



wwPDB EM Model Validation Summary Report ⓘ

Mar 9, 2020 – 11:26 PM EDT

PDB ID : 6QWJ
EMDB ID : EMD-4659
Title : The structure of tetrameric cyanobacterial Photosystem I of *Chroococcidiopsis* sp. TS-821
Authors : Semchonok, D.A.; Ramirez-Aportela, E.; Sorzano, C.O.S.; Boekema, E.J.; Bruce, B.D.; Guskov, A.
Deposited on : 2019-03-05
Resolution : 4.50 Å (reported)
Based on initial model : 1JB0

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

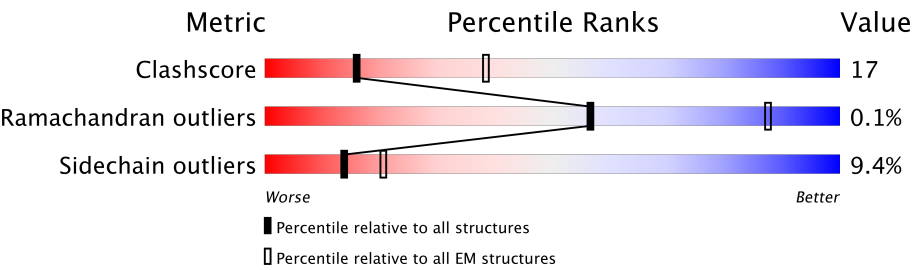
MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.50 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.






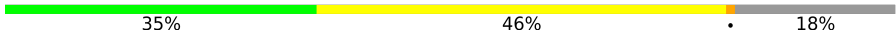
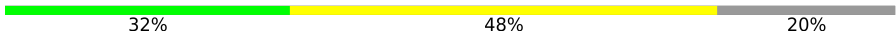






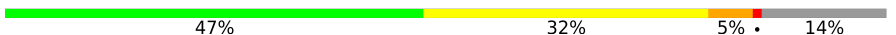
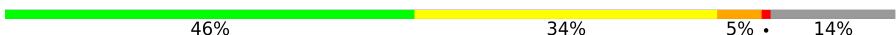












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	752	<div><div>43%</div><div>50%</div><div>..</div></div>
1	E	752	<div><div>44%</div><div>49%</div><div>..</div></div>
1	a	752	<div><div>91%</div><div>5%</div><div>.</div></div>
1	e	752	<div><div>91%</div><div>5%</div><div>.</div></div>
2	B	737	<div><div>45%</div><div>50%</div><div>.</div></div>
2	G	737	<div><div>44%</div><div>51%</div><div>.</div></div>
2	b	737	<div><div>92%</div><div>7%</div><div></div></div>
2	g	737	<div><div>92%</div><div>7%</div><div></div></div>
3	C	82	<div><div>40%</div><div>50%</div><div>7%..</div></div>







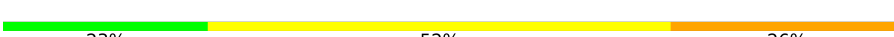
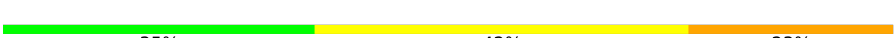


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Mol	Chain	Length	Quality of chain
3	H	82	
3	c	82	
3	h	82	
4	D	168	
4	N	168	
4	d	168	
4	n	168	
5	V	126	
5	W	126	
5	v	126	
5	w	126	
6	F	164	
6	O	164	
6	f	164	
6	o	164	
7	I	39	
7	P	39	
7	i	39	
7	p	39	
8	J	49	
8	Q	49	
8	j	49	
8	q	49	
9	K	93	
9	R	93	

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Mol	Chain	Length	Quality of chain
9	k	93	
9	r	93	
10	L	172	
10	S	172	
10	l	172	
10	s	172	
11	M	31	
11	T	31	
11	m	31	
11	t	31	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	801	X	-	-	-
12	CLA	A	802	X	-	-	-
12	CLA	A	803	X	-	-	-
12	CLA	A	804	X	-	-	-
12	CLA	A	805	X	-	-	-
12	CLA	A	806	X	-	-	-
12	CLA	A	807	X	-	-	-
12	CLA	A	808	X	-	-	-
12	CLA	A	809	X	-	-	-
12	CLA	A	810	X	-	-	-
12	CLA	A	811	X	-	-	-
12	CLA	A	812	X	-	-	-
12	CLA	A	813	X	-	-	-
12	CLA	A	814	X	-	-	-
12	CLA	A	815	X	-	-	-
12	CLA	A	816	X	-	-	-
12	CLA	A	817	X	-	-	-
12	CLA	A	818	X	-	-	-
12	CLA	A	819	X	-	-	-
12	CLA	A	820	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	A	821	X	-	-	-
12	CLA	A	822	X	-	-	-
12	CLA	A	823	X	-	-	-
12	CLA	A	824	X	-	-	-
12	CLA	A	825	X	-	-	-
12	CLA	A	826	X	-	-	-
12	CLA	A	827	X	-	-	-
12	CLA	A	828	X	-	-	-
12	CLA	A	829	X	-	-	-
12	CLA	A	830	X	-	-	-
12	CLA	A	831	X	-	-	-
12	CLA	A	832	X	-	-	-
12	CLA	A	833	X	-	-	-
12	CLA	A	834	X	-	-	-
12	CLA	A	835	X	-	-	-
12	CLA	A	836	X	-	-	-
12	CLA	A	837	X	-	-	-
12	CLA	A	838	X	-	-	-
12	CLA	A	839	X	-	-	-
12	CLA	A	840	X	-	-	-
12	CLA	A	841	X	-	-	-
12	CLA	B	801	X	-	-	-
12	CLA	B	802	X	-	-	-
12	CLA	B	803	X	-	-	-
12	CLA	B	805	X	-	-	-
12	CLA	B	806	X	-	-	-
12	CLA	B	807	X	-	-	-
12	CLA	B	808	X	-	-	-
12	CLA	B	809	X	-	-	-
12	CLA	B	810	X	-	-	-
12	CLA	B	811	X	-	-	-
12	CLA	B	812	X	-	-	-
12	CLA	B	813	X	-	-	-
12	CLA	B	814	X	-	-	-
12	CLA	B	815	X	-	-	-
12	CLA	B	816	X	-	-	-
12	CLA	B	817	X	-	-	-
12	CLA	B	818	X	-	-	-
12	CLA	B	819	X	-	-	-
12	CLA	B	820	X	-	-	-
12	CLA	B	821	X	-	-	-
12	CLA	B	822	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	B	823	X	-	-	-
12	CLA	B	824	X	-	-	-
12	CLA	B	825	X	-	-	-
12	CLA	B	826	X	-	-	-
12	CLA	B	827	X	-	-	-
12	CLA	B	828	X	-	-	-
12	CLA	B	829	X	-	-	-
12	CLA	B	830	X	-	-	-
12	CLA	B	831	X	-	-	-
12	CLA	B	832	X	-	-	-
12	CLA	B	833	X	-	-	-
12	CLA	B	834	X	-	-	-
12	CLA	B	835	X	-	-	-
12	CLA	B	836	X	-	-	-
12	CLA	B	837	X	-	-	-
12	CLA	B	838	X	-	-	-
12	CLA	B	839	X	-	-	-
12	CLA	B	840	X	-	-	-
12	CLA	B	841	X	-	-	-
12	CLA	B	842	X	-	-	-
12	CLA	B	843	X	-	-	-
12	CLA	E	801	X	-	-	-
12	CLA	E	802	X	-	-	-
12	CLA	E	803	X	-	-	-
12	CLA	E	804	X	-	-	-
12	CLA	E	805	X	-	-	-
12	CLA	E	806	X	-	-	-
12	CLA	E	807	X	-	-	-
12	CLA	E	808	X	-	-	-
12	CLA	E	809	X	-	-	-
12	CLA	E	810	X	-	-	-
12	CLA	E	811	X	-	-	-
12	CLA	E	812	X	-	-	-
12	CLA	E	813	X	-	-	-
12	CLA	E	814	X	-	-	-
12	CLA	E	815	X	-	-	-
12	CLA	E	816	X	-	-	-
12	CLA	E	817	X	-	-	-
12	CLA	E	818	X	-	-	-
12	CLA	E	819	X	-	-	-
12	CLA	E	820	X	-	-	-
12	CLA	E	821	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	E	822	X	-	-	-
12	CLA	E	823	X	-	-	-
12	CLA	E	824	X	-	-	-
12	CLA	E	825	X	-	-	-
12	CLA	E	826	X	-	-	-
12	CLA	E	827	X	-	-	-
12	CLA	E	828	X	-	-	-
12	CLA	E	829	X	-	-	-
12	CLA	E	830	X	-	-	-
12	CLA	E	831	X	-	-	-
12	CLA	E	832	X	-	-	-
12	CLA	E	833	X	-	-	-
12	CLA	E	834	X	-	-	-
12	CLA	E	835	X	-	-	-
12	CLA	E	836	X	-	-	-
12	CLA	E	837	X	-	-	-
12	CLA	E	838	X	-	-	-
12	CLA	E	839	X	-	-	-
12	CLA	E	840	X	-	-	-
12	CLA	E	841	X	-	-	-
12	CLA	E	842	X	-	-	-
12	CLA	E	843	X	-	-	-
12	CLA	E	844	X	-	-	-
12	CLA	F	1301	X	-	-	-
12	CLA	G	801	X	-	-	-
12	CLA	G	802	X	-	-	-
12	CLA	G	803	X	-	-	-
12	CLA	G	804	X	-	-	-
12	CLA	G	805	X	-	-	-
12	CLA	G	806	X	-	-	-
12	CLA	G	807	X	-	-	-
12	CLA	G	808	X	-	-	-
12	CLA	G	809	X	-	-	-
12	CLA	G	810	X	-	-	-
12	CLA	G	811	X	-	-	-
12	CLA	G	812	X	-	-	-
12	CLA	G	813	X	-	-	-
12	CLA	G	814	X	-	-	-
12	CLA	G	815	X	-	-	-
12	CLA	G	816	X	-	-	-
12	CLA	G	817	X	-	-	-
12	CLA	G	818	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	G	819	X	-	-	-
12	CLA	G	820	X	-	-	-
12	CLA	G	821	X	-	-	-
12	CLA	G	822	X	-	-	-
12	CLA	G	823	X	-	-	-
12	CLA	G	824	X	-	-	-
12	CLA	G	825	X	-	-	-
12	CLA	G	826	X	-	-	-
12	CLA	G	827	X	-	-	-
12	CLA	G	828	X	-	-	-
12	CLA	G	829	X	-	-	-
12	CLA	G	830	X	-	-	-
12	CLA	G	831	X	-	-	-
12	CLA	G	832	X	-	-	-
12	CLA	G	833	X	-	-	-
12	CLA	G	834	X	-	-	-
12	CLA	G	835	X	-	-	-
12	CLA	G	836	X	-	-	-
12	CLA	G	837	X	-	-	-
12	CLA	G	838	X	-	-	-
12	CLA	G	839	X	-	-	-
12	CLA	G	840	X	-	-	-
12	CLA	G	841	X	-	-	-
12	CLA	G	843	X	-	-	-
12	CLA	J	1101	X	-	-	-
12	CLA	J	1102	X	-	-	-
12	CLA	K	1401	X	-	-	-
12	CLA	L	201	X	-	-	-
12	CLA	L	202	X	-	-	-
12	CLA	L	203	X	-	-	-
12	CLA	L	204	X	-	-	-
12	CLA	O	1301	X	-	-	-
12	CLA	R	1401	X	-	-	-
12	CLA	S	1501	X	-	-	-
12	CLA	S	1502	X	-	-	-
12	CLA	a	801	X	-	-	-
12	CLA	a	802	X	-	-	-
12	CLA	a	803	X	-	-	-
12	CLA	a	804	X	-	-	-
12	CLA	a	805	X	-	-	-
12	CLA	a	806	X	-	-	-
12	CLA	a	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	a	808	X	-	-	-
12	CLA	a	809	X	-	-	-
12	CLA	a	810	X	-	-	-
12	CLA	a	811	X	-	-	-
12	CLA	a	812	X	-	-	-
12	CLA	a	813	X	-	-	-
12	CLA	a	814	X	-	-	-
12	CLA	a	815	X	-	-	-
12	CLA	a	816	X	-	-	-
12	CLA	a	817	X	-	-	-
12	CLA	a	818	X	-	-	-
12	CLA	a	819	X	-	-	-
12	CLA	a	820	X	-	-	-
12	CLA	a	821	X	-	-	-
12	CLA	a	822	X	-	-	-
12	CLA	a	823	X	-	-	-
12	CLA	a	824	X	-	-	-
12	CLA	a	825	X	-	-	-
12	CLA	a	826	X	-	-	-
12	CLA	a	827	X	-	-	-
12	CLA	a	828	X	-	-	-
12	CLA	a	829	X	-	-	-
12	CLA	a	830	X	-	-	-
12	CLA	a	831	X	-	-	-
12	CLA	a	832	X	-	-	-
12	CLA	a	833	X	-	-	-
12	CLA	a	834	X	-	-	-
12	CLA	a	835	X	-	-	-
12	CLA	a	836	X	-	-	-
12	CLA	a	837	X	-	-	-
12	CLA	a	838	X	-	-	-
12	CLA	a	839	X	-	-	-
12	CLA	a	840	X	-	-	-
12	CLA	a	841	X	-	-	-
12	CLA	a	842	X	-	-	-
12	CLA	b	801	X	-	-	-
12	CLA	b	802	X	-	-	-
12	CLA	b	803	X	-	-	-
12	CLA	b	804	X	-	-	-
12	CLA	b	805	X	-	-	-
12	CLA	b	806	X	-	-	-
12	CLA	b	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	b	808	X	-	-	-
12	CLA	b	809	X	-	-	-
12	CLA	b	810	X	-	-	-
12	CLA	b	811	X	-	-	-
12	CLA	b	812	X	-	-	-
12	CLA	b	813	X	-	-	-
12	CLA	b	814	X	-	-	-
12	CLA	b	815	X	-	-	-
12	CLA	b	816	X	-	-	-
12	CLA	b	817	X	-	-	-
12	CLA	b	818	X	-	-	-
12	CLA	b	819	X	-	-	-
12	CLA	b	820	X	-	-	-
12	CLA	b	821	X	-	-	-
12	CLA	b	822	X	-	-	-
12	CLA	b	823	X	-	-	-
12	CLA	b	824	X	-	-	-
12	CLA	b	825	X	-	-	-
12	CLA	b	826	X	-	-	-
12	CLA	b	827	X	-	-	-
12	CLA	b	828	X	-	-	-
12	CLA	b	829	X	-	-	-
12	CLA	b	830	X	-	-	-
12	CLA	b	831	X	-	-	-
12	CLA	b	832	X	-	-	-
12	CLA	b	833	X	-	-	-
12	CLA	b	834	X	-	-	-
12	CLA	b	835	X	-	-	-
12	CLA	b	836	X	-	-	-
12	CLA	b	837	X	-	-	-
12	CLA	b	838	X	-	-	-
12	CLA	b	839	X	-	-	-
12	CLA	b	840	X	-	-	-
12	CLA	b	841	X	-	-	-
12	CLA	b	842	X	-	-	-
12	CLA	e	801	X	-	-	-
12	CLA	e	802	X	-	-	-
12	CLA	e	803	X	-	-	-
12	CLA	e	804	X	-	-	-
12	CLA	e	805	X	-	-	-
12	CLA	e	806	X	-	-	-
12	CLA	e	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	e	808	X	-	-	-
12	CLA	e	809	X	-	-	-
12	CLA	e	810	X	-	-	-
12	CLA	e	811	X	-	-	-
12	CLA	e	812	X	-	-	-
12	CLA	e	813	X	-	-	-
12	CLA	e	814	X	-	-	-
12	CLA	e	815	X	-	-	-
12	CLA	e	816	X	-	-	-
12	CLA	e	817	X	-	-	-
12	CLA	e	818	X	-	-	-
12	CLA	e	819	X	-	-	-
12	CLA	e	820	X	-	-	-
12	CLA	e	821	X	-	-	-
12	CLA	e	822	X	-	-	-
12	CLA	e	823	X	-	-	-
12	CLA	e	824	X	-	-	-
12	CLA	e	825	X	-	-	-
12	CLA	e	826	X	-	-	-
12	CLA	e	827	X	-	-	-
12	CLA	e	828	X	-	-	-
12	CLA	e	829	X	-	-	-
12	CLA	e	830	X	-	-	-
12	CLA	e	831	X	-	-	-
12	CLA	e	832	X	-	-	-
12	CLA	e	833	X	-	-	-
12	CLA	e	834	X	-	-	-
12	CLA	e	835	X	-	-	-
12	CLA	e	836	X	-	-	-
12	CLA	e	837	X	-	-	-
12	CLA	e	838	X	-	-	-
12	CLA	e	839	X	-	-	-
12	CLA	e	840	X	-	-	-
12	CLA	e	841	X	-	-	-
12	CLA	e	842	X	-	-	-
12	CLA	e	844	X	-	-	-
12	CLA	e	845	X	-	-	-
12	CLA	f	1301	X	-	-	-
12	CLA	g	801	X	-	-	-
12	CLA	g	802	X	-	-	-
12	CLA	g	803	X	-	-	-
12	CLA	g	805	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	g	806	X	-	-	-
12	CLA	g	807	X	-	-	-
12	CLA	g	808	X	-	-	-
12	CLA	g	809	X	-	-	-
12	CLA	g	810	X	-	-	-
12	CLA	g	811	X	-	-	-
12	CLA	g	812	X	-	-	-
12	CLA	g	813	X	-	-	-
12	CLA	g	814	X	-	-	-
12	CLA	g	815	X	-	-	-
12	CLA	g	816	X	-	-	-
12	CLA	g	817	X	-	-	-
12	CLA	g	818	X	-	-	-
12	CLA	g	819	X	-	-	-
12	CLA	g	820	X	-	-	-
12	CLA	g	821	X	-	-	-
12	CLA	g	822	X	-	-	-
12	CLA	g	823	X	-	-	-
12	CLA	g	824	X	-	-	-
12	CLA	g	825	X	-	-	-
12	CLA	g	826	X	-	-	-
12	CLA	g	827	X	-	-	-
12	CLA	g	828	X	-	-	-
12	CLA	g	829	X	-	-	-
12	CLA	g	830	X	-	-	-
12	CLA	g	831	X	-	-	-
12	CLA	g	832	X	-	-	-
12	CLA	g	833	X	-	-	-
12	CLA	g	834	X	-	-	-
12	CLA	g	835	X	-	-	-
12	CLA	g	836	X	-	-	-
12	CLA	g	837	X	-	-	-
12	CLA	g	838	X	-	-	-
12	CLA	g	839	X	-	-	-
12	CLA	g	840	X	-	-	-
12	CLA	g	841	X	-	-	-
12	CLA	g	842	X	-	-	-
12	CLA	k	1401	X	-	-	-
12	CLA	l	201	X	-	-	-
12	CLA	l	202	X	-	-	-
12	CLA	l	203	X	-	-	-
12	CLA	l	204	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	CLA	o	1301	X	-	-	-
12	CLA	r	1401	X	-	-	-
12	CLA	s	201	X	-	-	-
12	CLA	s	202	X	-	-	-
12	CLA	s	203	X	-	-	-
12	CLA	s	204	X	-	-	-
13	PQN	A	842	X	-	-	-
13	PQN	B	844	X	-	-	-
13	PQN	E	846	X	-	-	-
13	PQN	G	842	X	-	-	-
13	PQN	a	844	X	-	-	-
13	PQN	b	843	X	-	-	-
13	PQN	e	843	X	-	-	-
13	PQN	g	843	X	-	-	-
14	SF4	C	102	-	-	X	-
14	SF4	H	102	-	-	X	-

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 87228 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	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	E	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	e	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		
1	a	728	Total	C	N	O	S	0	0
			5713	3744	976	968	25		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	G	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	g	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		
2	b	734	Total	C	N	O	S	0	0
			5857	3861	984	996	16		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	H	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	h	81	Total	C	N	O	S	0	0
			605	370	105	119	11		
3	c	81	Total	C	N	O	S	0	0
			605	370	105	119	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	N	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		
4	n	137	Total	C	N	O	S	0	0
			1080	689	189	198	4		
4	d	135	Total	C	N	O	S	0	0
			1066	680	187	195	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	V	61	Total	C	N	O	0	0
			494	315	86	93		
5	W	61	Total	C	N	O	0	0
			494	315	86	93		
5	v	61	Total	C	N	O	0	0
			494	315	86	93		
5	w	61	Total	C	N	O	0	0
			494	315	86	93		

- 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
			1093	700	188	202	3		
6	O	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	o	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		
6	f	141	Total	C	N	O	S	0	0
			1093	700	188	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	P	39	Total	C	N	O	S	0	0
			295	199	42	52	2		
7	p	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	i	39	Total	C	N	O	S	0	0
			295	199	42	52	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	37	Total	C	N	O		0	0
			311	218	44	49			
8	Q	37	Total	C	N	O		0	0
			311	218	44	49			
8	q	37	Total	C	N	O		0	0
			311	218	44	49			
8	j	37	Total	C	N	O		0	0
			311	218	44	49			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	R	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	r	65	Total	C	N	O	S	0	0
			474	316	80	77	1		
9	k	65	Total	C	N	O	S	0	0
			474	316	80	77	1		

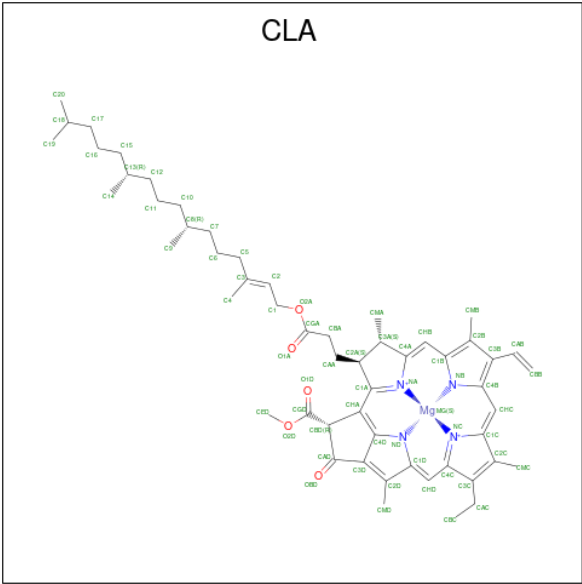
- Molecule 10 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	S	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	s	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		
10	l	150	Total	C	N	O	S	0	0
			1134	738	189	205	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	T	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	t	31	Total	C	N	O	S	0	0
			238	159	36	42	1		
11	m	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 12 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	
12	A	1	Total	C	Mg	N	O	0
			2016	1608	41	164	203	

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0

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Mol	Chain	Residues	Atoms					AltConf
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	A	1	Total 2016	C 1608	Mg 41	N 164	O 203	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	B	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	J	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	J	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	L	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	E	1	Total 2166	C 1728	Mg 44	N 176	O 218	0

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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Mol	Chain	Residues	Atoms					AltConf
12	G	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	O	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	R	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	S	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	S	1	Total 100	C 80	Mg 2	N 8	O 10	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0
12	e	1	Total 2165	C 1727	Mg 44	N 176	O 218	0

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Mol	Chain	Residues	Atoms					AltConf
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	e	1	Total	C	Mg	N	O	0
			2165	1727	44	176	218	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	
12	g	1	Total	C	Mg	N	O	0
			2000	1590	41	164	205	

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Mol	Chain	Residues	Atoms					AltConf
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0

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Mol	Chain	Residues	Atoms					AltConf
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	g	1	Total 2000	C 1590	Mg 41	N 164	O 205	0
12	o	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	r	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	s	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0

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Mol	Chain	Residues	Atoms					AltConf
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	a	1	Total 2066	C 1648	Mg 42	N 168	O 208	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
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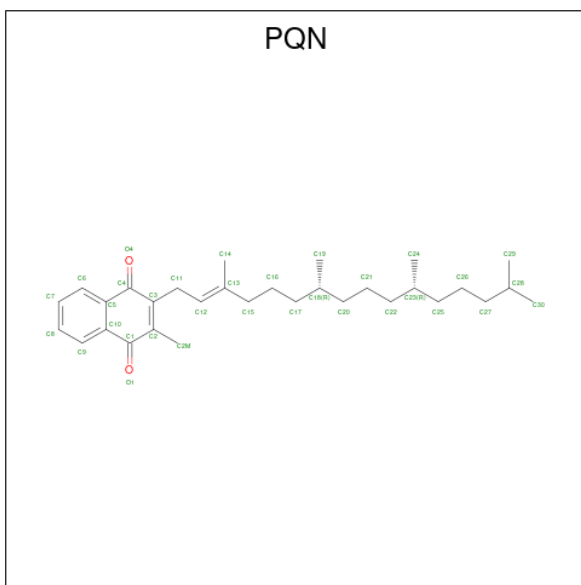
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12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0

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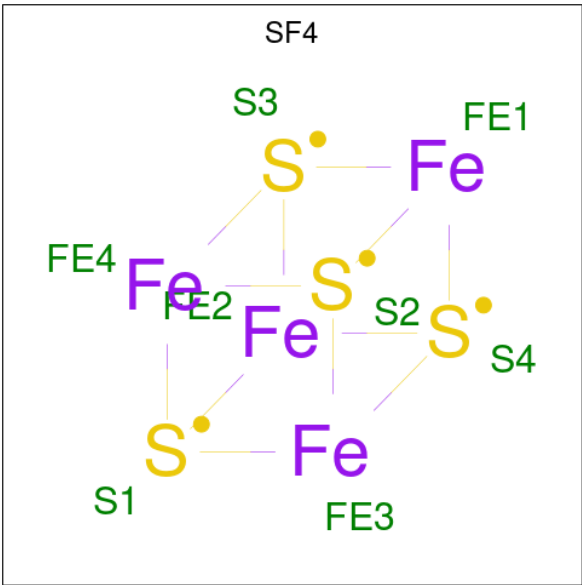
Mol	Chain	Residues	Atoms					AltConf
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	b	1	Total 2049	C 1629	Mg 42	N 168	O 210	0
12	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	k	1	Total 45	C 35	Mg 1	N 4	O 5	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0
12	l	1	Total 200	C 160	Mg 4	N 16	O 20	0

- Molecule 13 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total 33	C 31	O 2	0
13	B	1	Total 33	C 31	O 2	0
13	E	1	Total 33	C 31	O 2	0
13	G	1	Total 33	C 31	O 2	0
13	e	1	Total 33	C 31	O 2	0
13	g	1	Total 33	C 31	O 2	0
13	a	1	Total 33	C 31	O 2	0
13	b	1	Total 33	C 31	O 2	0

- Molecule 14 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

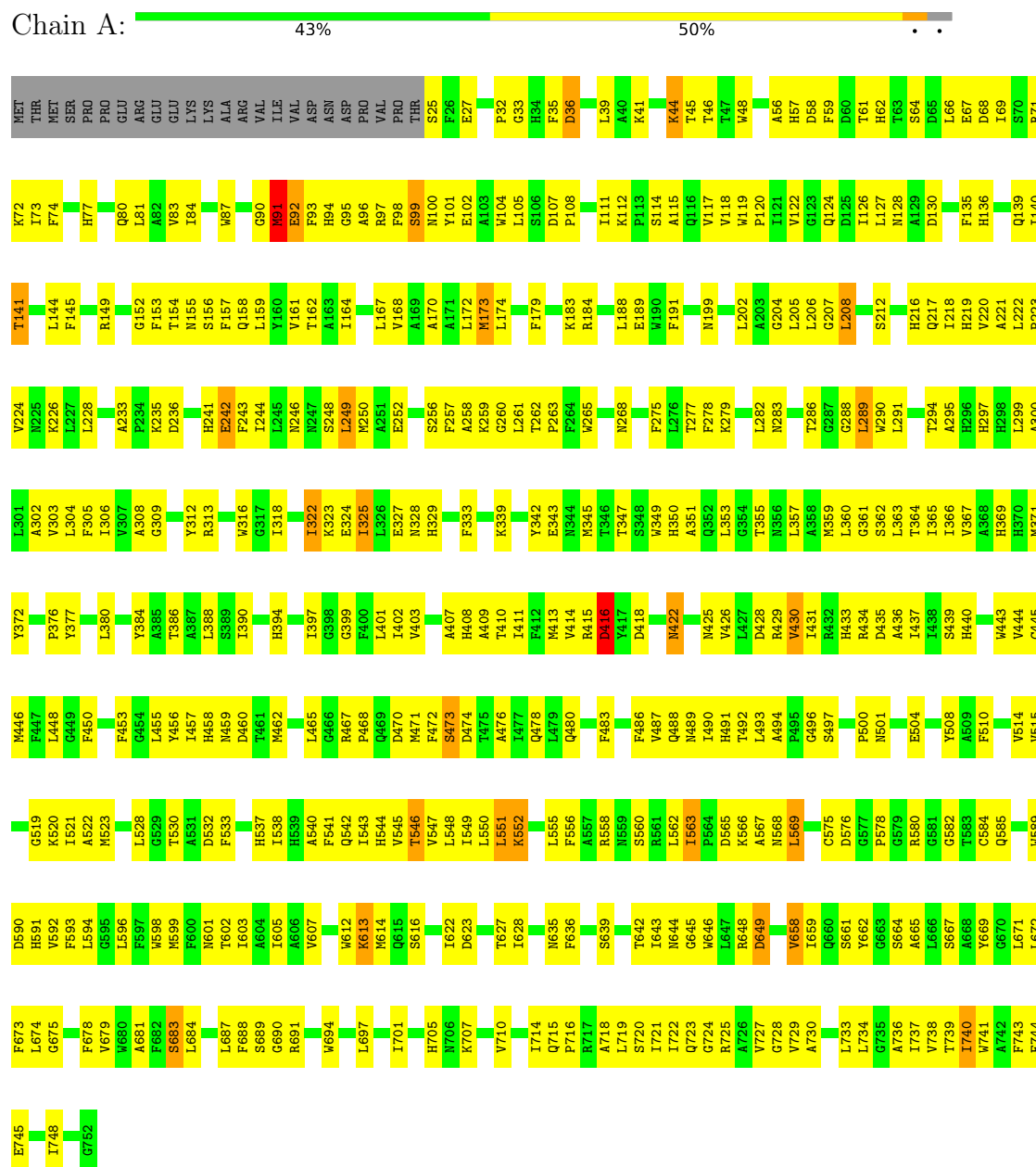


Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	Fe	S	0
			8	4	4	
14	C	1	Total	Fe	S	0
			16	8	8	
14	C	1	Total	Fe	S	0
			16	8	8	
14	E	1	Total	Fe	S	0
			8	4	4	
14	H	1	Total	Fe	S	0
			16	8	8	
14	H	1	Total	Fe	S	0
			16	8	8	
14	g	1	Total	Fe	S	0
			8	4	4	
14	h	1	Total	Fe	S	0
			16	8	8	
14	h	1	Total	Fe	S	0
			16	8	8	
14	a	1	Total	Fe	S	0
			8	4	4	
14	c	1	Total	Fe	S	0
			16	8	8	
14	c	1	Total	Fe	S	0
			16	8	8	

3 Residue-property plots

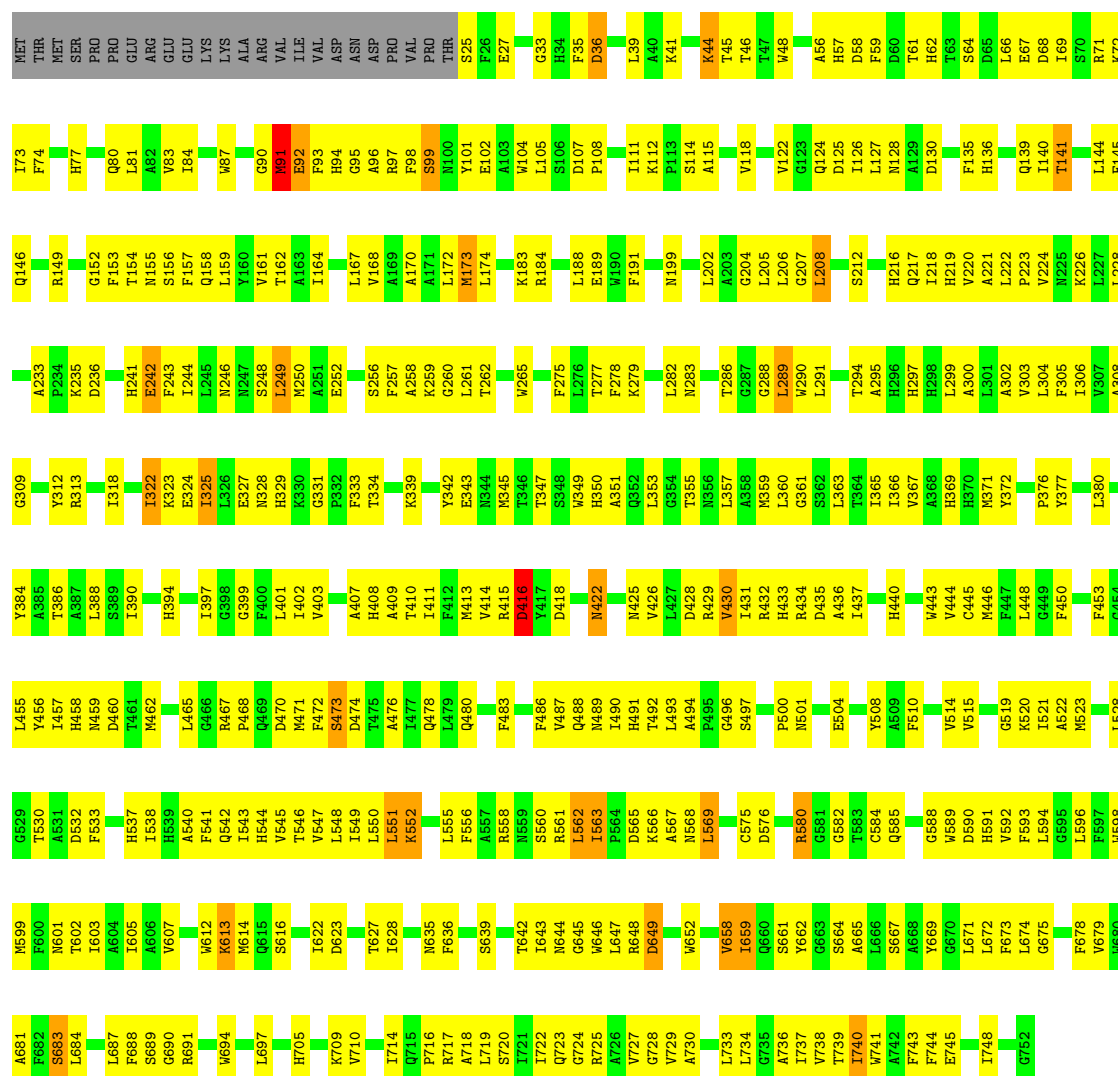
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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. 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



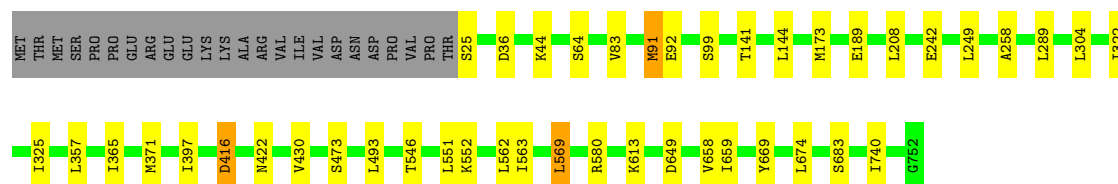
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain E: 



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain e: 



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

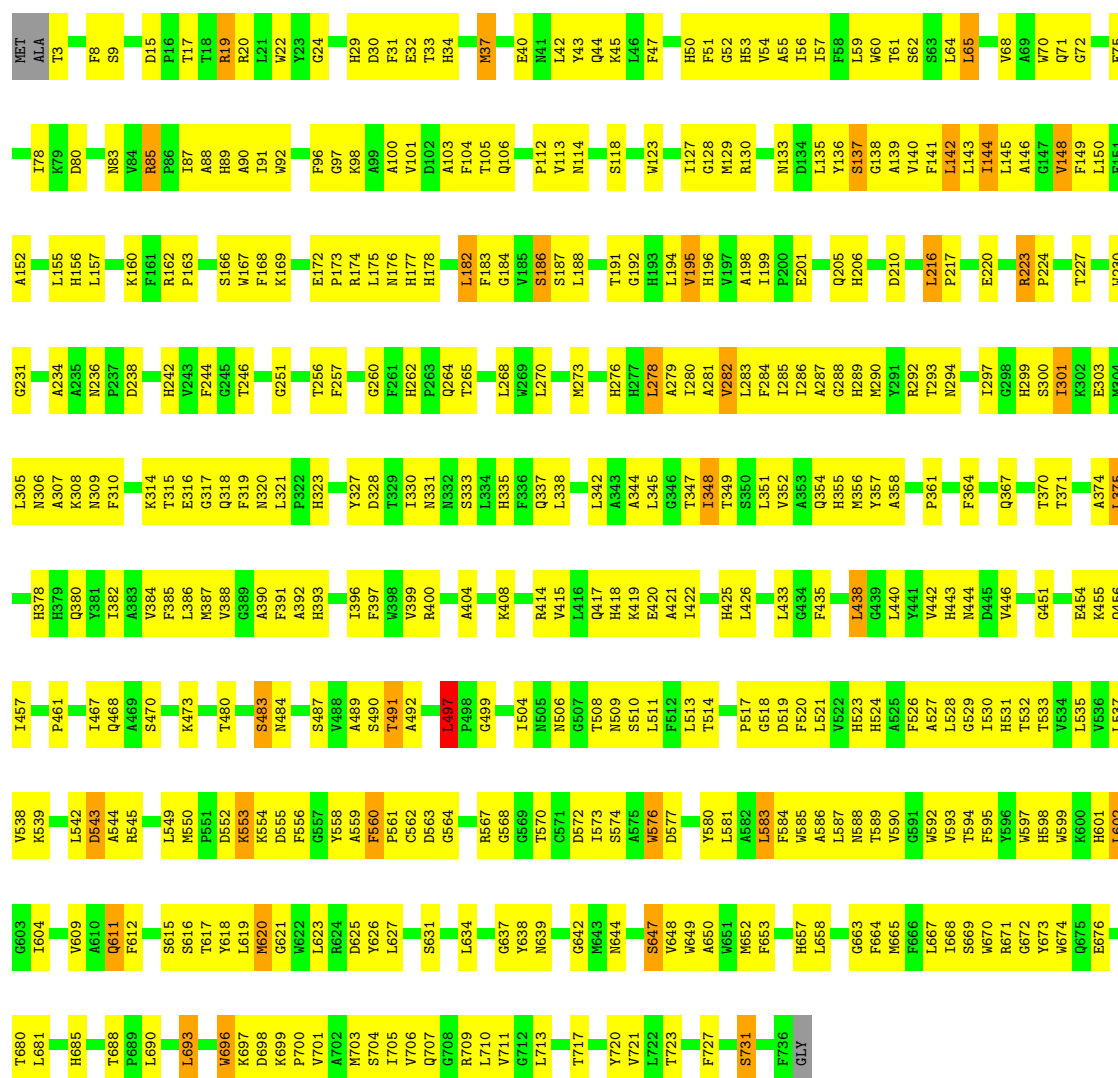
Chain a: 





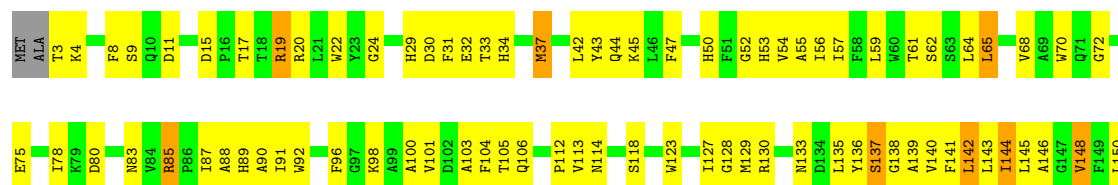
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

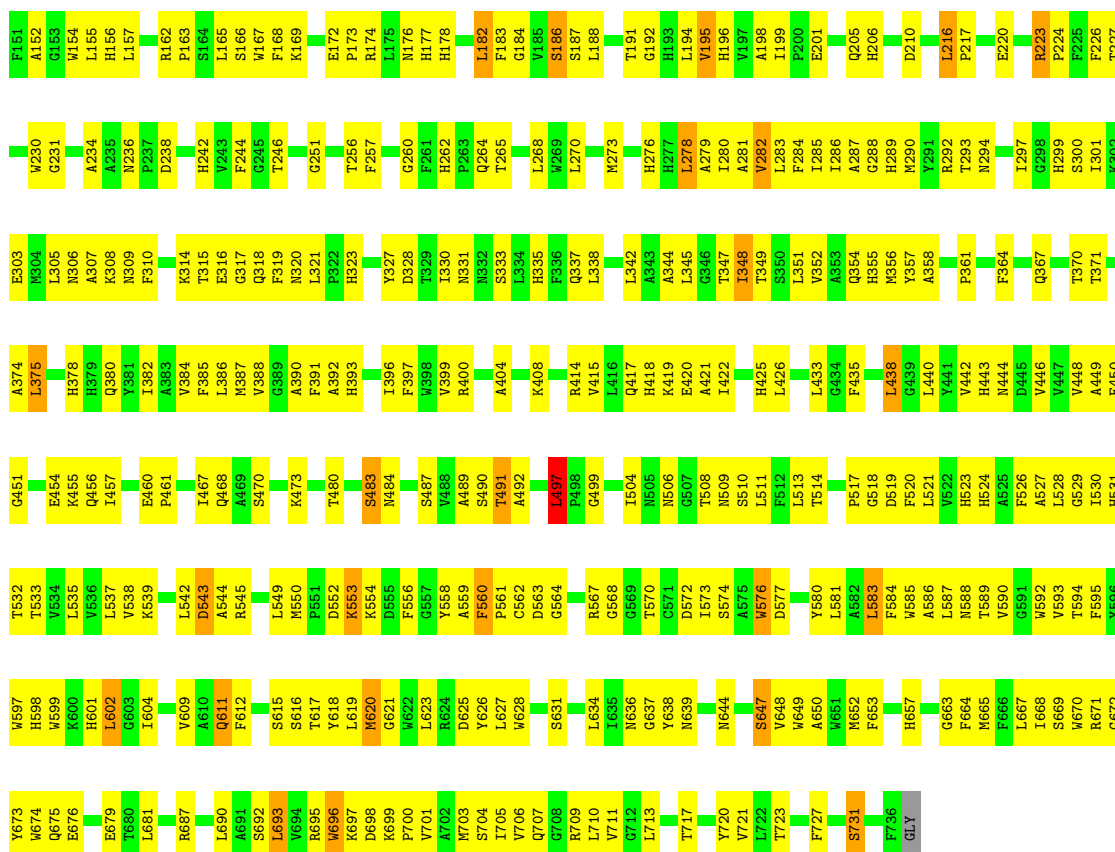
Chain B: 45% 50% .



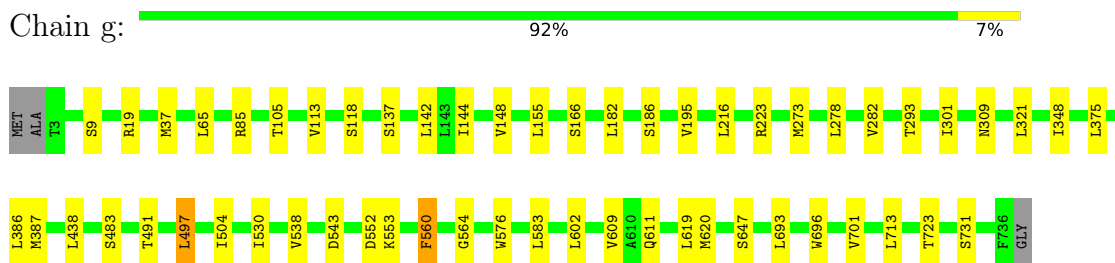
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain G: 44% 51% .

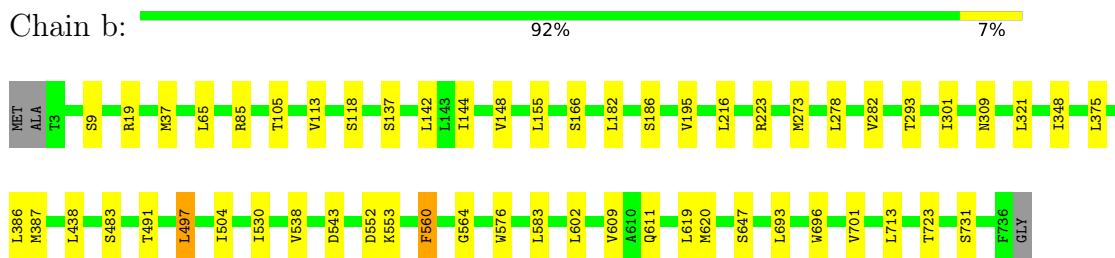




- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

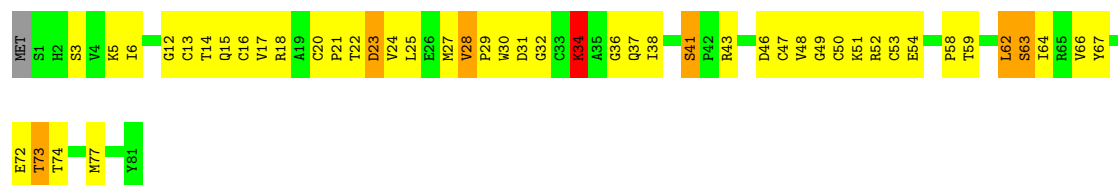


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



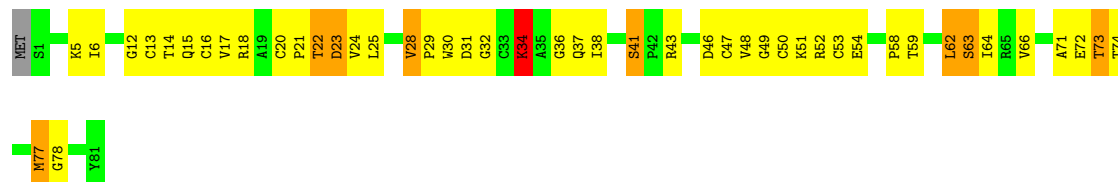
- Molecule 3: Photosystem I iron-sulfur center





• Molecule 3: Photosystem I iron-sulfur center

Chain H: 41% 46% 10% ..



• Molecule 3: Photosystem I iron-sulfur center

Chain h: 84% 13% ..



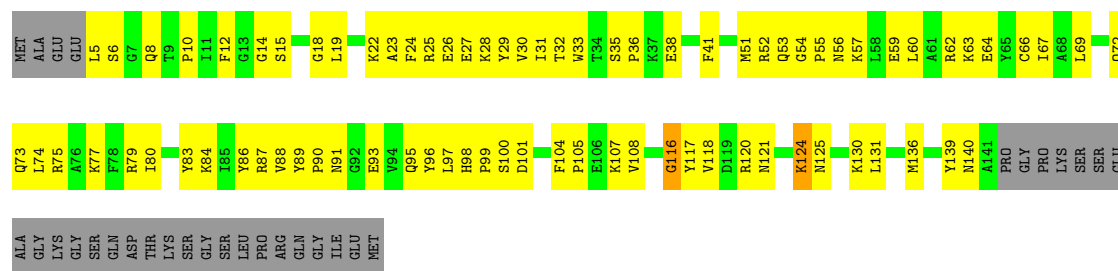
• Molecule 3: Photosystem I iron-sulfur center

Chain c: 84% 13% ..



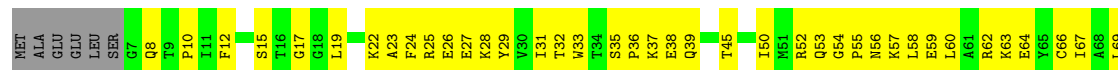
• Molecule 4: Photosystem I reaction center subunit II

Chain D: 35% 46% 18%

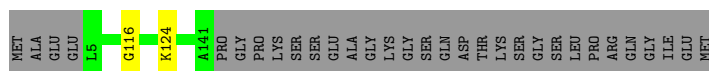
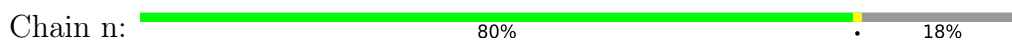


• Molecule 4: Photosystem I reaction center subunit II

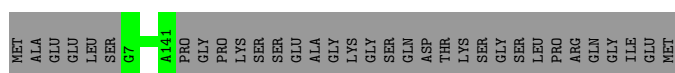
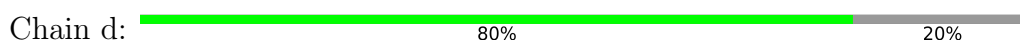
Chain N: 32% 48% 20%



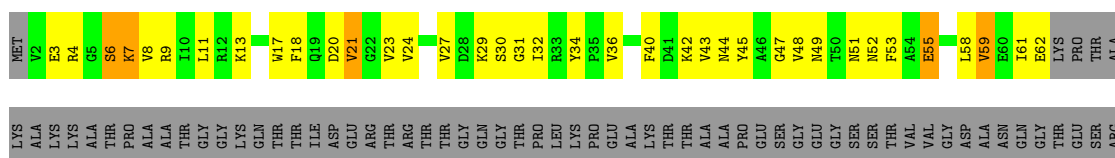
- Molecule 4: Photosystem I reaction center subunit II



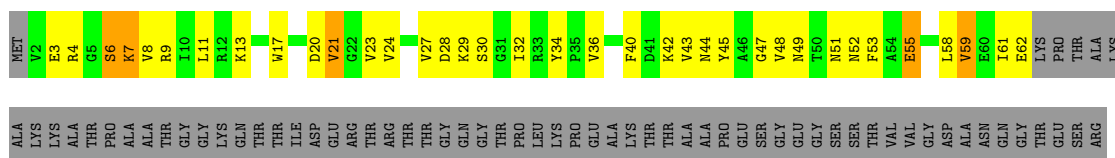
- Molecule 4: Photosystem I reaction center subunit II



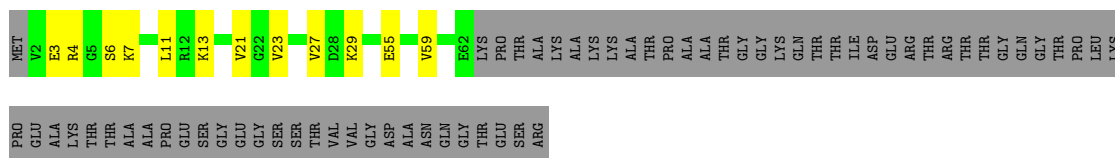
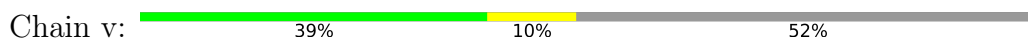
- Molecule 5: Photosystem I reaction center subunit IV



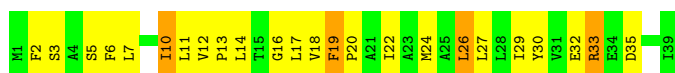
- Molecule 5: Photosystem I reaction center subunit IV



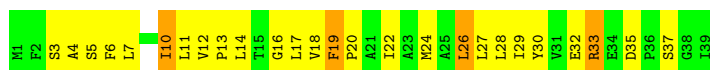
- Molecule 5: Photosystem I reaction center subunit IV



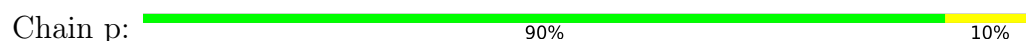
- Molecule 5: Photosystem I reaction center subunit IV



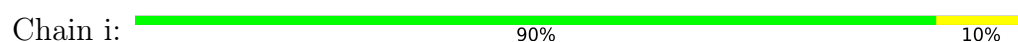
- Molecule 7: Photosystem I reaction center subunit VIII



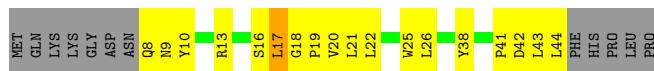
- Molecule 7: Photosystem I reaction center subunit VIII



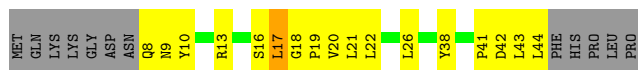
- Molecule 7: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

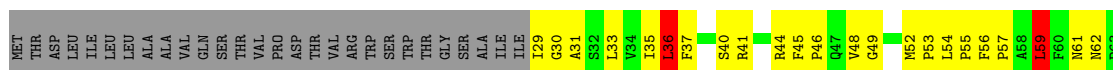


- Molecule 8: Photosystem I reaction center subunit IX

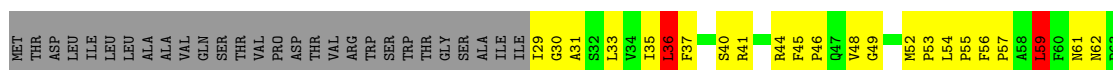




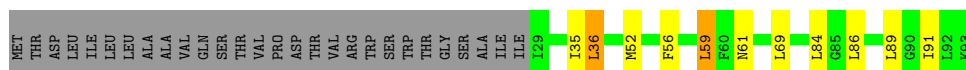
● Molecule 9: Photosystem I reaction center subunit PsaK



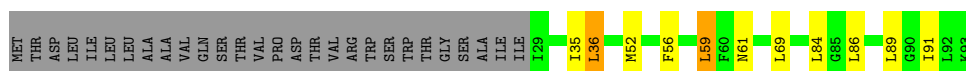
● Molecule 9: Photosystem I reaction center subunit PsaK



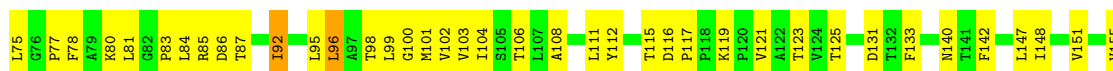
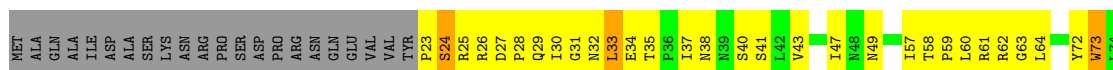
● Molecule 9: Photosystem I reaction center subunit PsaK



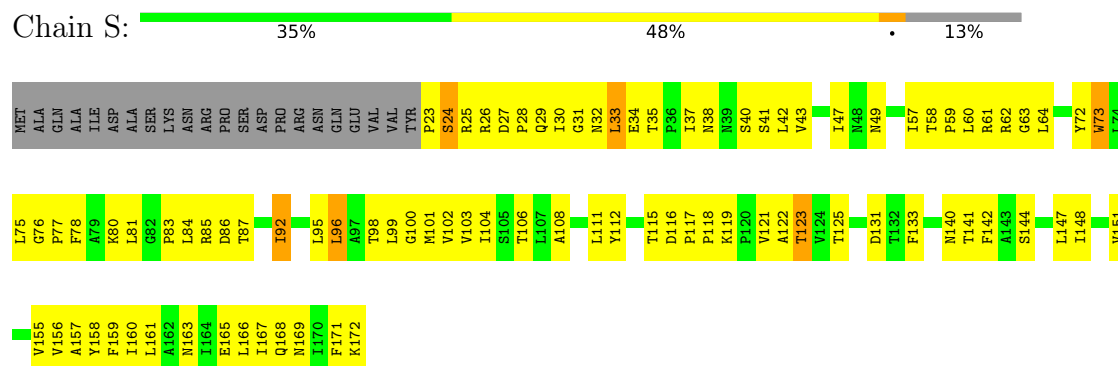
● Molecule 9: Photosystem I reaction center subunit PsaK



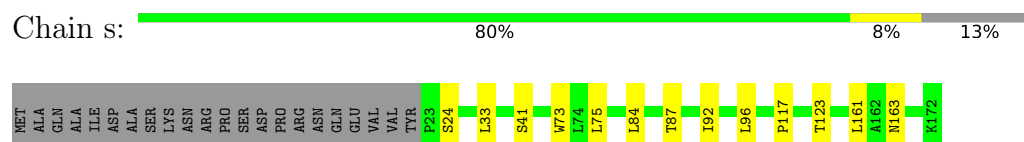
● Molecule 10: Photosystem I reaction center subunit XI



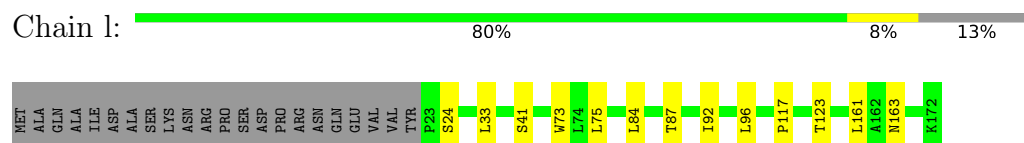
- Molecule 10: Photosystem I reaction center subunit XI



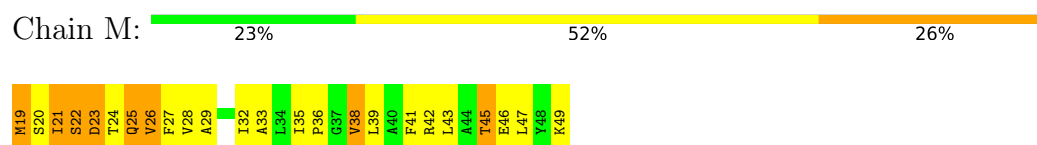
- Molecule 10: Photosystem I reaction center subunit XI



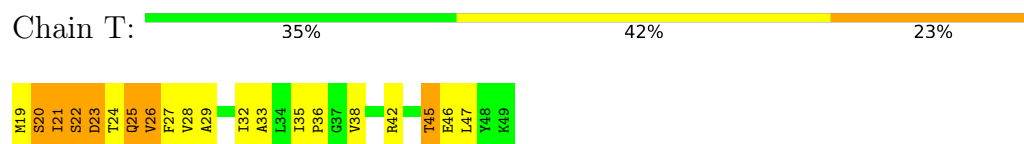
- Molecule 10: Photosystem I reaction center subunit XI



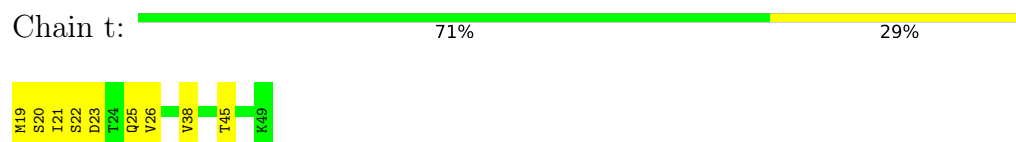
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	60561	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	4.3	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/5908	0.50	2/8056 (0.0%)
1	E	0.30	0/5908	0.50	2/8056 (0.0%)
1	a	0.30	0/5908	0.50	2/8056 (0.0%)
1	e	0.30	0/5908	0.50	2/8056 (0.0%)
2	B	0.30	0/6072	0.50	2/8301 (0.0%)
2	G	0.30	0/6072	0.50	2/8301 (0.0%)
2	b	0.30	0/6072	0.50	2/8301 (0.0%)
2	g	0.30	0/6072	0.50	2/8301 (0.0%)
3	C	0.32	0/615	0.53	0/833
3	H	0.32	0/615	0.53	0/833
3	c	0.32	0/615	0.53	0/833
3	h	0.32	0/615	0.52	0/833
4	D	0.28	0/1105	0.49	0/1489
4	N	0.27	0/1091	0.51	0/1470
4	d	0.30	0/1091	0.53	0/1470
4	n	0.28	0/1105	0.50	0/1489
5	V	0.33	0/502	0.57	0/678
5	W	0.33	0/502	0.57	0/678
5	v	0.33	0/502	0.57	0/678
5	w	0.33	0/502	0.57	0/678
6	F	0.27	0/1119	0.54	2/1522 (0.1%)
6	O	0.28	0/1119	0.54	2/1522 (0.1%)
6	f	0.27	0/1119	0.55	2/1522 (0.1%)
6	o	0.27	0/1119	0.54	2/1522 (0.1%)
7	I	0.30	0/302	0.60	0/411
7	P	0.30	0/302	0.60	0/411
7	i	0.29	0/302	0.60	0/411
7	p	0.30	0/302	0.60	0/411
8	J	0.27	0/321	0.49	0/441
8	Q	0.27	0/321	0.49	0/441
8	j	0.26	0/321	0.49	0/441
8	q	0.27	0/321	0.49	0/441

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	K	0.30	0/484	0.74	3/659 (0.5%)
9	R	0.30	0/484	0.74	3/659 (0.5%)
9	k	0.30	0/484	0.74	3/659 (0.5%)
9	r	0.30	0/484	0.74	3/659 (0.5%)
10	L	0.37	1/1165 (0.1%)	0.51	0/1597
10	S	0.37	1/1165 (0.1%)	0.51	0/1597
10	l	0.37	1/1165 (0.1%)	0.51	0/1597
10	s	0.37	1/1165 (0.1%)	0.51	0/1597
11	M	0.31	0/241	0.55	0/326
11	T	0.32	0/241	0.55	0/326
11	m	0.32	0/241	0.55	0/326
11	t	0.32	0/241	0.55	0/326
All	All	0.31	4/71308 (0.0%)	0.52	36/97214 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	E	0	3
1	a	0	3
1	e	0	3
2	B	0	3
2	G	0	3
2	b	0	3
2	g	0	3
3	C	0	1
3	H	0	1
3	c	0	1
3	h	0	1
4	D	0	1
4	n	0	1
7	I	0	1
7	P	0	1
7	i	0	1
7	p	0	1
9	K	0	1
9	R	0	1
9	k	0	1
9	r	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	L	0	1
10	S	0	1
10	l	0	1
10	s	0	1
All	All	0	42

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	s	73	TRP	C-N	7.98	1.52	1.34
10	S	73	TRP	C-N	7.96	1.52	1.34
10	L	73	TRP	C-N	7.96	1.52	1.34
10	l	73	TRP	C-N	7.95	1.52	1.34

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	r	36	LEU	CA-CB-CG	8.39	134.59	115.30
9	R	36	LEU	CA-CB-CG	8.39	134.59	115.30
9	K	36	LEU	CA-CB-CG	8.38	134.58	115.30
9	k	36	LEU	CA-CB-CG	8.38	134.57	115.30
2	G	497	LEU	CA-CB-CG	7.71	133.03	115.30

There are no chirality outliers.

5 of 42 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	258	ALA	Peptide
1	A	416	ASP	Peptide
1	A	669	TYR	Peptide
2	B	560	PHE	Peptide
2	B	576	TRP	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5713	0	5565	431	0
1	E	5713	0	5565	440	0
1	a	5713	0	5565	0	0
1	e	5713	0	5565	0	0
2	B	5857	0	5642	426	0
2	G	5857	0	5642	449	0
2	b	5857	0	5642	0	0
2	g	5857	0	5642	0	0
3	C	605	0	590	61	0
3	H	605	0	590	52	0
3	c	605	0	590	0	0
3	h	605	0	590	0	0
4	D	1080	0	1083	92	0
4	N	1066	0	1067	84	0
4	d	1066	0	1067	0	0
4	n	1080	0	1083	0	0
5	V	494	0	493	36	0
5	W	494	0	493	30	0
5	v	494	0	493	0	0
5	w	494	0	493	0	0
6	F	1093	0	1095	53	0
6	O	1093	0	1095	58	0
6	f	1093	0	1095	0	0
6	o	1093	0	1095	0	0
7	I	295	0	314	18	0
7	P	295	0	314	23	0
7	i	295	0	314	0	0
7	p	295	0	314	0	0
8	J	311	0	323	24	0
8	Q	311	0	323	18	0
8	j	311	0	323	0	0
8	q	311	0	323	0	0
9	K	474	0	521	30	0
9	R	474	0	521	33	0
9	k	474	0	521	0	0
9	r	474	0	521	0	0
10	L	1134	0	1151	75	0
10	S	1134	0	1151	85	0
10	l	1134	0	1151	0	0
10	s	1134	0	1151	0	0
11	M	238	0	257	29	0
11	T	238	0	257	19	0
11	m	238	0	257	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	t	238	0	257	0	0
12	A	2016	0	1561	231	0
12	B	2049	0	1576	241	0
12	E	2166	0	1678	250	0
12	F	45	0	33	4	0
12	G	2049	0	1576	250	0
12	J	100	0	78	13	0
12	K	45	0	33	2	0
12	L	200	0	156	14	0
12	O	45	0	33	1	0
12	R	45	0	33	3	0
12	S	100	0	78	6	0
12	a	2066	0	1600	0	0
12	b	2049	0	1576	0	0
12	e	2165	0	1678	0	0
12	f	45	0	33	0	0
12	g	2000	0	1537	0	0
12	k	45	0	33	0	0
12	l	200	0	156	0	0
12	o	45	0	33	0	0
12	r	45	0	33	0	0
12	s	200	0	156	0	0
13	A	33	0	46	7	0
13	B	33	0	46	4	0
13	E	33	0	46	9	0
13	G	33	0	46	4	0
13	a	33	0	46	0	0
13	b	33	0	46	0	0
13	e	33	0	46	0	0
13	g	33	0	46	0	0
14	B	8	0	0	0	0
14	C	16	0	0	7	0
14	E	8	0	0	0	0
14	H	16	0	0	7	0
14	a	8	0	0	0	0
14	c	16	0	0	0	0
14	g	8	0	0	0	0
14	h	16	0	0	0	0
All	All	87228	0	82142	2889	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 17.

The worst 5 of 2889 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)
2:B:417:GLN:HA	6:F:164:ARG:HH22	1.65	0.93
4:D:29:TYR:HB2	4:D:60:LEU:O	1.94	0.92
6:O:60:ARG:HH12	8:Q:43:LEU:HA	1.34	0.91
2:G:690:LEU:HD21	10:S:47:ILE:HD11	2.39	0.88
1:A:448:LEU:HD22	1:A:541:PHE:HB2	1.58	0.85

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	A	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	E	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	a	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
1	e	726/752 (96%)	636 (88%)	90 (12%)	0	100	100
2	B	732/737 (99%)	653 (89%)	78 (11%)	1 (0%)	53	88
2	G	732/737 (99%)	654 (89%)	77 (10%)	1 (0%)	53	88
2	b	732/737 (99%)	653 (89%)	78 (11%)	1 (0%)	53	88
2	g	732/737 (99%)	654 (89%)	77 (10%)	1 (0%)	53	88
3	C	79/82 (96%)	69 (87%)	9 (11%)	1 (1%)	13	53
3	H	79/82 (96%)	68 (86%)	10 (13%)	1 (1%)	13	53
3	c	79/82 (96%)	69 (87%)	9 (11%)	1 (1%)	13	53
3	h	79/82 (96%)	68 (86%)	10 (13%)	1 (1%)	13	53
4	D	135/168 (80%)	118 (87%)	17 (13%)	0	100	100
4	N	133/168 (79%)	116 (87%)	17 (13%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	d	133/168 (79%)	116 (87%)	17 (13%)	0	100	100
4	n	135/168 (80%)	118 (87%)	17 (13%)	0	100	100
5	V	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	W	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	v	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
5	w	59/126 (47%)	49 (83%)	10 (17%)	0	100	100
6	F	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	O	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	f	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
6	o	139/164 (85%)	128 (92%)	11 (8%)	0	100	100
7	I	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	P	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	i	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
7	p	37/39 (95%)	31 (84%)	6 (16%)	0	100	100
8	J	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	Q	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	j	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
8	q	35/49 (71%)	29 (83%)	6 (17%)	0	100	100
9	K	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	R	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	k	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
9	r	63/93 (68%)	46 (73%)	17 (27%)	0	100	100
10	L	148/172 (86%)	124 (84%)	24 (16%)	0	100	100
10	S	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
10	l	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
10	s	148/172 (86%)	125 (84%)	23 (16%)	0	100	100
11	M	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	T	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	m	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
11	t	29/31 (94%)	22 (76%)	6 (21%)	1 (3%)	4	34
All	All	8724/9652 (90%)	7619 (87%)	1093 (12%)	12 (0%)	56	88

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	62	LEU
11	M	23	ASP
3	H	62	LEU
11	T	23	ASP
3	h	62	LEU

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	A	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	E	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	a	578/601 (96%)	536 (93%)	42 (7%)	15	47
1	e	578/601 (96%)	536 (93%)	42 (7%)	15	47
2	B	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	G	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	b	594/595 (100%)	541 (91%)	53 (9%)	11	38
2	g	594/595 (100%)	541 (91%)	53 (9%)	11	38
3	C	68/70 (97%)	57 (84%)	11 (16%)	2	17
3	H	68/70 (97%)	57 (84%)	11 (16%)	2	17
3	c	68/70 (97%)	57 (84%)	11 (16%)	2	17
3	h	68/70 (97%)	57 (84%)	11 (16%)	2	17
4	D	113/137 (82%)	112 (99%)	1 (1%)	81	90
4	N	111/137 (81%)	111 (100%)	0	100	100
4	d	111/137 (81%)	111 (100%)	0	100	100
4	n	113/137 (82%)	112 (99%)	1 (1%)	81	90
5	V	54/102 (53%)	42 (78%)	12 (22%)	1	7
5	W	54/102 (53%)	42 (78%)	12 (22%)	1	7
5	v	54/102 (53%)	42 (78%)	12 (22%)	1	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	w	54/102 (53%)	42 (78%)	12 (22%)	1	7
6	F	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	O	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	f	116/135 (86%)	101 (87%)	15 (13%)	5	24
6	o	116/135 (86%)	101 (87%)	15 (13%)	5	24
7	I	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	P	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	i	33/33 (100%)	30 (91%)	3 (9%)	10	37
7	p	33/33 (100%)	30 (91%)	3 (9%)	10	37
8	J	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	Q	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	j	34/45 (76%)	31 (91%)	3 (9%)	11	39
8	q	34/45 (76%)	31 (91%)	3 (9%)	11	39
9	K	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	R	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	k	53/77 (69%)	44 (83%)	9 (17%)	2	15
9	r	53/77 (69%)	44 (83%)	9 (17%)	2	15
10	L	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	S	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	l	121/140 (86%)	110 (91%)	11 (9%)	10	37
10	s	121/140 (86%)	110 (91%)	11 (9%)	10	37
11	M	26/26 (100%)	18 (69%)	8 (31%)	0	2
11	T	26/26 (100%)	18 (69%)	8 (31%)	0	2
11	m	26/26 (100%)	18 (69%)	8 (31%)	0	2
11	t	26/26 (100%)	18 (69%)	8 (31%)	0	2
All	All	7156/7844 (91%)	6486 (91%)	670 (9%)	14	35

5 of 670 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	P	33	ARG
1	e	683	SER
5	w	55	GLU

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Mol	Chain	Res	Type
9	R	59	LEU
1	e	91	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 152 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	109	ASN
1	e	422	ASN
2	b	505	ASN
5	W	52	ASN
1	e	53	HIS

5.3.3 RNA [i](#)

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

382 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
12	CLA	A	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.70	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	802	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	A	803	-	42,58,73	1.19	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	A	804	1	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	A	805	1	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	A	806	1	42,58,73	1.19	4 (9%)	48,95,113	1.81	10 (20%)
12	CLA	A	807	1	42,58,73	1.16	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	A	808	-	34,53,73	1.27	4 (11%)	37,89,113	1.72	7 (18%)
12	CLA	A	809	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	A	810	1	42,58,73	1.14	4 (9%)	48,95,113	1.71	9 (18%)
12	CLA	A	811	1	42,58,73	1.18	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	A	812	-	34,53,73	1.29	5 (14%)	37,89,113	1.78	6 (16%)
12	CLA	A	813	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	A	814	1	41,57,73	1.18	4 (9%)	46,93,113	1.65	7 (15%)
12	CLA	A	815	1	42,58,73	1.17	5 (11%)	48,95,113	1.71	9 (18%)
12	CLA	A	816	1	42,58,73	1.14	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	A	817	-	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	A	818	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	A	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	A	820	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	A	821	1	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	A	822	1	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	A	823	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	A	824	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	A	825	-	42,58,73	1.15	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	A	826	1	42,58,73	1.16	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	A	827	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	9 (18%)
12	CLA	A	828	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	A	829	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	A	830	-	42,58,73	1.19	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	A	831	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	A	832	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	A	833	-	34,53,73	1.28	5 (14%)	37,89,113	1.84	8 (21%)
12	CLA	A	834	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	A	835	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)
12	CLA	A	836	-	39,55,73	1.22	5 (12%)	44,91,113	1.77	8 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	A	837	-	42,58,73	1.18	4 (9%)	48,95,113	1.64	10 (20%)
12	CLA	A	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	A	839	-	42,58,73	1.21	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	A	840	-	30,49,73	1.31	4 (13%)	31,83,113	1.89	7 (22%)
12	CLA	A	841	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
13	PQN	A	842	-	34,34,34	1.73	5 (14%)	42,45,45	1.29	6 (14%)
12	CLA	B	801	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	B	802	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	B	803	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
14	SF4	B	804	-	0,12,12	0.00	-	-	-	-
12	CLA	B	805	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	B	806	-	42,58,73	1.20	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	B	807	-	42,58,73	1.17	5 (11%)	48,95,113	1.78	11 (22%)
12	CLA	B	808	2	42,58,73	1.16	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	B	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	B	810	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	B	811	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	B	812	-	42,58,73	1.16	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	B	813	2	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	B	814	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	B	815	-	34,53,73	1.28	4 (11%)	37,89,113	1.70	7 (18%)
12	CLA	B	816	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	B	817	2	42,58,73	1.17	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	B	818	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	B	819	2	34,53,73	1.27	5 (14%)	37,89,113	1.75	7 (18%)
12	CLA	B	820	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	B	821	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	8 (16%)
12	CLA	B	822	-	42,58,73	1.18	5 (11%)	48,95,113	1.71	8 (16%)
12	CLA	B	823	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	B	824	2	39,55,73	1.22	5 (12%)	44,91,113	1.73	7 (15%)
12	CLA	B	825	-	34,53,73	1.27	4 (11%)	37,89,113	1.83	8 (21%)
12	CLA	B	826	2	42,58,73	1.19	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	B	827	-	34,53,73	1.28	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	B	828	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	B	829	-	38,54,73	1.21	4 (10%)	43,90,113	1.75	7 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	B	830	-	42,58,73	1.18	5 (11%)	48,95,113	1.60	8 (16%)
12	CLA	B	831	2	42,58,73	1.18	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	B	832	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	B	833	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	B	834	-	34,53,73	1.26	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	B	835	-	41,57,73	1.19	5 (12%)	46,93,113	1.61	8 (17%)
12	CLA	B	836	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	B	837	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	B	838	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	B	839	-	42,58,73	1.20	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	B	840	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	B	841	-	39,55,73	1.21	5 (12%)	44,91,113	1.81	7 (15%)
12	CLA	B	842	-	42,58,73	1.20	5 (11%)	48,95,113	1.77	9 (18%)
12	CLA	B	843	-	42,58,73	1.21	5 (11%)	48,95,113	1.60	8 (16%)
13	PQN	B	844	-	34,34,34	1.70	5 (14%)	42,45,45	1.19	2 (4%)
14	SF4	C	101	-	0,12,12	0.00	-	-	-	-
14	SF4	C	102	3	0,12,12	0.00	-	-	-	-
12	CLA	E	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.71	10 (20%)
12	CLA	E	802	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	E	803	-	42,58,73	1.18	5 (11%)	48,95,113	1.73	10 (20%)
12	CLA	E	804	-	42,58,73	1.20	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	E	805	-	42,58,73	1.17	5 (11%)	48,95,113	1.69	8 (16%)
12	CLA	E	806	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	E	807	1	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	E	808	1	42,58,73	1.16	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	E	809	1	42,58,73	1.19	4 (9%)	48,95,113	1.80	10 (20%)
12	CLA	E	810	1	42,58,73	1.16	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	E	811	-	34,53,73	1.27	4 (11%)	37,89,113	1.71	7 (18%)
12	CLA	E	812	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	8 (16%)
12	CLA	E	813	1	42,58,73	1.14	4 (9%)	48,95,113	1.72	9 (18%)
12	CLA	E	814	1	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	E	815	-	34,53,73	1.29	5 (14%)	37,89,113	1.77	7 (18%)
12	CLA	E	816	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	E	817	1	41,57,73	1.18	4 (9%)	46,93,113	1.63	7 (15%)
12	CLA	E	818	1	42,58,73	1.18	5 (11%)	48,95,113	1.72	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	E	819	1	42,58,73	1.15	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	E	820	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	E	821	-	42,58,73	1.18	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	E	822	-	42,58,73	1.20	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	E	823	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	E	824	1	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	E	825	1	42,58,73	1.18	4 (9%)	48,95,113	1.60	9 (18%)
12	CLA	E	826	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	E	827	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	E	828	-	42,58,73	1.15	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	E	829	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	E	830	-	42,58,73	1.20	5 (11%)	48,95,113	1.63	9 (18%)
12	CLA	E	831	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	E	832	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	E	833	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	E	834	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	E	835	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	E	836	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	E	837	-	34,53,73	1.28	5 (14%)	37,89,113	1.82	8 (21%)
12	CLA	E	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	E	839	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)
12	CLA	E	840	-	39,55,73	1.21	6 (15%)	44,91,113	1.76	8 (18%)
12	CLA	E	841	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	E	842	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	E	843	-	42,58,73	1.20	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	E	844	-	30,49,73	1.31	4 (13%)	31,83,113	1.89	7 (22%)
14	SF4	E	845	-	0,12,12	0.00	-	-	-	-
13	PQN	E	846	-	34,34,34	1.69	5 (14%)	42,45,45	1.32	7 (16%)
12	CLA	F	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	G	801	-	42,58,73	1.20	5 (11%)	48,95,113	1.67	9 (18%)
12	CLA	G	802	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	G	803	-	42,58,73	1.20	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	G	804	-	42,58,73	1.17	5 (11%)	48,95,113	1.77	11 (22%)
12	CLA	G	805	2	42,58,73	1.15	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	G	806	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	G	807	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	G	808	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	G	809	-	42,58,73	1.17	5 (11%)	48,95,113	1.73	9 (18%)
12	CLA	G	810	2	42,58,73	1.18	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	G	811	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	G	812	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	G	813	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	G	814	2	42,58,73	1.16	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	G	815	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	G	816	2	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	G	817	-	42,58,73	1.19	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	G	818	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	G	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	G	820	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	G	821	2	39,55,73	1.22	5 (12%)	44,91,113	1.74	7 (15%)
12	CLA	G	822	-	34,53,73	1.26	4 (11%)	37,89,113	1.82	8 (21%)
12	CLA	G	823	2	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	G	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	G	825	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	G	826	-	38,54,73	1.21	4 (10%)	43,90,113	1.76	7 (16%)
12	CLA	G	827	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	G	828	2	42,58,73	1.18	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	G	829	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	G	830	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	G	831	-	34,53,73	1.26	4 (11%)	37,89,113	1.68	7 (18%)
12	CLA	G	832	-	41,57,73	1.19	5 (12%)	46,93,113	1.61	8 (17%)
12	CLA	G	833	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	G	834	-	42,58,73	1.16	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	G	835	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	G	836	-	34,53,73	1.27	4 (11%)	37,89,113	1.83	7 (18%)
12	CLA	G	837	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	G	838	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	G	839	-	39,55,73	1.21	4 (10%)	44,91,113	1.80	8 (18%)
12	CLA	G	840	-	42,58,73	1.19	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	G	841	-	42,58,73	1.20	5 (11%)	48,95,113	1.62	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	PQN	G	842	-	34,34,34	1.71	5 (14%)	42,45,45	1.19	2 (4%)
12	CLA	G	843	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
14	SF4	H	101	-	0,12,12	0.00	-	-		
14	SF4	H	102	3	0,12,12	0.00	-	-		
12	CLA	J	1101	-	42,58,73	1.19	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	J	1102	-	42,58,73	1.15	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	K	1401	-	34,53,73	1.24	4 (11%)	37,89,113	1.86	8 (21%)
12	CLA	L	201	-	42,58,73	1.17	5 (11%)	48,95,113	1.68	9 (18%)
12	CLA	L	202	-	42,58,73	1.17	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	L	203	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	L	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	O	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	R	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.86	8 (21%)
12	CLA	S	1501	-	42,58,73	1.17	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	S	1502	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	a	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.70	10 (20%)
12	CLA	a	802	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	a	803	-	42,58,73	1.19	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	a	804	-	42,58,73	1.17	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	a	805	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	a	806	1	42,58,73	1.18	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	a	807	1	42,58,73	1.16	4 (9%)	48,95,113	1.70	8 (16%)
12	CLA	a	808	1	42,58,73	1.18	4 (9%)	48,95,113	1.79	10 (20%)
12	CLA	a	809	1	42,58,73	1.17	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	a	810	-	34,53,73	1.27	4 (11%)	37,89,113	1.71	7 (18%)
12	CLA	a	811	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	8 (16%)
12	CLA	a	812	1	42,58,73	1.13	4 (9%)	48,95,113	1.71	9 (18%)
12	CLA	a	813	1	42,58,73	1.18	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	a	814	-	34,53,73	1.29	5 (14%)	37,89,113	1.78	6 (16%)
12	CLA	a	815	-	34,53,73	1.26	4 (11%)	37,89,113	1.80	7 (18%)
12	CLA	a	816	1	41,57,73	1.18	4 (9%)	46,93,113	1.63	7 (15%)
12	CLA	a	817	1	42,58,73	1.18	5 (11%)	48,95,113	1.71	9 (18%)
12	CLA	a	818	1	42,58,73	1.14	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	a	819	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	a	820	-	42,58,73	1.18	5 (11%)	48,95,113	1.63	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	a	821	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	a	822	1	41,57,73	1.16	4 (9%)	46,93,113	1.80	10 (21%)
12	CLA	a	823	1	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	a	824	1	42,58,73	1.18	4 (9%)	48,95,113	1.61	9 (18%)
12	CLA	a	825	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	a	826	-	42,58,73	1.20	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	a	827	-	42,58,73	1.15	5 (11%)	48,95,113	1.70	8 (16%)
12	CLA	a	828	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	a	829	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	a	830	1	42,58,73	1.16	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	a	831	-	42,58,73	1.19	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	a	832	-	42,58,73	1.20	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	a	833	-	42,58,73	1.17	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	a	834	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	a	835	-	34,53,73	1.28	5 (14%)	37,89,113	1.83	8 (21%)
12	CLA	a	836	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	a	837	-	42,58,73	1.21	6 (14%)	48,95,113	1.65	9 (18%)
12	CLA	a	838	-	39,55,73	1.21	5 (12%)	44,91,113	1.76	8 (18%)
12	CLA	a	839	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	a	840	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	a	841	-	42,58,73	1.21	5 (11%)	48,95,113	1.69	8 (16%)
12	CLA	a	842	-	30,49,73	1.31	4 (13%)	31,83,113	1.92	7 (22%)
14	SF4	a	843	-	0,12,12	0.00	-	-		
13	PQN	a	844	-	34,34,34	1.68	5 (14%)	42,45,45	1.33	8 (19%)
12	CLA	b	801	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	10 (20%)
12	CLA	b	802	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
12	CLA	b	803	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	804	-	42,58,73	1.20	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	b	805	-	42,58,73	1.18	5 (11%)	48,95,113	1.79	11 (22%)
12	CLA	b	806	2	42,58,73	1.16	4 (9%)	48,95,113	1.78	10 (20%)
12	CLA	b	807	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	b	808	-	42,58,73	1.17	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	b	809	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	b	810	-	42,58,73	1.17	5 (11%)	48,95,113	1.73	9 (18%)
12	CLA	b	811	2	42,58,73	1.18	4 (9%)	48,95,113	1.68	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	b	812	-	42,58,73	1.18	4 (9%)	48,95,113	1.64	9 (18%)
12	CLA	b	813	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	6 (16%)
12	CLA	b	814	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	b	815	2	42,58,73	1.17	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	b	816	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	b	817	2	34,53,73	1.26	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	b	818	-	42,58,73	1.19	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	819	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	b	820	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	8 (16%)
12	CLA	b	821	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	b	822	2	39,55,73	1.22	5 (12%)	44,91,113	1.75	7 (15%)
12	CLA	b	823	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	b	824	2	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	b	825	-	34,53,73	1.27	4 (11%)	37,89,113	1.79	7 (18%)
12	CLA	b	826	-	42,58,73	1.19	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	b	827	-	38,54,73	1.22	4 (10%)	43,90,113	1.75	7 (16%)
12	CLA	b	828	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	b	829	2	42,58,73	1.18	5 (11%)	48,95,113	1.61	8 (16%)
12	CLA	b	830	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	b	831	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	b	832	-	34,53,73	1.26	4 (11%)	37,89,113	1.70	7 (18%)
12	CLA	b	833	-	41,57,73	1.19	5 (12%)	46,93,113	1.60	8 (17%)
12	CLA	b	834	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	b	835	-	42,58,73	1.16	4 (9%)	48,95,113	1.61	8 (16%)
12	CLA	b	836	2	34,53,73	1.30	5 (14%)	37,89,113	1.77	8 (21%)
12	CLA	b	837	-	34,53,73	1.28	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	b	838	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	b	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	b	840	-	39,55,73	1.21	5 (12%)	44,91,113	1.81	8 (18%)
12	CLA	b	841	-	42,58,73	1.20	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	b	842	-	42,58,73	1.20	6 (14%)	48,95,113	1.61	8 (16%)
13	PQN	b	843	-	34,34,34	1.71	5 (14%)	42,45,45	1.20	2 (4%)
14	SF4	c	101	-	0,12,12	0.00	-	-	-	-
14	SF4	c	102	3	0,12,12	0.00	-	-	-	-
12	CLA	e	801	-	42,58,73	1.14	4 (9%)	48,95,113	1.71	10 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	e	802	-	42,58,73	1.19	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	e	803	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	8 (16%)
12	CLA	e	804	-	42,58,73	1.18	5 (11%)	48,95,113	1.75	11 (22%)
12	CLA	e	805	1	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	e	806	1	42,58,73	1.16	4 (9%)	48,95,113	1.71	8 (16%)
12	CLA	e	807	1	42,58,73	1.18	4 (9%)	48,95,113	1.80	10 (20%)
12	CLA	e	808	1	42,58,73	1.17	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	e	809	-	34,53,73	1.27	4 (11%)	37,89,113	1.72	7 (18%)
12	CLA	e	810	-	42,58,73	1.19	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	e	811	1	42,58,73	1.14	4 (9%)	48,95,113	1.72	9 (18%)
12	CLA	e	812	1	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	e	813	-	34,53,73	1.29	5 (14%)	37,89,113	1.77	7 (18%)
12	CLA	e	814	-	34,53,73	1.26	4 (11%)	37,89,113	1.79	7 (18%)
12	CLA	e	815	1	41,57,73	1.18	4 (9%)	46,93,113	1.65	7 (15%)
12	CLA	e	816	1	42,58,73	1.17	5 (11%)	48,95,113	1.70	9 (18%)
12	CLA	e	817	1	42,58,73	1.15	4 (9%)	48,95,113	1.76	9 (18%)
12	CLA	e	818	-	42,58,73	1.17	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	e	819	-	42,58,73	1.19	5 (11%)	48,95,113	1.63	8 (16%)
12	CLA	e	820	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	8 (16%)
12	CLA	e	821	1	41,57,73	1.16	4 (9%)	46,93,113	1.81	10 (21%)
12	CLA	e	822	1	42,58,73	1.17	4 (9%)	48,95,113	1.66	9 (18%)
12	CLA	e	823	1	42,58,73	1.18	4 (9%)	48,95,113	1.60	9 (18%)
12	CLA	e	824	-	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	825	-	42,58,73	1.20	5 (11%)	48,95,113	1.68	8 (16%)
12	CLA	e	826	-	42,58,73	1.15	4 (9%)	48,95,113	1.69	8 (16%)
12	CLA	e	827	1	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	e	828	-	42,58,73	1.19	5 (11%)	48,95,113	1.64	9 (18%)
12	CLA	e	829	1	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	e	830	-	42,58,73	1.19	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	e	831	-	42,58,73	1.19	5 (11%)	48,95,113	1.62	8 (16%)
12	CLA	e	832	-	42,58,73	1.16	4 (9%)	48,95,113	1.66	7 (14%)
12	CLA	e	833	1	42,58,73	1.18	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	834	-	34,53,73	1.28	5 (14%)	37,89,113	1.83	8 (21%)
12	CLA	e	835	-	42,58,73	1.17	4 (9%)	48,95,113	1.74	9 (18%)
12	CLA	e	836	-	42,58,73	1.21	6 (14%)	48,95,113	1.66	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	e	837	-	39,55,73	1.22	5 (12%)	44,91,113	1.77	8 (18%)
12	CLA	e	838	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	10 (20%)
12	CLA	e	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.64	8 (16%)
12	CLA	e	840	-	42,58,73	1.21	5 (11%)	48,95,113	1.67	8 (16%)
12	CLA	e	841	-	30,49,73	1.31	4 (13%)	31,83,113	1.88	7 (22%)
12	CLA	e	842	-	42,58,73	1.18	4 (9%)	48,95,113	1.65	9 (18%)
13	PQN	e	843	-	34,34,34	1.73	5 (14%)	42,45,45	1.28	5 (11%)
12	CLA	e	844	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	e	845	-	41,57,73	1.19	5 (12%)	46,93,113	1.60	8 (17%)
12	CLA	f	1301	-	34,53,73	1.28	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	g	801	-	42,58,73	1.16	5 (11%)	48,95,113	1.80	10 (20%)
12	CLA	g	802	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	g	803	-	42,58,73	1.20	6 (14%)	48,95,113	1.67	9 (18%)
14	SF4	g	804	-	0,12,12	0.00	-	-	-	-
12	CLA	g	805	-	42,58,73	1.20	4 (9%)	48,95,113	1.62	9 (18%)
12	CLA	g	806	-	42,58,73	1.17	5 (11%)	48,95,113	1.79	11 (22%)
12	CLA	g	807	2	42,58,73	1.15	4 (9%)	48,95,113	1.77	10 (20%)
12	CLA	g	808	-	42,58,73	1.19	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	g	809	-	42,58,73	1.17	4 (9%)	48,95,113	1.72	8 (16%)
12	CLA	g	810	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	g	811	-	42,58,73	1.17	5 (11%)	48,95,113	1.72	9 (18%)
12	CLA	g	812	2	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	g	813	-	42,58,73	1.19	4 (9%)	48,95,113	1.63	9 (18%)
12	CLA	g	814	-	34,53,73	1.28	4 (11%)	37,89,113	1.69	6 (16%)
12	CLA	g	815	-	34,53,73	1.26	4 (11%)	37,89,113	1.78	7 (18%)
12	CLA	g	816	2	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	g	817	2	42,58,73	1.17	4 (9%)	48,95,113	1.68	8 (16%)
12	CLA	g	818	2	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	g	819	-	42,58,73	1.19	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	g	820	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	g	821	-	42,58,73	1.18	5 (11%)	48,95,113	1.72	8 (16%)
12	CLA	g	822	-	42,58,73	1.18	4 (9%)	48,95,113	1.67	9 (18%)
12	CLA	g	823	2	39,55,73	1.22	5 (12%)	44,91,113	1.73	7 (15%)
12	CLA	g	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	8 (21%)
12	CLA	g	825	2	42,58,73	1.18	4 (9%)	48,95,113	1.64	8 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	CLA	g	826	-	34,53,73	1.27	5 (14%)	37,89,113	1.80	7 (18%)
12	CLA	g	827	-	42,58,73	1.18	4 (9%)	48,95,113	1.63	8 (16%)
12	CLA	g	828	-	38,54,73	1.22	4 (10%)	43,90,113	1.76	7 (16%)
12	CLA	g	829	-	42,58,73	1.17	4 (9%)	48,95,113	1.60	8 (16%)
12	CLA	g	830	2	42,58,73	1.17	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	g	831	-	42,58,73	1.18	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	g	832	2	42,58,73	1.17	4 (9%)	48,95,113	1.67	8 (16%)
12	CLA	g	833	-	34,53,73	1.26	4 (11%)	37,89,113	1.69	7 (18%)
12	CLA	g	834	-	42,58,73	1.18	4 (9%)	48,95,113	1.66	8 (16%)
12	CLA	g	835	-	42,58,73	1.16	4 (9%)	48,95,113	1.62	8 (16%)
12	CLA	g	836	2	34,53,73	1.30	5 (14%)	37,89,113	1.76	8 (21%)
12	CLA	g	837	-	34,53,73	1.27	4 (11%)	37,89,113	1.82	7 (18%)
12	CLA	g	838	-	42,58,73	1.20	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	g	839	-	42,58,73	1.17	4 (9%)	48,95,113	1.75	9 (18%)
12	CLA	g	840	-	39,55,73	1.21	4 (10%)	44,91,113	1.80	8 (18%)
12	CLA	g	841	-	42,58,73	1.20	4 (9%)	48,95,113	1.76	10 (20%)
12	CLA	g	842	-	42,58,73	1.20	5 (11%)	48,95,113	1.60	8 (16%)
13	PQN	g	843	-	34,34,34	1.71	5 (14%)	42,45,45	1.19	2 (4%)
14	SF4	h	101	-	0,12,12	0.00	-	-		
14	SF4	h	102	3	0,12,12	0.00	-	-		
12	CLA	k	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.85	8 (21%)
12	CLA	l	201	-	42,58,73	1.17	4 (9%)	48,95,113	1.69	9 (18%)
12	CLA	l	202	-	42,58,73	1.18	5 (11%)	48,95,113	1.66	9 (18%)
12	CLA	l	203	10	42,58,73	1.18	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	l	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.65	9 (18%)
12	CLA	o	1301	-	34,53,73	1.27	4 (11%)	37,89,113	1.76	7 (18%)
12	CLA	r	1401	-	34,53,73	1.25	4 (11%)	37,89,113	1.84	7 (18%)
12	CLA	s	201	-	42,58,73	1.17	4 (9%)	48,95,113	1.68	9 (18%)
12	CLA	s	202	-	42,58,73	1.18	5 (11%)	48,95,113	1.65	9 (18%)
12	CLA	s	203	10	42,58,73	1.17	4 (9%)	48,95,113	1.73	8 (16%)
12	CLA	s	204	-	42,58,73	1.17	4 (9%)	48,95,113	1.65	9 (18%)

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
12	CLA	A	801	-	3/3/17/25	8/19/117/135	-
12	CLA	A	802	-	3/3/17/25	5/19/117/135	-
12	CLA	A	803	-	3/3/17/25	8/19/117/135	-
12	CLA	A	804	1	3/3/17/25	2/19/117/135	-
12	CLA	A	805	1	2/2/17/25	10/19/117/135	-
12	CLA	A	806	1	3/3/17/25	8/19/117/135	-
12	CLA	A	807	1	3/3/17/25	8/19/117/135	-
12	CLA	A	808	-	3/3/16/25	5/11/111/135	-
12	CLA	A	809	-	3/3/17/25	6/19/117/135	-
12	CLA	A	810	1	3/3/17/25	3/19/117/135	-
12	CLA	A	811	1	3/3/17/25	4/19/117/135	-
12	CLA	A	812	-	3/3/16/25	9/11/111/135	-
12	CLA	A	813	-	3/3/16/25	6/11/111/135	-
12	CLA	A	814	1	3/3/16/25	8/18/116/135	-
12	CLA	A	815	1	3/3/17/25	5/19/117/135	-
12	CLA	A	816	1	3/3/17/25	6/19/117/135	-
12	CLA	A	817	-	3/3/17/25	9/19/117/135	-
12	CLA	A	818	-	3/3/17/25	7/19/117/135	-
12	CLA	A	819	-	3/3/17/25	6/19/117/135	-
12	CLA	A	820	1	3/3/16/25	7/18/116/135	-
12	CLA	A	821	1	3/3/17/25	8/19/117/135	-
12	CLA	A	822	1	3/3/17/25	8/19/117/135	-
12	CLA	A	823	-	3/3/17/25	9/19/117/135	-
12	CLA	A	824	-	3/3/17/25	7/19/117/135	-
12	CLA	A	825	-	3/3/17/25	9/19/117/135	-
12	CLA	A	826	1	3/3/17/25	8/19/117/135	-
12	CLA	A	827	-	3/3/17/25	8/19/117/135	-
12	CLA	A	828	1	3/3/17/25	8/19/117/135	-
12	CLA	A	829	-	2/2/17/25	9/19/117/135	-
12	CLA	A	830	-	3/3/17/25	8/19/117/135	-
12	CLA	A	831	-	3/3/17/25	7/19/117/135	-
12	CLA	A	832	1	3/3/17/25	6/19/117/135	-
12	CLA	A	833	-	3/3/16/25	7/11/111/135	-
12	CLA	A	834	-	3/3/17/25	6/19/117/135	-
12	CLA	A	835	-	3/3/17/25	3/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	A	836	-	3/3/16/25	6/16/114/135	-
12	CLA	A	837	-	2/2/17/25	4/19/117/135	-
12	CLA	A	838	-	3/3/17/25	8/19/117/135	-
12	CLA	A	839	-	3/3/17/25	3/19/117/135	-
12	CLA	A	840	-	3/3/14/25	1/5/101/135	-
12	CLA	A	841	-	3/3/17/25	8/19/117/135	-
13	PQN	A	842	-	1/1/8/9	11/23/43/43	0/2/2/2
12	CLA	B	801	-	3/3/17/25	8/19/117/135	-
12	CLA	B	802	-	3/3/17/25	2/19/117/135	-
12	CLA	B	803	-	3/3/17/25	5/19/117/135	-
14	SF4	B	804	-	-	-	0/6/5/5
12	CLA	B	805	-	3/3/17/25	9/19/117/135	-
12	CLA	B	806	-	3/3/17/25	6/19/117/135	-
12	CLA	B	807	-	3/3/17/25	9/19/117/135	-
12	CLA	B	808	2	3/3/17/25	9/19/117/135	-
12	CLA	B	809	-	3/3/17/25	7/19/117/135	-
12	CLA	B	810	-	3/3/17/25	4/19/117/135	-
12	CLA	B	811	-	3/3/17/25	6/19/117/135	-
12	CLA	B	812	-	3/3/17/25	6/19/117/135	-
12	CLA	B	813	2	3/3/17/25	7/19/117/135	-
12	CLA	B	814	-	3/3/17/25	10/19/117/135	-
12	CLA	B	815	-	3/3/16/25	6/11/111/135	-
12	CLA	B	816	-	3/3/16/25	4/11/111/135	-
12	CLA	B	817	2	3/3/17/25	10/19/117/135	-
12	CLA	B	818	2	3/3/17/25	7/19/117/135	-
12	CLA	B	819	2	3/3/16/25	4/11/111/135	-
12	CLA	B	820	-	3/3/17/25	6/19/117/135	-
12	CLA	B	821	-	3/3/17/25	13/19/117/135	-
12	CLA	B	822	-	3/3/17/25	8/19/117/135	-
12	CLA	B	823	-	3/3/17/25	6/19/117/135	-
12	CLA	B	824	2	3/3/16/25	7/16/114/135	-
12	CLA	B	825	-	3/3/16/25	3/11/111/135	-
12	CLA	B	826	2	3/3/17/25	3/19/117/135	-
12	CLA	B	827	-	3/3/16/25	5/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	B	828	-	3/3/17/25	5/19/117/135	-
12	CLA	B	829	-	3/3/16/25	7/15/113/135	-
12	CLA	B	830	-	3/3/17/25	6/19/117/135	-
12	CLA	B	831	2	3/3/17/25	9/19/117/135	-
12	CLA	B	832	-	3/3/17/25	8/19/117/135	-
12	CLA	B	833	2	3/3/17/25	7/19/117/135	-
12	CLA	B	834	-	3/3/16/25	4/11/111/135	-
12	CLA	B	835	-	3/3/16/25	11/18/116/135	-
12	CLA	B	836	-	3/3/17/25	7/19/117/135	-
12	CLA	B	837	2	3/3/16/25	4/11/111/135	-
12	CLA	B	838	-	3/3/16/25	7/11/111/135	-
12	CLA	B	839	-	3/3/17/25	9/19/117/135	-
12	CLA	B	840	-	3/3/17/25	5/19/117/135	-
12	CLA	B	841	-	2/2/16/25	8/16/114/135	-
12	CLA	B	842	-	3/3/17/25	8/19/117/135	-
12	CLA	B	843	-	3/3/17/25	9/19/117/135	-
13	PQN	B	844	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	C	101	-	-	-	0/6/5/5
14	SF4	C	102	3	-	-	0/6/5/5
12	CLA	E	801	-	3/3/17/25	8/19/117/135	-
12	CLA	E	802	-	3/3/17/25	8/19/117/135	-
12	CLA	E	803	-	3/3/17/25	2/19/117/135	-
12	CLA	E	804	-	3/3/17/25	8/19/117/135	-
12	CLA	E	805	-	3/3/17/25	5/19/117/135	-
12	CLA	E	806	-	3/3/17/25	8/19/117/135	-
12	CLA	E	807	1	3/3/17/25	2/19/117/135	-
12	CLA	E	808	1	2/2/17/25	10/19/117/135	-
12	CLA	E	809	1	3/3/17/25	8/19/117/135	-
12	CLA	E	810	1	3/3/17/25	8/19/117/135	-
12	CLA	E	811	-	3/3/16/25	5/11/111/135	-
12	CLA	E	812	-	3/3/17/25	6/19/117/135	-
12	CLA	E	813	1	3/3/17/25	3/19/117/135	-
12	CLA	E	814	1	3/3/17/25	4/19/117/135	-
12	CLA	E	815	-	3/3/16/25	9/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	E	816	-	3/3/16/25	6/11/111/135	-
12	CLA	E	817	1	3/3/16/25	8/18/116/135	-
12	CLA	E	818	1	3/3/17/25	5/19/117/135	-
12	CLA	E	819	1	3/3/17/25	6/19/117/135	-
12	CLA	E	820	-	3/3/17/25	9/19/117/135	-
12	CLA	E	821	-	3/3/17/25	7/19/117/135	-
12	CLA	E	822	-	3/3/17/25	6/19/117/135	-
12	CLA	E	823	1	3/3/16/25	7/18/116/135	-
12	CLA	E	824	1	3/3/17/25	8/19/117/135	-
12	CLA	E	825	1	3/3/17/25	8/19/117/135	-
12	CLA	E	826	-	3/3/17/25	9/19/117/135	-
12	CLA	E	827	-	3/3/17/25	7/19/117/135	-
12	CLA	E	828	-	3/3/17/25	9/19/117/135	-
12	CLA	E	829	1	3/3/17/25	8/19/117/135	-
12	CLA	E	830	-	3/3/17/25	8/19/117/135	-
12	CLA	E	831	1	3/3/17/25	8/19/117/135	-
12	CLA	E	832	-	2/2/17/25	9/19/117/135	-
12	CLA	E	833	-	3/3/17/25	10/19/117/135	-
12	CLA	E	834	-	3/3/17/25	9/19/117/135	-
12	CLA	E	835	-	3/3/17/25	7/19/117/135	-
12	CLA	E	836	1	3/3/17/25	6/19/117/135	-
12	CLA	E	837	-	3/3/16/25	7/11/111/135	-
12	CLA	E	838	-	3/3/17/25	6/19/117/135	-
12	CLA	E	839	-	3/3/17/25	3/19/117/135	-
12	CLA	E	840	-	3/3/16/25	6/16/114/135	-
12	CLA	E	841	-	2/2/17/25	4/19/117/135	-
12	CLA	E	842	-	3/3/17/25	8/19/117/135	-
12	CLA	E	843	-	3/3/17/25	3/19/117/135	-
12	CLA	E	844	-	3/3/14/25	1/5/101/135	-
14	SF4	E	845	-	-	-	0/6/5/5
13	PQN	E	846	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	F	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	G	801	-	3/3/17/25	5/19/117/135	-
12	CLA	G	802	-	3/3/17/25	9/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	803	-	3/3/17/25	6/19/117/135	-
12	CLA	G	804	-	3/3/17/25	9/19/117/135	-
12	CLA	G	805	2	3/3/17/25	9/19/117/135	-
12	CLA	G	806	-	3/3/17/25	7/19/117/135	-
12	CLA	G	807	-	3/3/17/25	4/19/117/135	-
12	CLA	G	808	-	3/3/17/25	6/19/117/135	-
12	CLA	G	809	-	3/3/17/25	6/19/117/135	-
12	CLA	G	810	2	3/3/17/25	7/19/117/135	-
12	CLA	G	811	-	3/3/17/25	10/19/117/135	-
12	CLA	G	812	-	3/3/16/25	6/11/111/135	-
12	CLA	G	813	-	3/3/16/25	4/11/111/135	-
12	CLA	G	814	2	3/3/17/25	10/19/117/135	-
12	CLA	G	815	2	3/3/17/25	7/19/117/135	-
12	CLA	G	816	2	3/3/16/25	4/11/111/135	-
12	CLA	G	817	-	3/3/17/25	6/19/117/135	-
12	CLA	G	818	-	3/3/17/25	13/19/117/135	-
12	CLA	G	819	-	3/3/17/25	8/19/117/135	-
12	CLA	G	820	-	3/3/17/25	6/19/117/135	-
12	CLA	G	821	2	3/3/16/25	7/16/114/135	-
12	CLA	G	822	-	3/3/16/25	3/11/111/135	-
12	CLA	G	823	2	3/3/17/25	3/19/117/135	-
12	CLA	G	824	-	3/3/16/25	5/11/111/135	-
12	CLA	G	825	-	3/3/17/25	5/19/117/135	-
12	CLA	G	826	-	3/3/16/25	7/15/113/135	-
12	CLA	G	827	-	3/3/17/25	6/19/117/135	-
12	CLA	G	828	2	3/3/17/25	9/19/117/135	-
12	CLA	G	829	-	3/3/17/25	8/19/117/135	-
12	CLA	G	830	2	3/3/17/25	7/19/117/135	-
12	CLA	G	831	-	3/3/16/25	4/11/111/135	-
12	CLA	G	832	-	3/3/16/25	11/18/116/135	-
12	CLA	G	833	-	3/3/17/25	7/19/117/135	-
12	CLA	G	834	-	3/3/17/25	12/19/117/135	-
12	CLA	G	835	2	3/3/16/25	4/11/111/135	-
12	CLA	G	836	-	3/3/16/25	7/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	G	837	-	3/3/17/25	9/19/117/135	-
12	CLA	G	838	-	3/3/17/25	5/19/117/135	-
12	CLA	G	839	-	2/2/16/25	8/16/114/135	-
12	CLA	G	840	-	3/3/17/25	8/19/117/135	-
12	CLA	G	841	-	3/3/17/25	9/19/117/135	-
13	PQN	G	842	-	1/1/8/9	11/23/43/43	0/2/2/2
12	CLA	G	843	10	3/3/17/25	4/19/117/135	-
14	SF4	H	101	-	-	-	0/6/5/5
14	SF4	H	102	3	-	-	0/6/5/5
12	CLA	J	1101	-	3/3/17/25	8/19/117/135	-
12	CLA	J	1102	-	3/3/17/25	12/19/117/135	-
12	CLA	K	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	L	201	-	3/3/17/25	10/19/117/135	-
12	CLA	L	202	-	3/3/17/25	7/19/117/135	-
12	CLA	L	203	10	3/3/17/25	4/19/117/135	-
12	CLA	L	204	-	3/3/17/25	11/19/117/135	-
12	CLA	O	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	R	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	S	1501	-	3/3/17/25	7/19/117/135	-
12	CLA	S	1502	-	3/3/17/25	11/19/117/135	-
12	CLA	a	801	-	3/3/17/25	8/19/117/135	-
12	CLA	a	802	-	3/3/17/25	8/19/117/135	-
12	CLA	a	803	-	3/3/17/25	8/19/117/135	-
12	CLA	a	804	-	3/3/17/25	5/19/117/135	-
12	CLA	a	805	-	3/3/17/25	8/19/117/135	-
12	CLA	a	806	1	3/3/17/25	2/19/117/135	-
12	CLA	a	807	1	2/2/17/25	9/19/117/135	-
12	CLA	a	808	1	3/3/17/25	8/19/117/135	-
12	CLA	a	809	1	3/3/17/25	8/19/117/135	-
12	CLA	a	810	-	3/3/16/25	5/11/111/135	-
12	CLA	a	811	-	3/3/17/25	6/19/117/135	-
12	CLA	a	812	1	3/3/17/25	3/19/117/135	-
12	CLA	a	813	1	3/3/17/25	4/19/117/135	-
12	CLA	a	814	-	3/3/16/25	9/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	a	815	-	3/3/16/25	6/11/111/135	-
12	CLA	a	816	1	3/3/16/25	8/18/116/135	-
12	CLA	a	817	1	3/3/17/25	5/19/117/135	-
12	CLA	a	818	1	3/3/17/25	6/19/117/135	-
12	CLA	a	819	-	3/3/17/25	9/19/117/135	-
12	CLA	a	820	-	3/3/17/25	7/19/117/135	-
12	CLA	a	821	-	3/3/17/25	6/19/117/135	-
12	CLA	a	822	1	3/3/16/25	7/18/116/135	-
12	CLA	a	823	1	3/3/17/25	8/19/117/135	-
12	CLA	a	824	1	3/3/17/25	8/19/117/135	-
12	CLA	a	825	-	3/3/17/25	9/19/117/135	-
12	CLA	a	826	-	3/3/17/25	7/19/117/135	-
12	CLA	a	827	-	3/3/17/25	9/19/117/135	-
12	CLA	a	828	1	3/3/17/25	8/19/117/135	-
12	CLA	a	829	-	3/3/17/25	8/19/117/135	-
12	CLA	a	830	1	3/3/17/25	8/19/117/135	-
12	CLA	a	831	-	2/2/17/25	9/19/117/135	-
12	CLA	a	832	-	3/3/17/25	8/19/117/135	-
12	CLA	a	833	-	3/3/17/25	7/19/117/135	-
12	CLA	a	834	1	3/3/17/25	6/19/117/135	-
12	CLA	a	835	-	3/3/16/25	7/11/111/135	-
12	CLA	a	836	-	3/3/17/25	6/19/117/135	-
12	CLA	a	837	-	3/3/17/25	3/19/117/135	-
12	CLA	a	838	-	3/3/16/25	6/16/114/135	-
12	CLA	a	839	-	2/2/17/25	4/19/117/135	-
12	CLA	a	840	-	3/3/17/25	8/19/117/135	-
12	CLA	a	841	-	3/3/17/25	3/19/117/135	-
12	CLA	a	842	-	3/3/14/25	1/5/101/135	-
14	SF4	a	843	-	-	-	0/6/5/5
13	PQN	a	844	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	b	801	-	3/3/17/25	2/19/117/135	-
12	CLA	b	802	-	3/3/17/25	5/19/117/135	-
12	CLA	b	803	-	3/3/17/25	9/19/117/135	-
12	CLA	b	804	-	3/3/17/25	6/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	805	-	3/3/17/25	9/19/117/135	-
12	CLA	b	806	2	3/3/17/25	9/19/117/135	-
12	CLA	b	807	-	3/3/17/25	7/19/117/135	-
12	CLA	b	808	-	3/3/17/25	4/19/117/135	-
12	CLA	b	809	-	3/3/17/25	6/19/117/135	-
12	CLA	b	810	-	3/3/17/25	6/19/117/135	-
12	CLA	b	811	2	3/3/17/25	7/19/117/135	-
12	CLA	b	812	-	3/3/17/25	10/19/117/135	-
12	CLA	b	813	-	3/3/16/25	6/11/111/135	-
12	CLA	b	814	-	3/3/16/25	4/11/111/135	-
12	CLA	b	815	2	3/3/17/25	10/19/117/135	-
12	CLA	b	816	2	3/3/17/25	7/19/117/135	-
12	CLA	b	817	2	3/3/16/25	4/11/111/135	-
12	CLA	b	818	-	3/3/17/25	6/19/117/135	-
12	CLA	b	819	-	3/3/17/25	13/19/117/135	-
12	CLA	b	820	-	3/3/17/25	8/19/117/135	-
12	CLA	b	821	-	3/3/17/25	6/19/117/135	-
12	CLA	b	822	2	3/3/16/25	7/16/114/135	-
12	CLA	b	823	-	3/3/16/25	3/11/111/135	-
12	CLA	b	824	2	3/3/17/25	3/19/117/135	-
12	CLA	b	825	-	3/3/16/25	5/11/111/135	-
12	CLA	b	826	-	3/3/17/25	5/19/117/135	-
12	CLA	b	827	-	3/3/16/25	7/15/113/135	-
12	CLA	b	828	-	3/3/17/25	6/19/117/135	-
12	CLA	b	829	2	3/3/17/25	9/19/117/135	-
12	CLA	b	830	-	3/3/17/25	8/19/117/135	-
12	CLA	b	831	2	3/3/17/25	7/19/117/135	-
12	CLA	b	832	-	3/3/16/25	4/11/111/135	-
12	CLA	b	833	-	3/3/16/25	11/18/116/135	-
12	CLA	b	834	-	3/3/17/25	7/19/117/135	-
12	CLA	b	835	-	3/3/17/25	12/19/117/135	-
12	CLA	b	836	2	3/3/16/25	4/11/111/135	-
12	CLA	b	837	-	3/3/16/25	7/11/111/135	-
12	CLA	b	838	-	3/3/17/25	9/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	b	839	-	3/3/17/25	5/19/117/135	-
12	CLA	b	840	-	2/2/16/25	8/16/114/135	-
12	CLA	b	841	-	3/3/17/25	8/19/117/135	-
12	CLA	b	842	-	3/3/17/25	9/19/117/135	-
13	PQN	b	843	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	c	101	-	-	-	0/6/5/5
14	SF4	c	102	3	-	-	0/6/5/5
12	CLA	e	801	-	3/3/17/25	8/19/117/135	-
12	CLA	e	802	-	3/3/17/25	8/19/117/135	-
12	CLA	e	803	-	3/3/17/25	5/19/117/135	-
12	CLA	e	804	-	3/3/17/25	8/19/117/135	-
12	CLA	e	805	1	3/3/17/25	2/19/117/135	-
12	CLA	e	806	1	2/2/17/25	10/19/117/135	-
12	CLA	e	807	1	3/3/17/25	8/19/117/135	-
12	CLA	e	808	1	3/3/17/25	8/19/117/135	-
12	CLA	e	809	-	3/3/16/25	5/11/111/135	-
12	CLA	e	810	-	3/3/17/25	6/19/117/135	-
12	CLA	e	811	1	3/3/17/25	3/19/117/135	-
12	CLA	e	812	1	3/3/17/25	4/19/117/135	-
12	CLA	e	813	-	3/3/16/25	9/11/111/135	-
12	CLA	e	814	-	3/3/16/25	6/11/111/135	-
12	CLA	e	815	1	3/3/16/25	8/18/116/135	-
12	CLA	e	816	1	3/3/17/25	5/19/117/135	-
12	CLA	e	817	1	3/3/17/25	6/19/117/135	-
12	CLA	e	818	-	3/3/17/25	9/19/117/135	-
12	CLA	e	819	-	3/3/17/25	7/19/117/135	-
12	CLA	e	820	-	3/3/17/25	6/19/117/135	-
12	CLA	e	821	1	3/3/16/25	7/18/116/135	-
12	CLA	e	822	1	3/3/17/25	8/19/117/135	-
12	CLA	e	823	1	3/3/17/25	8/19/117/135	-
12	CLA	e	824	-	3/3/17/25	9/19/117/135	-
12	CLA	e	825	-	3/3/17/25	7/19/117/135	-
12	CLA	e	826	-	3/3/17/25	9/19/117/135	-
12	CLA	e	827	1	3/3/17/25	8/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	e	828	-	3/3/17/25	8/19/117/135	-
12	CLA	e	829	1	3/3/17/25	8/19/117/135	-
12	CLA	e	830	-	2/2/17/25	9/19/117/135	-
12	CLA	e	831	-	3/3/17/25	8/19/117/135	-
12	CLA	e	832	-	3/3/17/25	8/19/117/135	-
12	CLA	e	833	1	3/3/17/25	6/19/117/135	-
12	CLA	e	834	-	3/3/16/25	7/11/111/135	-
12	CLA	e	835	-	3/3/17/25	6/19/117/135	-
12	CLA	e	836	-	3/3/17/25	3/19/117/135	-
12	CLA	e	837	-	3/3/16/25	6/16/114/135	-
12	CLA	e	838	-	2/2/17/25	4/19/117/135	-
12	CLA	e	839	-	3/3/17/25	8/19/117/135	-
12	CLA	e	840	-	3/3/17/25	3/19/117/135	-
12	CLA	e	841	-	3/3/14/25	1/5/101/135	-
12	CLA	e	842	-	3/3/17/25	9/19/117/135	-
13	PQN	e	843	-	1/1/8/9	12/23/43/43	0/2/2/2
12	CLA	e	844	-	3/3/17/25	9/19/117/135	-
12	CLA	e	845	-	3/3/16/25	11/18/116/135	-
12	CLA	f	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	g	801	-	3/3/17/25	8/19/117/135	-
12	CLA	g	802	-	3/3/17/25	2/19/117/135	-
12	CLA	g	803	-	3/3/17/25	5/19/117/135	-
14	SF4	g	804	-	-	-	0/6/5/5
12	CLA	g	805	-	3/3/17/25	6/19/117/135	-
12	CLA	g	806	-	3/3/17/25	9/19/117/135	-
12	CLA	g	807	2	3/3/17/25	9/19/117/135	-
12	CLA	g	808	-	3/3/17/25	7/19/117/135	-
12	CLA	g	809	-	3/3/17/25	4/19/117/135	-
12	CLA	g	810	-	3/3/17/25	6/19/117/135	-
12	CLA	g	811	-	3/3/17/25	6/19/117/135	-
12	CLA	g	812	2	3/3/17/25	7/19/117/135	-
12	CLA	g	813	-	3/3/17/25	10/19/117/135	-
12	CLA	g	814	-	3/3/16/25	6/11/111/135	-
12	CLA	g	815	-	3/3/16/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	g	816	2	3/3/17/25	10/19/117/135	-
12	CLA	g	817	2	3/3/17/25	7/19/117/135	-
12	CLA	g	818	2	3/3/16/25	4/11/111/135	-
12	CLA	g	819	-	3/3/17/25	6/19/117/135	-
12	CLA	g	820	-	3/3/17/25	13/19/117/135	-
12	CLA	g	821	-	3/3/17/25	8/19/117/135	-
12	CLA	g	822	-	3/3/17/25	6/19/117/135	-
12	CLA	g	823	2	3/3/16/25	7/16/114/135	-
12	CLA	g	824	-	3/3/16/25	3/11/111/135	-
12	CLA	g	825	2	3/3/17/25	3/19/117/135	-
12	CLA	g	826	-	3/3/16/25	5/11/111/135	-
12	CLA	g	827	-	3/3/17/25	5/19/117/135	-
12	CLA	g	828	-	3/3/16/25	7/15/113/135	-
12	CLA	g	829	-	3/3/17/25	6/19/117/135	-
12	CLA	g	830	2	3/3/17/25	9/19/117/135	-
12	CLA	g	831	-	3/3/17/25	8/19/117/135	-
12	CLA	g	832	2	3/3/17/25	7/19/117/135	-
12	CLA	g	833	-	3/3/16/25	4/11/111/135	-
12	CLA	g	834	-	3/3/17/25	7/19/117/135	-
12	CLA	g	835	-	3/3/17/25	12/19/117/135	-
12	CLA	g	836	2	3/3/16/25	4/11/111/135	-
12	CLA	g	837	-	3/3/16/25	7/11/111/135	-
12	CLA	g	838	-	3/3/17/25	9/19/117/135	-
12	CLA	g	839	-	3/3/17/25	5/19/117/135	-
12	CLA	g	840	-	2/2/16/25	9/16/114/135	-
12	CLA	g	841	-	3/3/17/25	8/19/117/135	-
12	CLA	g	842	-	3/3/17/25	9/19/117/135	-
13	PQN	g	843	-	1/1/8/9	11/23/43/43	0/2/2/2
14	SF4	h	101	-	-	-	0/6/5/5
14	SF4	h	102	3	-	-	0/6/5/5
12	CLA	k	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	l	201	-	3/3/17/25	10/19/117/135	-
12	CLA	l	202	-	3/3/17/25	7/19/117/135	-
12	CLA	l	203	10	3/3/17/25	4/19/117/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
12	CLA	l	204	-	3/3/17/25	11/19/117/135	-
12	CLA	o	1301	-	3/3/16/25	7/11/111/135	-
12	CLA	r	1401	-	3/3/16/25	4/11/111/135	-
12	CLA	s	201	-	3/3/17/25	10/19/117/135	-
12	CLA	s	202	-	3/3/17/25	7/19/117/135	-
12	CLA	s	203	10	3/3/17/25	4/19/117/135	-
12	CLA	s	204	-	3/3/17/25	11/19/117/135	-

The worst 5 of 1612 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	842	PQN	C3-C2	6.28	1.48	1.35
13	b	843	PQN	C3-C2	6.24	1.48	1.35
13	e	843	PQN	C3-C2	6.23	1.48	1.35
13	g	843	PQN	C3-C2	6.20	1.48	1.35
13	G	842	PQN	C3-C2	6.19	1.48	1.35

The worst 5 of 3068 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	A	806	CLA	C4A-NA-C1A	7.42	110.04	106.71
12	e	807	CLA	C4A-NA-C1A	7.33	110.00	106.71
12	e	837	CLA	C4A-NA-C1A	7.30	109.99	106.71
12	E	809	CLA	C4A-NA-C1A	7.27	109.98	106.71
12	b	840	CLA	C4A-NA-C1A	7.24	109.96	106.71

5 of 1078 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
12	E	817	CLA	NC
12	E	817	CLA	ND
12	E	817	CLA	NA
12	a	812	CLA	NC
12	a	812	CLA	ND

5 of 2550 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	E	817	CLA	C1A-C2A-CAA-CBA
12	E	817	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
12	E	817	CLA	CHA-CBD-CGD-O2D
12	E	817	CLA	CBD-CGD-O2D-CED
12	E	840	CLA	C1A-C2A-CAA-CBA

There are no ring outliers.

188 monomers are involved in 1018 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	801	CLA	9	0
12	A	802	CLA	8	0
12	A	803	CLA	10	0
12	A	804	CLA	5	0
12	A	805	CLA	8	0
12	A	806	CLA	8	0
12	A	808	CLA	5	0
12	A	809	CLA	2	0
12	A	810	CLA	6	0
12	A	811	CLA	7	0
12	A	812	CLA	7	0
12	A	813	CLA	6	0
12	A	814	CLA	5	0
12	A	815	CLA	5	0
12	A	816	CLA	6	0
12	A	817	CLA	6	0
12	A	818	CLA	7	0
12	A	819	CLA	2	0
12	A	820	CLA	8	0
12	A	821	CLA	5	0
12	A	822	CLA	4	0
12	A	823	CLA	9	0
12	A	824	CLA	3	0
12	A	825	CLA	7	0
12	A	826	CLA	4	0
12	A	827	CLA	6	0
12	A	828	CLA	4	0
12	A	829	CLA	6	0
12	A	830	CLA	5	0
12	A	831	CLA	7	0
12	A	832	CLA	8	0
12	A	833	CLA	9	0
12	A	834	CLA	10	0
12	A	835	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	836	CLA	9	0
12	A	837	CLA	8	0
12	A	838	CLA	9	0
12	A	839	CLA	7	0
12	A	840	CLA	6	0
12	A	841	CLA	6	0
13	A	842	PQN	7	0
12	B	801	CLA	10	0
12	B	802	CLA	8	0
12	B	803	CLA	6	0
12	B	805	CLA	12	0
12	B	806	CLA	12	0
12	B	807	CLA	14	0
12	B	808	CLA	4	0
12	B	809	CLA	9	0
12	B	810	CLA	7	0
12	B	811	CLA	5	0
12	B	812	CLA	4	0
12	B	813	CLA	6	0
12	B	814	CLA	6	0
12	B	815	CLA	7	0
12	B	816	CLA	5	0
12	B	817	CLA	9	0
12	B	818	CLA	5	0
12	B	819	CLA	6	0
12	B	820	CLA	7	0
12	B	821	CLA	6	0
12	B	822	CLA	8	0
12	B	823	CLA	4	0
12	B	824	CLA	10	0
12	B	825	CLA	4	0
12	B	826	CLA	8	0
12	B	827	CLA	7	0
12	B	828	CLA	7	0
12	B	829	CLA	6	0
12	B	830	CLA	5	0
12	B	831	CLA	4	0
12	B	832	CLA	5	0
12	B	833	CLA	2	0
12	B	834	CLA	6	0
12	B	835	CLA	9	0
12	B	836	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	B	837	CLA	3	0
12	B	838	CLA	4	0
12	B	839	CLA	8	0
12	B	840	CLA	7	0
12	B	841	CLA	7	0
12	B	842	CLA	6	0
12	B	843	CLA	2	0
13	B	844	PQN	4	0
14	C	101	SF4	1	0
14	C	102	SF4	6	0
12	E	801	CLA	10	0
12	E	802	CLA	9	0
12	E	803	CLA	3	0
12	E	804	CLA	11	0
12	E	805	CLA	7	0
12	E	806	CLA	11	0
12	E	807	CLA	7	0
12	E	808	CLA	1	0
12	E	809	CLA	5	0
12	E	810	CLA	2	0
12	E	811	CLA	3	0
12	E	812	CLA	7	0
12	E	813	CLA	8	0
12	E	814	CLA	5	0
12	E	815	CLA	4	0
12	E	816	CLA	5	0
12	E	817	CLA	6	0
12	E	818	CLA	7	0
12	E	819	CLA	7	0
12	E	820	CLA	2	0
12	E	821	CLA	8	0
12	E	822	CLA	5	0
12	E	823	CLA	5	0
12	E	824	CLA	8	0
12	E	825	CLA	3	0
12	E	826	CLA	8	0
12	E	827	CLA	3	0
12	E	828	CLA	5	0
12	E	829	CLA	4	0
12	E	830	CLA	5	0
12	E	831	CLA	5	0
12	E	832	CLA	9	0

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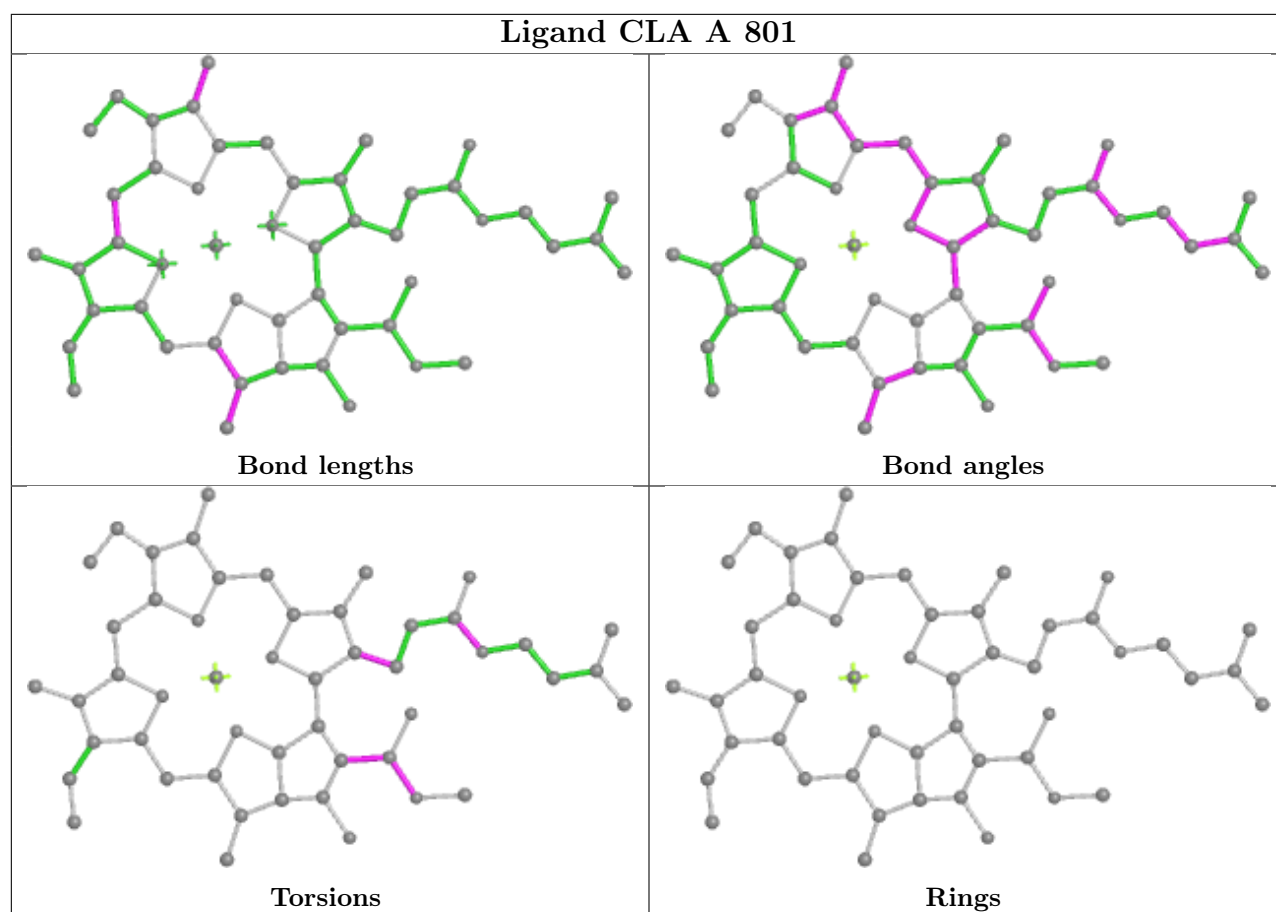
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	E	833	CLA	4	0
12	E	834	CLA	8	0
12	E	835	CLA	13	0
12	E	836	CLA	7	0
12	E	837	CLA	6	0
12	E	838	CLA	9	0
12	E	839	CLA	11	0
12	E	840	CLA	5	0
12	E	841	CLA	4	0
12	E	842	CLA	10	0
12	E	843	CLA	6	0
12	E	844	CLA	7	0
13	E	846	PQN	9	0
12	F	1301	CLA	4	0
12	G	801	CLA	18	0
12	G	802	CLA	5	0
12	G	803	CLA	1	0
12	G	804	CLA	8	0
12	G	805	CLA	11	0
12	G	806	CLA	13	0
12	G	807	CLA	2	0
12	G	808	CLA	12	0
12	G	809	CLA	4	0
12	G	810	CLA	4	0
12	G	811	CLA	5	0
12	G	812	CLA	6	0
12	G	813	CLA	6	0
12	G	814	CLA	10	0
12	G	815	CLA	6	0
12	G	816	CLA	7	0
12	G	817	CLA	6	0
12	G	818	CLA	6	0
12	G	819	CLA	7	0
12	G	820	CLA	6	0
12	G	821	CLA	8	0
12	G	822	CLA	3	0
12	G	823	CLA	10	0
12	G	824	CLA	4	0
12	G	825	CLA	7	0
12	G	826	CLA	6	0
12	G	827	CLA	7	0
12	G	828	CLA	5	0

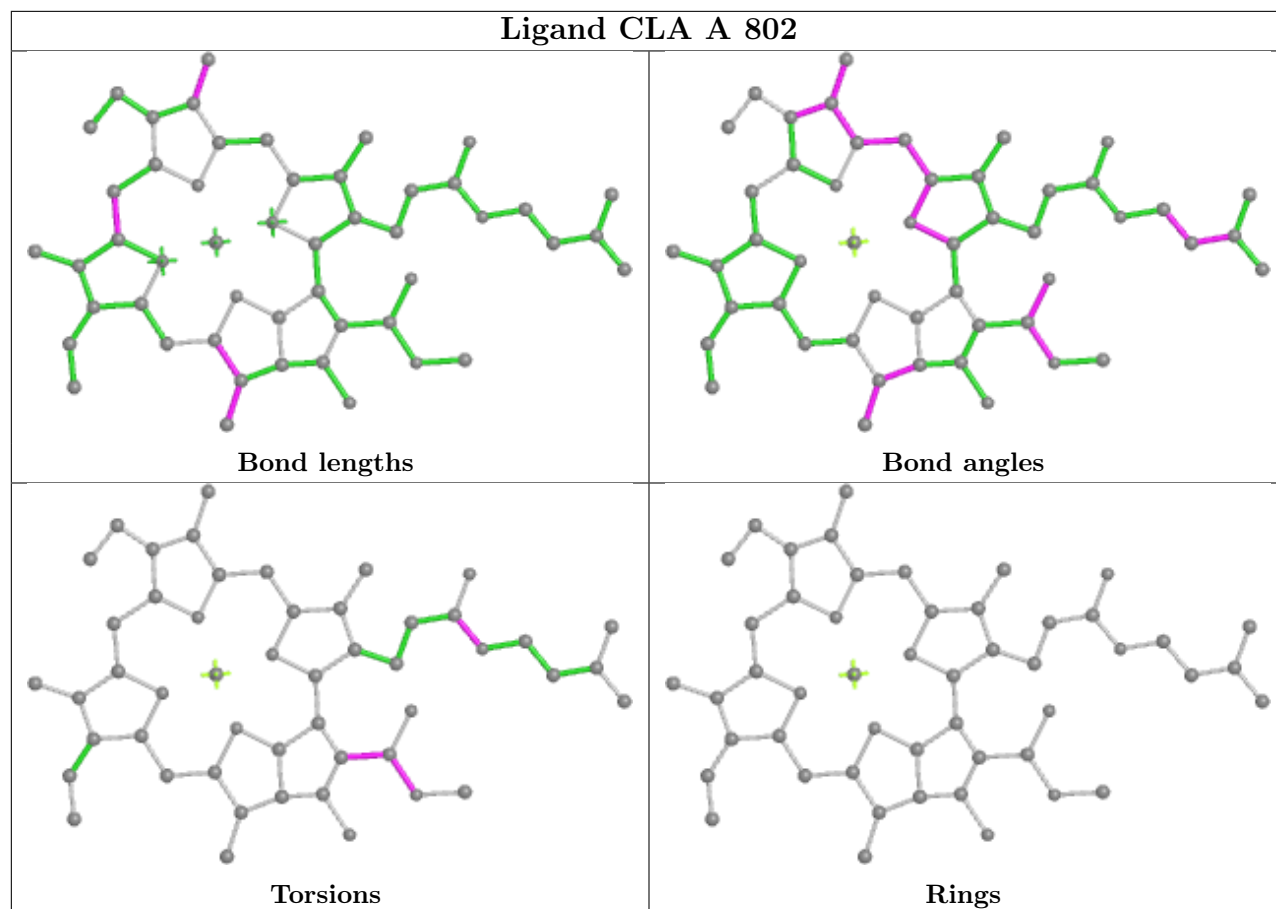
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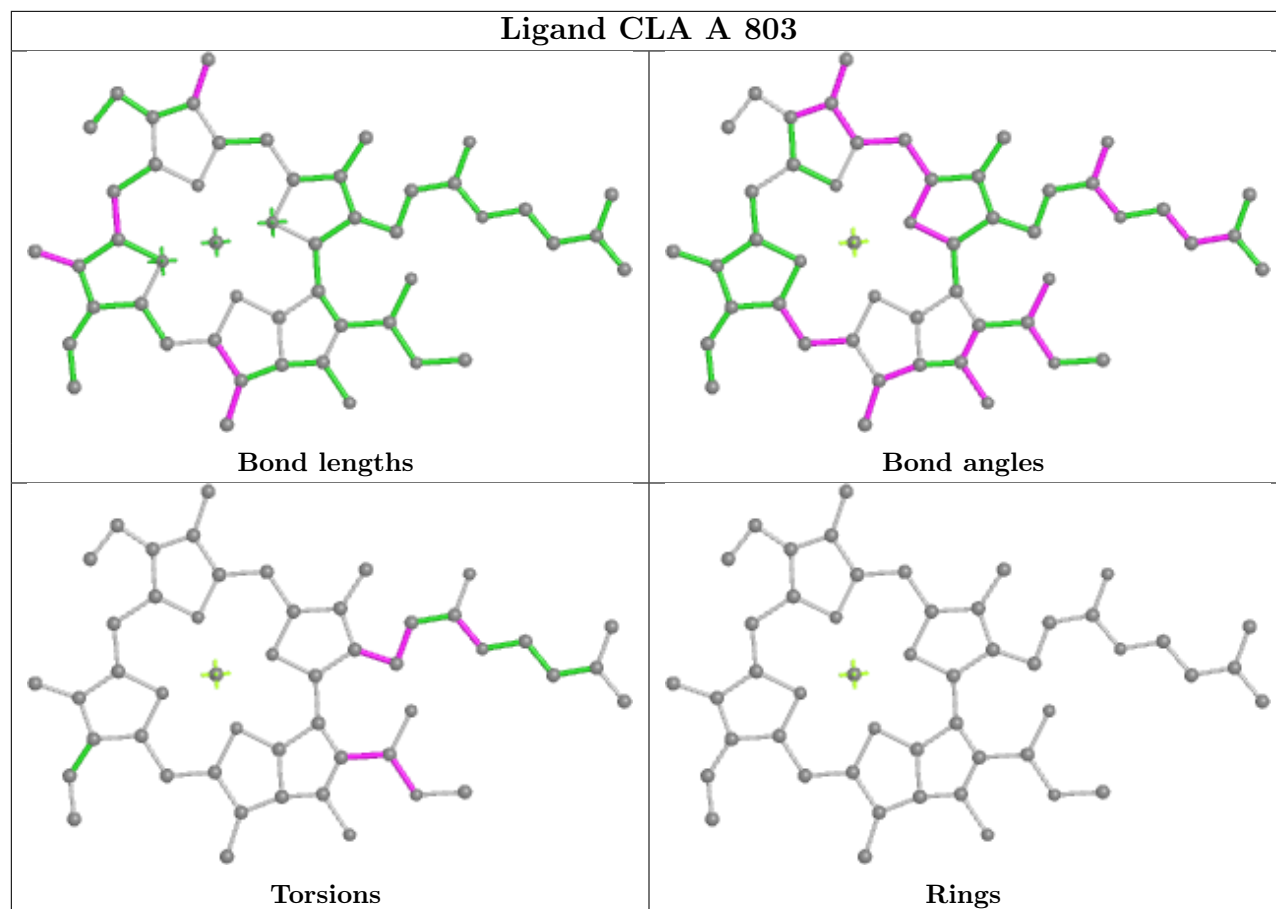
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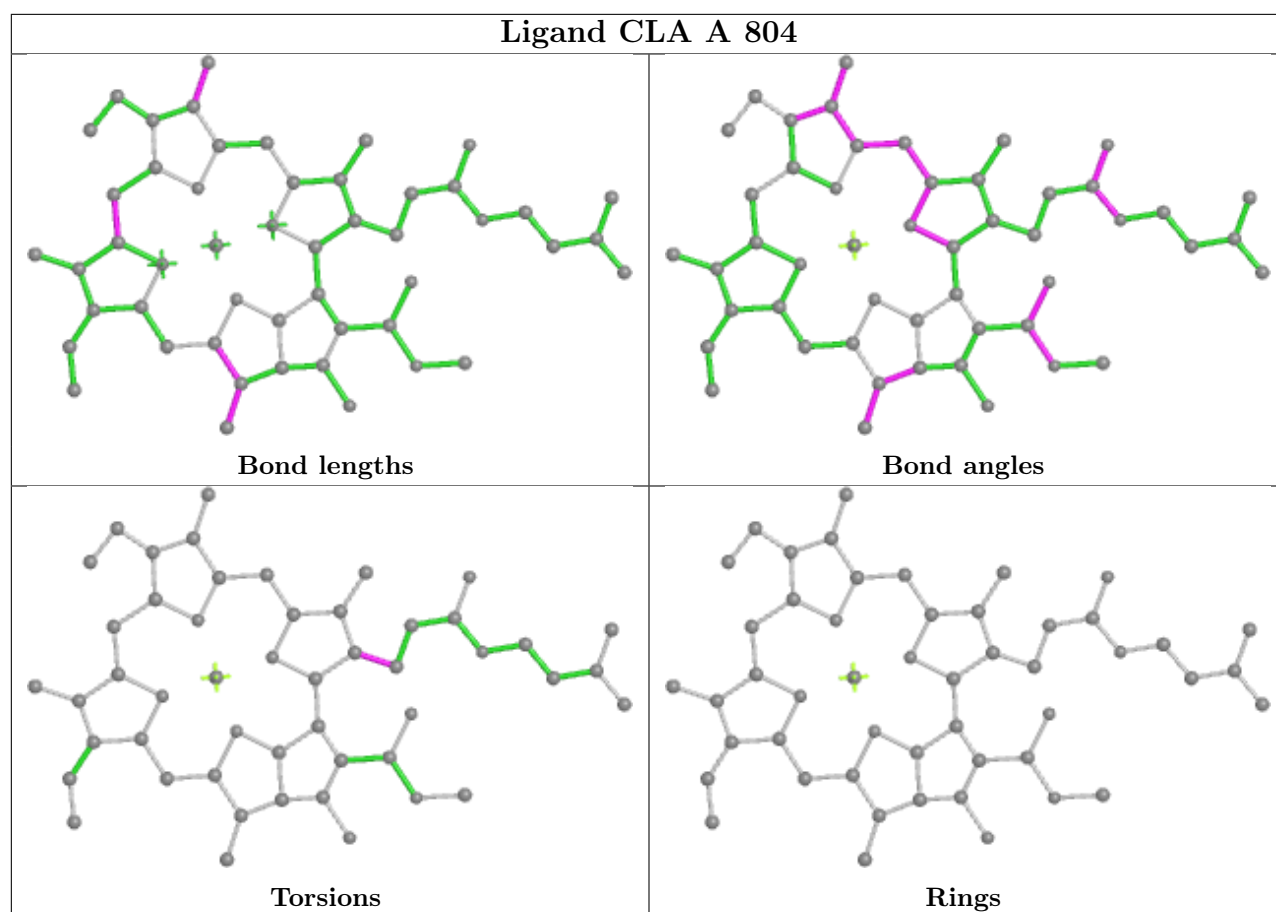
Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	G	829	CLA	6	0
12	G	830	CLA	3	0
12	G	831	CLA	6	0
12	G	832	CLA	2	0
12	G	833	CLA	6	0
12	G	834	CLA	10	0
12	G	835	CLA	11	0
12	G	836	CLA	4	0
12	G	837	CLA	5	0
12	G	838	CLA	9	0
12	G	839	CLA	7	0
12	G	840	CLA	11	0
12	G	841	CLA	7	0
13	G	842	PQN	4	0
12	G	843	CLA	3	0
14	H	101	SF4	1	0
14	H	102	SF4	6	0
12	J	1101	CLA	5	0
12	J	1102	CLA	8	0
12	K	1401	CLA	2	0
12	L	201	CLA	4	0
12	L	202	CLA	2	0
12	L	203	CLA	3	0
12	L	204	CLA	5	0
12	O	1301	CLA	1	0
12	R	1401	CLA	3	0
12	S	1501	CLA	2	0
12	S	1502	CLA	4	0

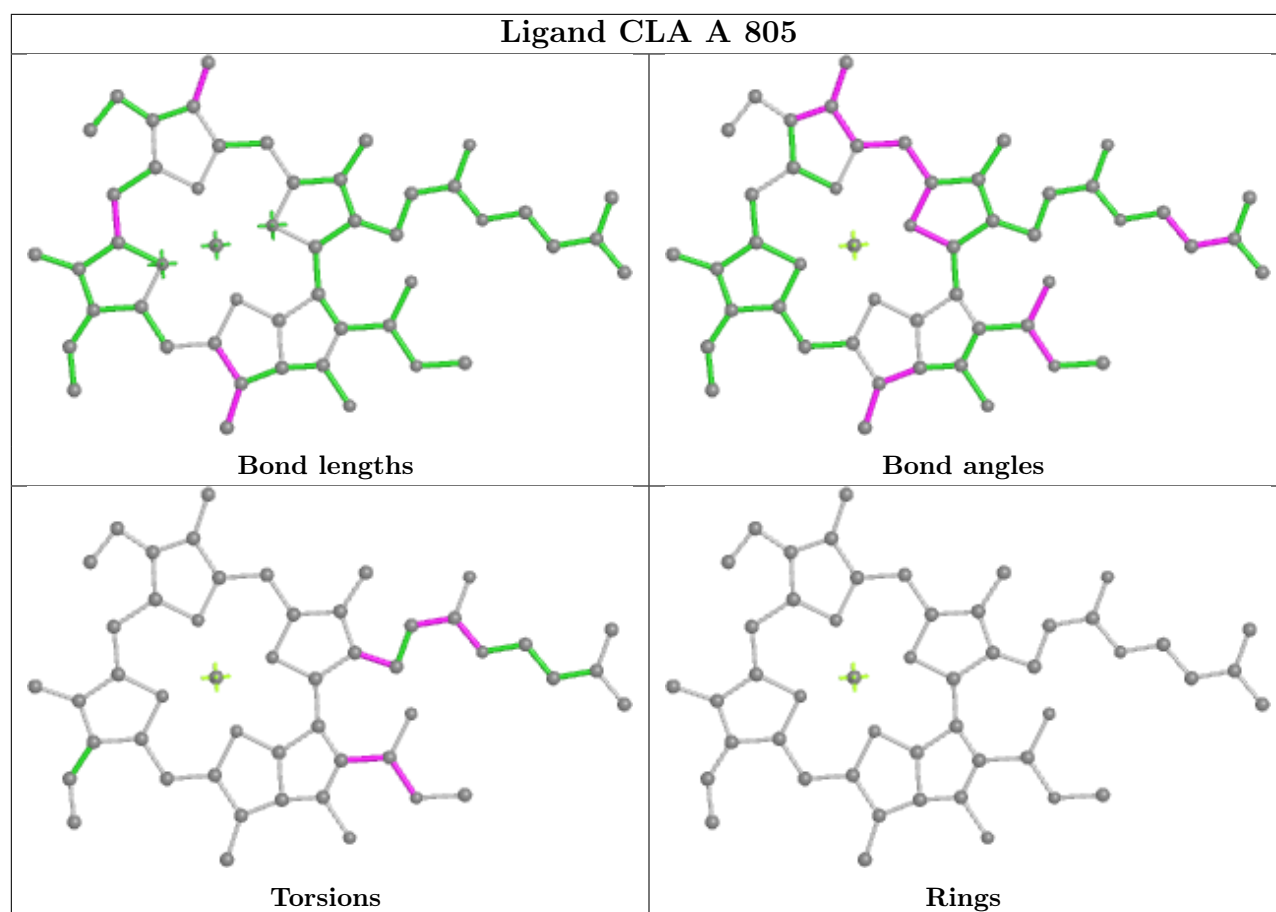
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

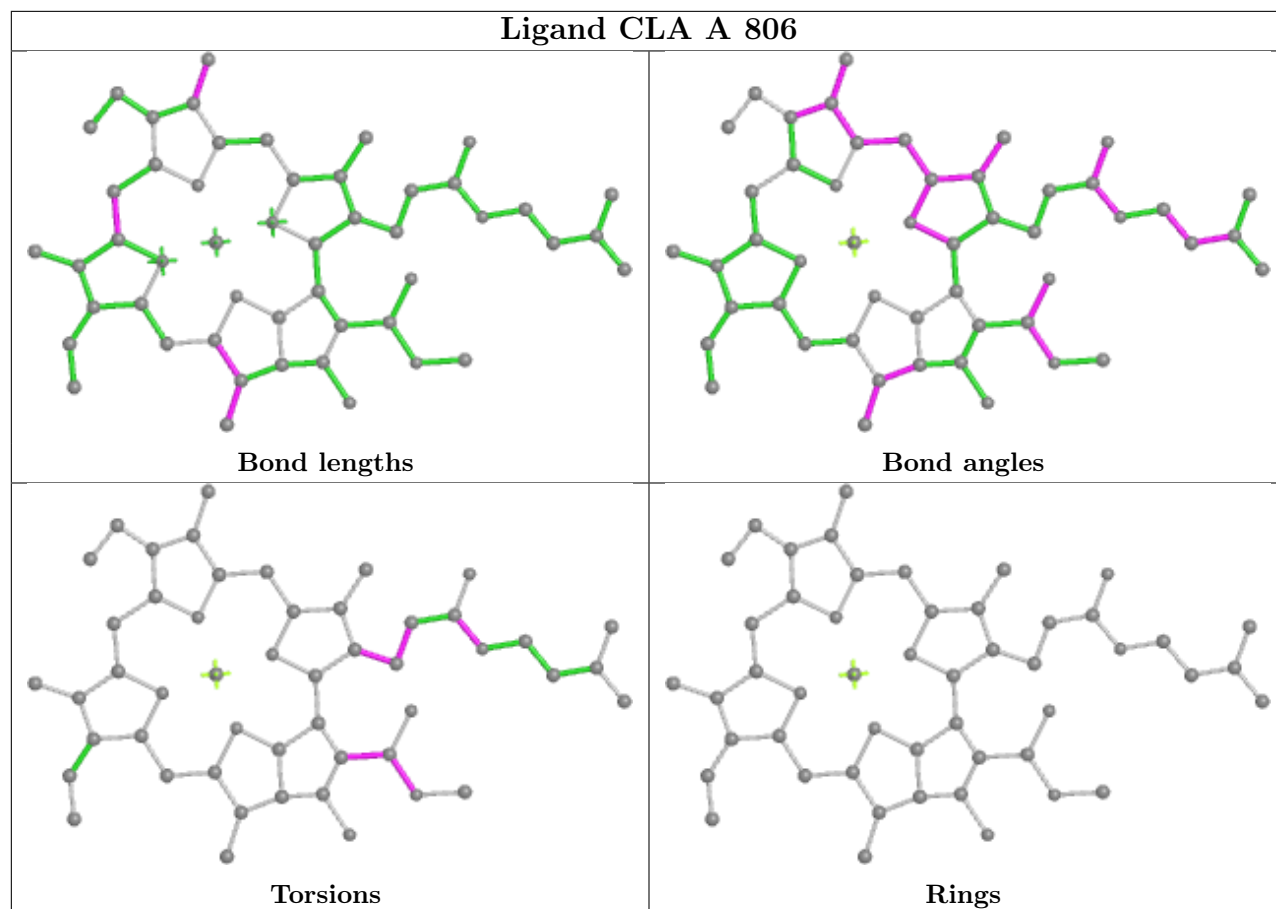


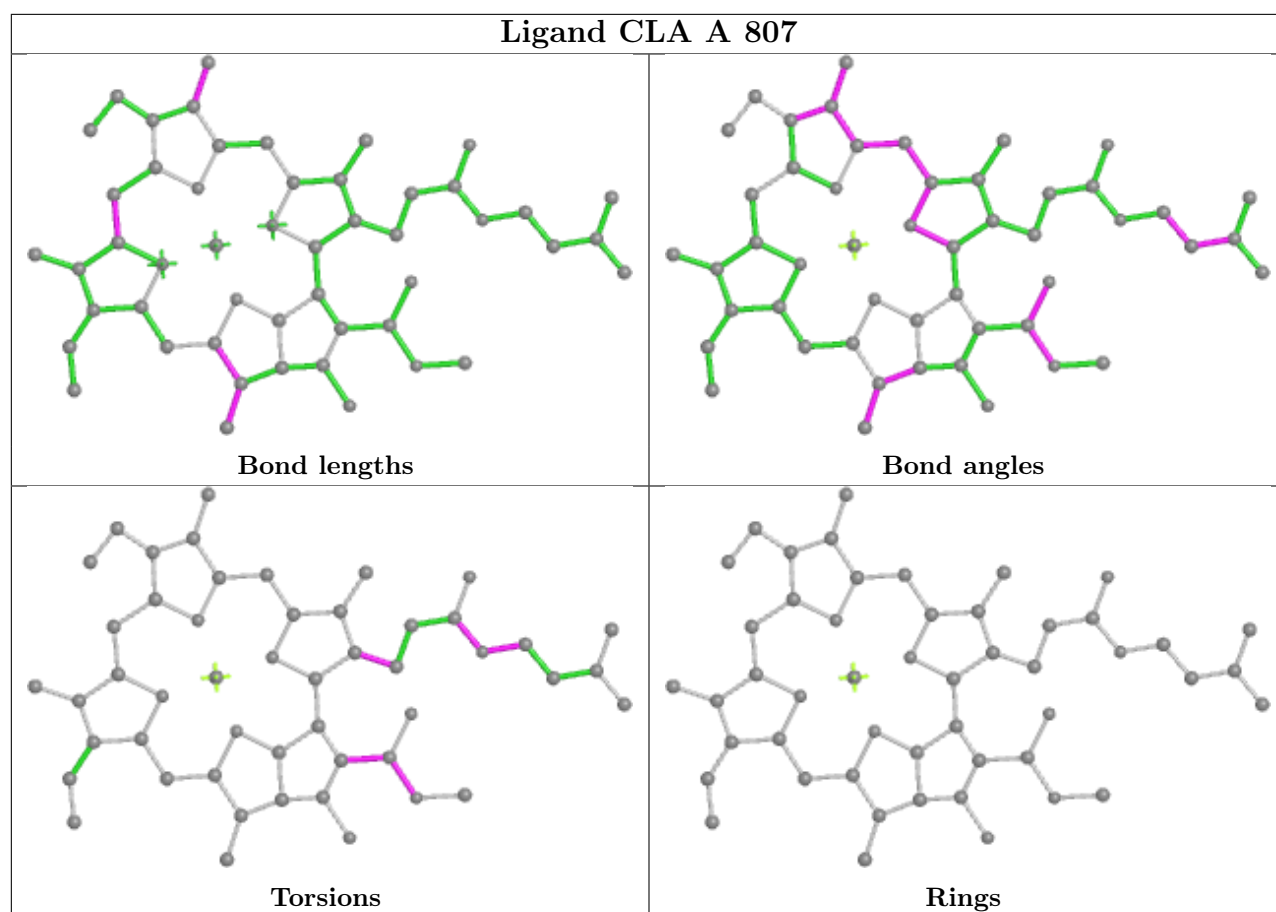




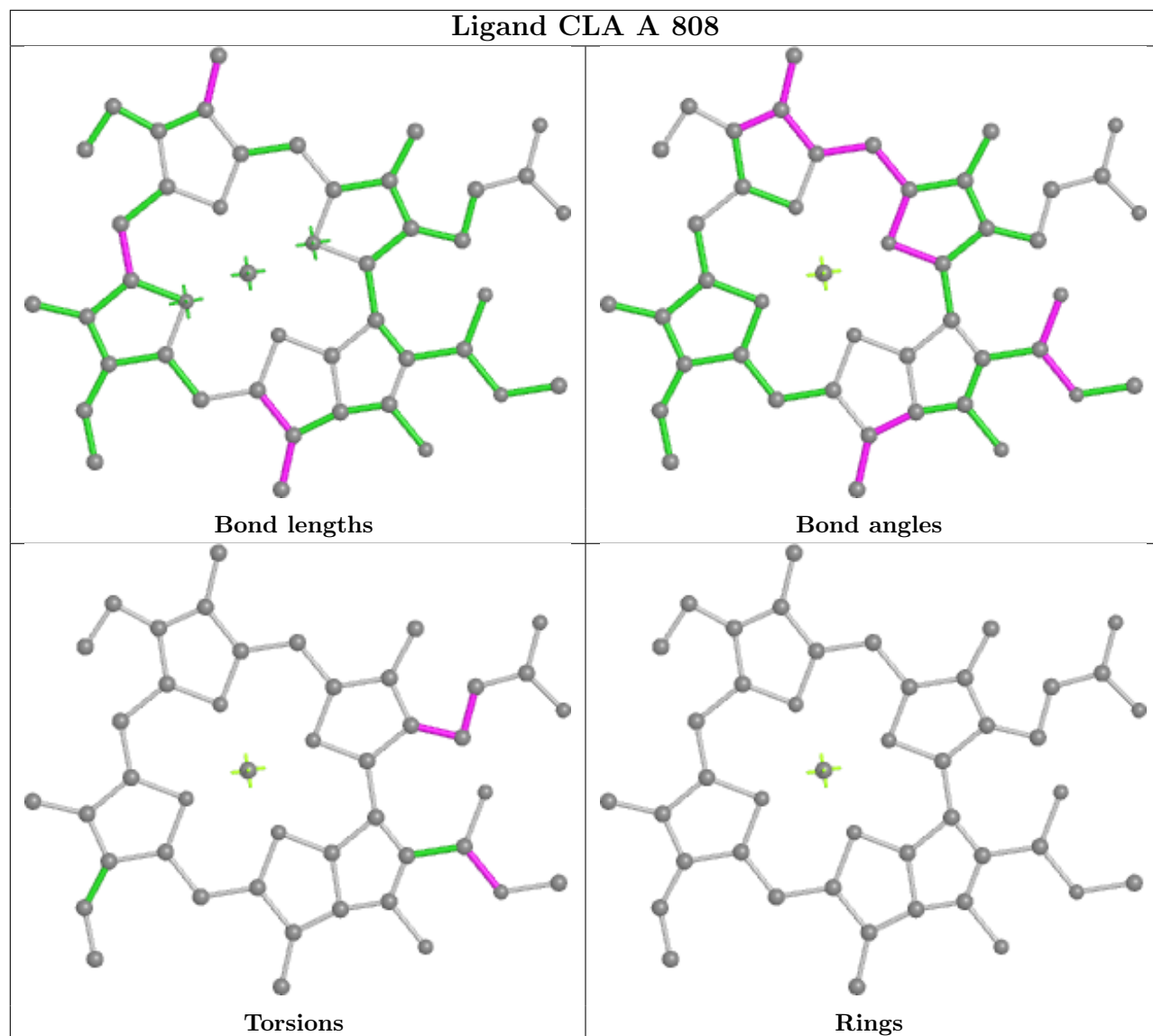


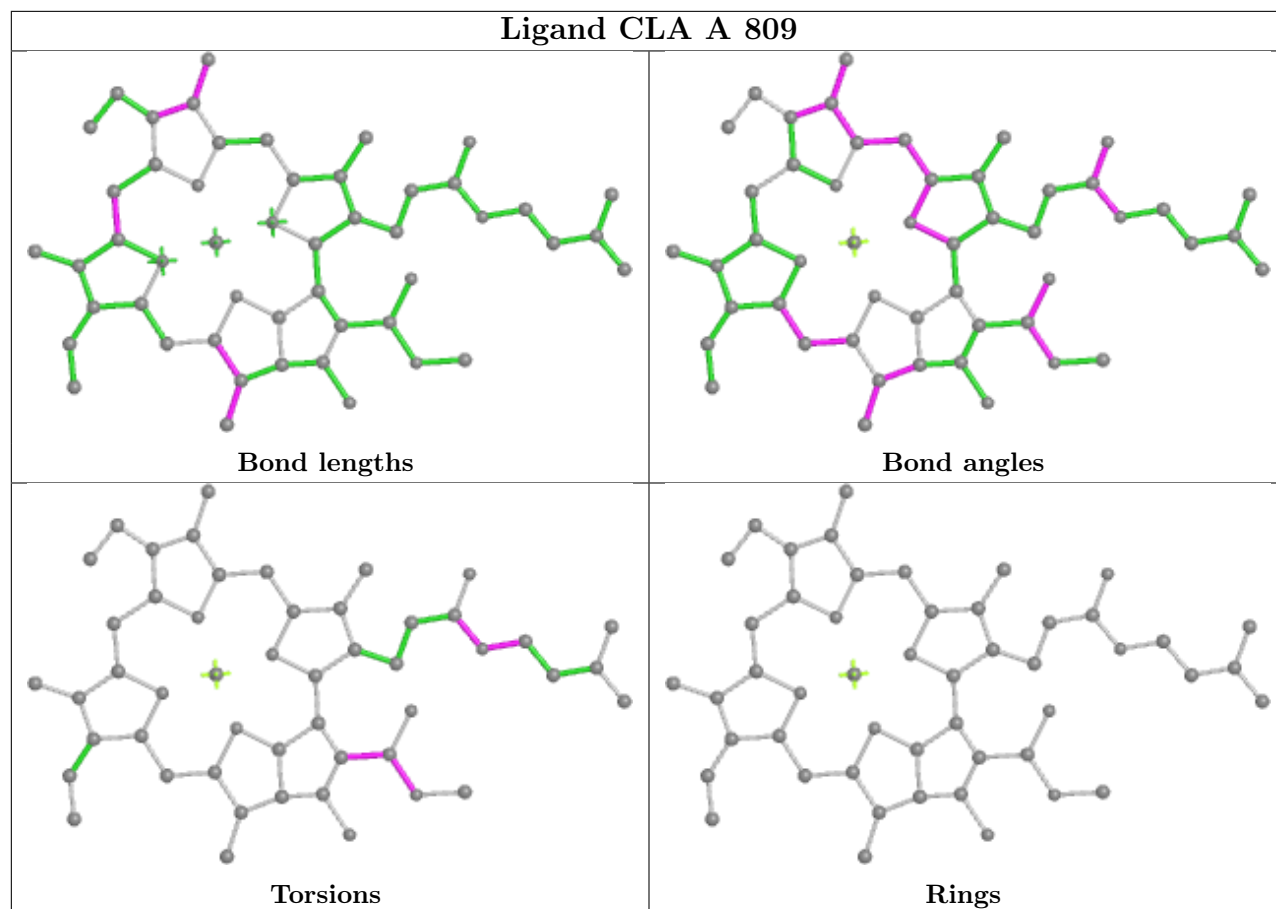


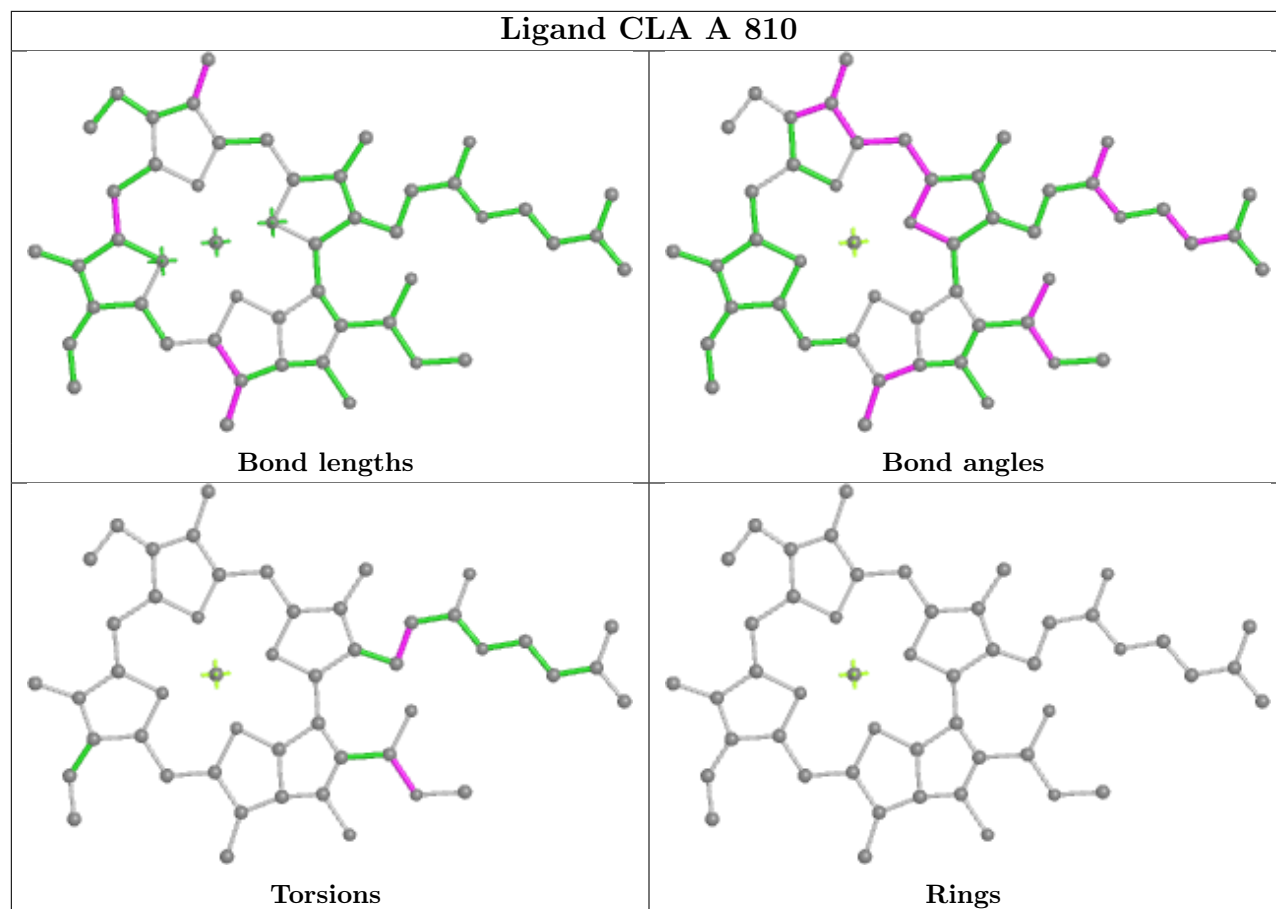


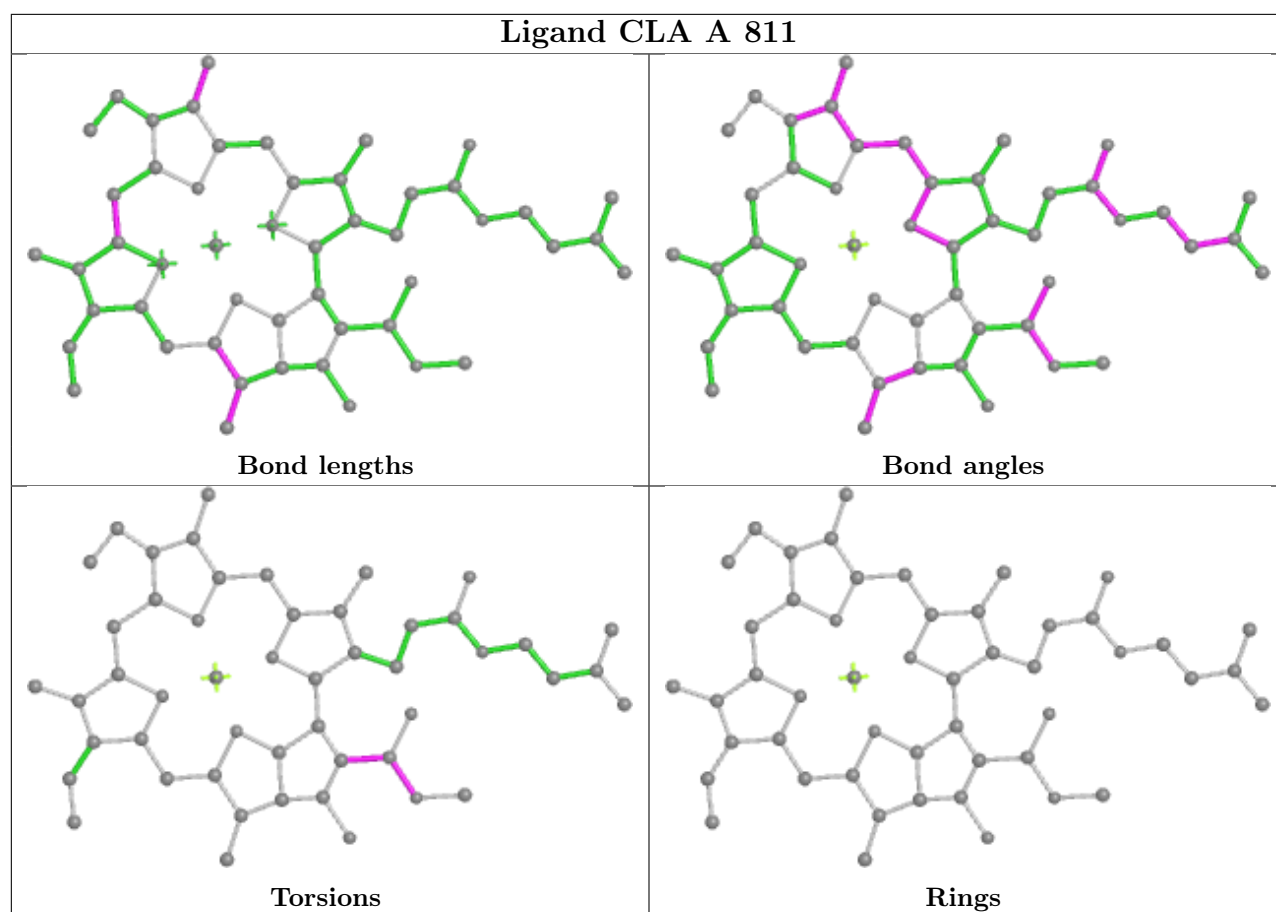


Ligand CLA A 808

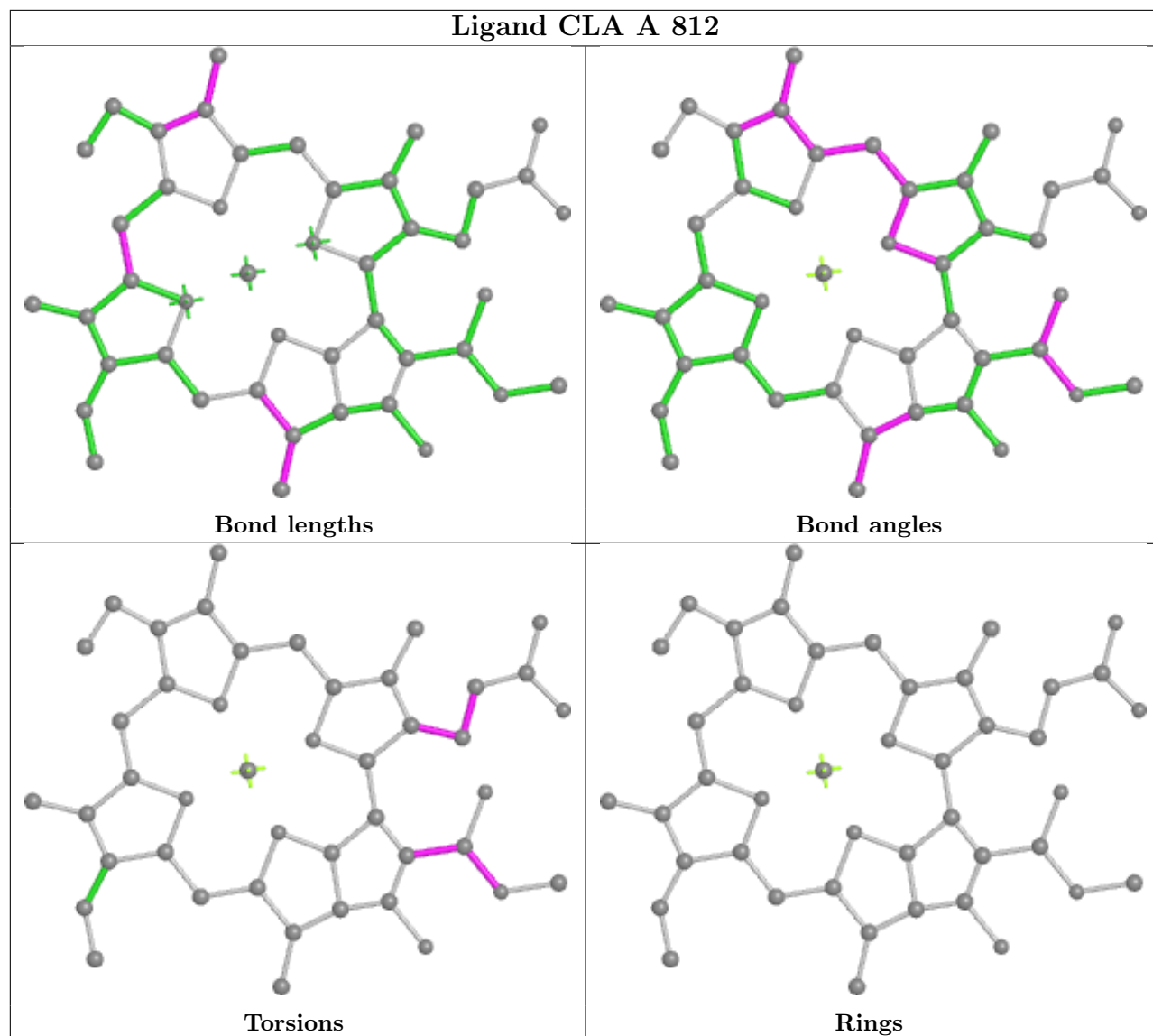




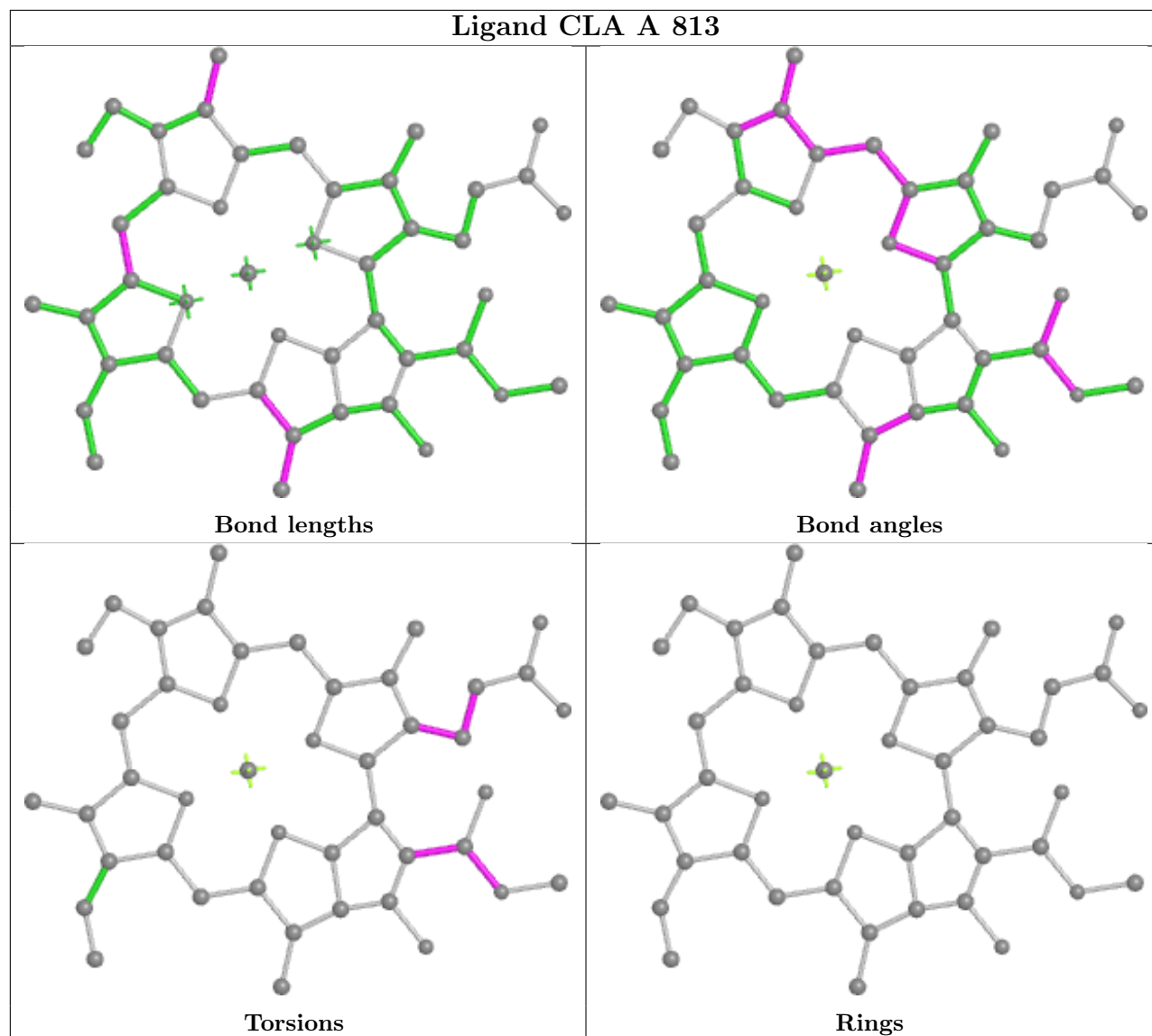


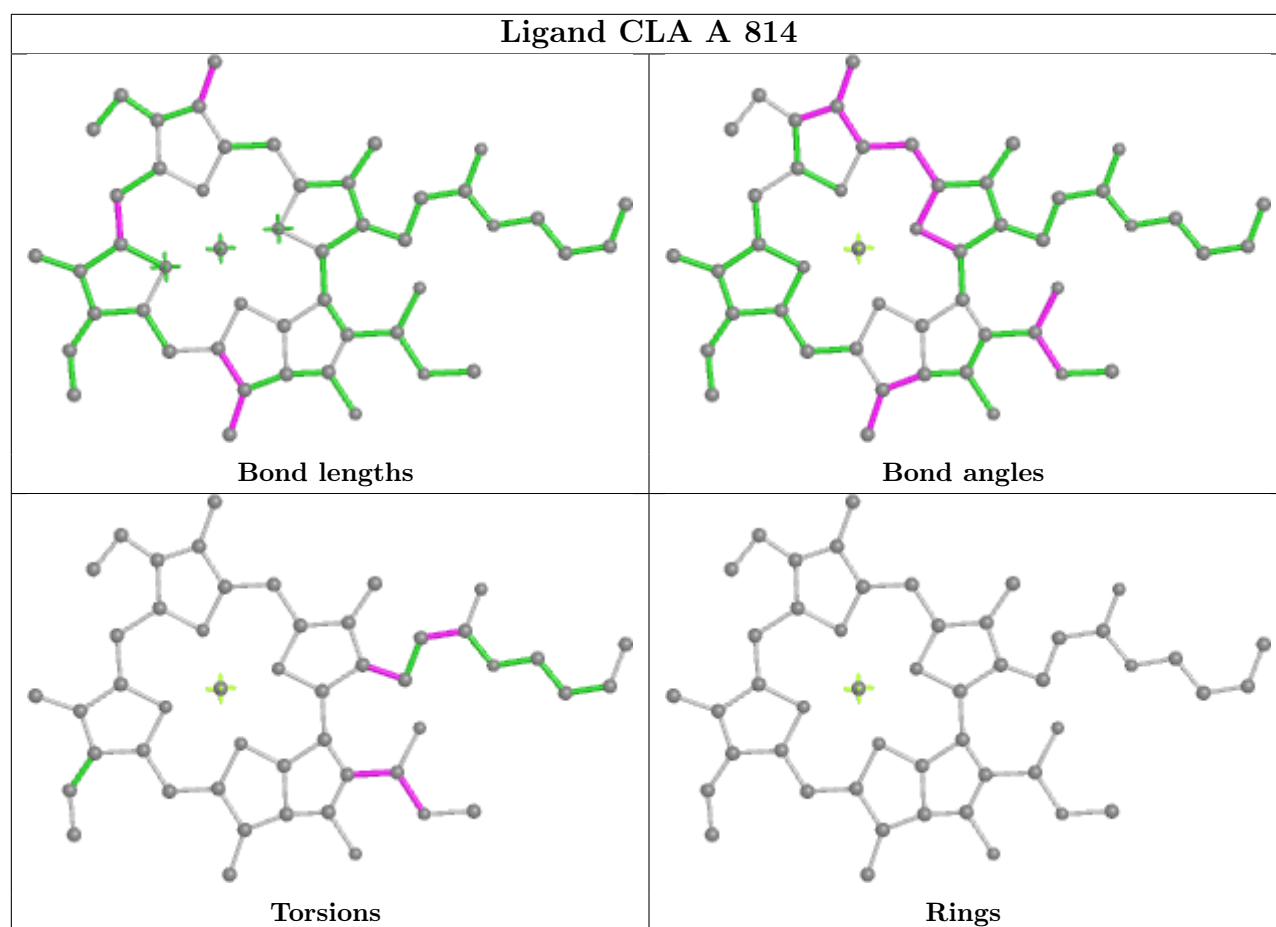


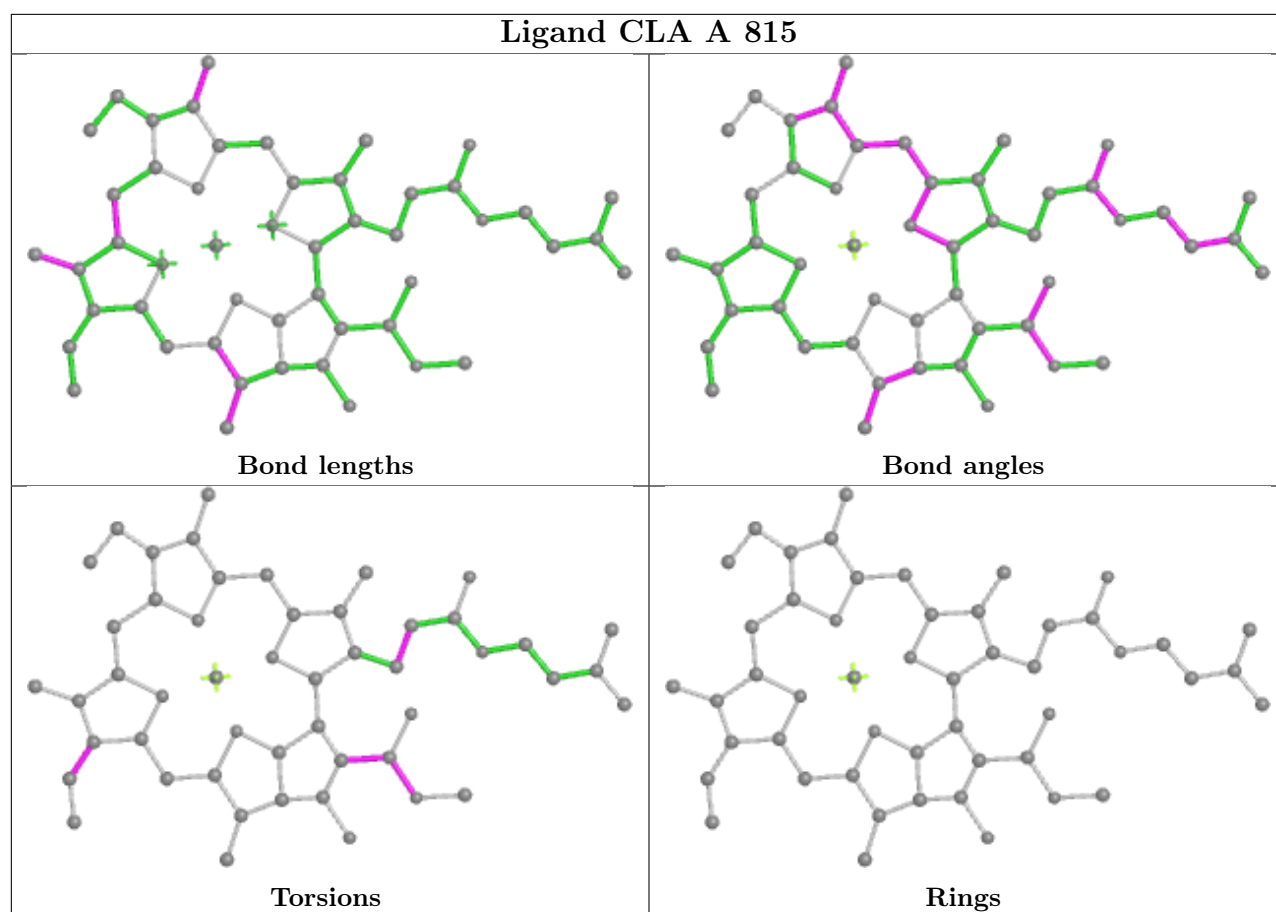
Ligand CLA A 812

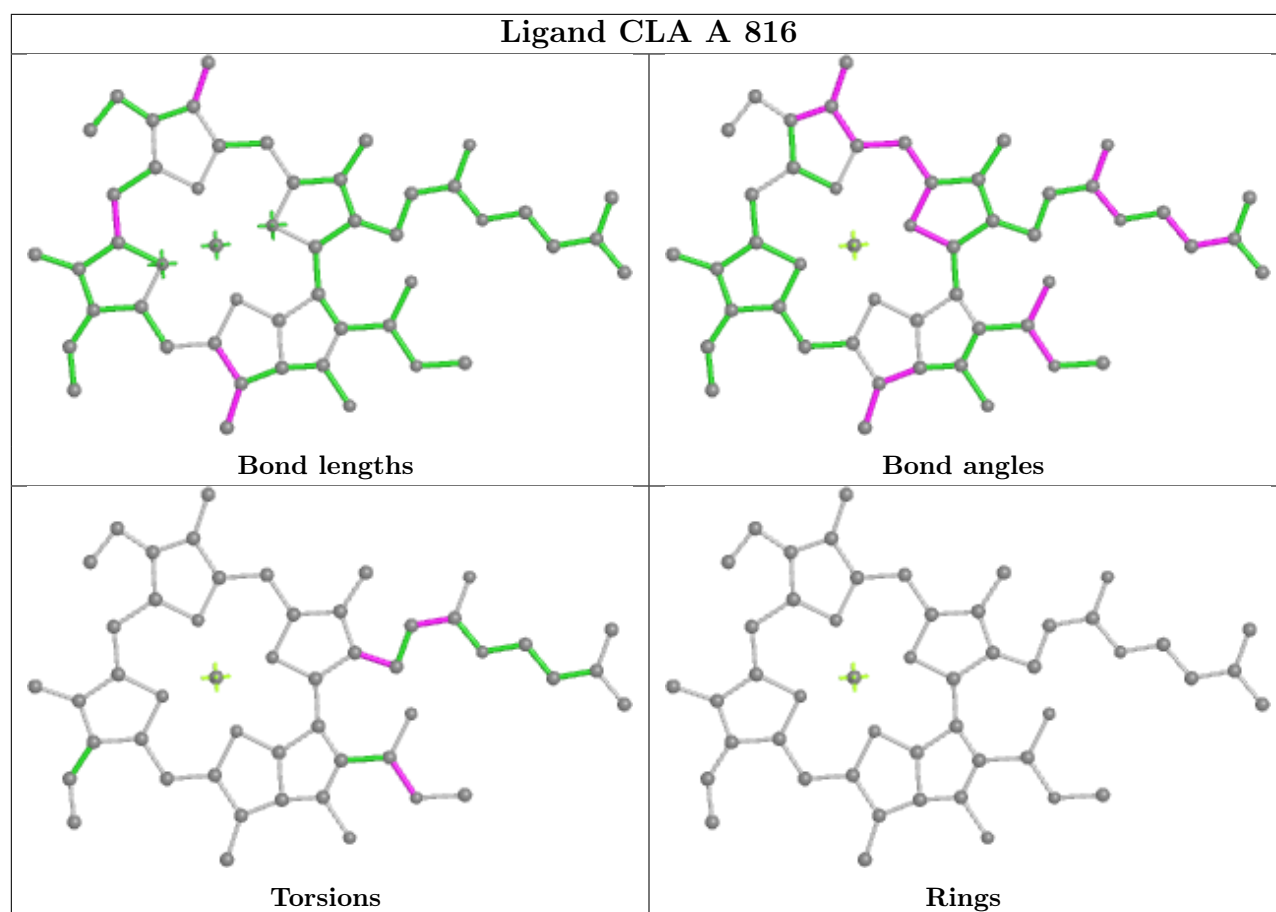


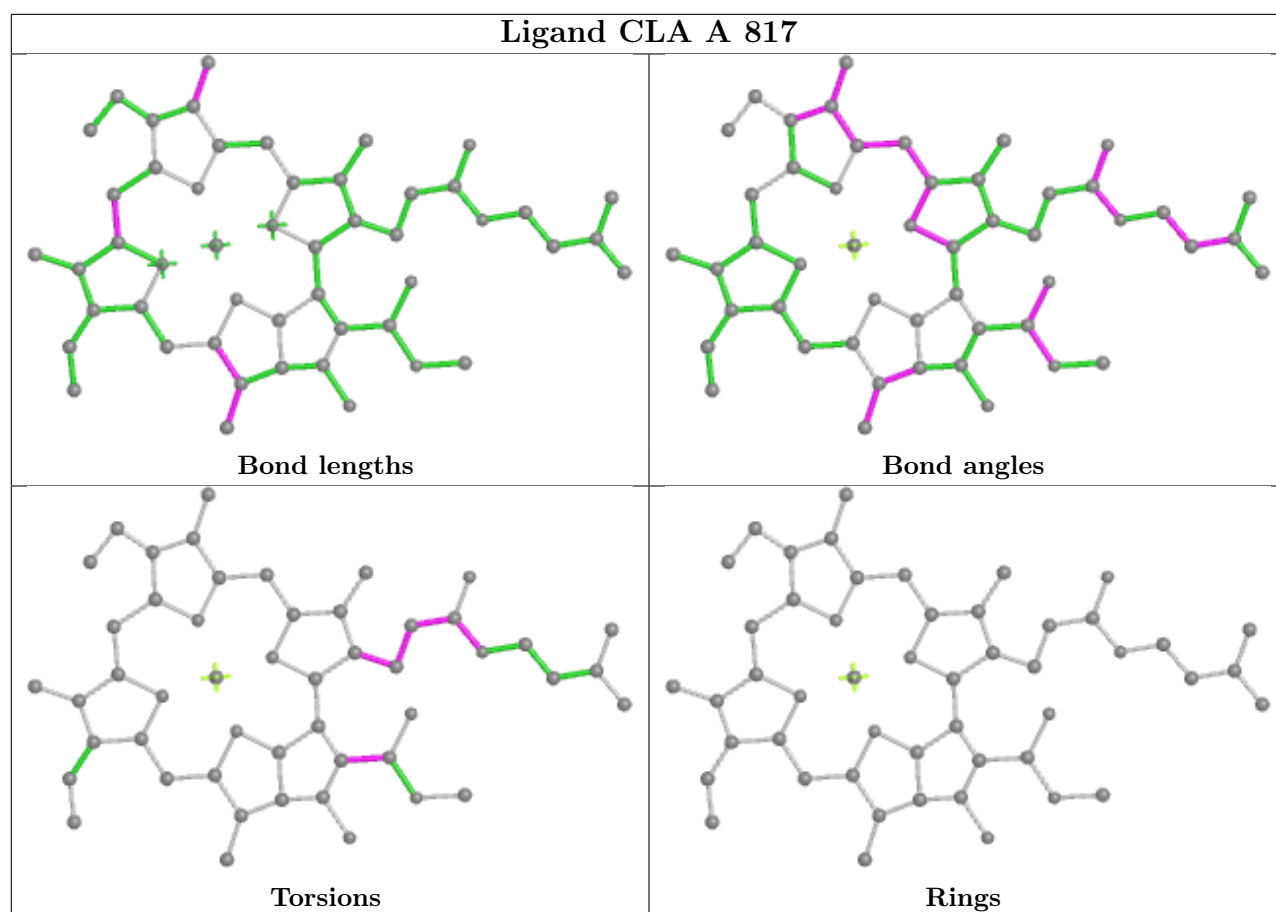
Ligand CLA A 813

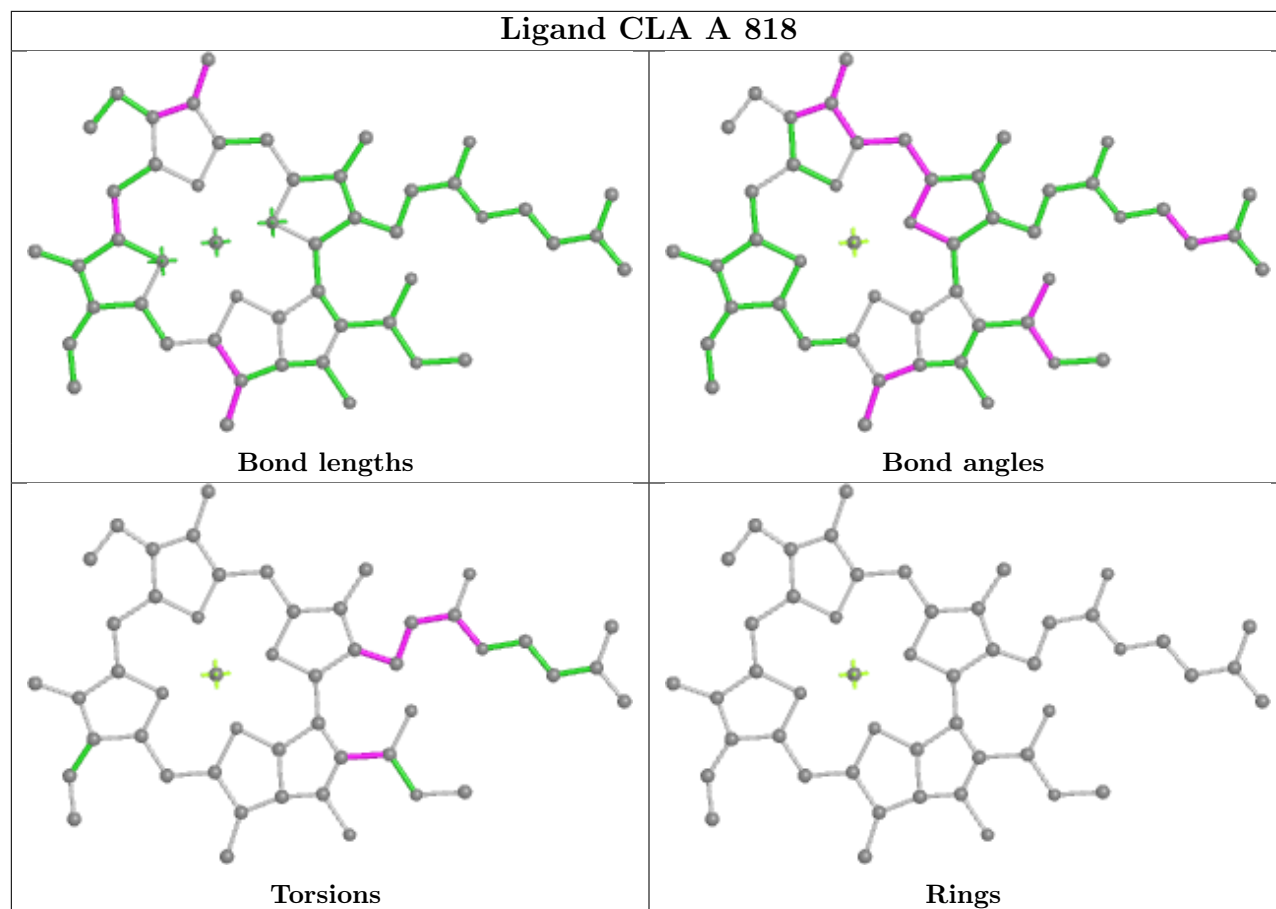


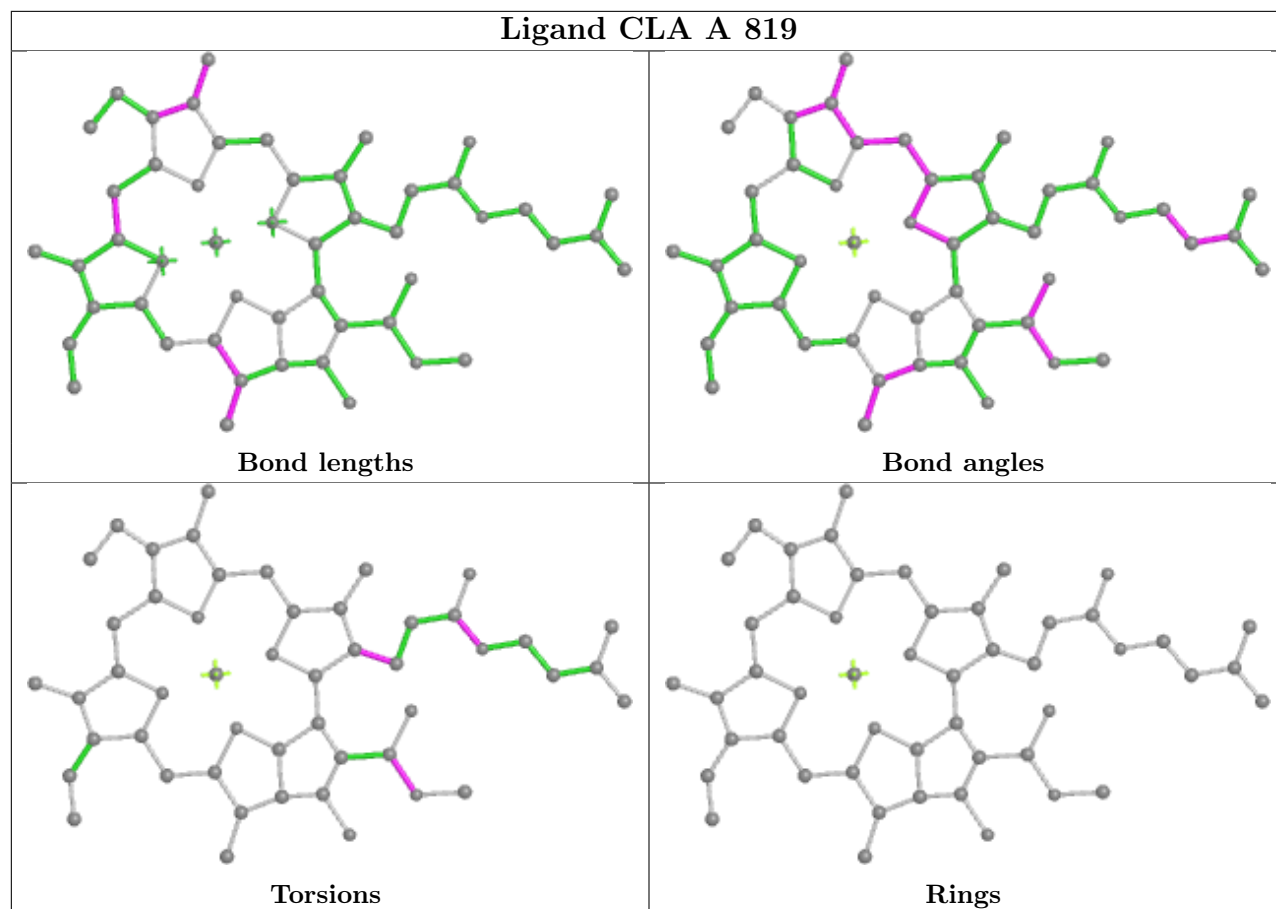


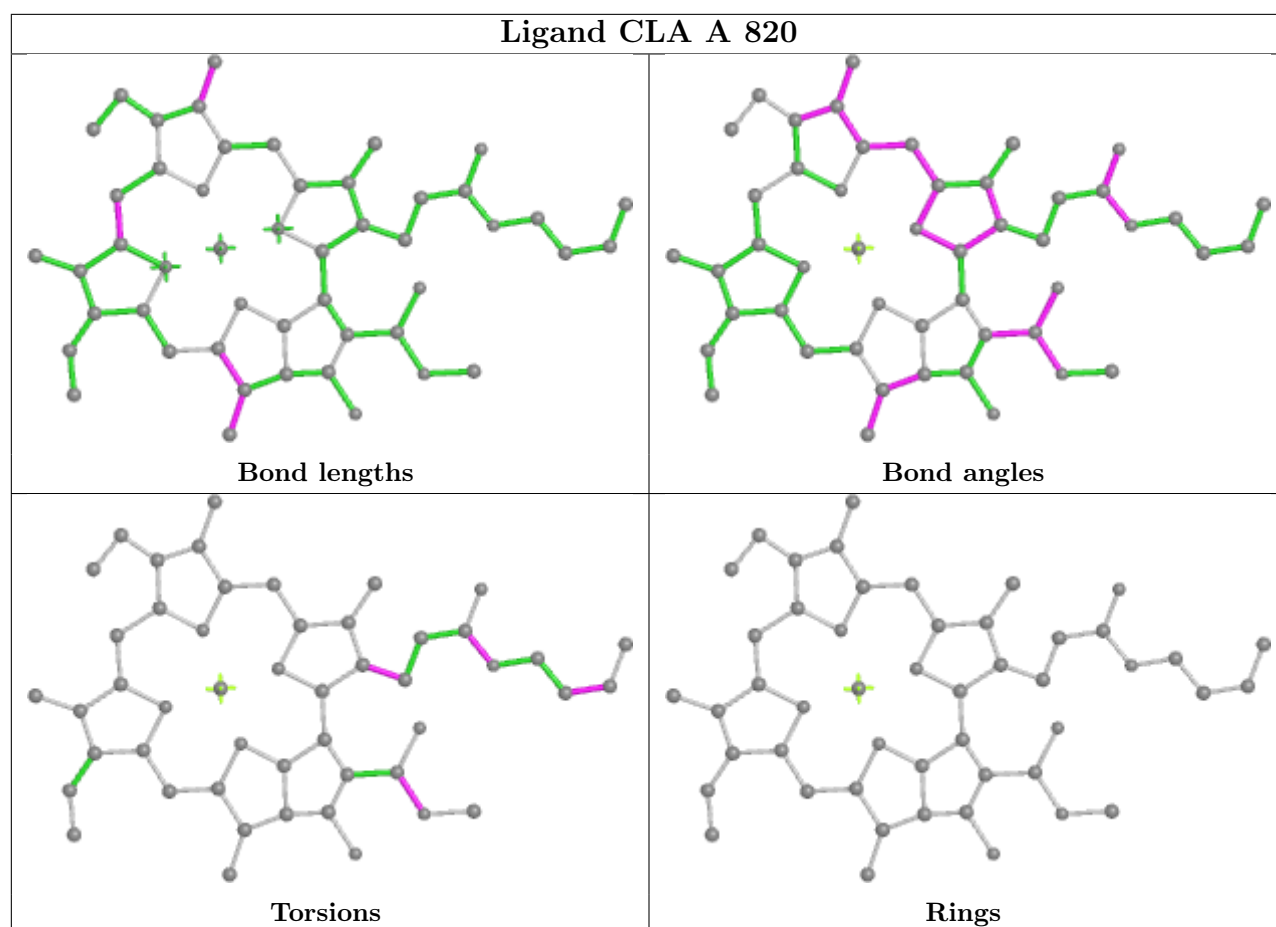


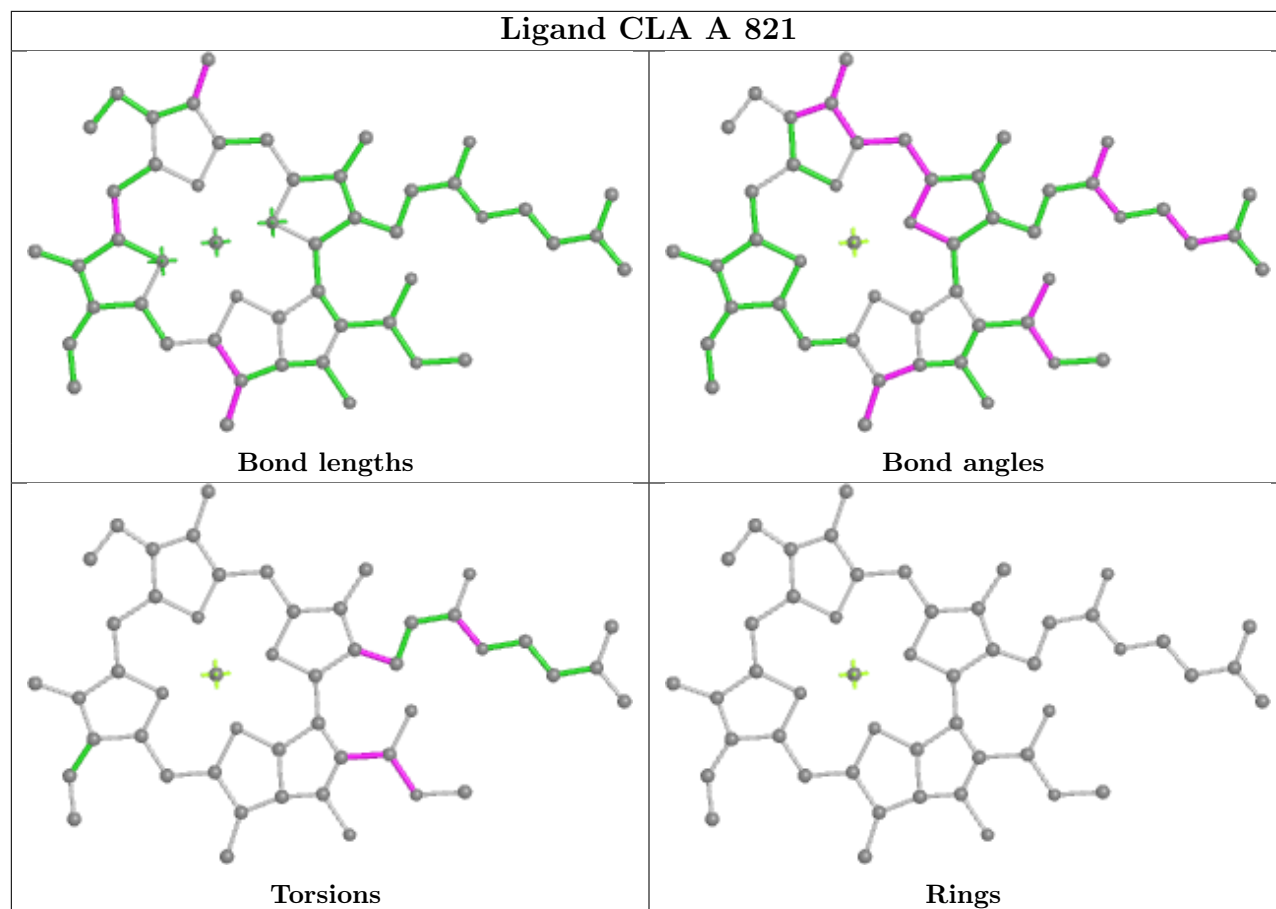


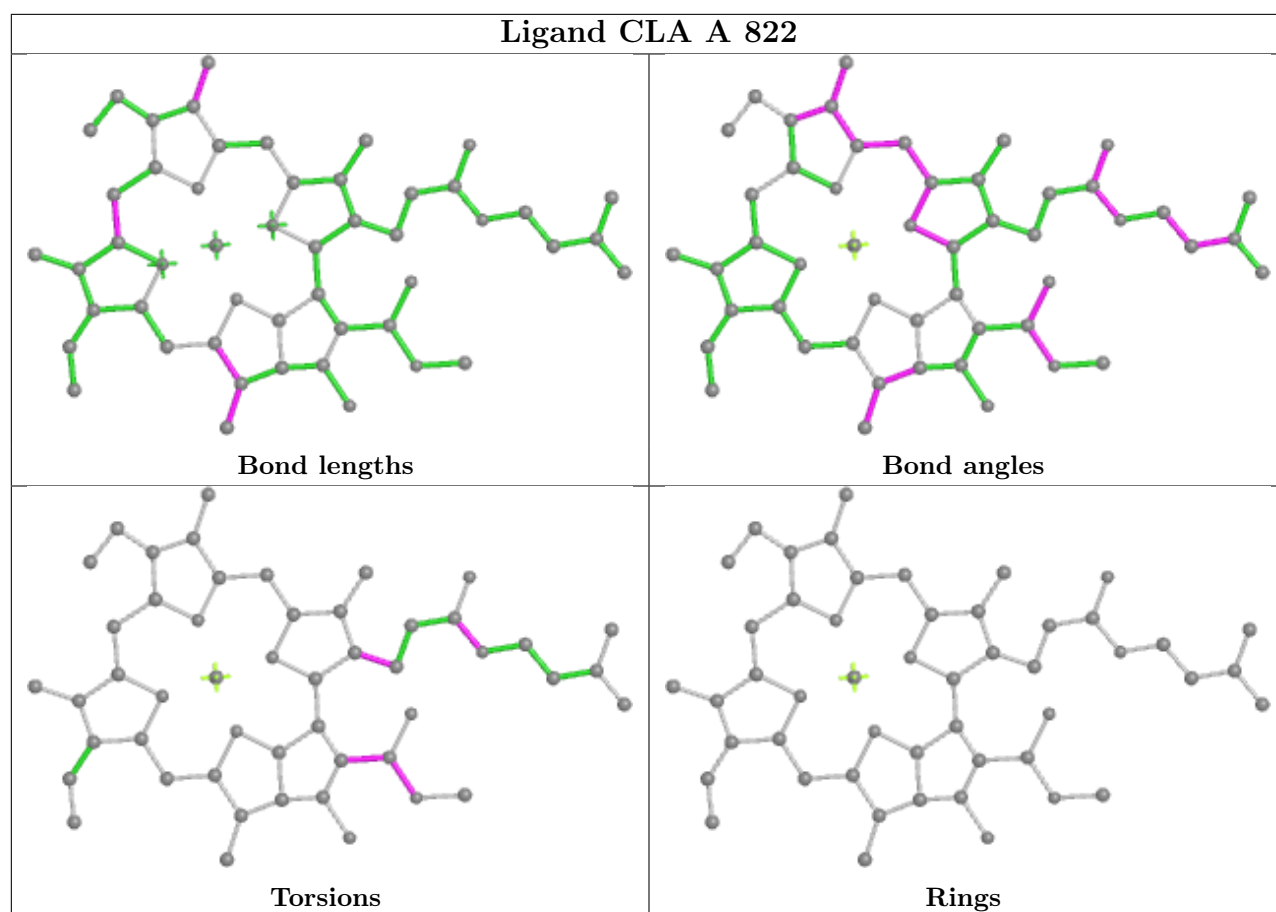


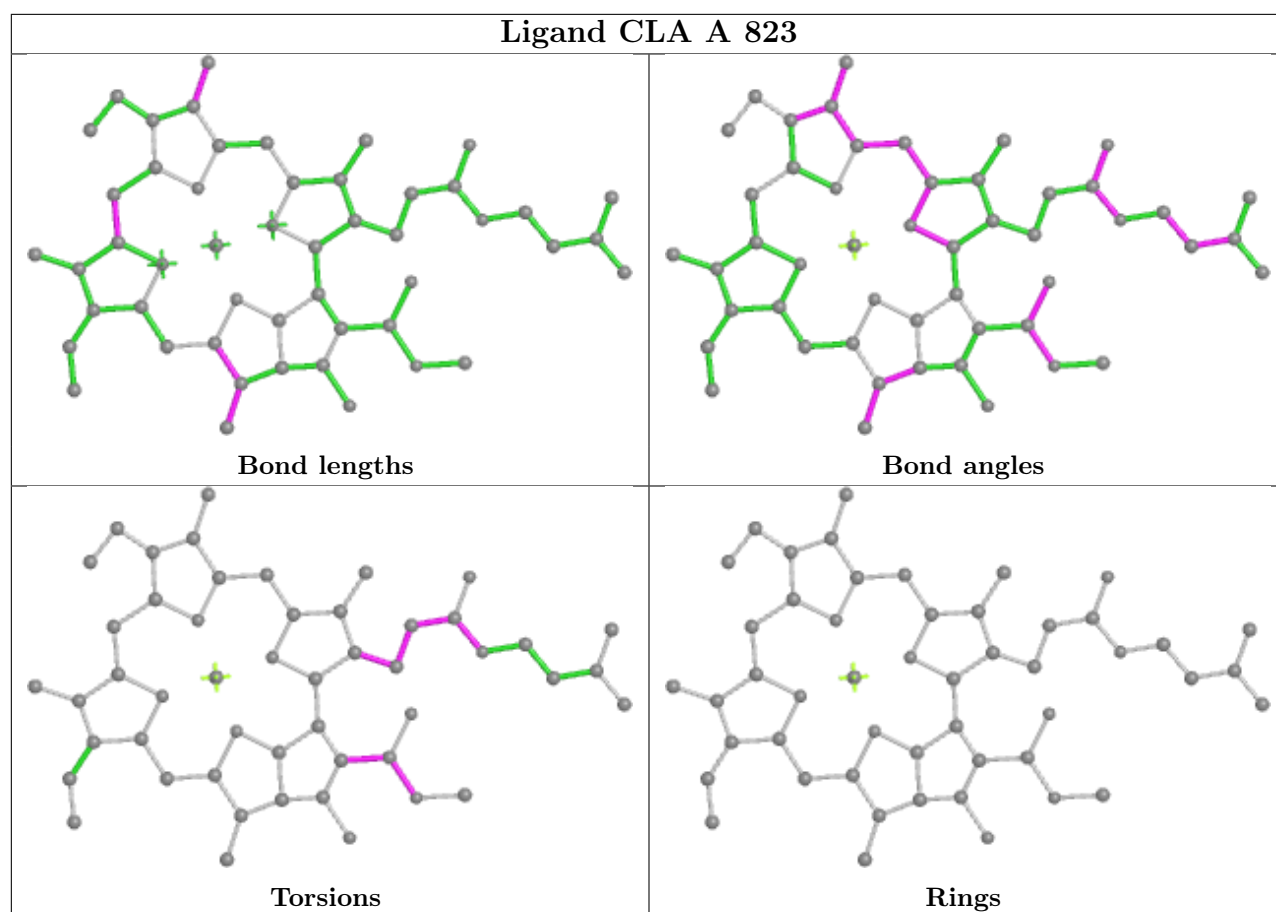


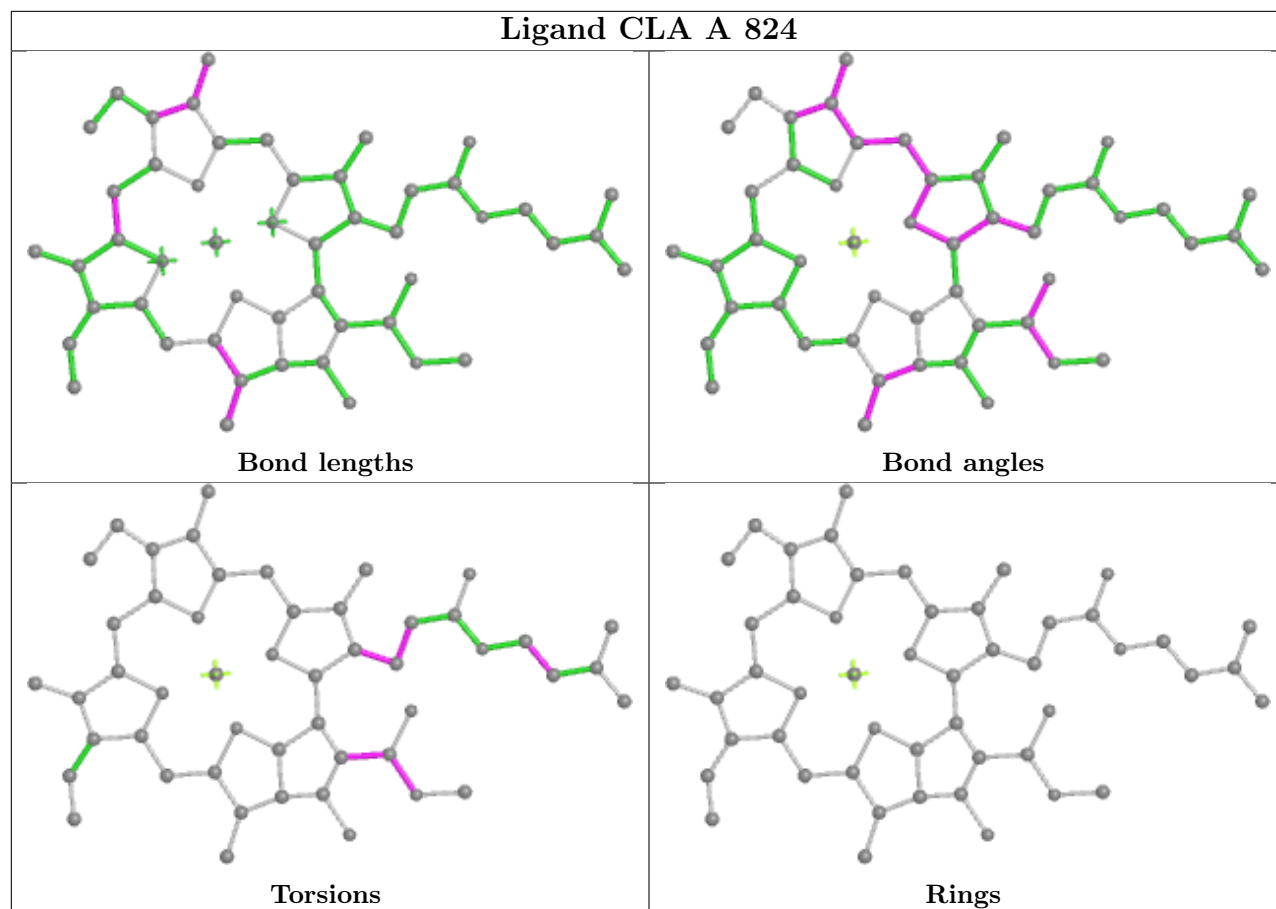


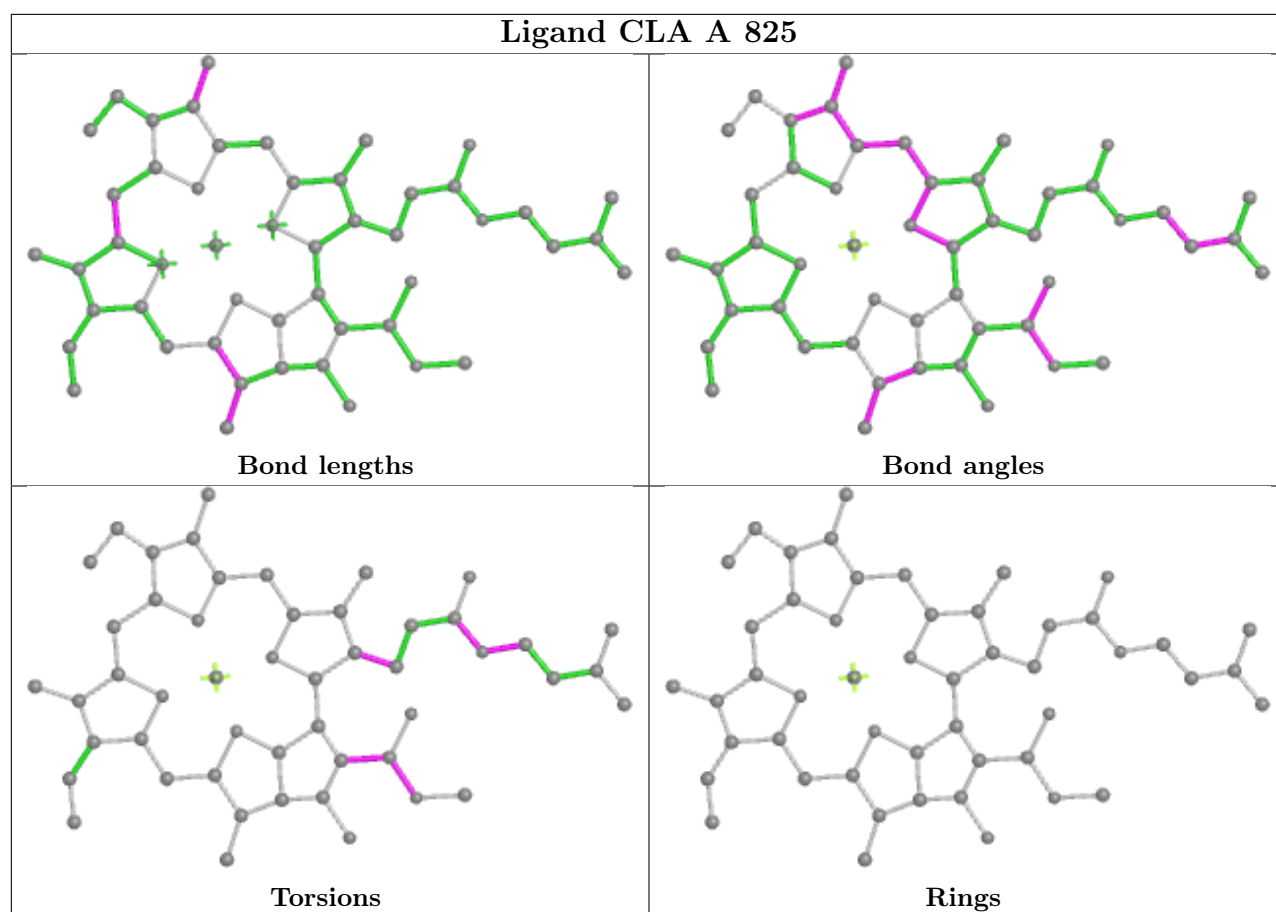


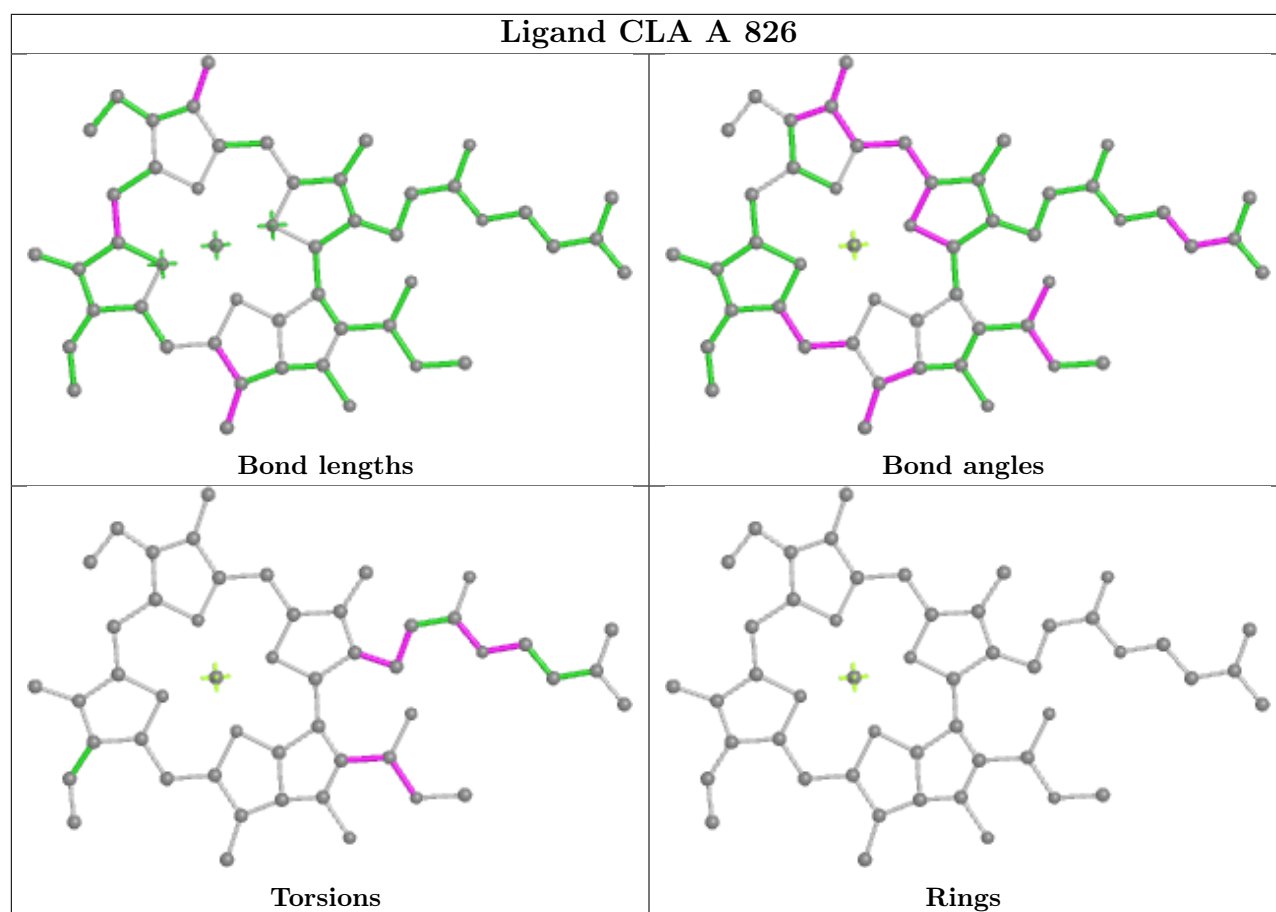


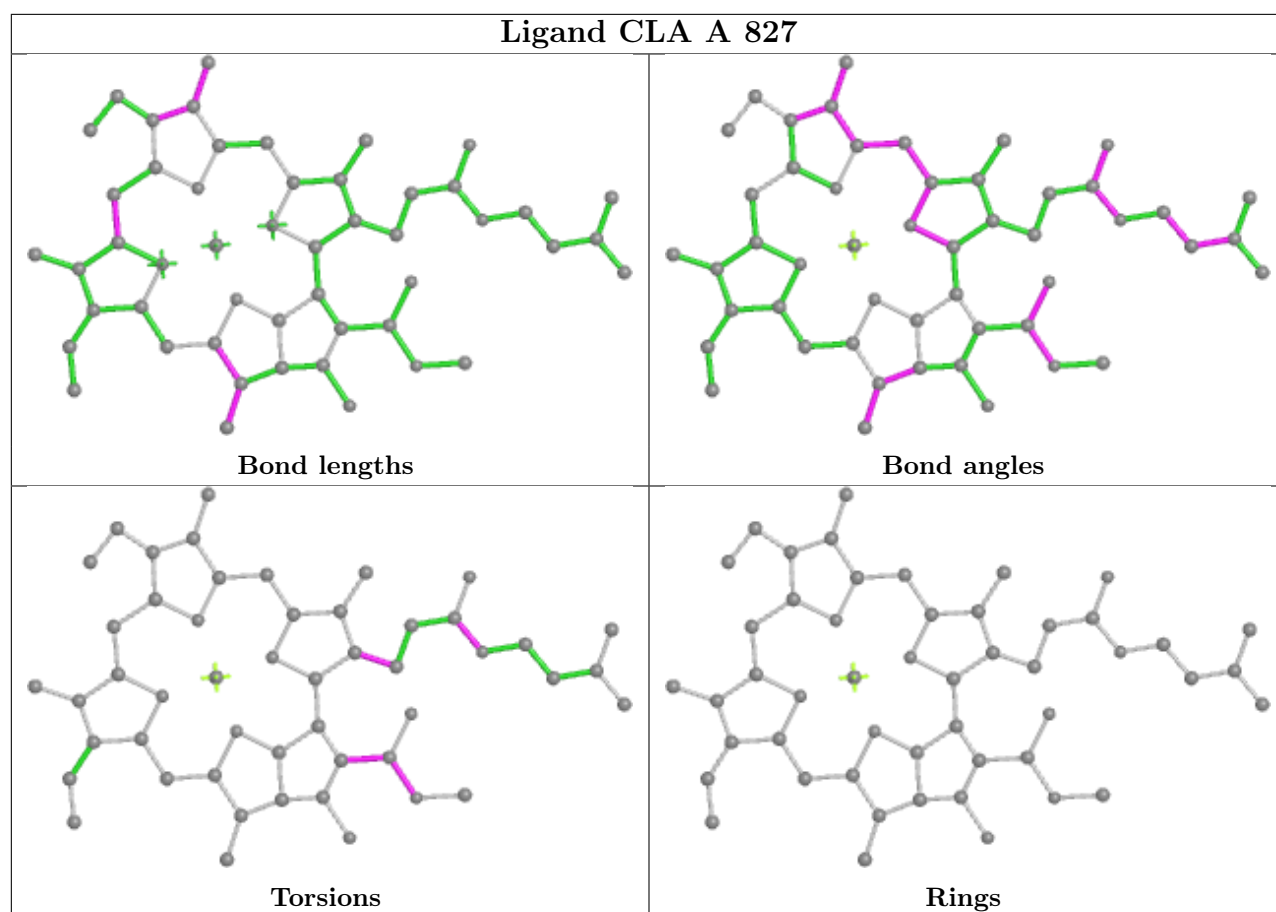


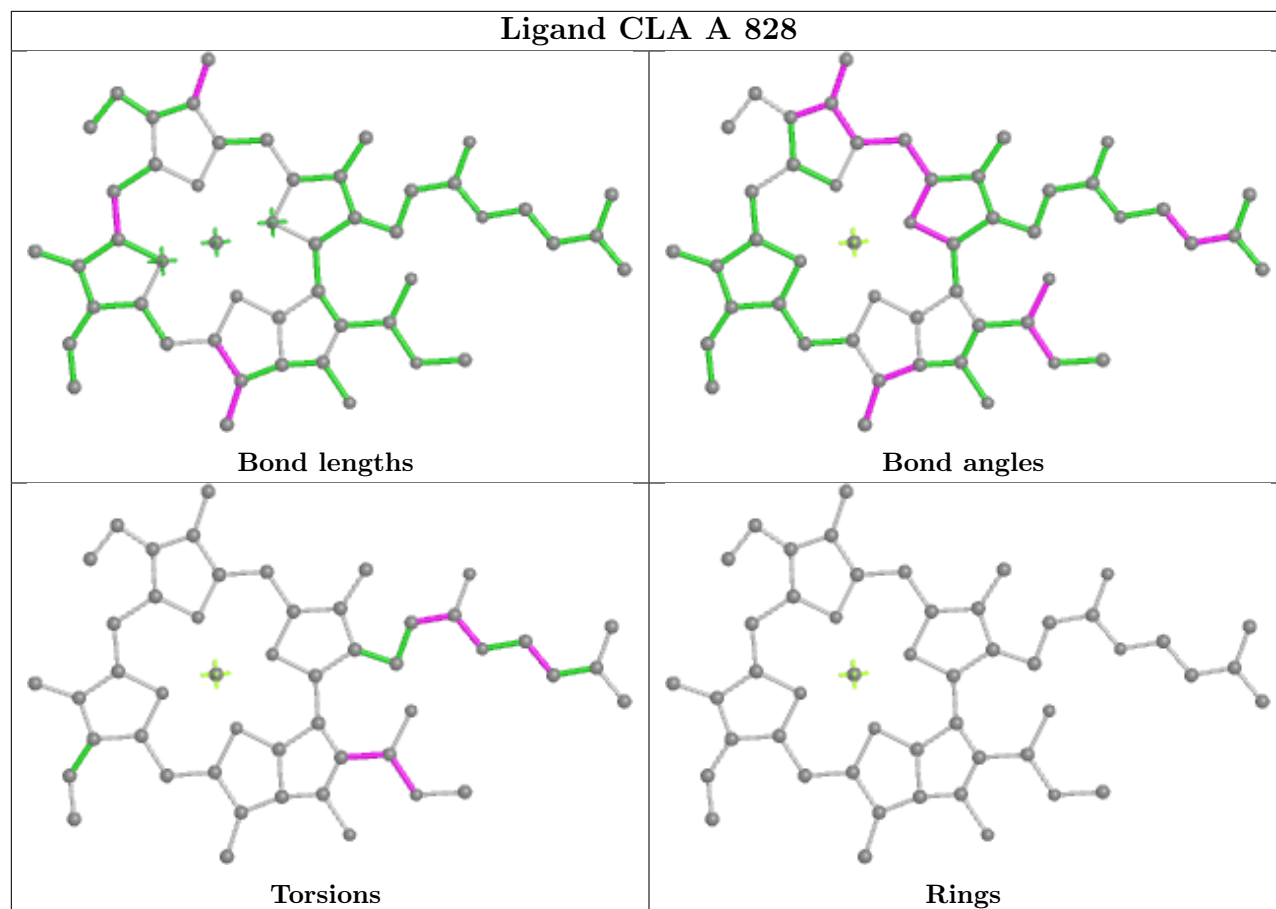


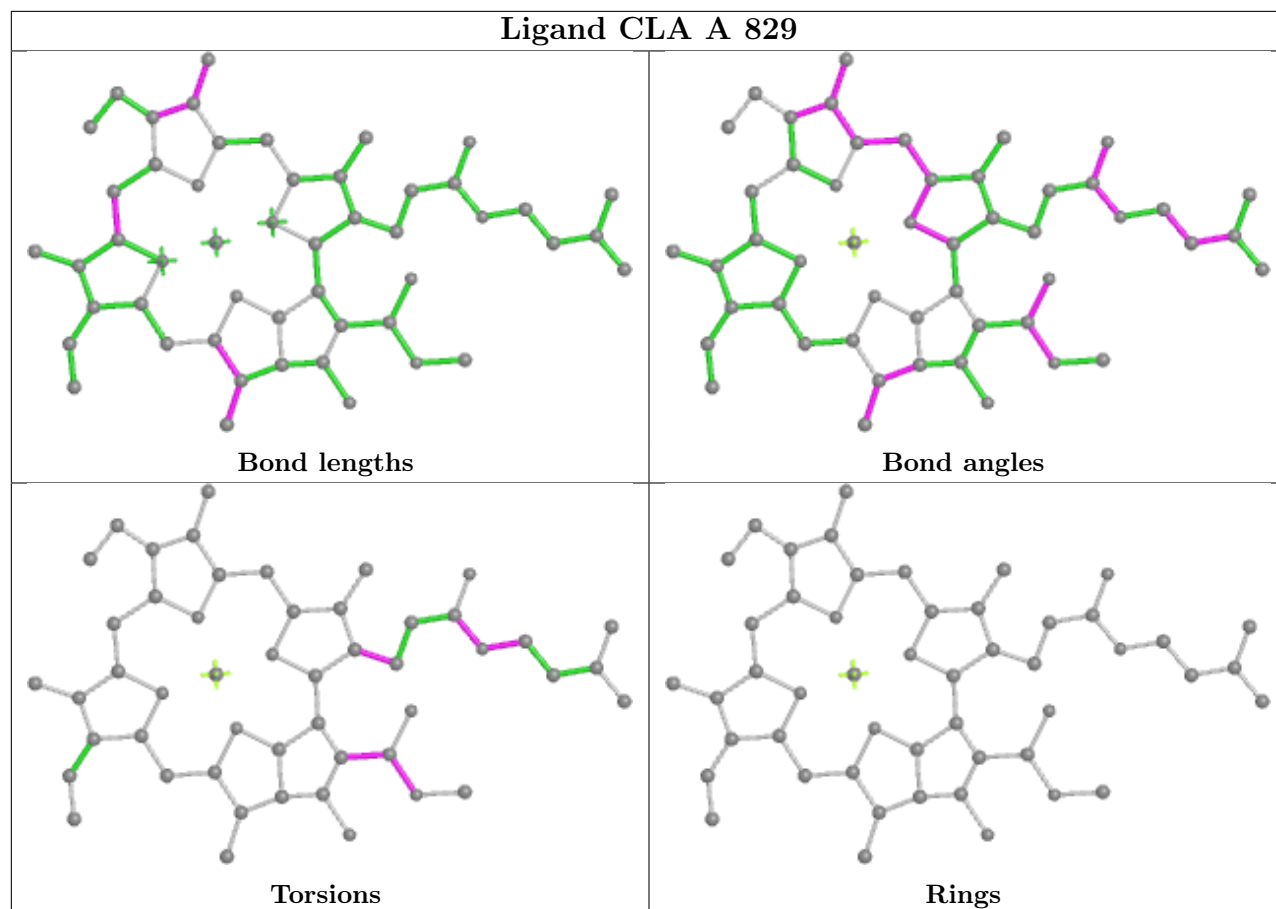


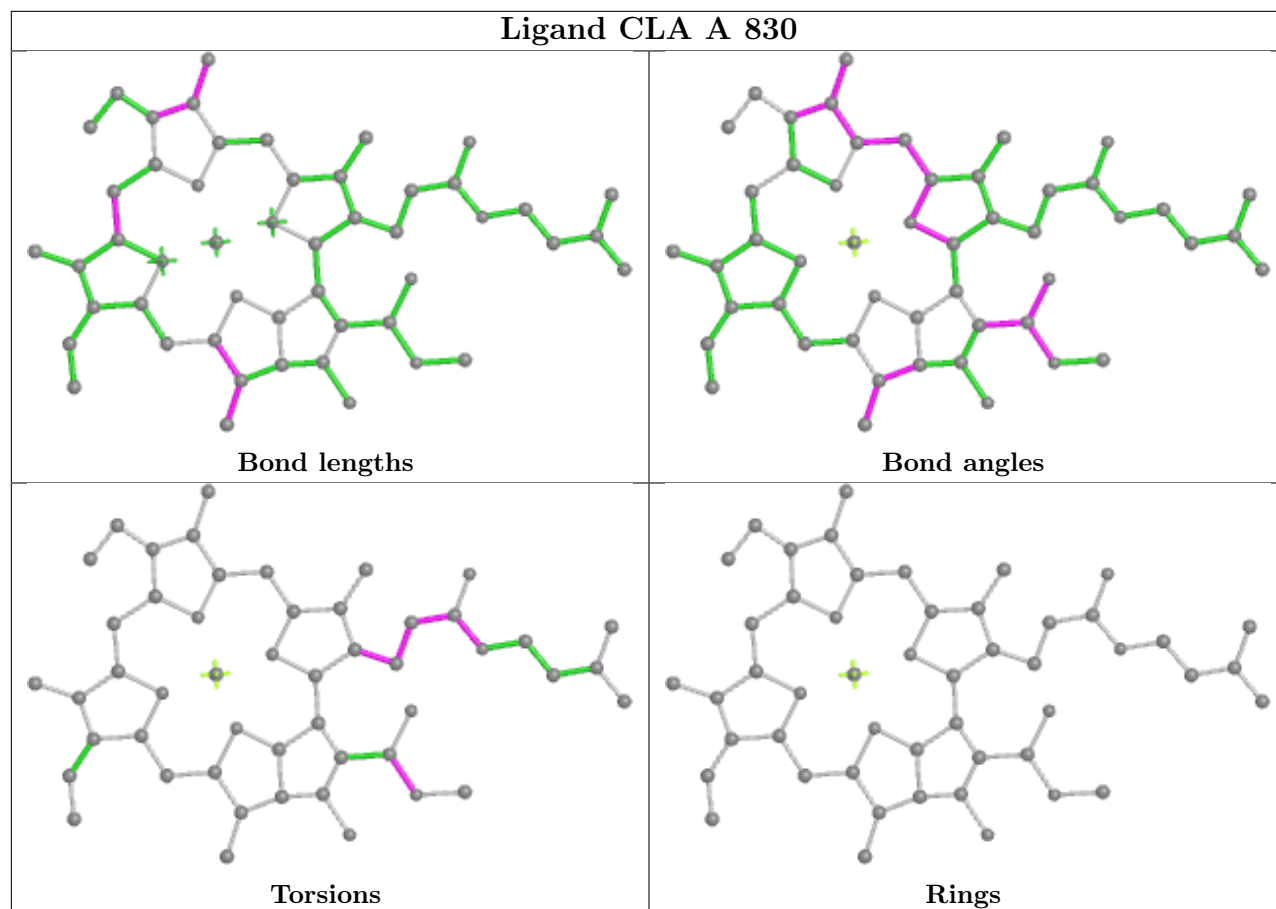


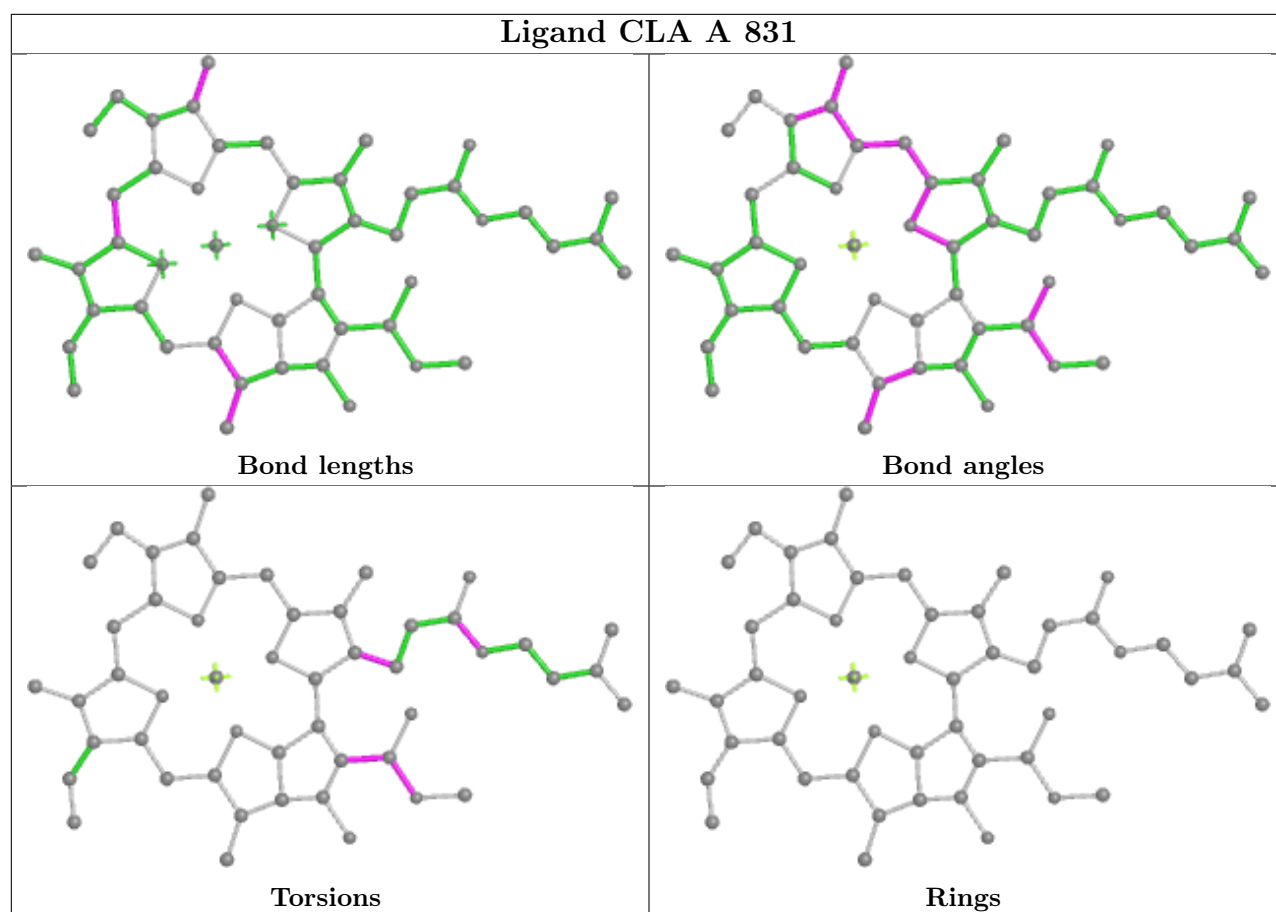


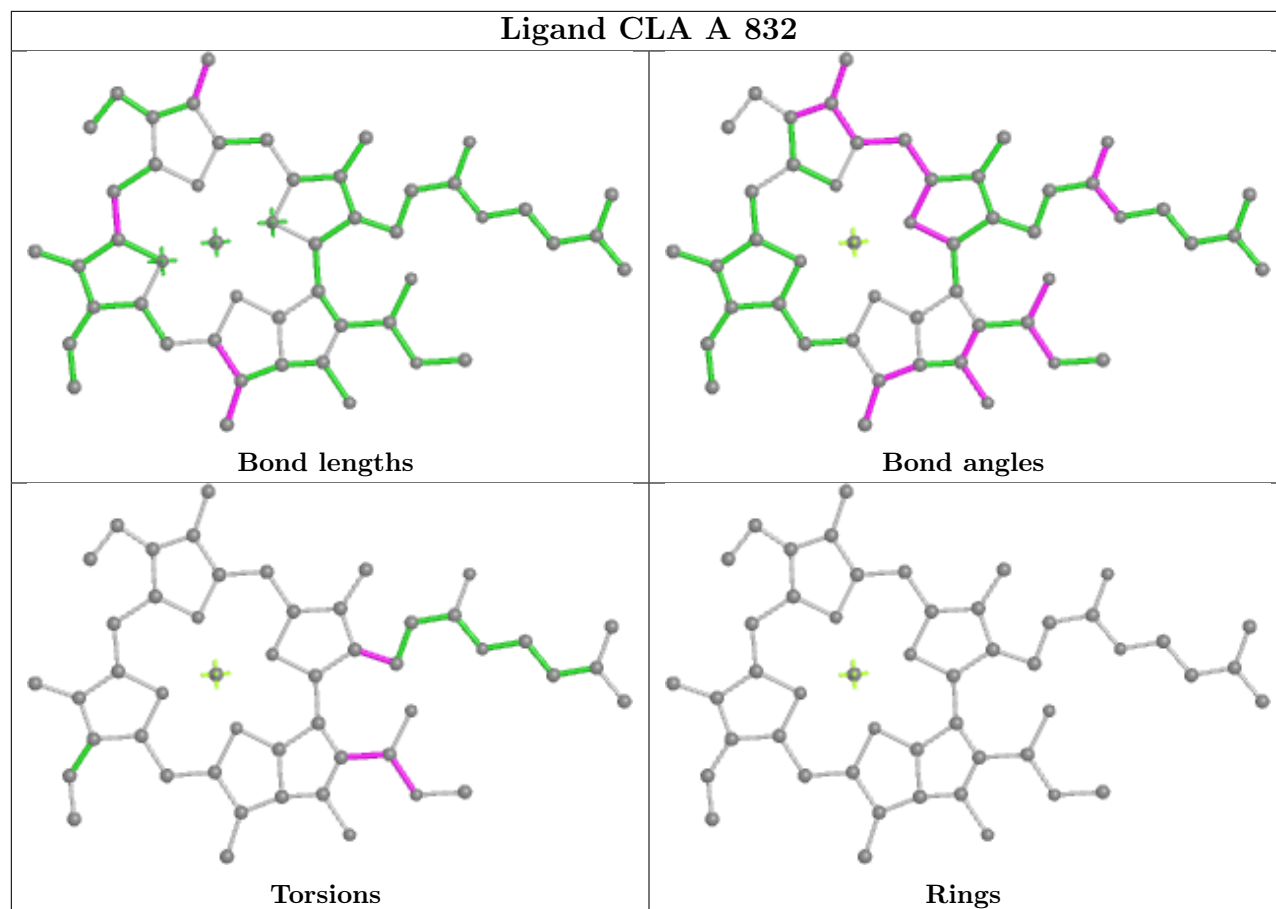




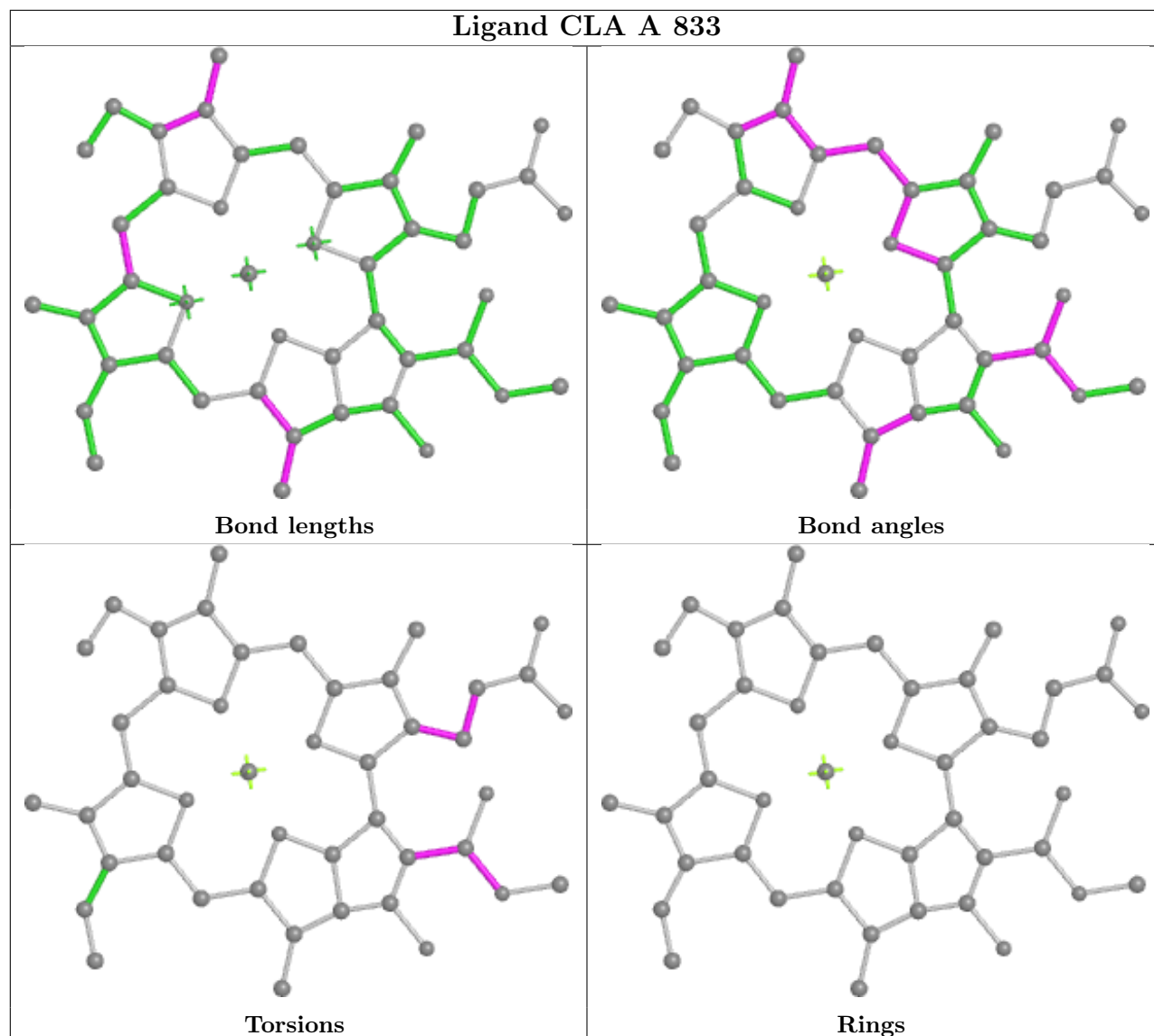


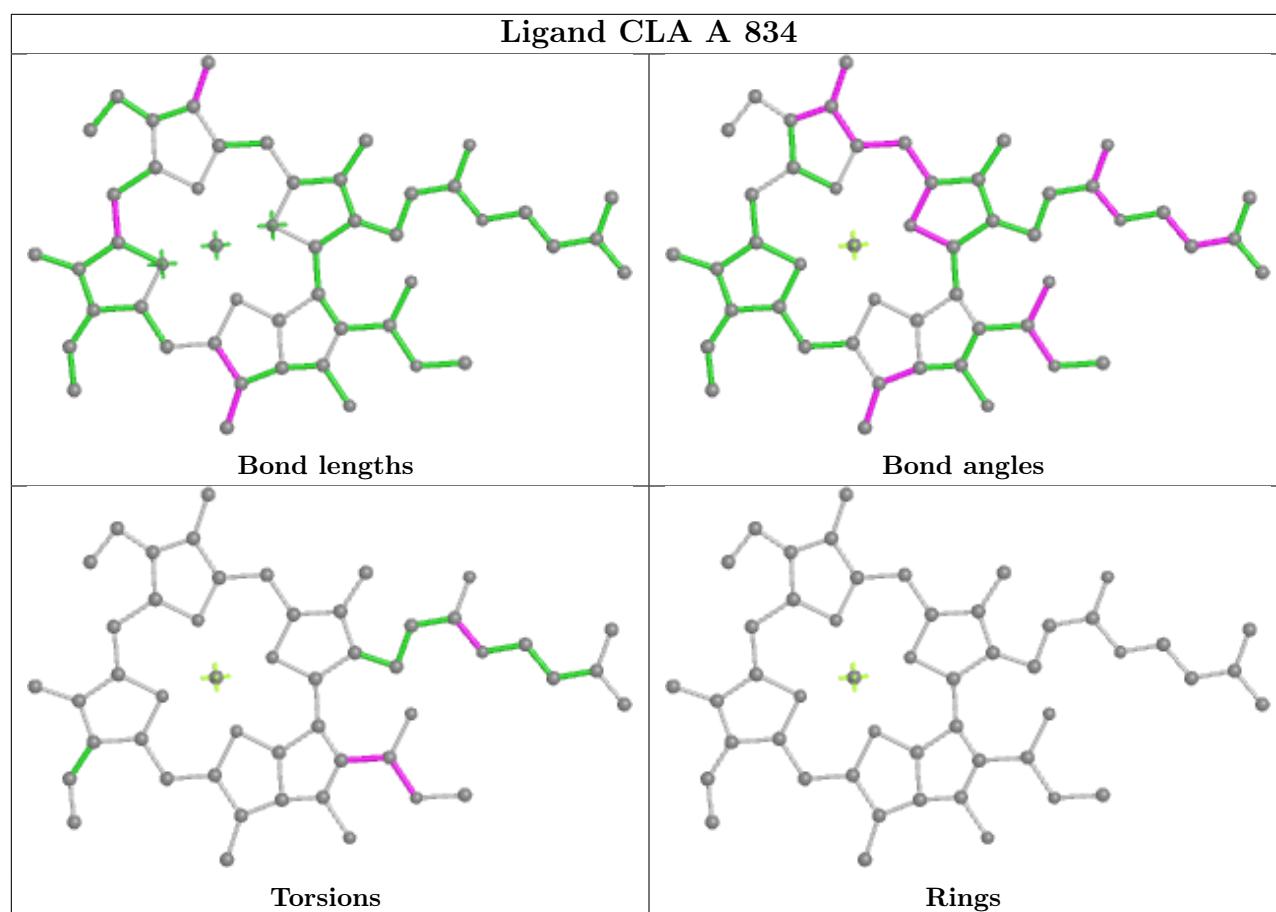


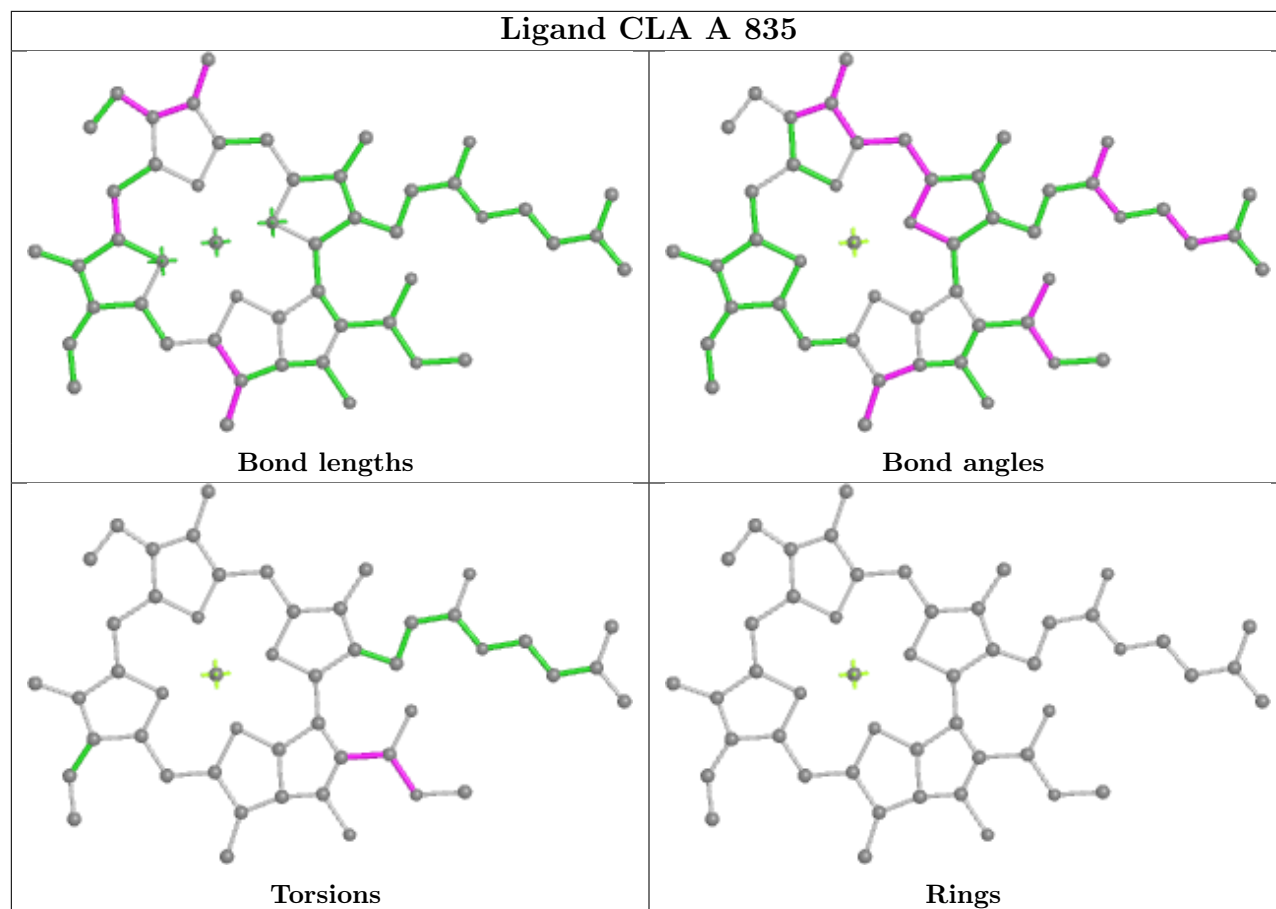




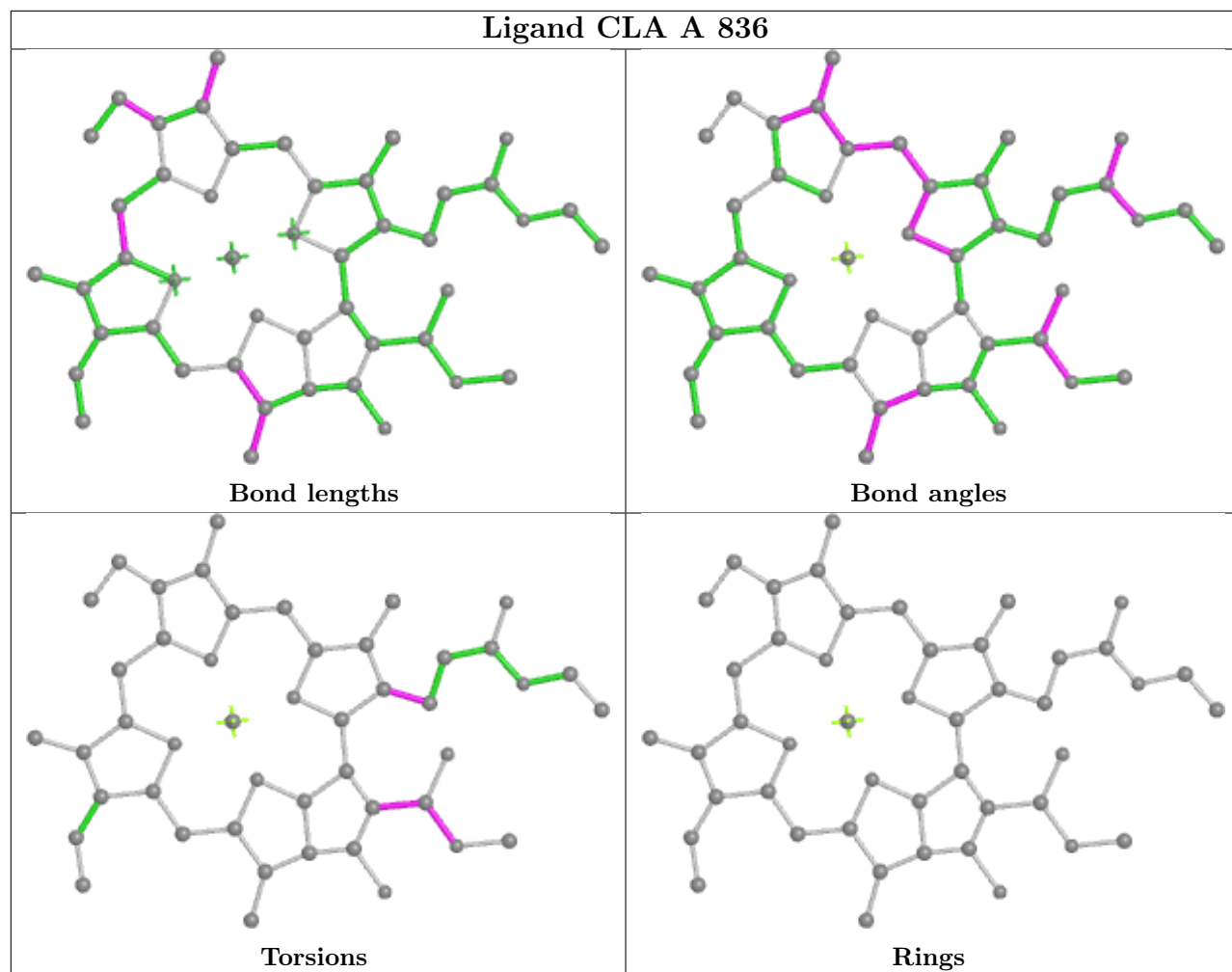
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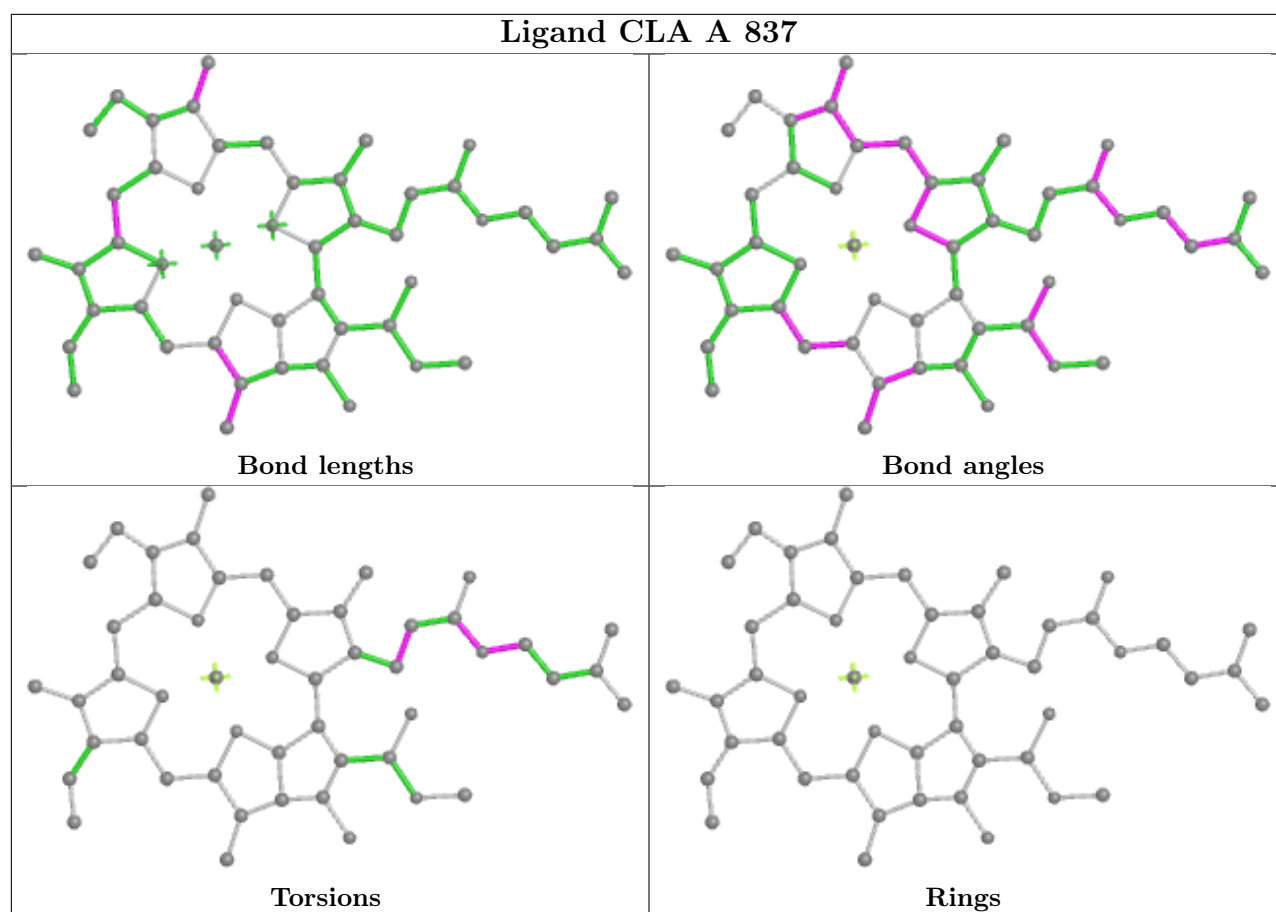


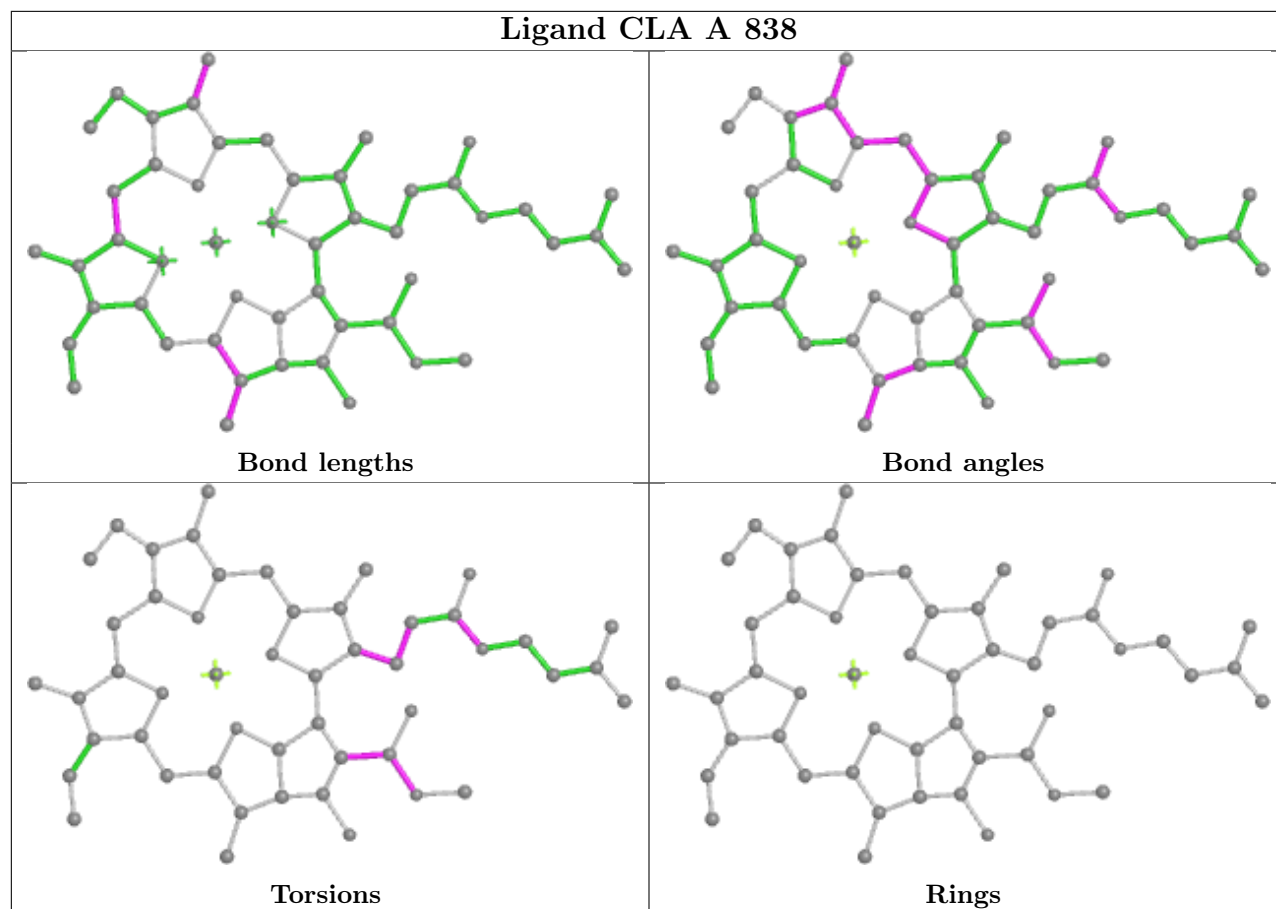


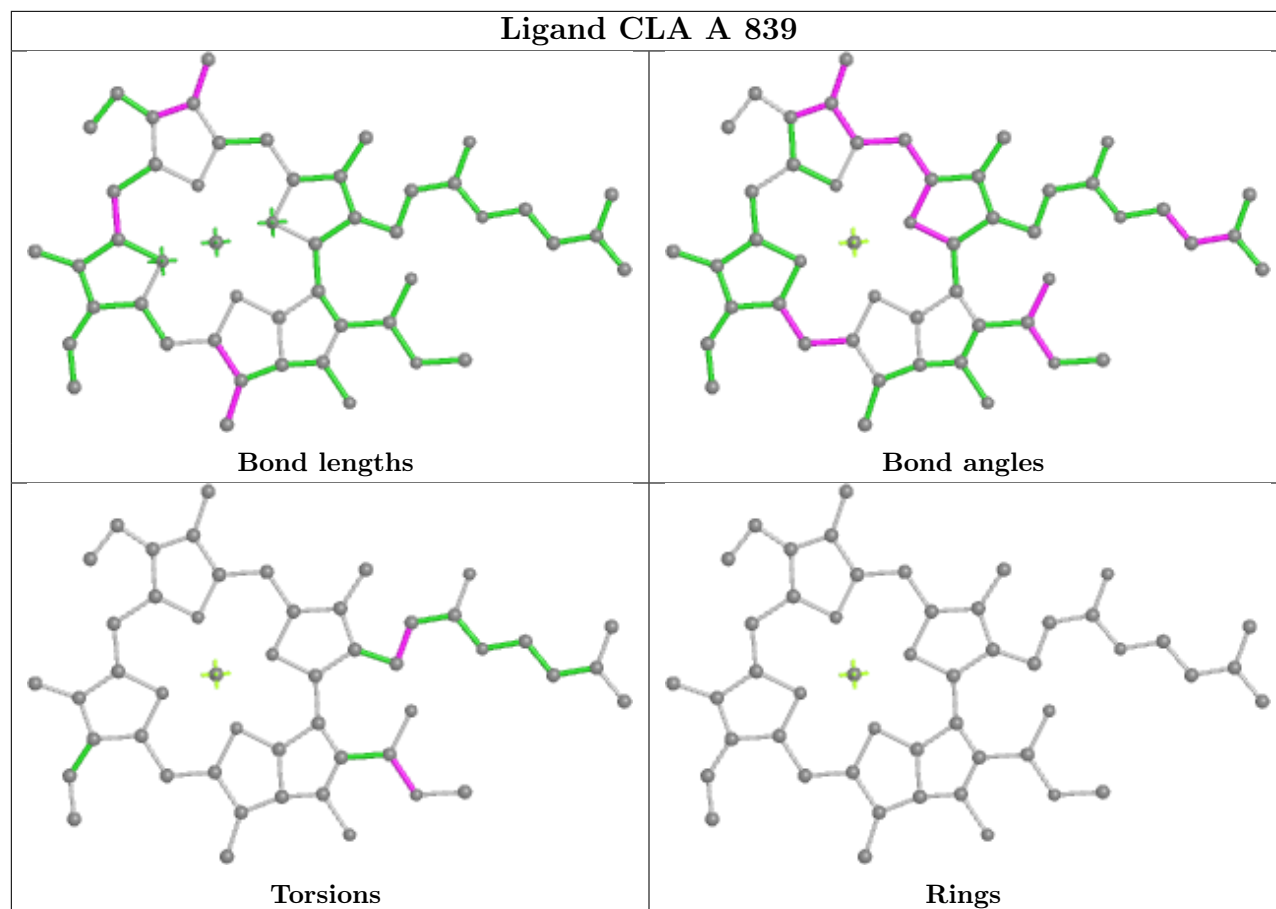


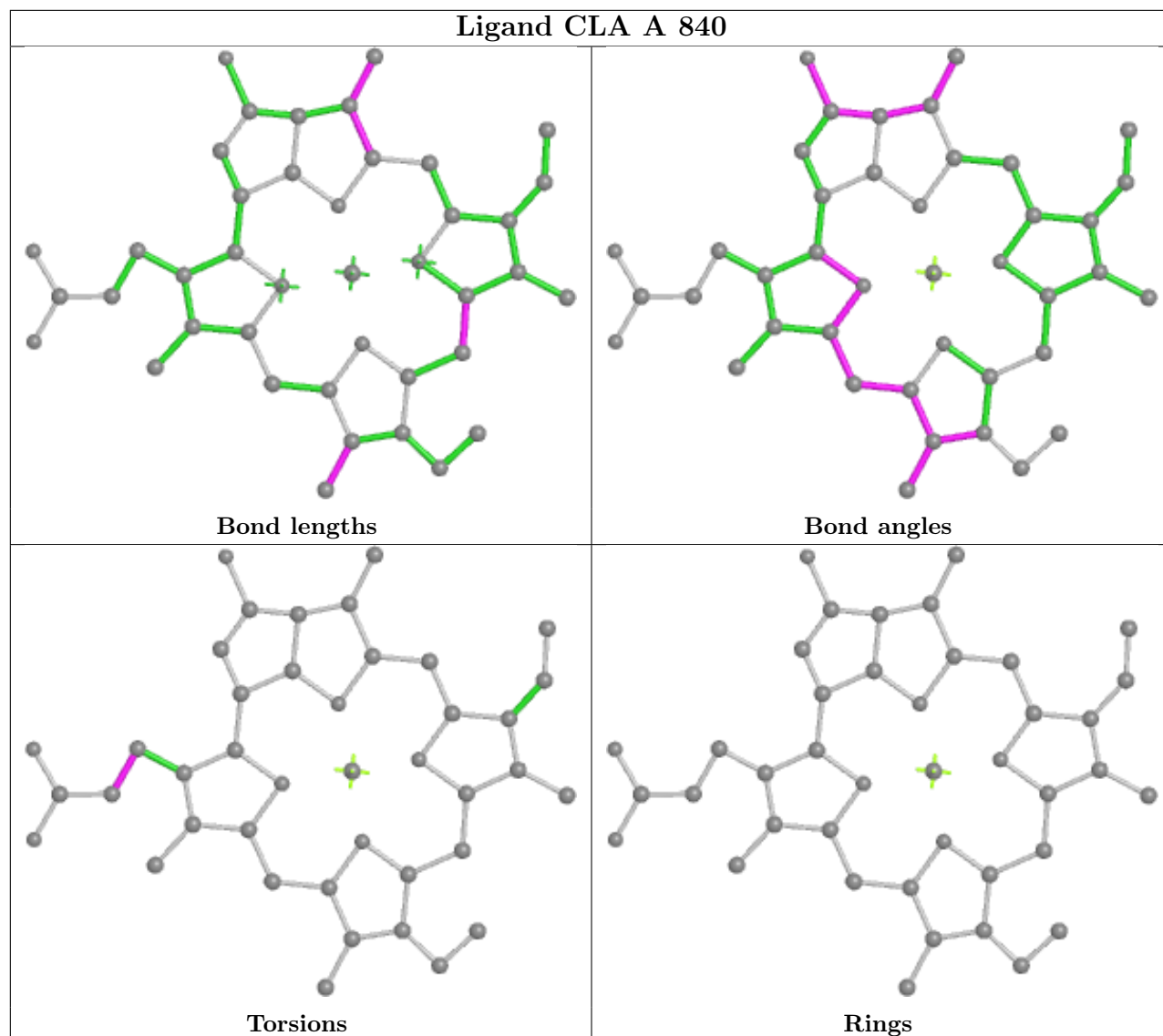
Ligand CLA A 836

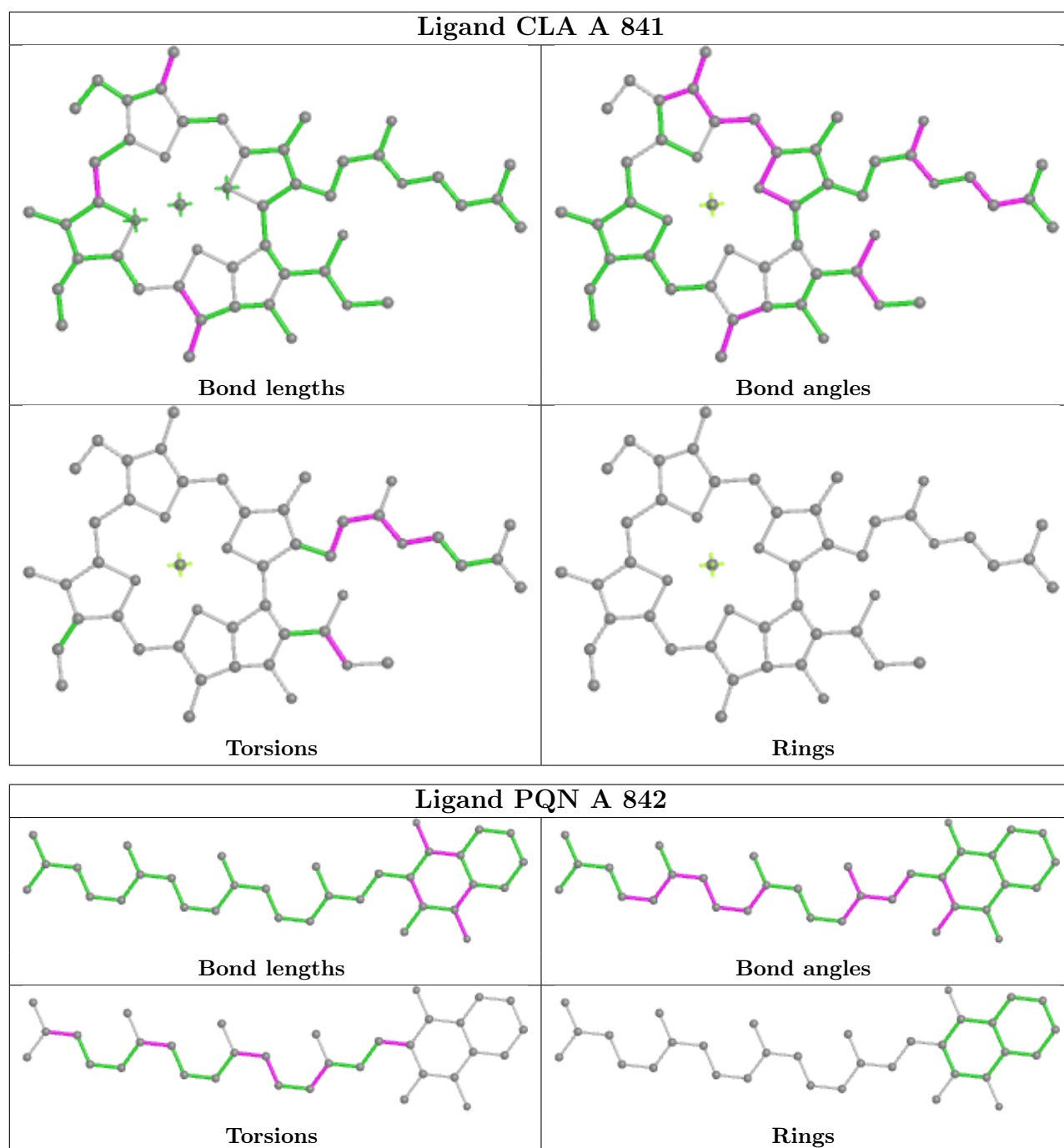


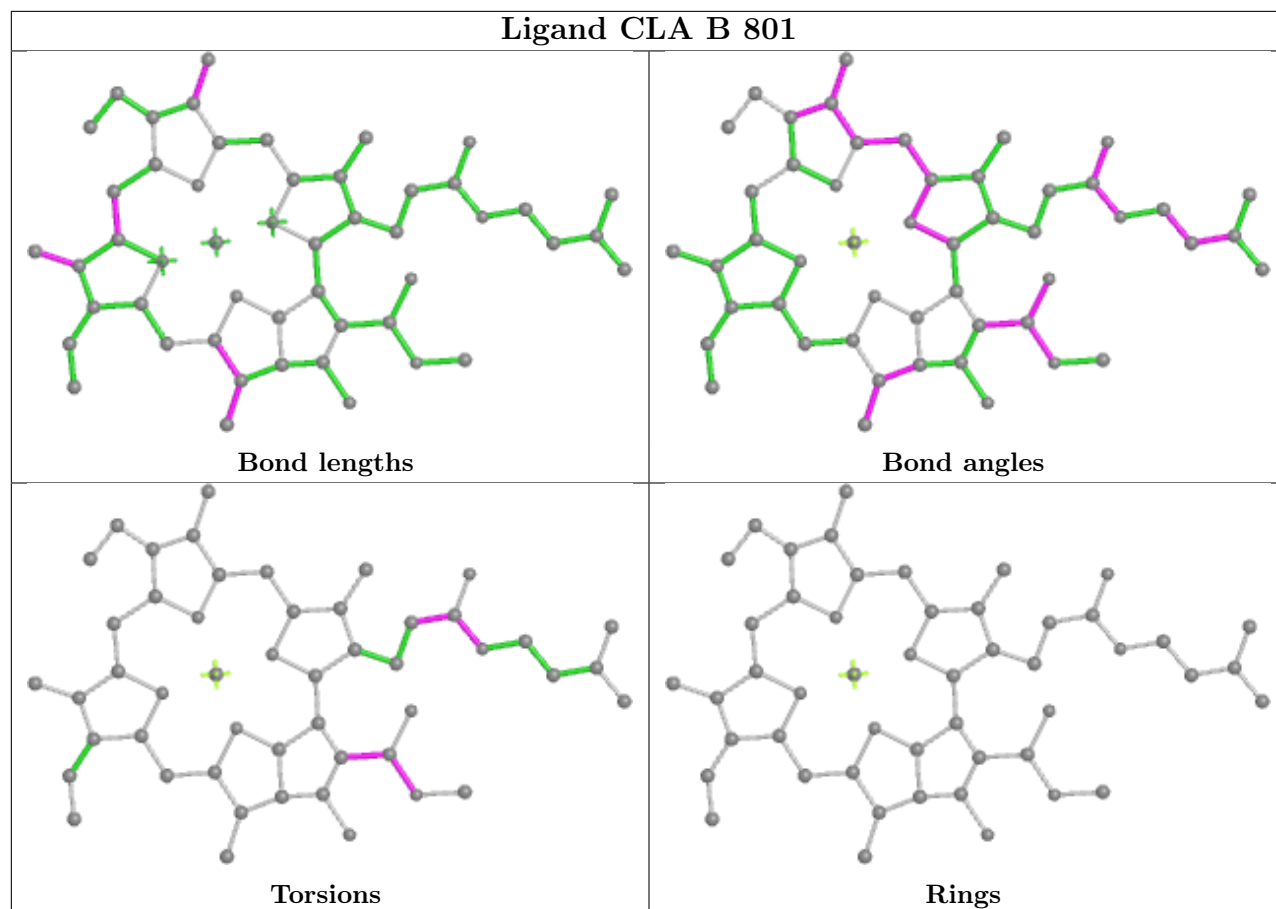


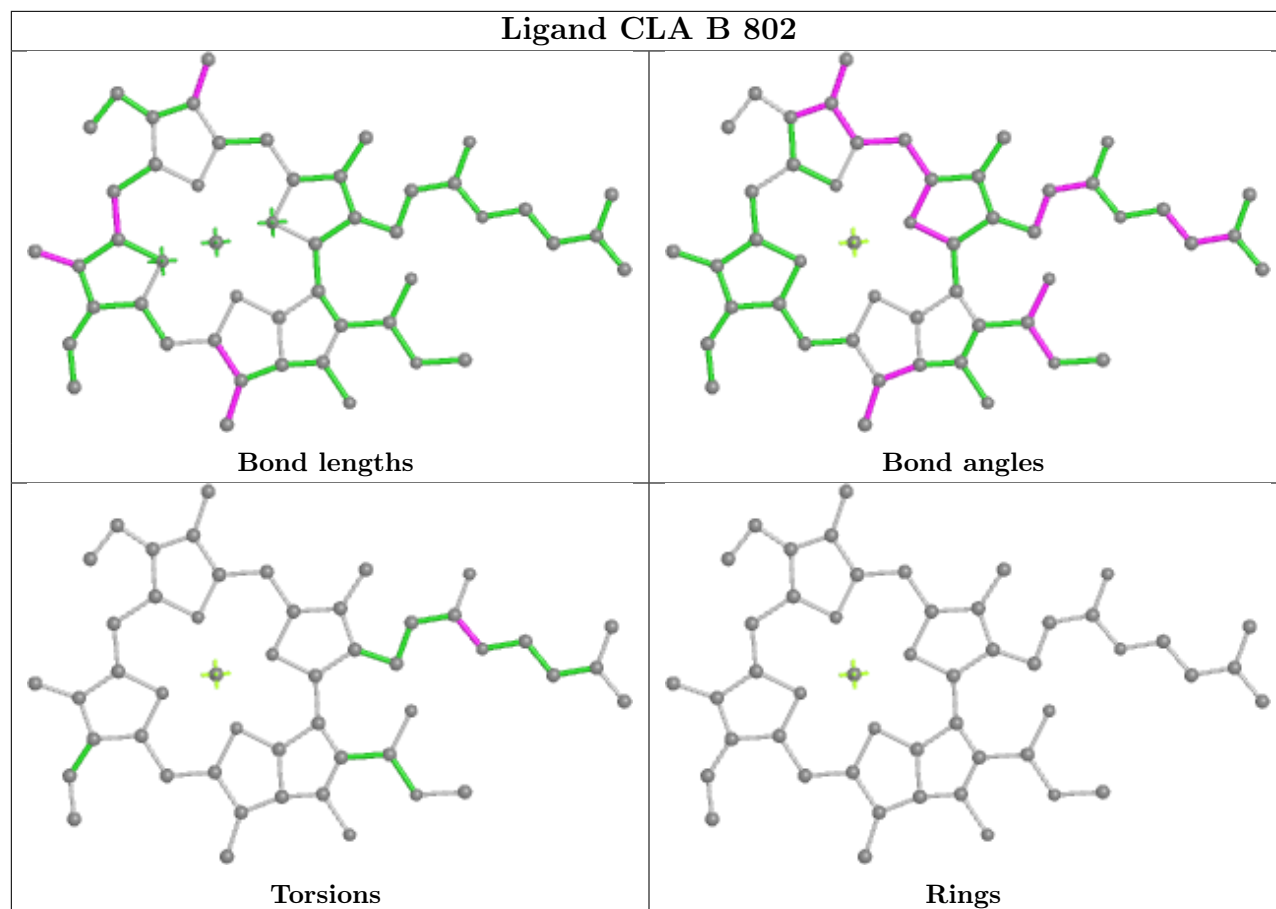


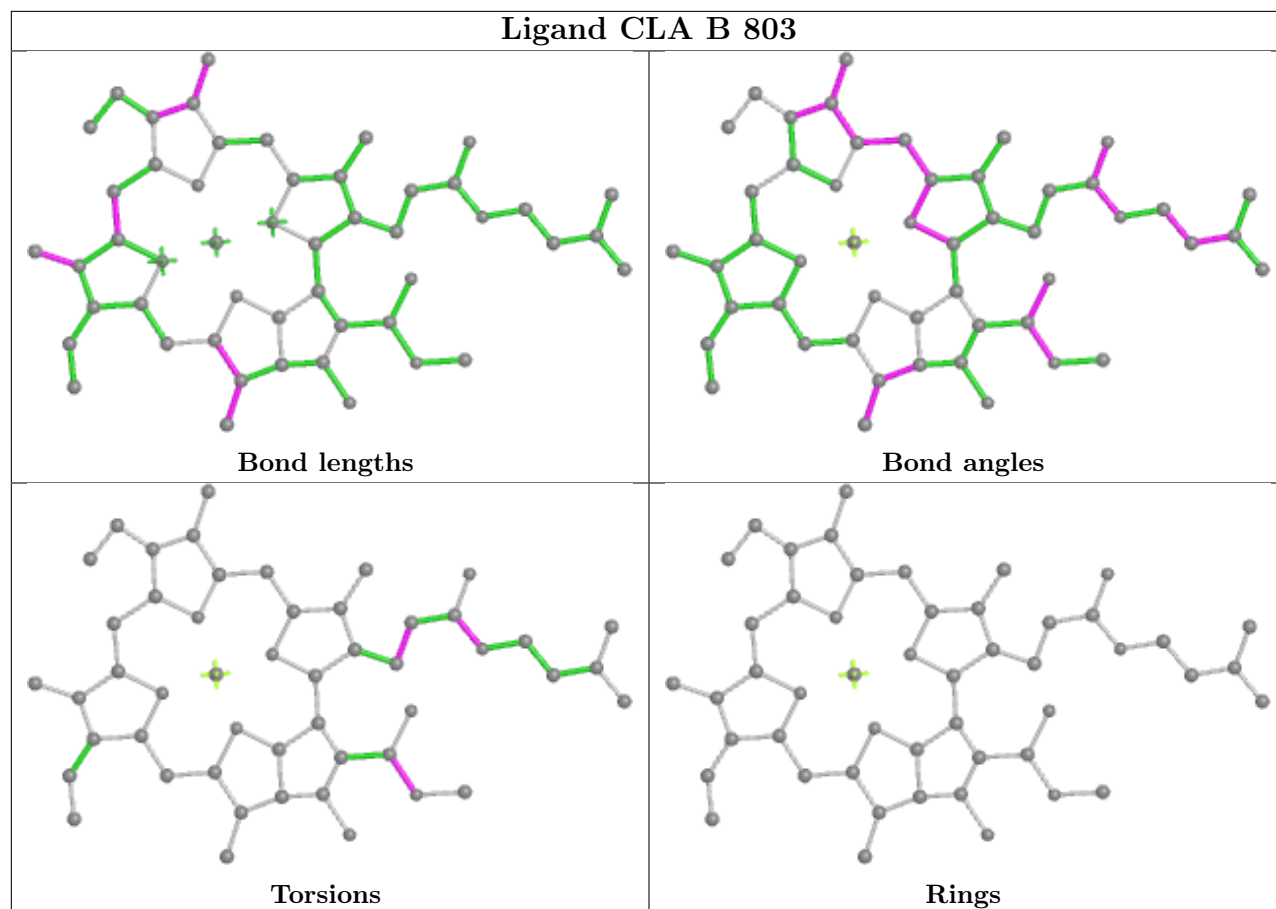


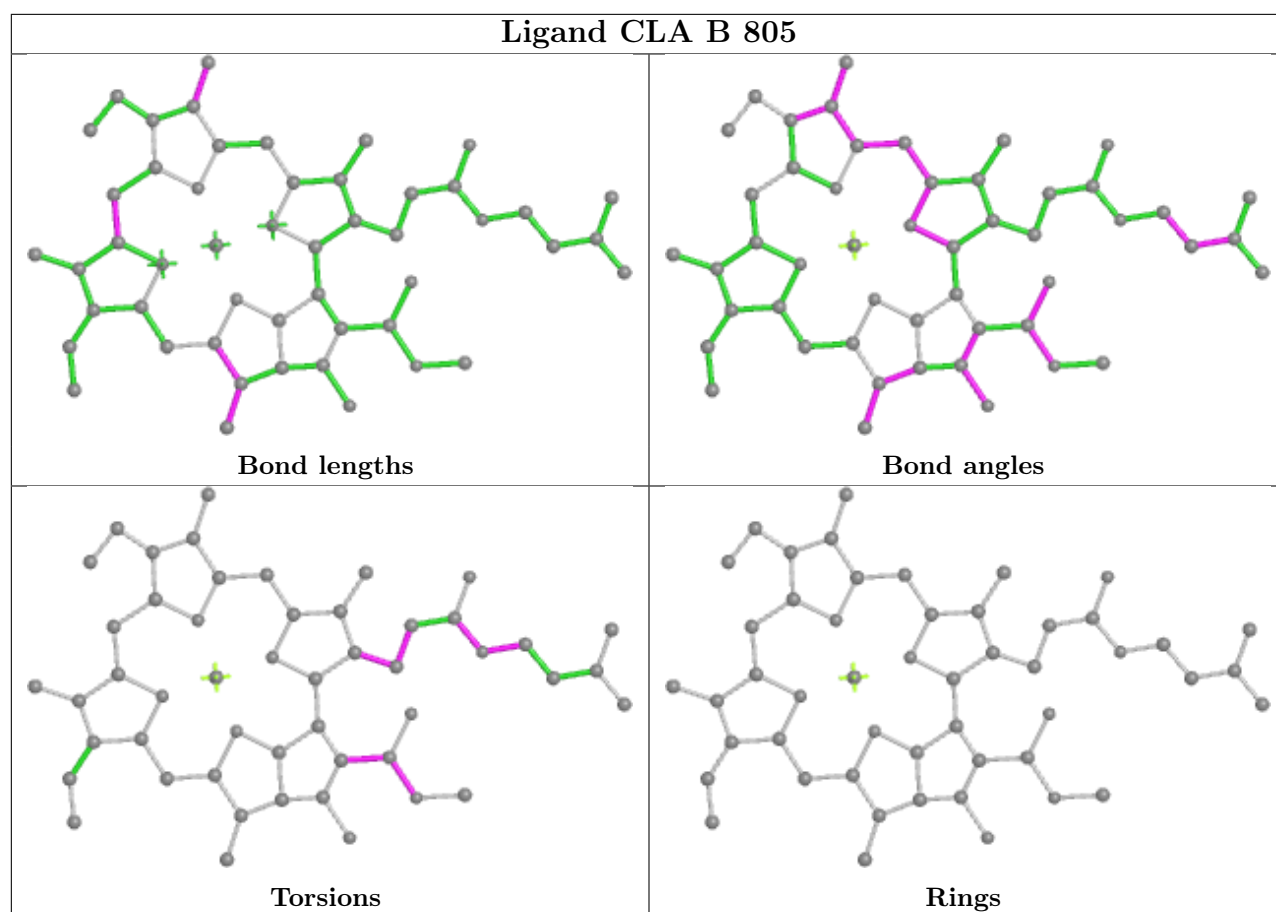


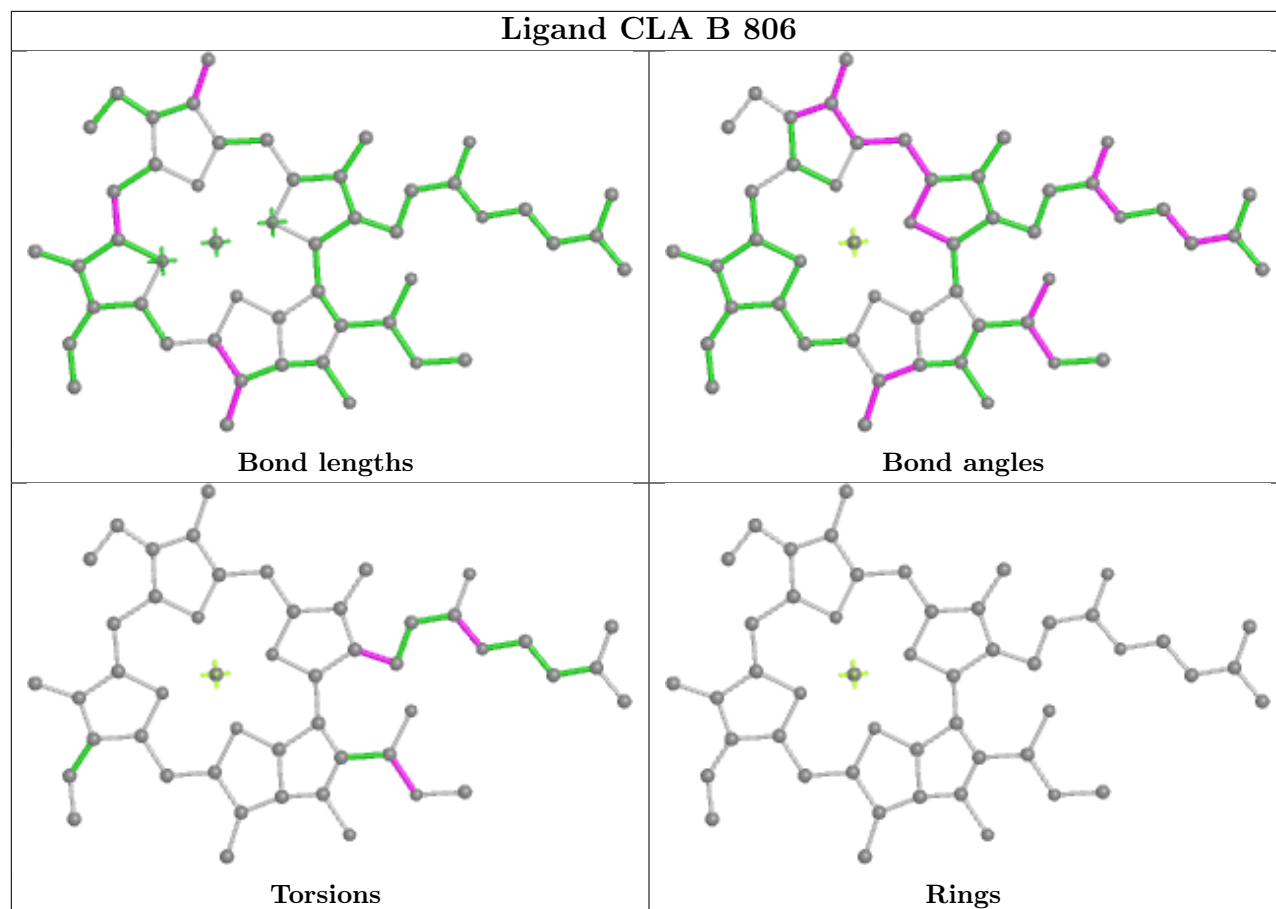


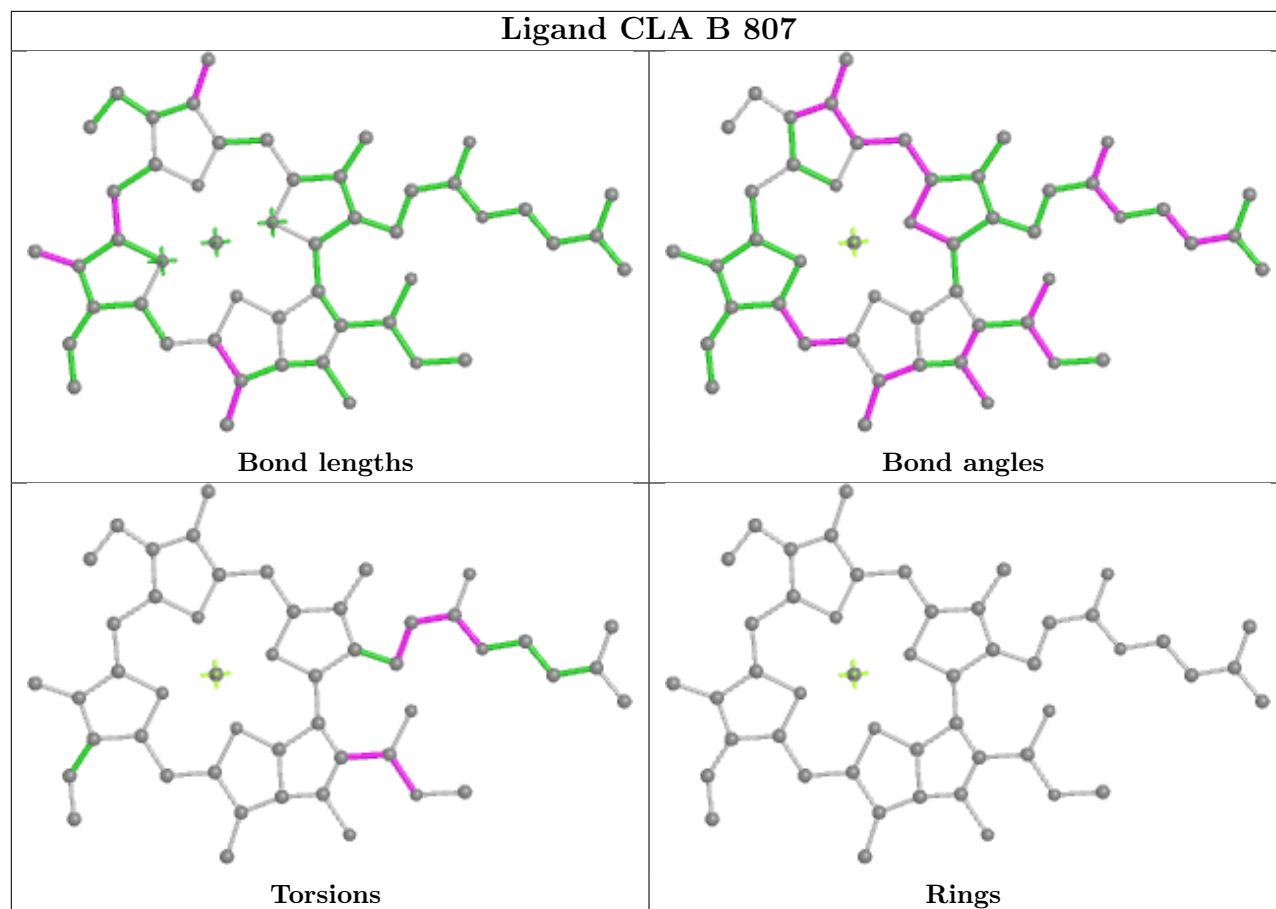


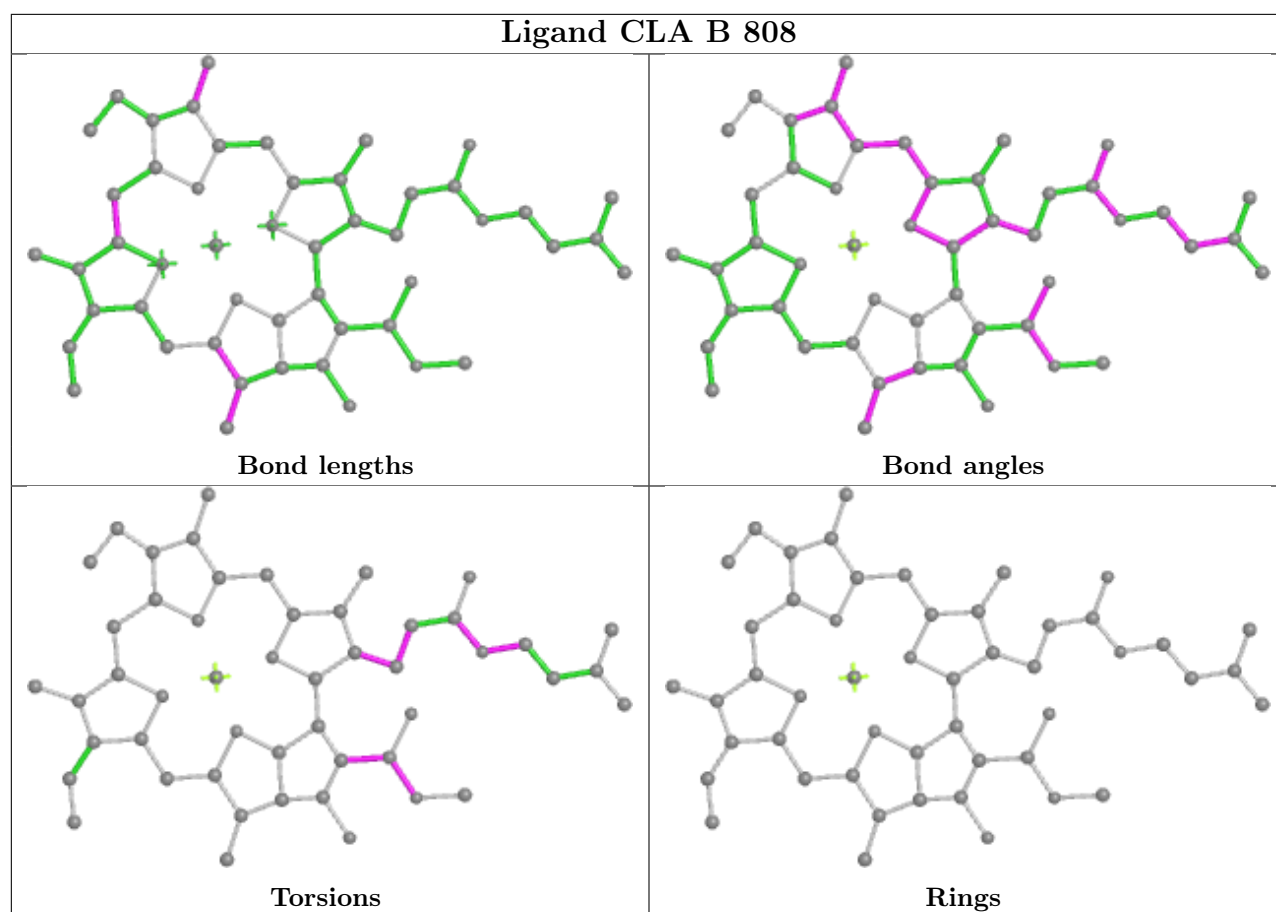


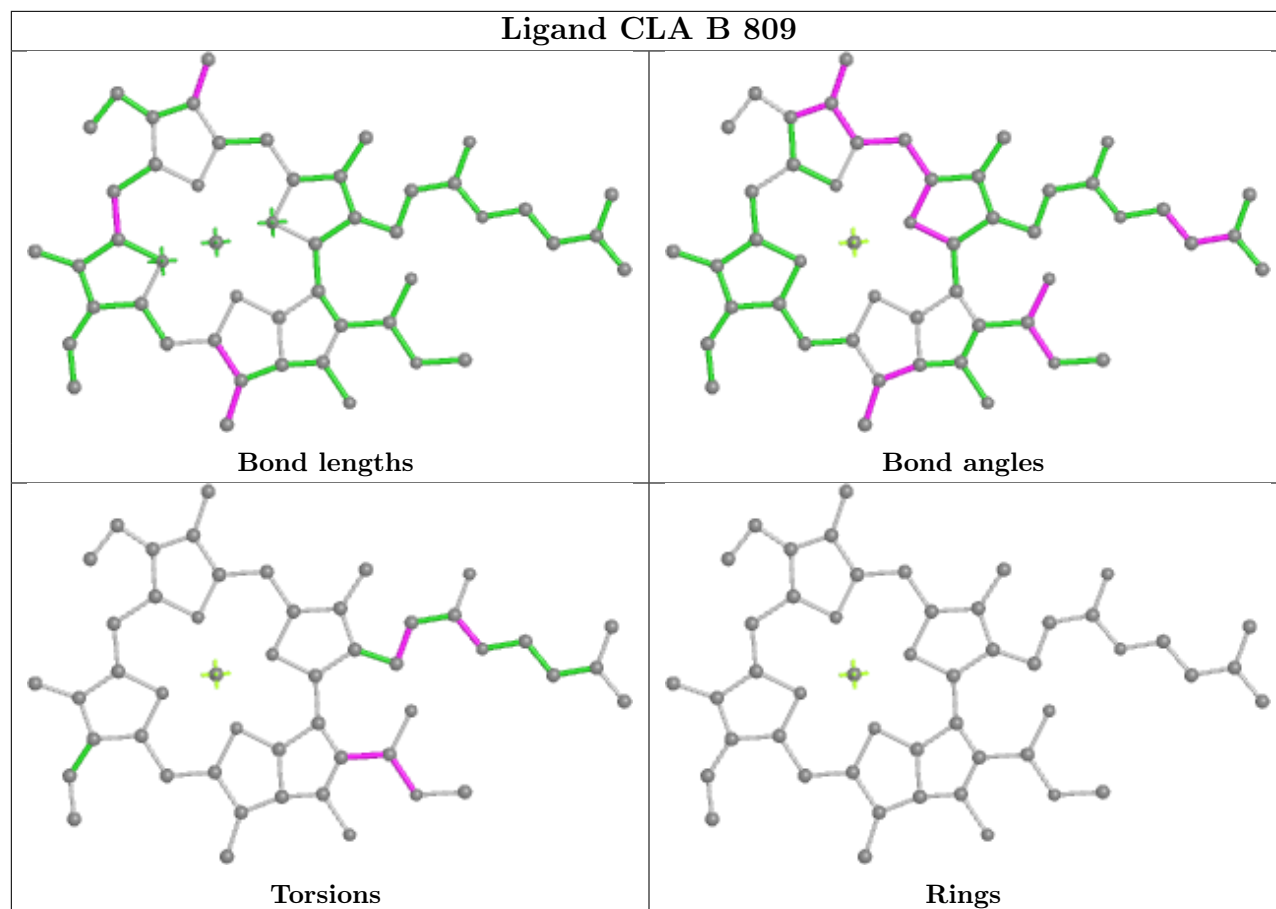


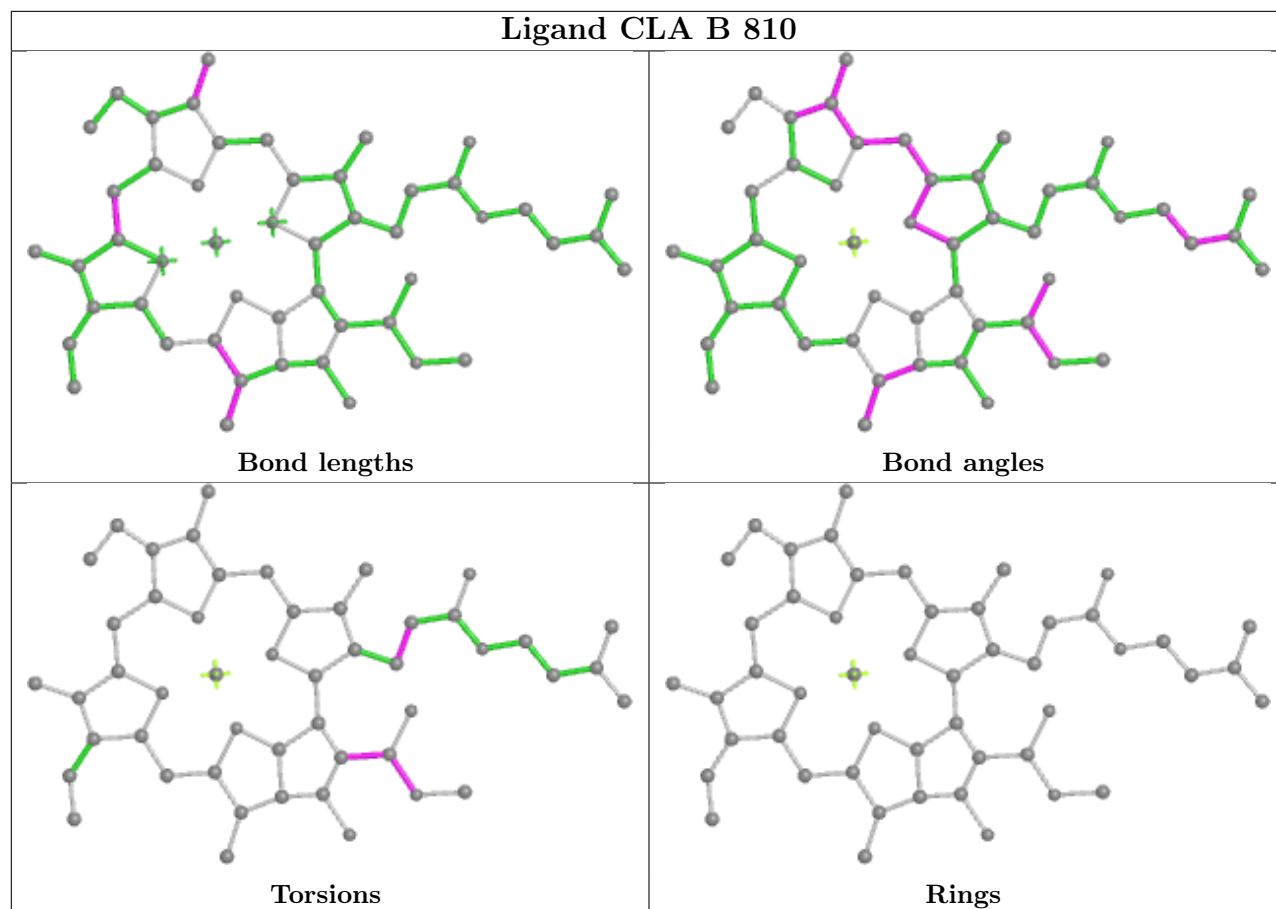


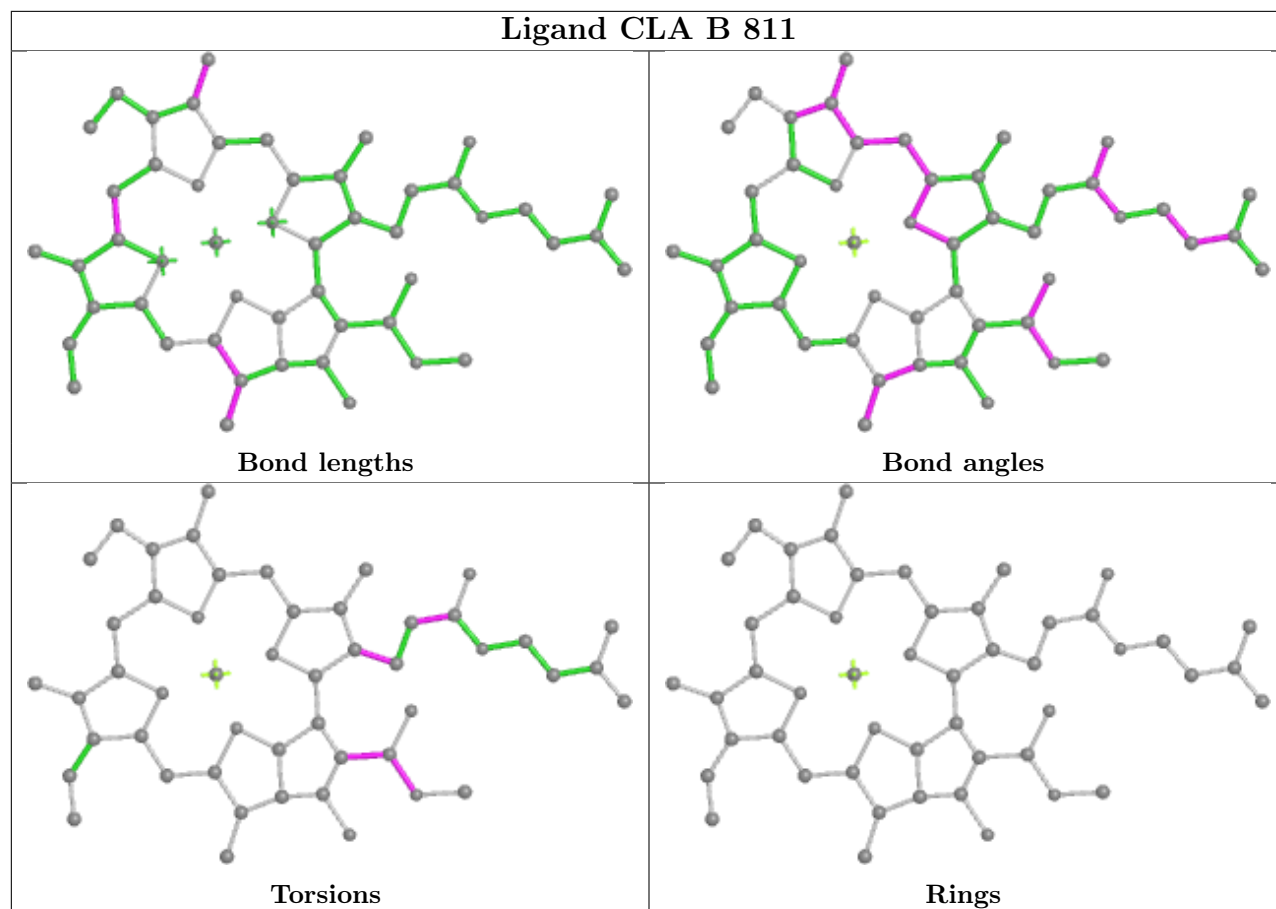


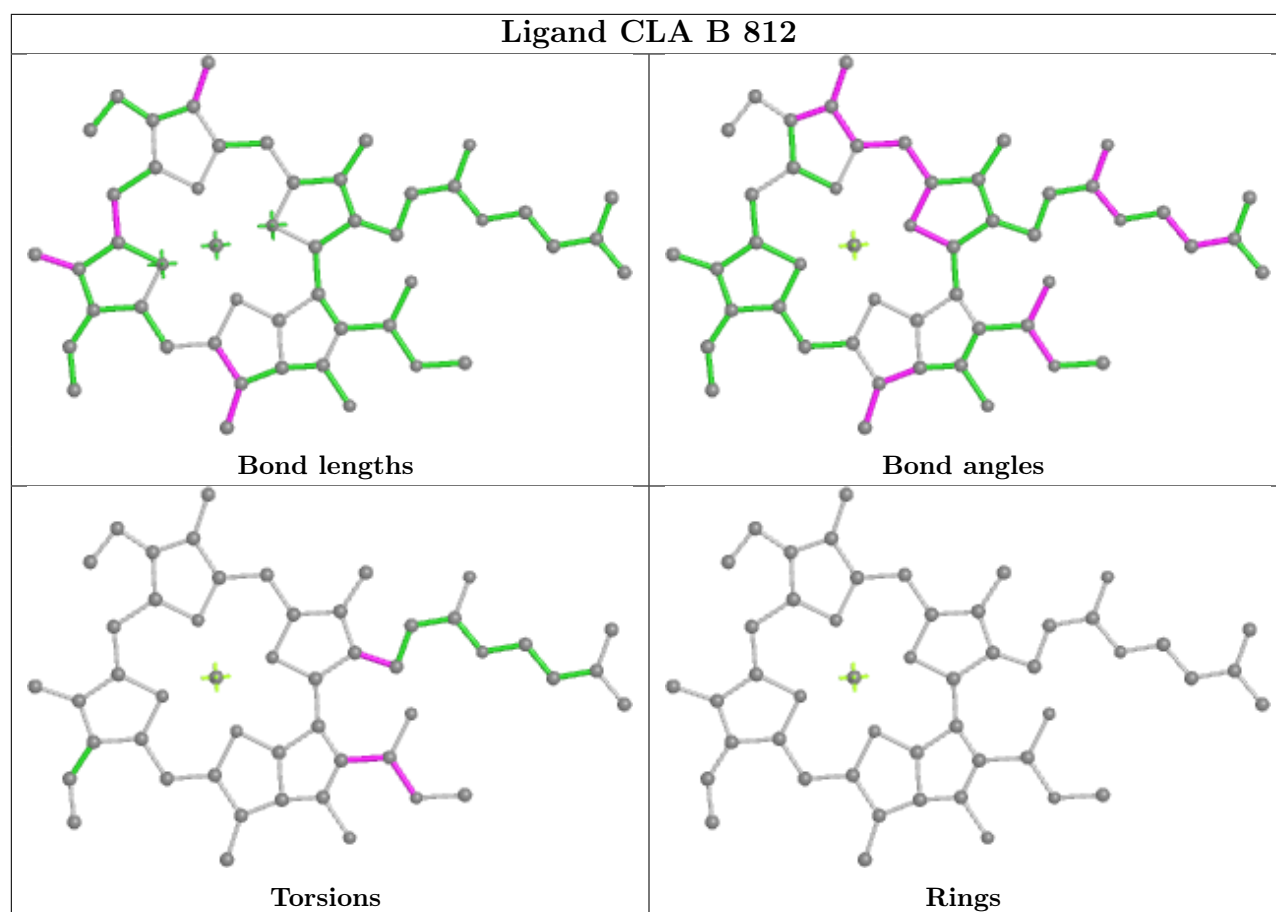


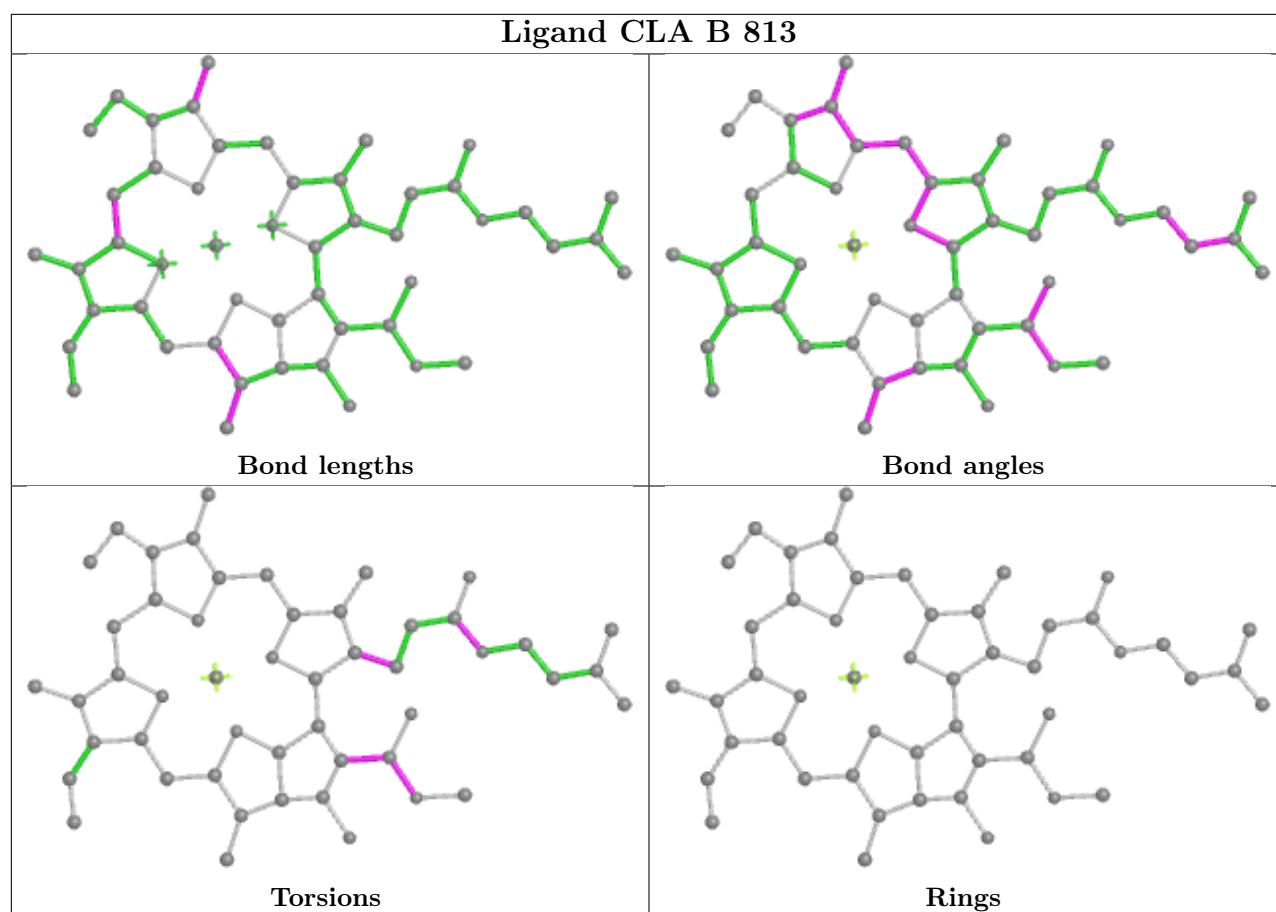


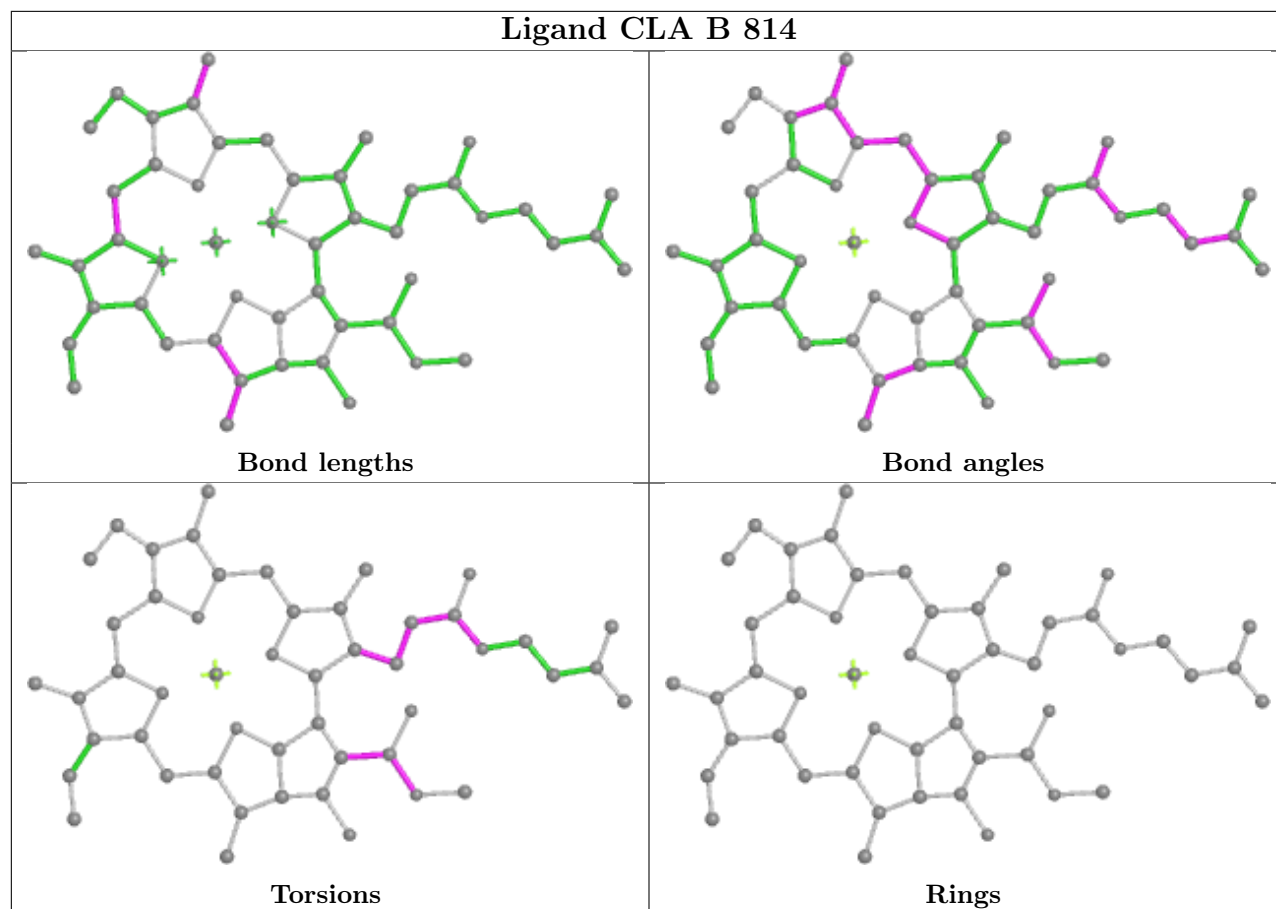




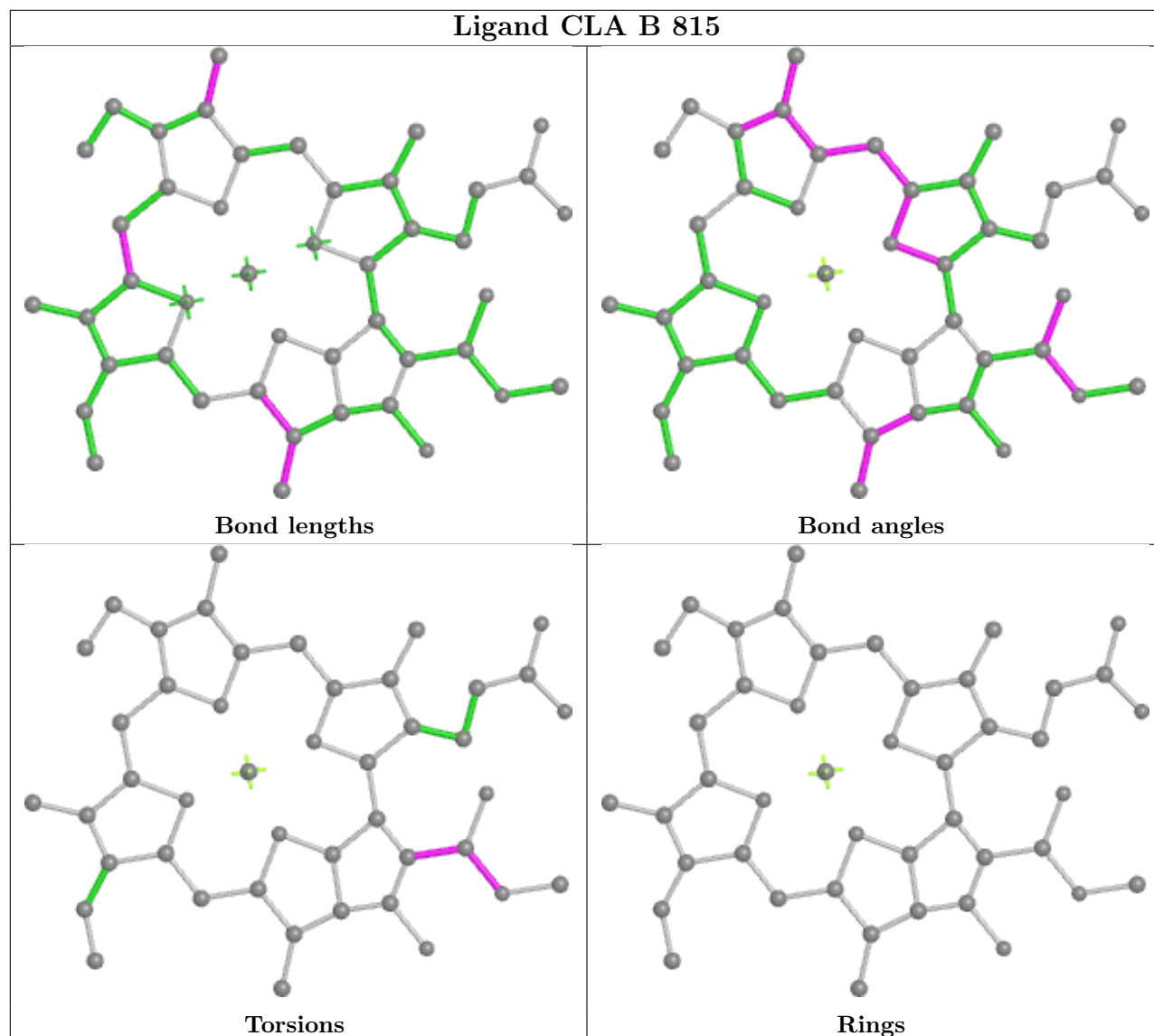




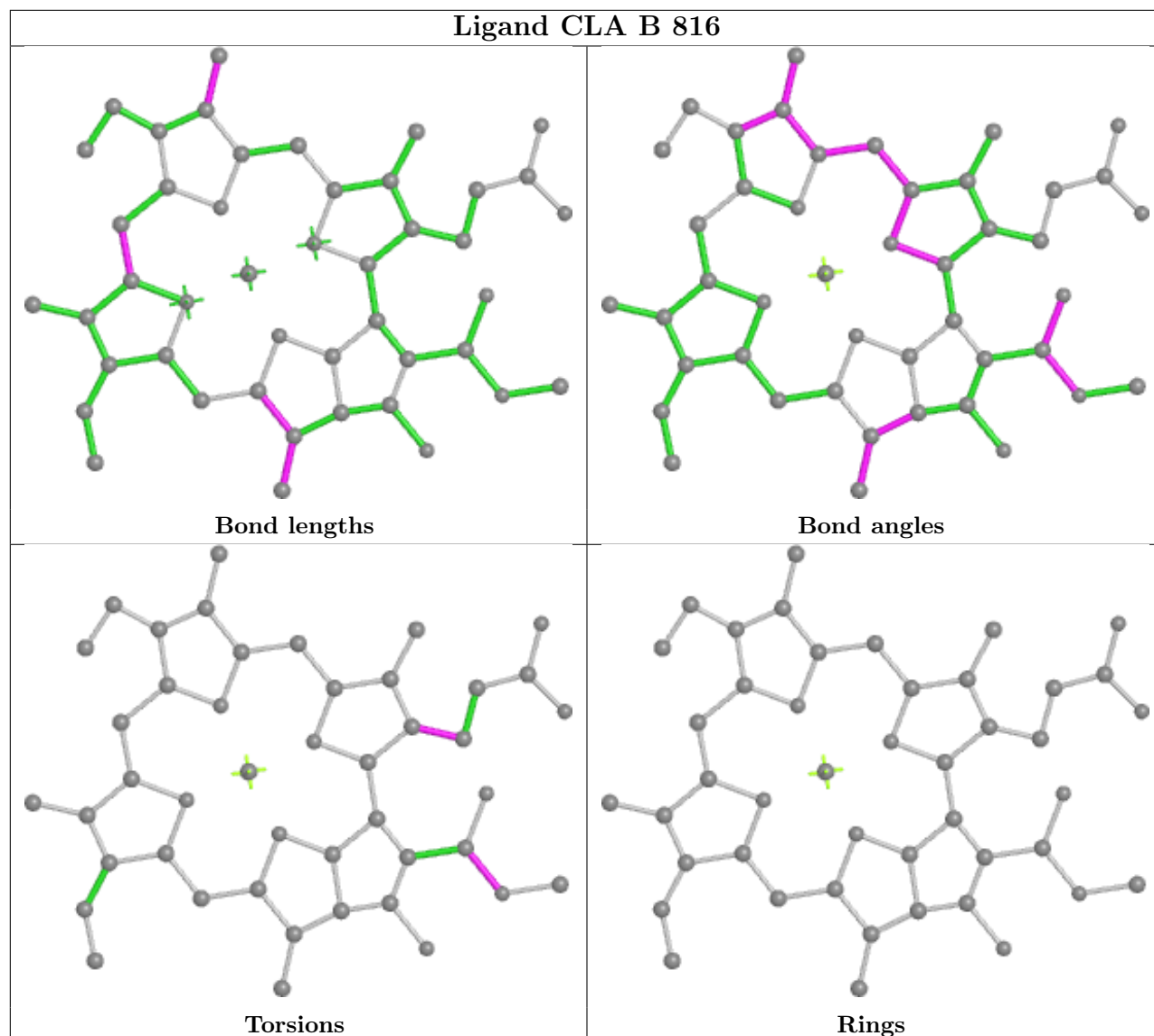


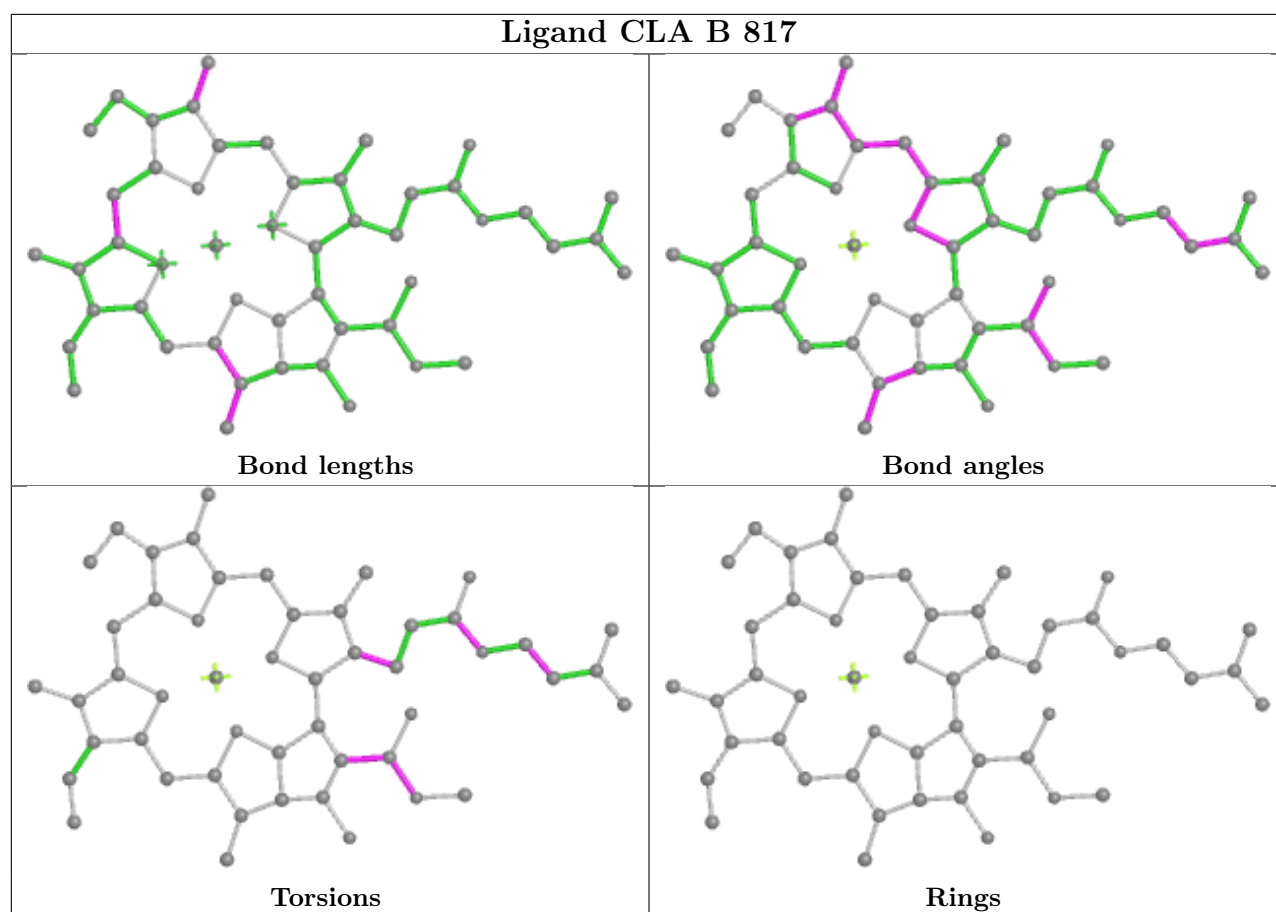


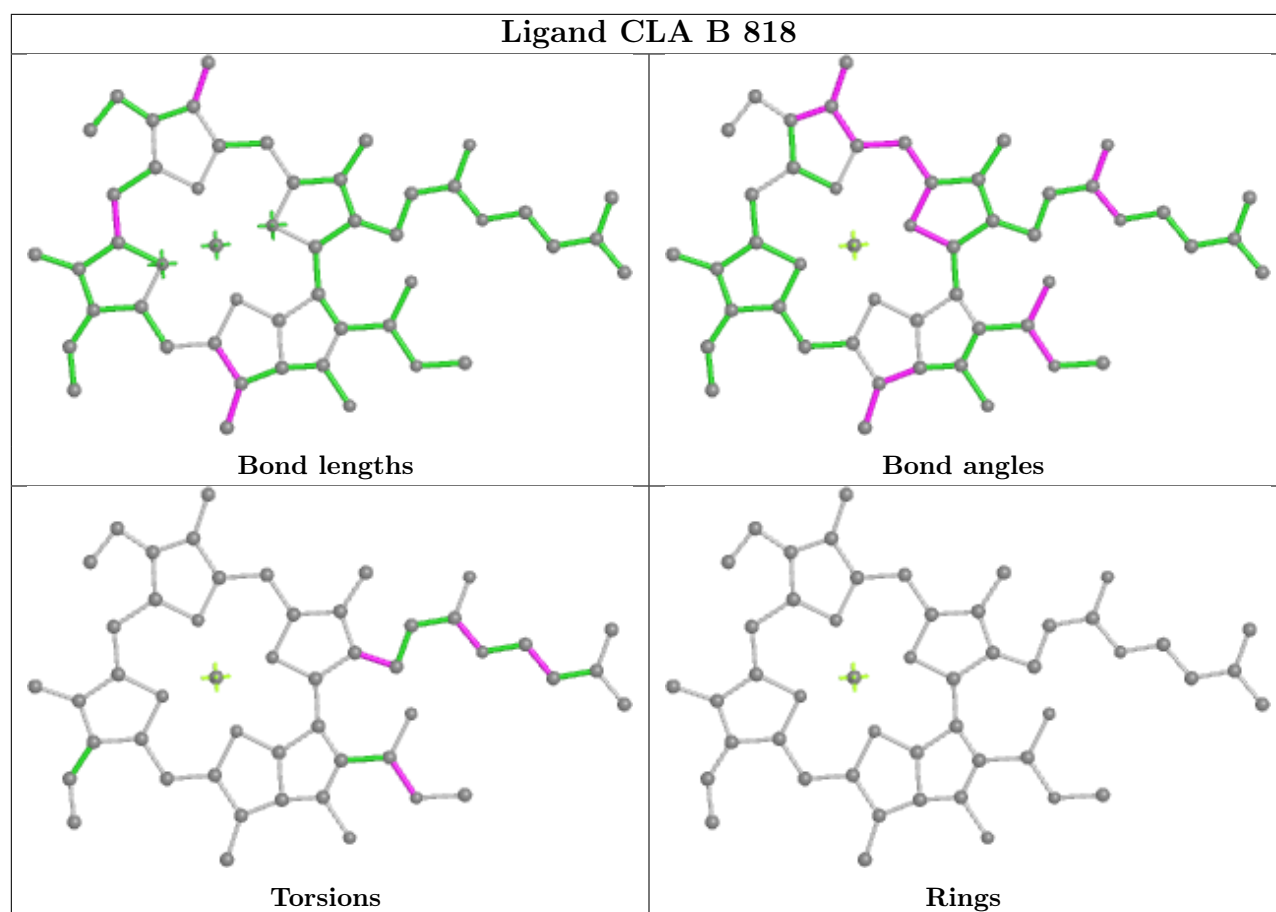
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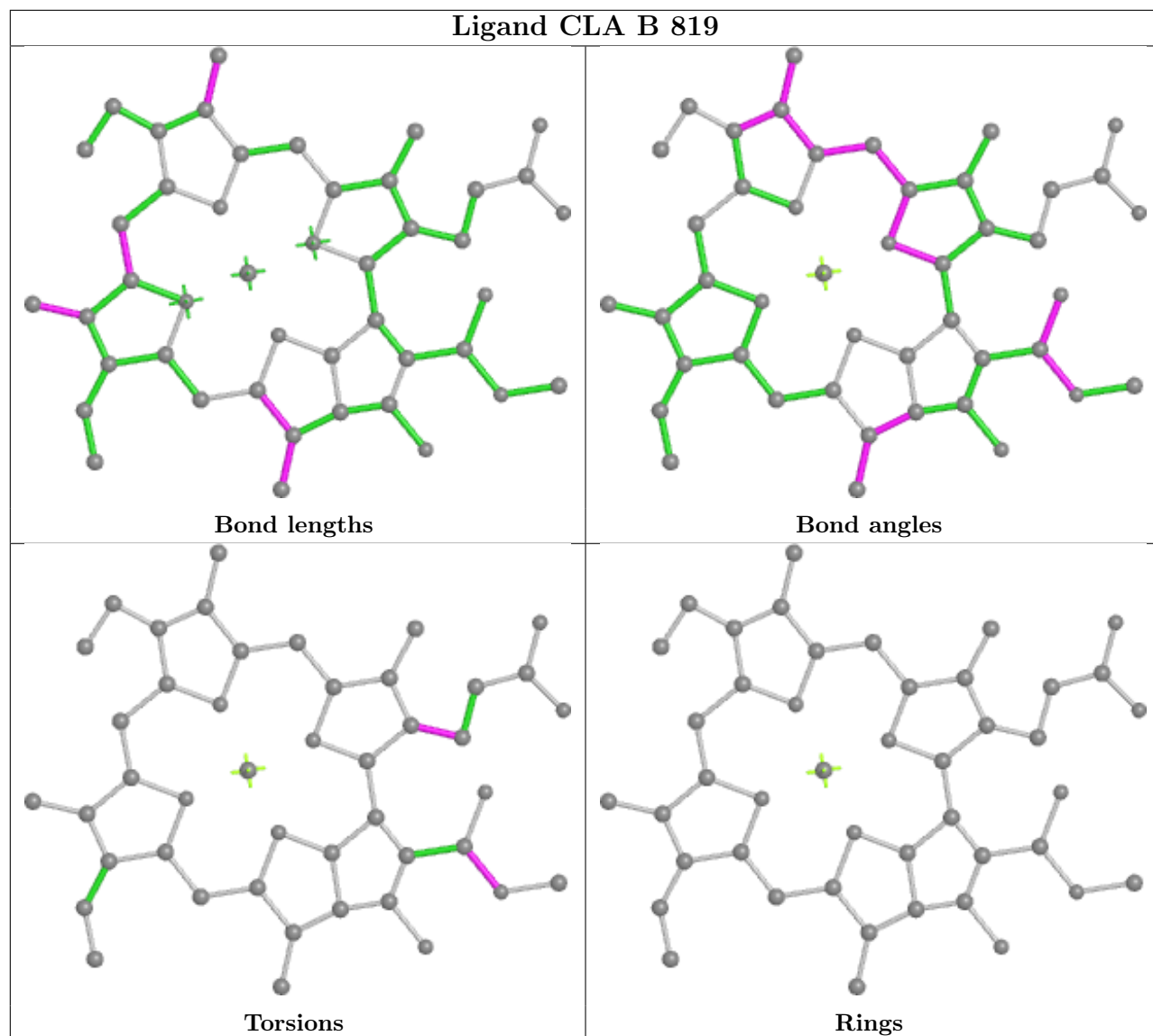
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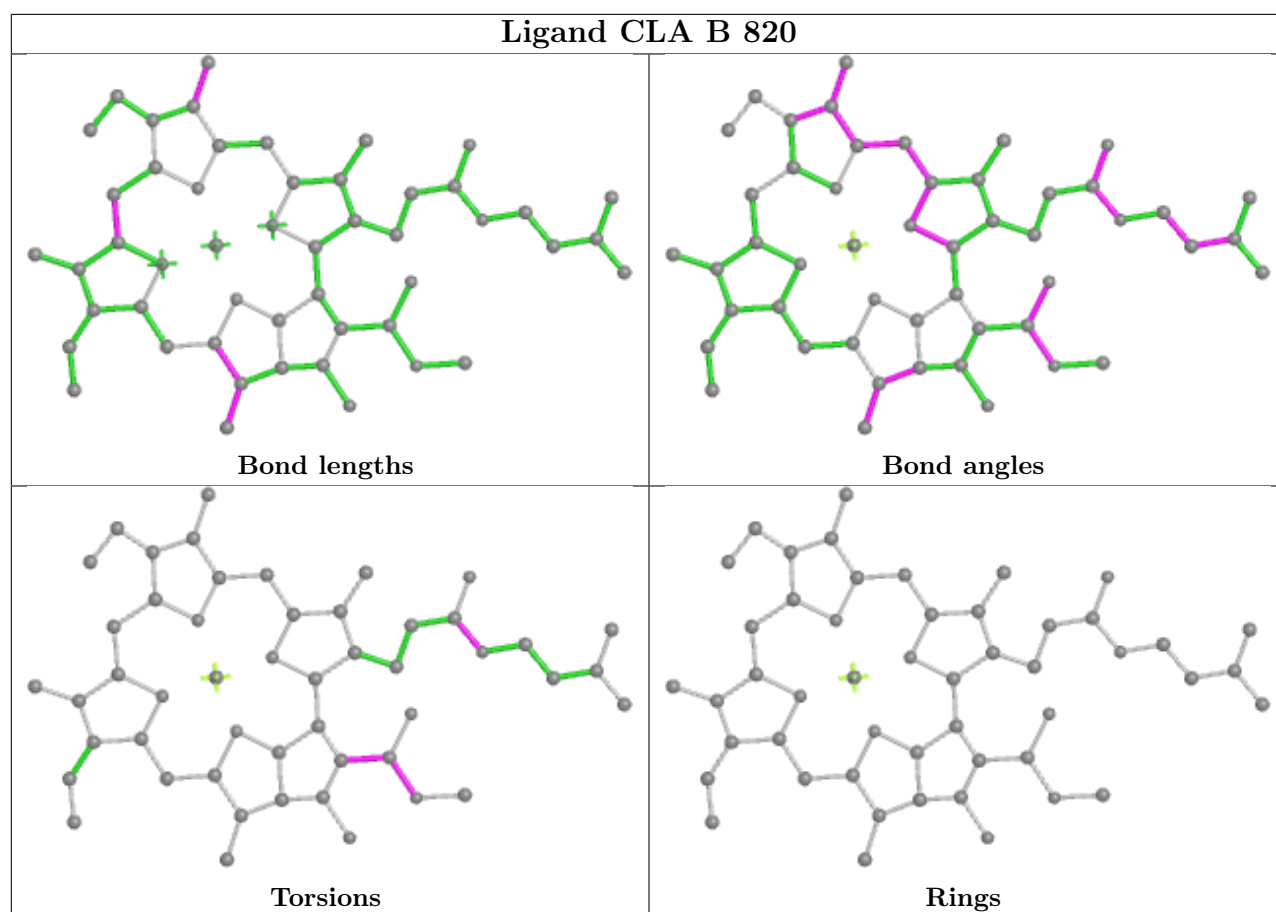


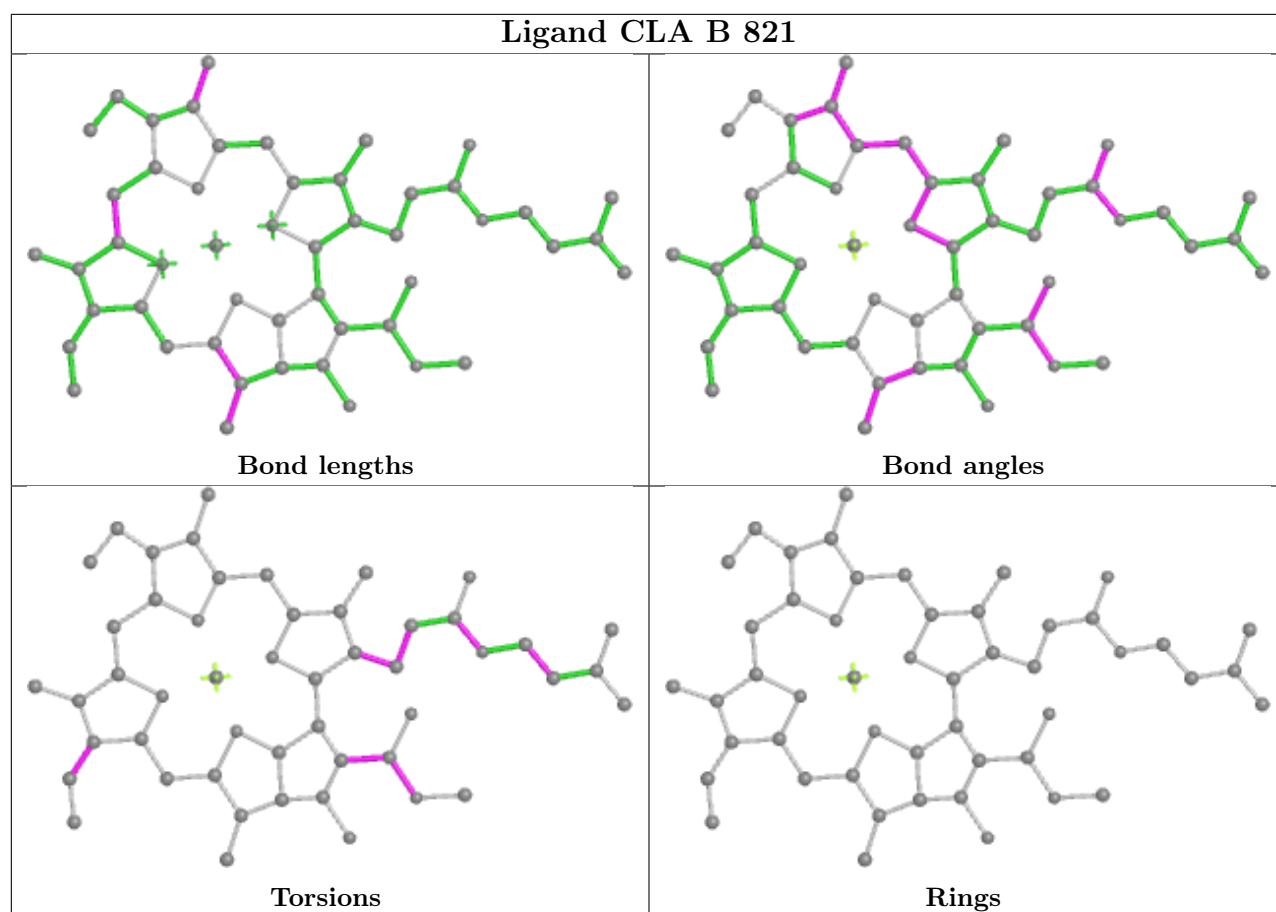


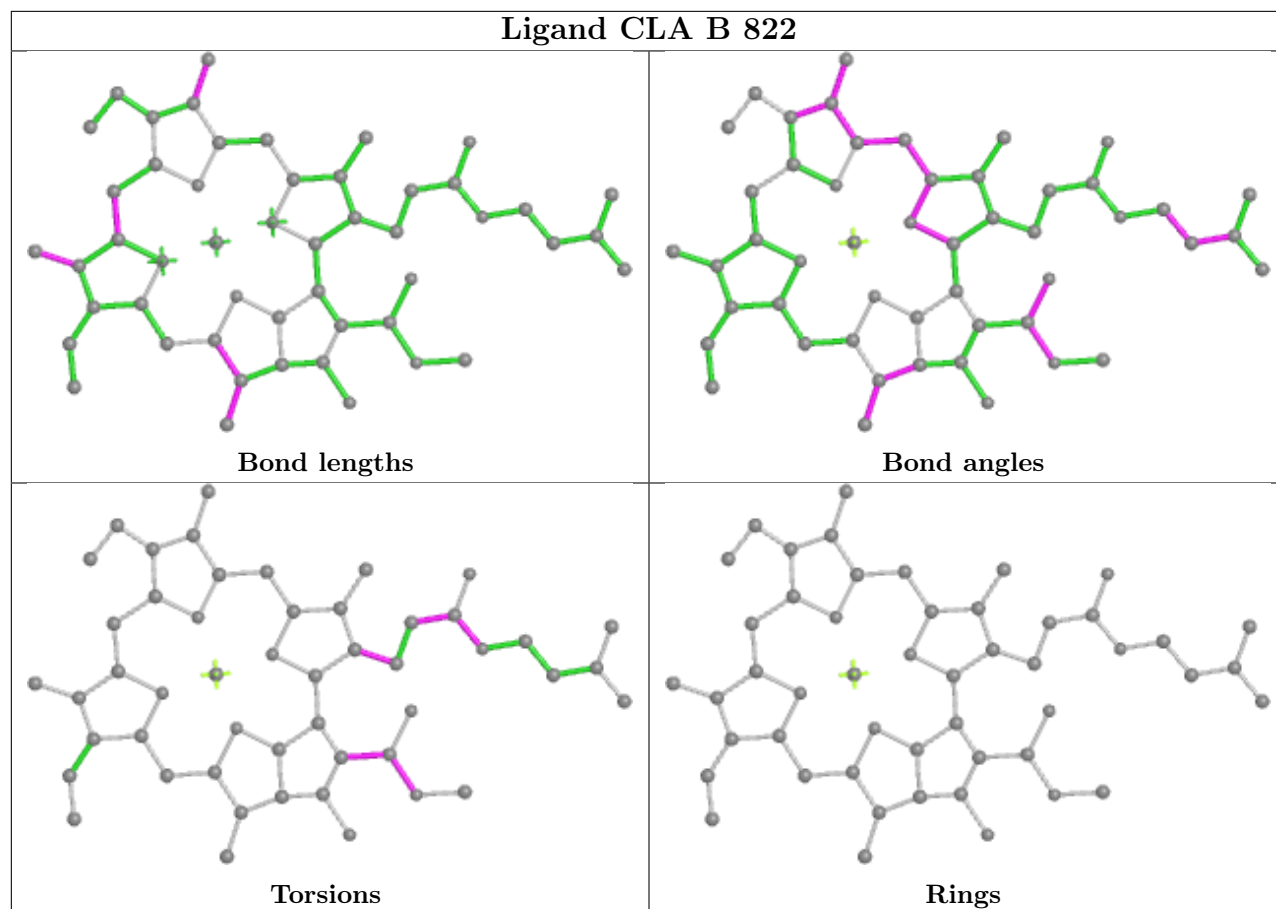


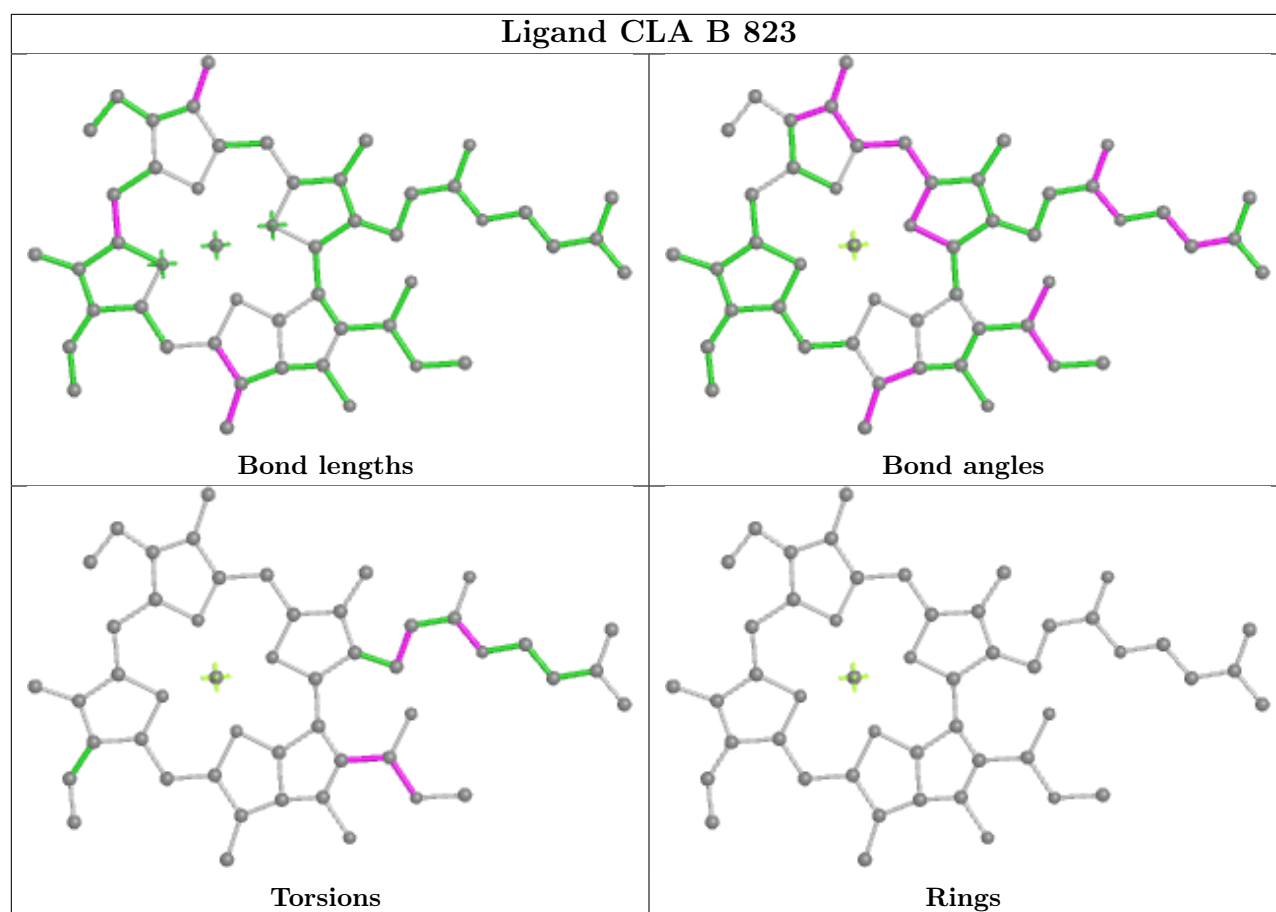
Ligand CLA B 819



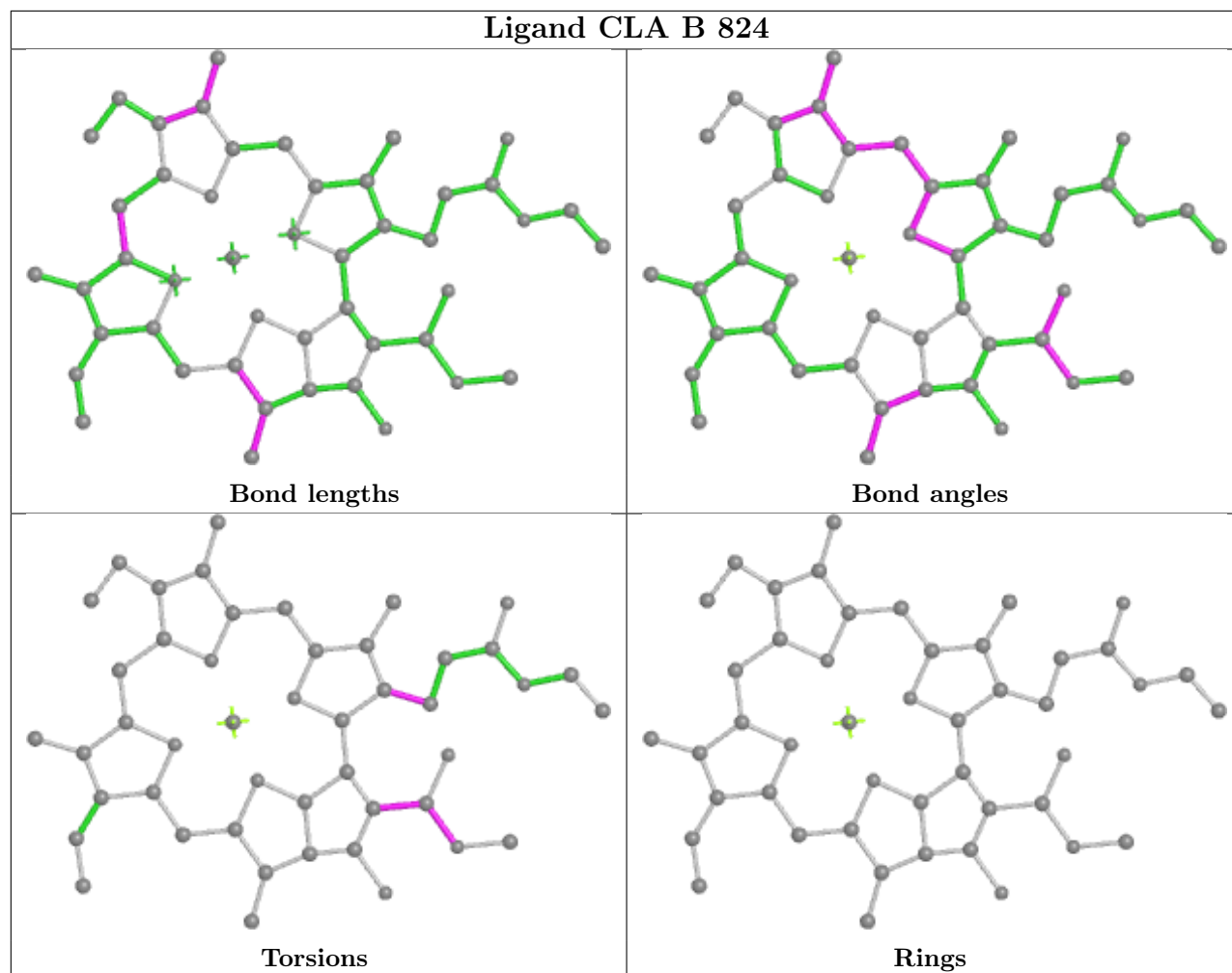




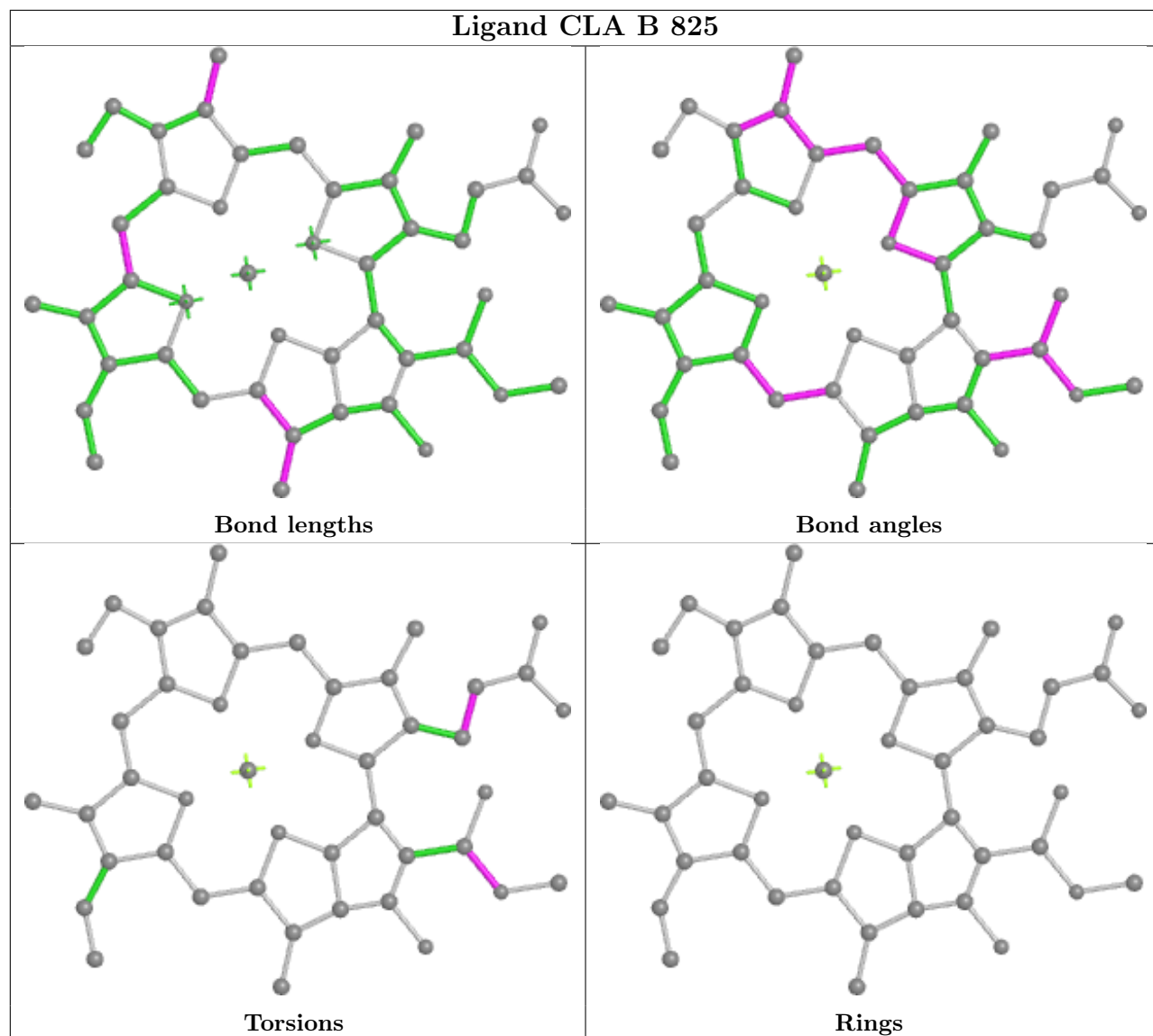


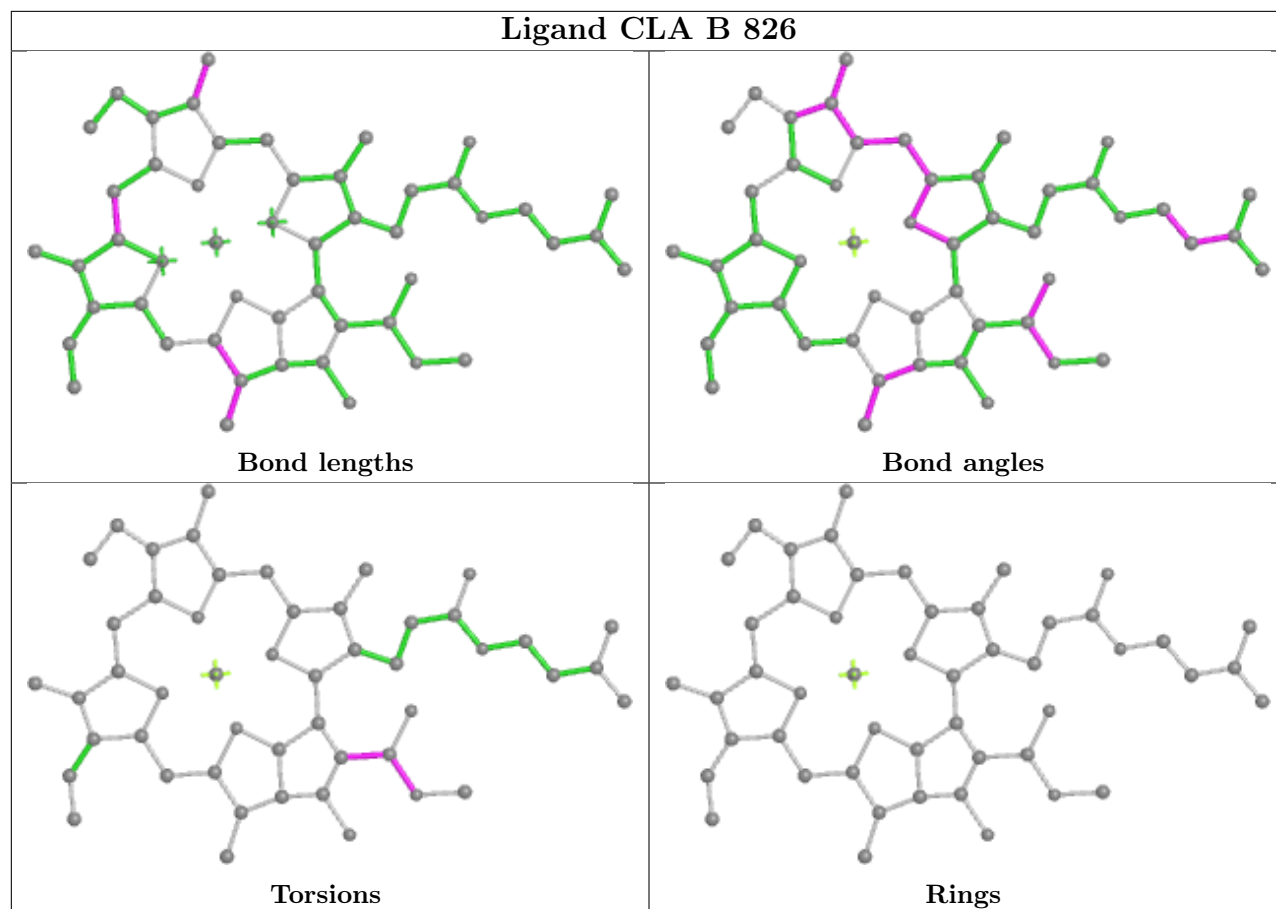


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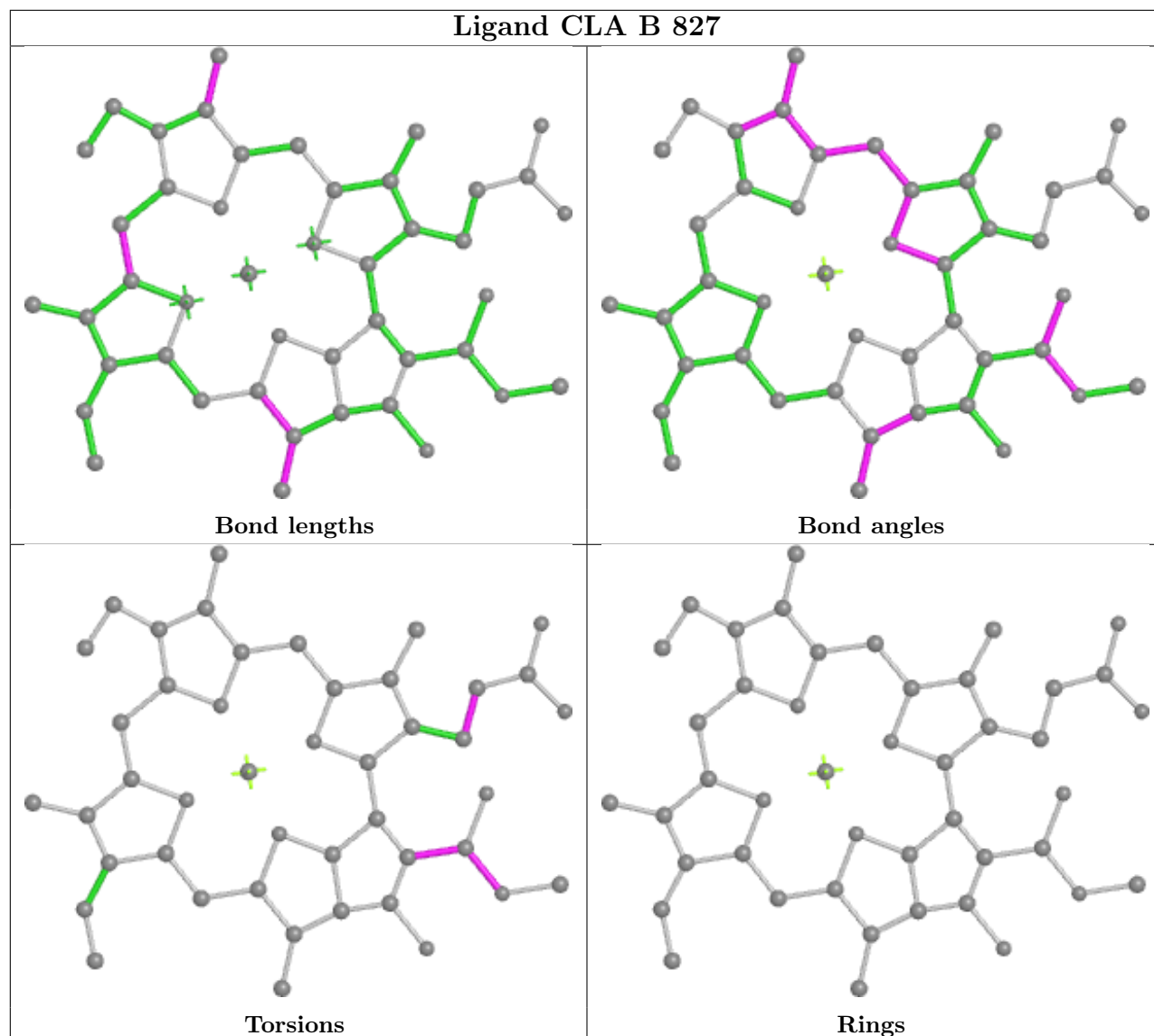


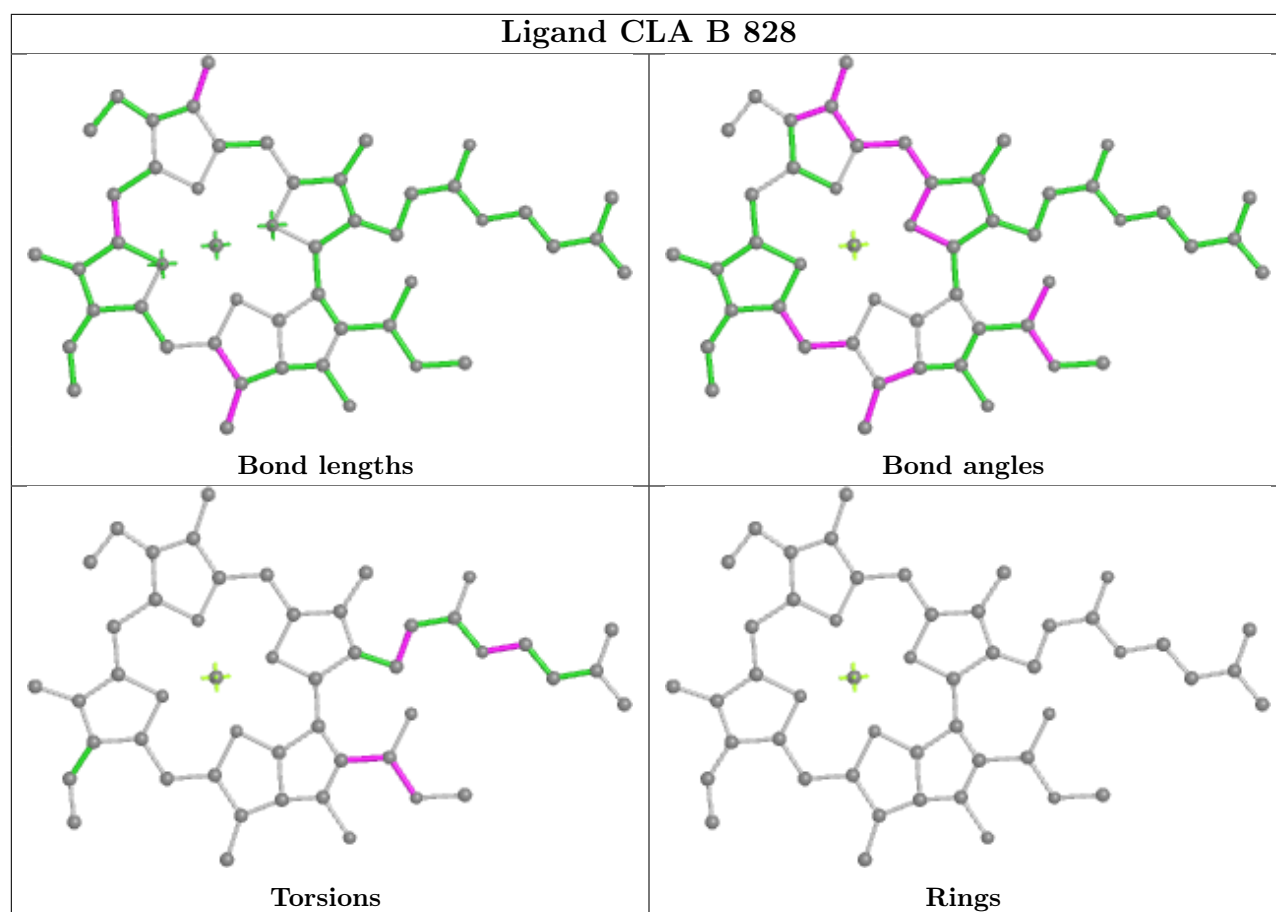
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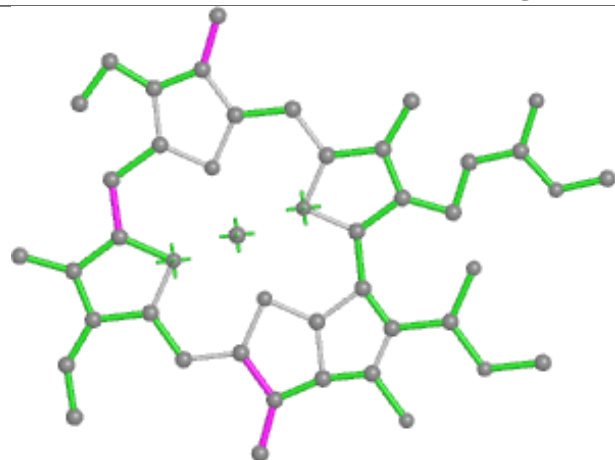


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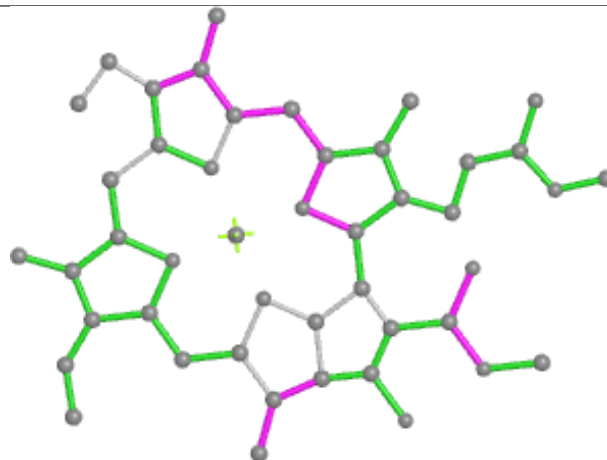




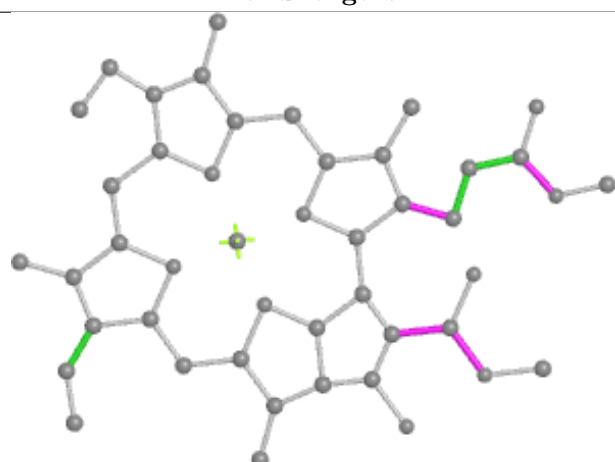
Ligand CLA B 829



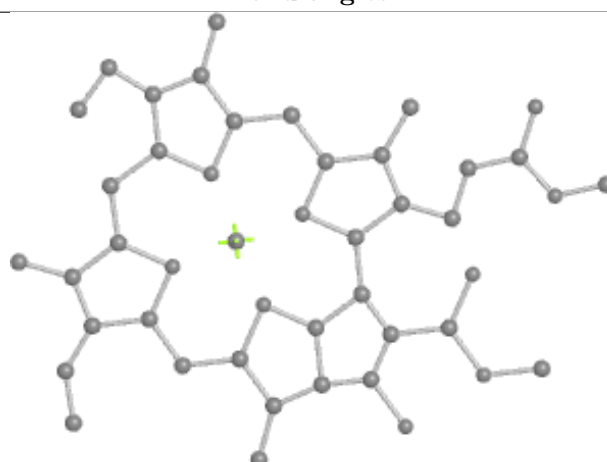
Bond lengths



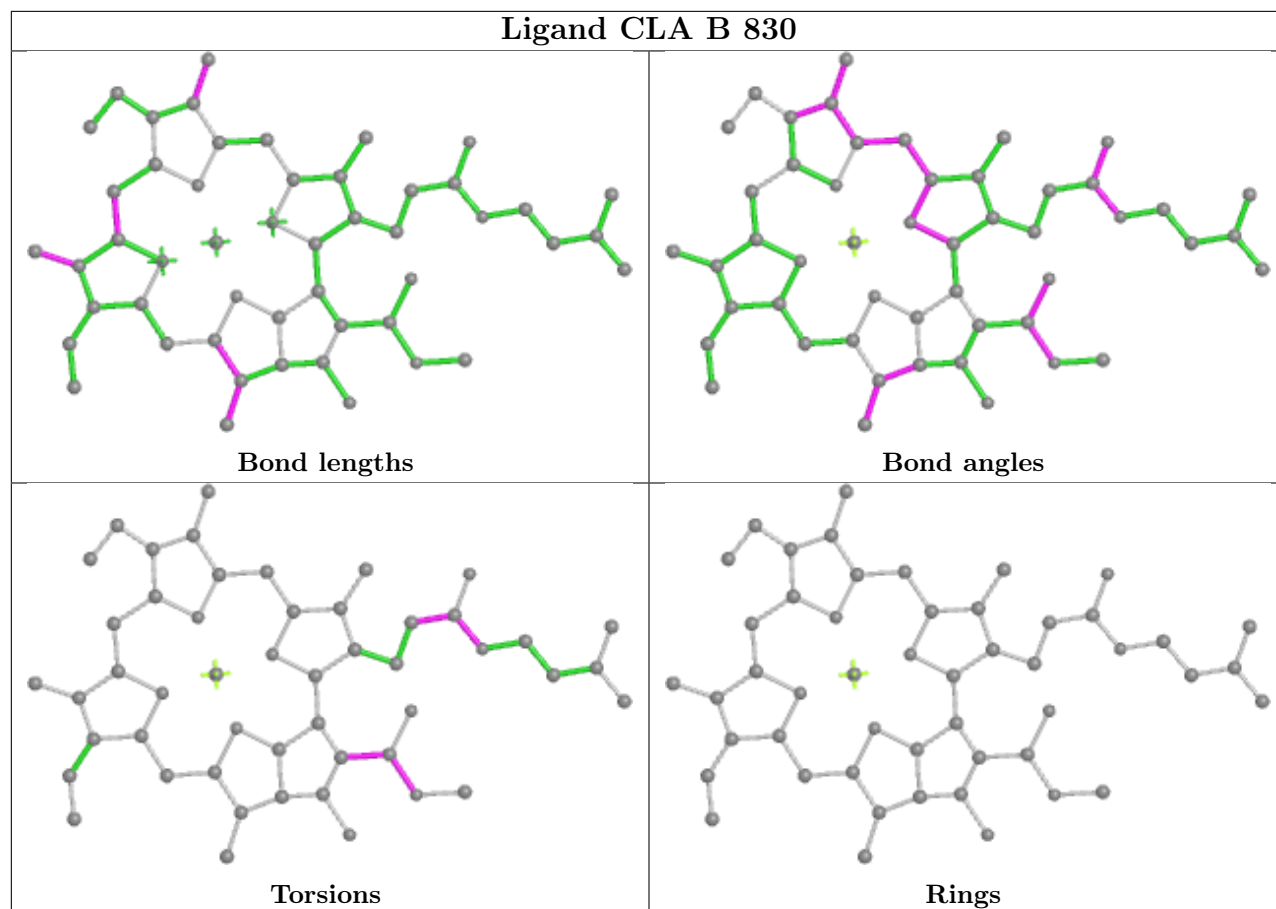
Bond angles

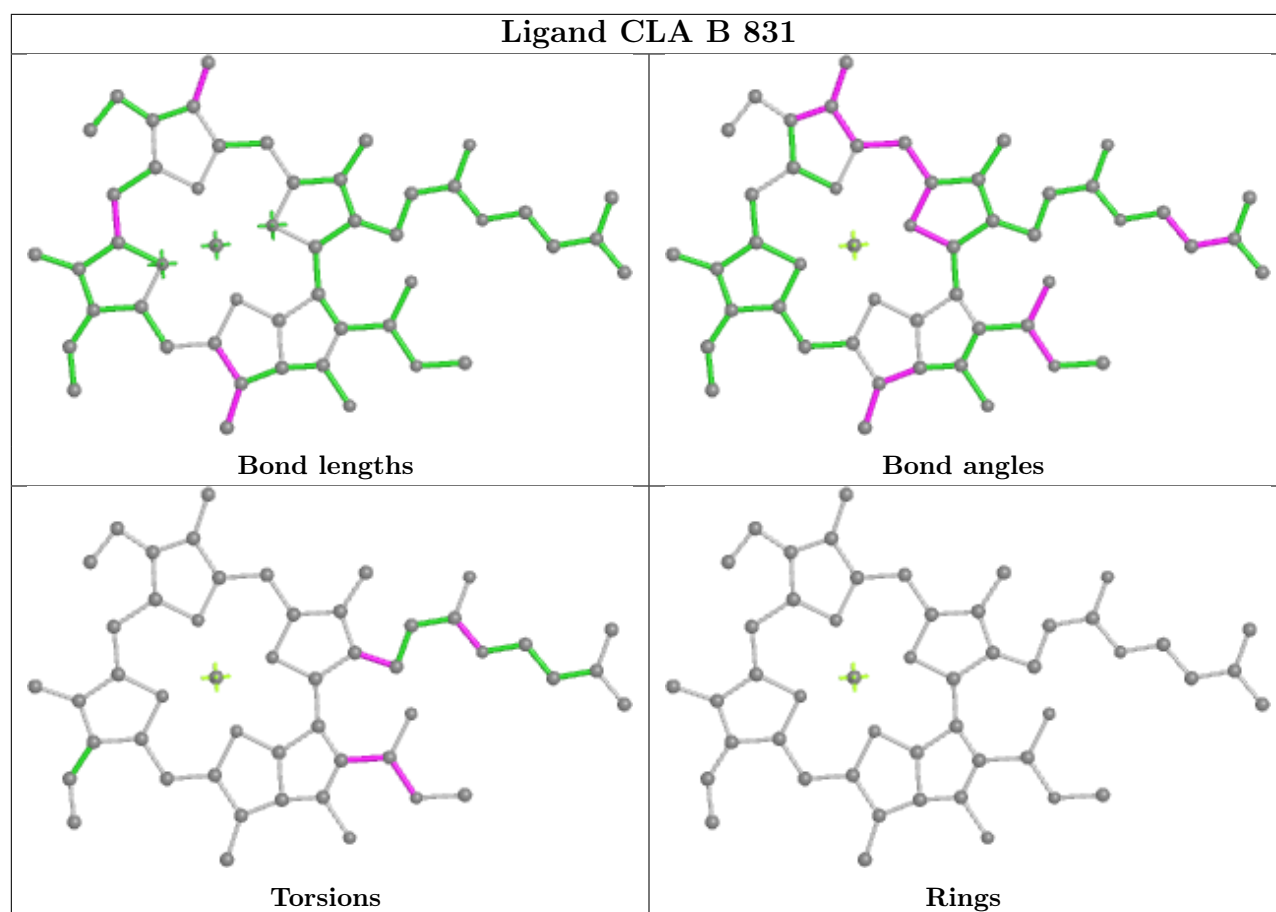


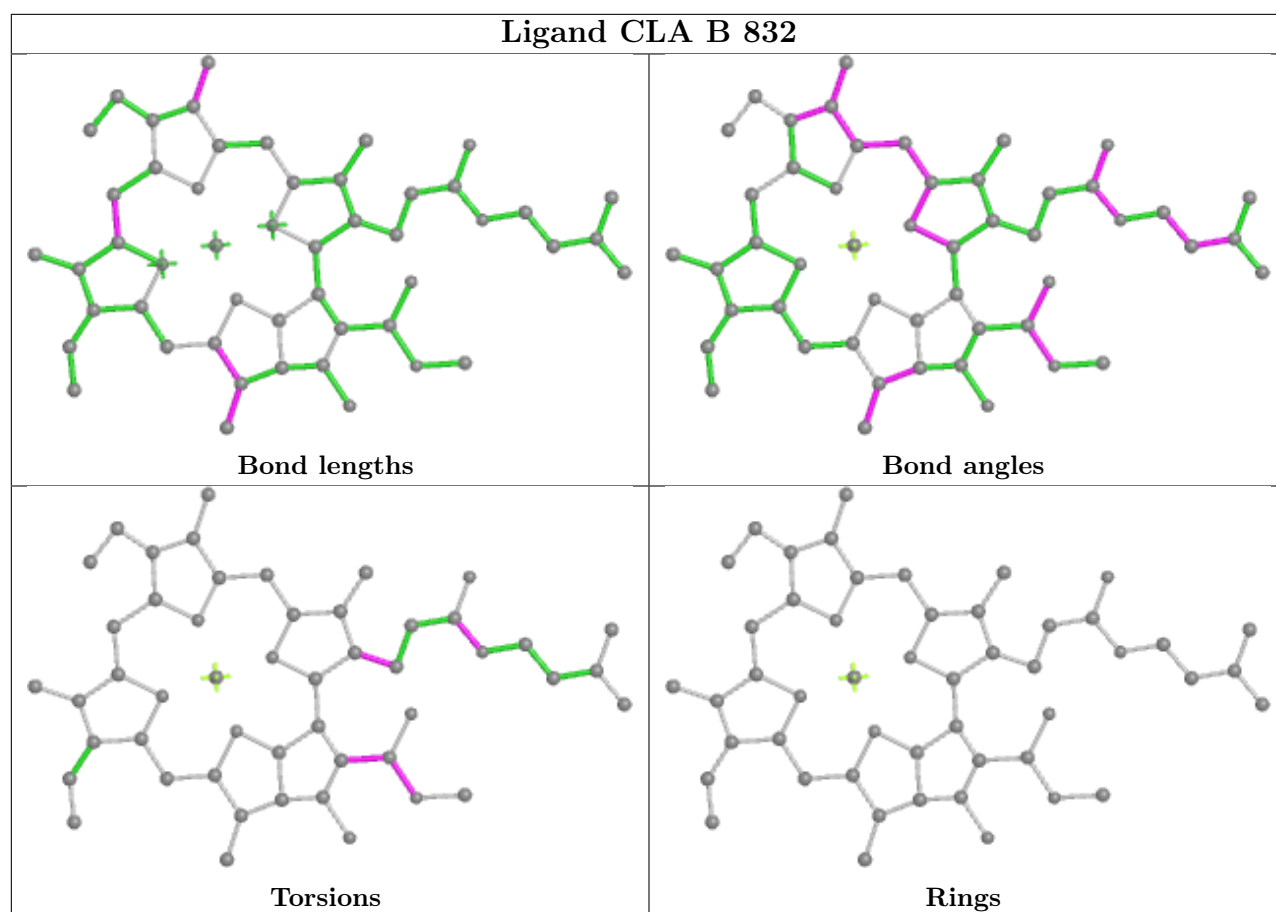
Torsions

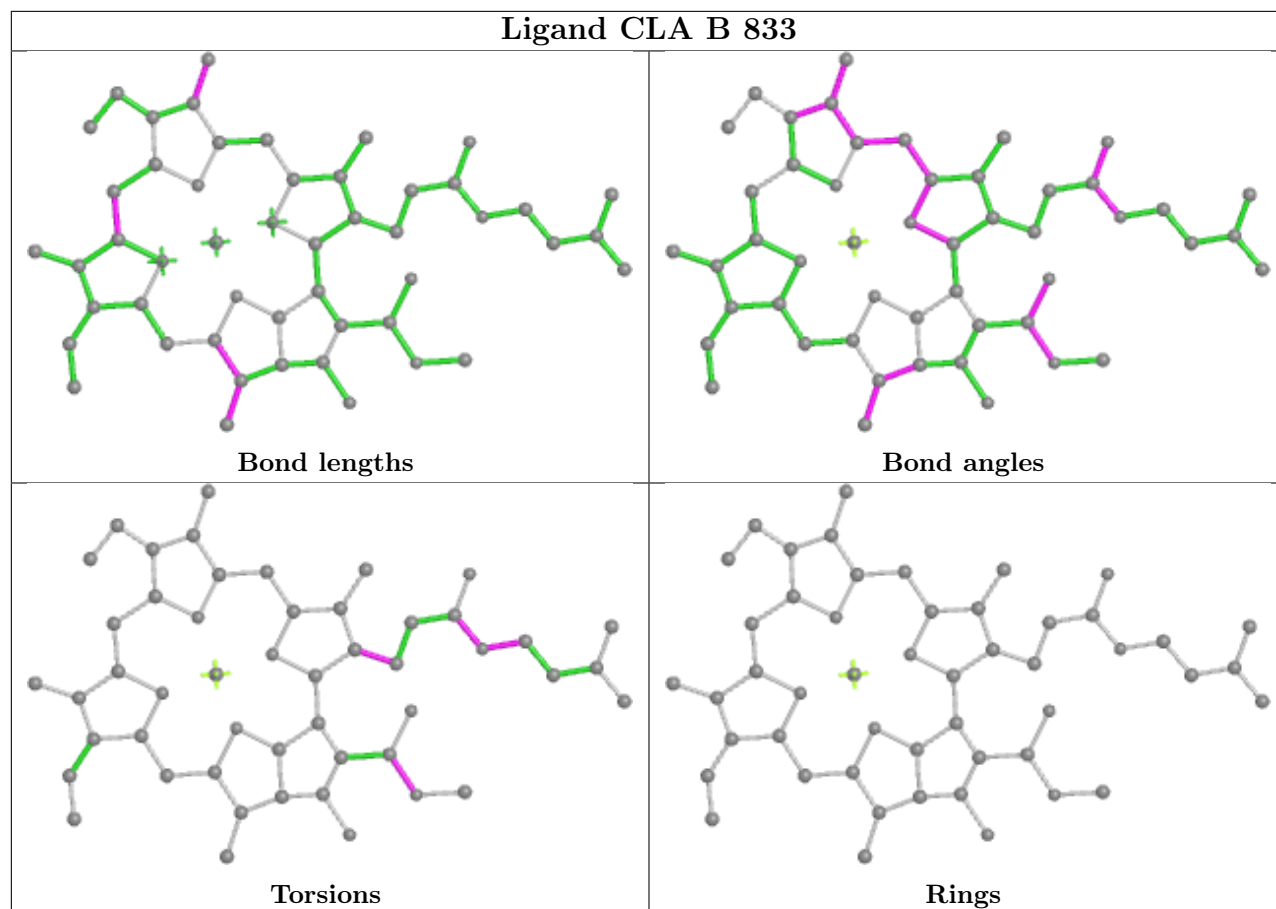


Rings

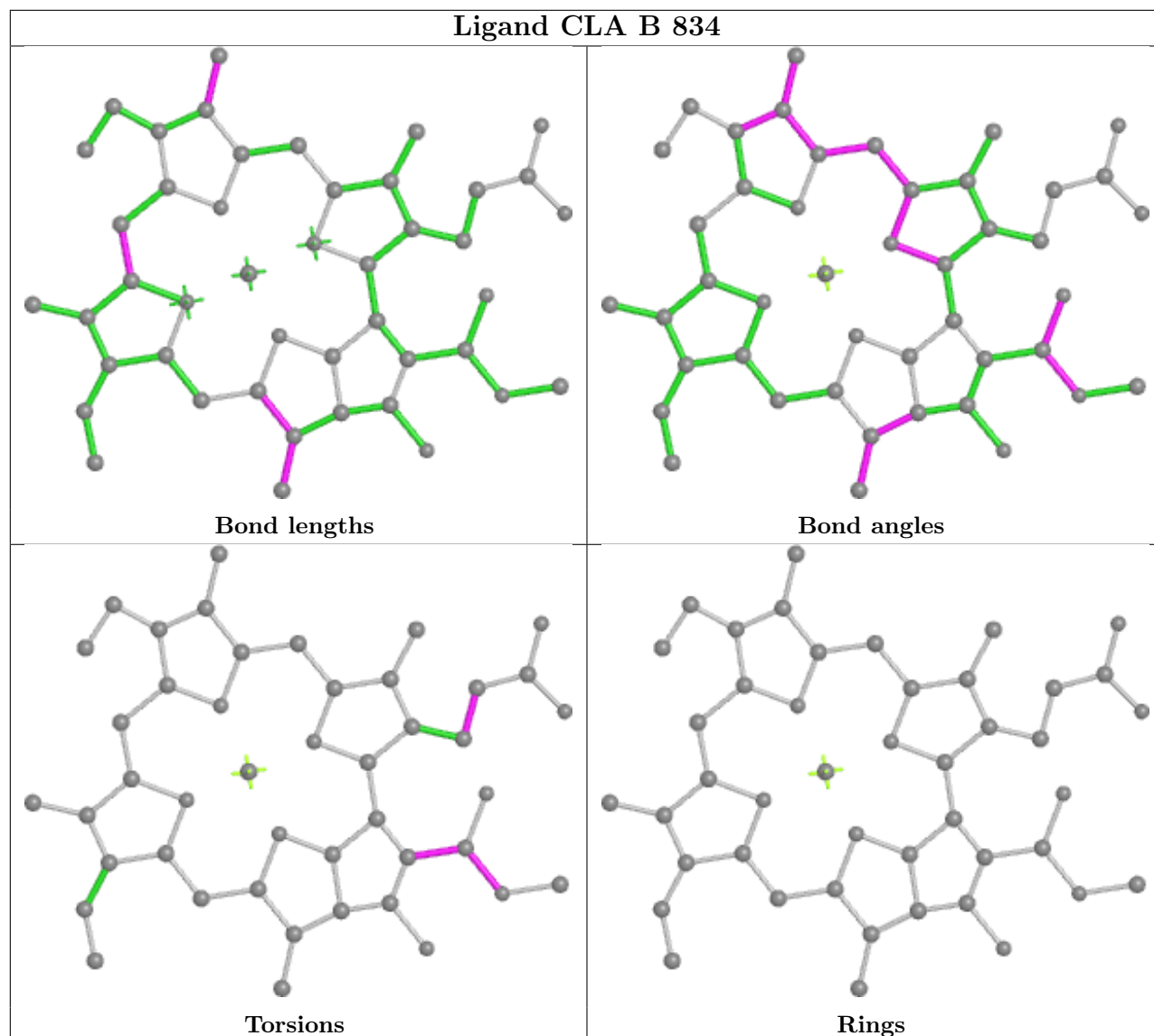


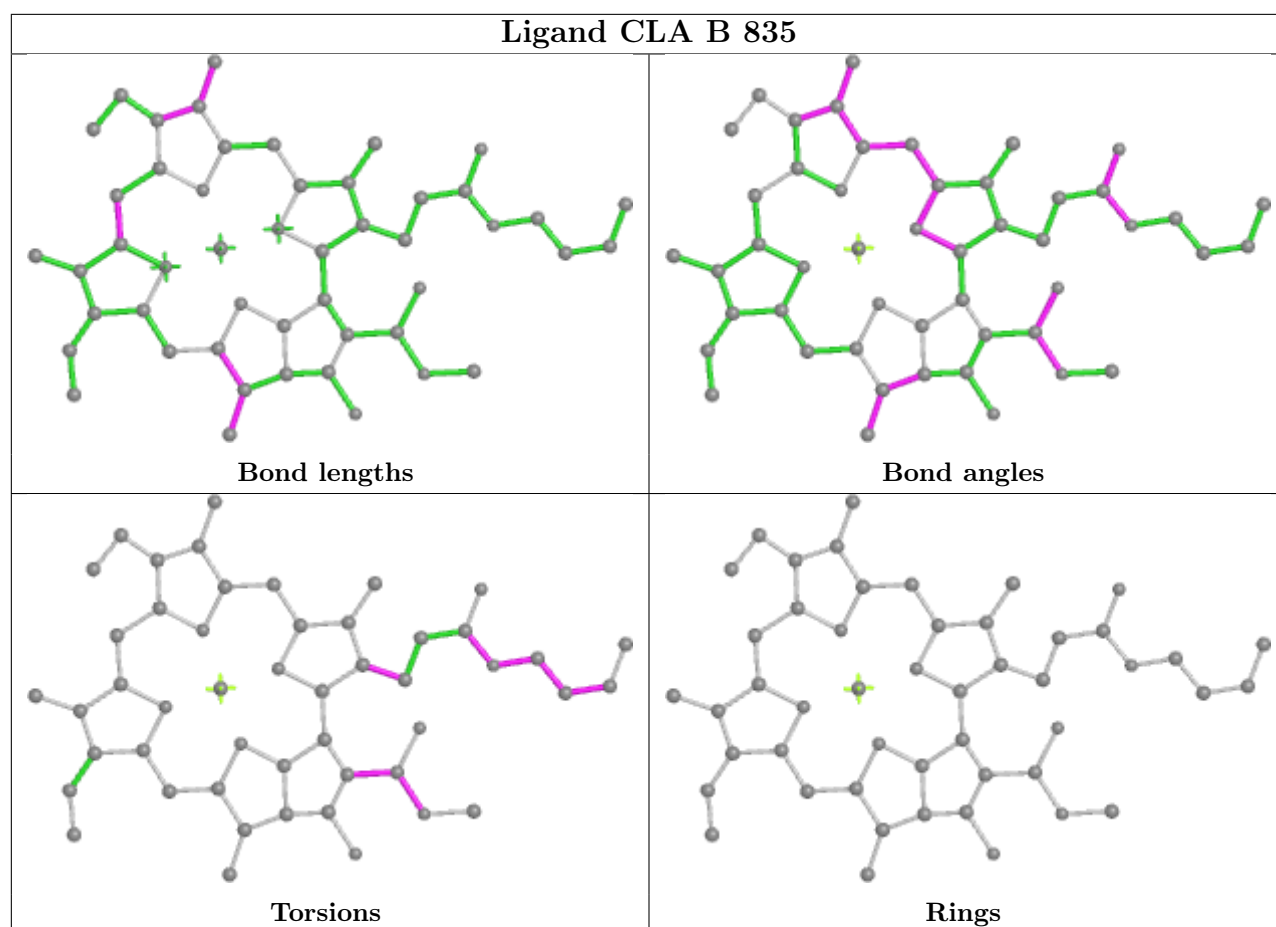


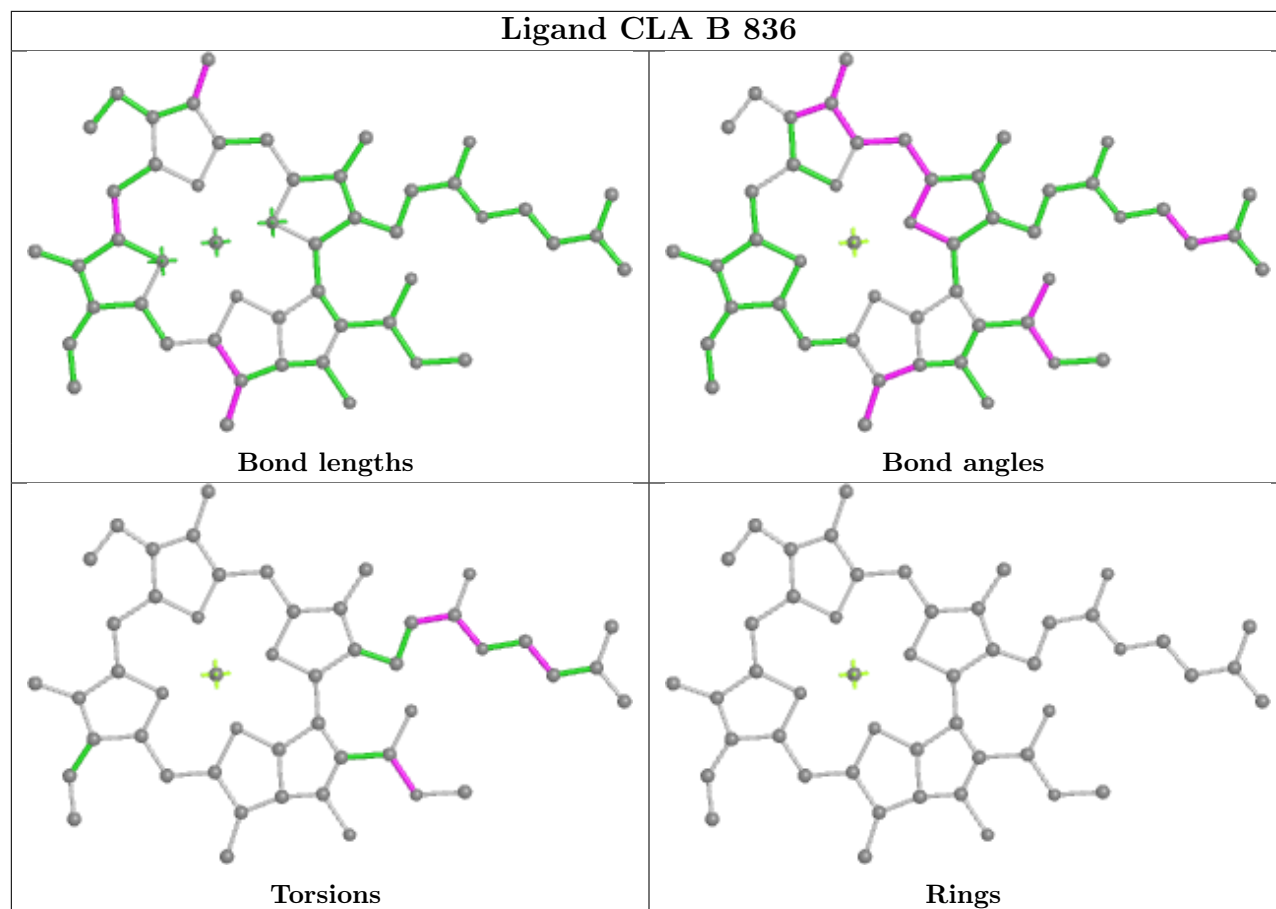




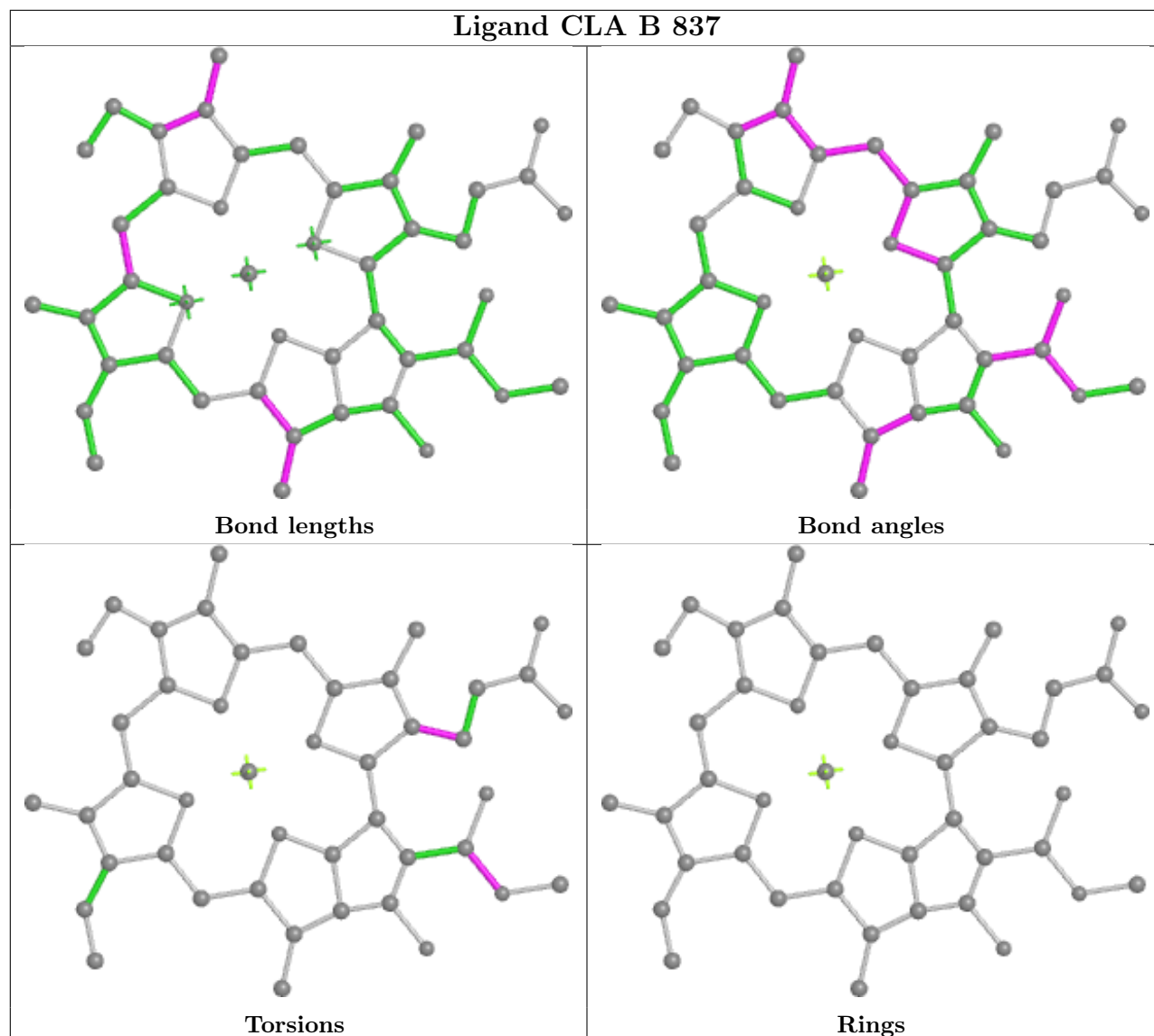
Ligand CLA B 834



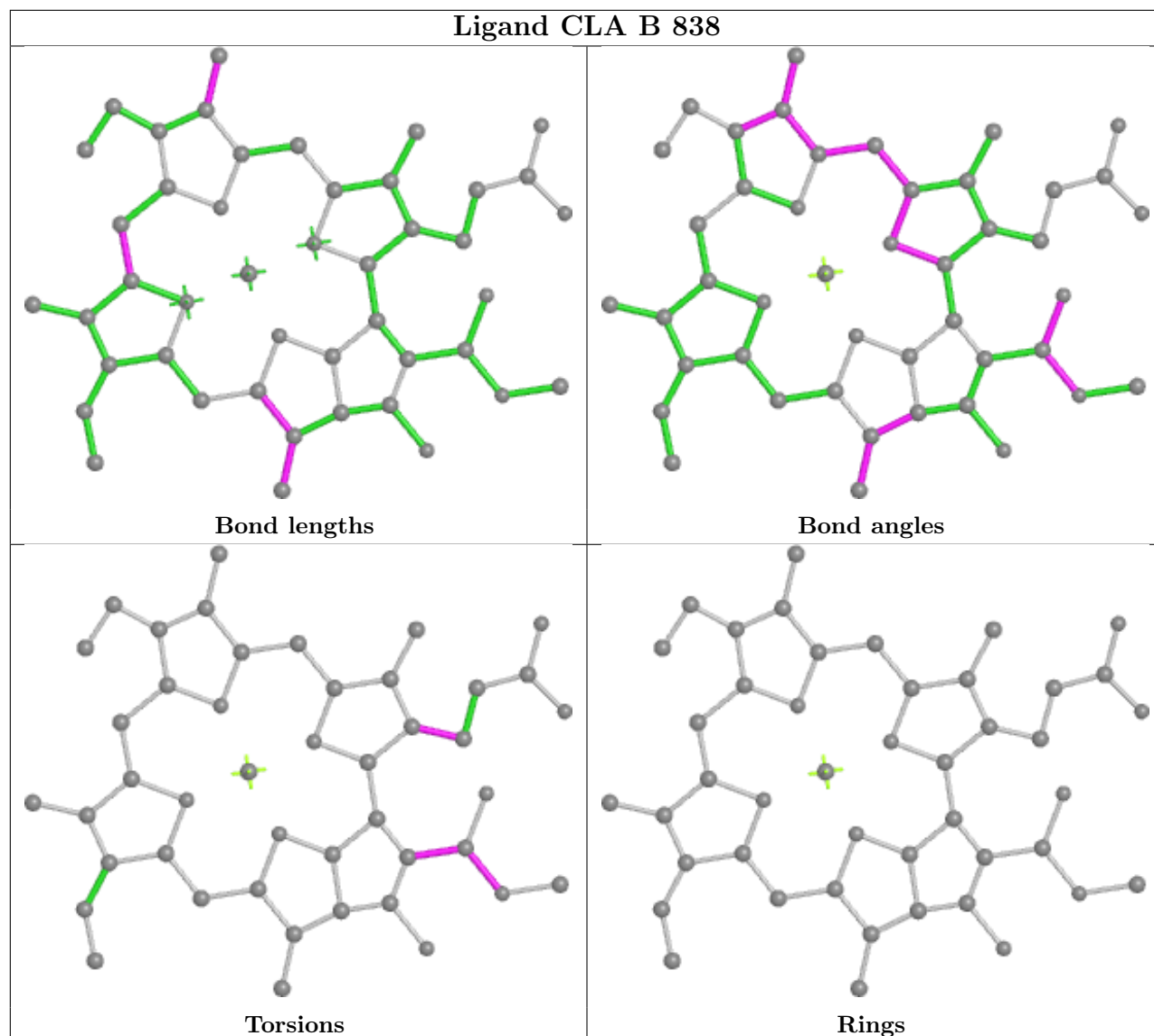


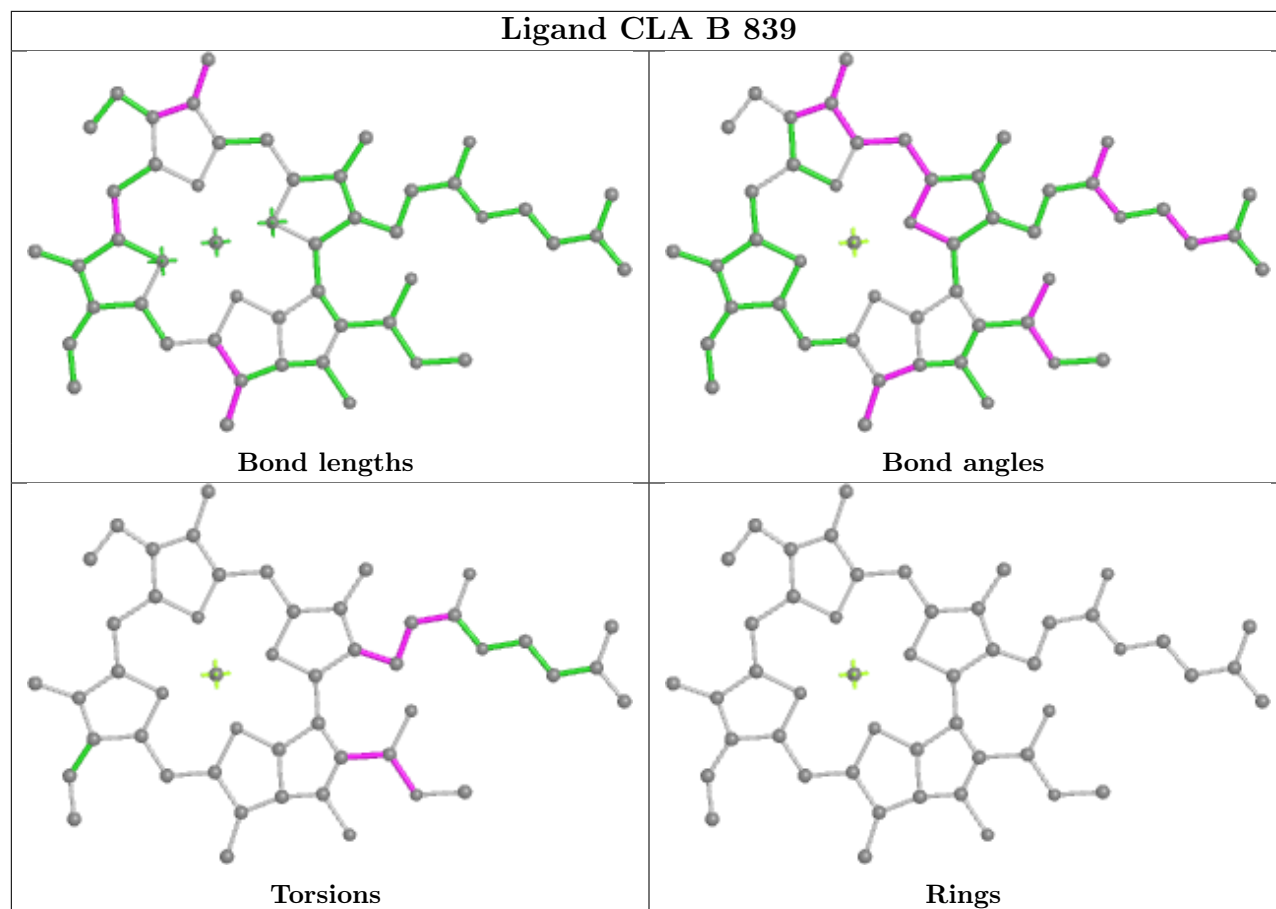


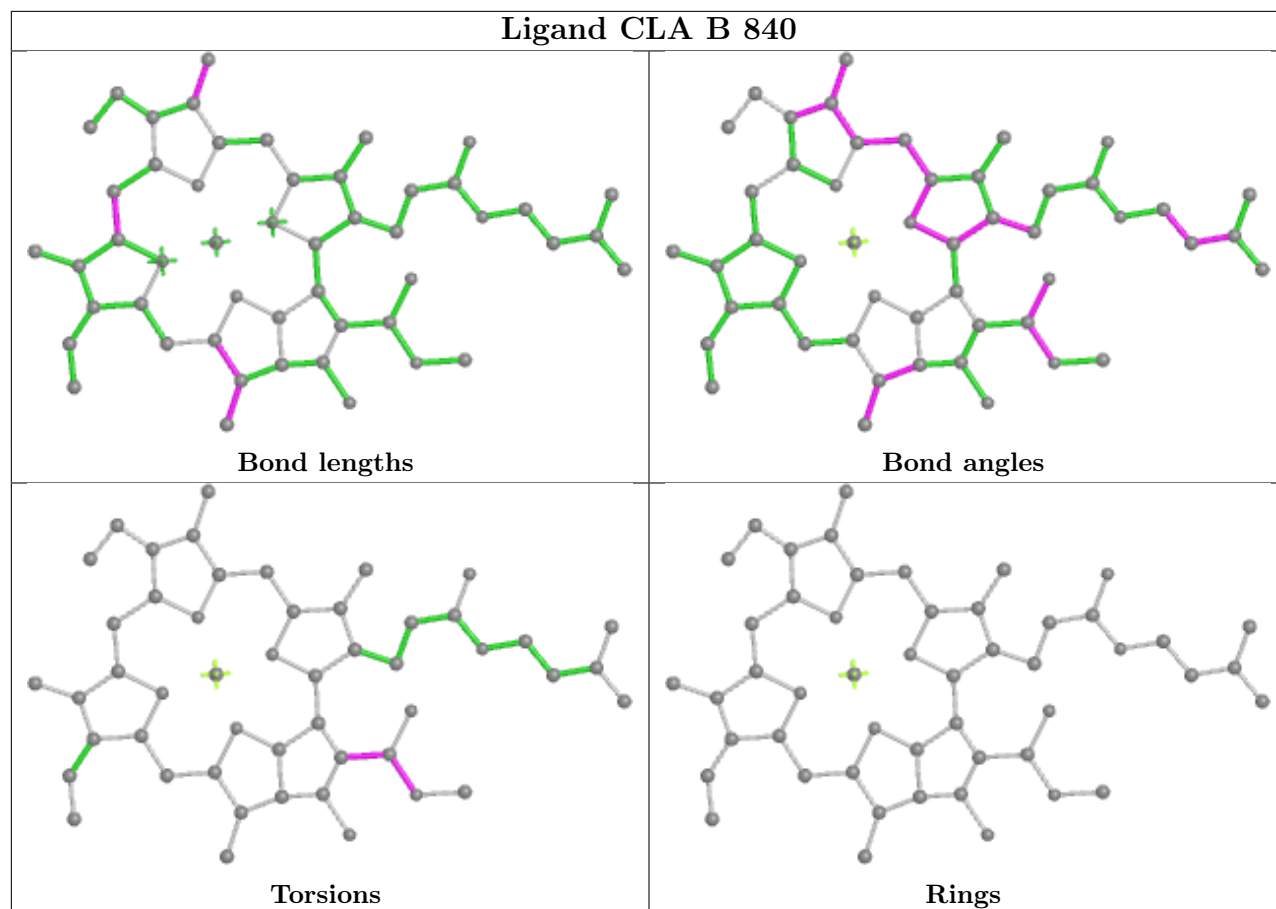
Ligand CLA B 837



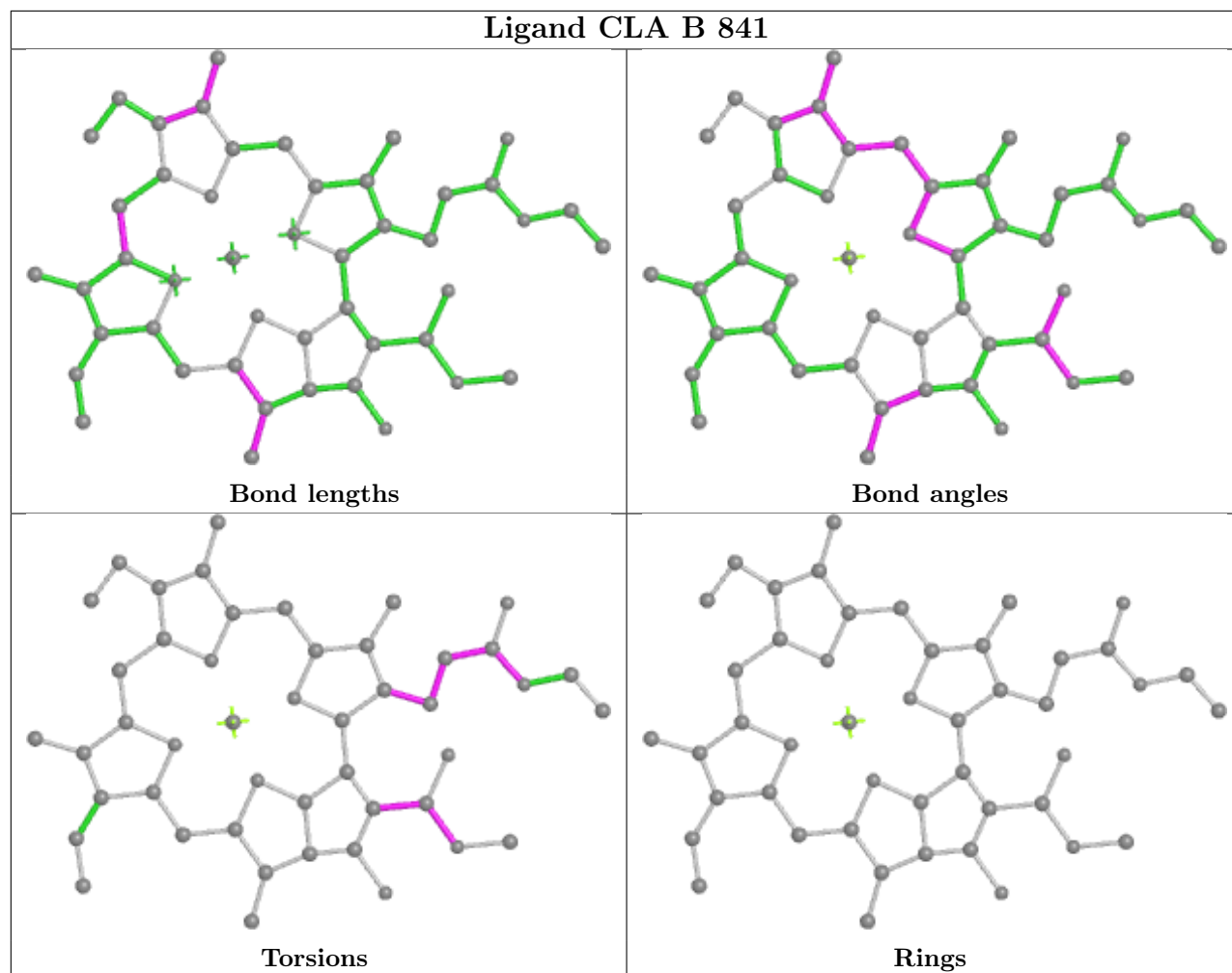
Ligand CLA B 838

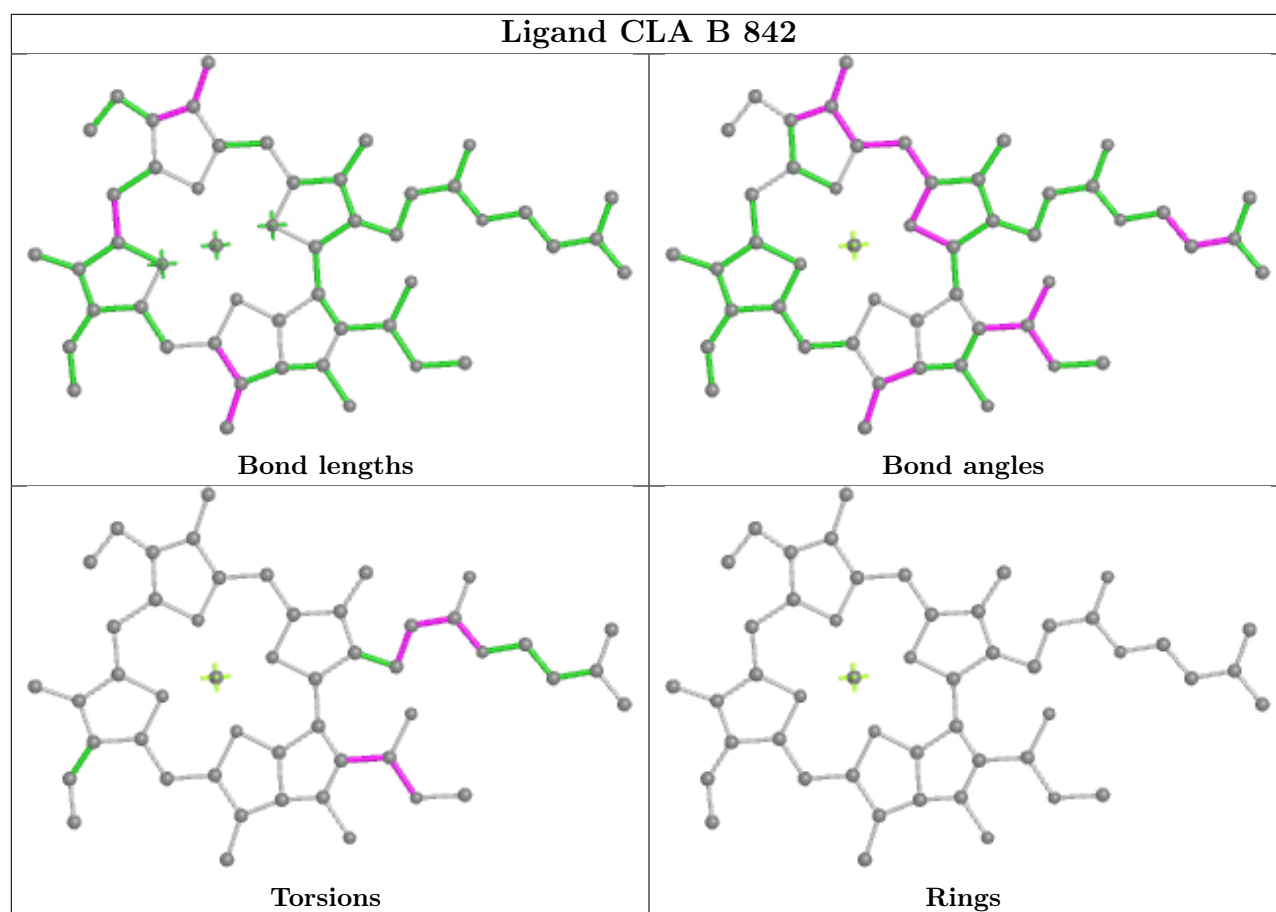


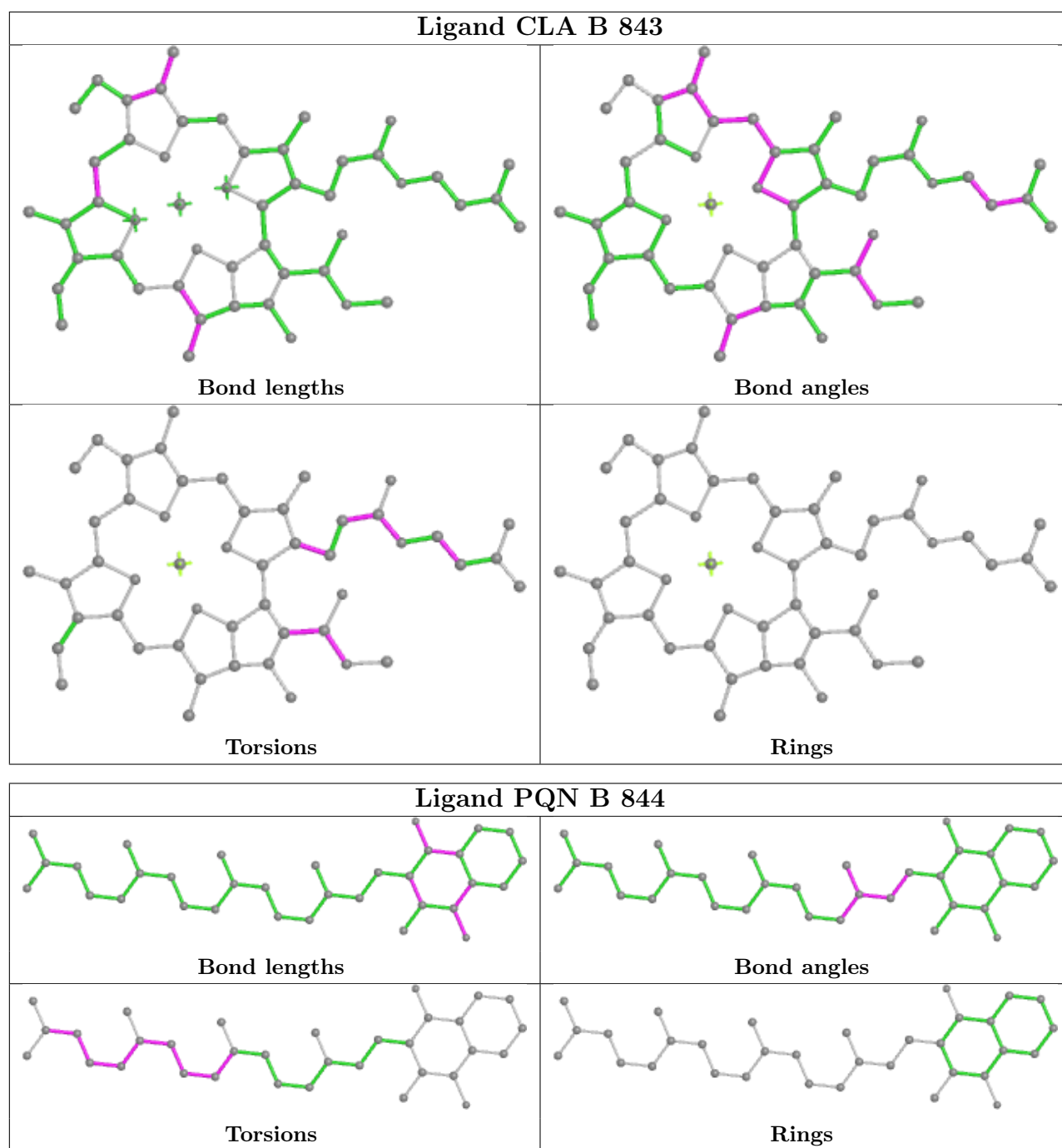


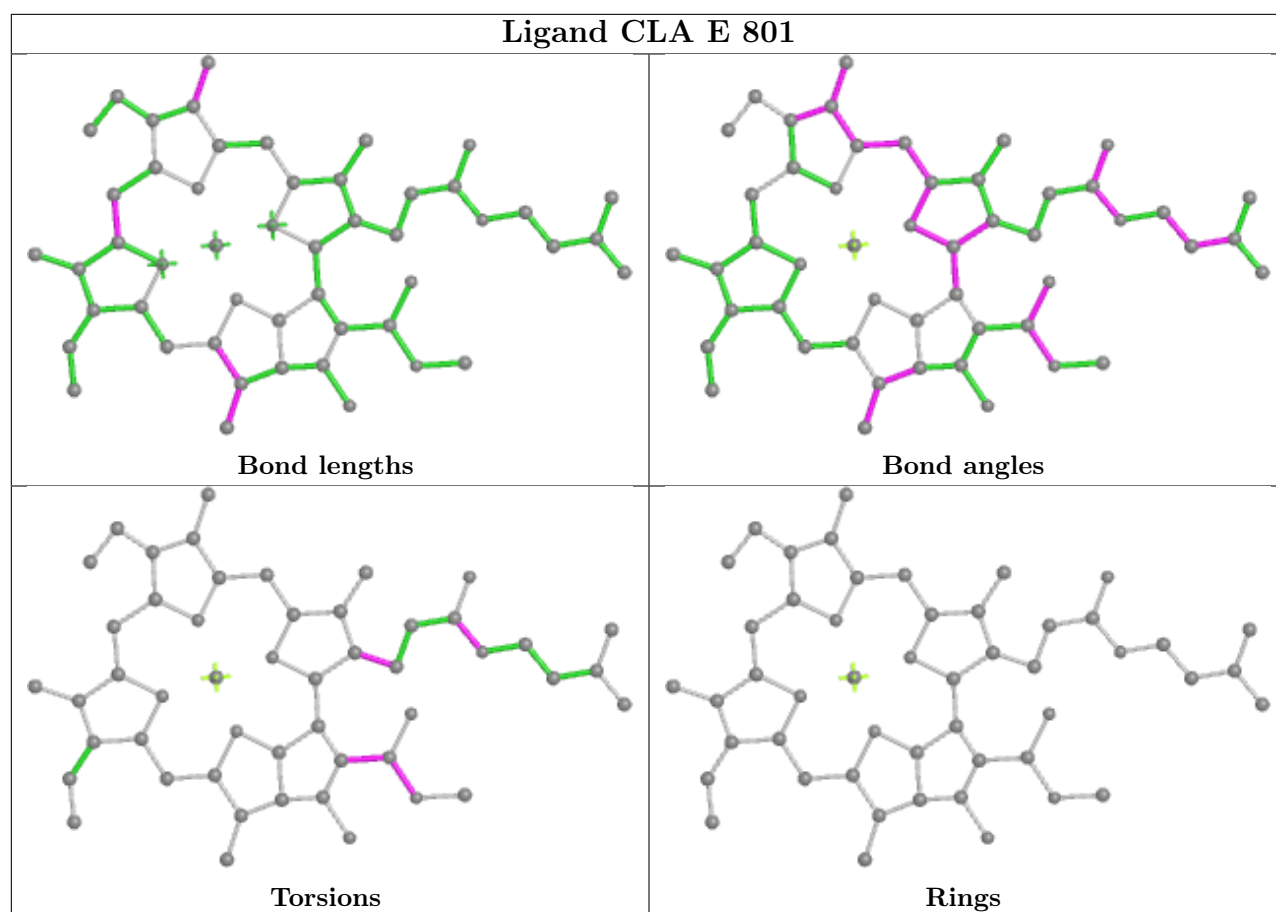


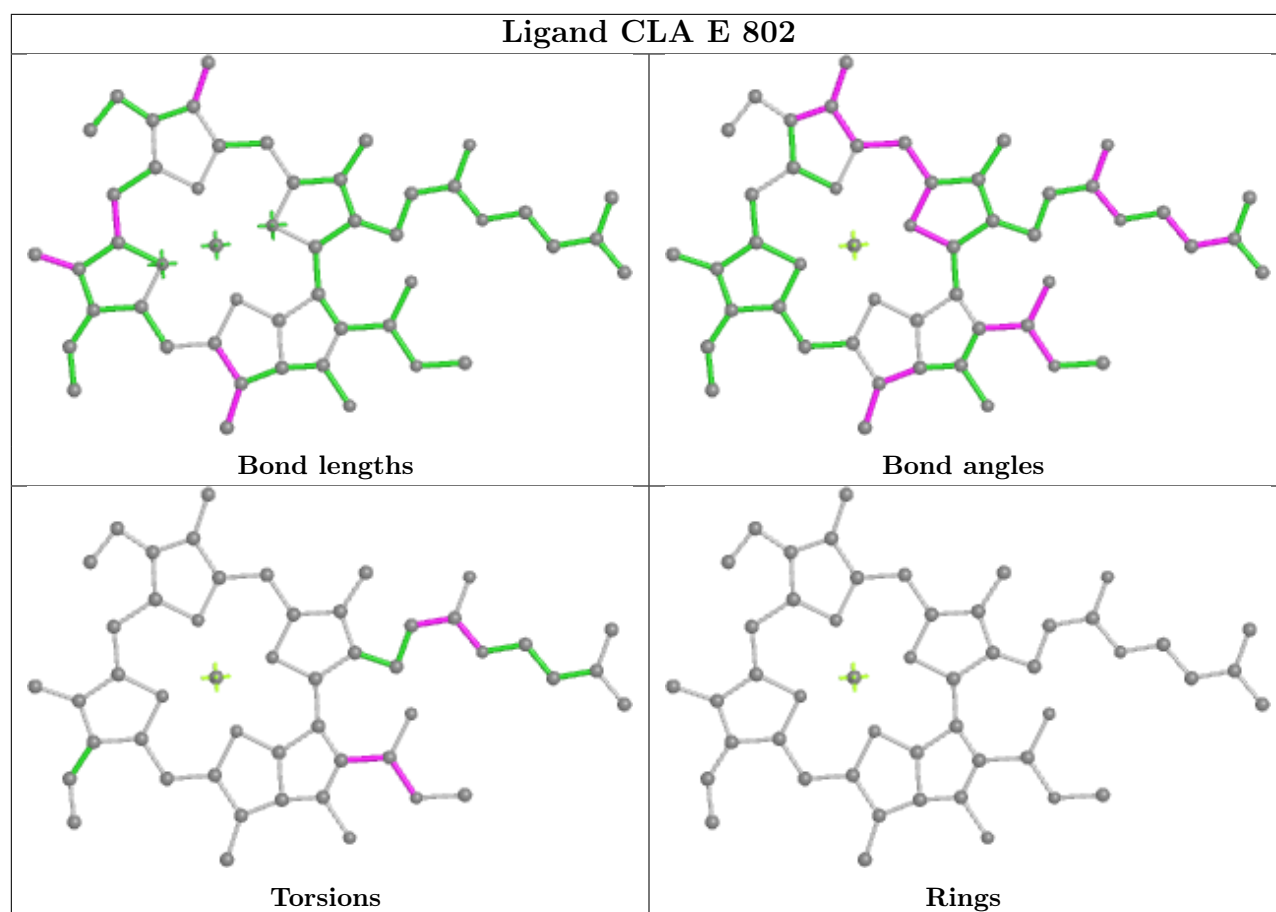
Ligand CLA B 841

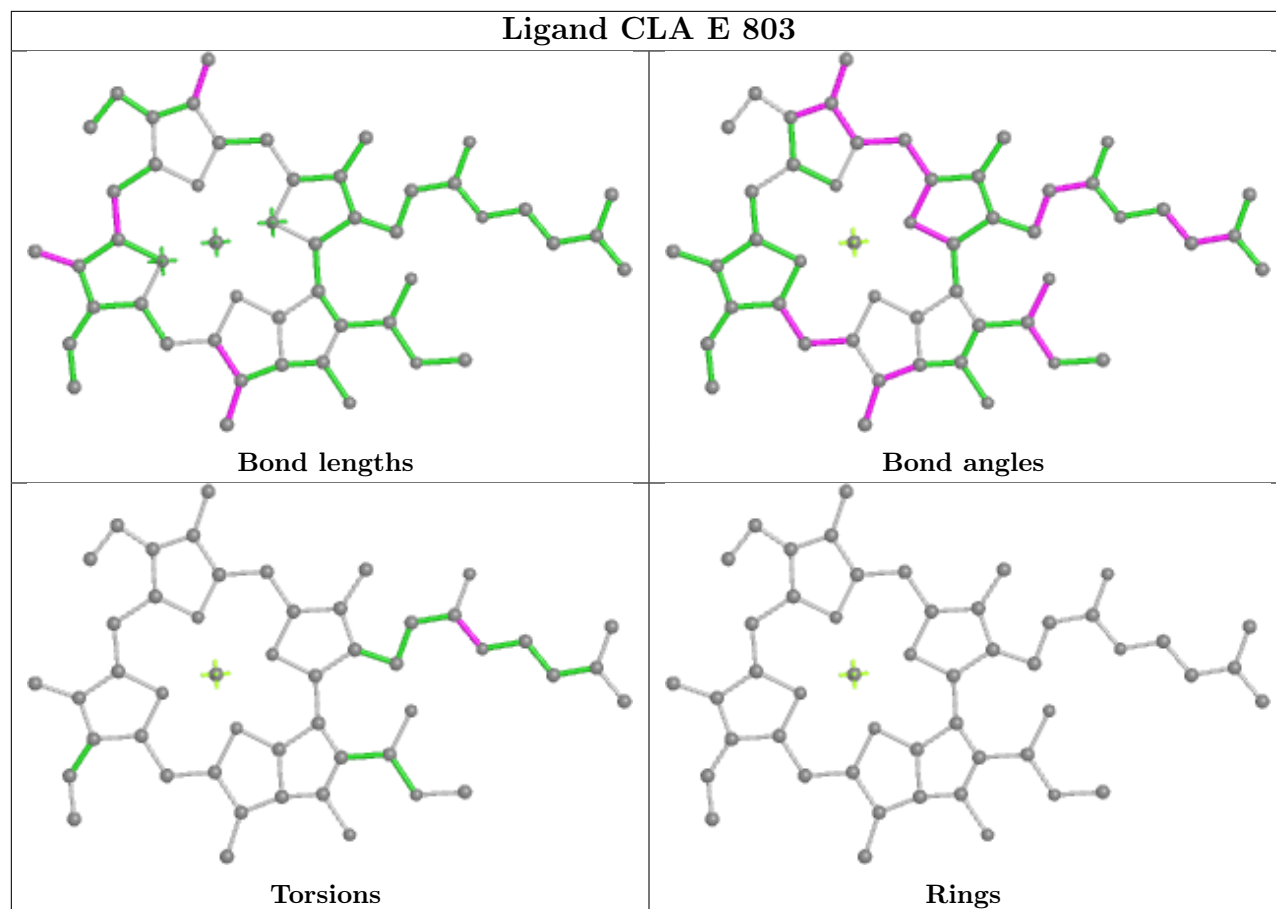


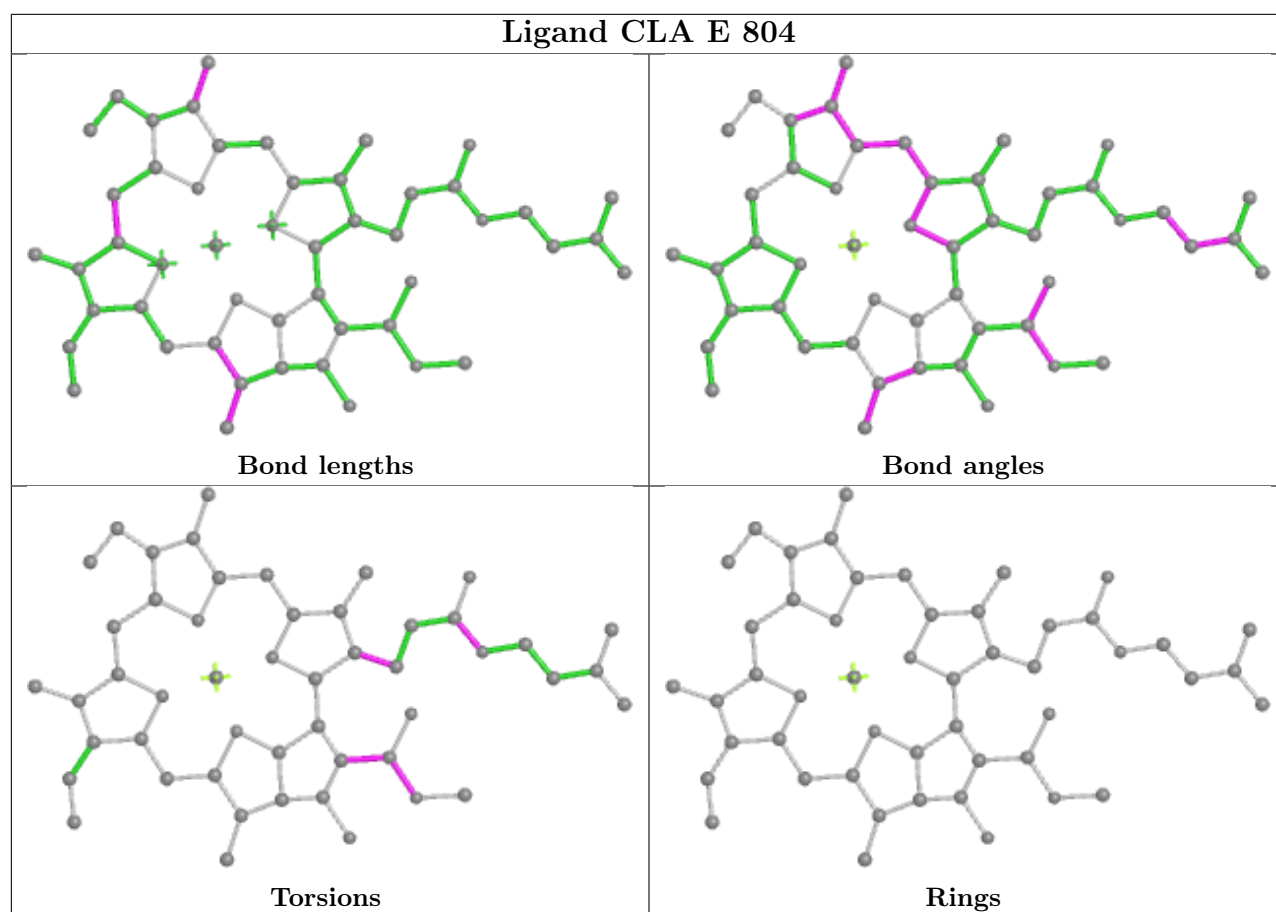


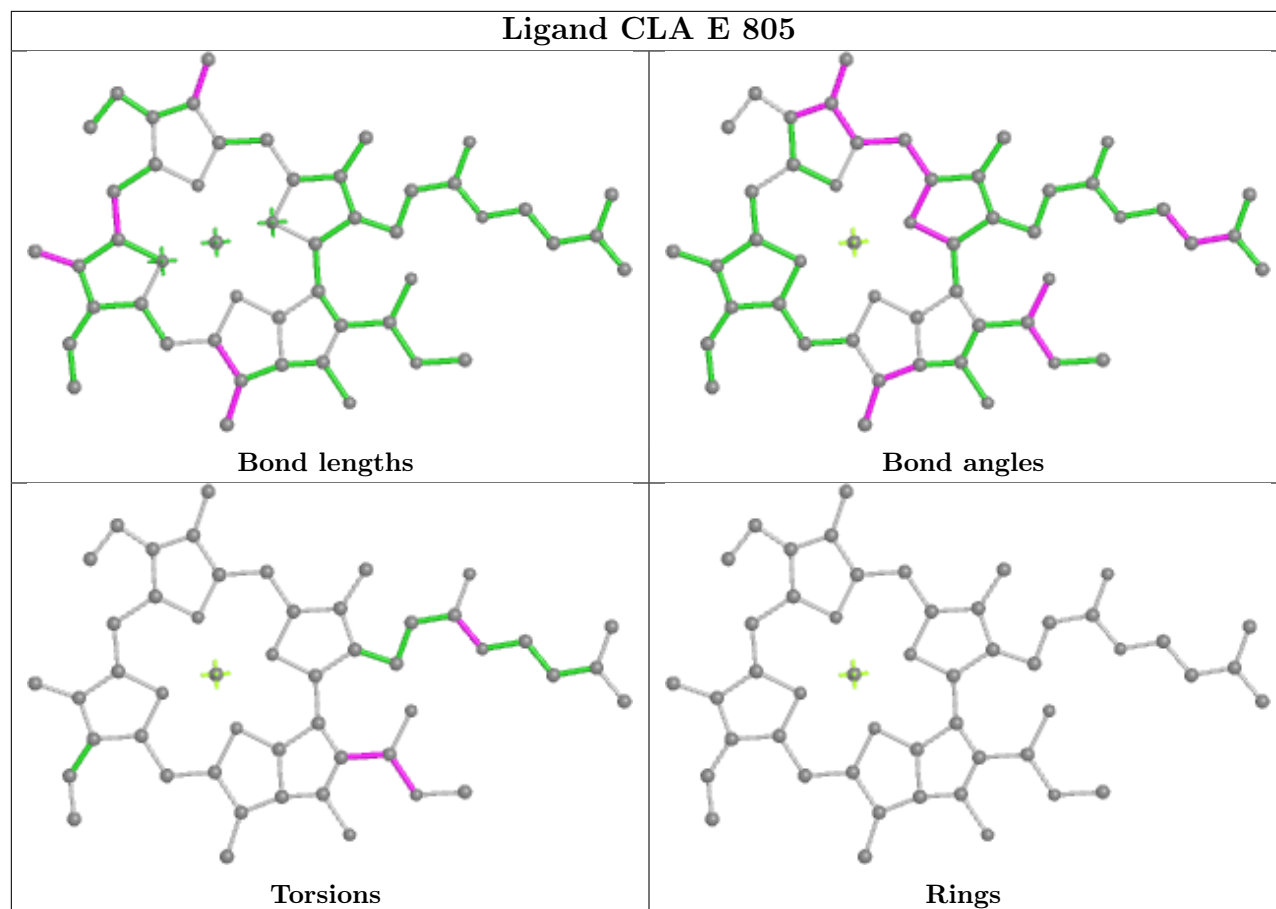




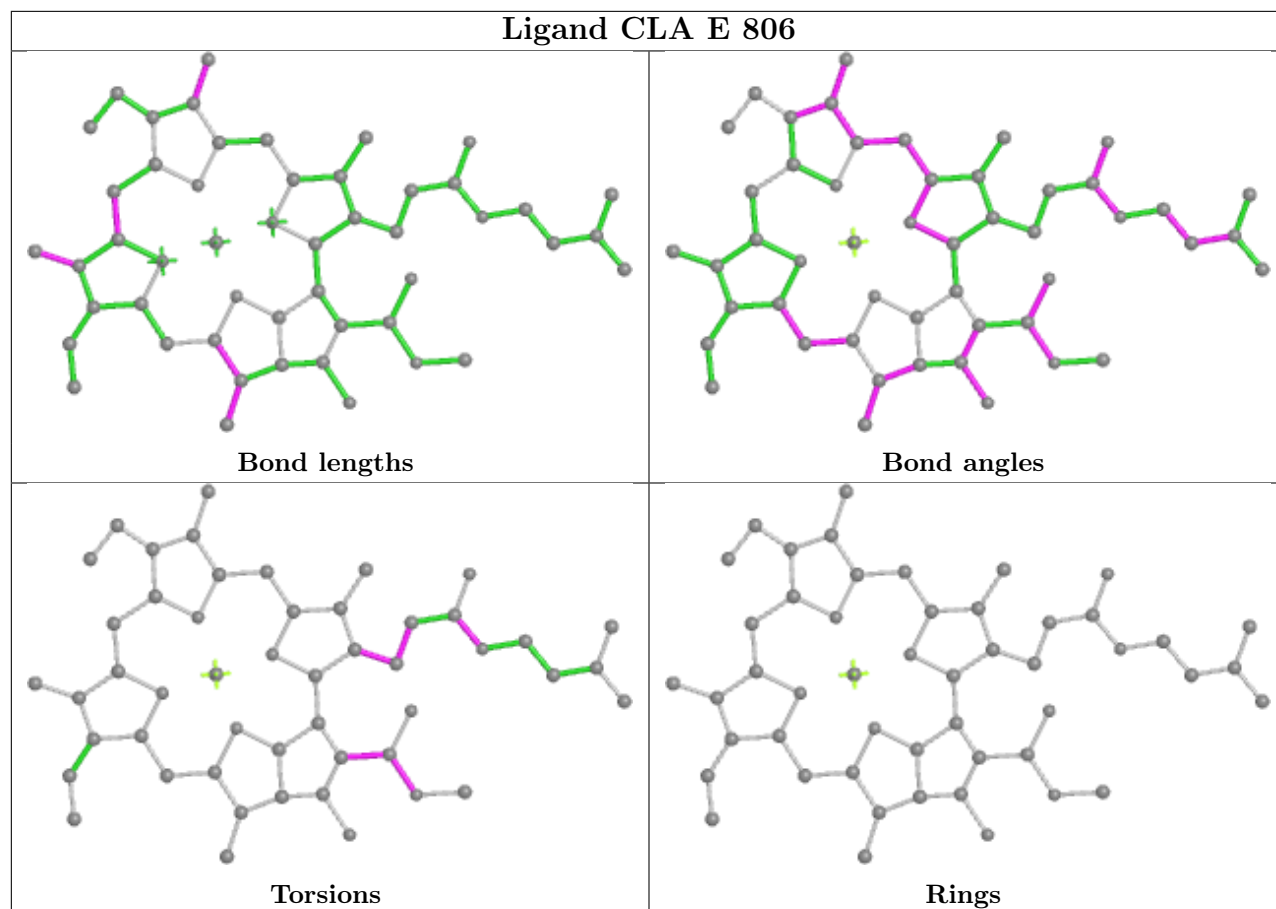


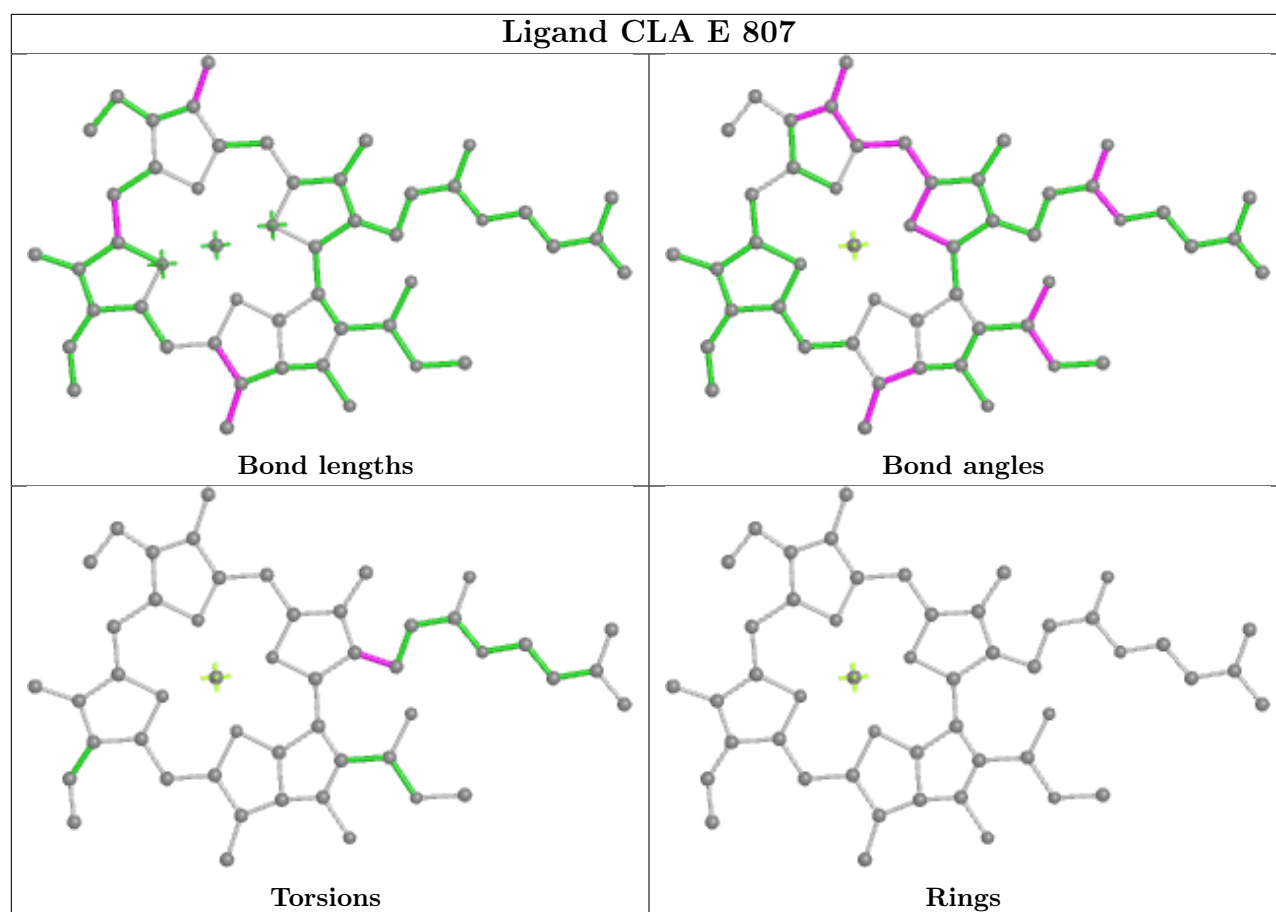




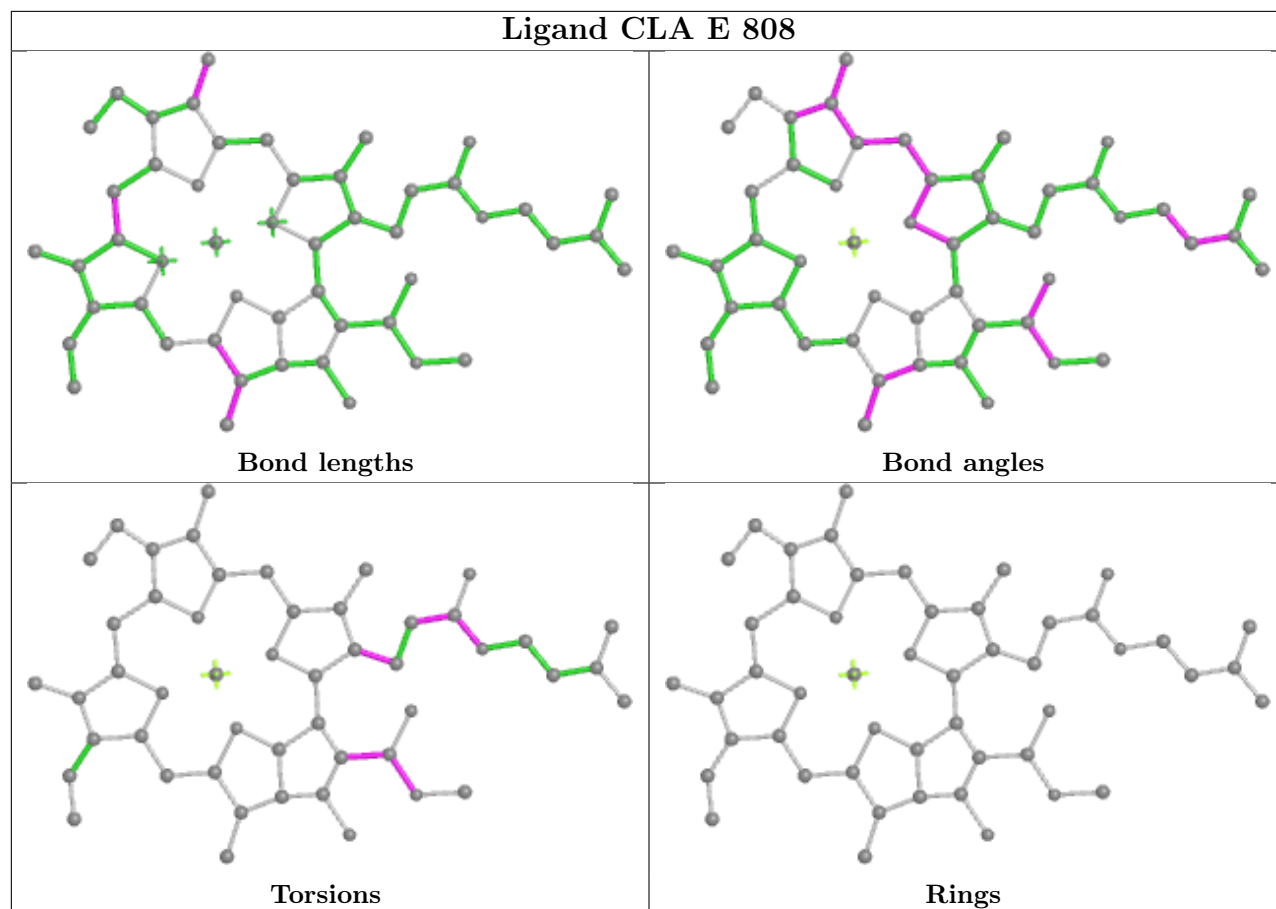


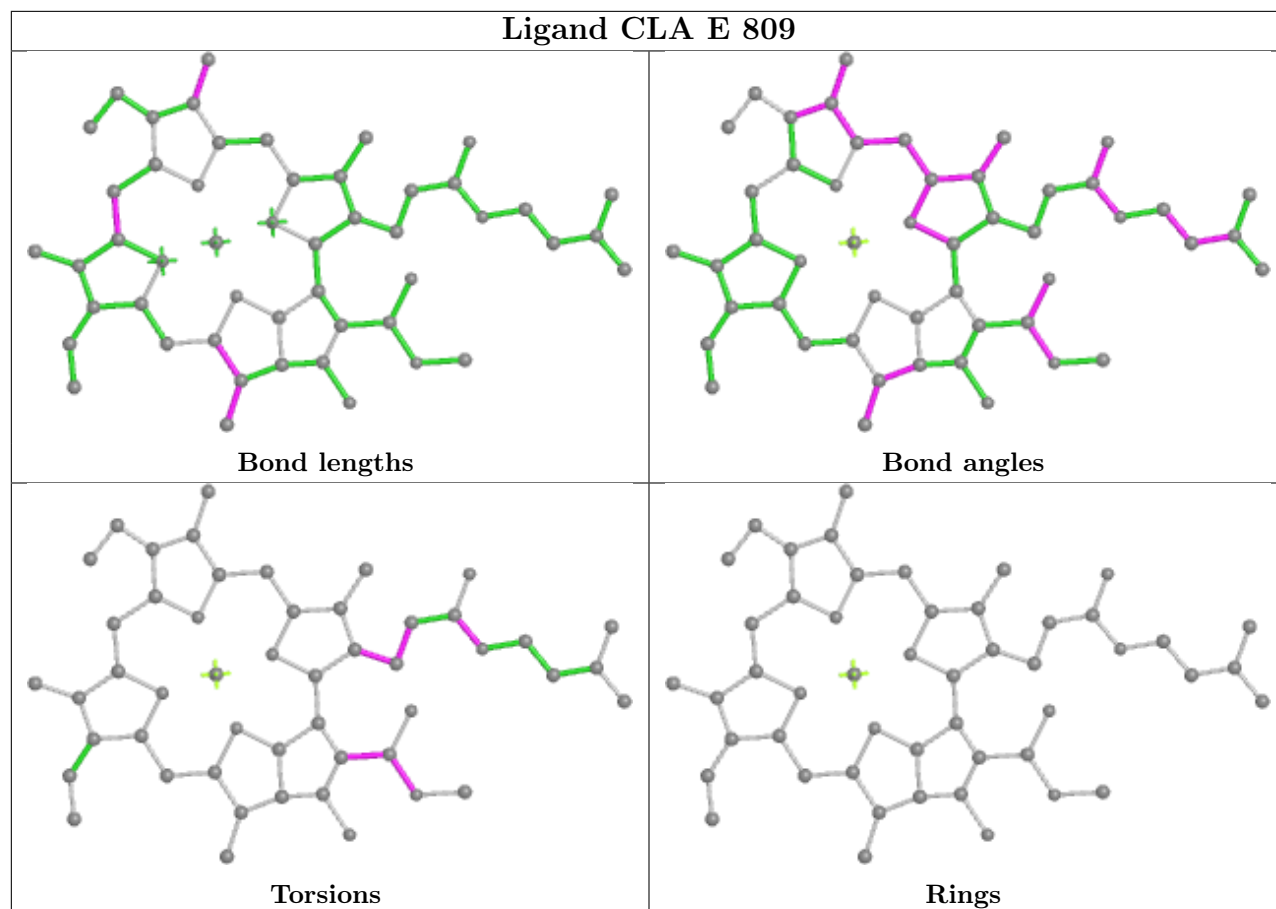
Ligand CLA E 806

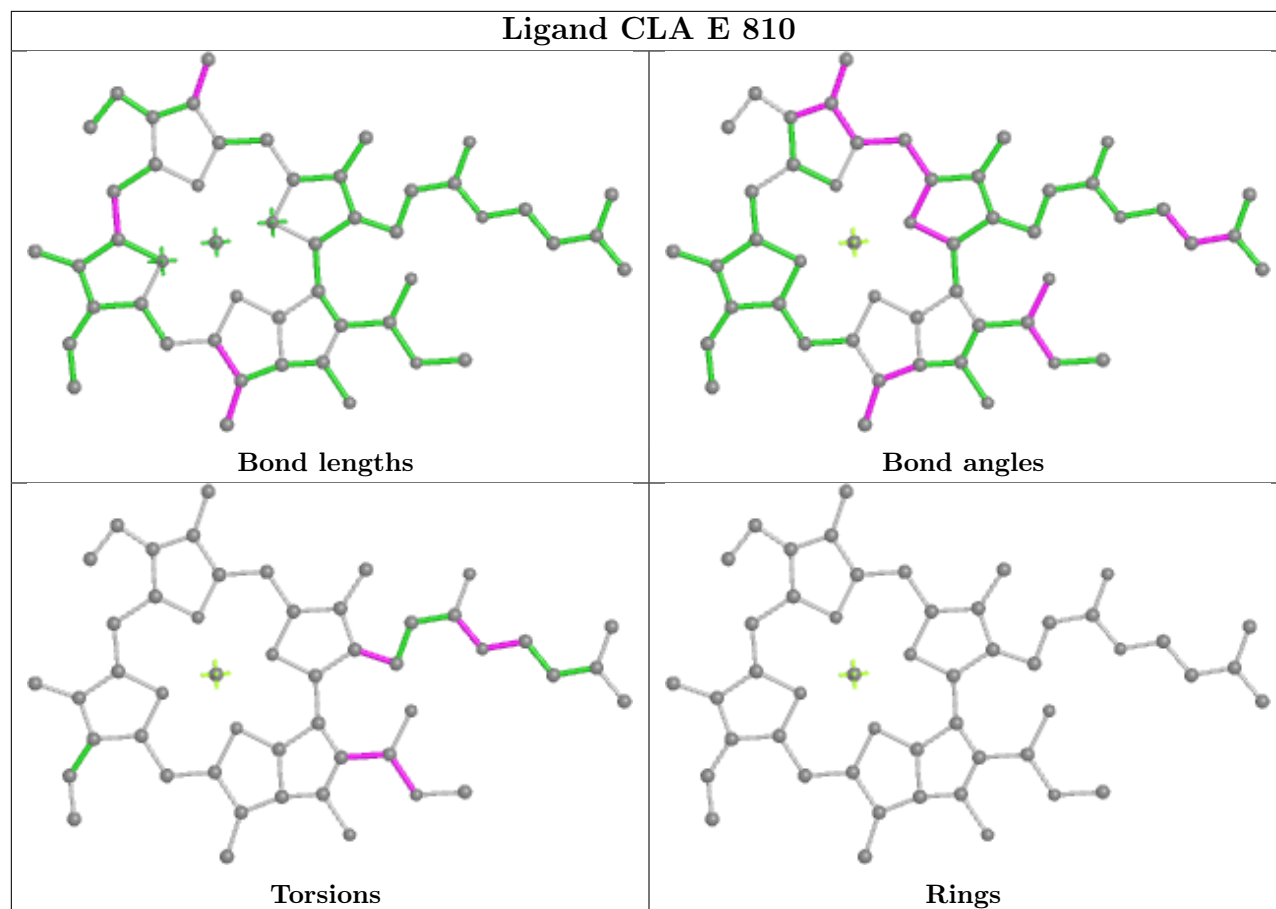




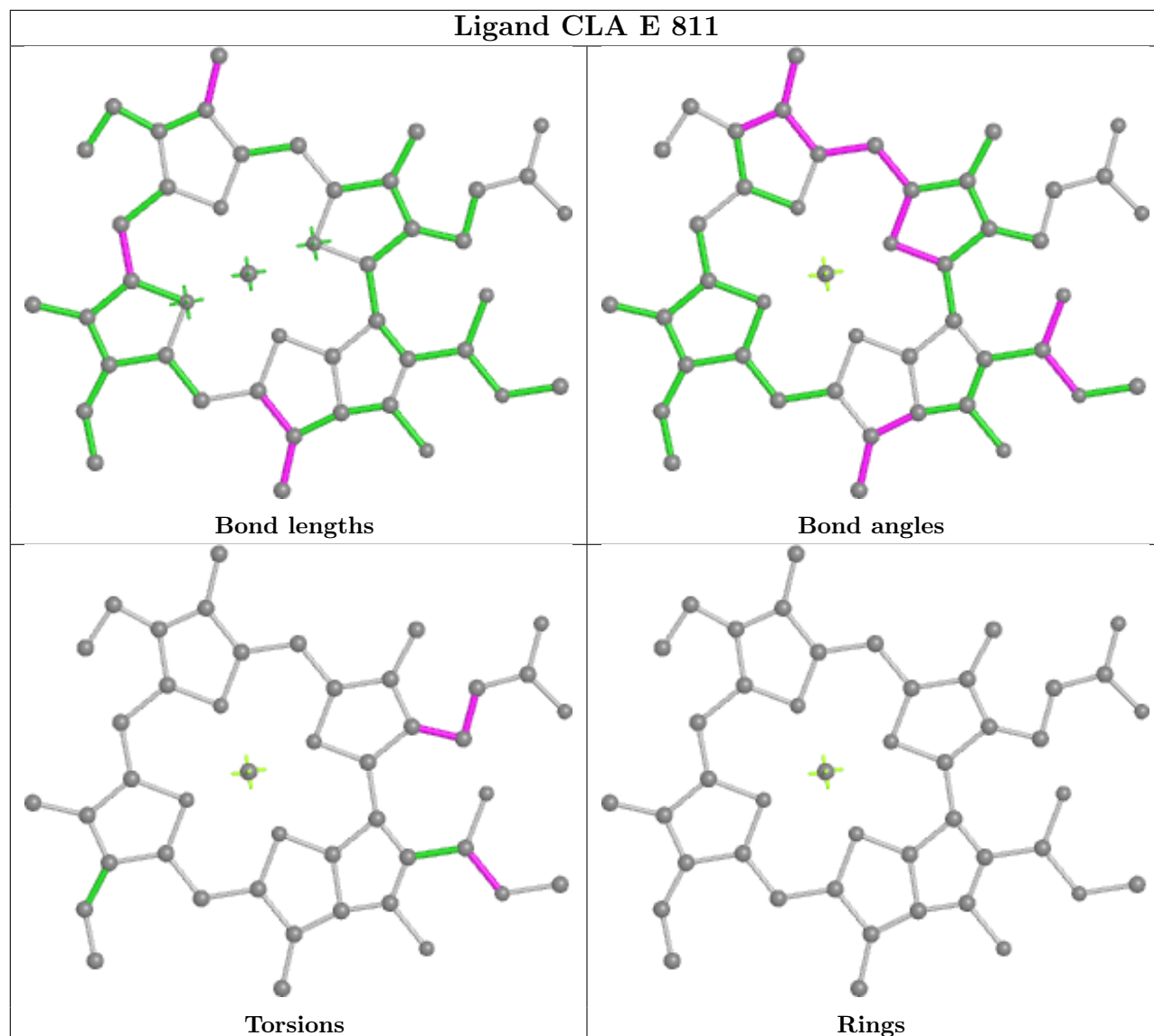
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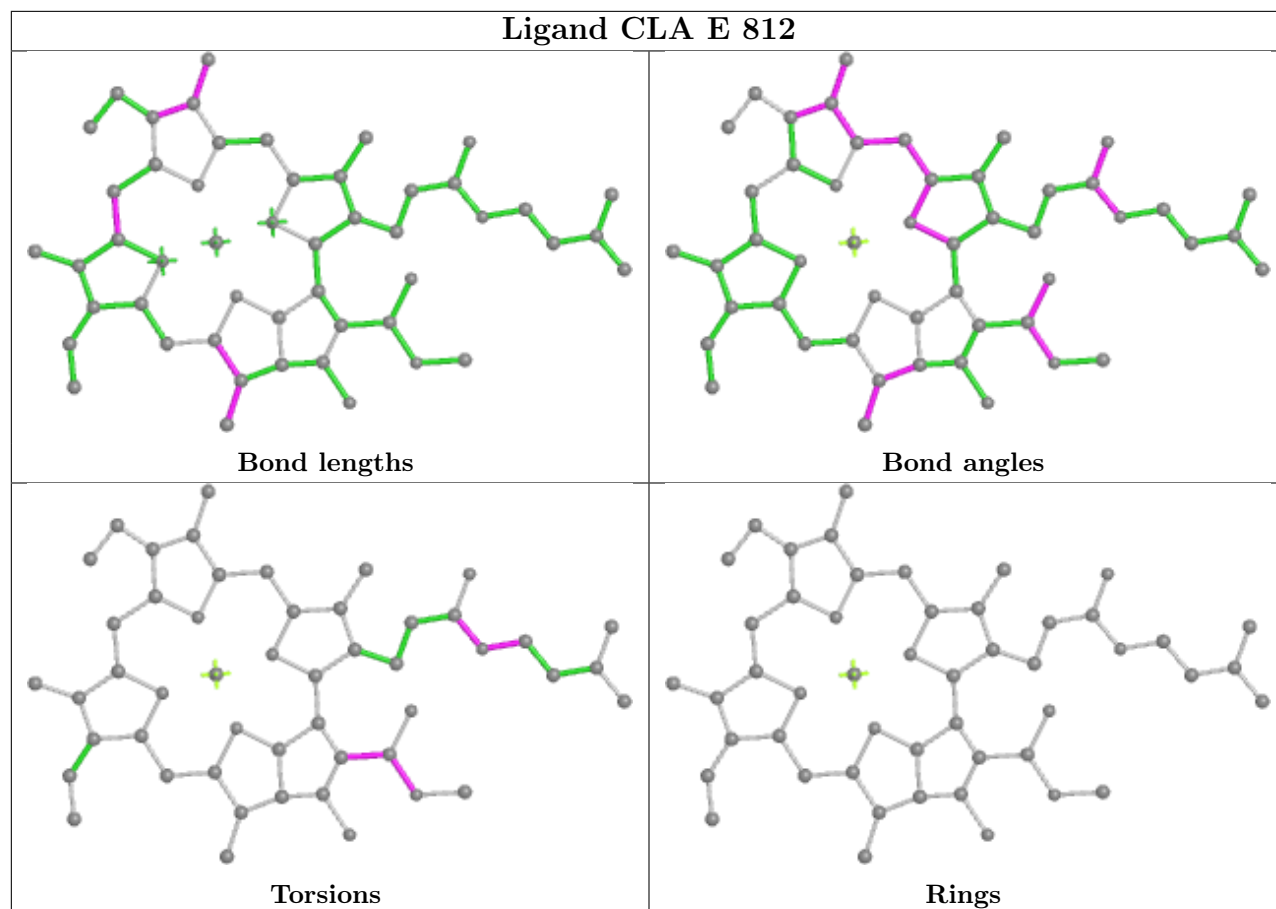


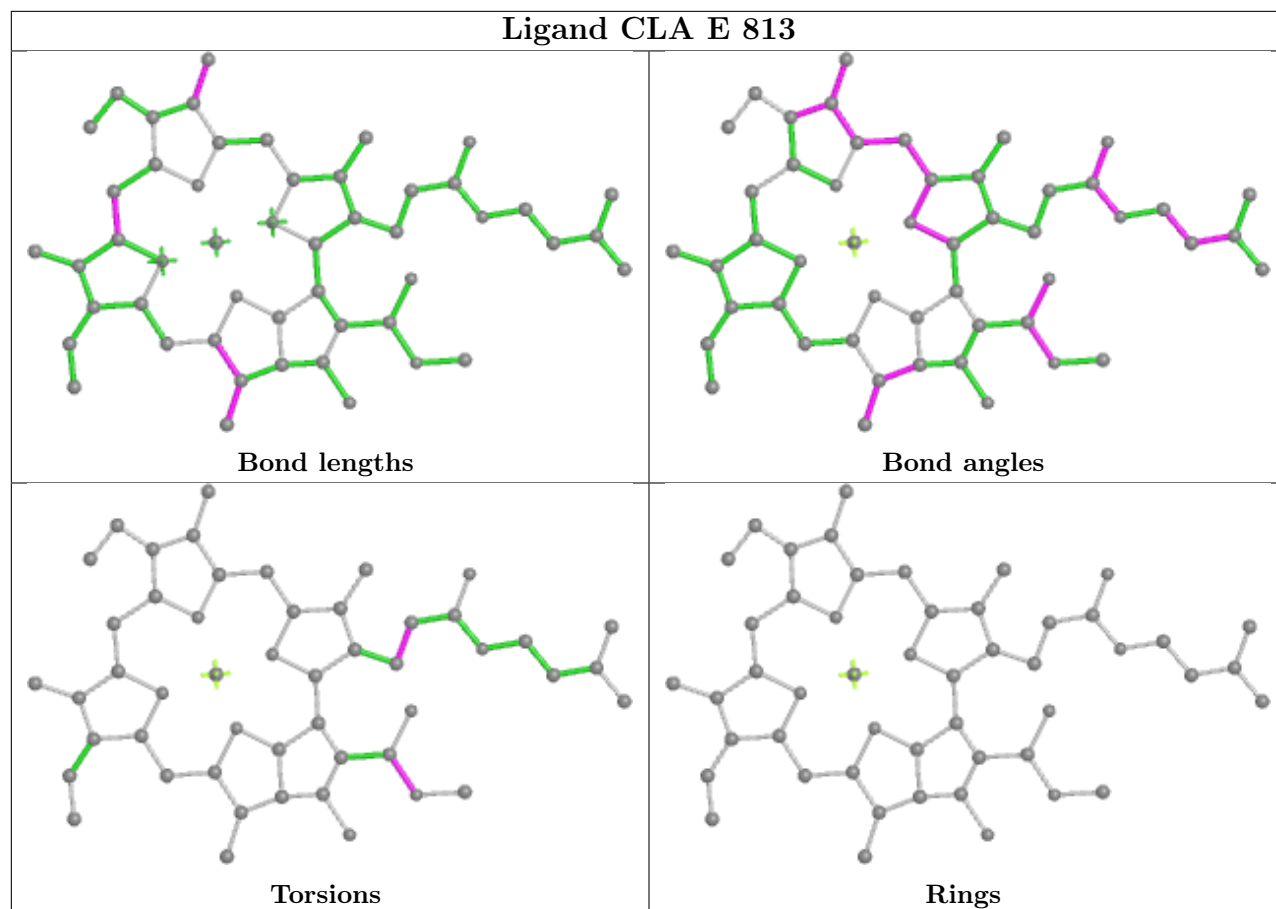


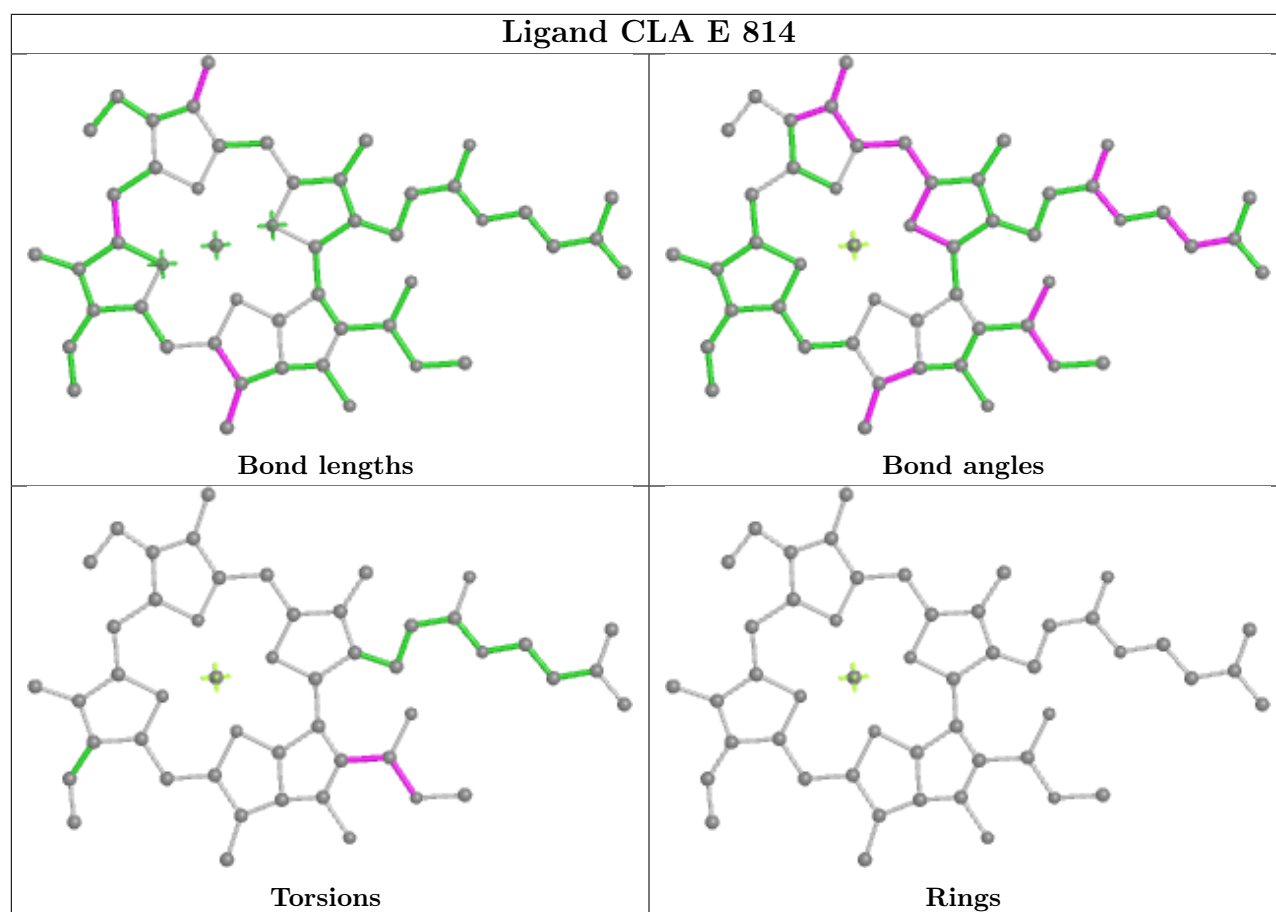


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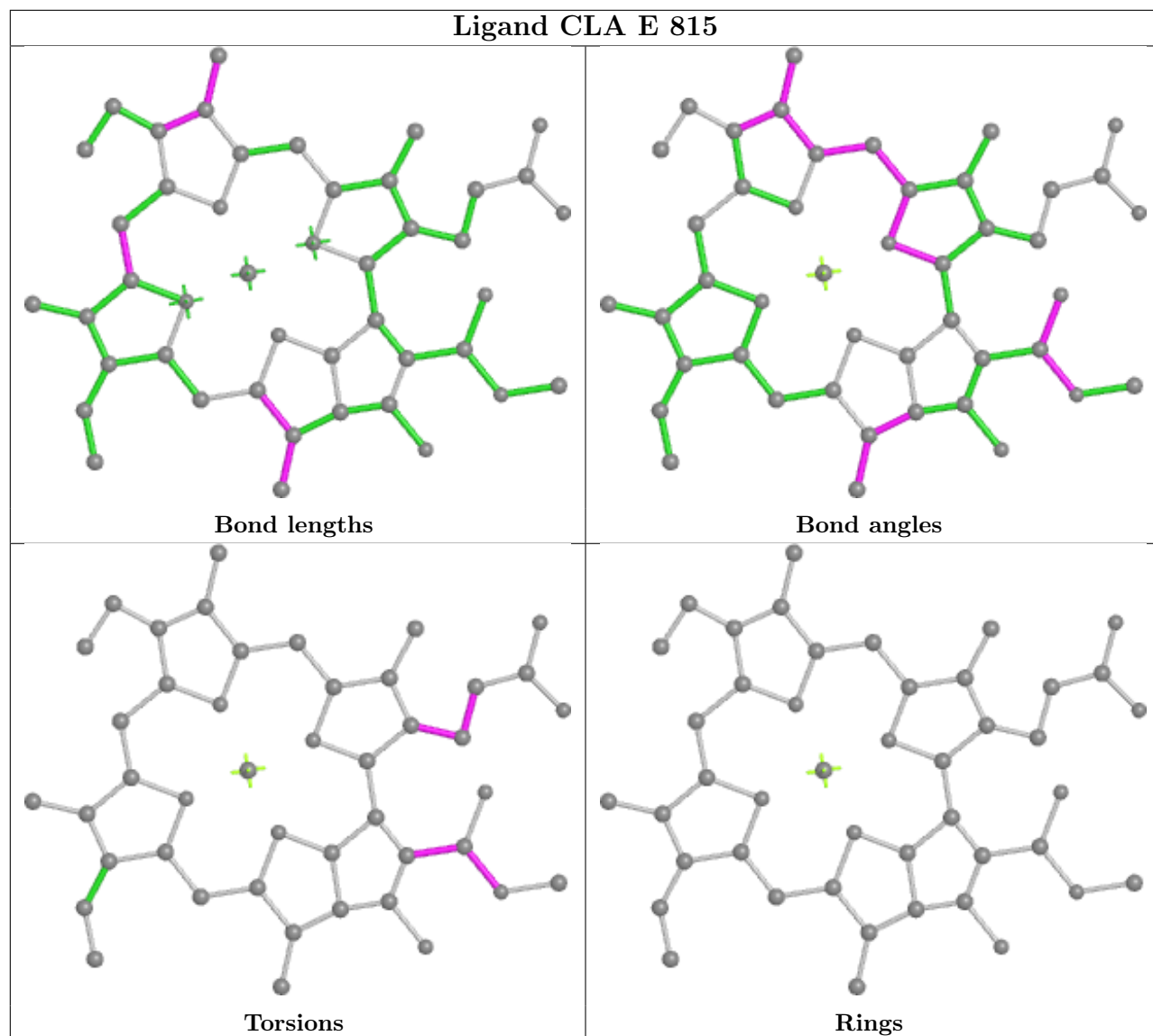




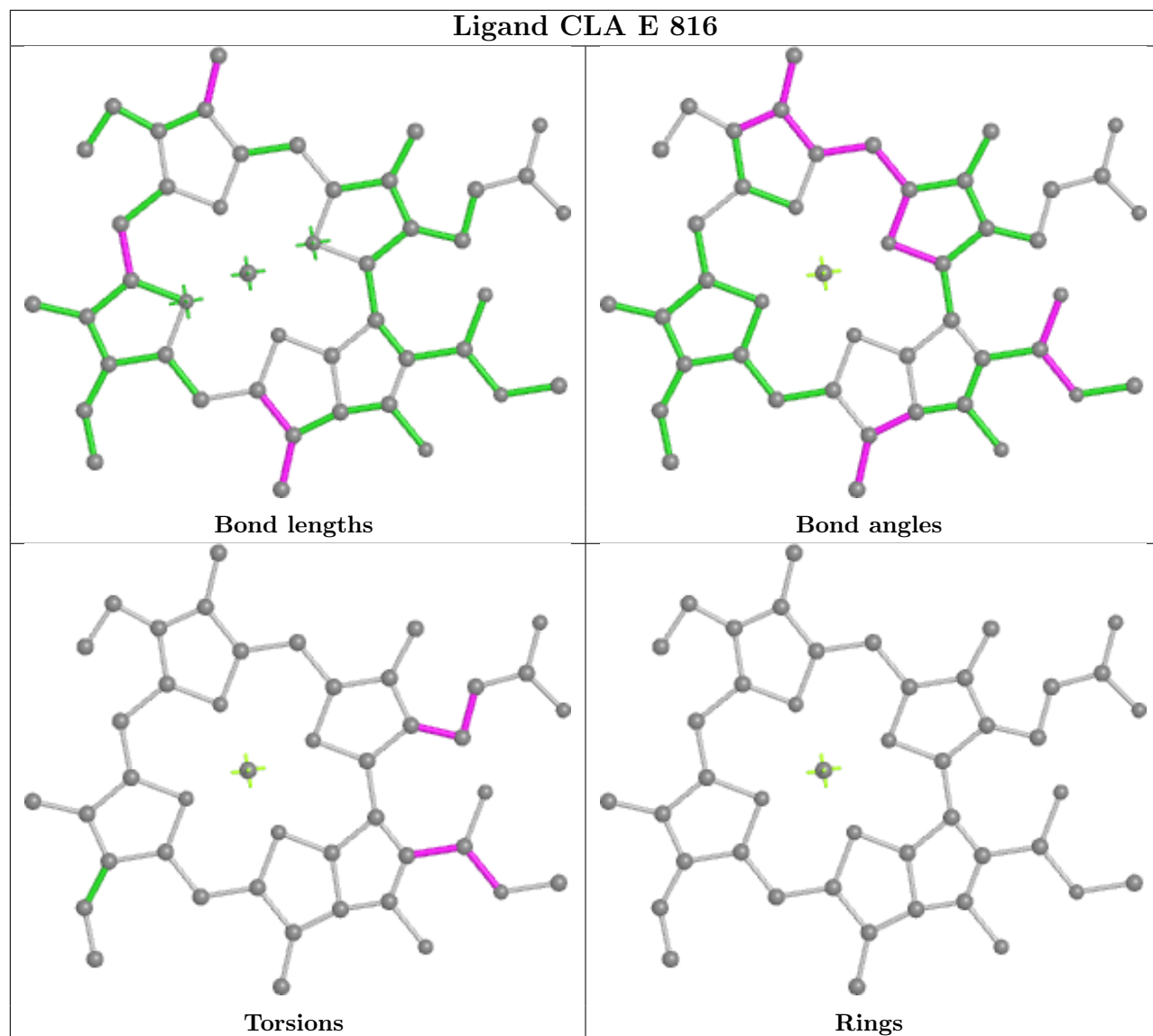


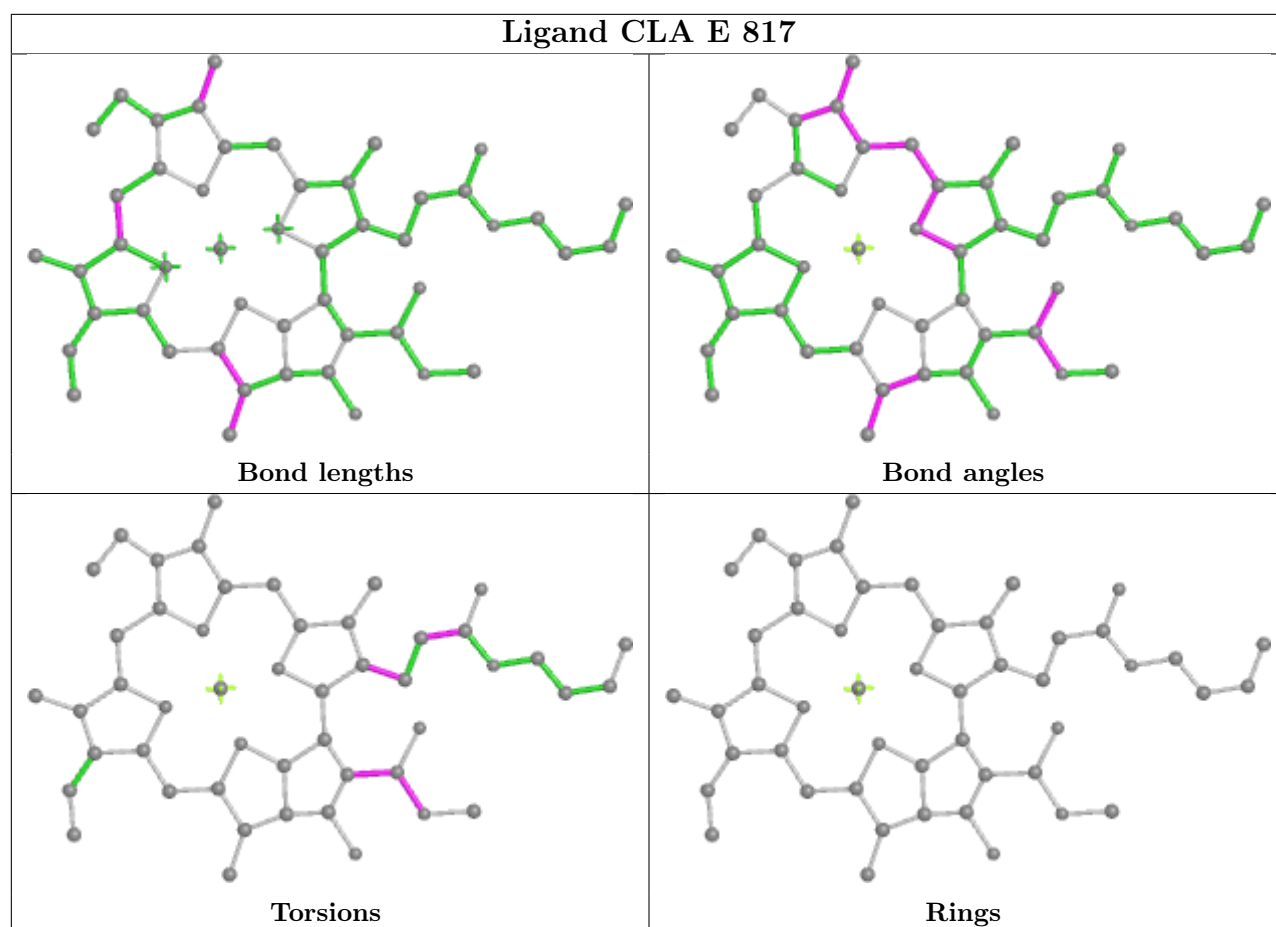


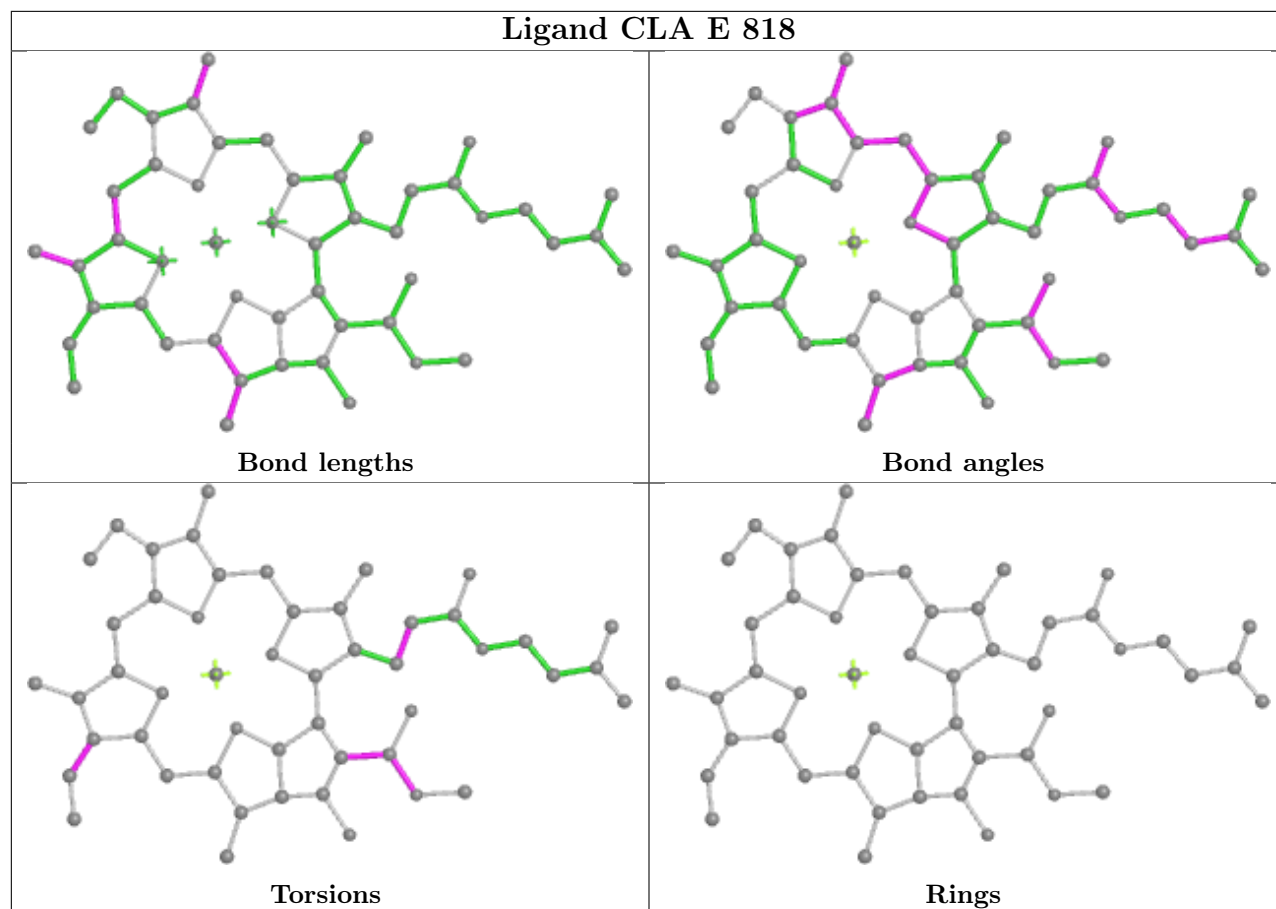
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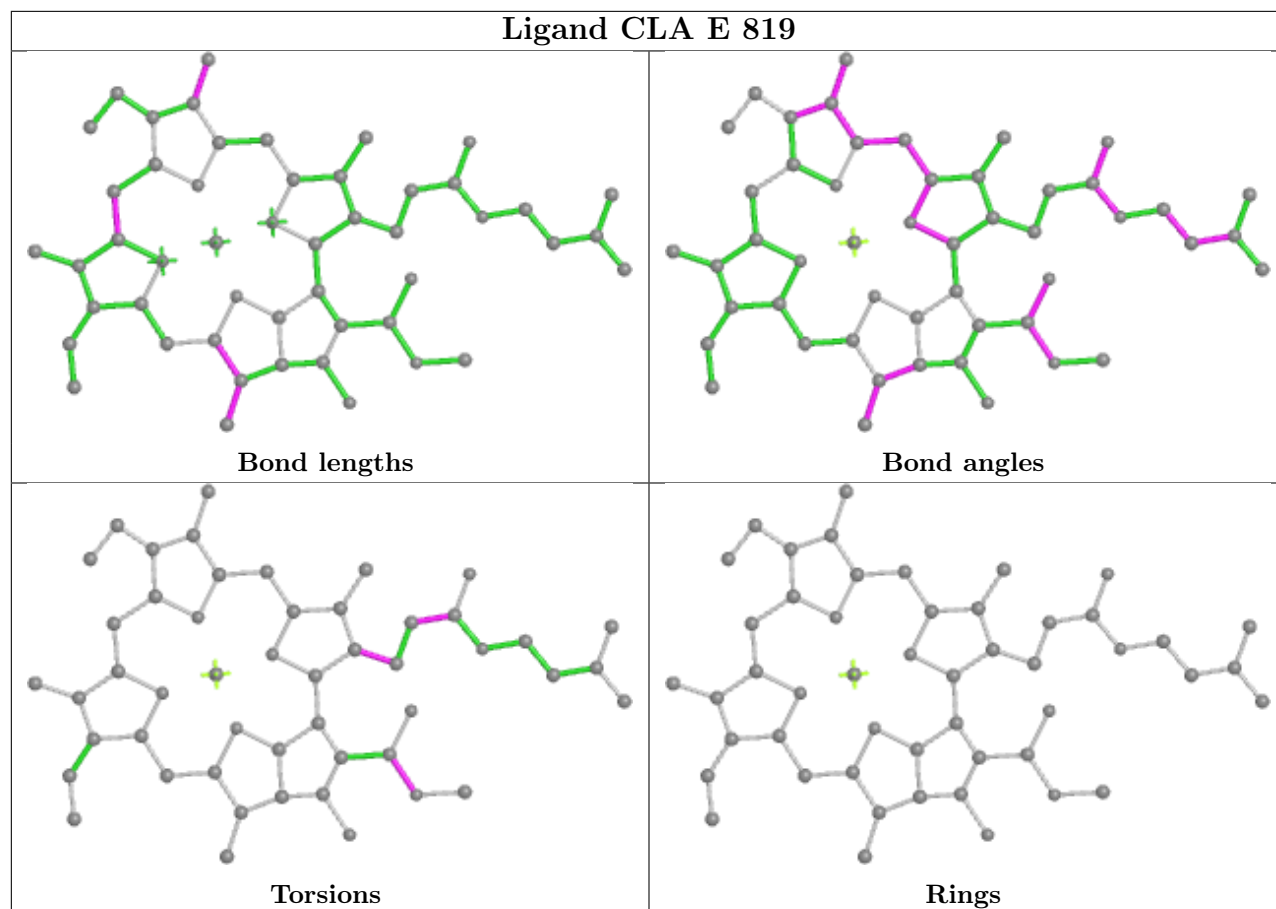


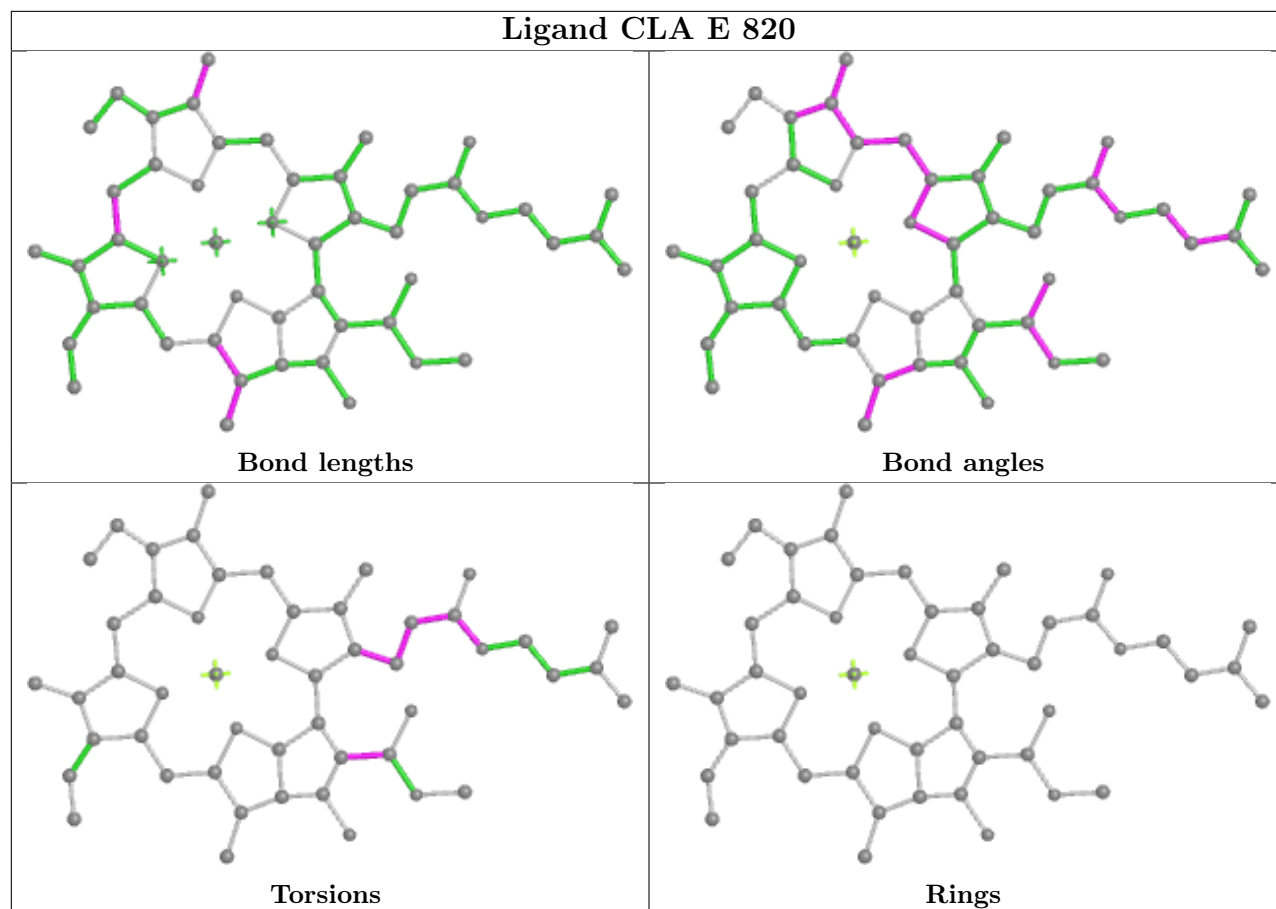
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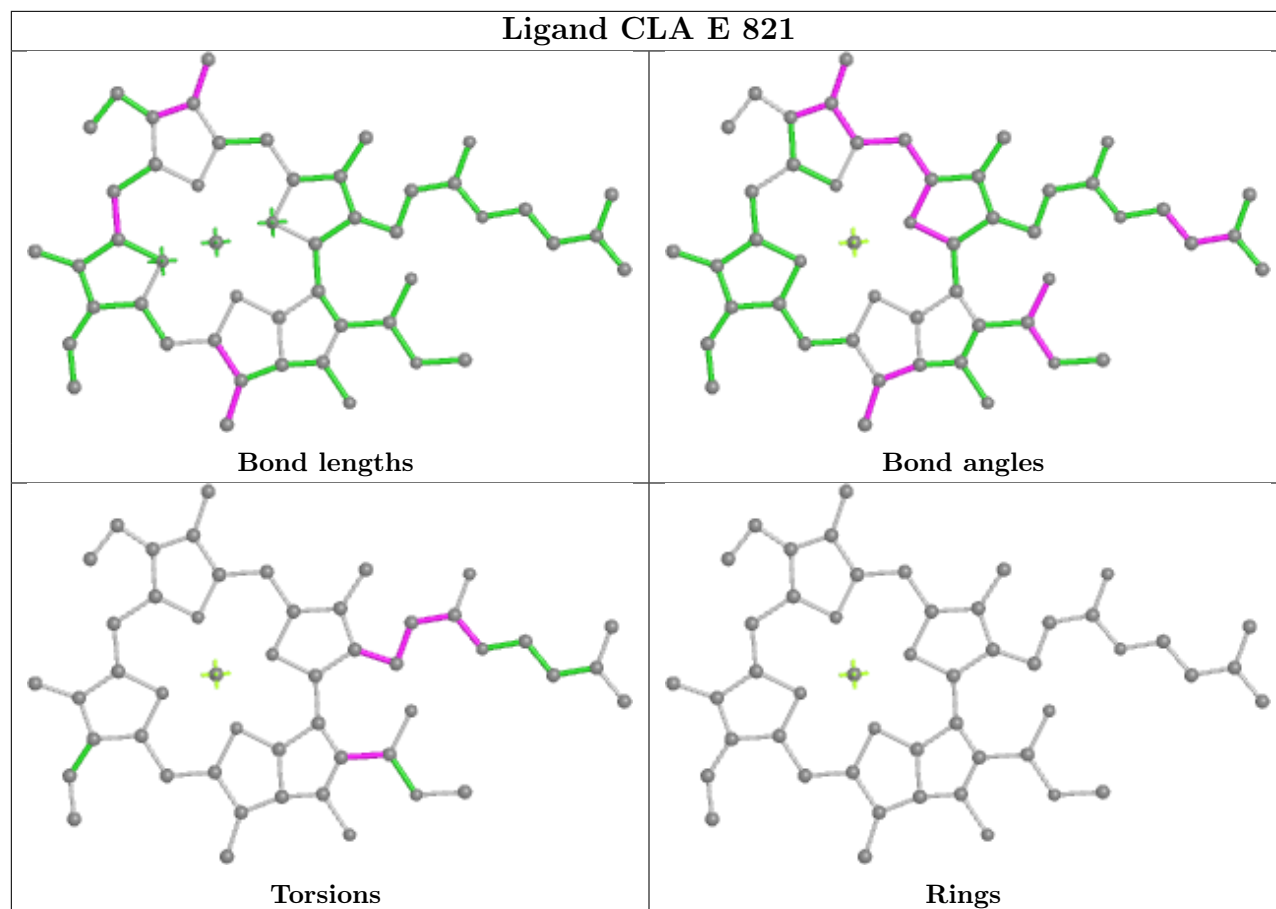


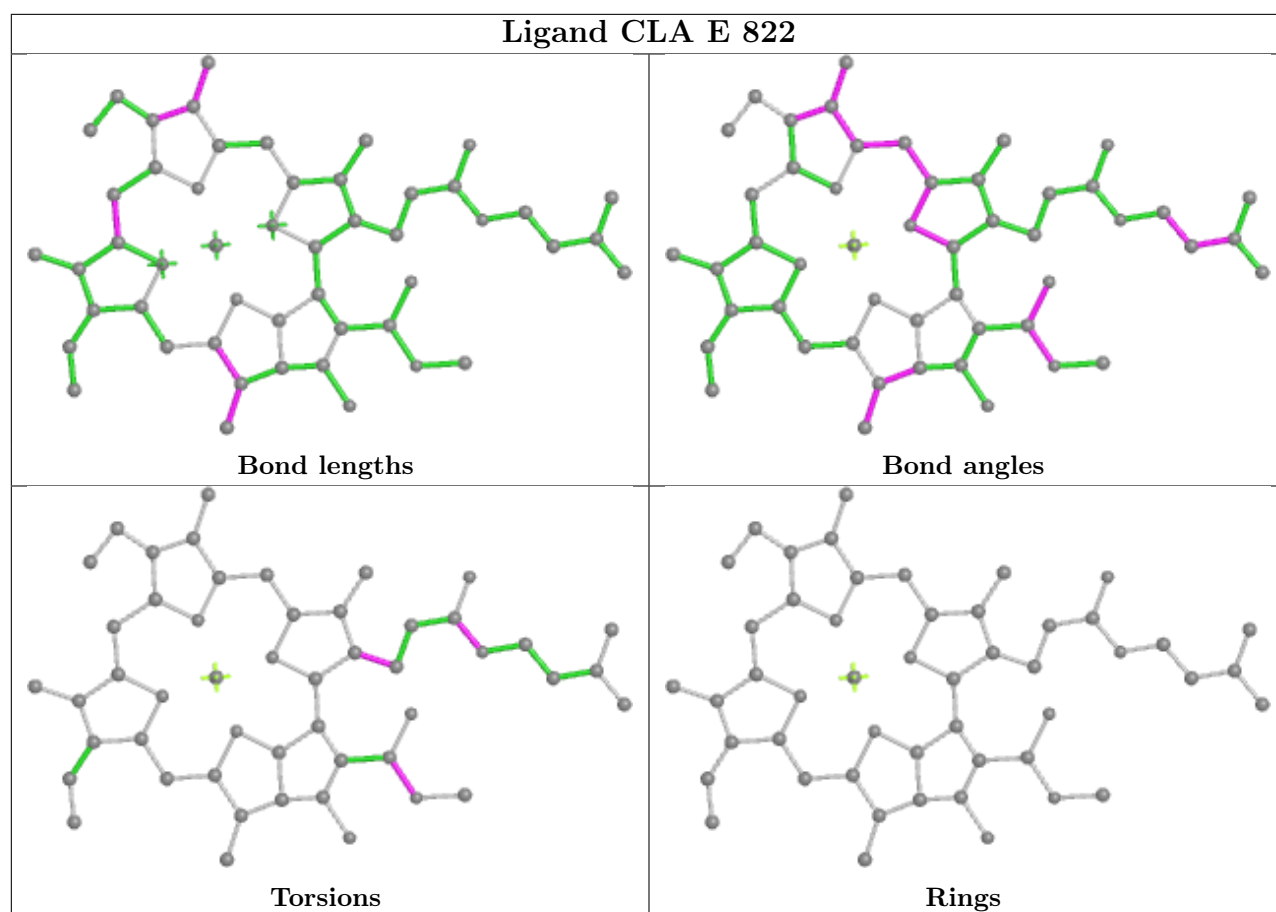


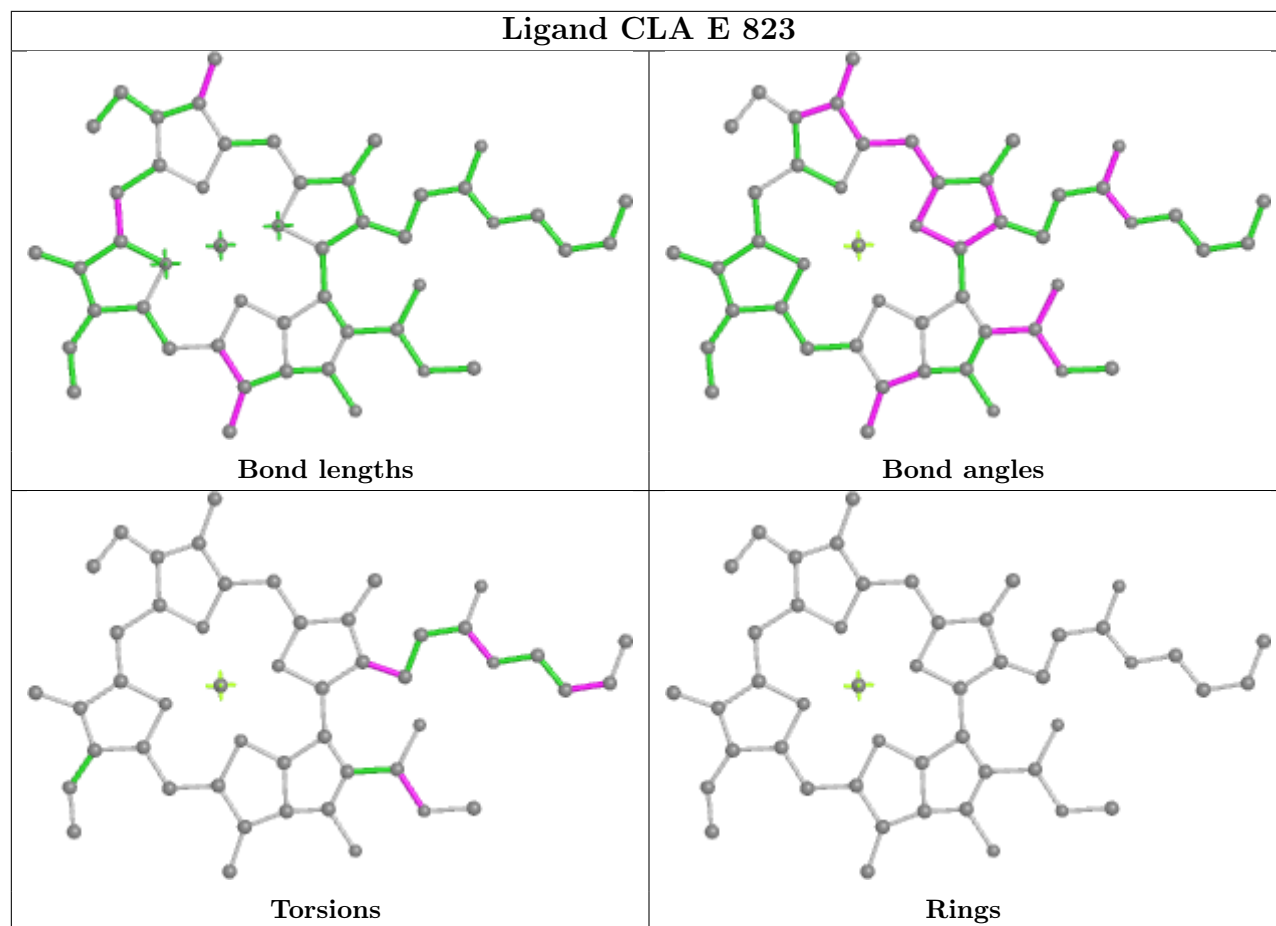


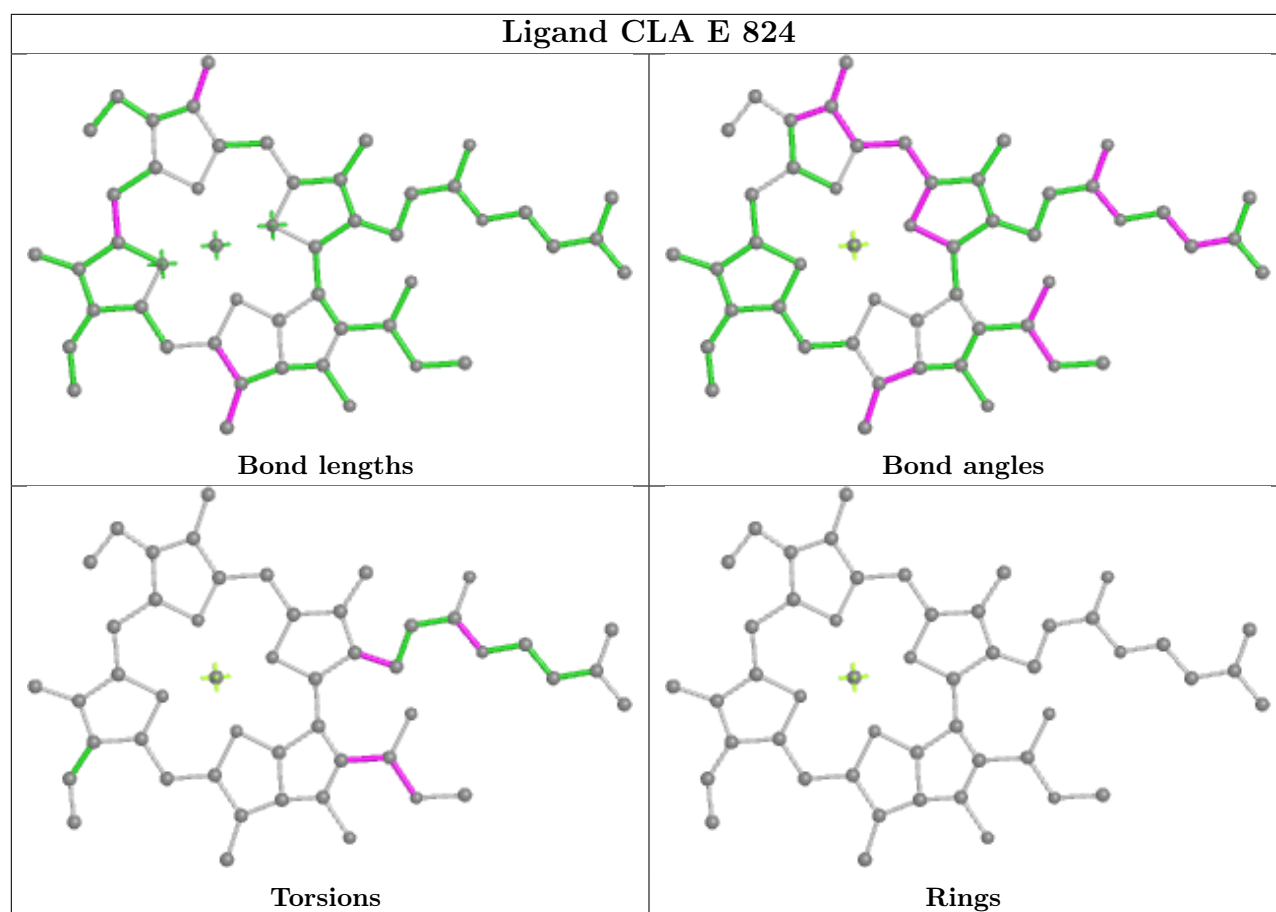


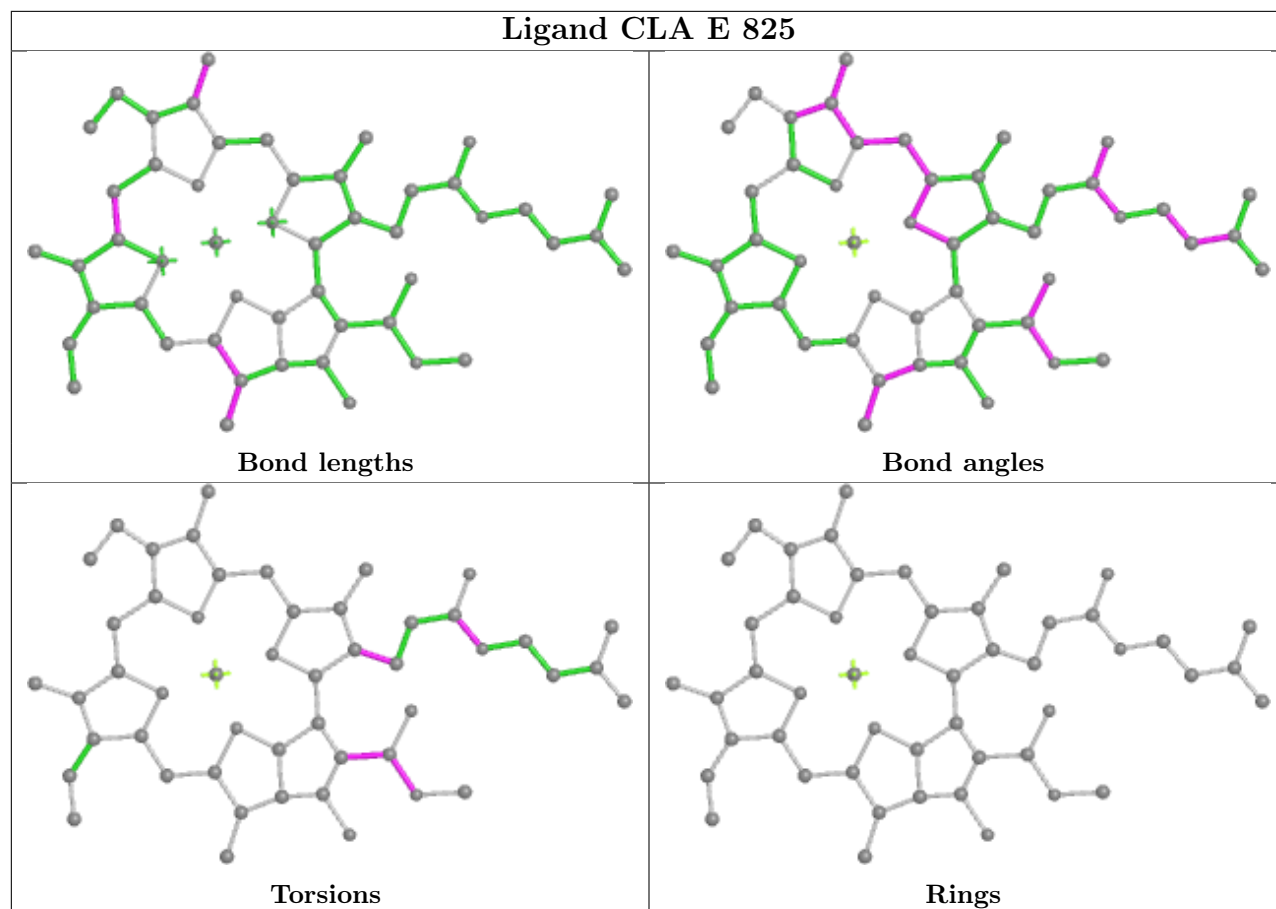


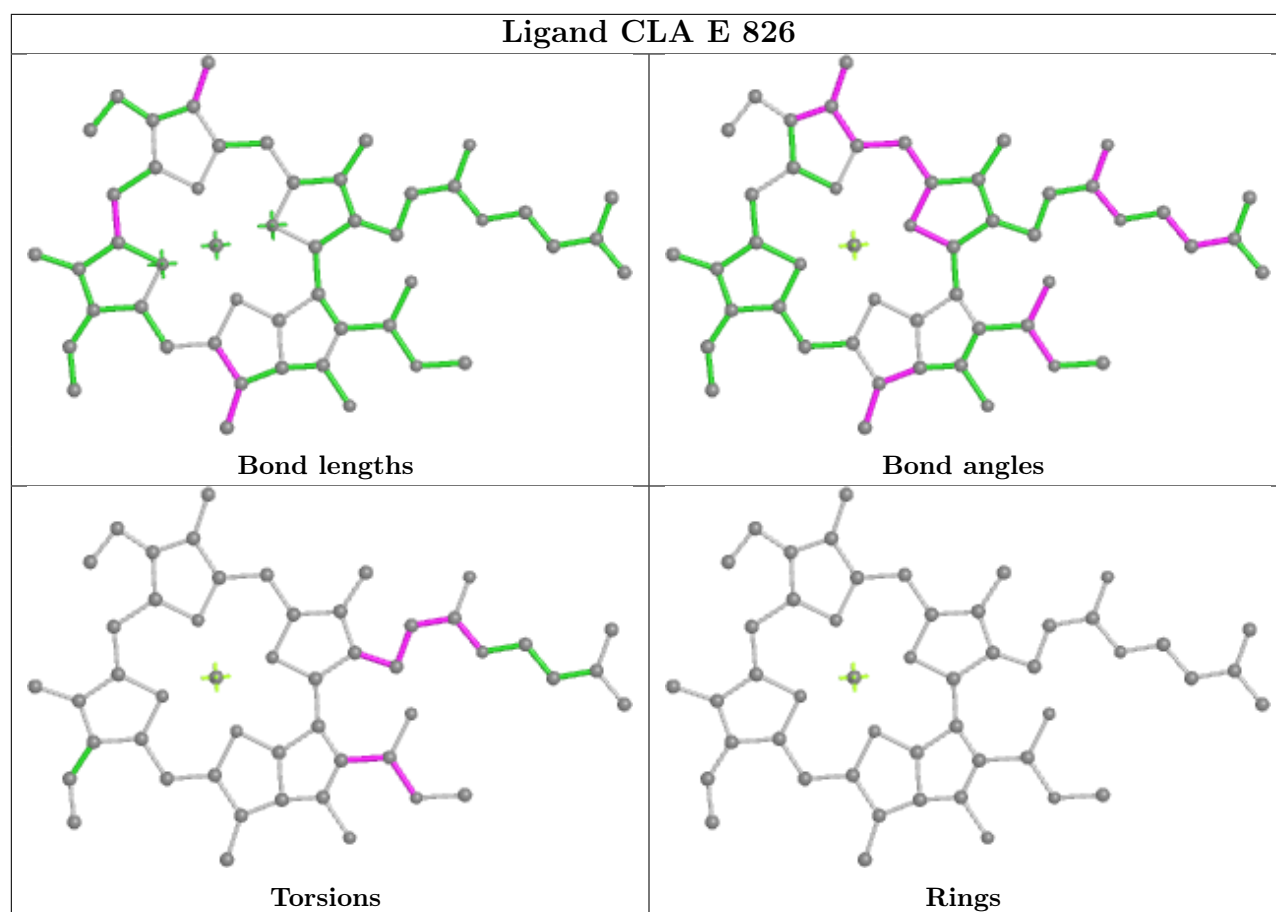


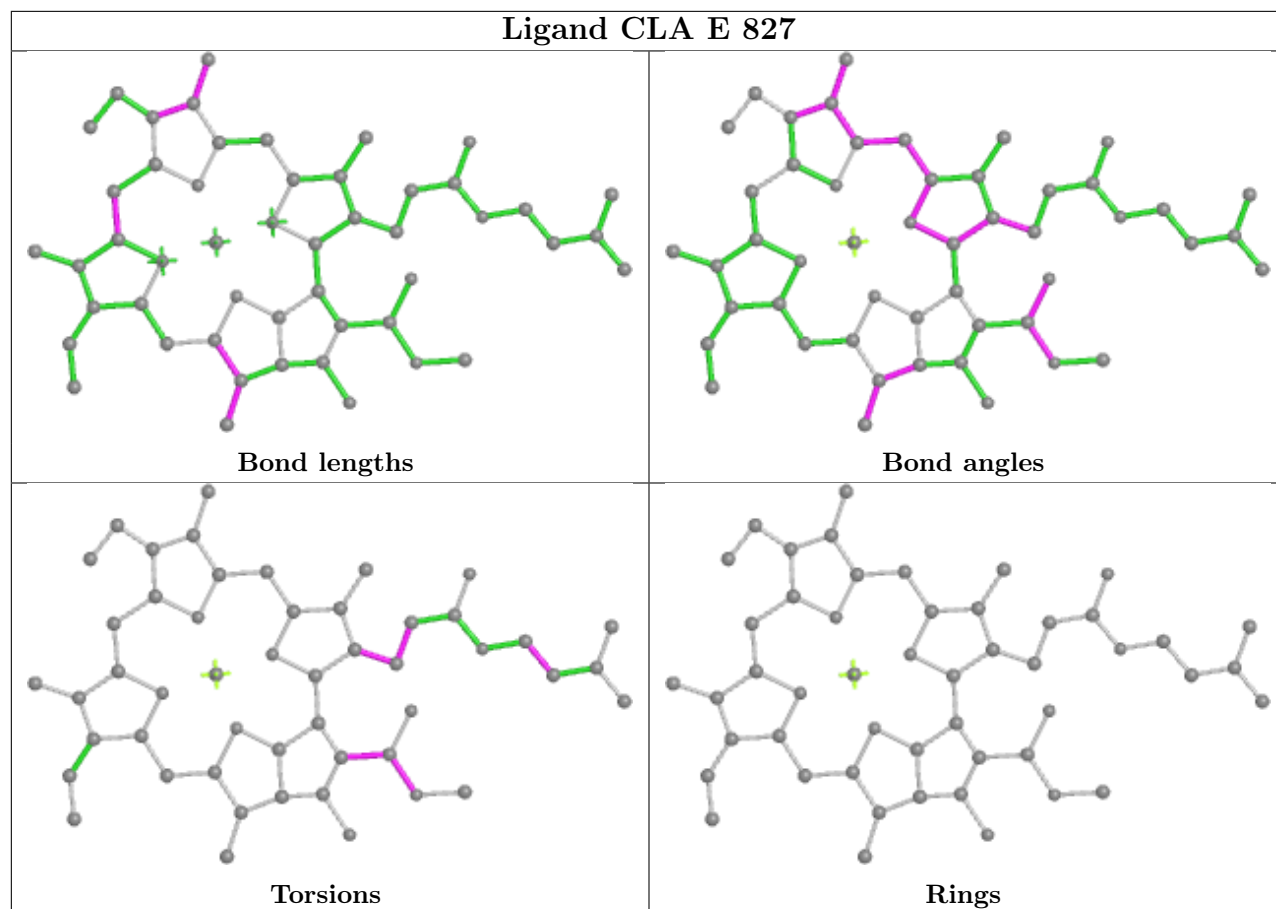


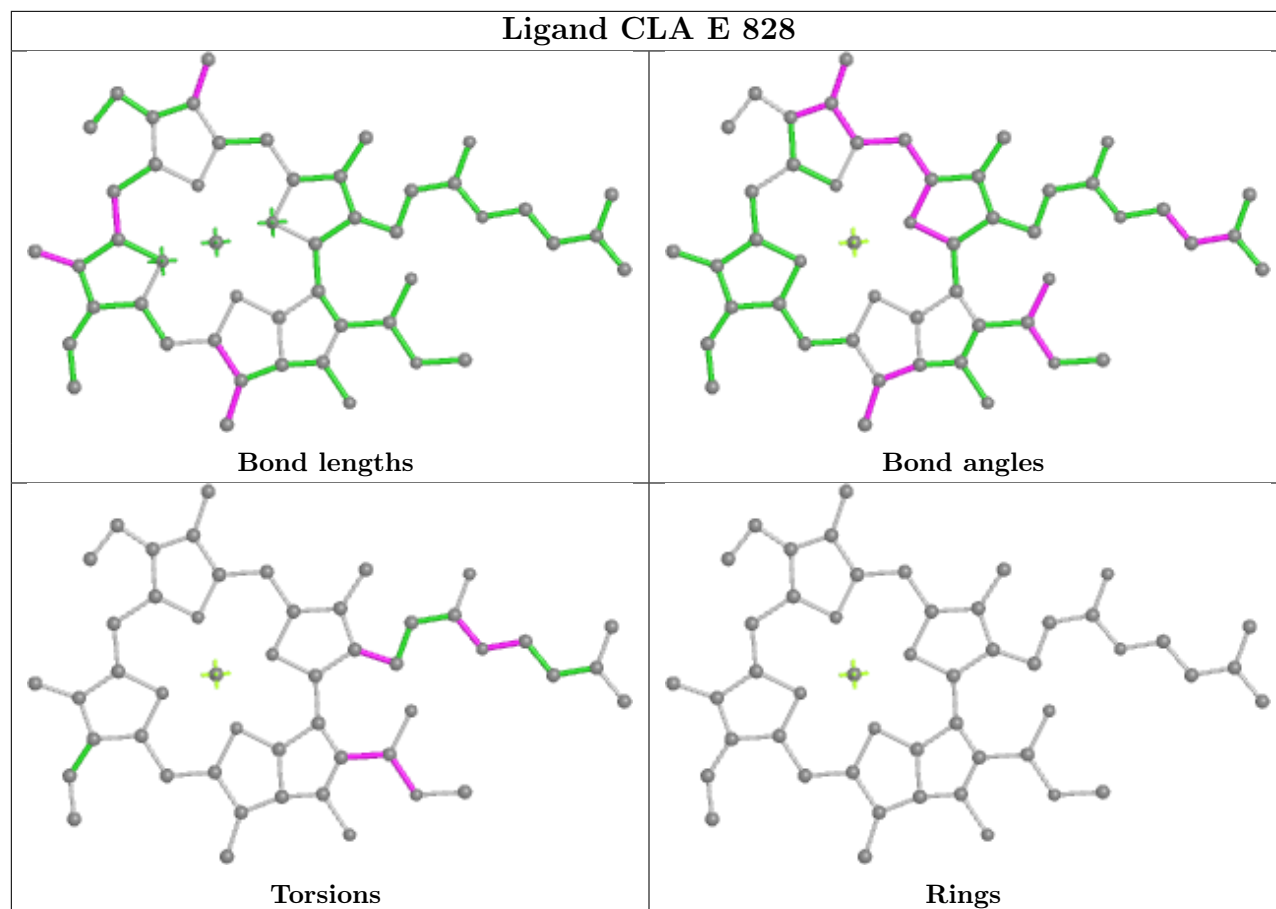


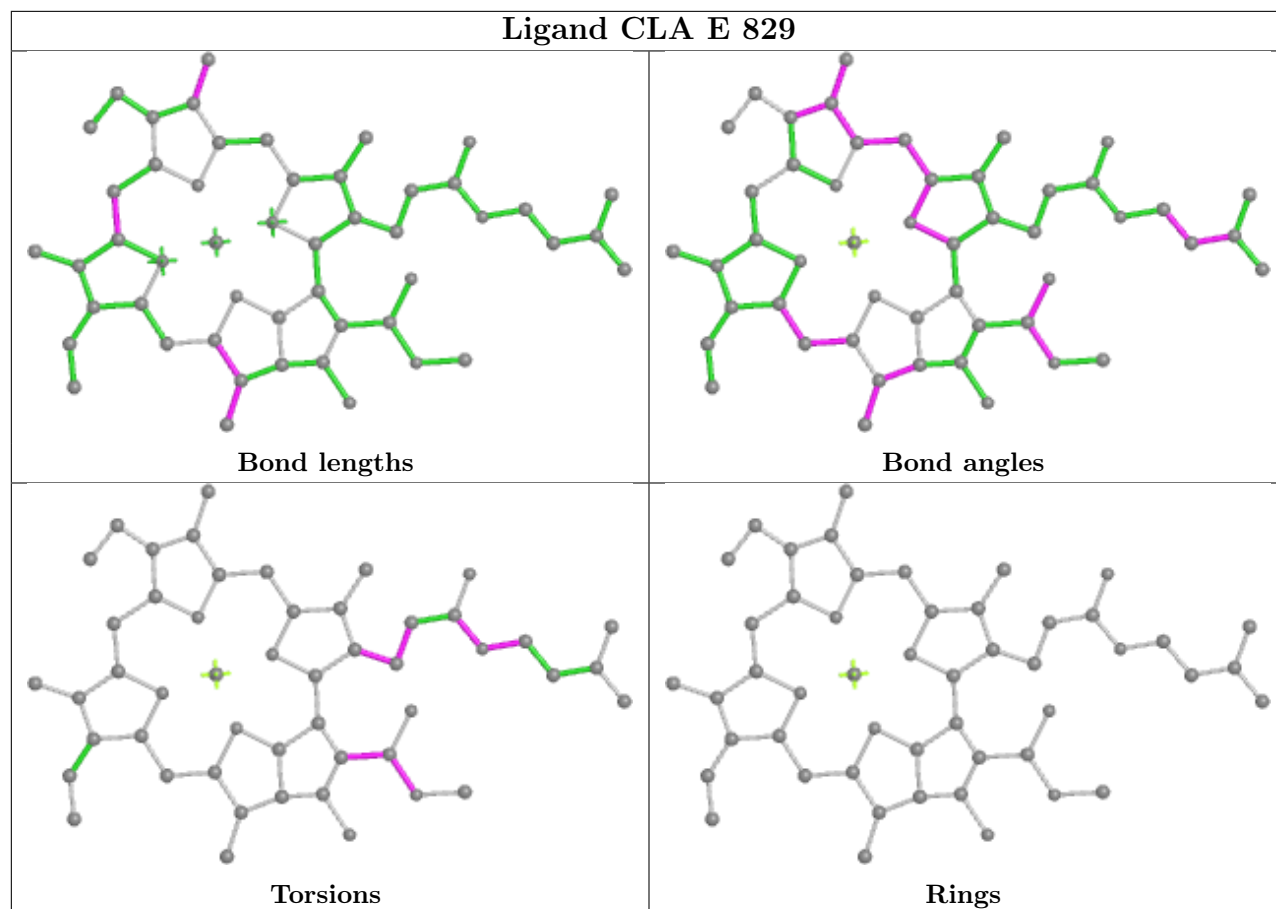


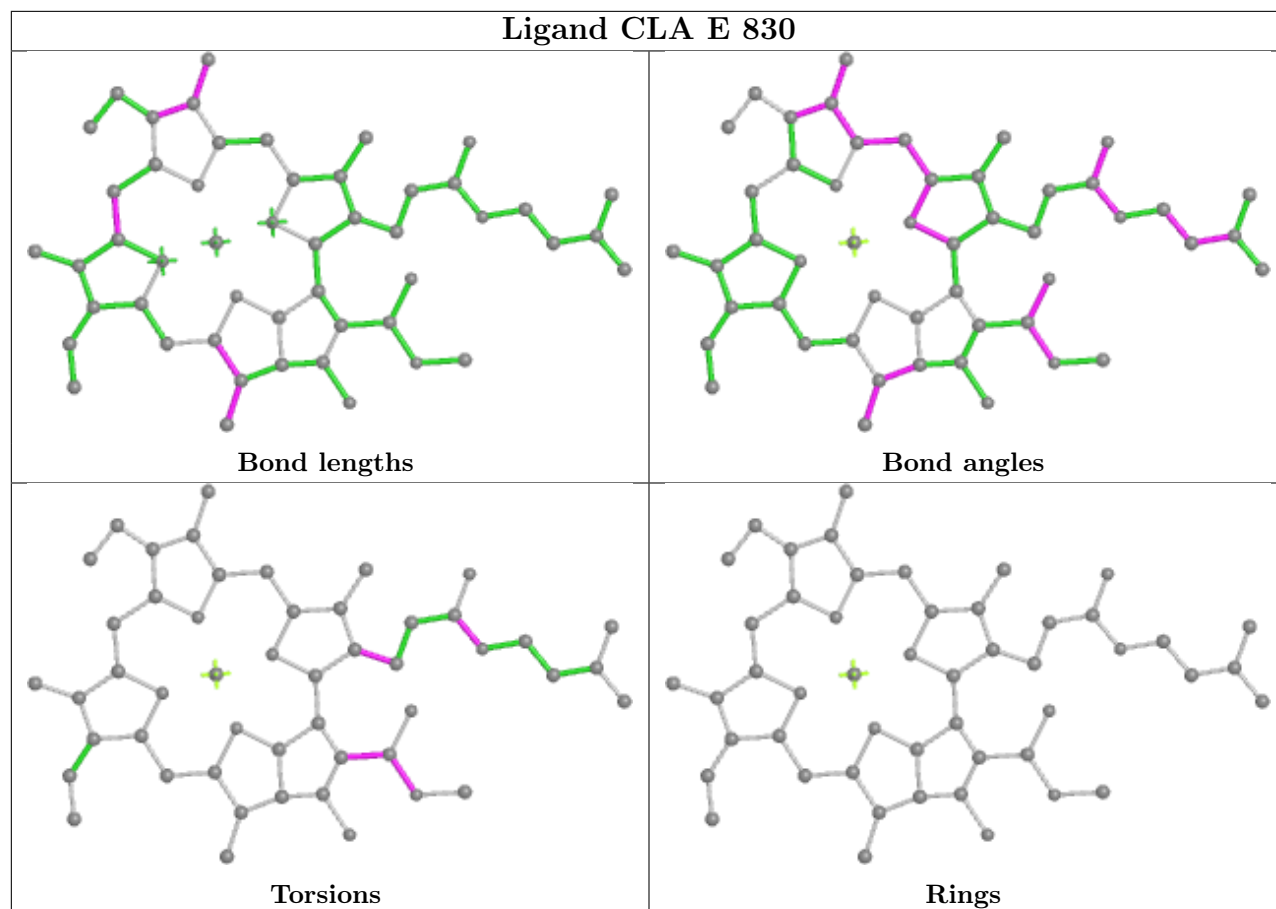


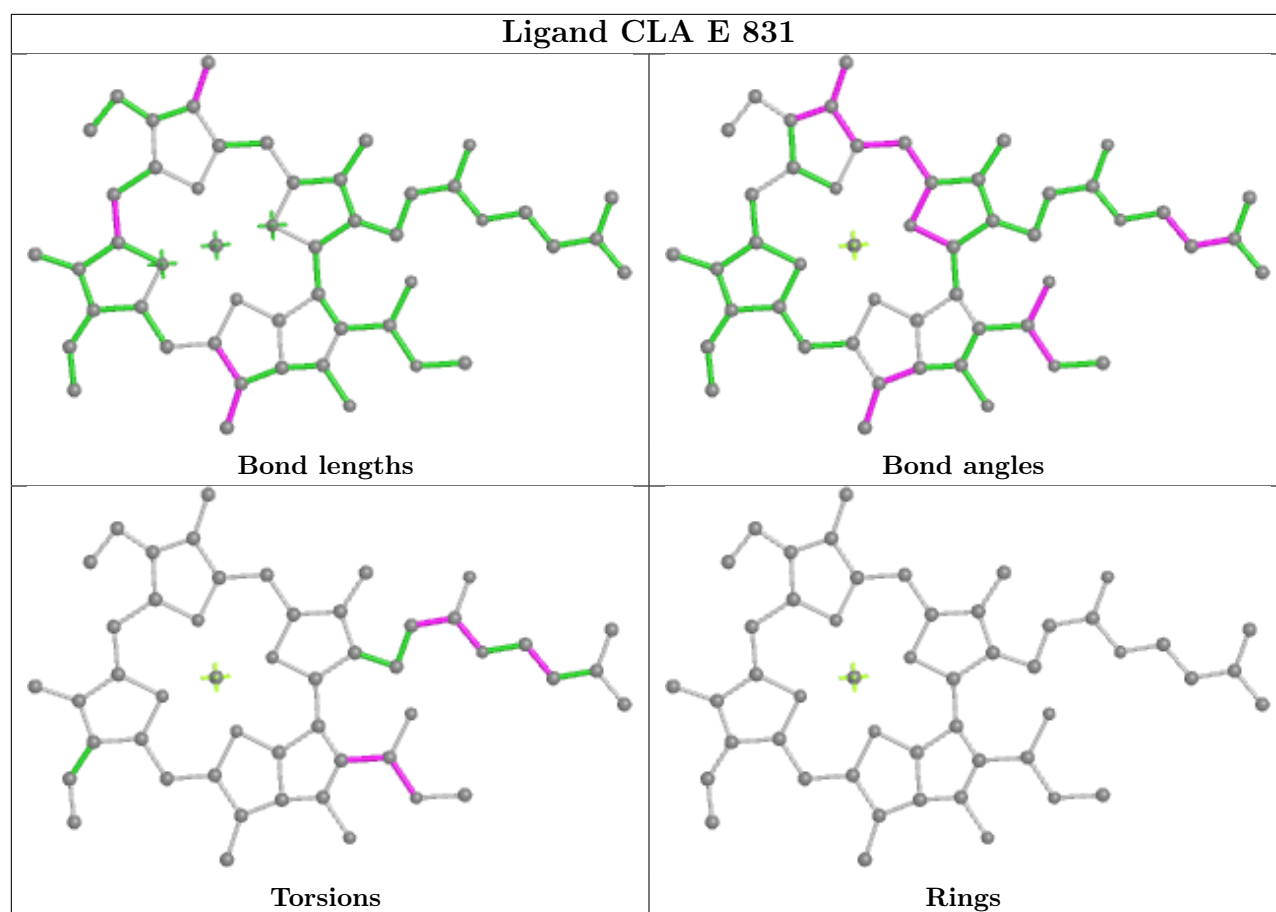


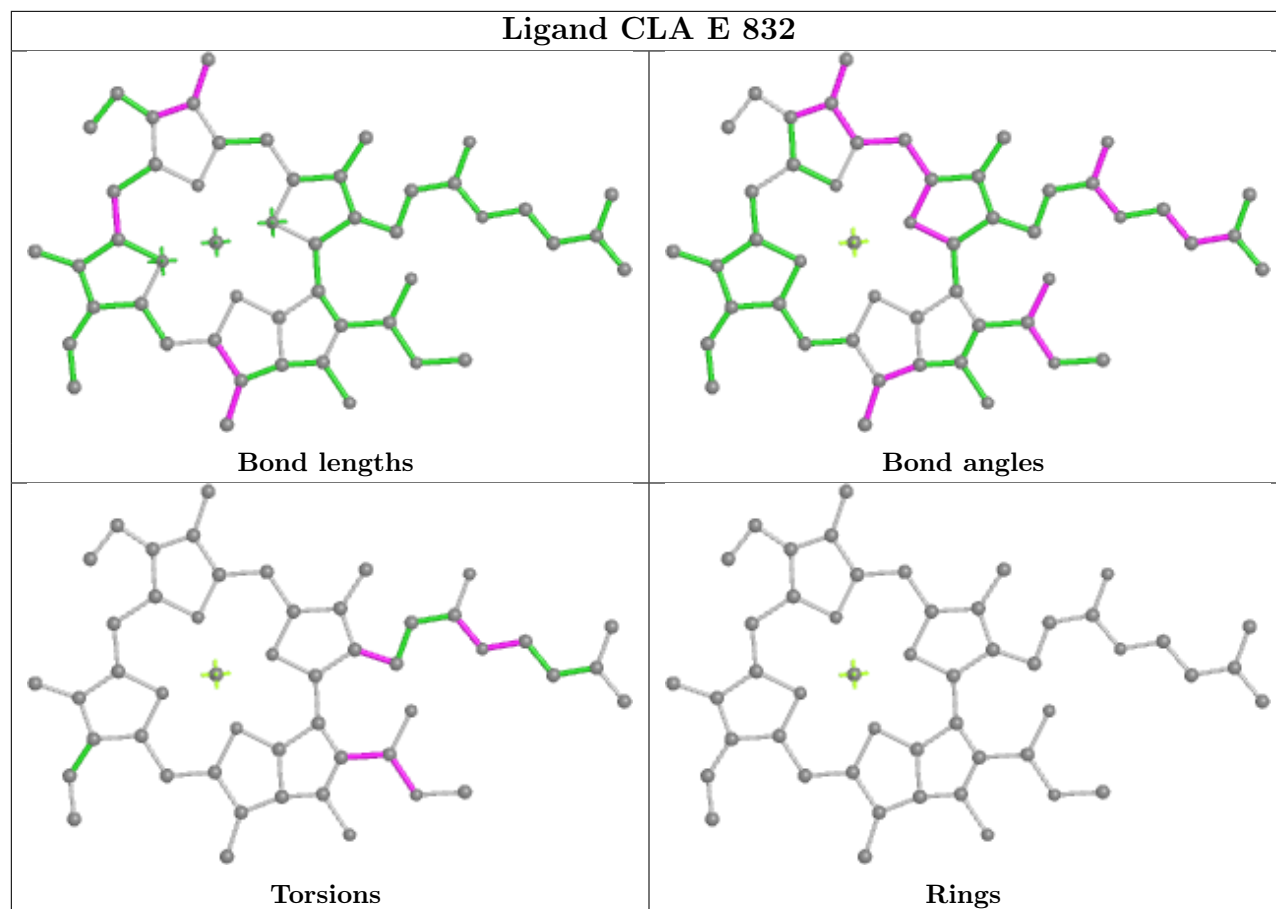


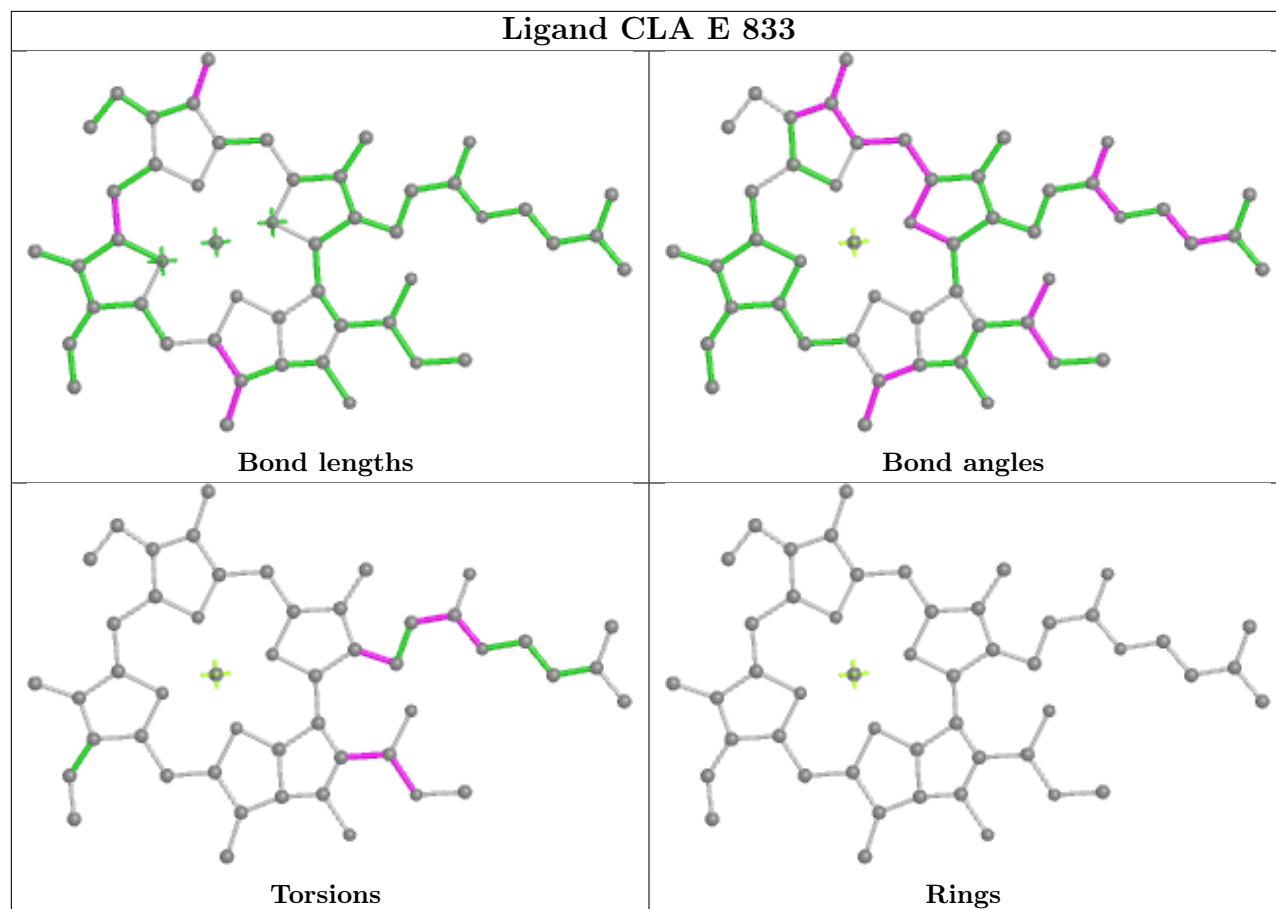


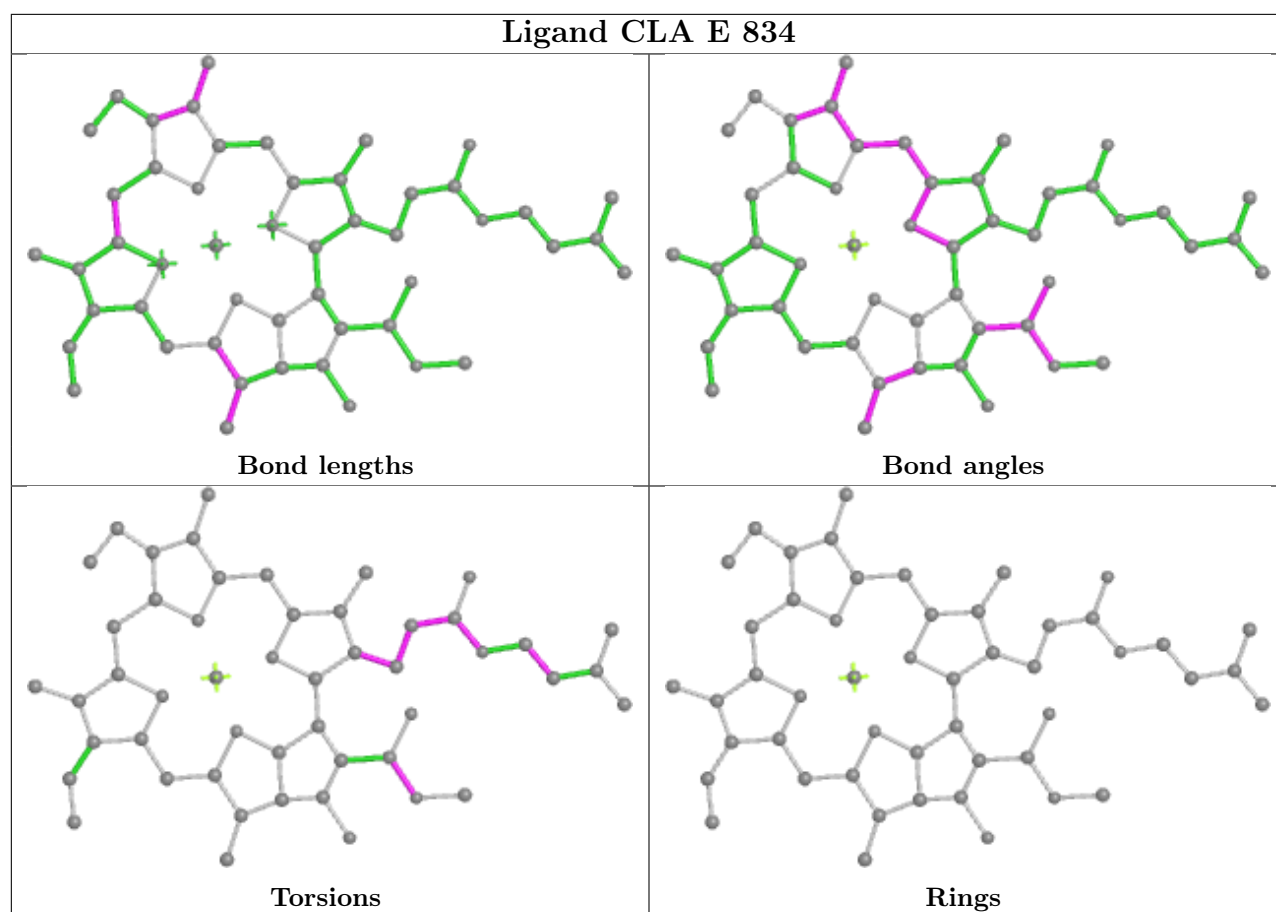


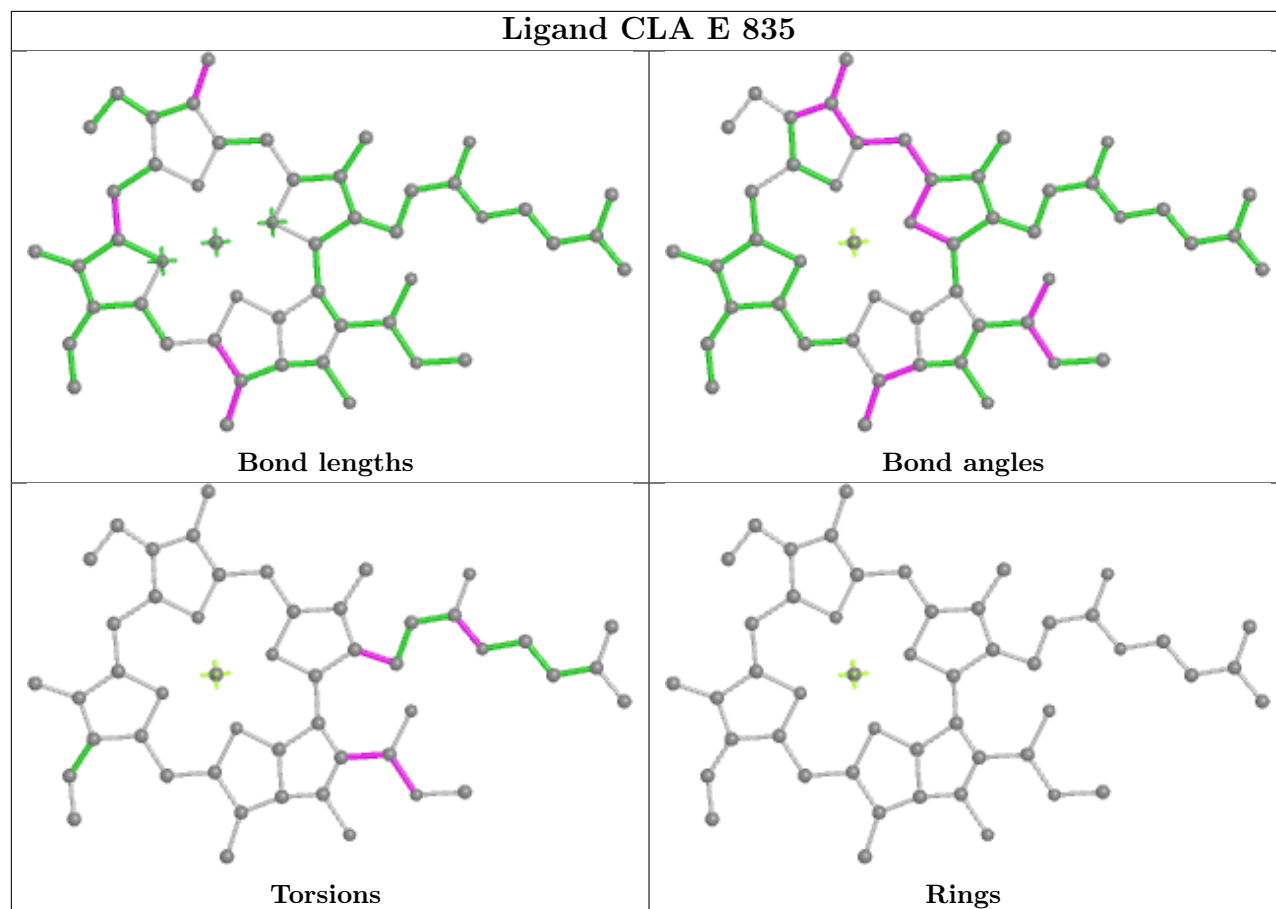


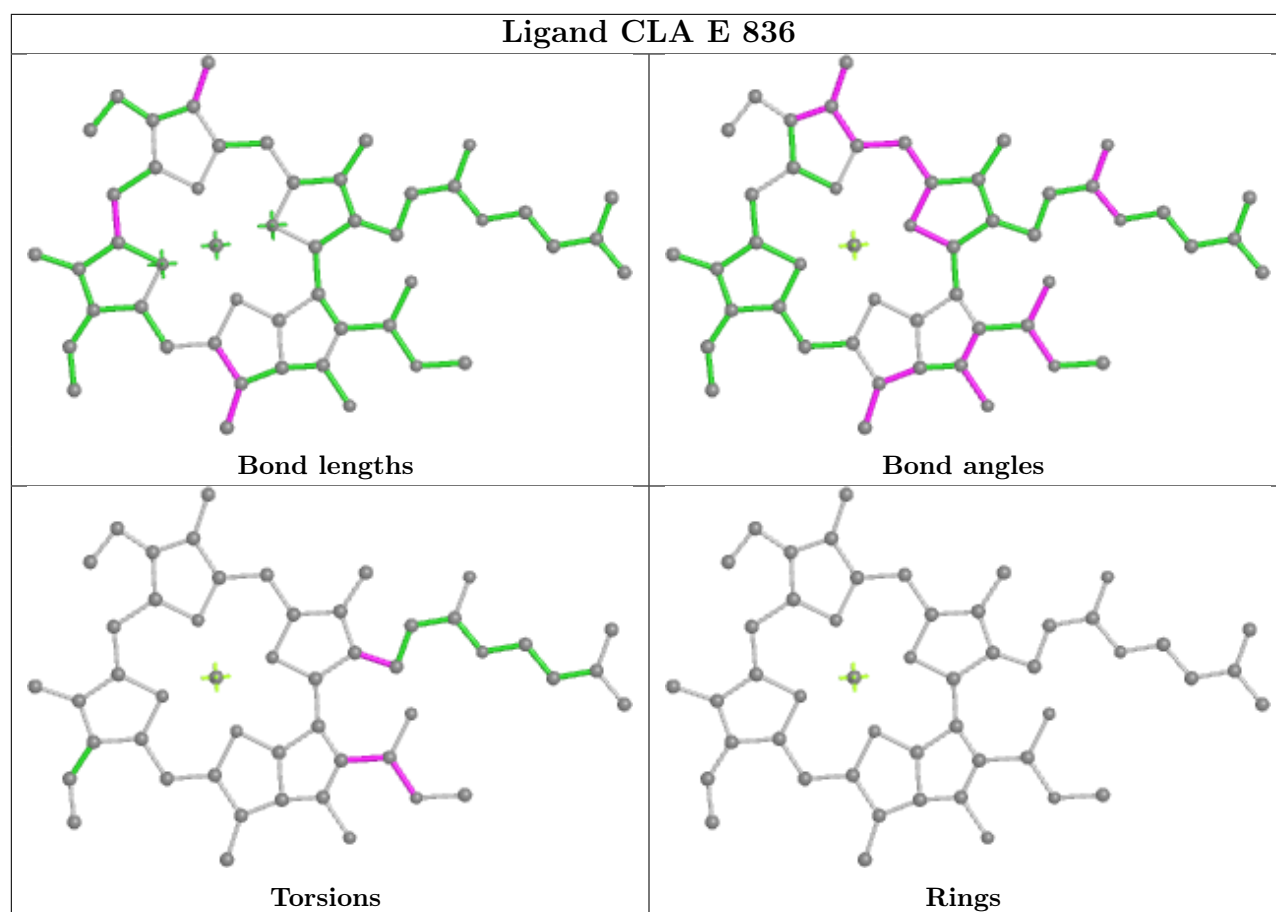




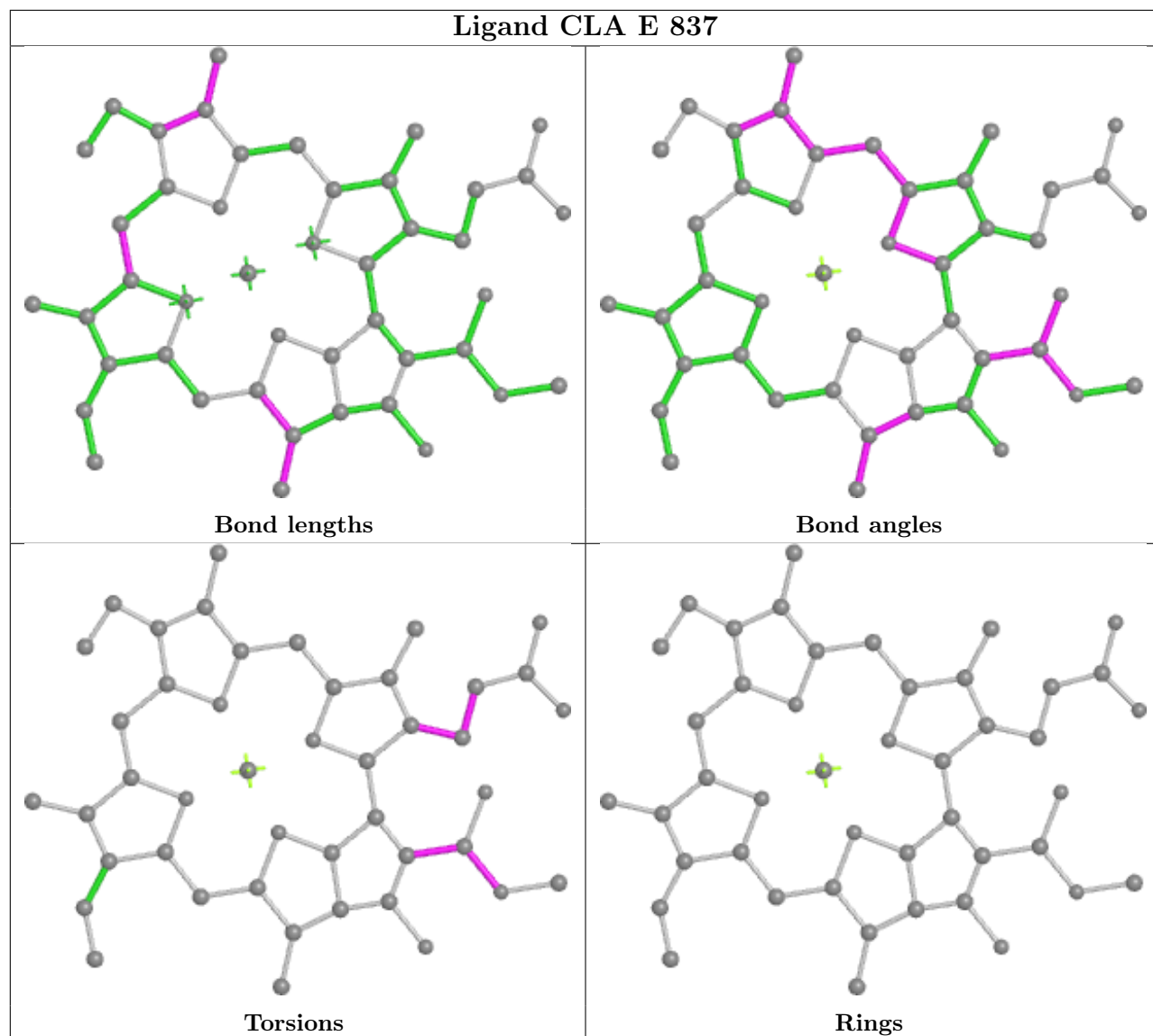


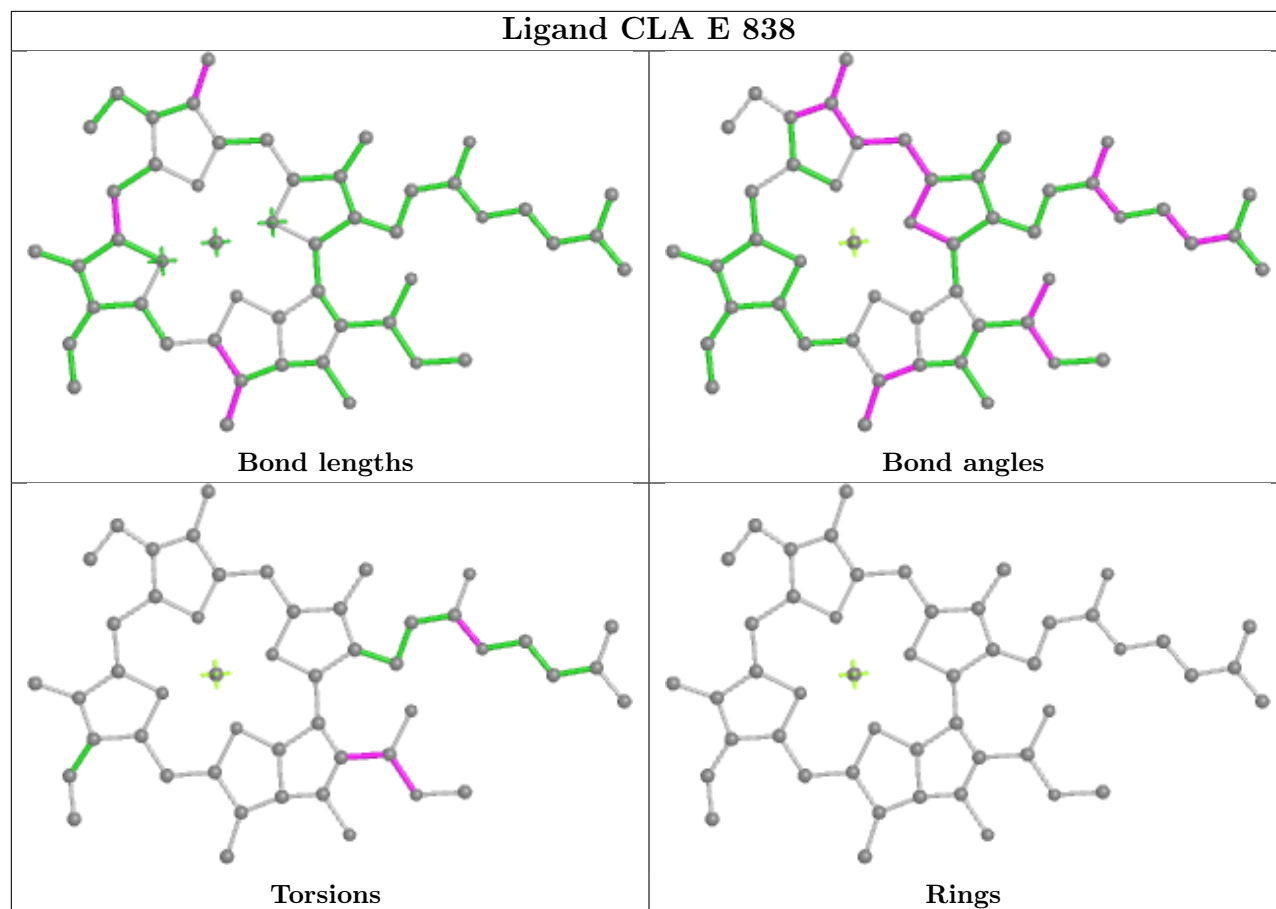


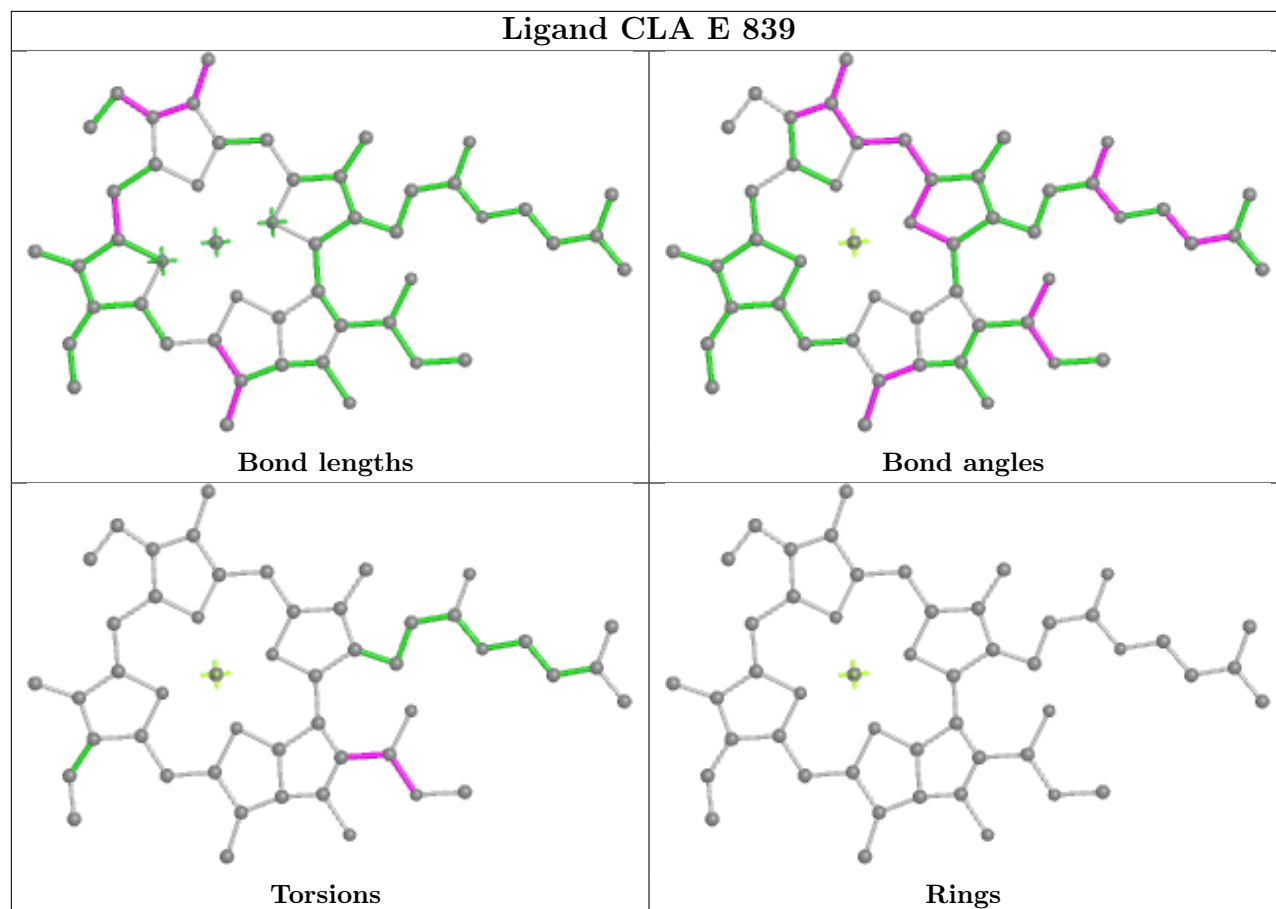




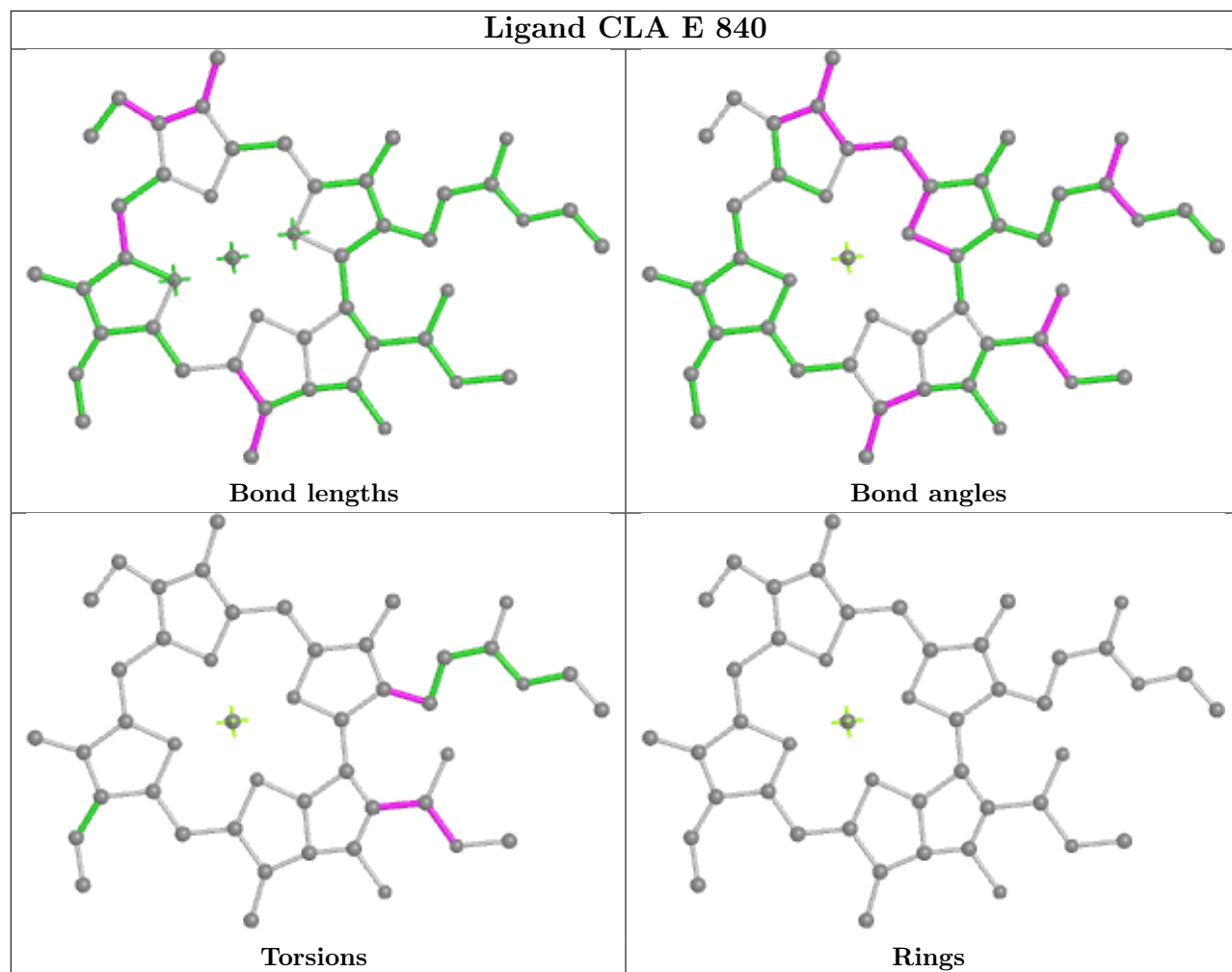
Ligand CLA E 837

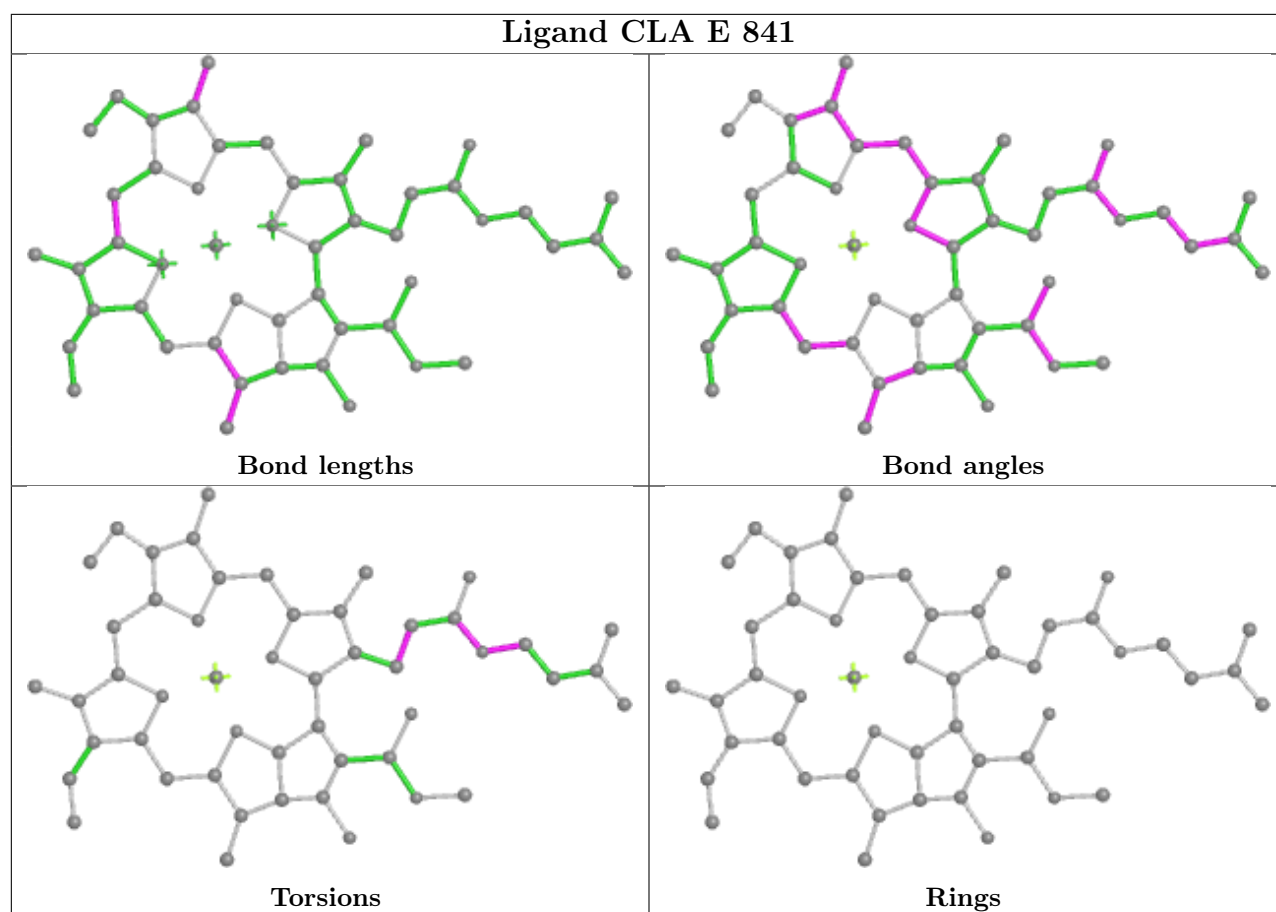


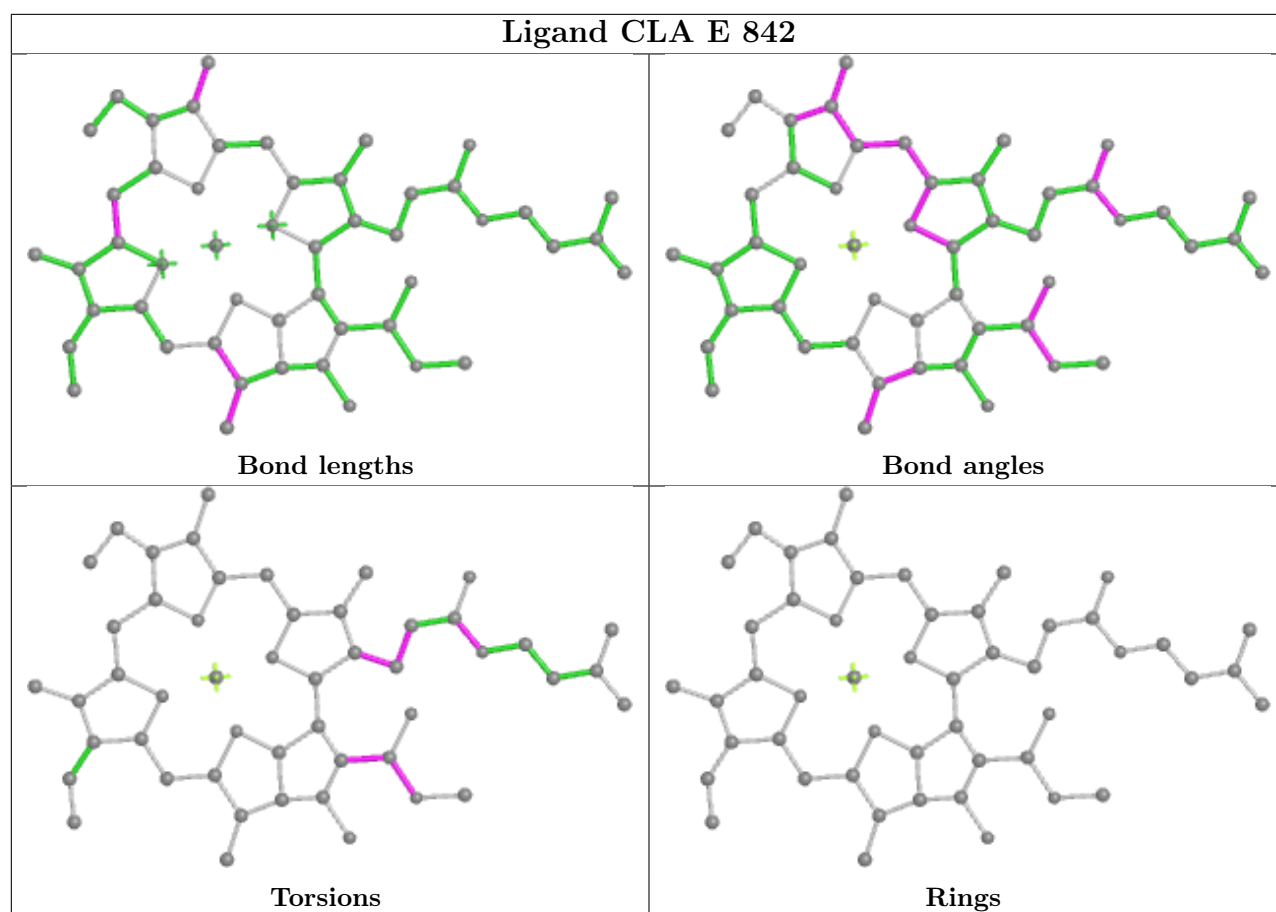


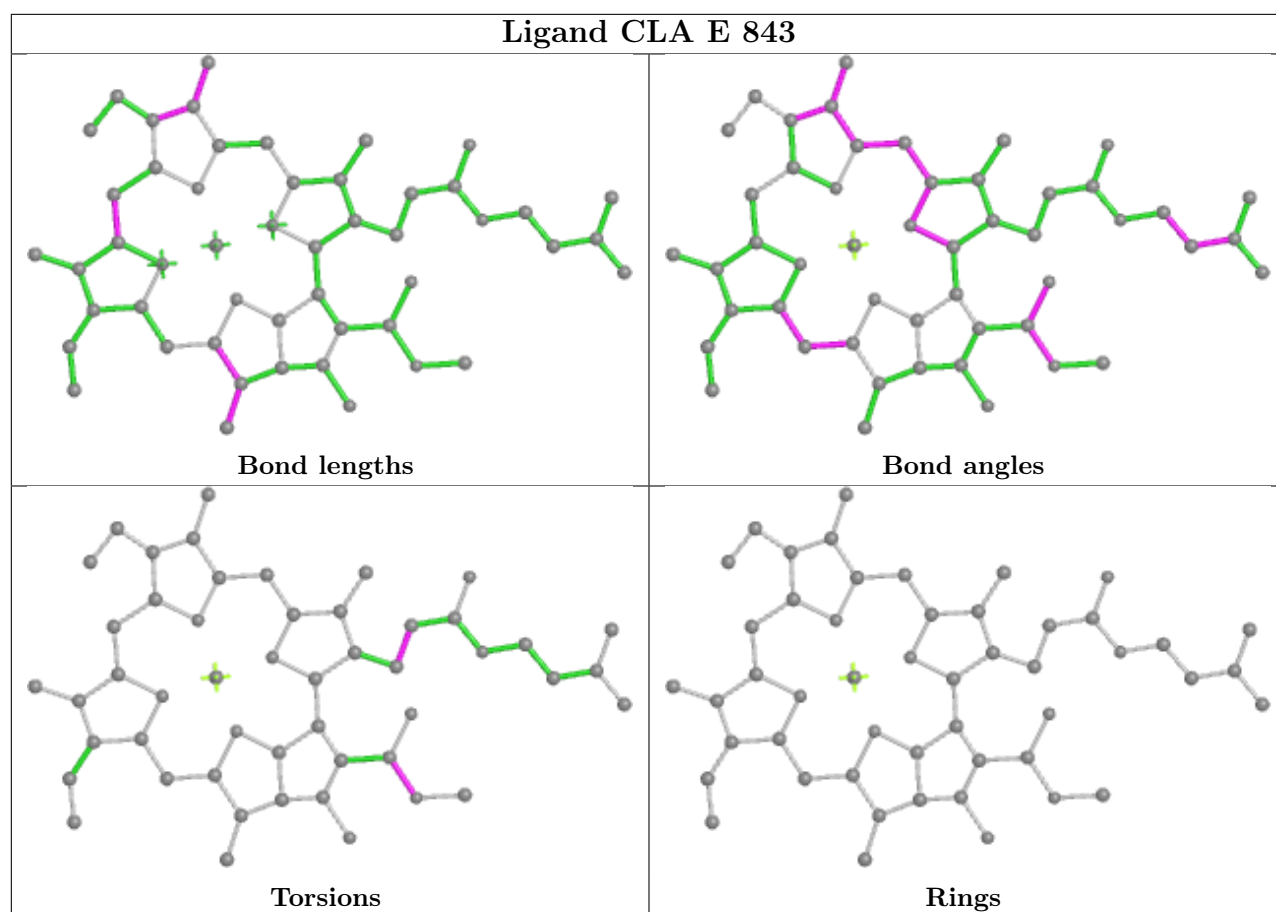


Ligand CLA E 840

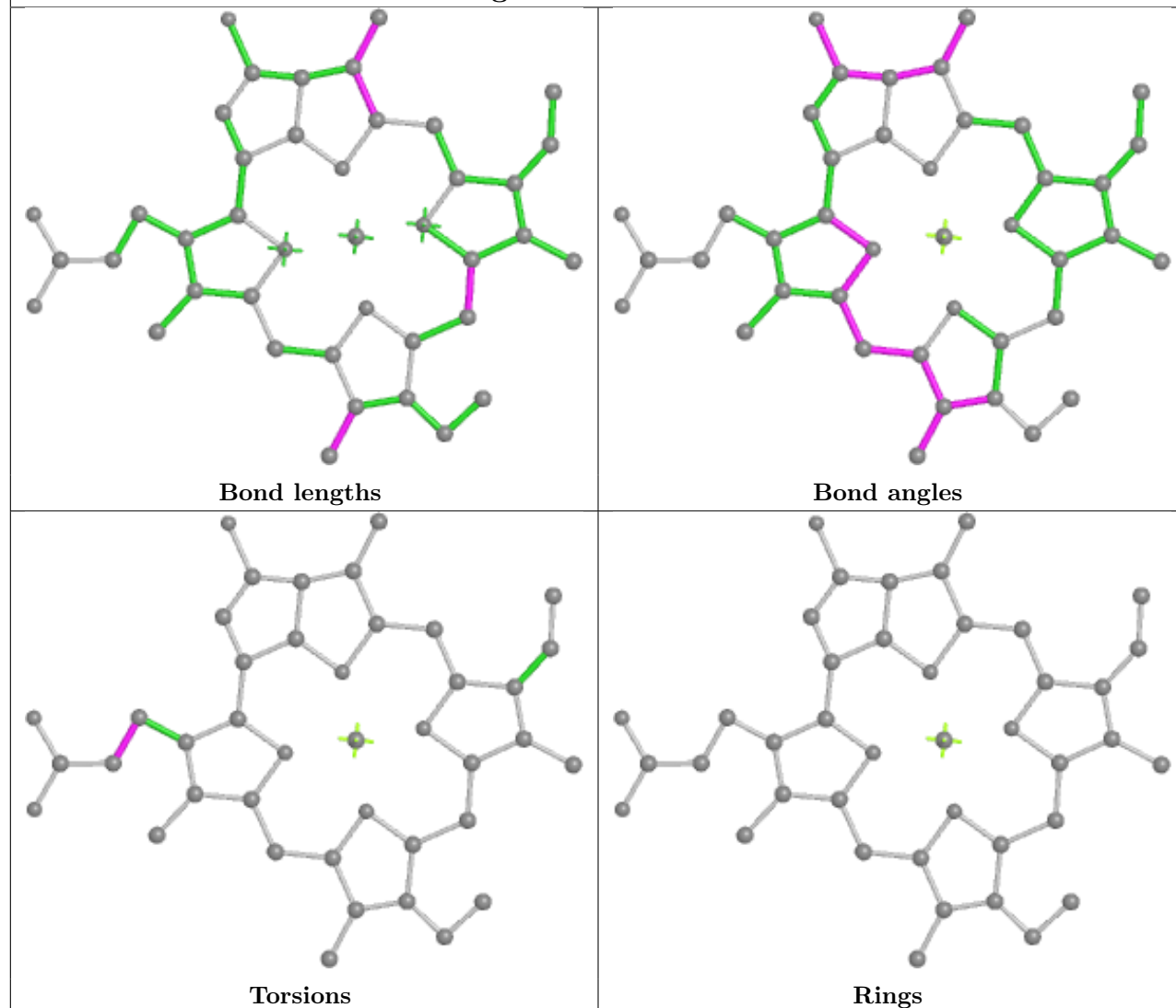




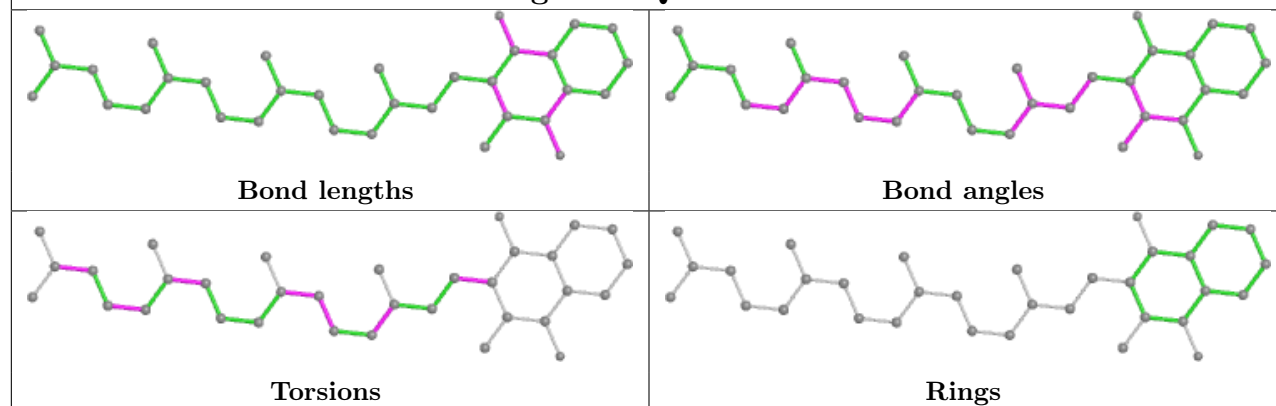


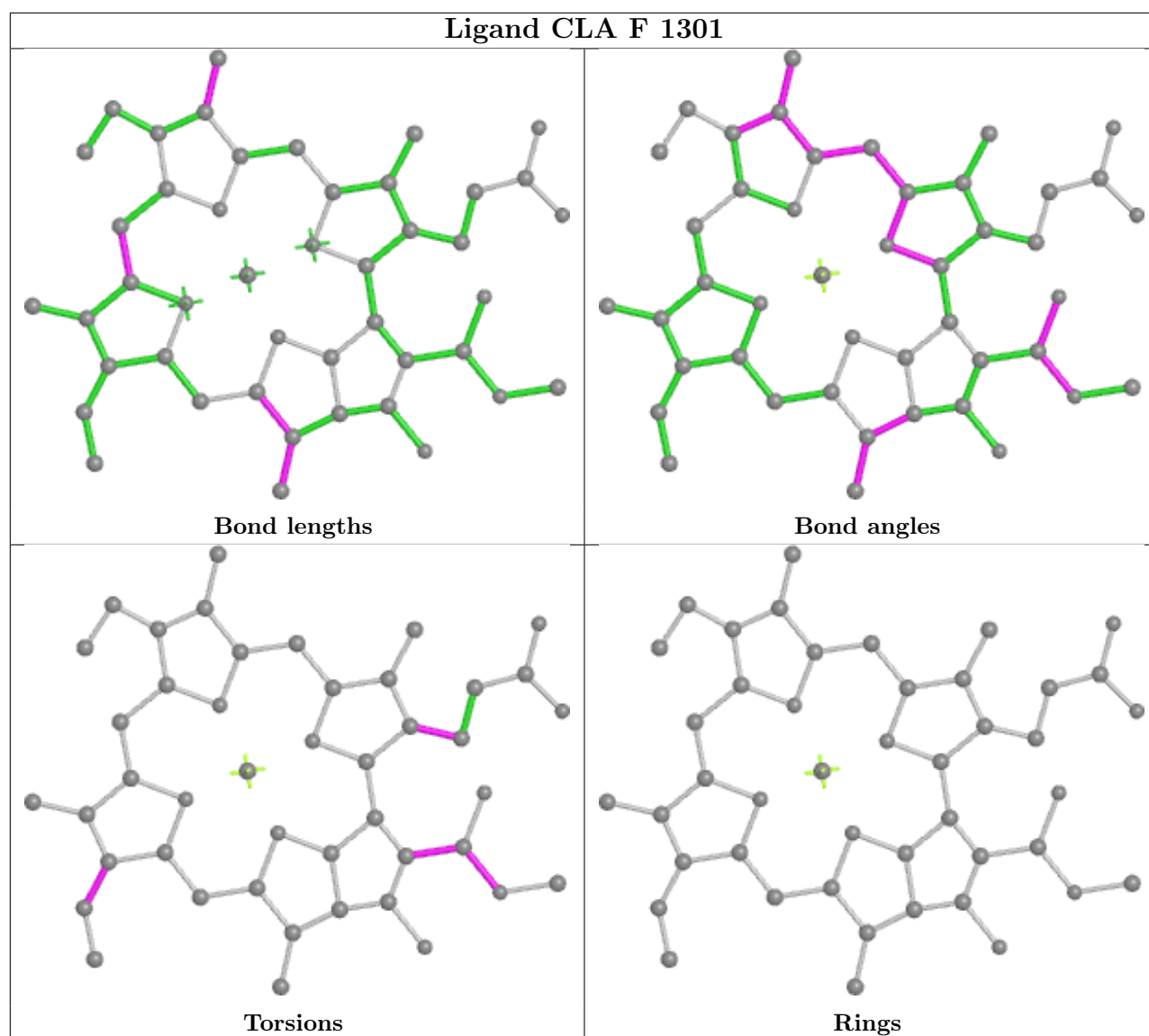


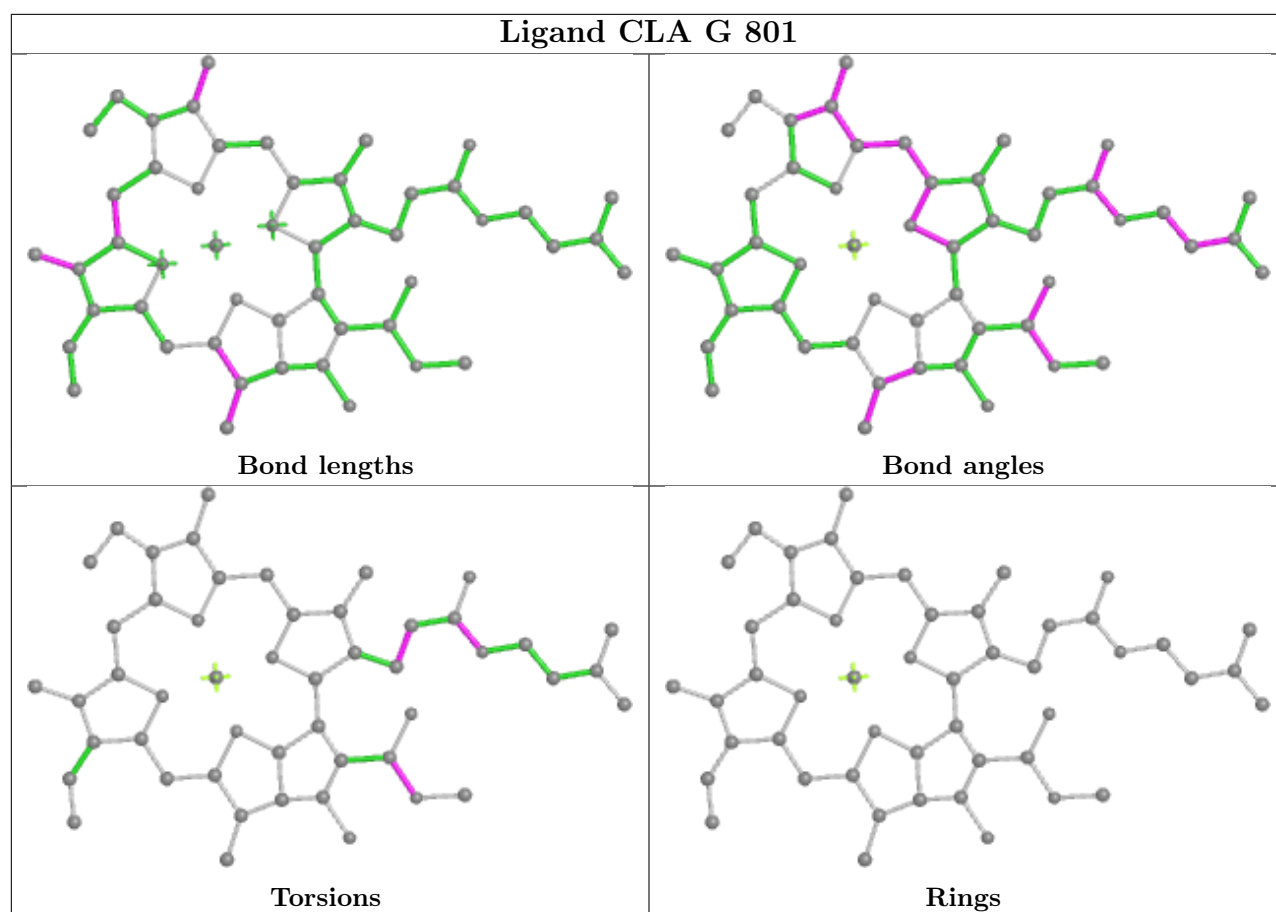
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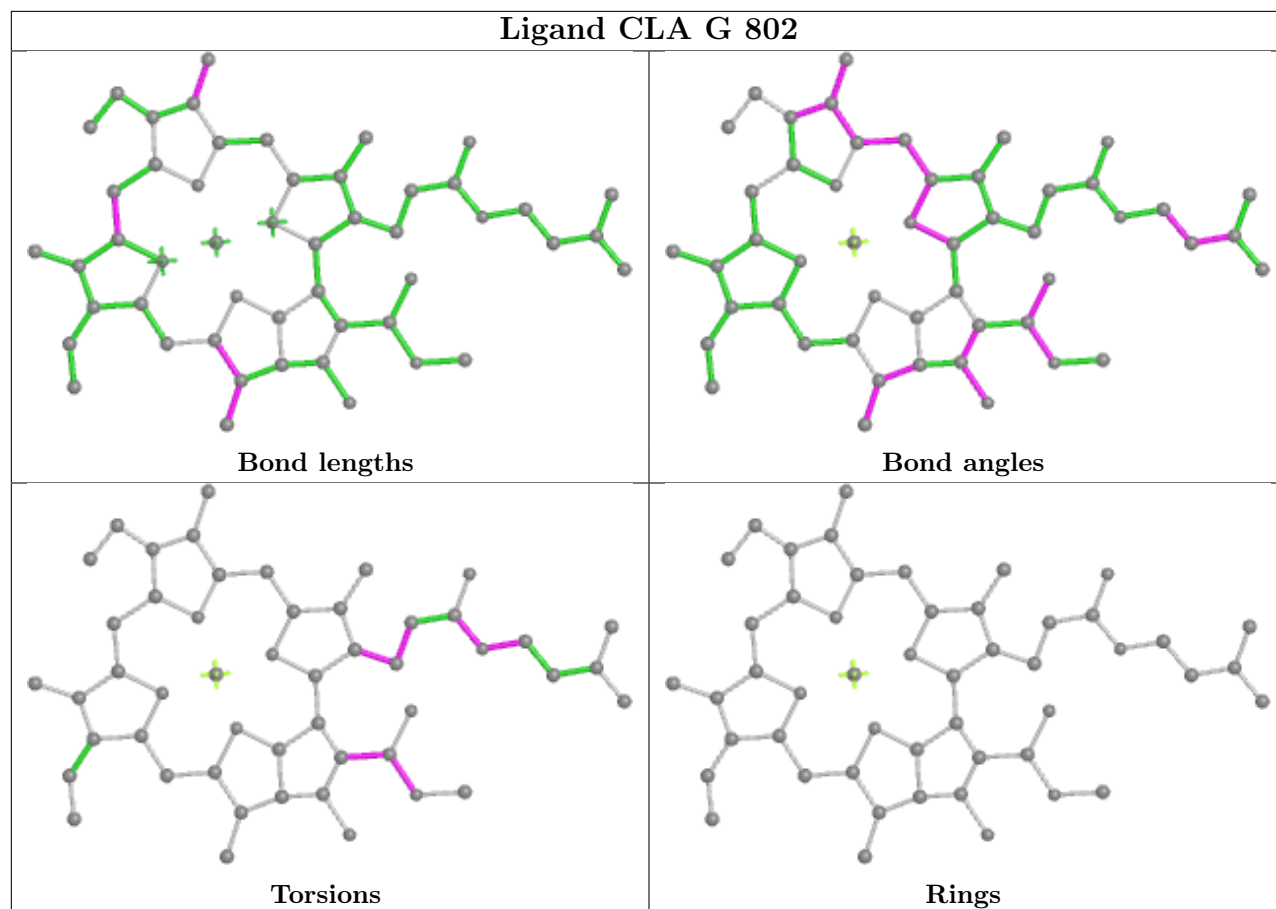


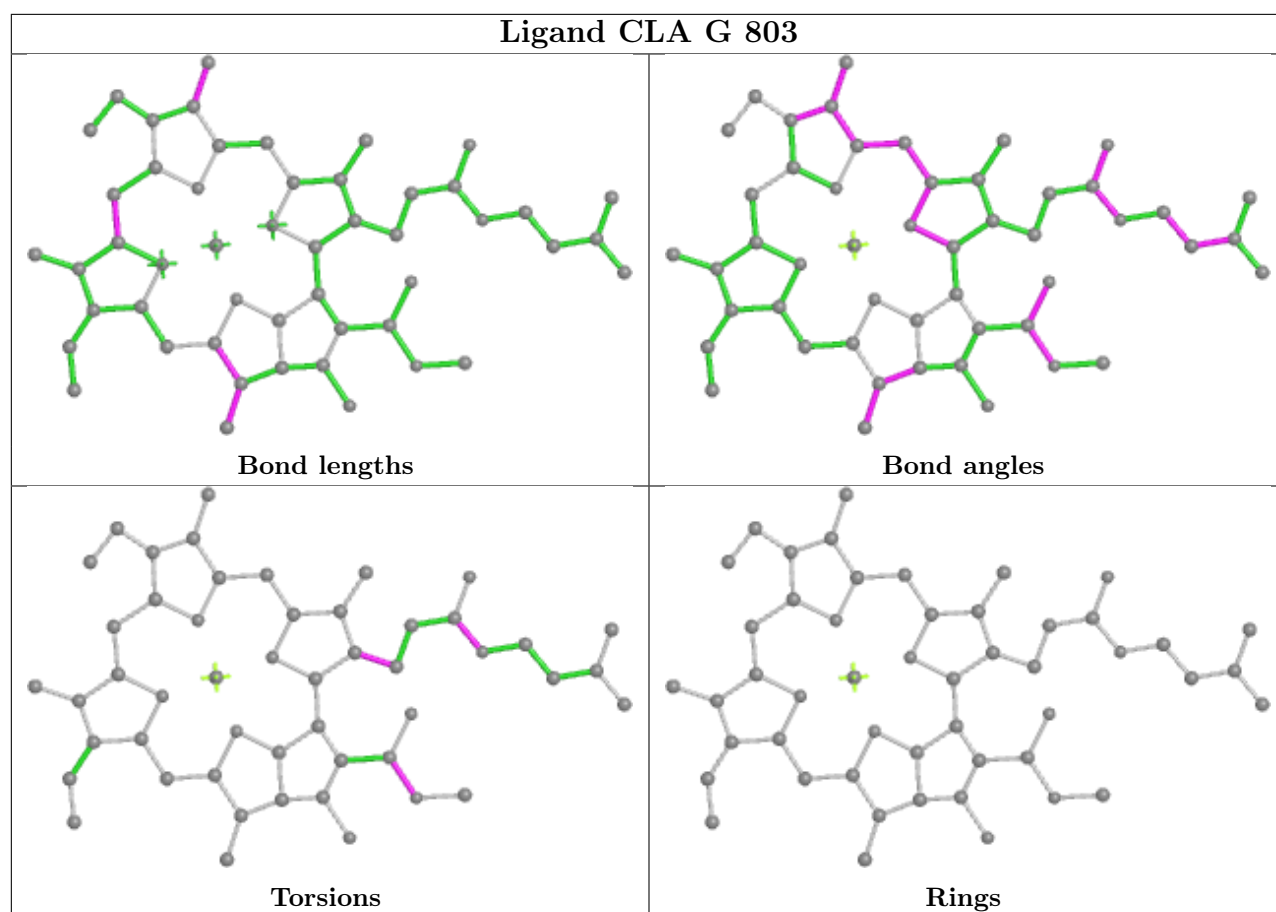
Ligand PQN E 846

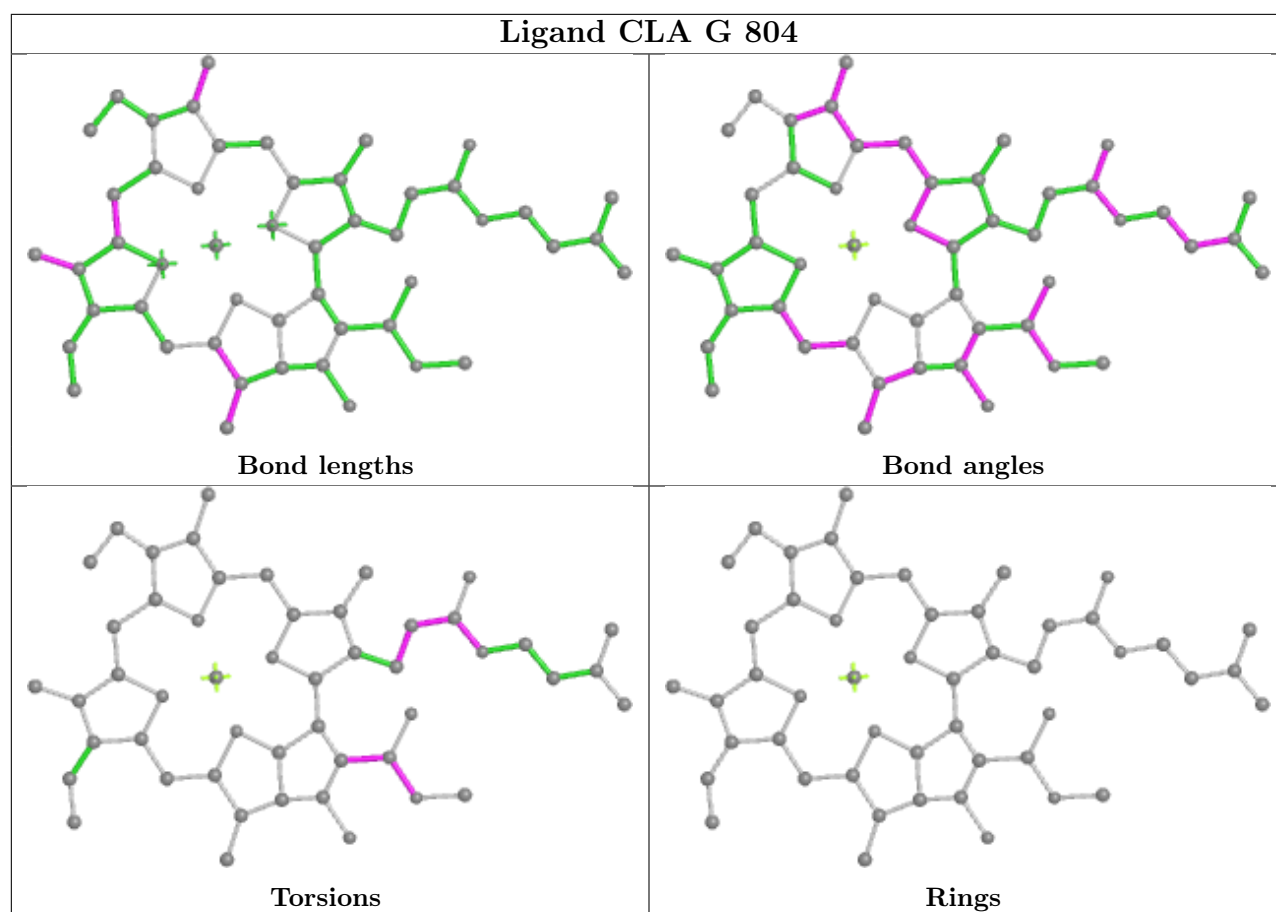


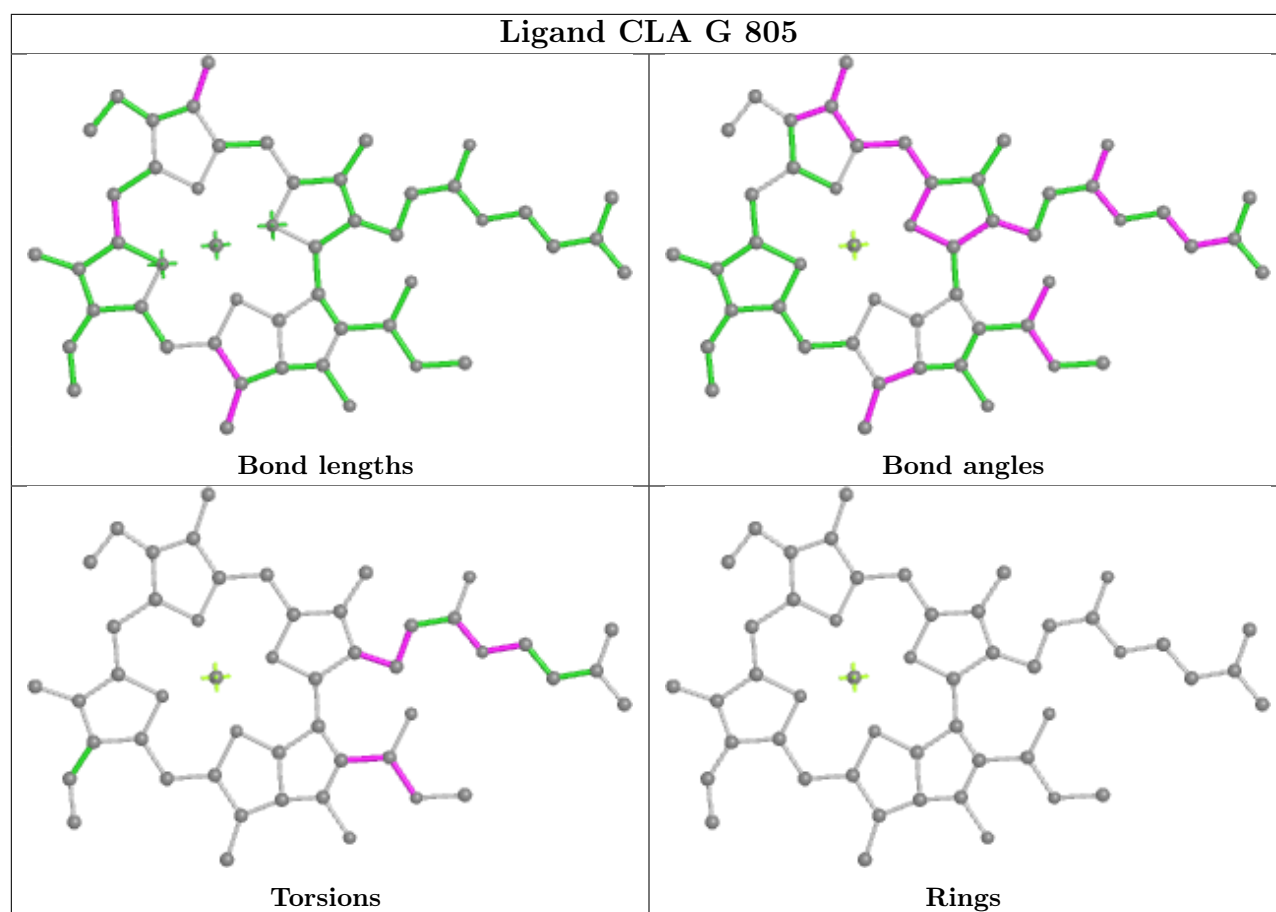


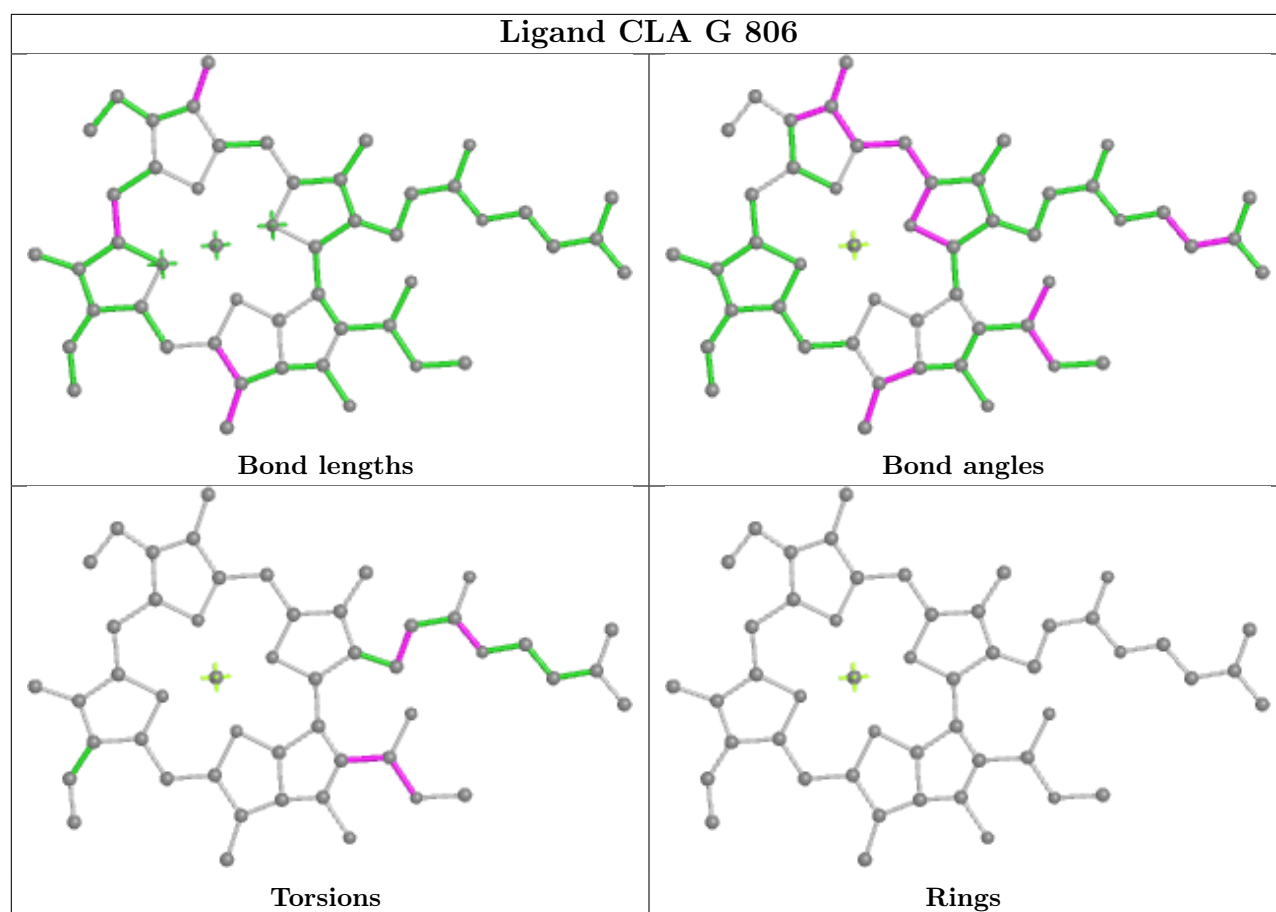


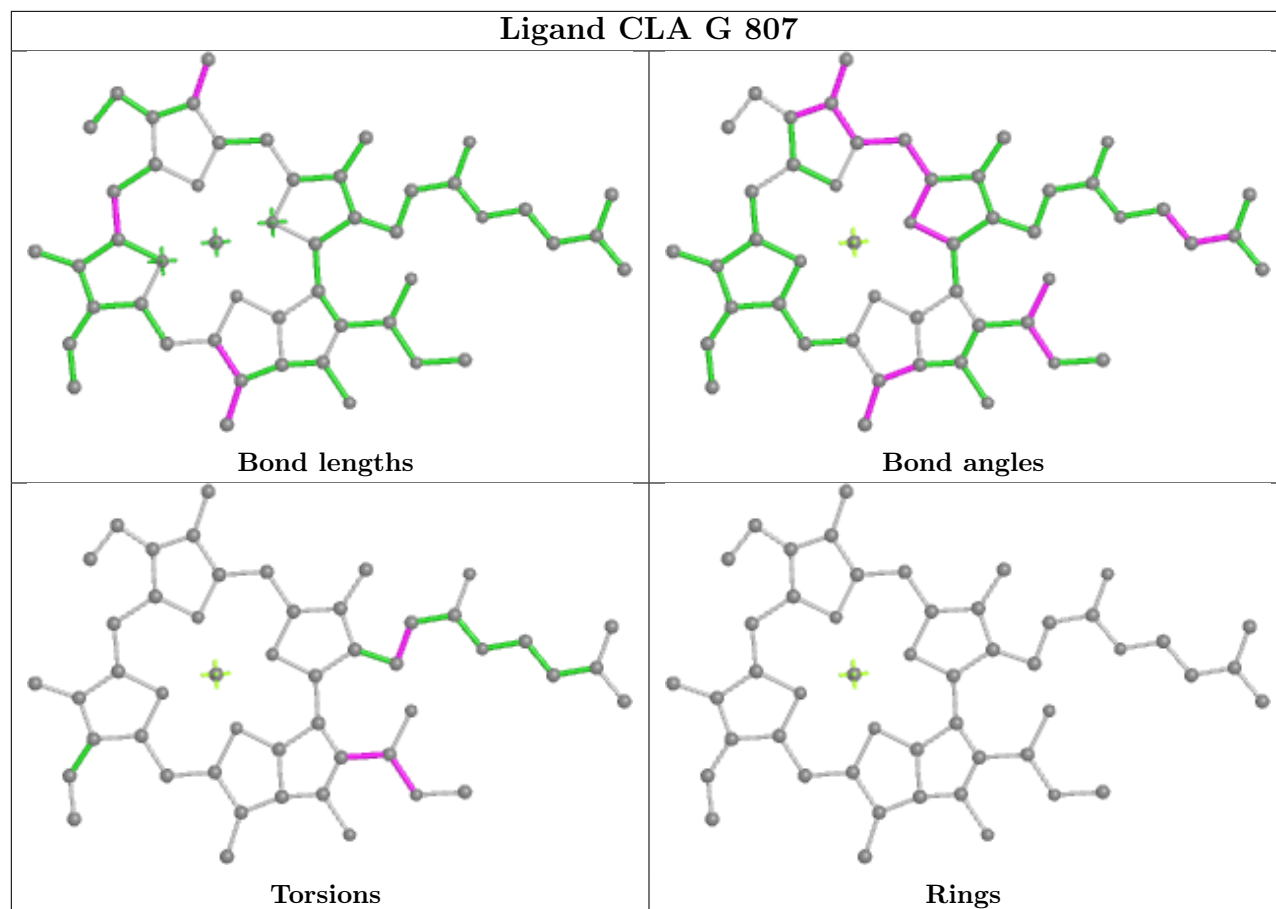


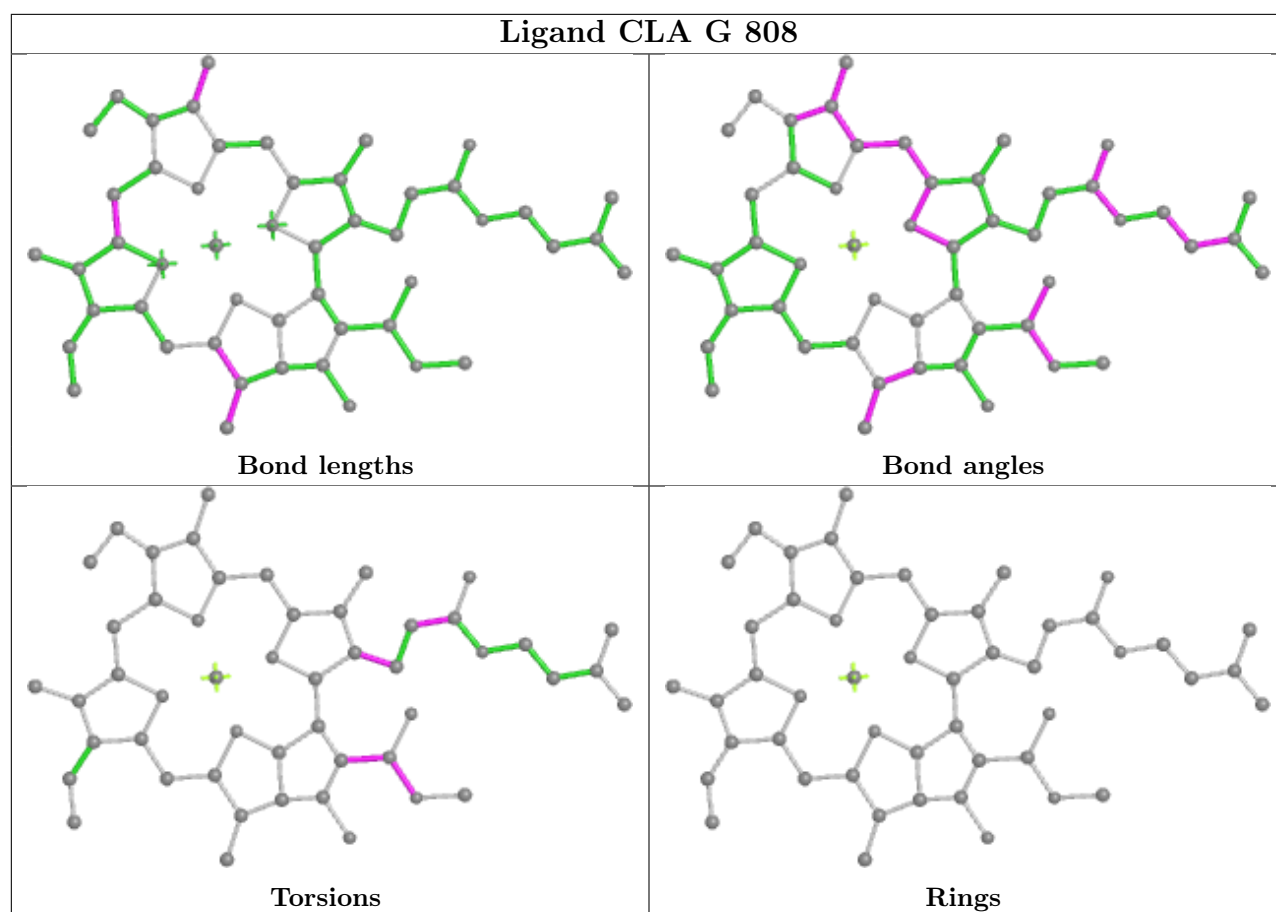


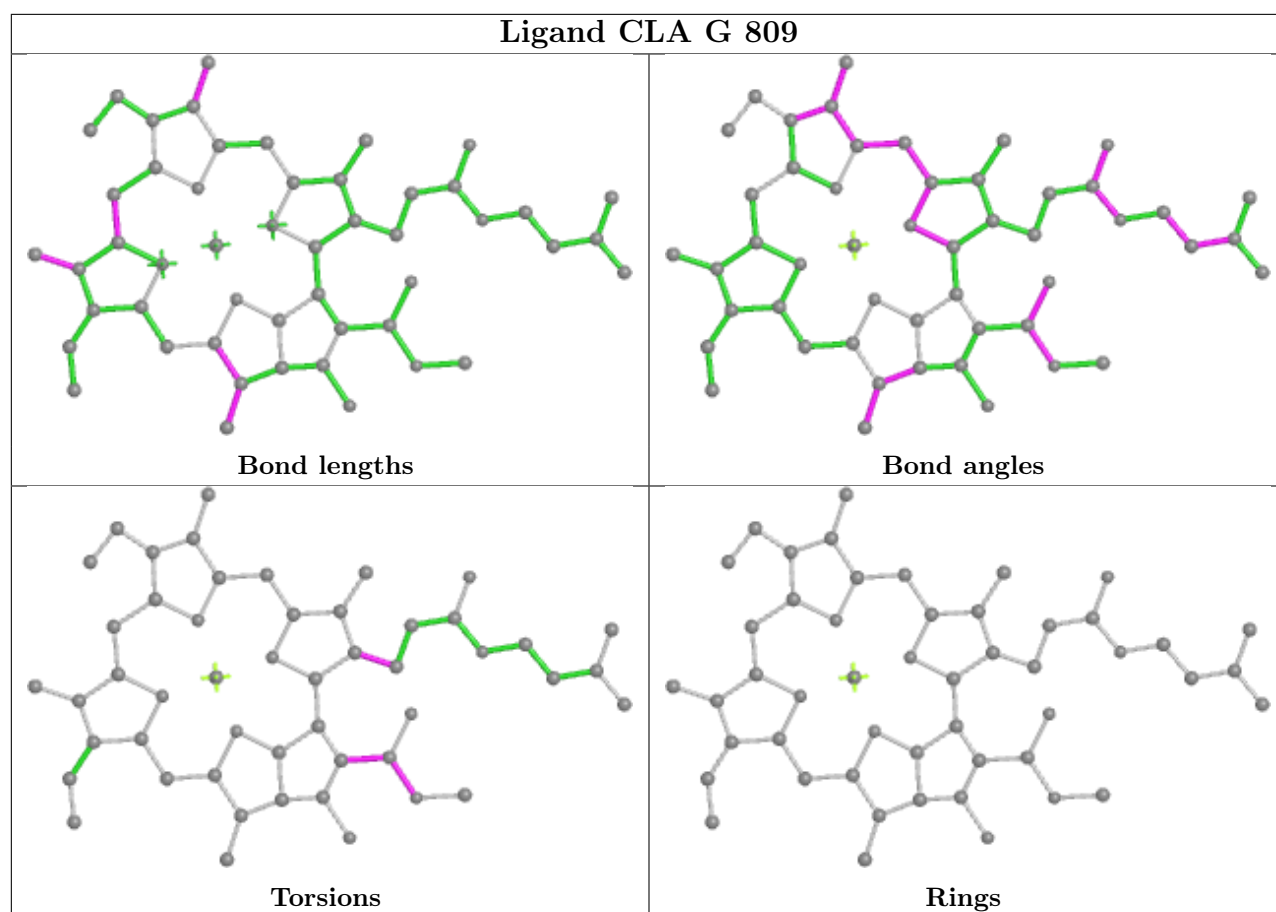


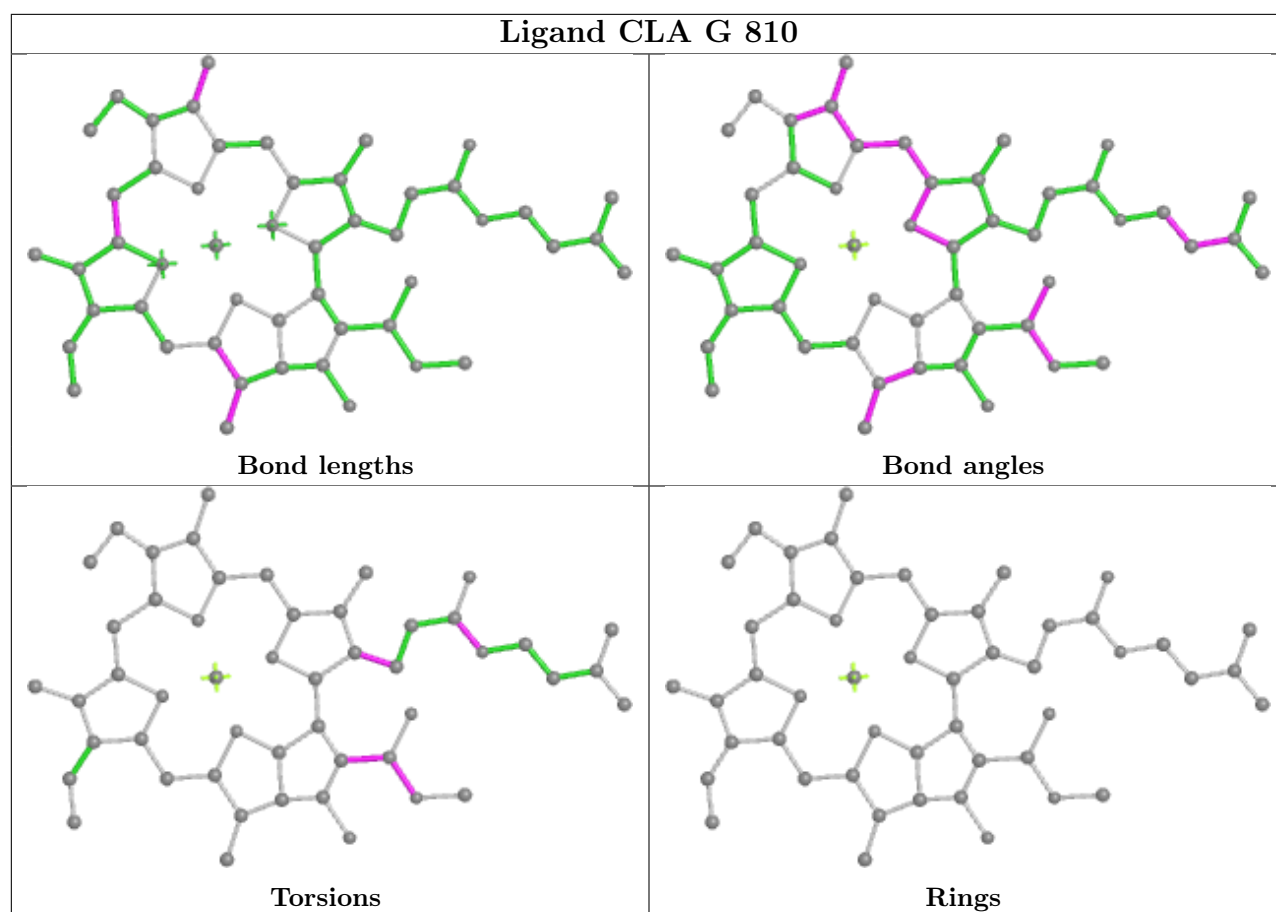


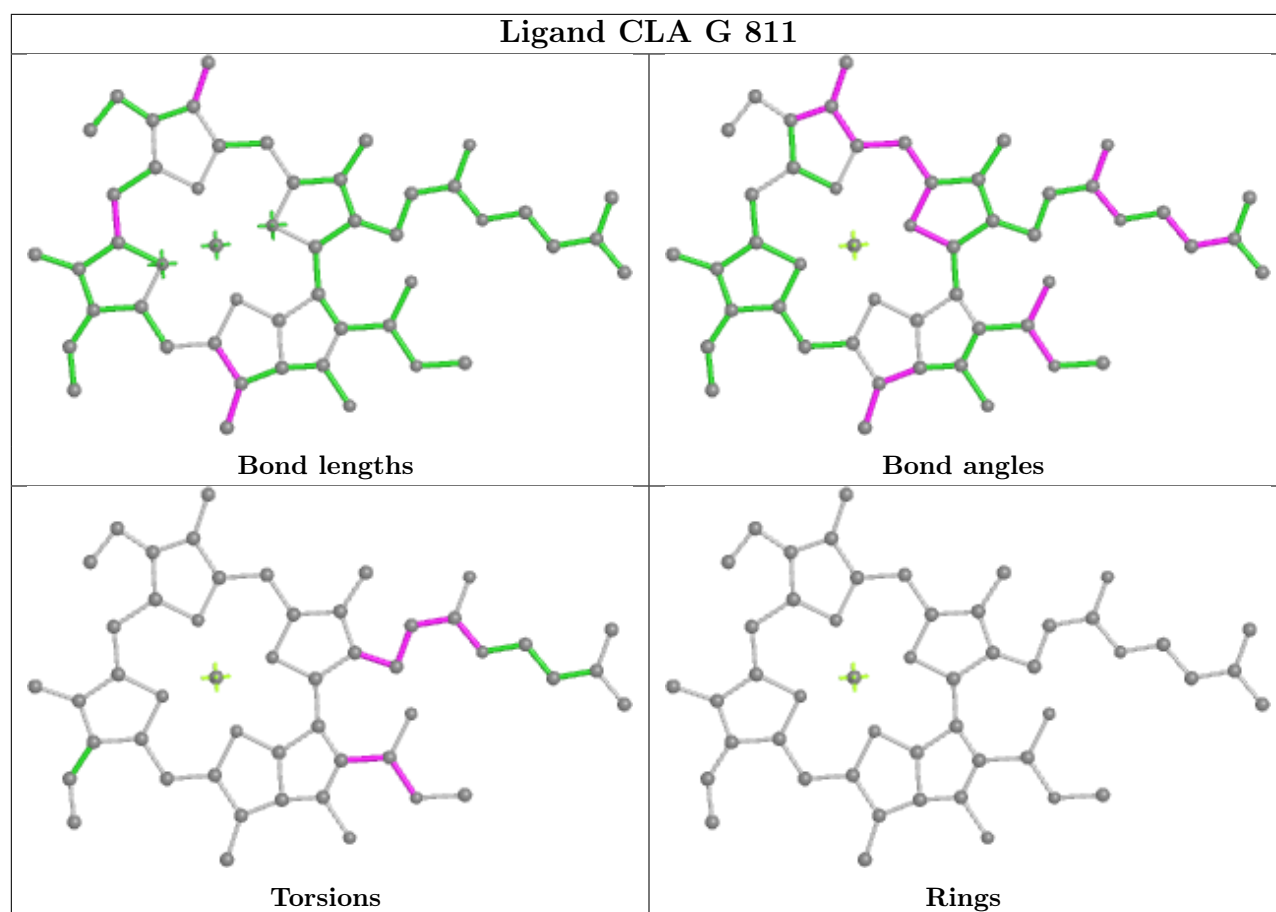


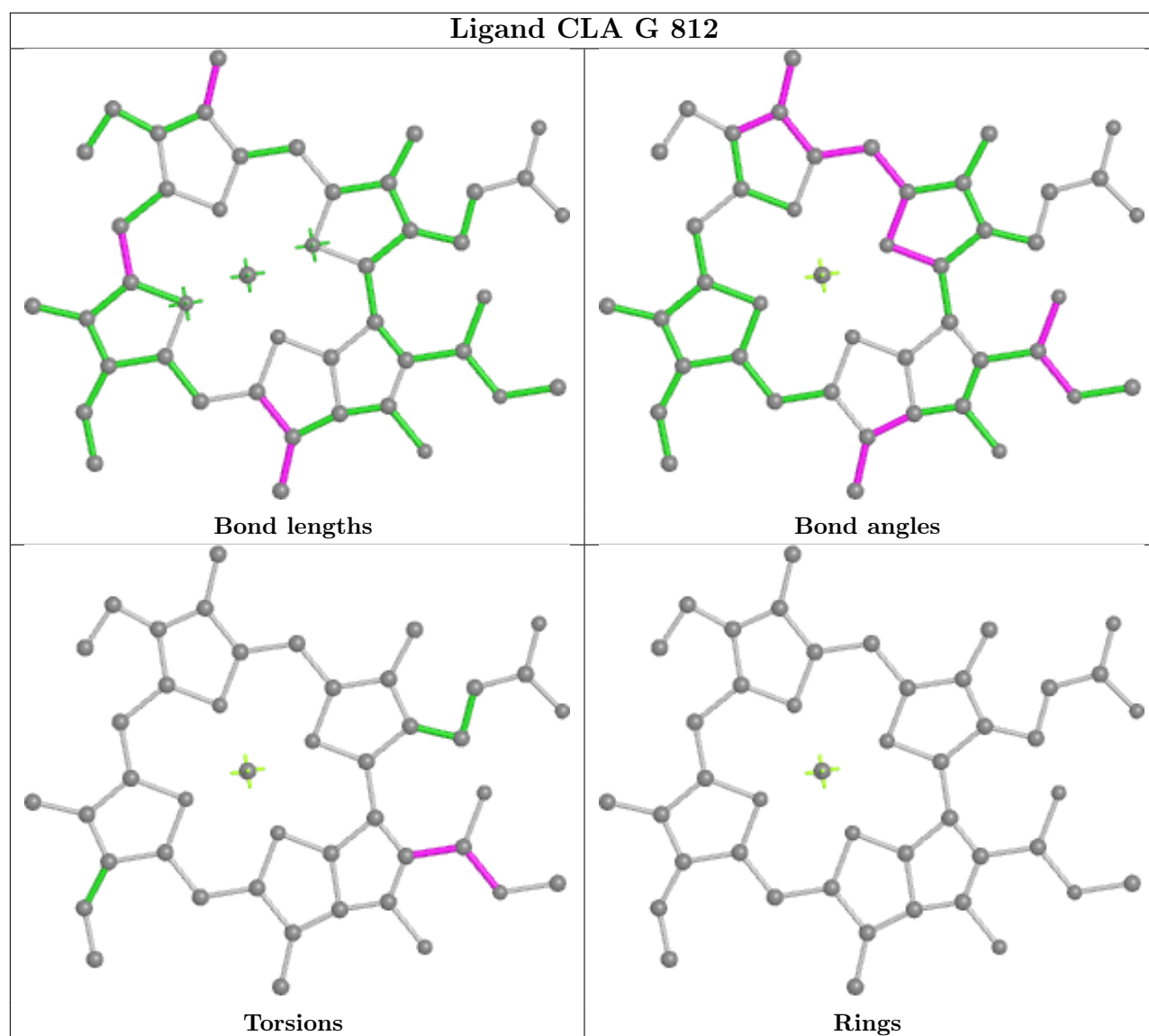




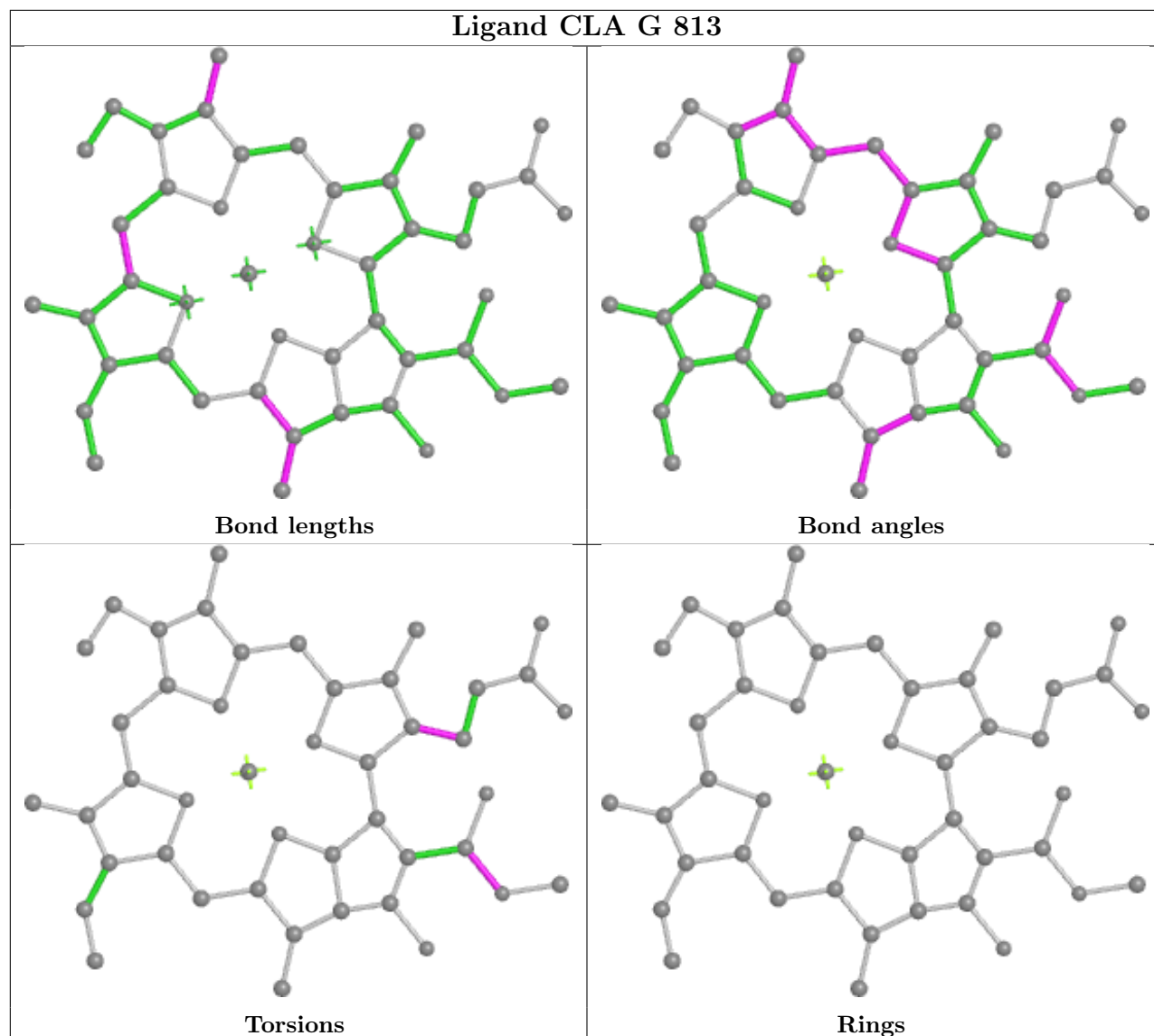


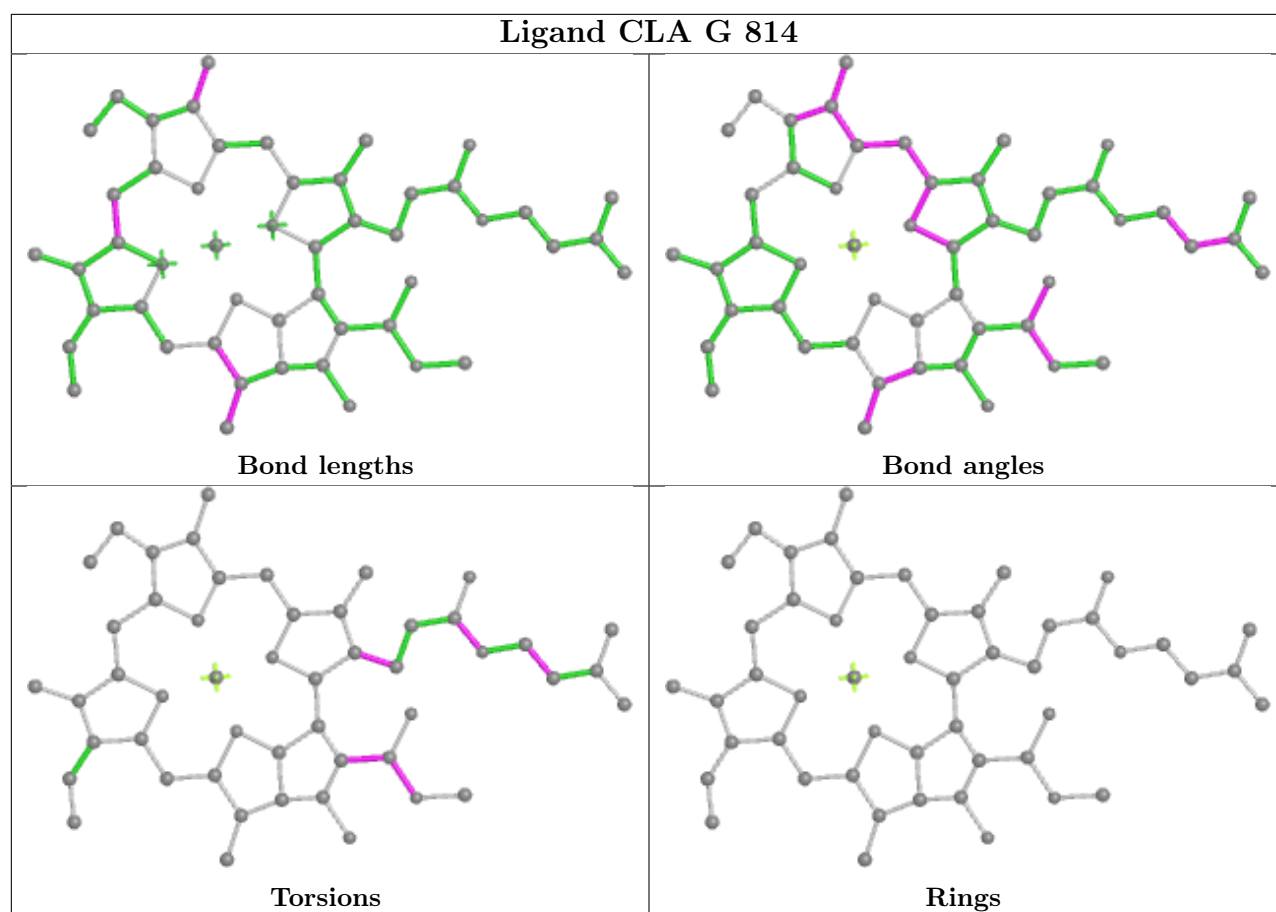


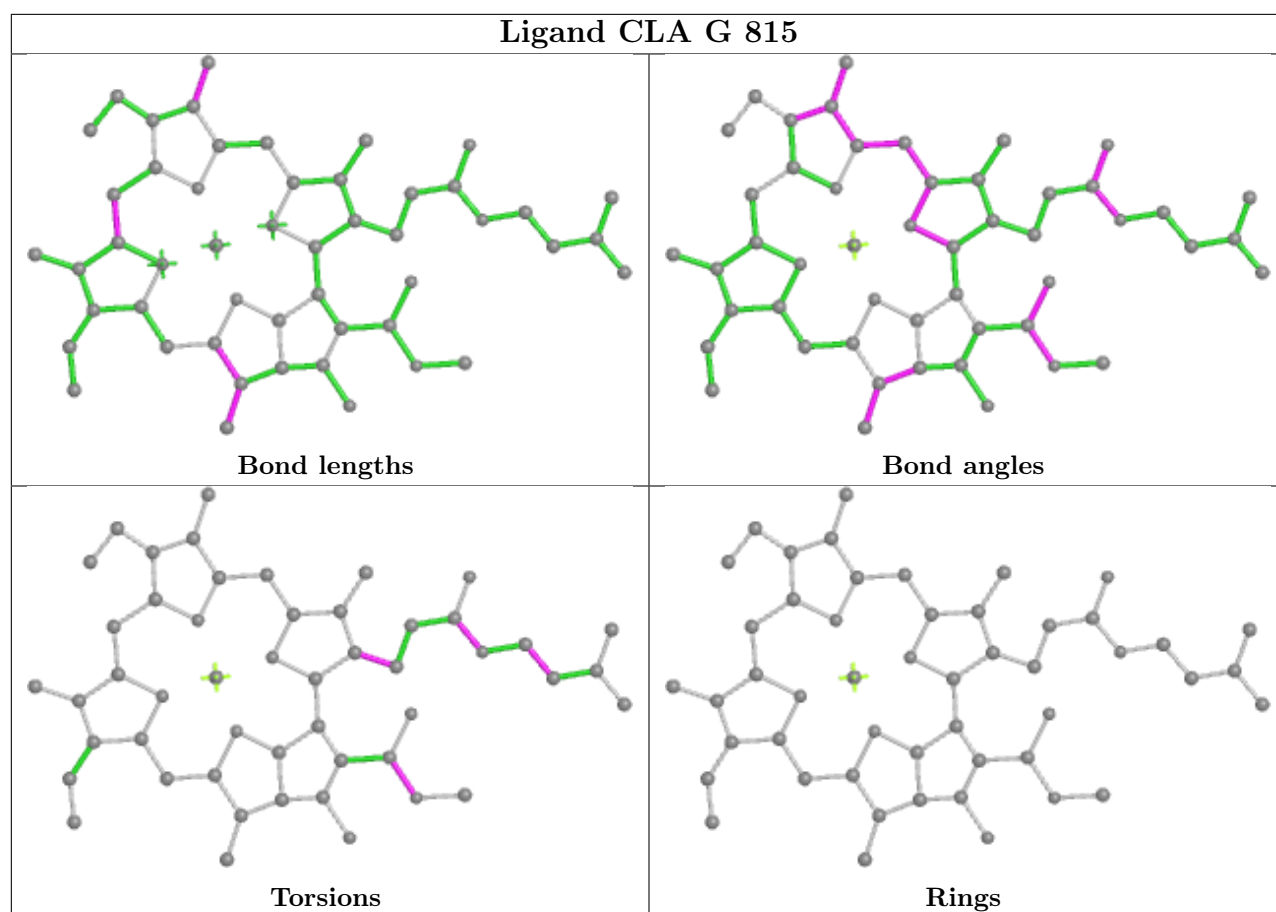




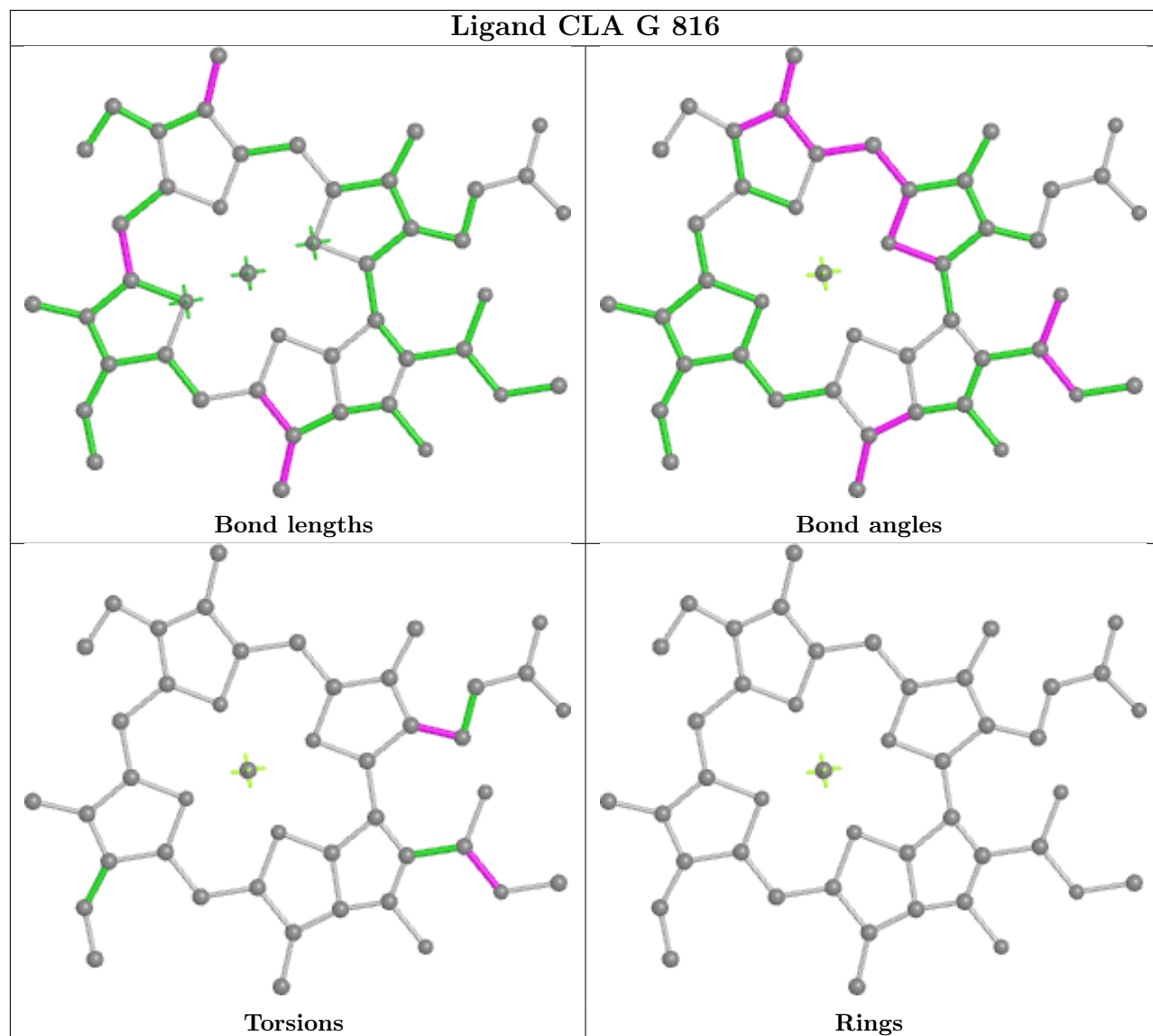
Ligand CLA G 813

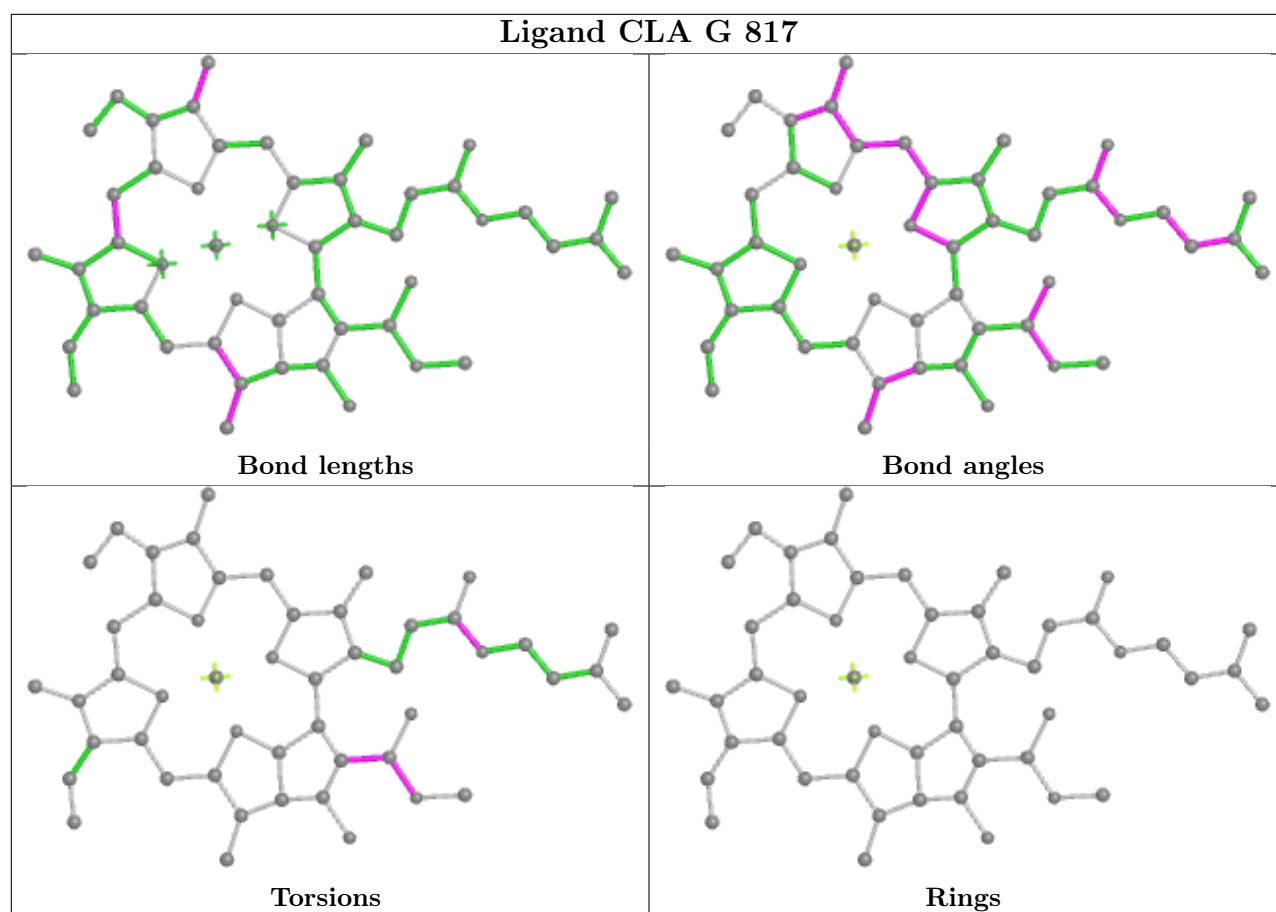


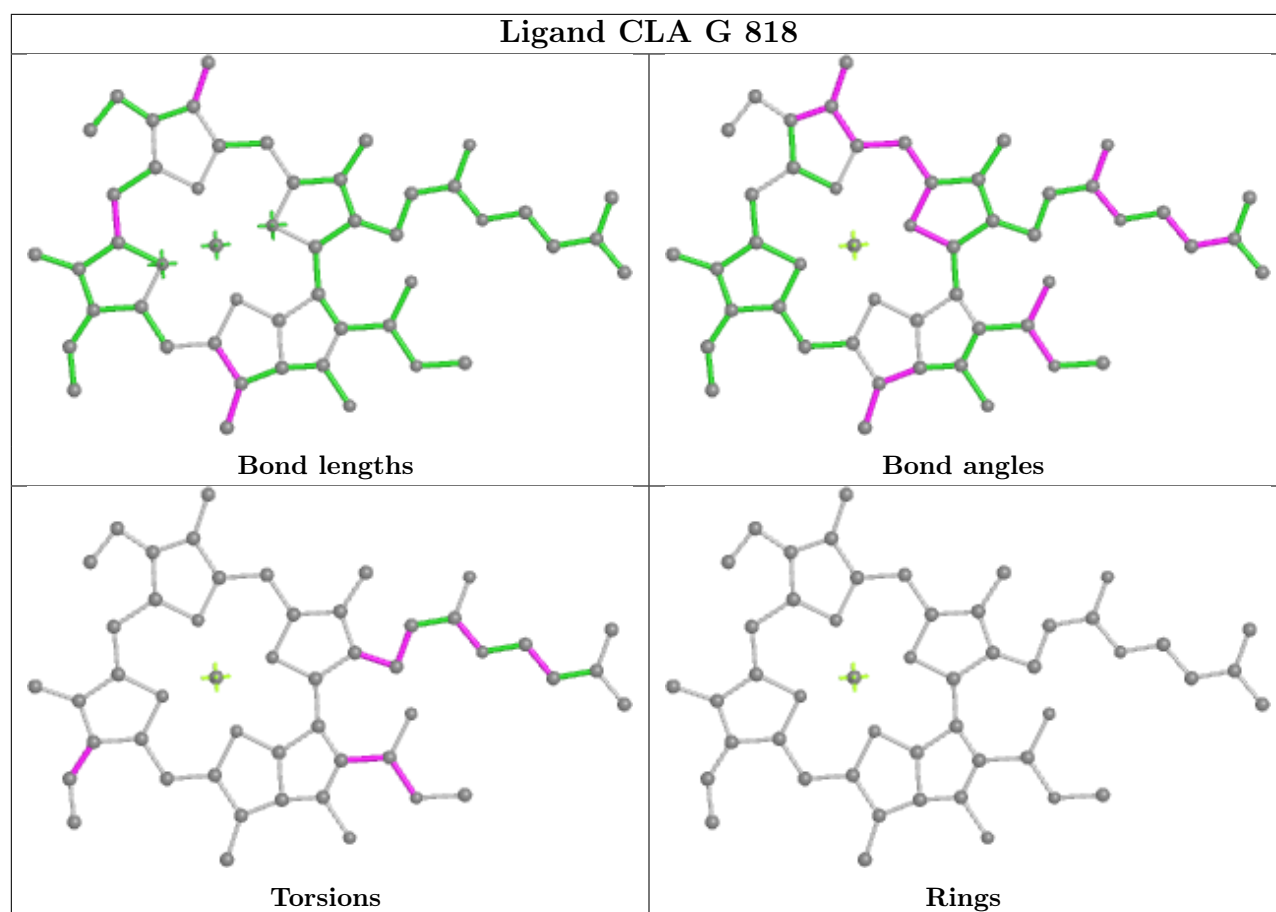


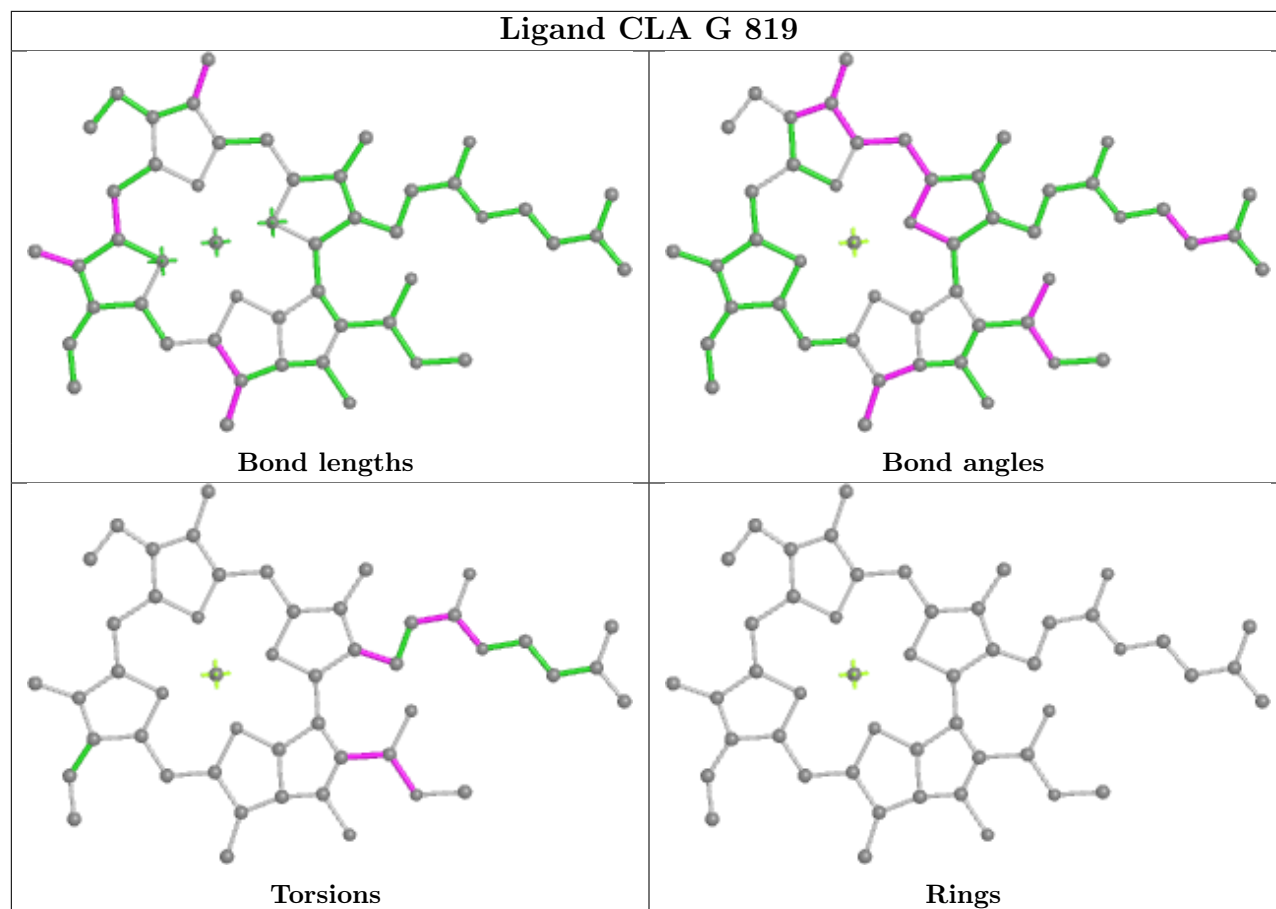


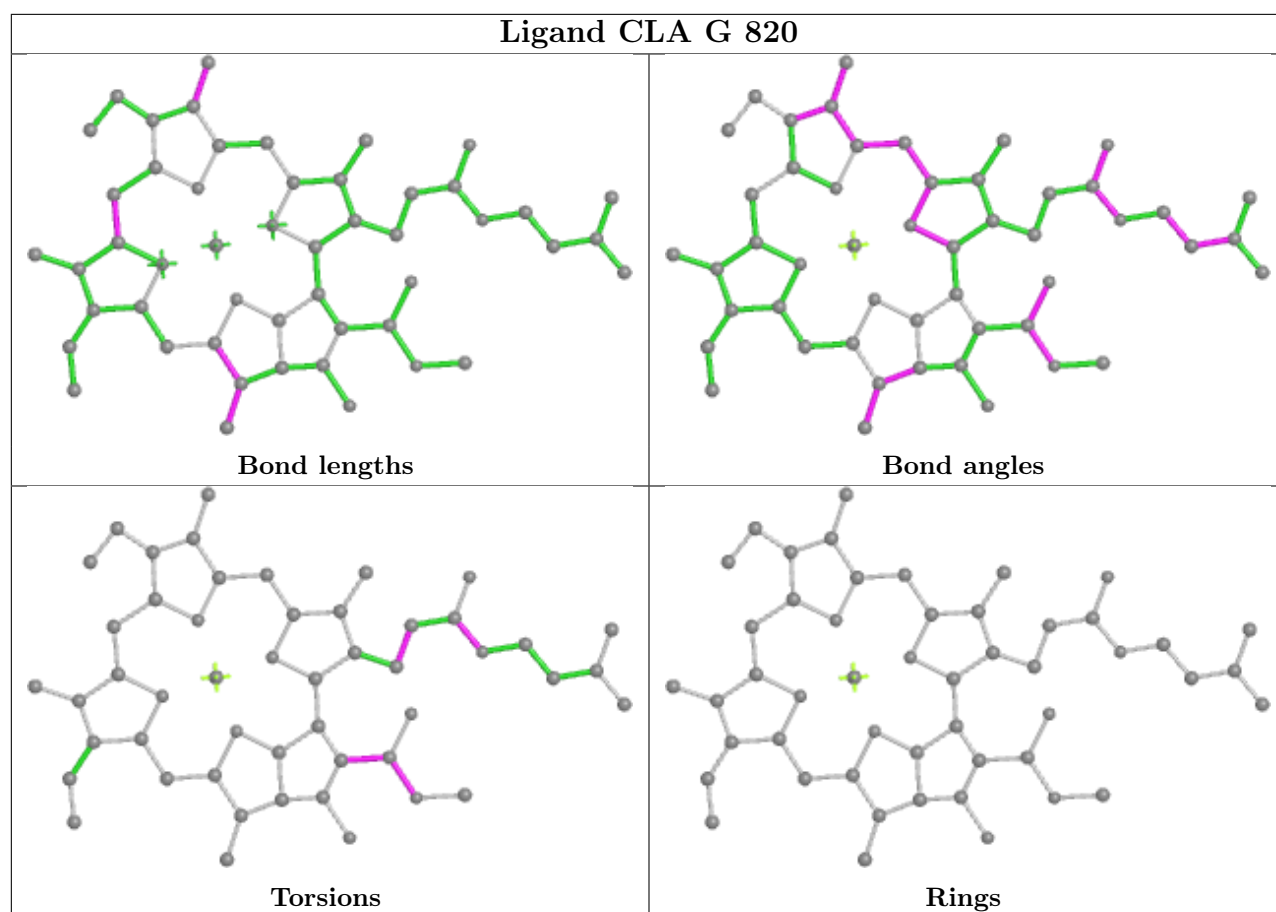
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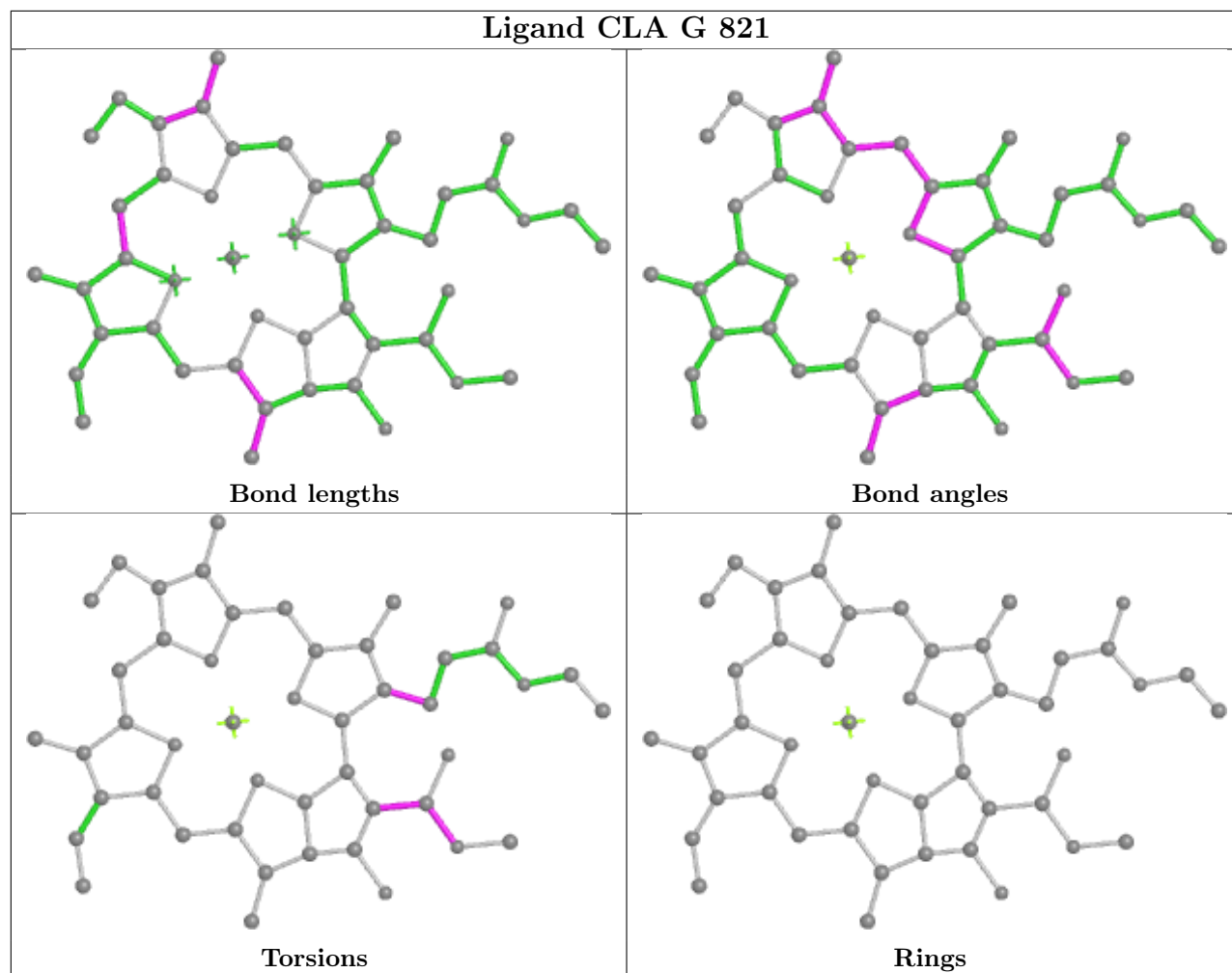




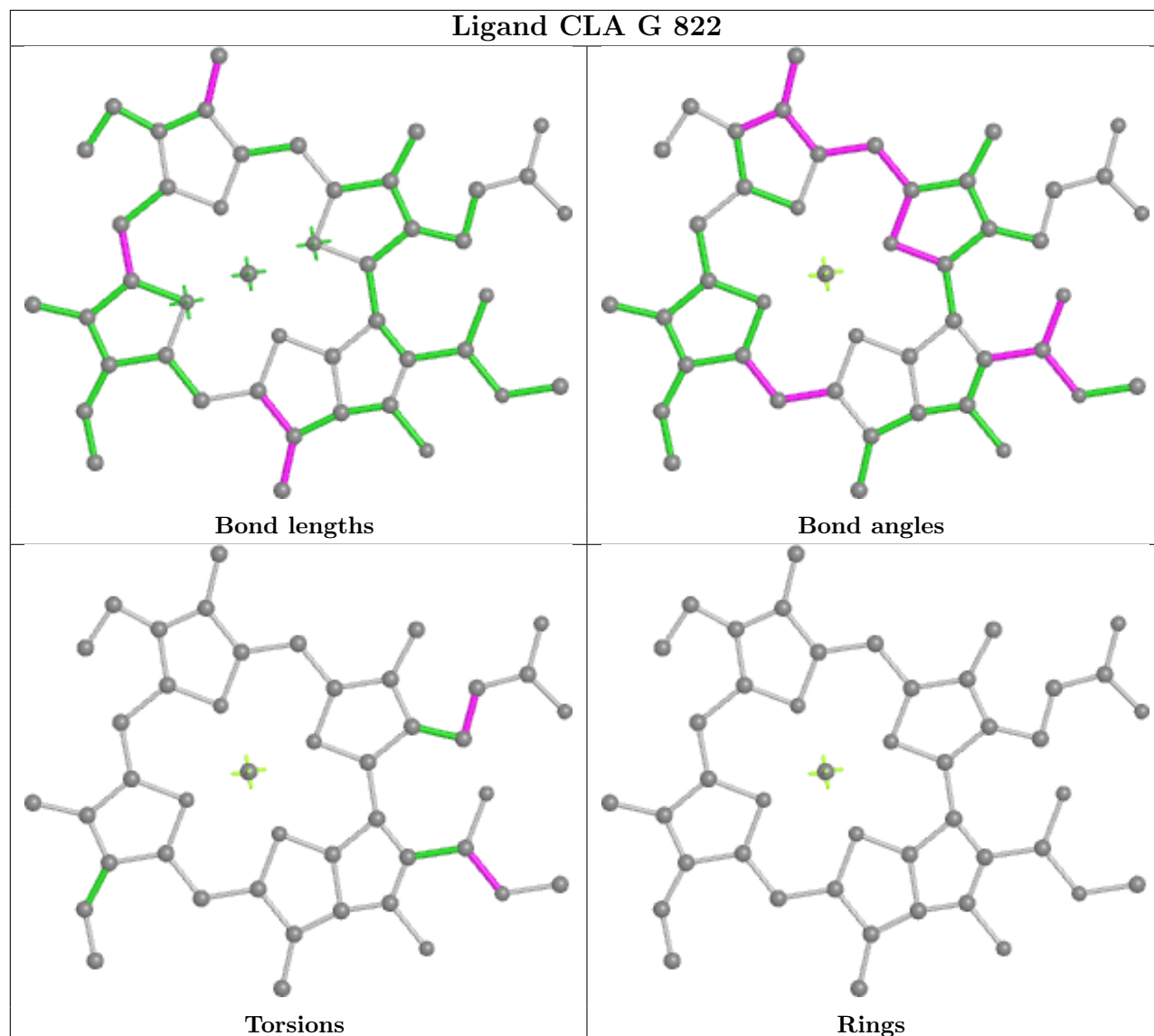


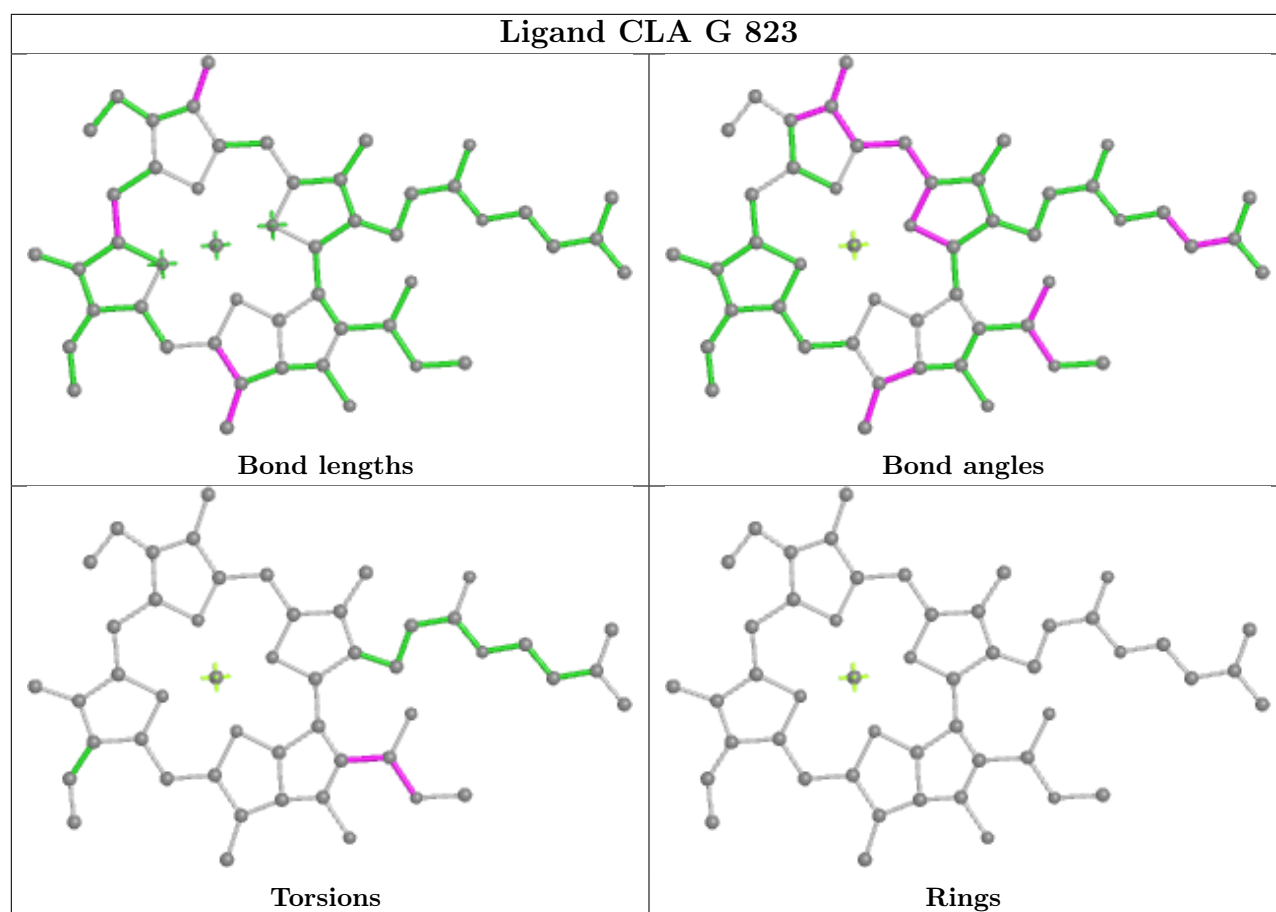


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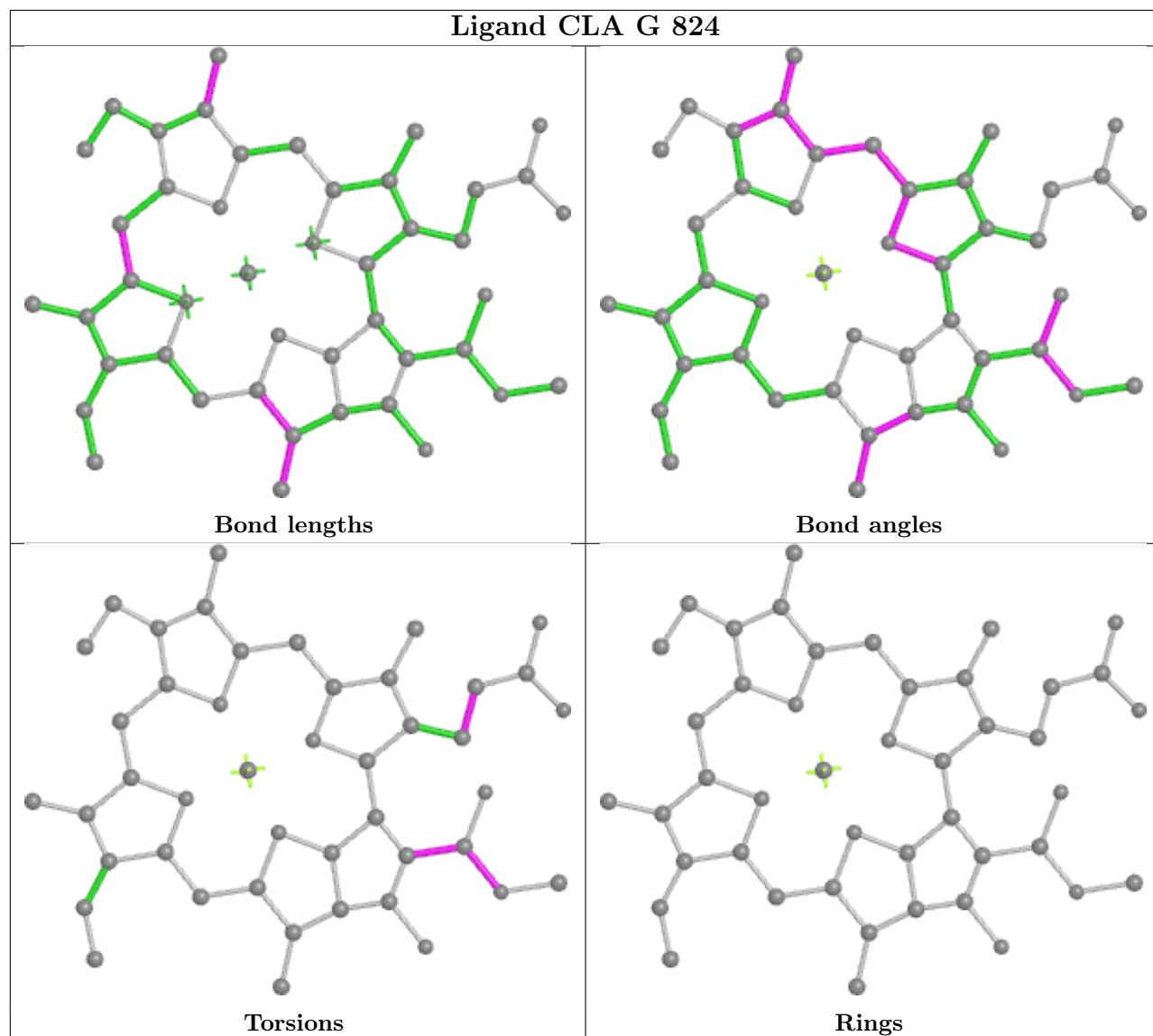


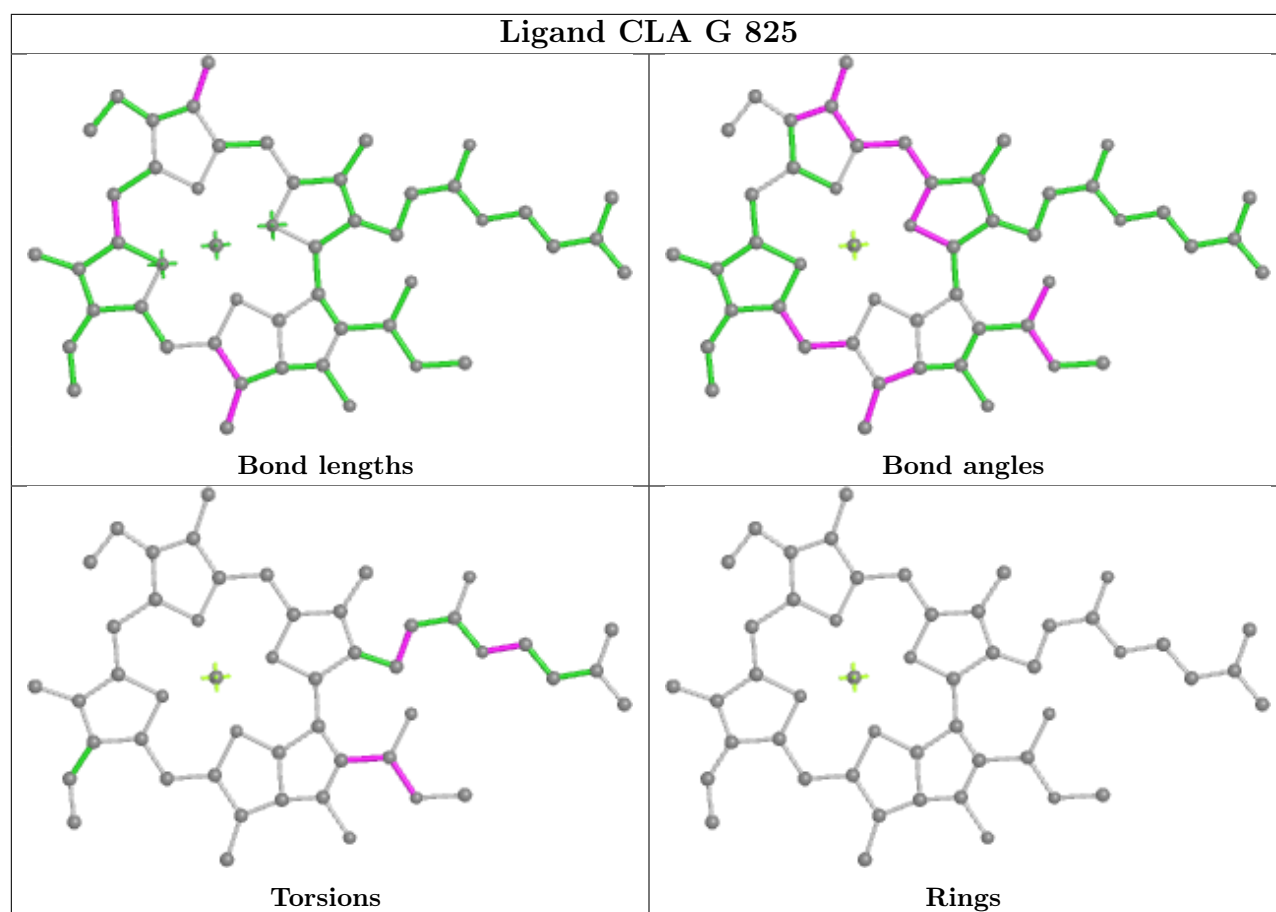
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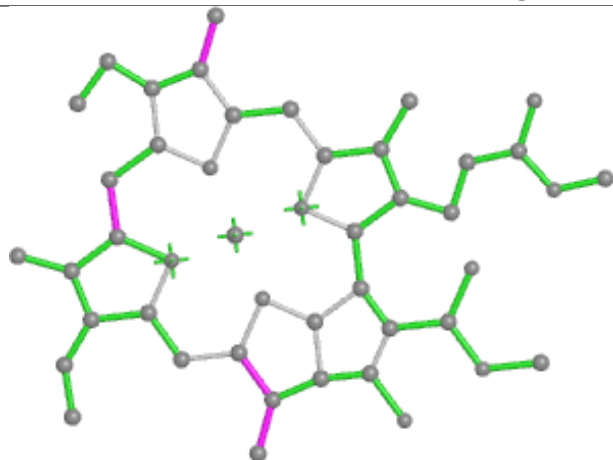


Ligand CLA G 824

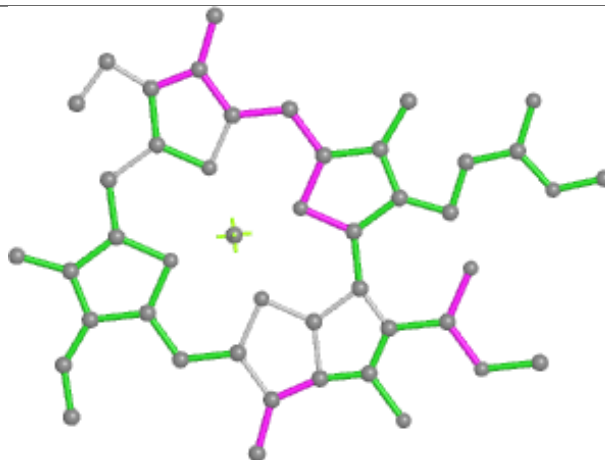




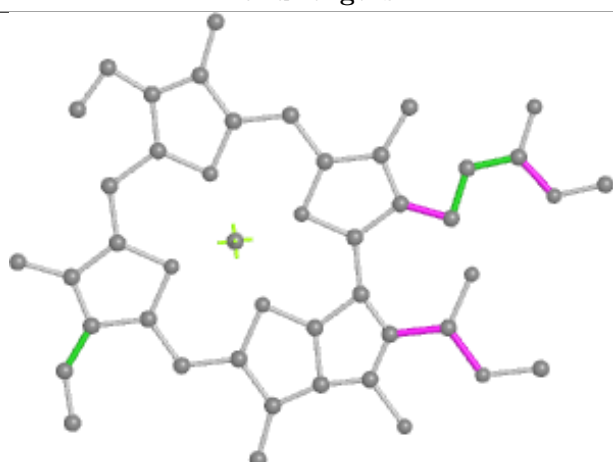
Ligand CLA G 826



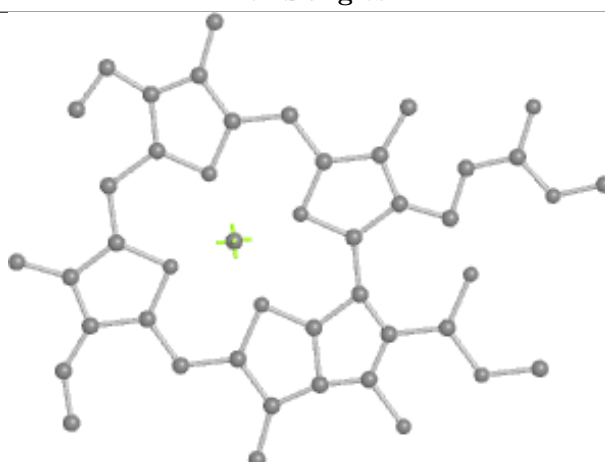
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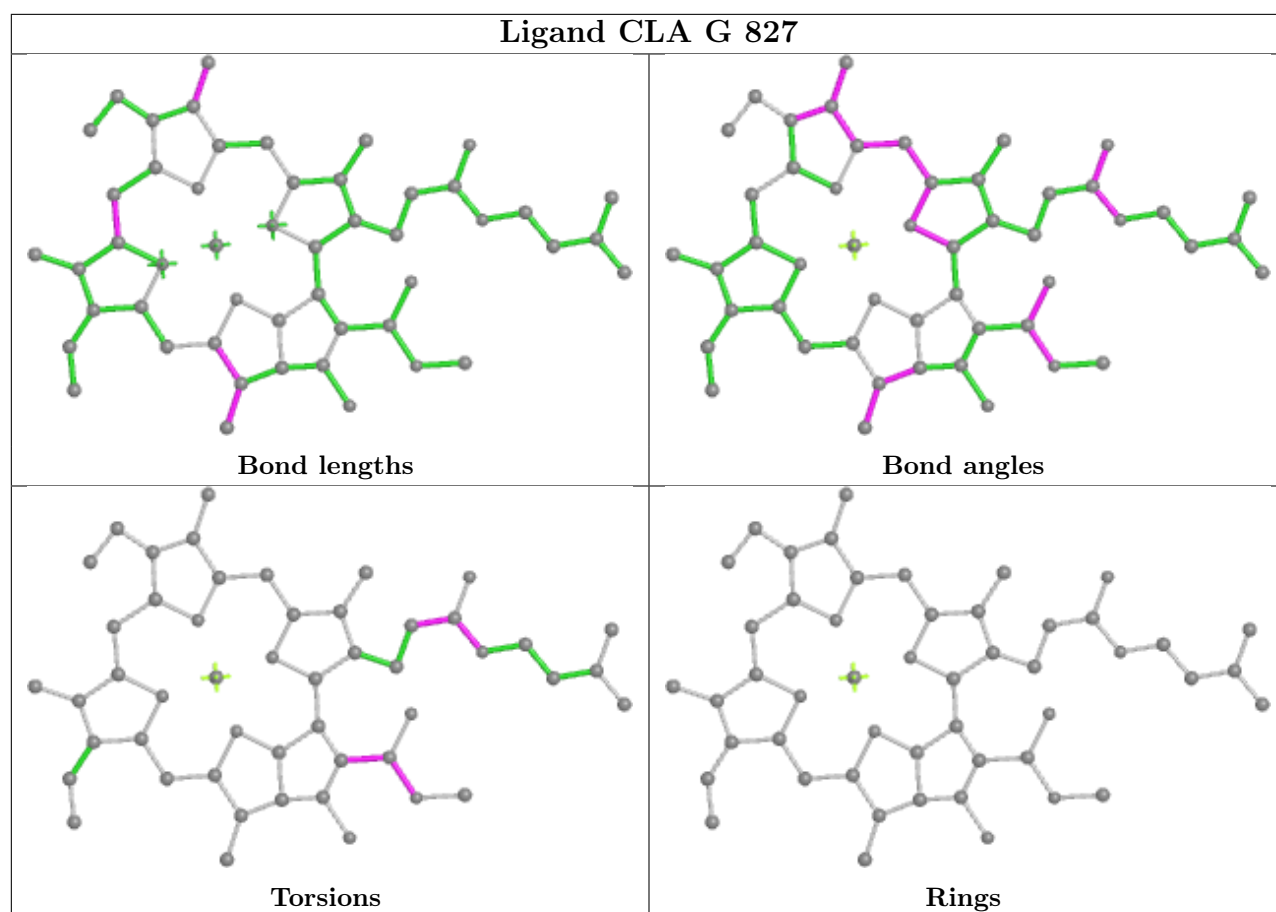
Bond angles

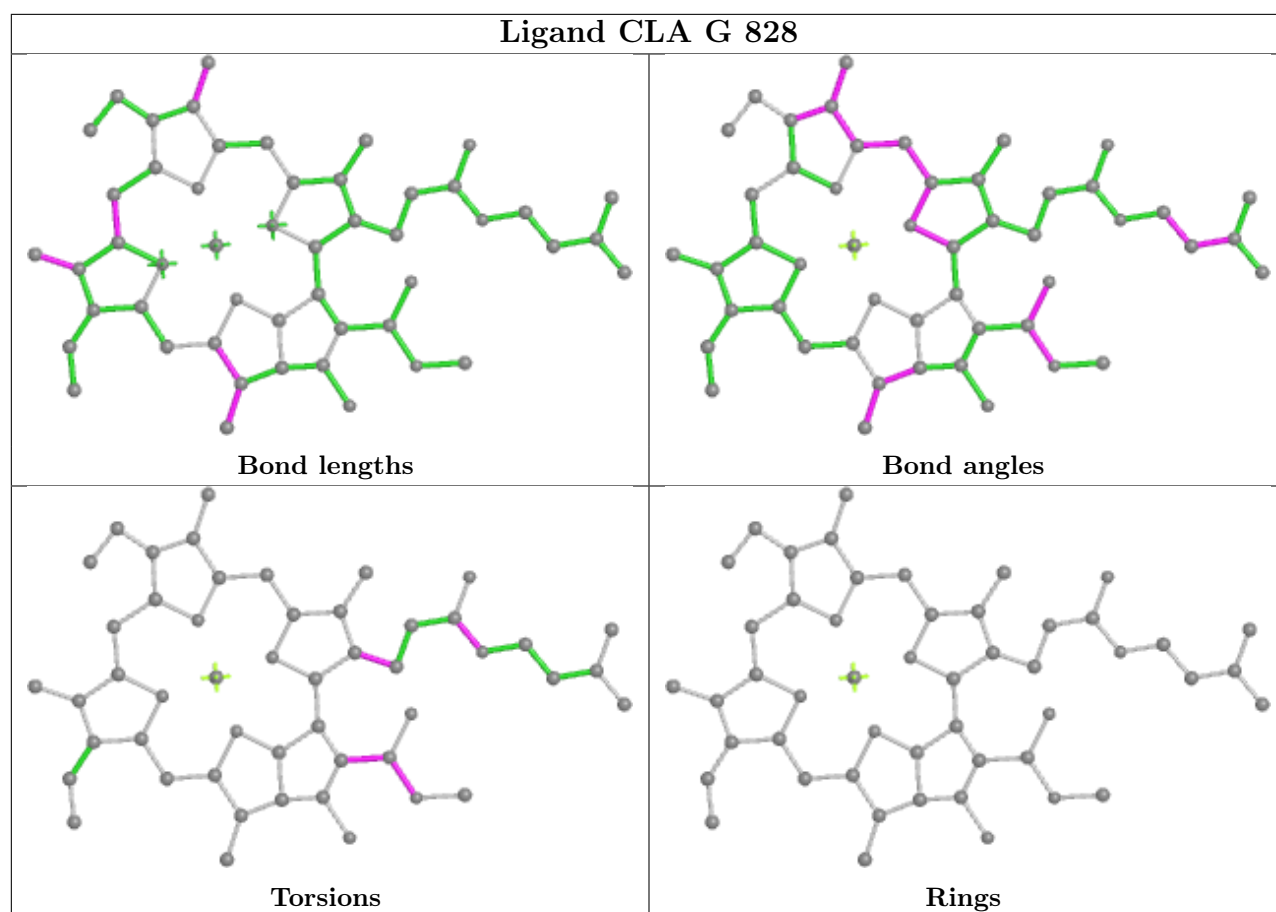


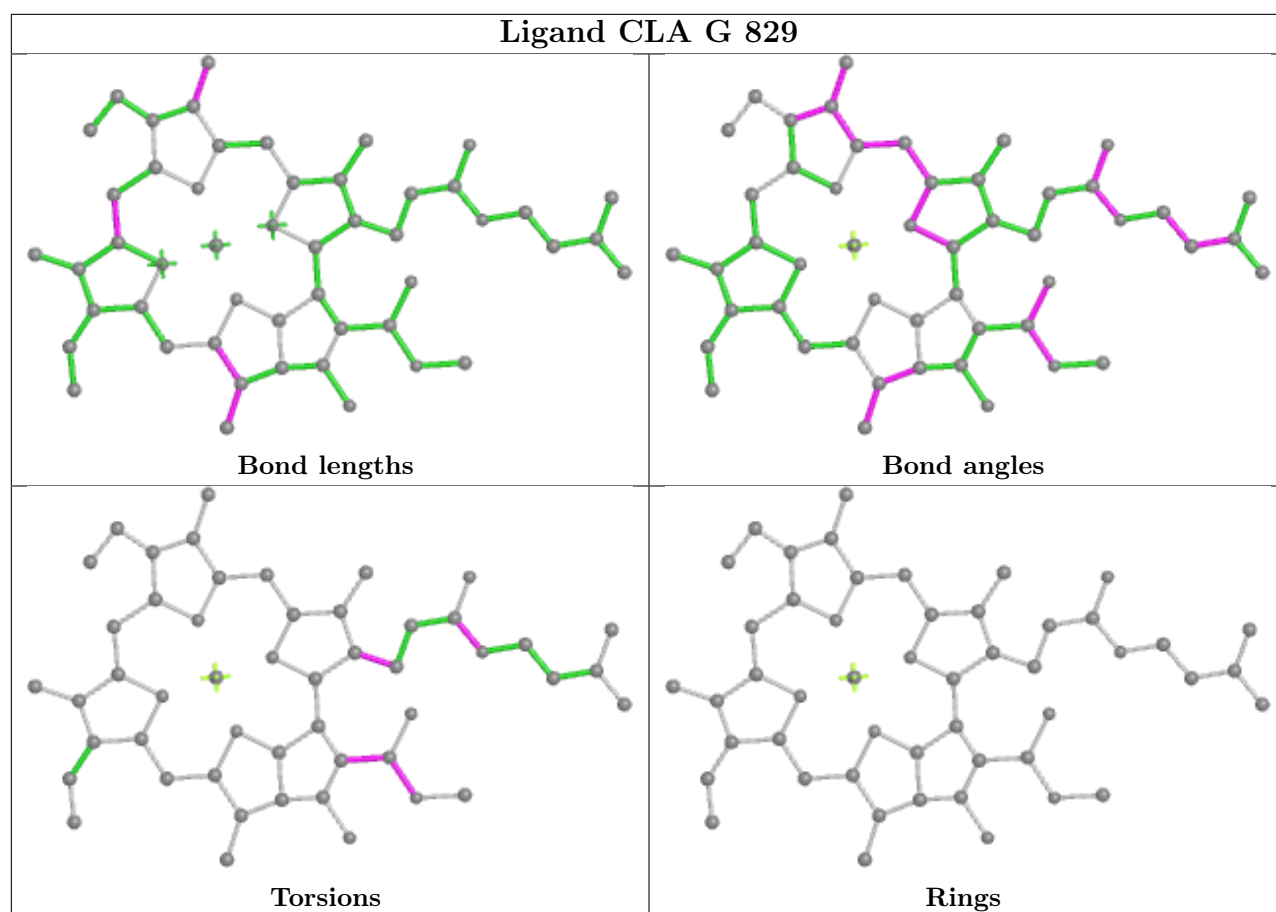
Torsions

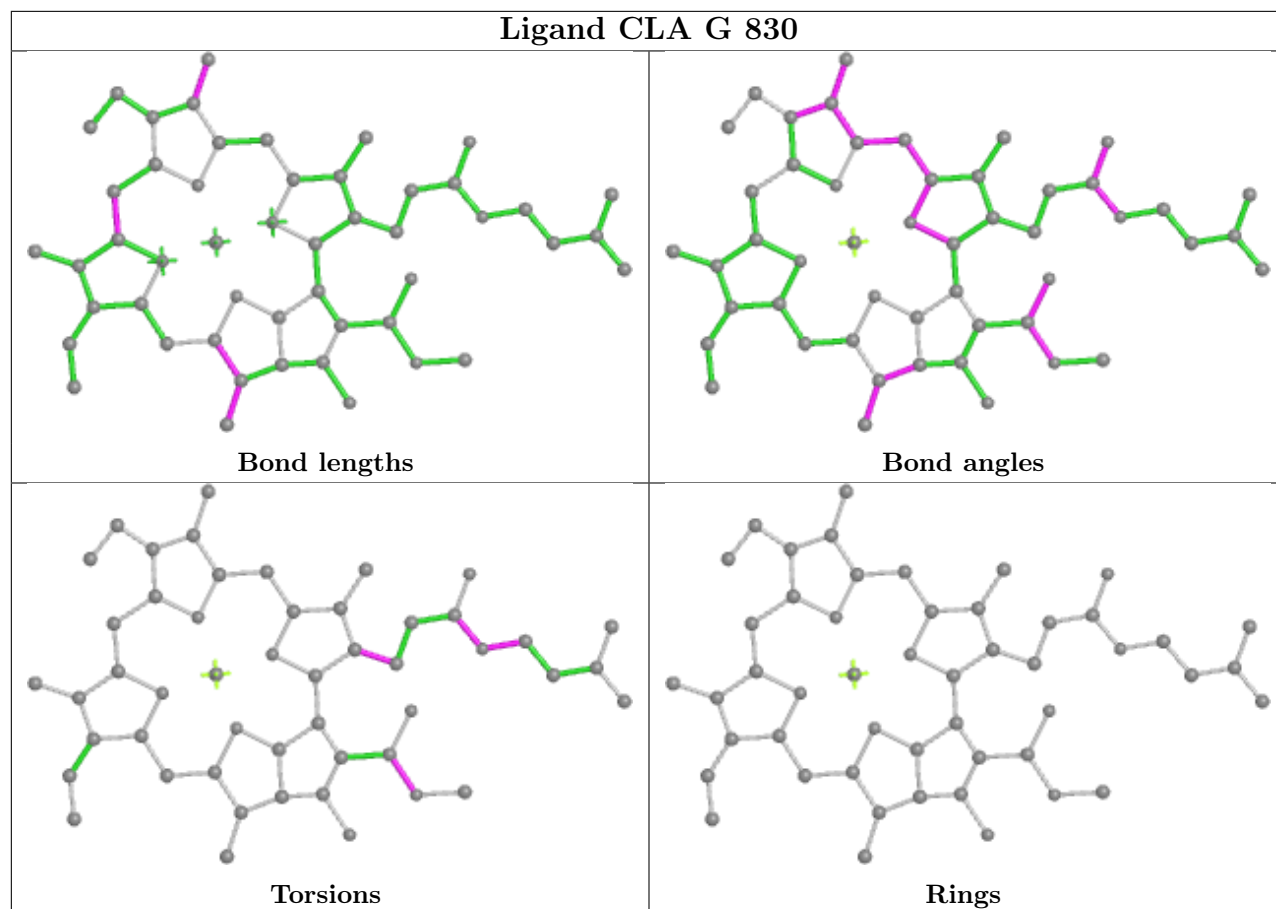


Rings

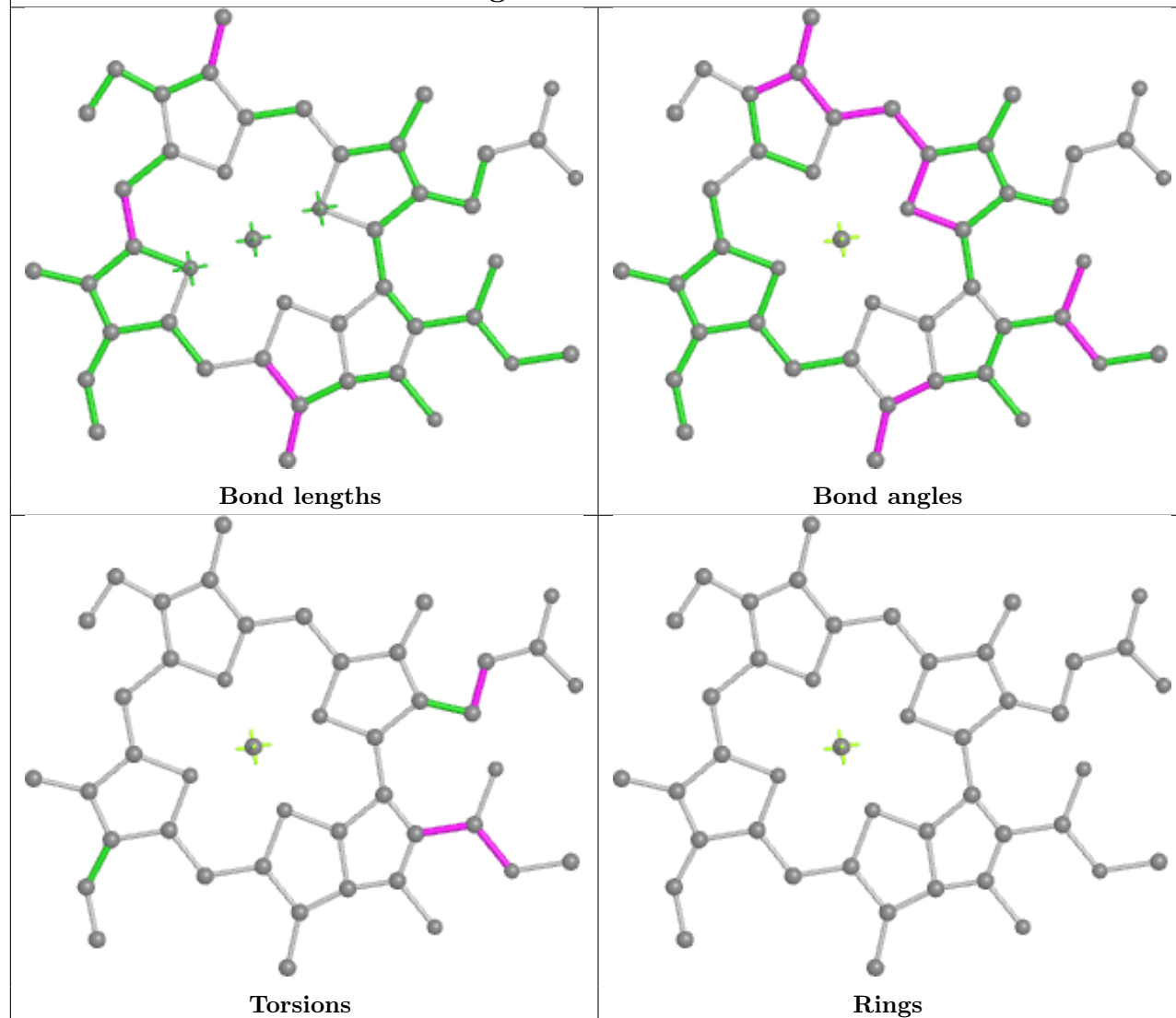


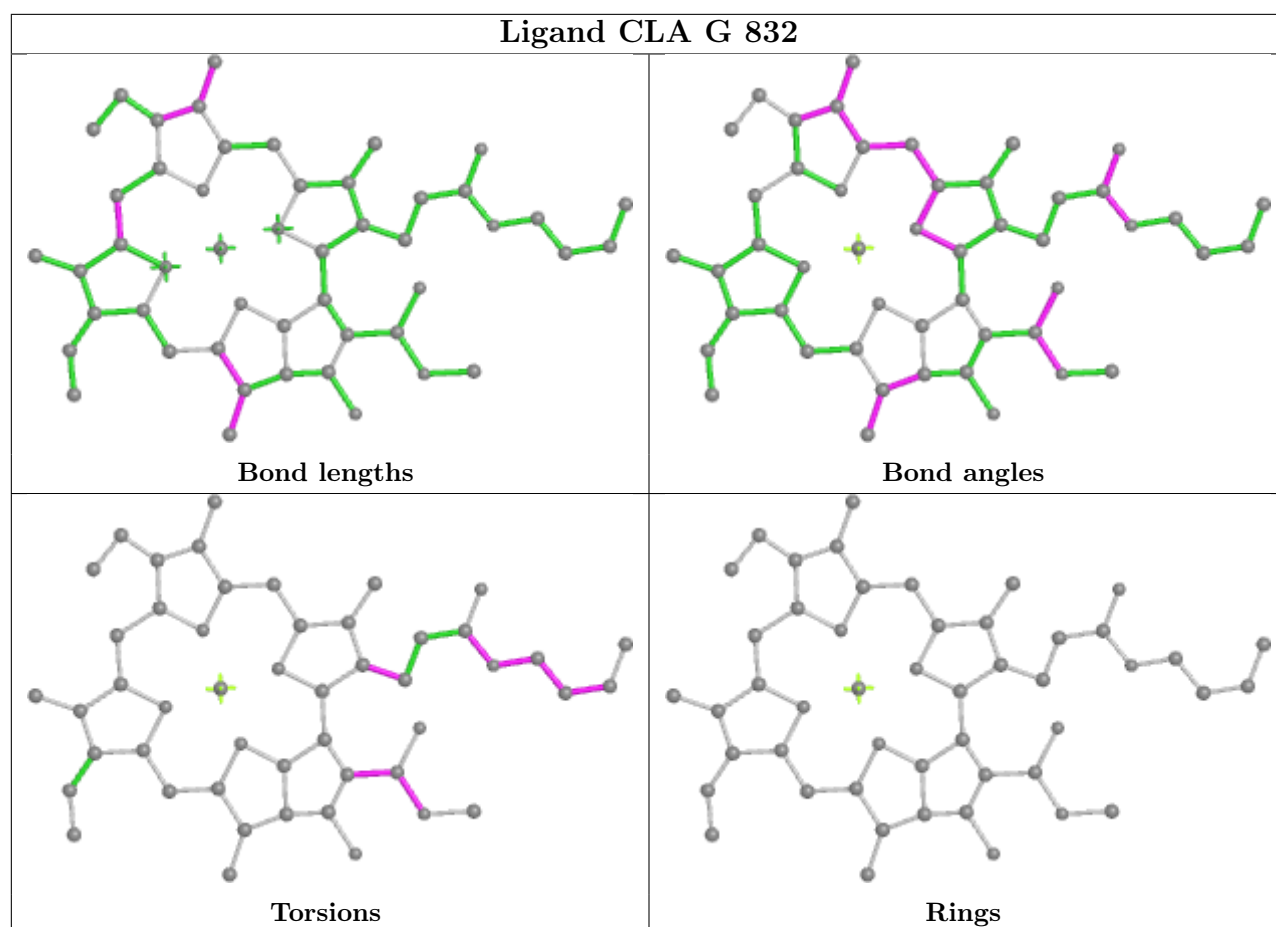


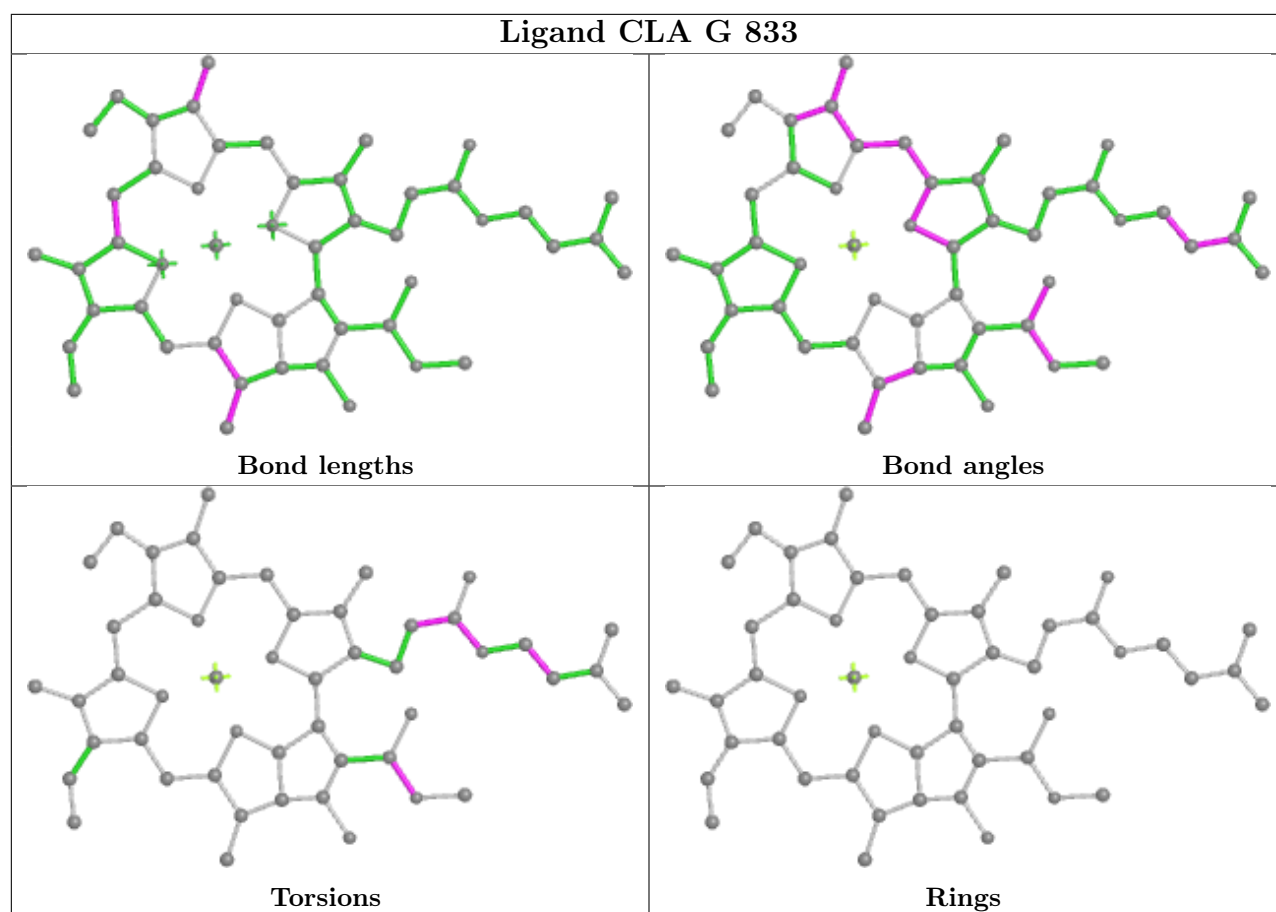


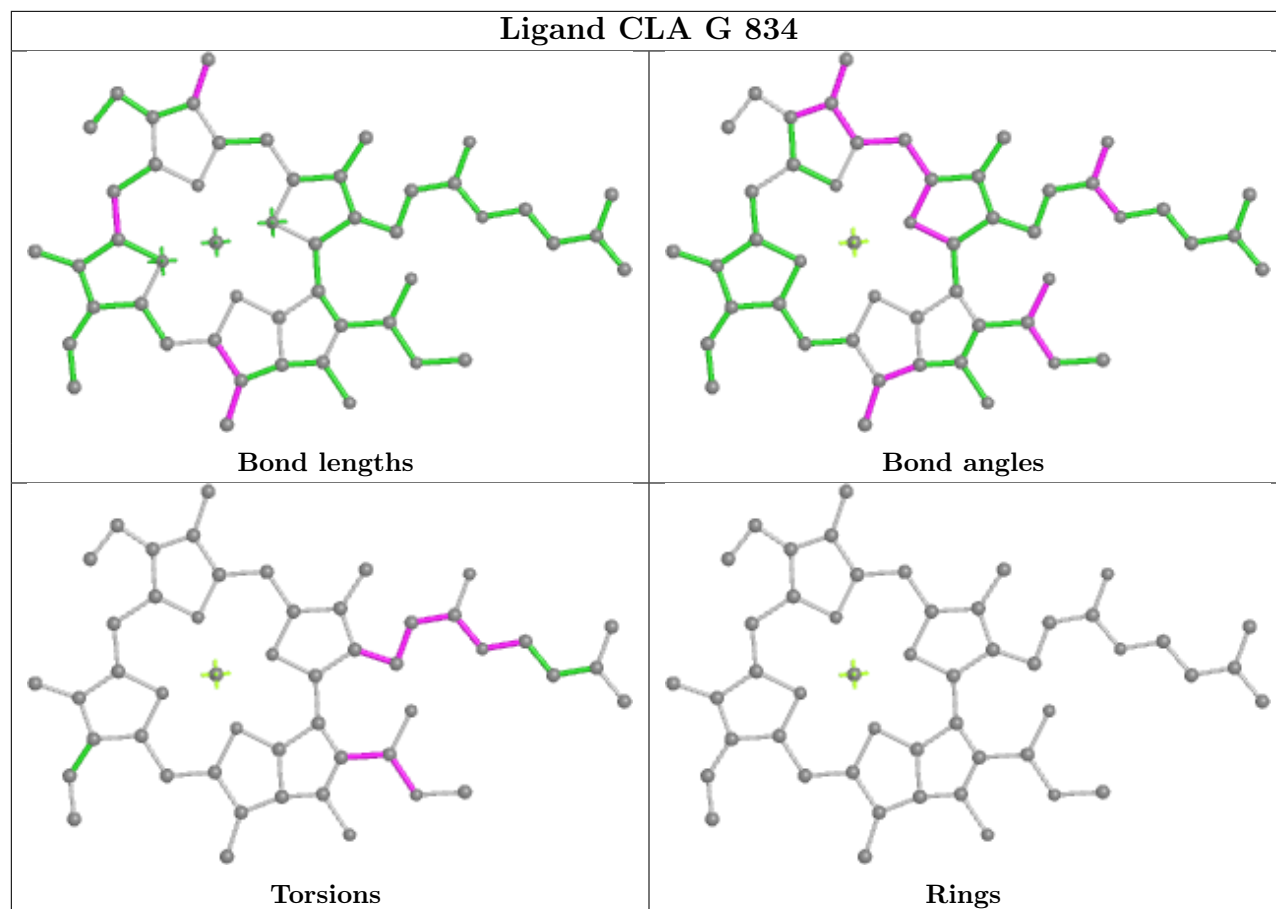


Ligand CLA G 831

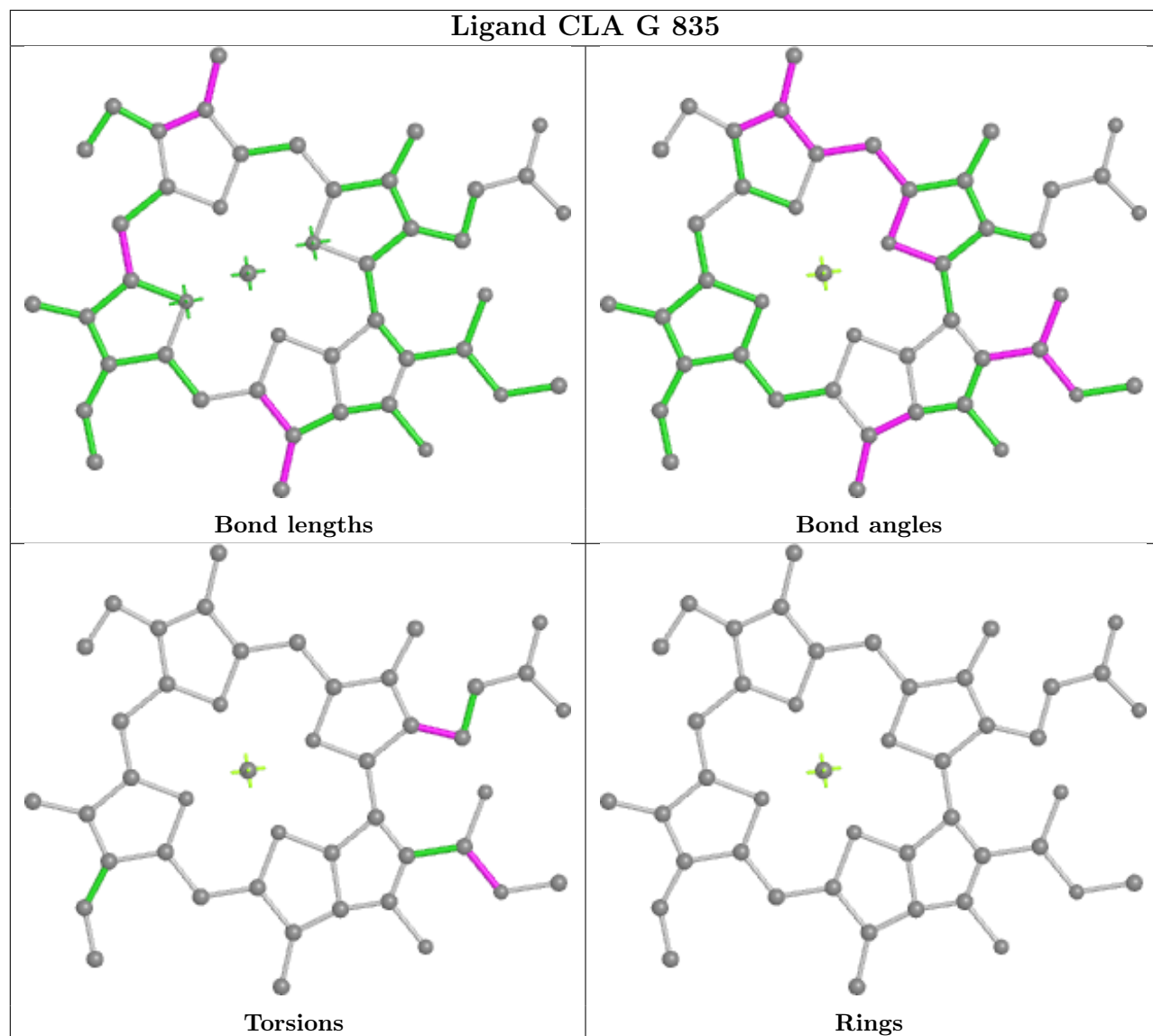




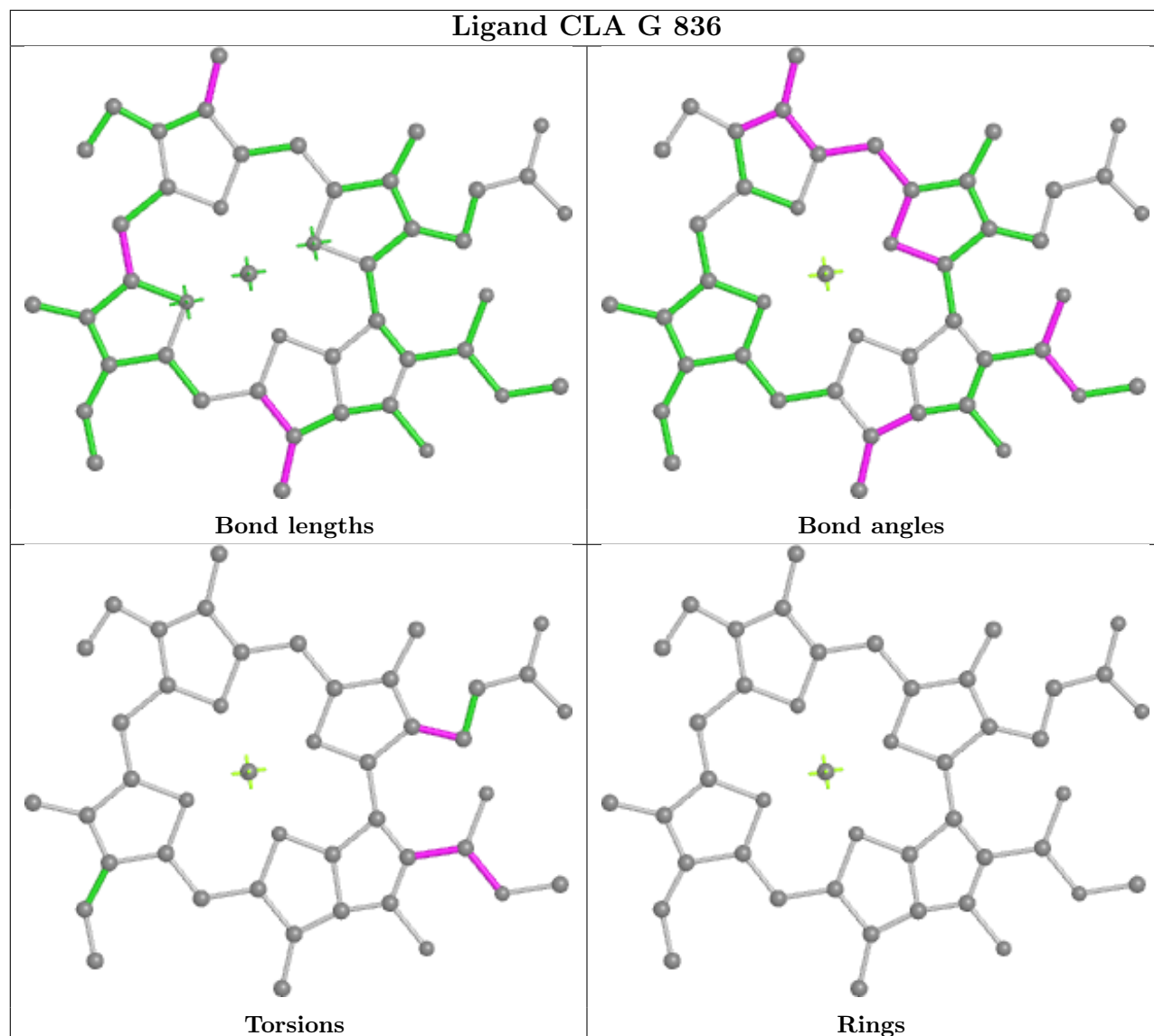


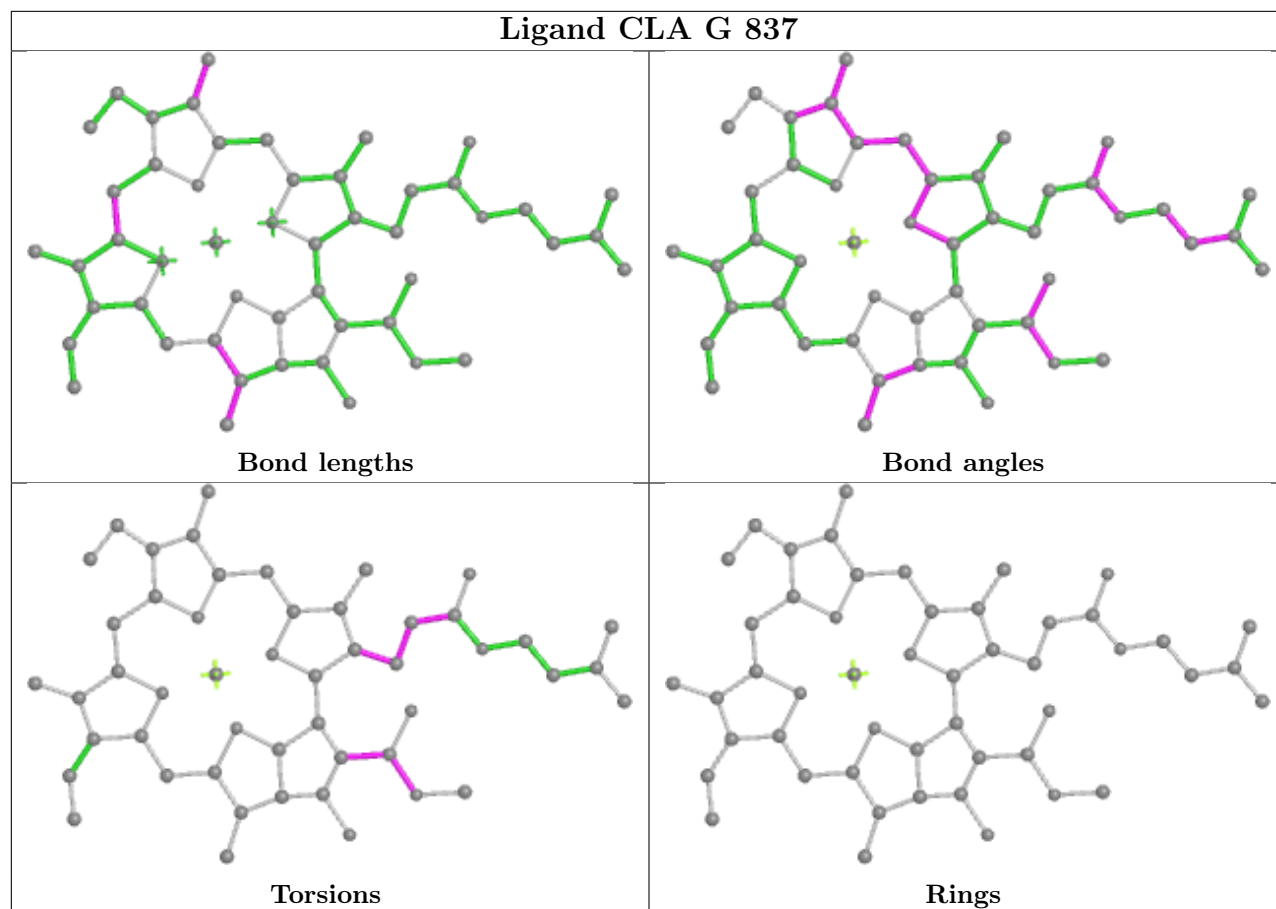


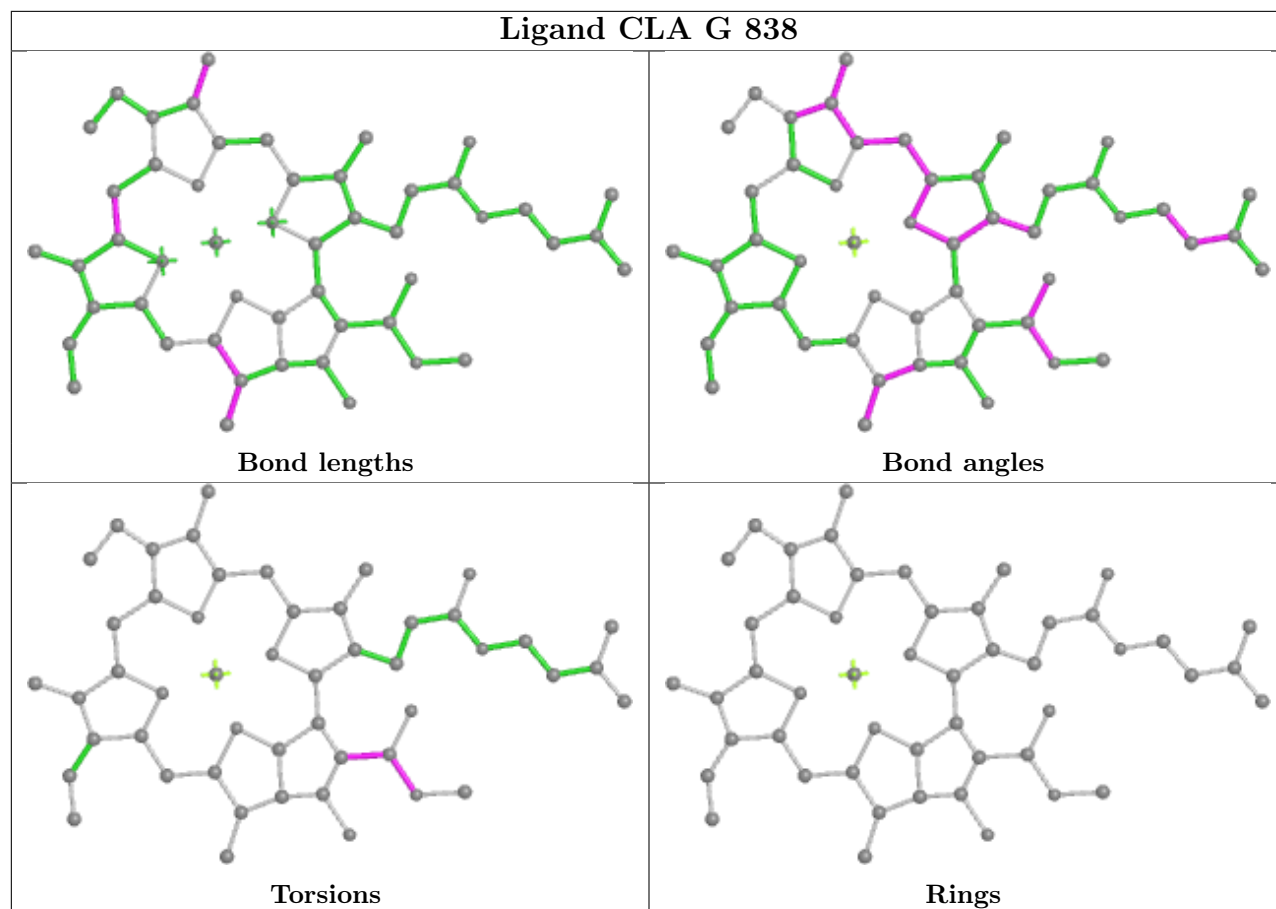
Ligand CLA G 835



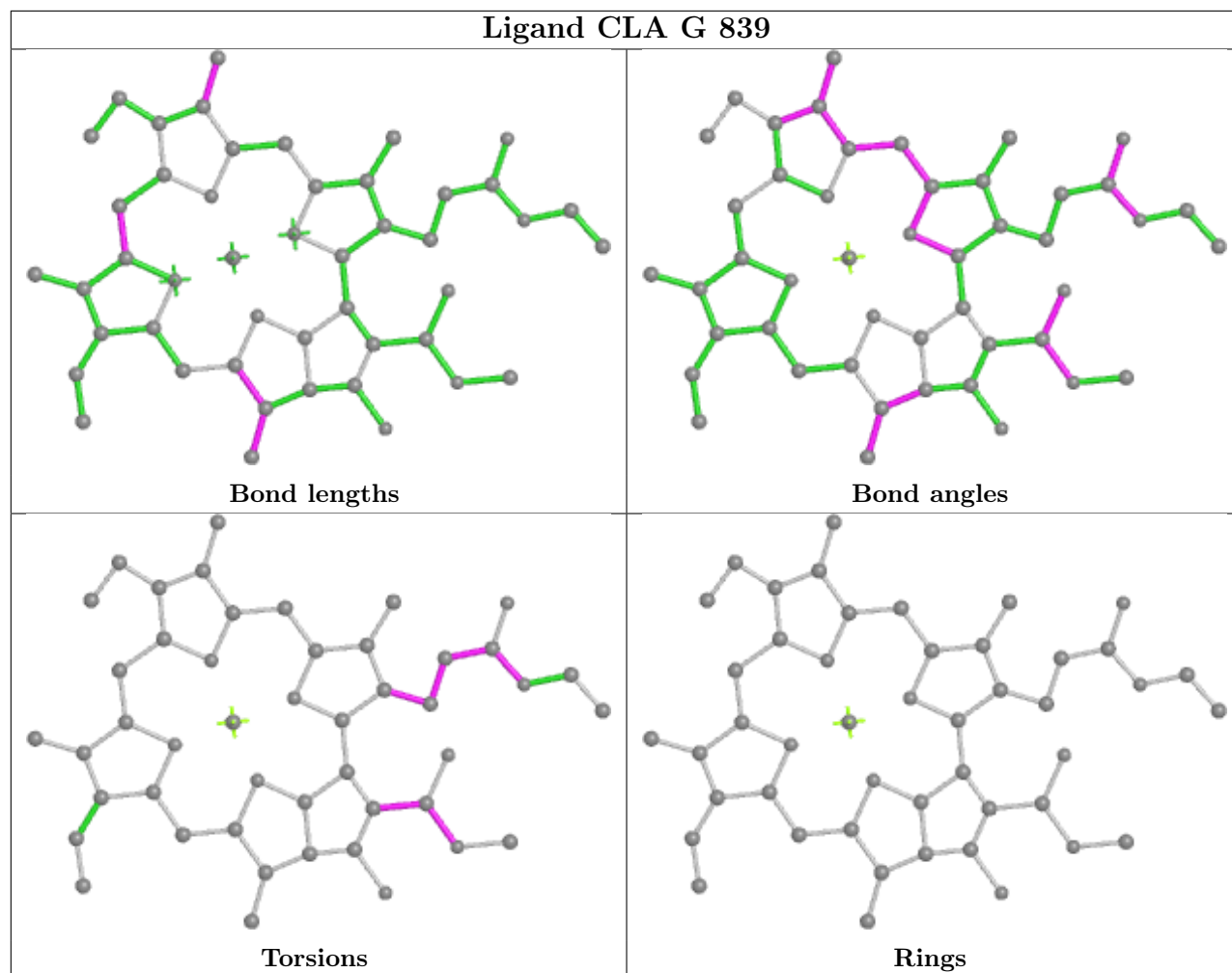
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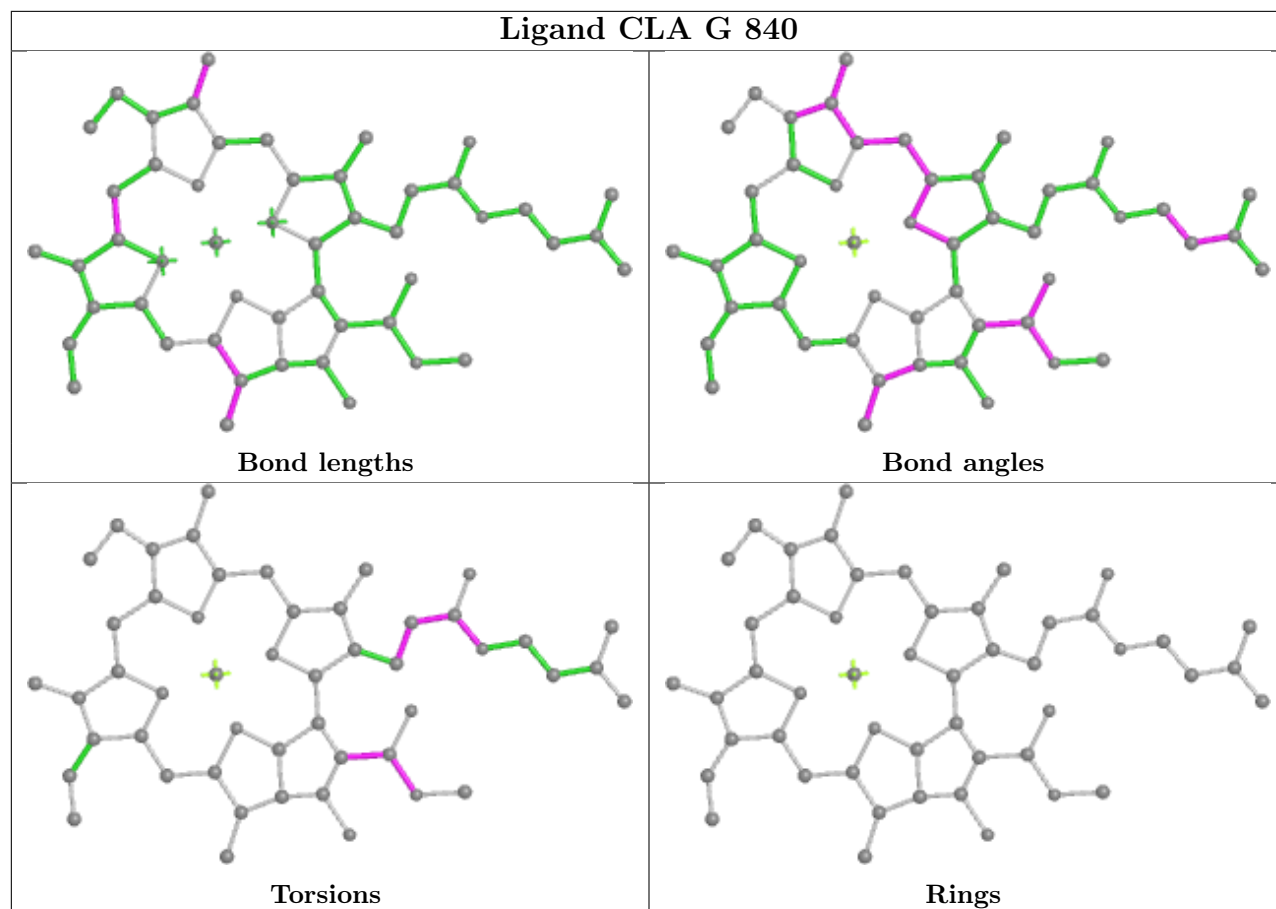


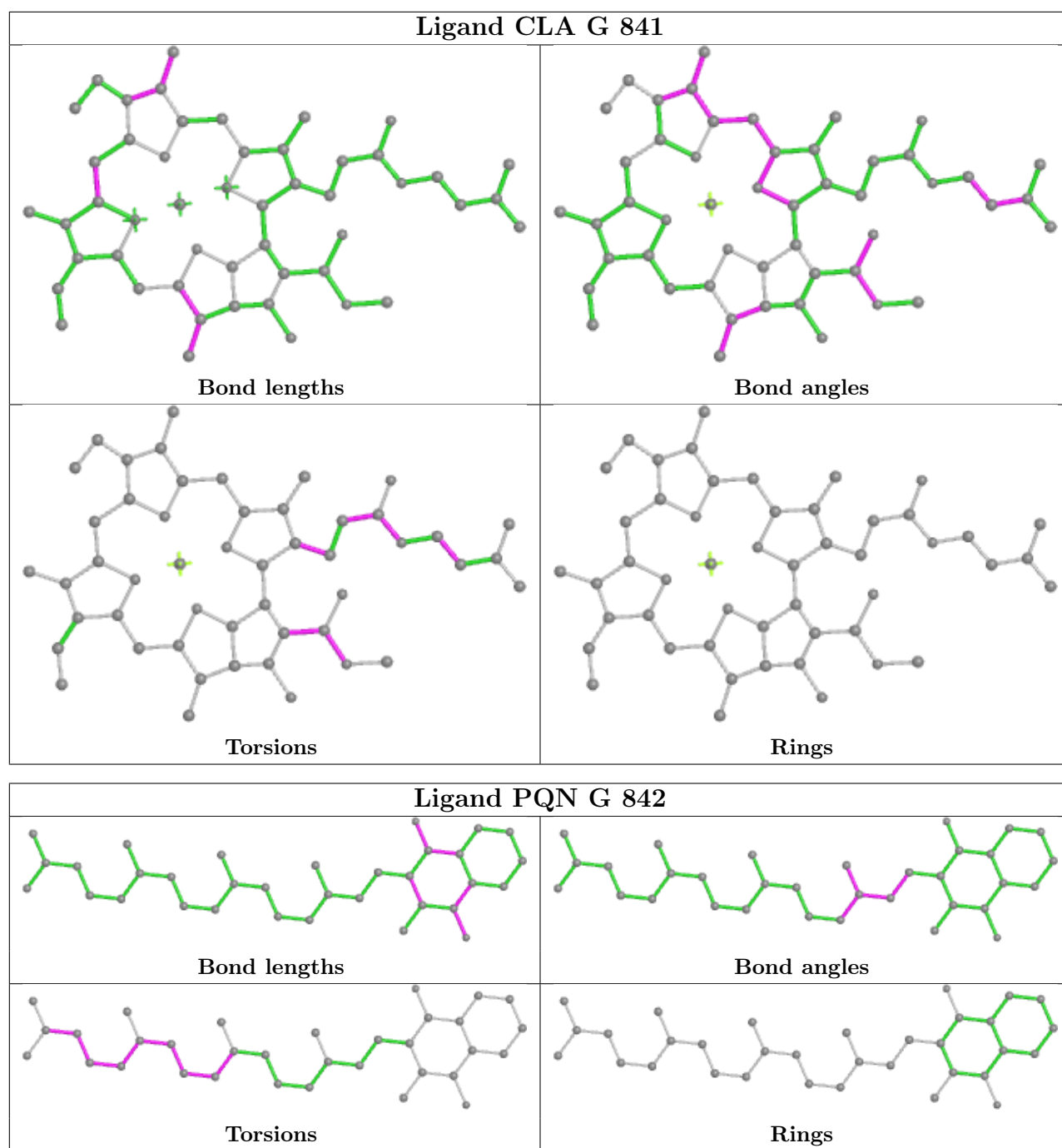


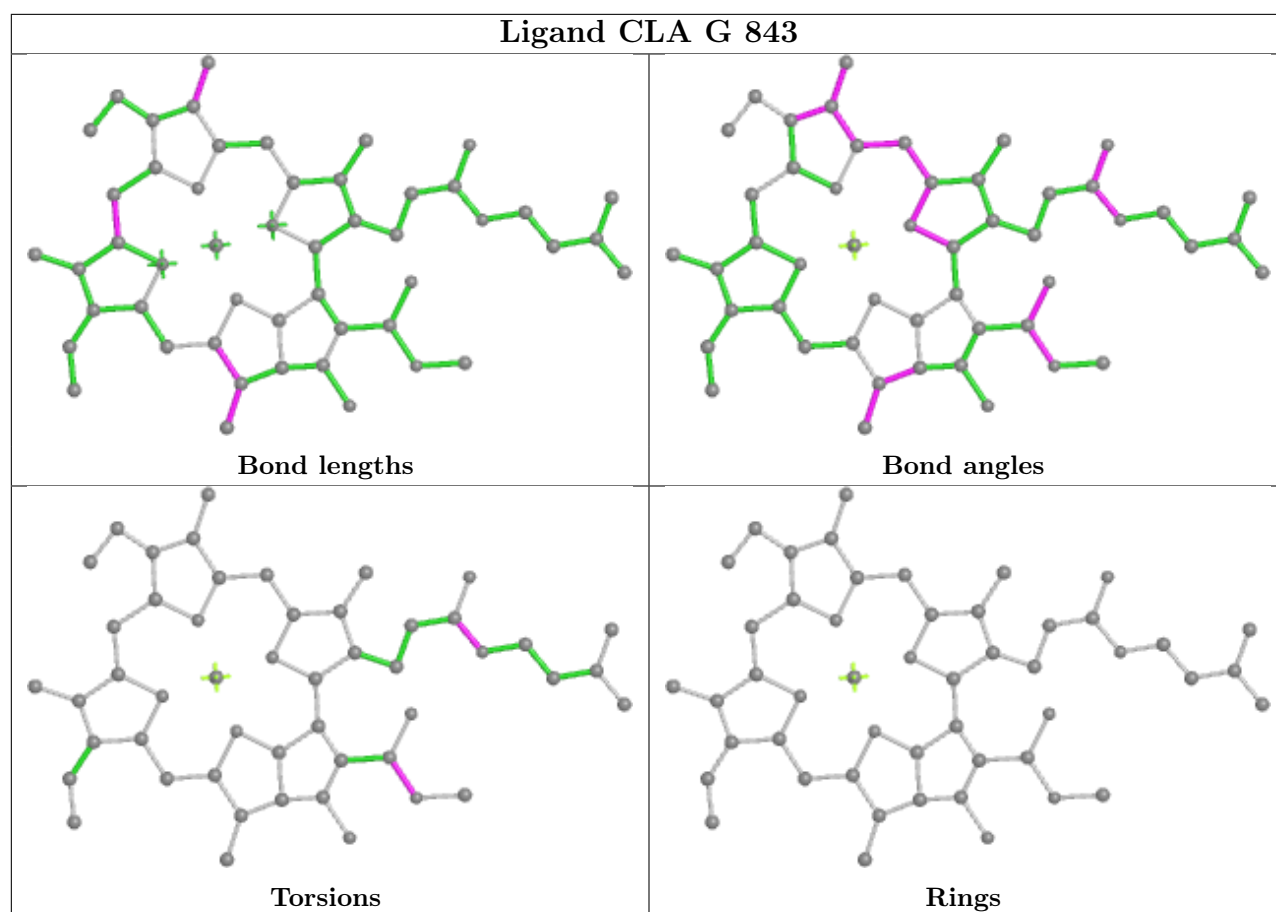


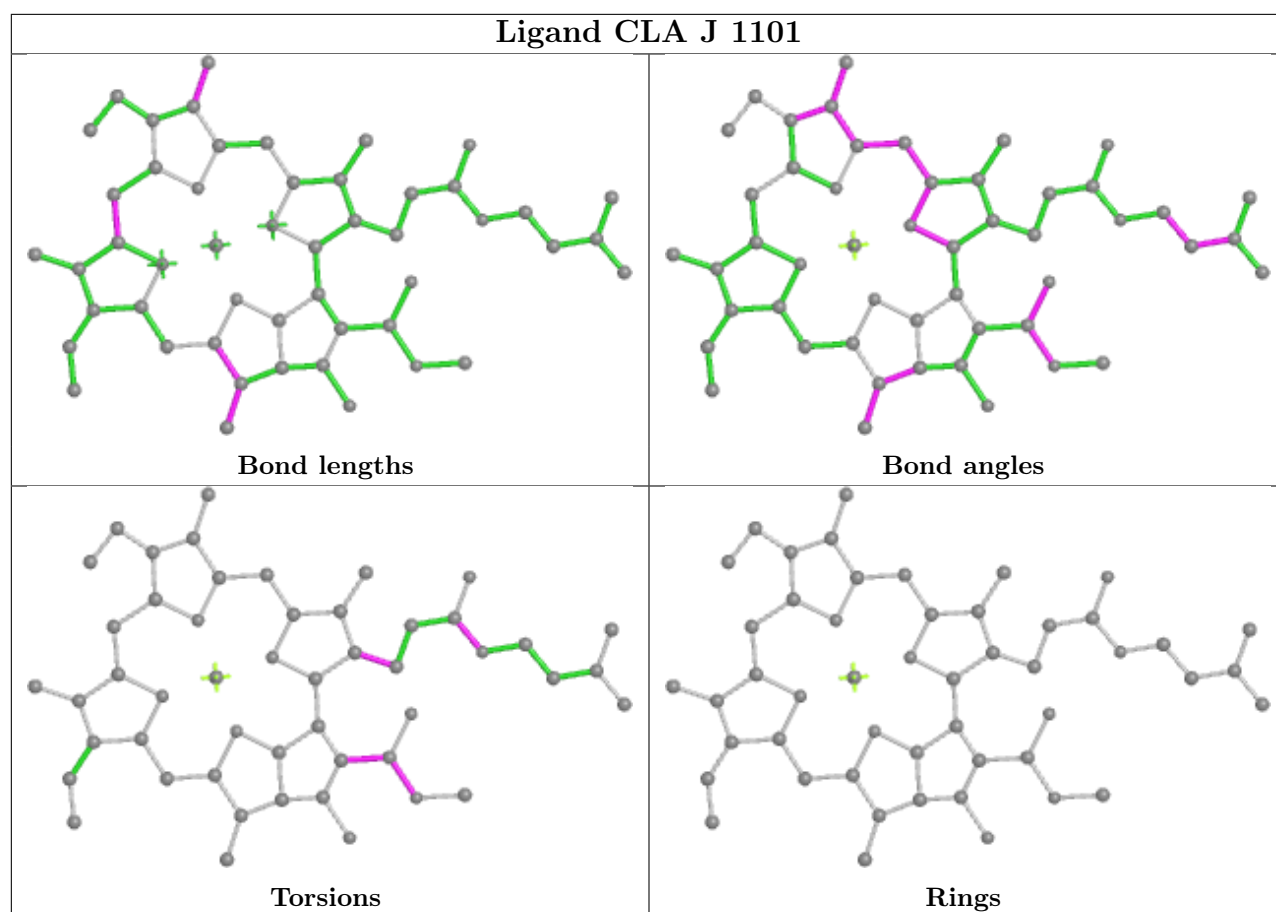
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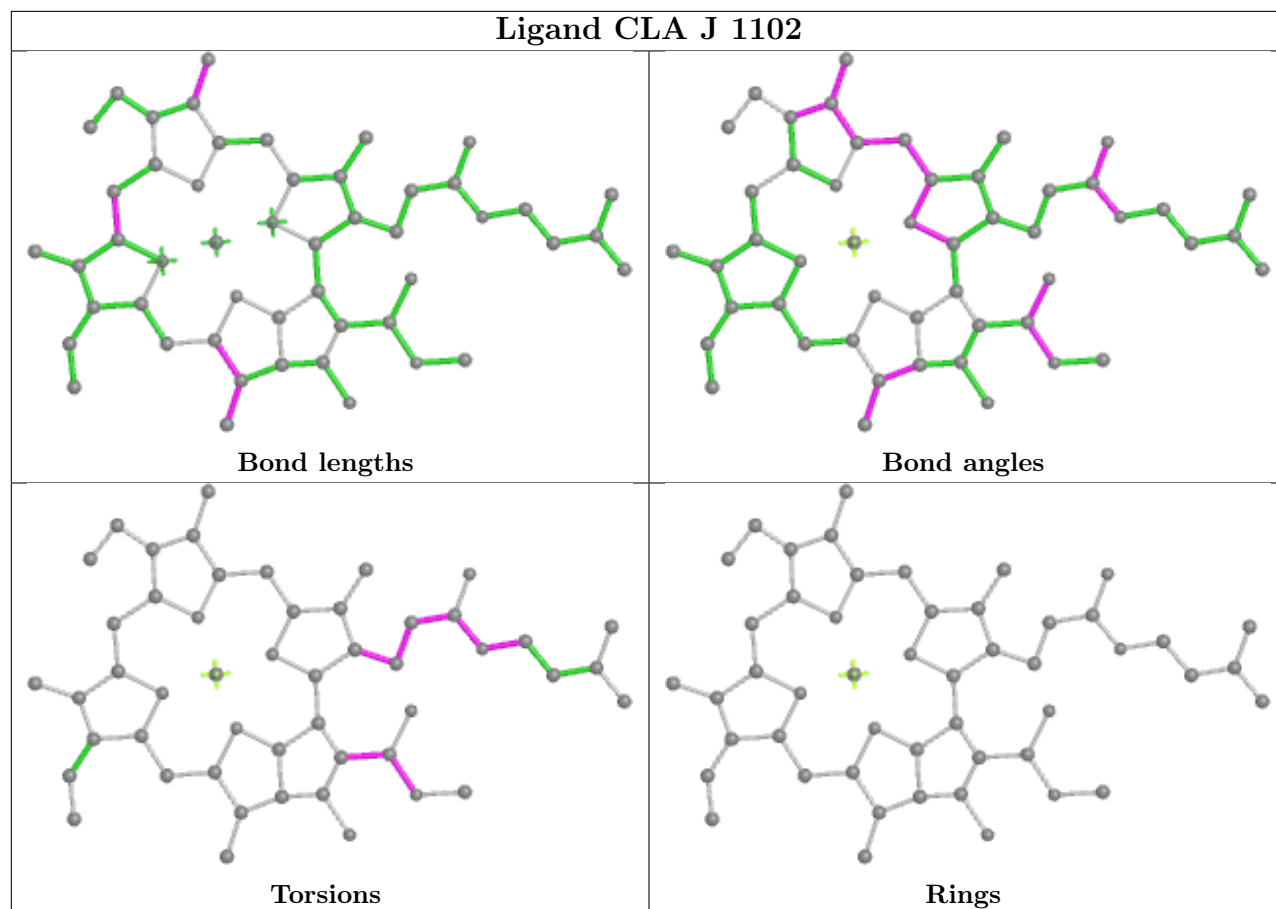




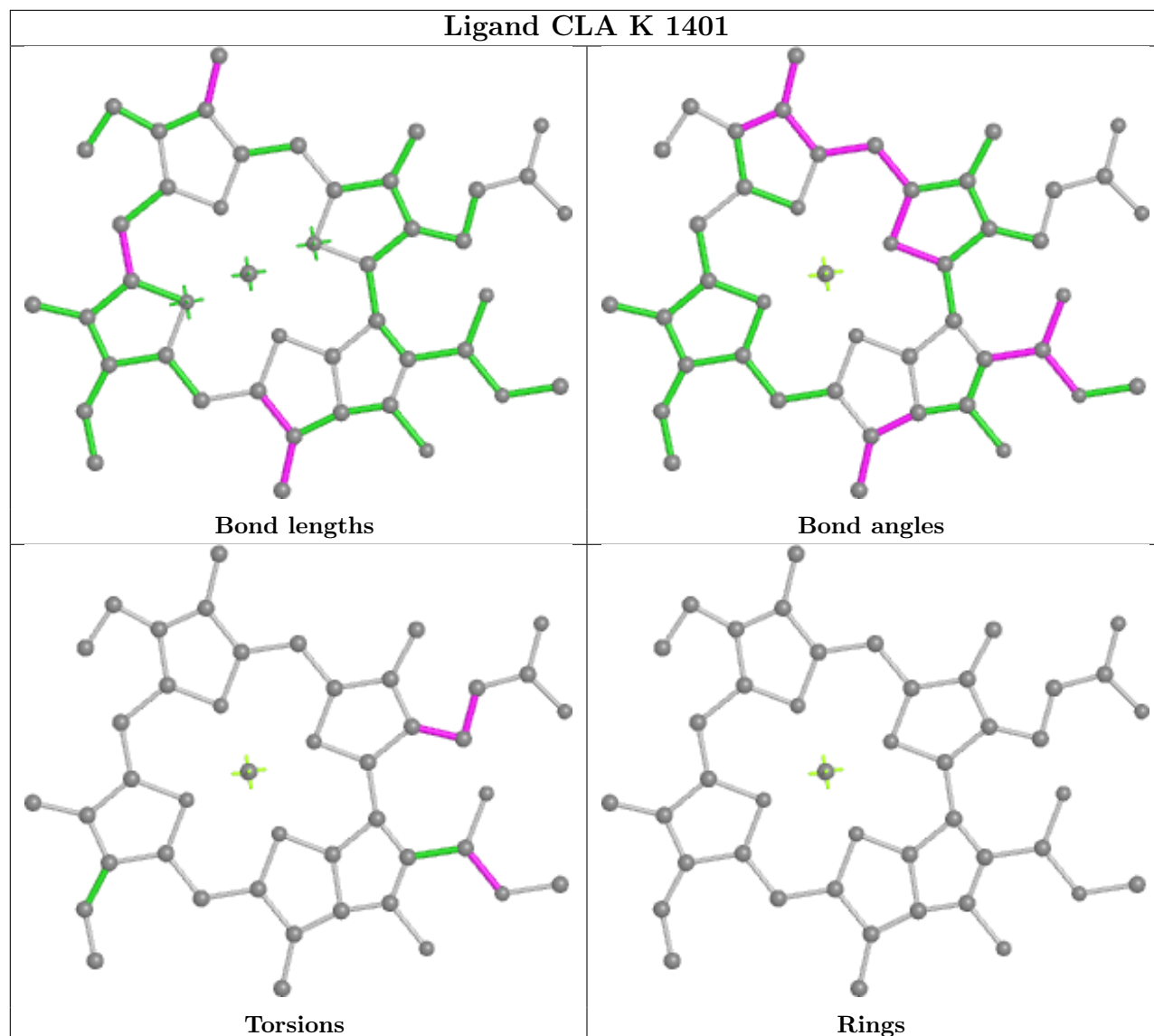


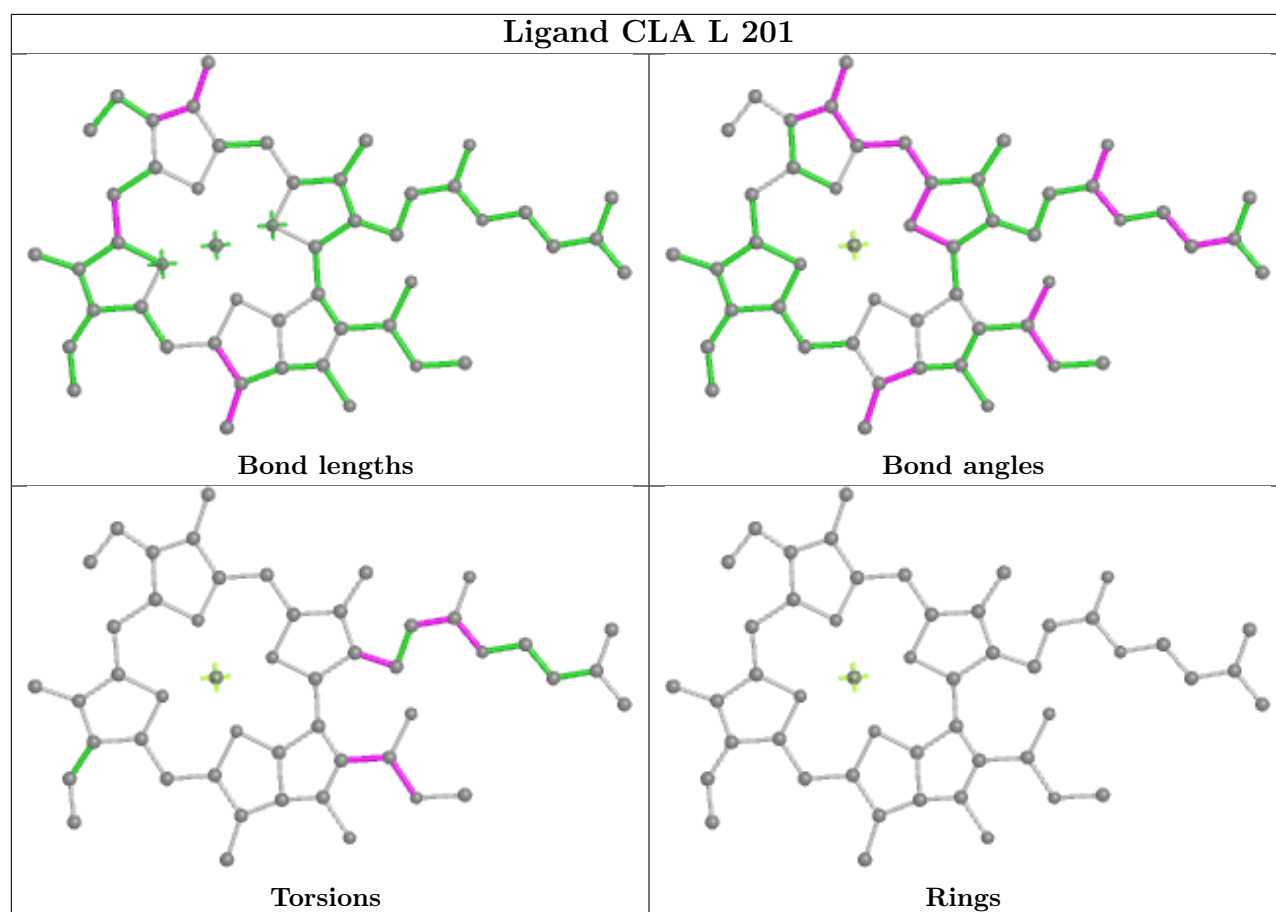


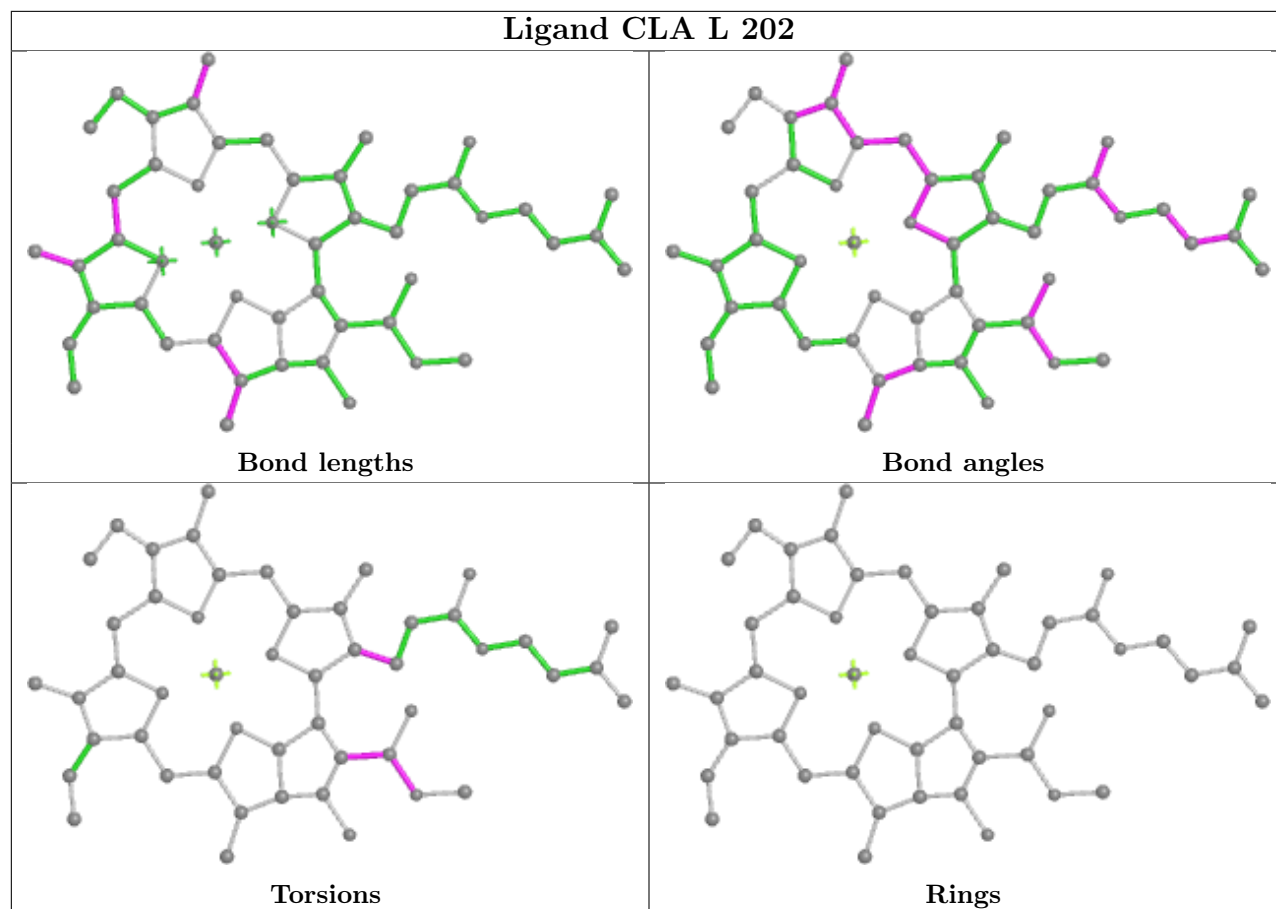


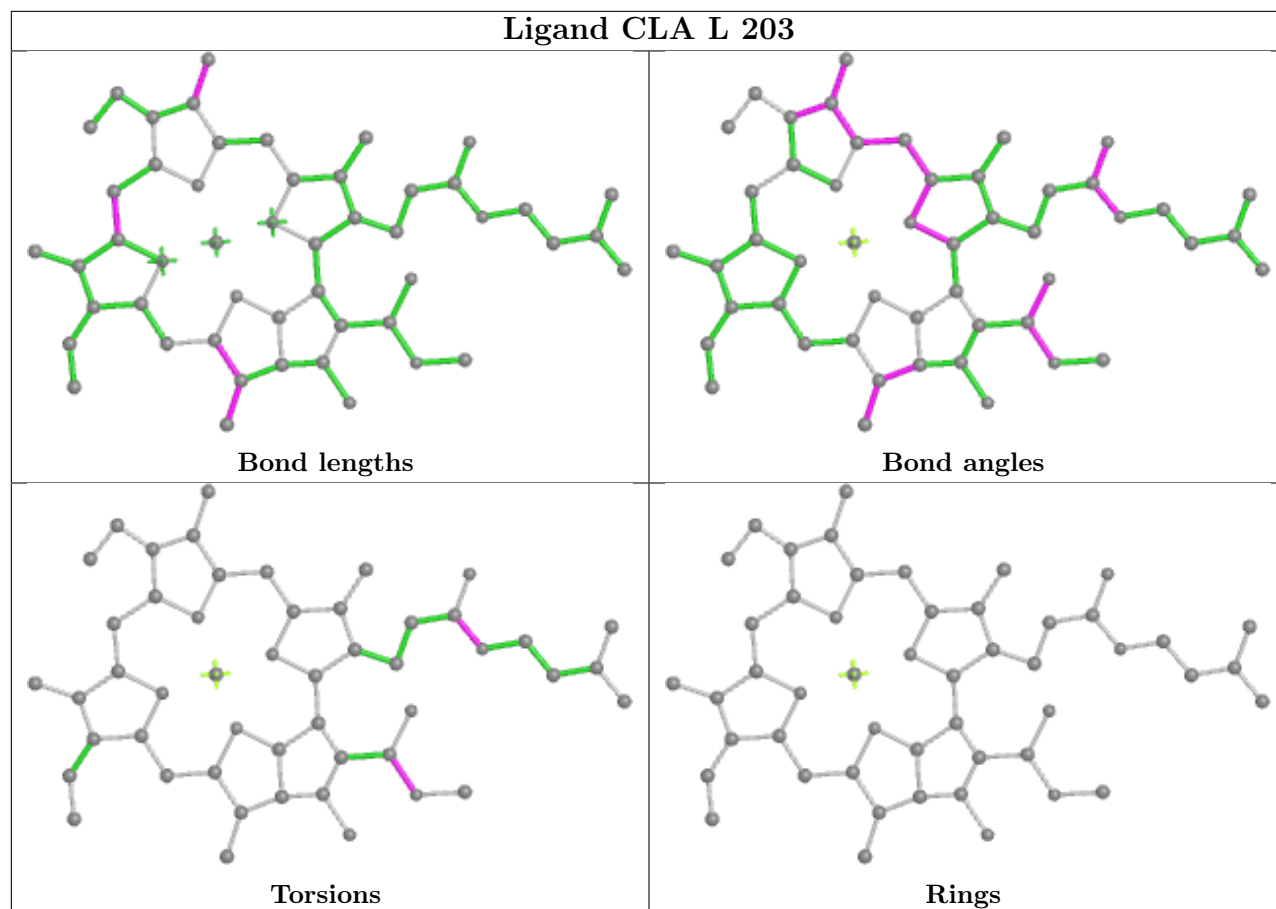


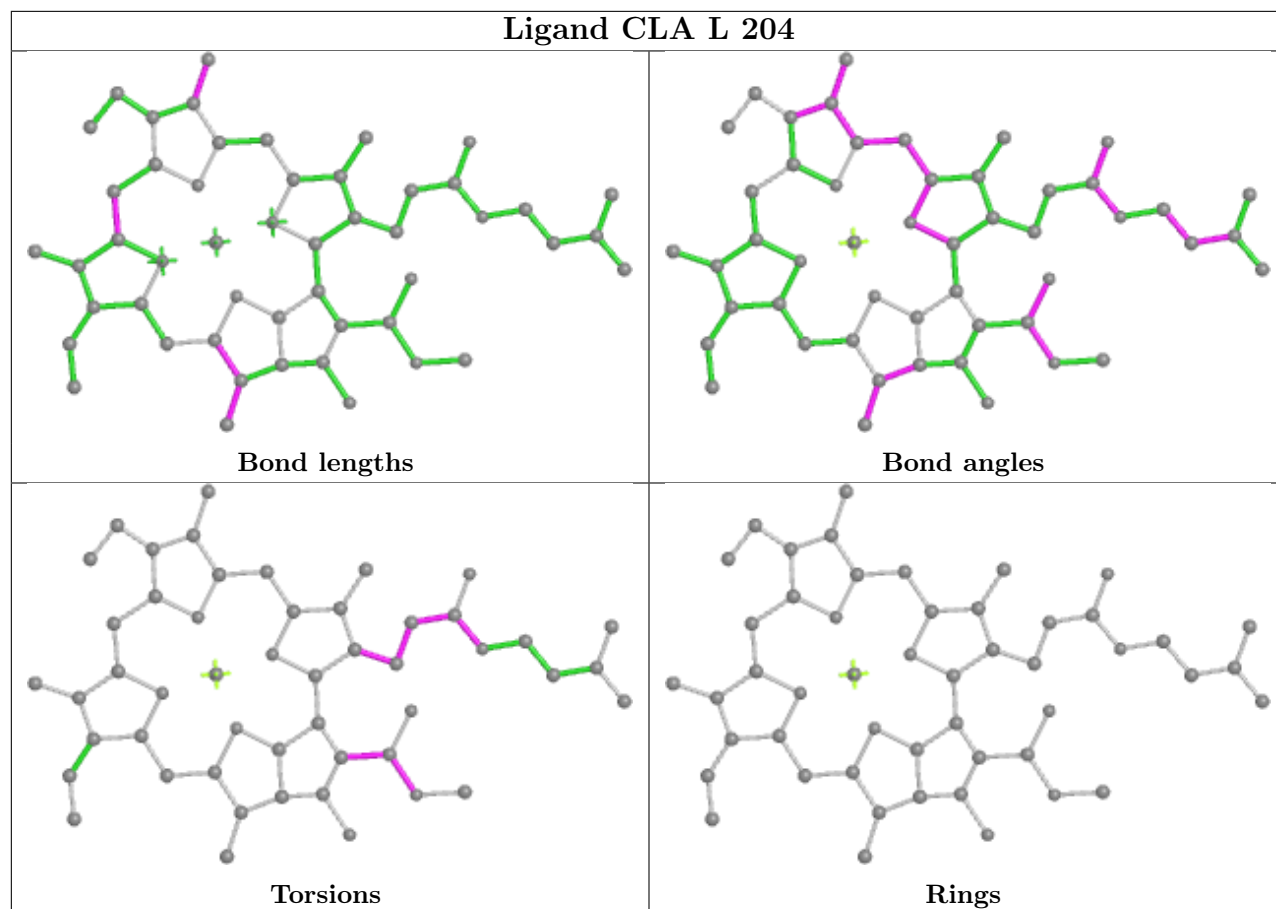
Ligand CLA K 1401



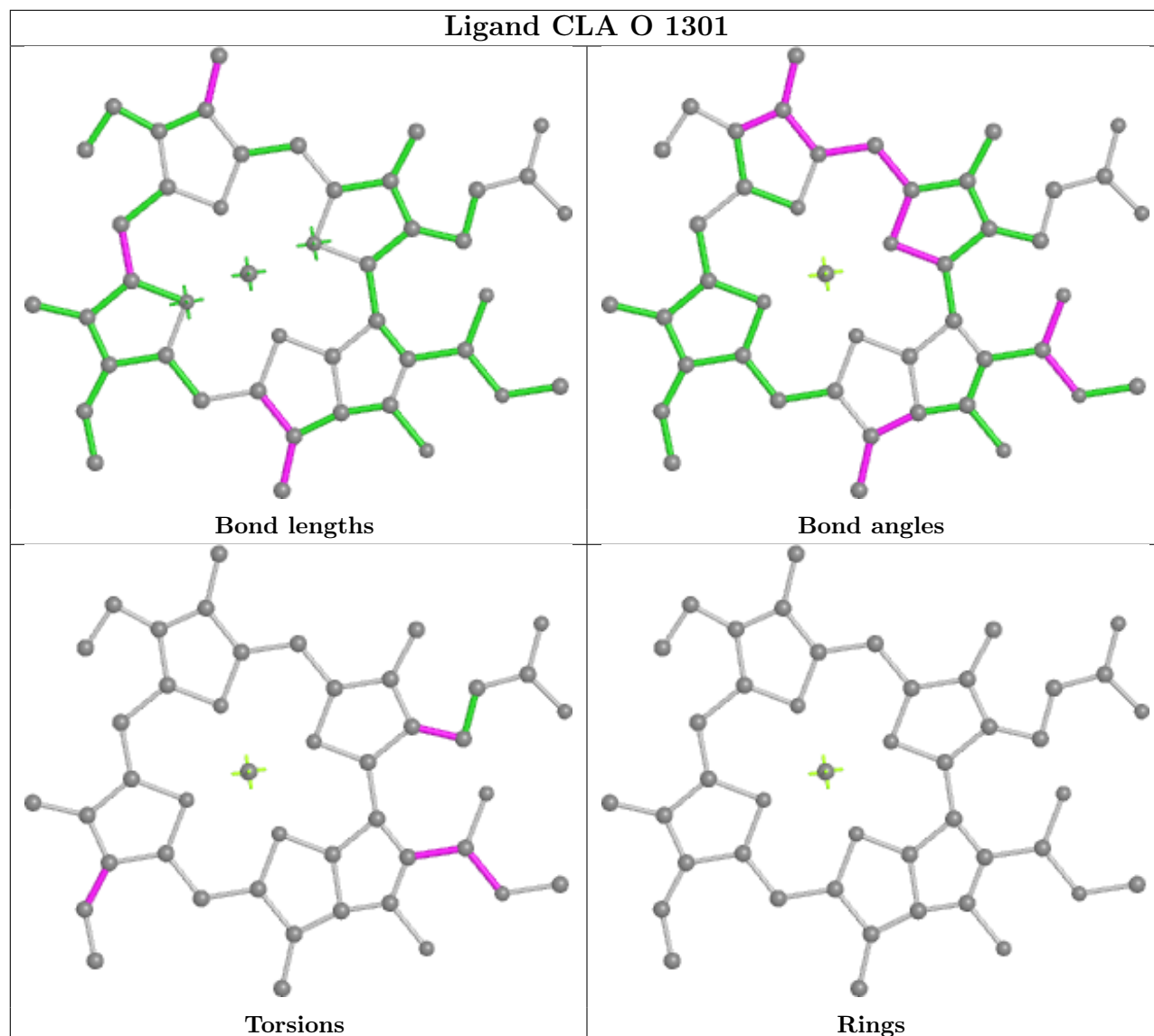




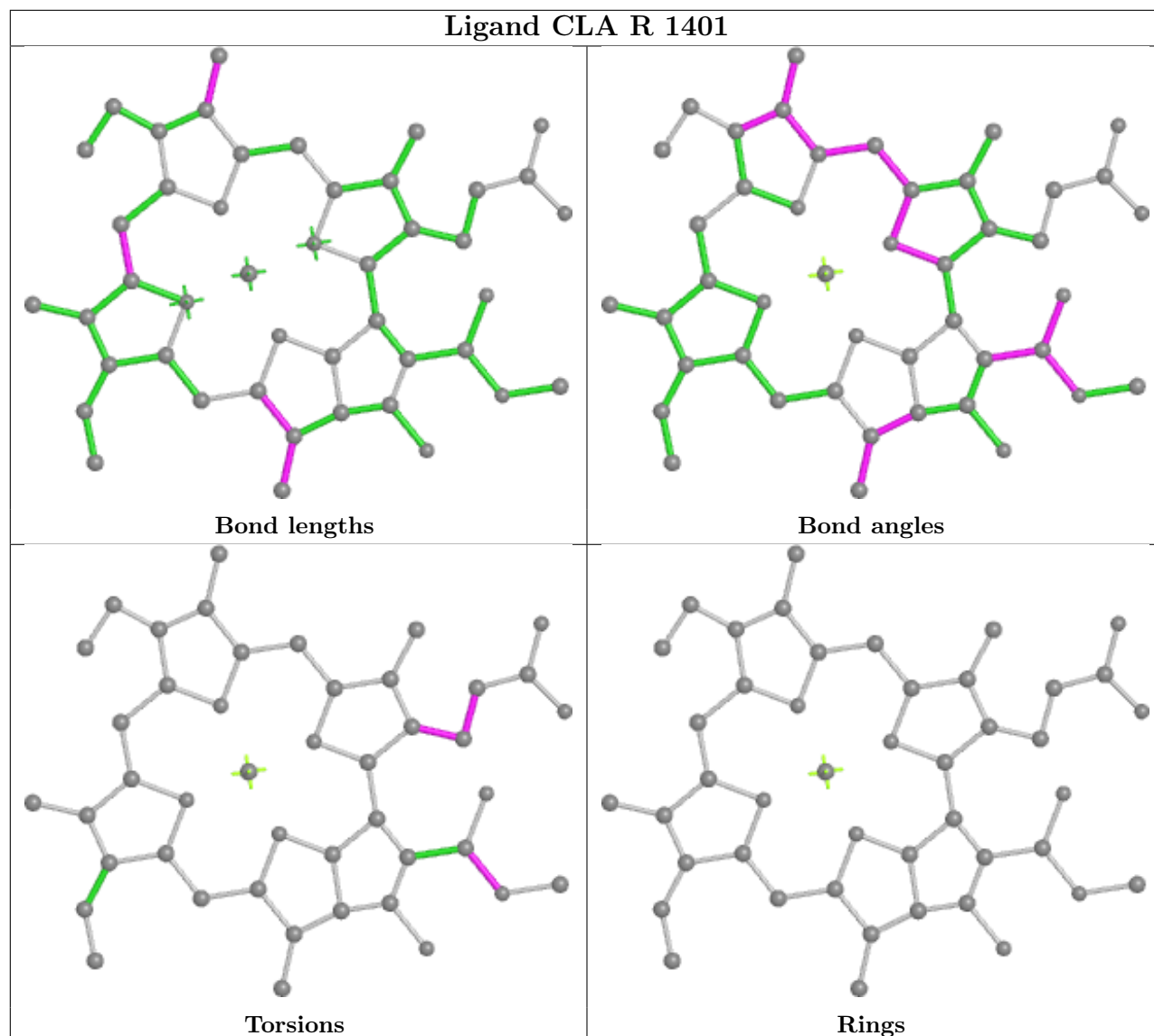


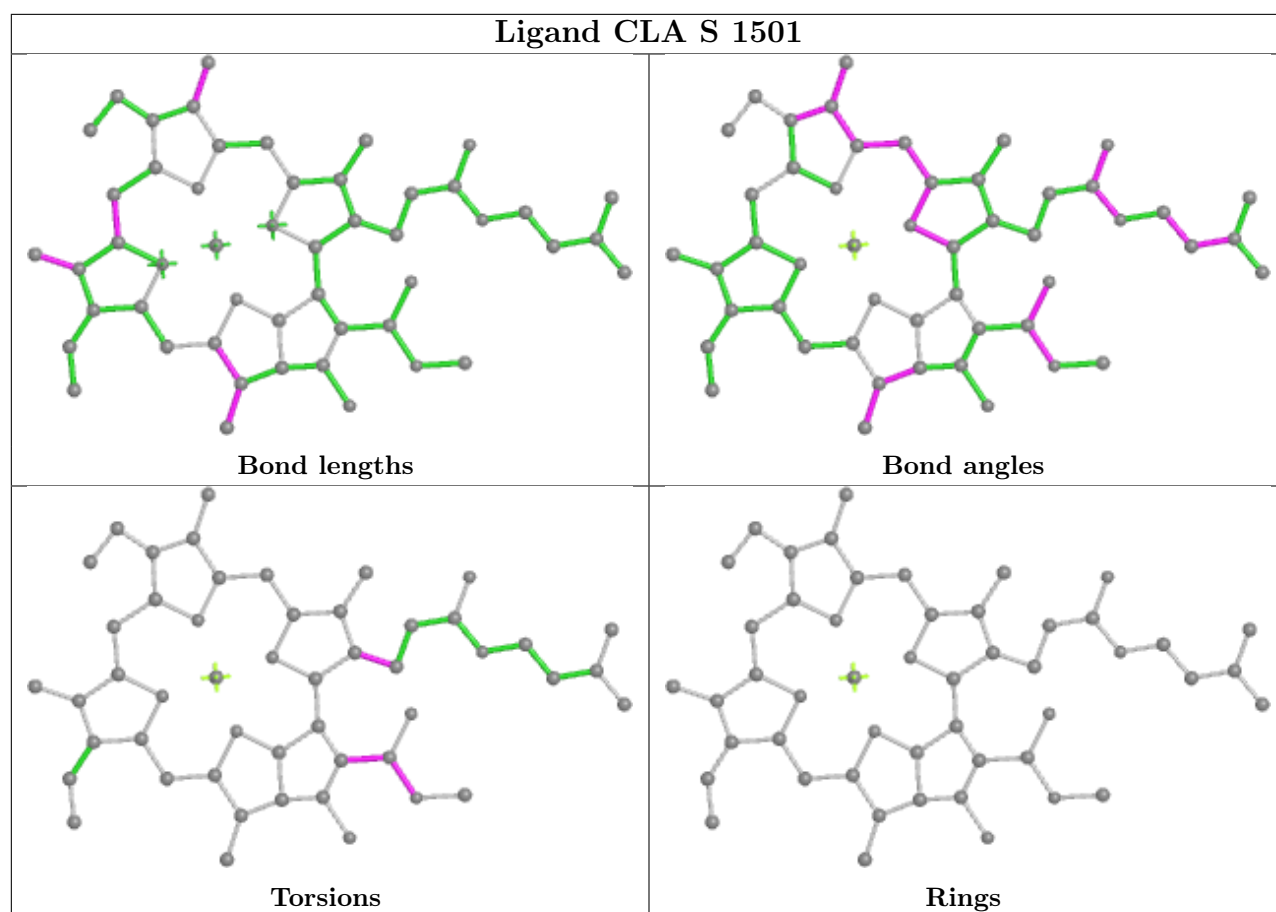


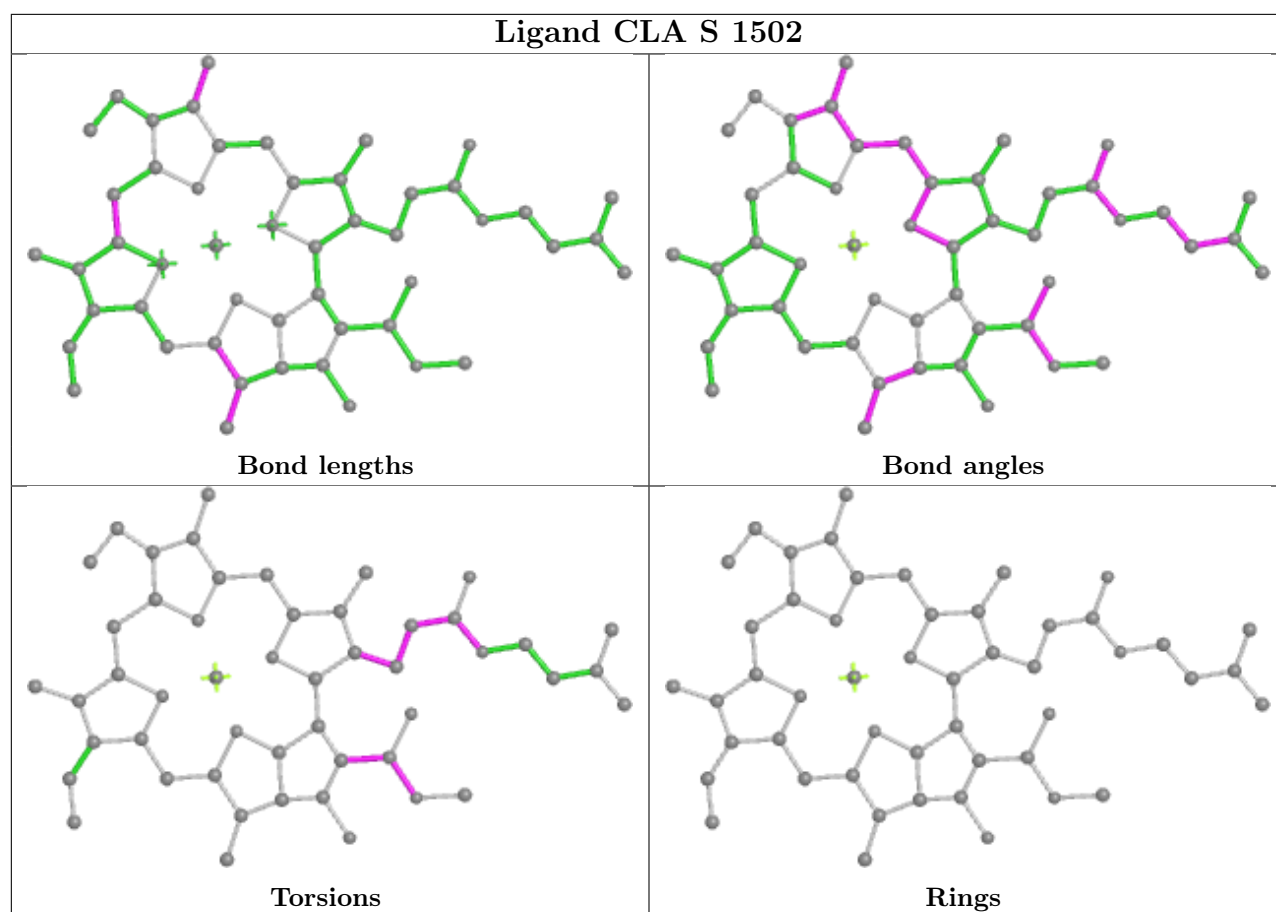
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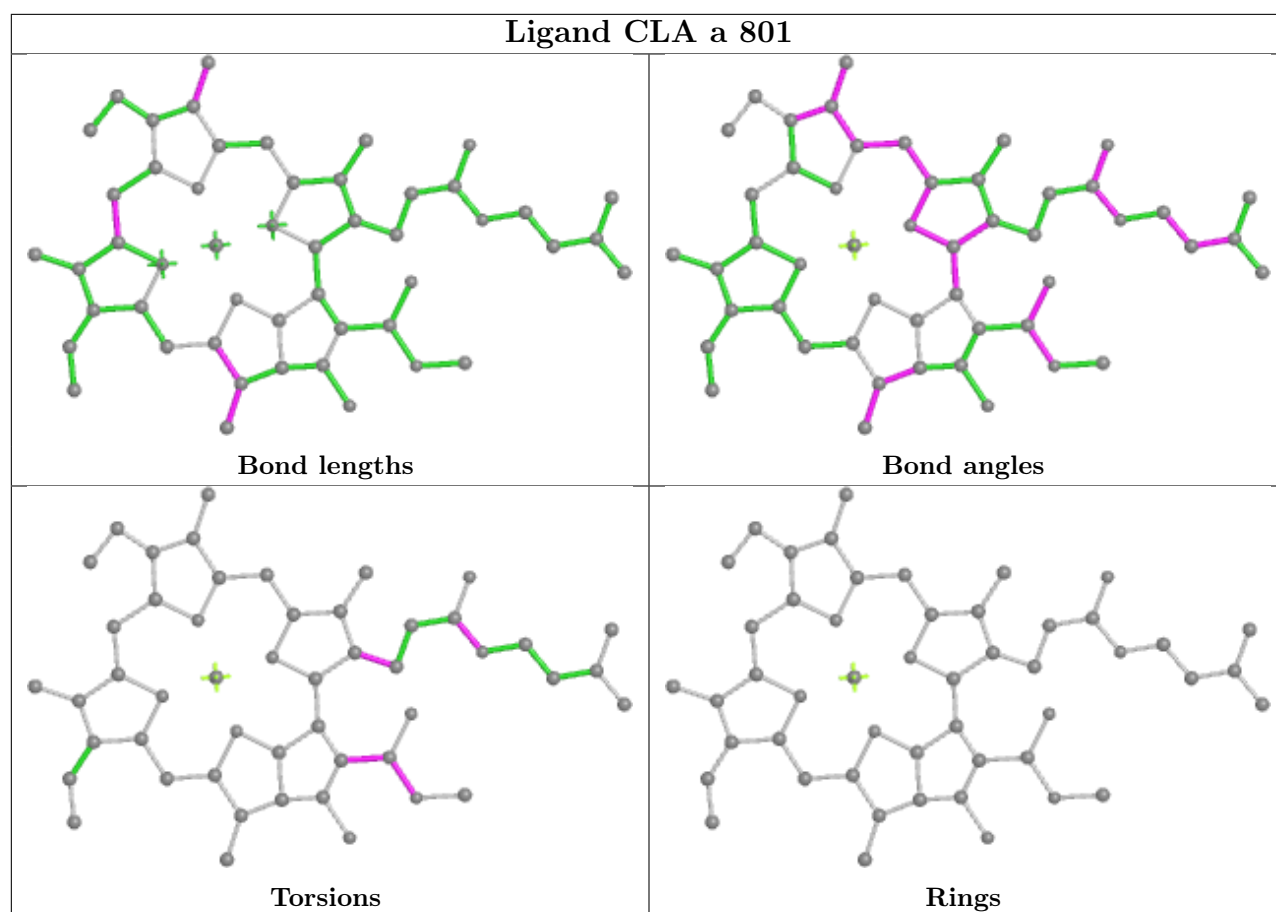


Ligand CLA R 1401

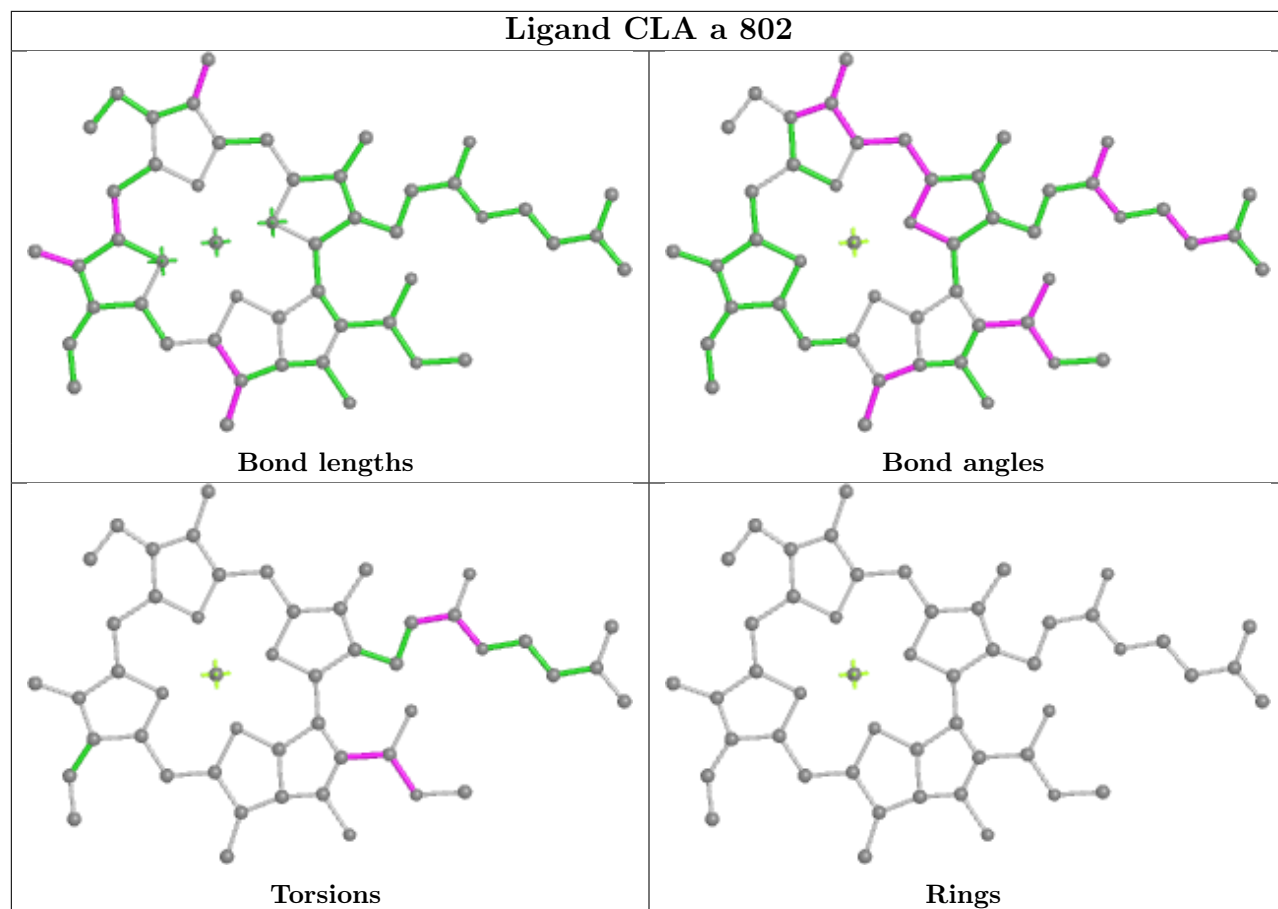




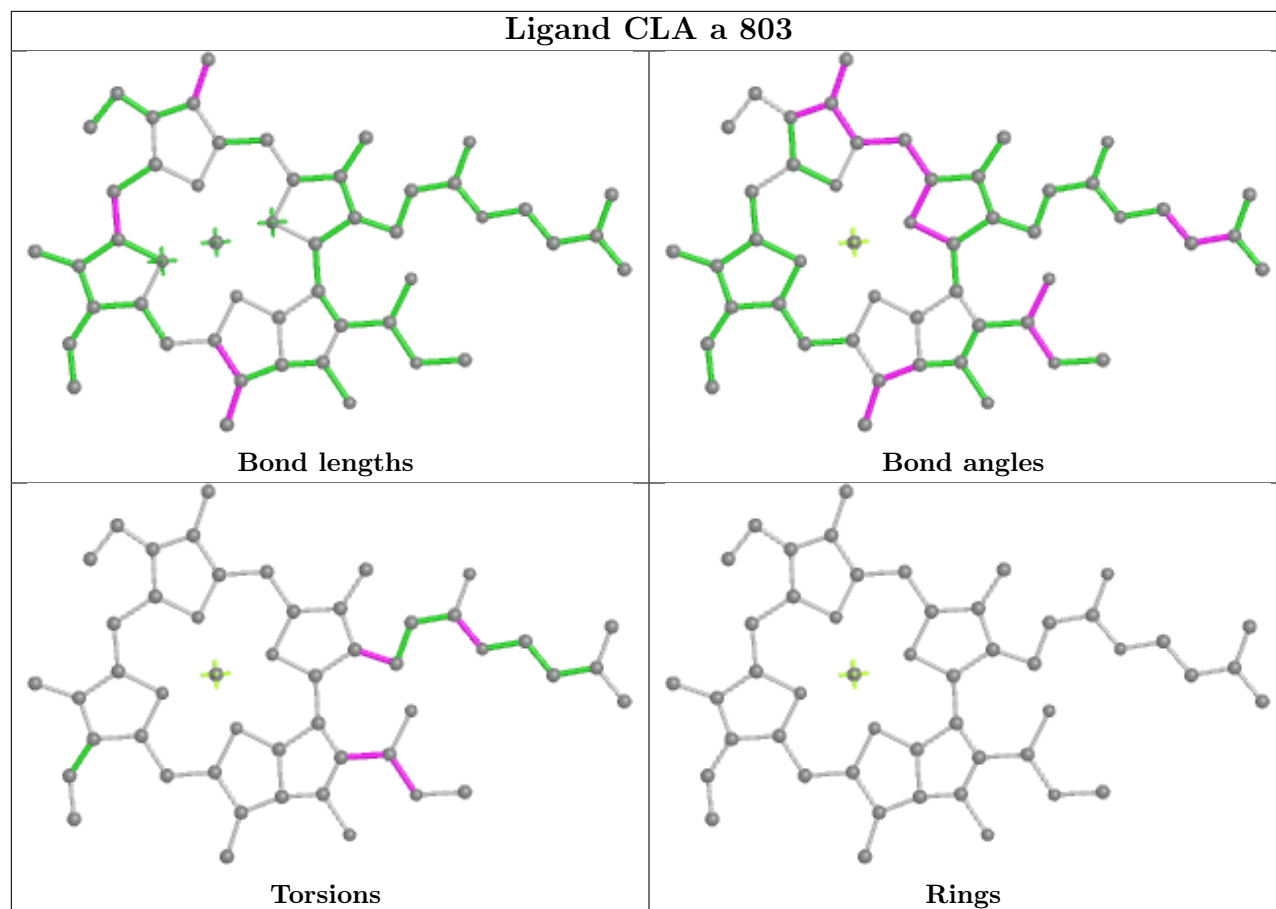




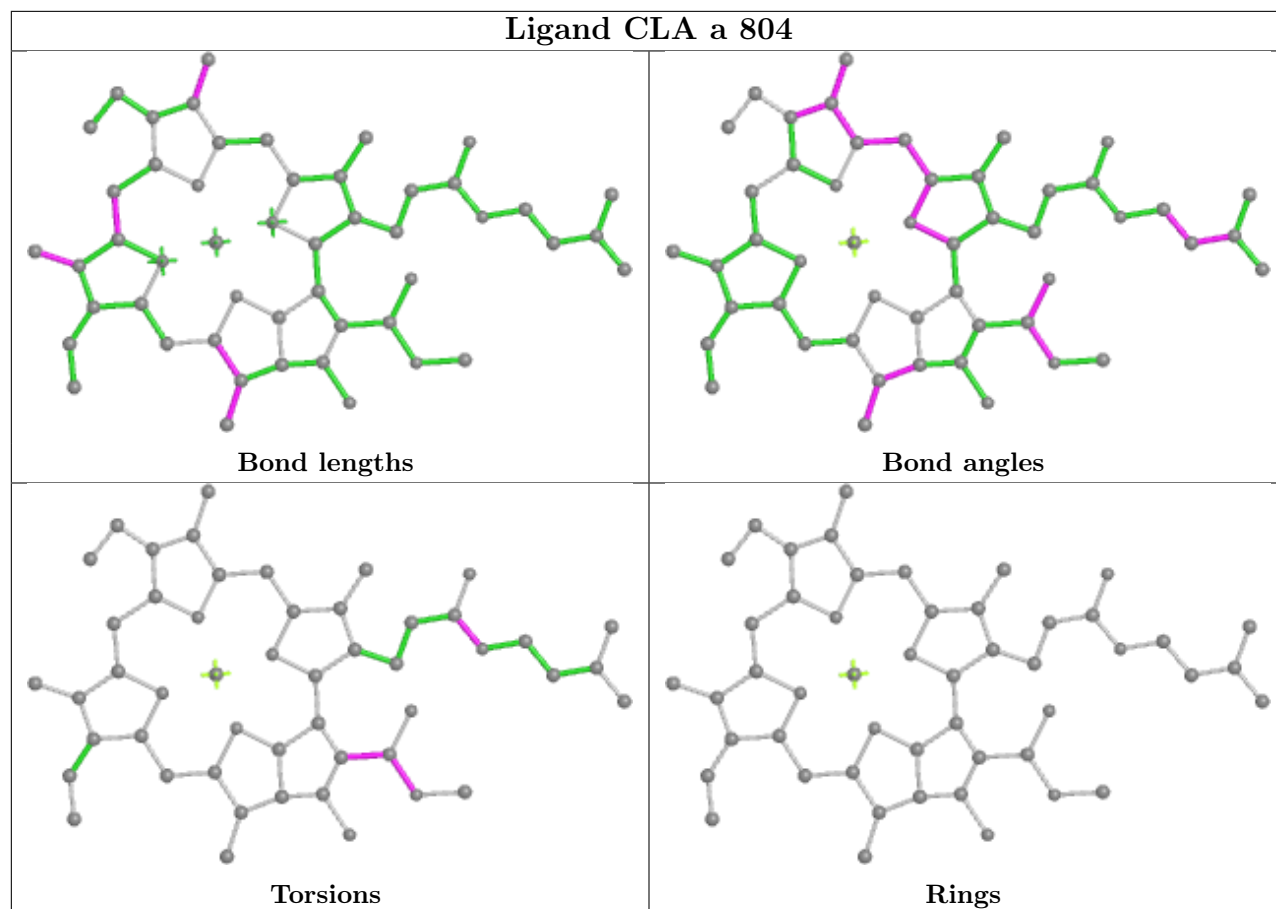
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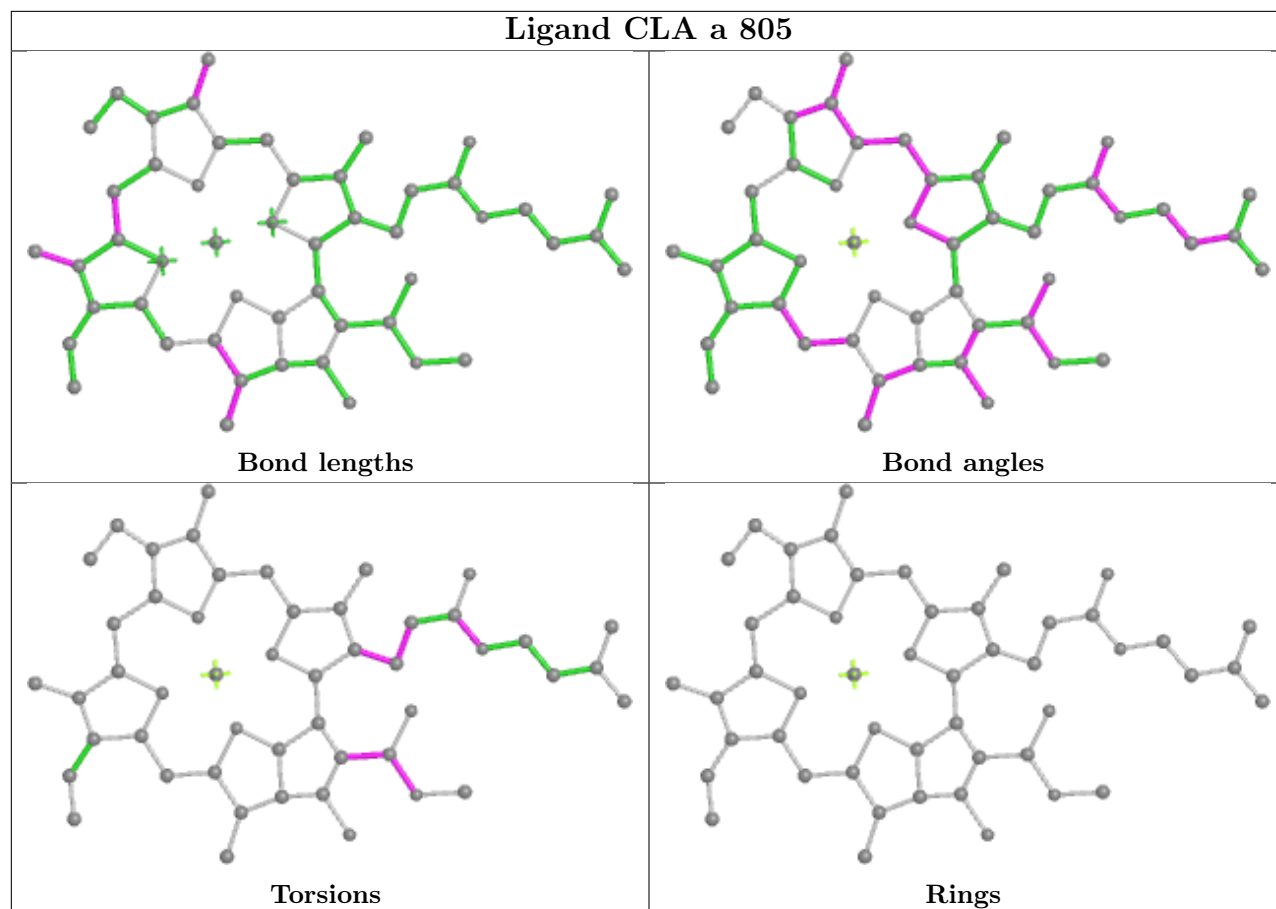
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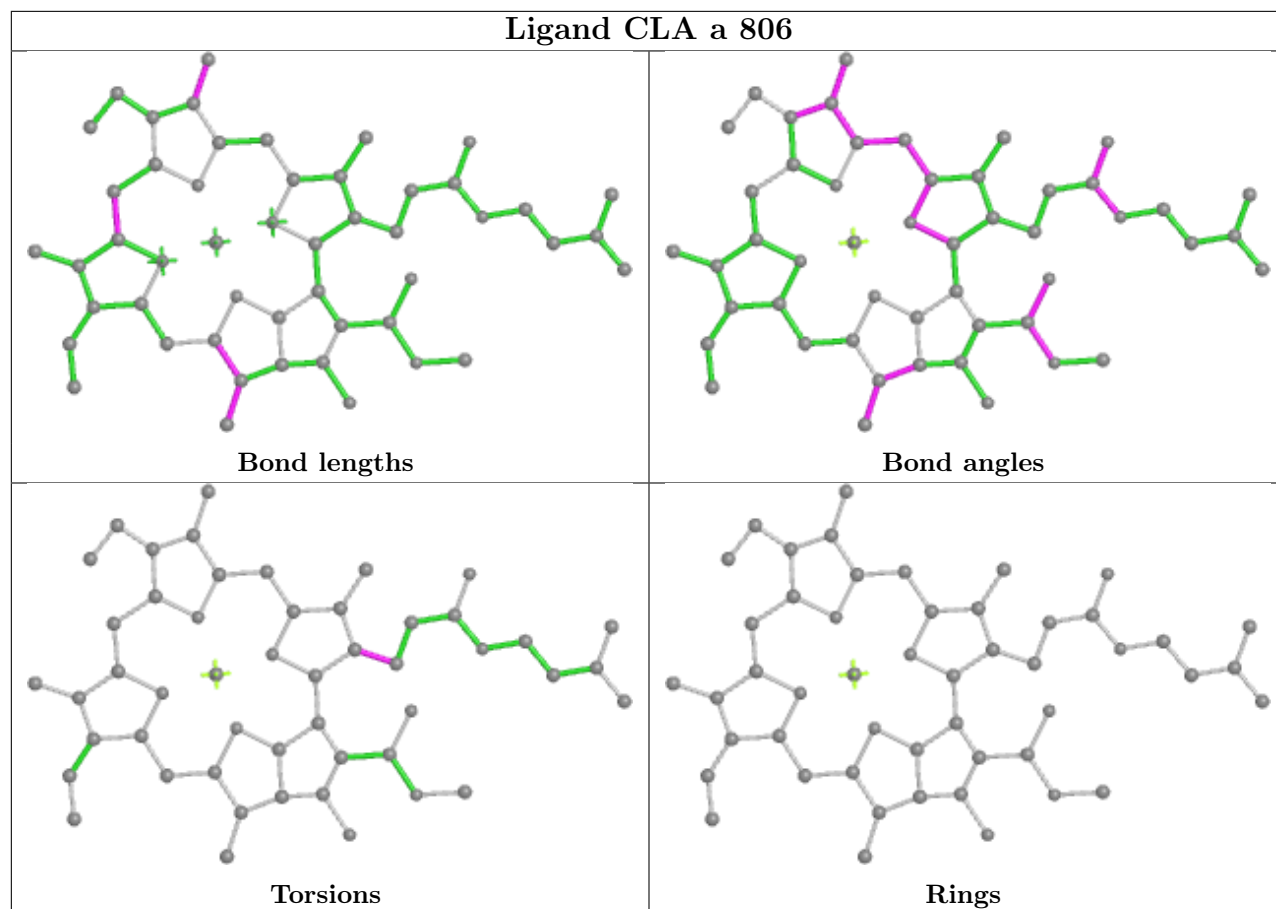
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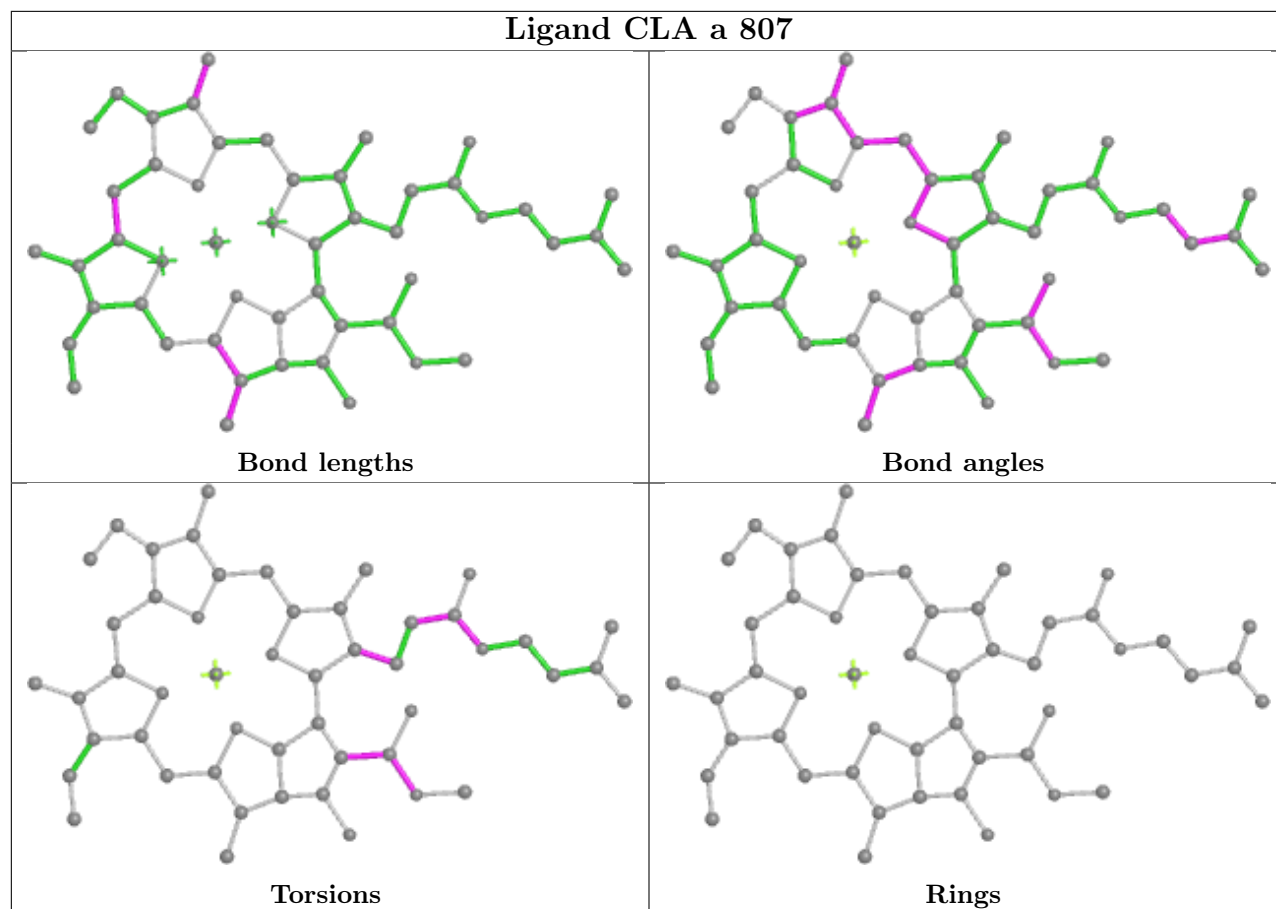
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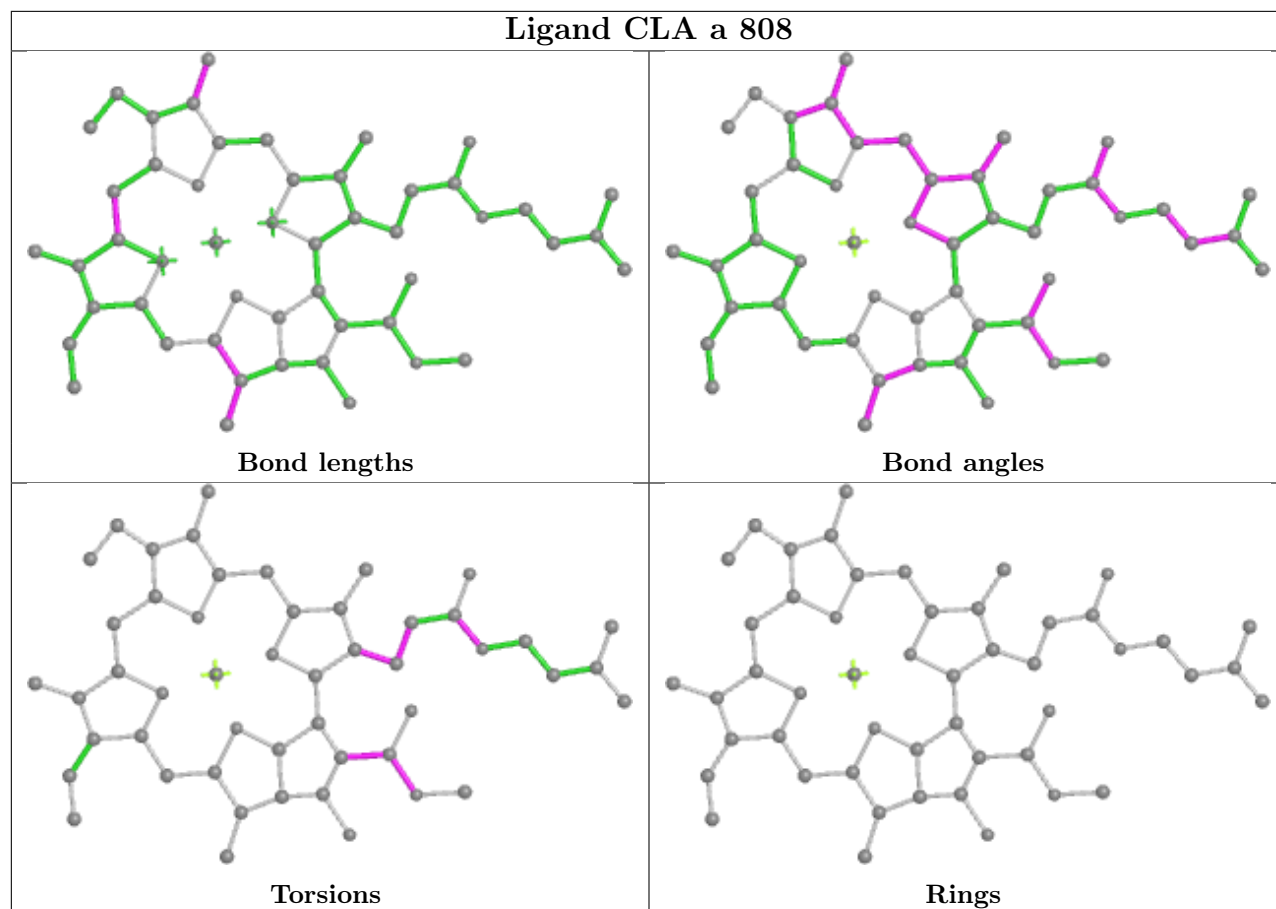
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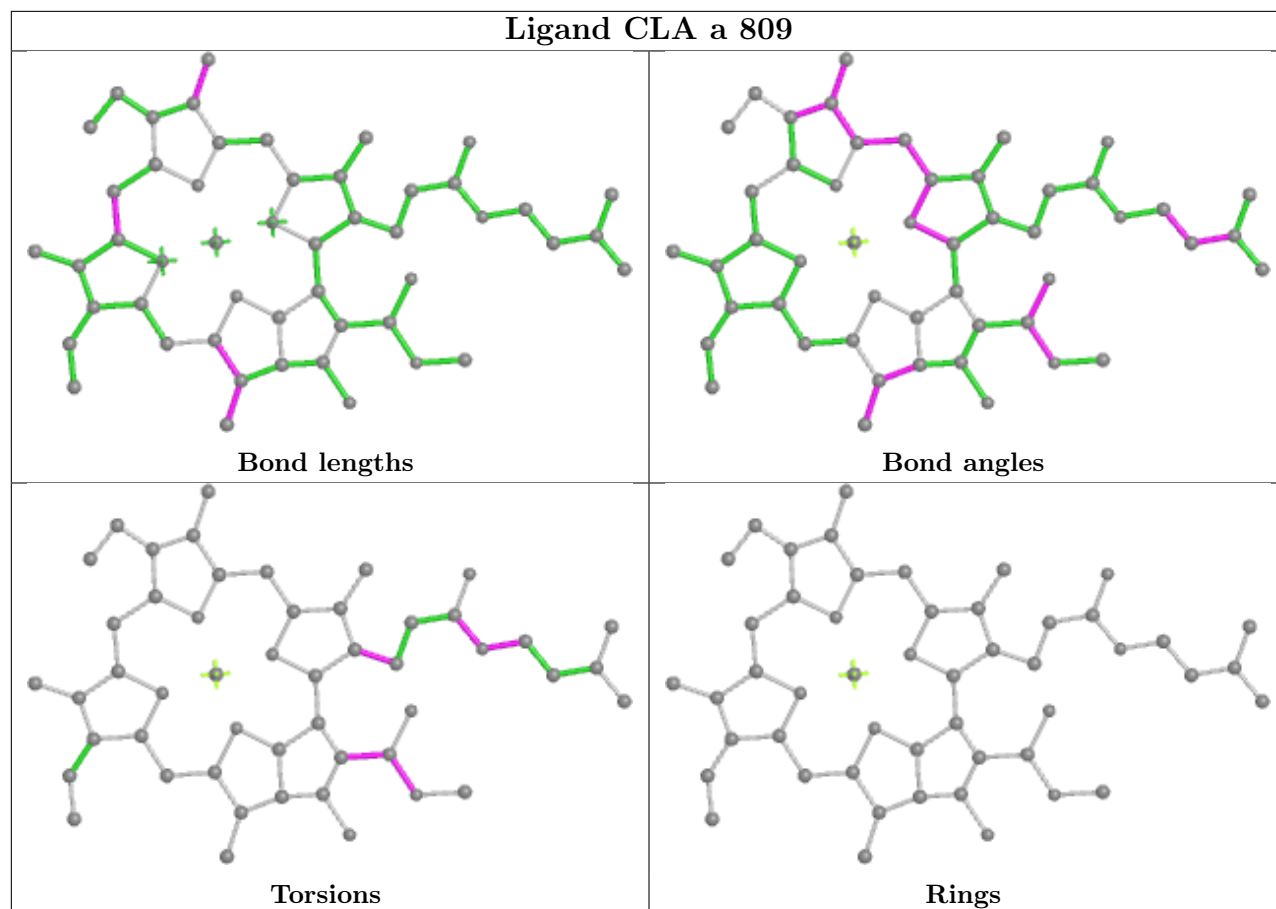


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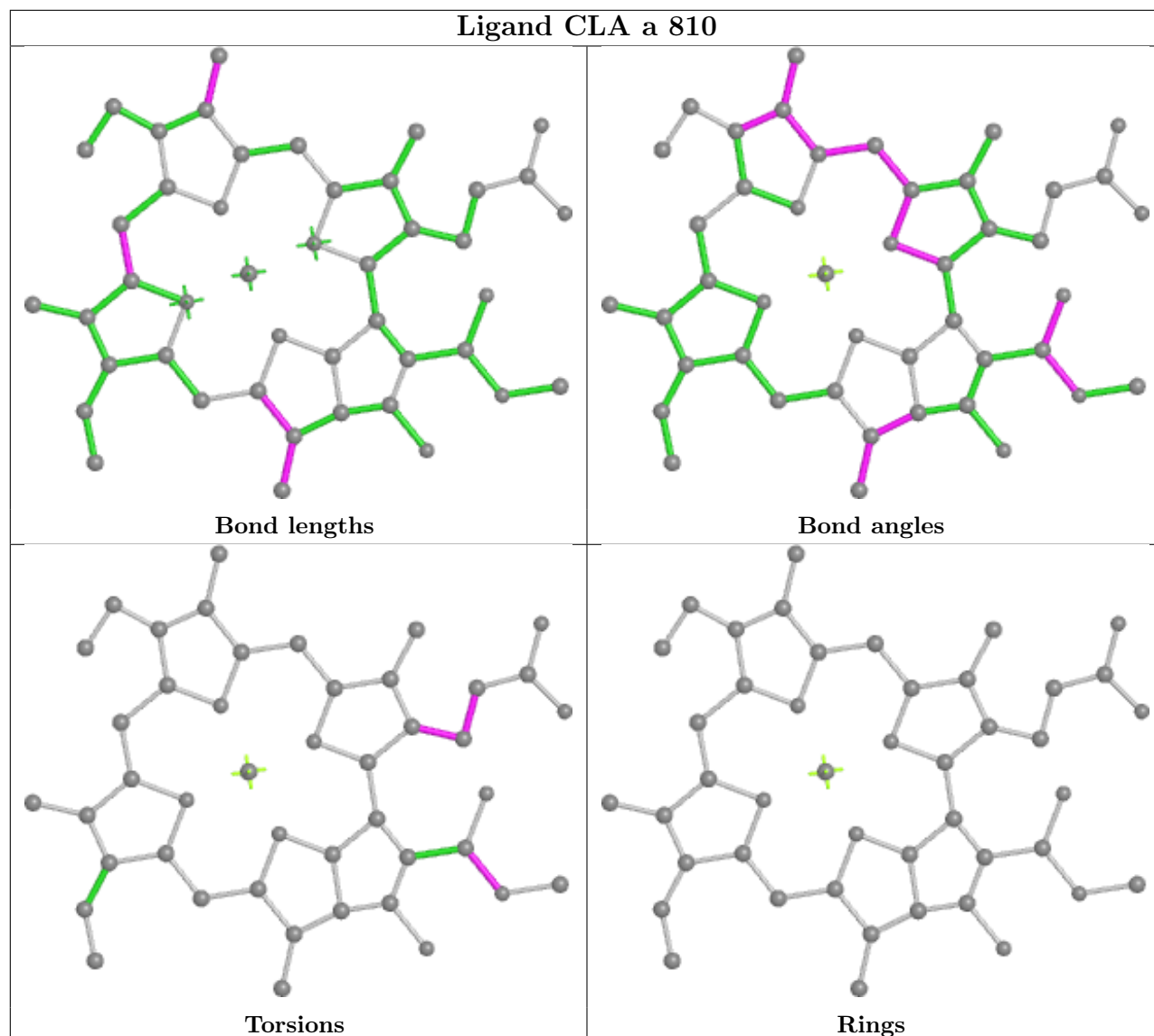


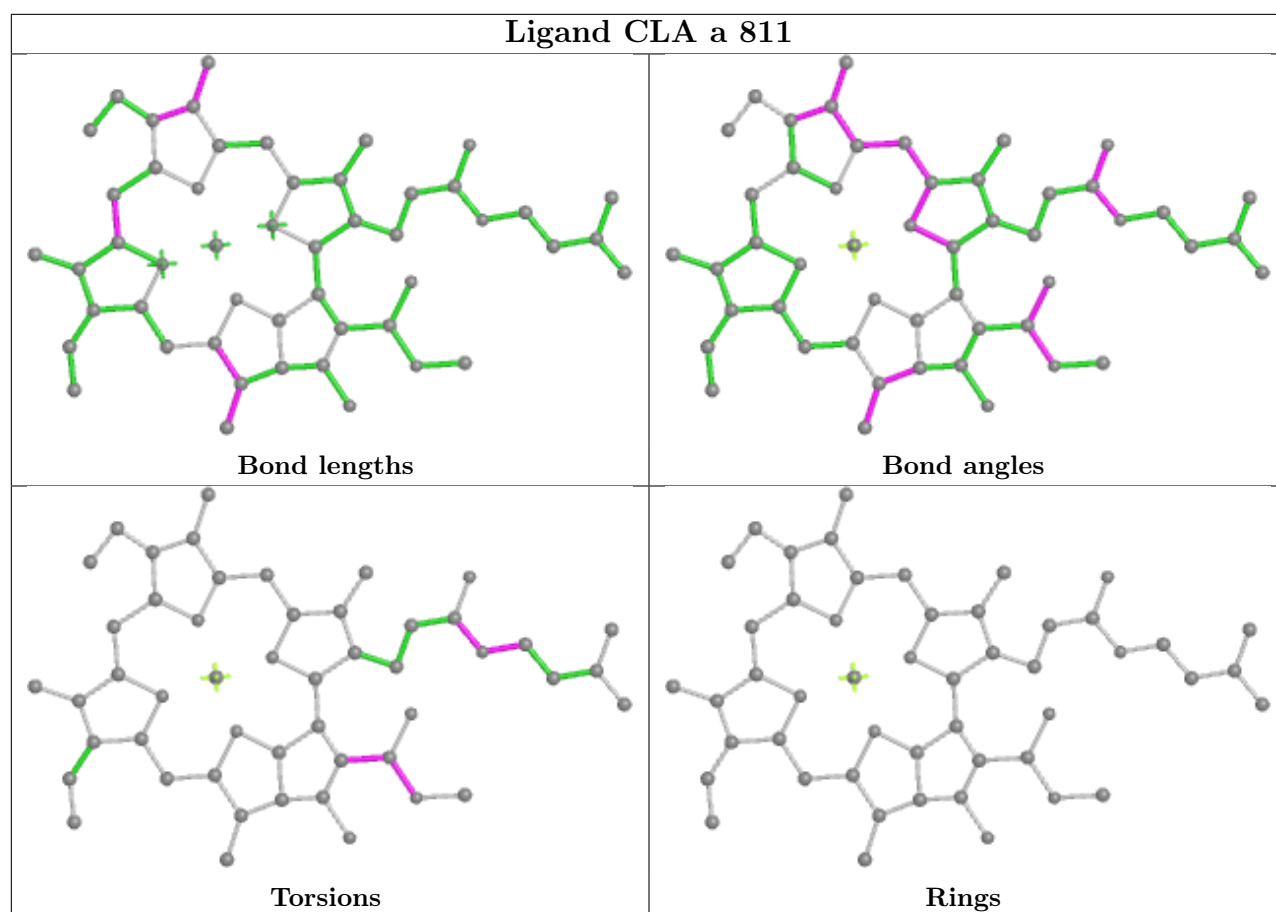
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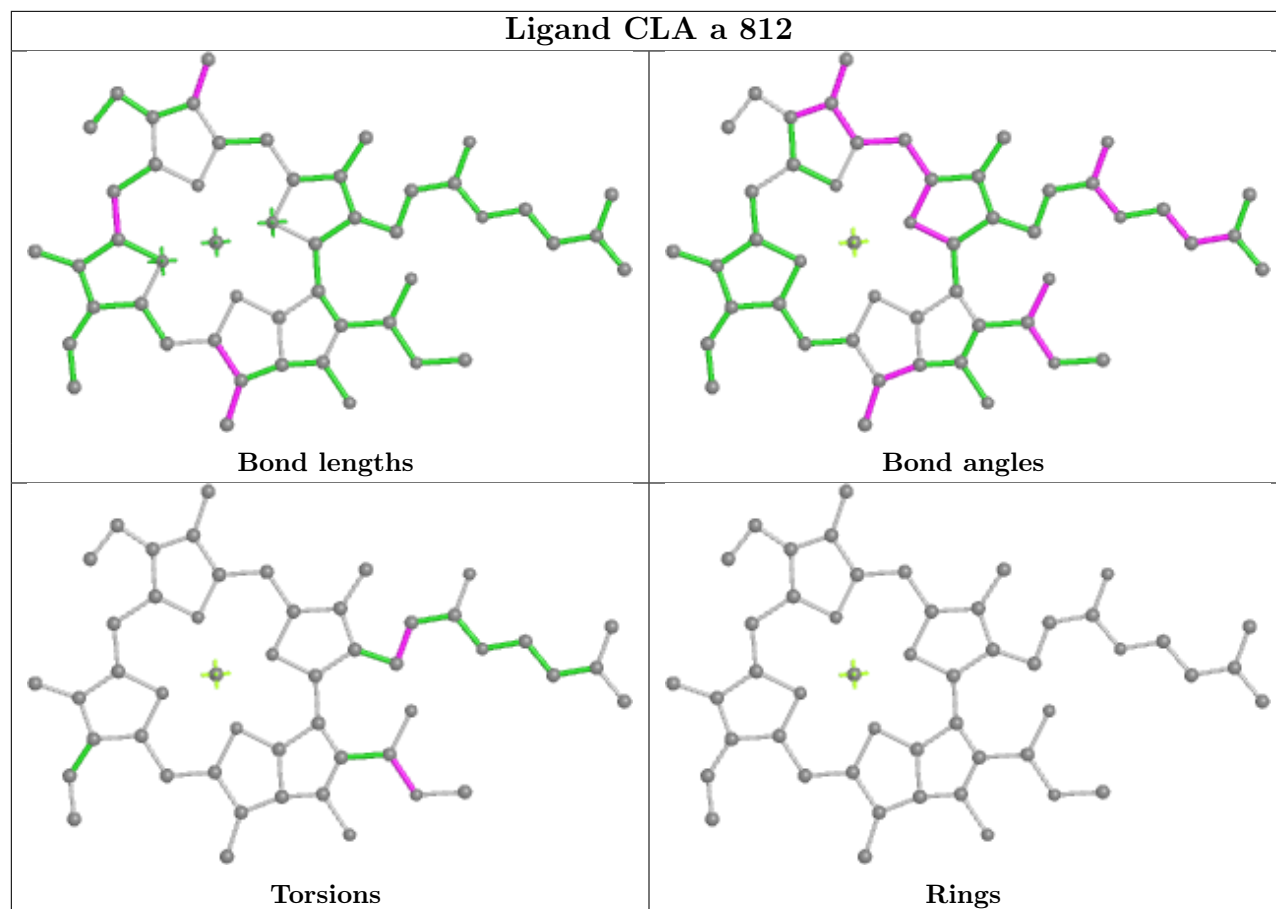


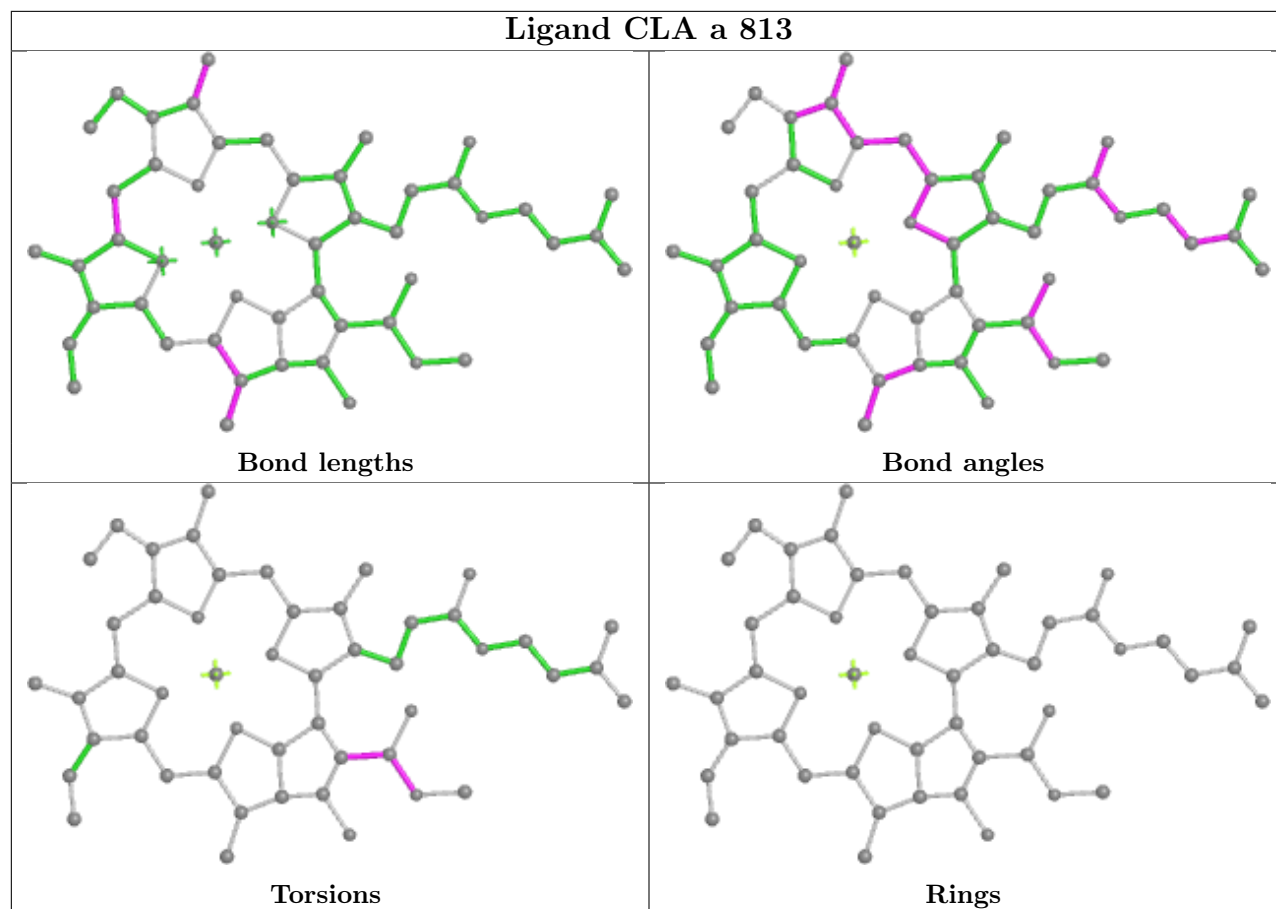
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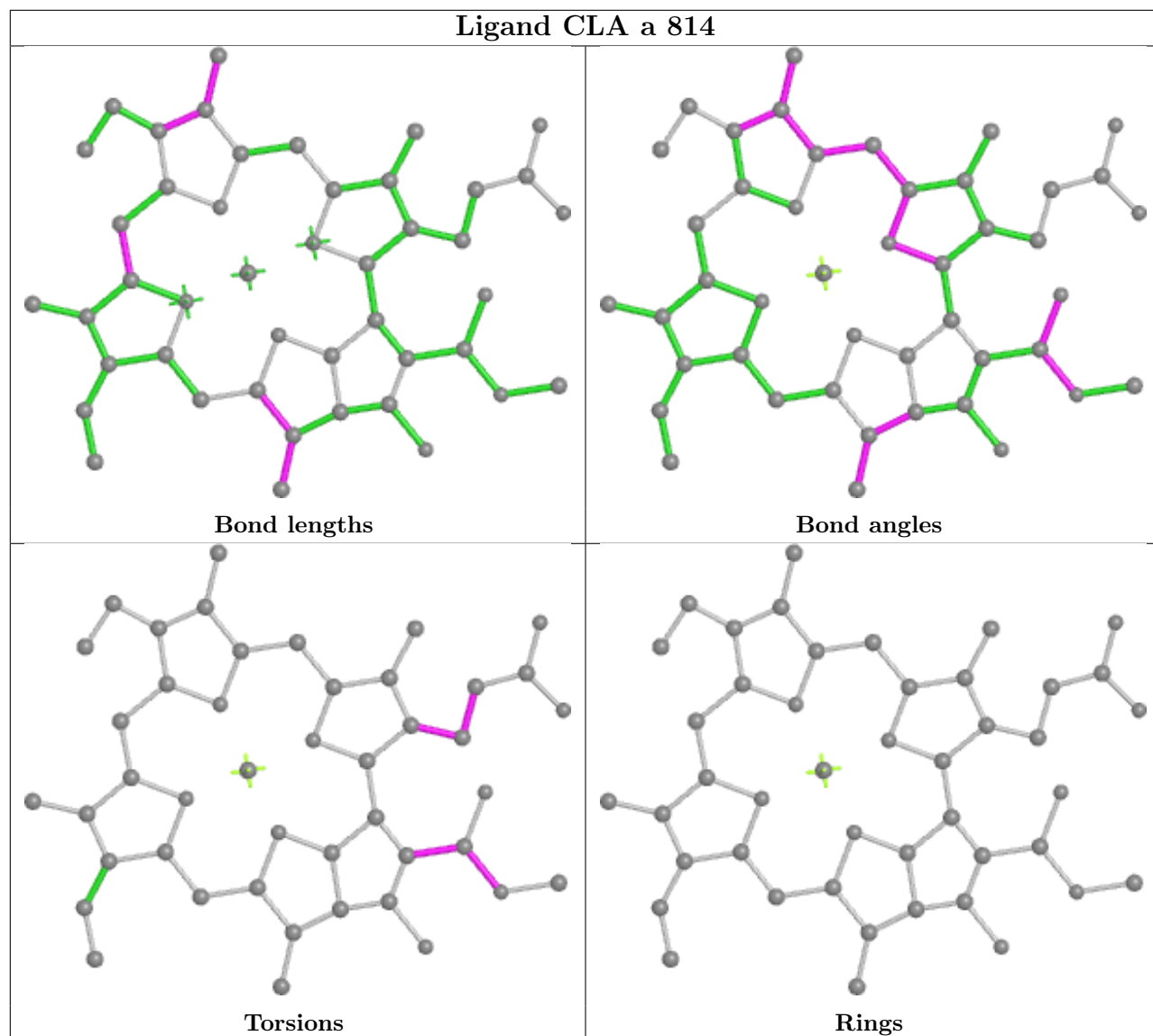


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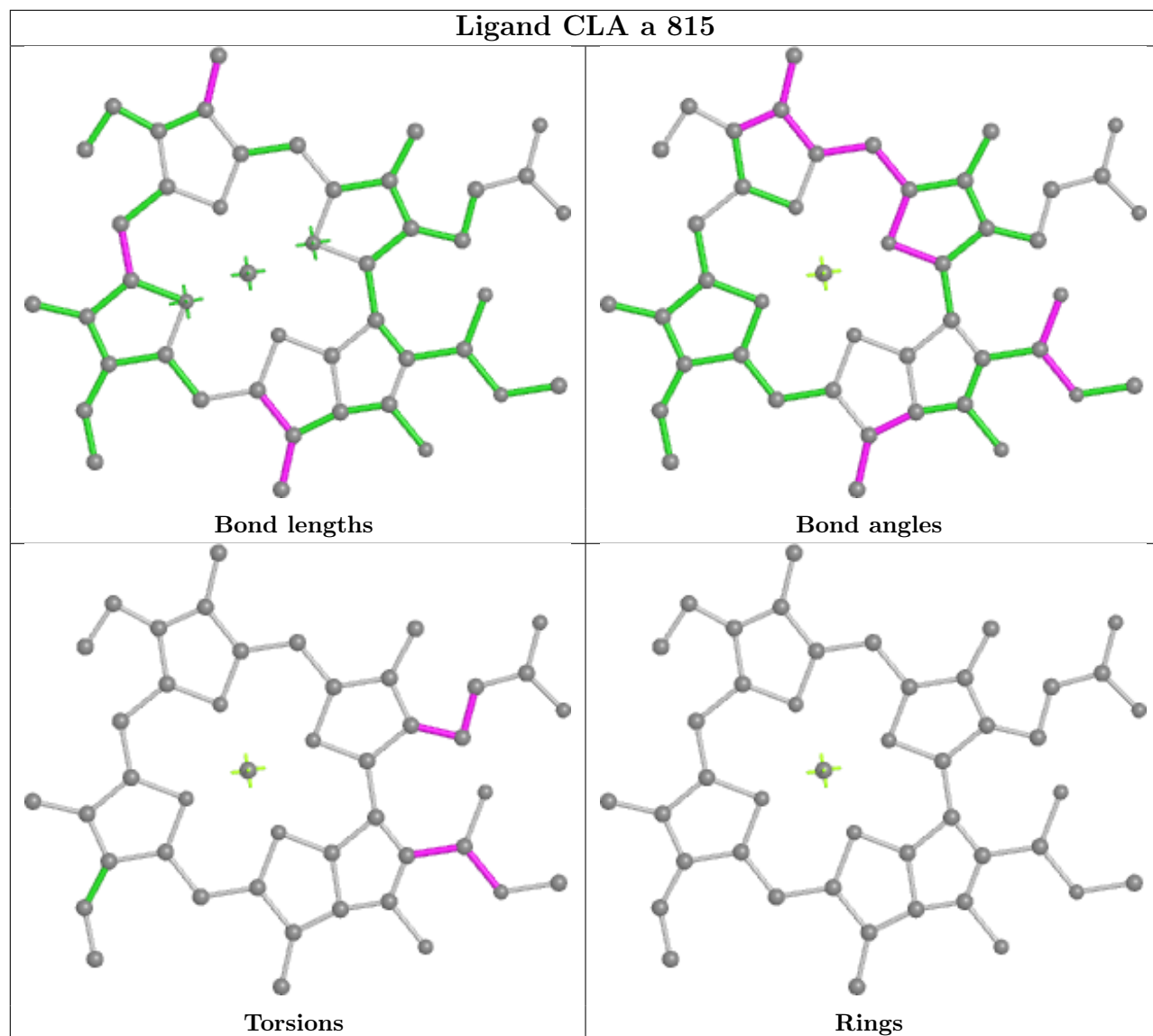


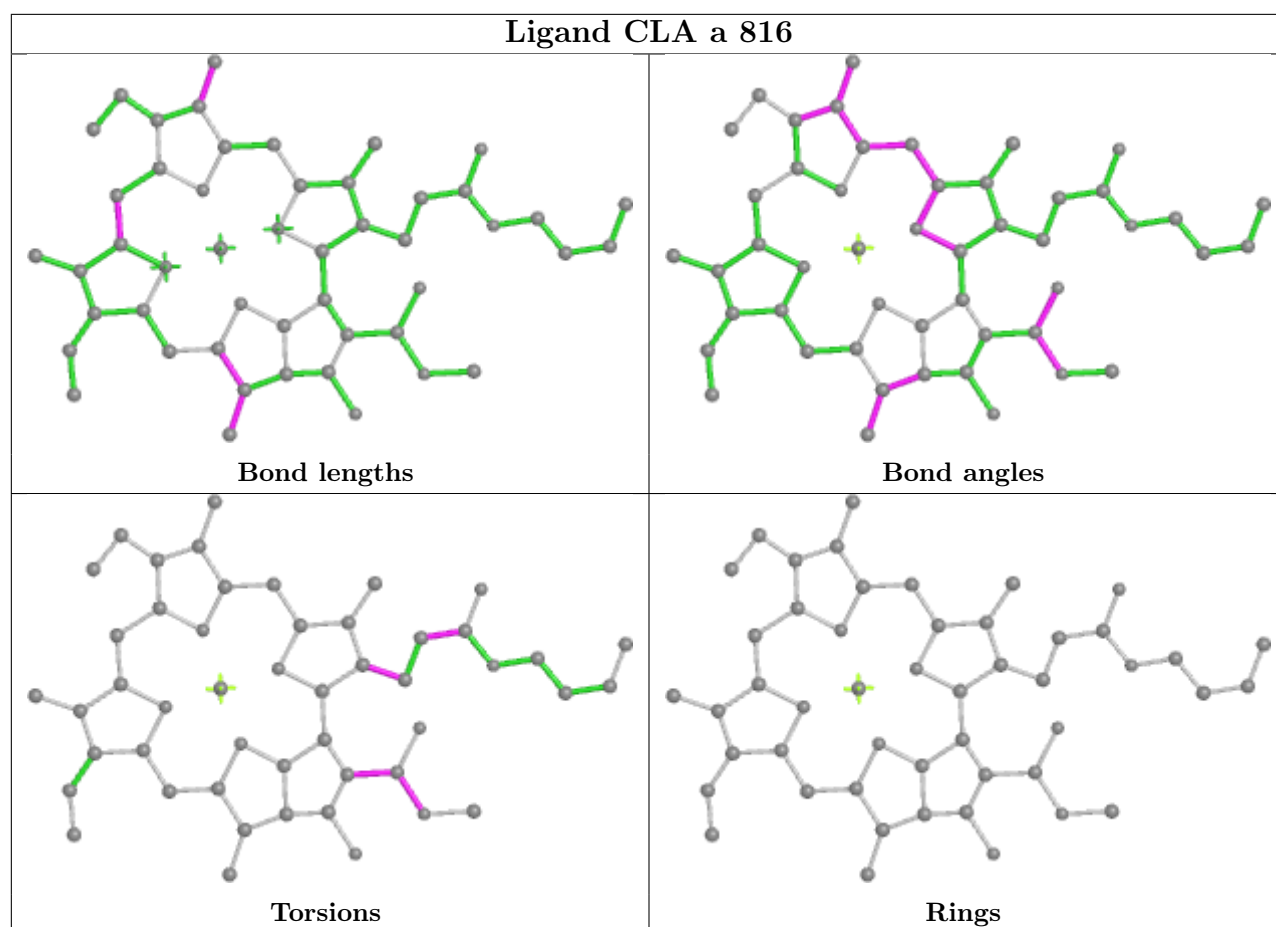


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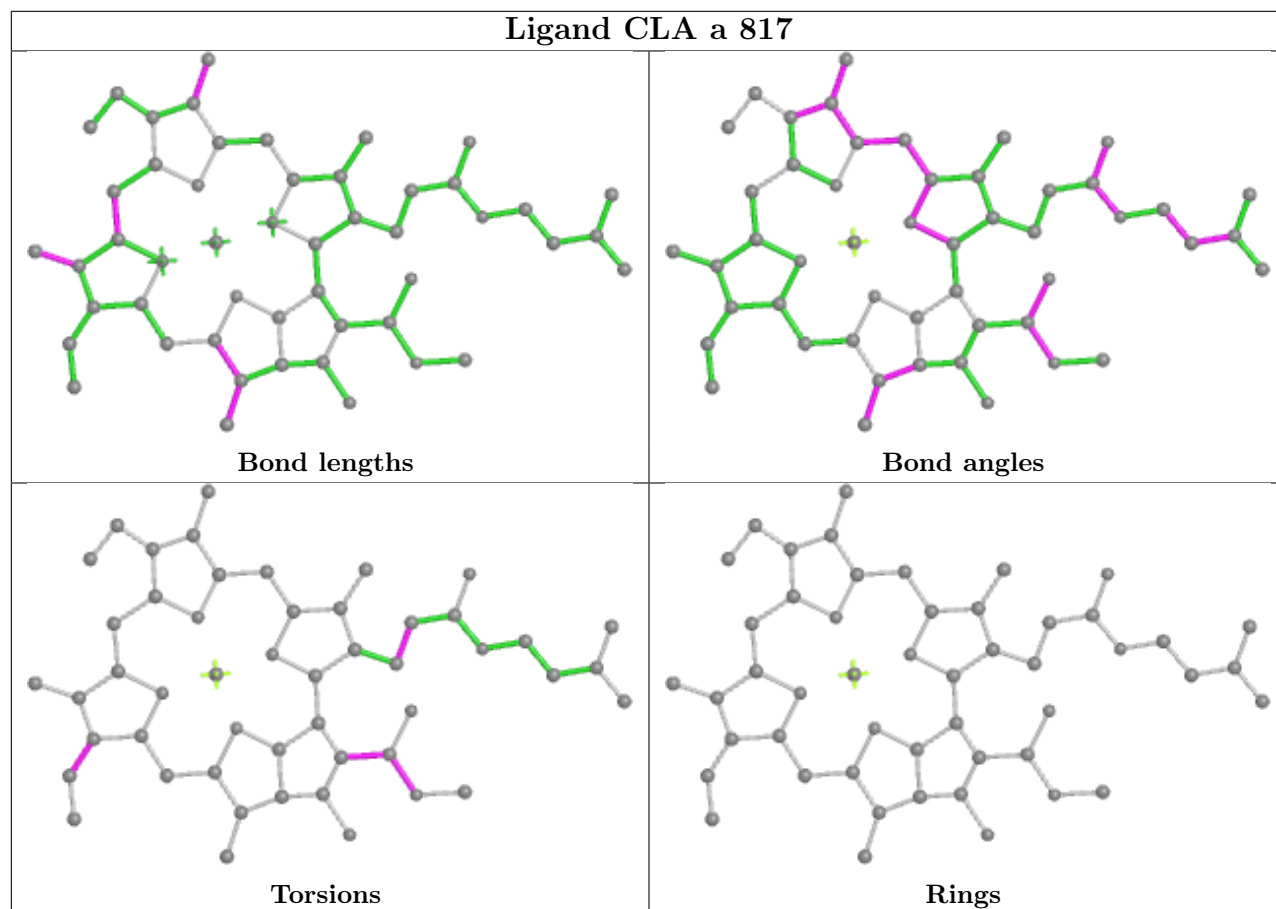


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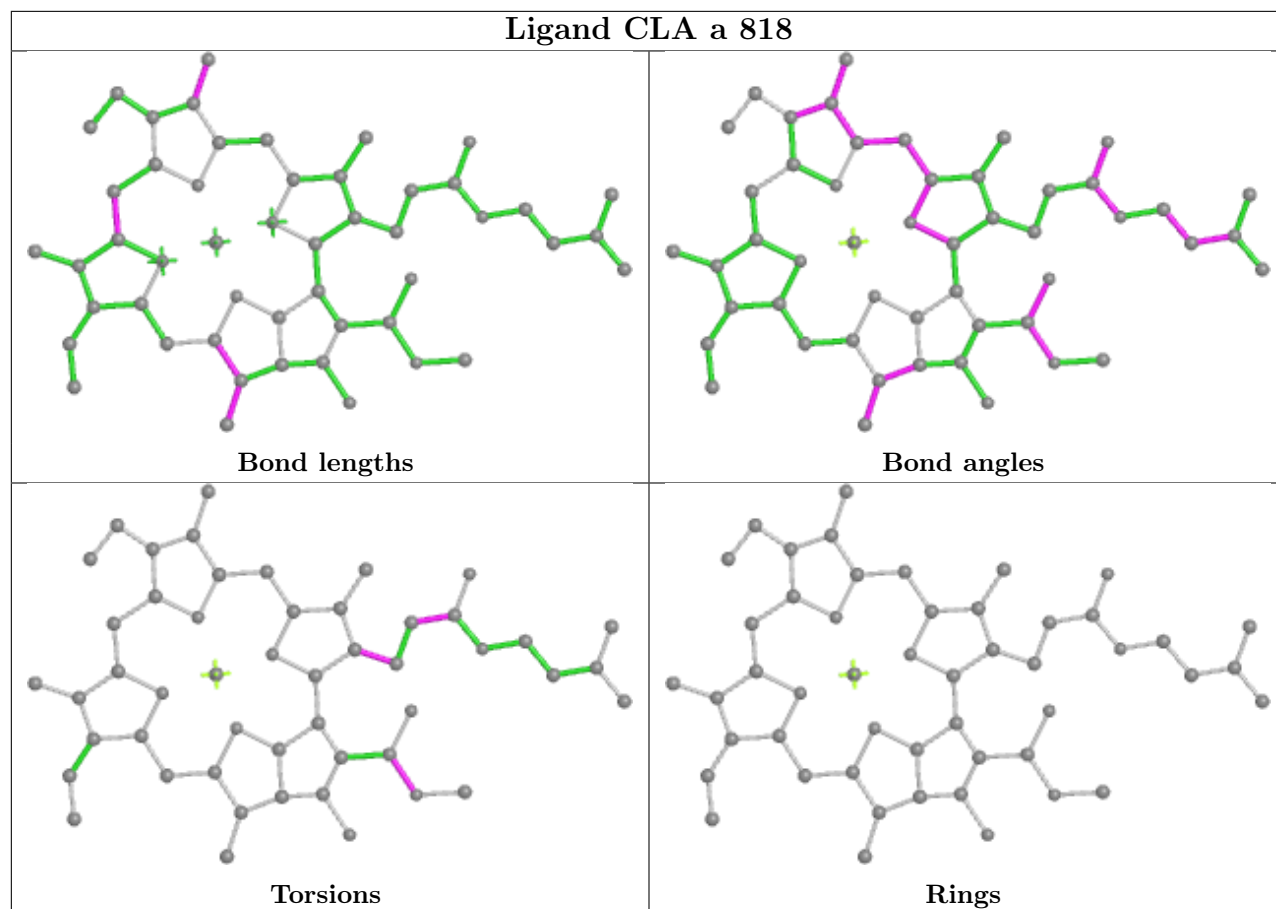




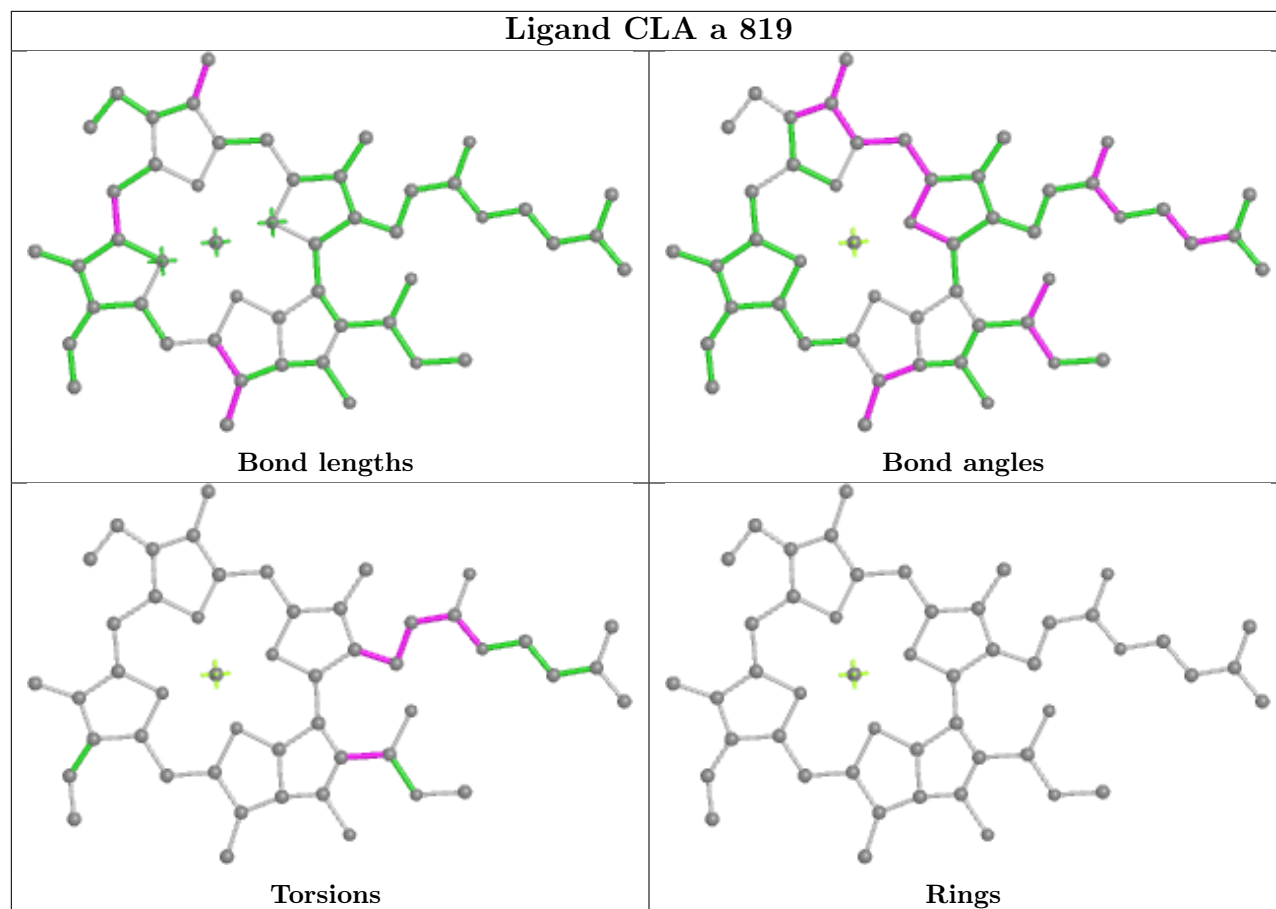
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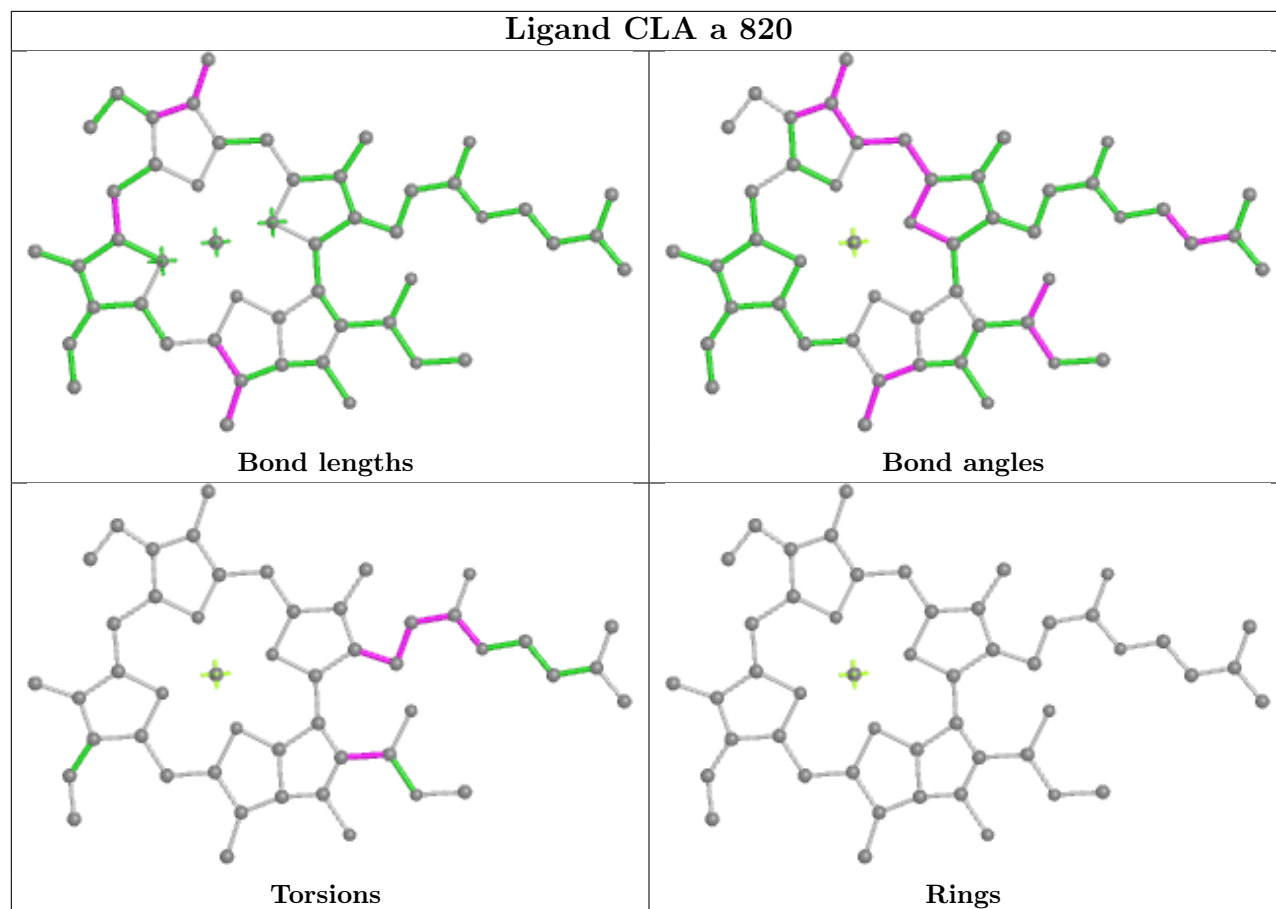


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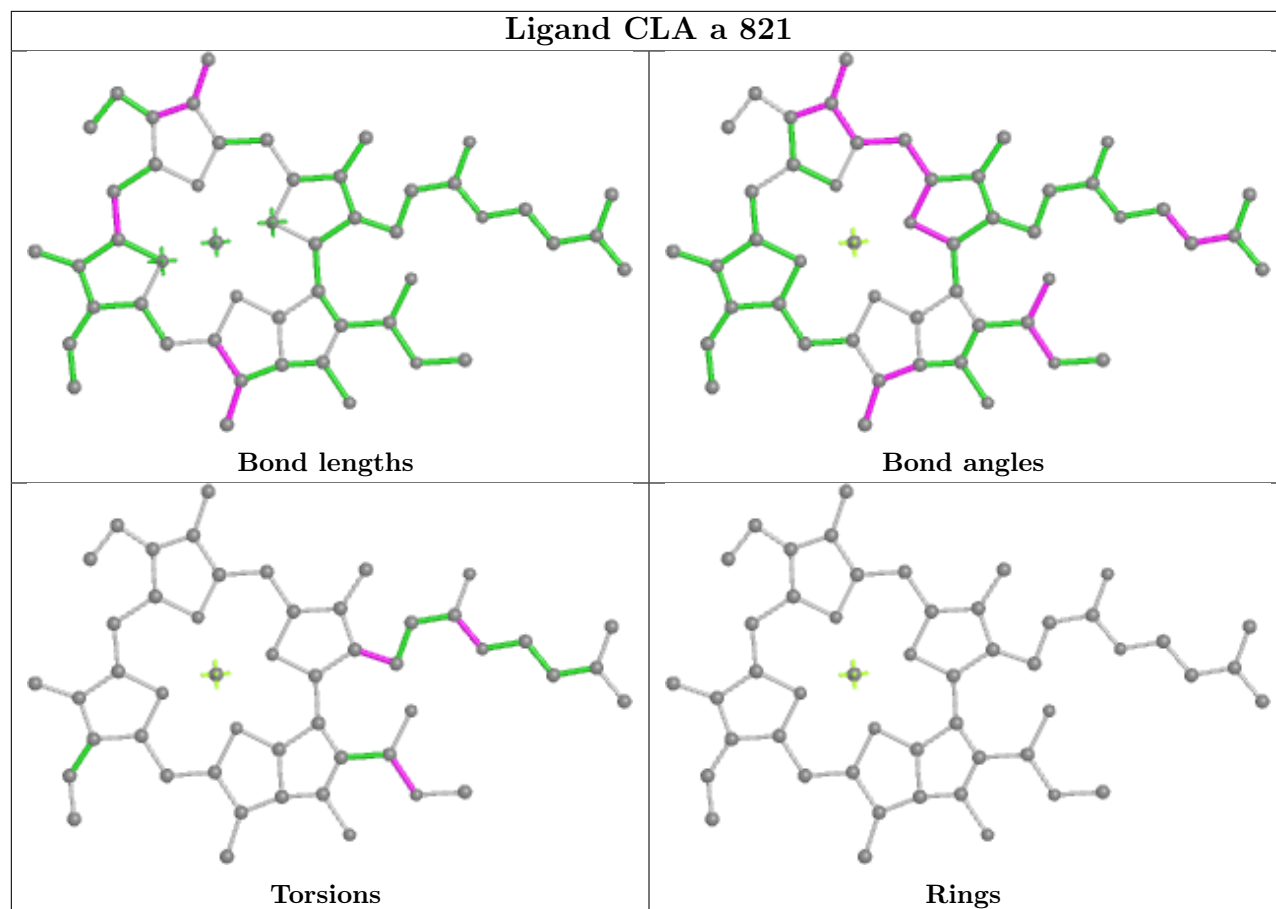


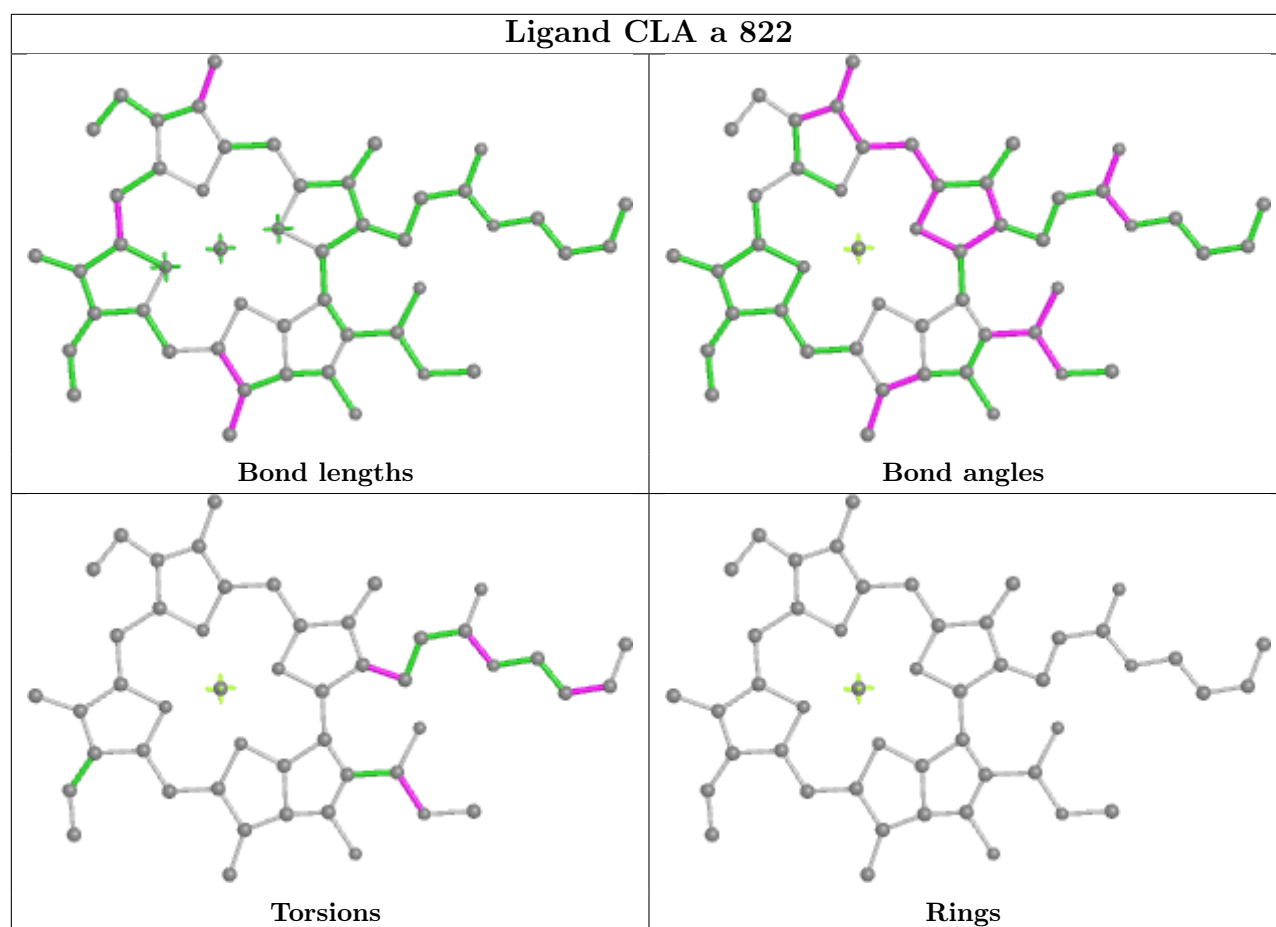
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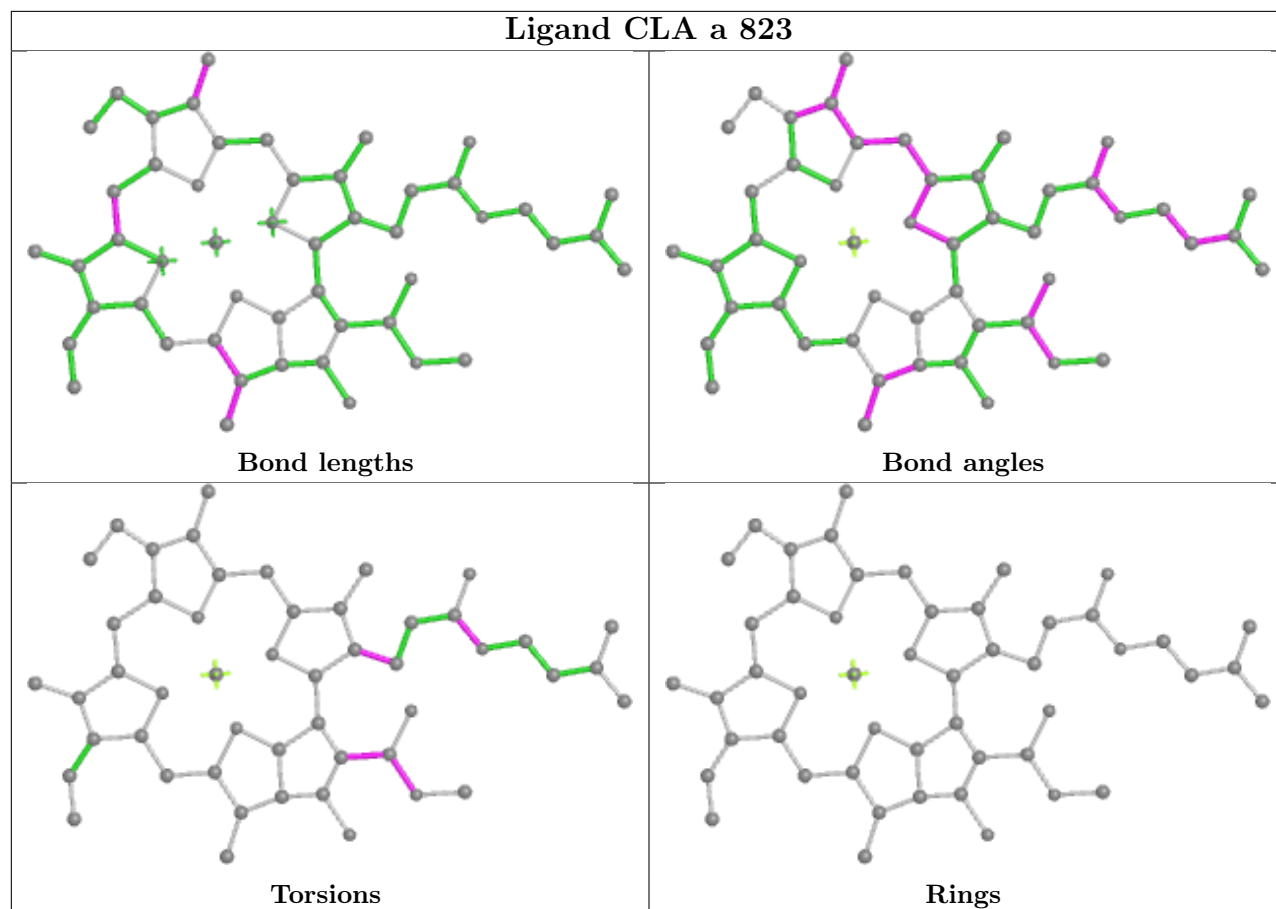


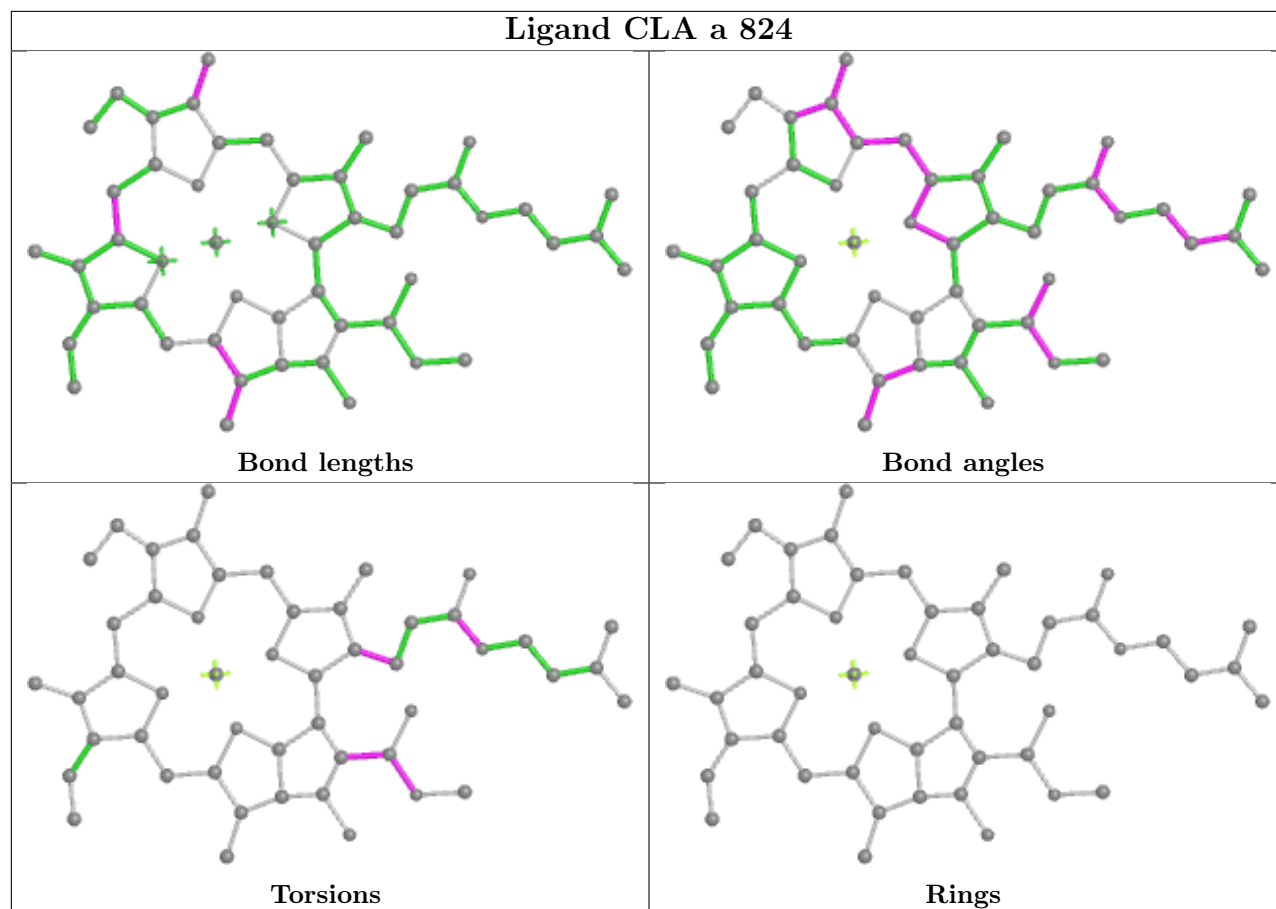
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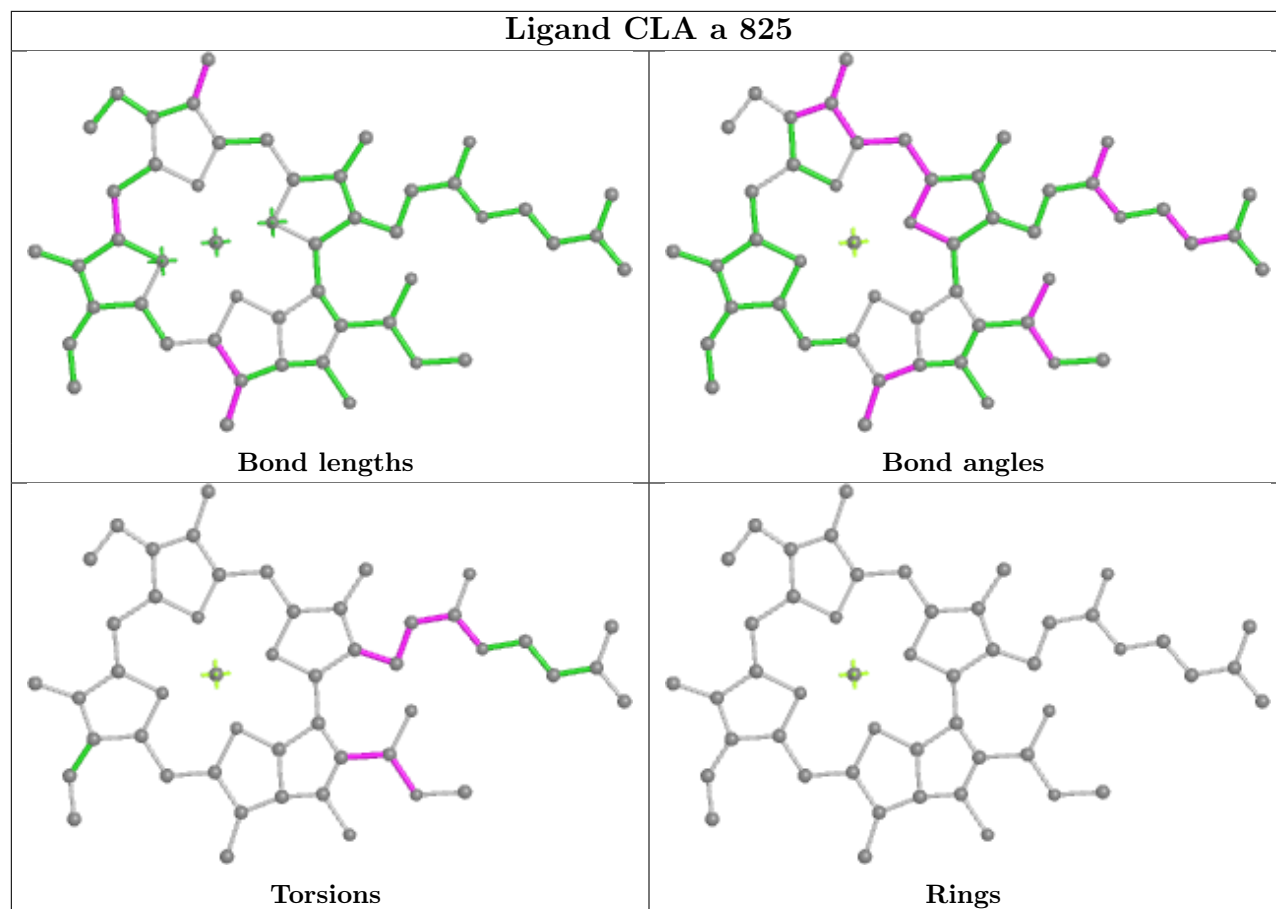


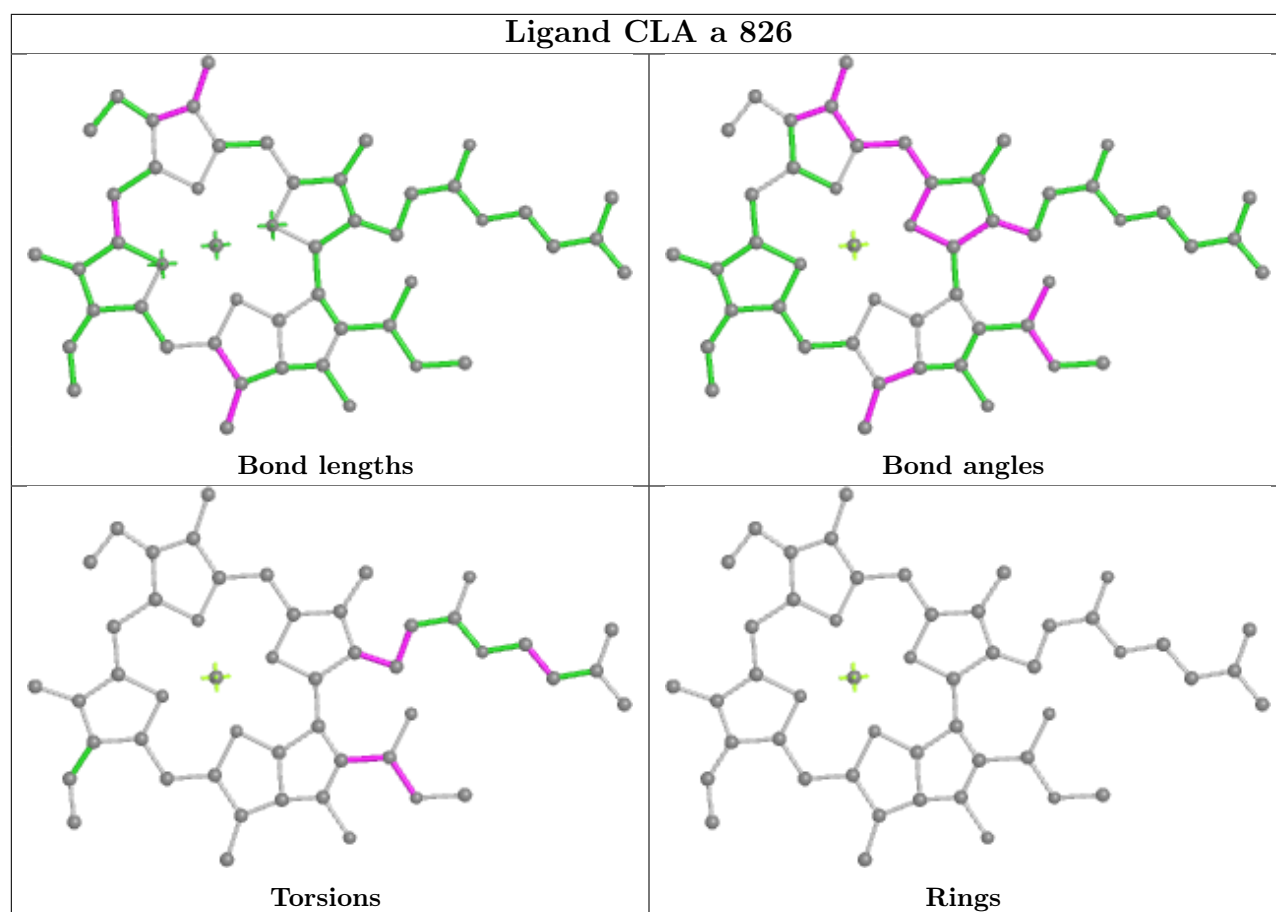
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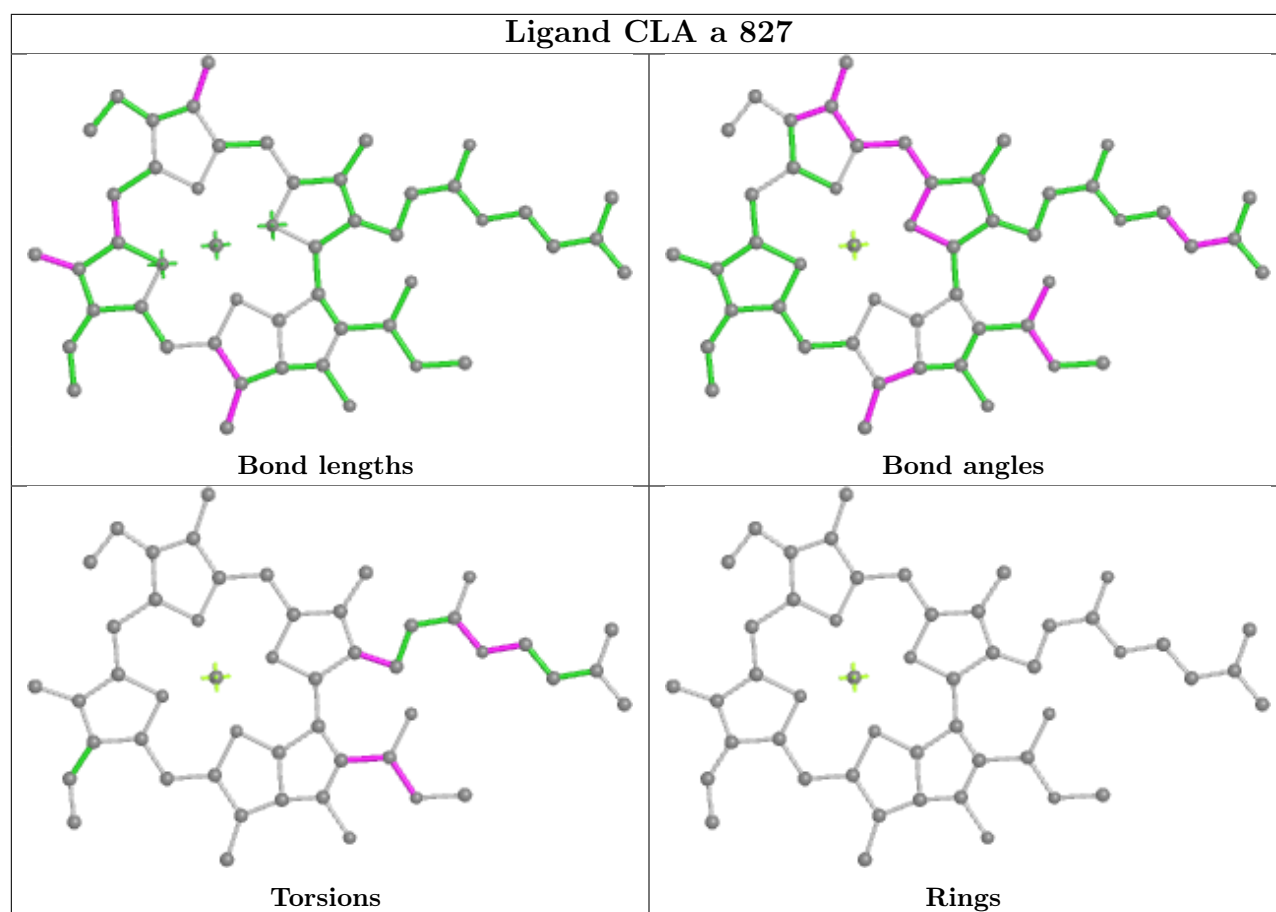




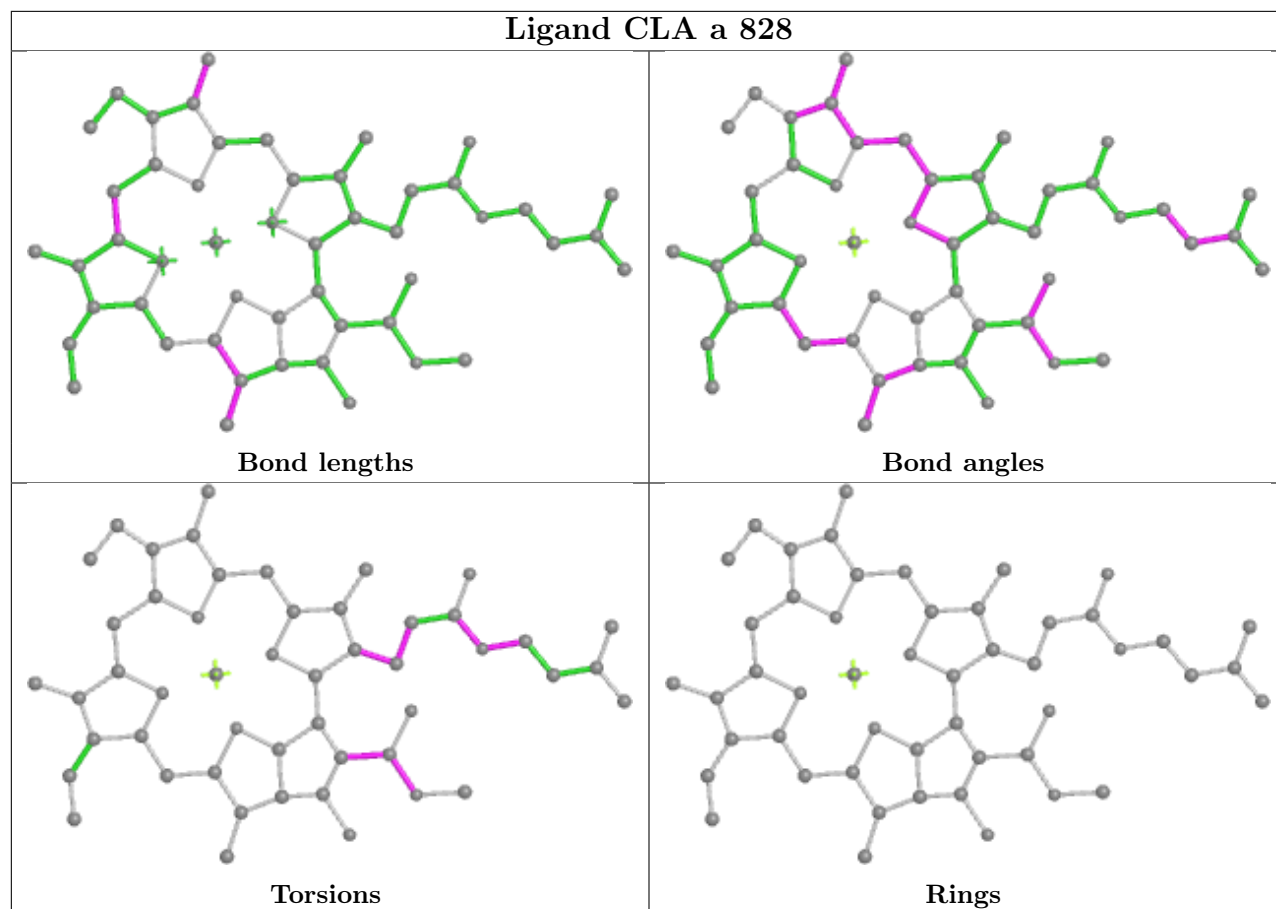
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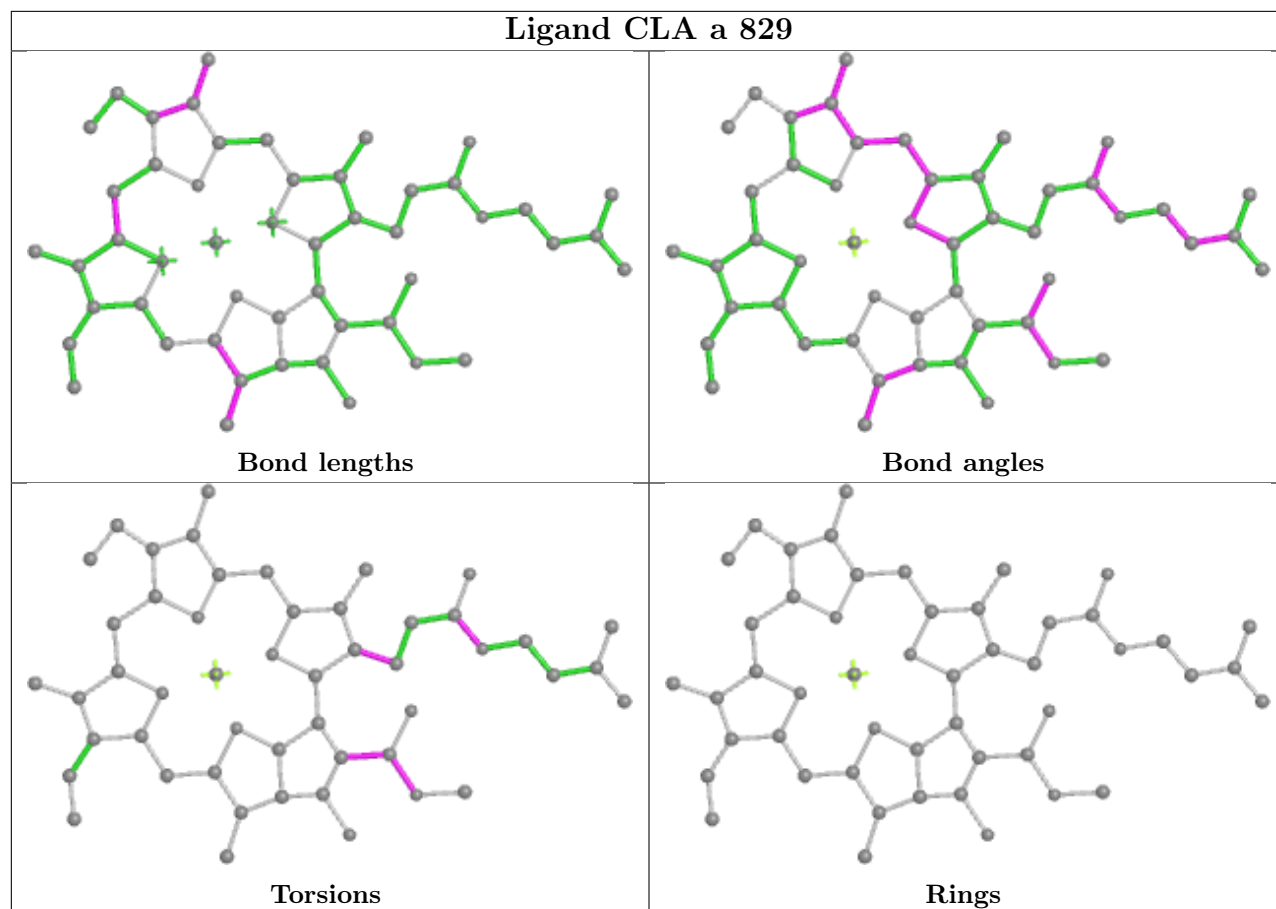




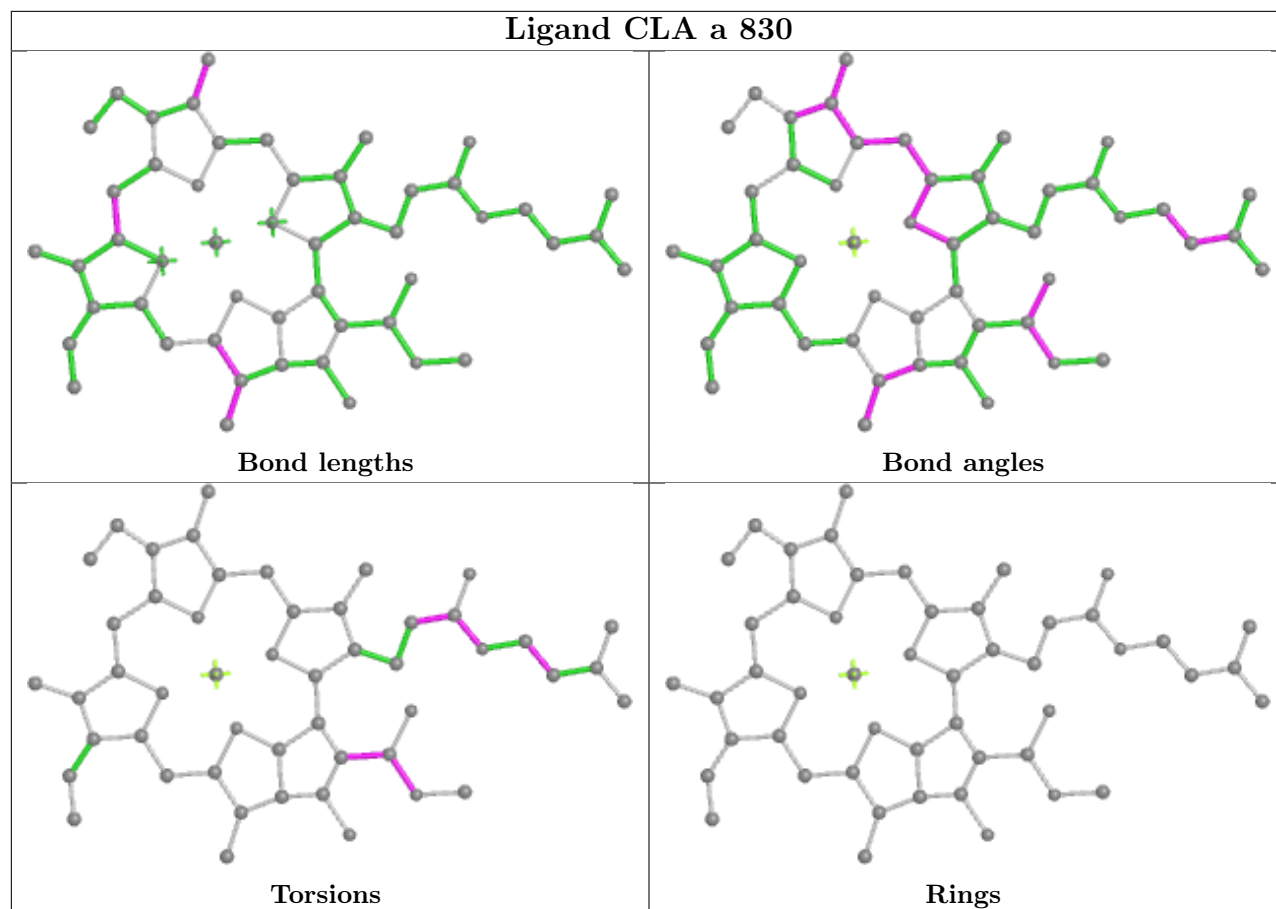
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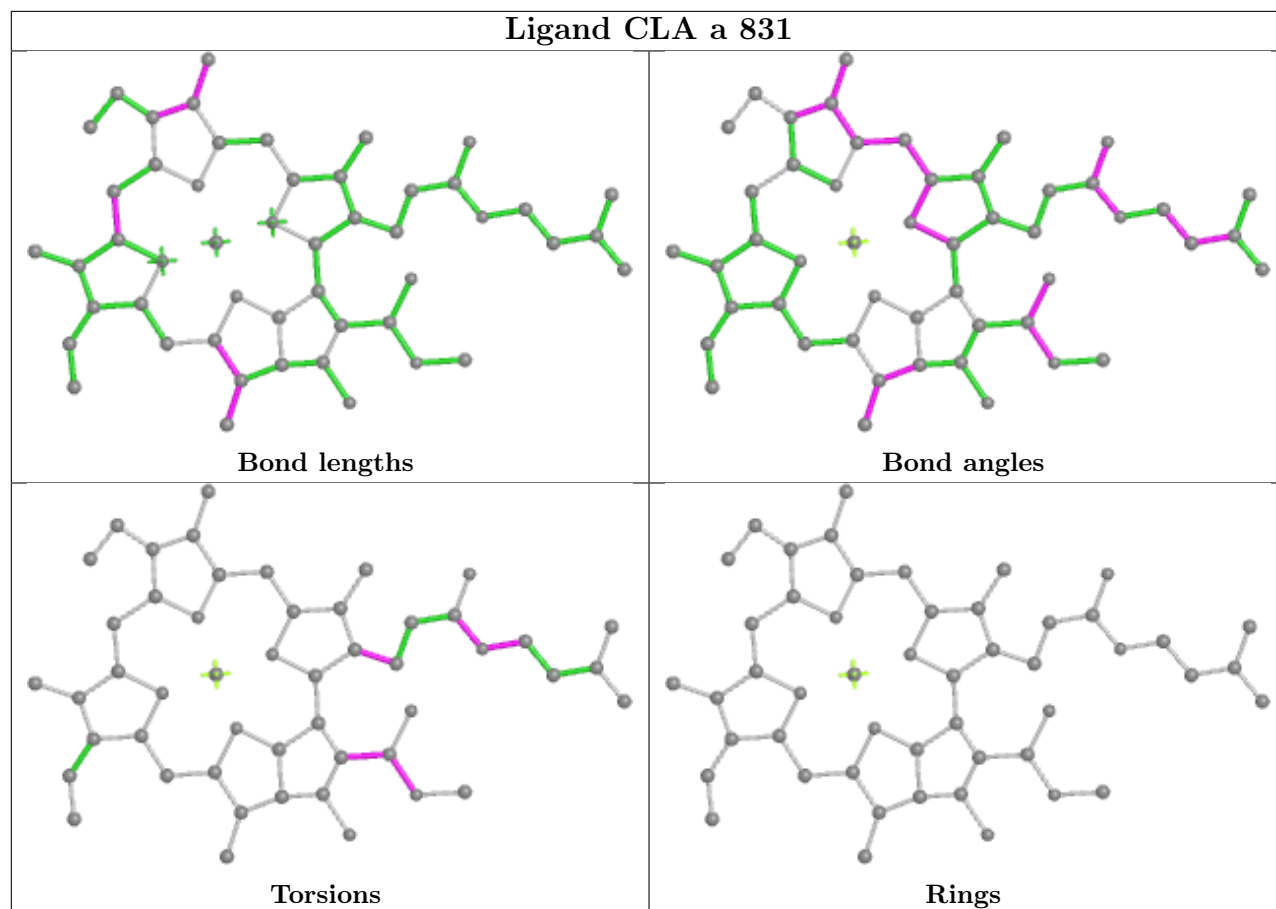
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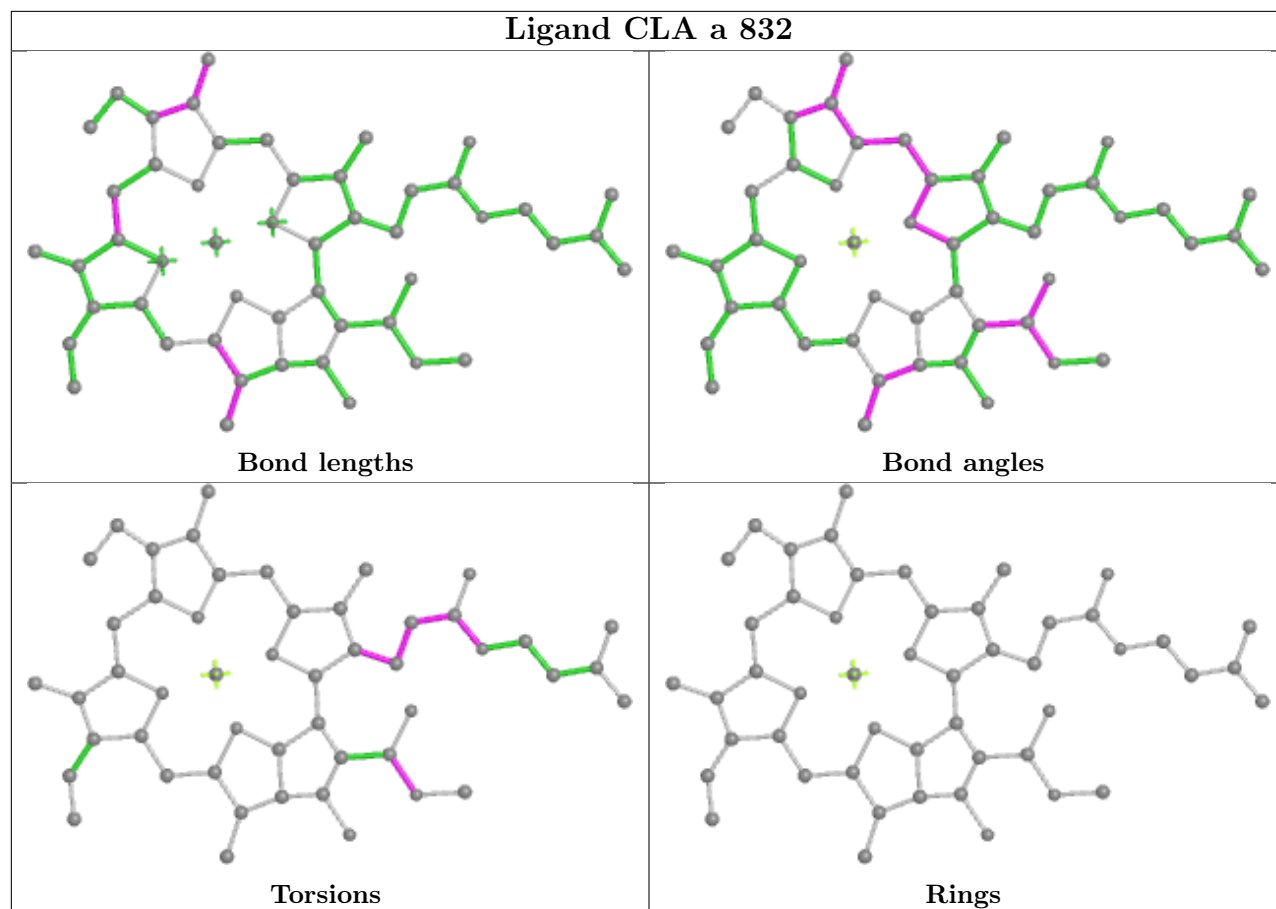
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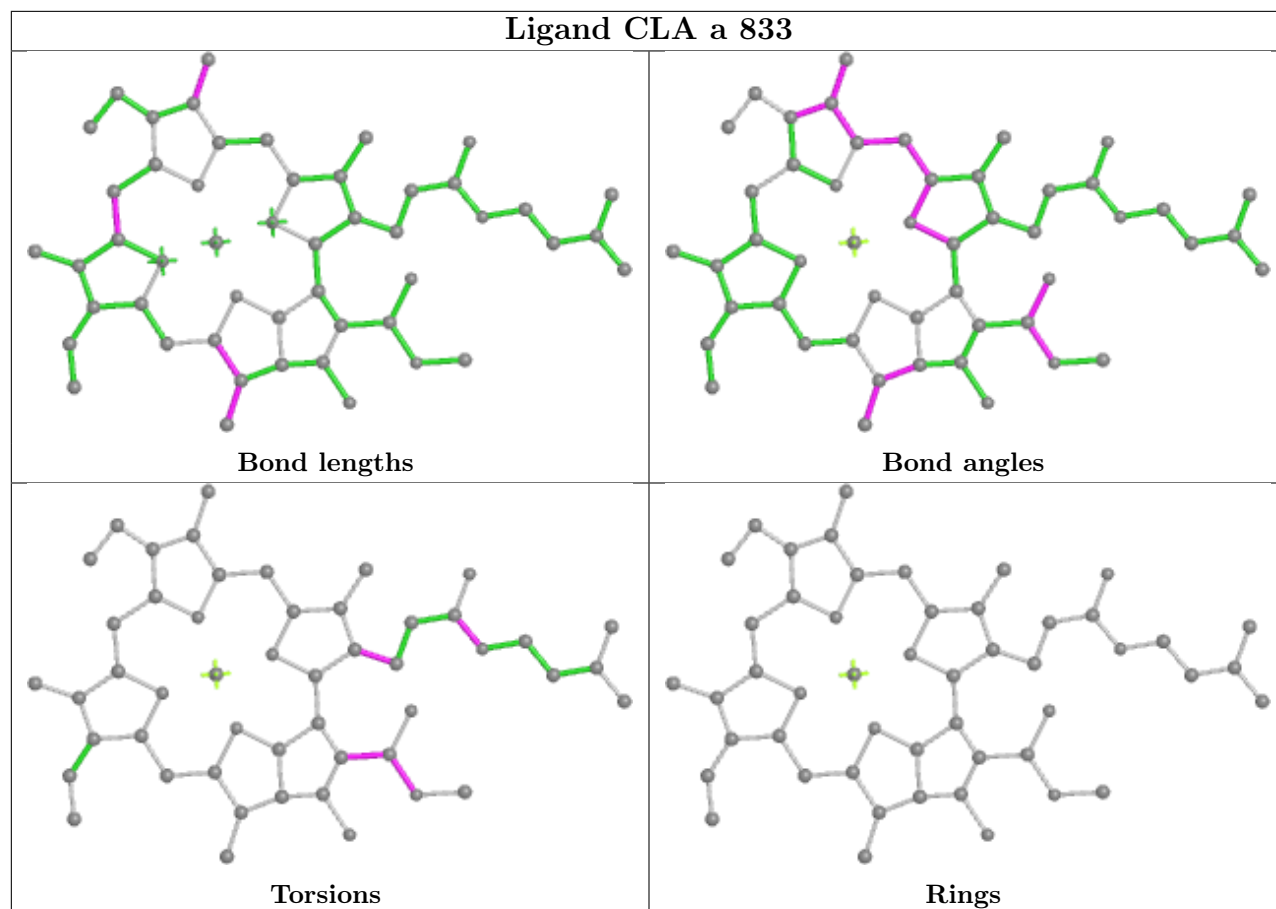
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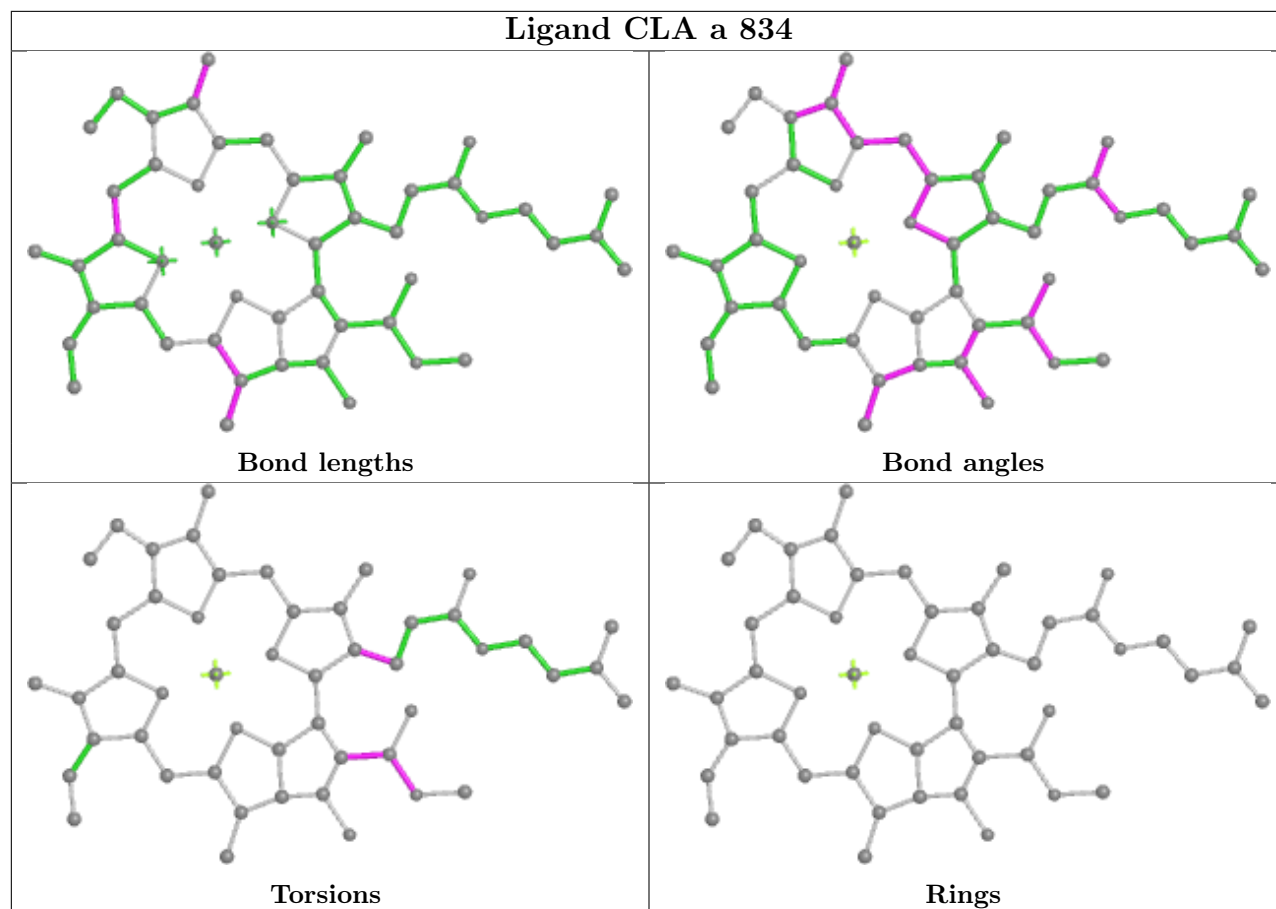
Ligand CLA a 832



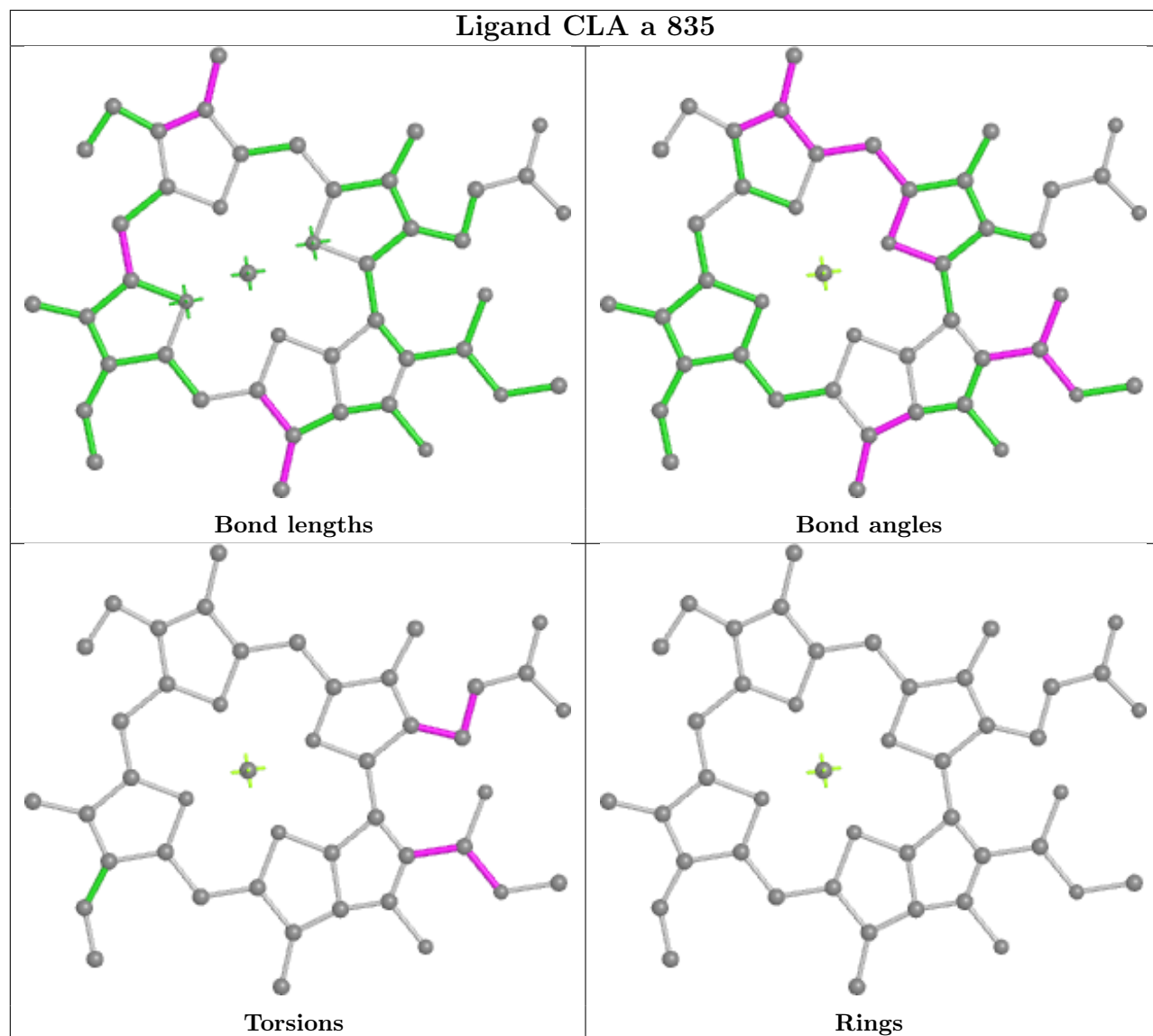
Ligand CLA a 833



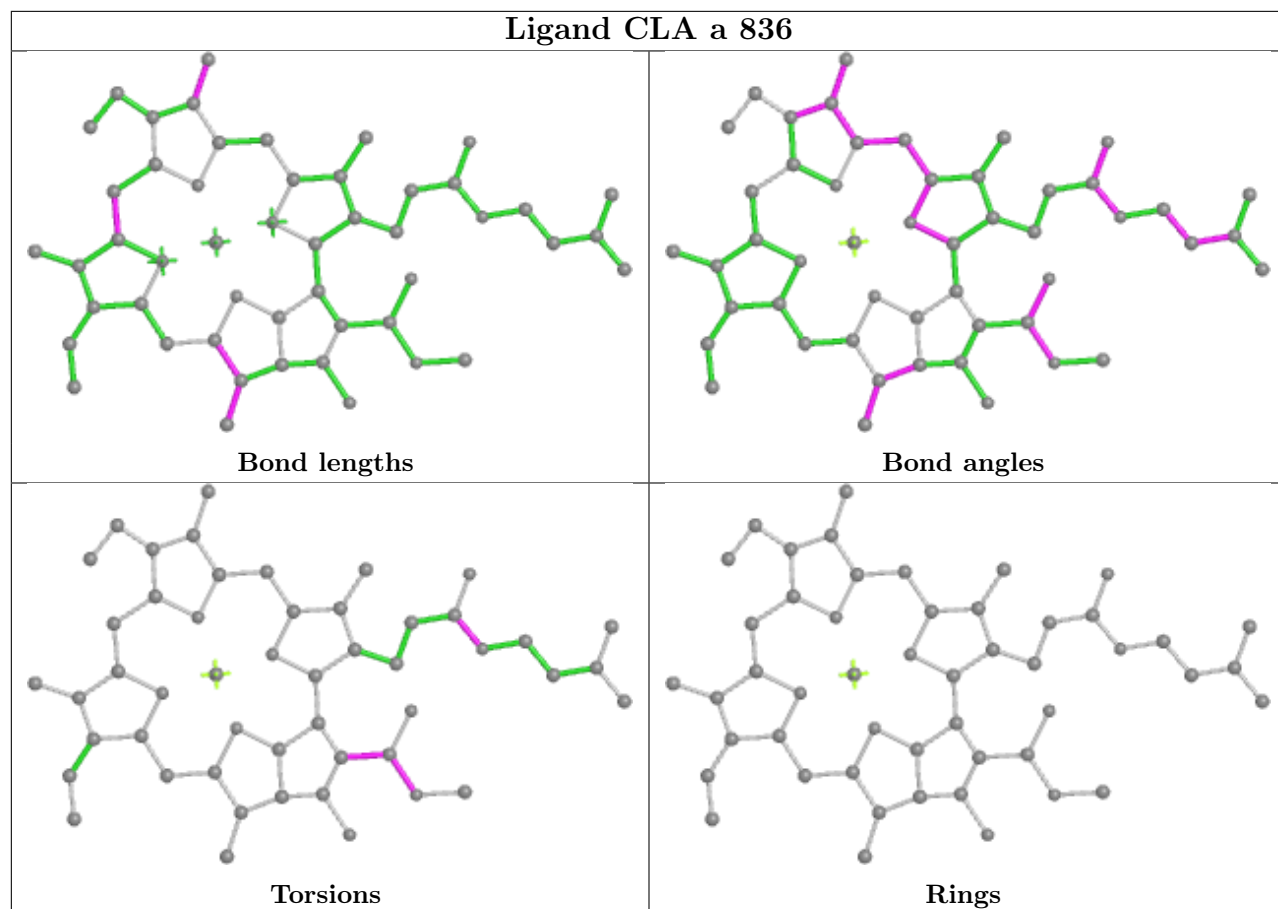
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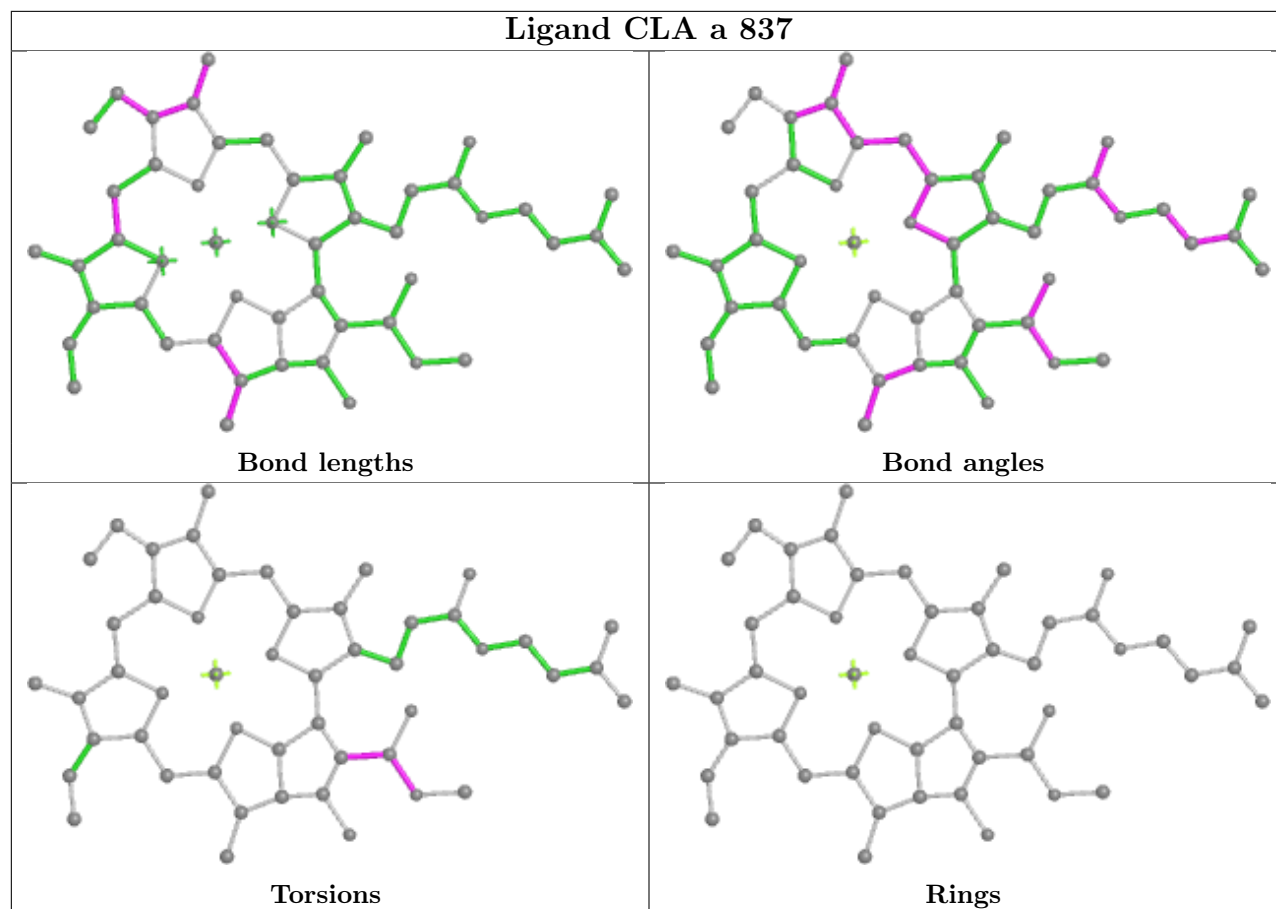


Ligand CLA a 835

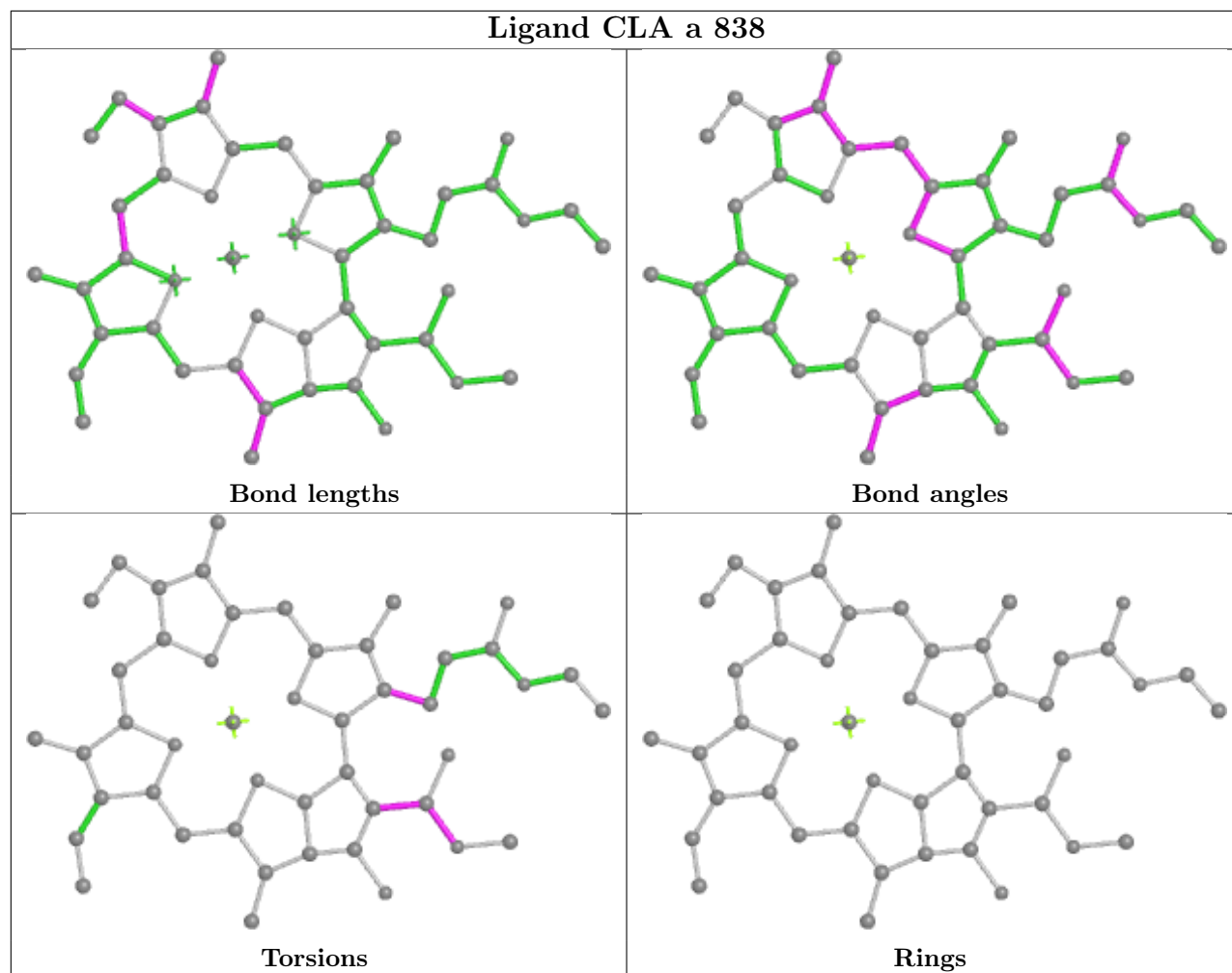


Ligand CLA a 836

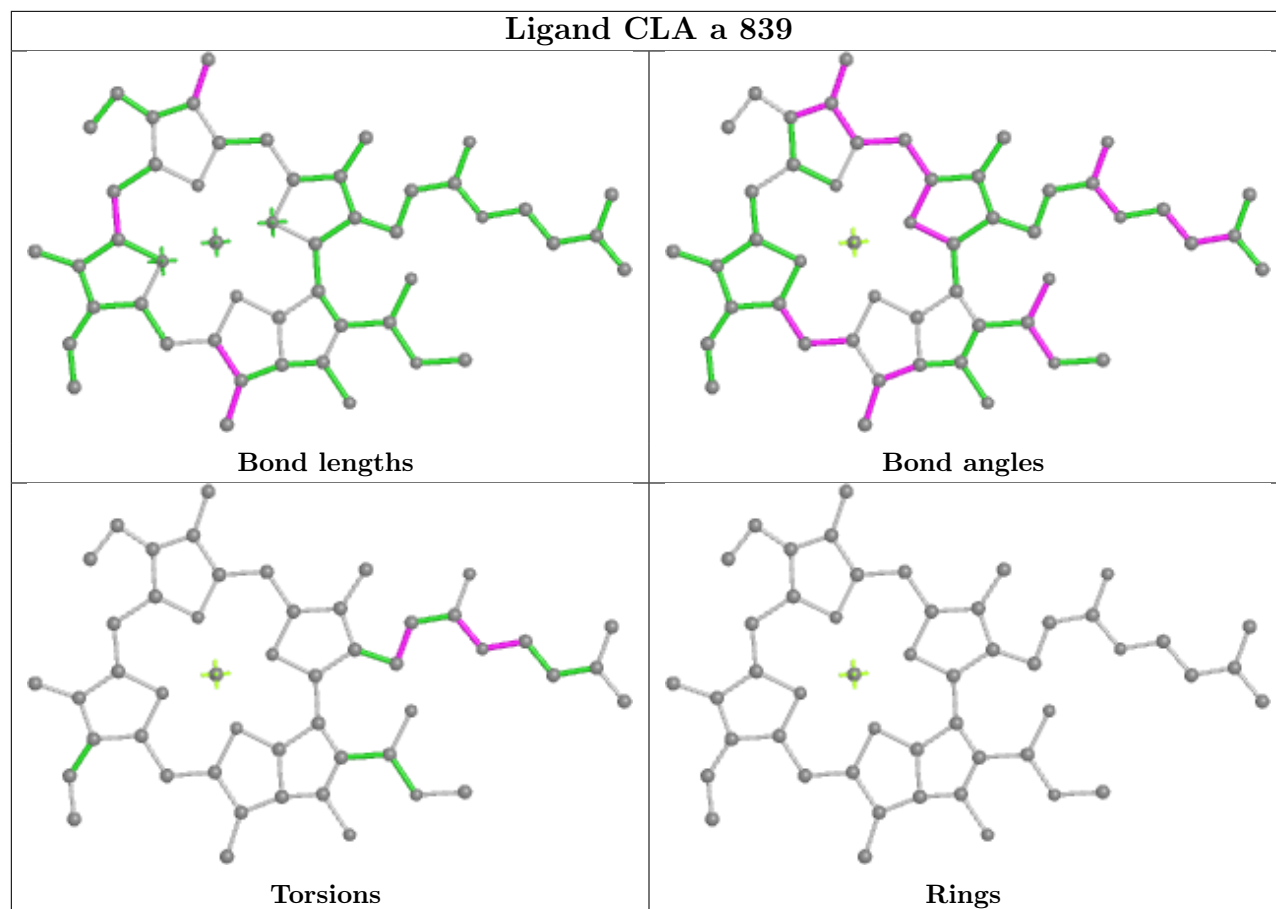




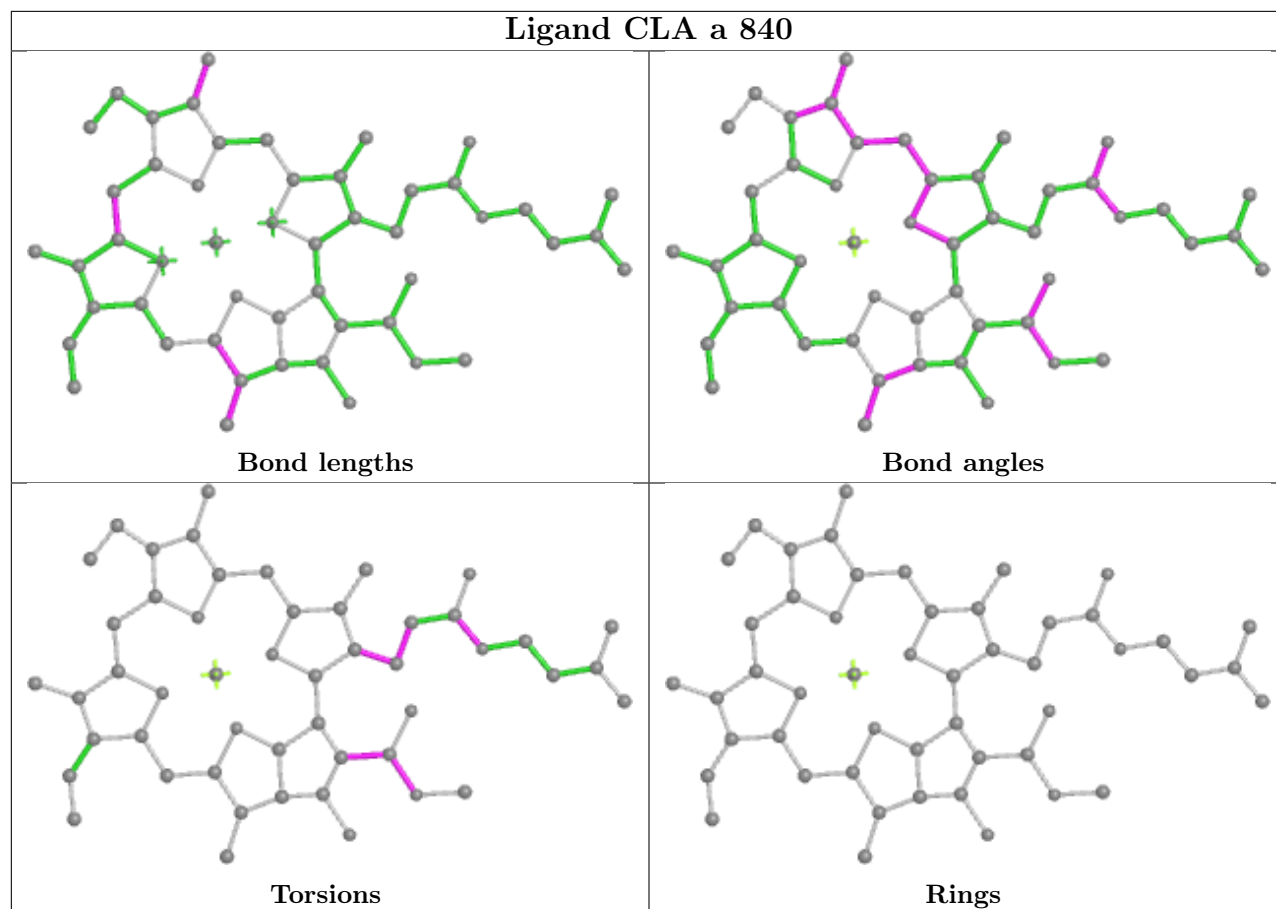
Ligand CLA a 838



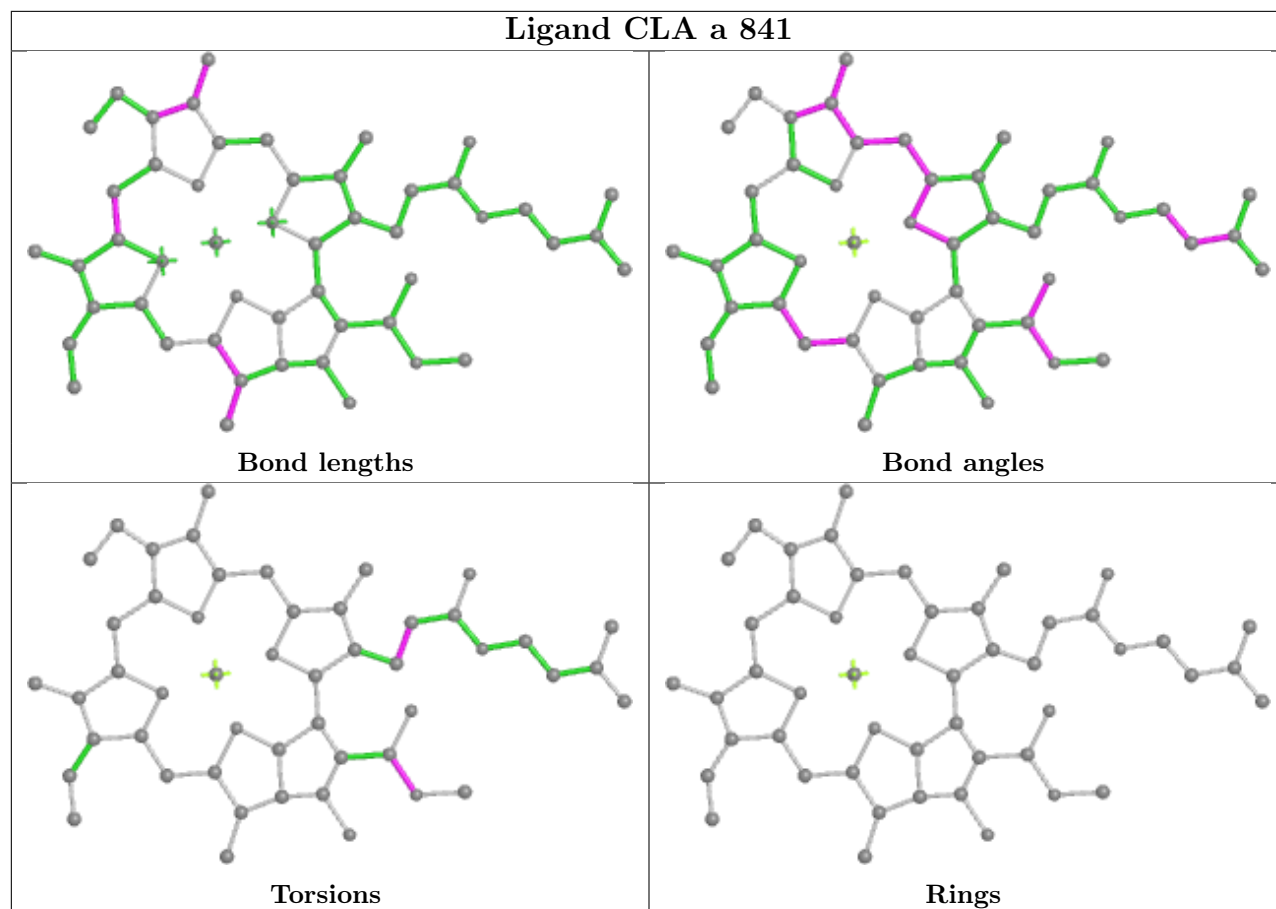
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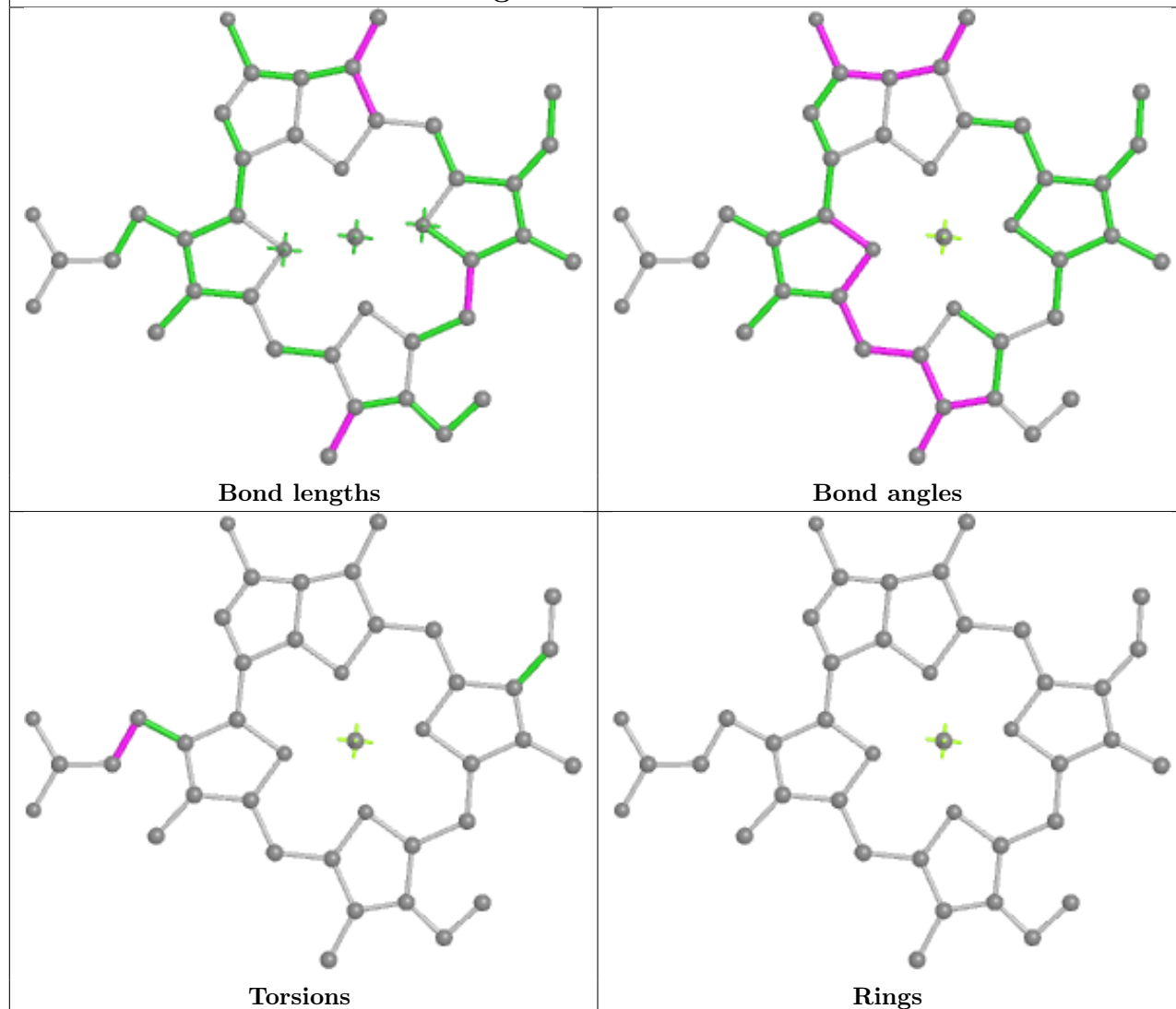
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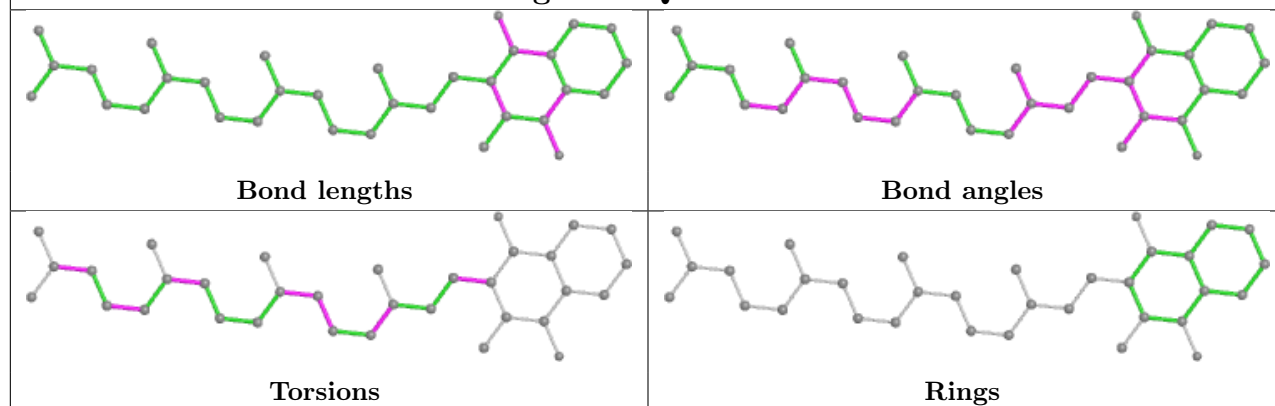
Ligand CLA a 841

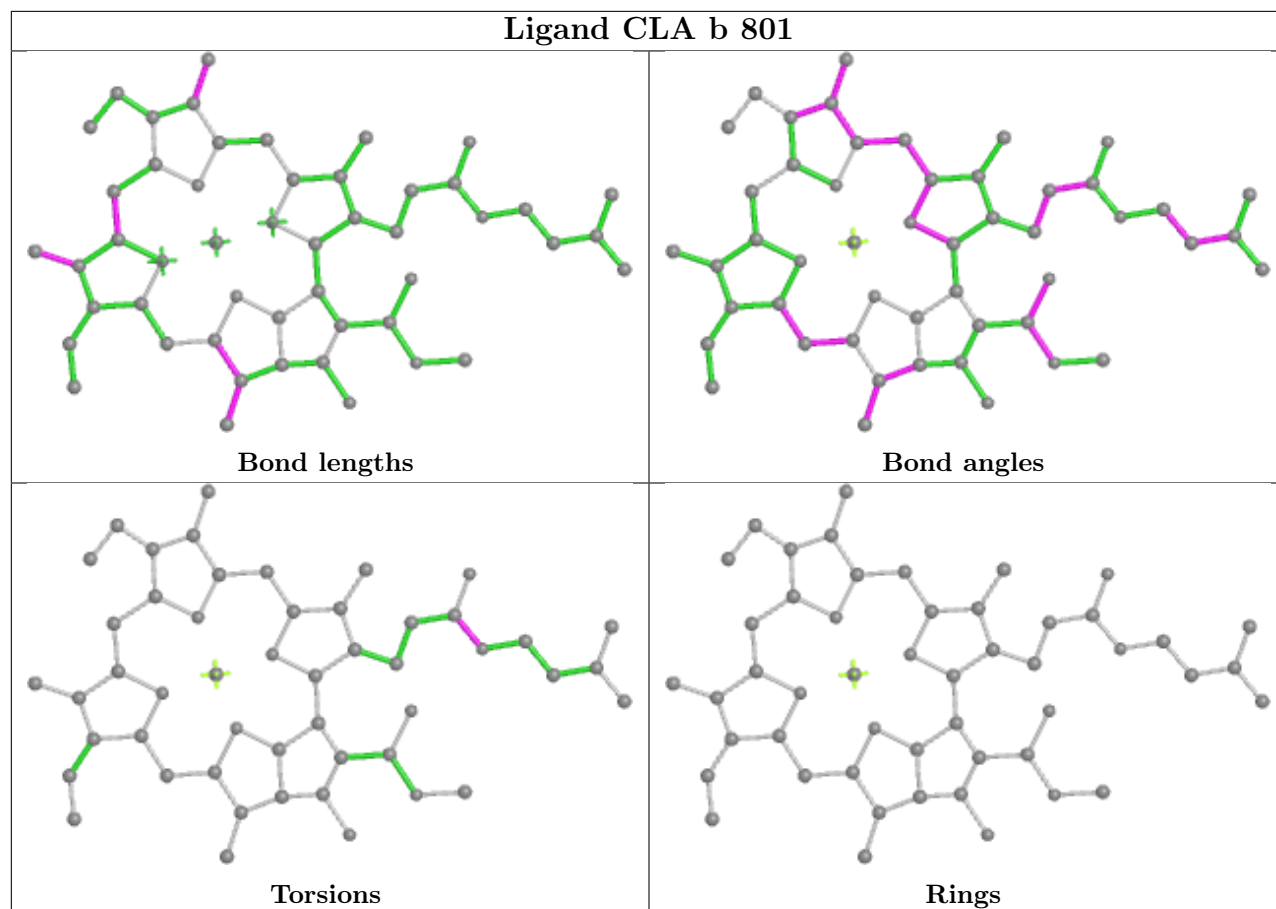


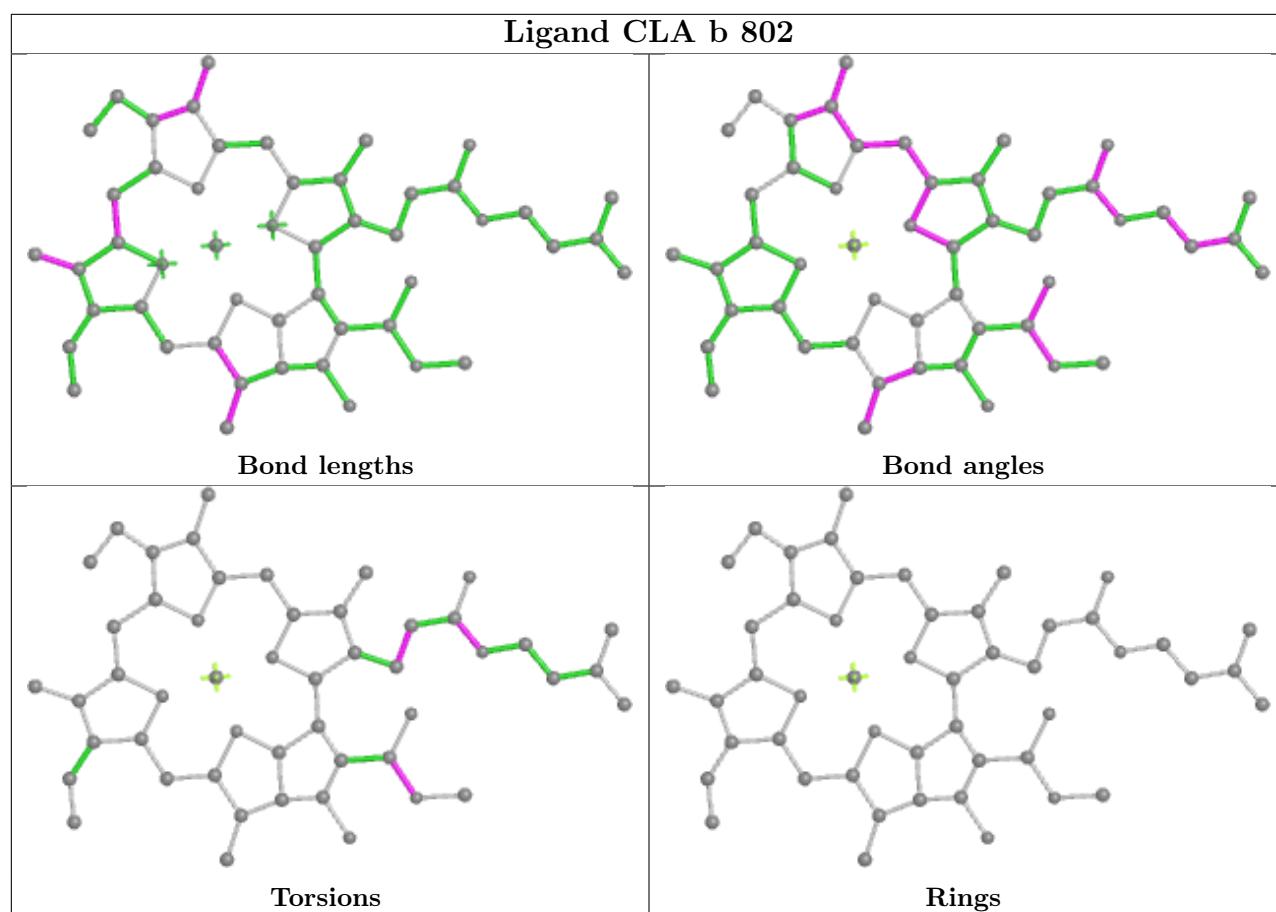
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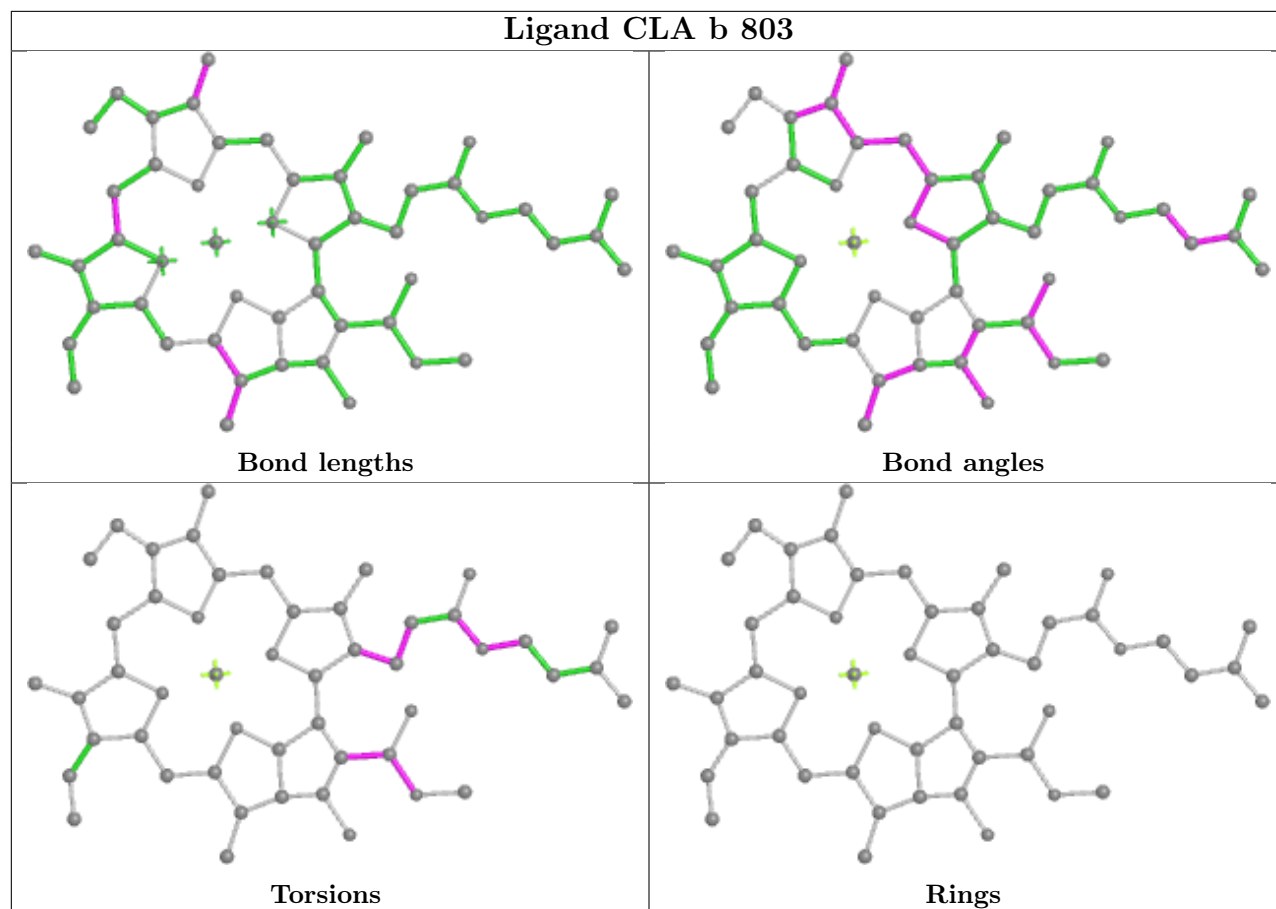
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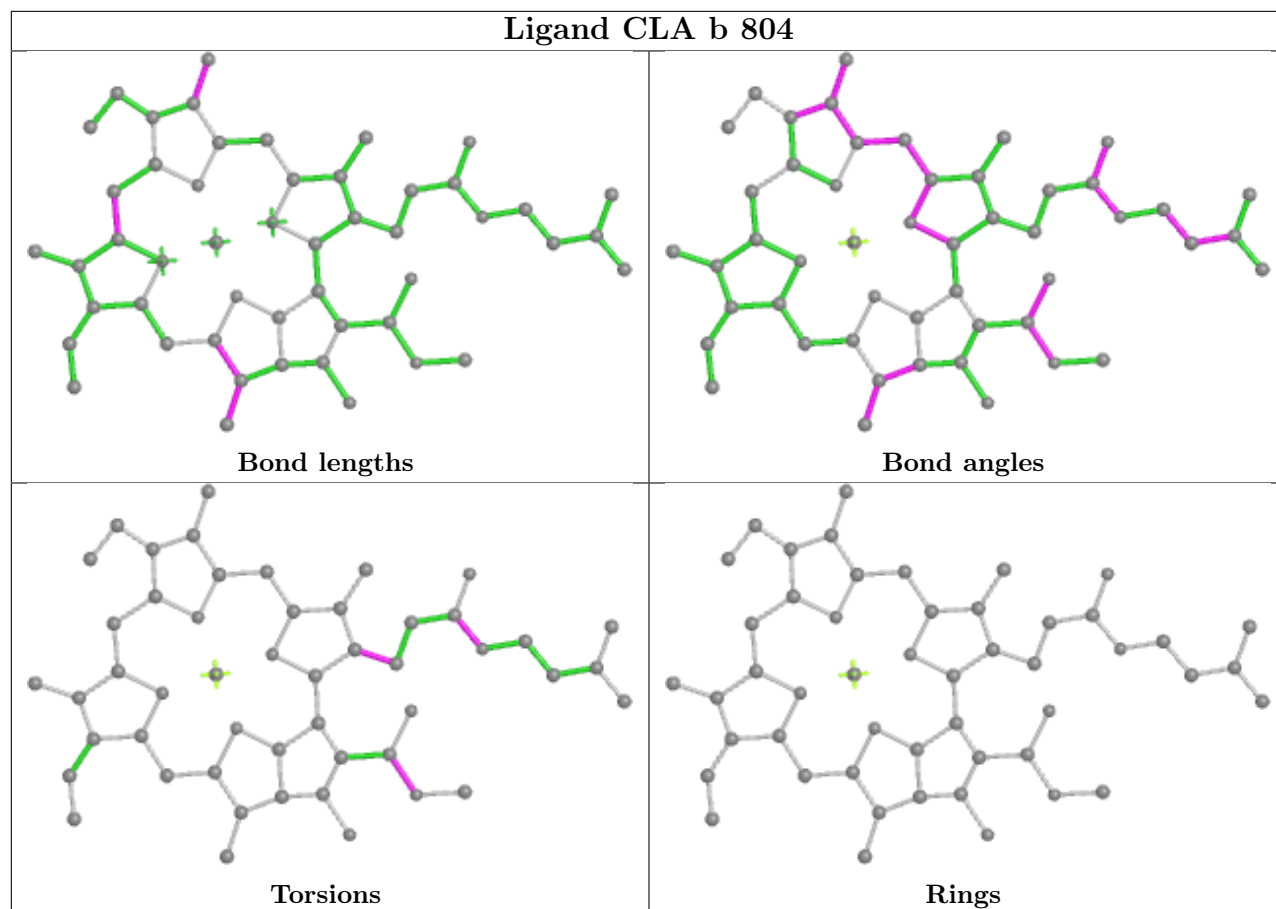


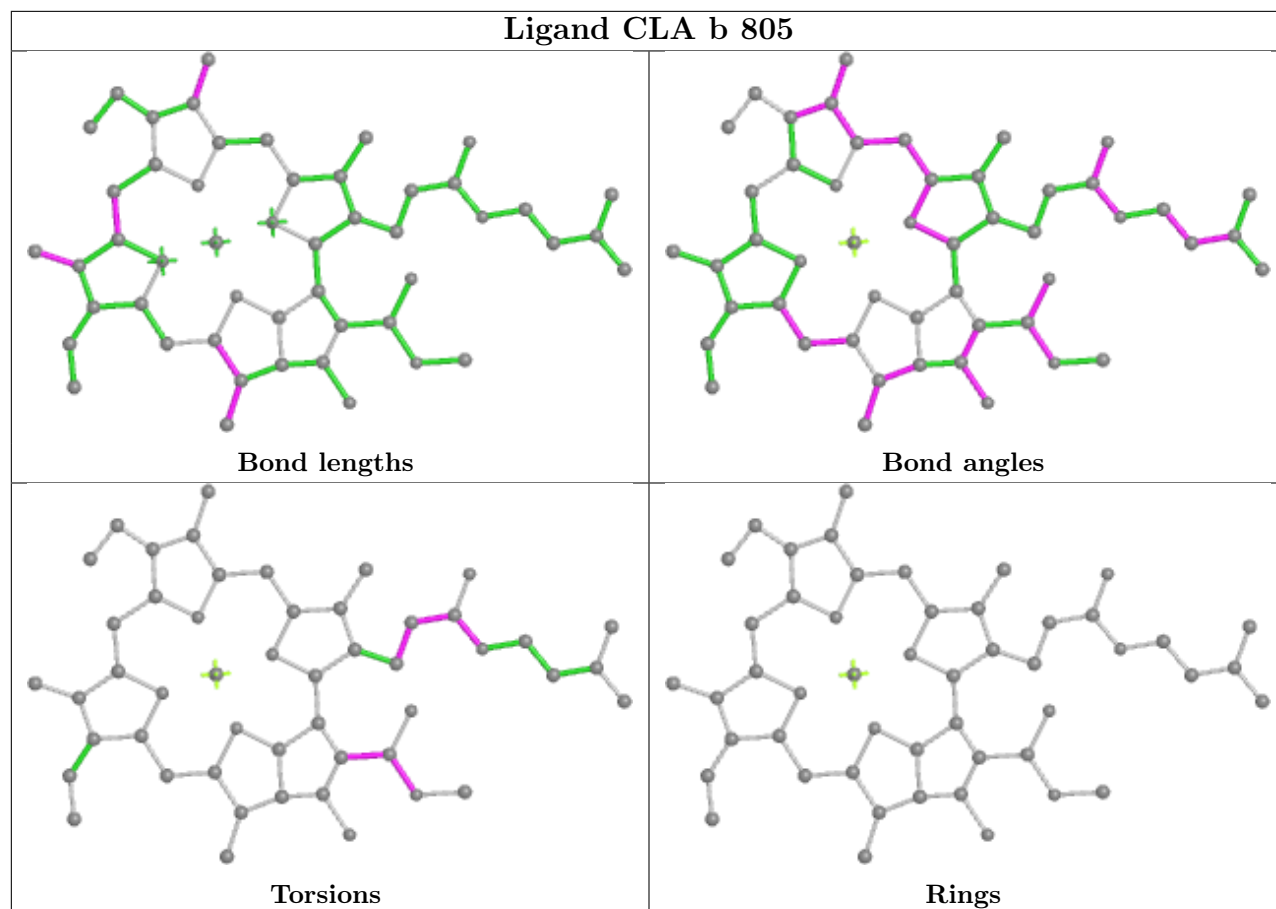




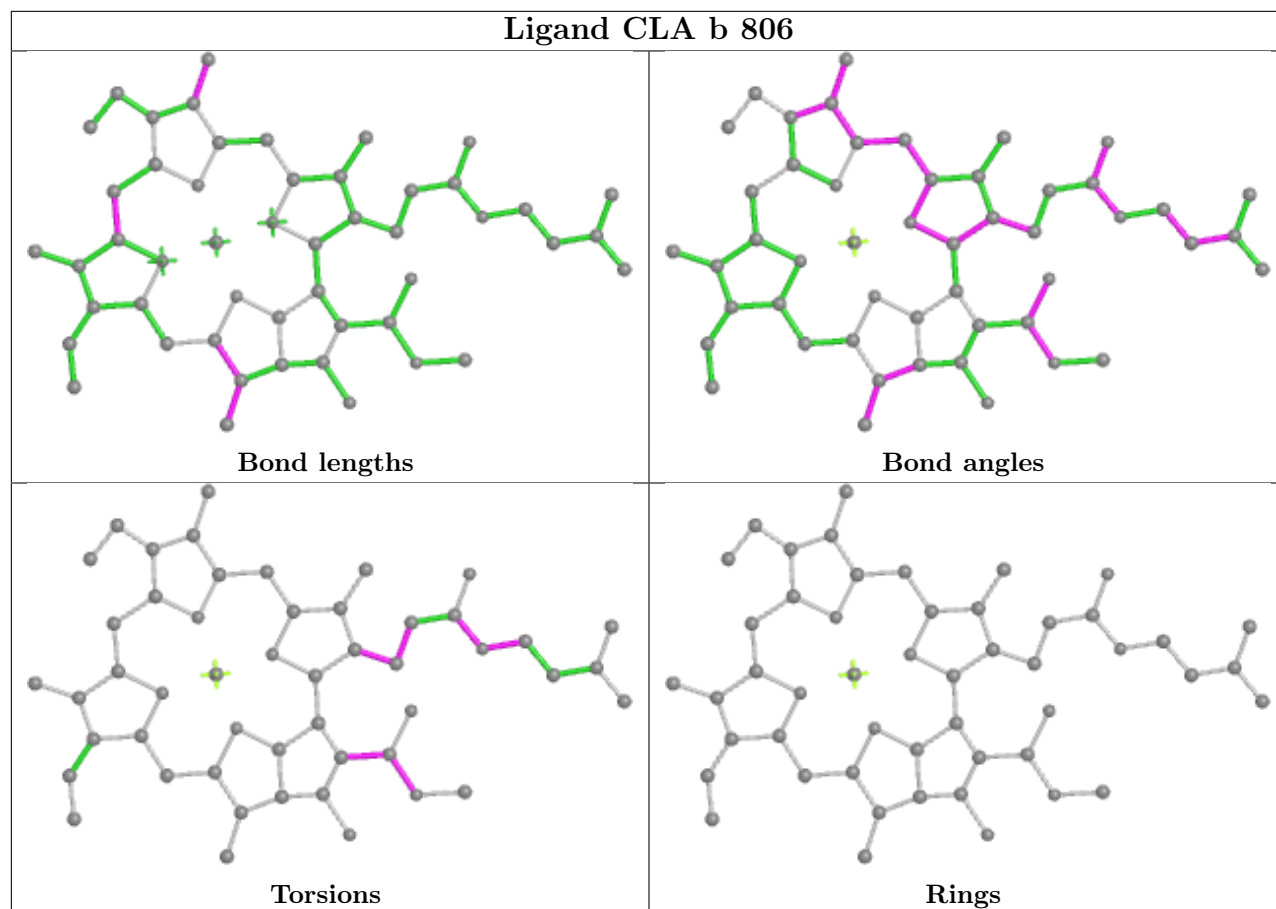
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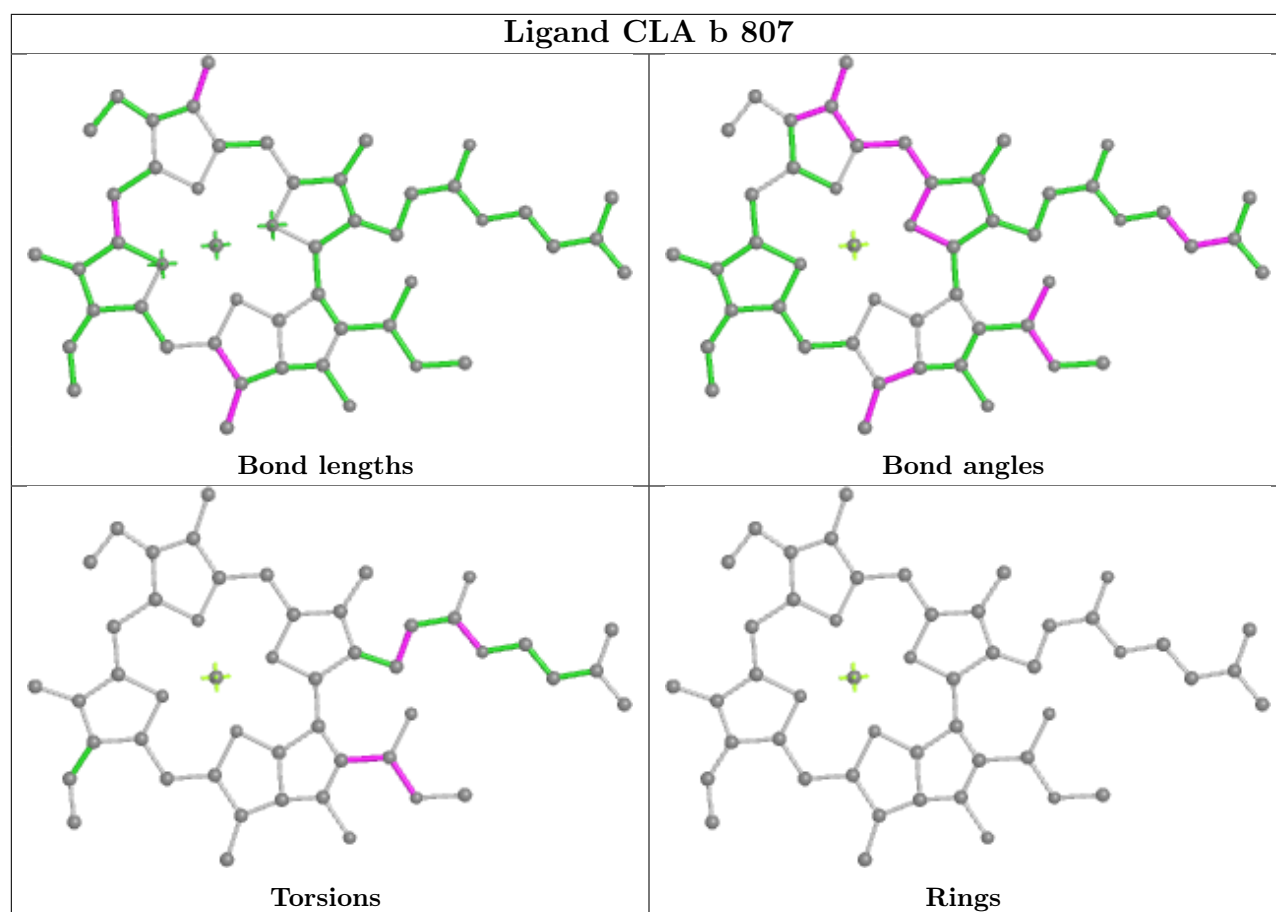




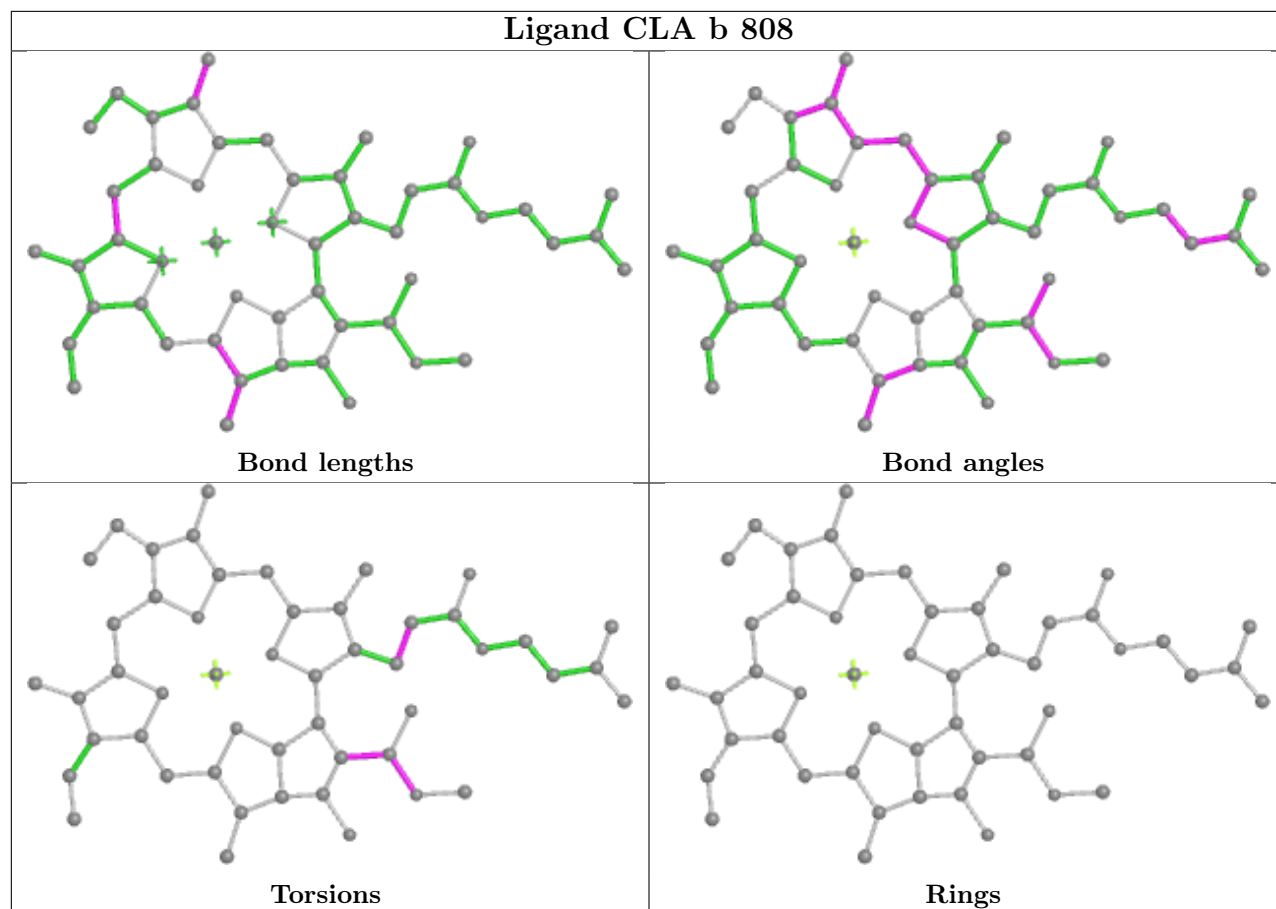


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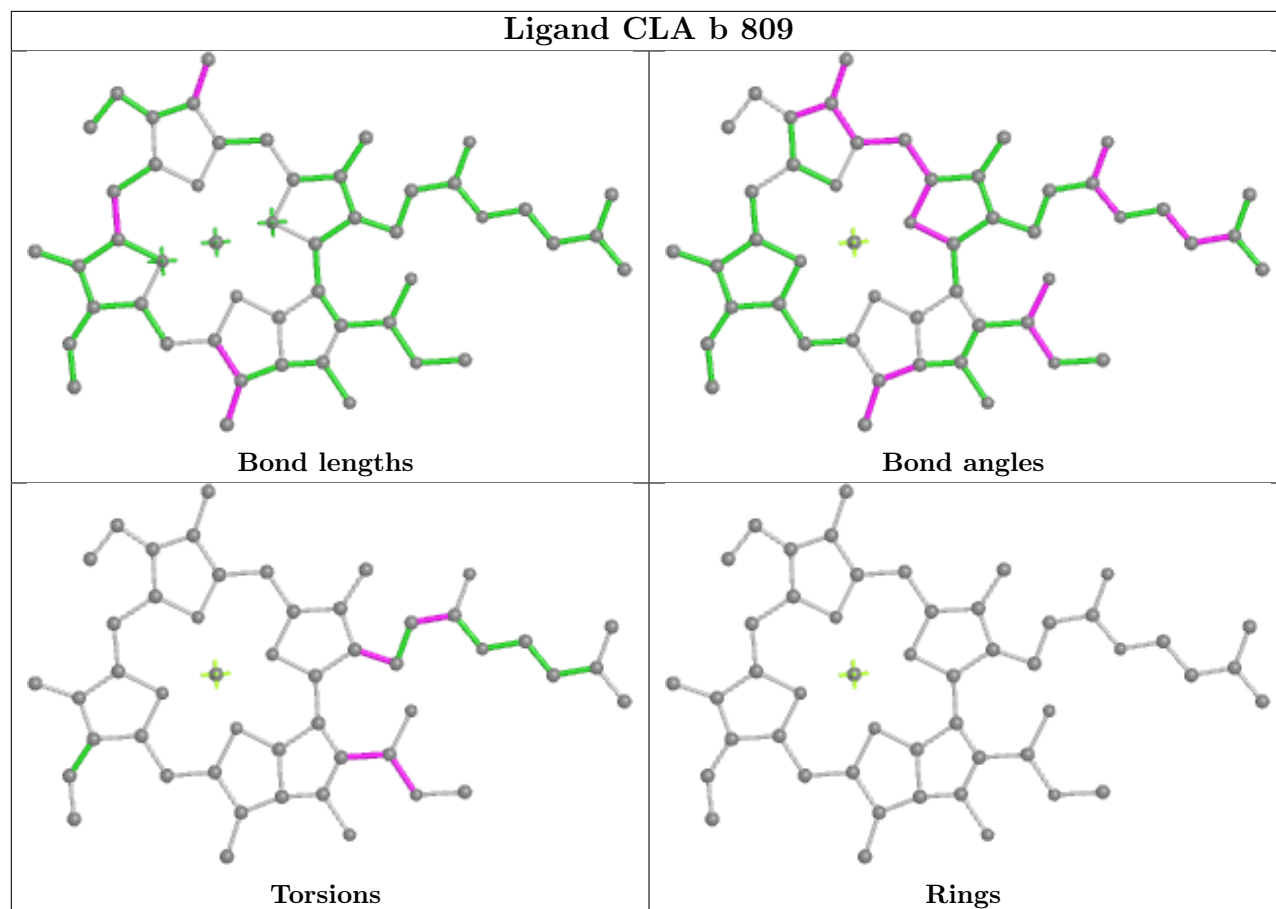




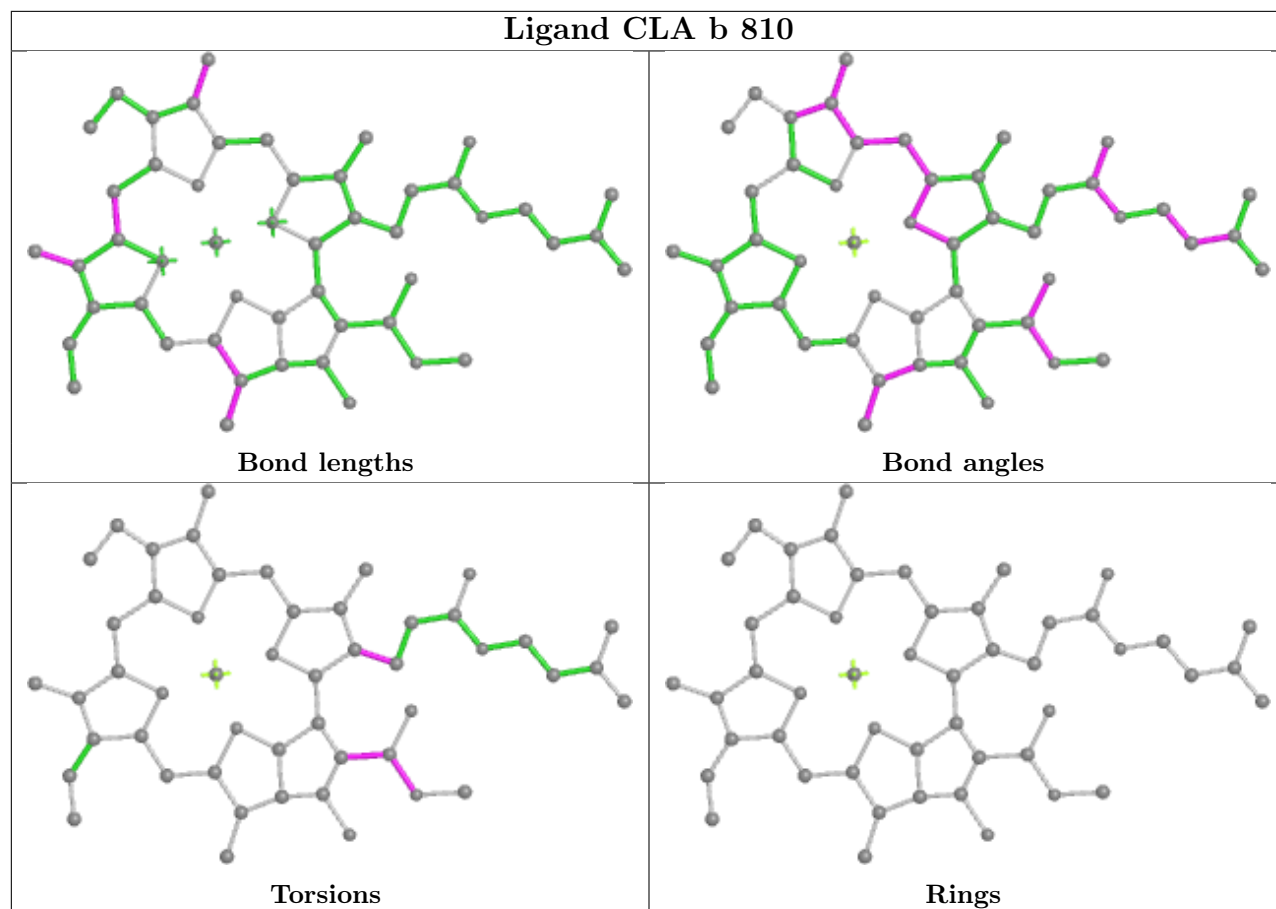
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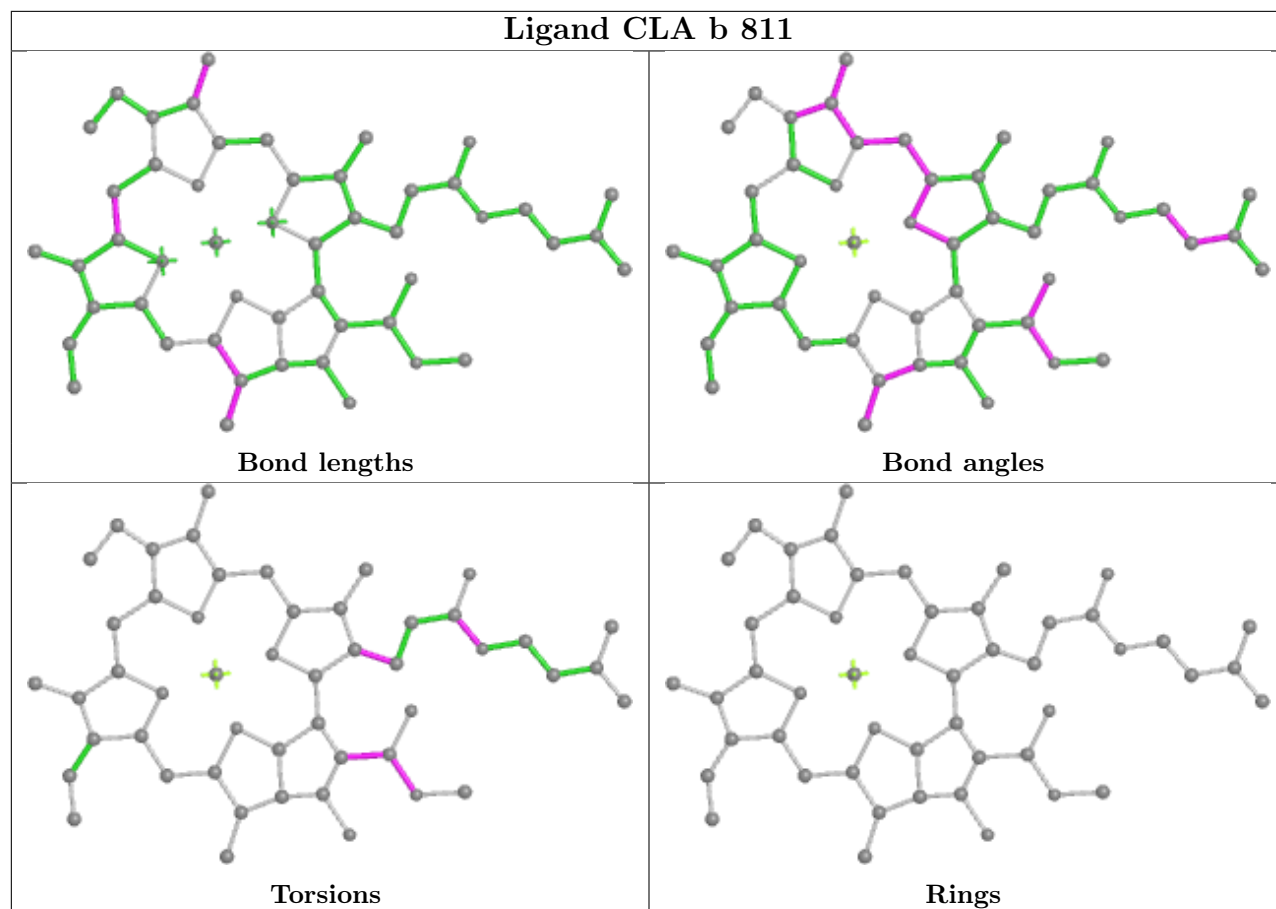
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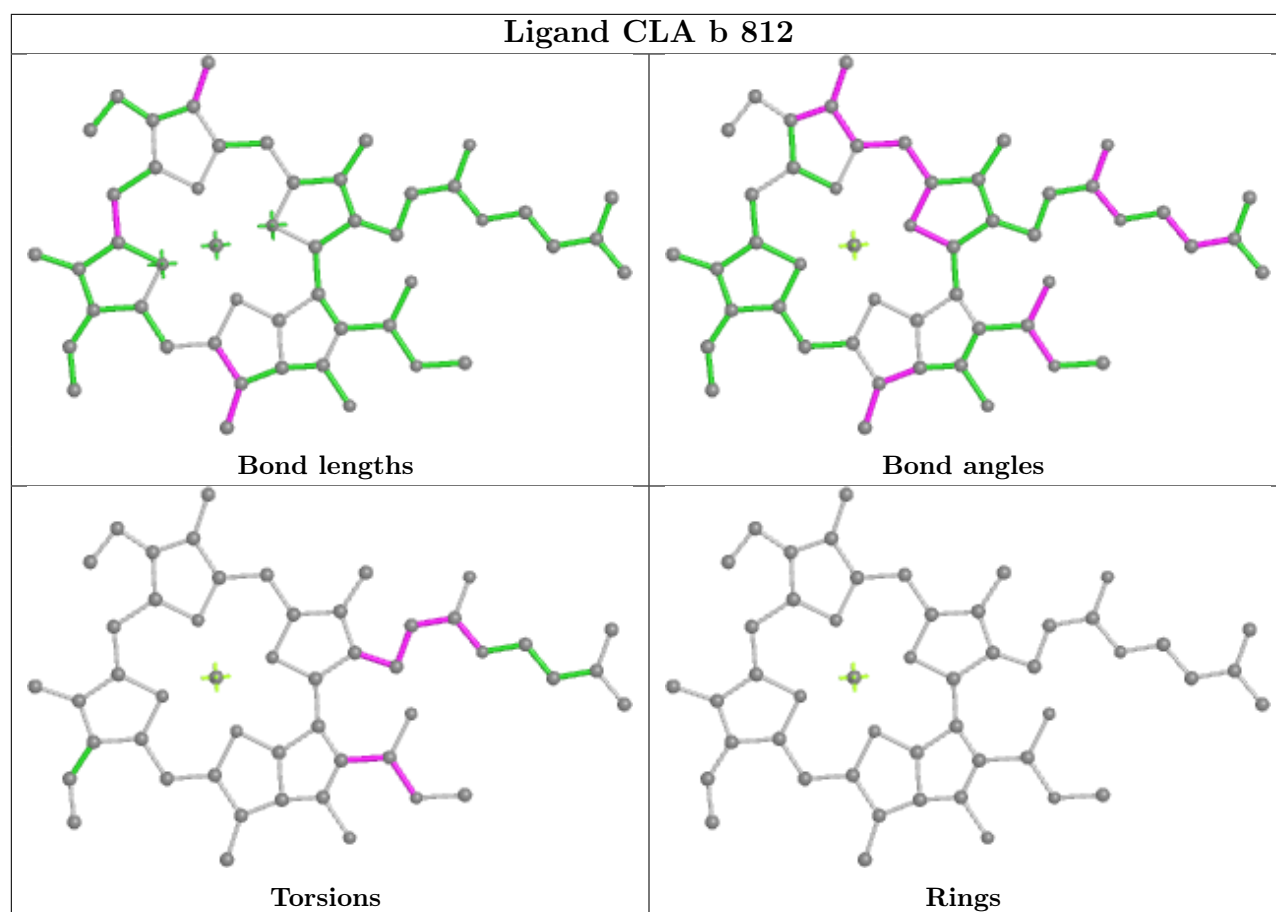


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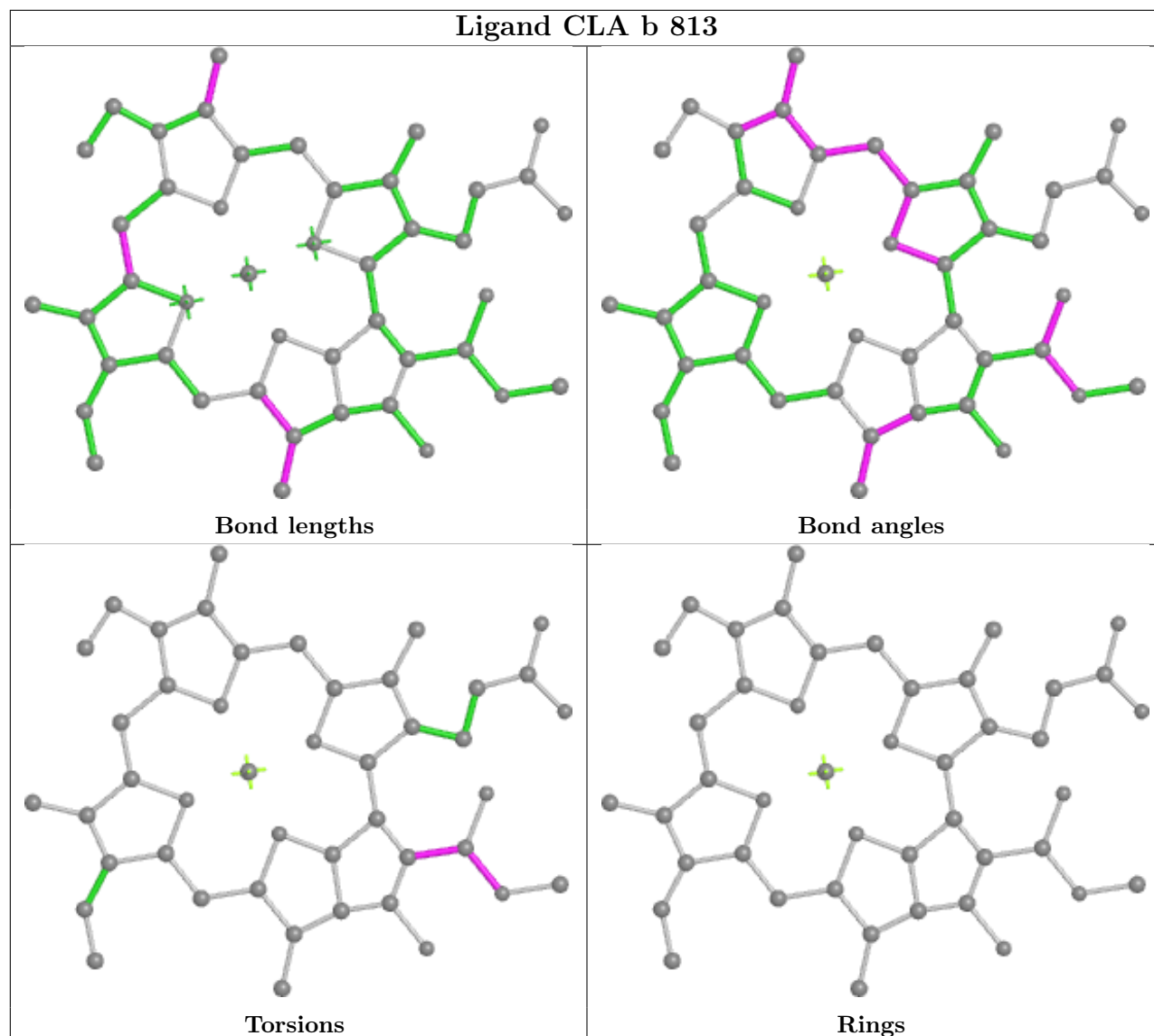


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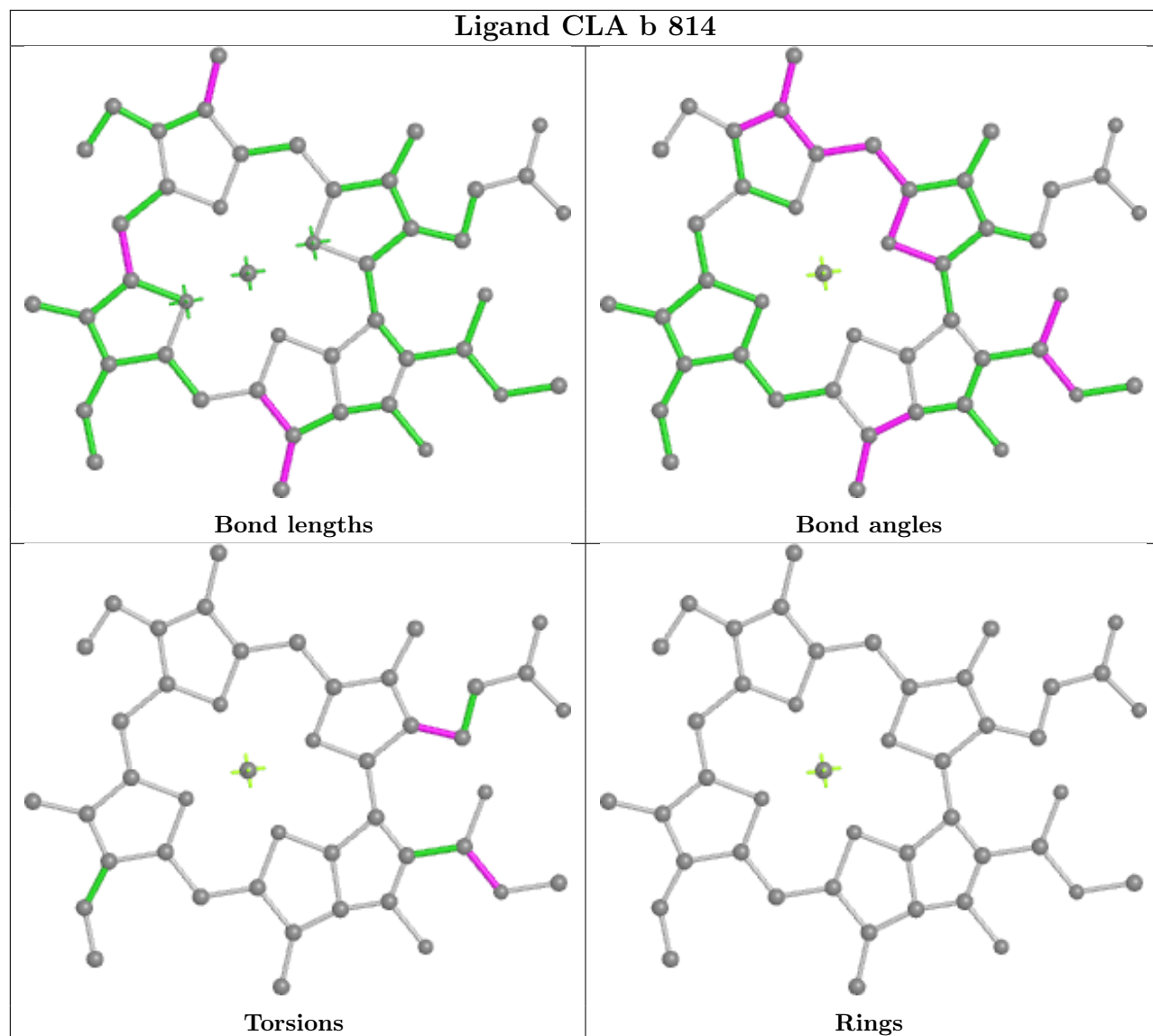


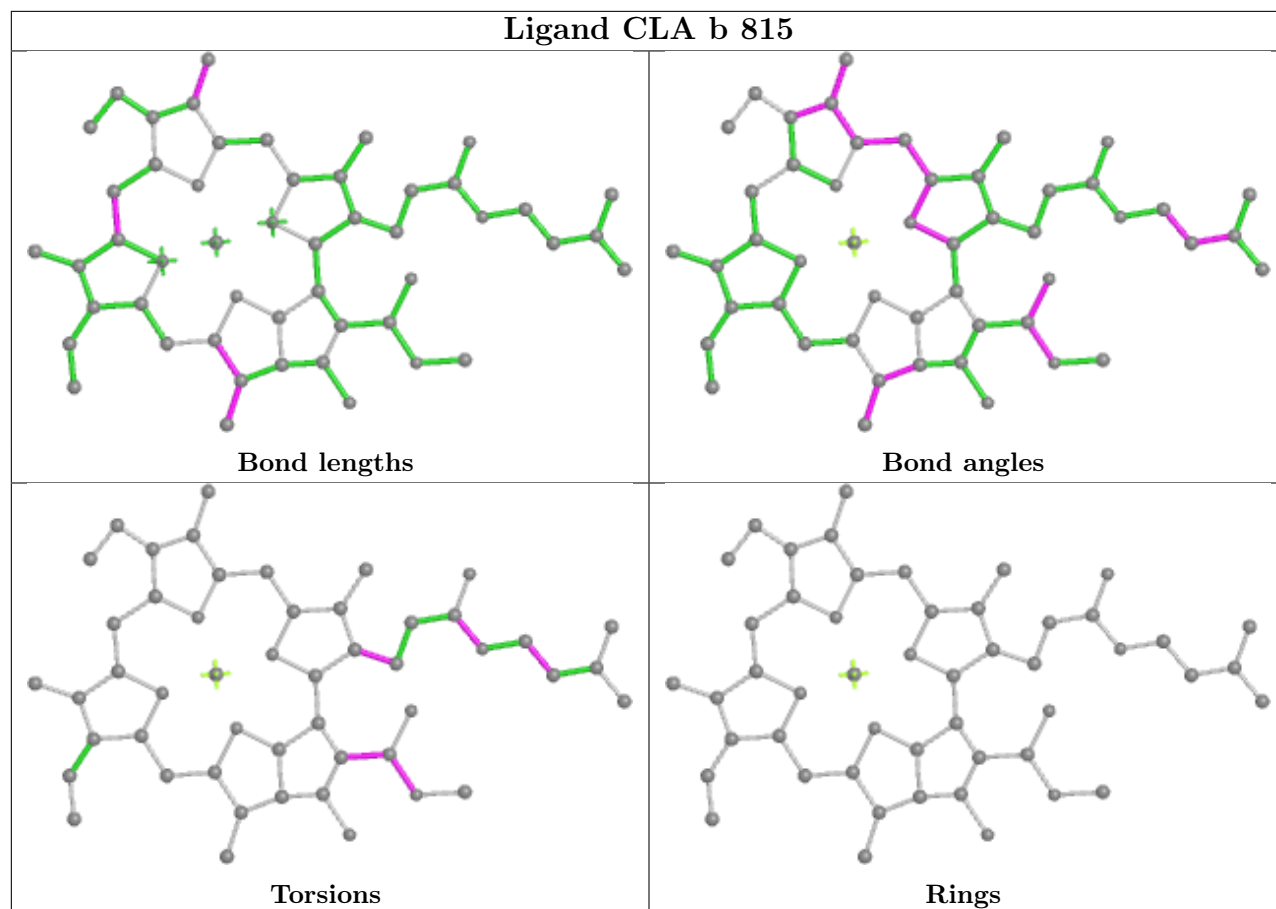


Ligand CLA b 813

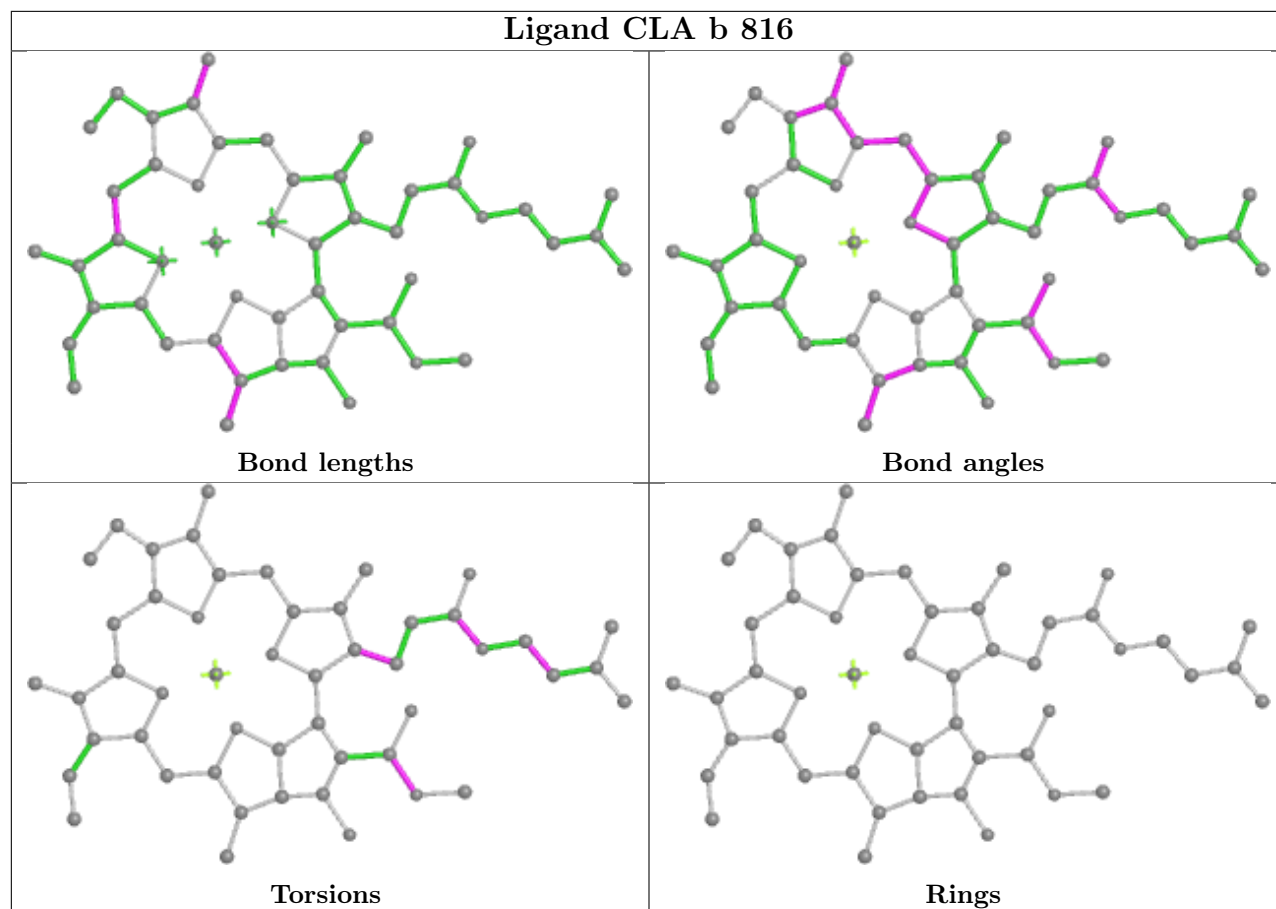


Ligand CLA b 814

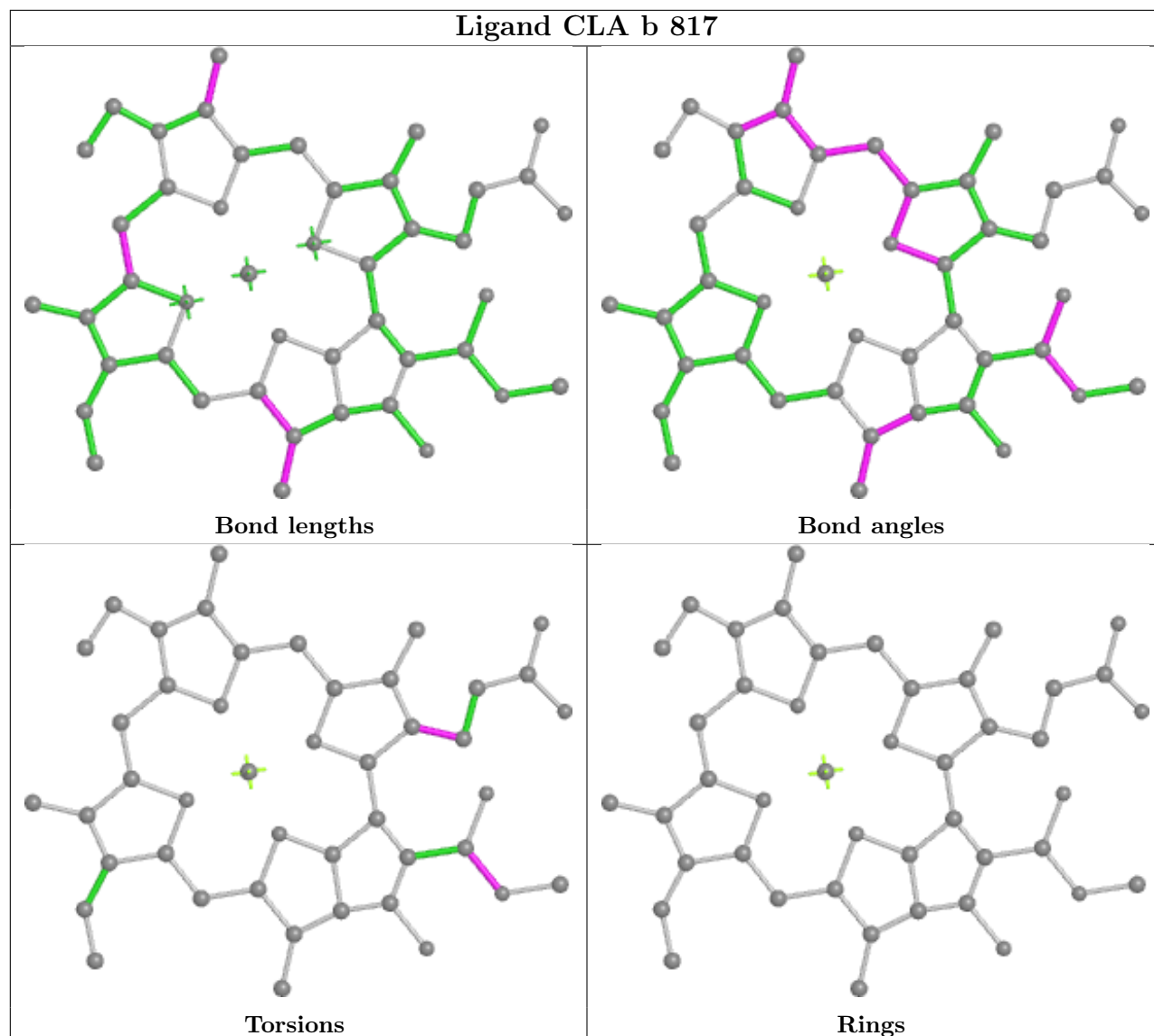


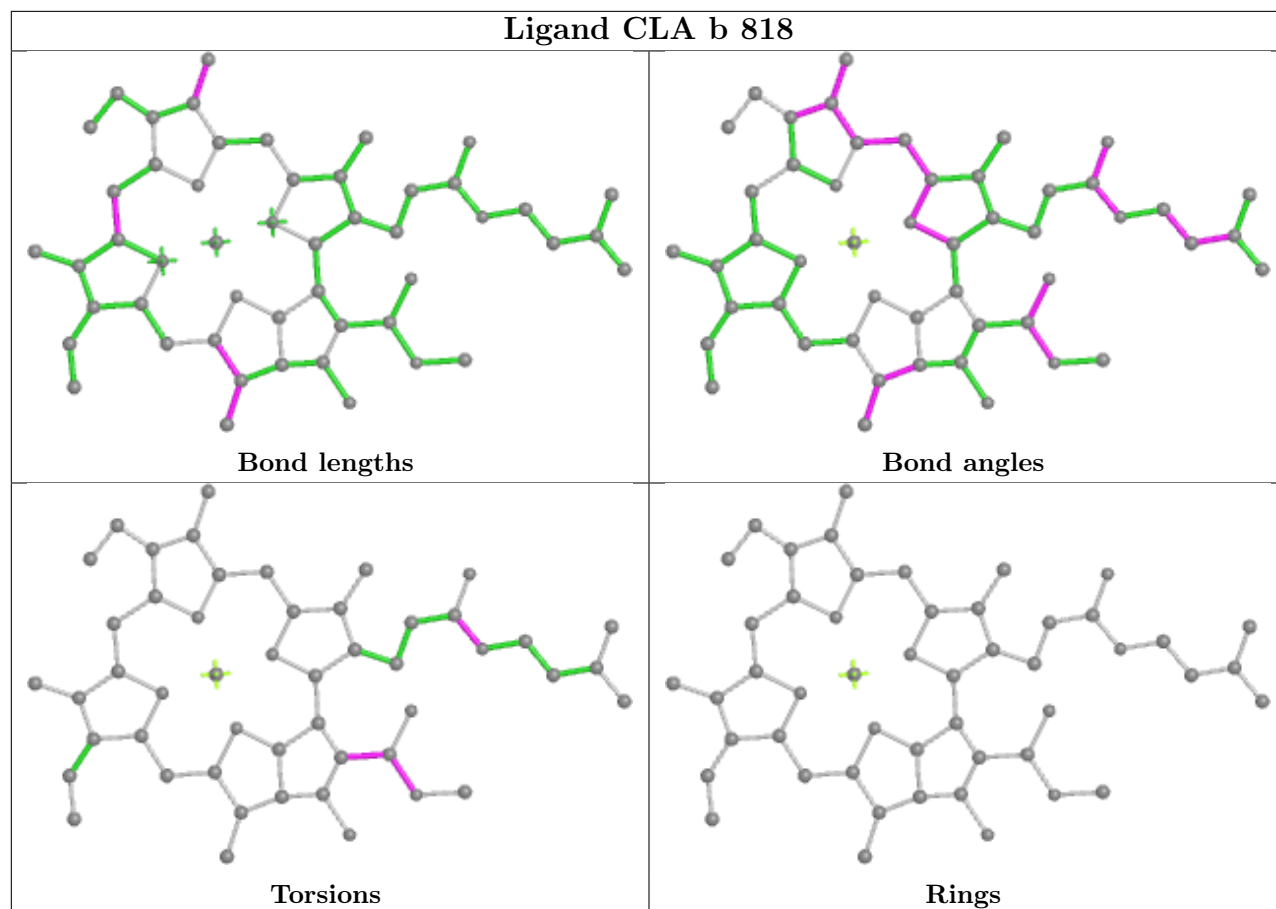


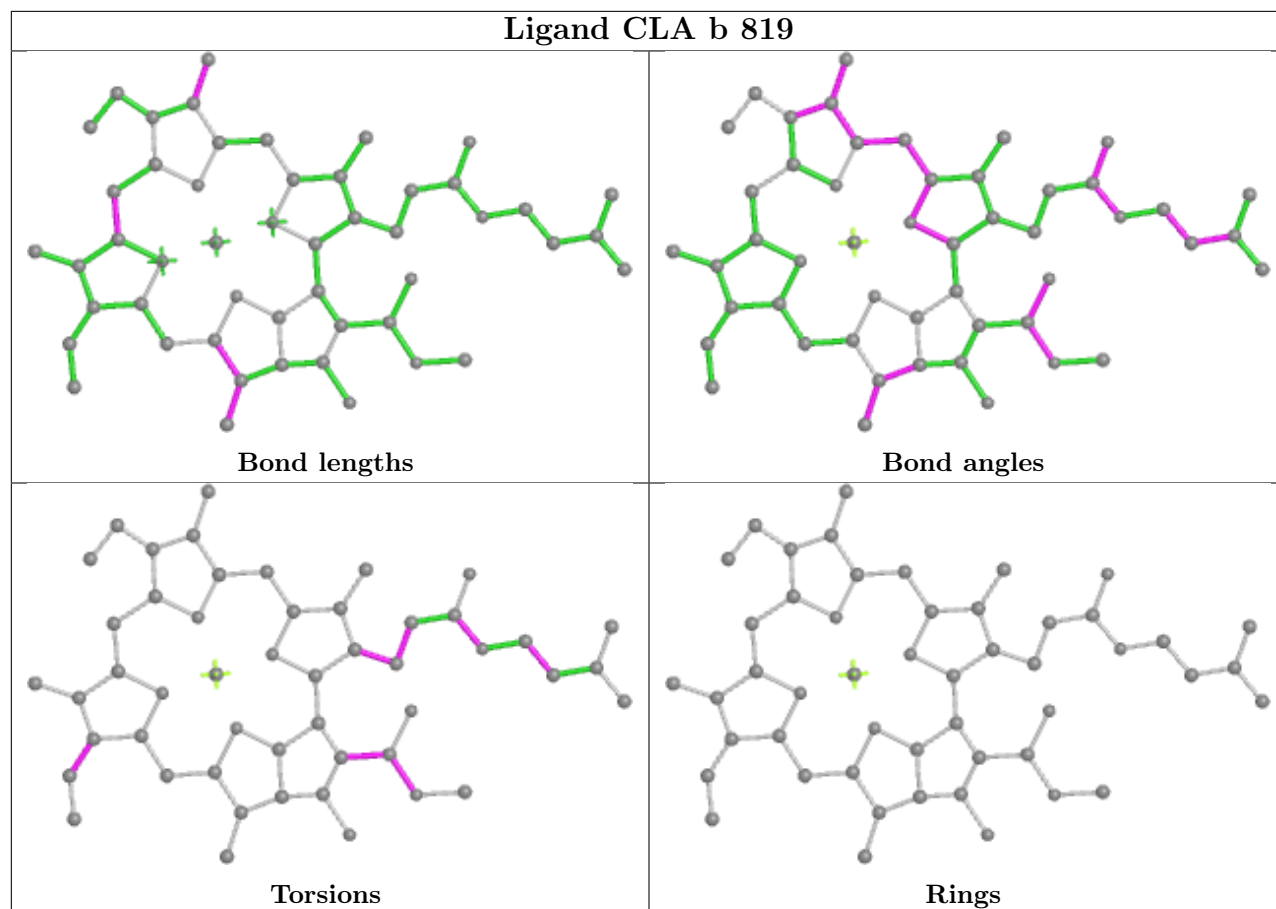
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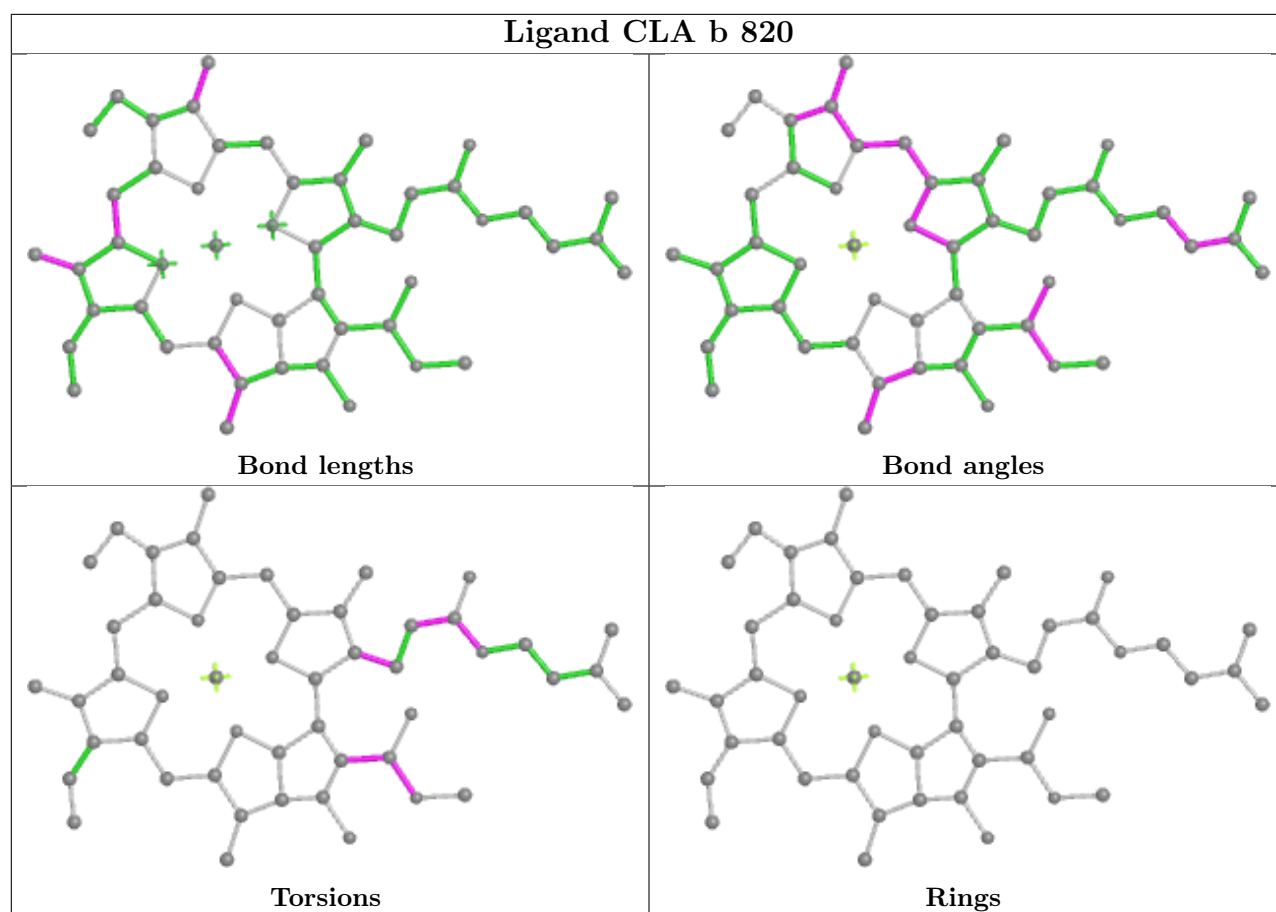


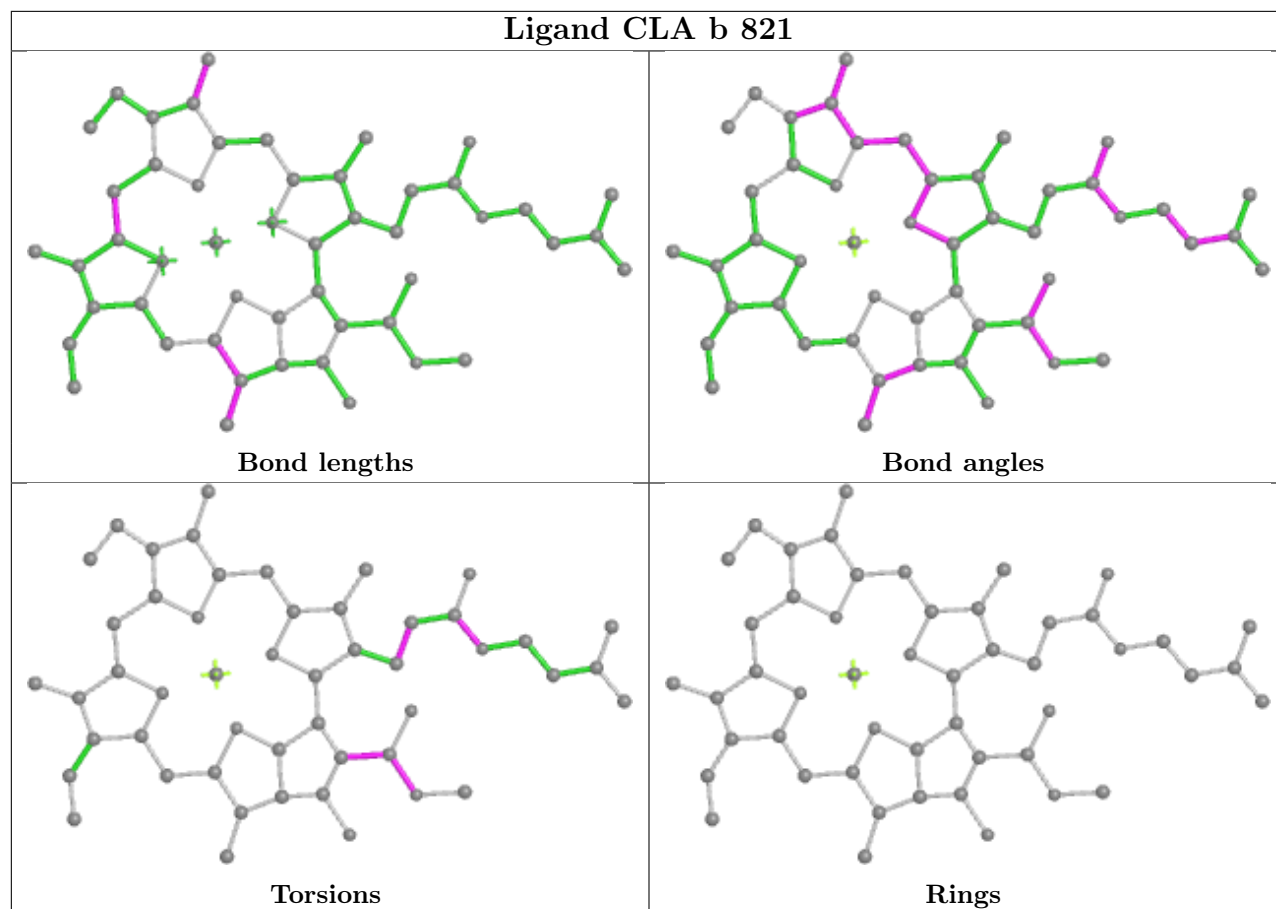
Ligand CLA b 817



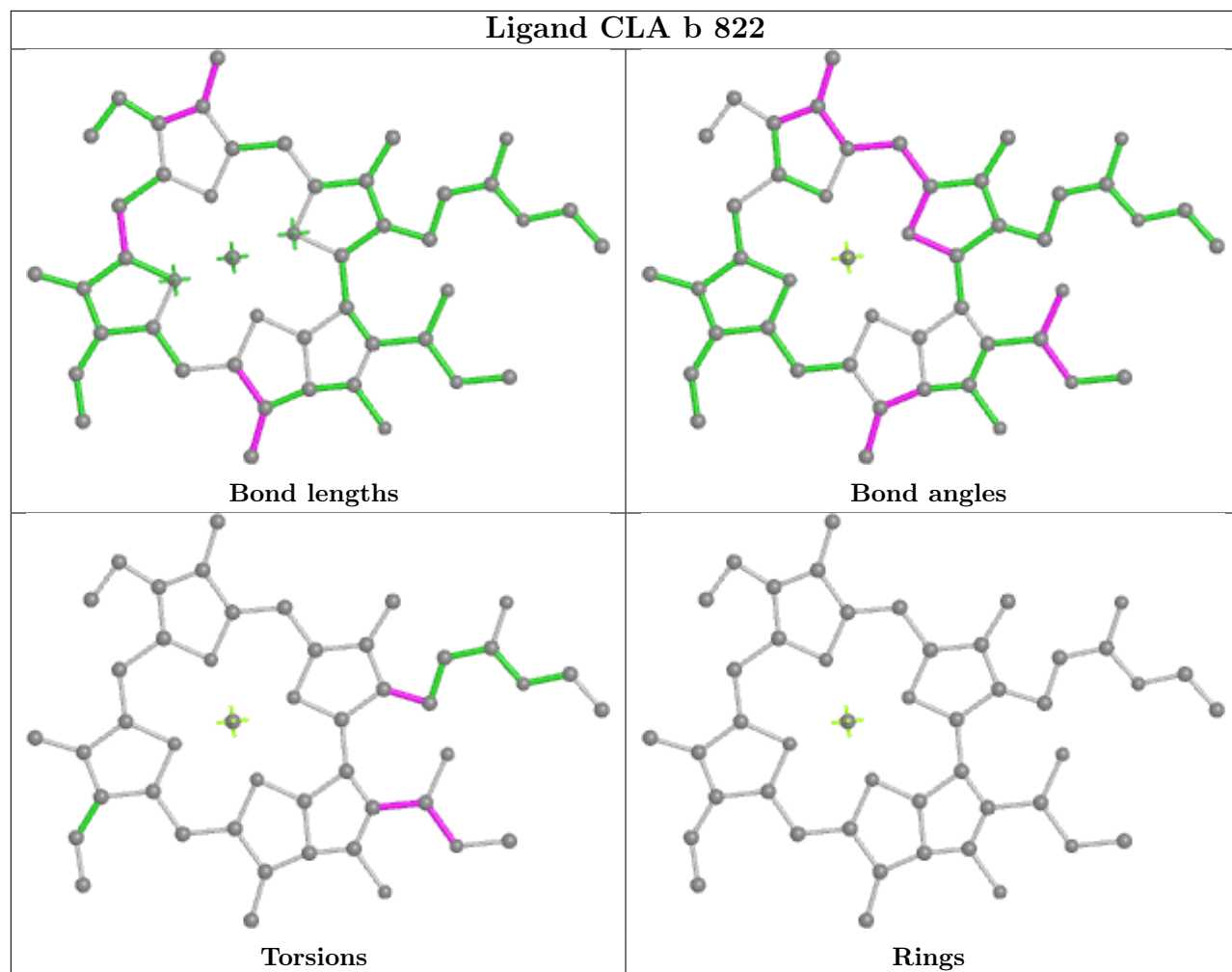




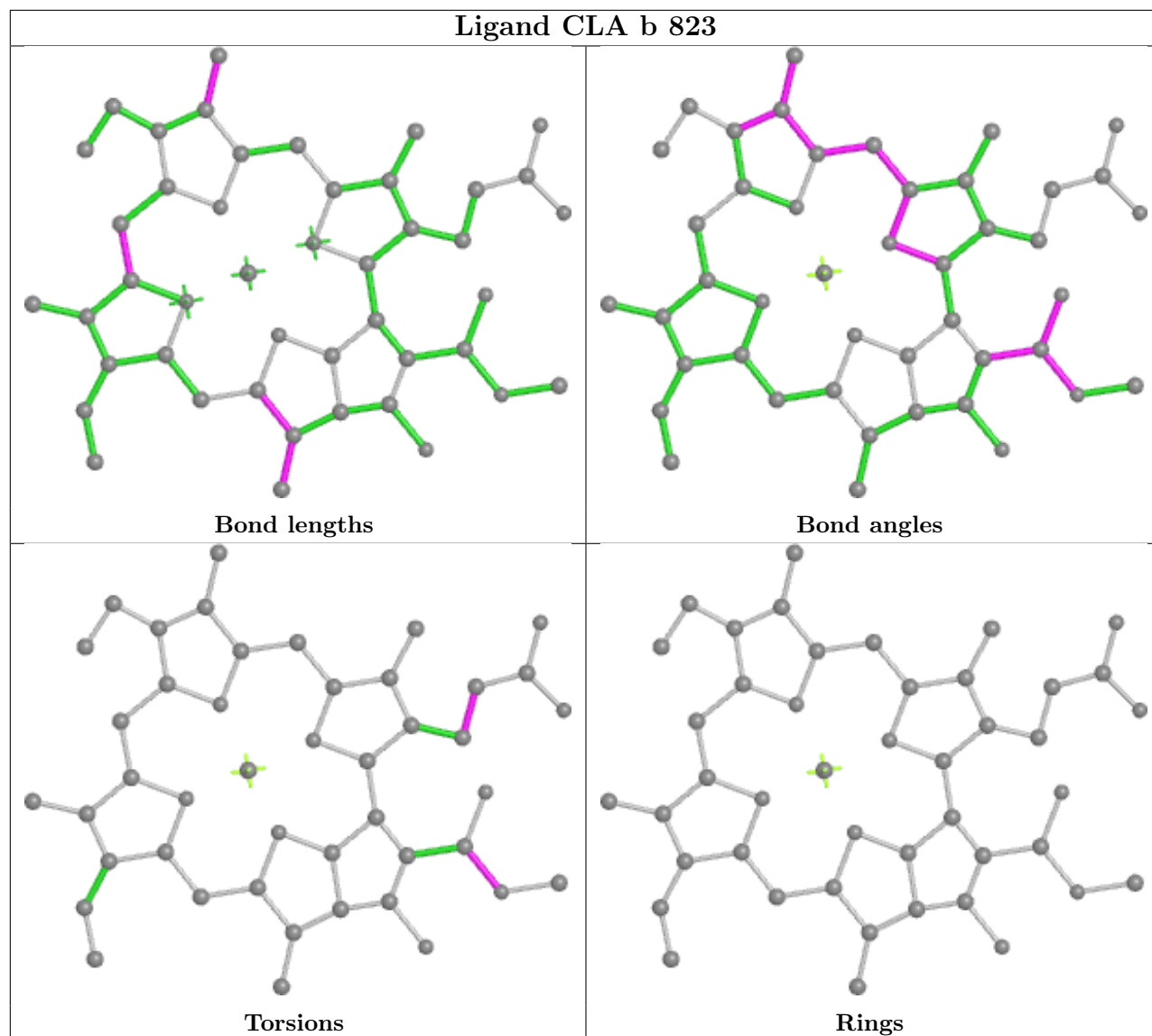


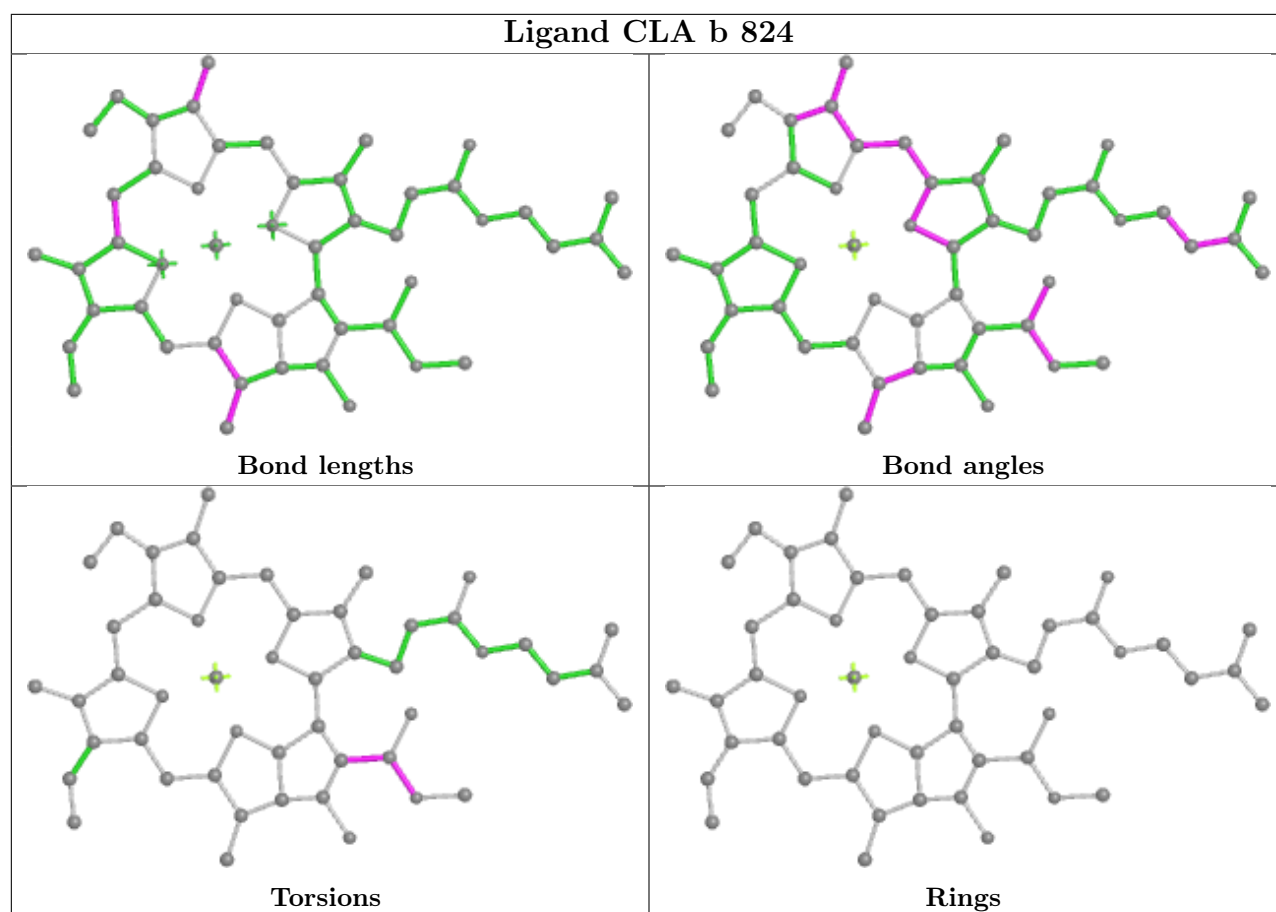


Ligand CLA b 822

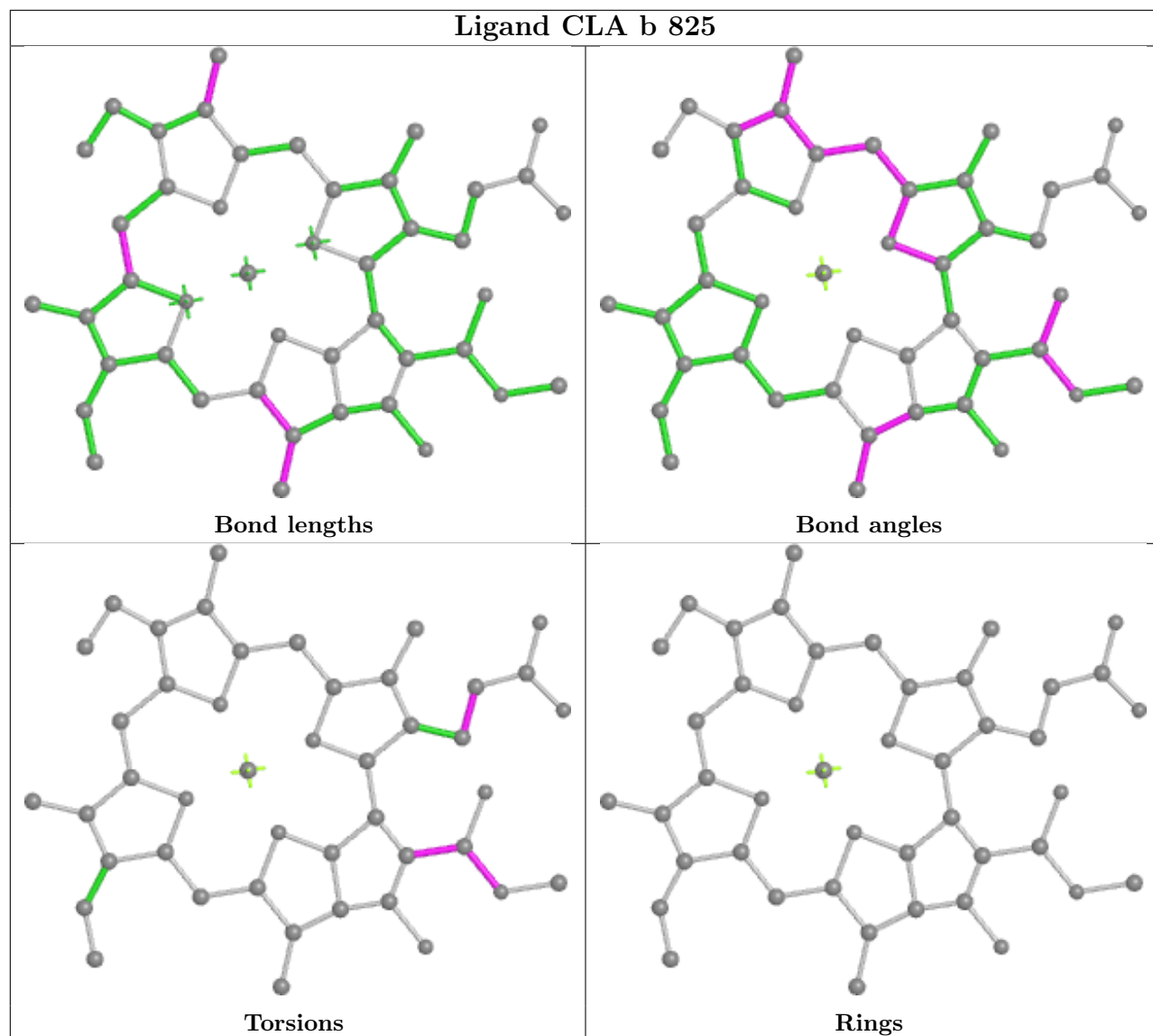


Ligand CLA b 823

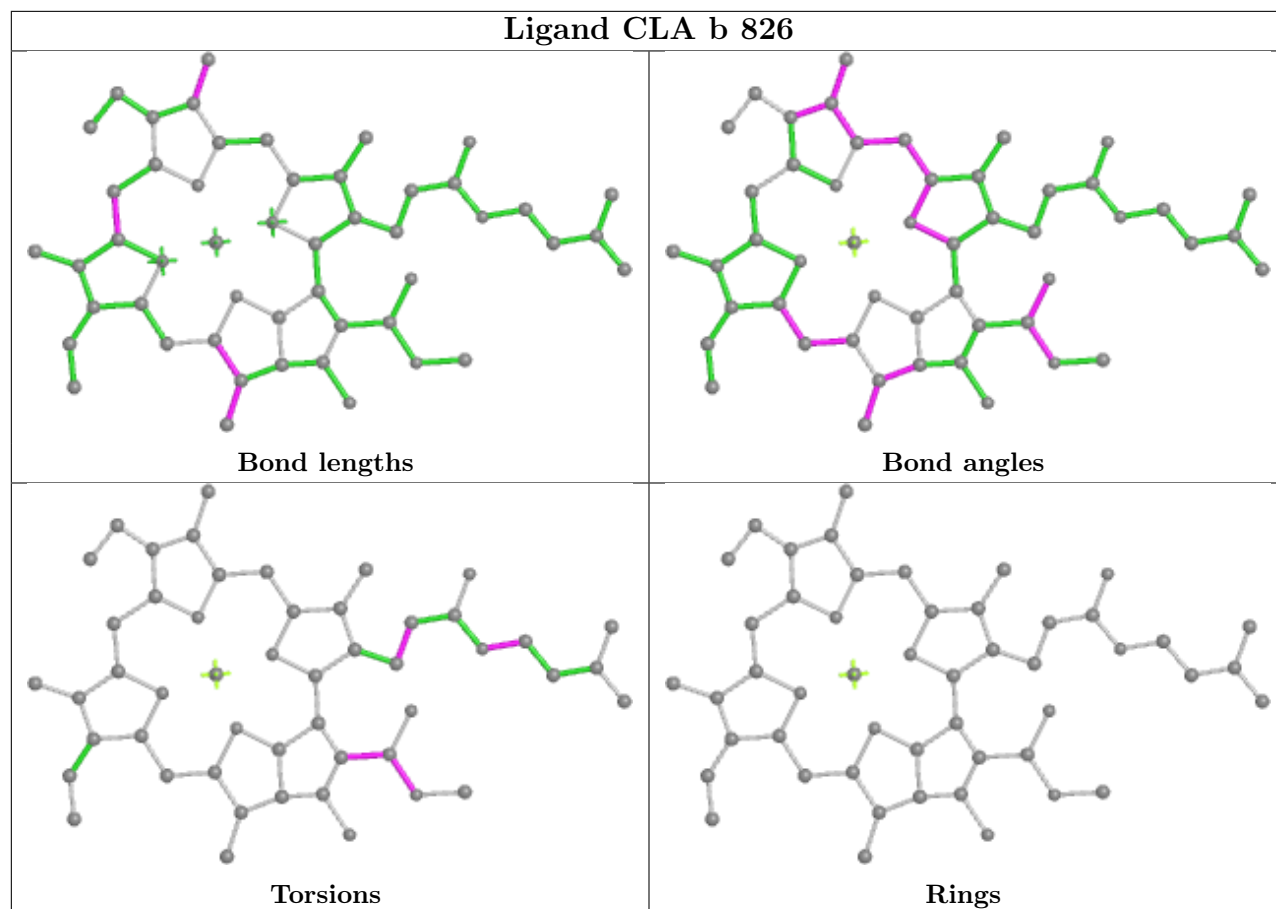




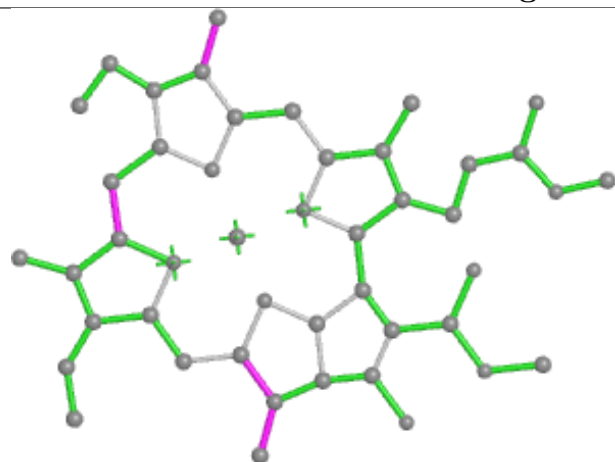
Ligand CLA b 825



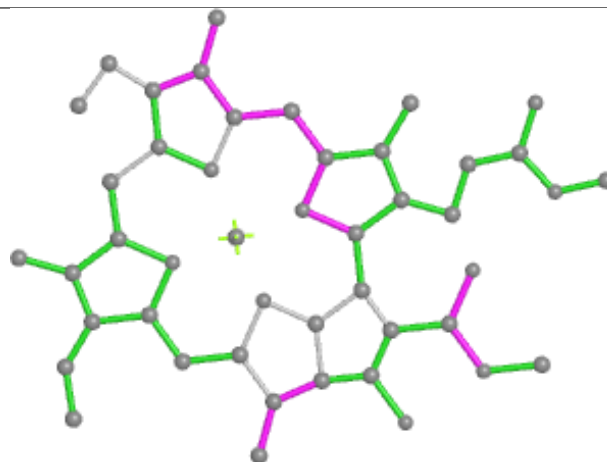
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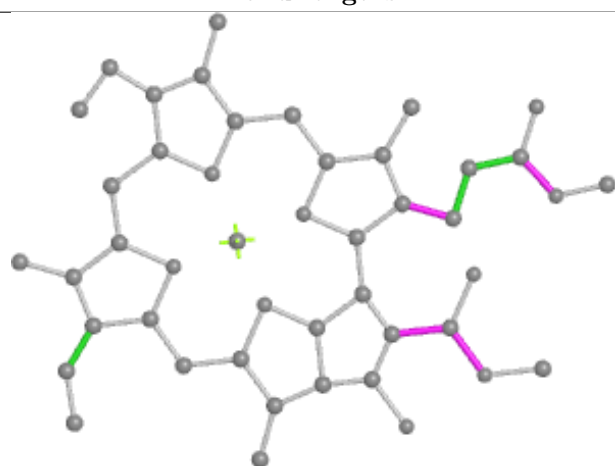
Ligand CLA b 827



Bond lengths



Bond angles

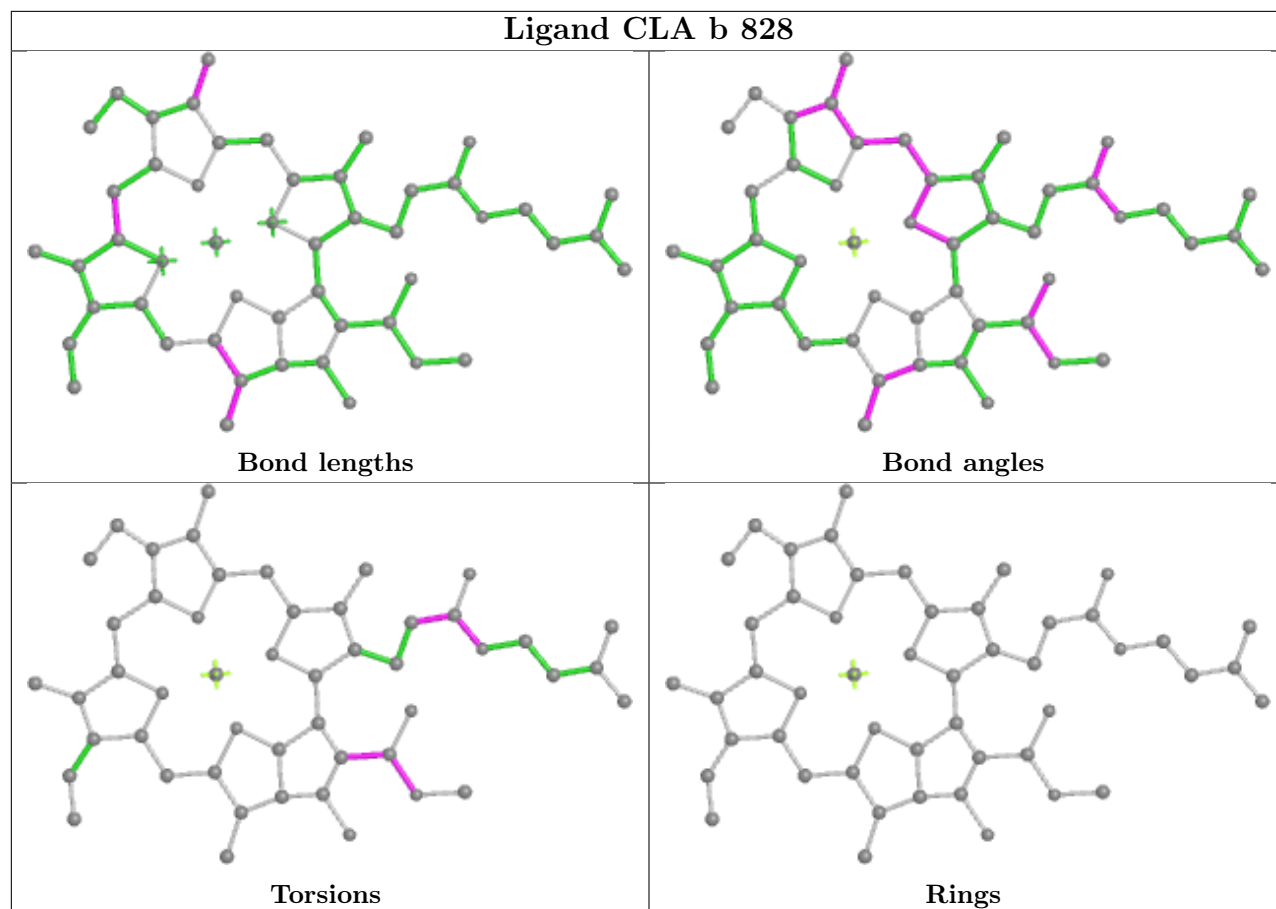


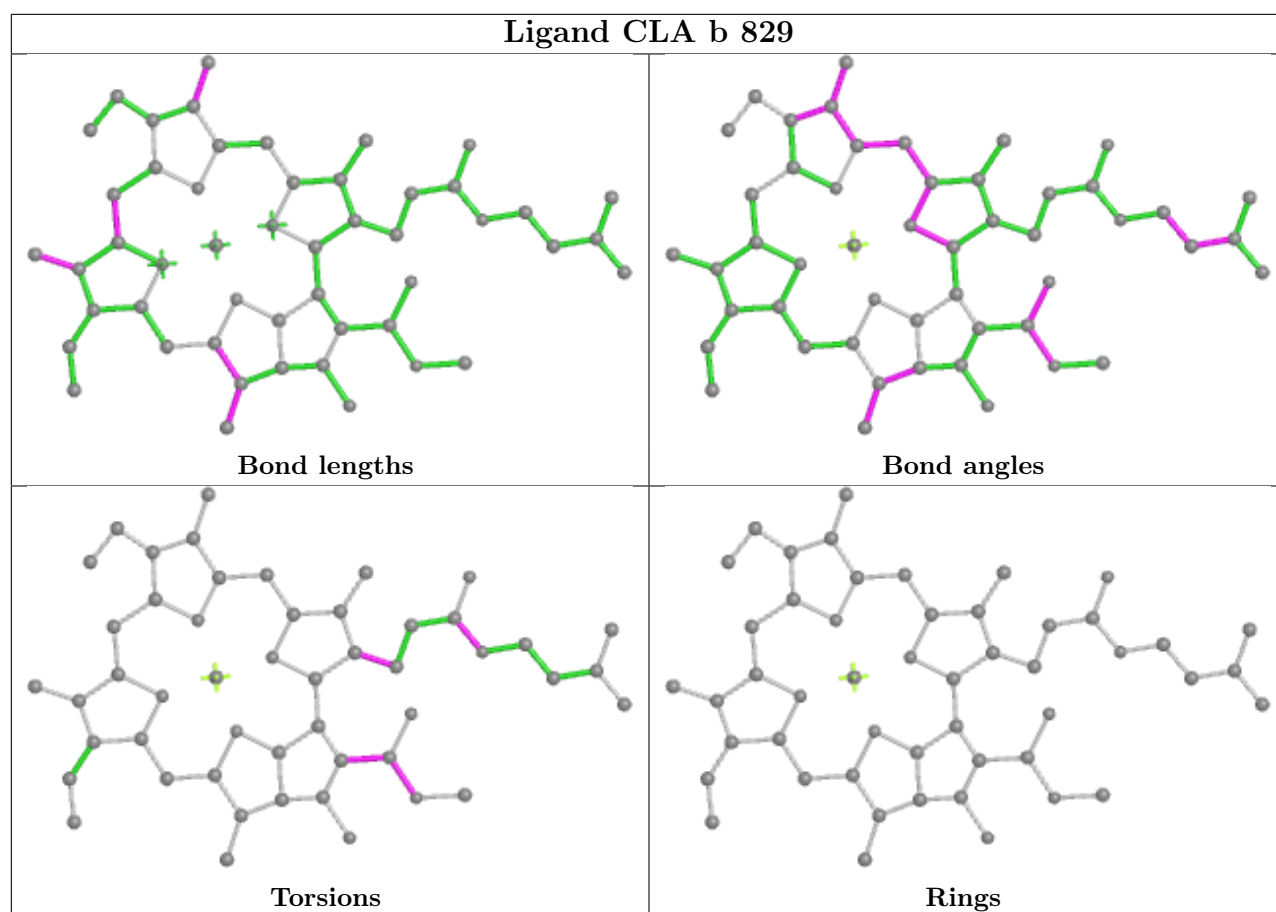
Torsions

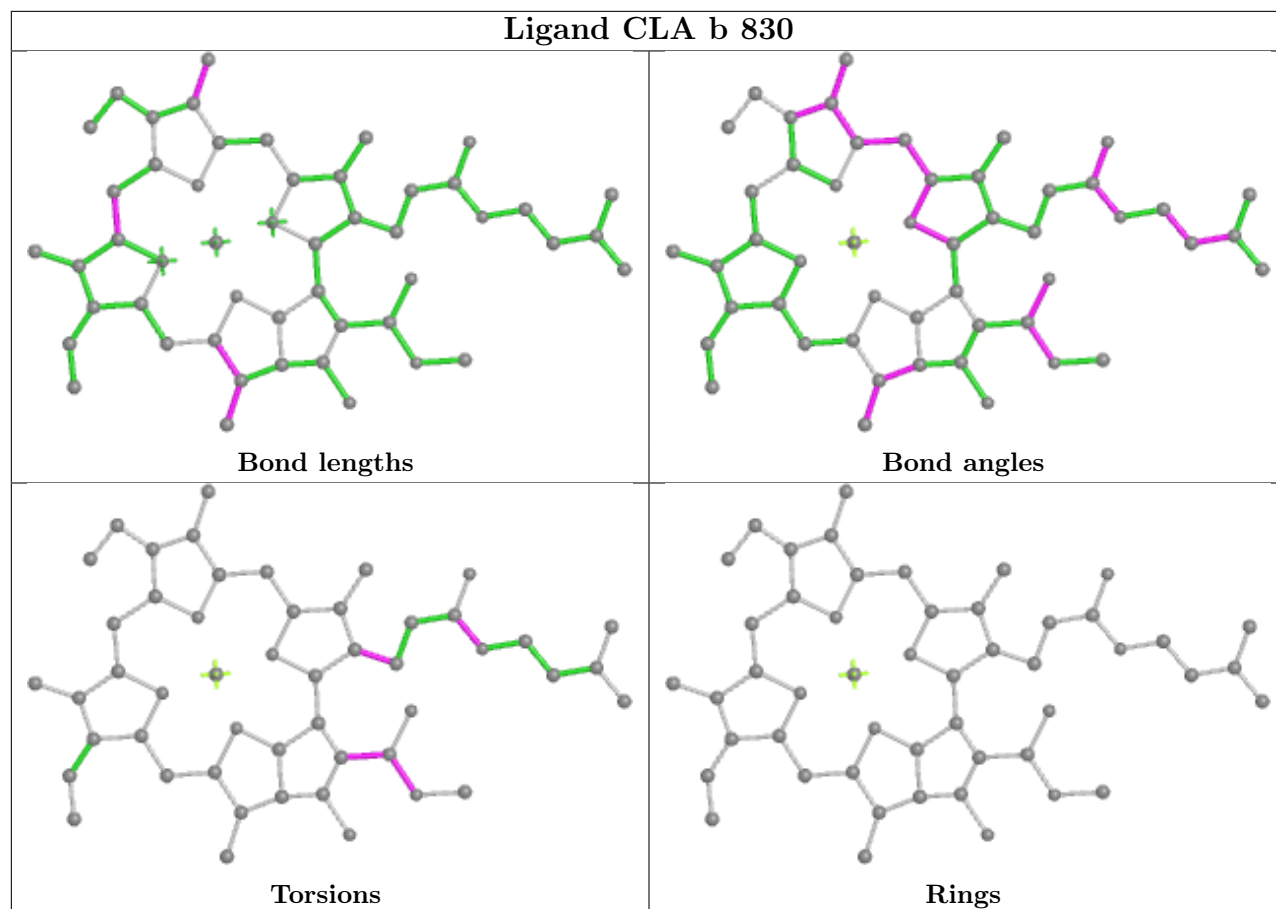


Rings

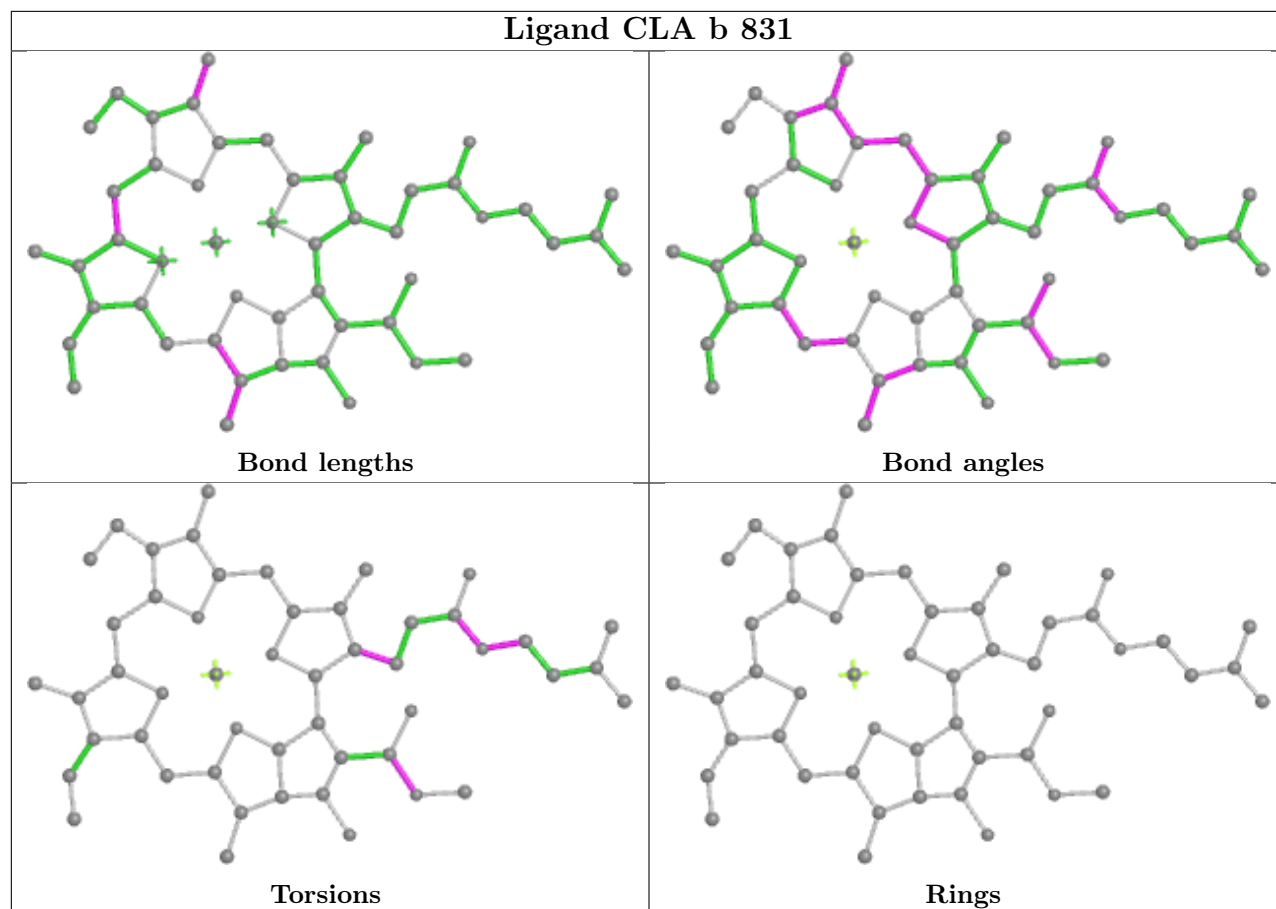
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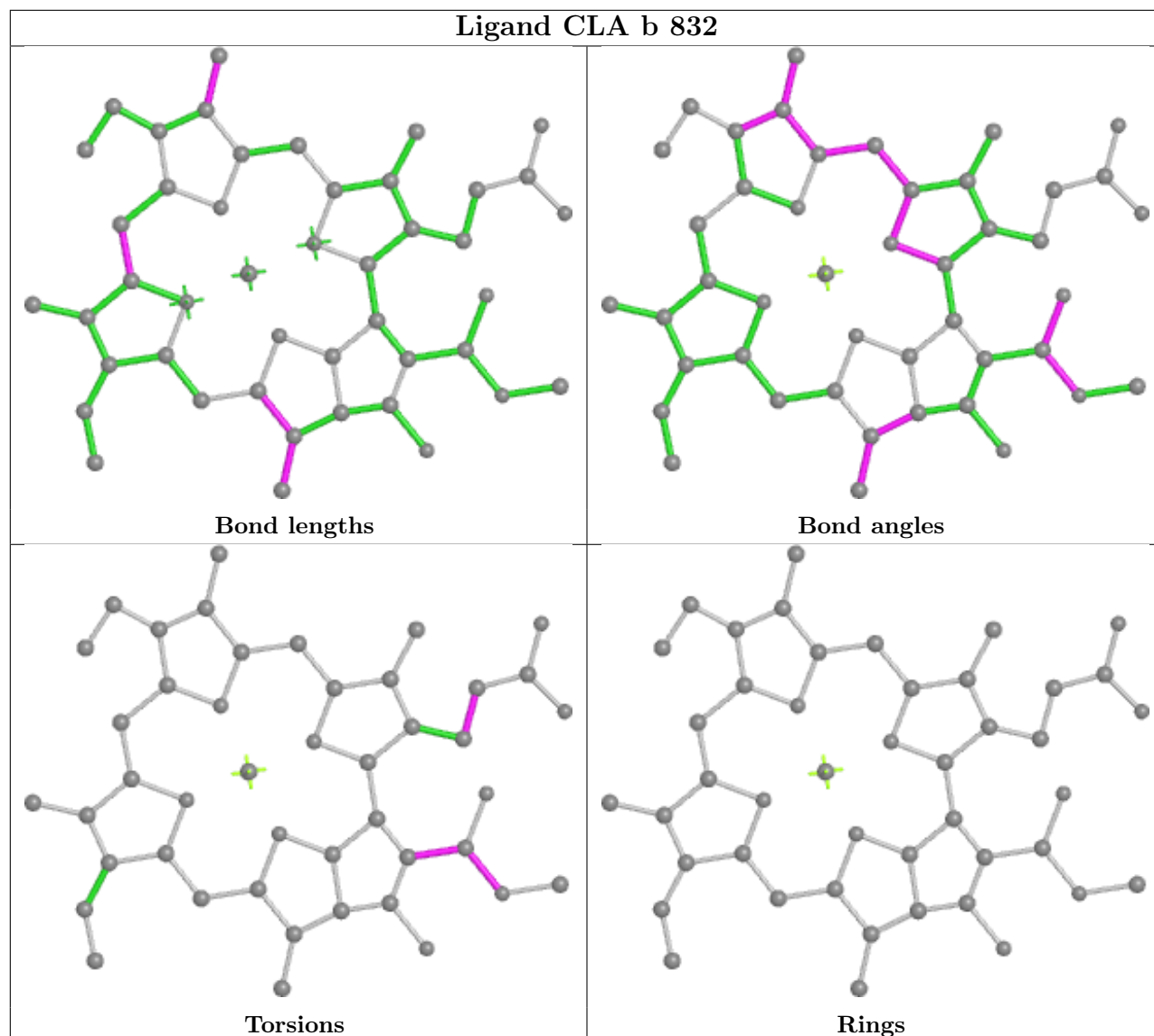




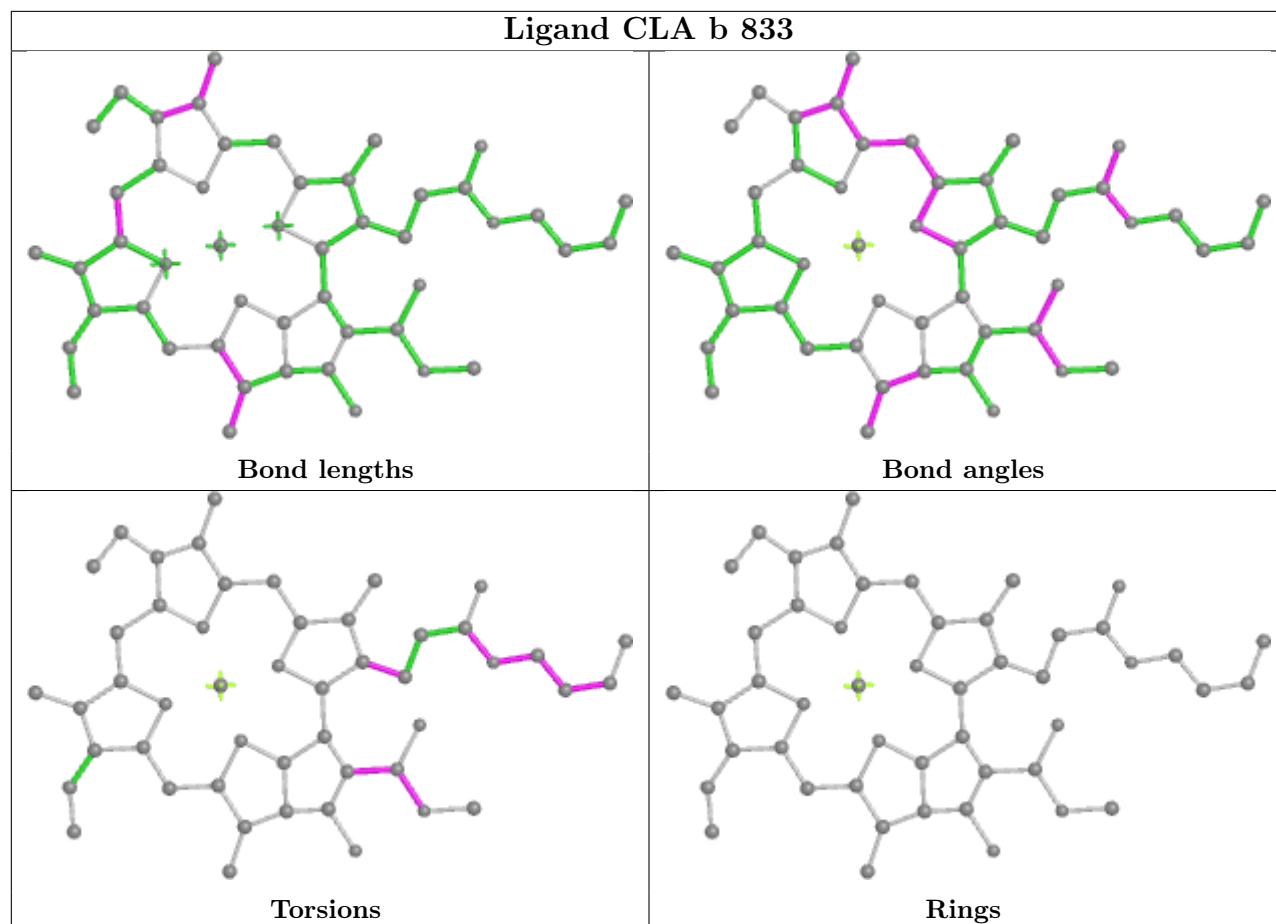
Ligand CLA b 831

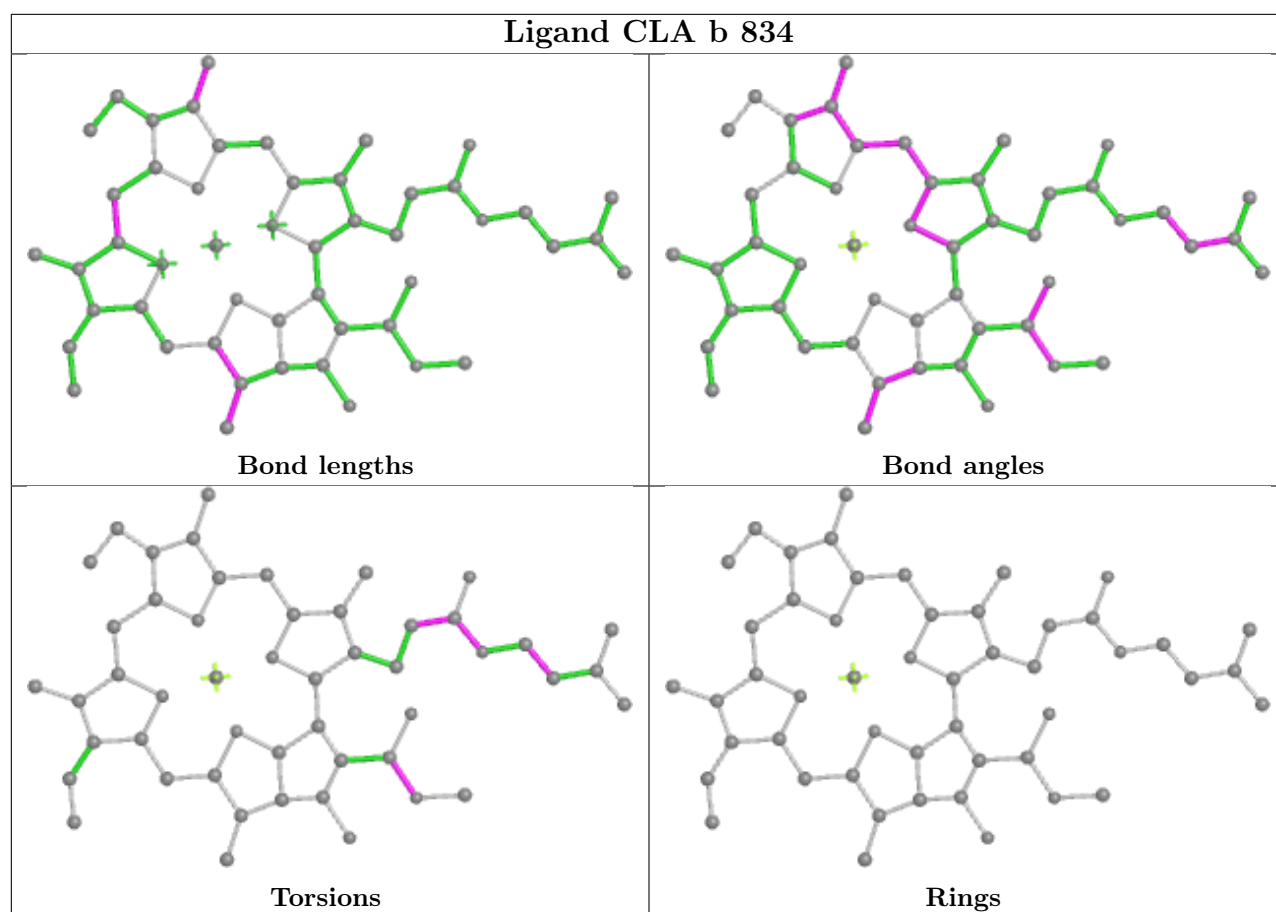


Ligand CLA b 832

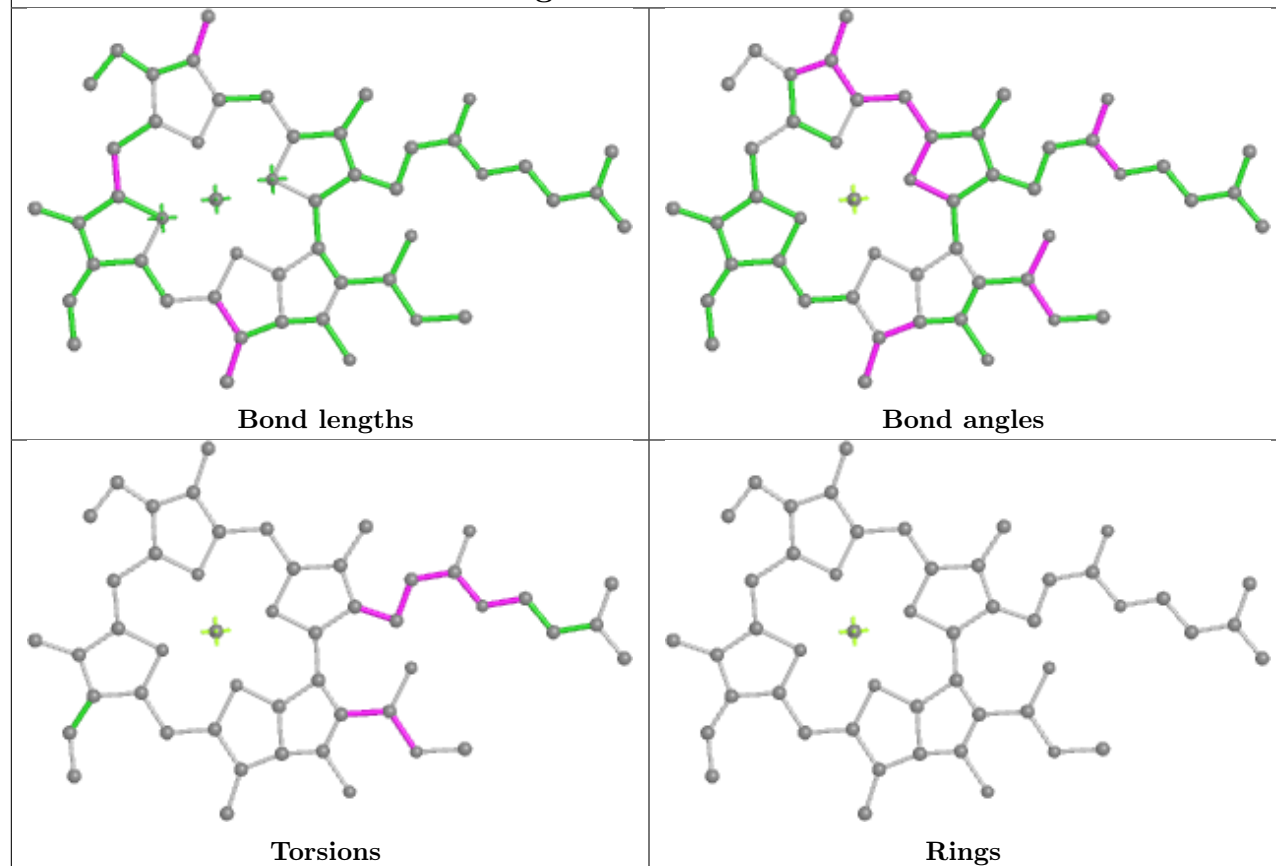


Ligand CLA b 833

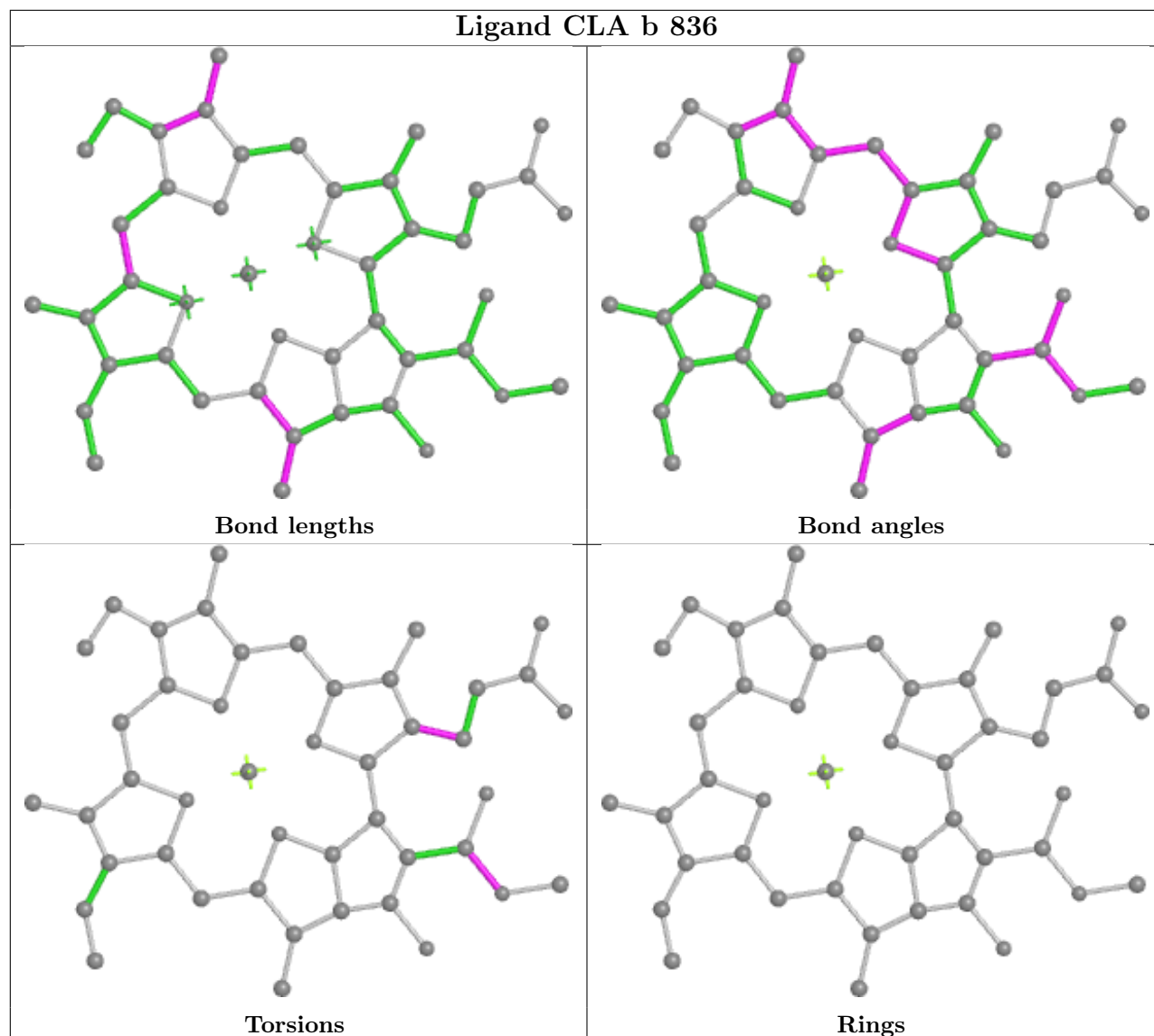




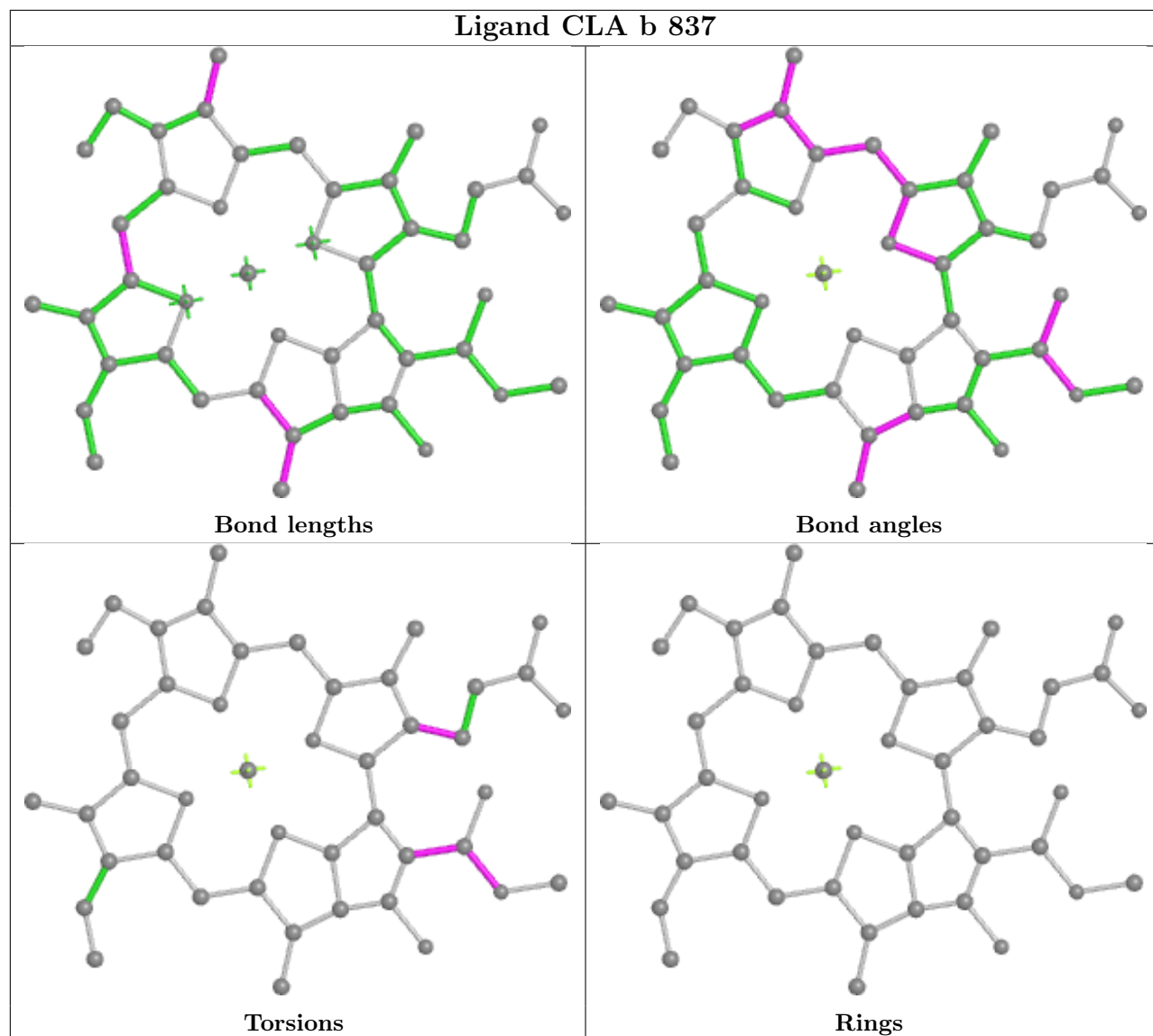
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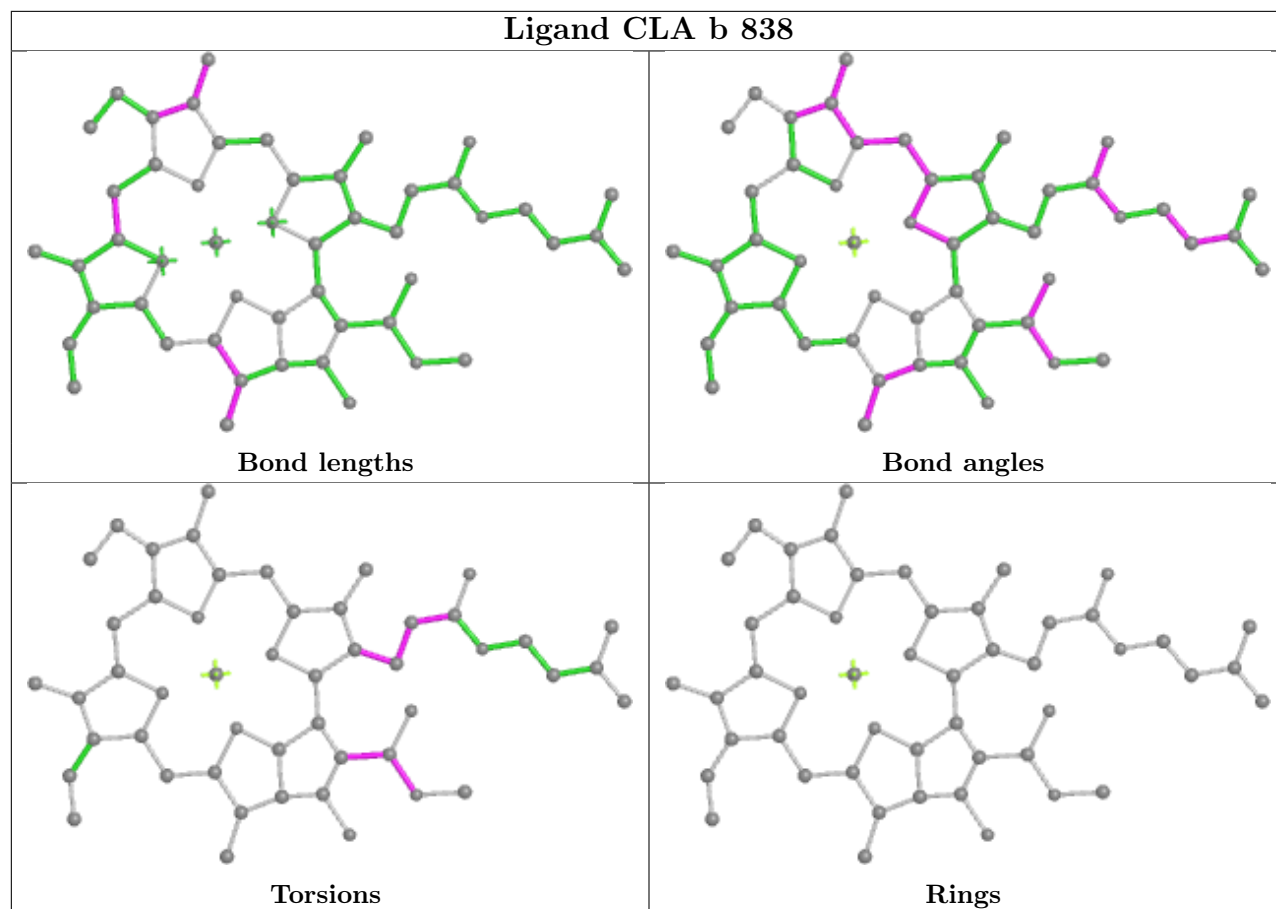
Ligand CLA b 836

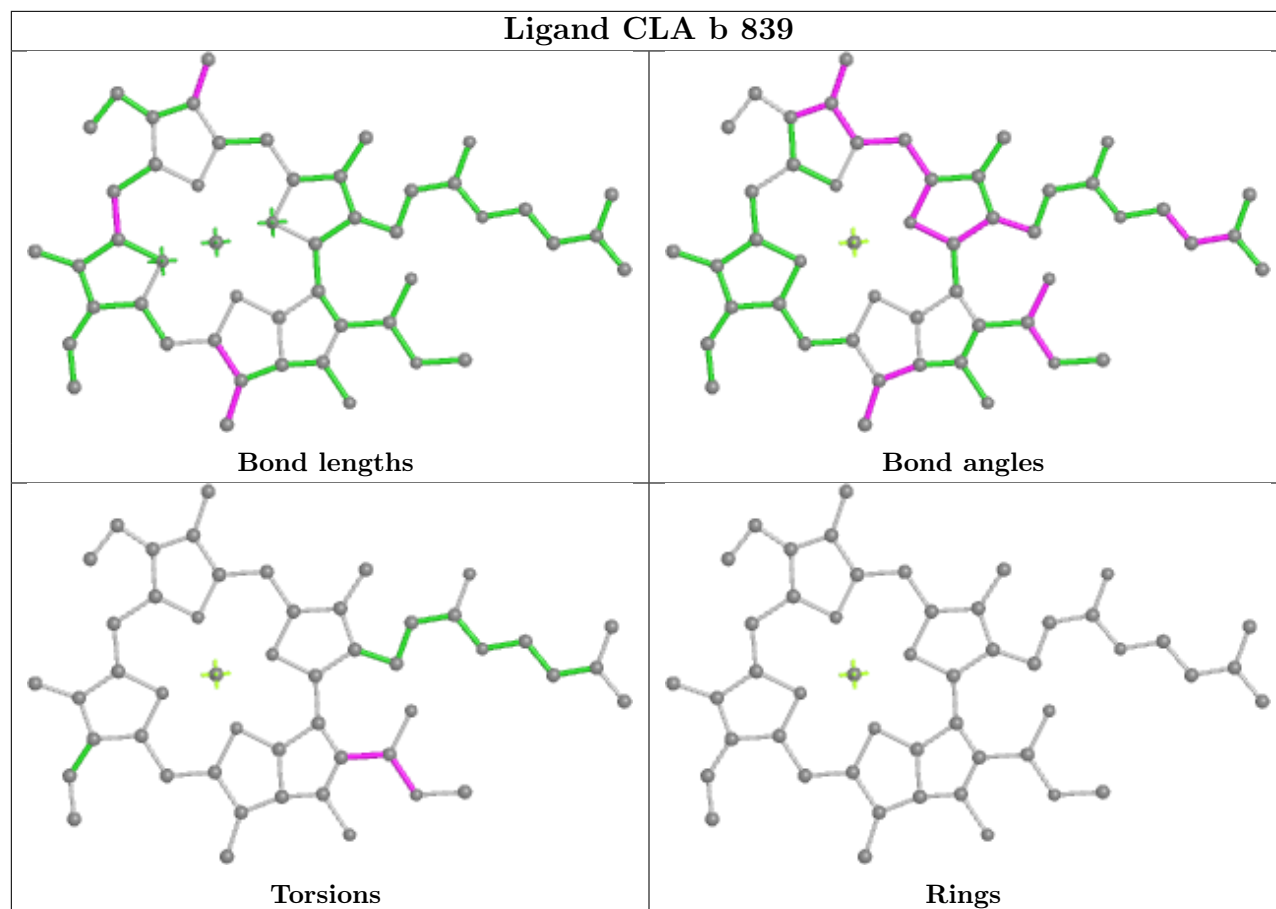


Ligand CLA b 837

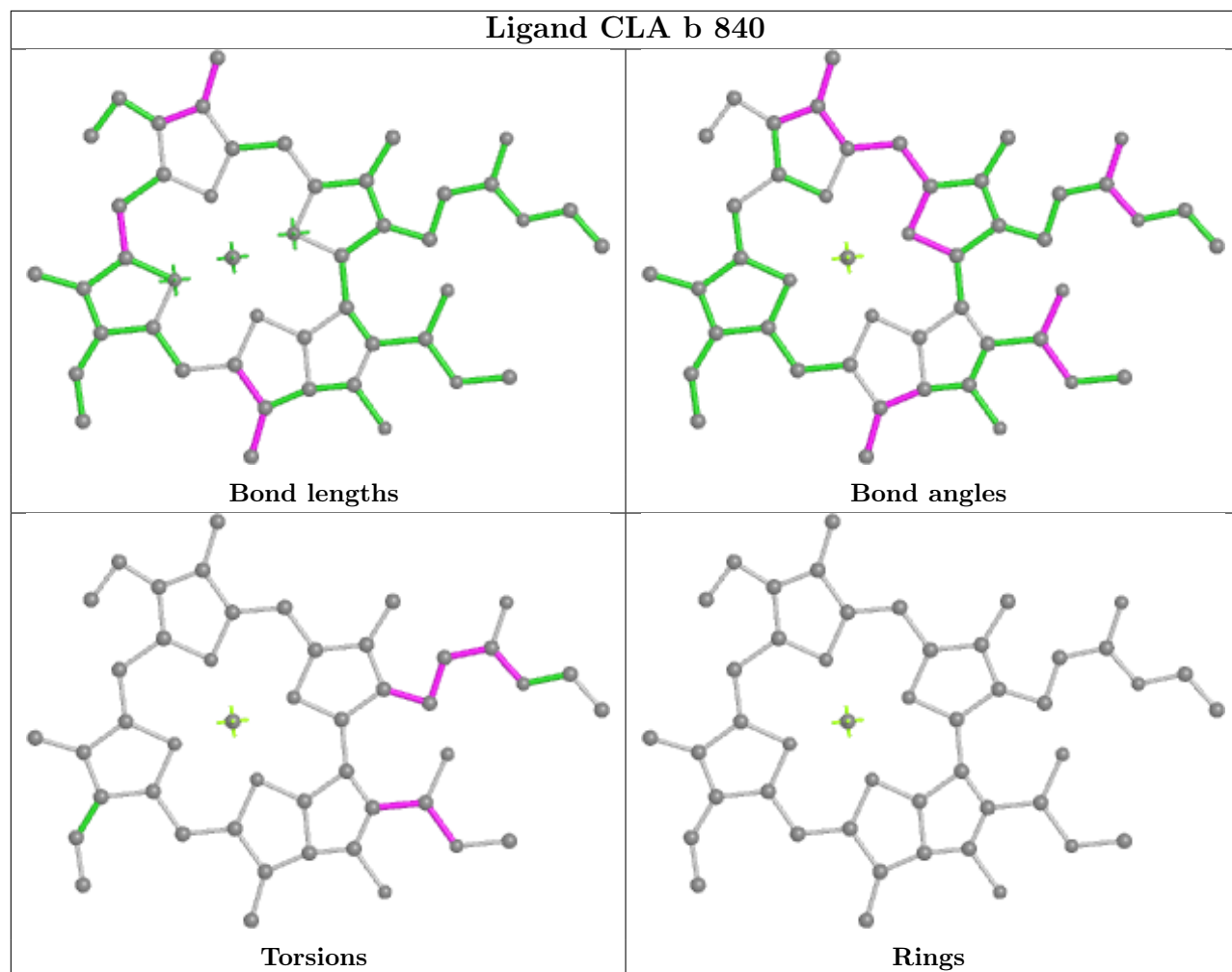


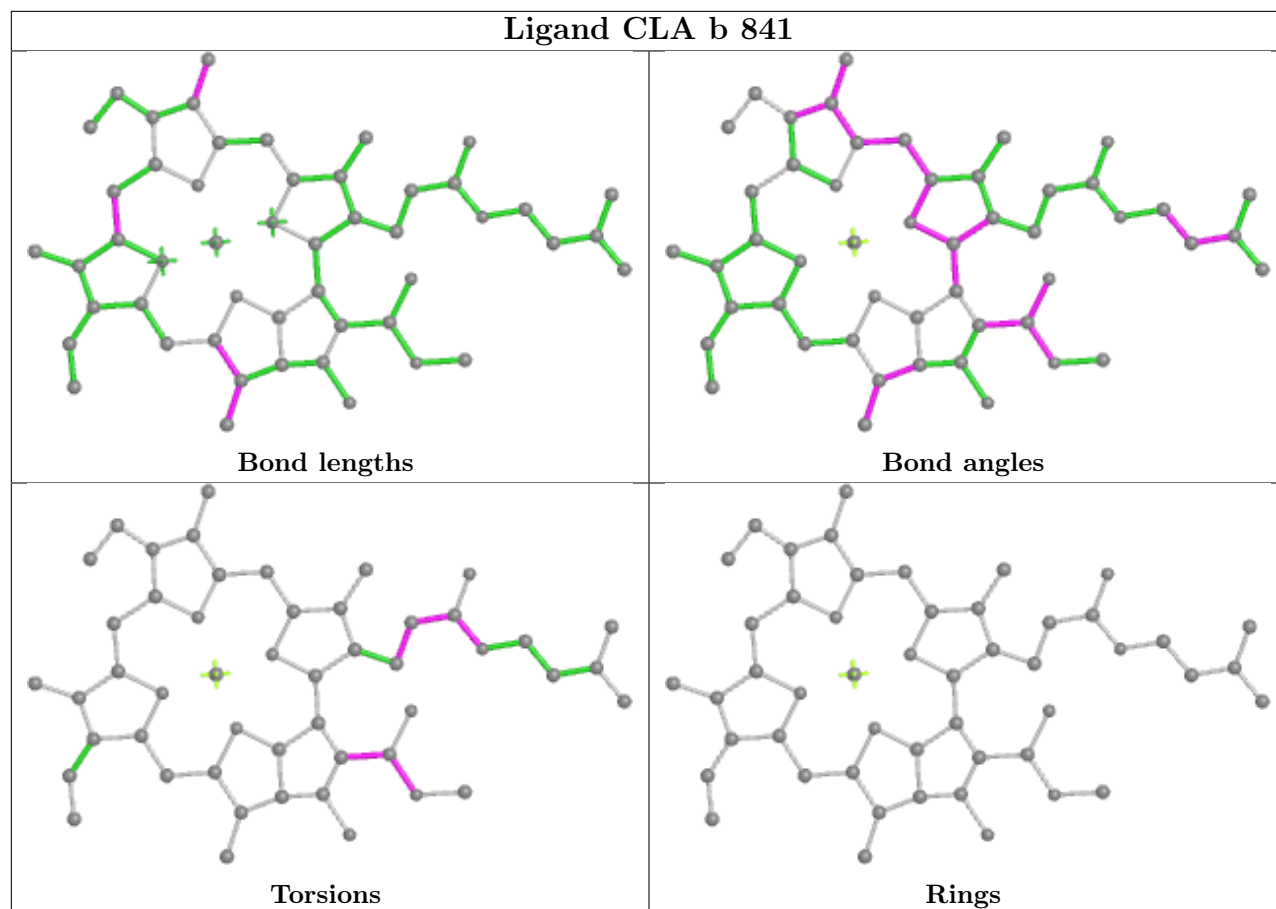
Ligand CLA b 838

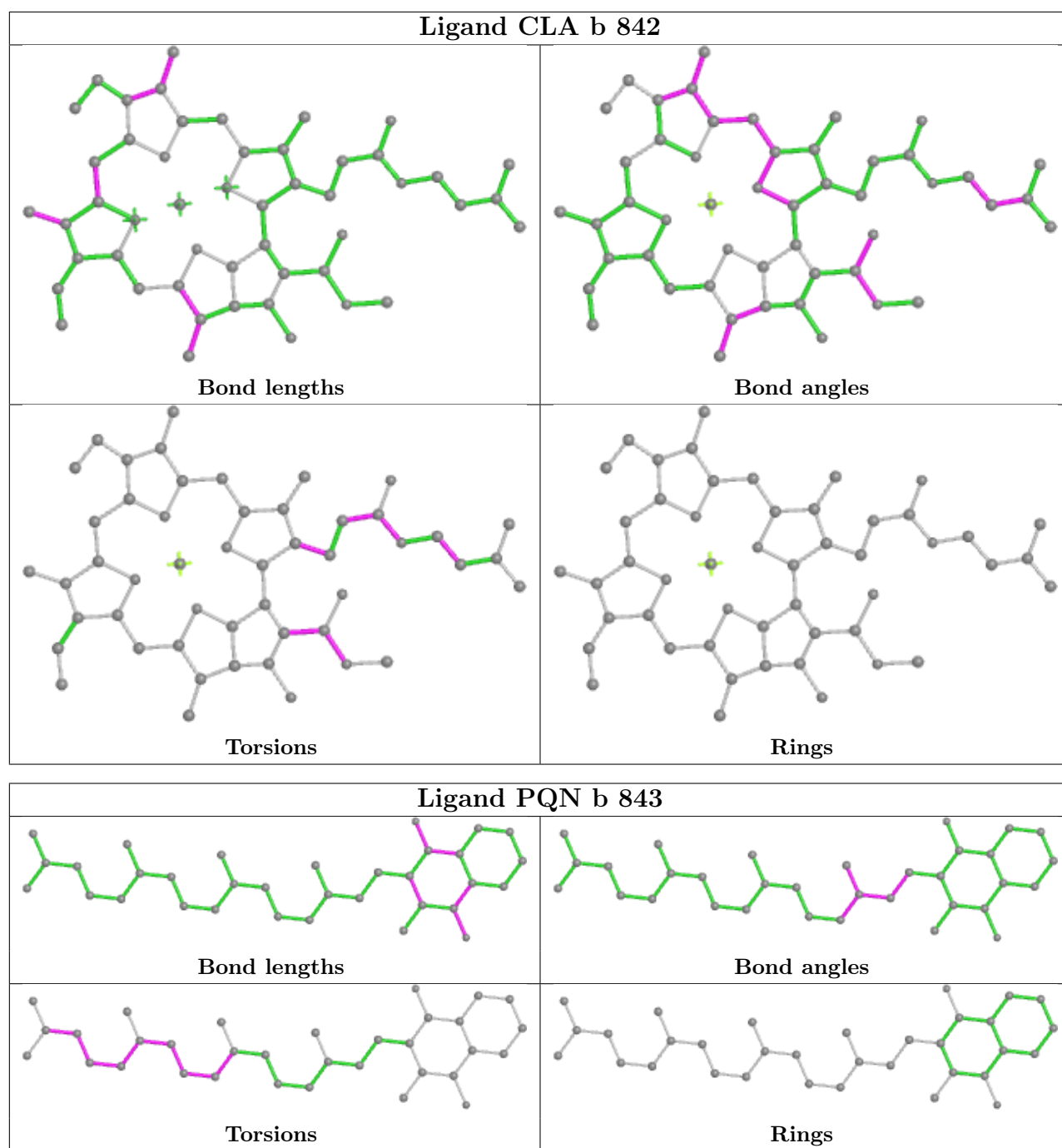




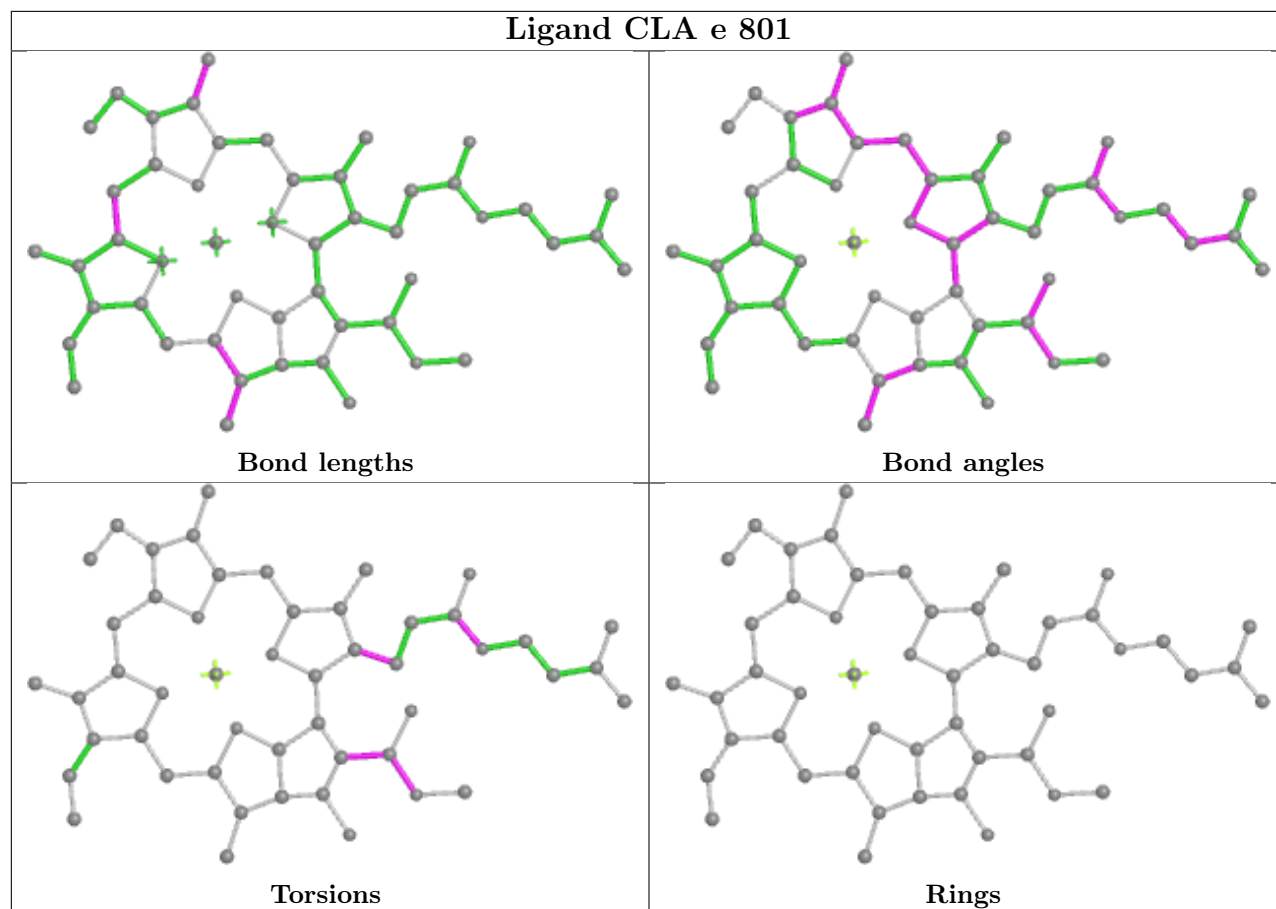
Ligand CLA b 840



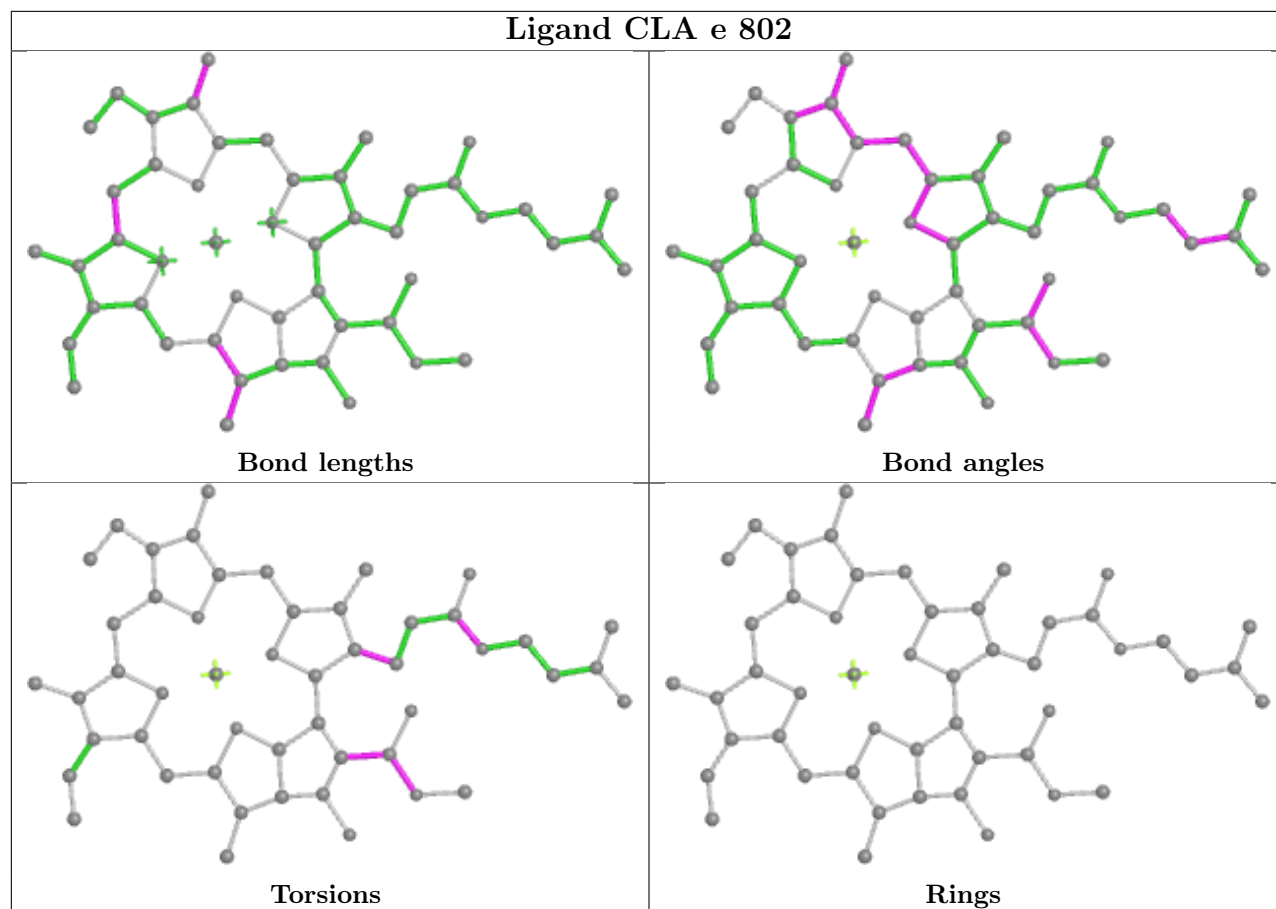




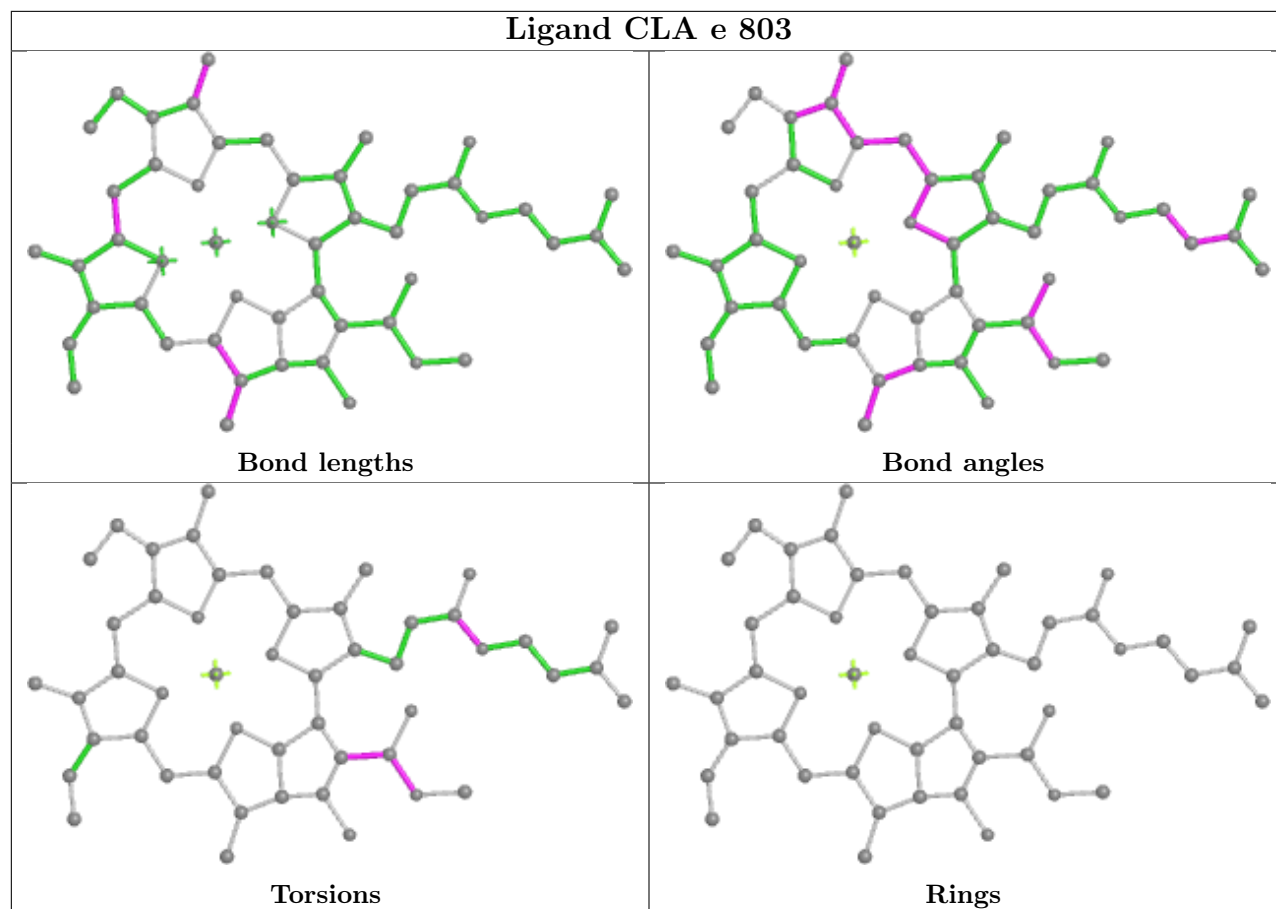
Ligand CLA e 801



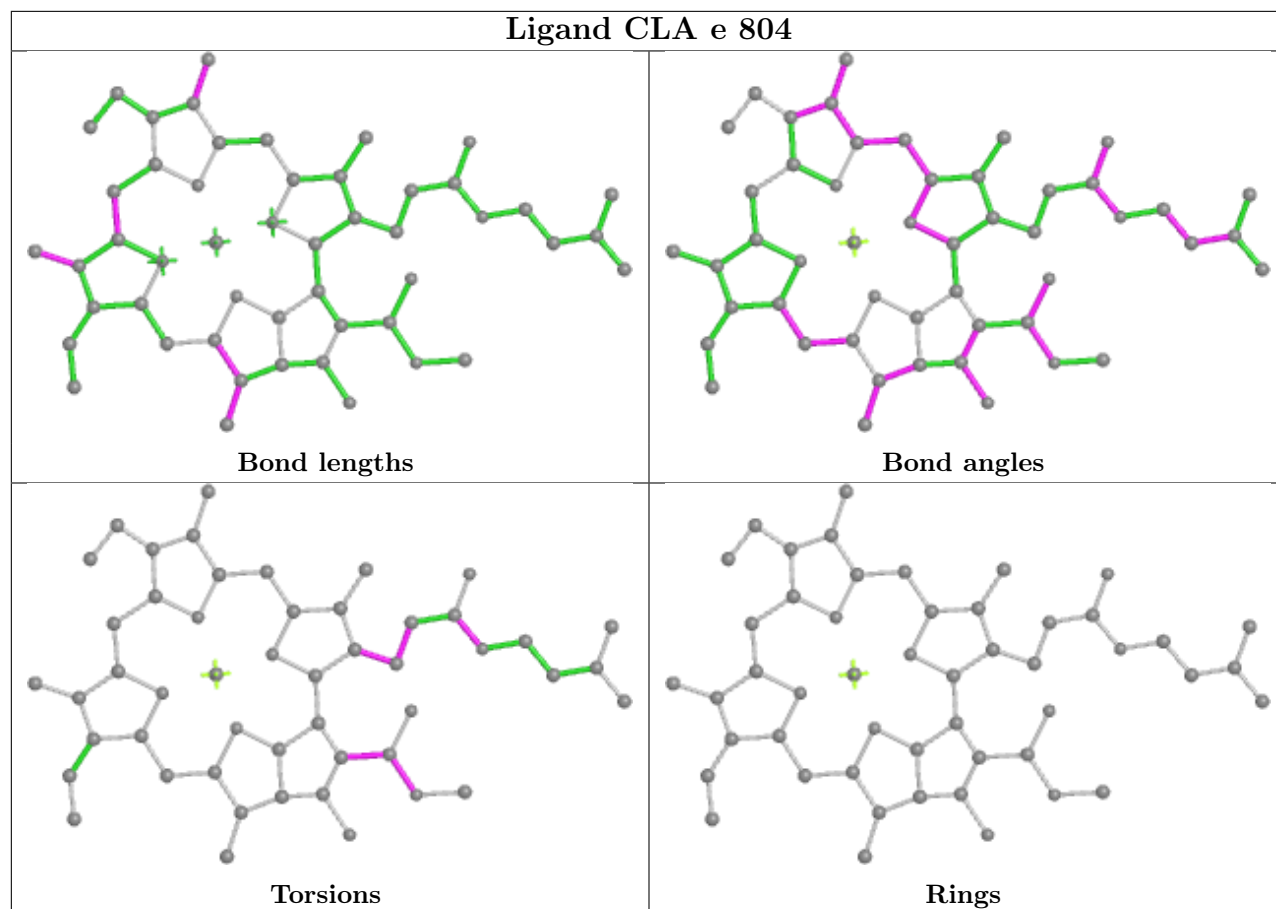
Ligand CLA e 802



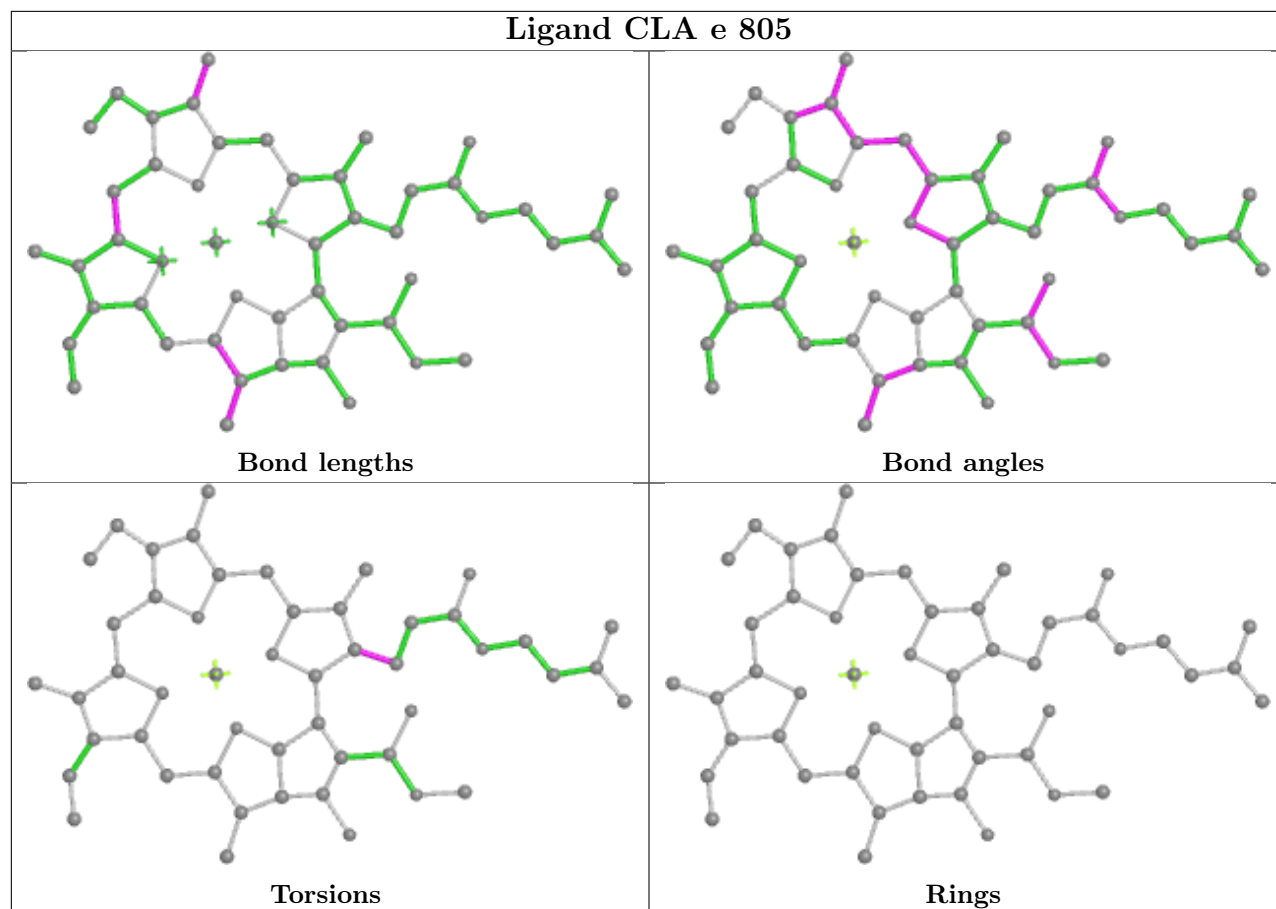
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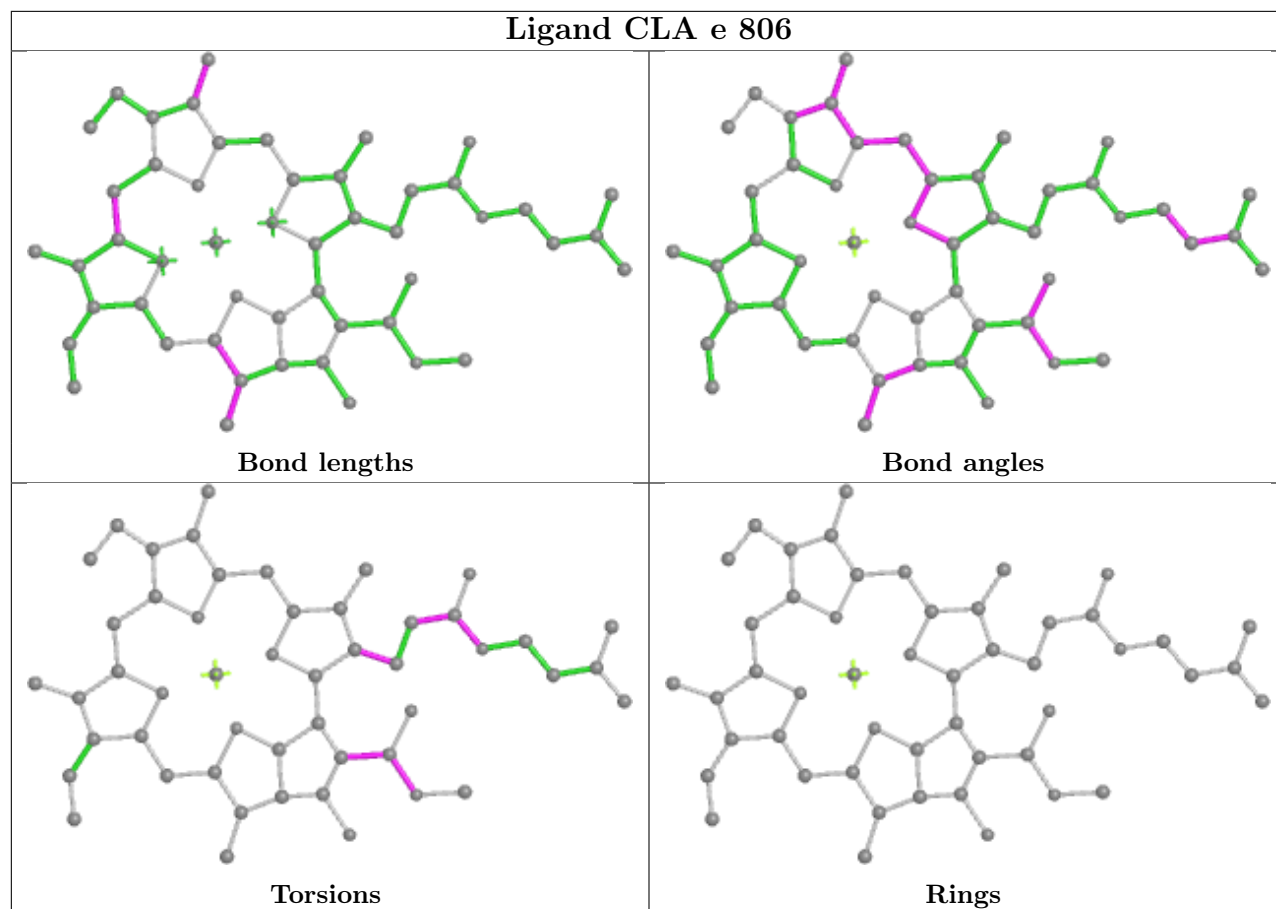
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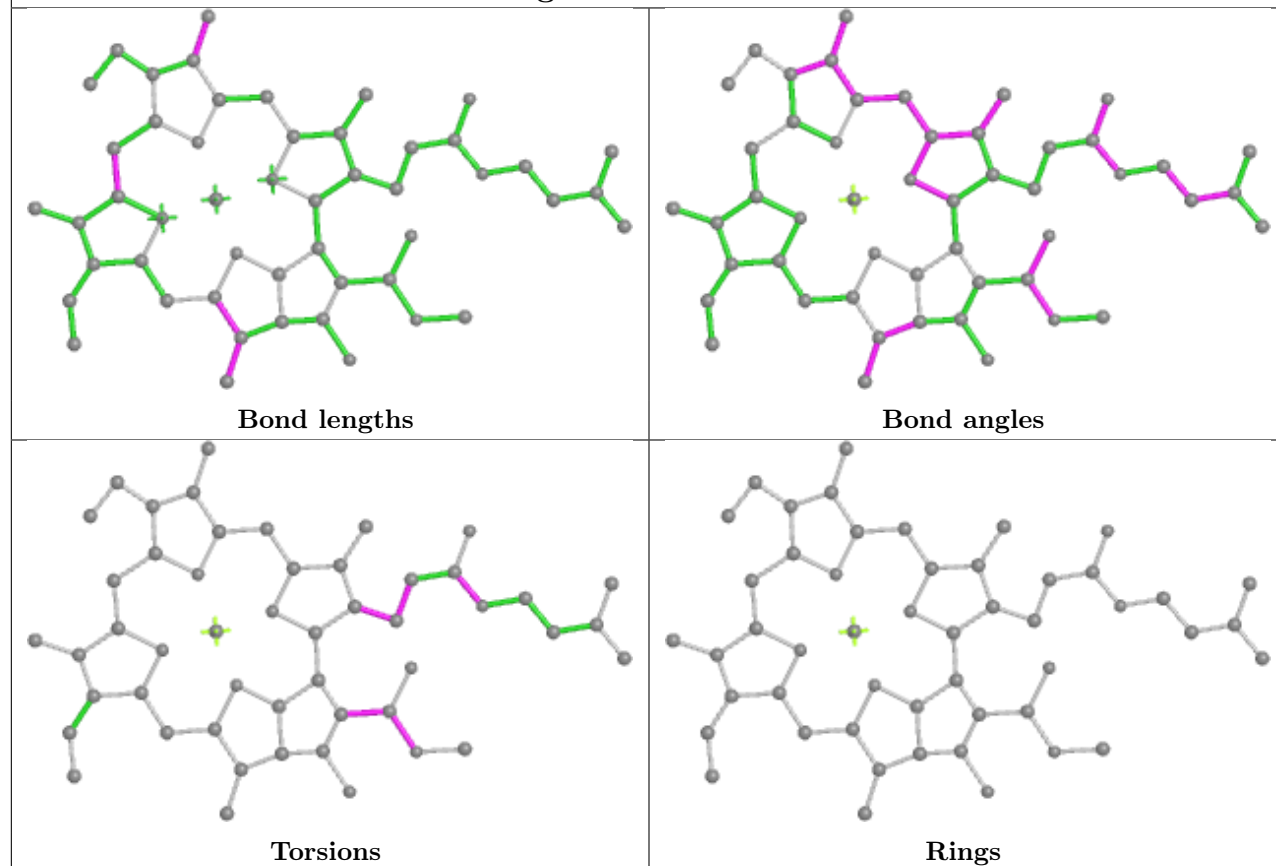
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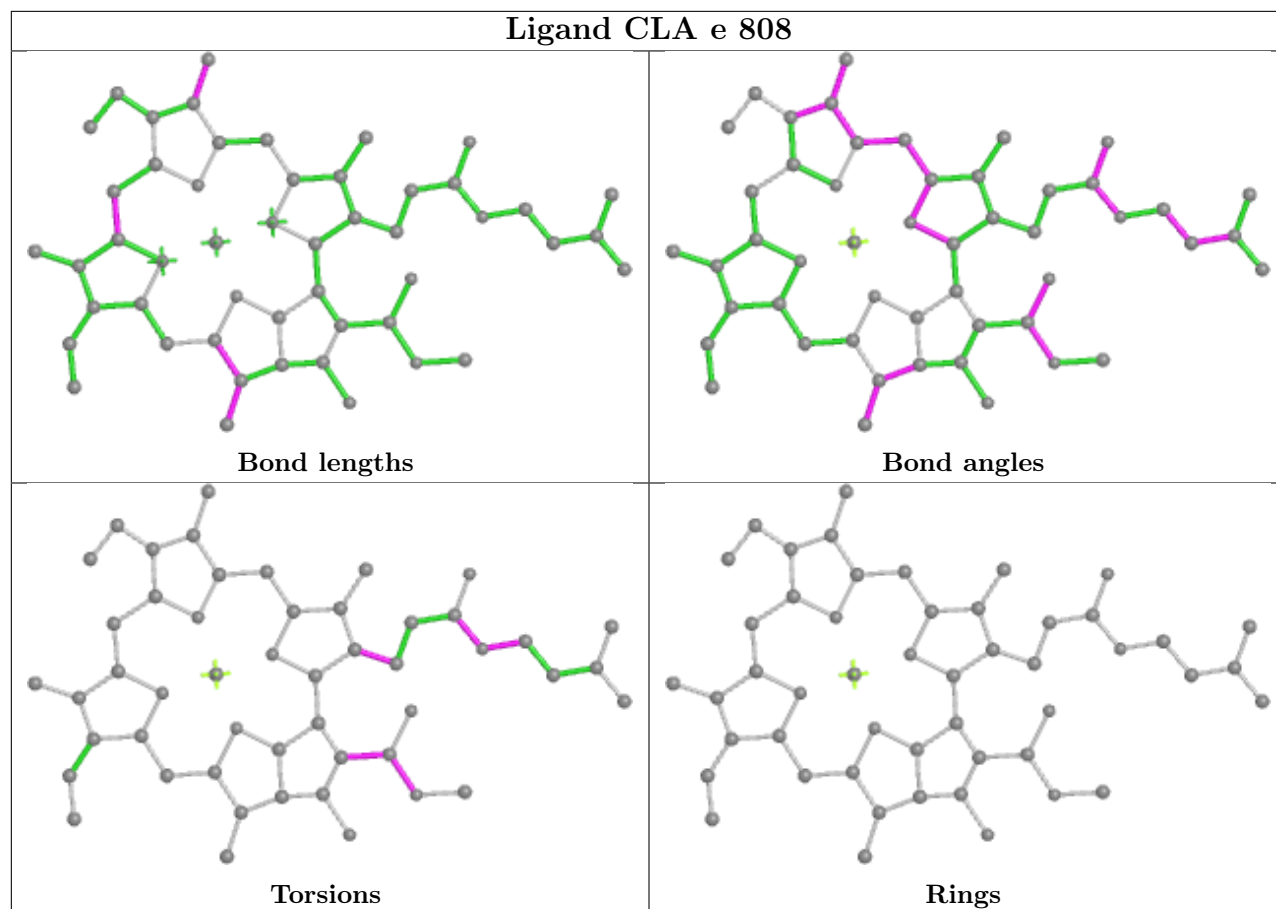
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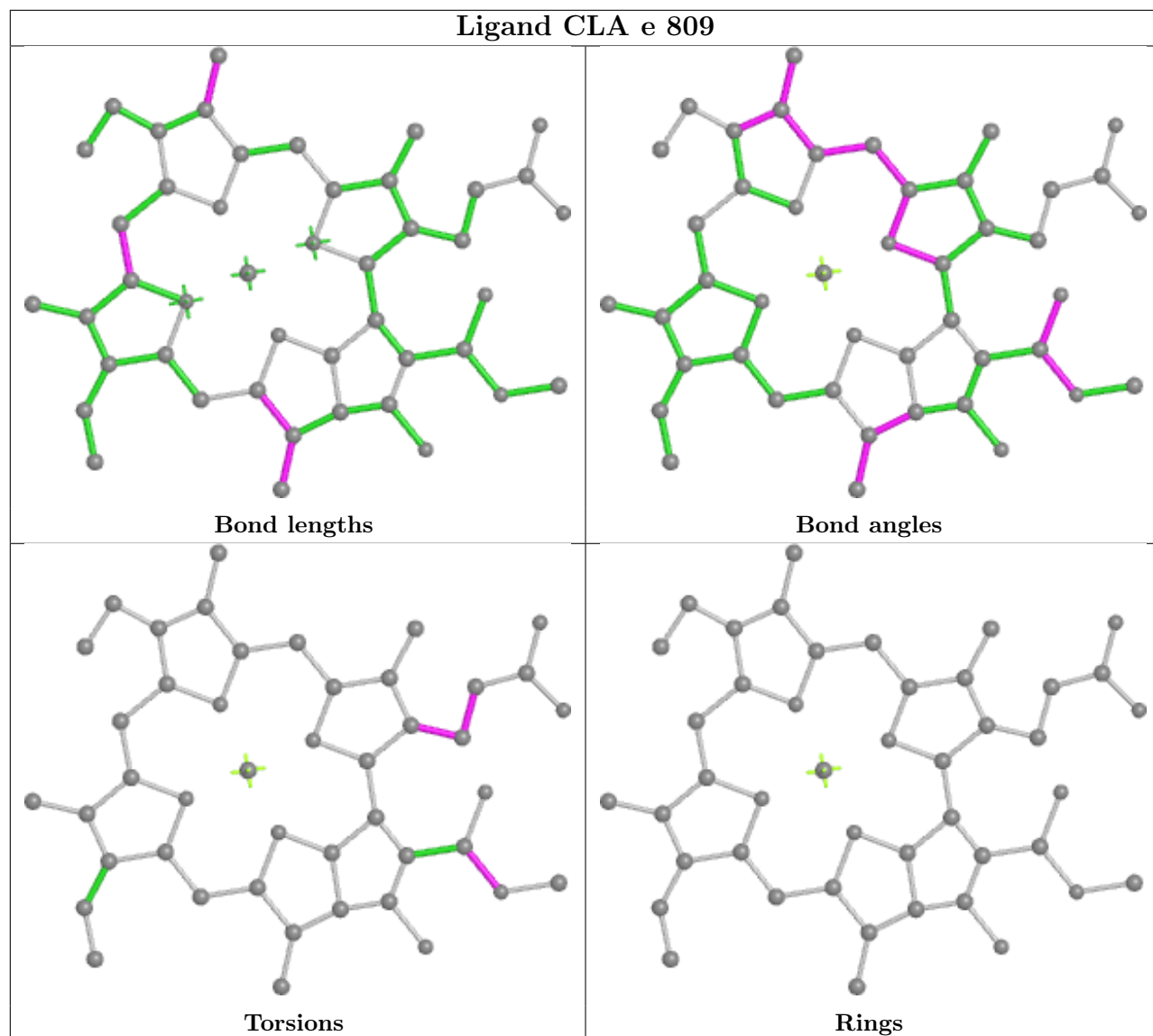
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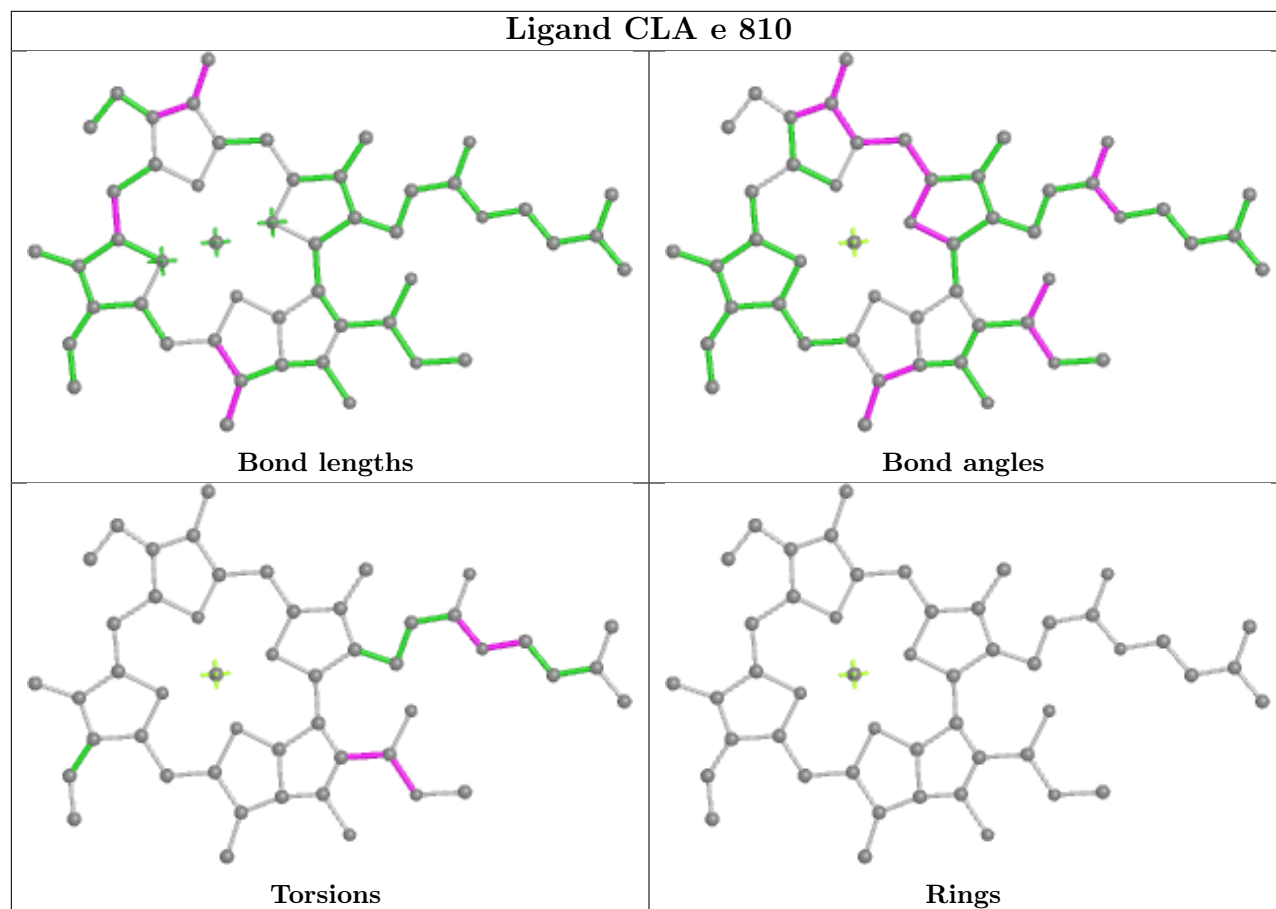
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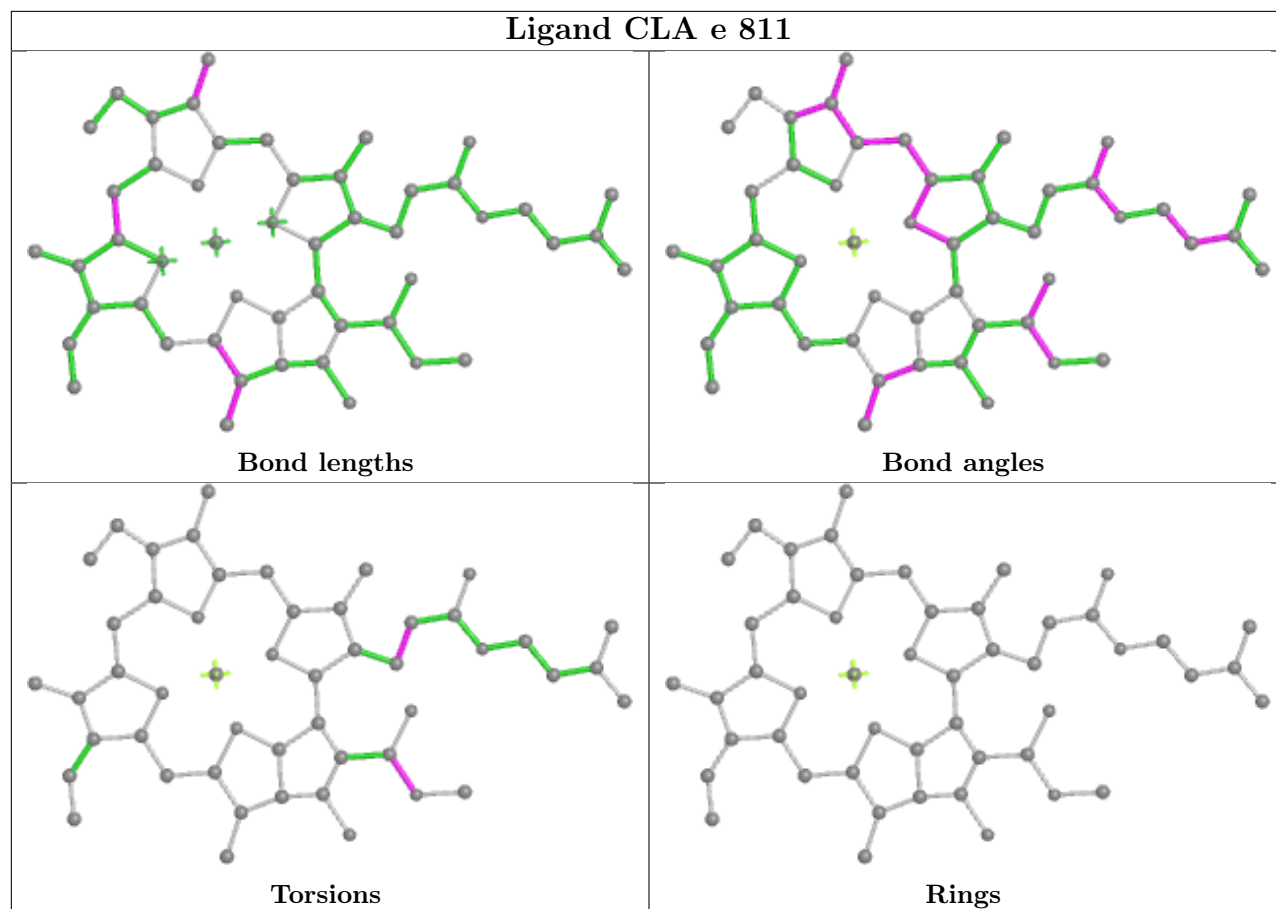
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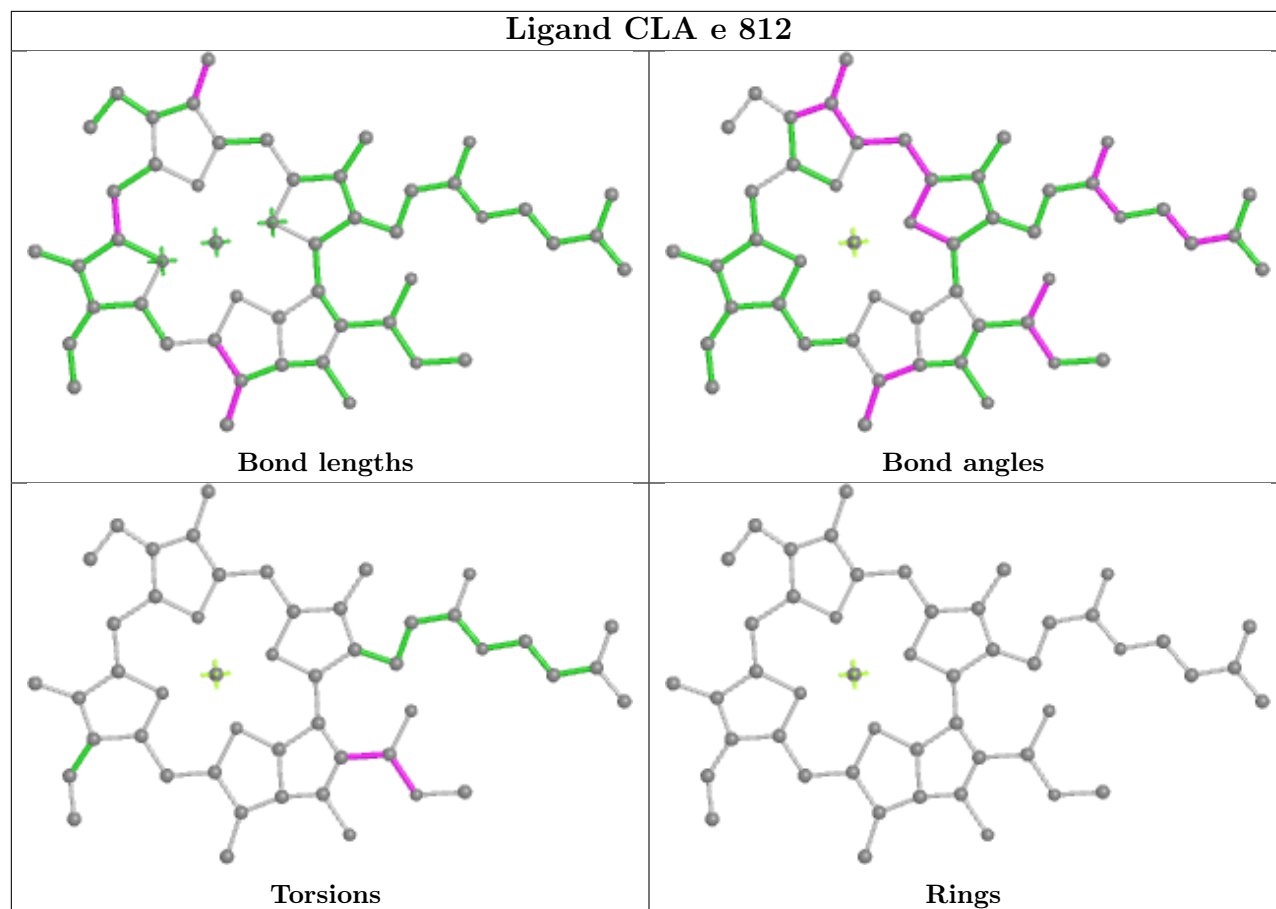
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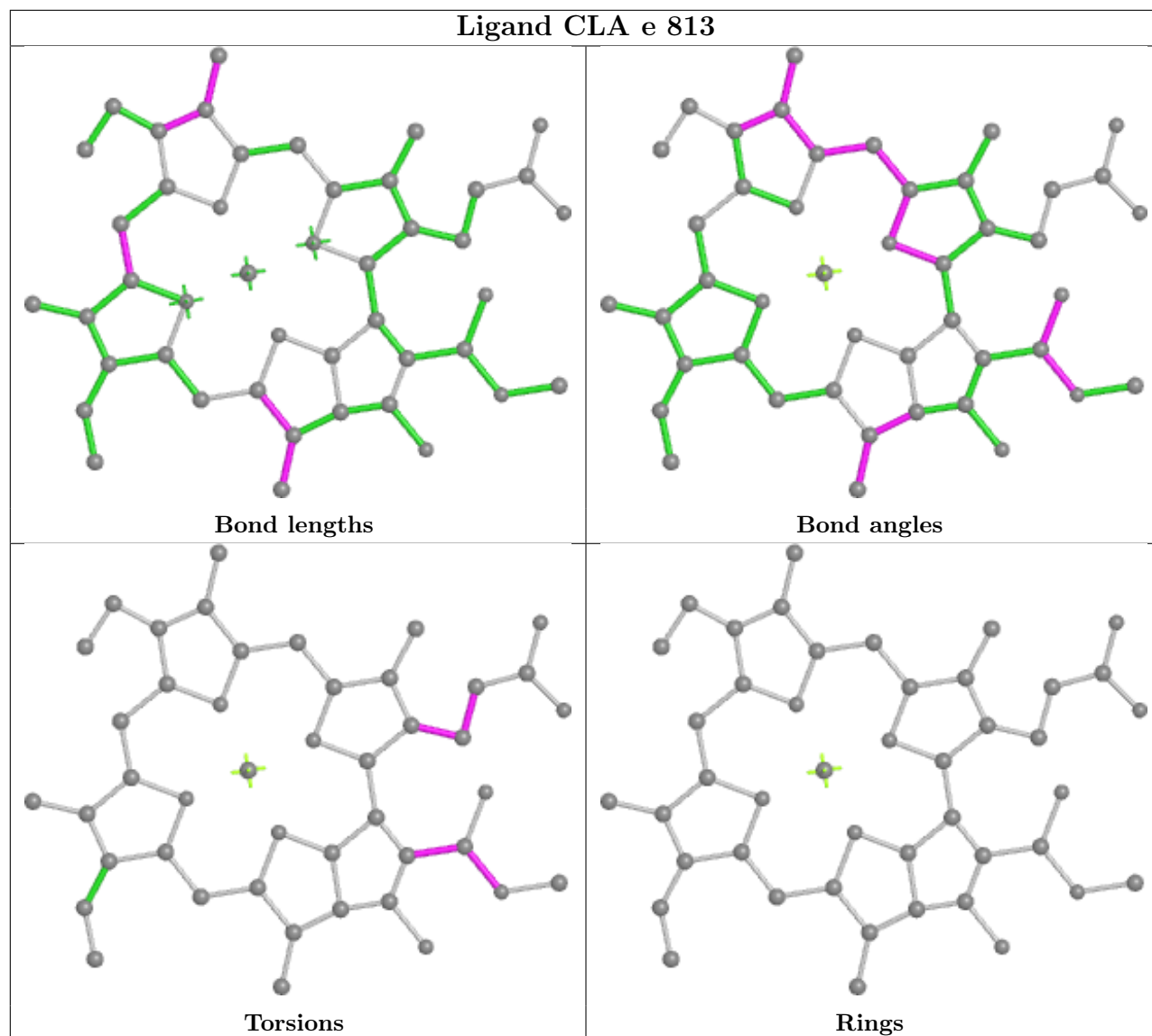
Ligand CLA e 811



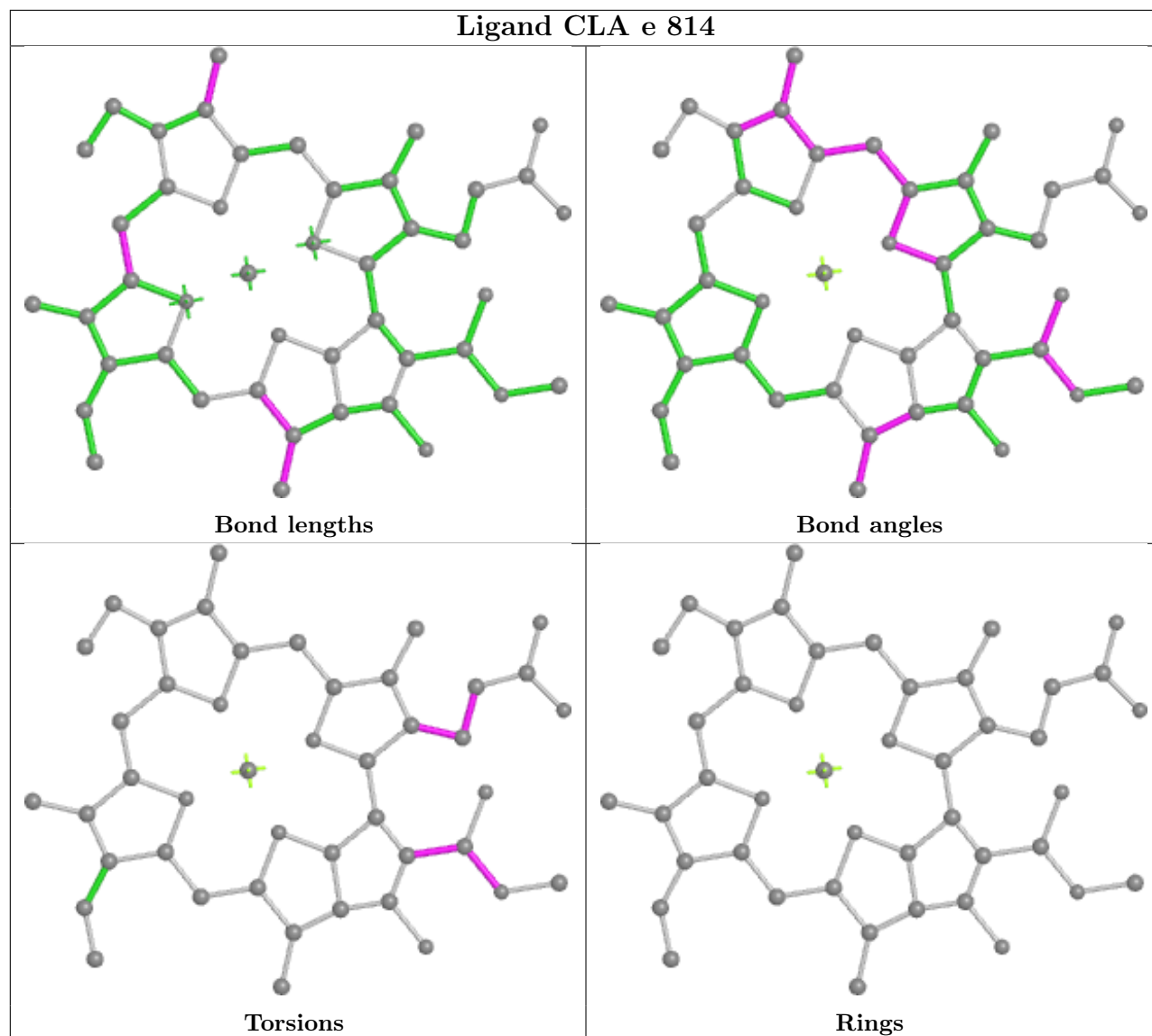
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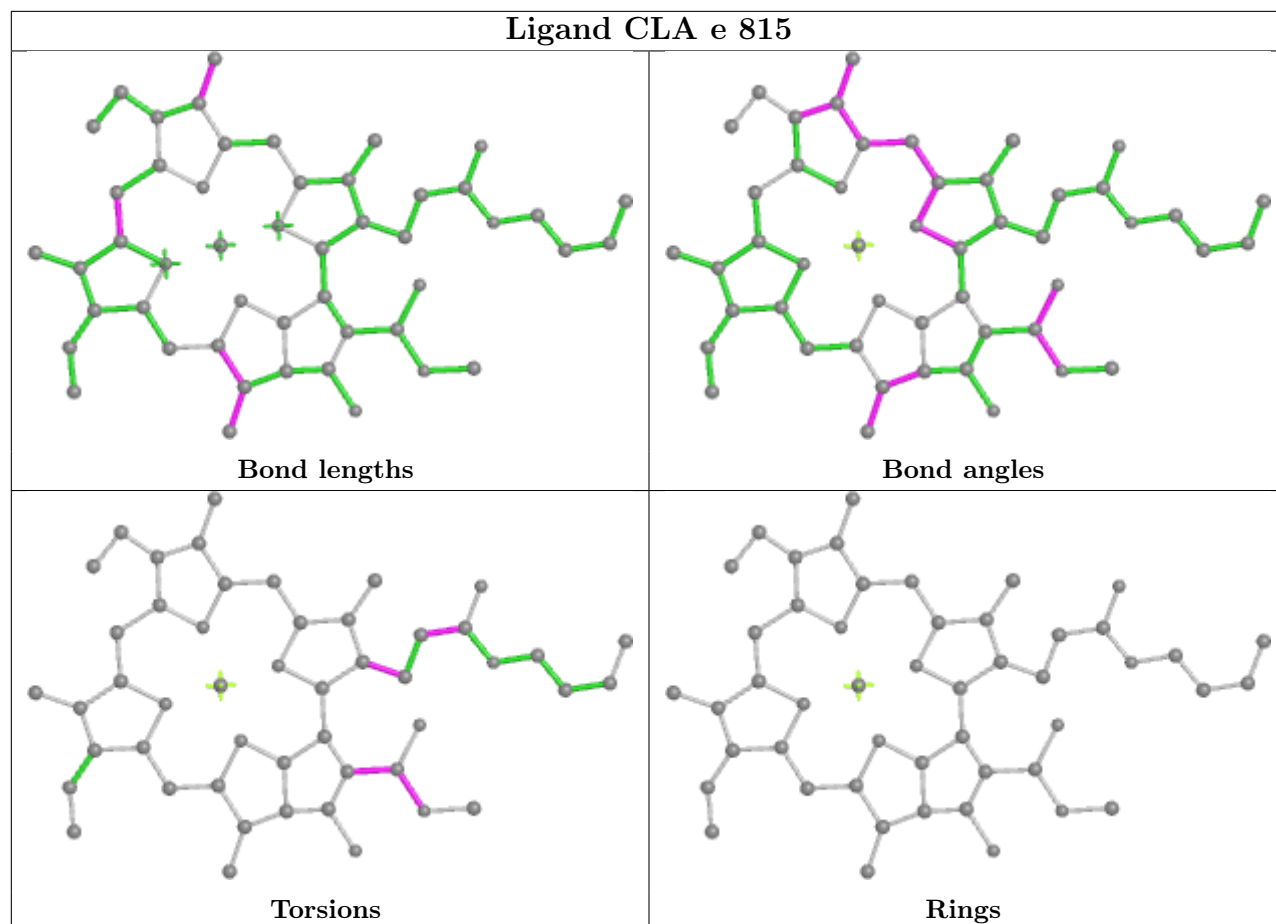
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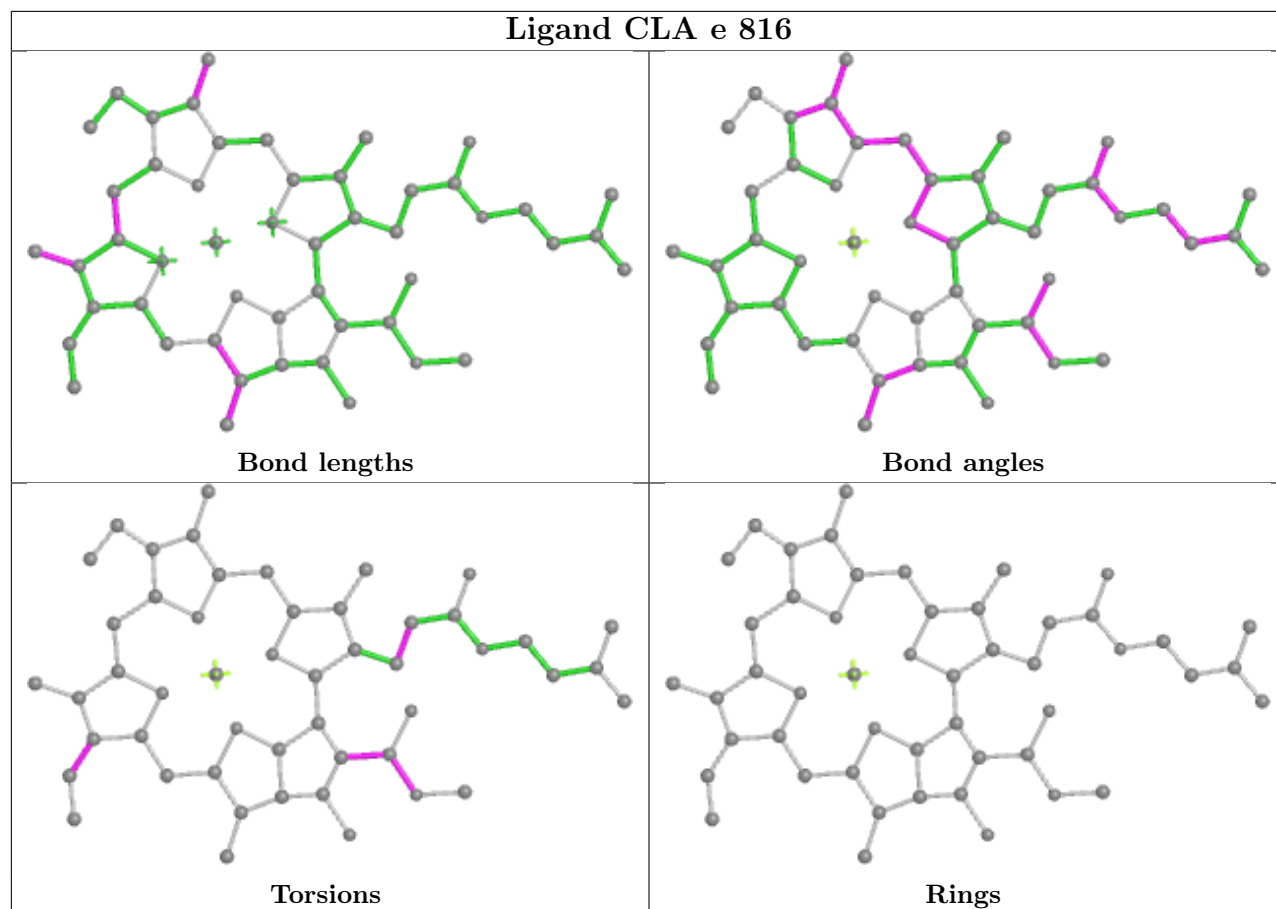
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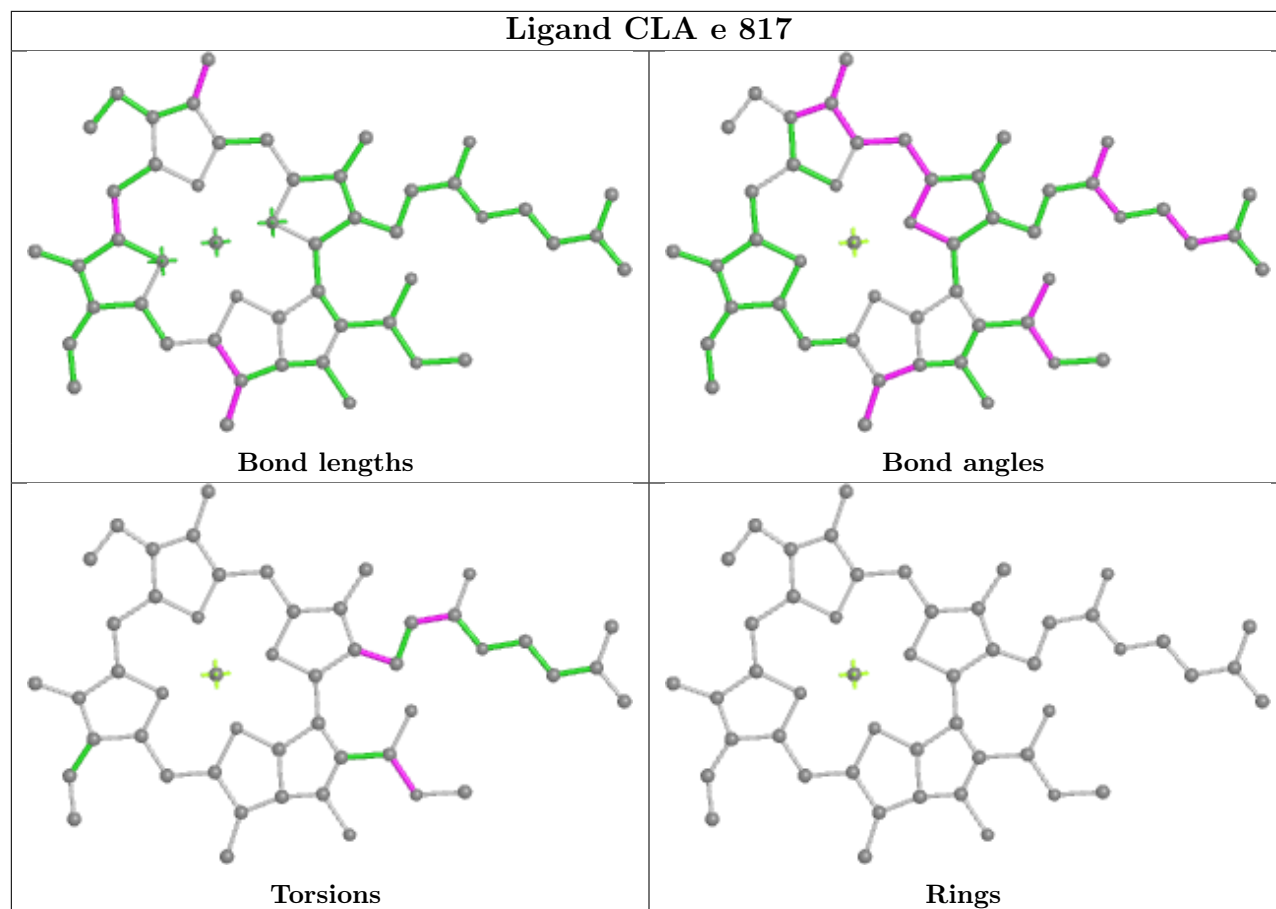
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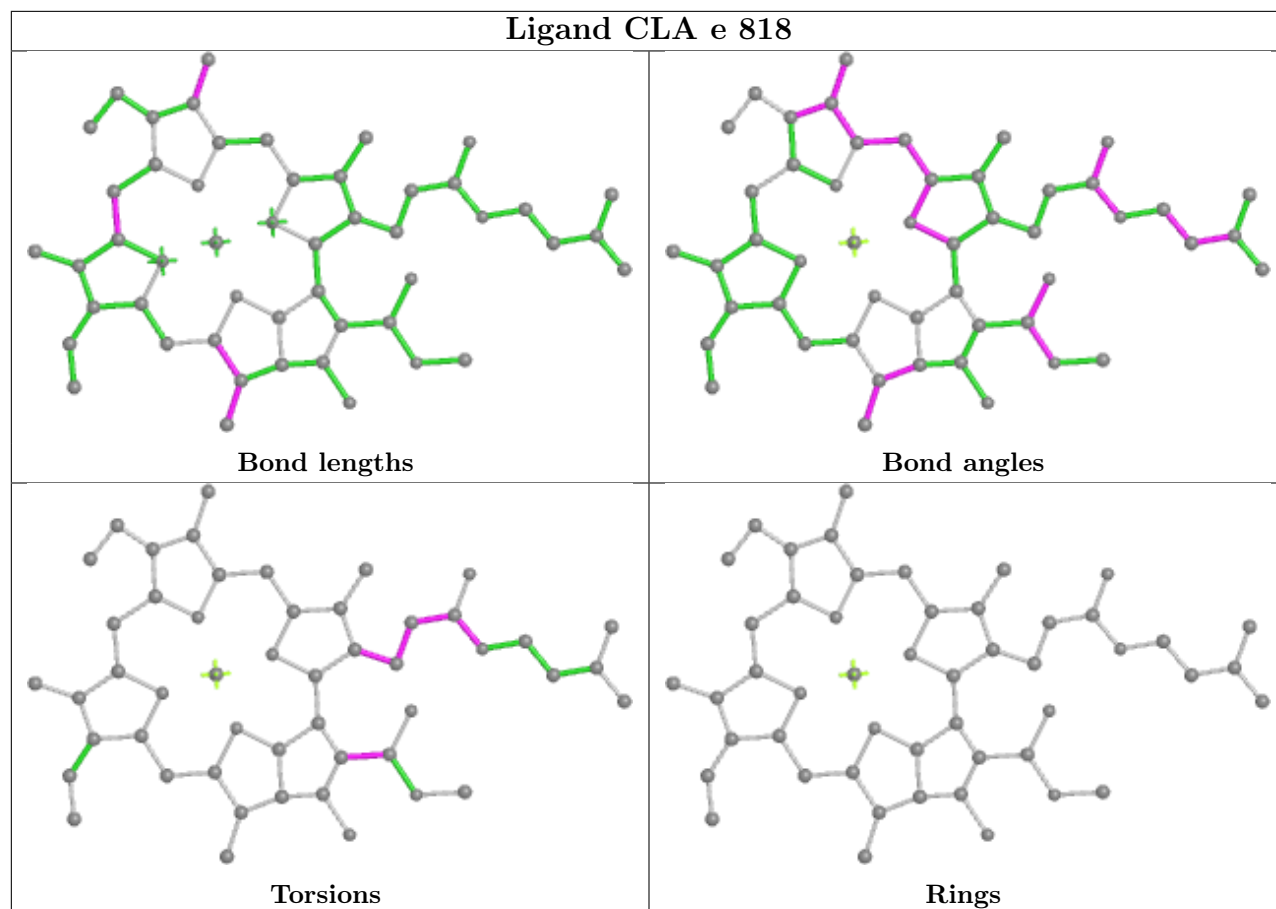
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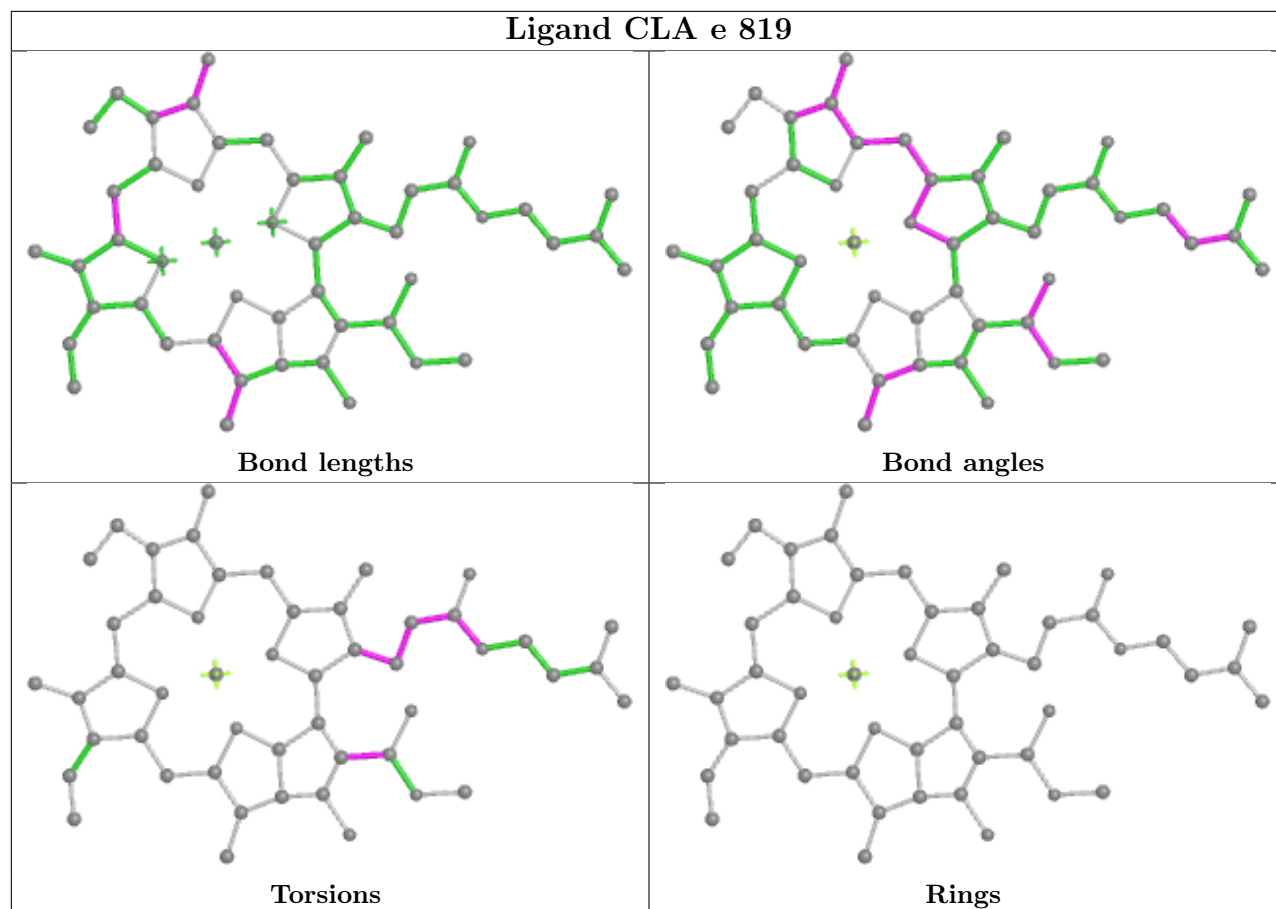
Ligand CLA e 817



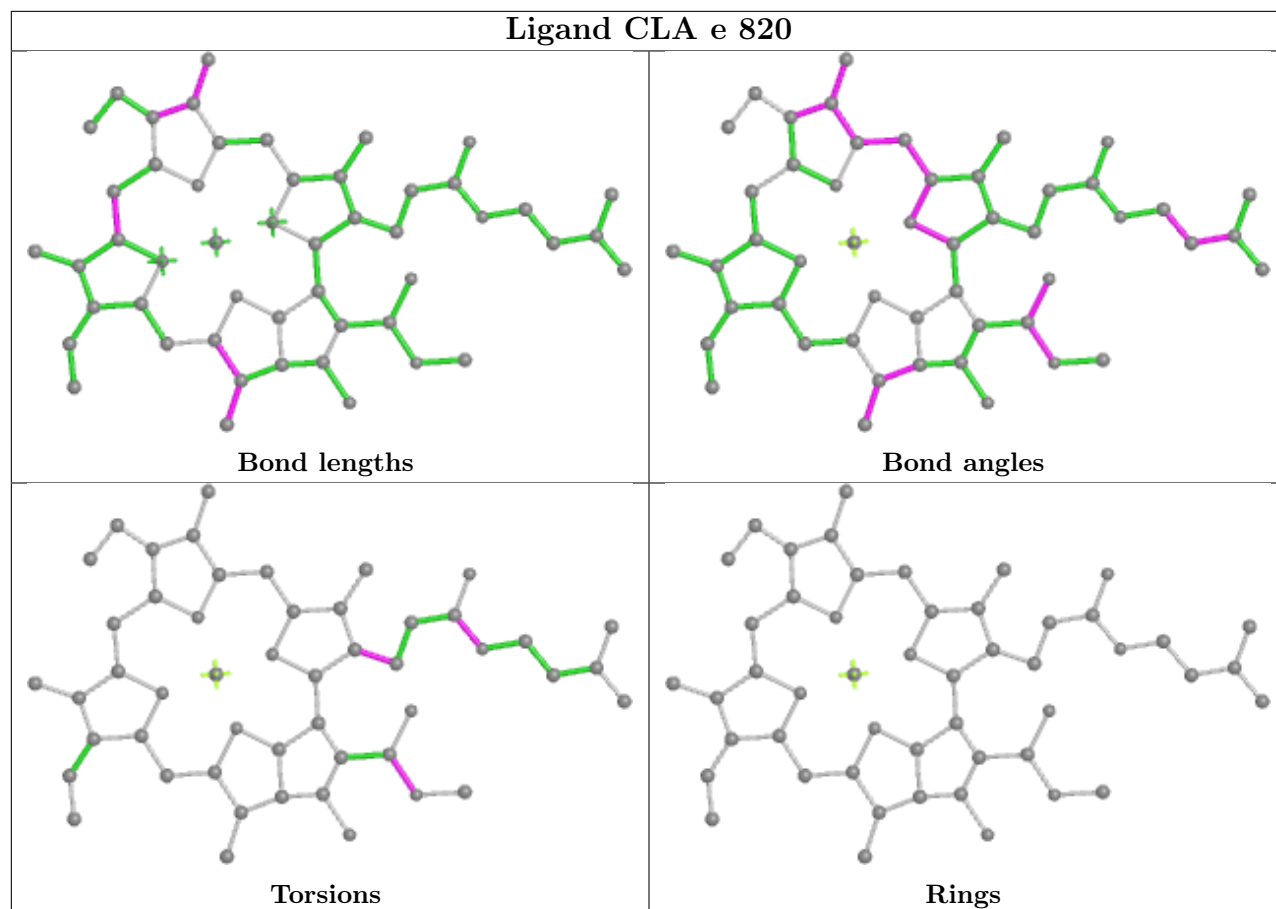
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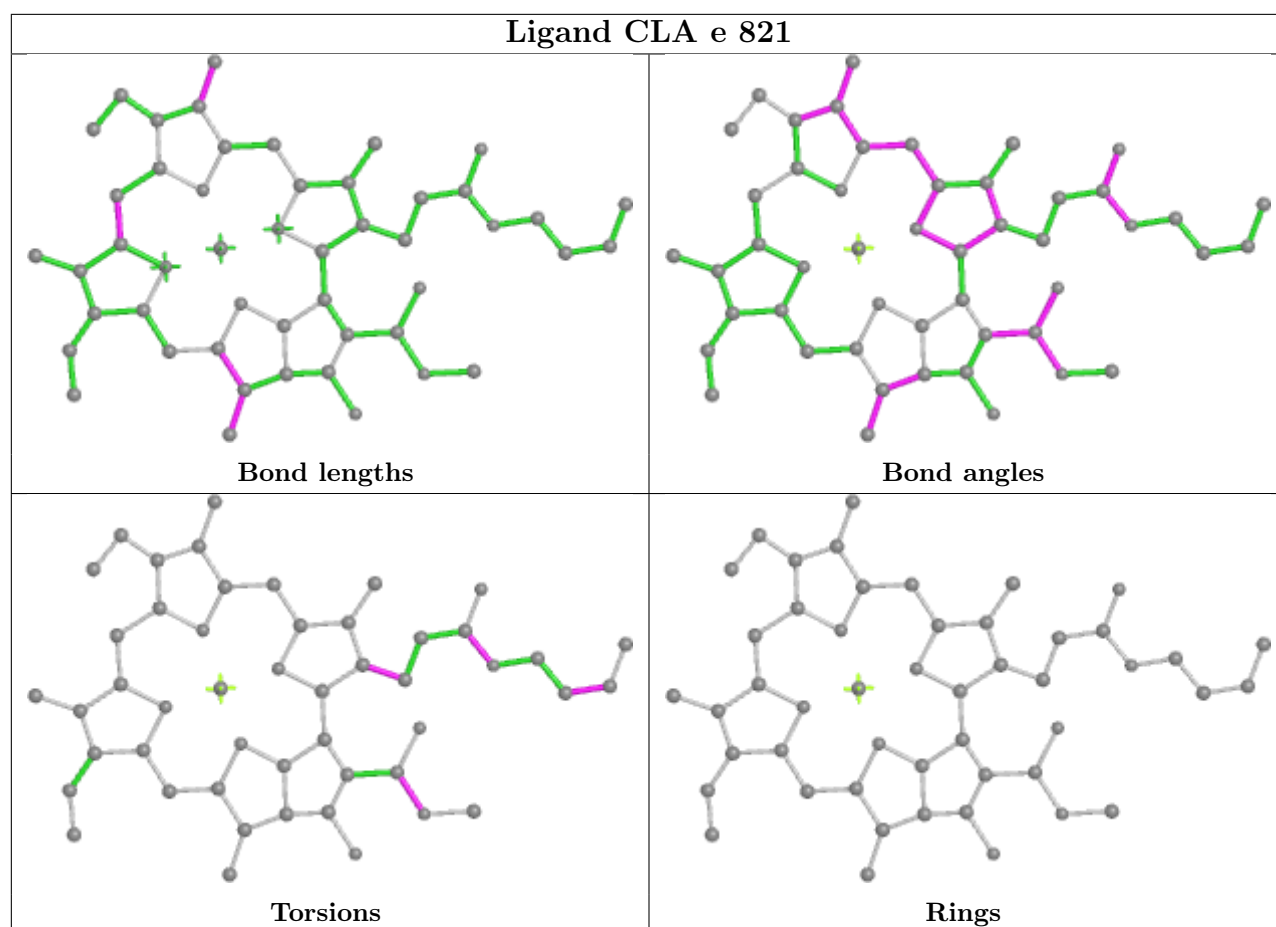


Ligand CLA e 819

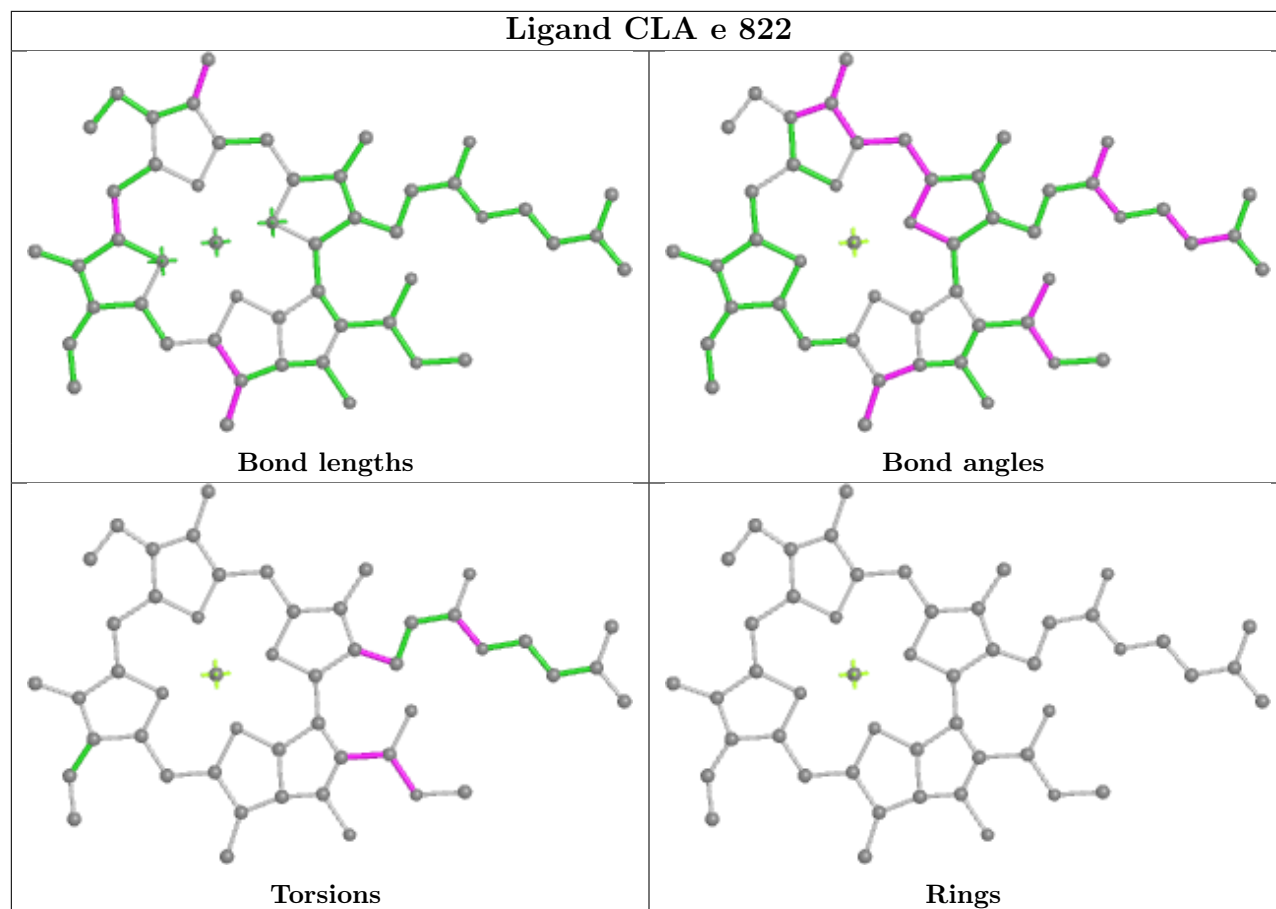


Ligand CLA e 820

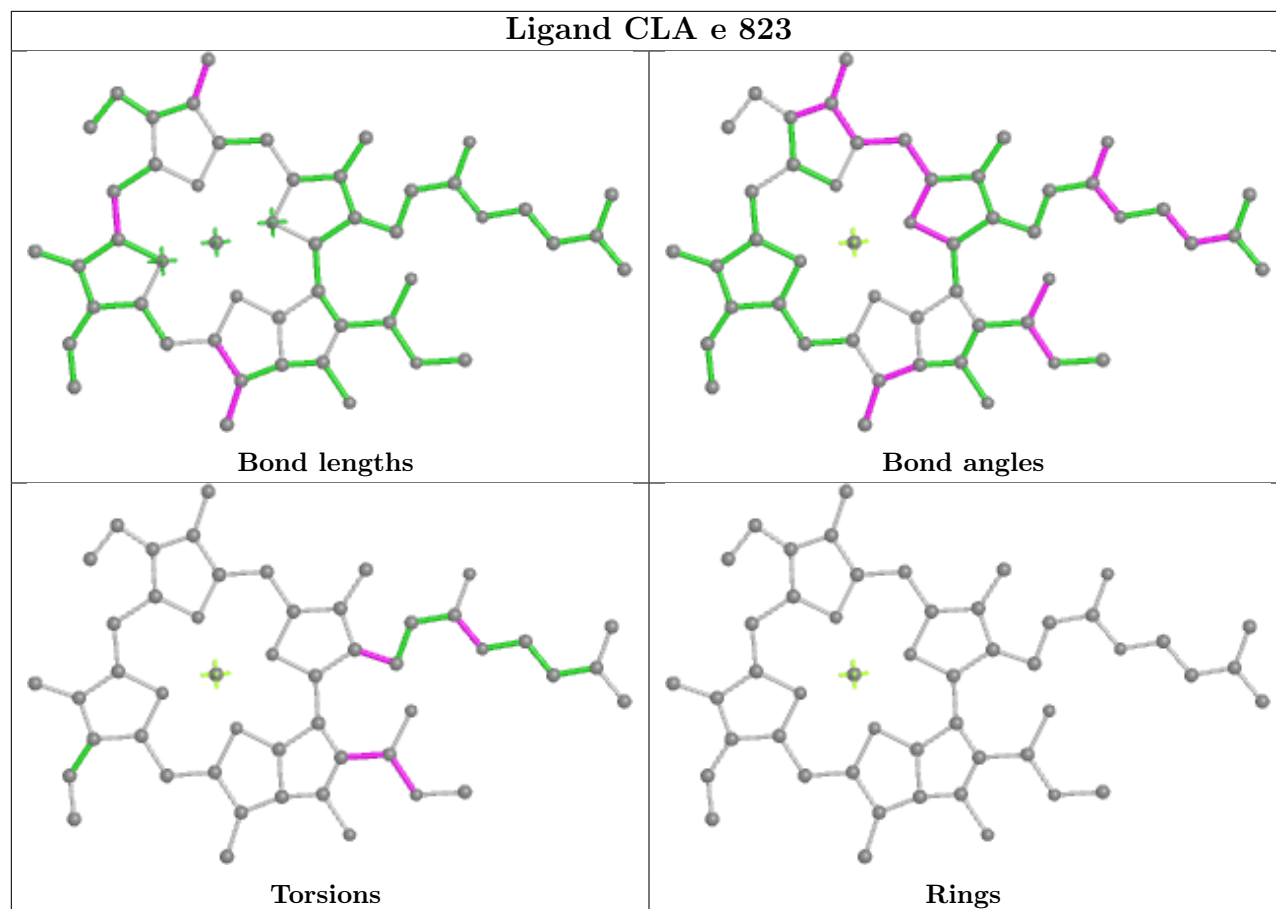




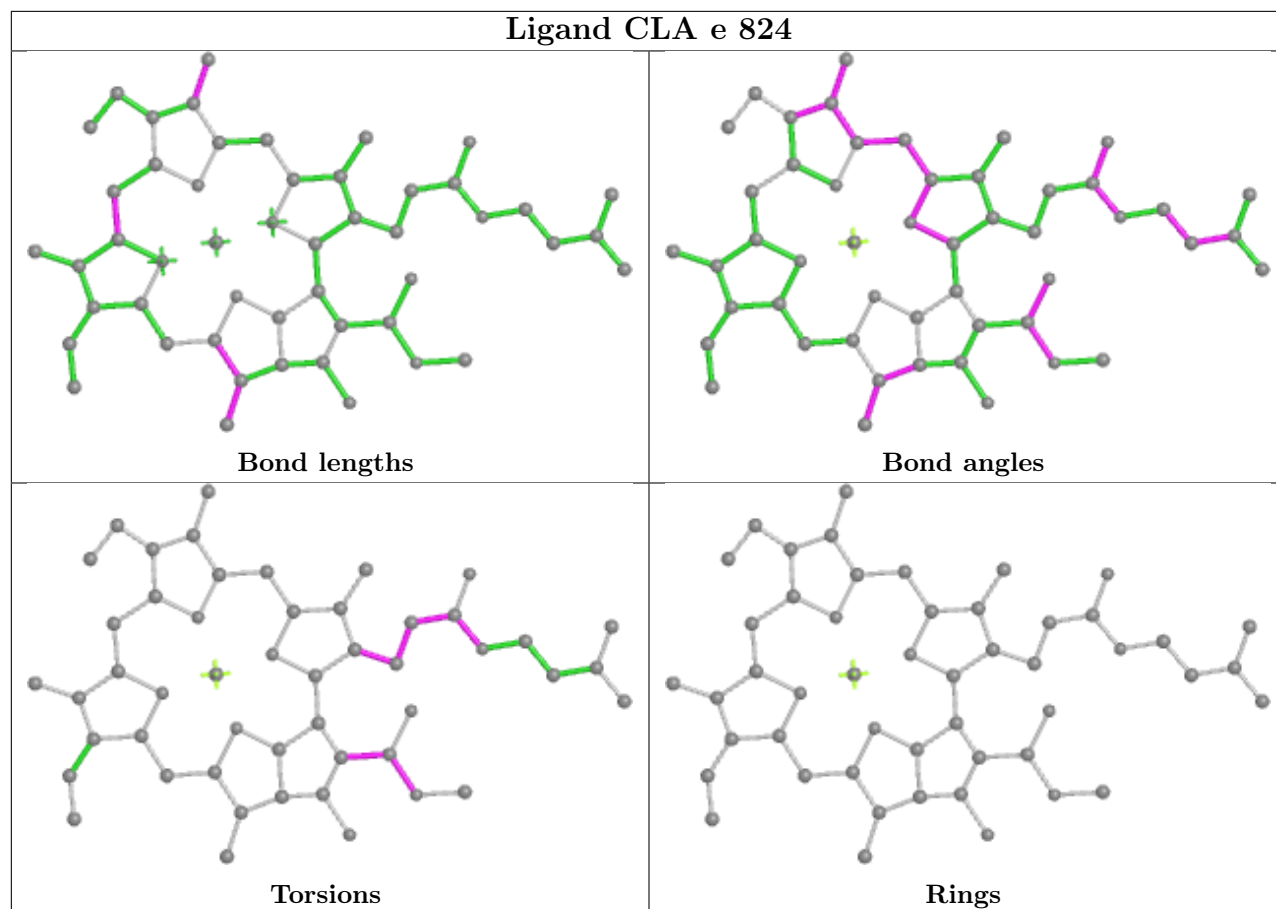
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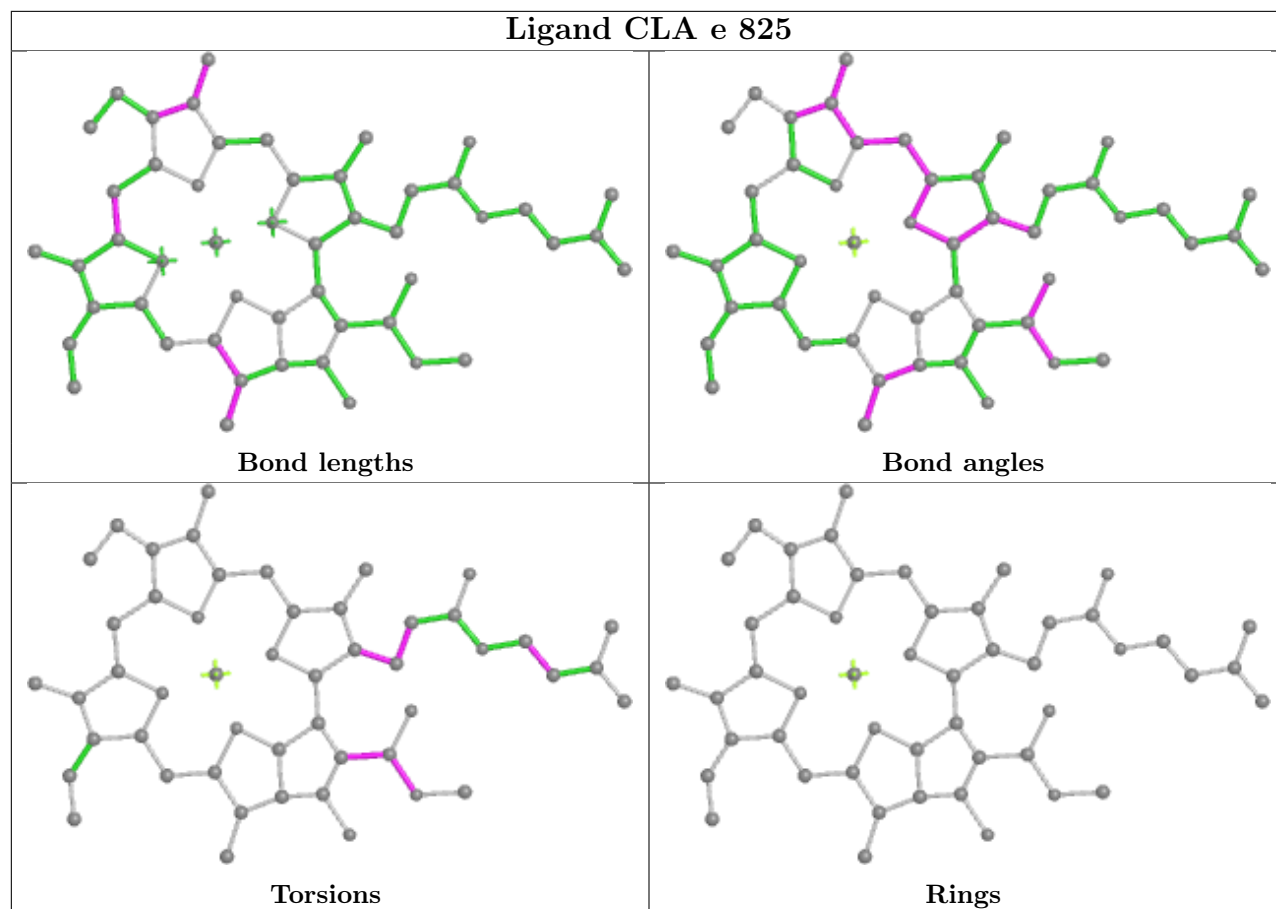
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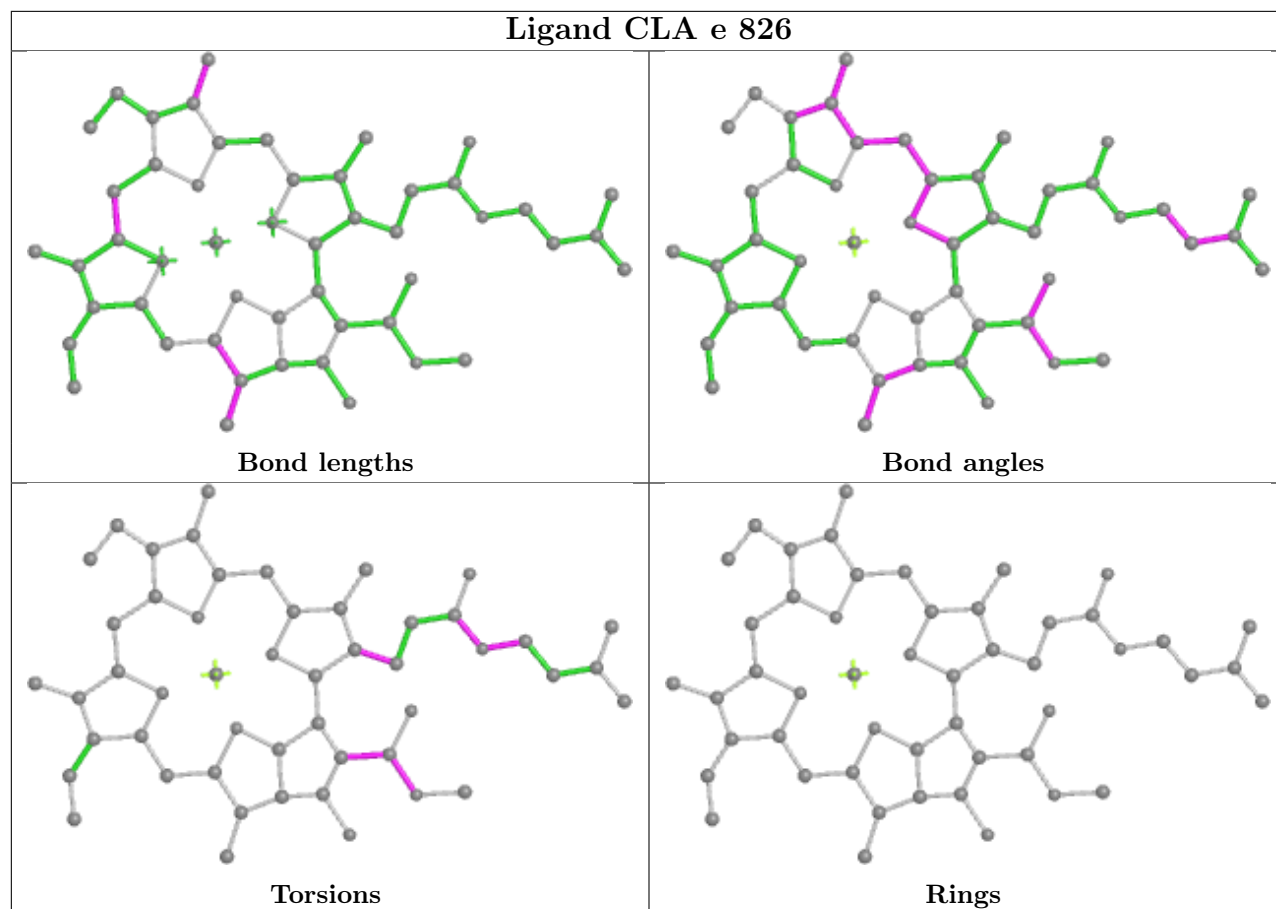
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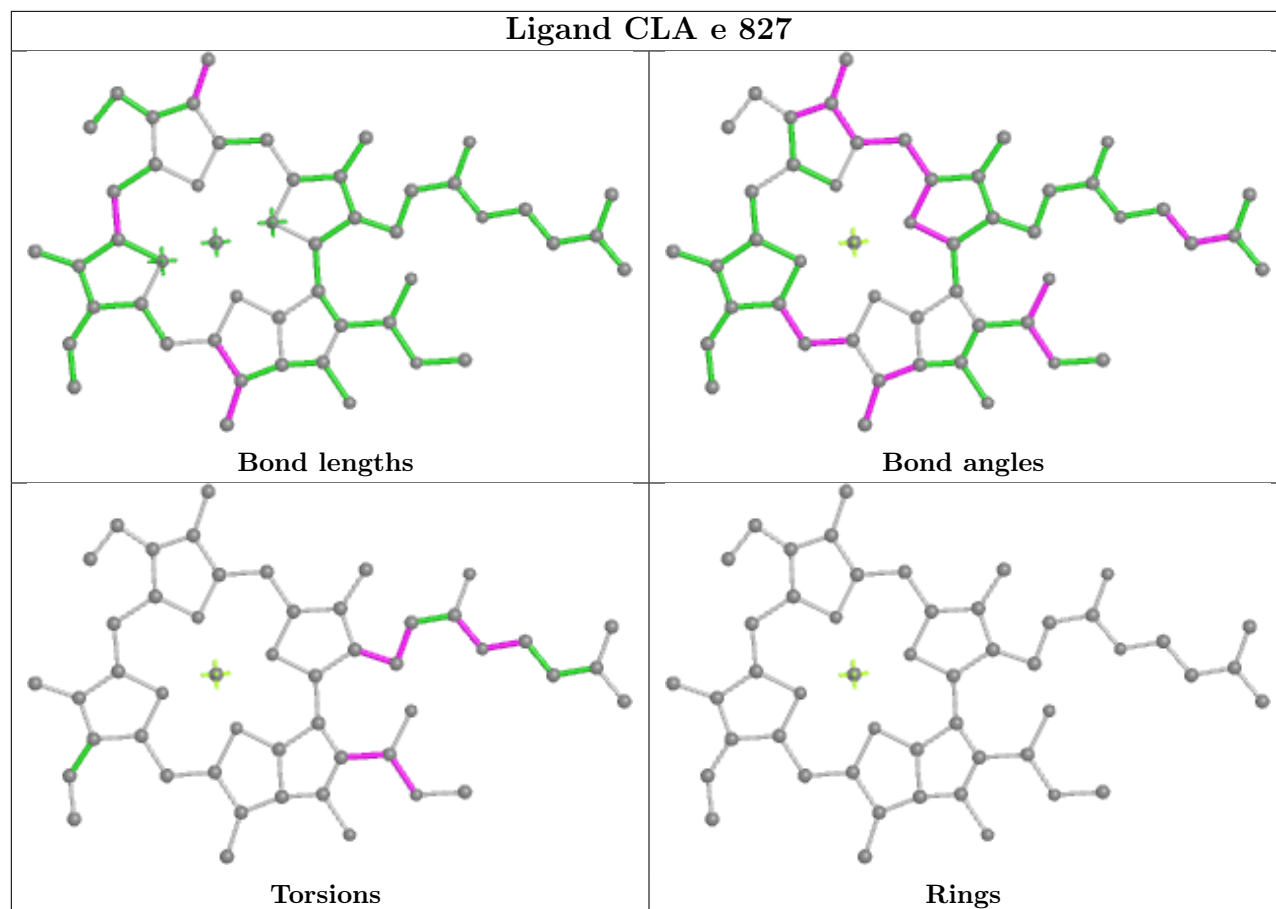
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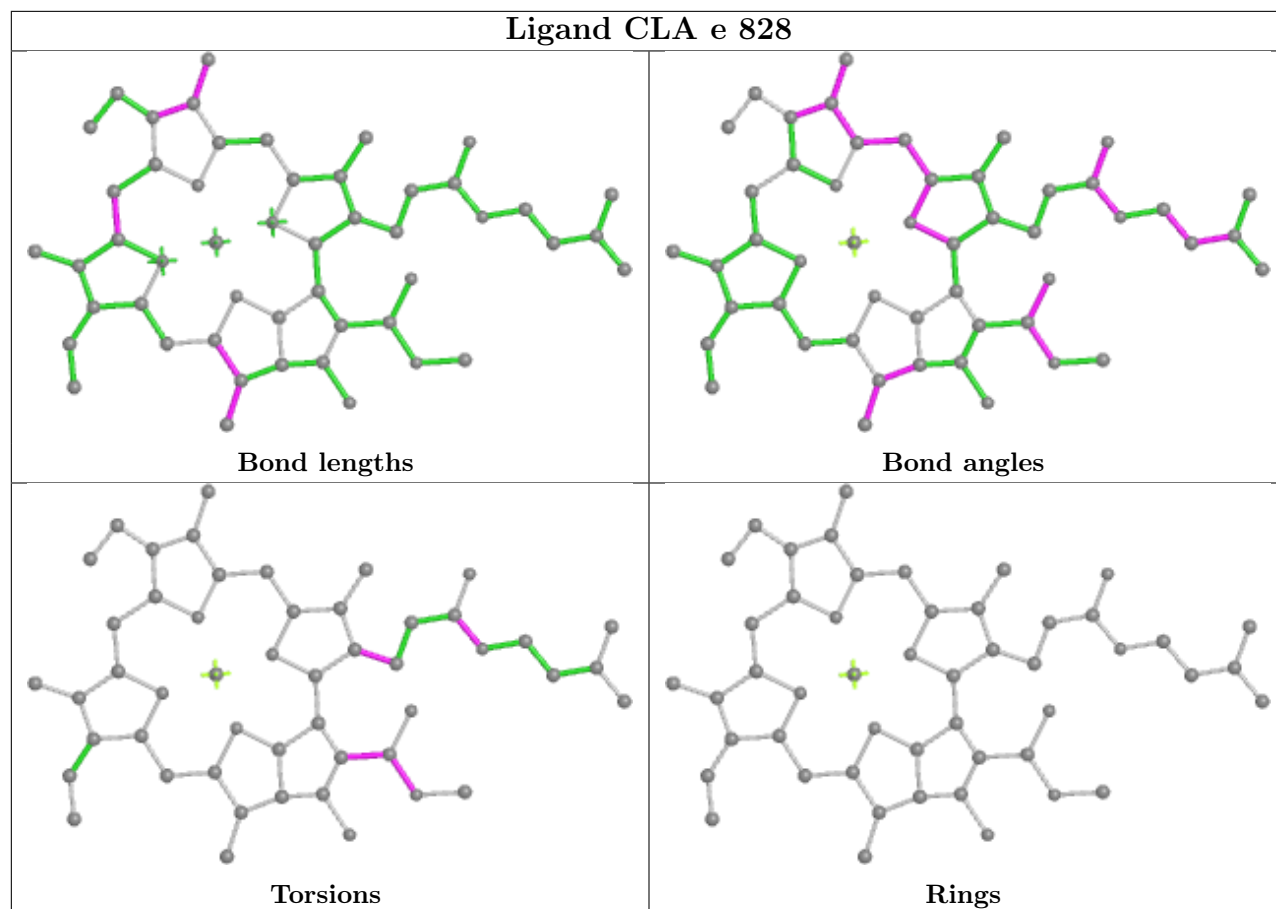
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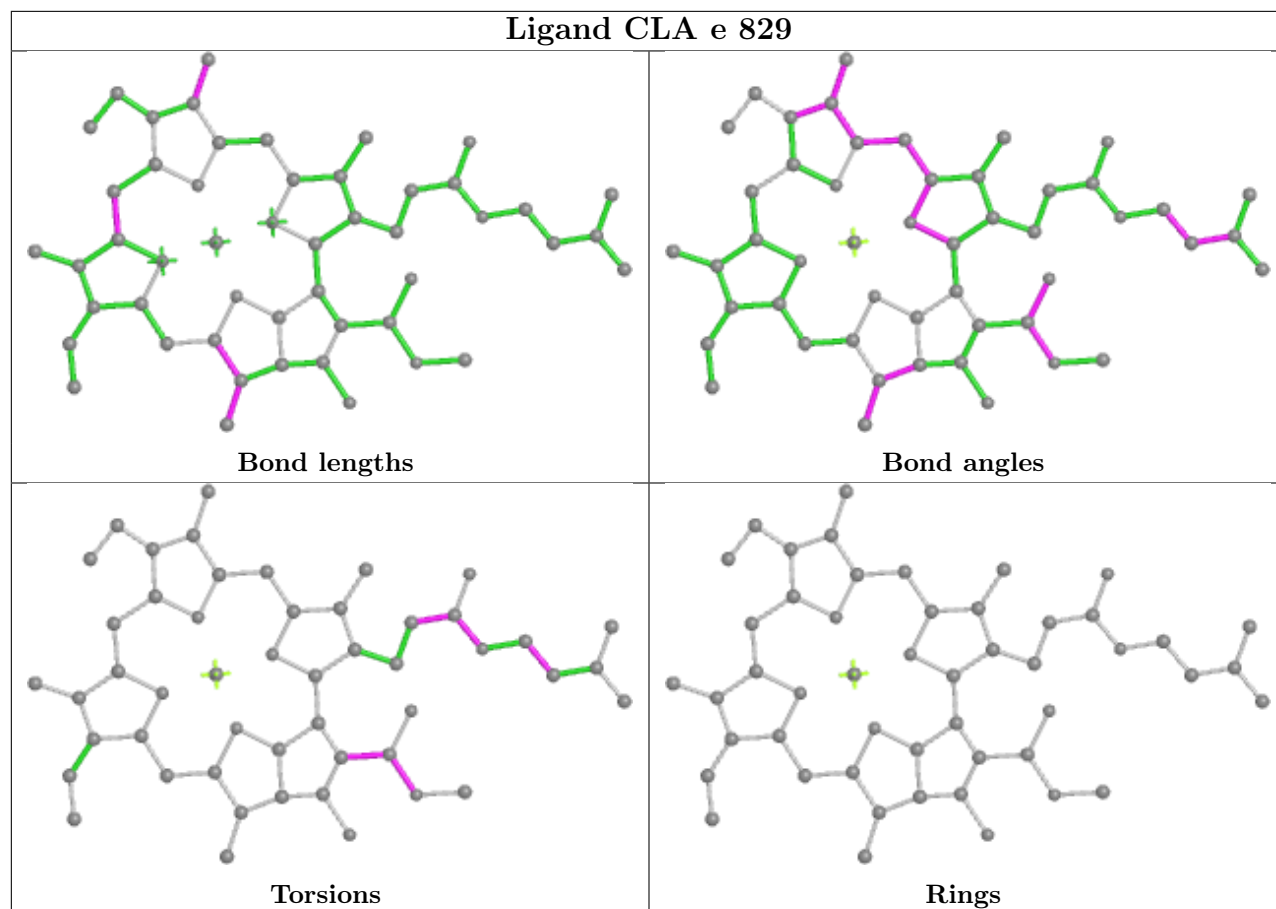
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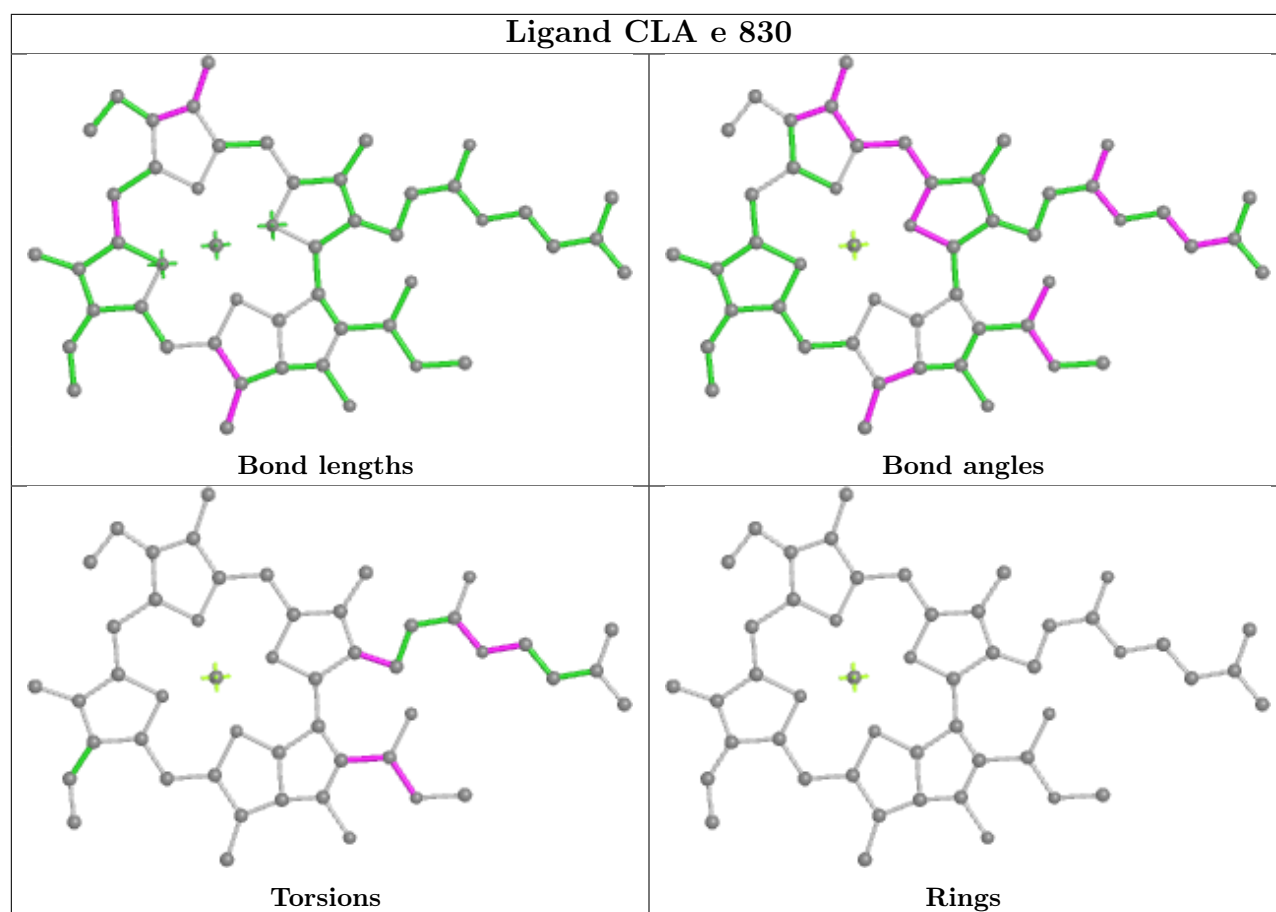


Ligand CLA e 828

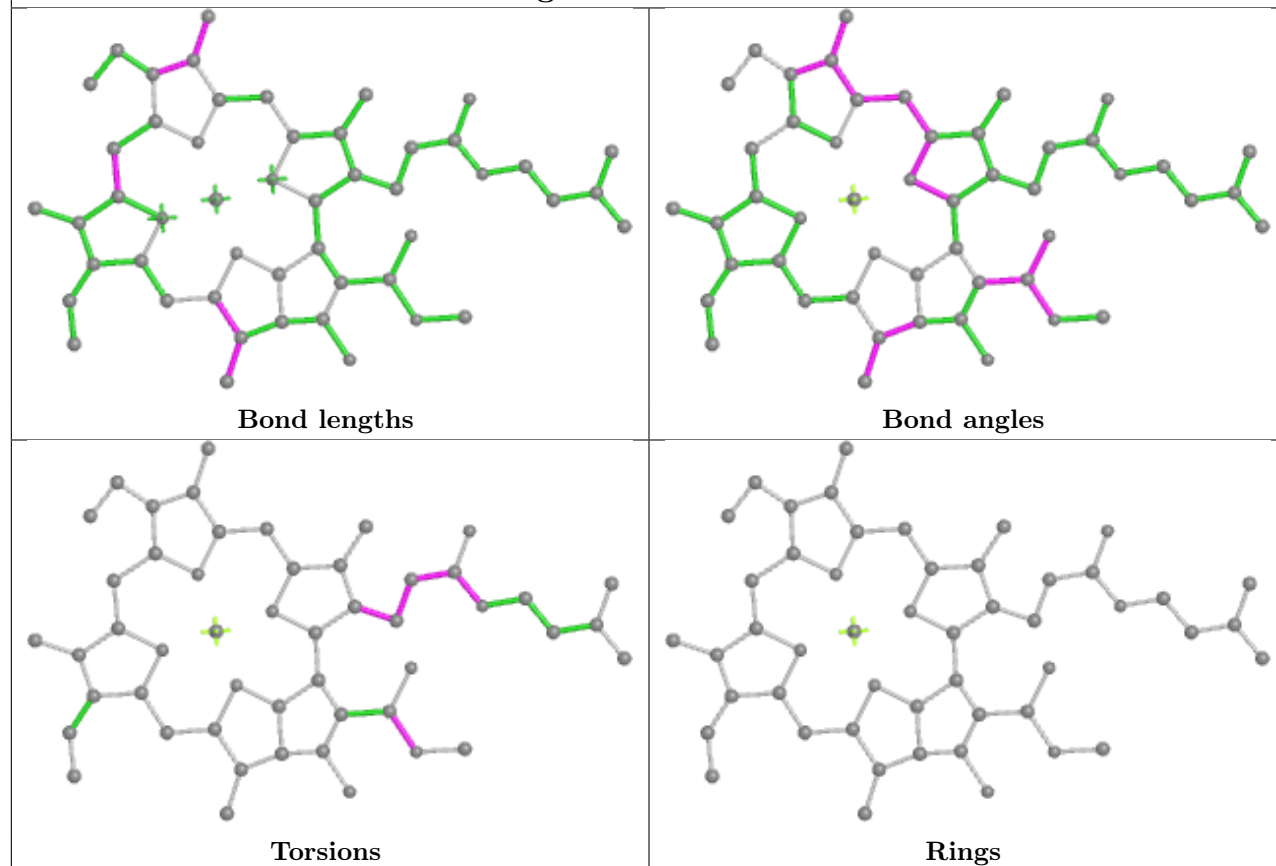


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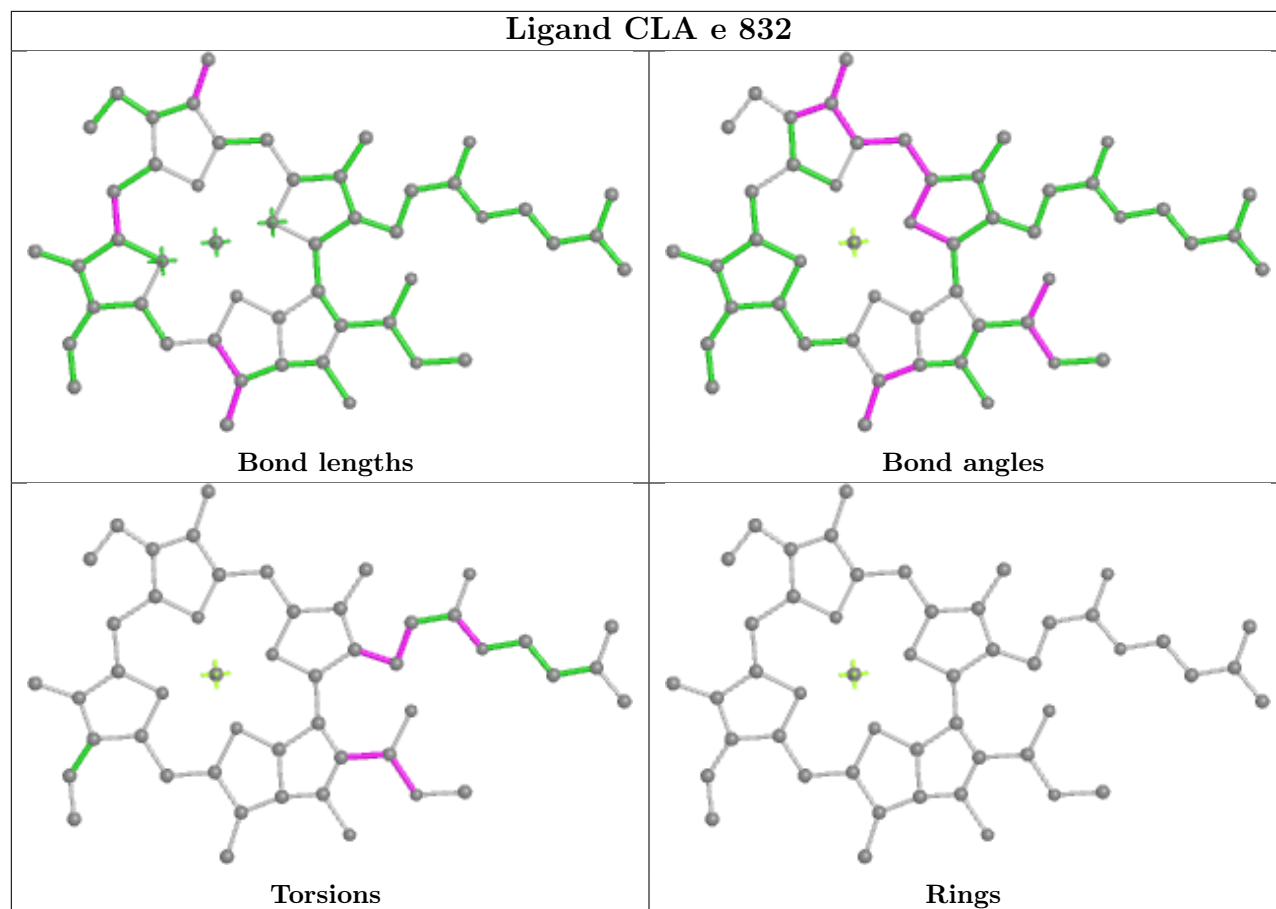




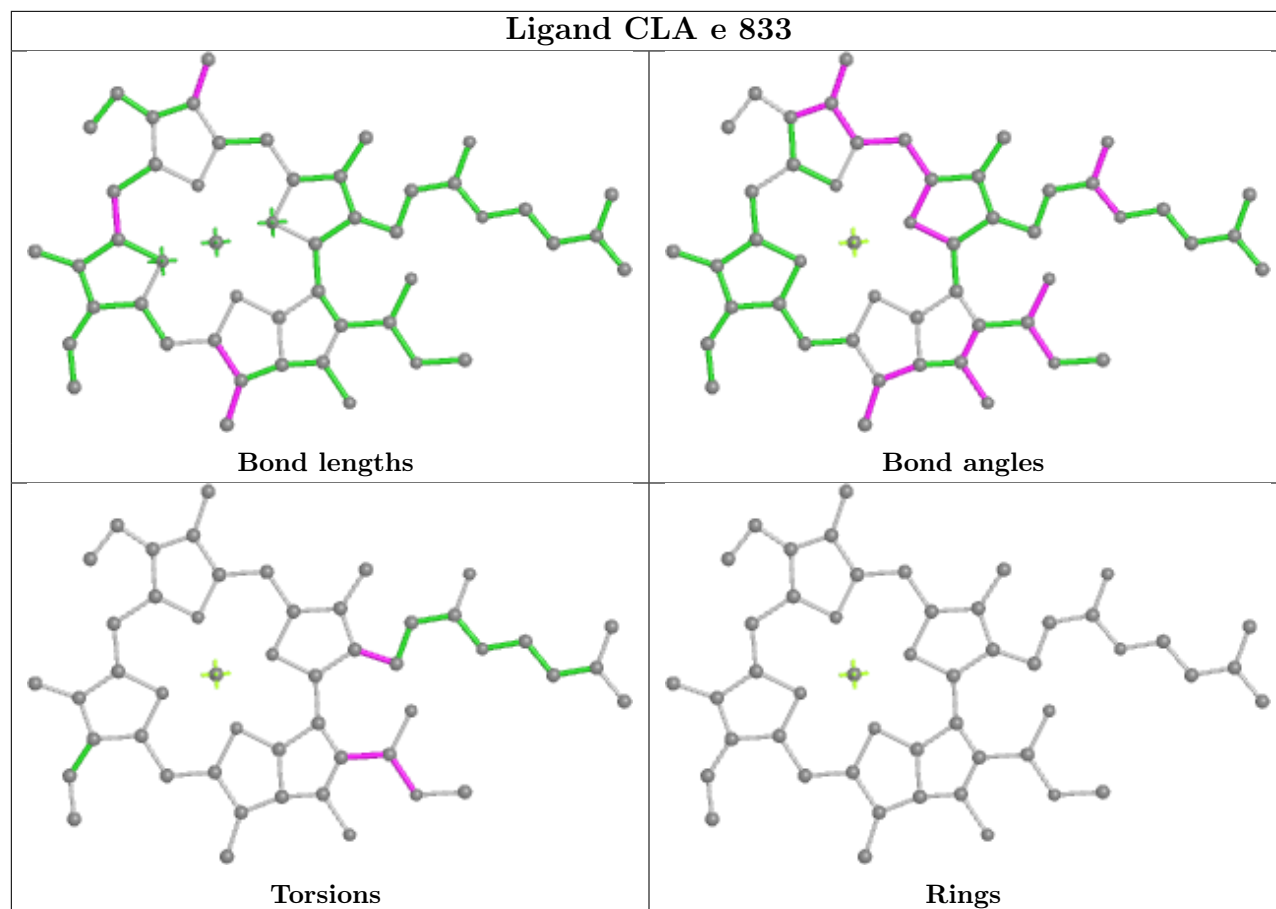
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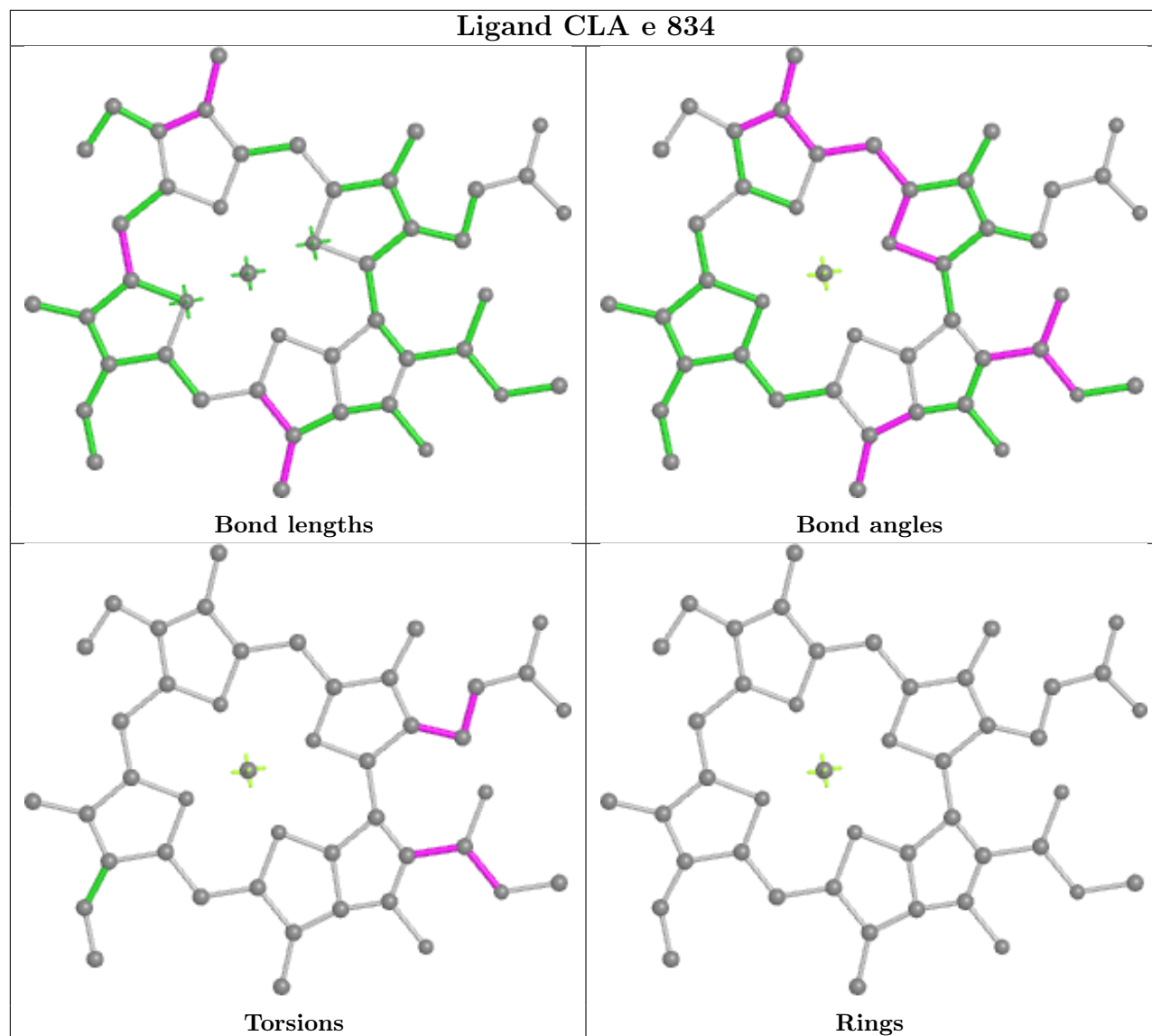
Ligand CLA e 832



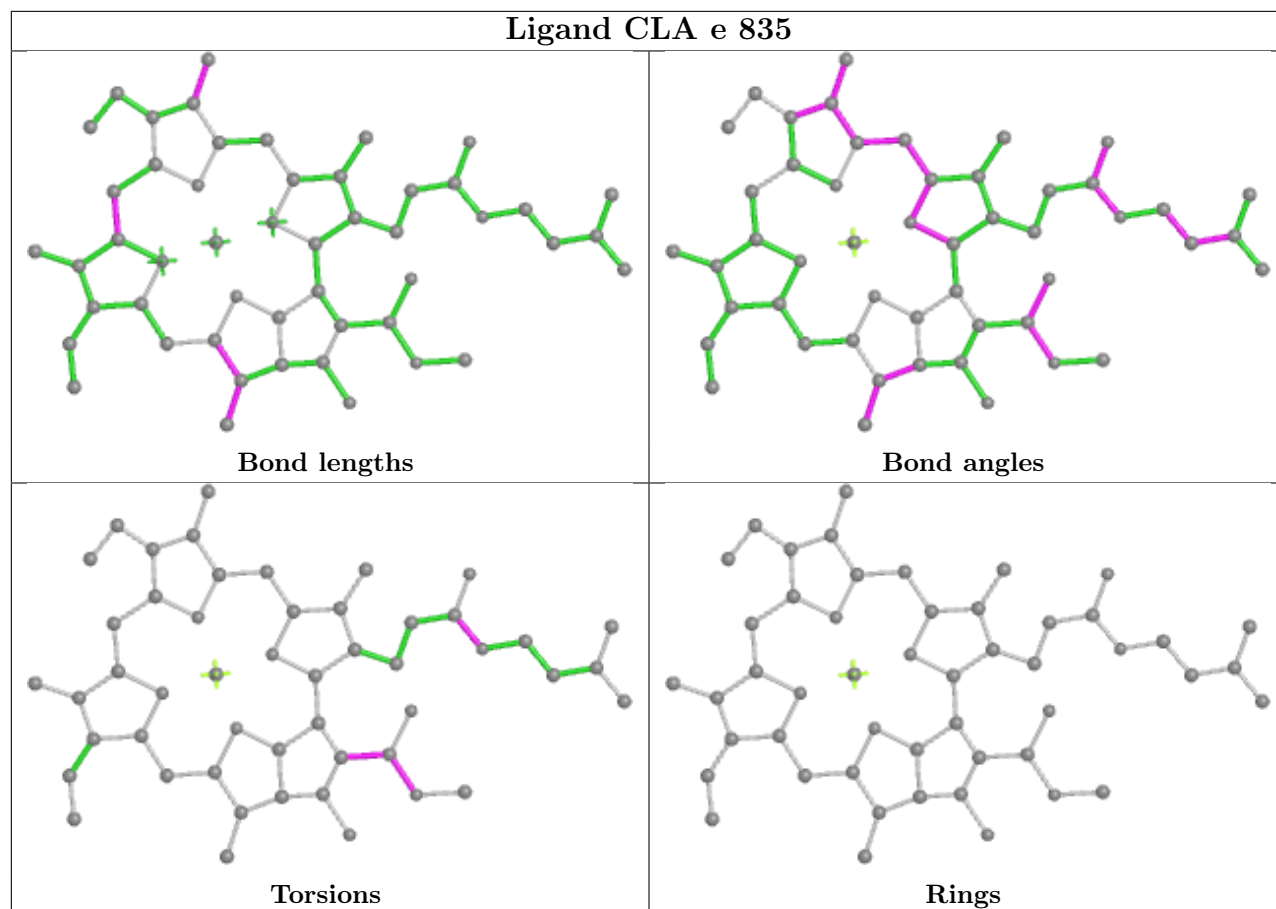
Ligand CLA e 833



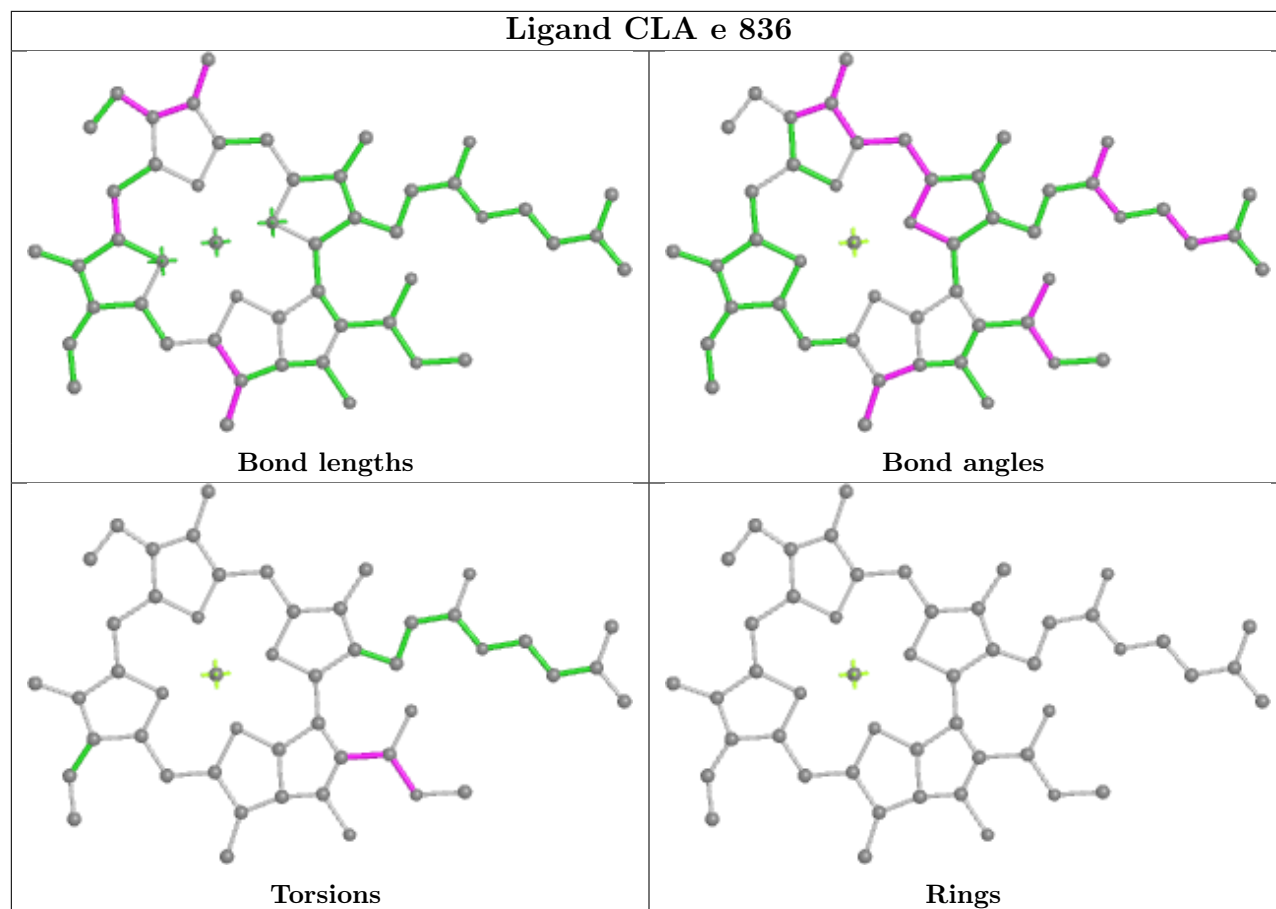
Ligand CLA e 834



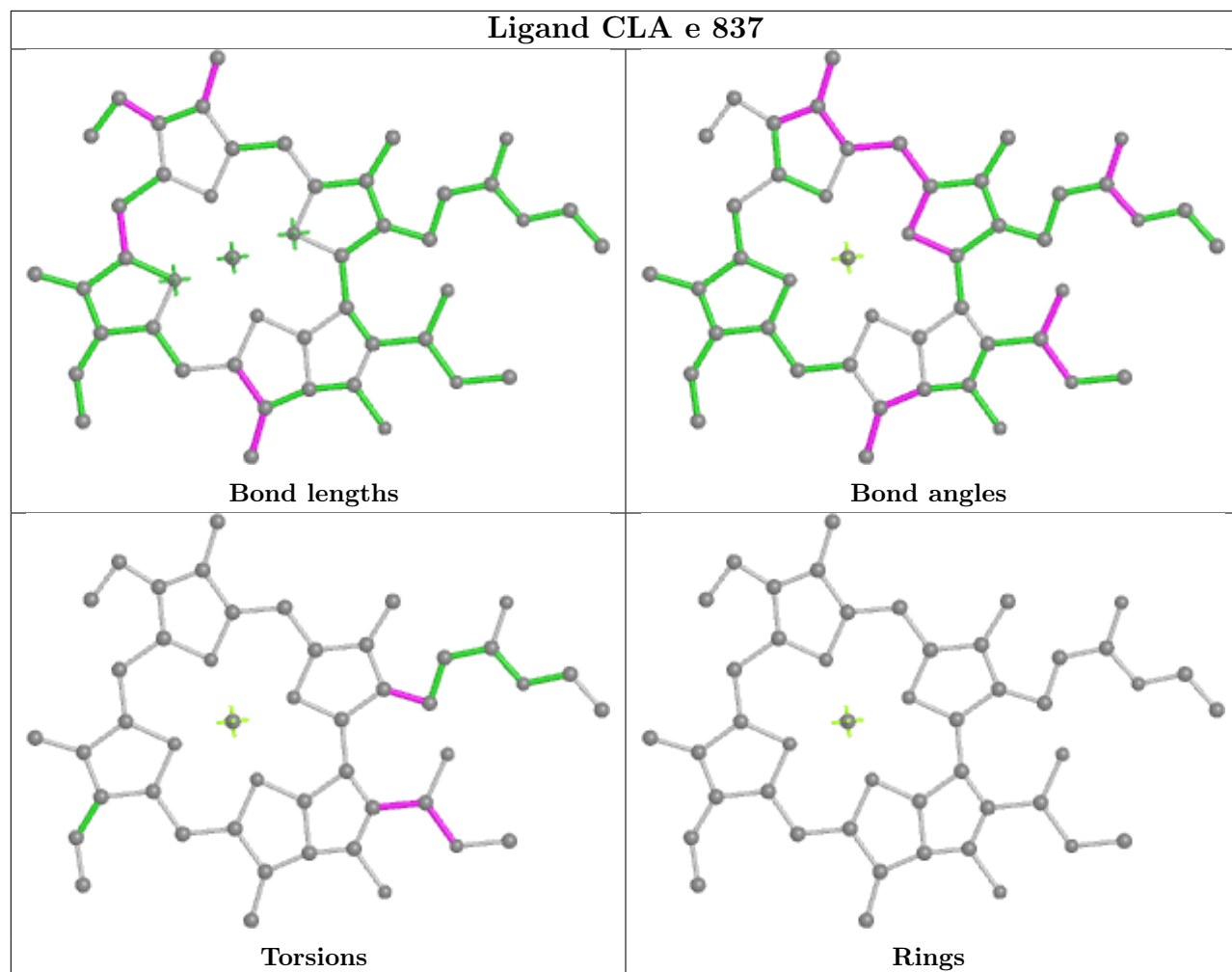
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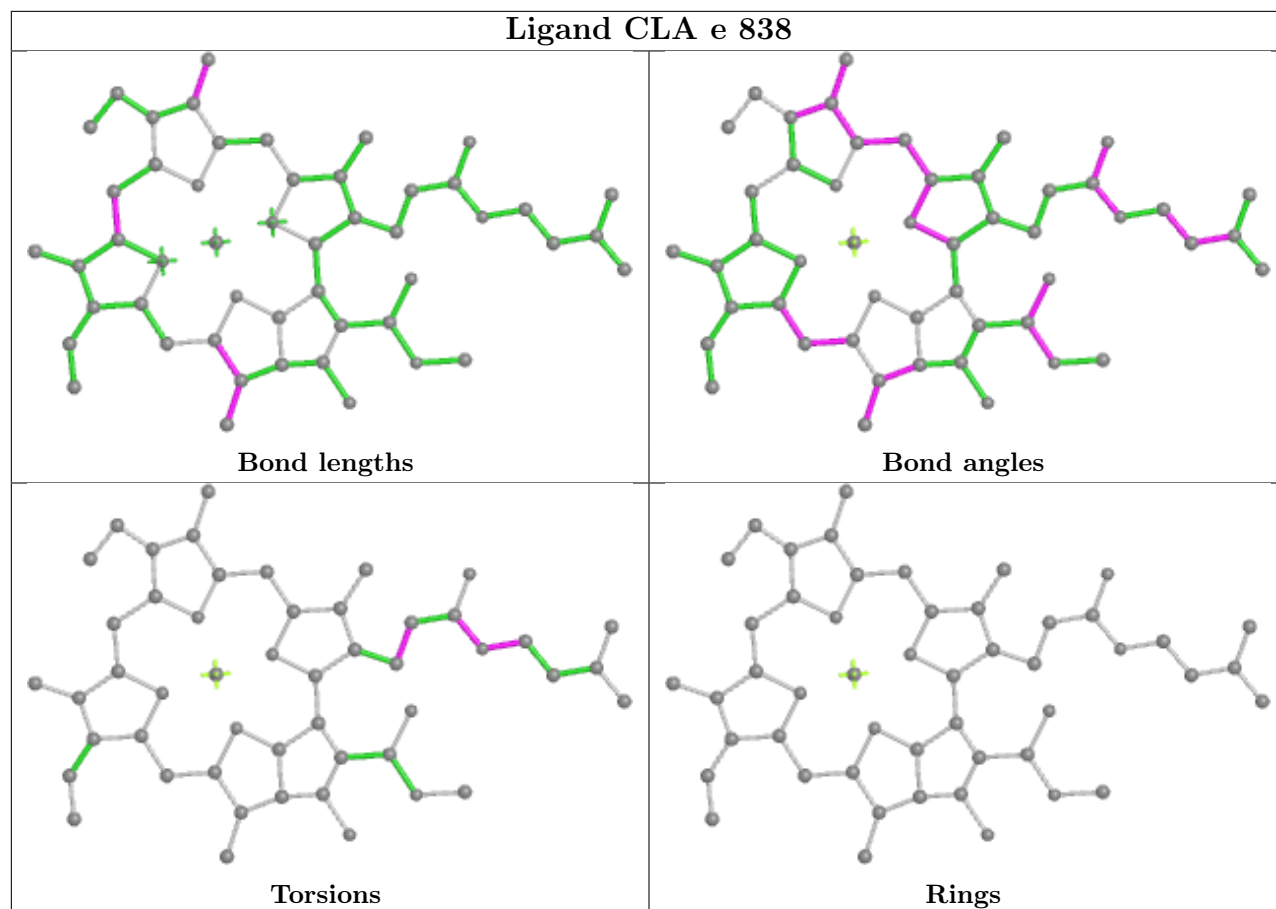
Ligand CLA e 836



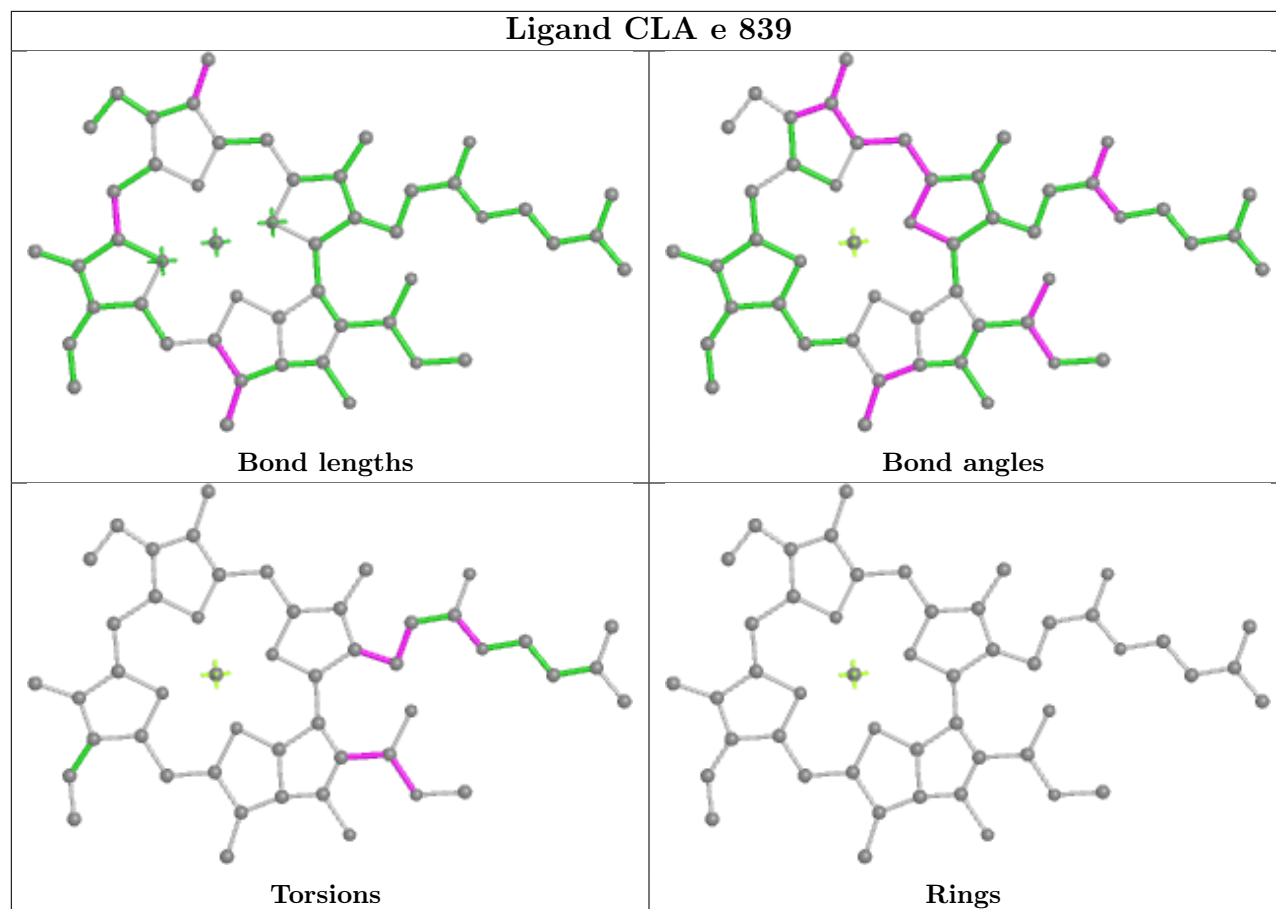
Ligand CLA e 837

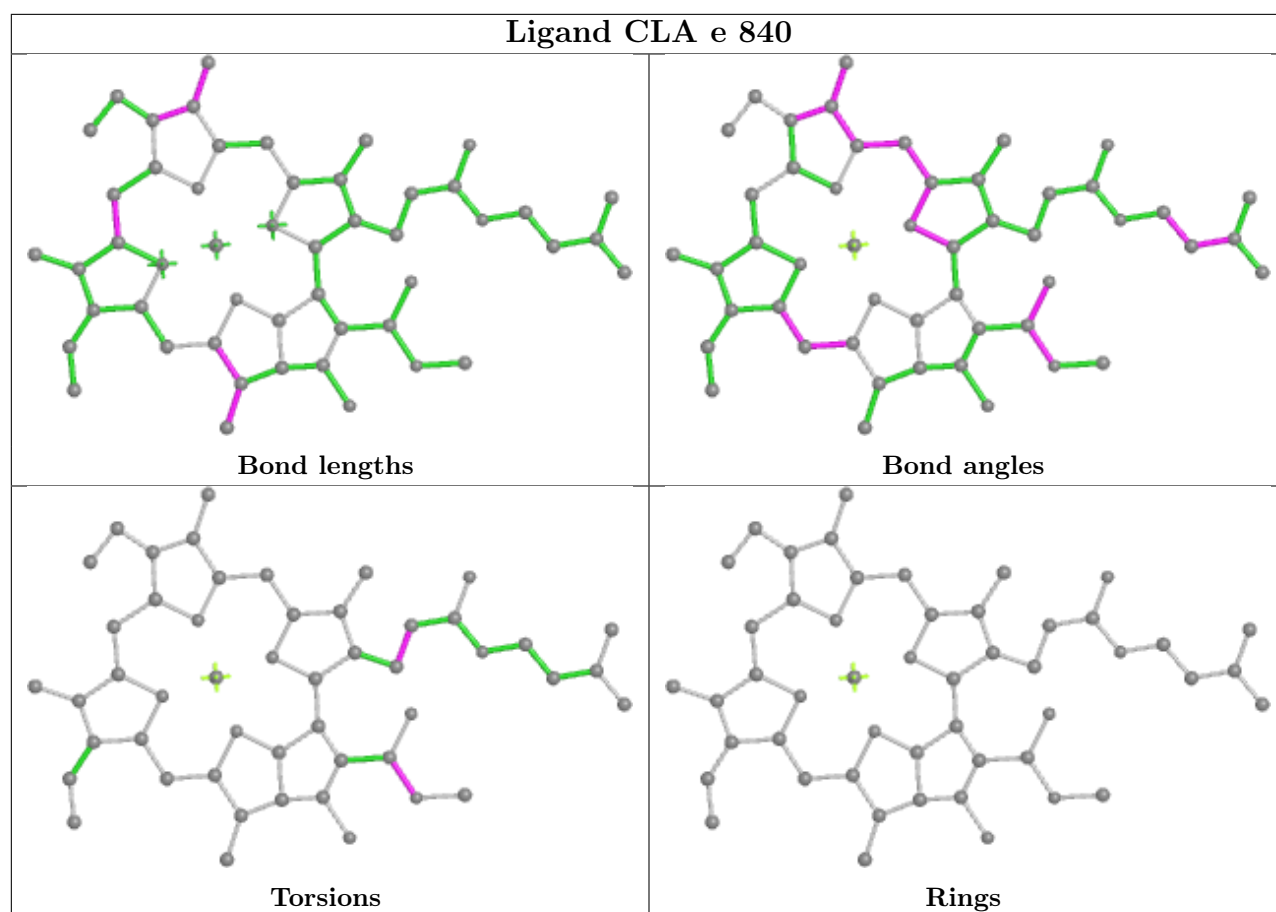


Ligand CLA e 838

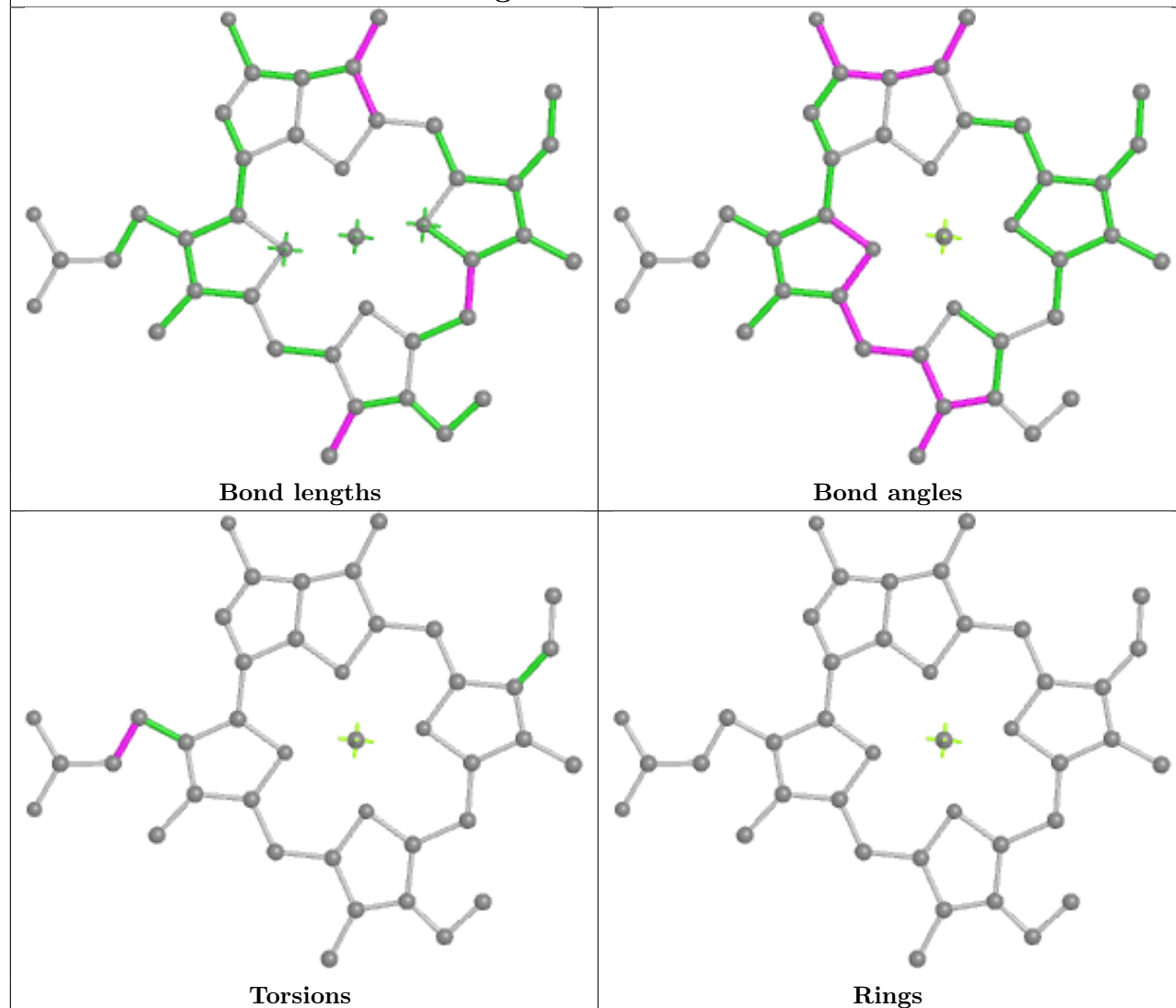


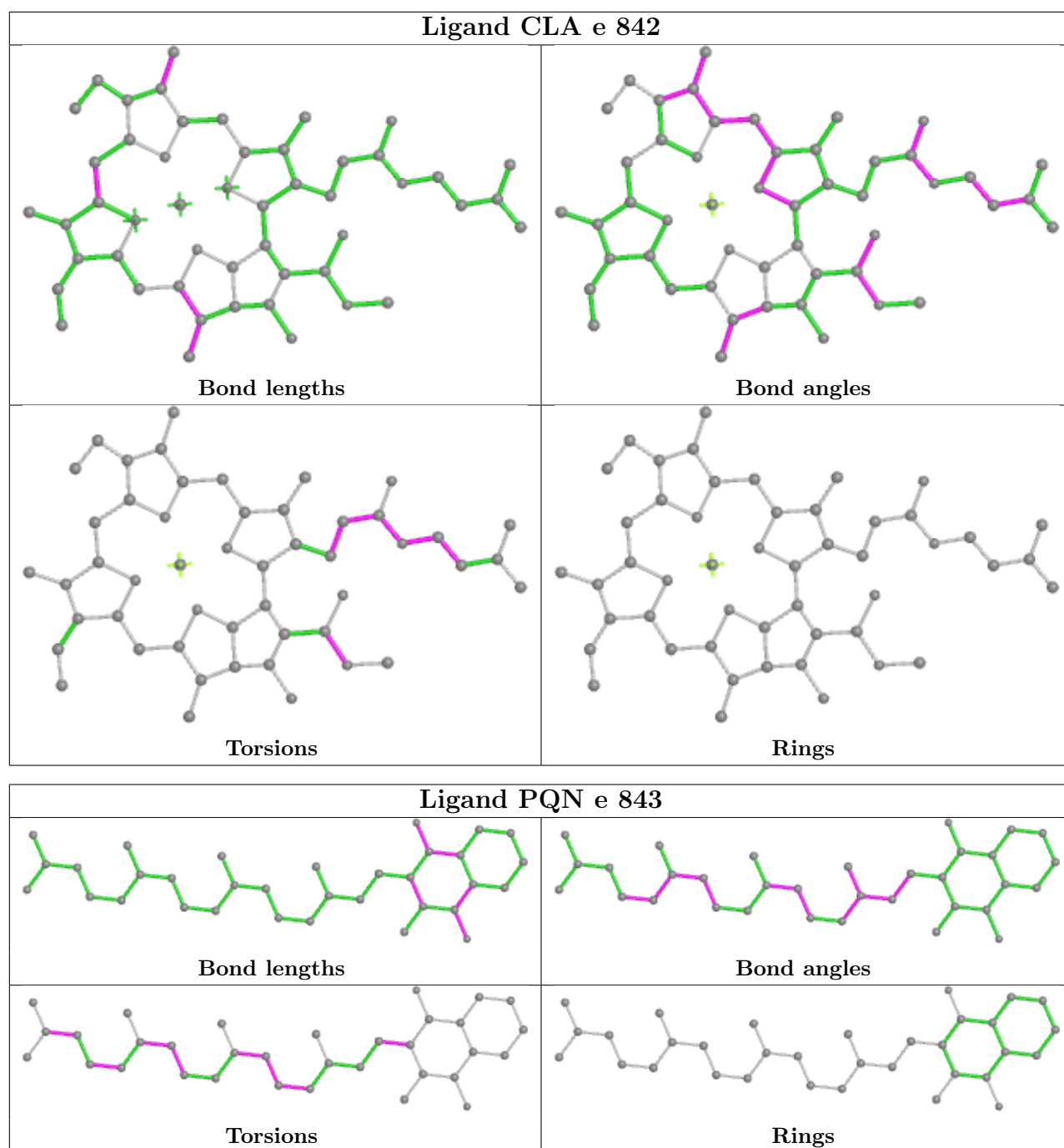
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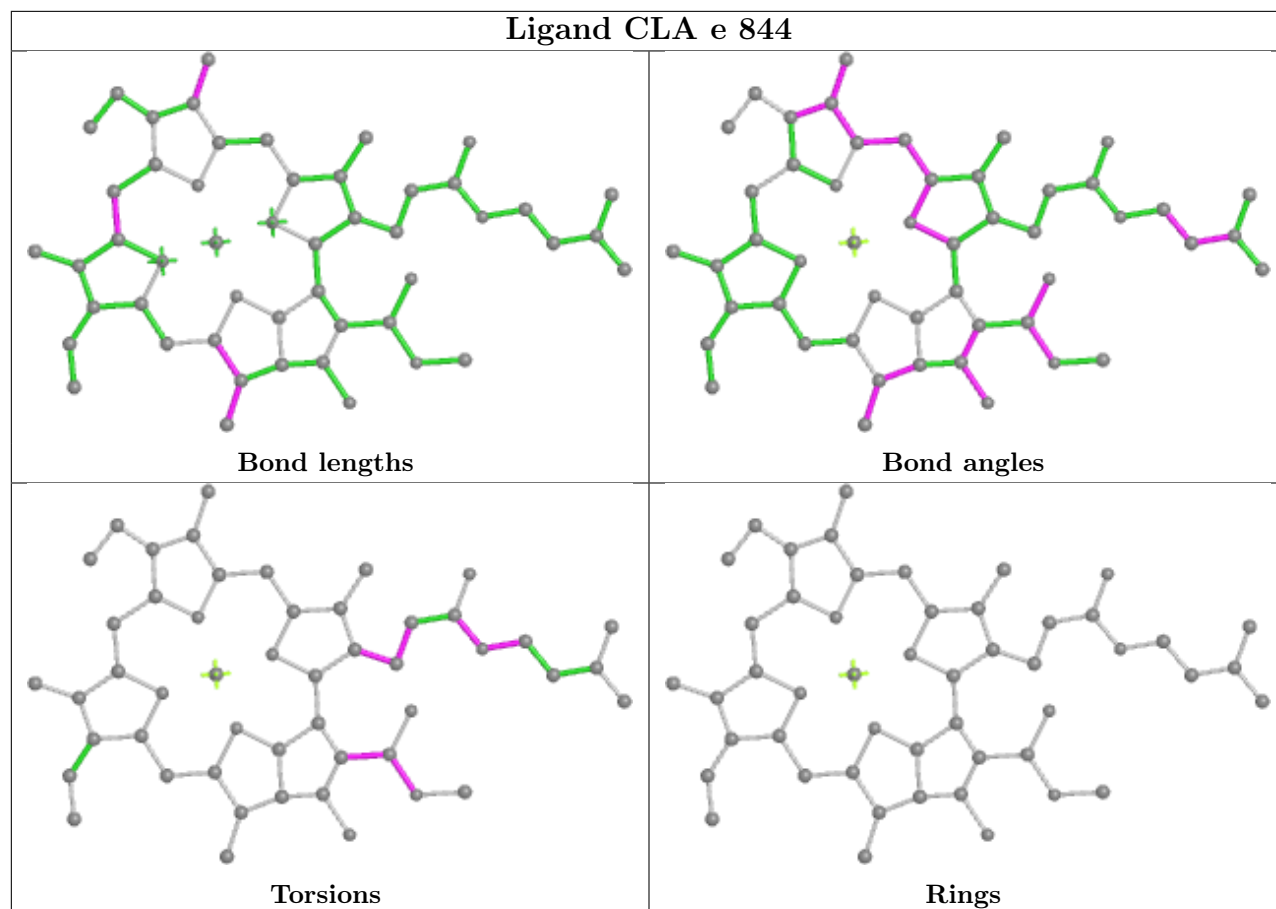




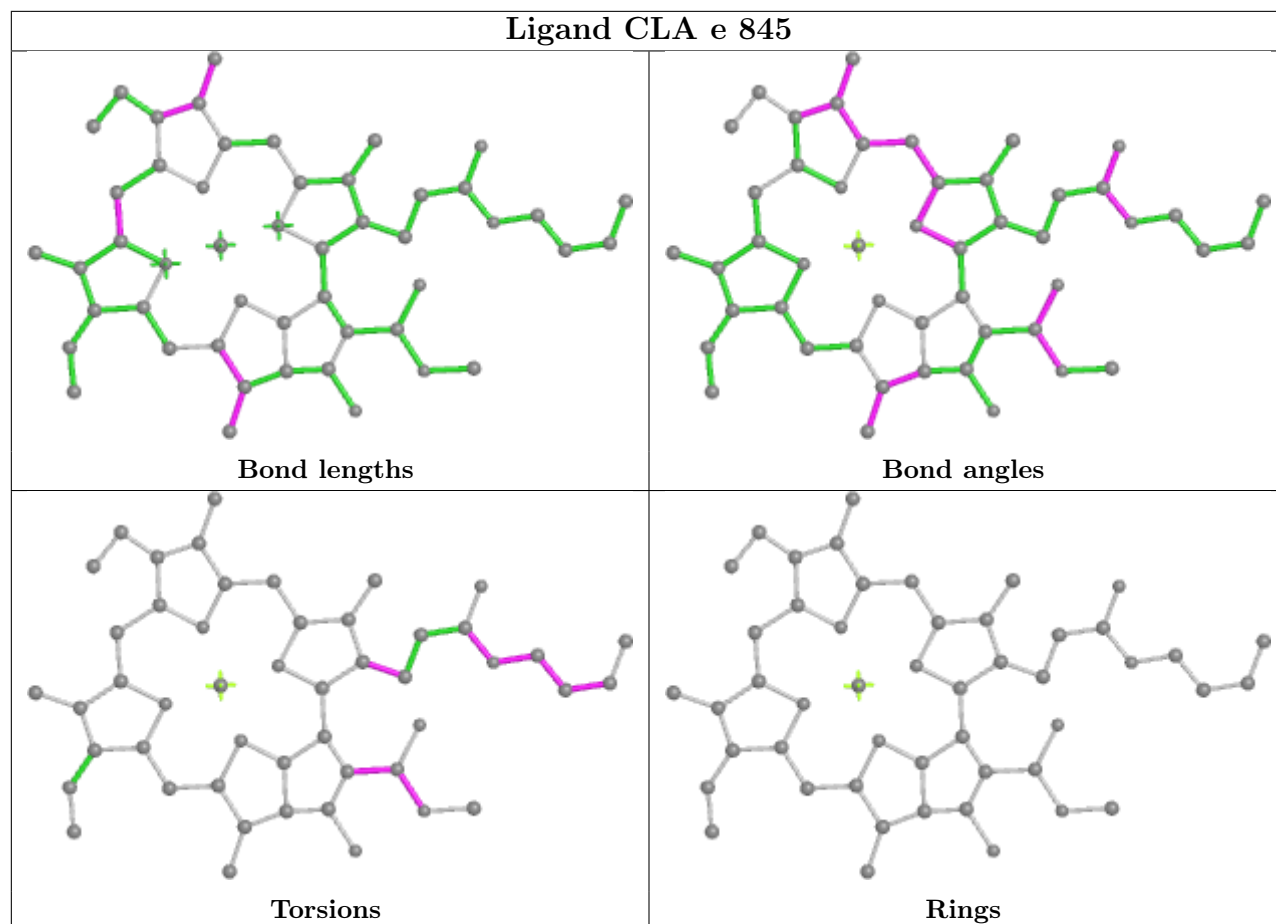
Ligand CLA e 841



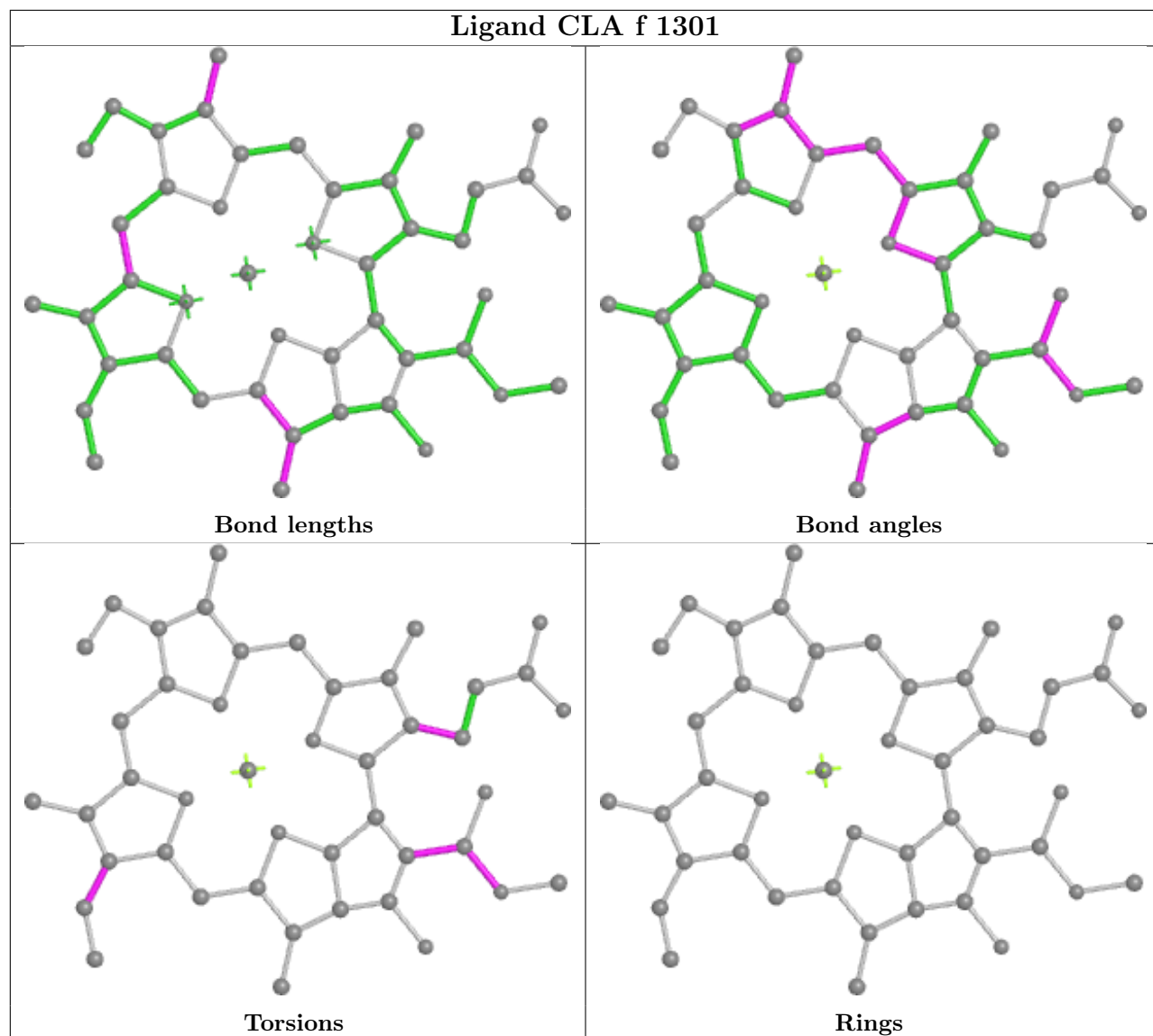


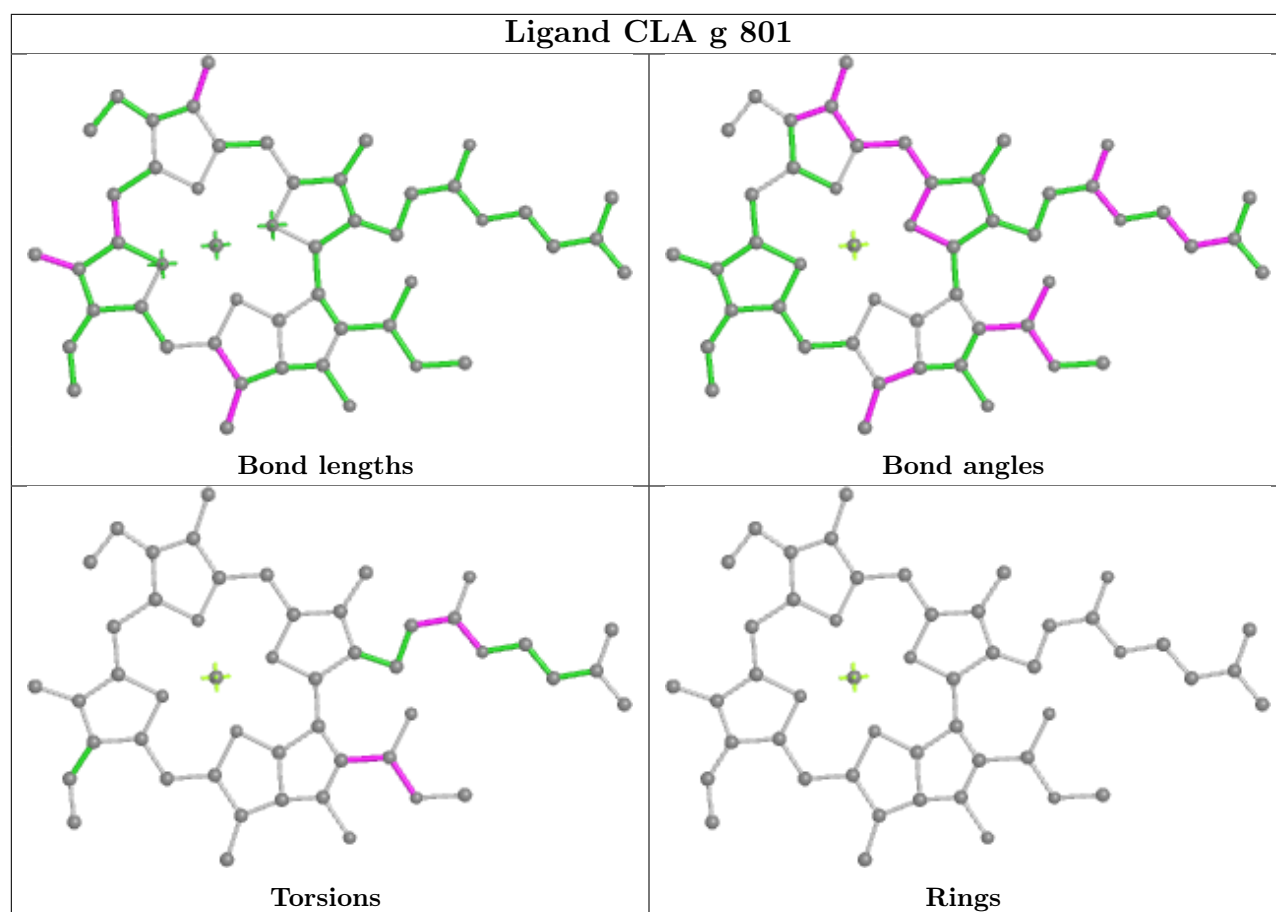


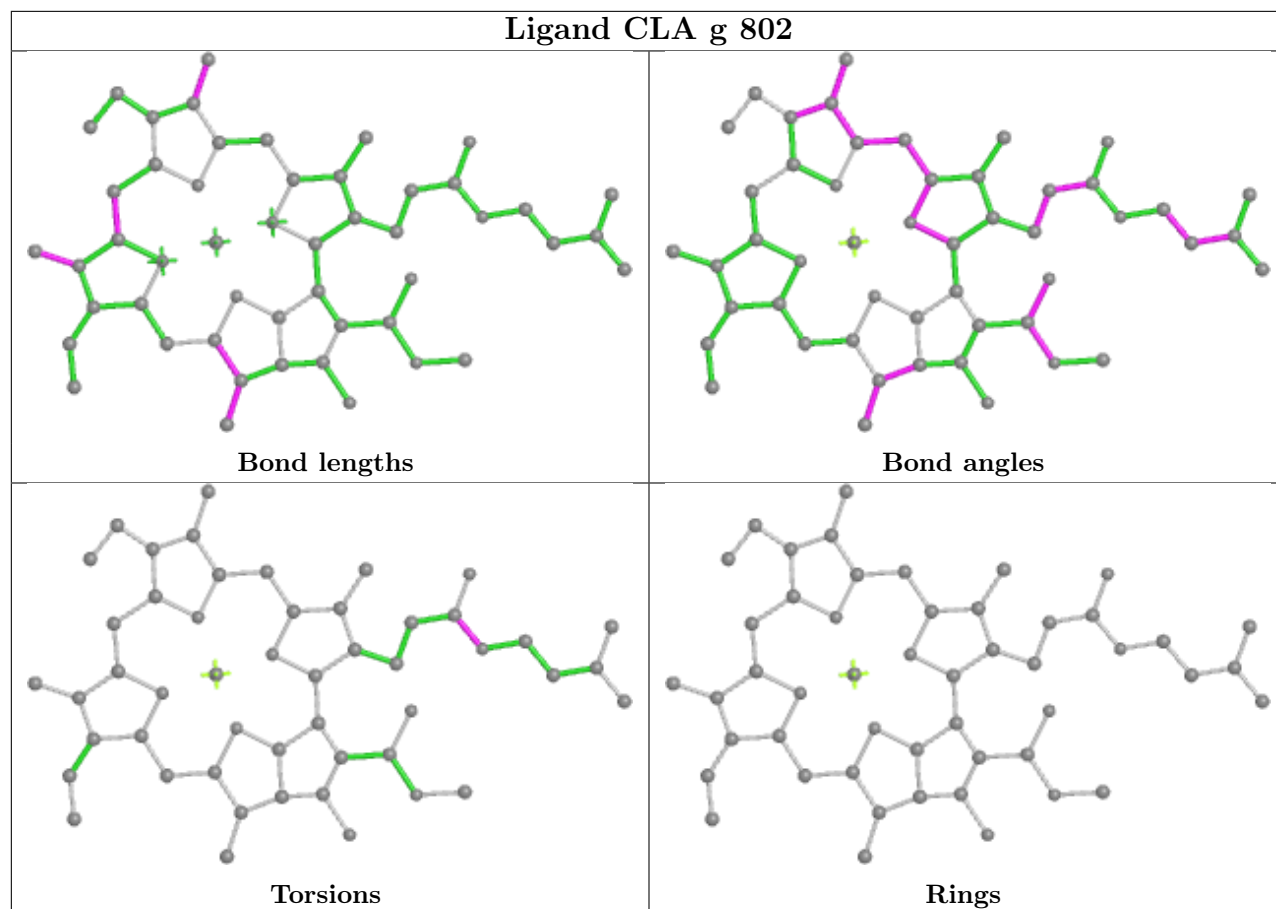
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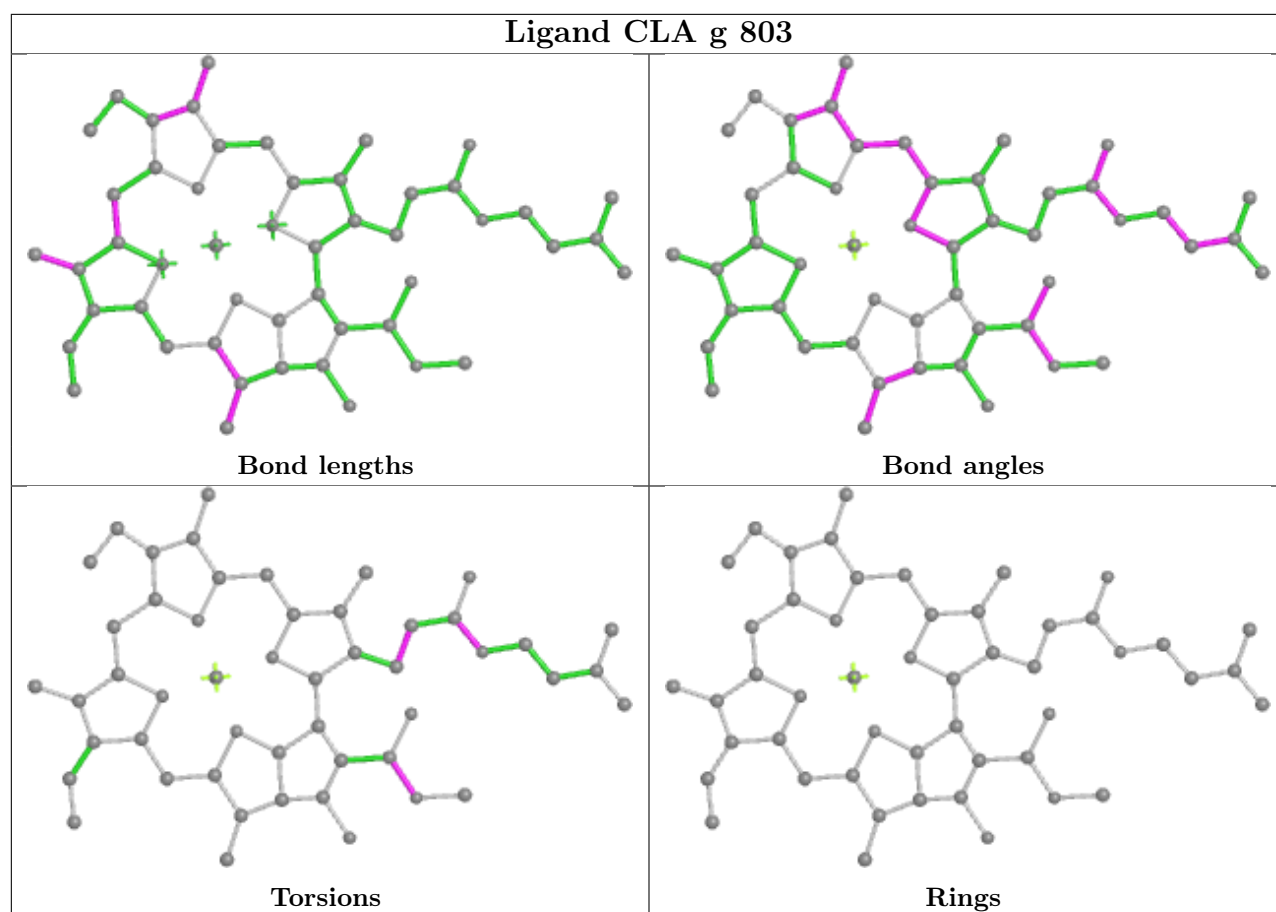


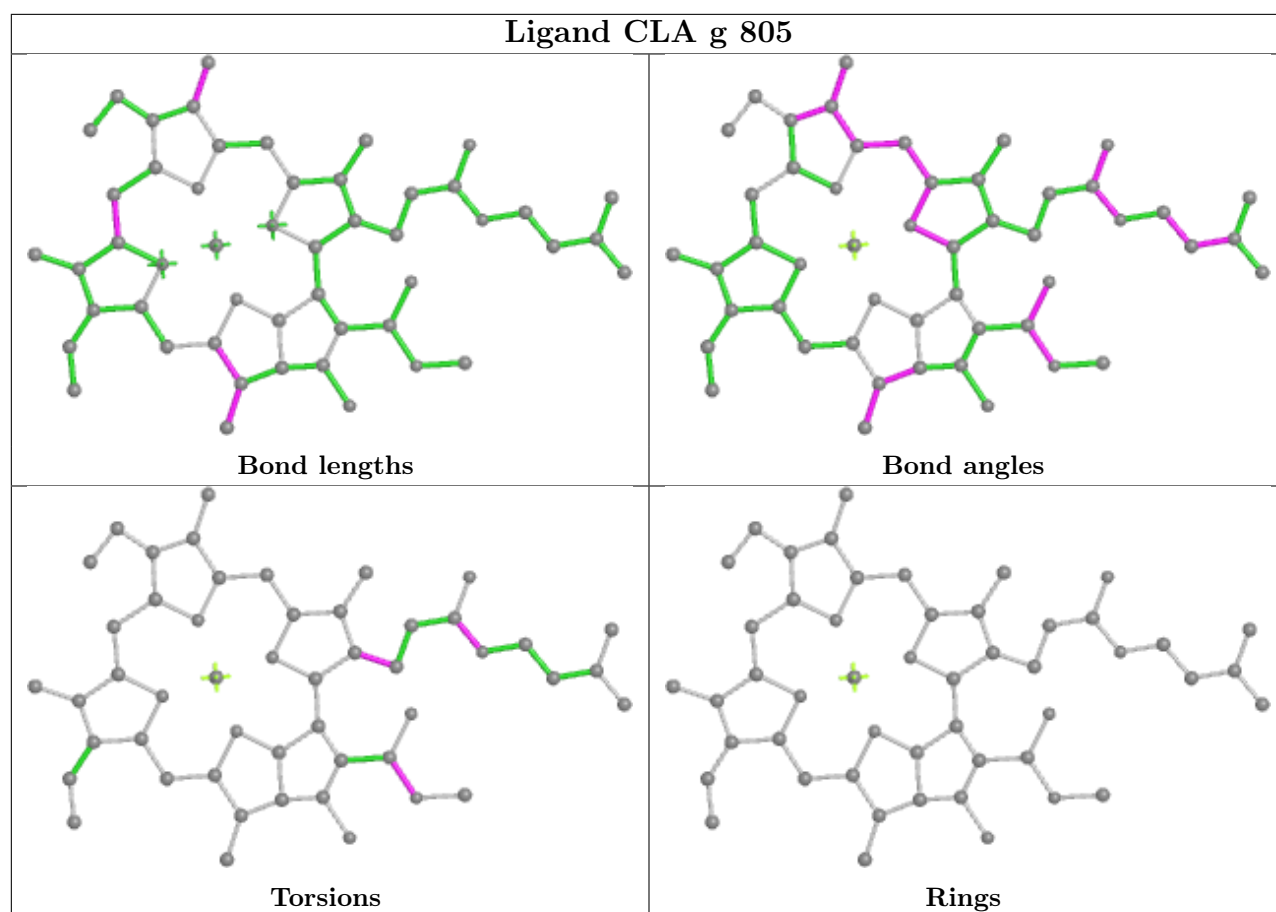
Ligand CLA f 1301

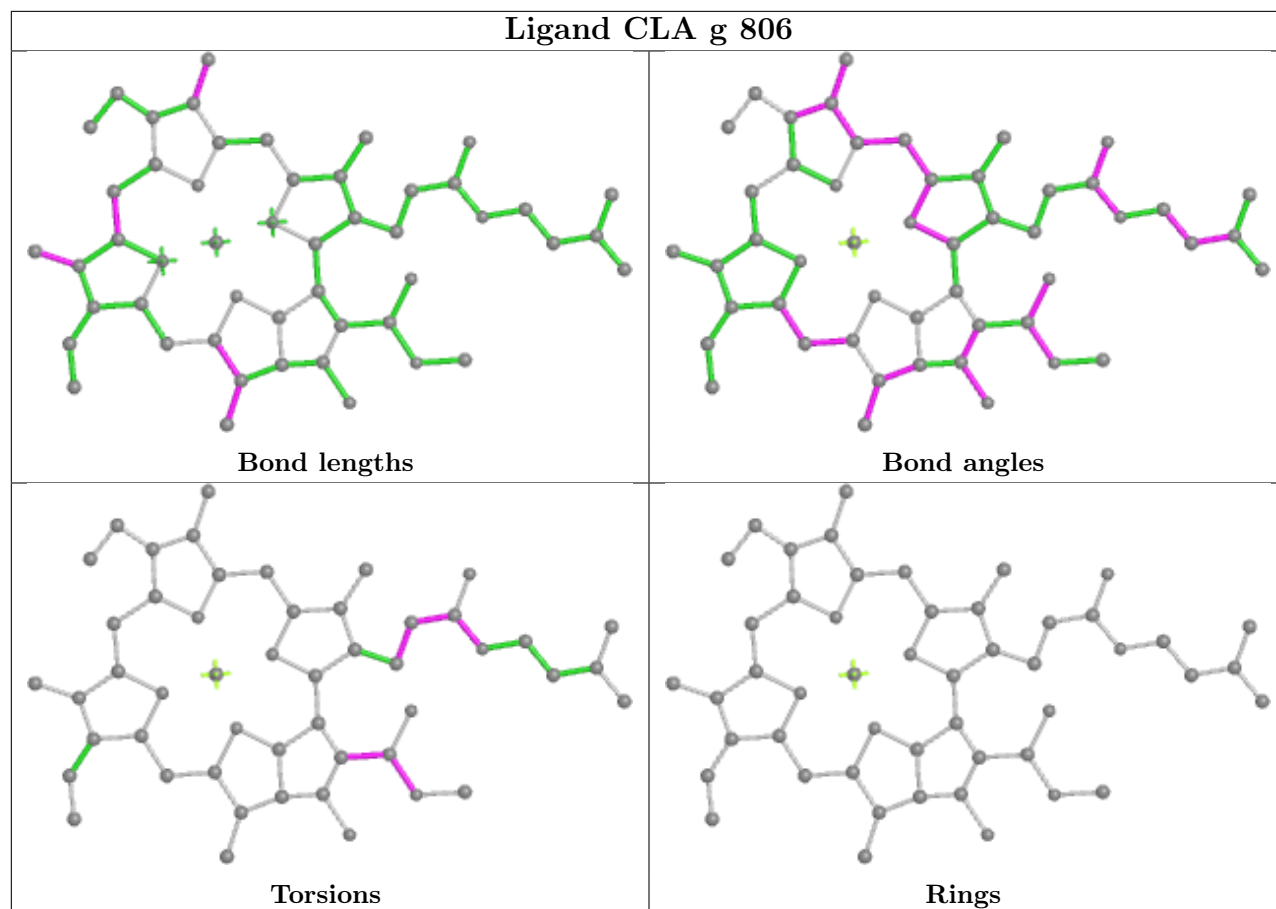


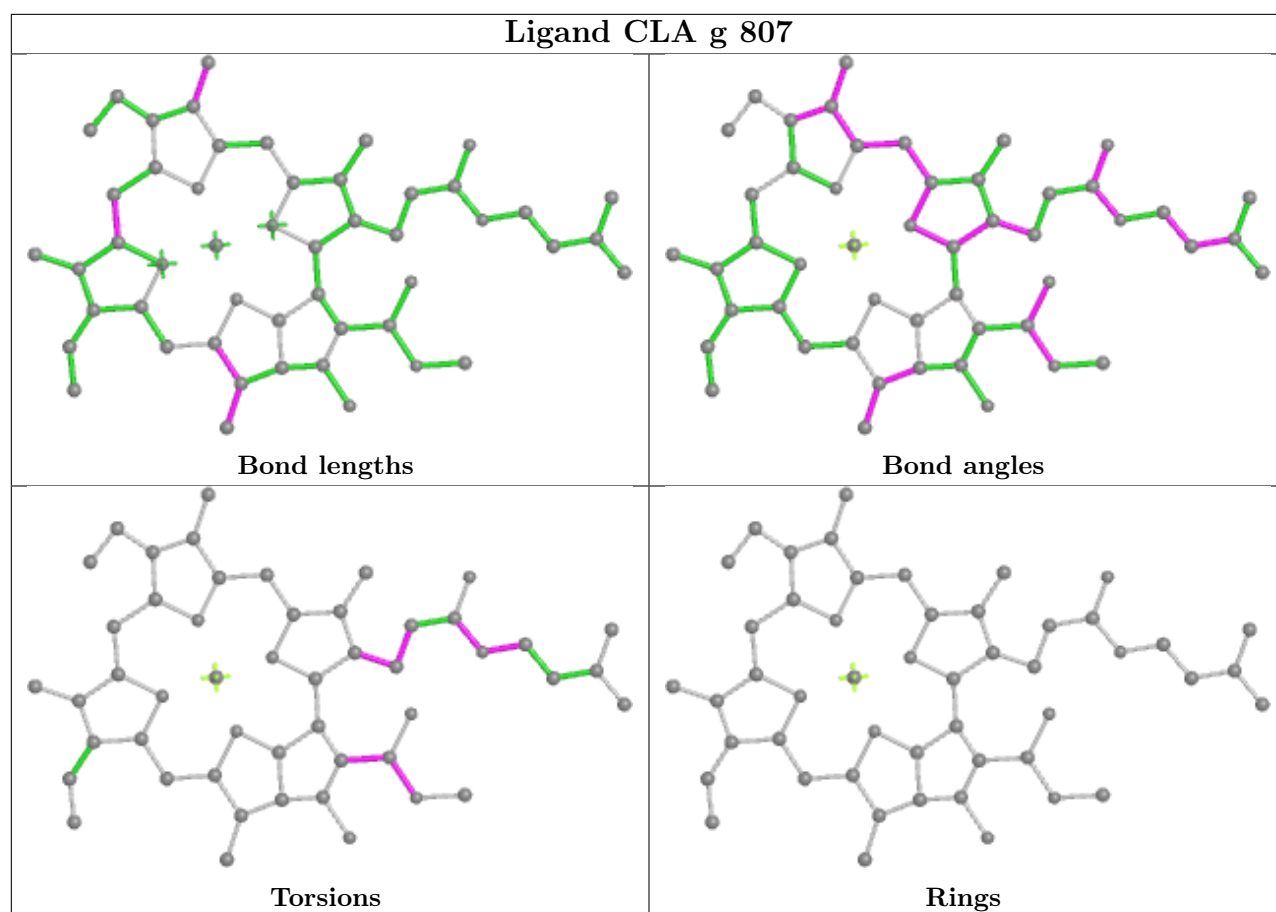


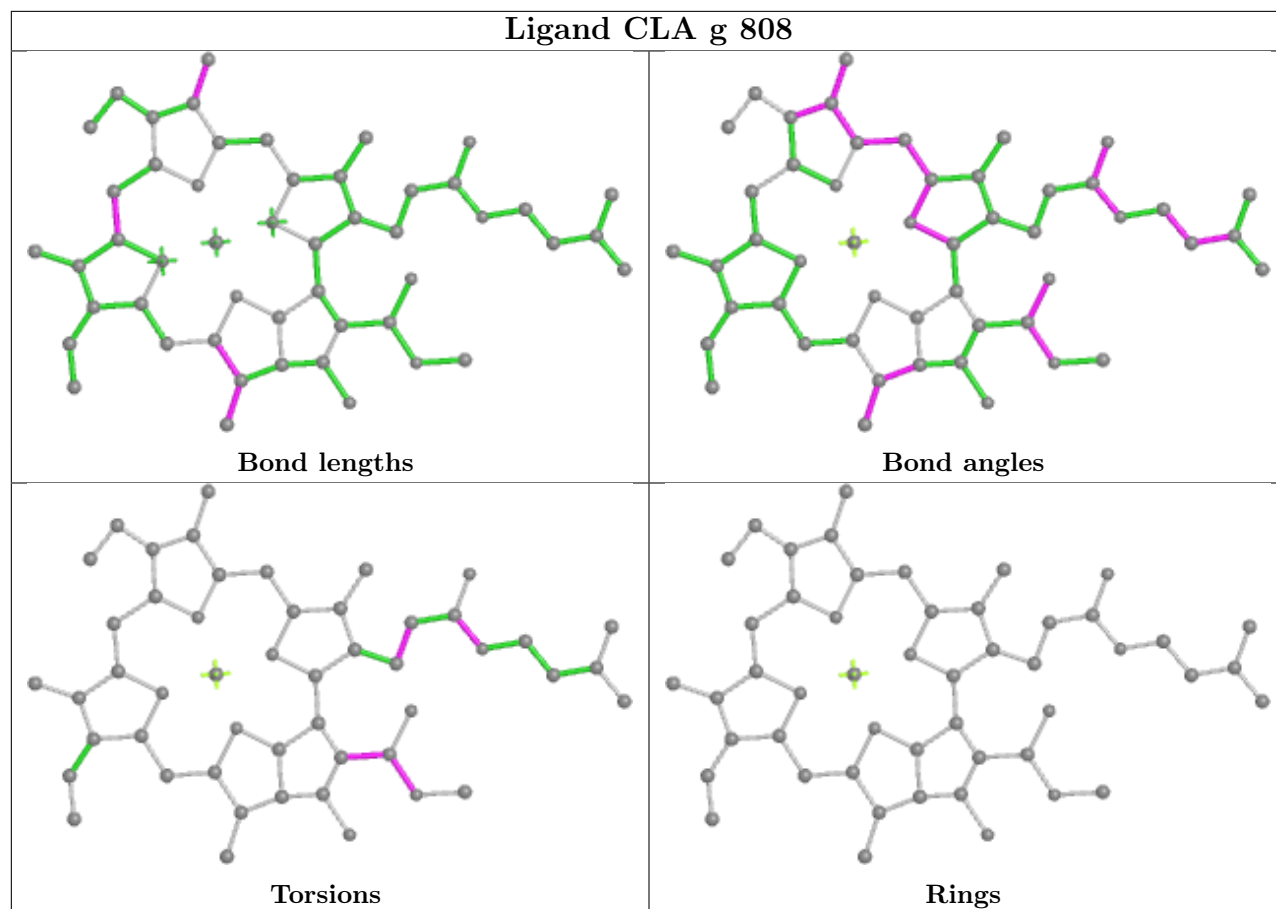


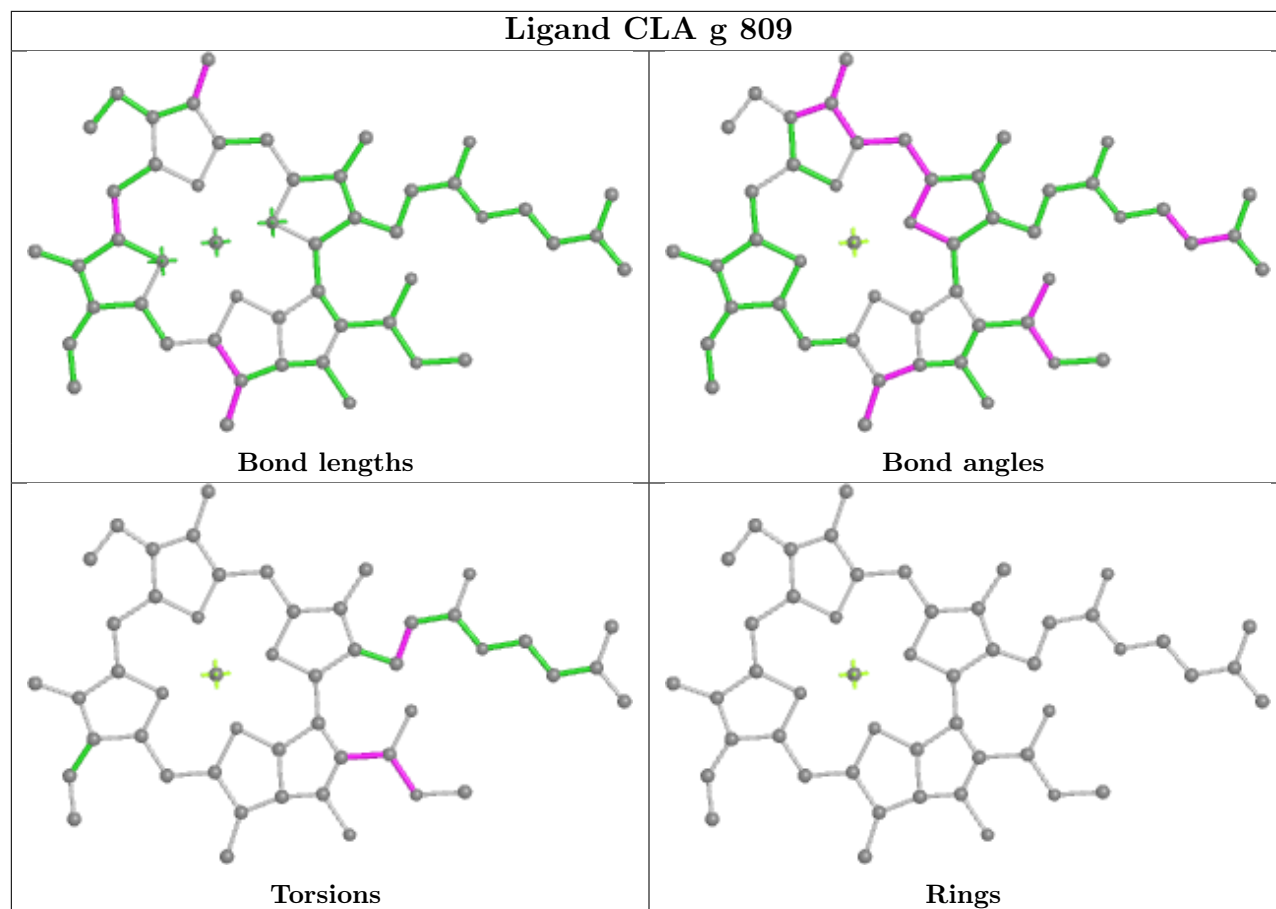


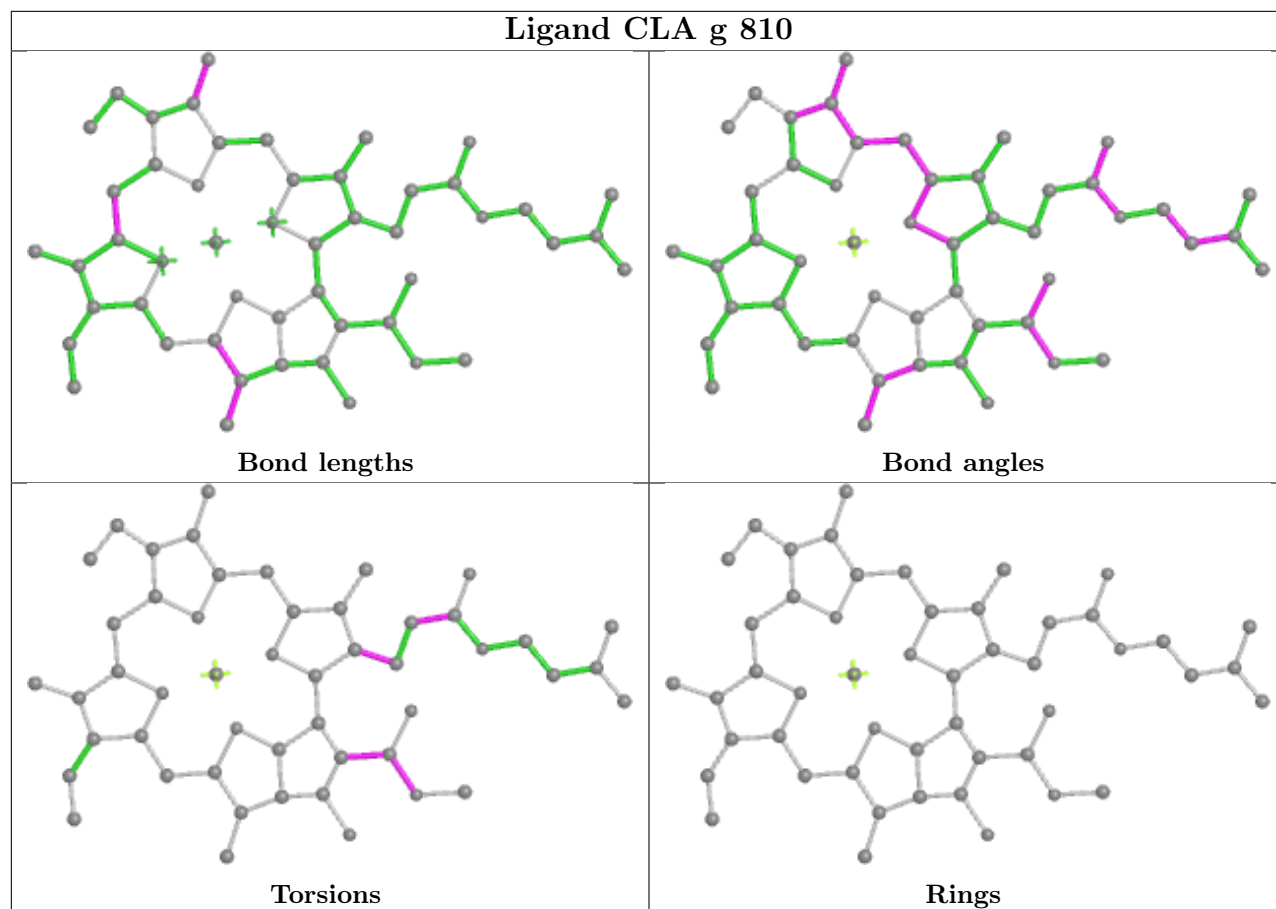


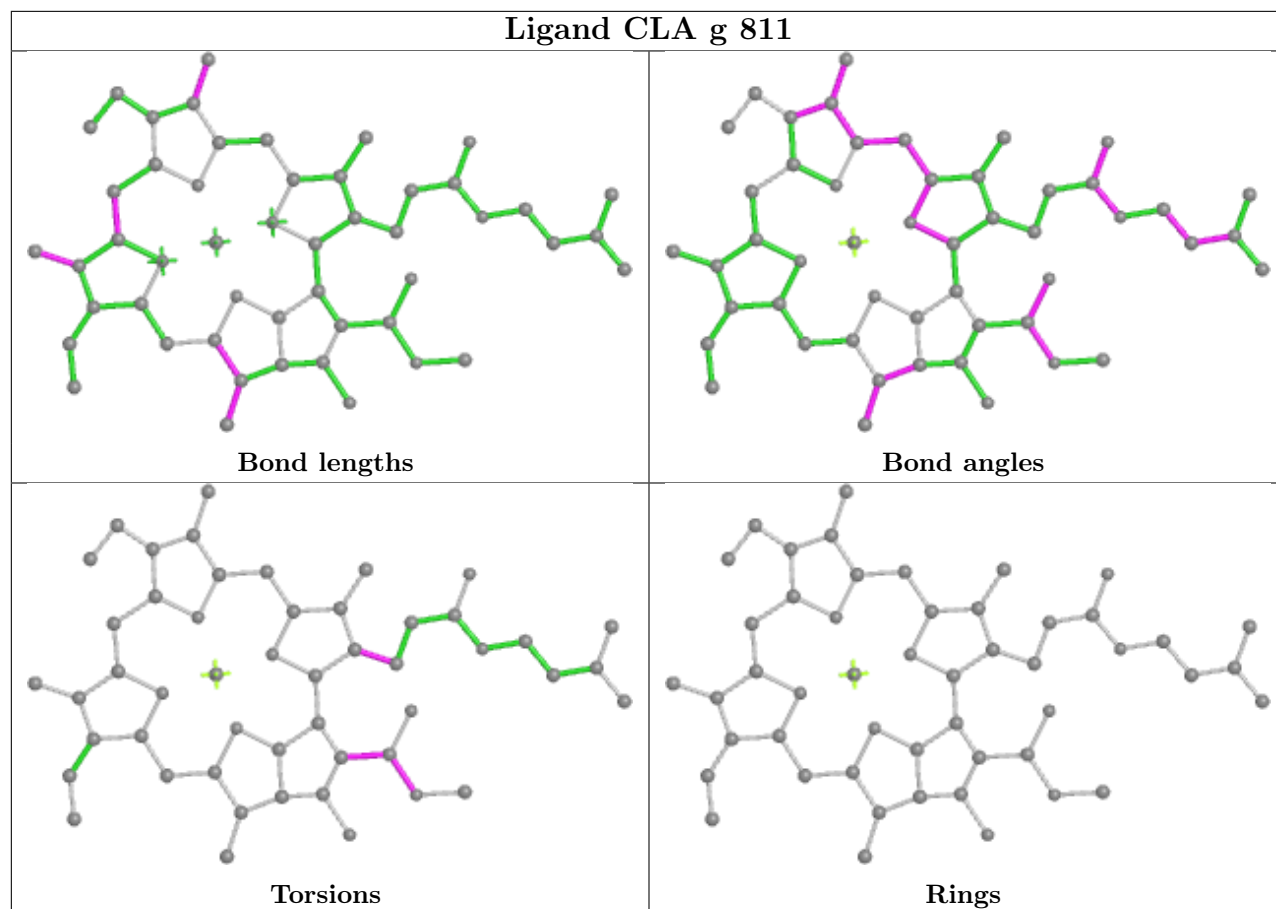


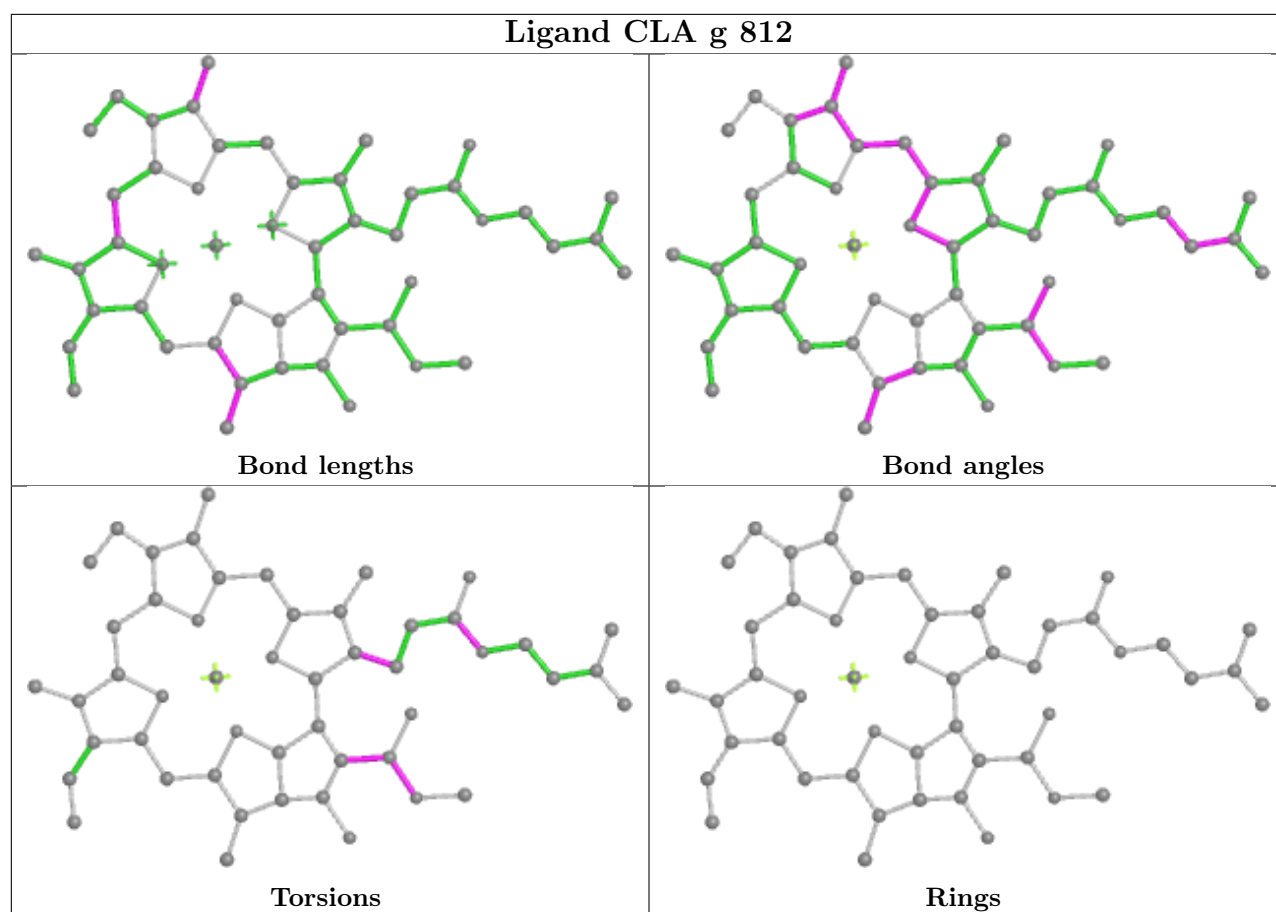




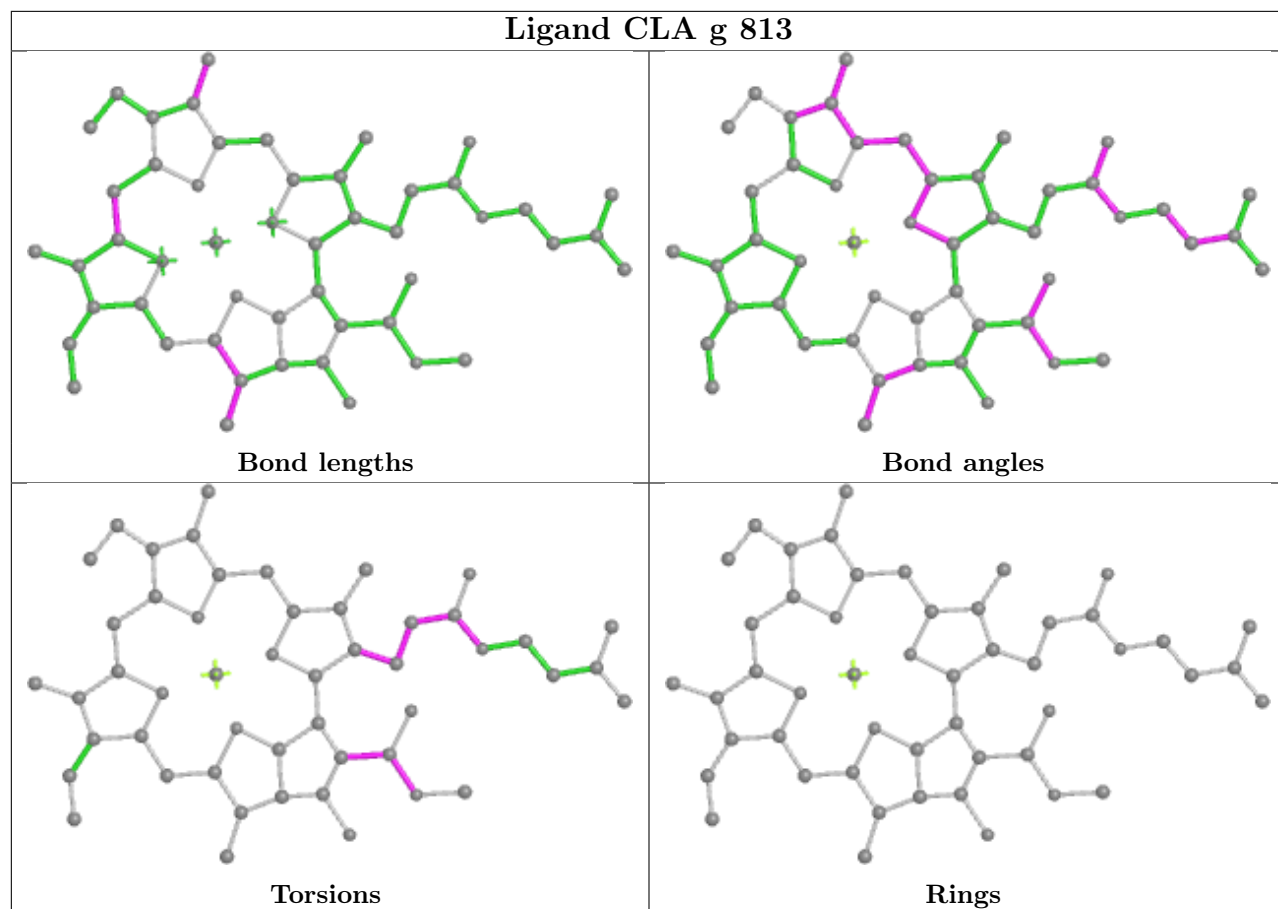




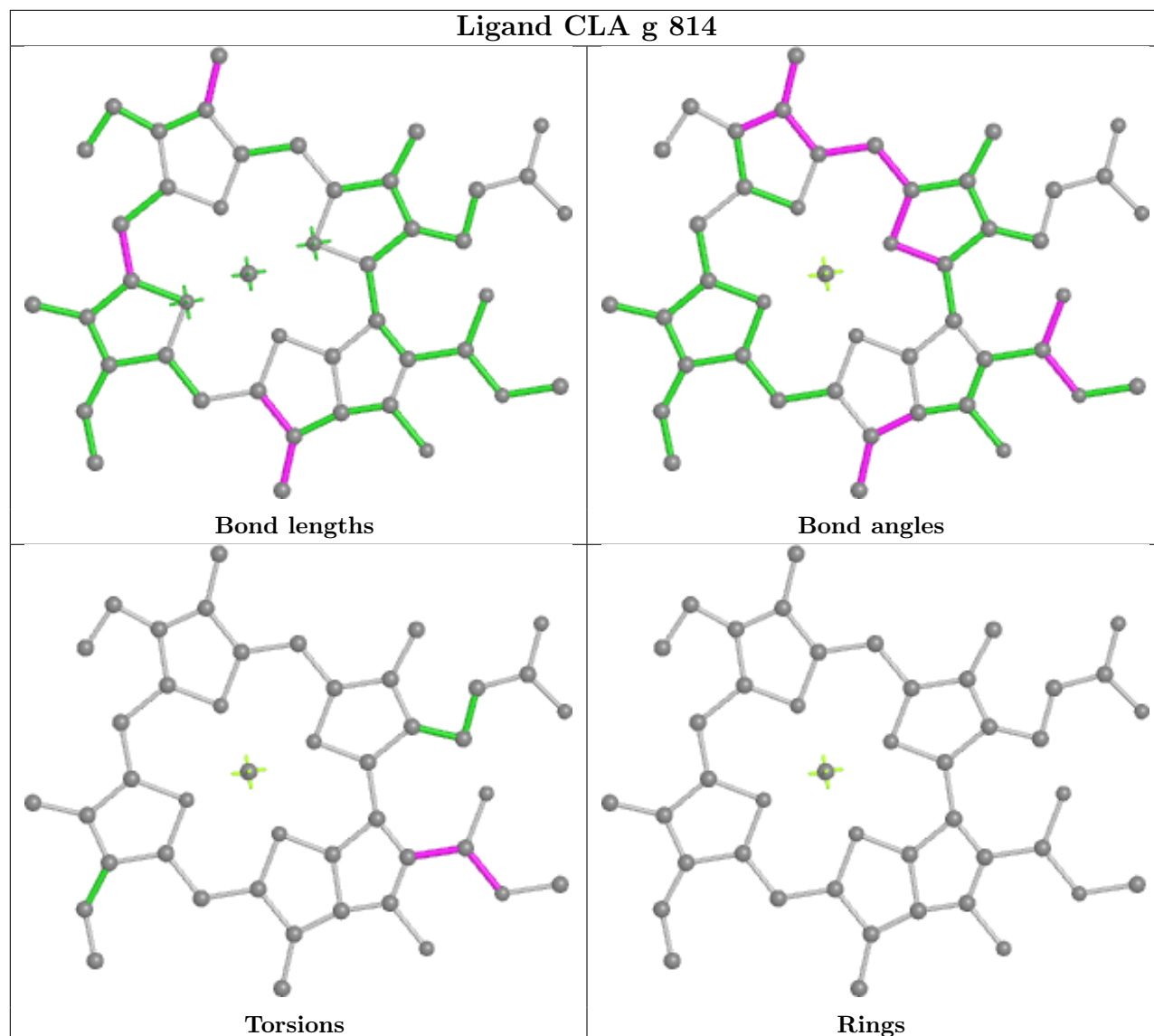




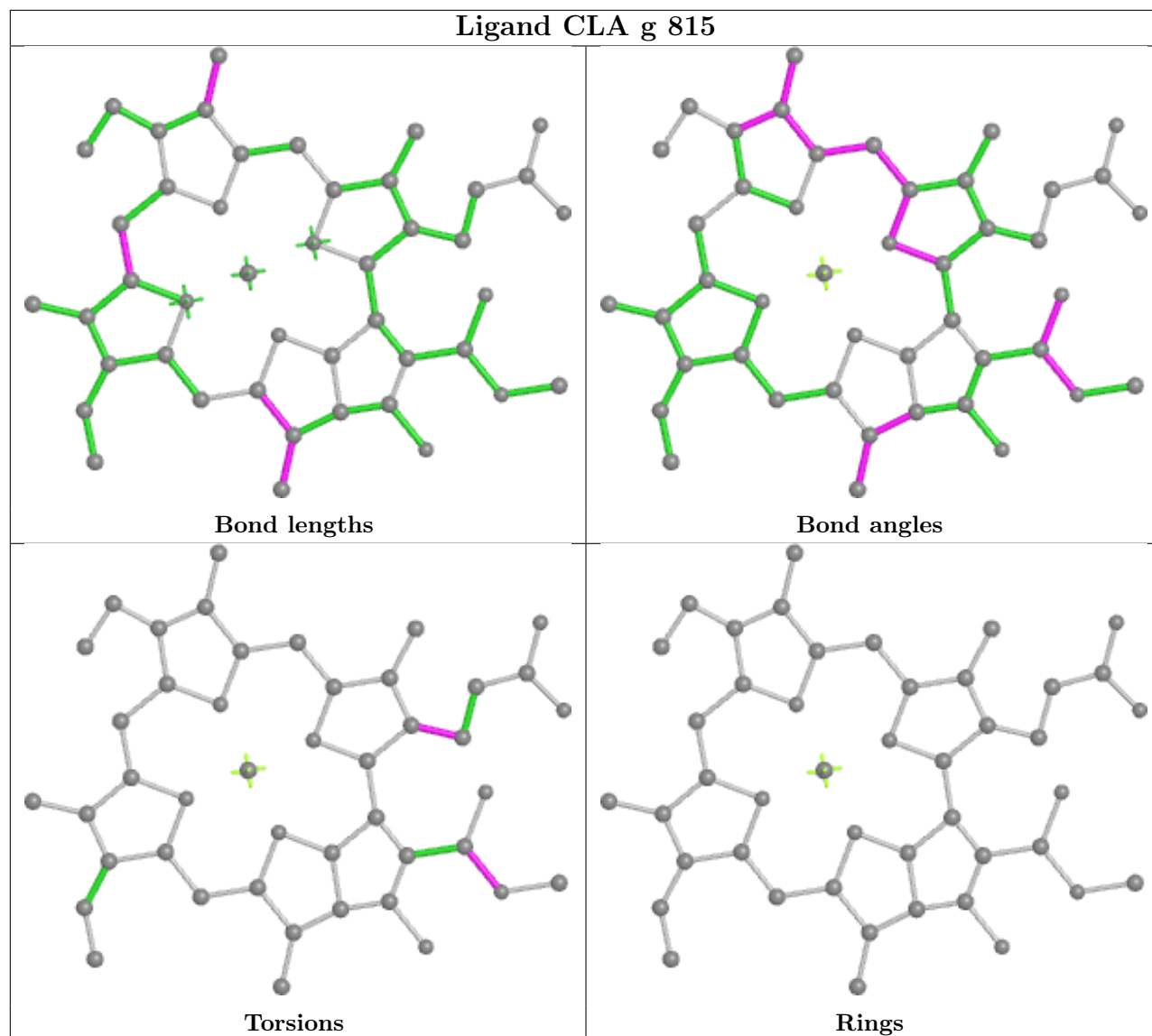
Ligand CLA g 813



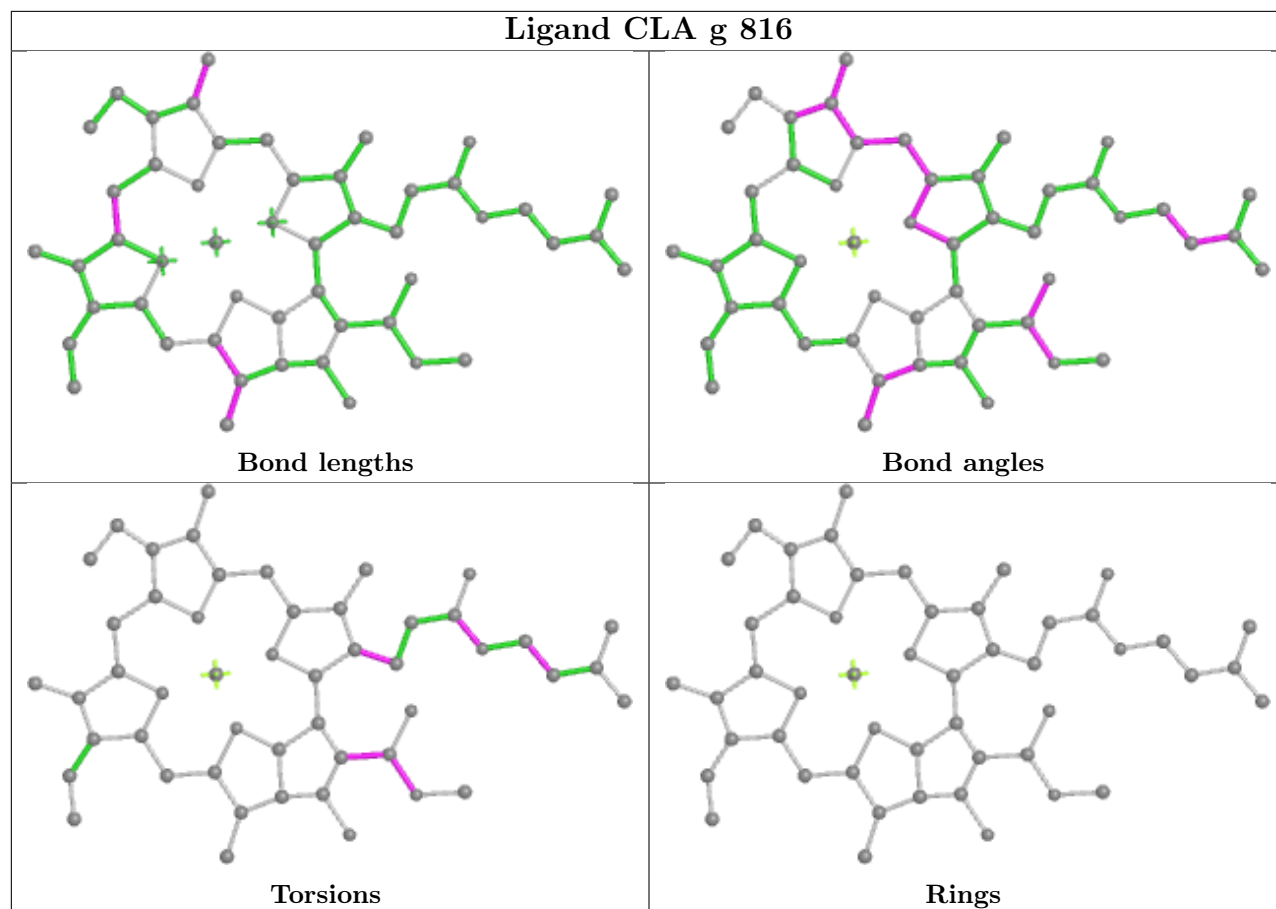
Ligand CLA g 814

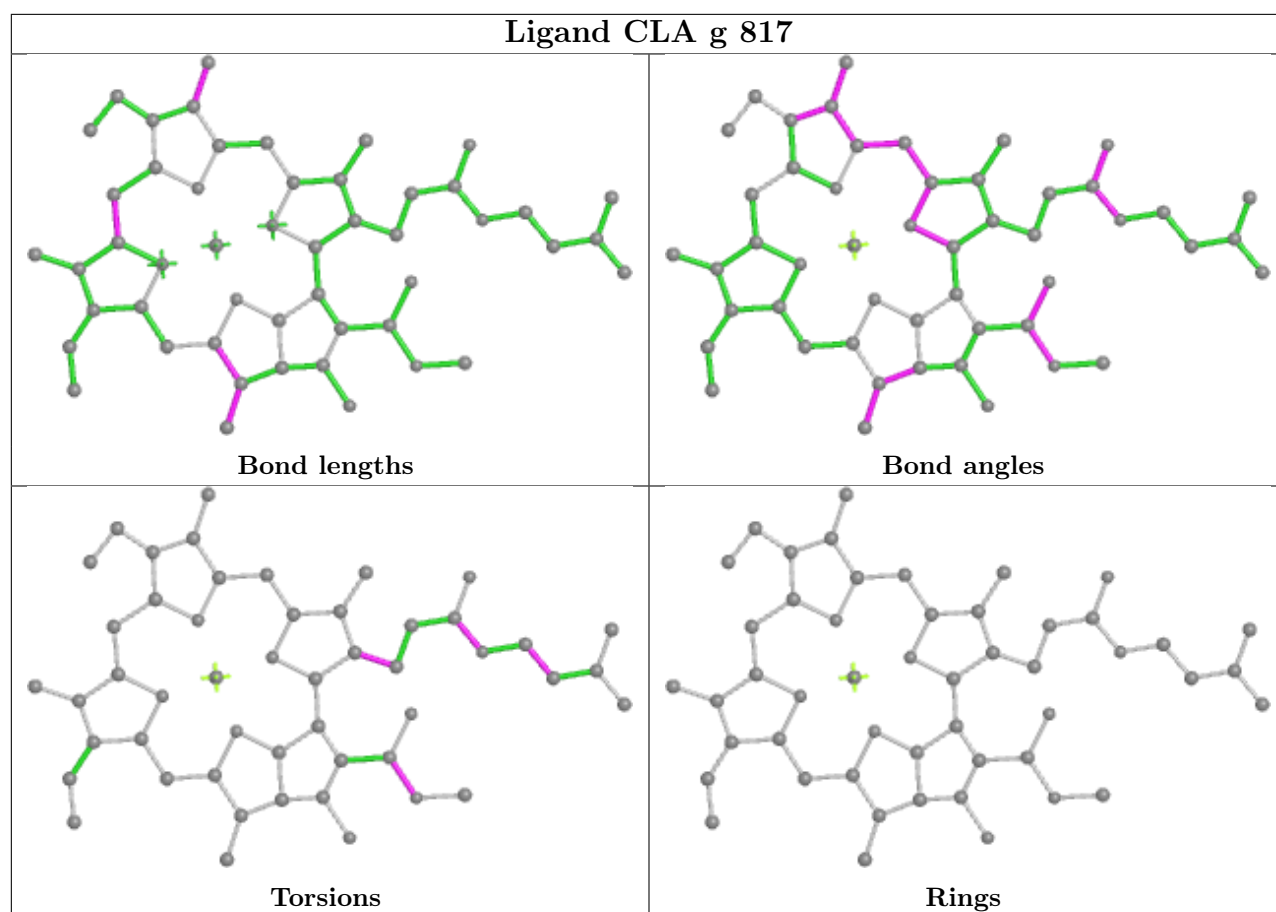


Ligand CLA g 815

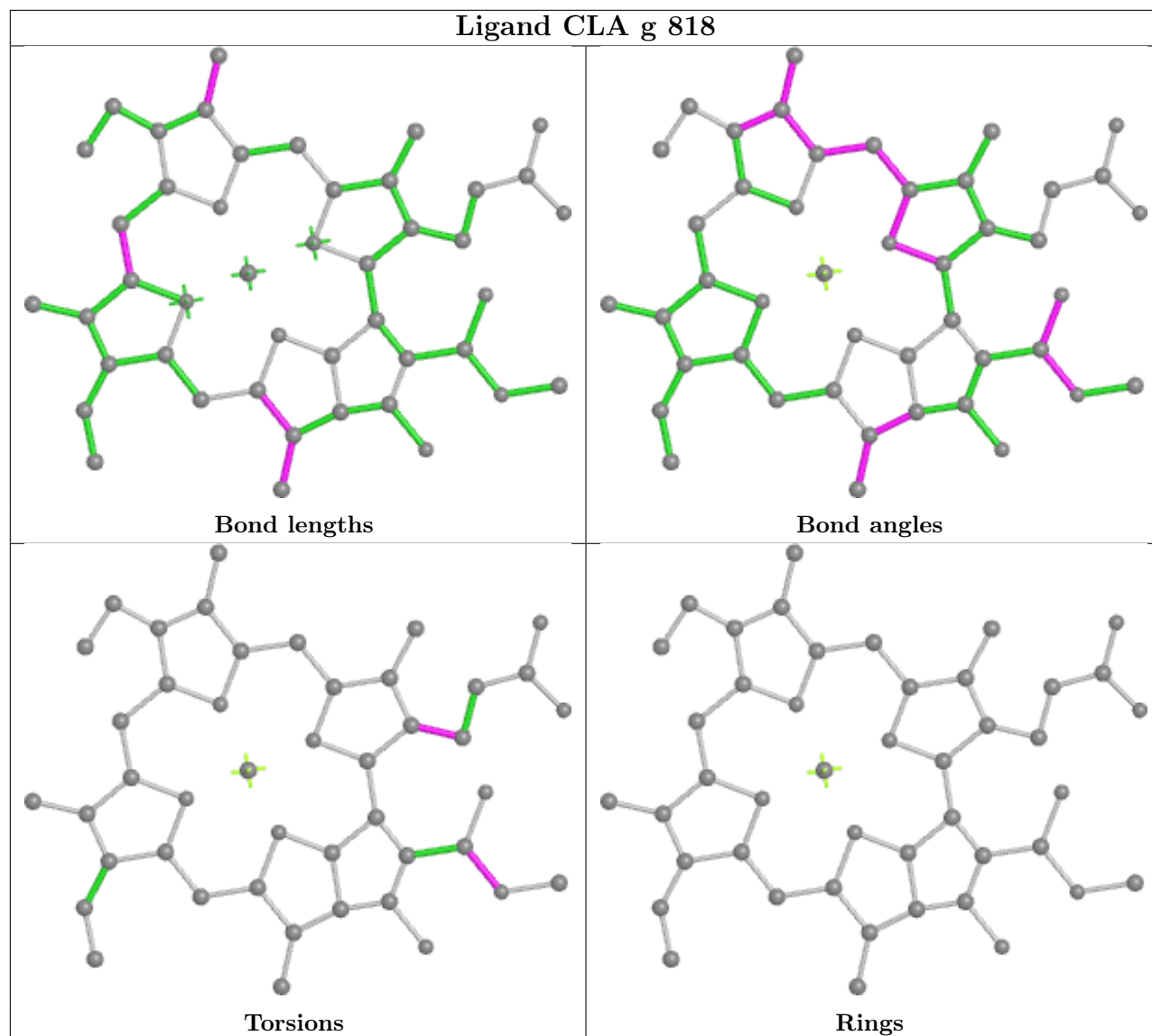


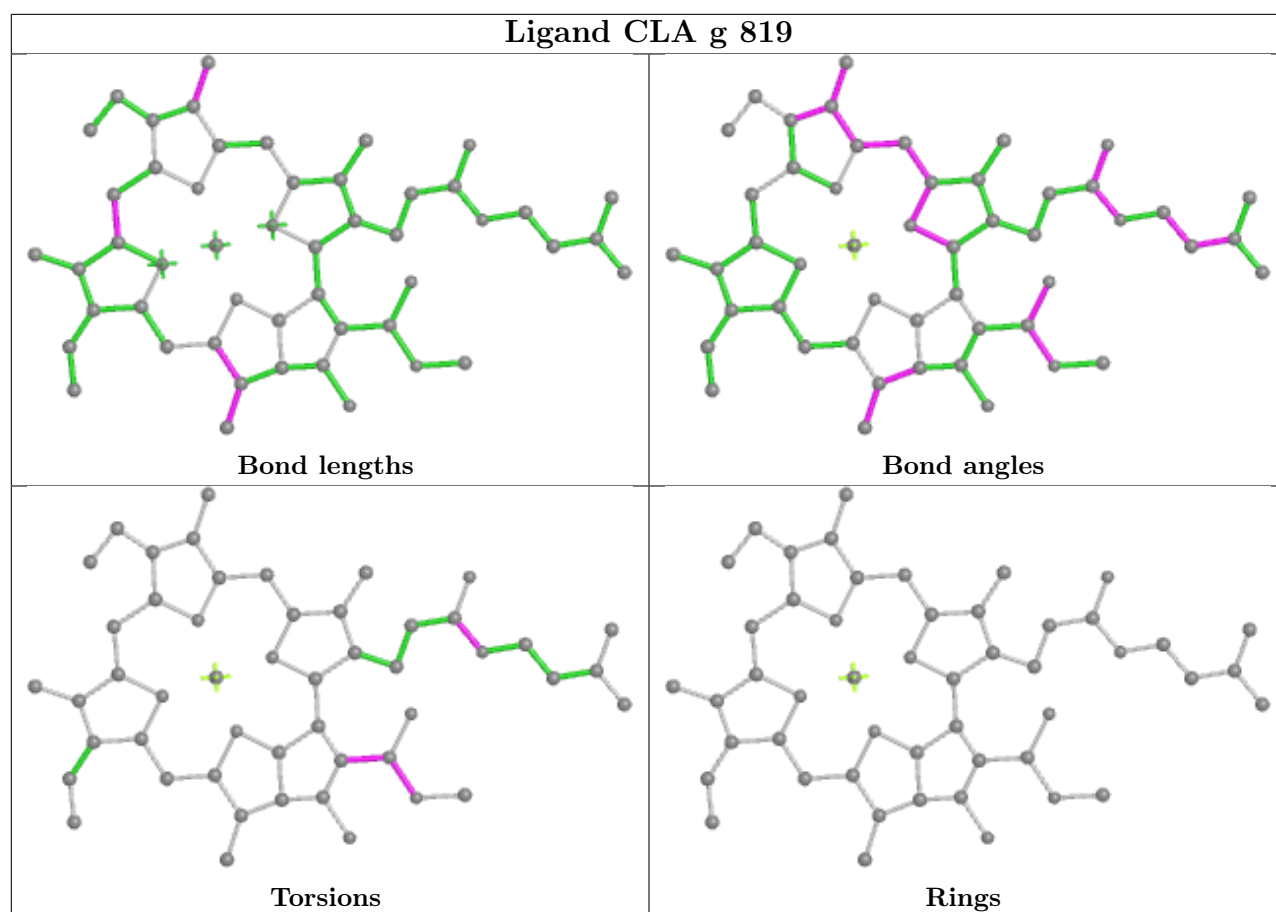
Ligand CLA g 816

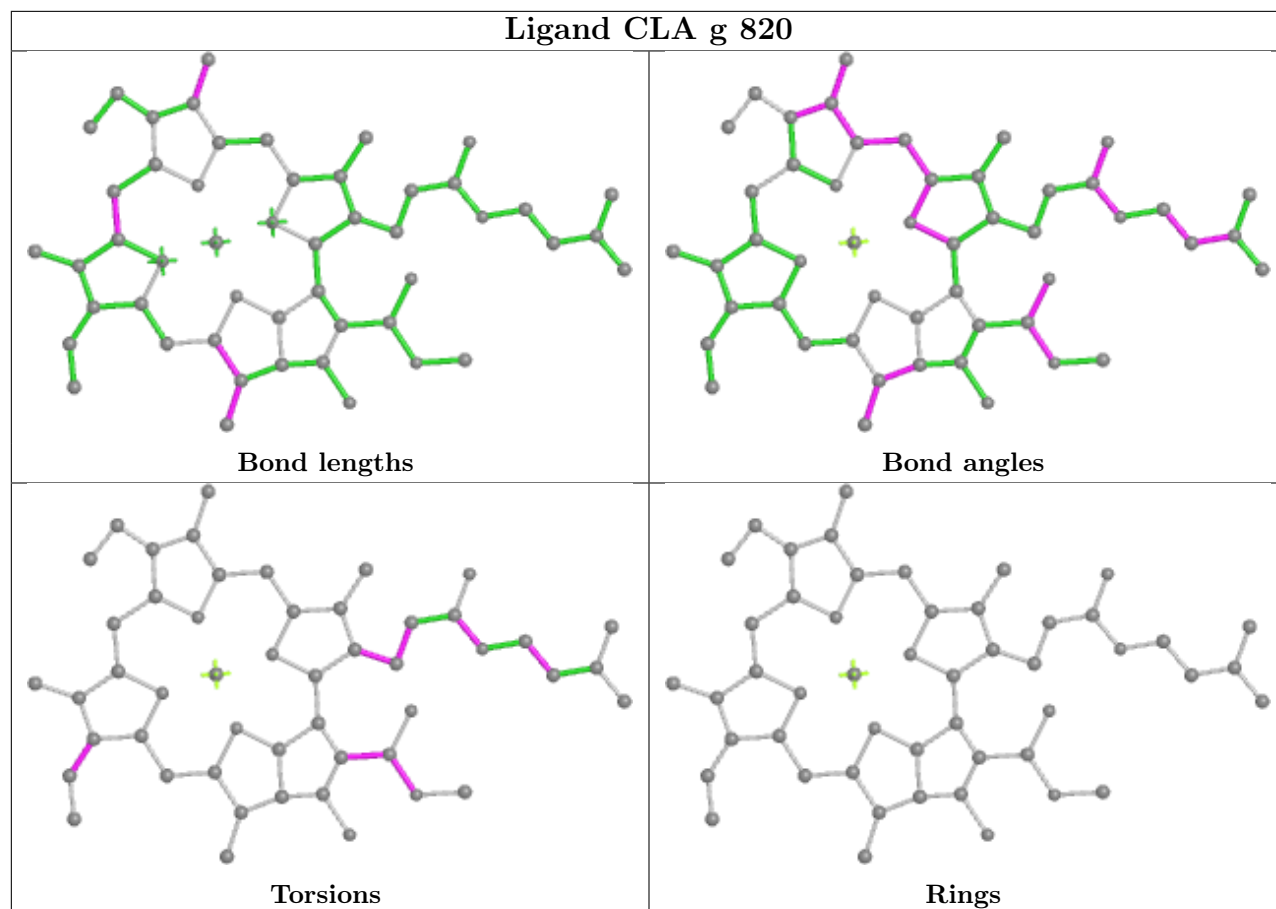


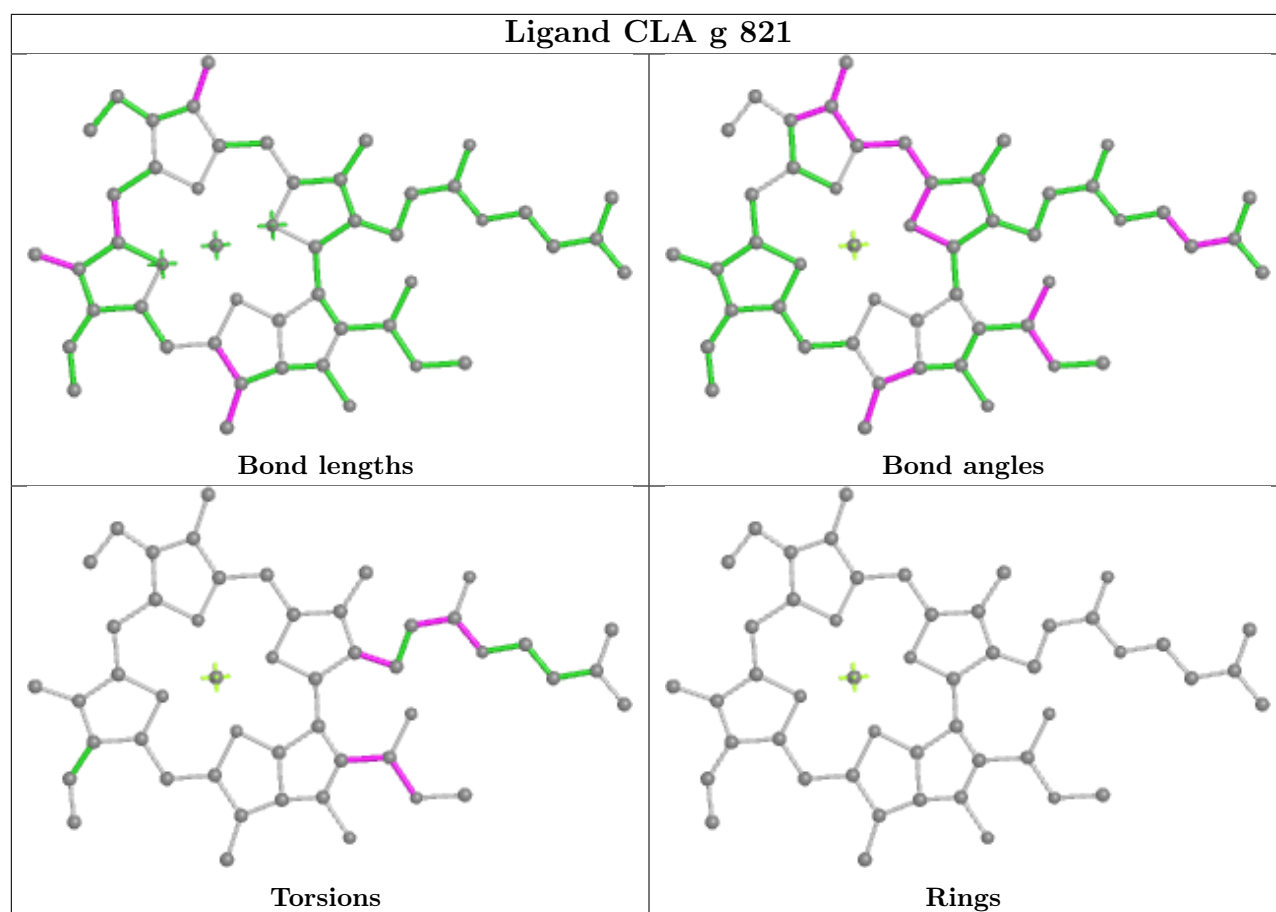


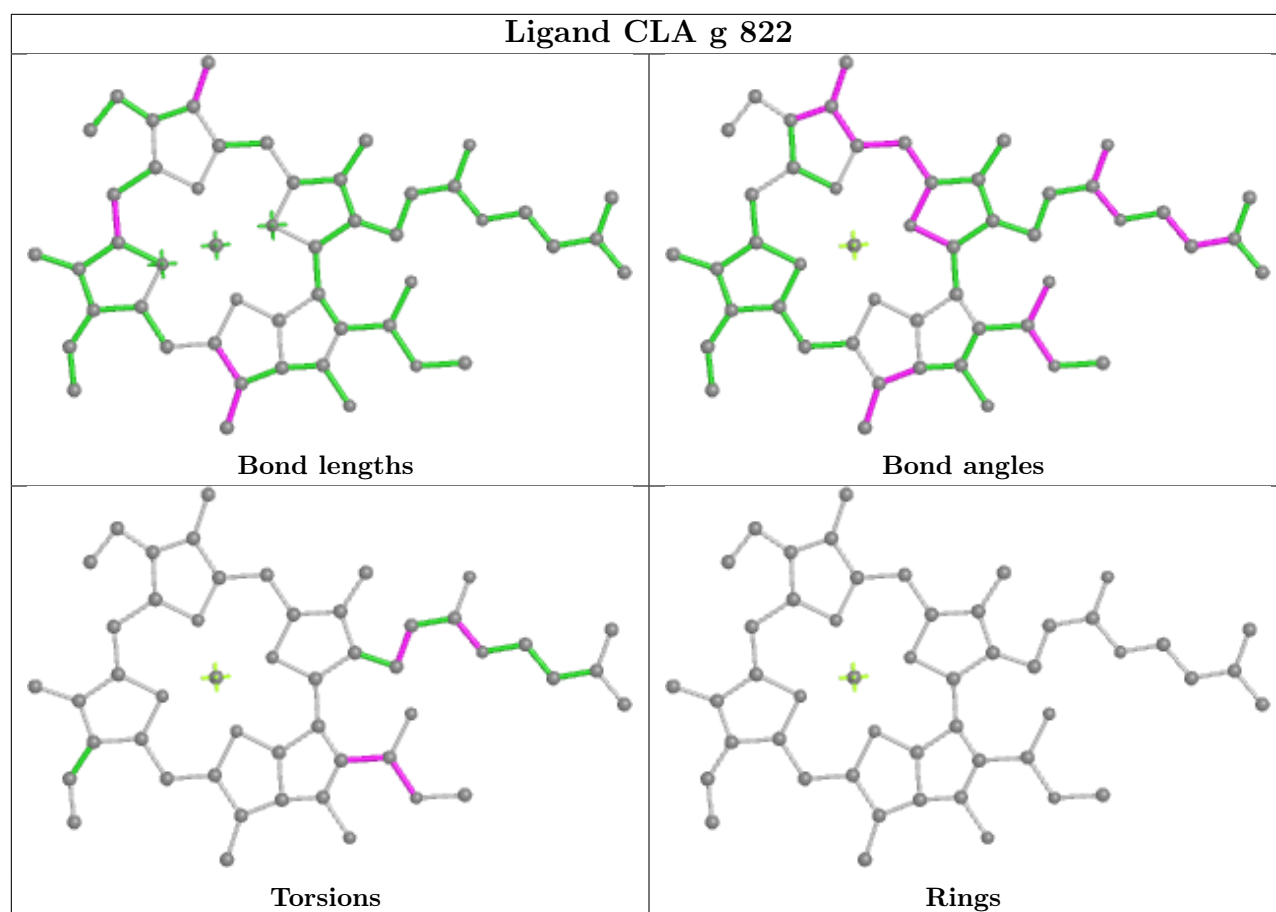
Ligand CLA g 818



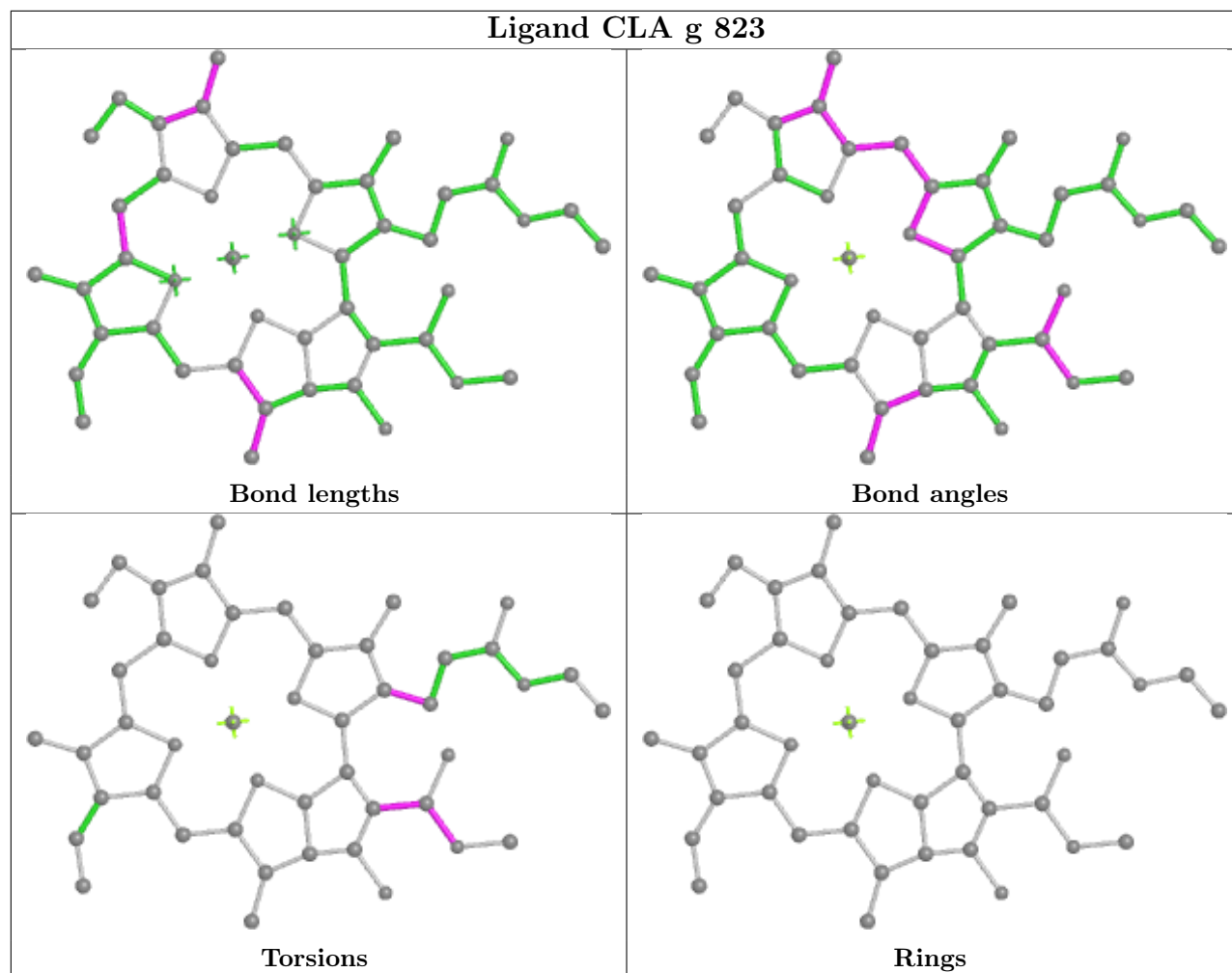




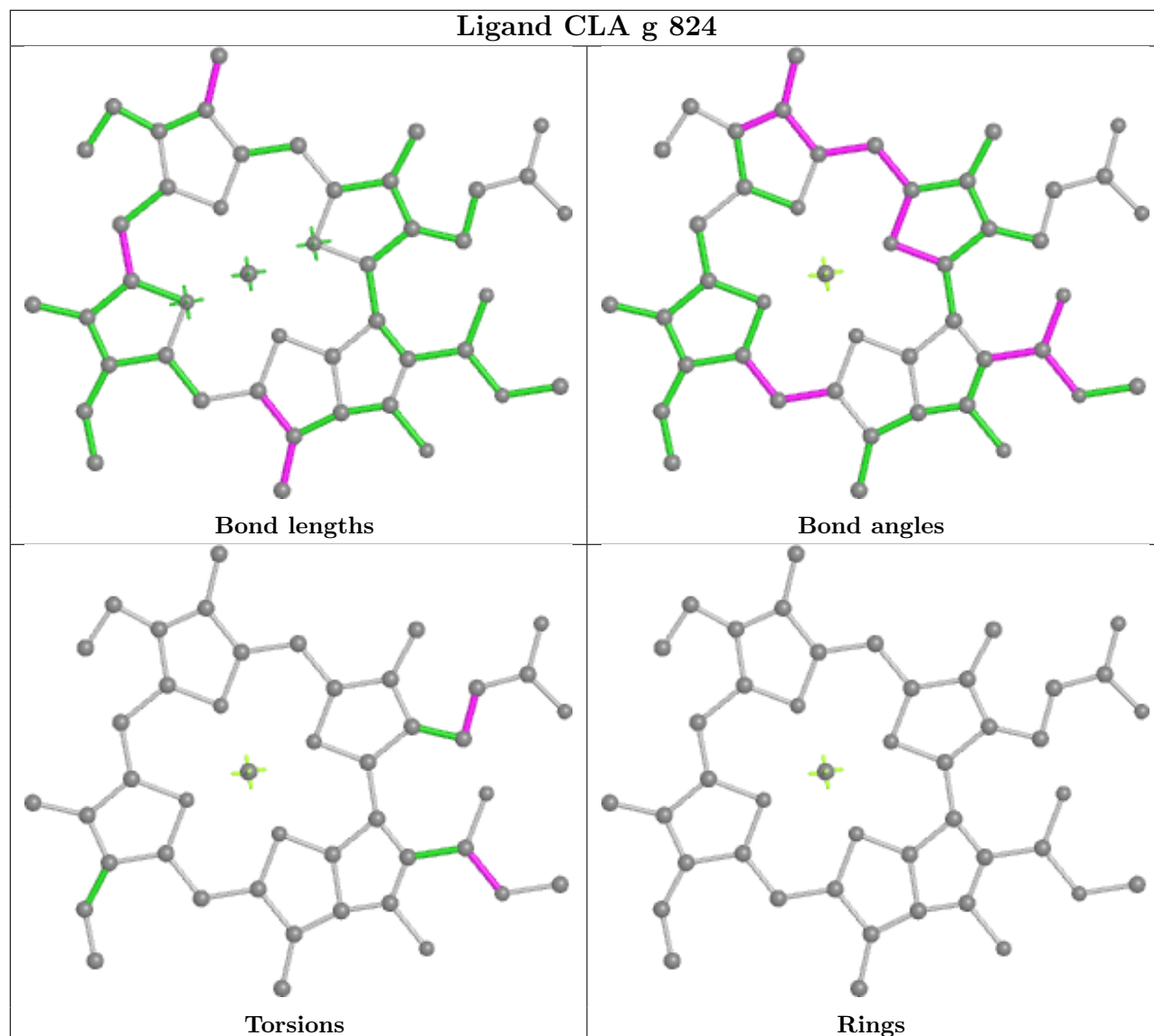


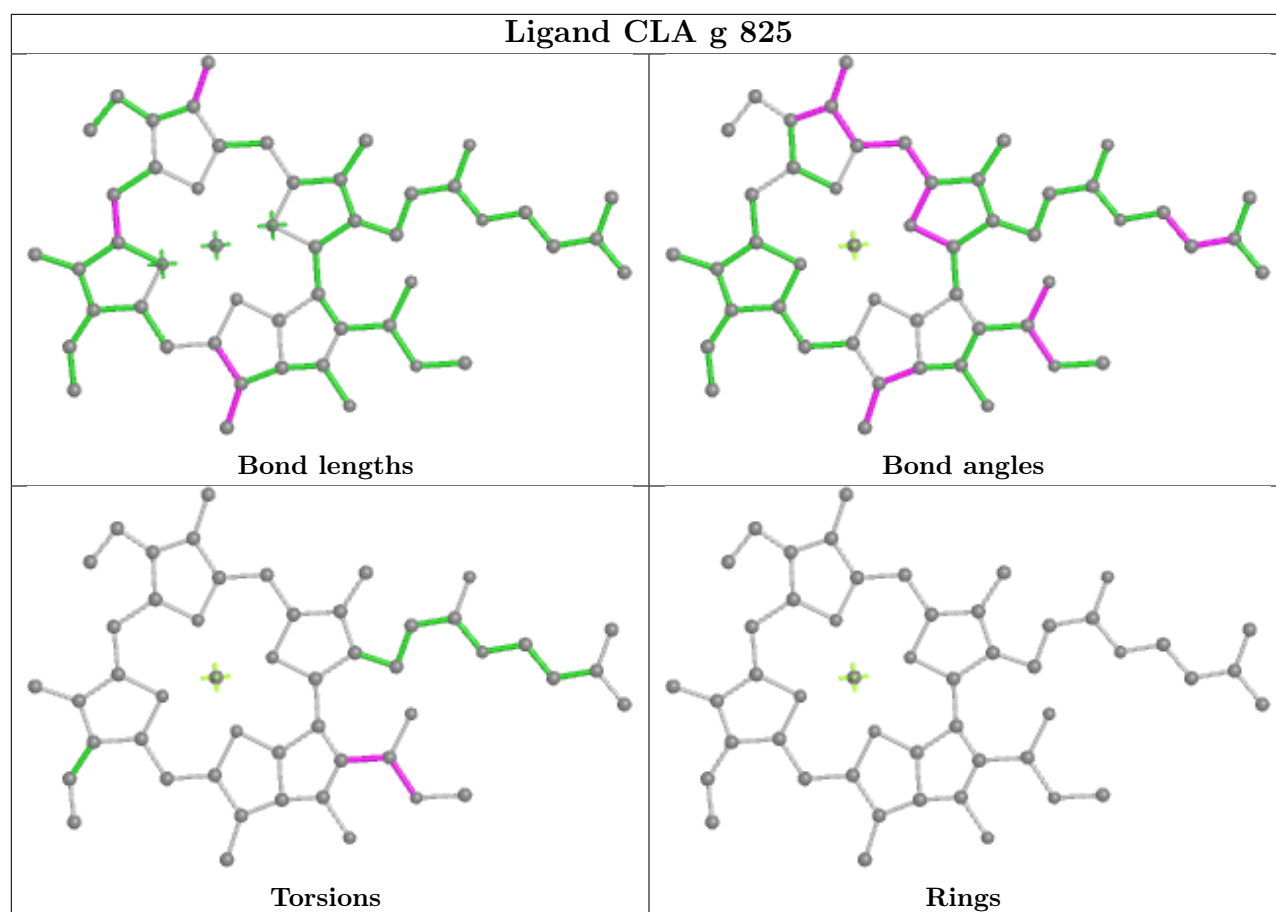


Ligand CLA g 823

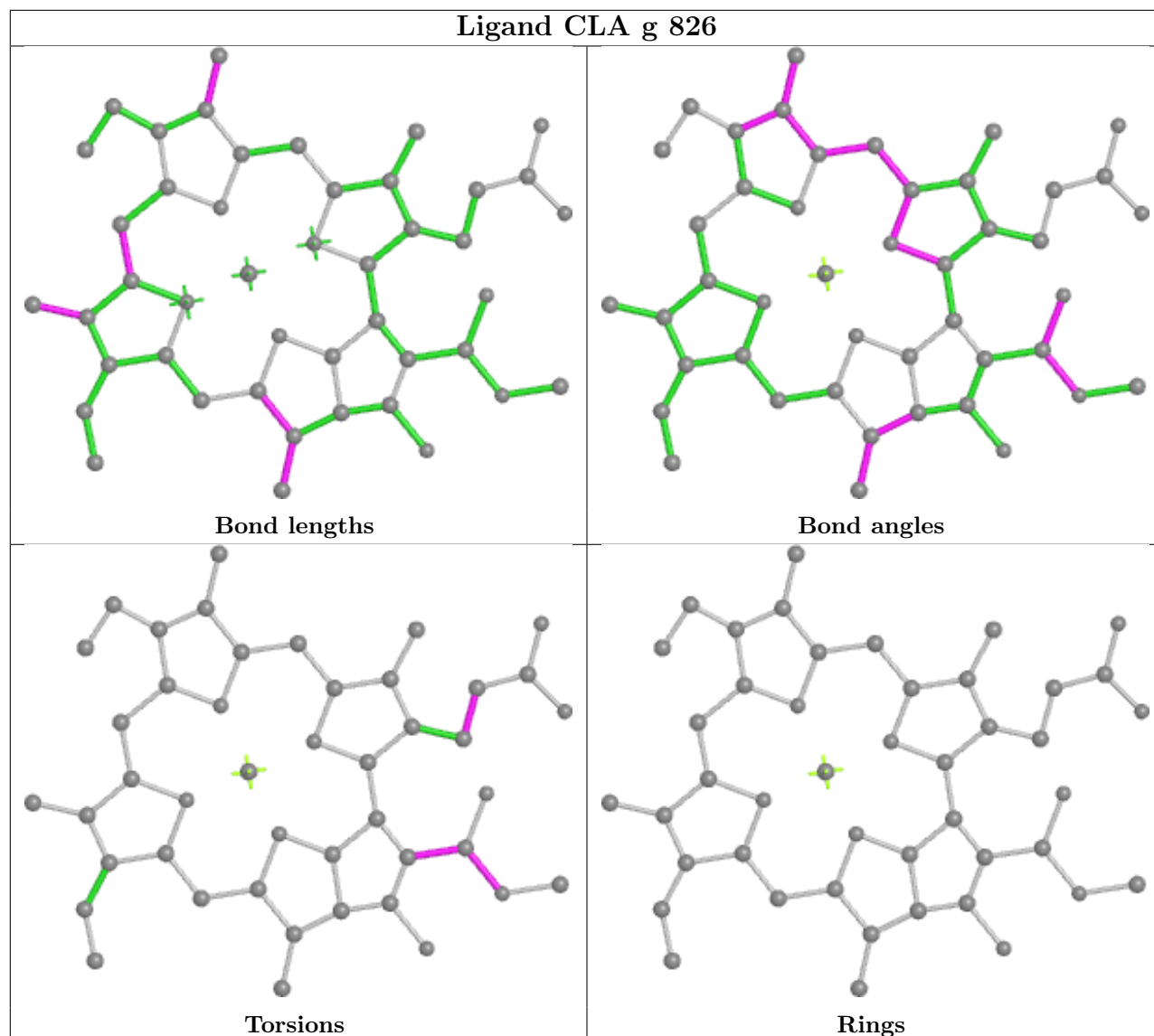


Ligand CLA g 824

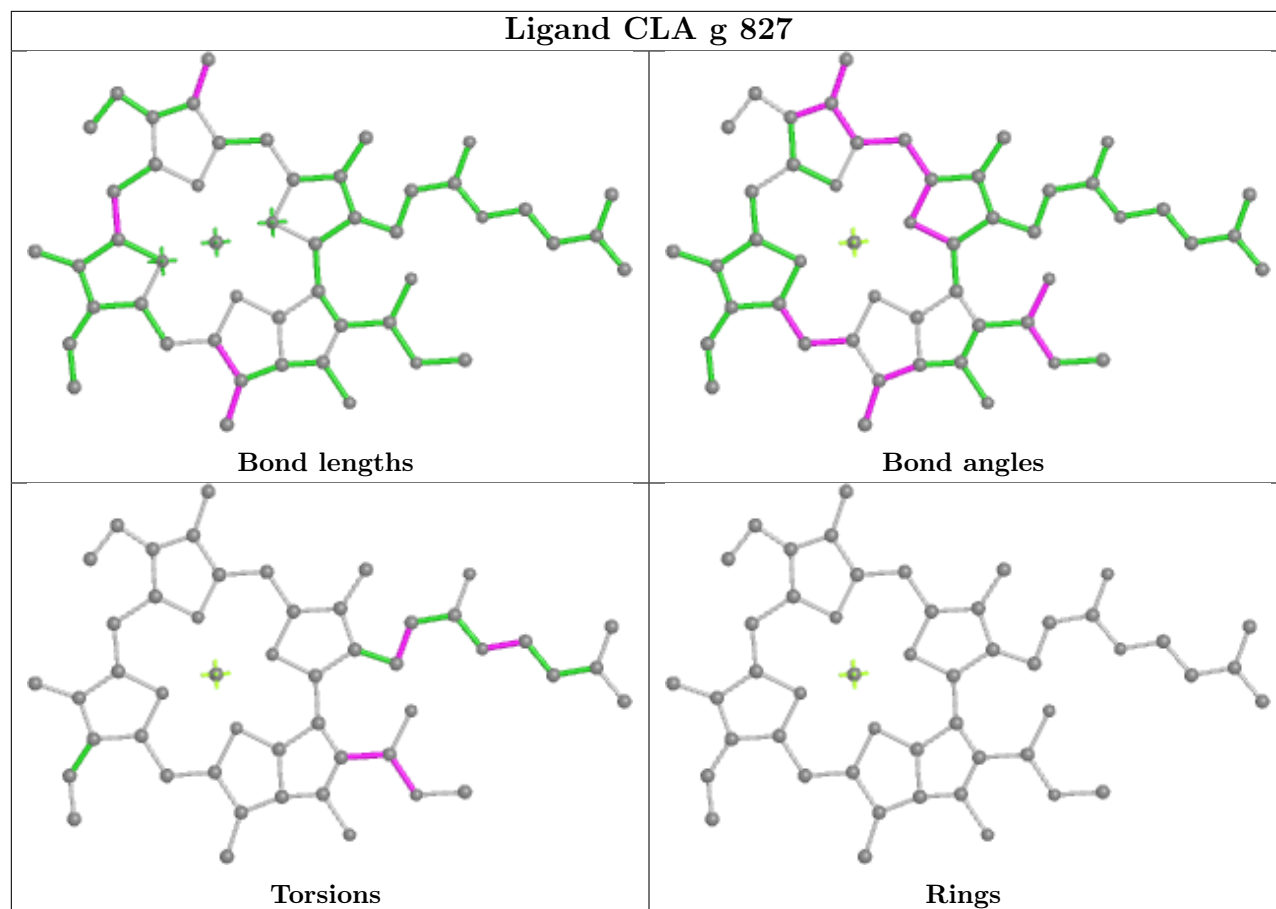




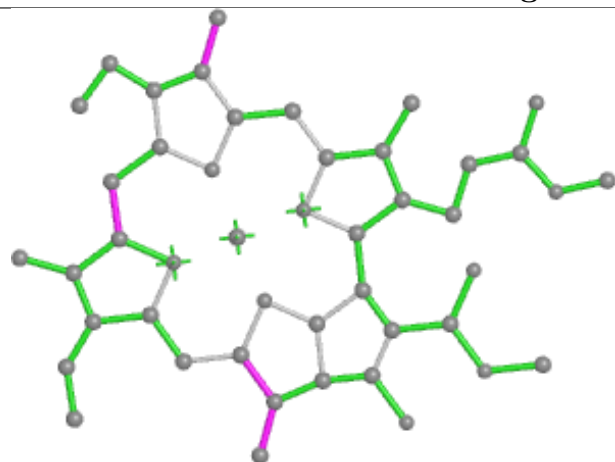
Ligand CLA g 826



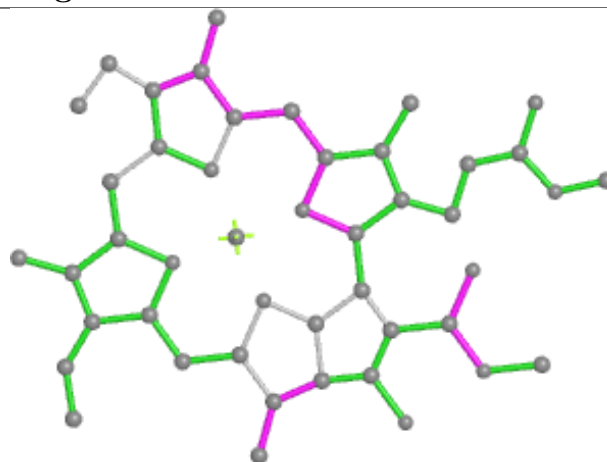
Ligand CLA g 827



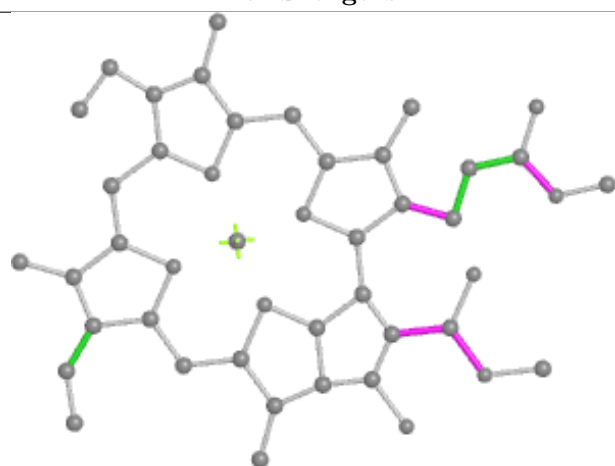
Ligand CLA g 828



Bond lengths



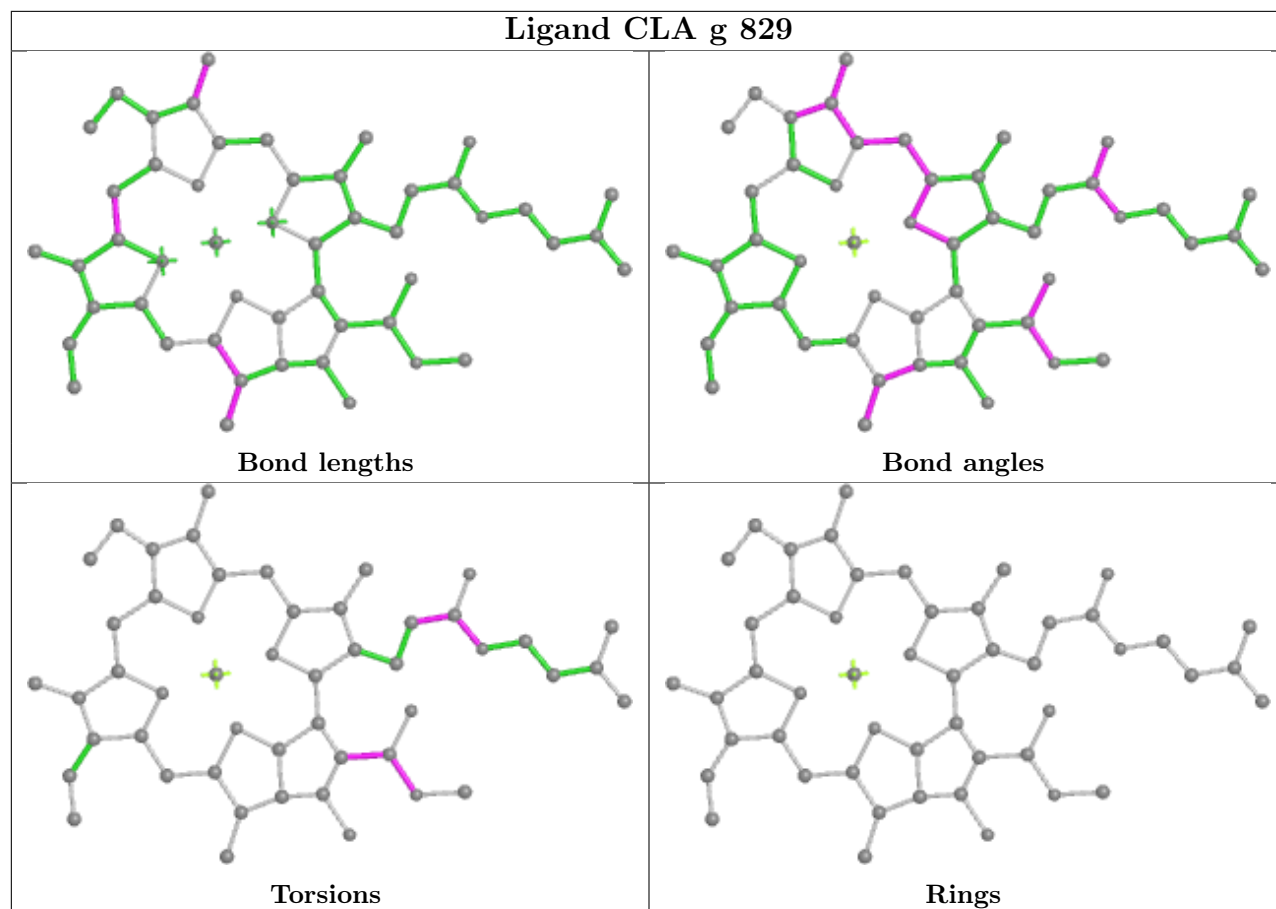
Bond angles

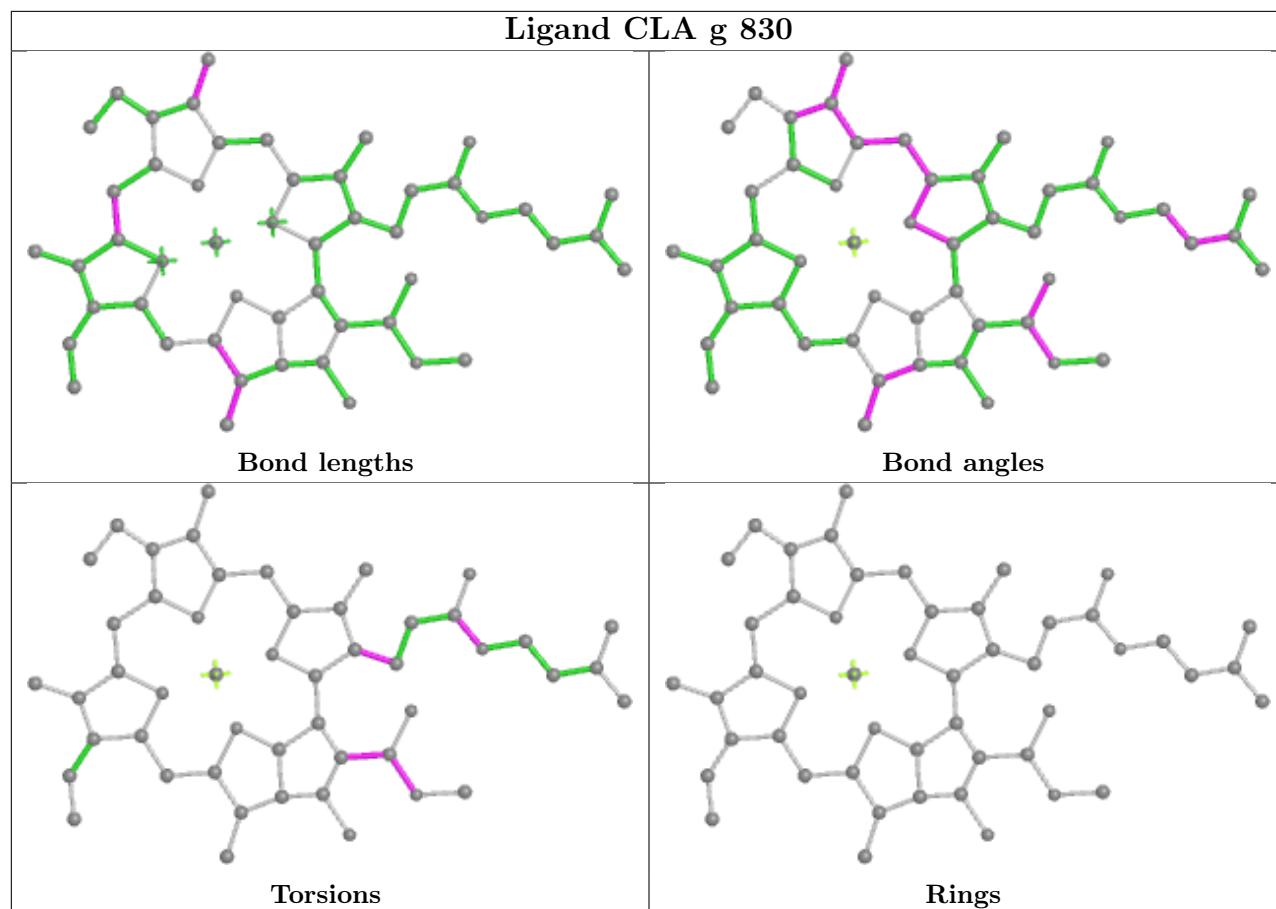


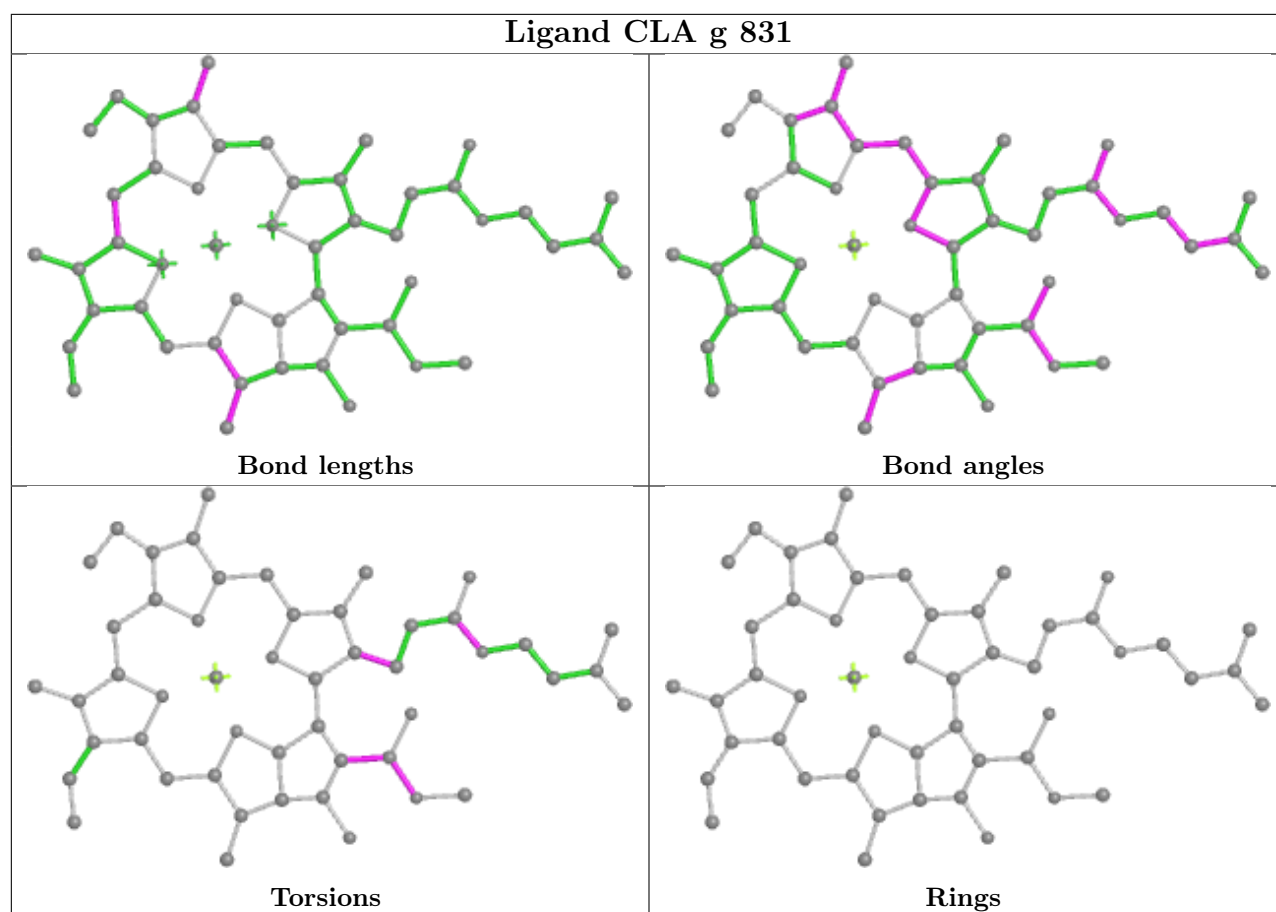
Torsions



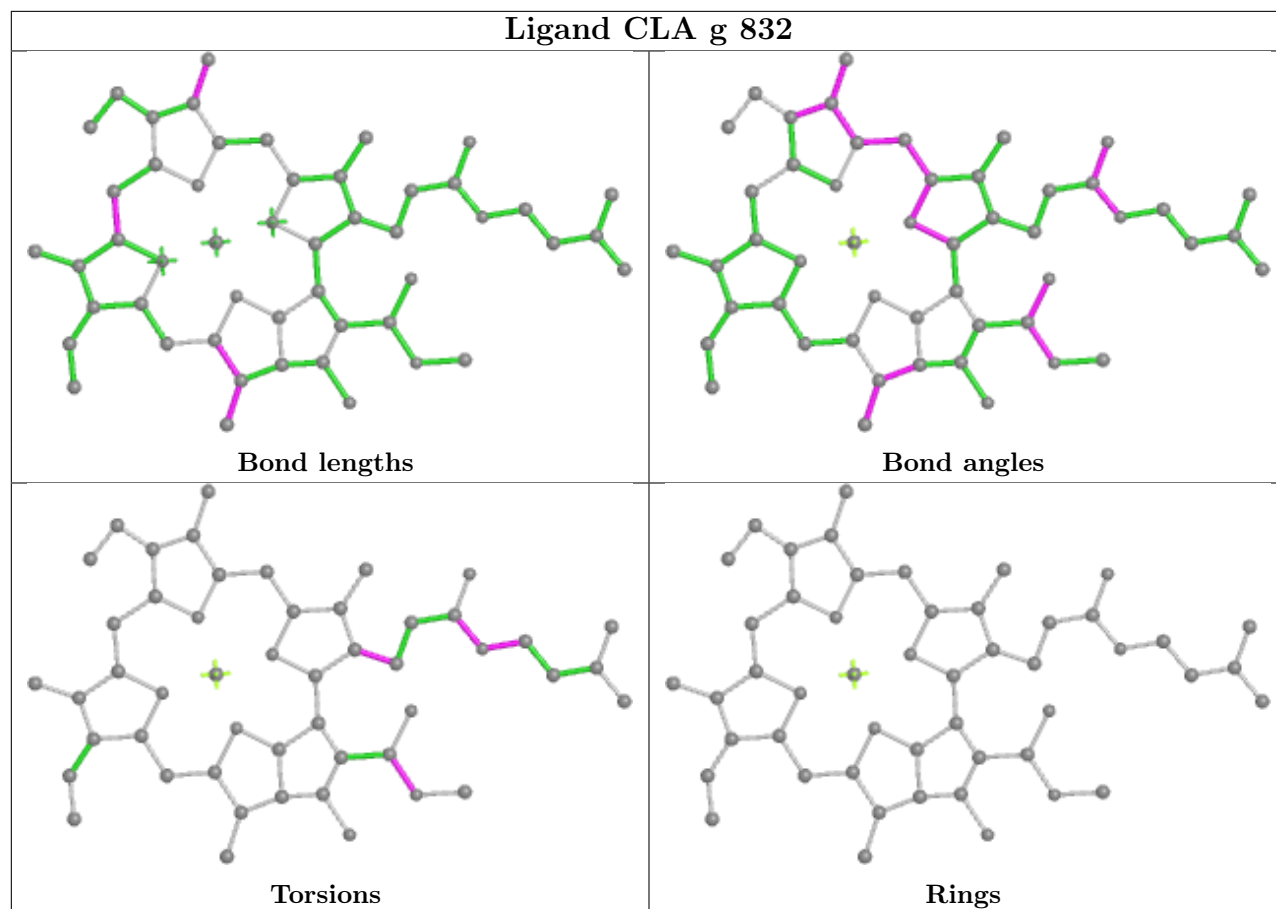
Rings



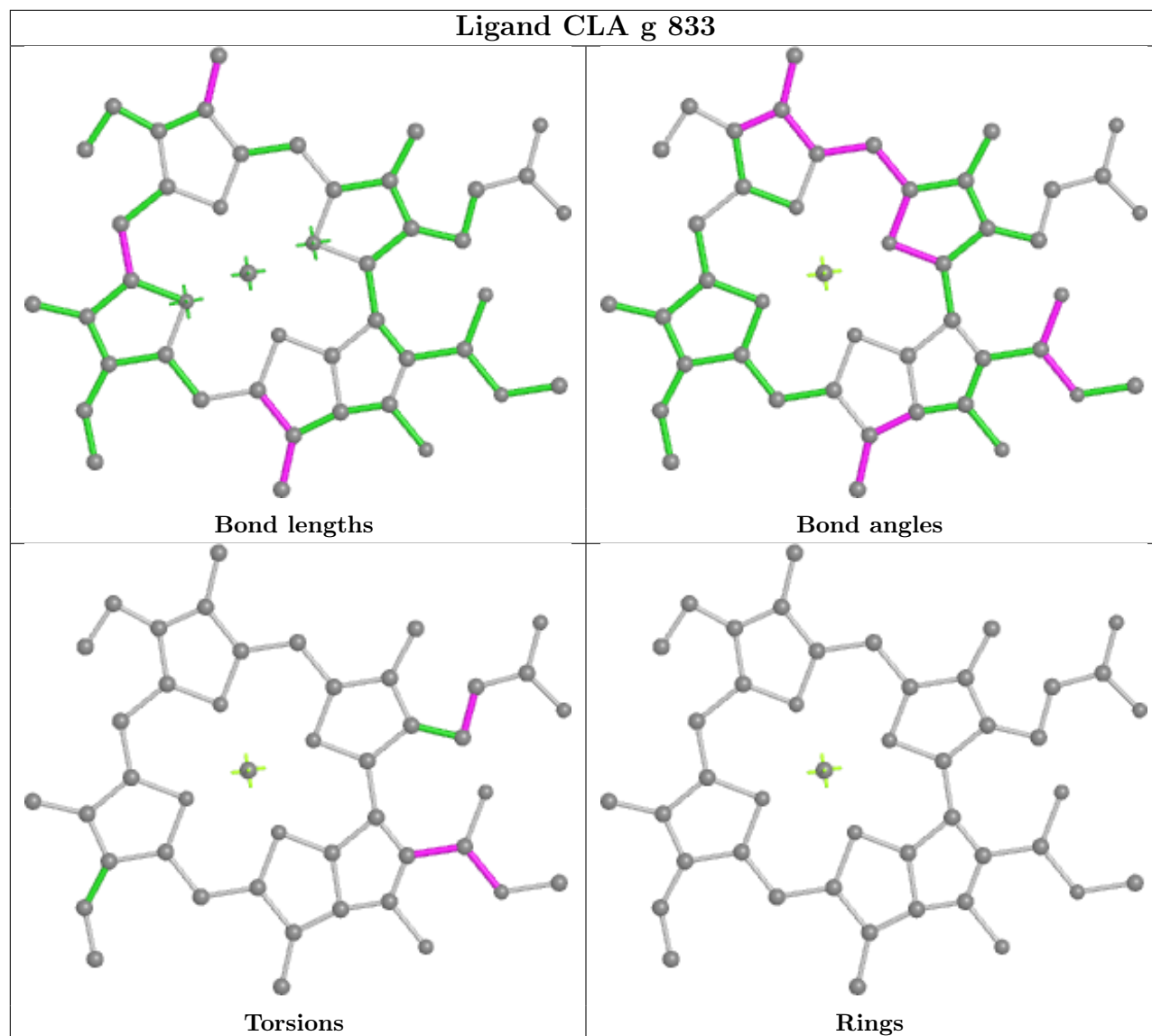




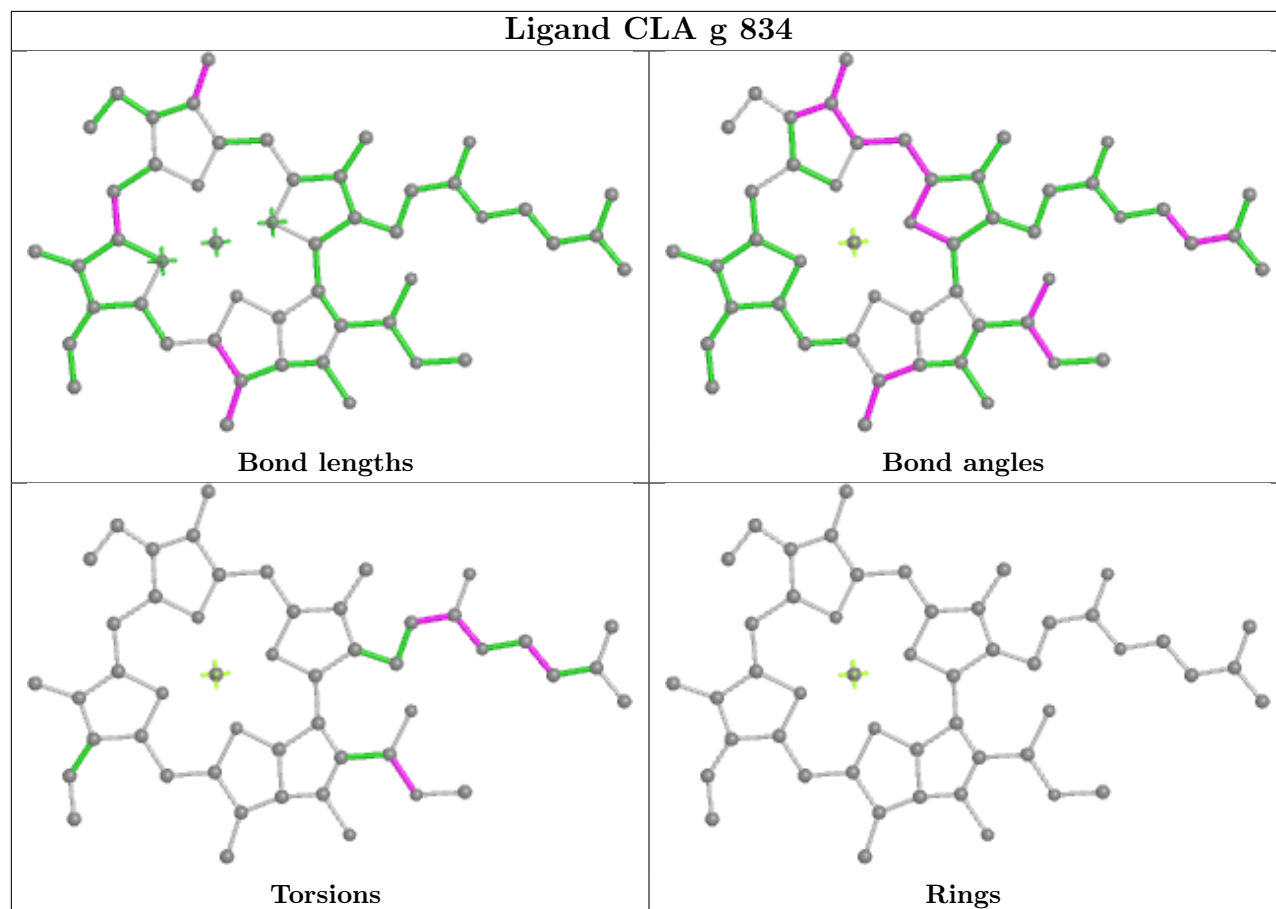
Ligand CLA g 832

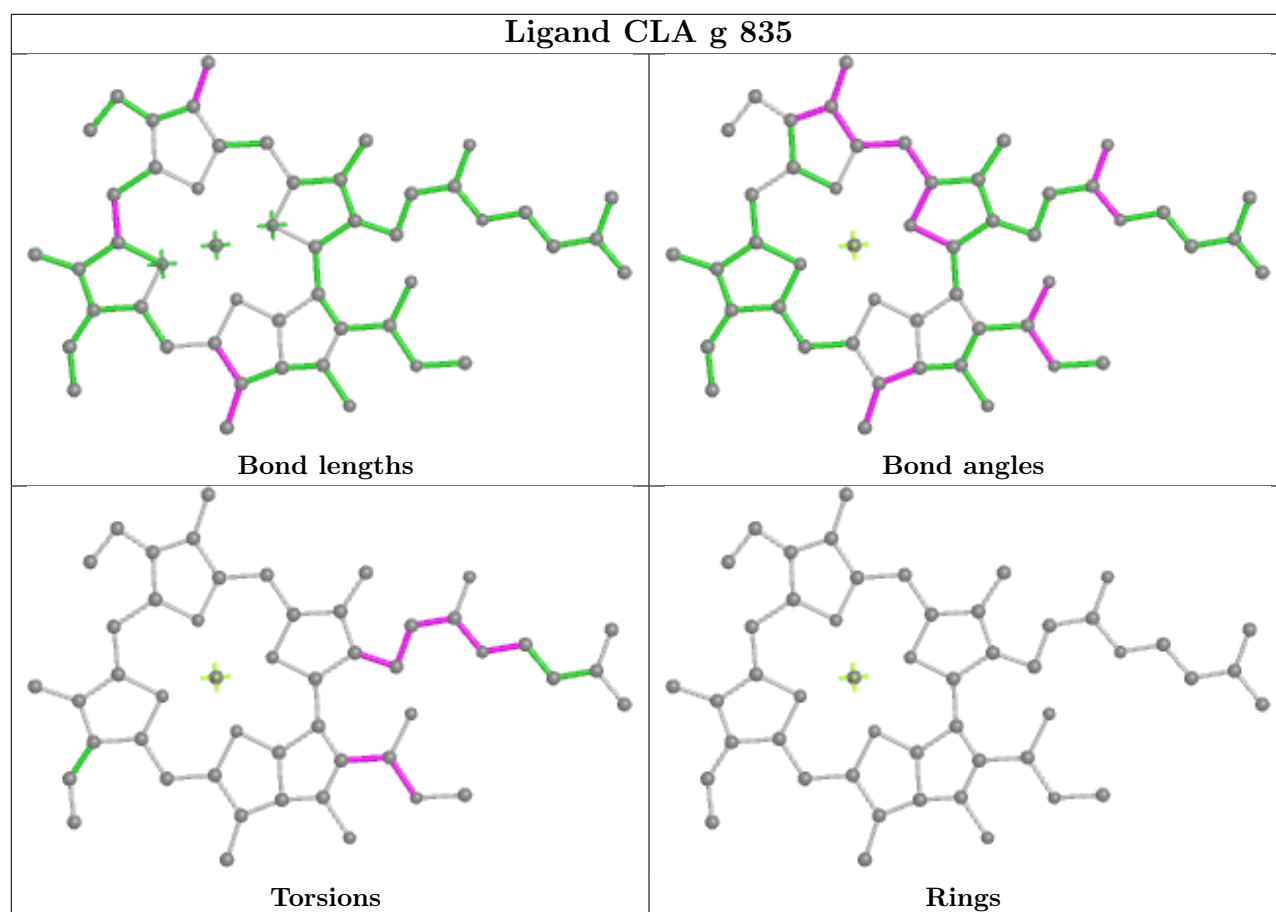


Ligand CLA g 833

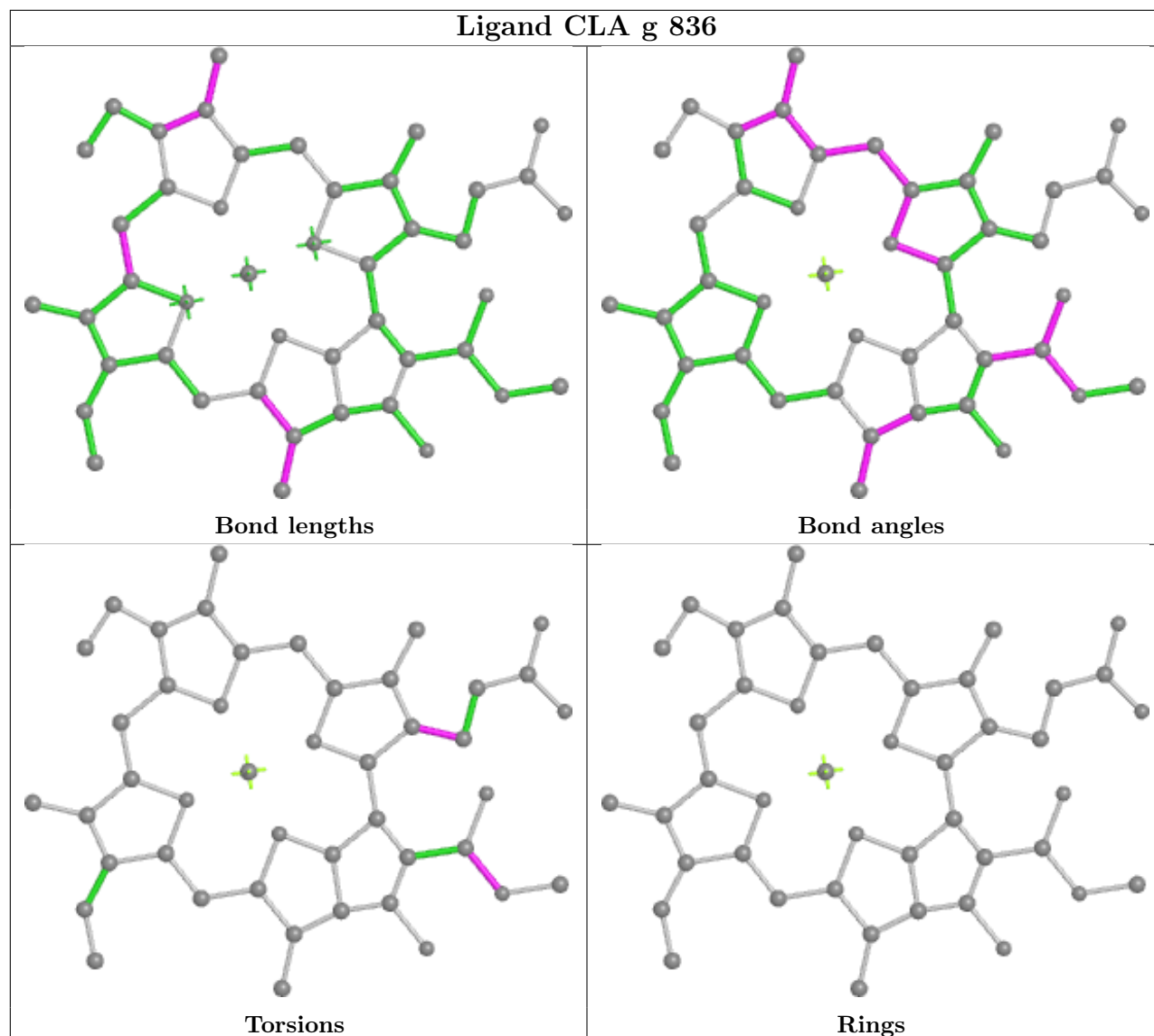


Ligand CLA g 834

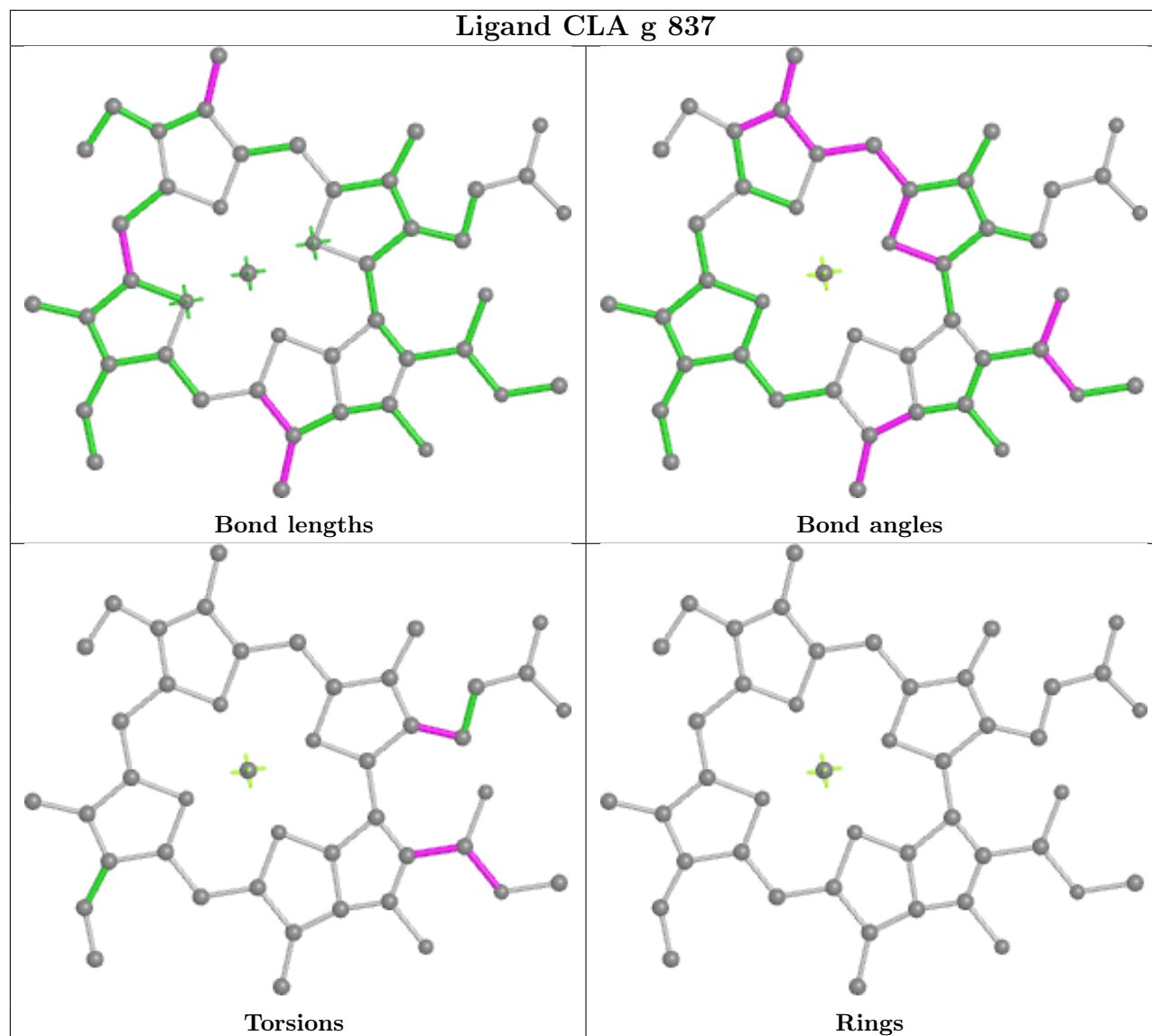


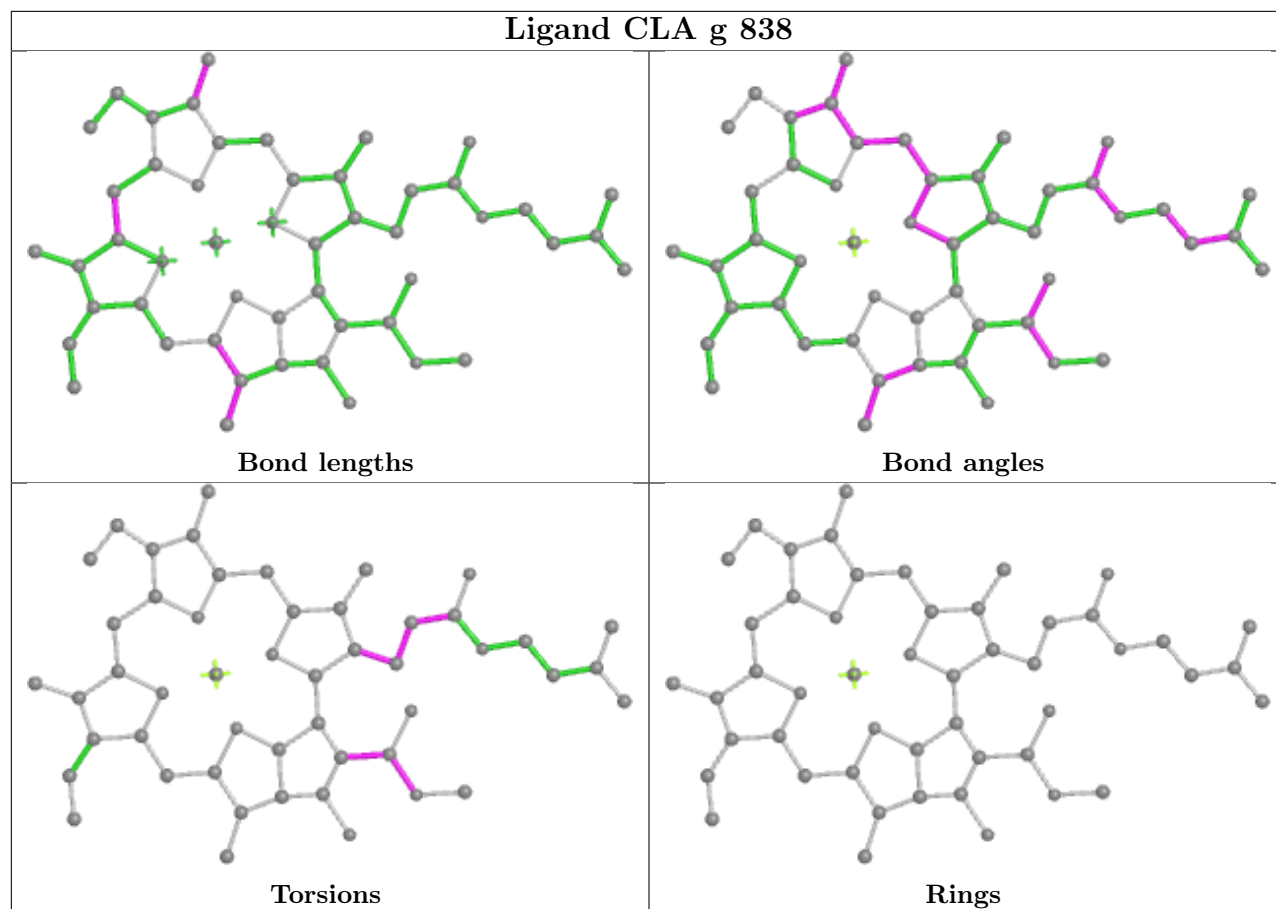


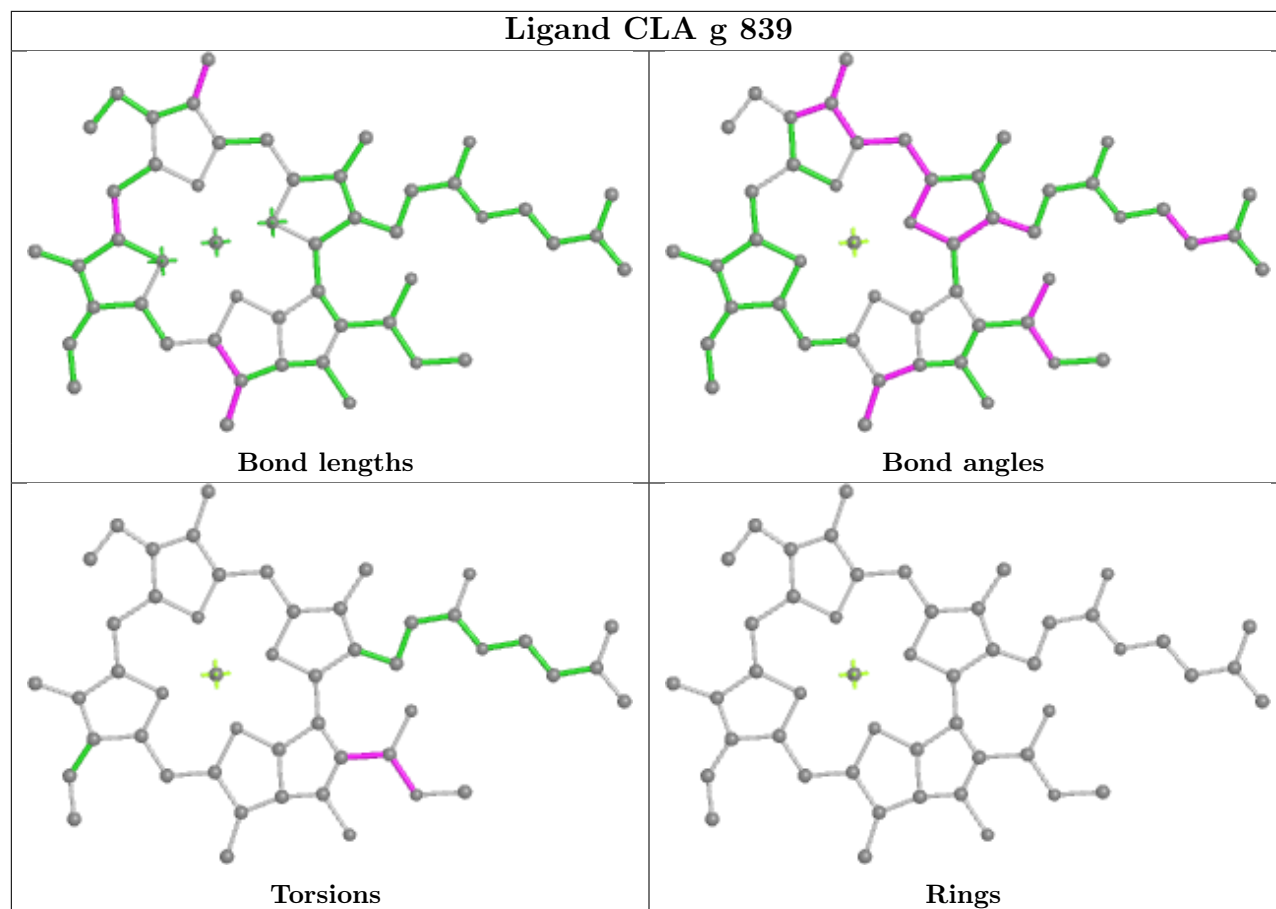
Ligand CLA g 836



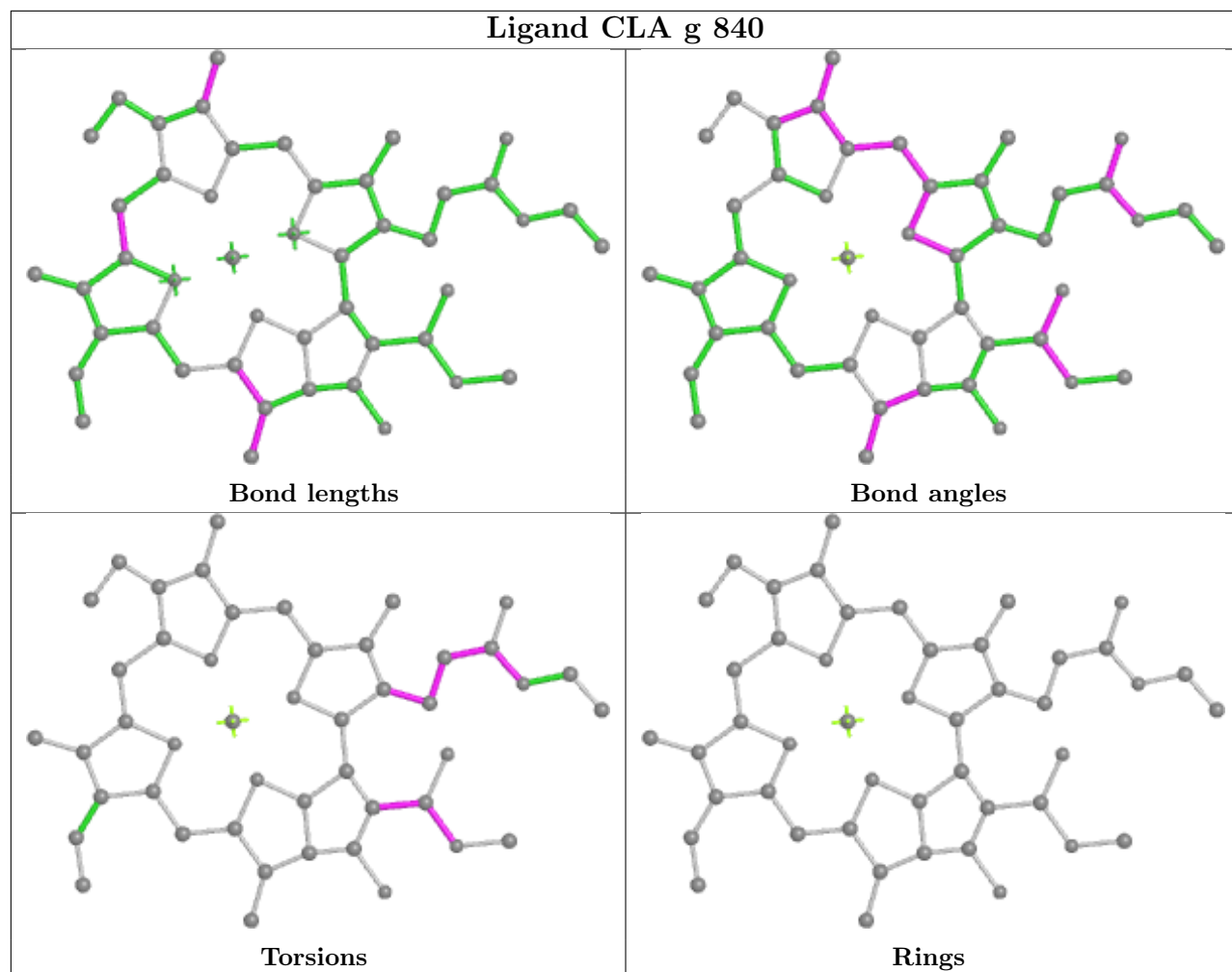
Ligand CLA g 837

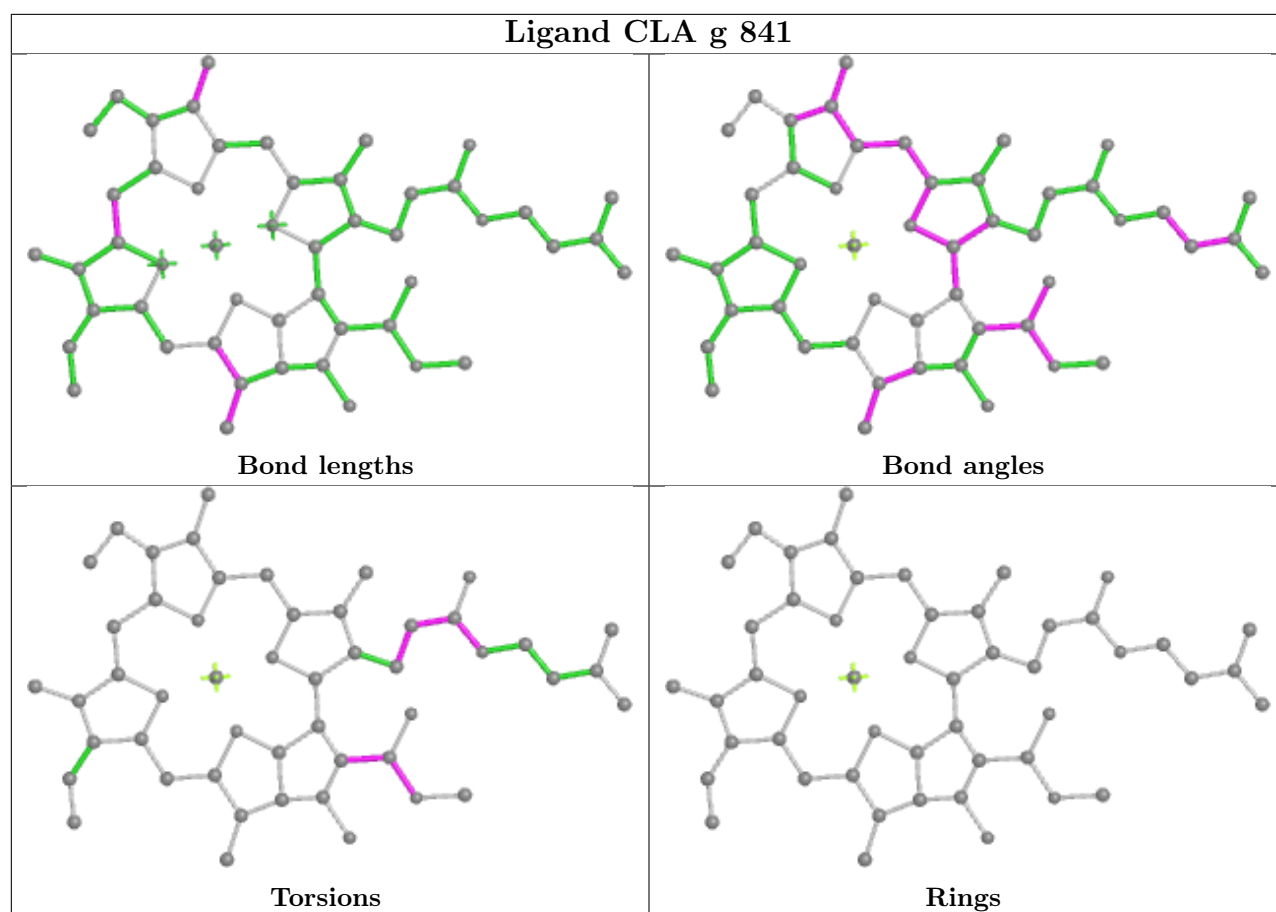


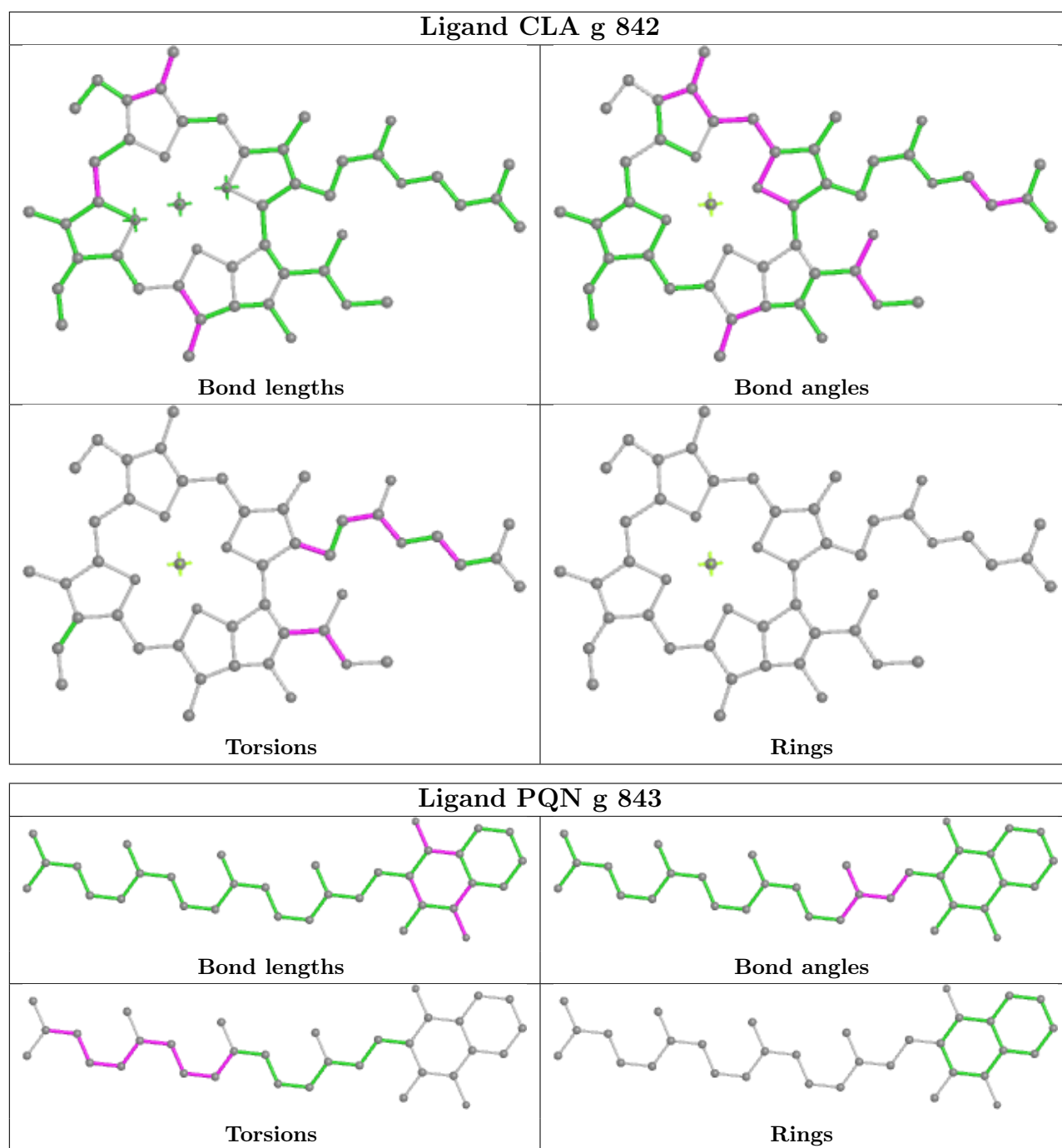


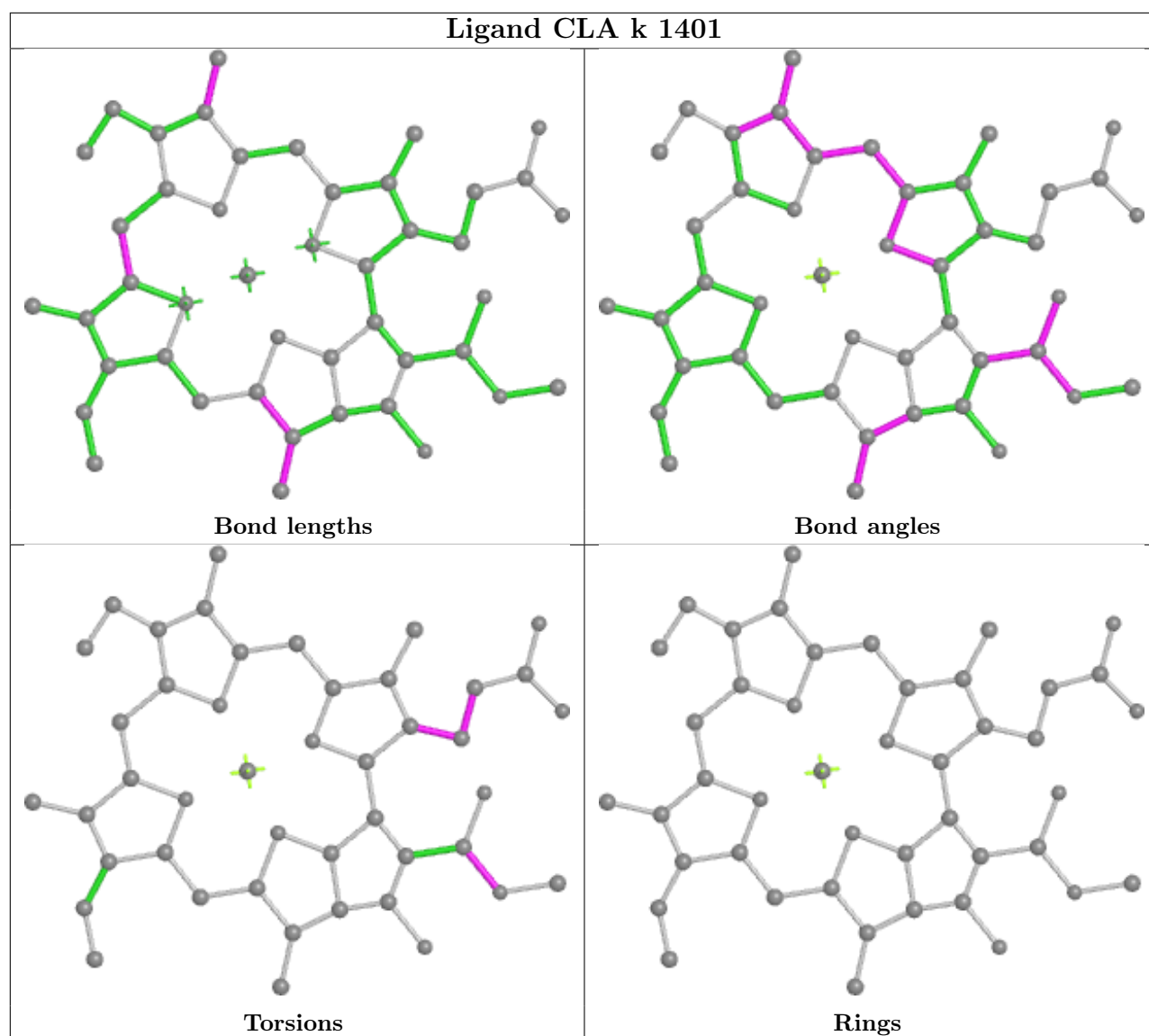


Ligand CLA g 840

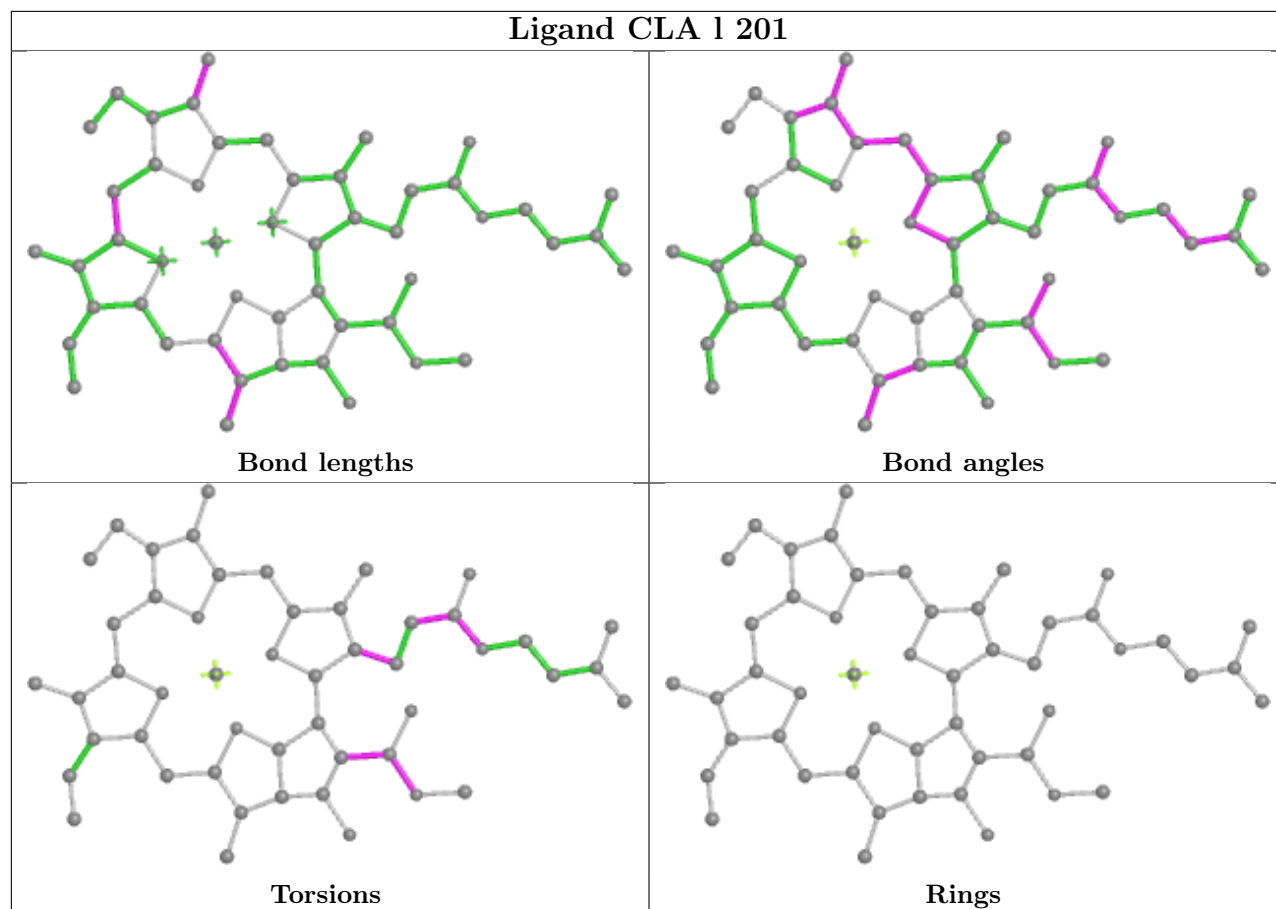




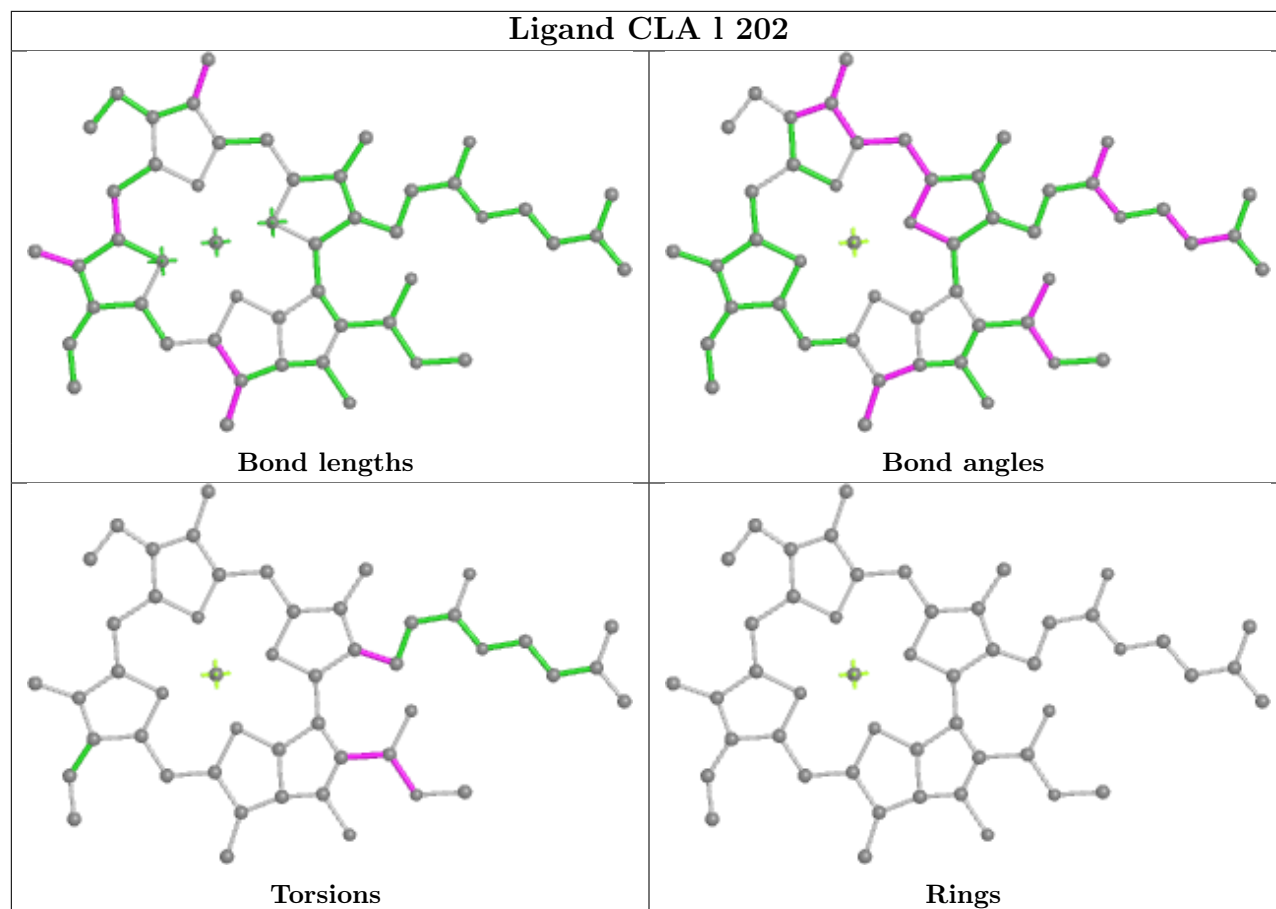




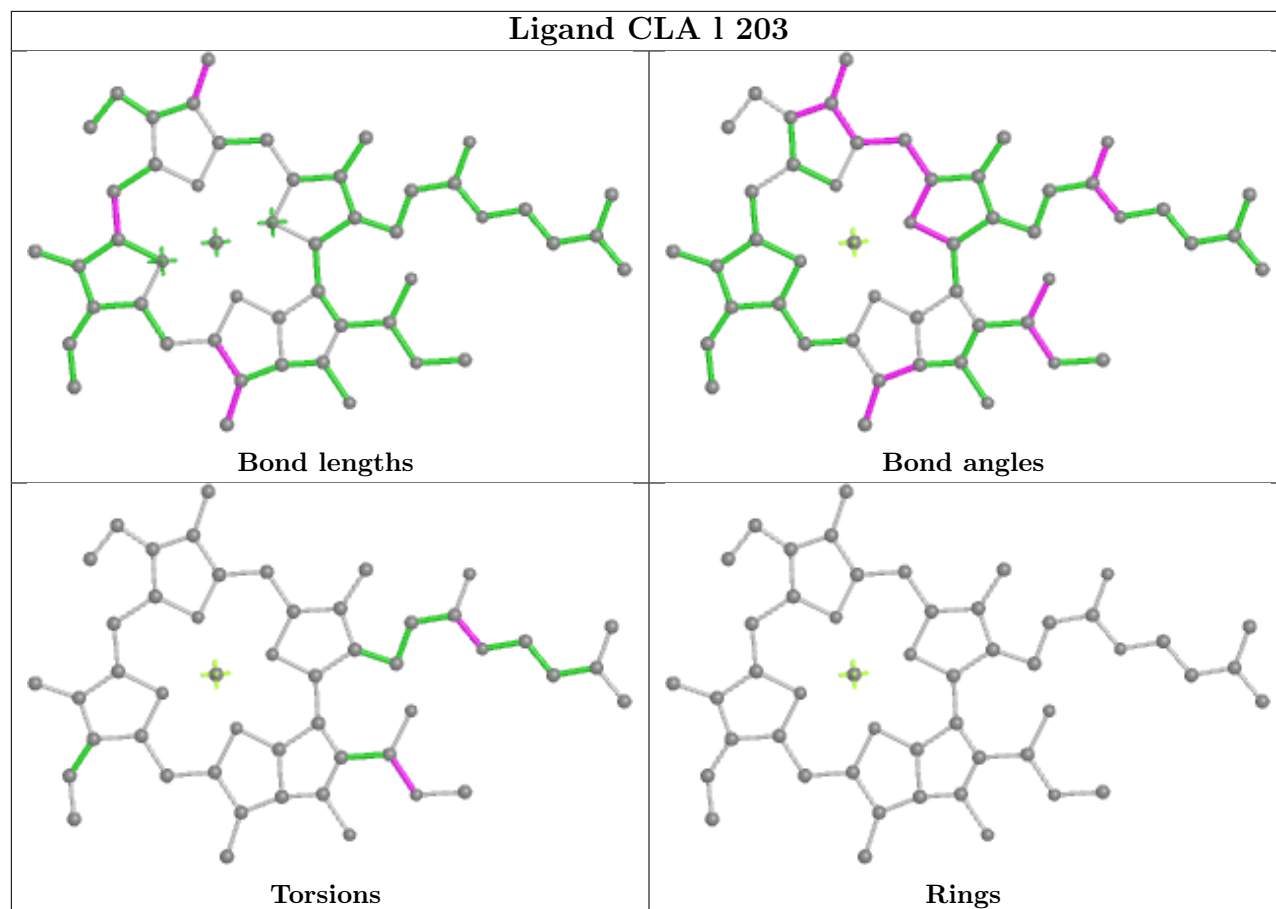
Ligand CLA 1 201

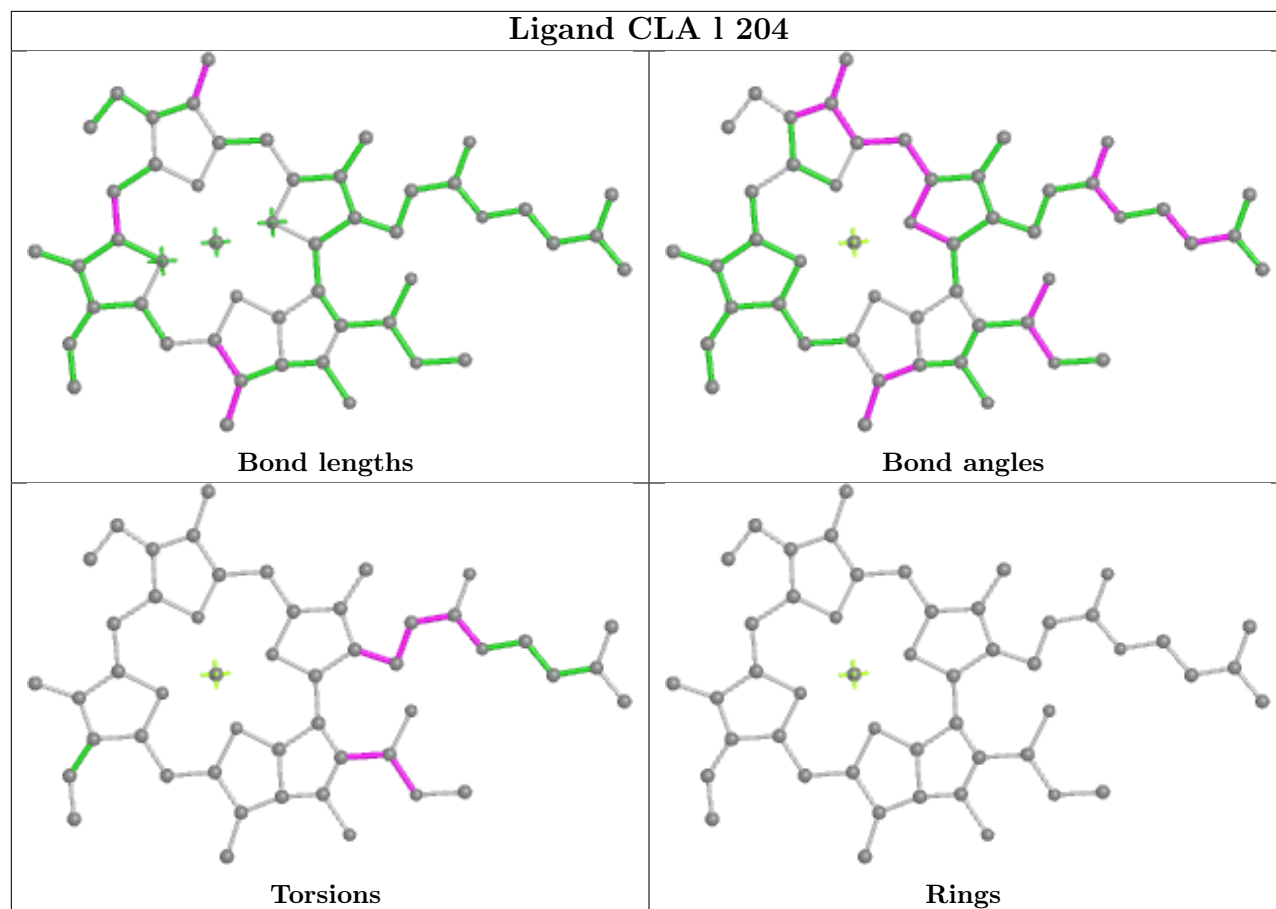


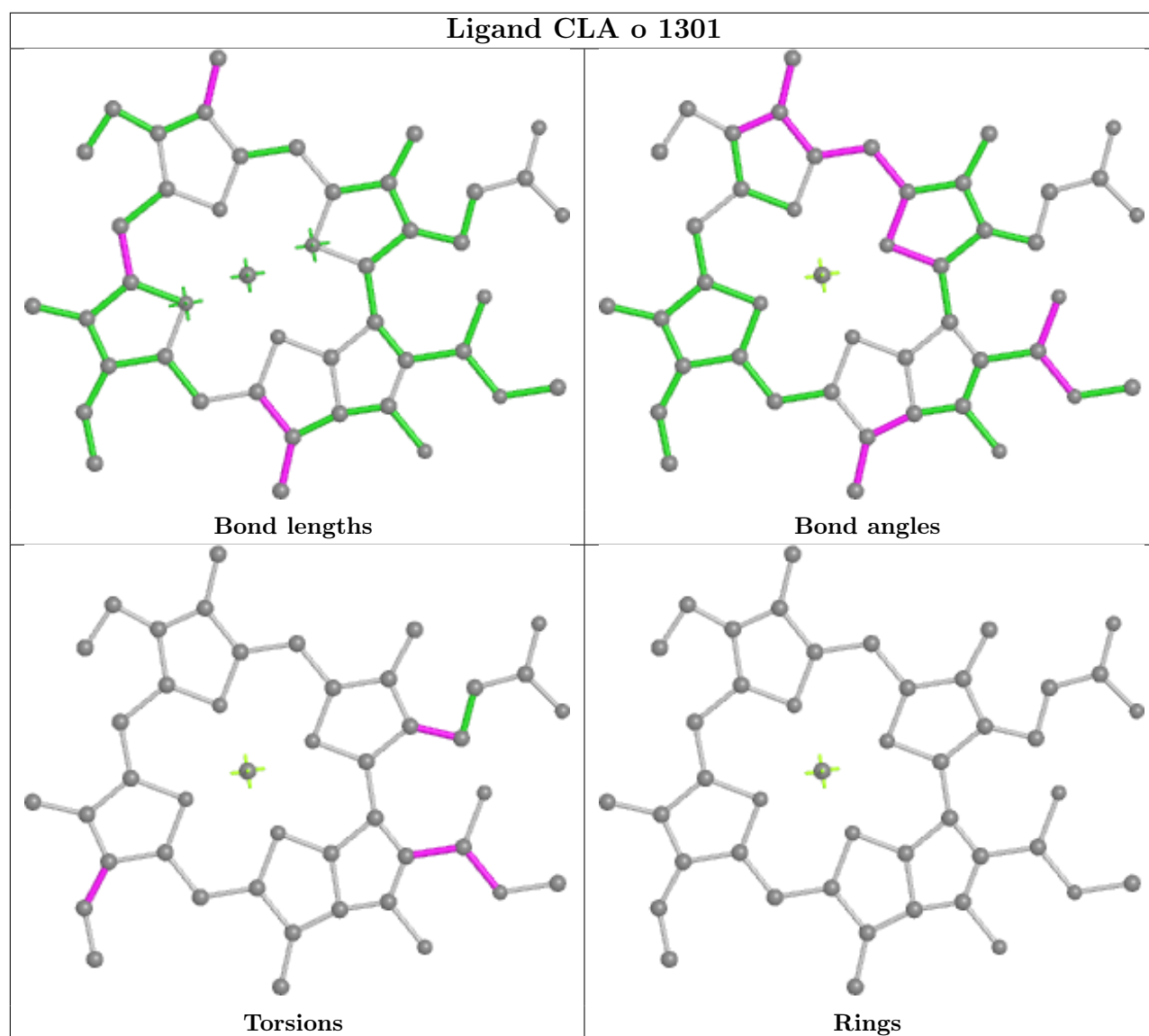
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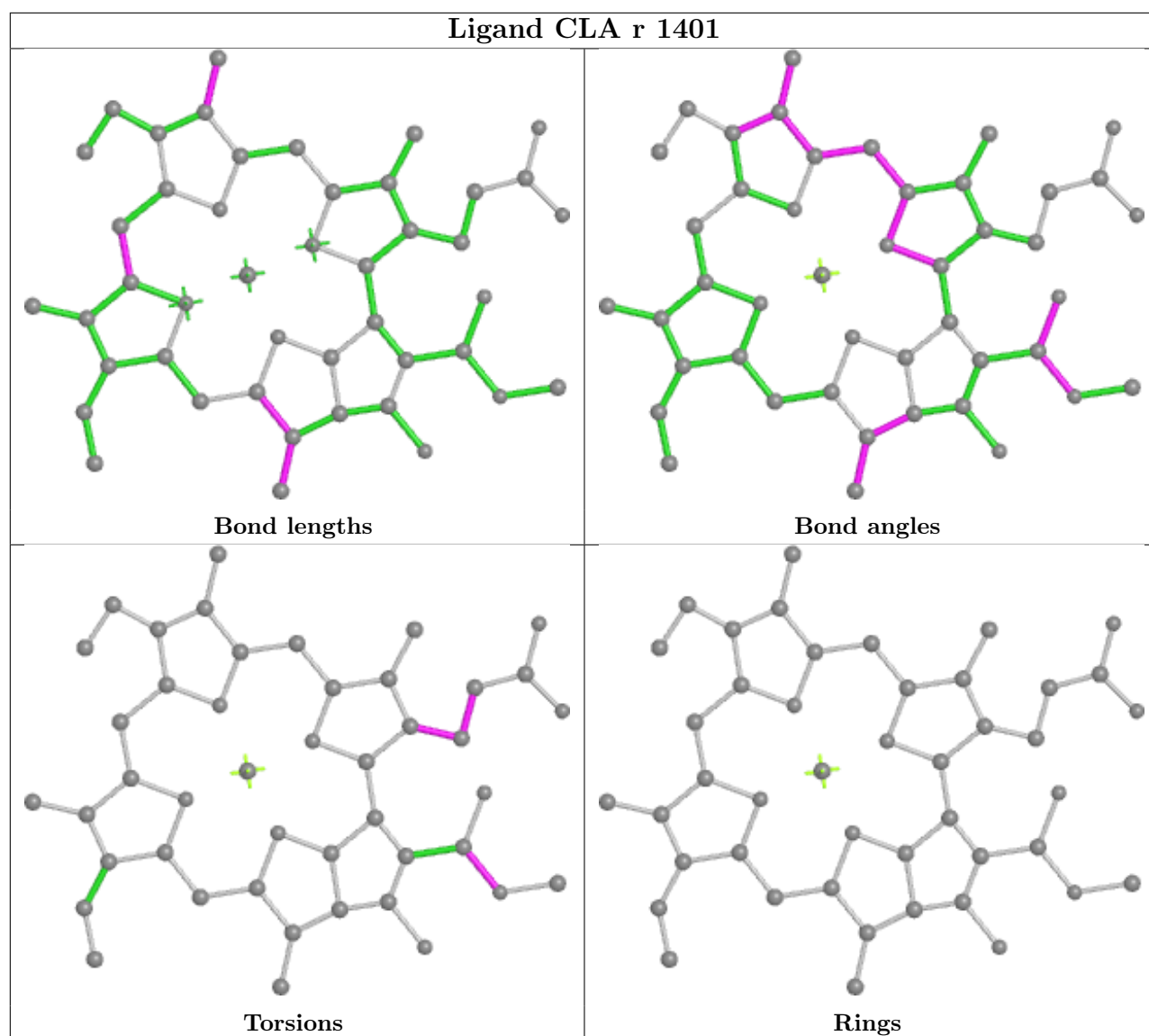


Ligand CLA 1 203

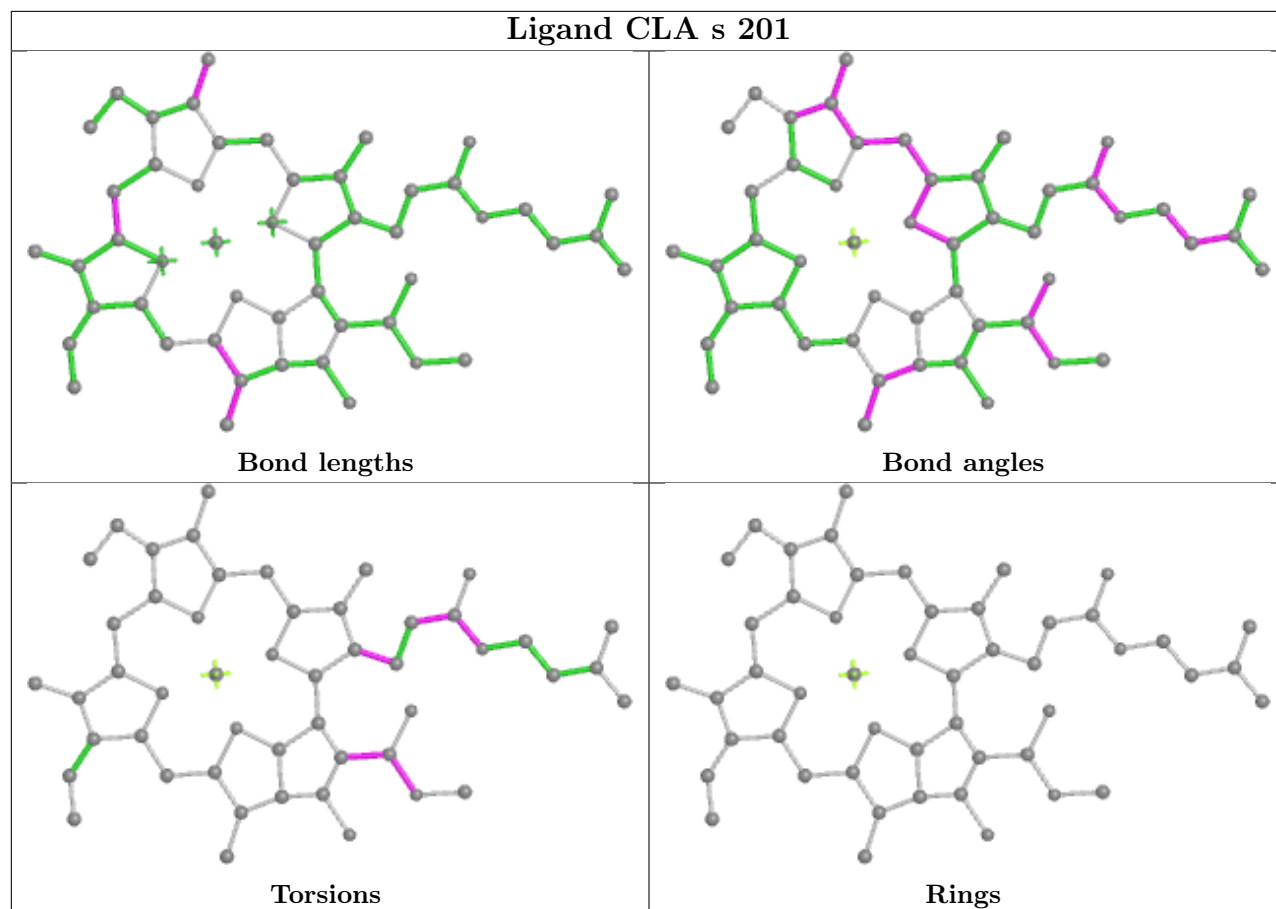


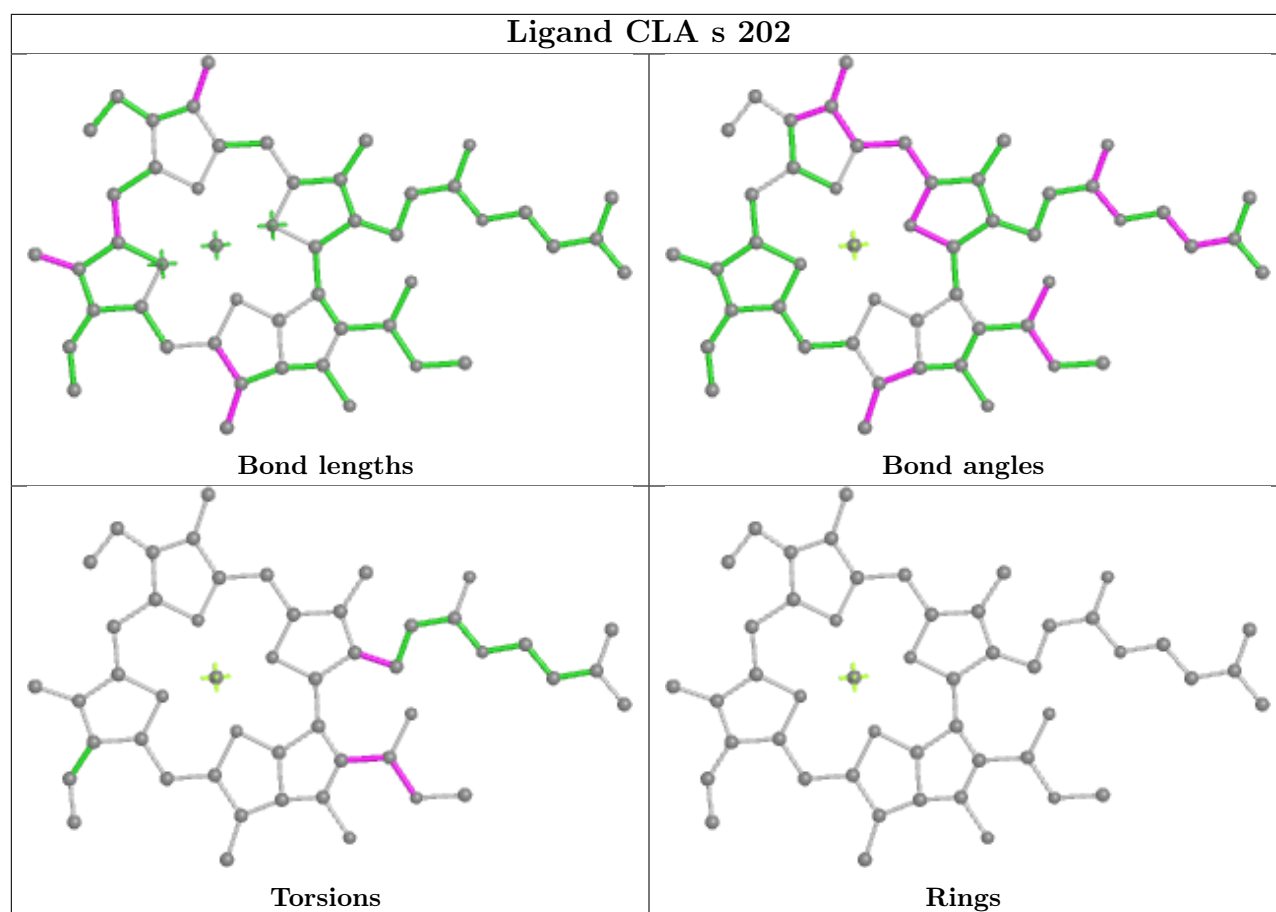


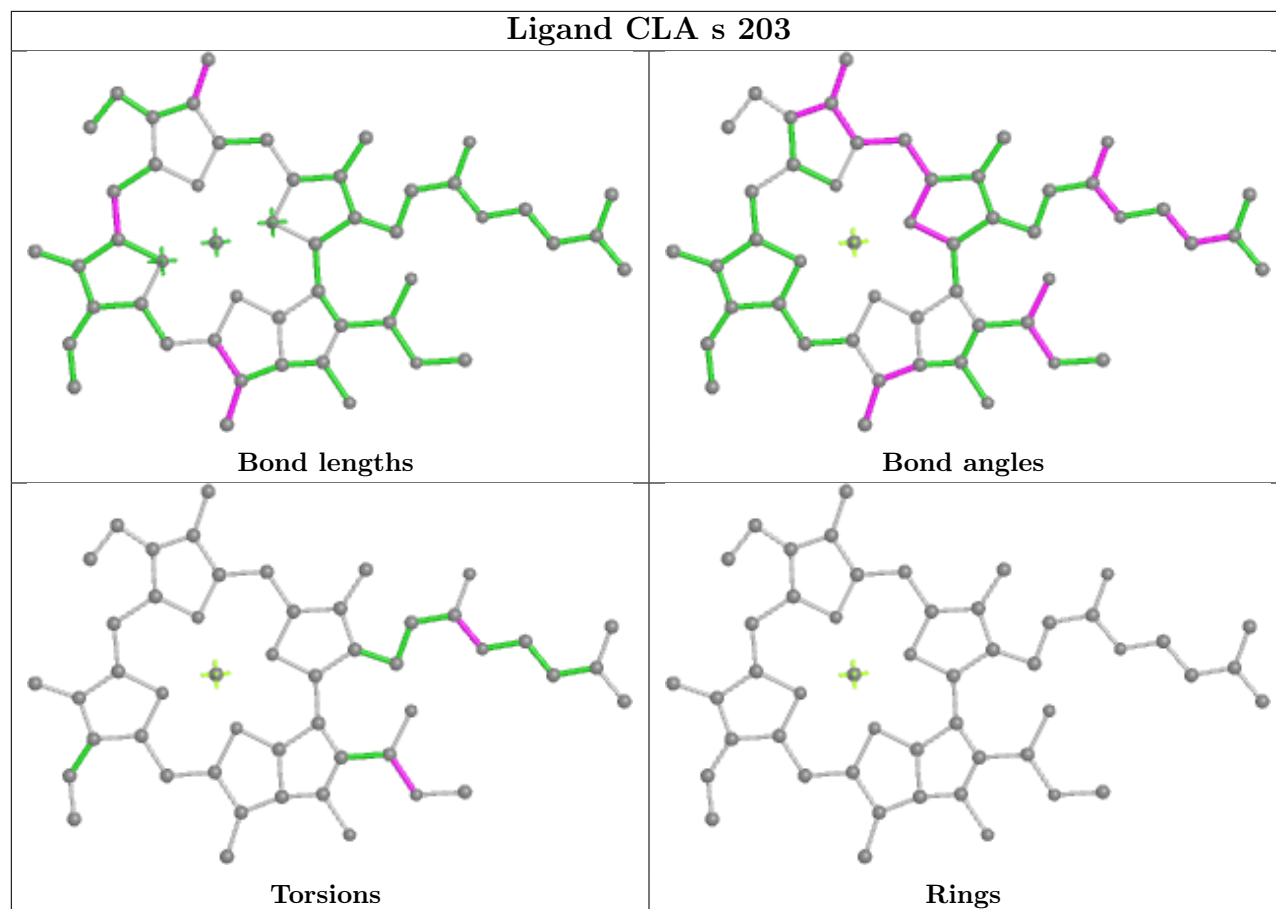


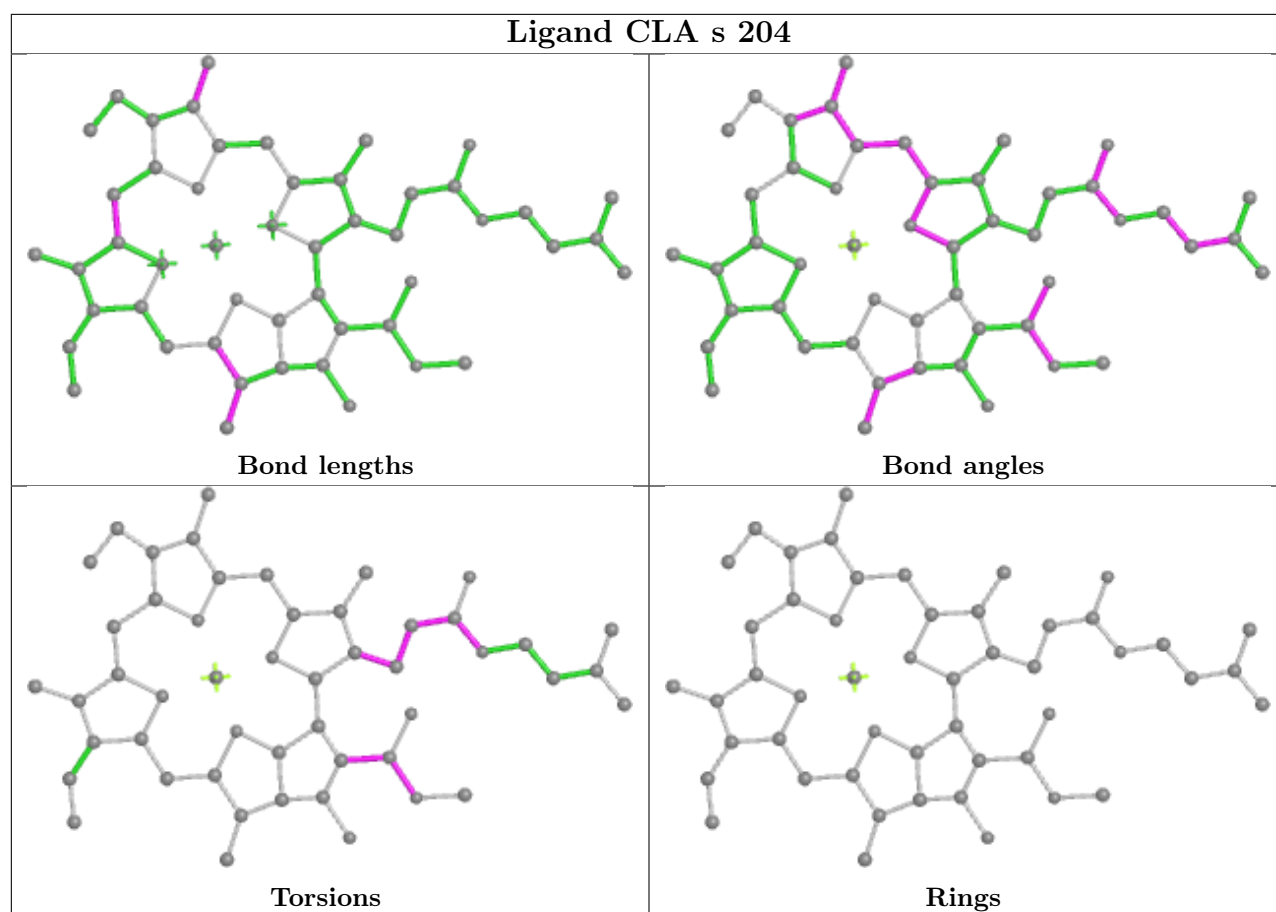


Ligand CLA s 201









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.