0	110	5	0
12	B	39	0	51	2	0
12	M	39	0	48	0	0
12	a	82	0	110	7	0
12	b	39	0	51	2	0
12	m	39	0	48	1	0
13	1	65	0	72	0	0
13	A	65	0	72	0	0
13	a	65	0	72	3	0
14	0	260	0	288	22	0
14	1	2331	0	2248	126	0
14	2	2342	0	2160	112	0
14	6	90	0	66	5	0
14	7	147	0	130	8	0
14	8	145	0	115	4	0
14	A	2345	0	2279	131	0
14	B	2407	0	2232	123	0
14	F	141	0	107	5	0
14	J	82	0	58	2	0
14	K	145	0	115	5	0
14	L	195	0	216	15	0
14	a	2395	0	2315	131	0
14	b	2347	0	2173	112	0
14	f	141	0	107	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	j	82	0	58	2	0
14	k	90	0	66	3	0
14	l	260	0	288	30	0
15	1	33	0	46	1	0
15	2	33	0	46	6	0
15	A	33	0	46	1	0
15	B	33	0	46	9	0
15	a	33	0	46	1	0
15	b	33	0	46	8	0
16	1	8	0	0	0	0
16	3	16	0	0	1	0
16	A	8	0	0	0	0
16	C	16	0	0	1	0
16	a	8	0	0	0	0
16	c	16	0	0	1	0
17	0	120	0	168	18	0
17	1	200	0	280	16	0
17	2	225	0	313	21	0
17	6	120	0	168	10	0
17	7	80	0	112	7	0
17	8	80	0	112	5	0
17	9	40	0	56	4	0
17	A	200	0	280	17	0
17	B	265	0	369	28	0
17	F	80	0	112	4	0
17	I	80	0	112	6	0
17	J	80	0	112	5	0
17	K	80	0	112	6	0
17	L	80	0	112	10	0
17	M	40	0	56	5	0
17	a	200	0	280	16	0
17	b	305	0	425	32	0
17	f	80	0	112	5	0
17	h	80	0	112	6	0
17	i	80	0	112	5	0
17	j	80	0	112	4	0
17	k	80	0	112	5	0
17	l	40	0	56	1	0
18	0	84	0	108	3	0
18	1	32	0	34	0	0
18	2	48	0	66	3	0
18	A	78	0	96	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	B	48	0	66	4	0
18	L	38	0	46	1	0
18	a	78	0	96	1	0
18	b	48	0	66	3	0
18	l	38	0	46	1	0
19	6	35	0	43	0	0
19	F	35	0	43	0	0
19	I	35	0	46	1	0
19	f	35	0	44	0	0
19	h	35	0	46	1	0
19	i	35	0	46	1	0
20	0	1	0	0	0	0
20	L	1	0	0	0	0
20	l	1	0	0	0	0
All	All	72606	0	71884	1622	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

The worst 5 of 1622 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:HB3	11:K:60:PRO:HB3	1.58	0.85
14:A:812:CLA:HBB2	14:A:815:CLA:HMA3	1.61	0.82
1:a:315:TRP:HB3	11:k:60:PRO:HB3	1.62	0.81
14:a:813:CLA:HBB2	14:a:816:CLA:HMA3	1.61	0.81
14:1:811:CLA:HBB2	14:1:814:CLA:HMA3	1.61	0.81

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	73	81
1	A	593/603 (98%)	588 (99%)	5 (1%)	73	81
1	a	539/603 (89%)	534 (99%)	5 (1%)	70	80
2	2	585/588 (100%)	584 (100%)	1 (0%)	87	89
2	B	585/588 (100%)	584 (100%)	1 (0%)	87	89
2	b	585/588 (100%)	584 (100%)	1 (0%)	87	89
3	3	68/69 (99%)	67 (98%)	1 (2%)	57	75
3	C	68/69 (99%)	67 (98%)	1 (2%)	57	75
3	c	68/69 (99%)	67 (98%)	1 (2%)	57	75
4	4	113/116 (97%)	108 (96%)	5 (4%)	25	56
4	D	113/116 (97%)	108 (96%)	5 (4%)	25	56
4	d	113/116 (97%)	108 (96%)	5 (4%)	25	56
5	5	58/60 (97%)	56 (97%)	2 (3%)	32	63
5	E	58/60 (97%)	56 (97%)	2 (3%)	32	63
5	e	58/60 (97%)	56 (97%)	2 (3%)	32	63
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	70	80
9	L	111/118 (94%)	110 (99%)	1 (1%)	70	80
9	l	111/118 (94%)	110 (99%)	1 (1%)	70	80
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%)	53	74
11	K	59/68 (87%)	58 (98%)	1 (2%)	53	74
11	k	59/68 (87%)	58 (98%)	1 (2%)	53	74
All	All	5316/5553 (96%)	5268 (99%)	48 (1%)	68	80

5 of 48 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	b	612	GLU
4	4	10	LYS
2	2	612	GLU
4	d	119	THR
4	4	119	THR

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

Mol	Chain	Res	Type
2	b	133	GLN
2	2	133	GLN
10	9	7	GLN
2	b	158	GLN
2	b	478	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	1	821	-	64,68,73	1.18	9 (14%)	76,107,113	1.24	7 (9%)
14	CLA	2	805	-	69,73,73	1.16	11 (15%)	82,113,113	1.46	7 (8%)
17	BCR	i	4103	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	8 (14%)
14	CLA	b	843	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	9 (10%)
14	CLA	A	832	-	69,73,73	1.20	9 (13%)	82,113,113	1.42	7 (8%)
17	BCR	1	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
17	BCR	b	846	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	1	829	-	69,73,73	1.13	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	1	826	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	F	204	-	49,53,73	1.35	8 (16%)	58,89,113	1.59	6 (10%)
14	CLA	2	819	-	59,63,73	1.26	9 (15%)	70,101,113	1.53	7 (10%)
14	CLA	A	820	-	58,62,73	1.27	9 (15%)	68,99,113	1.44	7 (10%)
14	CLA	A	828	-	59,63,73	1.23	9 (15%)	70,101,113	1.22	5 (7%)
14	CLA	b	816	-	50,54,73	1.32	9 (18%)	59,90,113	1.45	4 (6%)
14	CLA	b	833	-	59,63,73	1.22	9 (15%)	70,101,113	1.37	6 (8%)
14	CLA	a	829	-	59,63,73	1.23	9 (15%)	70,101,113	1.22	5 (7%)
17	BCR	J	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.31	7 (12%)
14	CLA	A	844	12	49,53,73	1.36	9 (18%)	58,89,113	1.45	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	822	-	51,55,73	1.36	8 (15%)	60,91,113	1.45	8 (13%)
14	CLA	B	830	-	64,68,73	1.19	9 (14%)	76,107,113	1.37	6 (7%)
14	CLA	2	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	5 (8%)
14	CLA	A	810	1	69,73,73	1.13	10 (14%)	82,113,113	1.20	8 (9%)
19	LMT	I	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	B	804	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	9 (10%)
17	BCR	B	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	B	817	-	50,54,73	1.32	9 (18%)	59,90,113	1.46	4 (6%)
14	CLA	B	835	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	a	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	a	842	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	l	823	-	53,57,73	1.27	8 (15%)	61,93,113	1.53	7 (11%)
19	LMT	f	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	a	813	-	49,53,73	1.37	10 (20%)	58,89,113	1.41	5 (8%)
14	CLA	l	4205	-	69,73,73	1.14	10 (14%)	82,113,113	1.38	8 (9%)
17	BCR	l	4207	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
17	BCR	I	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)
19	LMT	h	103	-	36,36,36	1.19	6 (16%)	47,47,47	1.19	3 (6%)
16	SF4	A	846	2,1	0,12,12	-	-	-	-	-
17	BCR	6	4402	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)
17	BCR	i	4102	-	41,41,41	1.23	2 (4%)	56,56,56	1.37	5 (8%)
13	CL0	A	803	-	58,73,73	2.14	15 (25%)	60,113,113	1.80	16 (26%)
17	BCR	9	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.32	8 (14%)
14	CLA	A	804	-	69,73,73	1.22	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	a	814	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	b	835	-	49,53,73	1.40	10 (20%)	58,89,113	1.60	7 (12%)
14	CLA	A	837	1	49,53,73	1.38	9 (18%)	58,89,113	1.55	5 (8%)
14	CLA	2	825	-	49,53,73	1.37	10 (20%)	58,89,113	1.51	4 (6%)
12	LHG	M	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	2	824	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	4 (6%)
14	CLA	2	844	-	27,35,73	1.81	6 (22%)	32,60,113	1.72	5 (15%)
14	CLA	A	817	-	49,53,73	1.36	8 (16%)	58,89,113	1.43	4 (6%)
14	CLA	2	831	-	64,68,73	1.28	8 (12%)	76,107,113	1.57	7 (9%)
14	CLA	7	1101	-	69,73,73	1.16	9 (13%)	82,113,113	1.20	6 (7%)
14	CLA	A	818	-	50,54,73	1.34	8 (16%)	59,90,113	1.33	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	830	-	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	2	803	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	8 (9%)
14	CLA	B	844	-	69,73,73	1.15	7 (10%)	82,113,113	1.37	9 (10%)
14	CLA	1	817	-	50,54,73	1.34	8 (16%)	59,90,113	1.33	5 (8%)
14	CLA	1	835	-	58,62,73	1.28	10 (17%)	68,99,113	1.39	6 (8%)
16	SF4	3	102	3	0,12,12	-	-	-	-	-
14	CLA	a	820	-	58,62,73	1.22	8 (13%)	68,99,113	1.41	6 (8%)
14	CLA	2	817	-	49,53,73	1.36	9 (18%)	58,89,113	1.47	5 (8%)
14	CLA	b	820	-	64,68,73	1.18	9 (14%)	76,107,113	1.37	9 (11%)
17	BCR	A	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.30	10 (17%)
17	BCR	J	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	b	804	-	69,73,73	1.20	9 (13%)	82,113,113	1.25	8 (9%)
14	CLA	b	844	-	27,35,73	1.80	6 (22%)	32,60,113	1.72	5 (15%)
17	BCR	b	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.35	7 (21%)
14	CLA	L	1502	-	69,73,73	1.15	11 (15%)	82,113,113	1.38	8 (9%)
14	CLA	J	101	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)
17	BCR	2	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.33	8 (14%)
14	CLA	B	825	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	A	821	-	69,73,73	1.15	11 (15%)	82,113,113	1.31	8 (9%)
17	BCR	M	102	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
14	CLA	8	4003	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
14	CLA	A	825	-	55,59,73	1.29	8 (14%)	64,96,113	1.54	4 (6%)
17	BCR	h	102	-	41,41,41	1.32	4 (9%)	56,56,56	1.42	9 (16%)
14	CLA	6	4403	-	49,53,73	1.35	8 (16%)	58,89,113	1.58	6 (10%)
14	CLA	a	840	-	69,73,73	1.17	11 (15%)	82,113,113	1.31	6 (7%)
14	CLA	2	827	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
12	LHG	b	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	2	821	-	51,55,73	1.35	9 (17%)	60,91,113	1.44	7 (11%)
15	PQN	a	845	-	34,34,34	0.41	0	43,45,45	1.23	4 (9%)
14	CLA	B	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (13%)
14	CLA	A	836	-	58,62,73	1.27	9 (15%)	68,99,113	1.39	6 (8%)
14	CLA	1	822	-	69,73,73	1.18	10 (14%)	82,113,113	1.35	8 (9%)
14	CLA	k	4003	-	49,53,73	1.39	8 (16%)	58,89,113	1.54	6 (10%)
17	BCR	1	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	F	205	-	49,53,73	1.37	11 (22%)	58,89,113	1.46	9 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	5 (6%)
16	SF4	a	846	2,1	0,12,12	-	-	-		
14	CLA	a	806	-	69,73,73	1.16	9 (13%)	82,113,113	1.21	6 (7%)
13	CL0	a	803	-	58,73,73	2.13	14 (24%)	60,113,113	1.81	16 (26%)
14	CLA	B	818	-	49,53,73	1.35	9 (18%)	58,89,113	1.46	4 (6%)
14	CLA	f	204	-	49,53,73	1.36	8 (16%)	58,89,113	1.59	6 (10%)
14	CLA	2	813	-	49,53,73	1.36	9 (18%)	58,89,113	1.40	6 (10%)
14	CLA	a	804	-	64,68,73	1.23	11 (17%)	76,107,113	1.46	10 (13%)
14	CLA	k	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	6 (10%)
14	CLA	B	836	-	49,53,73	1.40	10 (20%)	58,89,113	1.61	7 (12%)
14	CLA	A	808	-	69,73,73	1.17	9 (13%)	82,113,113	1.41	7 (8%)
14	CLA	a	834	-	54,58,73	1.30	8 (14%)	64,95,113	1.69	10 (15%)
14	CLA	a	837	-	58,62,73	1.27	10 (17%)	68,99,113	1.39	6 (8%)
14	CLA	J	102	-	41,45,73	1.46	9 (21%)	50,78,113	1.35	5 (10%)
14	CLA	B	808	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	8 (9%)
17	BCR	7	1104	-	41,41,41	1.23	3 (7%)	56,56,56	1.32	5 (8%)
15	PQN	A	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)
14	CLA	A	827	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	2	807	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	8 (9%)
14	CLA	2	833	-	59,63,73	1.23	9 (15%)	70,101,113	1.38	6 (8%)
17	BCR	B	854	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	8 (14%)
15	PQN	1	845	-	34,34,34	0.42	0	43,45,45	1.23	4 (9%)
14	CLA	2	841	-	50,54,73	1.30	11 (22%)	59,90,113	1.57	8 (13%)
18	LMG	L	1506	-	38,38,55	0.86	0	46,46,63	1.29	5 (10%)
18	LMG	a	852	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
19	LMT	6	4401	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
14	CLA	A	842	-	69,73,73	1.14	8 (11%)	82,113,113	1.32	5 (6%)
17	BCR	a	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
17	BCR	b	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.30	6 (10%)
14	CLA	2	811	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
14	CLA	7	1103	-	41,45,73	1.46	9 (21%)	50,78,113	1.36	5 (10%)
14	CLA	a	812	1	54,58,73	1.31	9 (16%)	64,95,113	1.53	8 (12%)
14	CLA	b	826	-	59,63,73	1.27	10 (16%)	70,101,113	1.45	9 (12%)
14	CLA	1	805	-	54,58,73	1.27	10 (18%)	64,95,113	1.51	8 (12%)
14	CLA	1	813	-	58,62,73	1.26	11 (18%)	68,99,113	1.45	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	7	1105	-	41,41,41	1.18	3 (7%)	56,56,56	1.32	7 (12%)
17	BCR	j	104	-	41,41,41	1.19	3 (7%)	56,56,56	1.31	6 (10%)
14	CLA	1	836	1	49,53,73	1.38	9 (18%)	58,89,113	1.55	6 (10%)
14	CLA	a	818	-	49,53,73	1.34	8 (16%)	58,89,113	1.43	4 (6%)
17	BCR	8	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
12	LHG	m	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	a	839	-	55,59,73	1.27	8 (14%)	64,96,113	1.40	9 (14%)
14	CLA	b	822	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	4 (6%)
14	CLA	b	802	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	b	828	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	843	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	4 (4%)
14	CLA	A	841	-	69,73,73	1.14	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	b	806	-	69,73,73	1.15	10 (14%)	82,113,113	1.47	7 (8%)
14	CLA	A	834	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	f	205	-	49,53,73	1.37	11 (22%)	58,89,113	1.45	9 (15%)
14	CLA	b	834	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	A	805	-	69,73,73	1.16	9 (13%)	82,113,113	1.21	6 (7%)
14	CLA	1	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	1	842	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	A	813	-	69,73,73	1.16	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	a	808	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	B	813	-	69,73,73	1.16	11 (15%)	82,113,113	1.38	8 (9%)
14	CLA	1	806	-	69,73,73	1.17	10 (14%)	82,113,113	1.30	5 (6%)
14	CLA	b	808	-	69,73,73	1.15	8 (11%)	82,113,113	1.34	8 (9%)
14	CLA	2	809	-	64,68,73	1.19	8 (12%)	76,107,113	1.25	6 (7%)
14	CLA	B	828	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
14	CLA	B	841	-	66,70,73	1.17	9 (13%)	78,109,113	1.25	6 (7%)
16	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	a	827	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	8 (10%)
15	PQN	b	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
14	CLA	A	833	-	54,58,73	1.30	8 (14%)	64,95,113	1.68	10 (15%)
14	CLA	1	837	-	55,59,73	1.26	9 (16%)	64,96,113	1.39	9 (14%)
18	LMG	l	4202	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
17	BCR	b	854	-	41,41,41	1.16	3 (7%)	56,56,56	1.32	8 (14%)
17	BCR	A	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	2	837	-	49,53,73	1.38	10 (20%)	58,89,113	1.49	4 (6%)
14	CLA	L	1503	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	B	833	-	49,53,73	1.37	11 (22%)	58,89,113	1.65	7 (12%)
17	BCR	1	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	5 (8%)
14	CLA	b	841	-	50,54,73	1.31	11 (22%)	59,90,113	1.58	8 (13%)
14	CLA	b	842	-	69,73,73	1.16	9 (13%)	82,113,113	1.16	5 (6%)
14	CLA	0	202	-	69,73,73	1.14	10 (14%)	82,113,113	1.26	8 (9%)
14	CLA	1	808	-	50,54,73	1.32	10 (20%)	59,90,113	1.48	6 (10%)
14	CLA	B	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.35	6 (7%)
17	BCR	B	852	-	41,41,41	1.23	3 (7%)	56,56,56	1.33	8 (14%)
14	CLA	l	4203	-	69,73,73	1.16	11 (15%)	82,113,113	1.36	8 (9%)
18	LMG	A	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	A	830	-	69,73,73	1.12	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	A	811	1	54,58,73	1.31	9 (16%)	64,95,113	1.52	8 (12%)
14	CLA	1	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.45	11 (13%)
17	BCR	B	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.30	7 (12%)
14	CLA	a	838	1	49,53,73	1.39	9 (18%)	58,89,113	1.55	5 (8%)
14	CLA	L	1501	9	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	2	810	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	6 (7%)
14	CLA	j	102	-	41,45,73	1.46	9 (21%)	50,78,113	1.36	5 (10%)
14	CLA	a	841	-	51,55,73	1.31	10 (19%)	60,91,113	1.46	5 (8%)
14	CLA	2	812	-	69,73,73	1.16	11 (15%)	82,113,113	1.37	8 (9%)
14	CLA	1	841	-	55,59,73	1.29	10 (18%)	64,96,113	1.39	6 (9%)
17	BCR	a	848	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
14	CLA	1	804	-	69,73,73	1.22	10 (14%)	82,113,113	1.14	5 (6%)
14	CLA	A	829	-	69,73,73	1.15	8 (11%)	82,113,113	1.45	6 (7%)
16	SF4	c	101	3	0,12,12	-	-	-	-	-
14	CLA	B	809	-	69,73,73	1.20	12 (17%)	82,113,113	1.40	6 (7%)
17	BCR	b	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.40	10 (17%)
14	CLA	A	838	-	55,59,73	1.27	9 (16%)	64,96,113	1.40	9 (14%)
14	CLA	b	813	-	49,53,73	1.35	8 (16%)	58,89,113	1.40	6 (10%)
14	CLA	B	845	-	27,35,73	1.80	6 (22%)	32,60,113	1.71	5 (15%)
14	CLA	A	822	-	64,68,73	1.19	9 (14%)	76,107,113	1.24	7 (9%)
14	CLA	1	820	-	69,73,73	1.15	10 (14%)	82,113,113	1.31	8 (9%)
14	CLA	a	816	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	812	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
14	CLA	a	833	-	69,73,73	1.20	9 (13%)	82,113,113	1.43	8 (9%)
14	CLA	1	811	-	49,53,73	1.37	10 (20%)	58,89,113	1.41	5 (8%)
14	CLA	B	824	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	5 (8%)
17	BCR	k	4004	-	41,41,41	1.12	2 (4%)	56,56,56	1.25	5 (8%)
14	CLA	b	814	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
14	CLA	2	806	-	58,62,73	1.21	9 (15%)	68,99,113	1.37	8 (11%)
14	CLA	1	844	12	49,53,73	1.35	9 (18%)	58,89,113	1.46	5 (8%)
17	BCR	K	4005	-	41,41,41	1.13	2 (4%)	56,56,56	1.25	5 (8%)
14	CLA	1	825	-	63,67,73	1.20	8 (12%)	74,105,113	1.46	8 (10%)
14	CLA	a	825	-	53,57,73	1.27	8 (15%)	61,93,113	1.53	7 (11%)
14	CLA	a	830	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	6 (7%)
14	CLA	a	811	1	69,73,73	1.13	9 (13%)	82,113,113	1.19	7 (8%)
14	CLA	1	831	-	69,73,73	1.19	8 (11%)	82,113,113	1.42	8 (9%)
14	CLA	a	819	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	5 (8%)
14	CLA	a	844	12	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	b	824	-	49,53,73	1.36	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.44	11 (13%)
14	CLA	a	810	-	50,54,73	1.32	10 (20%)	59,90,113	1.47	6 (10%)
18	LMG	A	852	-	46,46,55	0.86	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	l	4204	9	69,73,73	1.16	10 (14%)	82,113,113	1.34	8 (9%)
14	CLA	1	840	-	69,73,73	1.13	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	A	831	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	b	830	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
17	BCR	B	851	-	41,41,41	1.25	5 (12%)	56,56,56	1.56	10 (17%)
14	CLA	b	817	-	49,53,73	1.36	10 (20%)	58,89,113	1.47	4 (6%)
13	CL0	1	803	-	58,73,73	2.13	15 (25%)	60,113,113	1.81	16 (26%)
12	LHG	1	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	K	4003	-	49,53,73	1.38	8 (16%)	58,89,113	1.55	6 (10%)
14	CLA	b	805	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (13%)
14	CLA	1	812	-	69,73,73	1.17	11 (15%)	82,113,113	1.37	9 (10%)
14	CLA	a	854	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
17	BCR	A	848	-	41,41,41	1.19	2 (4%)	56,56,56	1.21	5 (8%)
14	CLA	2	834	-	62,66,73	1.23	10 (16%)	73,104,113	1.37	6 (8%)
14	CLA	1	824	-	55,59,73	1.29	9 (16%)	64,96,113	1.55	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	819	-	59,63,73	1.22	10 (16%)	70,101,113	1.45	7 (10%)
18	LMG	a	853	-	32,32,55	0.91	1 (3%)	40,40,63	1.21	4 (10%)
14	CLA	a	832	-	69,73,73	1.16	10 (14%)	82,113,113	1.35	8 (9%)
17	BCR	b	851	-	41,41,41	1.22	3 (7%)	56,56,56	1.34	8 (14%)
17	BCR	2	846	-	41,41,41	1.18	3 (7%)	56,56,56	1.29	7 (12%)
17	BCR	I	101	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	5 (8%)
14	CLA	1	818	-	58,62,73	1.23	7 (12%)	68,99,113	1.42	6 (8%)
14	CLA	A	823	-	69,73,73	1.18	10 (14%)	82,113,113	1.36	8 (9%)
14	CLA	a	822	-	69,73,73	1.15	11 (15%)	82,113,113	1.31	8 (9%)
17	BCR	2	848	-	25,25,41	1.18	2 (8%)	33,33,56	1.34	5 (15%)
17	BCR	F	203	-	41,41,41	1.26	2 (4%)	56,56,56	1.38	7 (12%)
17	BCR	6	4406	-	41,41,41	1.25	3 (7%)	56,56,56	1.39	8 (14%)
14	CLA	2	843	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	9 (10%)
14	CLA	b	819	-	59,63,73	1.27	9 (15%)	70,101,113	1.52	8 (11%)
14	CLA	a	821	-	58,62,73	1.27	9 (15%)	68,99,113	1.44	7 (10%)
14	CLA	b	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.52	5 (8%)
17	BCR	K	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	b	839	-	54,58,73	1.28	8 (14%)	64,95,113	1.52	10 (15%)
17	BCR	j	103	-	41,41,41	1.23	2 (4%)	56,56,56	1.32	5 (8%)
14	CLA	K	4004	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
17	BCR	1	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
14	CLA	2	801	-	64,68,73	1.23	10 (15%)	76,107,113	1.46	10 (13%)
14	CLA	B	831	-	69,73,73	1.14	9 (13%)	82,113,113	1.31	8 (9%)
14	CLA	2	822	-	49,53,73	1.35	9 (18%)	58,89,113	1.51	5 (8%)
14	CLA	B	840	-	54,58,73	1.28	9 (16%)	64,95,113	1.52	10 (15%)
12	LHG	9	101	-	38,38,48	0.68	0	41,44,54	1.27	4 (9%)
14	CLA	a	835	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	9 (10%)
16	SF4	c	102	3	0,12,12	-	-	-	-	-
14	CLA	K	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.49	6 (10%)
17	BCR	0	209	-	41,41,41	1.20	2 (4%)	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	7	1102	-	49,53,73	1.36	9 (18%)	58,89,113	1.53	6 (10%)
14	CLA	1	819	-	58,62,73	1.26	8 (13%)	68,99,113	1.44	7 (10%)
12	LHG	a	802	14	32,32,48	0.88	1 (3%)	35,38,54	1.30	3 (8%)
14	CLA	b	831	-	64,68,73	1.29	8 (12%)	76,107,113	1.56	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	6	4405	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	7 (12%)
17	BCR	2	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	825	-	49,53,73	1.37	9 (18%)	58,89,113	1.49	4 (6%)
14	CLA	B	827	-	59,63,73	1.27	10 (16%)	70,101,113	1.45	9 (12%)
14	CLA	A	809	-	50,54,73	1.32	10 (20%)	59,90,113	1.47	6 (10%)
17	BCR	h	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.36	5 (8%)
14	CLA	2	835	-	49,53,73	1.40	10 (20%)	58,89,113	1.60	7 (12%)
14	CLA	2	829	-	64,68,73	1.18	9 (14%)	76,107,113	1.38	6 (7%)
14	CLA	b	821	-	51,55,73	1.36	8 (15%)	60,91,113	1.44	8 (13%)
14	CLA	2	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.28	8 (9%)
14	CLA	2	826	-	59,63,73	1.27	10 (16%)	70,101,113	1.46	9 (12%)
14	CLA	0	208	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	A	816	-	49,53,73	1.37	10 (20%)	58,89,113	1.48	6 (10%)
14	CLA	b	829	-	64,68,73	1.19	9 (14%)	76,107,113	1.37	6 (7%)
14	CLA	8	4004	-	59,63,73	1.25	9 (15%)	70,101,113	1.26	8 (11%)
14	CLA	0	206	9	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	0	207	-	69,73,73	1.14	11 (15%)	82,113,113	1.39	8 (9%)
14	CLA	a	831	-	69,73,73	1.13	11 (15%)	82,113,113	1.47	11 (13%)
14	CLA	A	843	-	69,73,73	1.18	9 (13%)	82,113,113	1.27	7 (8%)
14	CLA	A	839	-	69,73,73	1.17	10 (14%)	82,113,113	1.31	6 (7%)
14	CLA	2	832	-	49,53,73	1.36	11 (22%)	58,89,113	1.65	7 (12%)
17	BCR	A	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.43	7 (12%)
14	CLA	F	201	-	55,59,73	1.29	10 (18%)	64,96,113	1.39	6 (9%)
17	BCR	B	849	-	25,25,41	1.17	2 (8%)	33,33,56	1.34	6 (18%)
14	CLA	B	842	-	50,54,73	1.31	11 (22%)	59,90,113	1.56	7 (11%)
14	CLA	B	810	-	64,68,73	1.19	9 (14%)	76,107,113	1.26	7 (9%)
14	CLA	1	809	1	69,73,73	1.13	9 (13%)	82,113,113	1.19	6 (7%)
17	BCR	2	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
14	CLA	1	816	-	49,53,73	1.35	8 (16%)	58,89,113	1.42	3 (5%)
14	CLA	a	809	-	69,73,73	1.17	9 (13%)	82,113,113	1.41	7 (8%)
14	CLA	2	816	-	50,54,73	1.33	9 (18%)	59,90,113	1.46	4 (6%)
14	CLA	1	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	2	838	-	50,54,73	1.35	9 (18%)	59,90,113	1.44	7 (11%)
14	CLA	b	810	-	64,68,73	1.19	8 (12%)	76,107,113	1.25	6 (7%)
14	CLA	8	4002	-	49,53,73	1.39	9 (18%)	58,89,113	1.50	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	SF4	C	102	3	0,12,12	-	-	-		
14	CLA	A	806	-	54,58,73	1.27	10 (18%)	64,95,113	1.53	8 (12%)
12	LHG	2	852	-	38,38,48	0.71	1 (2%)	41,44,54	1.22	3 (7%)
14	CLA	6	4404	-	49,53,73	1.37	11 (22%)	58,89,113	1.45	9 (15%)
14	CLA	b	827	-	54,58,73	1.28	10 (18%)	64,95,113	1.27	9 (14%)
14	CLA	B	832	-	64,68,73	1.29	8 (12%)	76,107,113	1.57	7 (9%)
14	CLA	B	807	-	58,62,73	1.21	9 (15%)	68,99,113	1.38	9 (13%)
14	CLA	b	809	-	69,73,73	1.19	11 (15%)	82,113,113	1.40	6 (7%)
14	CLA	B	839	-	50,54,73	1.34	9 (18%)	59,90,113	1.44	7 (11%)
17	BCR	8	4001	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	7 (12%)
14	CLA	b	832	-	49,53,73	1.37	11 (22%)	58,89,113	1.66	7 (12%)
14	CLA	B	837	-	49,53,73	1.35	10 (20%)	58,89,113	1.45	9 (15%)
14	CLA	b	807	-	58,62,73	1.21	9 (15%)	68,99,113	1.38	8 (11%)
14	CLA	1	827	-	59,63,73	1.23	10 (16%)	70,101,113	1.23	5 (7%)
14	CLA	2	814	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
14	CLA	b	811	-	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
17	BCR	a	849	-	41,41,41	1.26	3 (7%)	56,56,56	1.42	8 (14%)
17	BCR	a	850	-	41,41,41	1.29	4 (9%)	56,56,56	1.41	9 (16%)
14	CLA	f	201	-	55,59,73	1.29	10 (18%)	64,96,113	1.40	6 (9%)
14	CLA	A	812	-	49,53,73	1.37	8 (16%)	58,89,113	1.41	5 (8%)
14	CLA	1	807	-	69,73,73	1.17	9 (13%)	82,113,113	1.42	7 (8%)
14	CLA	B	801	-	64,68,73	1.23	10 (15%)	76,107,113	1.47	10 (13%)
14	CLA	A	840	-	51,55,73	1.31	10 (19%)	60,91,113	1.46	5 (8%)
14	CLA	1	810	1	54,58,73	1.31	9 (16%)	64,95,113	1.53	8 (12%)
14	CLA	1	832	-	54,58,73	1.31	8 (14%)	64,95,113	1.69	10 (15%)
14	CLA	A	824	-	53,57,73	1.28	9 (16%)	61,93,113	1.53	7 (11%)
14	CLA	2	820	-	64,68,73	1.19	9 (14%)	76,107,113	1.36	9 (11%)
14	CLA	B	816	-	69,73,73	1.16	9 (13%)	82,113,113	1.29	8 (9%)
17	BCR	F	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
16	SF4	3	101	3	0,12,12	-	-	-		
14	CLA	a	823	-	64,68,73	1.19	9 (14%)	76,107,113	1.24	7 (9%)
17	BCR	L	1504	-	41,41,41	1.21	2 (4%)	56,56,56	1.41	10 (17%)
14	CLA	b	837	-	49,53,73	1.38	10 (20%)	58,89,113	1.50	4 (6%)
14	CLA	A	807	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	B	820	-	59,63,73	1.27	9 (15%)	70,101,113	1.53	7 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	817	-	49,53,73	1.36	10 (20%)	58,89,113	1.48	6 (10%)
14	CLA	1	814	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)
14	CLA	2	840	-	66,70,73	1.17	8 (12%)	78,109,113	1.25	5 (6%)
15	PQN	2	845	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
17	BCR	L	1505	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	8 (14%)
12	LHG	B	853	-	38,38,48	0.72	1 (2%)	41,44,54	1.22	3 (7%)
17	BCR	b	853	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	8 (14%)
19	LMT	i	4101	-	36,36,36	1.20	6 (16%)	47,47,47	1.19	3 (6%)
14	CLA	A	814	-	58,62,73	1.25	11 (18%)	68,99,113	1.44	7 (10%)
14	CLA	B	806	-	69,73,73	1.16	11 (15%)	82,113,113	1.47	7 (8%)
14	CLA	B	814	-	49,53,73	1.35	7 (14%)	58,89,113	1.39	6 (10%)
14	CLA	B	821	-	64,68,73	1.18	9 (14%)	76,107,113	1.36	9 (11%)
14	CLA	l	4206	-	69,73,73	1.14	9 (13%)	82,113,113	1.24	7 (8%)
14	CLA	b	812	-	65,69,73	1.19	9 (13%)	77,108,113	1.48	8 (10%)
12	LHG	a	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	A	815	-	59,63,73	1.24	9 (15%)	70,101,113	1.38	7 (10%)
14	CLA	A	826	-	63,67,73	1.20	8 (12%)	74,105,113	1.47	7 (9%)
14	CLA	b	840	-	66,70,73	1.17	8 (12%)	78,109,113	1.25	5 (6%)
14	CLA	a	805	-	69,73,73	1.21	9 (13%)	82,113,113	1.14	5 (6%)
14	CLA	2	836	-	49,53,73	1.35	10 (20%)	58,89,113	1.46	9 (15%)
14	CLA	1	833	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	a	824	-	69,73,73	1.17	10 (14%)	82,113,113	1.35	8 (9%)
14	CLA	b	818	-	59,63,73	1.21	10 (16%)	70,101,113	1.44	7 (10%)
14	CLA	b	801	-	69,73,73	1.14	10 (14%)	82,113,113	1.27	8 (9%)
18	LMG	0	203	-	46,46,55	0.85	1 (2%)	54,54,63	1.30	6 (11%)
14	CLA	B	838	-	49,53,73	1.38	10 (20%)	58,89,113	1.50	4 (6%)
14	CLA	j	101	-	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)
17	BCR	k	4001	-	41,41,41	1.25	3 (7%)	56,56,56	1.42	7 (12%)
19	LMT	F	202	-	36,36,36	1.21	6 (16%)	47,47,47	0.95	1 (2%)
18	LMG	0	201	-	38,38,55	0.86	0	46,46,63	1.30	5 (10%)
17	BCR	2	847	-	41,41,41	1.16	2 (4%)	56,56,56	1.31	6 (10%)
14	CLA	B	815	-	49,53,73	1.35	10 (20%)	58,89,113	1.49	6 (10%)
17	BCR	f	206	-	41,41,41	1.16	2 (4%)	56,56,56	1.34	7 (12%)
14	CLA	B	802	-	69,73,73	1.14	10 (14%)	82,113,113	1.26	8 (9%)
16	SF4	1	846	2,1	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	BCR	1	847	-	41,41,41	1.22	2 (4%)	56,56,56	1.31	9 (16%)
17	BCR	a	851	-	41,41,41	1.20	2 (4%)	56,56,56	1.39	8 (14%)
17	BCR	0	204	-	41,41,41	1.12	2 (4%)	56,56,56	1.39	9 (16%)
14	CLA	1	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.44	6 (7%)
14	CLA	B	834	-	59,63,73	1.23	9 (15%)	70,101,113	1.37	6 (8%)
14	CLA	b	815	-	69,73,73	1.16	9 (13%)	82,113,113	1.30	8 (9%)
14	CLA	a	807	-	54,58,73	1.28	10 (18%)	64,95,113	1.52	8 (12%)
14	CLA	2	818	-	59,63,73	1.22	10 (16%)	70,101,113	1.45	7 (10%)
14	CLA	2	828	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	2	839	-	54,58,73	1.28	8 (14%)	64,95,113	1.51	10 (15%)
17	BCR	A	850	-	41,41,41	1.29	3 (7%)	56,56,56	1.41	9 (16%)
14	CLA	2	830	-	69,73,73	1.15	8 (11%)	82,113,113	1.30	8 (9%)
14	CLA	a	828	-	69,73,73	1.17	9 (13%)	82,113,113	1.27	8 (9%)
14	CLA	1	839	-	51,55,73	1.31	10 (19%)	60,91,113	1.47	5 (8%)
17	BCR	B	850	-	41,41,41	1.14	2 (4%)	56,56,56	1.41	10 (17%)
18	LMG	1	852	-	32,32,55	0.90	1 (3%)	40,40,63	1.21	4 (10%)
17	BCR	f	203	-	41,41,41	1.25	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	B	829	-	69,73,73	1.18	9 (13%)	82,113,113	1.22	5 (6%)
14	CLA	B	826	-	49,53,73	1.36	10 (20%)	58,89,113	1.49	4 (6%)
12	LHG	A	801	-	48,48,48	0.69	1 (2%)	51,54,54	1.28	7 (13%)
14	CLA	2	808	-	69,73,73	1.19	11 (15%)	82,113,113	1.40	6 (7%)
12	LHG	A	802	14	32,32,48	0.87	1 (3%)	35,38,54	1.30	3 (8%)
18	LMG	B	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	A	819	-	58,62,73	1.22	7 (12%)	68,99,113	1.42	6 (8%)
14	CLA	1	815	-	49,53,73	1.36	10 (20%)	58,89,113	1.49	6 (10%)
17	BCR	b	850	-	41,41,41	1.25	5 (12%)	56,56,56	1.55	10 (17%)
17	BCR	0	210	-	41,41,41	1.13	2 (4%)	56,56,56	1.38	9 (16%)
14	CLA	a	815	-	58,62,73	1.26	11 (18%)	68,99,113	1.45	7 (10%)
14	CLA	a	826	-	55,59,73	1.29	10 (18%)	64,96,113	1.54	4 (6%)
15	PQN	B	846	-	34,34,34	0.50	0	43,45,45	1.26	4 (9%)
18	LMG	2	802	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)
14	CLA	a	836	-	69,73,73	1.14	7 (10%)	82,113,113	1.45	11 (13%)
14	CLA	b	836	-	49,53,73	1.35	10 (20%)	58,89,113	1.46	9 (15%)
14	CLA	b	838	-	50,54,73	1.35	9 (18%)	59,90,113	1.45	7 (11%)
18	LMG	b	803	-	48,48,55	0.79	2 (4%)	56,56,63	1.36	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	823	-	49,53,73	1.35	9 (18%)	58,89,113	1.50	4 (6%)
14	CLA	2	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.48	11 (13%)

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	1	821	-	1/1/14/20	8/33/109/115	-
14	CLA	2	805	-	1/1/15/20	14/39/115/115	-
17	BCR	i	4103	-	-	20/29/63/63	0/2/2/2
14	CLA	b	843	-	-	20/39/115/115	-
14	CLA	A	832	-	1/1/15/20	20/39/115/115	-
17	BCR	1	850	-	-	19/29/63/63	0/2/2/2
17	BCR	b	846	-	-	12/29/63/63	0/2/2/2
14	CLA	1	829	-	1/1/15/20	10/39/115/115	-
14	CLA	1	826	-	1/1/15/20	14/39/115/115	-
14	CLA	F	204	-	1/1/11/20	6/15/91/115	-
14	CLA	2	819	-	-	8/27/103/115	-
14	CLA	A	820	-	1/1/12/20	6/26/102/115	-
14	CLA	A	828	-	1/1/13/20	6/27/103/115	-
14	CLA	b	816	-	1/1/11/20	7/17/93/115	-
14	CLA	b	833	-	1/1/13/20	14/27/103/115	-
14	CLA	a	829	-	1/1/13/20	6/27/103/115	-
17	BCR	J	104	-	-	10/29/63/63	0/2/2/2
14	CLA	A	844	12	1/1/11/20	6/15/91/115	-
14	CLA	B	822	-	1/1/11/20	5/18/94/115	-
14	CLA	B	830	-	1/1/14/20	7/33/109/115	-
14	CLA	2	823	-	-	8/15/91/115	-
14	CLA	A	810	1	1/1/15/20	23/39/115/115	-
19	LMT	I	103	-	-	8/21/61/61	0/2/2/2
14	CLA	B	804	-	1/1/15/20	13/39/115/115	-
17	BCR	B	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	817	-	1/1/11/20	7/17/93/115	-
14	CLA	B	835	-	1/1/13/20	15/31/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	843	-	1/1/15/20	18/39/115/115	-
14	CLA	a	842	-	-	13/39/115/115	-
14	CLA	1	823	-	1/1/11/20	13/20/96/115	-
19	LMT	f	202	-	-	3/21/61/61	0/2/2/2
14	CLA	a	813	-	1/1/11/20	8/15/91/115	-
14	CLA	l	4205	-	1/1/15/20	11/39/115/115	-
17	BCR	l	4207	-	-	14/29/63/63	0/2/2/2
17	BCR	I	102	-	-	20/29/63/63	0/2/2/2
19	LMT	h	103	-	-	8/21/61/61	0/2/2/2
16	SF4	A	846	2,1	-	-	0/6/5/5
17	BCR	6	4402	-	-	13/29/63/63	0/2/2/2
17	BCR	i	4102	-	-	16/29/63/63	0/2/2/2
13	CL0	A	803	-	3/3/20/25	13/37/135/135	-
17	BCR	9	102	-	-	15/29/63/63	0/2/2/2
14	CLA	A	804	-	1/1/15/20	10/39/115/115	-
14	CLA	a	814	-	1/1/15/20	19/39/115/115	-
14	CLA	b	835	-	1/1/11/20	4/15/91/115	-
14	CLA	A	837	1	1/1/11/20	6/15/91/115	-
14	CLA	2	825	-	-	6/15/91/115	-
12	LHG	M	101	-	-	20/43/43/53	-
14	CLA	2	824	-	1/1/11/20	7/15/91/115	-
14	CLA	2	844	-	1/1/5/20	-	-
14	CLA	A	817	-	-	3/15/91/115	-
14	CLA	2	831	-	1/1/14/20	12/33/109/115	-
14	CLA	7	1101	-	1/1/15/20	16/39/115/115	-
14	CLA	A	818	-	1/1/11/20	7/17/93/115	-
14	CLA	1	830	-	1/1/15/20	7/39/115/115	-
14	CLA	2	803	-	1/1/15/20	13/39/115/115	-
14	CLA	B	844	-	-	20/39/115/115	-
14	CLA	1	817	-	1/1/11/20	7/17/93/115	-
14	CLA	1	835	-	1/1/12/20	10/26/102/115	-
16	SF4	3	102	3	-	-	0/6/5/5
14	CLA	a	820	-	1/1/12/20	7/26/102/115	-
14	CLA	2	817	-	1/1/11/20	3/15/91/115	-
14	CLA	b	820	-	1/1/14/20	15/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	A	847	-	-	11/29/63/63	0/2/2/2
17	BCR	J	103	-	-	13/29/63/63	0/2/2/2
14	CLA	b	804	-	1/1/15/20	13/39/115/115	-
14	CLA	b	844	-	1/1/5/20	-	-
17	BCR	b	848	-	-	4/18/35/63	0/1/1/2
14	CLA	L	1502	-	1/1/15/20	11/39/115/115	-
14	CLA	J	101	-	1/1/11/20	8/15/91/115	-
17	BCR	2	851	-	-	10/29/63/63	0/2/2/2
14	CLA	B	825	-	1/1/11/20	7/15/91/115	-
14	CLA	A	821	-	1/1/15/20	19/39/115/115	-
17	BCR	M	102	-	-	15/29/63/63	0/2/2/2
14	CLA	8	4003	-	1/1/11/20	10/15/91/115	-
14	CLA	A	825	-	1/1/12/20	10/23/99/115	-
17	BCR	h	102	-	-	20/29/63/63	0/2/2/2
14	CLA	6	4403	-	1/1/11/20	6/15/91/115	-
14	CLA	a	840	-	1/1/15/20	11/39/115/115	-
12	LHG	b	852	-	-	22/43/43/53	-
14	CLA	2	827	-	1/1/12/20	2/21/97/115	-
14	CLA	2	821	-	1/1/11/20	5/18/94/115	-
15	PQN	a	845	-	-	4/23/43/43	0/2/2/2
14	CLA	B	805	-	1/1/15/20	13/39/115/115	-
14	CLA	A	836	-	1/1/12/20	10/26/102/115	-
14	CLA	1	822	-	1/1/15/20	13/39/115/115	-
14	CLA	k	4003	-	1/1/11/20	10/15/91/115	-
17	BCR	1	849	-	-	7/29/63/63	0/2/2/2
14	CLA	F	205	-	1/1/11/20	7/15/91/115	-
14	CLA	2	842	-	1/1/15/20	13/39/115/115	-
16	SF4	a	846	2,1	-	-	0/6/5/5
14	CLA	a	806	-	1/1/15/20	16/39/115/115	-
13	CL0	a	803	-	3/3/20/25	13/37/135/135	-
14	CLA	B	818	-	1/1/11/20	3/15/91/115	-
14	CLA	f	204	-	1/1/11/20	7/15/91/115	-
14	CLA	2	813	-	1/1/11/20	5/15/91/115	-
14	CLA	a	804	-	1/1/14/20	11/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	k	4002	-	-	8/15/91/115	-
14	CLA	B	836	-	1/1/11/20	4/15/91/115	-
14	CLA	A	808	-	1/1/15/20	14/39/115/115	-
14	CLA	a	834	-	1/1/12/20	3/21/97/115	-
14	CLA	a	837	-	1/1/12/20	10/26/102/115	-
14	CLA	J	102	-	1/1/8/20	3/4/76/115	-
14	CLA	B	808	-	-	11/39/115/115	-
17	BCR	7	1104	-	-	13/29/63/63	0/2/2/2
15	PQN	A	845	-	-	4/23/43/43	0/2/2/2
14	CLA	A	827	-	1/1/15/20	14/39/115/115	-
14	CLA	2	807	-	-	11/39/115/115	-
14	CLA	2	833	-	1/1/13/20	14/27/103/115	-
17	BCR	B	854	-	-	13/29/63/63	0/2/2/2
15	PQN	1	845	-	-	4/23/43/43	0/2/2/2
14	CLA	2	841	-	1/1/11/20	4/17/93/115	-
18	LMG	L	1506	-	-	20/33/53/70	0/1/1/1
18	LMG	a	852	-	-	21/41/61/70	0/1/1/1
19	LMT	6	4401	-	-	3/21/61/61	0/2/2/2
14	CLA	A	842	-	-	13/39/115/115	-
17	BCR	a	847	-	-	11/29/63/63	0/2/2/2
17	BCR	b	847	-	-	7/29/63/63	0/2/2/2
14	CLA	2	811	-	1/1/14/20	13/35/111/115	-
14	CLA	7	1103	-	1/1/8/20	3/4/76/115	-
14	CLA	a	812	1	1/1/12/20	8/21/97/115	-
14	CLA	b	826	-	1/1/13/20	4/27/103/115	-
14	CLA	1	805	-	1/1/12/20	3/21/97/115	-
14	CLA	1	813	-	1/1/12/20	11/26/102/115	-
17	BCR	7	1105	-	-	10/29/63/63	0/2/2/2
17	BCR	j	104	-	-	10/29/63/63	0/2/2/2
14	CLA	1	836	1	1/1/11/20	6/15/91/115	-
14	CLA	a	818	-	-	3/15/91/115	-
17	BCR	8	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	a	839	-	1/1/12/20	8/23/99/115	-
12	LHG	m	101	-	-	20/43/43/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	822	-	-	7/15/91/115	-
14	CLA	b	802	-	1/1/15/20	9/39/115/115	-
14	CLA	b	828	-	1/1/15/20	9/39/115/115	-
14	CLA	B	843	-	1/1/15/20	13/39/115/115	-
14	CLA	A	841	-	1/1/15/20	9/39/115/115	-
14	CLA	b	806	-	1/1/15/20	14/39/115/115	-
14	CLA	A	834	-	1/1/15/20	16/39/115/115	-
14	CLA	f	205	-	1/1/11/20	7/15/91/115	-
14	CLA	b	834	-	1/1/13/20	15/31/107/115	-
14	CLA	A	805	-	1/1/15/20	16/39/115/115	-
14	CLA	1	843	-	1/1/15/20	18/39/115/115	-
14	CLA	1	842	-	-	13/39/115/115	-
14	CLA	A	813	-	1/1/15/20	19/39/115/115	-
14	CLA	a	808	-	1/1/15/20	17/39/115/115	-
14	CLA	B	813	-	1/1/15/20	8/39/115/115	-
14	CLA	1	806	-	1/1/15/20	17/39/115/115	-
14	CLA	b	808	-	-	11/39/115/115	-
14	CLA	2	809	-	1/1/14/20	9/33/109/115	-
14	CLA	B	828	-	1/1/12/20	2/21/97/115	-
14	CLA	B	841	-	1/1/14/20	8/36/112/115	-
16	SF4	C	101	3	-	-	0/6/5/5
14	CLA	a	827	-	1/1/13/20	15/32/108/115	-
15	PQN	b	845	-	-	10/23/43/43	0/2/2/2
14	CLA	A	833	-	1/1/12/20	3/21/97/115	-
14	CLA	1	837	-	1/1/12/20	8/23/99/115	-
18	LMG	l	4202	-	-	20/33/53/70	0/1/1/1
17	BCR	b	854	-	-	15/29/63/63	0/2/2/2
17	BCR	A	851	-	-	21/29/63/63	0/2/2/2
14	CLA	2	837	-	1/1/11/20	4/15/91/115	-
14	CLA	L	1503	-	1/1/15/20	14/39/115/115	-
14	CLA	B	833	-	1/1/11/20	6/15/91/115	-
17	BCR	1	848	-	-	11/29/63/63	0/2/2/2
14	CLA	b	841	-	1/1/11/20	4/17/93/115	-
14	CLA	b	842	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	0	202	-	1/1/15/20	11/39/115/115	-
14	CLA	1	808	-	1/1/11/20	6/17/93/115	-
14	CLA	B	811	-	1/1/15/20	16/39/115/115	-
17	BCR	B	852	-	-	10/29/63/63	0/2/2/2
14	CLA	l	4203	-	1/1/15/20	8/39/115/115	-
18	LMG	A	853	-	-	8/27/47/70	0/1/1/1
14	CLA	A	830	-	1/1/15/20	10/39/115/115	-
14	CLA	A	811	1	1/1/12/20	8/21/97/115	-
14	CLA	1	834	-	1/1/15/20	7/39/115/115	-
17	BCR	B	847	-	-	12/29/63/63	0/2/2/2
14	CLA	a	838	1	1/1/11/20	6/15/91/115	-
14	CLA	L	1501	9	1/1/15/20	14/39/115/115	-
14	CLA	2	810	-	1/1/15/20	17/39/115/115	-
14	CLA	j	102	-	1/1/8/20	3/4/76/115	-
14	CLA	a	841	-	1/1/11/20	3/18/94/115	-
14	CLA	2	812	-	1/1/15/20	8/39/115/115	-
14	CLA	1	841	-	1/1/12/20	11/23/99/115	-
17	BCR	a	848	-	-	10/29/63/63	0/2/2/2
14	CLA	1	804	-	1/1/15/20	10/39/115/115	-
14	CLA	A	829	-	1/1/15/20	11/39/115/115	-
16	SF4	c	101	3	-	-	0/6/5/5
14	CLA	B	809	-	1/1/15/20	24/39/115/115	-
17	BCR	b	849	-	-	15/29/63/63	0/2/2/2
14	CLA	A	838	-	1/1/12/20	8/23/99/115	-
14	CLA	b	813	-	1/1/11/20	5/15/91/115	-
14	CLA	B	845	-	1/1/5/20	-	-
14	CLA	A	822	-	1/1/14/20	8/33/109/115	-
14	CLA	1	820	-	1/1/15/20	19/39/115/115	-
14	CLA	a	816	-	1/1/13/20	10/27/103/115	-
14	CLA	B	812	-	1/1/14/20	13/35/111/115	-
14	CLA	a	833	-	1/1/15/20	20/39/115/115	-
14	CLA	1	811	-	1/1/11/20	8/15/91/115	-
14	CLA	B	824	-	-	8/15/91/115	-
17	BCR	k	4004	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	814	-	1/1/11/20	11/15/91/115	-
14	CLA	2	806	-	1/1/12/20	10/26/102/115	-
14	CLA	1	844	12	1/1/11/20	6/15/91/115	-
17	BCR	K	4005	-	-	10/29/63/63	0/2/2/2
14	CLA	1	825	-	1/1/13/20	15/32/108/115	-
14	CLA	a	825	-	1/1/11/20	13/20/96/115	-
14	CLA	a	830	-	1/1/15/20	11/39/115/115	-
14	CLA	a	811	1	1/1/15/20	23/39/115/115	-
14	CLA	1	831	-	1/1/15/20	20/39/115/115	-
14	CLA	a	819	-	1/1/11/20	7/17/93/115	-
14	CLA	a	844	12	1/1/11/20	6/15/91/115	-
14	CLA	b	824	-	1/1/11/20	7/15/91/115	-
14	CLA	A	835	-	1/1/15/20	7/39/115/115	-
14	CLA	a	810	-	1/1/11/20	6/17/93/115	-
18	LMG	A	852	-	-	21/41/61/70	0/1/1/1
14	CLA	l	4204	9	1/1/15/20	14/39/115/115	-
14	CLA	1	840	-	1/1/15/20	9/39/115/115	-
14	CLA	A	831	-	1/1/15/20	7/39/115/115	-
14	CLA	b	830	-	1/1/15/20	8/39/115/115	-
17	BCR	B	851	-	-	19/29/63/63	0/2/2/2
14	CLA	b	817	-	1/1/11/20	3/15/91/115	-
13	CL0	1	803	-	3/3/20/25	13/37/135/135	-
12	LHG	1	801	-	-	22/53/53/53	-
14	CLA	K	4003	-	1/1/11/20	10/15/91/115	-
14	CLA	b	805	-	1/1/15/20	13/39/115/115	-
14	CLA	1	812	-	1/1/15/20	19/39/115/115	-
14	CLA	a	854	-	1/1/13/20	7/27/103/115	-
17	BCR	A	848	-	-	11/29/63/63	0/2/2/2
14	CLA	2	834	-	1/1/13/20	15/31/107/115	-
14	CLA	1	824	-	1/1/12/20	10/23/99/115	-
14	CLA	B	819	-	1/1/13/20	10/27/103/115	-
18	LMG	a	853	-	-	8/27/47/70	0/1/1/1
14	CLA	a	832	-	1/1/15/20	7/39/115/115	-
17	BCR	b	851	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	2	846	-	-	12/29/63/63	0/2/2/2
17	BCR	I	101	-	-	16/29/63/63	0/2/2/2
14	CLA	1	818	-	1/1/12/20	7/26/102/115	-
14	CLA	A	823	-	1/1/15/20	13/39/115/115	-
14	CLA	a	822	-	1/1/15/20	19/39/115/115	-
17	BCR	2	848	-	-	4/18/35/63	0/1/1/2
17	BCR	F	203	-	-	13/29/63/63	0/2/2/2
17	BCR	6	4406	-	-	13/29/63/63	0/2/2/2
14	CLA	2	843	-	-	20/39/115/115	-
14	CLA	b	819	-	-	8/27/103/115	-
14	CLA	a	821	-	1/1/12/20	6/26/102/115	-
14	CLA	b	823	-	-	8/15/91/115	-
17	BCR	K	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	839	-	1/1/12/20	7/21/97/115	-
17	BCR	j	103	-	-	13/29/63/63	0/2/2/2
14	CLA	K	4004	-	1/1/13/20	7/27/103/115	-
17	BCR	1	851	-	-	21/29/63/63	0/2/2/2
14	CLA	2	801	-	1/1/14/20	11/33/109/115	-
14	CLA	B	831	-	1/1/15/20	8/39/115/115	-
14	CLA	2	822	-	-	7/15/91/115	-
14	CLA	B	840	-	1/1/12/20	7/21/97/115	-
12	LHG	9	101	-	-	20/43/43/53	-
14	CLA	a	835	-	1/1/15/20	16/39/115/115	-
16	SF4	c	102	3	-	-	0/6/5/5
14	CLA	K	4002	-	-	8/15/91/115	-
17	BCR	0	209	-	-	14/29/63/63	0/2/2/2
14	CLA	7	1102	-	1/1/11/20	8/15/91/115	-
12	LHG	1	802	14	-	13/37/37/53	-
14	CLA	1	819	-	1/1/12/20	6/26/102/115	-
12	LHG	a	802	14	-	13/37/37/53	-
14	CLA	b	831	-	1/1/14/20	12/33/109/115	-
17	BCR	6	4405	-	-	13/29/63/63	0/2/2/2
17	BCR	2	849	-	-	15/29/63/63	0/2/2/2
14	CLA	b	825	-	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	827	-	1/1/13/20	4/27/103/115	-
14	CLA	A	809	-	1/1/11/20	6/17/93/115	-
17	BCR	h	101	-	-	16/29/63/63	0/2/2/2
14	CLA	2	835	-	1/1/11/20	4/15/91/115	-
14	CLA	2	829	-	1/1/14/20	7/33/109/115	-
14	CLA	b	821	-	1/1/11/20	5/18/94/115	-
14	CLA	2	815	-	1/1/15/20	22/39/115/115	-
14	CLA	2	826	-	1/1/13/20	4/27/103/115	-
14	CLA	0	208	-	1/1/15/20	14/39/115/115	-
14	CLA	A	816	-	1/1/11/20	4/15/91/115	-
14	CLA	b	829	-	1/1/14/20	7/33/109/115	-
14	CLA	8	4004	-	1/1/13/20	7/27/103/115	-
14	CLA	0	206	9	1/1/15/20	14/39/115/115	-
14	CLA	0	207	-	1/1/15/20	11/39/115/115	-
14	CLA	a	831	-	1/1/15/20	10/39/115/115	-
14	CLA	A	843	-	1/1/15/20	18/39/115/115	-
14	CLA	A	839	-	1/1/15/20	11/39/115/115	-
14	CLA	2	832	-	1/1/11/20	6/15/91/115	-
17	BCR	A	849	-	-	7/29/63/63	0/2/2/2
14	CLA	F	201	-	1/1/12/20	11/23/99/115	-
17	BCR	B	849	-	-	4/18/35/63	0/1/1/2
14	CLA	B	842	-	1/1/11/20	4/17/93/115	-
14	CLA	B	810	-	1/1/14/20	9/33/109/115	-
14	CLA	1	809	1	1/1/15/20	23/39/115/115	-
17	BCR	2	850	-	-	19/29/63/63	0/2/2/2
14	CLA	1	816	-	-	3/15/91/115	-
14	CLA	a	809	-	1/1/15/20	14/39/115/115	-
14	CLA	2	816	-	1/1/11/20	7/17/93/115	-
14	CLA	1	838	-	1/1/15/20	11/39/115/115	-
14	CLA	2	838	-	1/1/11/20	5/17/93/115	-
14	CLA	b	810	-	1/1/14/20	9/33/109/115	-
14	CLA	8	4002	-	-	8/15/91/115	-
16	SF4	C	102	3	-	-	0/6/5/5
14	CLA	A	806	-	1/1/12/20	3/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	LHG	2	852	-	-	22/43/43/53	-
14	CLA	6	4404	-	1/1/11/20	7/15/91/115	-
14	CLA	b	827	-	1/1/12/20	2/21/97/115	-
14	CLA	B	832	-	1/1/14/20	12/33/109/115	-
14	CLA	B	807	-	1/1/12/20	10/26/102/115	-
14	CLA	b	809	-	1/1/15/20	24/39/115/115	-
14	CLA	B	839	-	1/1/11/20	5/17/93/115	-
17	BCR	8	4001	-	-	12/29/63/63	0/2/2/2
14	CLA	b	832	-	1/1/11/20	6/15/91/115	-
14	CLA	B	837	-	1/1/11/20	4/15/91/115	-
14	CLA	b	807	-	1/1/12/20	10/26/102/115	-
14	CLA	1	827	-	1/1/13/20	6/27/103/115	-
14	CLA	2	814	-	1/1/11/20	11/15/91/115	-
14	CLA	b	811	-	1/1/15/20	16/39/115/115	-
17	BCR	a	849	-	-	7/29/63/63	0/2/2/2
17	BCR	a	850	-	-	19/29/63/63	0/2/2/2
14	CLA	f	201	-	1/1/12/20	11/23/99/115	-
14	CLA	A	812	-	1/1/11/20	8/15/91/115	-
14	CLA	1	807	-	1/1/15/20	14/39/115/115	-
14	CLA	B	801	-	1/1/14/20	11/33/109/115	-
14	CLA	A	840	-	1/1/11/20	3/18/94/115	-
14	CLA	1	810	1	1/1/12/20	8/21/97/115	-
14	CLA	1	832	-	1/1/12/20	3/21/97/115	-
14	CLA	A	824	-	1/1/11/20	13/20/96/115	-
14	CLA	2	820	-	1/1/14/20	15/33/109/115	-
14	CLA	B	816	-	1/1/15/20	22/39/115/115	-
17	BCR	F	206	-	-	14/29/63/63	0/2/2/2
16	SF4	3	101	3	-	-	0/6/5/5
14	CLA	a	823	-	1/1/14/20	8/33/109/115	-
17	BCR	L	1504	-	-	14/29/63/63	0/2/2/2
14	CLA	b	837	-	1/1/11/20	4/15/91/115	-
14	CLA	A	807	-	1/1/15/20	17/39/115/115	-
14	CLA	B	820	-	-	8/27/103/115	-
14	CLA	a	817	-	1/1/11/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	814	-	1/1/13/20	10/27/103/115	-
14	CLA	2	840	-	1/1/14/20	8/36/112/115	-
15	PQN	2	845	-	-	10/23/43/43	0/2/2/2
17	BCR	L	1505	-	-	13/29/63/63	0/2/2/2
12	LHG	B	853	-	-	22/43/43/53	-
17	BCR	b	853	-	-	13/29/63/63	0/2/2/2
19	LMT	i	4101	-	-	8/21/61/61	0/2/2/2
14	CLA	A	814	-	1/1/12/20	11/26/102/115	-
14	CLA	B	806	-	1/1/15/20	14/39/115/115	-
14	CLA	B	814	-	1/1/11/20	5/15/91/115	-
14	CLA	B	821	-	1/1/14/20	15/33/109/115	-
14	CLA	l	4206	-	1/1/15/20	14/39/115/115	-
14	CLA	b	812	-	1/1/14/20	13/35/111/115	-
12	LHG	a	801	-	-	22/53/53/53	-
14	CLA	A	815	-	1/1/13/20	10/27/103/115	-
14	CLA	A	826	-	1/1/13/20	15/32/108/115	-
14	CLA	b	840	-	1/1/14/20	8/36/112/115	-
14	CLA	a	805	-	1/1/15/20	10/39/115/115	-
14	CLA	2	836	-	1/1/11/20	4/15/91/115	-
14	CLA	1	833	-	1/1/15/20	16/39/115/115	-
14	CLA	a	824	-	1/1/15/20	13/39/115/115	-
14	CLA	b	818	-	1/1/13/20	10/27/103/115	-
14	CLA	b	801	-	1/1/15/20	11/39/115/115	-
18	LMG	0	203	-	-	21/41/61/70	0/1/1/1
14	CLA	B	838	-	1/1/11/20	4/15/91/115	-
14	CLA	j	101	-	1/1/11/20	8/15/91/115	-
17	BCR	k	4001	-	-	12/29/63/63	0/2/2/2
19	LMT	F	202	-	-	3/21/61/61	0/2/2/2
18	LMG	0	201	-	-	20/33/53/70	0/1/1/1
17	BCR	2	847	-	-	7/29/63/63	0/2/2/2
14	CLA	B	815	-	1/1/11/20	11/15/91/115	-
17	BCR	f	206	-	-	13/29/63/63	0/2/2/2
14	CLA	B	802	-	1/1/15/20	11/39/115/115	-
16	SF4	1	846	2,1	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	BCR	1	847	-	-	11/29/63/63	0/2/2/2
17	BCR	a	851	-	-	21/29/63/63	0/2/2/2
17	BCR	0	204	-	-	13/29/63/63	0/2/2/2
14	CLA	1	828	-	1/1/15/20	11/39/115/115	-
14	CLA	B	834	-	1/1/13/20	14/27/103/115	-
14	CLA	b	815	-	1/1/15/20	22/39/115/115	-
14	CLA	a	807	-	1/1/12/20	3/21/97/115	-
14	CLA	2	818	-	1/1/13/20	10/27/103/115	-
14	CLA	2	828	-	1/1/15/20	9/39/115/115	-
14	CLA	2	839	-	1/1/12/20	7/21/97/115	-
17	BCR	A	850	-	-	19/29/63/63	0/2/2/2
14	CLA	2	830	-	1/1/15/20	8/39/115/115	-
14	CLA	a	828	-	1/1/15/20	14/39/115/115	-
14	CLA	1	839	-	1/1/11/20	3/18/94/115	-
17	BCR	B	850	-	-	15/29/63/63	0/2/2/2
18	LMG	1	852	-	-	8/27/47/70	0/1/1/1
17	BCR	f	203	-	-	13/29/63/63	0/2/2/2
14	CLA	B	829	-	1/1/15/20	9/39/115/115	-
14	CLA	B	826	-	-	6/15/91/115	-
12	LHG	A	801	-	-	22/53/53/53	-
14	CLA	2	808	-	1/1/15/20	24/39/115/115	-
12	LHG	A	802	14	-	13/37/37/53	-
18	LMG	B	803	-	-	20/43/63/70	0/1/1/1
14	CLA	A	819	-	1/1/12/20	7/26/102/115	-
14	CLA	1	815	-	1/1/11/20	4/15/91/115	-
17	BCR	b	850	-	-	19/29/63/63	0/2/2/2
17	BCR	0	210	-	-	13/29/63/63	0/2/2/2
14	CLA	a	815	-	1/1/12/20	11/26/102/115	-
14	CLA	a	826	-	1/1/12/20	10/23/99/115	-
15	PQN	B	846	-	-	10/23/43/43	0/2/2/2
18	LMG	2	802	-	-	20/43/63/70	0/1/1/1
14	CLA	a	836	-	1/1/15/20	7/39/115/115	-
14	CLA	b	836	-	1/1/11/20	4/15/91/115	-
14	CLA	b	838	-	1/1/11/20	5/17/93/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	LMG	b	803	-	-	20/43/63/70	0/1/1/1
14	CLA	B	823	-	-	7/15/91/115	-
14	CLA	2	804	-	1/1/15/20	13/39/115/115	-

The worst 5 of 2926 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	803	CL0	C1B-C2B	8.20	1.48	1.39
13	1	803	CL0	C1B-C2B	8.13	1.48	1.39
13	a	803	CL0	C1B-C2B	8.09	1.48	1.39
13	a	803	CL0	C3B-C4B	6.64	1.47	1.41
13	A	803	CL0	C3B-C4B	6.63	1.47	1.41

The worst 5 of 2695 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	NA
13	A	803	CL0	NC
13	A	803	CL0	ND
13	a	803	CL0	NA
13	a	803	CL0	NC

5 of 4268 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.

359 monomers are involved in 953 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	821	CLA	4	0
14	2	805	CLA	3	0
17	i	4103	BCR	3	0
14	b	843	CLA	5	0
14	A	832	CLA	7	0
17	1	850	BCR	6	0
17	b	846	BCR	2	0
14	1	829	CLA	11	0
14	1	826	CLA	8	0
14	2	819	CLA	3	0
14	A	820	CLA	4	0
14	A	828	CLA	4	0
14	b	816	CLA	1	0
14	b	833	CLA	1	0
14	a	829	CLA	3	0
17	J	104	BCR	2	0
14	B	822	CLA	2	0
14	B	830	CLA	2	0
14	A	810	CLA	7	0
19	I	103	LMT	1	0
14	B	804	CLA	7	0
17	B	848	BCR	2	0
14	B	817	CLA	1	0
14	B	835	CLA	1	0
14	a	843	CLA	5	0
14	a	842	CLA	7	0
14	1	823	CLA	1	0
14	a	813	CLA	2	0
14	l	4205	CLA	4	0
17	l	4207	BCR	1	0
17	I	102	BCR	4	0
19	h	103	LMT	1	0
17	6	4402	BCR	4	0
17	i	4102	BCR	2	0
17	9	102	BCR	4	0
14	A	804	CLA	5	0
14	a	814	CLA	4	0
14	b	835	CLA	3	0
14	A	837	CLA	1	0
14	2	825	CLA	5	0
14	A	817	CLA	1	0
14	2	831	CLA	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	7	1101	CLA	7	0
14	1	830	CLA	4	0
14	2	803	CLA	9	0
14	B	844	CLA	5	0
14	1	835	CLA	6	0
16	3	102	SF4	1	0
14	a	820	CLA	1	0
14	2	817	CLA	2	0
14	b	820	CLA	2	0
17	A	847	BCR	2	0
17	J	103	BCR	3	0
14	b	804	CLA	8	0
14	L	1502	CLA	2	0
14	J	101	CLA	1	0
17	2	851	BCR	5	0
14	B	825	CLA	1	0
14	A	821	CLA	3	0
17	M	102	BCR	5	0
14	8	4003	CLA	1	0
14	A	825	CLA	1	0
17	h	102	BCR	3	0
14	6	4403	CLA	3	0
14	a	840	CLA	5	0
14	2	827	CLA	1	0
12	b	852	LHG	2	0
14	2	821	CLA	2	0
15	a	845	PQN	1	0
14	B	805	CLA	2	0
14	A	836	CLA	6	0
14	1	822	CLA	4	0
14	k	4003	CLA	1	0
17	1	849	BCR	1	0
14	F	205	CLA	2	0
14	2	842	CLA	5	0
14	a	806	CLA	6	0
13	a	803	CL0	3	0
14	B	818	CLA	2	0
14	f	204	CLA	1	0
14	2	813	CLA	1	0
14	a	804	CLA	10	0
14	k	4002	CLA	2	0
14	B	836	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	808	CLA	7	0
14	a	834	CLA	1	0
14	a	837	CLA	6	0
14	J	102	CLA	1	0
14	B	808	CLA	4	0
17	7	1104	BCR	7	0
15	A	845	PQN	1	0
14	A	827	CLA	8	0
14	2	807	CLA	2	0
14	2	833	CLA	1	0
17	B	854	BCR	6	0
15	1	845	PQN	1	0
14	2	841	CLA	2	0
18	L	1506	LMG	1	0
18	a	852	LMG	1	0
14	A	842	CLA	9	0
17	a	847	BCR	4	0
17	b	847	BCR	2	0
14	2	811	CLA	6	0
14	7	1103	CLA	1	0
14	a	812	CLA	2	0
14	b	826	CLA	2	0
14	1	813	CLA	2	0
14	1	836	CLA	1	0
14	a	818	CLA	1	0
17	8	4005	BCR	3	0
12	m	101	LHG	1	0
14	a	839	CLA	2	0
14	b	822	CLA	2	0
14	b	802	CLA	5	0
14	b	828	CLA	1	0
14	B	843	CLA	6	0
14	A	841	CLA	4	0
14	b	806	CLA	4	0
14	A	834	CLA	3	0
14	f	205	CLA	2	0
14	b	834	CLA	2	0
14	A	805	CLA	7	0
14	1	843	CLA	6	0
14	1	842	CLA	8	0
14	A	813	CLA	4	0
14	a	808	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	813	CLA	9	0
14	1	806	CLA	5	0
14	b	808	CLA	4	0
14	2	809	CLA	4	0
14	B	828	CLA	1	0
14	B	841	CLA	3	0
14	a	827	CLA	2	0
15	b	845	PQN	8	0
14	A	833	CLA	1	0
14	1	837	CLA	2	0
18	l	4202	LMG	1	0
17	b	854	BCR	5	0
17	A	851	BCR	4	0
14	2	837	CLA	2	0
14	L	1503	CLA	8	0
14	B	833	CLA	3	0
17	1	848	BCR	4	0
14	b	841	CLA	2	0
14	b	842	CLA	5	0
14	0	202	CLA	2	0
14	1	808	CLA	1	0
14	B	811	CLA	5	0
17	B	852	BCR	7	0
14	l	4203	CLA	9	0
14	A	830	CLA	9	0
14	A	811	CLA	2	0
14	1	834	CLA	4	0
17	B	847	BCR	2	0
14	a	838	CLA	1	0
14	L	1501	CLA	6	0
14	2	810	CLA	3	0
14	j	102	CLA	1	0
14	a	841	CLA	2	0
14	2	812	CLA	8	0
14	1	841	CLA	4	0
17	a	848	BCR	3	0
14	1	804	CLA	6	0
14	A	829	CLA	5	0
14	B	809	CLA	10	0
17	b	849	BCR	4	0
14	A	838	CLA	2	0
14	b	813	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	A	822	CLA	5	0
14	1	820	CLA	3	0
14	a	816	CLA	5	0
14	B	812	CLA	4	0
14	a	833	CLA	7	0
14	1	811	CLA	2	0
17	k	4004	BCR	3	0
14	2	806	CLA	2	0
17	K	4005	BCR	4	0
14	1	825	CLA	2	0
14	a	825	CLA	1	0
14	a	830	CLA	5	0
14	a	811	CLA	7	0
14	1	831	CLA	5	0
14	b	824	CLA	1	0
14	A	835	CLA	4	0
14	a	810	CLA	1	0
18	A	852	LMG	1	0
14	1	4204	CLA	6	0
14	1	840	CLA	4	0
14	A	831	CLA	5	0
14	b	830	CLA	3	0
17	B	851	BCR	8	0
14	b	817	CLA	2	0
12	1	801	LHG	4	0
14	K	4003	CLA	1	0
14	b	805	CLA	3	0
14	1	812	CLA	3	0
14	a	854	CLA	2	0
17	A	848	BCR	4	0
14	2	834	CLA	2	0
14	1	824	CLA	1	0
14	B	819	CLA	2	0
14	a	832	CLA	5	0
17	b	851	BCR	5	0
17	2	846	BCR	3	0
17	I	101	BCR	2	0
14	1	818	CLA	1	0
14	A	823	CLA	5	0
14	a	822	CLA	3	0
17	2	848	BCR	1	0
17	F	203	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
17	6	4406	BCR	6	0
14	2	843	CLA	4	0
14	b	819	CLA	2	0
14	a	821	CLA	4	0
17	K	4001	BCR	2	0
14	b	839	CLA	3	0
17	j	103	BCR	4	0
14	K	4004	CLA	2	0
17	1	851	BCR	3	0
14	2	801	CLA	8	0
14	B	831	CLA	4	0
14	2	822	CLA	2	0
14	B	840	CLA	4	0
14	a	835	CLA	4	0
16	c	102	SF4	1	0
14	K	4002	CLA	2	0
17	0	209	BCR	2	0
12	1	802	LHG	1	0
14	1	819	CLA	4	0
12	a	802	LHG	1	0
14	b	831	CLA	5	0
17	6	4405	BCR	1	0
17	2	849	BCR	4	0
14	b	825	CLA	6	0
14	B	827	CLA	2	0
14	A	809	CLA	1	0
17	h	101	BCR	3	0
14	2	835	CLA	2	0
14	2	829	CLA	2	0
14	b	821	CLA	2	0
14	2	815	CLA	9	0
14	2	826	CLA	2	0
14	0	208	CLA	12	0
14	b	829	CLA	2	0
14	8	4004	CLA	1	0
14	0	206	CLA	6	0
14	0	207	CLA	3	0
14	a	831	CLA	12	0
14	A	843	CLA	7	0
14	A	839	CLA	6	0
14	2	832	CLA	3	0
17	A	849	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	F	201	CLA	3	0
17	B	849	BCR	1	0
14	B	842	CLA	3	0
14	B	810	CLA	5	0
14	1	809	CLA	8	0
17	2	850	BCR	7	0
14	1	816	CLA	1	0
14	a	809	CLA	5	0
14	2	816	CLA	1	0
14	1	838	CLA	5	0
14	b	810	CLA	7	0
14	8	4002	CLA	2	0
16	C	102	SF4	1	0
12	2	852	LHG	2	0
14	6	4404	CLA	2	0
14	b	827	CLA	1	0
14	B	832	CLA	7	0
14	B	807	CLA	2	0
14	b	809	CLA	8	0
17	8	4001	BCR	2	0
14	b	832	CLA	3	0
14	B	837	CLA	1	0
14	b	807	CLA	1	0
14	1	827	CLA	3	0
14	b	811	CLA	5	0
17	a	849	BCR	1	0
17	a	850	BCR	6	0
14	f	201	CLA	4	0
14	A	812	CLA	2	0
14	1	807	CLA	7	0
14	B	801	CLA	9	0
14	A	840	CLA	2	0
14	1	810	CLA	2	0
14	1	832	CLA	1	0
14	A	824	CLA	1	0
14	2	820	CLA	1	0
14	B	816	CLA	8	0
17	F	206	BCR	1	0
14	a	823	CLA	3	0
17	L	1504	BCR	1	0
14	b	837	CLA	3	0
14	A	807	CLA	6	0

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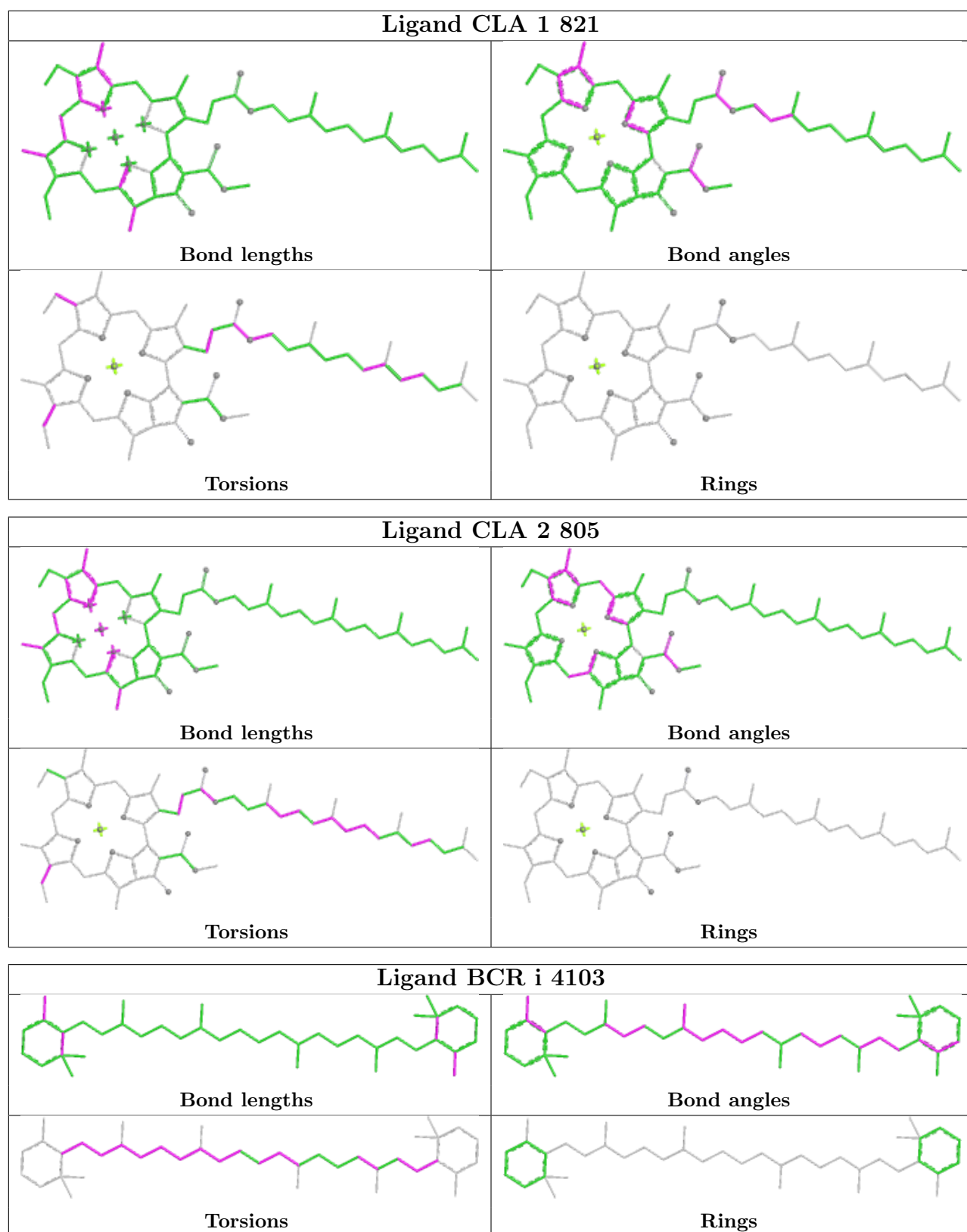
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	B	820	CLA	3	0
14	1	814	CLA	5	0
14	2	840	CLA	3	0
15	2	845	PQN	6	0
17	L	1505	BCR	9	0
12	B	853	LHG	2	0
17	b	853	BCR	8	0
19	i	4101	LMT	1	0
14	A	814	CLA	2	0
14	B	806	CLA	4	0
14	B	814	CLA	1	0
14	B	821	CLA	2	0
14	l	4206	CLA	12	0
14	b	812	CLA	5	0
12	a	801	LHG	6	0
14	A	815	CLA	5	0
14	A	826	CLA	2	0
14	b	840	CLA	2	0
14	a	805	CLA	5	0
14	2	836	CLA	1	0
14	1	833	CLA	4	0
14	a	824	CLA	5	0
14	b	818	CLA	2	0
14	b	801	CLA	2	0
18	0	203	LMG	1	0
14	B	838	CLA	2	0
14	j	101	CLA	1	0
17	k	4001	BCR	2	0
18	0	201	LMG	2	0
17	2	847	BCR	3	0
17	f	206	BCR	1	0
14	B	802	CLA	3	0
17	1	847	BCR	2	0
17	a	851	BCR	2	0
17	0	204	BCR	8	0
14	1	828	CLA	5	0
14	B	834	CLA	1	0
14	b	815	CLA	9	0
14	2	818	CLA	1	0
14	2	828	CLA	1	0
14	2	839	CLA	3	0
17	A	850	BCR	6	0

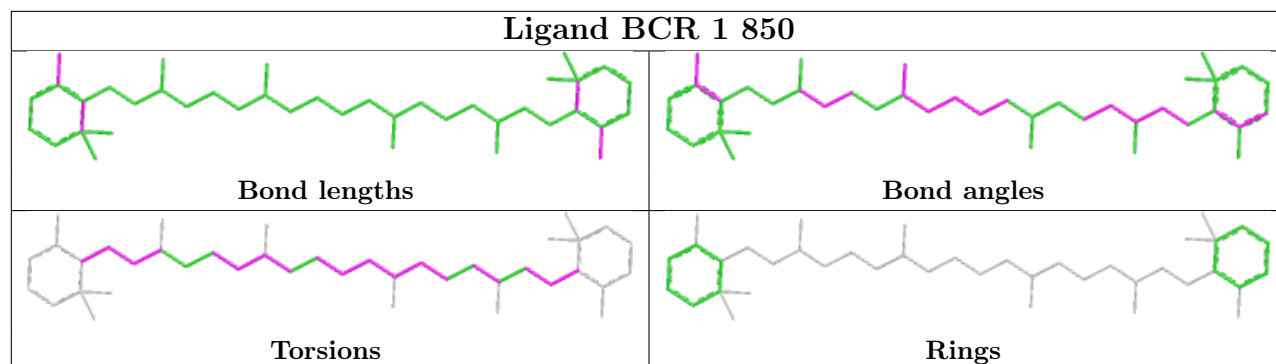
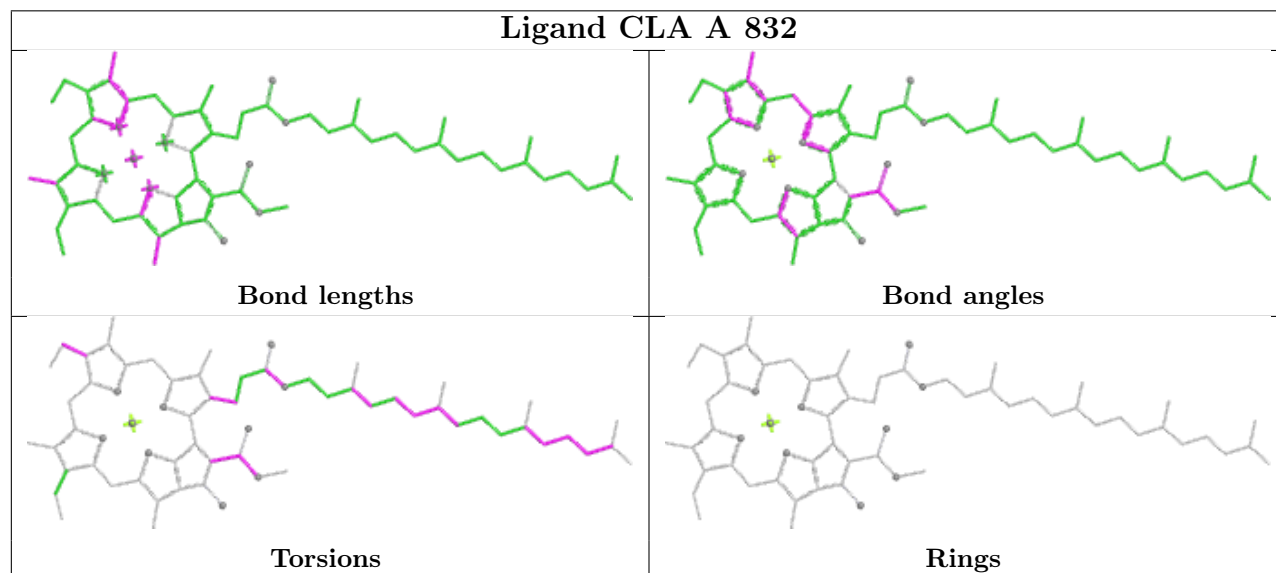
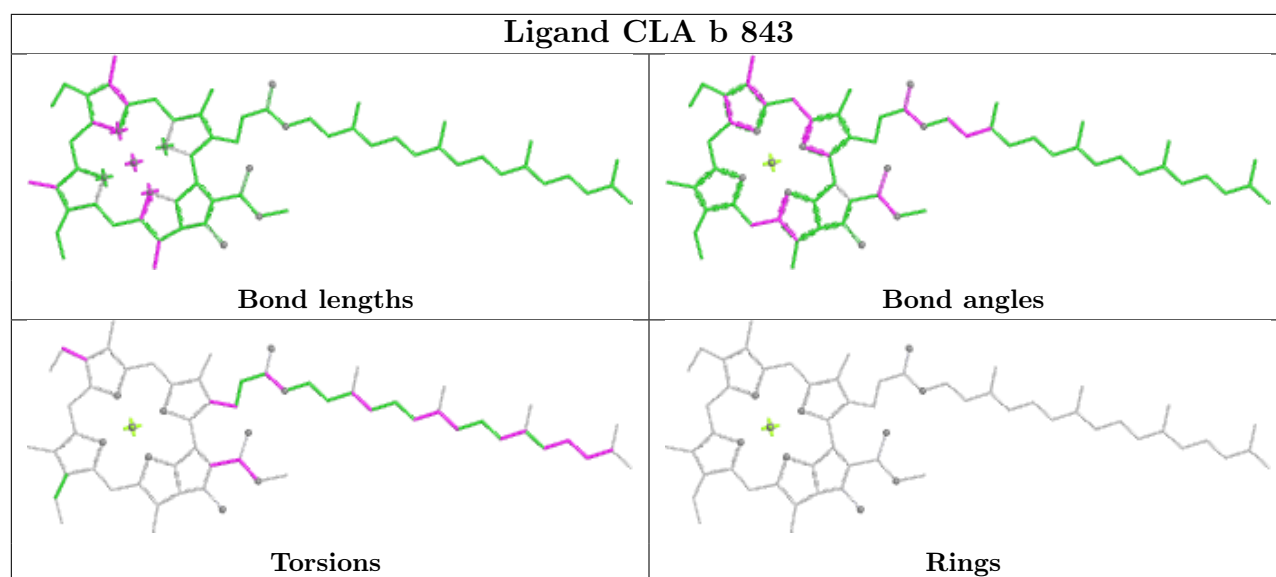
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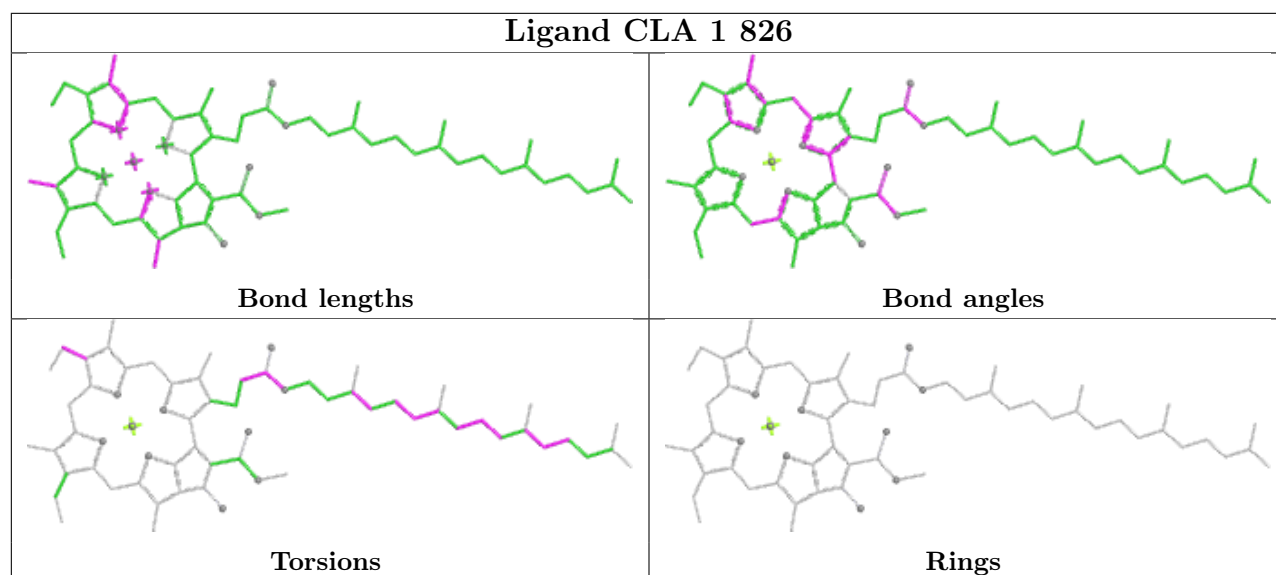
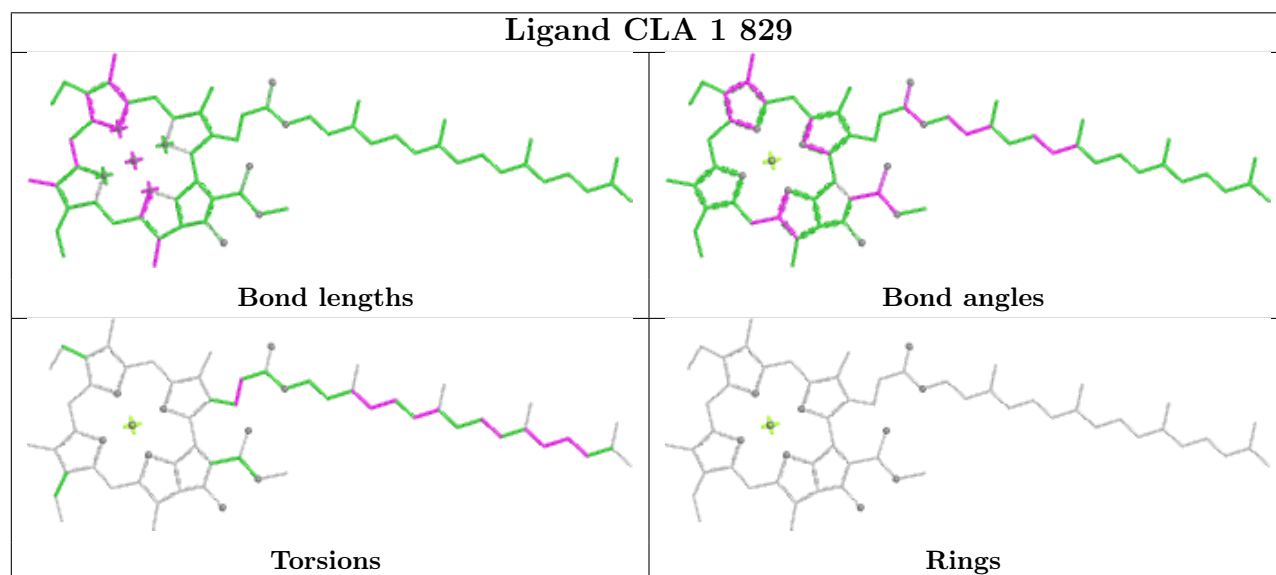
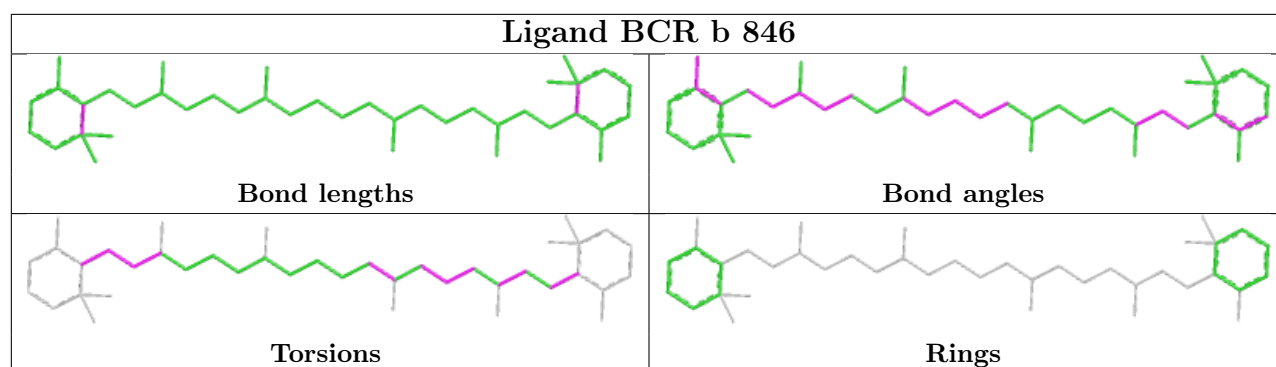
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	830	CLA	4	0
14	a	828	CLA	7	0
14	1	839	CLA	2	0
17	B	850	BCR	4	0
17	f	203	BCR	4	0
14	B	829	CLA	2	0
14	B	826	CLA	5	0
12	A	801	LHG	4	0
14	2	808	CLA	10	0
12	A	802	LHG	1	0
18	B	803	LMG	4	0
14	A	819	CLA	1	0
17	b	850	BCR	8	0
17	0	210	BCR	8	0
14	a	815	CLA	2	0
14	a	826	CLA	1	0
15	B	846	PQN	9	0
18	2	802	LMG	3	0
14	a	836	CLA	5	0
14	b	836	CLA	2	0
18	b	803	LMG	3	0
14	B	823	CLA	2	0
14	2	804	CLA	1	0

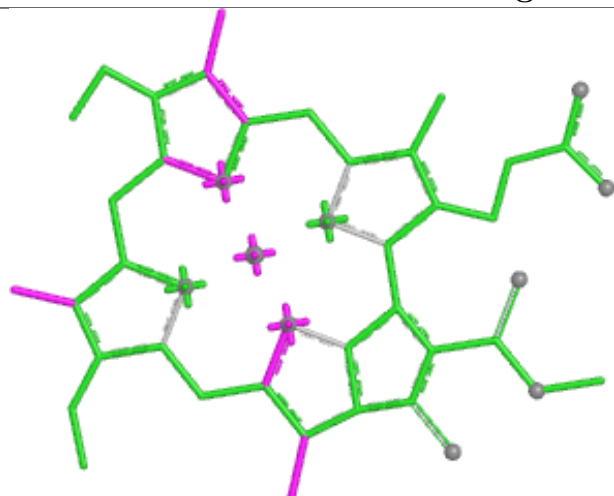
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



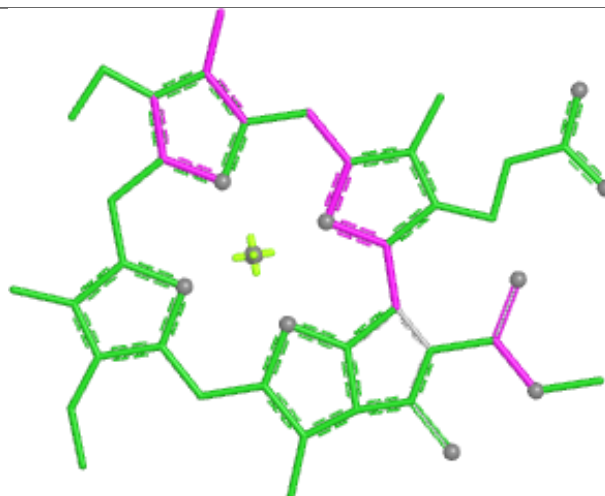




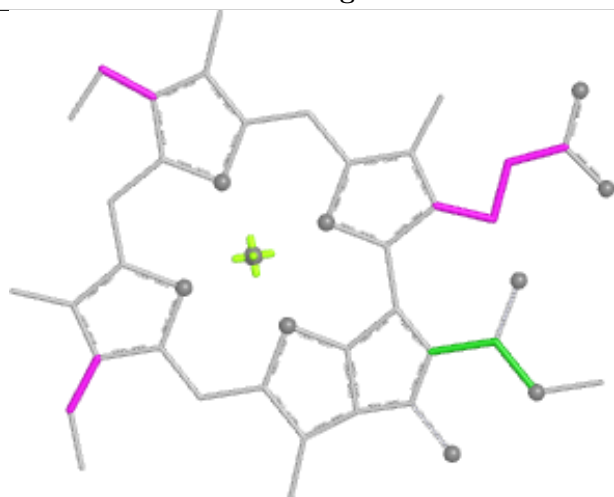
Ligand CLA F 204



Bond lengths



Bond angles

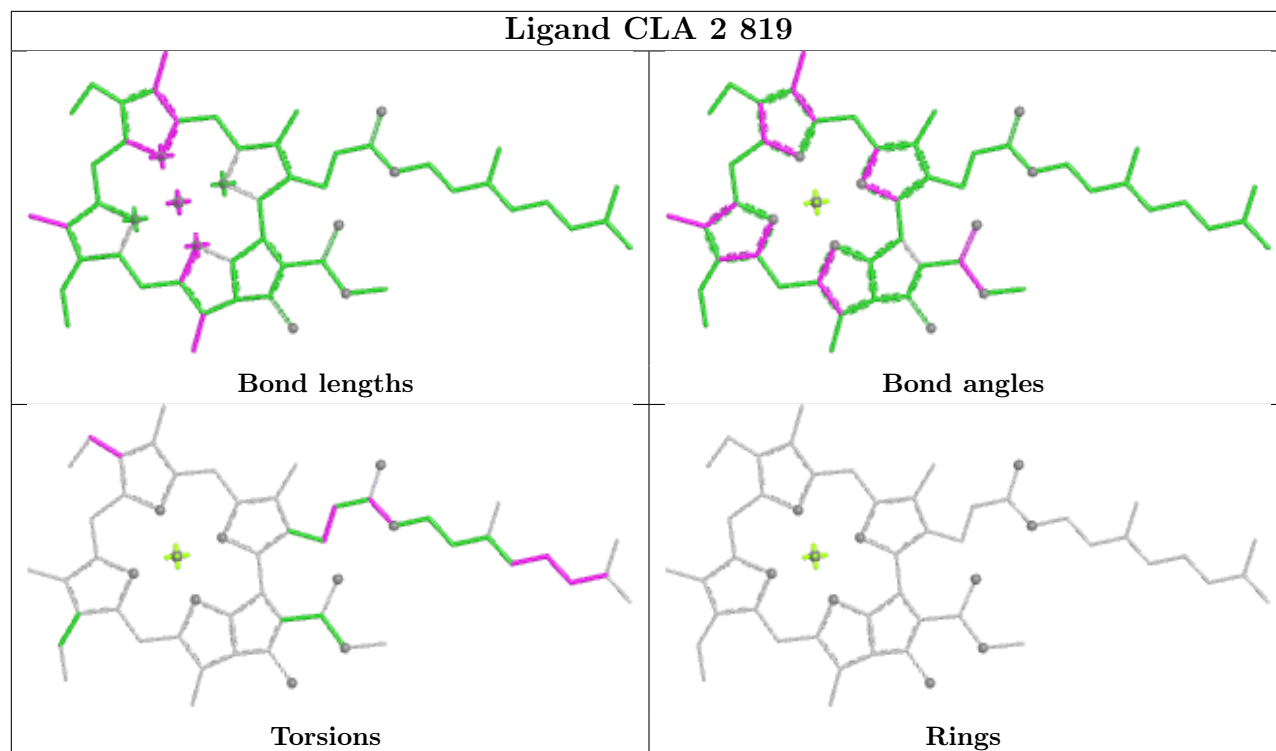


Torsions

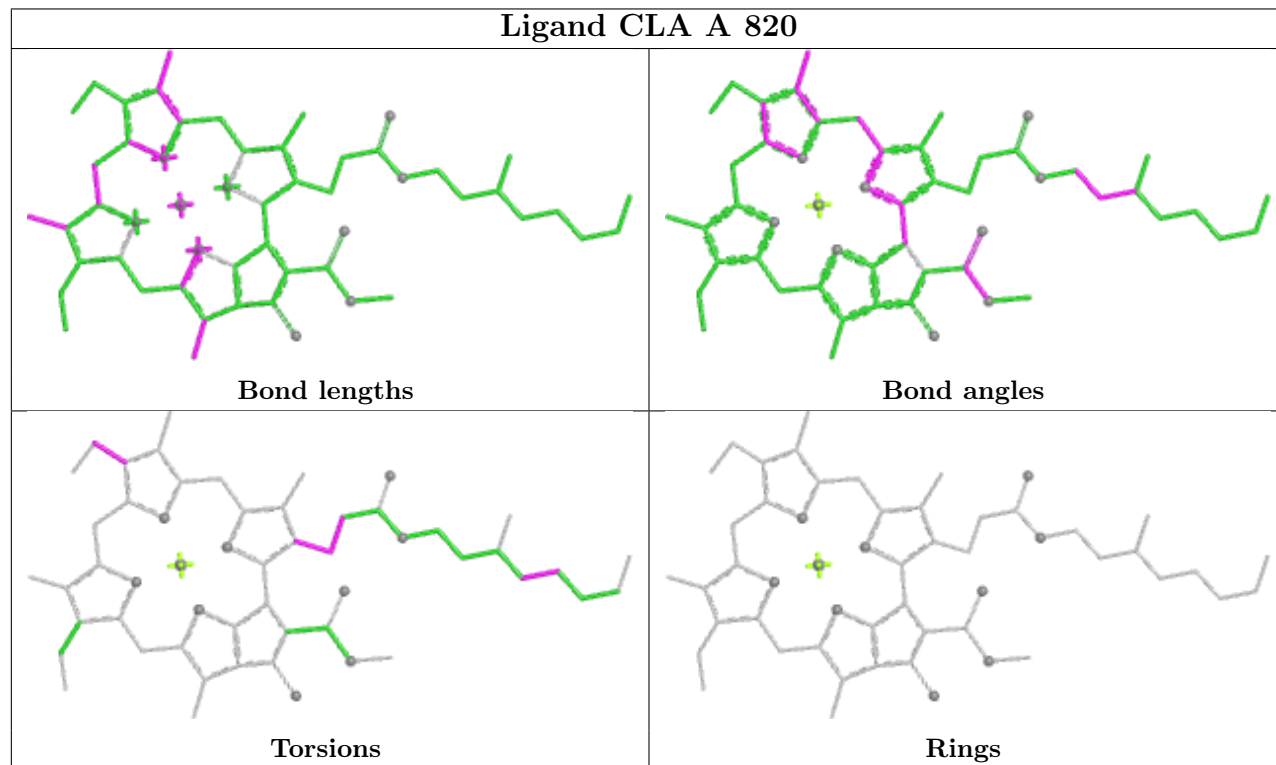


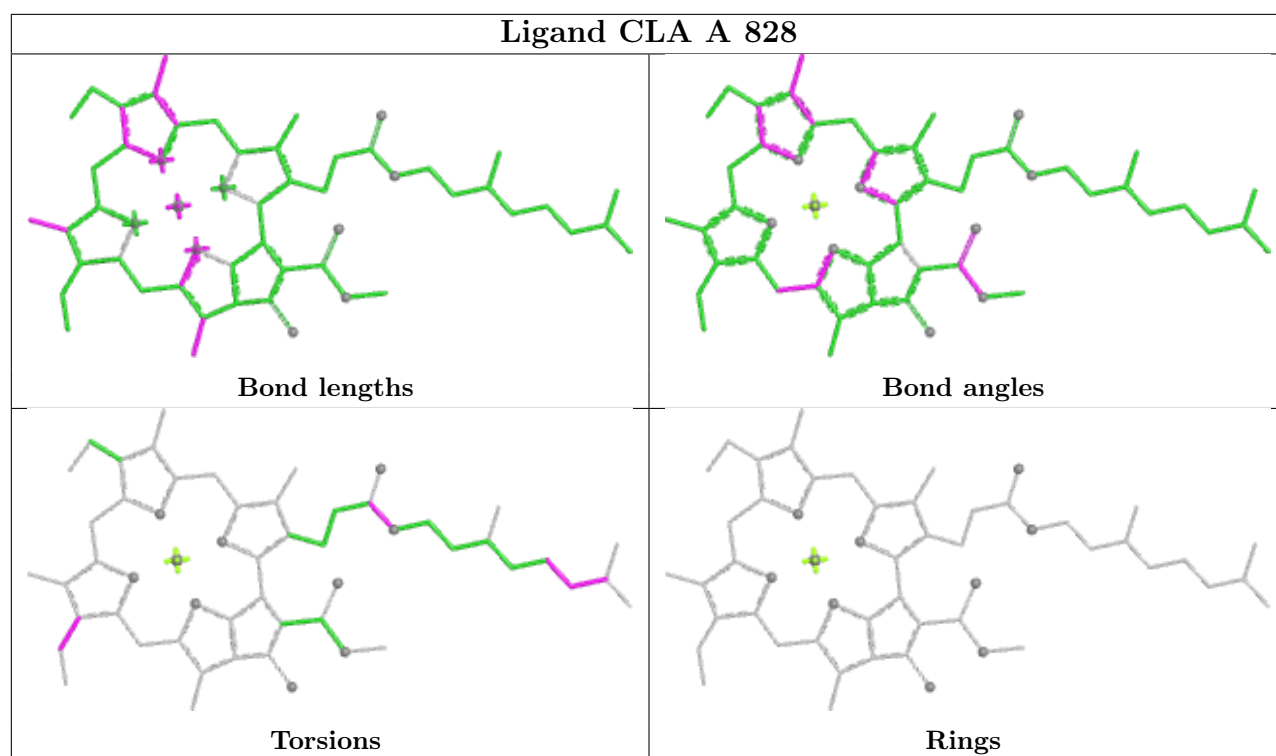
Rings

Ligand CLA 2 819

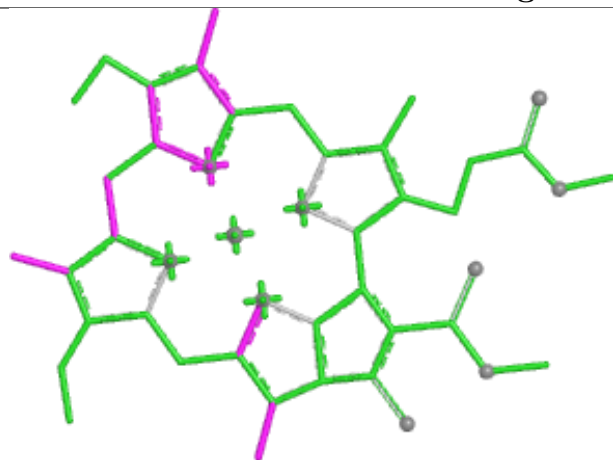


Ligand CLA A 820

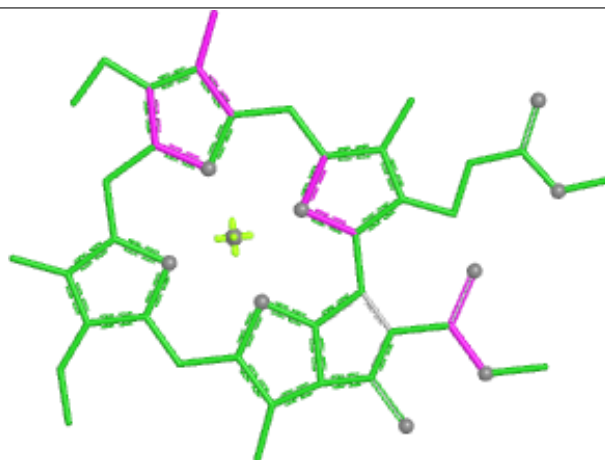




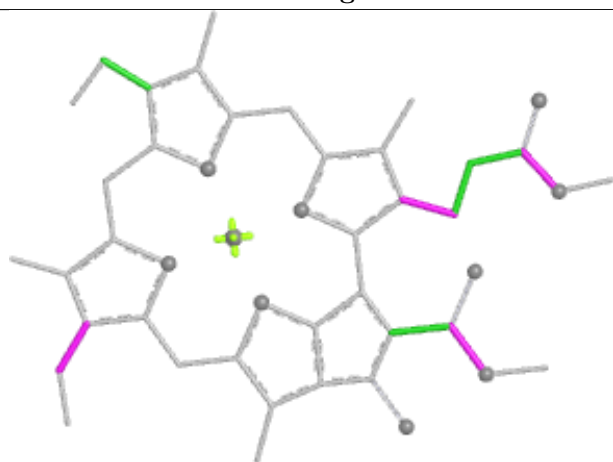
Ligand CLA b 816



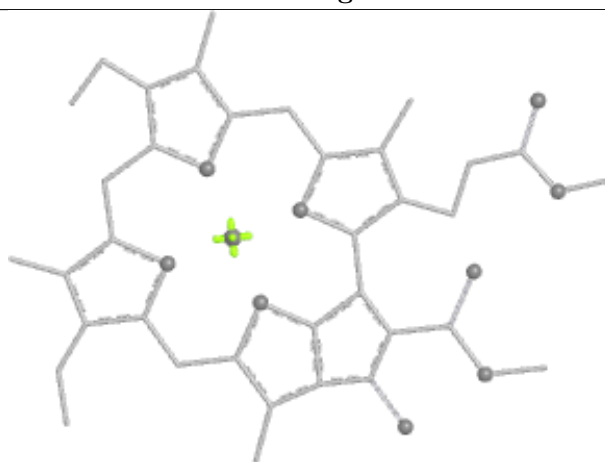
Bond lengths



Bond angles

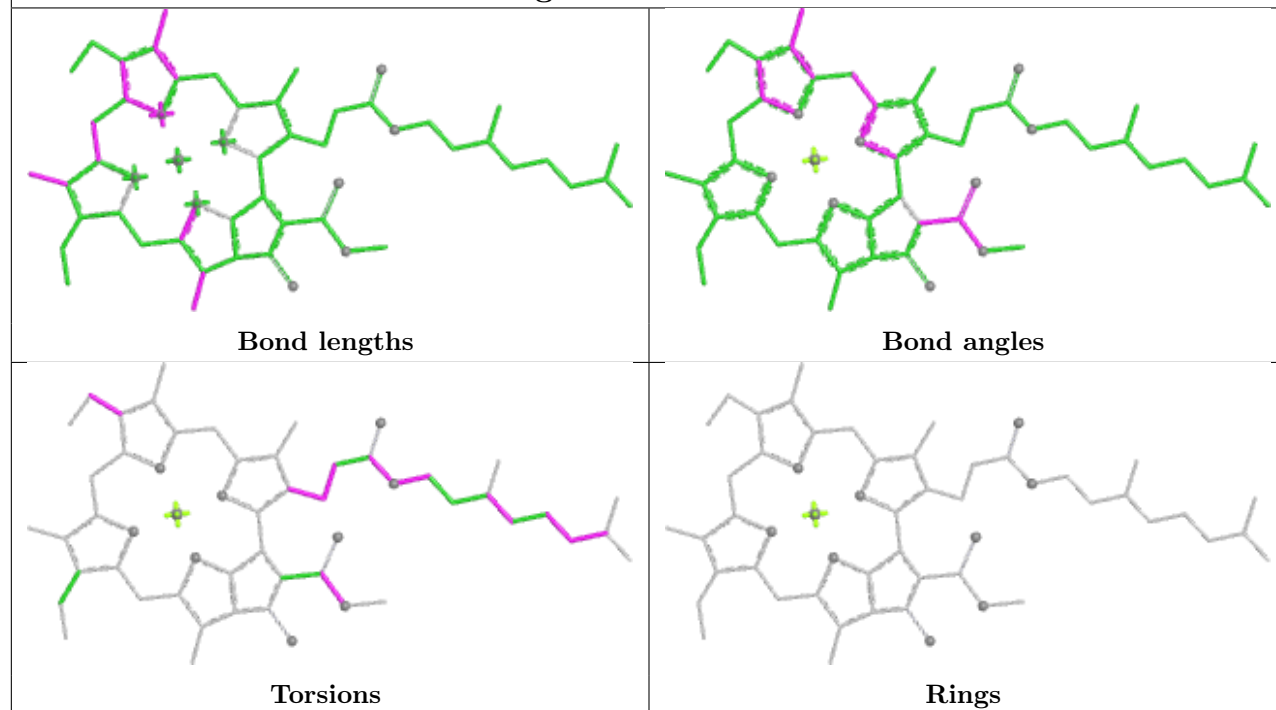


Torsions

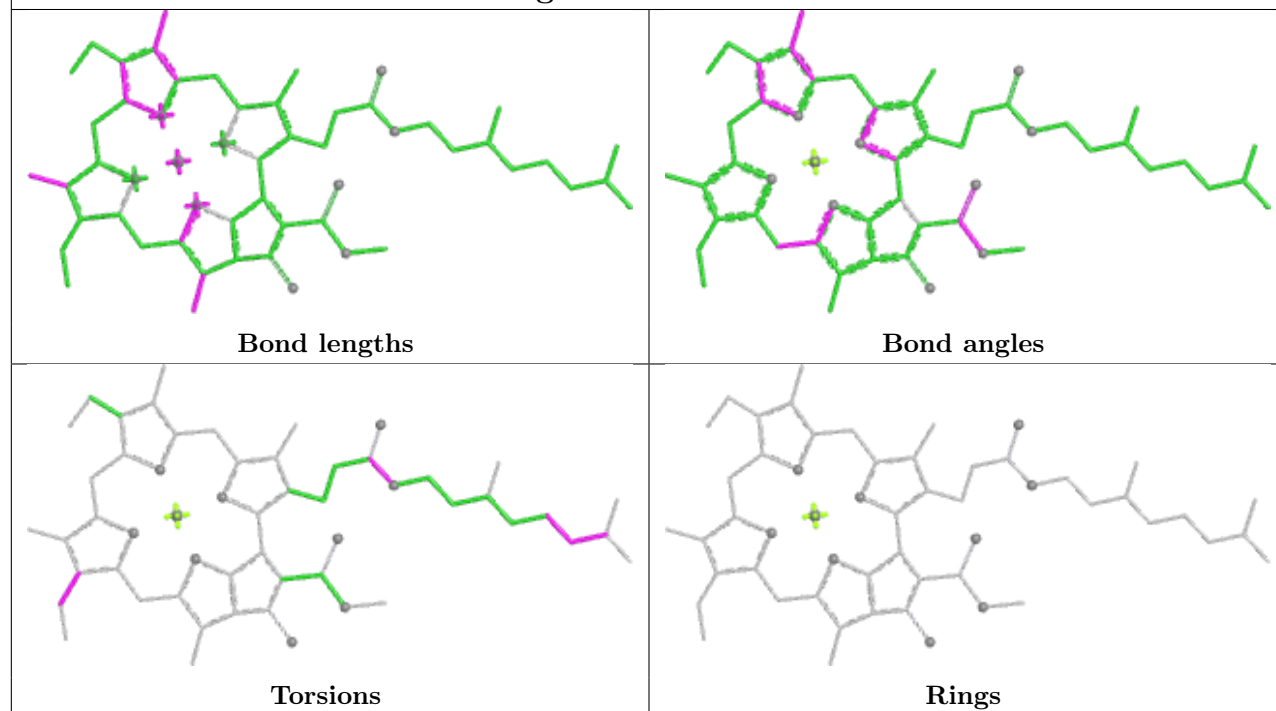


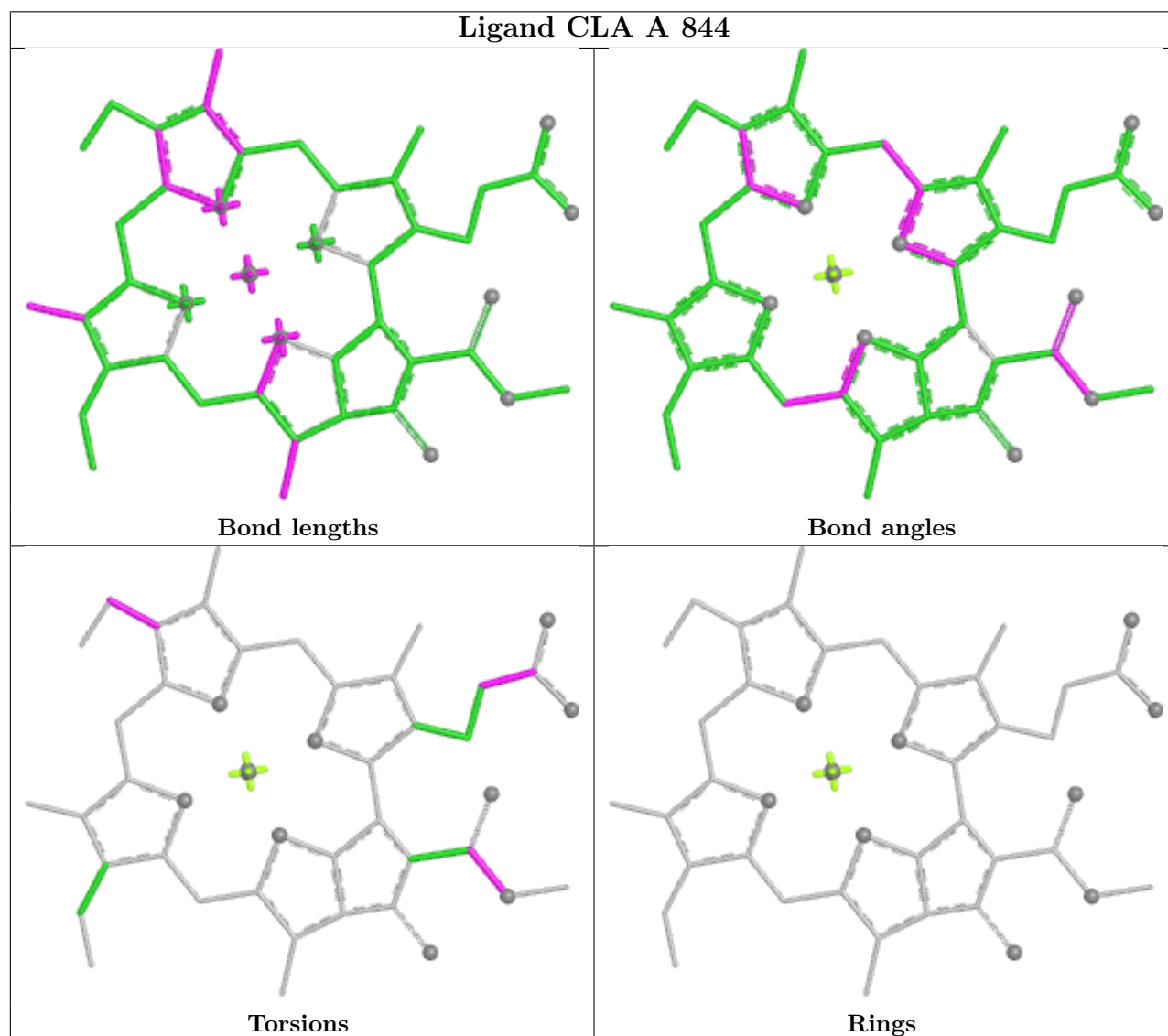
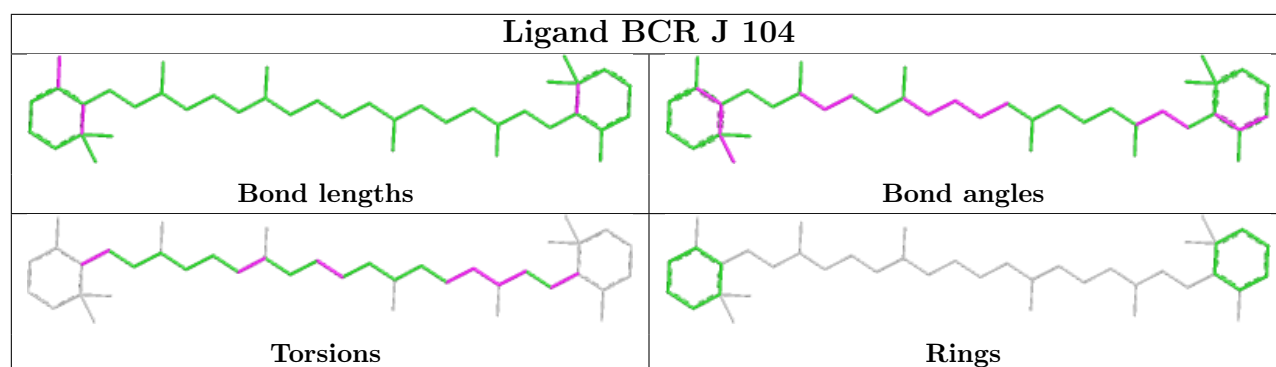
Rings

Ligand CLA b 833

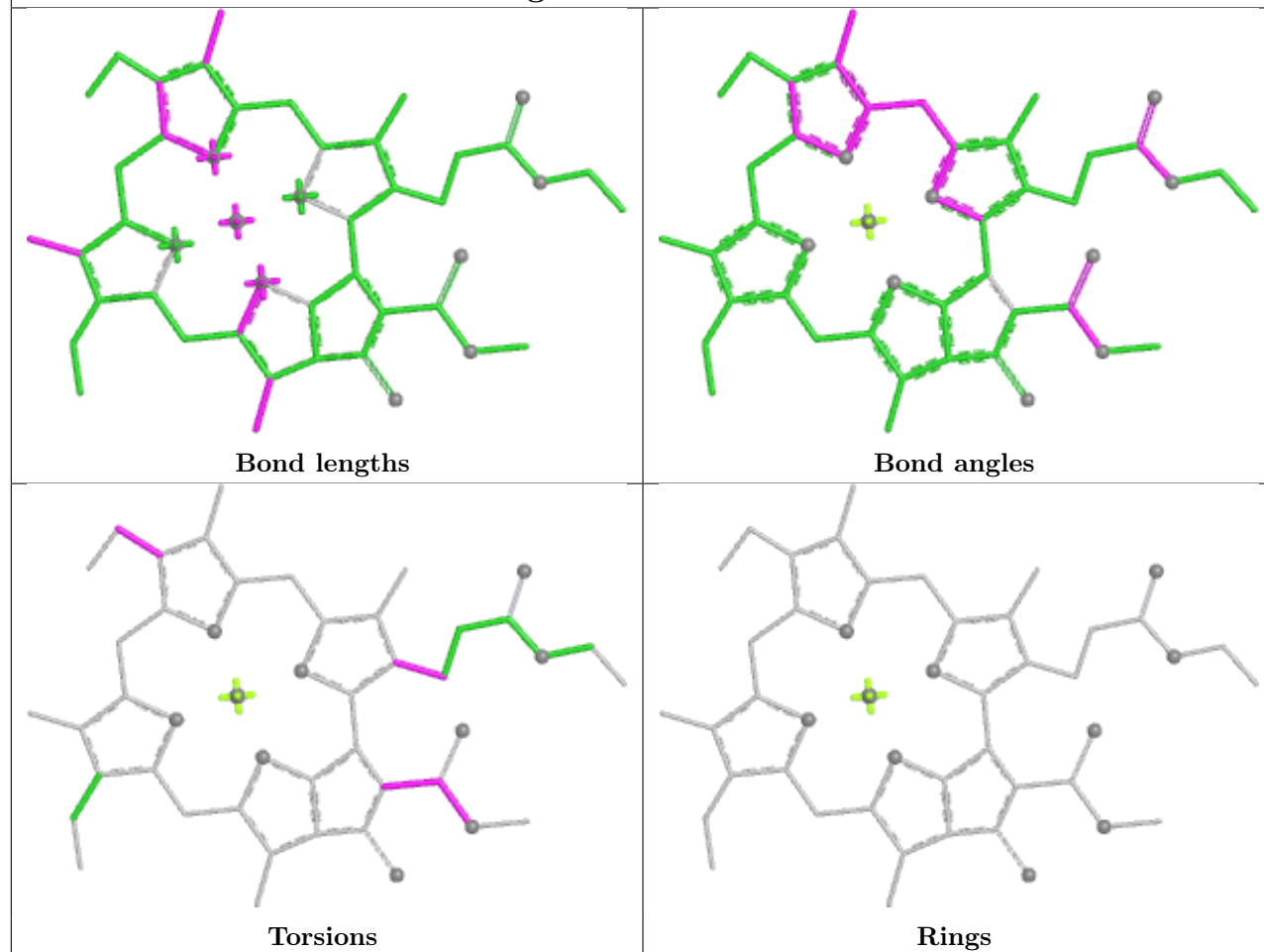


Ligand CLA a 829

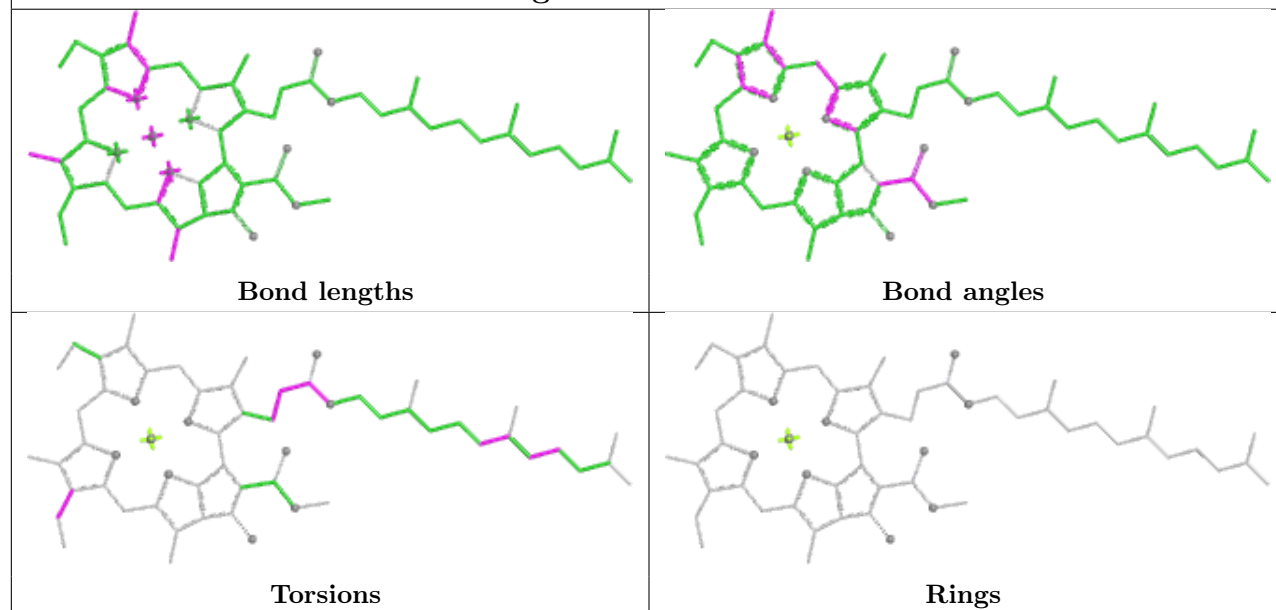




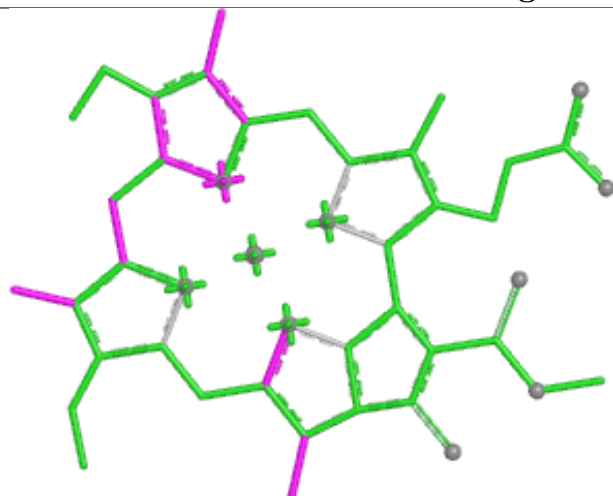
Ligand CLA B 822



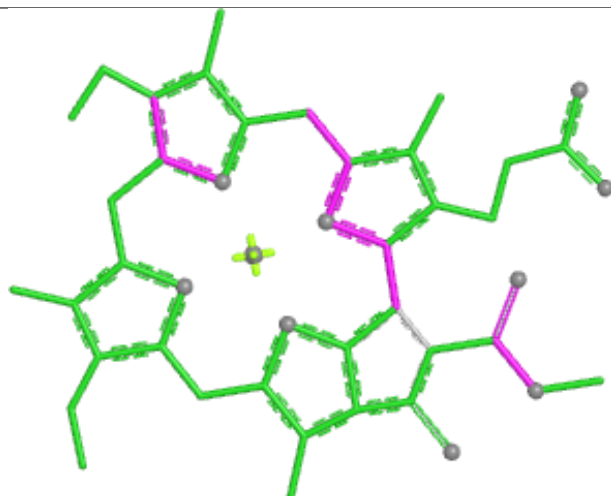
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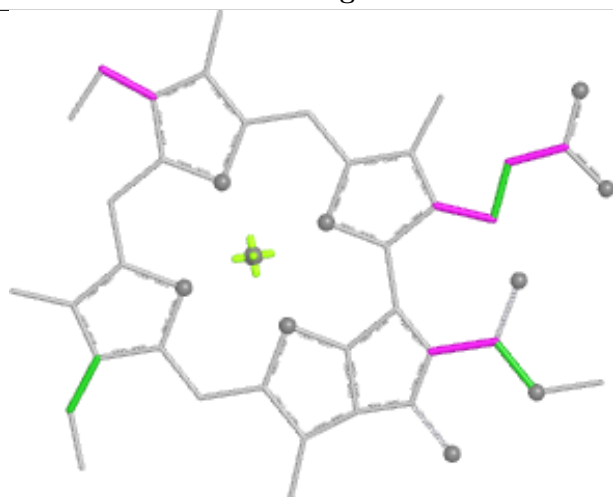
Ligand CLA 2 823



Bond lengths



Bond angles

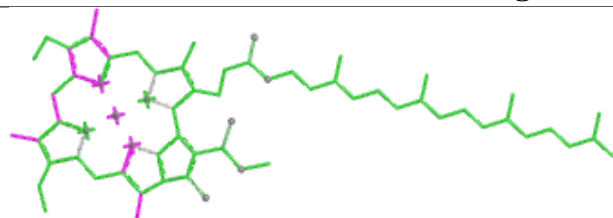


Torsions

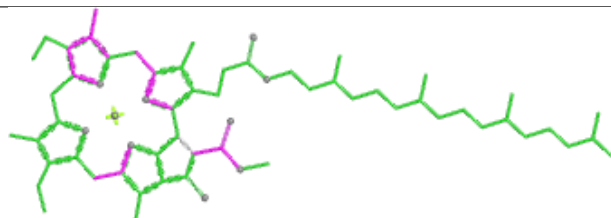


Rings

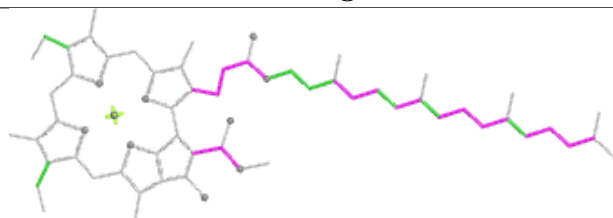
Ligand CLA A 810



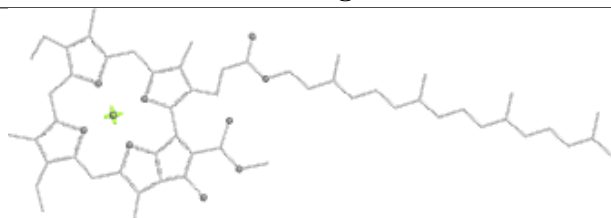
Bond lengths



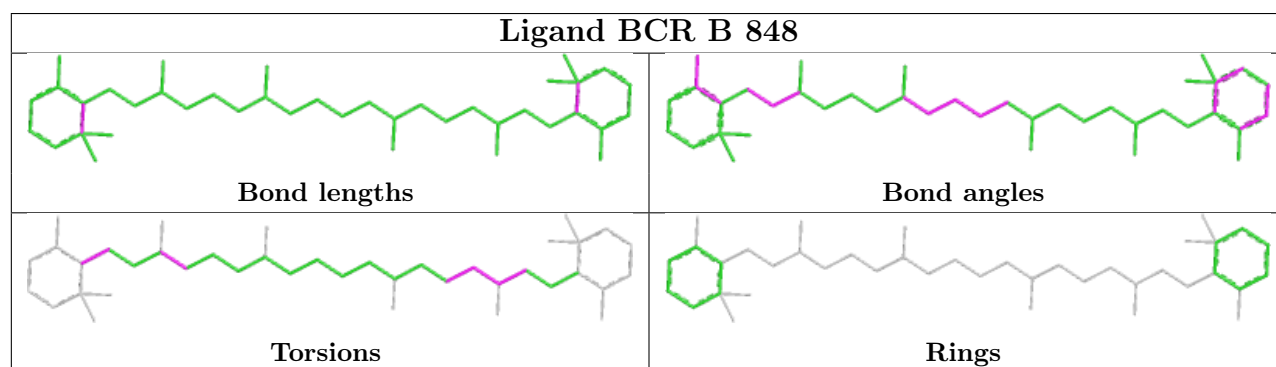
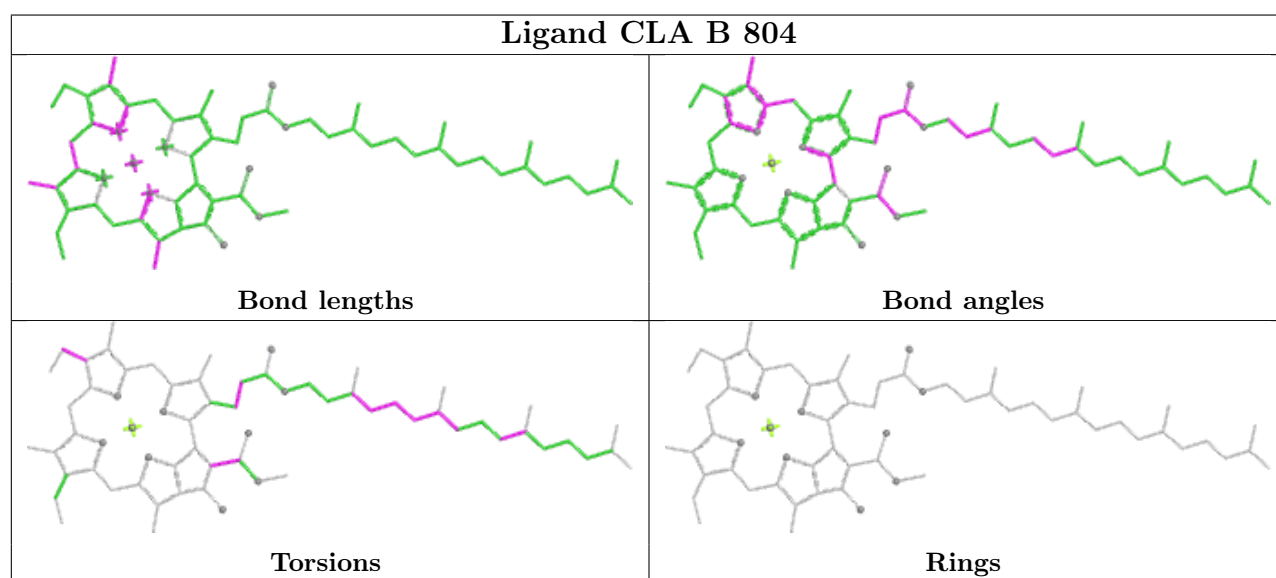
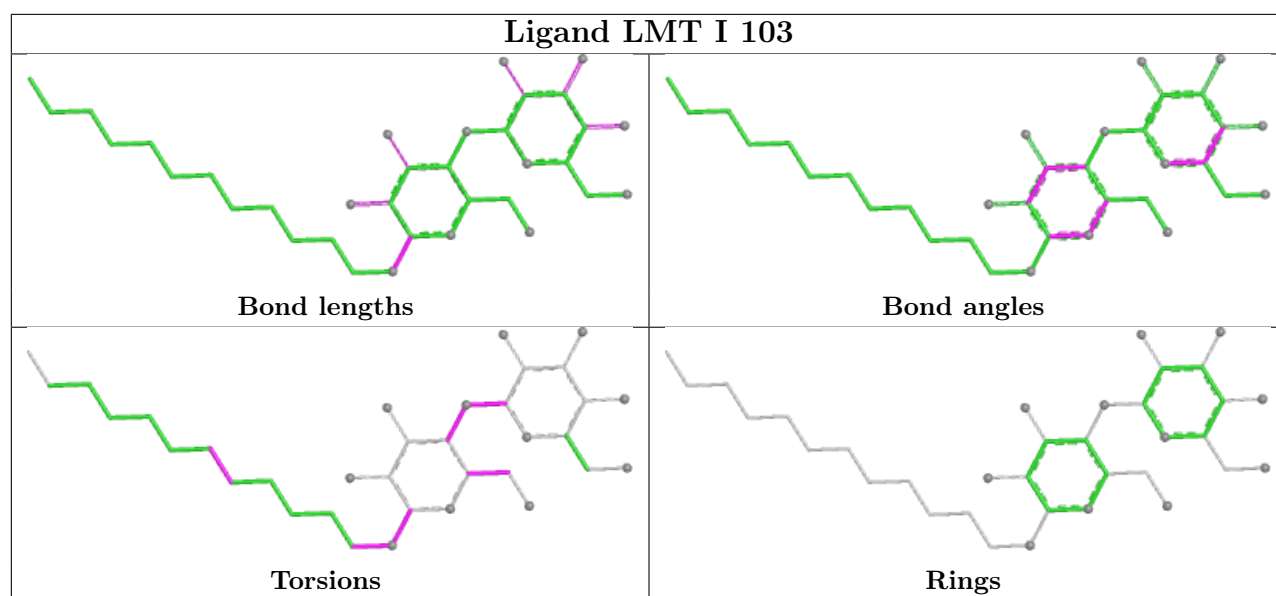
Bond angles



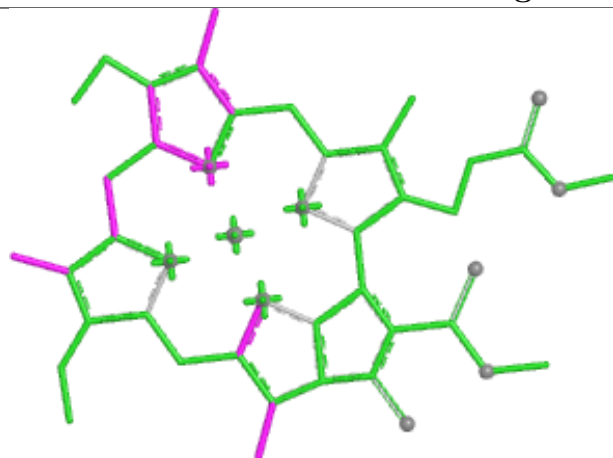
Torsions



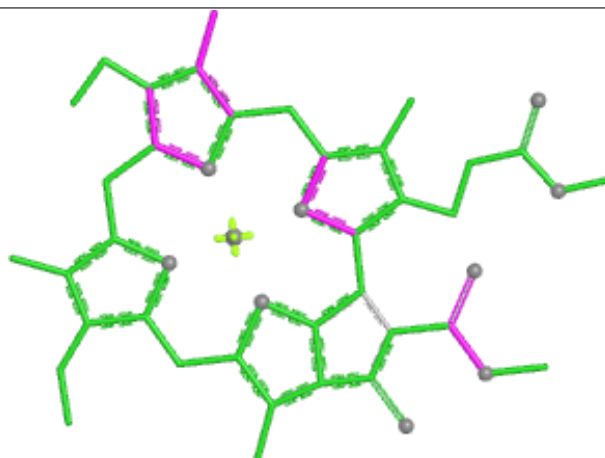
Rings



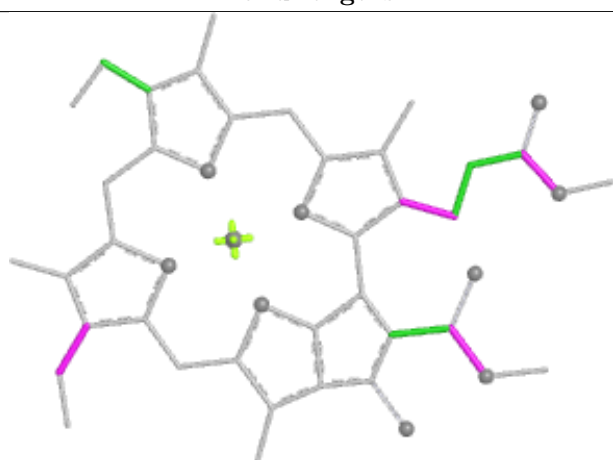
Ligand CLA B 817



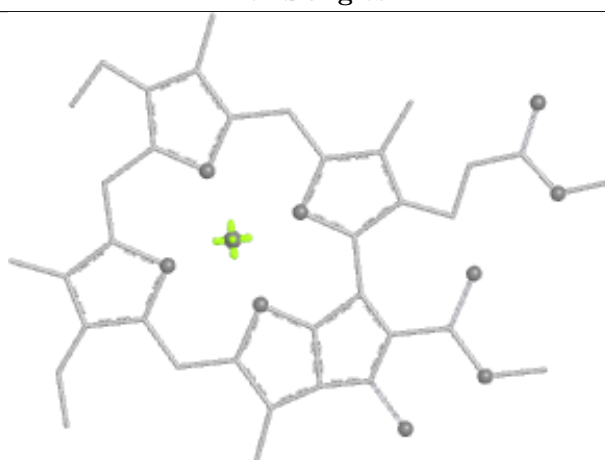
Bond lengths



Bond angles

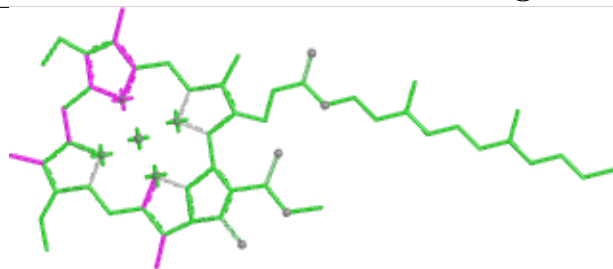


Torsions

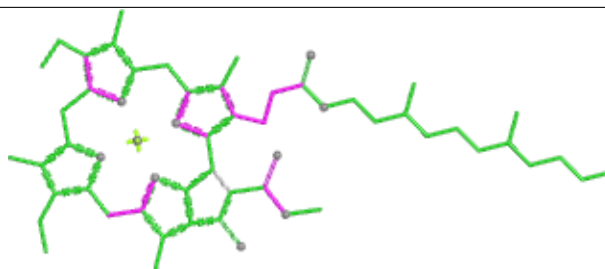


Rings

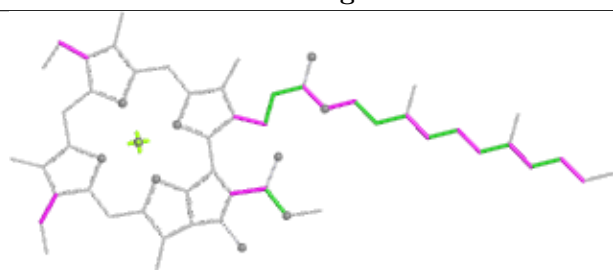
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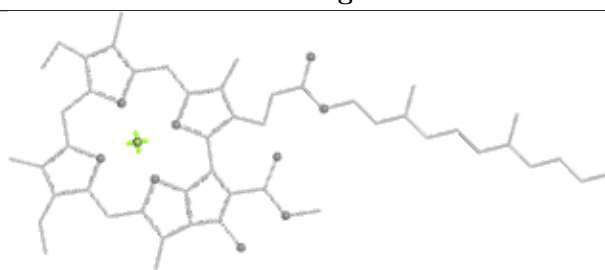
Bond lengths



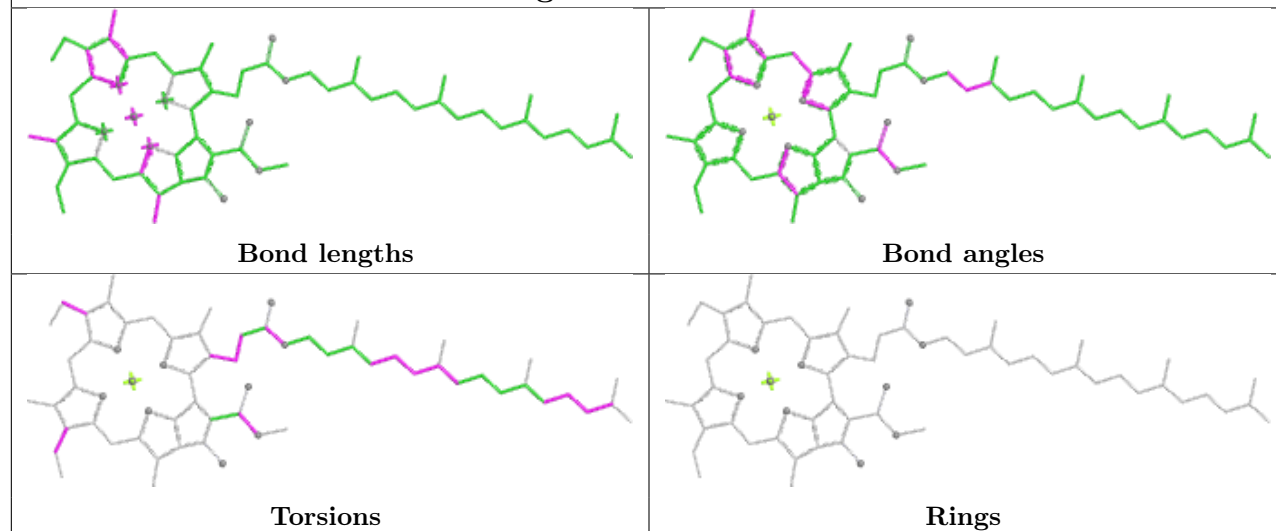
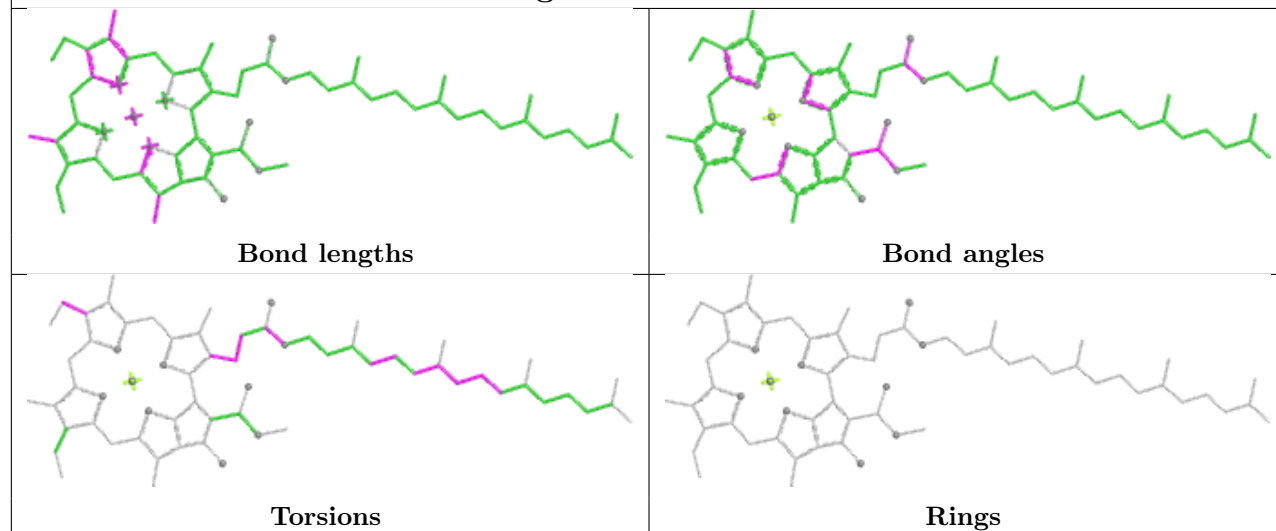
Bond angles



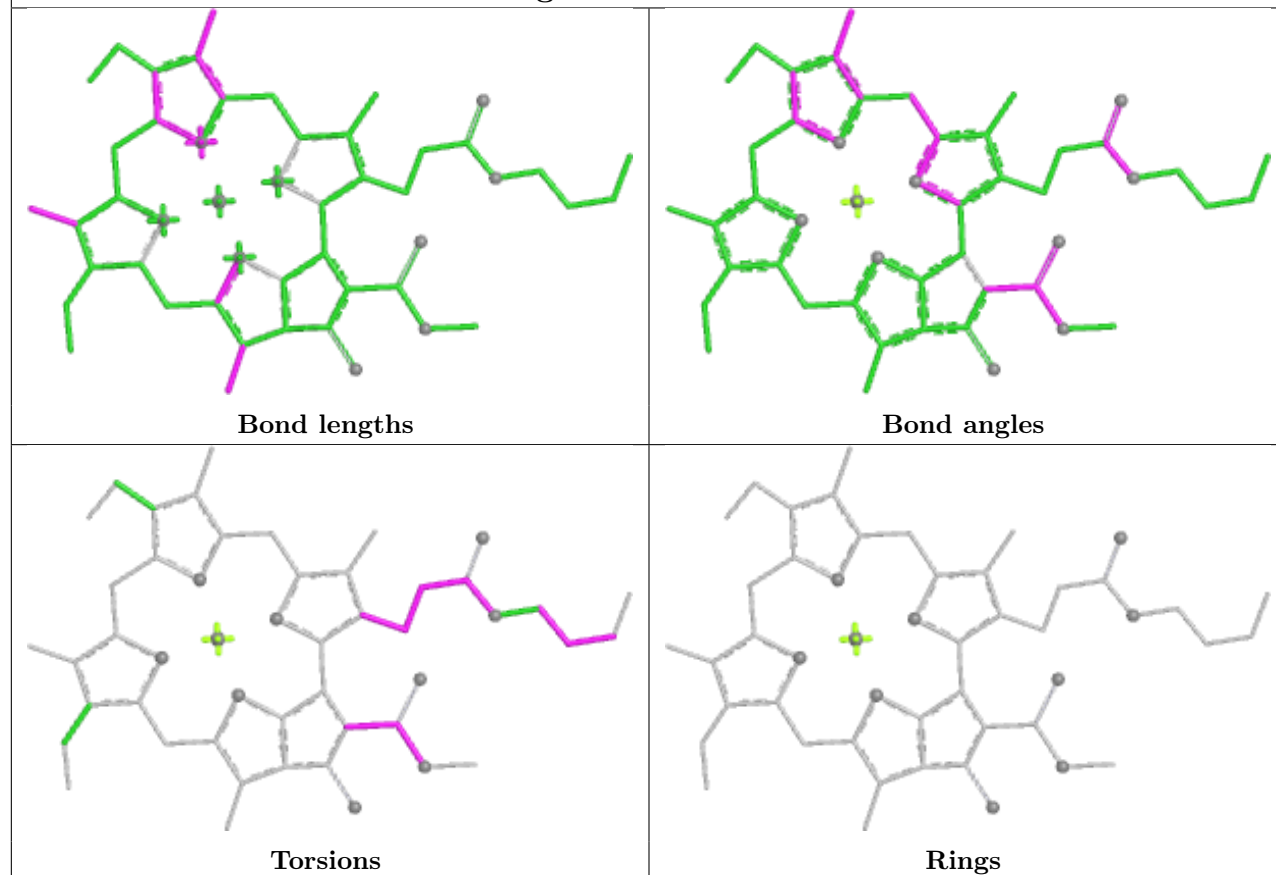
Torsions



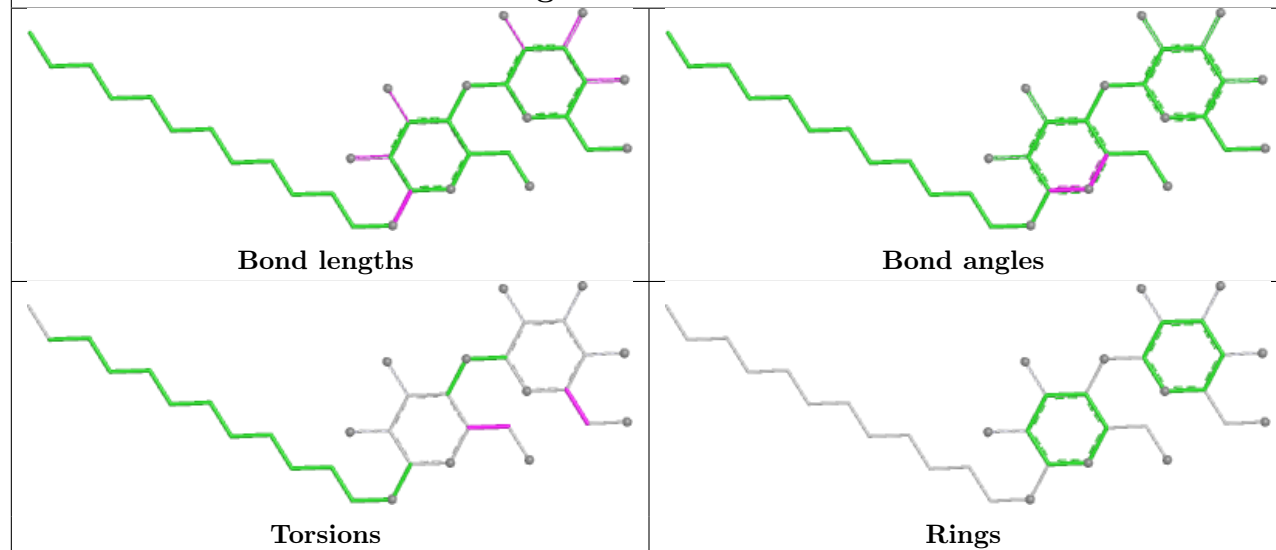
Rings

Ligand CLA a 843**Ligand CLA a 842**

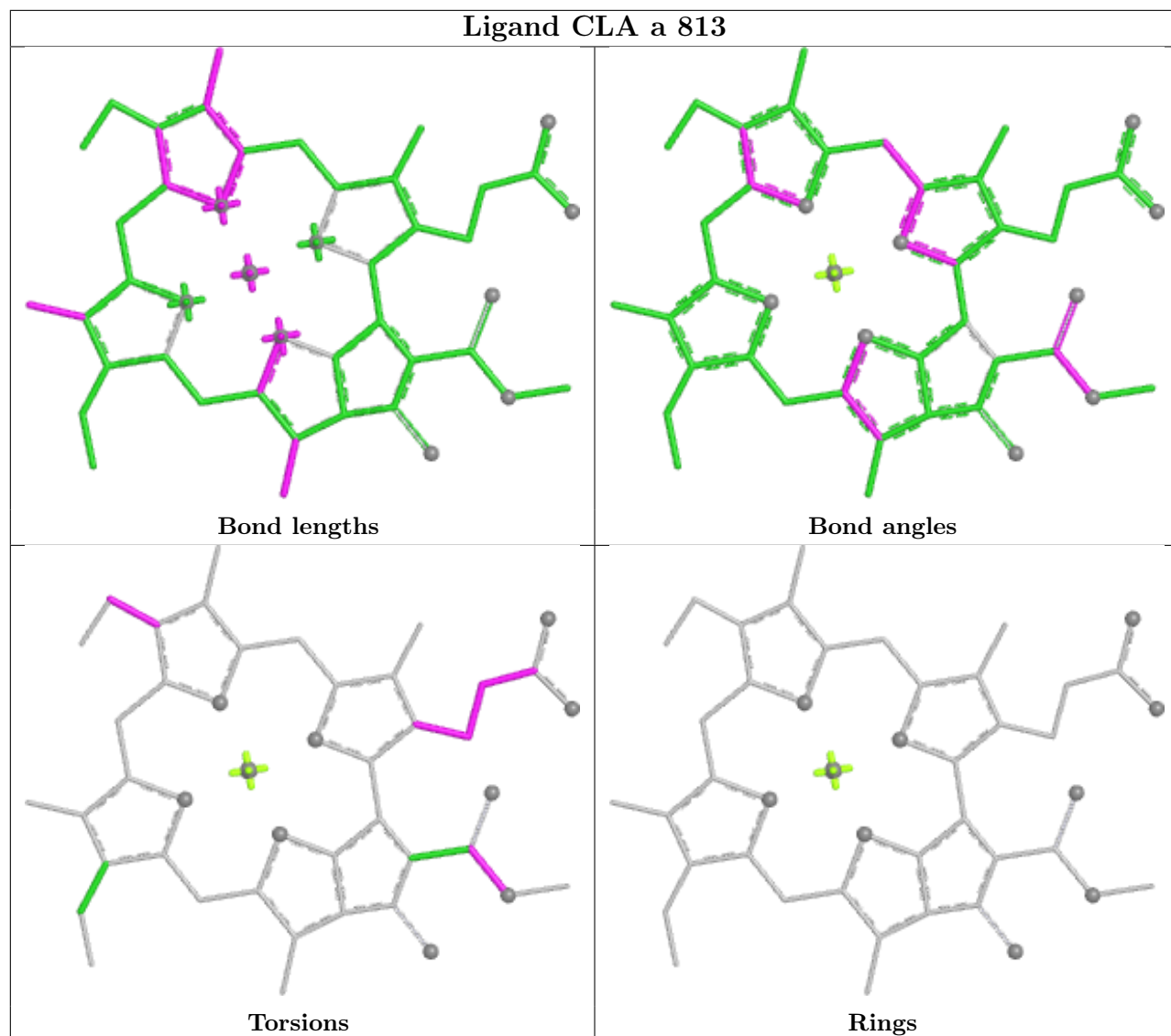
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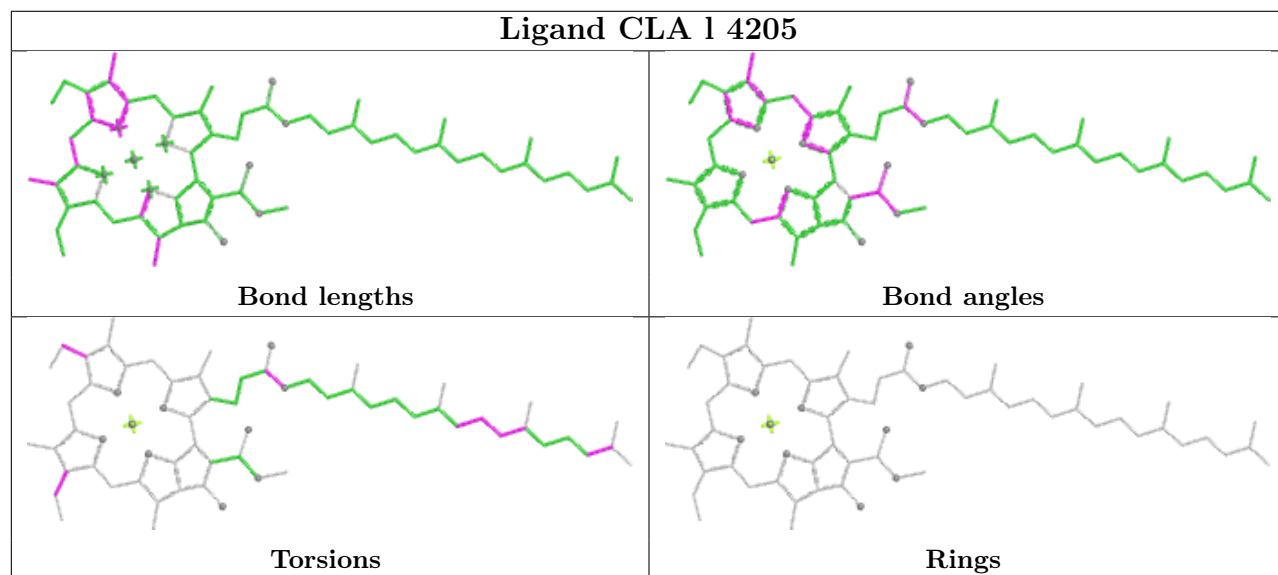
Ligand LMT f 202

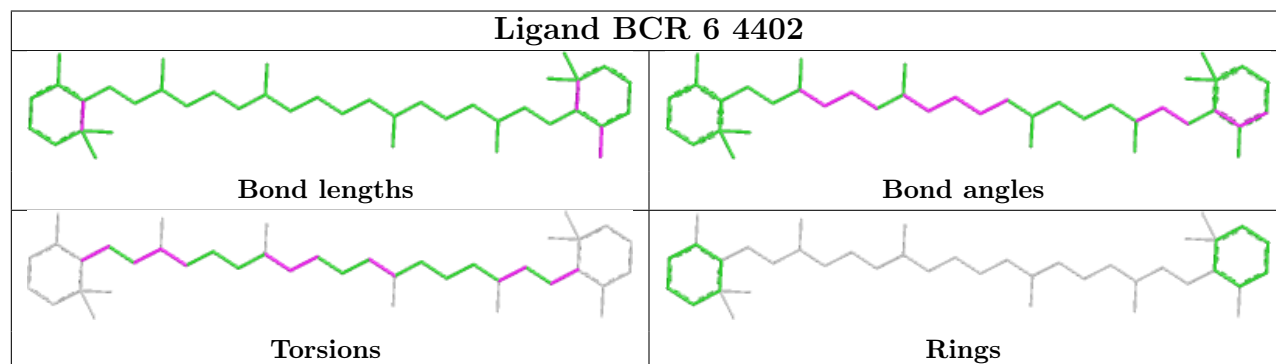
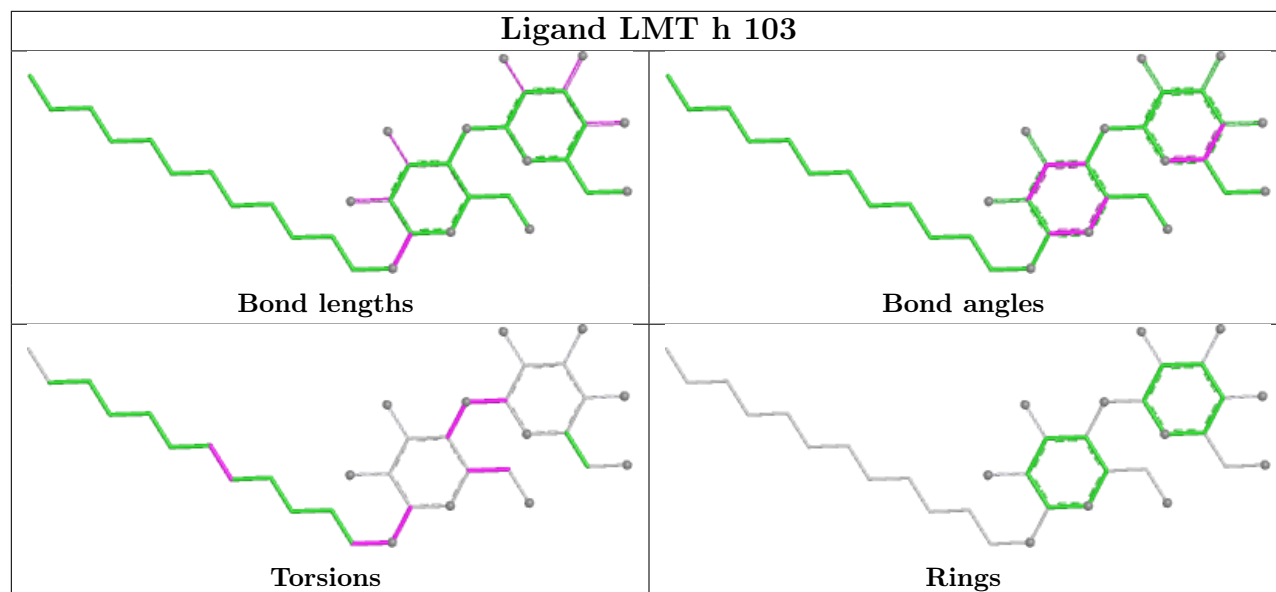
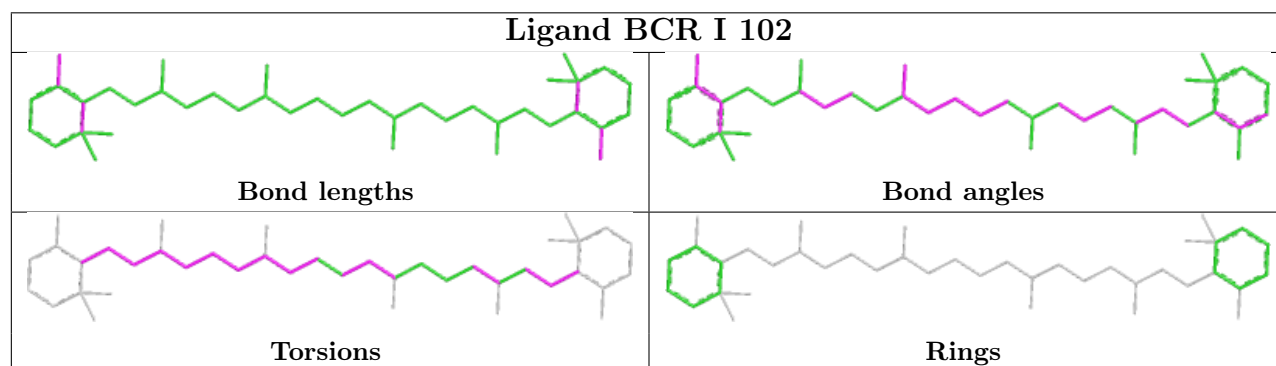
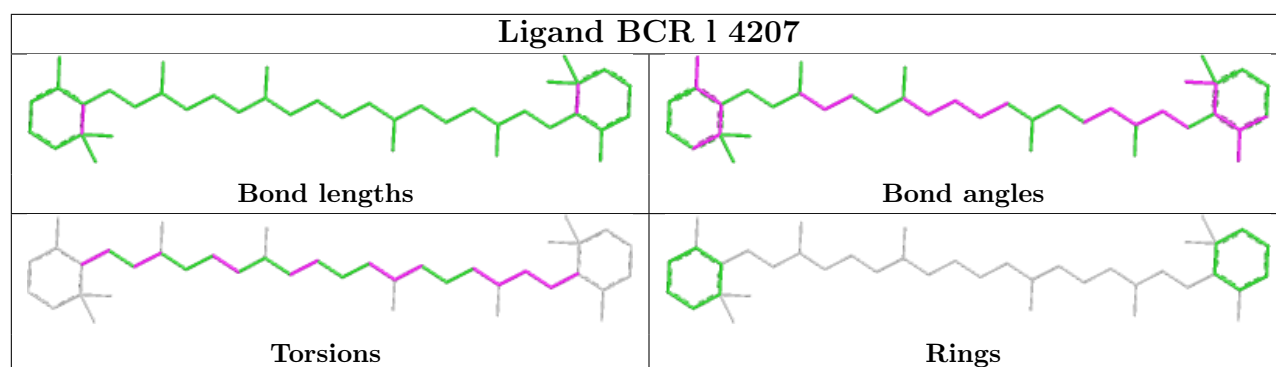


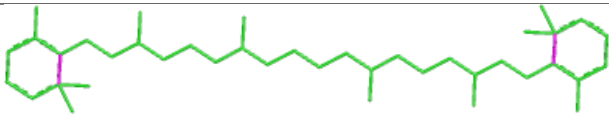
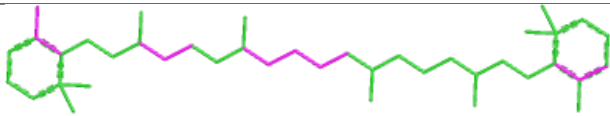
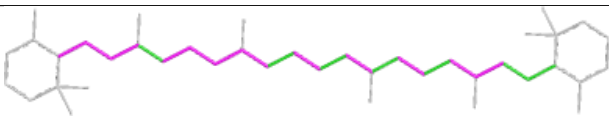
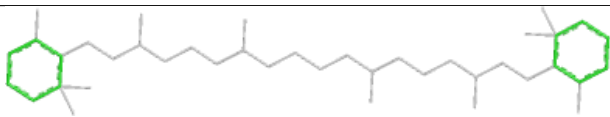
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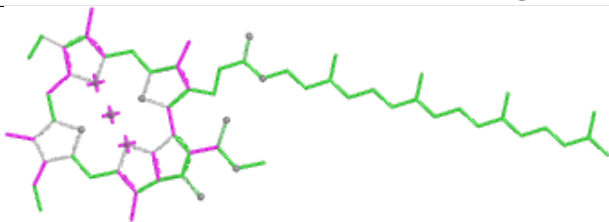
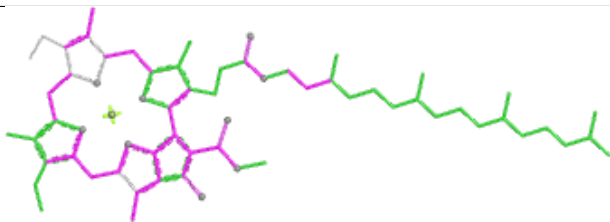
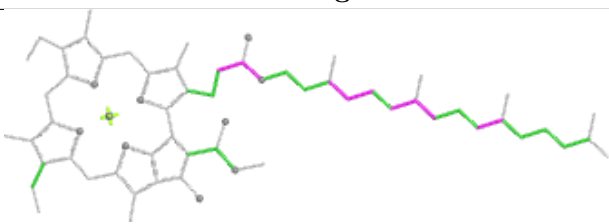
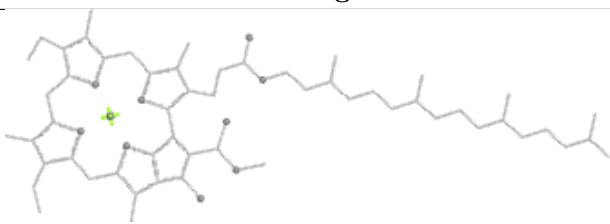


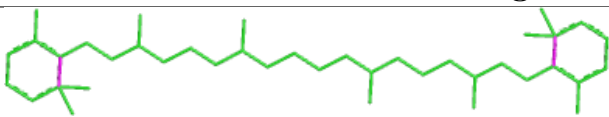
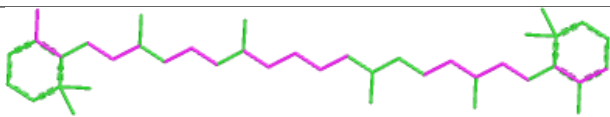
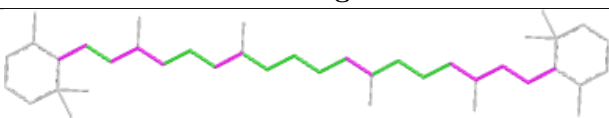
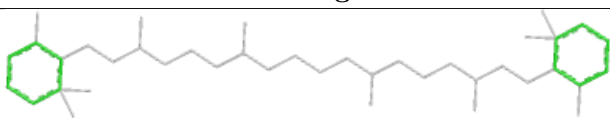
Ligand CLA l 4205

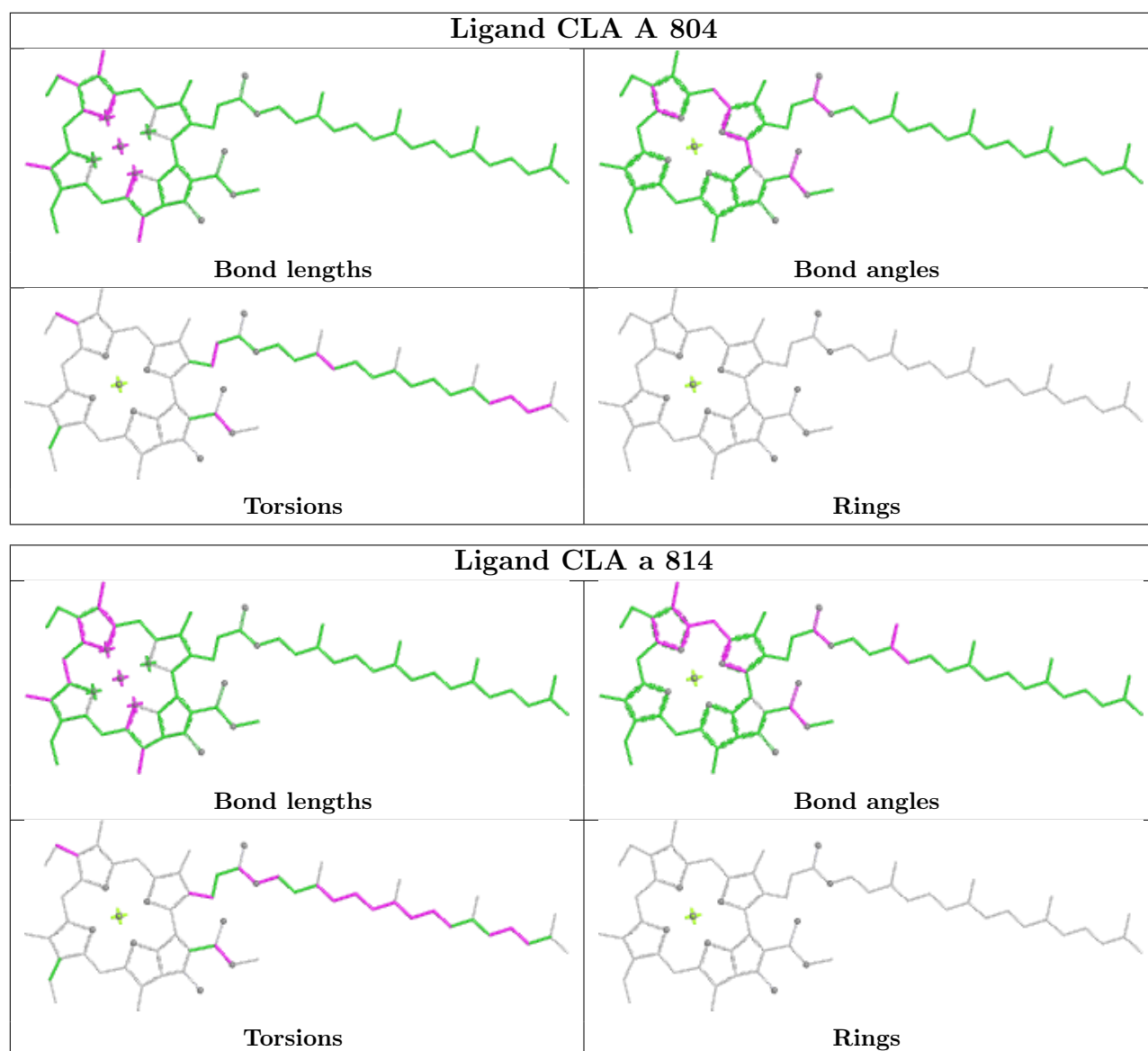




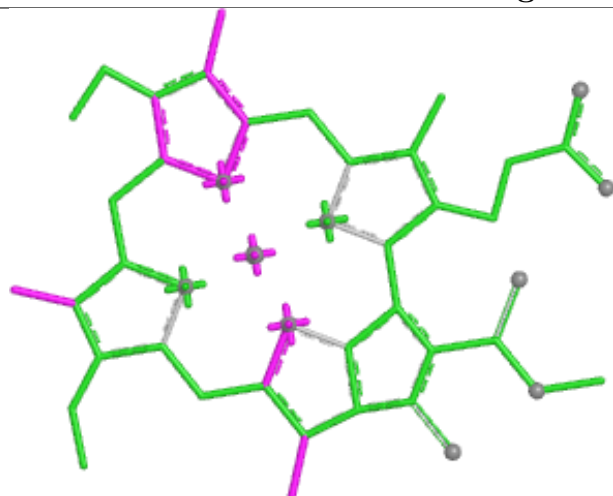
Ligand BCR i 4102	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CL0 A 803	
	
Bond lengths	Bond angles
	
Torsions	Rings

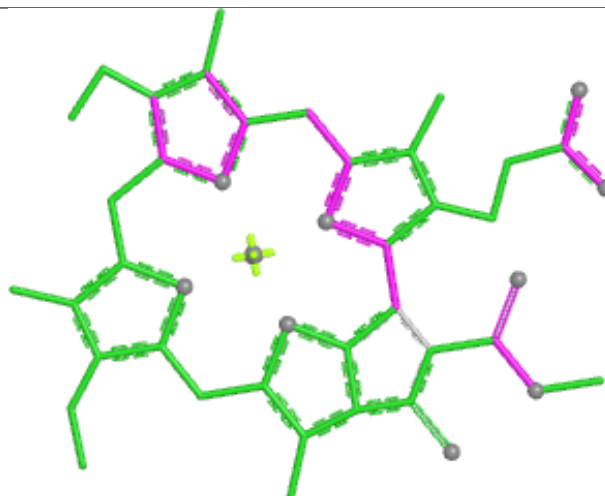
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Bond lengths	Bond angles
	
Torsions	Rings



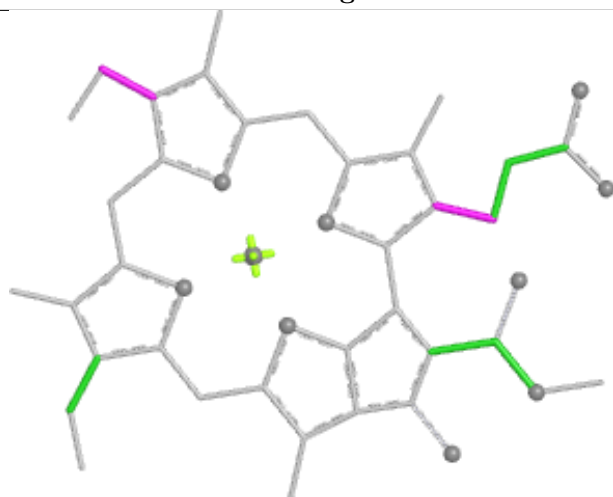
Ligand CLA b 835



Bond lengths



Bond angles

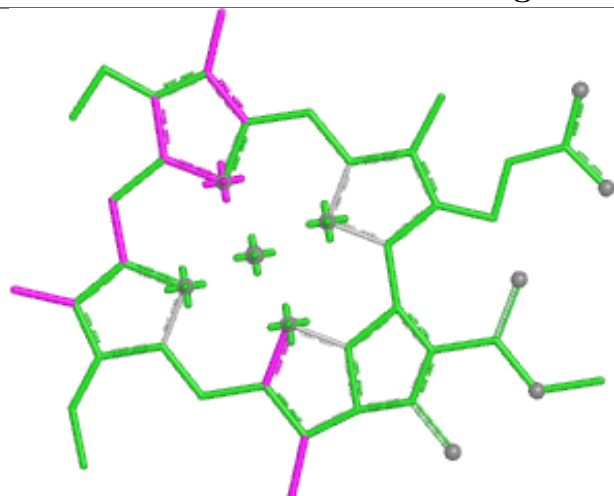


Torsions

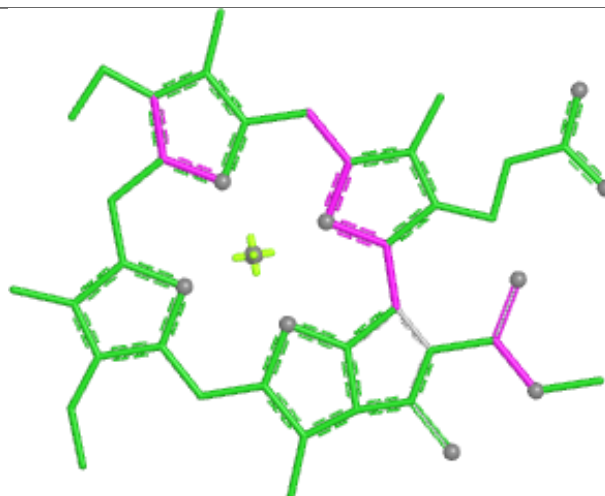


Rings

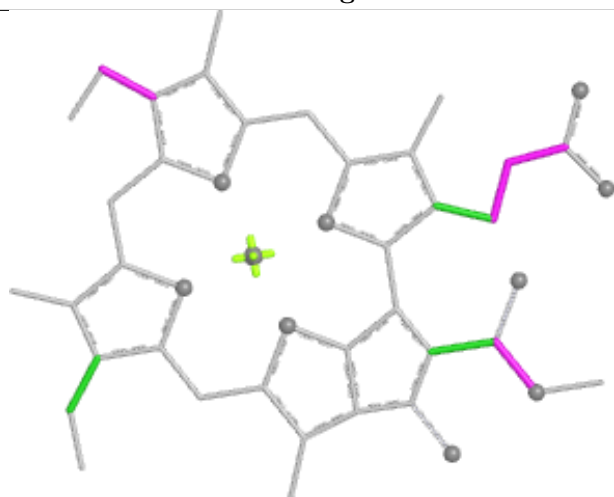
Ligand CLA A 837



Bond lengths



Bond angles

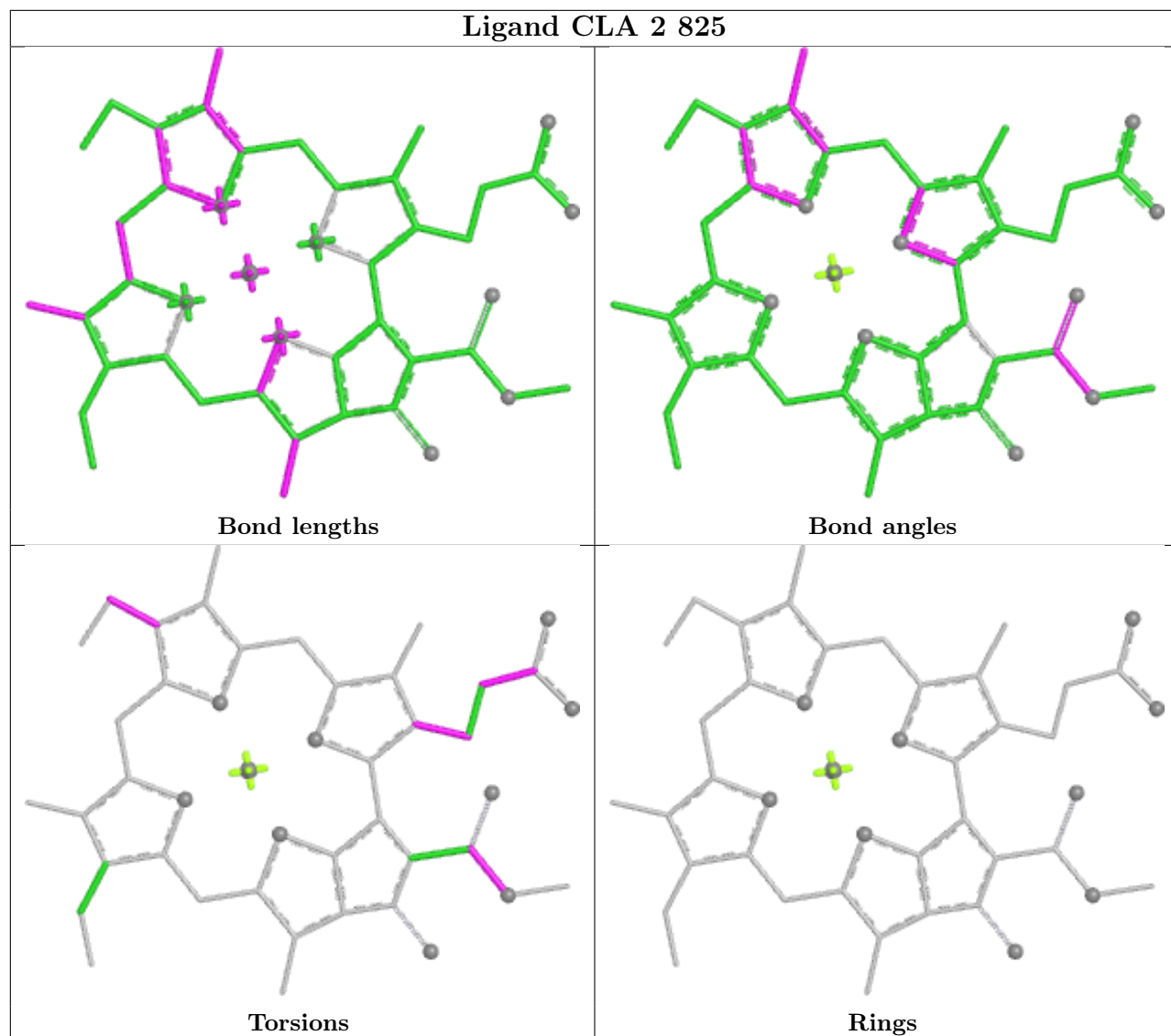


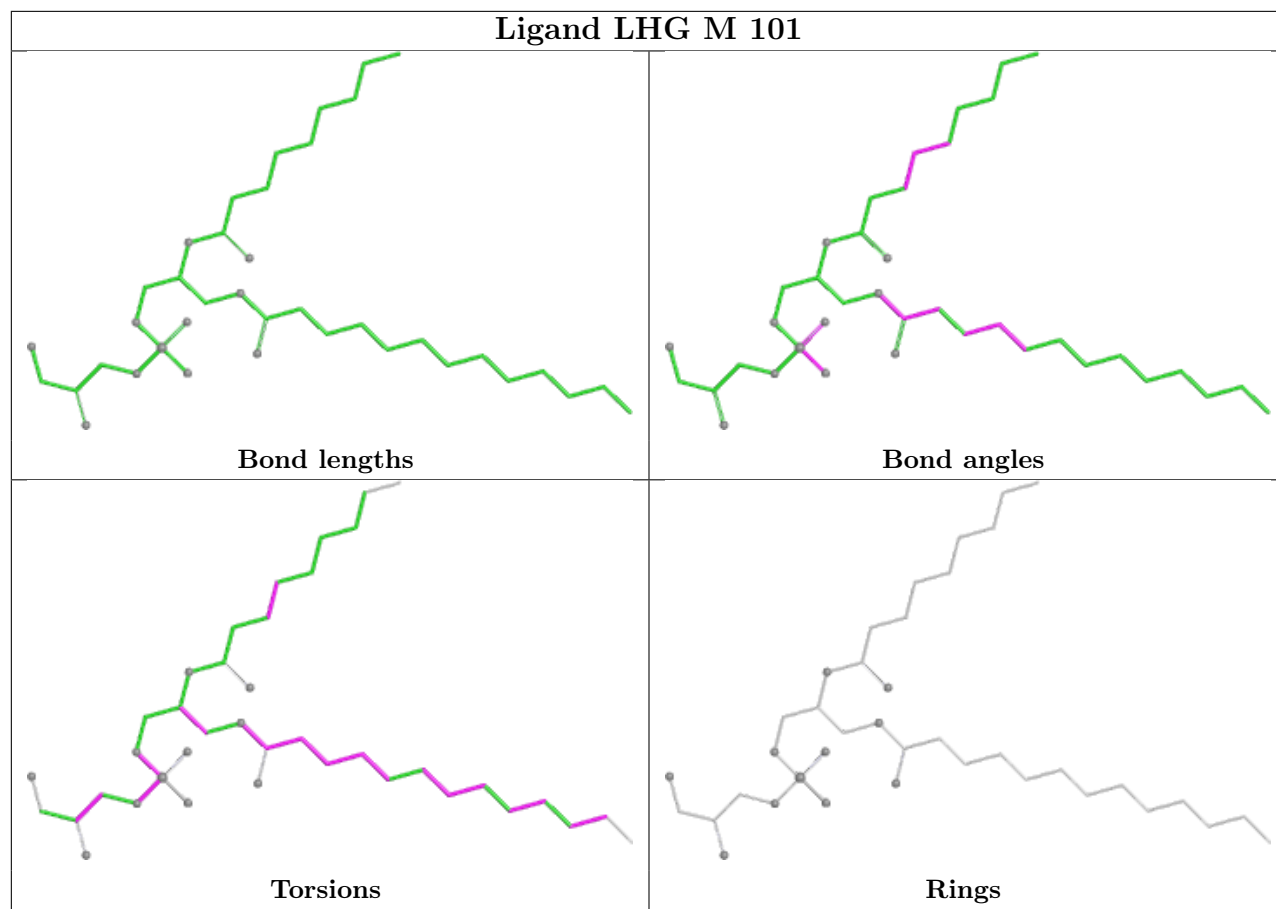
Torsions



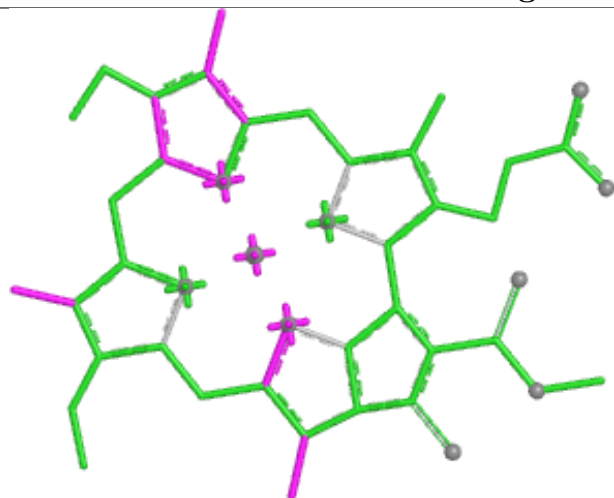
Rings

Ligand CLA 2 825

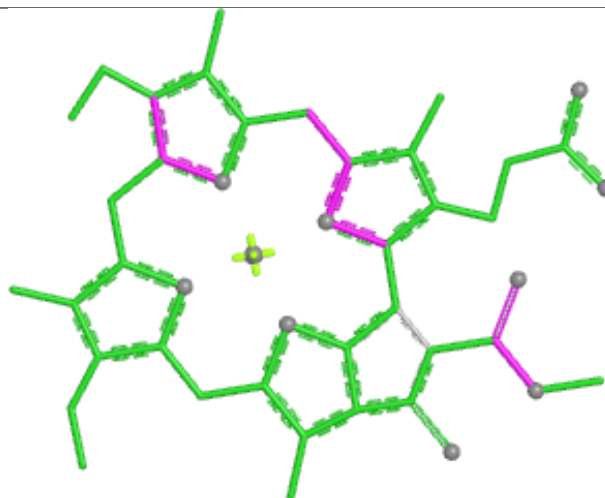




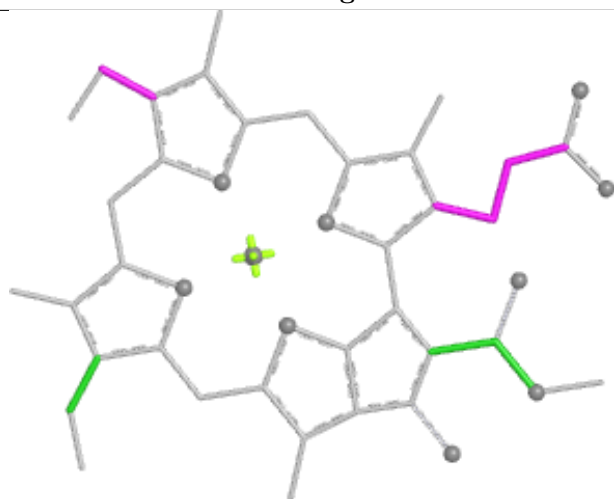
Ligand CLA 2 824



Bond lengths



Bond angles

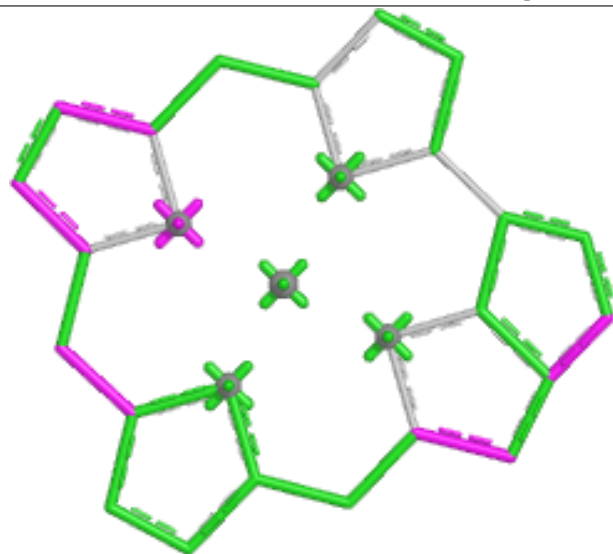


Torsions

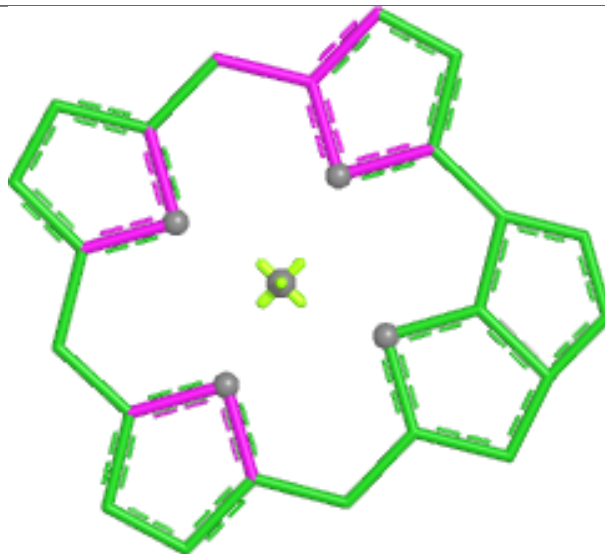


Rings

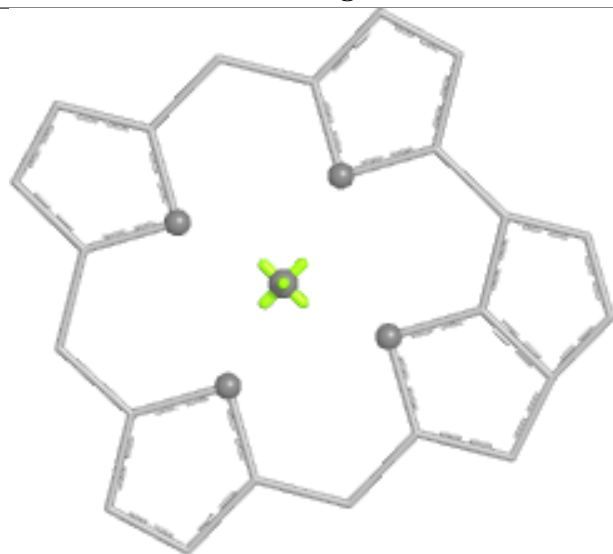
Ligand CLA 2 844



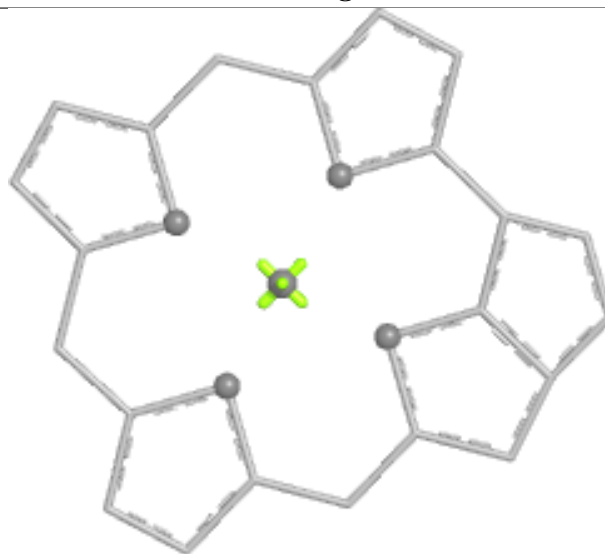
Bond lengths



Bond angles

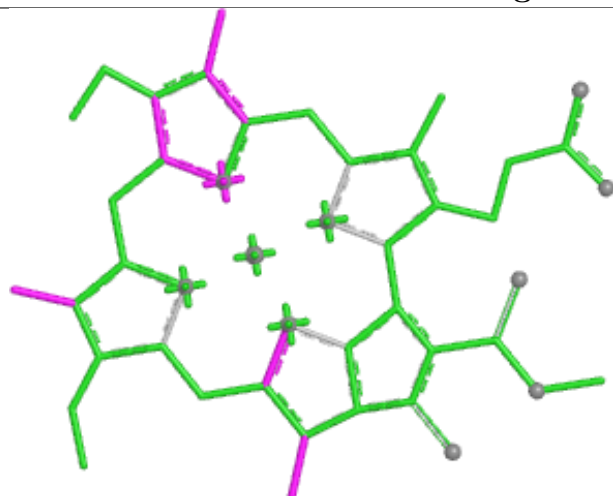


Torsions

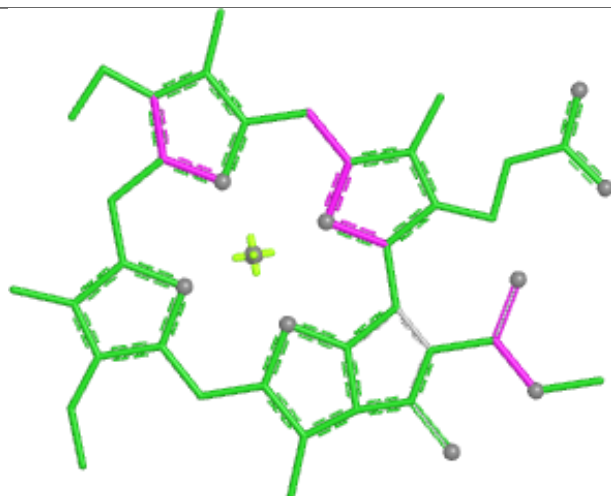


Rings

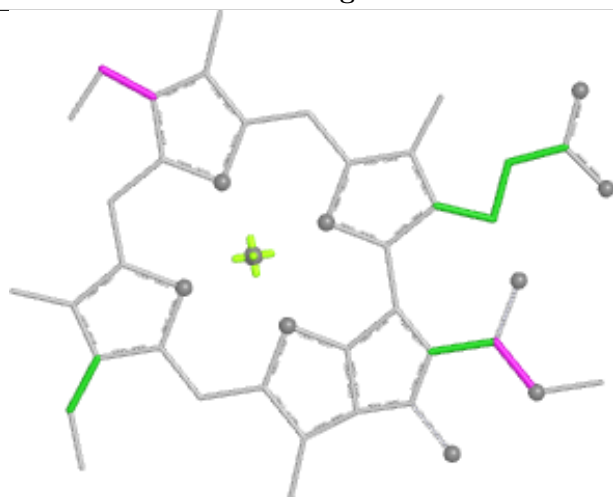
Ligand CLA A 817



Bond lengths



Bond angles

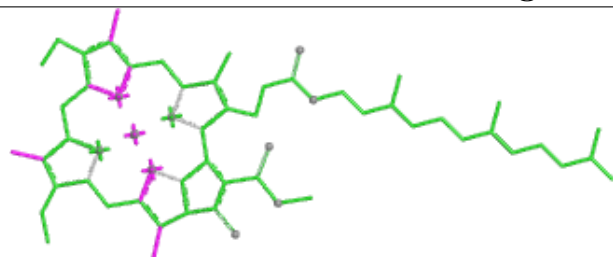


Torsions

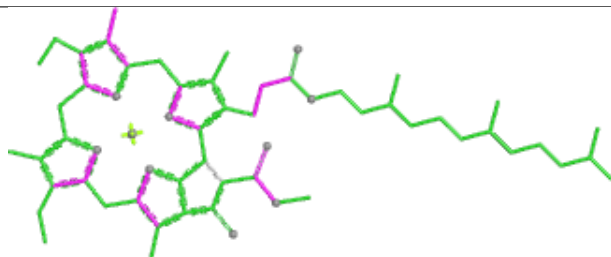


Rings

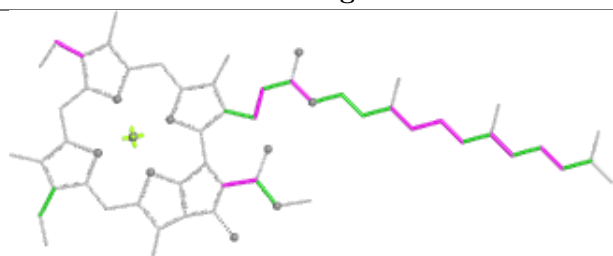
Ligand CLA 2 831



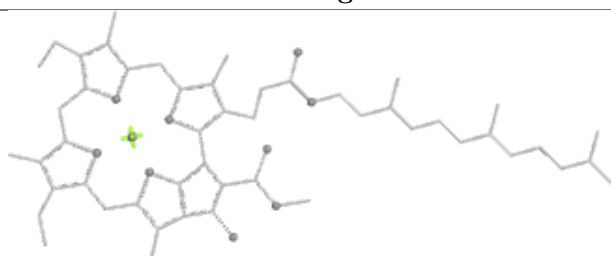
Bond lengths



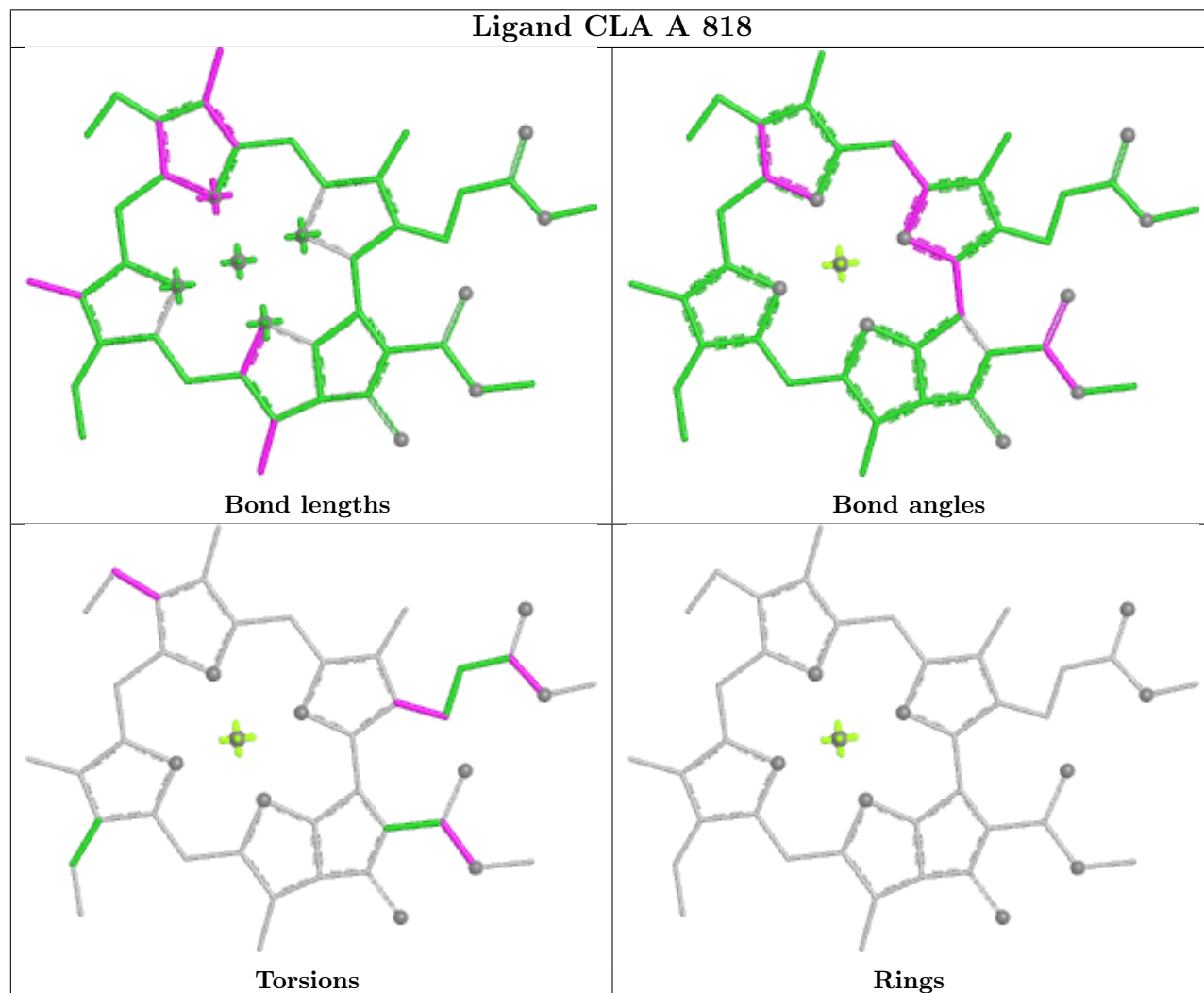
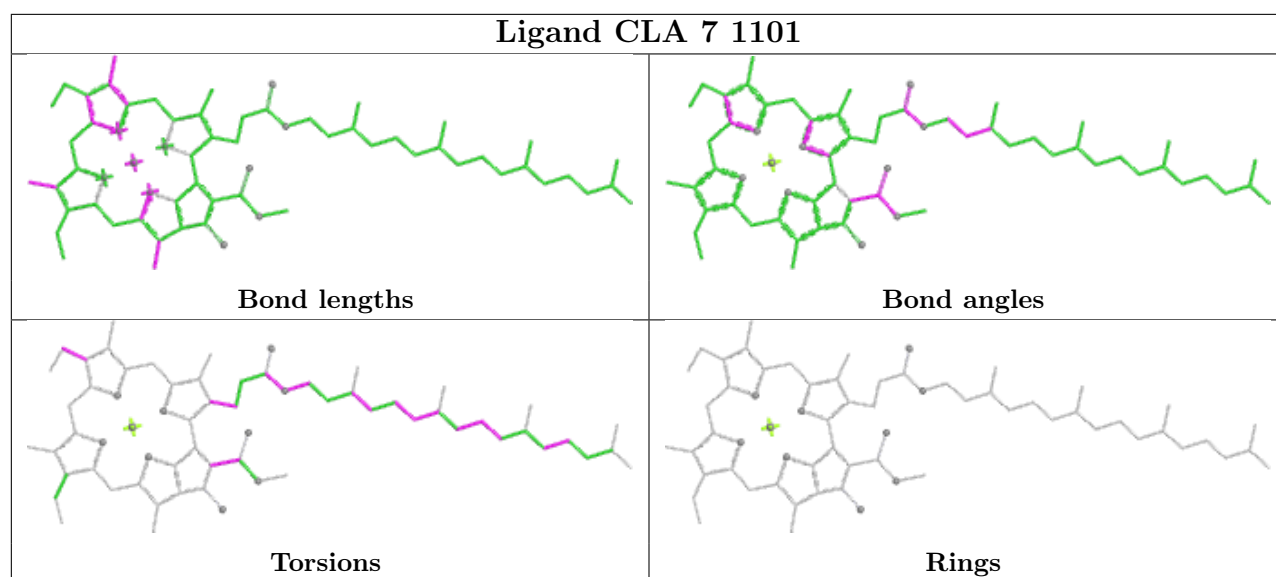
Bond angles

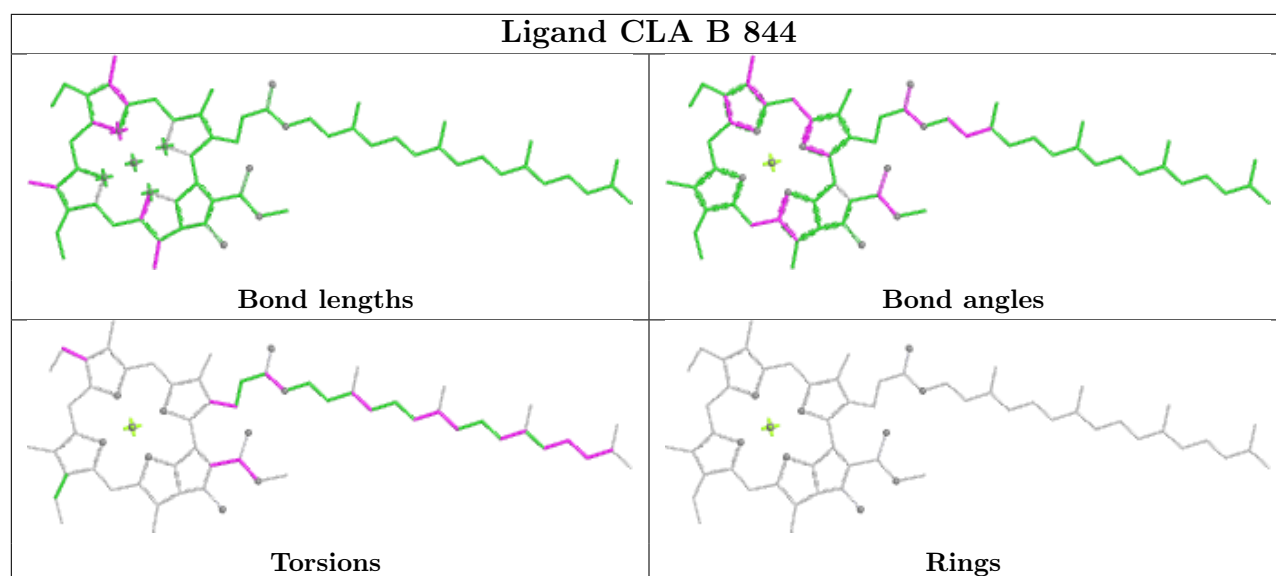
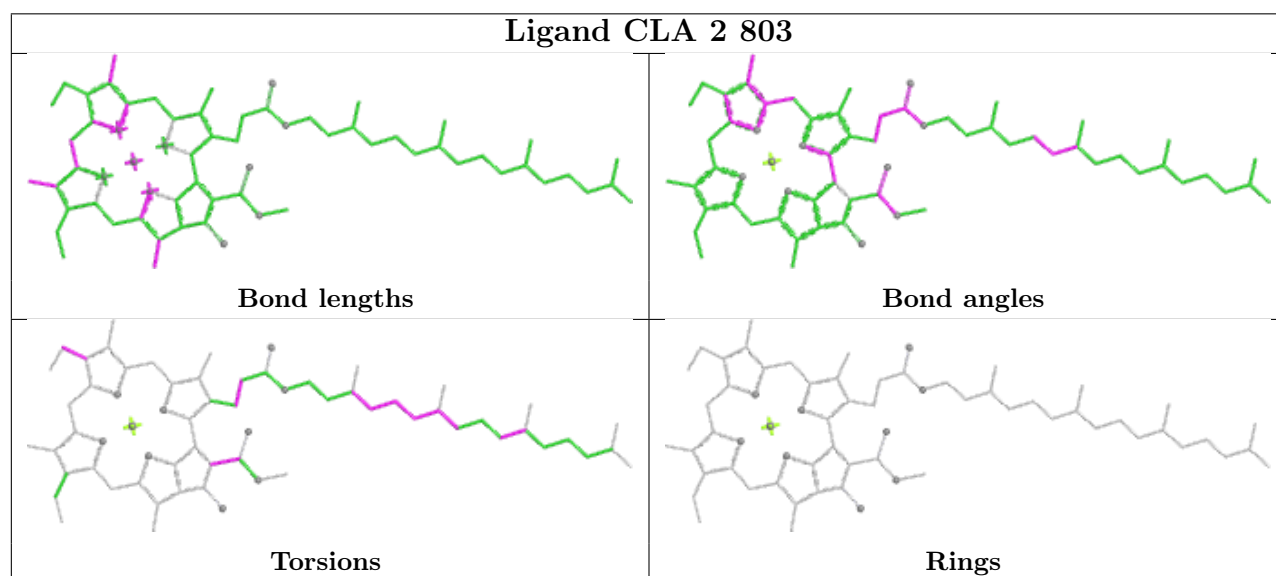
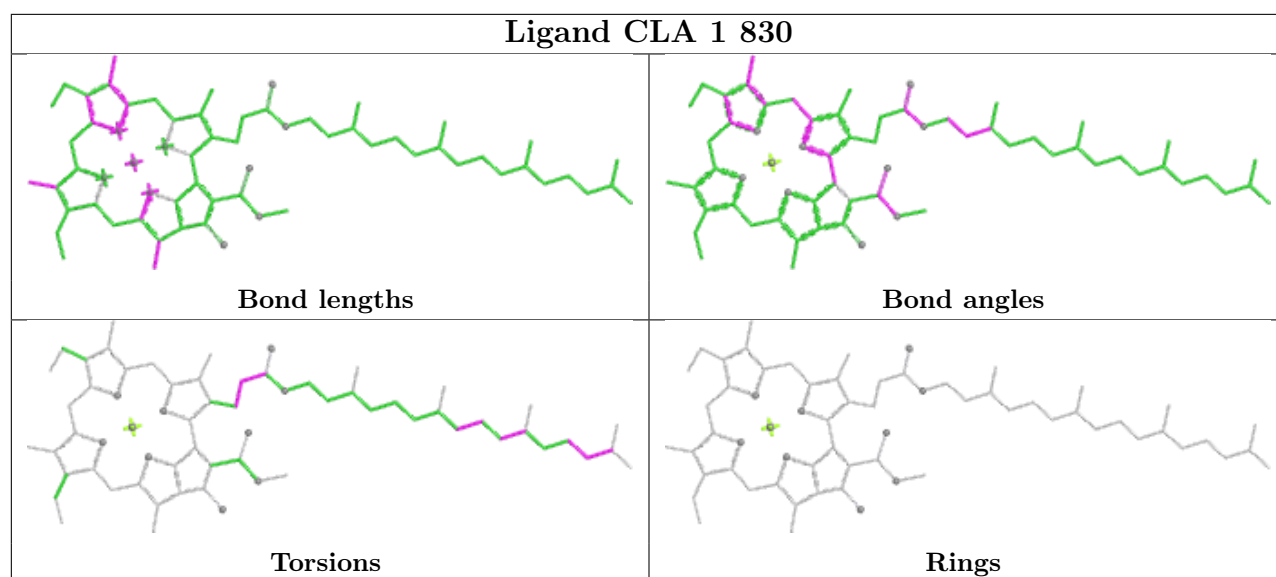


Torsions

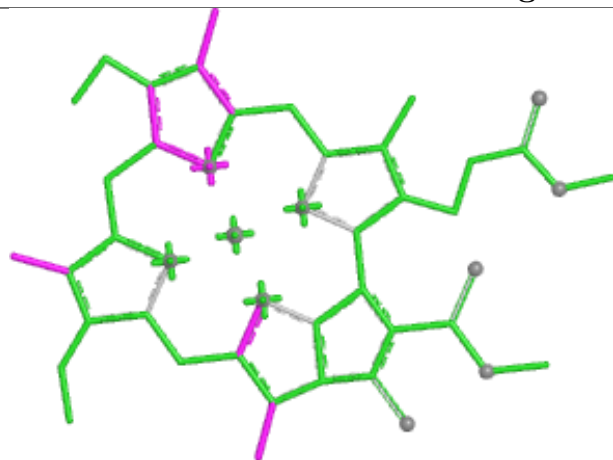


Rings

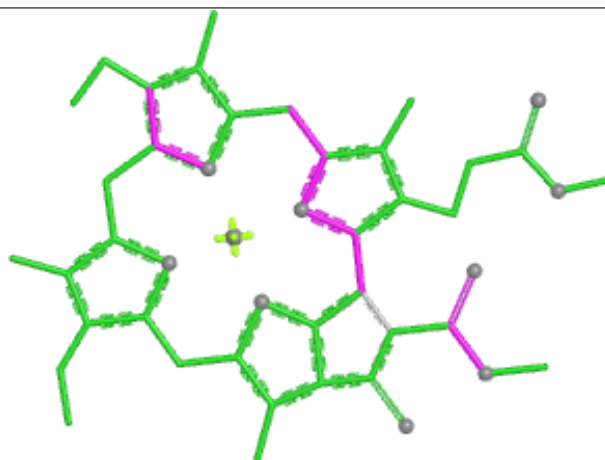




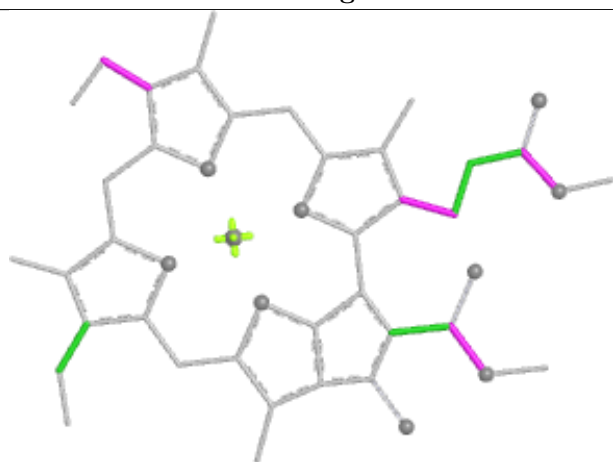
Ligand CLA 1 817



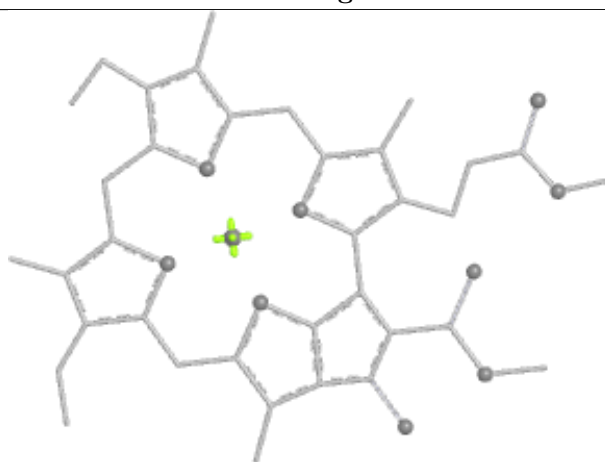
Bond lengths



Bond angles

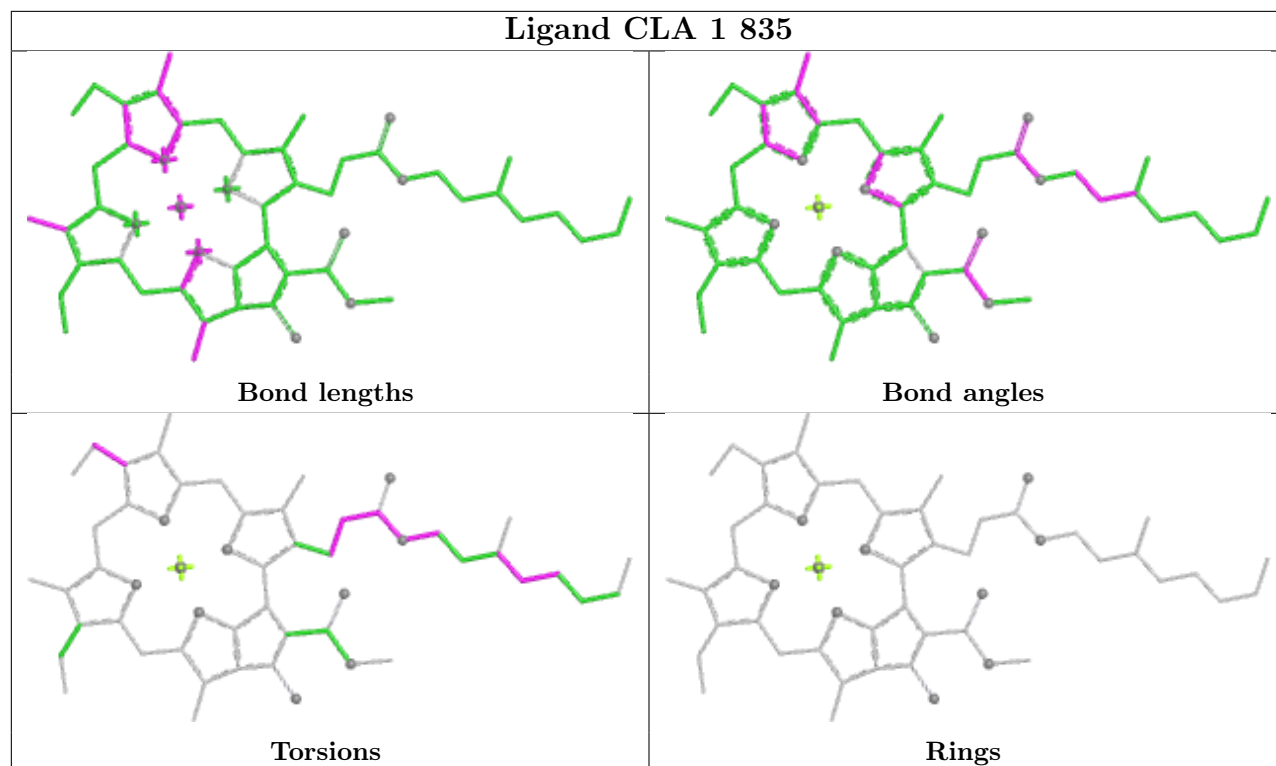


Torsions

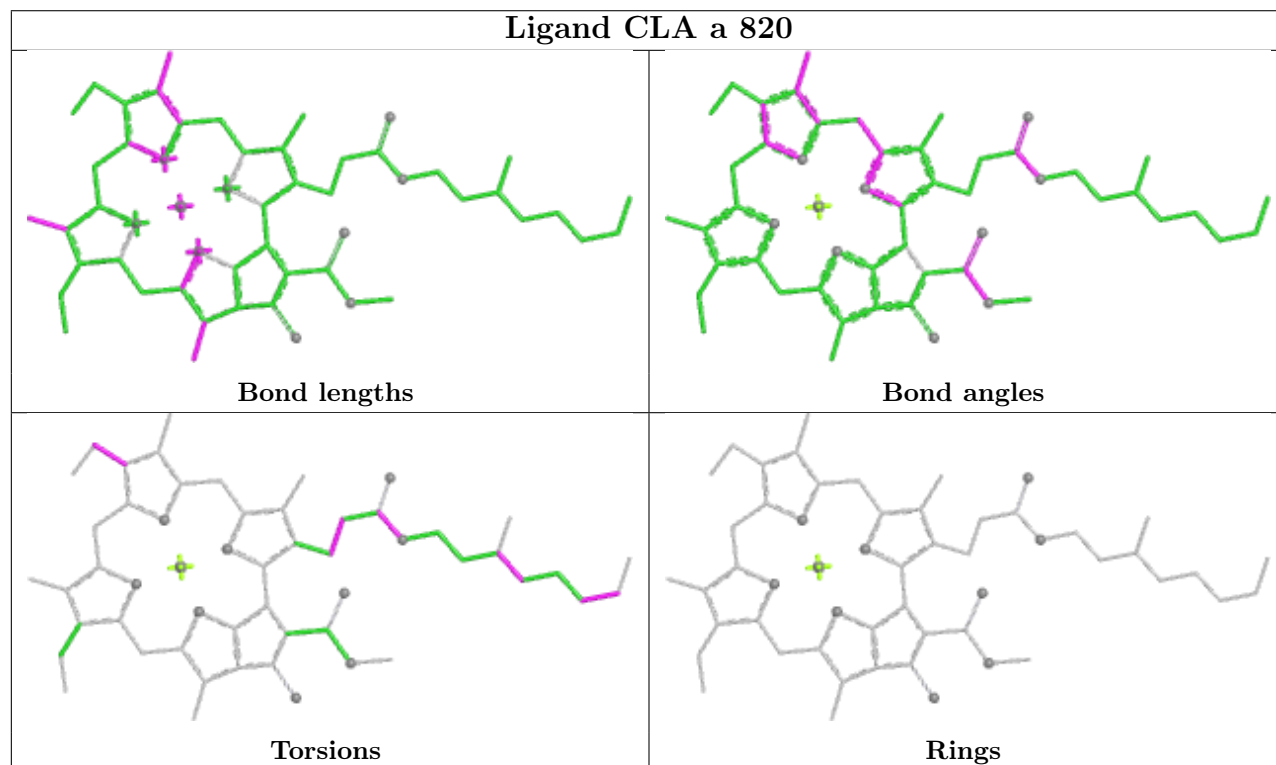


Rings

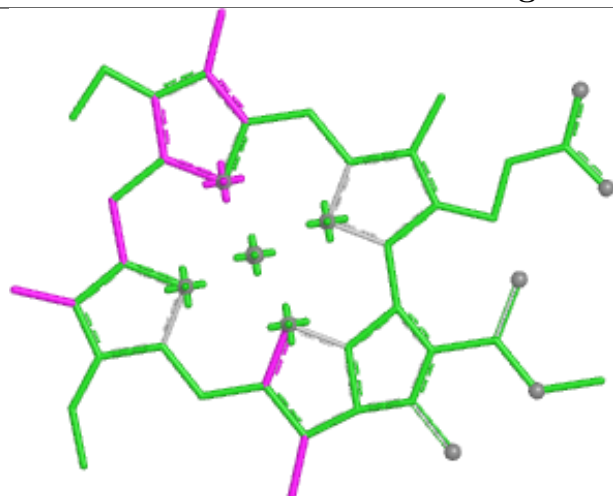
Ligand CLA 1 835



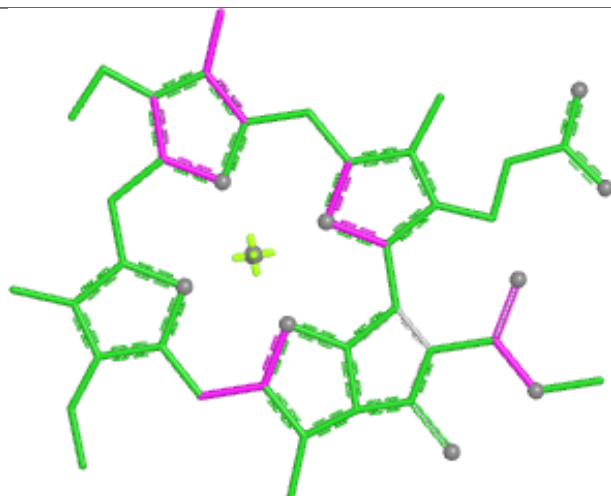
Ligand CLA a 820



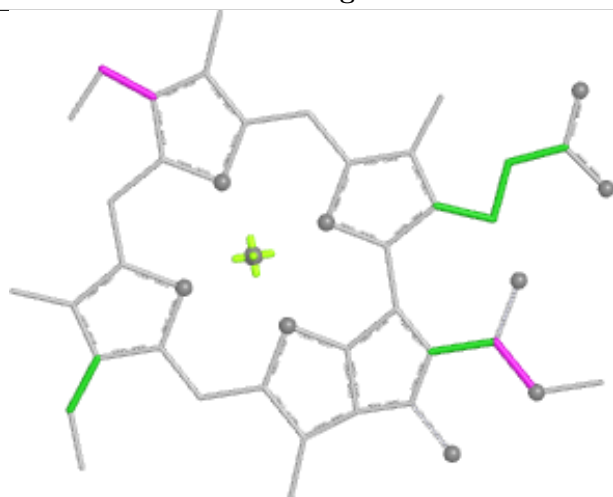
Ligand CLA 2 817



Bond lengths



Bond angles

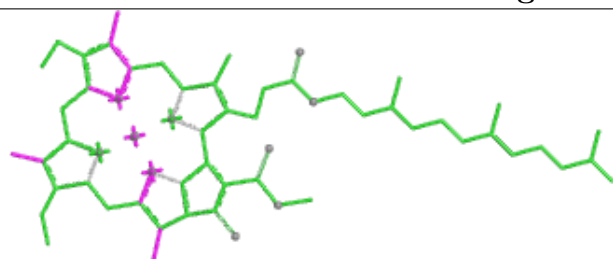


Torsions

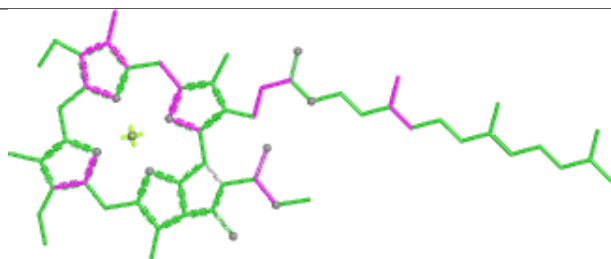


Rings

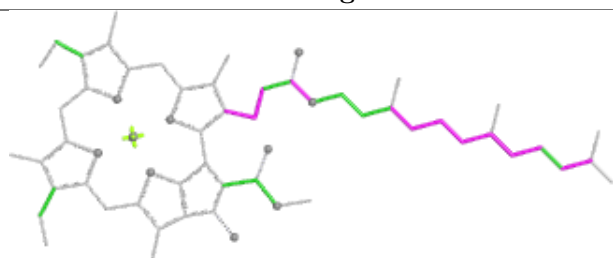
Ligand CLA b 820



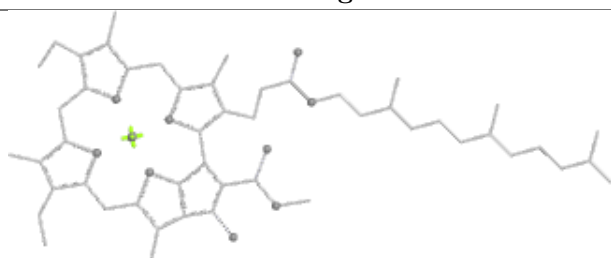
Bond lengths



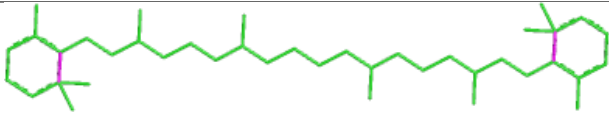
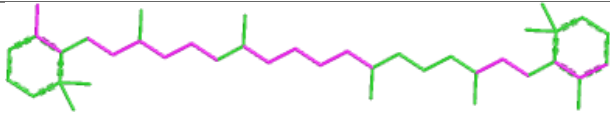
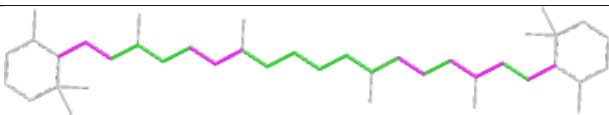
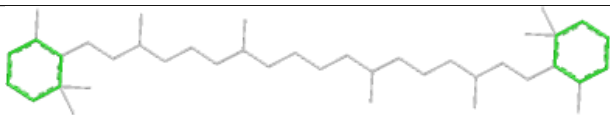
Bond angles

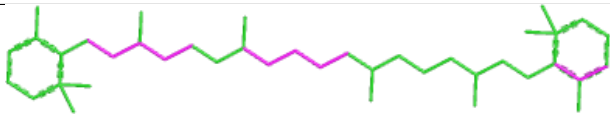
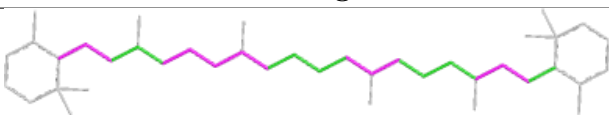
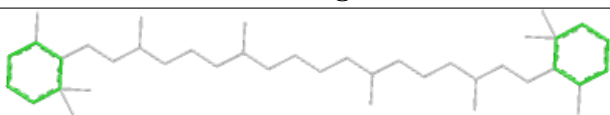


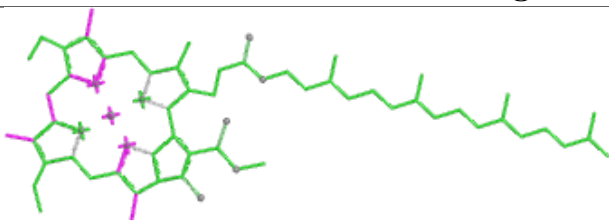
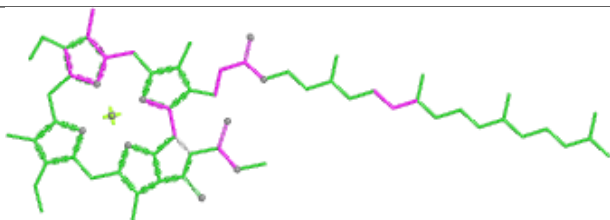
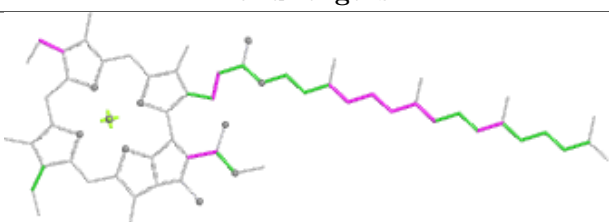
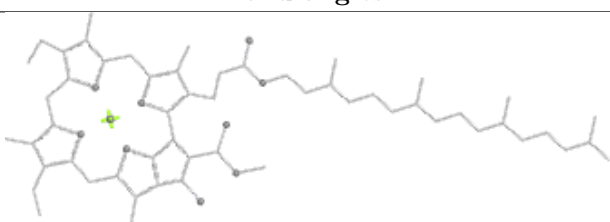
Torsions



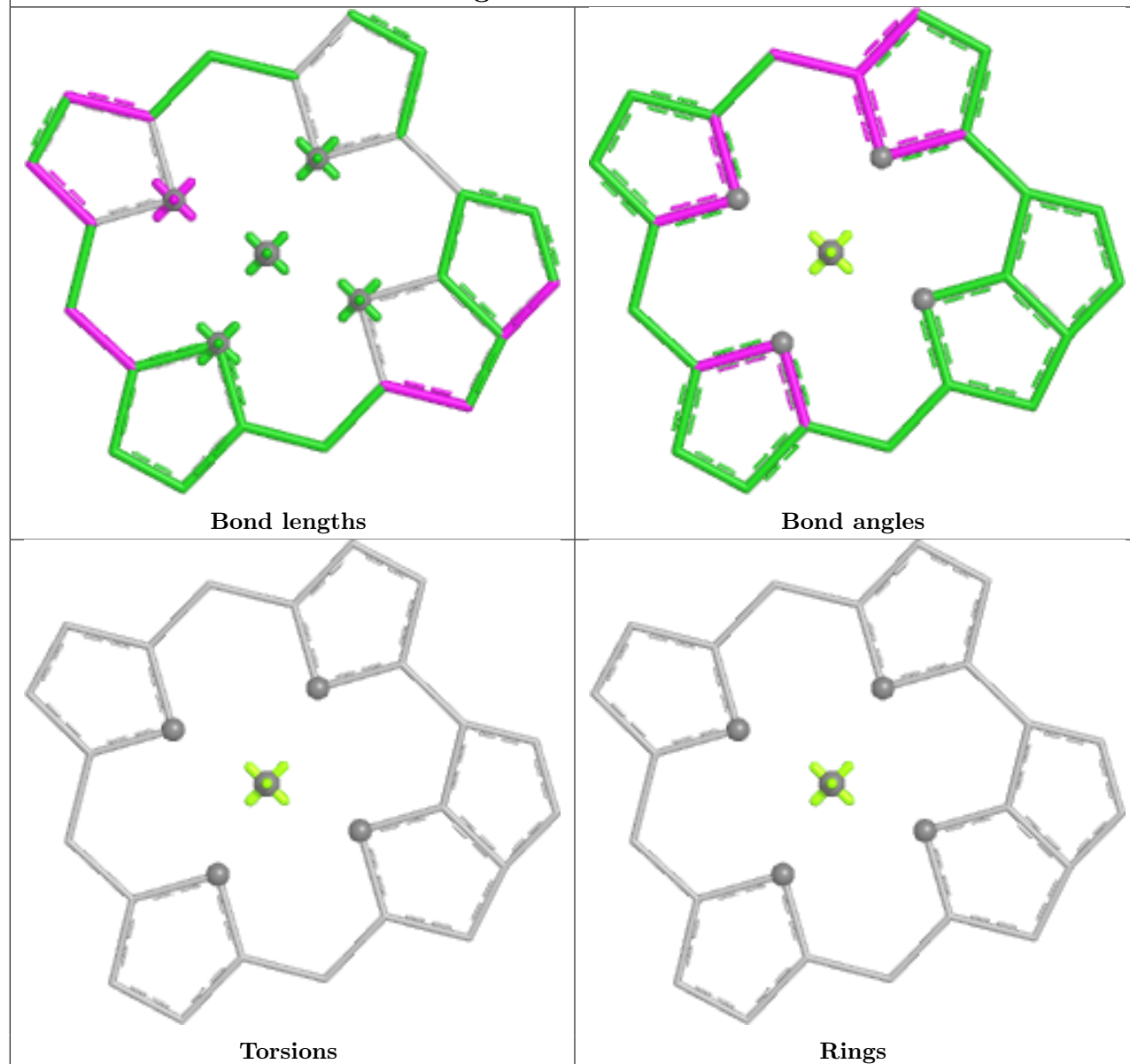
Rings

Ligand BCR A 847	
	
Bond lengths	Bond angles
	
Torsions	Rings

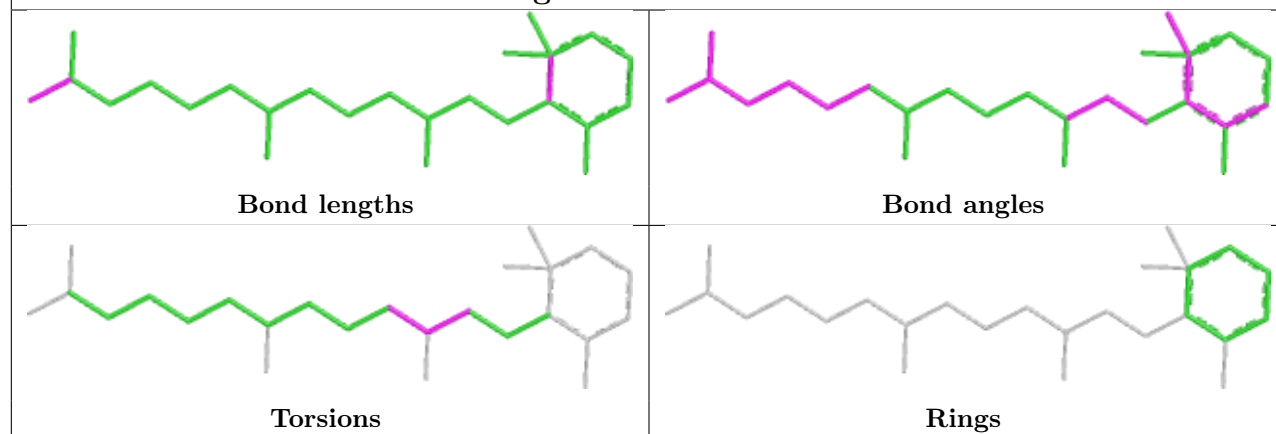
Ligand BCR J 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

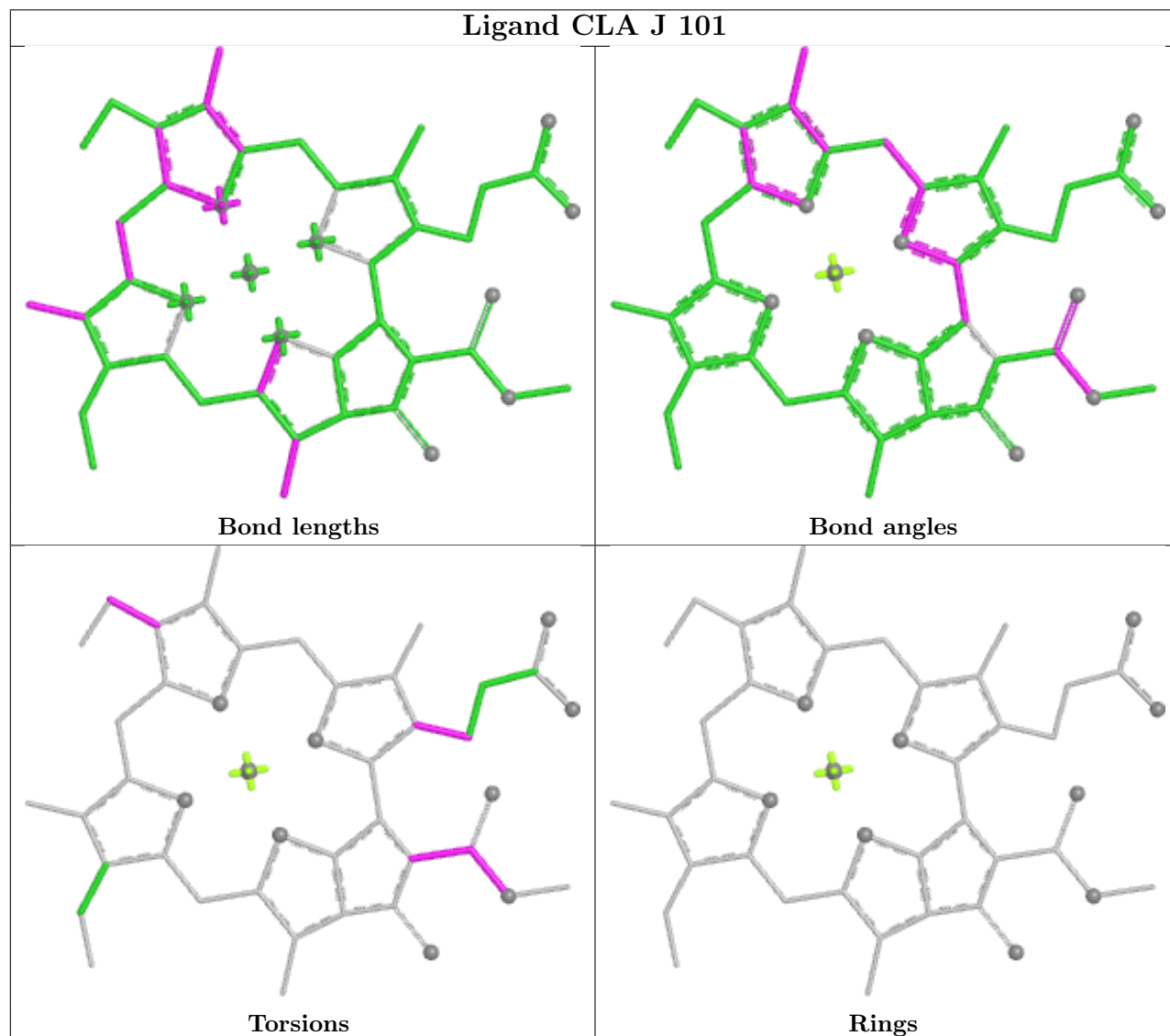
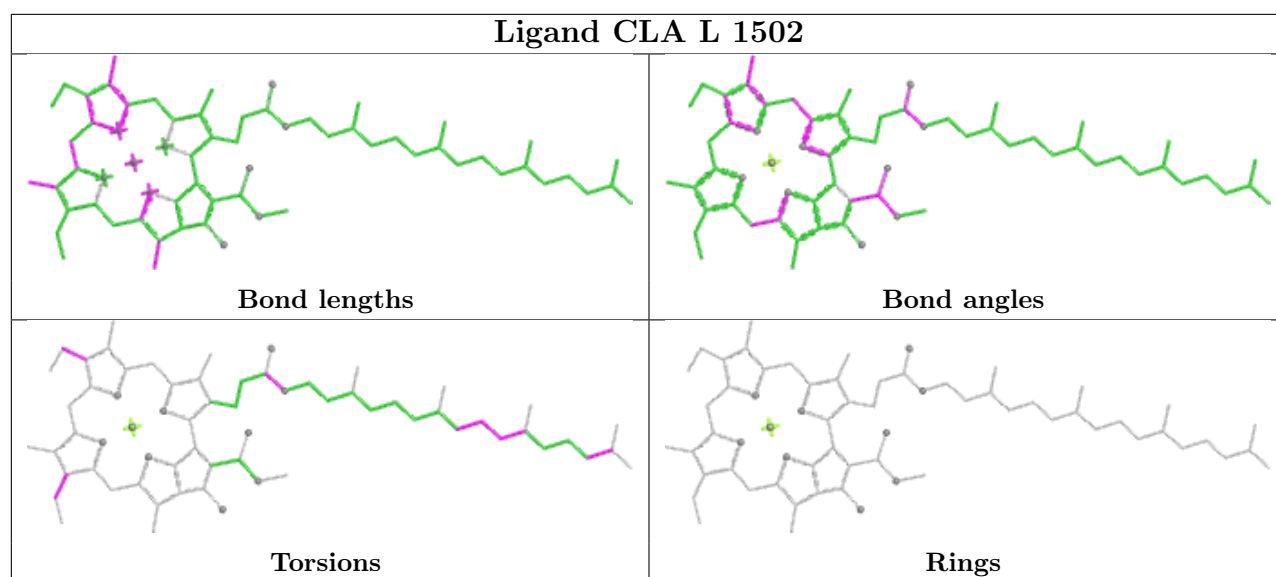
Ligand CLA b 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

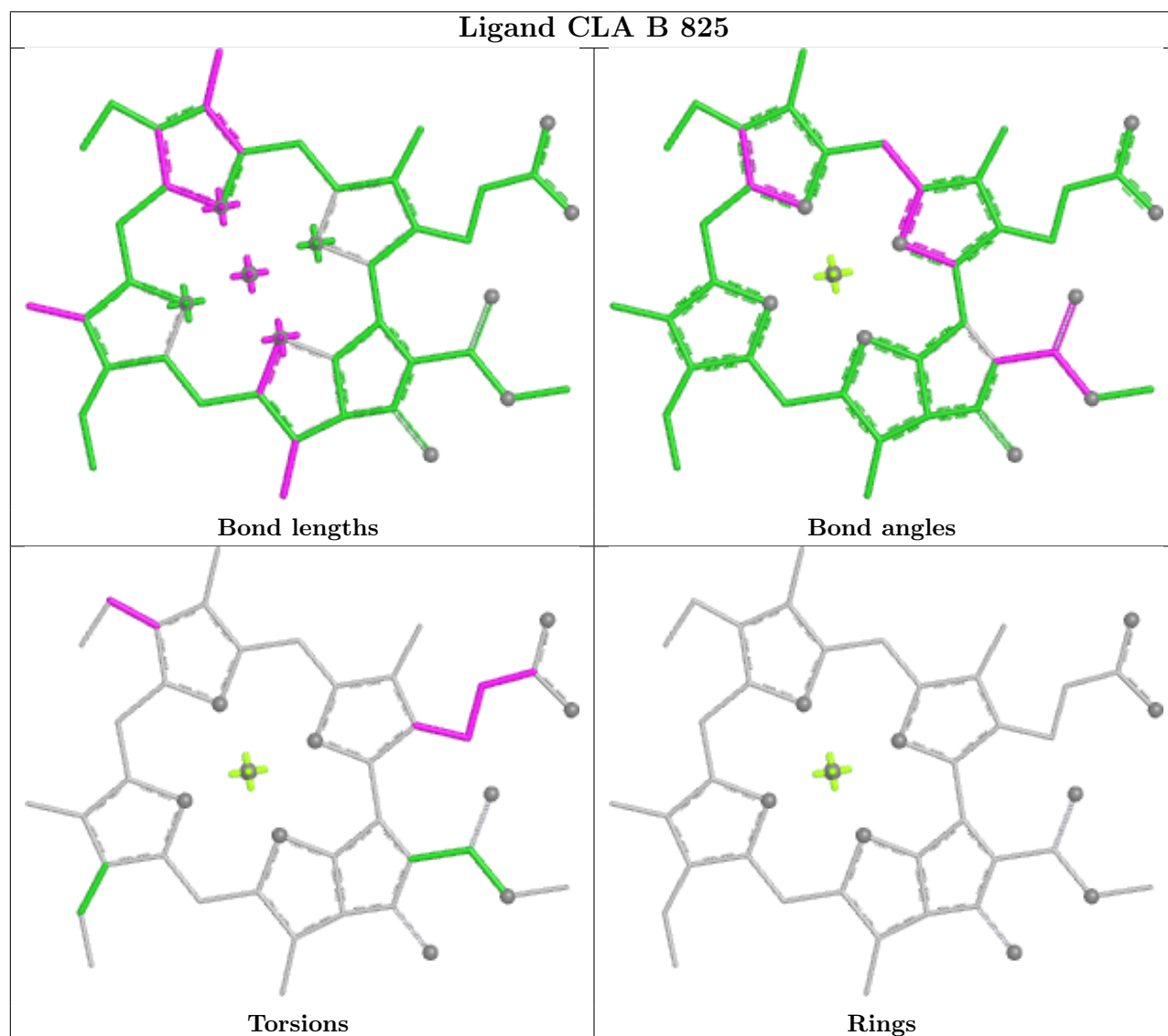
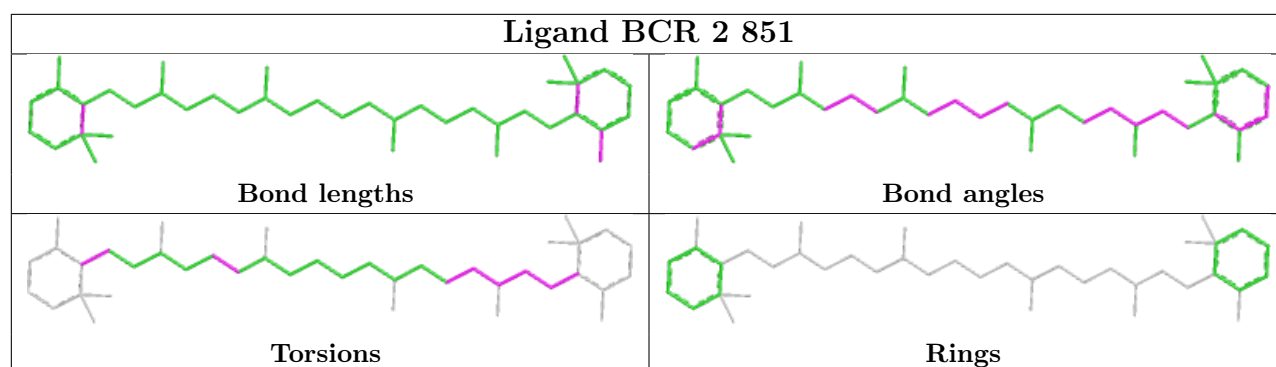
Ligand CLA b 844

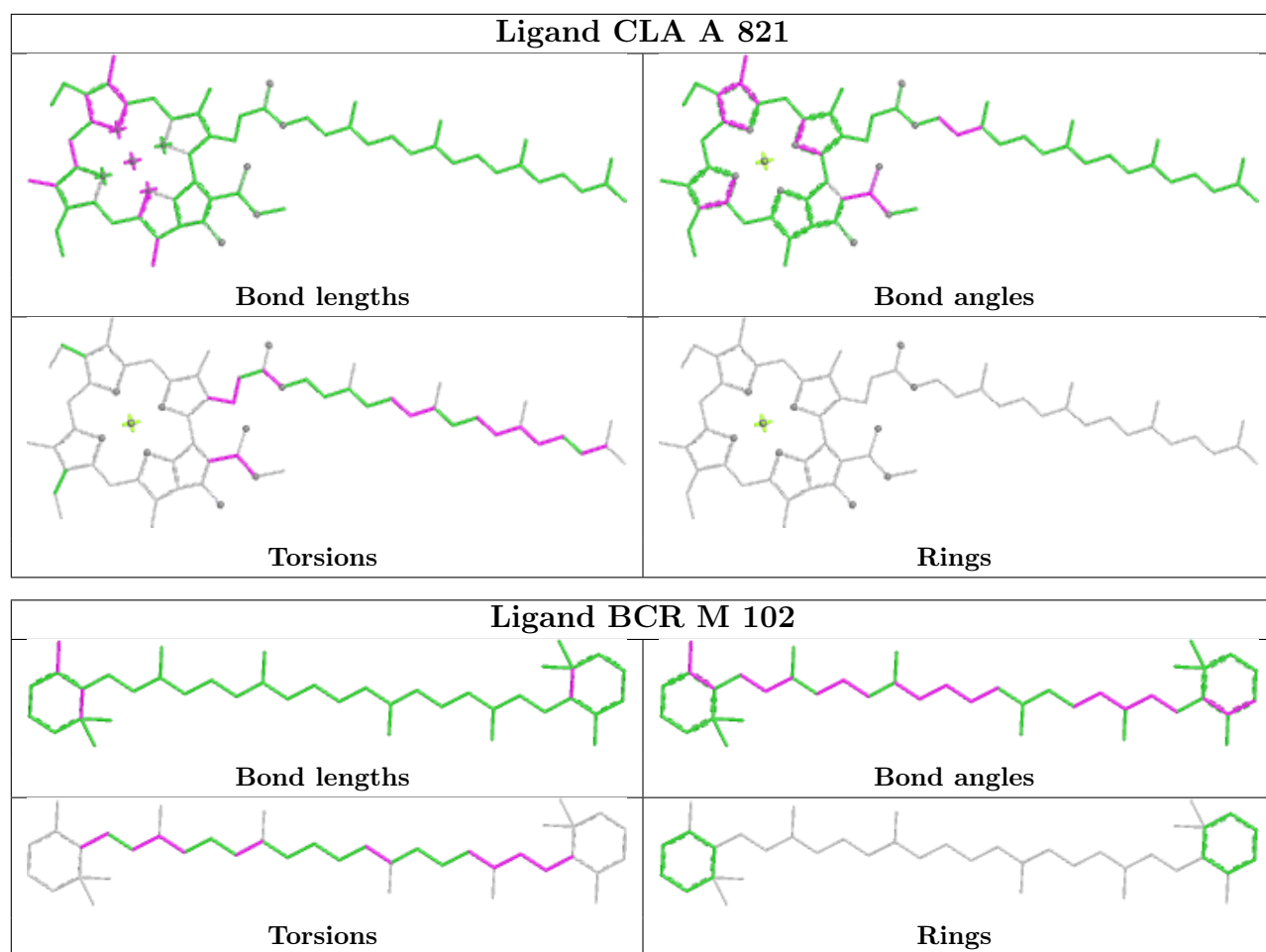


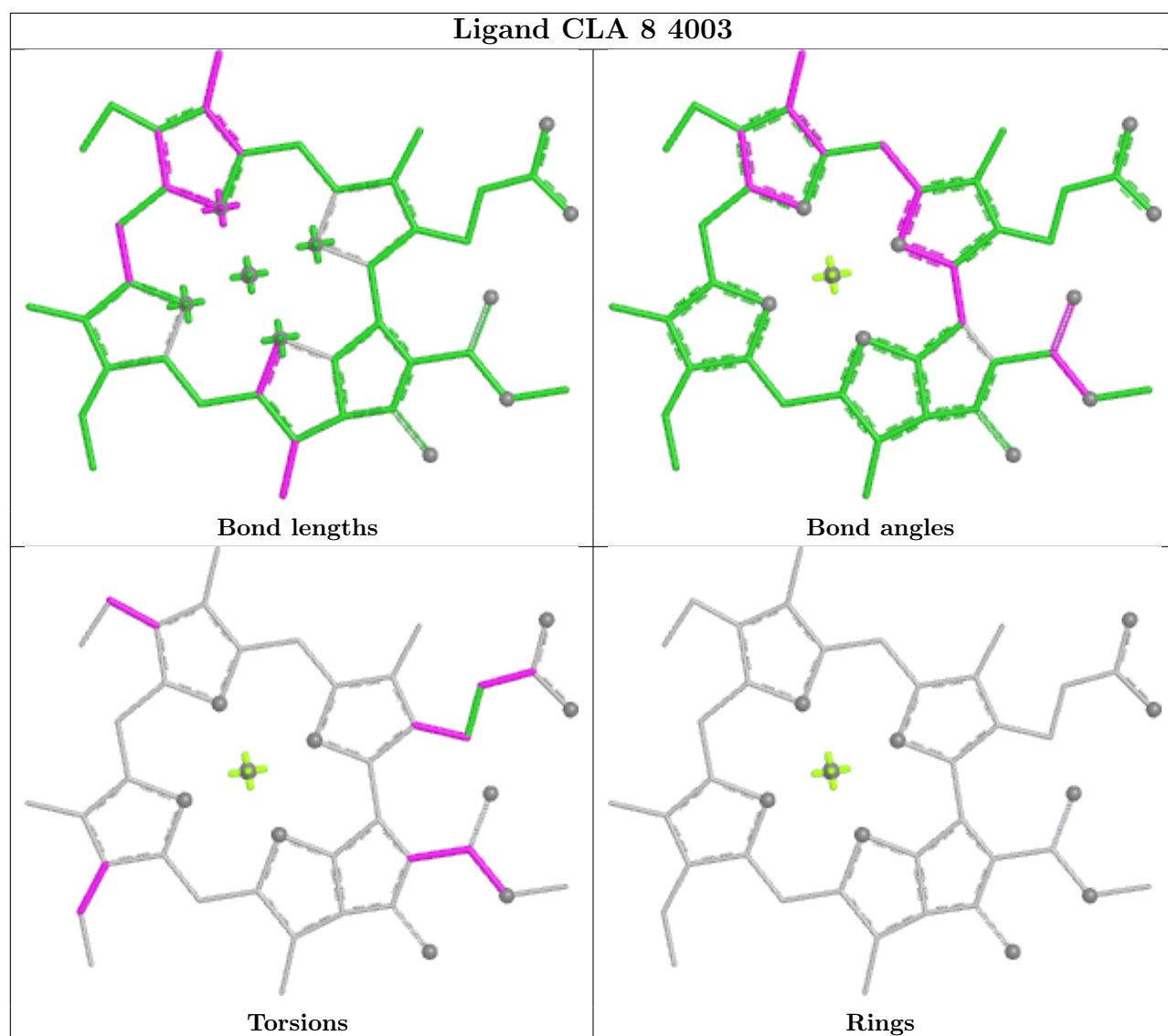
Ligand BCR b 848

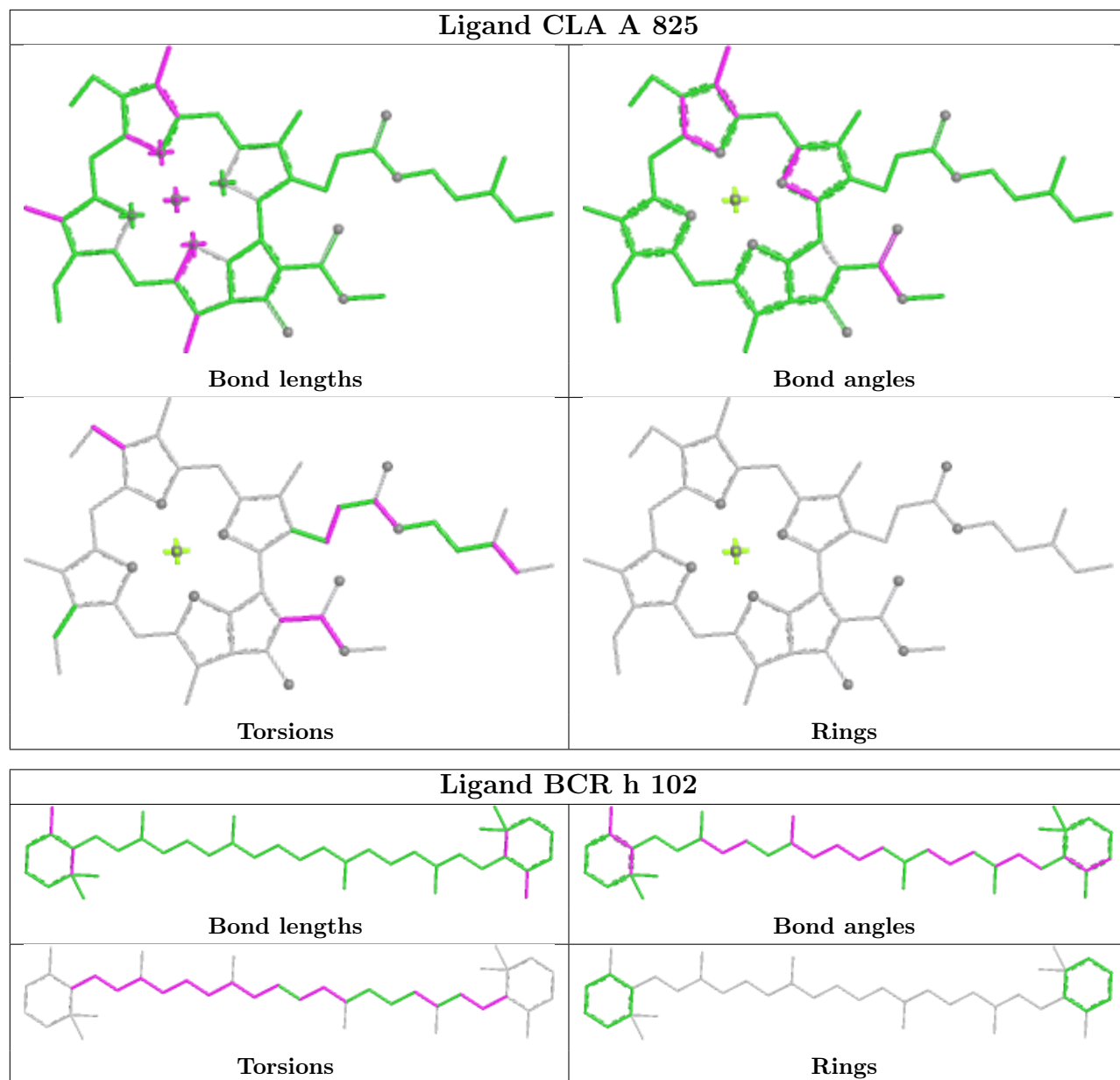


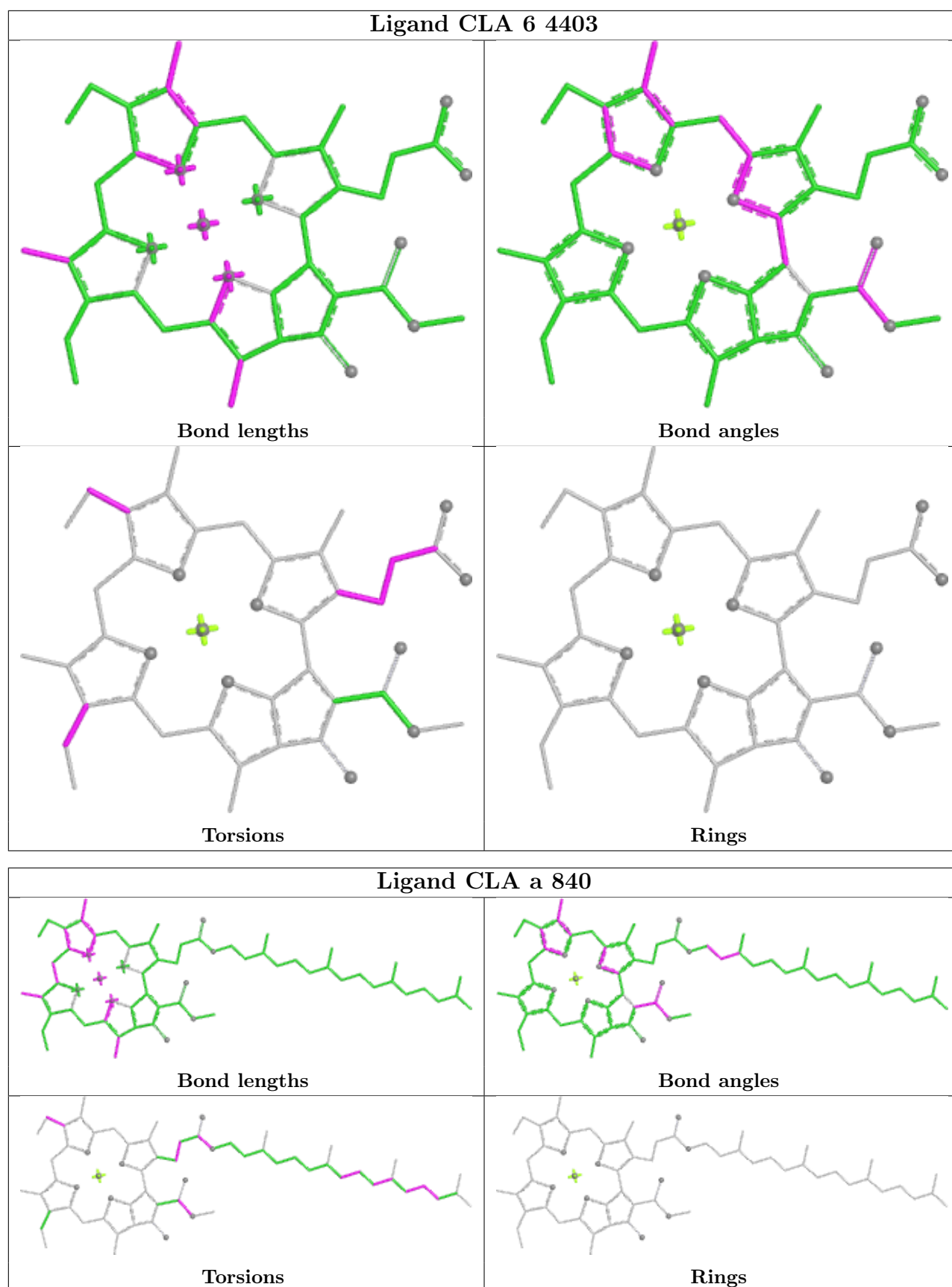




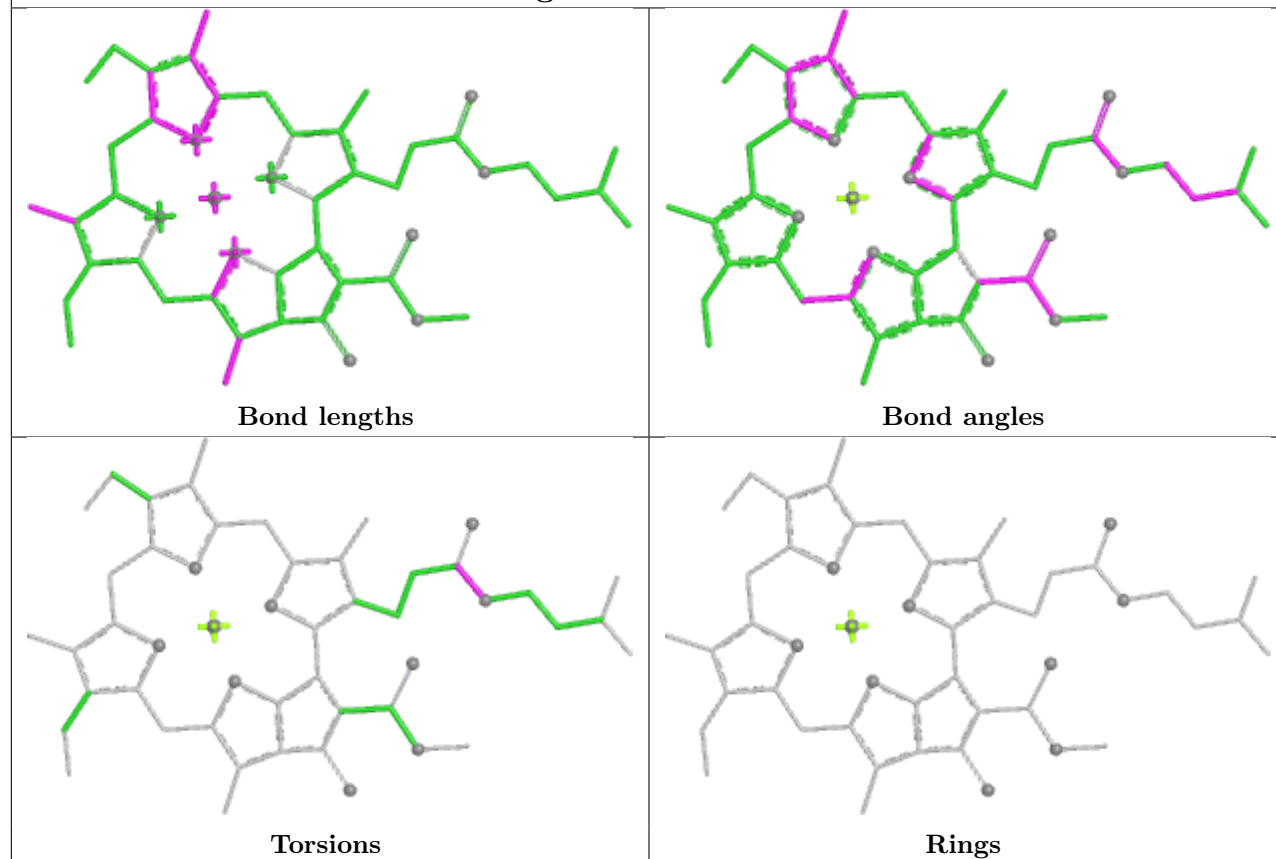




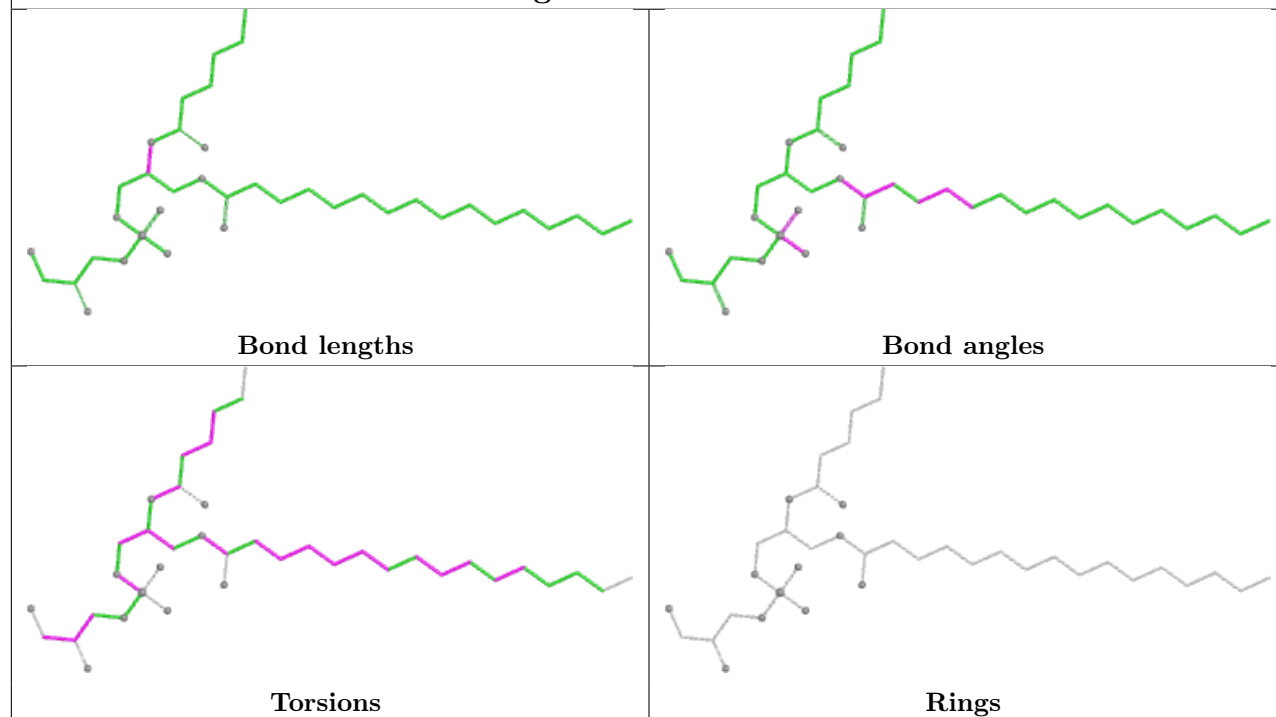


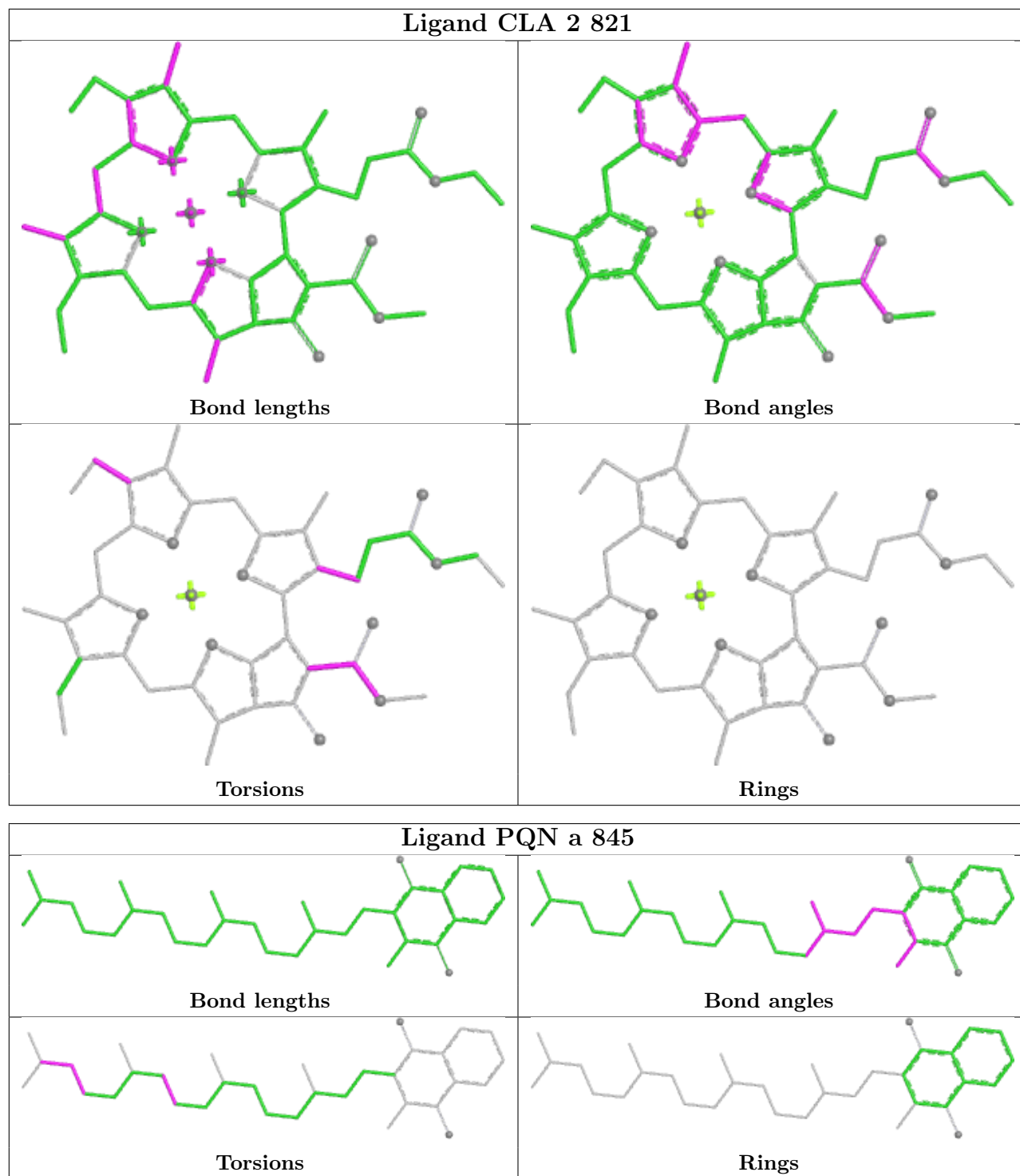


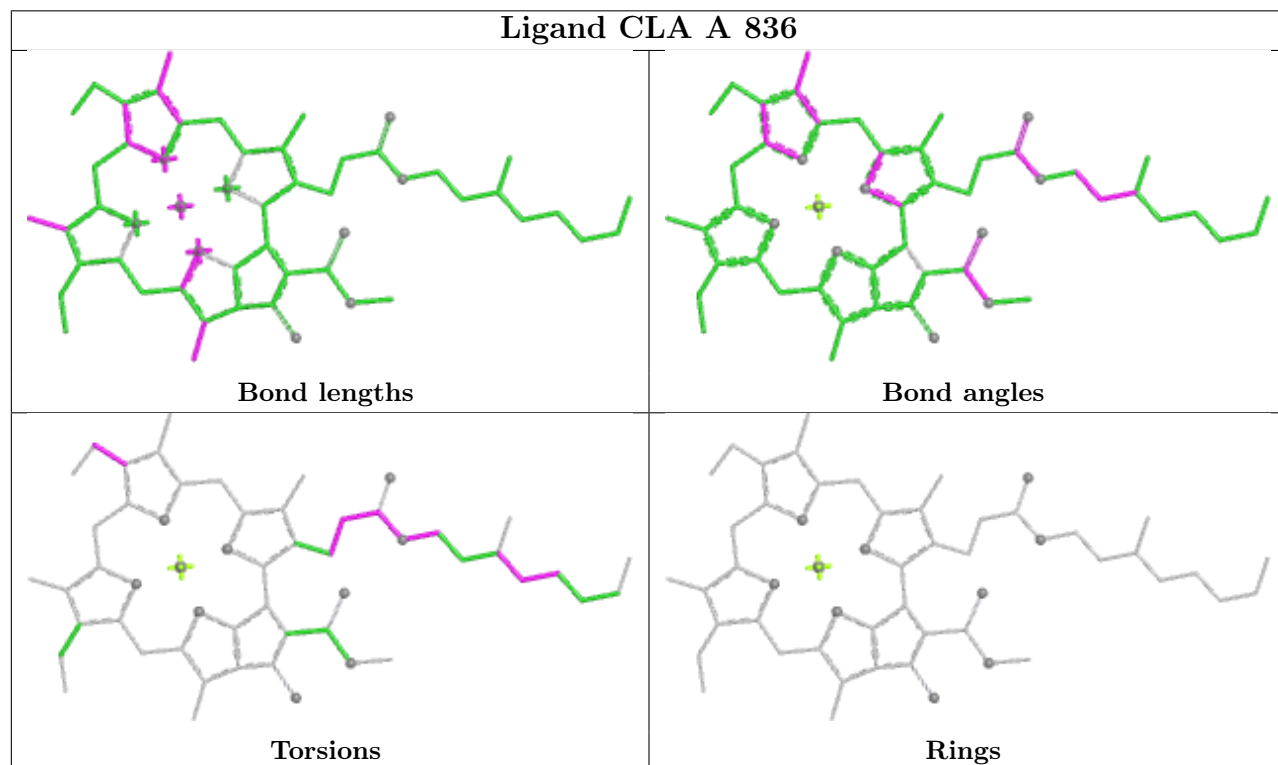
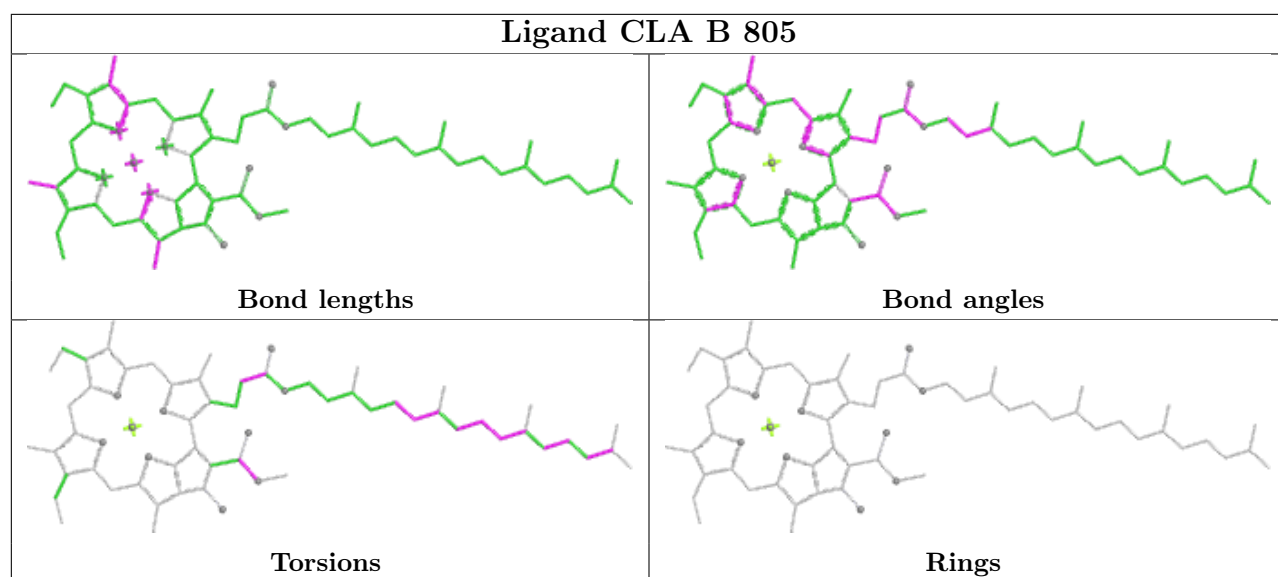
Ligand CLA 2 827



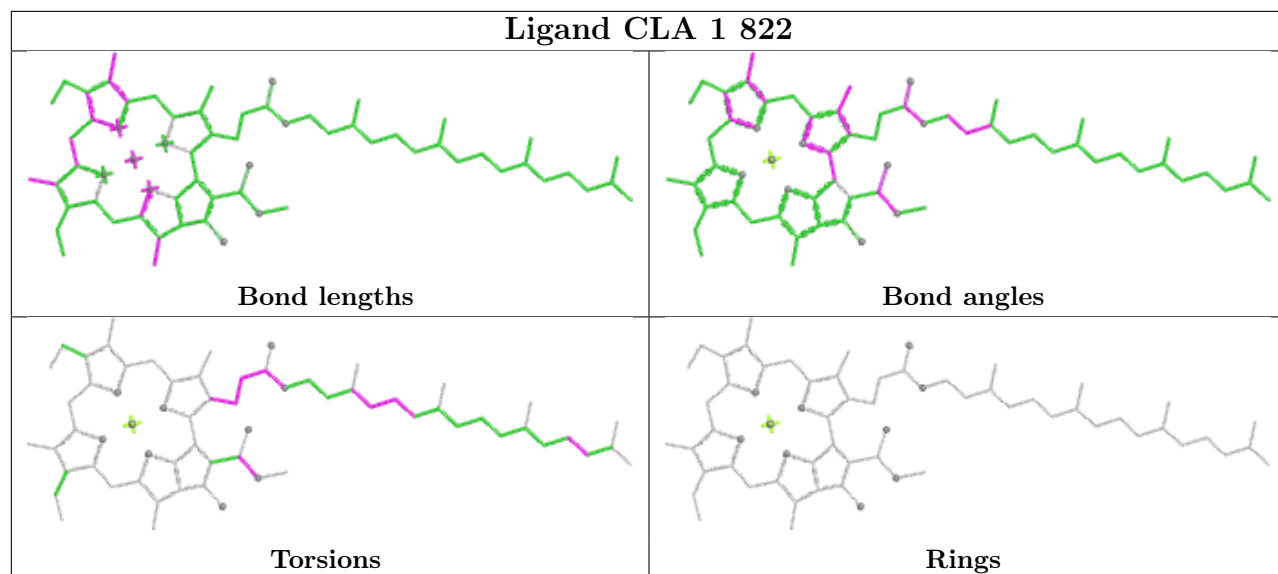
Ligand LHG b 852



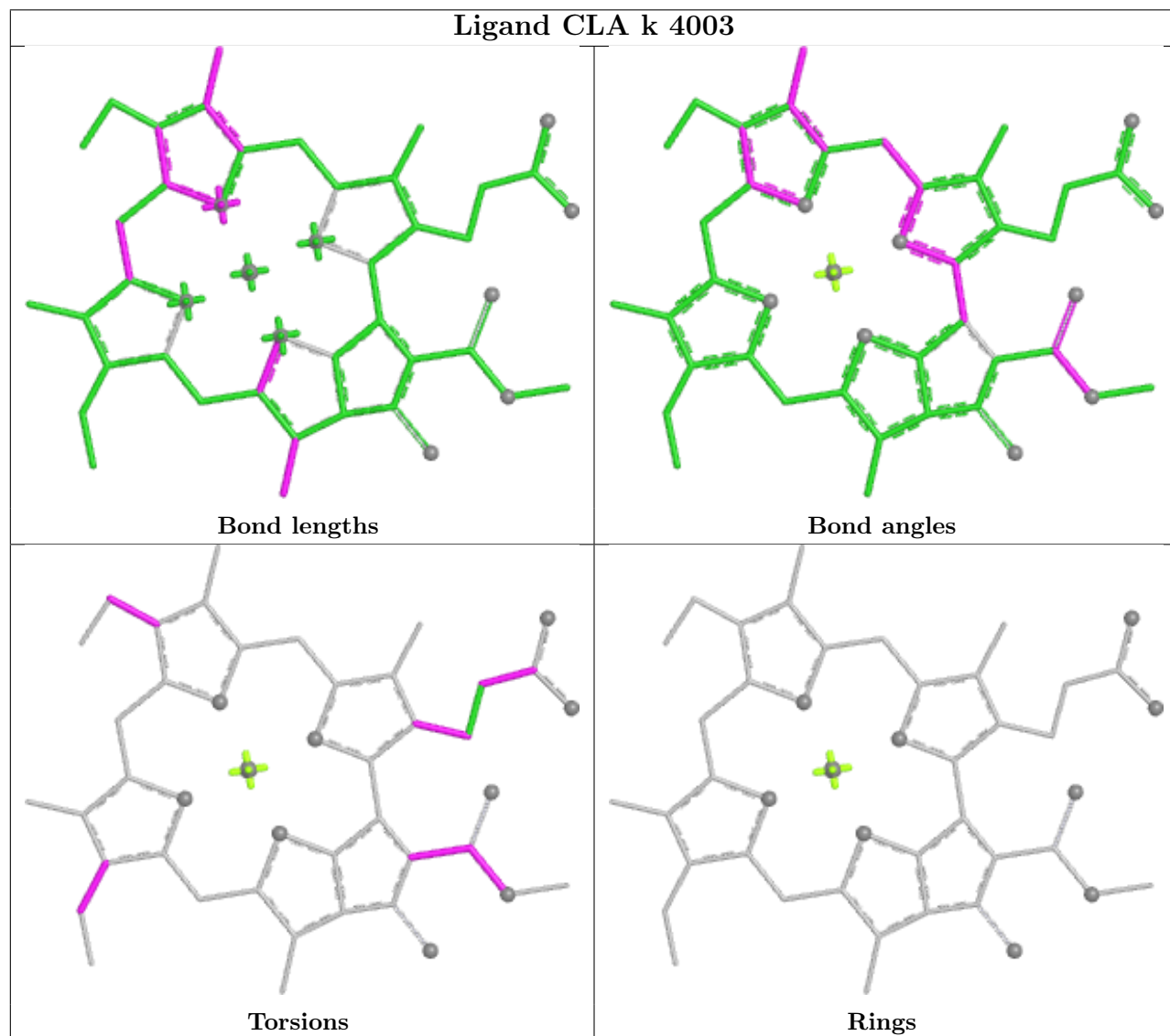


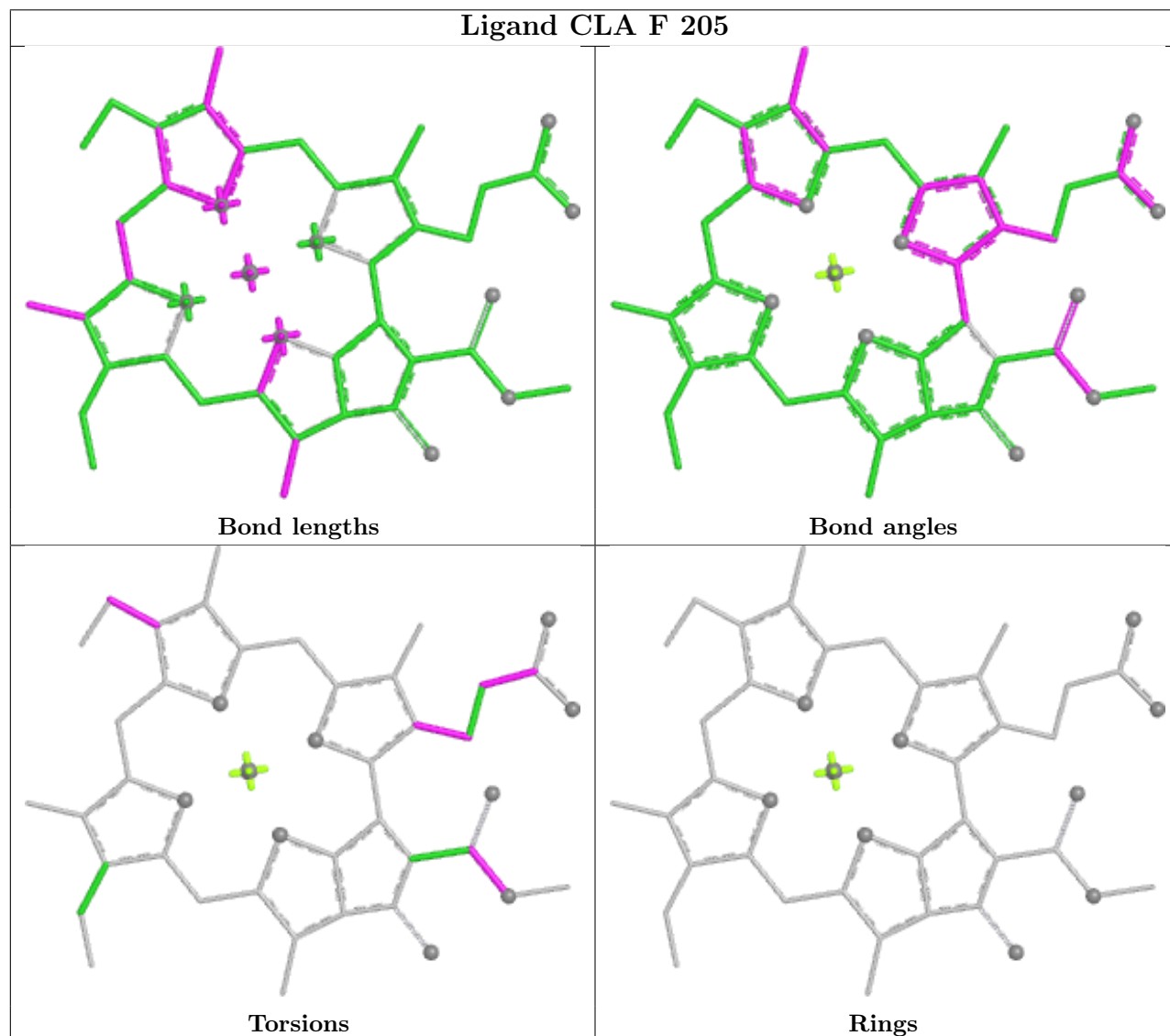
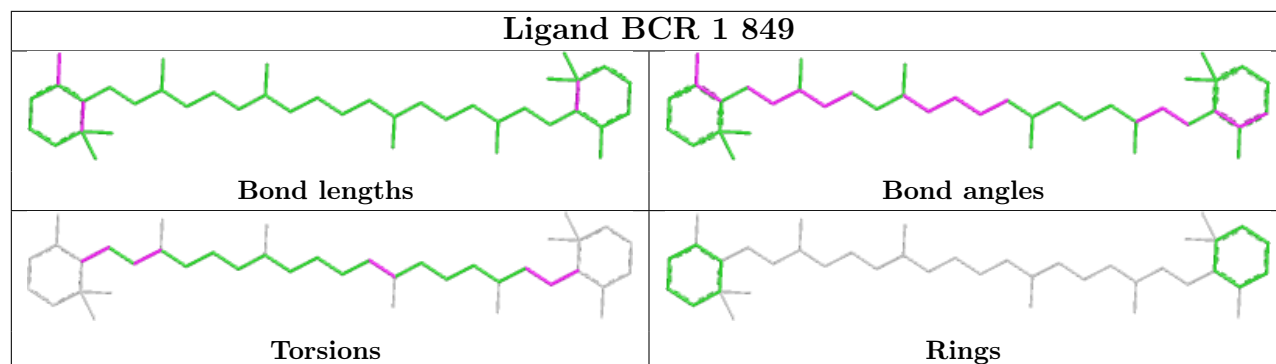


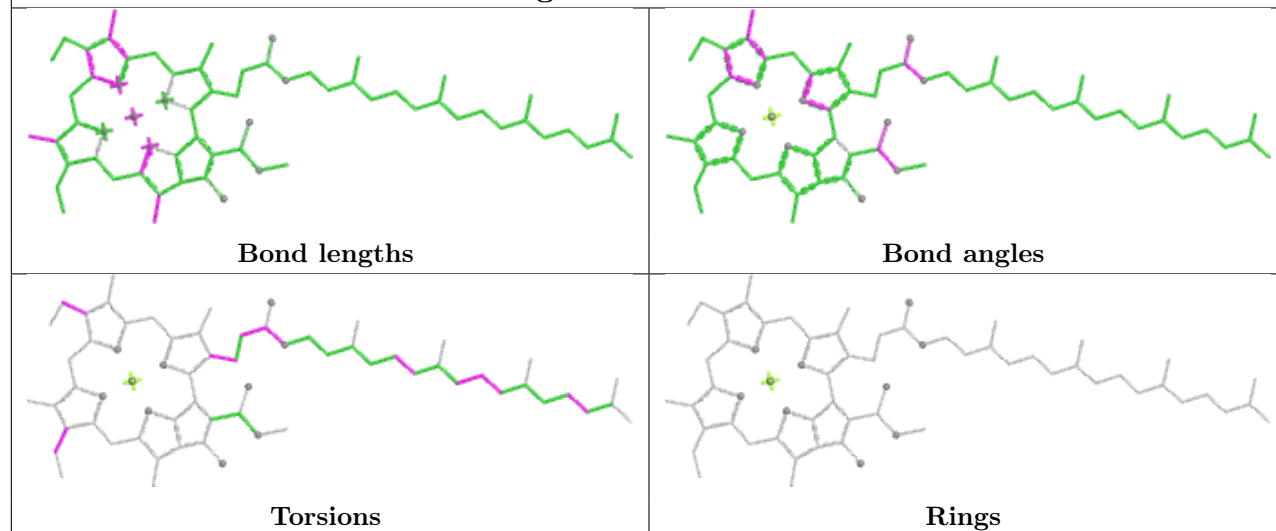
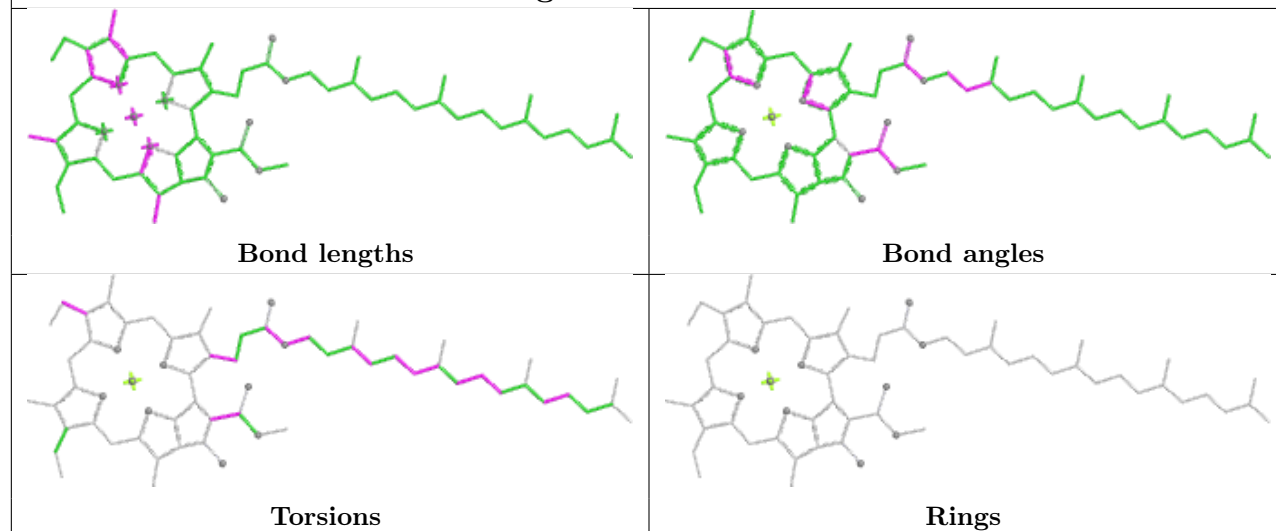
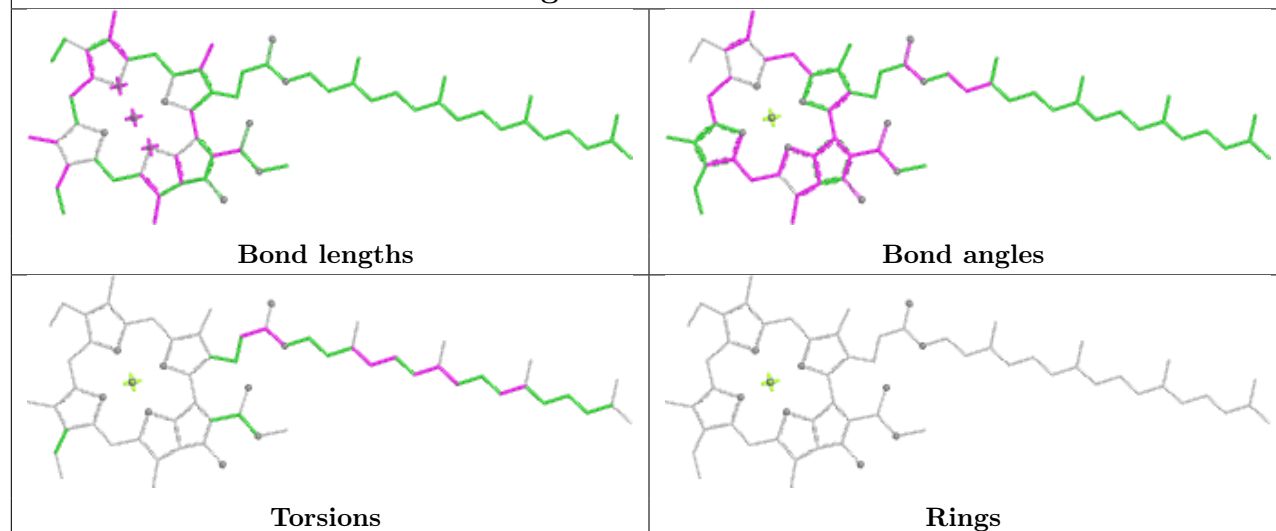
Ligand CLA 1 822



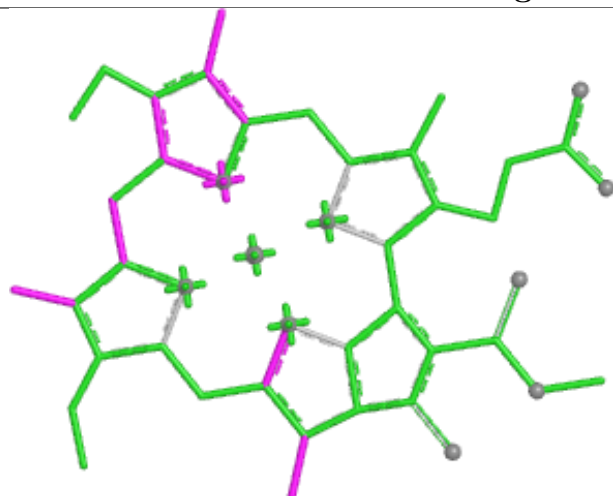
Ligand CLA k 4003



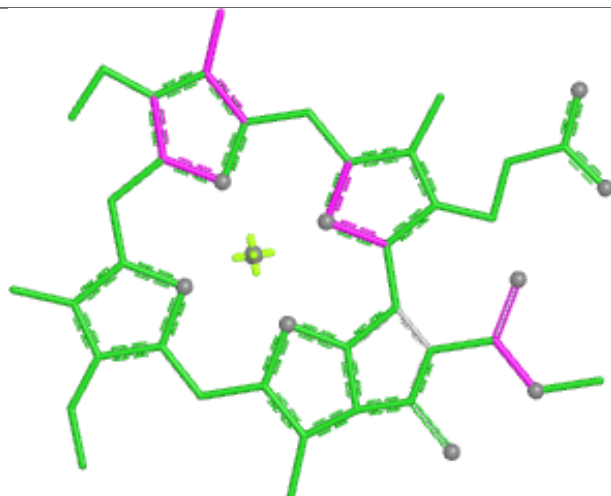


Ligand CLA 2 842**Ligand CLA a 806****Ligand CL0 a 803**

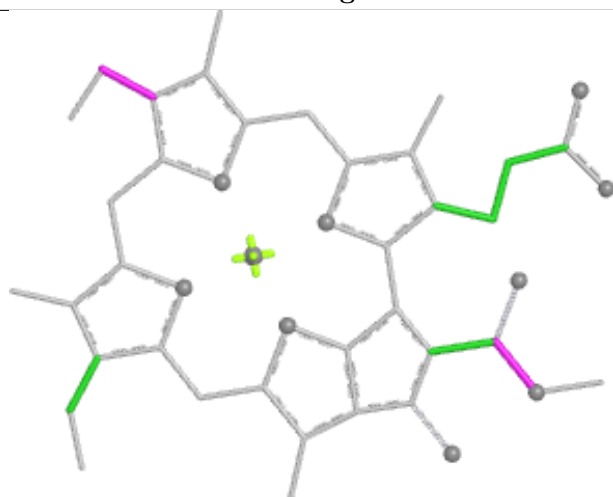
Ligand CLA B 818



Bond lengths



Bond angles

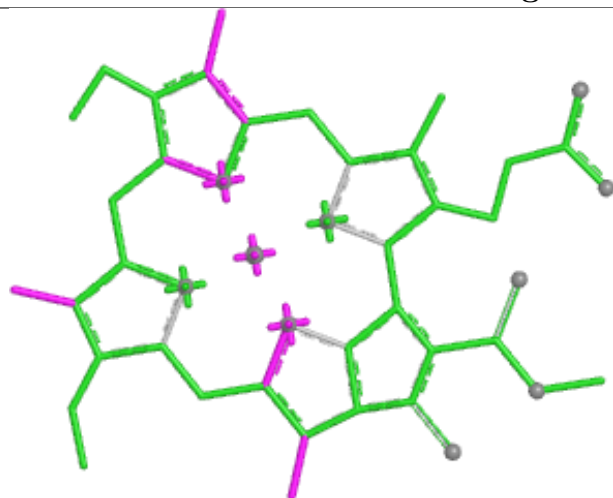


Torsions

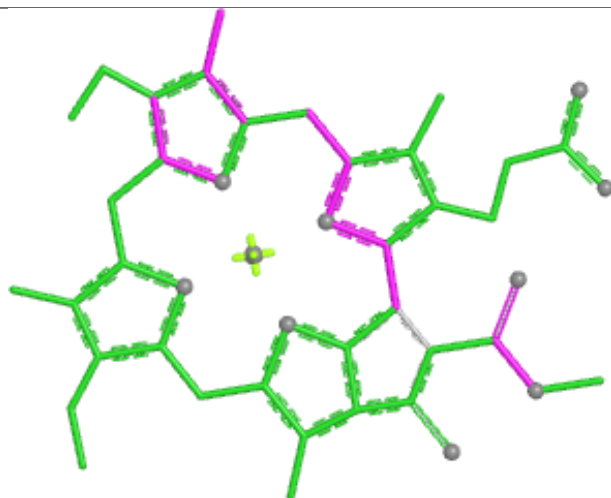


Rings

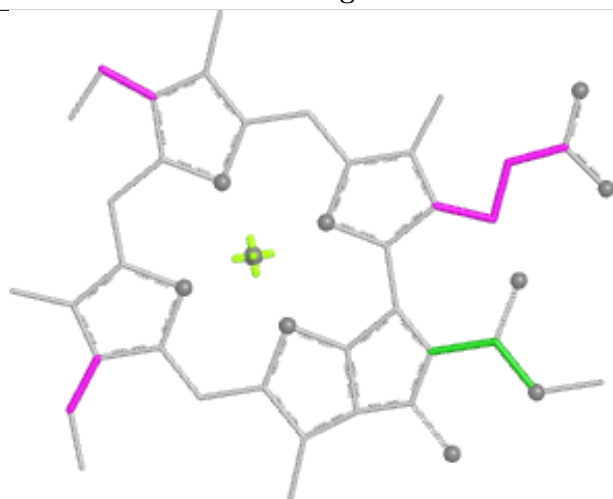
Ligand CLA f 204



Bond lengths



Bond angles

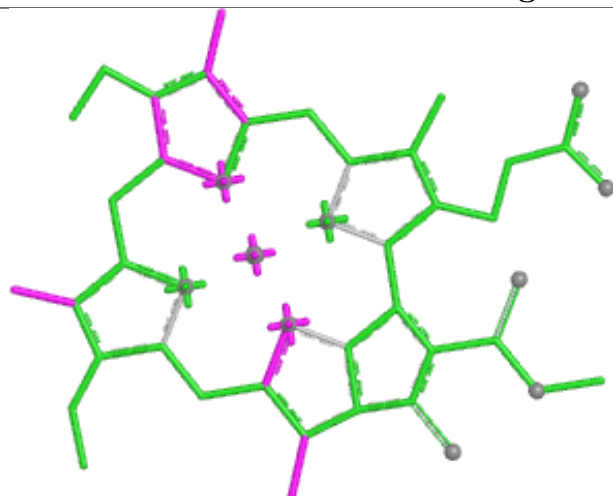


Torsions

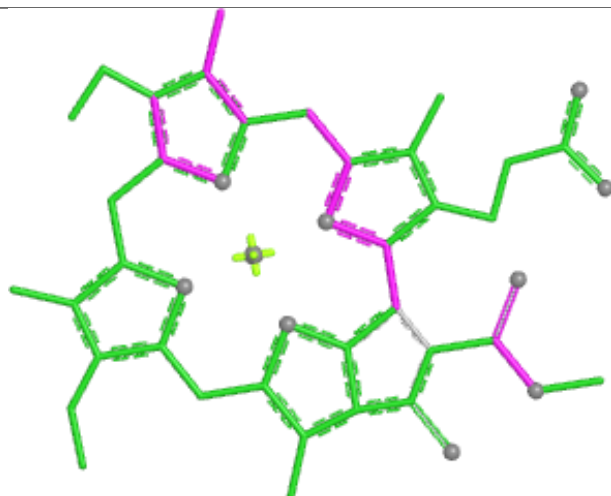


Rings

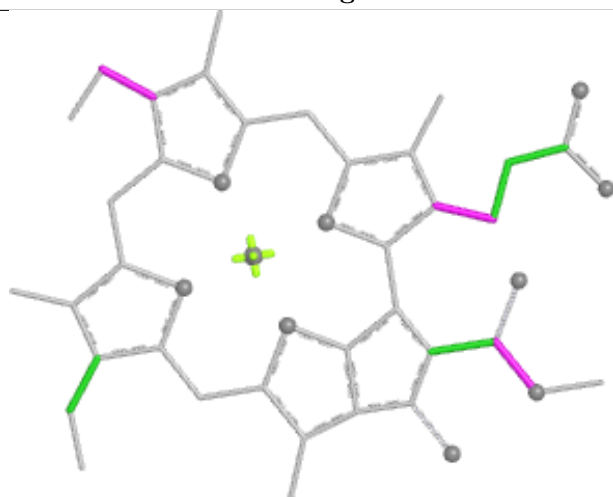
Ligand CLA 2 813



Bond lengths



Bond angles

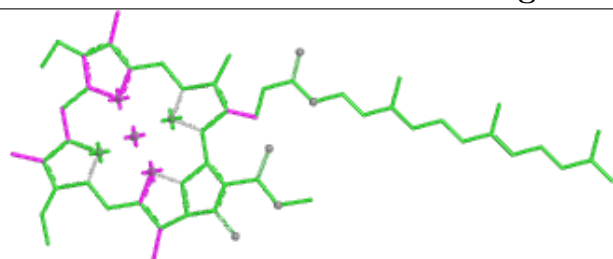


Torsions

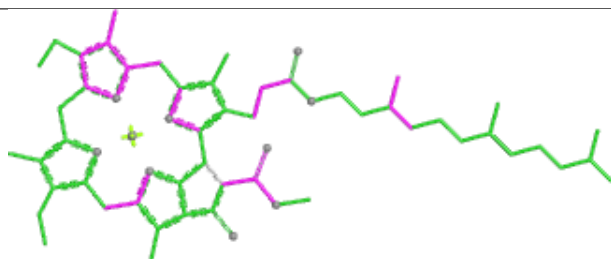


Rings

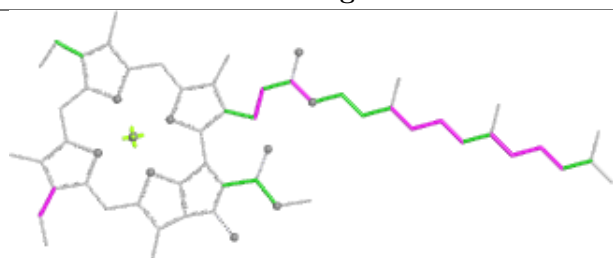
Ligand CLA a 804



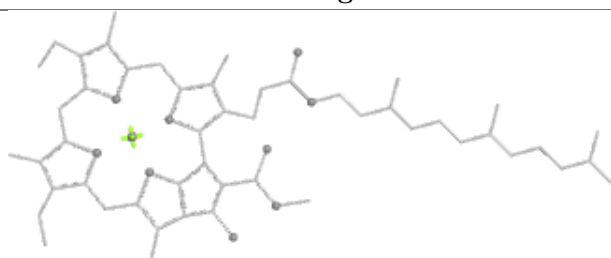
Bond lengths



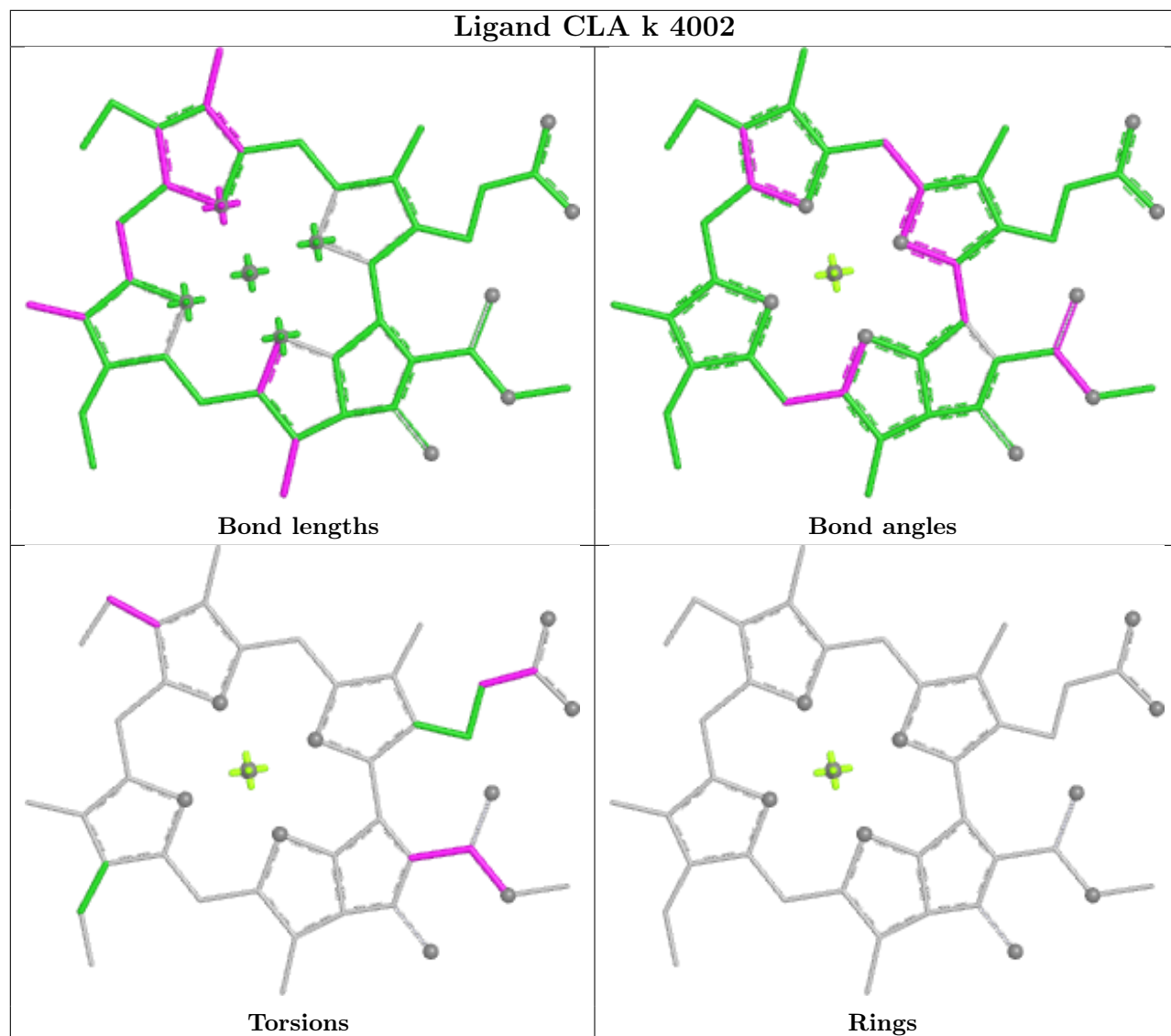
Bond angles



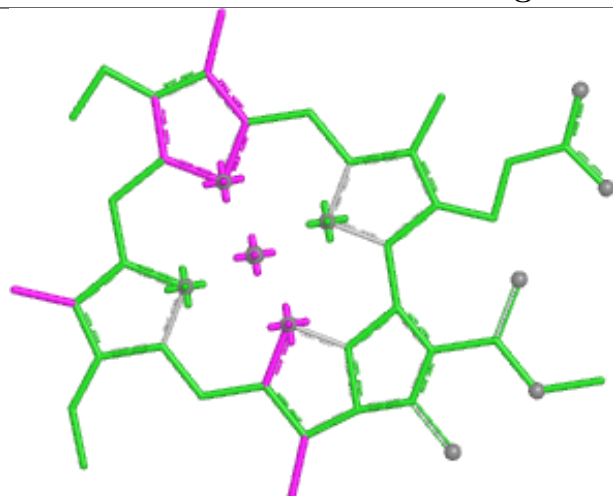
Torsions



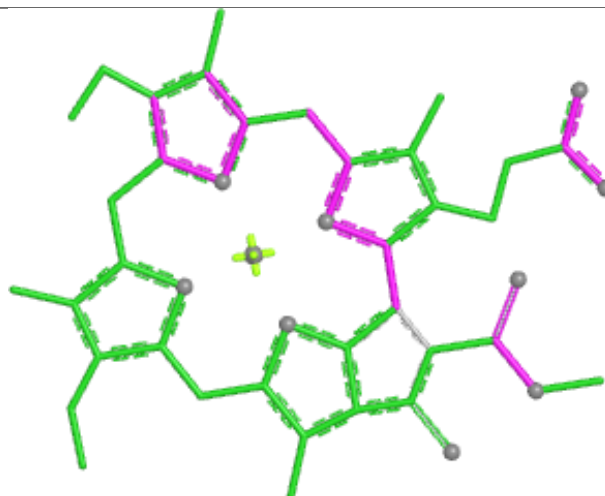
Rings



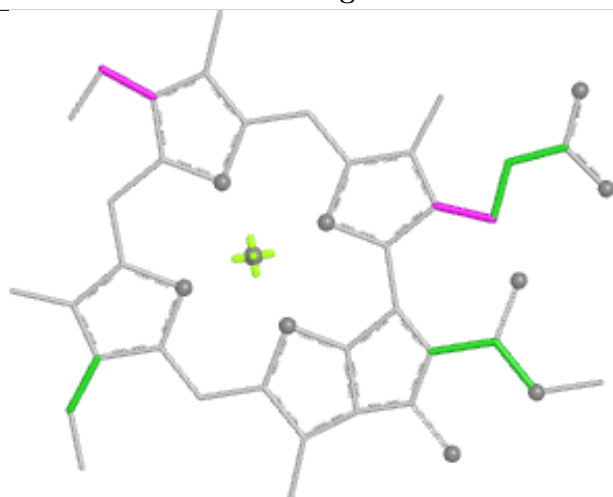
Ligand CLA B 836



Bond lengths



Bond angles

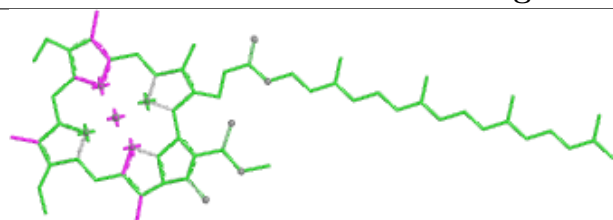


Torsions

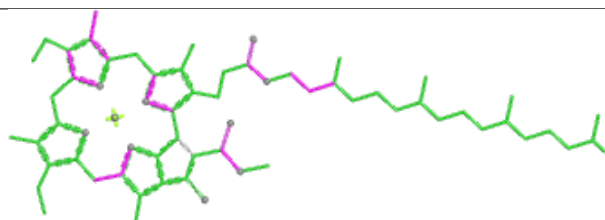


Rings

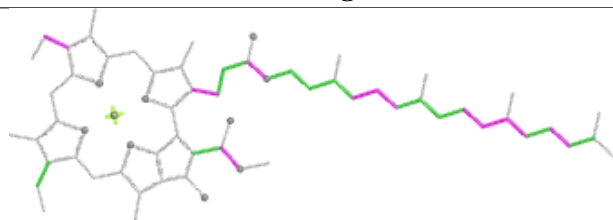
Ligand CLA A 808



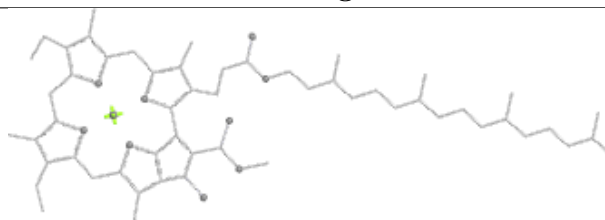
Bond lengths



Bond angles

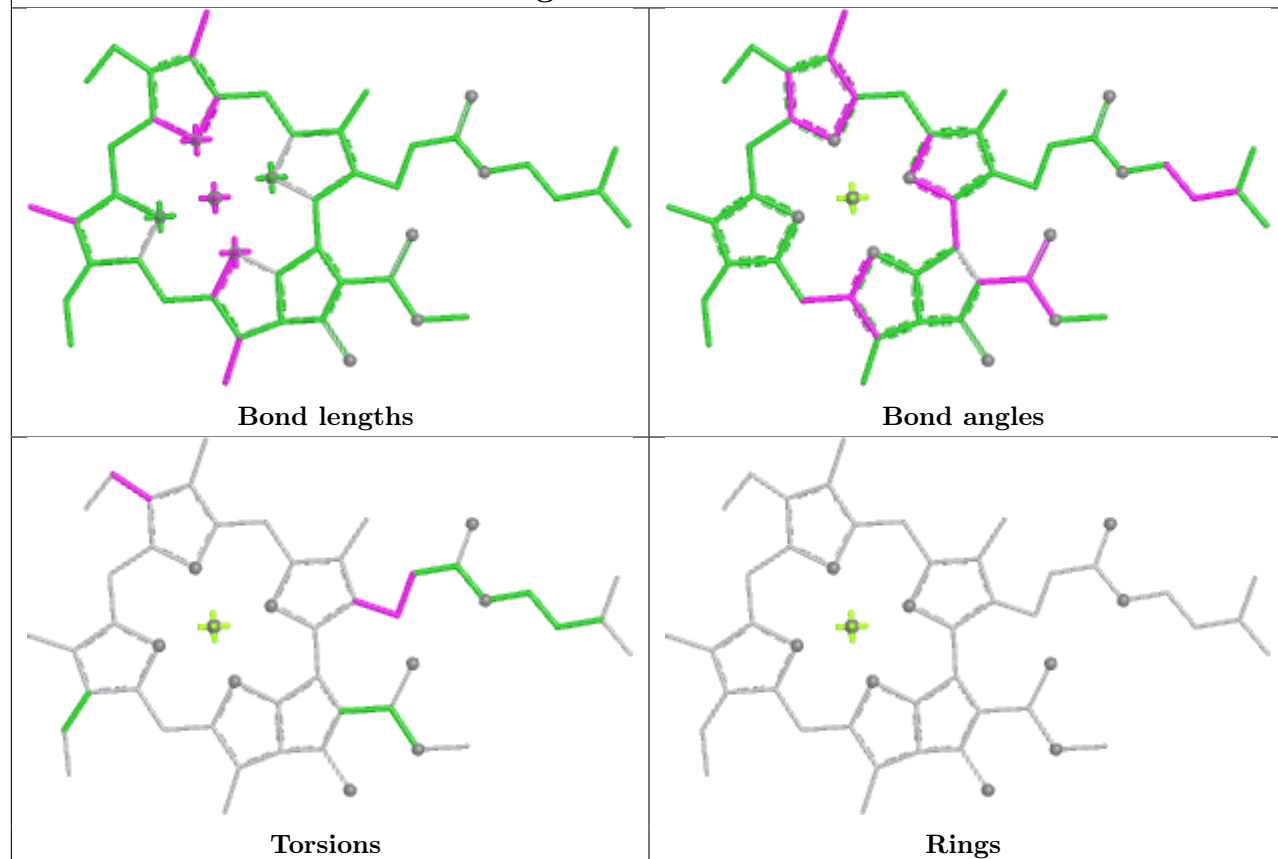


Torsions

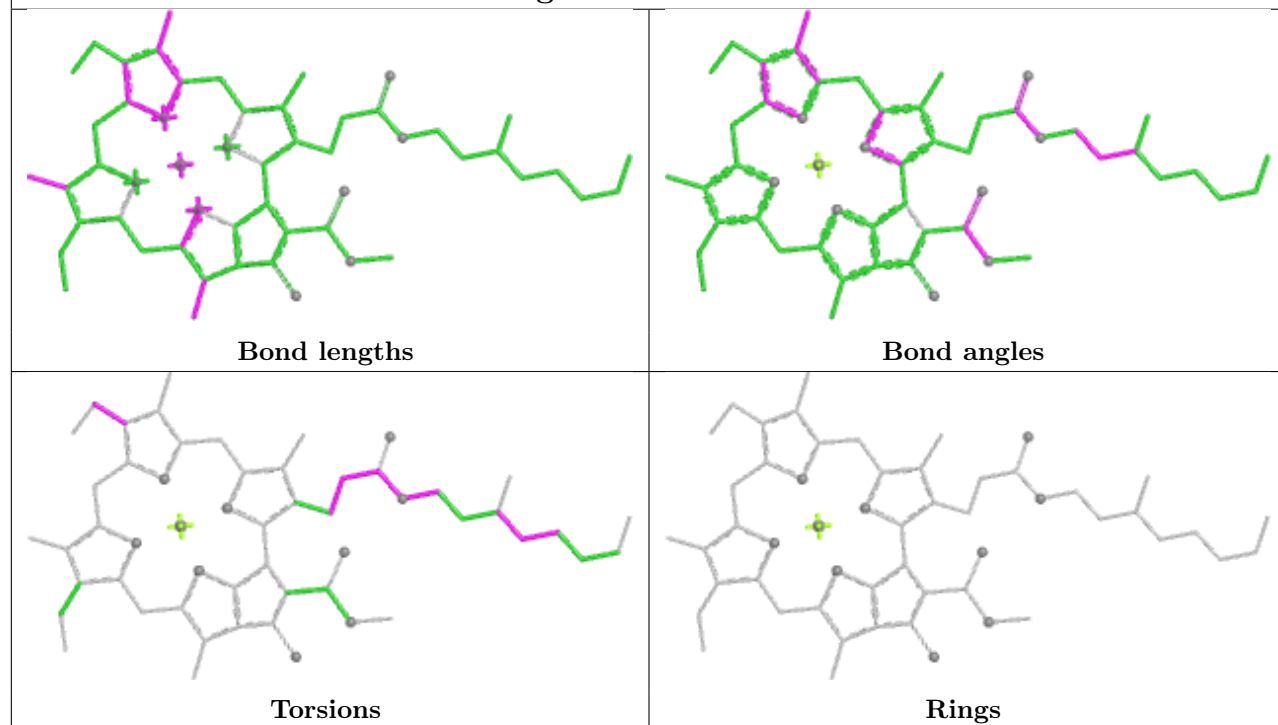


Rings

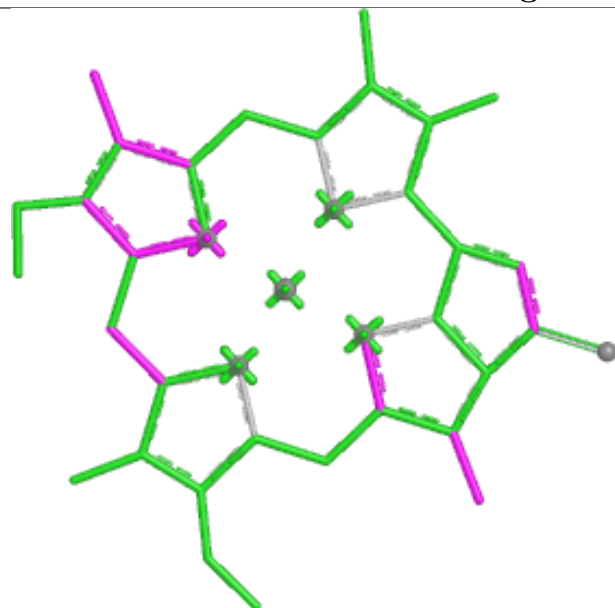
Ligand CLA a 834



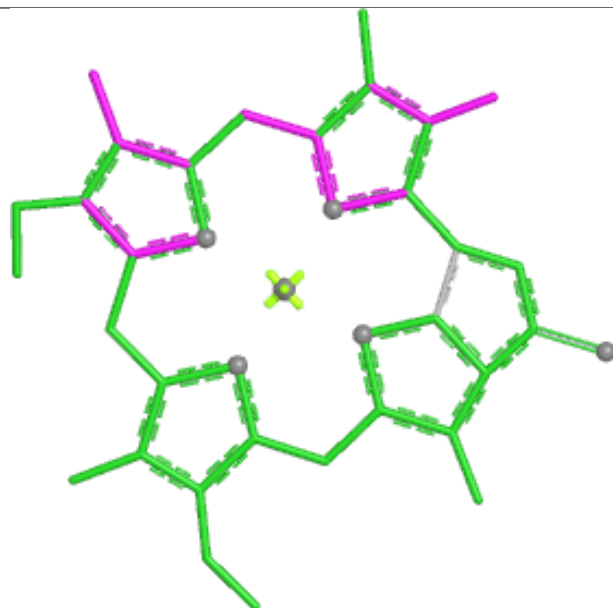
Ligand CLA a 837



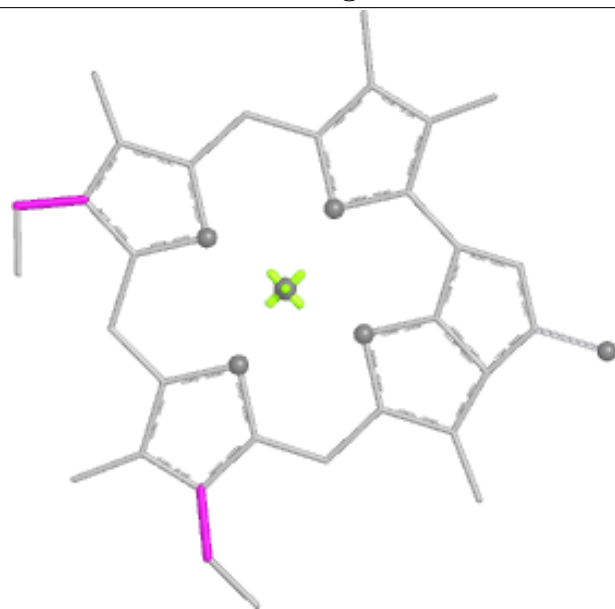
Ligand CLA J 102



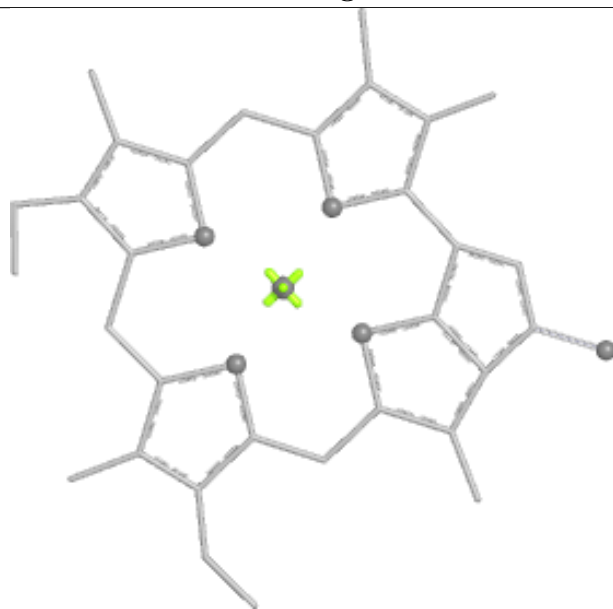
Bond lengths



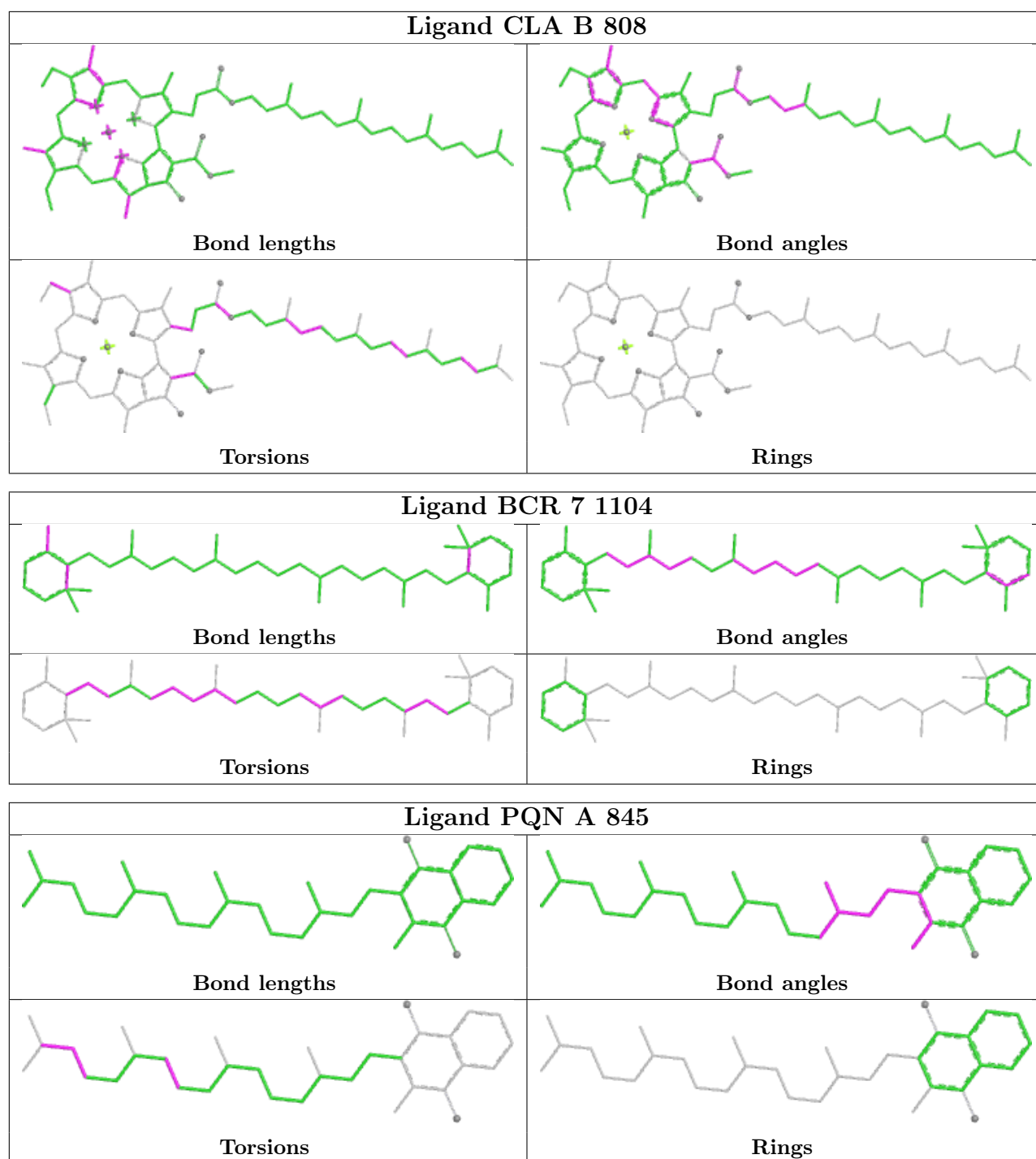
Bond angles

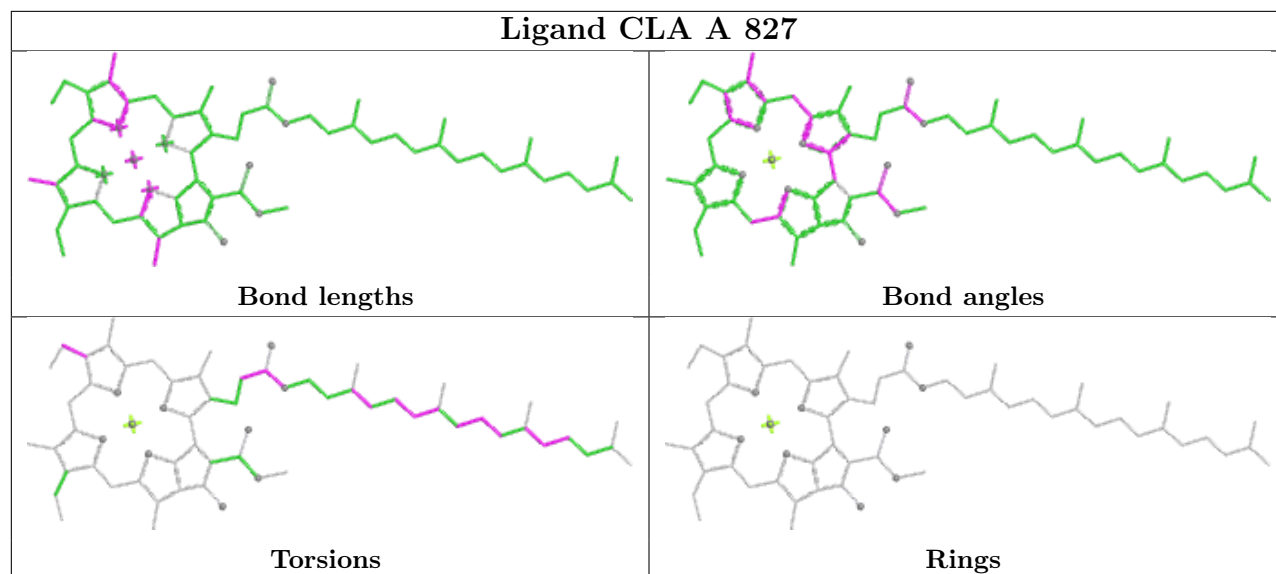
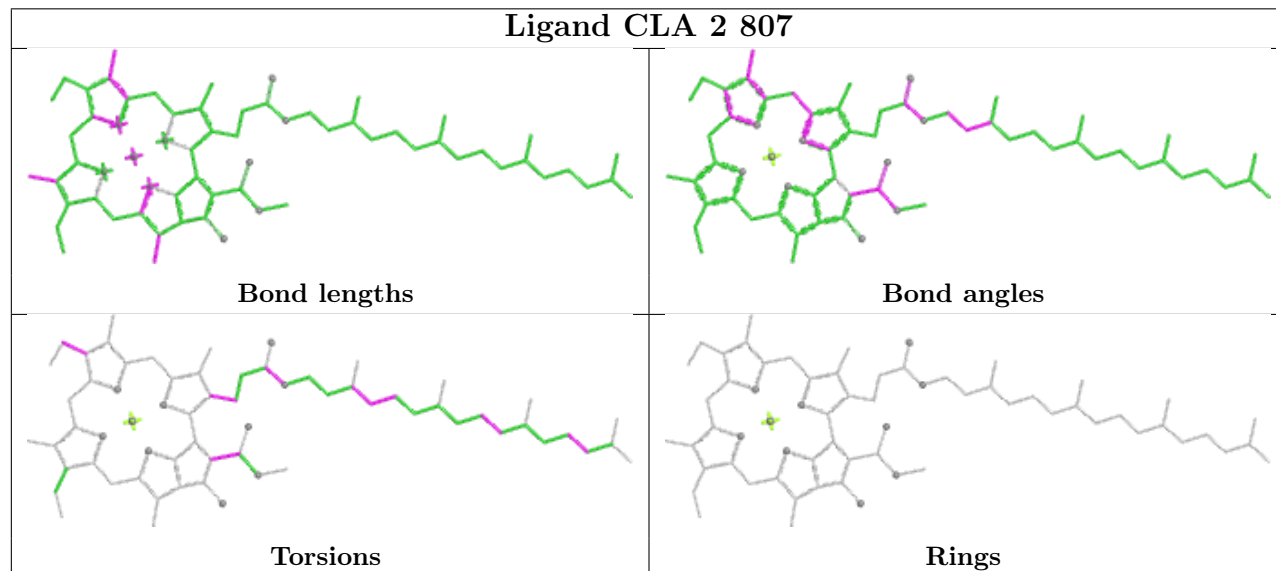


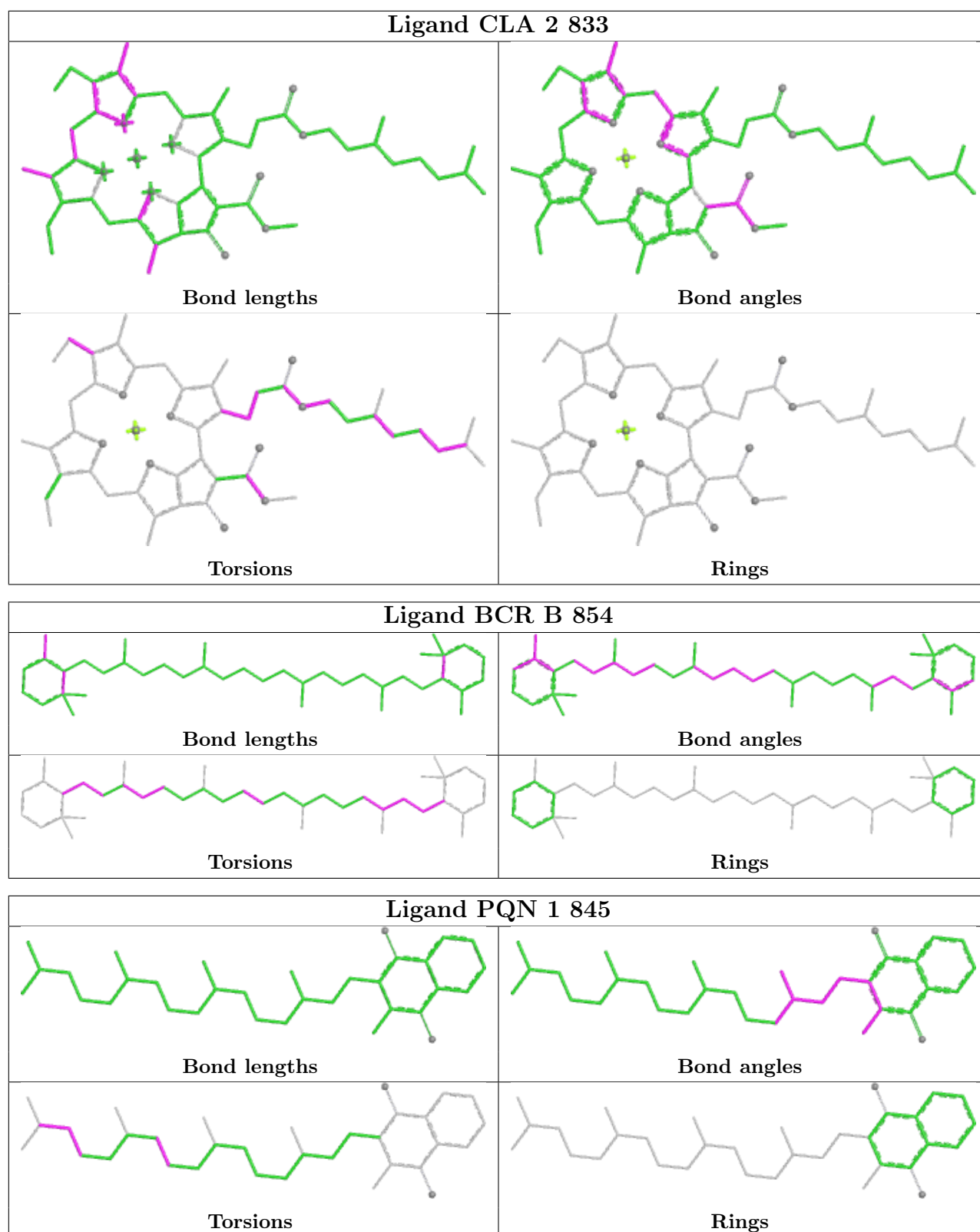
Torsions



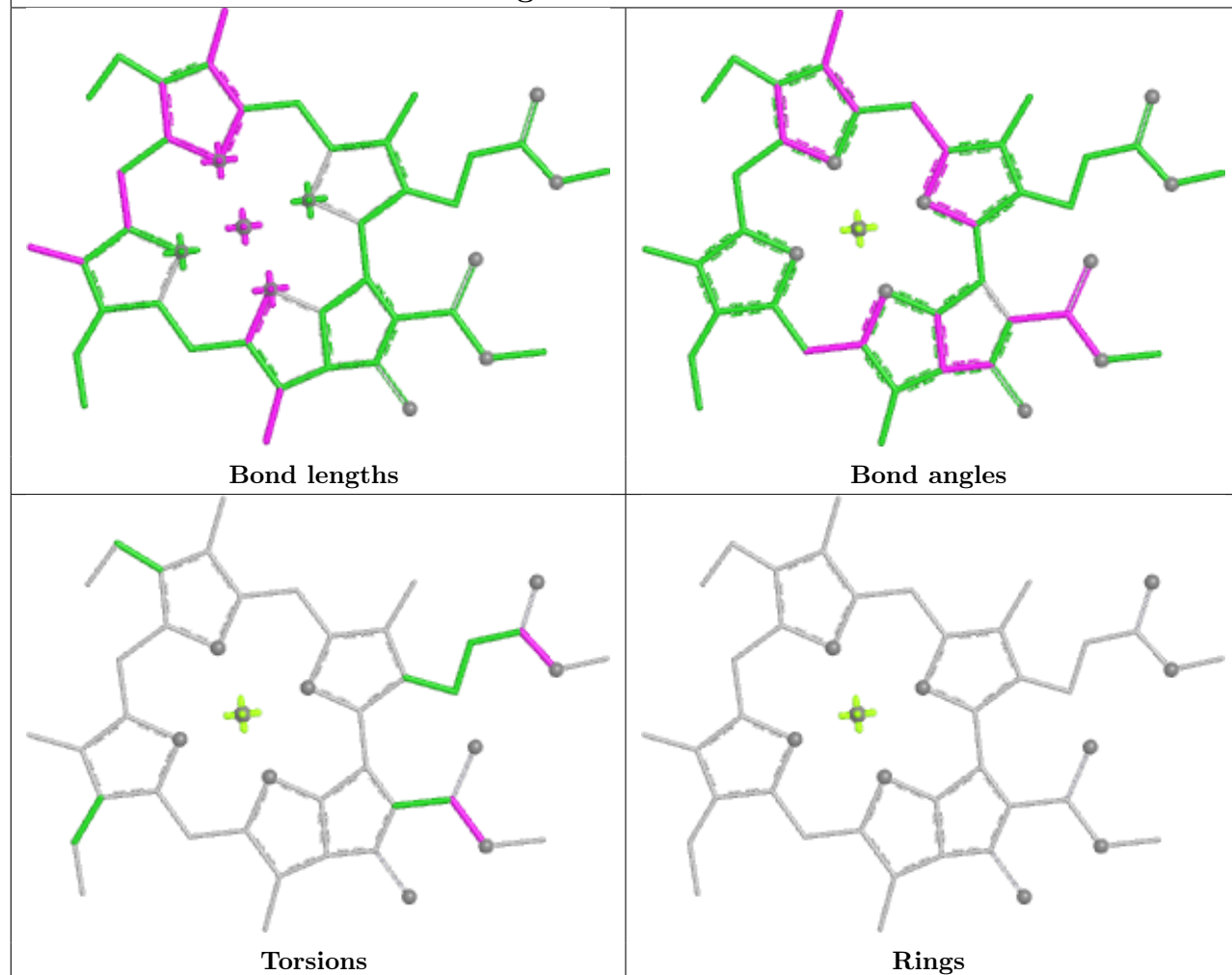
Rings



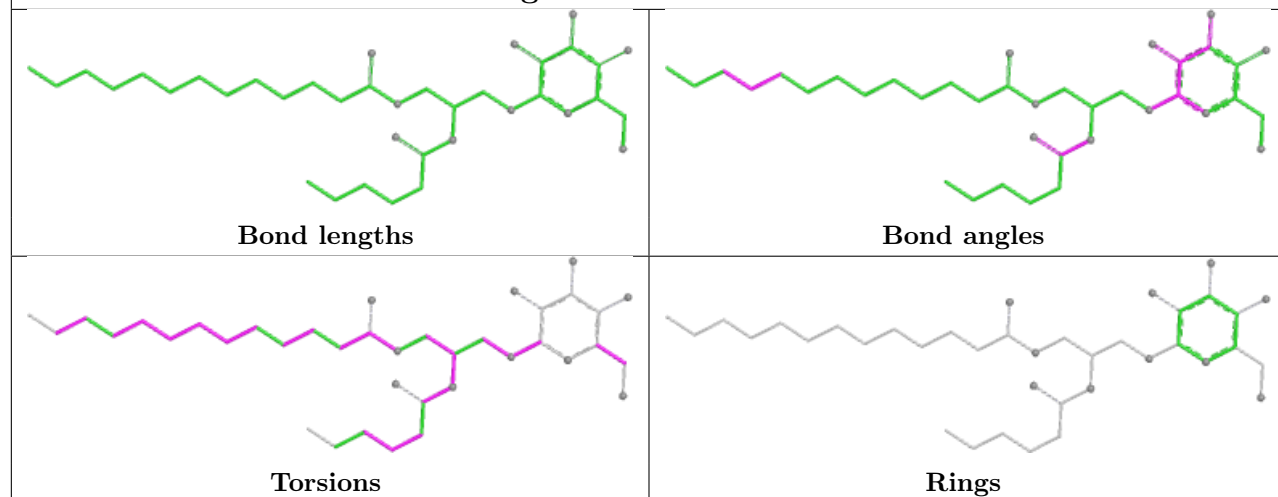
Ligand CLA A 827**Ligand CLA 2 807**

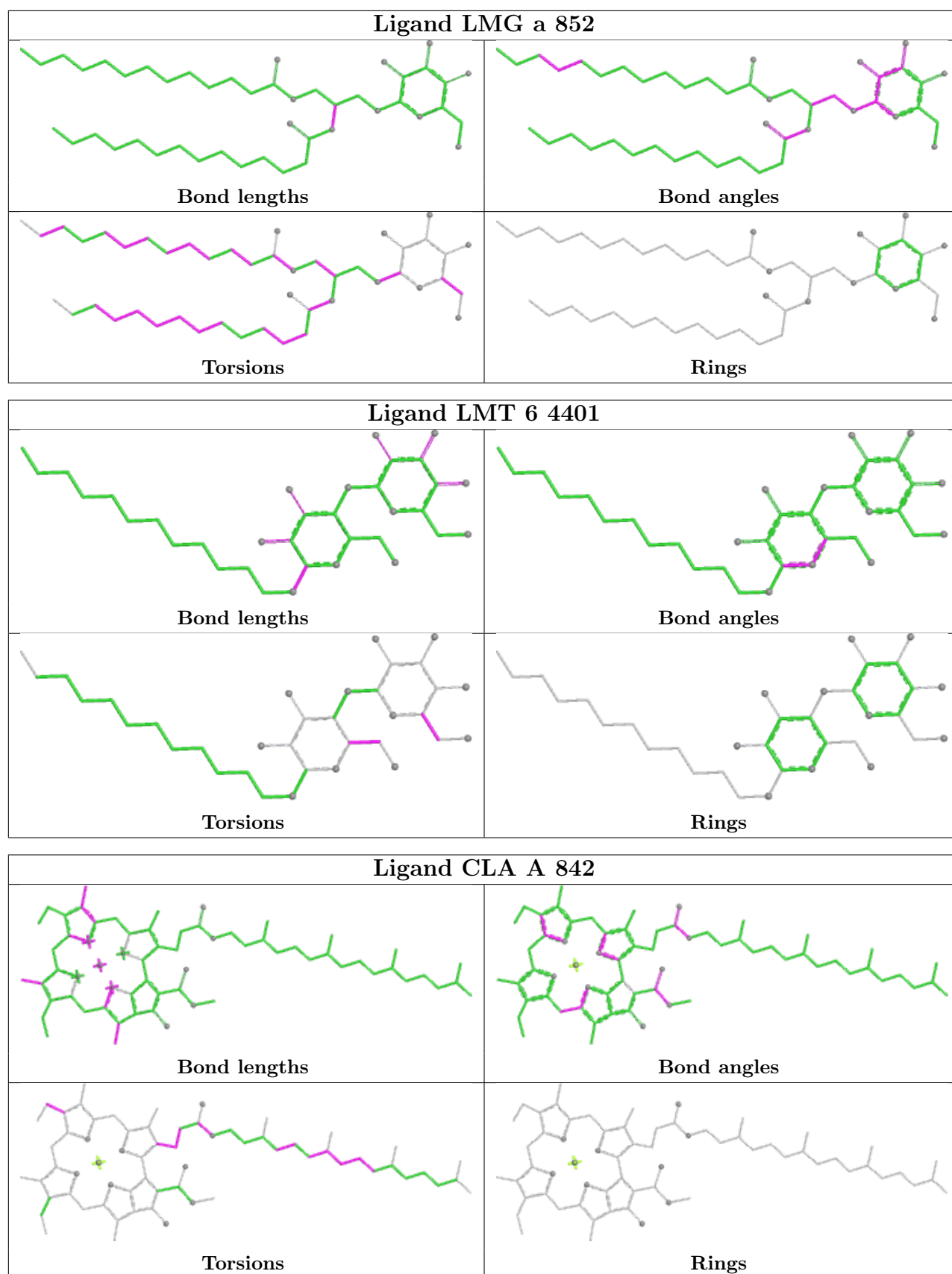


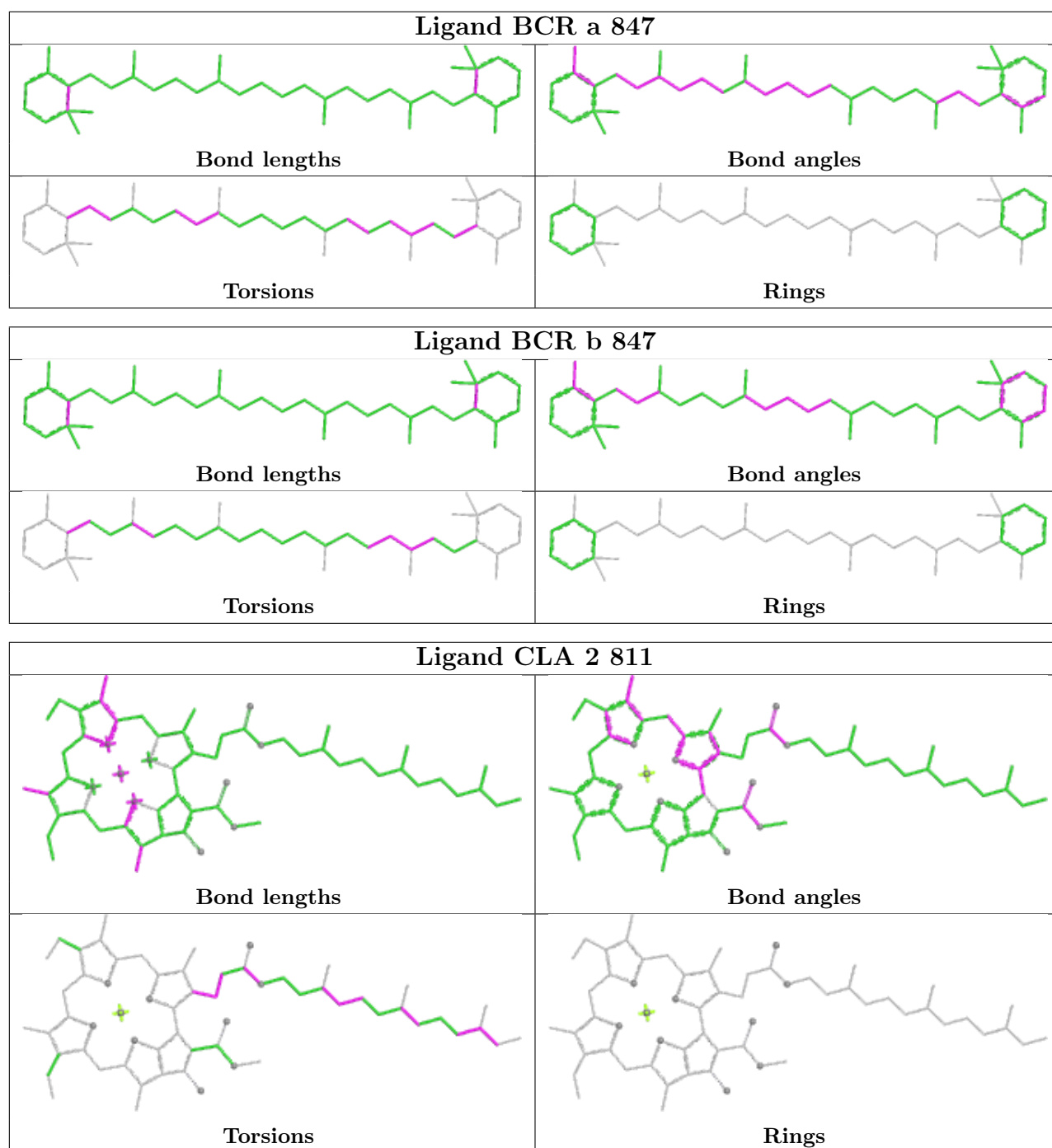
Ligand CLA 2 841

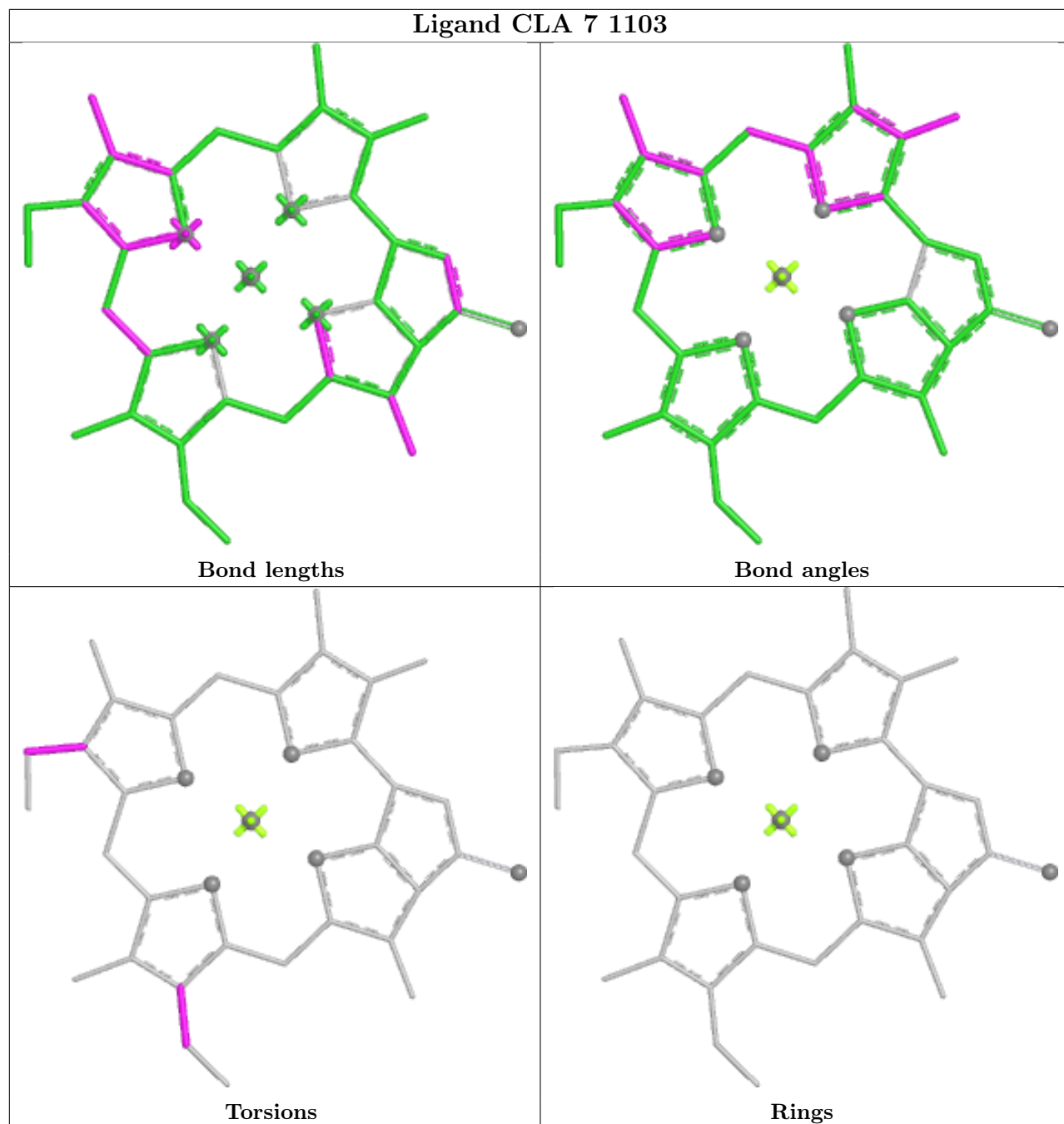


Ligand LMG L 1506

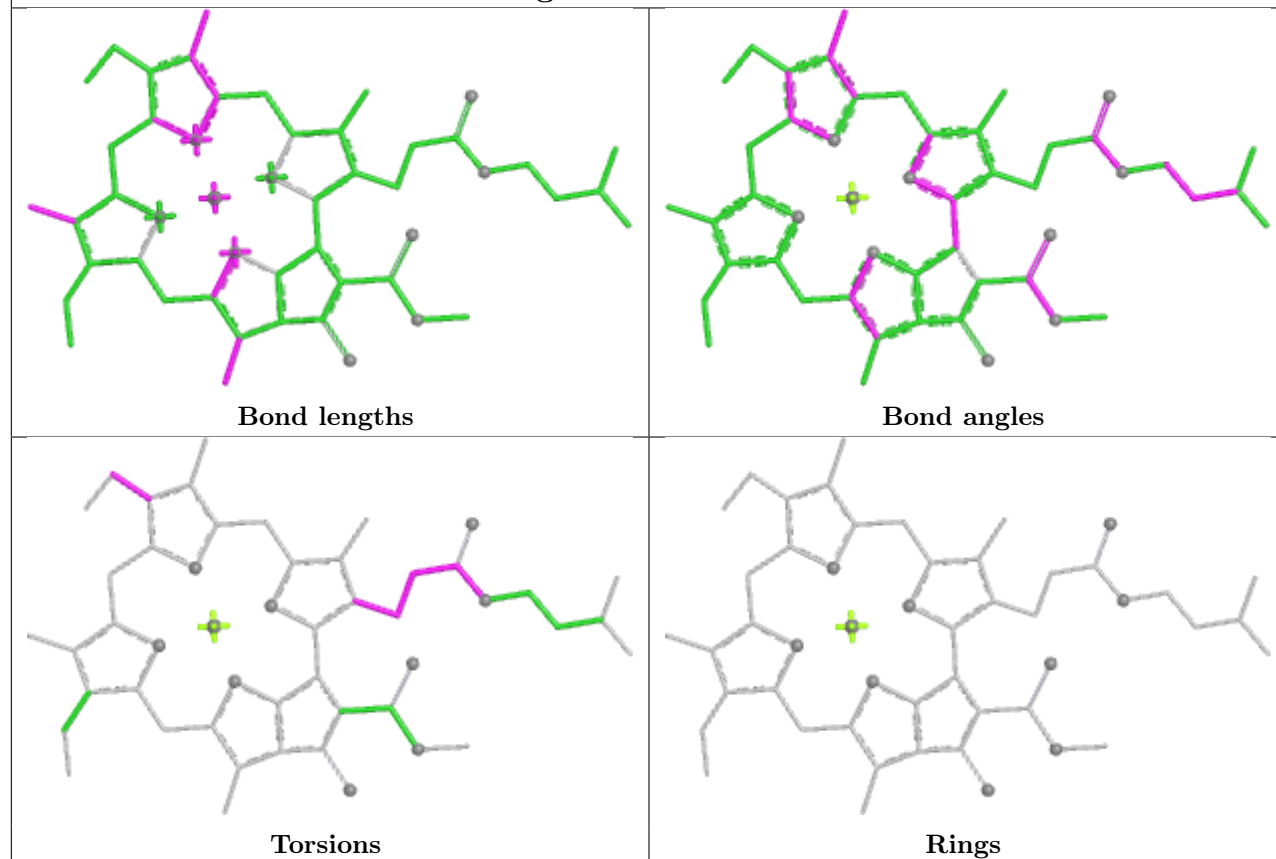




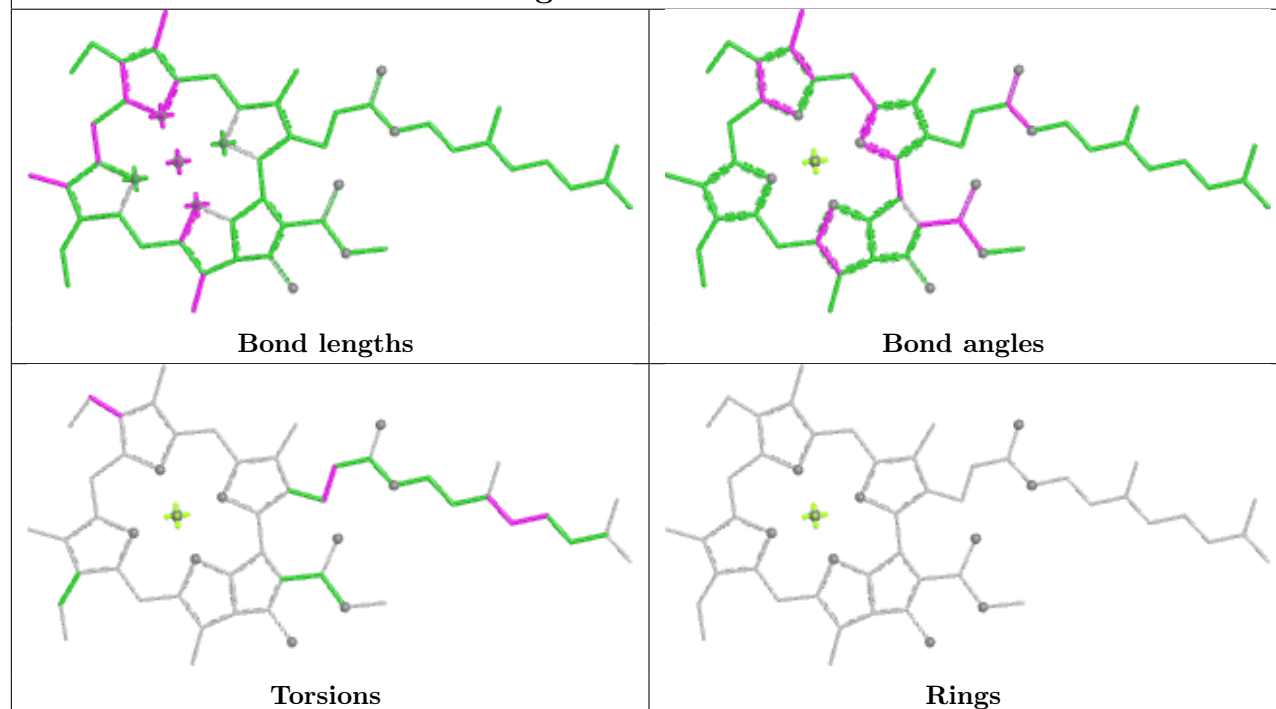




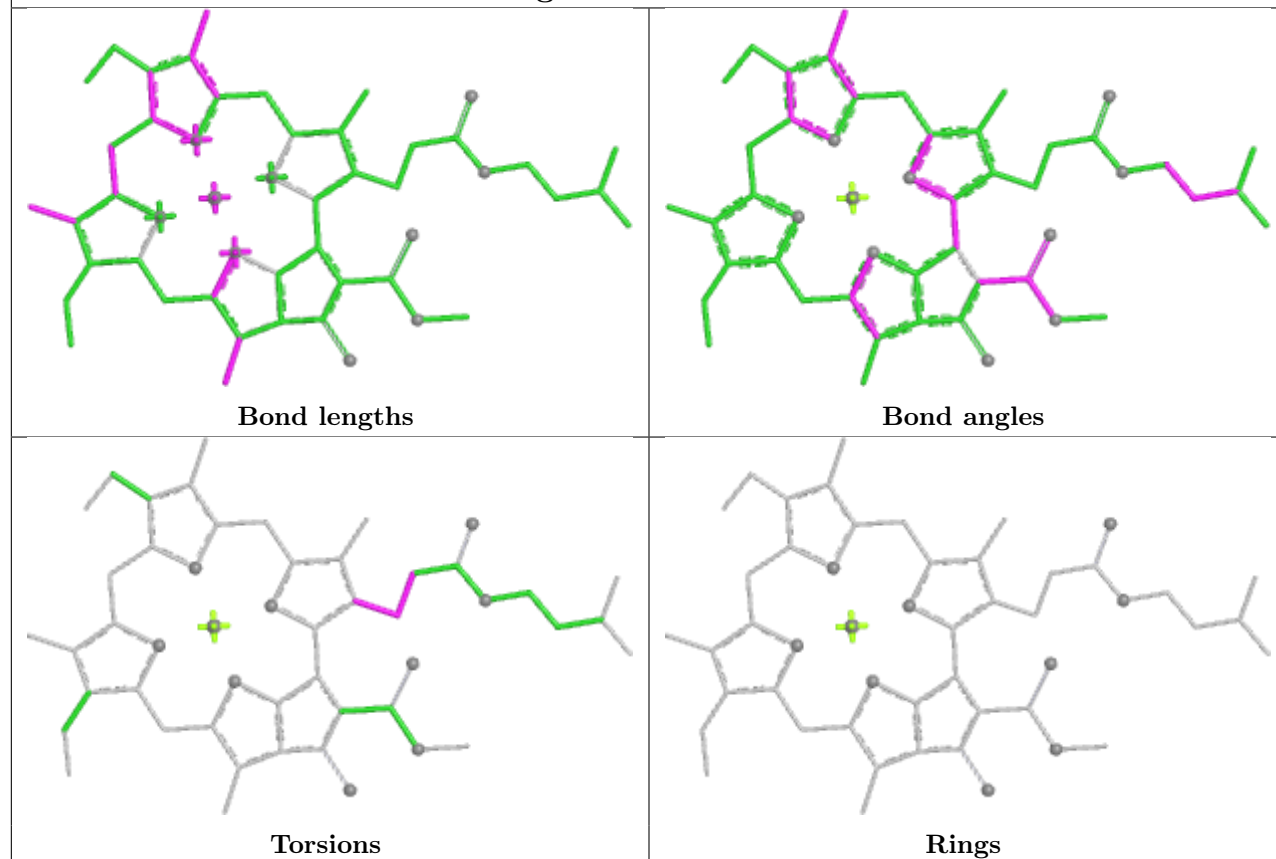
Ligand CLA a 812



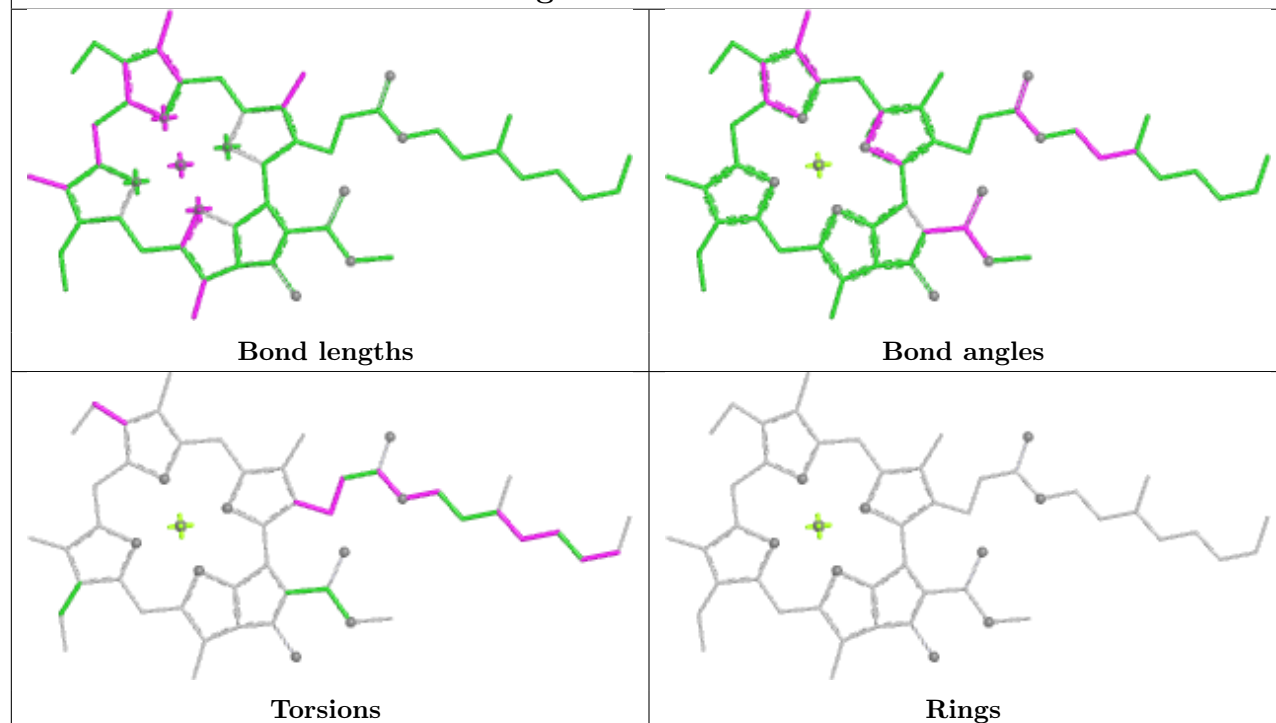
Ligand CLA b 826

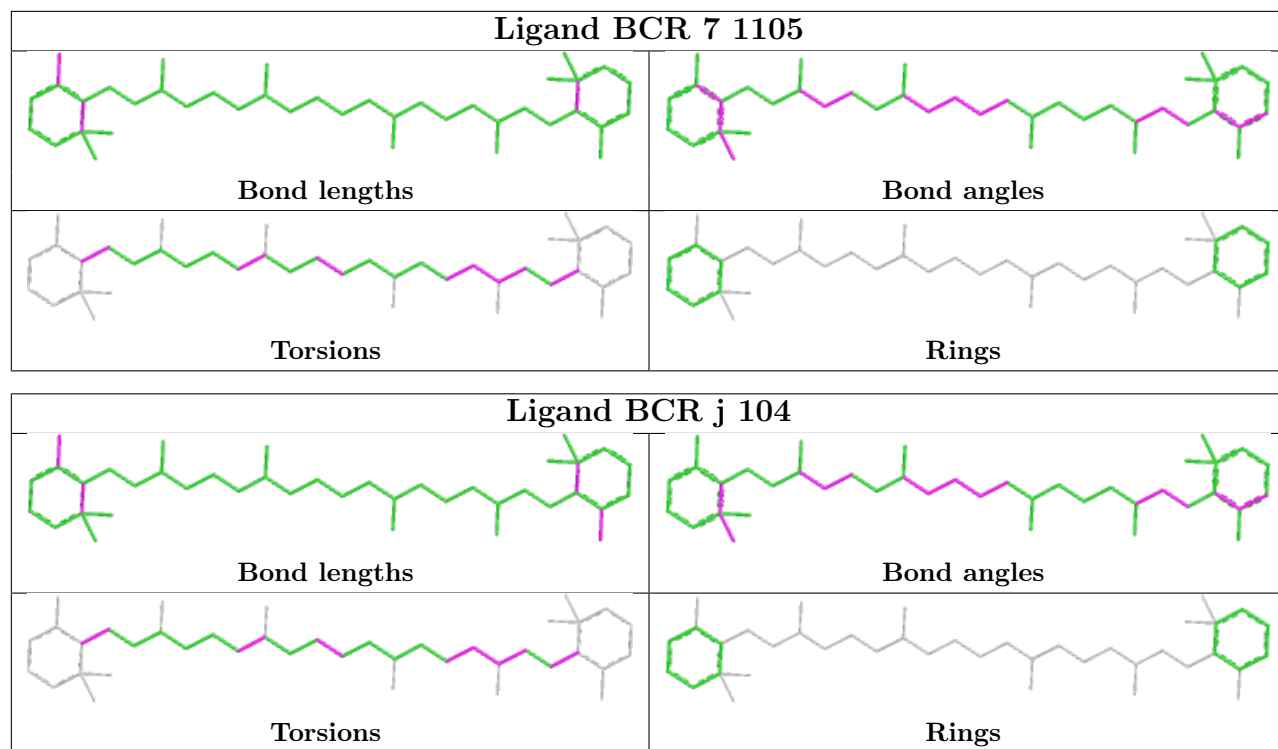


Ligand CLA 1 805

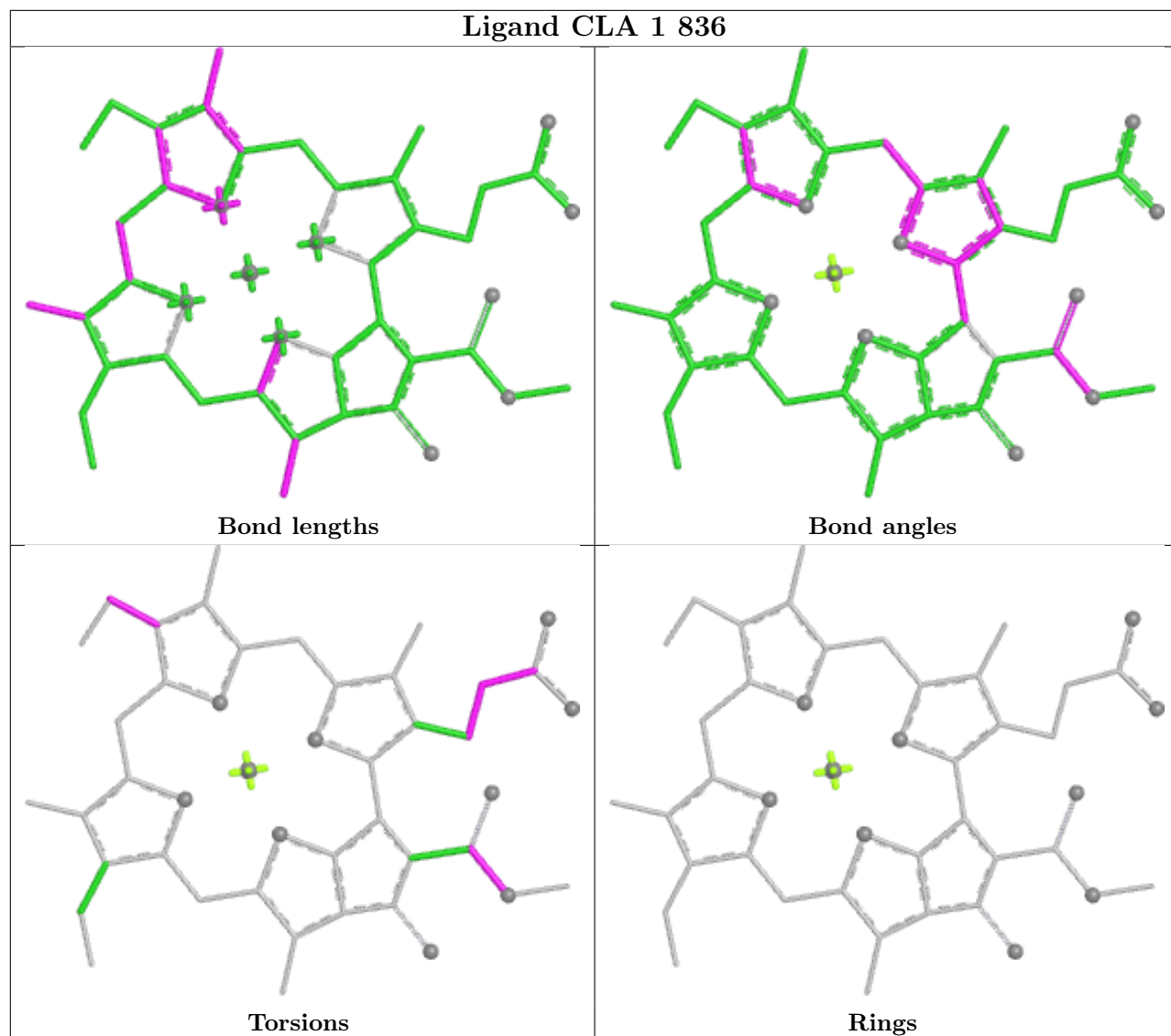


Ligand CLA 1 813

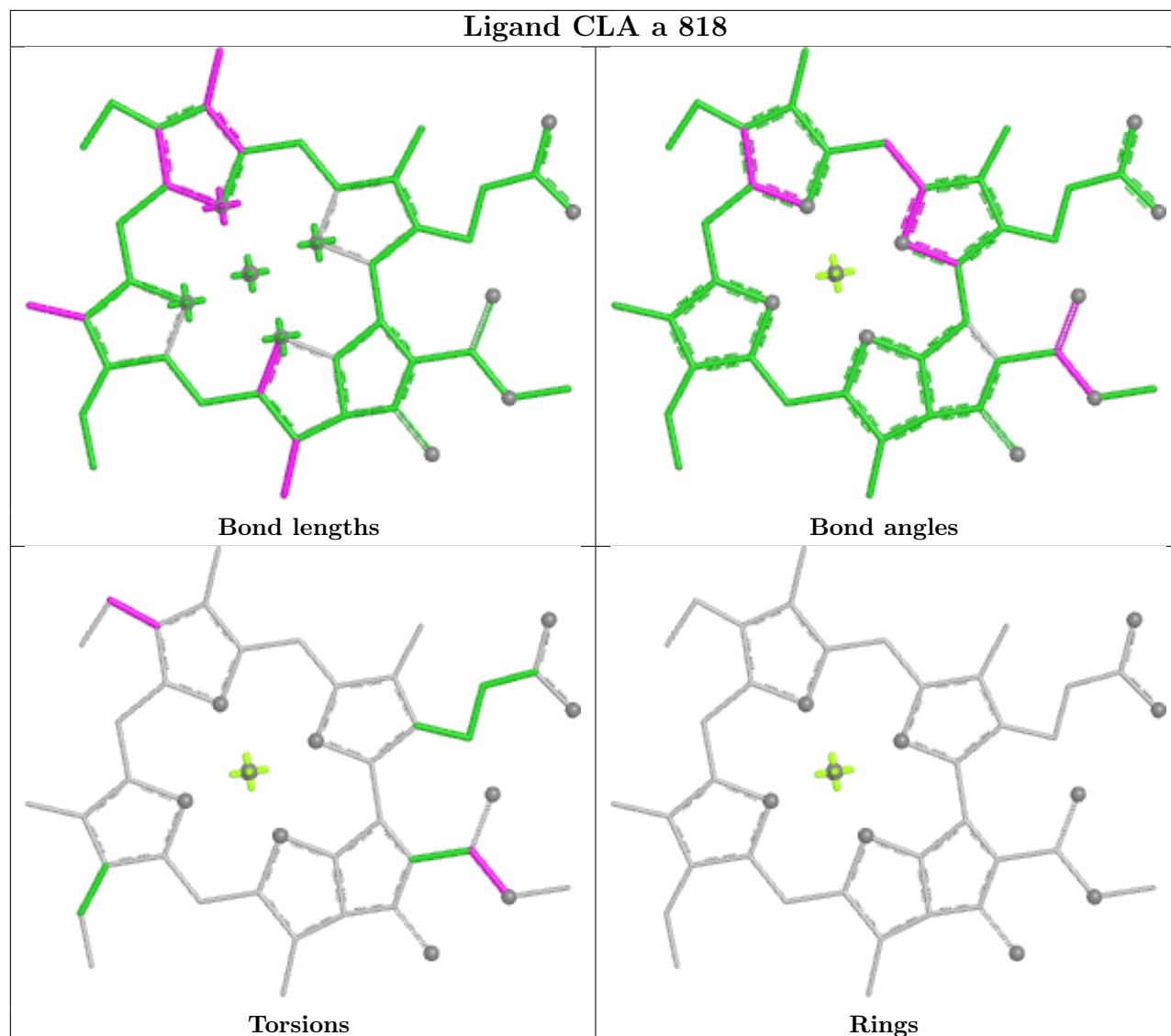




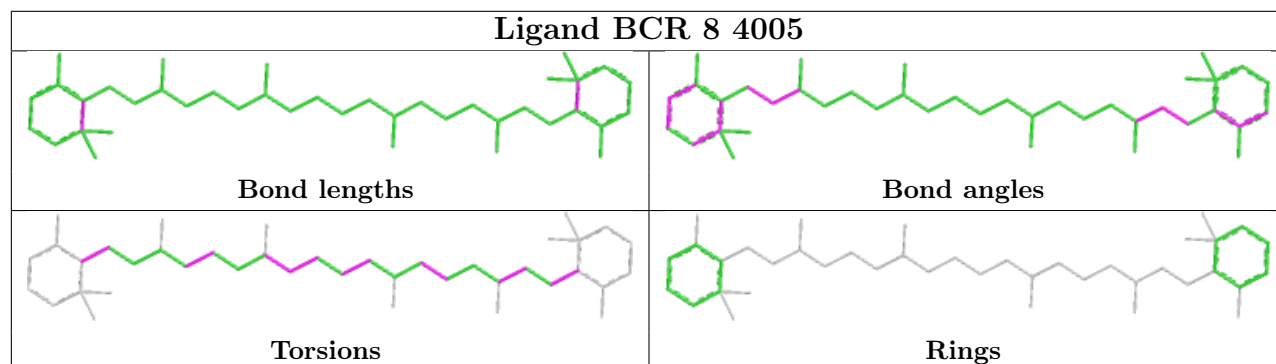
Ligand CLA 1 836

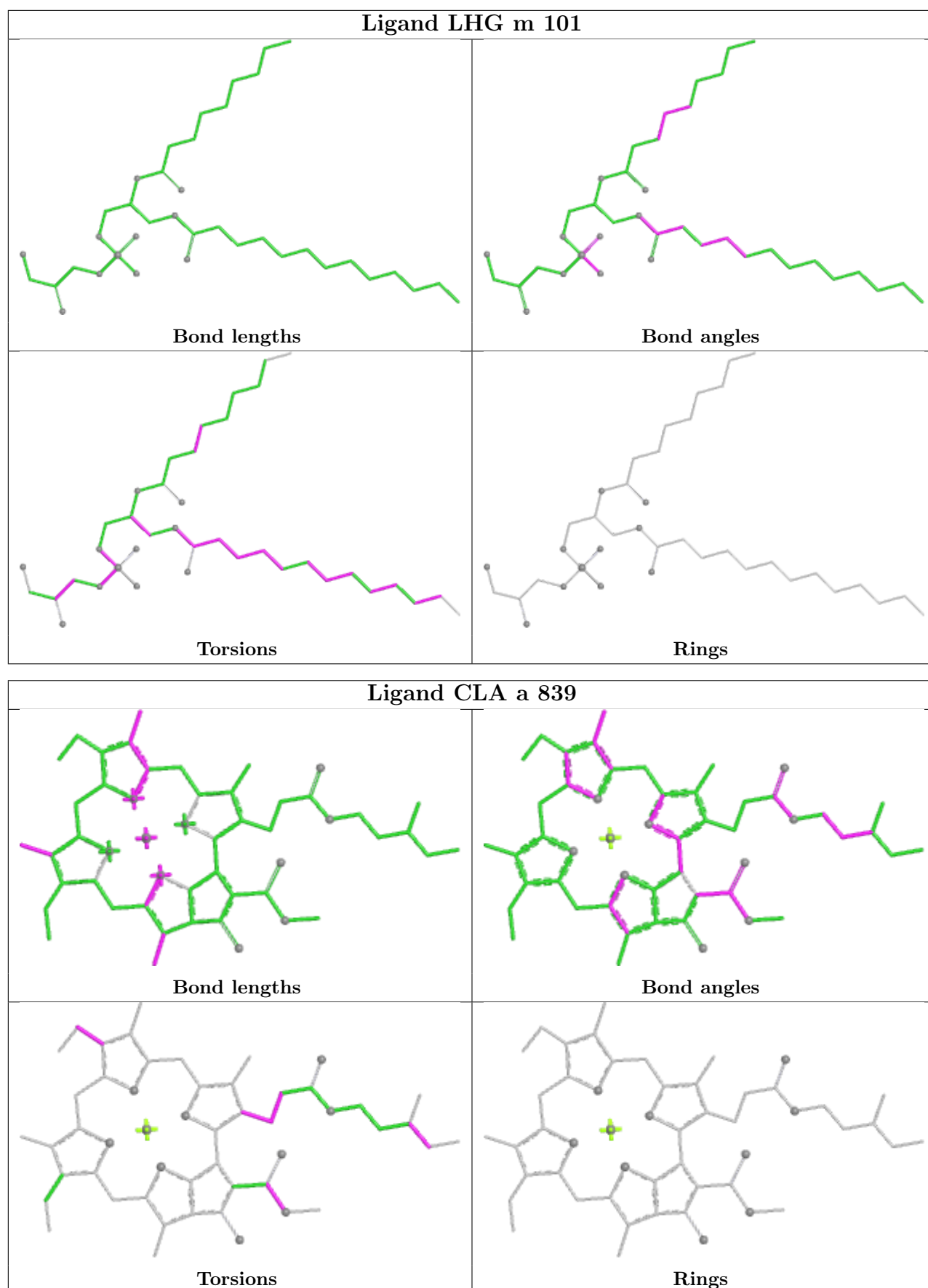


Ligand CLA a 818

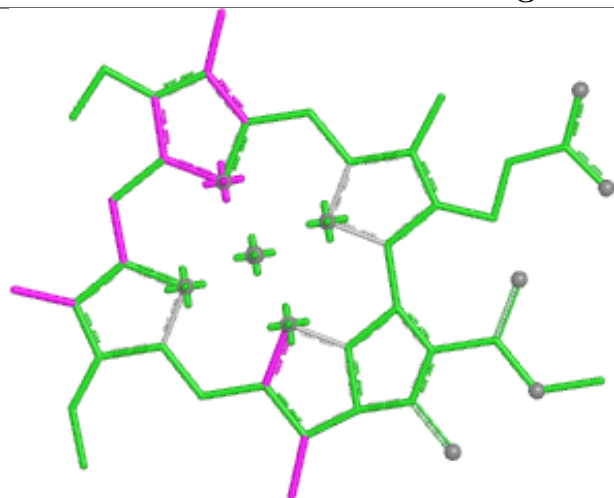


Ligand BCR 8 4005

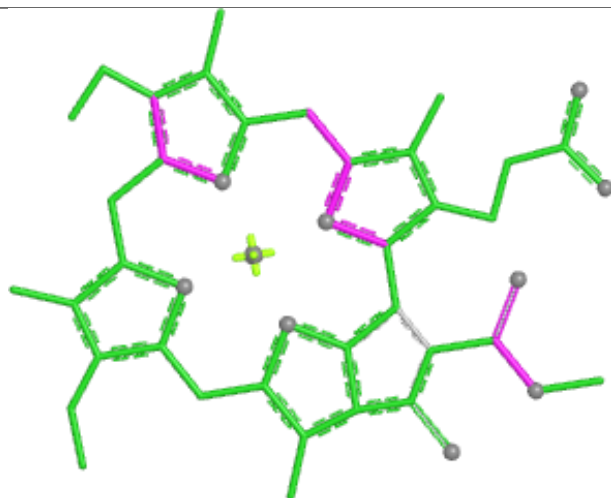




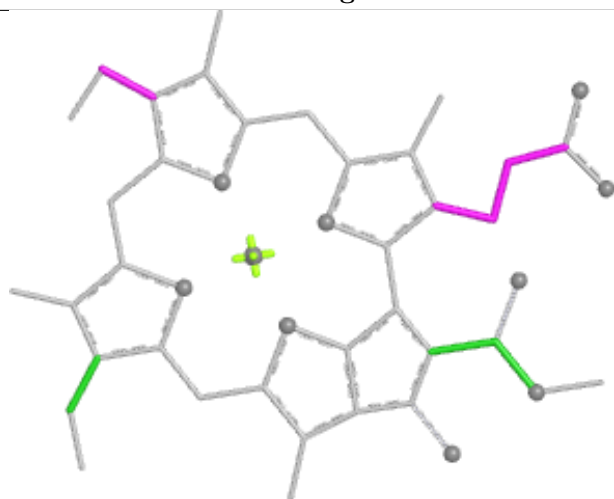
Ligand CLA b 822



Bond lengths



Bond angles

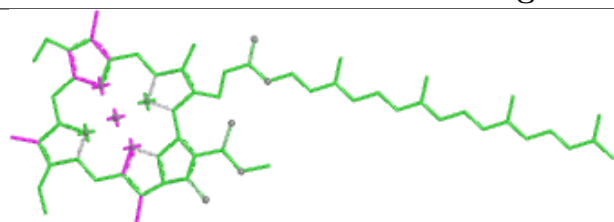


Torsions

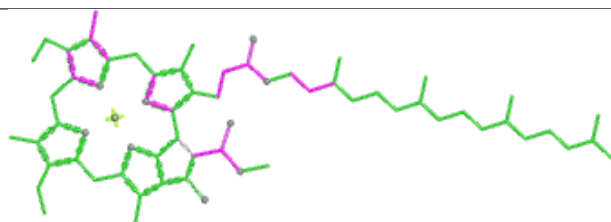


Rings

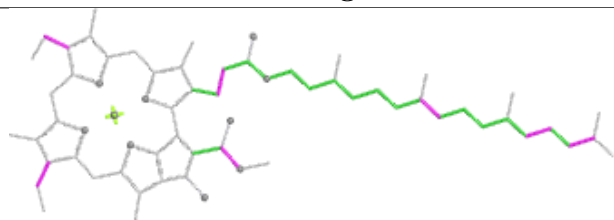
Ligand CLA b 802



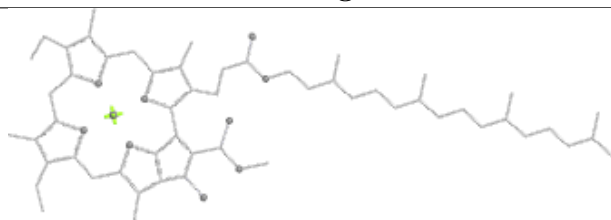
Bond lengths



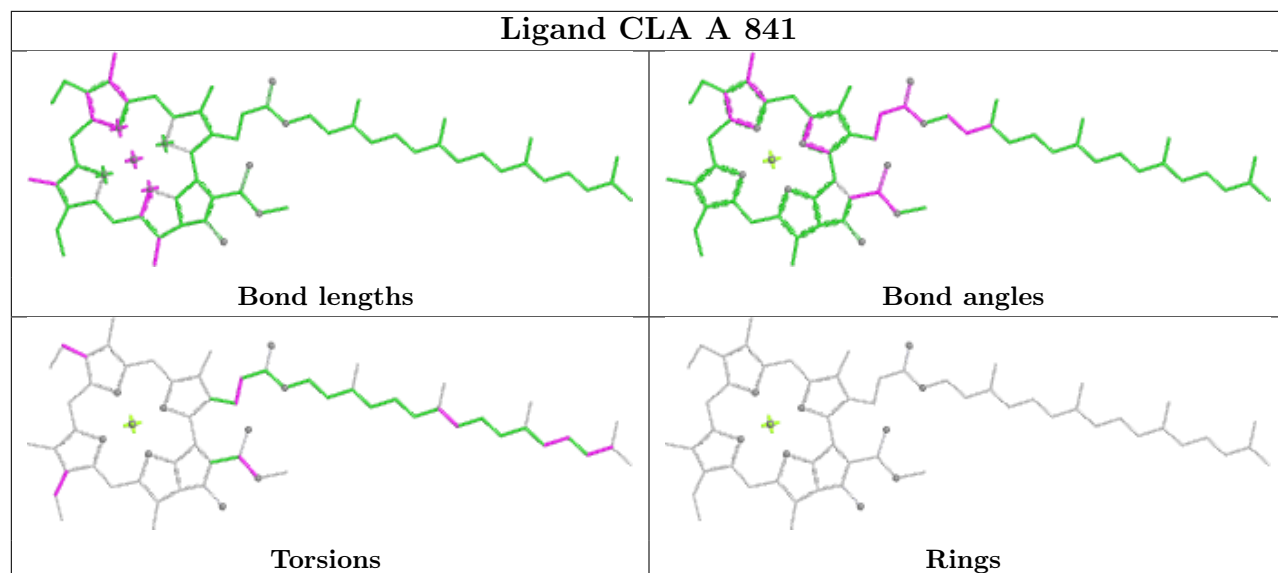
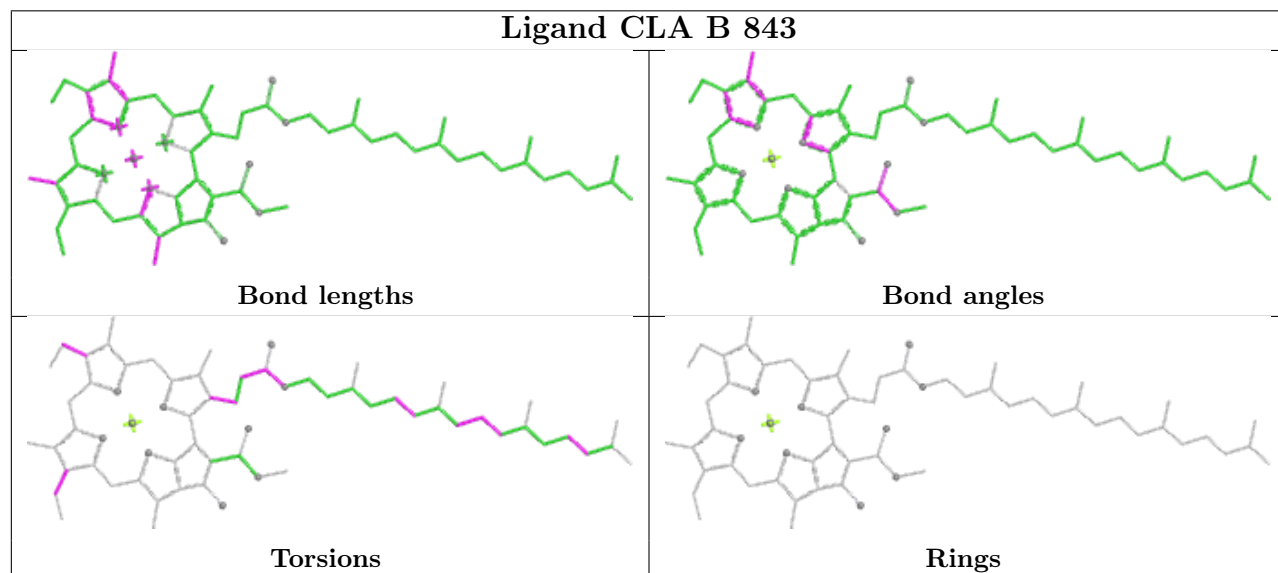
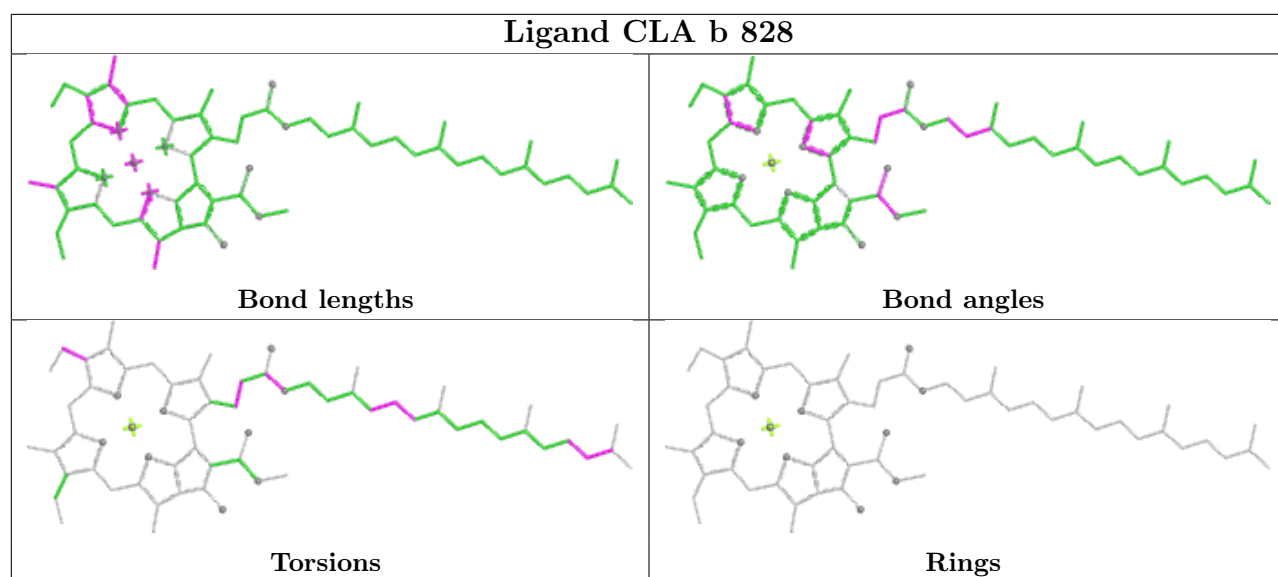
Bond angles

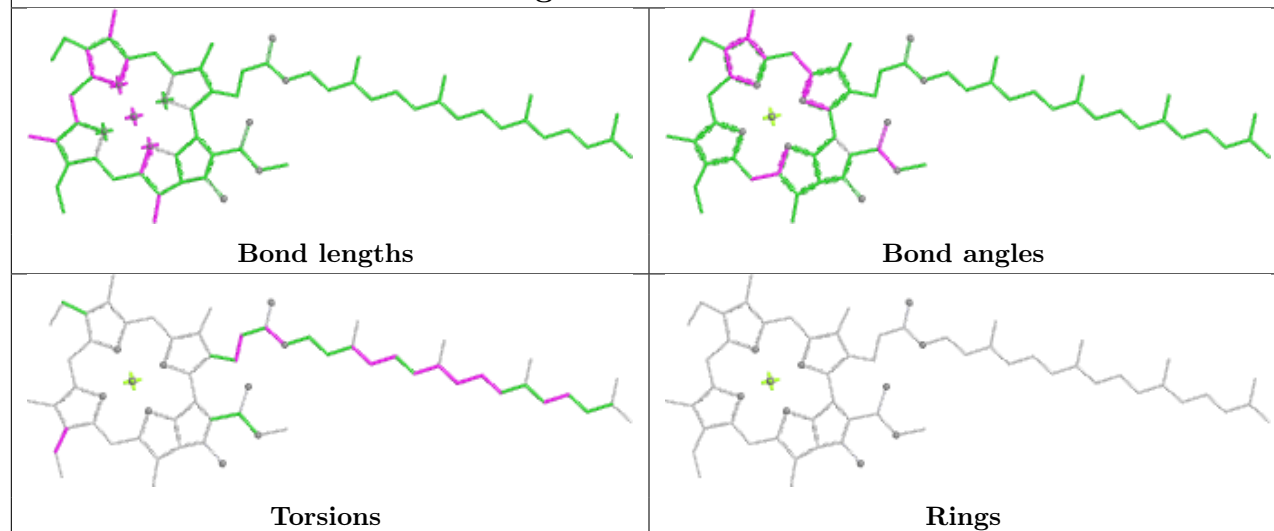
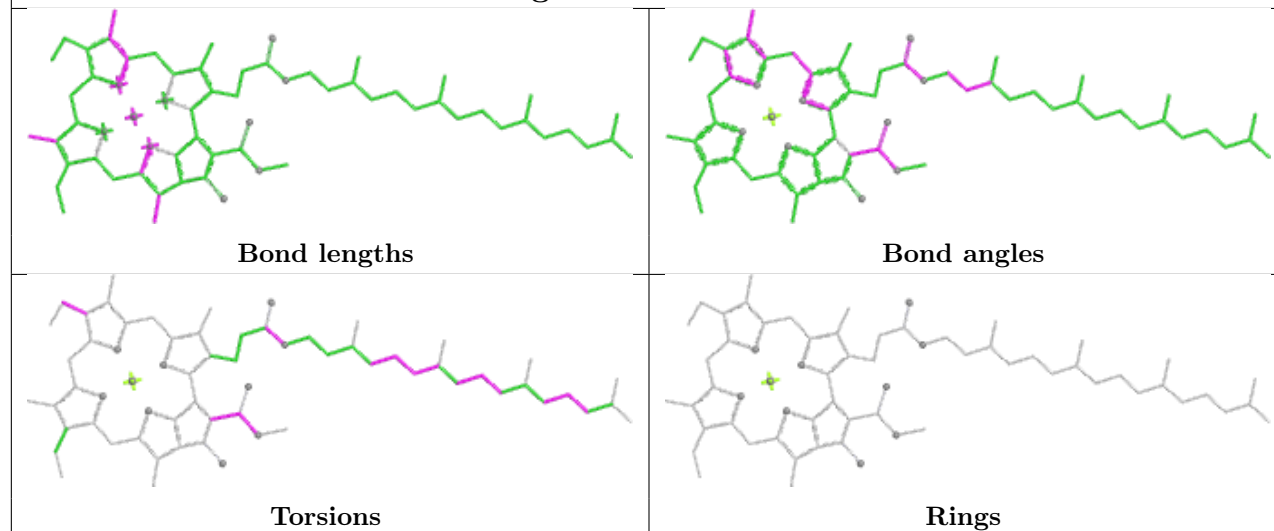


Torsions

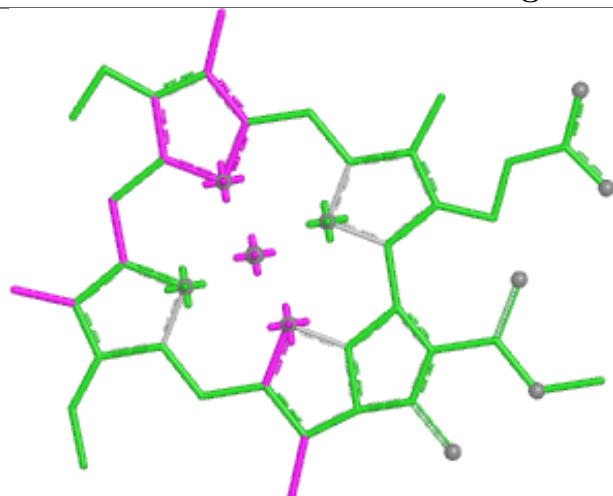


Rings

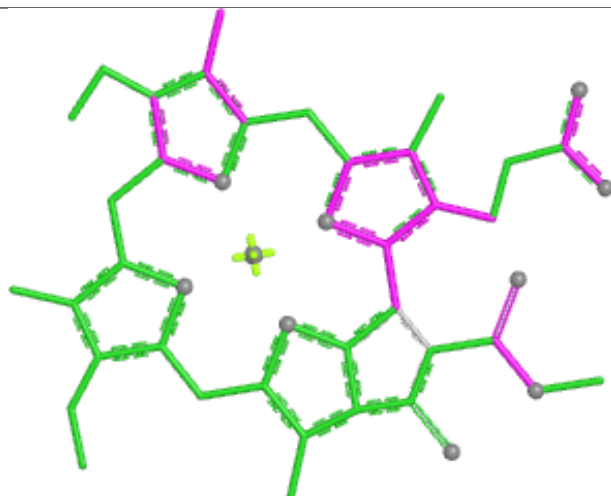


Ligand CLA b 806**Ligand CLA A 834**

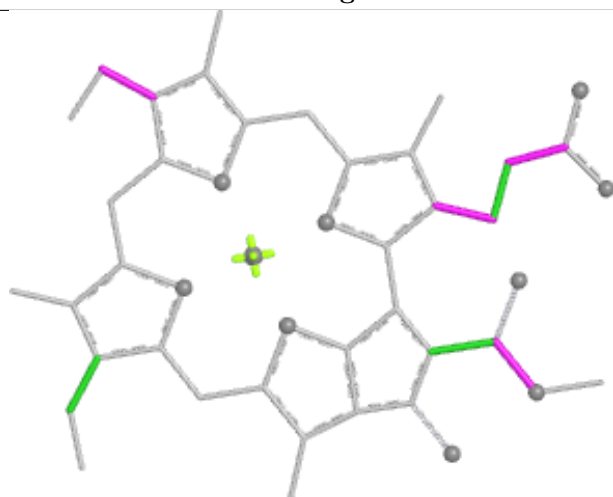
Ligand CLA f 205



Bond lengths



Bond angles

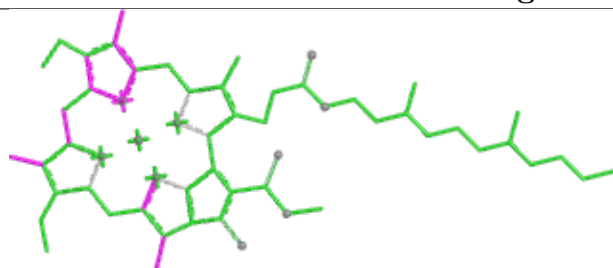


Torsions

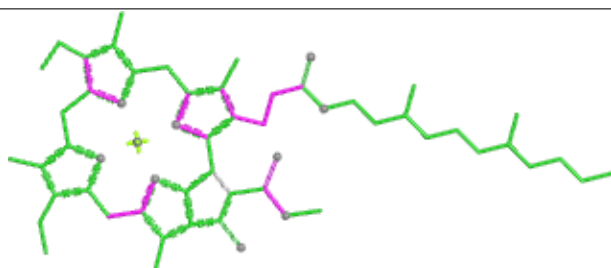


Rings

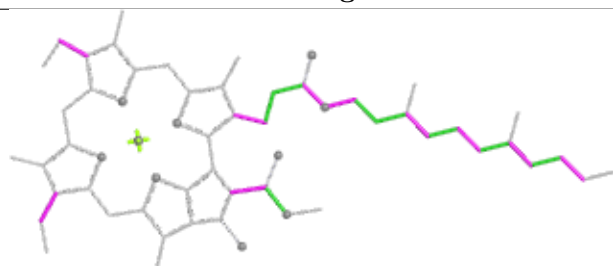
Ligand CLA b 834



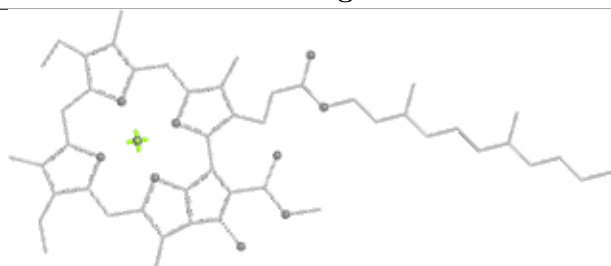
Bond lengths



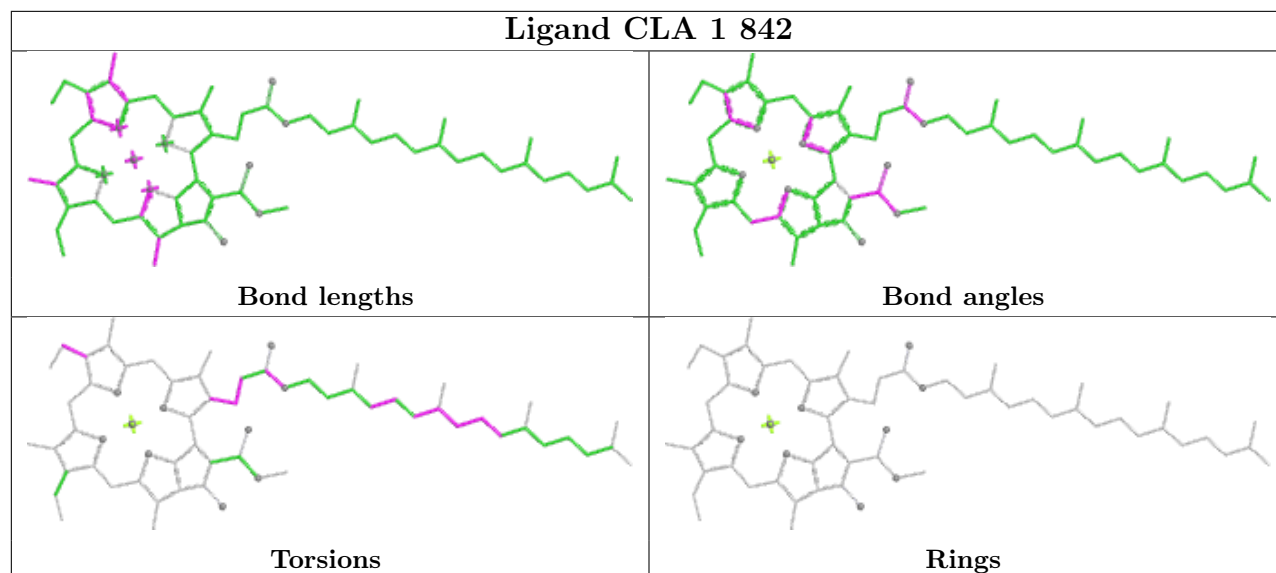
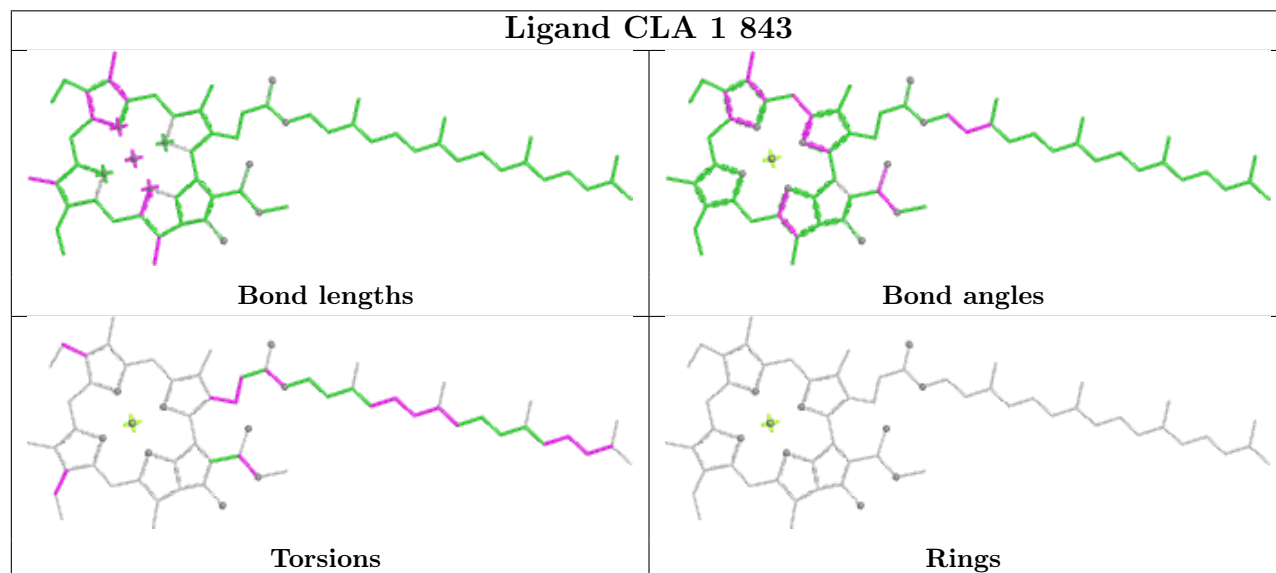
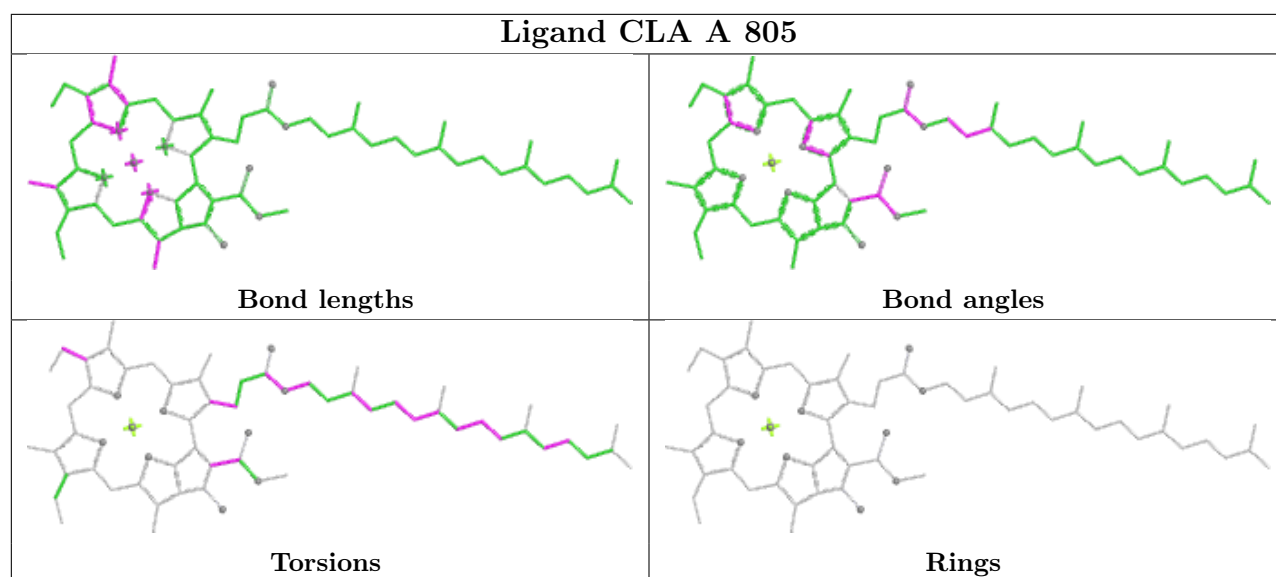
Bond angles

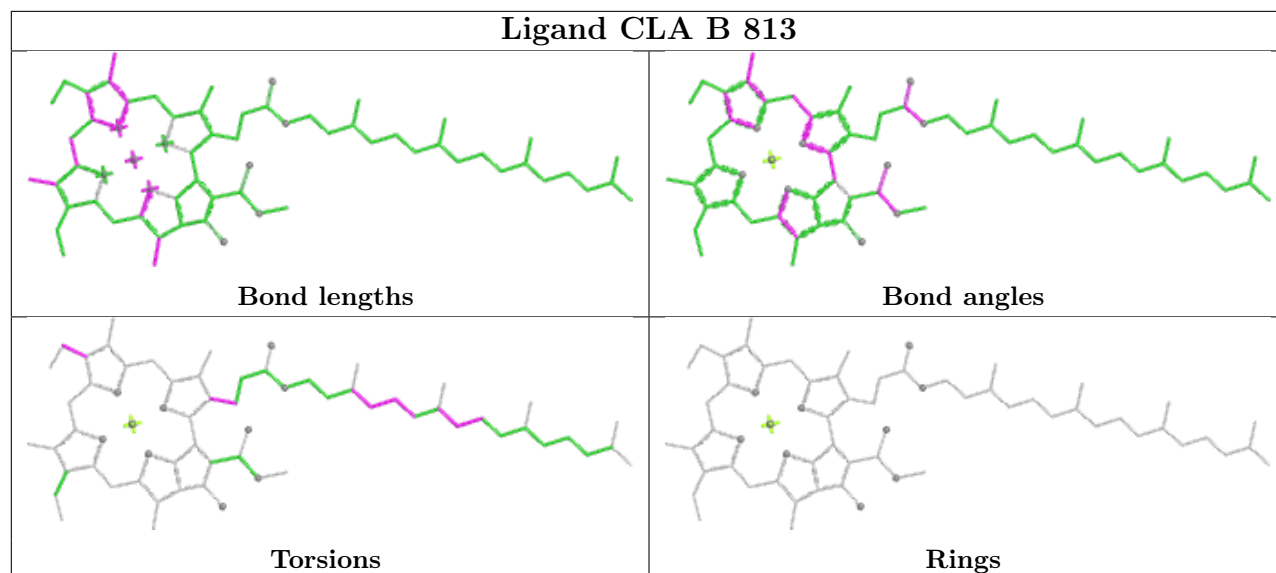
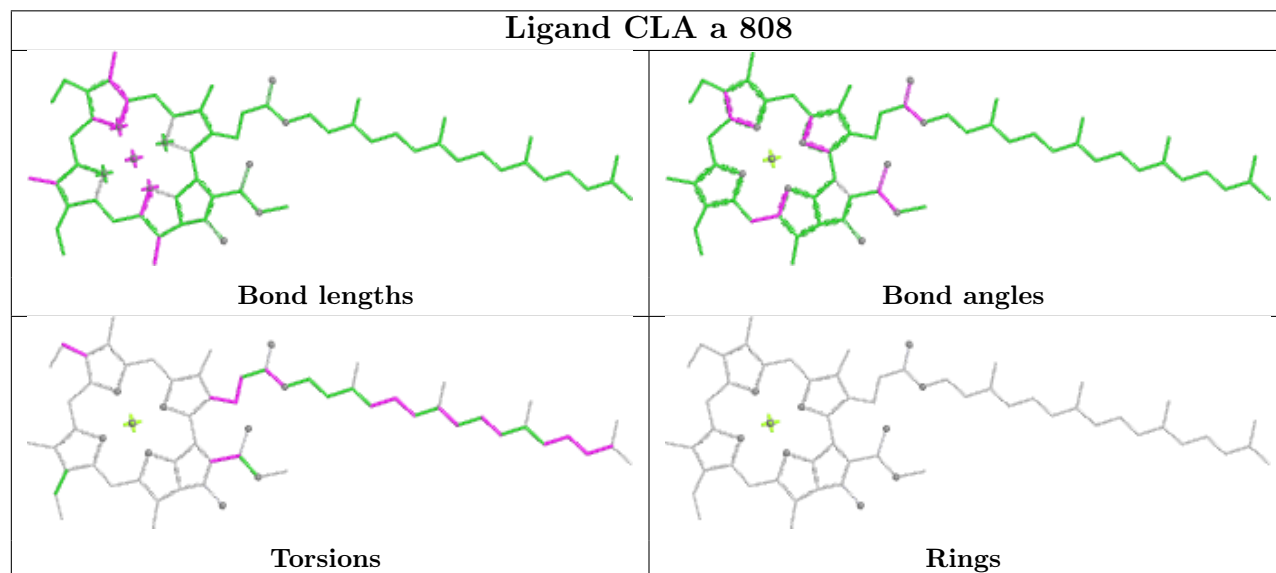
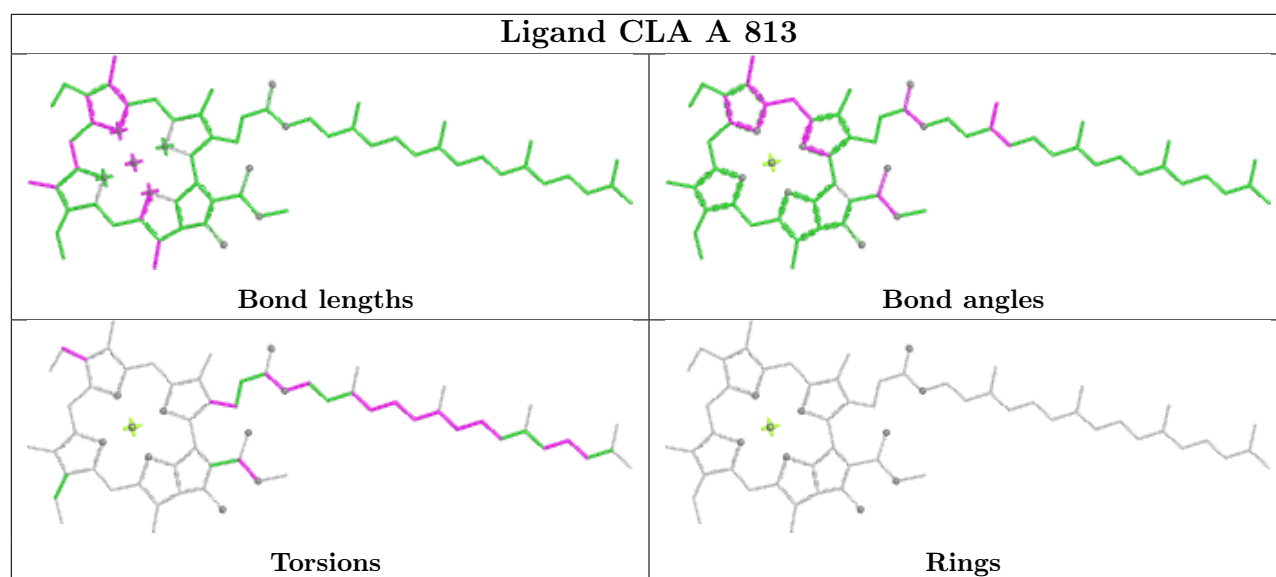


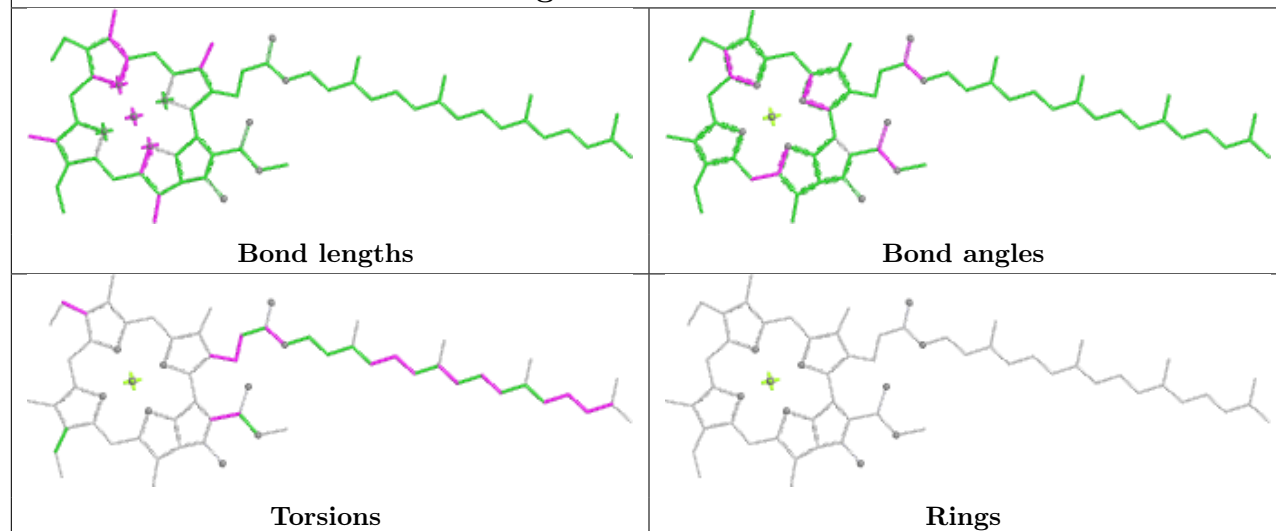
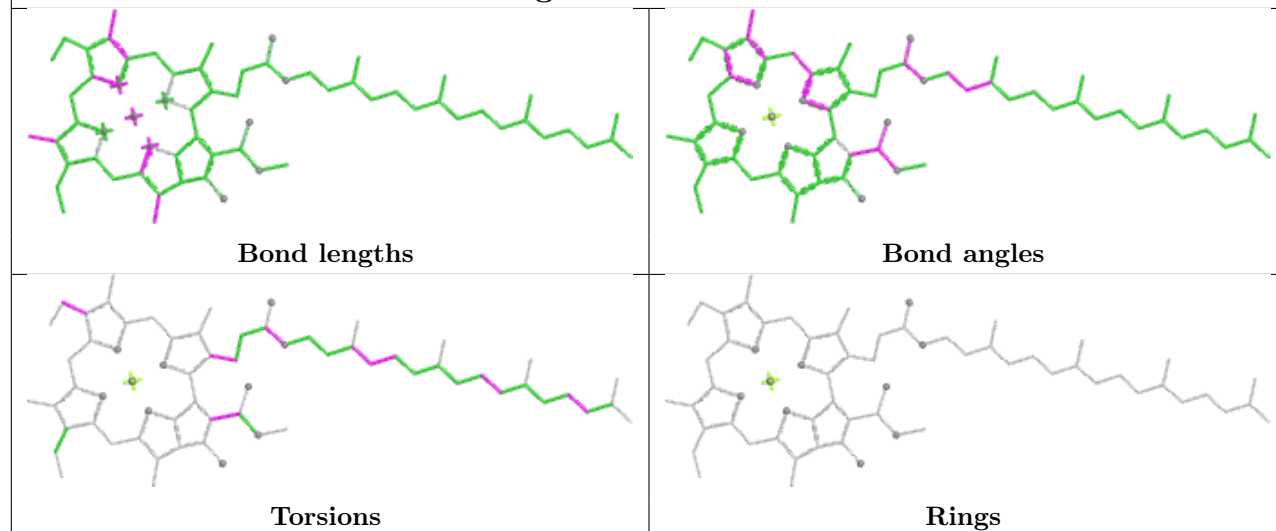
Torsions



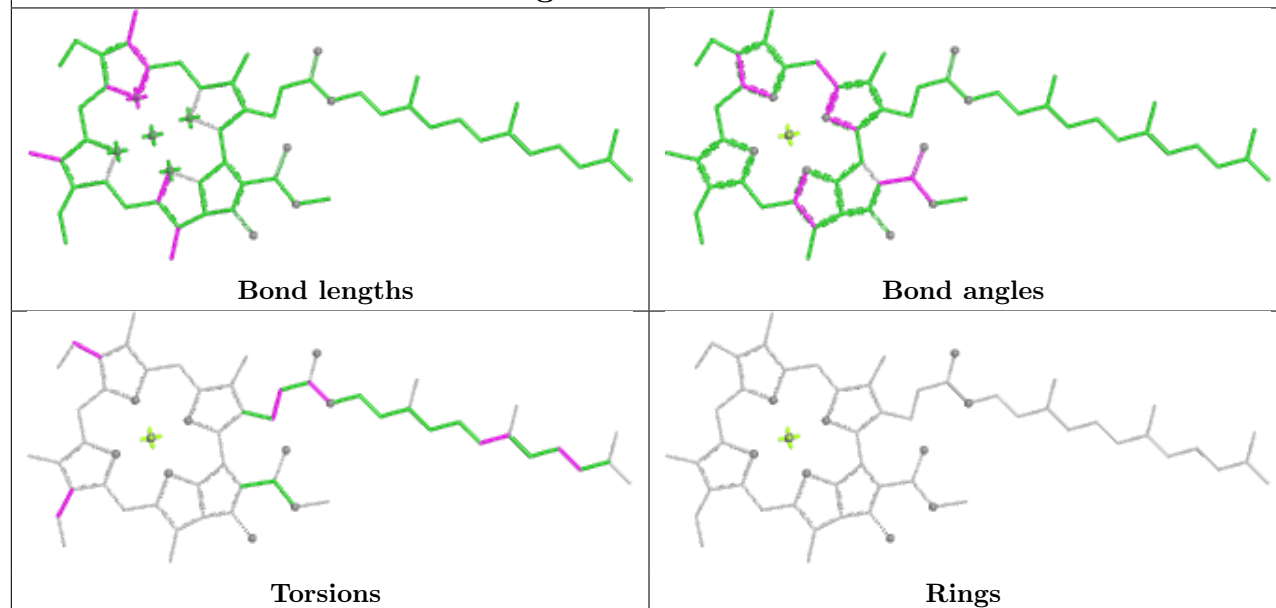
Rings



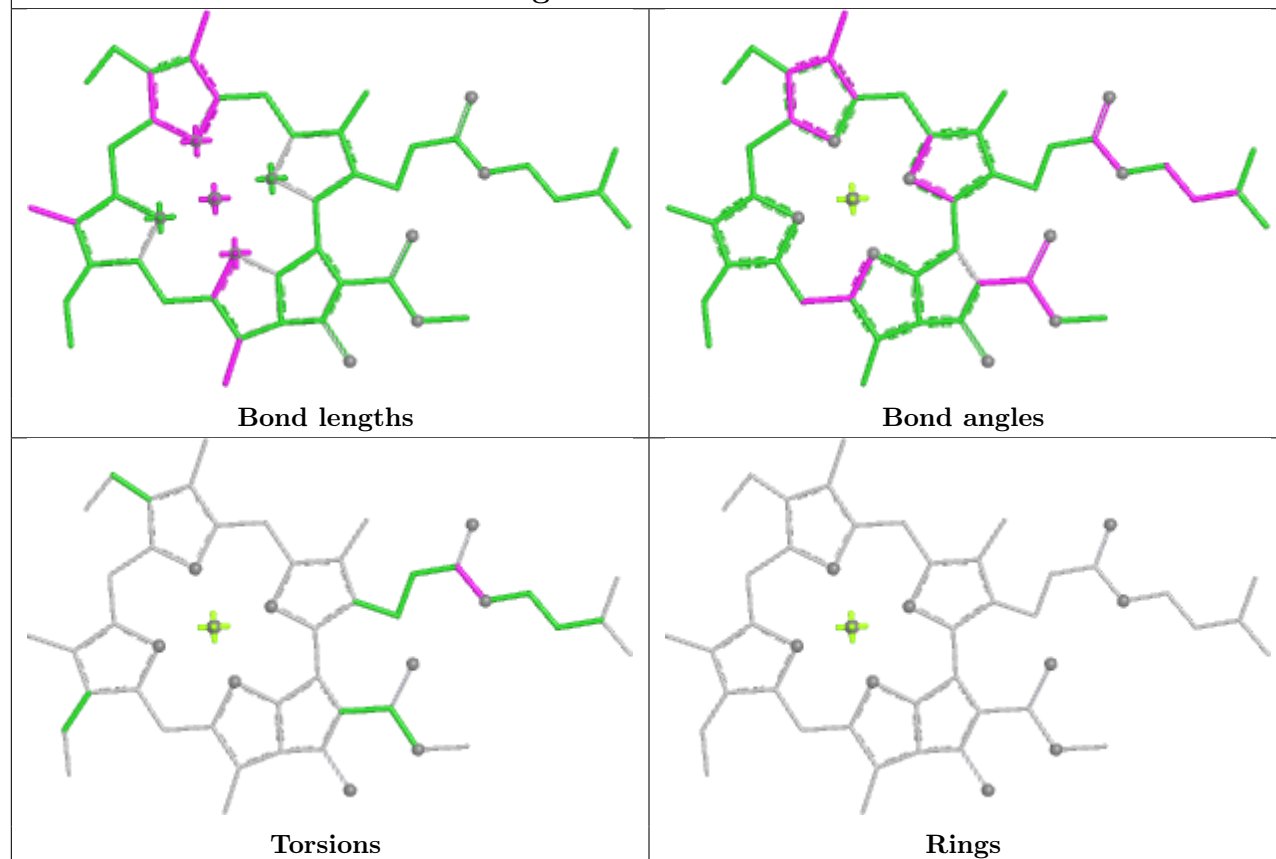


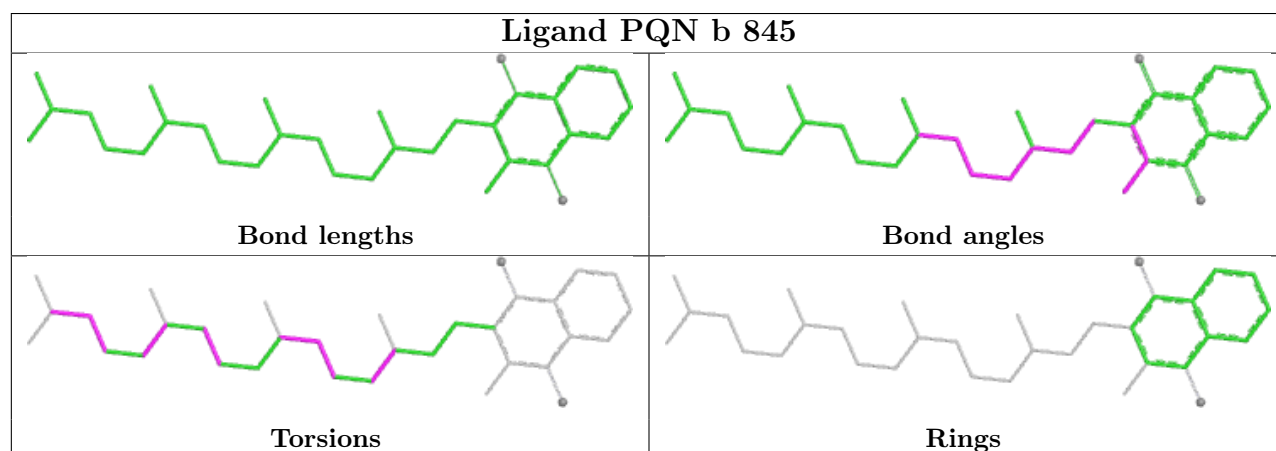
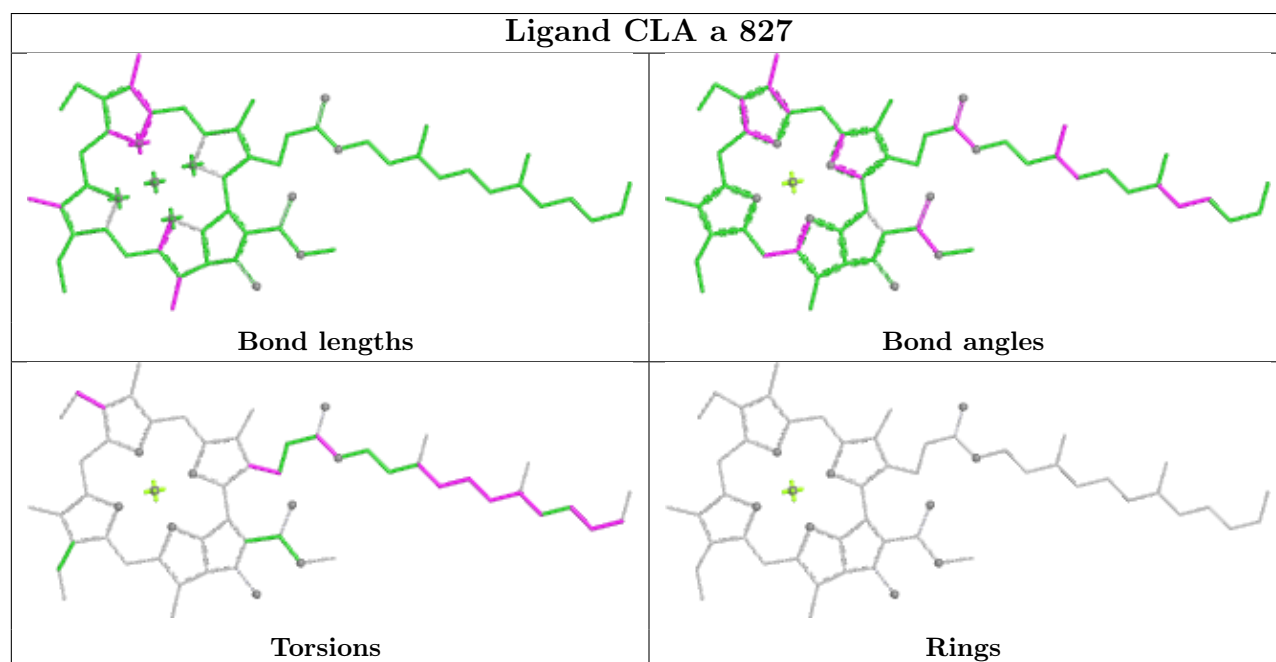
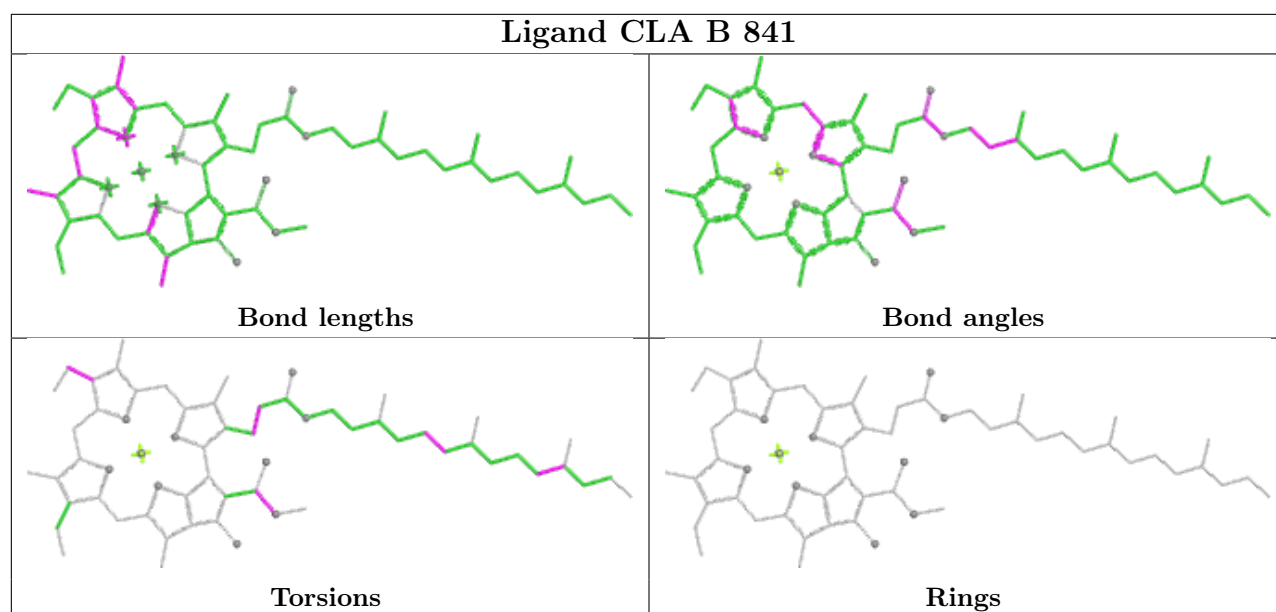
Ligand CLA 1 806**Ligand CLA b 808**

Ligand CLA 2 809

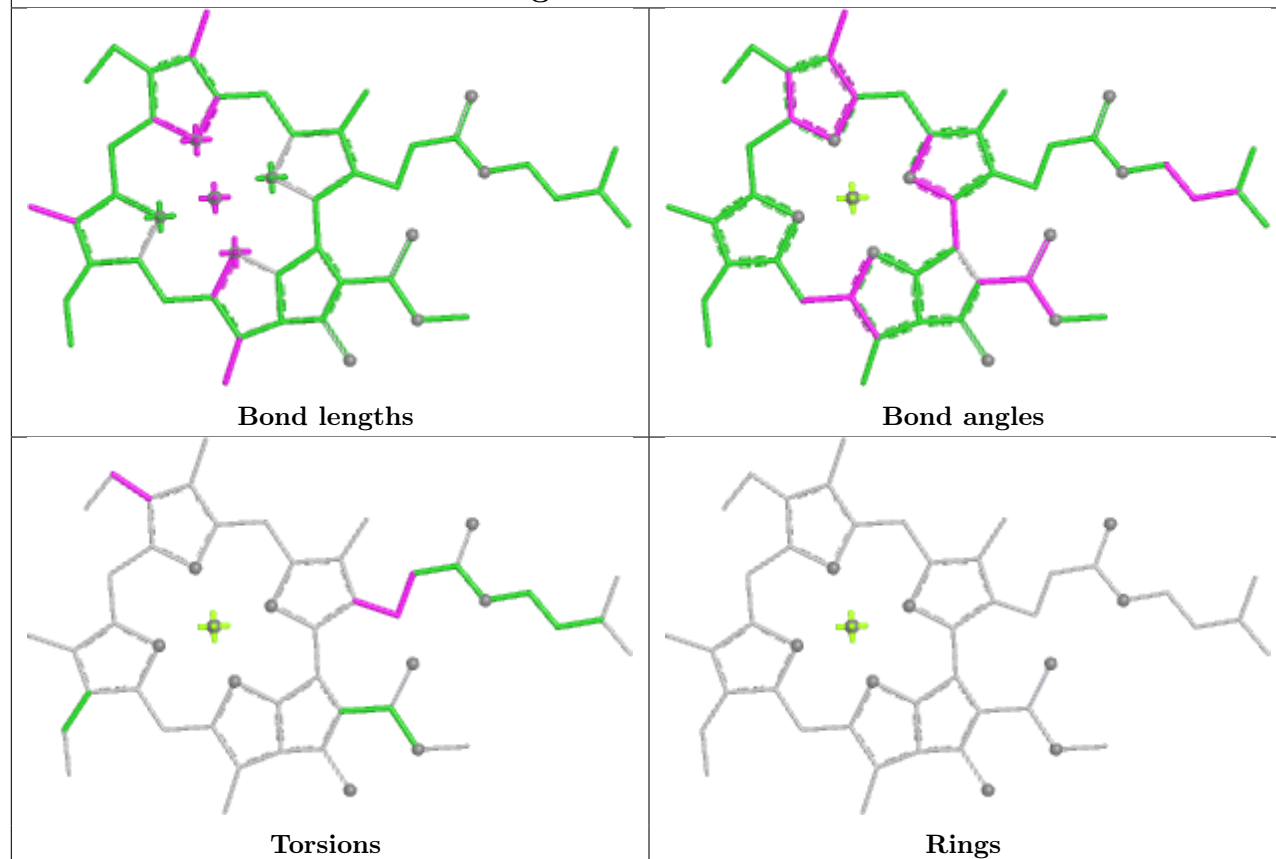


Ligand CLA B 828

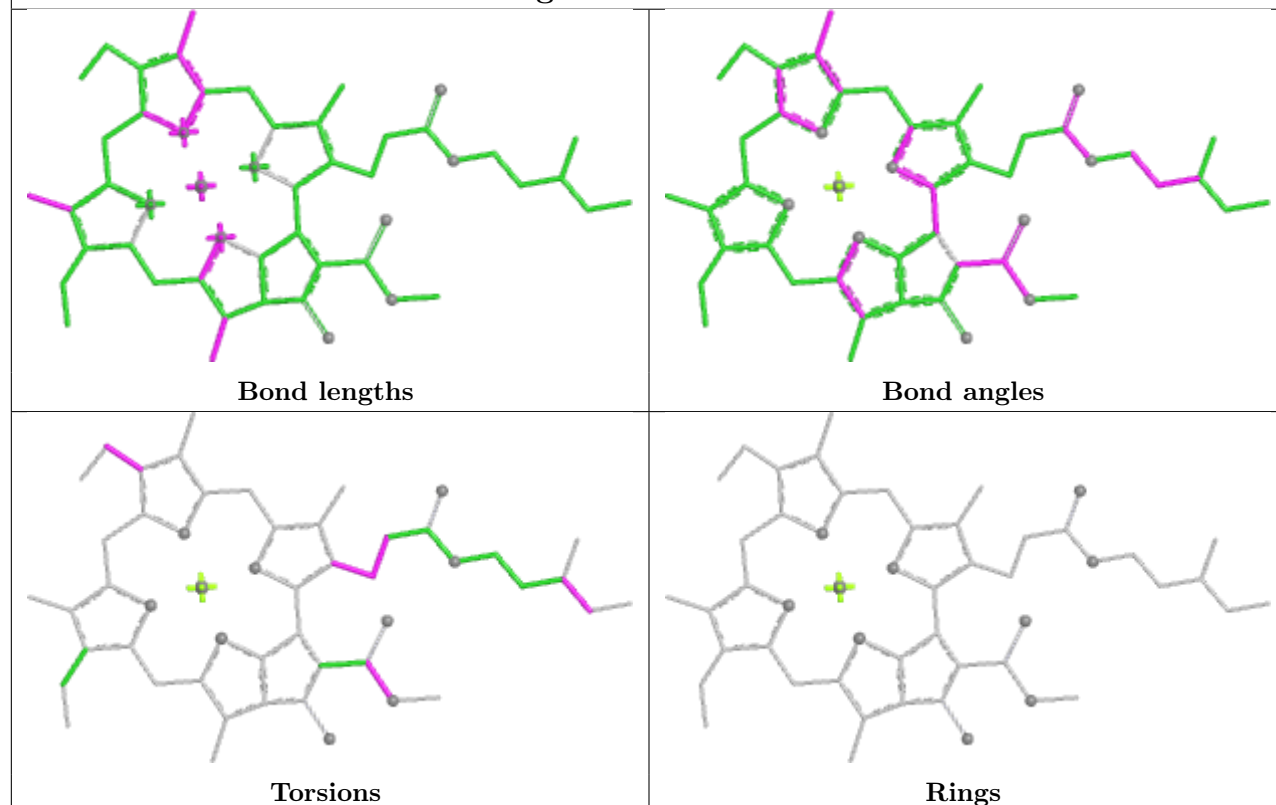


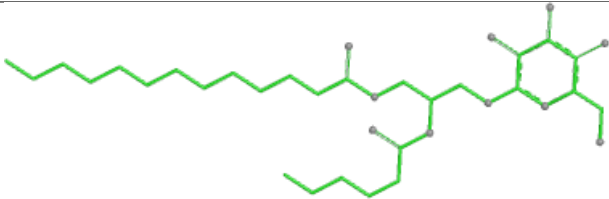
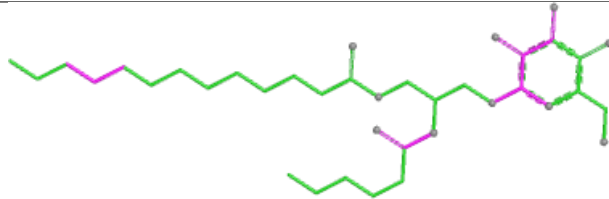
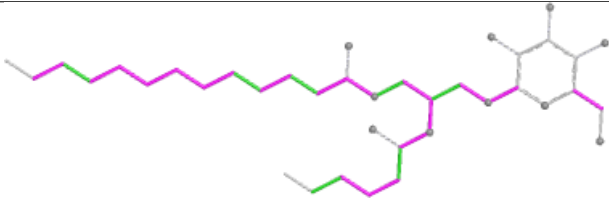
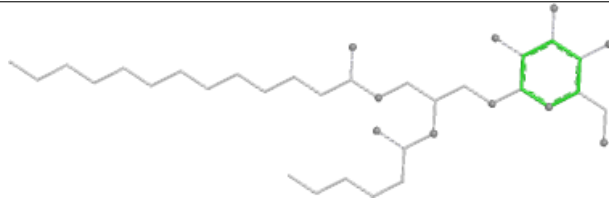


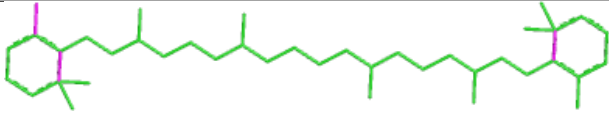
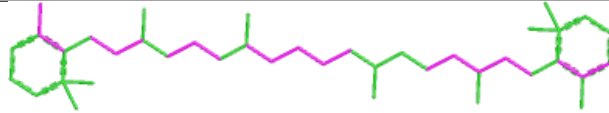
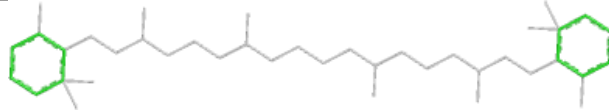
Ligand CLA A 833

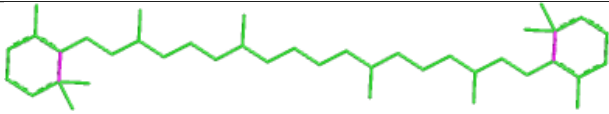
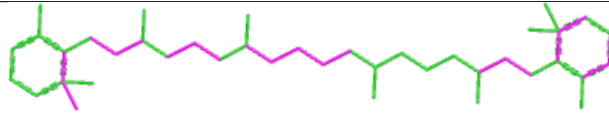
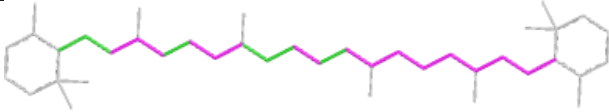
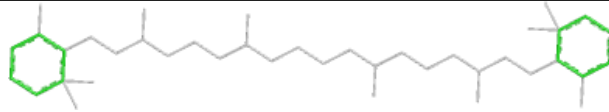


Ligand CLA 1 837

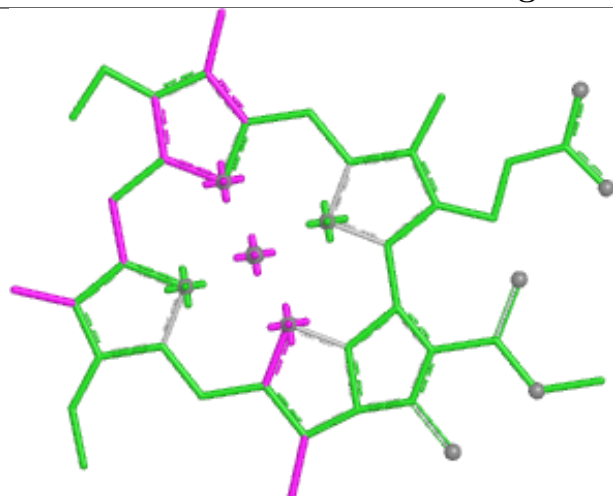


Ligand LMG 1 4202	
	
Bond lengths	Bond angles
	
Torsions	Rings

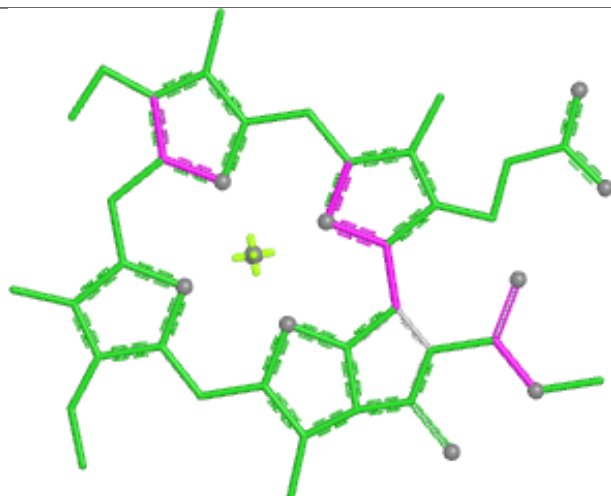
Ligand BCR b 854	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 851	
	
Bond lengths	Bond angles
	
Torsions	Rings

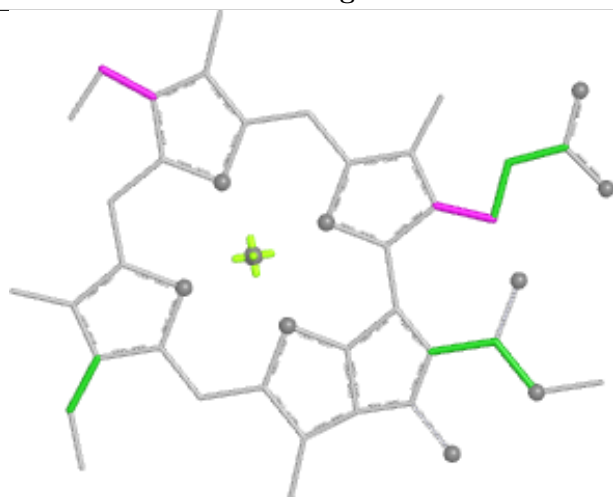
Ligand CLA 2 837



Bond lengths



Bond angles

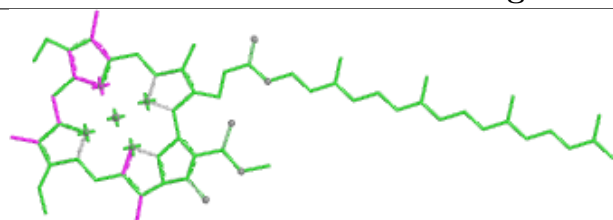


Torsions

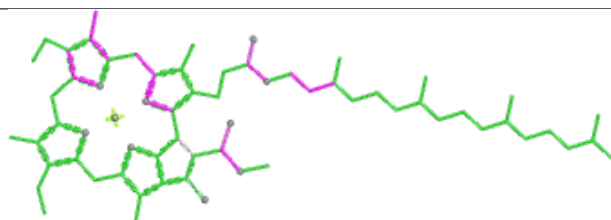


Rings

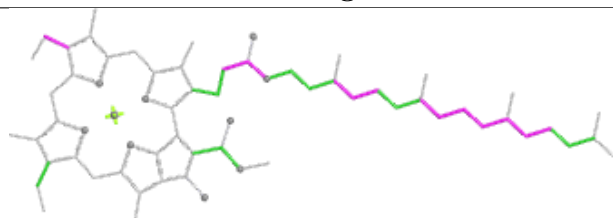
Ligand CLA L 1503



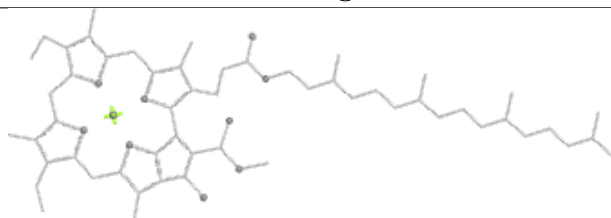
Bond lengths



Bond angles

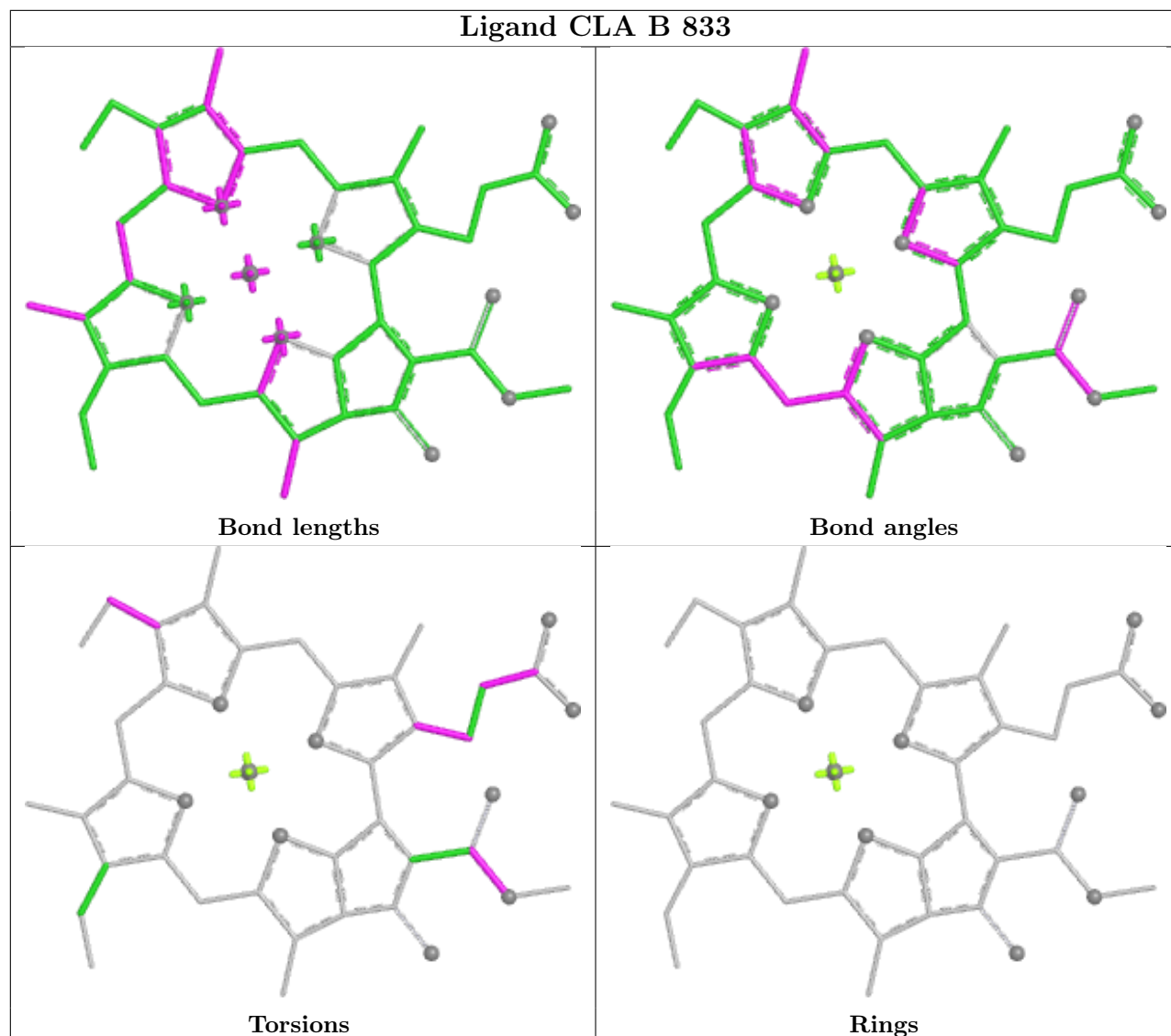


Torsions

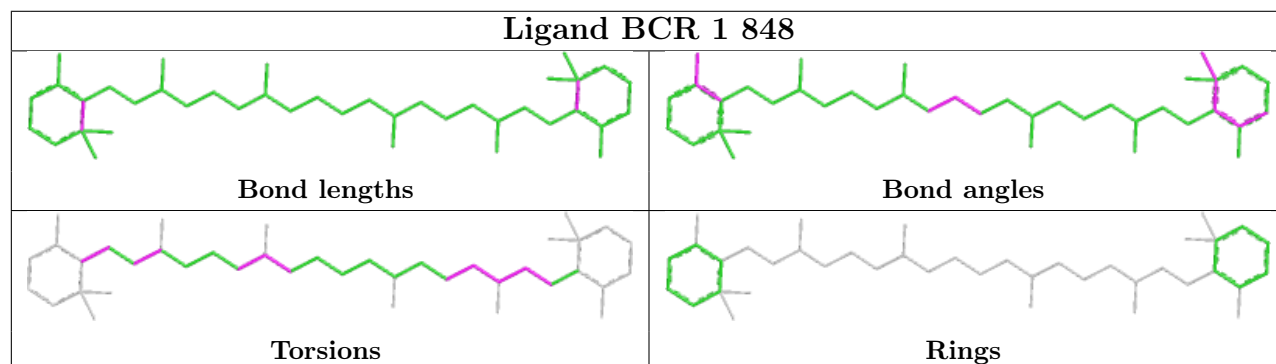


Rings

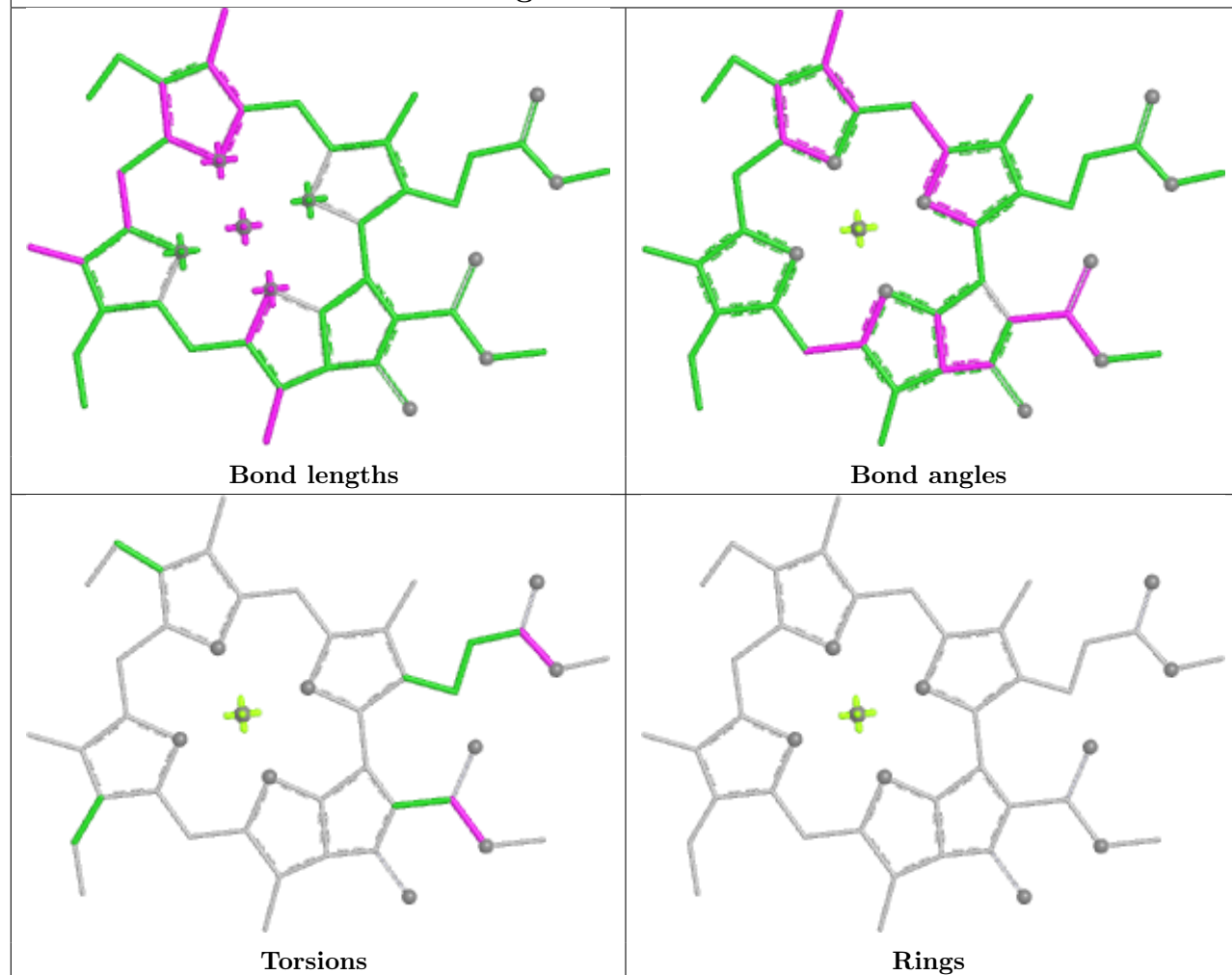
Ligand CLA B 833



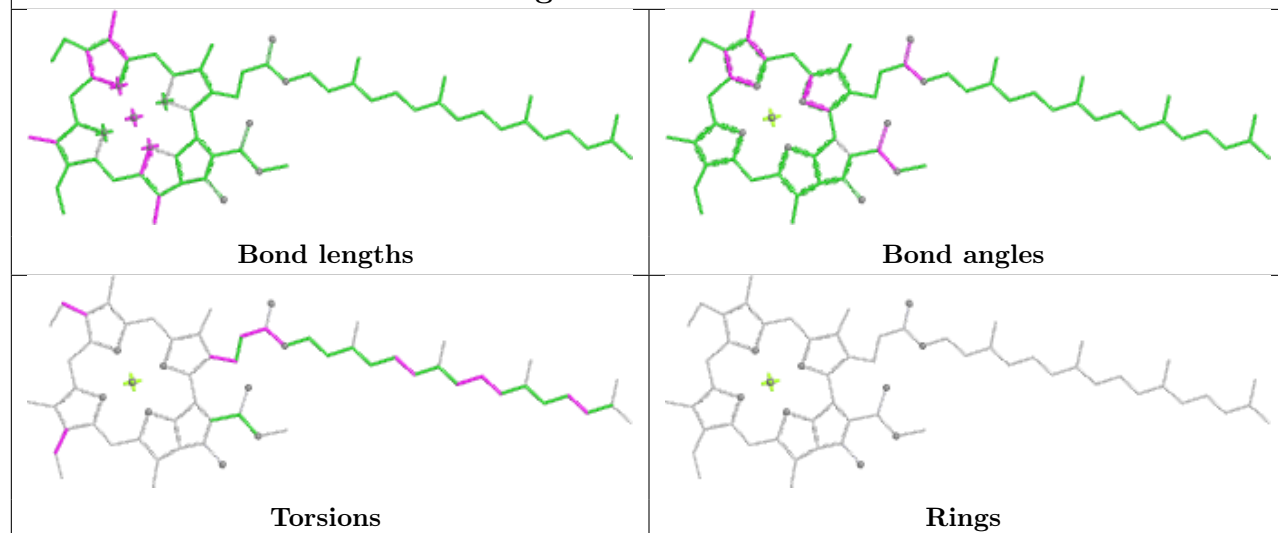
Ligand BCR 1 848



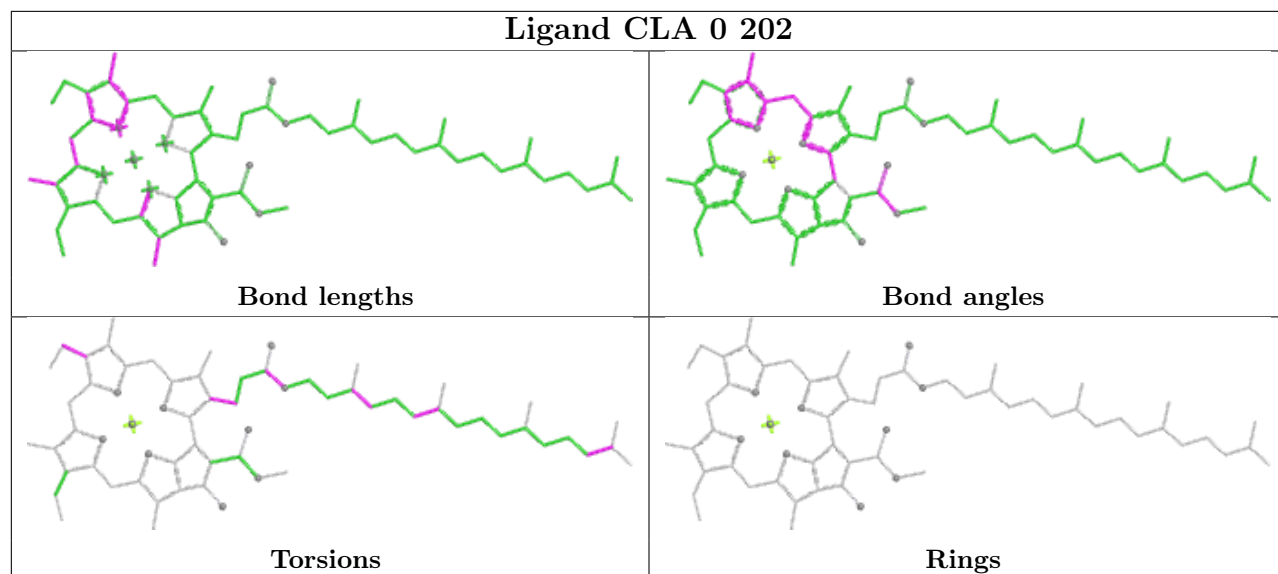
Ligand CLA b 841



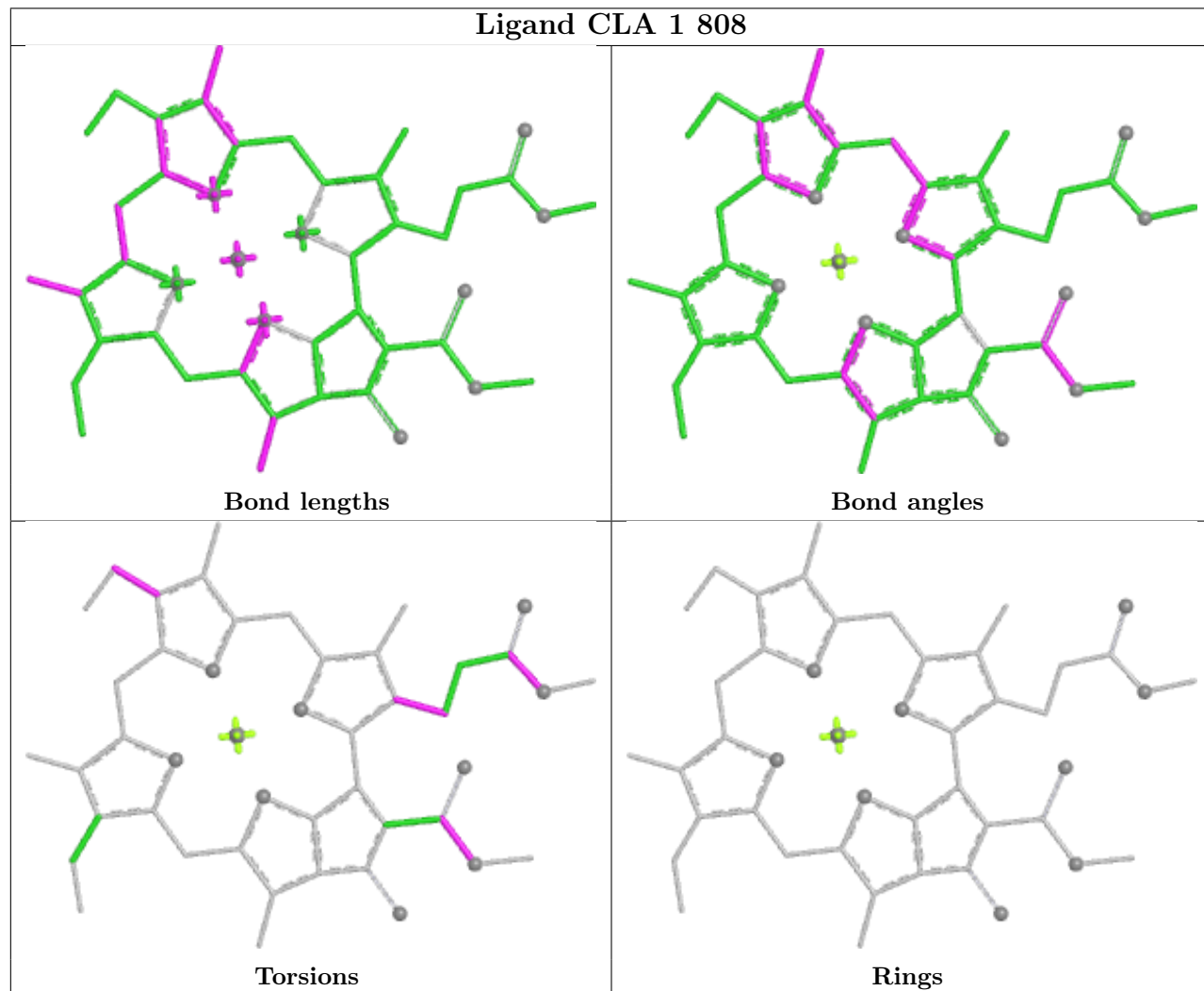
Ligand CLA b 842

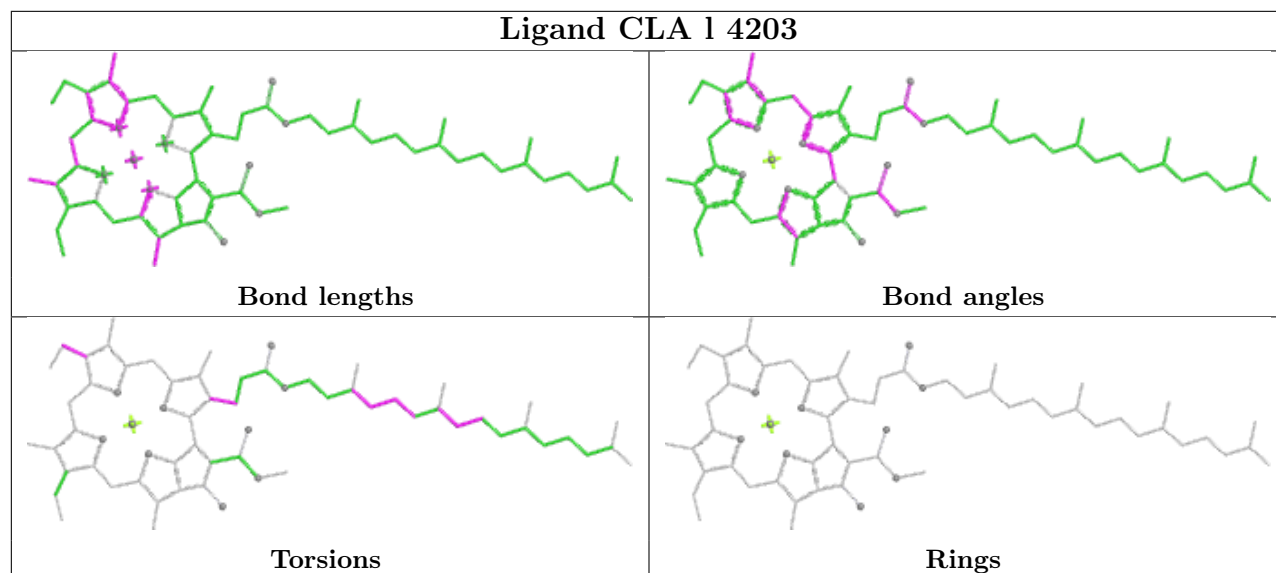
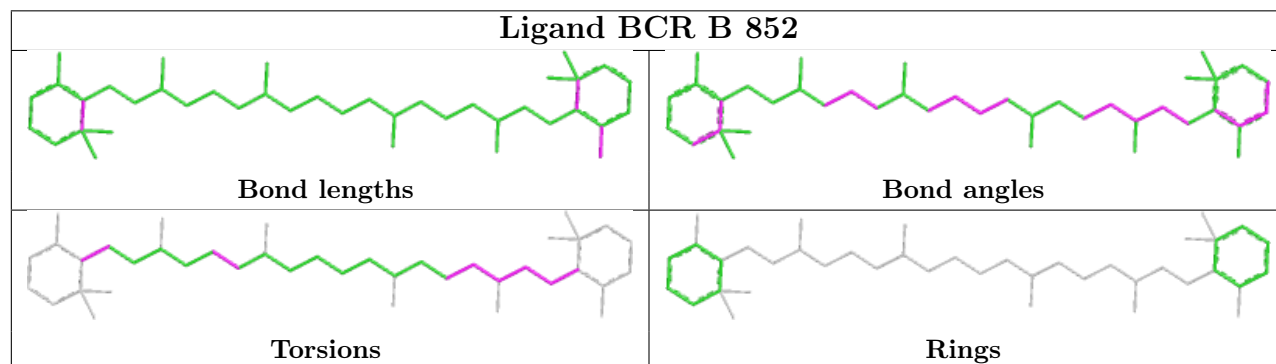
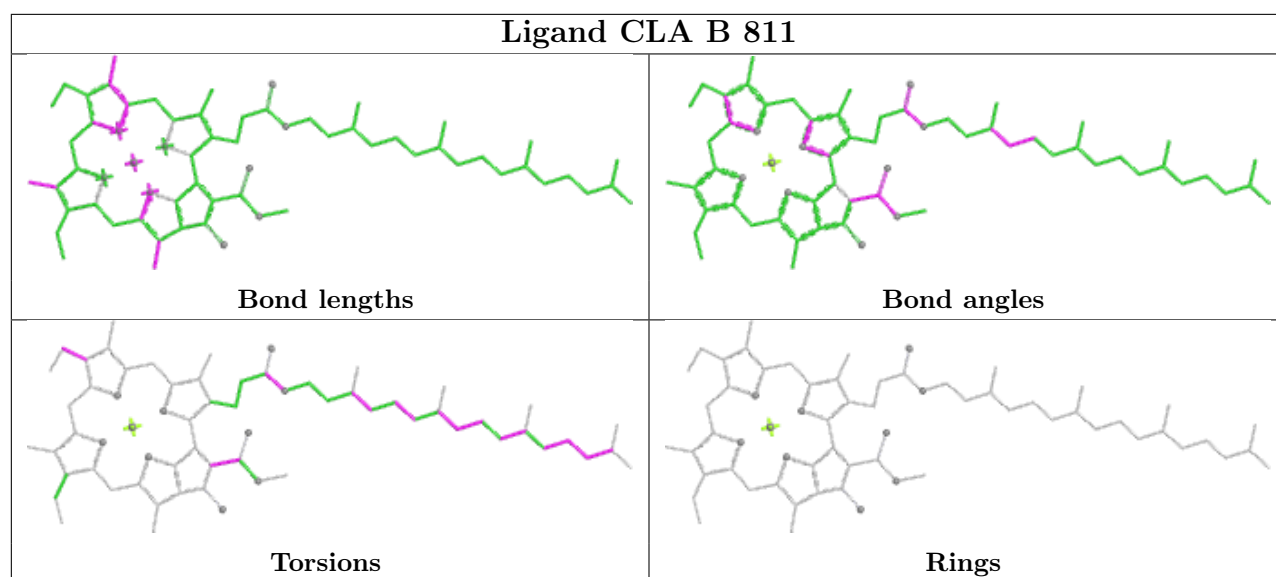


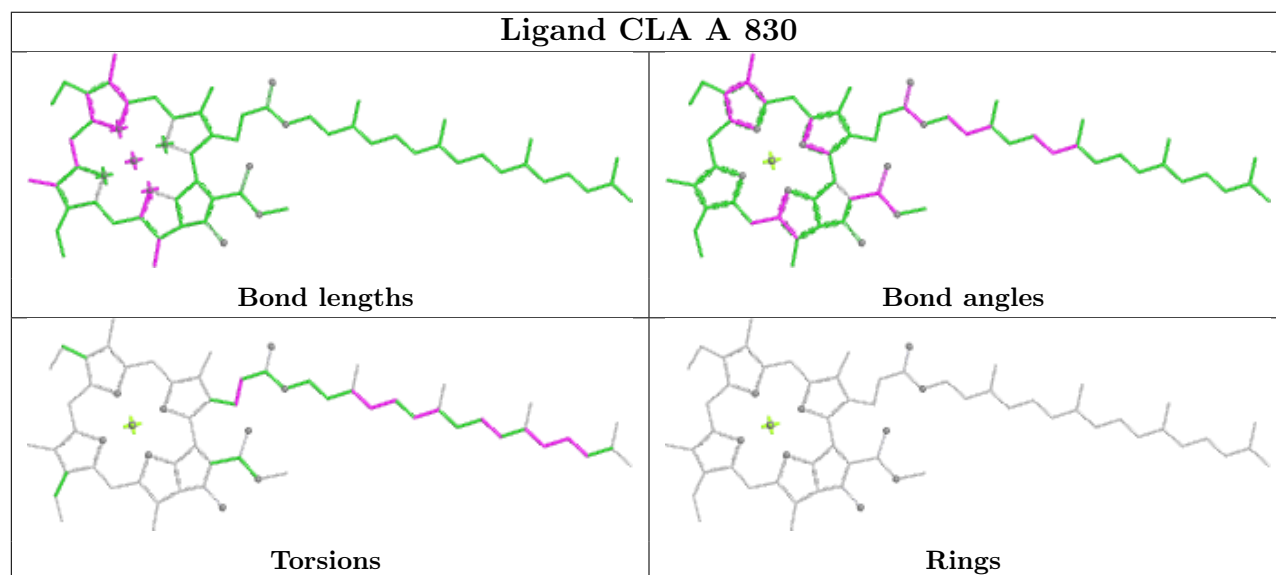
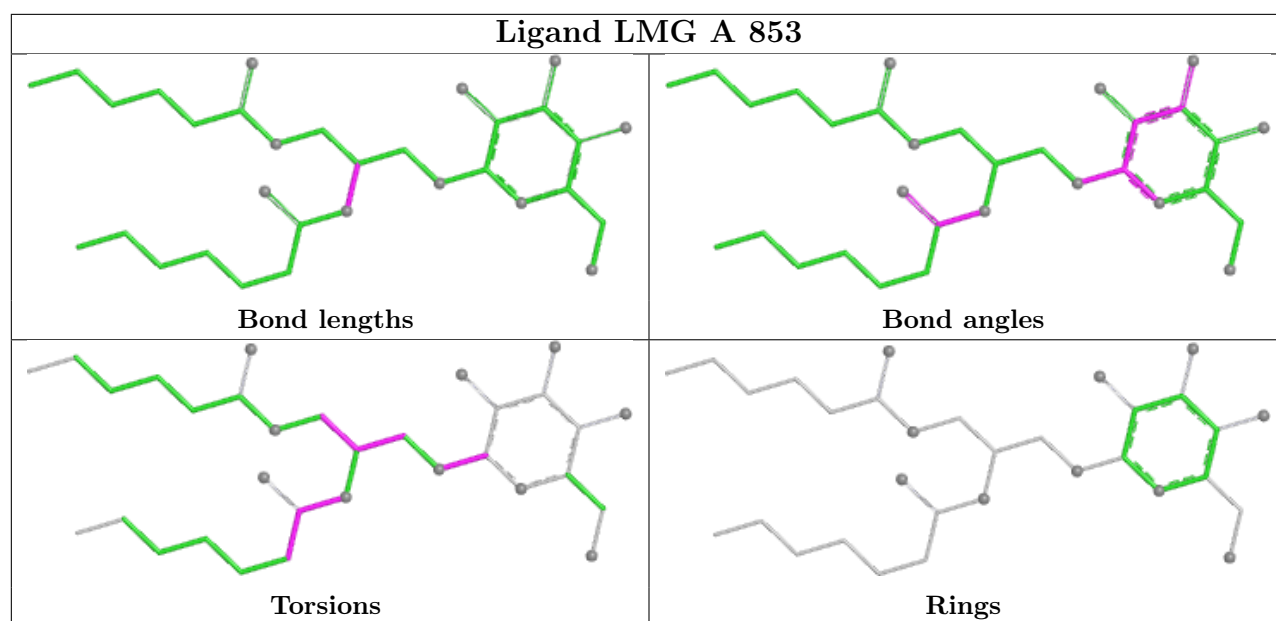
Ligand CLA 0 202



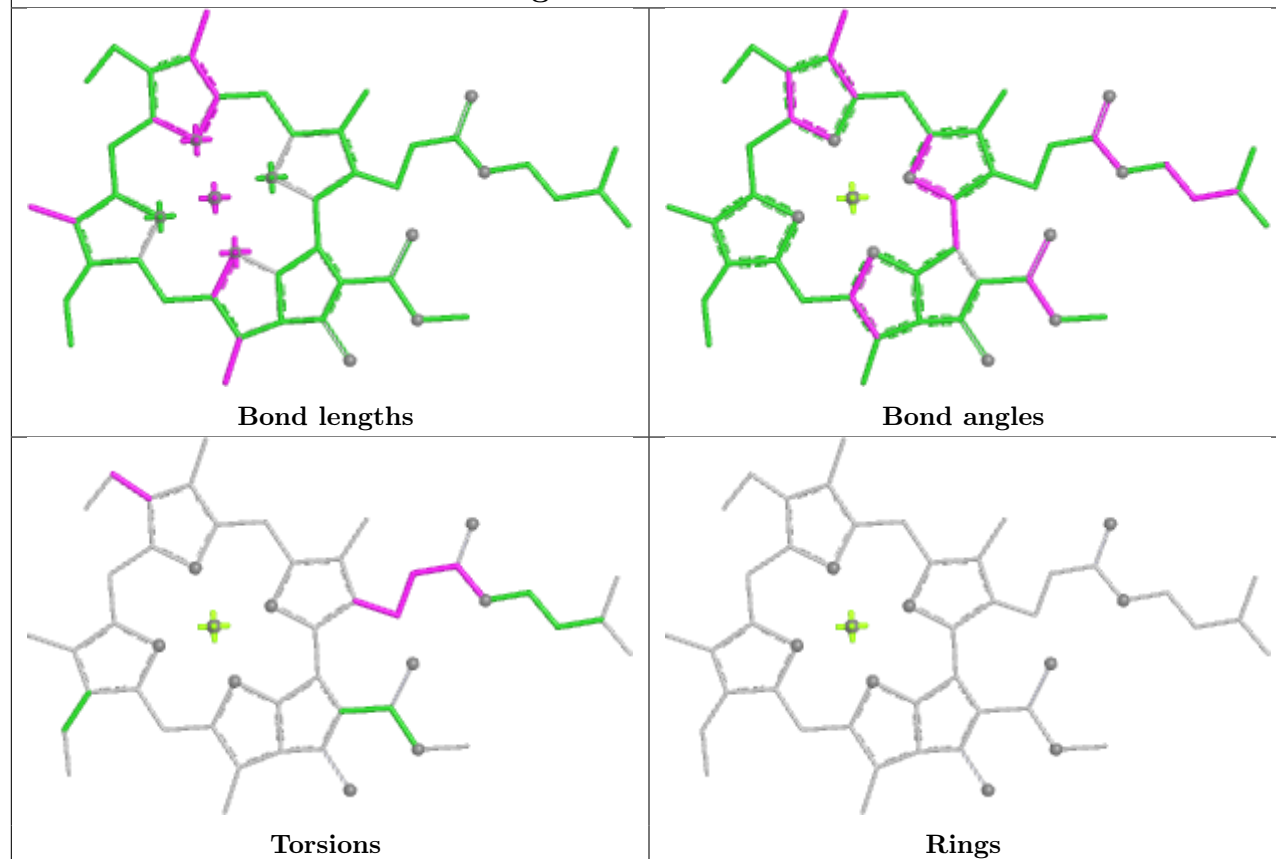
Ligand CLA 1 808



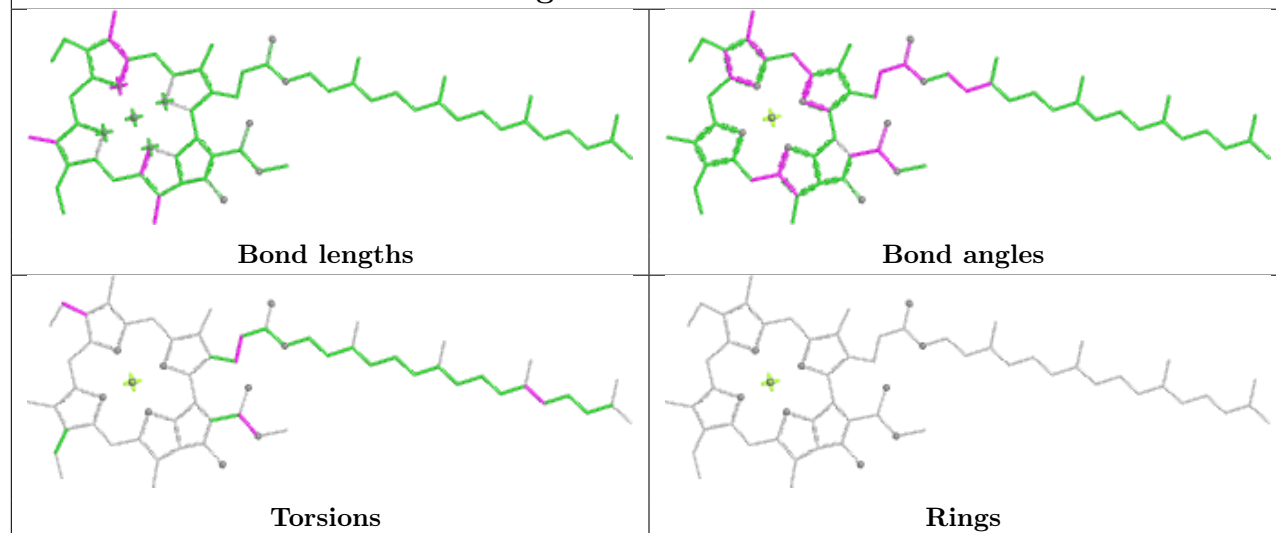


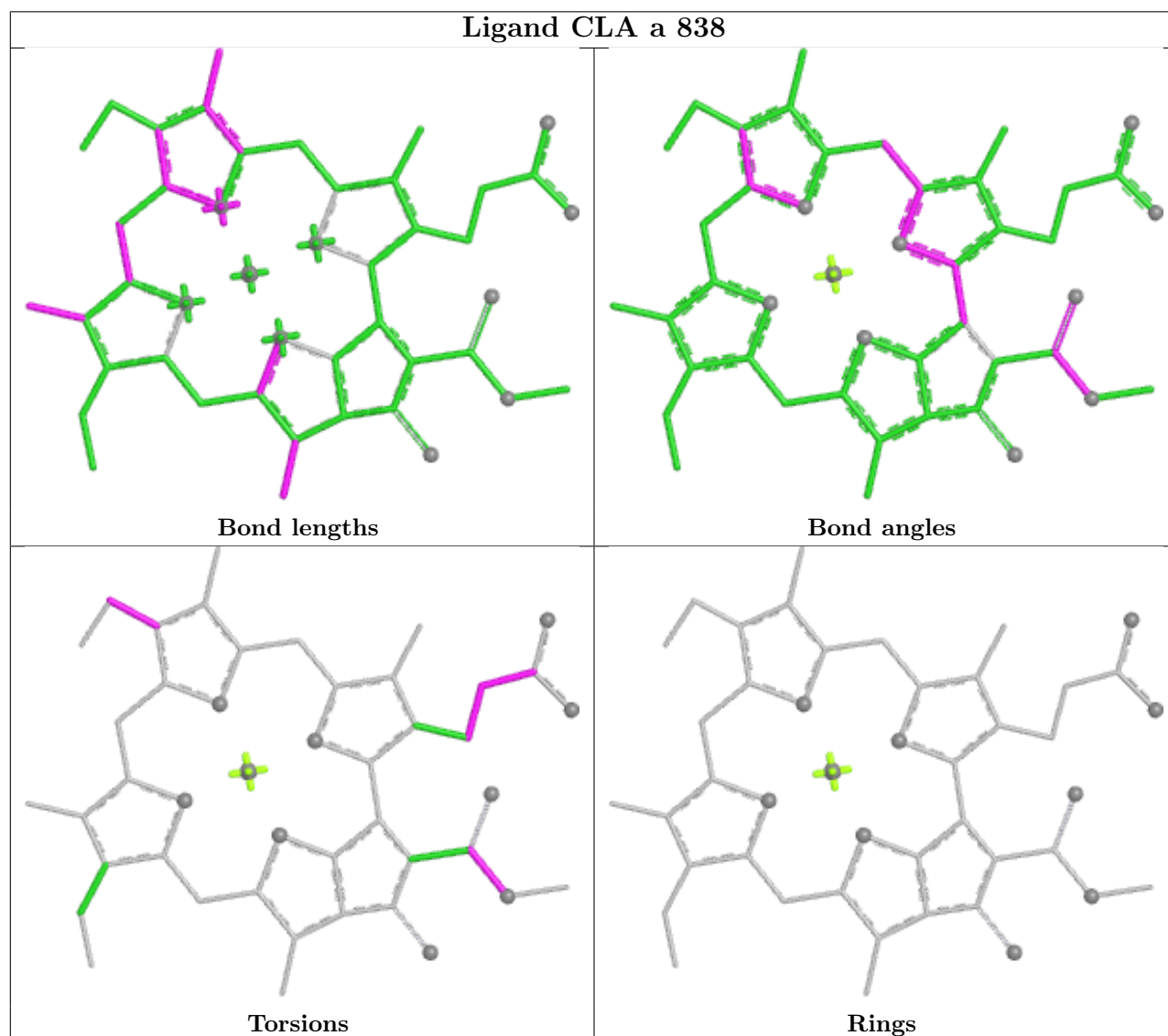
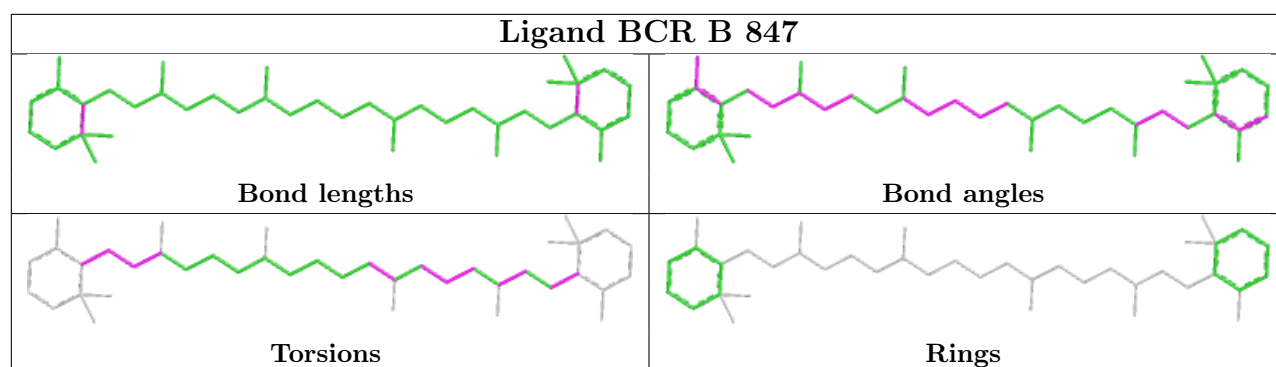


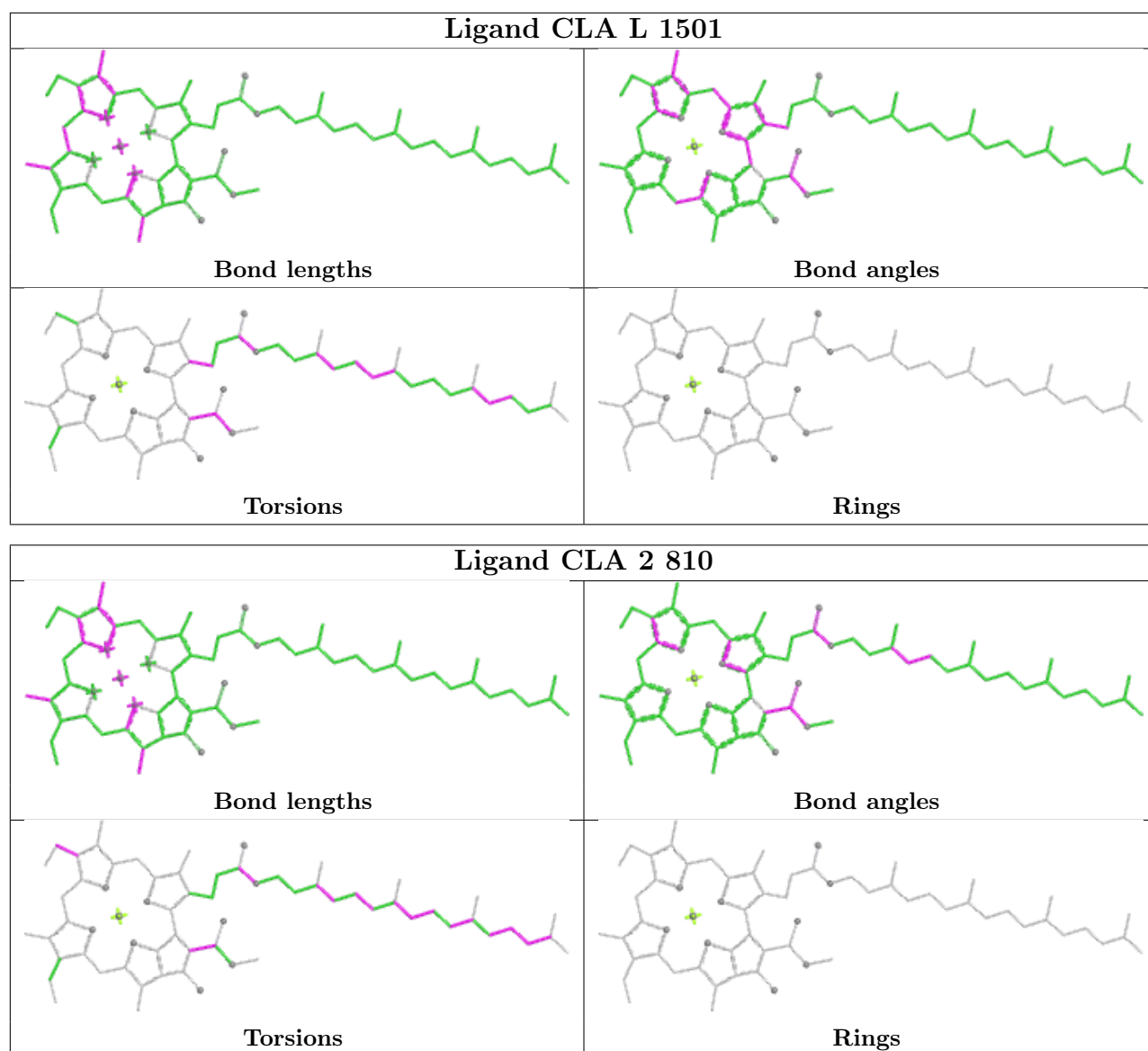
Ligand CLA A 811



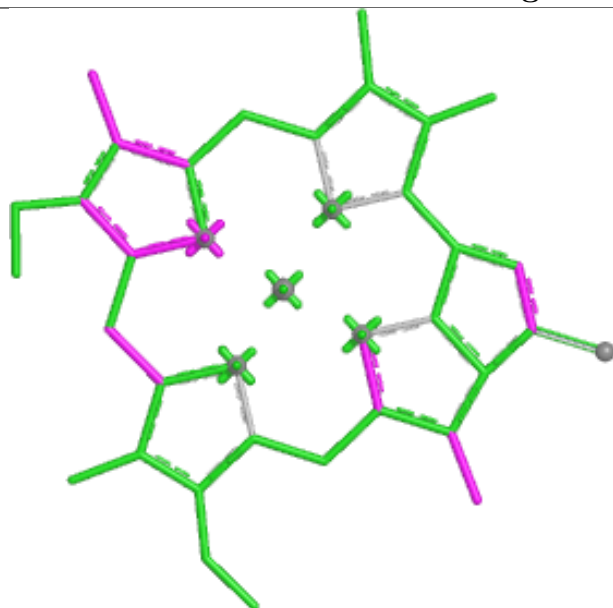
Ligand CLA 1 834



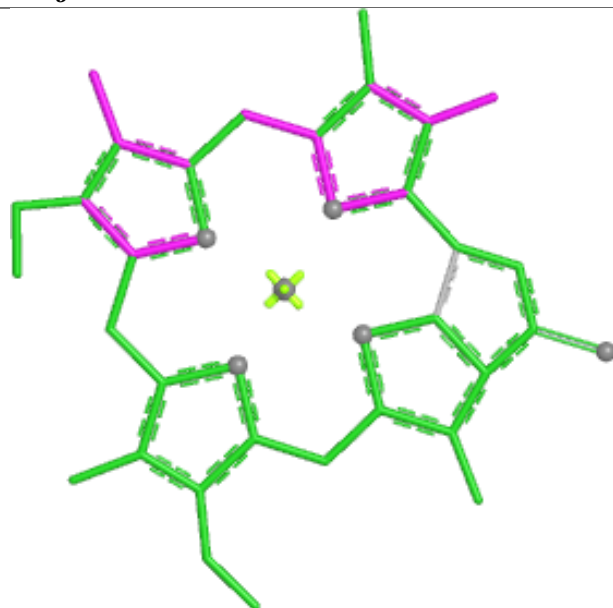




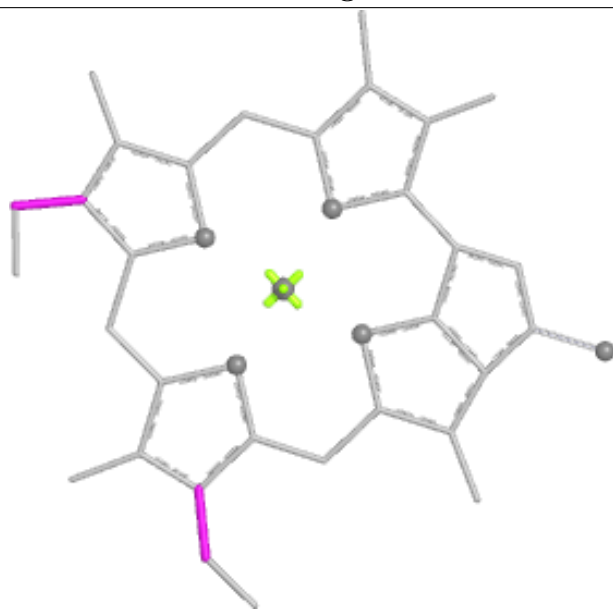
Ligand CLA j 102



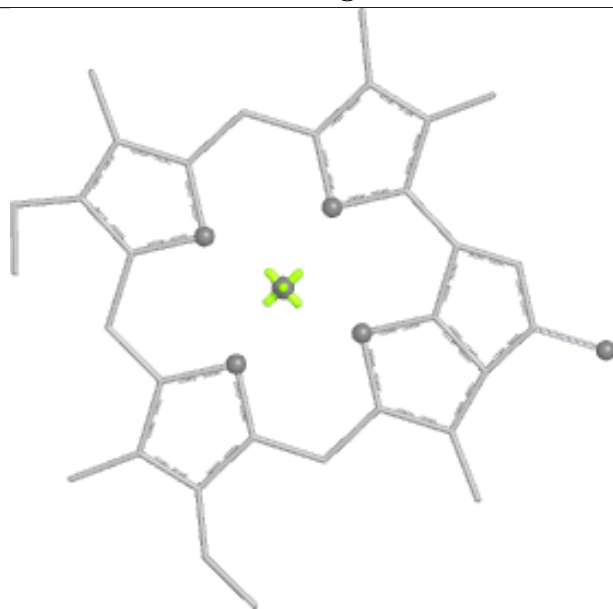
Bond lengths



Bond angles

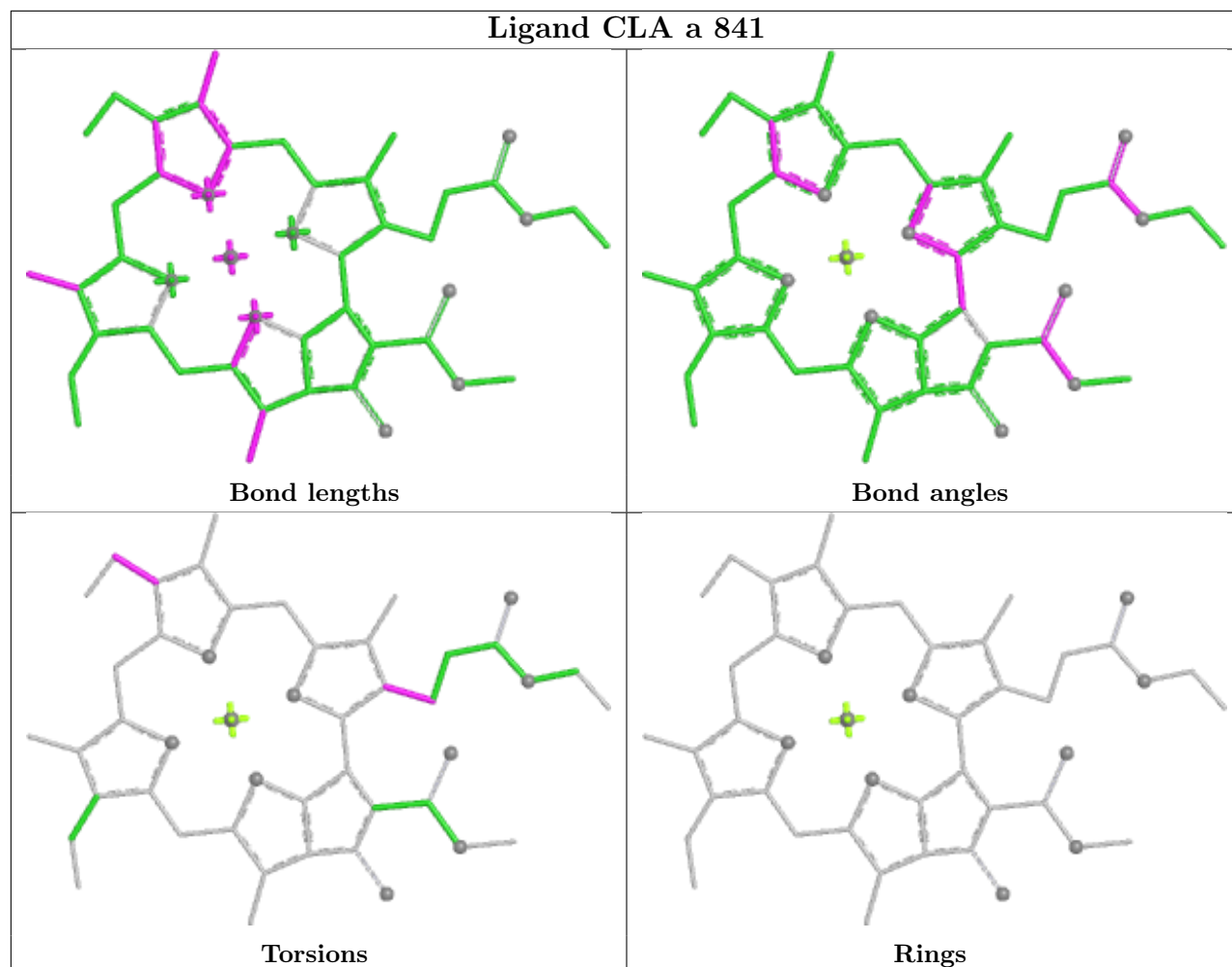


Torsions

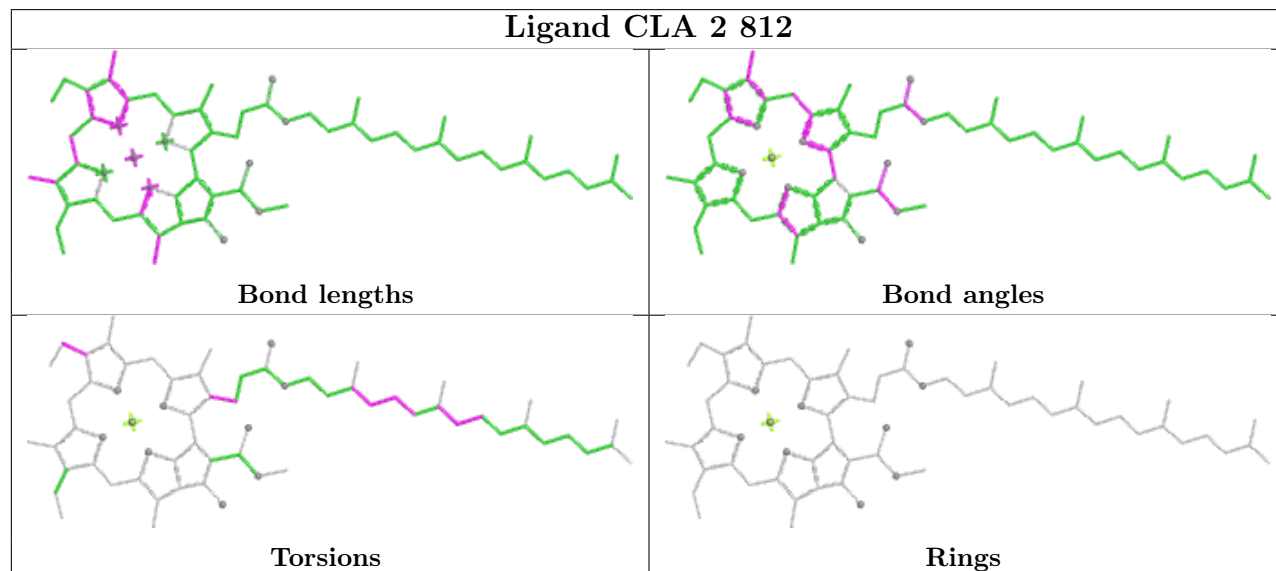


Rings

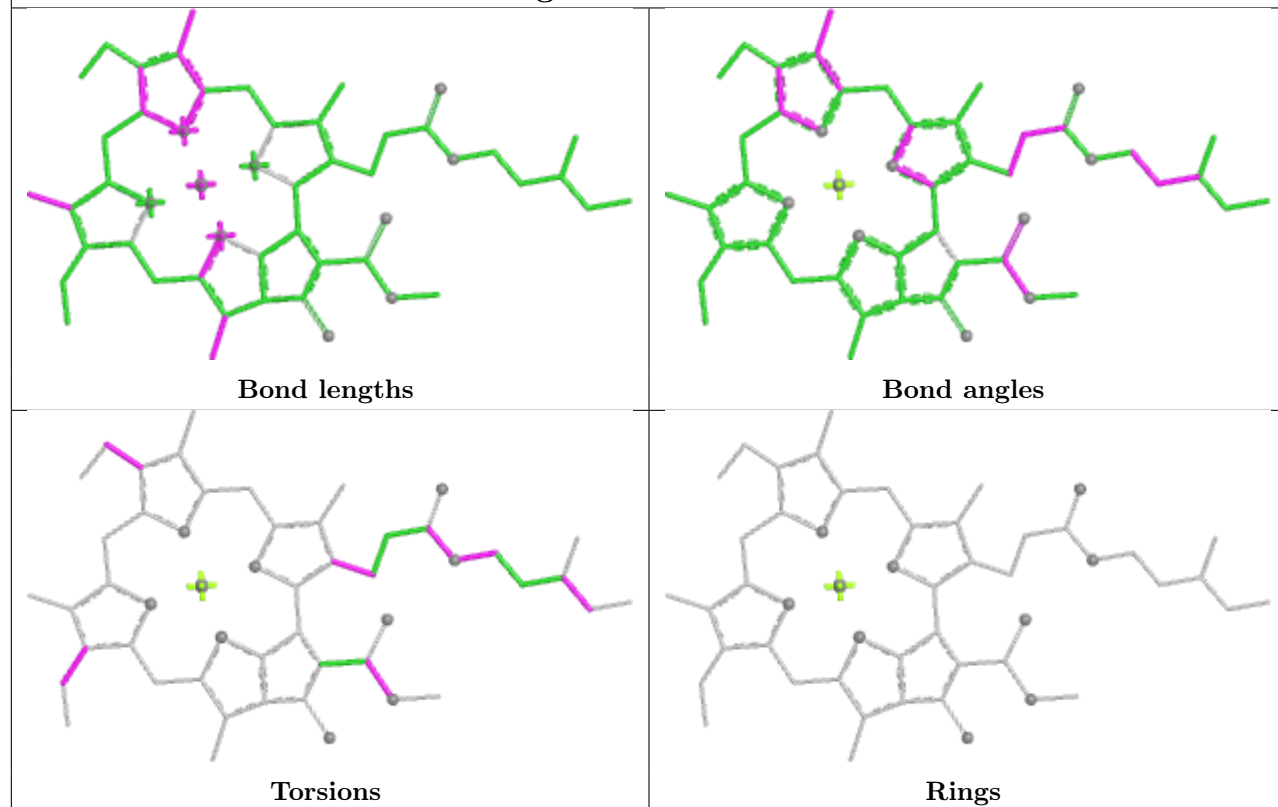
Ligand CLA a 841



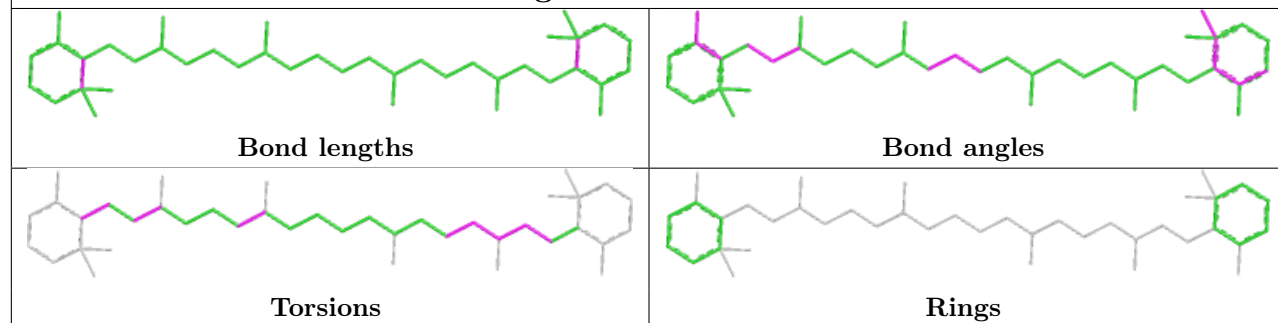
Ligand CLA 2 812

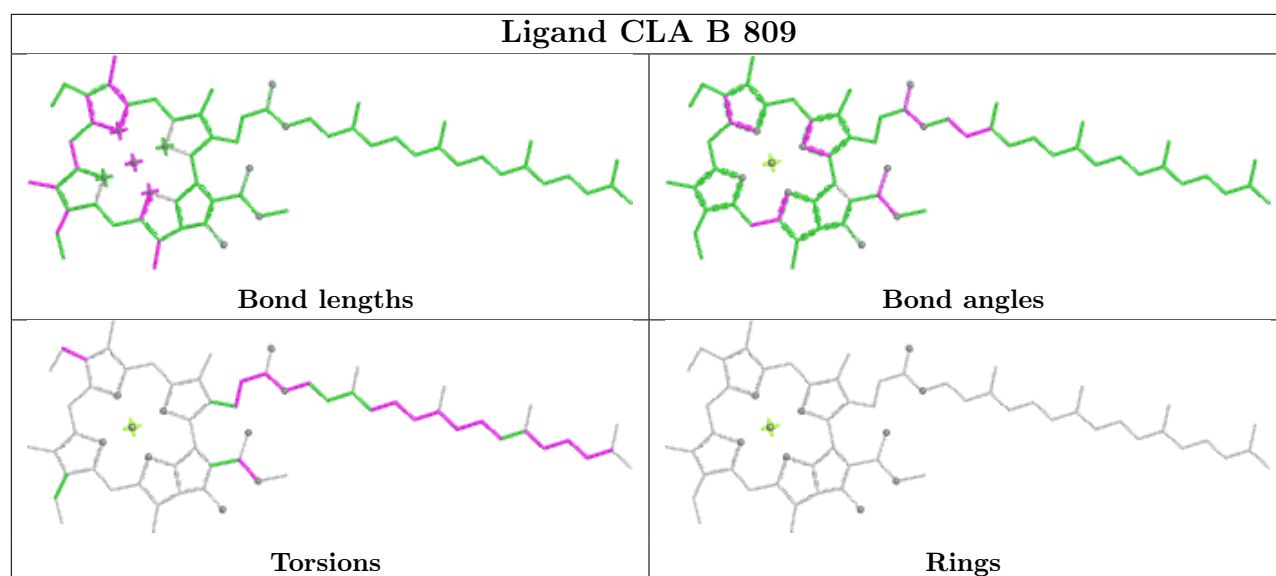
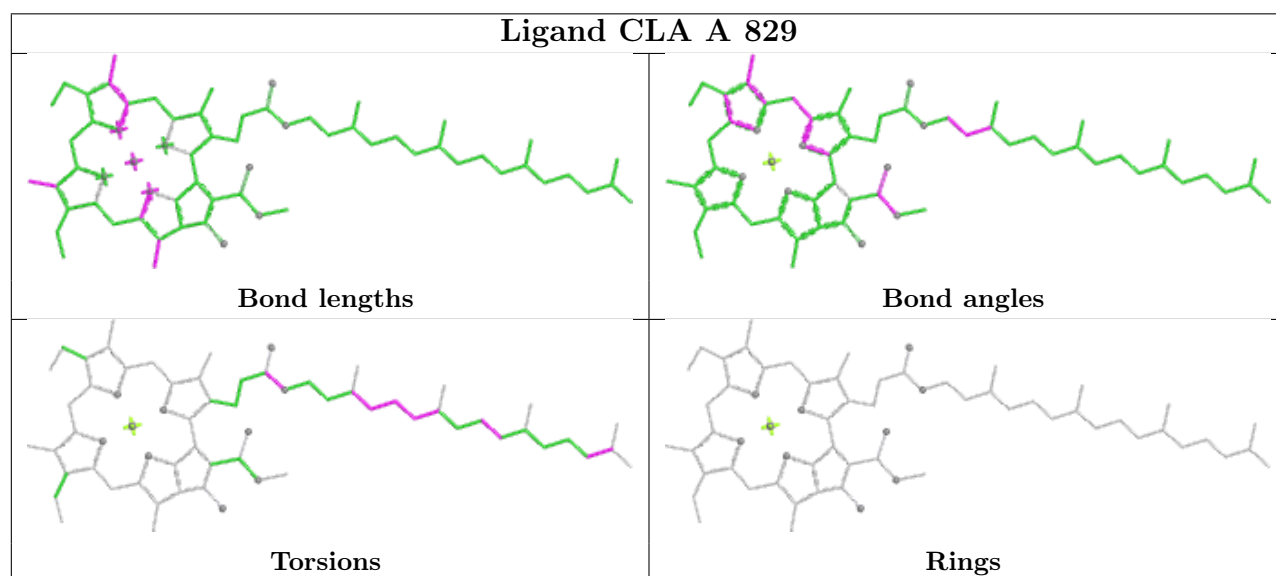
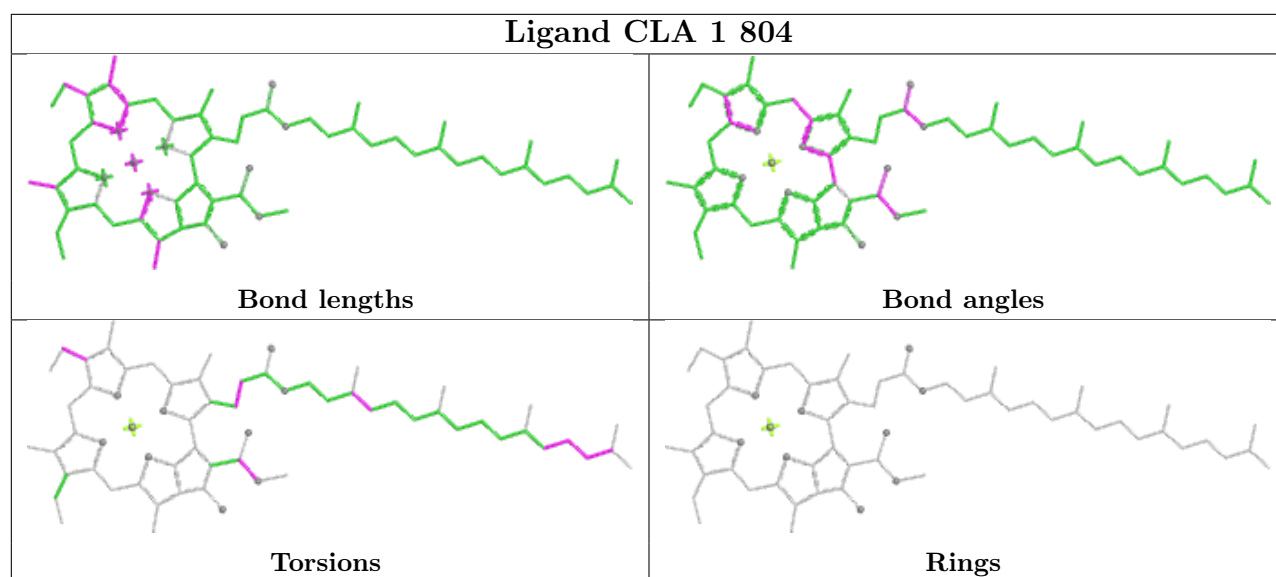


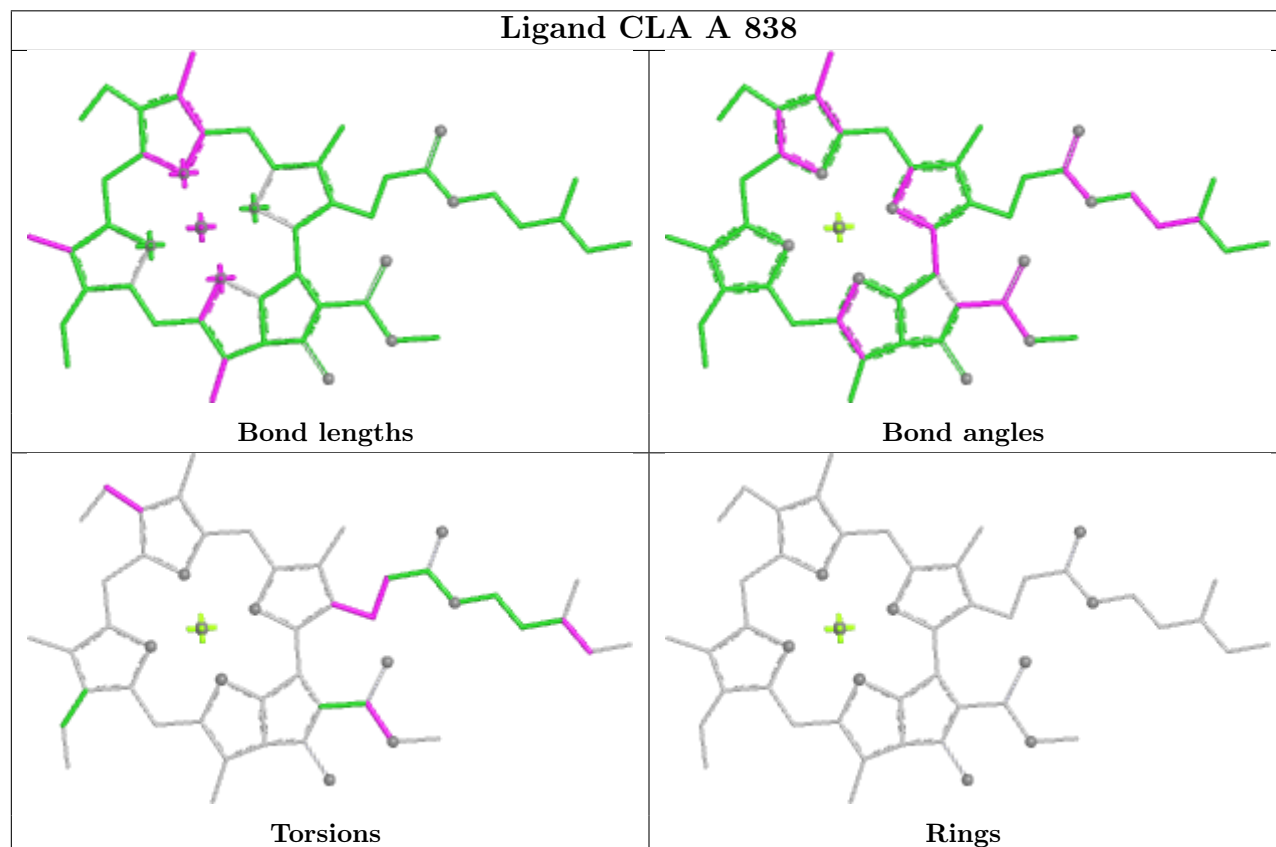
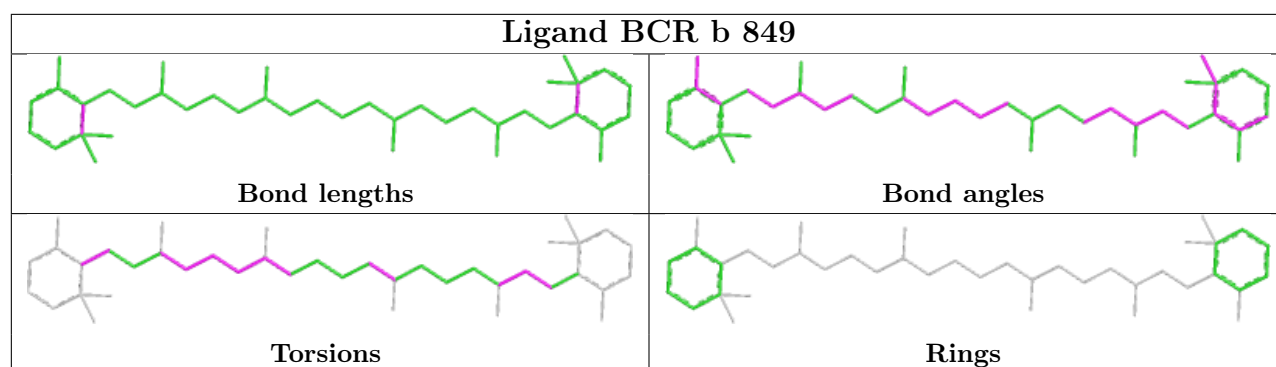
Ligand CLA 1 841



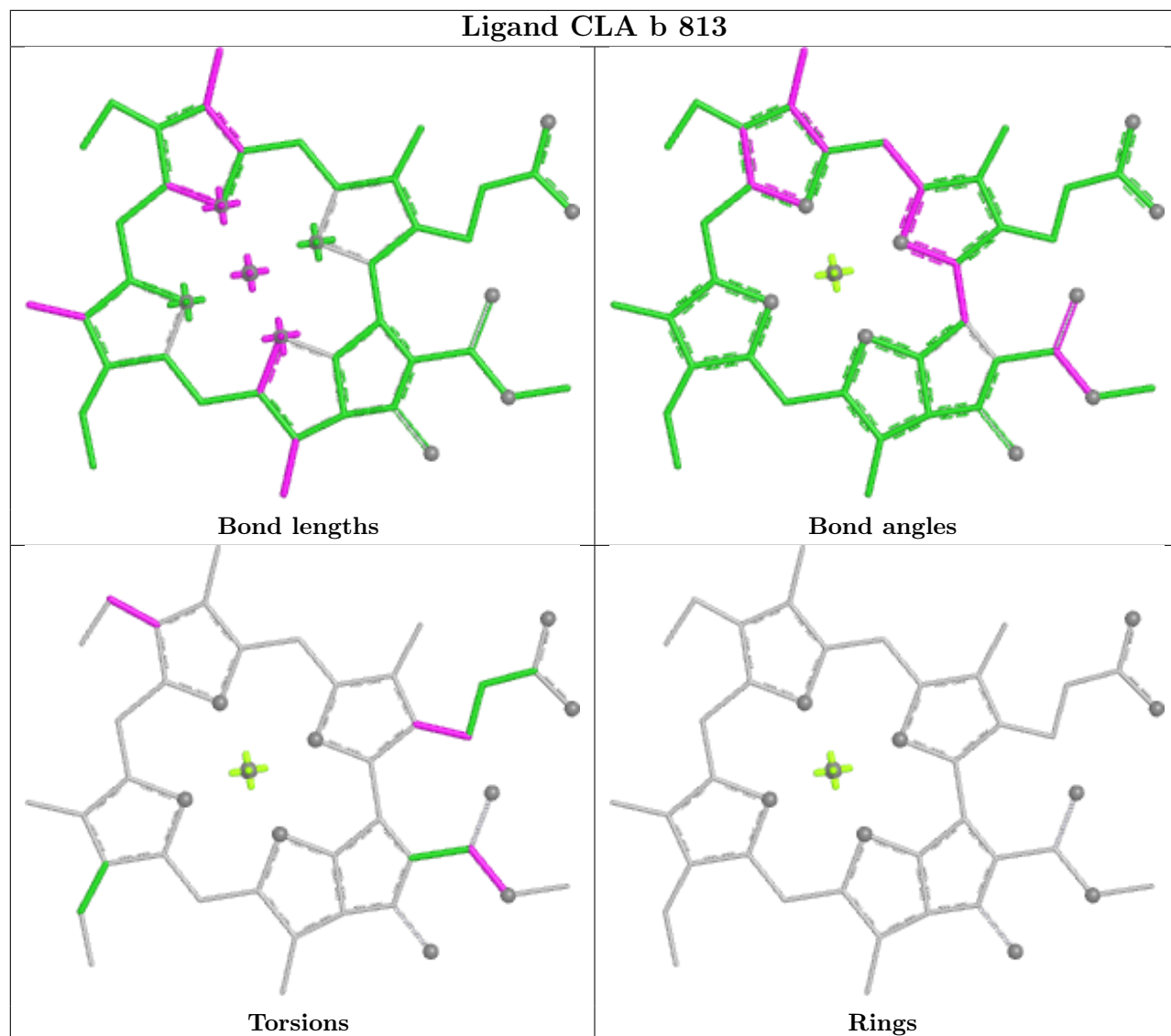
Ligand BCR a 848



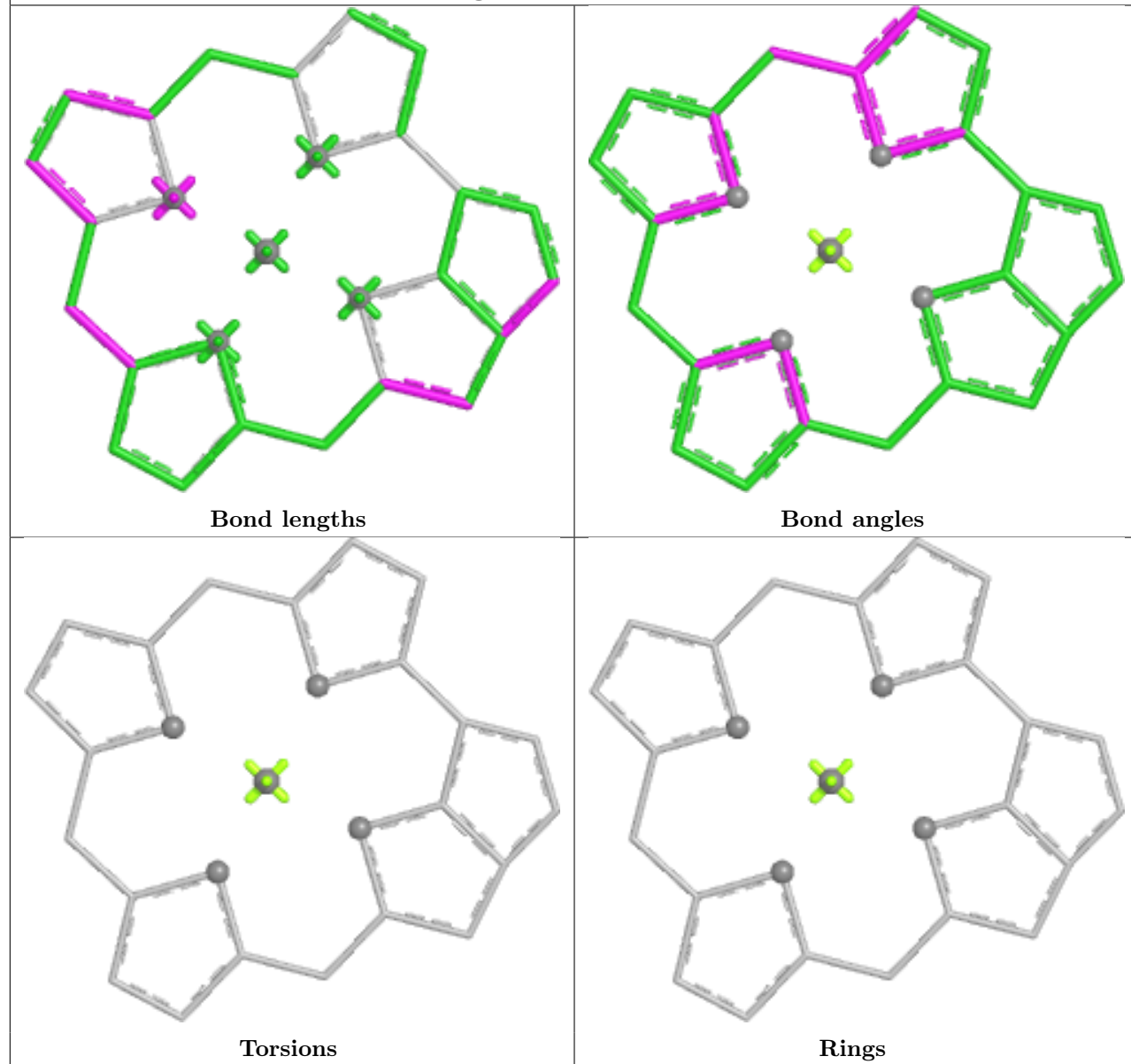


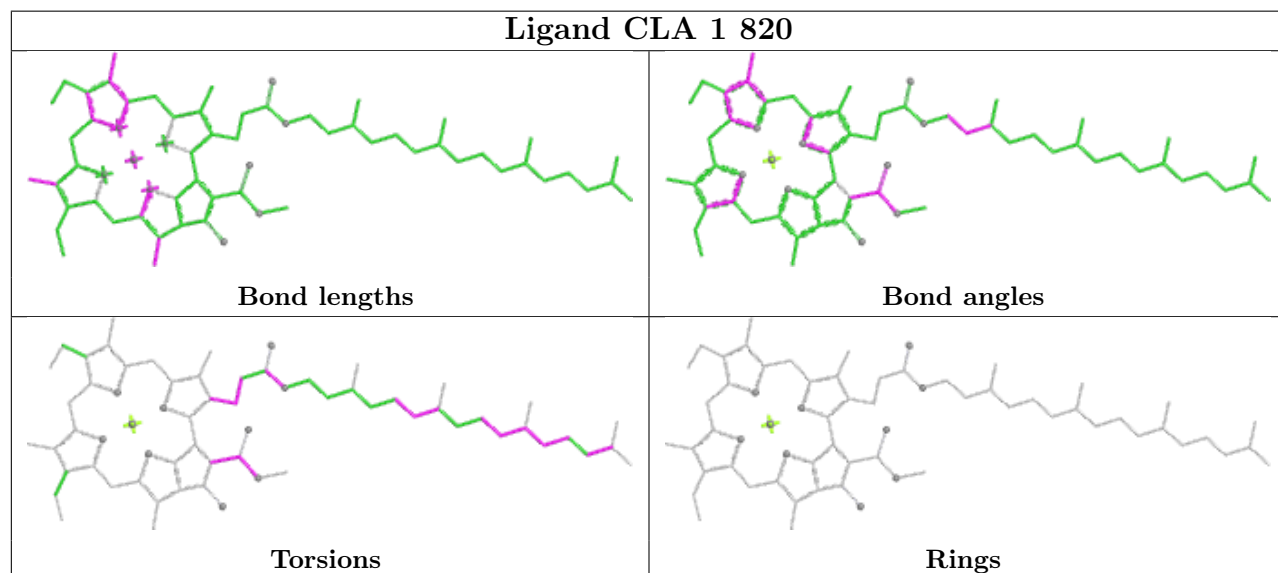
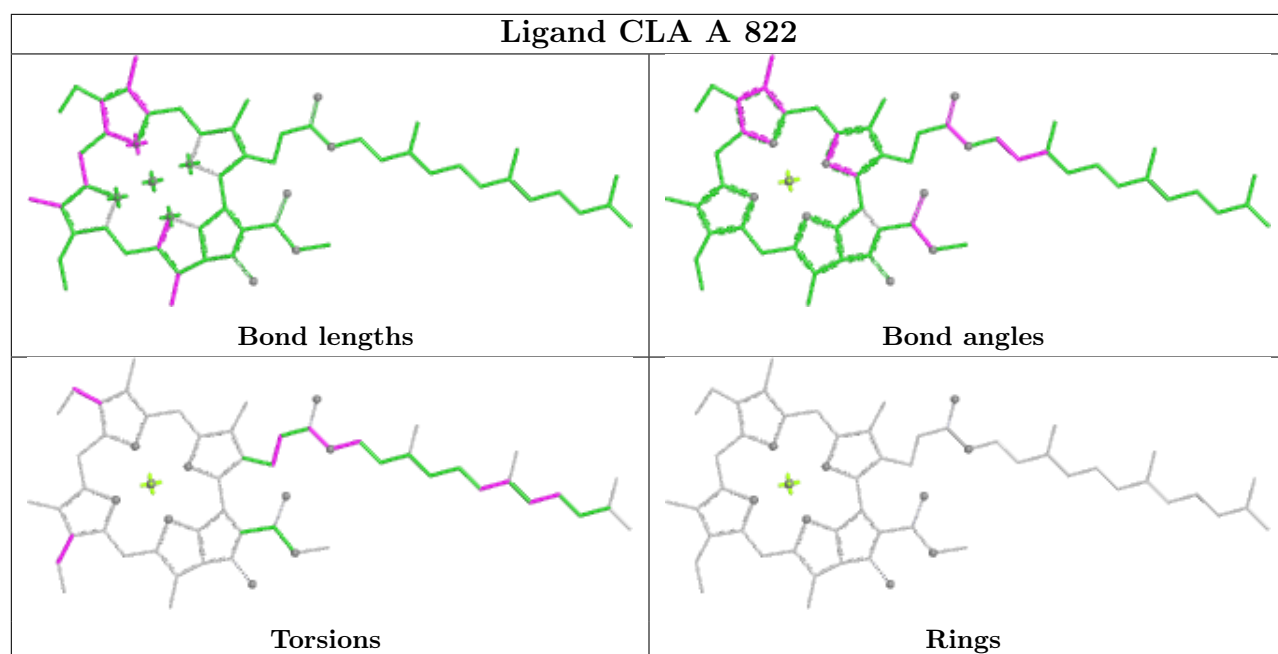


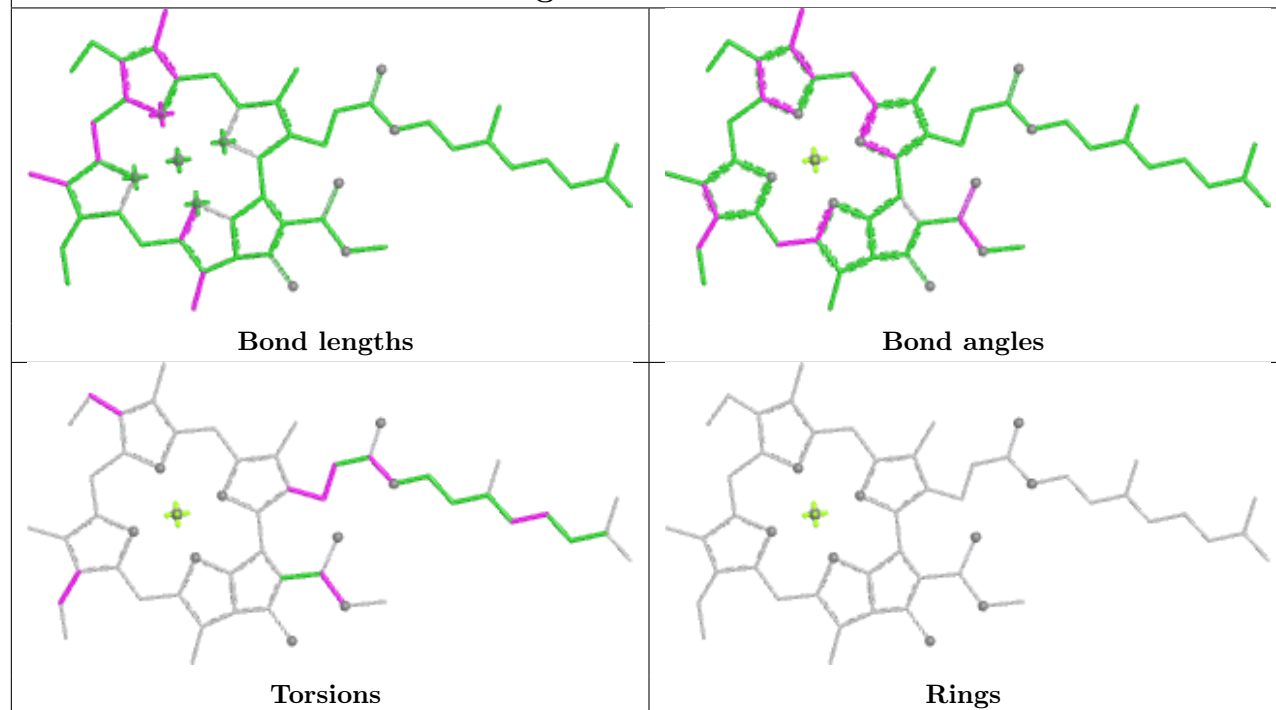
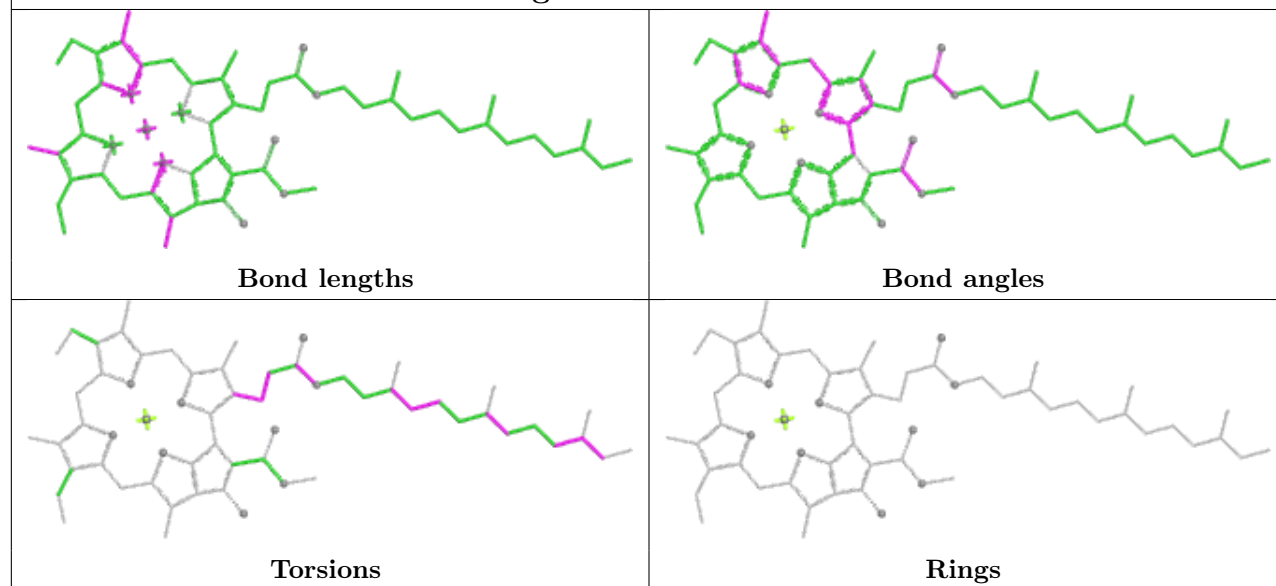
Ligand CLA b 813

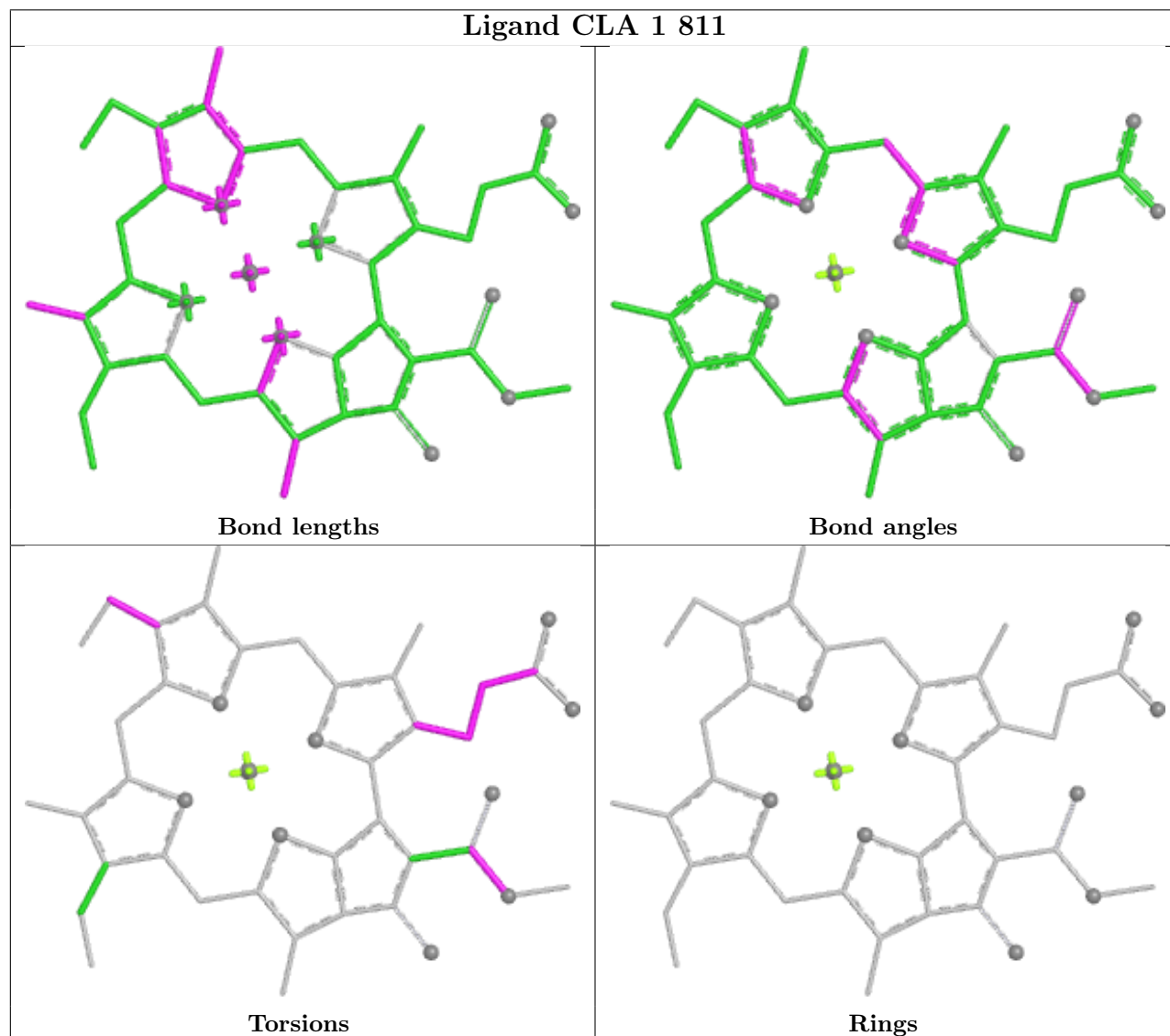
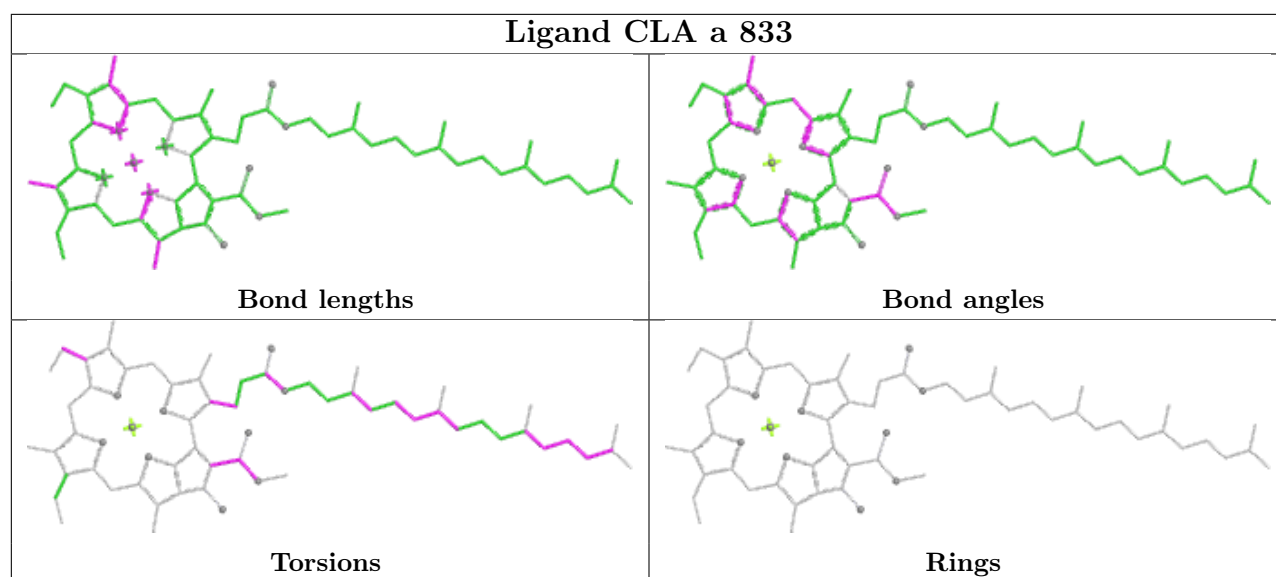


Ligand CLA B 845

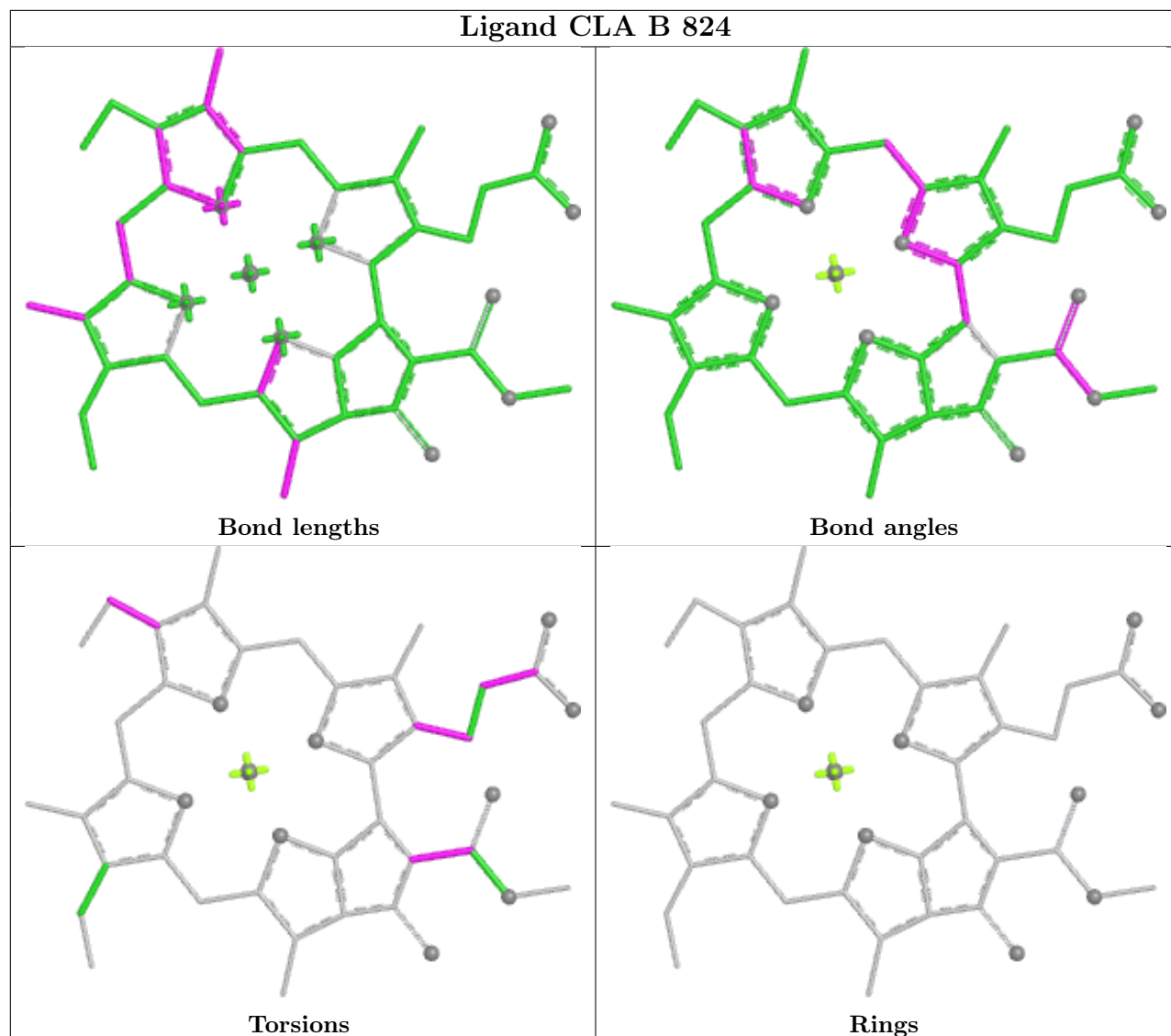




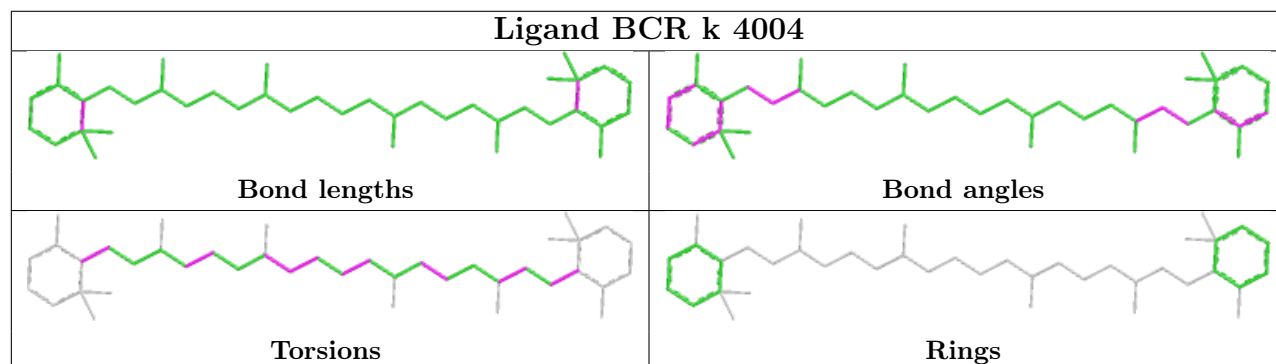
Ligand CLA a 816**Ligand CLA B 812**



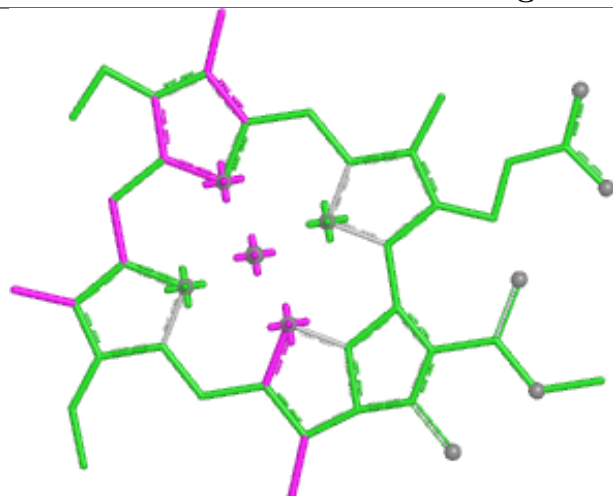
Ligand CLA B 824



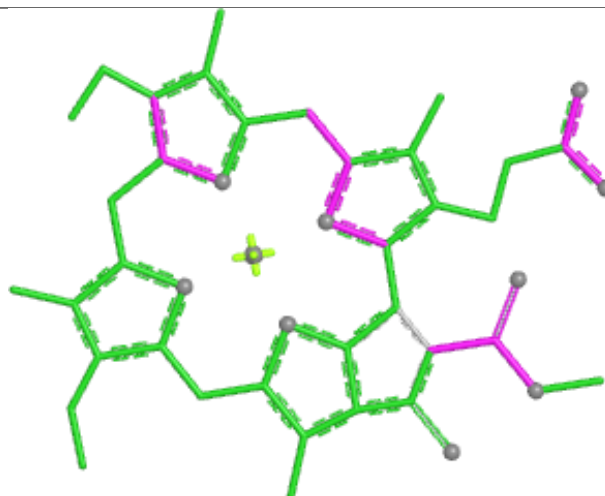
Ligand BCR k 4004



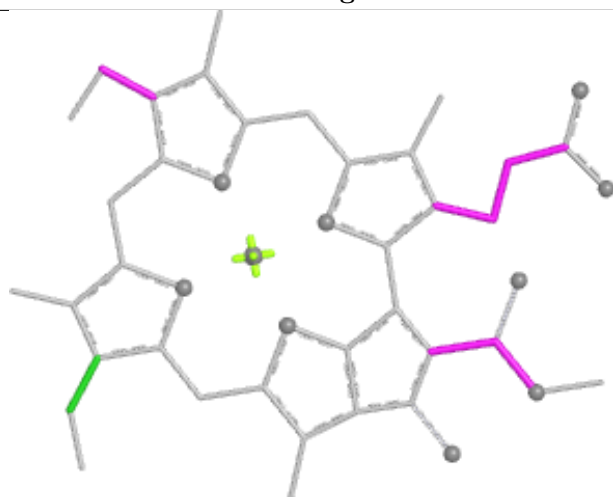
Ligand CLA b 814



Bond lengths



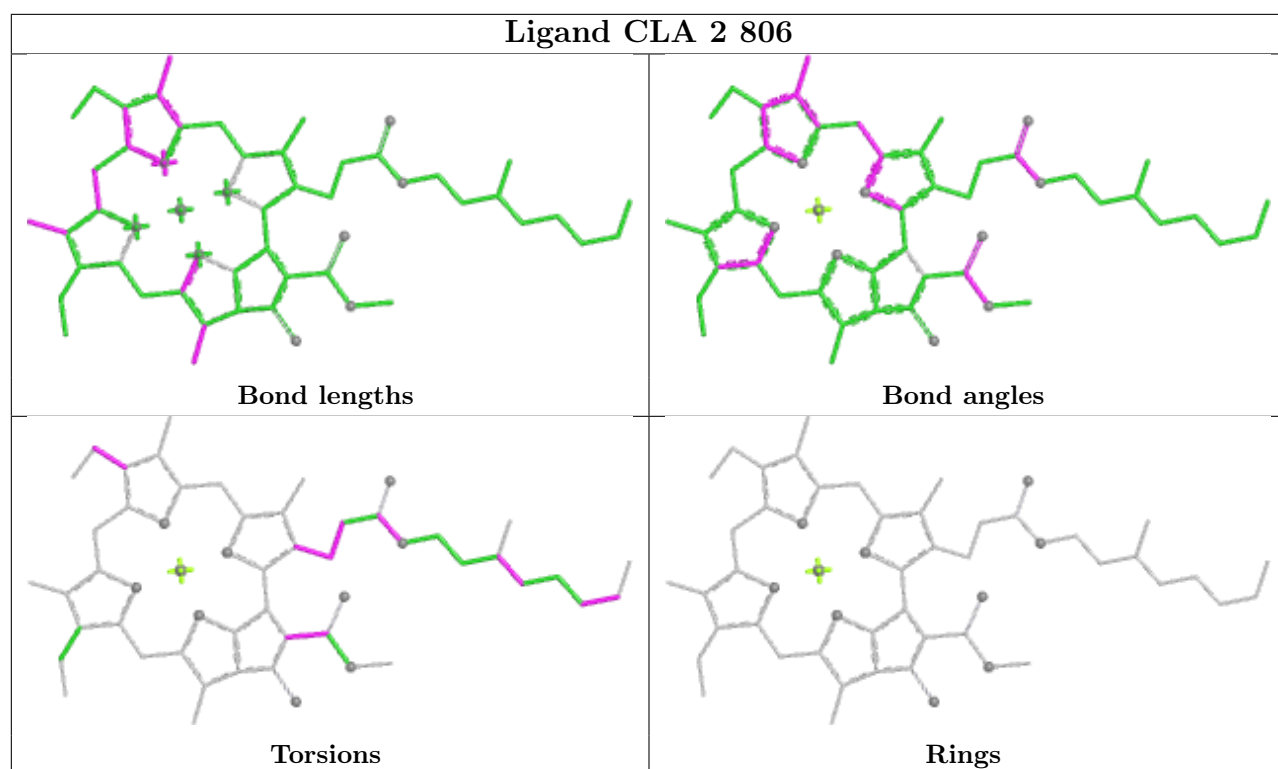
Bond angles



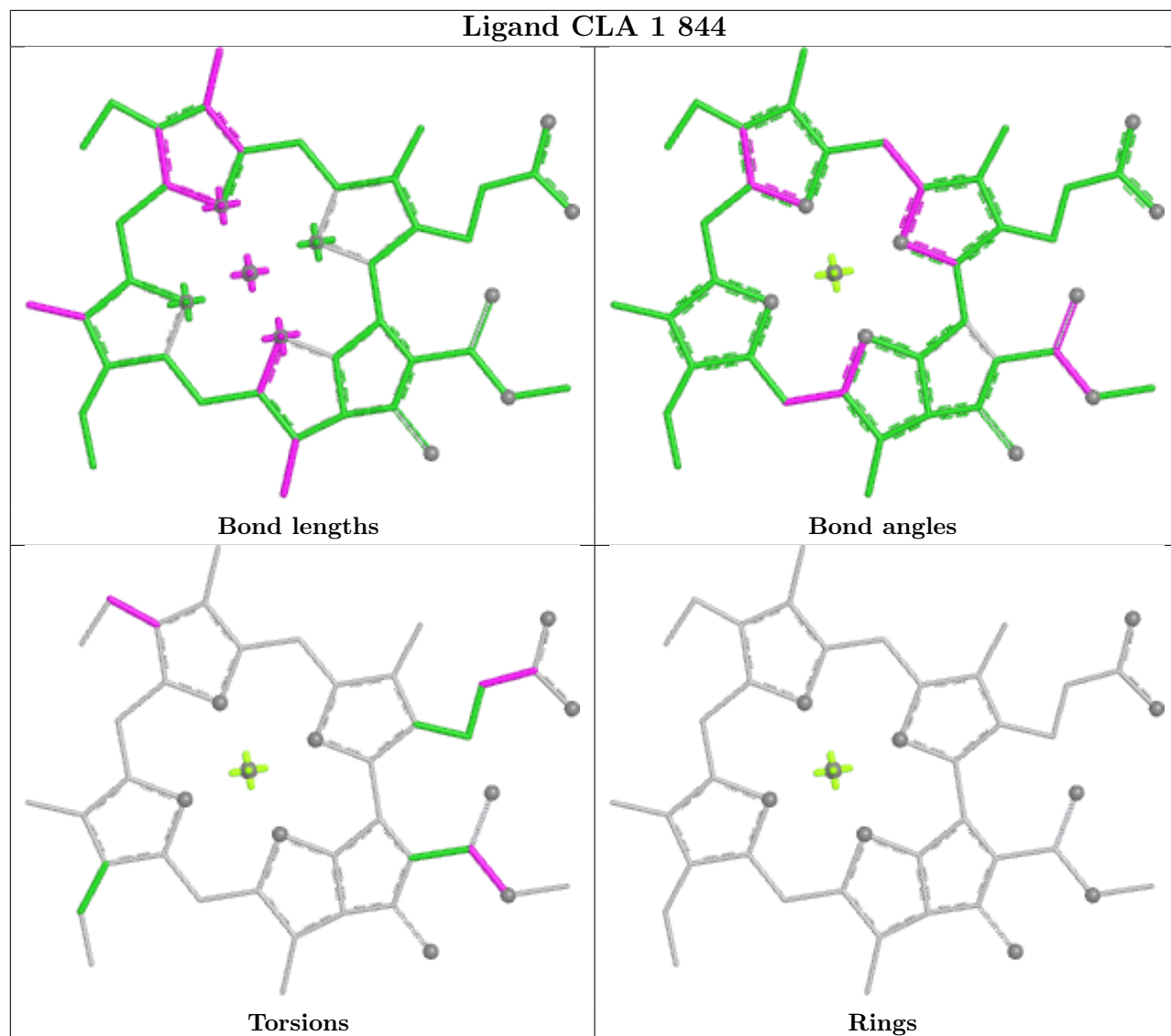
Torsions



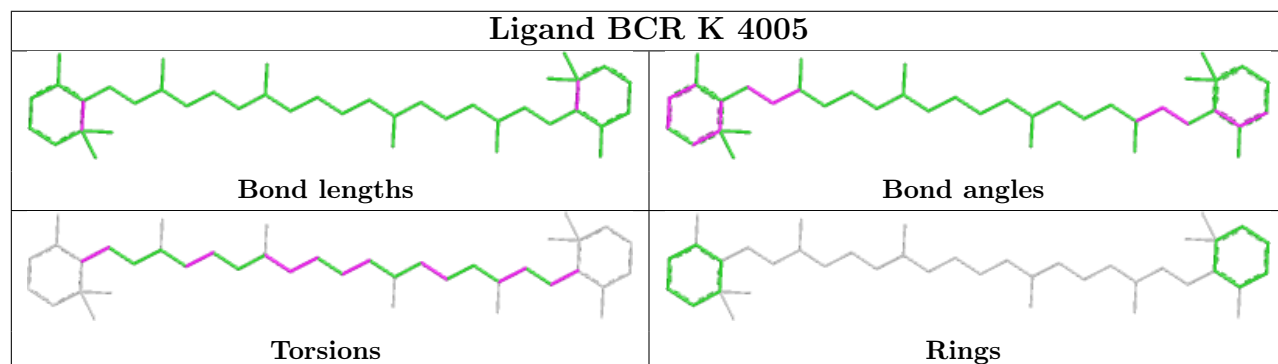
Rings



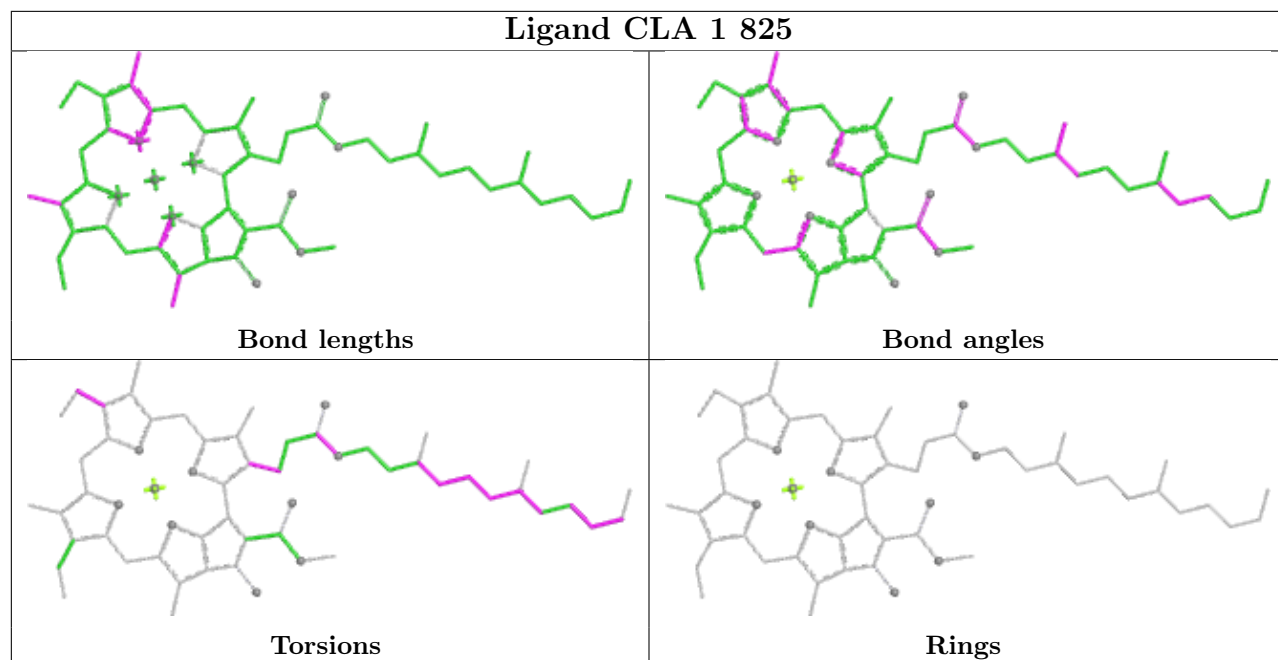
Ligand CLA 1 844



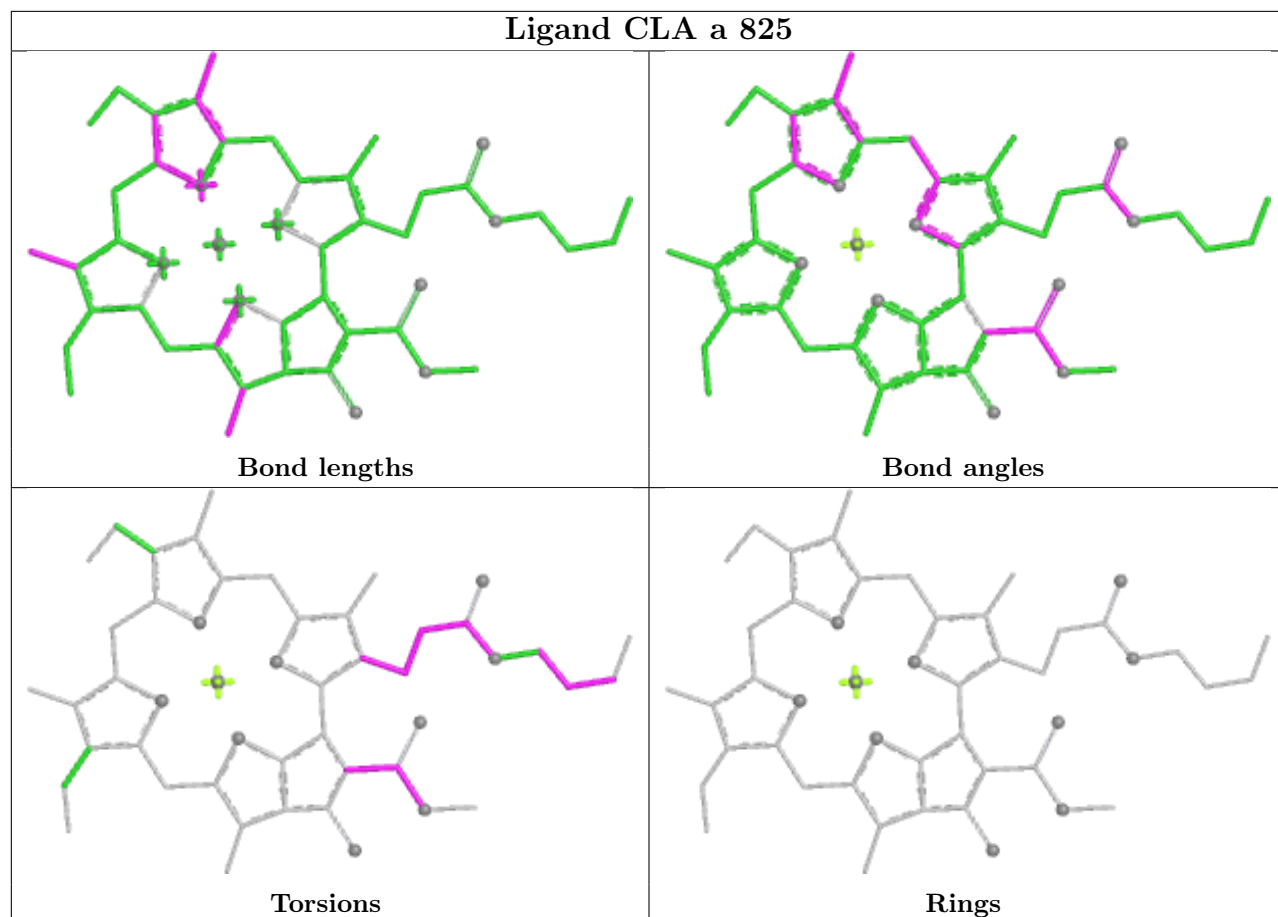
Ligand BCR K 4005

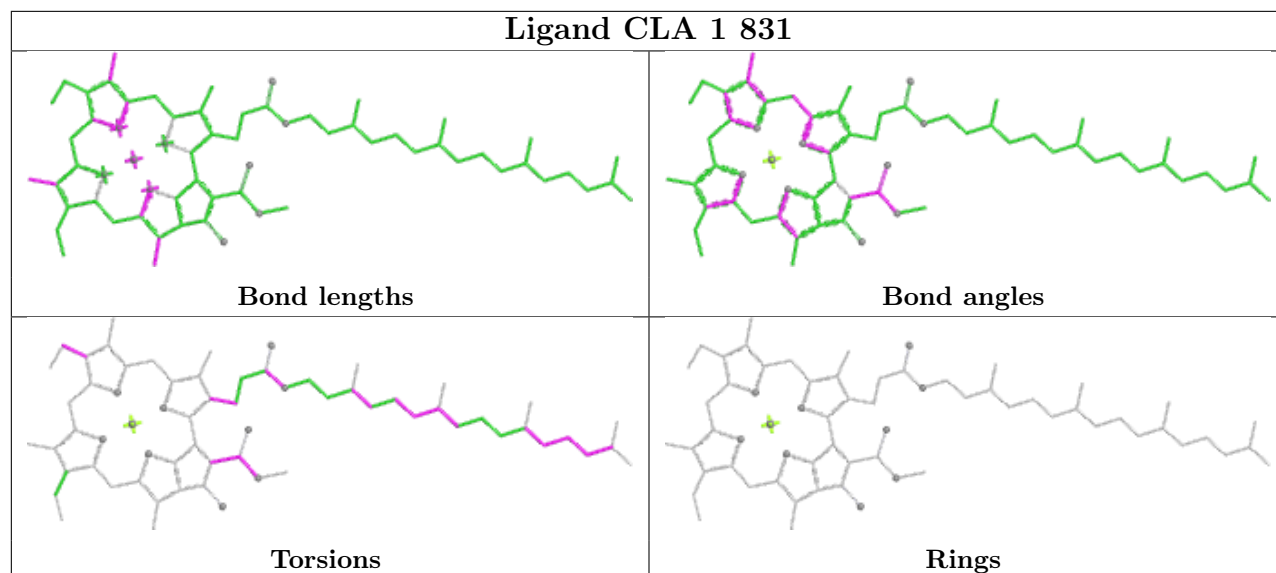
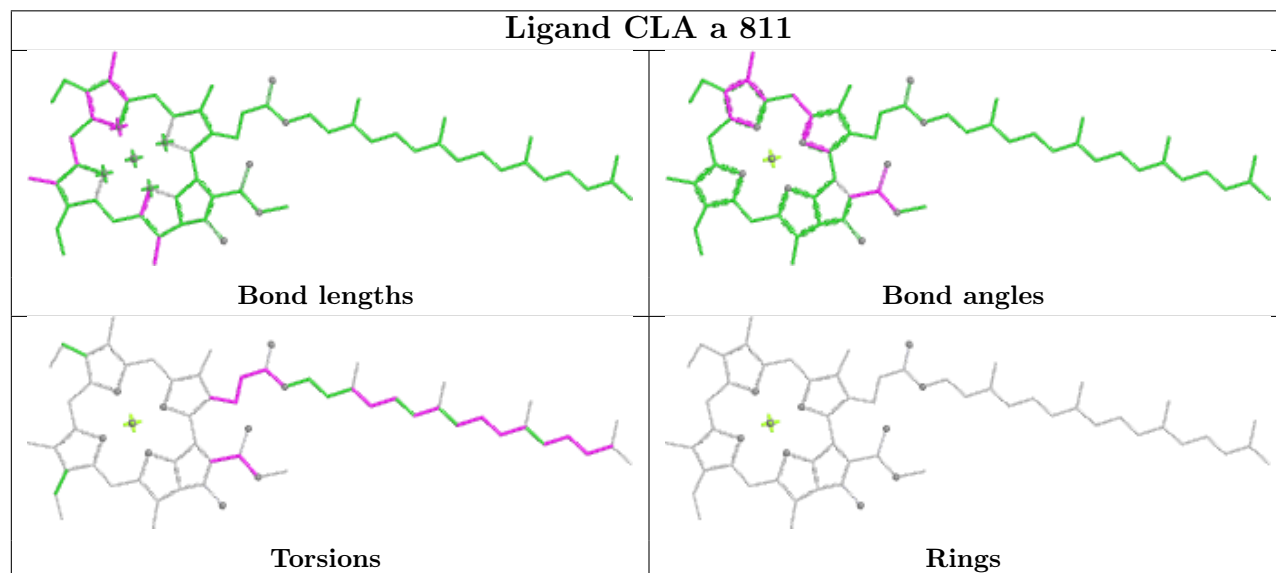
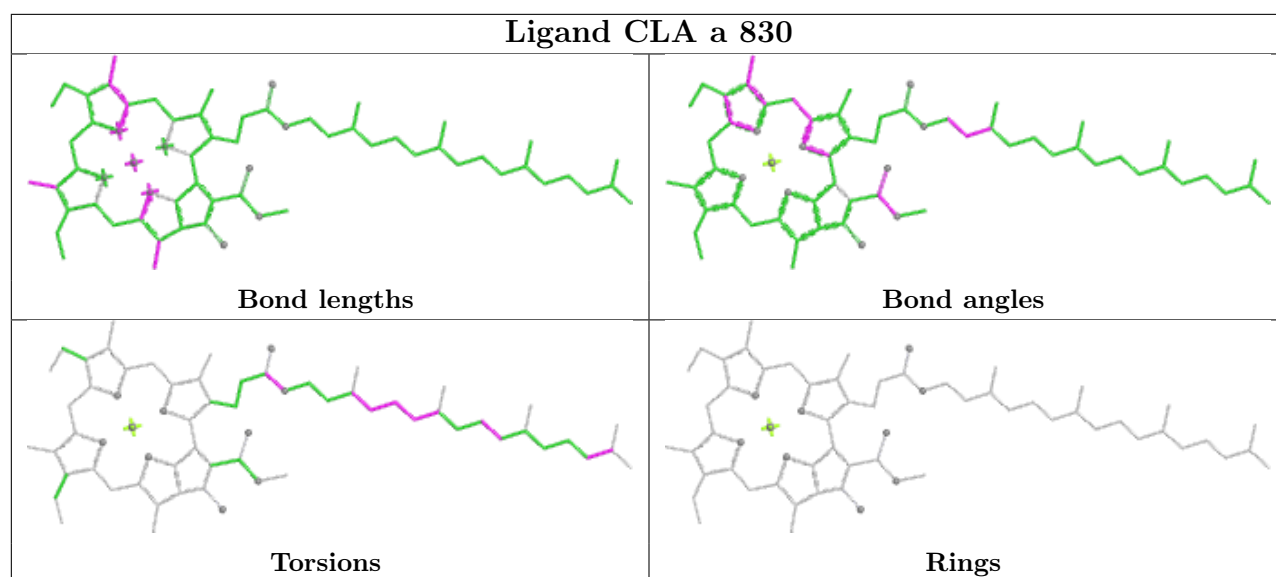


Ligand CLA 1 825

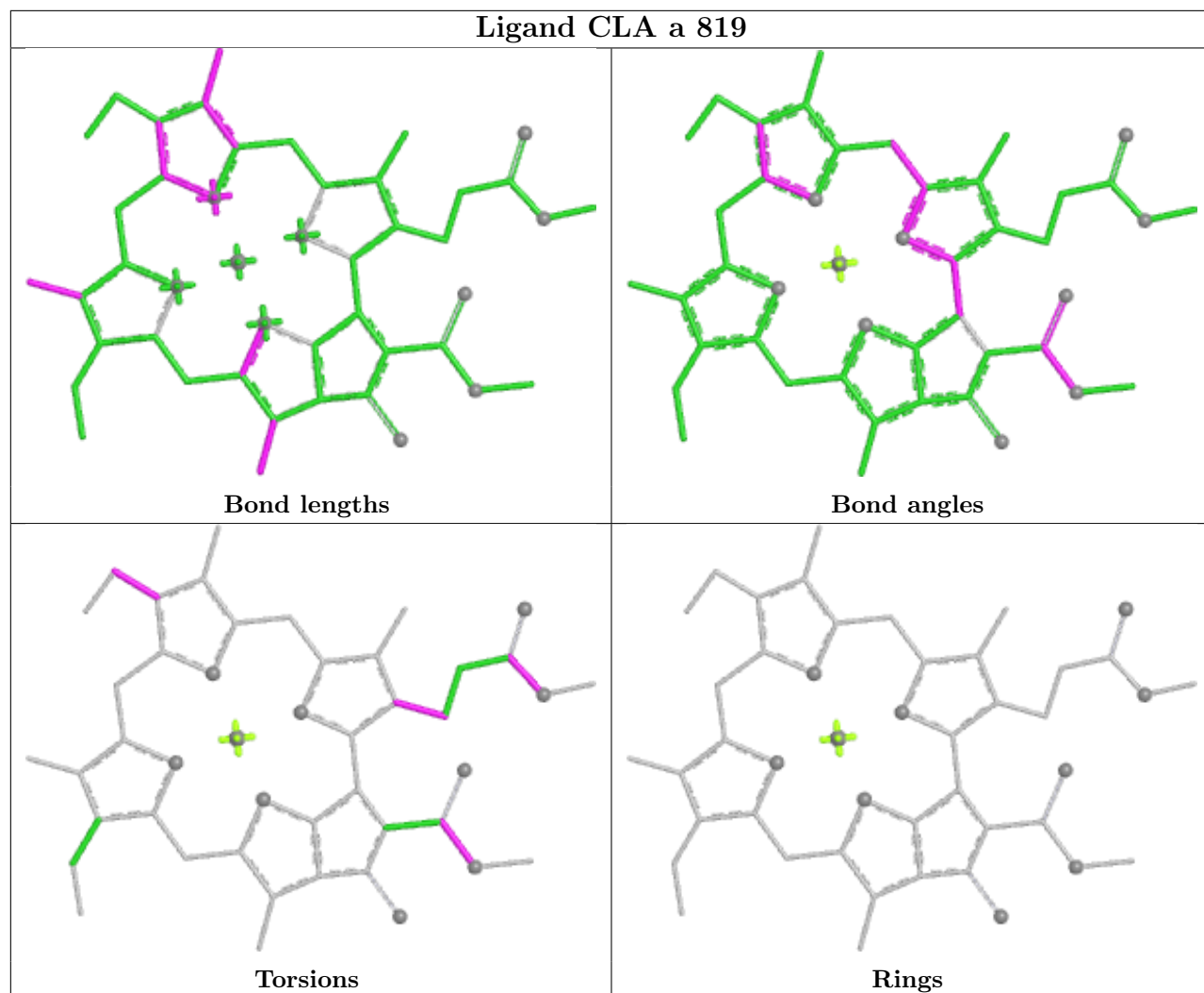


Ligand CLA a 825

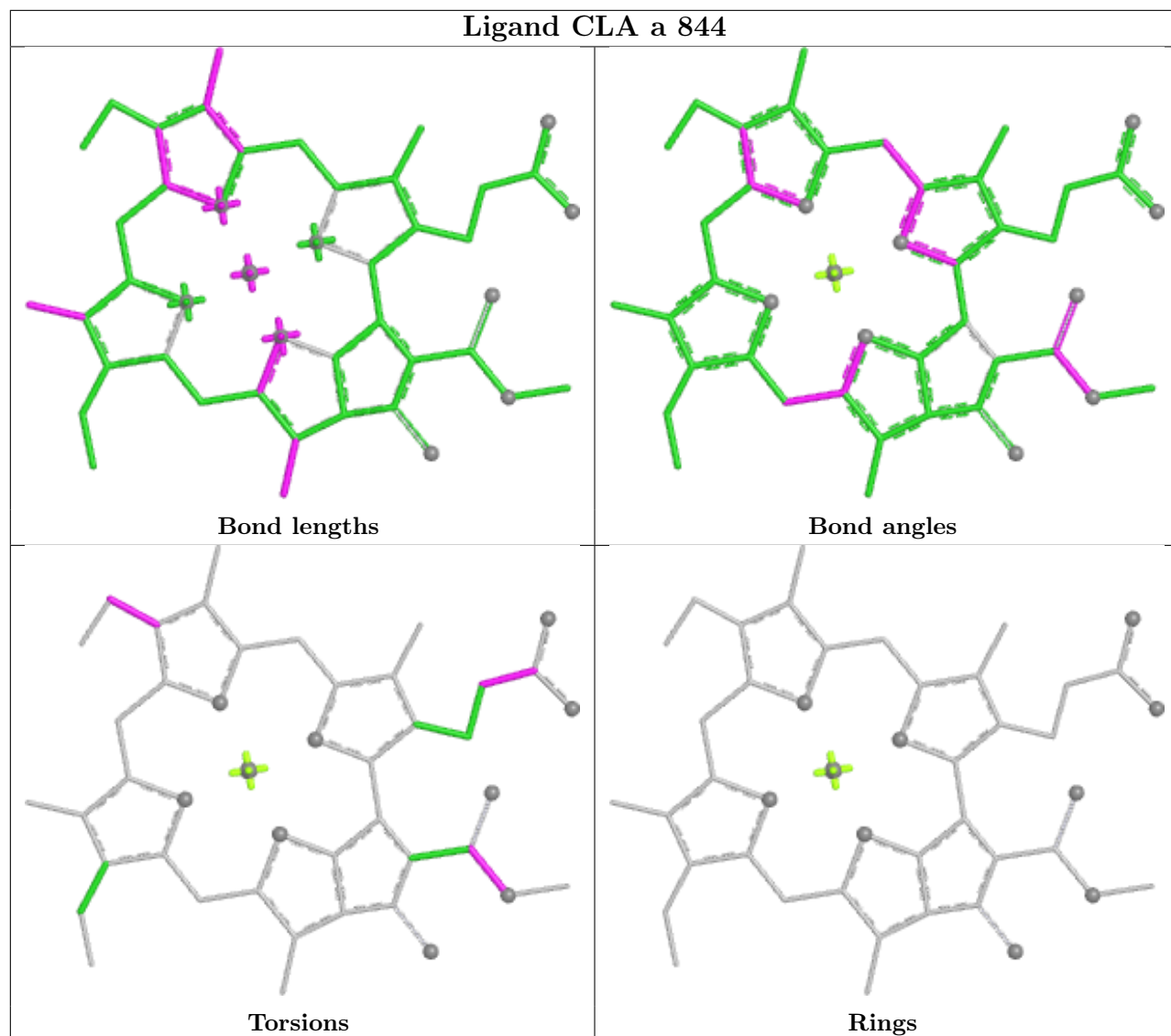




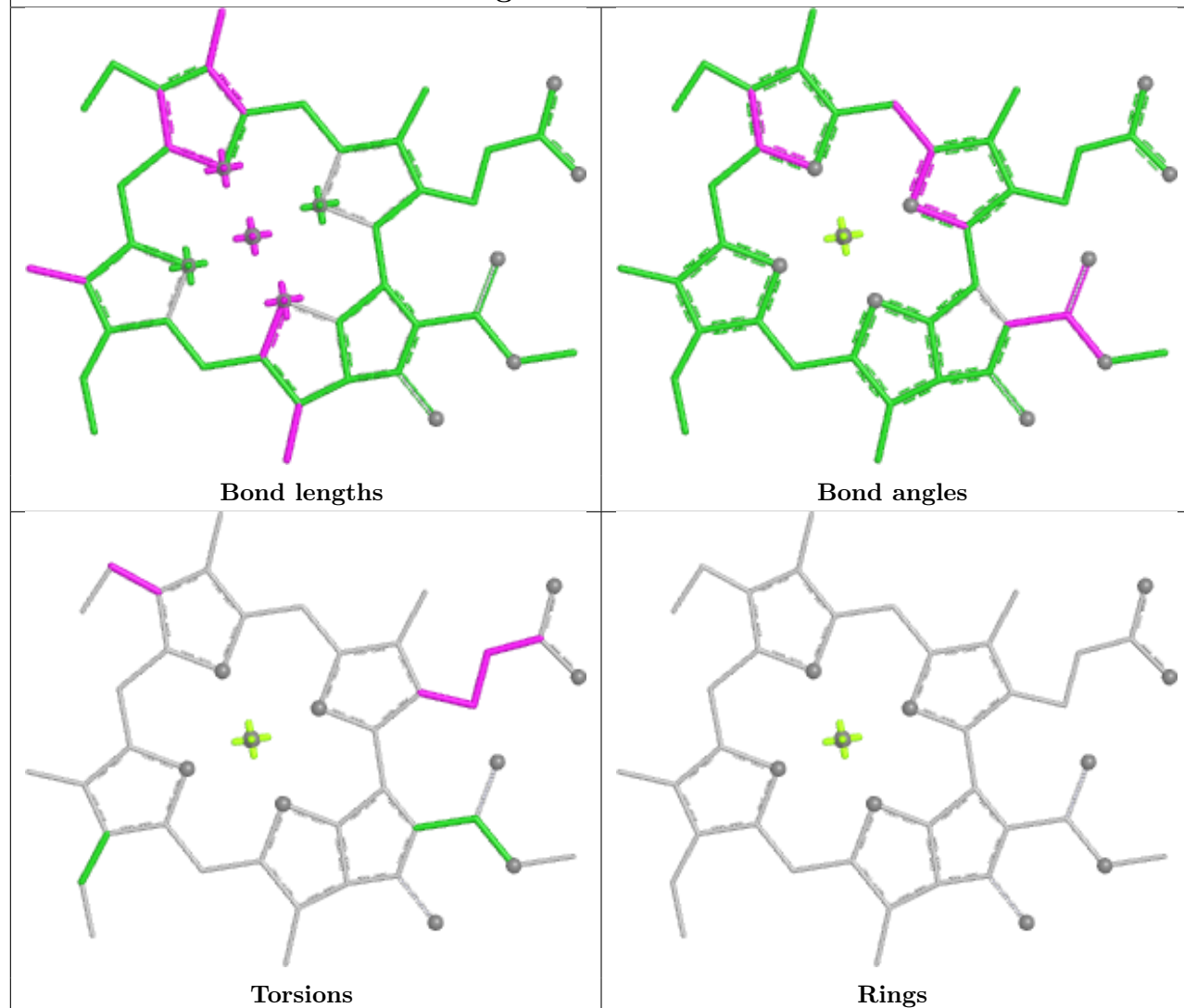
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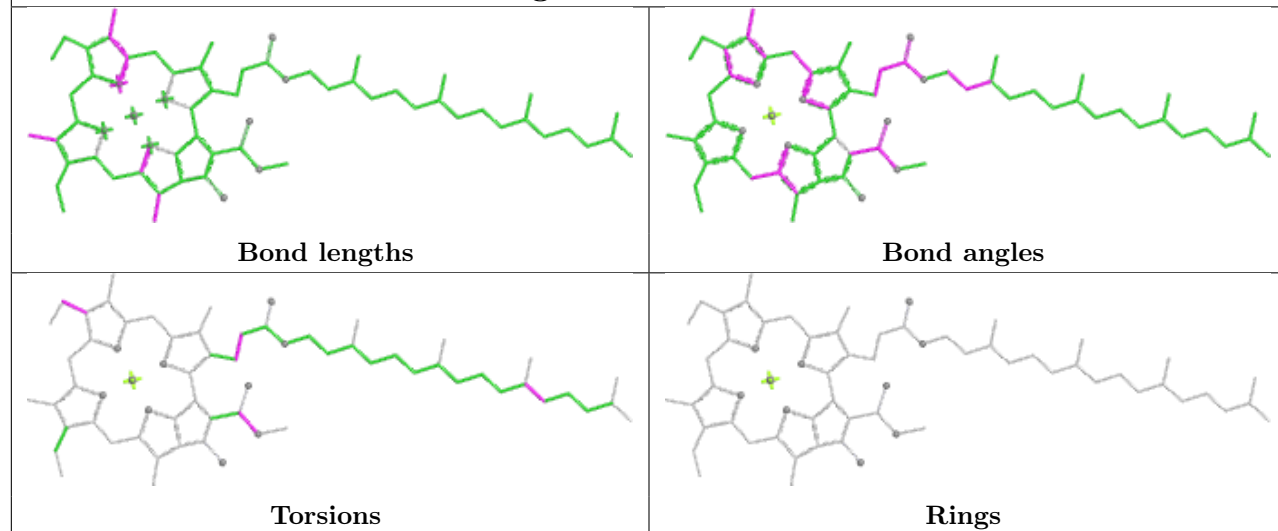
Ligand CLA a 844



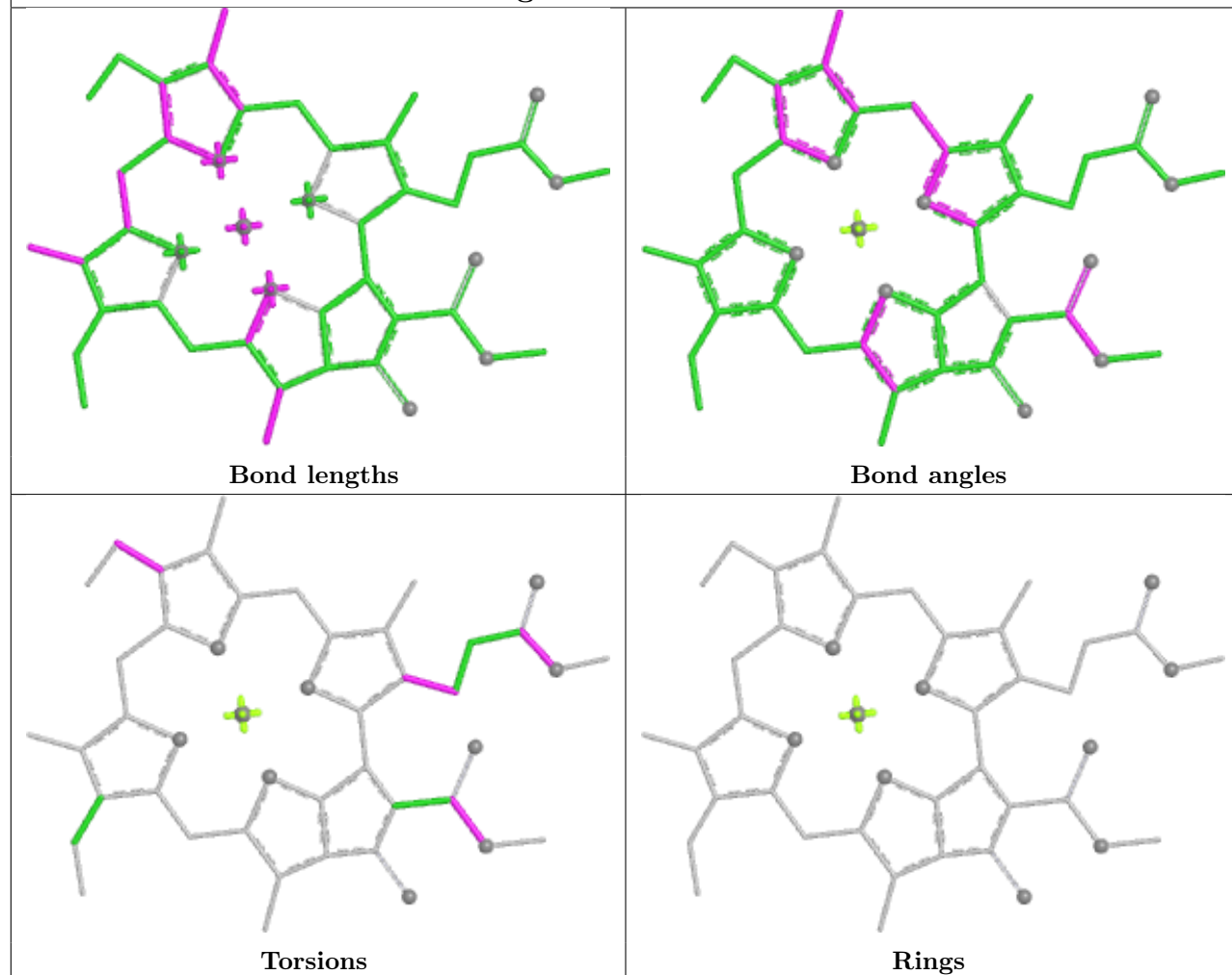
Ligand CLA b 824



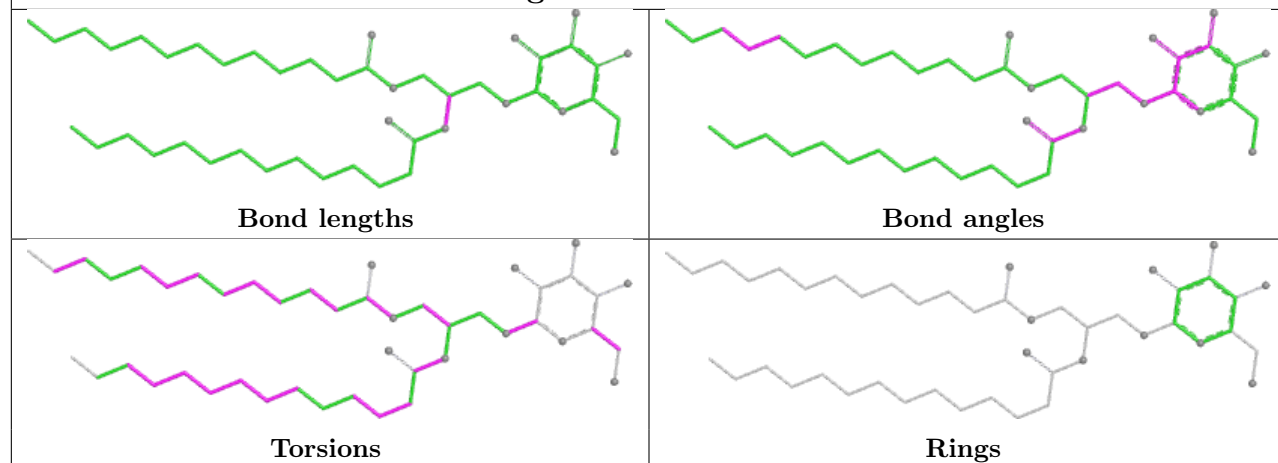
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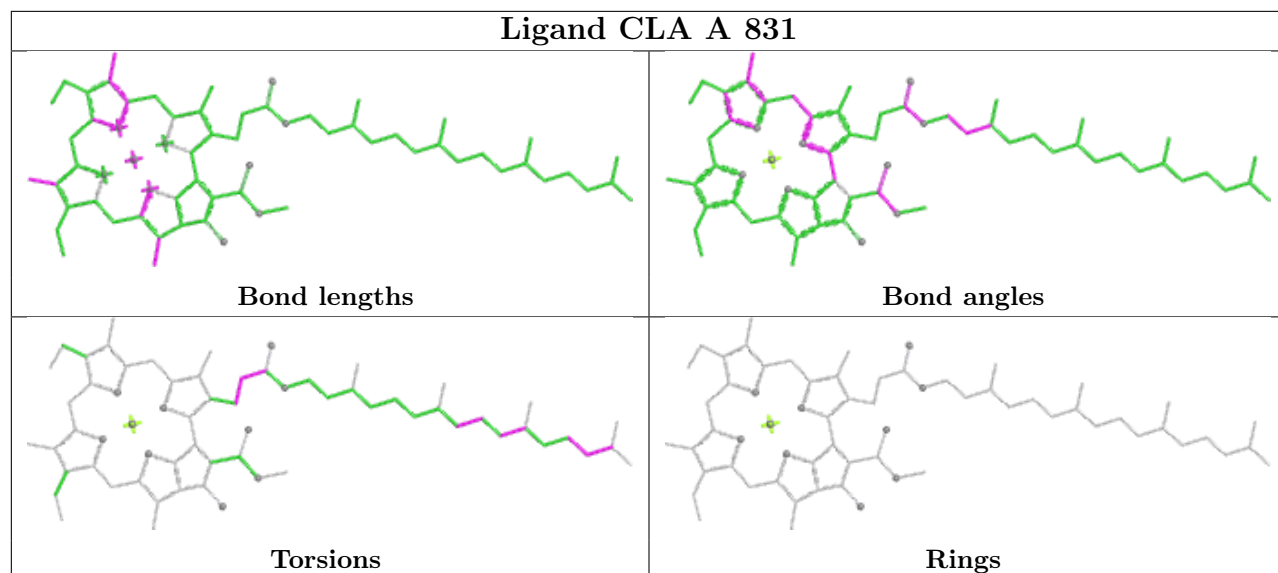
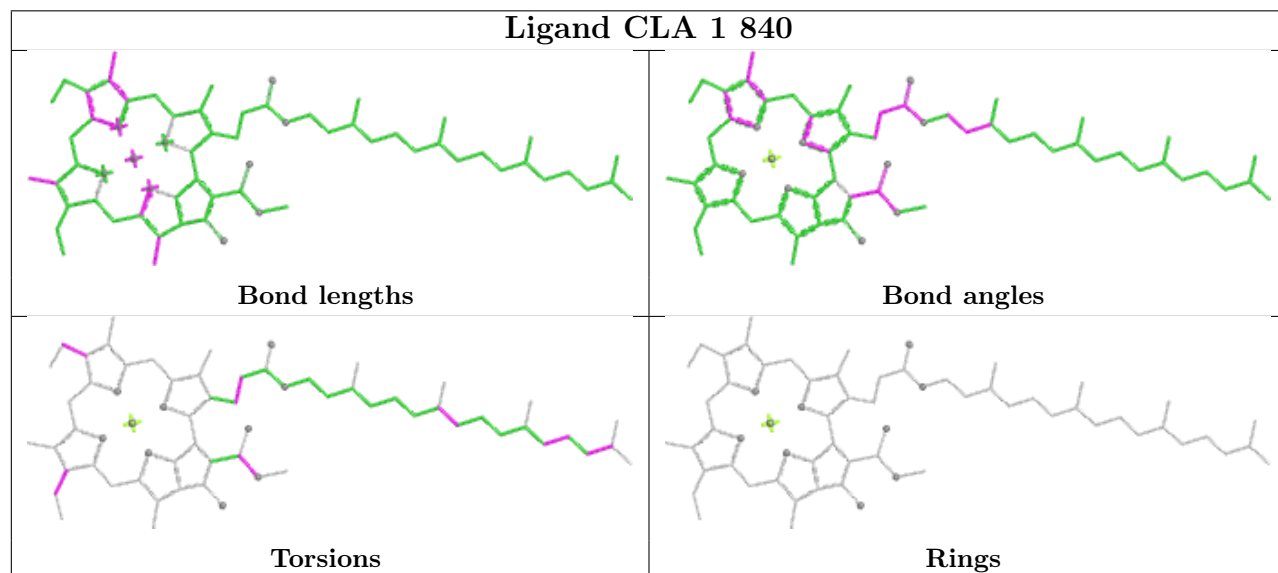
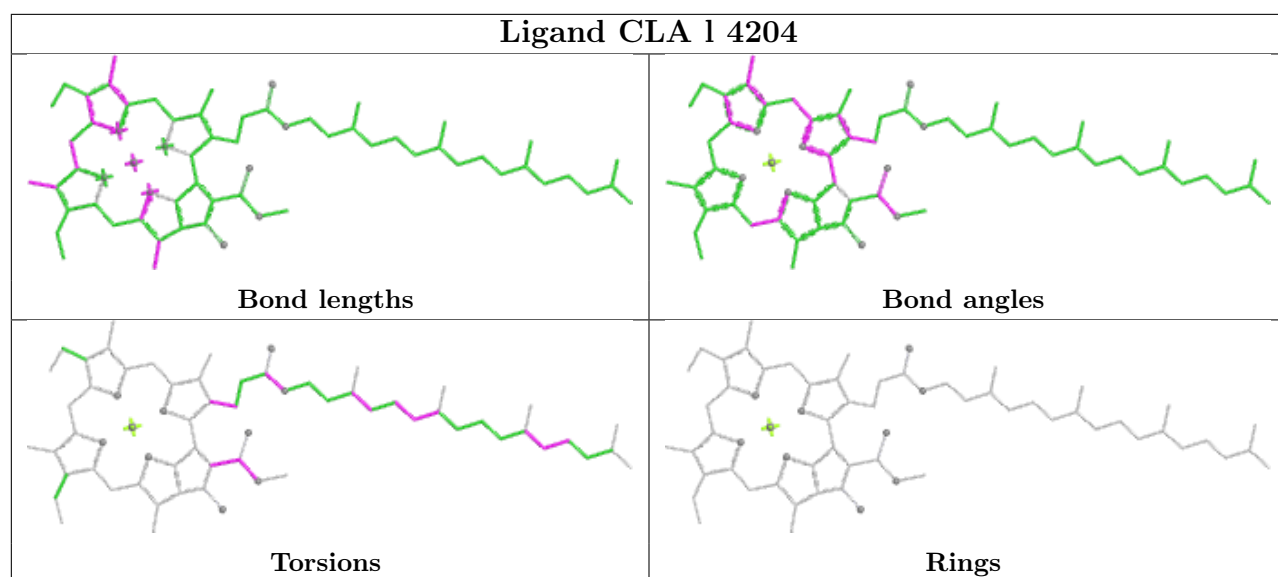


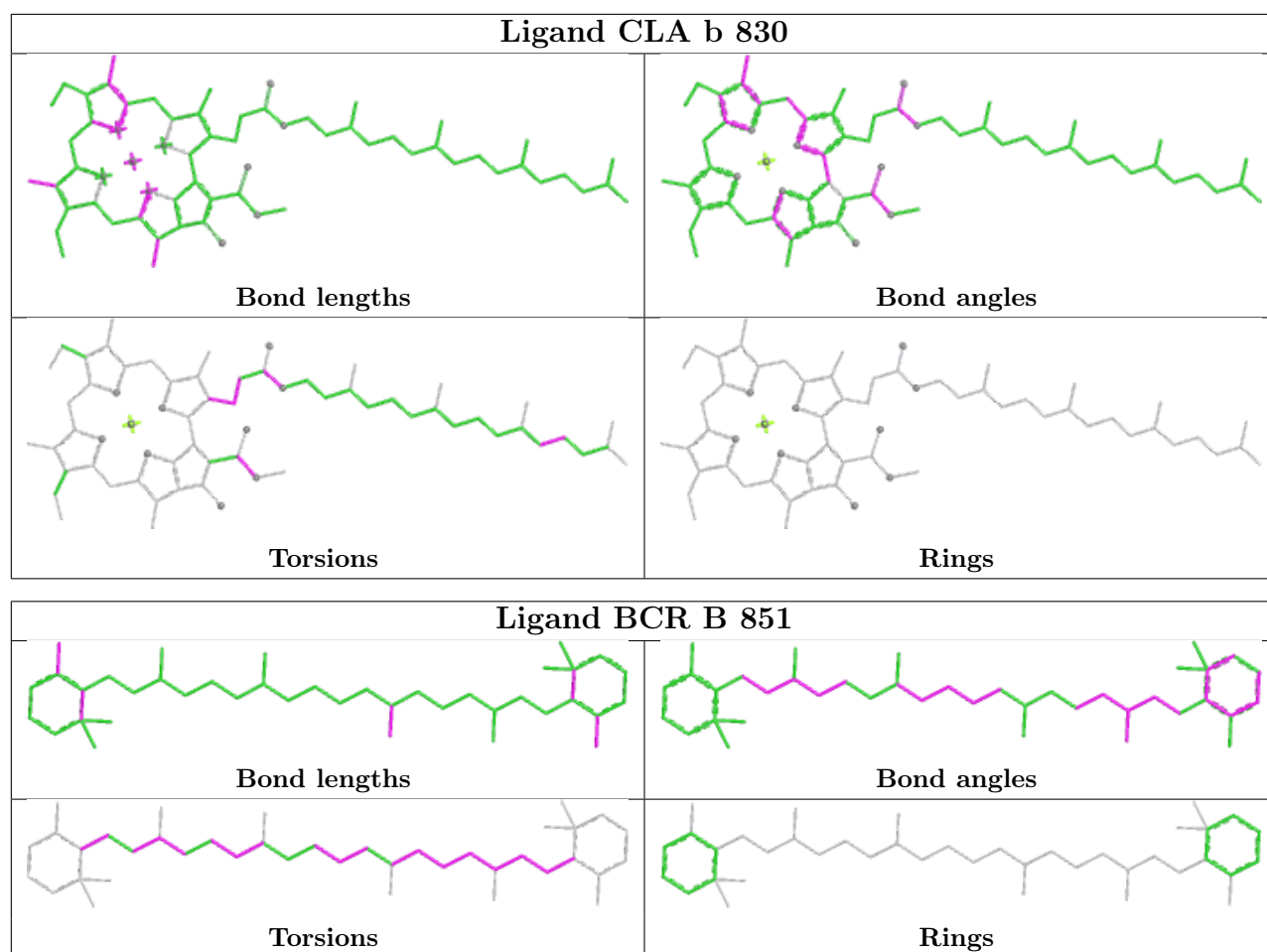
Ligand CLA a 810



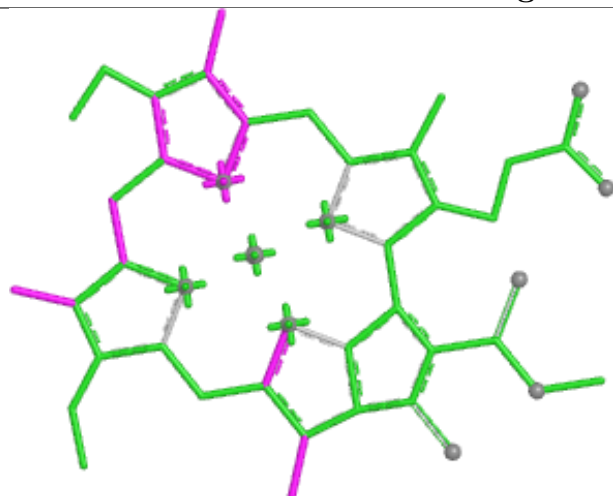
Ligand LMG A 852



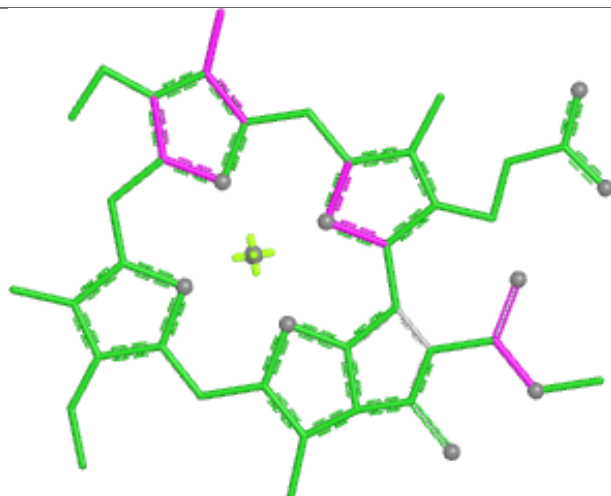




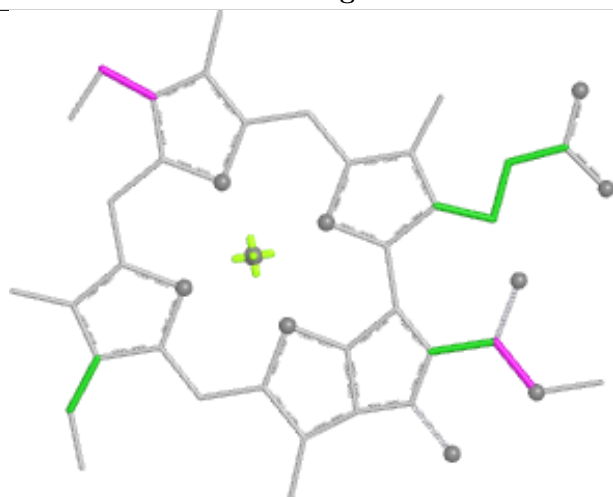
Ligand CLA b 817



Bond lengths



Bond angles

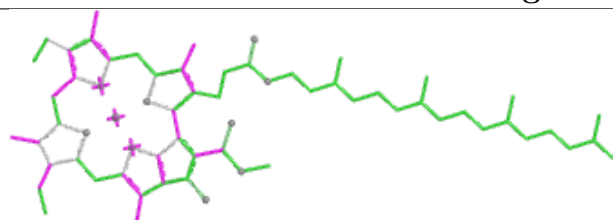


Torsions

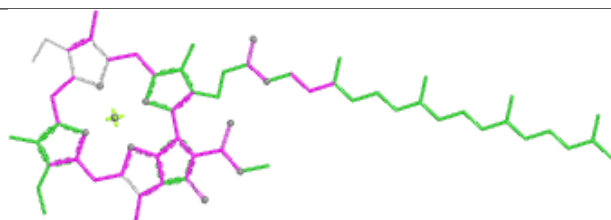


Rings

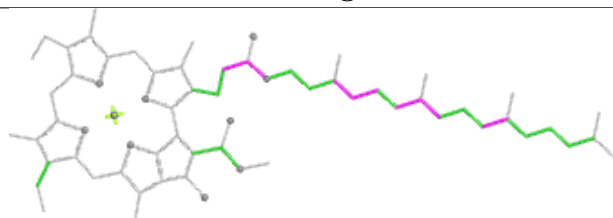
Ligand CL0 1 803



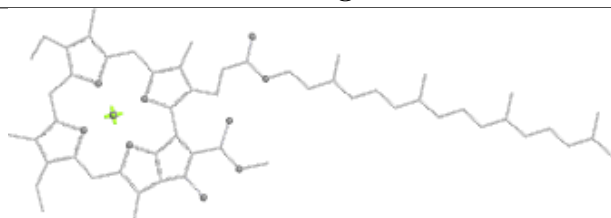
Bond lengths



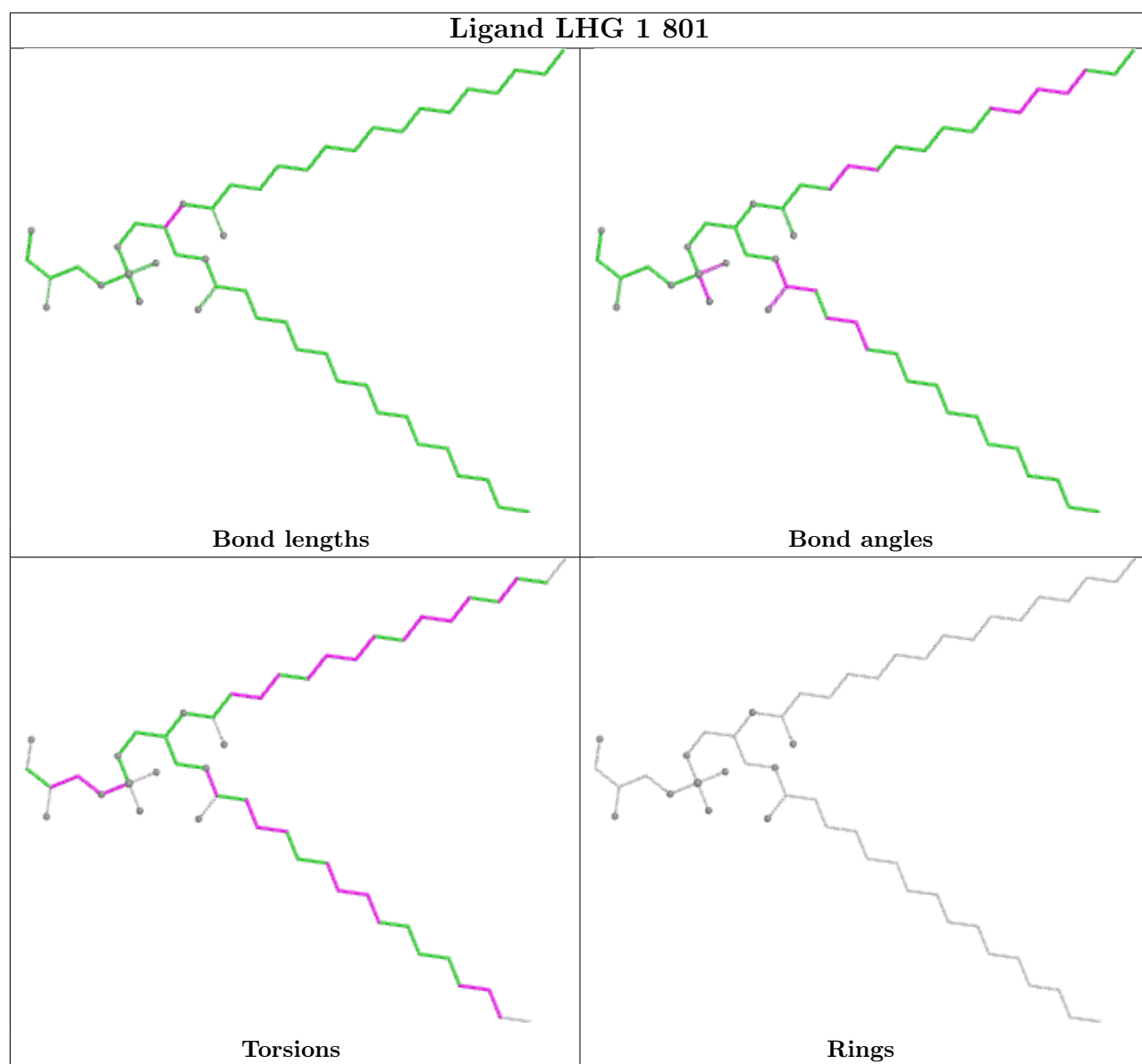
Bond angles



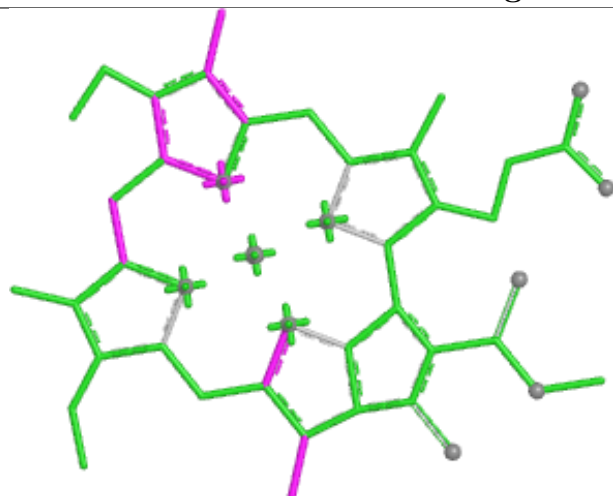
Torsions



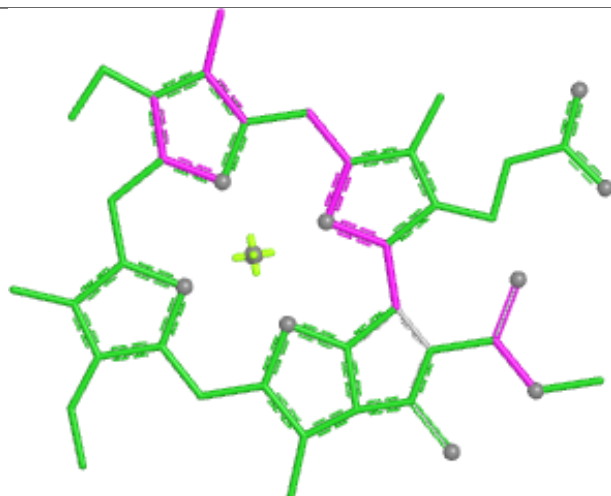
Rings



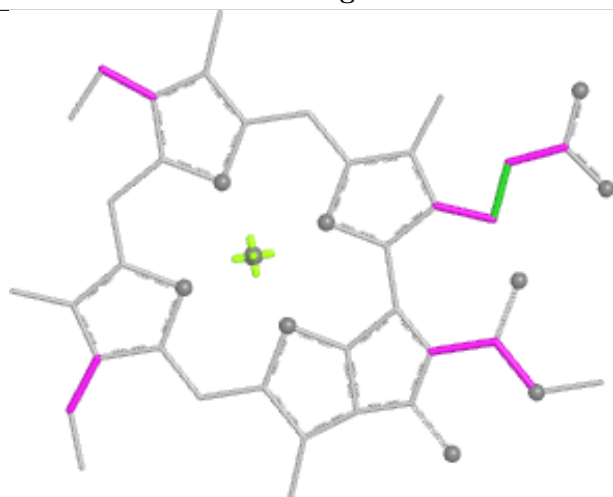
Ligand CLA K 4003



Bond lengths



Bond angles

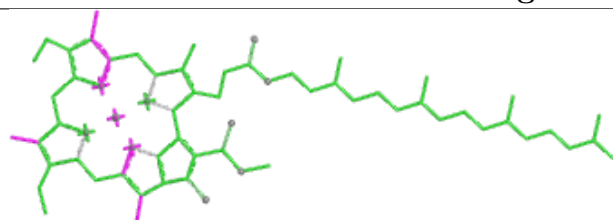


Torsions

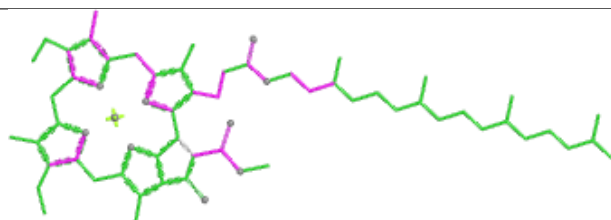


Rings

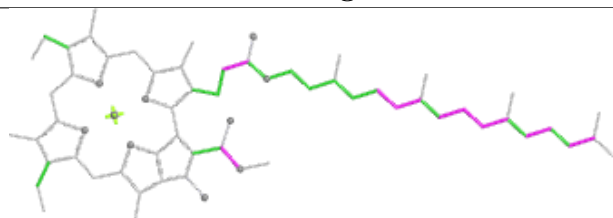
Ligand CLA b 805



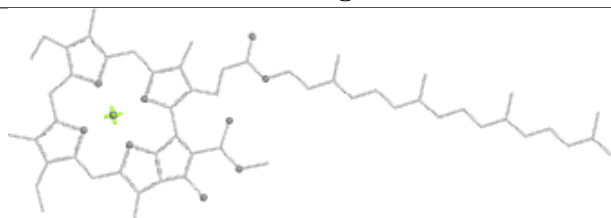
Bond lengths



Bond angles

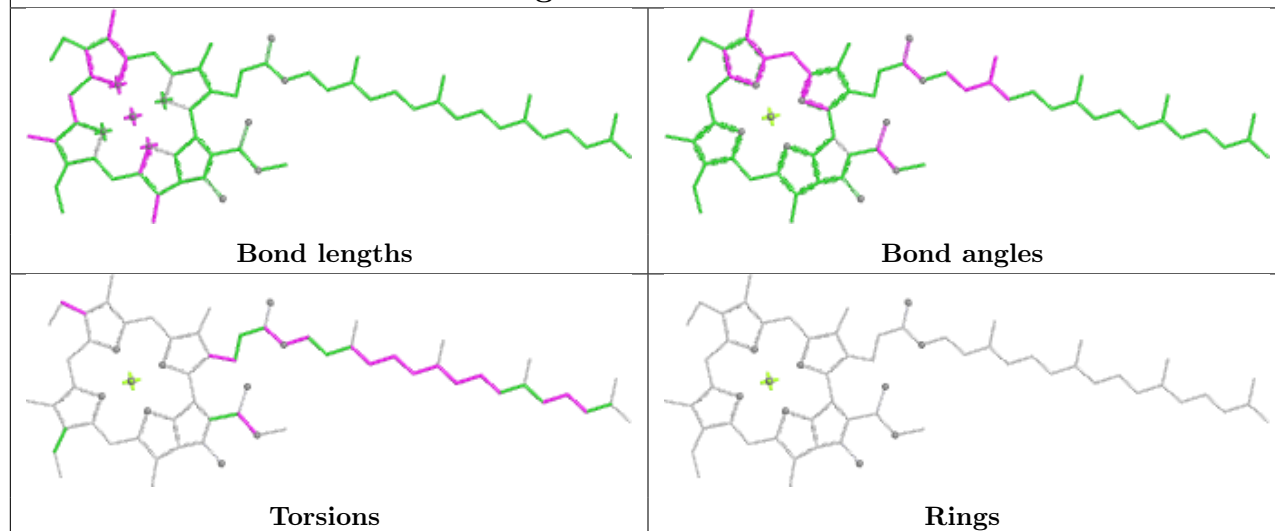


Torsions

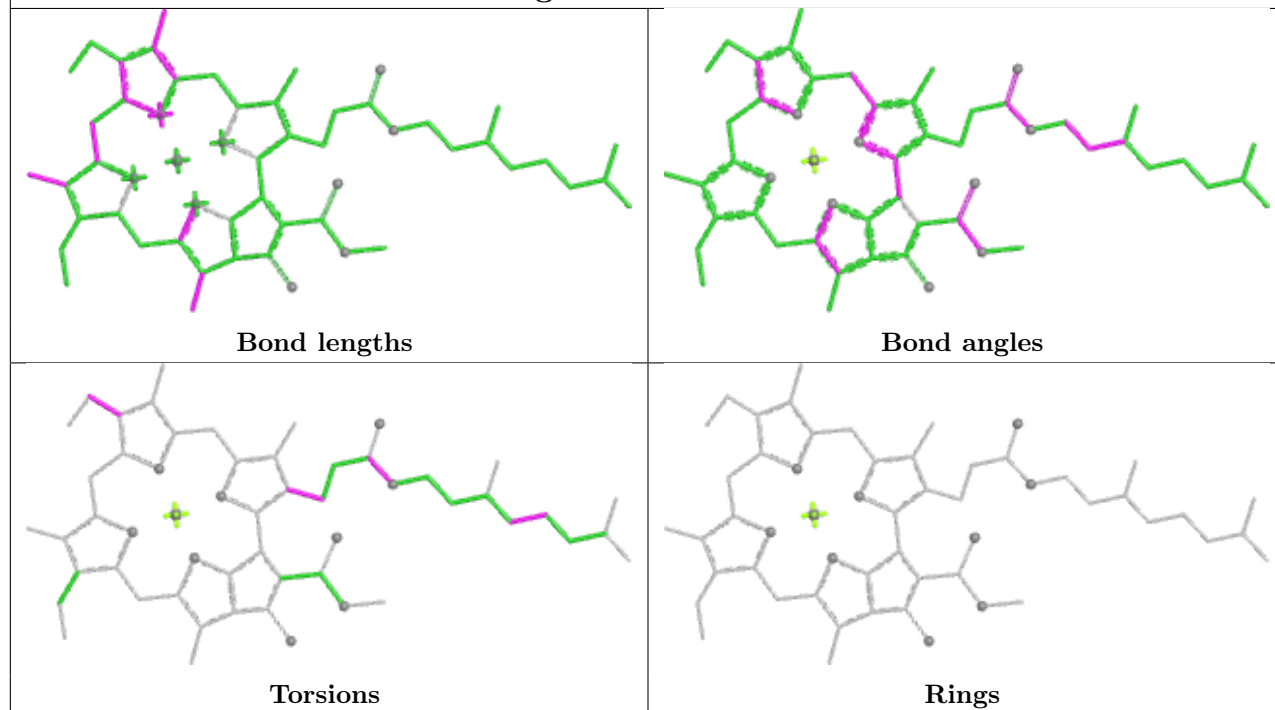


Rings

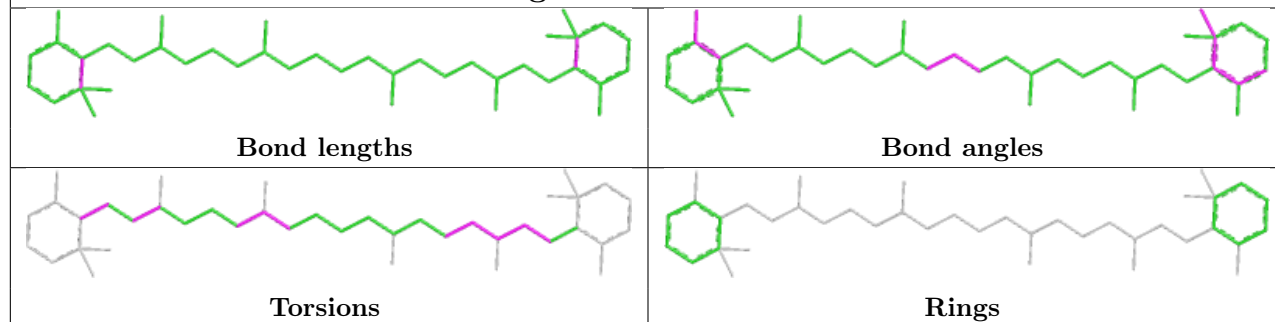
Ligand CLA 1 812



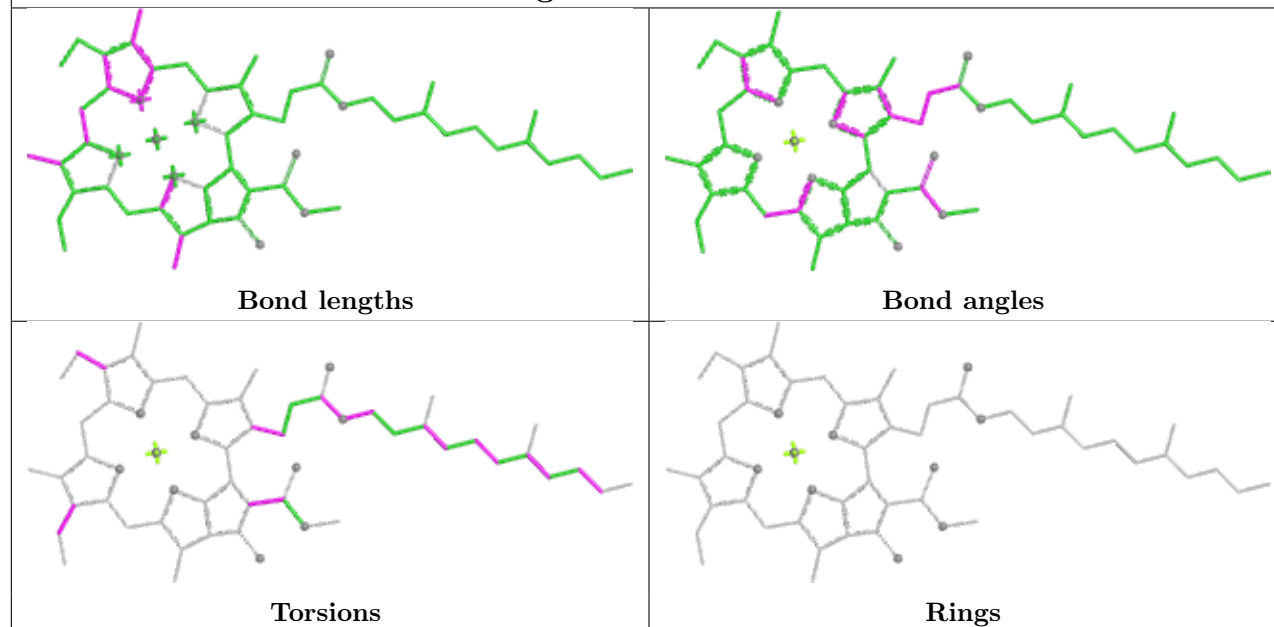
Ligand CLA a 854



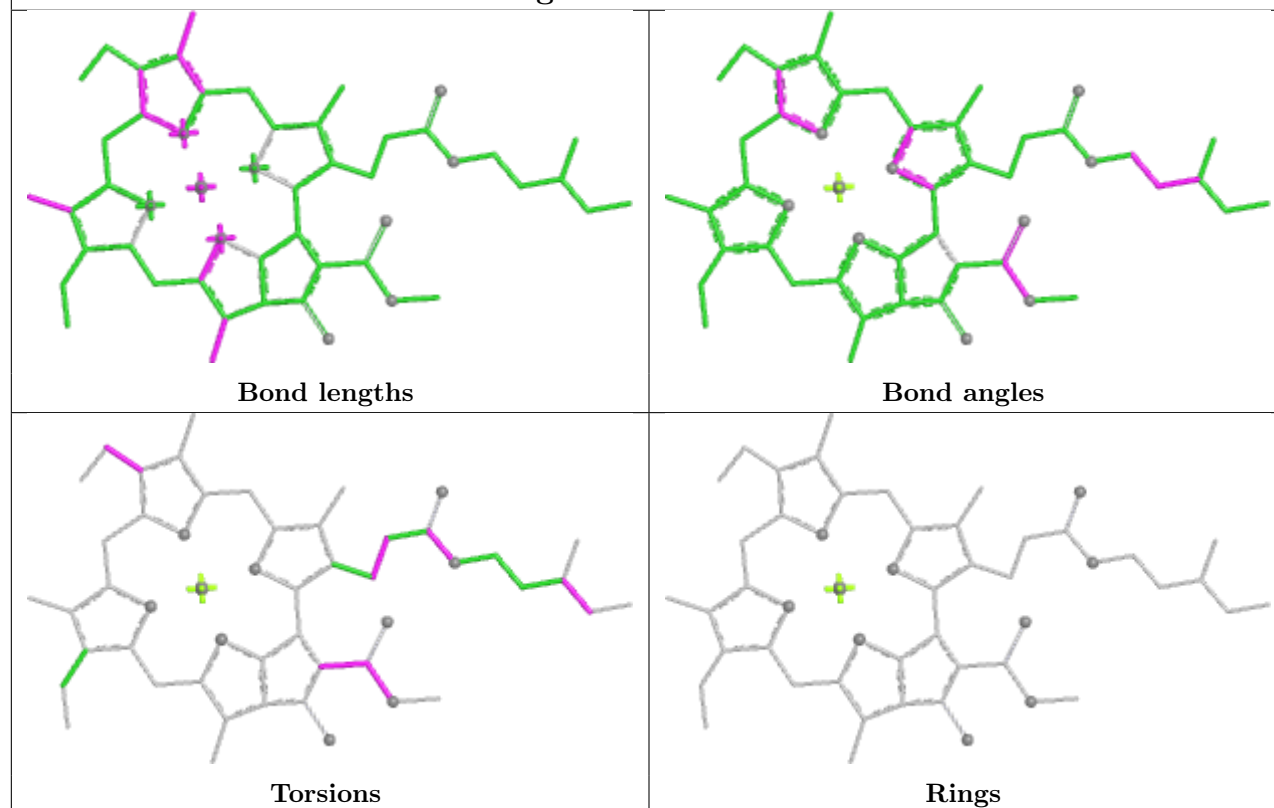
Ligand BCR A 848

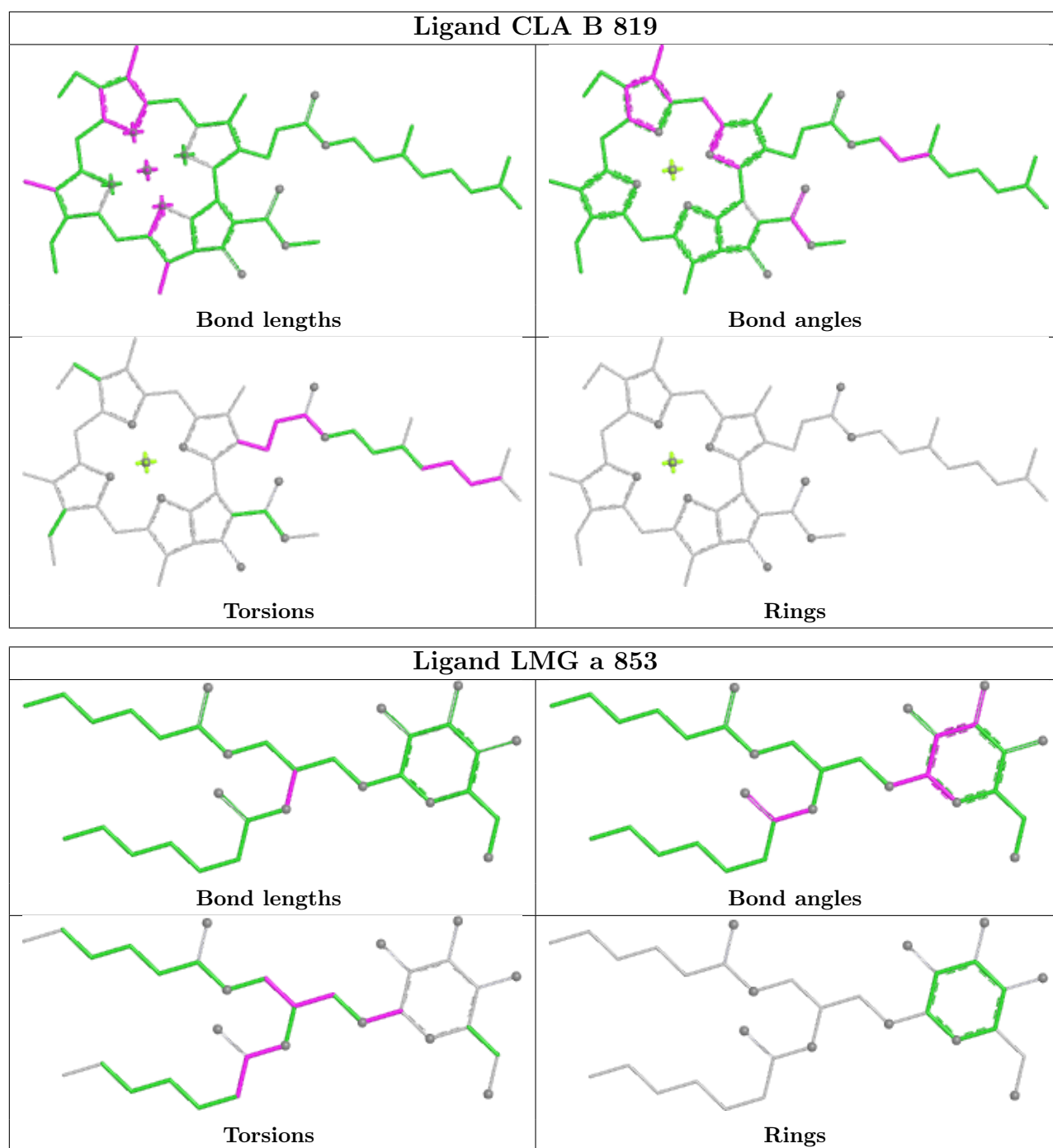


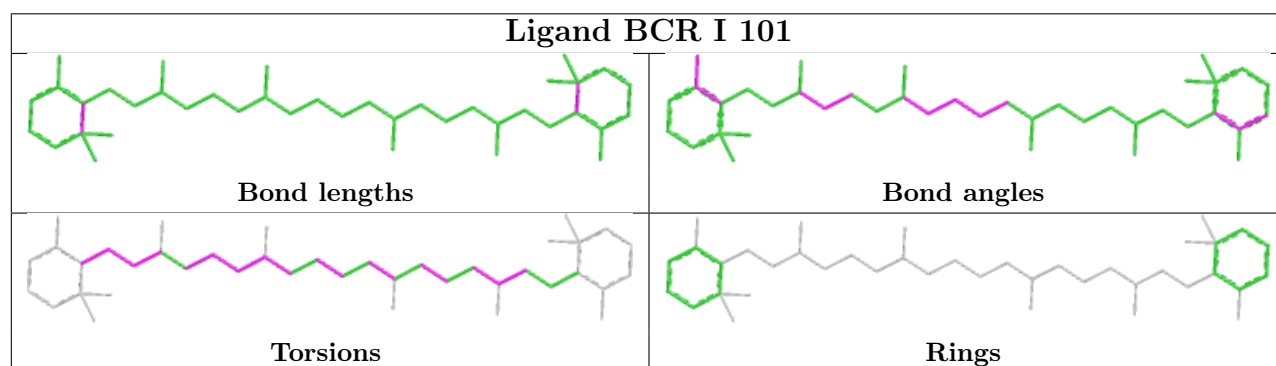
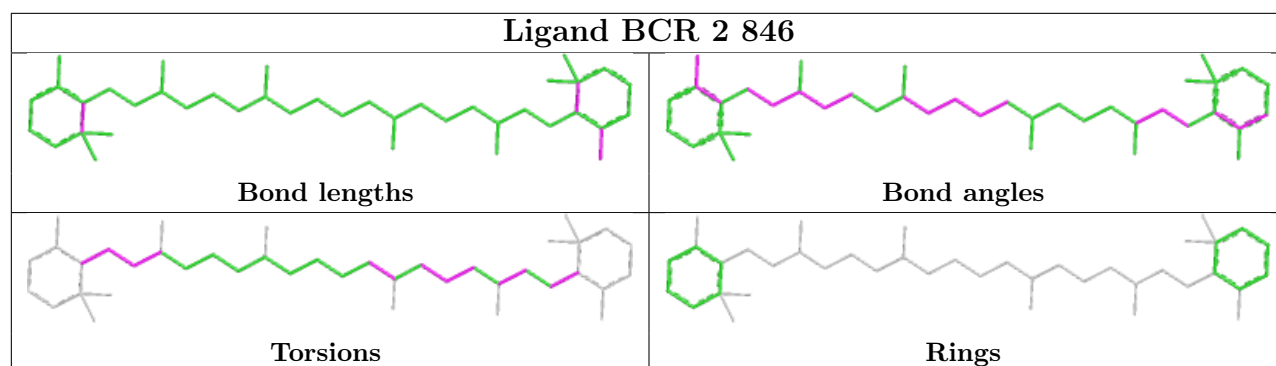
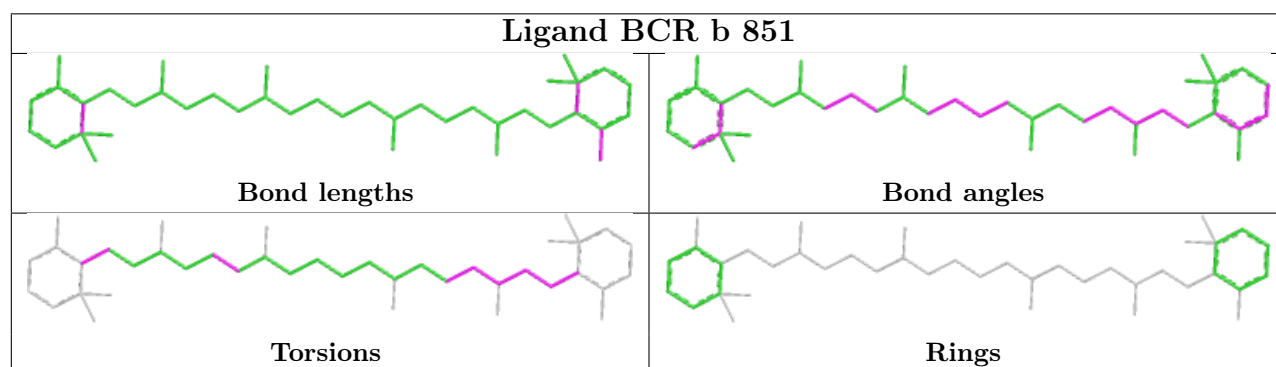
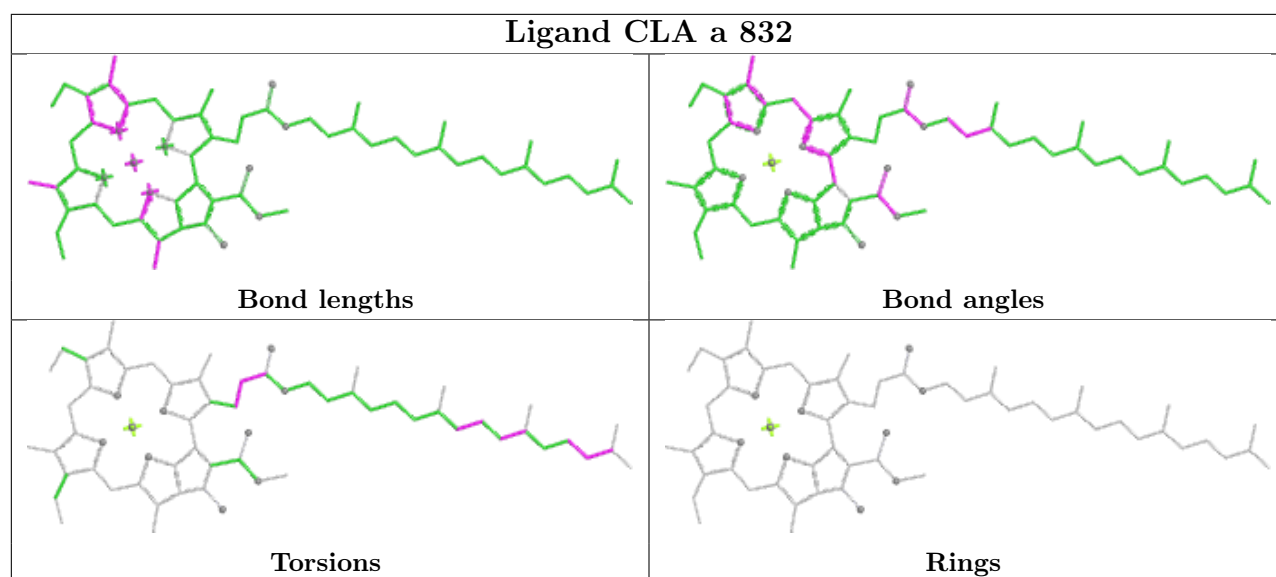
Ligand CLA 2 834



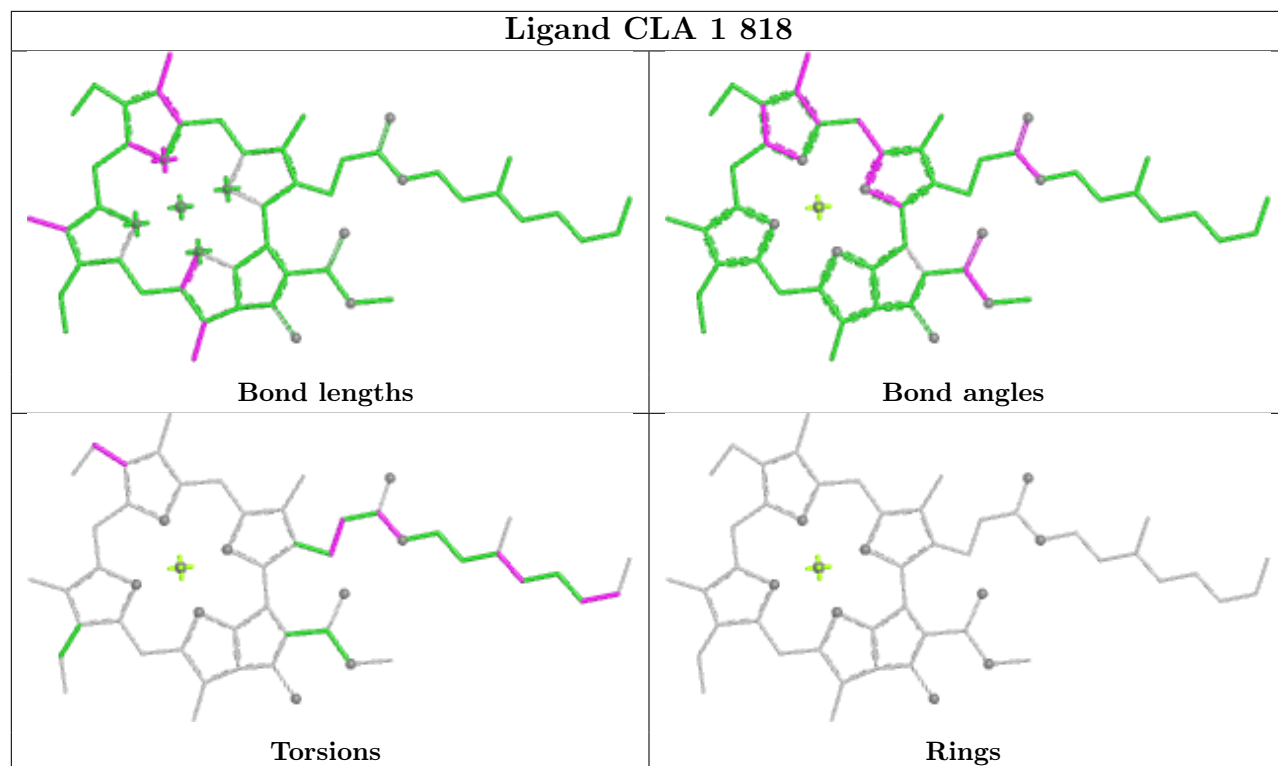
Ligand CLA 1 824



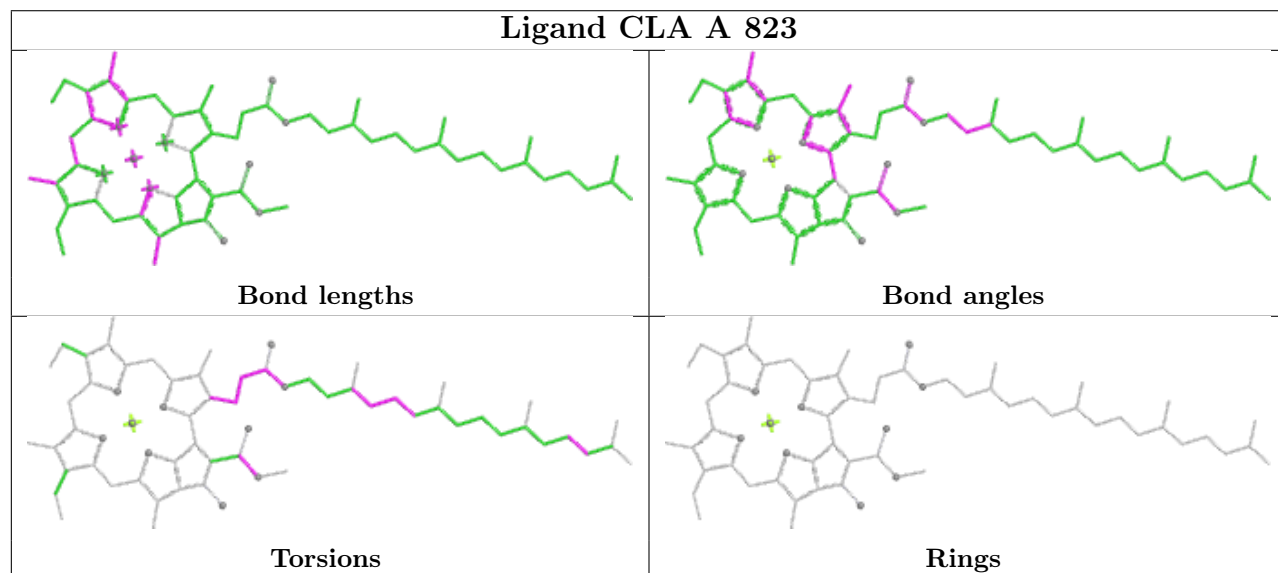


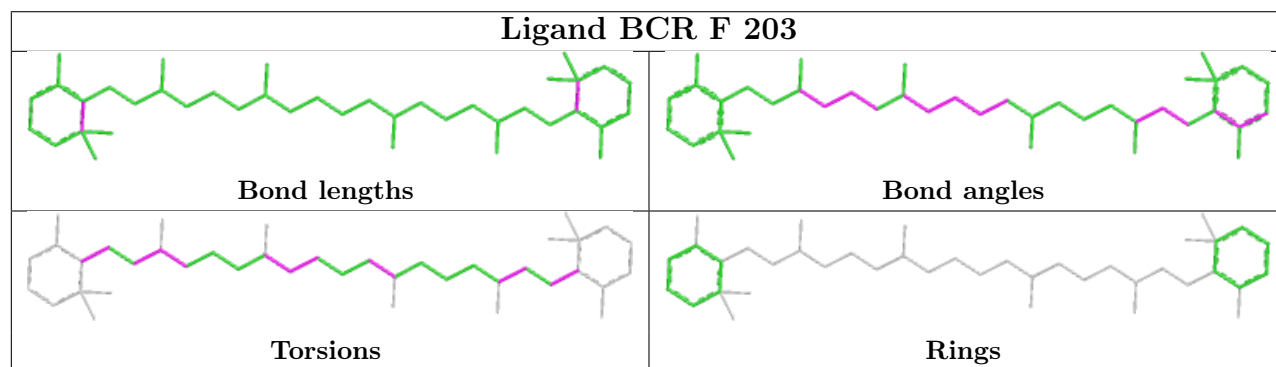
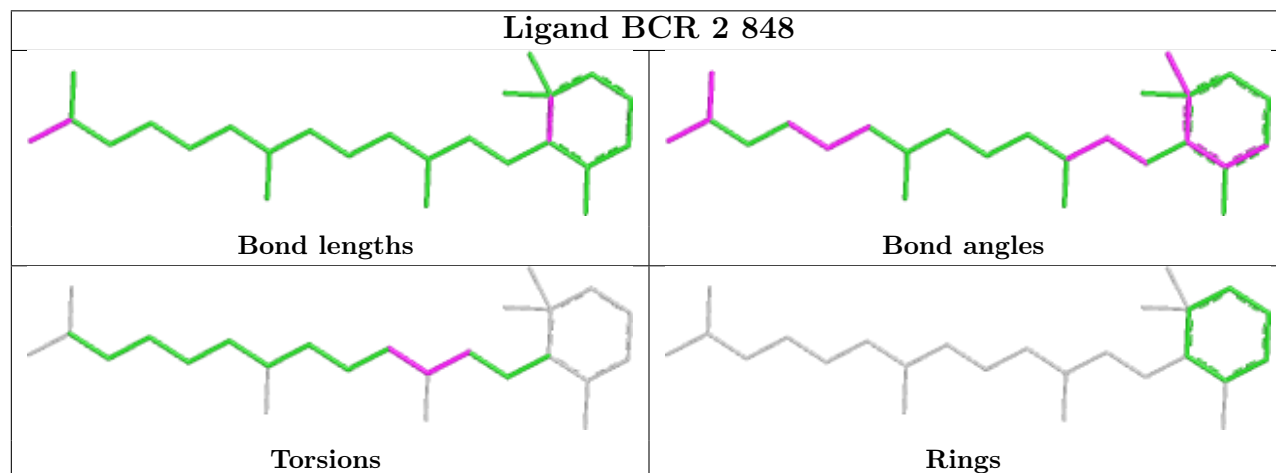
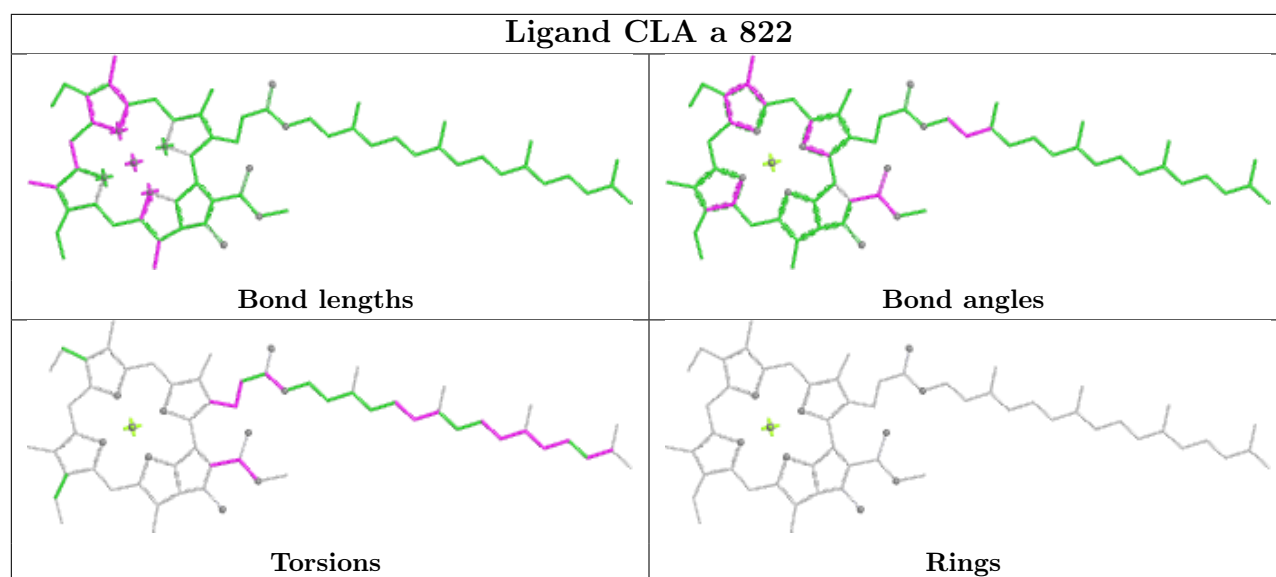


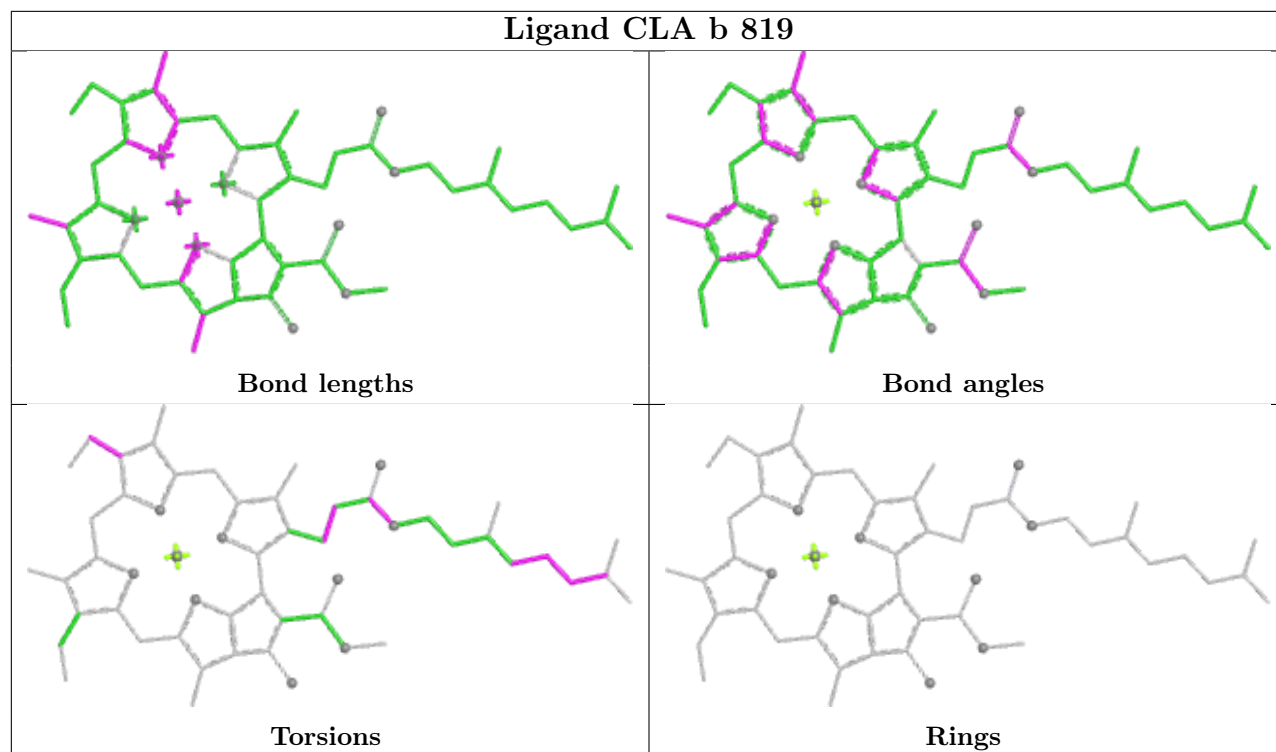
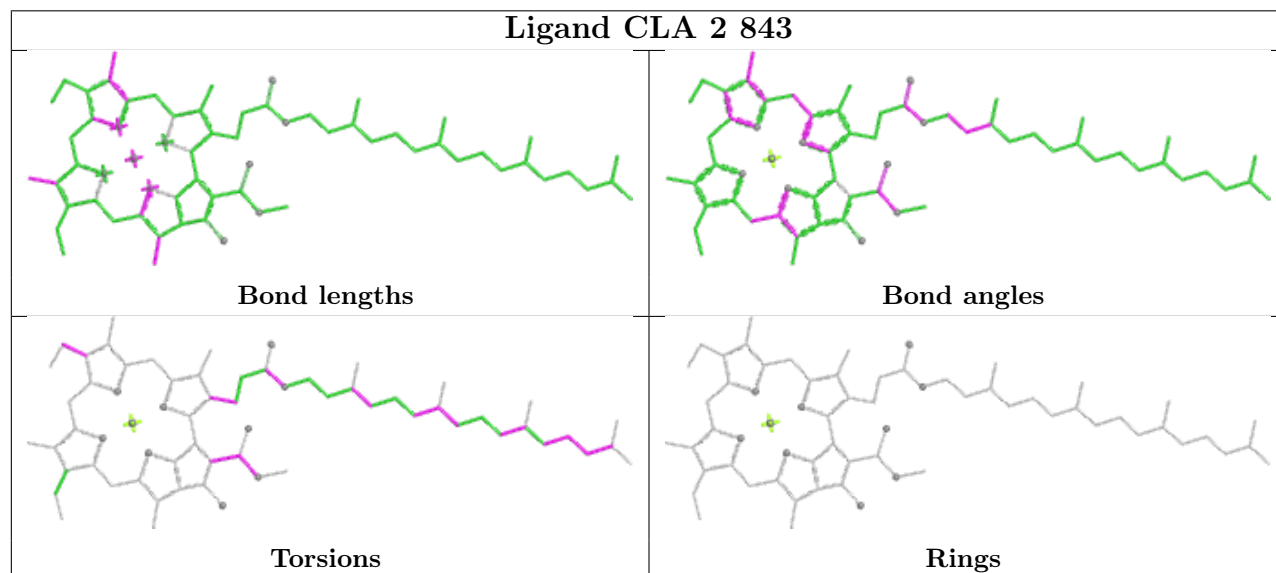
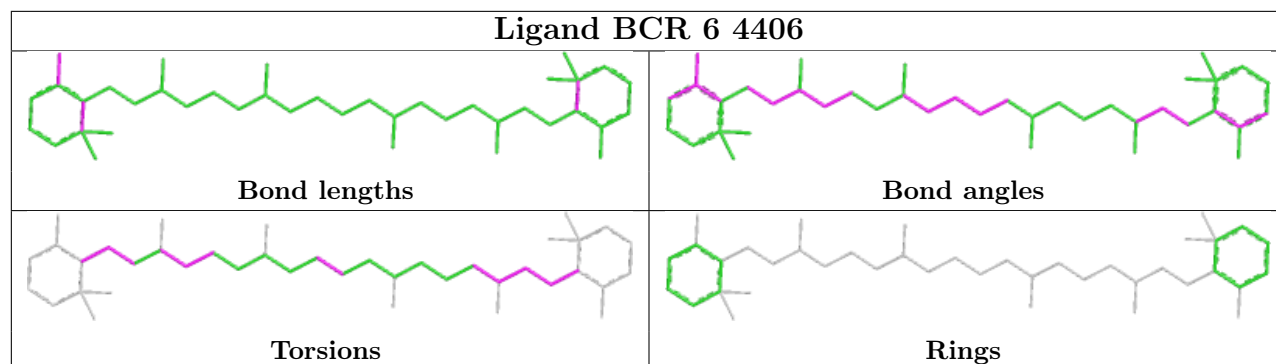
Ligand CLA 1 818

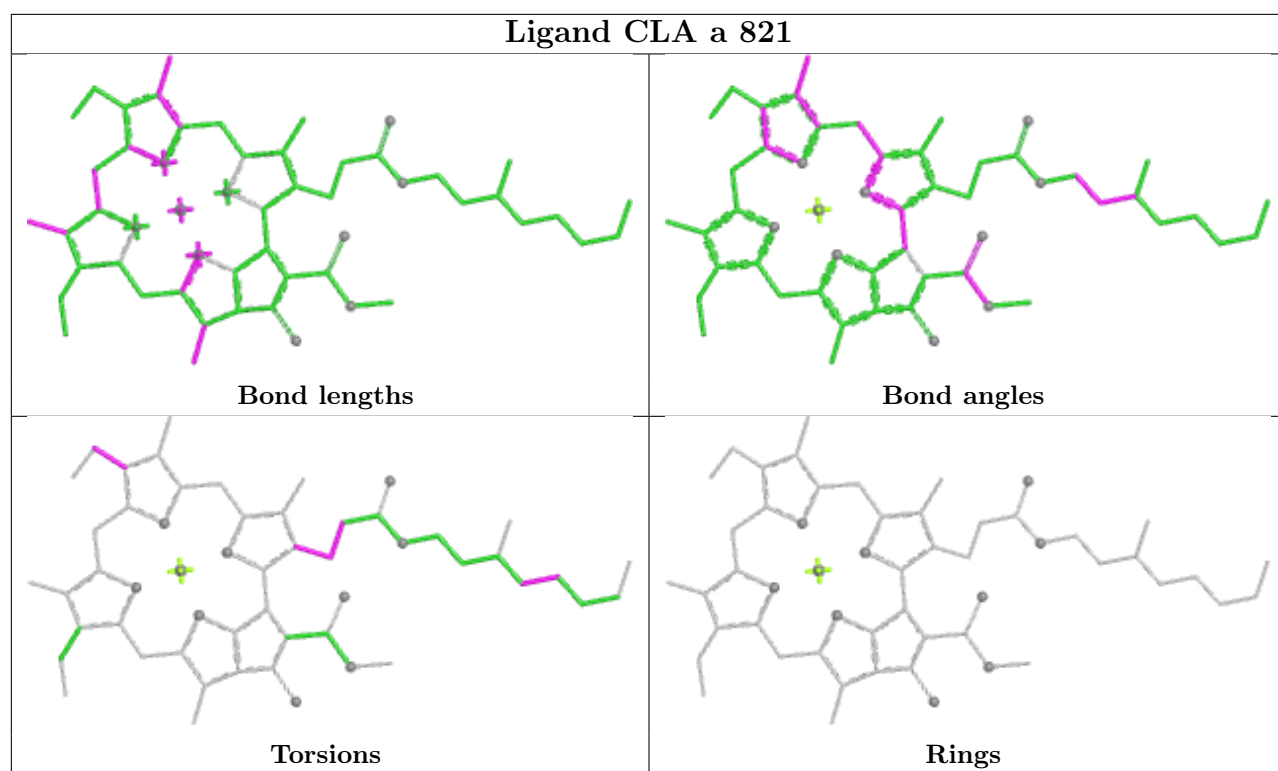


Ligand CLA A 823

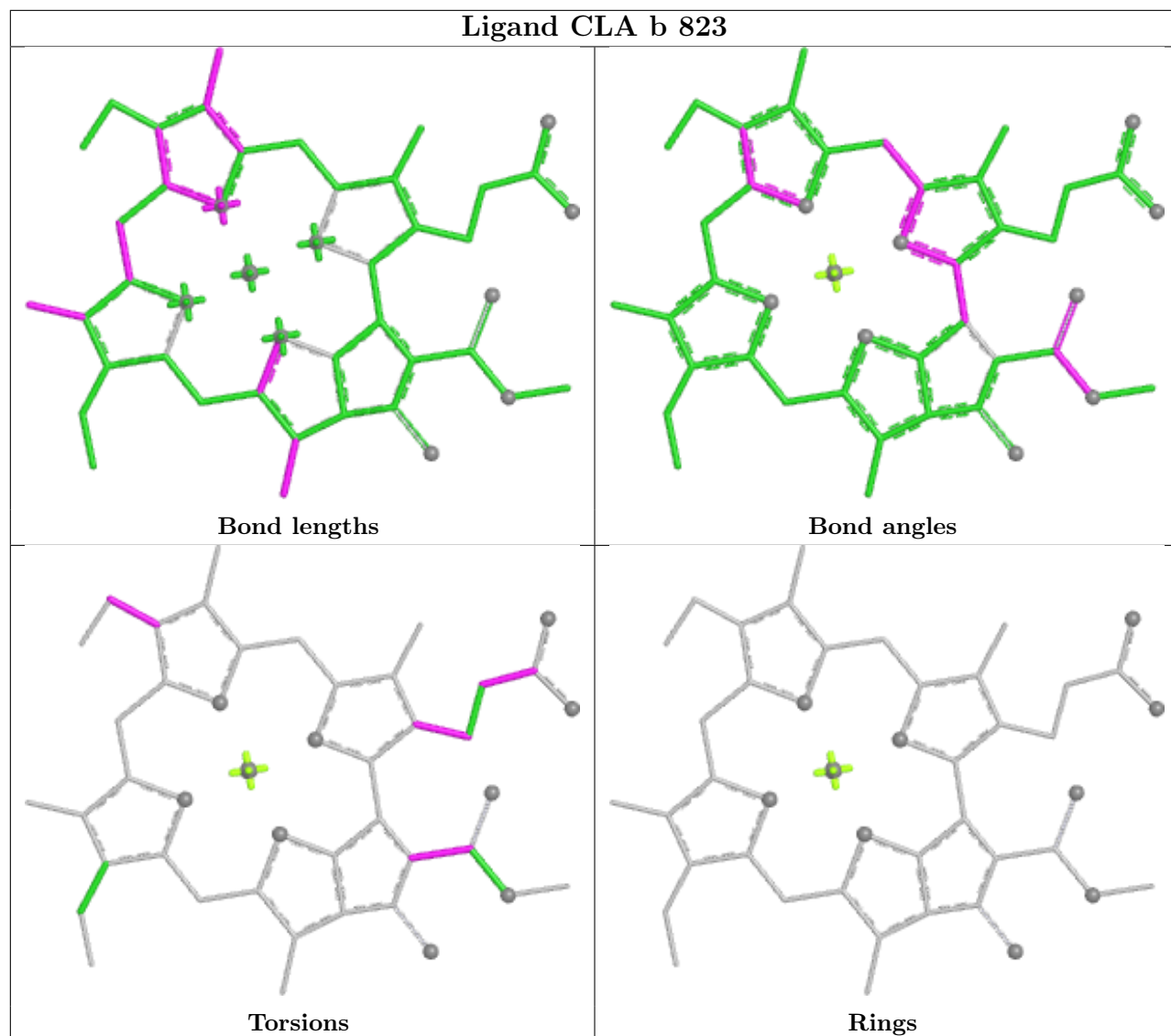




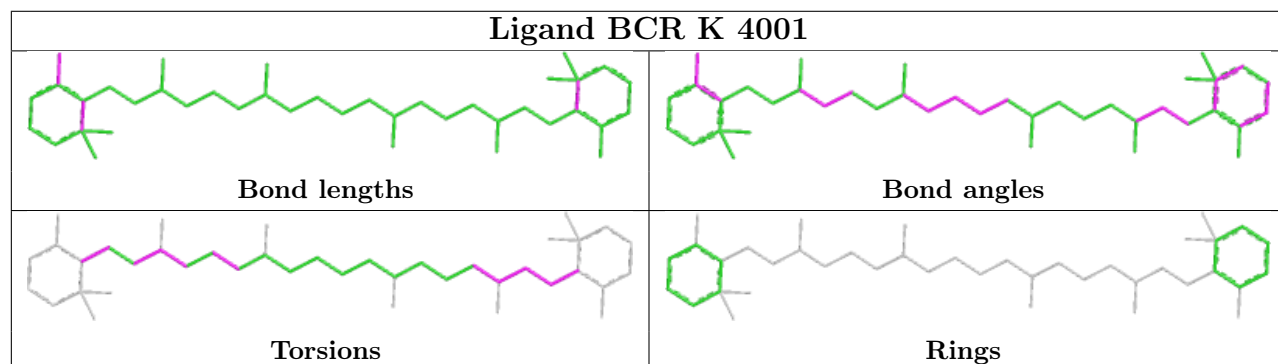




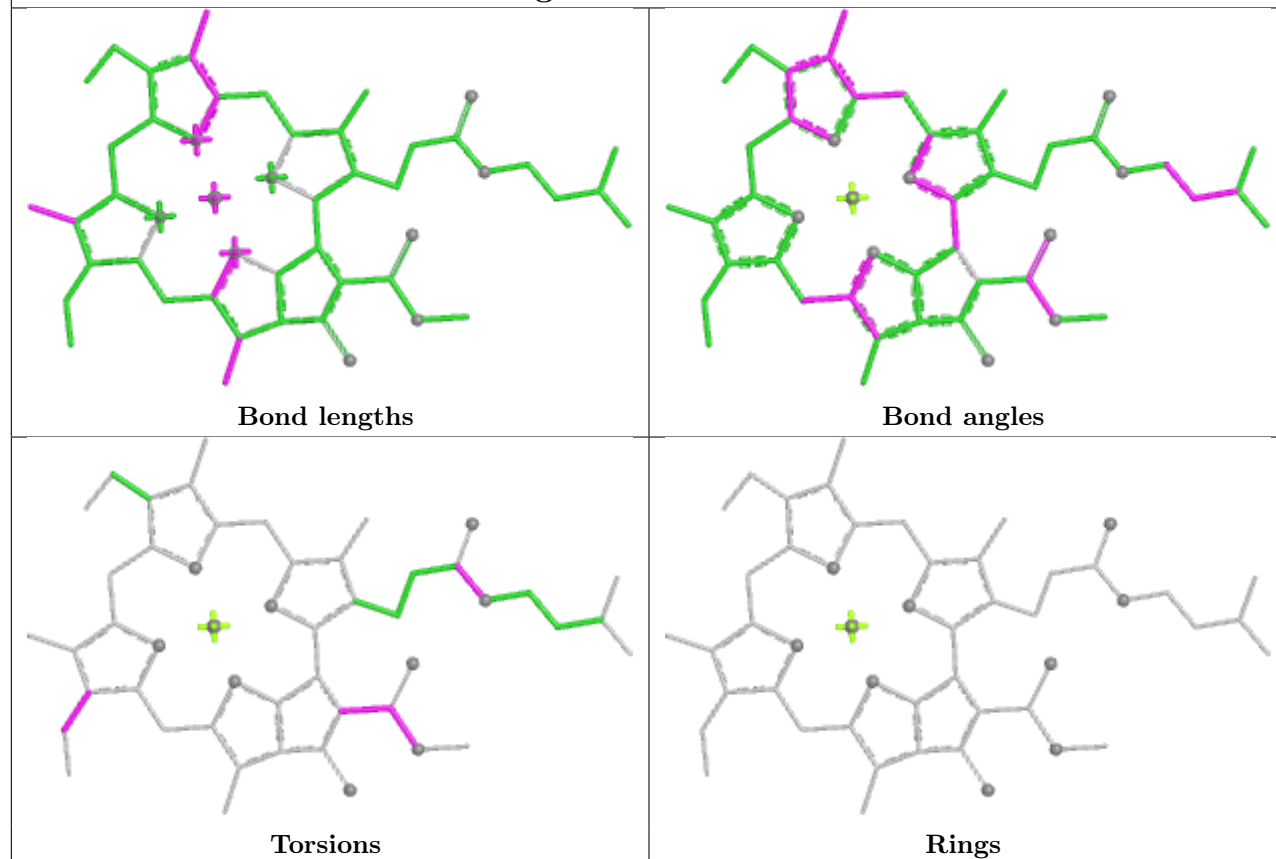
Ligand CLA b 823



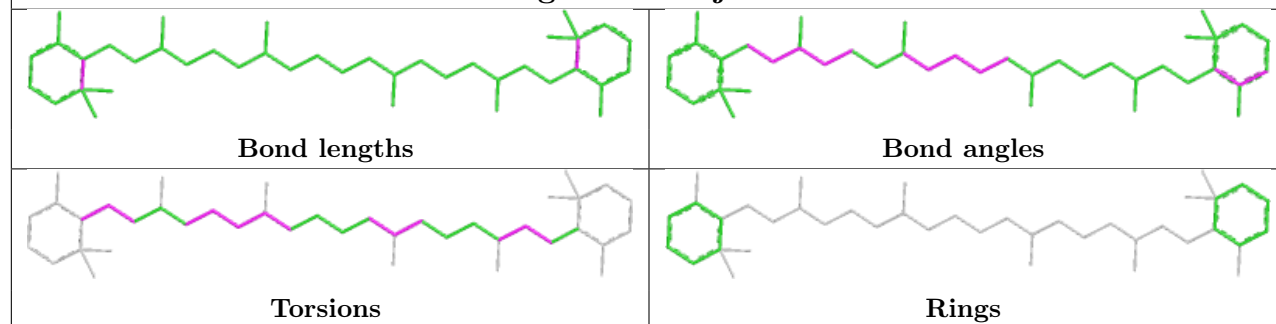
Ligand BCR K 4001

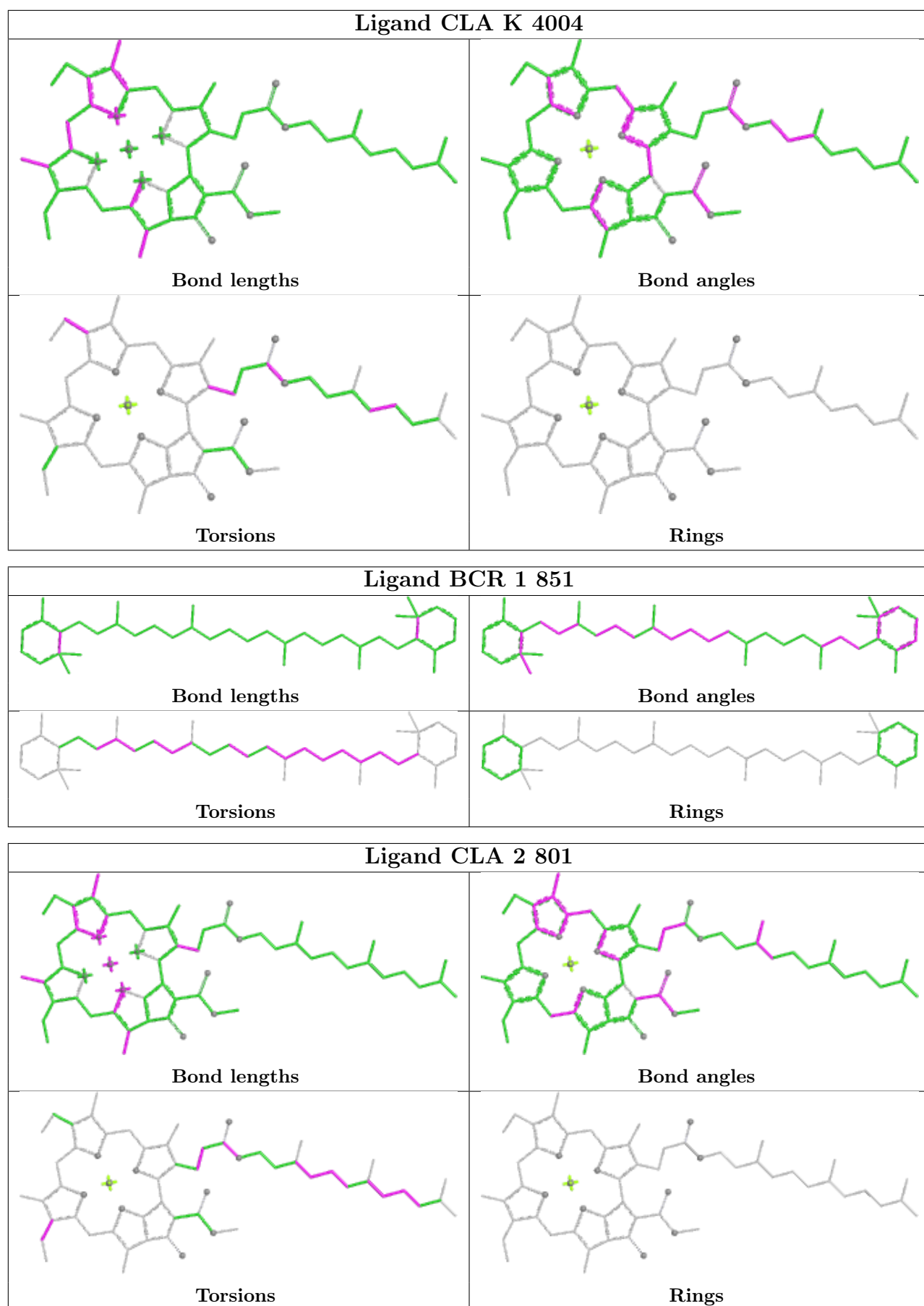


Ligand CLA b 839

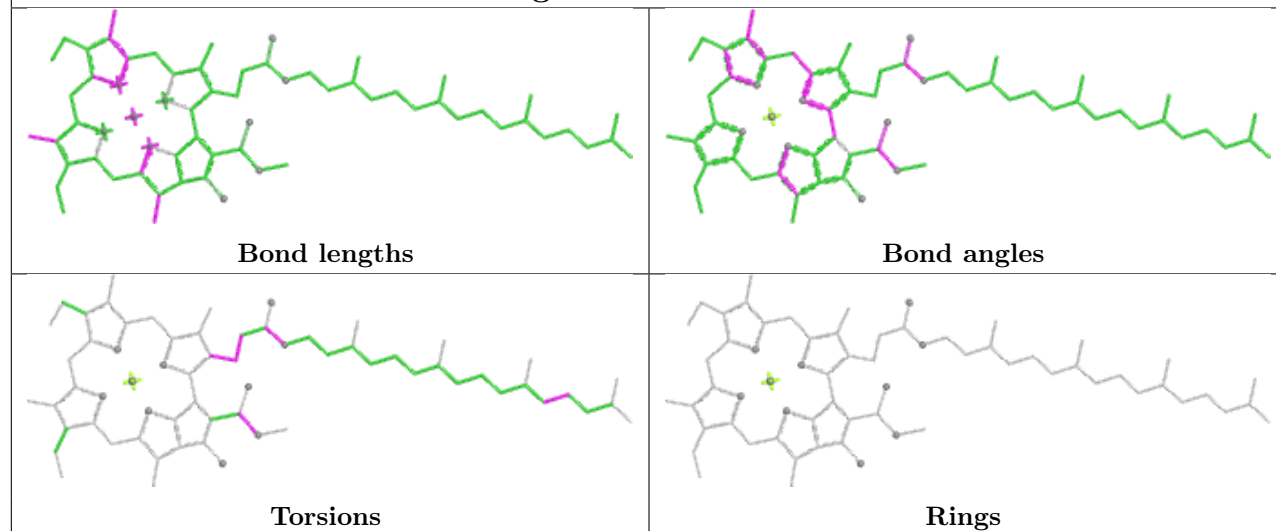


Ligand BCR j 103

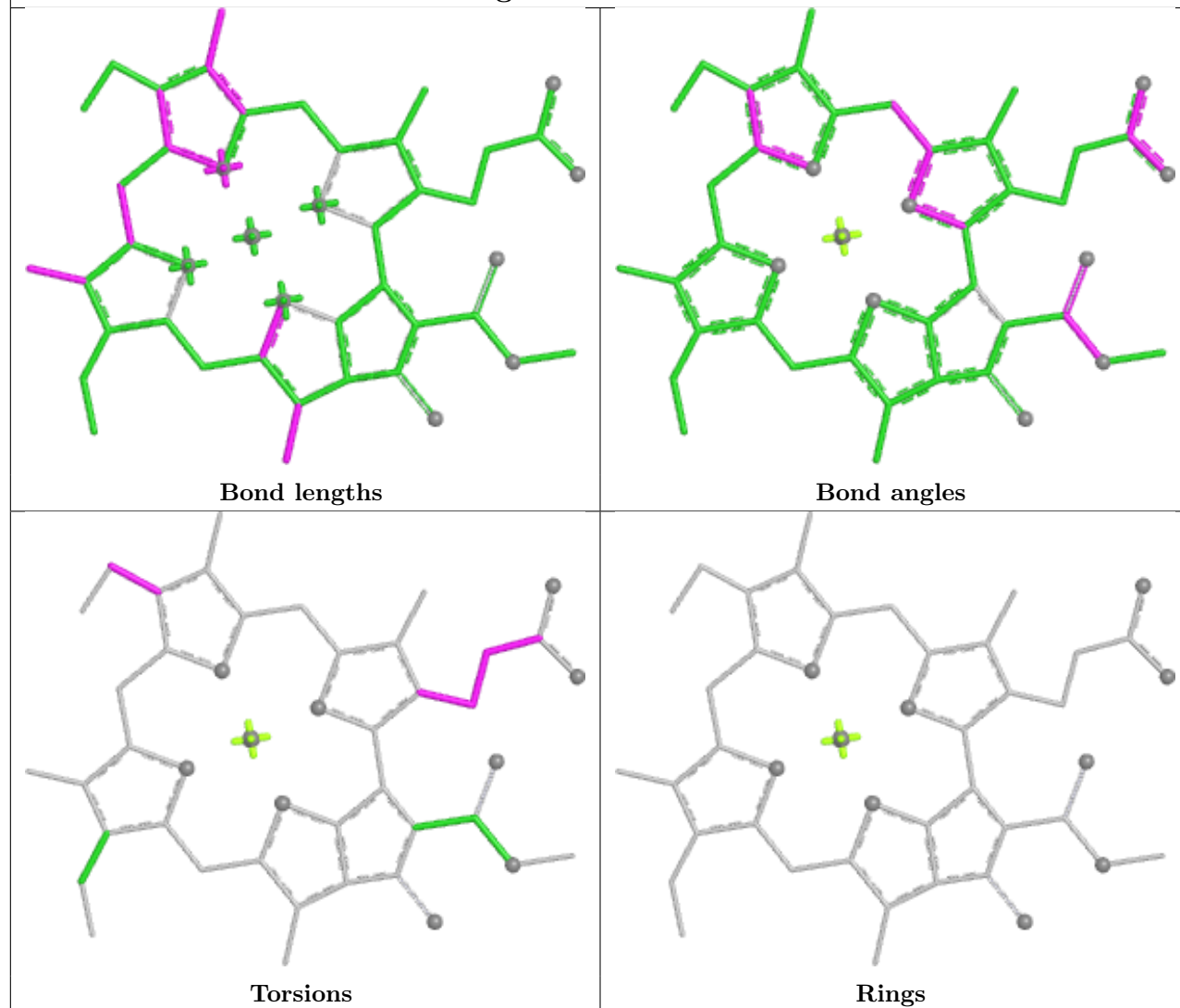


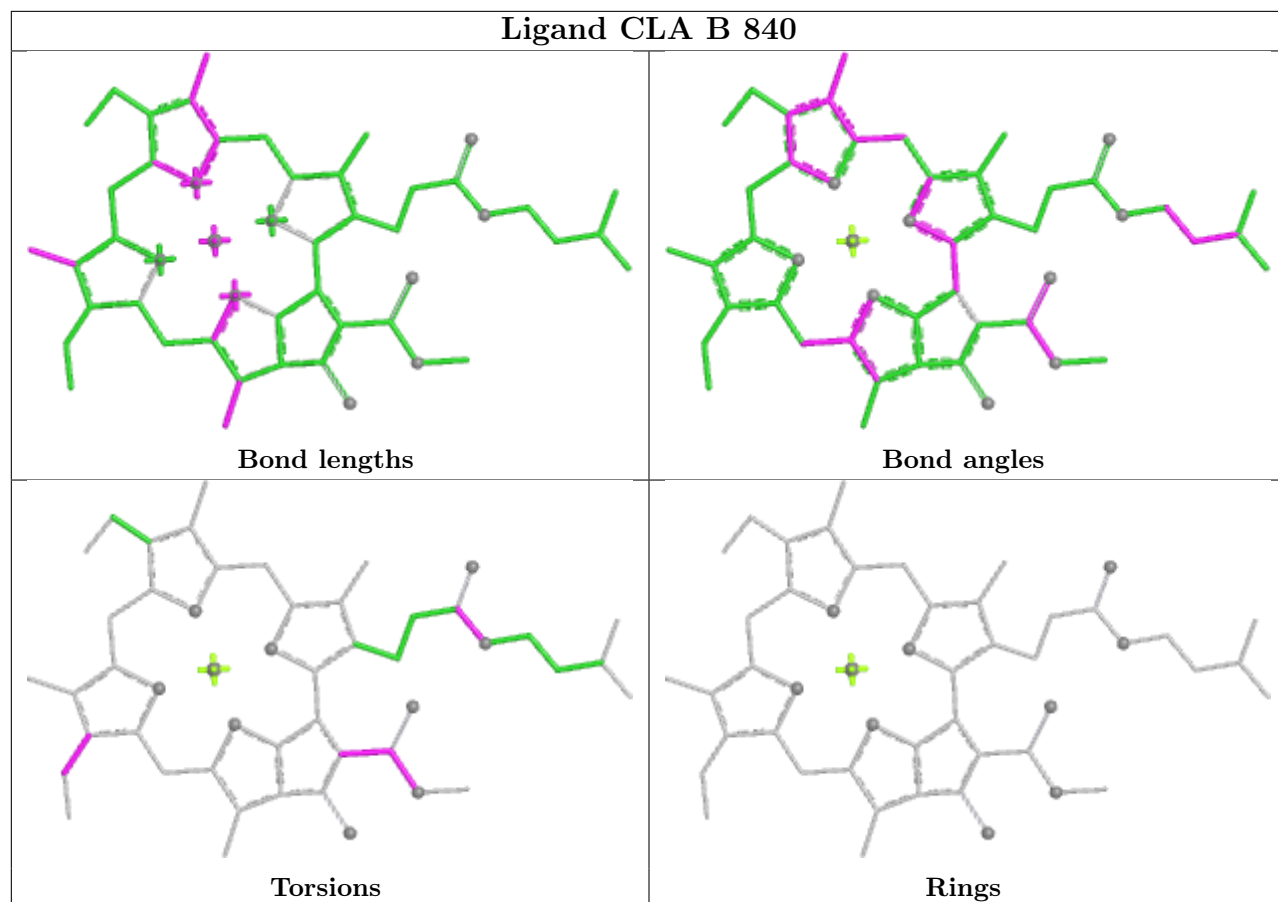


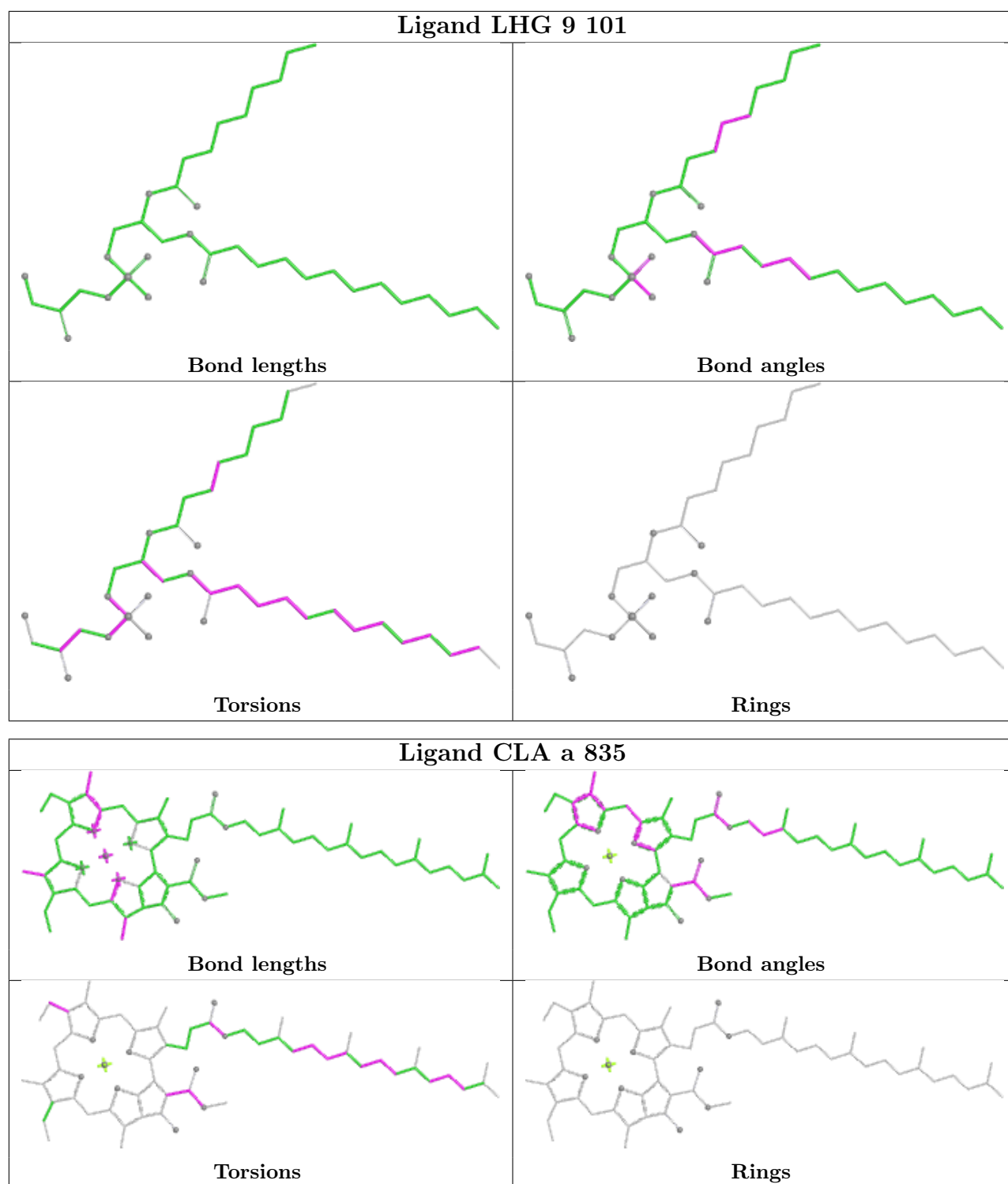
Ligand CLA B 831

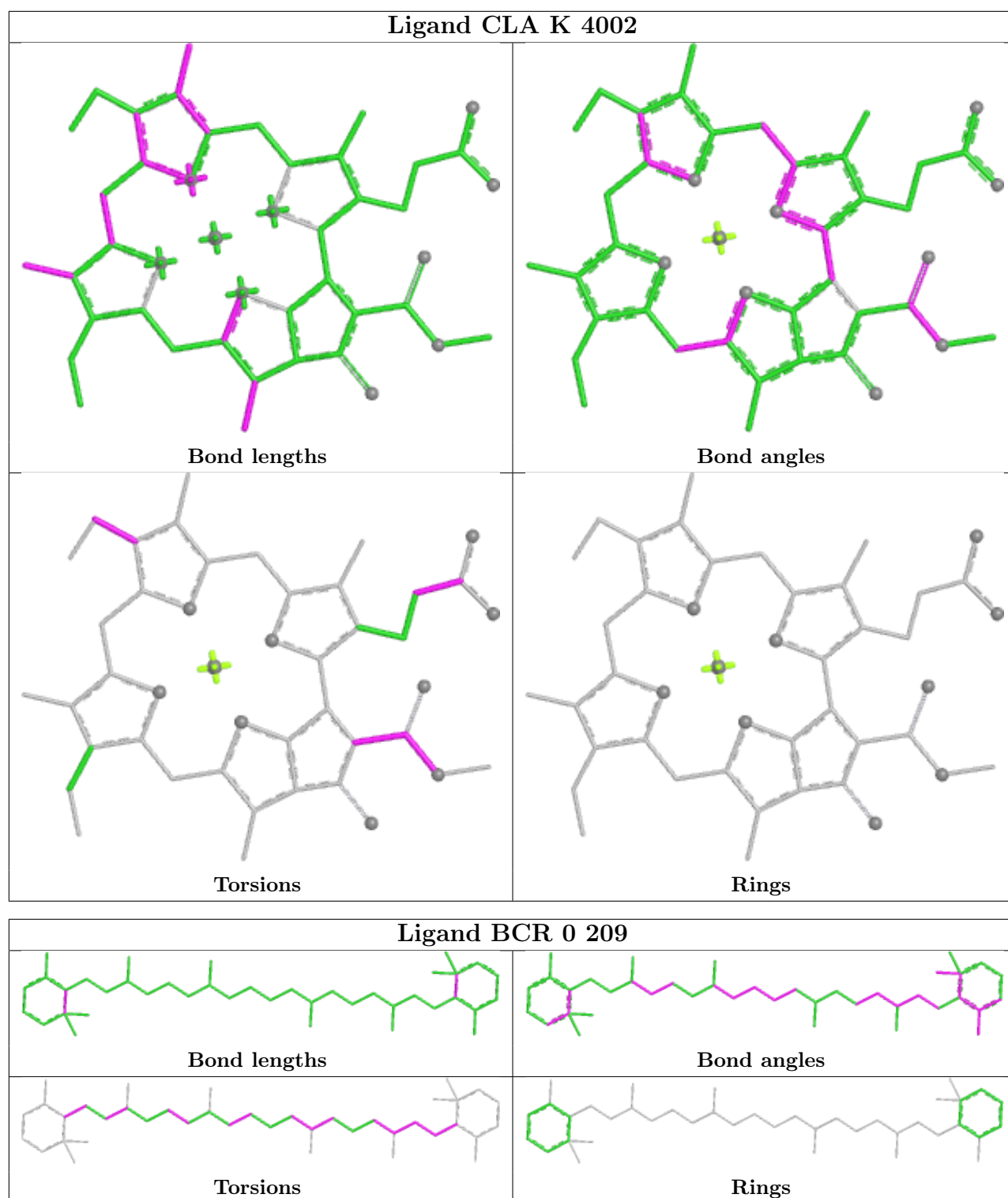


Ligand CLA 2 822

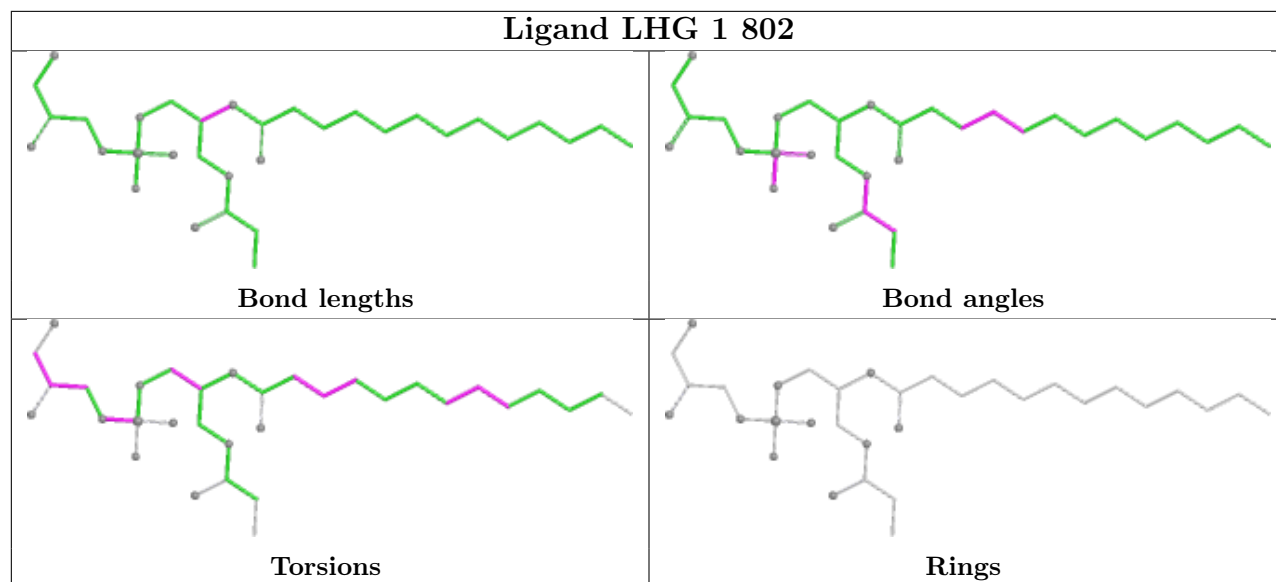




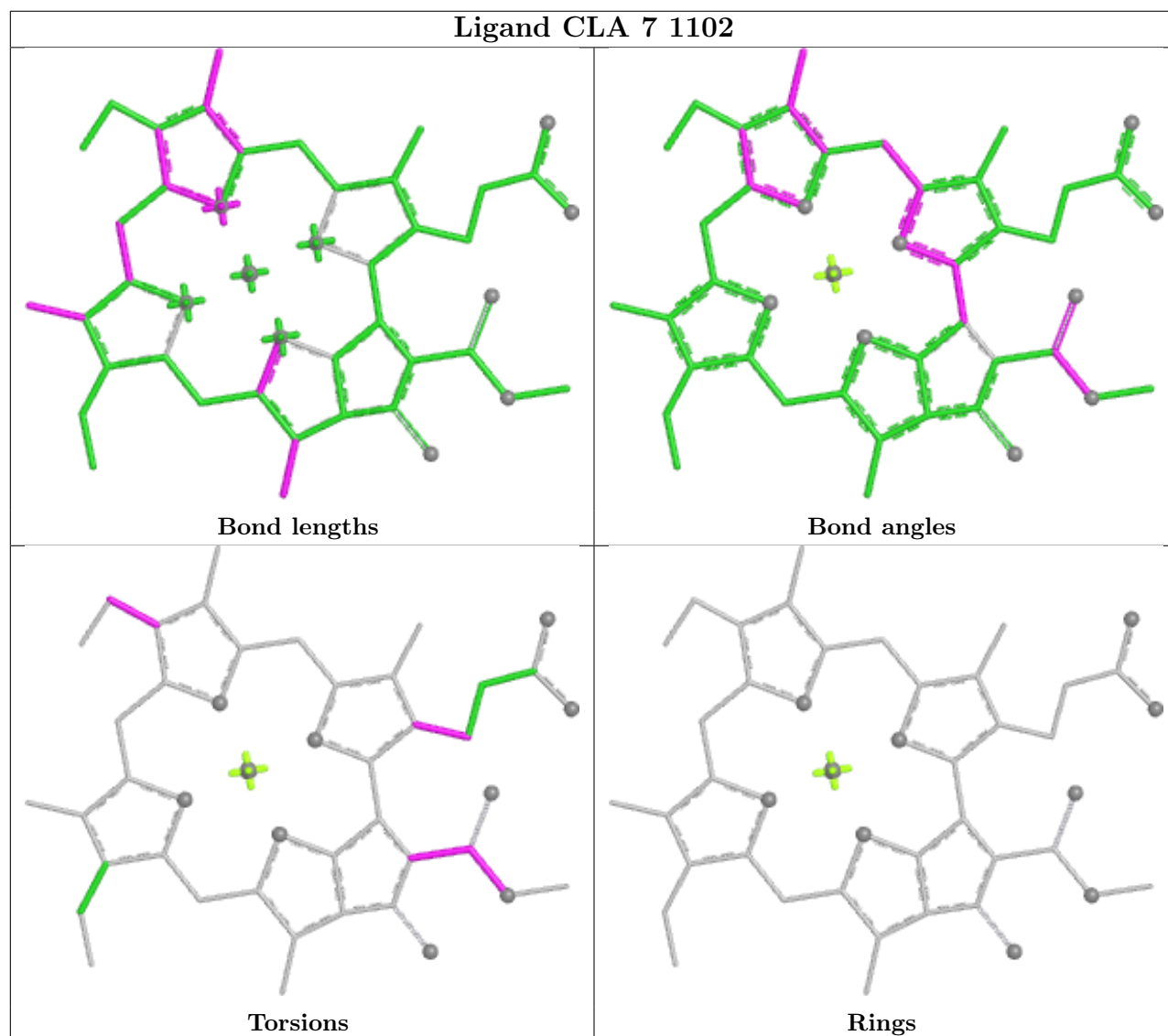




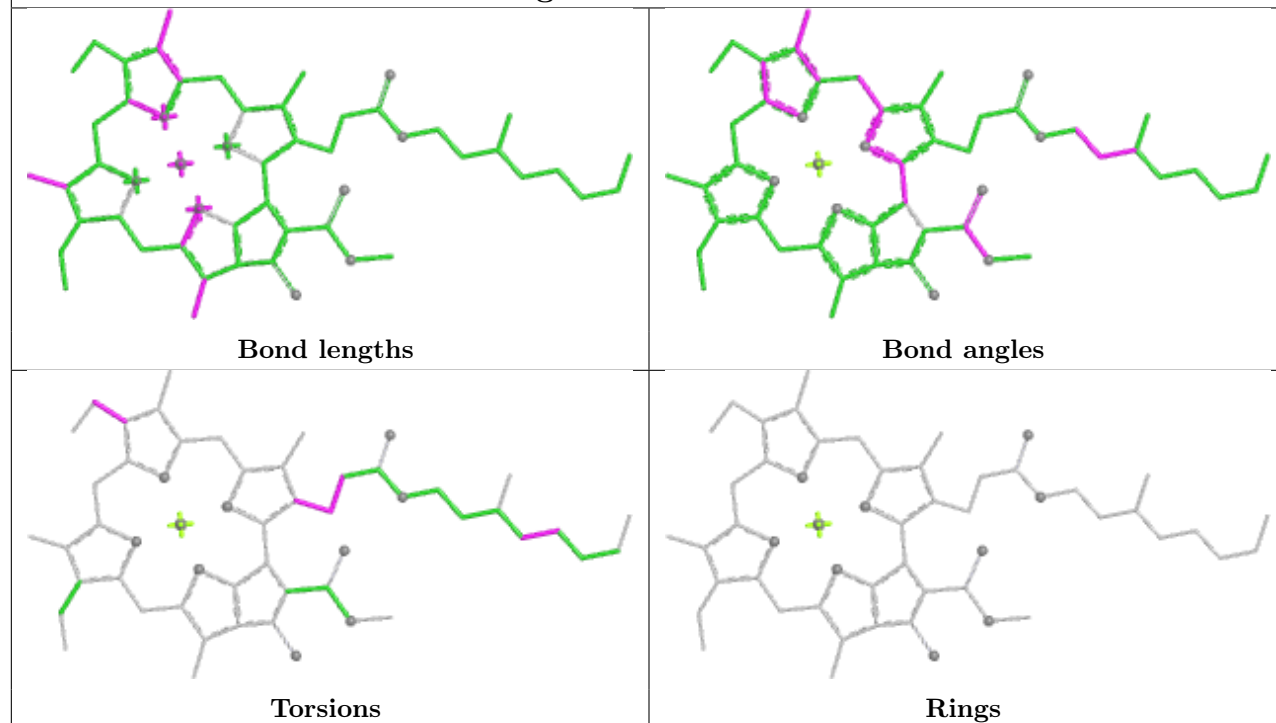
Ligand LHG 1 802



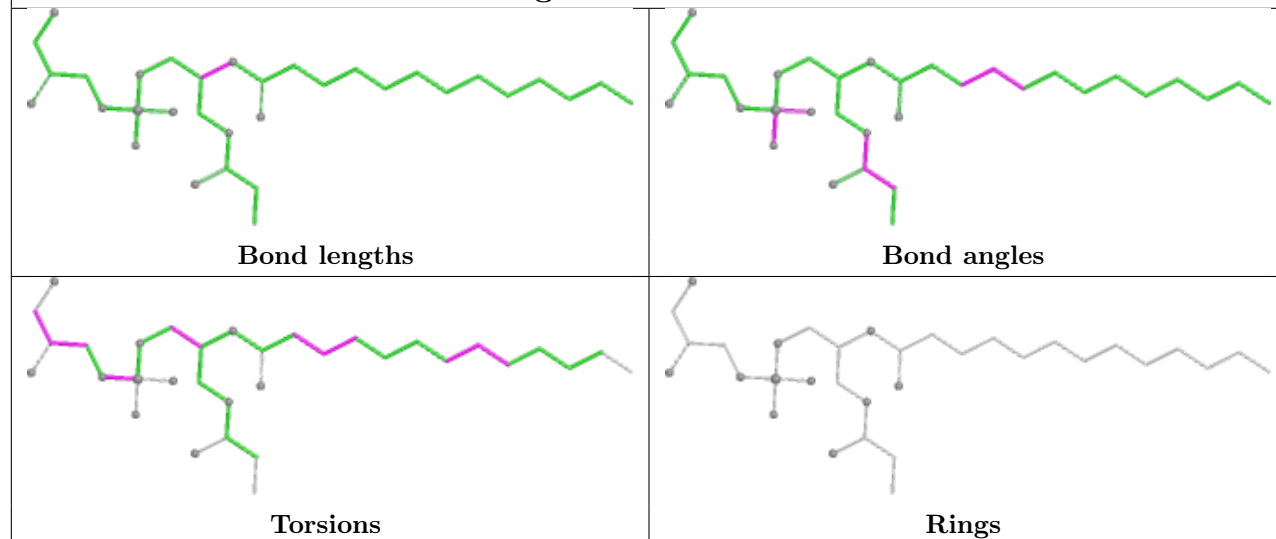
Ligand CLA 7 1102

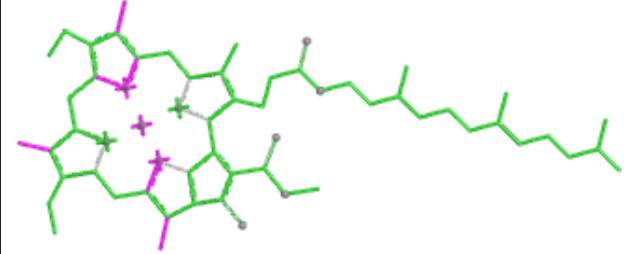
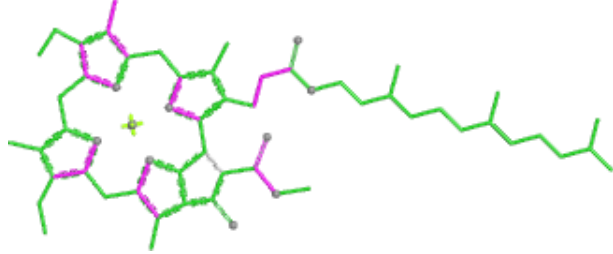
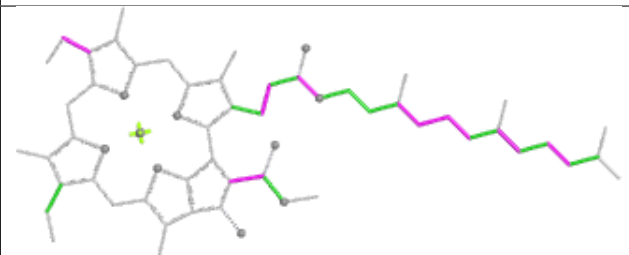
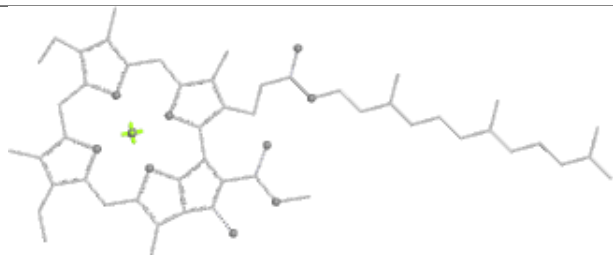
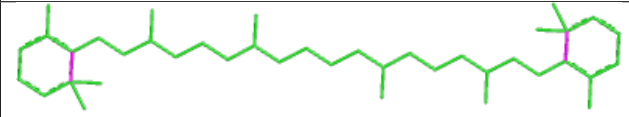
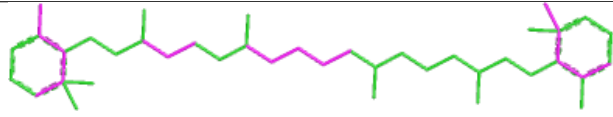
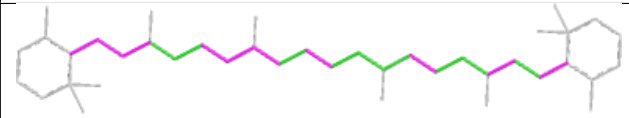
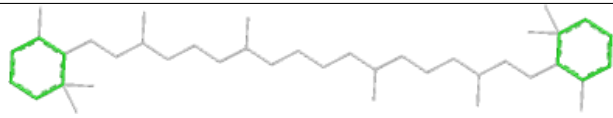
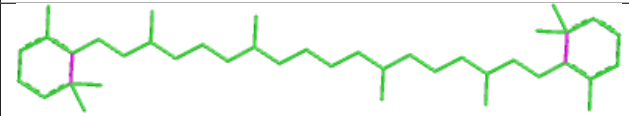
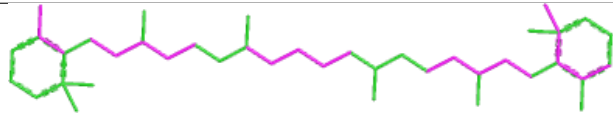
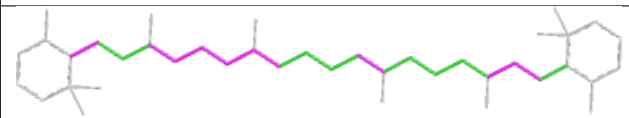
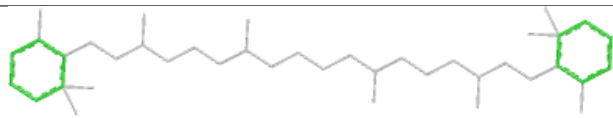


Ligand CLA 1 819

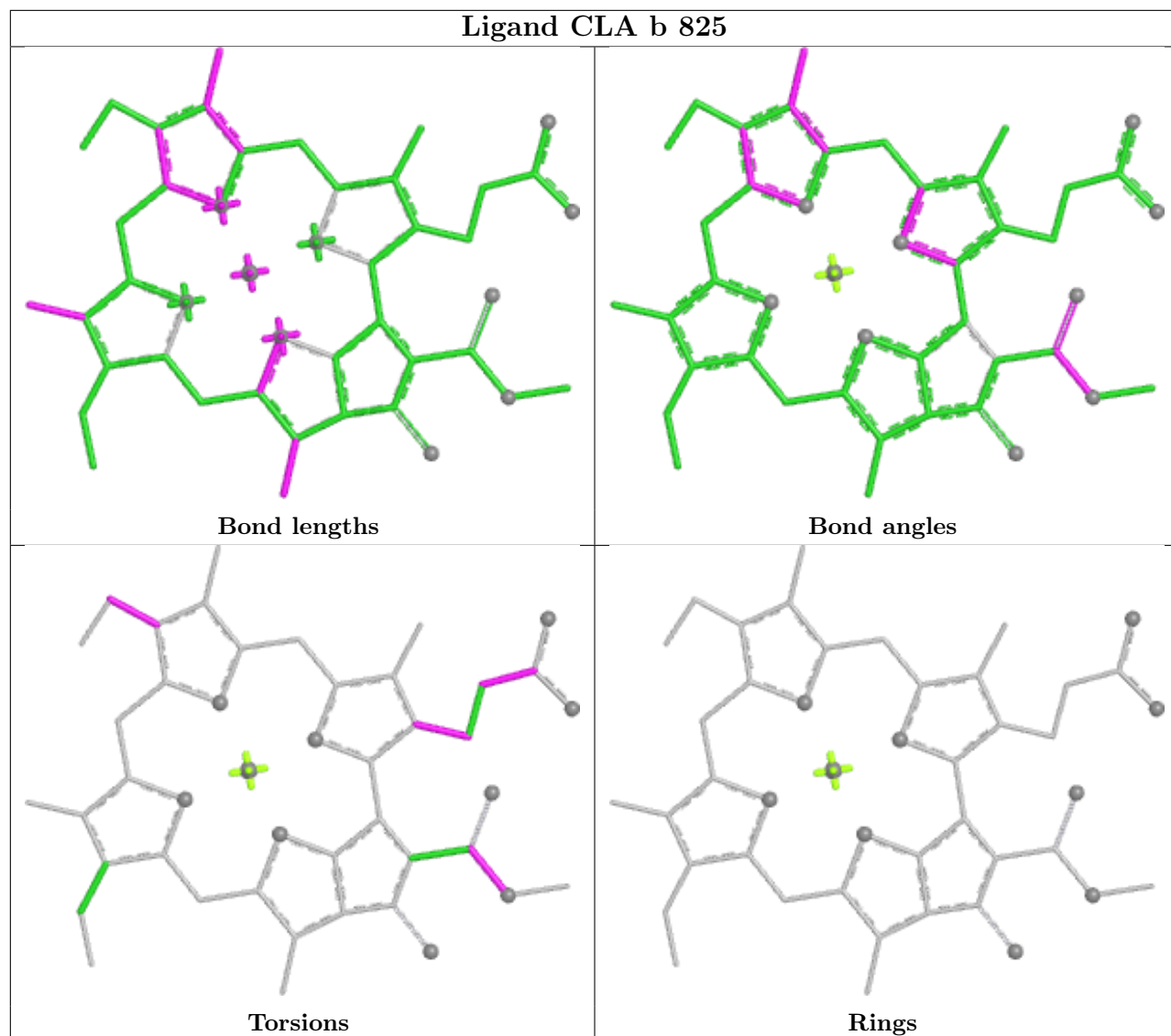


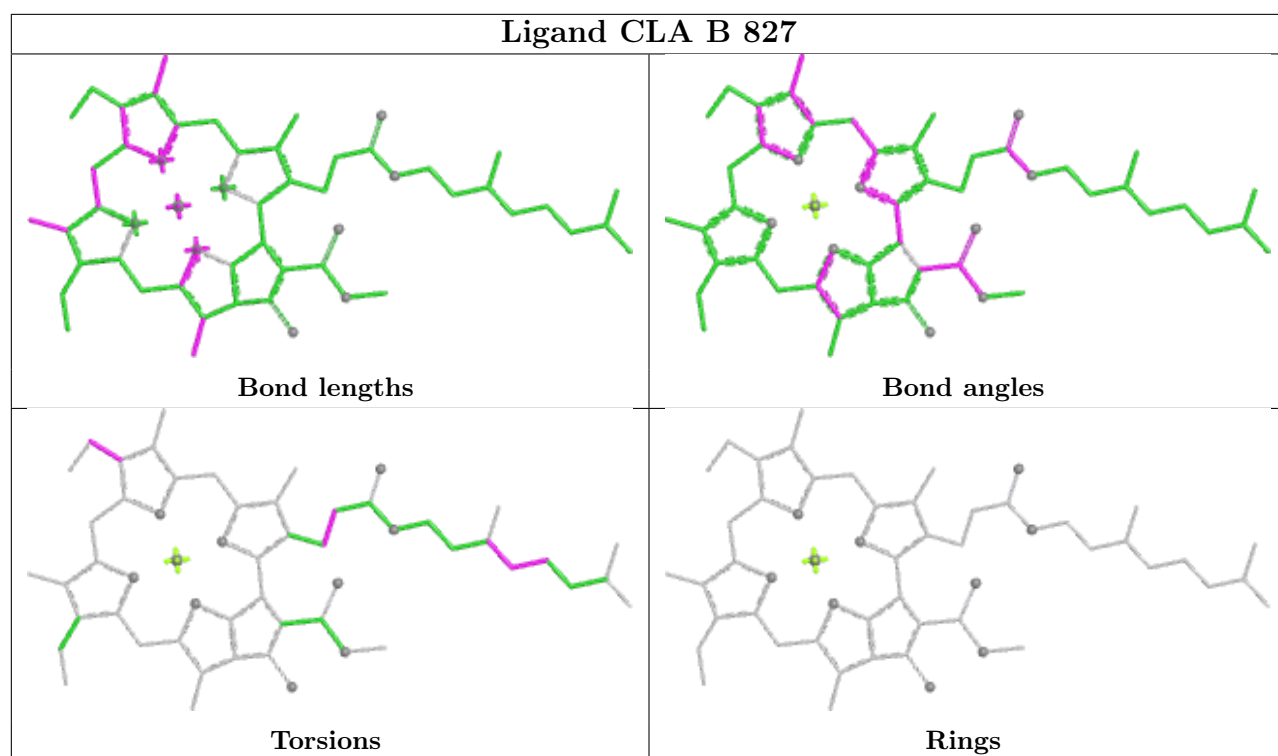
Ligand LHG a 802

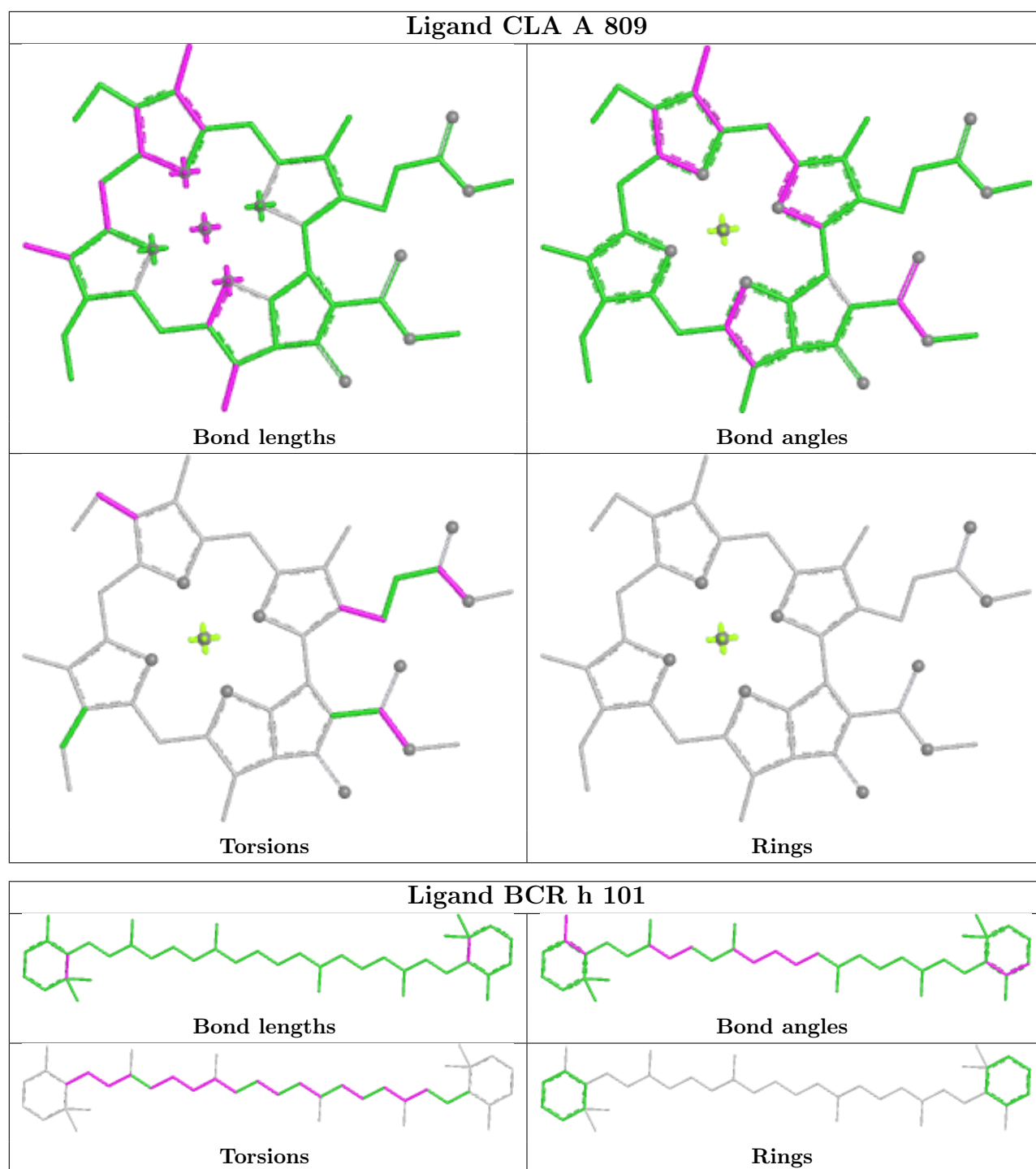


Ligand CLA b 831	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 6 4405	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 2 849	
 Bond lengths	 Bond angles
 Torsions	 Rings

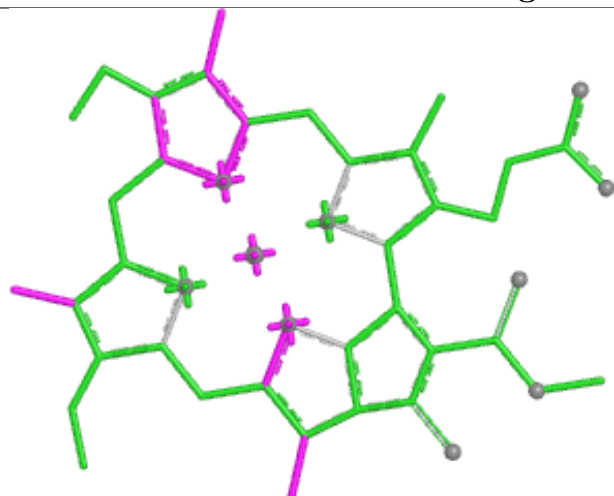
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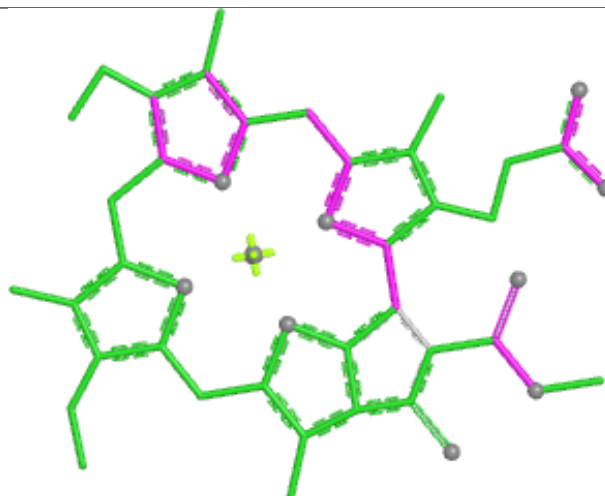




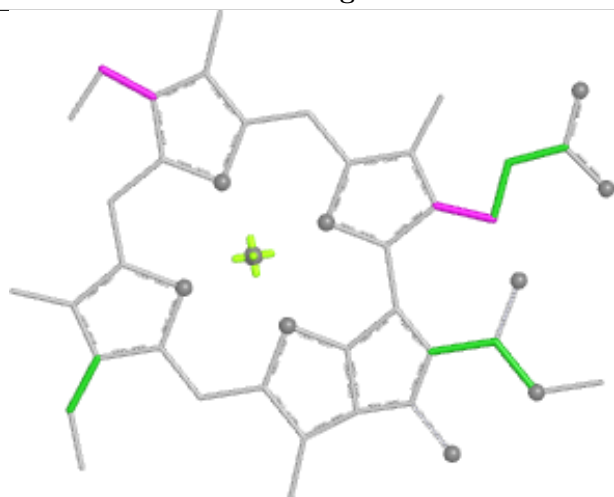
Ligand CLA 2 835



Bond lengths



Bond angles

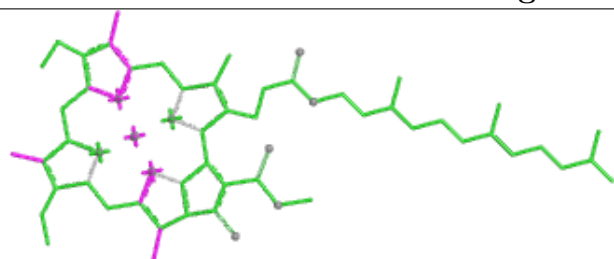


Torsions

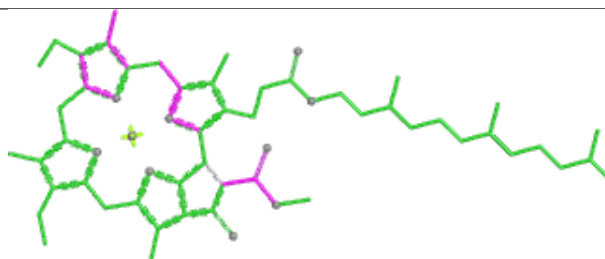


Rings

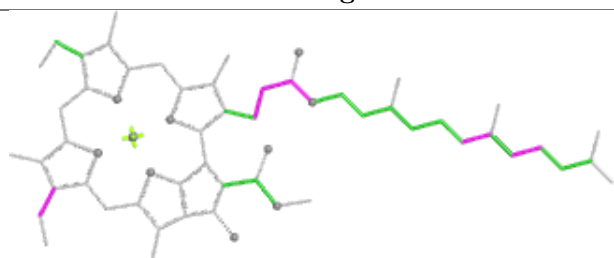
Ligand CLA 2 829



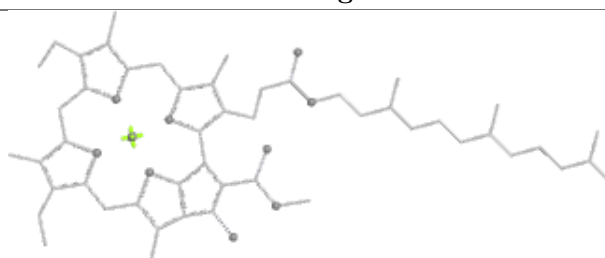
Bond lengths



Bond angles

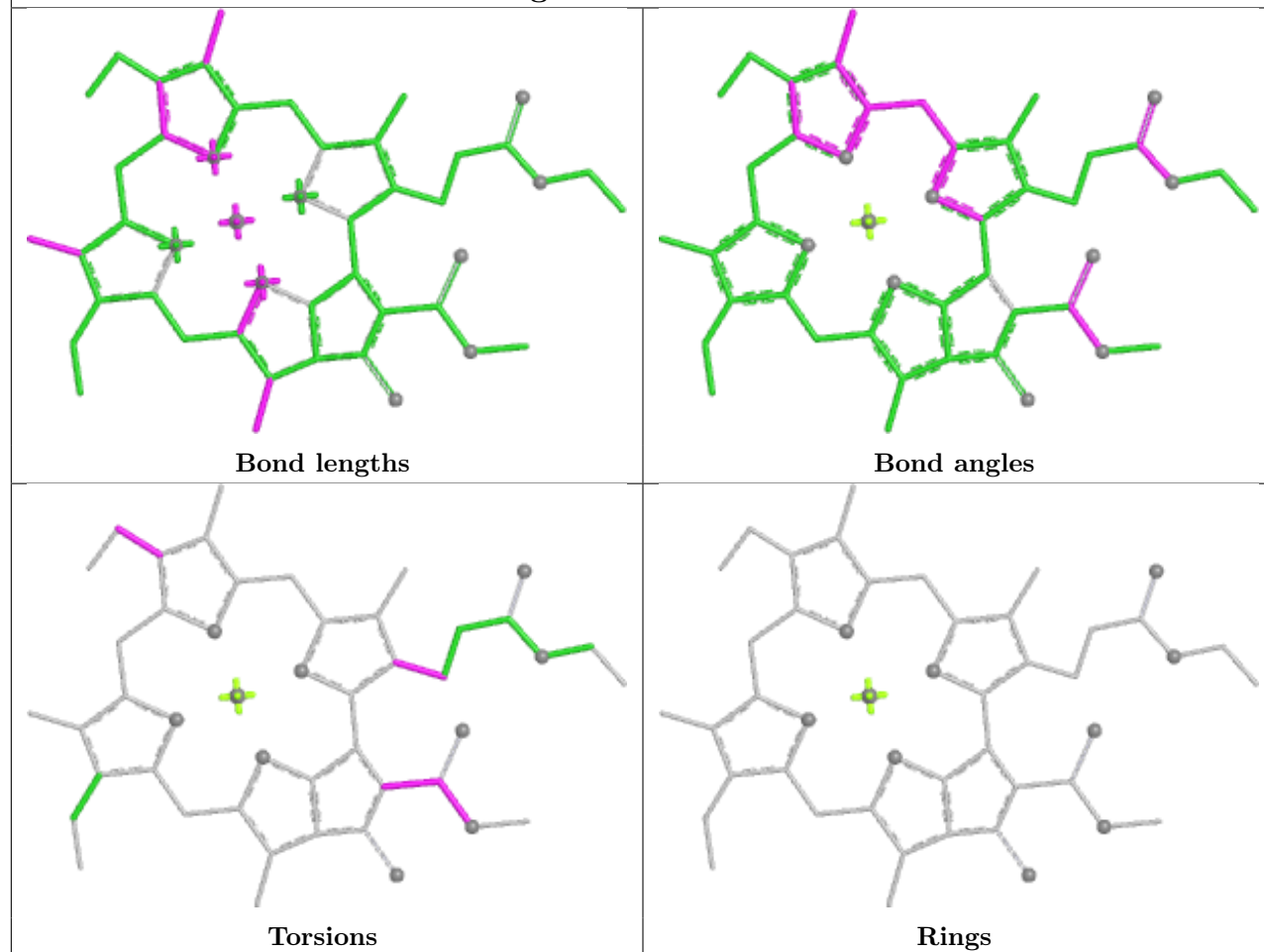


Torsions

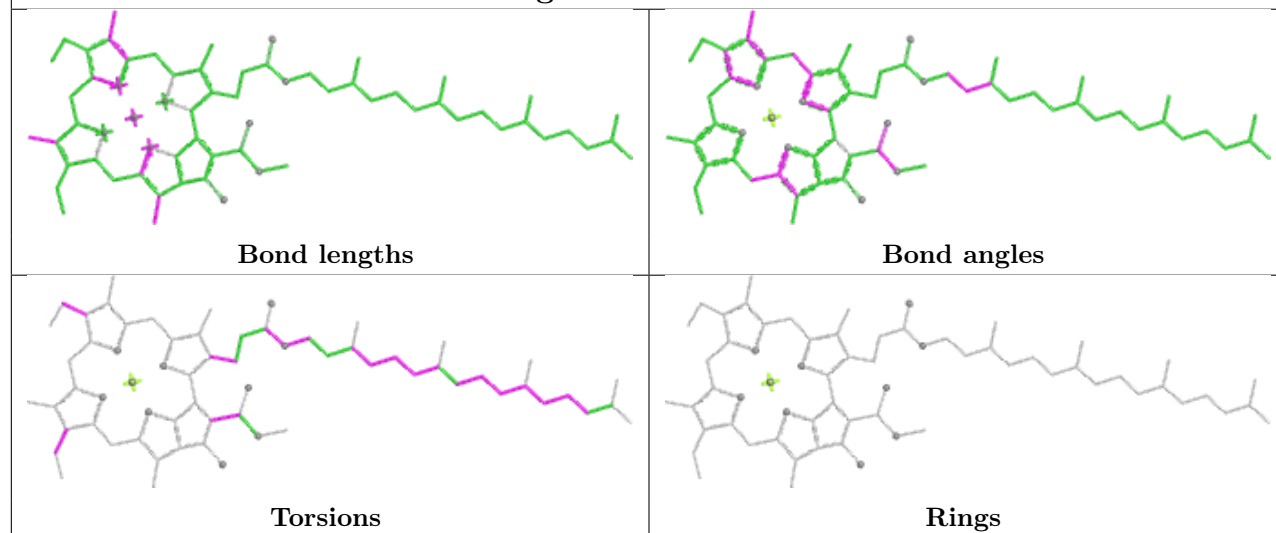


Rings

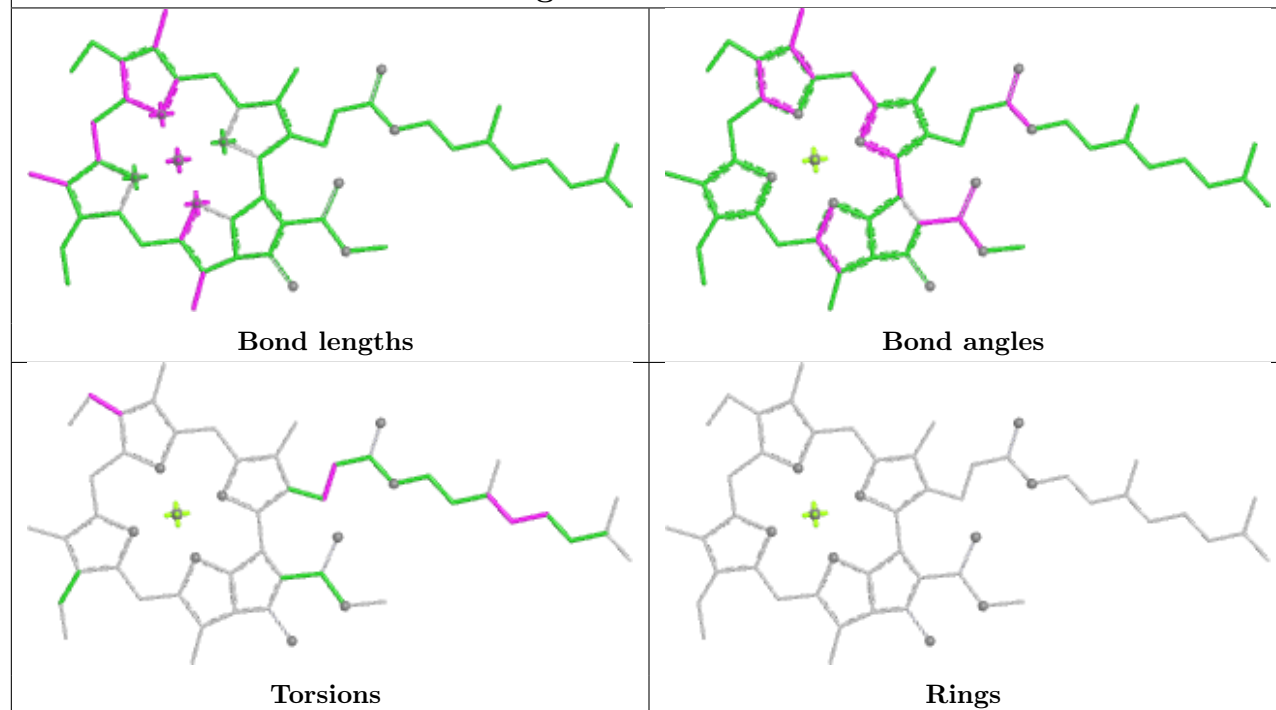
Ligand CLA b 821



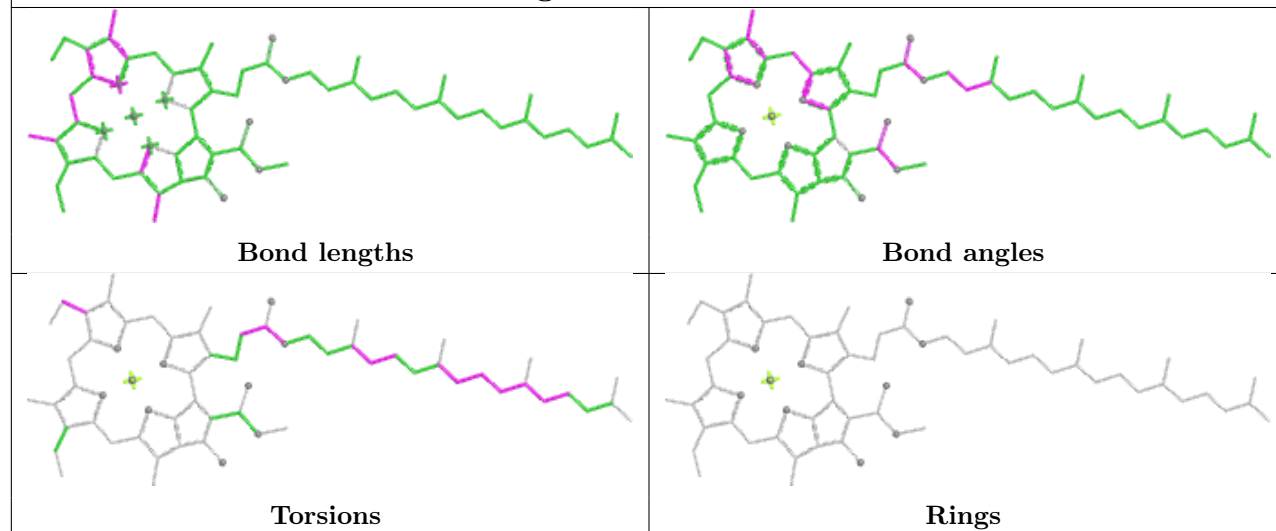
Ligand CLA 2 815



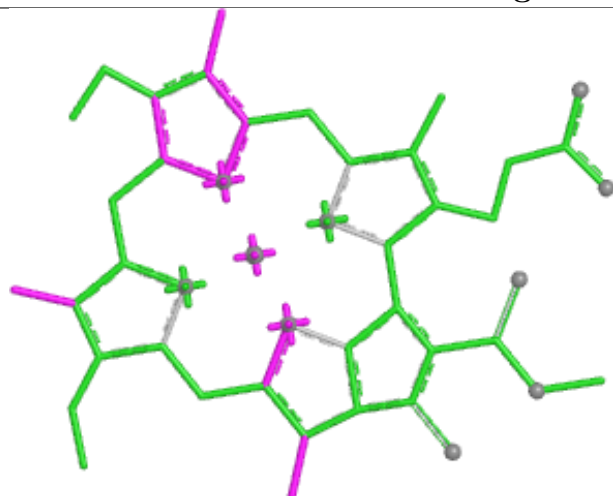
Ligand CLA 2 826



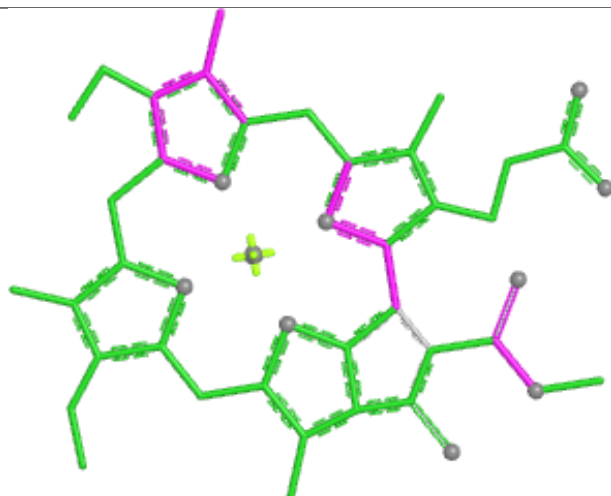
Ligand CLA 0 208



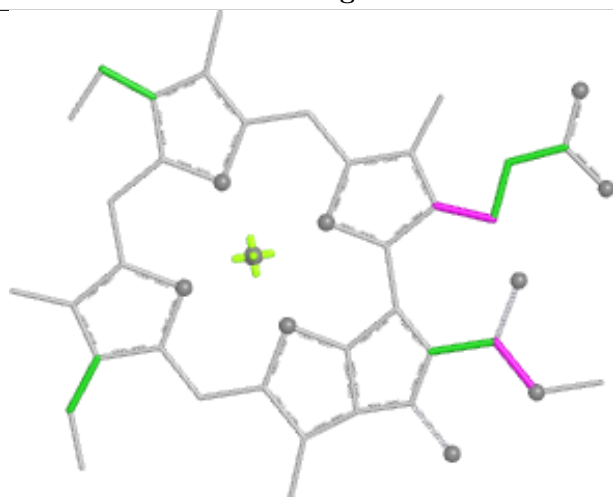
Ligand CLA A 816



Bond lengths



Bond angles

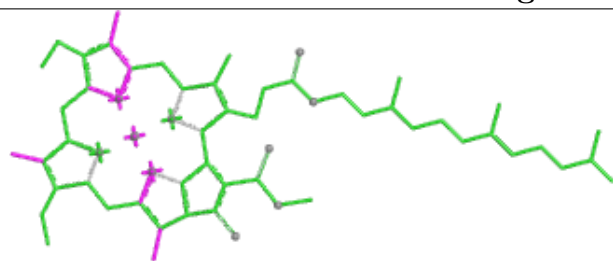


Torsions

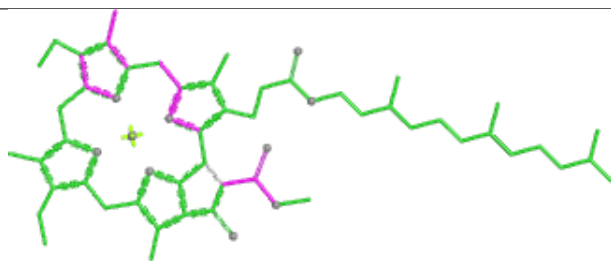


Rings

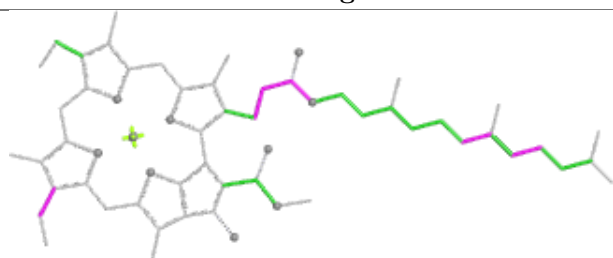
Ligand CLA b 829



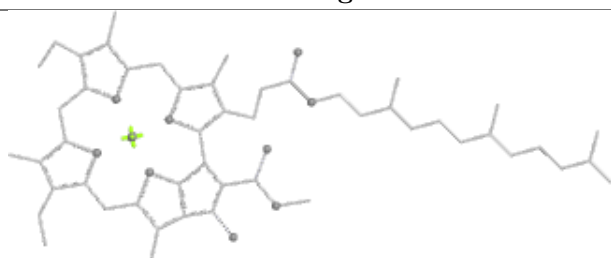
Bond lengths



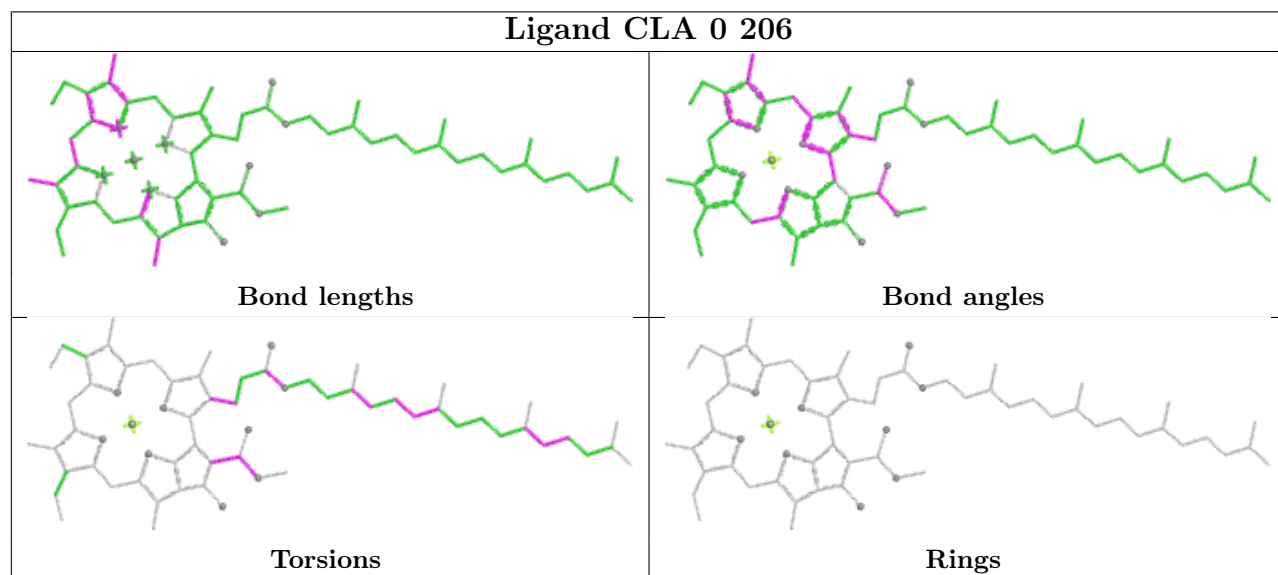
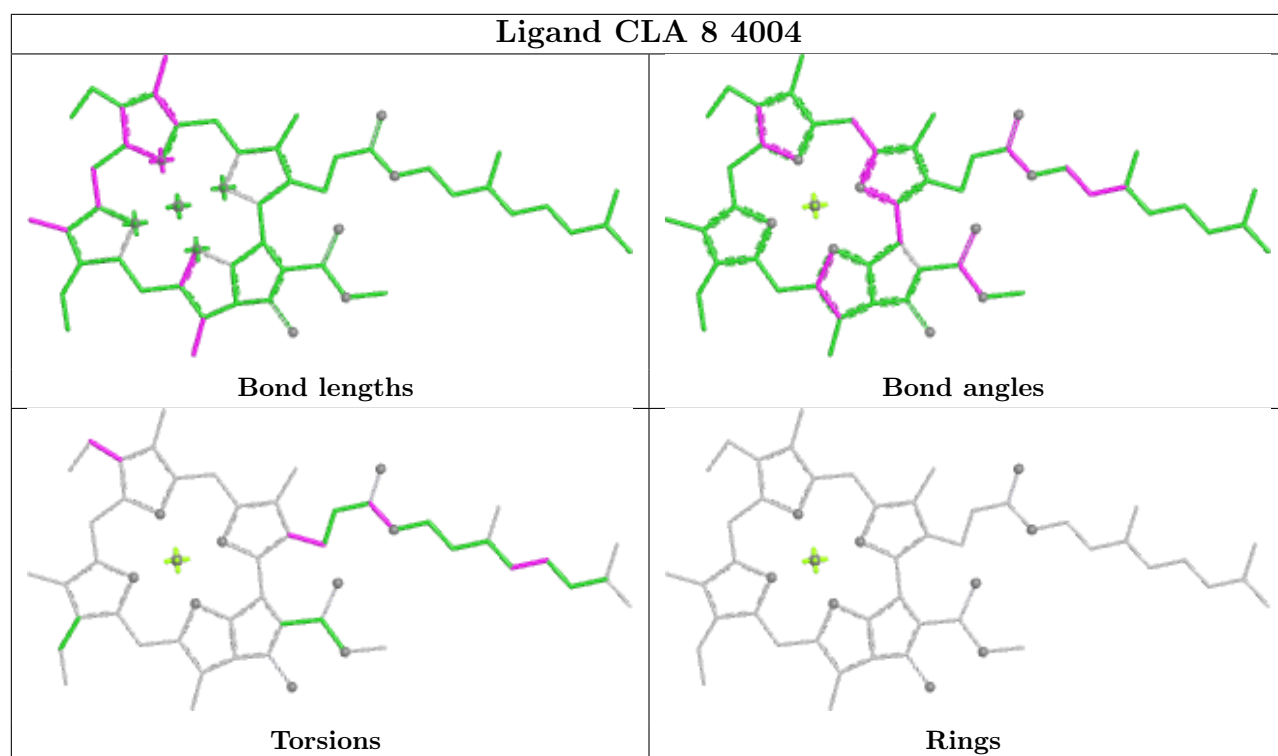
Bond angles

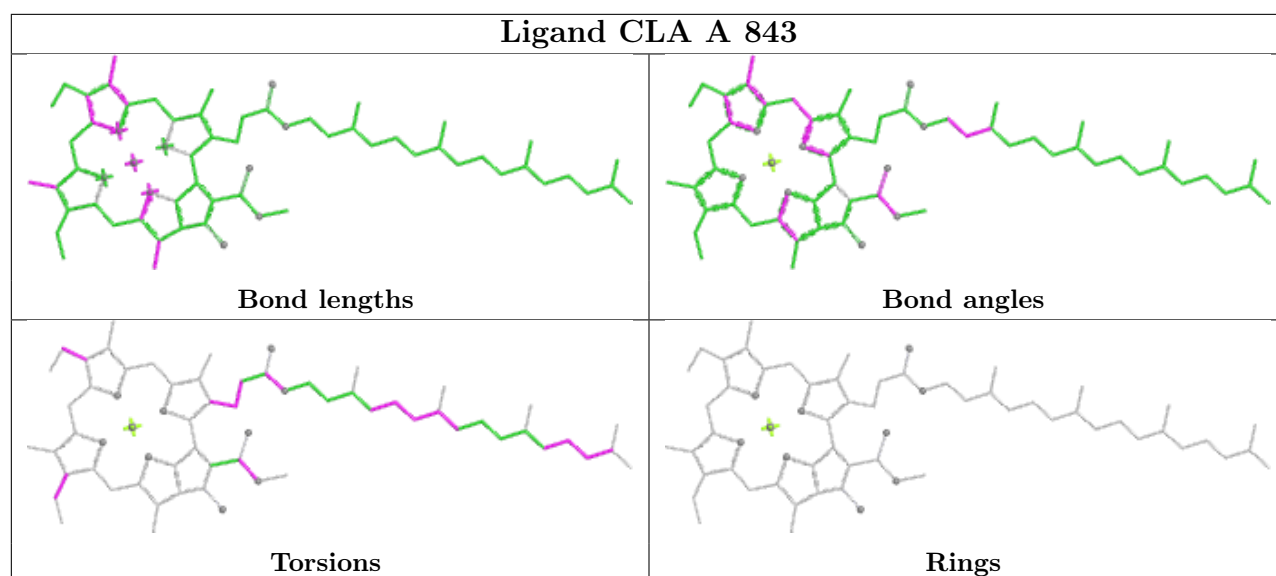
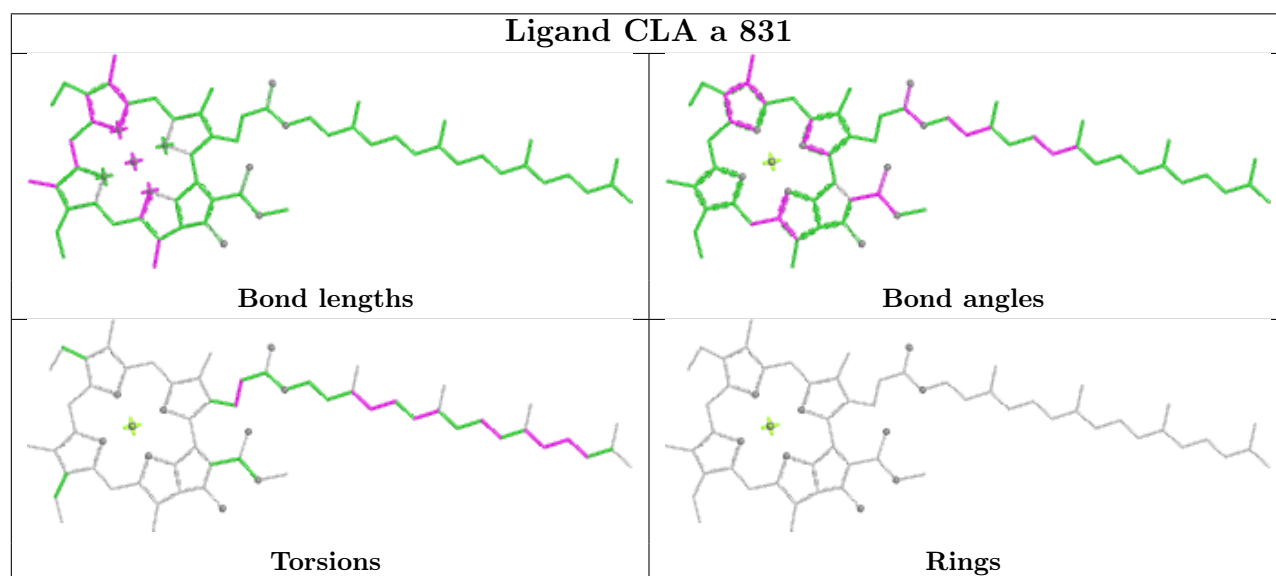
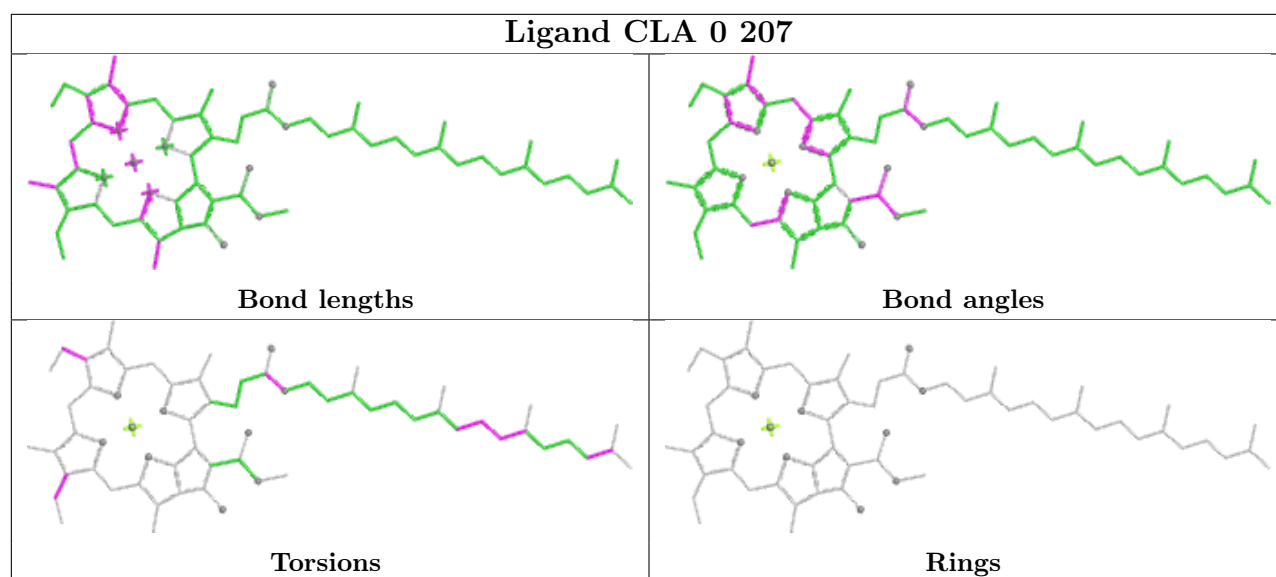


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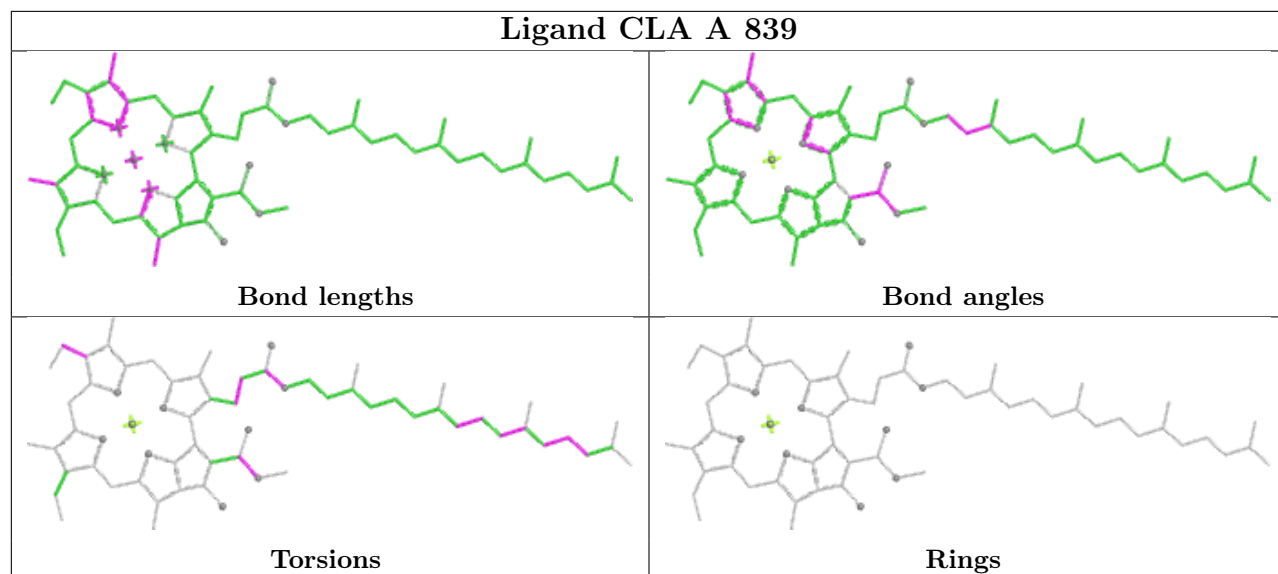


Rings

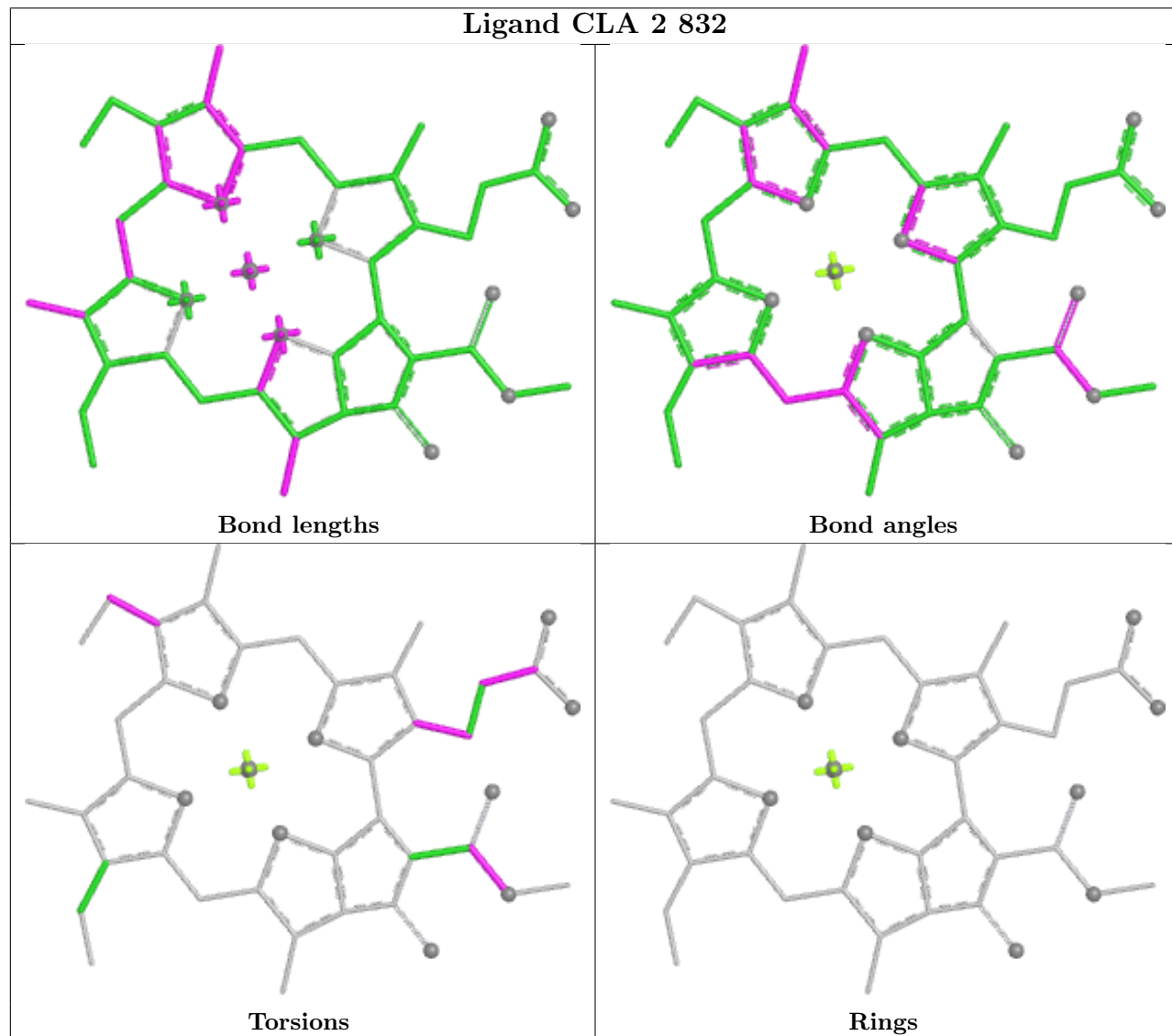


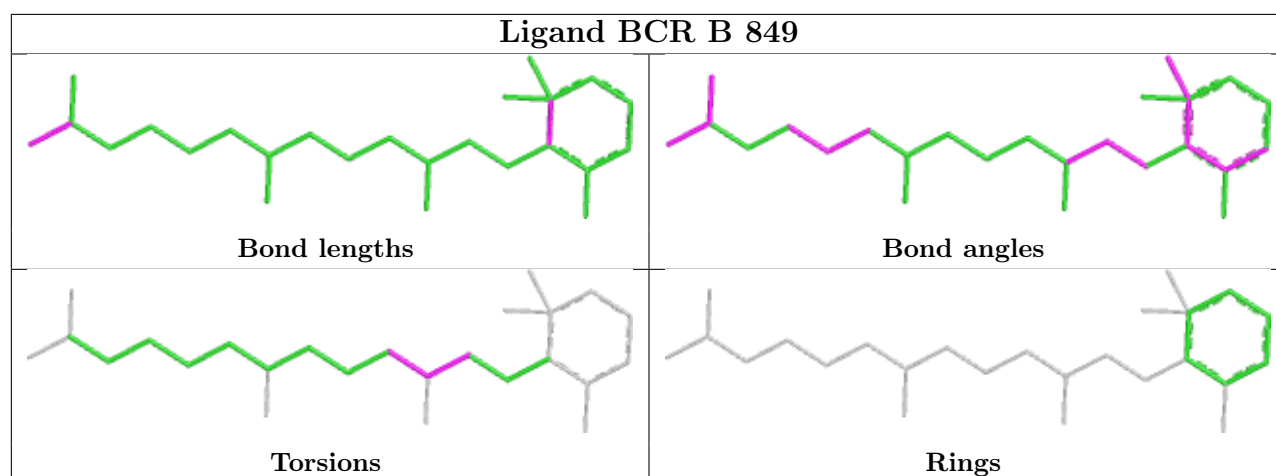
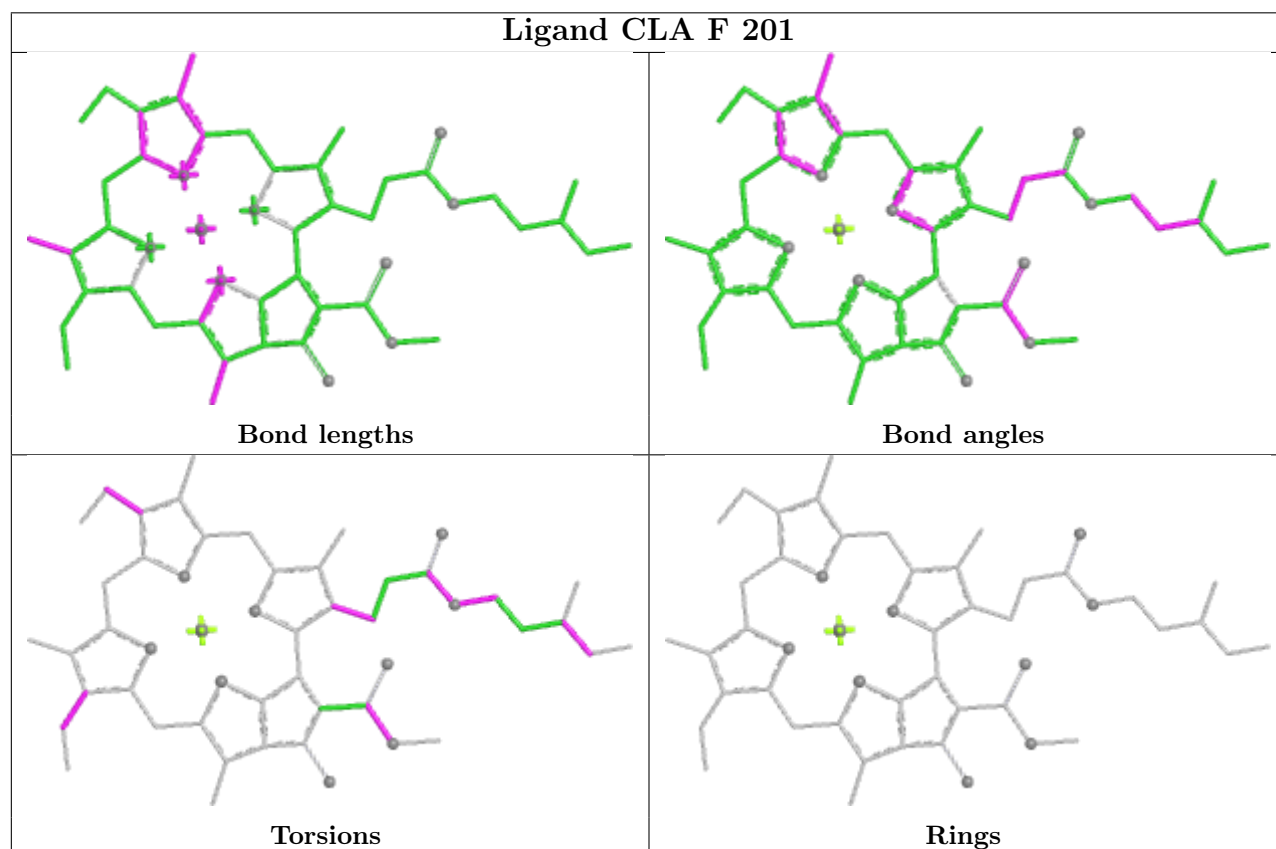
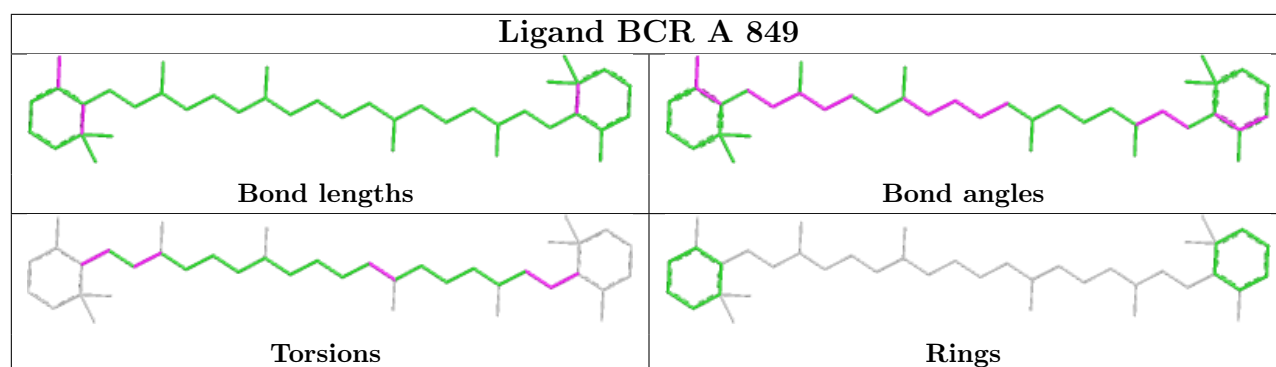


Ligand CLA A 839

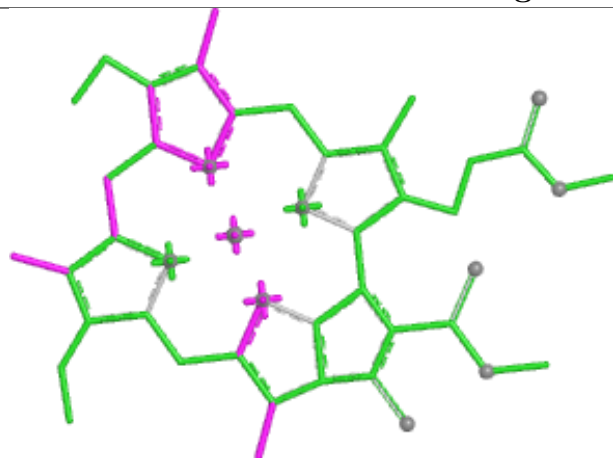


Ligand CLA 2 832

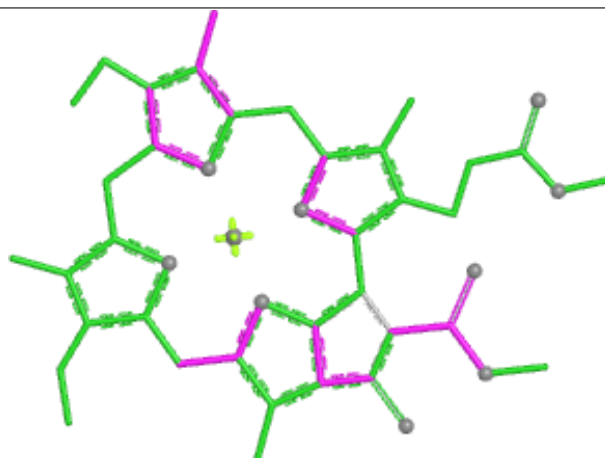




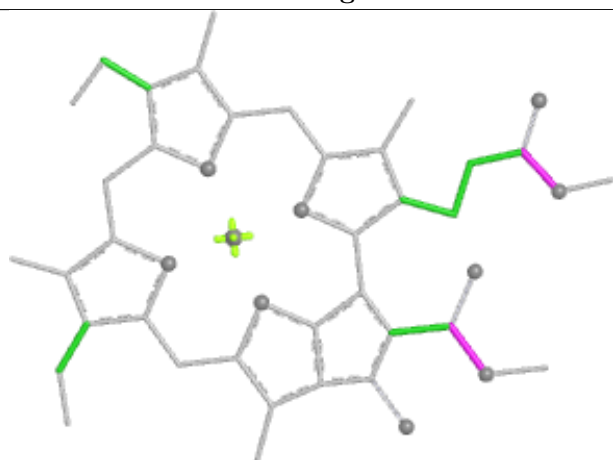
Ligand CLA B 842



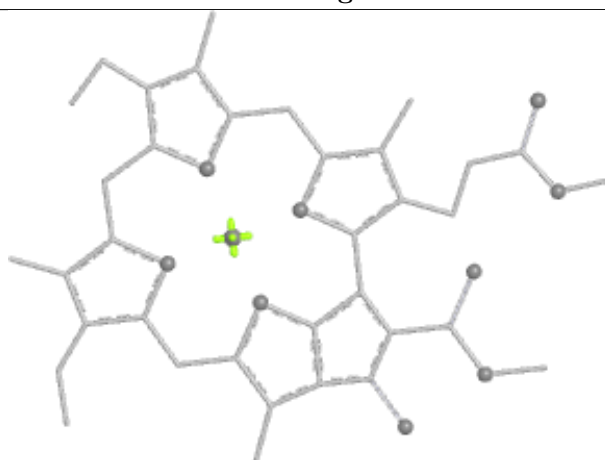
Bond lengths



Bond angles

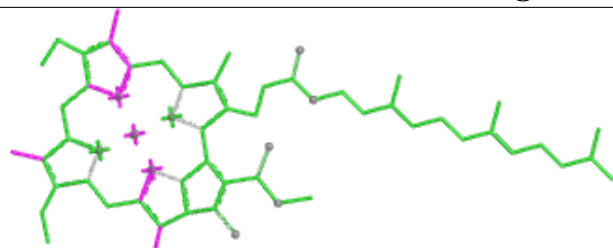


Torsions

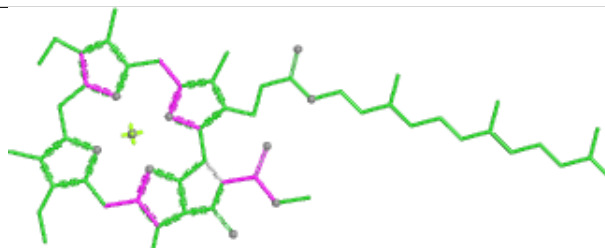


Rings

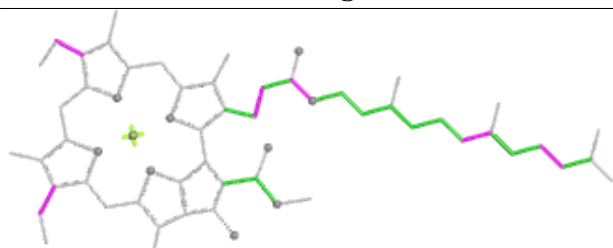
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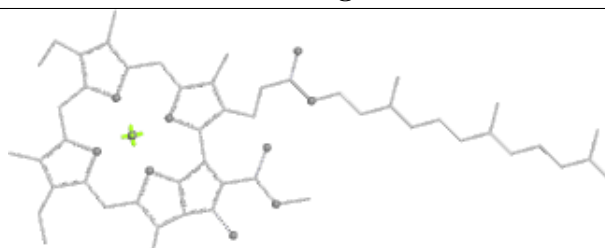
Bond lengths



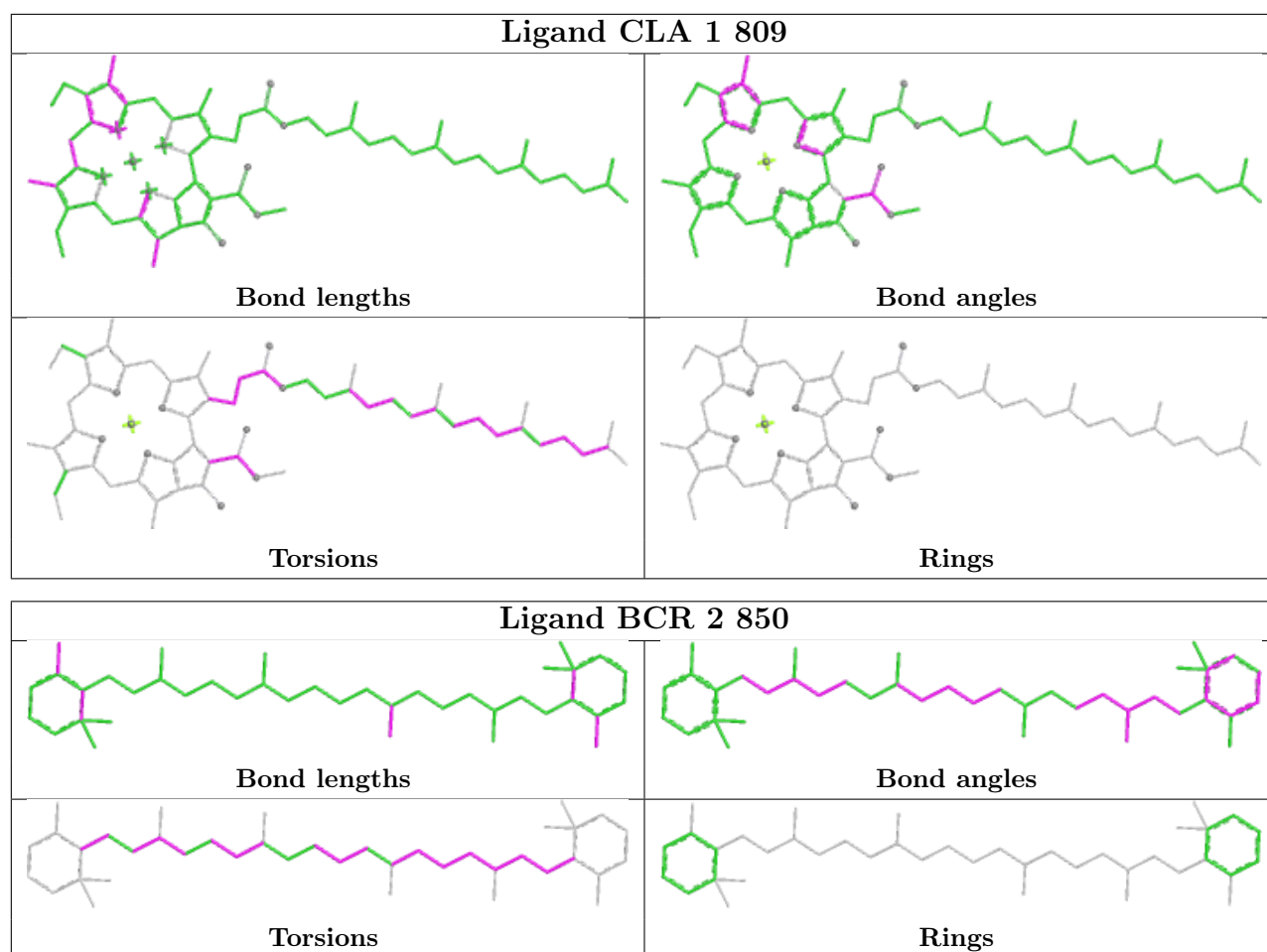
Bond angles



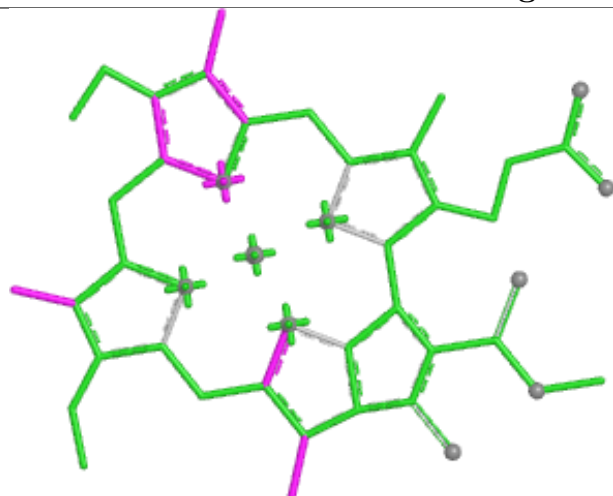
Torsions



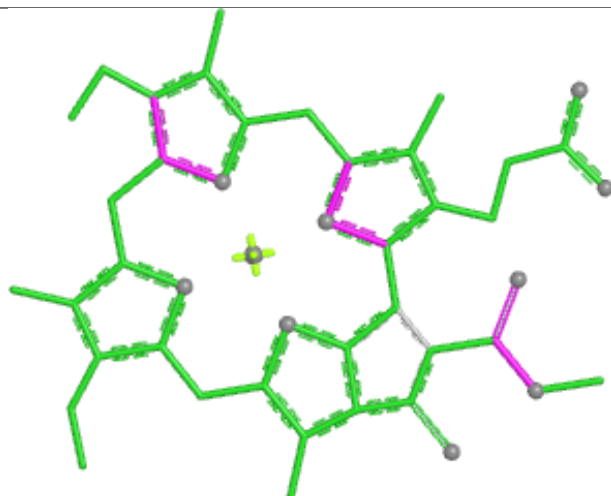
Rings



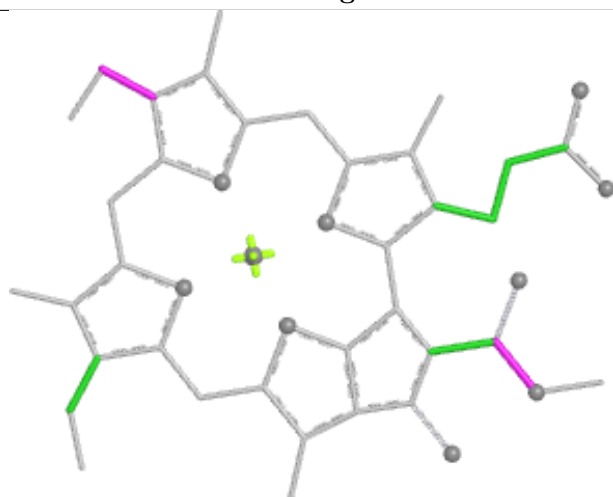
Ligand CLA 1 816



Bond lengths



Bond angles

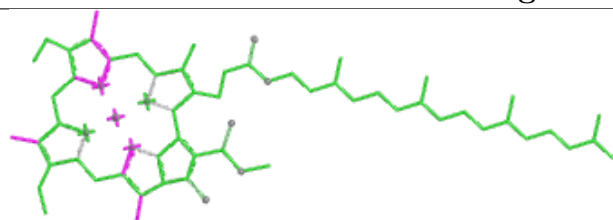


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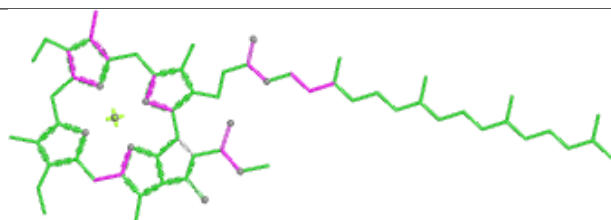


Rings

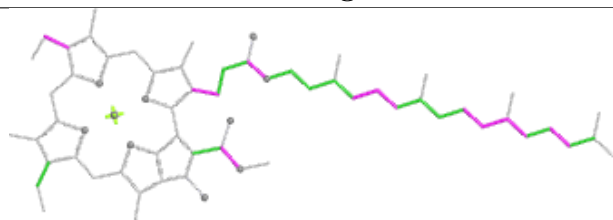
Ligand CLA a 809



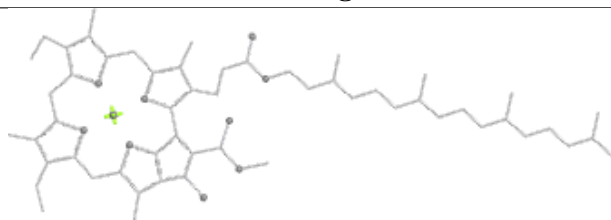
Bond lengths



Bond angles

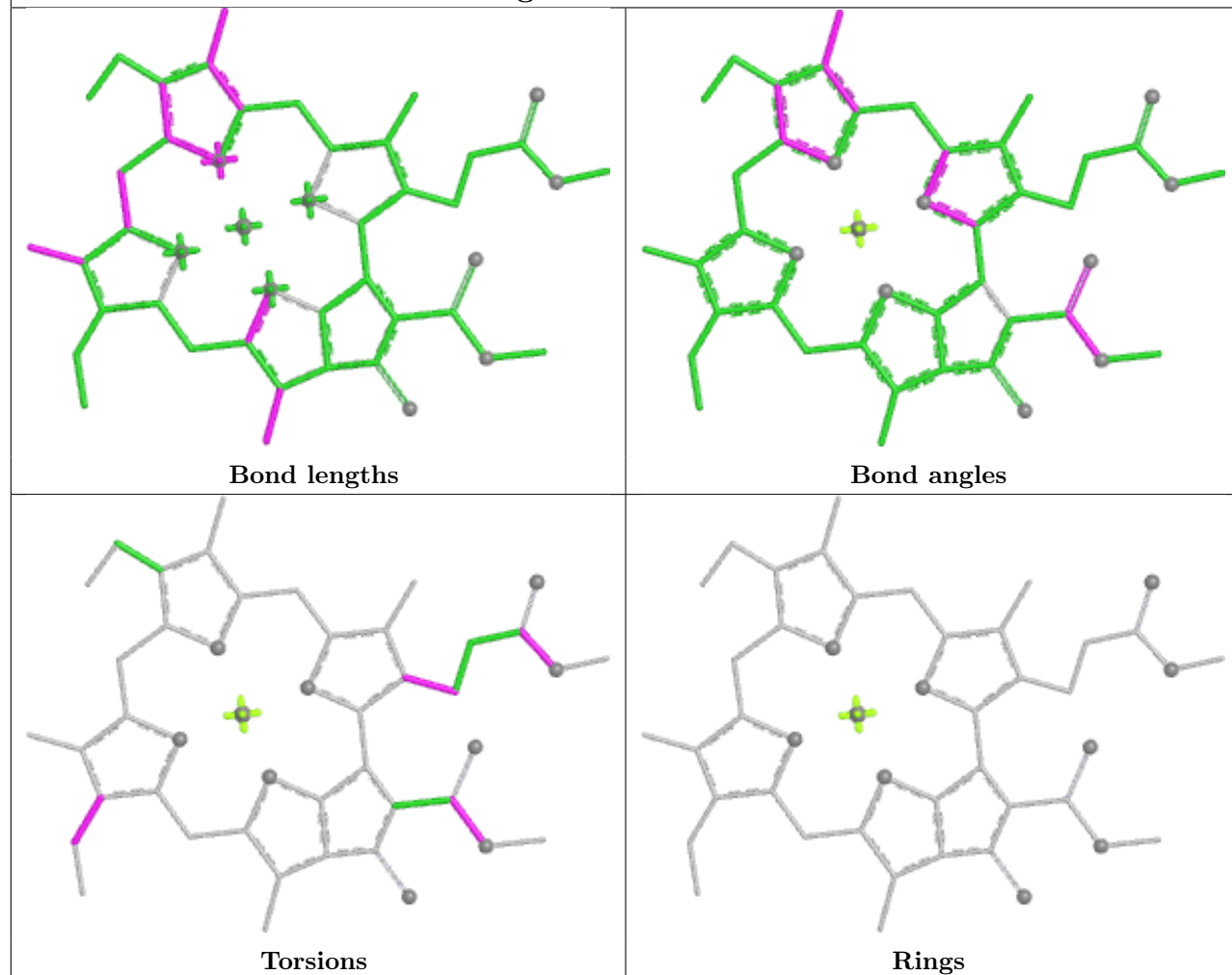


Torsions

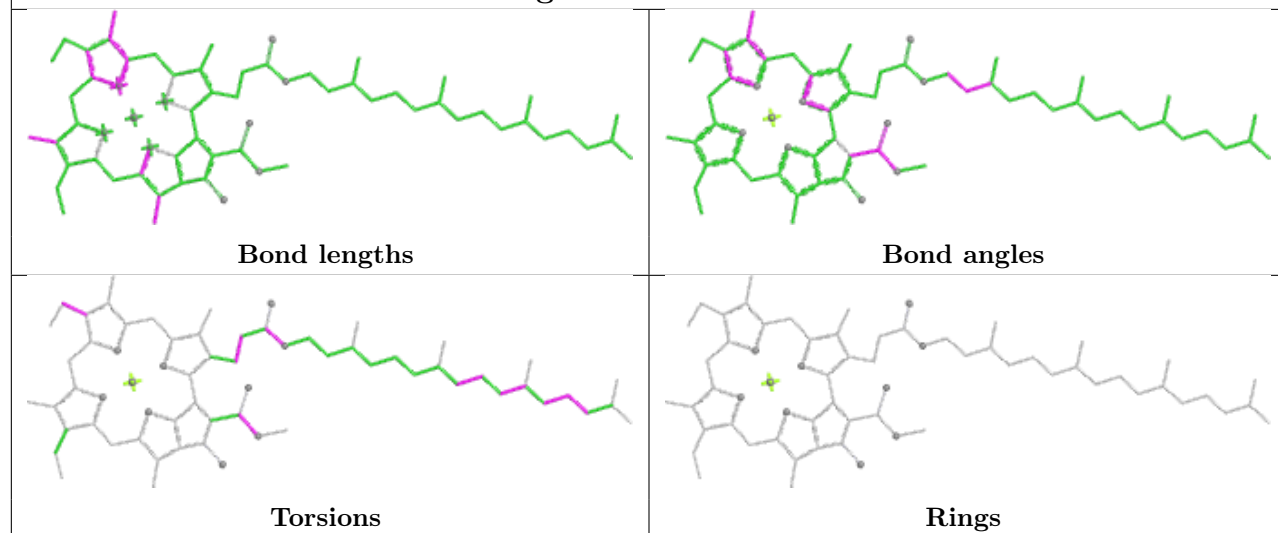


Rings

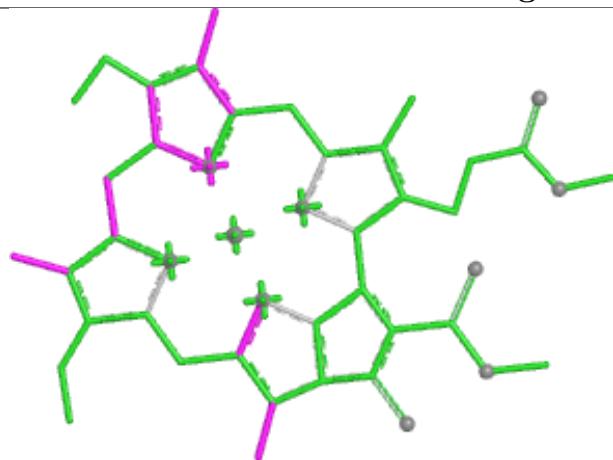
Ligand CLA 2 816



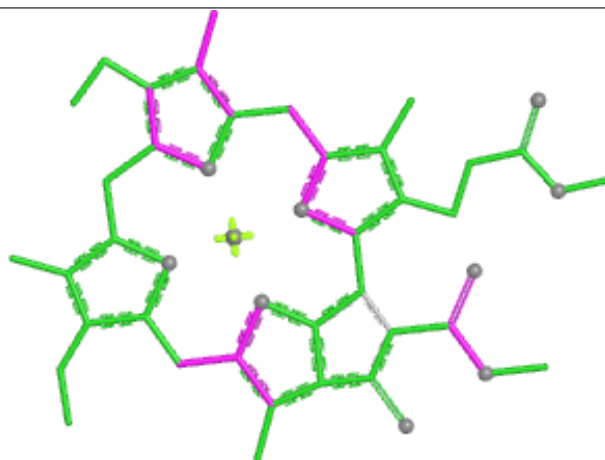
Ligand CLA 1 838



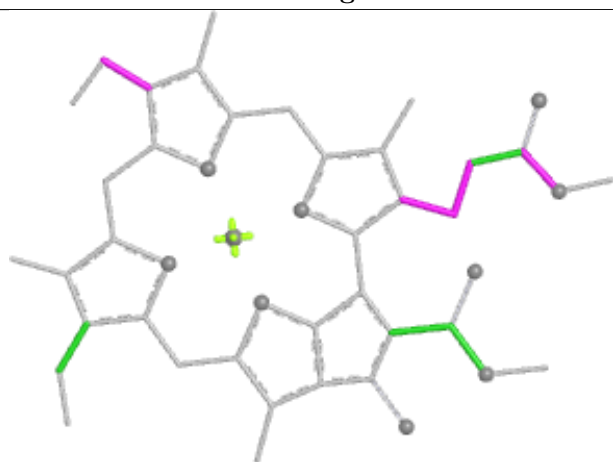
Ligand CLA 2 838



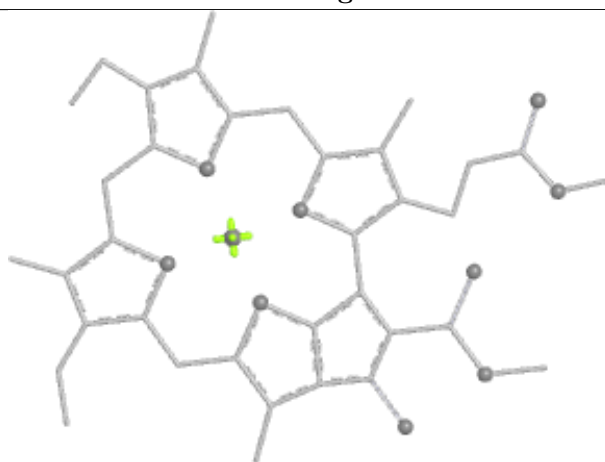
Bond lengths



Bond angles

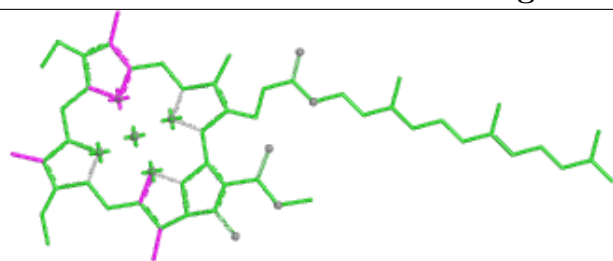


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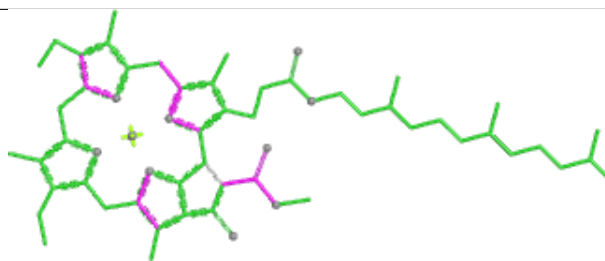


Rings

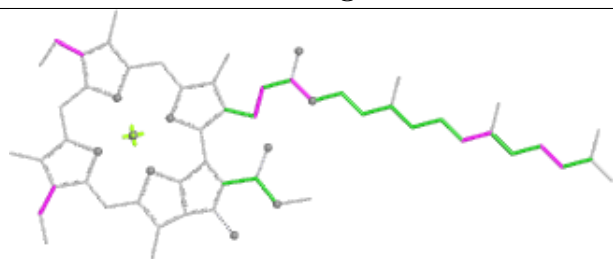
Ligand CLA b 810



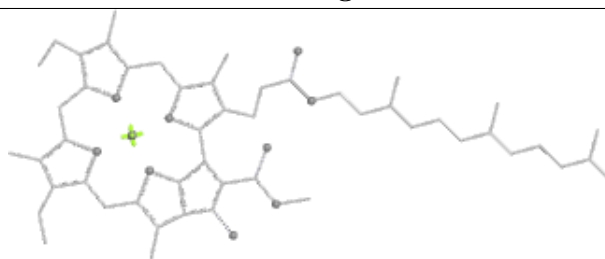
Bond lengths



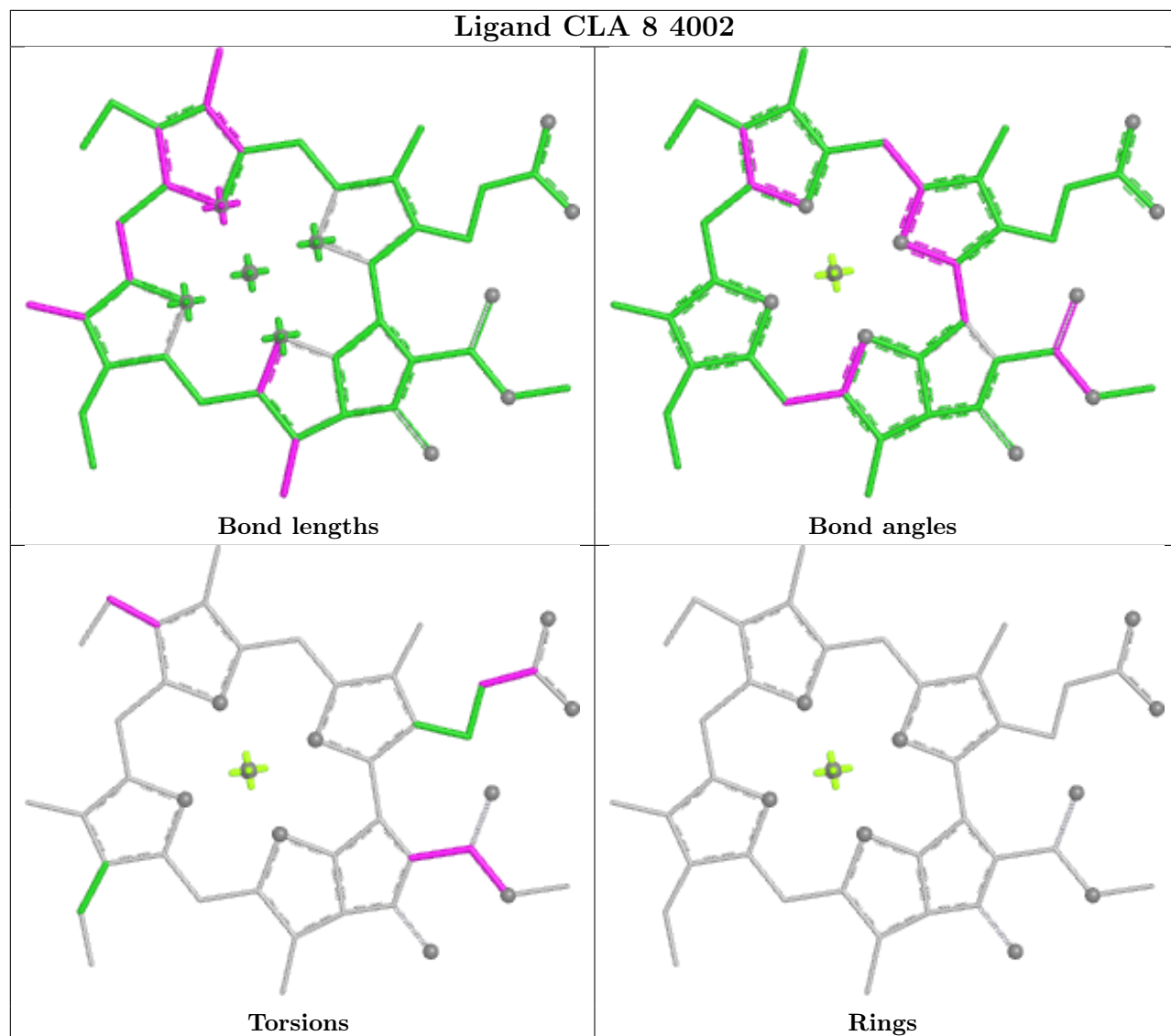
Bond angles



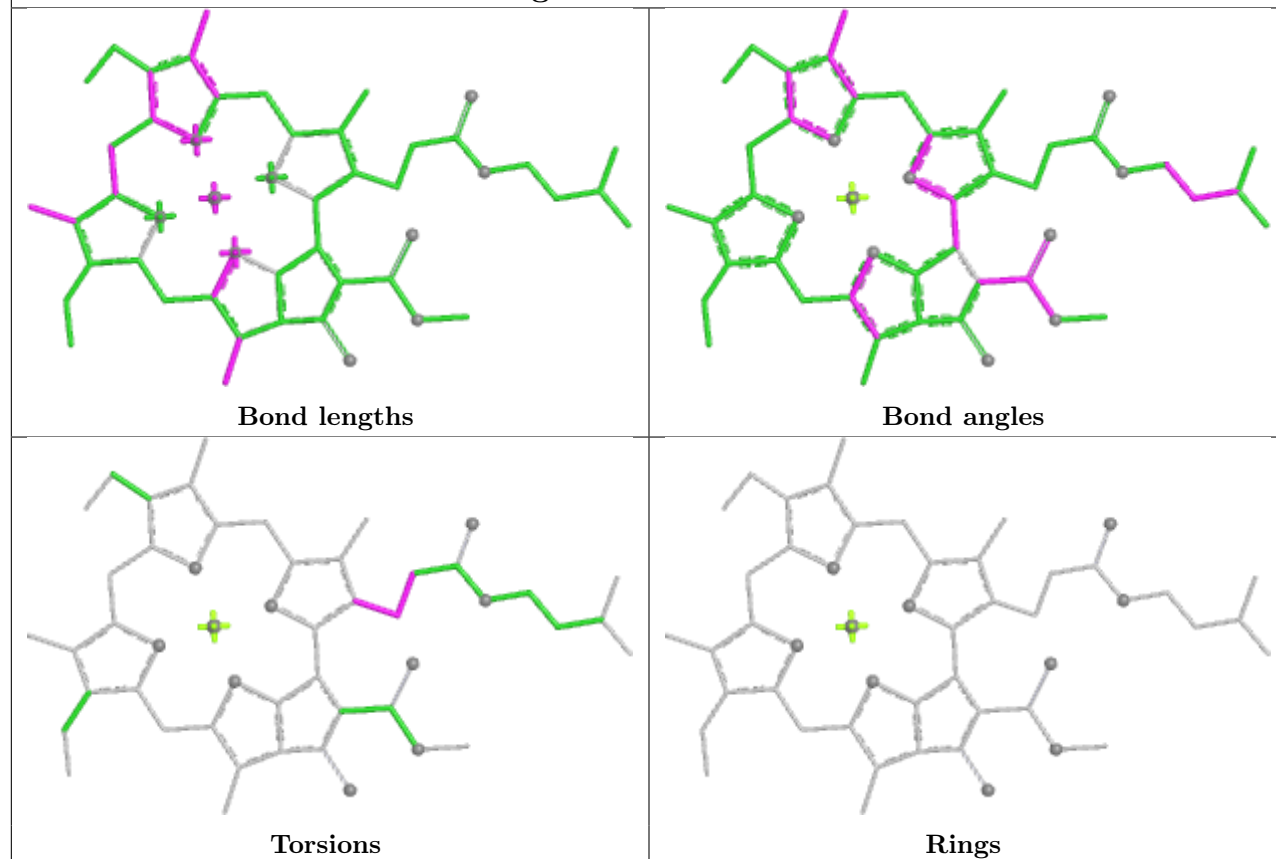
Torsions



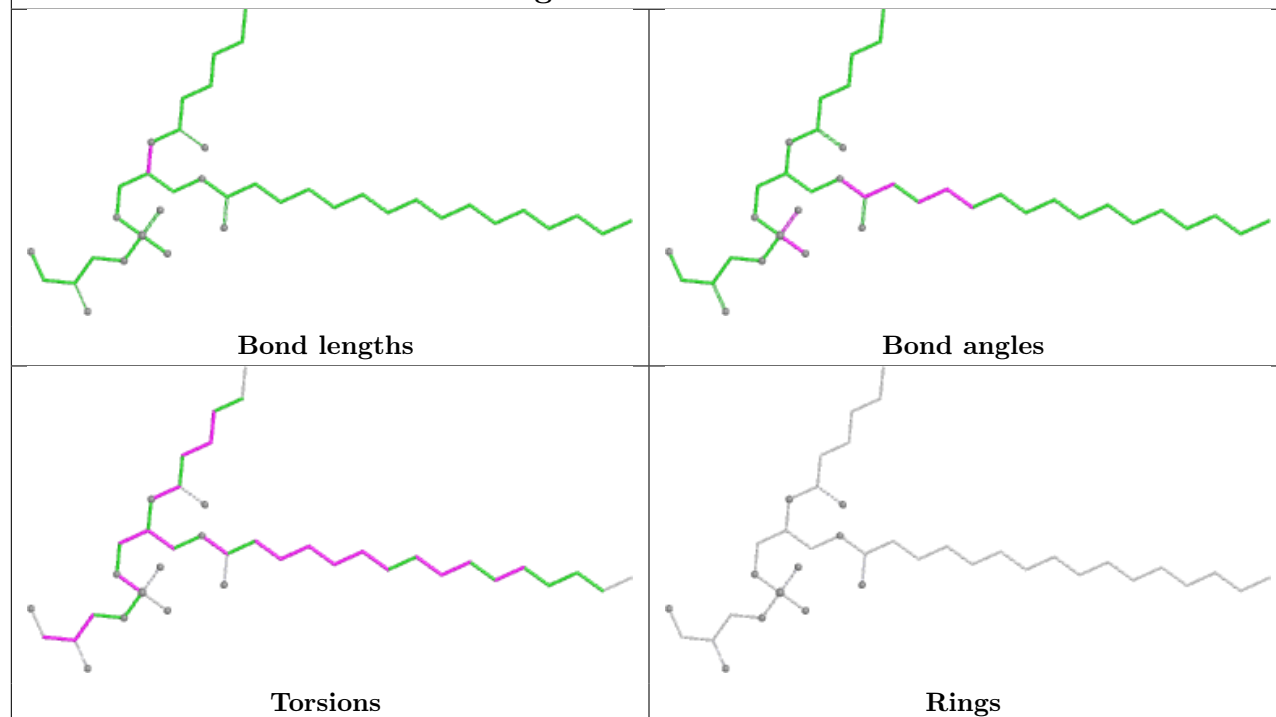
Rings

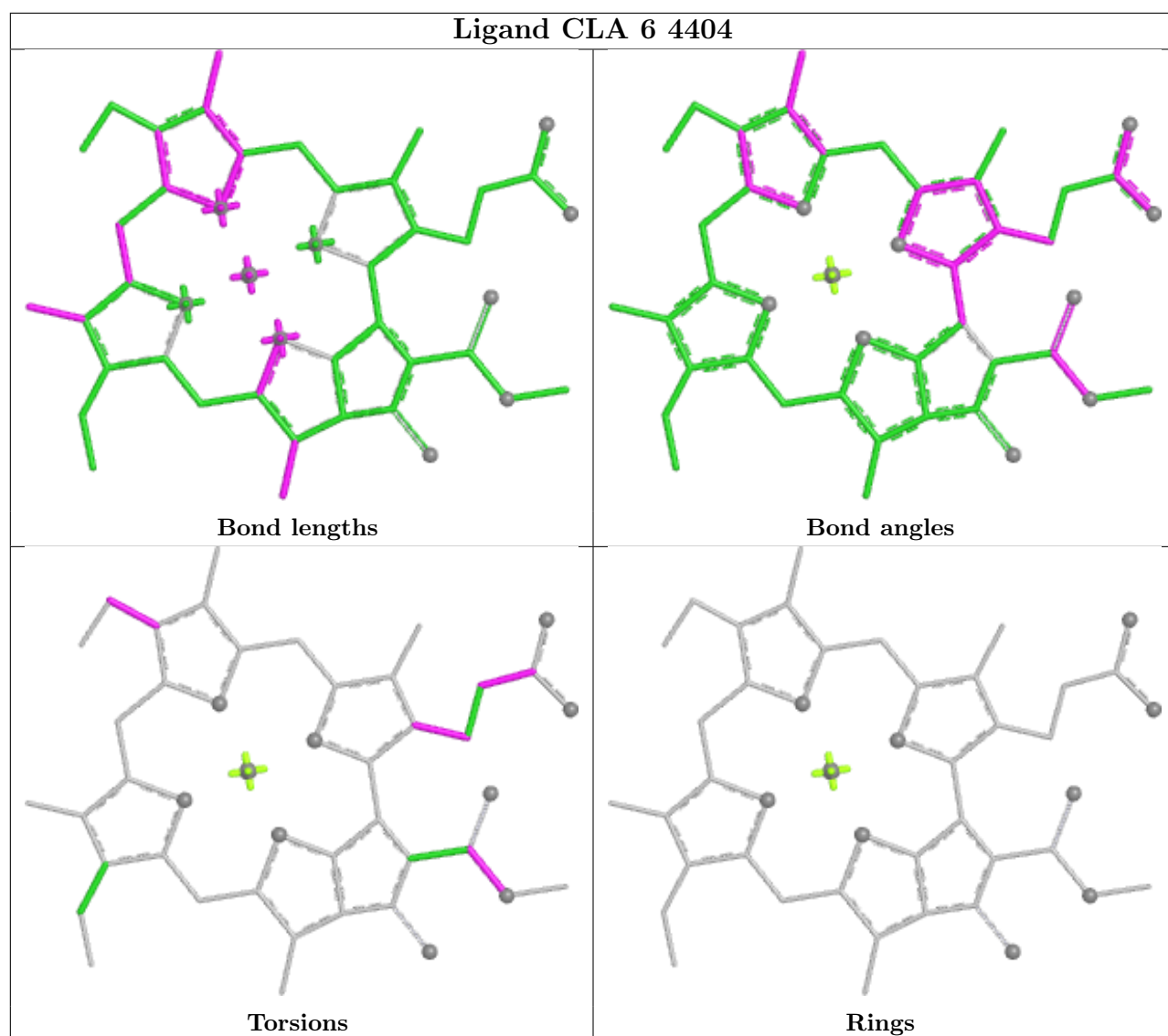


Ligand CLA A 806

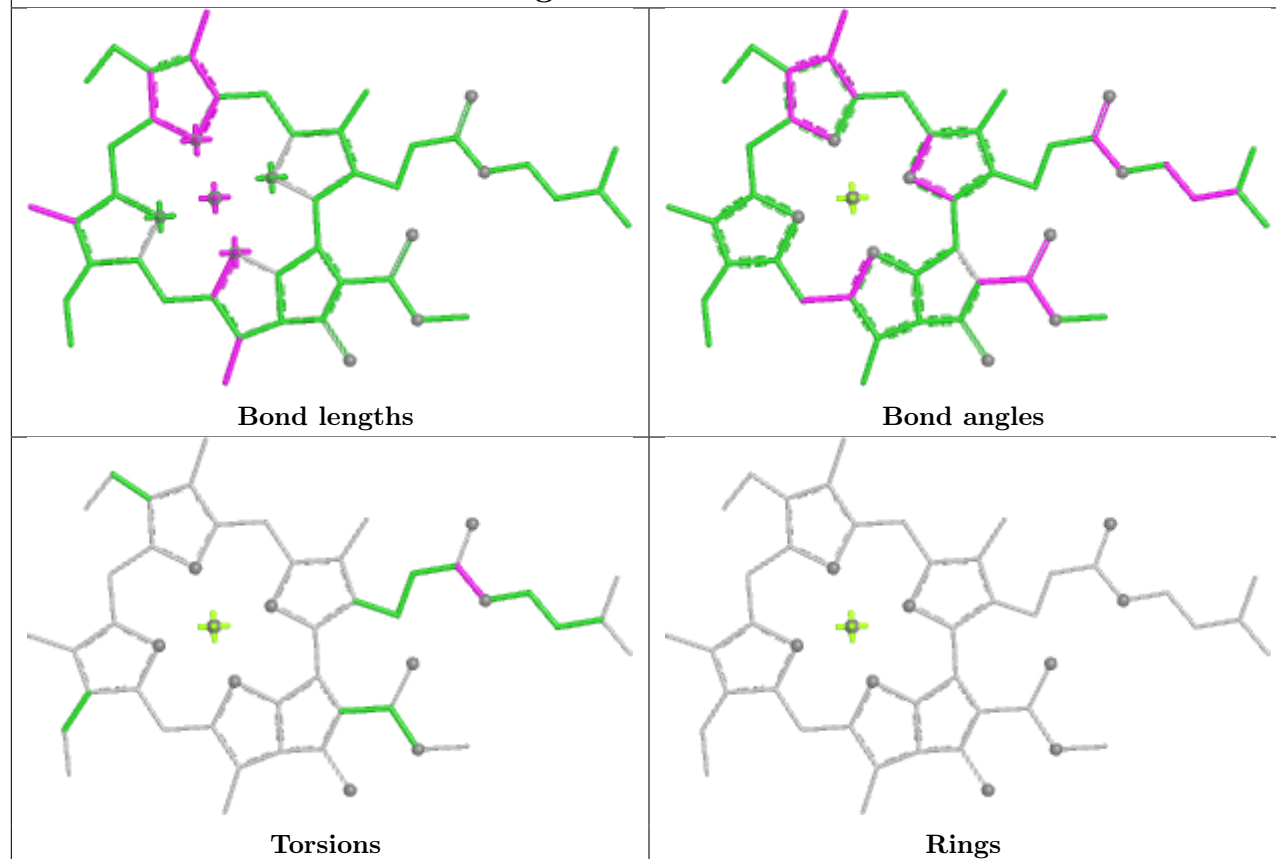


Ligand LHG 2 852

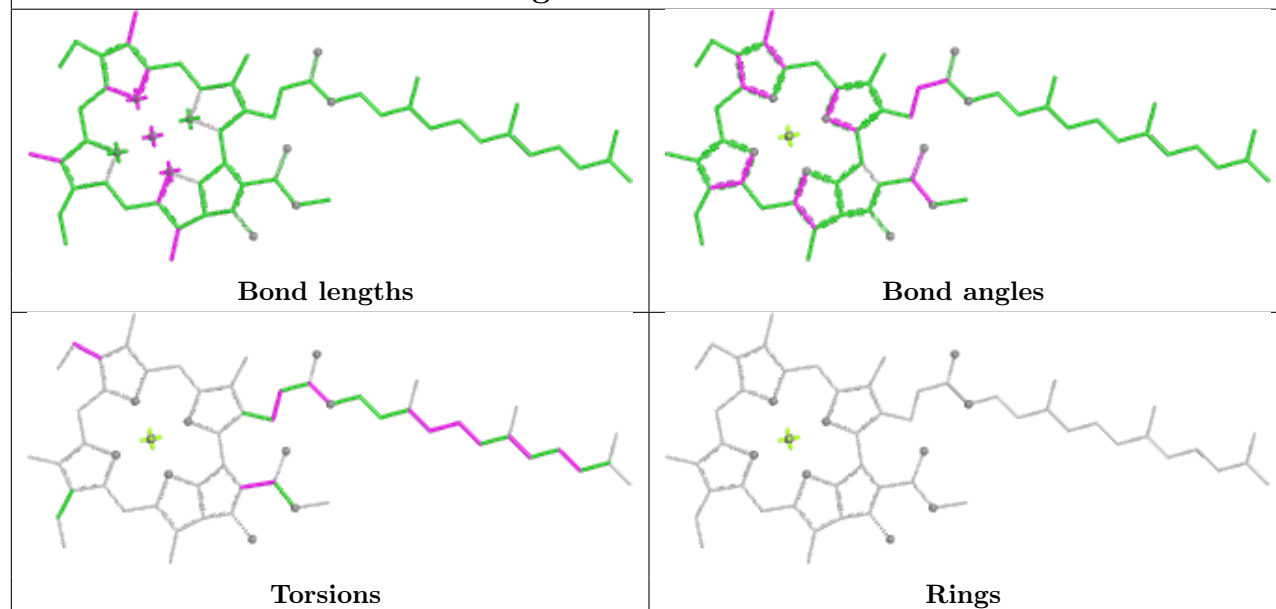




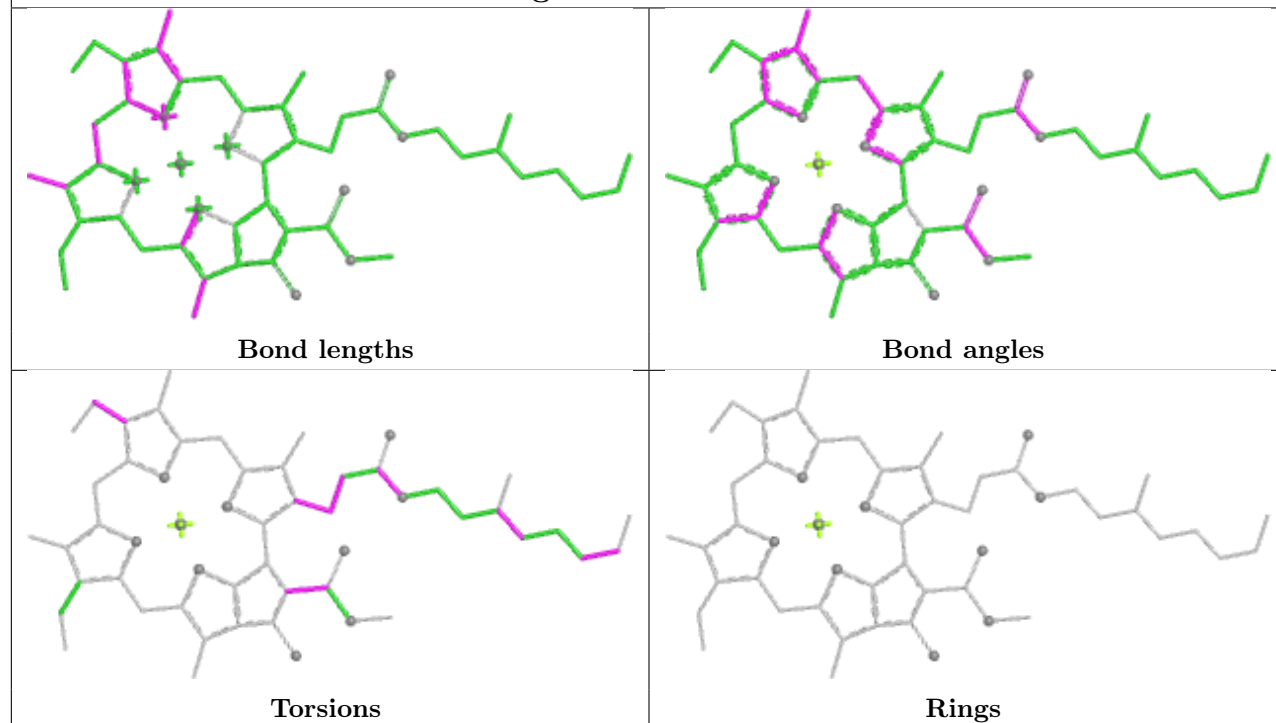
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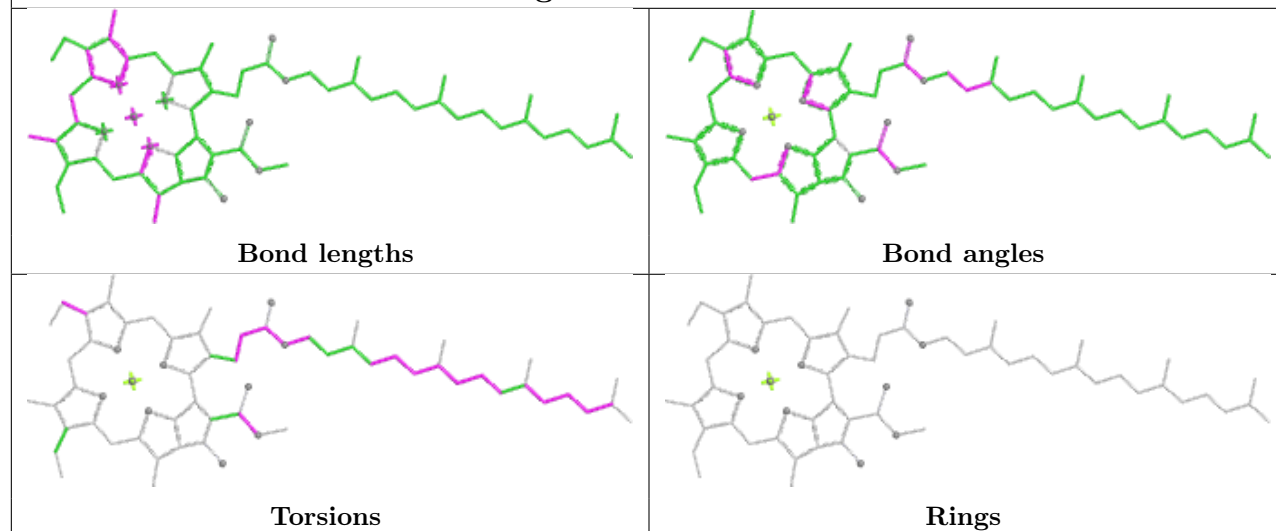
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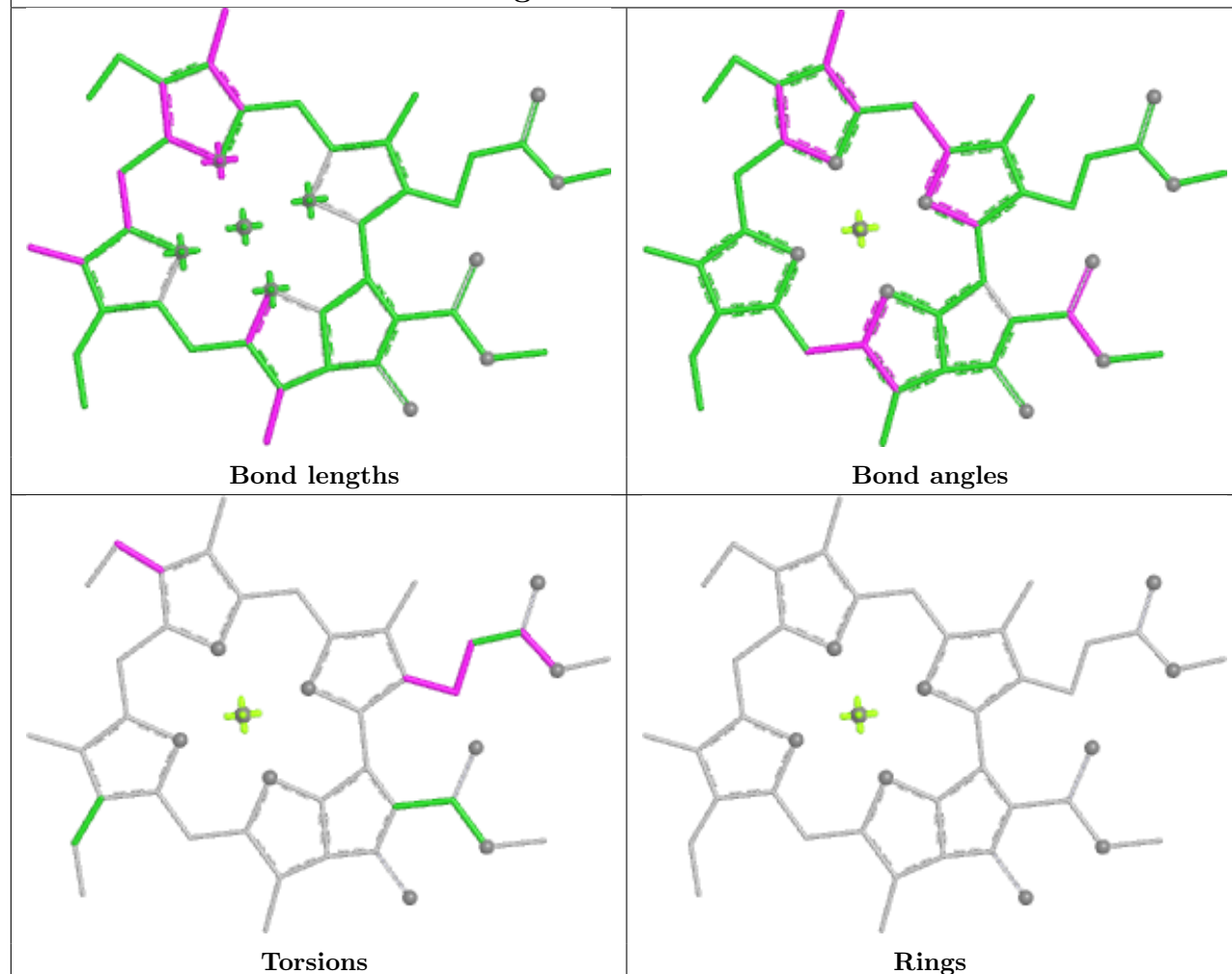
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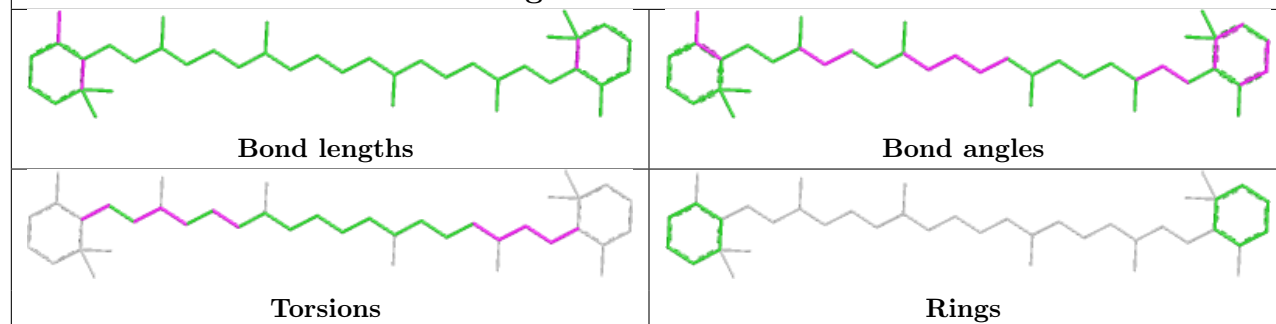
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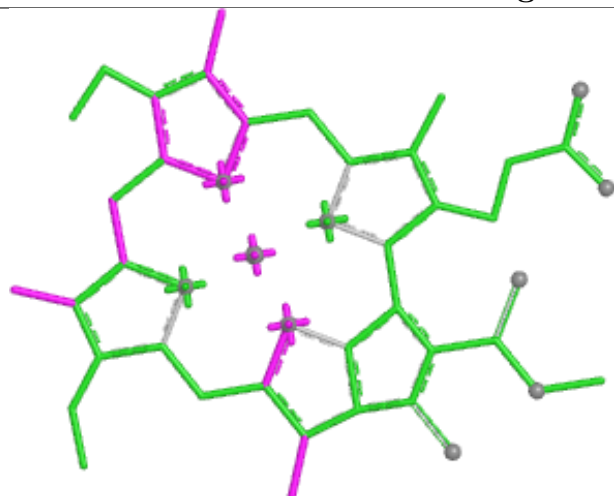
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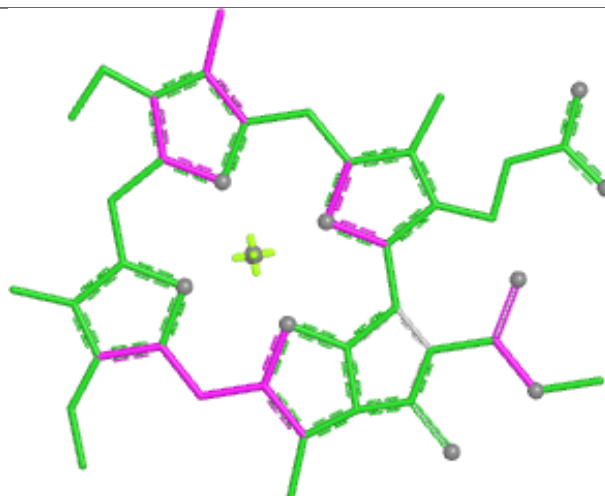
Ligand BCR 8 4001



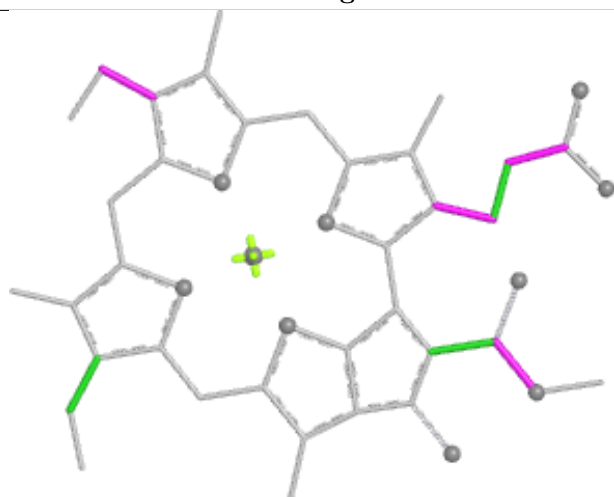
Ligand CLA b 832



Bond lengths



Bond angles

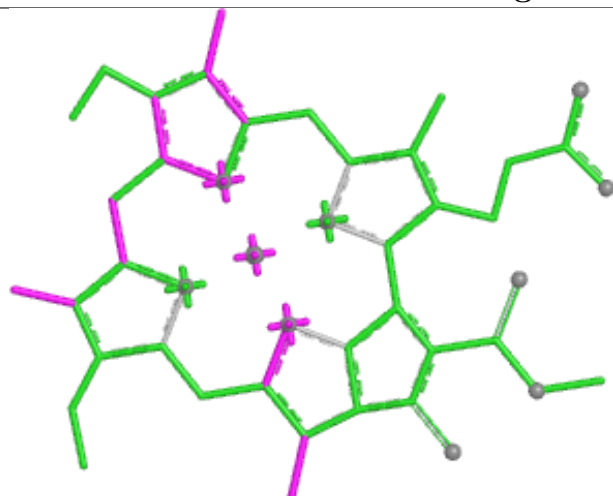


Torsions

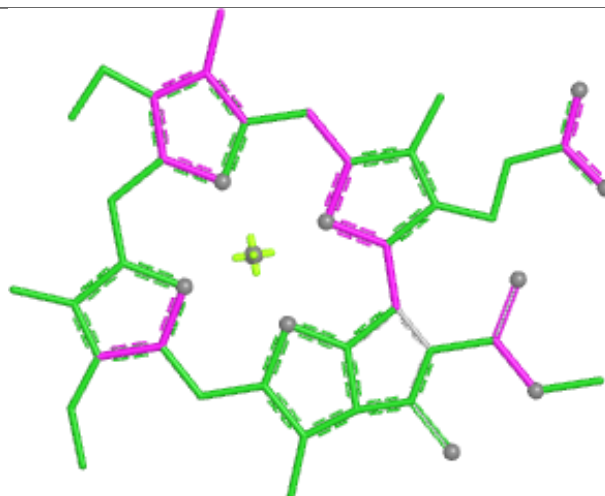


Rings

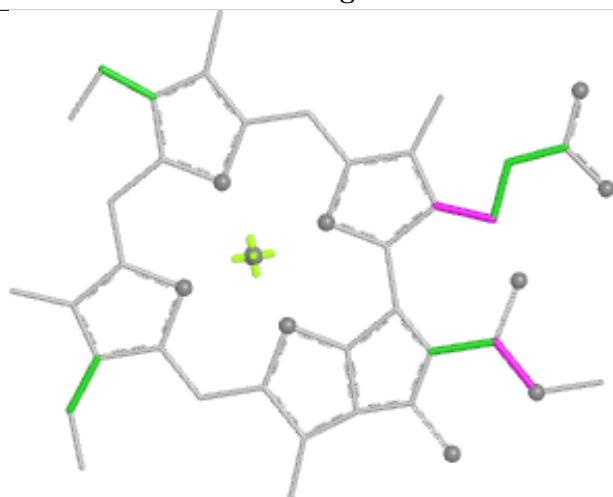
Ligand CLA B 837



Bond lengths



Bond angles

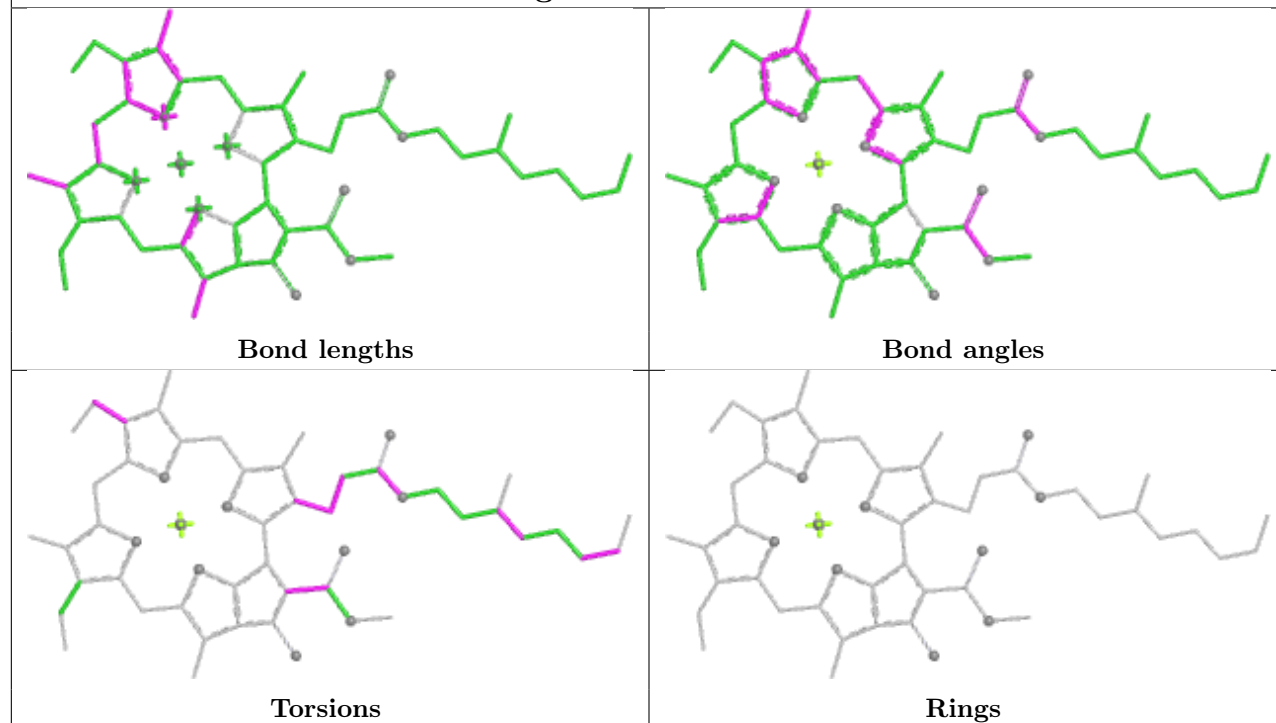


Torsions

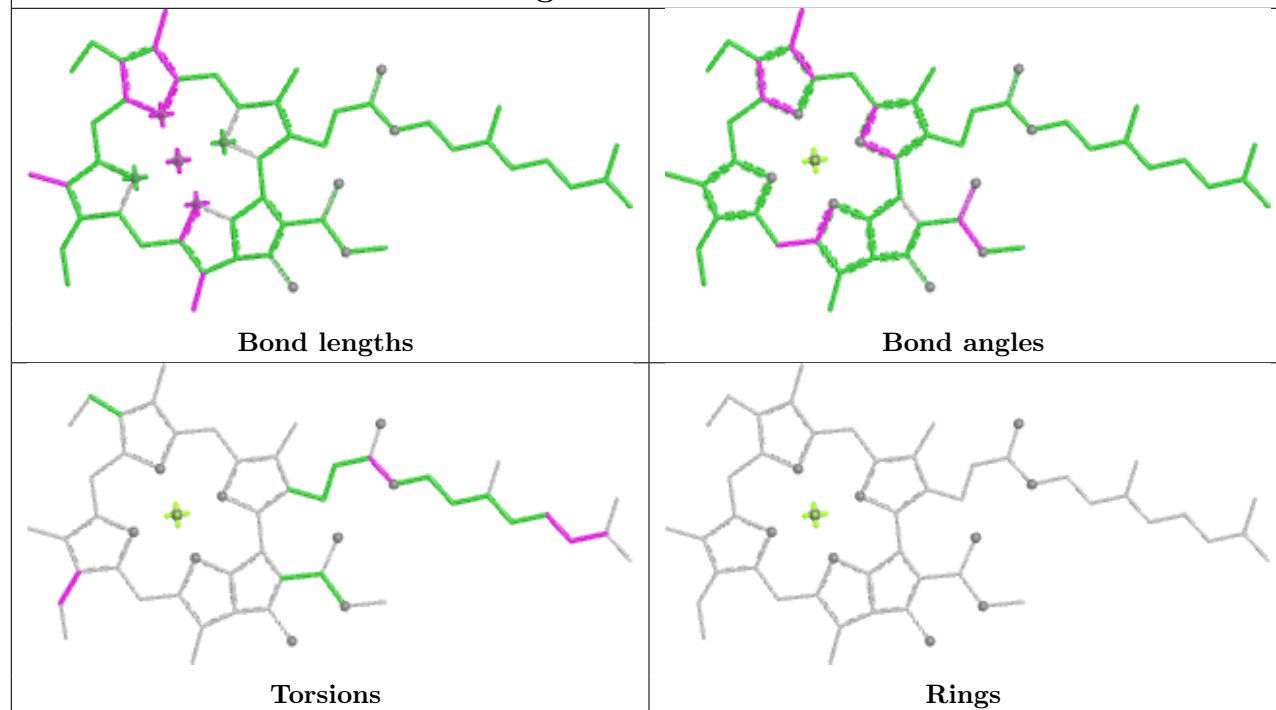


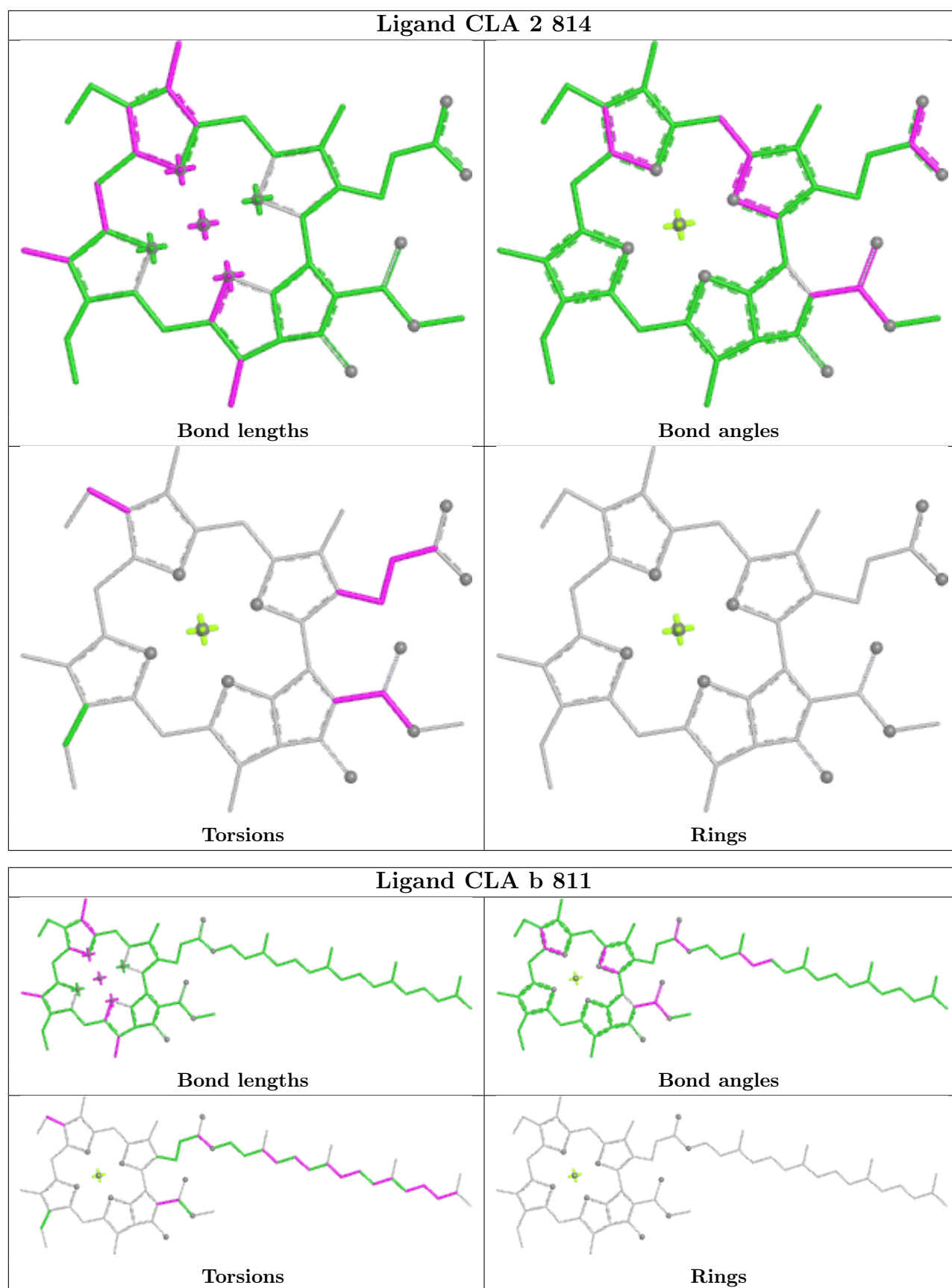
Rings

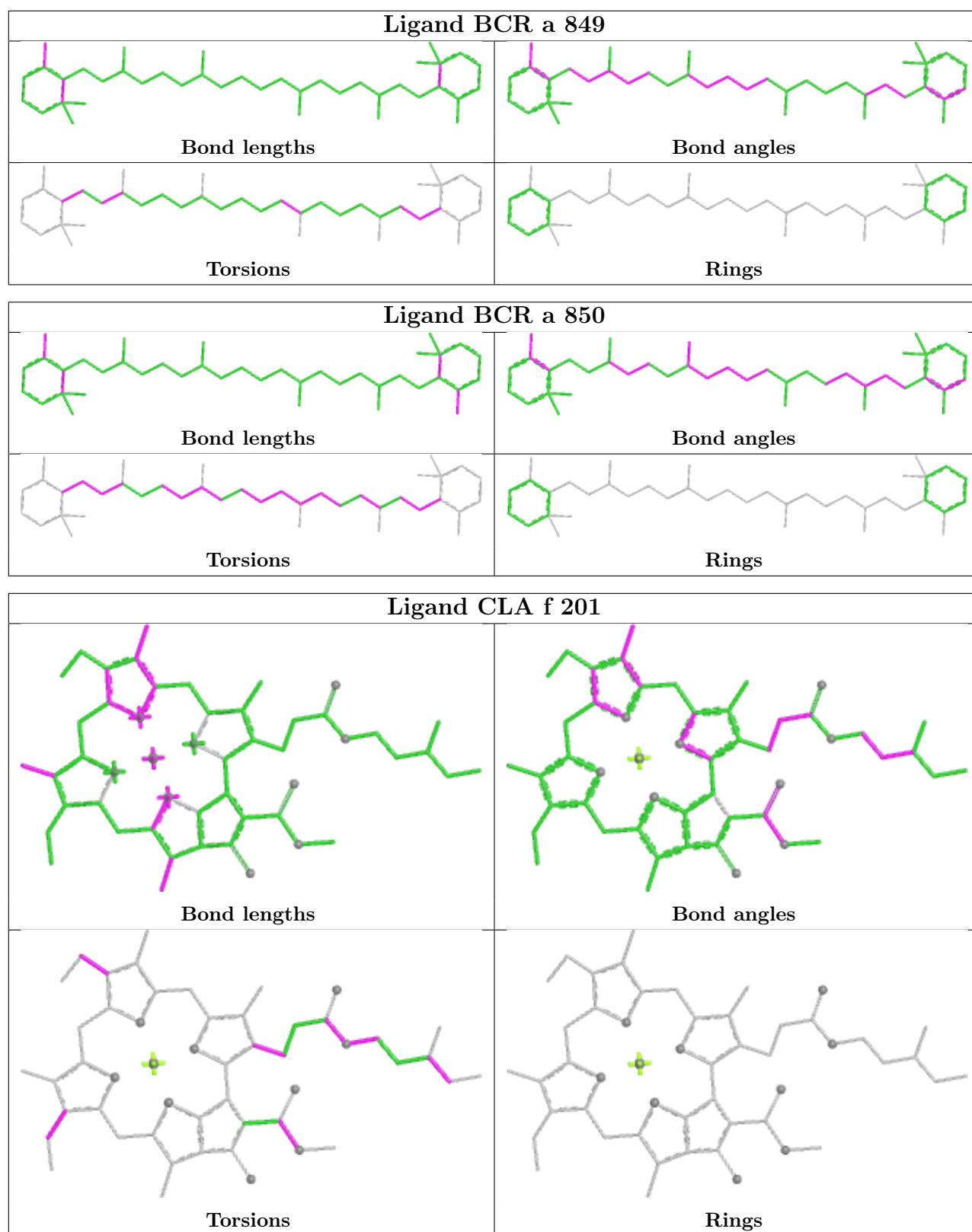
Ligand CLA b 807



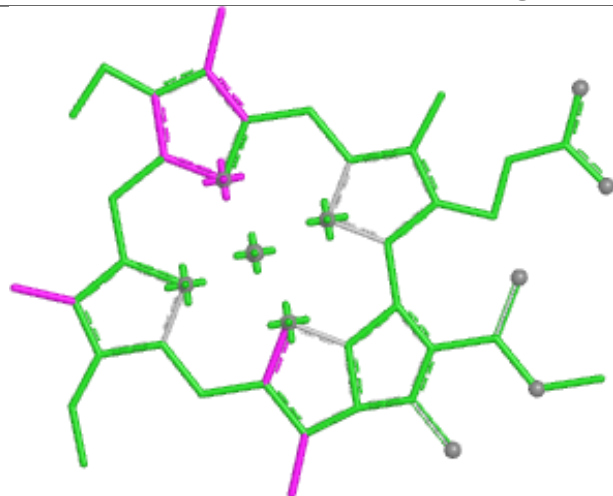
Ligand CLA 1 827



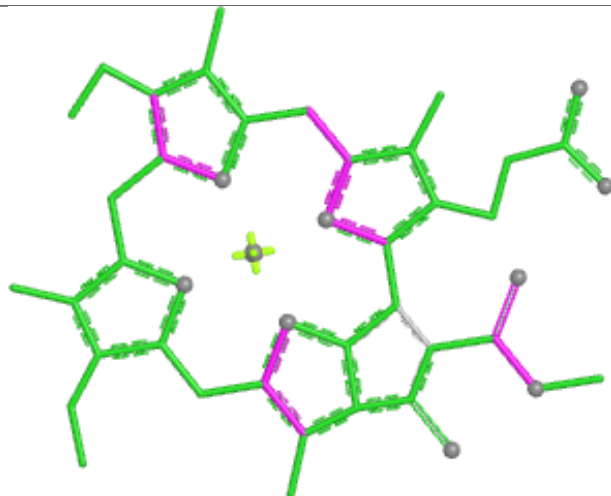




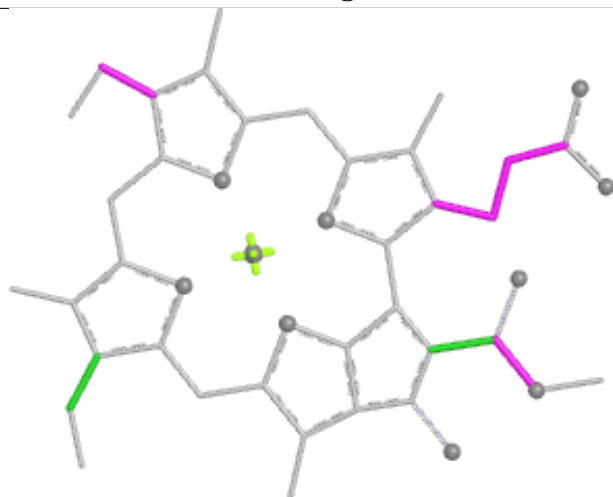
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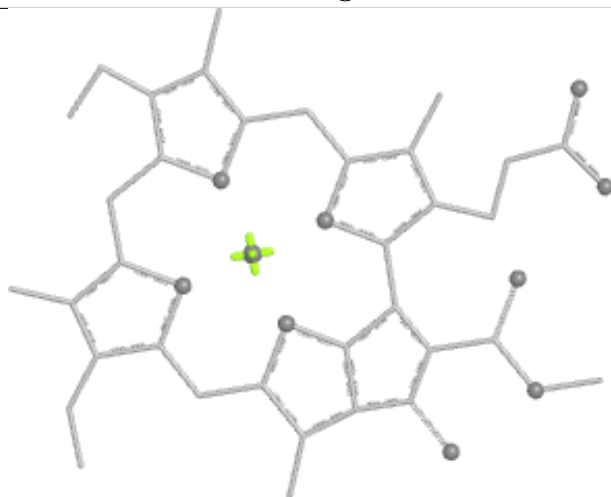
Bond lengths



Bond angles

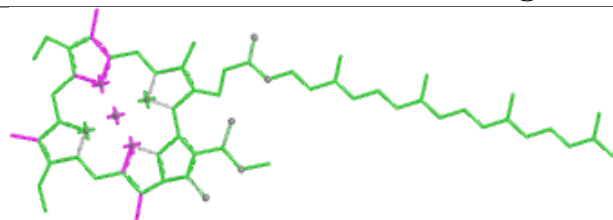


Torsions

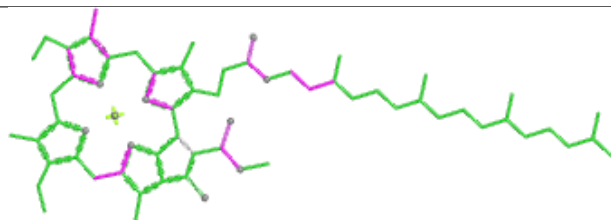


Rings

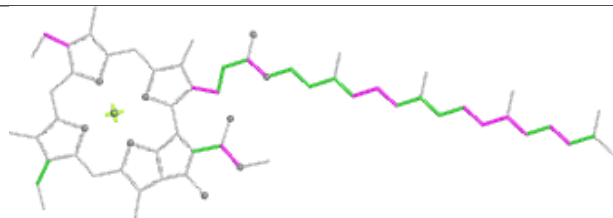
Ligand CLA 1 807



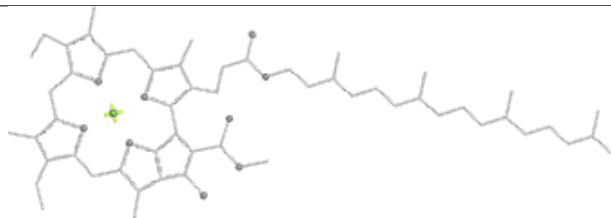
Bond lengths



Bond angles

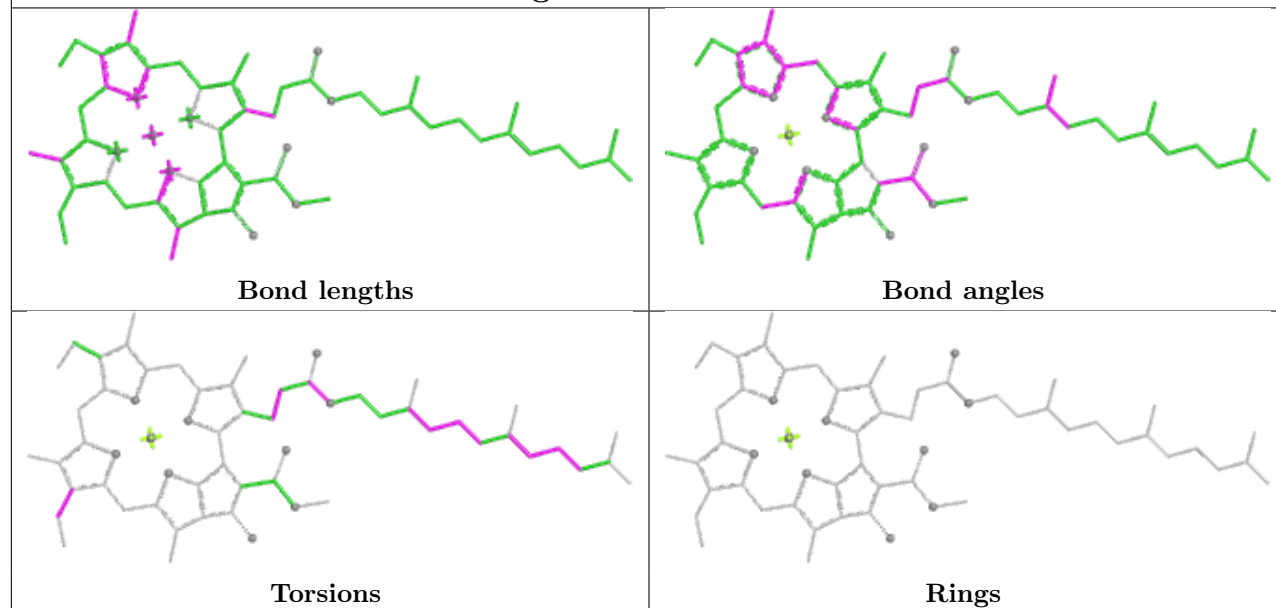


Torsions

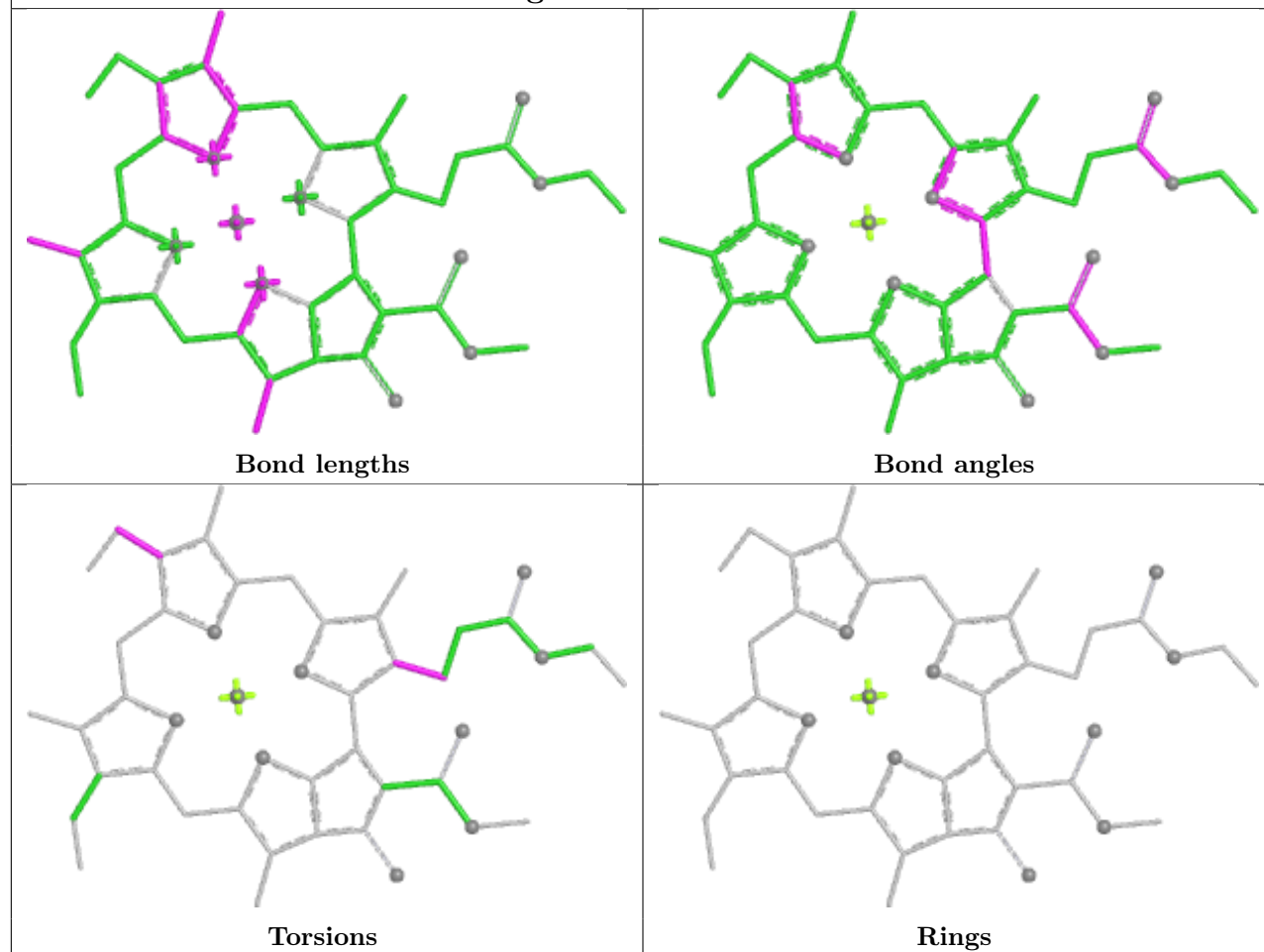


Rings

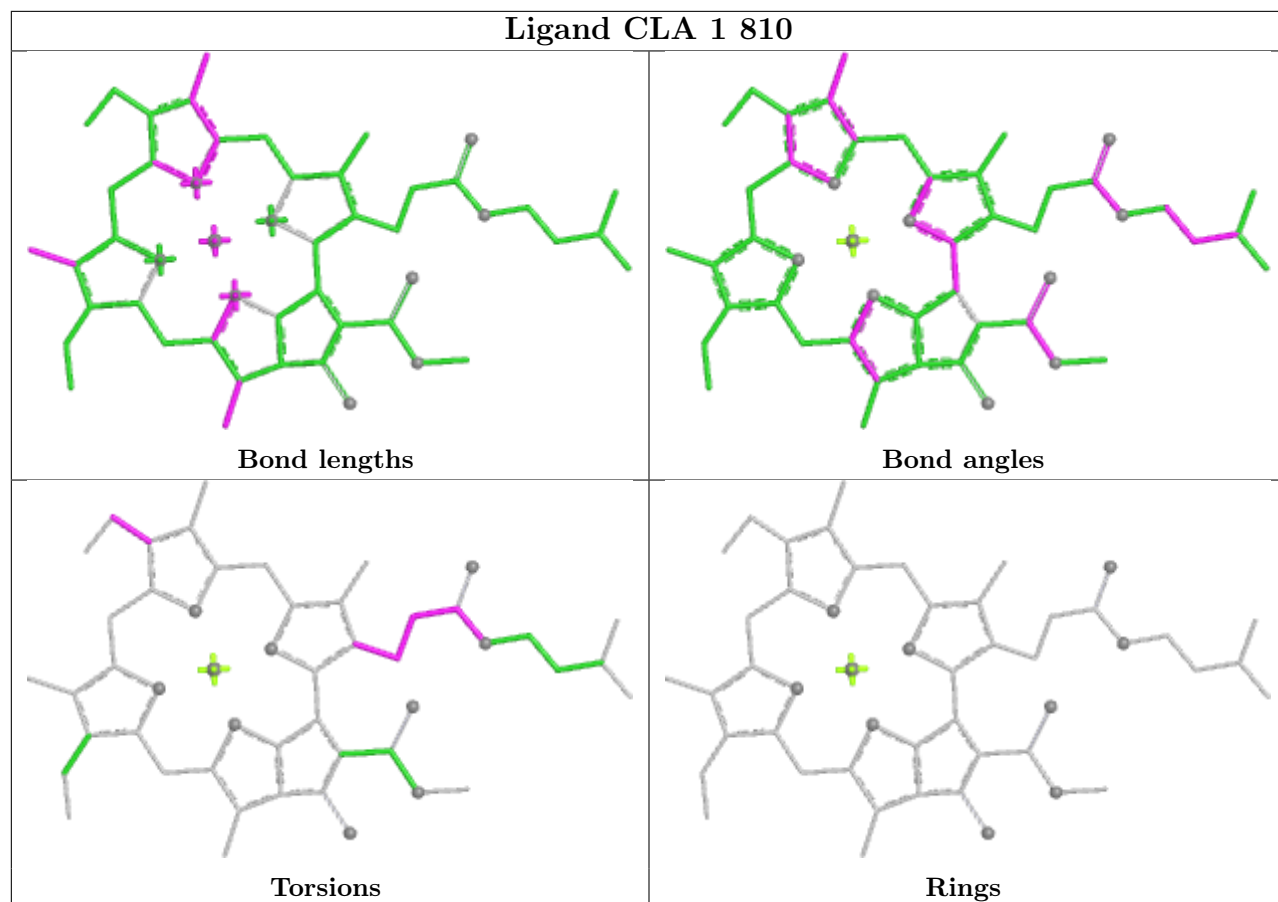
Ligand CLA B 801



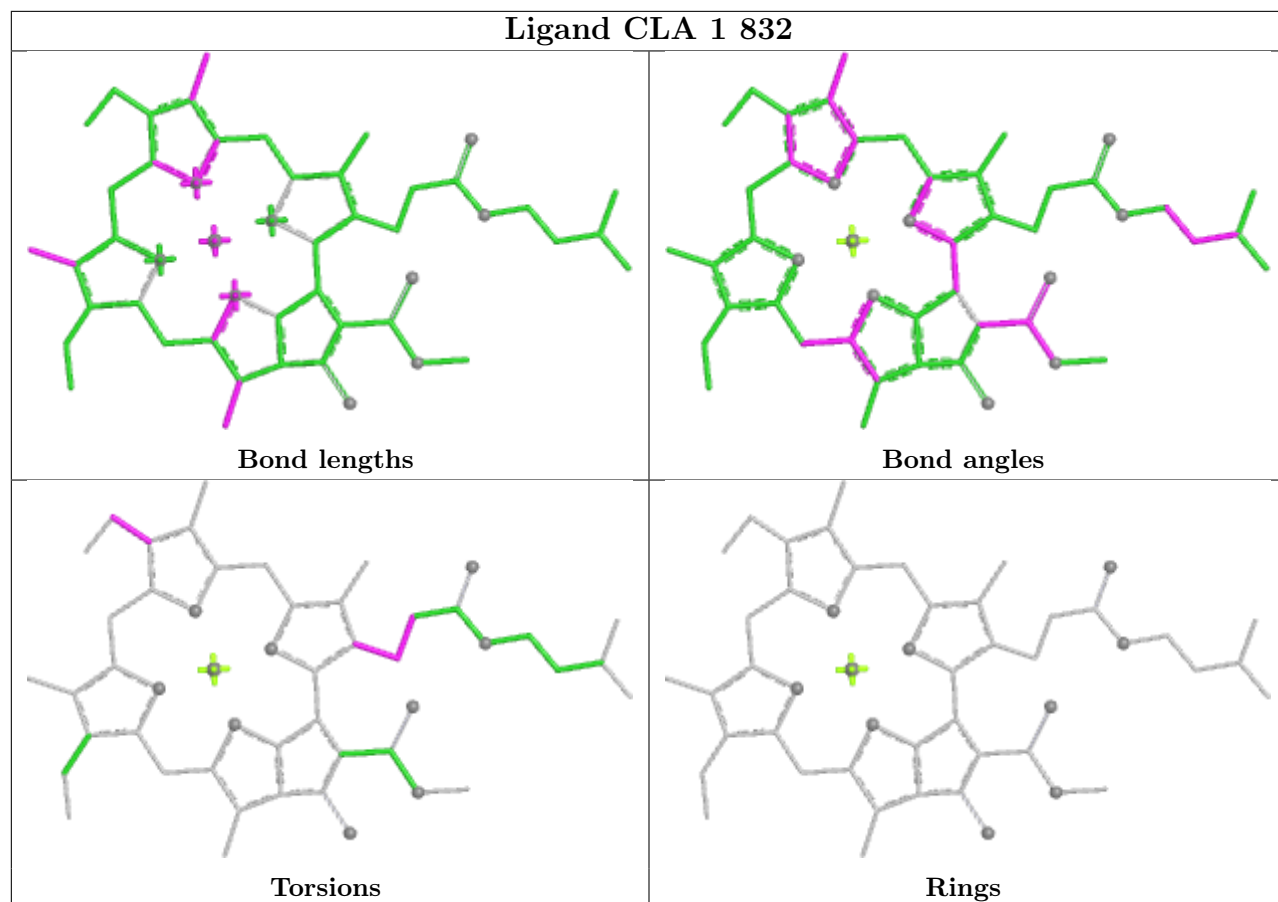
Ligand CLA A 840



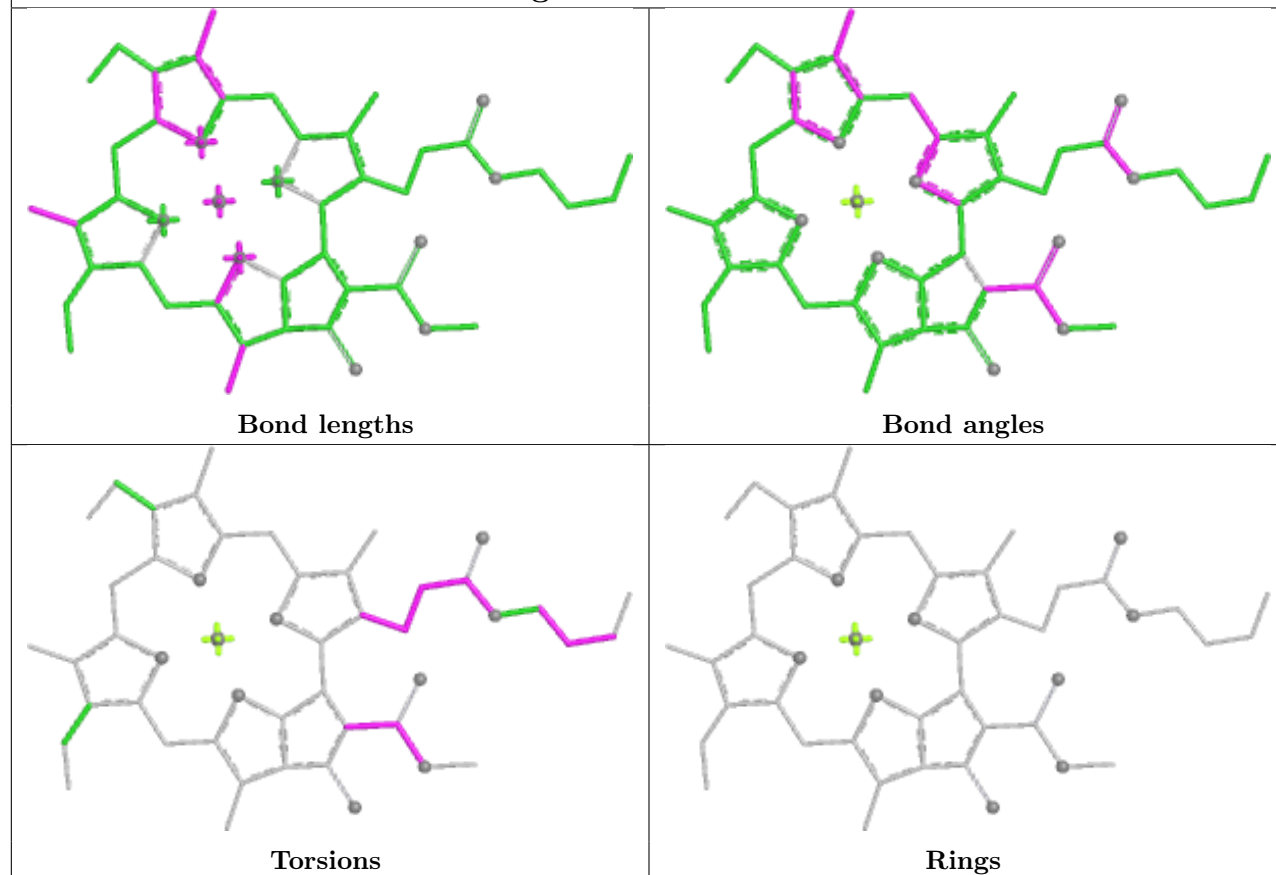
Ligand CLA 1 810



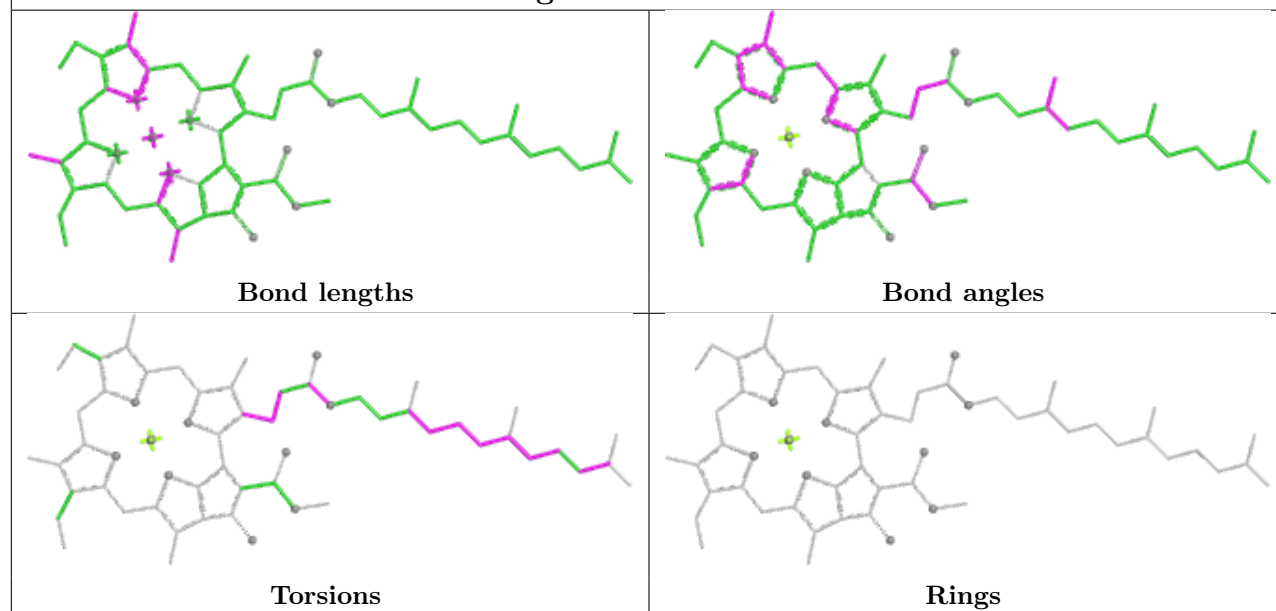
Ligand CLA 1 832

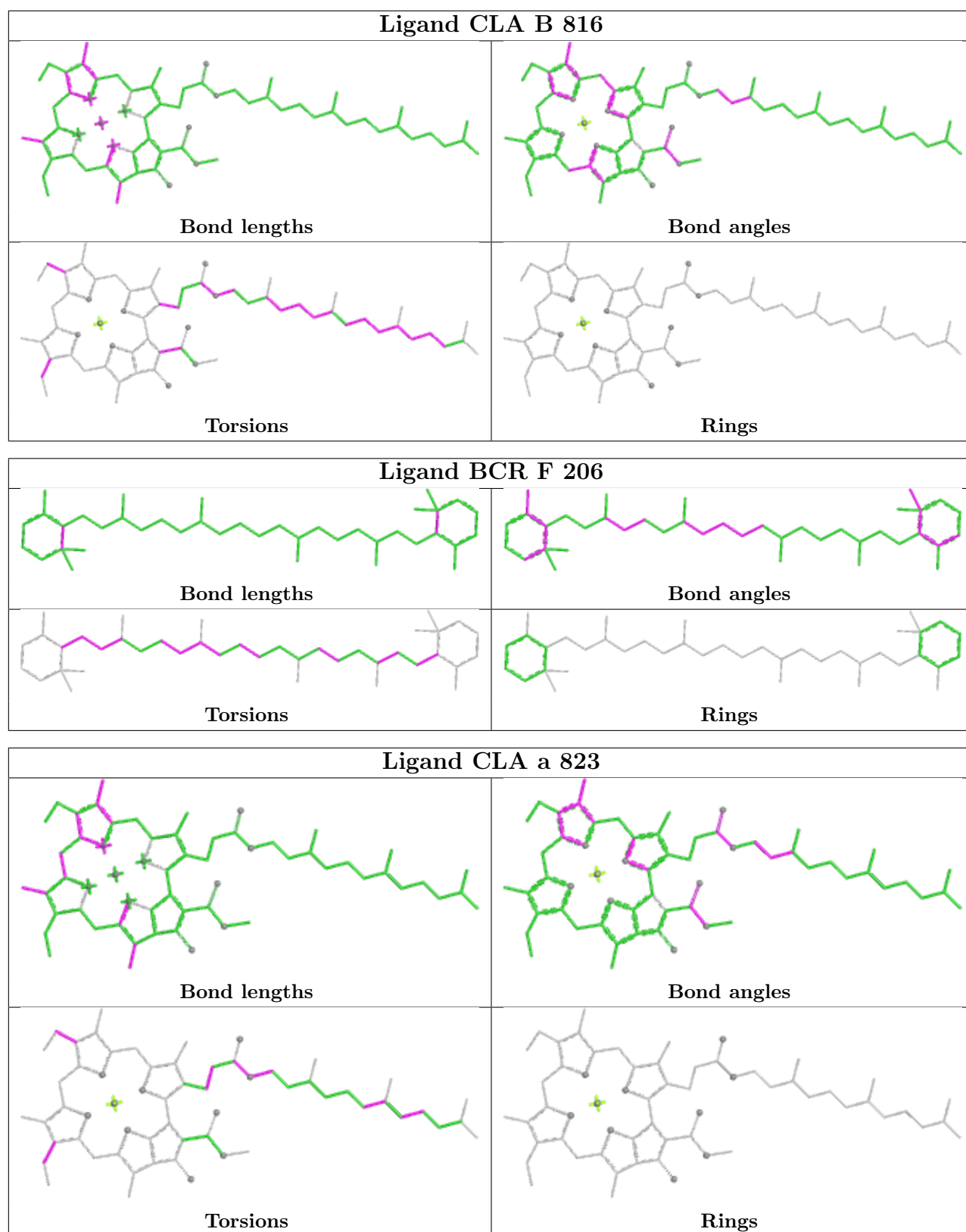


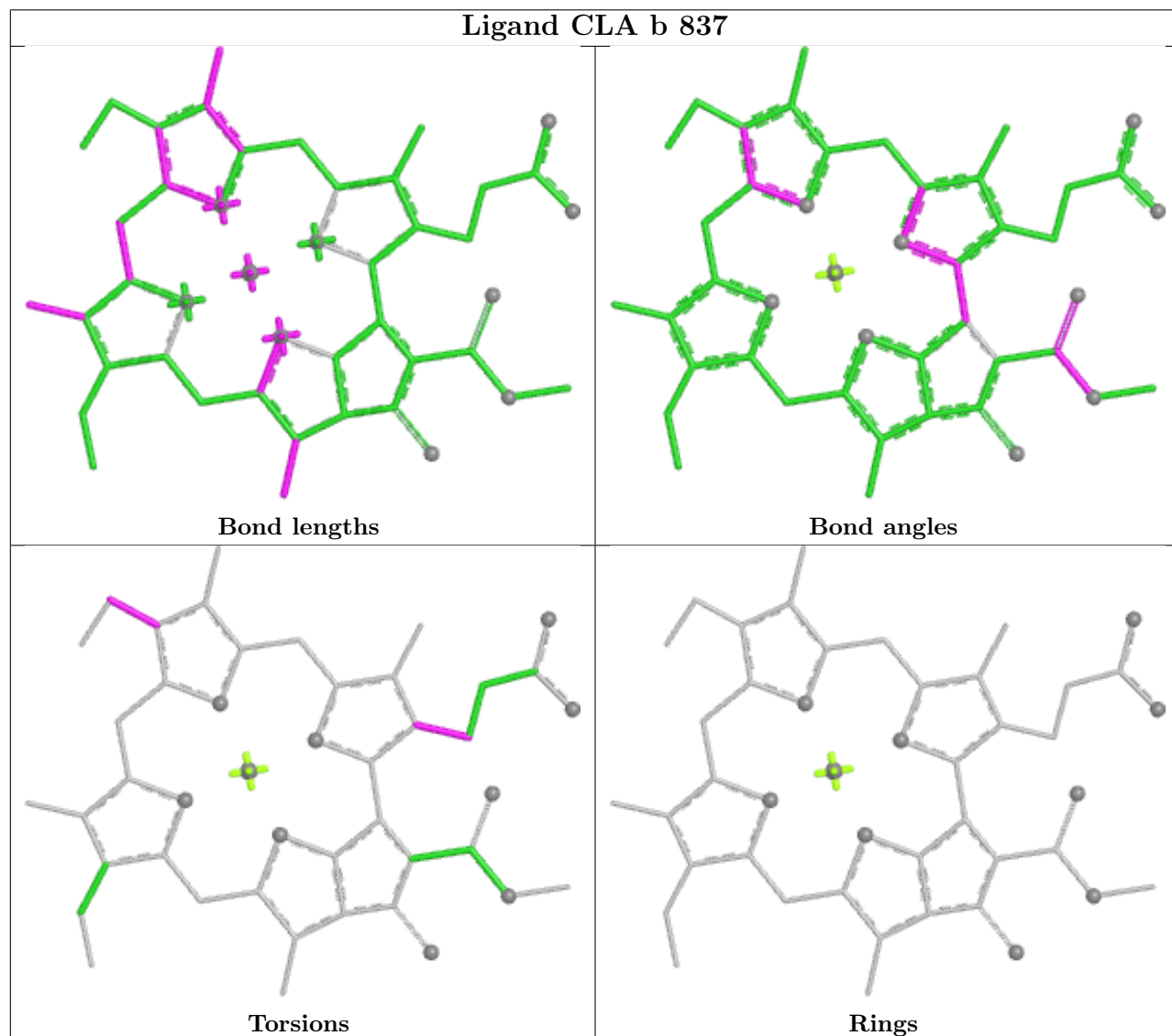
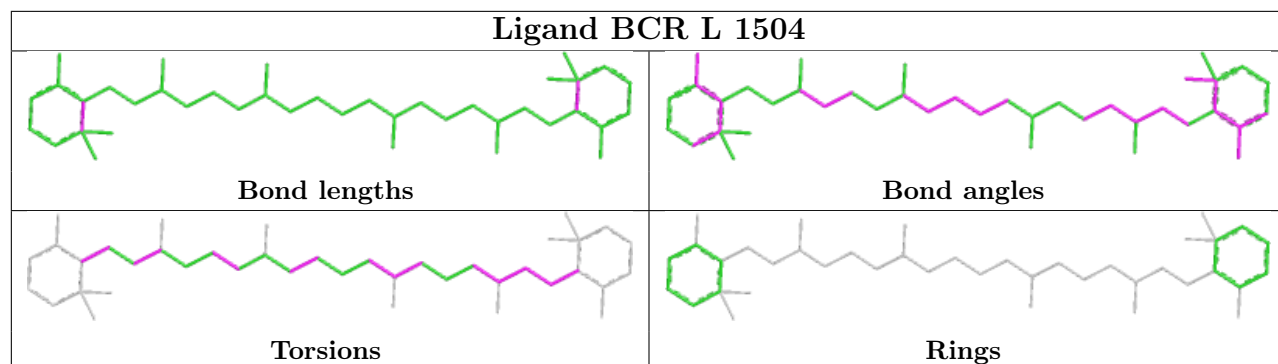
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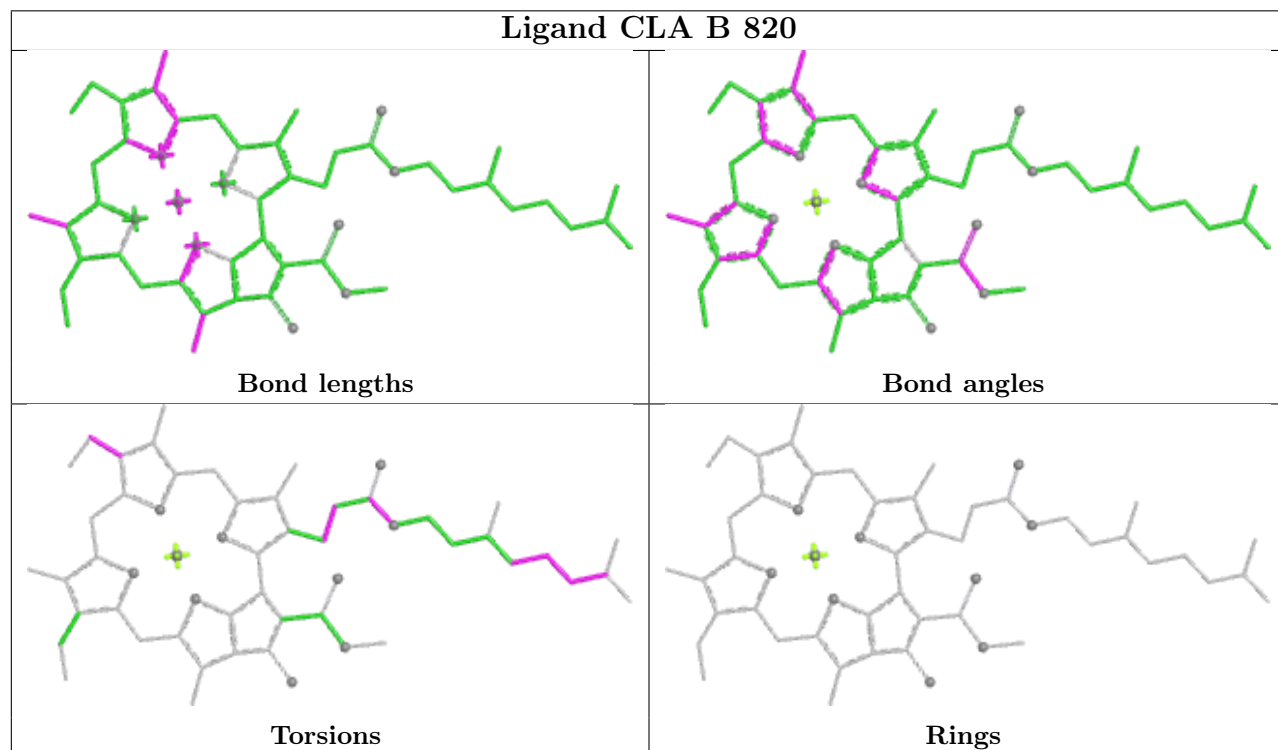
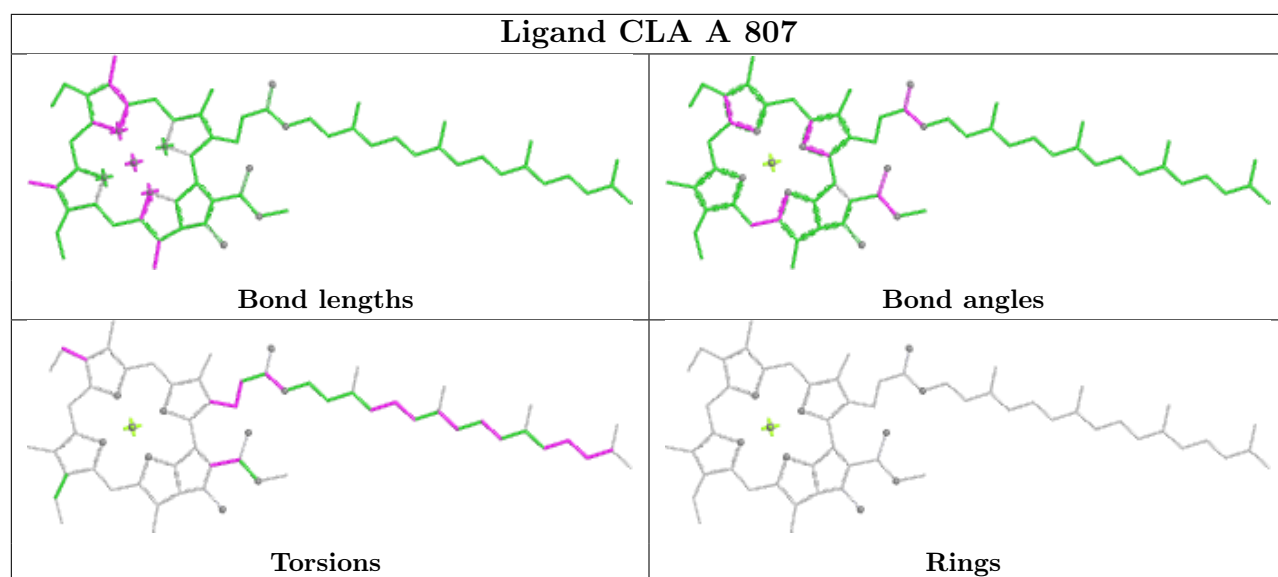


Ligand CLA 2 820

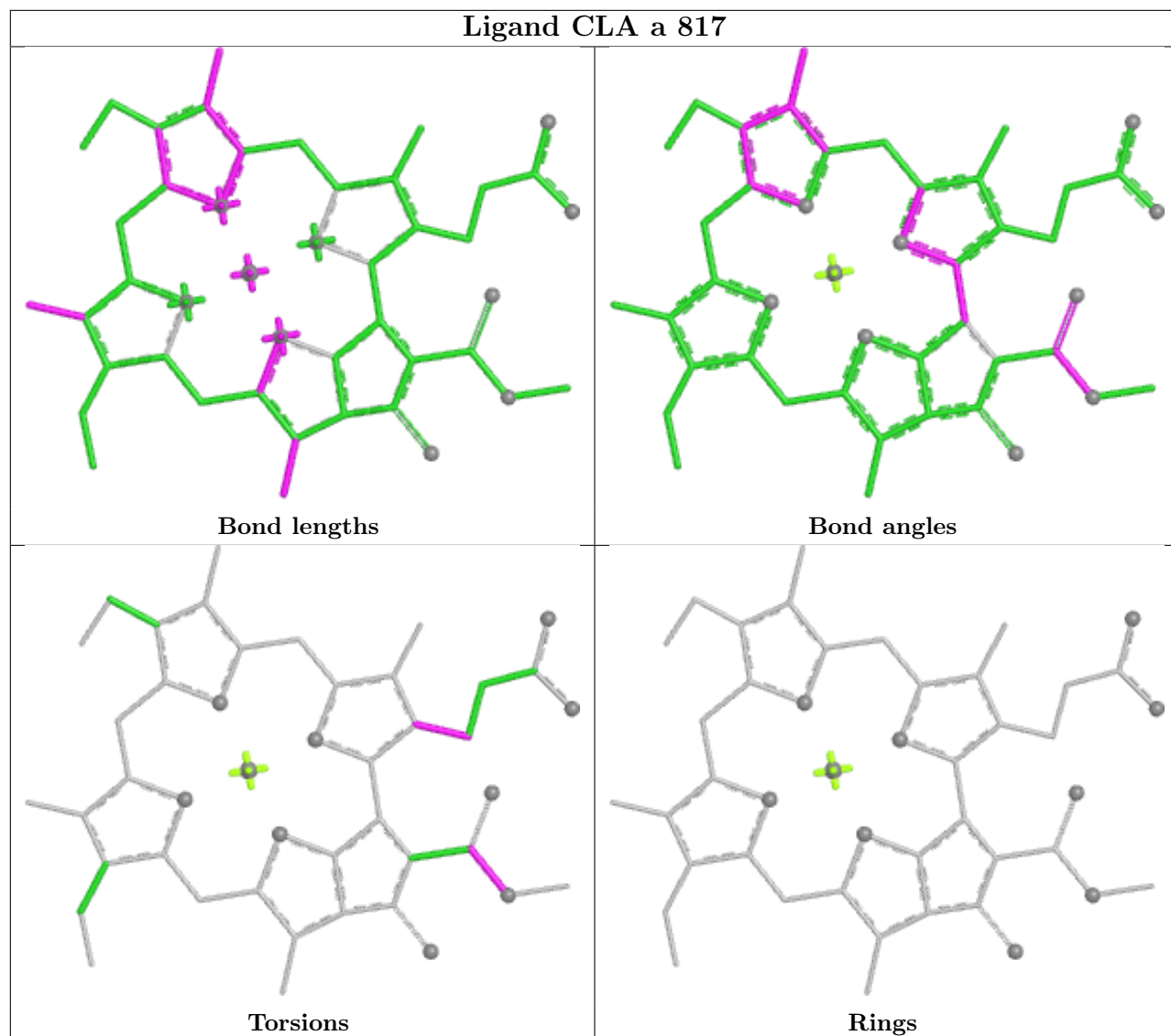




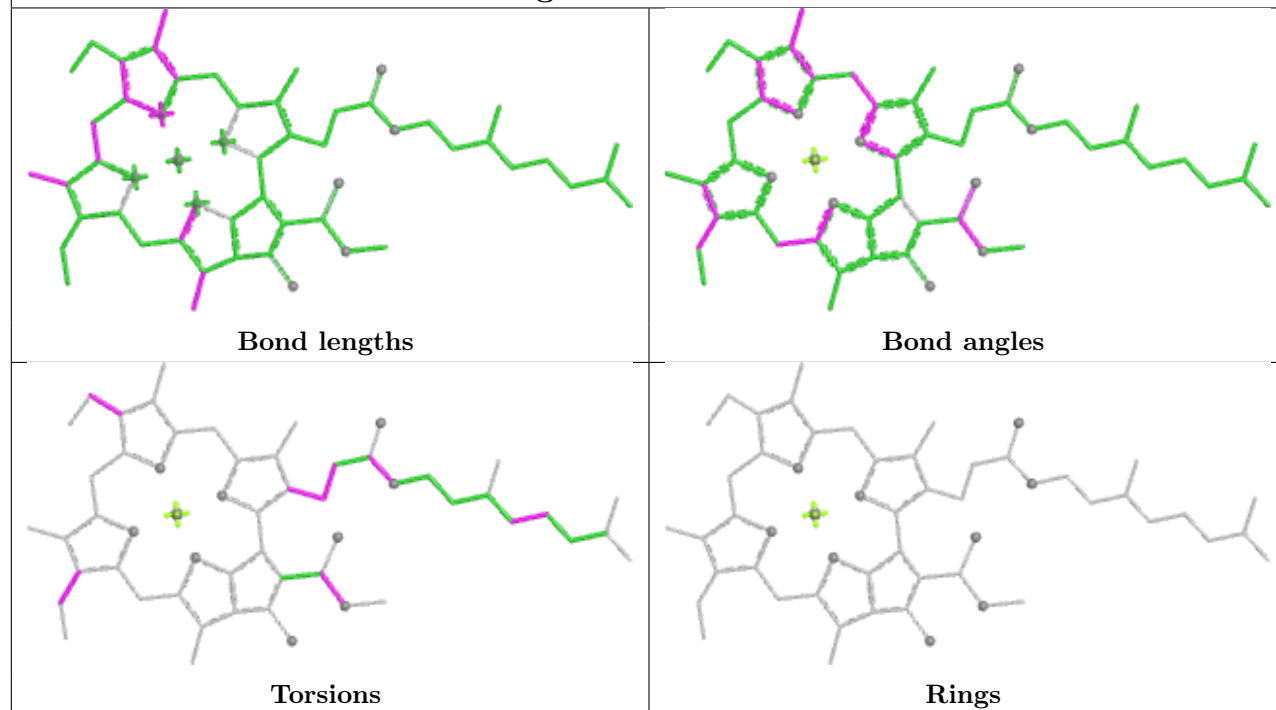




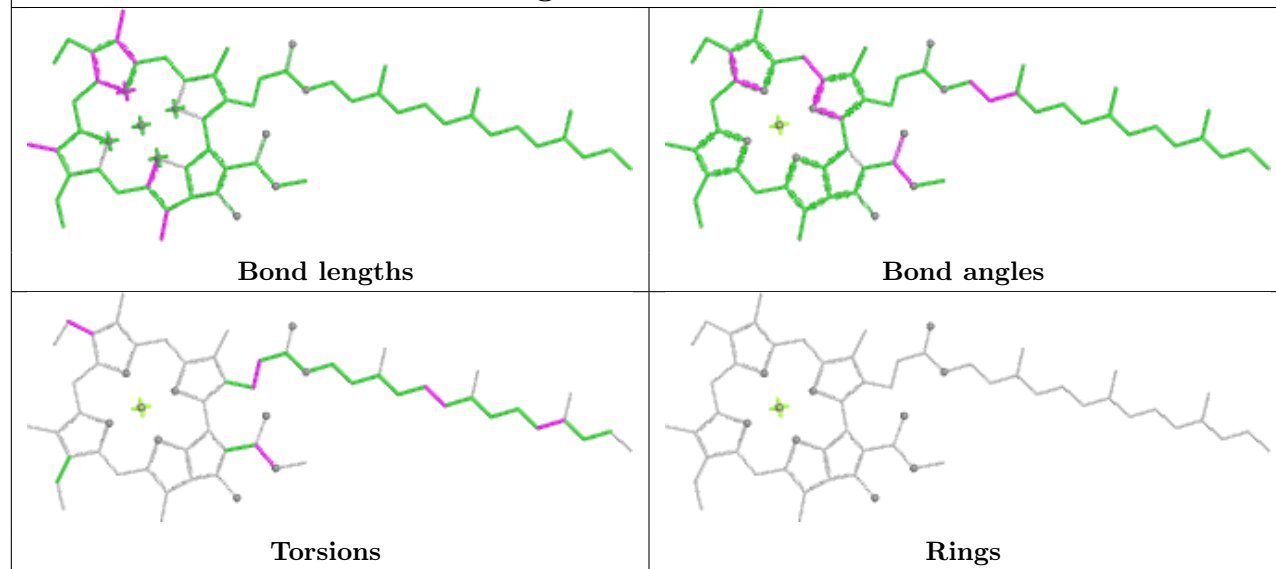
Ligand CLA a 817

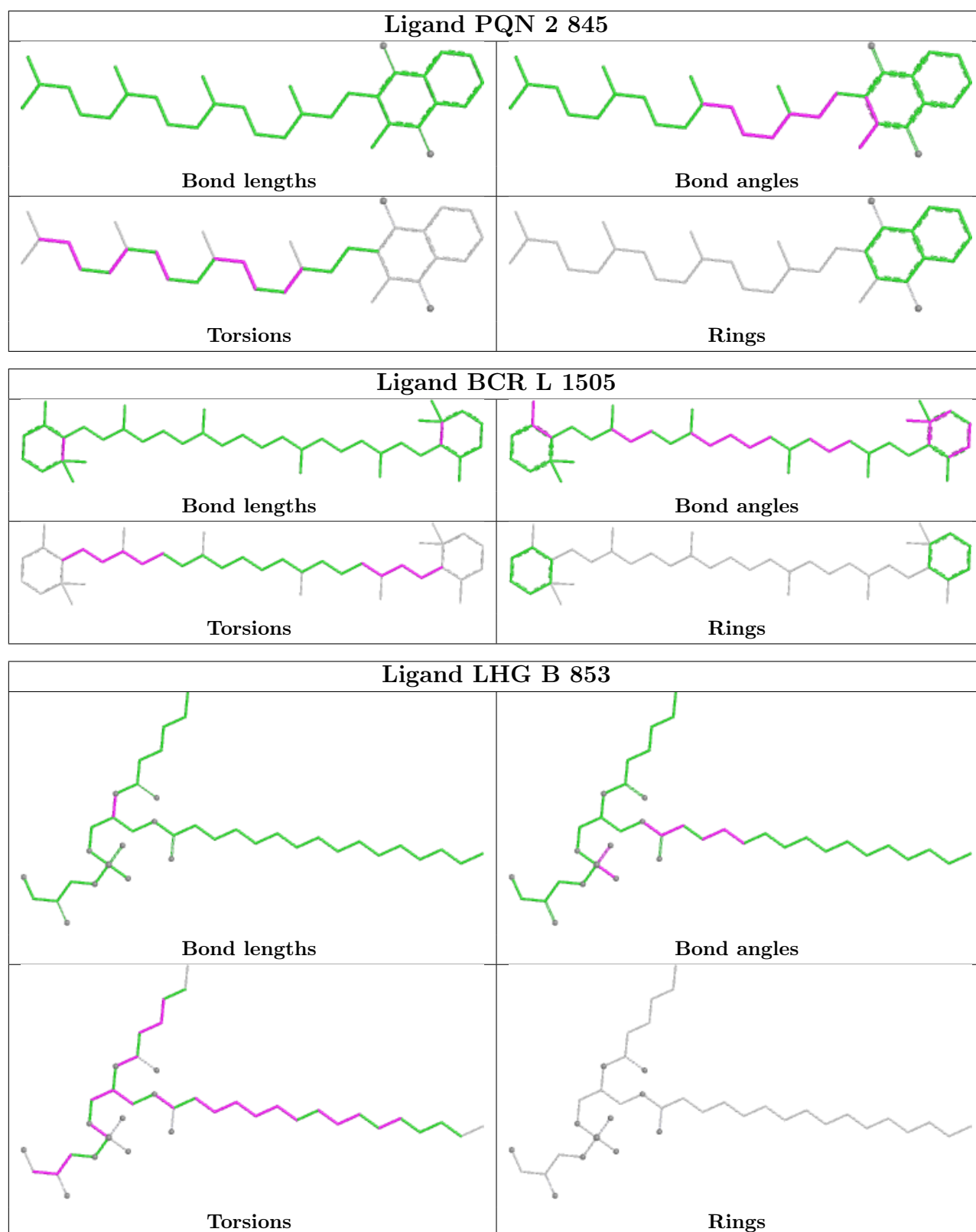


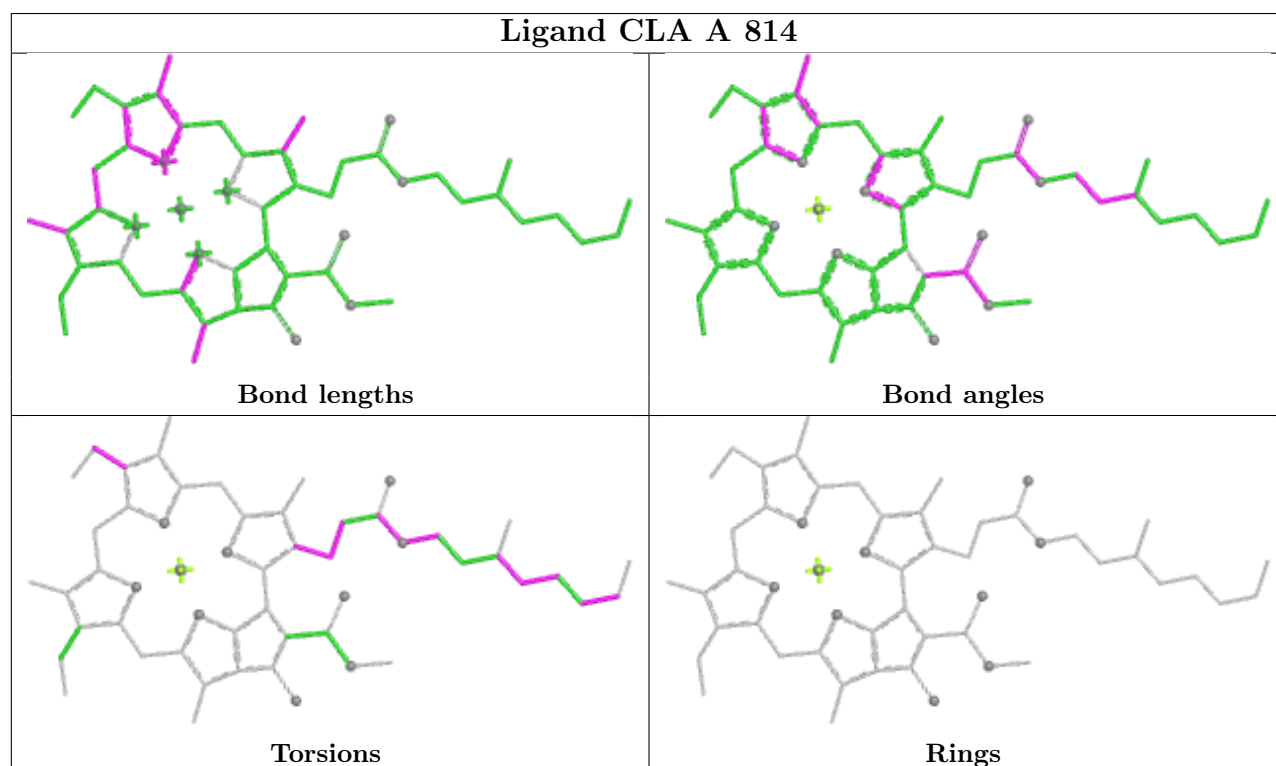
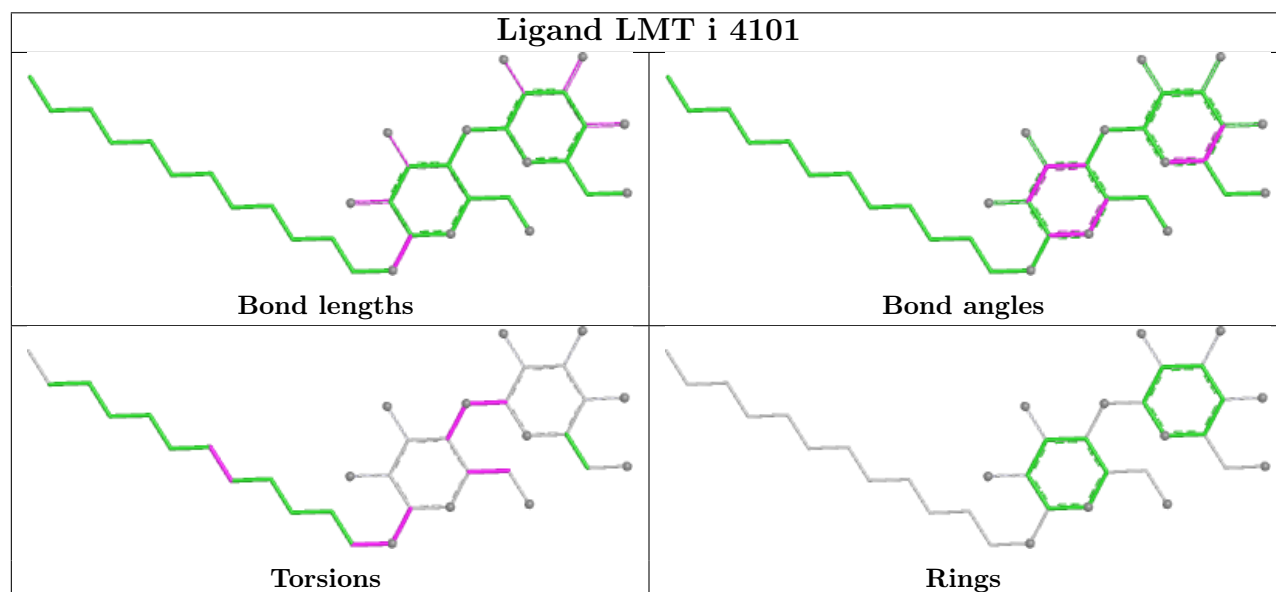
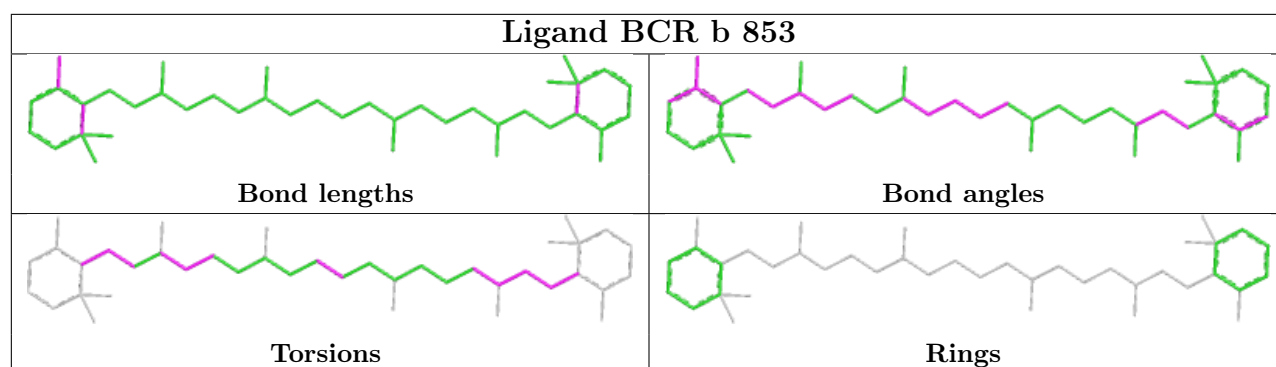
Ligand CLA 1 814



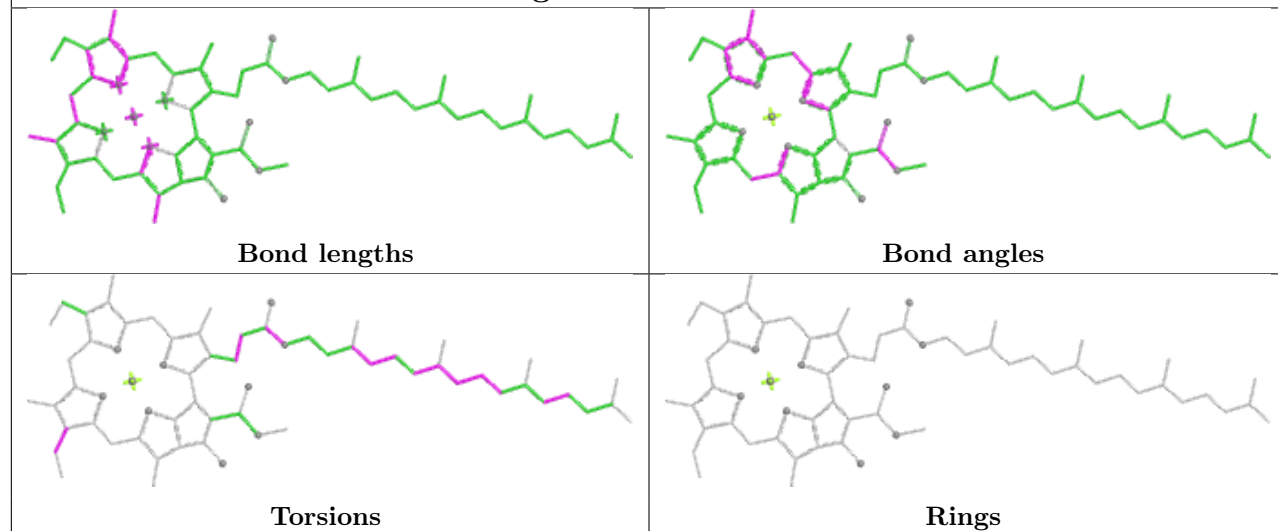
Ligand CLA 2 840



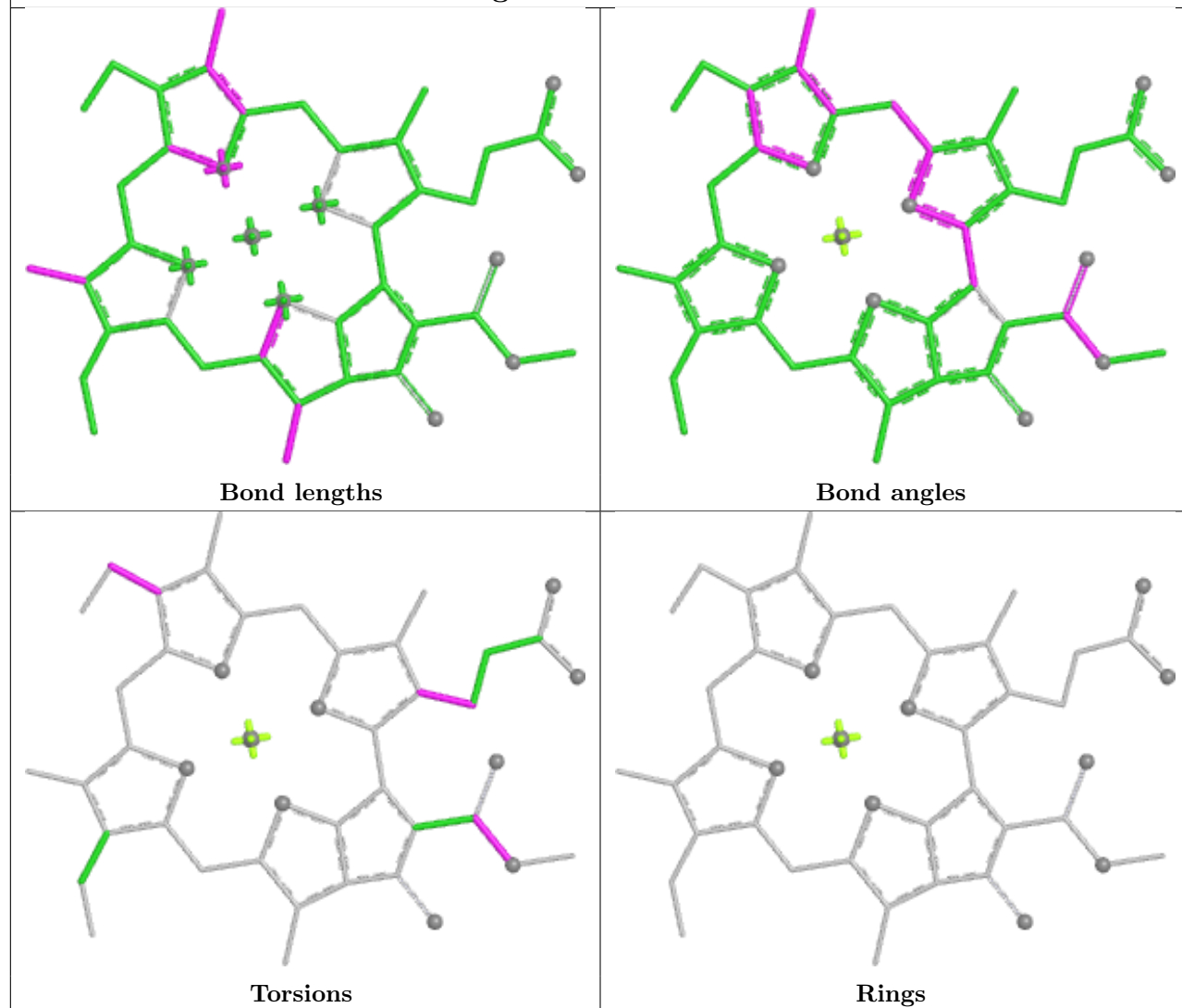


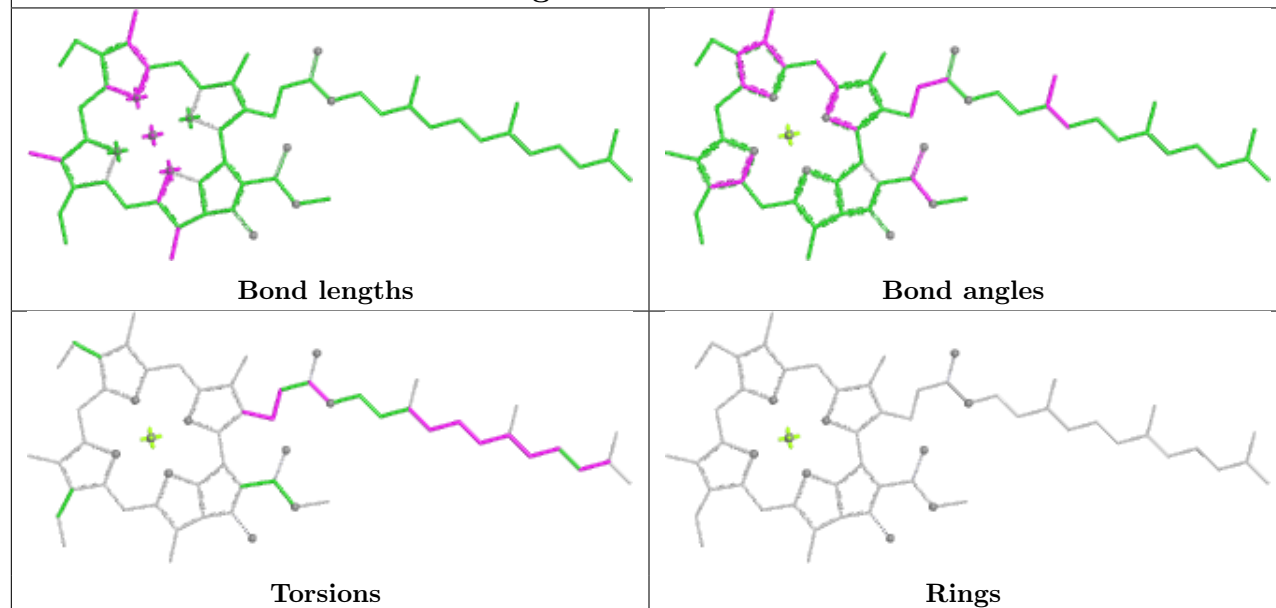
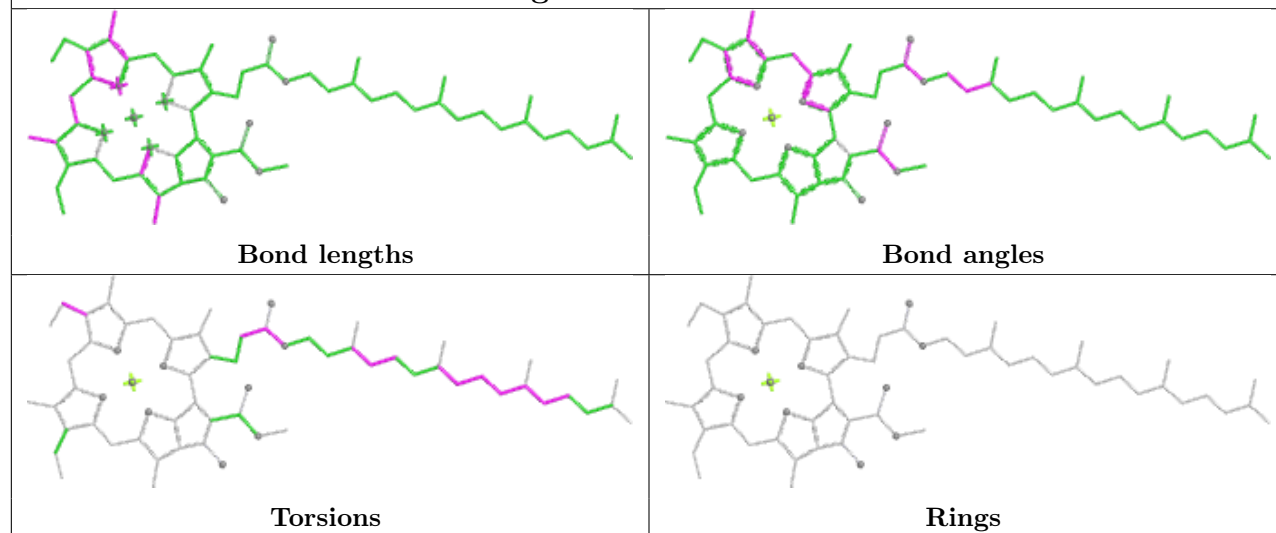


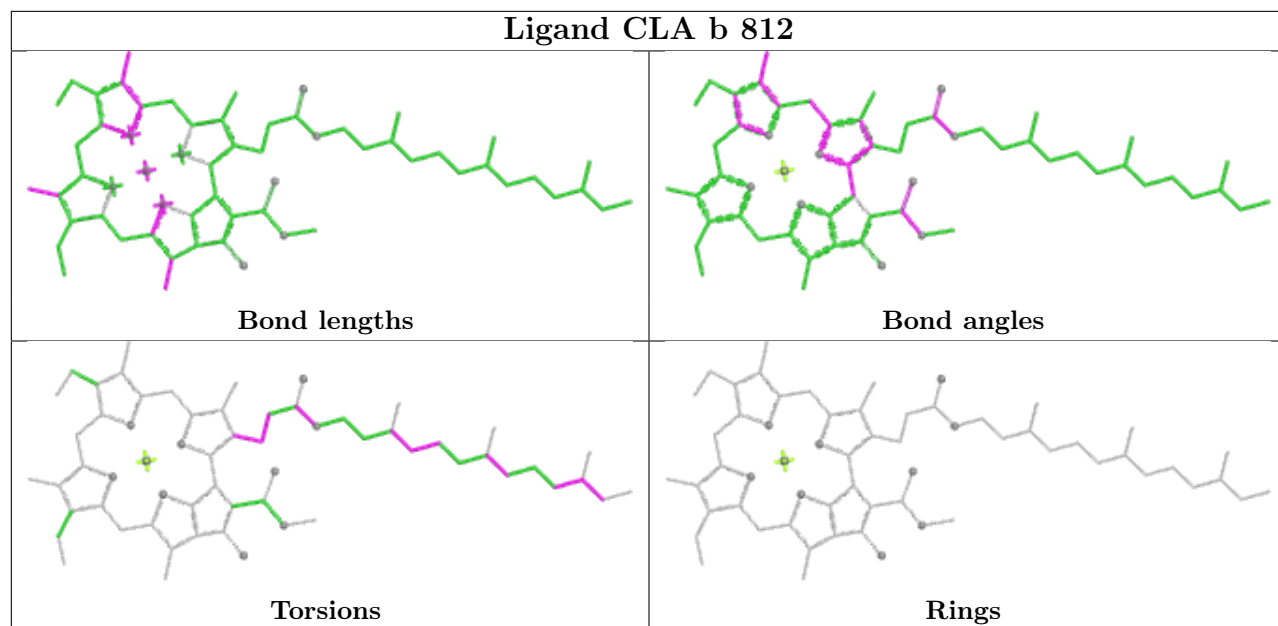
Ligand CLA B 806

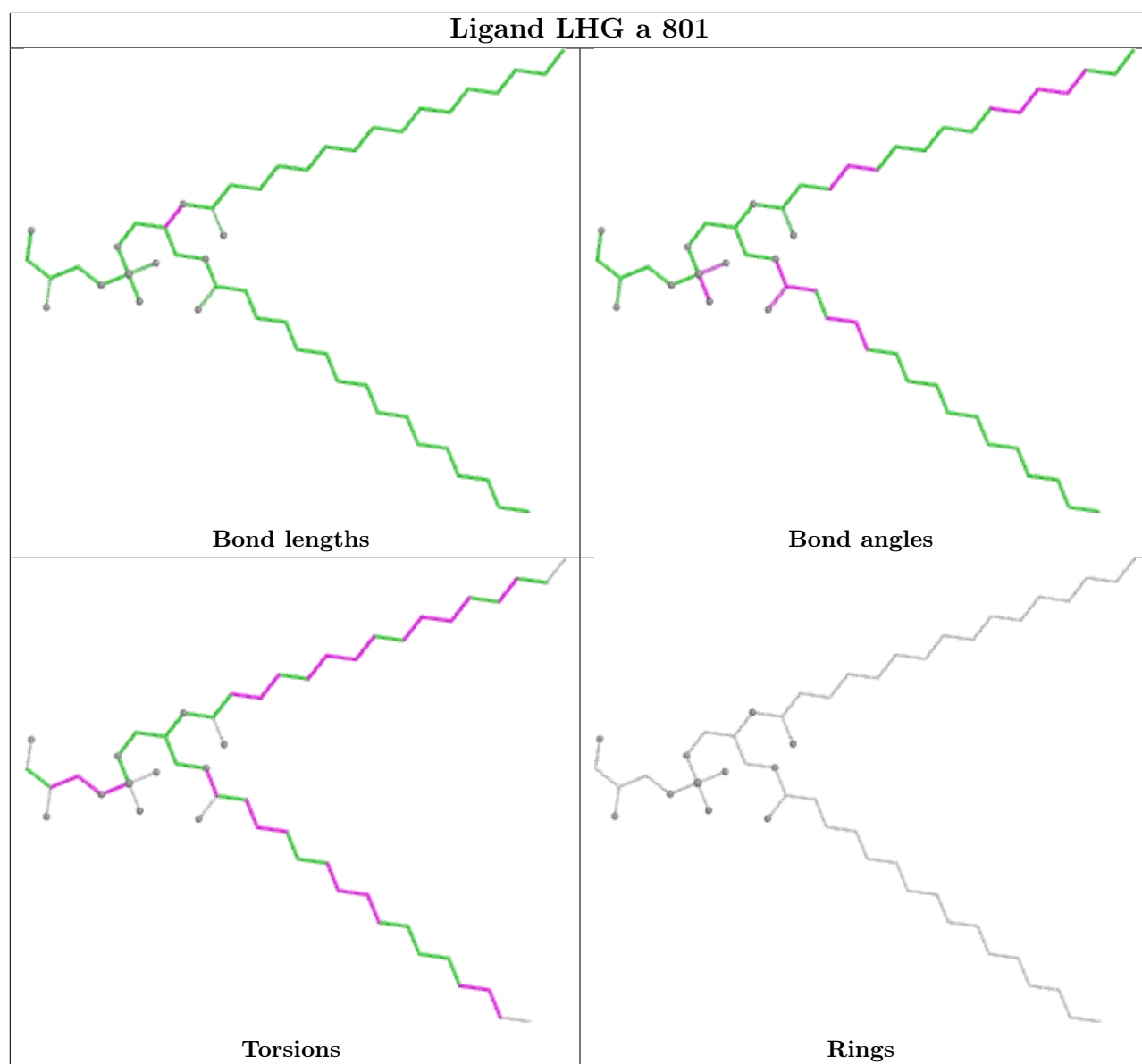


Ligand CLA B 814

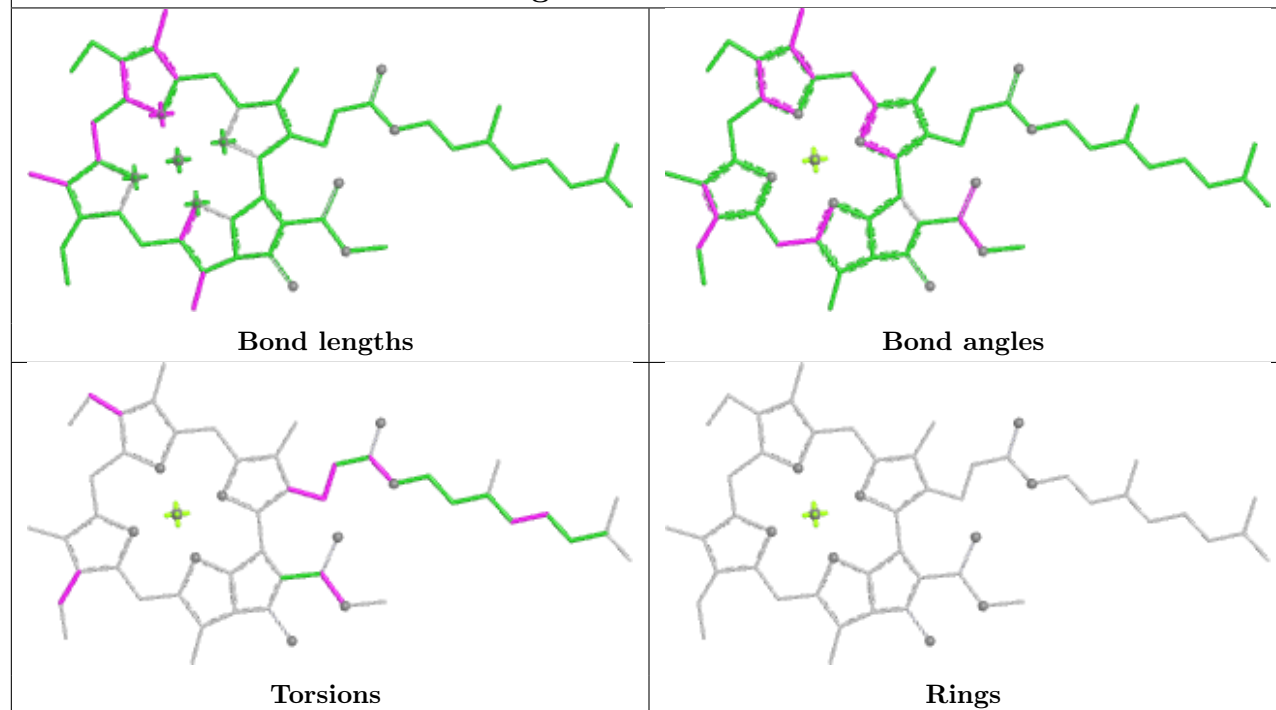


Ligand CLA B 821**Ligand CLA I 4206**

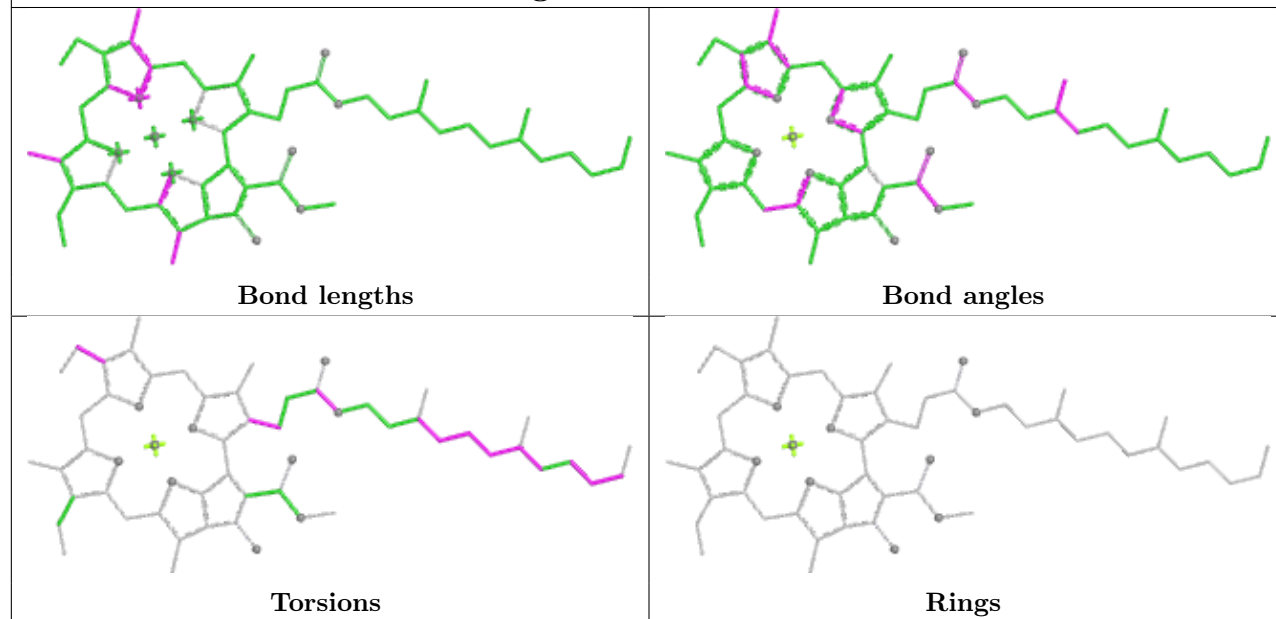


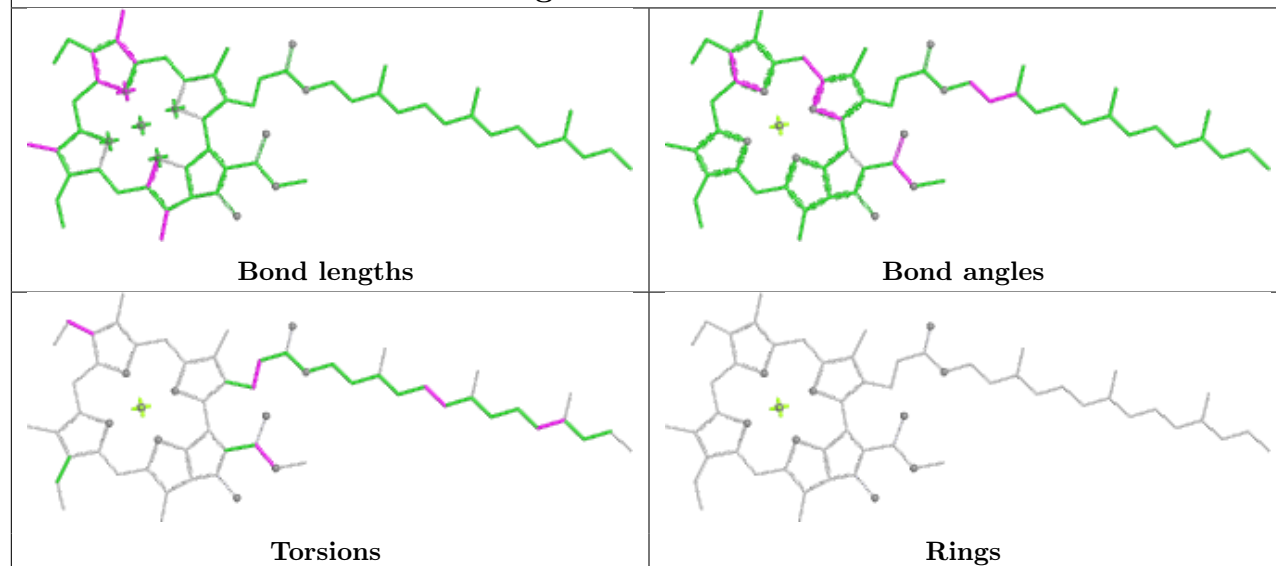
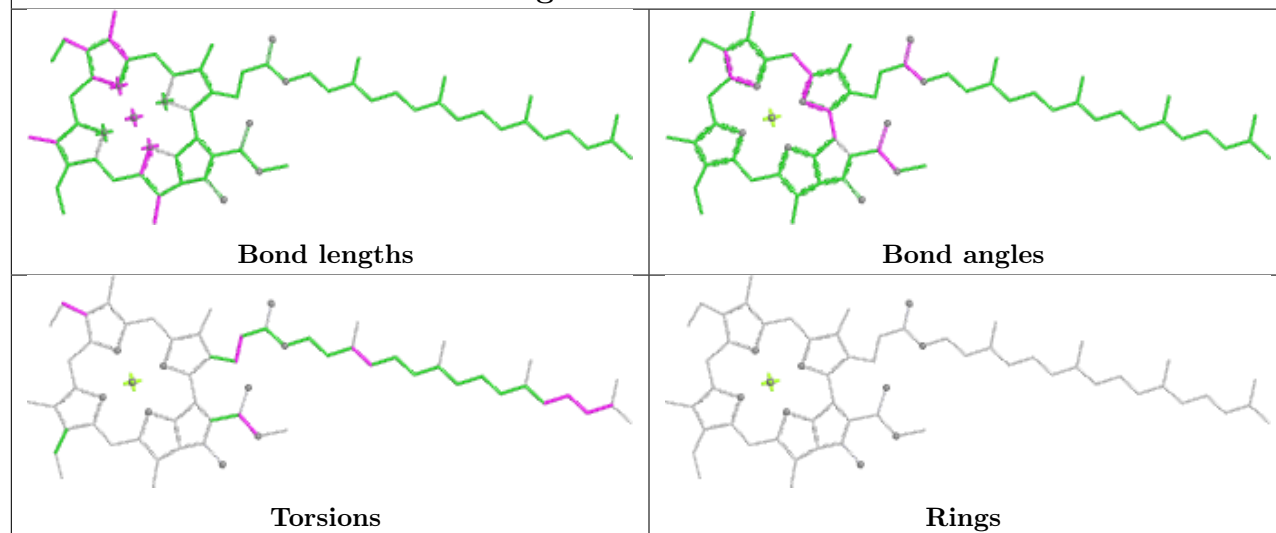


Ligand CLA A 815

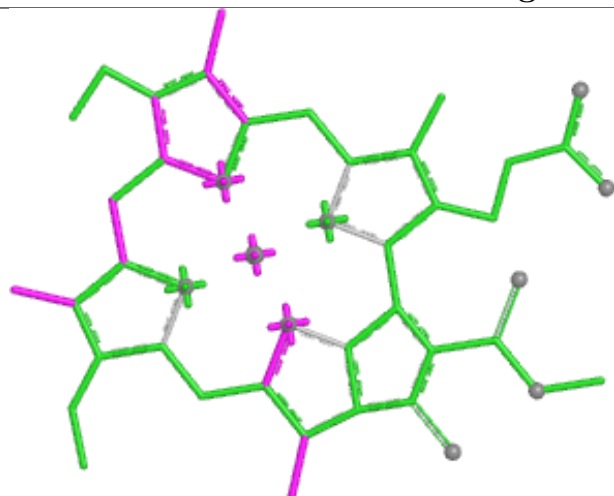


Ligand CLA A 826

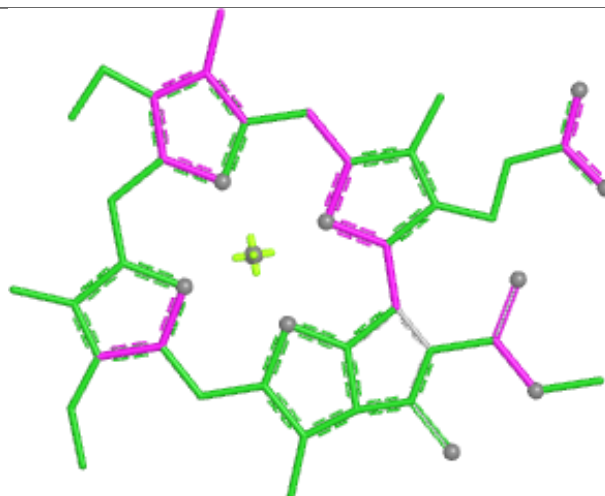


Ligand CLA b 840**Ligand CLA a 805**

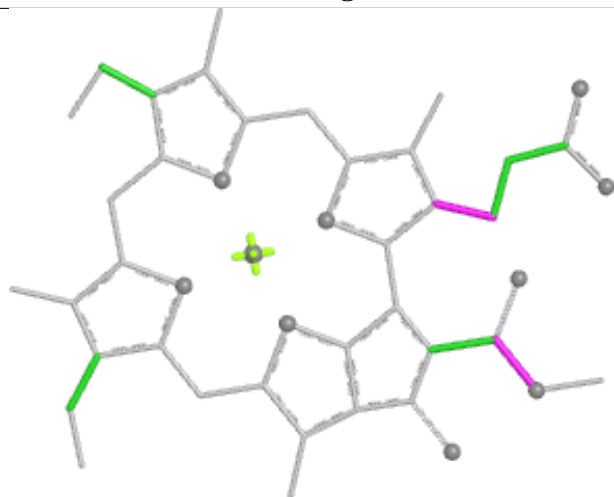
Ligand CLA 2 836



Bond lengths



Bond angles

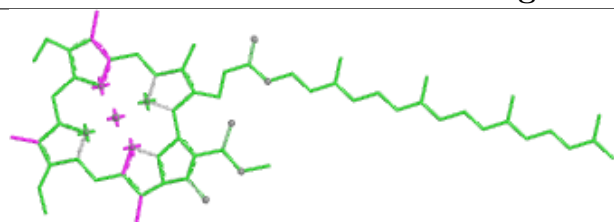


Torsions

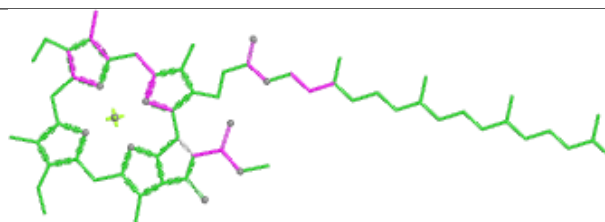


Rings

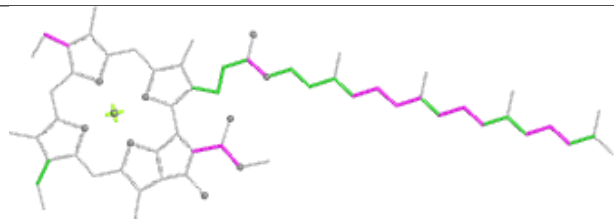
Ligand CLA 1 833



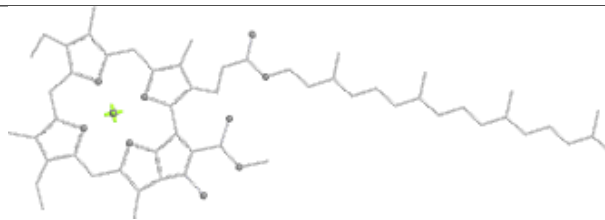
Bond lengths



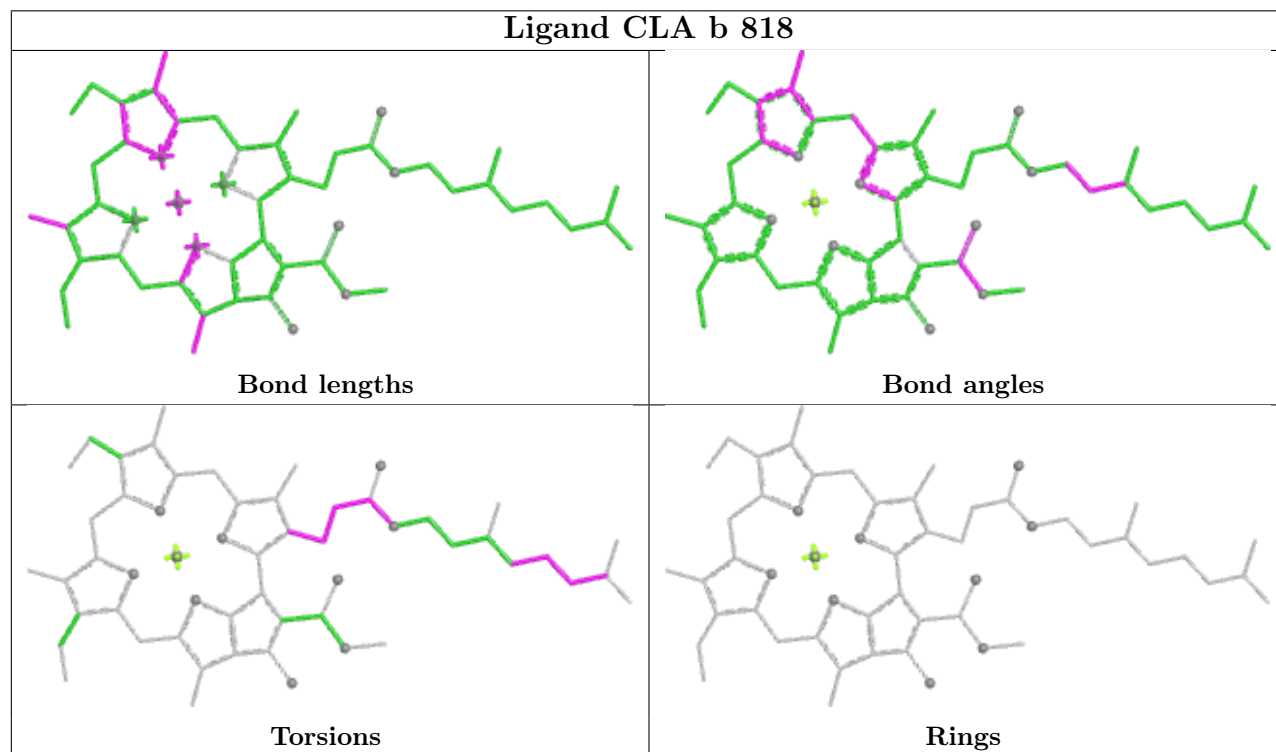
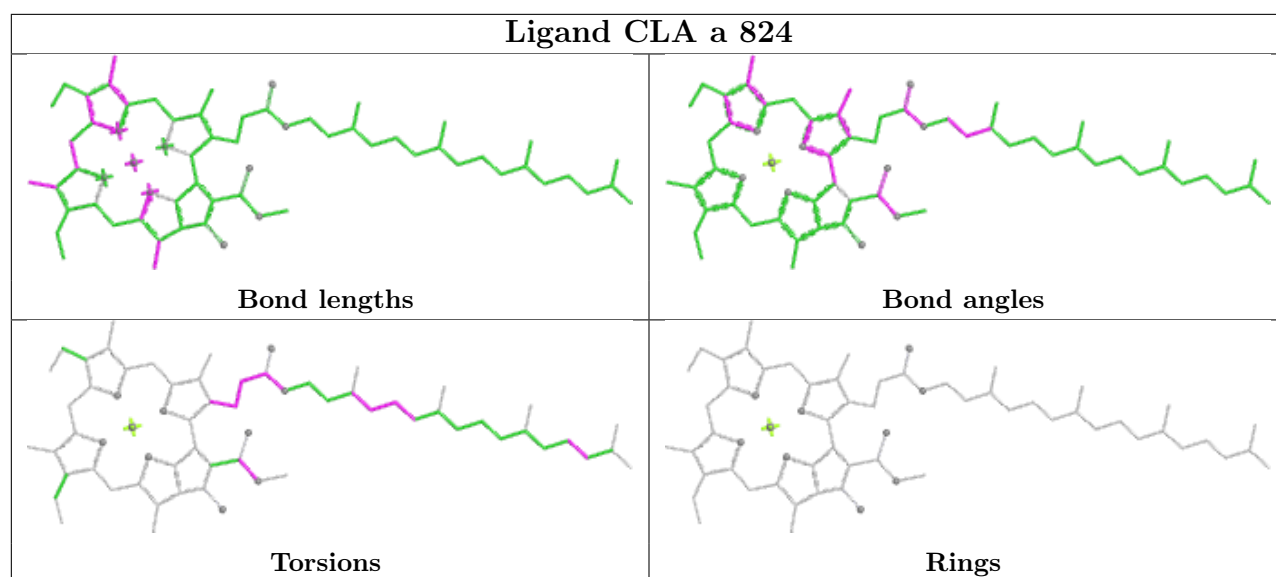
Bond angles

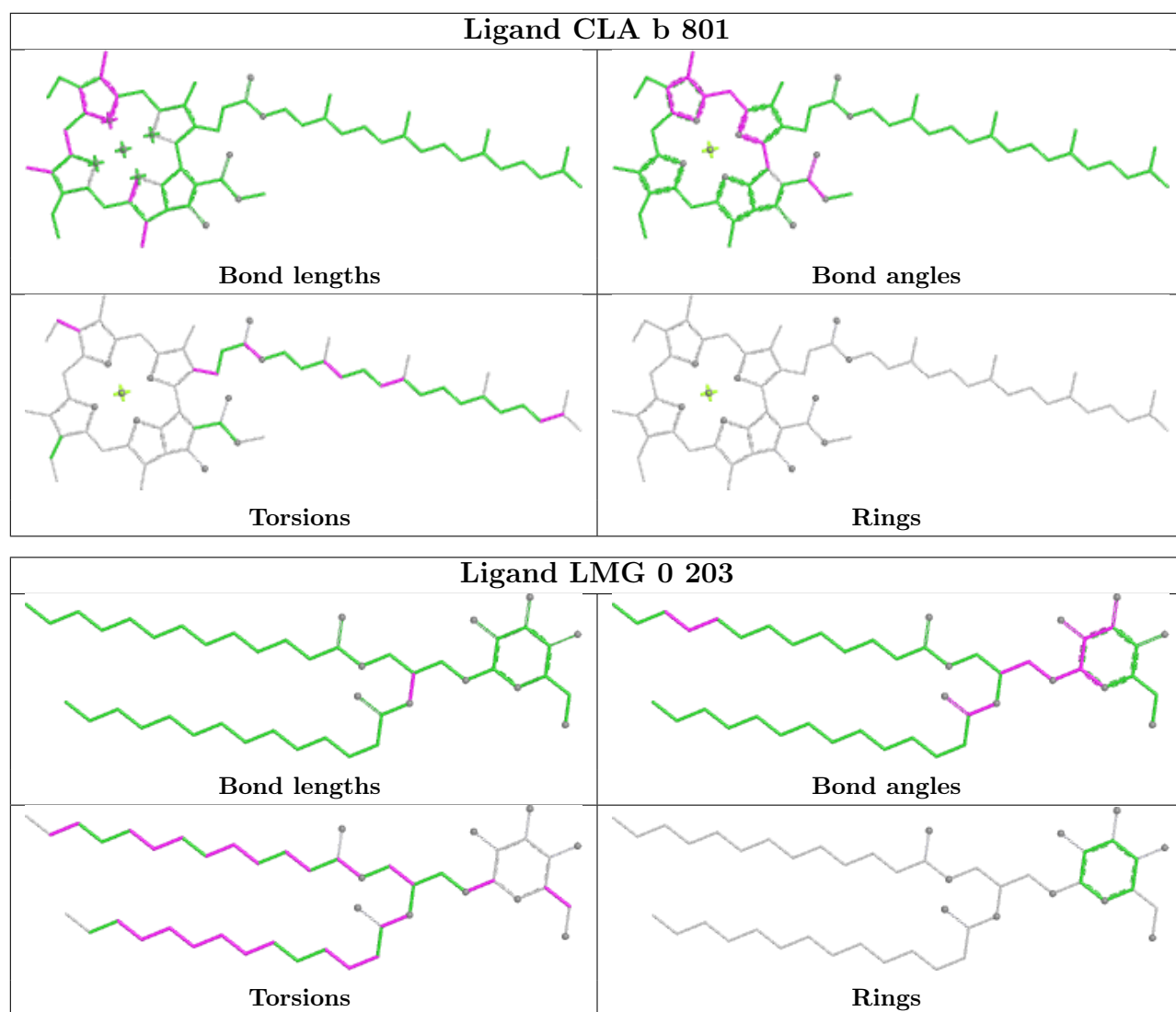


Torsions

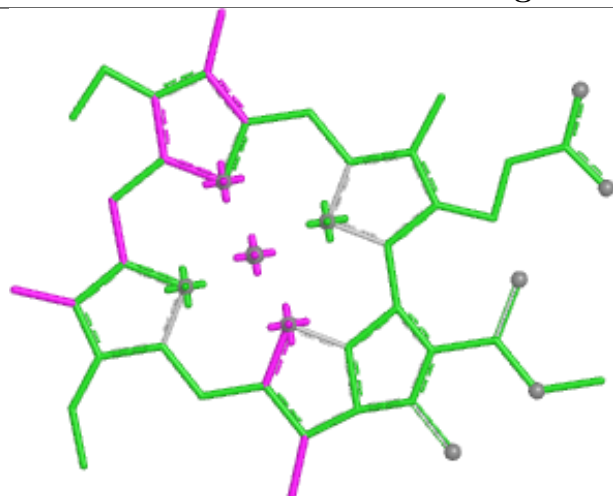


Rings

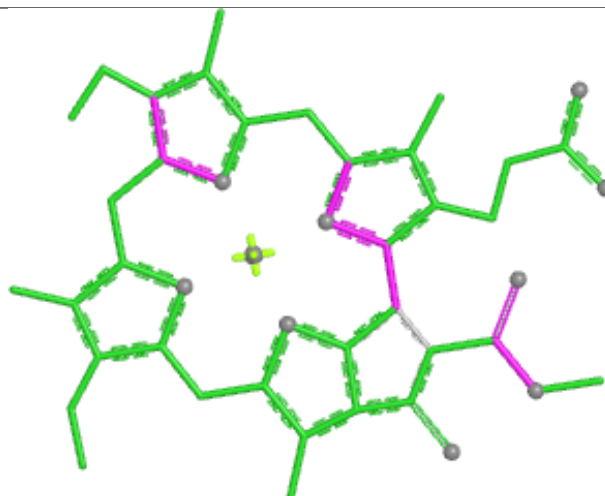




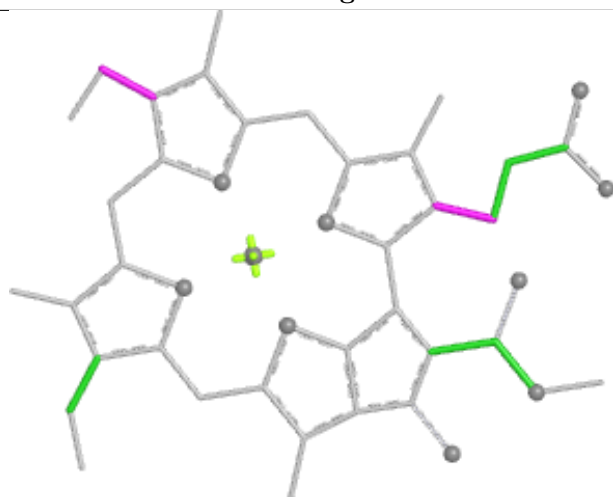
Ligand CLA B 838



Bond lengths



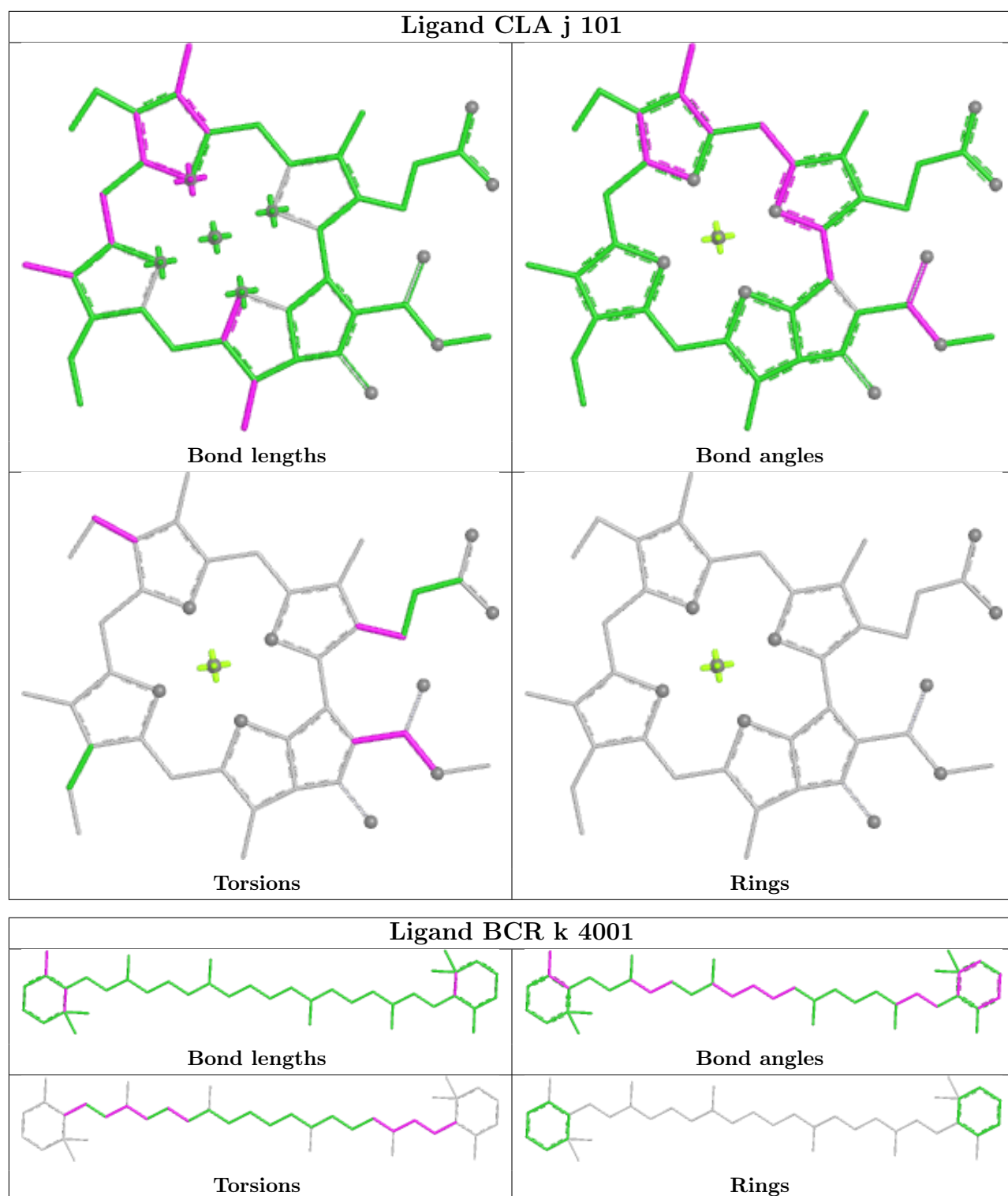
Bond angles

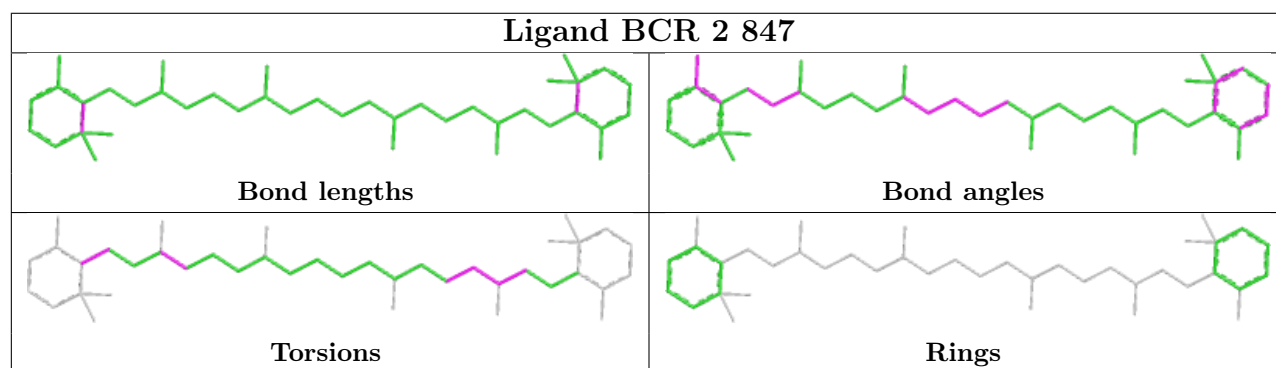
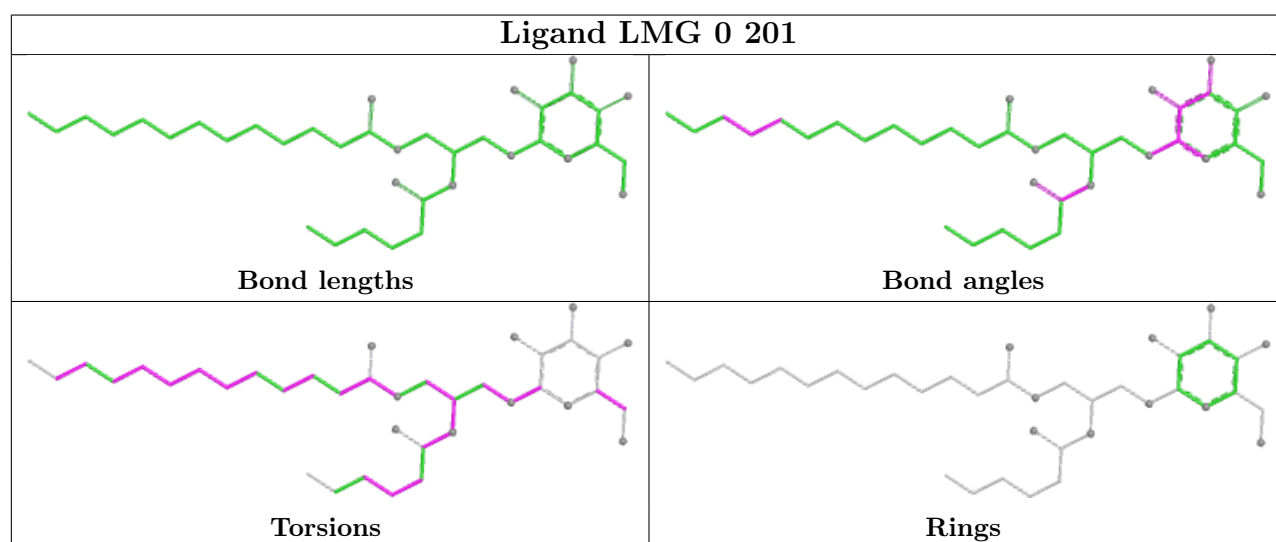
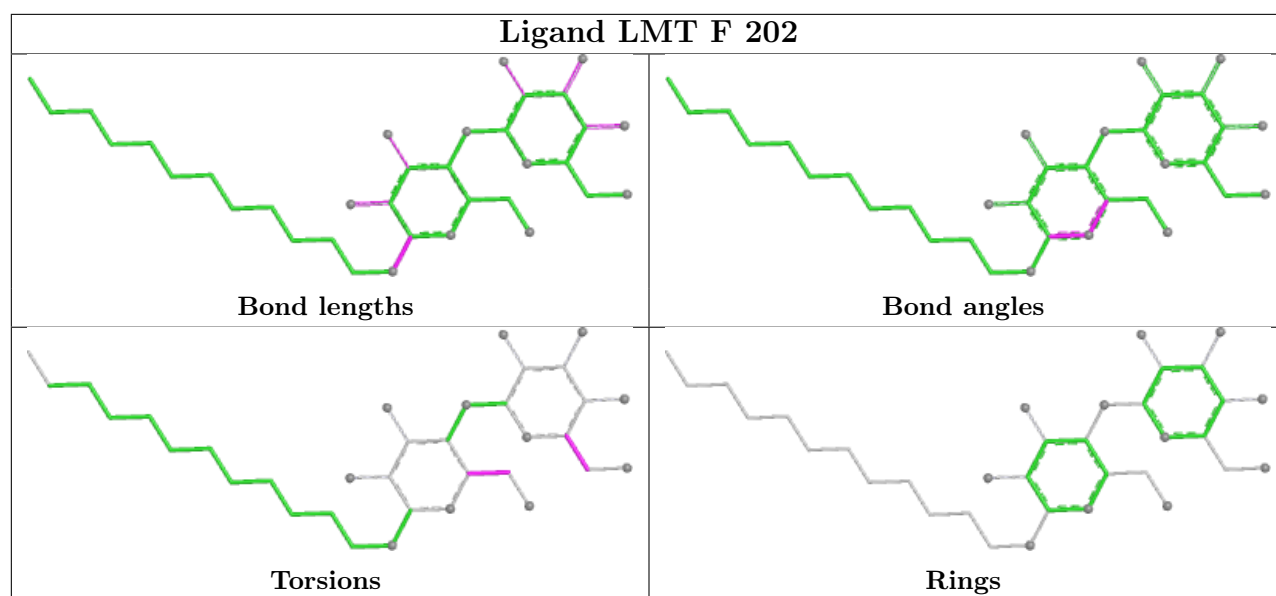


Torsions

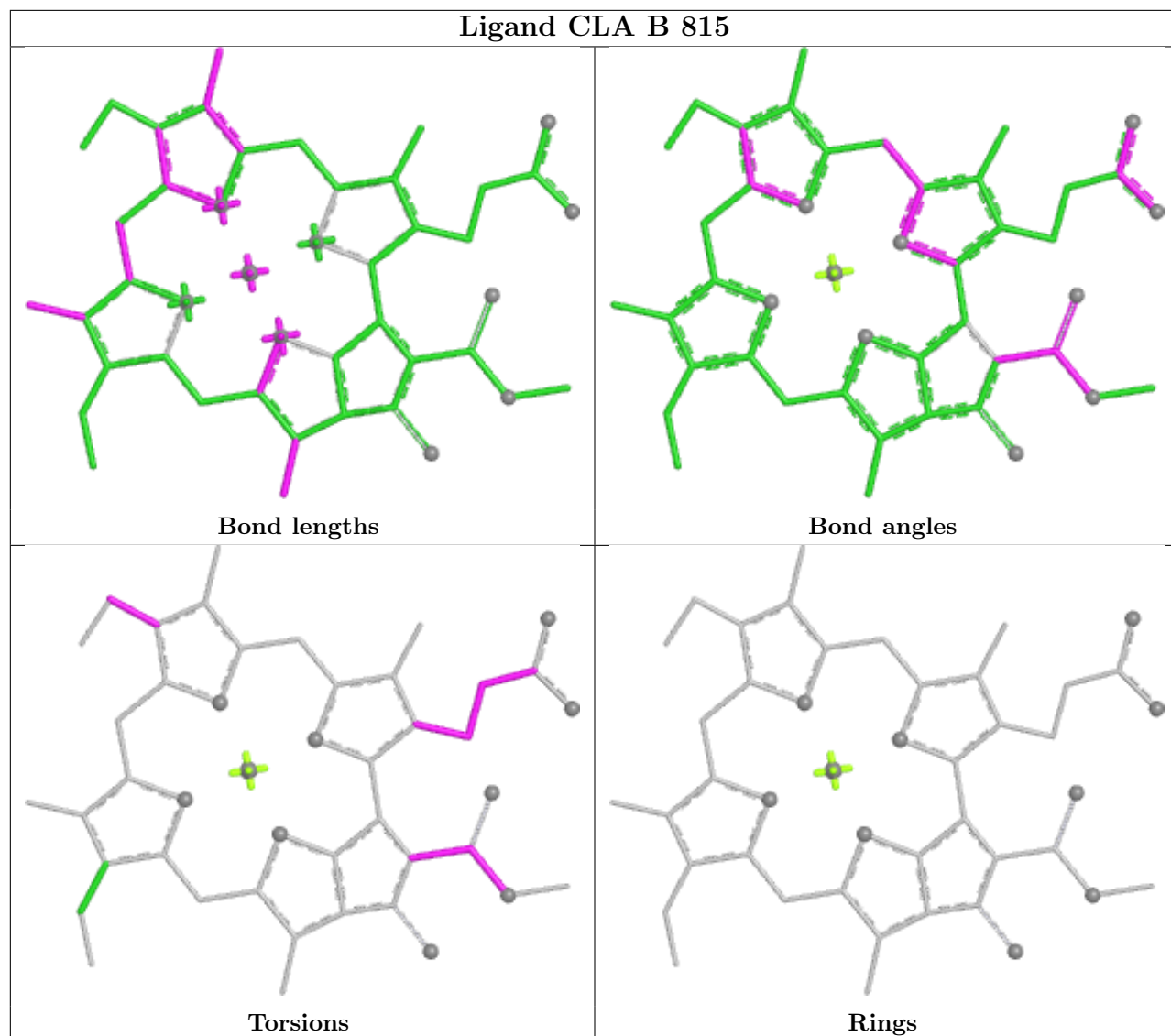


Rings

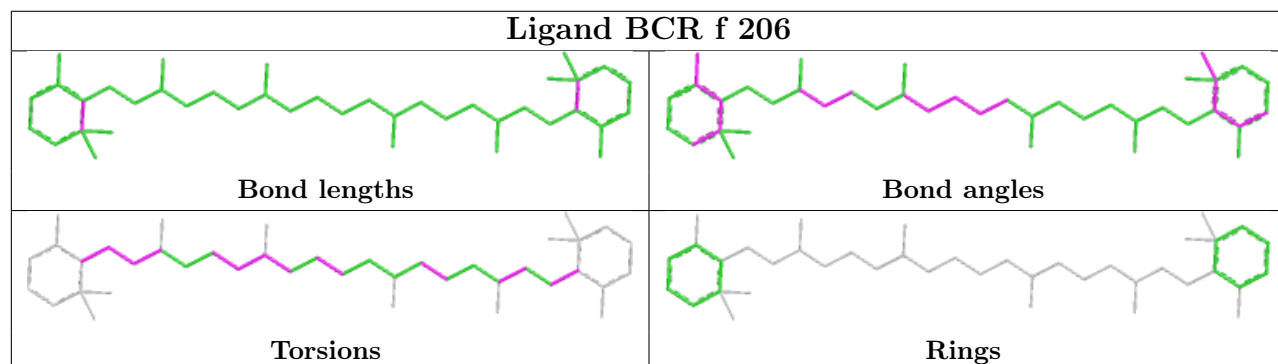


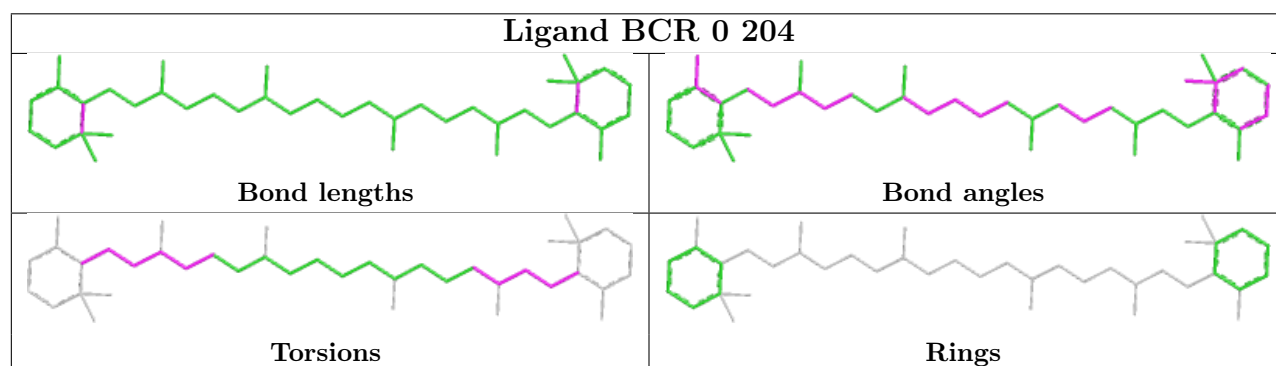
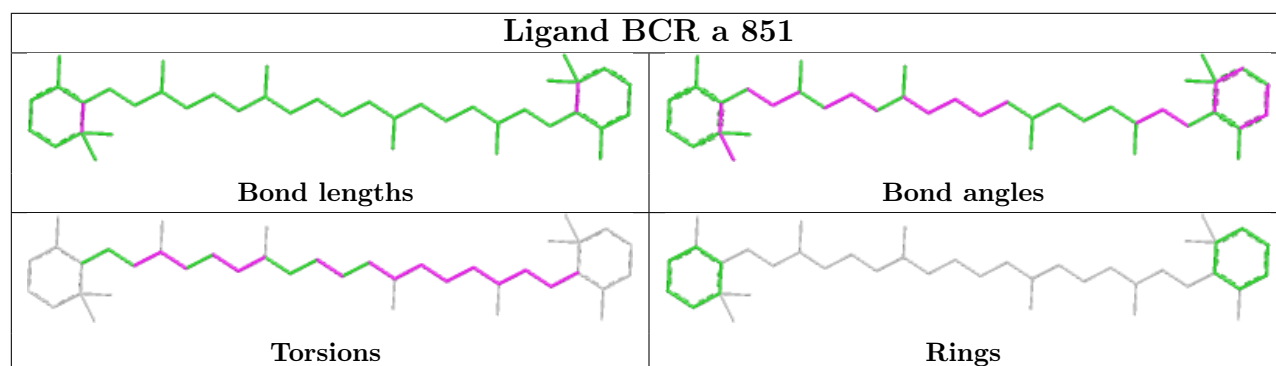
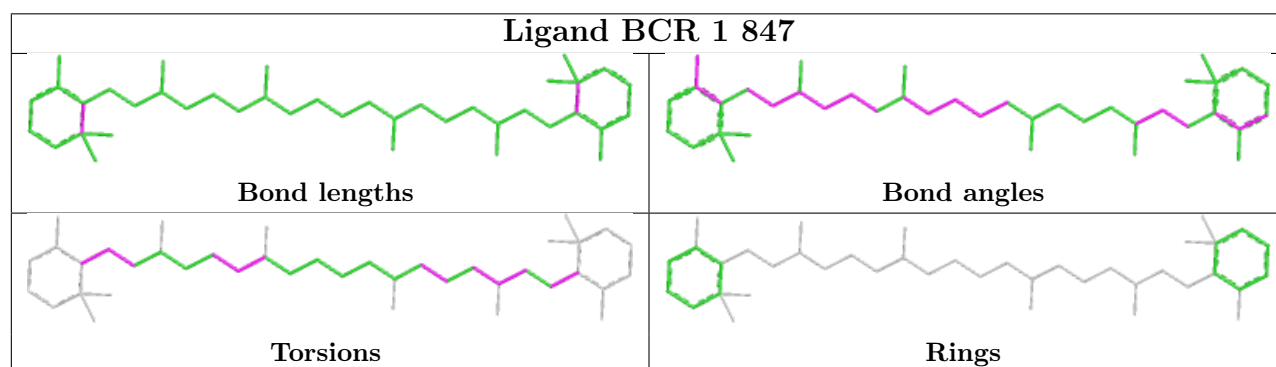
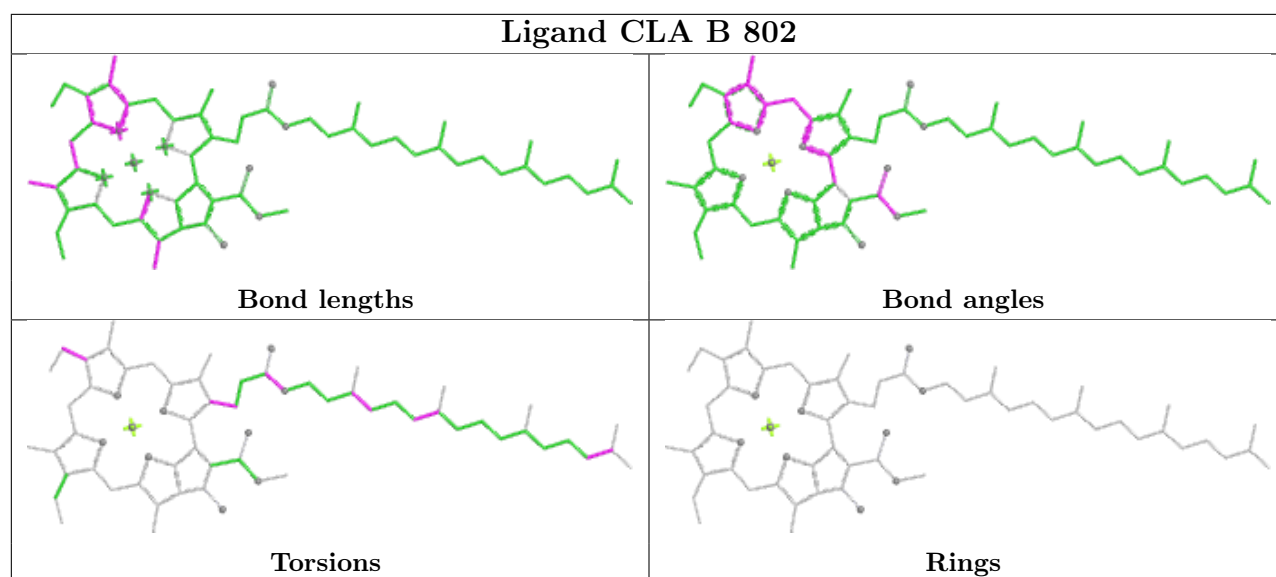


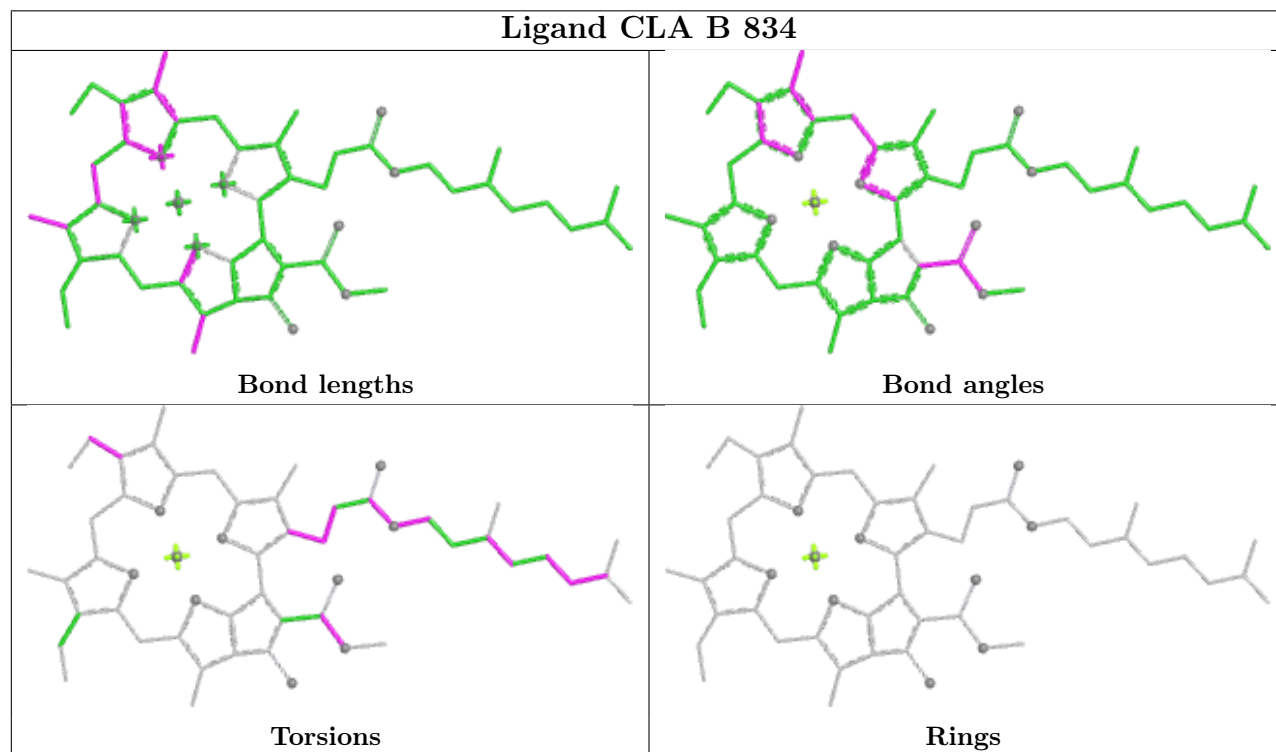
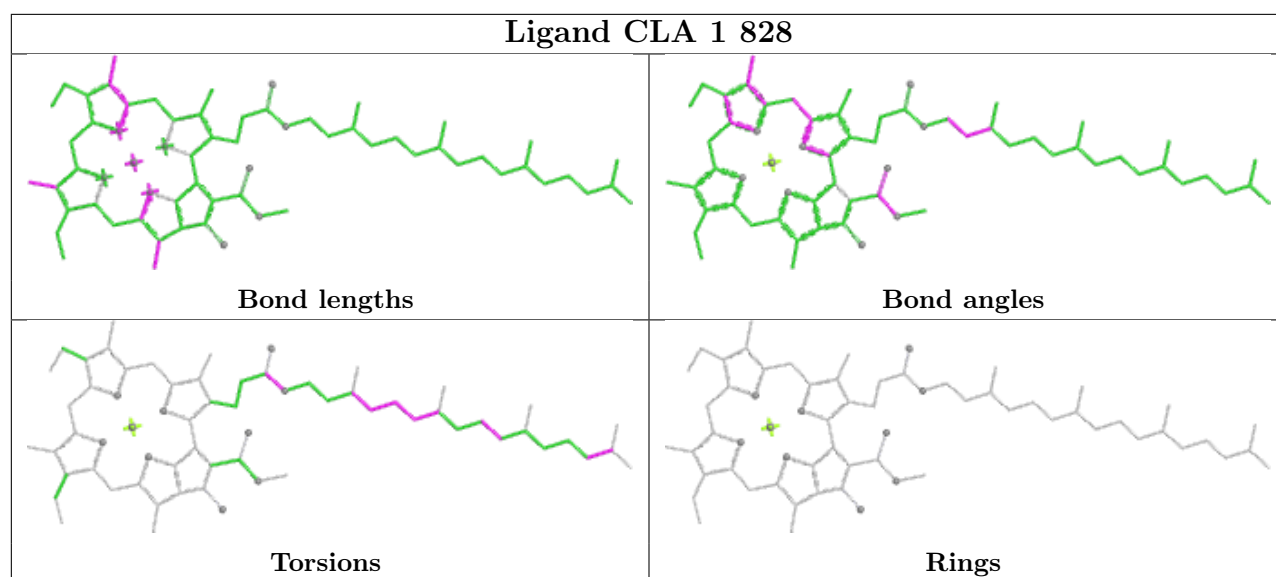
Ligand CLA B 815



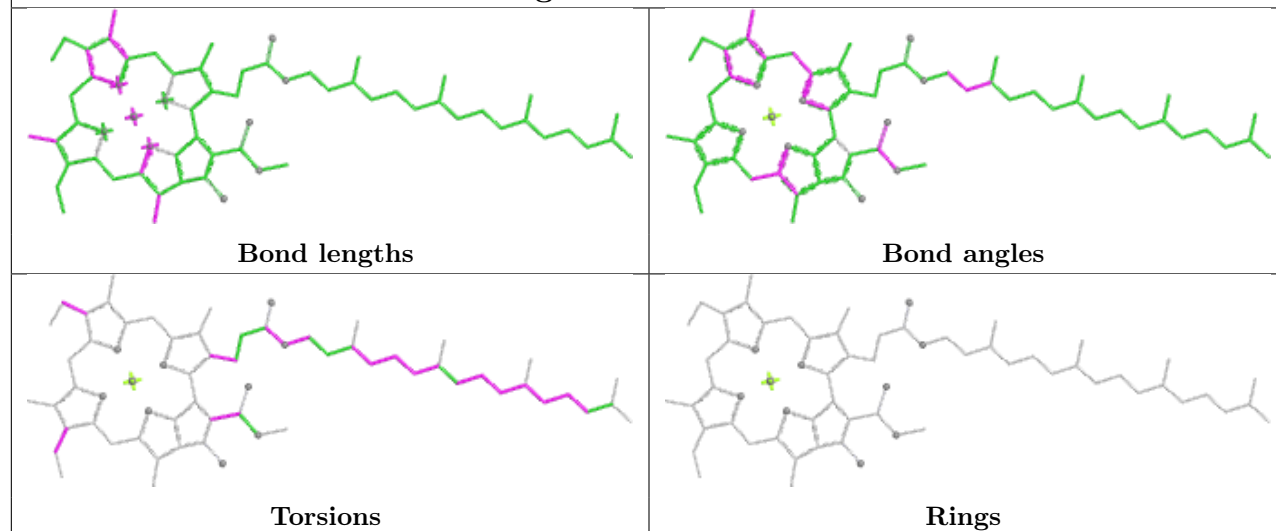
Ligand BCR f 206



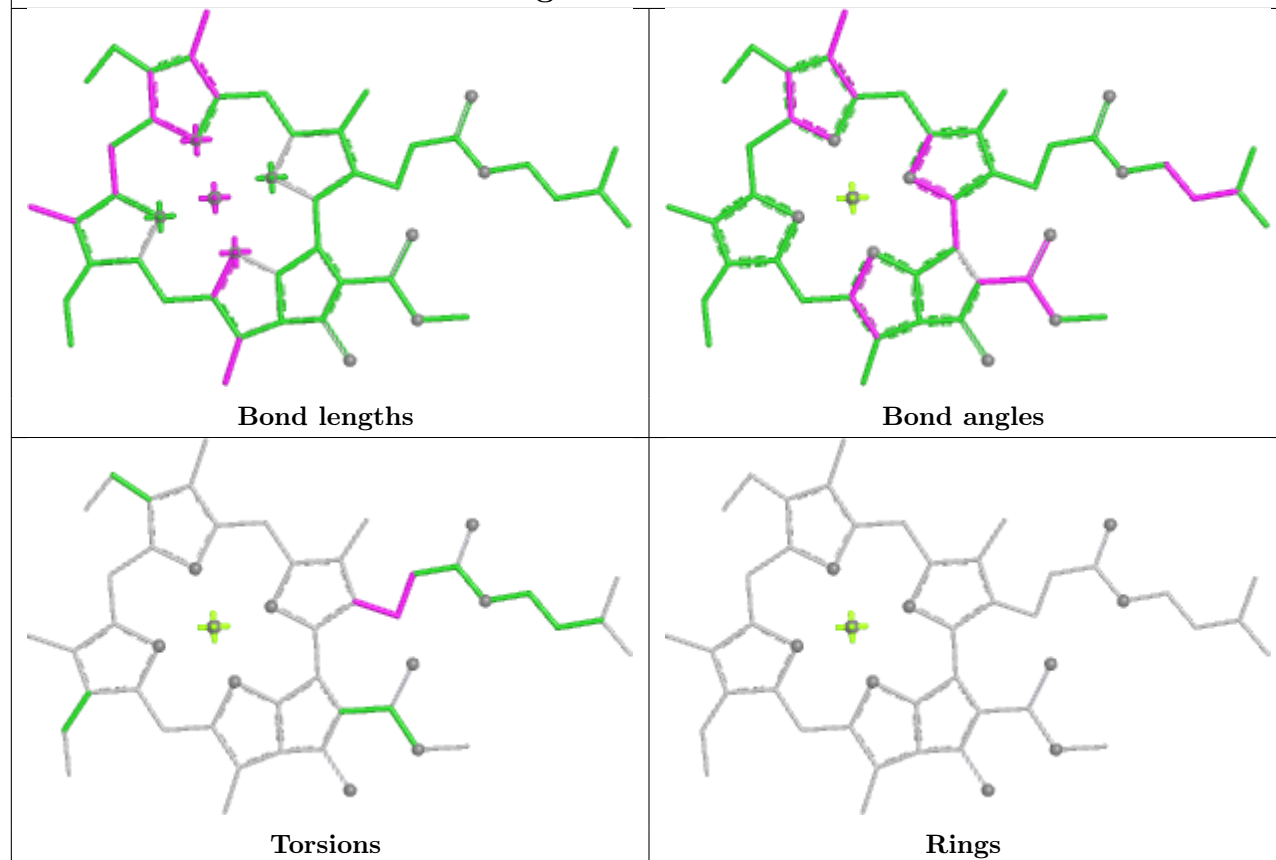




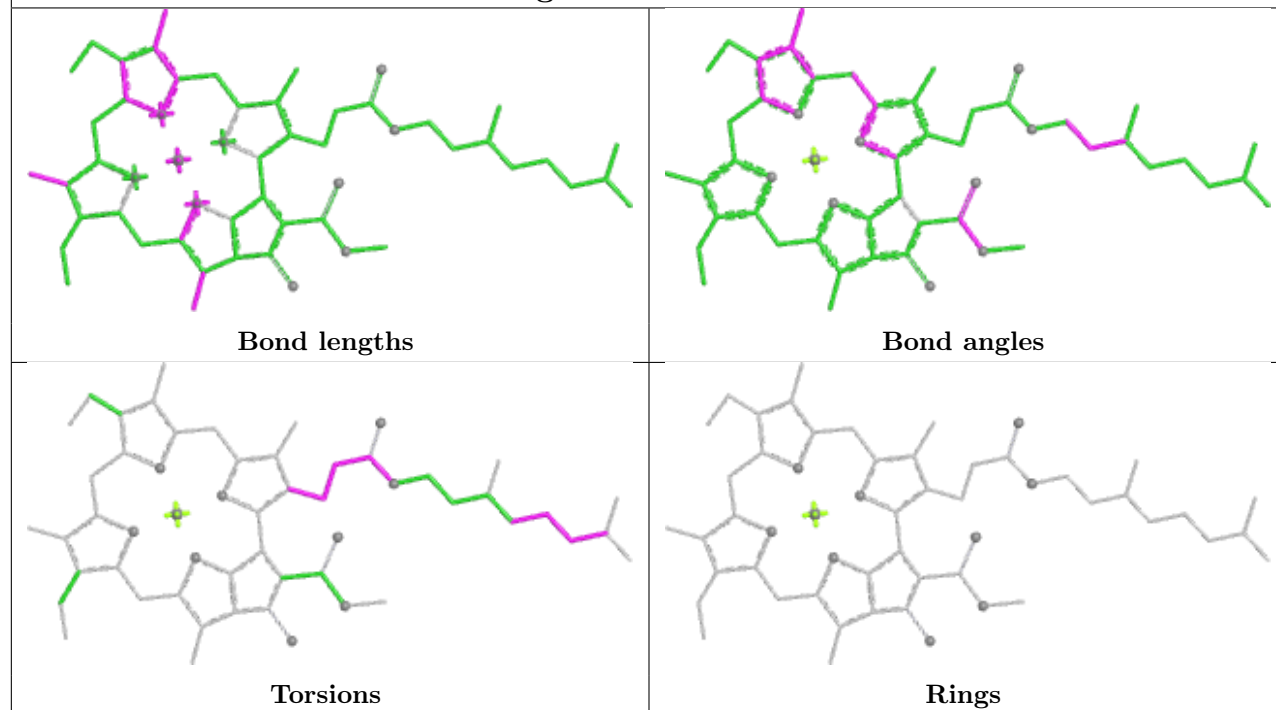
Ligand CLA b 815



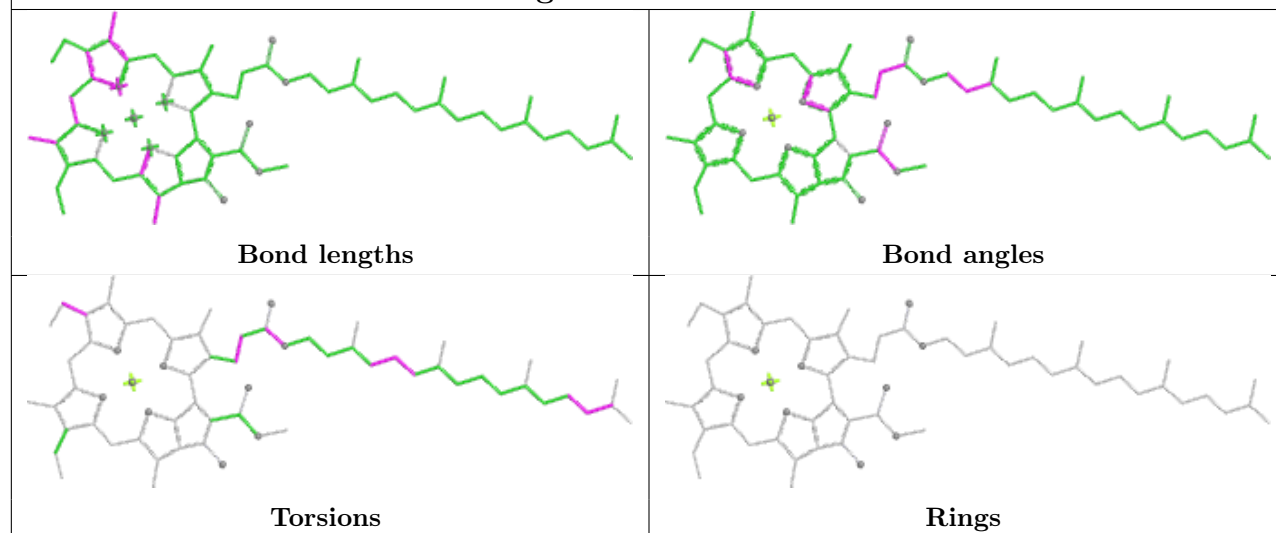
Ligand CLA a 807



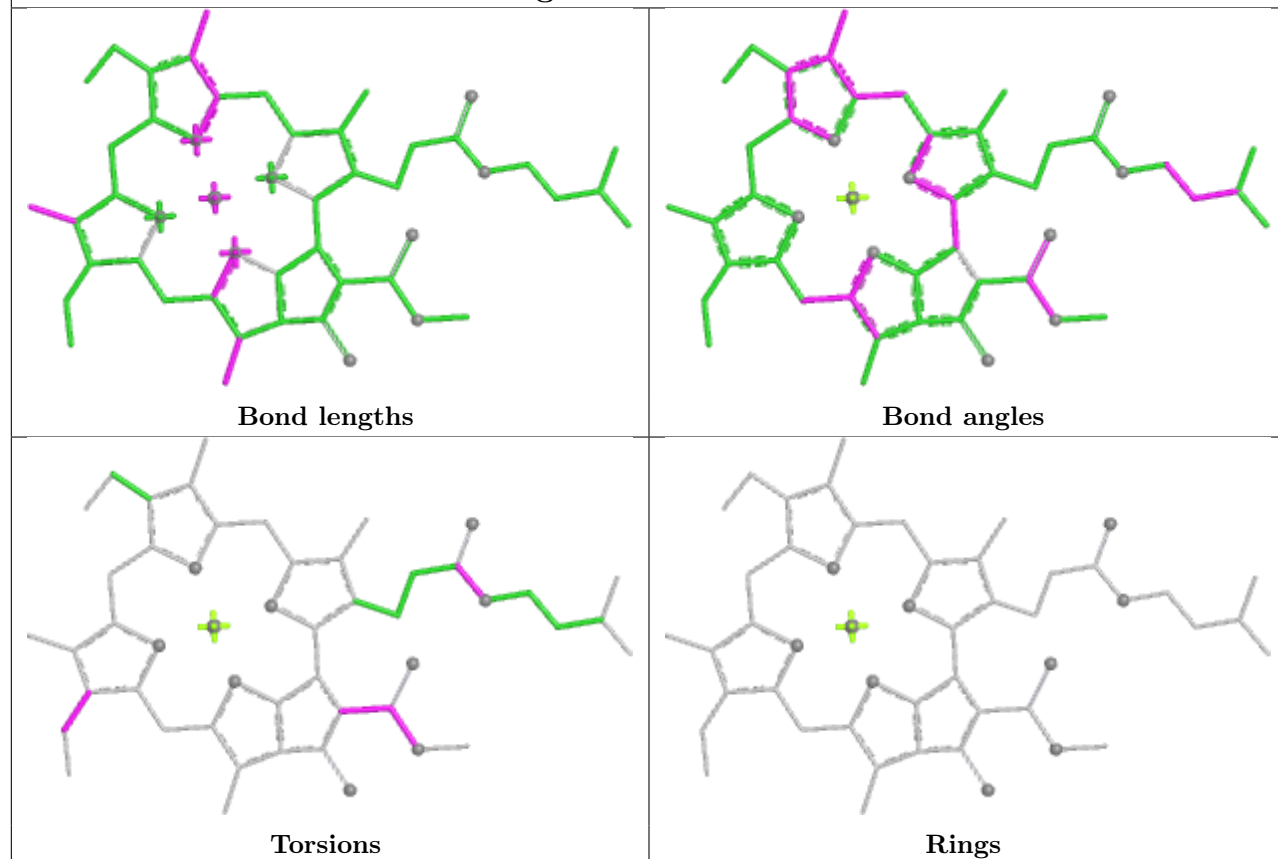
Ligand CLA 2 818



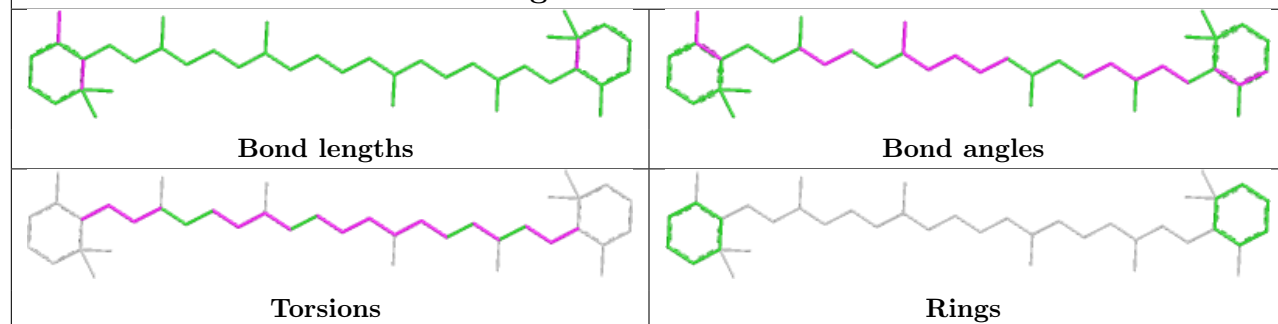
Ligand CLA 2 828

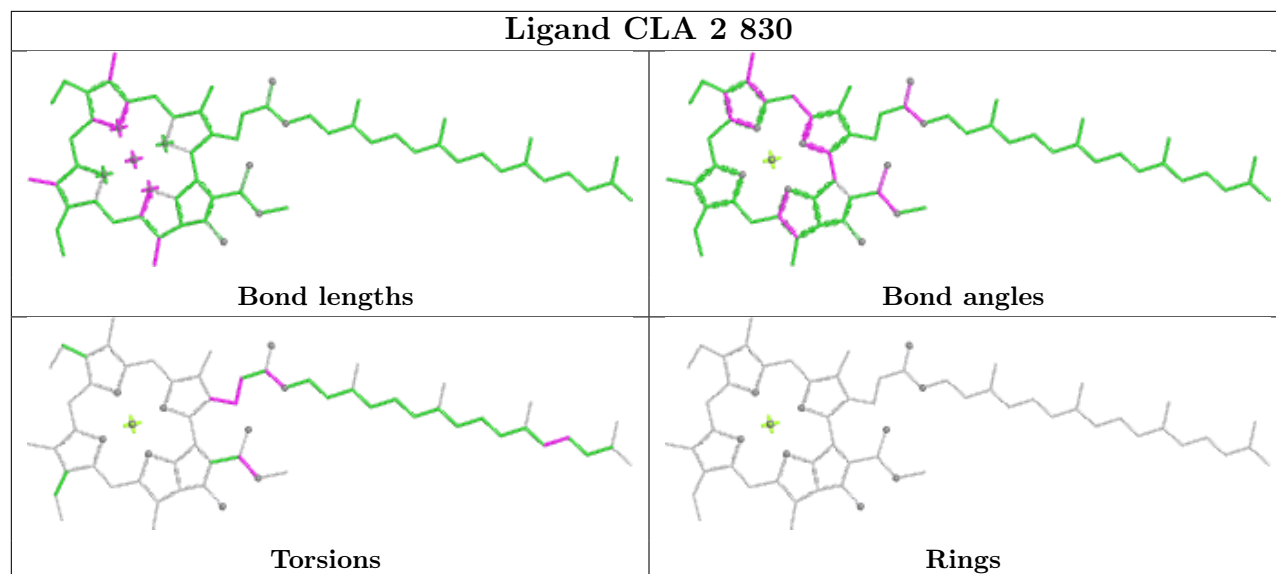
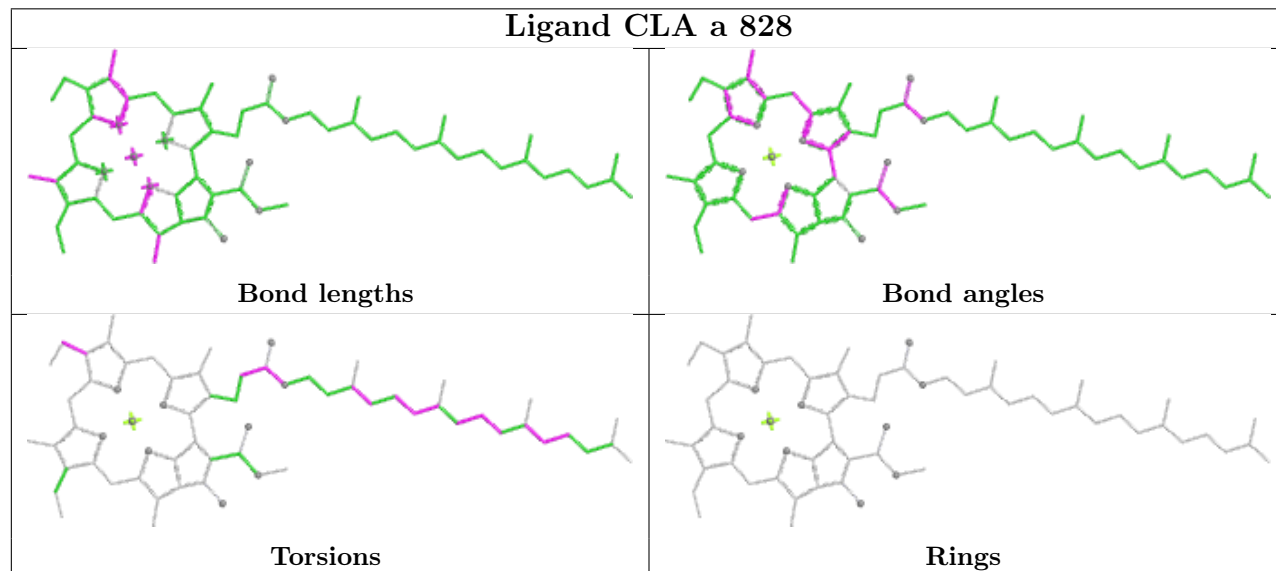


Ligand CLA 2 839

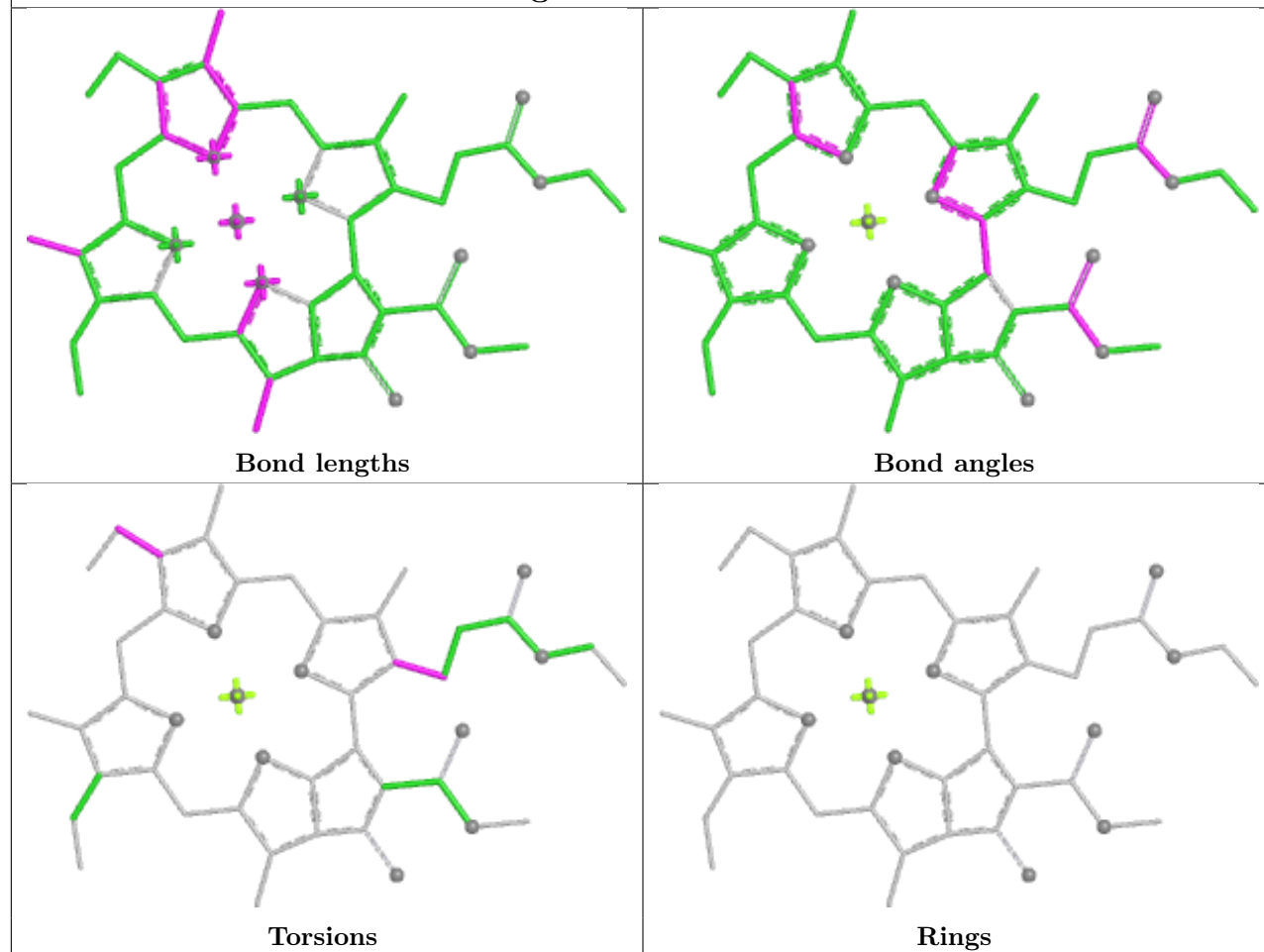


Ligand BCR A 850

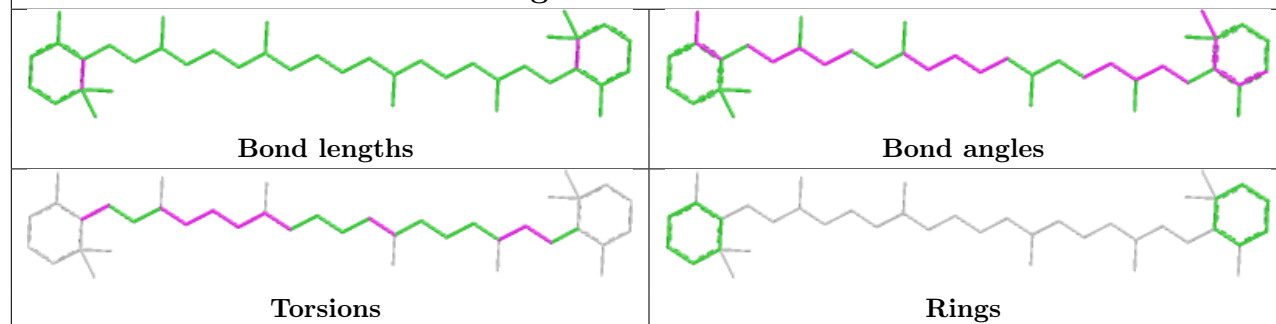


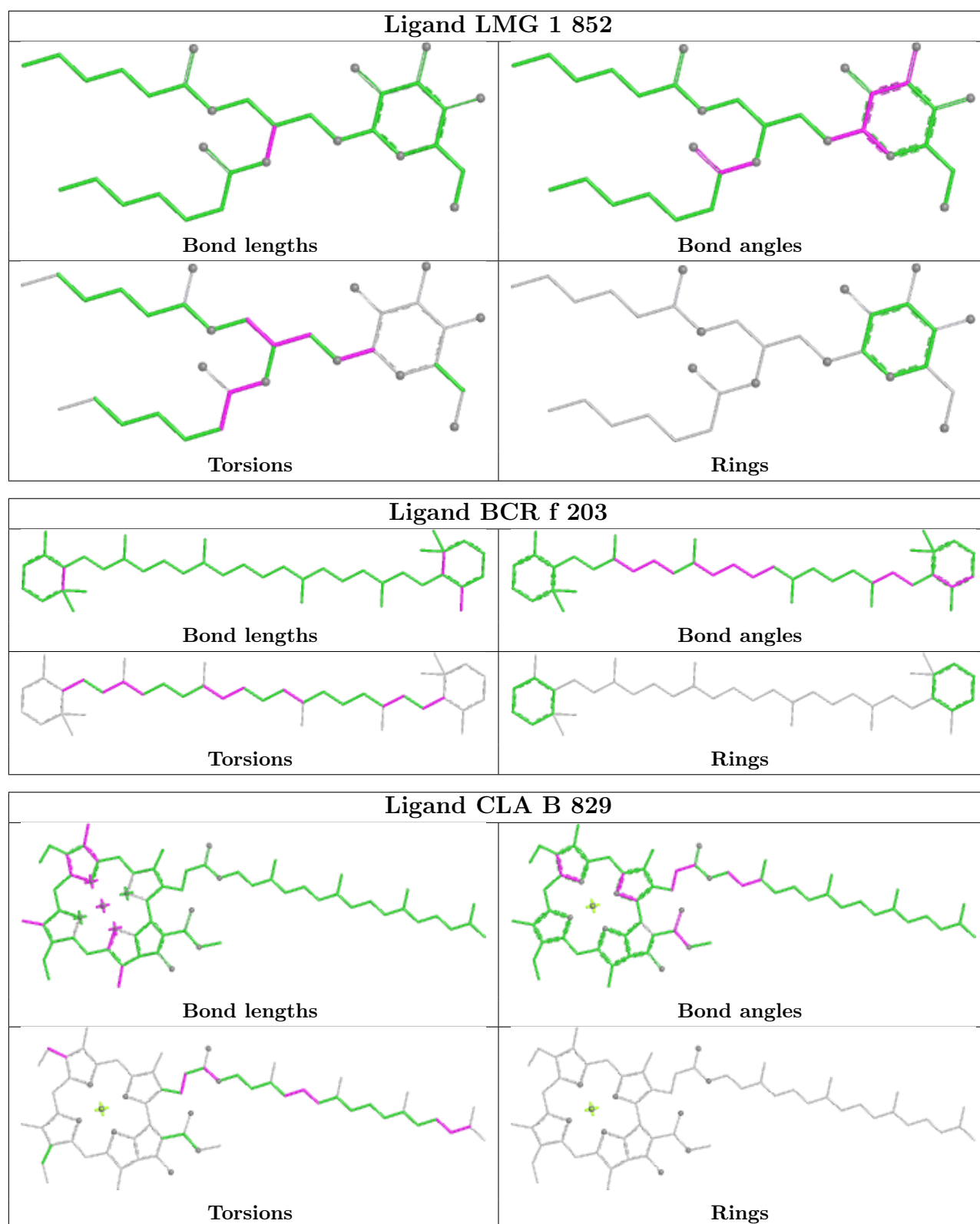
Ligand CLA 2 830**Ligand CLA a 828**

Ligand CLA 1 839

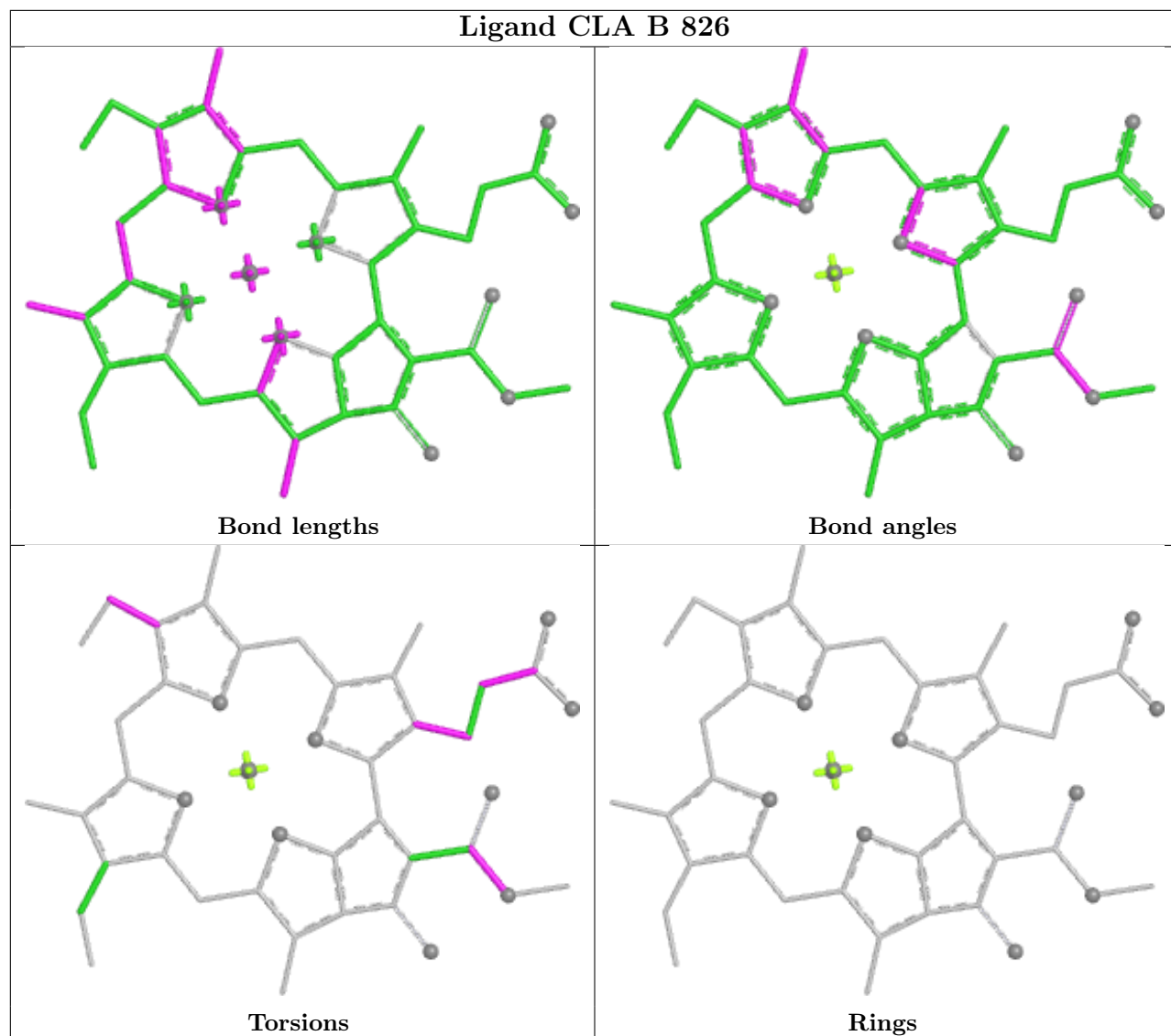


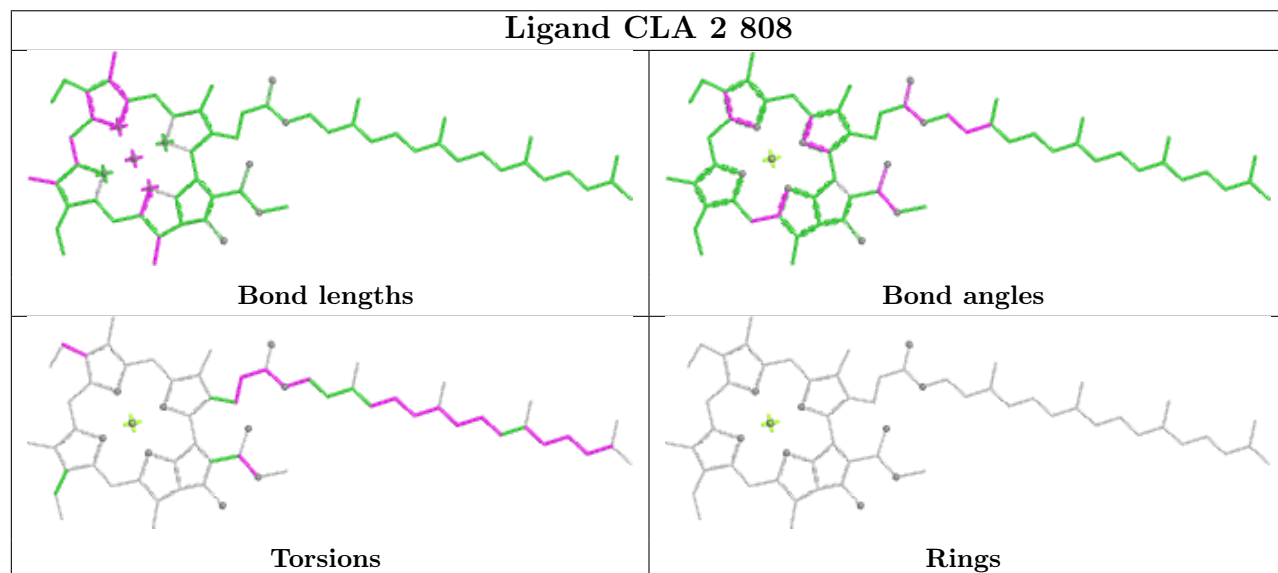
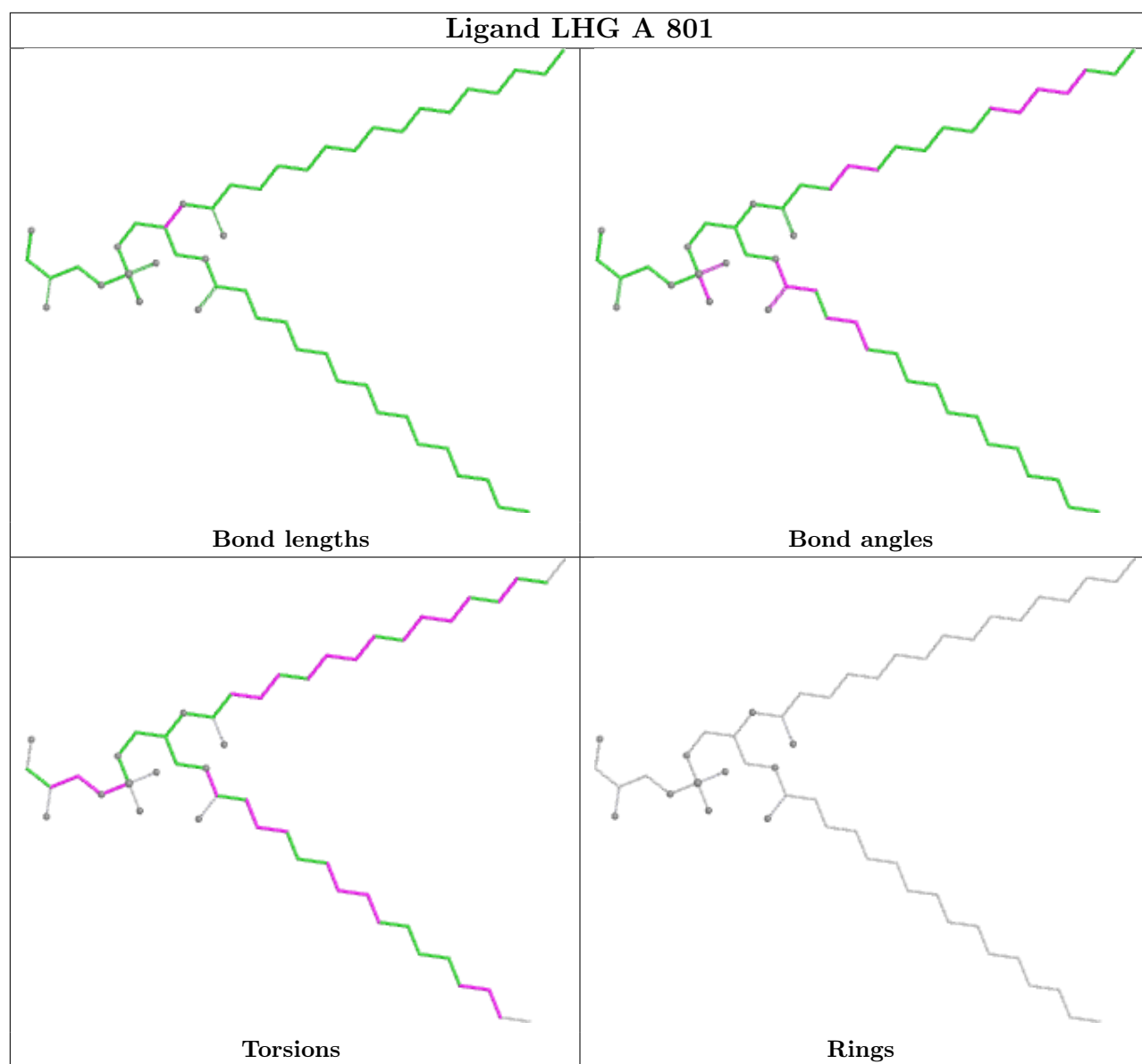
Ligand BCR B 850

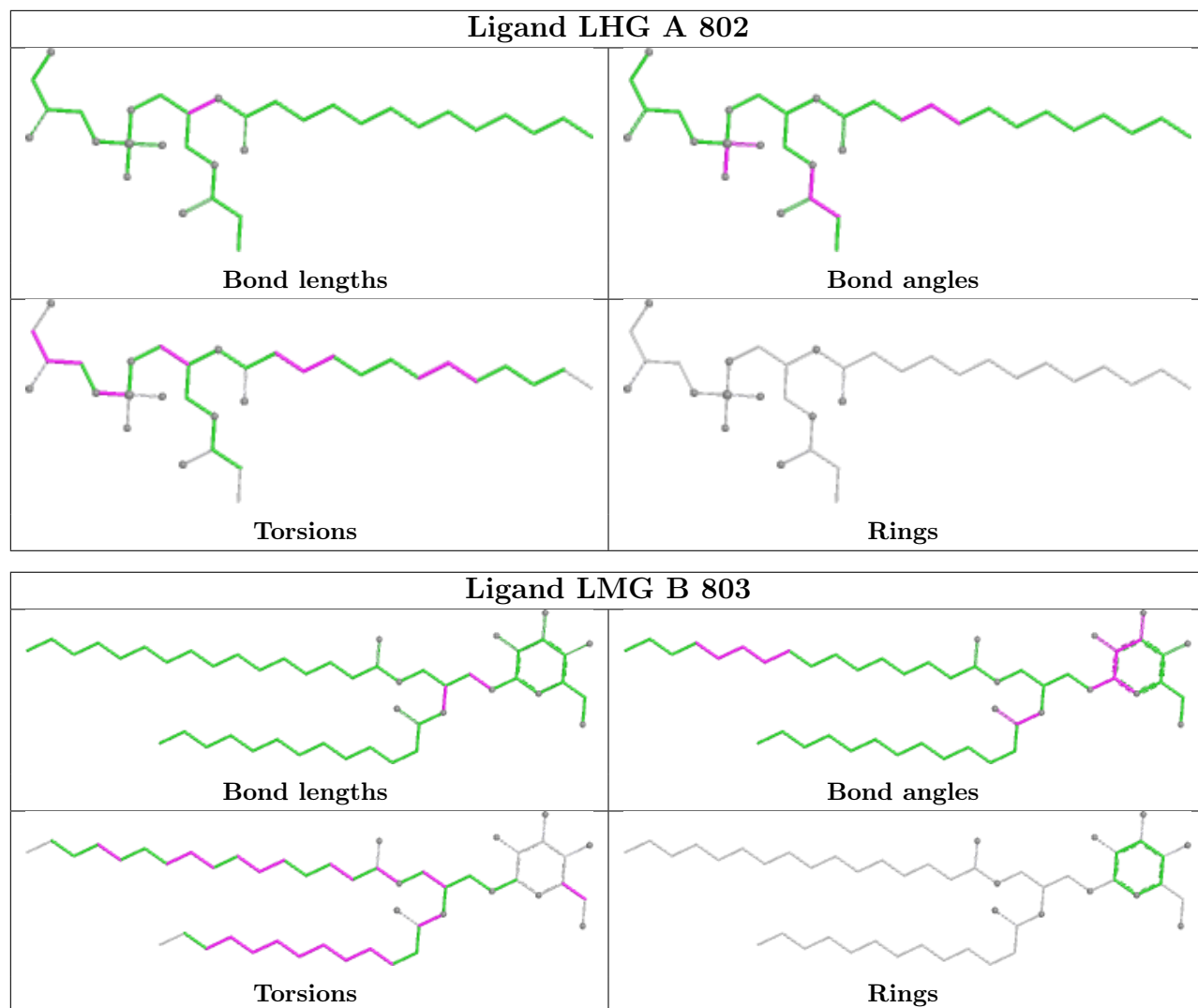


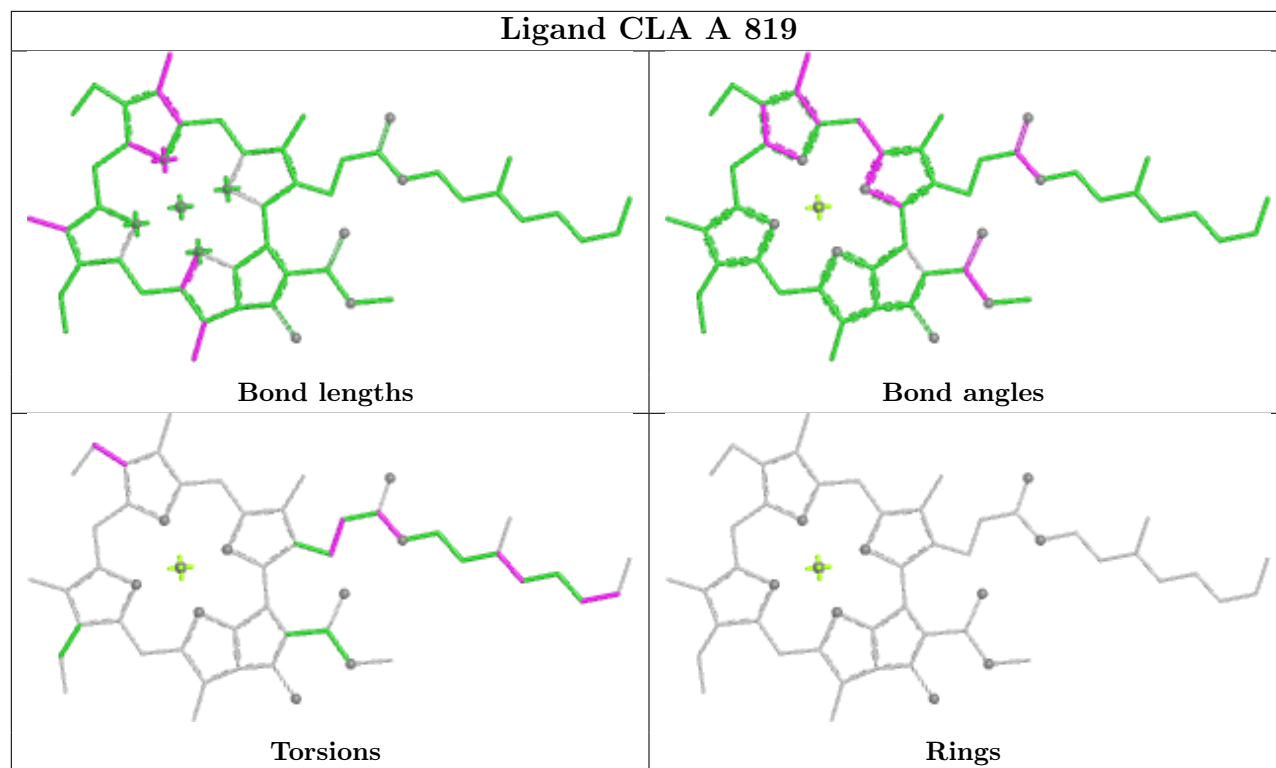


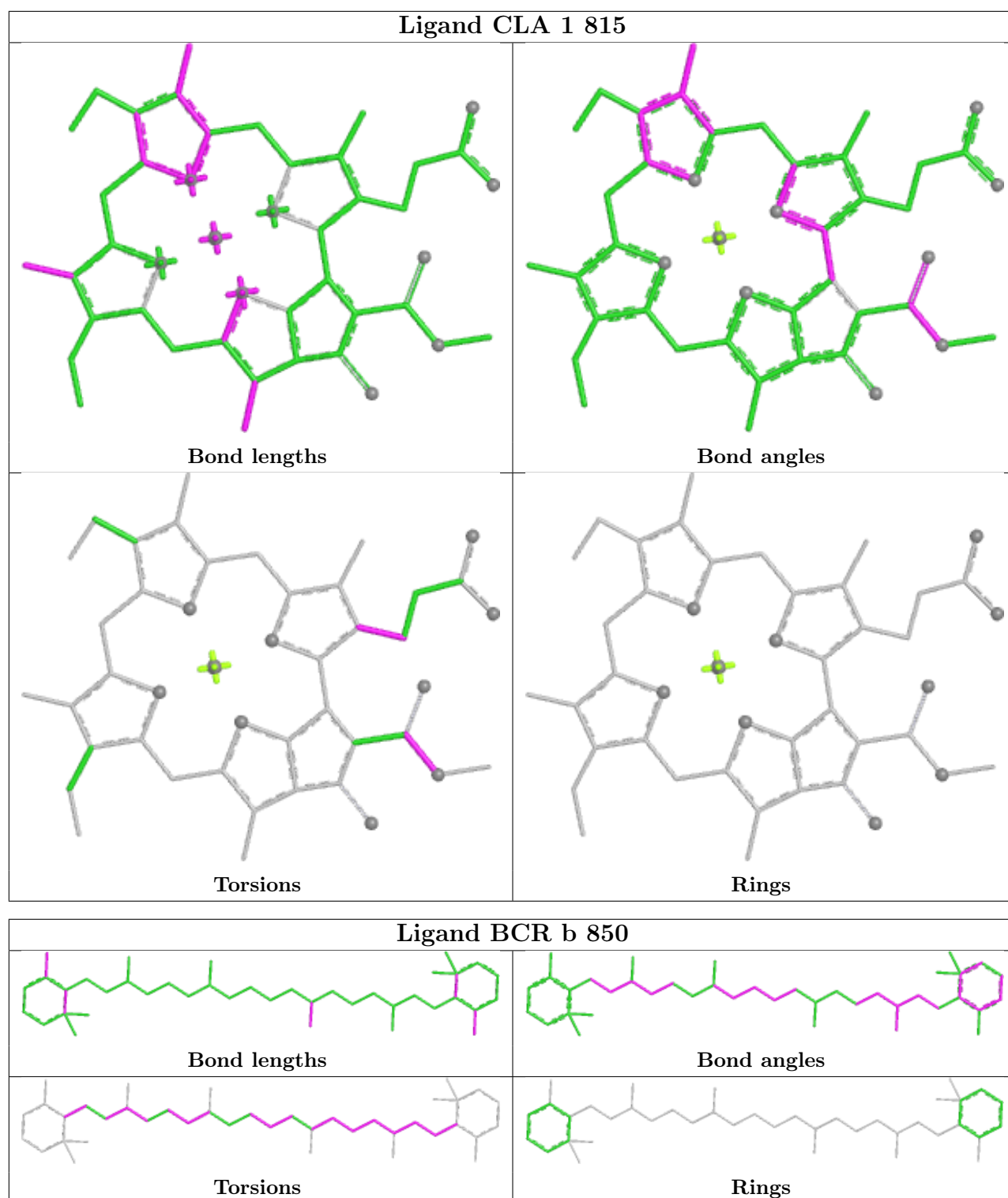
Ligand CLA B 826

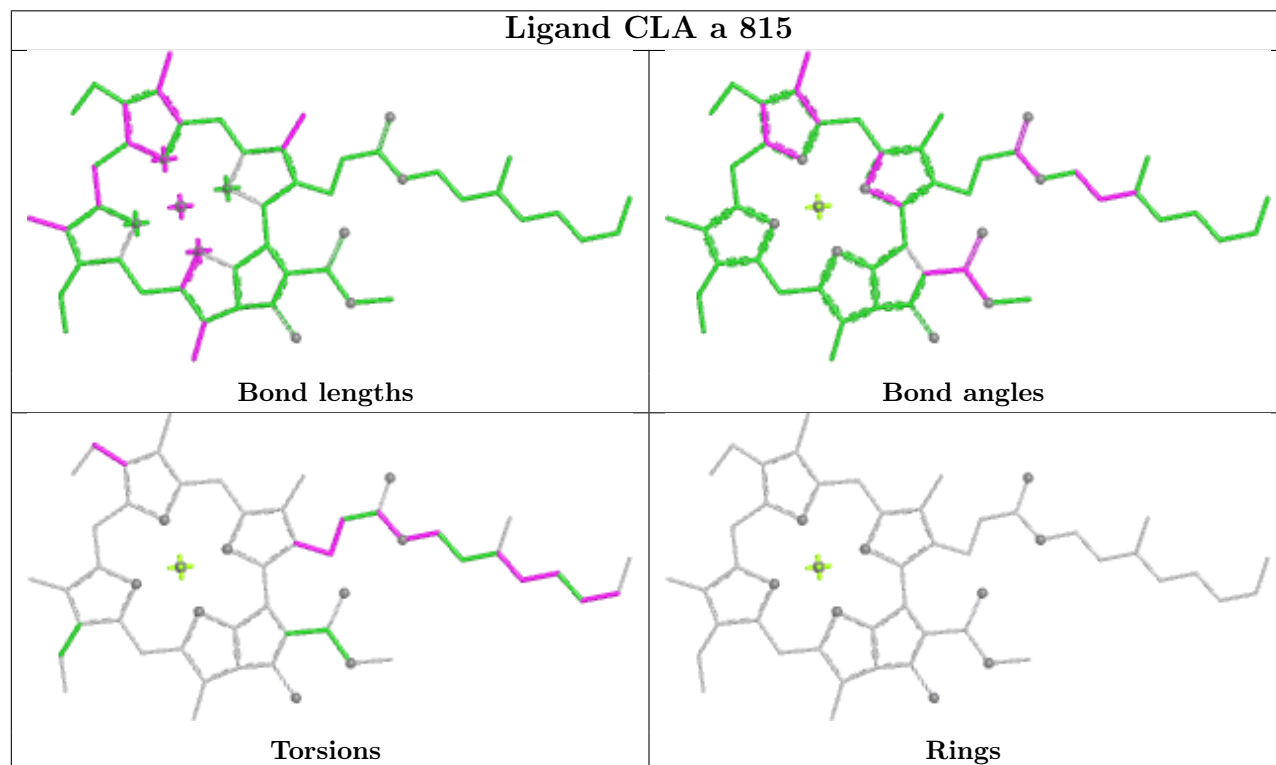
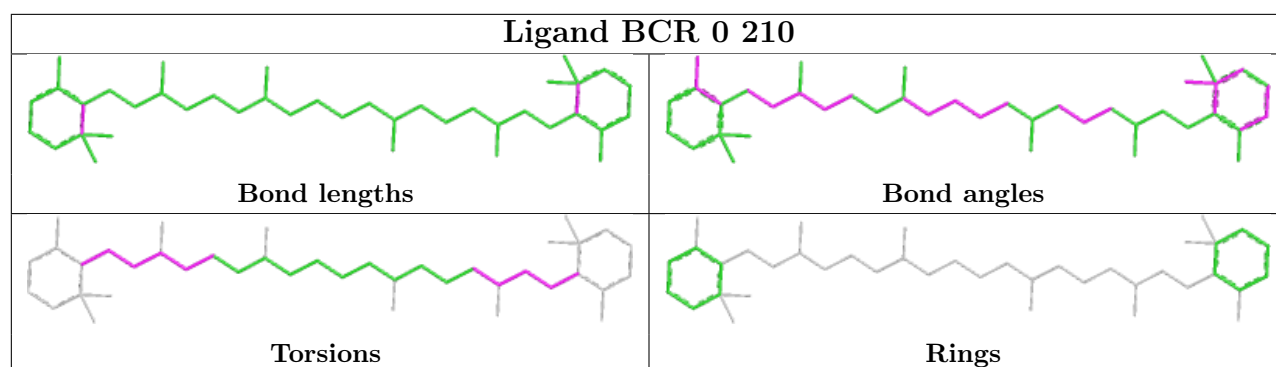


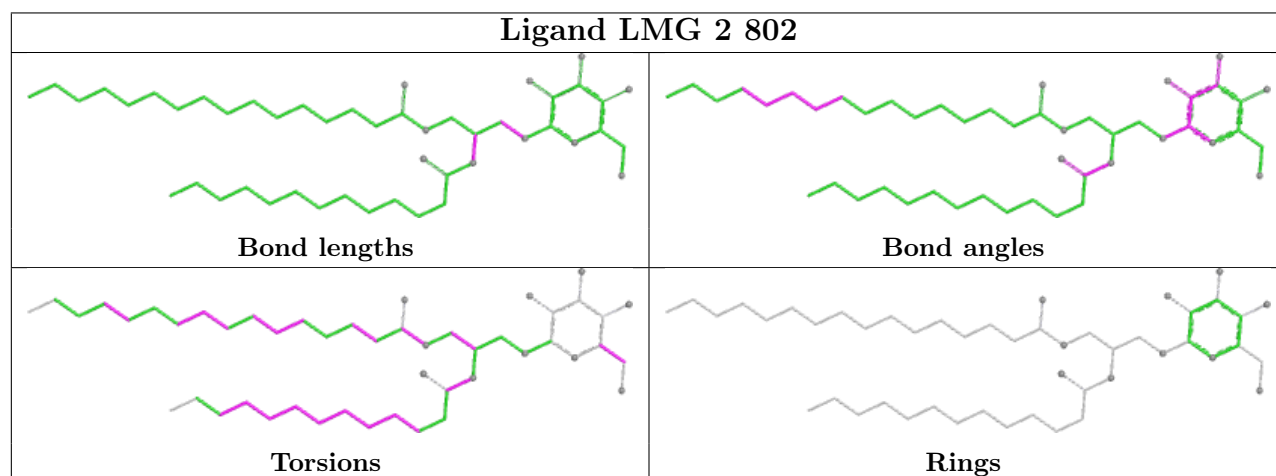
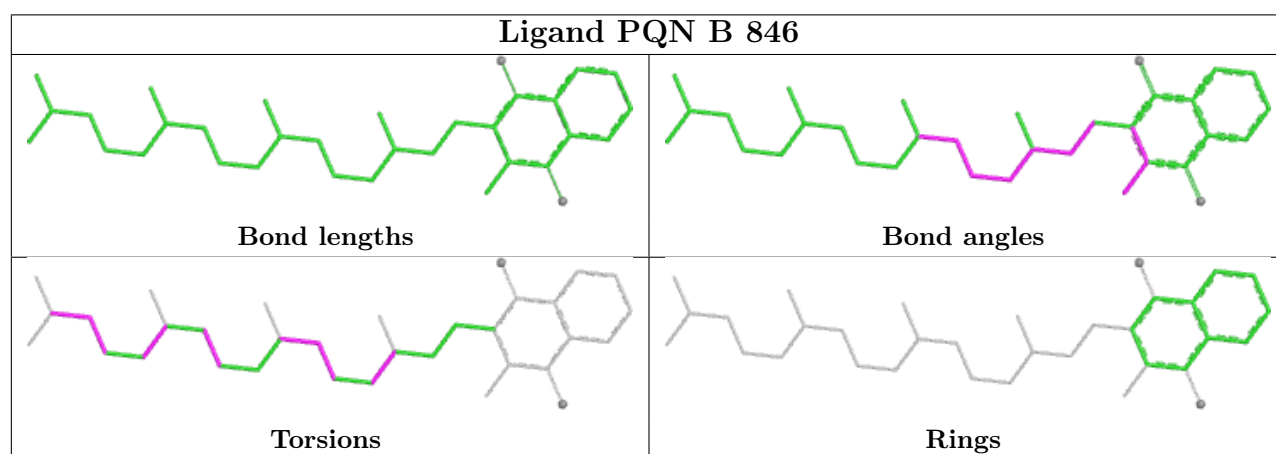
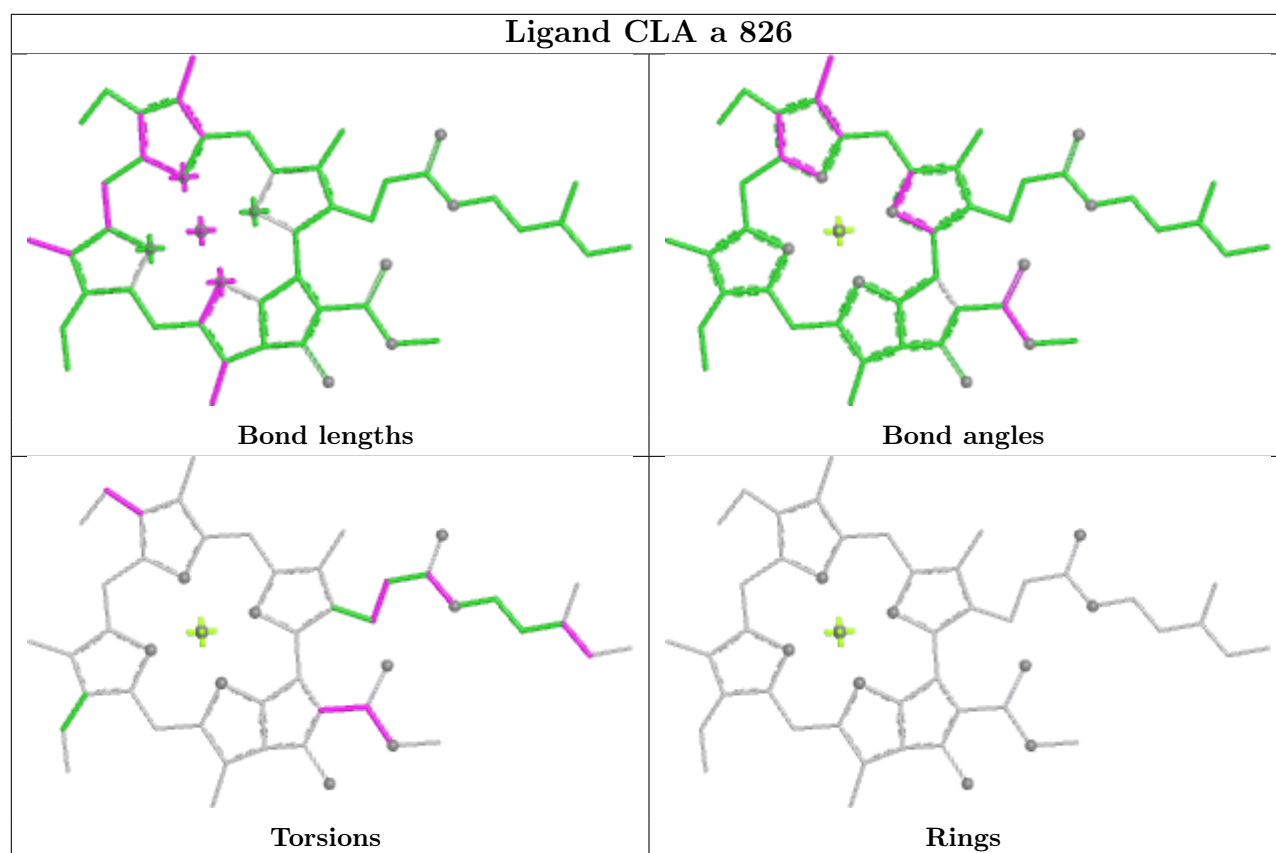




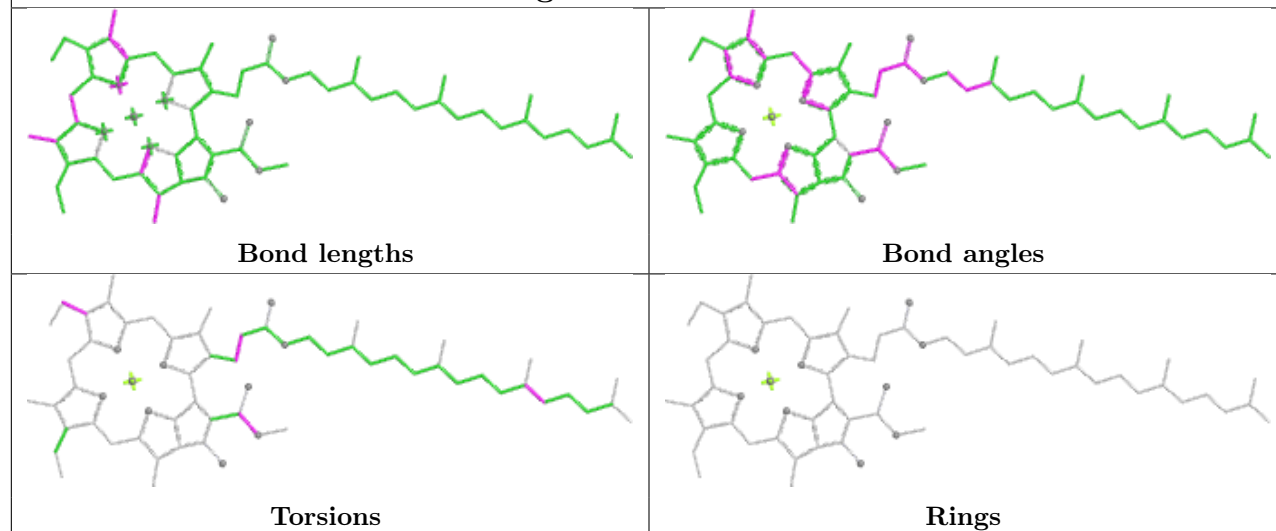




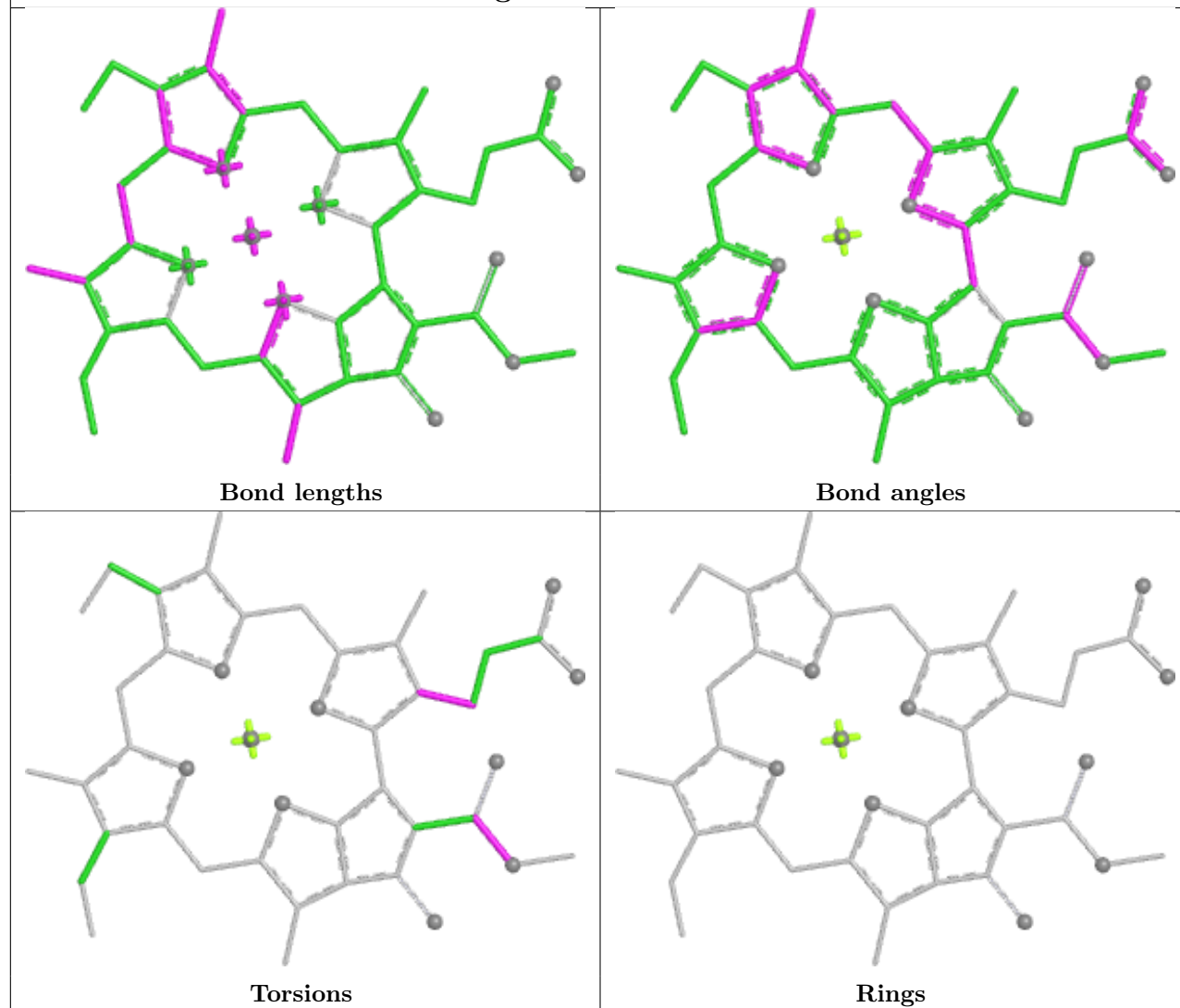




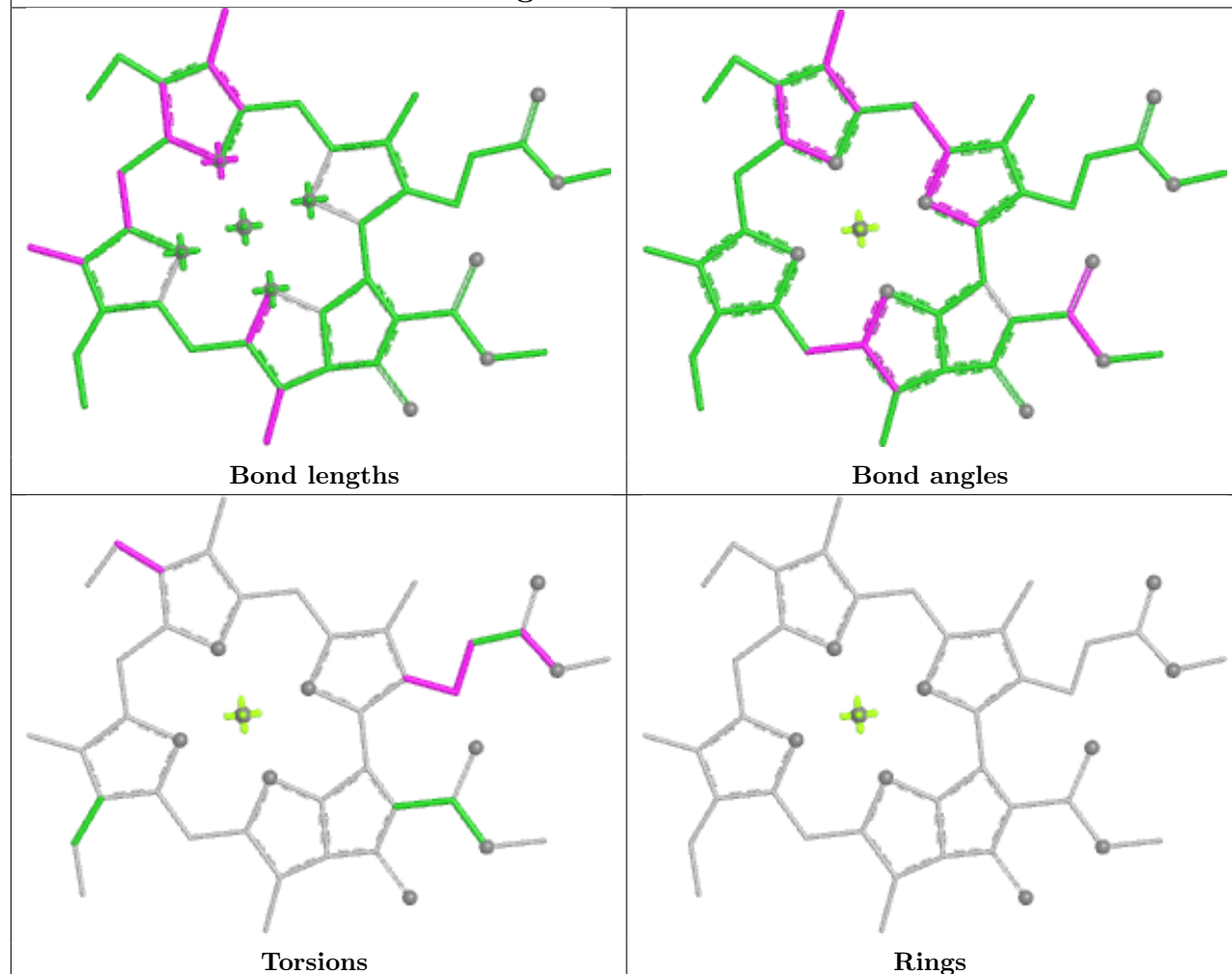
Ligand CLA a 836



Ligand CLA b 836



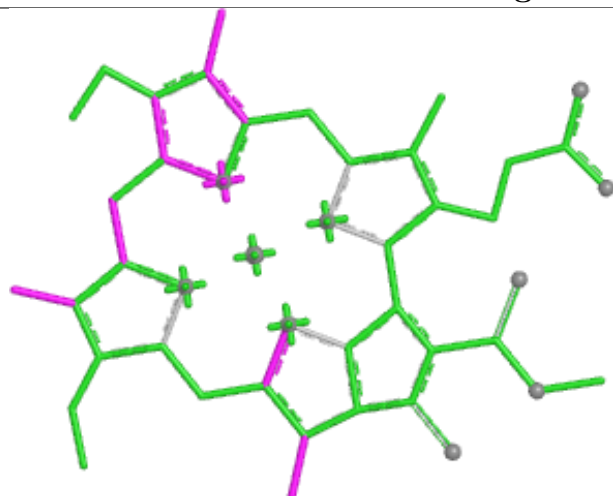
Ligand CLA b 838



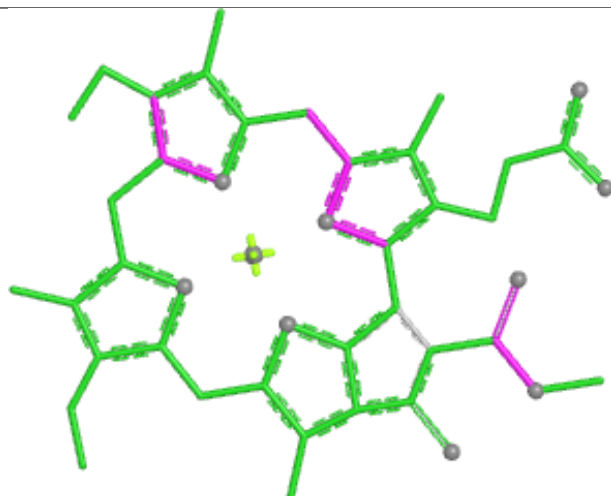
Ligand LMG b 803



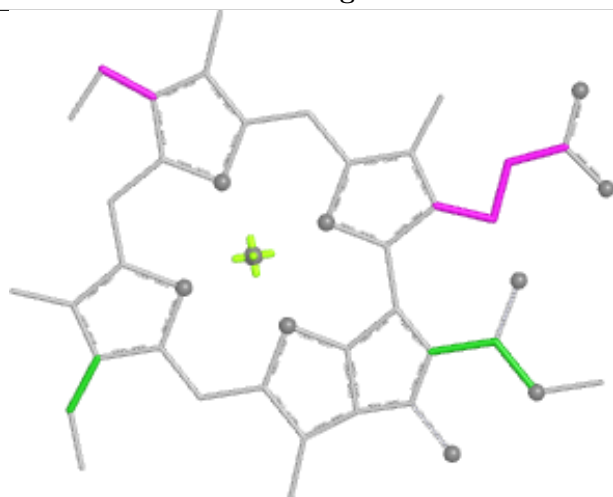
Ligand CLA B 823



Bond lengths



Bond angles

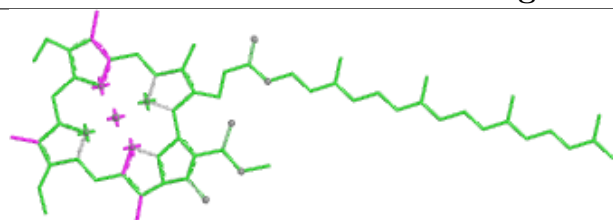


Torsions

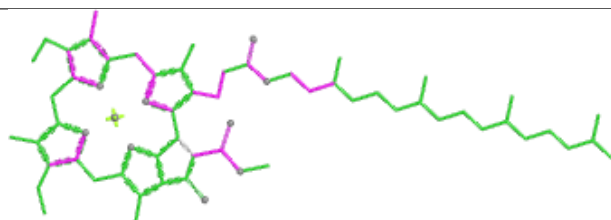


Rings

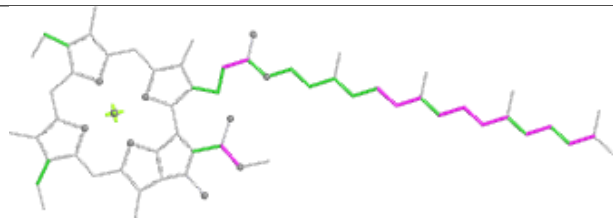
Ligand CLA 2 804



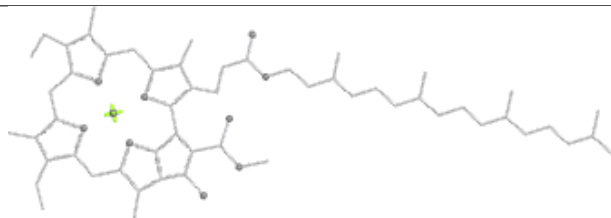
Bond lengths



Bond angles



Torsions



Rings

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.

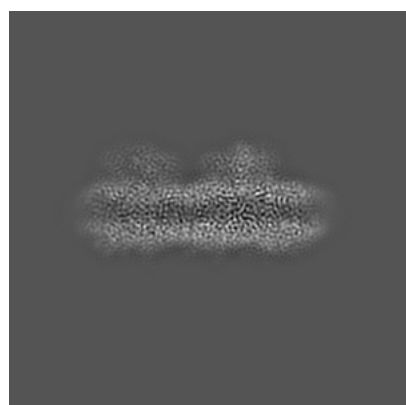
6 Map visualisation [i](#)

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.

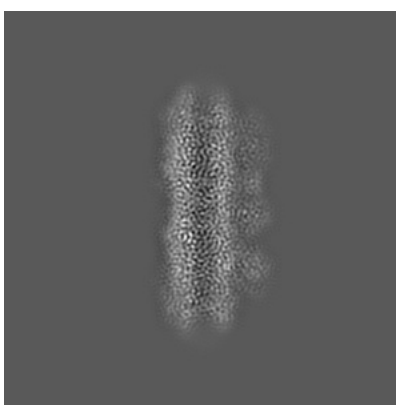
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

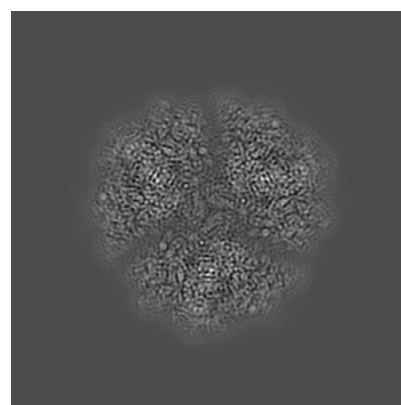
6.1.1 Primary map



X



Y



Z

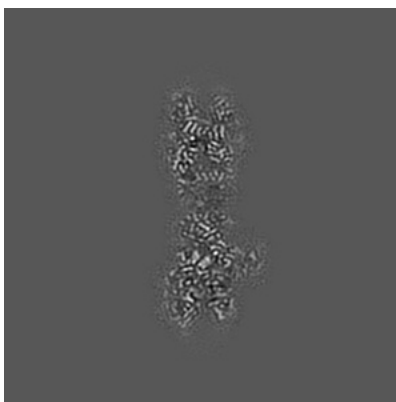
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

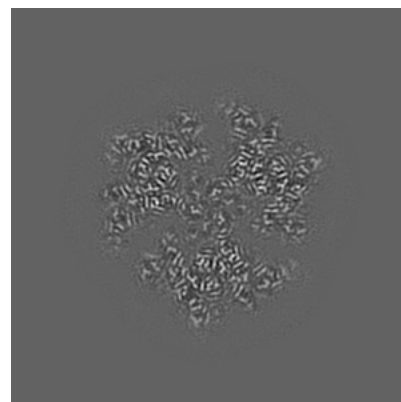
6.2.1 Primary map



X Index: 155



Y Index: 155



Z Index: 155

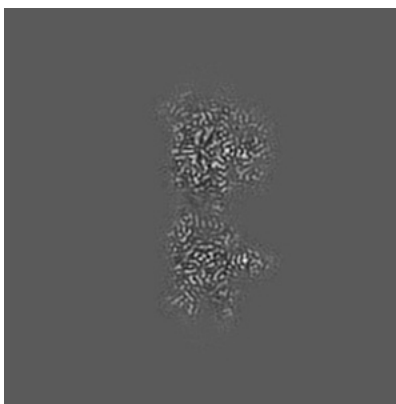
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

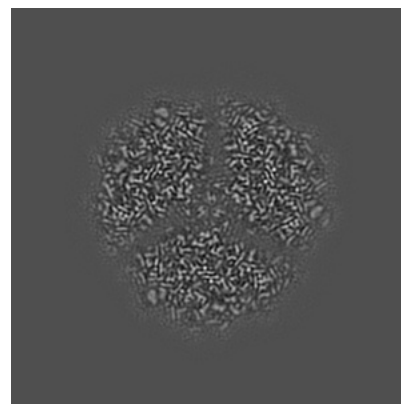
6.3.1 Primary map



X Index: 113



Y Index: 179

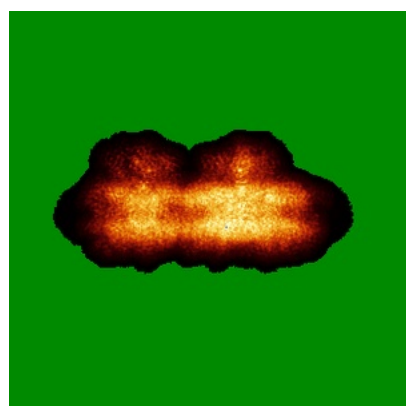


Z Index: 143

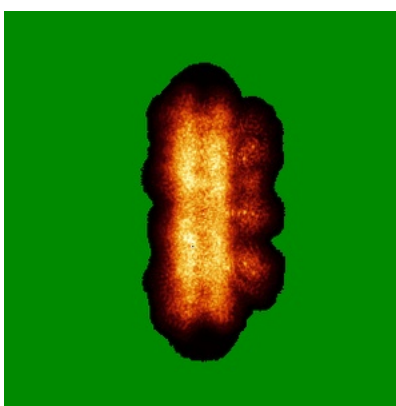
The images above show the largest variance slices of the map in three orthogonal directions.

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

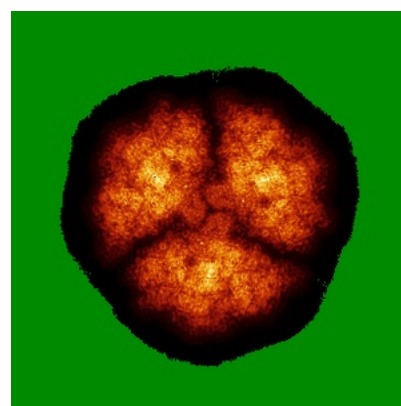
6.4.1 Primary map



X



Y

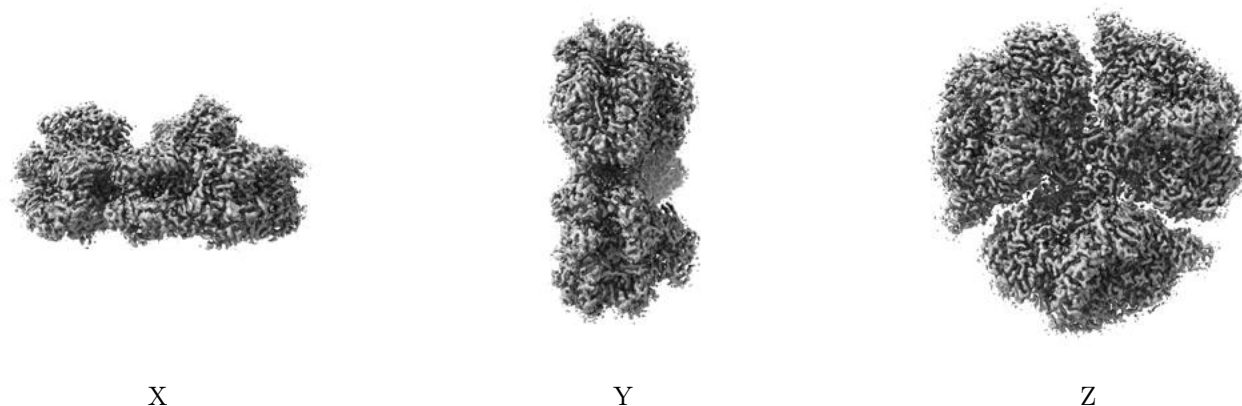


Z

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.

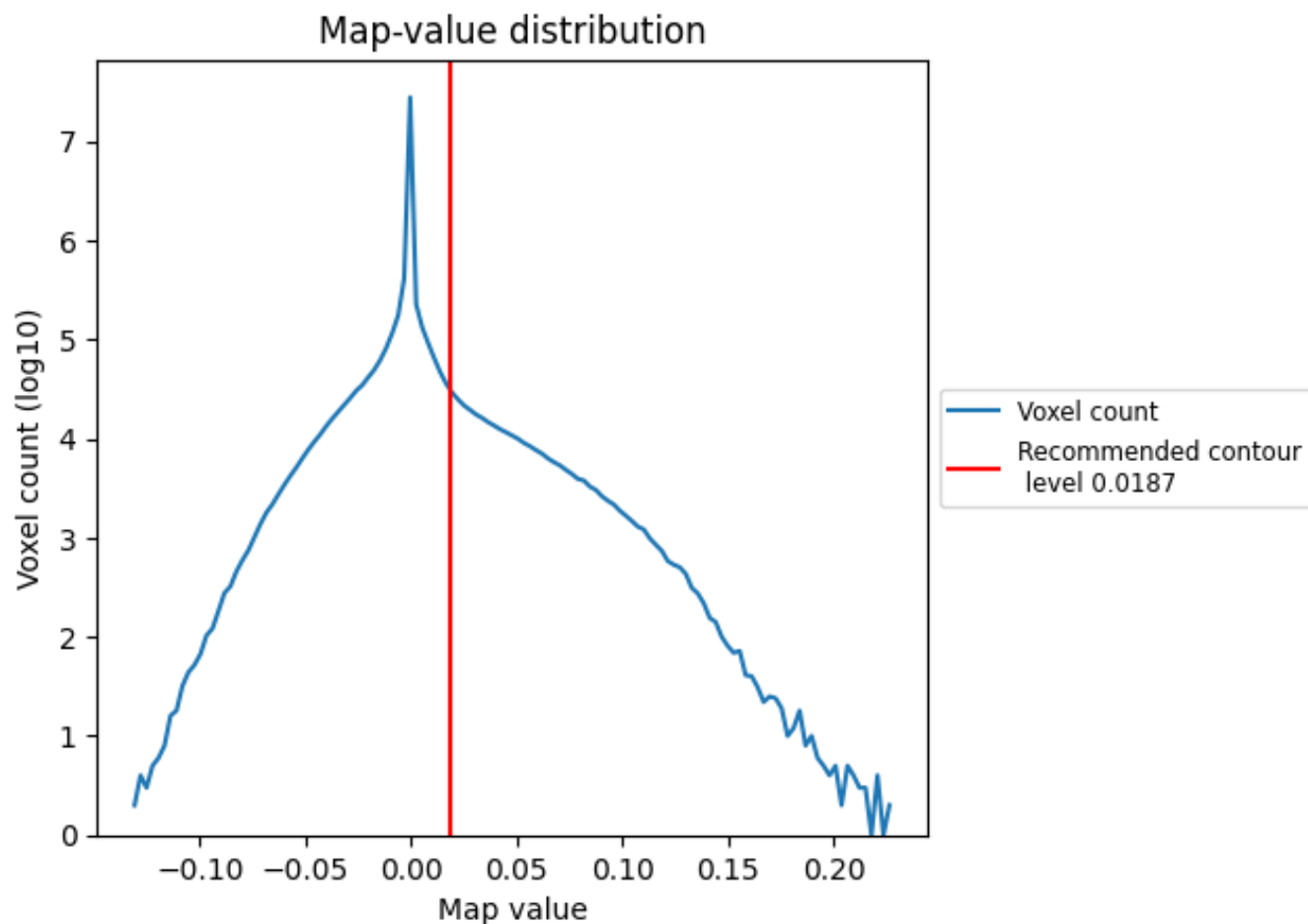
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

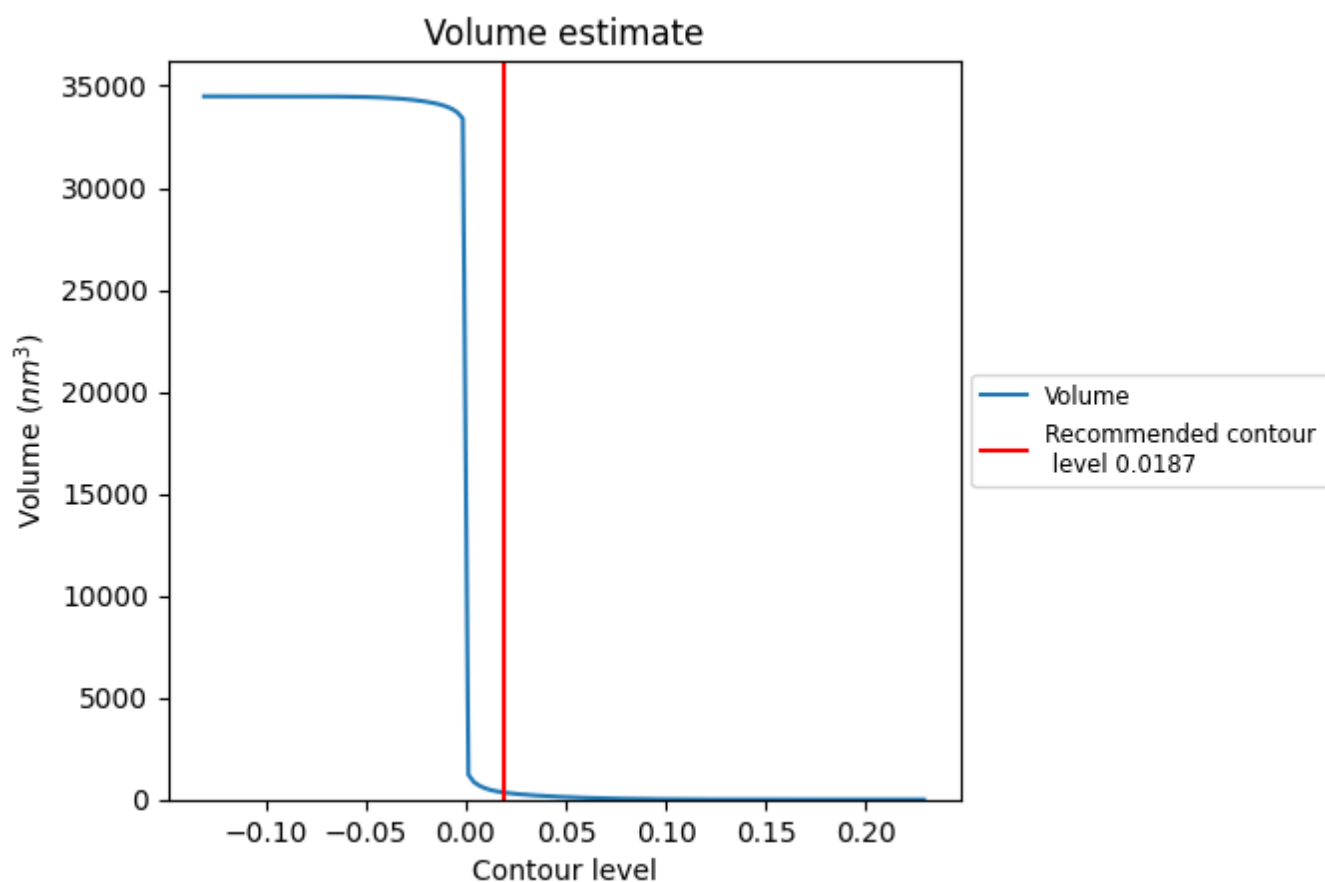
This section contains the results of statistical analysis of the map.

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.

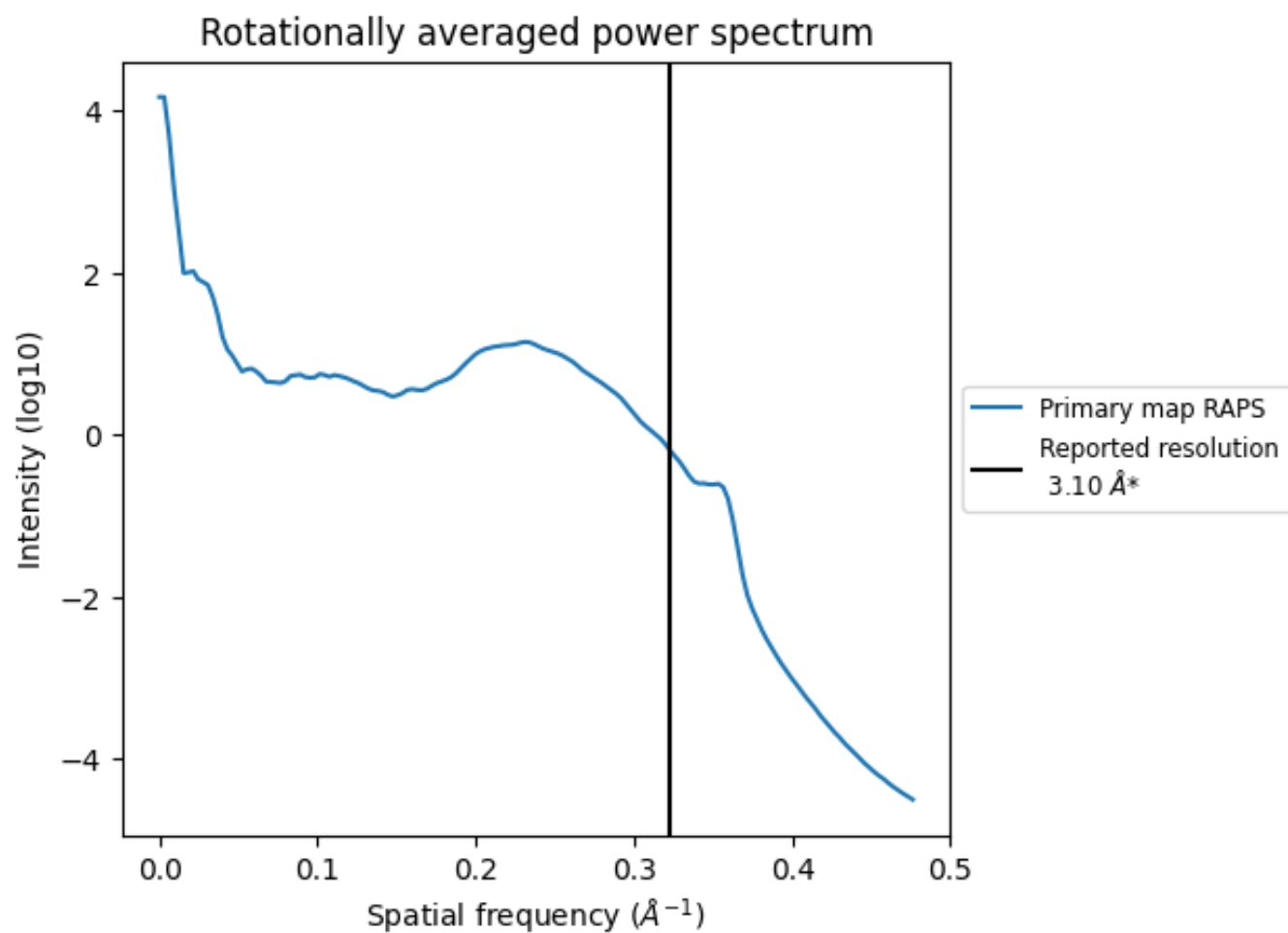
7.2 Volume estimate [i](#)



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

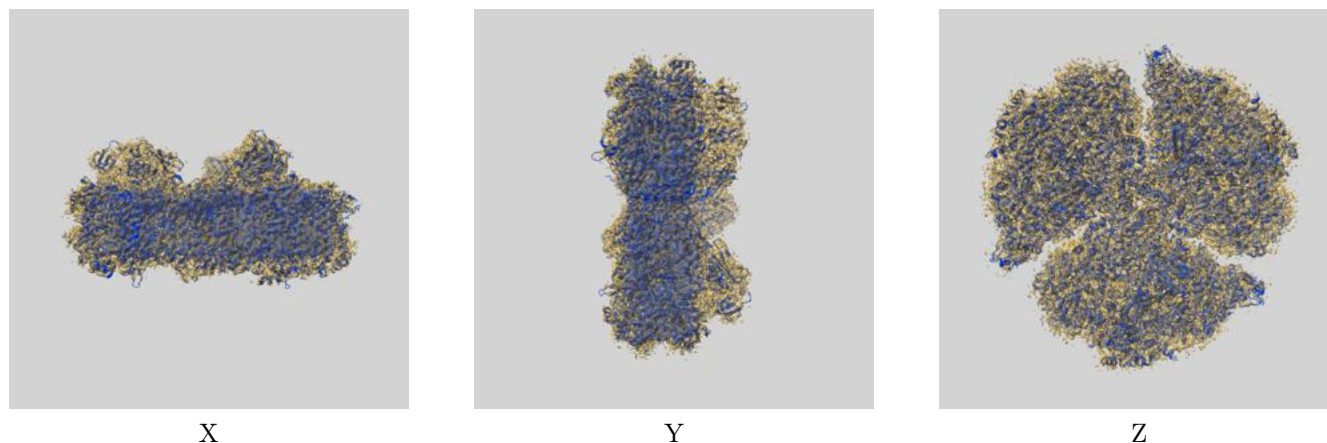
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

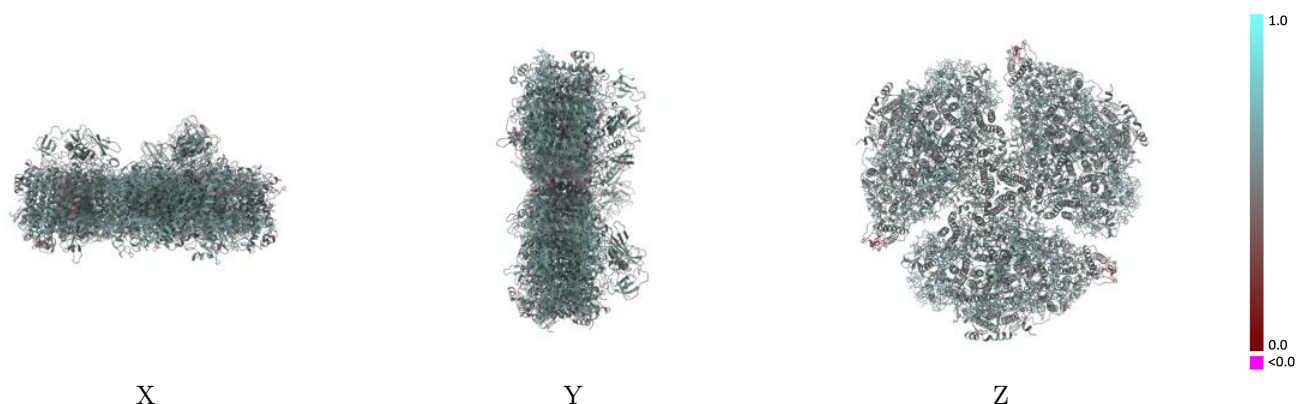
This section contains information regarding the fit between EMDB map EMD-20963 and PDB model 6UZV. Per-residue inclusion information can be found in section 3 on page 38.

9.1 Map-model overlay [i](#)



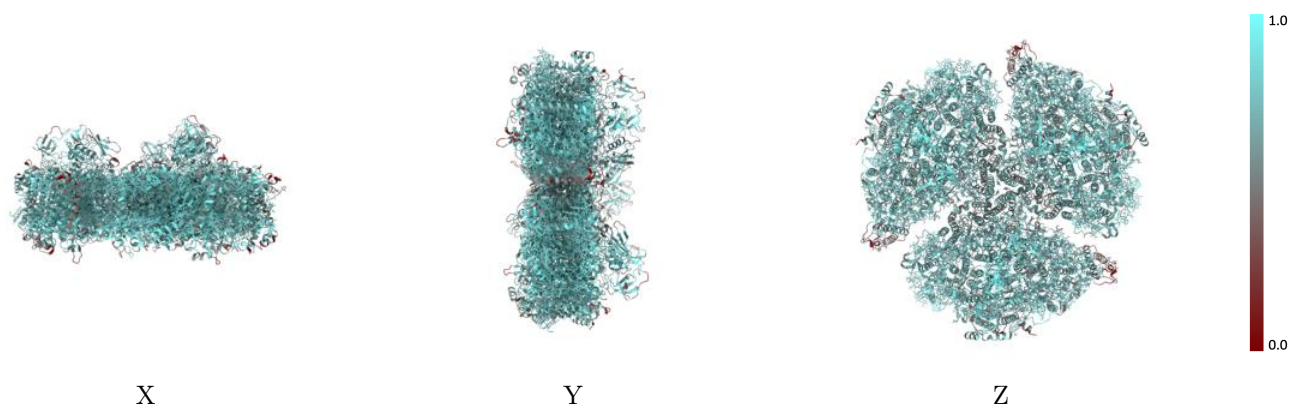
The images above show the 3D surface view of the map at the recommended contour level 0.0187 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



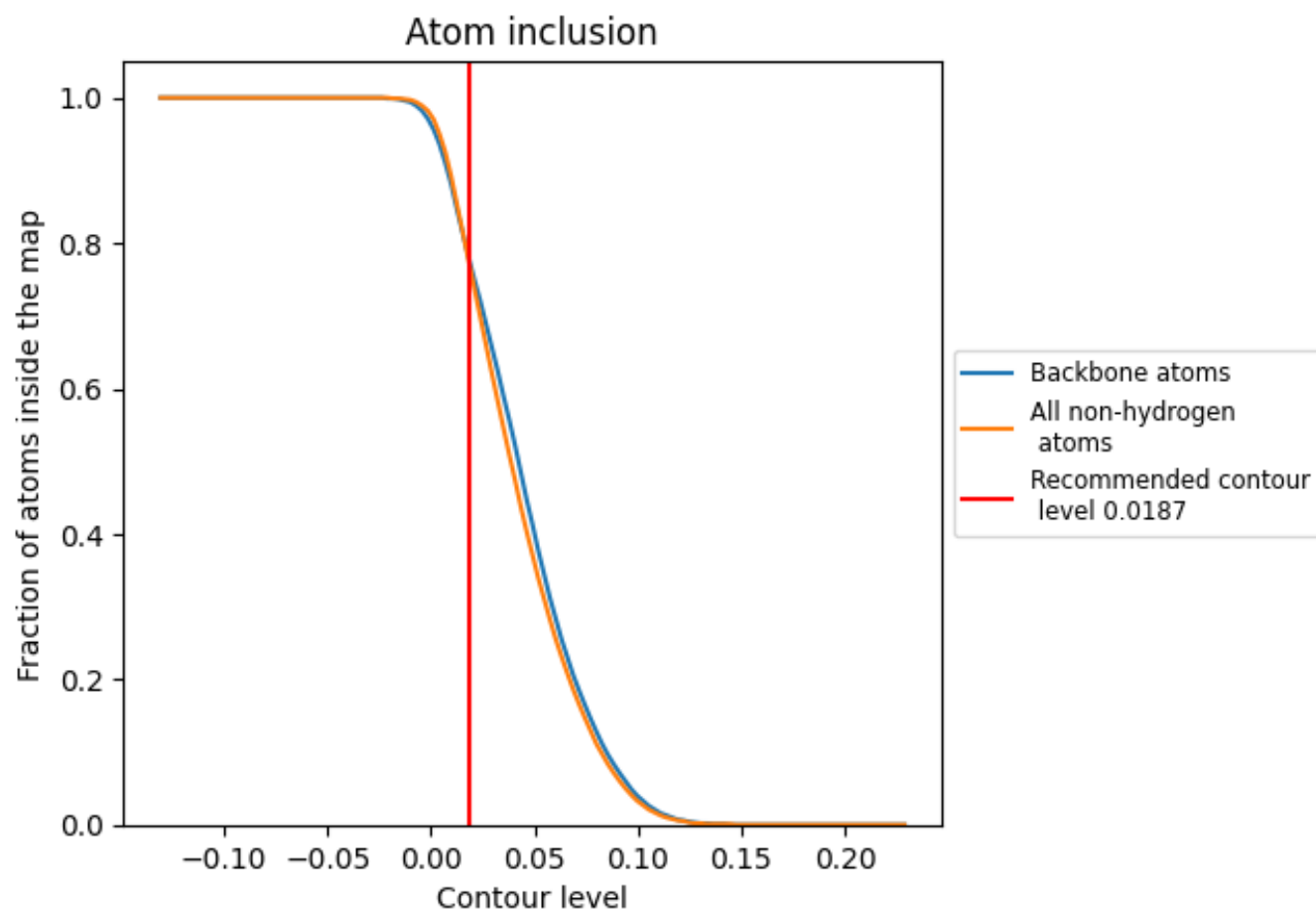
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

