



wwPDB EM Validation Summary Report ⓘ

Oct 13, 2024 – 08:50 pm BST

PDB ID : 6TRC
EMDB ID : EMD-10558
Title : Cryo- EM structure of the Thermosynechococcus elongatus photosystem I in the presence of cytochrome c6
Authors : Koelsch, A.; Radon, C.; Baumert, A.; Buerger, J.; Mielke, T.; Lisdat, F.; Zouni, A.; Wendler, P.
Deposited on : 2019-12-18
Resolution : 2.98 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

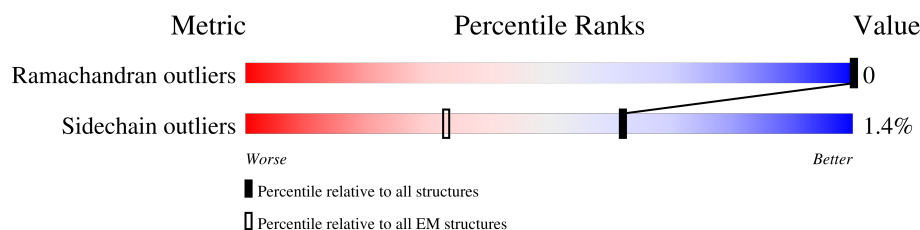
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

1 Overall quality at a glance

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

The reported resolution of this entry is 2.98 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	1	755	<div> <div>25%</div> <div>98%</div> </div>
1	A	755	<div> <div>25%</div> <div>98%</div> </div>
1	a	755	<div> <div>24%</div> <div>98%</div> </div>
2	2	741	<div> <div>18%</div> <div>99%</div> </div>
2	B	741	<div> <div>17%</div> <div>99%</div> </div>
2	b	741	<div> <div>18%</div> <div>99%</div> </div>
3	3	81	<div> <div>98%</div> </div>
3	C	81	<div> <div>98%</div> </div>
3	c	81	<div> <div>98%</div> </div>

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Mol	Chain	Length	Quality of chain
4	4	139	19% 98% ..
4	D	139	18% 98% ..
4	d	139	18% 98% ..
5	5	76	39% 88% . 8%
5	E	76	41% 88% . 8%
5	e	76	41% 88% . 8%
6	6	141	82% 99% .
6	F	141	83% 99% .
6	f	141	82% 99% .
7	7	38	5% 97% .
7	I	38	5% 97% .
7	i	38	5% 97% .
8	8	41	85% 93% 7%
8	J	41	88% 93% 7%
8	j	41	90% 93% 7%
9	9	83	88% 92% .. 5%
9	K	83	87% 92% .. 5%
9	k	83	90% 92% .. 5%
10	0	155	6% 97% ..
10	L	155	7% 97% ..
10	l	155	6% 97% ..
11	M	31	13% 100%
11	m	31	13% 100%
11	y	31	6% 100%
12	X	36	75% 67% 6% . 25%

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Mol	Chain	Length	Quality of chain
12	x	36	
12	z	36	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CL0	1	801	X	-	-	-
13	CL0	A	801	X	-	-	-
13	CL0	a	801	X	-	-	-
14	CLA	0	203	X	-	-	-
14	CLA	0	204	X	-	-	-
14	CLA	0	207	X	-	-	-
14	CLA	0	208	X	-	-	-
14	CLA	0	209	X	-	-	-
14	CLA	1	802	X	-	-	-
14	CLA	1	803	X	-	-	-
14	CLA	1	804	X	-	-	-
14	CLA	1	805	X	-	-	-
14	CLA	1	806	X	-	-	-
14	CLA	1	807	X	-	-	-
14	CLA	1	808	X	-	-	-
14	CLA	1	809	X	-	-	-
14	CLA	1	810	X	-	-	-
14	CLA	1	811	X	-	-	-
14	CLA	1	812	X	-	-	-
14	CLA	1	813	X	-	-	-
14	CLA	1	814	X	-	-	-
14	CLA	1	815	X	-	-	-
14	CLA	1	816	X	-	-	-
14	CLA	1	817	X	-	-	-
14	CLA	1	818	X	-	-	-
14	CLA	1	819	X	-	-	-
14	CLA	1	820	X	-	-	-
14	CLA	1	821	X	-	-	-
14	CLA	1	822	X	-	-	-
14	CLA	1	823	X	-	-	-
14	CLA	1	824	X	-	-	-
14	CLA	1	825	X	-	-	-
14	CLA	1	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	827	X	-	-	-
14	CLA	1	828	X	-	-	-
14	CLA	1	829	X	-	-	-
14	CLA	1	830	X	-	-	-
14	CLA	1	831	X	-	-	-
14	CLA	1	832	X	-	-	-
14	CLA	1	833	X	-	-	-
14	CLA	1	834	X	-	-	-
14	CLA	1	835	X	-	-	-
14	CLA	1	836	X	-	-	-
14	CLA	1	837	X	-	-	-
14	CLA	1	838	X	-	-	-
14	CLA	1	839	X	-	-	-
14	CLA	1	840	X	-	-	-
14	CLA	1	841	X	-	-	-
14	CLA	1	842	X	-	-	-
14	CLA	1	843	X	-	-	-
14	CLA	1	844	X	-	-	-
14	CLA	2	3003	X	-	-	-
14	CLA	2	3004	X	-	-	-
14	CLA	2	3005	X	-	-	-
14	CLA	2	3006	X	-	-	-
14	CLA	2	3007	X	-	-	-
14	CLA	2	3008	X	-	-	-
14	CLA	2	3009	X	-	-	-
14	CLA	2	3010	X	-	-	-
14	CLA	2	3011	X	-	-	-
14	CLA	2	3012	X	-	-	-
14	CLA	2	3014	X	-	-	-
14	CLA	2	3015	X	-	-	-
14	CLA	2	3016	X	-	-	-
14	CLA	2	3017	X	-	-	-
14	CLA	2	3019	X	-	-	-
14	CLA	2	3020	X	-	-	-
14	CLA	2	3021	X	-	-	-
14	CLA	2	3022	X	-	-	-
14	CLA	2	3023	X	-	-	-
14	CLA	2	3025	X	-	-	-
14	CLA	2	3026	X	-	-	-
14	CLA	2	3027	X	-	-	-
14	CLA	2	3028	X	-	-	-
14	CLA	2	3029	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	2	3030	X	-	-	-
14	CLA	2	3031	X	-	-	-
14	CLA	2	3032	X	-	-	-
14	CLA	2	3033	X	-	-	-
14	CLA	2	3034	X	-	-	-
14	CLA	2	3035	X	-	-	-
14	CLA	2	3036	X	-	-	-
14	CLA	2	3037	X	-	-	-
14	CLA	2	3038	X	-	-	-
14	CLA	2	3039	X	-	-	-
14	CLA	2	3041	X	-	-	-
14	CLA	2	3042	X	-	-	-
14	CLA	6	201	X	-	-	-
14	CLA	6	203	X	-	-	-
14	CLA	6	204	X	-	-	-
14	CLA	8	101	X	-	-	-
14	CLA	8	102	X	-	-	-
14	CLA	9	101	X	-	-	-
14	CLA	9	103	X	-	-	-
14	CLA	A	802	X	-	-	-
14	CLA	A	803	X	-	-	-
14	CLA	A	804	X	-	-	-
14	CLA	A	805	X	-	-	-
14	CLA	A	806	X	-	-	-
14	CLA	A	807	X	-	-	-
14	CLA	A	808	X	-	-	-
14	CLA	A	809	X	-	-	-
14	CLA	A	810	X	-	-	-
14	CLA	A	811	X	-	-	-
14	CLA	A	812	X	-	-	-
14	CLA	A	813	X	-	-	-
14	CLA	A	814	X	-	-	-
14	CLA	A	815	X	-	-	-
14	CLA	A	816	X	-	-	-
14	CLA	A	817	X	-	-	-
14	CLA	A	818	X	-	-	-
14	CLA	A	819	X	-	-	-
14	CLA	A	820	X	-	-	-
14	CLA	A	821	X	-	-	-
14	CLA	A	822	X	-	-	-
14	CLA	A	823	X	-	-	-
14	CLA	A	824	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	A	825	X	-	-	-
14	CLA	A	826	X	-	-	-
14	CLA	A	827	X	-	-	-
14	CLA	A	828	X	-	-	-
14	CLA	A	829	X	-	-	-
14	CLA	A	830	X	-	-	-
14	CLA	A	831	X	-	-	-
14	CLA	A	832	X	-	-	-
14	CLA	A	833	X	-	-	-
14	CLA	A	834	X	-	-	-
14	CLA	A	835	X	-	-	-
14	CLA	A	836	X	-	-	-
14	CLA	A	837	X	-	-	-
14	CLA	A	838	X	-	-	-
14	CLA	A	839	X	-	-	-
14	CLA	A	840	X	-	-	-
14	CLA	A	841	X	-	-	-
14	CLA	A	842	X	-	-	-
14	CLA	A	843	X	-	-	-
14	CLA	A	844	X	-	-	-
14	CLA	A	855	X	-	-	-
14	CLA	B	3003	X	-	-	-
14	CLA	B	3004	X	-	-	-
14	CLA	B	3005	X	-	-	-
14	CLA	B	3006	X	-	-	-
14	CLA	B	3007	X	-	-	-
14	CLA	B	3008	X	-	-	-
14	CLA	B	3009	X	-	-	-
14	CLA	B	3010	X	-	-	-
14	CLA	B	3011	X	-	-	-
14	CLA	B	3012	X	-	-	-
14	CLA	B	3014	X	-	-	-
14	CLA	B	3015	X	-	-	-
14	CLA	B	3016	X	-	-	-
14	CLA	B	3017	X	-	-	-
14	CLA	B	3019	X	-	-	-
14	CLA	B	3020	X	-	-	-
14	CLA	B	3021	X	-	-	-
14	CLA	B	3022	X	-	-	-
14	CLA	B	3023	X	-	-	-
14	CLA	B	3025	X	-	-	-
14	CLA	B	3026	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	B	3027	X	-	-	-
14	CLA	B	3028	X	-	-	-
14	CLA	B	3029	X	-	-	-
14	CLA	B	3030	X	-	-	-
14	CLA	B	3031	X	-	-	-
14	CLA	B	3032	X	-	-	-
14	CLA	B	3033	X	-	-	-
14	CLA	B	3034	X	-	-	-
14	CLA	B	3035	X	-	-	-
14	CLA	B	3036	X	-	-	-
14	CLA	B	3037	X	-	-	-
14	CLA	B	3038	X	-	-	-
14	CLA	B	3039	X	-	-	-
14	CLA	B	3041	X	-	-	-
14	CLA	B	3042	X	-	-	-
14	CLA	F	201	X	-	-	-
14	CLA	F	203	X	-	-	-
14	CLA	F	204	X	-	-	-
14	CLA	J	101	X	-	-	-
14	CLA	J	102	X	-	-	-
14	CLA	K	101	X	-	-	-
14	CLA	K	102	X	-	-	-
14	CLA	L	201	X	-	-	-
14	CLA	L	203	X	-	-	-
14	CLA	L	204	X	-	-	-
14	CLA	L	205	X	-	-	-
14	CLA	M	1601	X	-	-	-
14	CLA	X	1701	X	-	-	-
14	CLA	a	802	X	-	-	-
14	CLA	a	803	X	-	-	-
14	CLA	a	804	X	-	-	-
14	CLA	a	805	X	-	-	-
14	CLA	a	806	X	-	-	-
14	CLA	a	807	X	-	-	-
14	CLA	a	808	X	-	-	-
14	CLA	a	809	X	-	-	-
14	CLA	a	810	X	-	-	-
14	CLA	a	811	X	-	-	-
14	CLA	a	812	X	-	-	-
14	CLA	a	813	X	-	-	-
14	CLA	a	814	X	-	-	-
14	CLA	a	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	a	816	X	-	-	-
14	CLA	a	817	X	-	-	-
14	CLA	a	818	X	-	-	-
14	CLA	a	819	X	-	-	-
14	CLA	a	820	X	-	-	-
14	CLA	a	821	X	-	-	-
14	CLA	a	822	X	-	-	-
14	CLA	a	823	X	-	-	-
14	CLA	a	824	X	-	-	-
14	CLA	a	825	X	-	-	-
14	CLA	a	826	X	-	-	-
14	CLA	a	827	X	-	-	-
14	CLA	a	828	X	-	-	-
14	CLA	a	829	X	-	-	-
14	CLA	a	830	X	-	-	-
14	CLA	a	831	X	-	-	-
14	CLA	a	832	X	-	-	-
14	CLA	a	833	X	-	-	-
14	CLA	a	834	X	-	-	-
14	CLA	a	835	X	-	-	-
14	CLA	a	836	X	-	-	-
14	CLA	a	837	X	-	-	-
14	CLA	a	838	X	-	-	-
14	CLA	a	839	X	-	-	-
14	CLA	a	840	X	-	-	-
14	CLA	a	841	X	-	-	-
14	CLA	a	842	X	-	-	-
14	CLA	a	843	X	-	-	-
14	CLA	b	3003	X	-	-	-
14	CLA	b	3004	X	-	-	-
14	CLA	b	3005	X	-	-	-
14	CLA	b	3006	X	-	-	-
14	CLA	b	3007	X	-	-	-
14	CLA	b	3008	X	-	-	-
14	CLA	b	3009	X	-	-	-
14	CLA	b	3010	X	-	-	-
14	CLA	b	3011	X	-	-	-
14	CLA	b	3012	X	-	-	-
14	CLA	b	3014	X	-	-	-
14	CLA	b	3015	X	-	-	-
14	CLA	b	3016	X	-	-	-
14	CLA	b	3017	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	b	3019	X	-	-	-
14	CLA	b	3020	X	-	-	-
14	CLA	b	3021	X	-	-	-
14	CLA	b	3022	X	-	-	-
14	CLA	b	3023	X	-	-	-
14	CLA	b	3025	X	-	-	-
14	CLA	b	3026	X	-	-	-
14	CLA	b	3027	X	-	-	-
14	CLA	b	3028	X	-	-	-
14	CLA	b	3029	X	-	-	-
14	CLA	b	3030	X	-	-	-
14	CLA	b	3031	X	-	-	-
14	CLA	b	3032	X	-	-	-
14	CLA	b	3033	X	-	-	-
14	CLA	b	3034	X	-	-	-
14	CLA	b	3035	X	-	-	-
14	CLA	b	3036	X	-	-	-
14	CLA	b	3037	X	-	-	-
14	CLA	b	3038	X	-	-	-
14	CLA	b	3039	X	-	-	-
14	CLA	b	3041	X	-	-	-
14	CLA	b	3042	X	-	-	-
14	CLA	f	201	X	-	-	-
14	CLA	f	203	X	-	-	-
14	CLA	f	204	X	-	-	-
14	CLA	j	1101	X	-	-	-
14	CLA	j	1102	X	-	-	-
14	CLA	j	1103	X	-	-	-
14	CLA	k	101	X	-	-	-
14	CLA	k	102	X	-	-	-
14	CLA	l	203	X	-	-	-
14	CLA	l	206	X	-	-	-
14	CLA	l	207	X	-	-	-
14	CLA	l	208	X	-	-	-
14	CLA	x	1701	X	-	-	-
14	CLA	z	1701	X	-	-	-

2 Entry composition [i](#)

There are 21 unique types of molecules in this entry. The entry contains 75591 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	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	a	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		
1	1	746	Total	C	N	O	S	0	0
			5826	3823	995	982	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	b	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		
2	2	740	Total	C	N	O	S	0	0
			5894	3878	988	1007	21		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	c	80	Total	C	N	O	S	0	0
			598	367	103	117	11		
3	3	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		
4	4	138	Total	C	N	O	S	0	0
			1075	682	186	204	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	70	Total	C	N	O		0	0
			546	347	94	105			
5	e	70	Total	C	N	O		0	0
			546	347	94	105			
5	5	70	Total	C	N	O		0	0
			546	347	94	105			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	f	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		
6	6	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	i	38	Total	C	N	O	S	0	0
			303	209	40	49	5		
7	7	38	Total	C	N	O	S	0	0
			303	209	40	49	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J	41	Total	C	N	O	S	0	0
			340	232	51	55	2		
8	j	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	8	41	Total	C	N	O	S	0	0
			340	232	51	55	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	K	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	k	79	Total	C	N	O	S	0	0
			571	377	92	101	1		
9	9	79	Total	C	N	O	S	0	0
			571	377	92	101	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	L	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	l	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		
10	0	152	Total	C	N	O	S	0	0
			1124	738	180	202	4		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	143	LEU	SER	conflict	UNP Q8DGB4
l	143	LEU	SER	conflict	UNP Q8DGB4
0	143	LEU	SER	conflict	UNP Q8DGB4

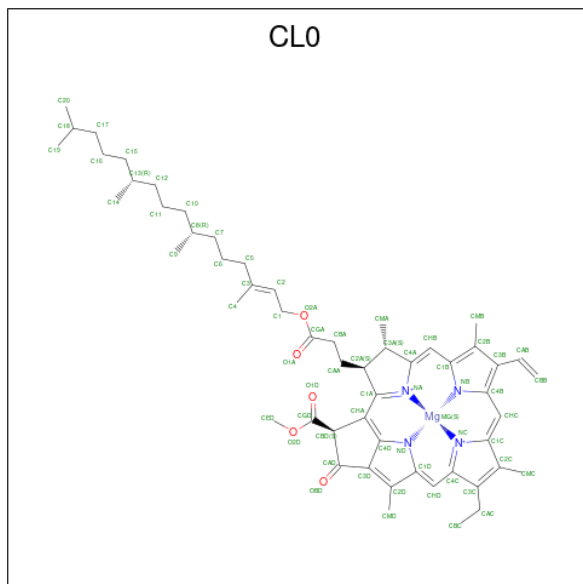
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	m	31	Total	C	N	O	S	0	0
			241	161	36	43	1		
11	y	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		
12	x	27	Total	C	N	O	0	0
			228	163	33	32		
12	z	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 14 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	A	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	B	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	F	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	F	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	F	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	J	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	J	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	K	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	L	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	M	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	a	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	b	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	b	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	b	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	b	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	f	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	f	1	Total 50	C 40	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	j	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	j	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	j	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	k	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	k	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	l	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	x	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 59	C 49	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 51	C 41	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 55	C 45	Mg 1	N 4	O 5	0
14	2	1	Total 49	C 39	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0

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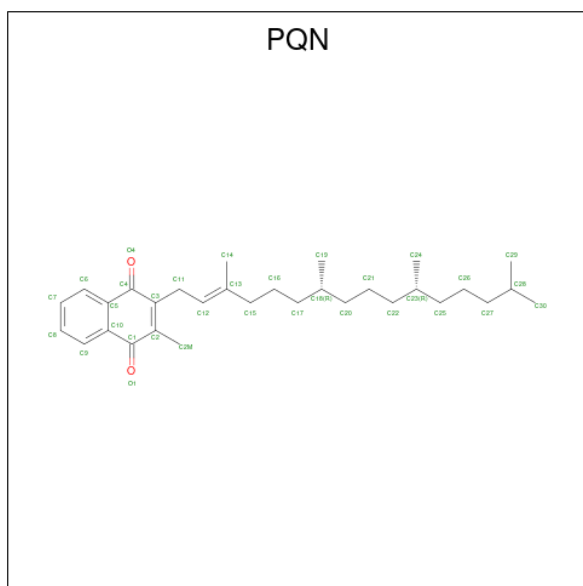
Mol	Chain	Residues	Atoms					AltConf
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	2	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	2	1	Total 60	C 50	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 47	C 37	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	2	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
14	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
14	8	1	Total 37	C 31	Mg 1	N 4	O 1	0
14	9	1	Total 46	C 36	Mg 1	N 4	O 5	0
14	9	1	Total 58	C 48	Mg 1	N 4	O 5	0
14	0	1	Total 36	C 30	Mg 1	N 4	O 1	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0
14	0	1	Total 65	C 55	Mg 1	N 4	O 5	0

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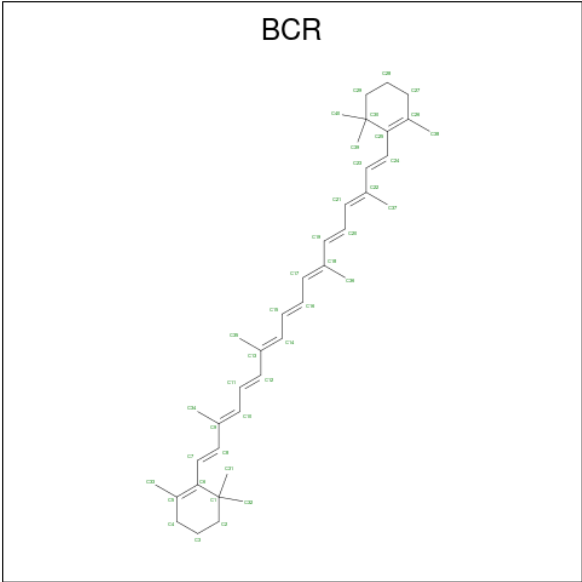
Mol	Chain	Residues	Atoms					AltConf
14	z	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 15 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 16 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



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

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Mol	Chain	Residues	Atoms	AltConf
16	B	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	F	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	I	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	J	1	Total C 40 40	0
16	K	1	Total C 25 25	0
16	L	1	Total C 40 40	0
16	M	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 40 40	0
16	a	1	Total C 25 25	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0

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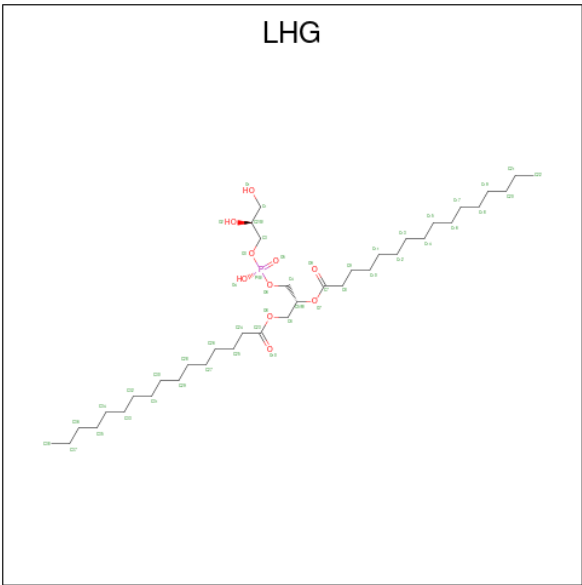
Mol	Chain	Residues	Atoms	AltConf
16	b	1	Total C 40 40	0
16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 25 25	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	l	1	Total C 40 40	0
16	m	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 40 40	0
16	1	1	Total C 25 25	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	2	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	6	1	Total C 40 40	0
16	7	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	8	1	Total C 40 40	0
16	9	1	Total C 40 40	0
16	9	1	Total C 25 25	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	0	1	Total C 40 40	0
16	y	1	Total C 40 40	0

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



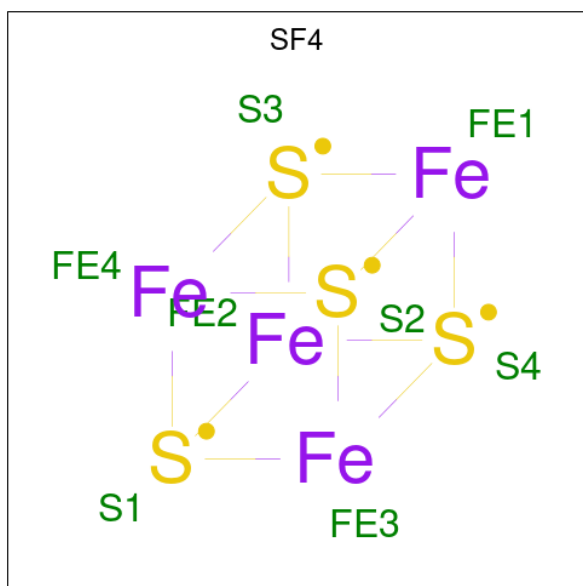
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	B	1	Total	C	O	P	0
			49	38	10	1	
17	L	1	Total	C	O	P	0
			49	38	10	1	
17	L	1	Total	C	O	P	0
			39	28	10	1	
17	a	1	Total	C	O	P	0
			49	38	10	1	
17	a	1	Total	C	O	P	0
			41	30	10	1	
17	b	1	Total	C	O	P	0
			49	38	10	1	
17	l	1	Total	C	O	P	0
			49	38	10	1	
17	l	1	Total	C	O	P	0
			39	28	10	1	
17	l	1	Total	C	O	P	0
			49	38	10	1	
17	l	1	Total	C	O	P	0
			41	30	10	1	
17	2	1	Total	C	O	P	0
			49	38	10	1	
17	0	1	Total	C	O	P	0
			49	38	10	1	

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Mol	Chain	Residues	Atoms				AltConf
17	0	1	Total	C	O	P	0
			39	28	10	1	

- Molecule 18 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).

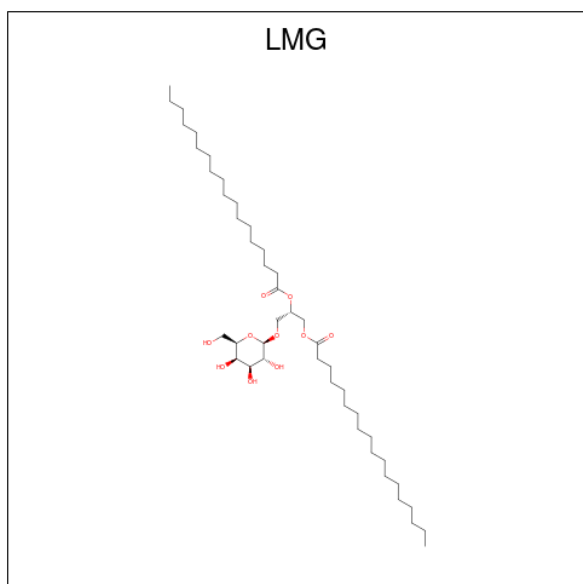


Mol	Chain	Residues	Atoms			AltConf
18	B	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	C	1	Total	Fe	S	0
			8	4	4	
18	b	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	c	1	Total	Fe	S	0
			8	4	4	
18	2	1	Total	Fe	S	0
			8	4	4	
18	3	1	Total	Fe	S	0
			8	4	4	
18	3	1	Total	Fe	S	0
			8	4	4	

- Molecule 19 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		AltConf
19	B	1	Total	Ca	0
			1	1	
19	L	1	Total	Ca	0
			1	1	
19	b	1	Total	Ca	0
			1	1	
19	1	1	Total	Ca	0
			1	1	
19	2	1	Total	Ca	0
			1	1	
19	0	1	Total	Ca	0
			1	1	

- Molecule 20 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms			AltConf
20	B	1	Total	C	O	0
			55	45	10	
20	b	1	Total	C	O	0
			55	45	10	
20	2	1	Total	C	O	0
			55	45	10	

- Molecule 21 is water.

Mol	Chain	Residues	Atoms		AltConf
21	A	65	Total 65	O 65	0
21	B	77	Total 77	O 77	0
21	C	28	Total 28	O 28	0
21	D	22	Total 22	O 22	0
21	E	7	Total 7	O 7	0
21	F	4	Total 4	O 4	0
21	I	1	Total 1	O 1	0
21	J	1	Total 1	O 1	0
21	K	1	Total 1	O 1	0
21	L	10	Total 10	O 10	0
21	M	1	Total 1	O 1	0
21	a	65	Total 65	O 65	0
21	b	74	Total 74	O 74	0
21	c	28	Total 28	O 28	0
21	d	19	Total 19	O 19	0
21	e	9	Total 9	O 9	0
21	f	5	Total 5	O 5	0
21	i	2	Total 2	O 2	0
21	j	1	Total 1	O 1	0
21	k	1	Total 1	O 1	0
21	l	11	Total 11	O 11	0
21	m	2	Total 2	O 2	0

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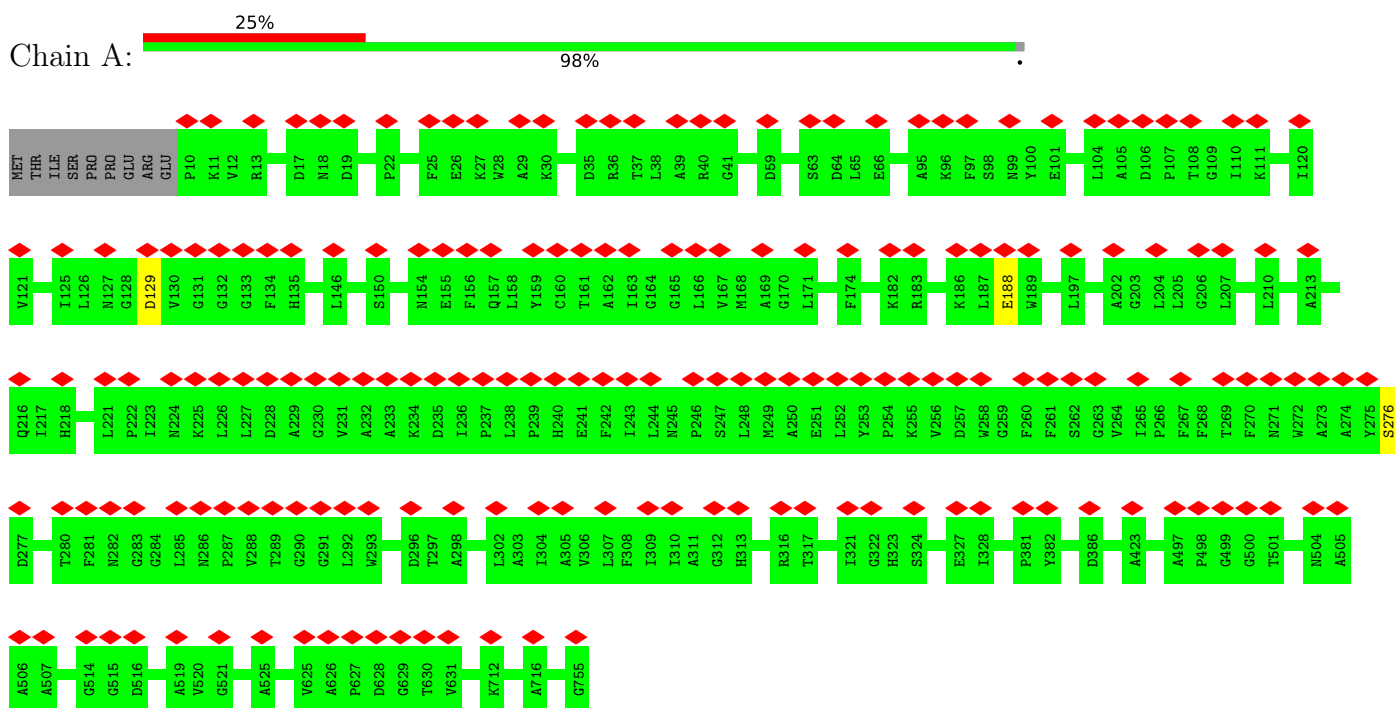
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Mol	Chain	Residues	Atoms		AltConf
21	1	65	Total 65	O 65	0
21	2	75	Total 75	O 75	0
21	3	27	Total 27	O 27	0
21	4	22	Total 22	O 22	0
21	5	8	Total 8	O 8	0
21	6	4	Total 4	O 4	0
21	7	2	Total 2	O 2	0
21	8	1	Total 1	O 1	0
21	9	1	Total 1	O 1	0
21	0	10	Total 10	O 10	0
21	y	2	Total 2	O 2	0

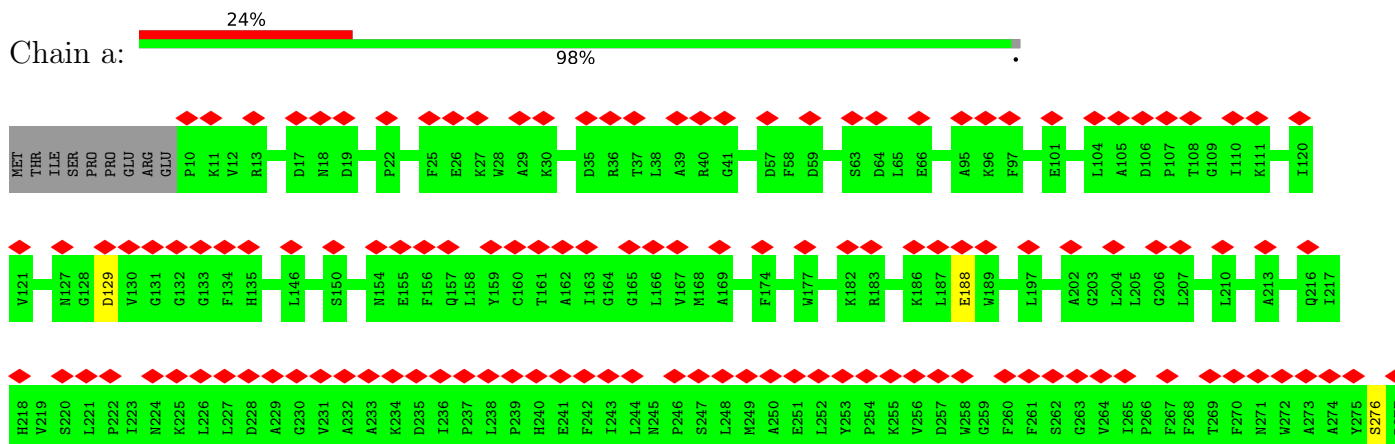
3 Residue-property plots [i](#)

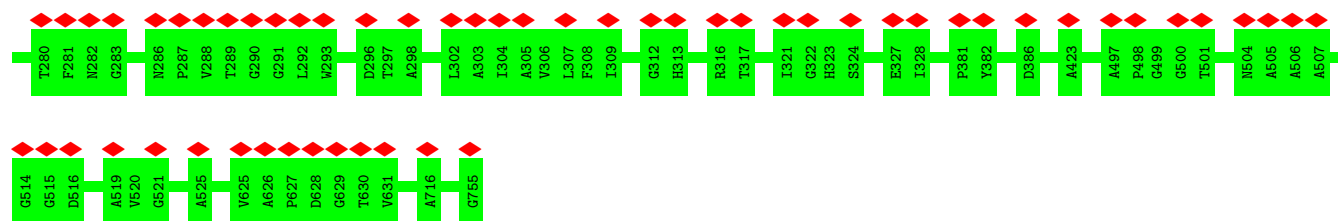
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



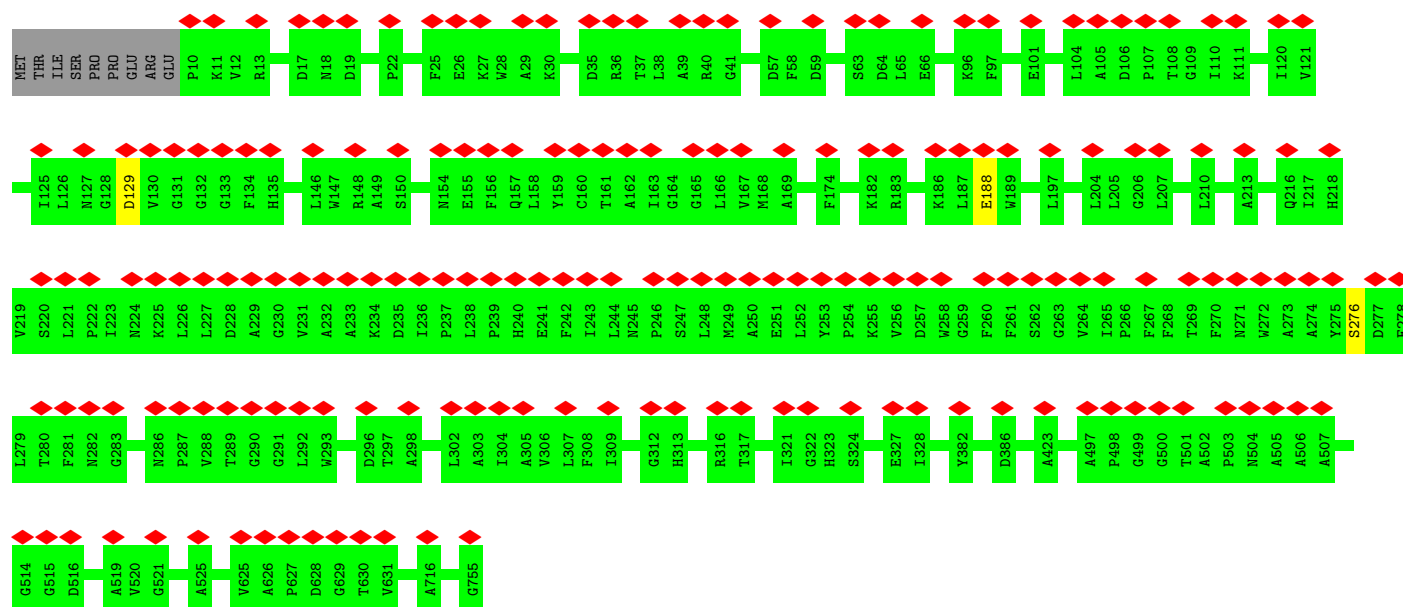
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





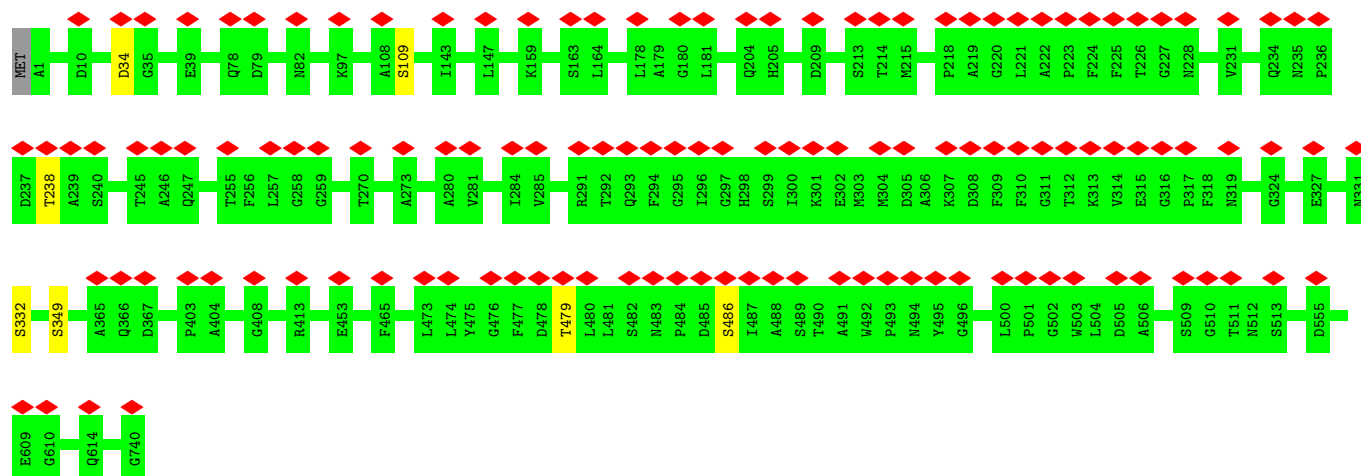
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain 1: 25% 98%

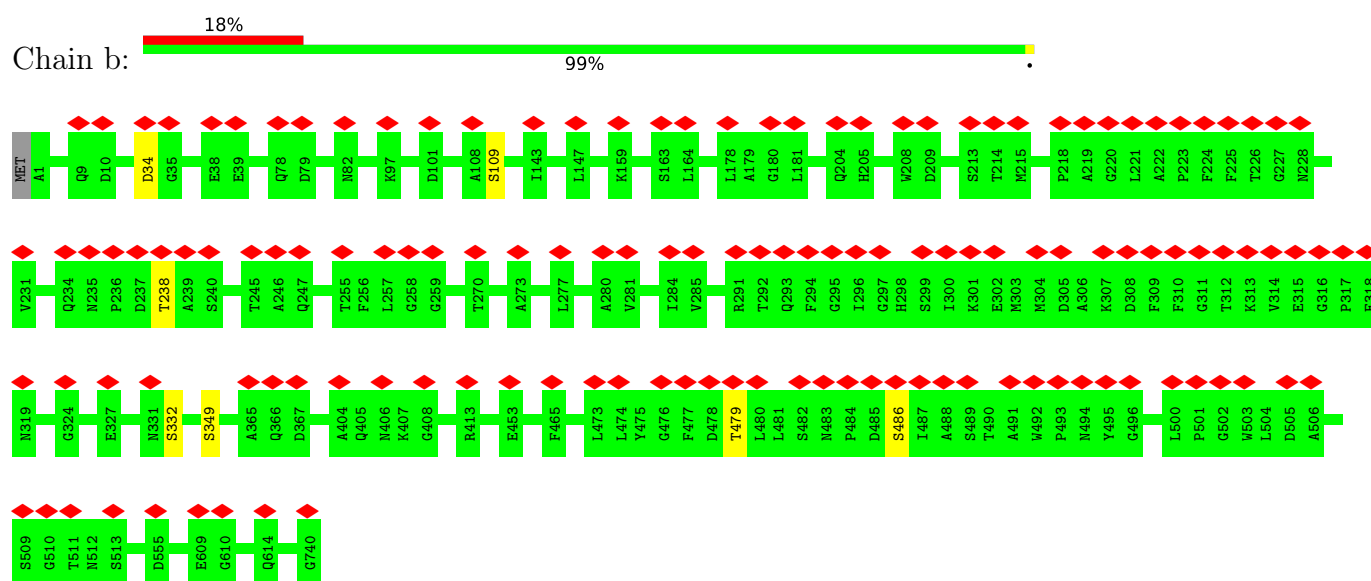


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

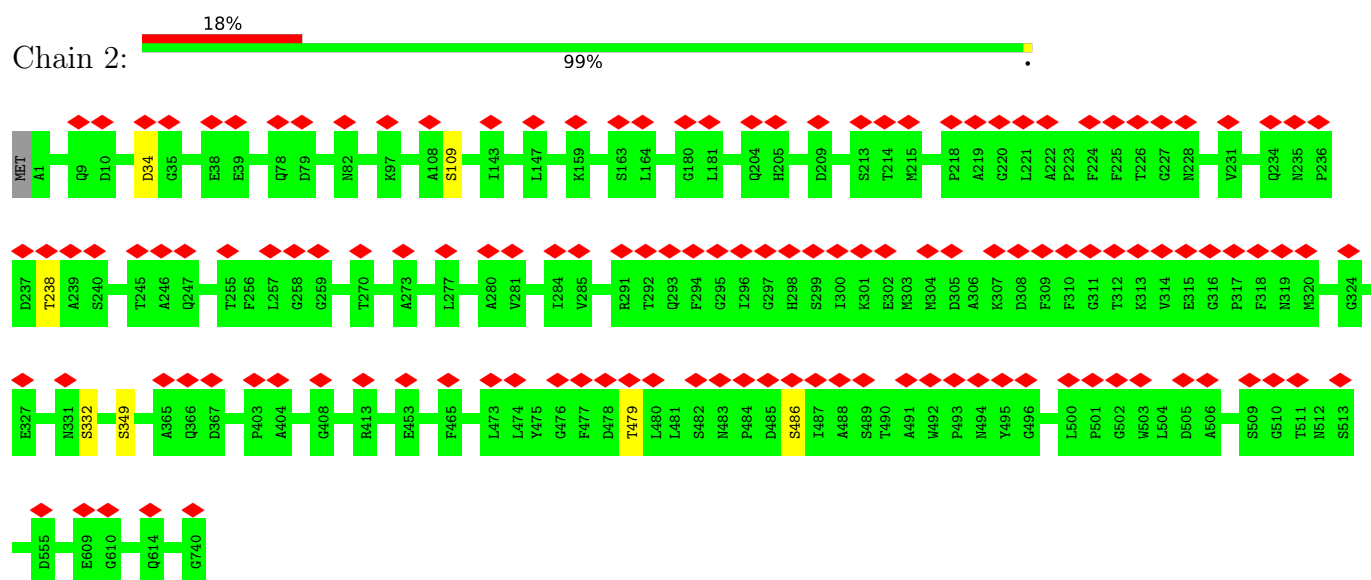
Chain B: 17% 99%



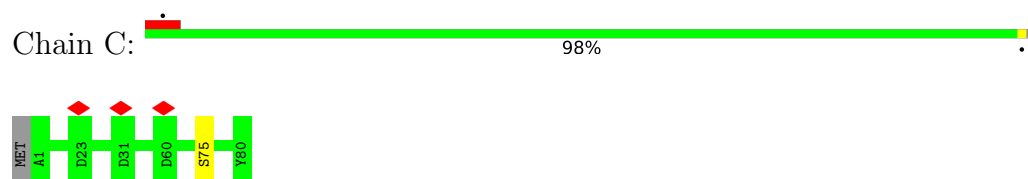
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



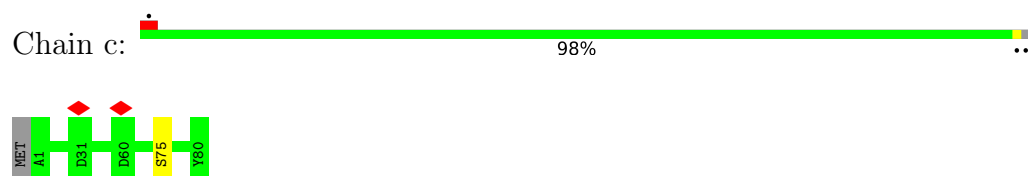
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



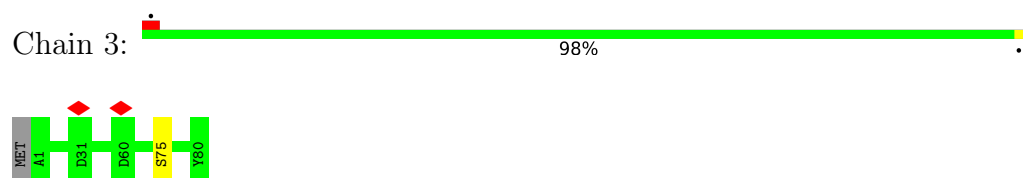
- Molecule 3: Photosystem I iron-sulfur center



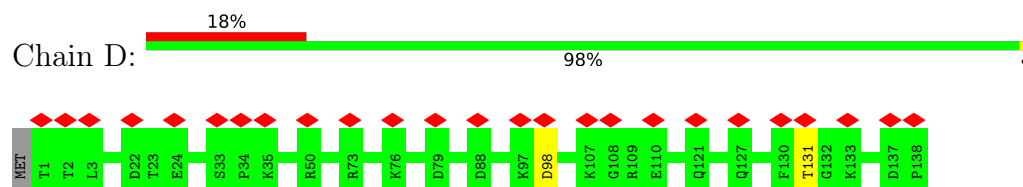
- Molecule 3: Photosystem I iron-sulfur center



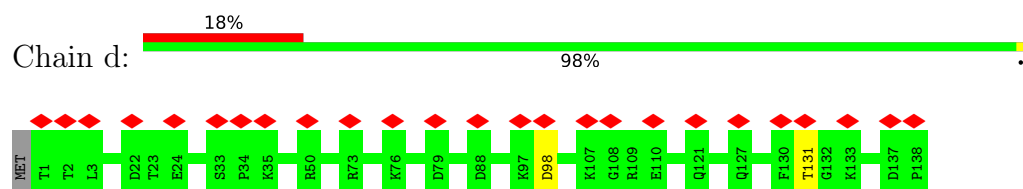
- Molecule 3: Photosystem I iron-sulfur center



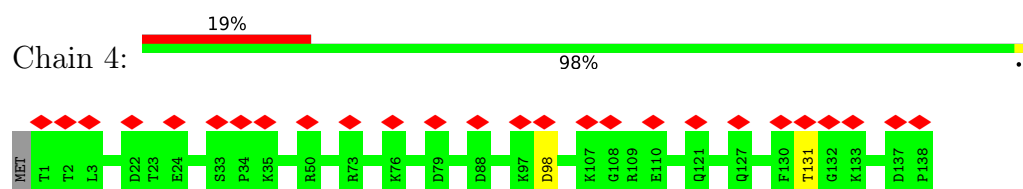
- Molecule 4: Photosystem I reaction center subunit II



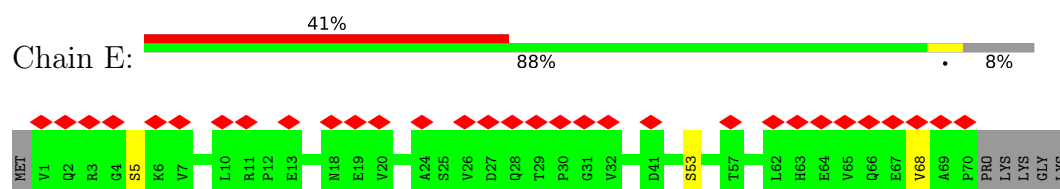
- Molecule 4: Photosystem I reaction center subunit II



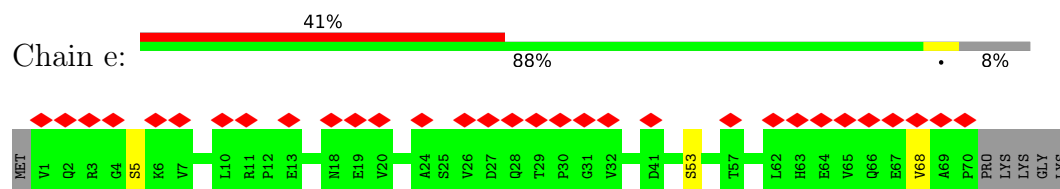
- Molecule 4: Photosystem I reaction center subunit II



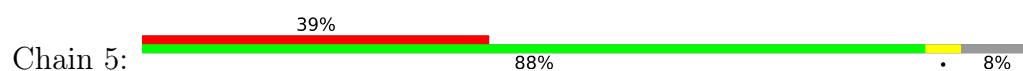
- Molecule 5: Photosystem I reaction center subunit IV

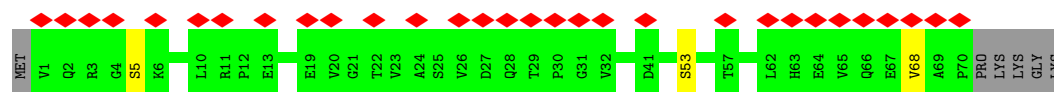


- Molecule 5: Photosystem I reaction center subunit IV

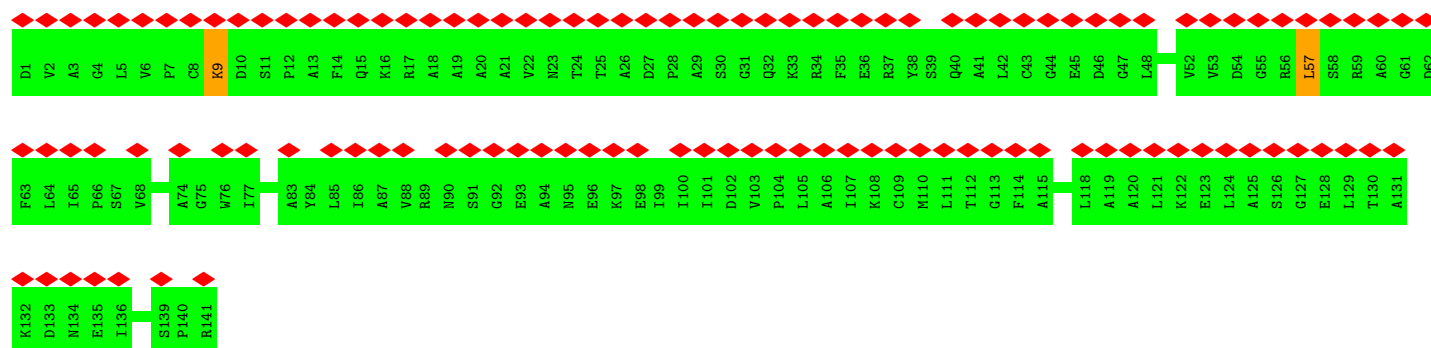
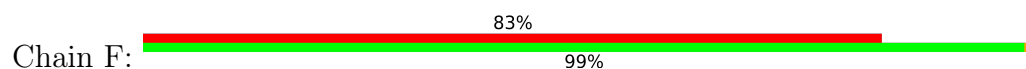


- Molecule 5: Photosystem I reaction center subunit IV

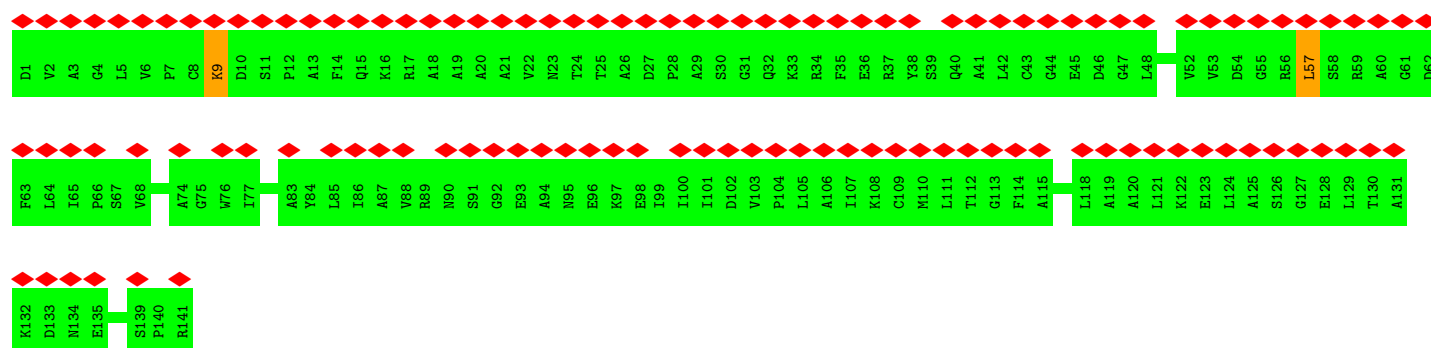
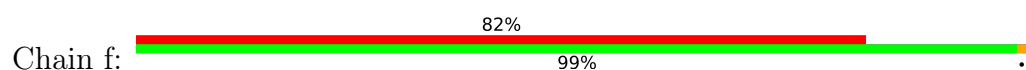




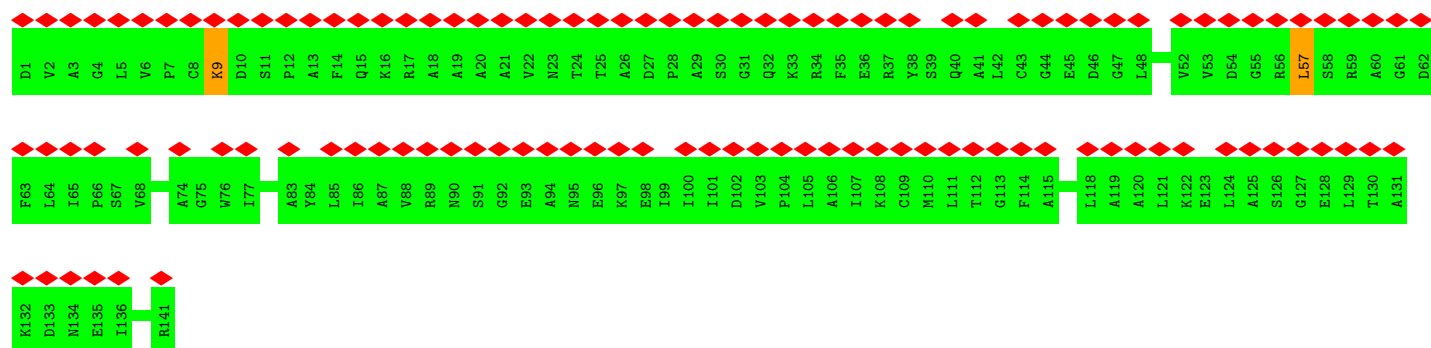
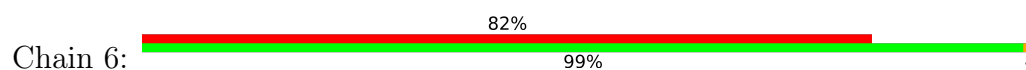
- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 6: Photosystem I reaction center subunit III



- Molecule 7: Photosystem I reaction center subunit VIII



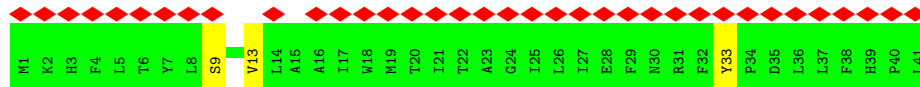
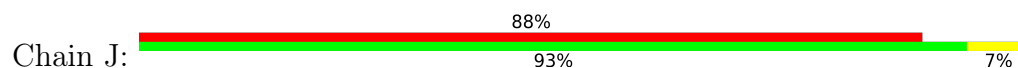
- Molecule 7: Photosystem I reaction center subunit VIII



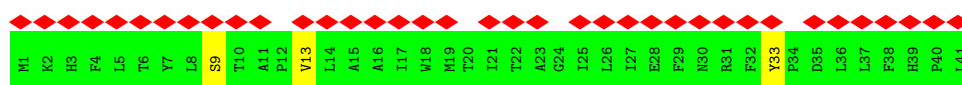
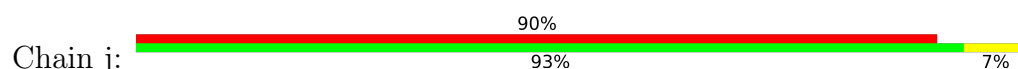
- Molecule 7: Photosystem I reaction center subunit VIII



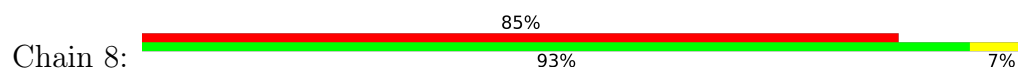
- Molecule 8: Photosystem I reaction center subunit IX



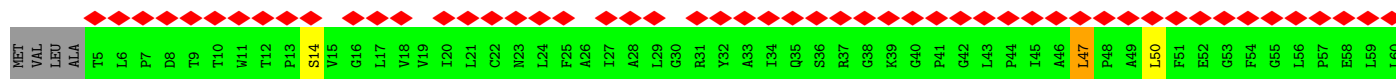
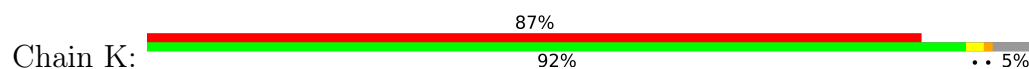
- Molecule 8: Photosystem I reaction center subunit IX



- Molecule 8: Photosystem I reaction center subunit IX

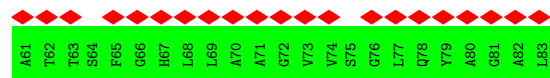
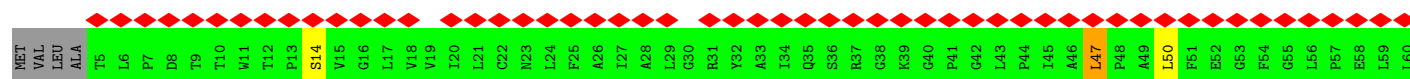
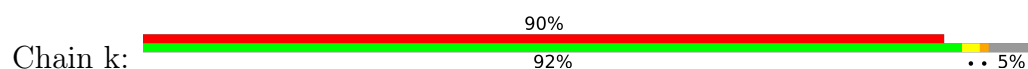


- Molecule 9: Photosystem I reaction center subunit Psak

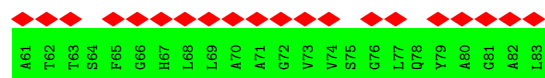
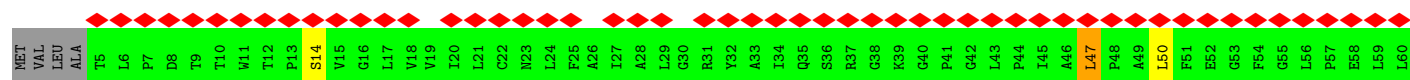
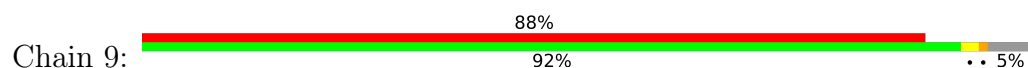




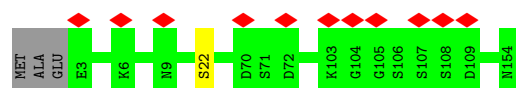
- Molecule 9: Photosystem I reaction center subunit PsaK



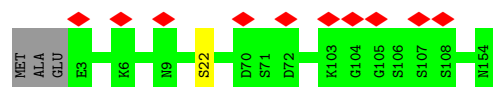
- Molecule 9: Photosystem I reaction center subunit PsaK



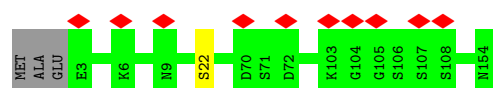
- Molecule 10: Photosystem I reaction center subunit XI



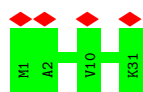
- Molecule 10: Photosystem I reaction center subunit XI



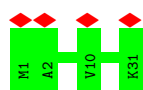
- Molecule 10: Photosystem I reaction center subunit XI



- Molecule 11: Photosystem I reaction center subunit XII



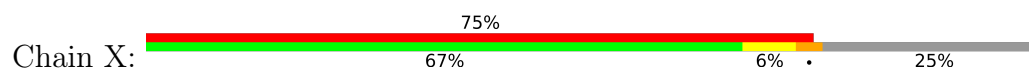
- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 11: Photosystem I reaction center subunit XII



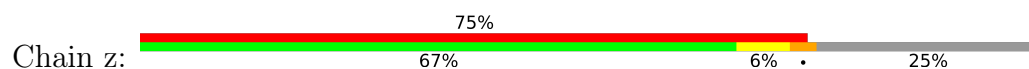
- Molecule 12: Photosystem I 4.8K protein



- Molecule 12: Photosystem I 4.8K protein



- Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	175999	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTFFIND4 was used to estimate contrast transfer function parameters. CTF correction was done in Relion 3.0.	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	32	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.105	Depositor
Minimum map value	-0.076	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.015	Depositor
Map size (\AA)	351.68002, 351.68002, 351.68002	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.628, 0.628, 0.628	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.44	0/6027	0.51	0/8220
1	A	0.44	0/6027	0.51	0/8220
1	a	0.44	0/6027	0.51	0/8220
2	2	0.46	0/6112	0.50	0/8350
2	B	0.46	0/6112	0.50	0/8350
2	b	0.46	0/6112	0.50	0/8350
3	3	0.49	0/608	0.56	0/824
3	C	0.49	0/608	0.56	0/824
3	c	0.49	0/608	0.56	0/824
4	4	0.46	0/1101	0.52	0/1492
4	D	0.46	0/1101	0.52	0/1492
4	d	0.46	0/1101	0.52	0/1492
5	5	0.42	0/559	0.46	0/762
5	E	0.41	0/559	0.46	0/762
5	e	0.42	0/559	0.46	0/762
6	6	0.32	0/1087	0.59	2/1476 (0.1%)
6	F	0.32	0/1087	0.59	2/1476 (0.1%)
6	f	0.32	0/1087	0.59	2/1476 (0.1%)
7	7	0.48	0/304	0.48	0/415
7	I	0.48	0/304	0.48	0/415
7	i	0.48	0/304	0.48	0/415
8	8	0.45	0/342	0.62	0/467
8	J	0.45	0/342	0.62	0/467
8	j	0.45	0/342	0.62	0/467
9	9	0.32	0/585	0.66	1/800 (0.1%)
9	K	0.32	0/585	0.66	1/800 (0.1%)
9	k	0.33	0/585	0.66	1/800 (0.1%)
10	0	0.50	0/1153	0.49	0/1565
10	L	0.50	0/1153	0.49	0/1565
10	l	0.50	0/1153	0.49	0/1565
11	M	0.43	0/244	0.55	0/332
11	m	0.43	0/244	0.55	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
11	y	0.43	0/244	0.55	0/332
12	X	0.38	0/236	0.80	2/321 (0.6%)
12	x	0.38	0/236	0.80	2/321 (0.6%)
12	z	0.38	0/236	0.80	2/321 (0.6%)
All	All	0.44	0/55074	0.53	15/75072 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	2	0	1
2	B	0	1
2	b	0	1
6	6	0	1
6	F	0	1
6	f	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	9	LYS	CD-CE-NZ	7.35	128.60	111.70
6	f	9	LYS	CD-CE-NZ	7.34	128.58	111.70
6	6	9	LYS	CD-CE-NZ	7.33	128.55	111.70
9	k	47	LEU	CB-CG-CD1	5.70	120.69	111.00
9	K	47	LEU	CB-CG-CD1	5.69	120.67	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	2	479	THR	Peptide
2	B	479	THR	Peptide
6	F	57	LEU	Peptide
2	b	479	THR	Peptide
6	f	57	LEU	Peptide

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
1	A	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
1	a	744/755 (98%)	688 (92%)	56 (8%)	0	100	100
2	2	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
2	B	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
2	b	738/741 (100%)	685 (93%)	53 (7%)	0	100	100
3	3	78/81 (96%)	66 (85%)	12 (15%)	0	100	100
3	C	78/81 (96%)	66 (85%)	12 (15%)	0	100	100
3	c	78/81 (96%)	67 (86%)	11 (14%)	0	100	100
4	4	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
4	D	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
4	d	136/139 (98%)	119 (88%)	17 (12%)	0	100	100
5	5	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
5	E	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
5	e	68/76 (90%)	67 (98%)	1 (2%)	0	100	100
6	6	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
6	F	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
6	f	139/141 (99%)	117 (84%)	22 (16%)	0	100	100
7	7	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	I	36/38 (95%)	33 (92%)	3 (8%)	0	100	100
7	i	36/38 (95%)	33 (92%)	3 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	8	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	J	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
8	j	39/41 (95%)	37 (95%)	2 (5%)	0	100	100
9	9	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
9	K	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
9	k	77/83 (93%)	73 (95%)	4 (5%)	0	100	100
10	0	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	L	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
10	l	150/155 (97%)	143 (95%)	7 (5%)	0	100	100
11	M	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	m	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
11	y	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
12	X	25/36 (69%)	25 (100%)	0	0	100	100
12	x	25/36 (69%)	25 (100%)	0	0	100	100
12	z	25/36 (69%)	25 (100%)	0	0	100	100
All	All	6777/6951 (98%)	6241 (92%)	536 (8%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	594/603 (98%)	591 (100%)	3 (0%)	86	94
1	A	594/603 (98%)	591 (100%)	3 (0%)	86	94
1	a	594/603 (98%)	591 (100%)	3 (0%)	86	94
2	2	597/598 (100%)	591 (99%)	6 (1%)	73	87
2	B	597/598 (100%)	591 (99%)	6 (1%)	73	87
2	b	597/598 (100%)	591 (99%)	6 (1%)	73	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	3	67/68 (98%)	66 (98%)	1 (2%)	60	82
3	C	67/68 (98%)	66 (98%)	1 (2%)	60	82
3	c	67/68 (98%)	66 (98%)	1 (2%)	60	82
4	4	115/116 (99%)	113 (98%)	2 (2%)	56	80
4	D	115/116 (99%)	113 (98%)	2 (2%)	56	80
4	d	115/116 (99%)	113 (98%)	2 (2%)	56	80
5	5	60/65 (92%)	57 (95%)	3 (5%)	20	51
5	E	60/65 (92%)	57 (95%)	3 (5%)	20	51
5	e	60/65 (92%)	57 (95%)	3 (5%)	20	51
6	6	109/109 (100%)	108 (99%)	1 (1%)	75	88
6	F	109/109 (100%)	108 (99%)	1 (1%)	75	88
6	f	109/109 (100%)	108 (99%)	1 (1%)	75	88
7	7	31/31 (100%)	31 (100%)	0	100	100
7	I	31/31 (100%)	31 (100%)	0	100	100
7	i	31/31 (100%)	31 (100%)	0	100	100
8	8	35/35 (100%)	32 (91%)	3 (9%)	8	30
8	J	35/35 (100%)	32 (91%)	3 (9%)	8	30
8	j	35/35 (100%)	32 (91%)	3 (9%)	8	30
9	9	58/61 (95%)	55 (95%)	3 (5%)	19	50
9	K	58/61 (95%)	55 (95%)	3 (5%)	19	50
9	k	58/61 (95%)	55 (95%)	3 (5%)	19	50
10	0	117/120 (98%)	116 (99%)	1 (1%)	75	88
10	L	117/120 (98%)	116 (99%)	1 (1%)	75	88
10	l	117/120 (98%)	116 (99%)	1 (1%)	75	88
11	M	26/26 (100%)	26 (100%)	0	100	100
11	m	26/26 (100%)	26 (100%)	0	100	100
11	y	26/26 (100%)	26 (100%)	0	100	100
12	X	21/28 (75%)	19 (90%)	2 (10%)	7	26
12	x	21/28 (75%)	19 (90%)	2 (10%)	7	26
12	z	21/28 (75%)	19 (90%)	2 (10%)	7	26
All	All	5490/5580 (98%)	5415 (99%)	75 (1%)	62	83

5 of 75 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	349	SER
9	9	50	LEU
3	3	75	SER
6	6	9	LYS
12	X	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 72 such sidechains are listed below:

Mol	Chain	Res	Type
2	2	157	GLN
12	z	23	ASN
2	2	405	GLN
4	4	71	GLN
1	a	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
8	FME	8	1	8	8,9,10	0.95	0	7,9,11	0.87	0
8	FME	J	1	8	8,9,10	0.95	0	7,9,11	0.87	0
8	FME	j	1	8	8,9,10	0.95	0	7,9,11	0.88	0
7	FME	7	1	7	8,9,10	1.00	0	7,9,11	1.23	1 (14%)
7	FME	I	1	7	8,9,10	1.00	0	7,9,11	1.23	1 (14%)
7	FME	i	1	7	8,9,10	1.00	0	7,9,11	1.24	1 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FME	8	1	8	-	1/7/9/11	-
8	FME	J	1	8	-	1/7/9/11	-
8	FME	j	1	8	-	1/7/9/11	-
7	FME	7	1	7	-	3/7/9/11	-
7	FME	I	1	7	-	3/7/9/11	-
7	FME	i	1	7	-	3/7/9/11	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	1	FME	C-CA-N	2.69	114.58	109.73
7	7	1	FME	C-CA-N	2.68	114.57	109.73
7	I	1	FME	C-CA-N	2.67	114.56	109.73

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	I	1	FME	C-CA-CB-CG
7	i	1	FME	C-CA-CB-CG
7	7	1	FME	C-CA-CB-CG
8	J	1	FME	CB-CG-SD-CE
8	j	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 402 ligands modelled in this entry, 6 are monoatomic - leaving 396 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
14	CLA	L	204	-	65,73,73	1.43	10 (15%)	76,113,113	1.54	11 (14%)
14	CLA	A	817	21	65,73,73	1.50	8 (12%)	76,113,113	1.49	9 (11%)
16	BCR	l	209	-	41,41,41	1.22	4 (9%)	56,56,56	1.30	6 (10%)
14	CLA	A	837	1	45,53,73	1.80	6 (13%)	52,89,113	1.52	8 (15%)
14	CLA	b	3004	-	65,73,73	1.41	9 (13%)	76,113,113	1.46	7 (9%)
16	BCR	F	205	-	41,41,41	1.17	2 (4%)	56,56,56	1.37	9 (16%)
14	CLA	B	3003	21	65,73,73	1.43	8 (12%)	76,113,113	1.70	10 (13%)
14	CLA	a	802	-	65,73,73	1.43	8 (12%)	76,113,113	1.64	11 (14%)
14	CLA	A	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.36	7 (9%)
14	CLA	A	820	-	65,73,73	1.45	8 (12%)	76,113,113	1.57	10 (13%)
14	CLA	2	3028	-	65,73,73	1.49	9 (13%)	76,113,113	1.40	9 (11%)
14	CLA	a	831	-	60,68,73	1.53	10 (16%)	70,107,113	1.47	8 (11%)
14	CLA	b	3028	-	65,73,73	1.49	9 (13%)	76,113,113	1.40	9 (11%)
16	BCR	J	103	-	41,41,41	1.14	2 (4%)	56,56,56	1.15	4 (7%)
14	CLA	2	3007	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	9 (11%)
14	CLA	1	843	21	65,73,73	1.48	9 (13%)	76,113,113	1.47	8 (10%)
14	CLA	X	1701	-	45,53,73	1.83	6 (13%)	52,89,113	1.57	6 (11%)
16	BCR	B	3052	-	41,41,41	1.41	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	1	807	-	65,73,73	1.43	8 (12%)	76,113,113	1.50	6 (7%)
14	CLA	0	209	21	65,73,73	1.44	8 (12%)	76,113,113	1.48	8 (10%)
14	CLA	a	813	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	6 (7%)
14	CLA	b	3029	-	65,73,73	1.48	10 (15%)	76,113,113	1.33	8 (10%)
14	CLA	2	3013	-	45,53,73	1.76	8 (17%)	52,89,113	1.61	7 (13%)
16	BCR	f	205	-	41,41,41	1.17	2 (4%)	56,56,56	1.37	9 (16%)
17	LHG	l	201	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	5 (9%)
14	CLA	2	3024	-	45,53,73	1.76	7 (15%)	52,89,113	1.71	7 (13%)
14	CLA	2	3025	2	65,73,73	1.48	7 (10%)	76,113,113	1.38	6 (7%)
14	CLA	8	101	-	45,53,73	1.78	5 (11%)	52,89,113	1.62	8 (15%)
14	CLA	a	824	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	8 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	A	855	-	36,44,73	1.94	7 (19%)	40,76,113	1.60	6 (15%)
14	CLA	A	825	-	65,73,73	1.45	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	a	819	-	65,73,73	1.46	8 (12%)	76,113,113	1.57	11 (14%)
14	CLA	B	3026	21	65,73,73	1.50	8 (12%)	76,113,113	1.64	14 (18%)
14	CLA	a	841	-	65,73,73	1.49	7 (10%)	76,113,113	1.41	8 (10%)
17	LHG	l	202	-	38,38,48	0.76	0	41,44,54	1.28	4 (9%)
16	BCR	k	103	-	25,25,41	1.07	1 (4%)	33,33,56	1.22	2 (6%)
14	CLA	B	3012	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	10 (13%)
14	CLA	1	832	-	60,68,73	1.53	10 (16%)	70,107,113	1.47	8 (11%)
14	CLA	1	811	-	49,57,73	1.68	7 (14%)	55,93,113	1.44	5 (9%)
14	CLA	b	3030	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	8 (10%)
14	CLA	2	3012	-	65,73,73	1.45	10 (15%)	76,113,113	1.55	10 (13%)
14	CLA	a	835	-	65,73,73	1.47	9 (13%)	76,113,113	1.45	7 (9%)
16	BCR	b	3047	-	41,41,41	1.19	2 (4%)	56,56,56	1.22	7 (12%)
14	CLA	2	3008	-	65,73,73	1.48	9 (13%)	76,113,113	1.44	9 (11%)
14	CLA	A	833	-	65,73,73	1.42	10 (15%)	76,113,113	1.36	6 (7%)
14	CLA	1	837	1	45,53,73	1.81	6 (13%)	52,89,113	1.53	8 (15%)
14	CLA	A	843	21	65,73,73	1.50	9 (13%)	76,113,113	1.47	8 (10%)
16	BCR	A	846	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	11 (19%)
14	CLA	B	3030	-	65,73,73	1.44	9 (13%)	76,113,113	1.46	9 (11%)
14	CLA	1	829	-	65,73,73	1.46	7 (10%)	76,113,113	1.57	7 (9%)
16	BCR	J	104	-	41,41,41	1.20	2 (4%)	56,56,56	1.28	7 (12%)
14	CLA	A	823	-	45,53,73	1.74	6 (13%)	52,89,113	1.68	7 (13%)
14	CLA	1	840	-	65,73,73	1.47	8 (12%)	76,113,113	1.39	9 (11%)
14	CLA	2	3027	-	65,73,73	1.49	8 (12%)	76,113,113	1.42	6 (7%)
16	BCR	j	1104	-	41,41,41	1.13	2 (4%)	56,56,56	1.15	4 (7%)
16	BCR	2	3046	-	41,41,41	1.26	3 (7%)	56,56,56	1.21	6 (10%)
14	CLA	A	830	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
14	CLA	b	3033	-	65,73,73	1.49	8 (12%)	76,113,113	1.54	10 (13%)
14	CLA	1	842	-	65,73,73	1.50	8 (12%)	76,113,113	1.42	8 (10%)
14	CLA	A	805	-	59,67,73	1.50	7 (11%)	68,105,113	1.58	7 (10%)
14	CLA	a	808	1	65,73,73	1.43	8 (12%)	76,113,113	1.48	8 (10%)
14	CLA	a	810	-	49,57,73	1.69	7 (14%)	55,93,113	1.44	5 (9%)
13	CL0	a	801	-	65,73,73	1.44	8 (12%)	76,113,113	1.50	8 (10%)
14	CLA	A	839	-	65,73,73	1.46	9 (13%)	76,113,113	1.45	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
17	LHG	a	852	-	48,48,48	0.78	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	b	3006	-	65,73,73	1.47	9 (13%)	76,113,113	1.50	10 (13%)
14	CLA	b	3009	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	1	844	17	45,53,73	1.71	6 (13%)	52,89,113	1.78	7 (13%)
14	CLA	B	3033	-	65,73,73	1.49	7 (10%)	76,113,113	1.54	10 (13%)
14	CLA	b	3025	2	65,73,73	1.48	7 (10%)	76,113,113	1.38	6 (7%)
14	CLA	B	3038	-	60,68,73	1.54	8 (13%)	70,107,113	1.46	8 (11%)
14	CLA	F	201	21	58,66,73	1.58	7 (12%)	67,104,113	1.48	7 (10%)
14	CLA	A	838	-	65,73,73	1.43	7 (10%)	76,113,113	1.61	10 (13%)
14	CLA	F	204	-	50,58,73	1.71	6 (12%)	58,95,113	1.61	8 (13%)
14	CLA	A	818	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	10 (13%)
14	CLA	A	842	-	65,73,73	1.50	8 (12%)	76,113,113	1.42	8 (10%)
14	CLA	2	3042	-	65,73,73	1.50	7 (10%)	76,113,113	1.49	10 (13%)
14	CLA	A	827	21	65,73,73	1.43	7 (10%)	76,113,113	1.58	9 (11%)
18	SF4	2	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	1	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	b	3012	-	65,73,73	1.45	10 (15%)	76,113,113	1.56	10 (13%)
14	CLA	A	832	-	60,68,73	1.54	10 (16%)	70,107,113	1.47	8 (11%)
14	CLA	1	803	21	65,73,73	1.55	10 (15%)	76,113,113	1.35	6 (7%)
14	CLA	2	3020	21	65,73,73	1.50	8 (12%)	76,113,113	1.46	7 (9%)
14	CLA	1	826	21	65,73,73	1.45	9 (13%)	76,113,113	1.52	8 (10%)
14	CLA	B	3009	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	1	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.40	7 (9%)
14	CLA	2	3014	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	6 (7%)
14	CLA	b	3027	-	65,73,73	1.49	8 (12%)	76,113,113	1.43	6 (7%)
14	CLA	B	3041	21	65,73,73	1.45	9 (13%)	76,113,113	1.45	8 (10%)
16	BCR	b	3046	-	41,41,41	1.25	3 (7%)	56,56,56	1.22	6 (10%)
16	BCR	0	205	-	41,41,41	1.42	4 (9%)	56,56,56	1.30	6 (10%)
14	CLA	2	3035	-	65,73,73	1.45	7 (10%)	76,113,113	1.46	8 (10%)
14	CLA	B	3024	-	45,53,73	1.76	7 (15%)	52,89,113	1.71	8 (15%)
14	CLA	2	3029	-	65,73,73	1.49	10 (15%)	76,113,113	1.32	8 (10%)
14	CLA	A	824	-	65,73,73	1.47	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	6	204	-	50,58,73	1.70	6 (12%)	58,95,113	1.61	8 (13%)
18	SF4	b	3001	1,2	0,12,12	-	-	-	-	-
14	CLA	B	3021	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	822	-	45,53,73	1.74	6 (13%)	52,89,113	1.69	6 (11%)
14	CLA	a	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.56	7 (9%)
14	CLA	b	3008	-	65,73,73	1.47	9 (13%)	76,113,113	1.43	9 (11%)
16	BCR	A	849	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	6 (10%)
14	CLA	A	829	-	65,73,73	1.47	7 (10%)	76,113,113	1.56	7 (9%)
14	CLA	A	840	-	65,73,73	1.47	8 (12%)	76,113,113	1.38	9 (11%)
16	BCR	1	849	-	41,41,41	1.34	4 (9%)	56,56,56	1.30	6 (10%)
17	LHG	1	853	14	40,40,48	0.77	2 (5%)	43,46,54	1.17	3 (6%)
14	CLA	K	101	-	46,54,73	1.78	7 (15%)	53,90,113	1.51	6 (11%)
14	CLA	6	203	21	45,53,73	1.75	7 (15%)	52,89,113	1.66	7 (13%)
16	BCR	f	202	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	b	3003	21	65,73,73	1.43	8 (12%)	76,113,113	1.70	10 (13%)
14	CLA	a	818	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	8 (10%)
14	CLA	1	815	-	65,73,73	1.48	7 (10%)	76,113,113	1.37	7 (9%)
14	CLA	2	3032	-	49,57,73	1.65	7 (14%)	55,93,113	1.62	7 (12%)
14	CLA	a	833	-	65,73,73	1.44	8 (12%)	76,113,113	1.55	9 (11%)
16	BCR	a	846	-	41,41,41	1.13	3 (7%)	56,56,56	1.27	8 (14%)
14	CLA	a	814	-	65,73,73	1.49	7 (10%)	76,113,113	1.38	7 (9%)
14	CLA	1	806	-	65,73,73	1.44	11 (16%)	76,113,113	1.60	11 (14%)
14	CLA	a	811	-	65,73,73	1.47	7 (10%)	76,113,113	1.35	7 (9%)
14	CLA	1	833	-	65,73,73	1.43	9 (13%)	76,113,113	1.37	6 (7%)
14	CLA	2	3040	-	47,55,73	1.77	8 (17%)	54,91,113	1.47	7 (12%)
14	CLA	B	3027	-	65,73,73	1.49	8 (12%)	76,113,113	1.43	6 (7%)
16	BCR	1	847	-	41,41,41	1.23	3 (7%)	56,56,56	1.39	8 (14%)
18	SF4	c	102	3	0,12,12	-	-	-	-	-
14	CLA	2	3010	-	65,73,73	1.47	8 (12%)	76,113,113	1.61	13 (17%)
14	CLA	2	3019	-	65,73,73	1.44	7 (10%)	76,113,113	1.52	8 (10%)
14	CLA	6	201	21	58,66,73	1.58	7 (12%)	67,104,113	1.48	7 (10%)
14	CLA	2	3037	21	45,53,73	1.82	6 (13%)	52,89,113	1.61	6 (11%)
14	CLA	A	828	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
16	BCR	0	211	-	41,41,41	1.16	3 (7%)	56,56,56	1.20	5 (8%)
16	BCR	a	845	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	11 (19%)
13	CL0	A	801	-	65,73,73	1.44	9 (13%)	76,113,113	1.49	8 (10%)
14	CLA	1	817	21	65,73,73	1.49	7 (10%)	76,113,113	1.49	9 (11%)
16	BCR	A	851	-	41,41,41	1.31	3 (7%)	56,56,56	1.30	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	805	-	59,67,73	1.50	7 (11%)	68,105,113	1.58	7 (10%)
14	CLA	B	3004	-	65,73,73	1.42	8 (12%)	76,113,113	1.46	7 (9%)
16	BCR	j	1106	-	41,41,41	1.26	2 (4%)	56,56,56	1.43	11 (19%)
18	SF4	3	101	3	0,12,12	-	-	-	-	-
16	BCR	l	210	-	41,41,41	1.17	3 (7%)	56,56,56	1.20	5 (8%)
14	CLA	b	3011	2	65,73,73	1.44	9 (13%)	76,113,113	1.58	10 (13%)
14	CLA	a	832	-	65,73,73	1.43	10 (15%)	76,113,113	1.37	6 (7%)
14	CLA	A	803	21	65,73,73	1.54	9 (13%)	76,113,113	1.35	6 (7%)
16	BCR	9	104	-	25,25,41	1.07	1 (4%)	33,33,56	1.22	2 (6%)
14	CLA	B	3042	-	65,73,73	1.49	7 (10%)	76,113,113	1.49	10 (13%)
15	PQN	1	845	-	34,34,34	0.42	0	42,45,45	0.34	0
14	CLA	f	204	-	50,58,73	1.70	6 (12%)	58,95,113	1.61	8 (13%)
14	CLA	b	3023	21	55,63,73	1.59	6 (10%)	64,101,113	1.59	7 (10%)
14	CLA	1	810	1	65,73,73	1.46	7 (10%)	76,113,113	1.46	8 (10%)
14	CLA	B	3020	21	65,73,73	1.51	8 (12%)	76,113,113	1.46	7 (9%)
17	LHG	b	3051	-	48,48,48	0.67	1 (2%)	51,54,54	1.18	5 (9%)
16	BCR	2	3047	-	41,41,41	1.19	3 (7%)	56,56,56	1.23	8 (14%)
14	CLA	A	806	-	65,73,73	1.43	10 (15%)	76,113,113	1.61	11 (14%)
14	CLA	J	102	-	38,45,73	1.92	8 (21%)	43,78,113	1.62	5 (11%)
14	CLA	1	819	-	65,73,73	1.49	8 (12%)	76,113,113	1.47	8 (10%)
14	CLA	B	3014	-	65,73,73	1.46	7 (10%)	76,113,113	1.43	6 (7%)
14	CLA	b	3040	-	47,55,73	1.78	8 (17%)	54,91,113	1.46	7 (12%)
16	BCR	y	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	5 (8%)
16	BCR	2	3044	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	5 (8%)
16	BCR	i	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.26	5 (8%)
14	CLA	a	826	21	65,73,73	1.44	7 (10%)	76,113,113	1.58	9 (11%)
14	CLA	b	3019	-	65,73,73	1.45	7 (10%)	76,113,113	1.52	8 (10%)
17	LHG	B	3051	-	48,48,48	0.67	1 (2%)	51,54,54	1.18	5 (9%)
14	CLA	a	838	-	65,73,73	1.46	9 (13%)	76,113,113	1.46	9 (11%)
16	BCR	I	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	l	208	21	65,73,73	1.45	8 (12%)	76,113,113	1.48	8 (10%)
17	LHG	2	3051	-	48,48,48	0.67	1 (2%)	51,54,54	1.18	5 (9%)
14	CLA	B	3039	-	65,73,73	1.45	7 (10%)	76,113,113	1.59	10 (13%)
16	BCR	B	3044	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	1	823	-	45,53,73	1.74	6 (13%)	52,89,113	1.69	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	B	3007	-	65,73,73	1.45	8 (12%)	76,113,113	1.52	9 (11%)
16	BCR	A	847	-	41,41,41	1.14	3 (7%)	56,56,56	1.27	7 (12%)
14	CLA	1	809	1	65,73,73	1.44	8 (12%)	76,113,113	1.48	8 (10%)
14	CLA	b	3018	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	10 (13%)
14	CLA	1	820	-	65,73,73	1.46	8 (12%)	76,113,113	1.57	10 (13%)
16	BCR	0	210	-	41,41,41	1.22	4 (9%)	56,56,56	1.30	6 (10%)
16	BCR	A	850	-	41,41,41	1.34	3 (7%)	56,56,56	1.29	6 (10%)
14	CLA	A	802	-	65,73,73	1.42	9 (13%)	76,113,113	1.64	10 (13%)
14	CLA	A	814	-	65,73,73	1.48	8 (12%)	76,113,113	1.42	6 (7%)
14	CLA	M	1601	-	36,44,73	1.95	8 (22%)	40,76,113	1.59	6 (15%)
16	BCR	a	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	6 (10%)
14	CLA	F	203	21	45,53,73	1.77	7 (15%)	52,89,113	1.66	6 (11%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	B	3010	-	65,73,73	1.46	8 (12%)	76,113,113	1.61	13 (17%)
14	CLA	B	3019	-	65,73,73	1.43	7 (10%)	76,113,113	1.51	8 (10%)
14	CLA	A	816	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
14	CLA	b	3013	-	45,53,73	1.75	8 (17%)	52,89,113	1.61	7 (13%)
14	CLA	a	815	-	65,73,73	1.50	6 (9%)	76,113,113	1.42	8 (10%)
16	BCR	b	3044	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	a	816	21	65,73,73	1.49	7 (10%)	76,113,113	1.48	9 (11%)
14	CLA	1	822	21	65,73,73	1.47	7 (10%)	76,113,113	1.52	6 (7%)
14	CLA	2	3017	-	65,73,73	1.44	7 (10%)	76,113,113	1.65	11 (14%)
14	CLA	1	836	-	65,73,73	1.47	9 (13%)	76,113,113	1.45	7 (9%)
14	CLA	b	3041	21	65,73,73	1.44	9 (13%)	76,113,113	1.45	8 (10%)
14	CLA	j	1103	-	38,45,73	1.93	8 (21%)	43,78,113	1.62	5 (11%)
14	CLA	B	3013	-	45,53,73	1.76	8 (17%)	52,89,113	1.60	7 (13%)
16	BCR	L	206	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	5 (8%)
14	CLA	2	3016	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	9 (11%)
16	BCR	K	103	-	25,25,41	1.07	1 (4%)	33,33,56	1.21	2 (6%)
15	PQN	A	845	-	34,34,34	0.42	0	42,45,45	0.35	0
14	CLA	1	821	-	65,73,73	1.45	6 (9%)	76,113,113	1.49	7 (9%)
16	BCR	1	851	-	25,25,41	1.14	1 (4%)	33,33,56	1.27	4 (12%)
14	CLA	b	3021	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
14	CLA	z	1701	-	45,53,73	1.83	6 (13%)	52,89,113	1.57	6 (11%)
14	CLA	1	838	-	65,73,73	1.44	7 (10%)	76,113,113	1.60	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	0	204	2	65,73,73	1.44	7 (10%)	76,113,113	1.49	10 (13%)
16	BCR	2	3049	-	41,41,41	1.39	4 (9%)	56,56,56	1.27	7 (12%)
14	CLA	a	809	1	65,73,73	1.46	7 (10%)	76,113,113	1.47	9 (11%)
14	CLA	A	836	-	65,73,73	1.47	9 (13%)	76,113,113	1.46	7 (9%)
14	CLA	A	831	-	65,73,73	1.49	11 (16%)	76,113,113	1.42	7 (9%)
14	CLA	a	830	-	65,73,73	1.50	11 (16%)	76,113,113	1.43	7 (9%)
14	CLA	2	3011	2	65,73,73	1.44	10 (15%)	76,113,113	1.59	10 (13%)
15	PQN	2	3043	-	34,34,34	0.44	0	42,45,45	0.37	0
17	LHG	a	853	14	40,40,48	0.77	2 (5%)	43,46,54	1.17	3 (6%)
14	CLA	B	3028	-	65,73,73	1.48	9 (13%)	76,113,113	1.40	9 (11%)
14	CLA	1	827	21	65,73,73	1.44	7 (10%)	76,113,113	1.57	9 (11%)
14	CLA	A	819	-	65,73,73	1.48	7 (10%)	76,113,113	1.46	8 (10%)
14	CLA	2	3034	-	65,73,73	1.44	7 (10%)	76,113,113	1.49	8 (10%)
14	CLA	A	841	-	65,73,73	1.43	9 (13%)	76,113,113	1.48	8 (10%)
14	CLA	1	839	-	65,73,73	1.45	9 (13%)	76,113,113	1.45	9 (11%)
14	CLA	A	835	-	65,73,73	1.42	9 (13%)	76,113,113	1.50	7 (9%)
16	BCR	2	3048	-	41,41,41	1.29	4 (9%)	56,56,56	1.23	7 (12%)
14	CLA	0	203	-	36,44,73	1.96	7 (19%)	40,76,113	1.59	6 (15%)
16	BCR	B	3045	-	41,41,41	1.15	3 (7%)	56,56,56	1.20	3 (5%)
14	CLA	1	825	-	65,73,73	1.45	7 (10%)	76,113,113	1.48	8 (10%)
14	CLA	A	813	-	45,53,73	1.75	6 (13%)	52,89,113	1.65	6 (11%)
14	CLA	2	3026	21	65,73,73	1.50	8 (12%)	76,113,113	1.64	14 (18%)
14	CLA	B	3029	-	65,73,73	1.48	10 (15%)	76,113,113	1.33	8 (10%)
14	CLA	L	203	10	65,73,73	1.51	8 (12%)	76,113,113	1.45	8 (10%)
17	LHG	1	852	-	48,48,48	0.78	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	a	817	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	10 (13%)
14	CLA	A	808	-	51,59,73	1.64	7 (13%)	59,96,113	1.54	9 (15%)
16	BCR	2	3045	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	4 (7%)
16	BCR	8	104	-	41,41,41	1.21	3 (7%)	56,56,56	1.27	7 (12%)
14	CLA	B	3005	-	65,73,73	1.39	9 (13%)	76,113,113	1.62	12 (15%)
14	CLA	a	837	-	65,73,73	1.44	7 (10%)	76,113,113	1.61	11 (14%)
16	BCR	j	1105	-	41,41,41	1.20	3 (7%)	56,56,56	1.28	7 (12%)
16	BCR	6	202	-	41,41,41	1.16	3 (7%)	56,56,56	1.23	6 (10%)
14	CLA	a	834	-	65,73,73	1.42	9 (13%)	76,113,113	1.49	8 (10%)
16	BCR	b	3049	-	41,41,41	1.39	4 (9%)	56,56,56	1.27	7 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	820	-	65,73,73	1.45	6 (9%)	76,113,113	1.48	7 (9%)
16	BCR	7	101	-	41,41,41	1.27	3 (7%)	56,56,56	1.25	5 (8%)
14	CLA	B	3032	-	49,57,73	1.67	7 (14%)	55,93,113	1.62	7 (12%)
14	CLA	8	102	-	38,45,73	1.93	8 (21%)	43,78,113	1.62	5 (11%)
14	CLA	a	803	21	65,73,73	1.54	9 (13%)	76,113,113	1.36	6 (7%)
16	BCR	M	1602	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	5 (8%)
15	PQN	b	3043	-	34,34,34	0.45	0	42,45,45	0.37	0
14	CLA	2	3018	-	65,73,73	1.51	8 (12%)	76,113,113	1.43	10 (13%)
14	CLA	2	3006	-	65,73,73	1.47	9 (13%)	76,113,113	1.51	11 (14%)
14	CLA	b	3020	21	65,73,73	1.50	8 (12%)	76,113,113	1.46	7 (9%)
14	CLA	b	3042	-	65,73,73	1.49	7 (10%)	76,113,113	1.49	10 (13%)
14	CLA	B	3037	21	45,53,73	1.83	6 (13%)	52,89,113	1.61	6 (11%)
14	CLA	a	804	-	59,67,73	1.50	7 (11%)	68,105,113	1.58	7 (10%)
14	CLA	b	3014	-	65,73,73	1.47	7 (10%)	76,113,113	1.43	6 (7%)
14	CLA	j	1102	-	45,53,73	1.78	5 (11%)	52,89,113	1.62	7 (13%)
14	CLA	b	3016	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	9 (11%)
14	CLA	A	821	-	65,73,73	1.44	6 (9%)	76,113,113	1.49	7 (9%)
14	CLA	2	3021	-	65,73,73	1.50	6 (9%)	76,113,113	1.33	8 (10%)
14	CLA	B	3017	-	65,73,73	1.43	7 (10%)	76,113,113	1.65	11 (14%)
14	CLA	B	3006	-	65,73,73	1.48	9 (13%)	76,113,113	1.51	11 (14%)
14	CLA	B	3016	-	65,73,73	1.42	7 (10%)	76,113,113	1.52	9 (11%)
16	BCR	b	3045	-	41,41,41	1.16	3 (7%)	56,56,56	1.19	4 (7%)
14	CLA	1	802	-	65,73,73	1.43	8 (12%)	76,113,113	1.64	10 (13%)
14	CLA	B	3015	-	65,73,73	1.46	6 (9%)	76,113,113	1.46	10 (13%)
14	CLA	a	805	-	65,73,73	1.44	11 (16%)	76,113,113	1.61	11 (14%)
14	CLA	a	836	1	45,53,73	1.81	6 (13%)	52,89,113	1.52	8 (15%)
14	CLA	B	3040	-	47,55,73	1.77	8 (17%)	54,91,113	1.47	7 (12%)
14	CLA	B	3031	-	55,63,73	1.60	10 (18%)	64,101,113	1.51	8 (12%)
15	PQN	B	3043	-	34,34,34	0.44	0	42,45,45	0.37	0
16	BCR	a	851	-	25,25,41	1.13	1 (4%)	33,33,56	1.27	4 (12%)
16	BCR	a	850	-	41,41,41	1.32	2 (4%)	56,56,56	1.31	7 (12%)
16	BCR	a	849	-	41,41,41	1.34	4 (9%)	56,56,56	1.30	6 (10%)
14	CLA	b	3032	-	49,57,73	1.66	7 (14%)	55,93,113	1.62	7 (12%)
16	BCR	B	3048	-	41,41,41	1.28	3 (7%)	56,56,56	1.23	7 (12%)
16	BCR	a	847	-	41,41,41	1.23	3 (7%)	56,56,56	1.39	8 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	a	823	-	65,73,73	1.47	7 (10%)	76,113,113	1.49	9 (11%)
14	CLA	2	3031	-	55,63,73	1.60	10 (18%)	64,101,113	1.52	8 (12%)
14	CLA	a	842	21	65,73,73	1.49	9 (13%)	76,113,113	1.47	8 (10%)
14	CLA	B	3025	2	65,73,73	1.48	7 (10%)	76,113,113	1.39	6 (7%)
14	CLA	b	3010	-	65,73,73	1.47	8 (12%)	76,113,113	1.61	13 (17%)
17	LHG	0	201	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	5 (9%)
14	CLA	b	3035	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	8 (10%)
14	CLA	A	807	-	65,73,73	1.43	7 (10%)	76,113,113	1.50	6 (7%)
20	LMG	2	3050	-	55,55,55	0.88	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	1	813	-	45,53,73	1.75	6 (13%)	52,89,113	1.66	6 (11%)
14	CLA	l	206	10	65,73,73	1.50	8 (12%)	76,113,113	1.45	8 (10%)
14	CLA	b	3037	21	45,53,73	1.82	6 (13%)	52,89,113	1.60	6 (11%)
14	CLA	B	3035	-	65,73,73	1.45	8 (12%)	76,113,113	1.46	8 (10%)
16	BCR	2	3052	-	41,41,41	1.26	2 (4%)	56,56,56	1.42	11 (19%)
16	BCR	B	3049	-	41,41,41	1.39	4 (9%)	56,56,56	1.27	7 (12%)
14	CLA	9	101	-	46,54,73	1.77	7 (15%)	53,90,113	1.51	6 (11%)
14	CLA	2	3022	-	45,53,73	1.74	6 (13%)	52,89,113	1.73	7 (13%)
14	CLA	2	3041	21	65,73,73	1.45	9 (13%)	76,113,113	1.45	8 (10%)
17	LHG	L	208	-	38,38,48	0.76	0	41,44,54	1.28	4 (9%)
16	BCR	1	848	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	6 (10%)
14	CLA	a	827	-	65,73,73	1.46	7 (10%)	76,113,113	1.41	7 (9%)
14	CLA	a	843	17	45,53,73	1.72	7 (15%)	52,89,113	1.78	7 (13%)
14	CLA	b	3007	-	65,73,73	1.45	8 (12%)	76,113,113	1.51	9 (11%)
15	PQN	a	844	-	34,34,34	0.42	0	42,45,45	0.35	0
14	CLA	A	811	-	49,57,73	1.69	7 (14%)	55,93,113	1.45	5 (9%)
17	LHG	0	202	-	38,38,48	0.76	0	41,44,54	1.28	4 (9%)
14	CLA	B	3022	-	45,53,73	1.74	6 (13%)	52,89,113	1.73	7 (13%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-
14	CLA	1	830	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
16	BCR	9	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.35	10 (17%)
14	CLA	b	3031	-	55,63,73	1.60	10 (18%)	64,101,113	1.52	8 (12%)
14	CLA	2	3036	21	50,58,73	1.73	7 (14%)	58,95,113	1.54	9 (15%)
14	CLA	2	3038	-	60,68,73	1.56	9 (15%)	70,107,113	1.47	8 (11%)
14	CLA	a	839	-	65,73,73	1.47	8 (12%)	76,113,113	1.39	9 (11%)
20	LMG	b	3050	-	55,55,55	0.88	4 (7%)	63,63,63	1.35	9 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	834	-	65,73,73	1.44	8 (12%)	76,113,113	1.56	10 (13%)
16	BCR	B	3053	-	41,41,41	1.26	2 (4%)	56,56,56	1.42	11 (19%)
14	CLA	b	3024	-	45,53,73	1.76	7 (15%)	52,89,113	1.71	8 (15%)
16	BCR	6	205	-	41,41,41	1.17	2 (4%)	56,56,56	1.37	9 (16%)
20	LMG	B	3050	-	55,55,55	0.88	4 (7%)	63,63,63	1.35	9 (14%)
18	SF4	B	3001	1,2	0,12,12	-	-	-		
14	CLA	1	824	-	65,73,73	1.48	7 (10%)	76,113,113	1.48	9 (11%)
14	CLA	f	203	21	45,53,73	1.75	7 (15%)	52,89,113	1.66	7 (13%)
14	CLA	b	3005	-	65,73,73	1.39	9 (13%)	76,113,113	1.62	11 (14%)
14	CLA	A	844	17	45,53,73	1.71	7 (15%)	52,89,113	1.78	7 (13%)
16	BCR	B	3046	-	41,41,41	1.25	3 (7%)	56,56,56	1.22	6 (10%)
14	CLA	2	3015	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	10 (13%)
14	CLA	a	829	-	65,73,73	1.42	9 (13%)	76,113,113	1.51	8 (10%)
13	CL0	1	801	-	65,73,73	1.44	9 (13%)	76,113,113	1.50	8 (10%)
14	CLA	b	3038	-	60,68,73	1.55	9 (15%)	70,107,113	1.46	8 (11%)
14	CLA	2	3009	-	65,73,73	1.46	9 (13%)	76,113,113	1.48	9 (11%)
14	CLA	a	825	21	65,73,73	1.45	9 (13%)	76,113,113	1.52	8 (10%)
18	SF4	3	102	3	0,12,12	-	-	-		
16	BCR	8	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.15	4 (7%)
14	CLA	1	841	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
16	BCR	B	3047	-	41,41,41	1.19	2 (4%)	56,56,56	1.23	8 (14%)
14	CLA	a	821	21	65,73,73	1.46	7 (10%)	76,113,113	1.52	6 (7%)
14	CLA	2	3033	-	65,73,73	1.49	8 (12%)	76,113,113	1.53	10 (13%)
14	CLA	1	203	2	65,73,73	1.45	8 (12%)	76,113,113	1.49	10 (13%)
14	CLA	2	3003	21	65,73,73	1.42	8 (12%)	76,113,113	1.70	10 (13%)
14	CLA	J	101	-	45,53,73	1.76	5 (11%)	52,89,113	1.63	7 (13%)
14	CLA	2	3023	21	55,63,73	1.60	7 (12%)	64,101,113	1.58	7 (10%)
14	CLA	B	3023	21	55,63,73	1.59	6 (10%)	64,101,113	1.58	7 (10%)
14	CLA	A	826	21	65,73,73	1.44	9 (13%)	76,113,113	1.53	8 (10%)
14	CLA	b	3017	-	65,73,73	1.43	7 (10%)	76,113,113	1.66	11 (14%)
14	CLA	b	3034	-	65,73,73	1.44	7 (10%)	76,113,113	1.48	8 (10%)
14	CLA	1	831	-	65,73,73	1.50	11 (16%)	76,113,113	1.43	7 (9%)
16	BCR	1	204	-	41,41,41	1.42	4 (9%)	56,56,56	1.29	6 (10%)
14	CLA	A	822	21	65,73,73	1.47	7 (10%)	76,113,113	1.51	6 (7%)
14	CLA	1	804	-	65,73,73	1.43	7 (10%)	76,113,113	1.54	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	1	808	-	51,59,73	1.64	7 (13%)	59,96,113	1.54	9 (15%)
16	BCR	A	848	-	41,41,41	1.23	3 (7%)	56,56,56	1.39	8 (14%)
16	BCR	1	846	-	41,41,41	1.13	3 (7%)	56,56,56	1.28	7 (12%)
14	CLA	b	3022	-	45,53,73	1.74	5 (11%)	52,89,113	1.74	7 (13%)
14	CLA	0	208	-	65,73,73	1.43	10 (15%)	76,113,113	1.54	10 (13%)
14	CLA	B	3034	-	65,73,73	1.43	7 (10%)	76,113,113	1.49	8 (10%)
14	CLA	l	207	-	65,73,73	1.43	10 (15%)	76,113,113	1.54	11 (14%)
14	CLA	b	3039	-	65,73,73	1.45	7 (10%)	76,113,113	1.59	10 (13%)
14	CLA	f	201	21	58,66,73	1.58	6 (10%)	67,104,113	1.48	7 (10%)
16	BCR	F	202	-	41,41,41	1.16	3 (7%)	56,56,56	1.24	6 (10%)
14	CLA	L	205	21	65,73,73	1.45	8 (12%)	76,113,113	1.47	8 (10%)
16	BCR	I	102	-	41,41,41	1.22	4 (9%)	56,56,56	1.30	6 (10%)
14	CLA	B	3018	-	65,73,73	1.52	8 (12%)	76,113,113	1.44	10 (13%)
14	CLA	a	840	-	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
14	CLA	A	810	1	65,73,73	1.46	7 (10%)	76,113,113	1.47	8 (10%)
14	CLA	B	3011	2	65,73,73	1.44	8 (12%)	76,113,113	1.58	10 (13%)
14	CLA	b	3015	-	65,73,73	1.46	6 (9%)	76,113,113	1.47	10 (13%)
14	CLA	a	812	-	45,53,73	1.76	6 (13%)	52,89,113	1.66	7 (13%)
14	CLA	2	3004	-	65,73,73	1.41	9 (13%)	76,113,113	1.47	7 (9%)
14	CLA	B	3008	-	65,73,73	1.48	9 (13%)	76,113,113	1.45	9 (11%)
14	CLA	1	835	-	65,73,73	1.42	9 (13%)	76,113,113	1.50	8 (10%)
14	CLA	k	102	21	58,66,73	1.58	5 (8%)	67,104,113	1.47	8 (11%)
14	CLA	b	3036	21	50,58,73	1.73	7 (14%)	58,95,113	1.55	9 (15%)
16	BCR	b	3048	-	41,41,41	1.28	4 (9%)	56,56,56	1.23	7 (12%)
14	CLA	A	804	-	65,73,73	1.43	7 (10%)	76,113,113	1.54	9 (11%)
17	LHG	A	854	14	40,40,48	0.77	2 (5%)	43,46,54	1.17	3 (6%)
17	LHG	L	207	-	48,48,48	0.68	1 (2%)	51,54,54	1.30	5 (9%)
14	CLA	x	1701	-	45,53,73	1.83	6 (13%)	52,89,113	1.56	6 (11%)
14	CLA	A	809	1	65,73,73	1.44	9 (13%)	76,113,113	1.48	8 (10%)
18	SF4	c	101	3	0,12,12	-	-	-	-	-
14	CLA	2	3005	-	65,73,73	1.38	9 (13%)	76,113,113	1.61	11 (14%)
14	CLA	a	806	-	65,73,73	1.42	7 (10%)	76,113,113	1.50	6 (7%)
14	CLA	A	834	-	65,73,73	1.44	8 (12%)	76,113,113	1.56	10 (13%)
17	LHG	A	853	-	48,48,48	0.78	2 (4%)	51,54,54	1.23	4 (7%)
14	CLA	b	3026	21	65,73,73	1.50	8 (12%)	76,113,113	1.65	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	CLA	j	1101	-	65,73,73	1.42	7 (10%)	76,113,113	1.54	9 (11%)
14	CLA	B	3036	21	50,58,73	1.73	7 (14%)	58,95,113	1.55	9 (15%)
16	BCR	m	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	4 (7%)
14	CLA	k	101	-	46,54,73	1.77	7 (15%)	53,90,113	1.51	6 (11%)
14	CLA	A	815	-	65,73,73	1.49	5 (7%)	76,113,113	1.37	7 (9%)
14	CLA	0	207	10	65,73,73	1.51	8 (12%)	76,113,113	1.45	8 (10%)
14	CLA	2	3030	-	65,73,73	1.44	10 (15%)	76,113,113	1.46	9 (11%)
14	CLA	a	807	-	51,59,73	1.65	7 (13%)	59,96,113	1.55	9 (15%)
14	CLA	9	103	21	58,66,73	1.57	5 (8%)	67,104,113	1.47	8 (11%)
14	CLA	1	818	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	10 (13%)
16	BCR	1	850	-	41,41,41	1.31	4 (9%)	56,56,56	1.30	6 (10%)
14	CLA	1	816	-	65,73,73	1.50	6 (9%)	76,113,113	1.42	8 (10%)
14	CLA	L	201	2	65,73,73	1.45	9 (13%)	76,113,113	1.49	10 (13%)
16	BCR	A	852	-	25,25,41	1.14	1 (4%)	33,33,56	1.27	4 (12%)
14	CLA	1	814	-	65,73,73	1.47	8 (12%)	76,113,113	1.42	6 (7%)
14	CLA	K	102	21	58,66,73	1.58	5 (8%)	67,104,113	1.47	8 (11%)
14	CLA	2	3039	-	65,73,73	1.44	7 (10%)	76,113,113	1.59	10 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	L	204	-	1/1/15/20	10/37/115/115	-
14	CLA	A	817	21	1/1/15/20	16/37/115/115	-
16	BCR	l	209	-	-	9/29/63/63	0/2/2/2
14	CLA	A	837	1	1/1/11/20	4/13/91/115	-
14	CLA	b	3004	-	1/1/15/20	15/37/115/115	-
16	BCR	F	205	-	-	8/29/63/63	0/2/2/2
14	CLA	B	3003	21	1/1/15/20	19/37/115/115	-
14	CLA	a	802	-	1/1/15/20	18/37/115/115	-
14	CLA	A	812	-	1/1/15/20	13/37/115/115	-
14	CLA	A	820	-	1/1/15/20	9/37/115/115	-
14	CLA	2	3028	-	1/1/15/20	20/37/115/115	-
14	CLA	a	831	-	1/1/14/20	9/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3028	-	1/1/15/20	20/37/115/115	-
16	BCR	J	103	-	-	9/29/63/63	0/2/2/2
14	CLA	2	3007	-	1/1/15/20	14/37/115/115	-
14	CLA	1	843	21	1/1/15/20	14/37/115/115	-
14	CLA	X	1701	-	1/1/11/20	6/13/91/115	-
16	BCR	B	3052	-	-	13/29/63/63	0/2/2/2
14	CLA	1	807	-	1/1/15/20	15/37/115/115	-
14	CLA	0	209	21	1/1/15/20	13/37/115/115	-
14	CLA	a	813	-	1/1/15/20	17/37/115/115	-
14	CLA	b	3029	-	1/1/15/20	8/37/115/115	-
14	CLA	2	3013	-	-	2/13/91/115	-
16	BCR	f	205	-	-	8/29/63/63	0/2/2/2
17	LHG	l	201	-	-	25/53/53/53	-
14	CLA	2	3024	-	-	6/13/91/115	-
14	CLA	2	3025	2	1/1/15/20	11/37/115/115	-
14	CLA	8	101	-	1/1/11/20	5/13/91/115	-
14	CLA	a	824	-	1/1/15/20	17/37/115/115	-
14	CLA	A	855	-	1/1/7/20	0/2/72/115	-
14	CLA	A	825	-	1/1/15/20	17/37/115/115	-
14	CLA	a	819	-	1/1/15/20	9/37/115/115	-
14	CLA	B	3026	21	1/1/15/20	15/37/115/115	-
14	CLA	a	841	-	1/1/15/20	8/37/115/115	-
17	LHG	l	202	-	-	28/43/43/53	-
16	BCR	k	103	-	-	2/18/35/63	0/1/1/2
14	CLA	B	3012	-	1/1/15/20	16/37/115/115	-
14	CLA	1	832	-	1/1/14/20	9/31/109/115	-
14	CLA	1	811	-	1/1/11/20	6/18/96/115	-
14	CLA	b	3030	-	1/1/15/20	6/37/115/115	-
14	CLA	2	3012	-	1/1/15/20	16/37/115/115	-
14	CLA	a	835	-	1/1/15/20	12/37/115/115	-
16	BCR	b	3047	-	-	14/29/63/63	0/2/2/2
14	CLA	2	3008	-	1/1/15/20	10/37/115/115	-
14	CLA	A	833	-	1/1/15/20	15/37/115/115	-
14	CLA	1	837	1	1/1/11/20	4/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	843	21	1/1/15/20	14/37/115/115	-
16	BCR	A	846	-	-	6/29/63/63	0/2/2/2
14	CLA	B	3030	-	1/1/15/20	6/37/115/115	-
14	CLA	1	829	-	1/1/15/20	13/37/115/115	-
16	BCR	J	104	-	-	14/29/63/63	0/2/2/2
14	CLA	A	823	-	1/1/11/20	4/13/91/115	-
14	CLA	1	840	-	1/1/15/20	13/37/115/115	-
14	CLA	2	3027	-	1/1/15/20	12/37/115/115	-
16	BCR	j	1104	-	-	9/29/63/63	0/2/2/2
16	BCR	2	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	A	830	-	1/1/15/20	17/37/115/115	-
14	CLA	b	3033	-	1/1/15/20	14/37/115/115	-
14	CLA	1	842	-	1/1/15/20	8/37/115/115	-
14	CLA	A	805	-	1/1/13/20	11/30/108/115	-
14	CLA	a	808	1	1/1/15/20	17/37/115/115	-
14	CLA	a	810	-	1/1/11/20	6/18/96/115	-
13	CL0	a	801	-	3/3/20/25	8/37/135/135	-
14	CLA	A	839	-	1/1/15/20	18/37/115/115	-
17	LHG	a	852	-	-	21/53/53/53	-
14	CLA	b	3006	-	1/1/15/20	17/37/115/115	-
14	CLA	b	3009	-	1/1/15/20	8/37/115/115	-
14	CLA	1	844	17	1/1/11/20	5/13/91/115	-
14	CLA	B	3033	-	1/1/15/20	14/37/115/115	-
14	CLA	b	3025	2	1/1/15/20	11/37/115/115	-
14	CLA	B	3038	-	1/1/14/20	12/31/109/115	-
14	CLA	F	201	21	1/1/13/20	7/29/107/115	-
14	CLA	A	838	-	1/1/15/20	17/37/115/115	-
14	CLA	F	204	-	1/1/12/20	8/19/97/115	-
14	CLA	A	818	-	1/1/15/20	13/37/115/115	-
14	CLA	A	842	-	1/1/15/20	8/37/115/115	-
14	CLA	2	3042	-	1/1/15/20	15/37/115/115	-
14	CLA	A	827	21	1/1/15/20	14/37/115/115	-
18	SF4	2	3001	1,2	-	-	0/6/5/5
14	CLA	1	812	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3012	-	1/1/15/20	16/37/115/115	-
14	CLA	A	832	-	1/1/14/20	9/31/109/115	-
14	CLA	1	803	21	1/1/15/20	7/37/115/115	-
14	CLA	2	3020	21	1/1/15/20	12/37/115/115	-
14	CLA	1	826	21	1/1/15/20	18/37/115/115	-
14	CLA	B	3009	-	1/1/15/20	8/37/115/115	-
14	CLA	1	828	-	1/1/15/20	6/37/115/115	-
14	CLA	2	3014	-	1/1/15/20	15/37/115/115	-
14	CLA	b	3027	-	1/1/15/20	12/37/115/115	-
14	CLA	B	3041	21	1/1/15/20	6/37/115/115	-
16	BCR	b	3046	-	-	11/29/63/63	0/2/2/2
16	BCR	0	205	-	-	13/29/63/63	0/2/2/2
14	CLA	2	3035	-	1/1/15/20	14/37/115/115	-
14	CLA	B	3024	-	-	6/13/91/115	-
14	CLA	2	3029	-	1/1/15/20	8/37/115/115	-
14	CLA	A	824	-	1/1/15/20	17/37/115/115	-
14	CLA	6	204	-	1/1/12/20	8/19/97/115	-
18	SF4	b	3001	1,2	-	-	0/6/5/5
14	CLA	B	3021	-	1/1/15/20	9/37/115/115	-
14	CLA	a	822	-	1/1/11/20	4/13/91/115	-
14	CLA	a	828	-	1/1/15/20	13/37/115/115	-
14	CLA	b	3008	-	1/1/15/20	10/37/115/115	-
16	BCR	A	849	-	-	7/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	13/37/115/115	-
14	CLA	A	840	-	1/1/15/20	13/37/115/115	-
16	BCR	1	849	-	-	4/29/63/63	0/2/2/2
17	LHG	1	853	14	-	21/45/45/53	-
14	CLA	K	101	-	1/1/11/20	10/15/93/115	-
14	CLA	6	203	21	1/1/11/20	5/13/91/115	-
16	BCR	f	202	-	-	12/29/63/63	0/2/2/2
14	CLA	b	3003	21	1/1/15/20	19/37/115/115	-
14	CLA	a	818	-	1/1/15/20	14/37/115/115	-
14	CLA	1	815	-	1/1/15/20	15/37/115/115	-
14	CLA	2	3032	-	1/1/11/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	833	-	1/1/15/20	12/37/115/115	-
16	BCR	a	846	-	-	17/29/63/63	0/2/2/2
14	CLA	a	814	-	1/1/15/20	15/37/115/115	-
14	CLA	1	806	-	1/1/15/20	21/37/115/115	-
14	CLA	a	811	-	1/1/15/20	13/37/115/115	-
14	CLA	1	833	-	1/1/15/20	15/37/115/115	-
14	CLA	2	3040	-	-	2/16/94/115	-
14	CLA	B	3027	-	1/1/15/20	12/37/115/115	-
16	BCR	1	847	-	-	17/29/63/63	0/2/2/2
18	SF4	c	102	3	-	-	0/6/5/5
14	CLA	2	3010	-	1/1/15/20	9/37/115/115	-
14	CLA	2	3019	-	1/1/15/20	13/37/115/115	-
14	CLA	6	201	21	1/1/13/20	7/29/107/115	-
14	CLA	2	3037	21	1/1/11/20	7/13/91/115	-
14	CLA	A	828	-	1/1/15/20	6/37/115/115	-
16	BCR	0	211	-	-	6/29/63/63	0/2/2/2
16	BCR	a	845	-	-	6/29/63/63	0/2/2/2
13	CL0	A	801	-	3/3/20/25	8/37/135/135	-
14	CLA	1	817	21	1/1/15/20	16/37/115/115	-
16	BCR	A	851	-	-	21/29/63/63	0/2/2/2
14	CLA	1	805	-	1/1/13/20	11/30/108/115	-
14	CLA	B	3004	-	1/1/15/20	15/37/115/115	-
16	BCR	j	1106	-	-	16/29/63/63	0/2/2/2
18	SF4	3	101	3	-	-	0/6/5/5
16	BCR	l	210	-	-	6/29/63/63	0/2/2/2
14	CLA	b	3011	2	1/1/15/20	9/37/115/115	-
14	CLA	a	832	-	1/1/15/20	15/37/115/115	-
14	CLA	A	803	21	1/1/15/20	7/37/115/115	-
16	BCR	9	104	-	-	2/18/35/63	0/1/1/2
14	CLA	B	3042	-	1/1/15/20	15/37/115/115	-
15	PQN	1	845	-	-	2/23/43/43	0/2/2/2
14	CLA	f	204	-	1/1/12/20	8/19/97/115	-
14	CLA	b	3023	21	1/1/13/20	10/25/103/115	-
14	CLA	1	810	1	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3020	21	1/1/15/20	12/37/115/115	-
17	LHG	b	3051	-	-	24/53/53/53	-
16	BCR	2	3047	-	-	14/29/63/63	0/2/2/2
14	CLA	A	806	-	1/1/15/20	21/37/115/115	-
14	CLA	J	102	-	1/1/8/20	0/2/76/115	-
14	CLA	1	819	-	1/1/15/20	14/37/115/115	-
14	CLA	B	3014	-	1/1/15/20	15/37/115/115	-
14	CLA	b	3040	-	-	2/16/94/115	-
16	BCR	y	101	-	-	13/29/63/63	0/2/2/2
16	BCR	2	3044	-	-	7/29/63/63	0/2/2/2
16	BCR	i	101	-	-	7/29/63/63	0/2/2/2
14	CLA	a	826	21	1/1/15/20	14/37/115/115	-
14	CLA	b	3019	-	1/1/15/20	13/37/115/115	-
17	LHG	B	3051	-	-	24/53/53/53	-
14	CLA	a	838	-	1/1/15/20	18/37/115/115	-
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
14	CLA	l	208	21	1/1/15/20	13/37/115/115	-
17	LHG	2	3051	-	-	24/53/53/53	-
14	CLA	B	3039	-	1/1/15/20	16/37/115/115	-
16	BCR	B	3044	-	-	6/29/63/63	0/2/2/2
14	CLA	1	823	-	1/1/11/20	4/13/91/115	-
14	CLA	B	3007	-	1/1/15/20	14/37/115/115	-
16	BCR	A	847	-	-	17/29/63/63	0/2/2/2
14	CLA	1	809	1	1/1/15/20	17/37/115/115	-
14	CLA	b	3018	-	-	16/37/115/115	-
14	CLA	1	820	-	1/1/15/20	9/37/115/115	-
16	BCR	0	210	-	-	9/29/63/63	0/2/2/2
16	BCR	A	850	-	-	4/29/63/63	0/2/2/2
14	CLA	A	802	-	1/1/15/20	18/37/115/115	-
14	CLA	A	814	-	1/1/15/20	17/37/115/115	-
14	CLA	M	1601	-	1/1/7/20	0/2/72/115	-
16	BCR	a	848	-	-	7/29/63/63	0/2/2/2
14	CLA	F	203	21	1/1/11/20	5/13/91/115	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	B	3010	-	1/1/15/20	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	B	3019	-	1/1/15/20	13/37/115/115	-
14	CLA	A	816	-	1/1/15/20	22/37/115/115	-
14	CLA	b	3013	-	-	2/13/91/115	-
14	CLA	a	815	-	1/1/15/20	22/37/115/115	-
16	BCR	b	3044	-	-	6/29/63/63	0/2/2/2
14	CLA	a	816	21	1/1/15/20	16/37/115/115	-
14	CLA	1	822	21	1/1/15/20	9/37/115/115	-
14	CLA	2	3017	-	1/1/15/20	14/37/115/115	-
14	CLA	1	836	-	1/1/15/20	12/37/115/115	-
14	CLA	b	3041	21	1/1/15/20	6/37/115/115	-
14	CLA	B	3013	-	-	2/13/91/115	-
14	CLA	j	1103	-	1/1/8/20	0/2/76/115	-
16	BCR	L	206	-	-	6/29/63/63	0/2/2/2
14	CLA	2	3016	-	1/1/15/20	11/37/115/115	-
16	BCR	K	103	-	-	2/18/35/63	0/1/1/2
15	PQN	A	845	-	-	2/23/43/43	0/2/2/2
14	CLA	1	821	-	1/1/15/20	19/37/115/115	-
16	BCR	1	851	-	-	15/18/35/63	0/1/1/2
14	CLA	b	3021	-	1/1/15/20	9/37/115/115	-
14	CLA	z	1701	-	1/1/11/20	6/13/91/115	-
14	CLA	1	838	-	1/1/15/20	17/37/115/115	-
14	CLA	0	204	2	1/1/15/20	10/37/115/115	-
16	BCR	2	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	a	809	1	1/1/15/20	14/37/115/115	-
14	CLA	A	836	-	1/1/15/20	12/37/115/115	-
14	CLA	A	831	-	1/1/15/20	8/37/115/115	-
14	CLA	a	830	-	1/1/15/20	8/37/115/115	-
14	CLA	2	3011	2	1/1/15/20	9/37/115/115	-
15	PQN	2	3043	-	-	4/23/43/43	0/2/2/2
17	LHG	a	853	14	-	21/45/45/53	-
14	CLA	B	3028	-	1/1/15/20	20/37/115/115	-
14	CLA	1	827	21	1/1/15/20	14/37/115/115	-
14	CLA	A	819	-	1/1/15/20	14/37/115/115	-
14	CLA	2	3034	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	841	-	1/1/15/20	10/37/115/115	-
14	CLA	1	839	-	1/1/15/20	18/37/115/115	-
14	CLA	A	835	-	1/1/15/20	10/37/115/115	-
16	BCR	2	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	0	203	-	1/1/7/20	0/2/72/115	-
16	BCR	B	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	1	825	-	1/1/15/20	17/37/115/115	-
14	CLA	A	813	-	1/1/11/20	5/13/91/115	-
14	CLA	2	3026	21	1/1/15/20	15/37/115/115	-
14	CLA	B	3029	-	1/1/15/20	8/37/115/115	-
14	CLA	L	203	10	1/1/15/20	15/37/115/115	-
17	LHG	1	852	-	-	21/53/53/53	-
14	CLA	a	817	-	1/1/15/20	13/37/115/115	-
14	CLA	A	808	-	1/1/12/20	3/21/99/115	-
16	BCR	2	3045	-	-	8/29/63/63	0/2/2/2
16	BCR	8	104	-	-	14/29/63/63	0/2/2/2
14	CLA	B	3005	-	1/1/15/20	14/37/115/115	-
14	CLA	a	837	-	1/1/15/20	17/37/115/115	-
16	BCR	j	1105	-	-	14/29/63/63	0/2/2/2
16	BCR	6	202	-	-	12/29/63/63	0/2/2/2
14	CLA	a	834	-	1/1/15/20	10/37/115/115	-
16	BCR	b	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	a	820	-	1/1/15/20	19/37/115/115	-
16	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3032	-	1/1/11/20	8/18/96/115	-
14	CLA	8	102	-	1/1/8/20	0/2/76/115	-
14	CLA	a	803	21	1/1/15/20	7/37/115/115	-
16	BCR	M	1602	-	-	13/29/63/63	0/2/2/2
15	PQN	b	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	2	3018	-	-	16/37/115/115	-
14	CLA	2	3006	-	1/1/15/20	17/37/115/115	-
14	CLA	b	3020	21	1/1/15/20	12/37/115/115	-
14	CLA	b	3042	-	1/1/15/20	15/37/115/115	-
14	CLA	B	3037	21	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	804	-	1/1/13/20	11/30/108/115	-
14	CLA	b	3014	-	1/1/15/20	15/37/115/115	-
14	CLA	j	1102	-	1/1/11/20	5/13/91/115	-
14	CLA	b	3016	-	1/1/15/20	11/37/115/115	-
14	CLA	A	821	-	1/1/15/20	19/37/115/115	-
14	CLA	2	3021	-	1/1/15/20	9/37/115/115	-
14	CLA	B	3017	-	1/1/15/20	14/37/115/115	-
14	CLA	B	3006	-	1/1/15/20	17/37/115/115	-
14	CLA	B	3016	-	1/1/15/20	11/37/115/115	-
16	BCR	b	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	1	802	-	1/1/15/20	18/37/115/115	-
14	CLA	B	3015	-	1/1/15/20	14/37/115/115	-
14	CLA	a	805	-	1/1/15/20	21/37/115/115	-
14	CLA	a	836	1	1/1/11/20	4/13/91/115	-
14	CLA	B	3040	-	-	2/16/94/115	-
14	CLA	B	3031	-	1/1/13/20	13/25/103/115	-
15	PQN	B	3043	-	-	4/23/43/43	0/2/2/2
16	BCR	a	851	-	-	15/18/35/63	0/1/1/2
16	BCR	a	850	-	-	21/29/63/63	0/2/2/2
16	BCR	a	849	-	-	4/29/63/63	0/2/2/2
14	CLA	b	3032	-	1/1/11/20	8/18/96/115	-
16	BCR	B	3048	-	-	10/29/63/63	0/2/2/2
16	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	a	823	-	1/1/15/20	17/37/115/115	-
14	CLA	2	3031	-	1/1/13/20	13/25/103/115	-
14	CLA	a	842	21	1/1/15/20	14/37/115/115	-
14	CLA	B	3025	2	1/1/15/20	12/37/115/115	-
14	CLA	b	3010	-	1/1/15/20	9/37/115/115	-
17	LHG	0	201	-	-	25/53/53/53	-
14	CLA	b	3035	-	1/1/15/20	14/37/115/115	-
14	CLA	A	807	-	1/1/15/20	15/37/115/115	-
20	LMG	2	3050	-	-	22/50/70/70	0/1/1/1
14	CLA	1	813	-	1/1/11/20	5/13/91/115	-
14	CLA	l	206	10	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3037	21	1/1/11/20	7/13/91/115	-
14	CLA	B	3035	-	1/1/15/20	14/37/115/115	-
16	BCR	2	3052	-	-	16/29/63/63	0/2/2/2
16	BCR	B	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	9	101	-	1/1/11/20	10/15/93/115	-
14	CLA	2	3022	-	1/1/11/20	5/13/91/115	-
14	CLA	2	3041	21	1/1/15/20	6/37/115/115	-
17	LHG	L	208	-	-	28/43/43/53	-
16	BCR	1	848	-	-	7/29/63/63	0/2/2/2
14	CLA	a	827	-	1/1/15/20	6/37/115/115	-
14	CLA	a	843	17	1/1/11/20	5/13/91/115	-
14	CLA	b	3007	-	1/1/15/20	14/37/115/115	-
15	PQN	a	844	-	-	2/23/43/43	0/2/2/2
14	CLA	A	811	-	1/1/11/20	6/18/96/115	-
17	LHG	0	202	-	-	28/43/43/53	-
14	CLA	B	3022	-	1/1/11/20	5/13/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
14	CLA	1	830	-	1/1/15/20	17/37/115/115	-
16	BCR	9	102	-	-	6/29/63/63	0/2/2/2
14	CLA	b	3031	-	1/1/13/20	13/25/103/115	-
14	CLA	2	3036	21	1/1/12/20	10/19/97/115	-
14	CLA	2	3038	-	1/1/14/20	12/31/109/115	-
14	CLA	a	839	-	1/1/15/20	13/37/115/115	-
20	LMG	b	3050	-	-	22/50/70/70	0/1/1/1
14	CLA	1	834	-	1/1/15/20	12/37/115/115	-
16	BCR	B	3053	-	-	16/29/63/63	0/2/2/2
14	CLA	b	3024	-	-	6/13/91/115	-
16	BCR	6	205	-	-	8/29/63/63	0/2/2/2
20	LMG	B	3050	-	-	22/50/70/70	0/1/1/1
18	SF4	B	3001	1,2	-	-	0/6/5/5
14	CLA	1	824	-	1/1/15/20	17/37/115/115	-
14	CLA	f	203	21	1/1/11/20	5/13/91/115	-
14	CLA	b	3005	-	1/1/15/20	14/37/115/115	-
14	CLA	A	844	17	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	2	3015	-	1/1/15/20	14/37/115/115	-
14	CLA	a	829	-	1/1/15/20	17/37/115/115	-
13	CL0	1	801	-	3/3/20/25	8/37/135/135	-
14	CLA	b	3038	-	1/1/14/20	12/31/109/115	-
14	CLA	2	3009	-	1/1/15/20	8/37/115/115	-
14	CLA	a	825	21	1/1/15/20	18/37/115/115	-
18	SF4	3	102	3	-	-	0/6/5/5
16	BCR	8	103	-	-	9/29/63/63	0/2/2/2
14	CLA	1	841	-	1/1/15/20	10/37/115/115	-
16	BCR	B	3047	-	-	14/29/63/63	0/2/2/2
14	CLA	a	821	21	1/1/15/20	9/37/115/115	-
14	CLA	2	3033	-	1/1/15/20	14/37/115/115	-
14	CLA	l	203	2	1/1/15/20	10/37/115/115	-
14	CLA	2	3003	21	1/1/15/20	19/37/115/115	-
14	CLA	J	101	-	1/1/11/20	5/13/91/115	-
14	CLA	2	3023	21	1/1/13/20	10/25/103/115	-
14	CLA	B	3023	21	1/1/13/20	10/25/103/115	-
14	CLA	A	826	21	1/1/15/20	18/37/115/115	-
14	CLA	b	3017	-	1/1/15/20	14/37/115/115	-
14	CLA	b	3034	-	1/1/15/20	15/37/115/115	-
14	CLA	1	831	-	1/1/15/20	8/37/115/115	-
16	BCR	l	204	-	-	13/29/63/63	0/2/2/2
14	CLA	A	822	21	1/1/15/20	9/37/115/115	-
14	CLA	1	804	-	1/1/15/20	14/37/115/115	-
14	CLA	1	808	-	1/1/12/20	3/21/99/115	-
16	BCR	A	848	-	-	17/29/63/63	0/2/2/2
16	BCR	1	846	-	-	17/29/63/63	0/2/2/2
14	CLA	b	3022	-	1/1/11/20	5/13/91/115	-
14	CLA	0	208	-	1/1/15/20	10/37/115/115	-
14	CLA	B	3034	-	1/1/15/20	15/37/115/115	-
14	CLA	l	207	-	1/1/15/20	10/37/115/115	-
14	CLA	b	3039	-	1/1/15/20	16/37/115/115	-
14	CLA	f	201	21	1/1/13/20	7/29/107/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	F	202	-	-	12/29/63/63	0/2/2/2
14	CLA	L	205	21	1/1/15/20	13/37/115/115	-
16	BCR	I	102	-	-	9/29/63/63	0/2/2/2
14	CLA	B	3018	-	-	16/37/115/115	-
14	CLA	a	840	-	1/1/15/20	10/37/115/115	-
14	CLA	A	810	1	1/1/15/20	14/37/115/115	-
14	CLA	B	3011	2	1/1/15/20	9/37/115/115	-
14	CLA	b	3015	-	1/1/15/20	14/37/115/115	-
14	CLA	a	812	-	1/1/11/20	5/13/91/115	-
14	CLA	2	3004	-	1/1/15/20	15/37/115/115	-
14	CLA	B	3008	-	1/1/15/20	10/37/115/115	-
14	CLA	l	835	-	1/1/15/20	10/37/115/115	-
14	CLA	k	102	21	1/1/13/20	11/29/107/115	-
14	CLA	b	3036	21	1/1/12/20	10/19/97/115	-
16	BCR	b	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	A	804	-	1/1/15/20	14/37/115/115	-
17	LHG	A	854	14	-	21/45/45/53	-
17	LHG	L	207	-	-	25/53/53/53	-
14	CLA	x	1701	-	1/1/11/20	6/13/91/115	-
14	CLA	A	809	1	1/1/15/20	17/37/115/115	-
18	SF4	c	101	3	-	-	0/6/5/5
14	CLA	2	3005	-	1/1/15/20	14/37/115/115	-
14	CLA	a	806	-	1/1/15/20	15/37/115/115	-
14	CLA	A	834	-	1/1/15/20	12/37/115/115	-
17	LHG	A	853	-	-	21/53/53/53	-
14	CLA	b	3026	21	1/1/15/20	15/37/115/115	-
14	CLA	j	1101	-	1/1/15/20	14/37/115/115	-
14	CLA	B	3036	21	1/1/12/20	10/19/97/115	-
16	BCR	m	101	-	-	13/29/63/63	0/2/2/2
14	CLA	k	101	-	1/1/11/20	10/15/93/115	-
14	CLA	A	815	-	1/1/15/20	15/37/115/115	-
14	CLA	0	207	10	1/1/15/20	15/37/115/115	-
14	CLA	2	3030	-	1/1/15/20	6/37/115/115	-
14	CLA	a	807	-	1/1/12/20	3/21/99/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	9	103	21	1/1/13/20	11/29/107/115	-
14	CLA	1	818	-	1/1/15/20	13/37/115/115	-
16	BCR	1	850	-	-	21/29/63/63	0/2/2/2
14	CLA	1	816	-	1/1/15/20	22/37/115/115	-
14	CLA	L	201	2	1/1/15/20	10/37/115/115	-
16	BCR	A	852	-	-	15/18/35/63	0/1/1/2
14	CLA	1	814	-	1/1/15/20	17/37/115/115	-
14	CLA	K	102	21	1/1/13/20	11/29/107/115	-
14	CLA	2	3039	-	1/1/15/20	16/37/115/115	-

The worst 5 of 2467 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	2	3037	CLA	C4B-NB	8.11	1.42	1.35
14	B	3037	CLA	C4B-NB	8.10	1.42	1.35
14	b	3037	CLA	C4B-NB	8.09	1.42	1.35
14	z	1701	CLA	C4B-NB	7.83	1.42	1.35
14	F	204	CLA	C4B-NB	7.81	1.42	1.35

The worst 5 of 2918 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3005	CLA	C4A-NA-C1A	8.29	110.43	106.71
14	B	3005	CLA	C4A-NA-C1A	8.29	110.43	106.71
14	2	3005	CLA	C4A-NA-C1A	8.27	110.42	106.71
14	a	805	CLA	C4A-NA-C1A	8.18	110.38	106.71
14	A	806	CLA	C4A-NA-C1A	8.07	110.33	106.71

5 of 285 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	A	801	CL0	NC
13	A	801	CL0	NA
13	A	801	CL0	ND
13	a	801	CL0	NC
13	a	801	CL0	NA

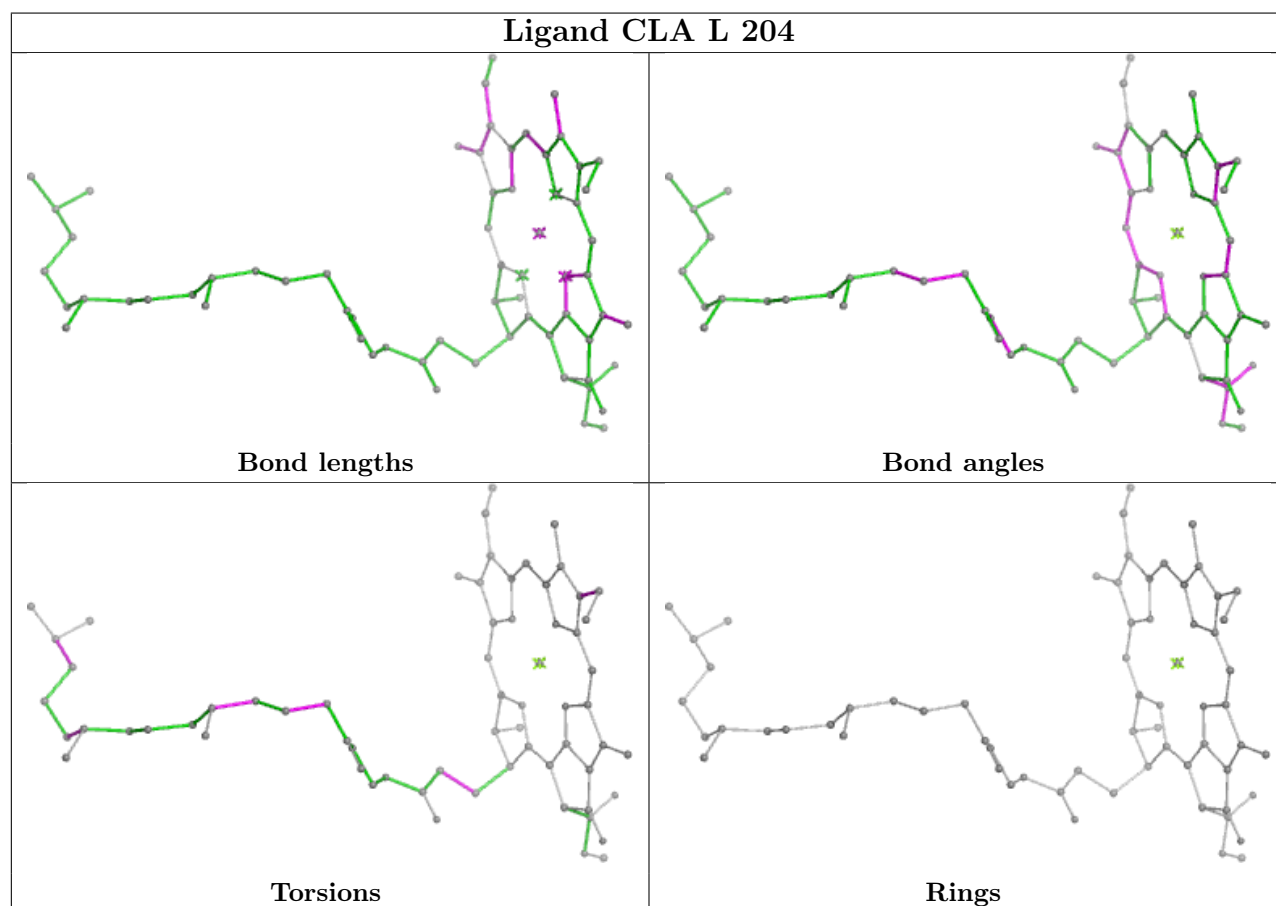
5 of 4512 torsion outliers are listed below:

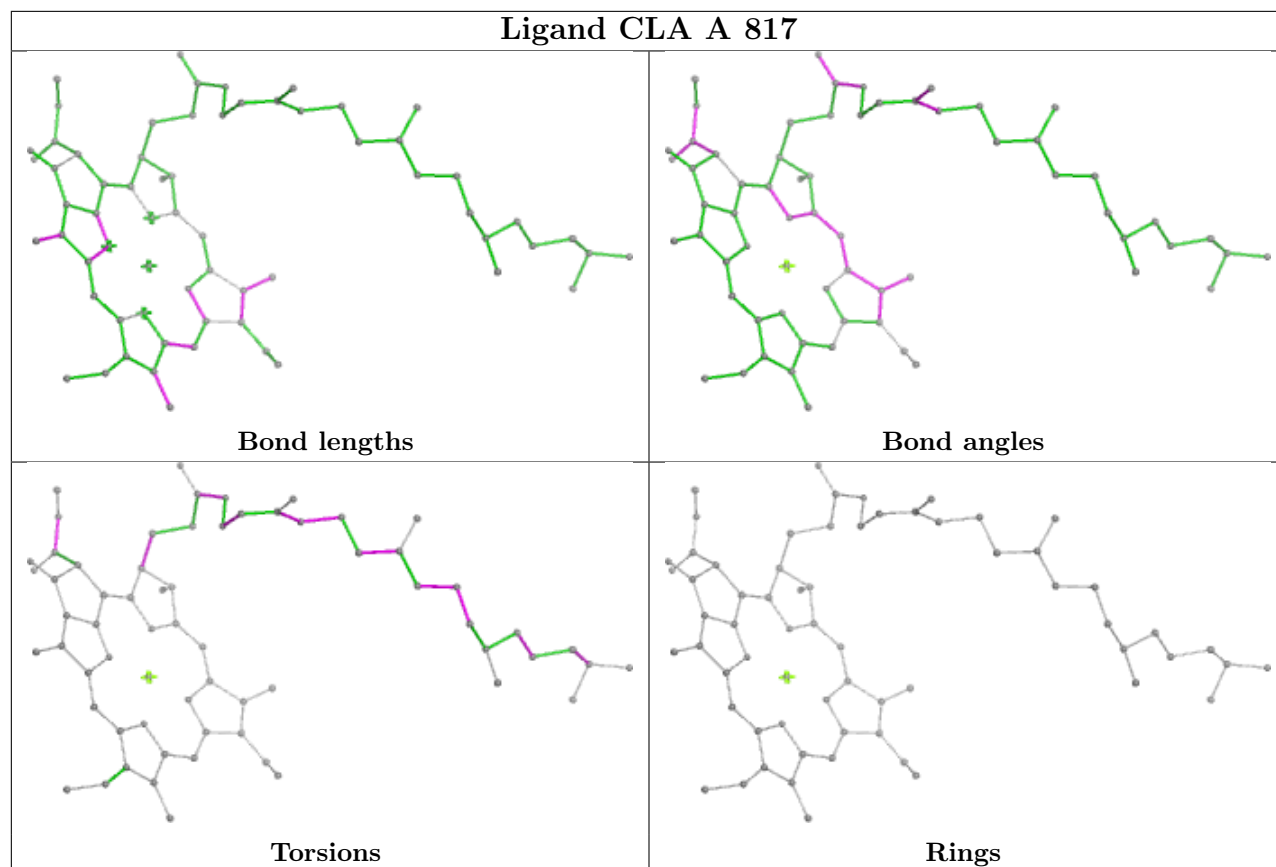
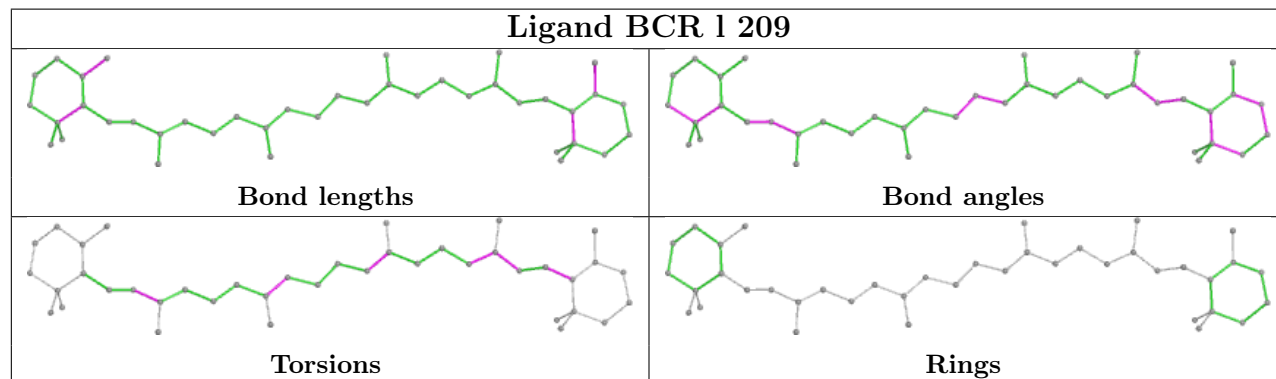
Mol	Chain	Res	Type	Atoms
14	A	802	CLA	C14-C13-C15-C16
14	A	804	CLA	C1A-C2A-CAA-CBA
14	A	804	CLA	C3A-C2A-CAA-CBA
14	A	805	CLA	C1A-C2A-CAA-CBA
14	A	805	CLA	C3A-C2A-CAA-CBA

There are no ring outliers.

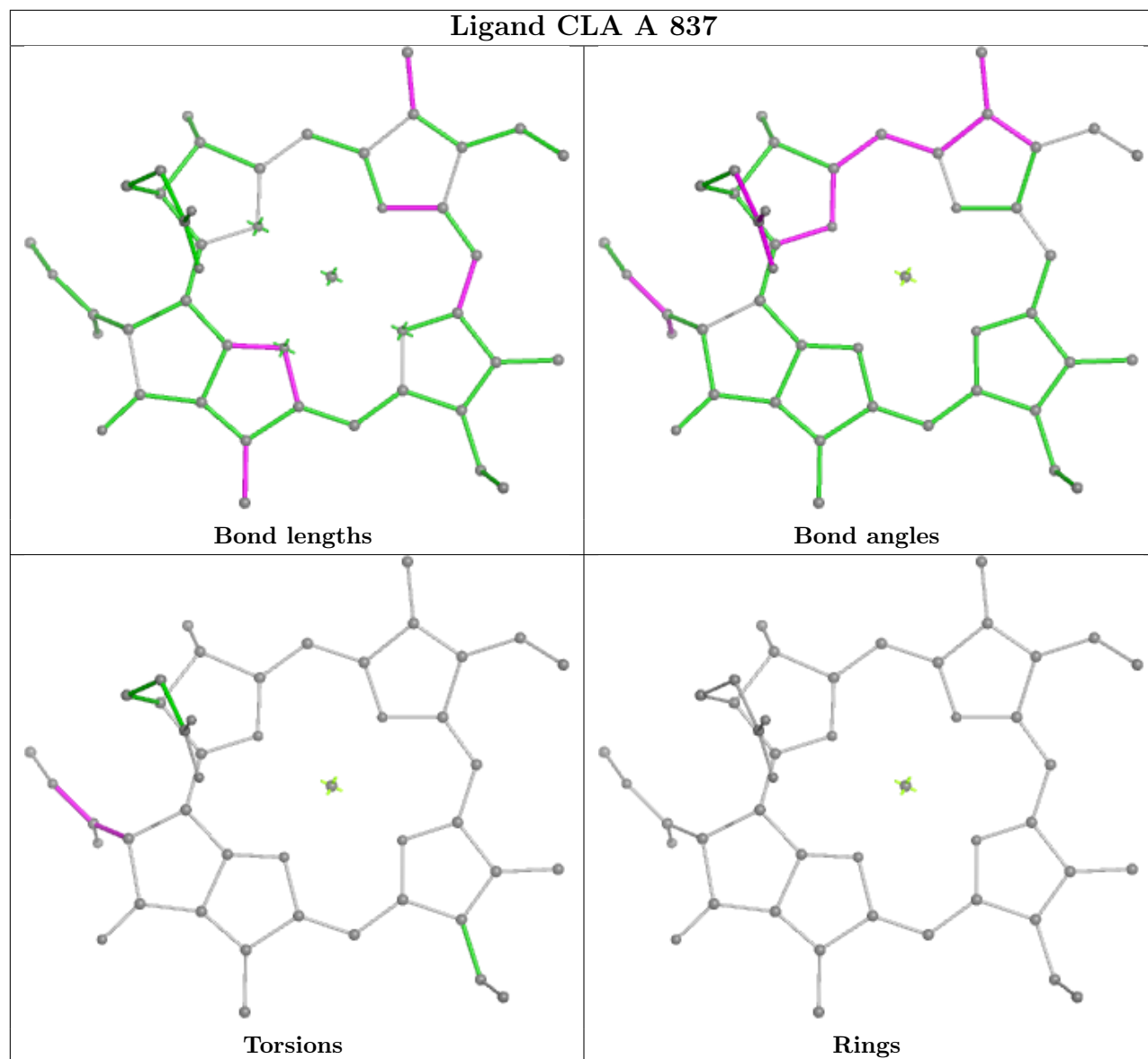
No monomer is involved in short contacts.

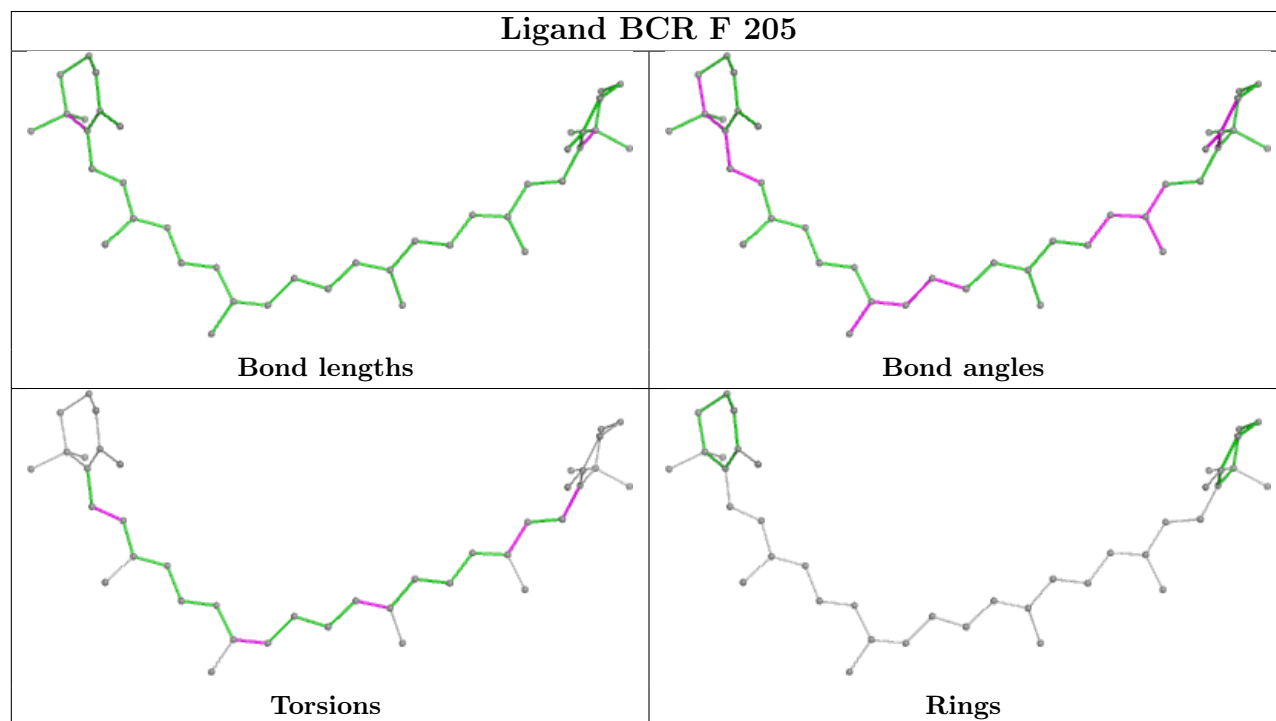
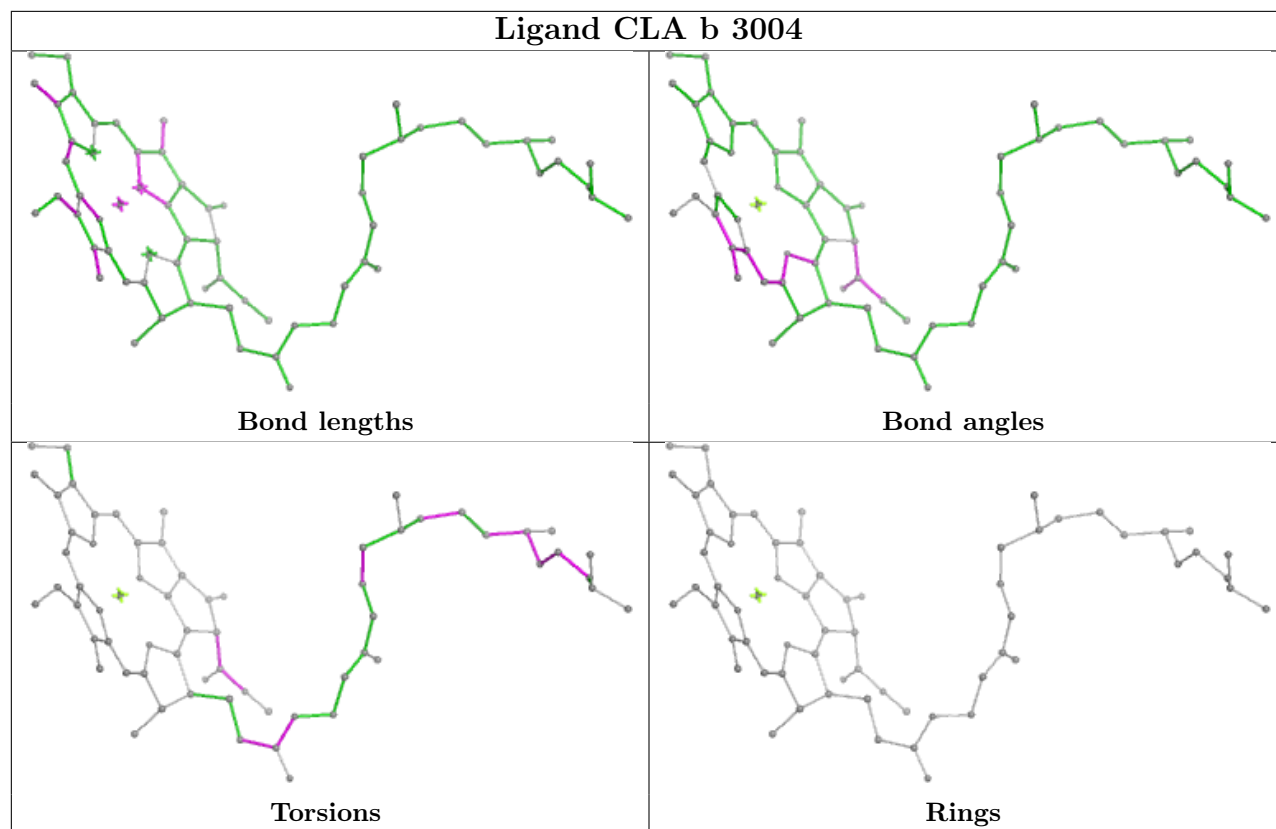
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

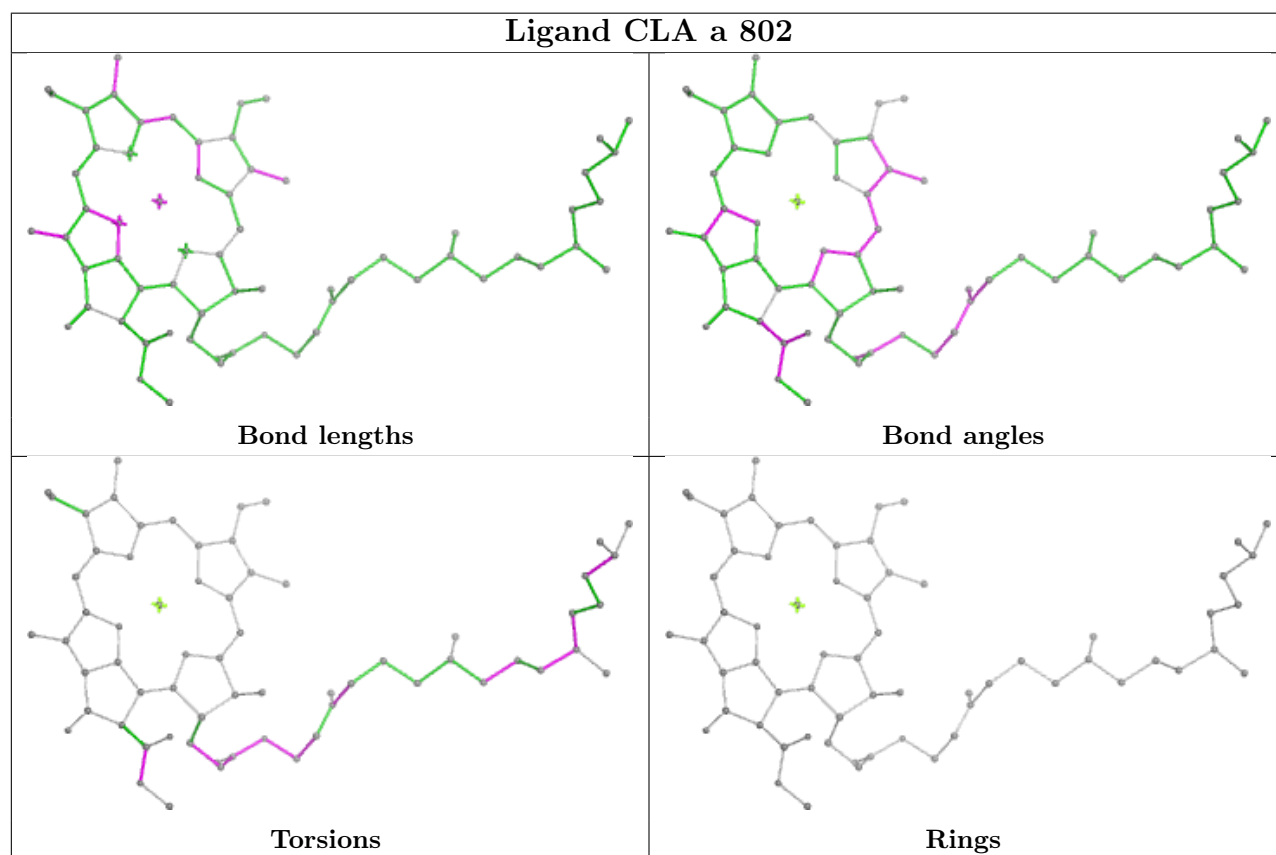
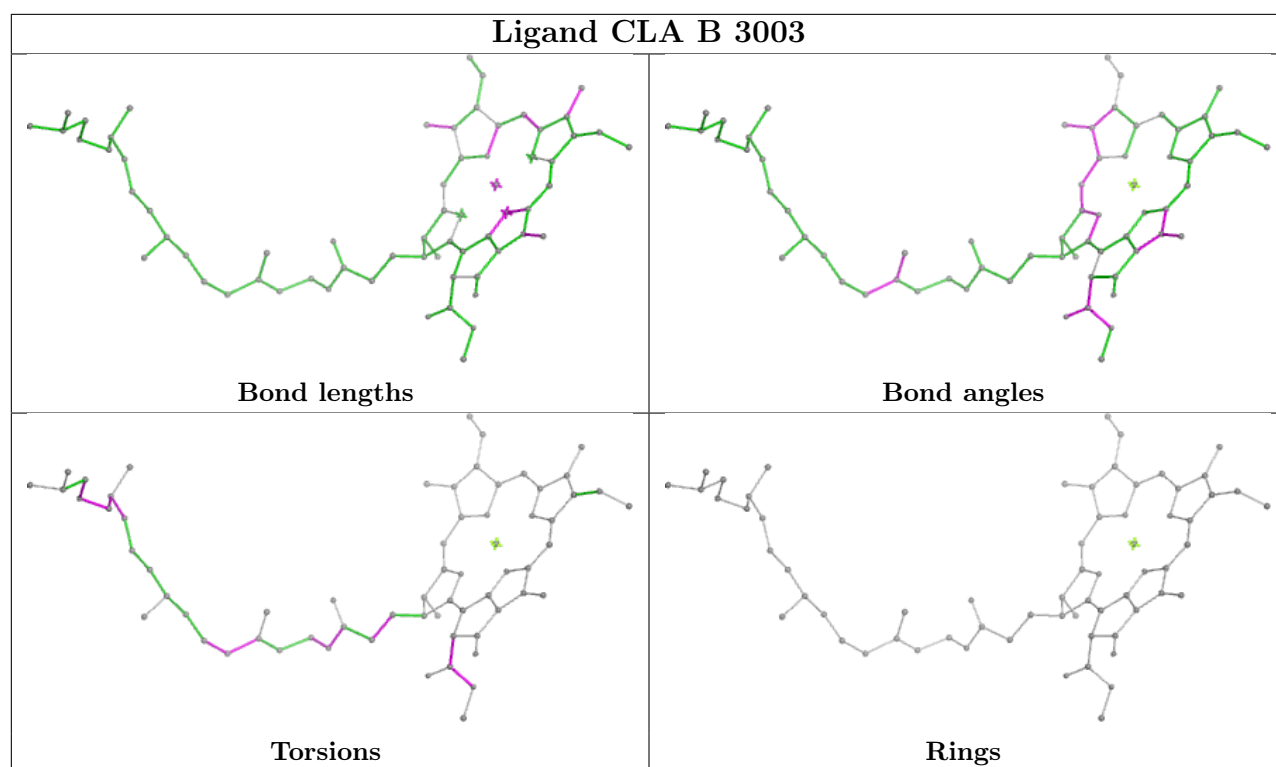


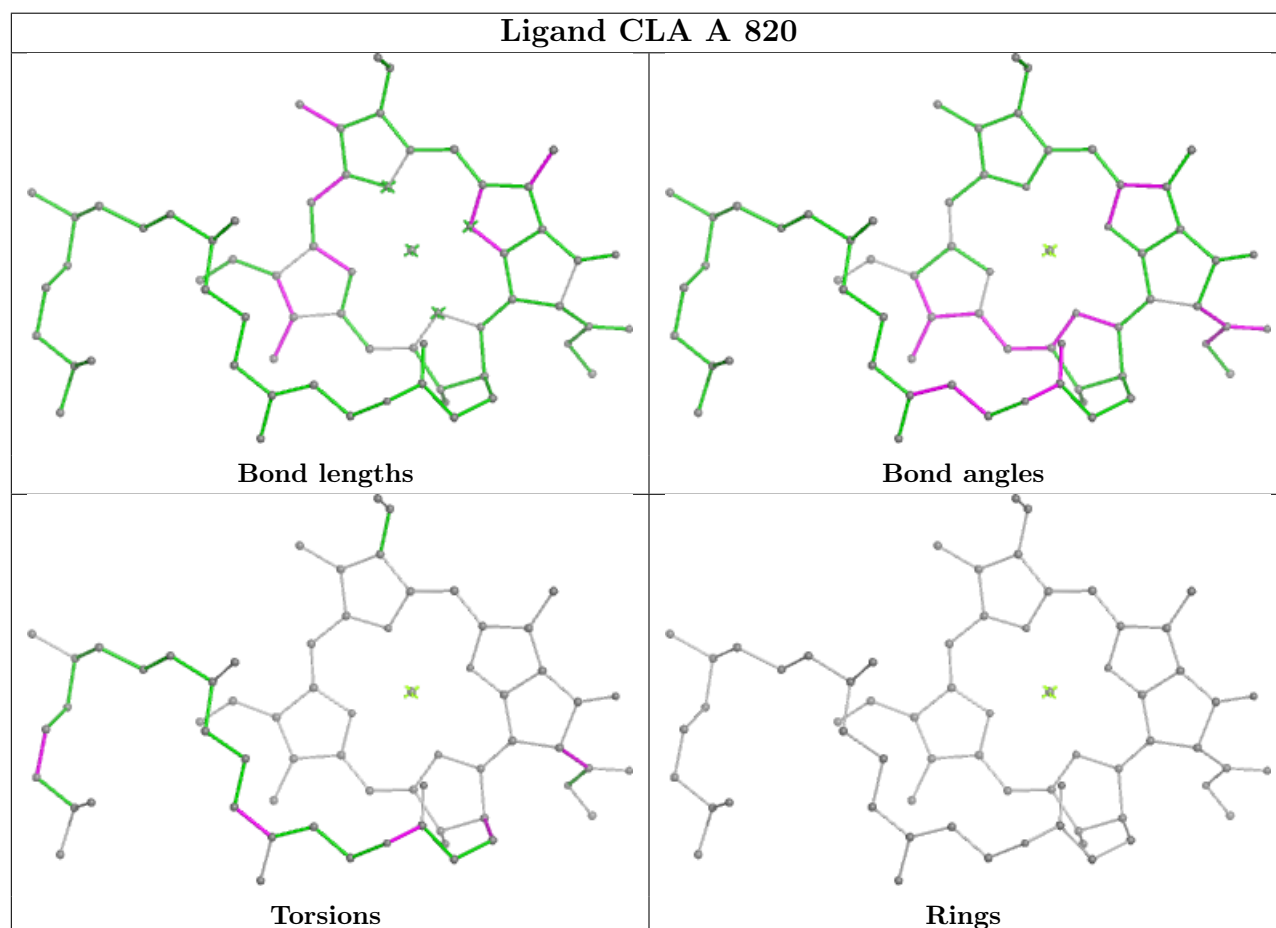
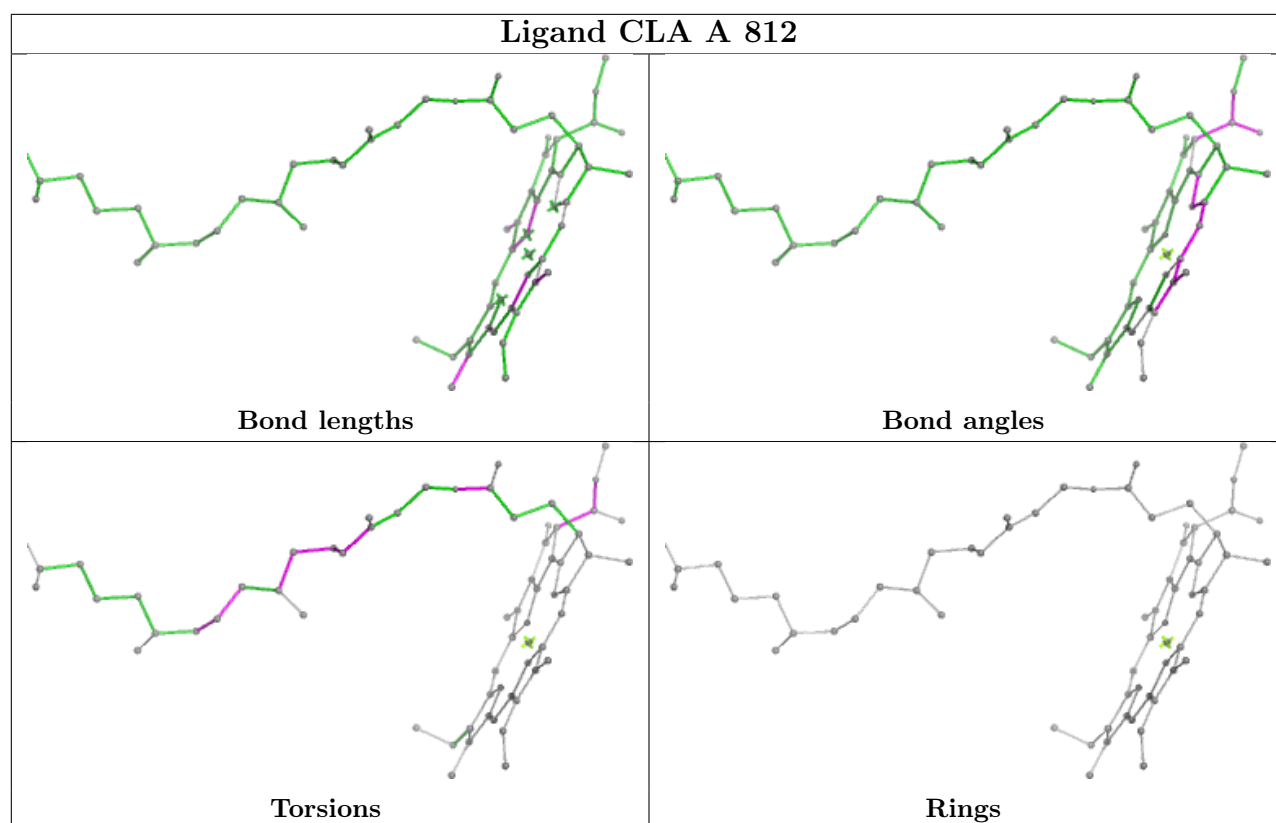
Ligand CLA A 817**Ligand BCR 1 209**

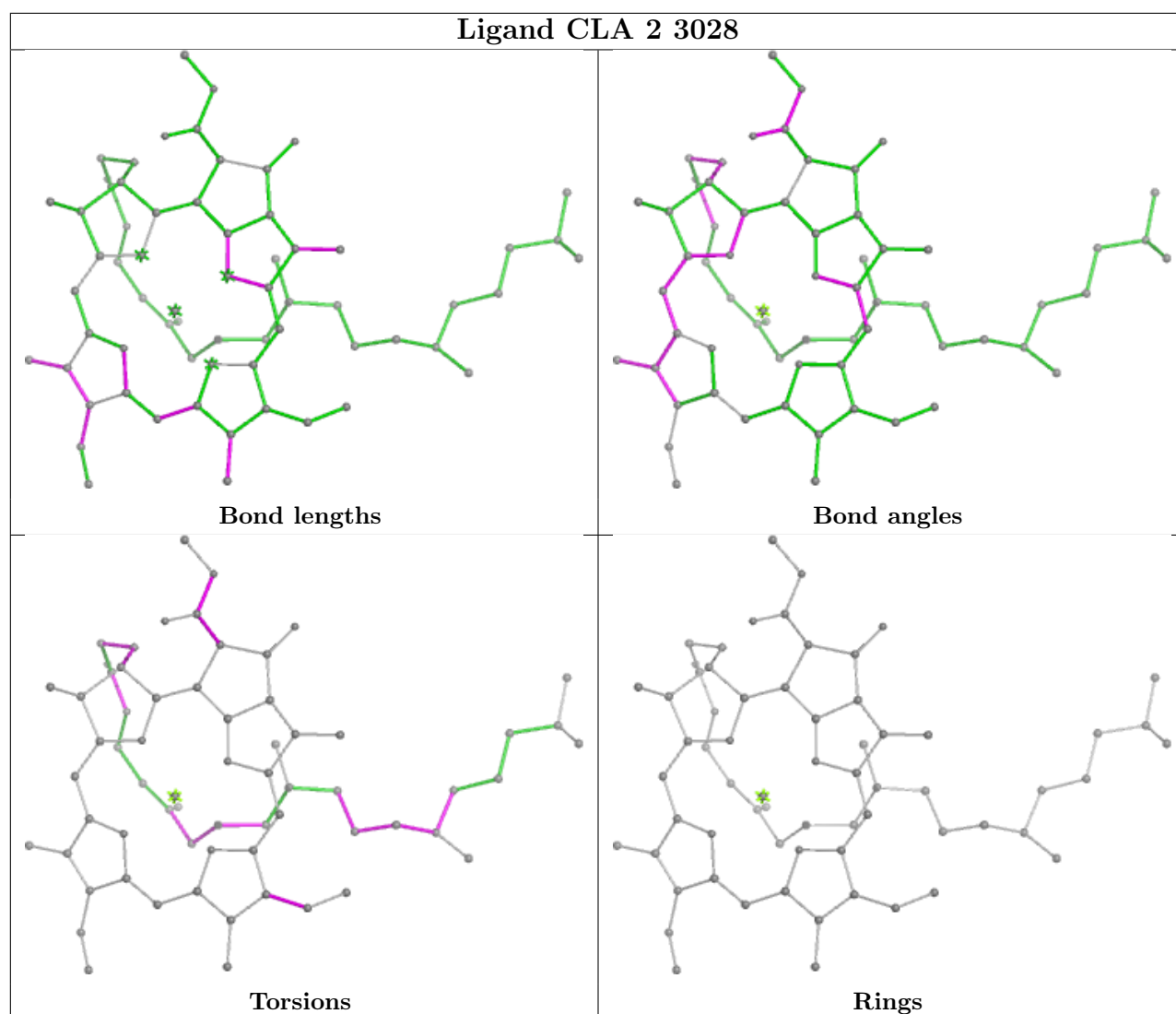
Ligand CLA A 837

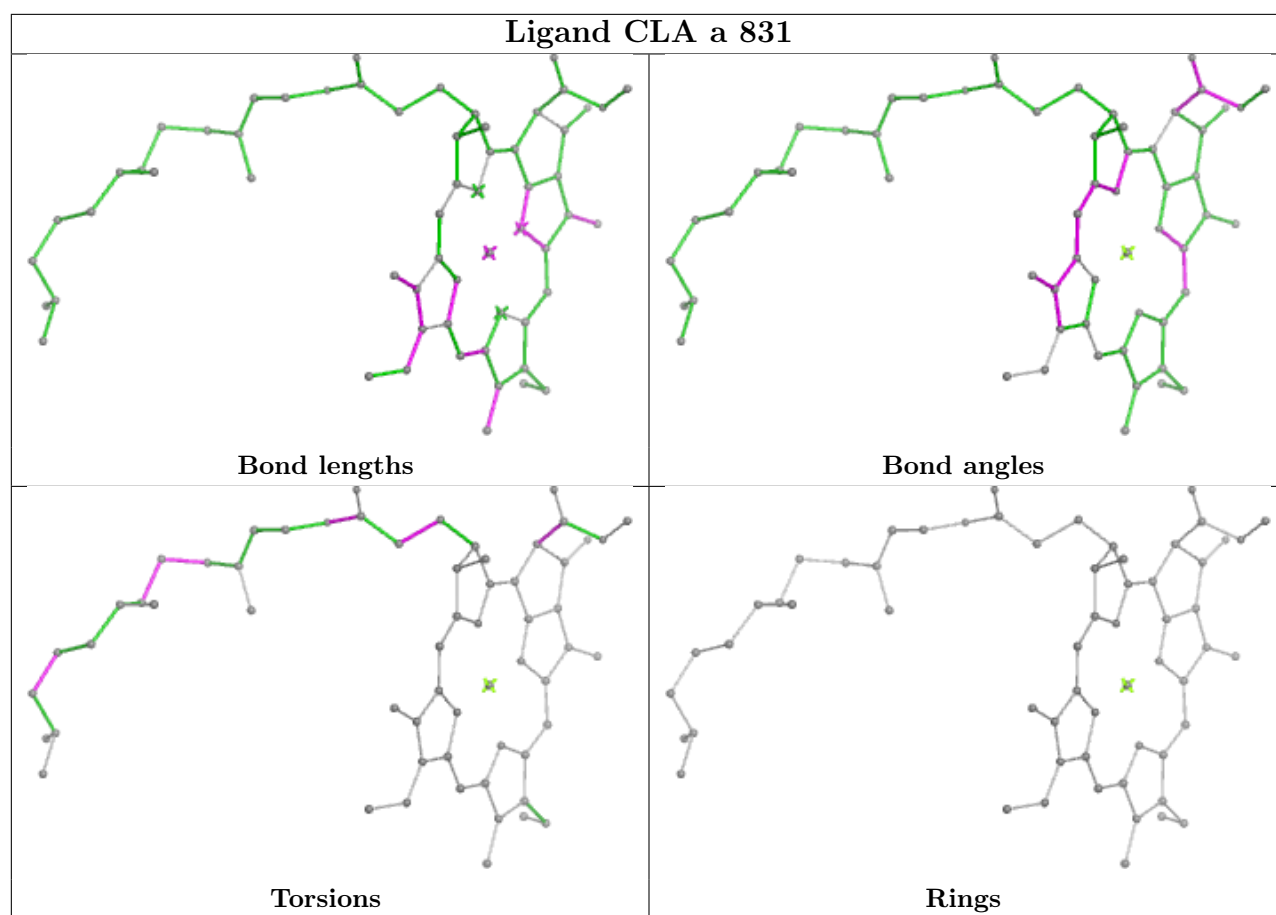


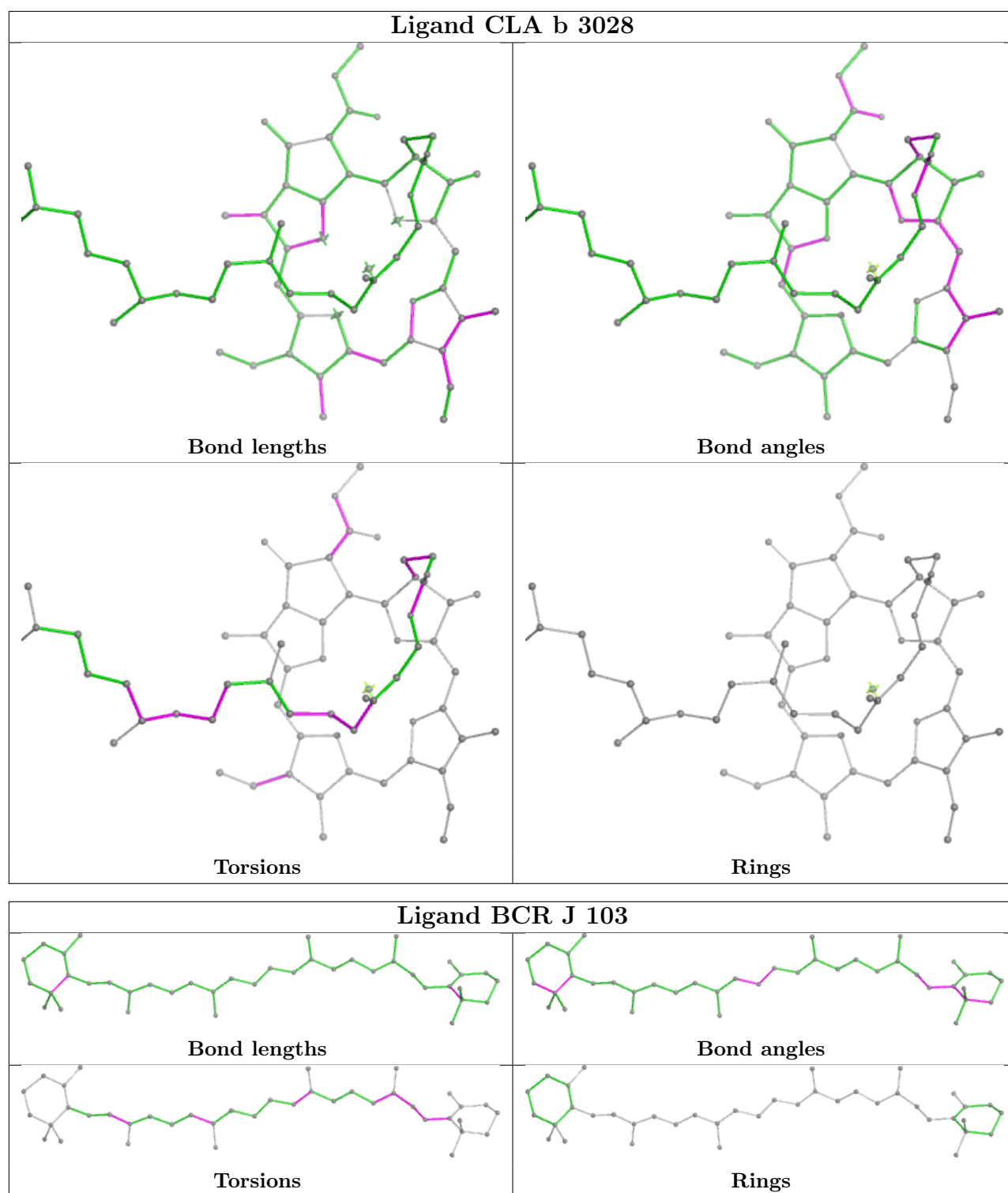


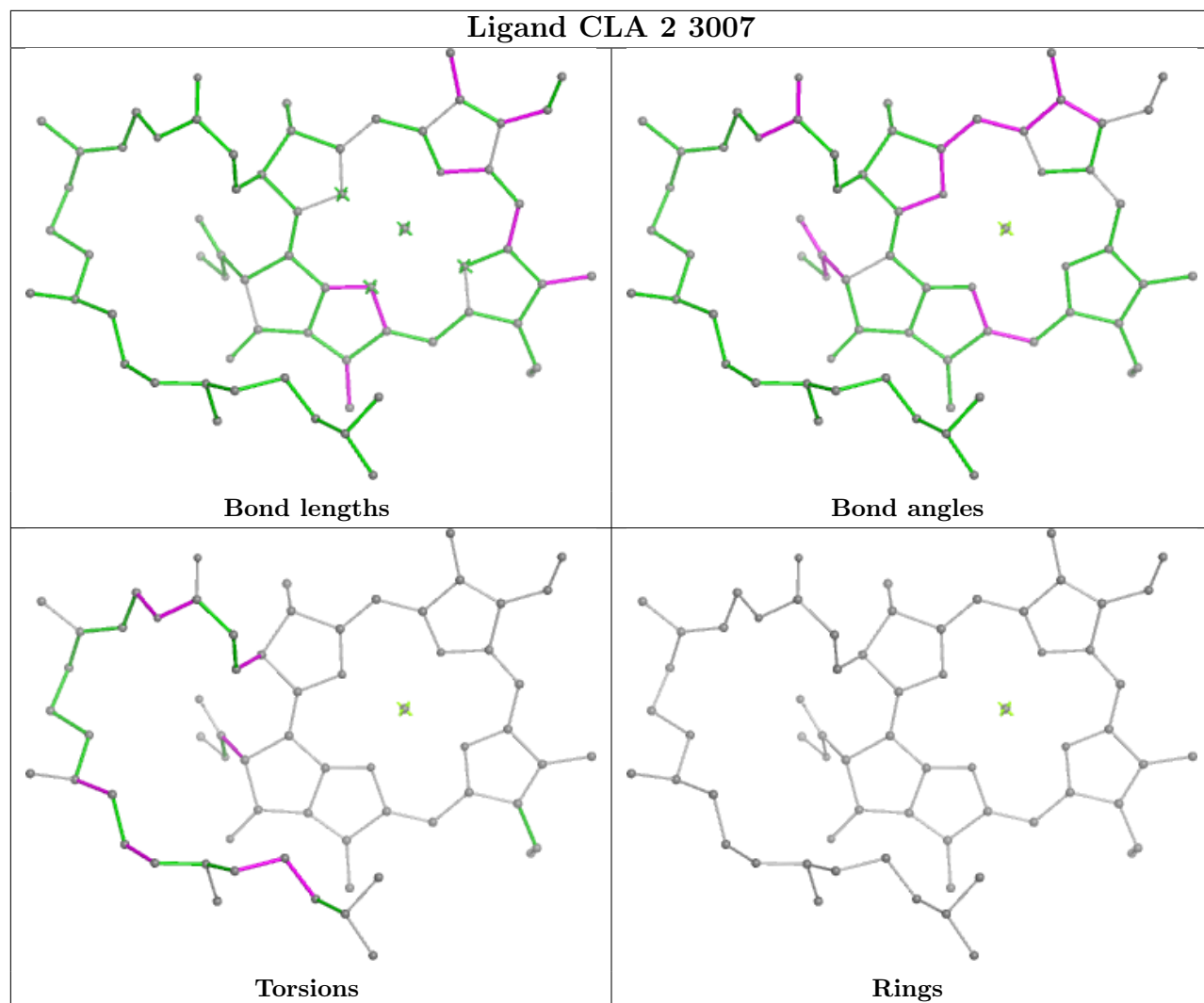




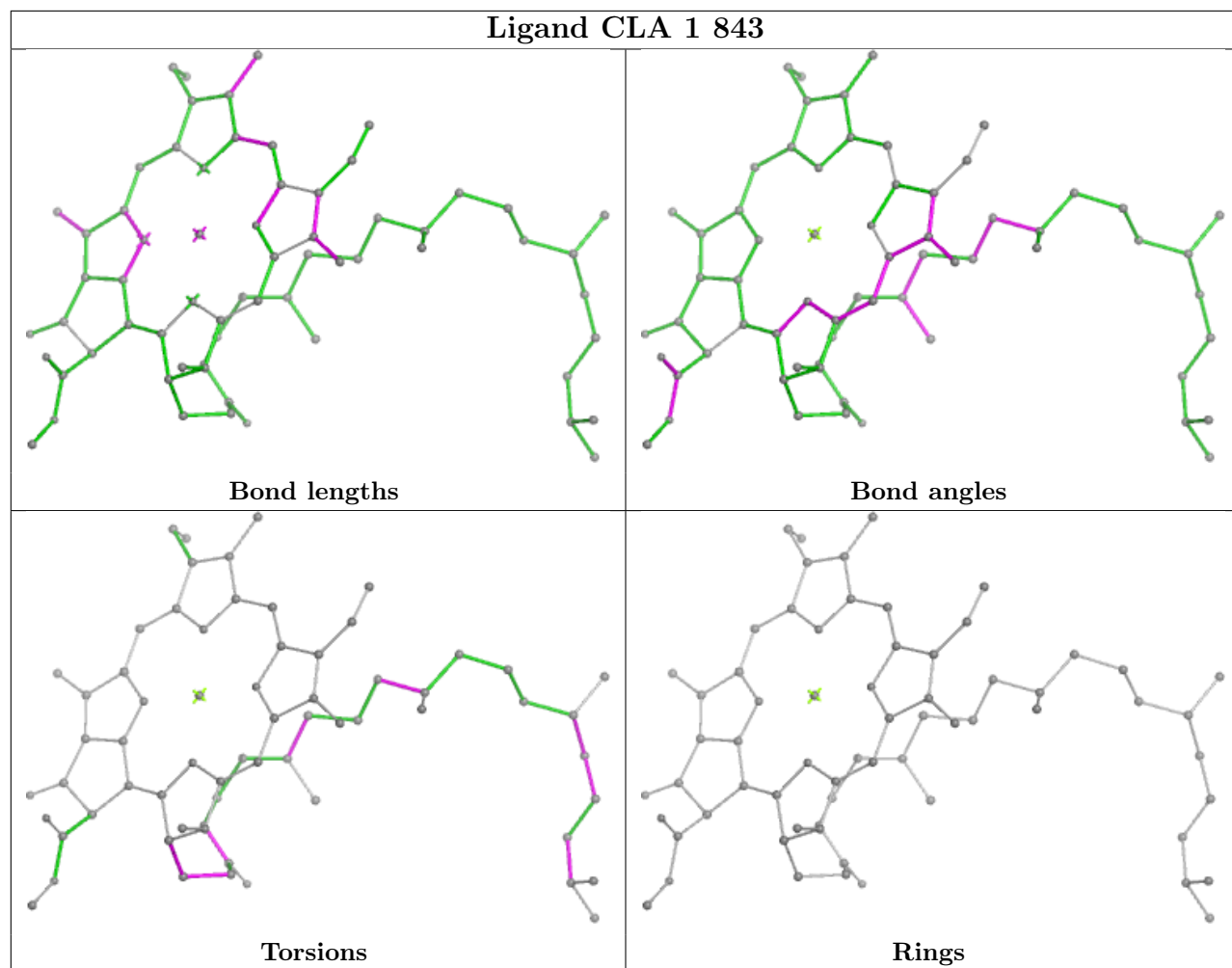




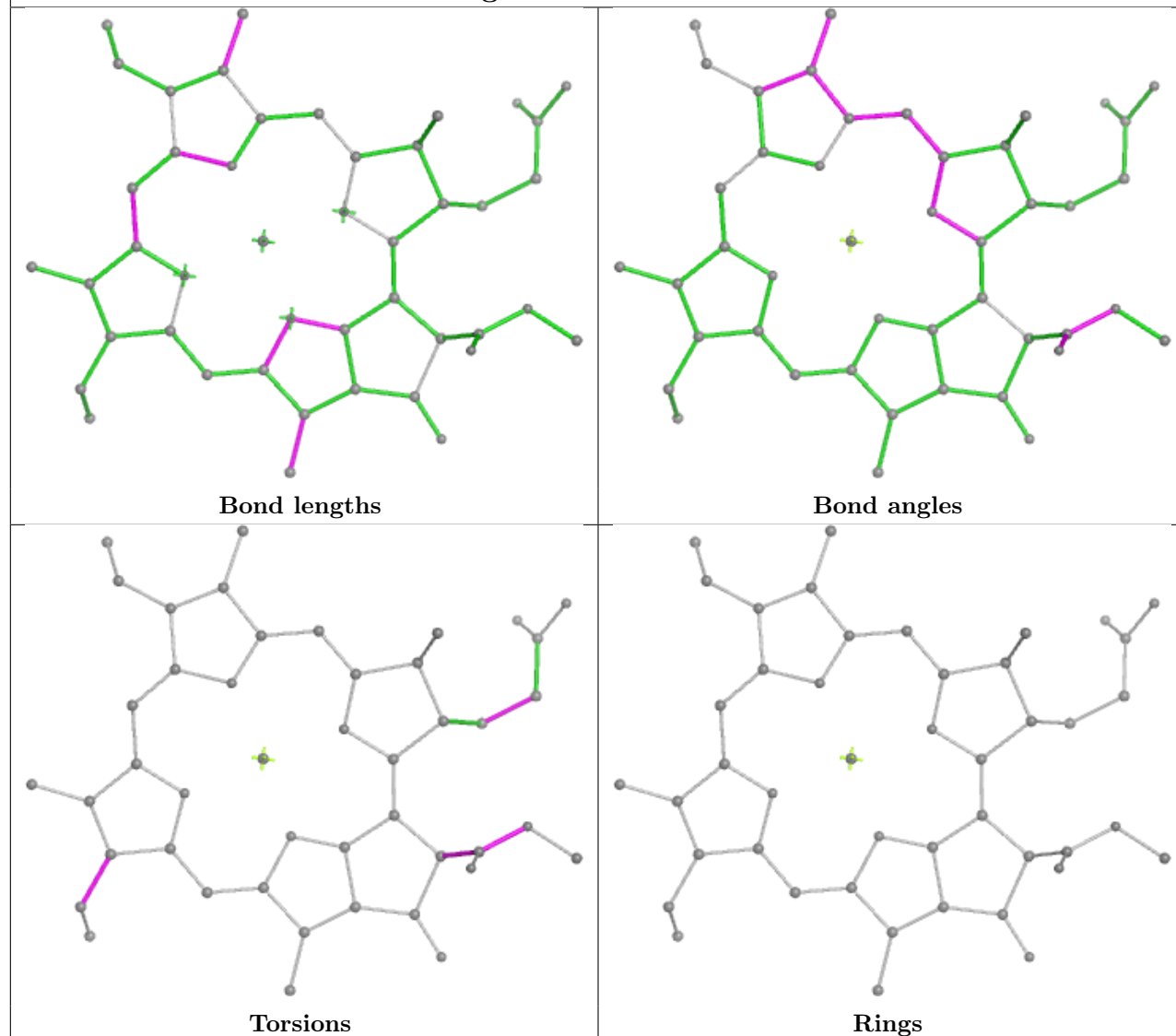




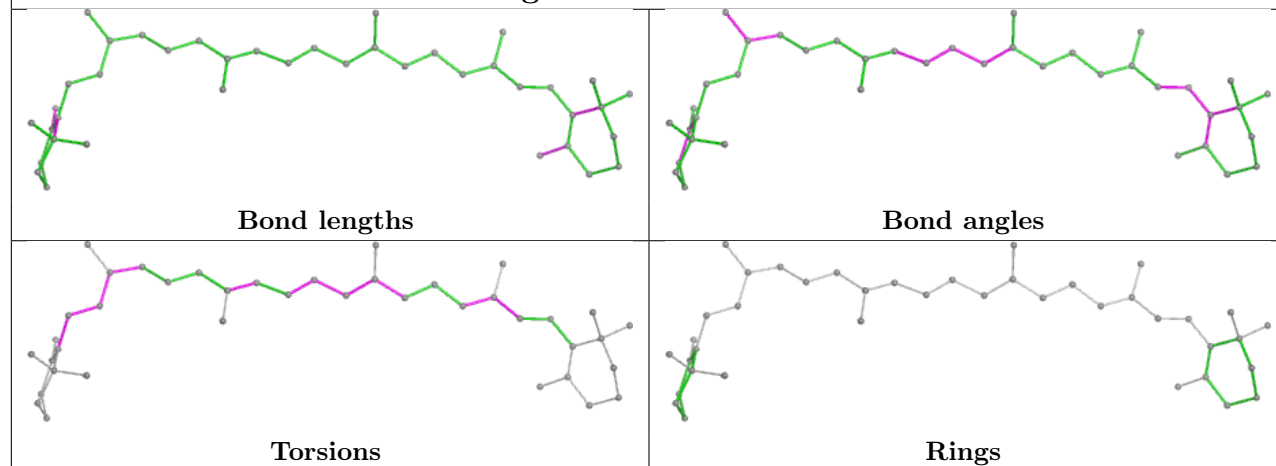
Ligand CLA 1 843



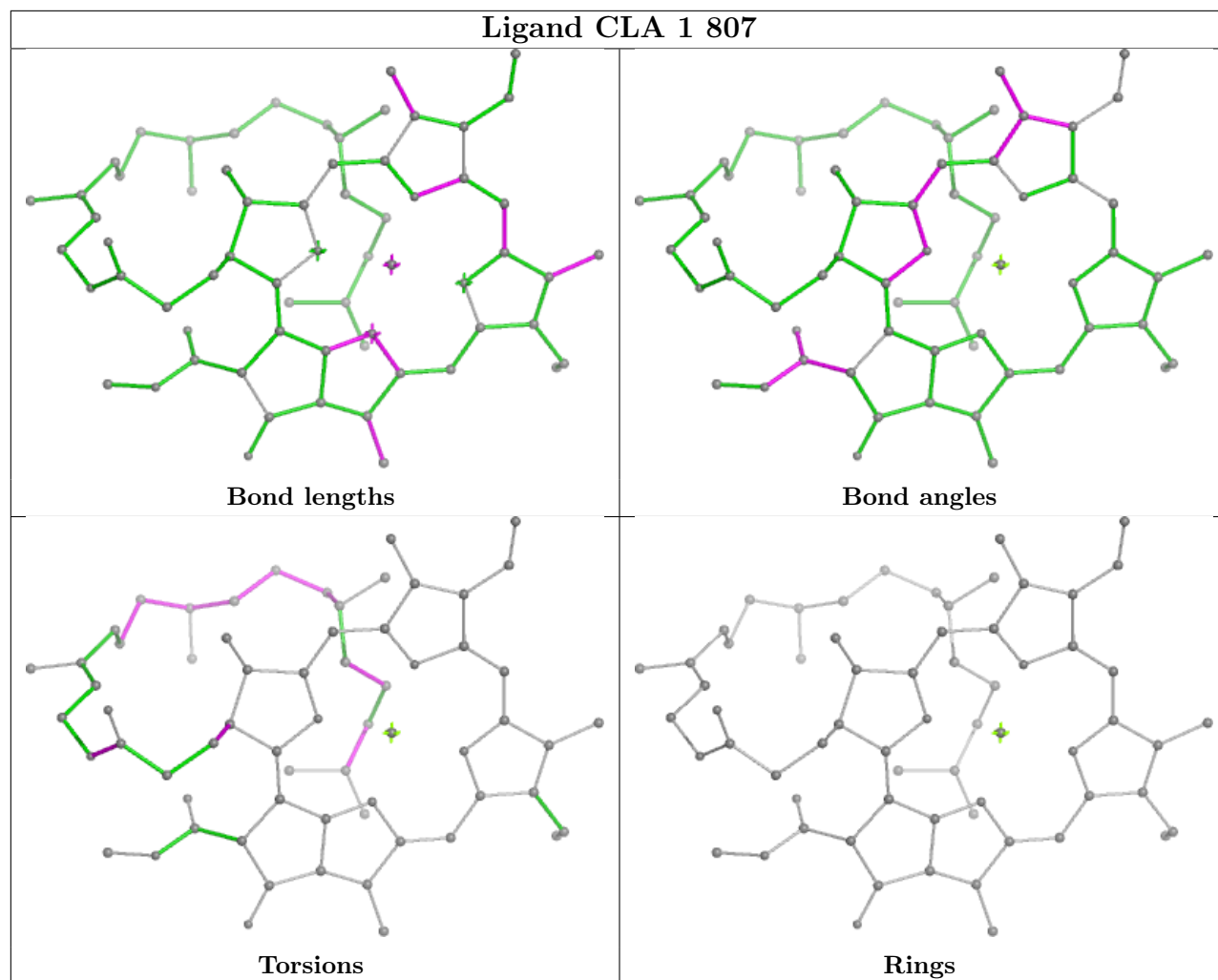
Ligand CLA X 1701



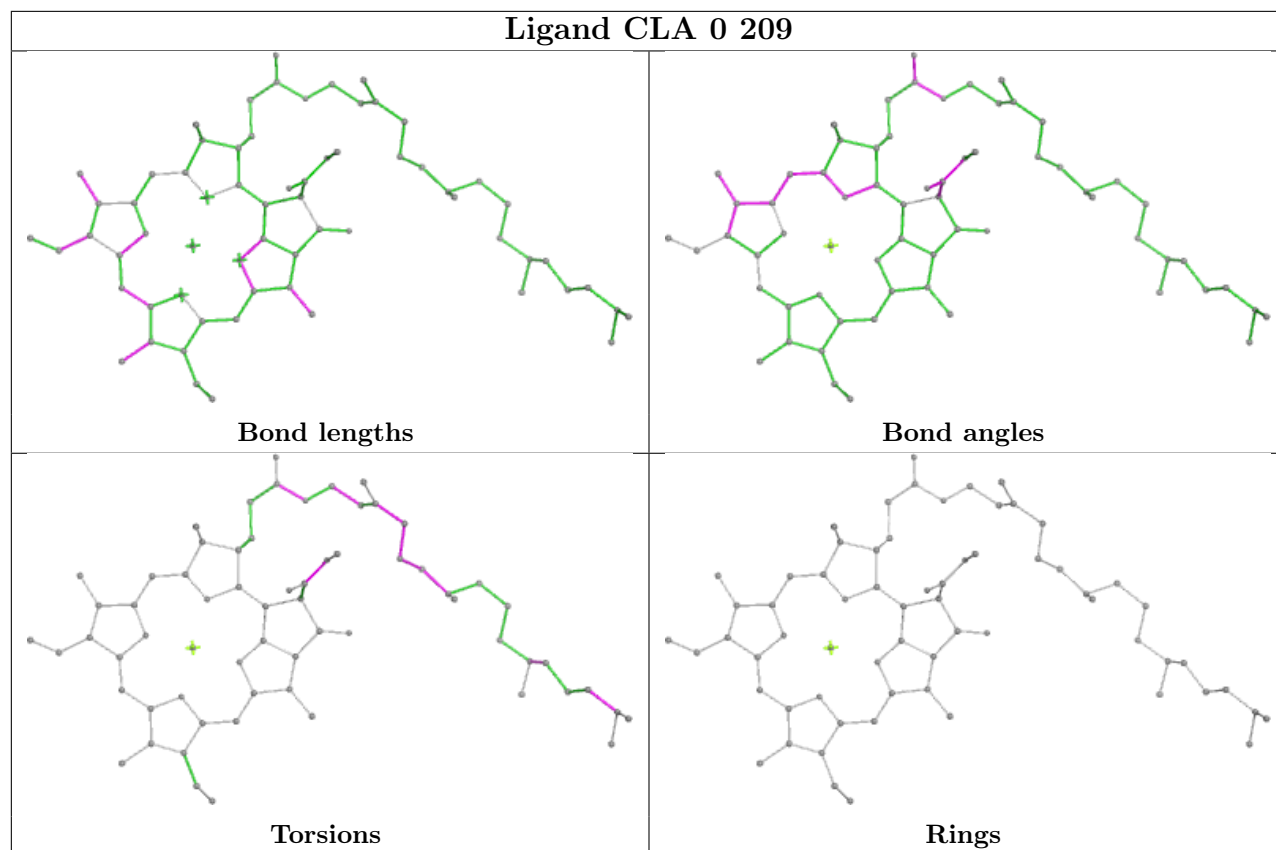
Ligand BCR B 3052



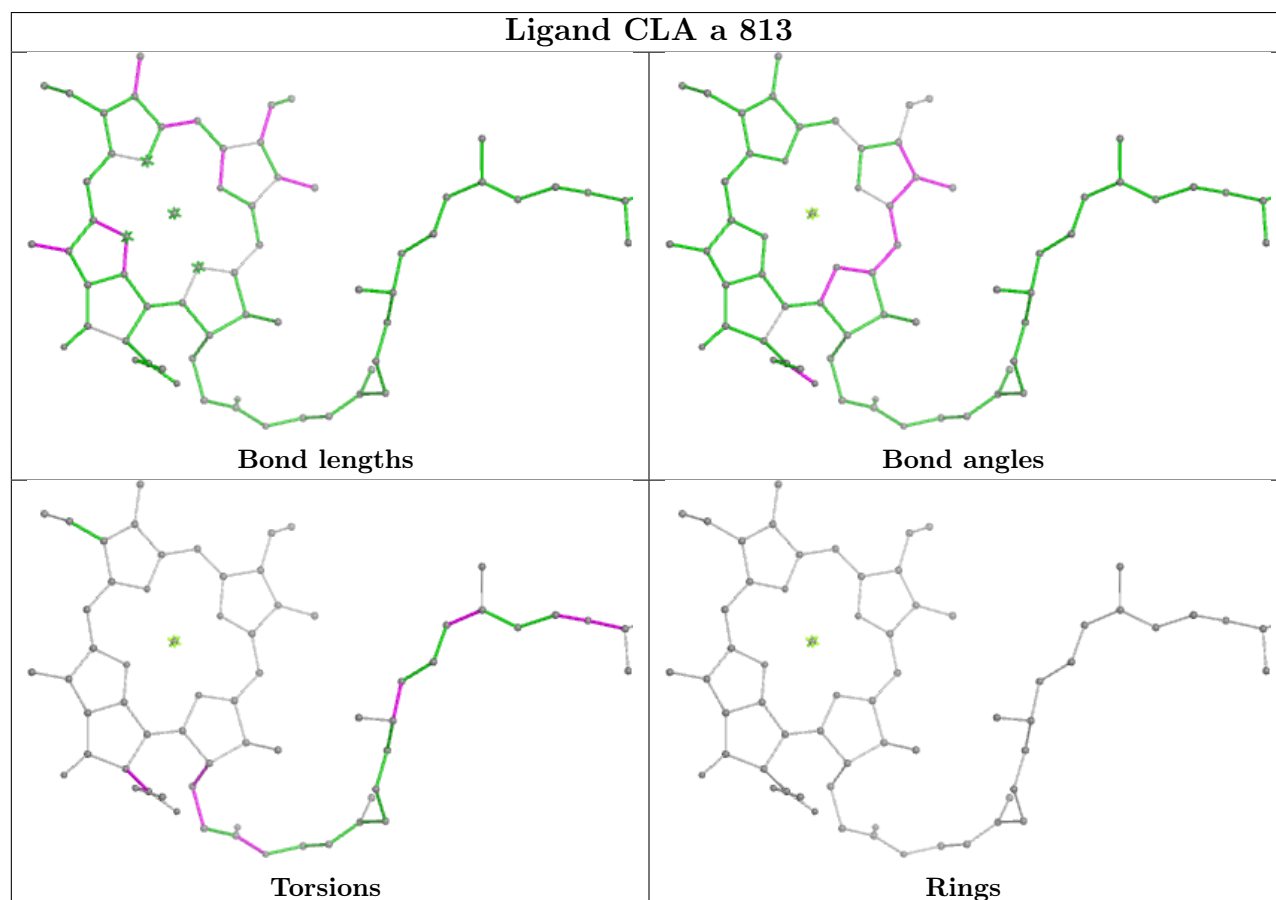
Ligand CLA 1 807

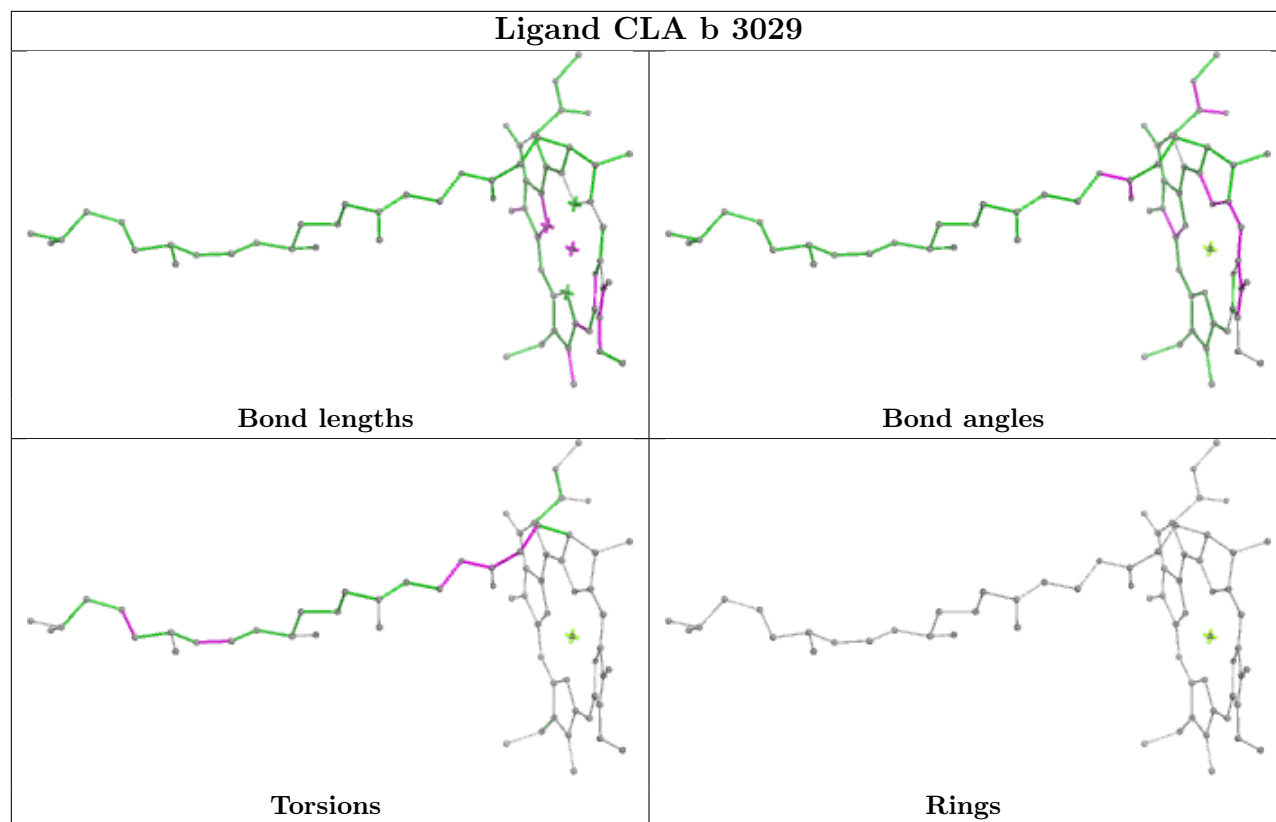


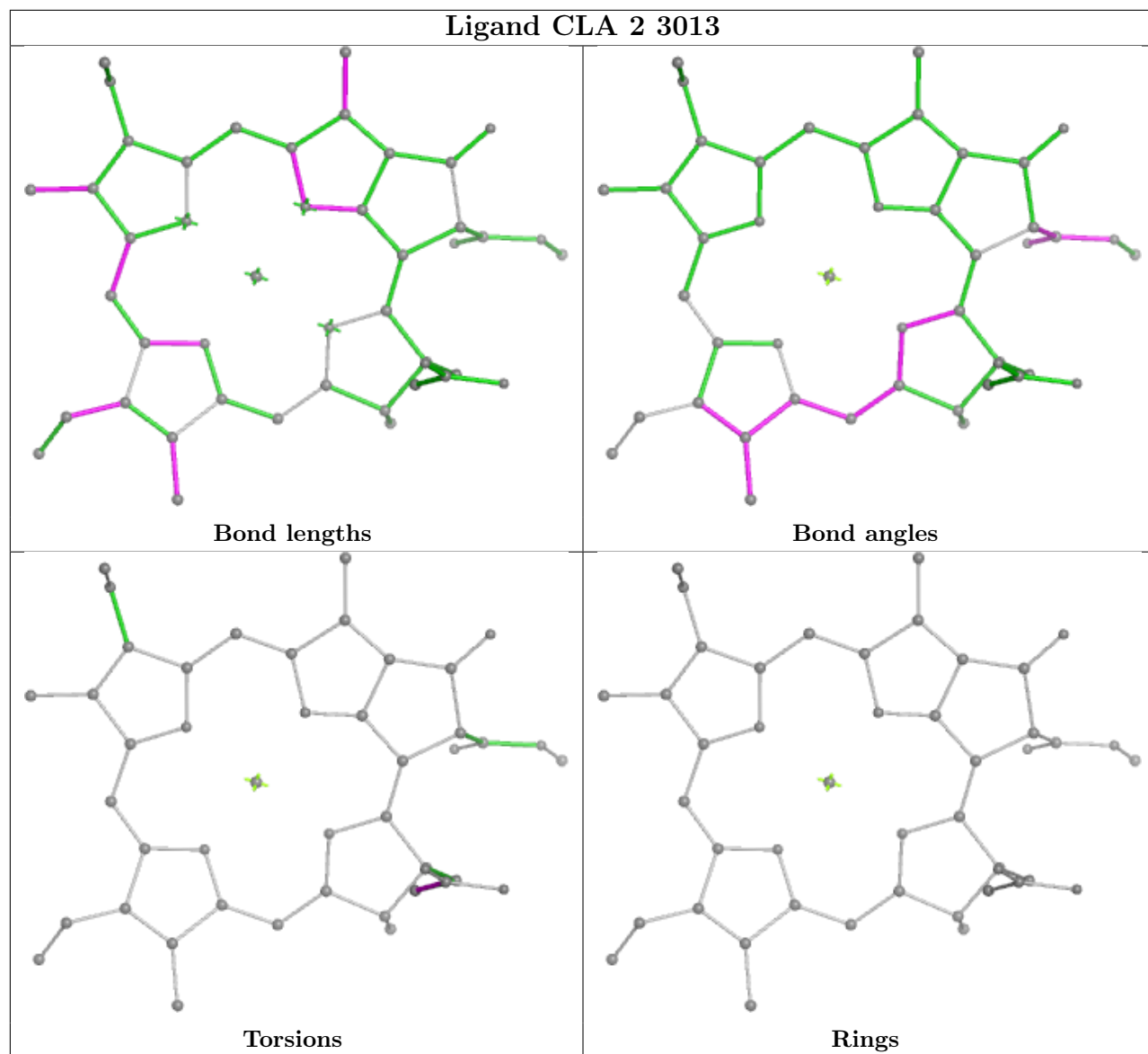
Ligand CLA 0 209

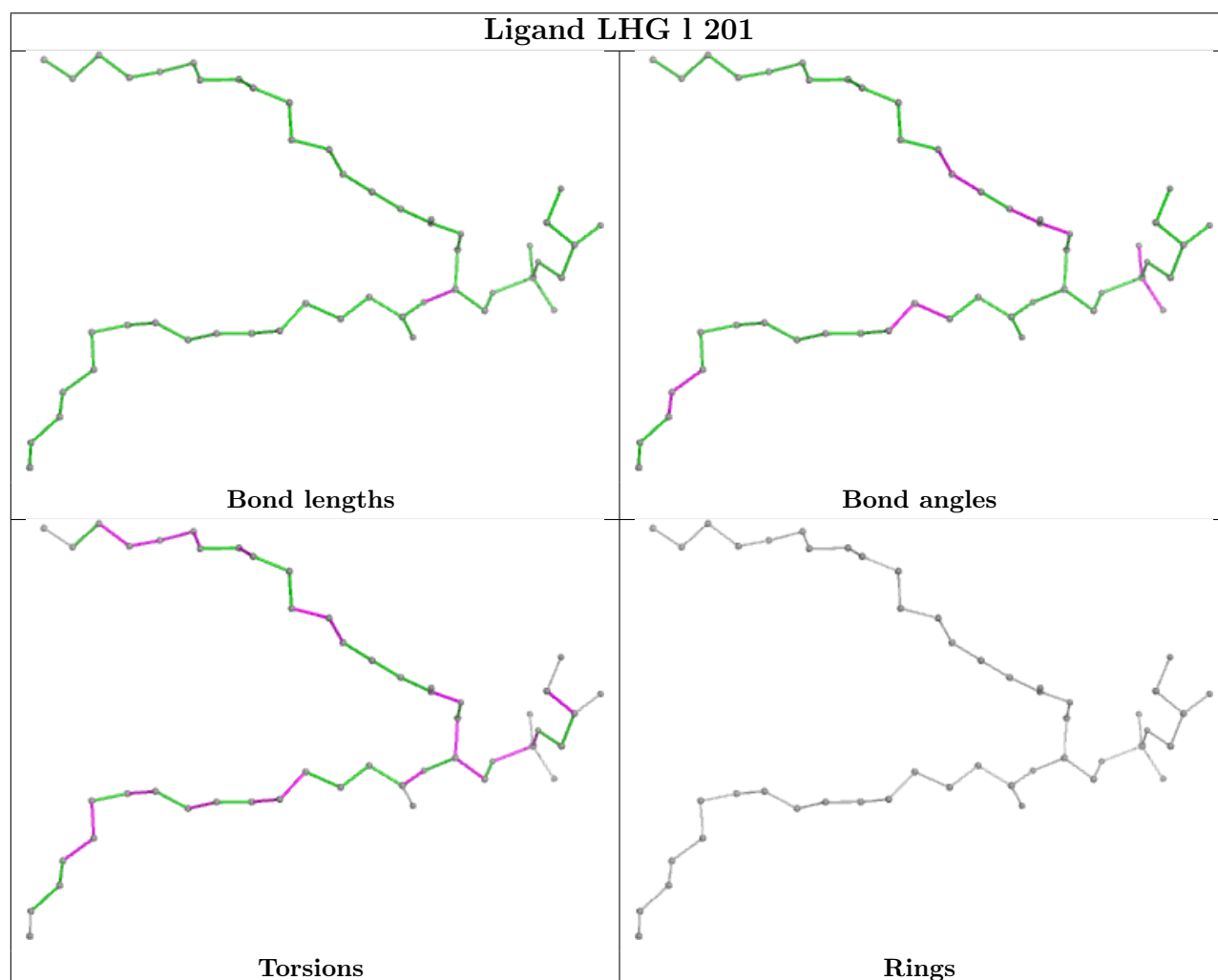
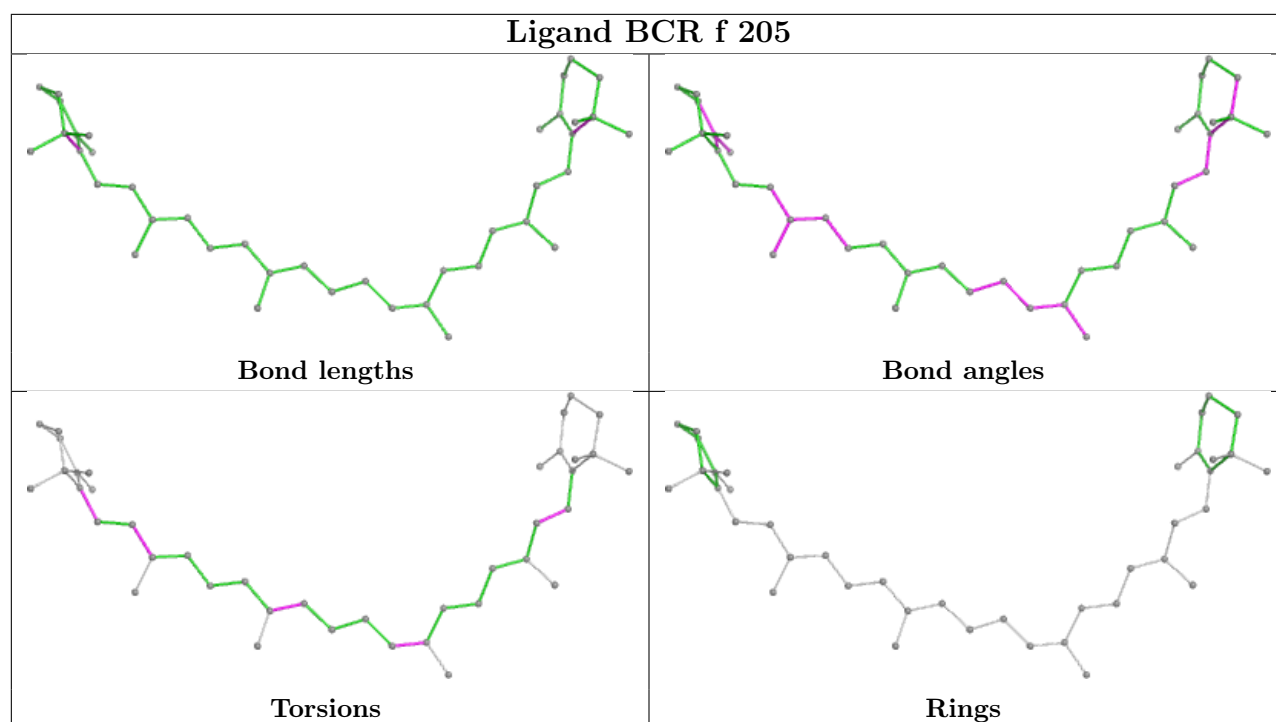


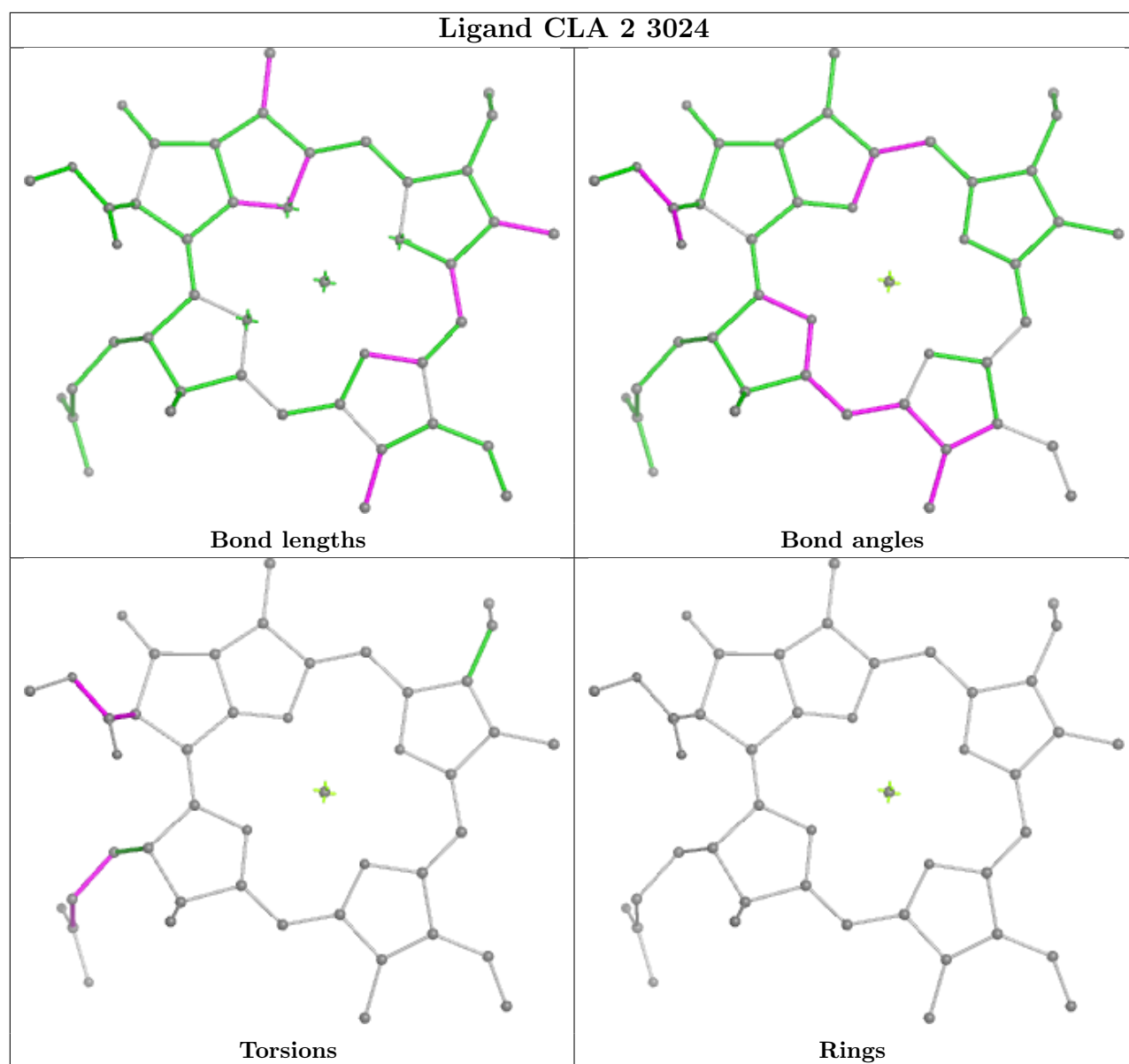
Ligand CLA a 813

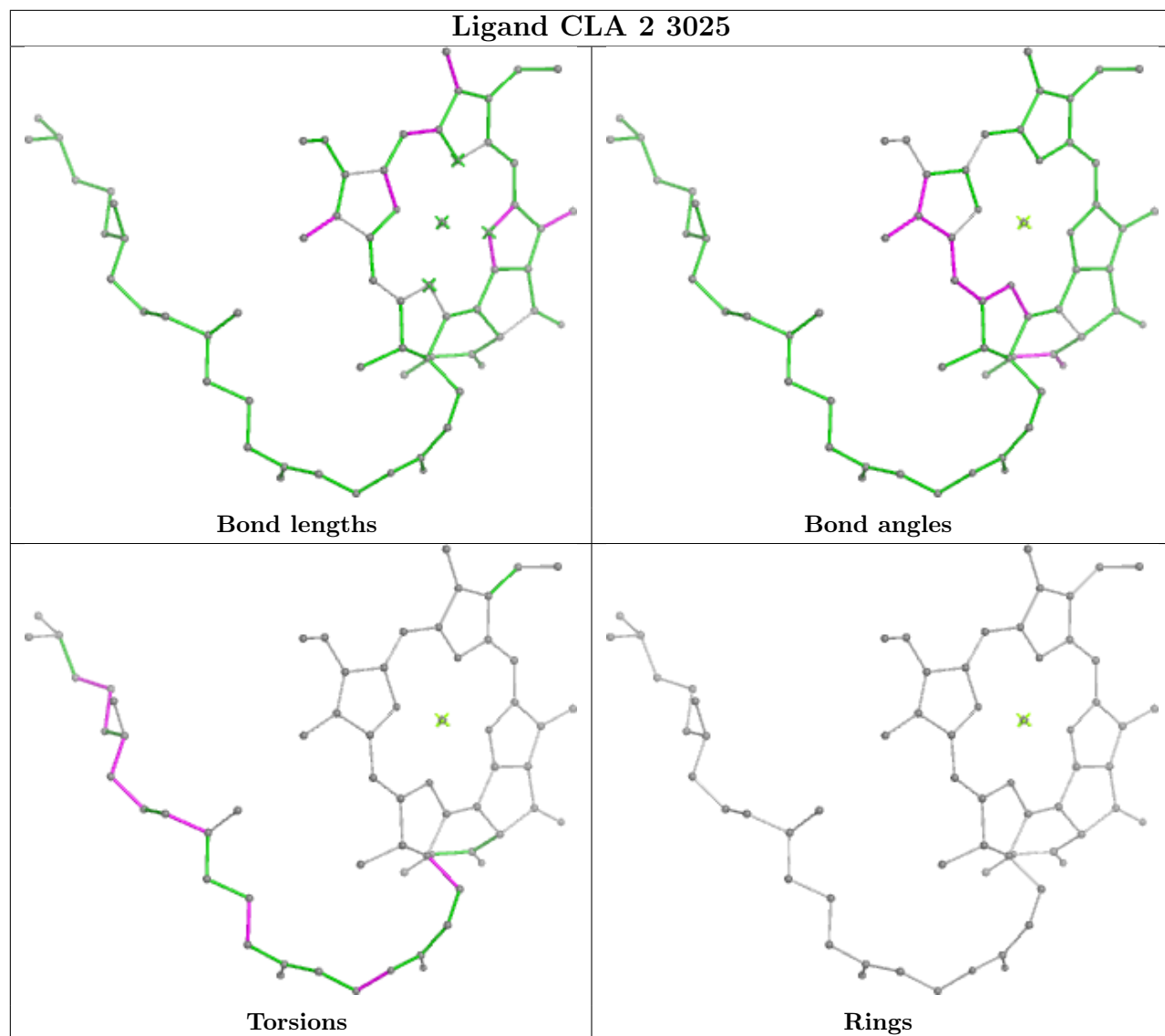




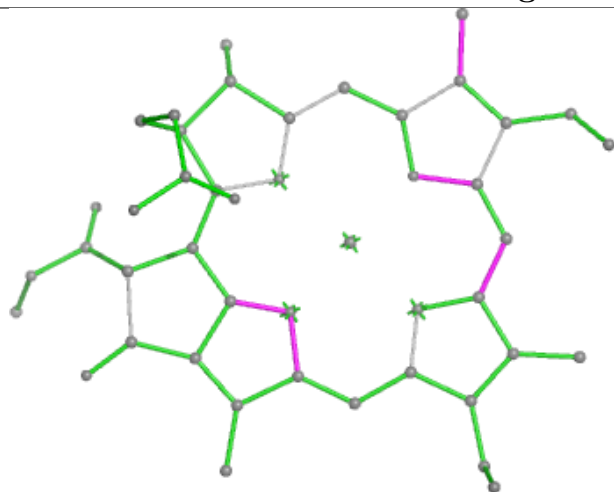




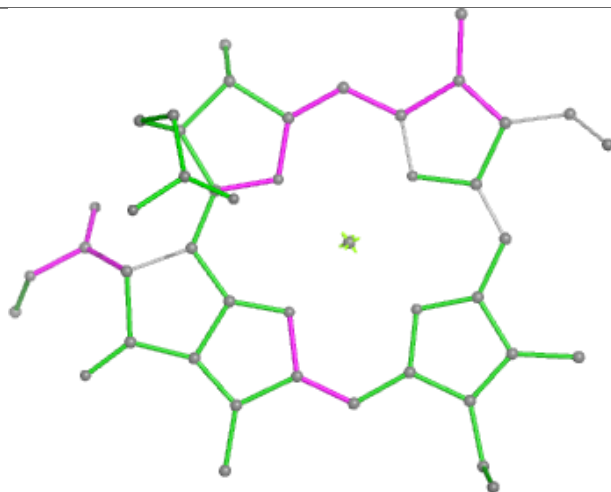




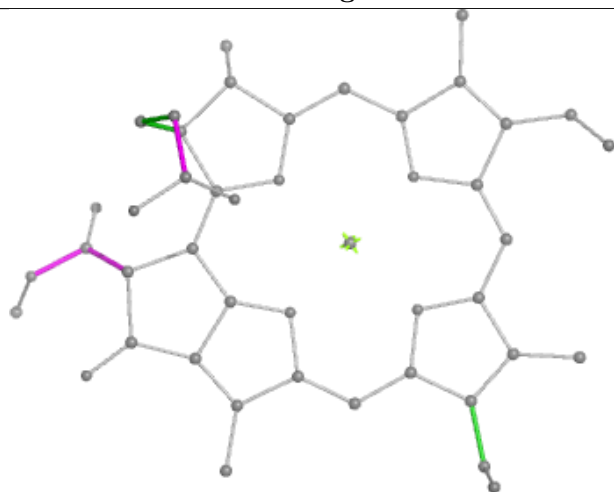
Ligand CLA 8 101



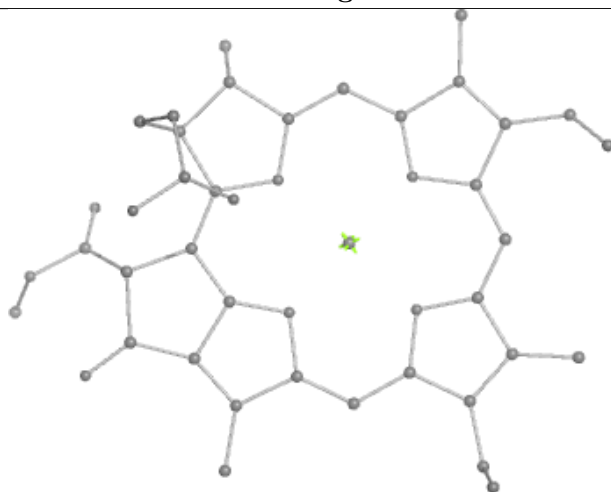
Bond lengths



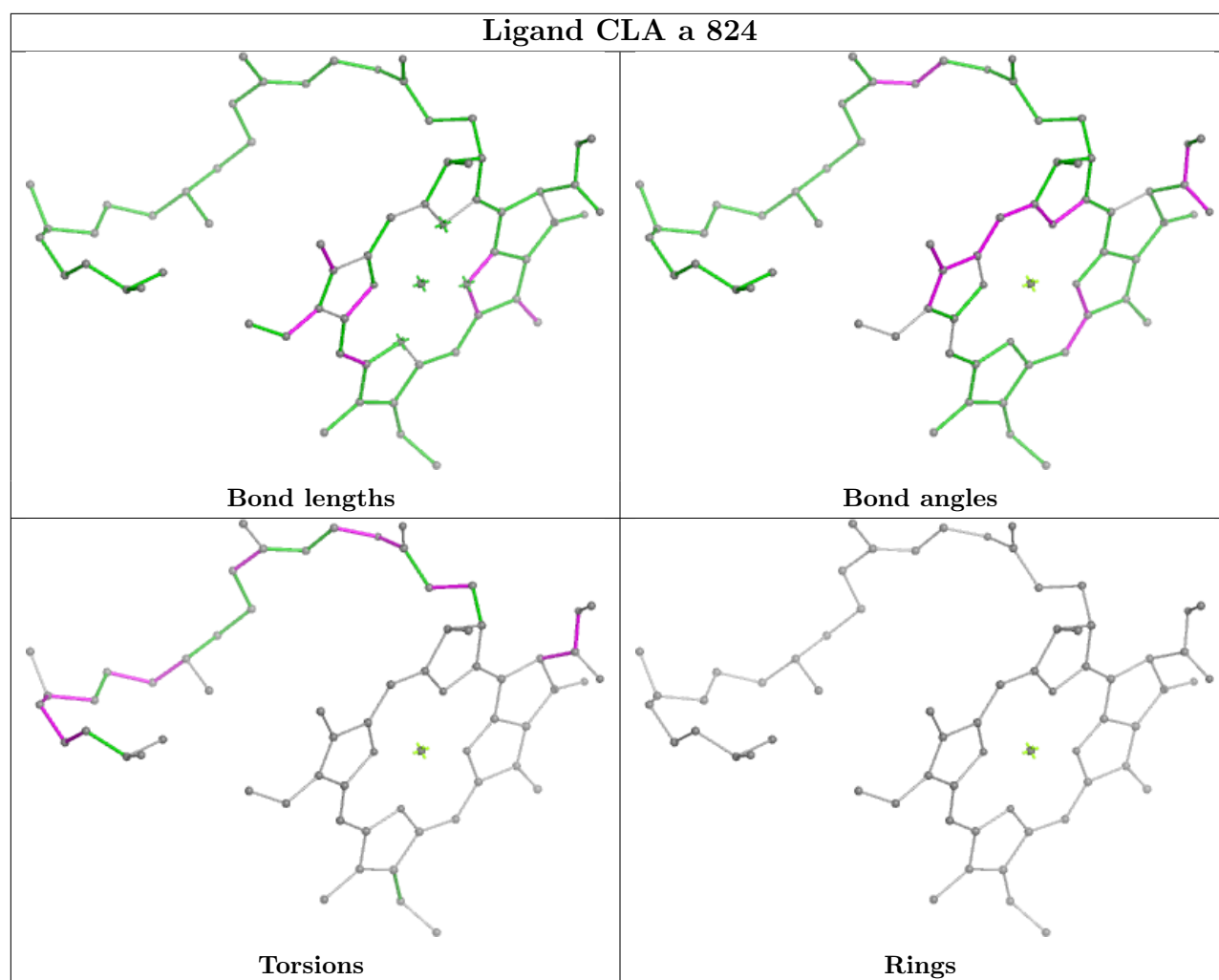
Bond angles



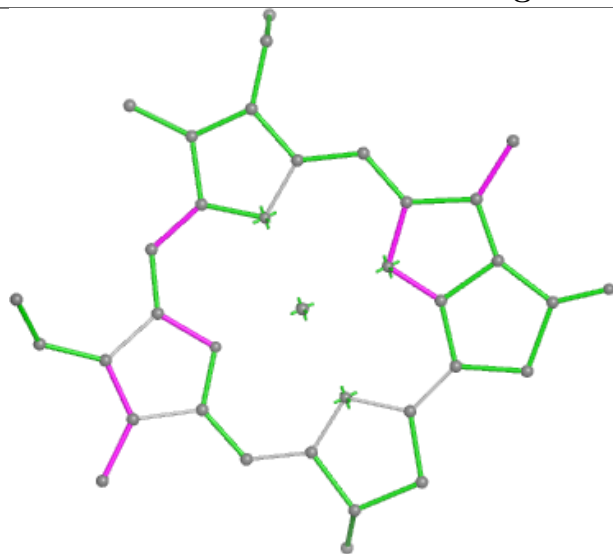
Torsions



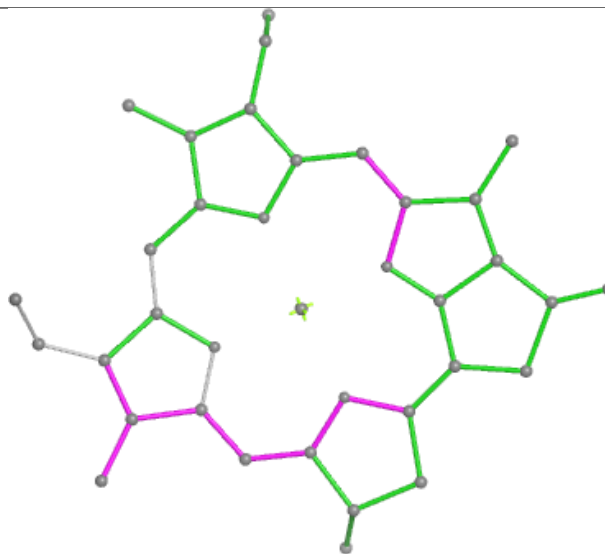
Rings



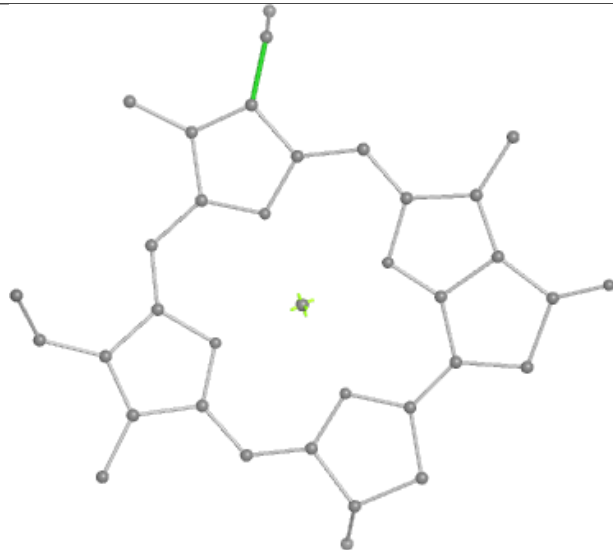
Ligand CLA A 855



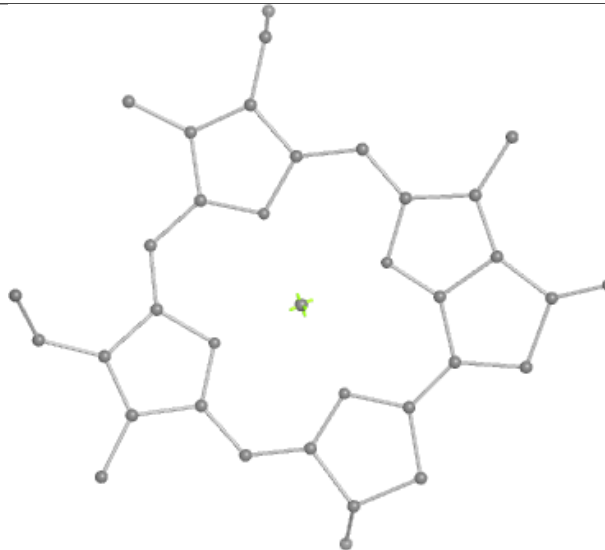
Bond lengths



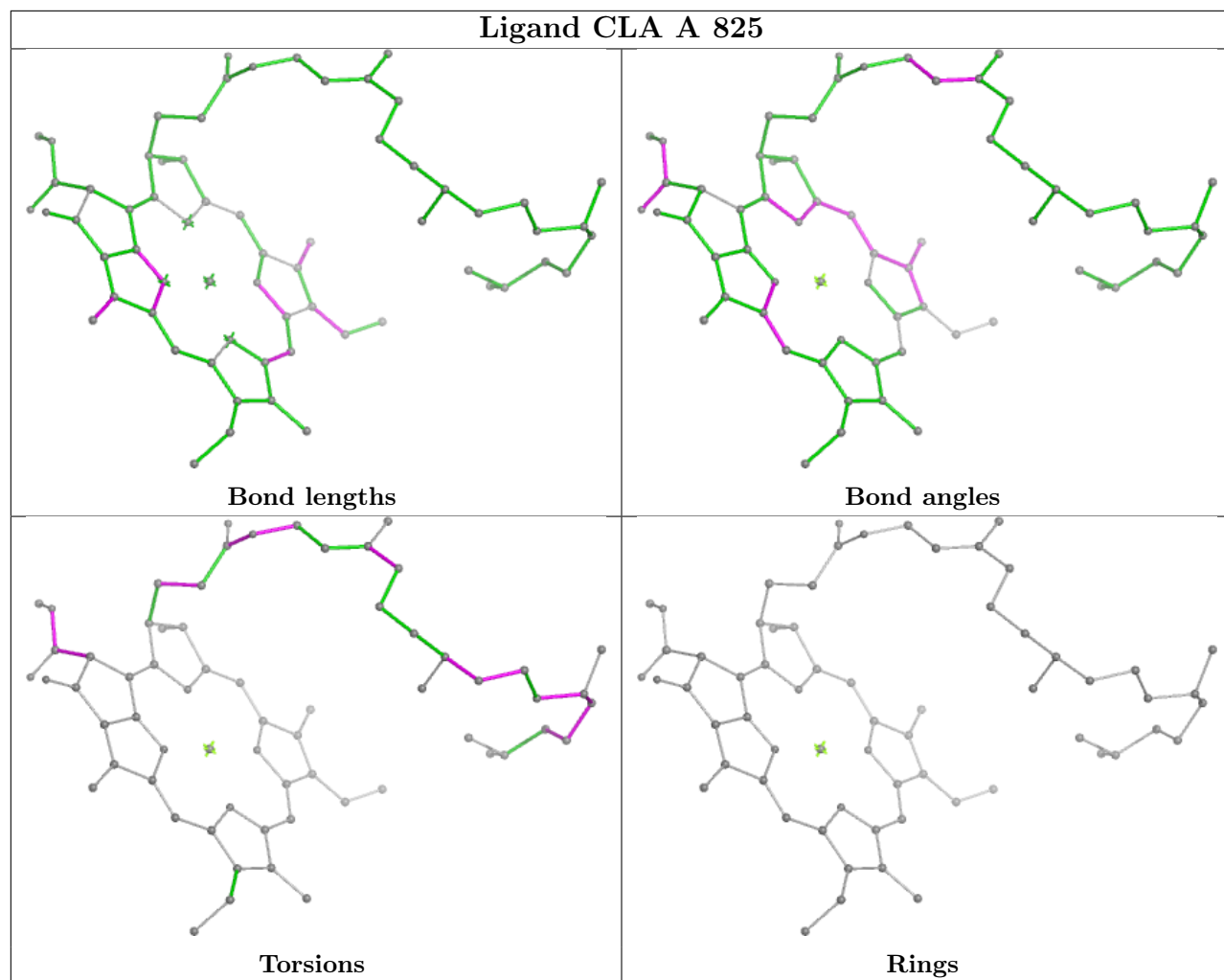
Bond angles



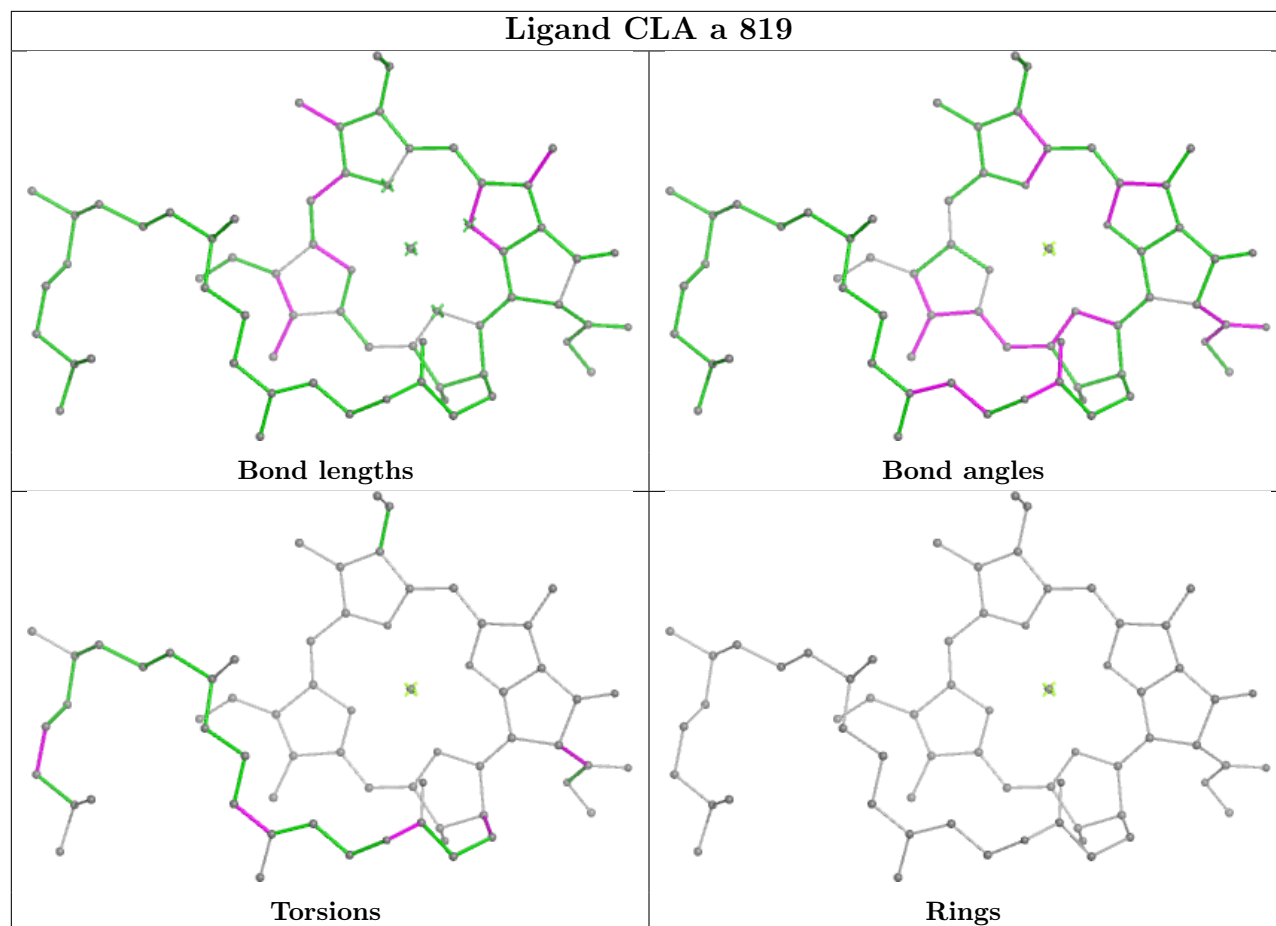
Torsions



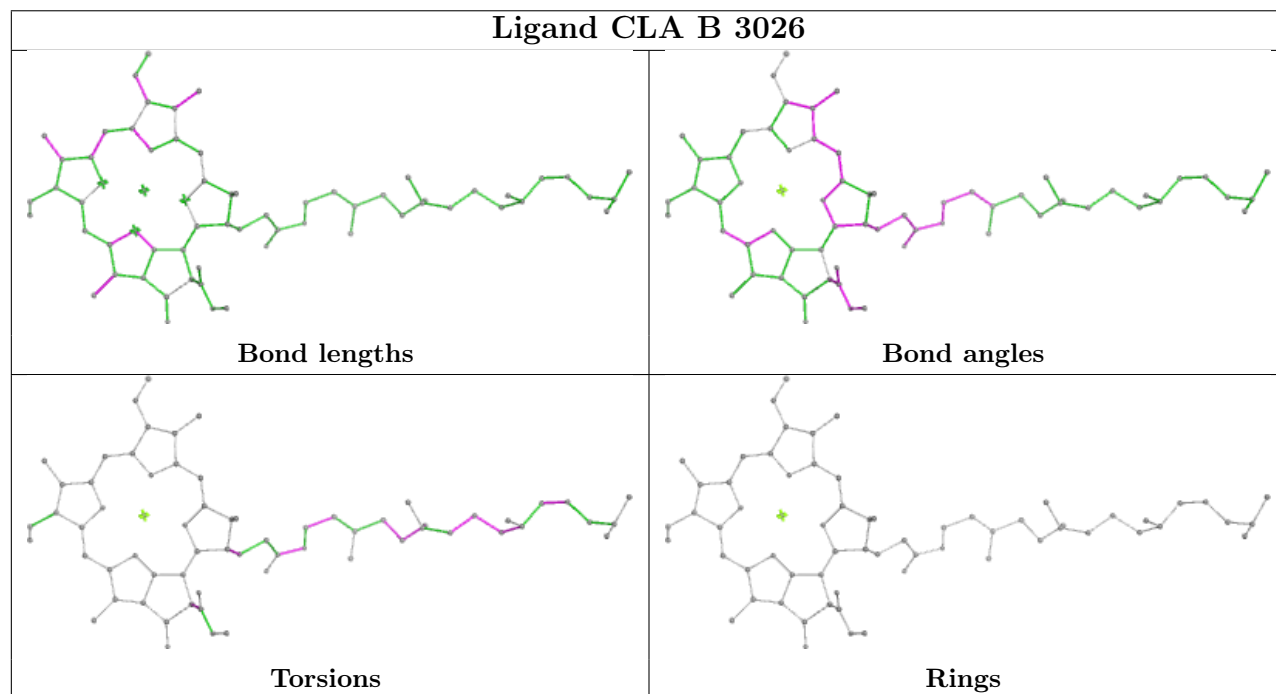
Rings

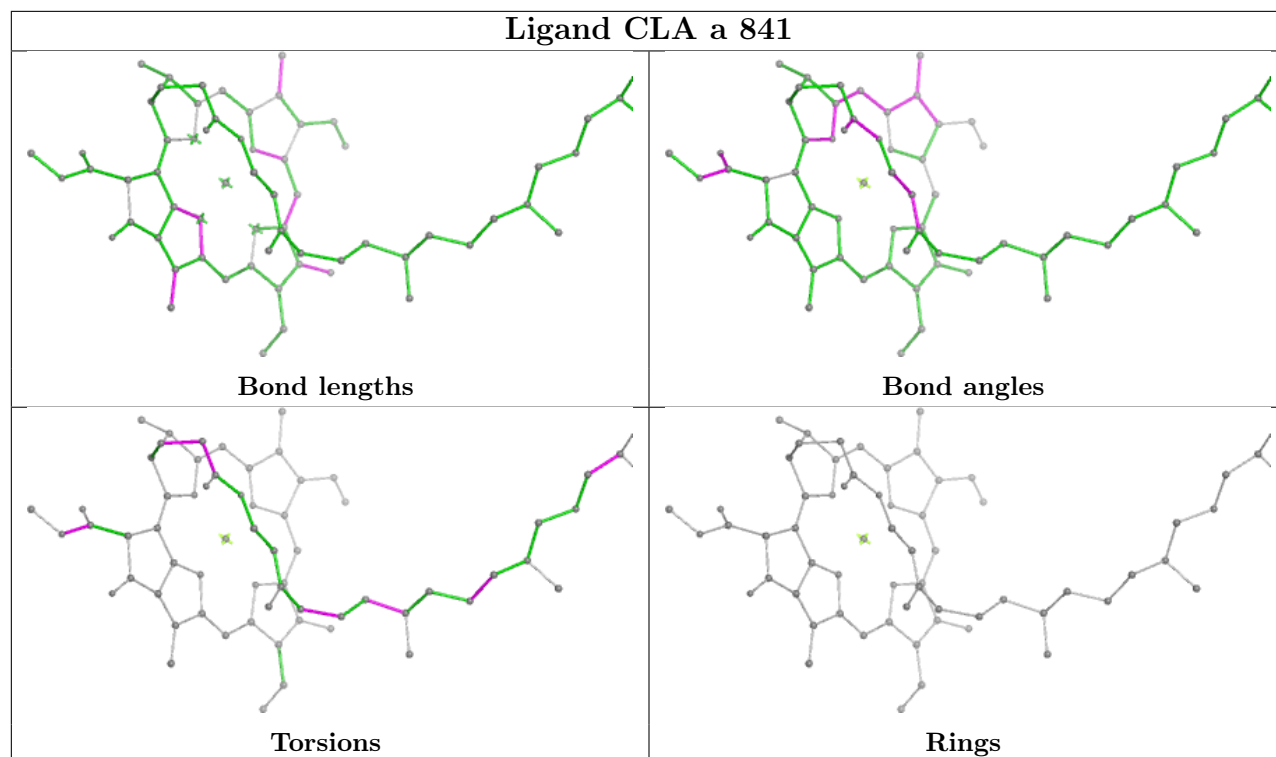
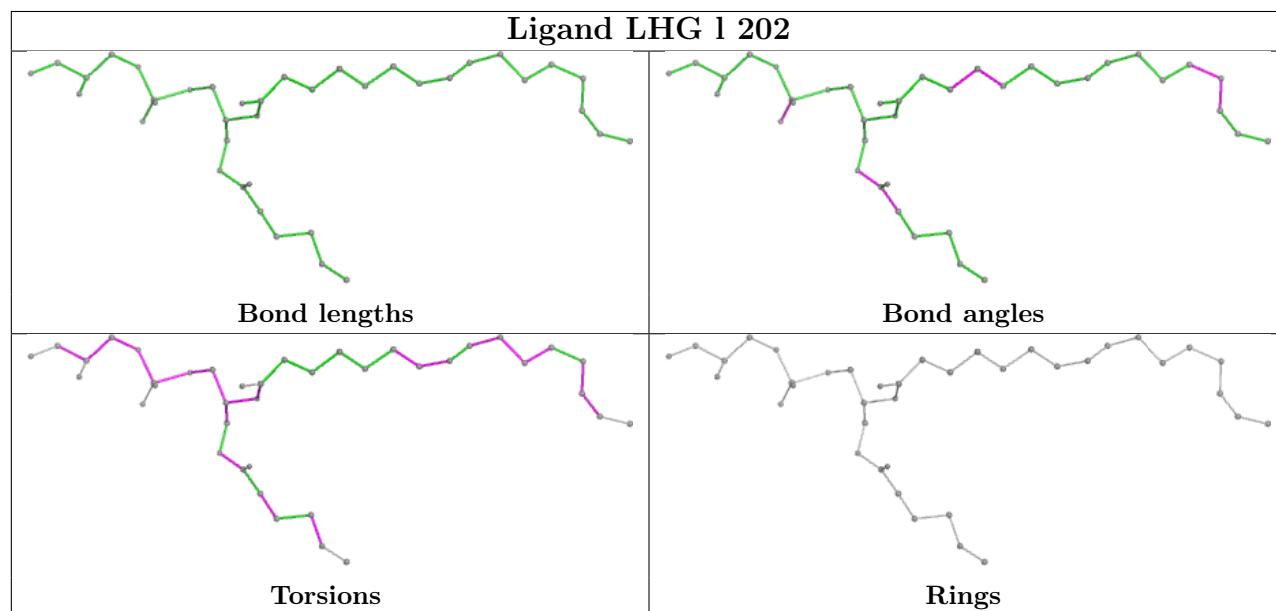


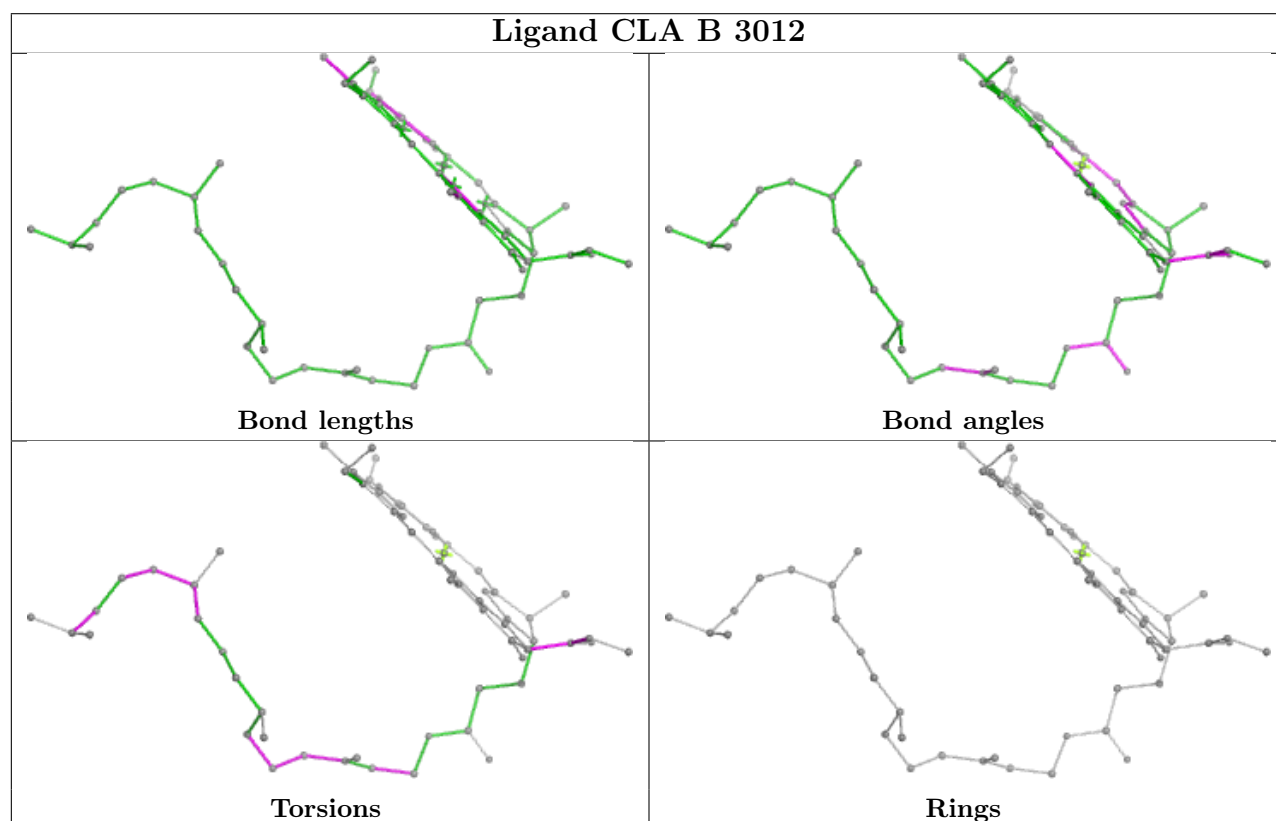
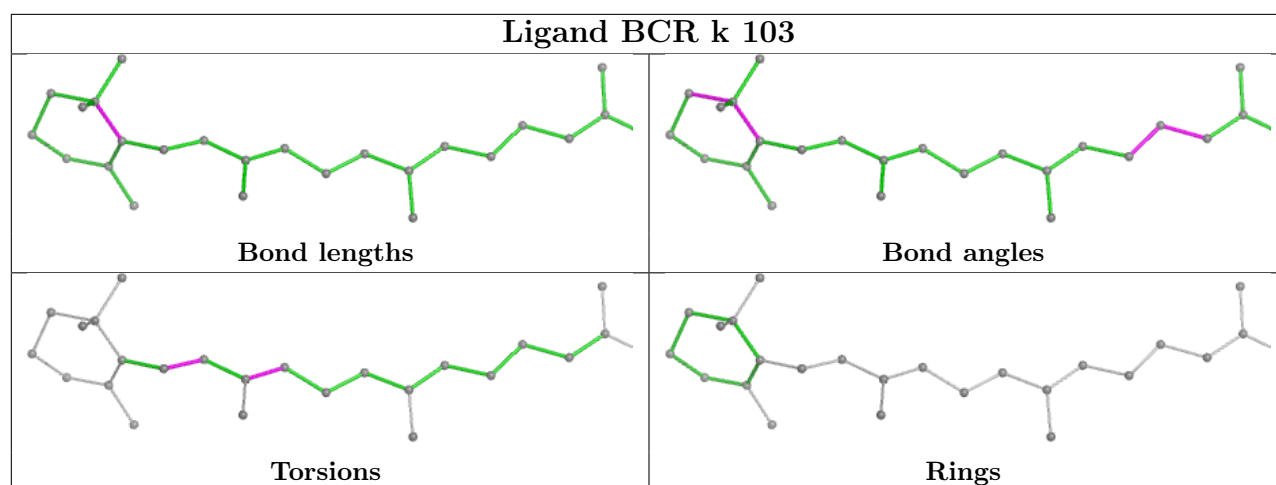
Ligand CLA a 819



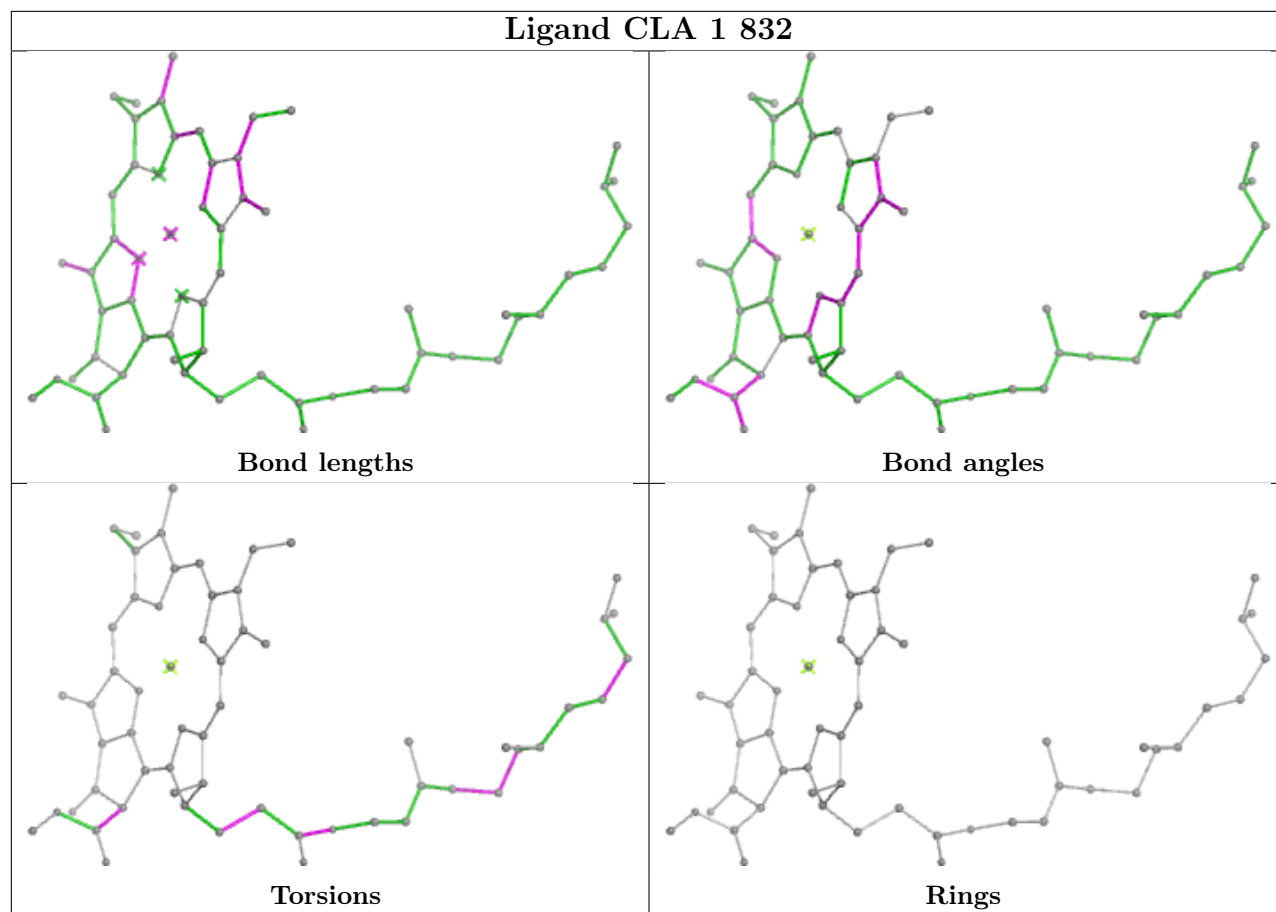
Ligand CLA B 3026

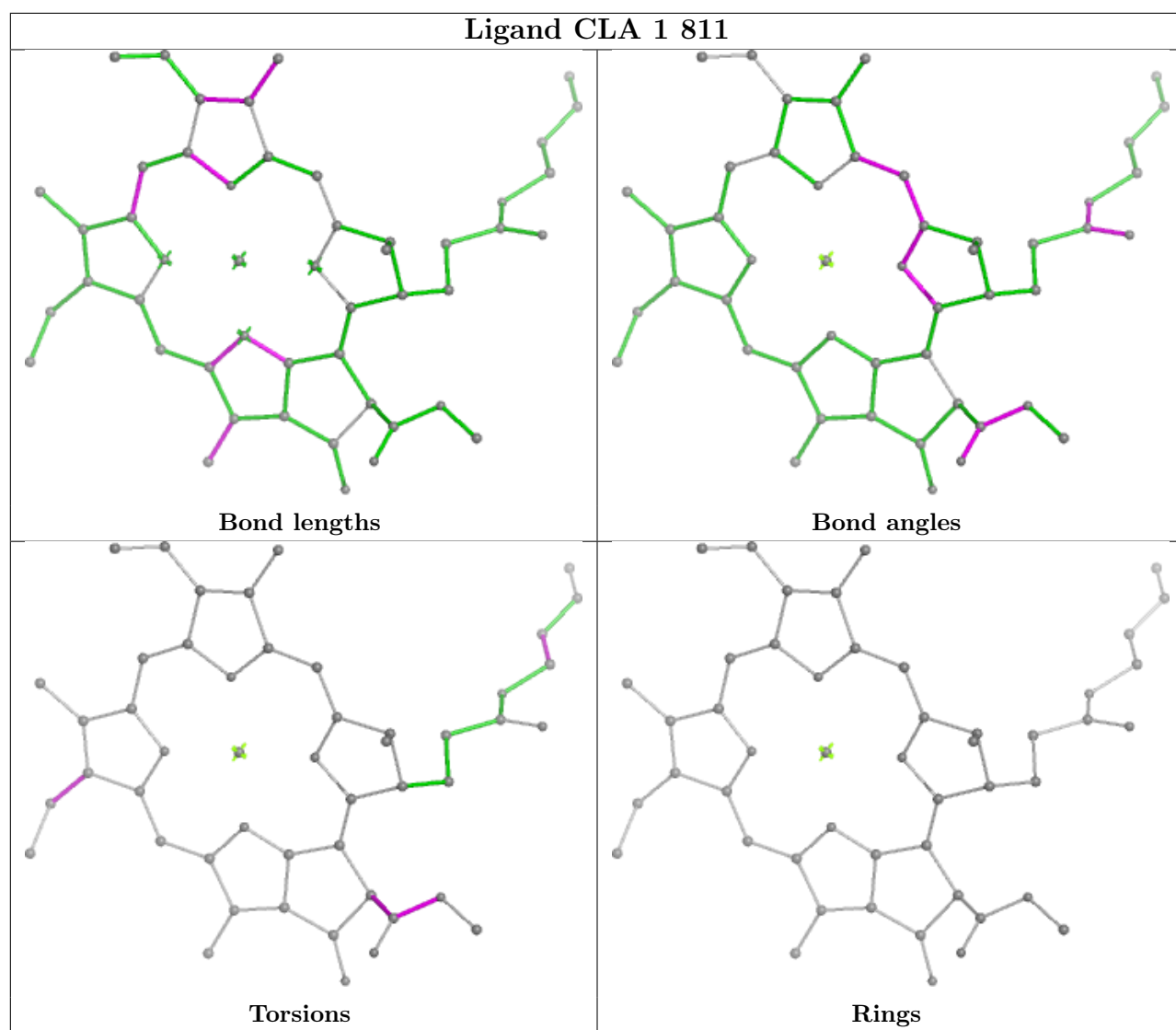


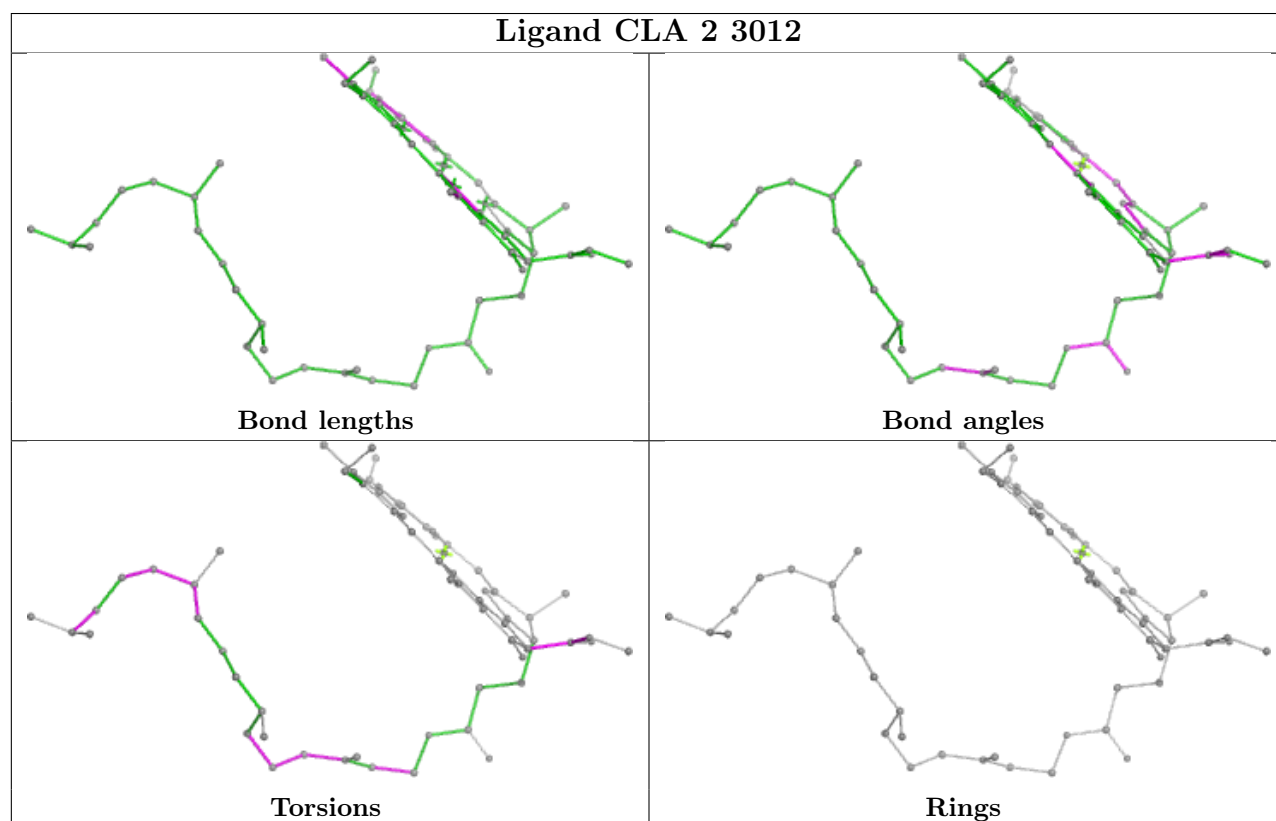
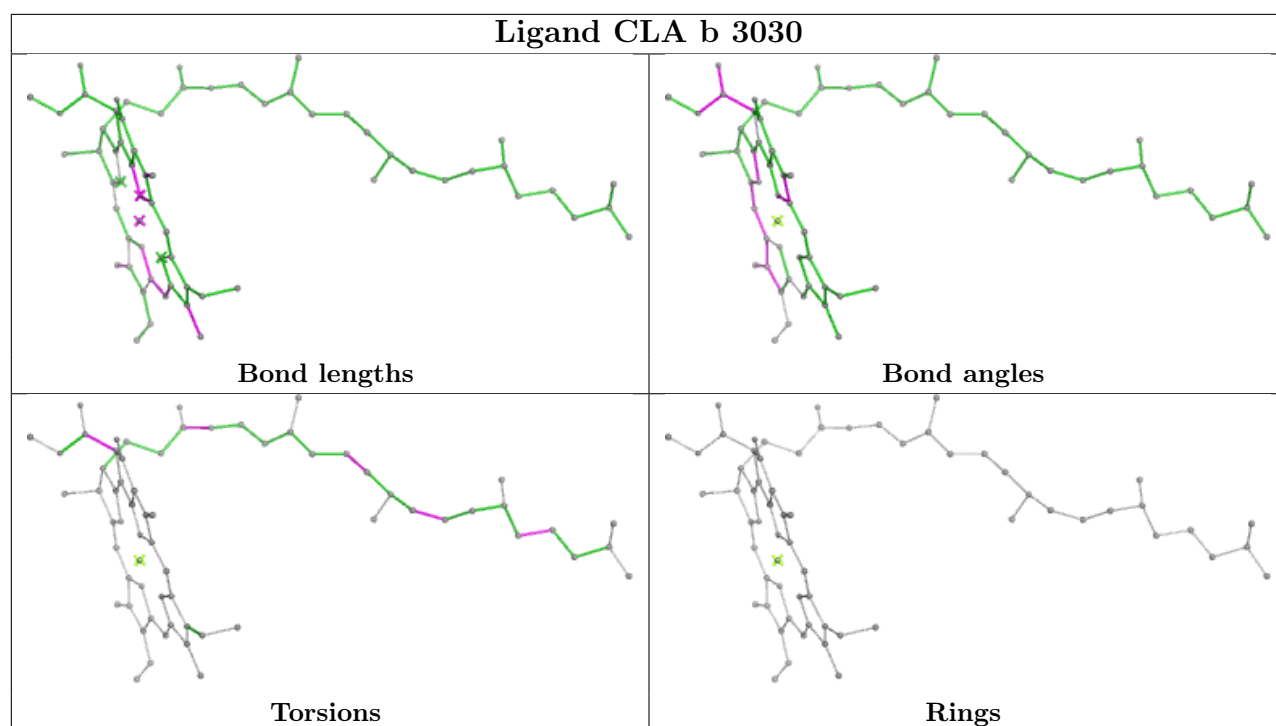
Ligand CLA a 841**Ligand LHG 1 202**

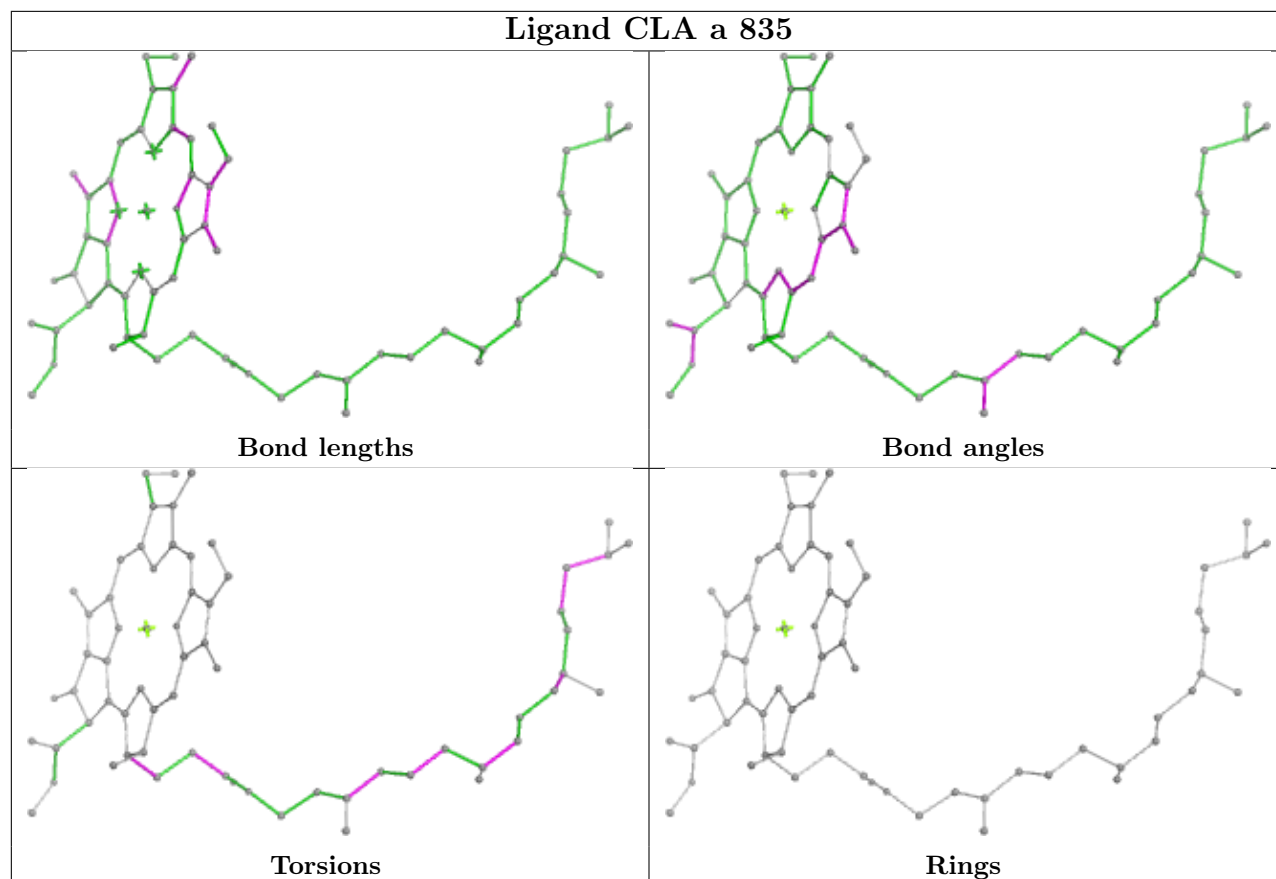
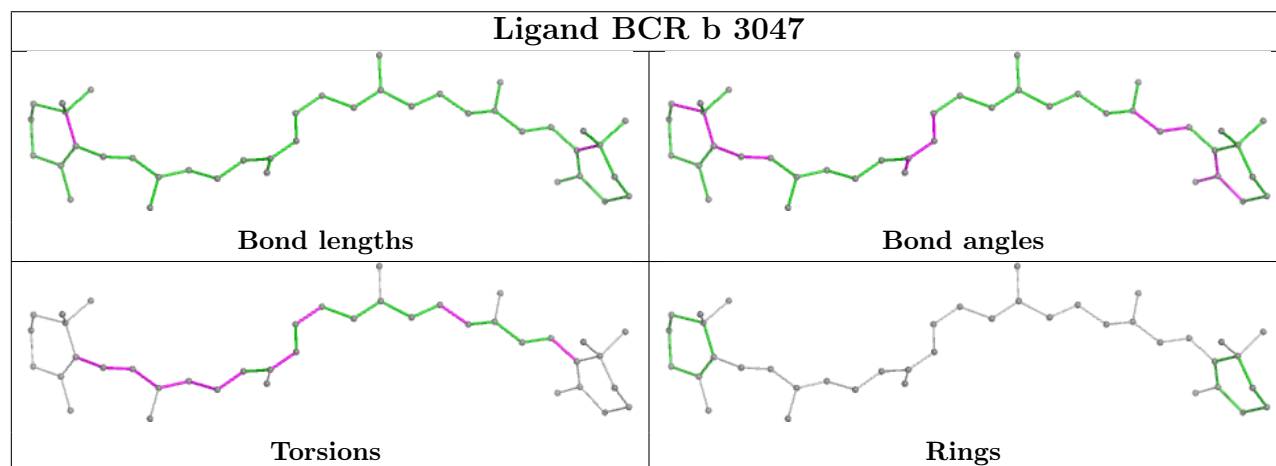


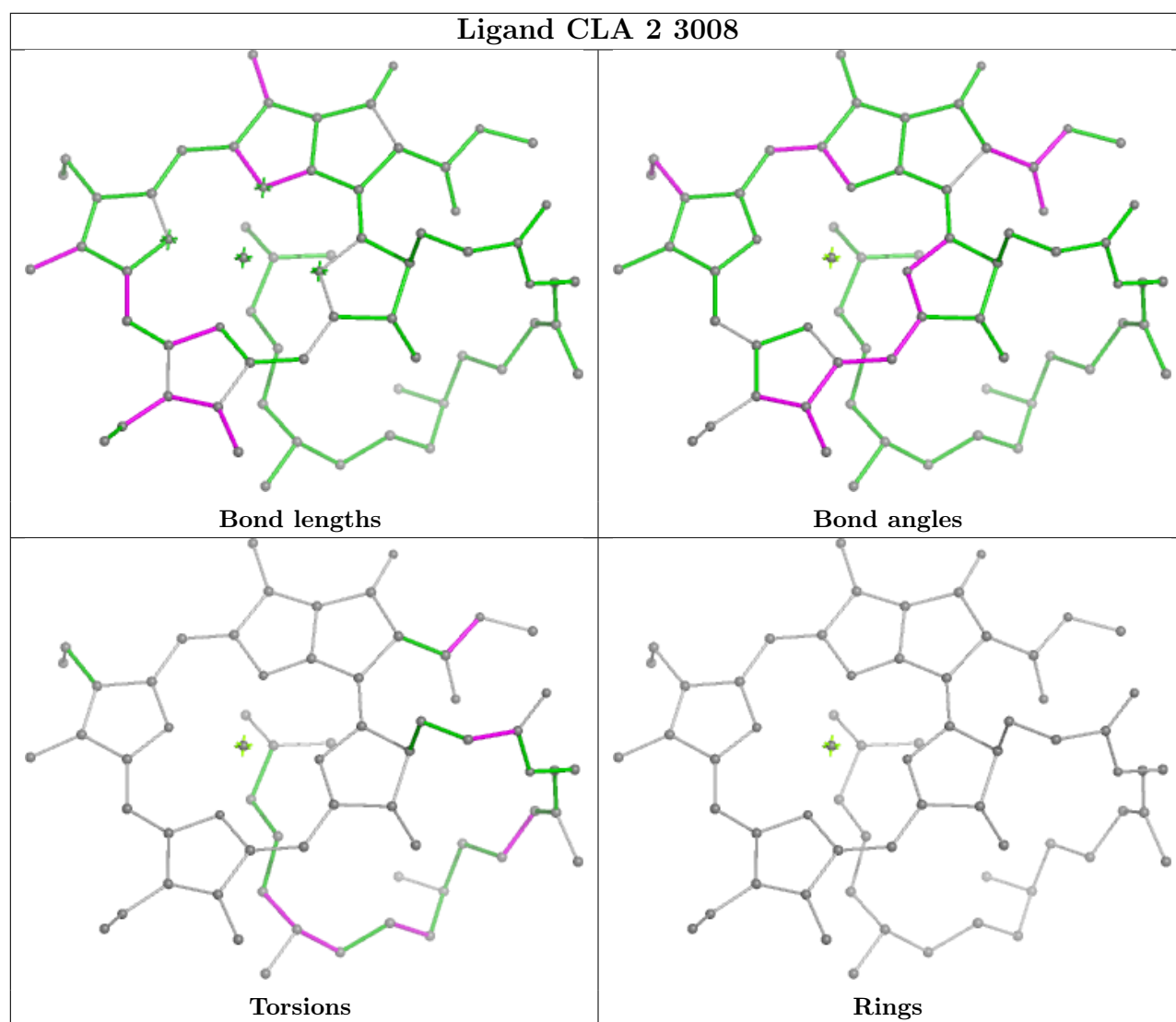
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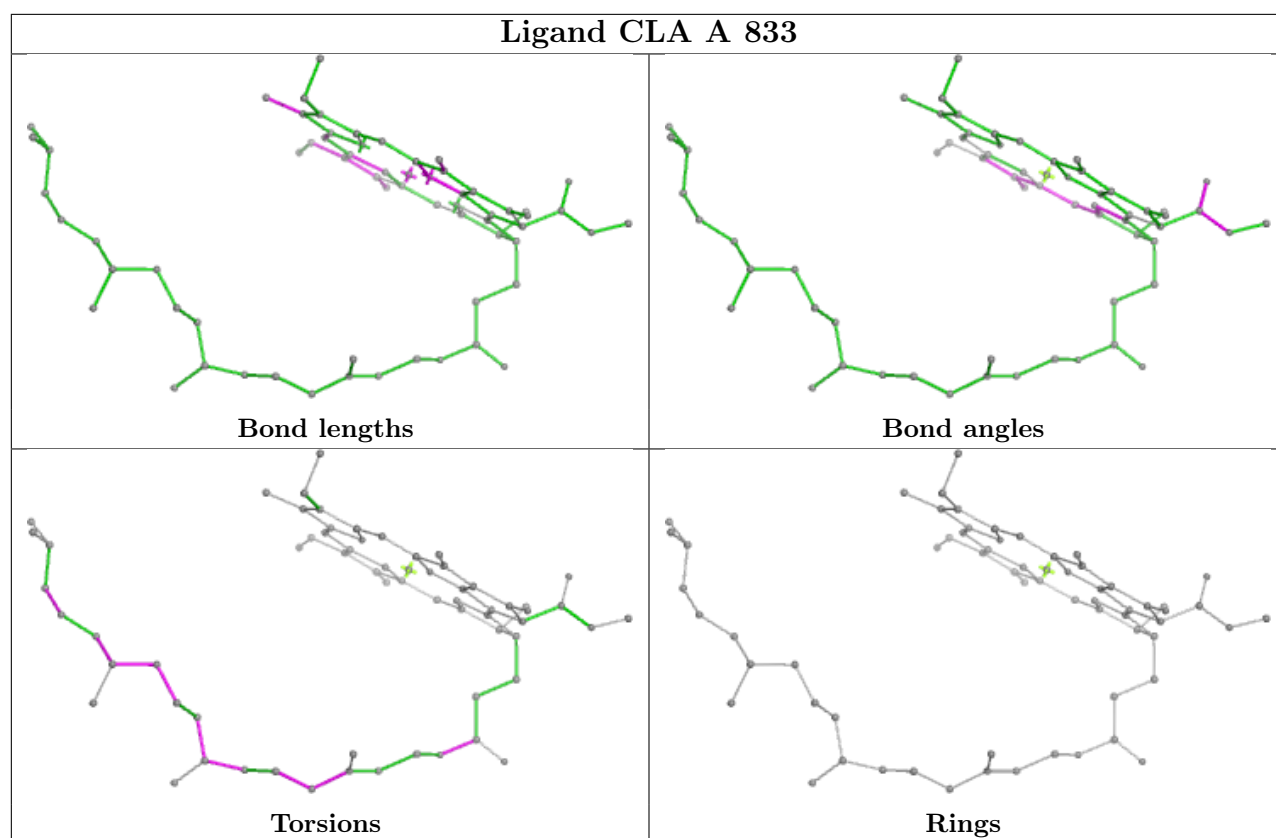




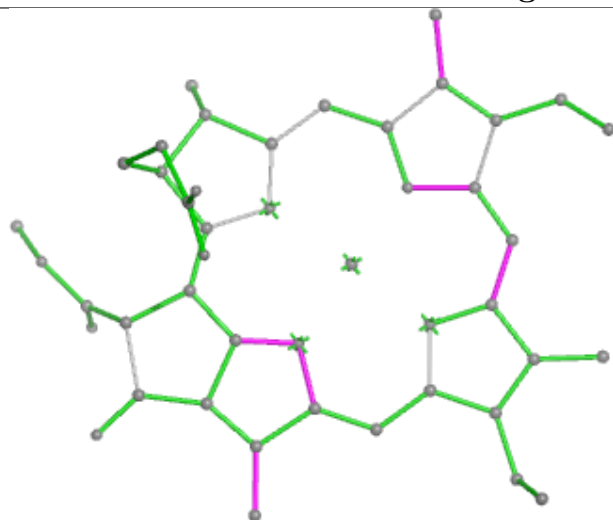


Ligand CLA a 835**Ligand BCR b 3047**

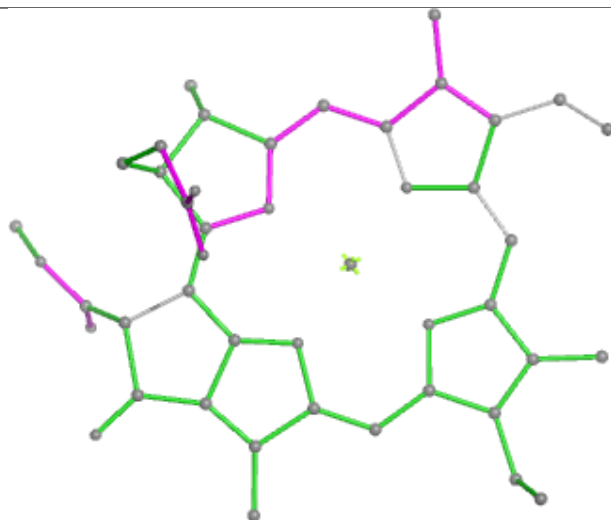




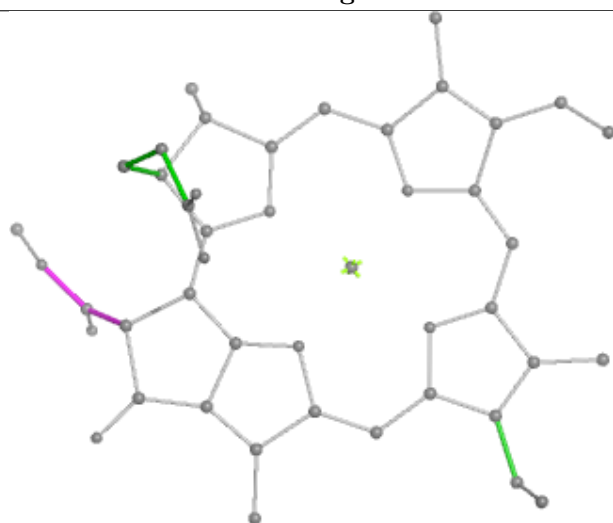
Ligand CLA 1 837



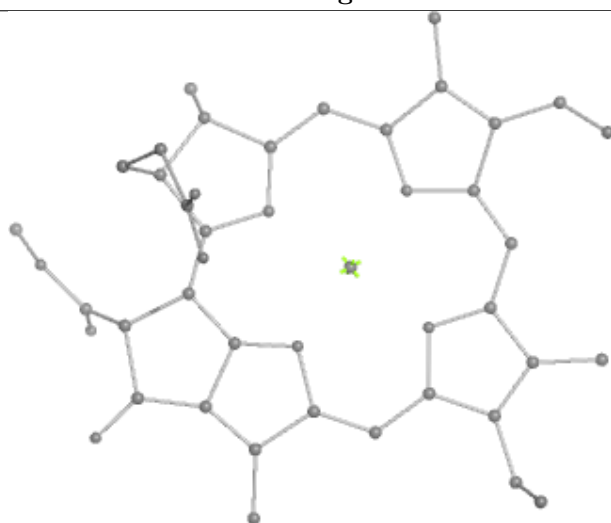
Bond lengths



Bond angles

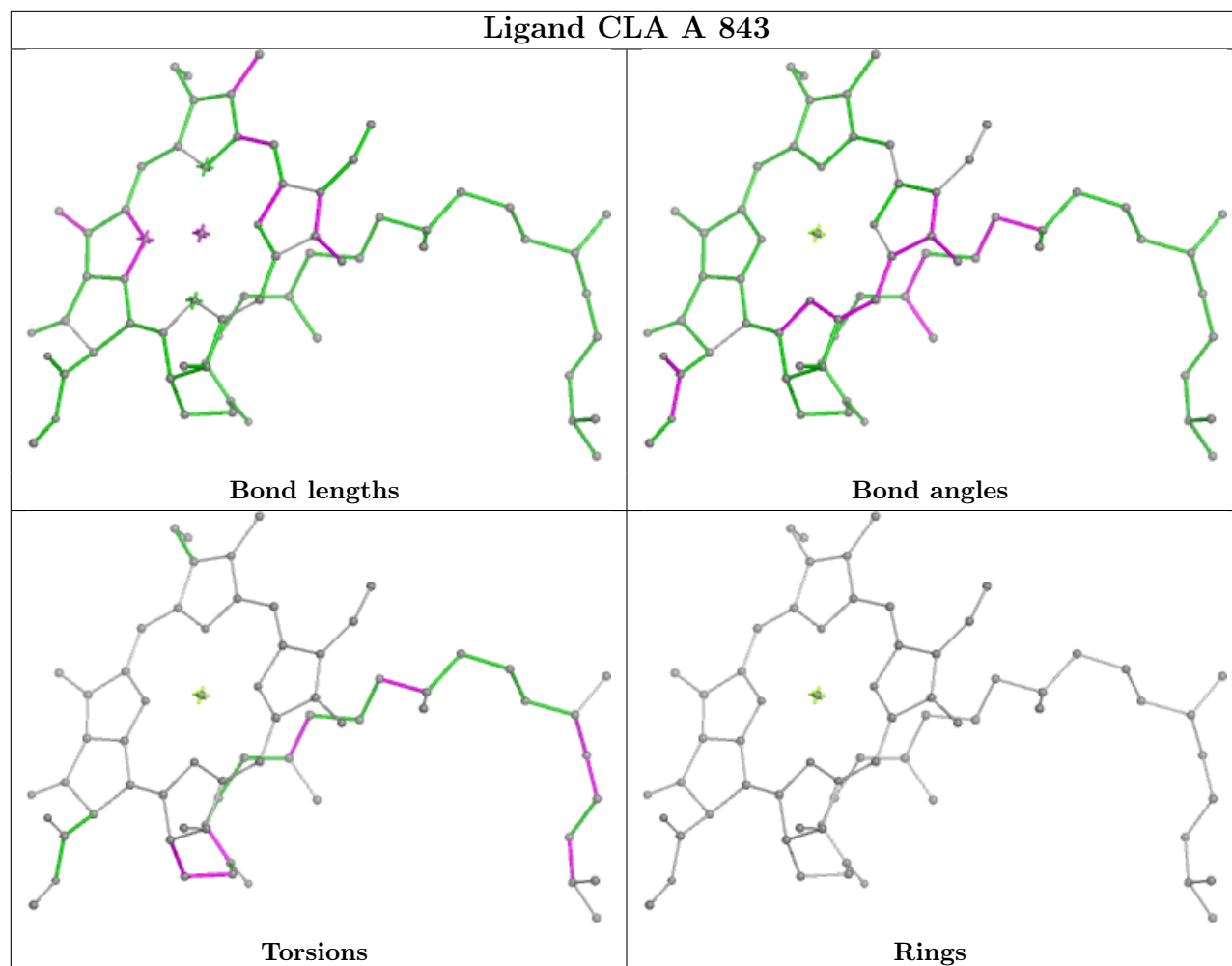


Torsions

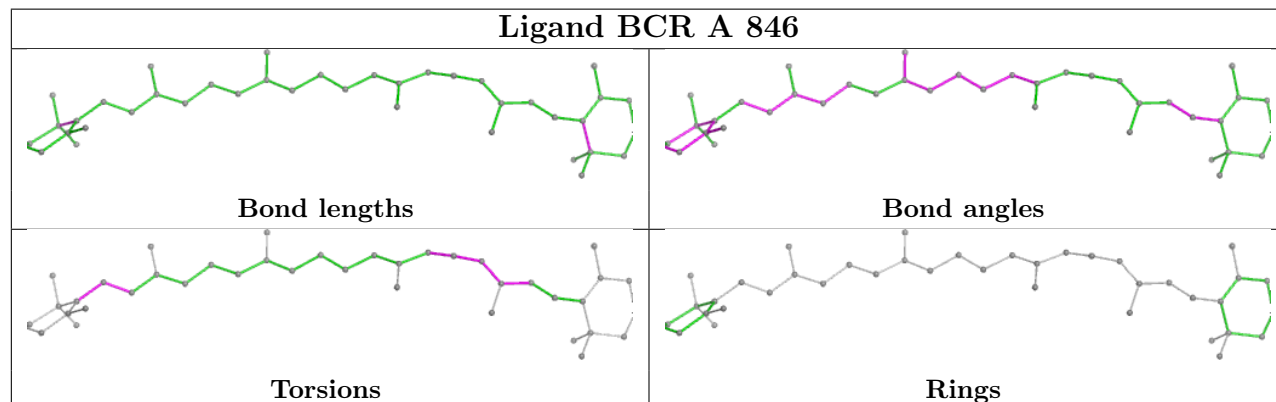


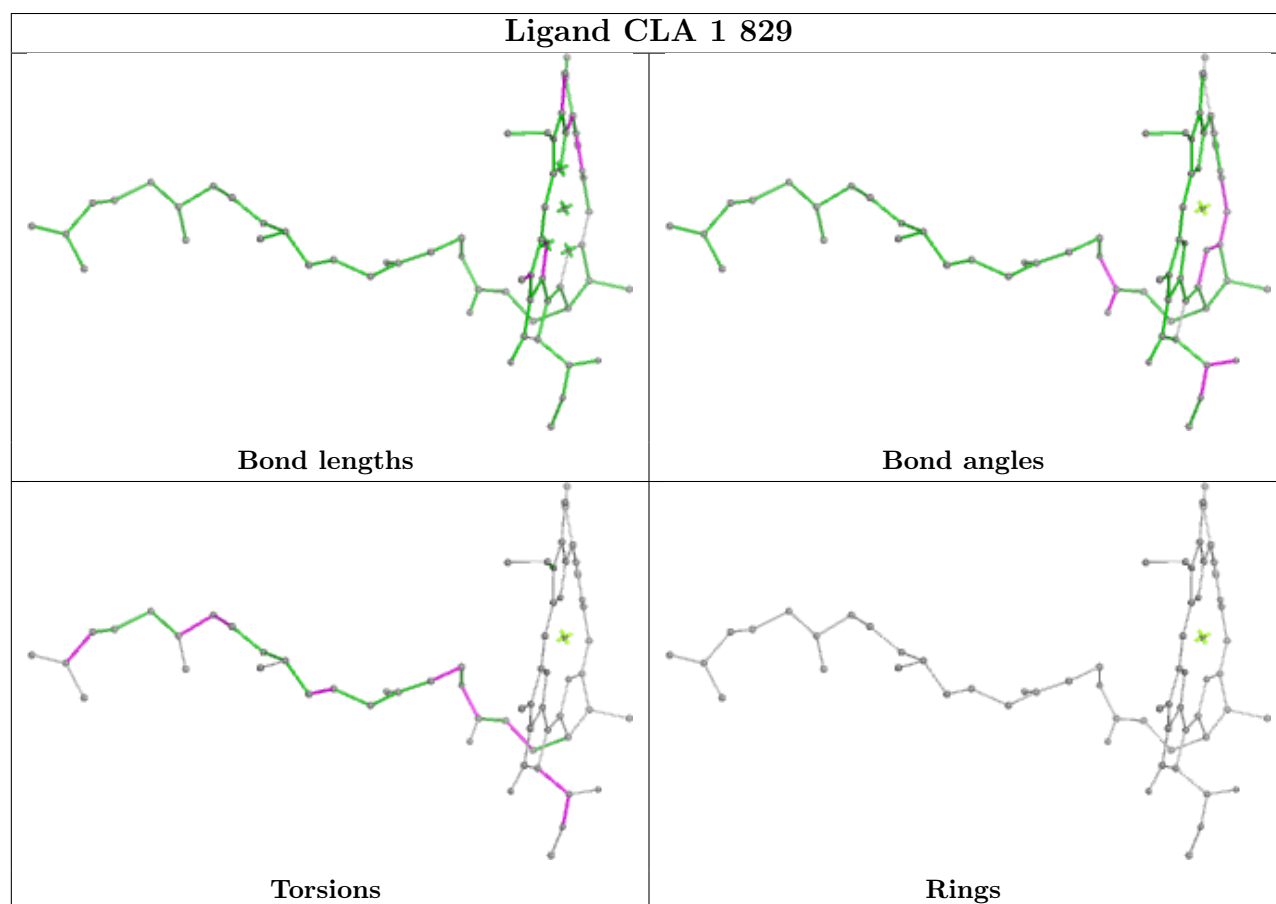
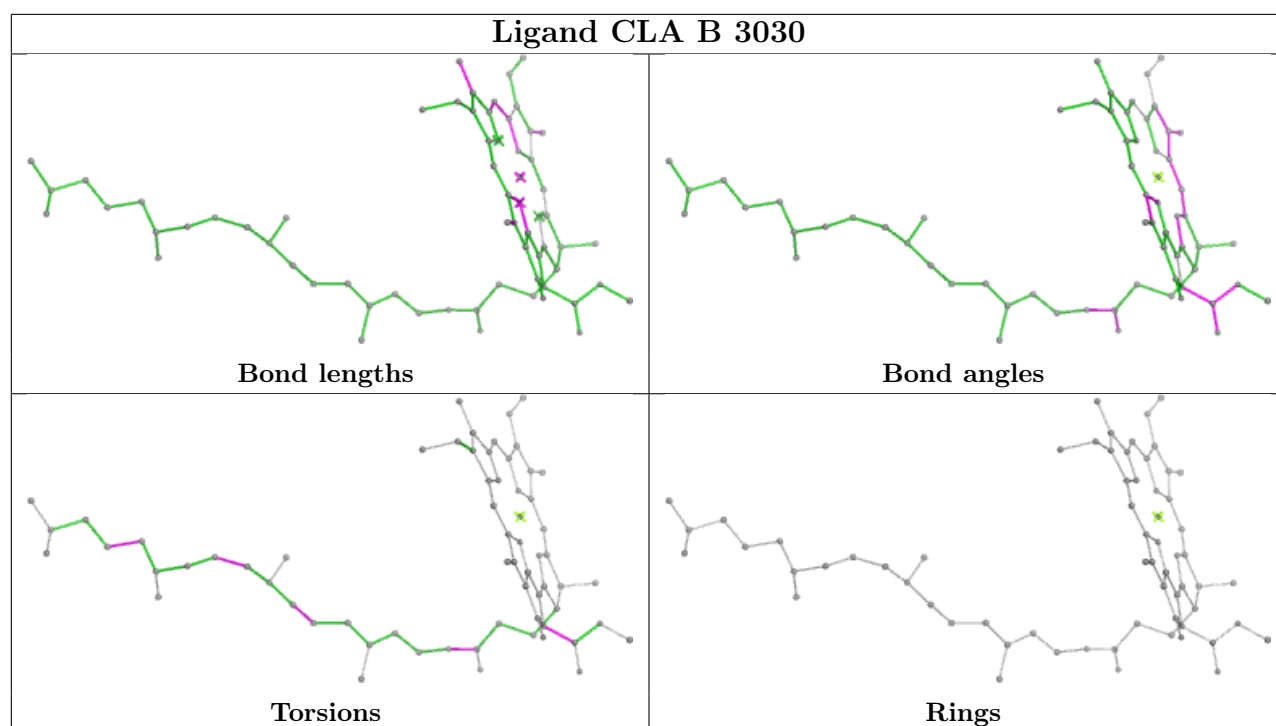
Rings

Ligand CLA A 843

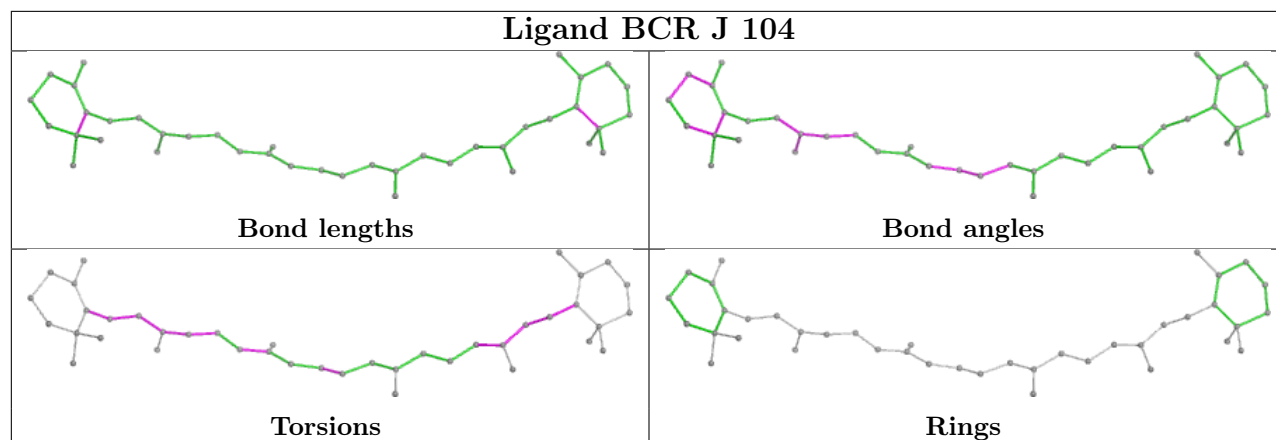


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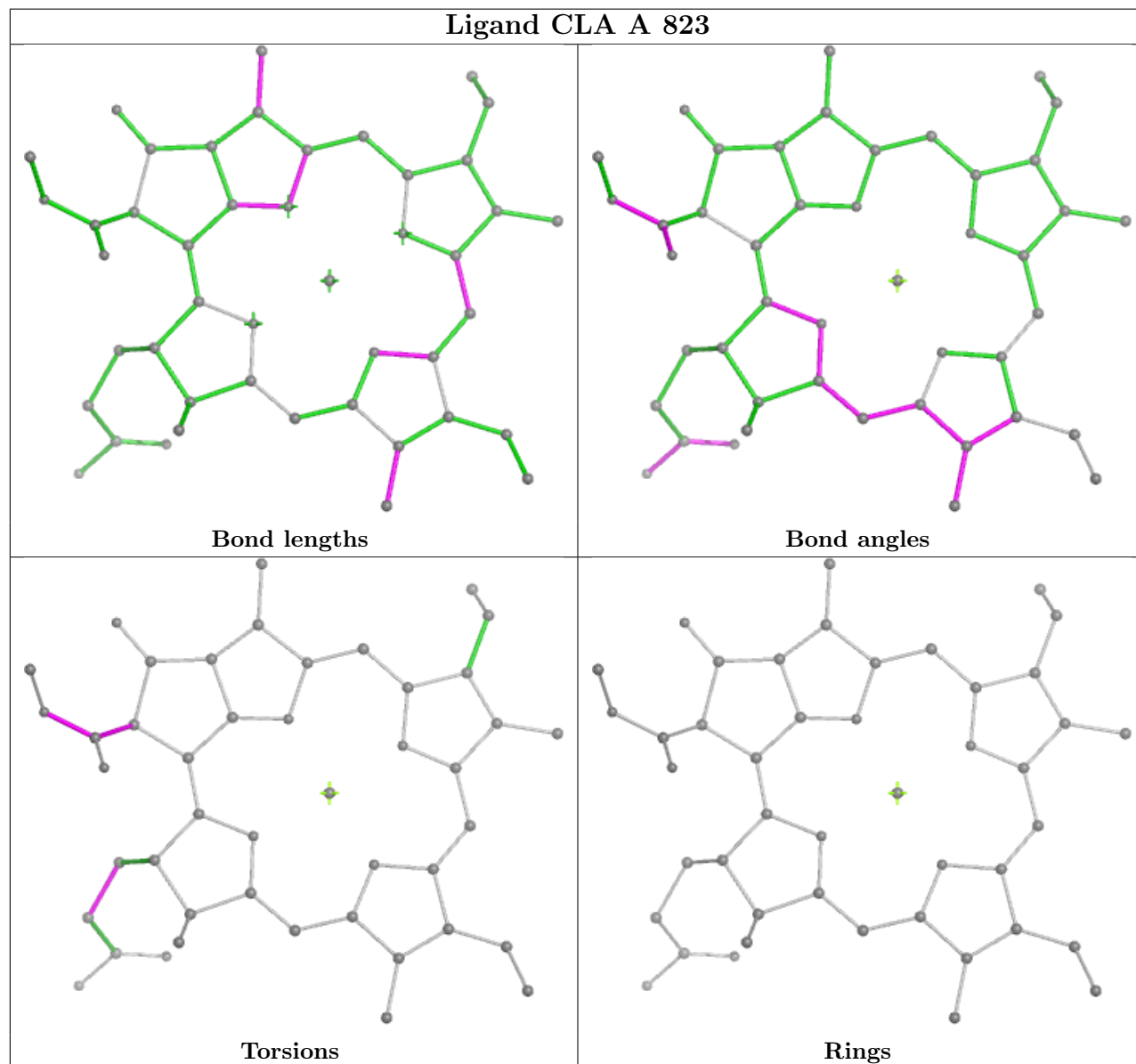




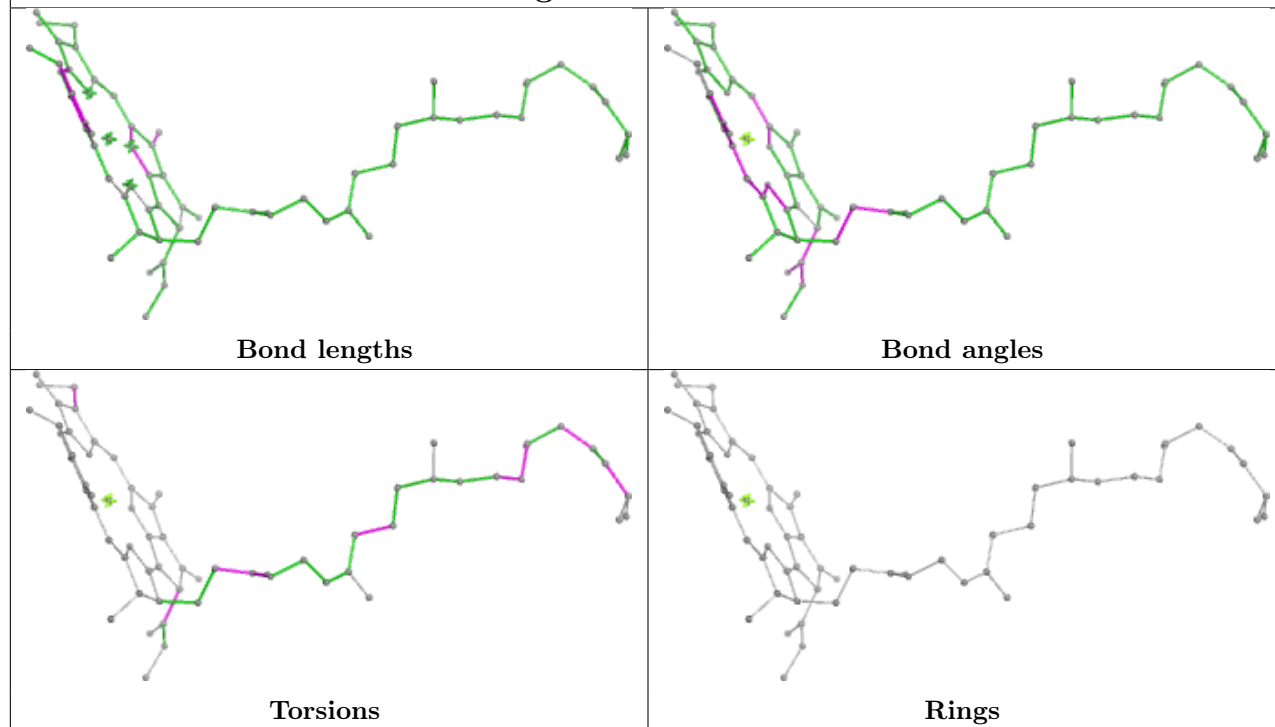
Ligand BCR J 104



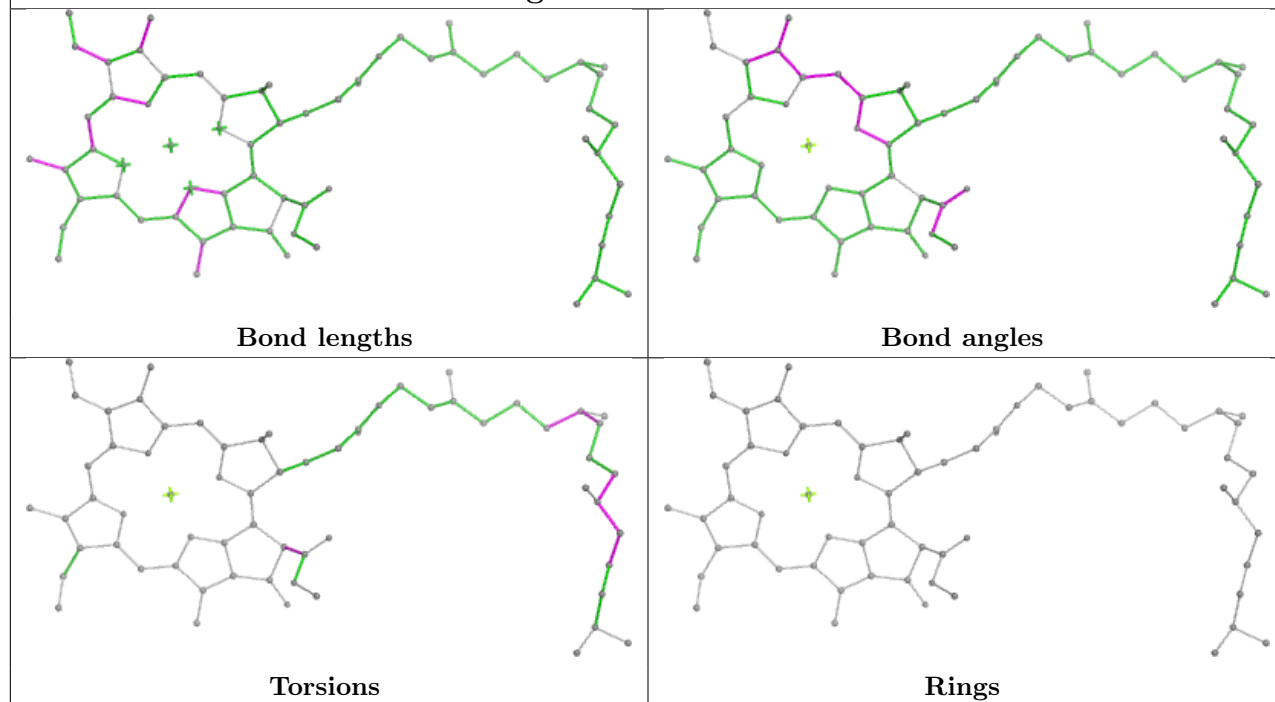
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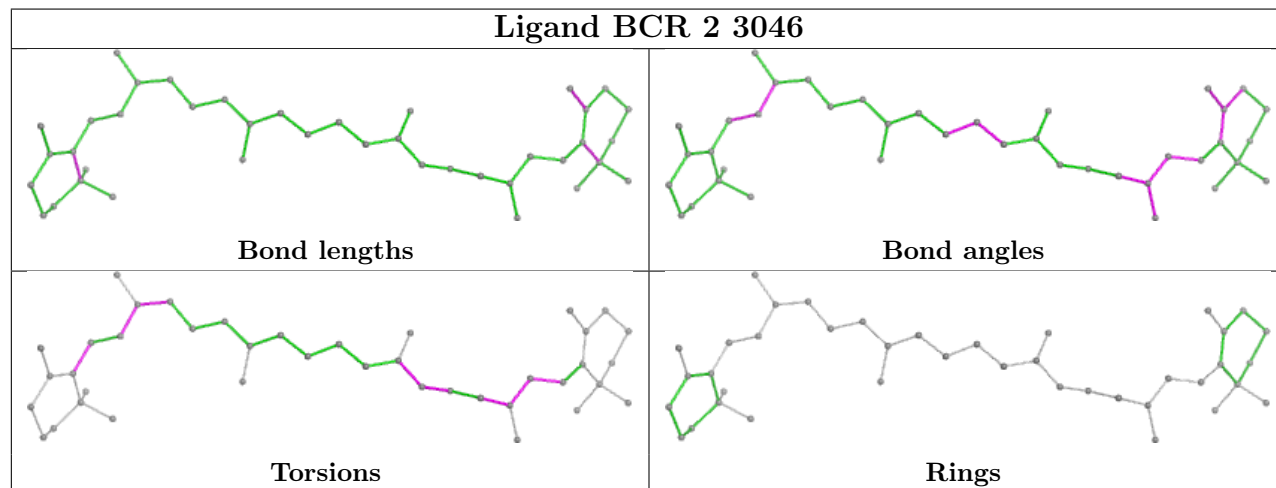
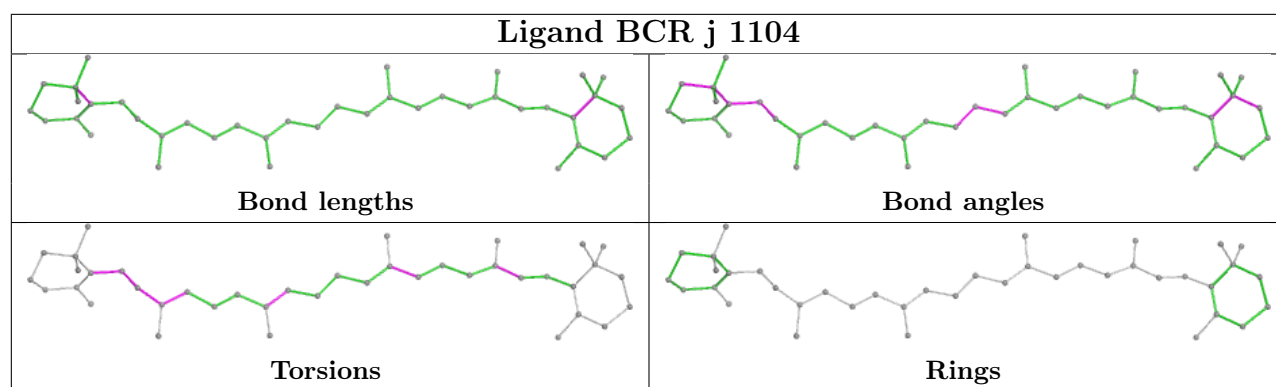


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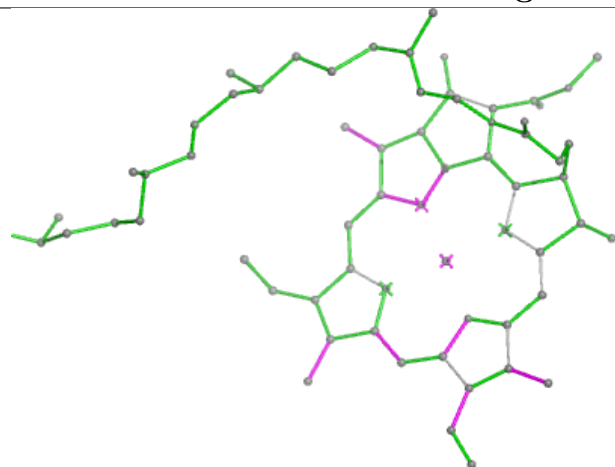


Ligand CLA 2 3027

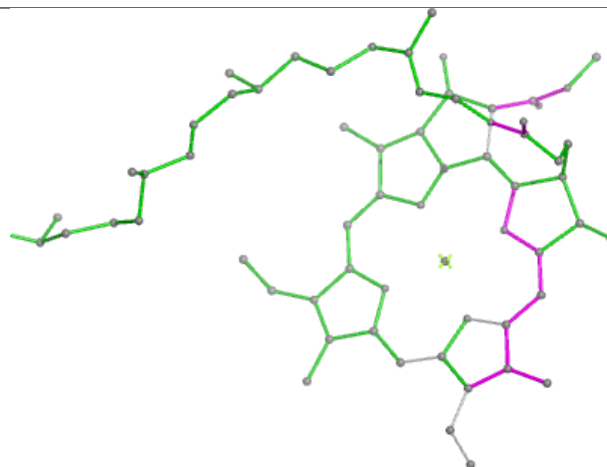




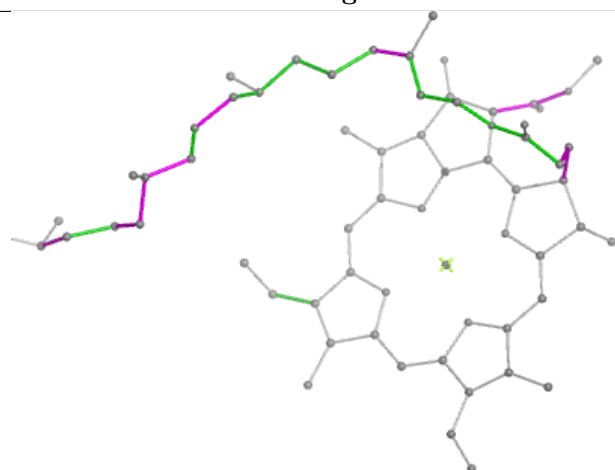
Ligand CLA A 830



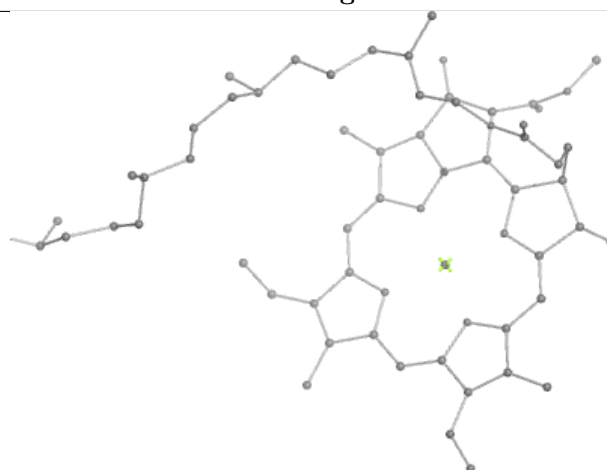
Bond lengths



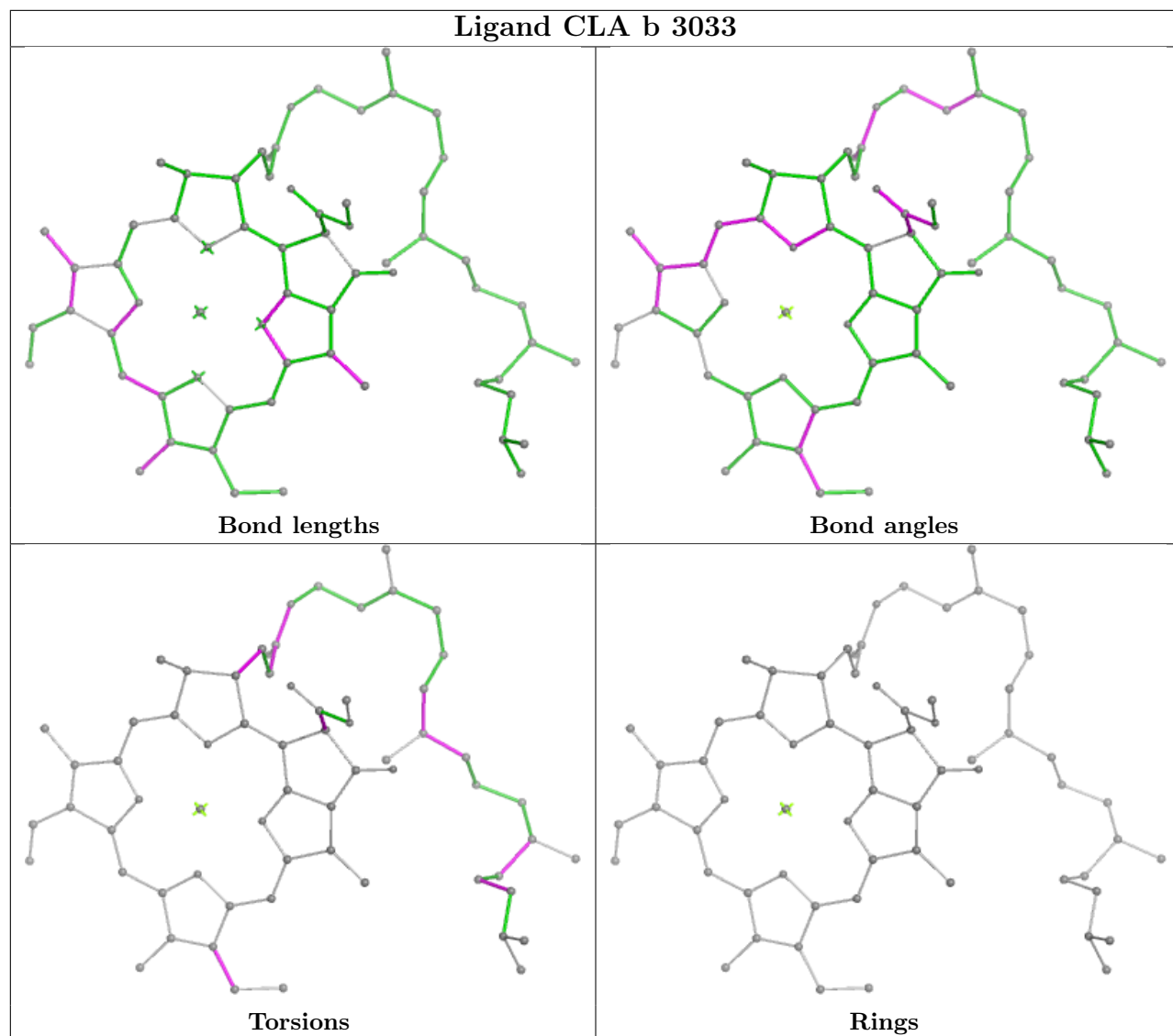
Bond angles

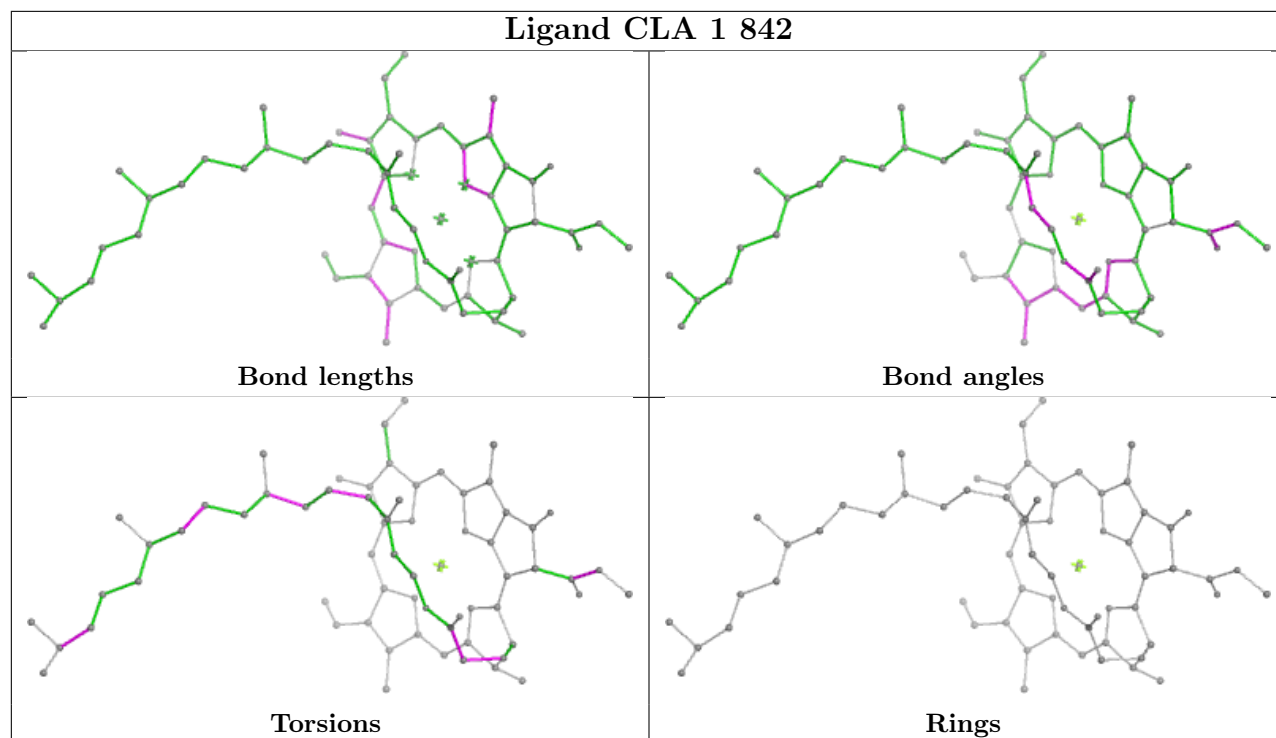


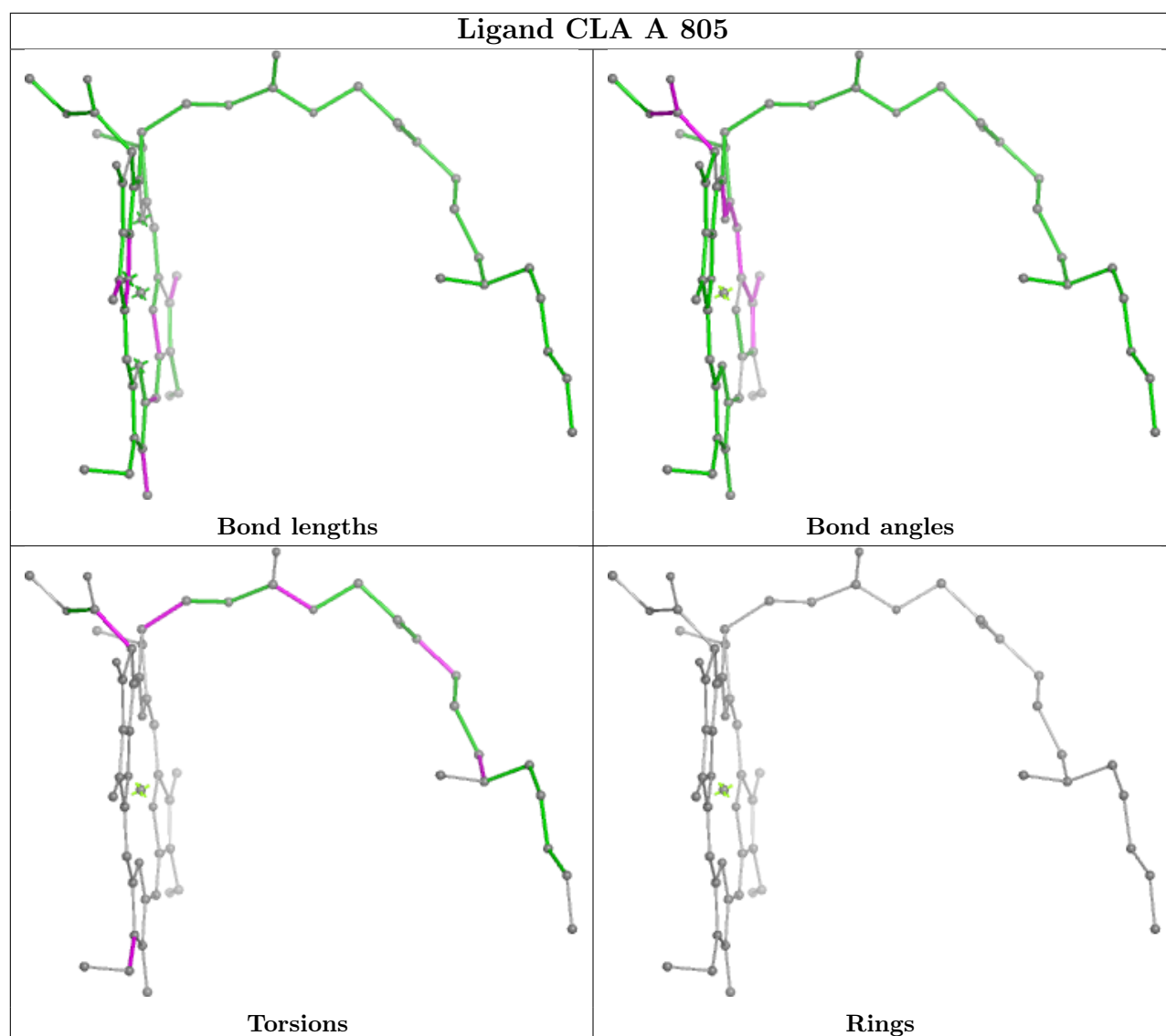
Torsions

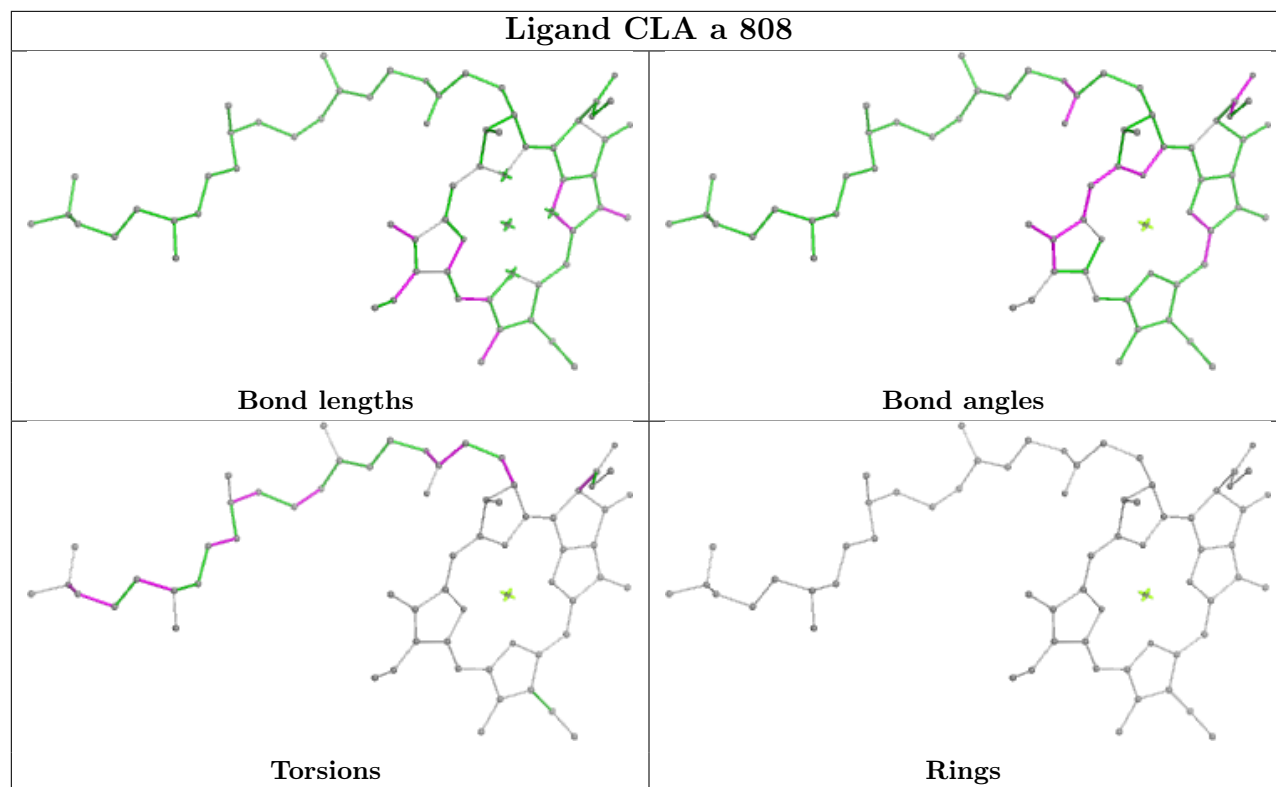


Rings

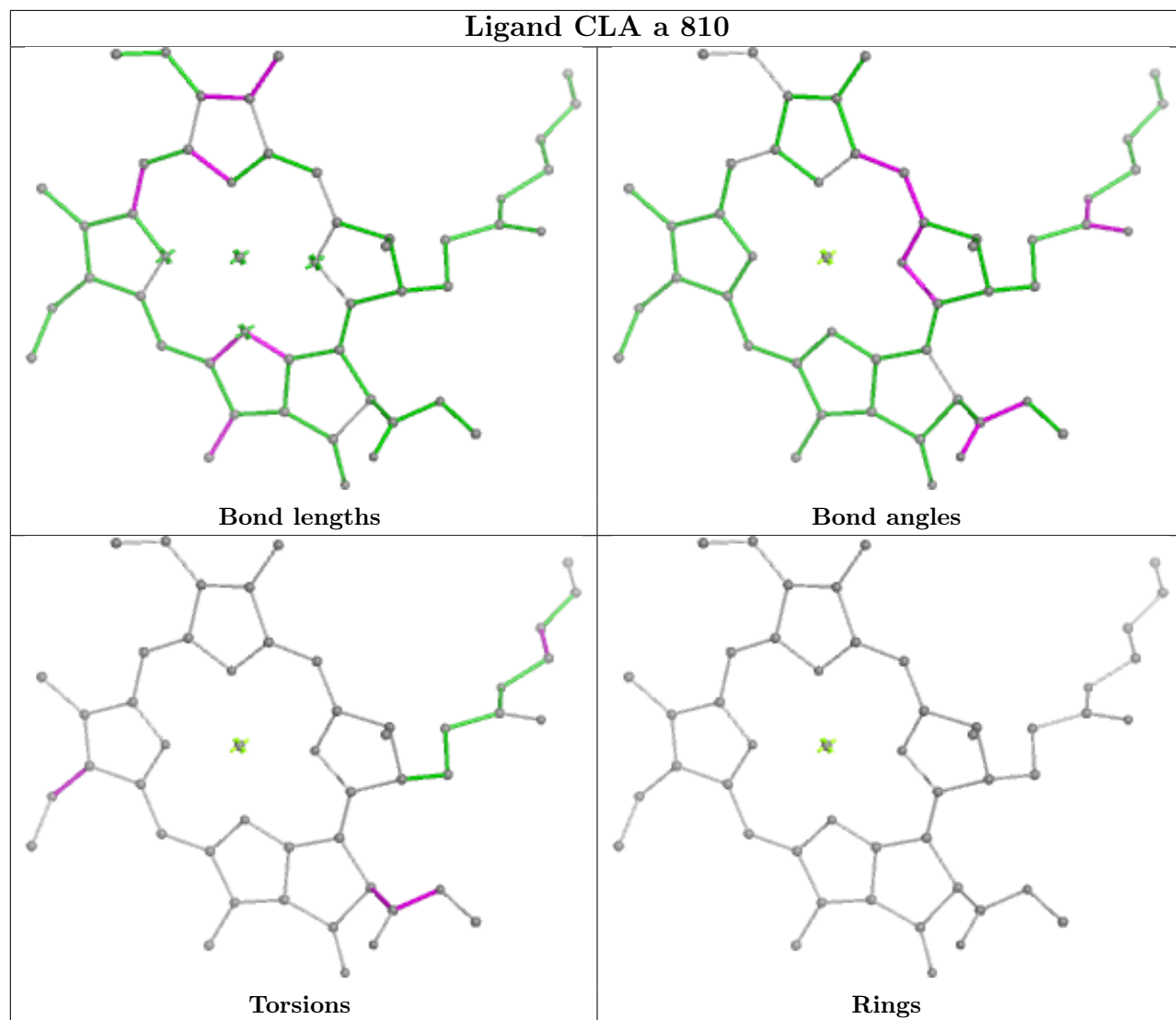


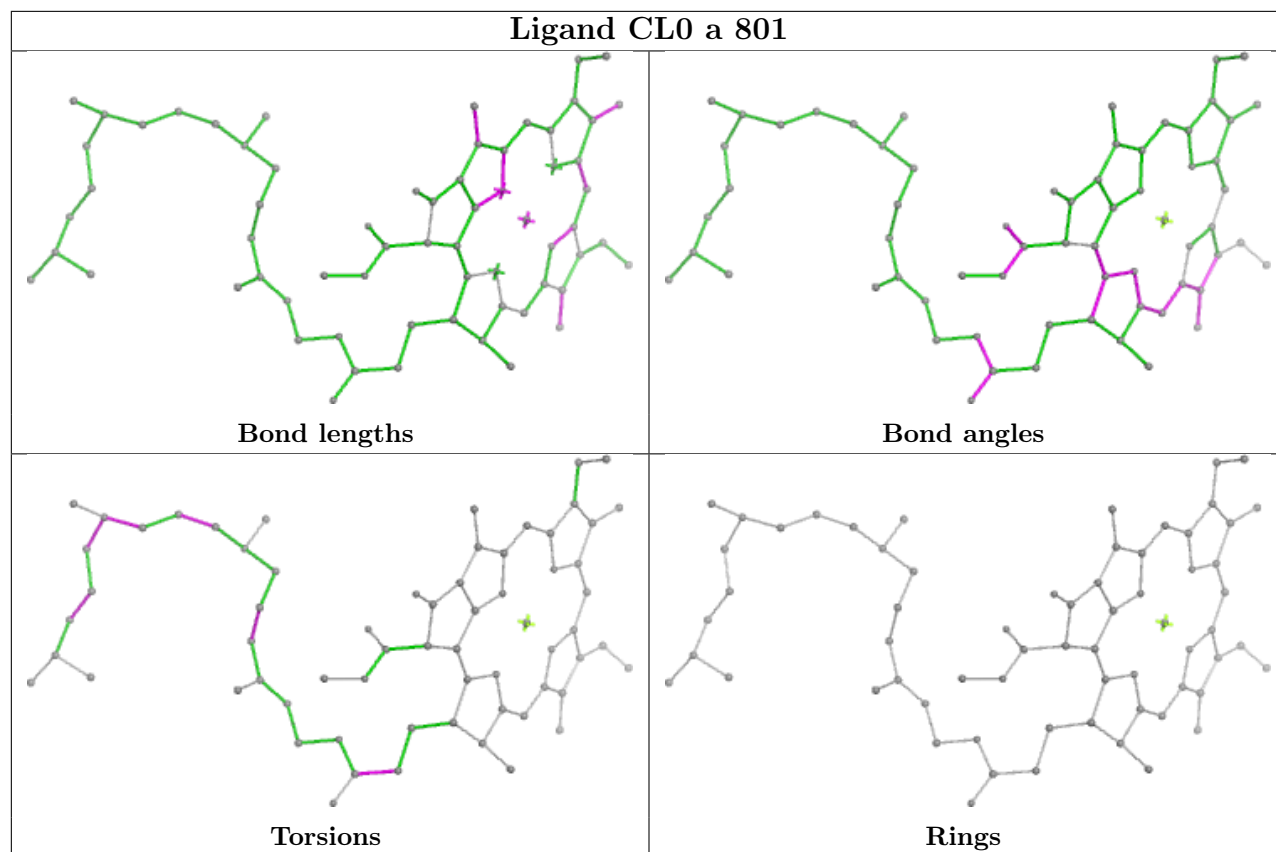
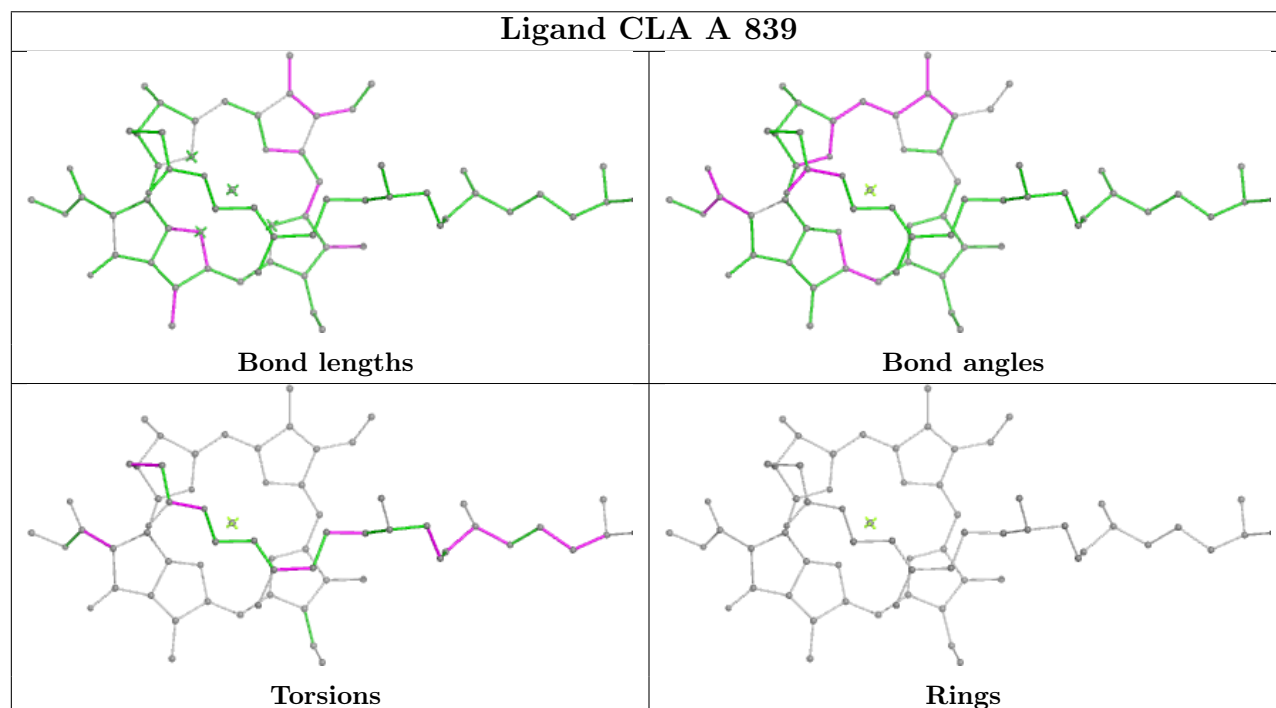


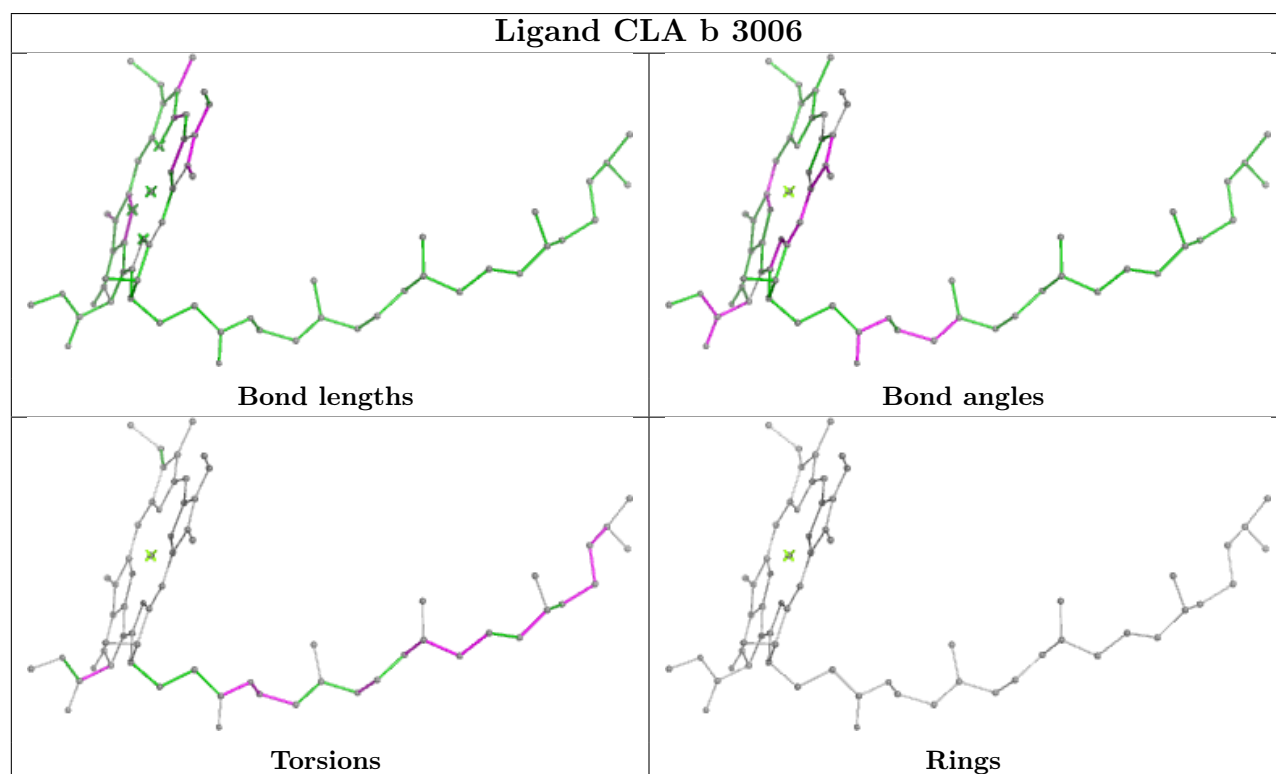
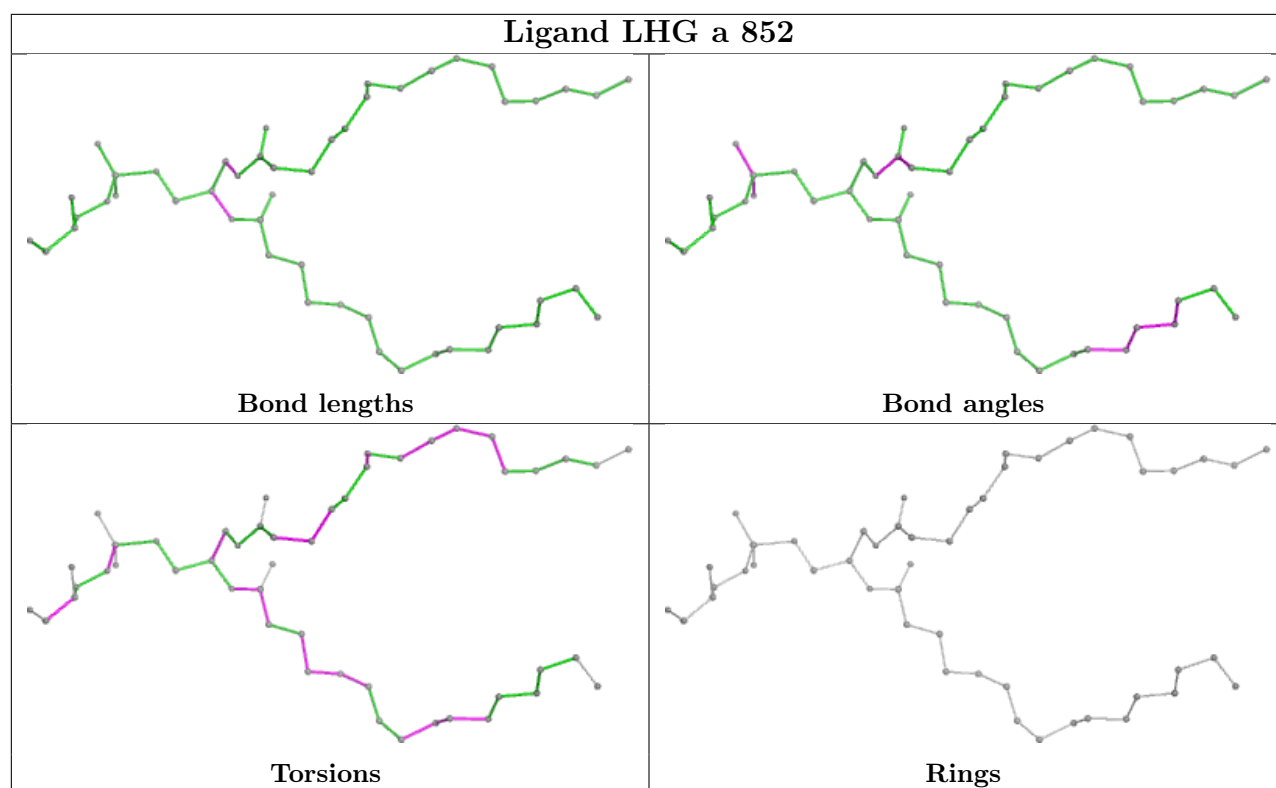


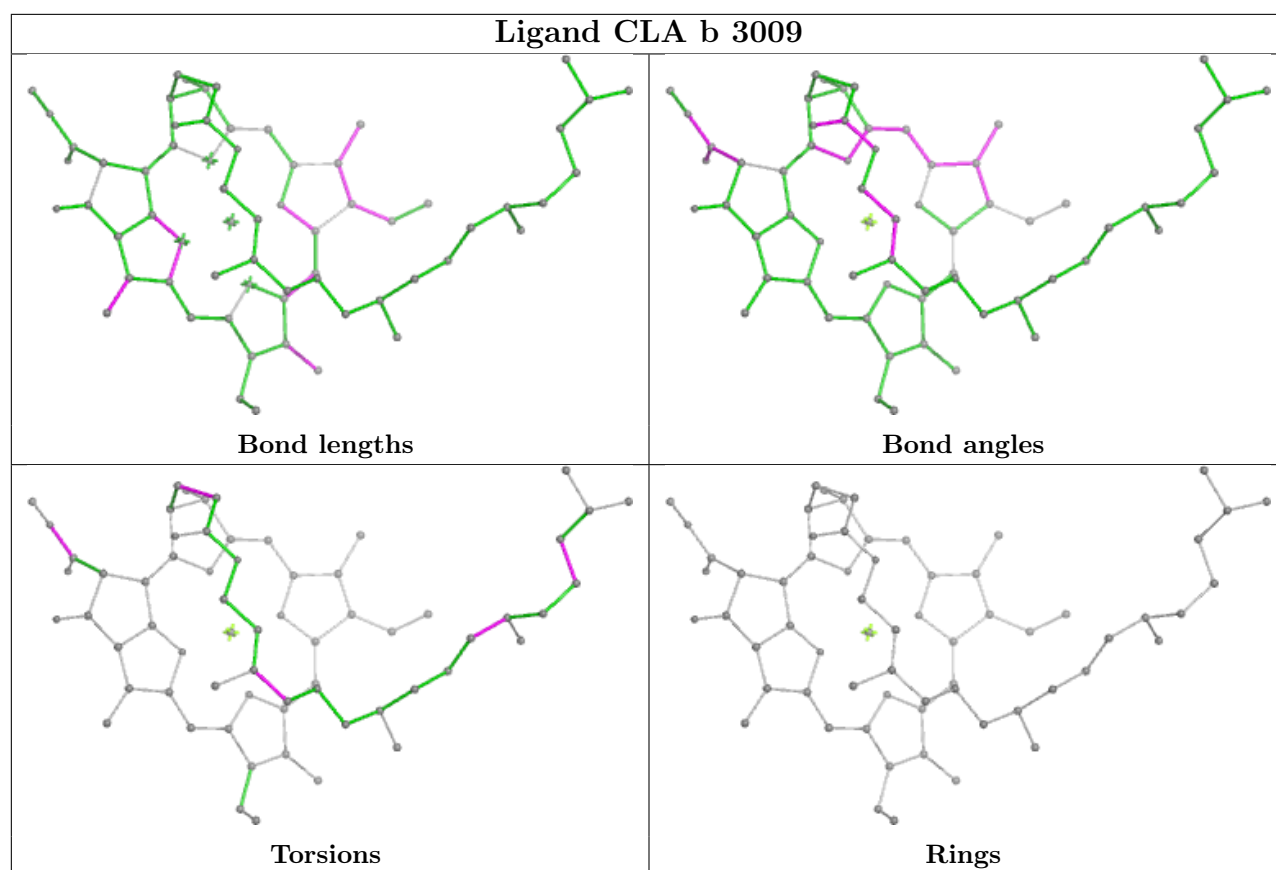


Ligand CLA a 810

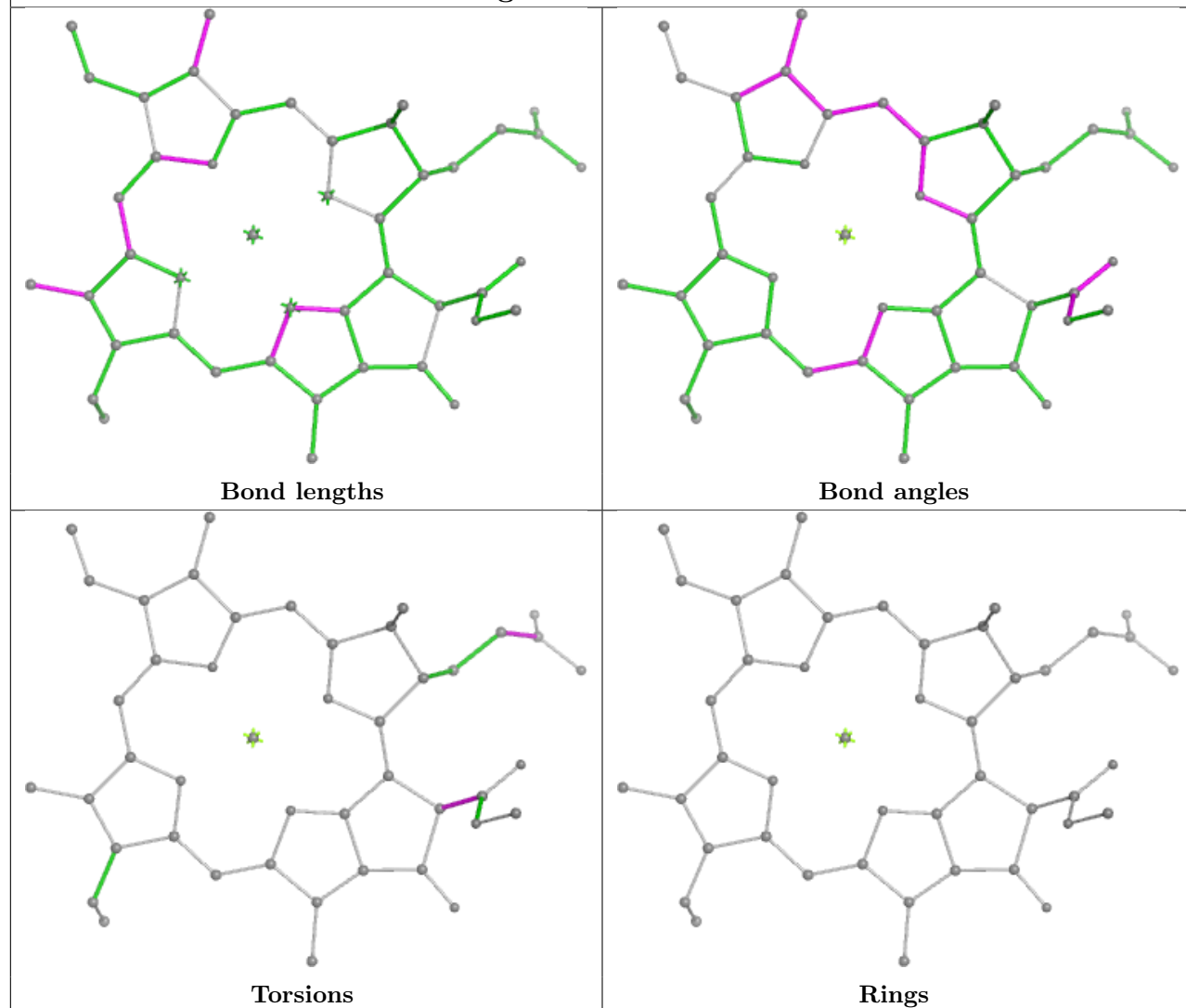


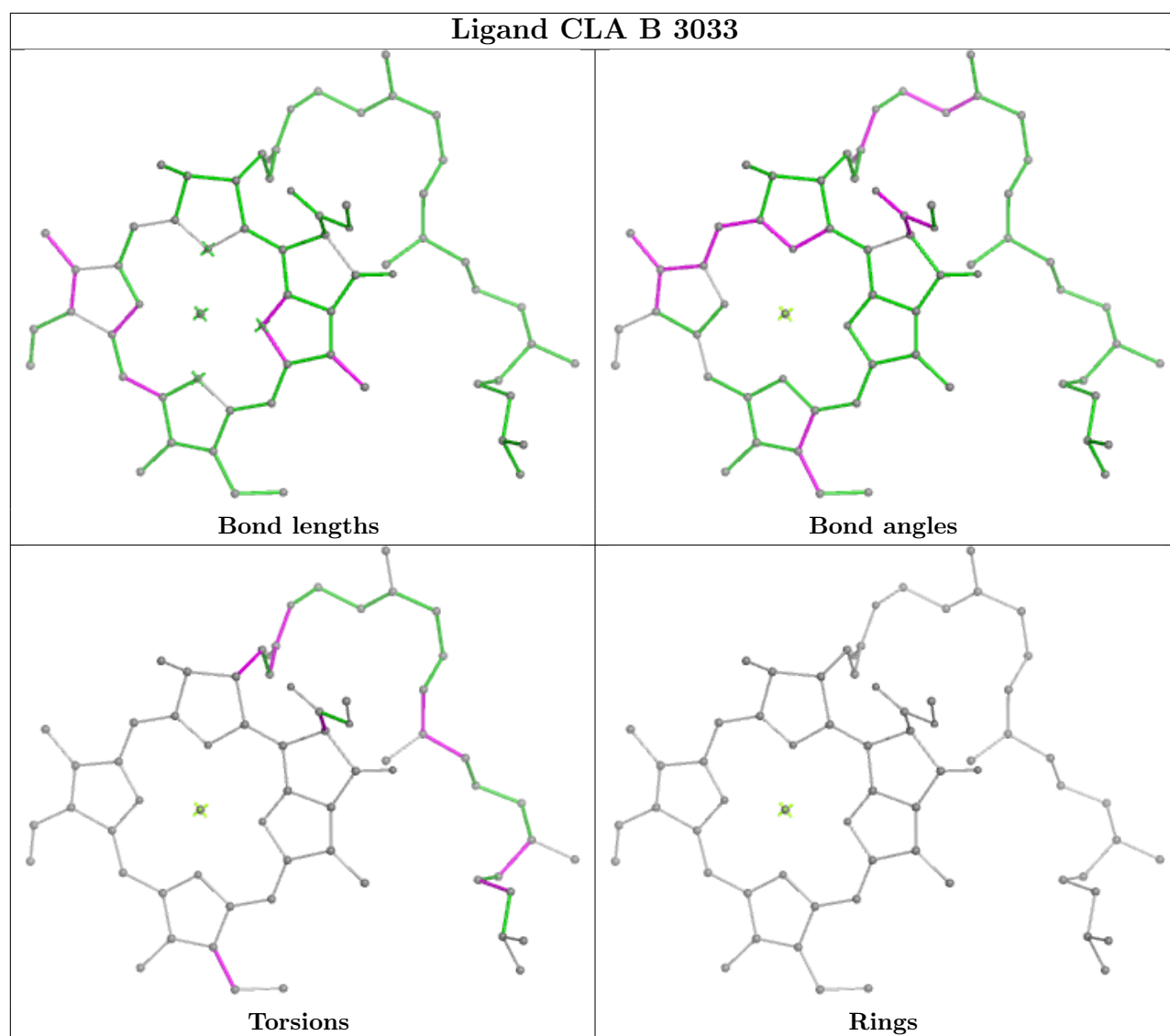
Ligand CL0 a 801**Ligand CLA A 839**

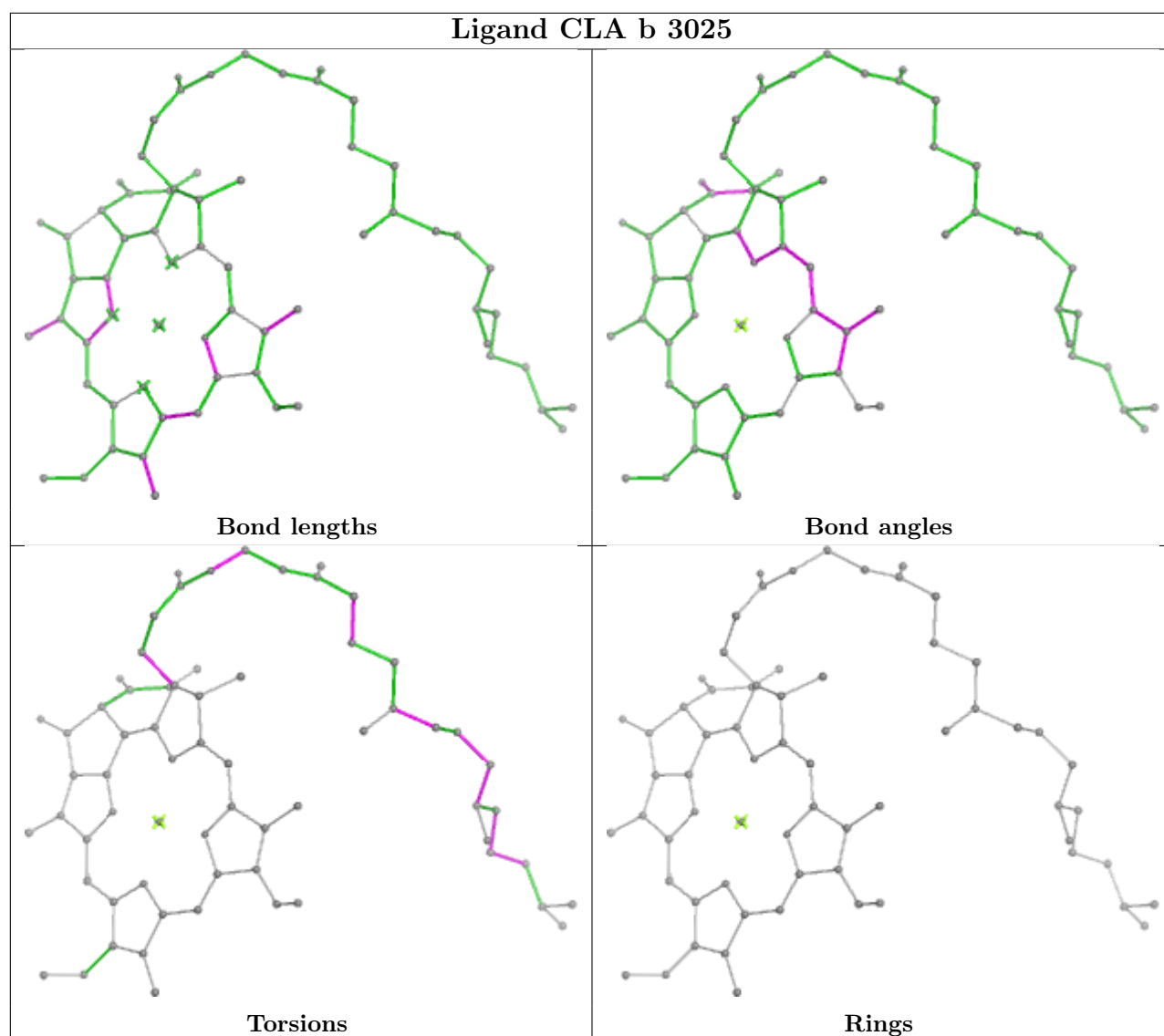


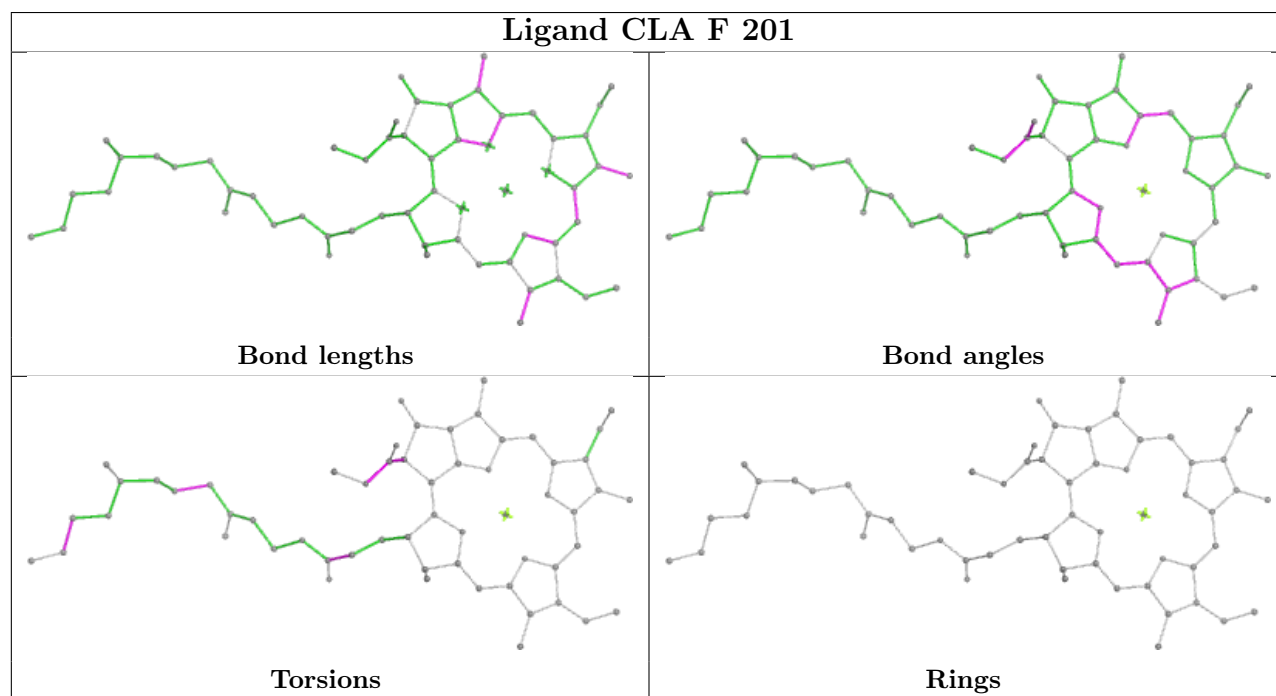
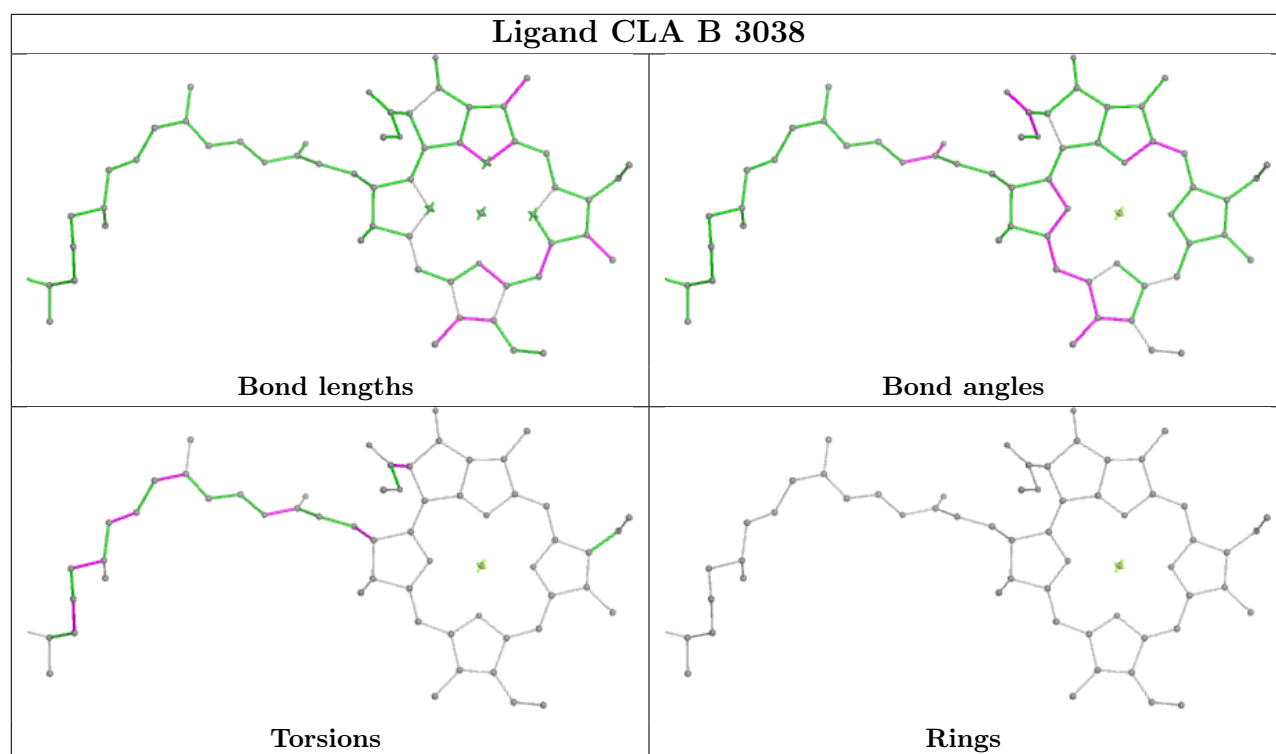


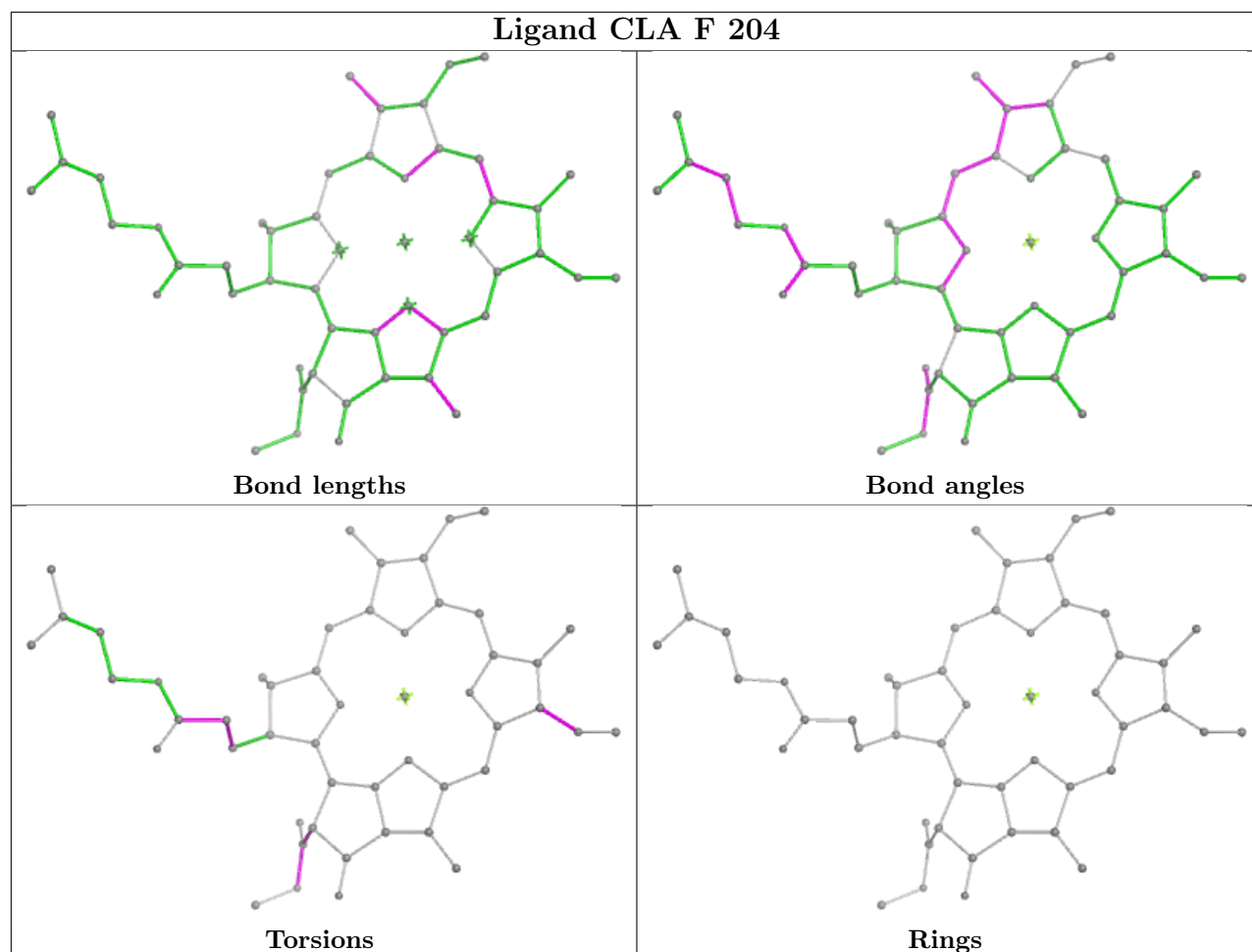
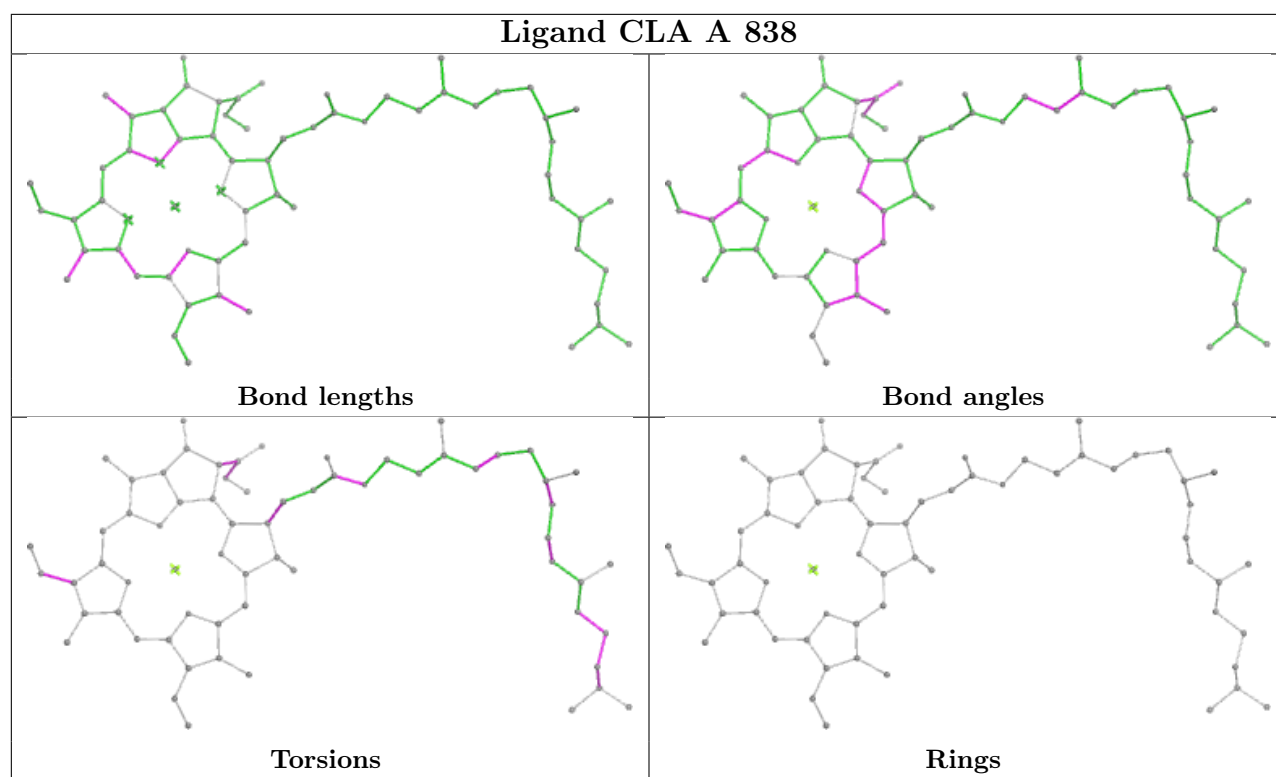
Ligand CLA 1 844

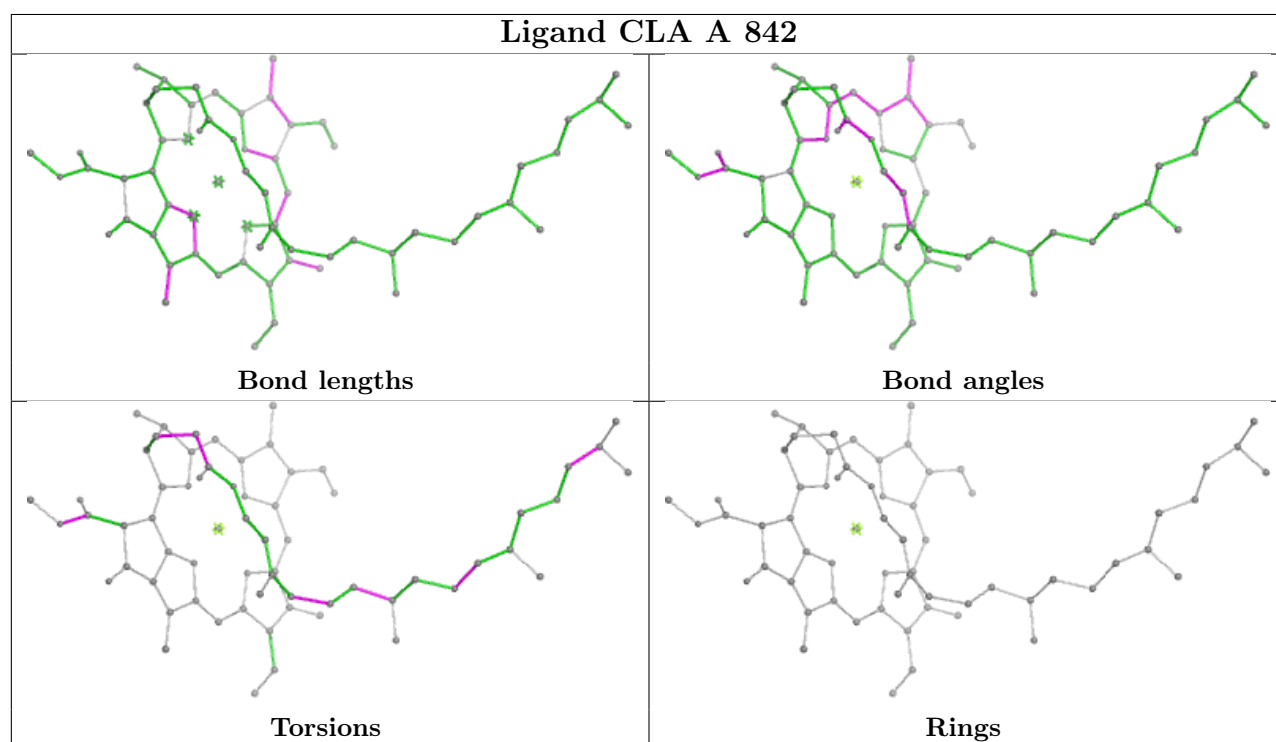
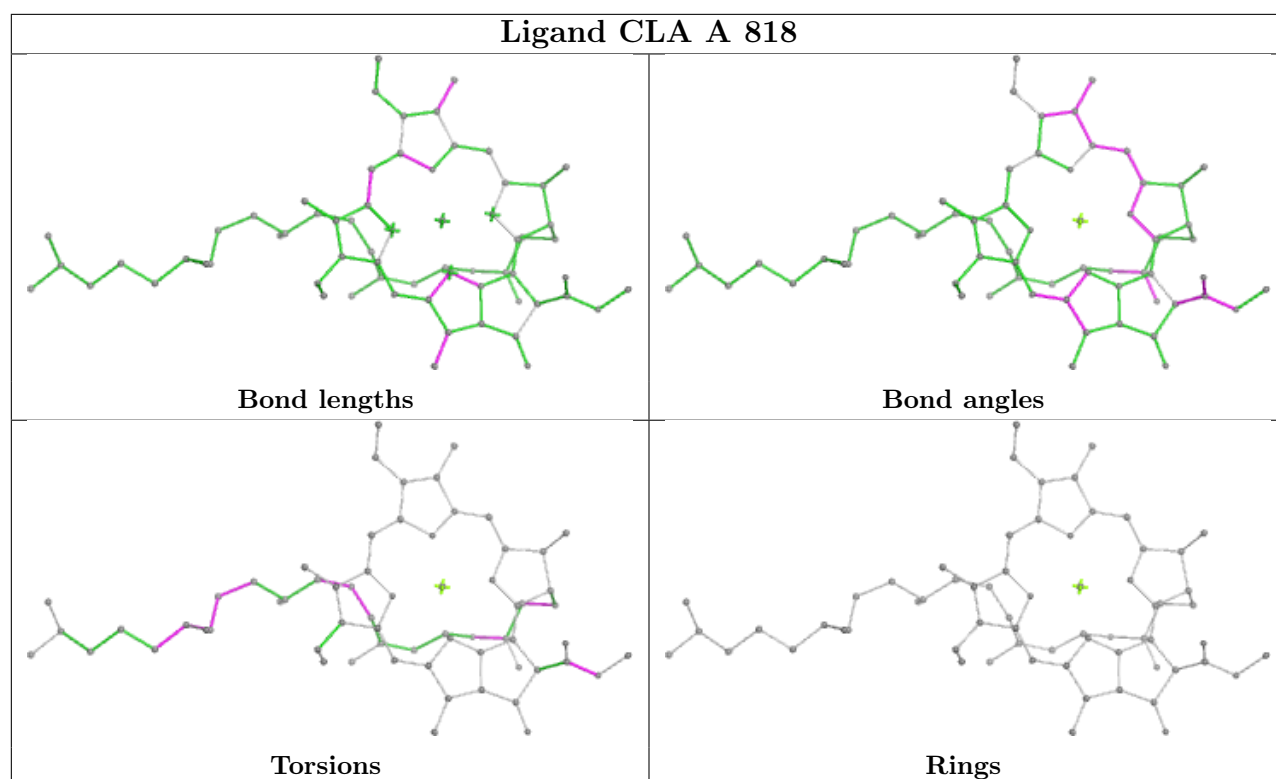


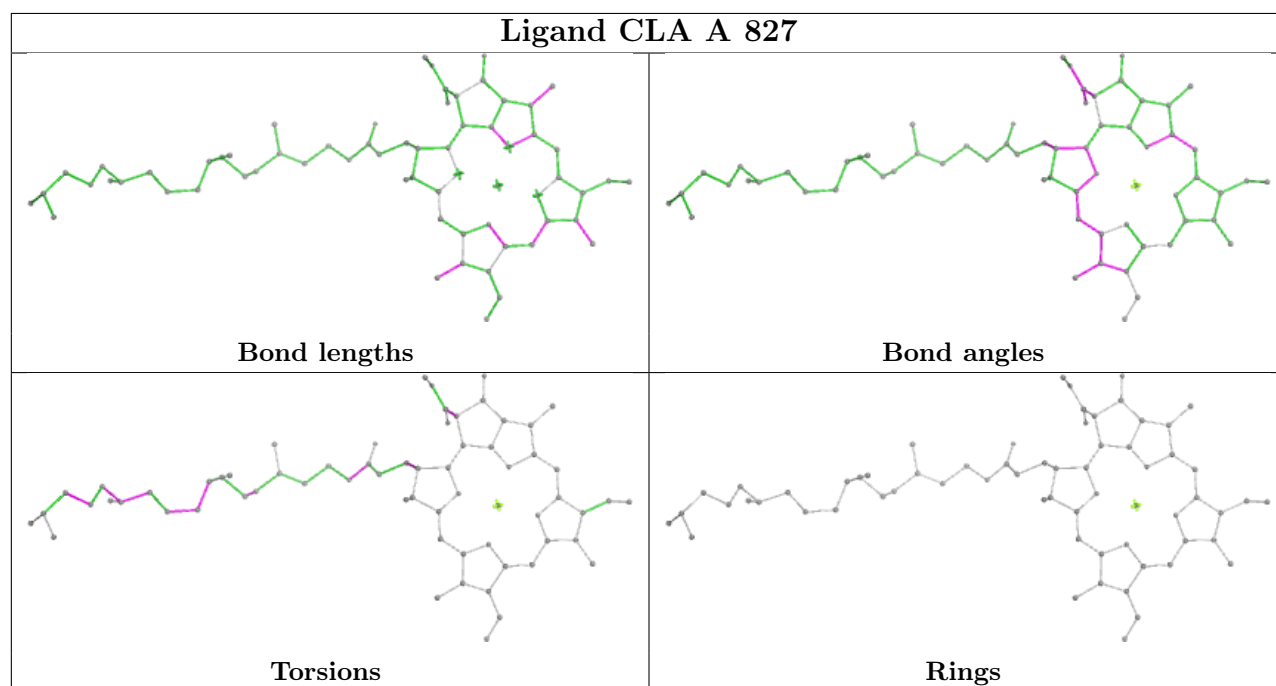
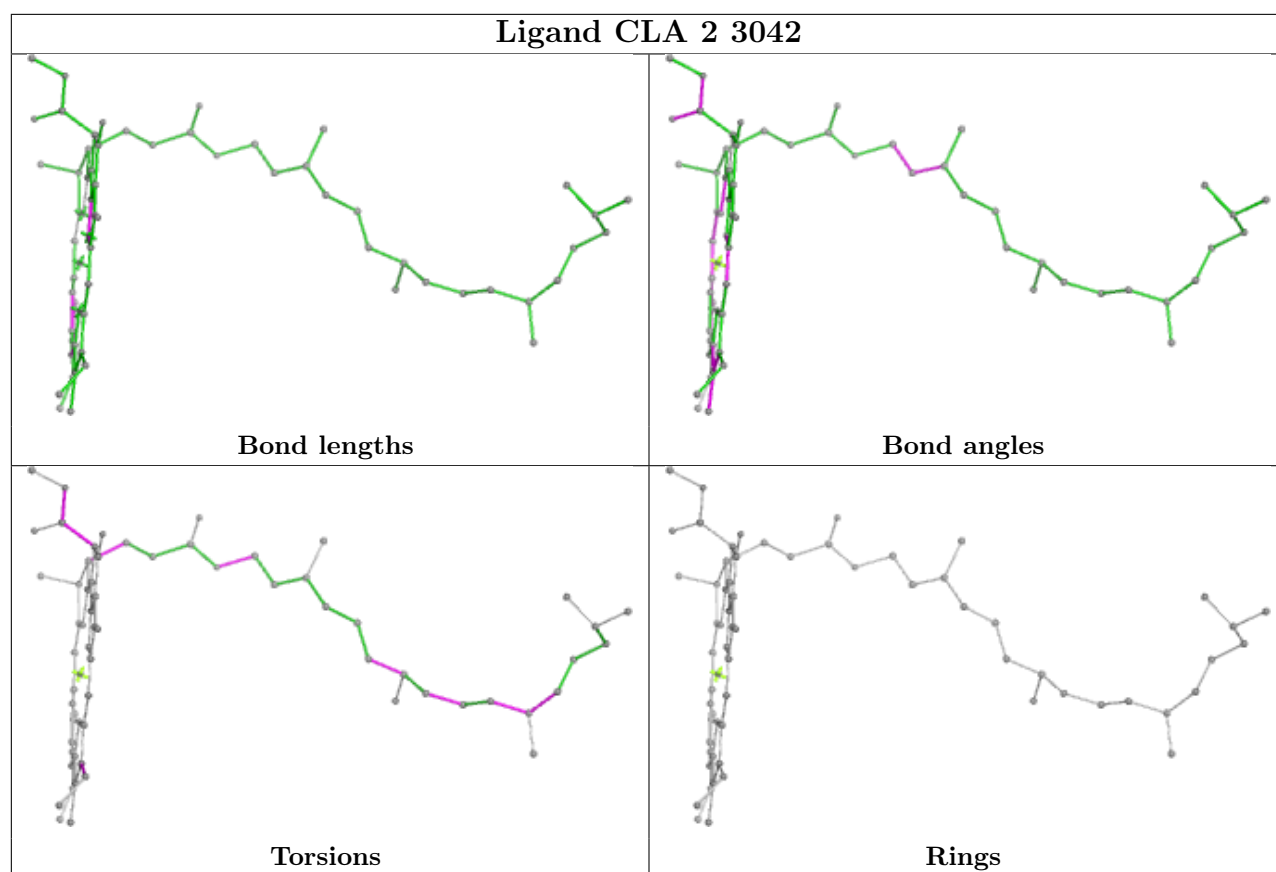


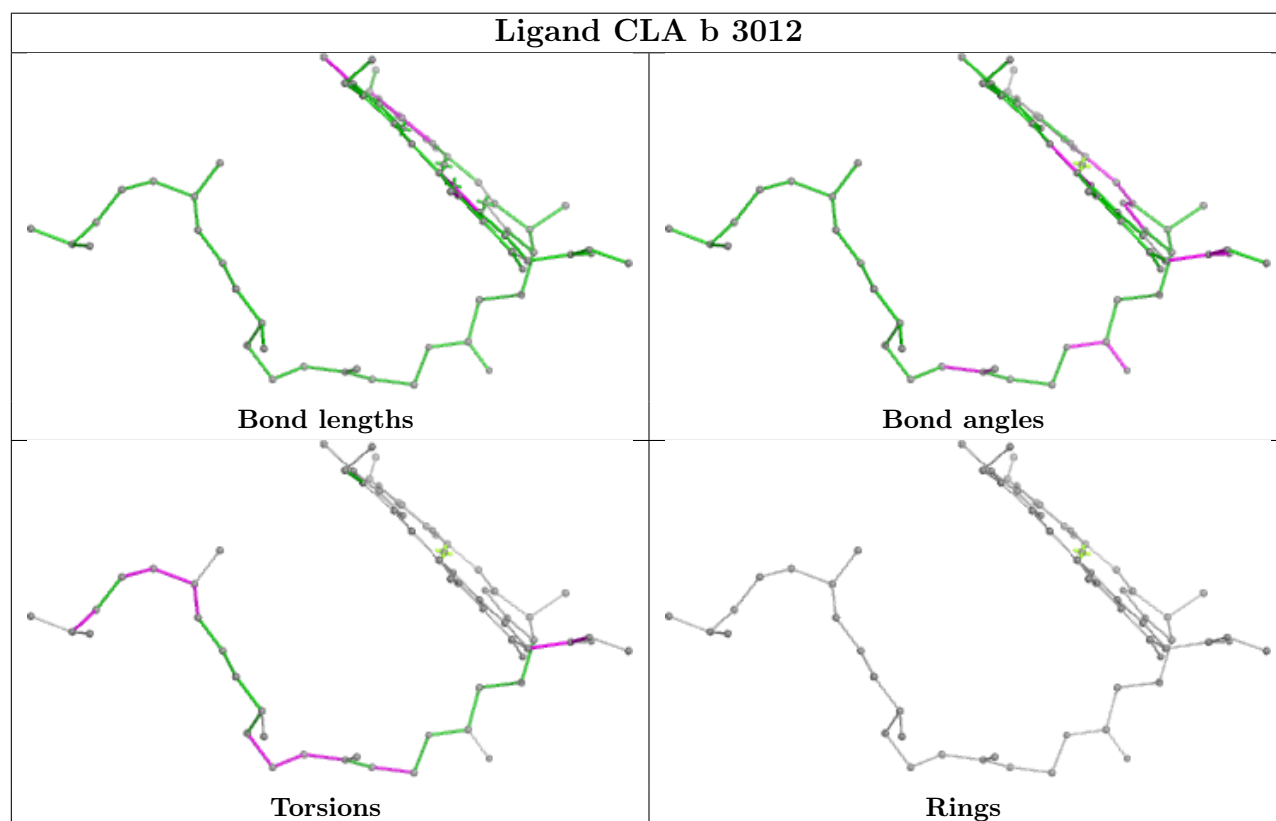
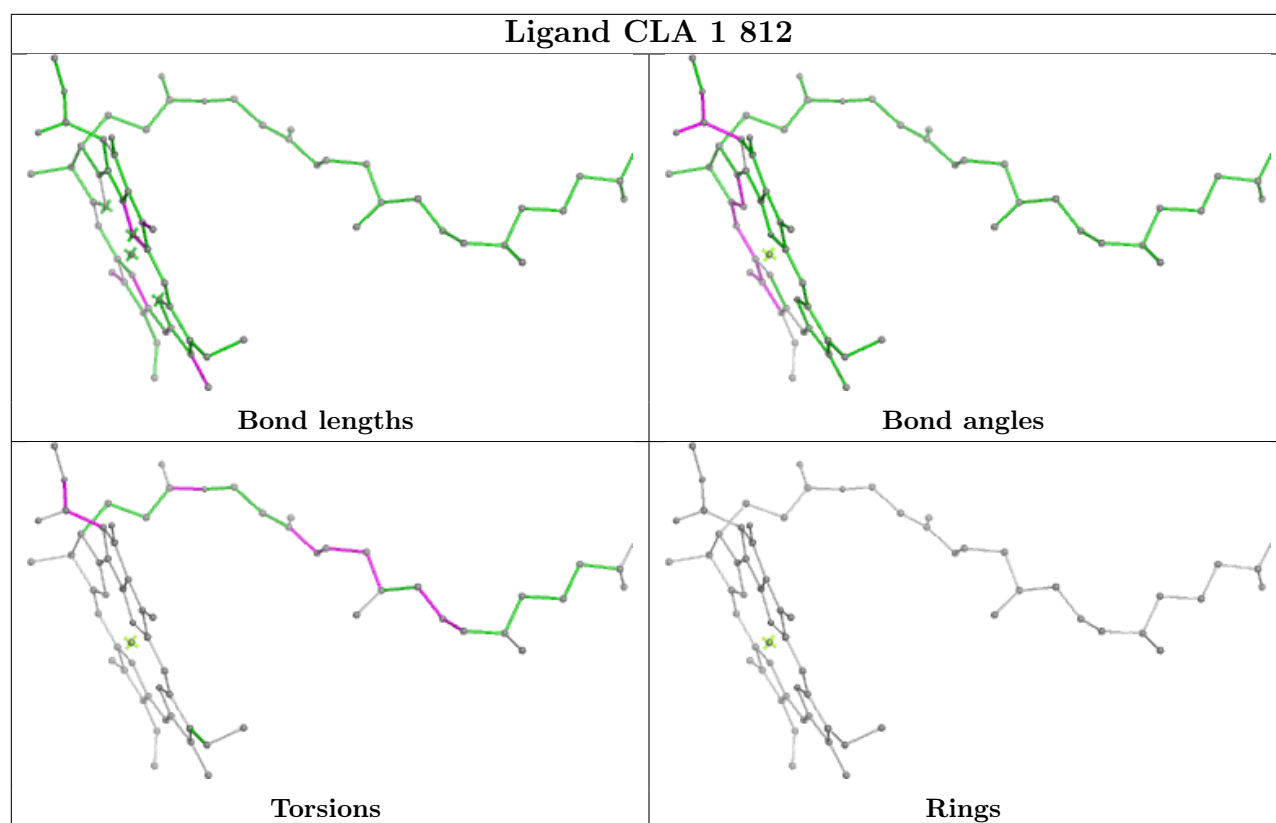


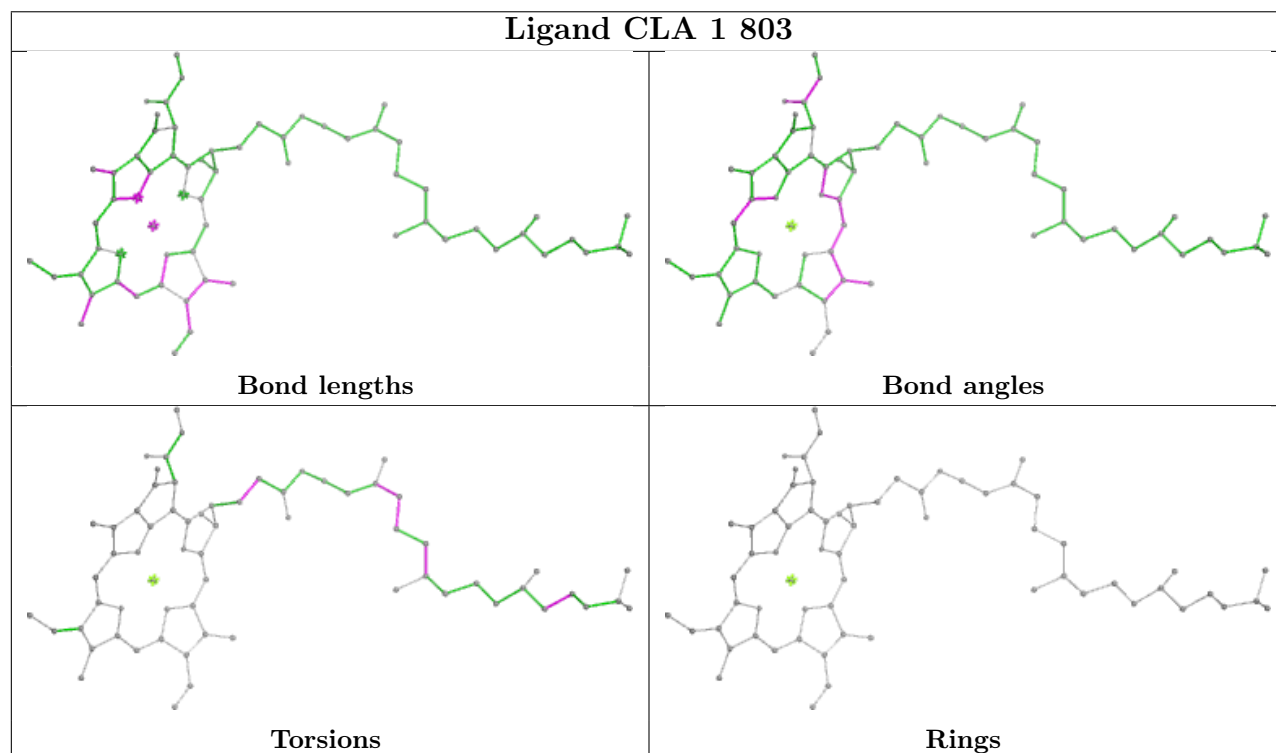
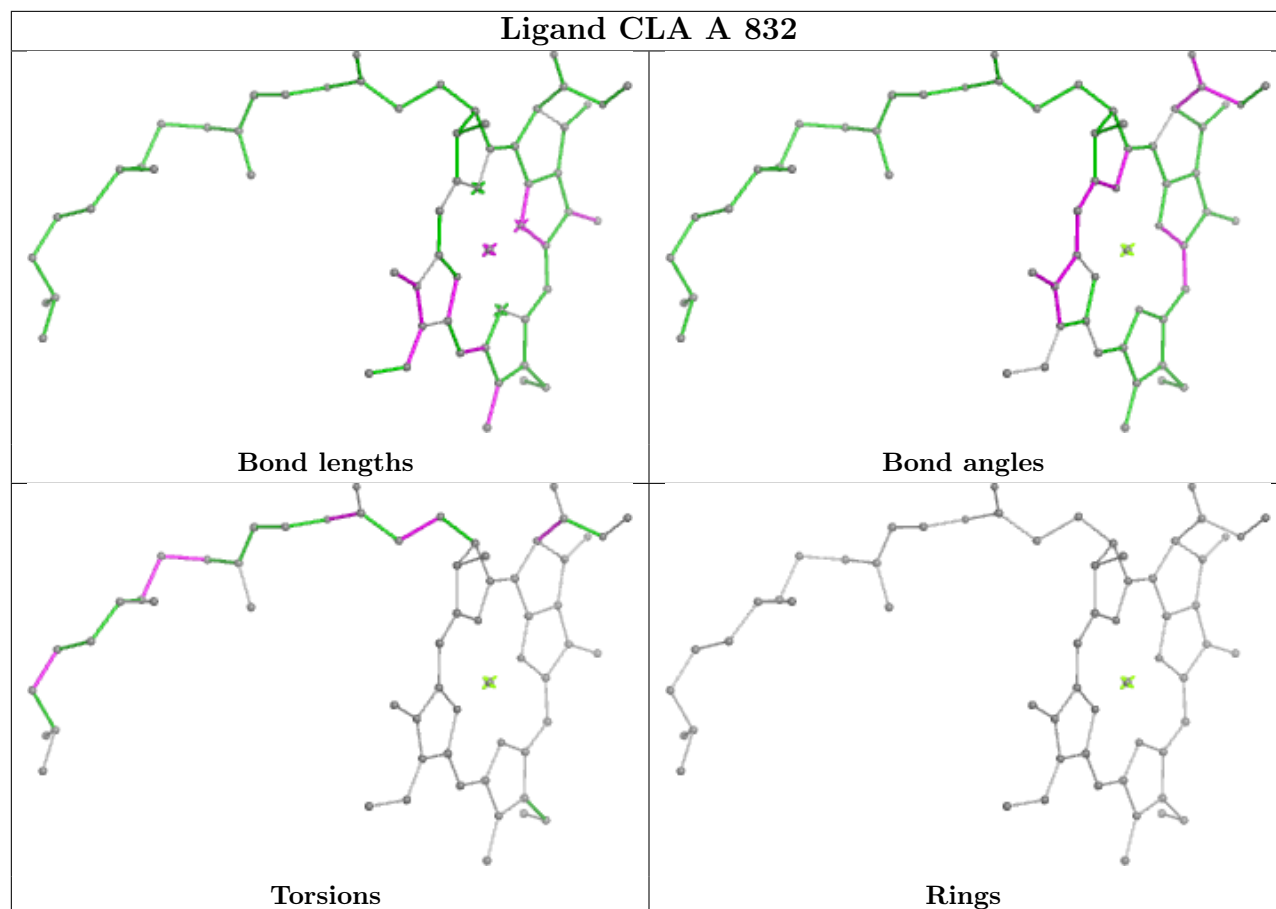


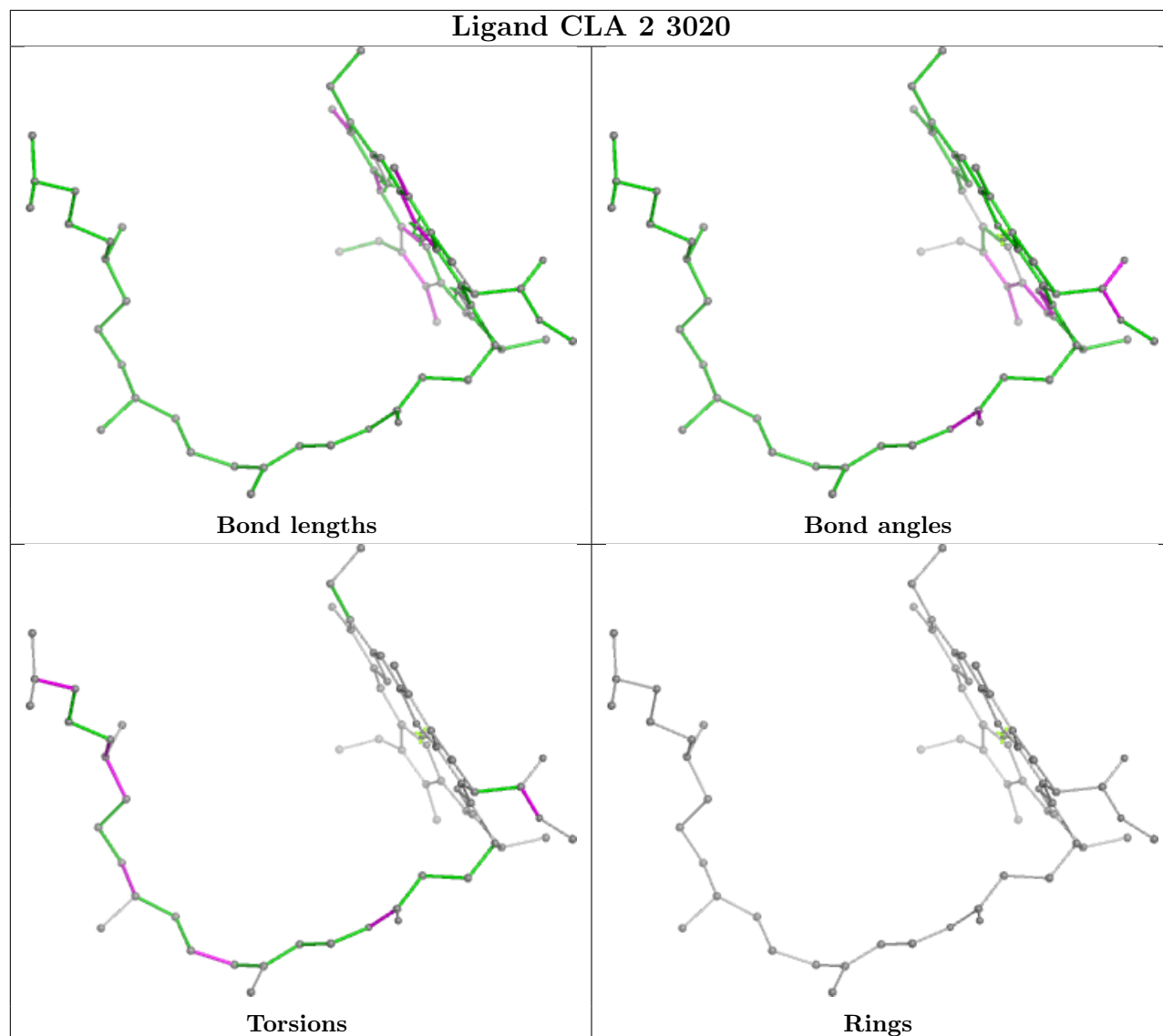




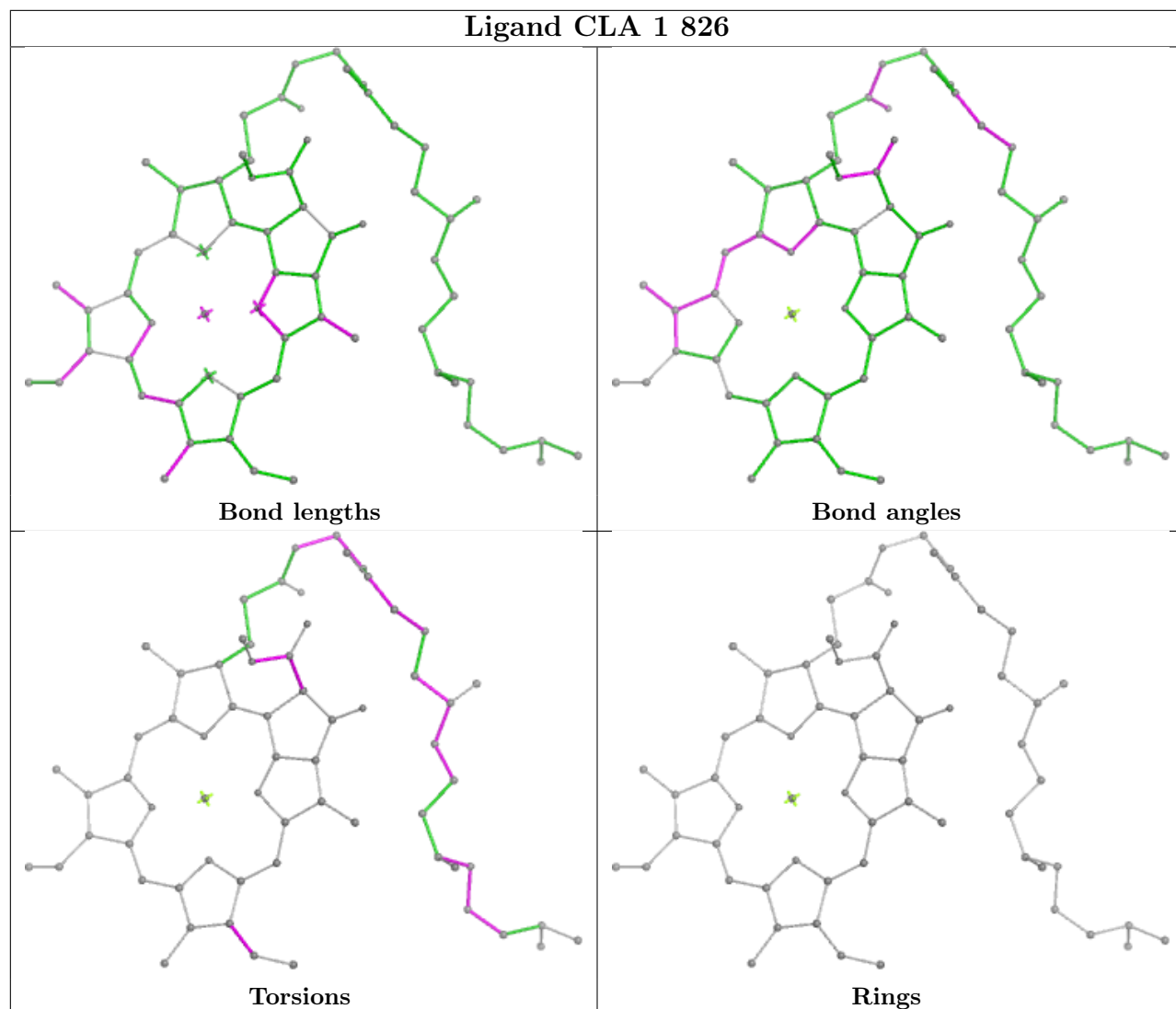


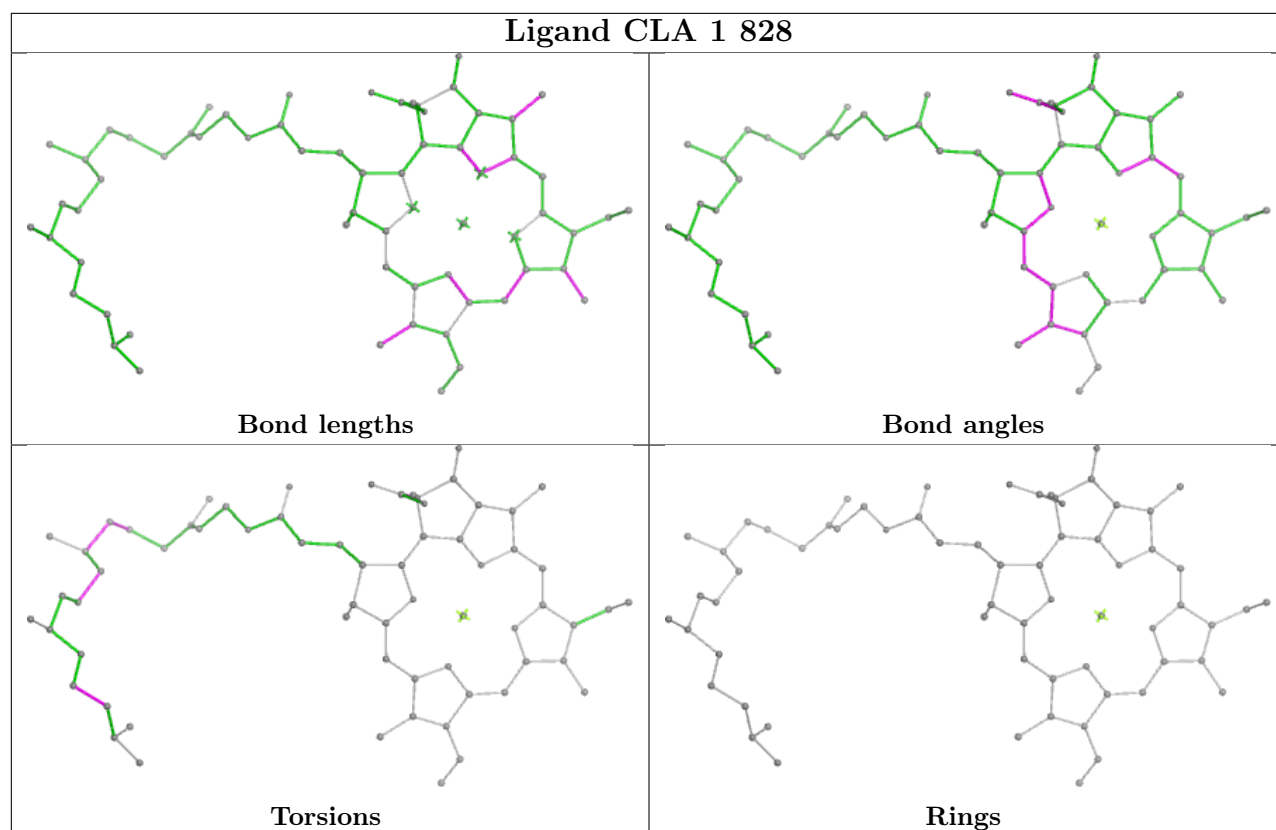
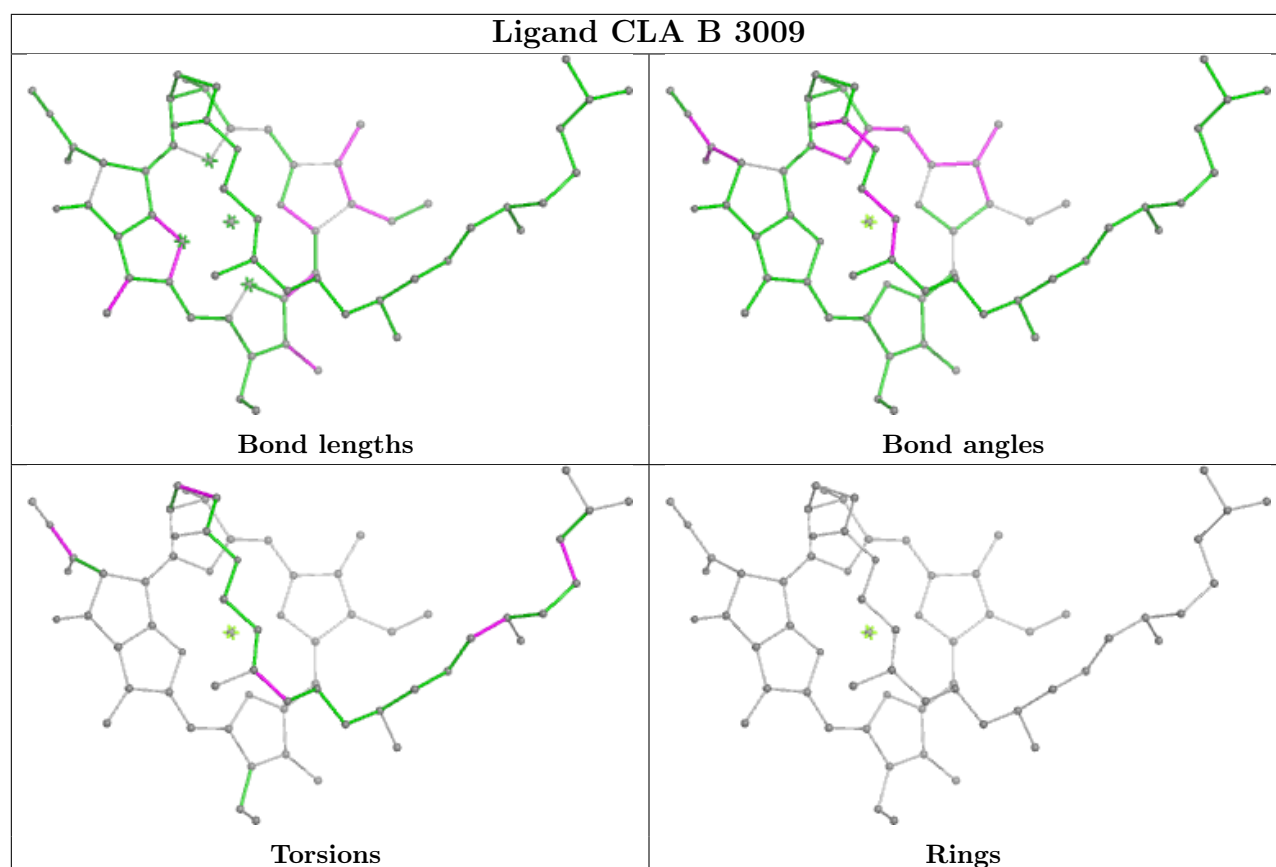


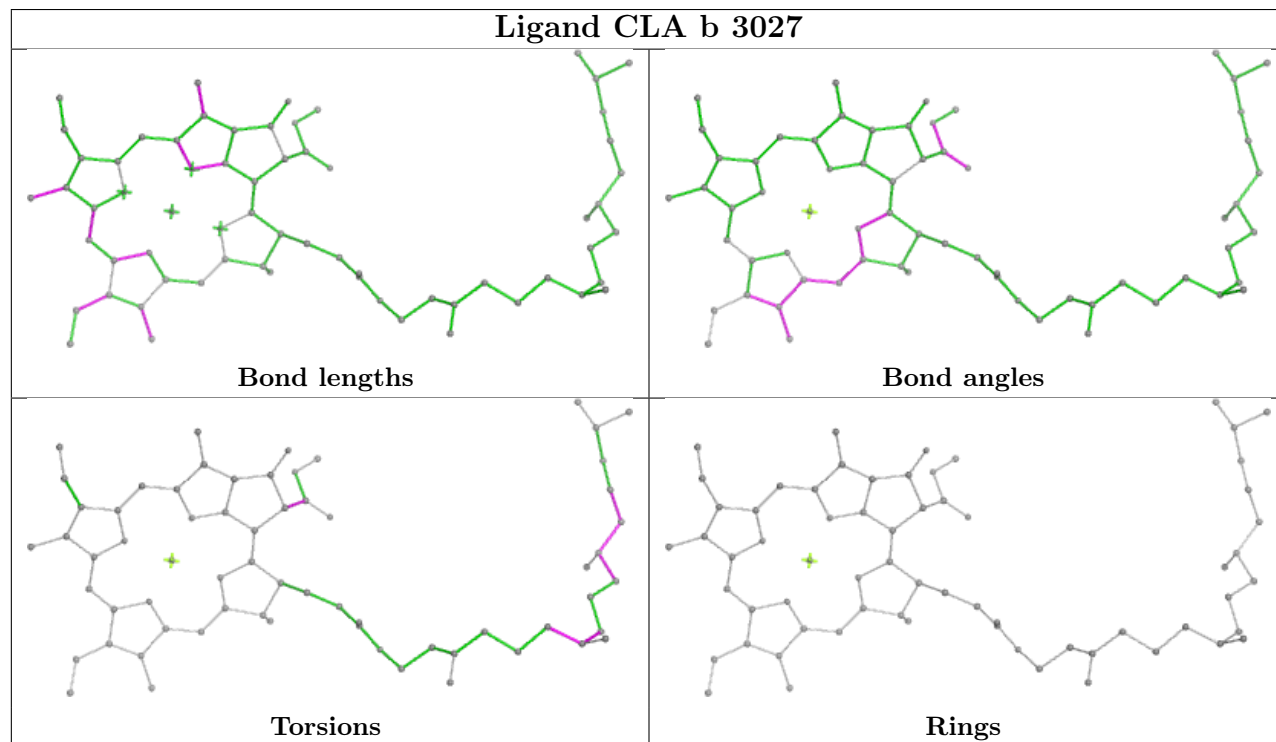
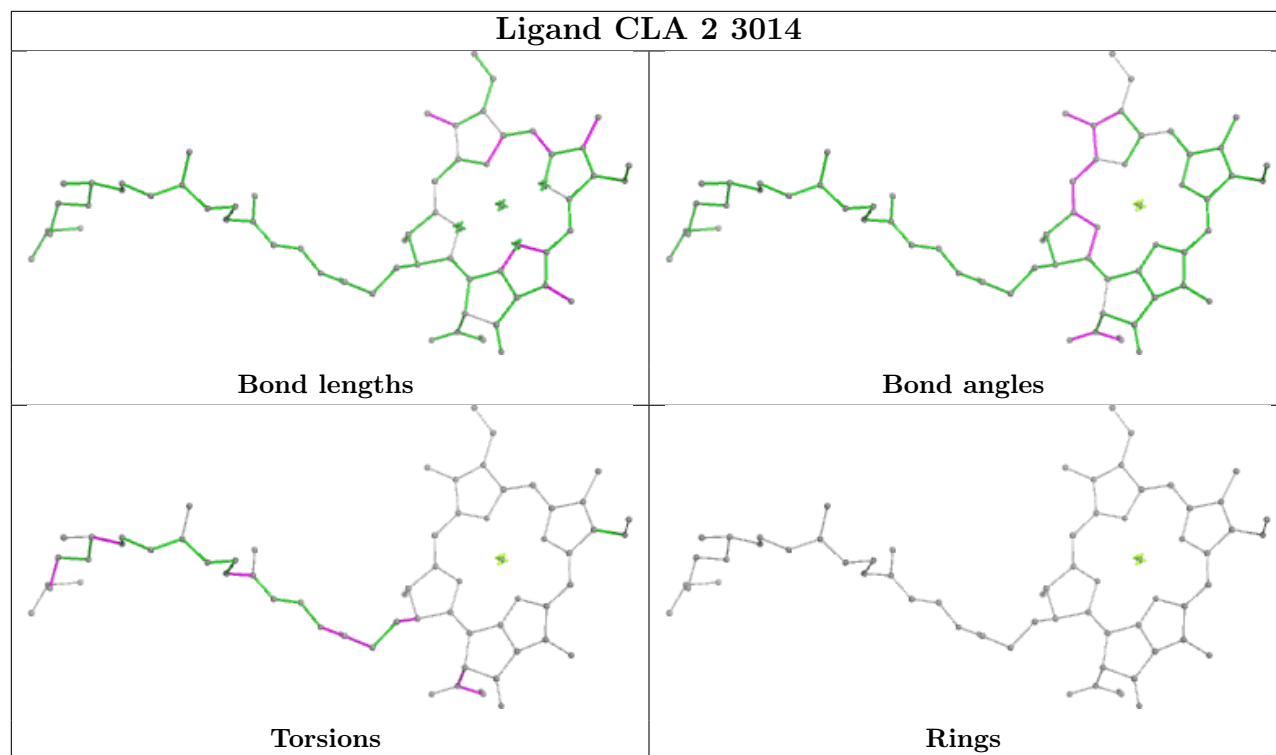


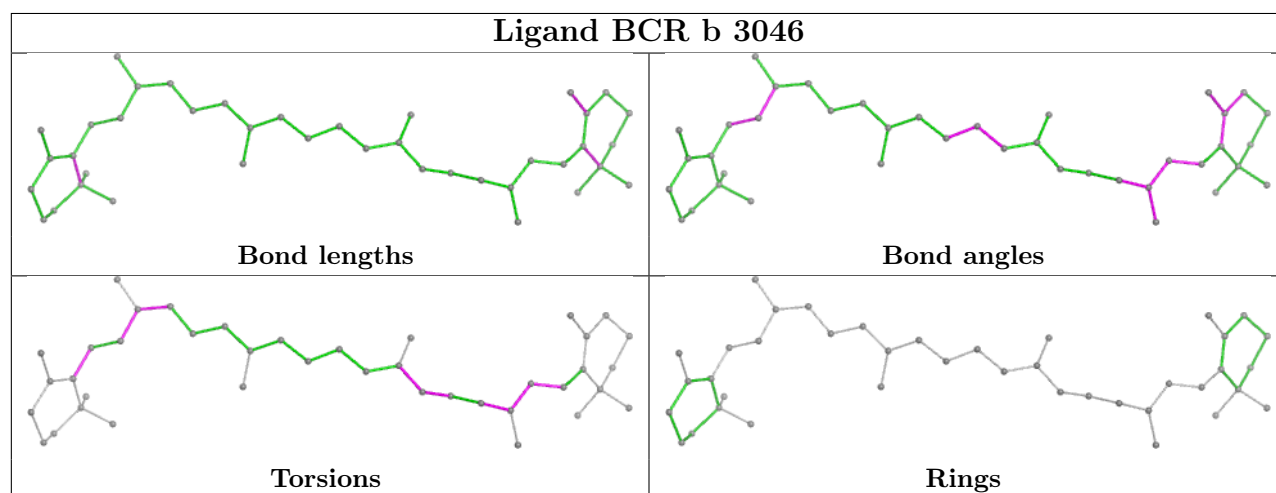
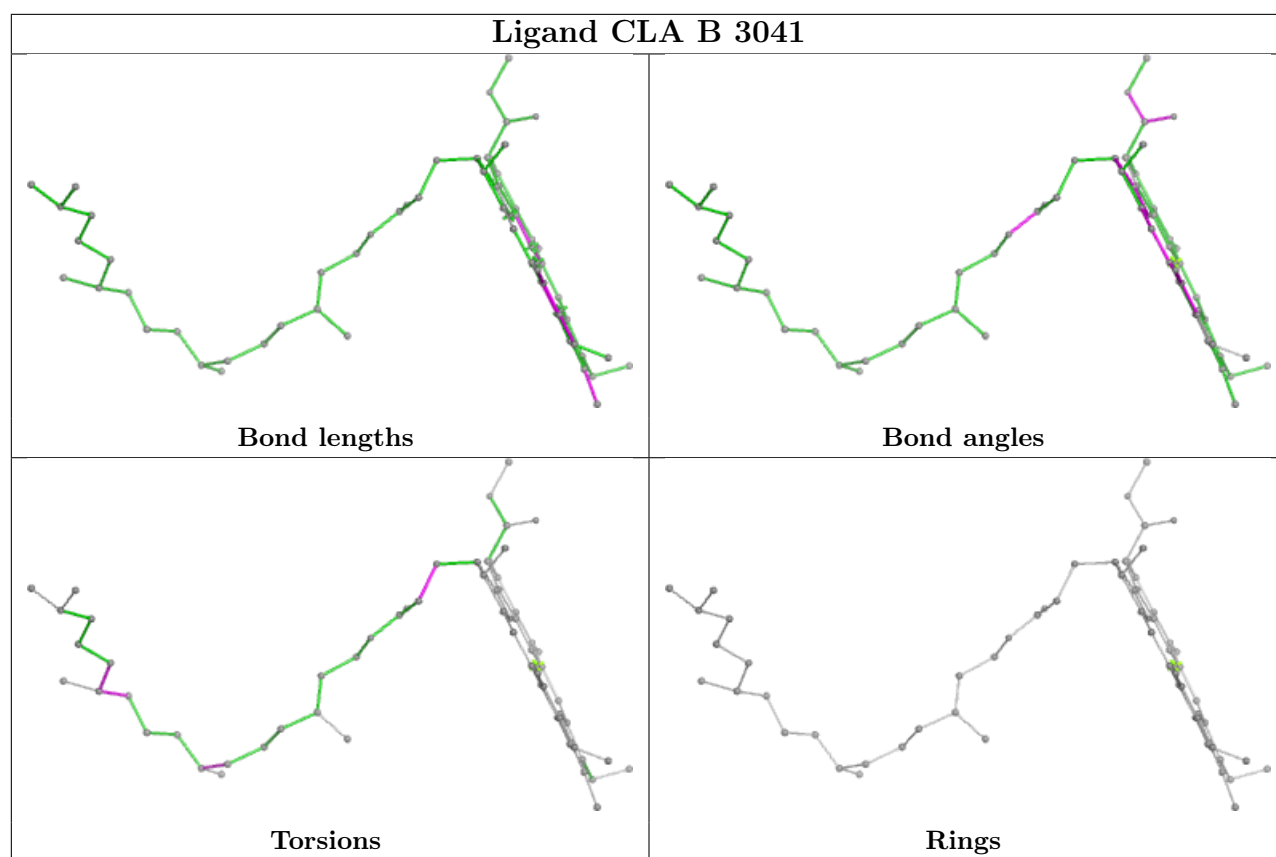


Ligand CLA 1 826

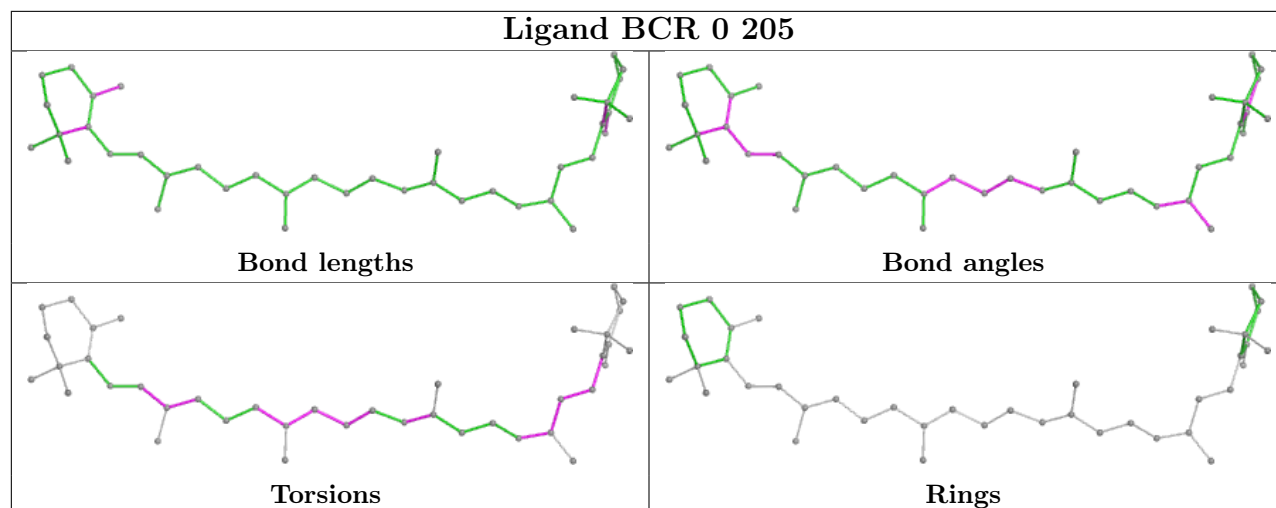




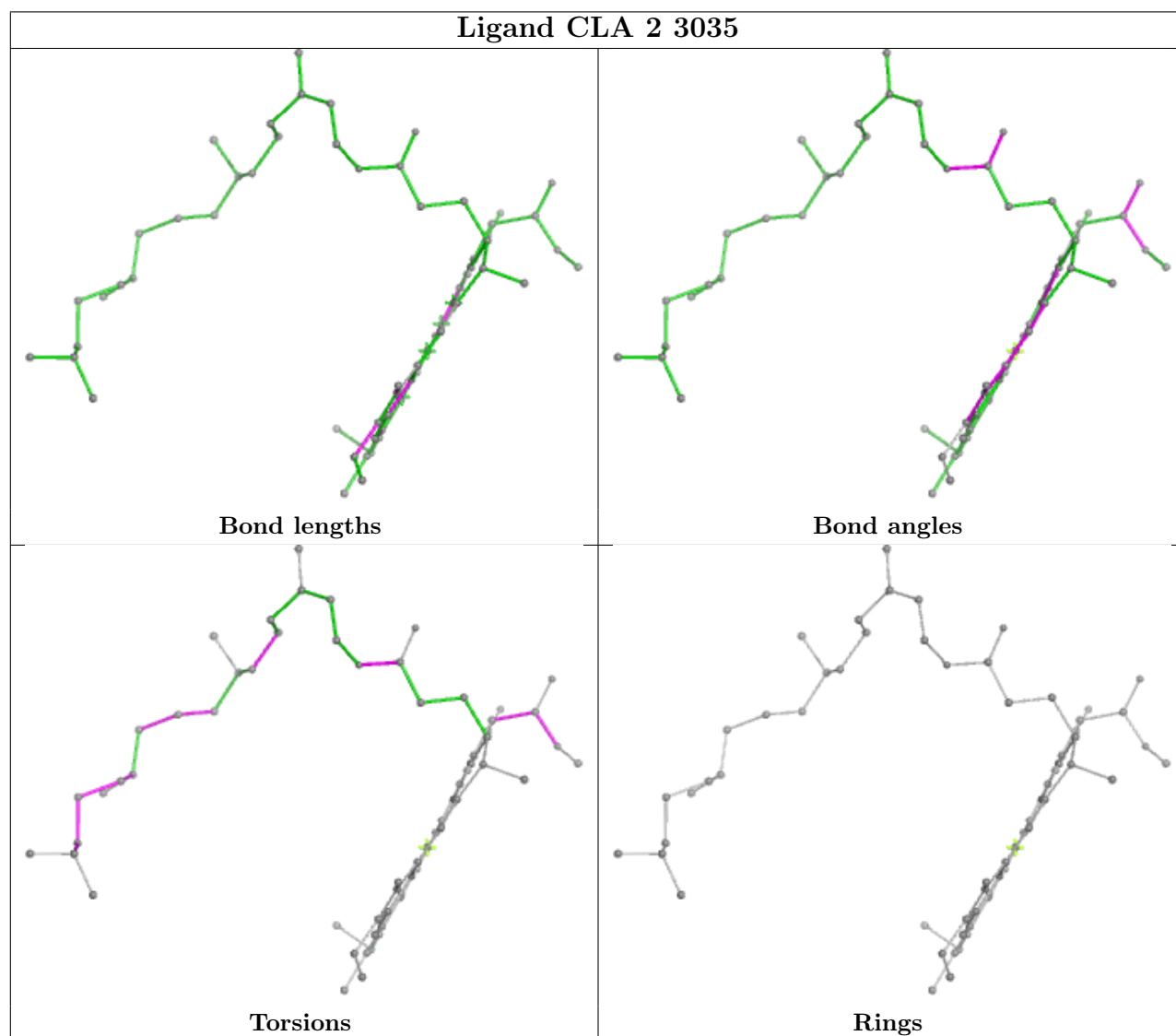


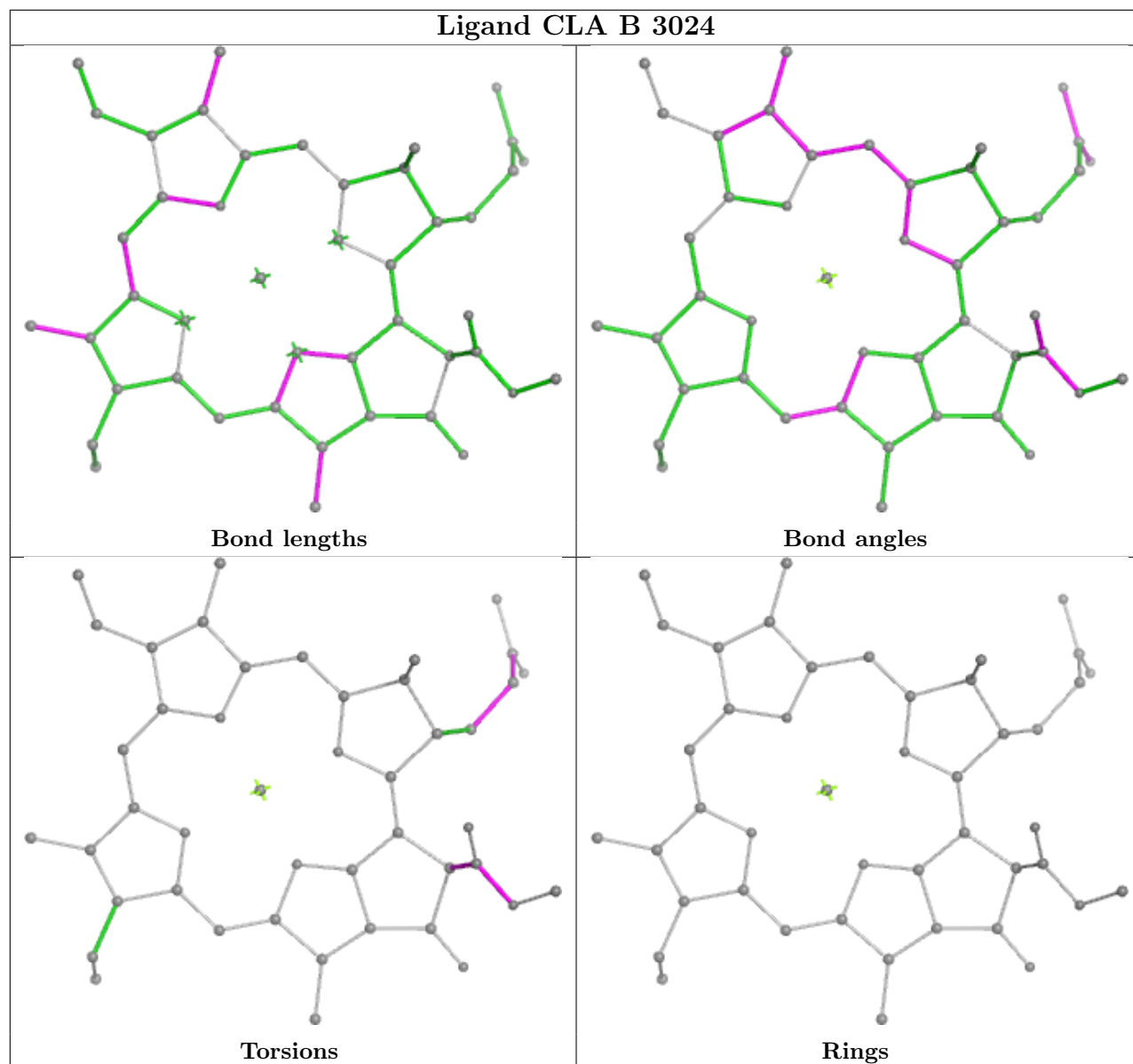


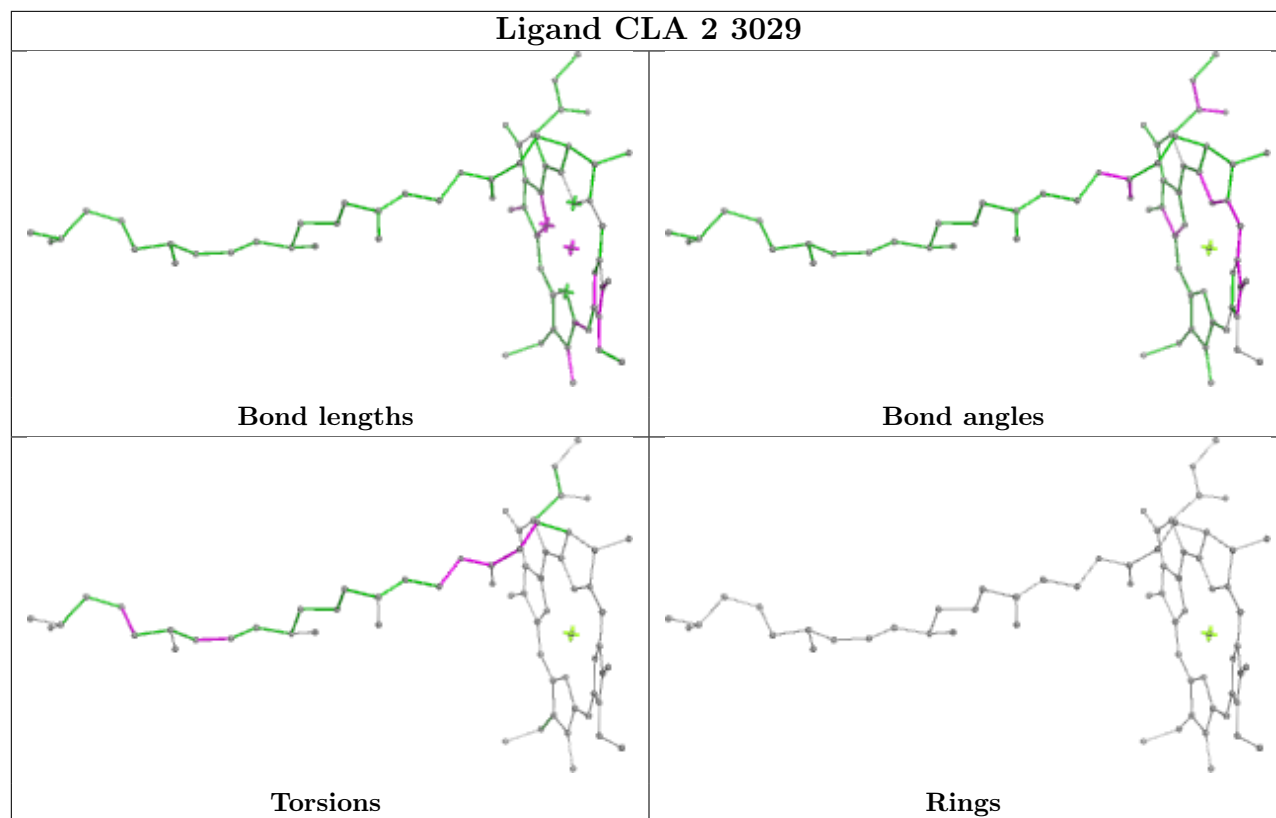
Ligand BCR 0 205



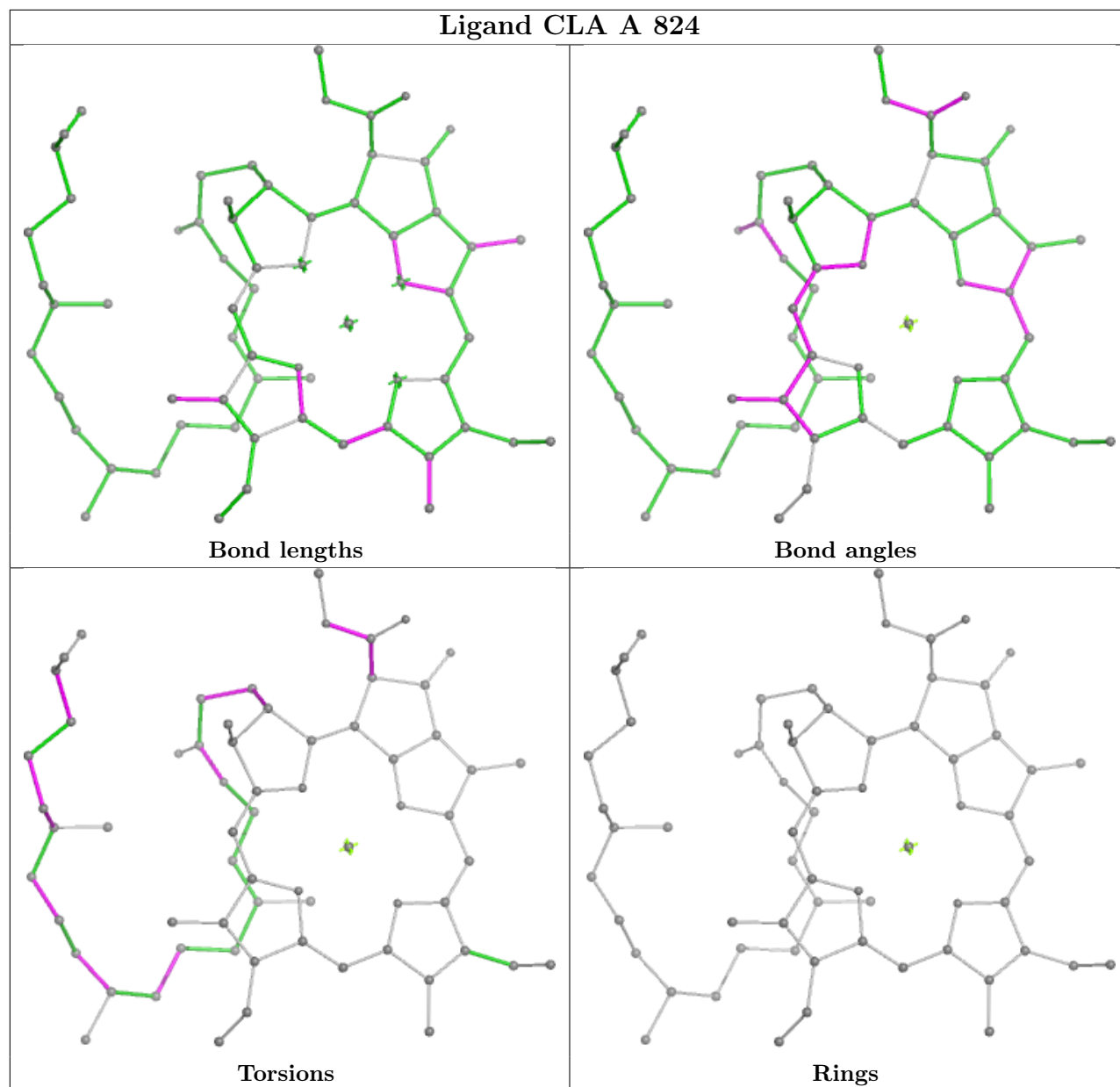
Ligand CLA 2 3035



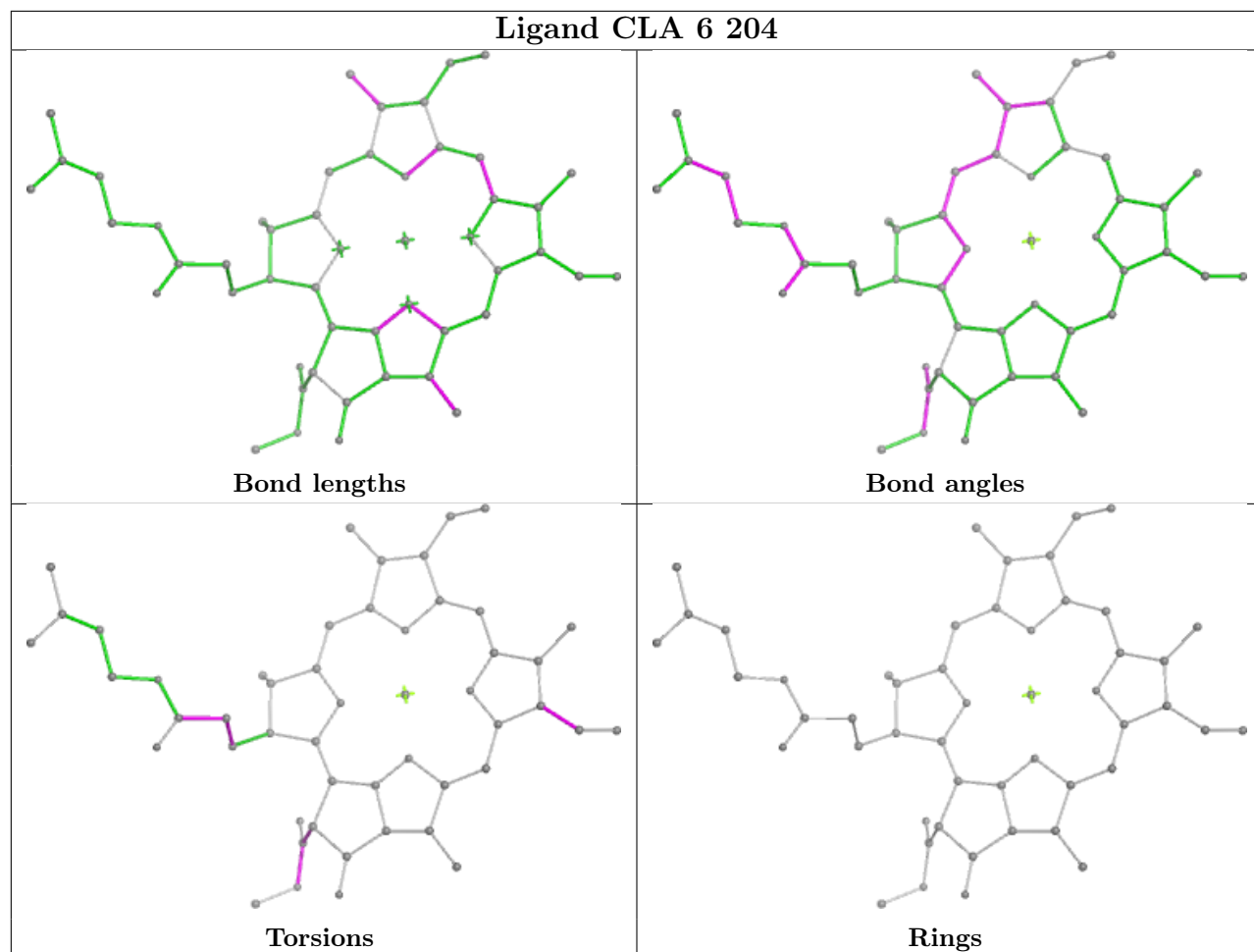


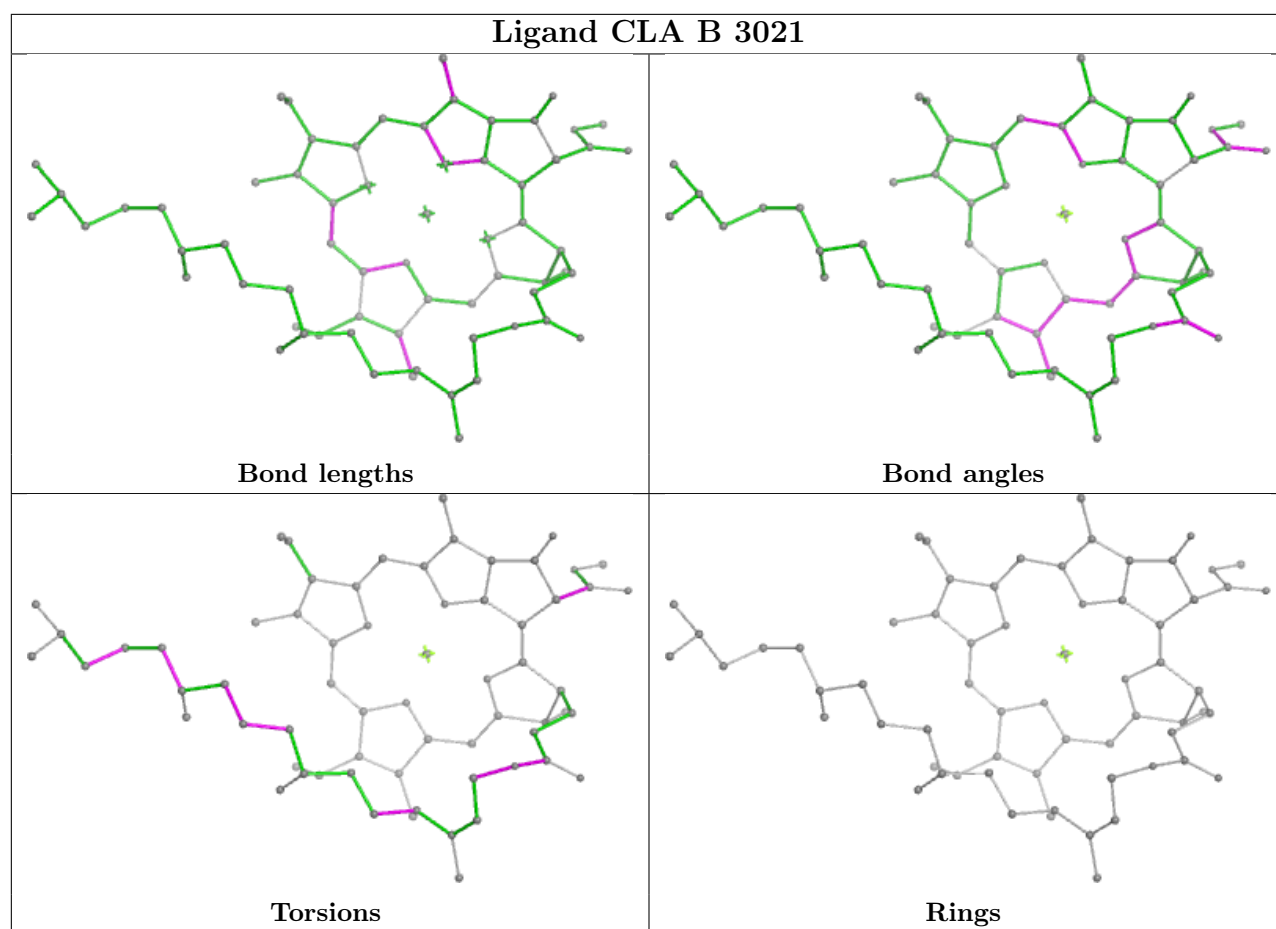


Ligand CLA A 824

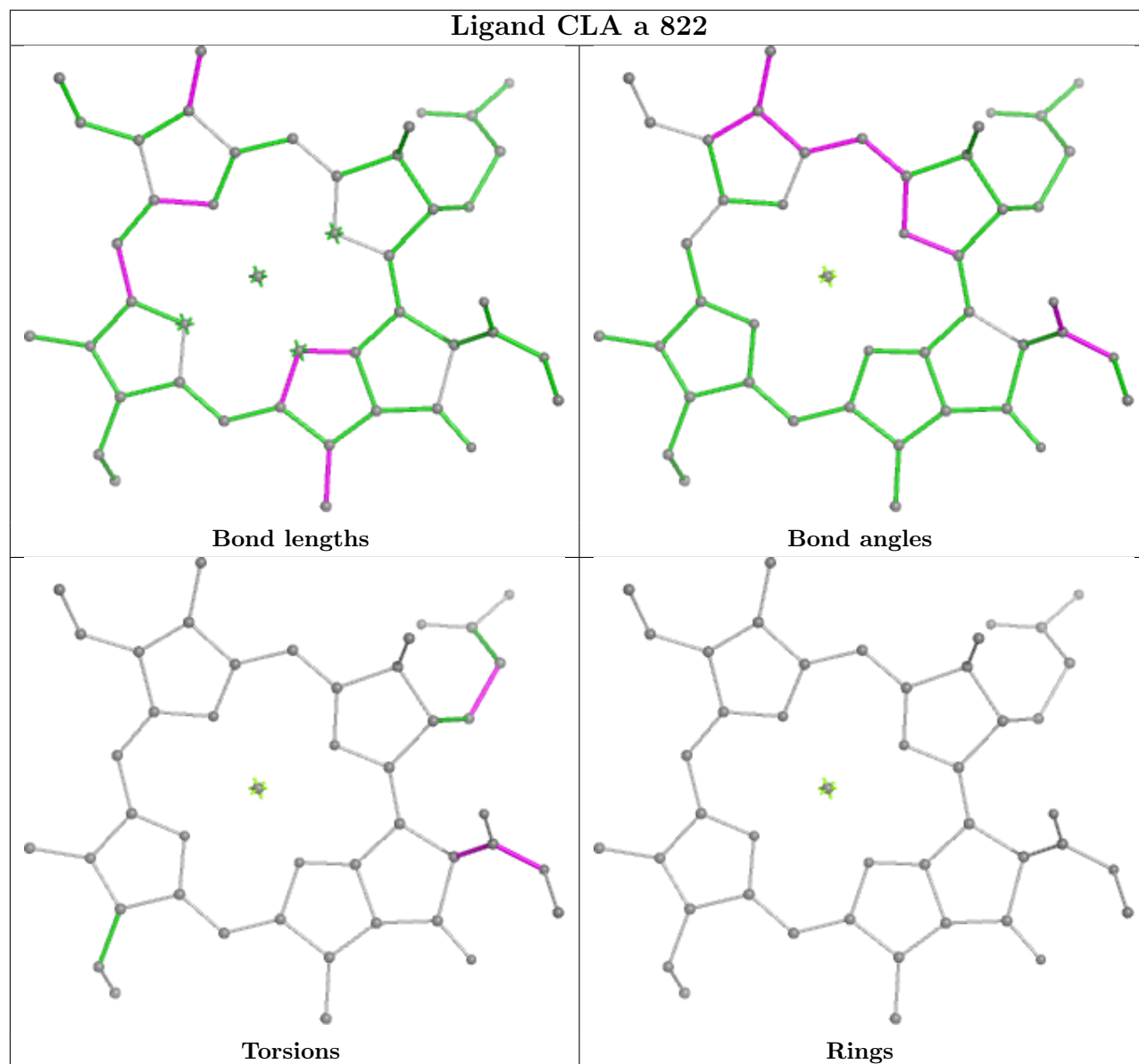


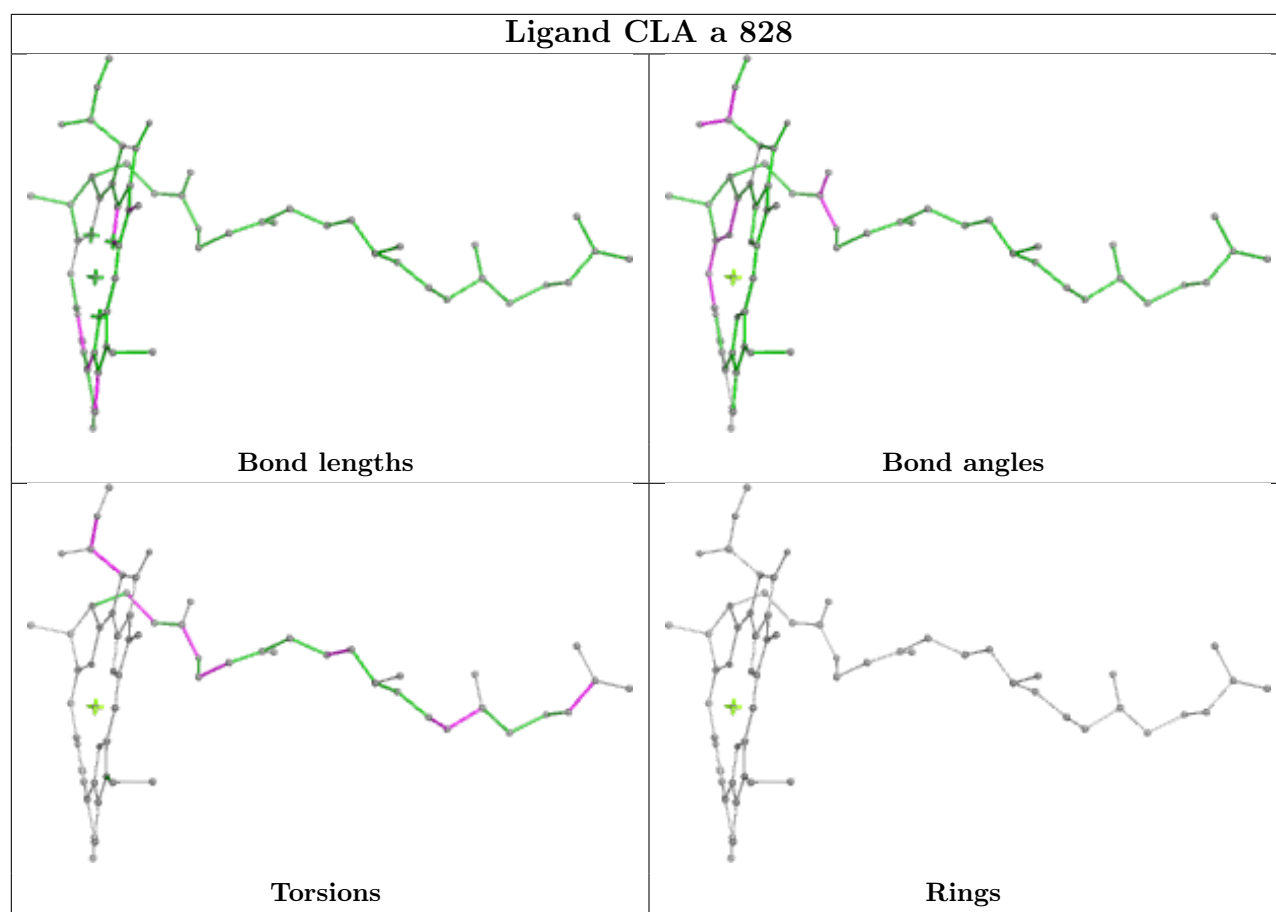
Ligand CLA 6 204

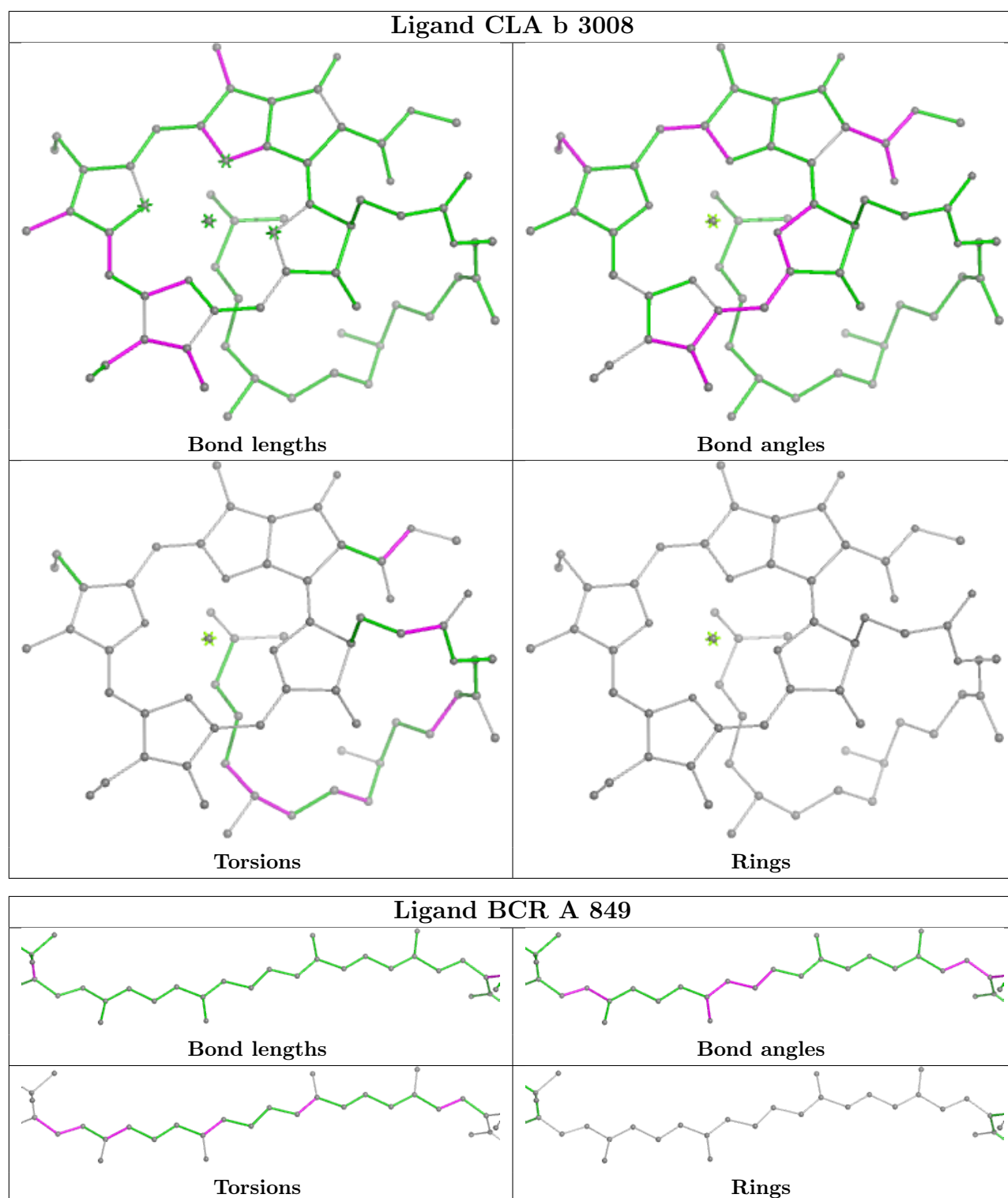


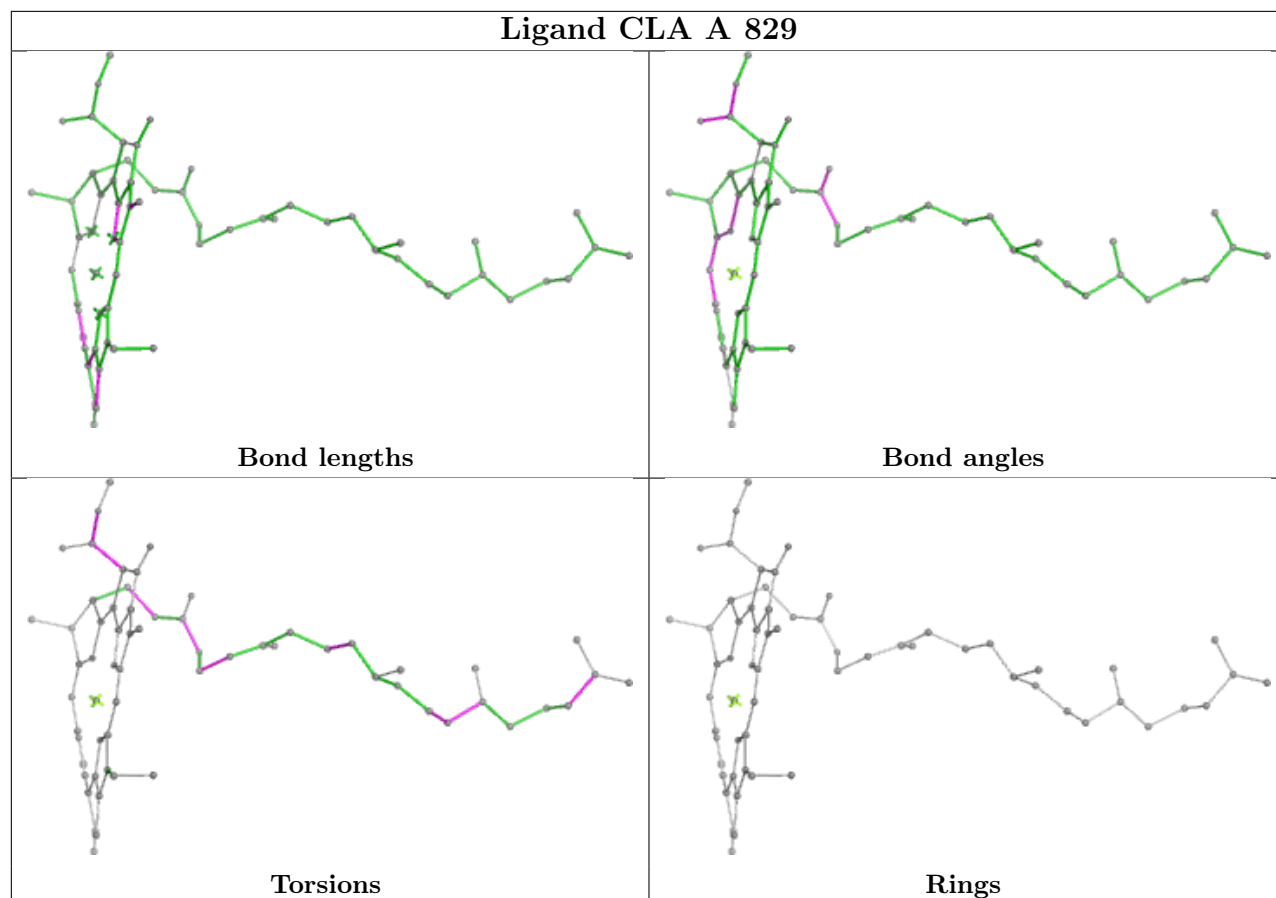
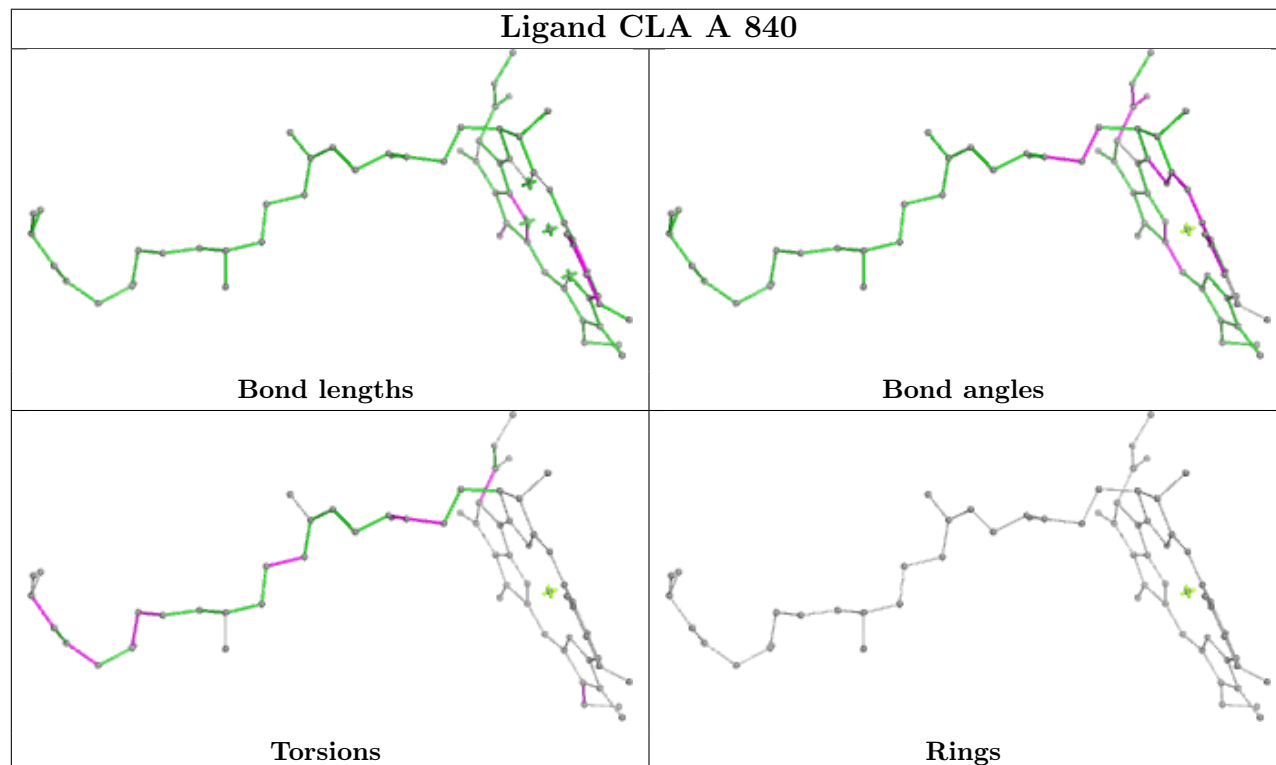


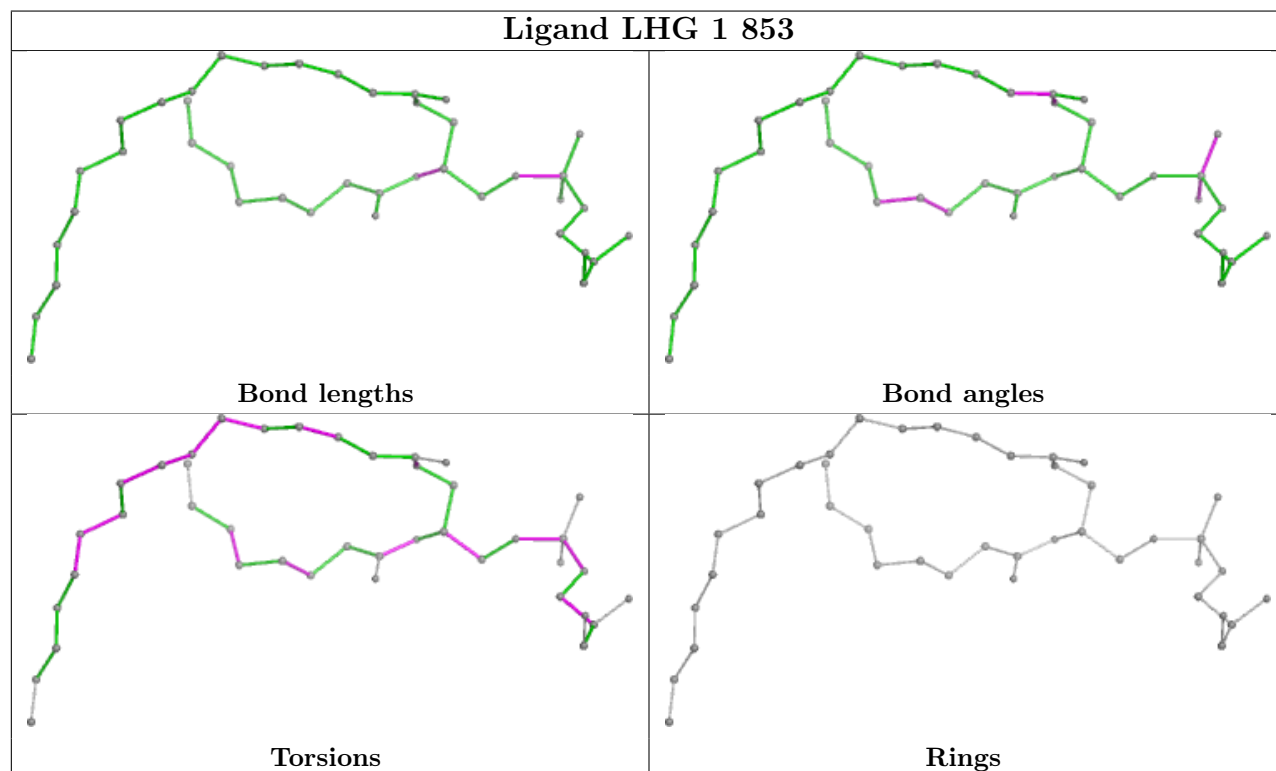
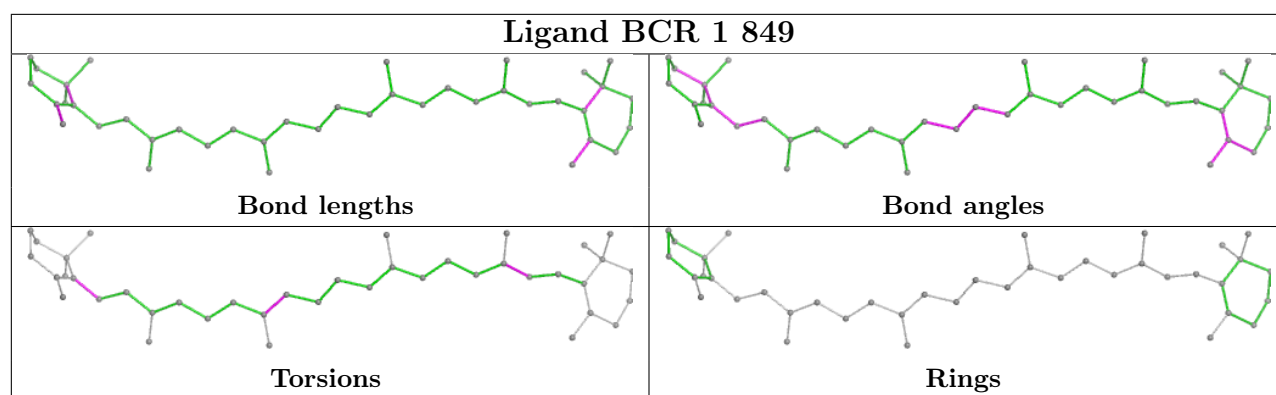
Ligand CLA a 822



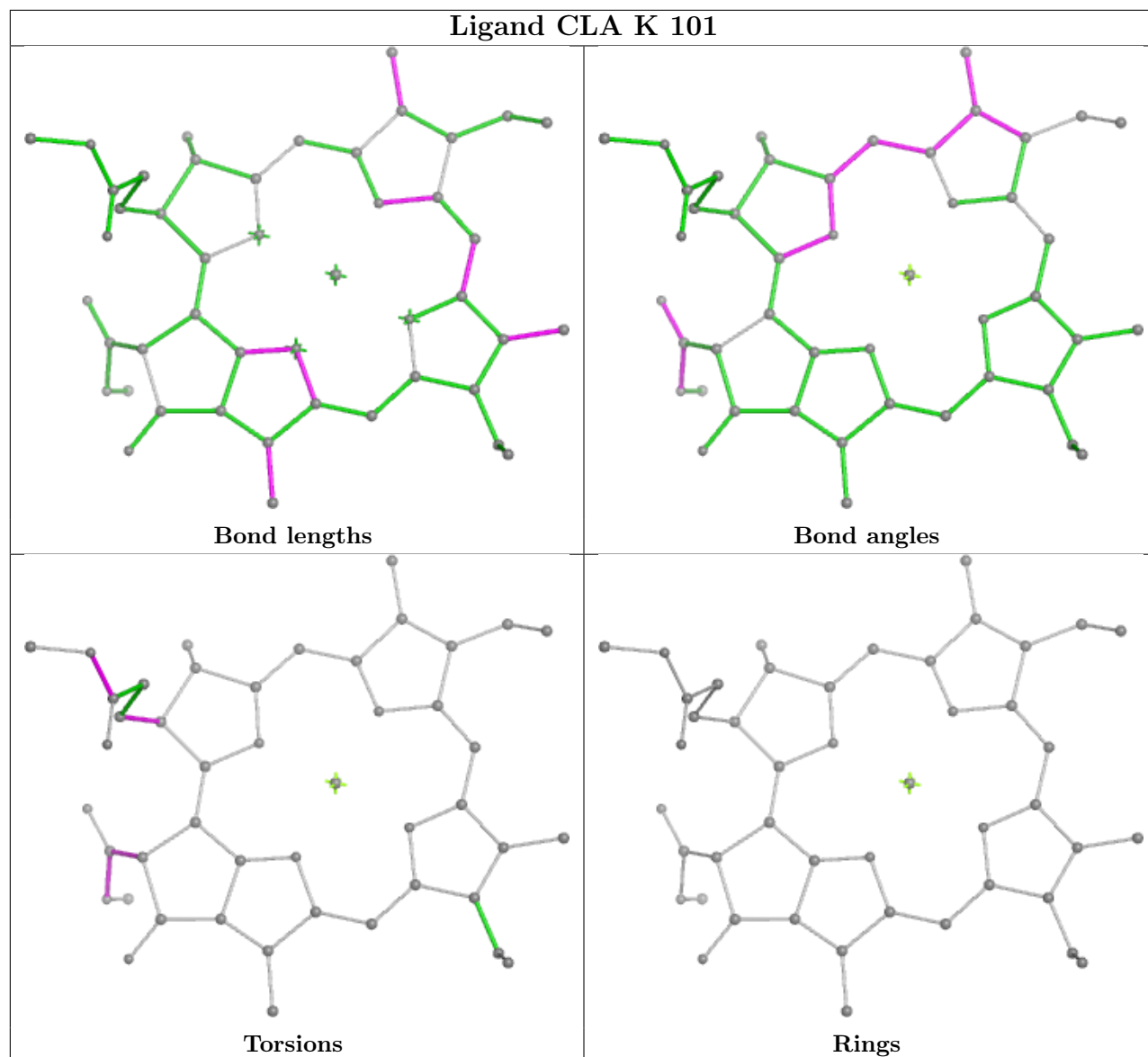




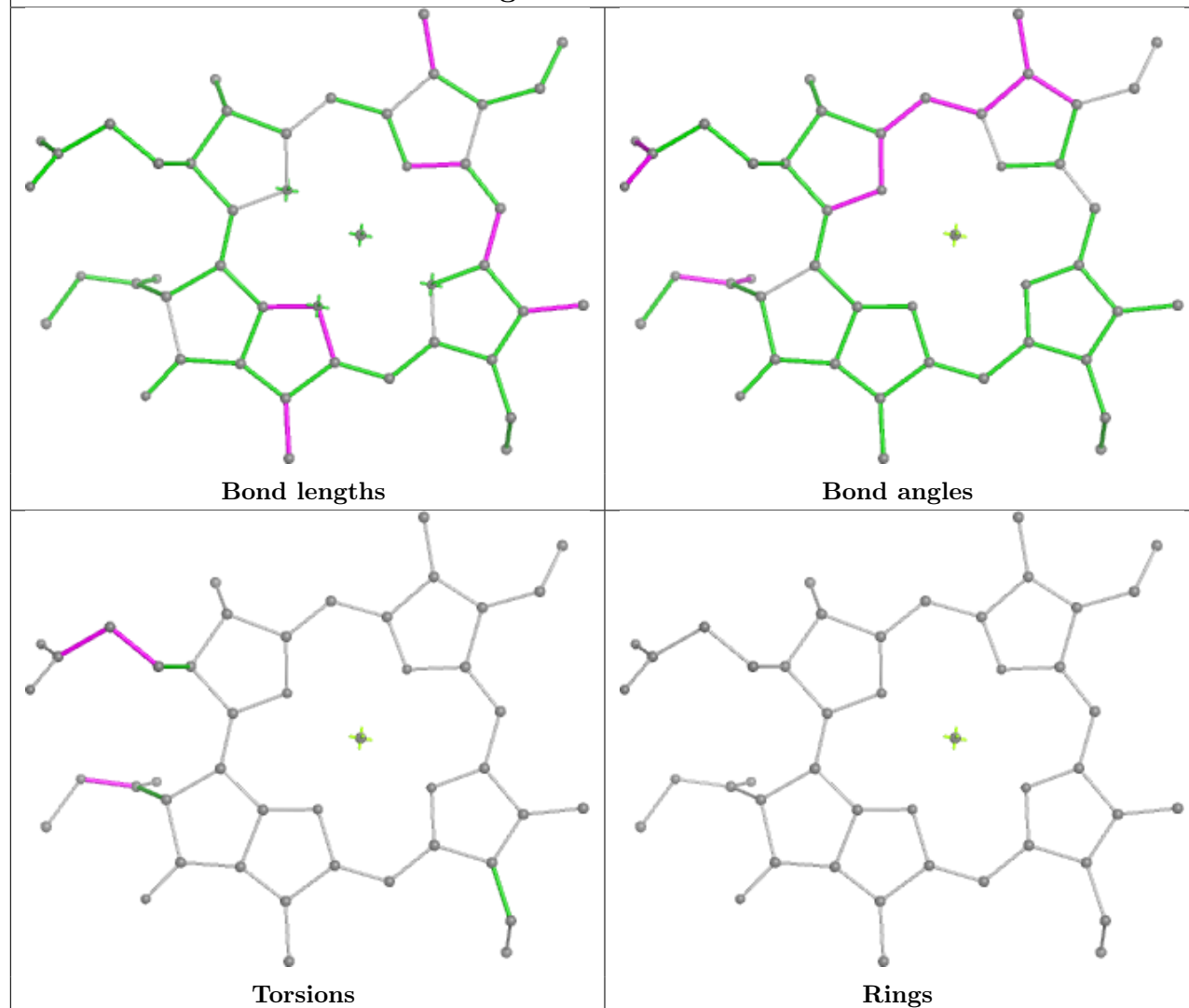
Ligand CLA A 829**Ligand CLA A 840**



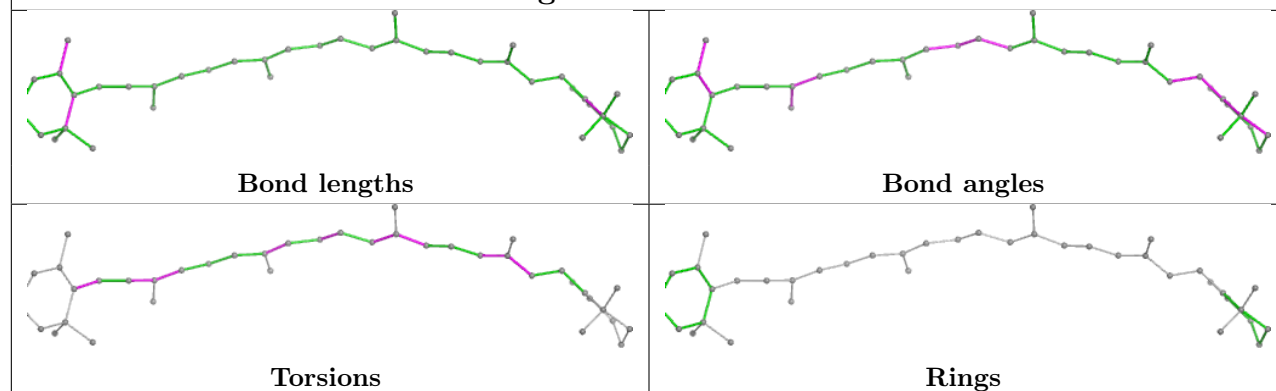
Ligand CLA K 101

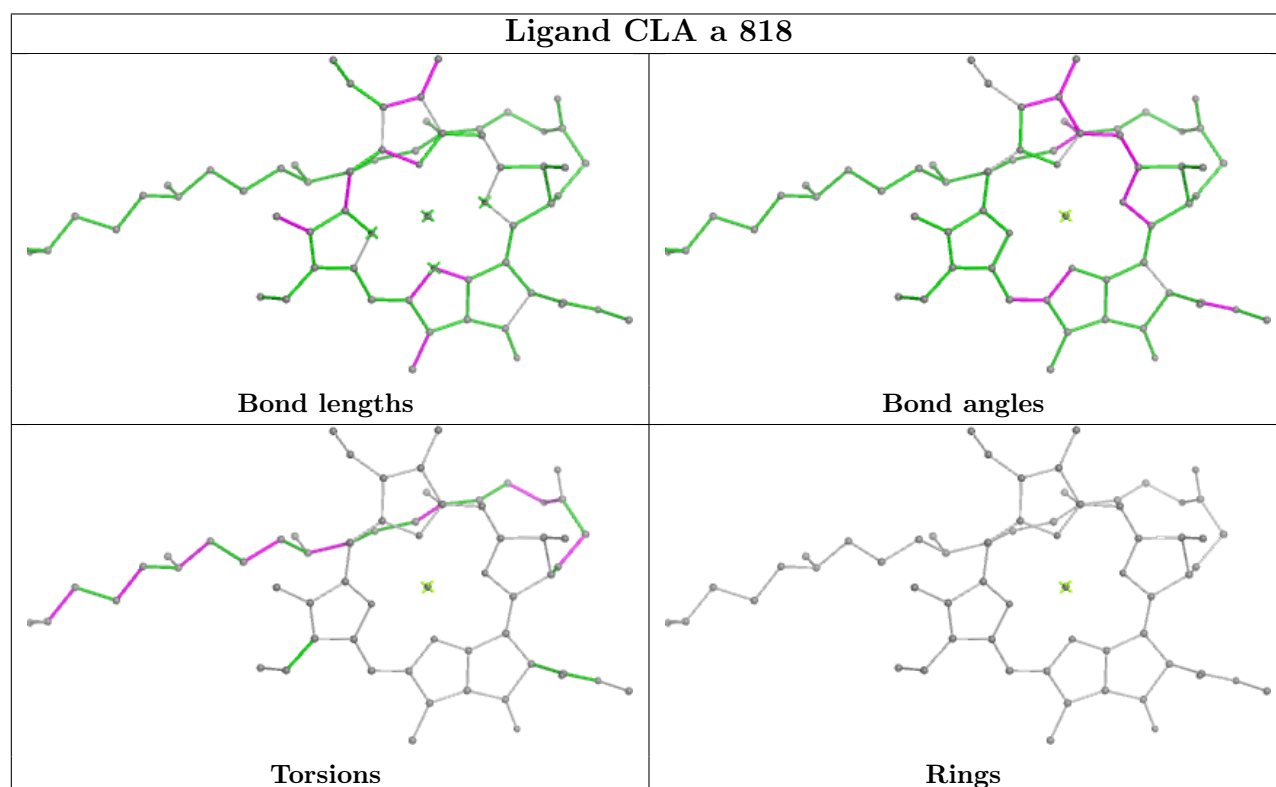
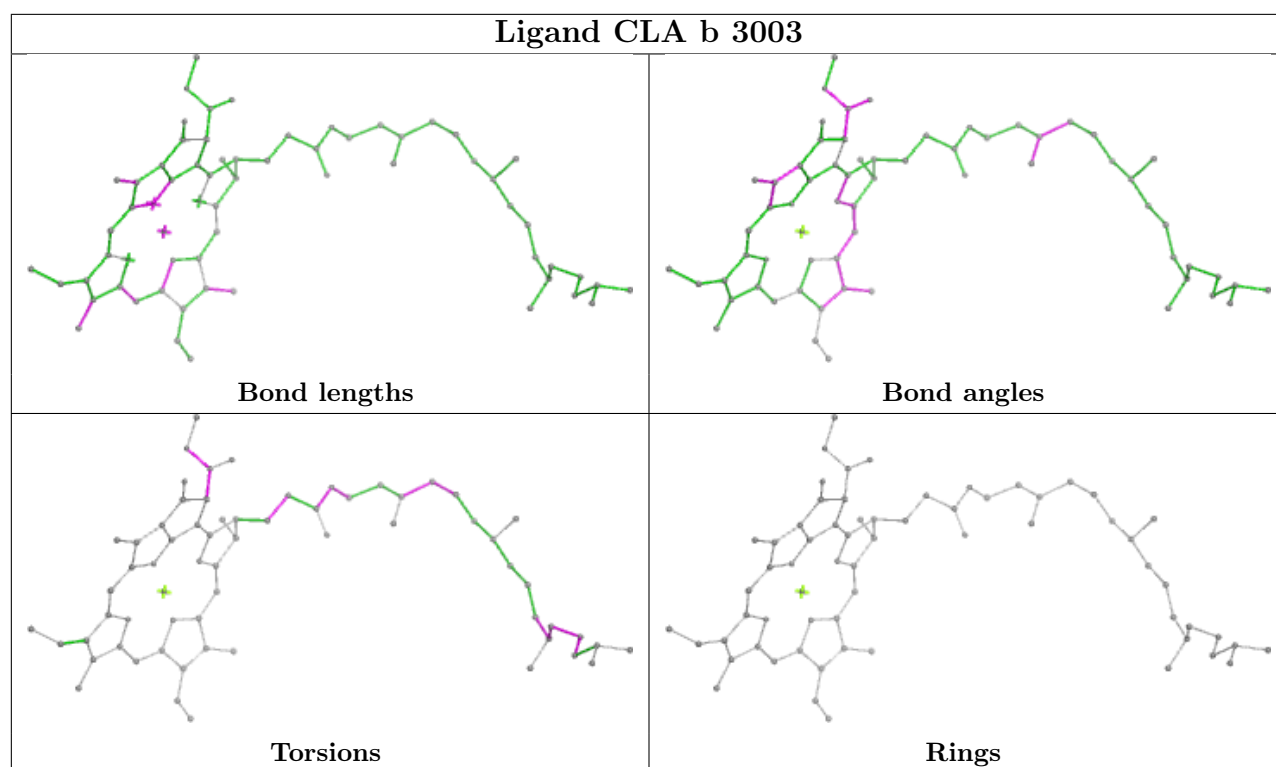


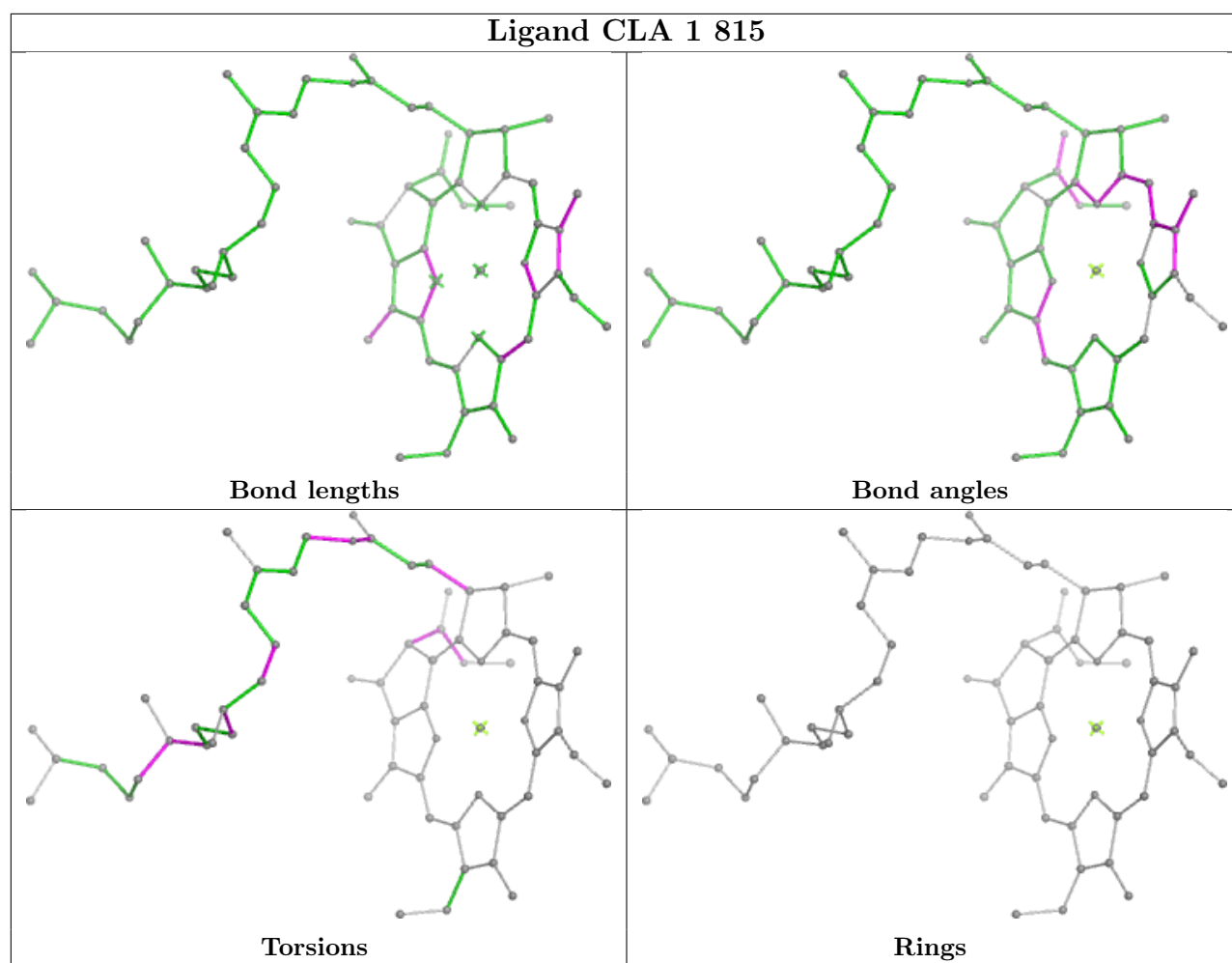
Ligand CLA 6 203

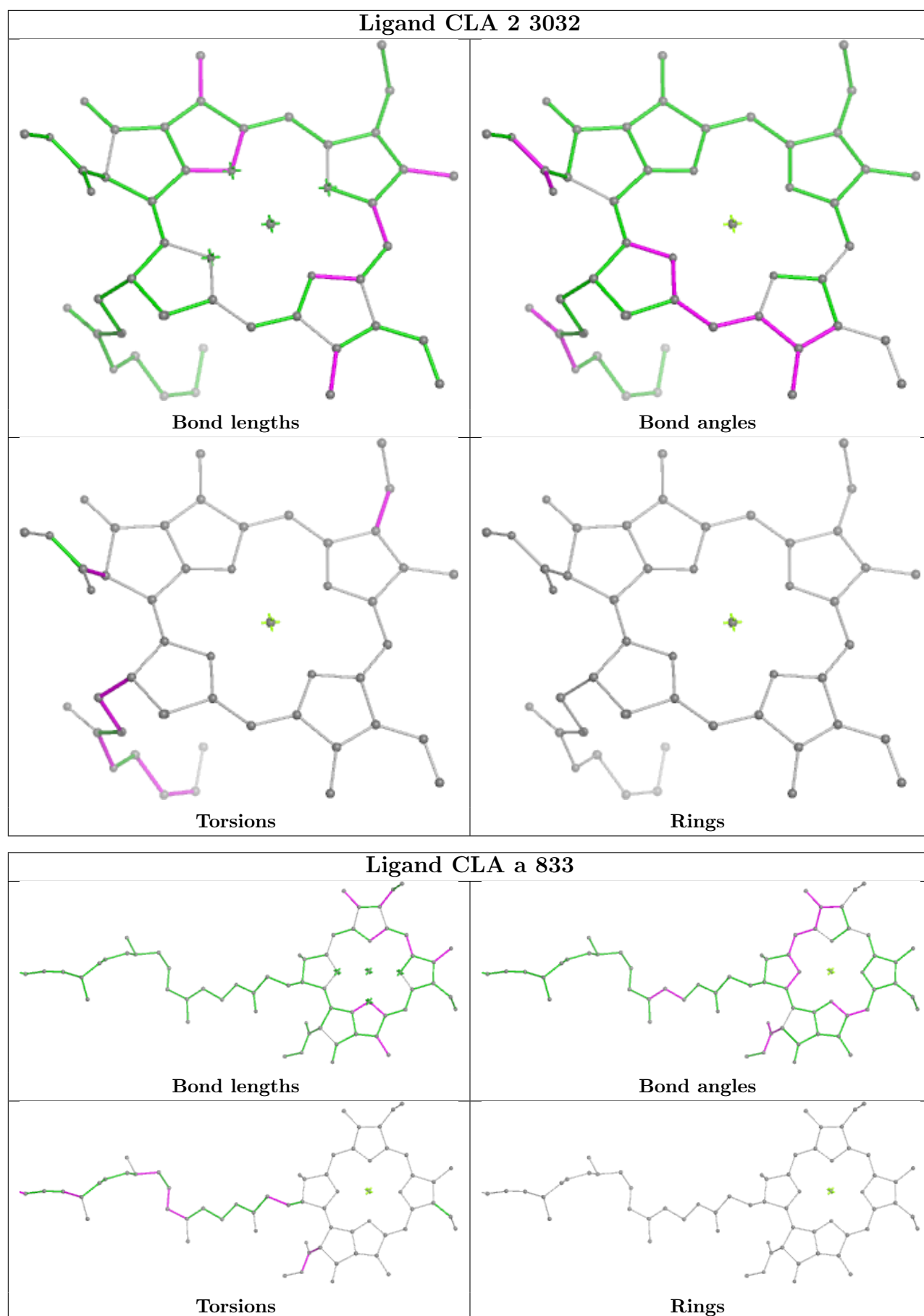


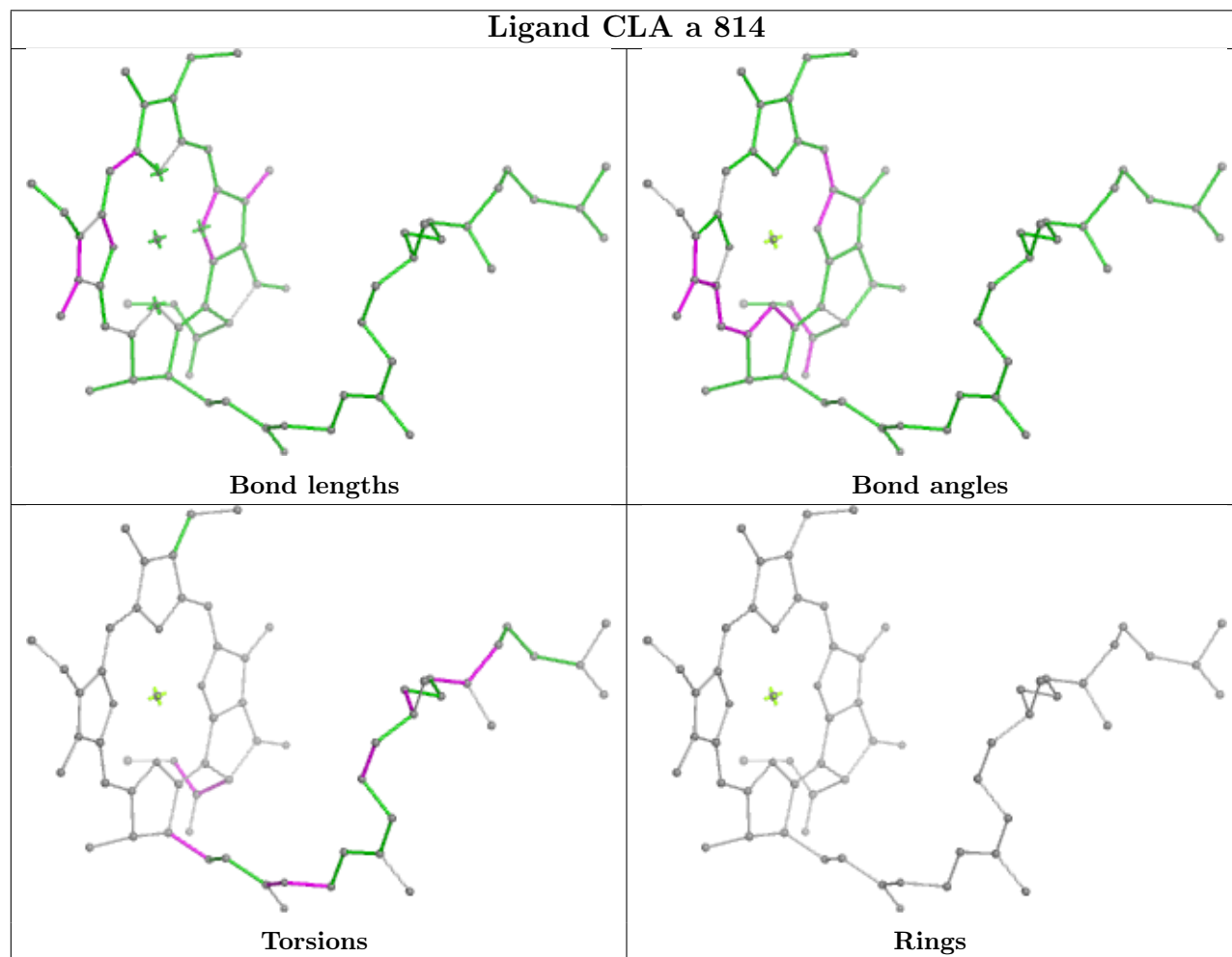
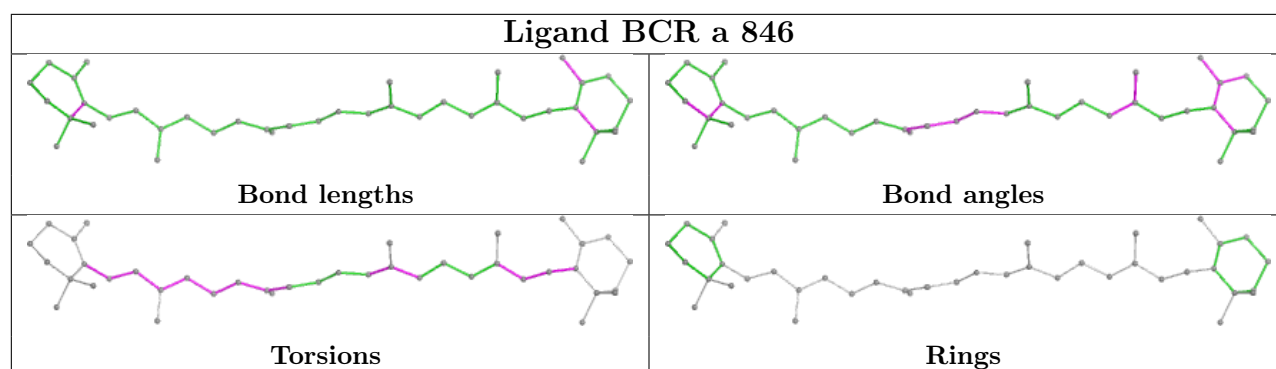
Ligand BCR f 202

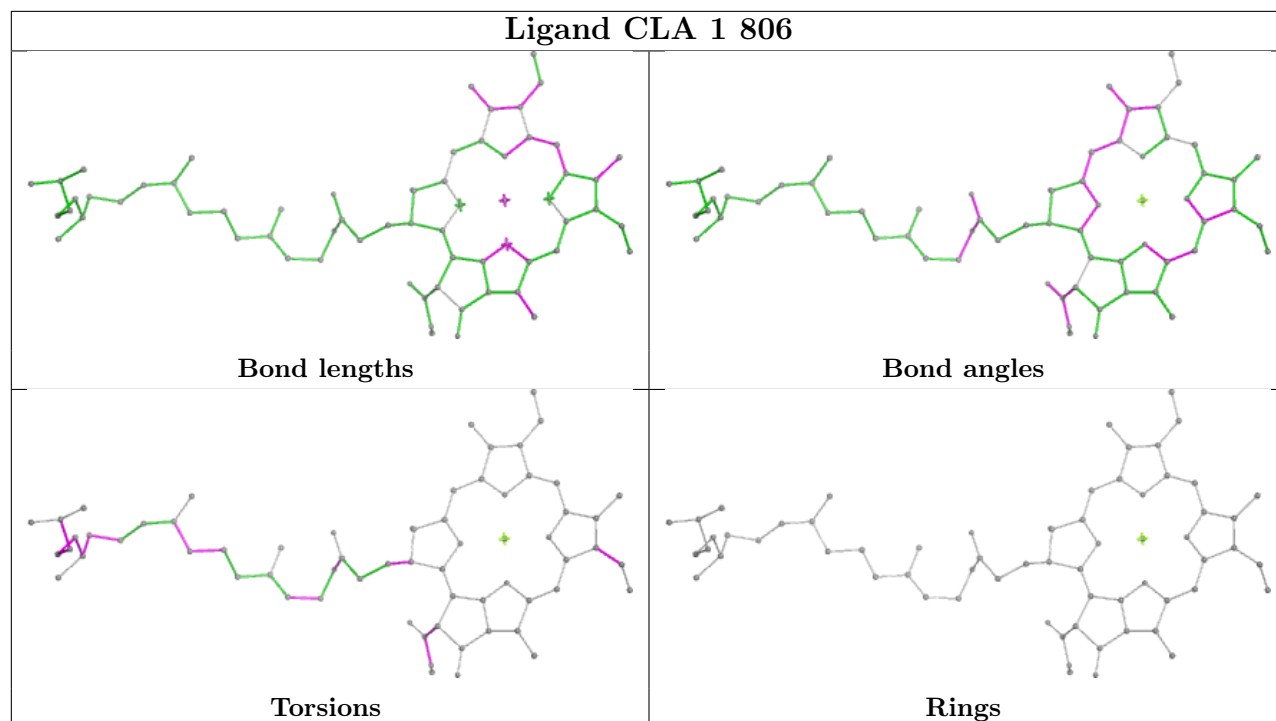
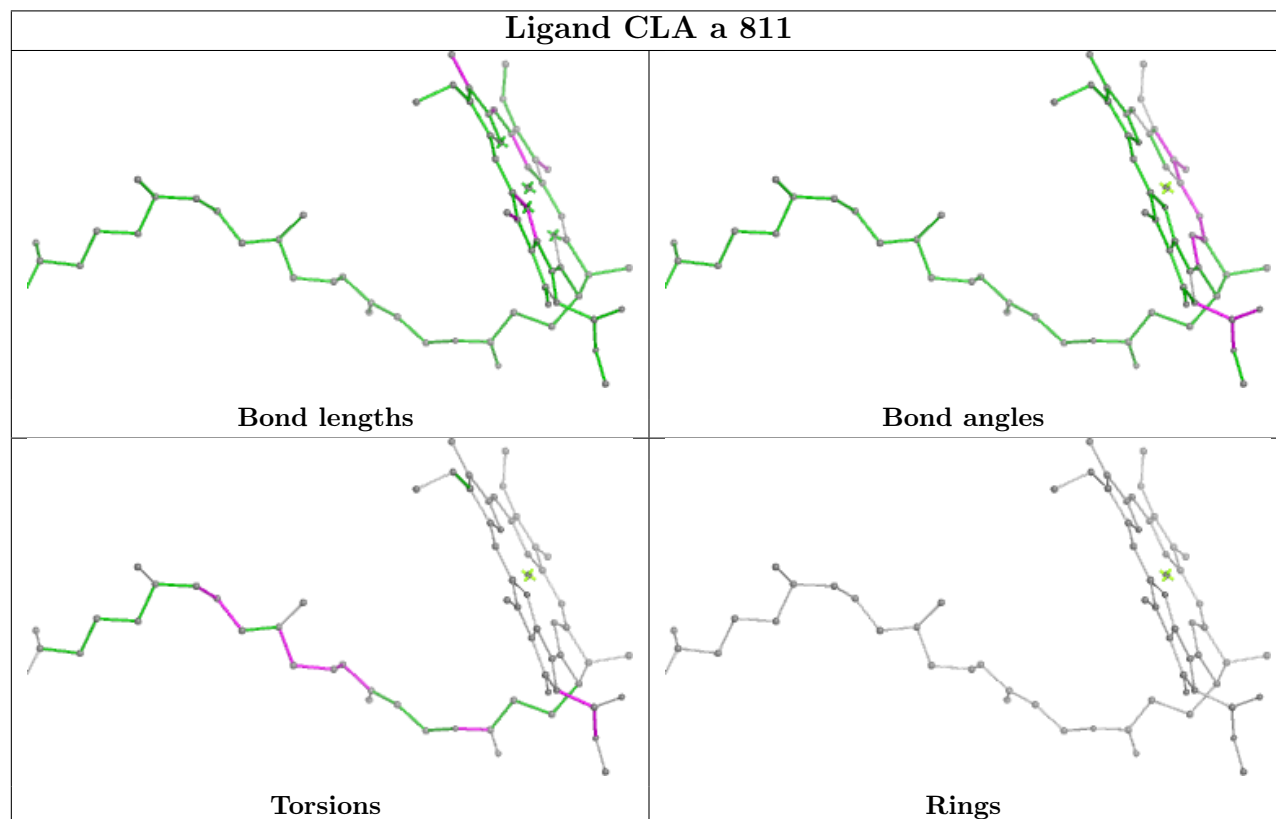


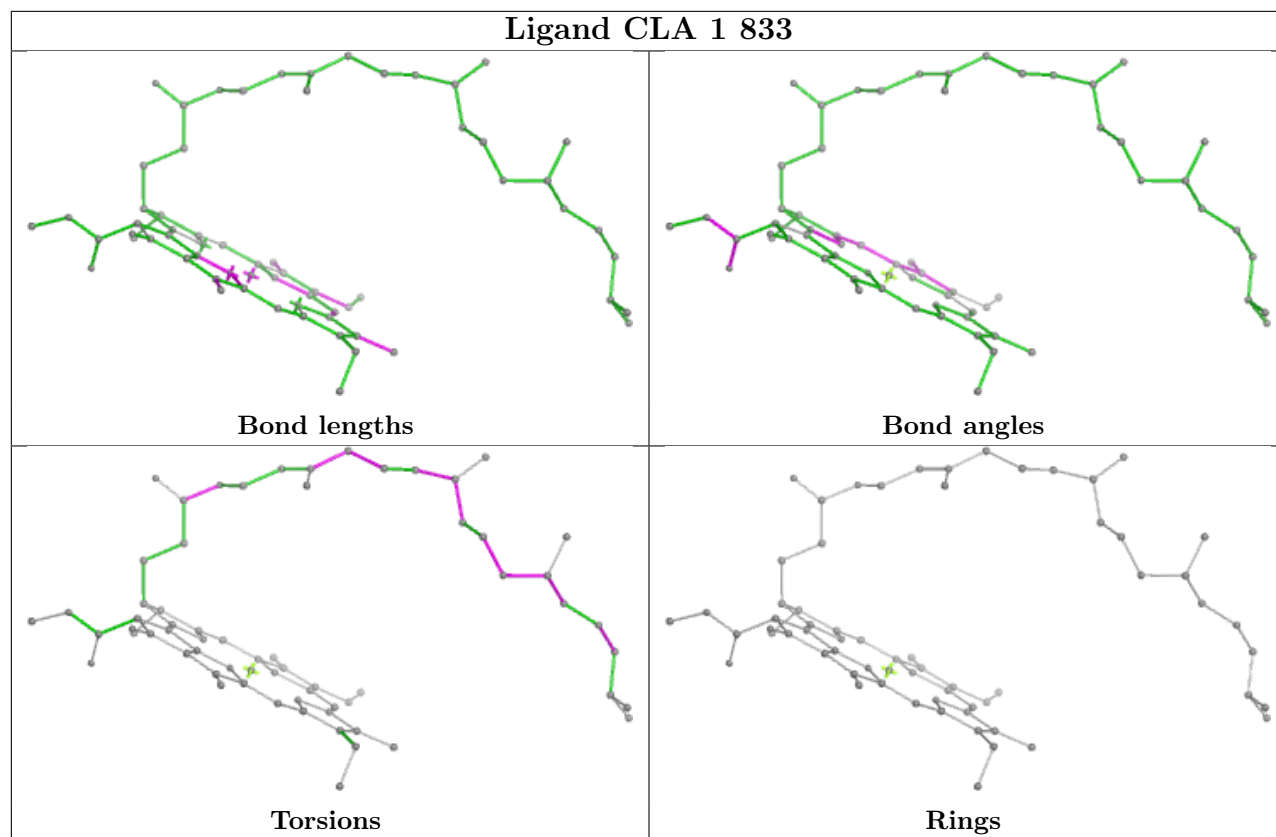


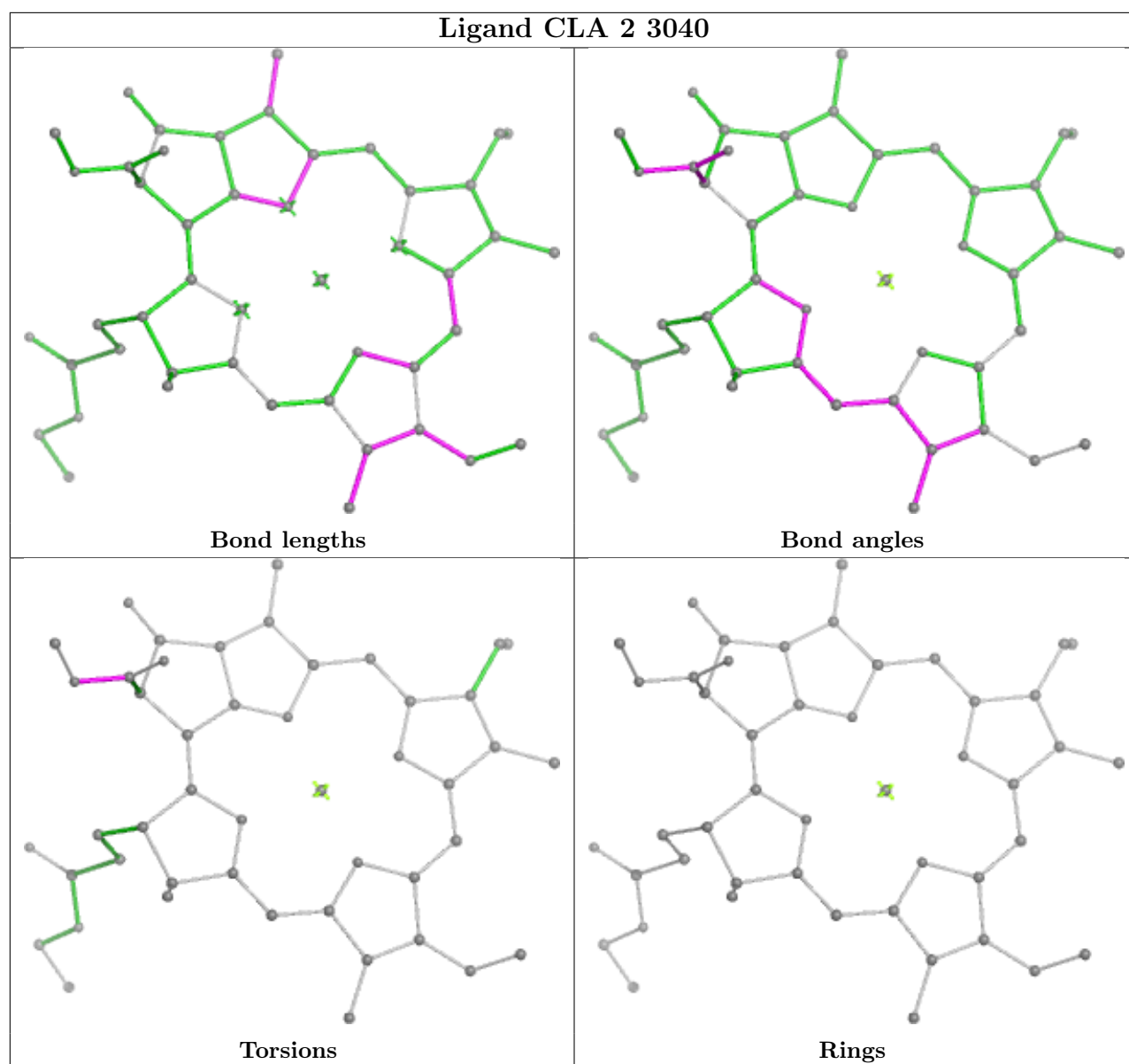


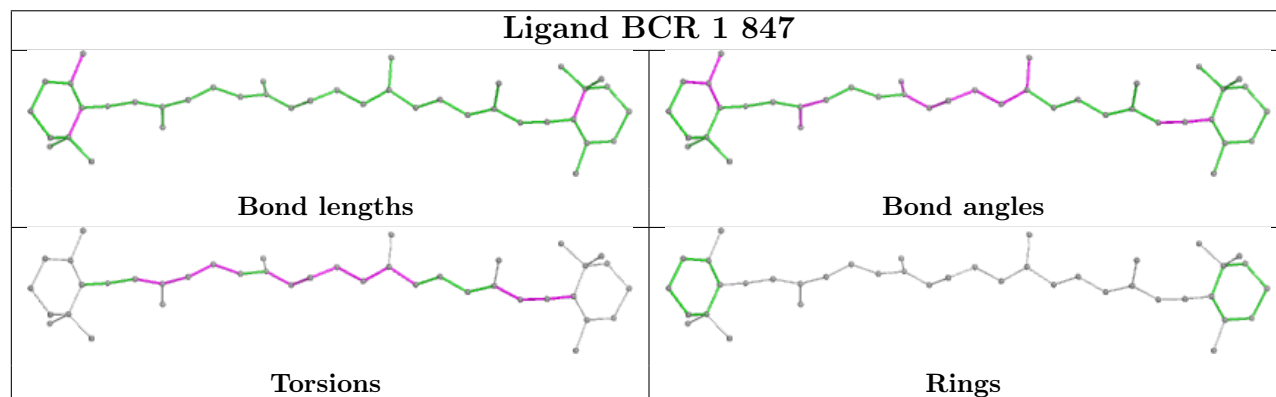
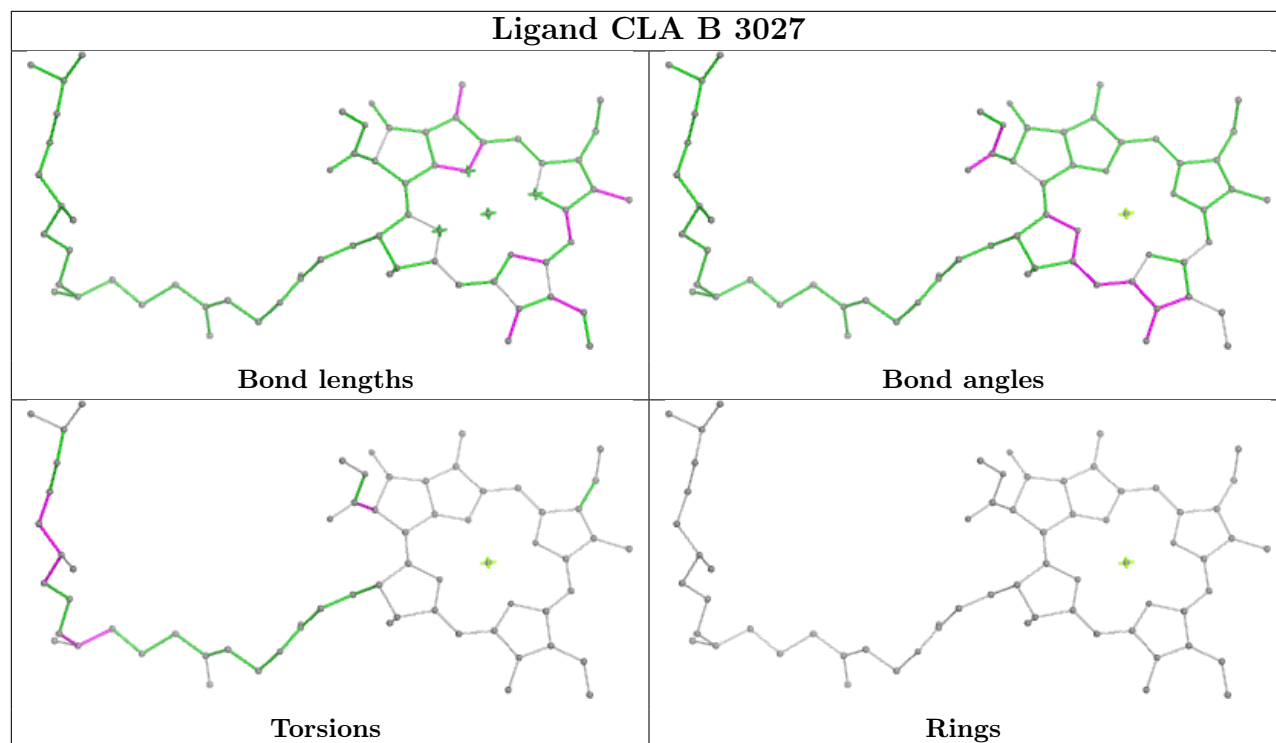


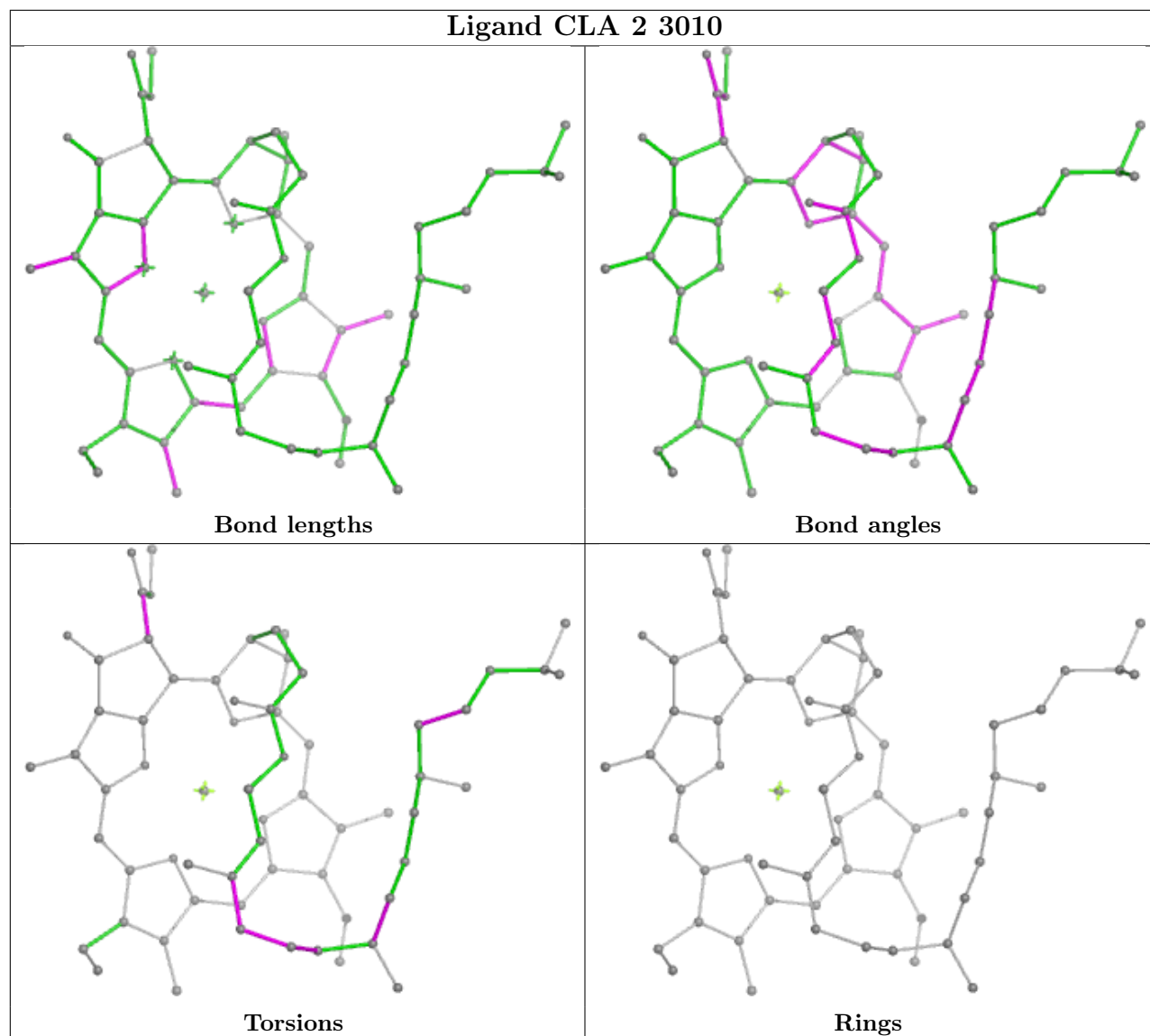


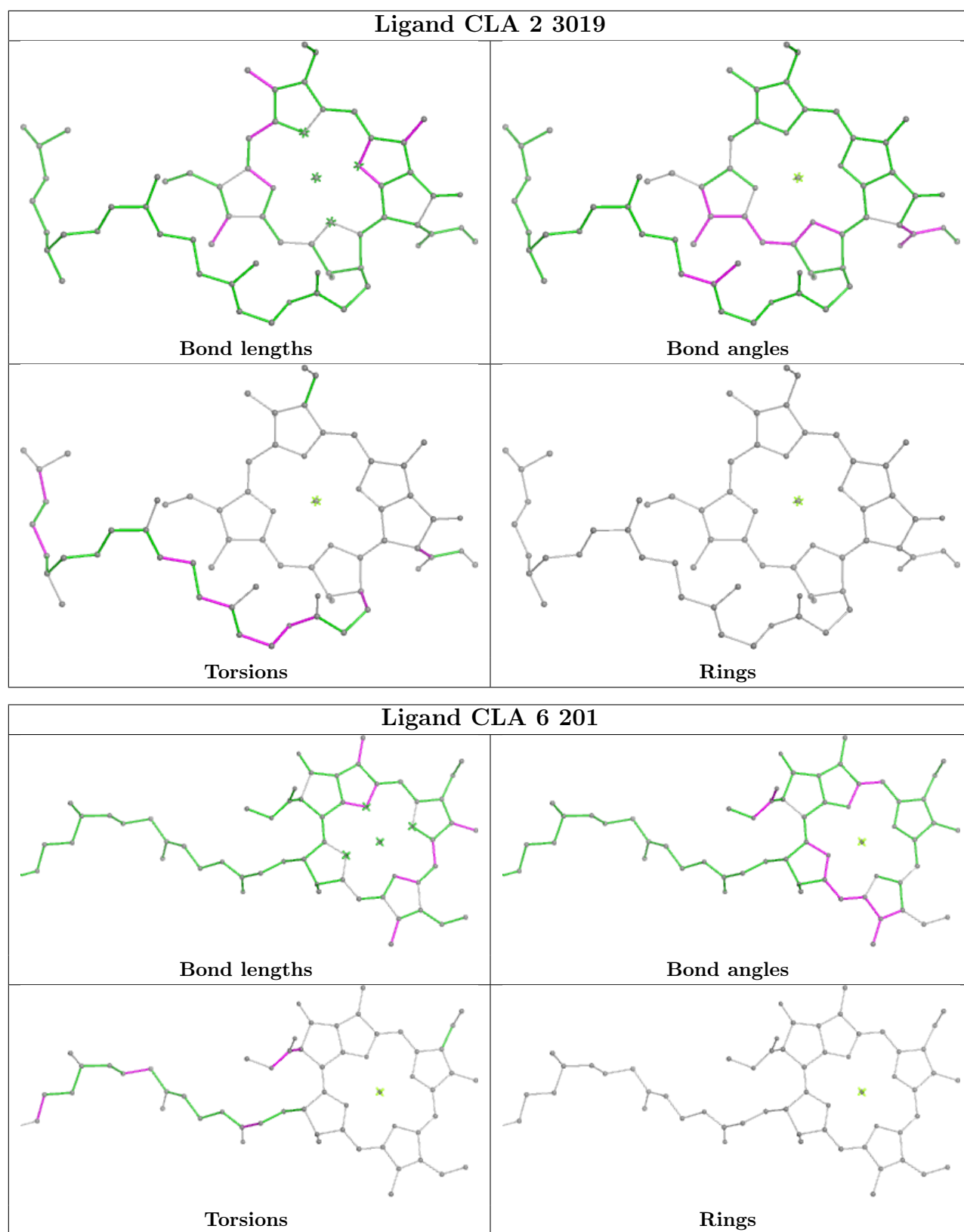
Ligand CLA 1 806**Ligand CLA a 811**

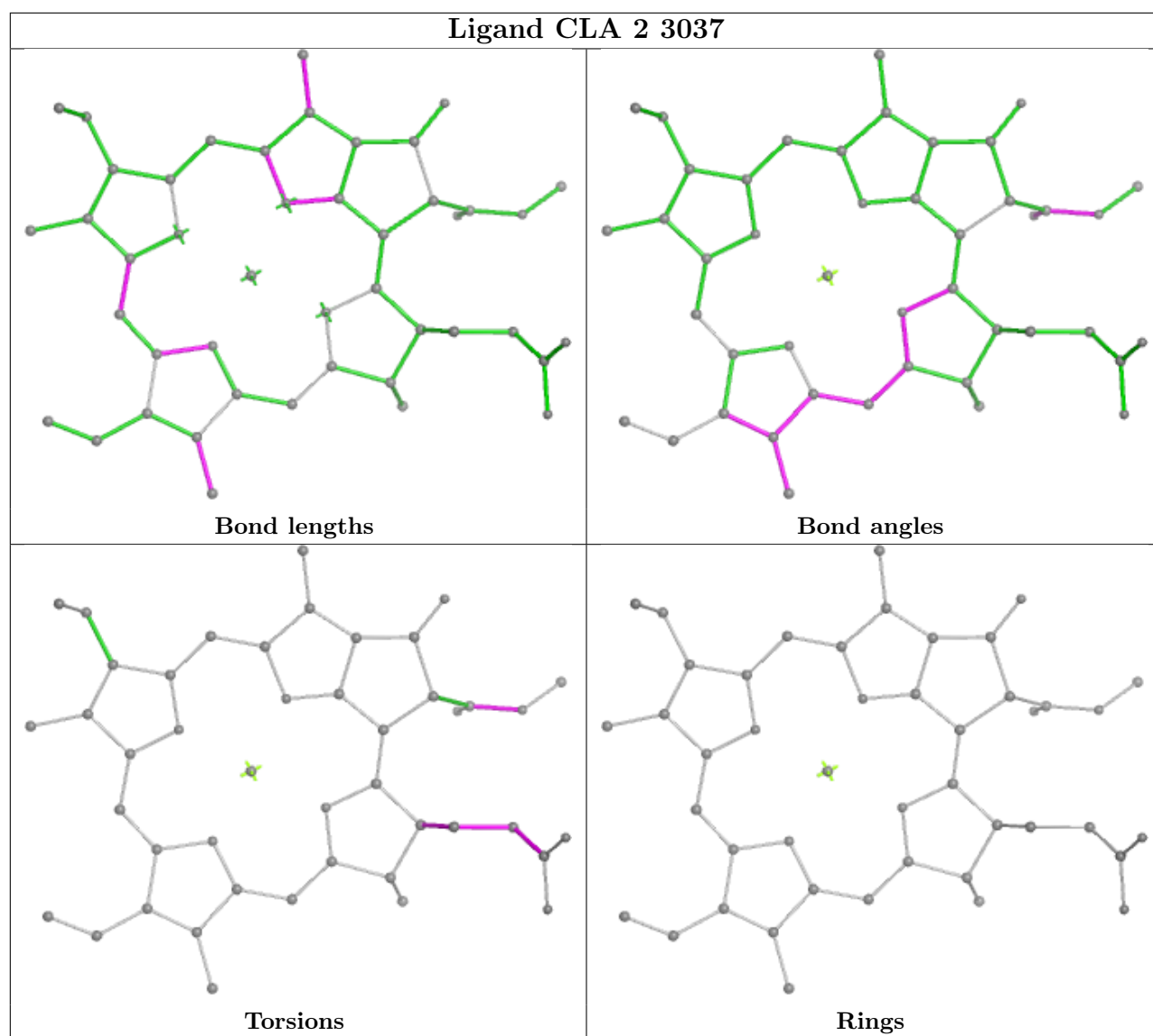


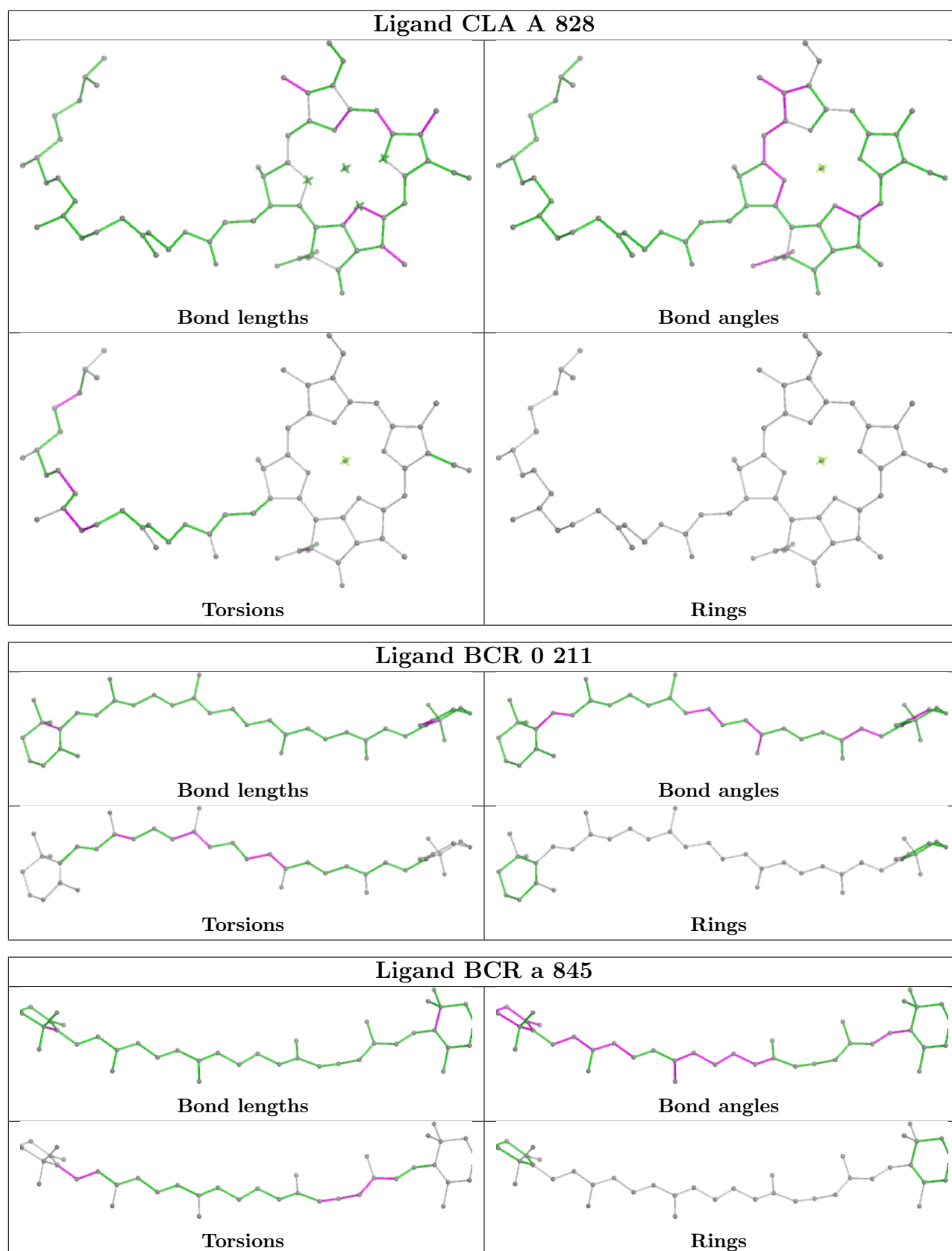




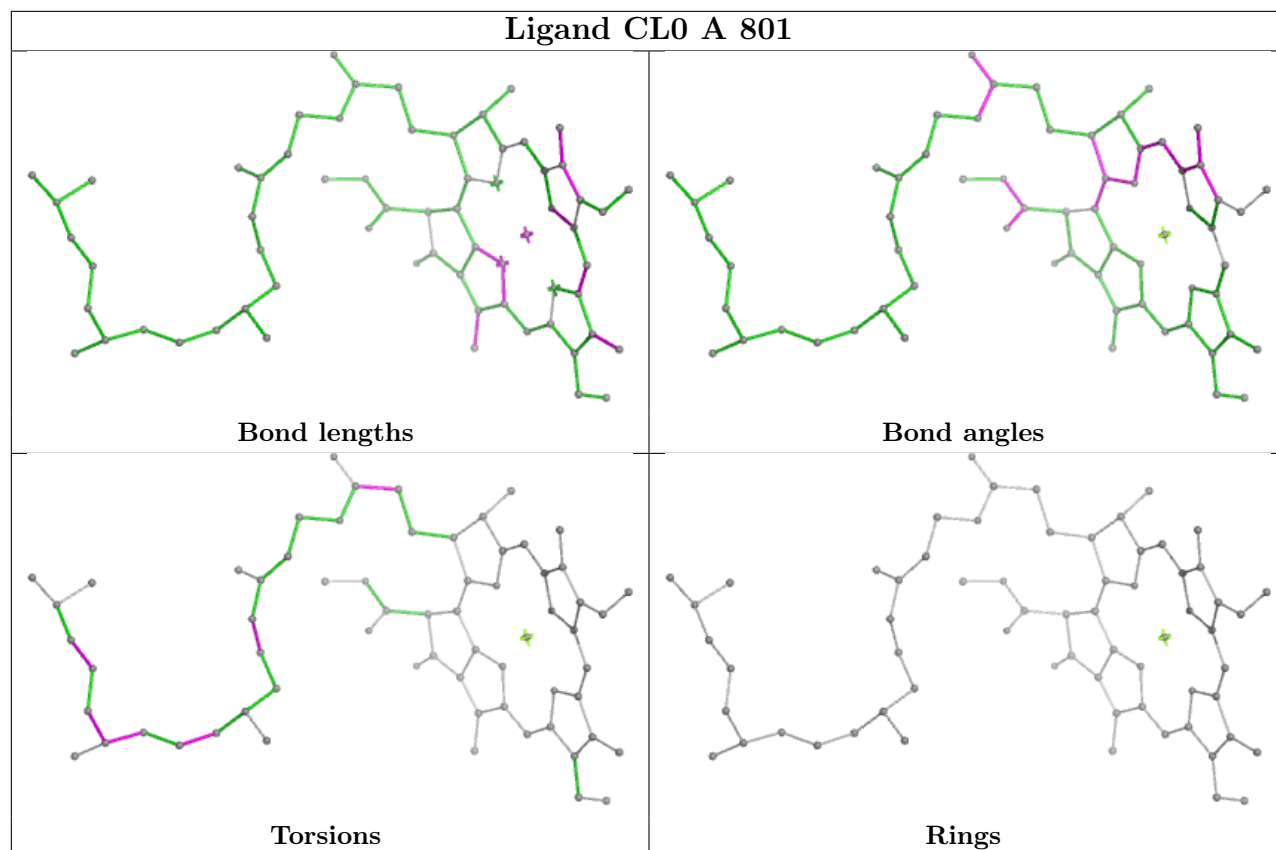




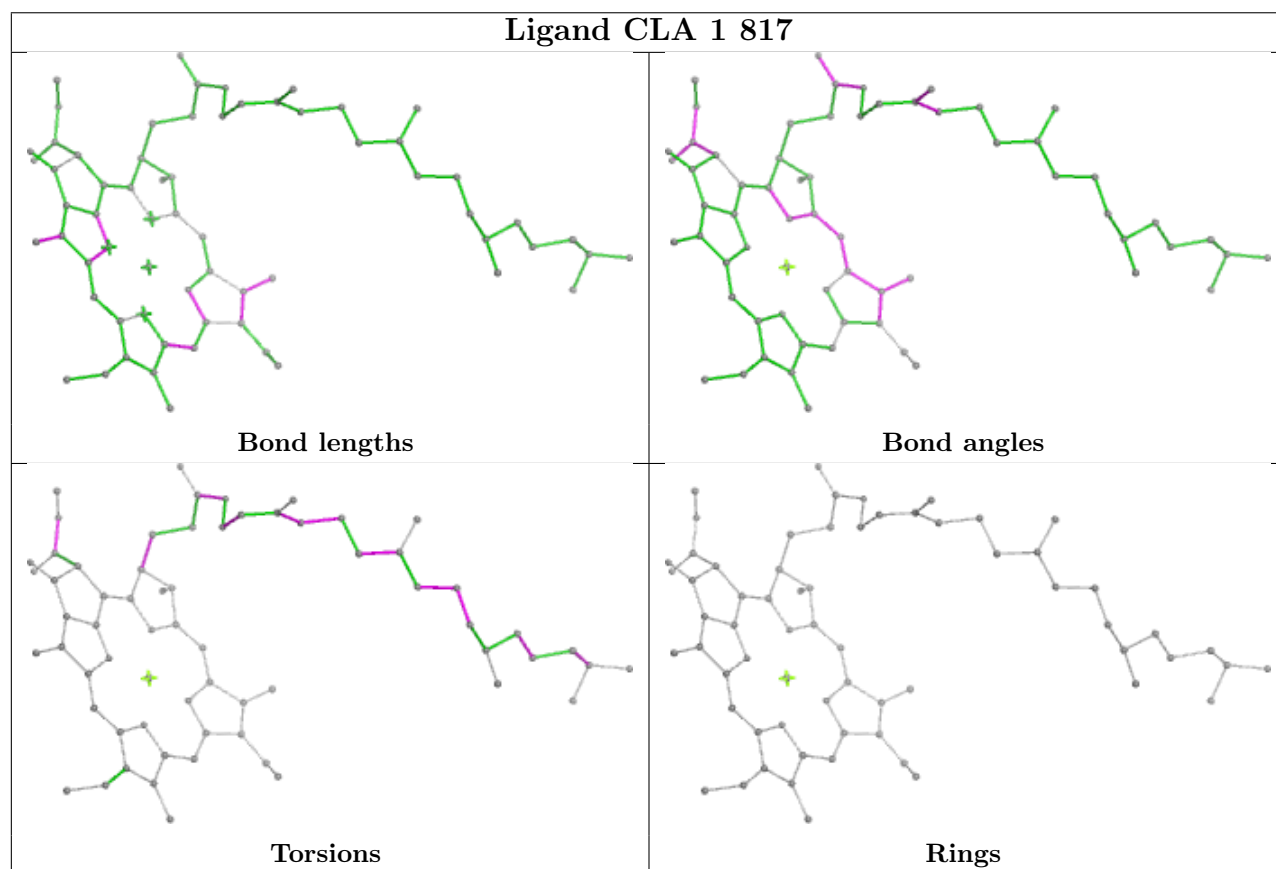


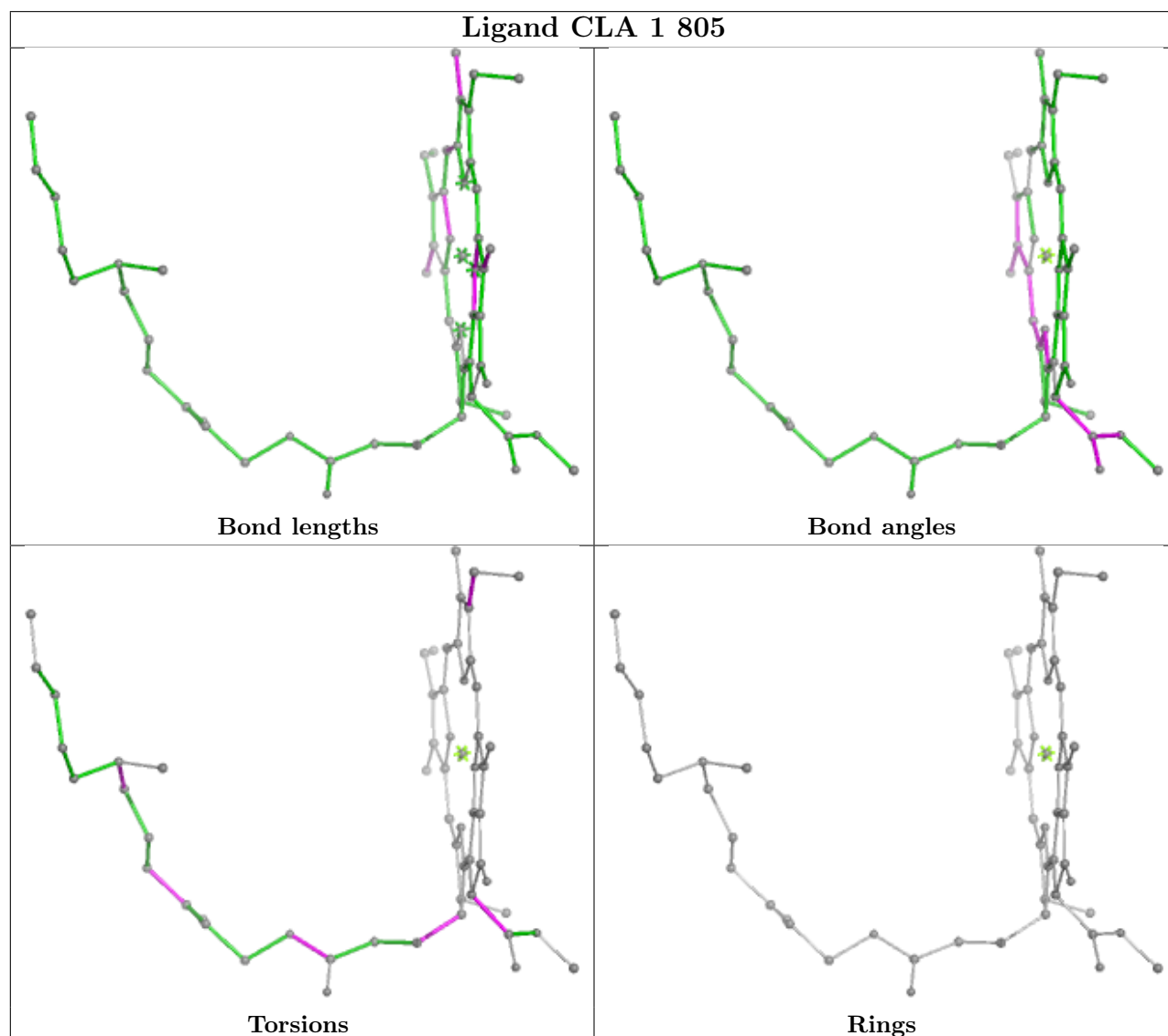
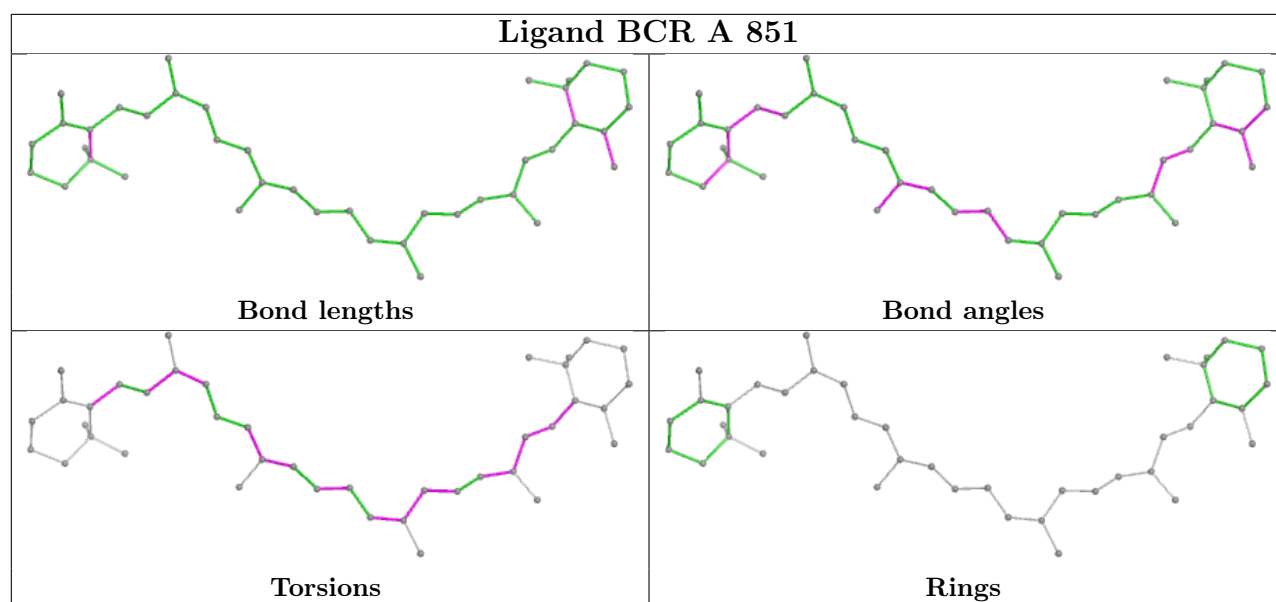


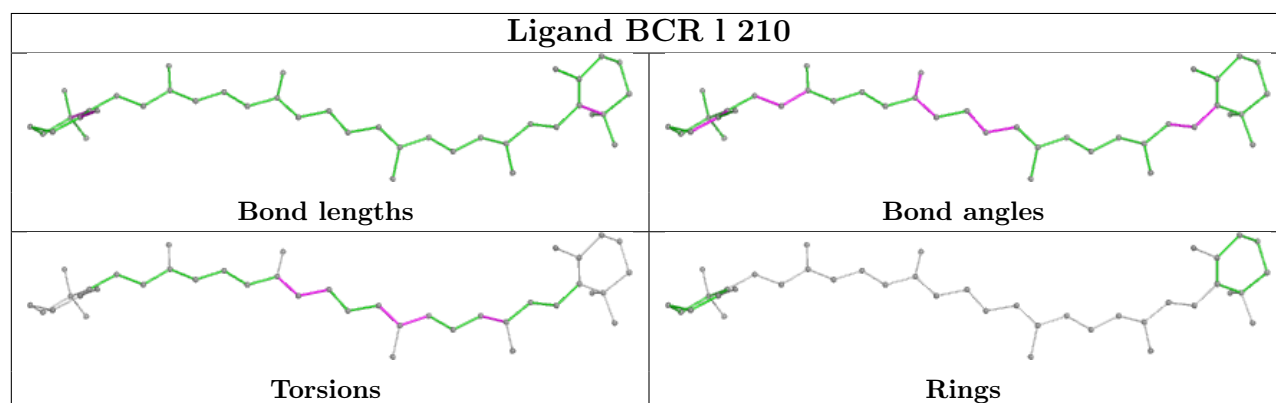
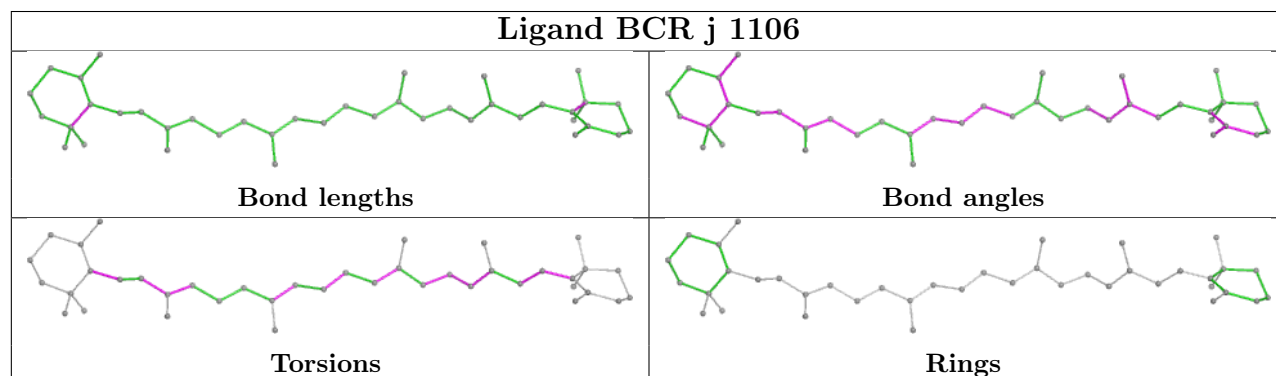
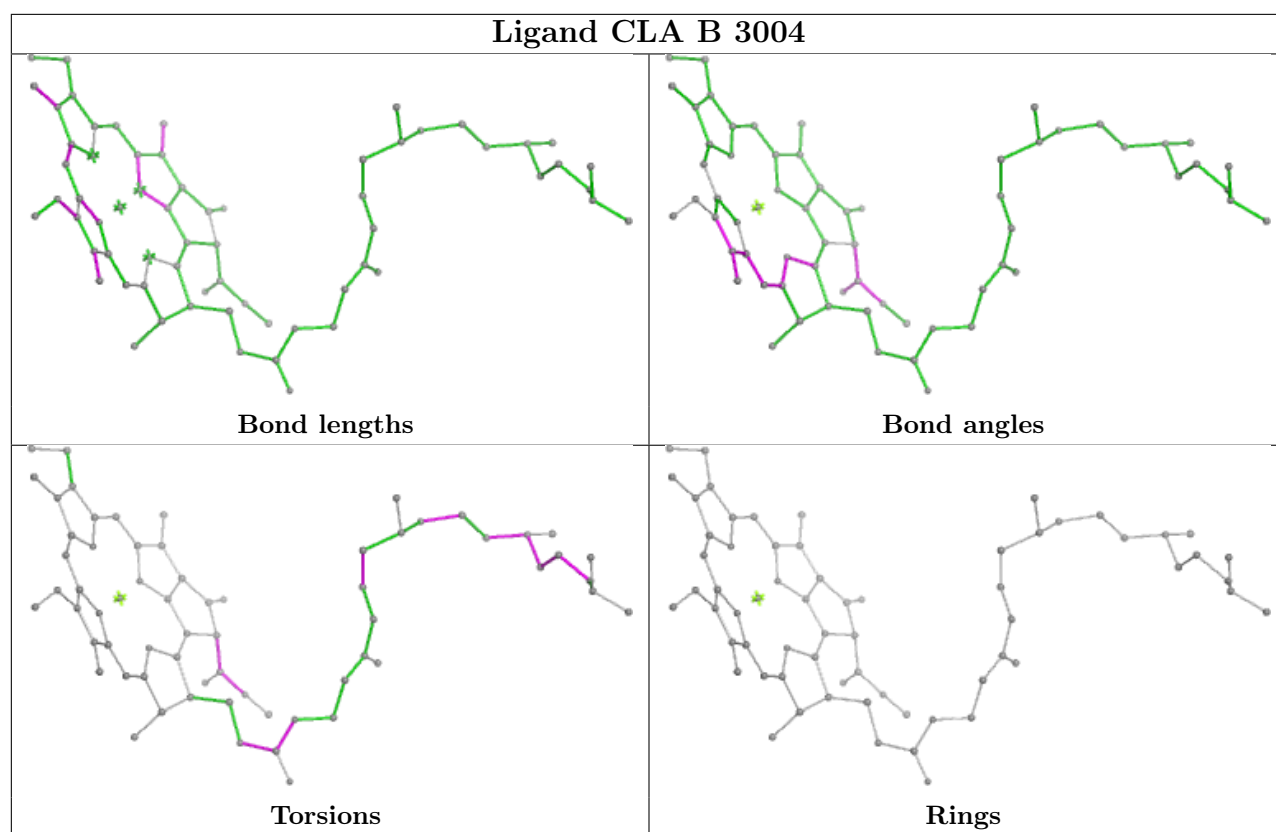
Ligand CL0 A 801

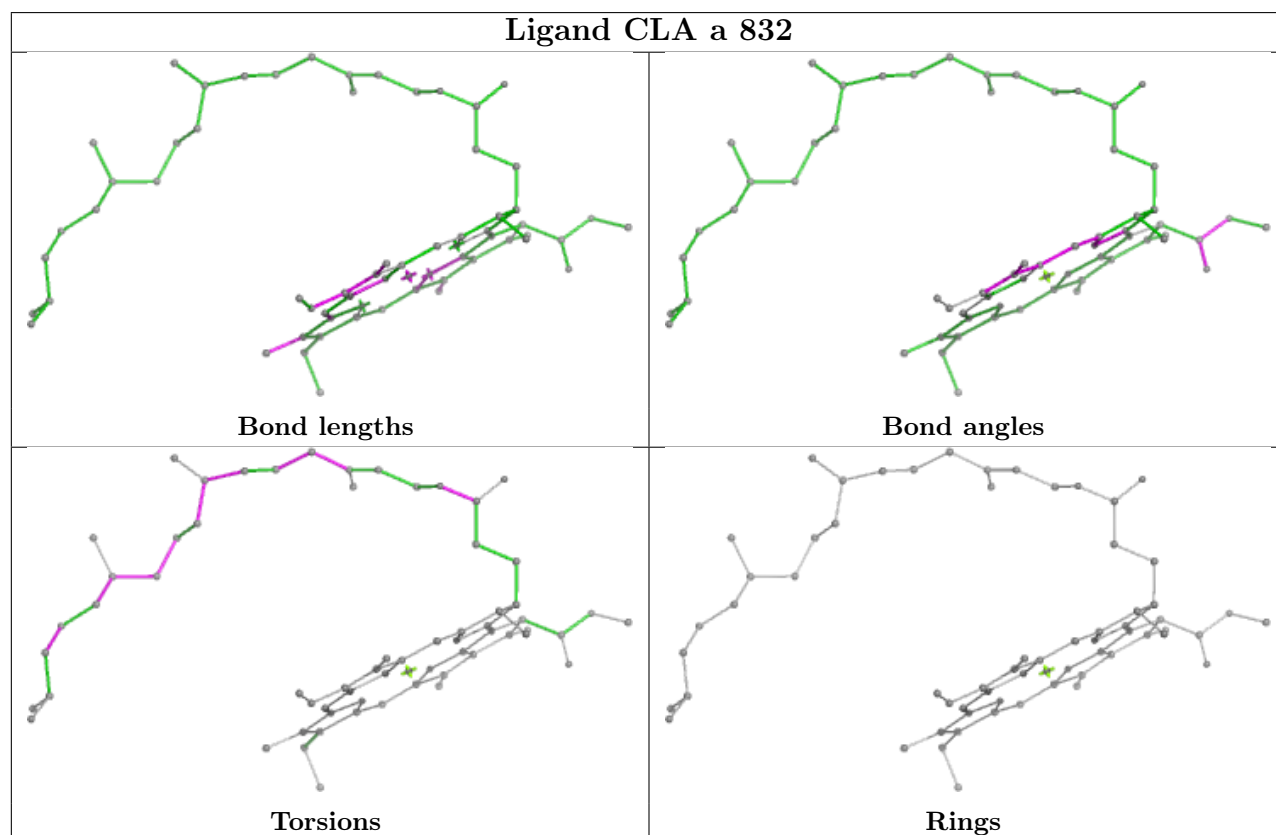
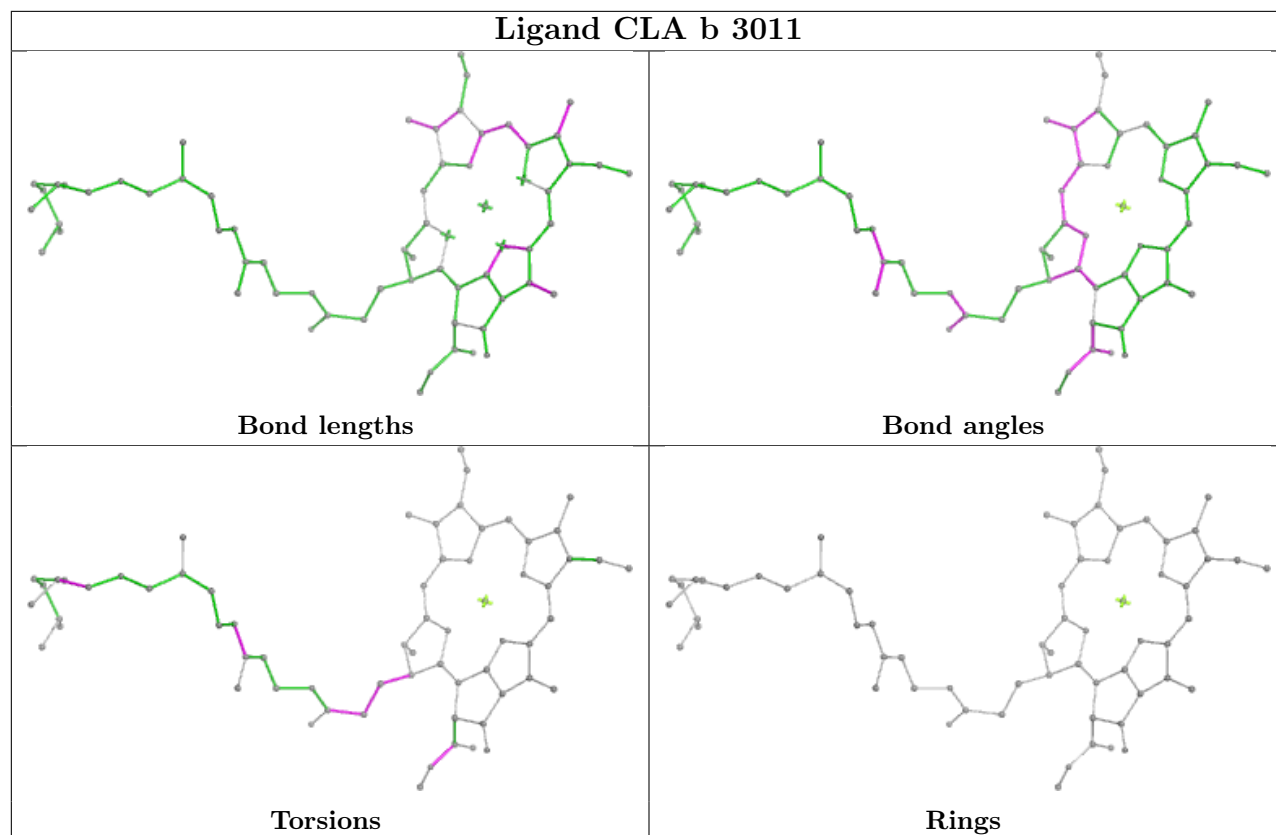


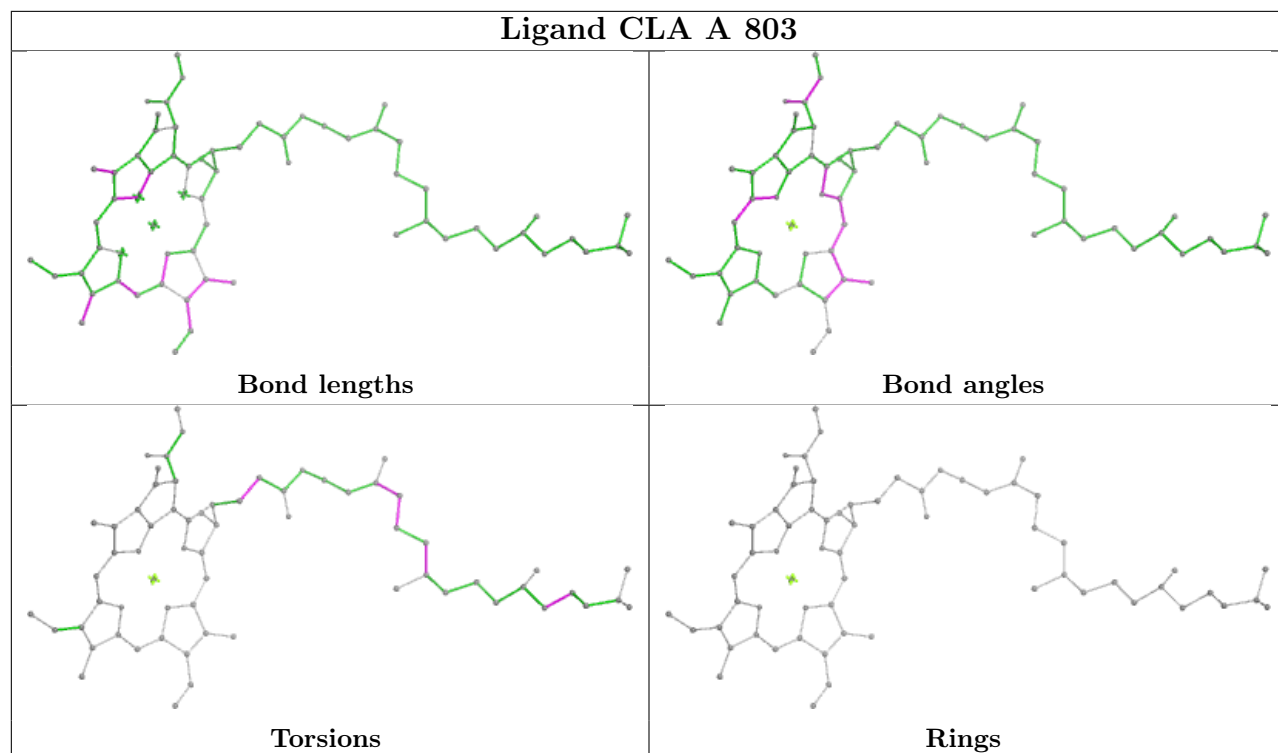
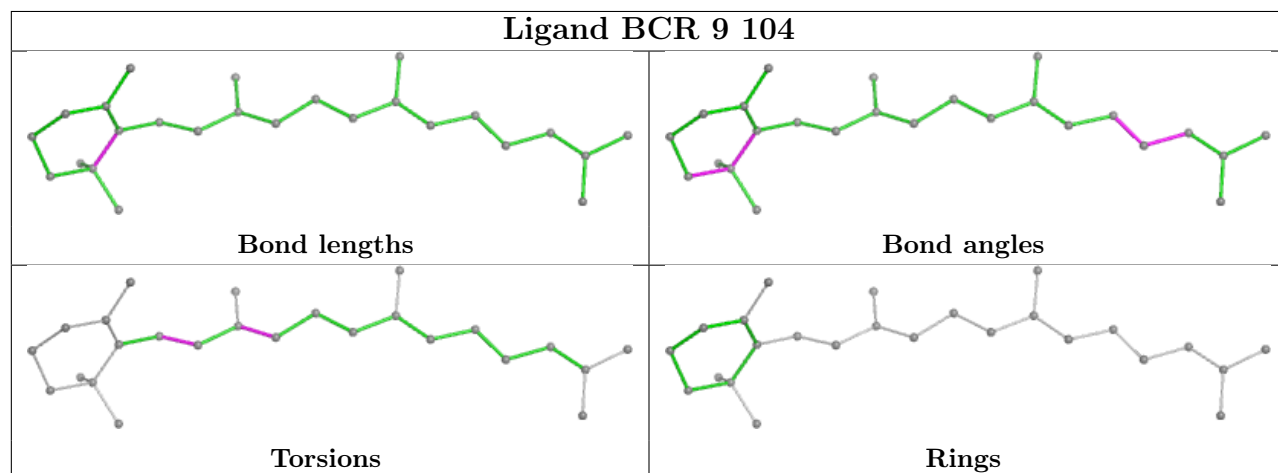
Ligand CLA 1 817

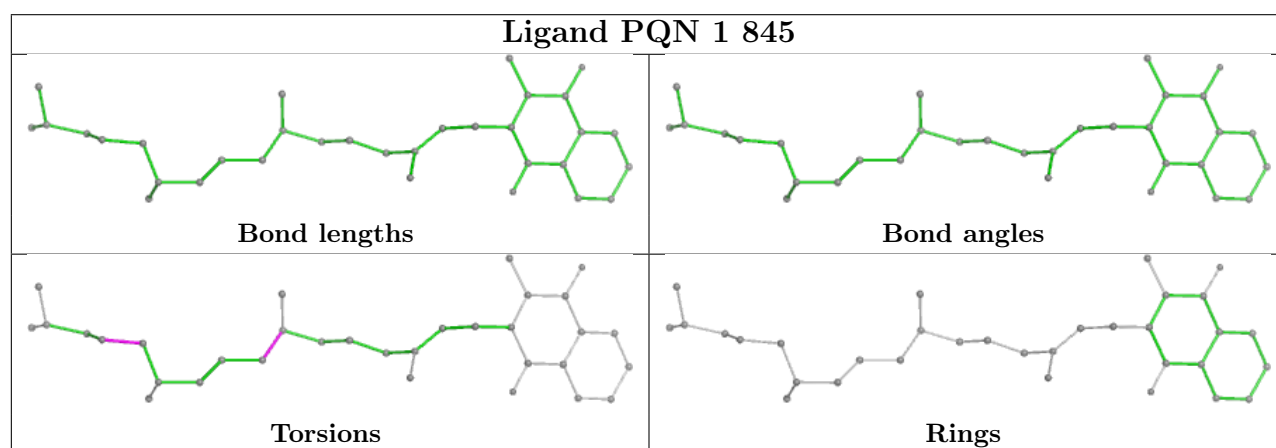
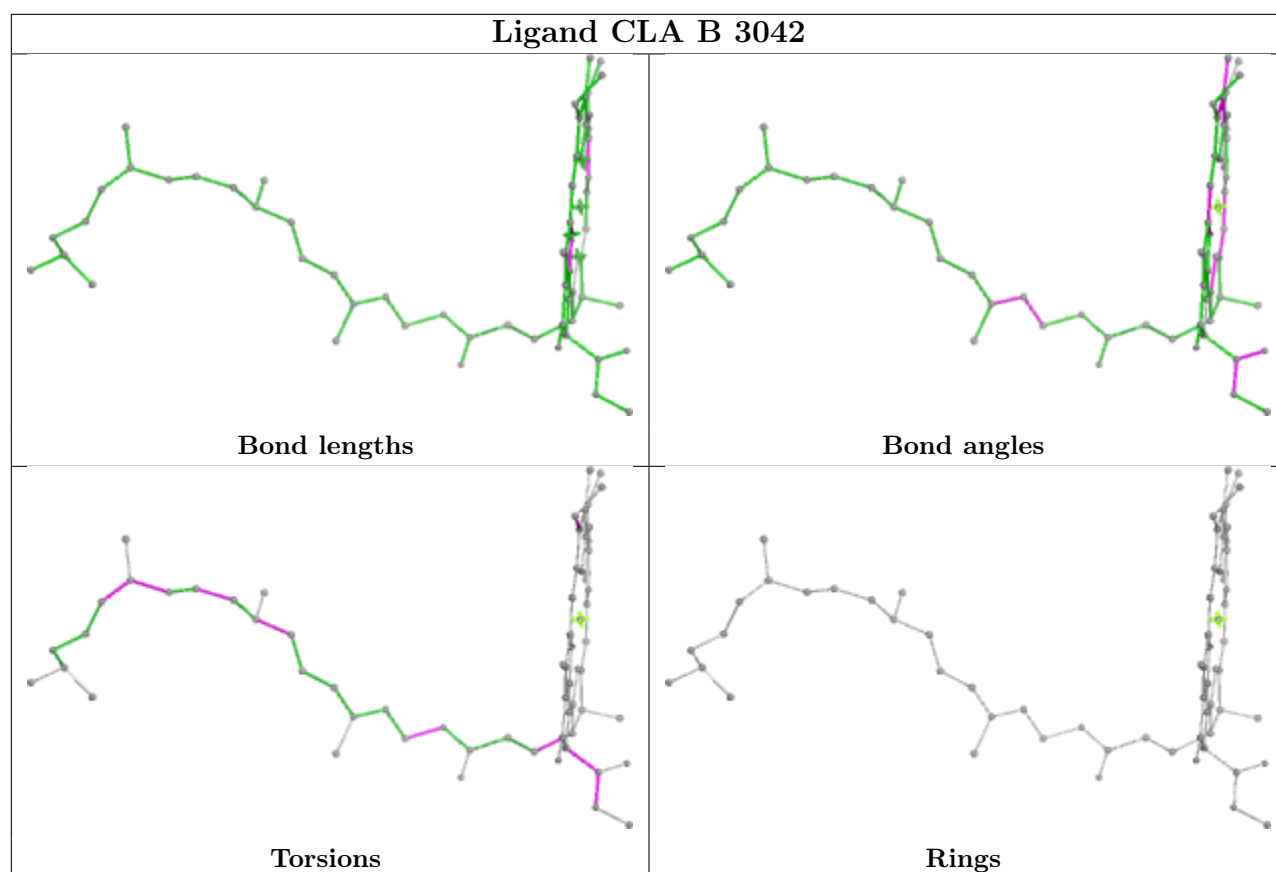




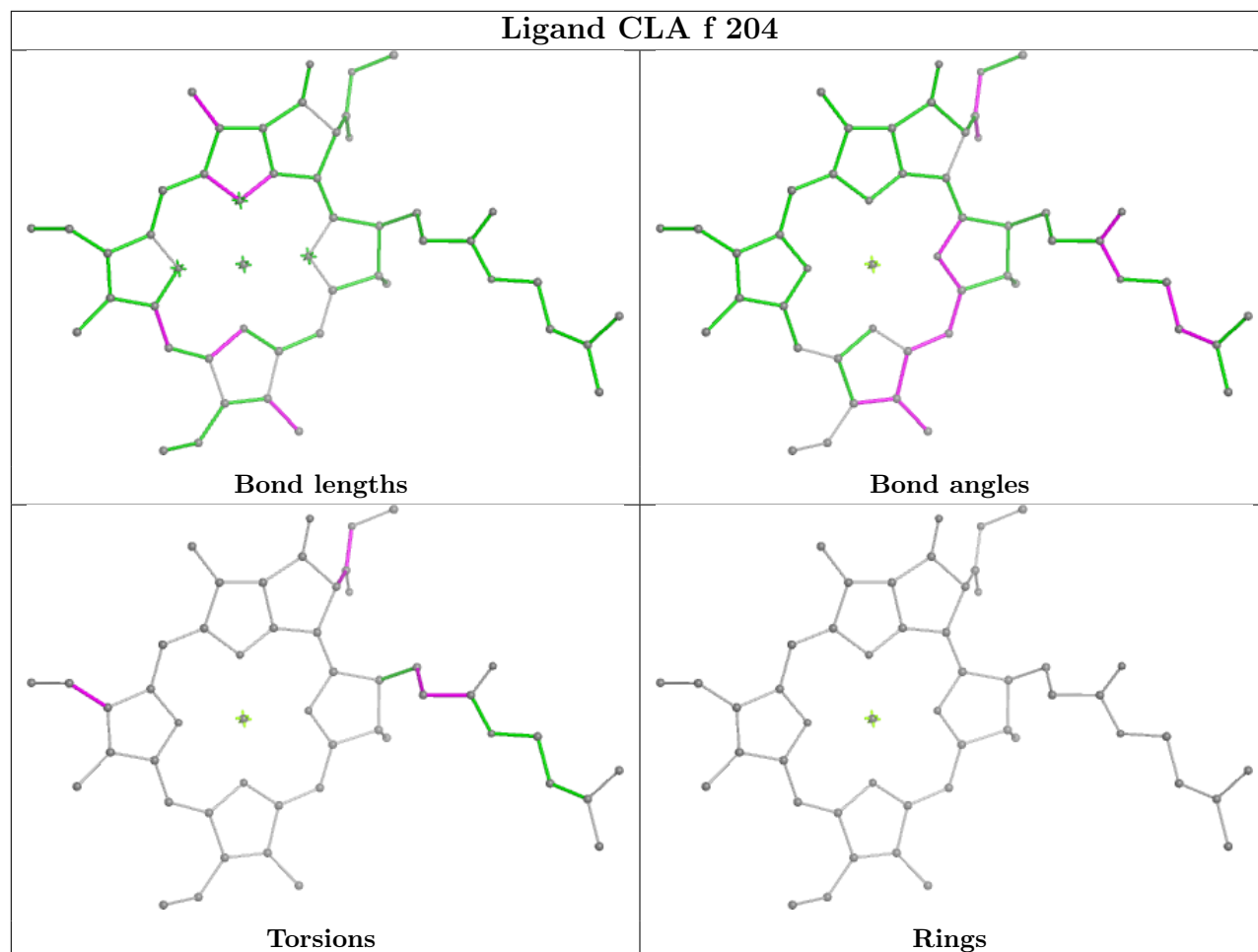


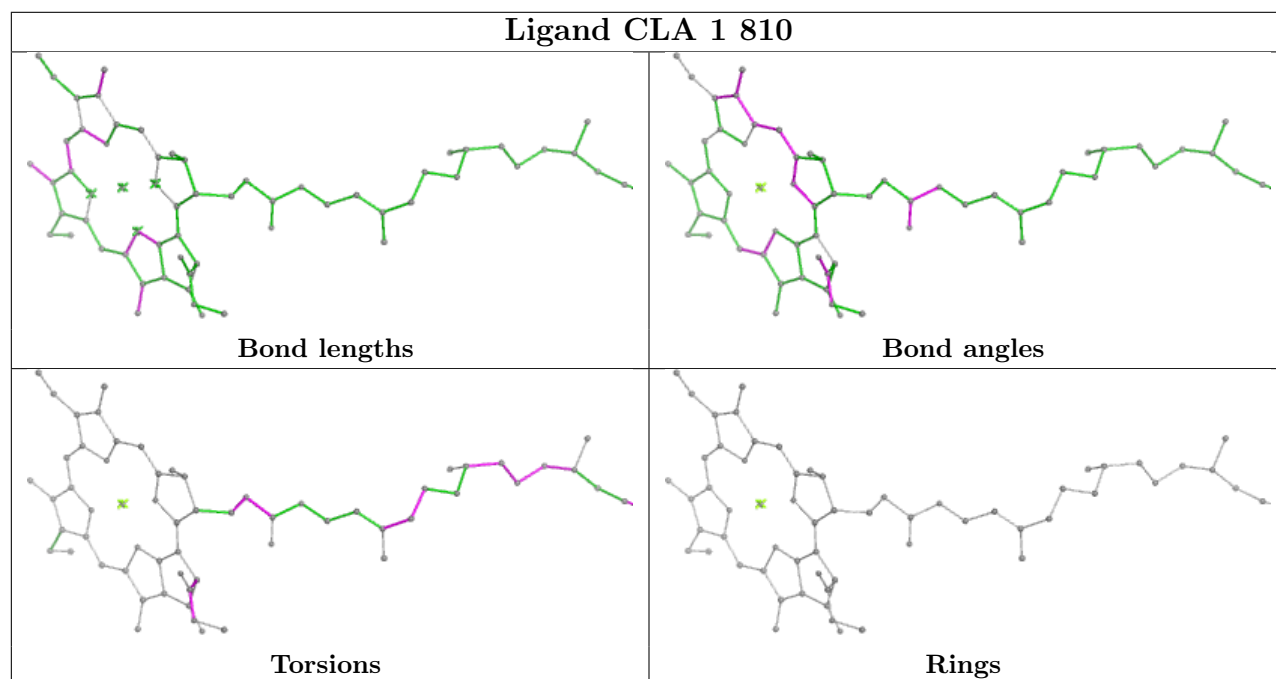
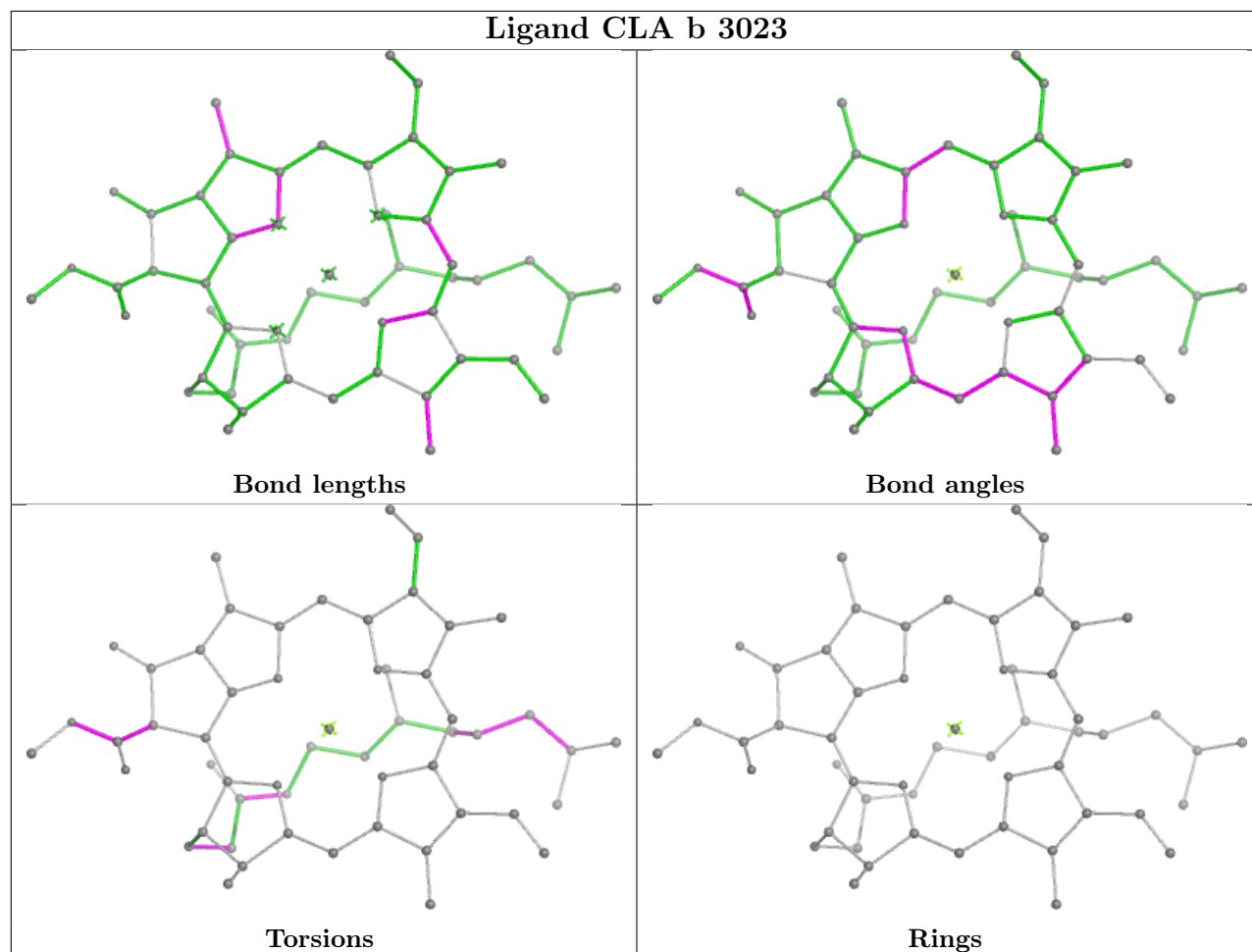


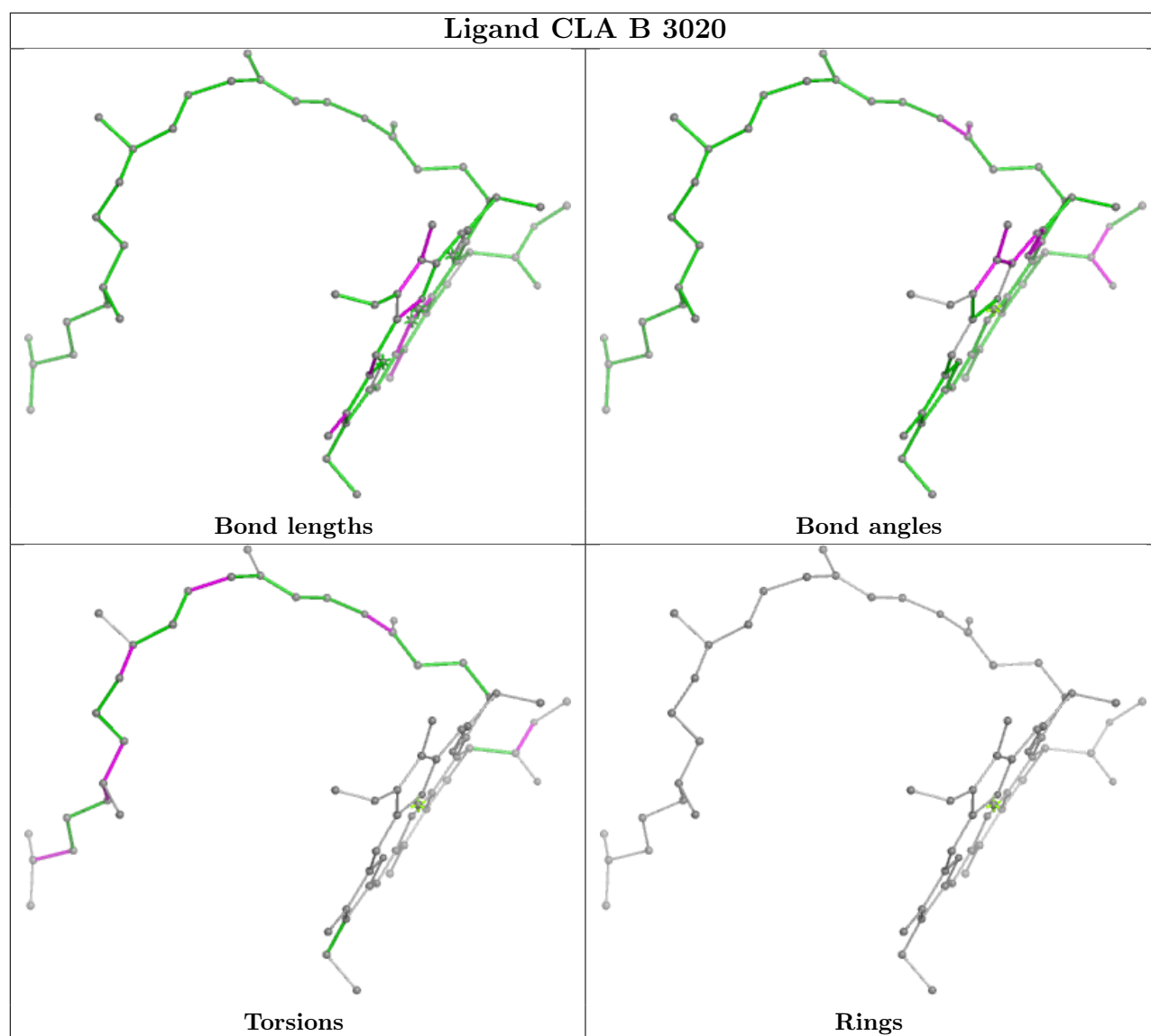
Ligand CLA A 803**Ligand BCR 9 104**

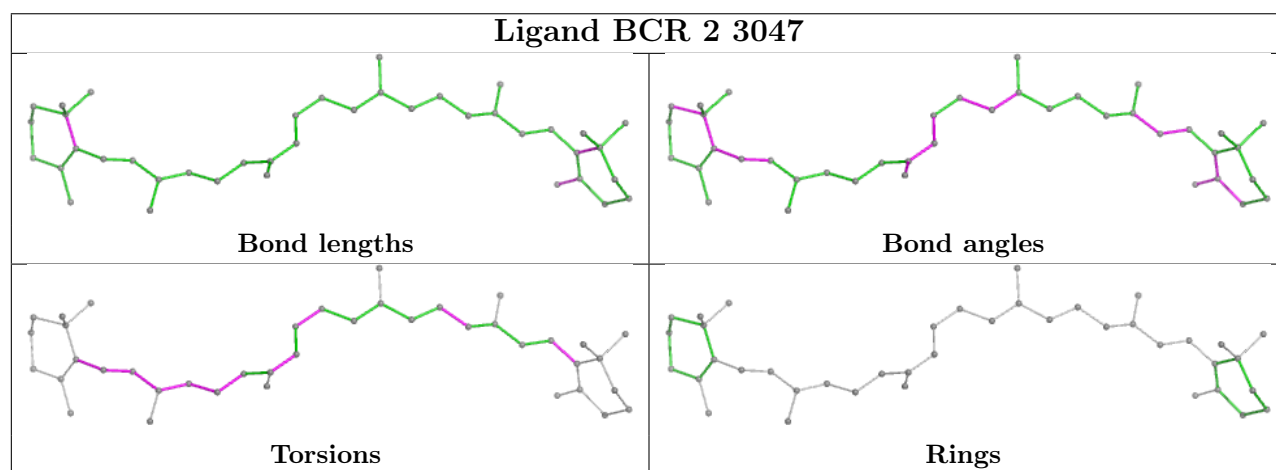
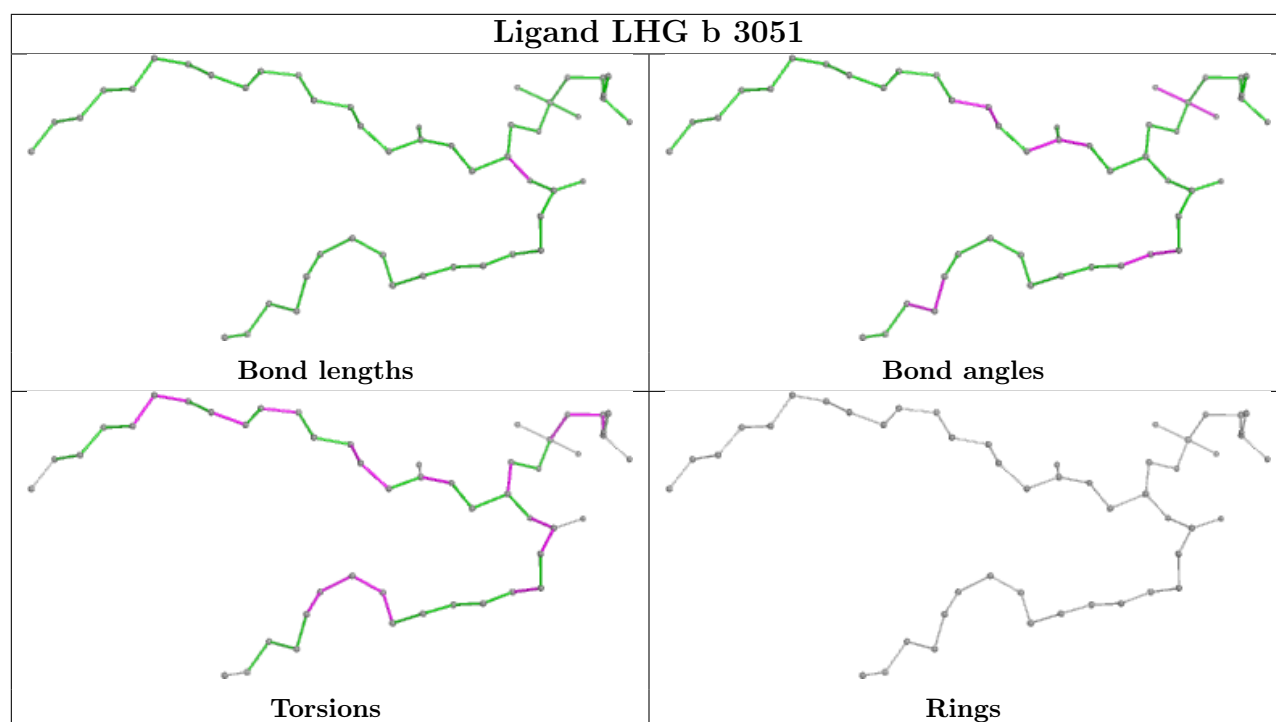


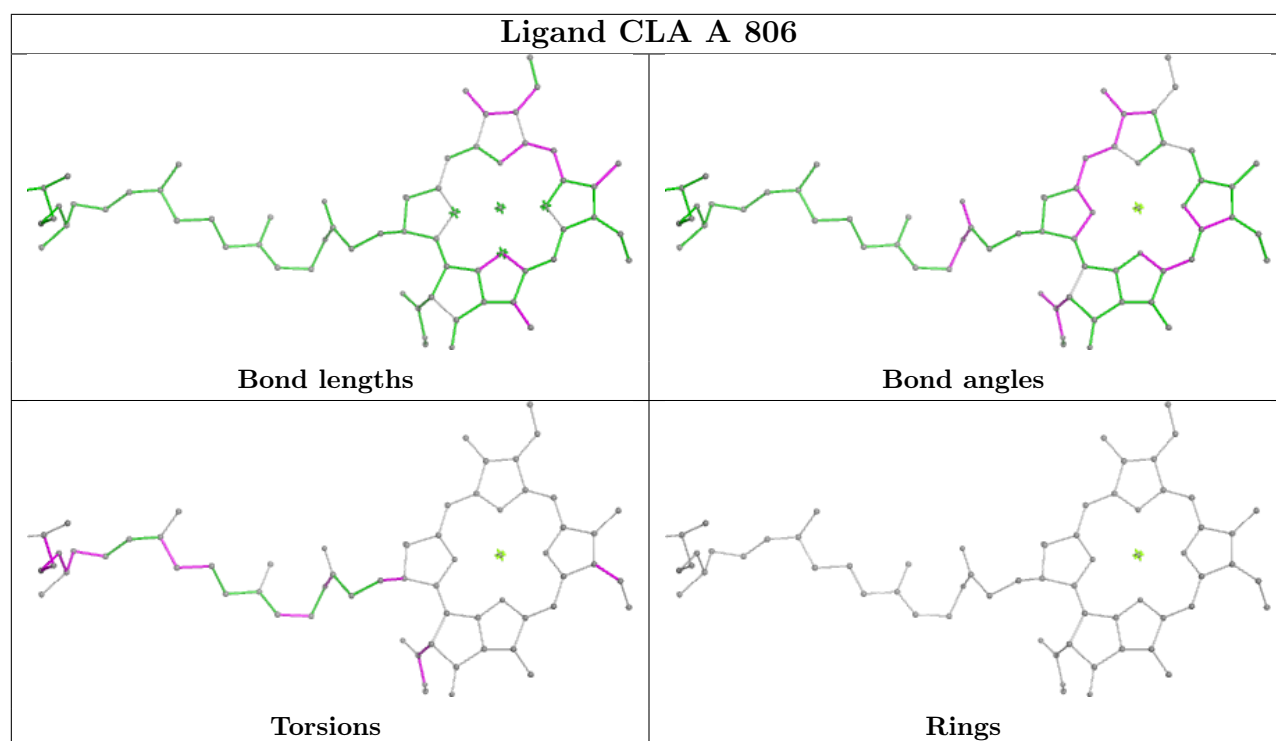
Ligand CLA f 204



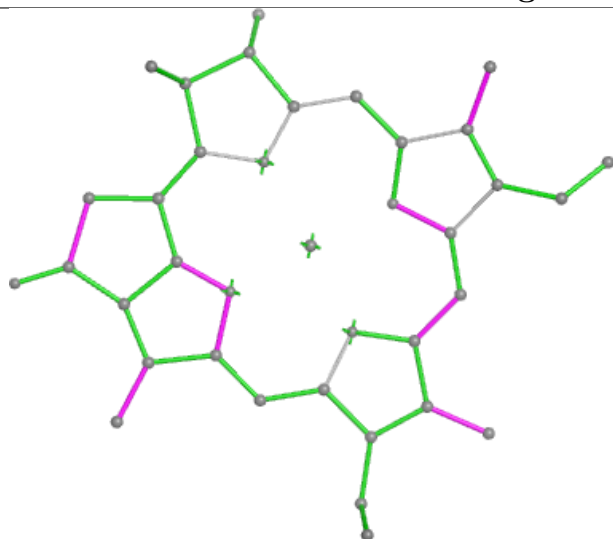




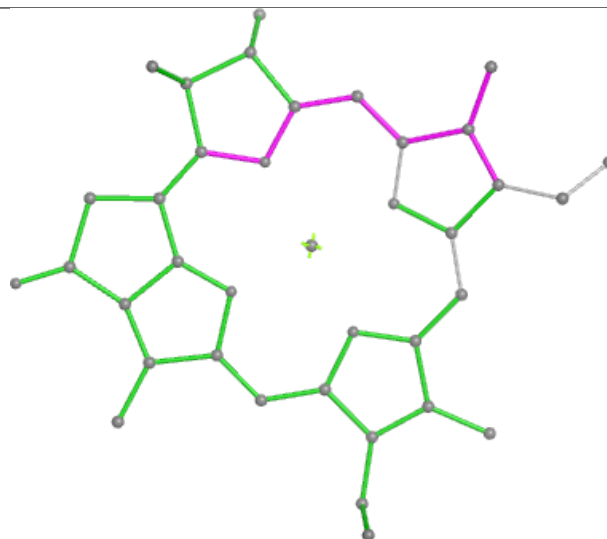




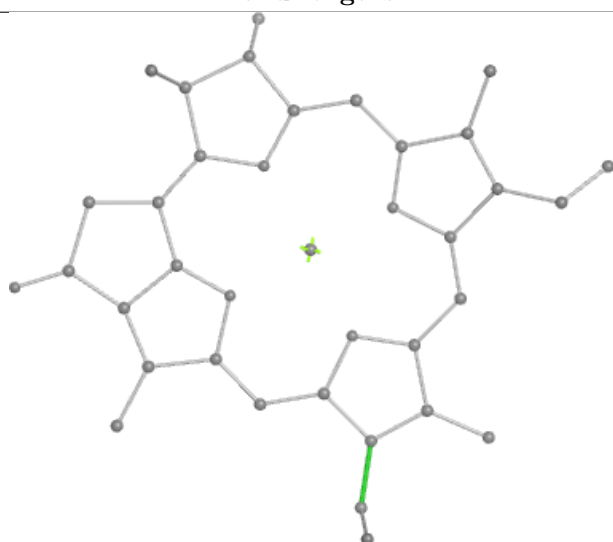
Ligand CLA J 102



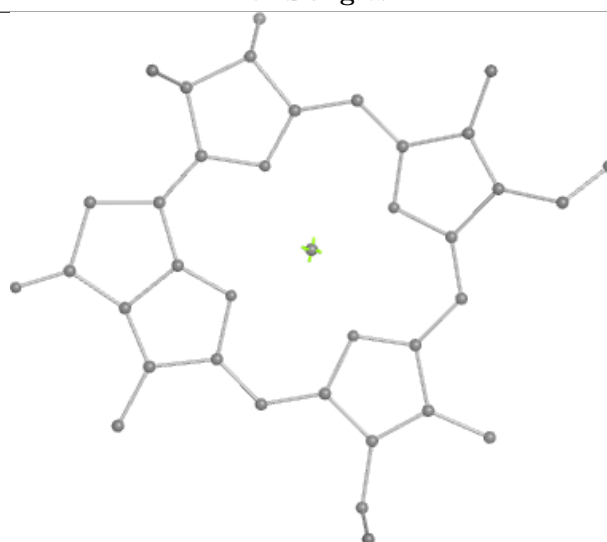
Bond lengths



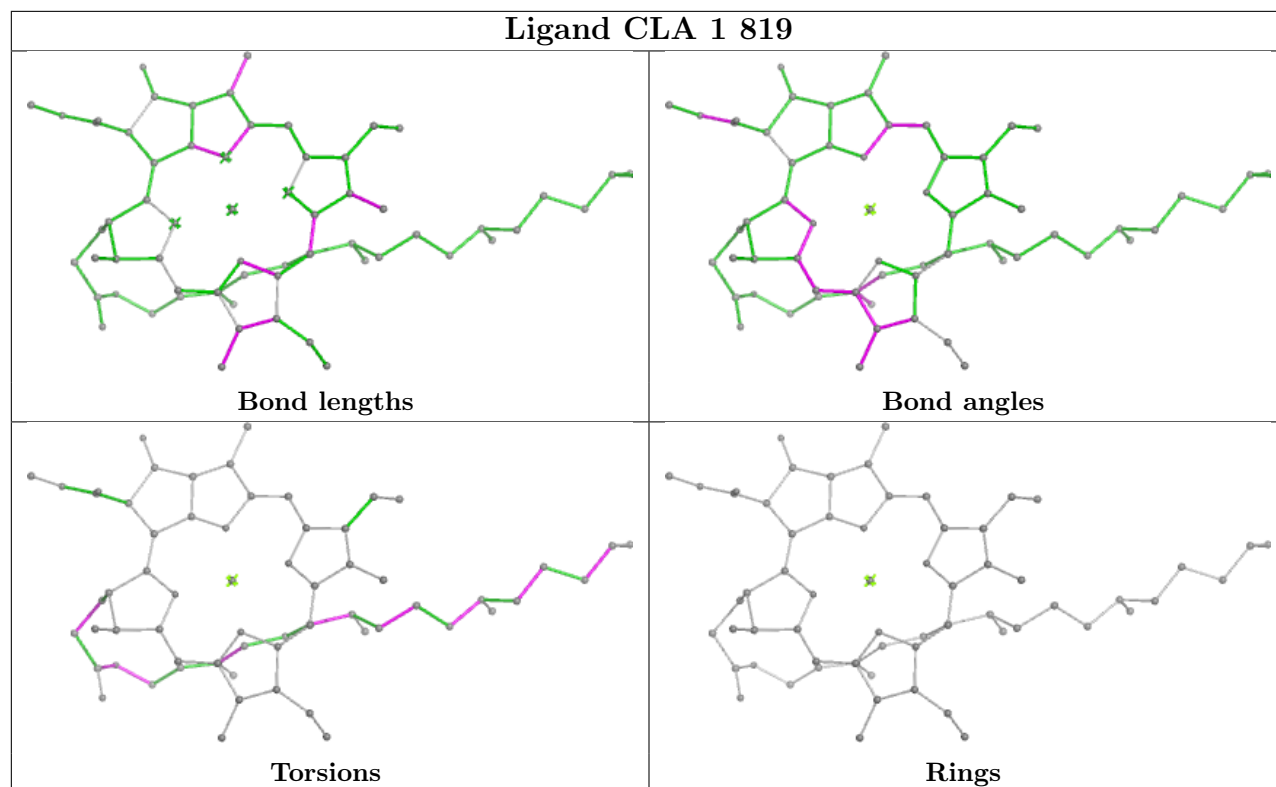
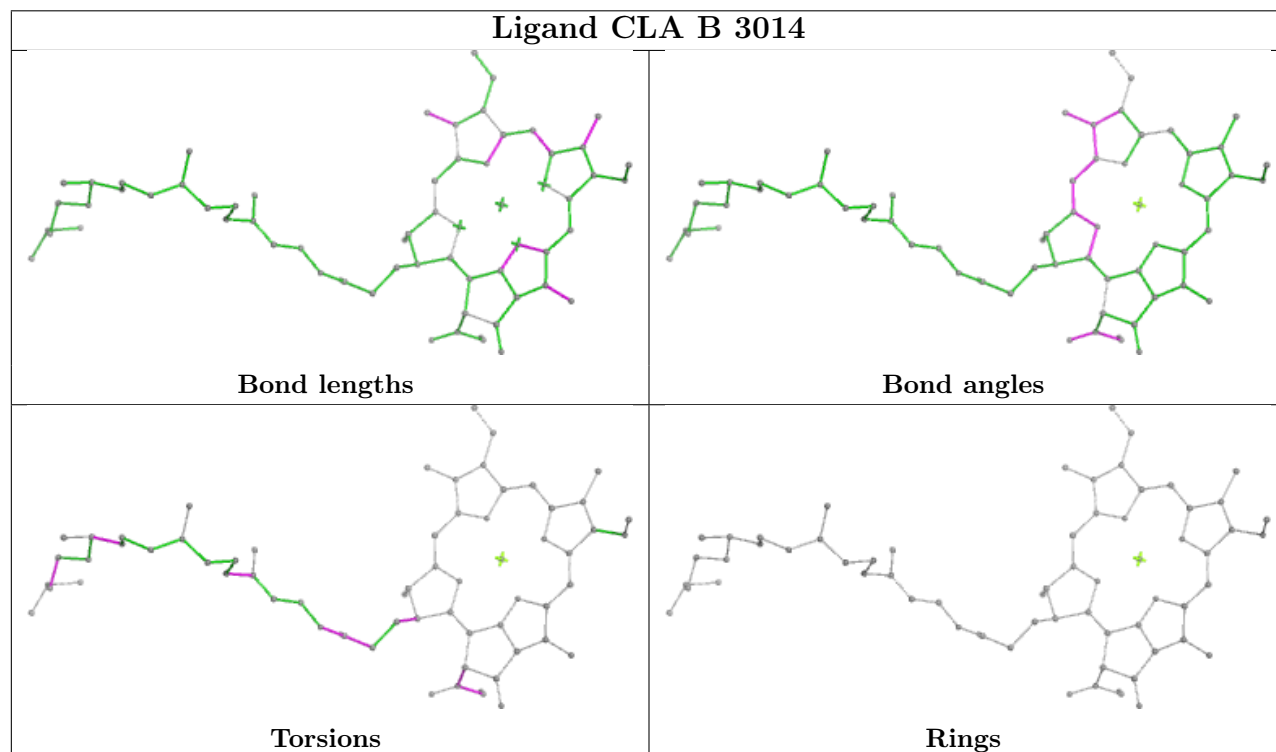
Bond angles

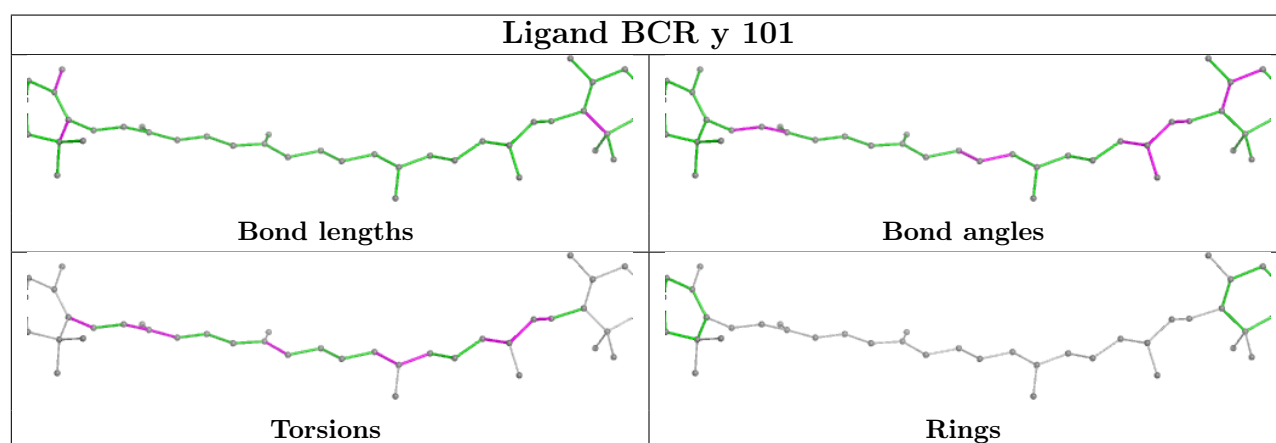
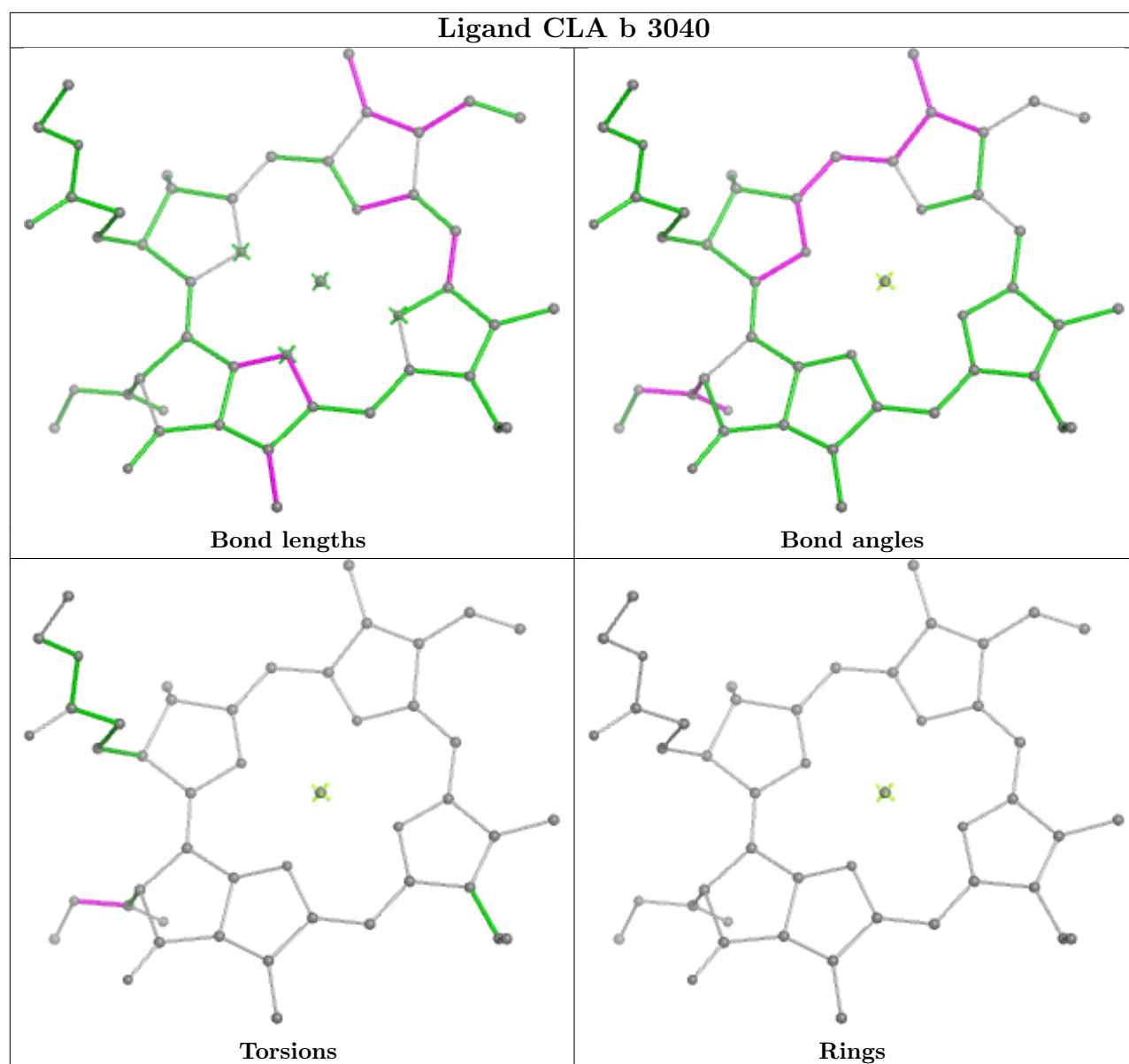


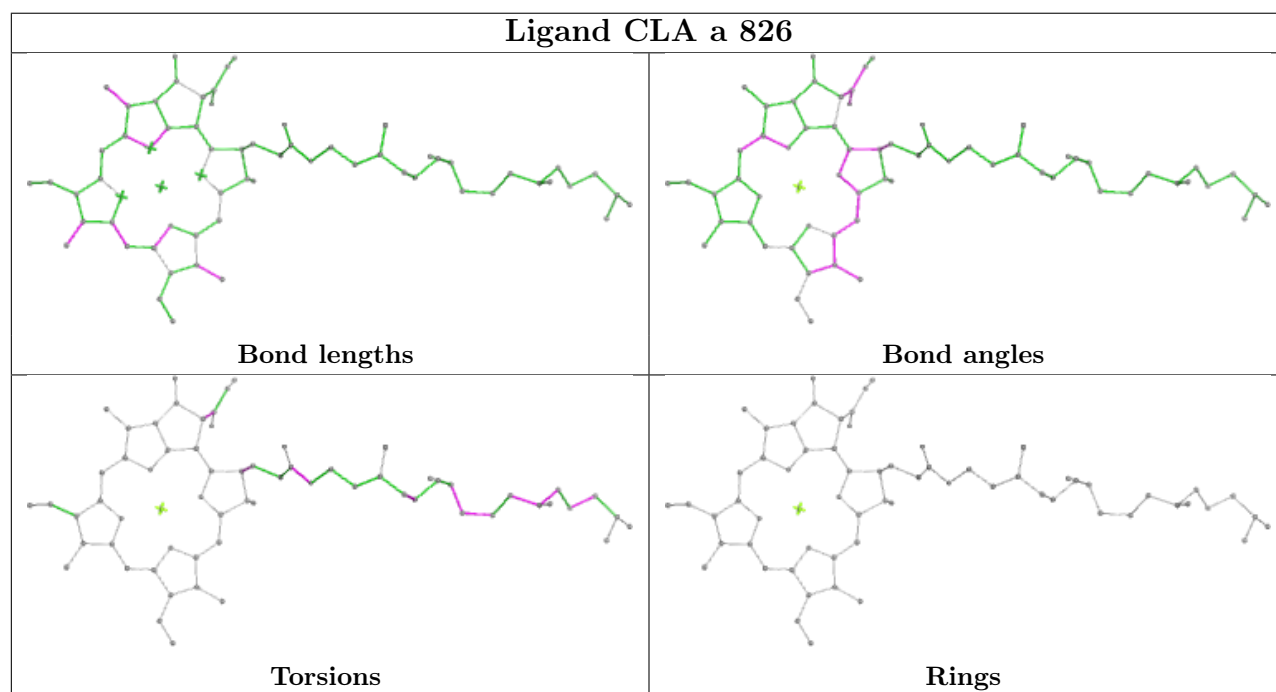
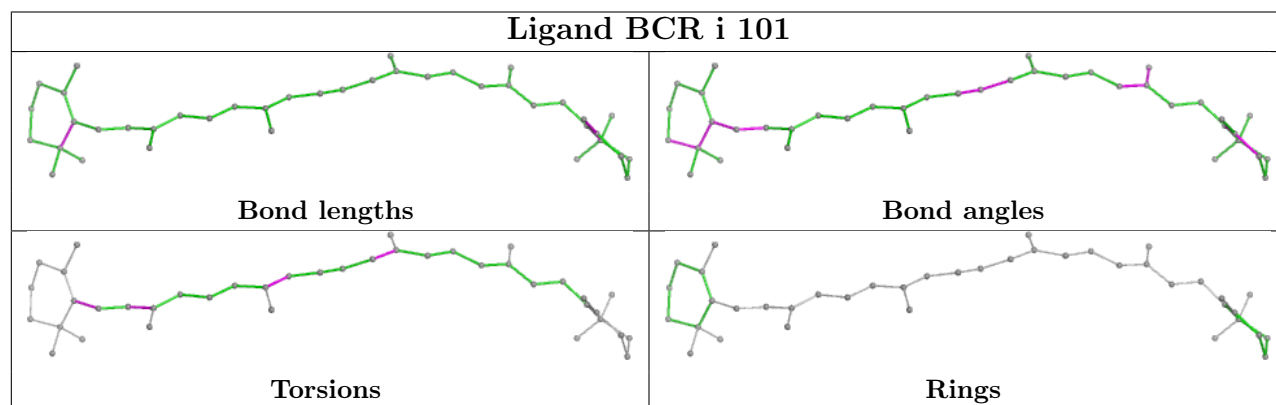
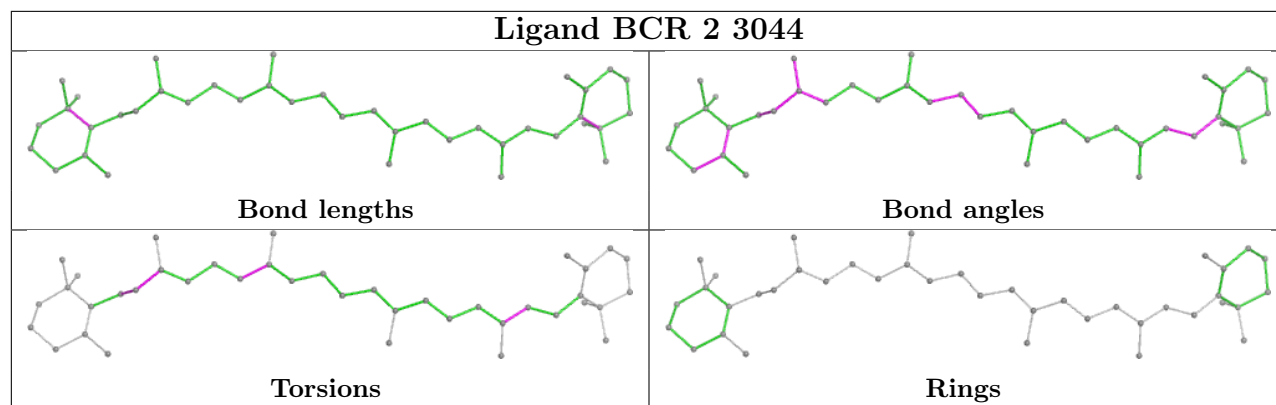
Torsions

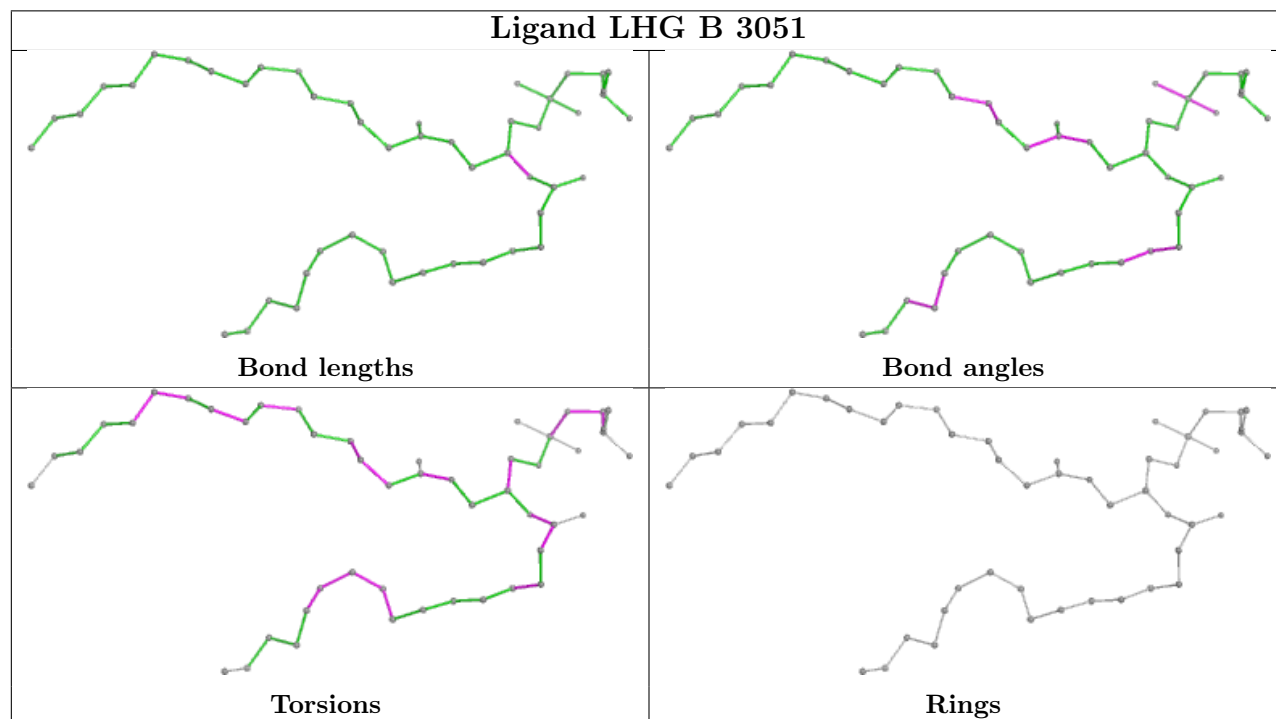
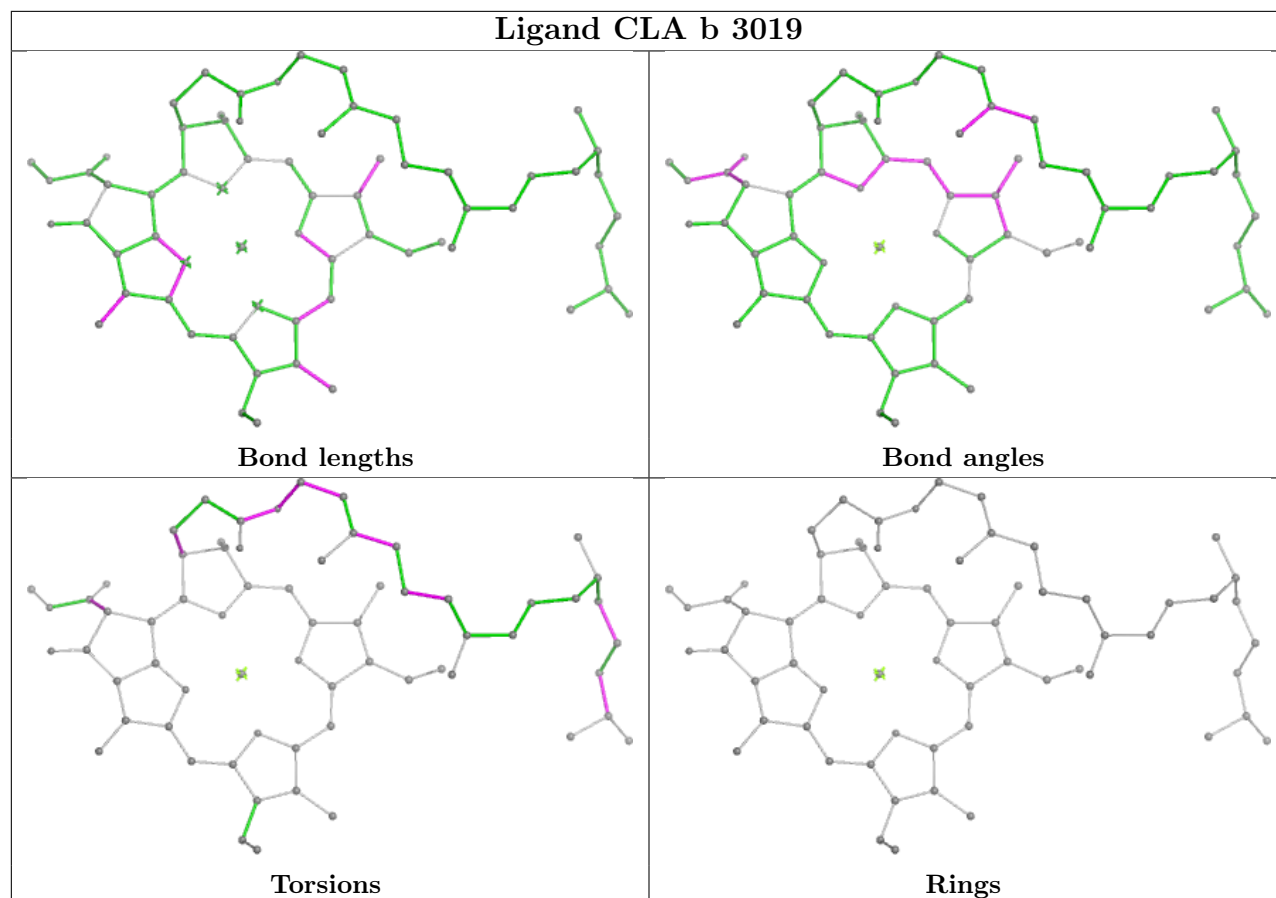


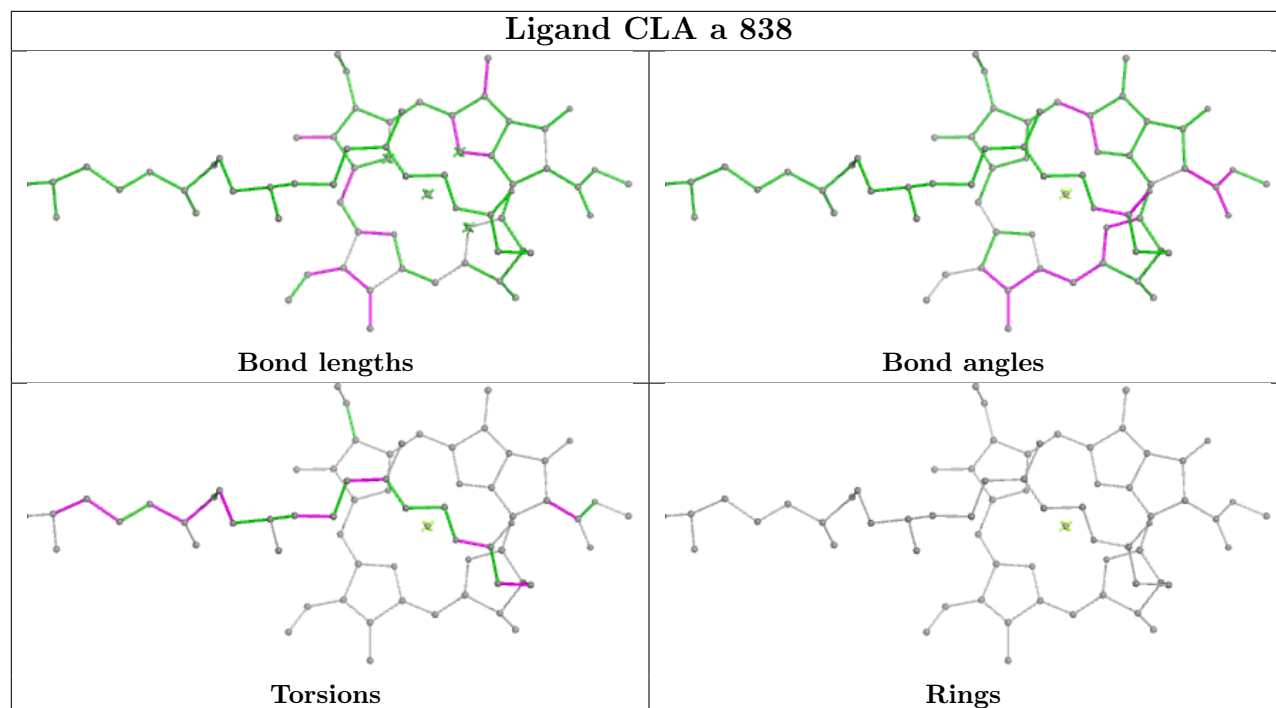
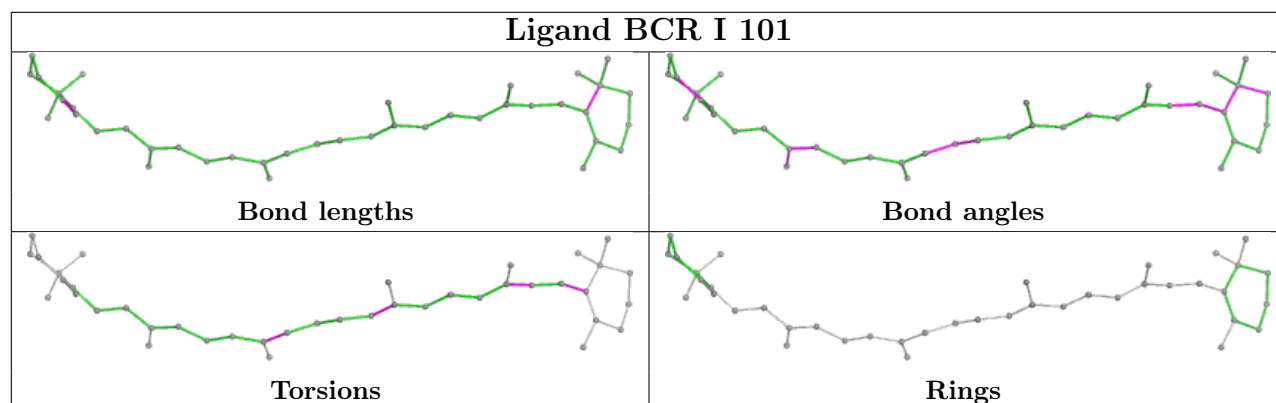
Rings

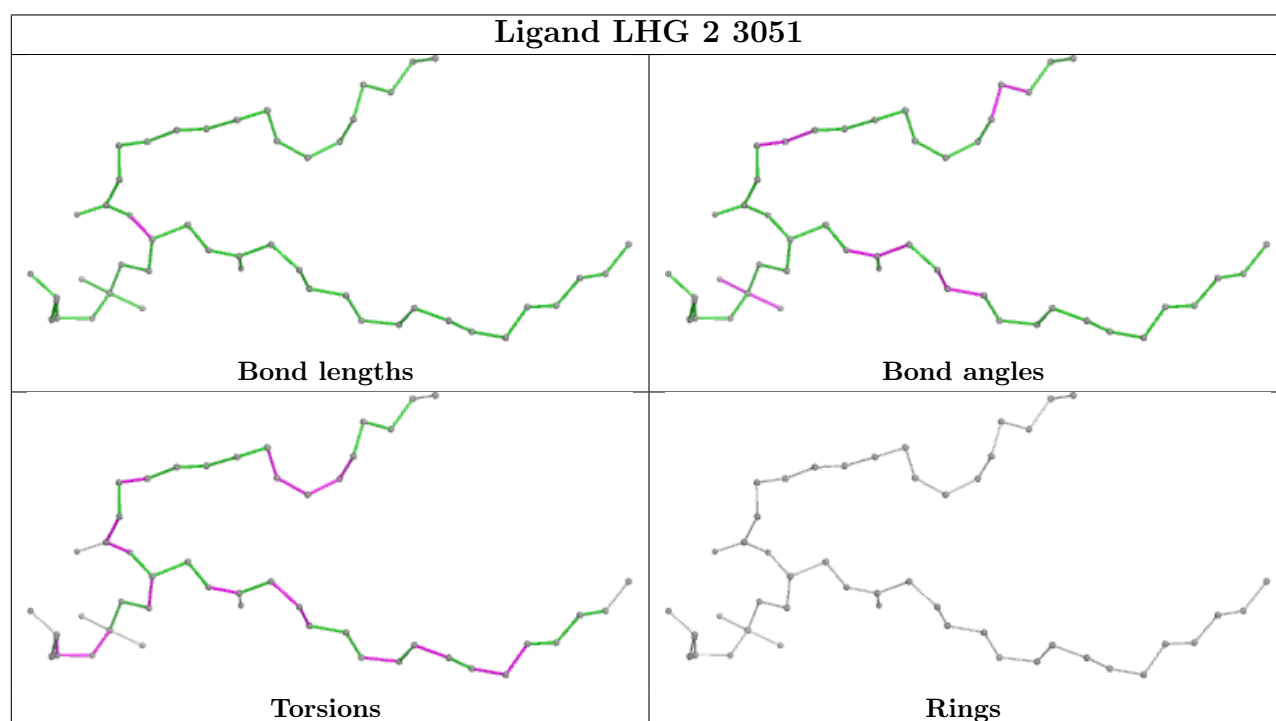
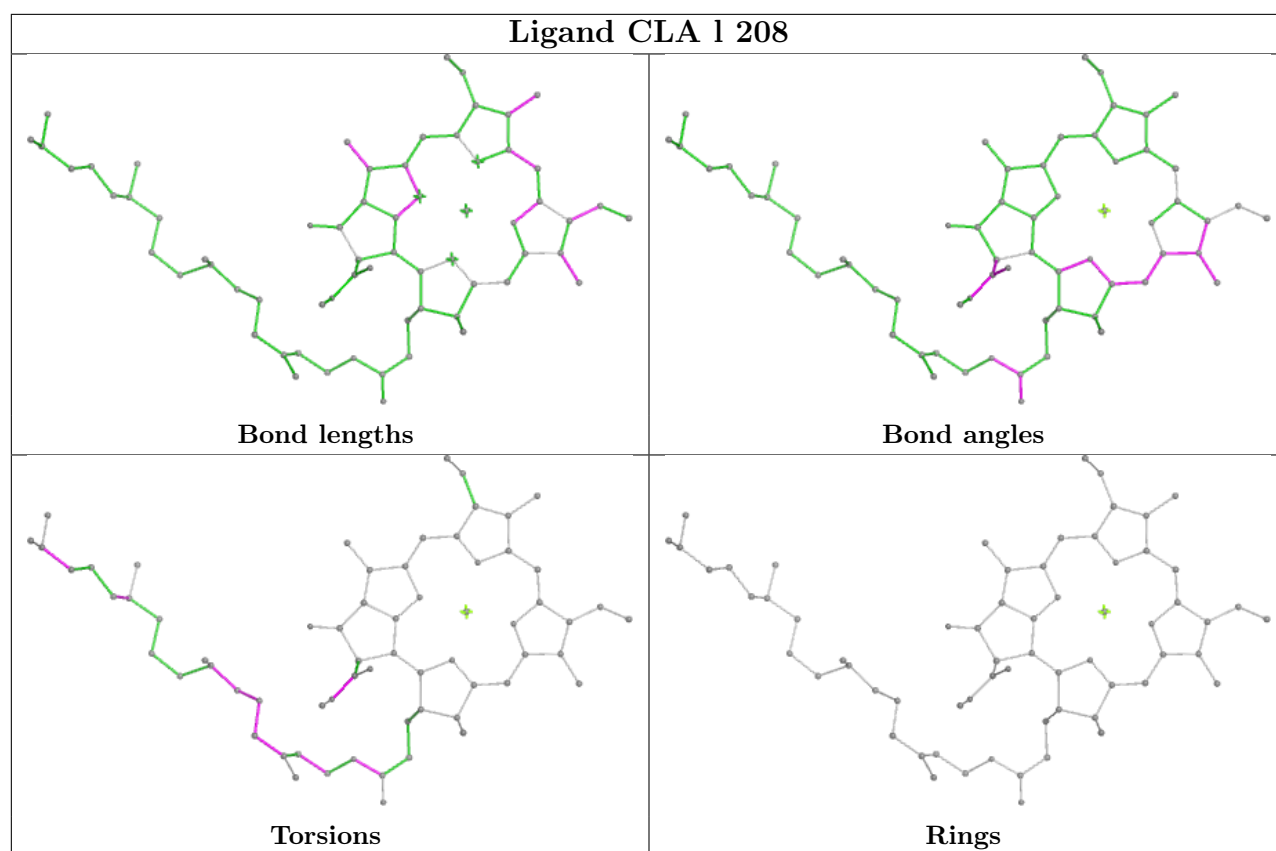
Ligand CLA 1 819**Ligand CLA B 3014**

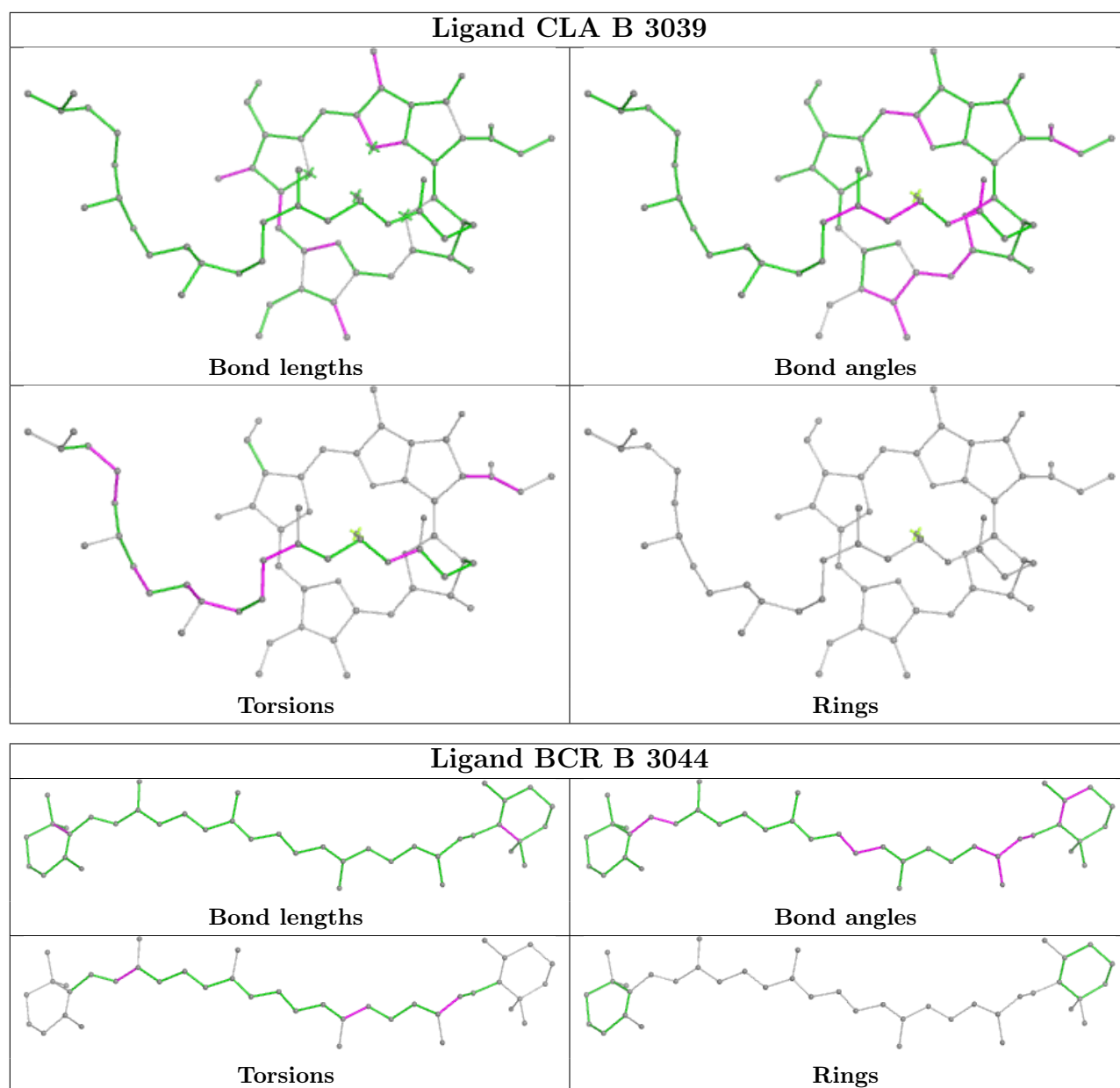




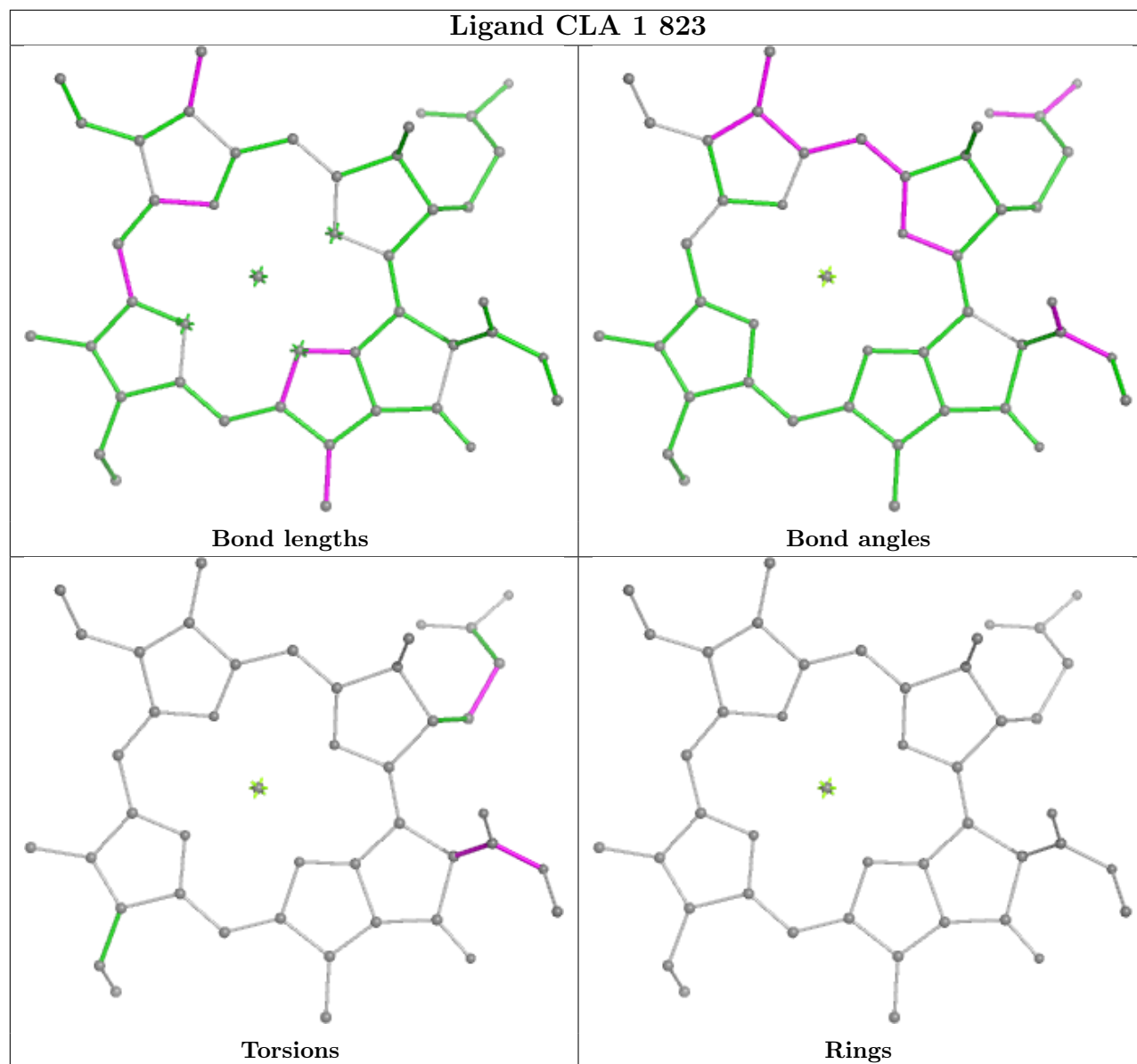


Ligand CLA a 838**Ligand BCR I 101**

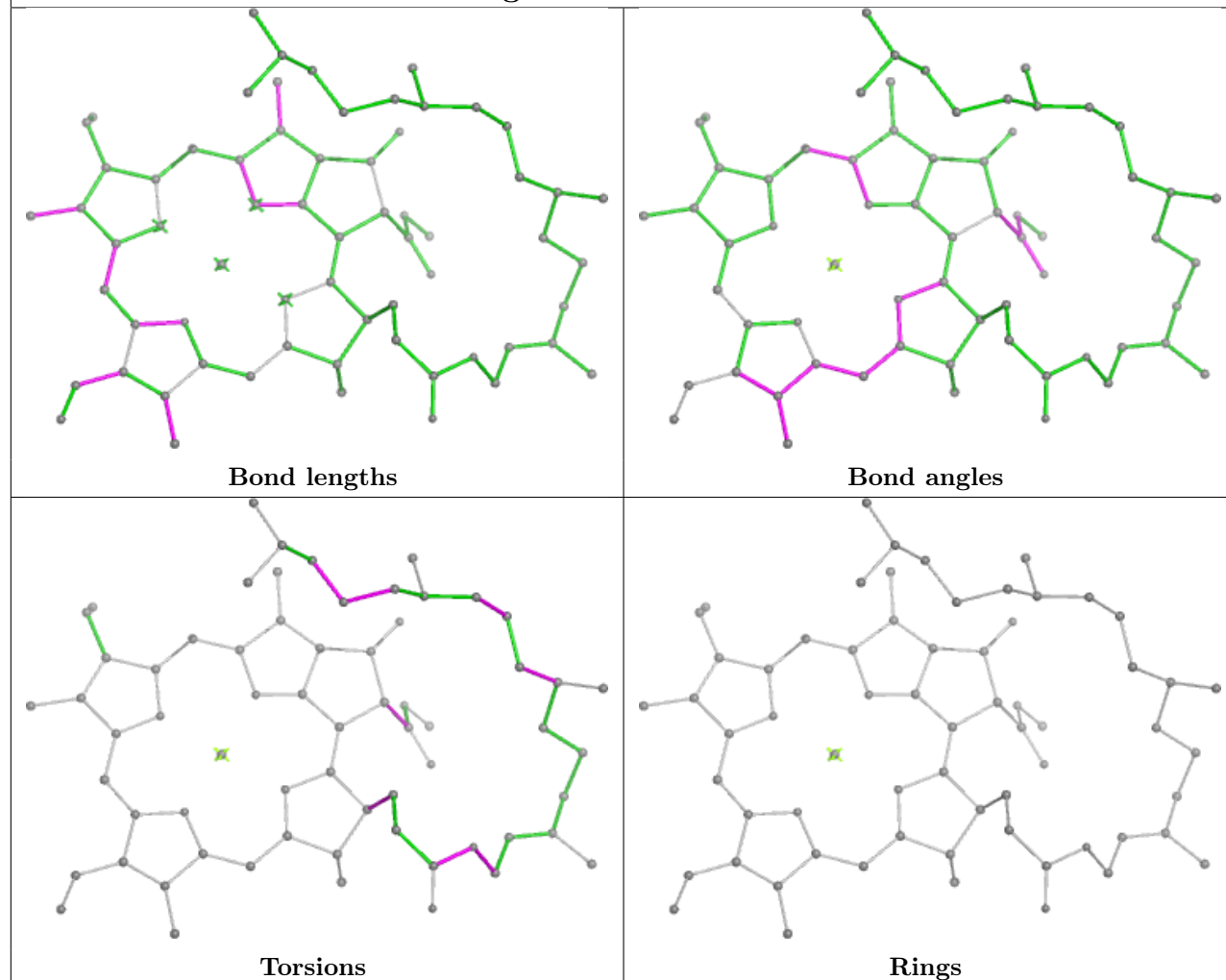




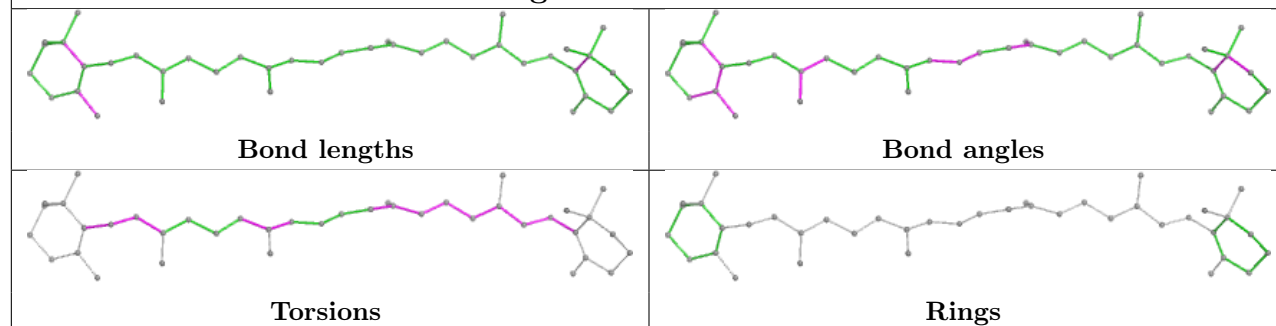
Ligand CLA 1 823

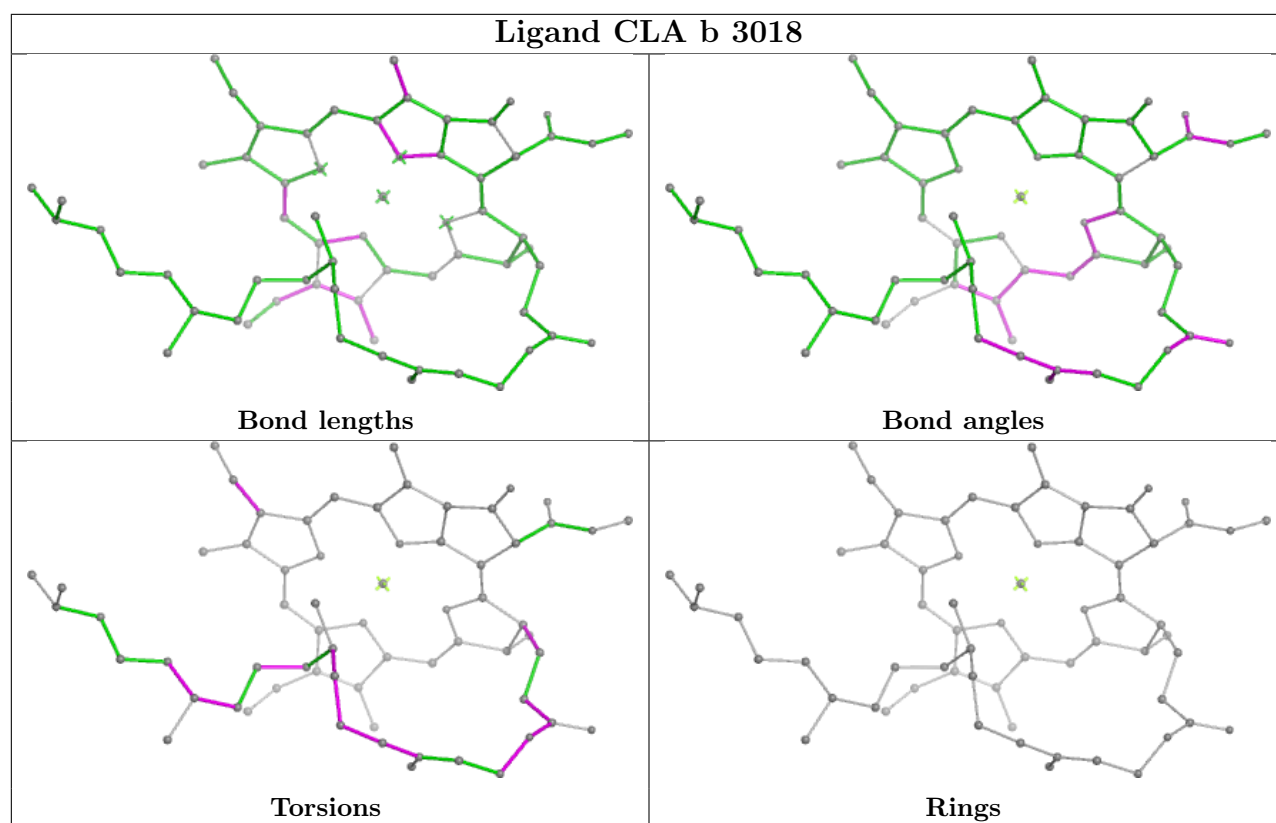
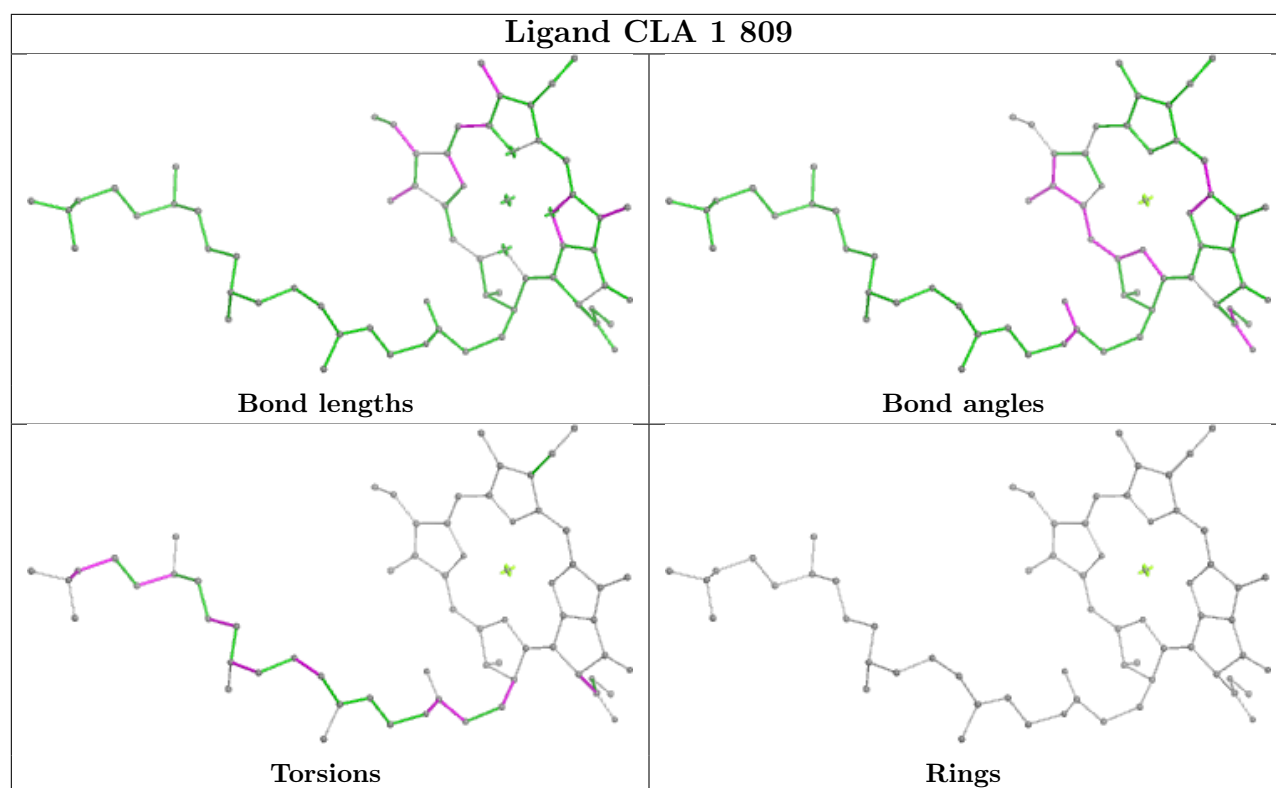


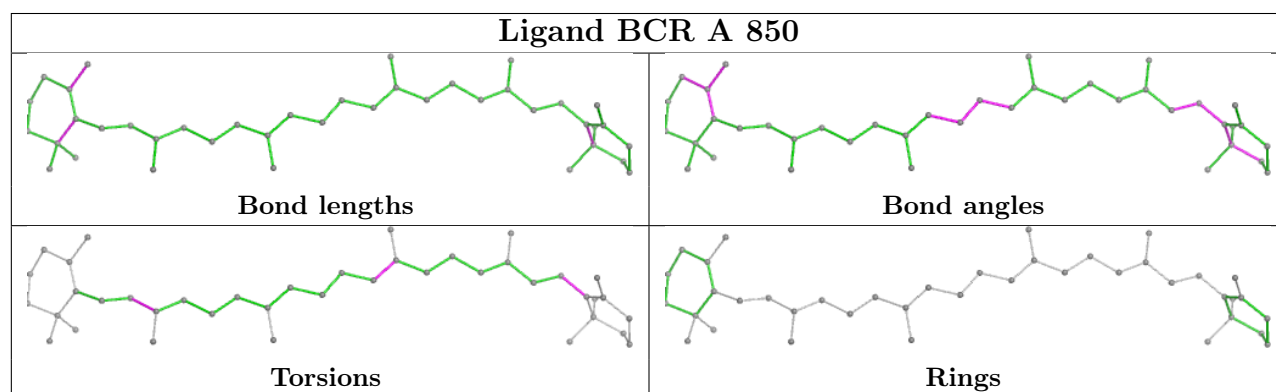
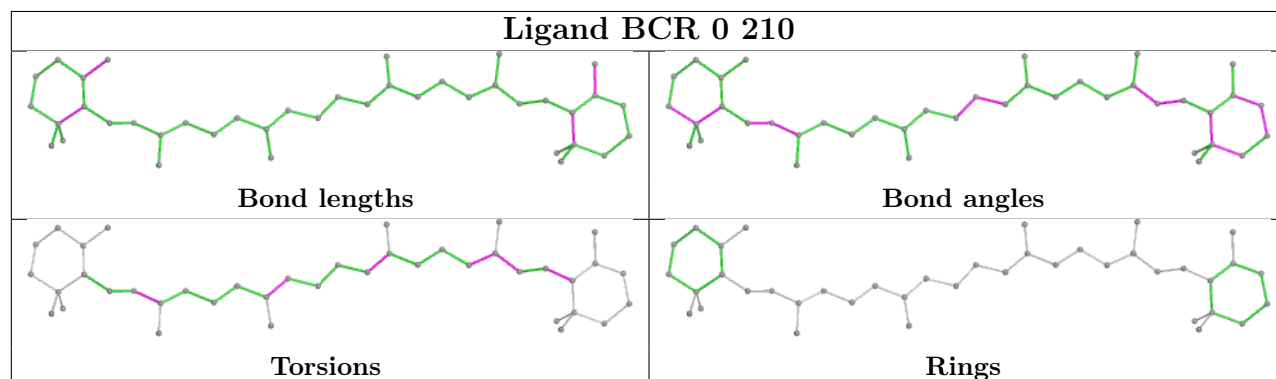
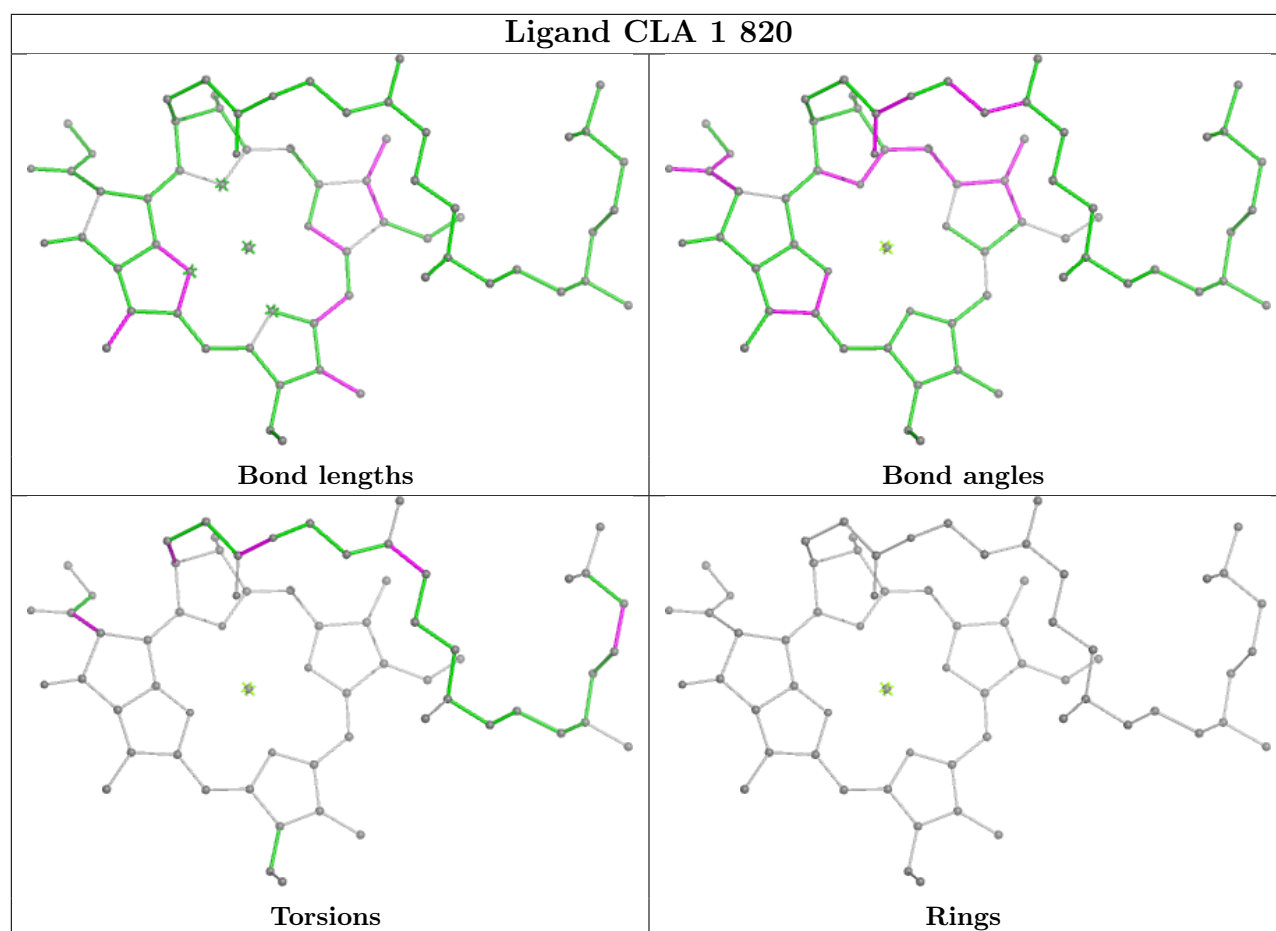
Ligand CLA B 3007

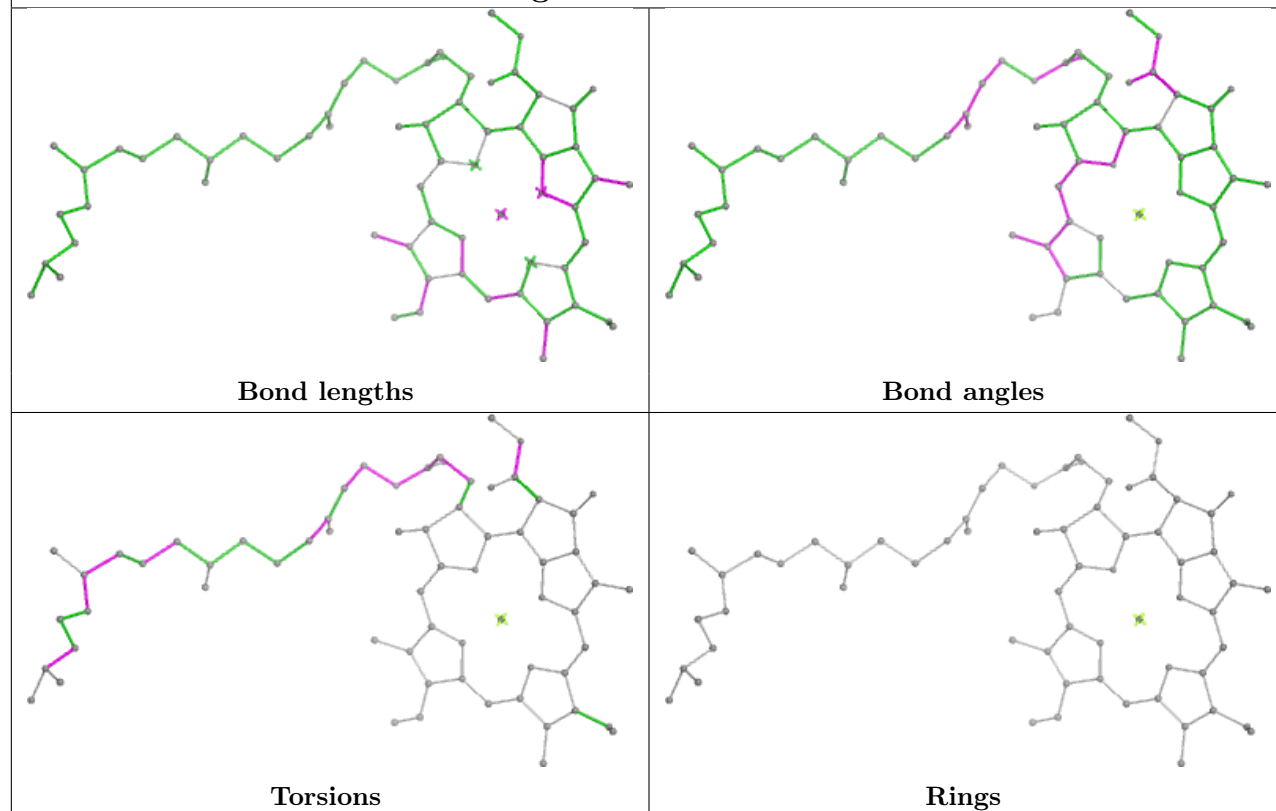
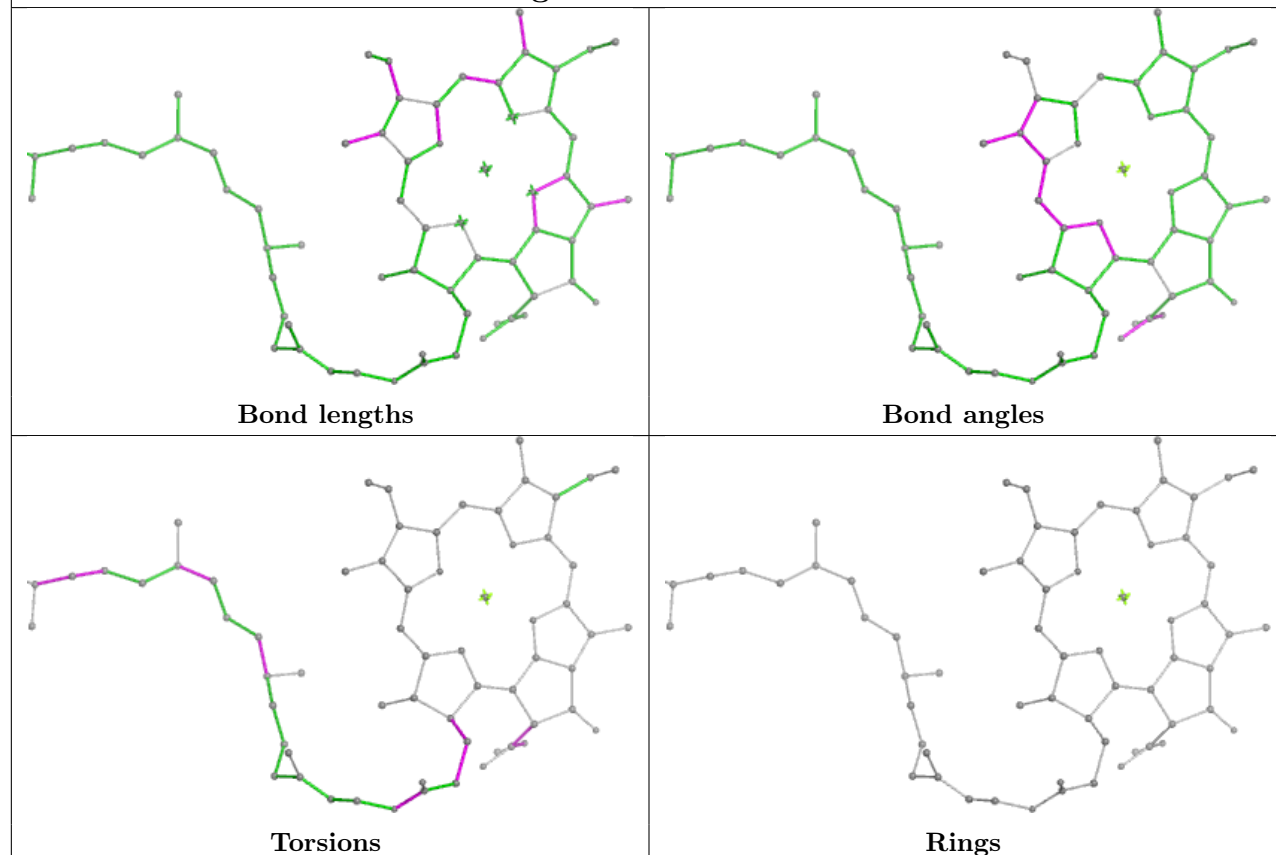


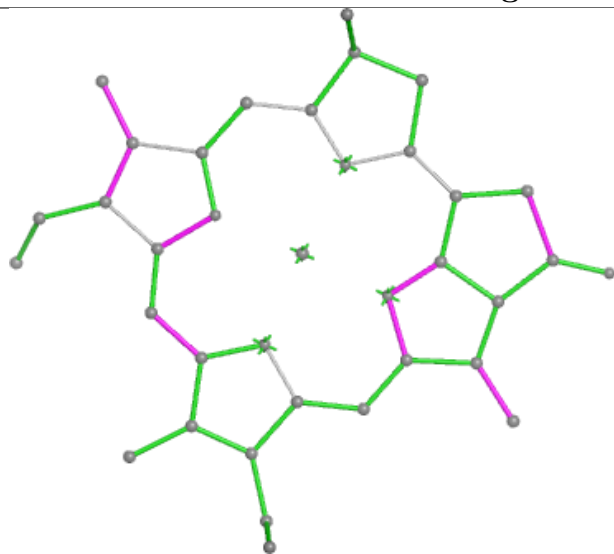
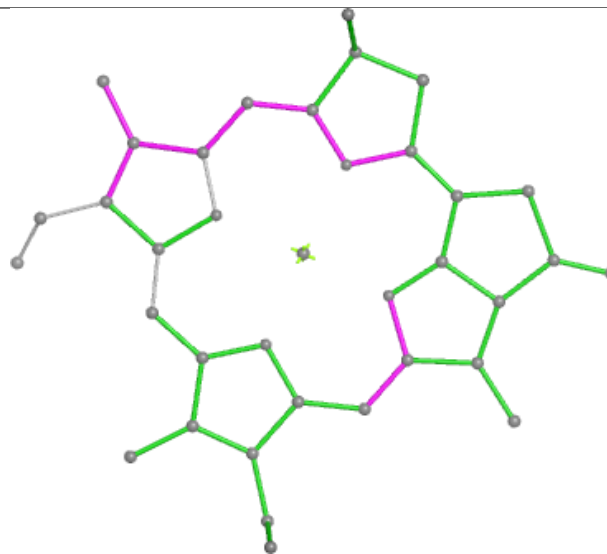
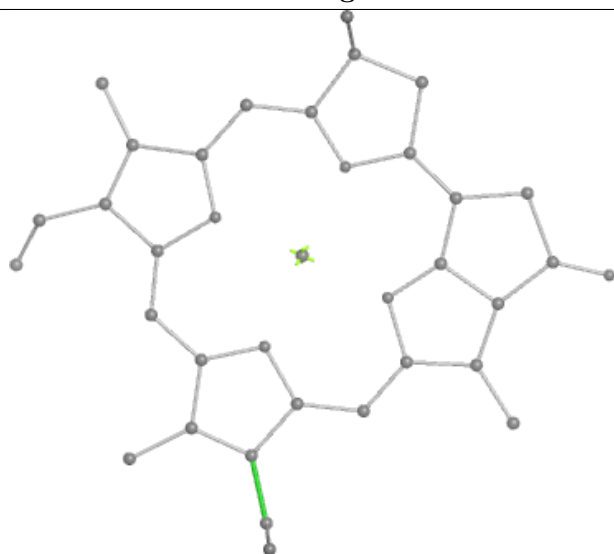
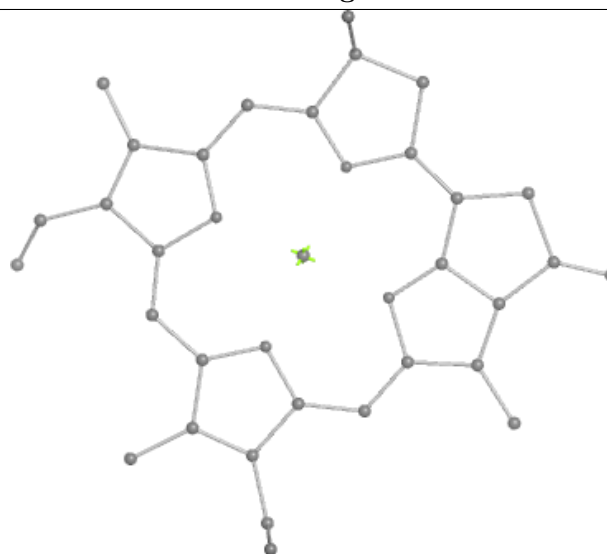
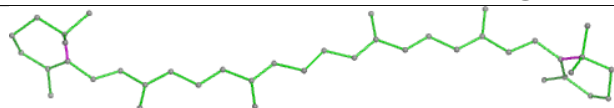
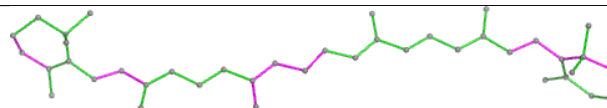
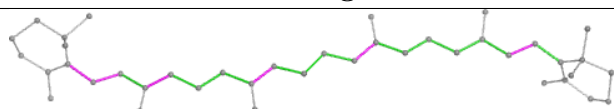
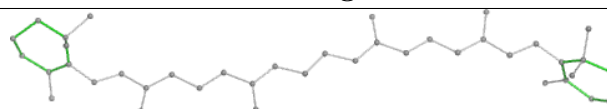
Ligand BCR A 847



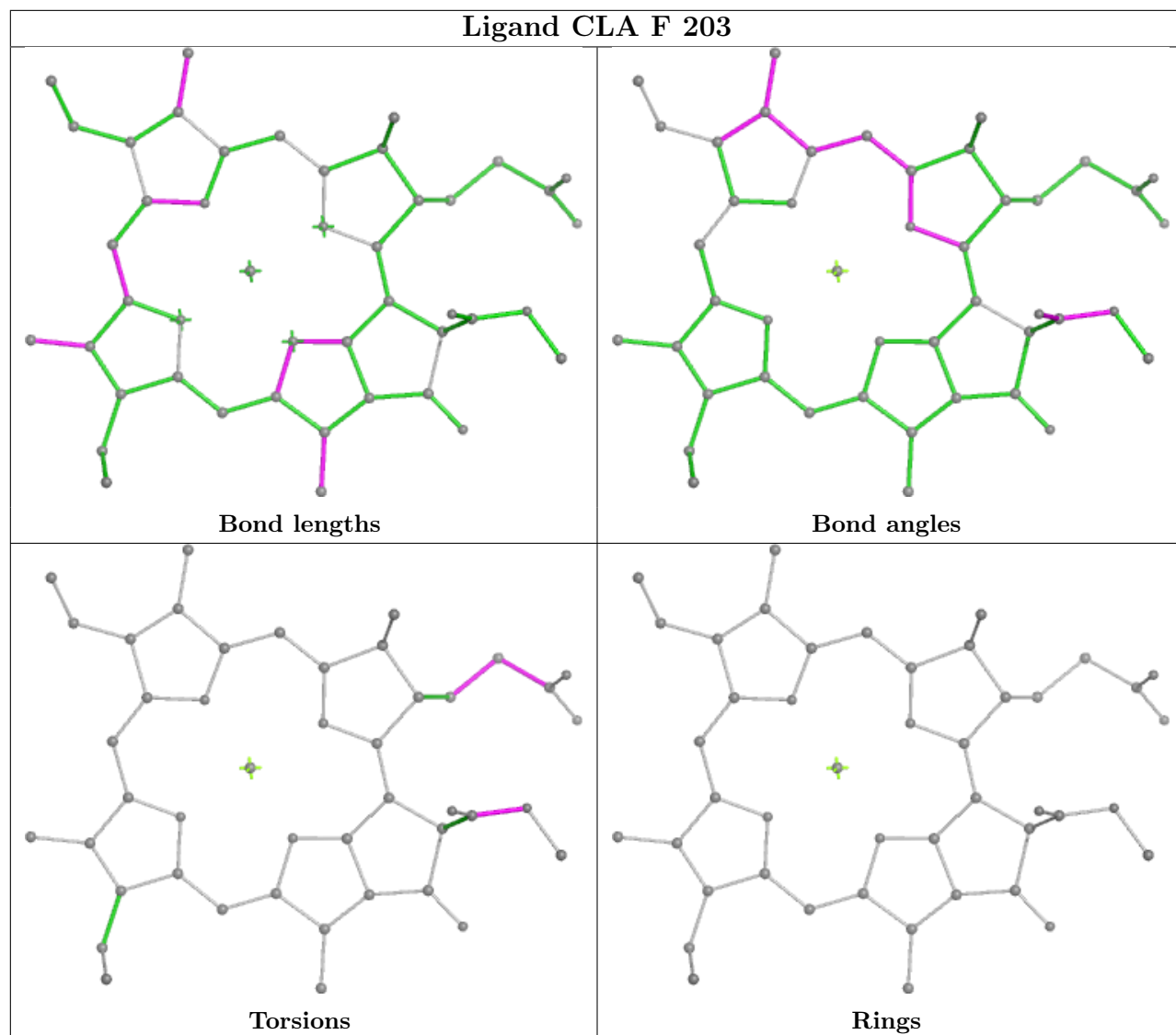




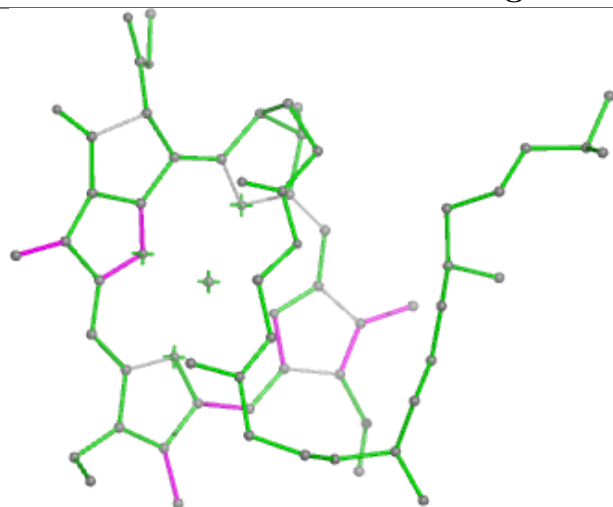
Ligand CLA A 802**Ligand CLA A 814**

Ligand CLA M 1601**Bond lengths****Bond angles****Torsions****Rings****Ligand BCR a 848****Bond lengths****Bond angles****Torsions****Rings**

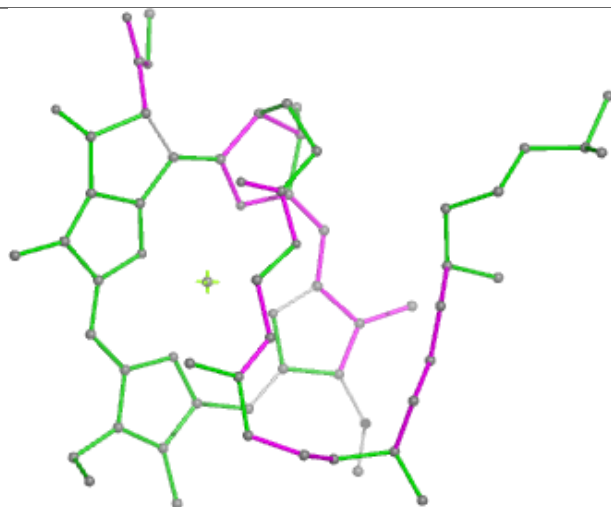
Ligand CLA F 203



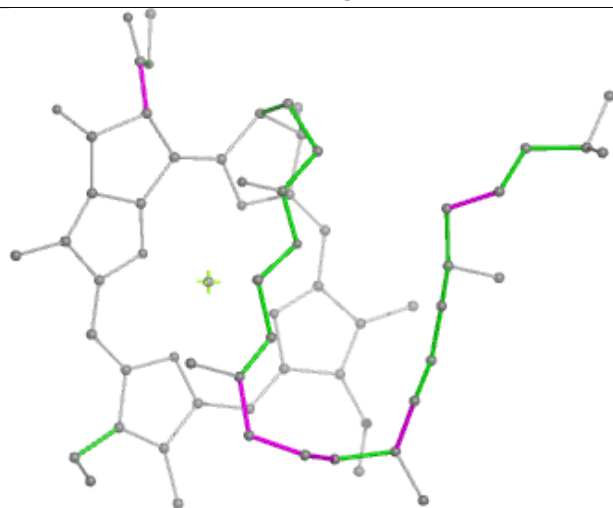
Ligand CLA B 3010



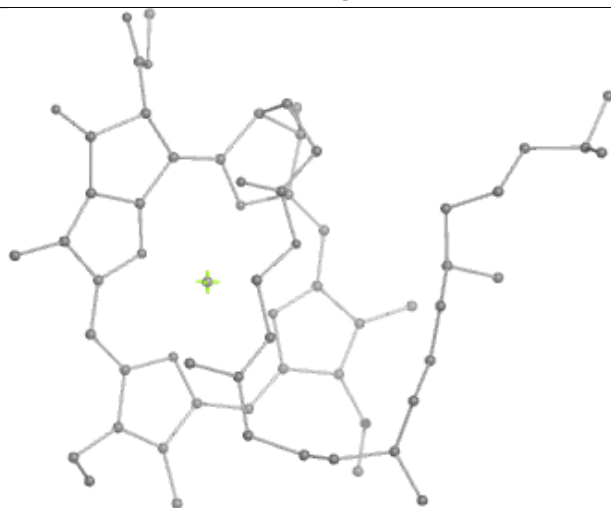
Bond lengths



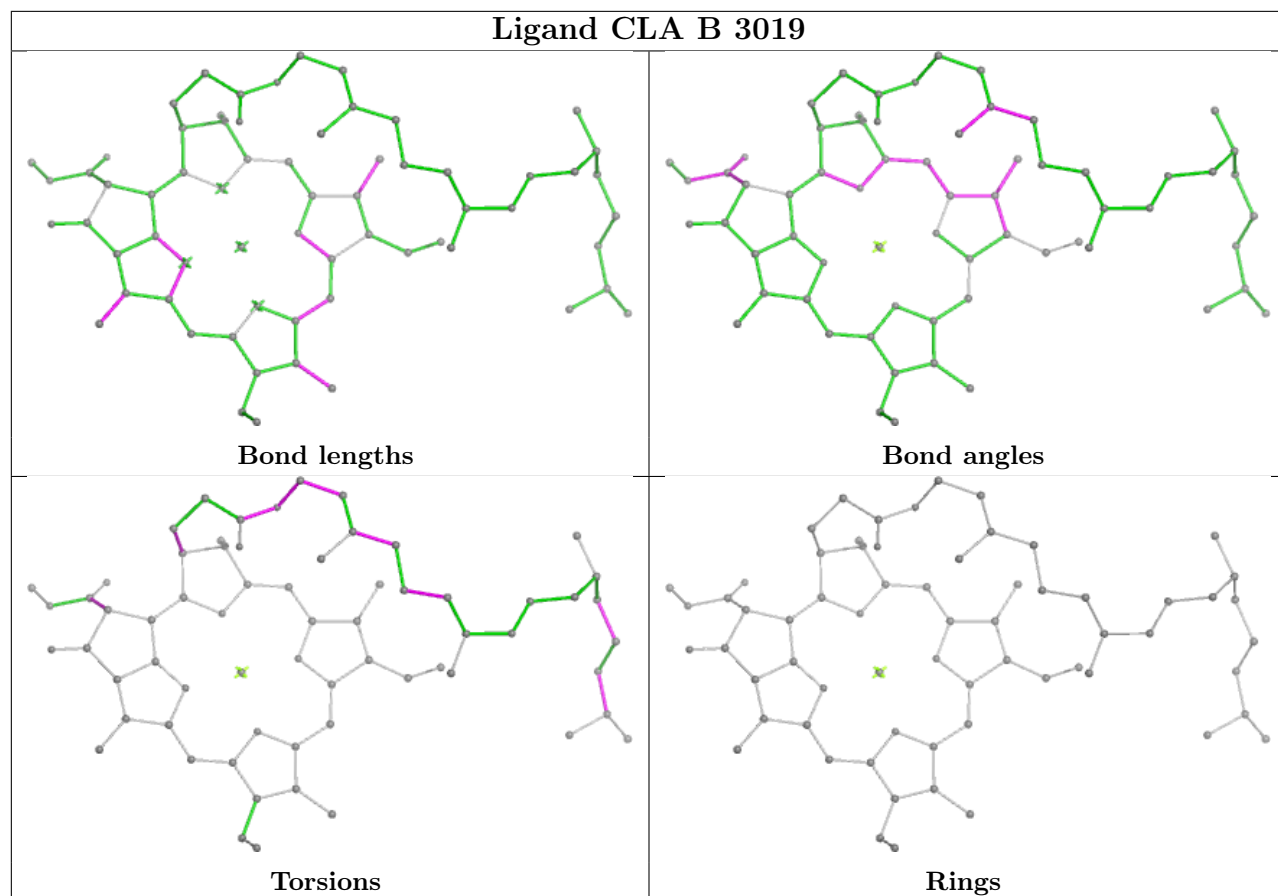
Bond angles



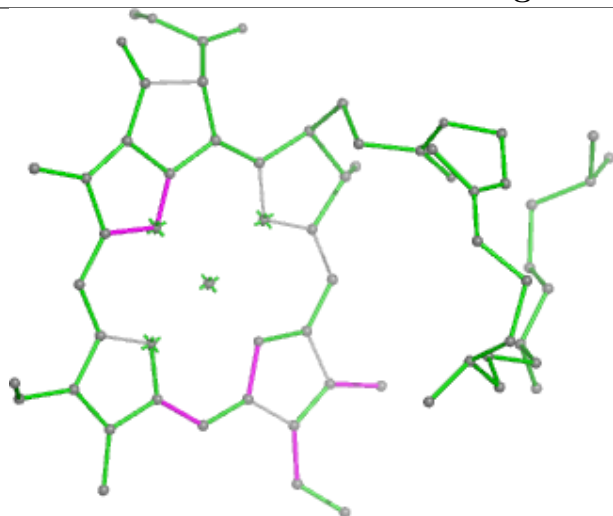
Torsions



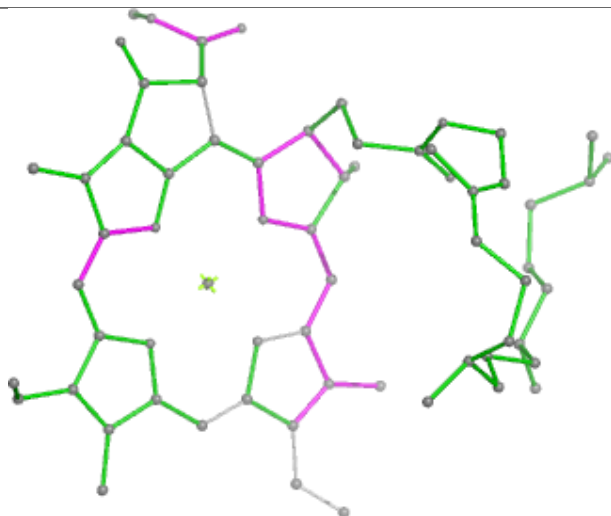
Rings



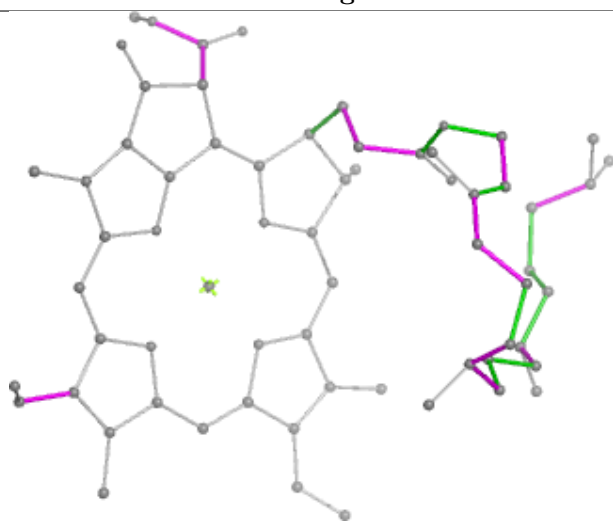
Ligand CLA A 816



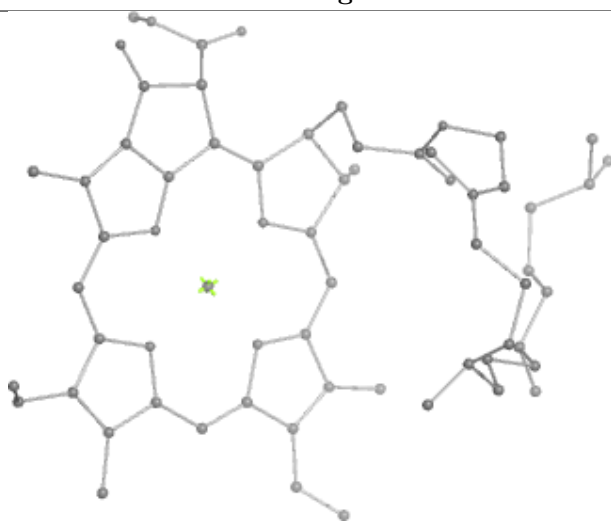
Bond lengths



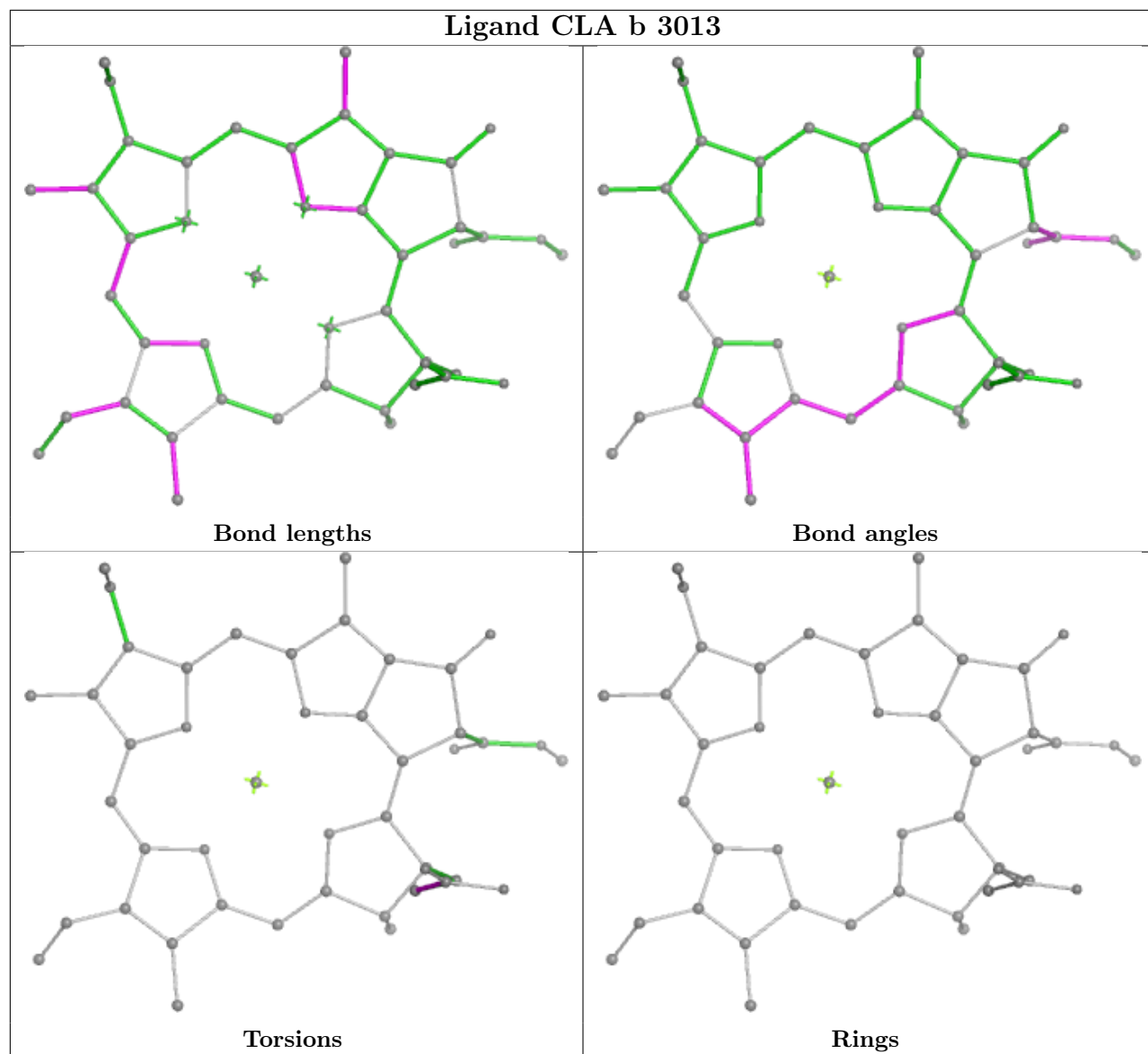
Bond angles



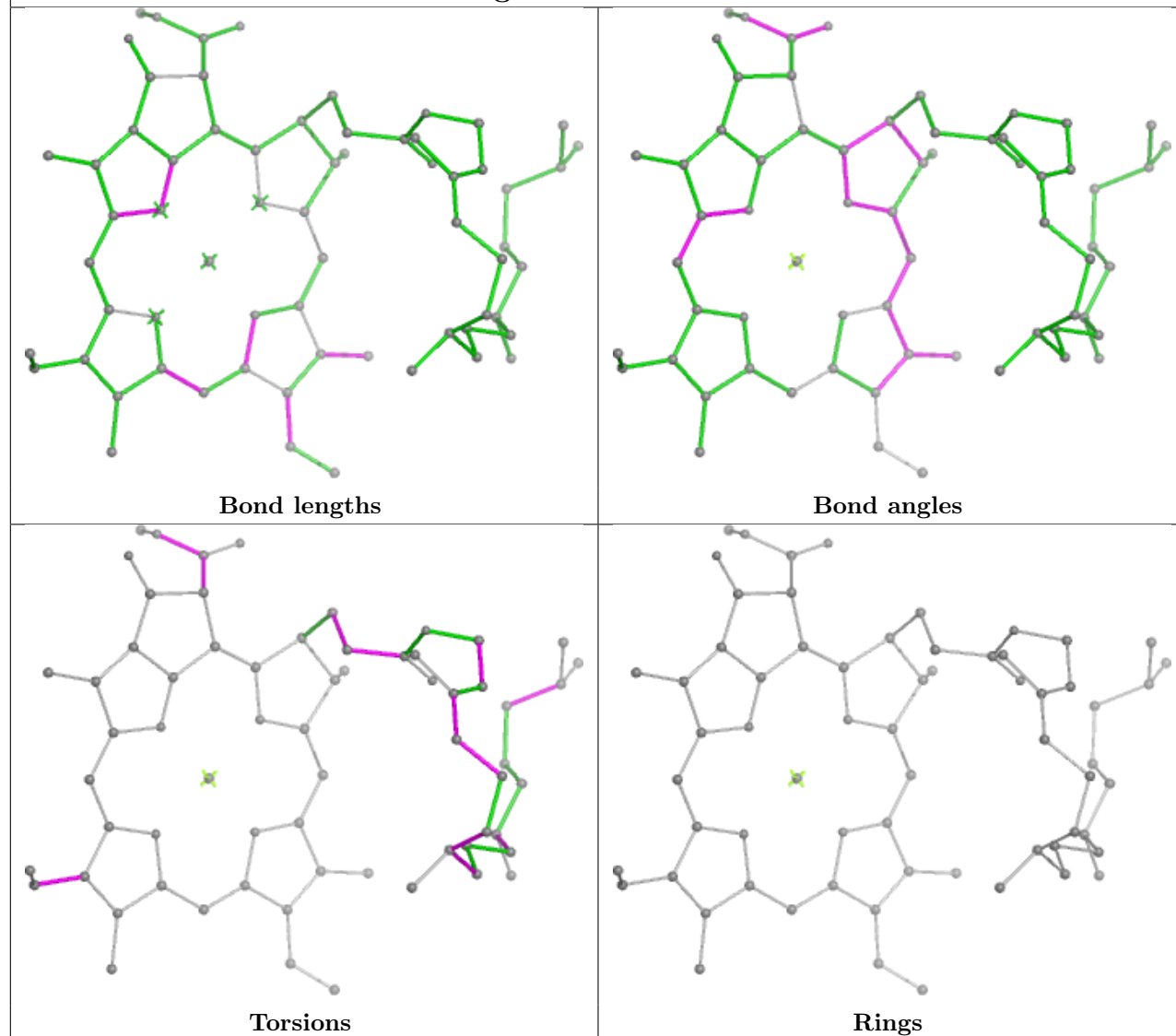
Torsions



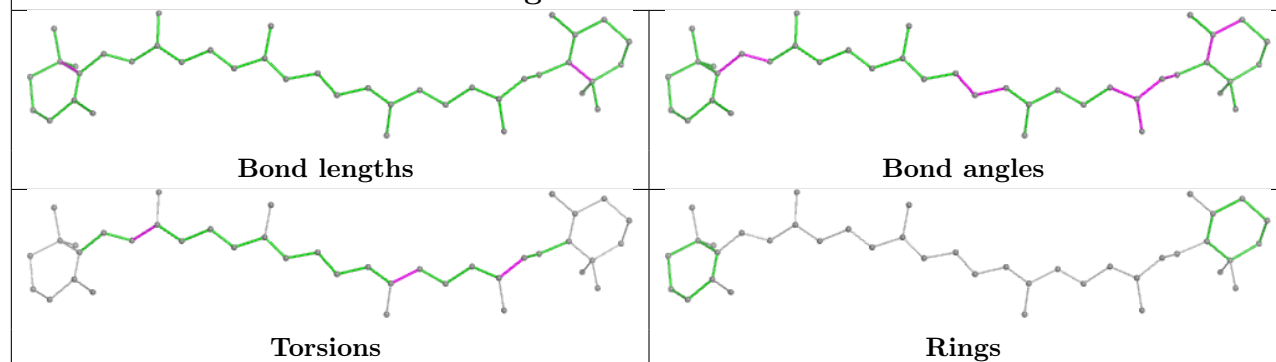
Rings

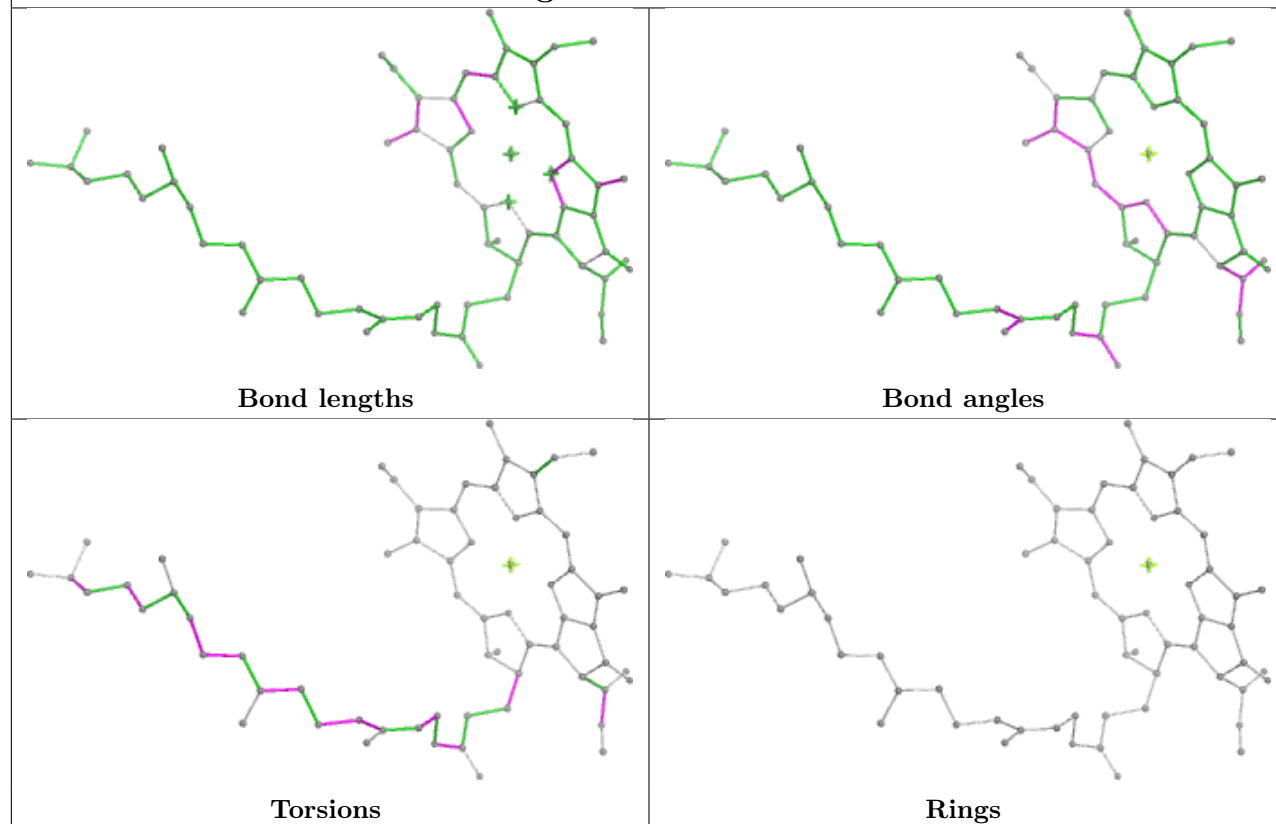
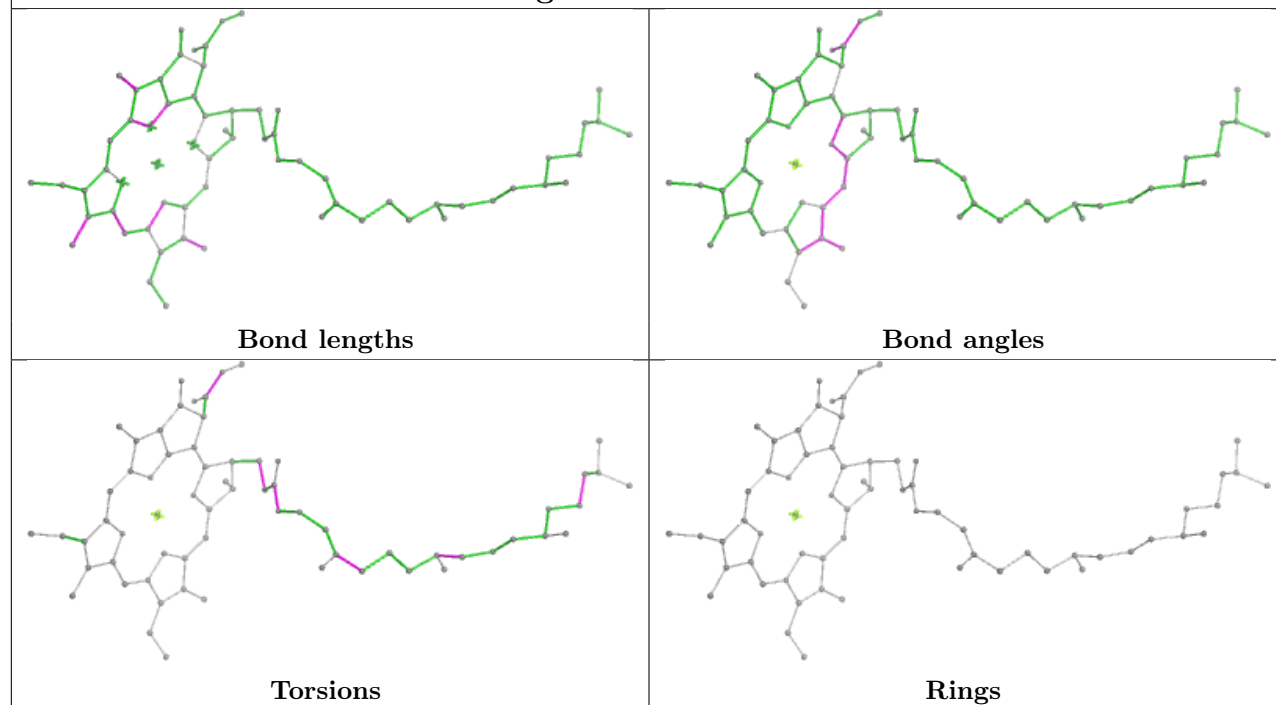


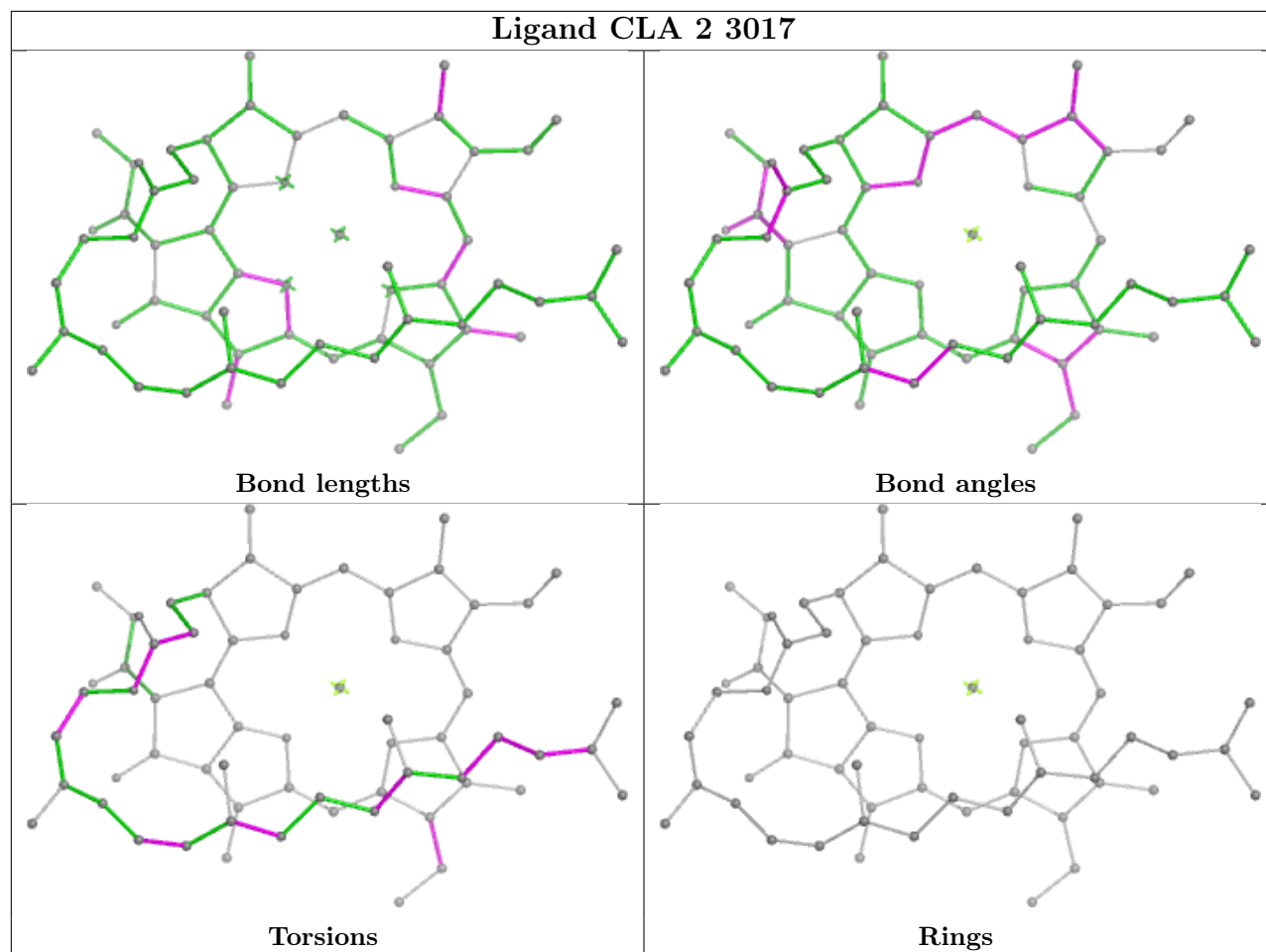
Ligand CLA a 815



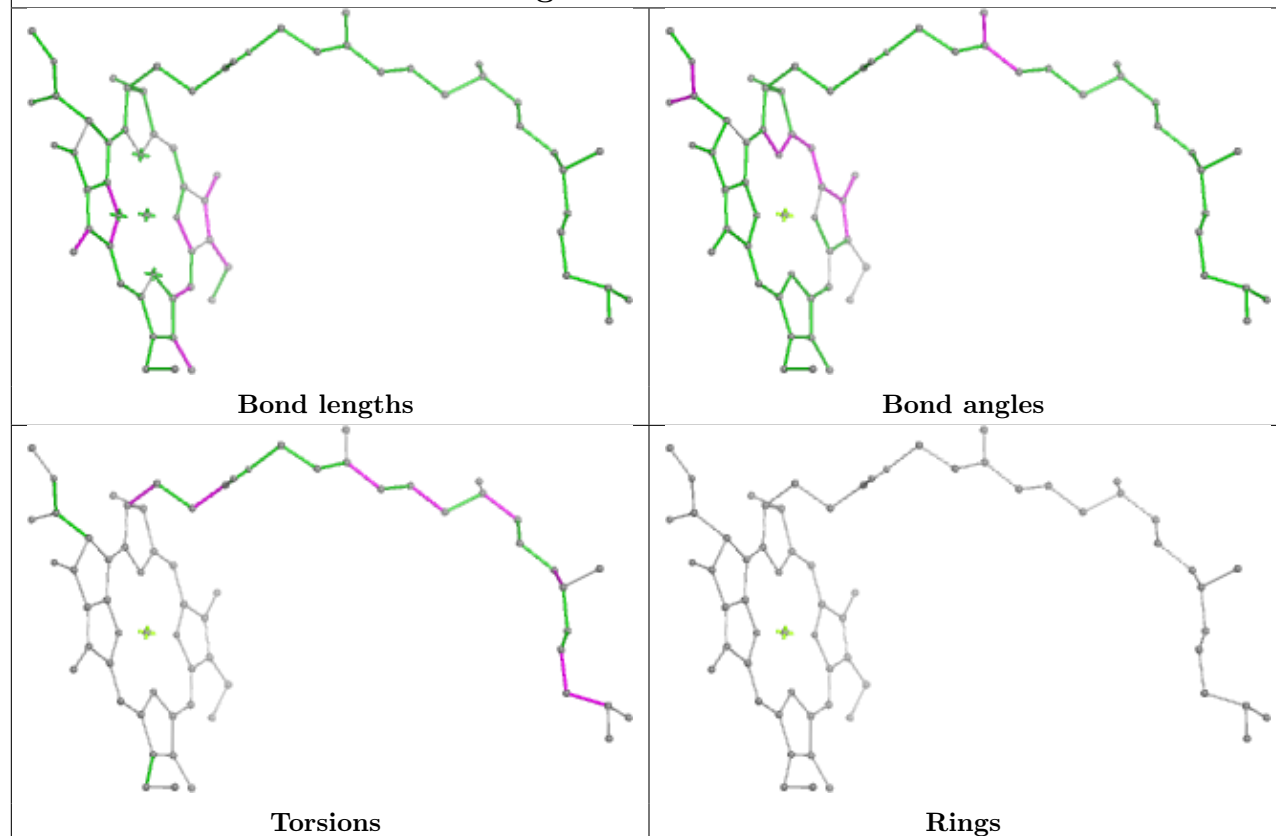
Ligand BCR b 3044



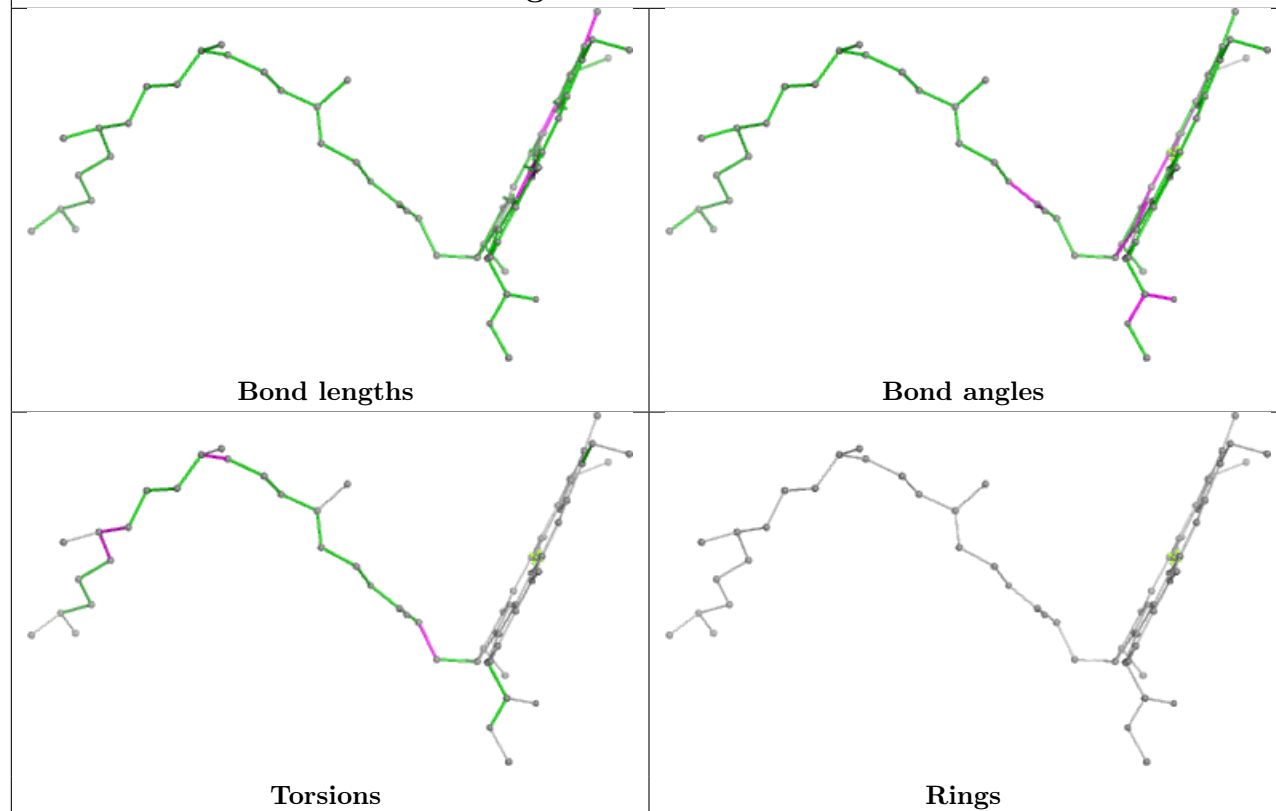
Ligand CLA a 816**Ligand CLA 1 822**

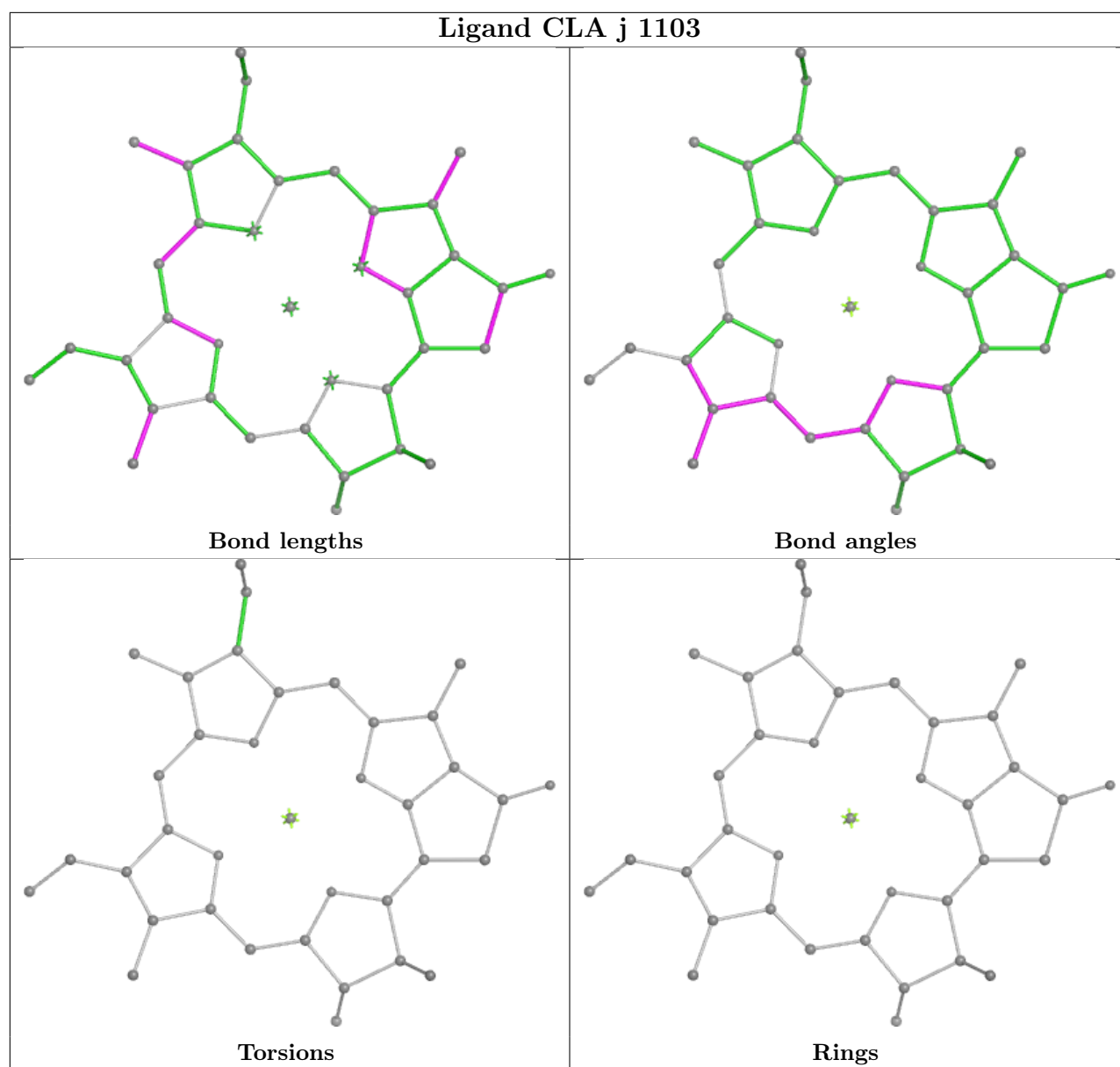


Ligand CLA 1 836

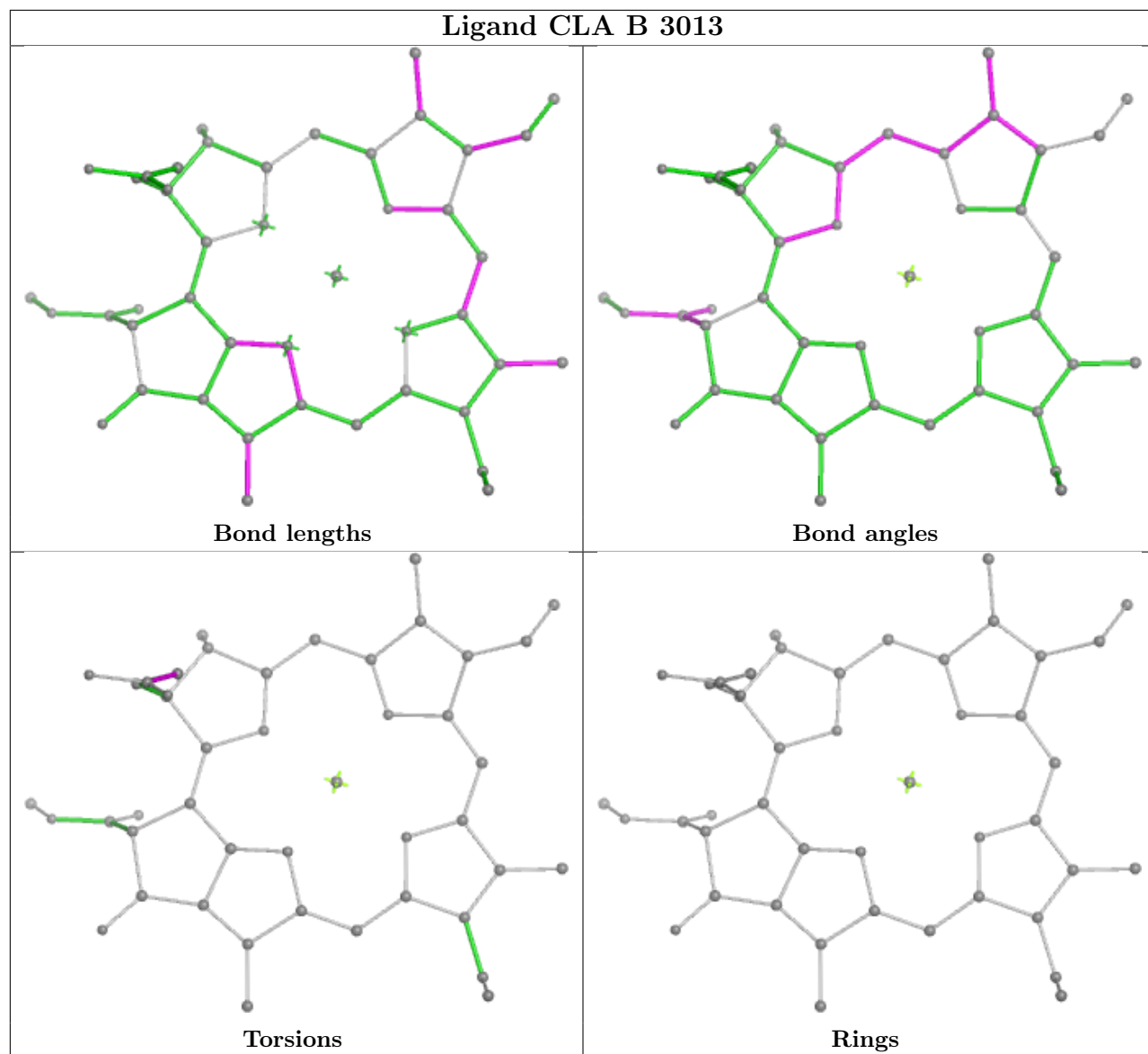


Ligand CLA b 3041

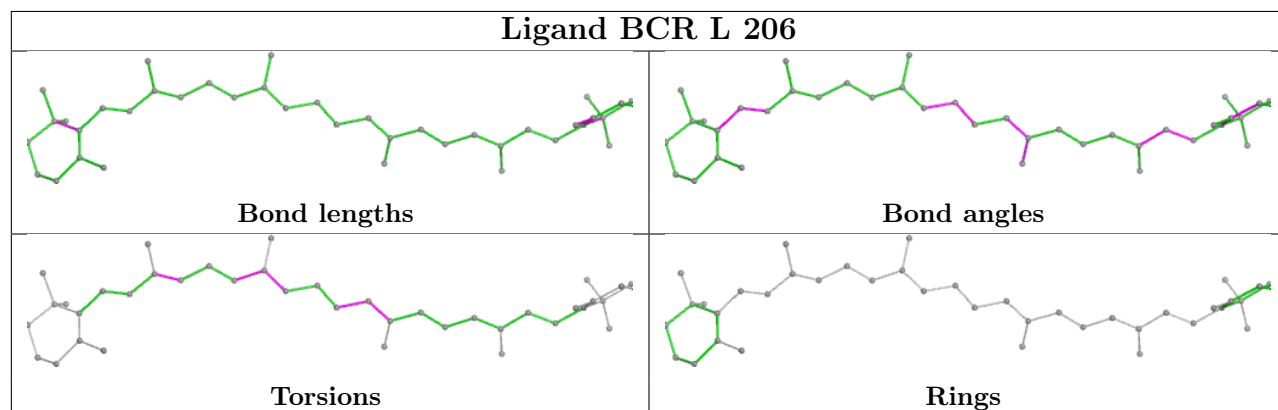


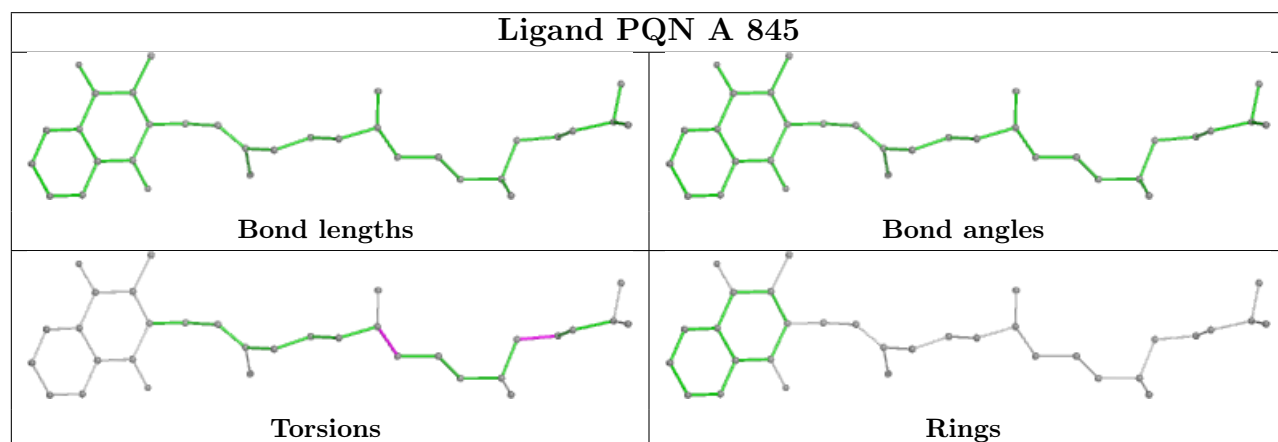
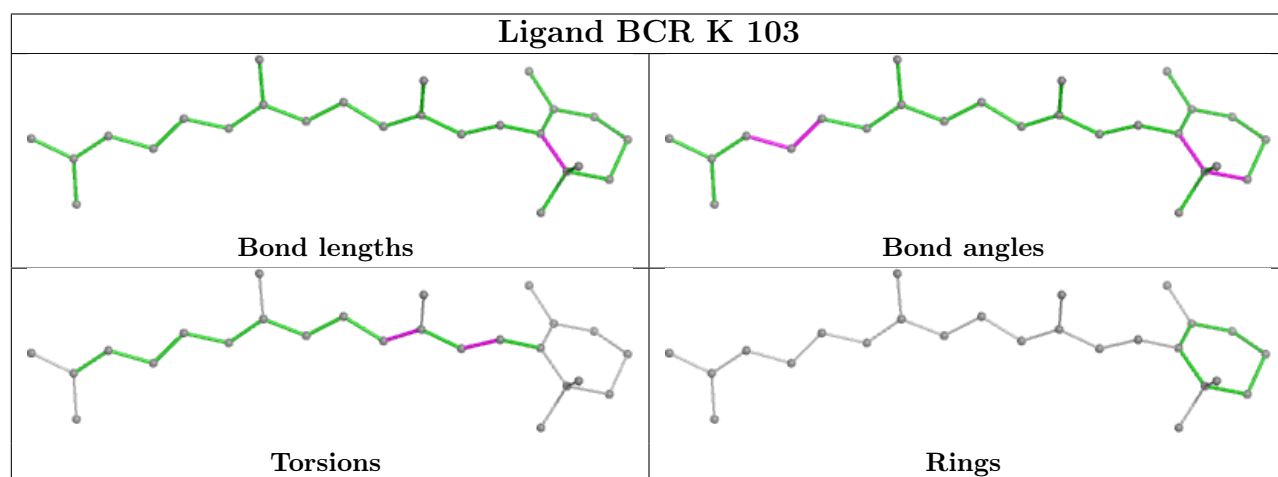
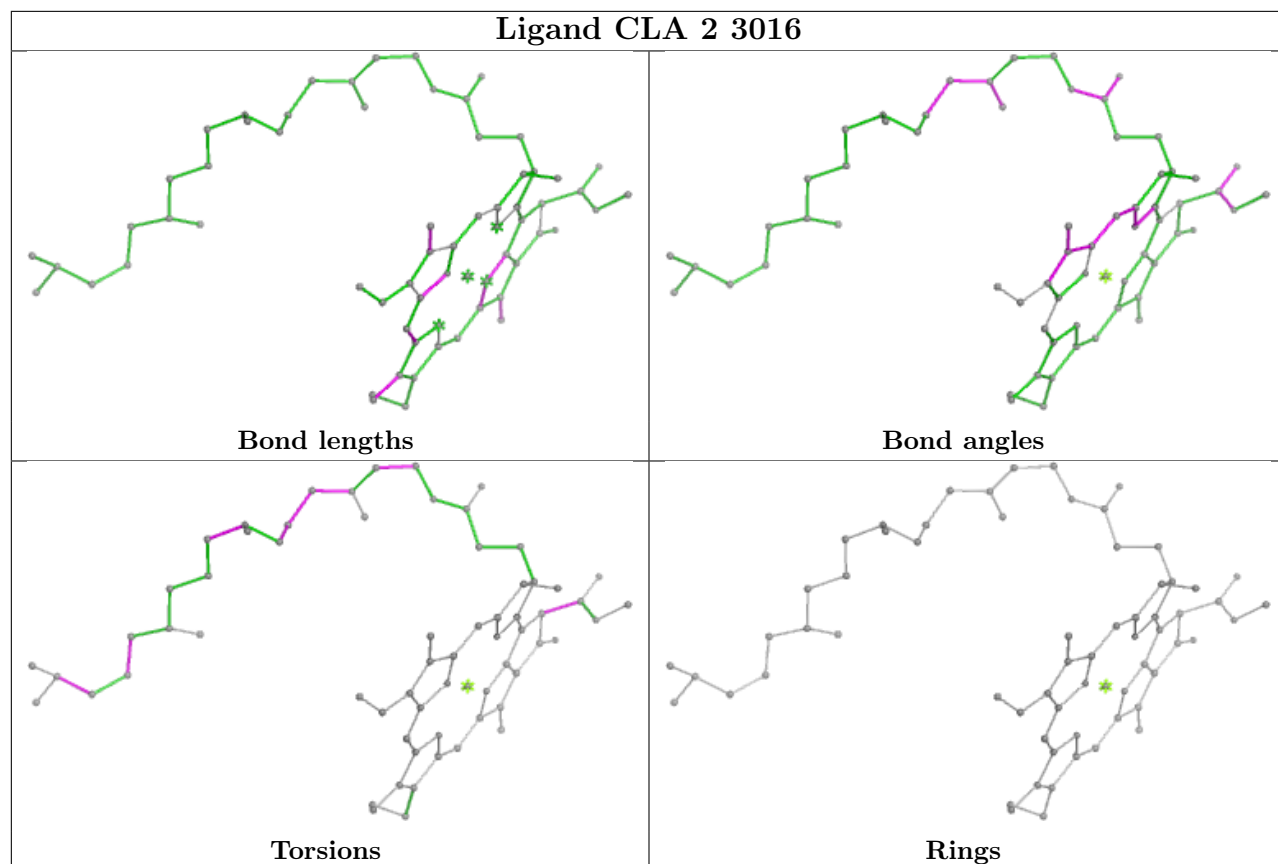


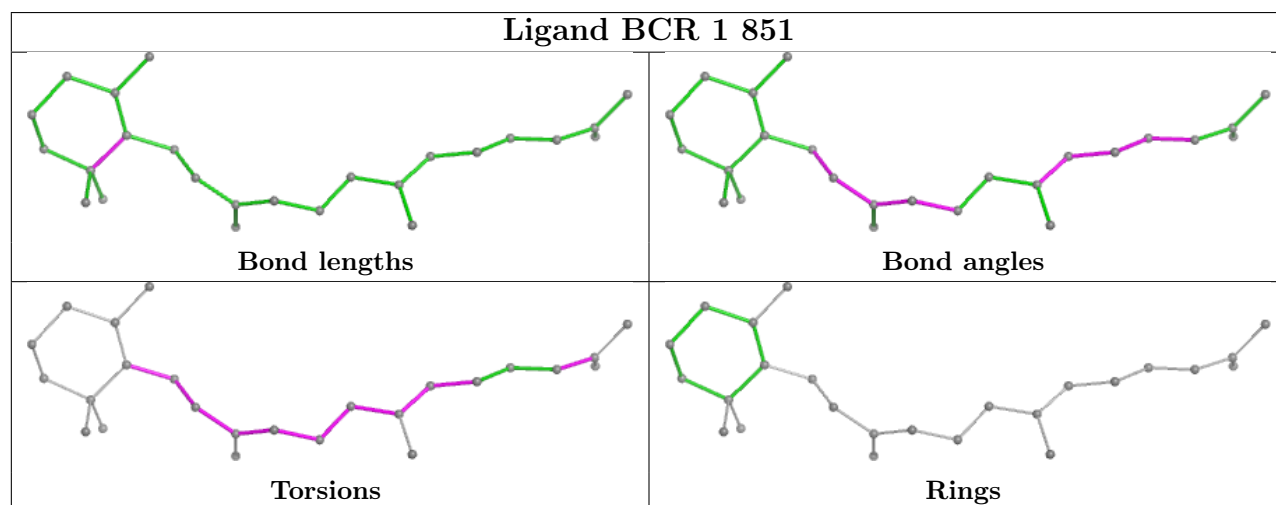
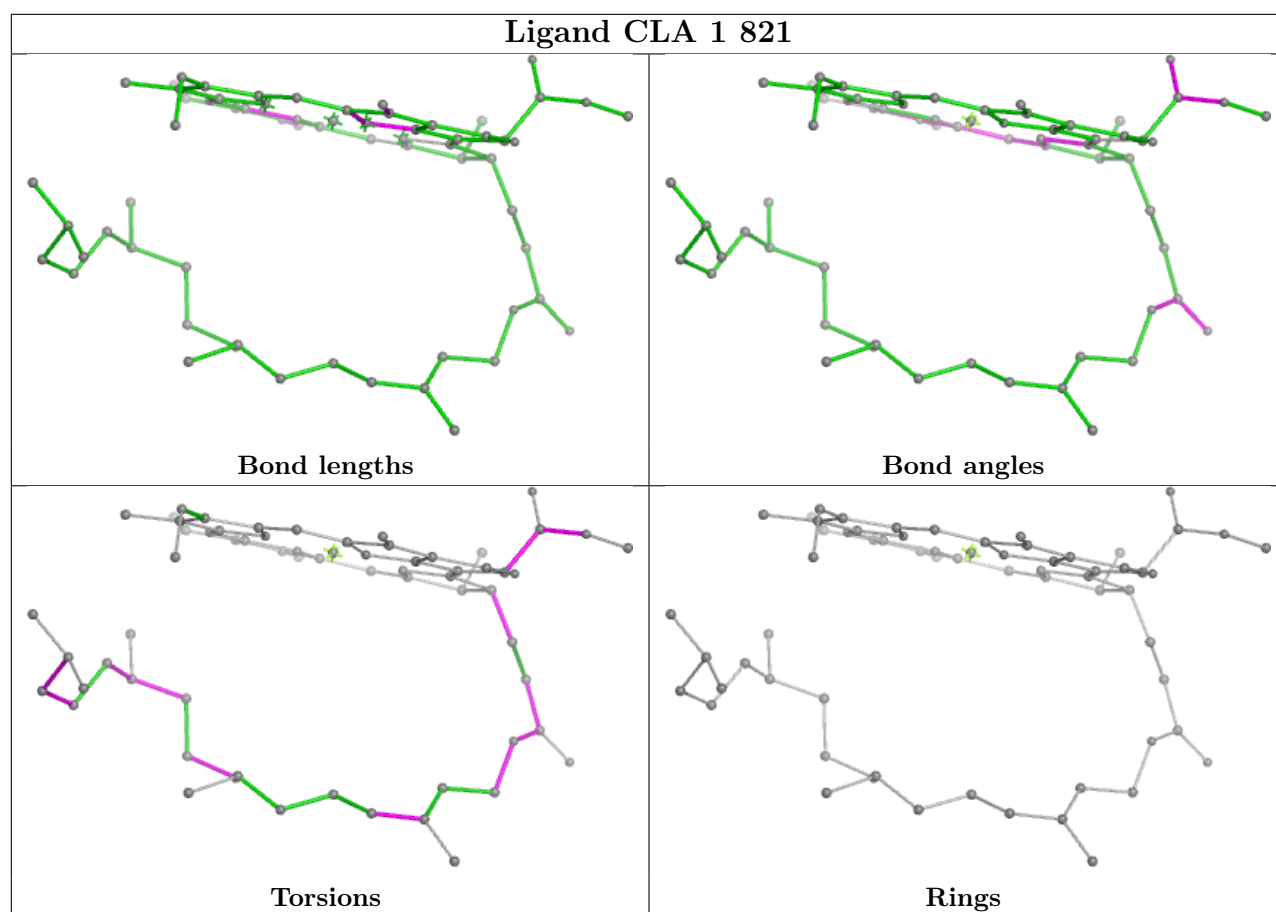
Ligand CLA B 3013

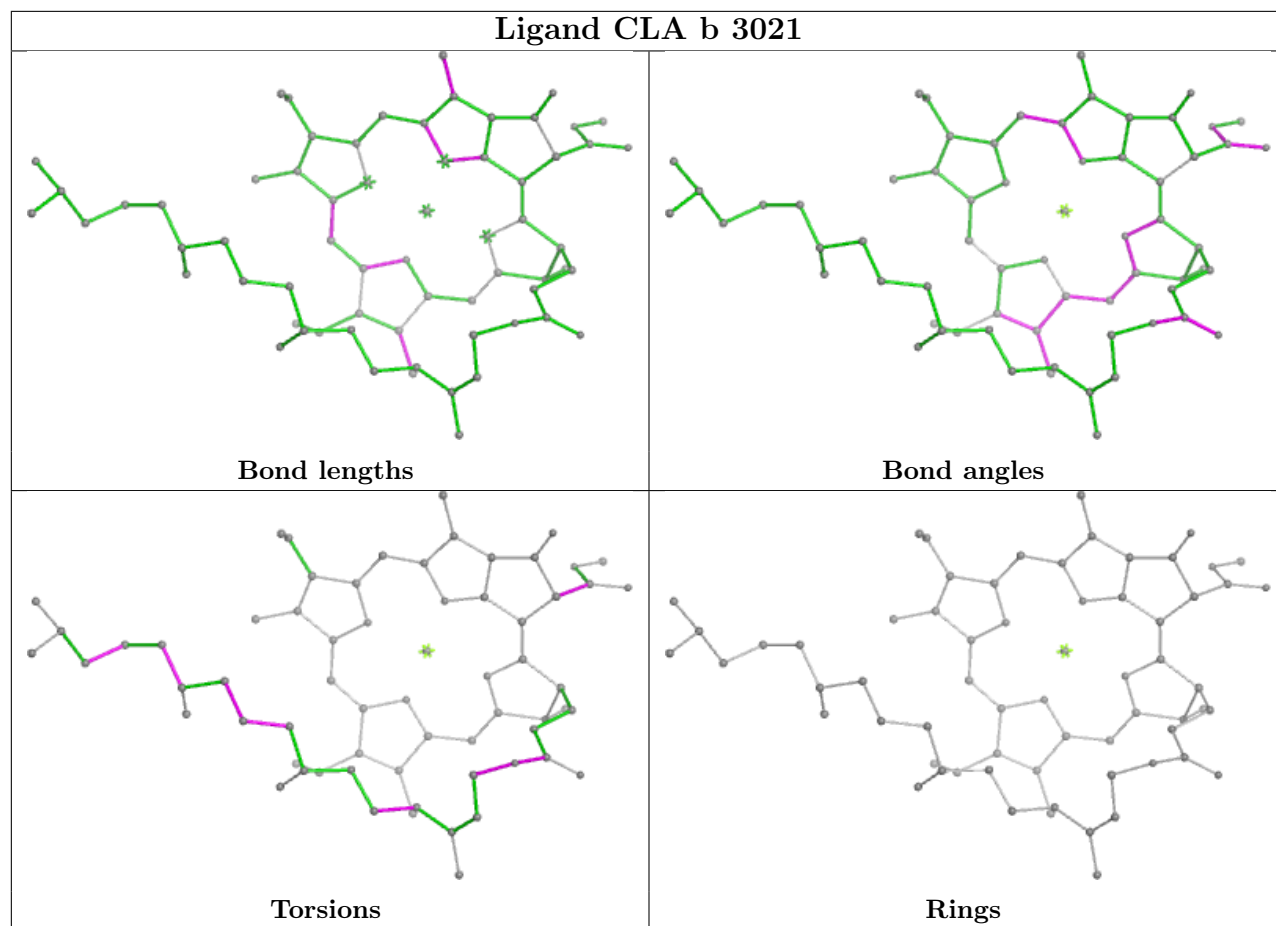


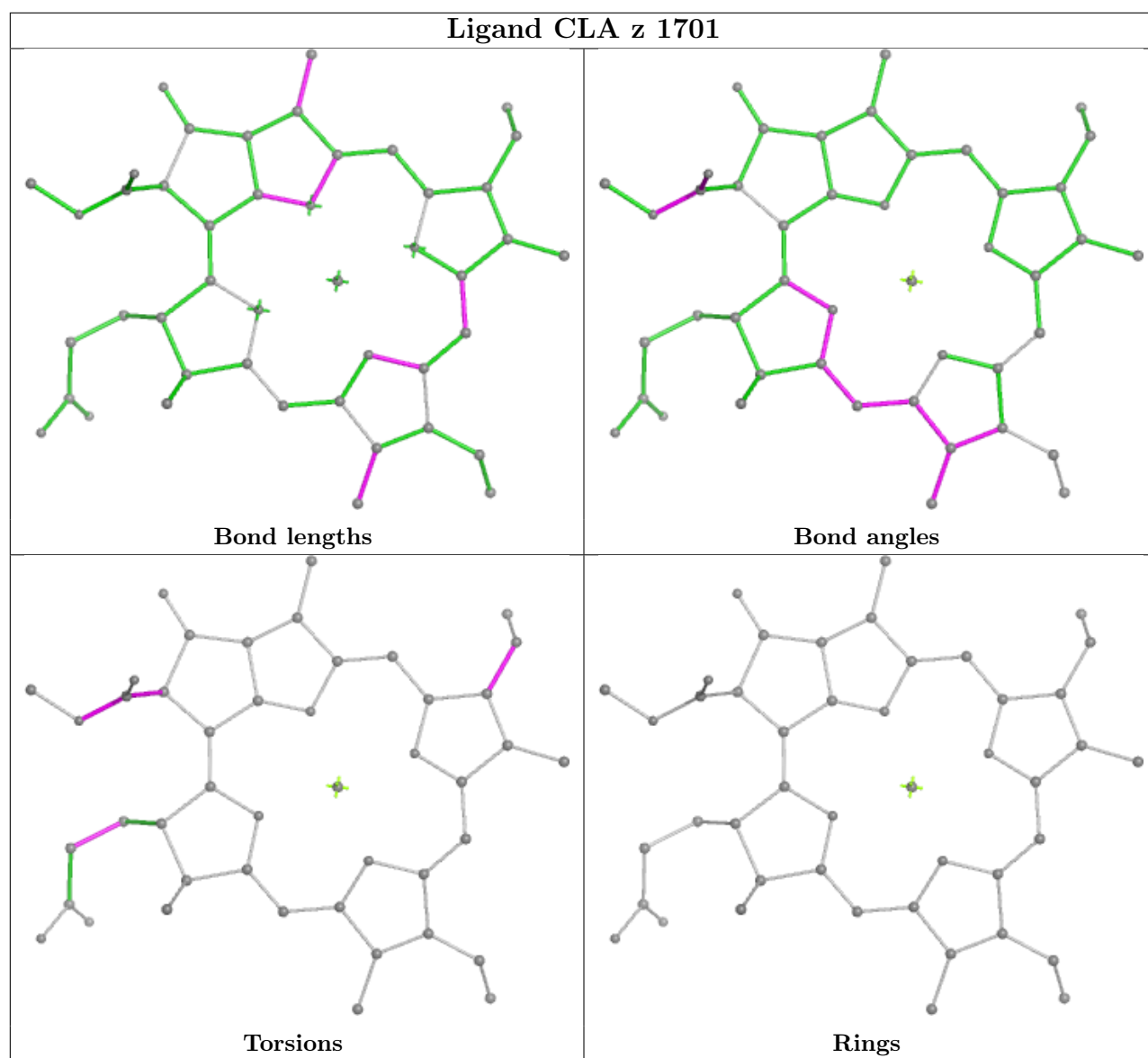
Ligand BCR L 206

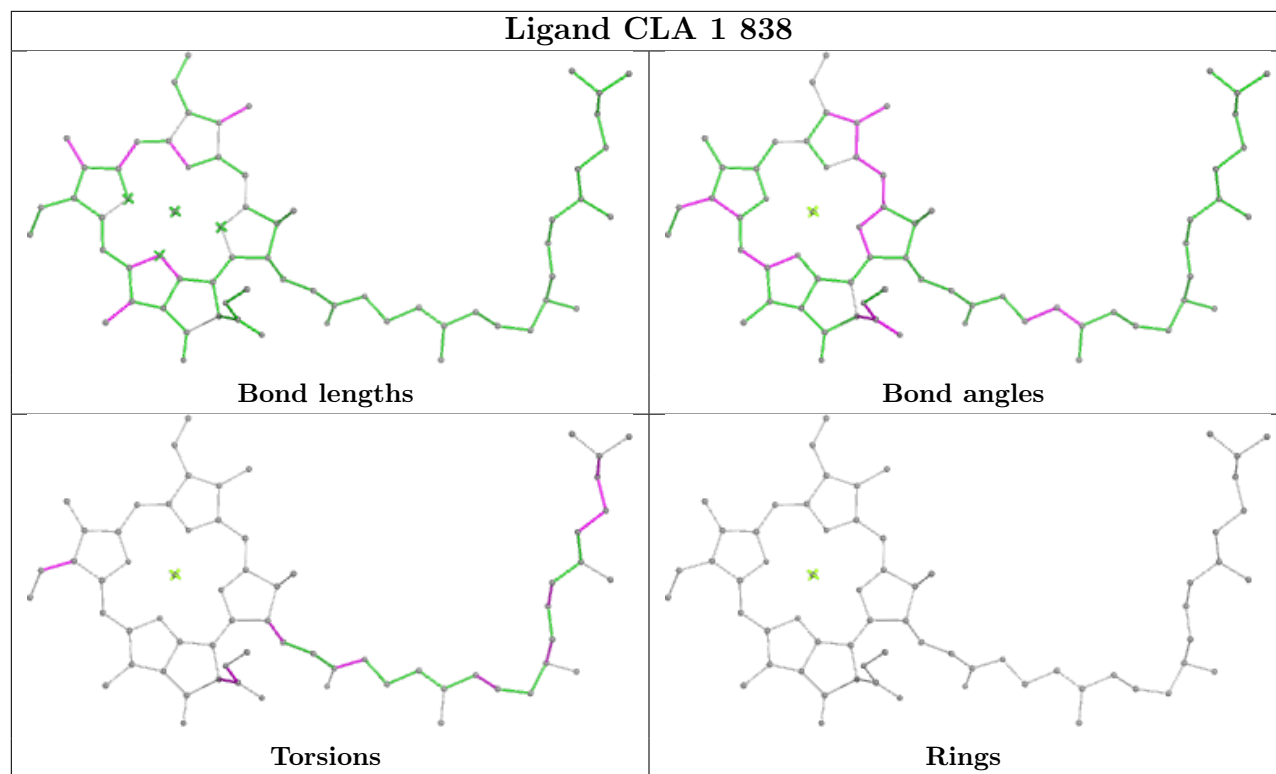
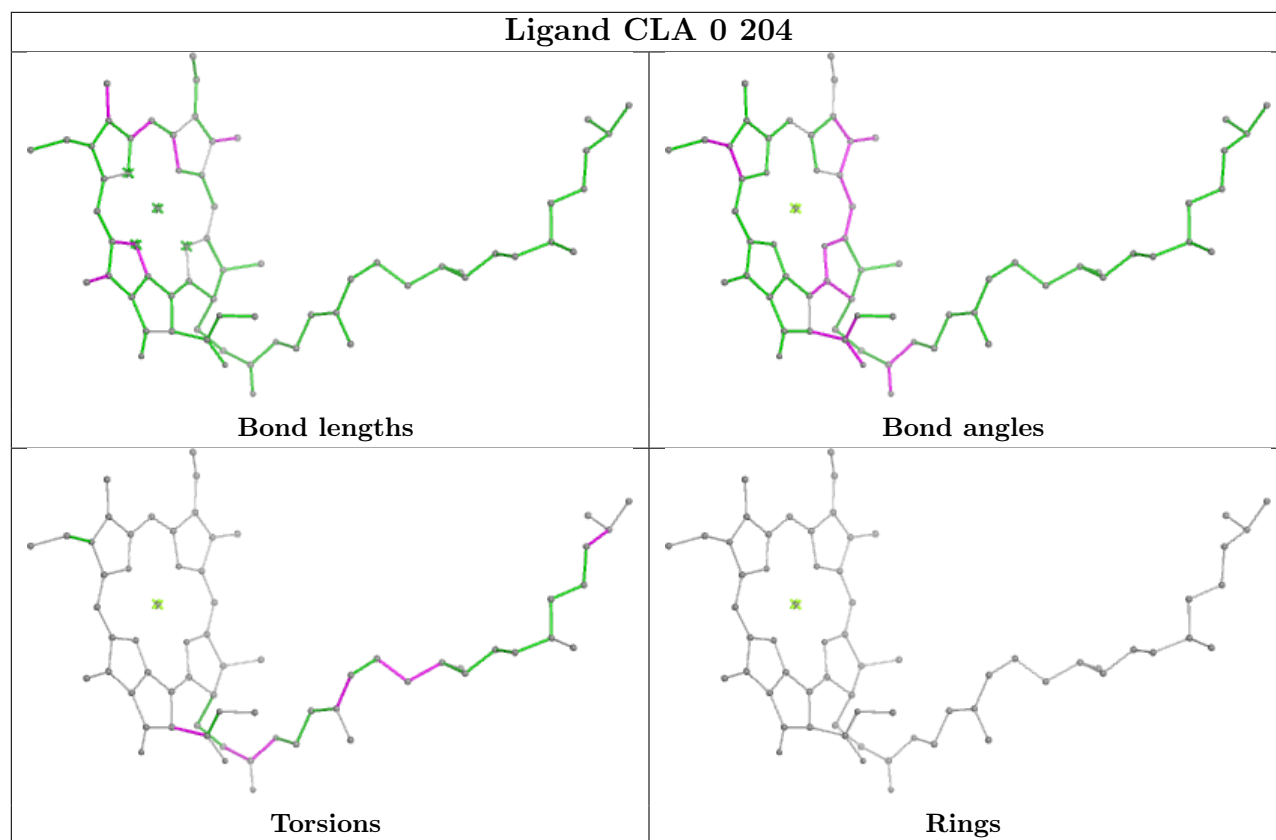


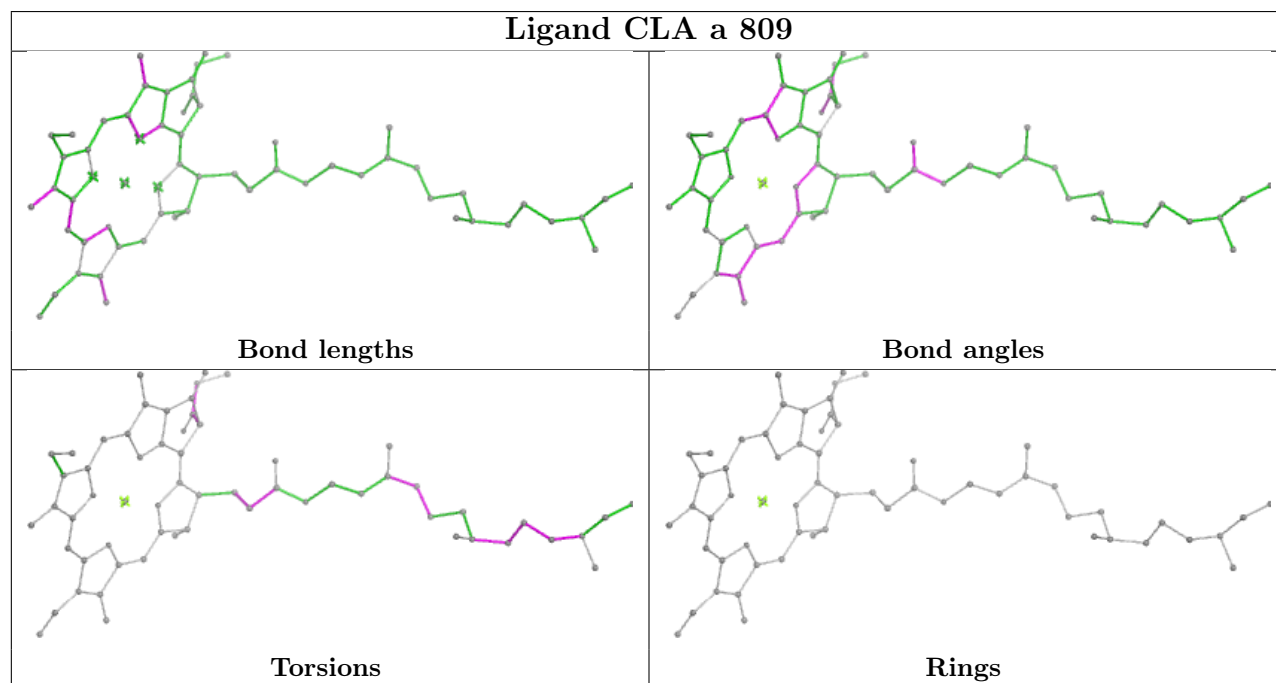
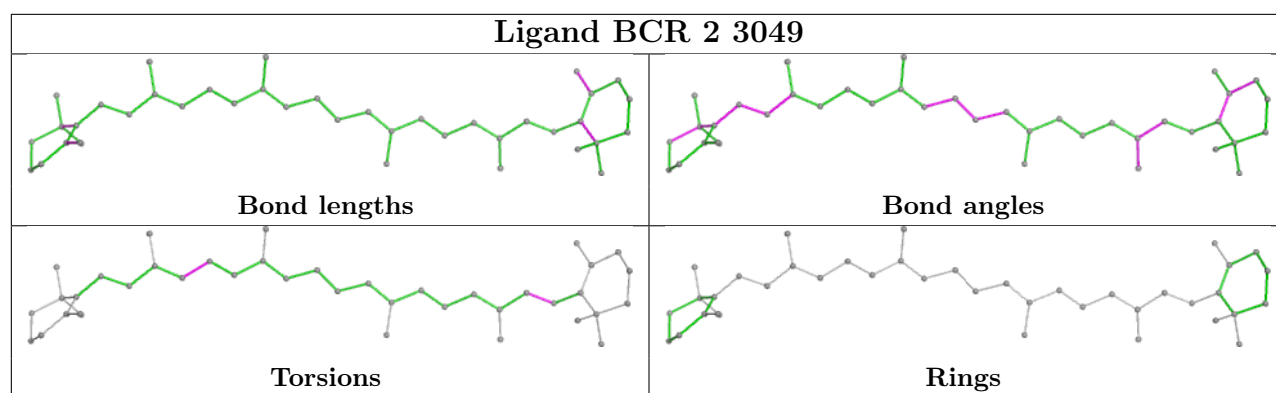


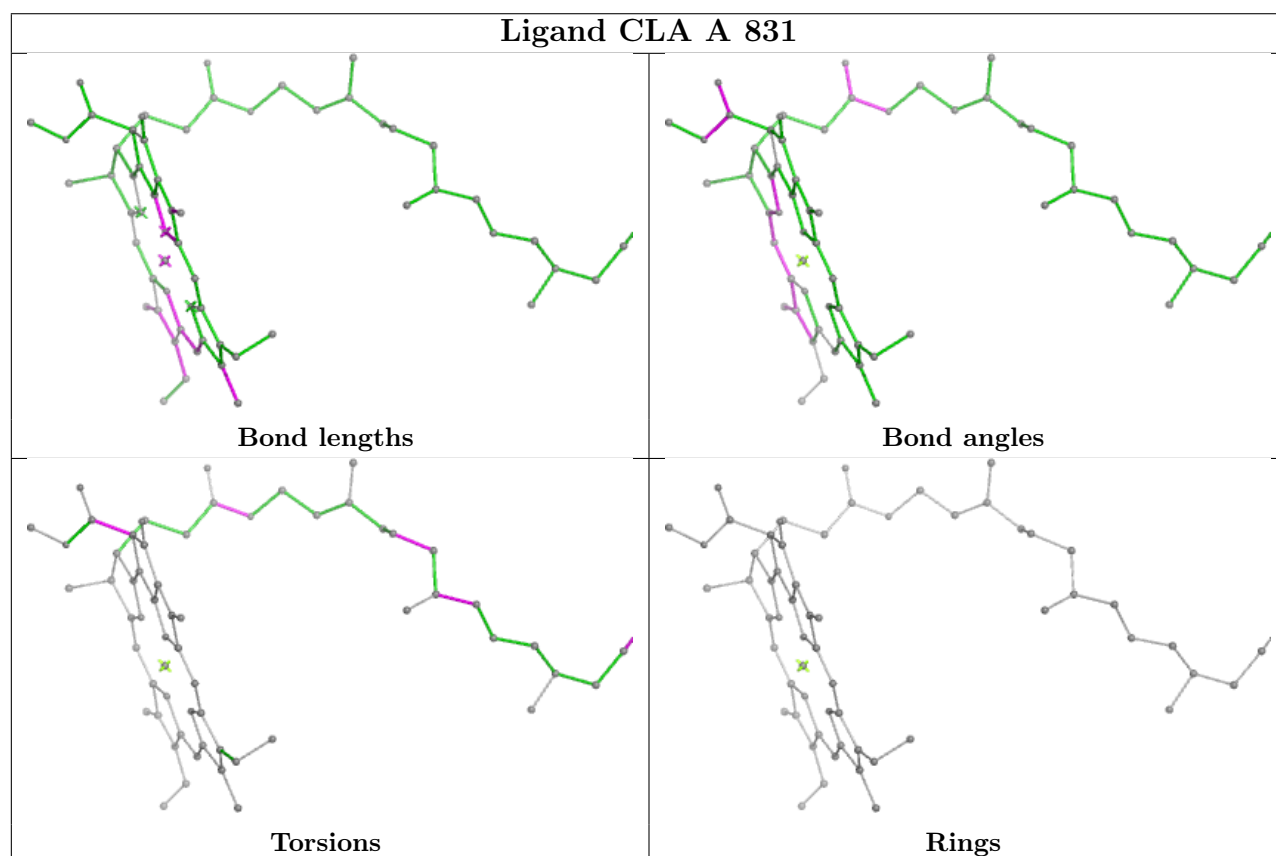
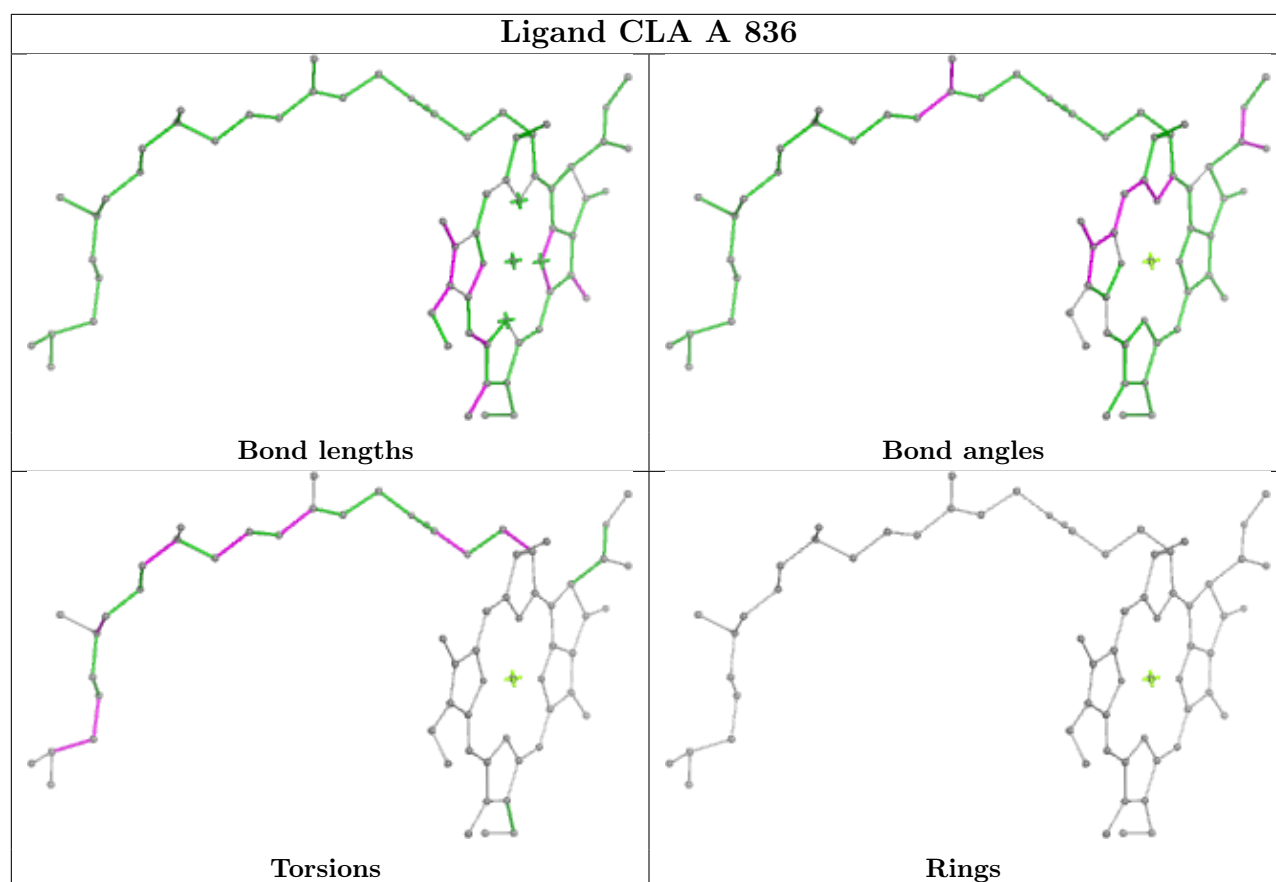


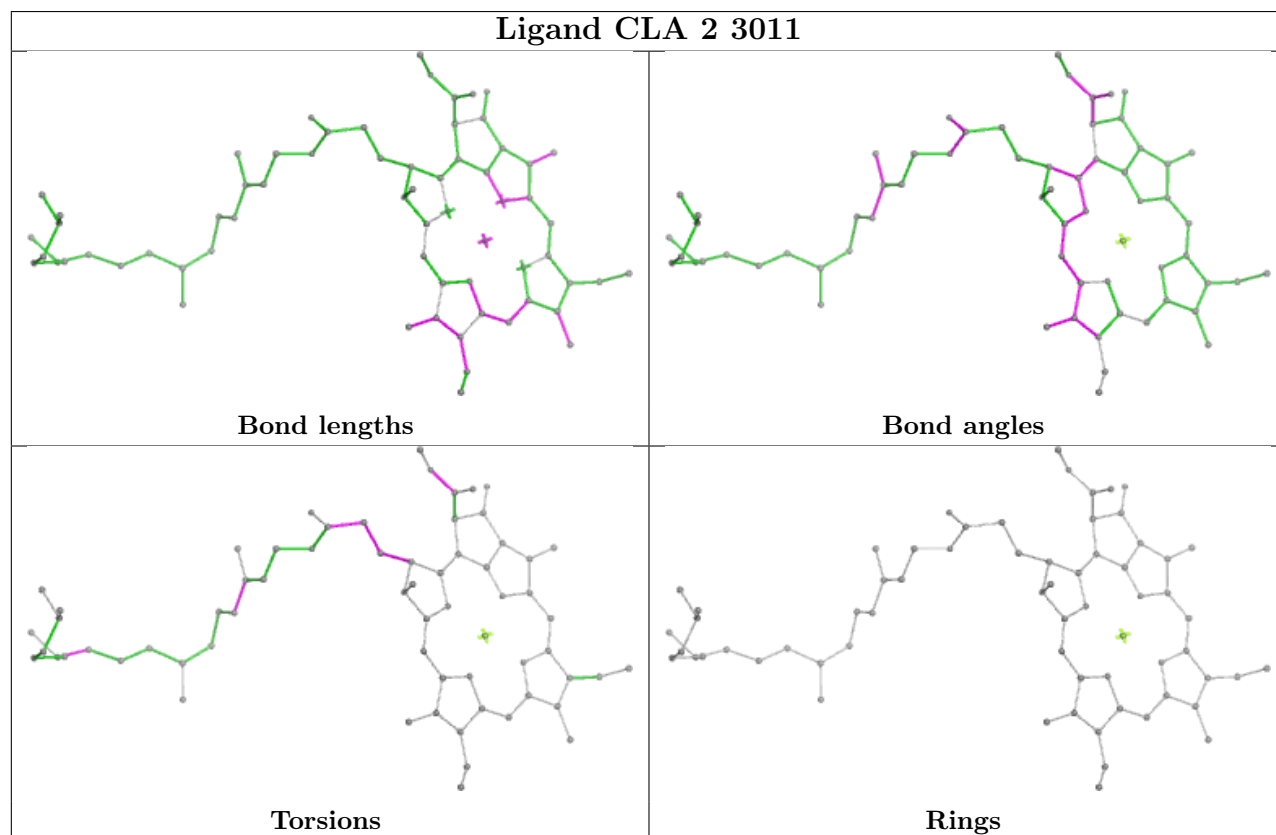
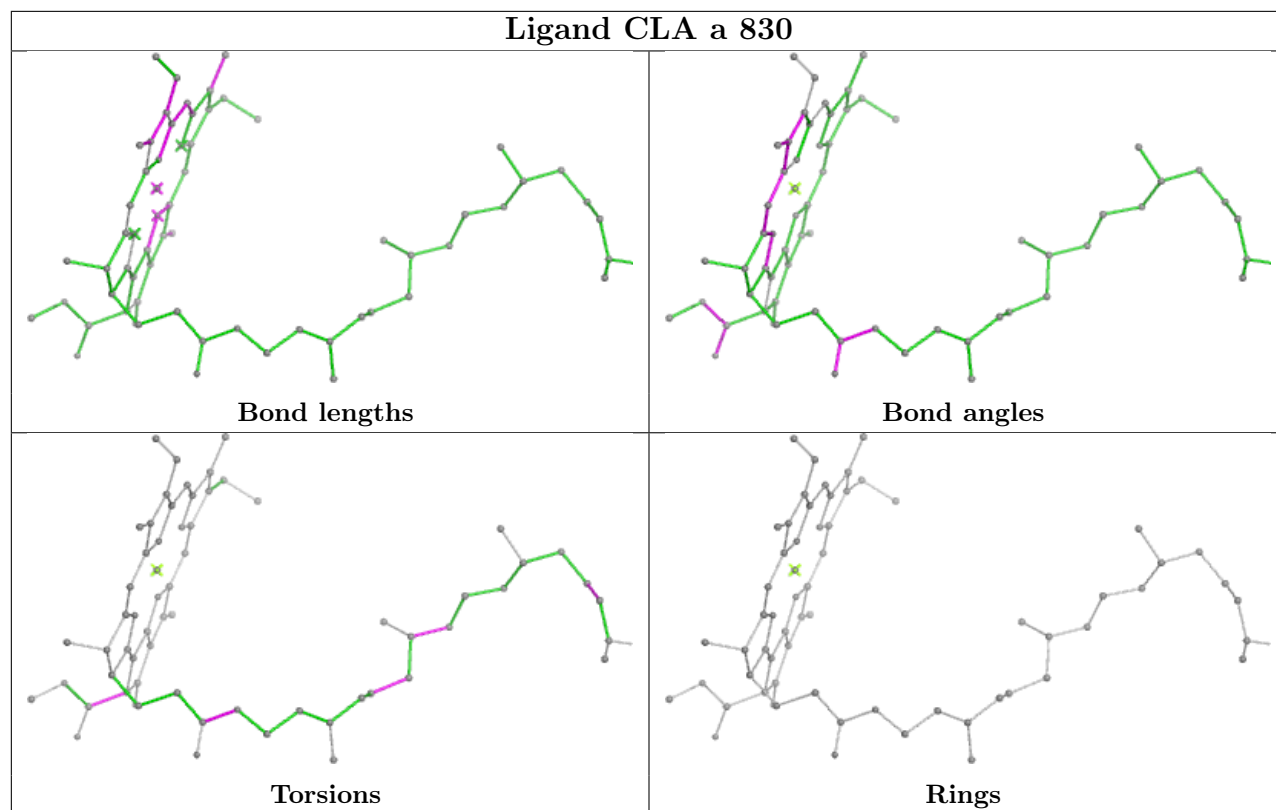


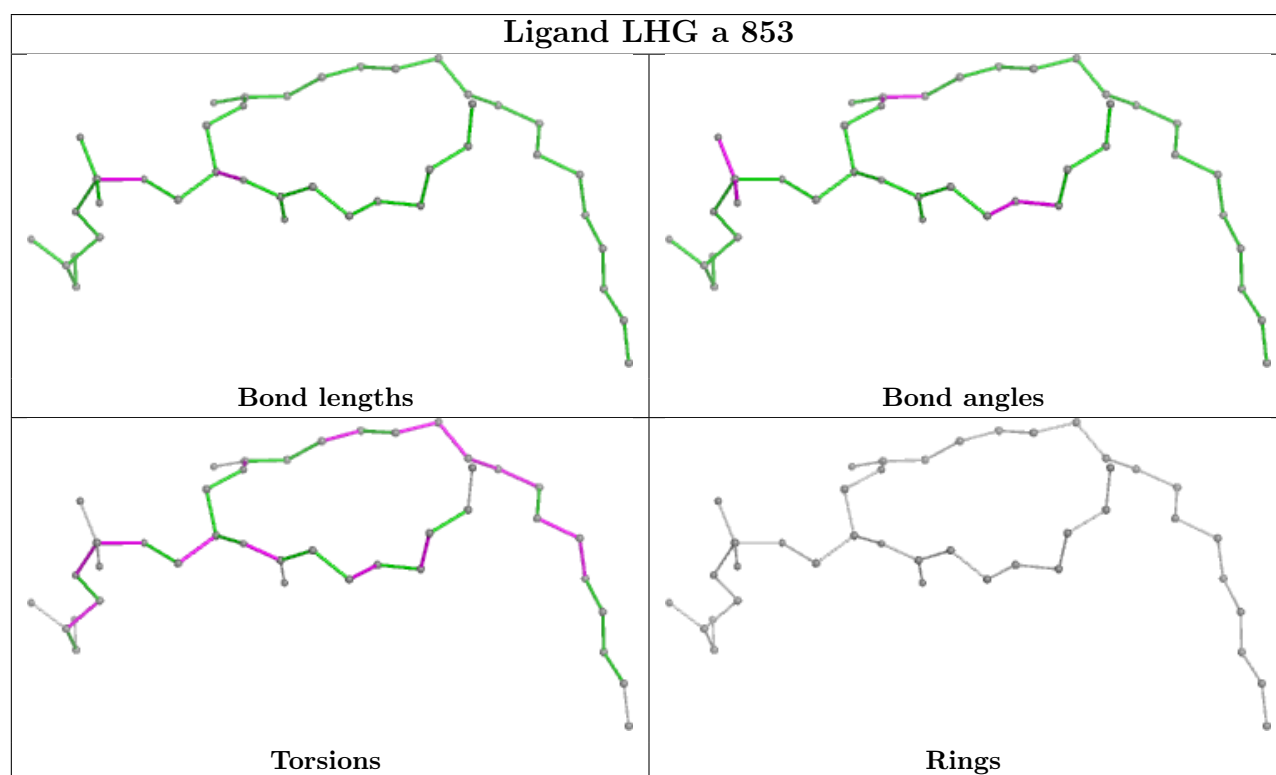
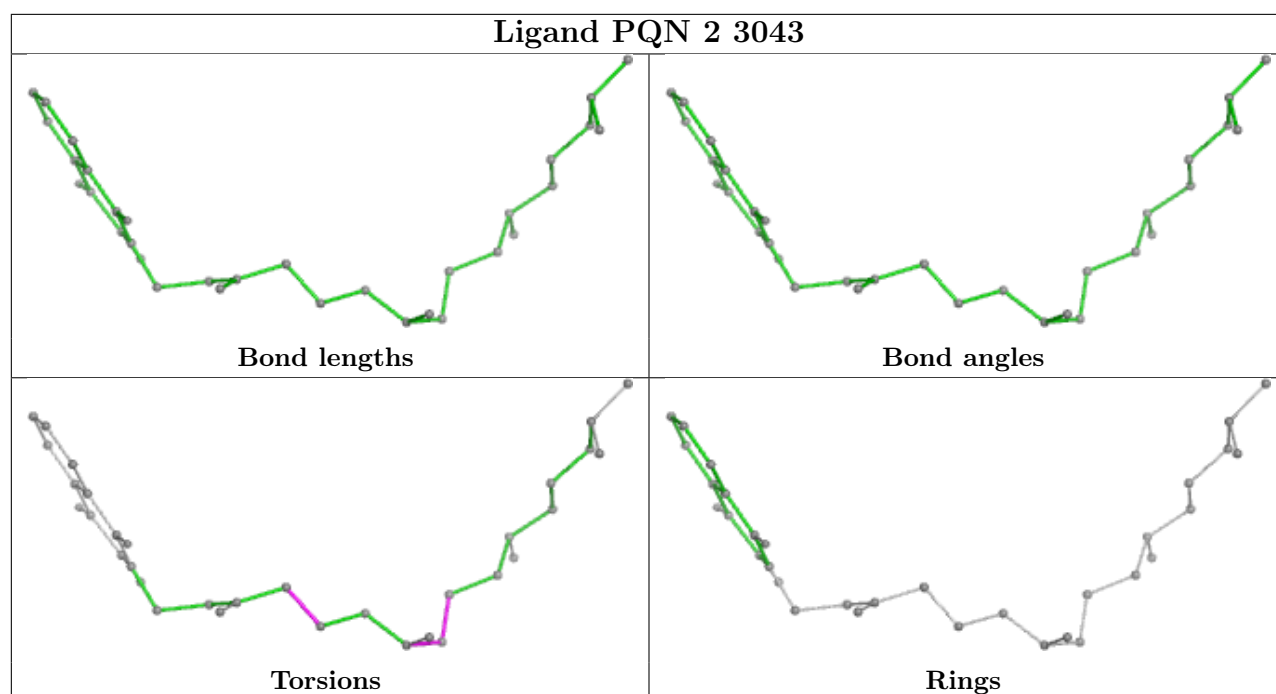


Ligand CLA 1 838**Ligand CLA 0 204**

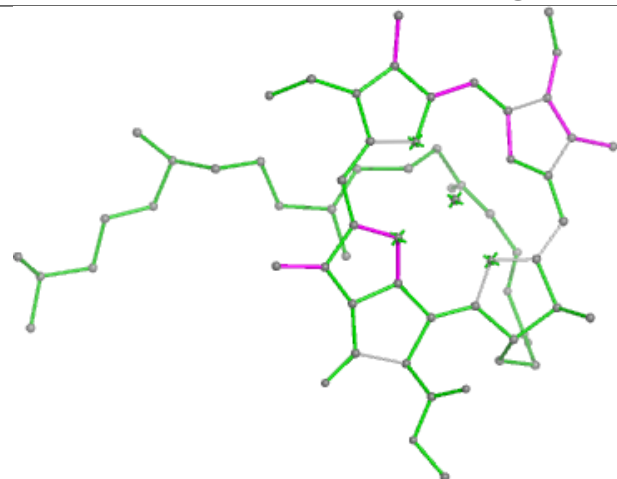




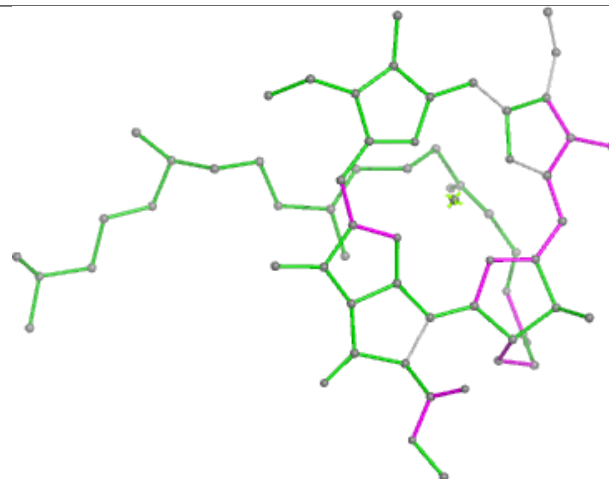




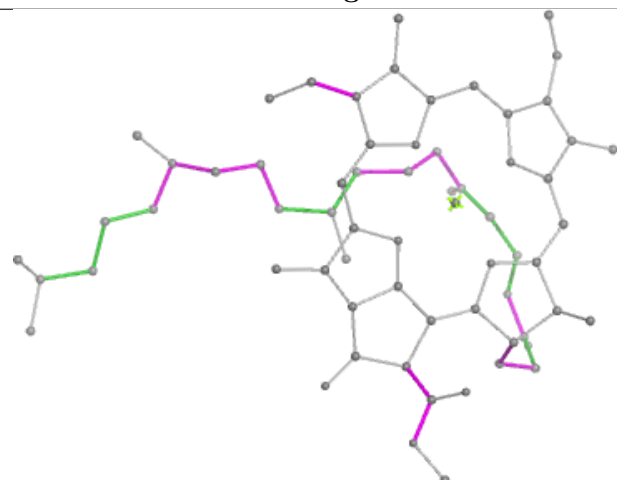
Ligand CLA B 3028



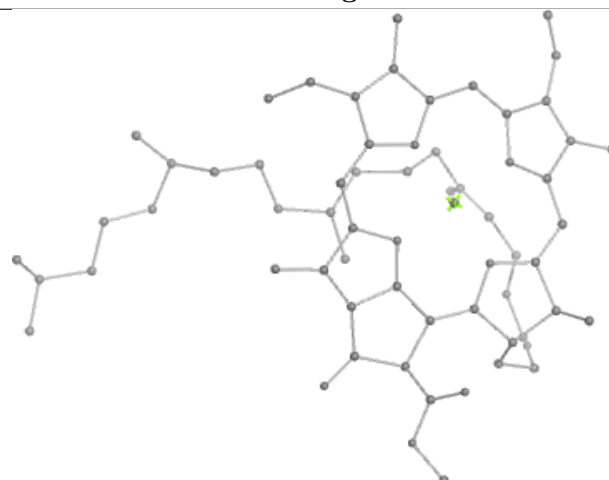
Bond lengths



Bond angles

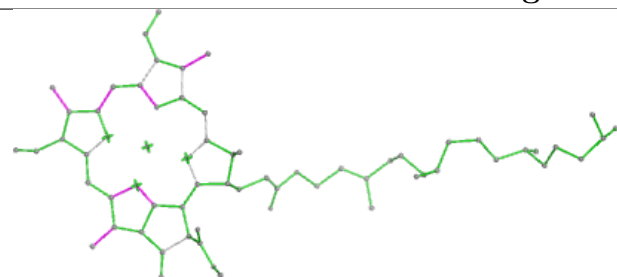


Torsions

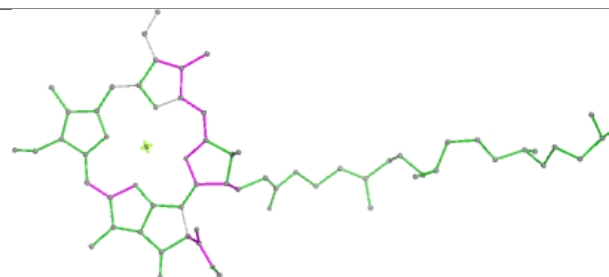


Rings

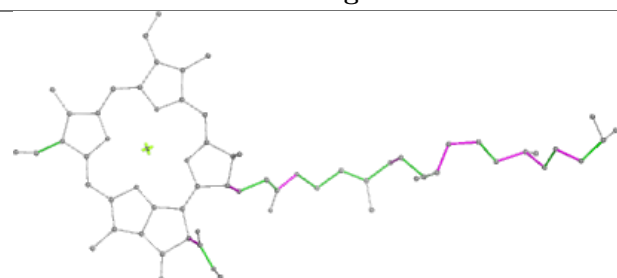
Ligand CLA 1 827



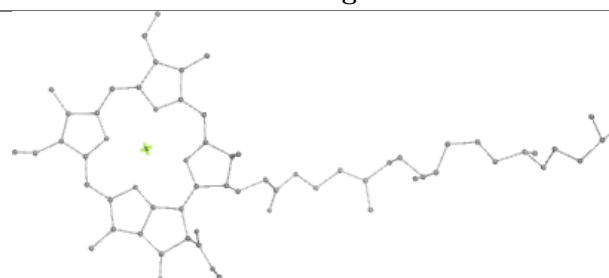
Bond lengths



Bond angles

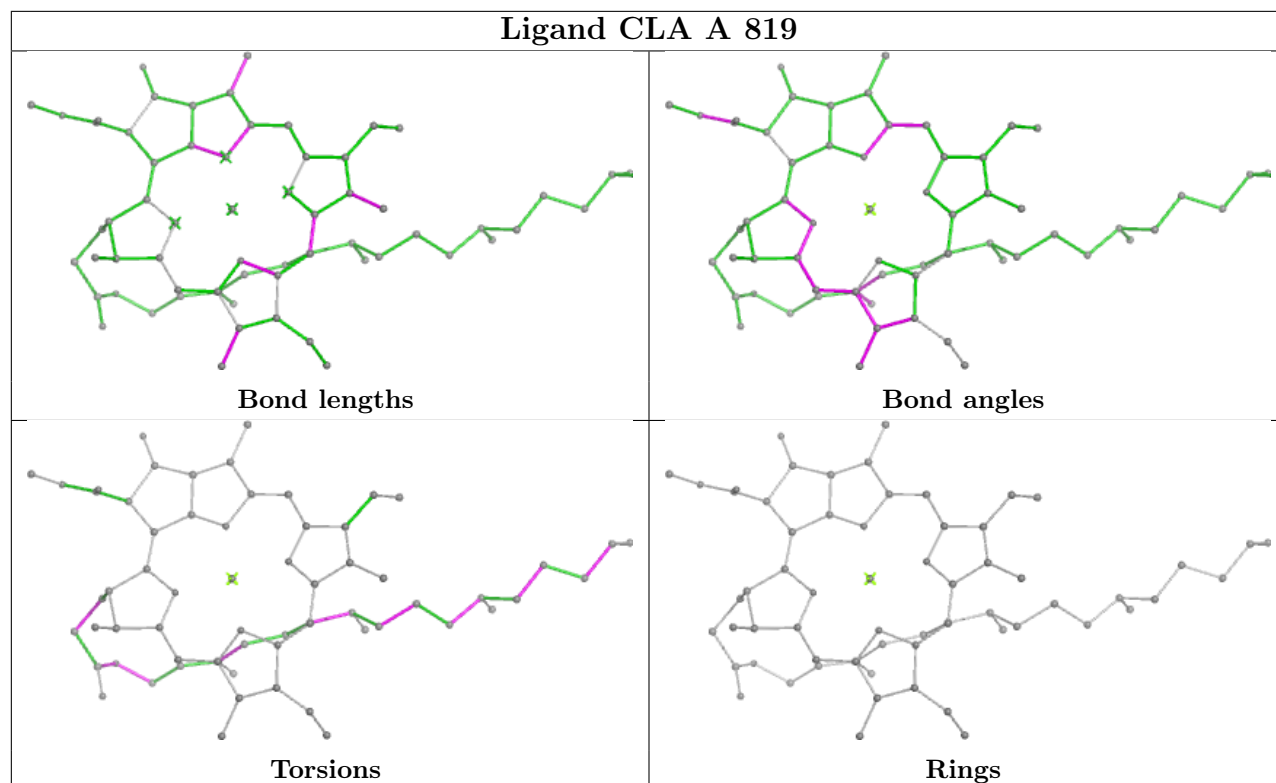


Torsions

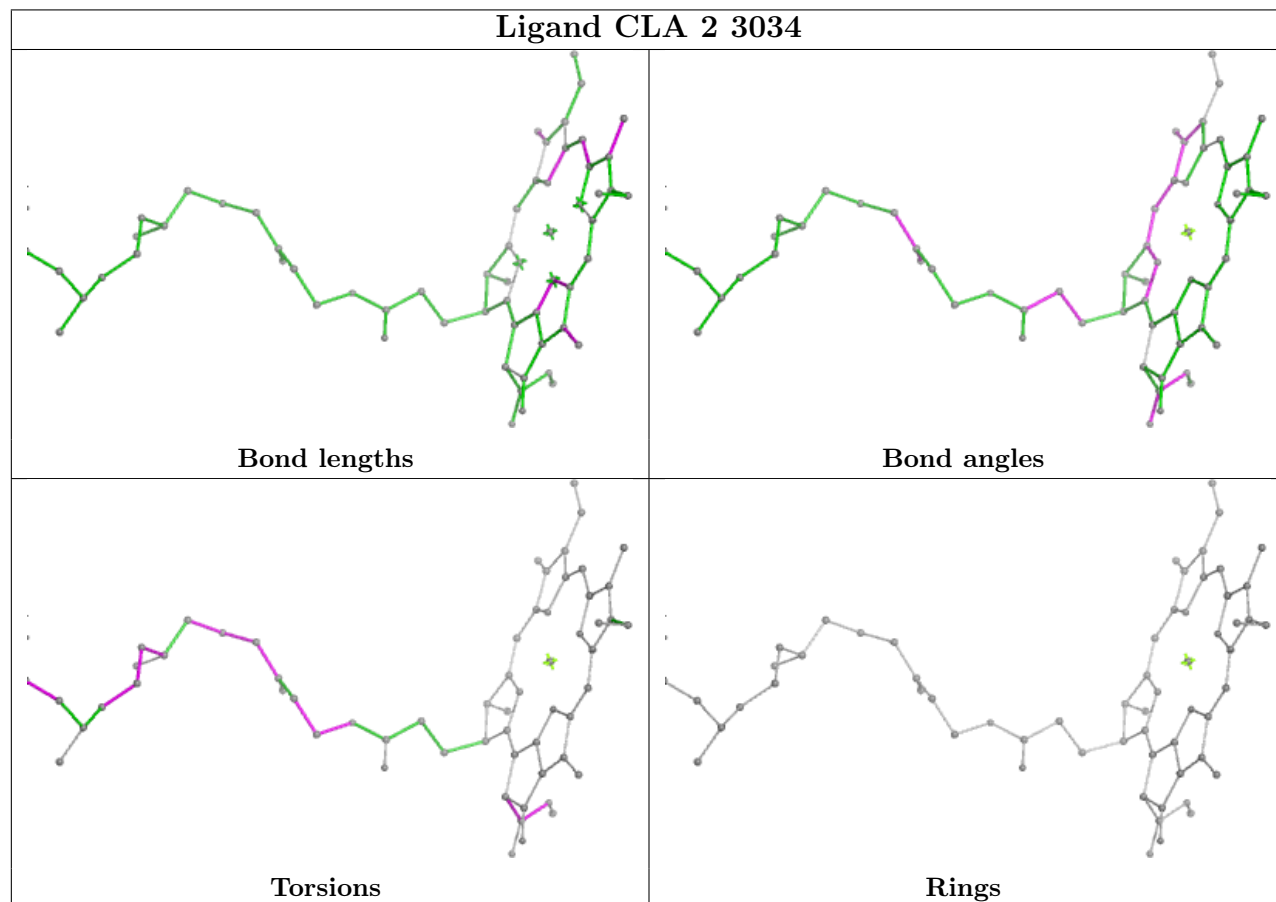


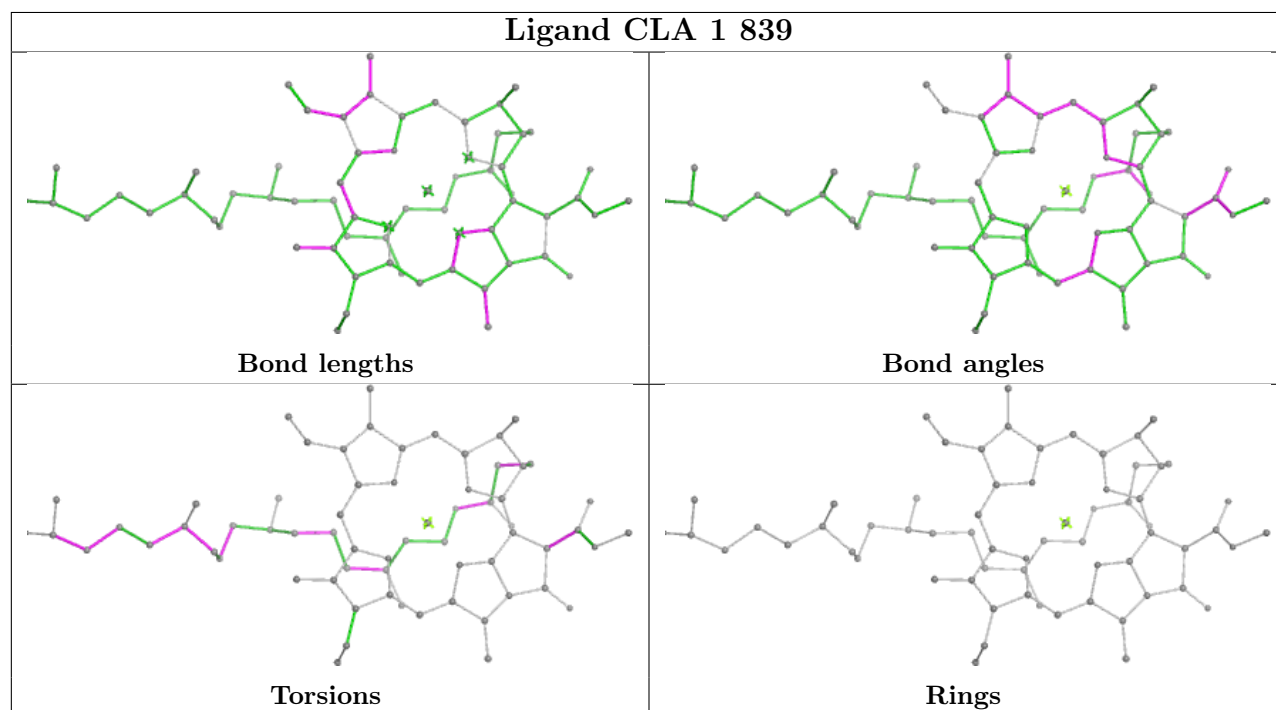
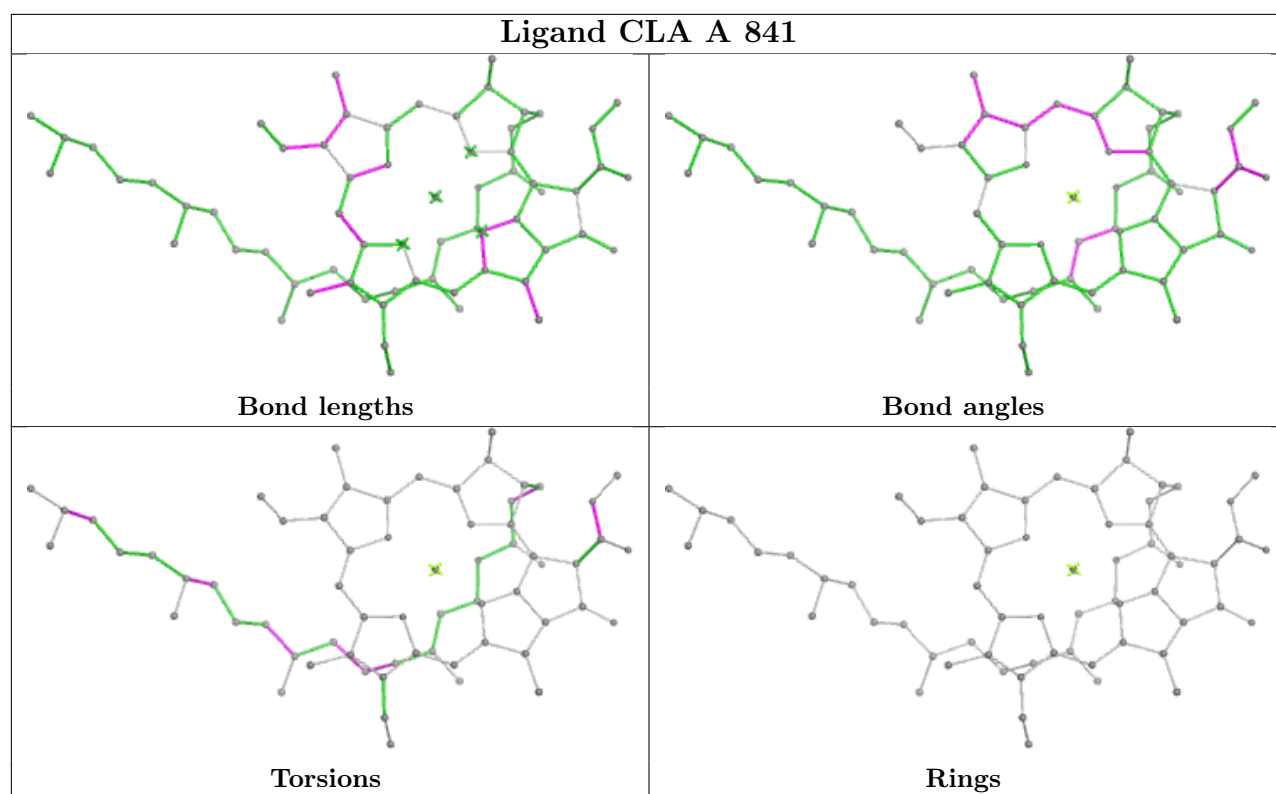
Rings

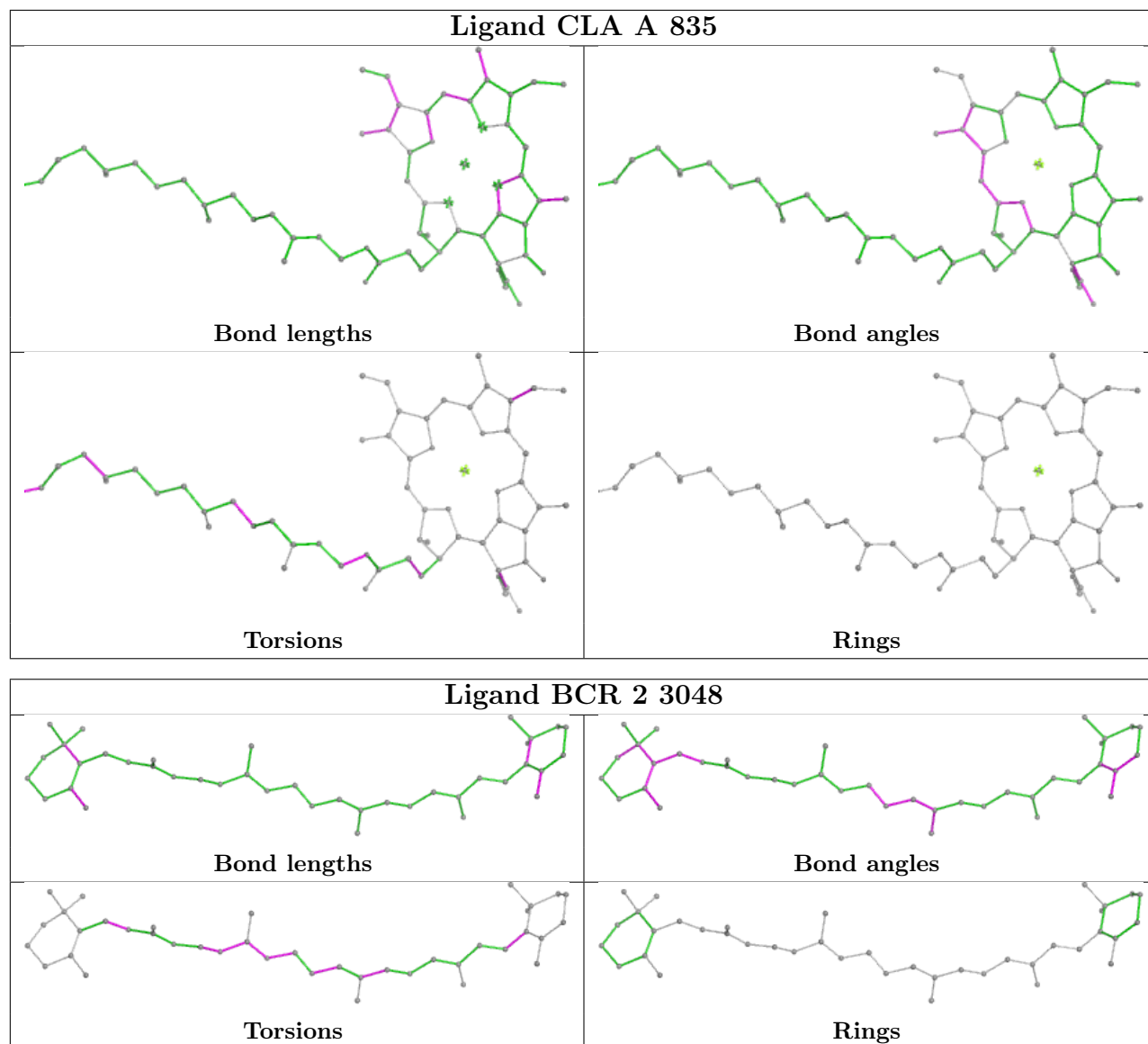
Ligand CLA A 819

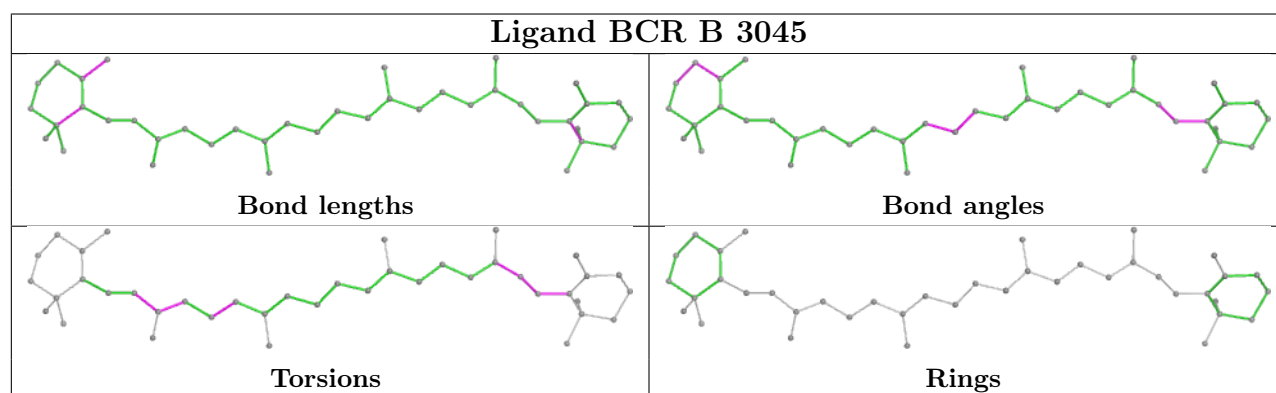
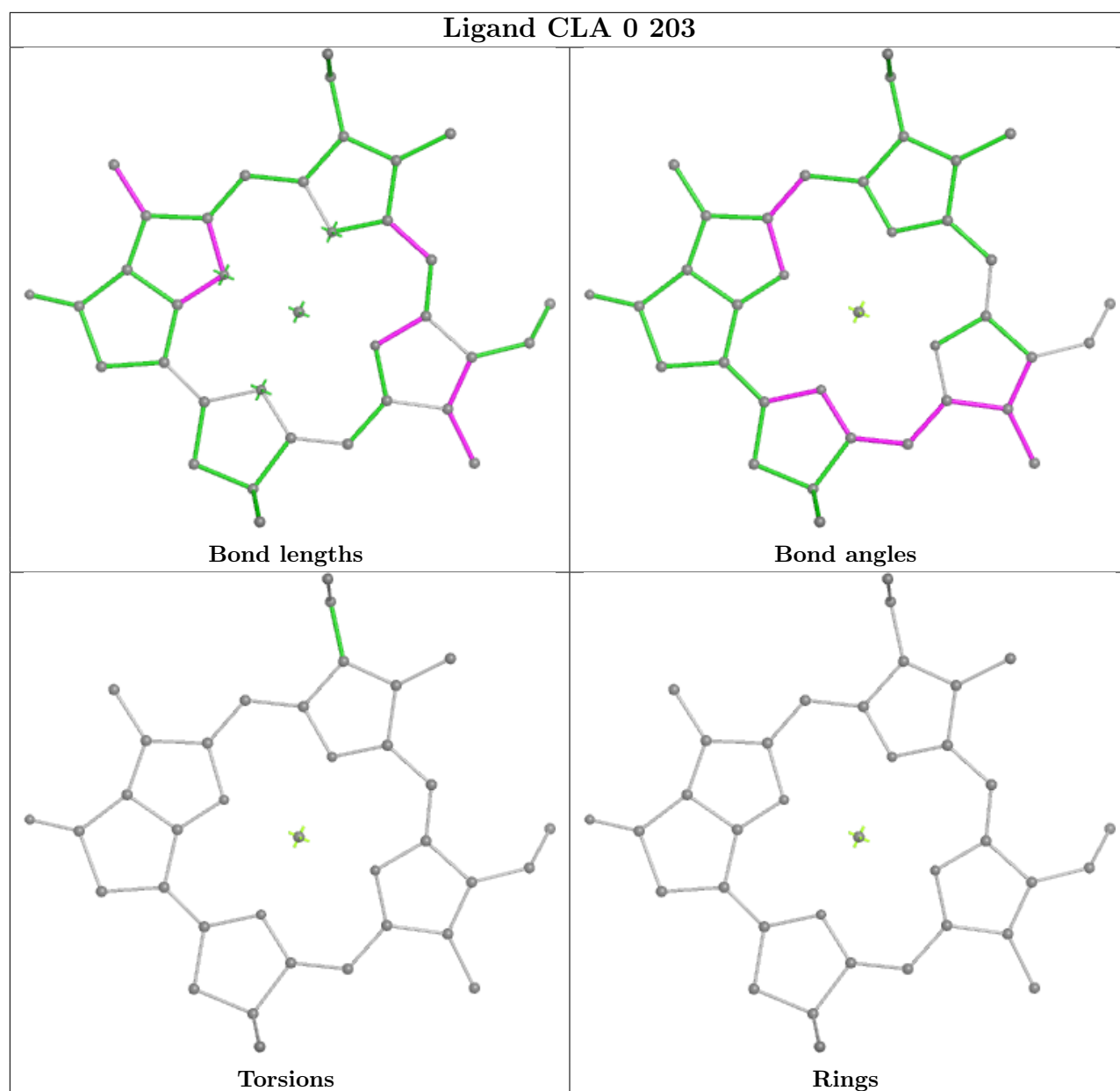


Ligand CLA 2 3034

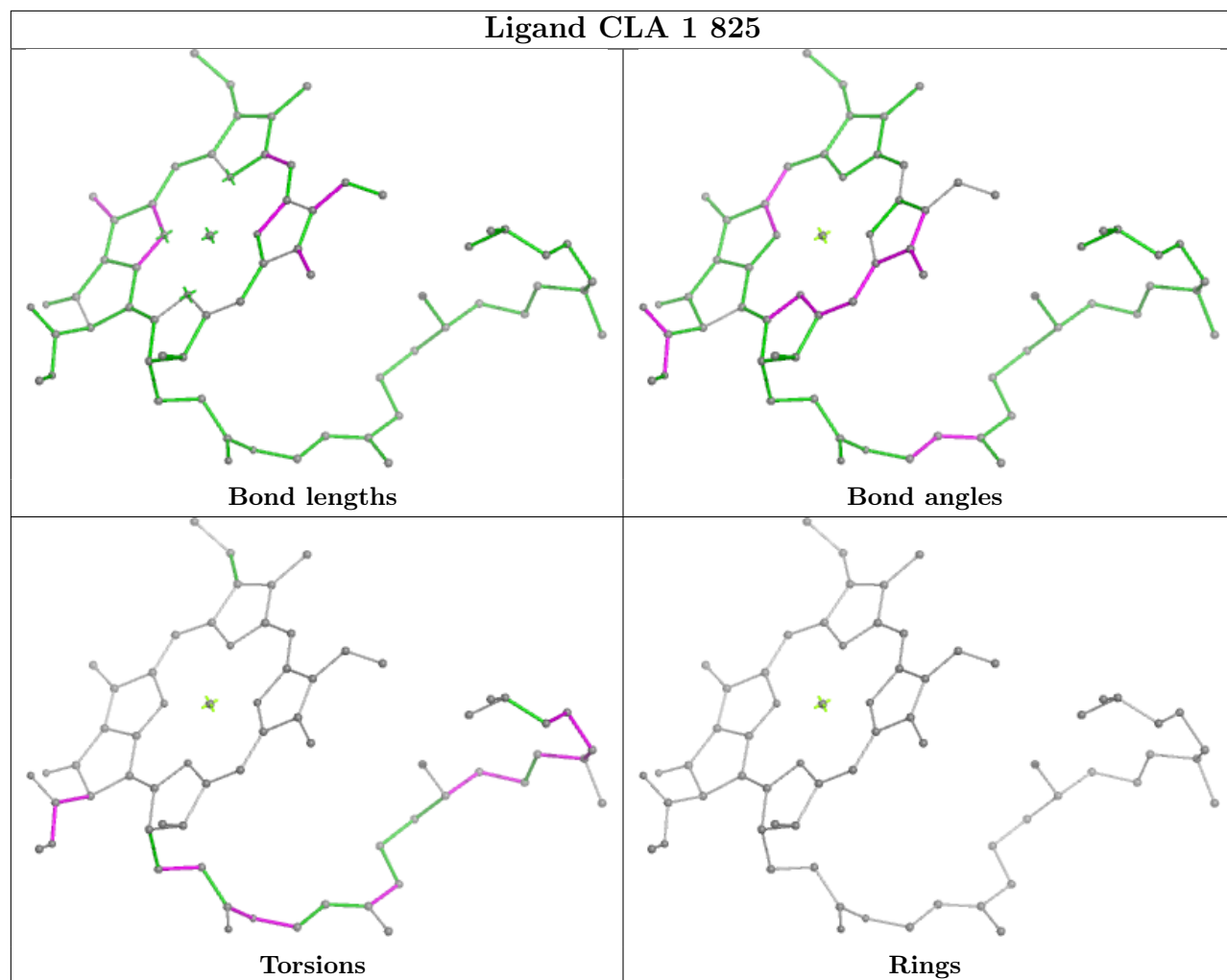




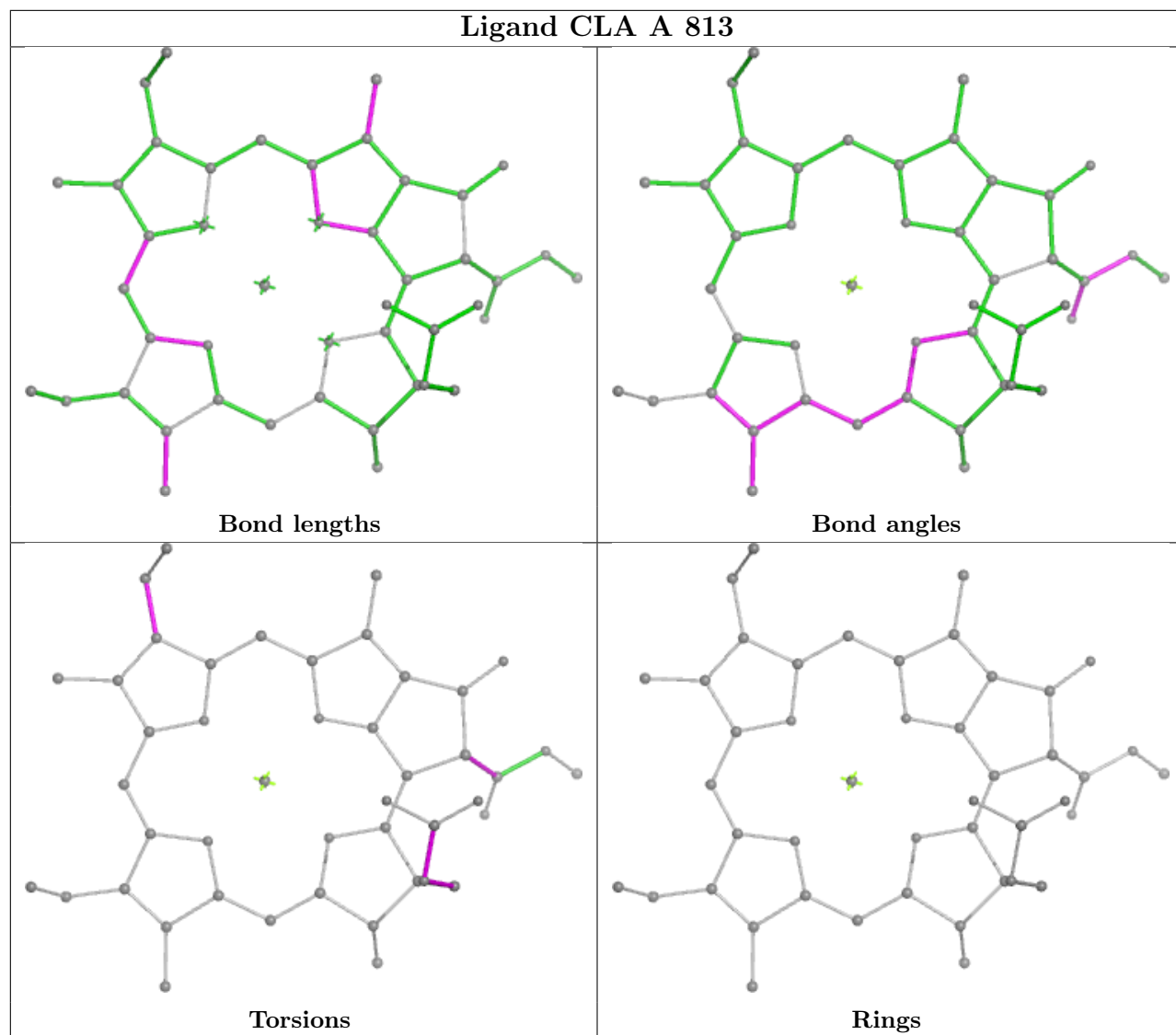


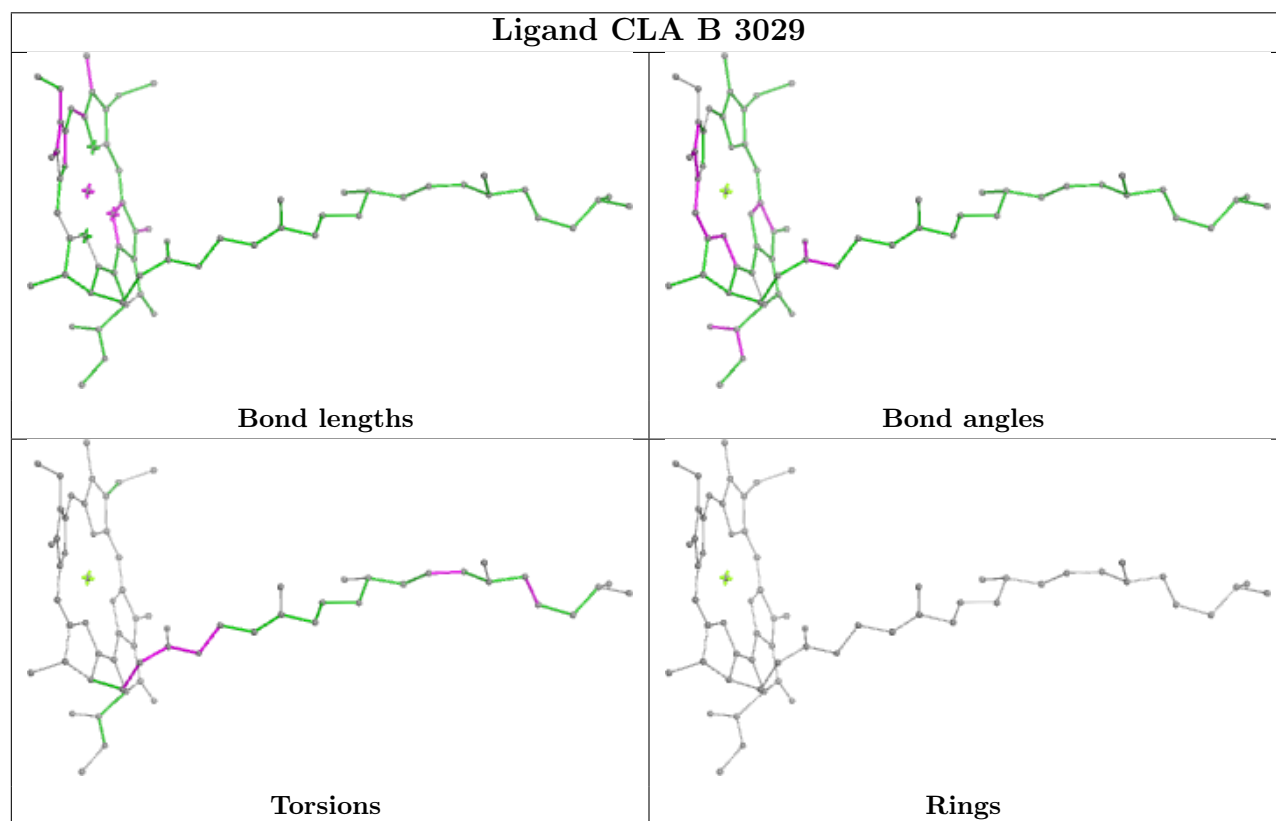
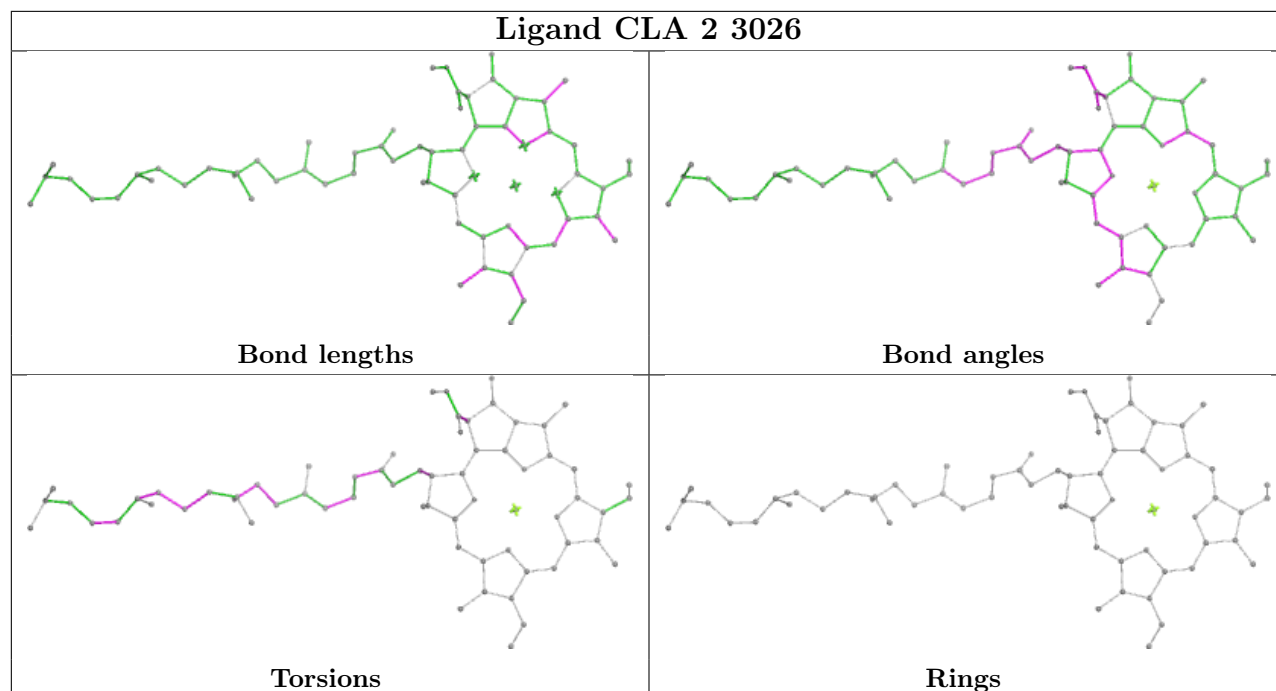


Ligand CLA 1 825

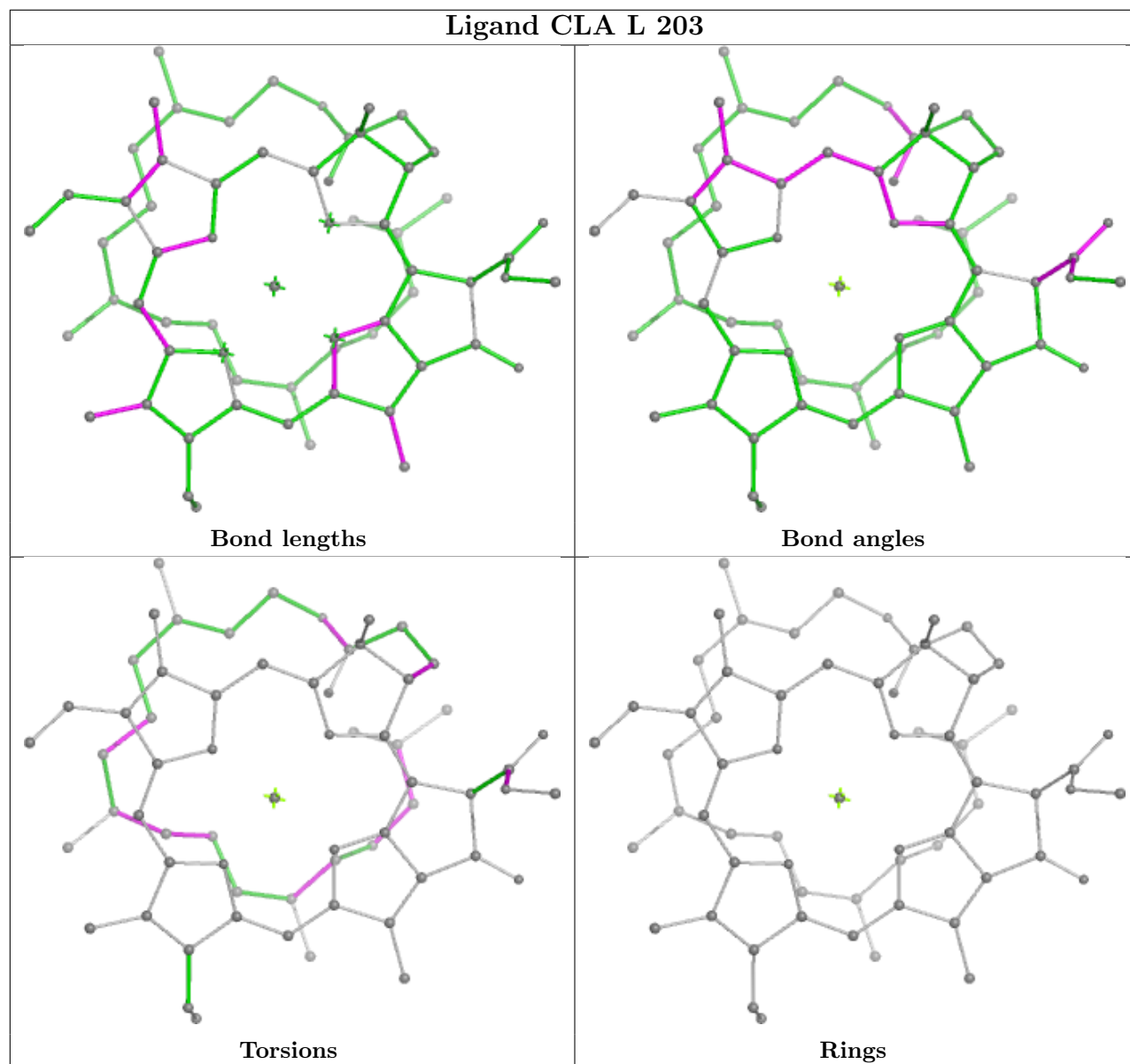


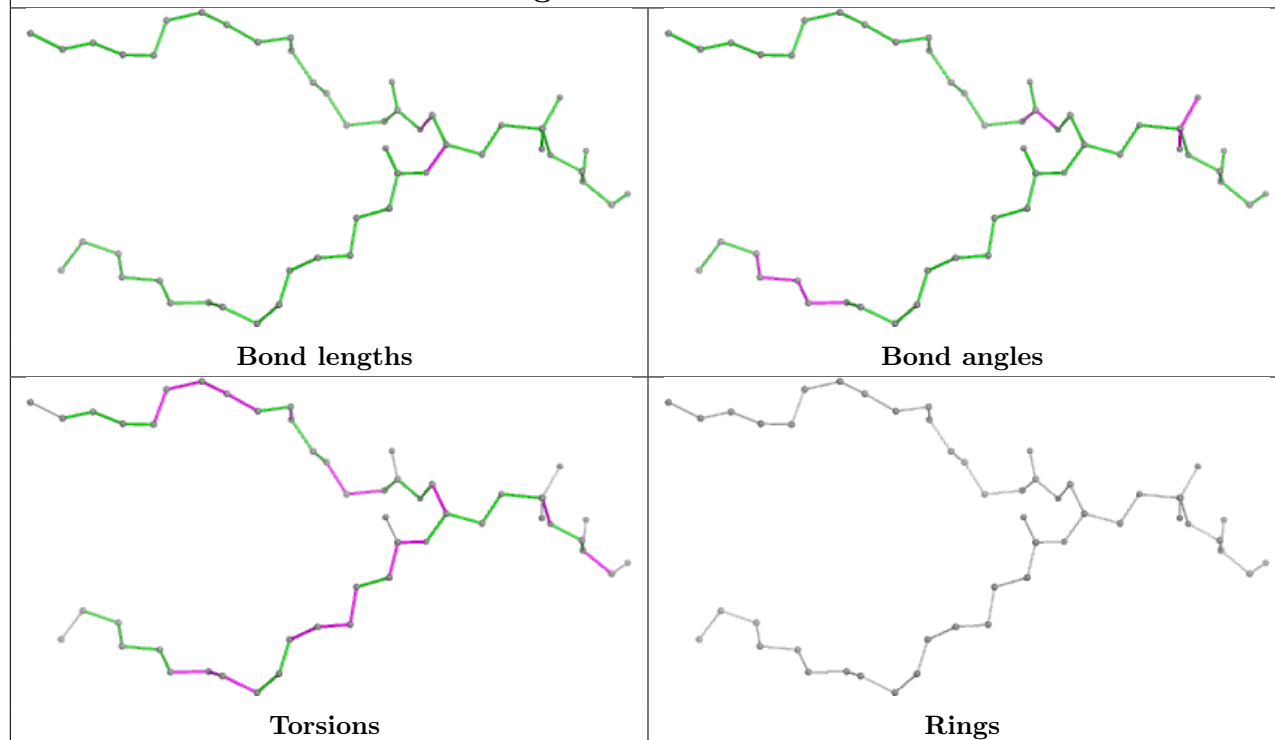
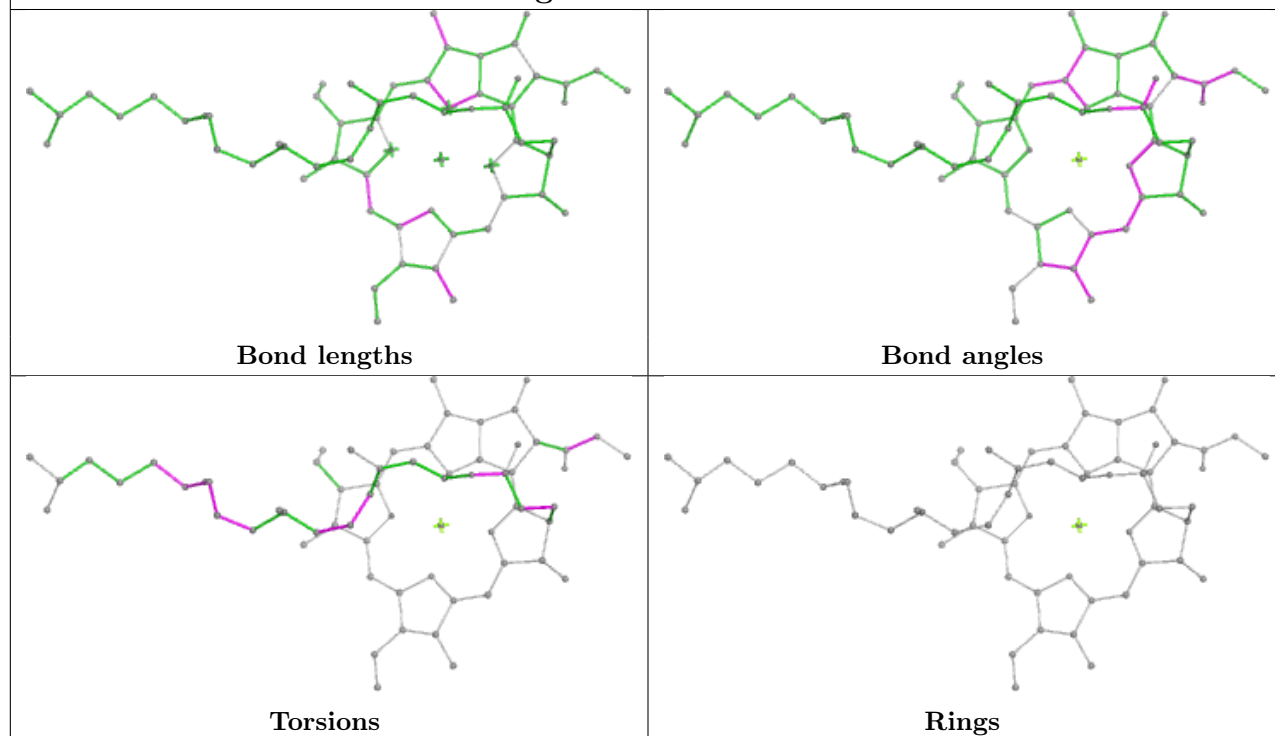
Ligand CLA A 813



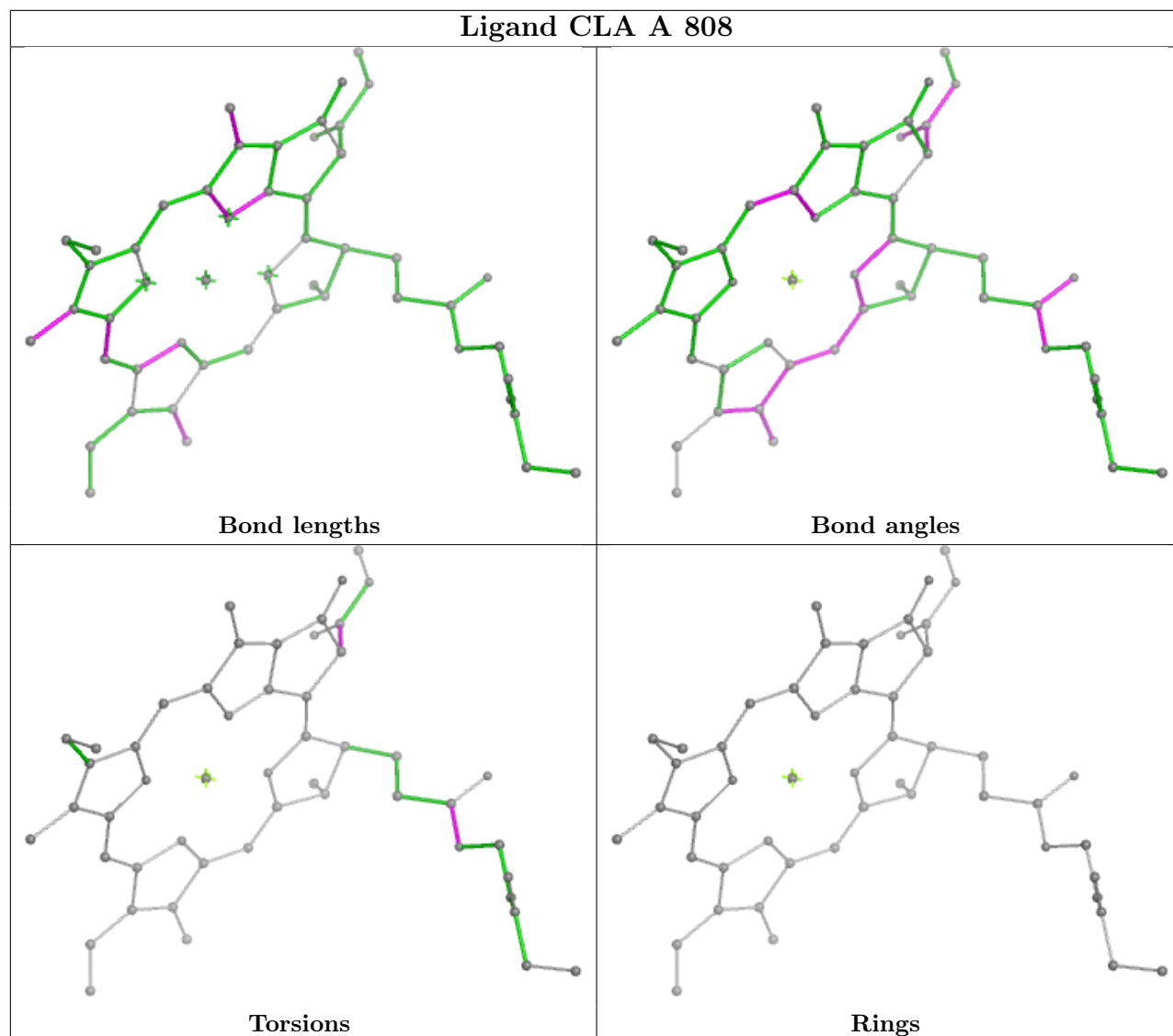


Ligand CLA L 203

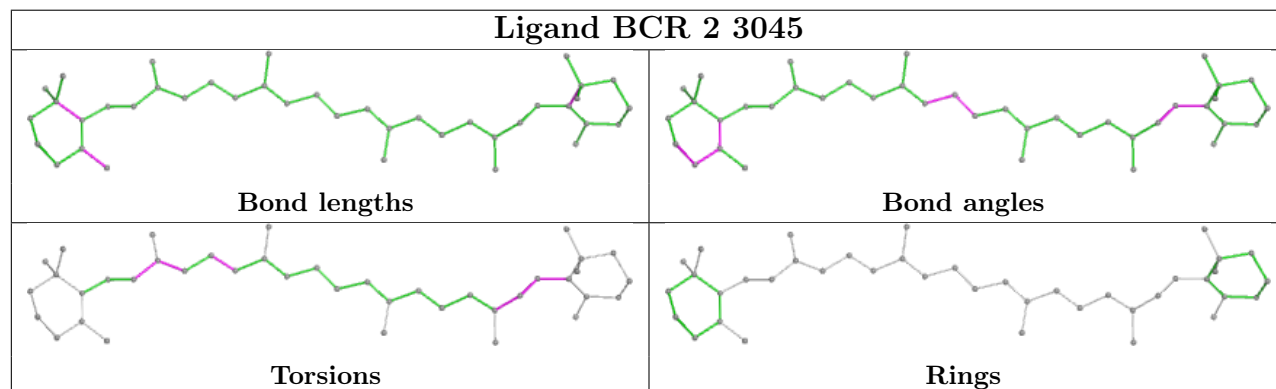


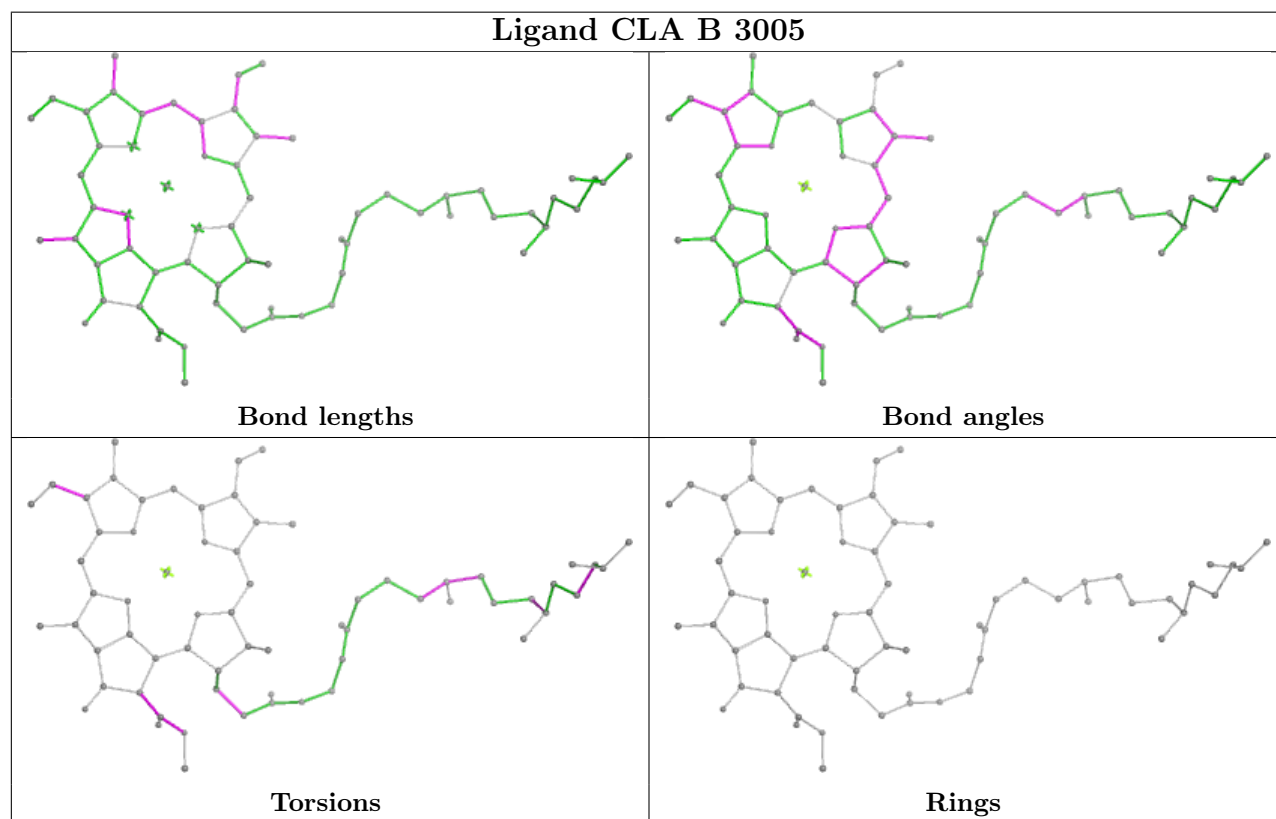
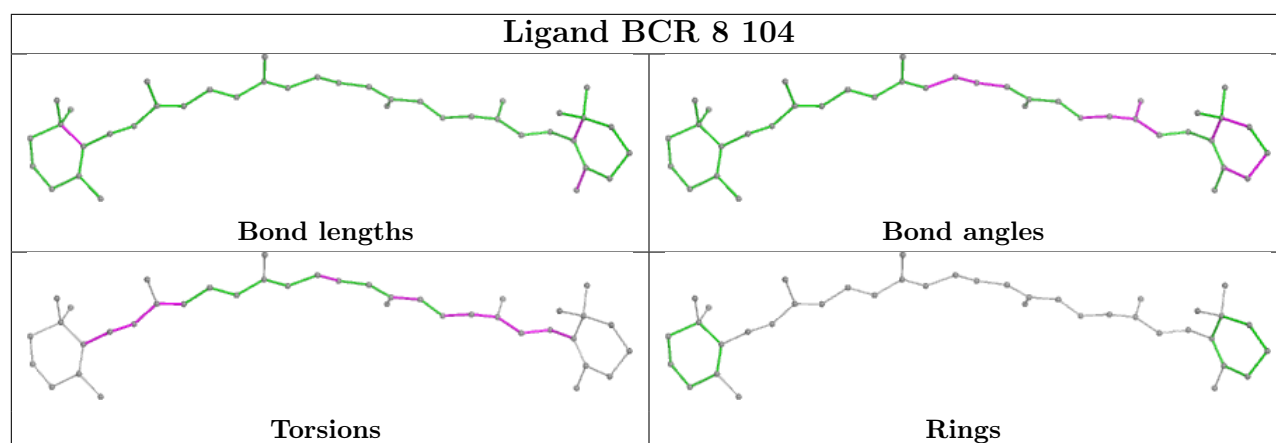
Ligand LHG 1 852**Ligand CLA a 817**

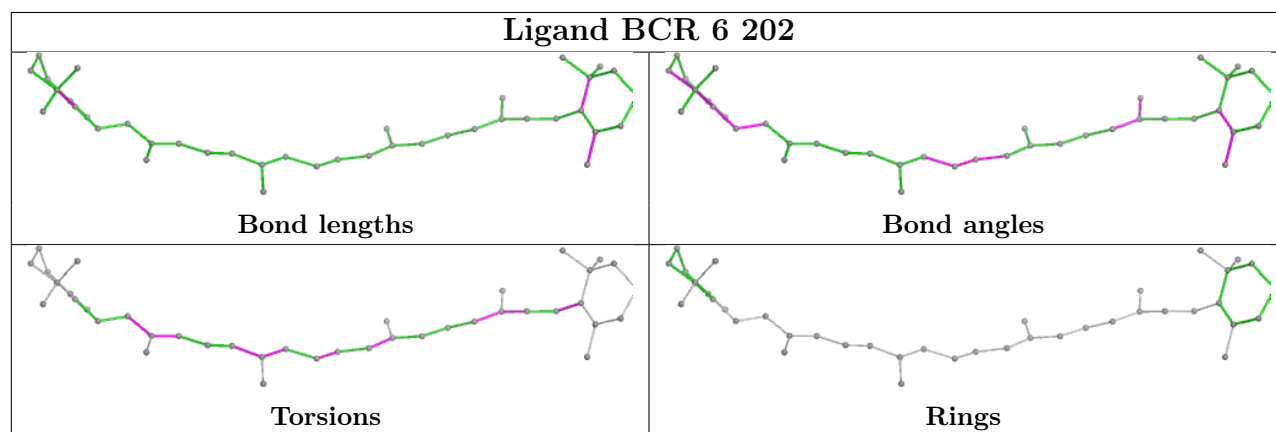
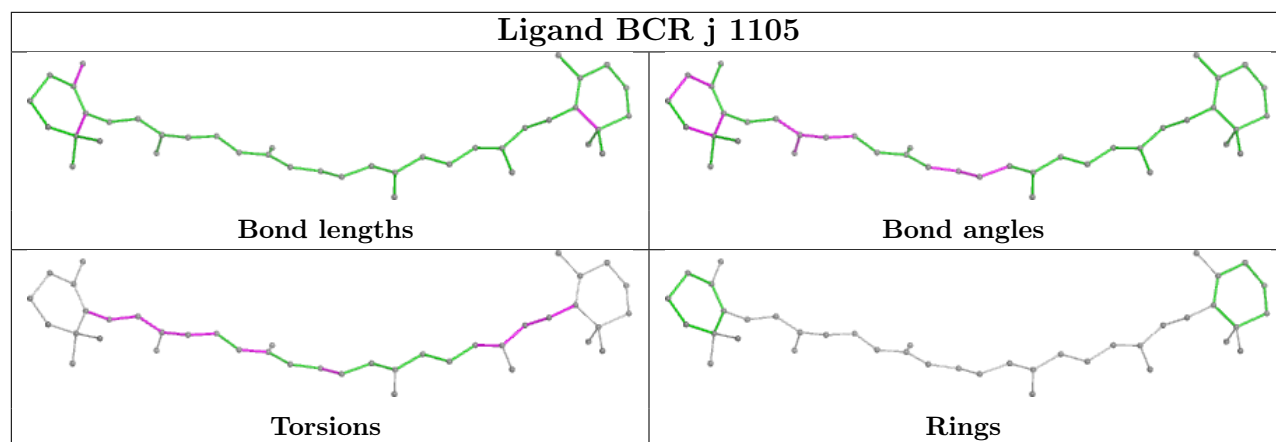
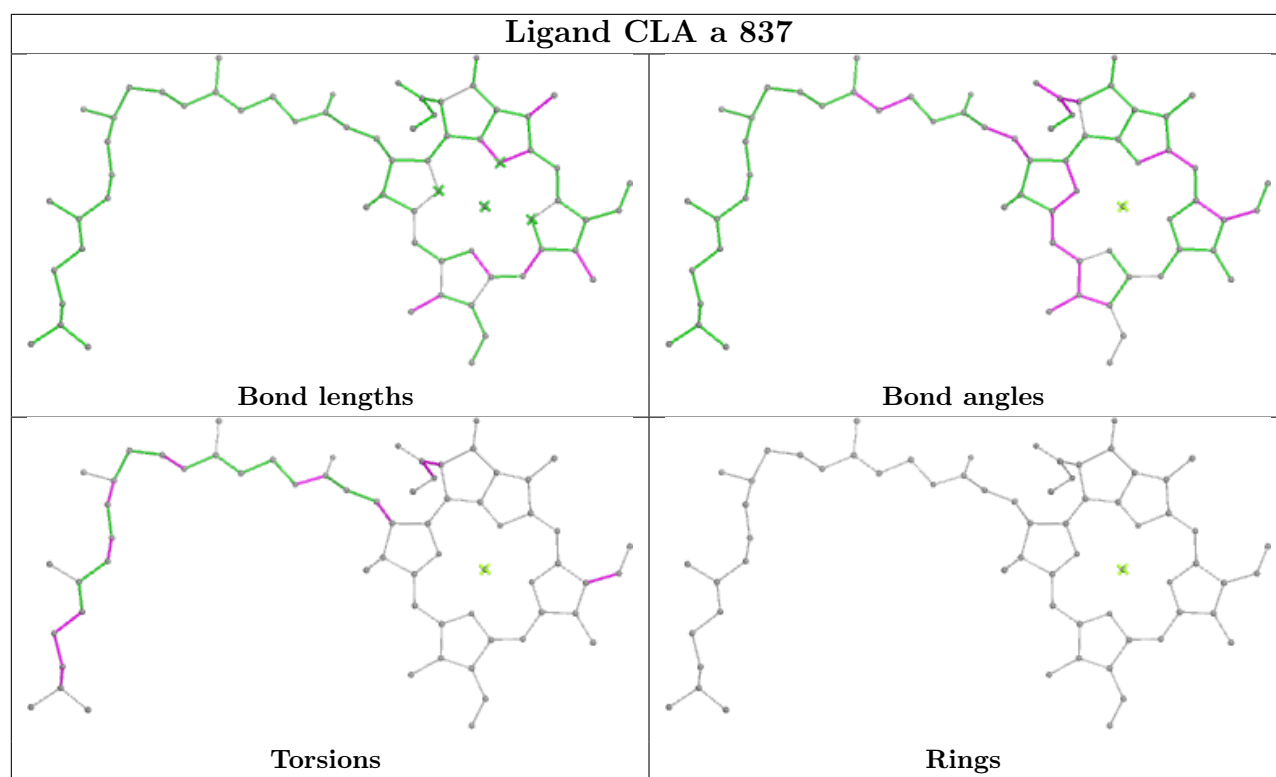
Ligand CLA A 808

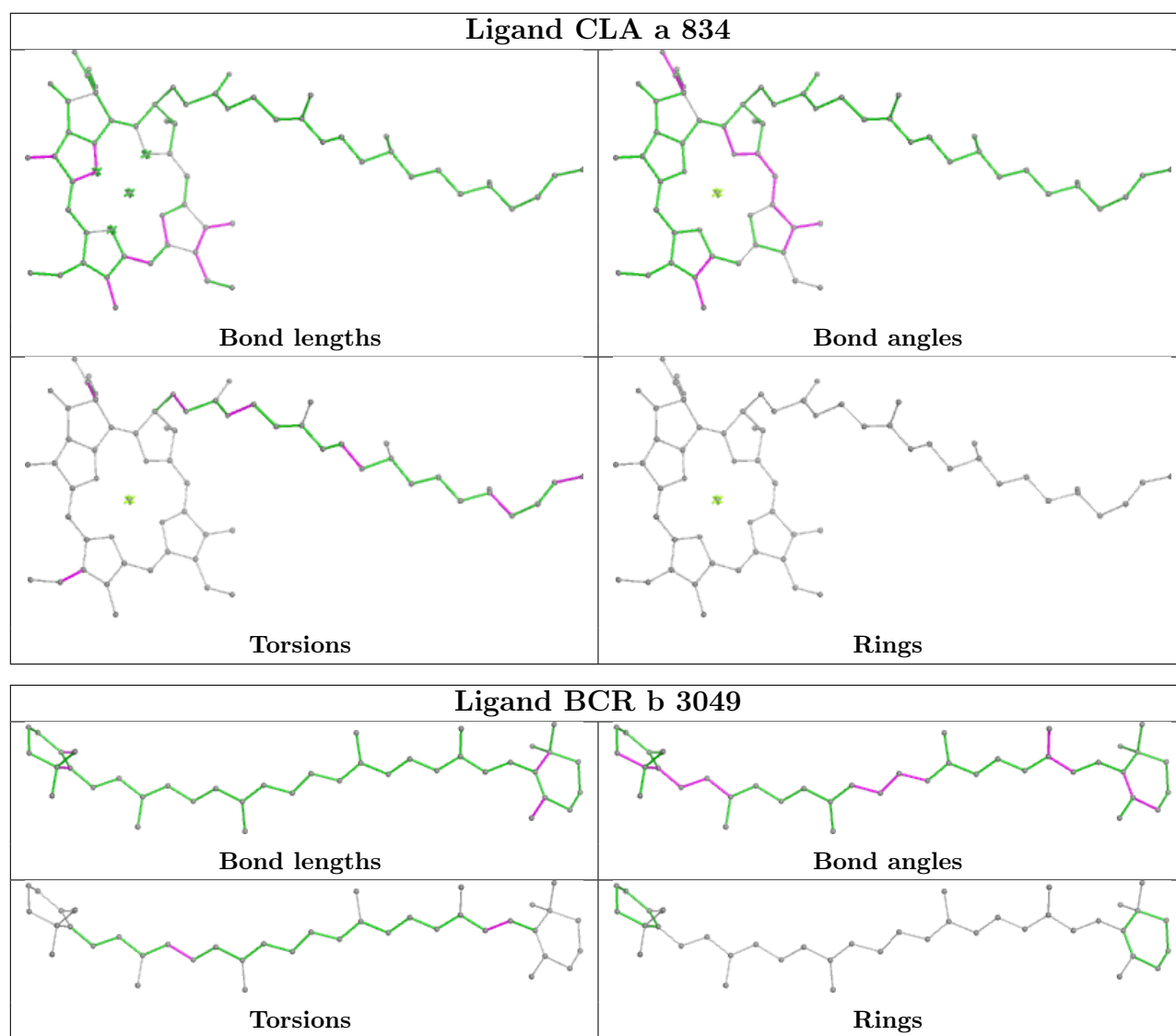


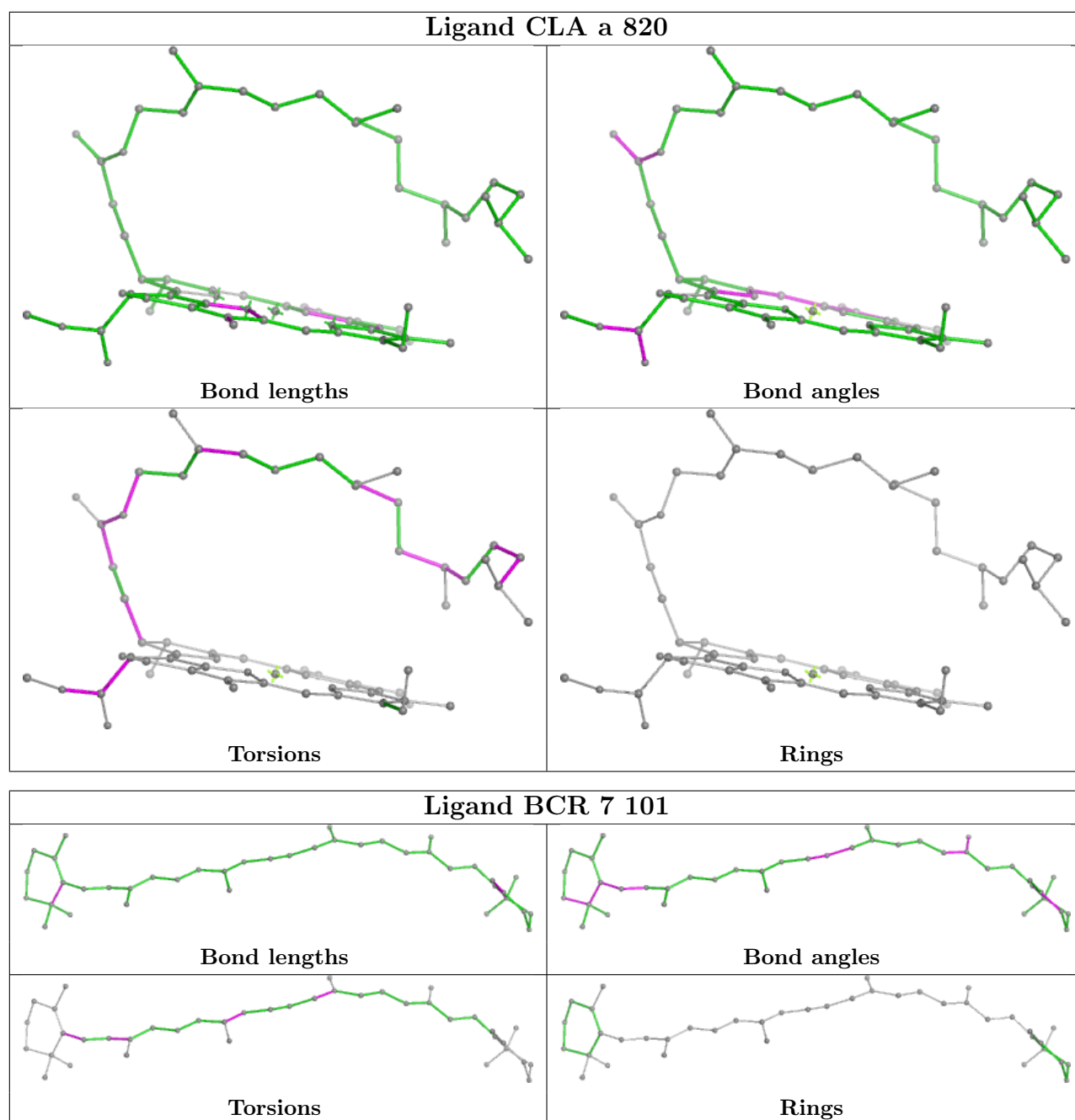
Ligand BCR 2 3045

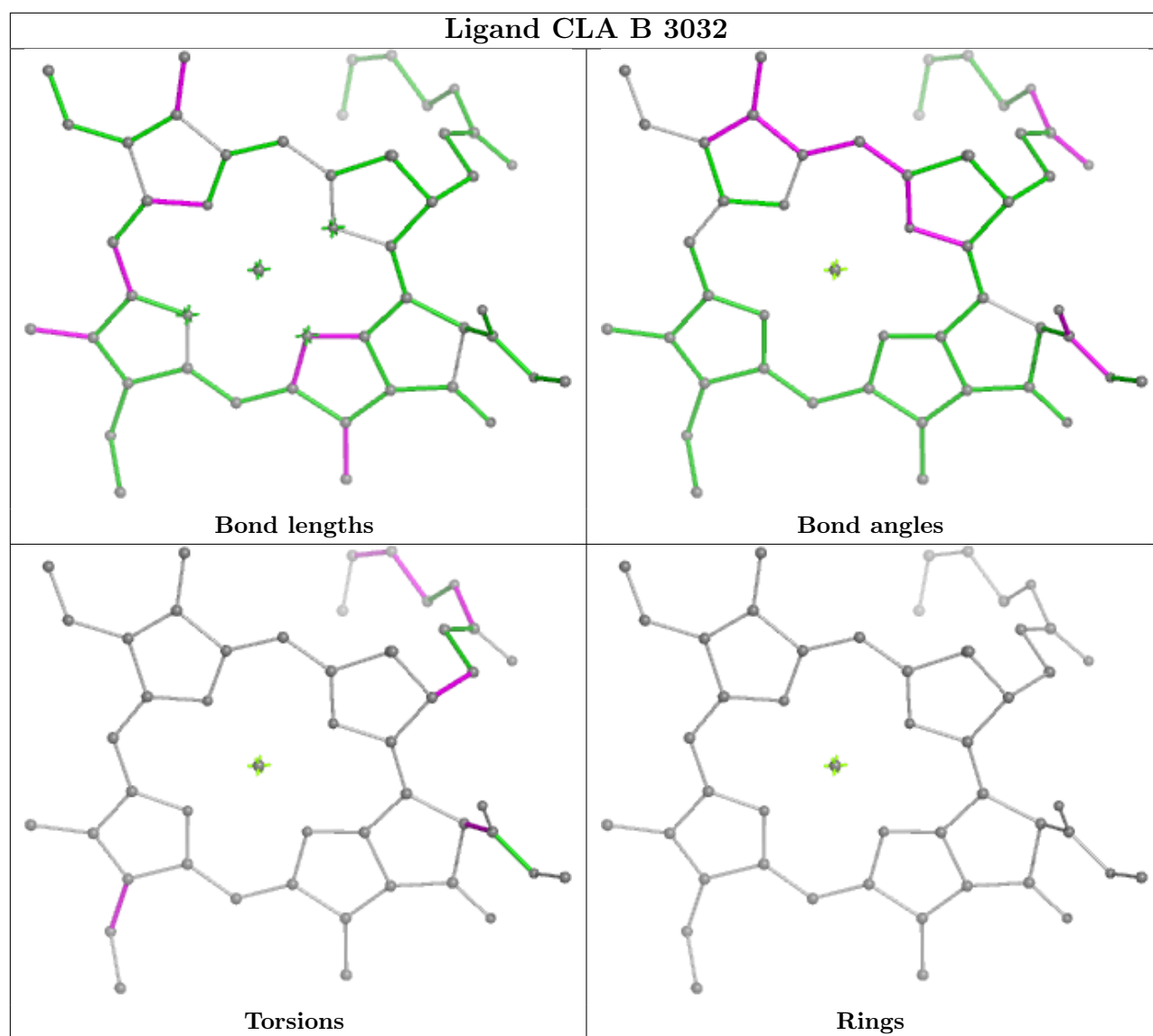




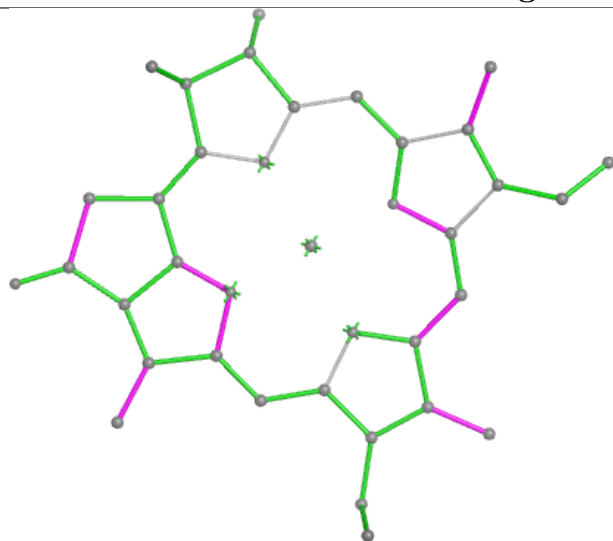




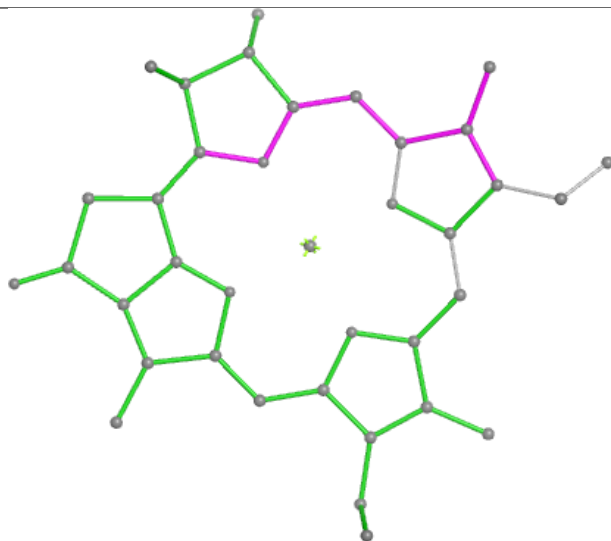




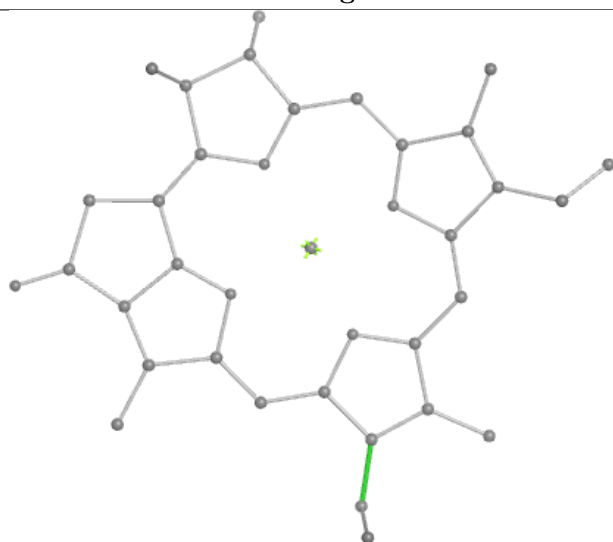
Ligand CLA 8 102



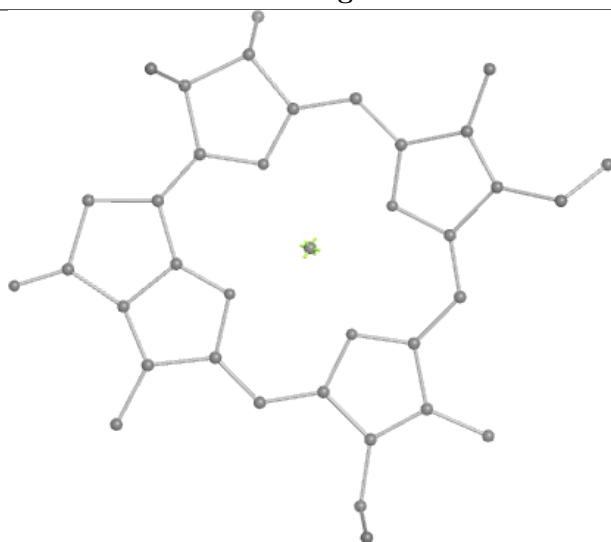
Bond lengths



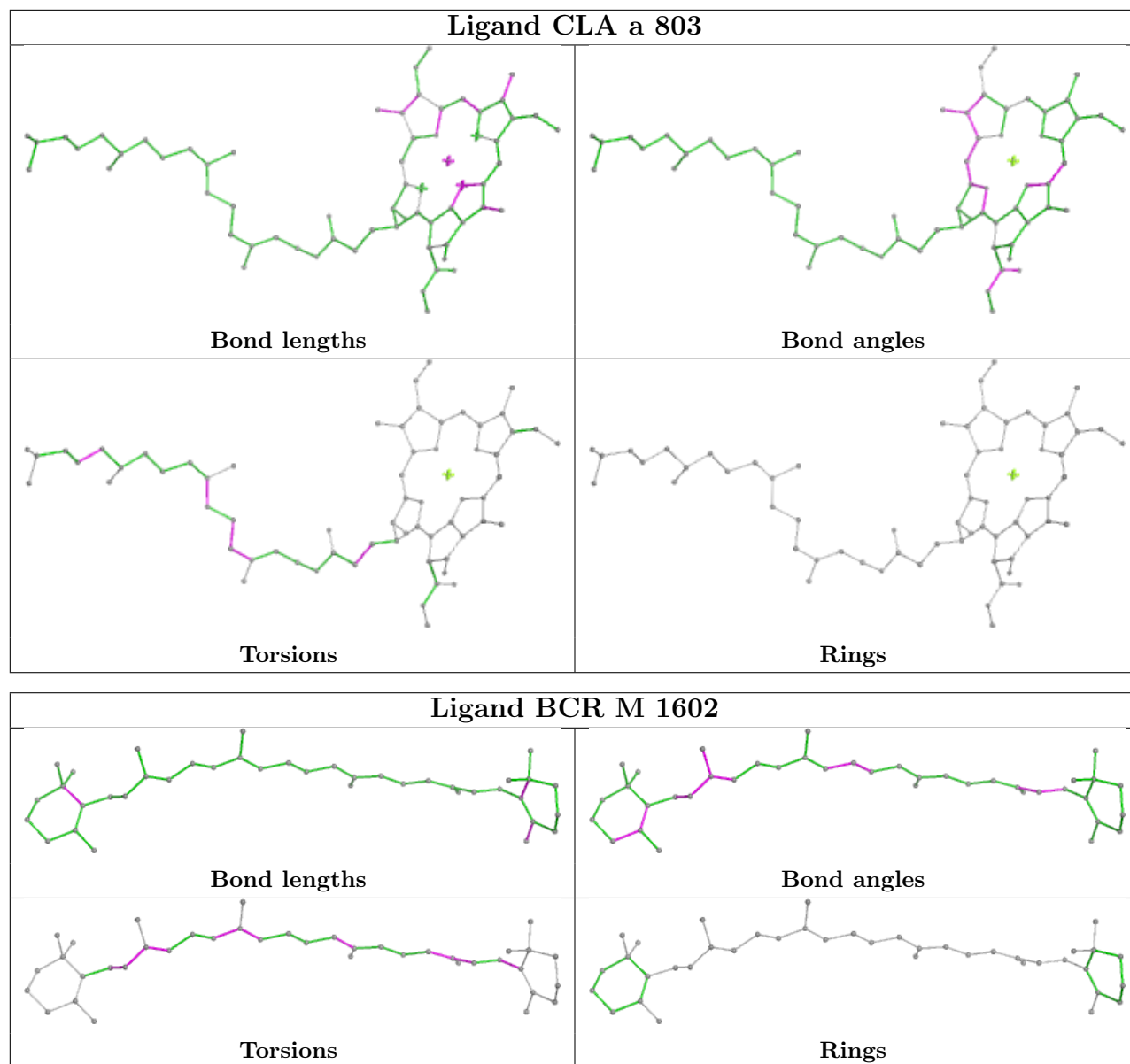
Bond angles

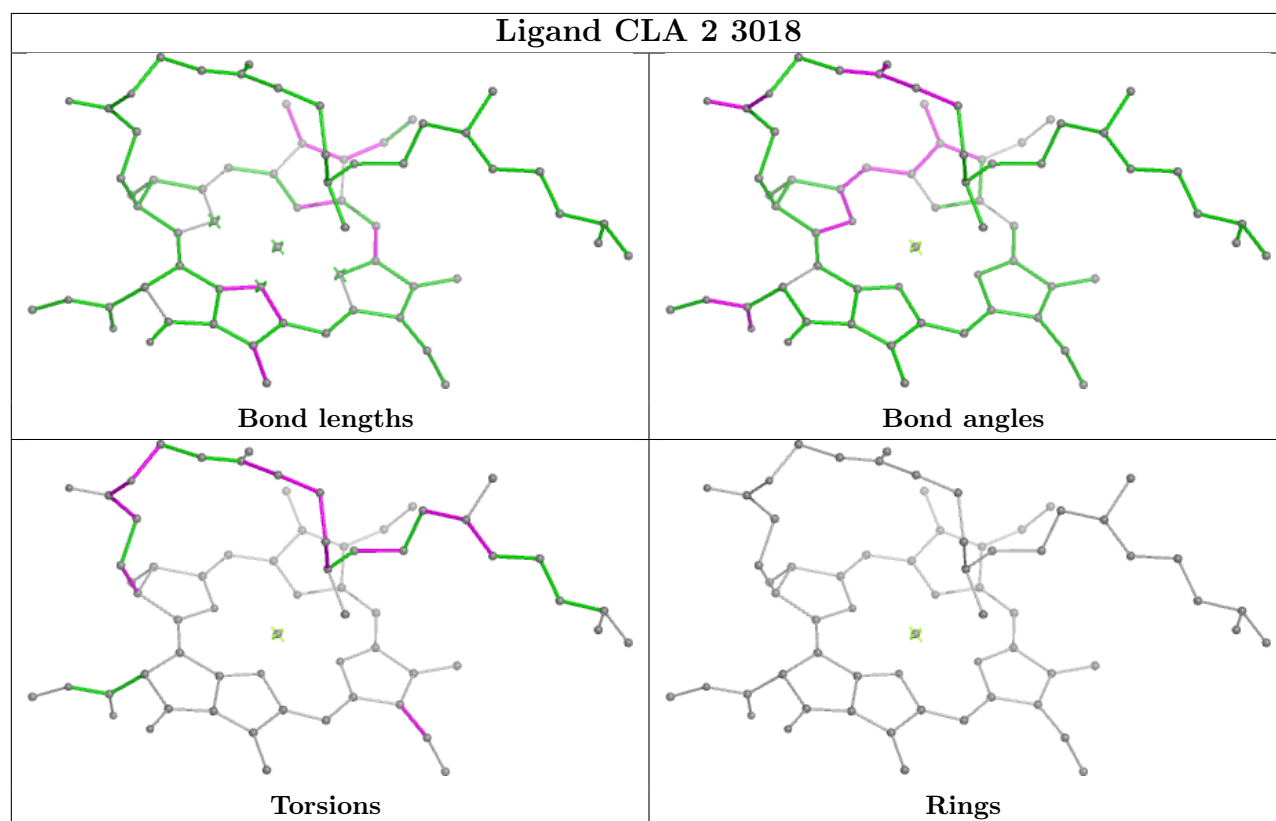
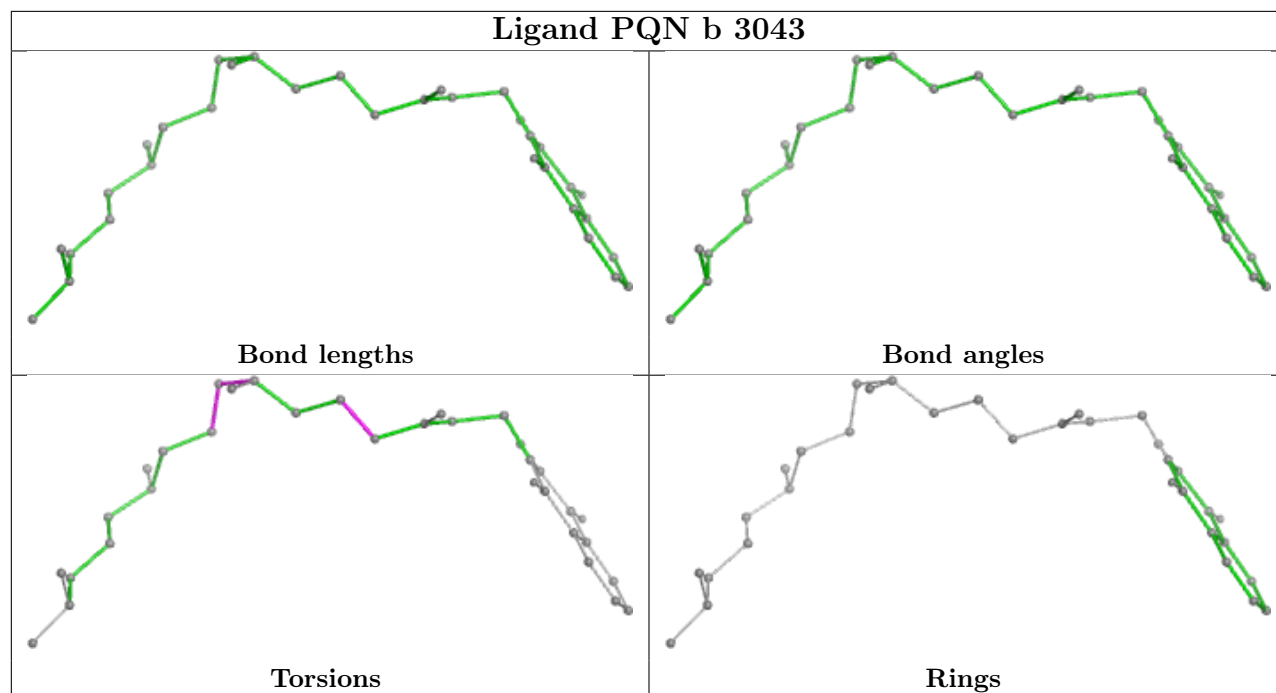


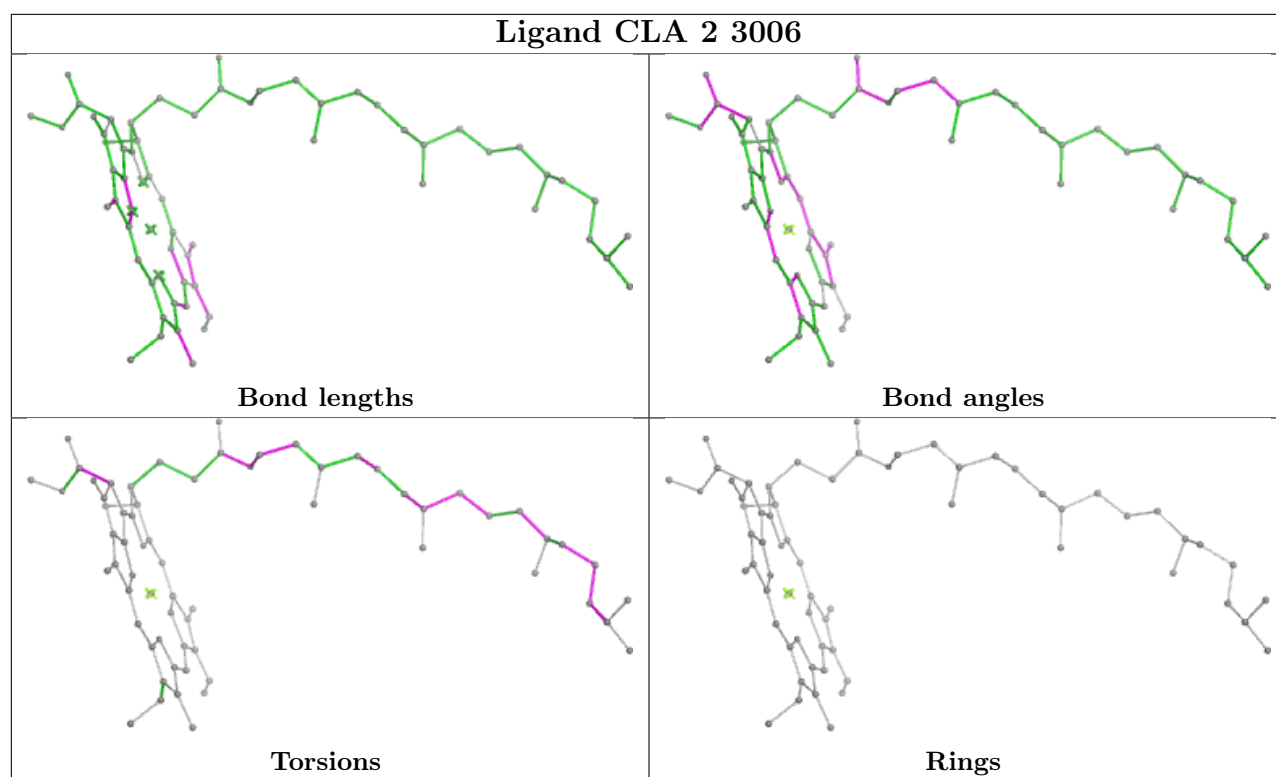
Torsions

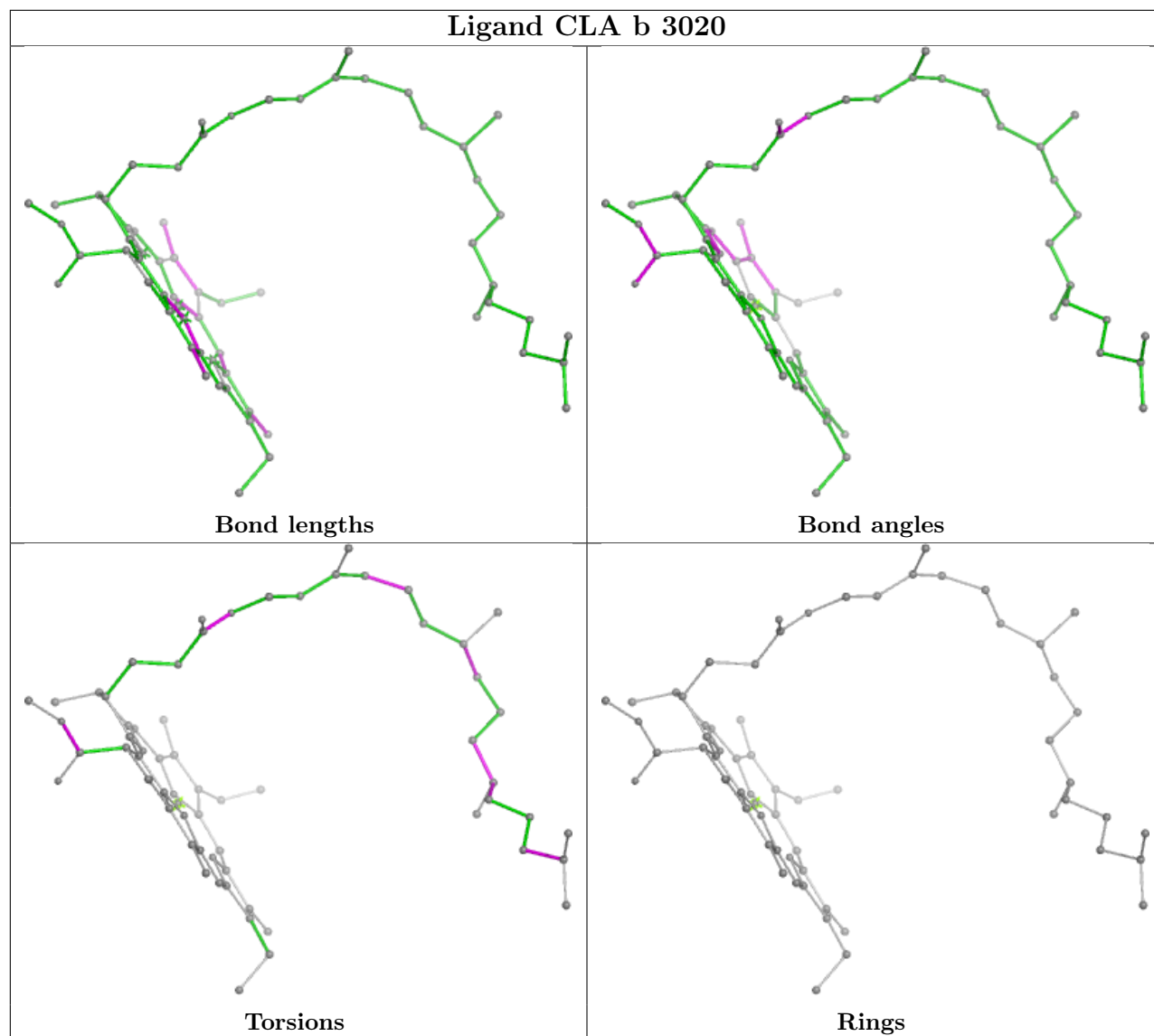


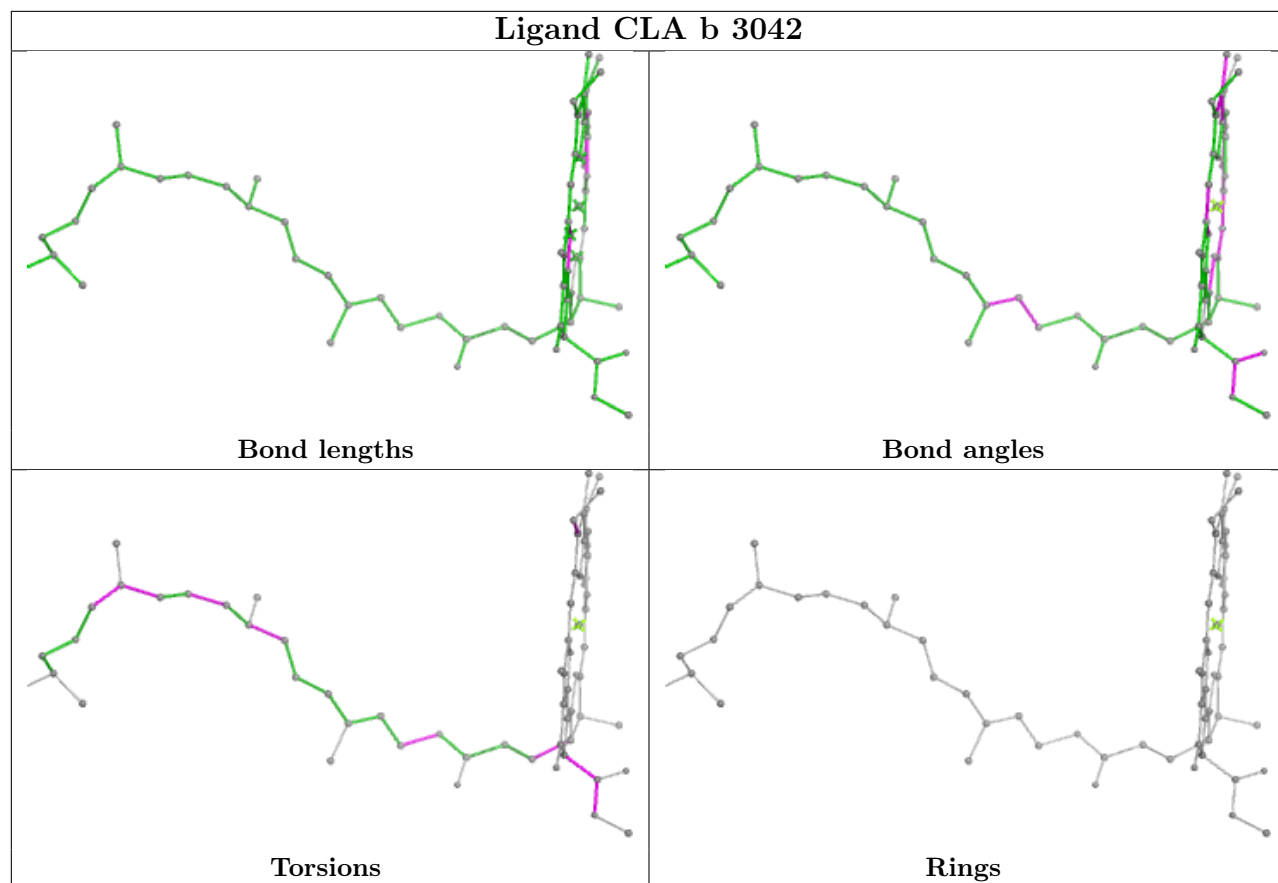
Rings

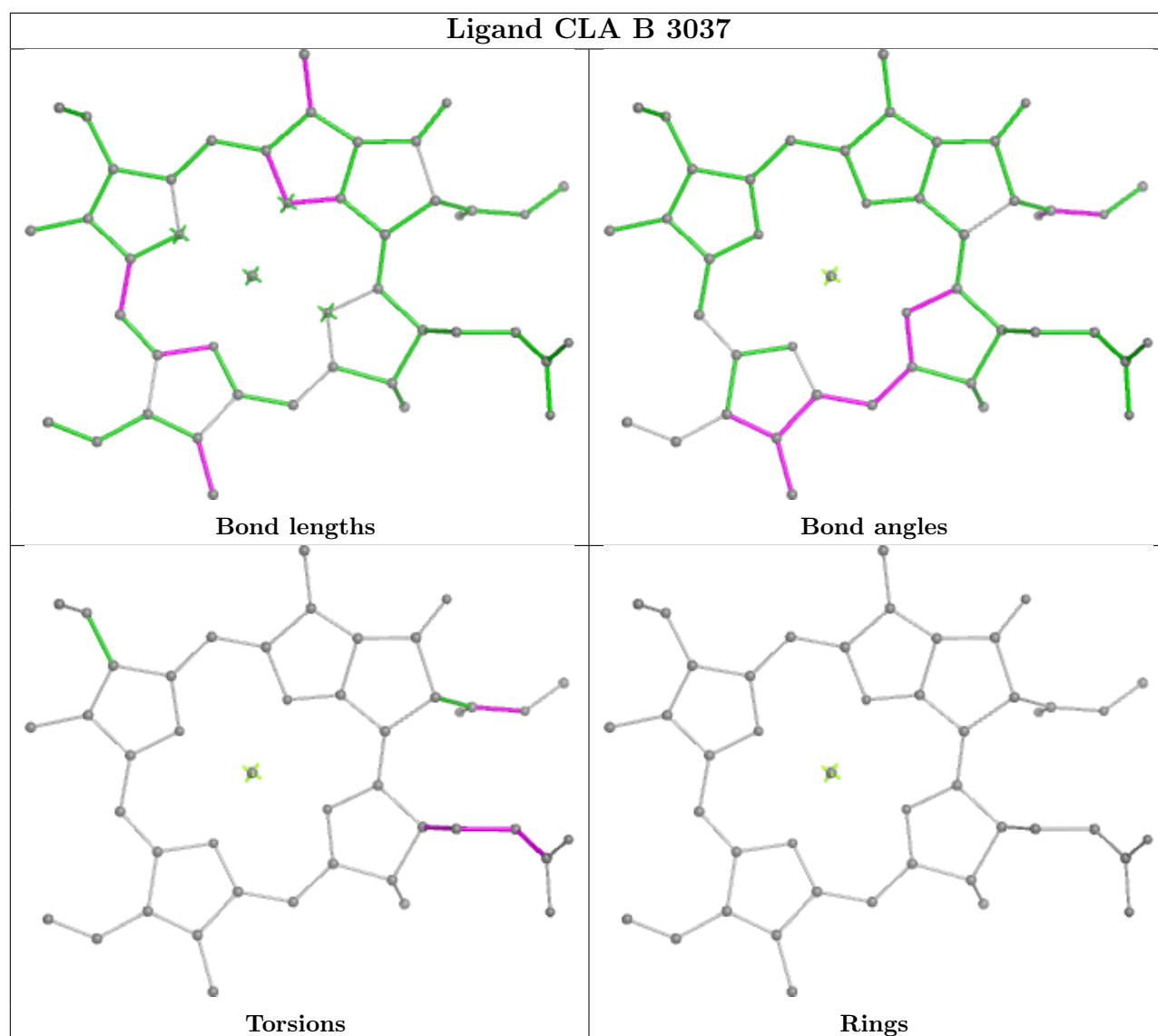


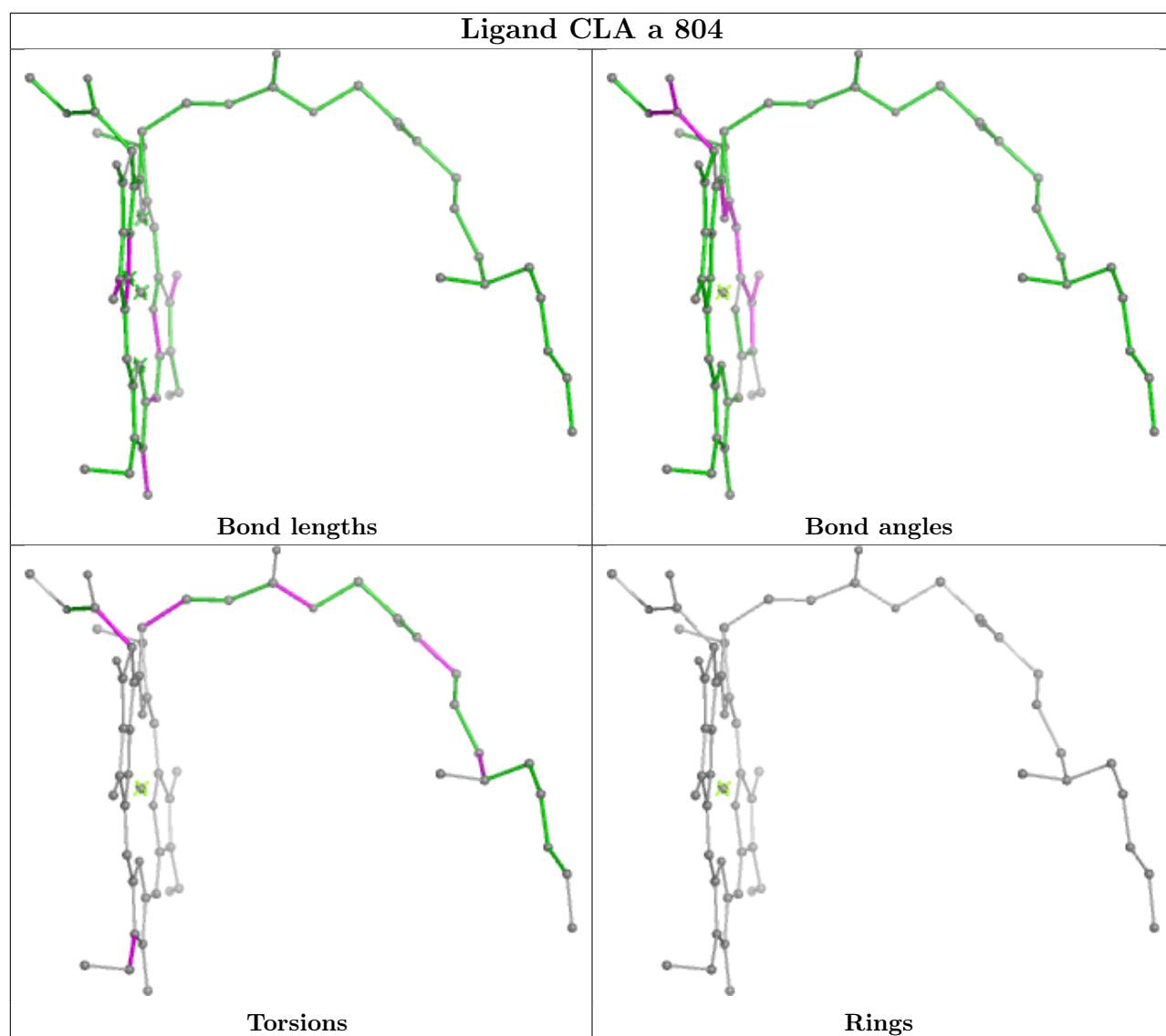


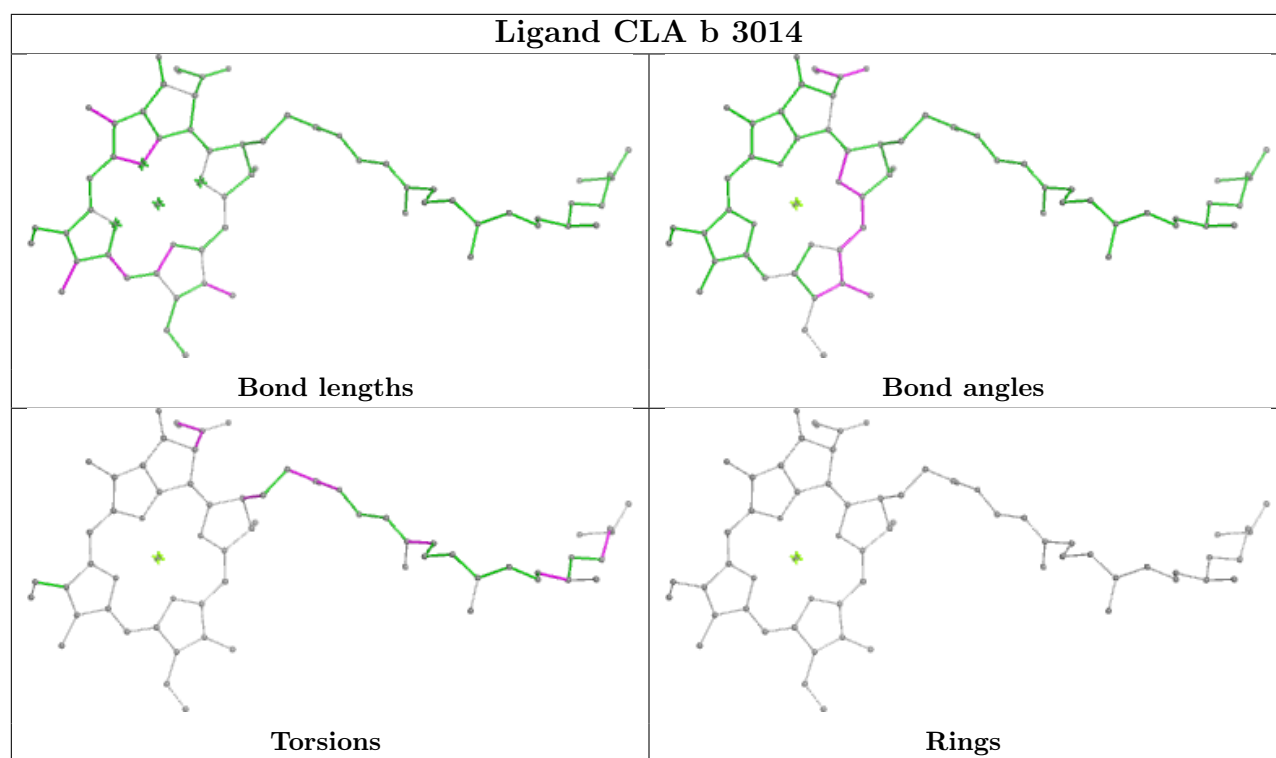




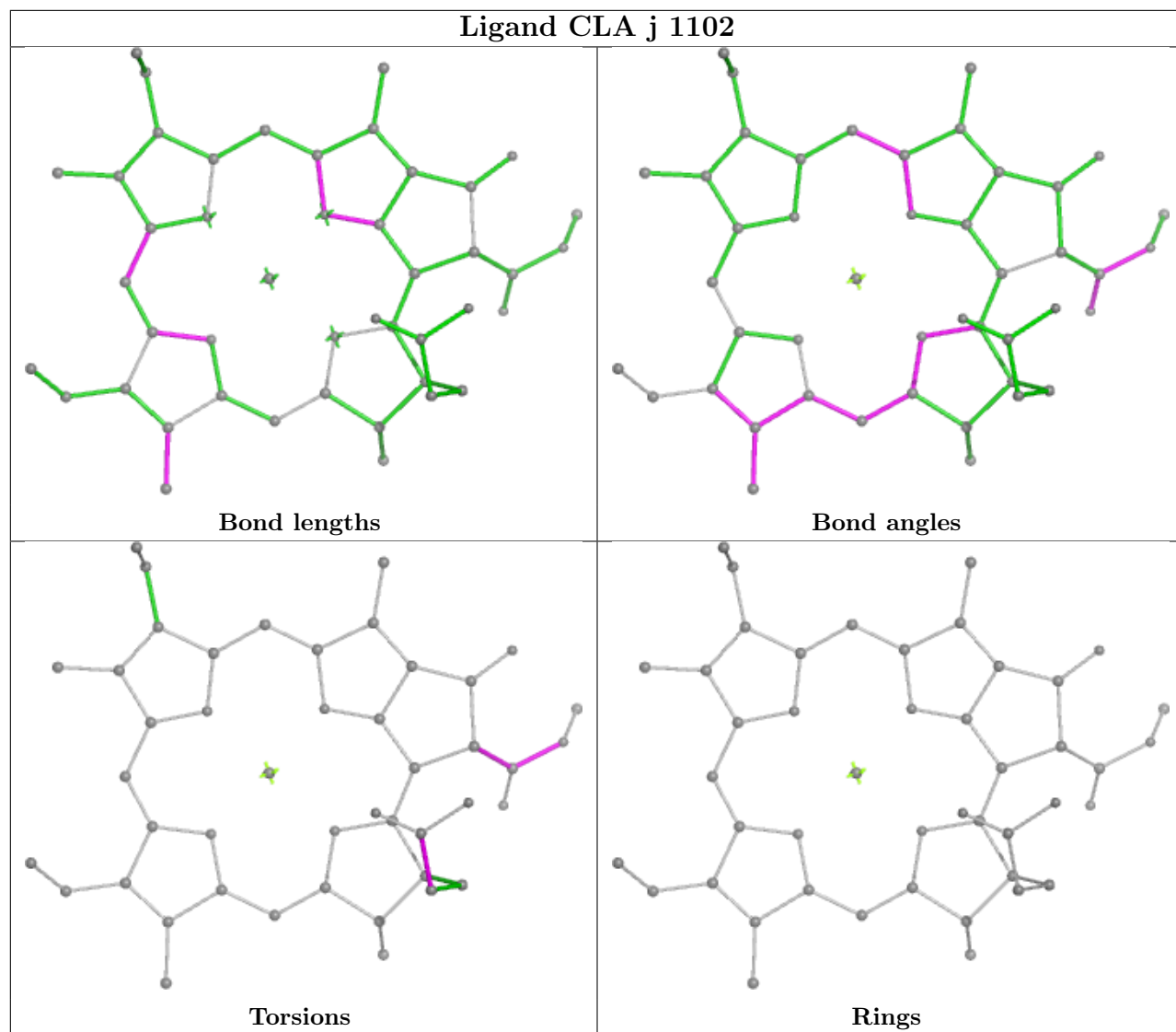


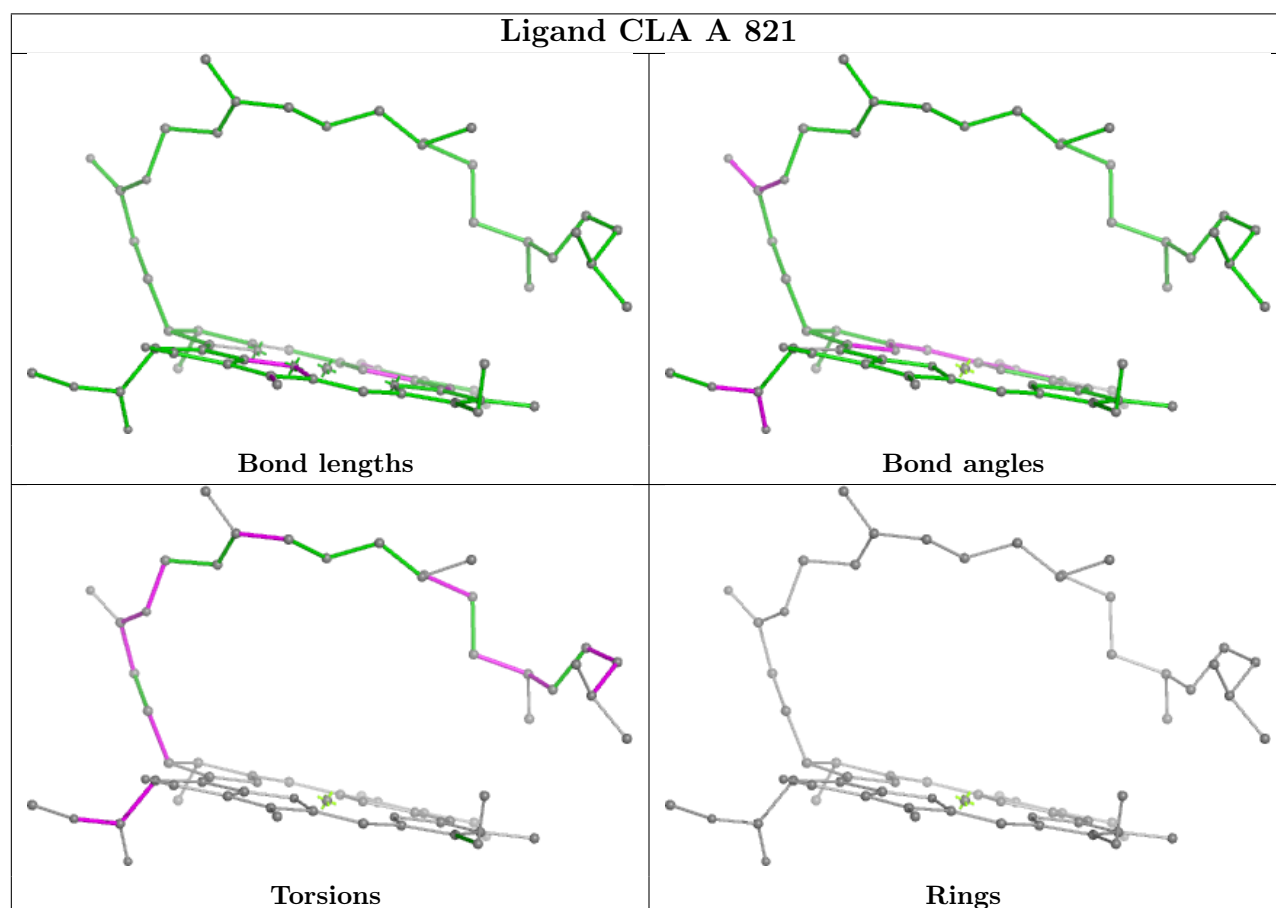
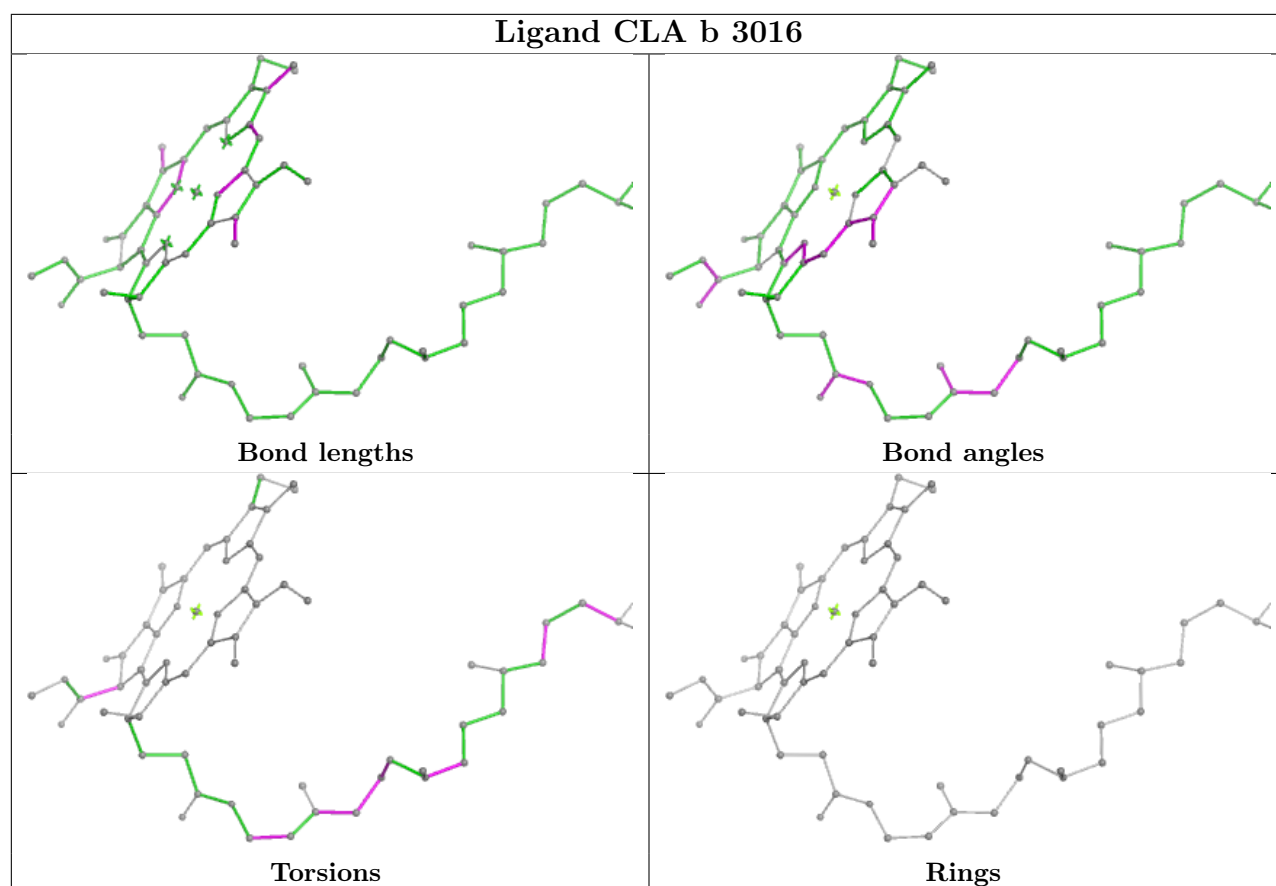


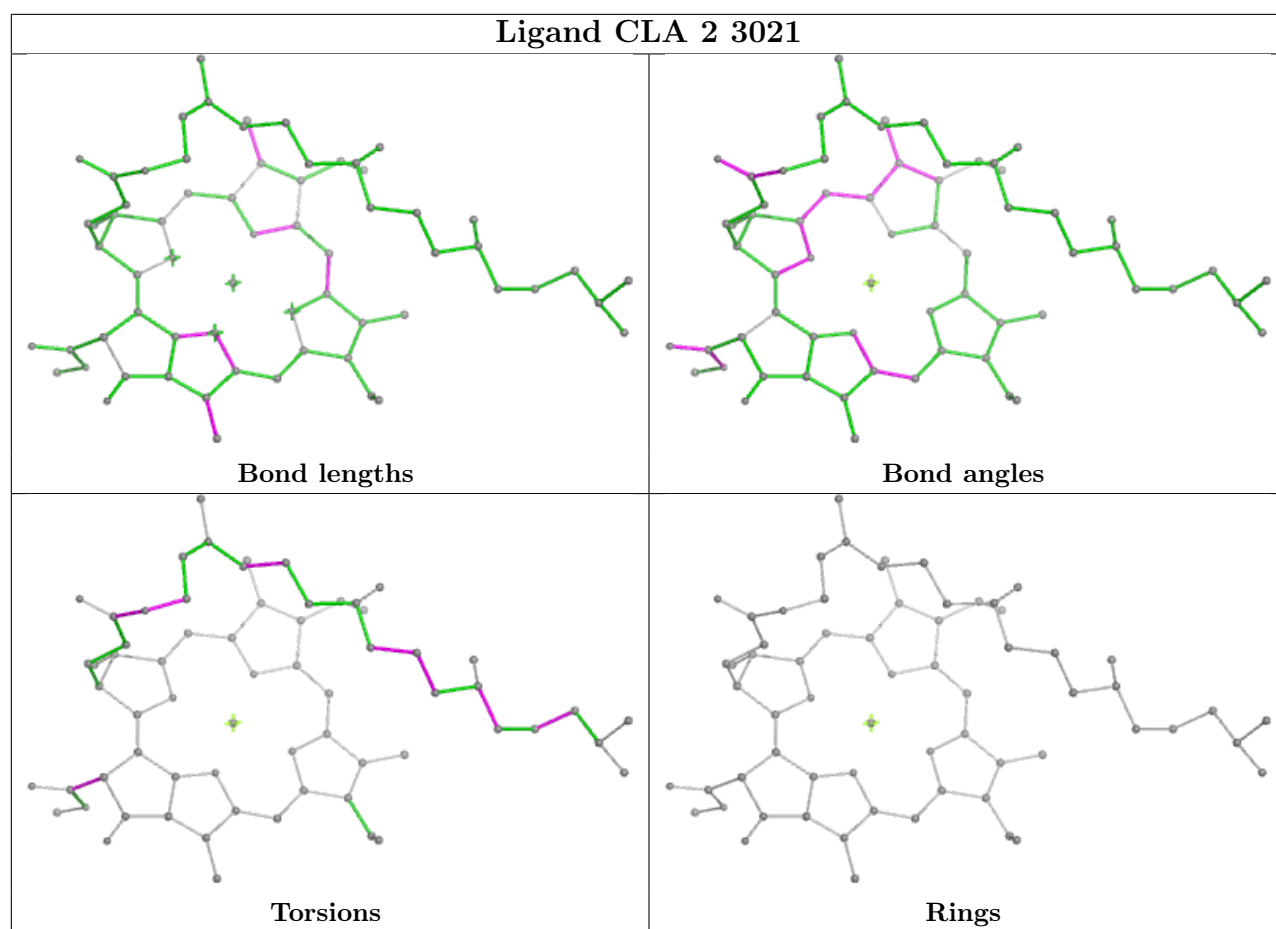




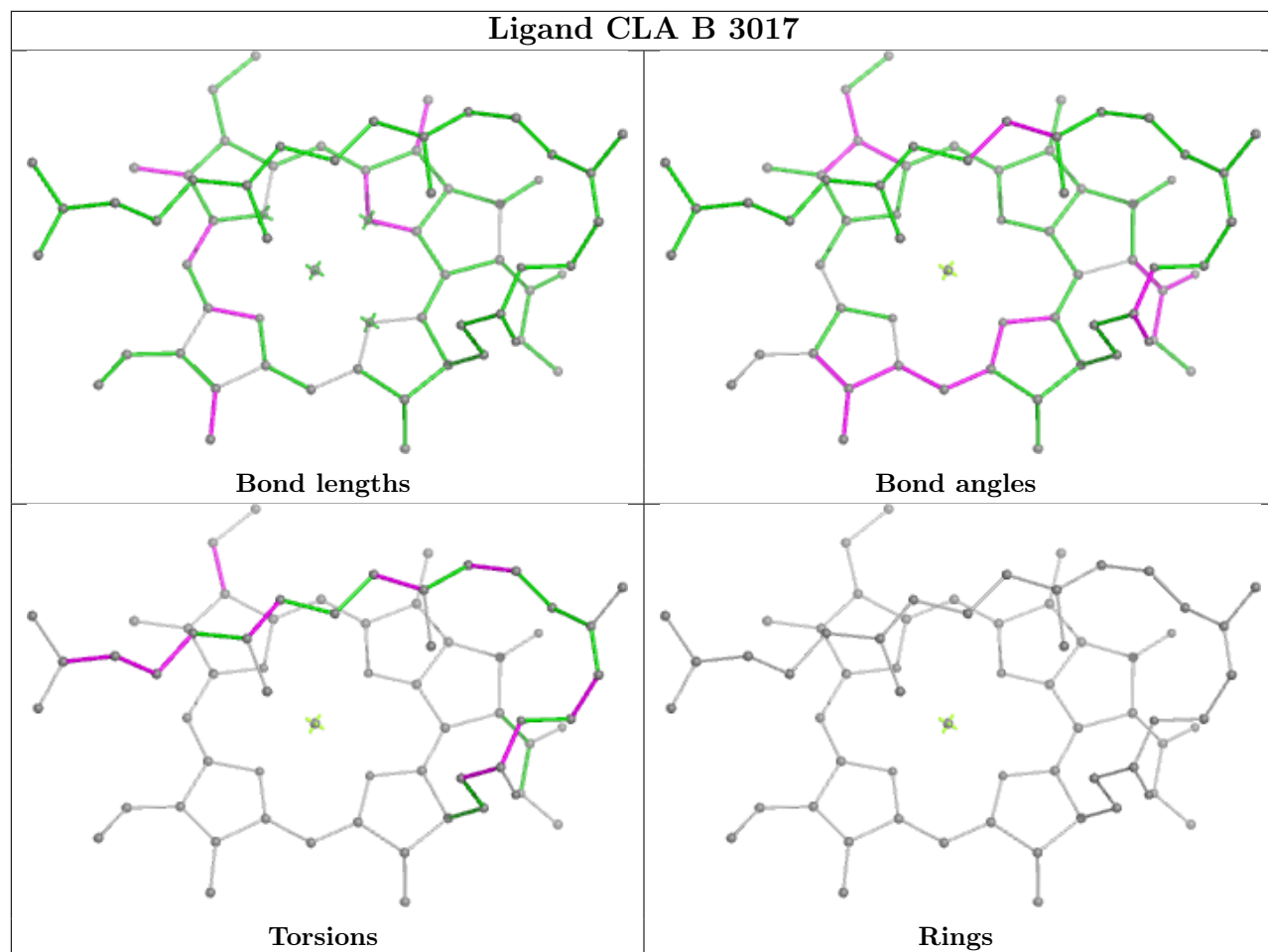
Ligand CLA j 1102



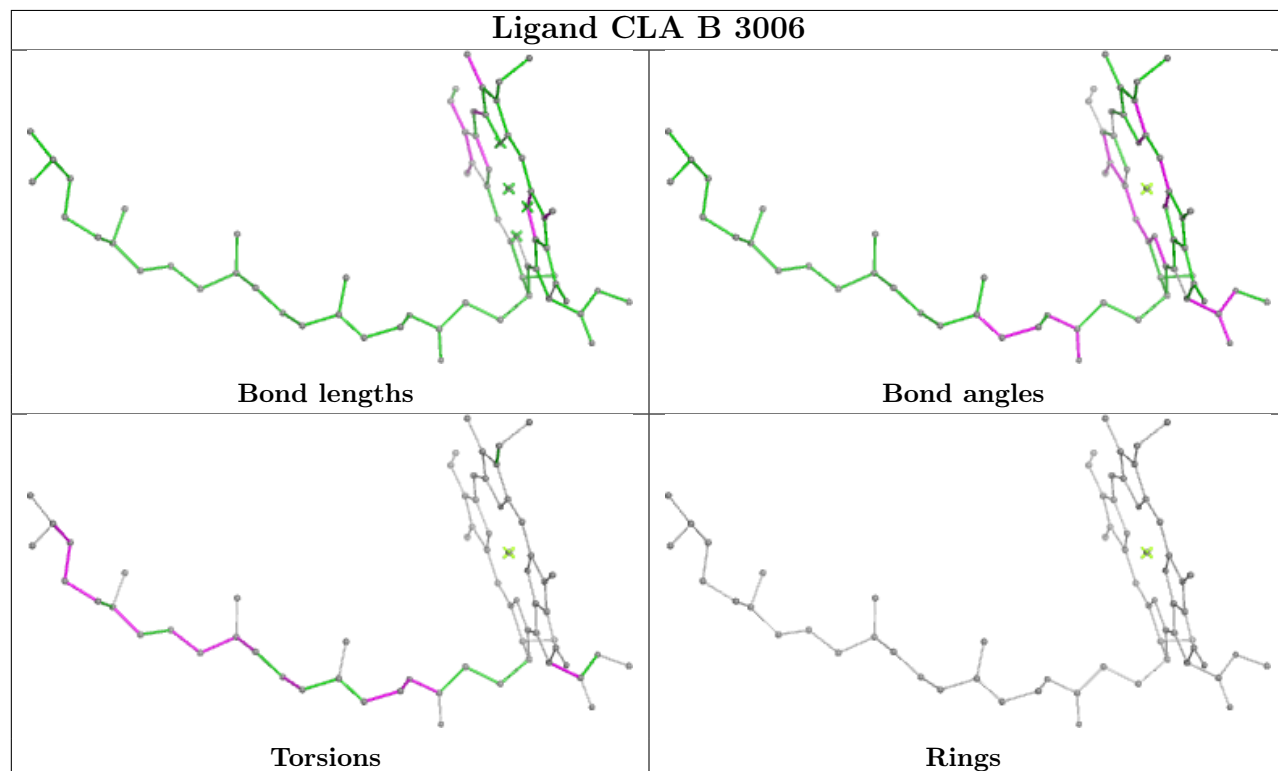


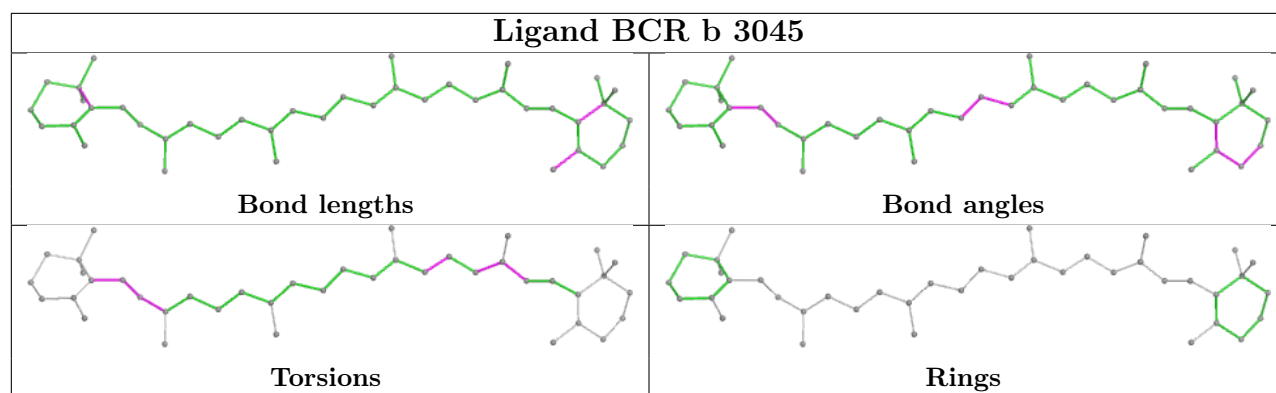
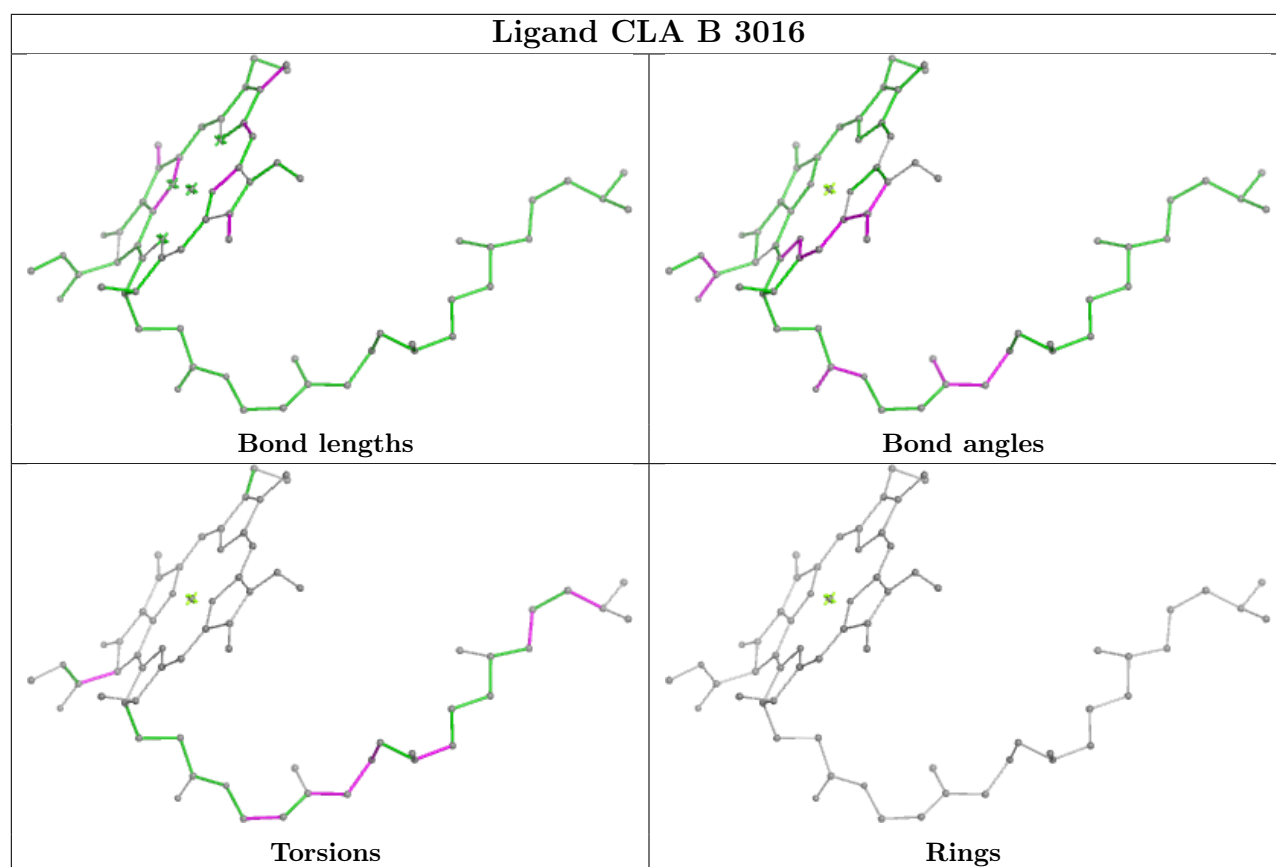


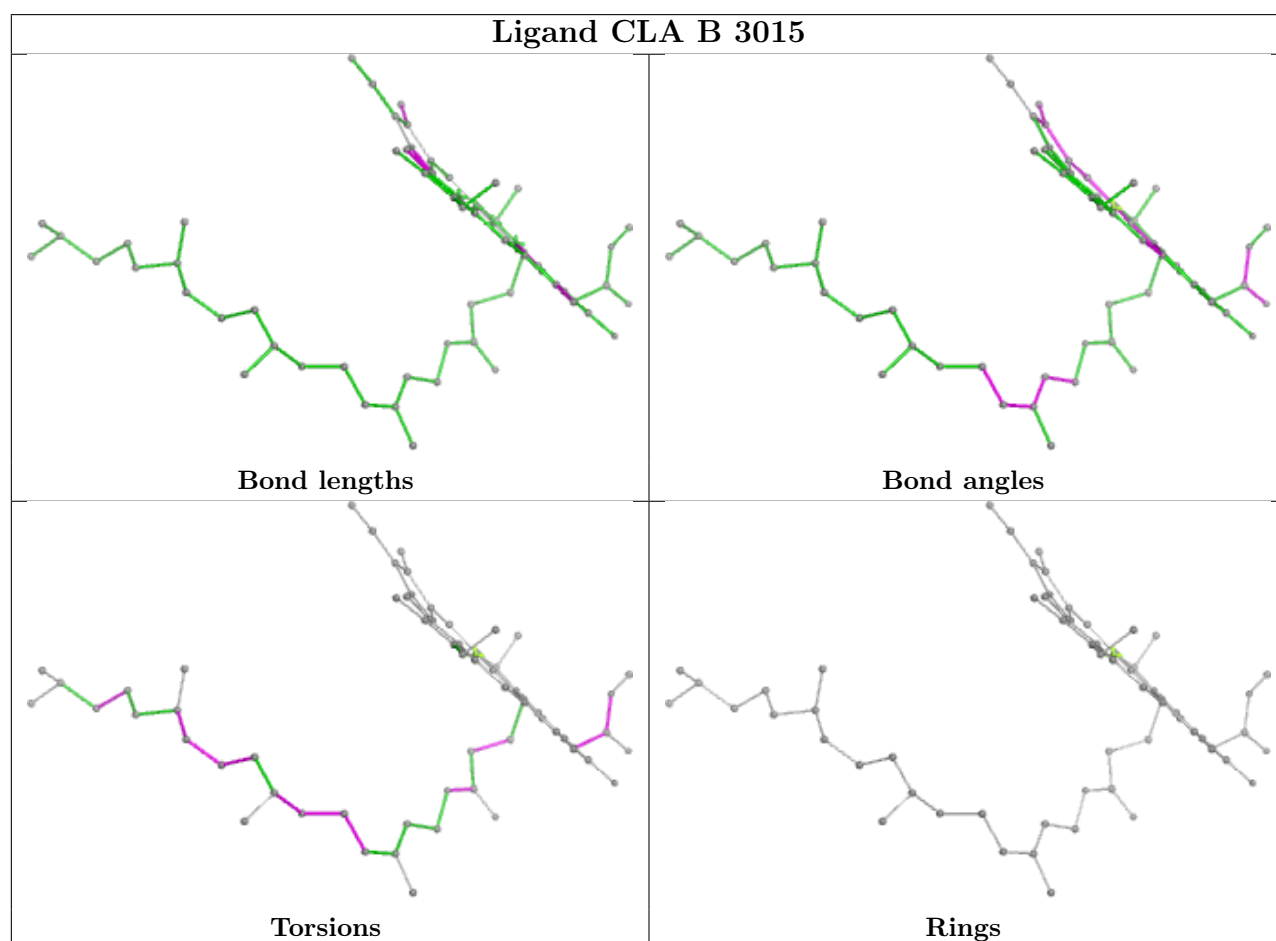
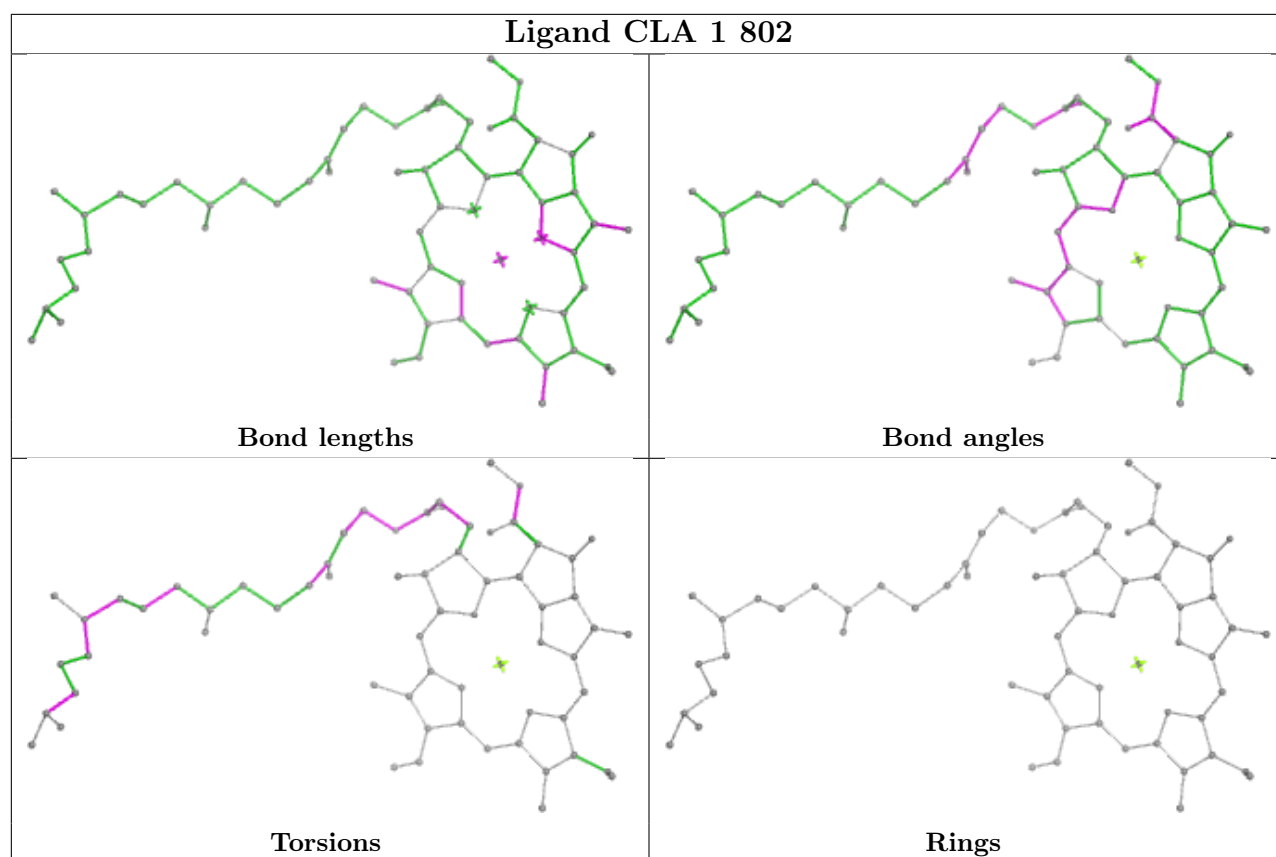
Ligand CLA B 3017

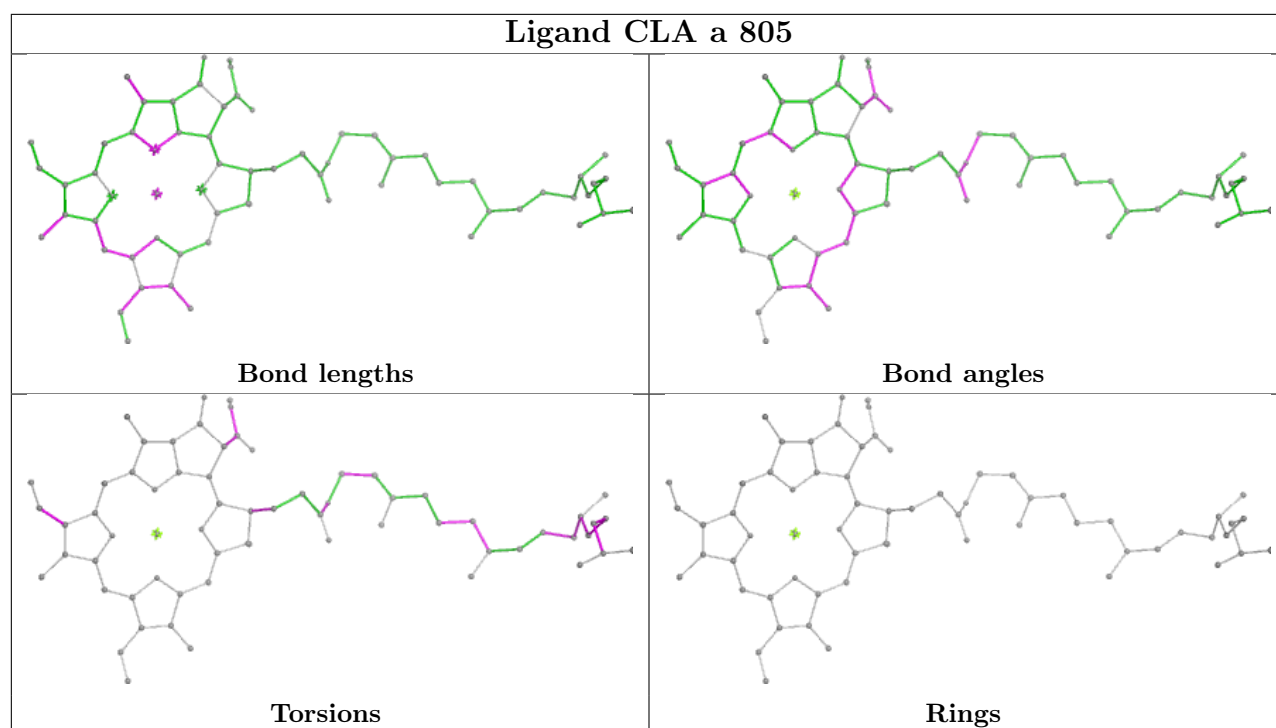


Ligand CLA B 3006

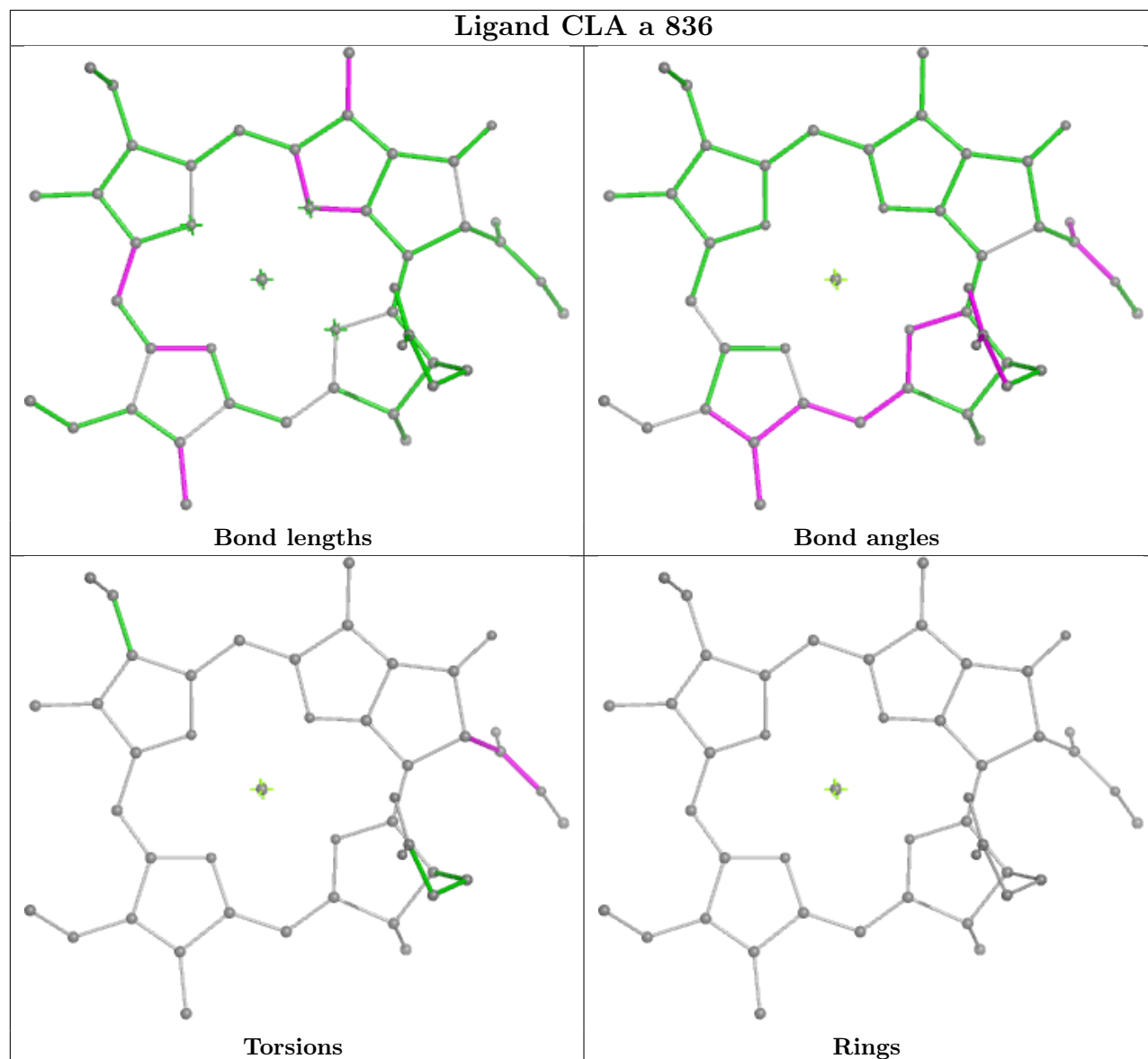


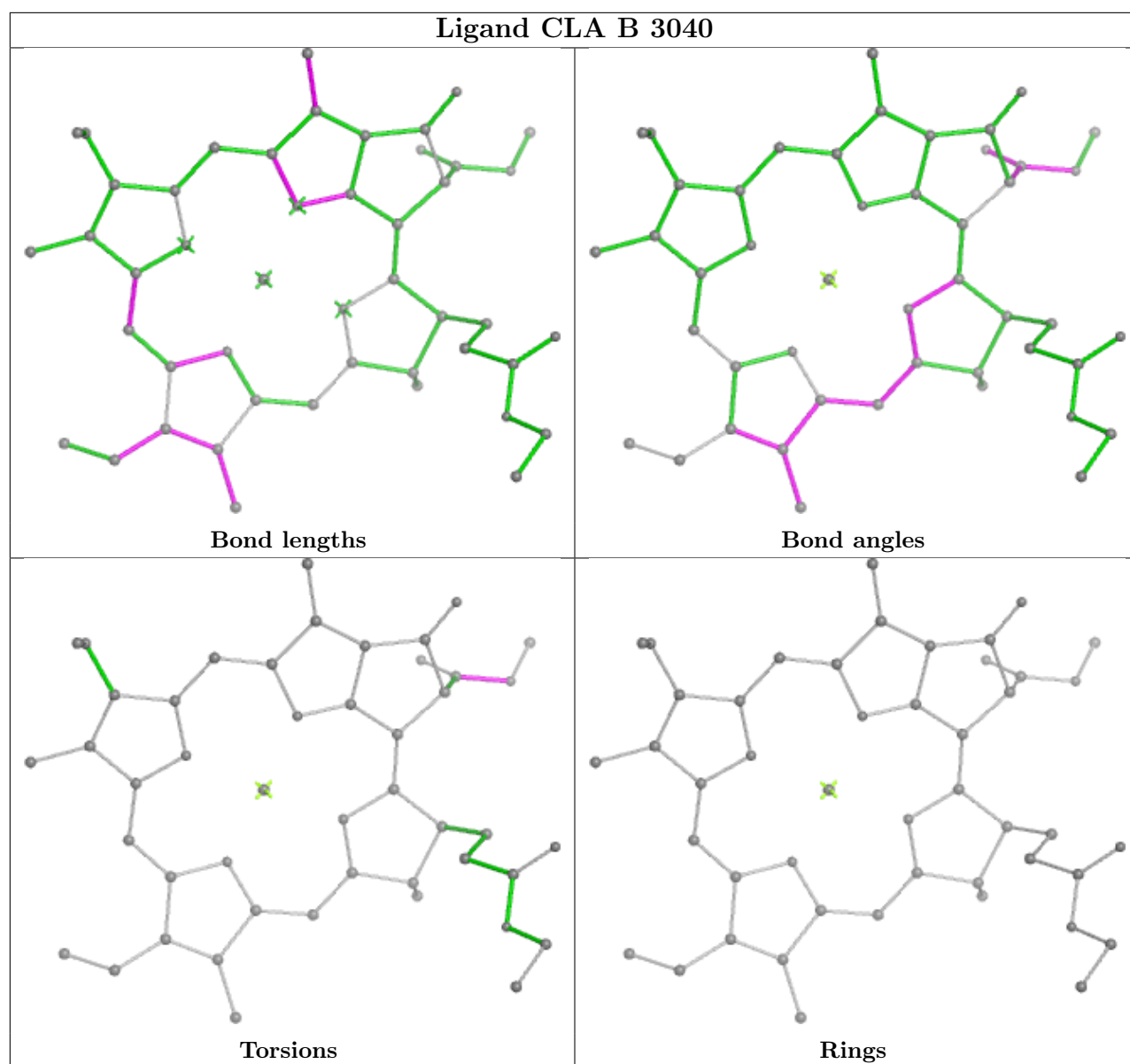


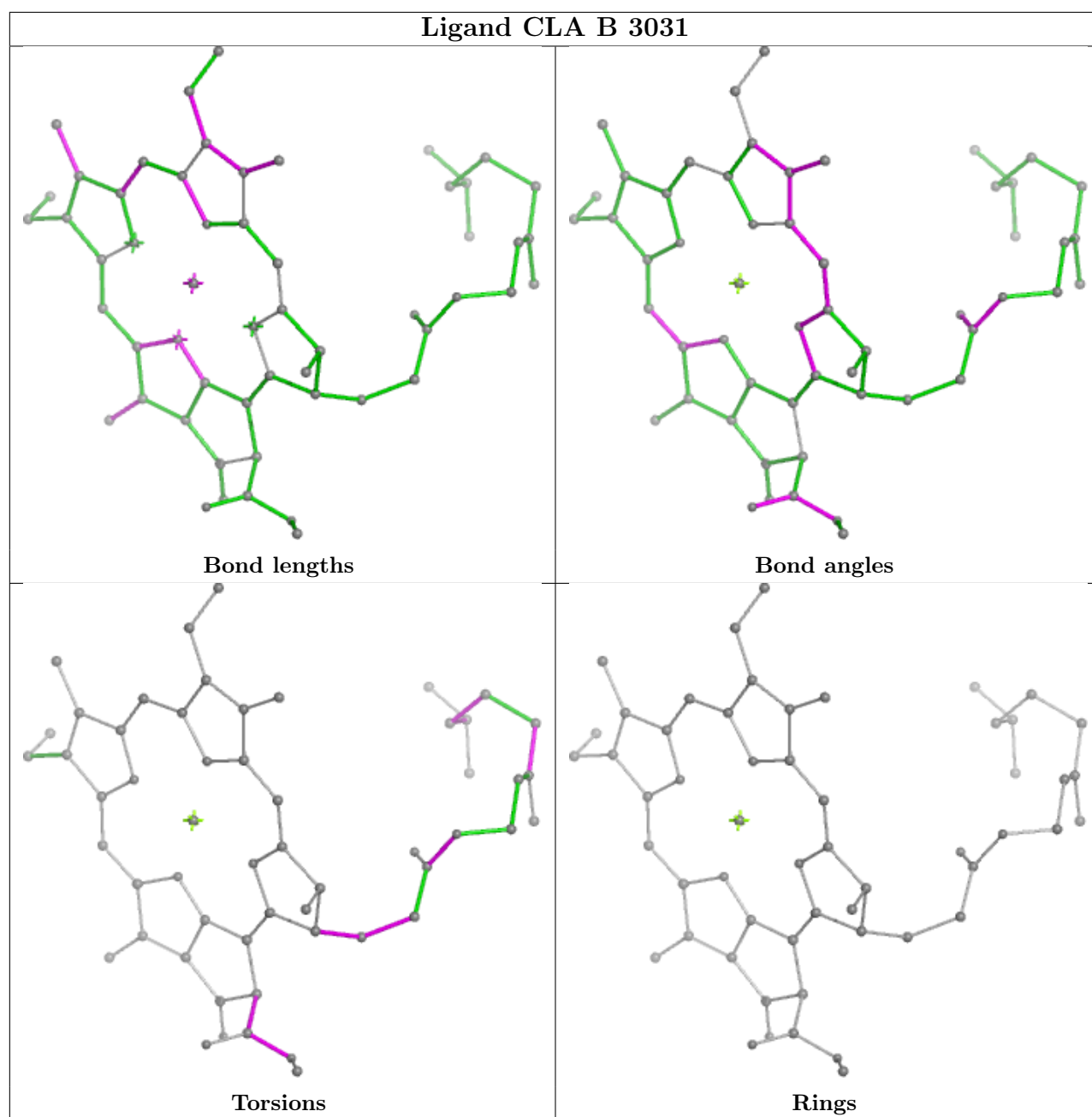


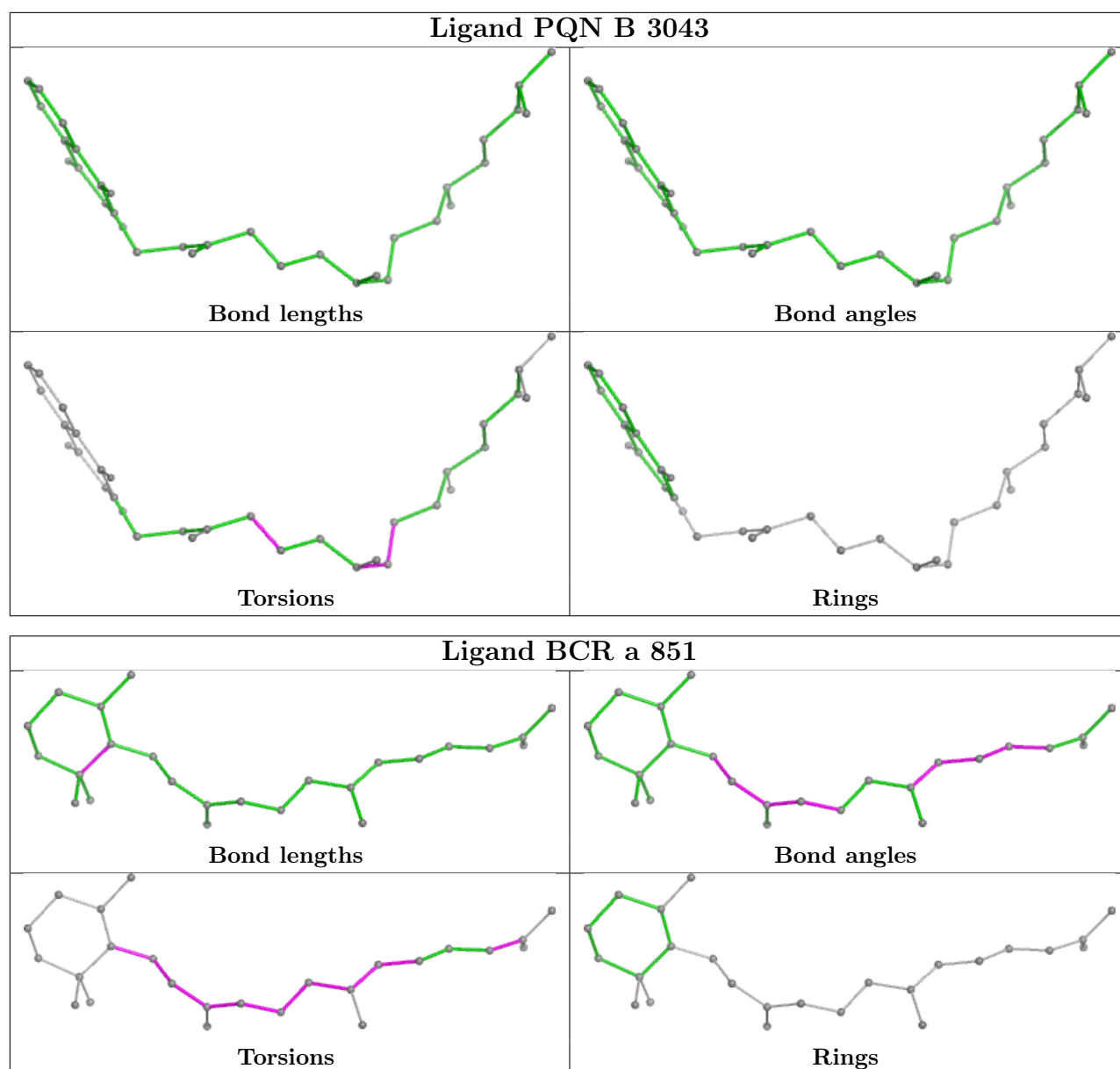


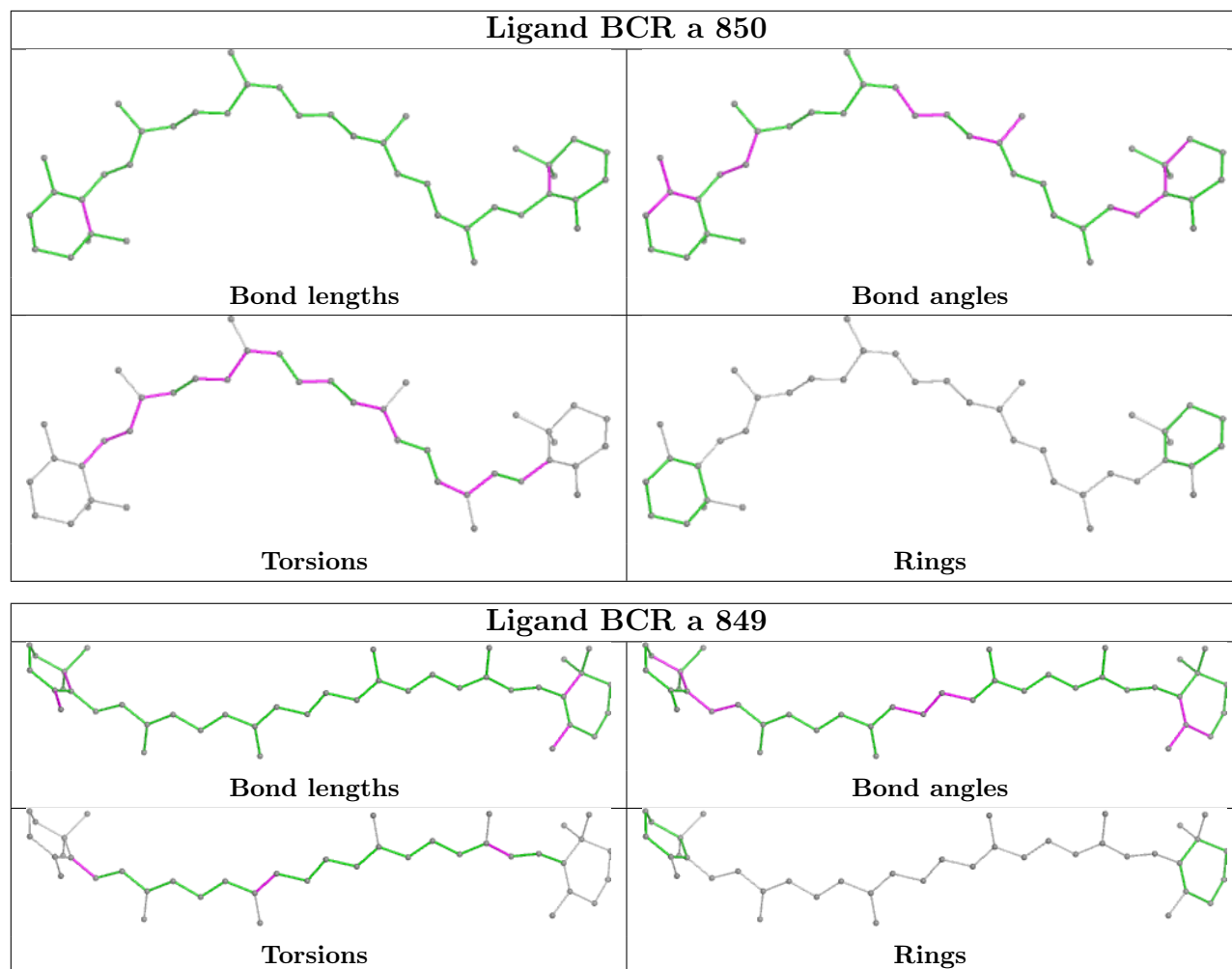
Ligand CLA a 836

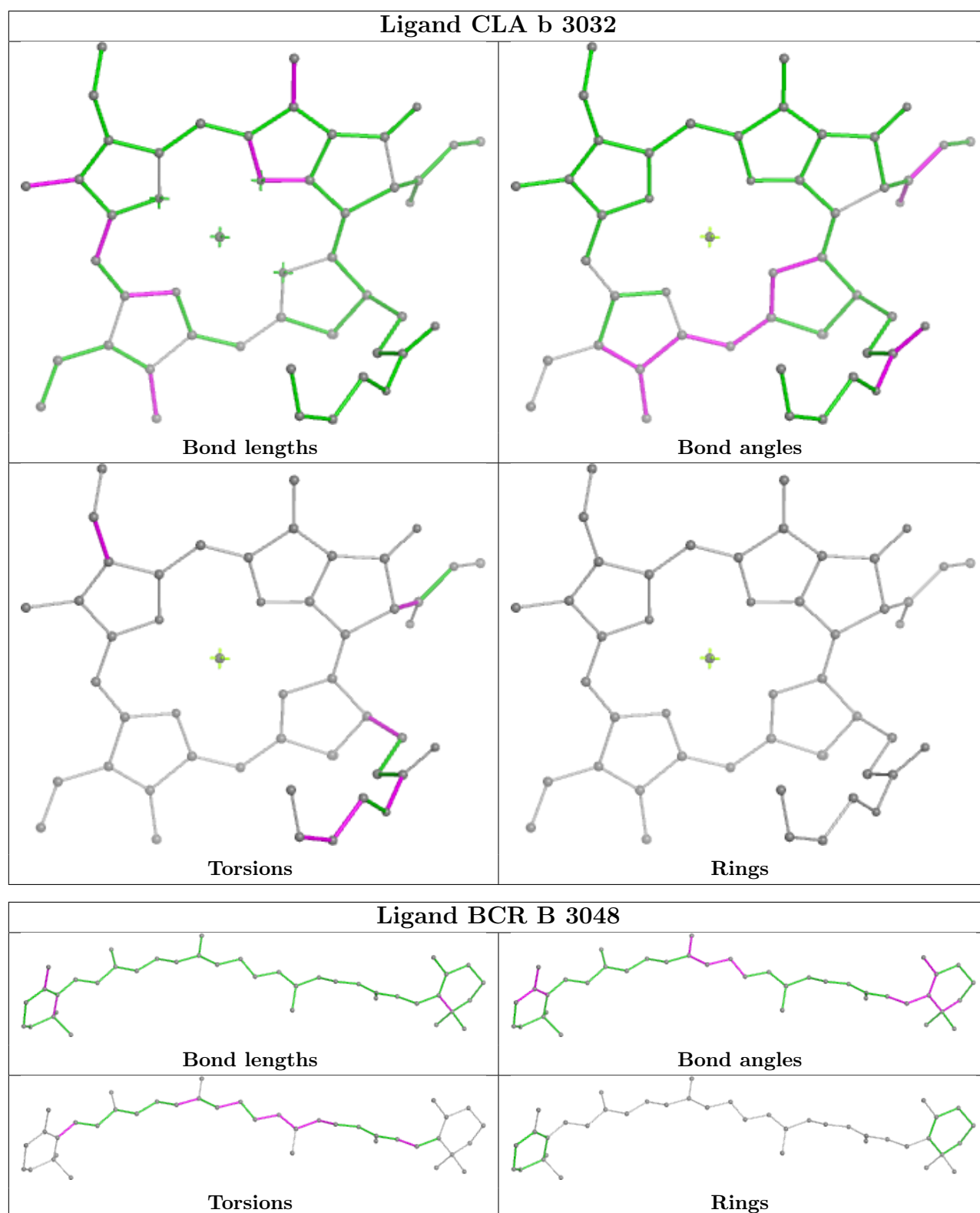


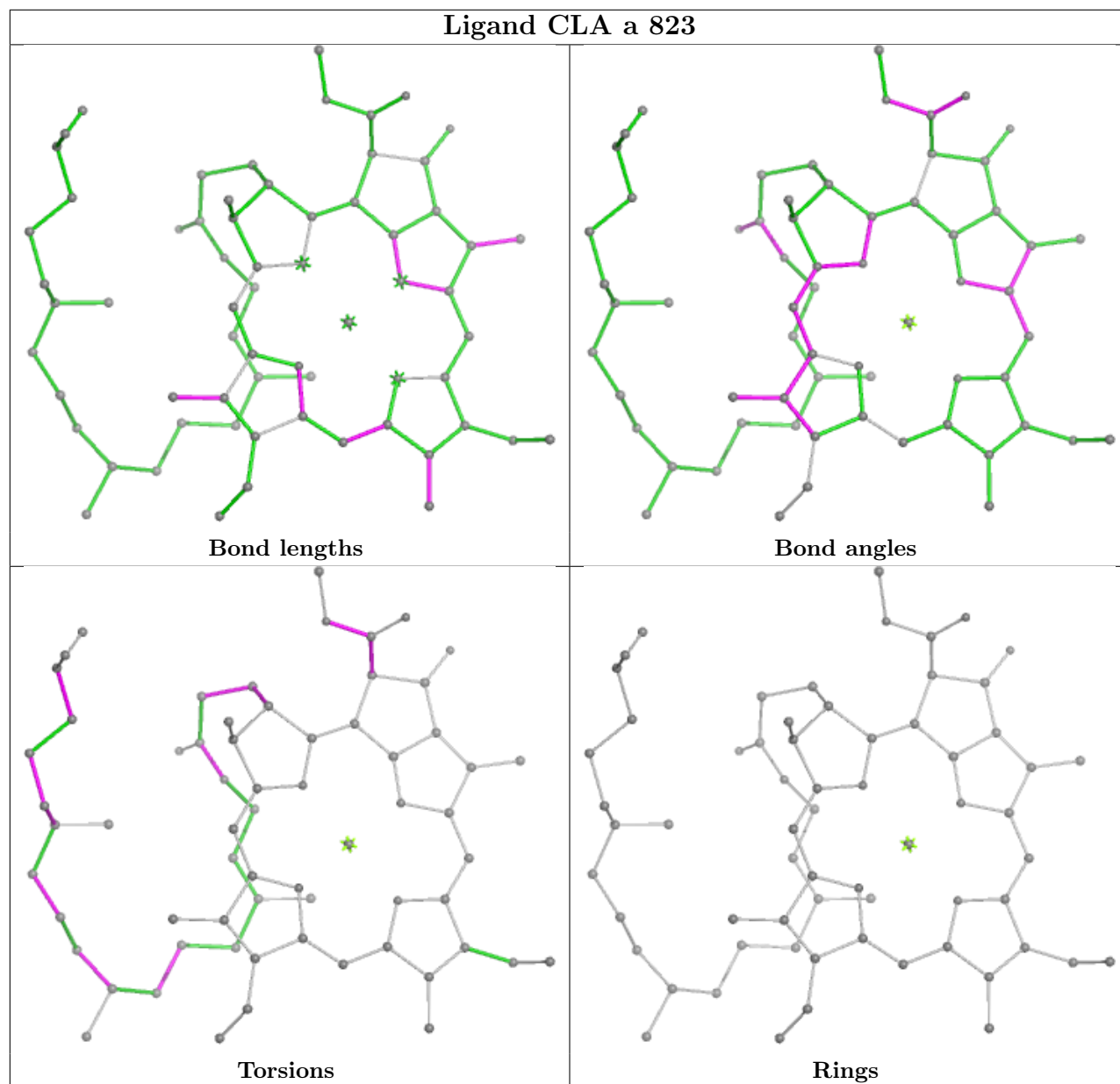
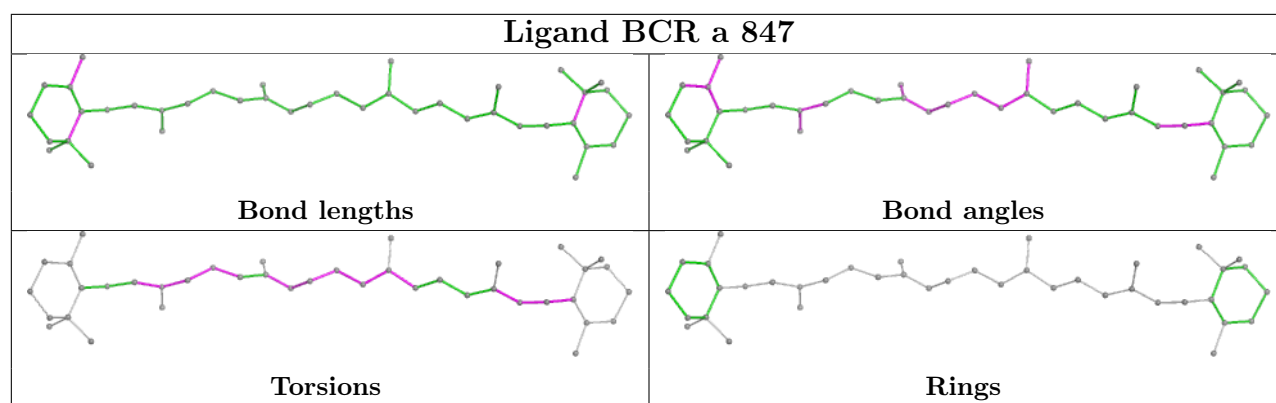


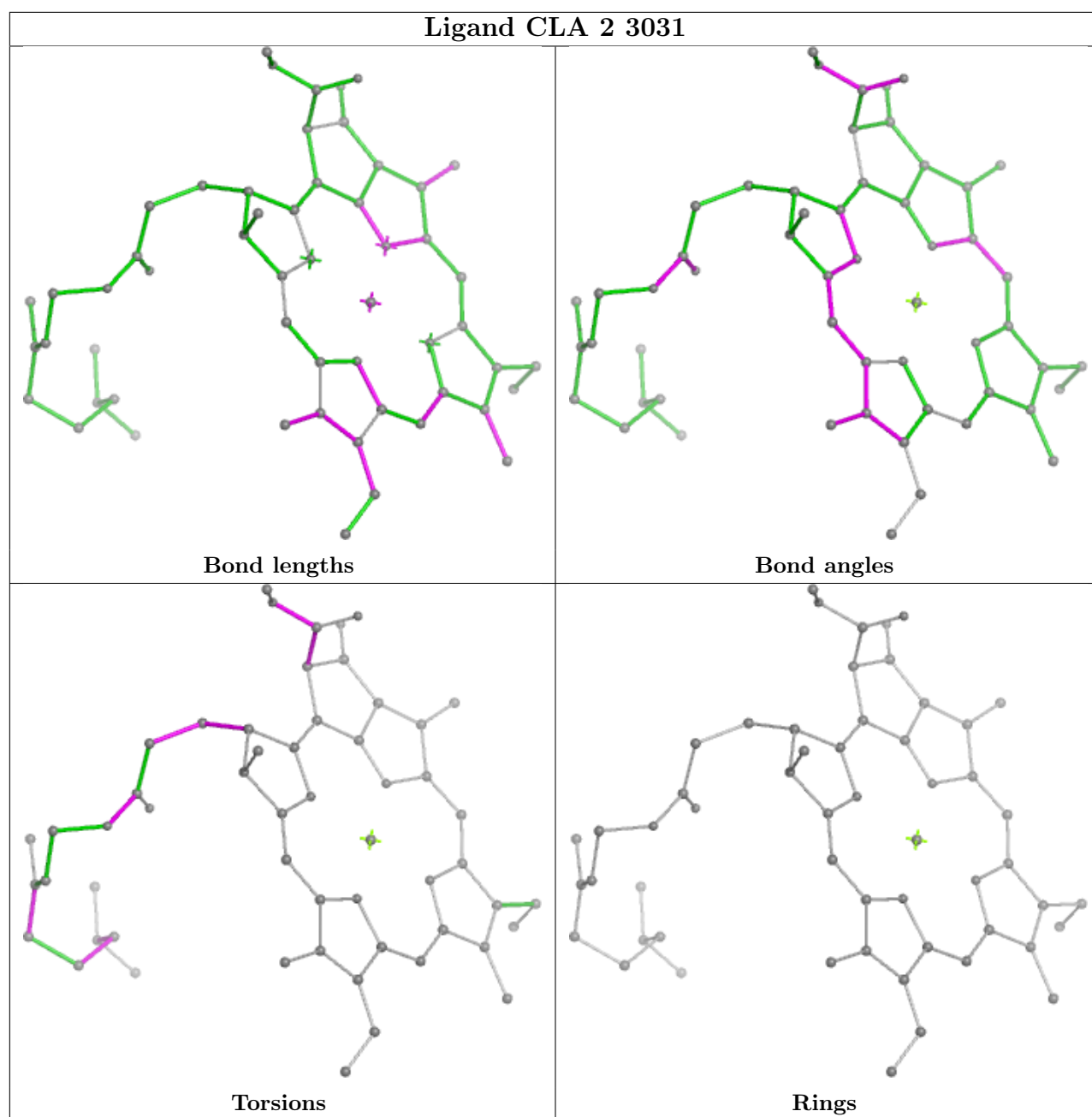


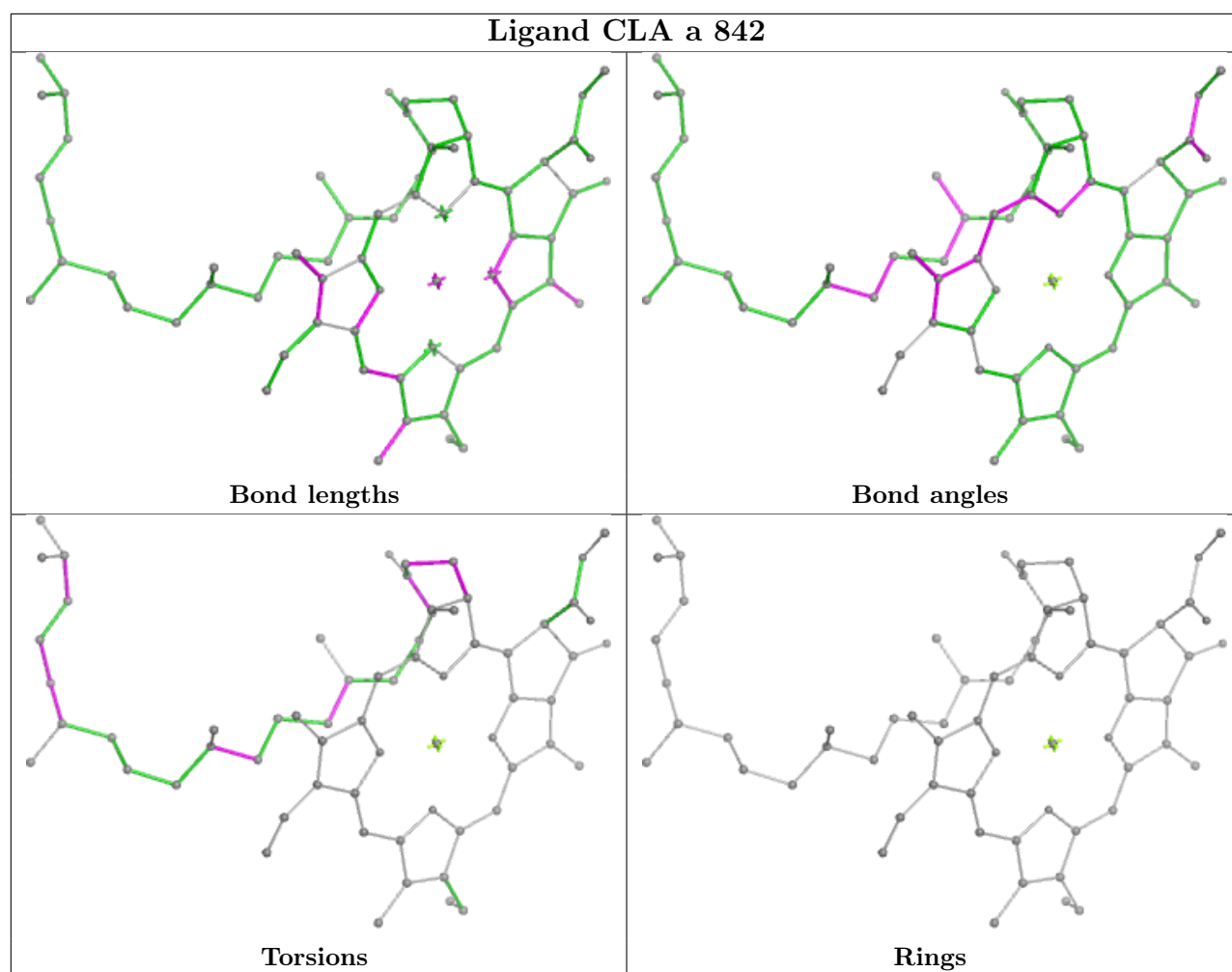


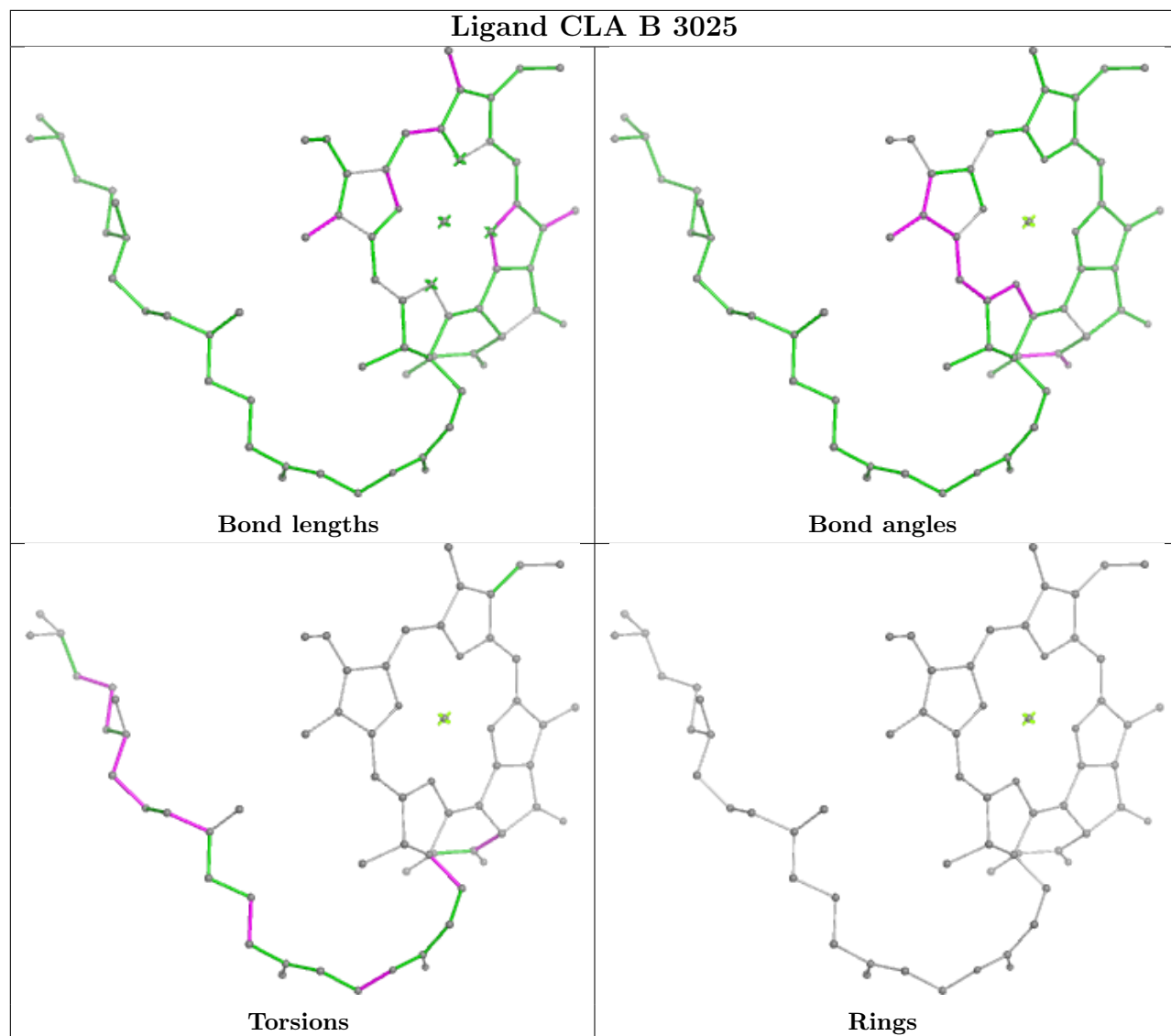


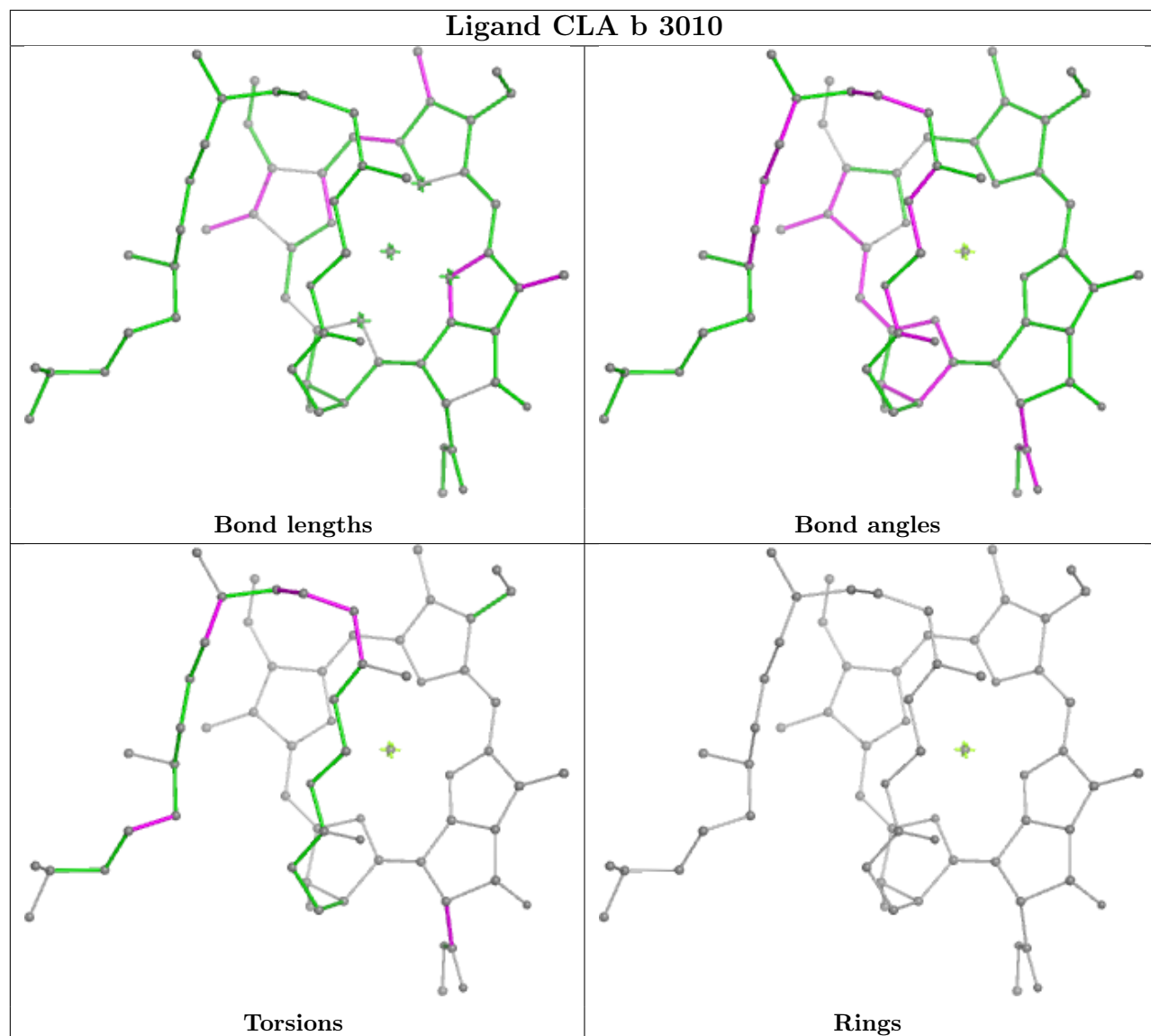


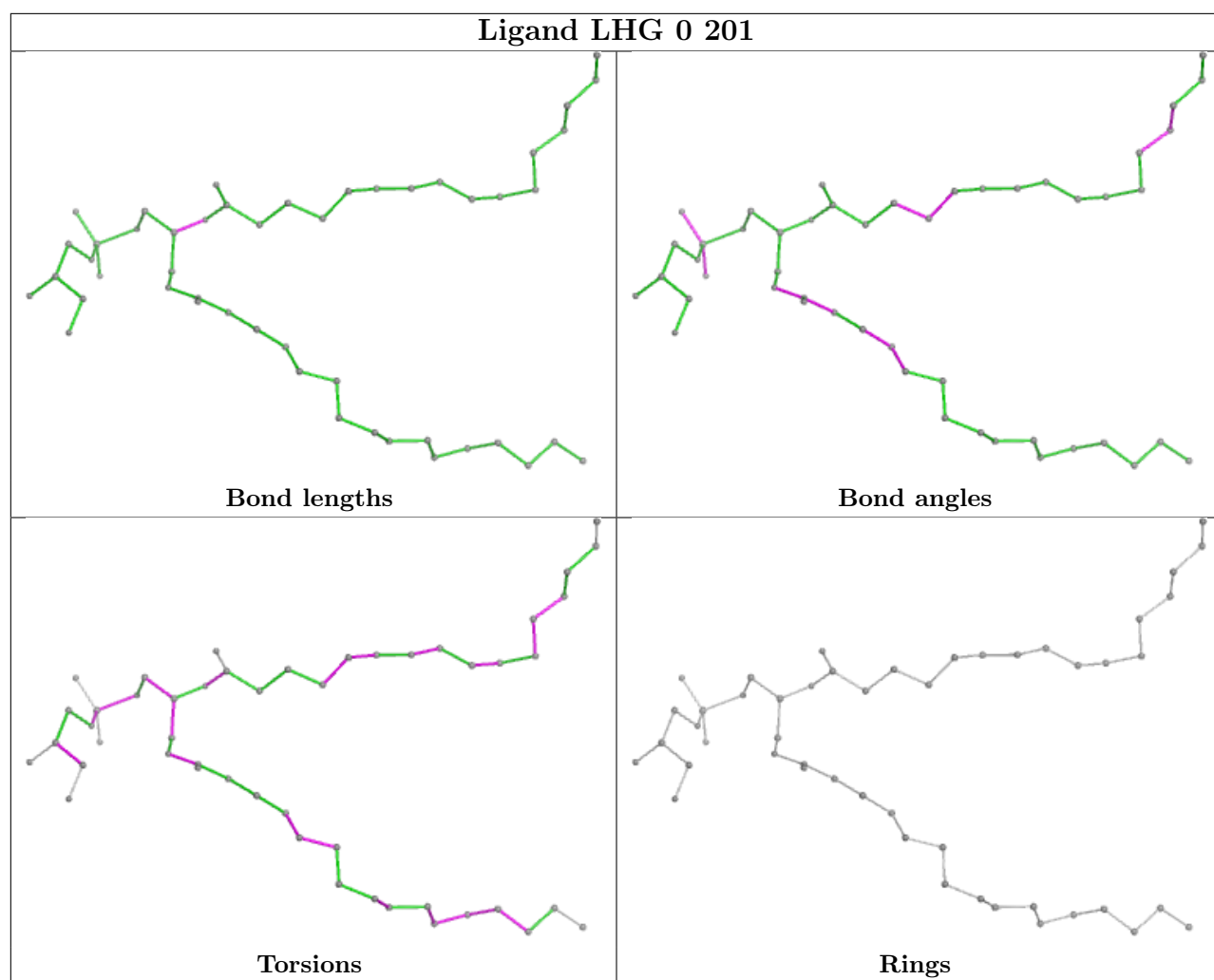


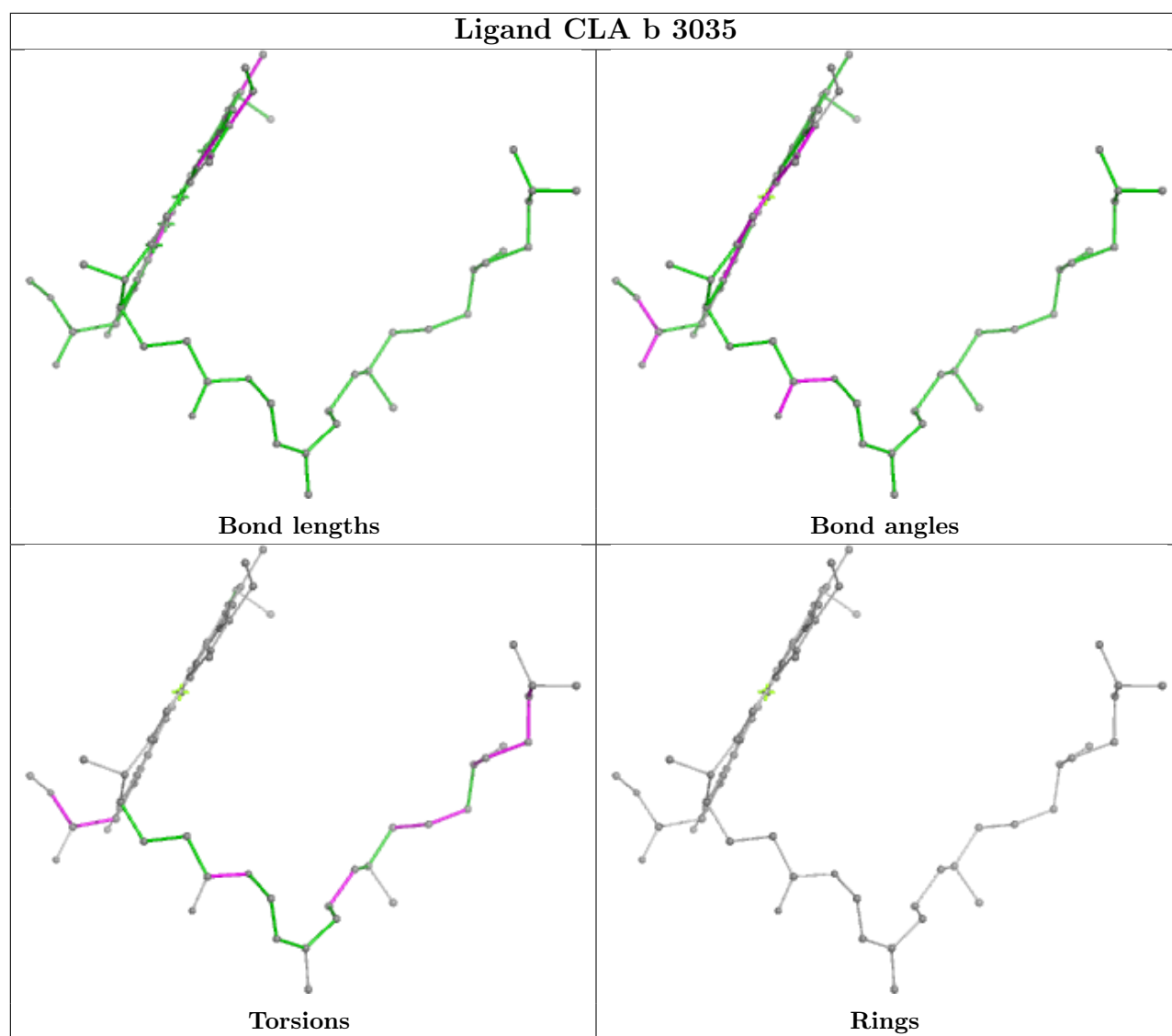




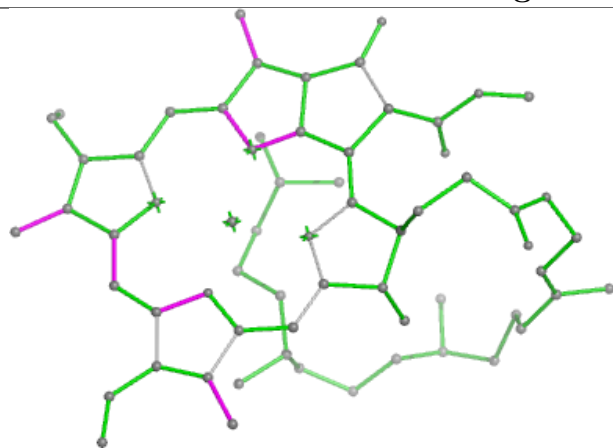




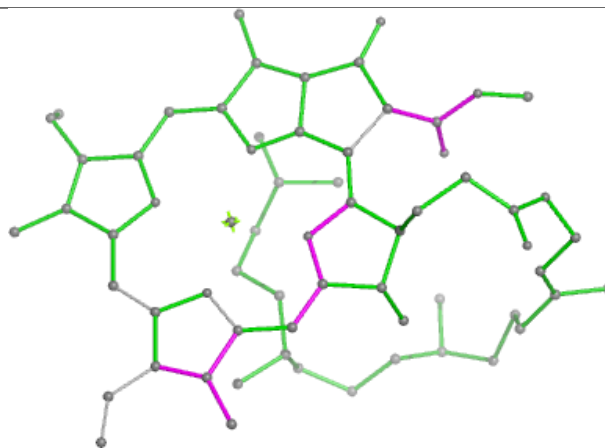




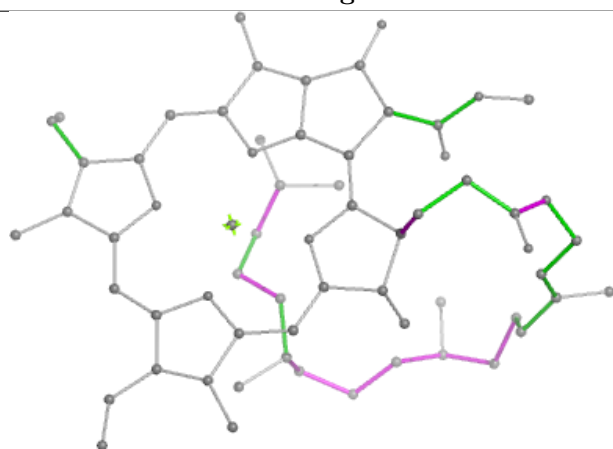
Ligand CLA A 807



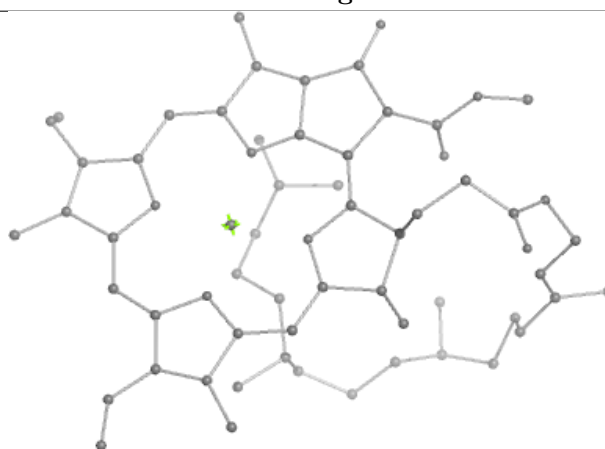
Bond lengths



Bond angles

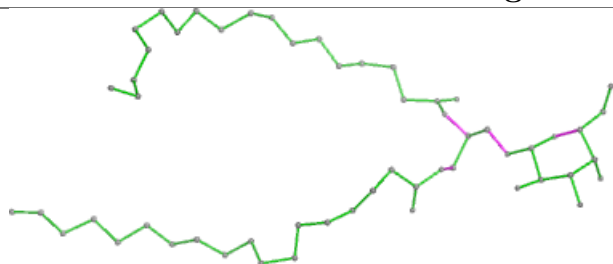


Torsions

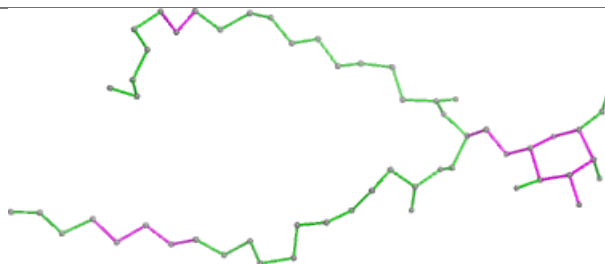


Rings

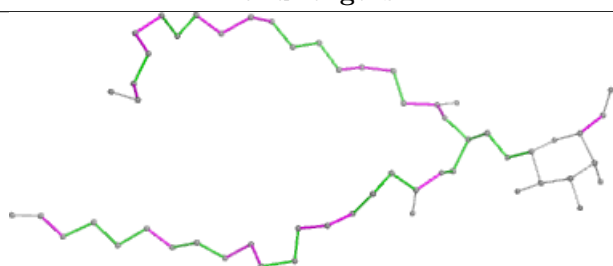
Ligand LMG 2 3050



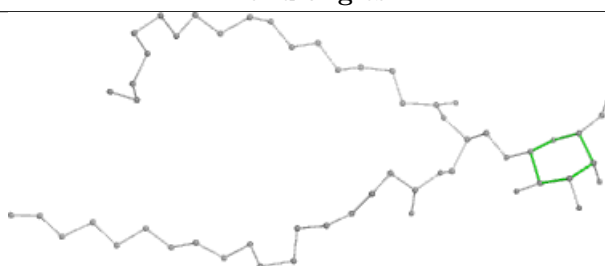
Bond lengths



Bond angles

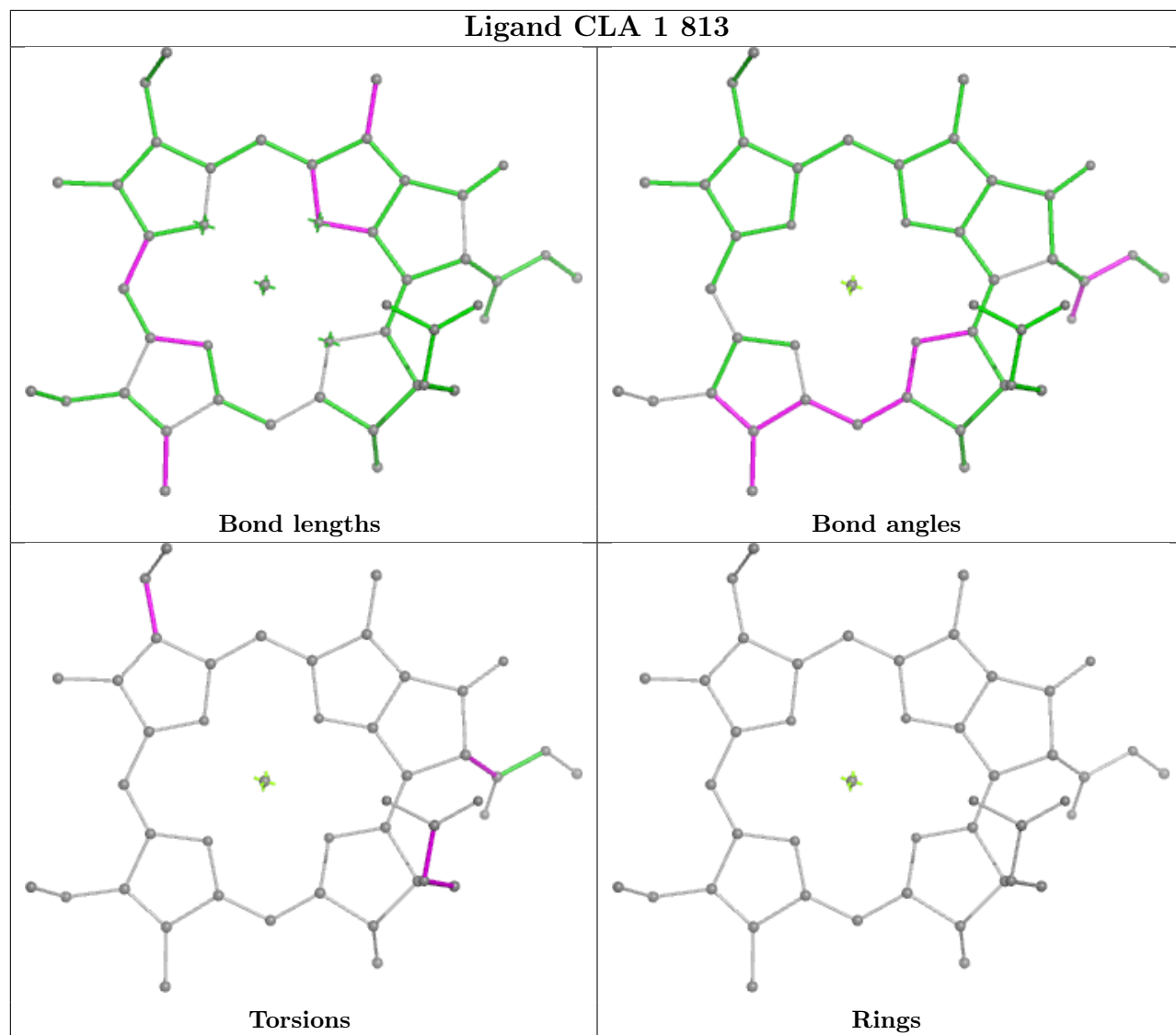


Torsions

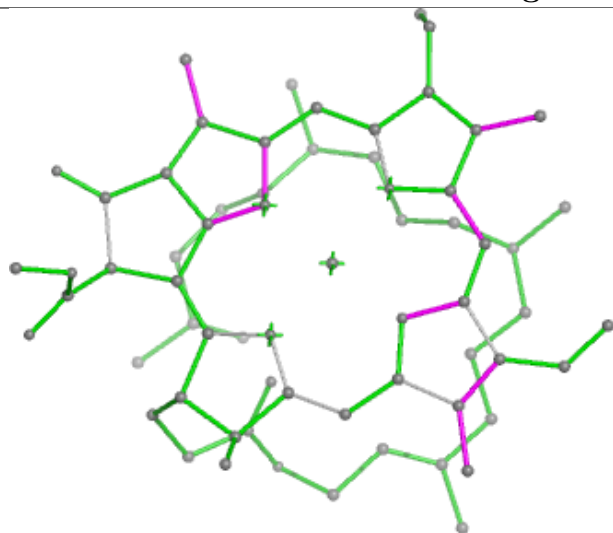


Rings

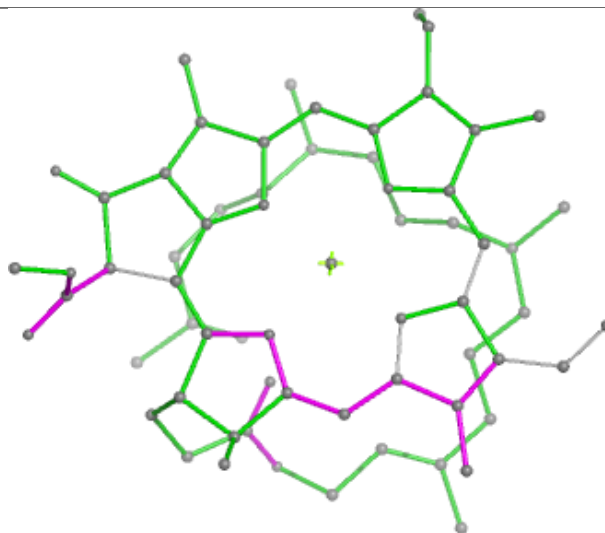
Ligand CLA 1 813



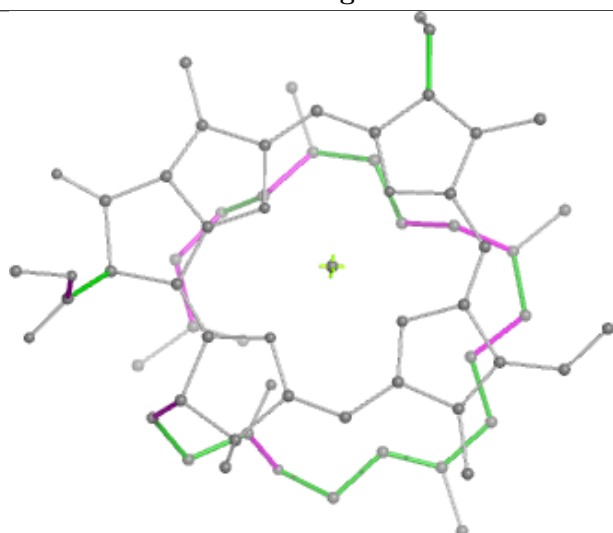
Ligand CLA 1 206



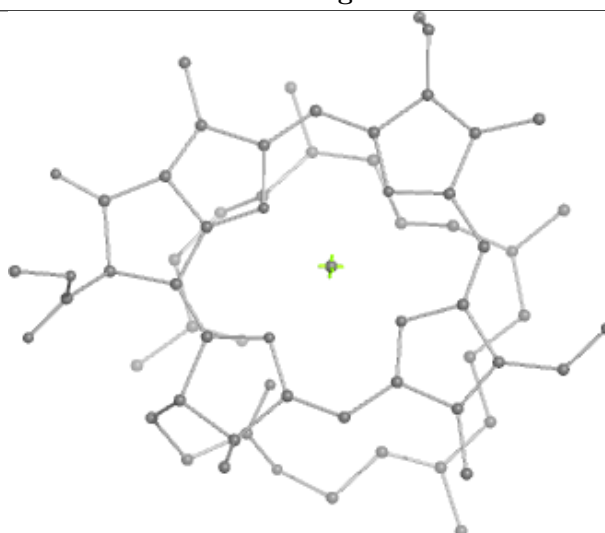
Bond lengths



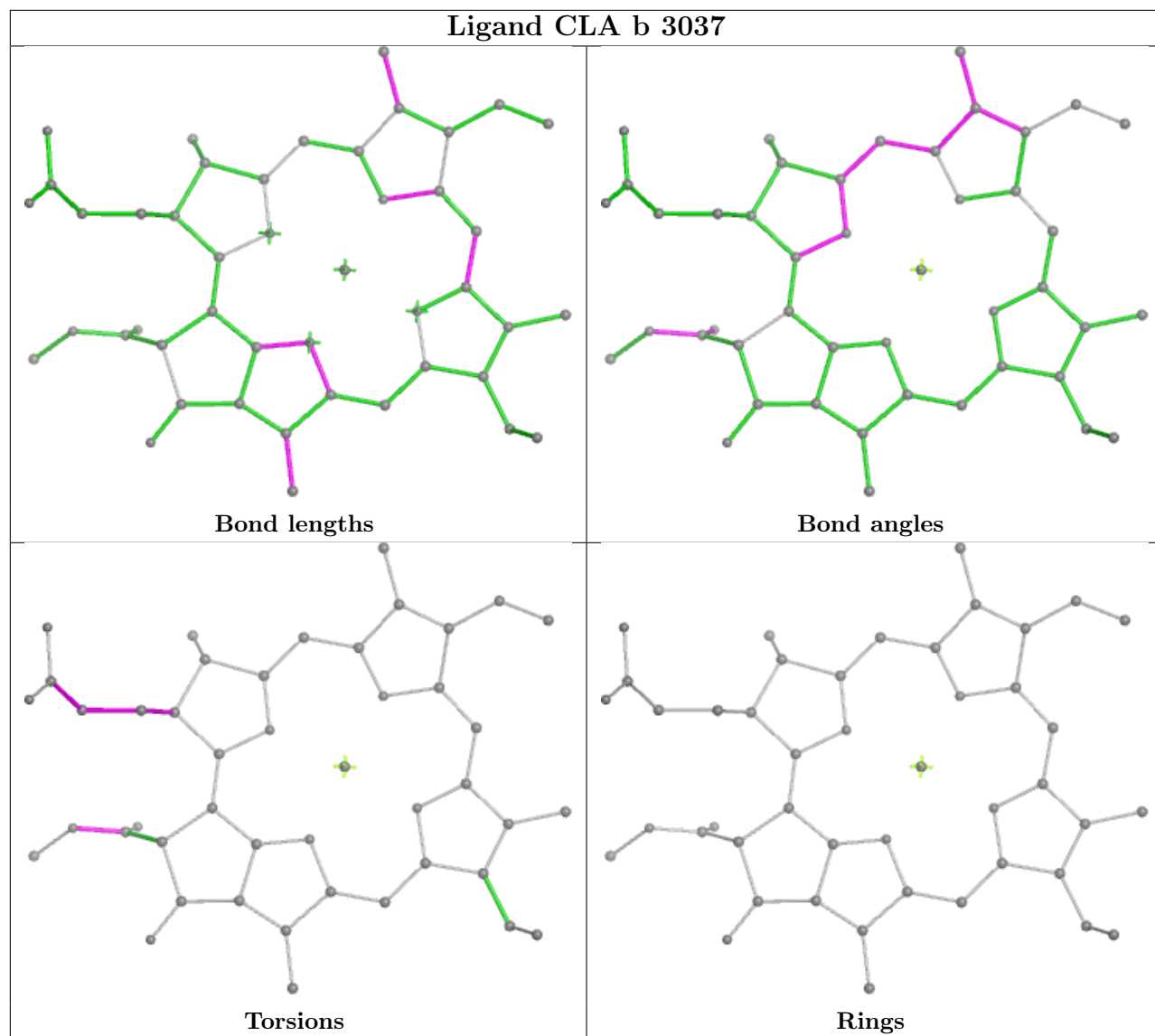
Bond angles



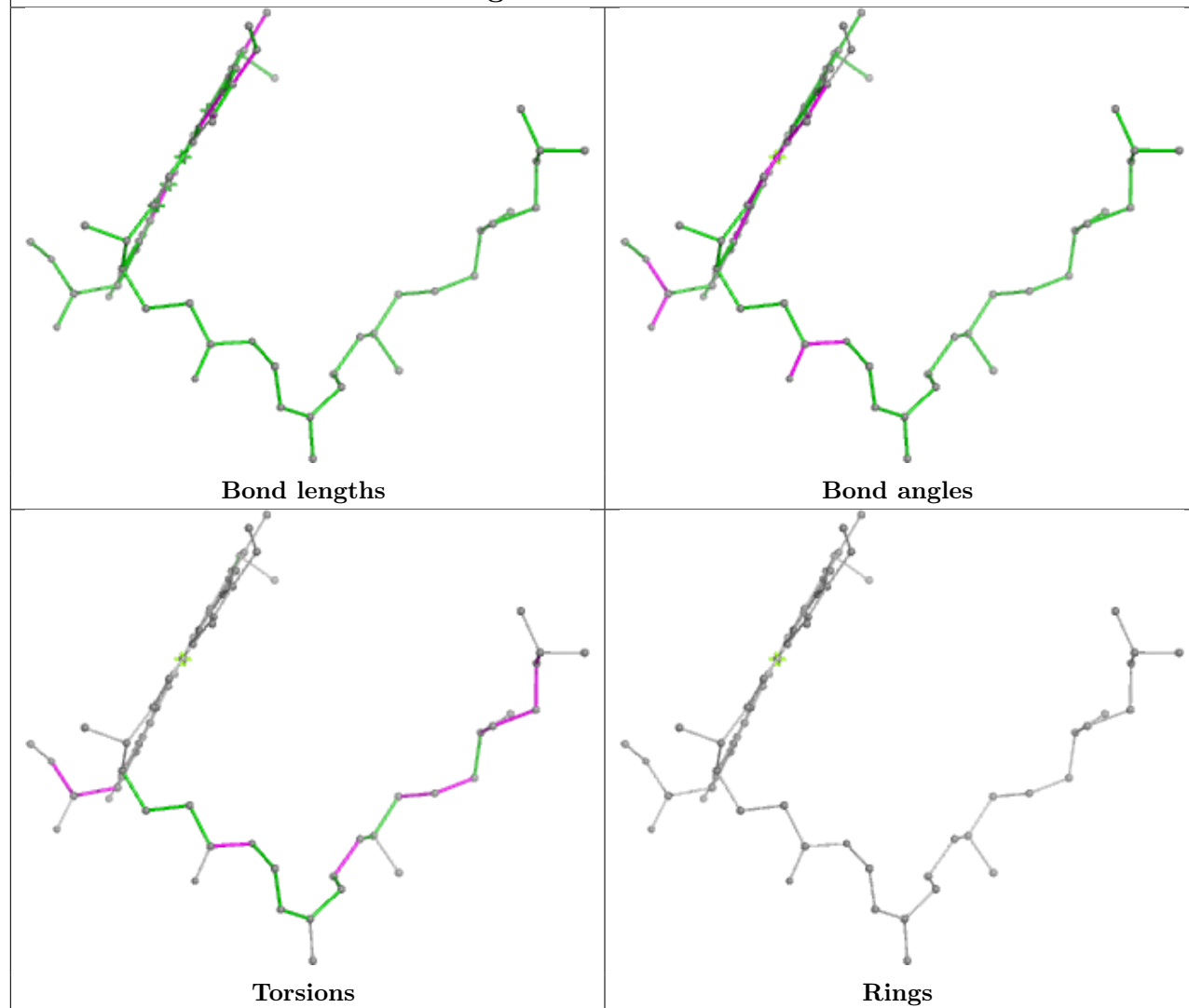
Torsions



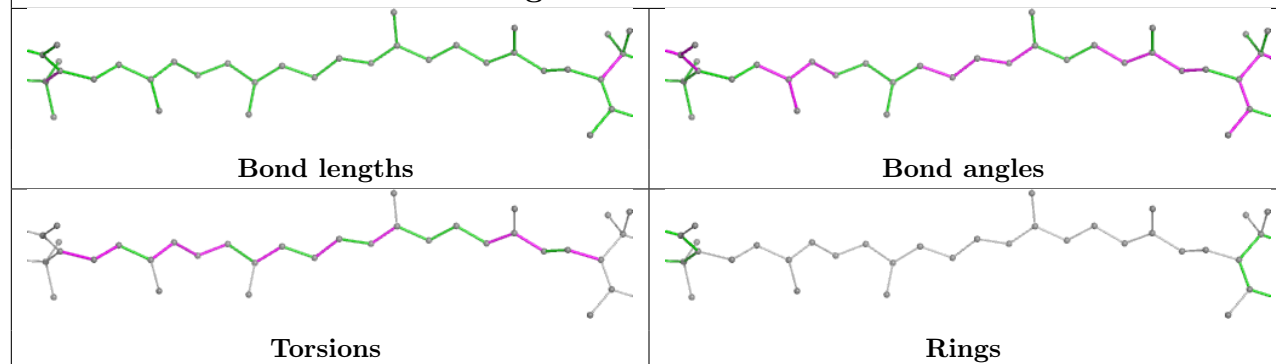
Rings



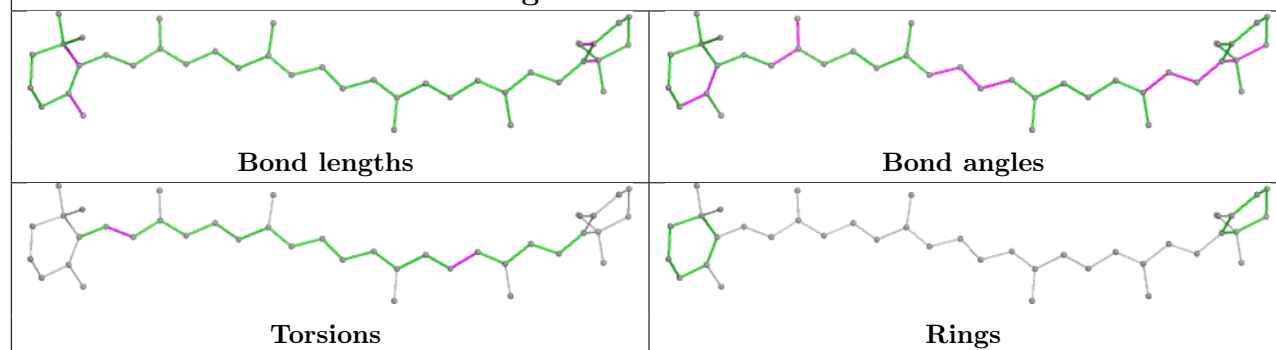
Ligand CLA B 3035



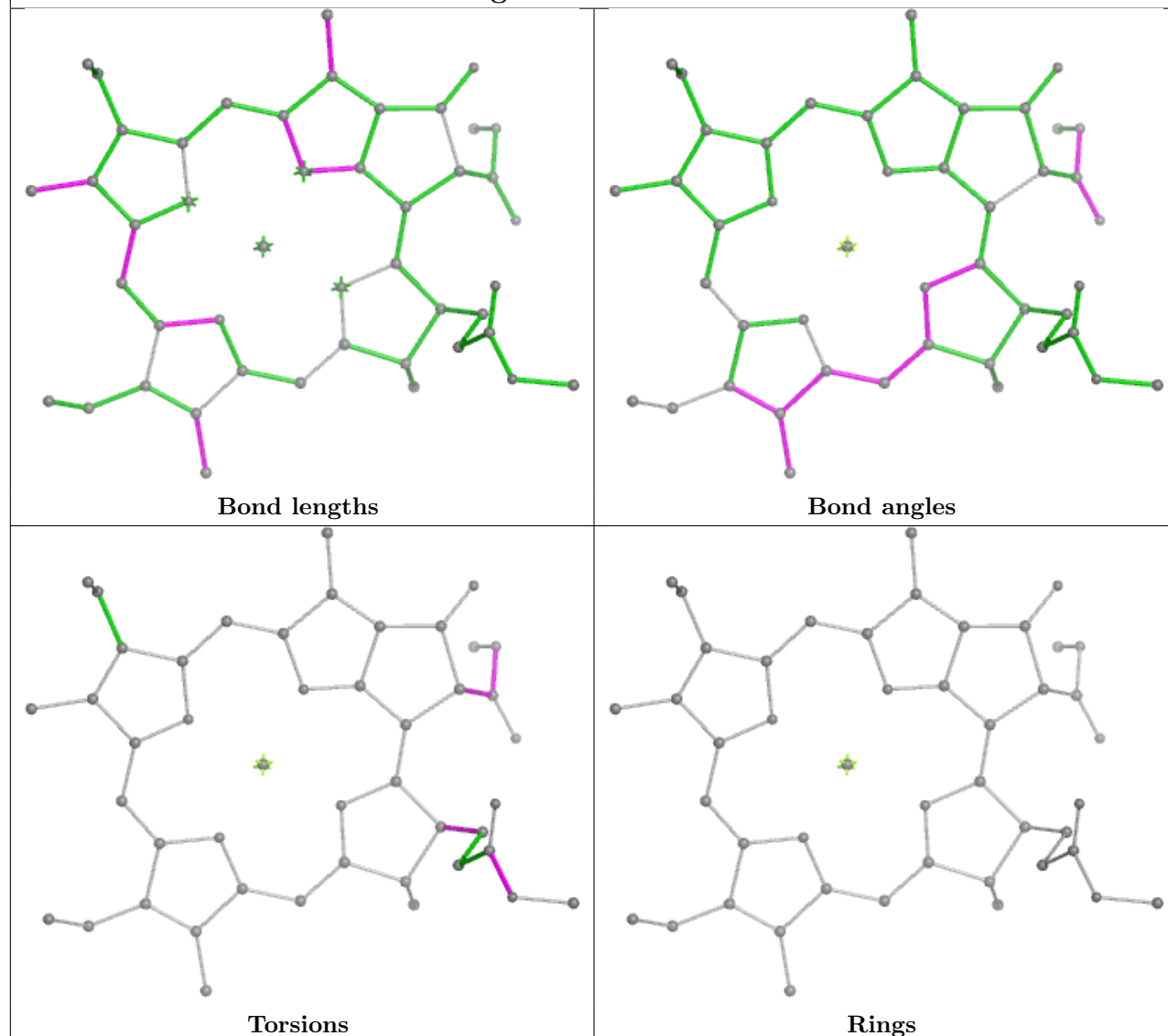
Ligand BCR 2 3052

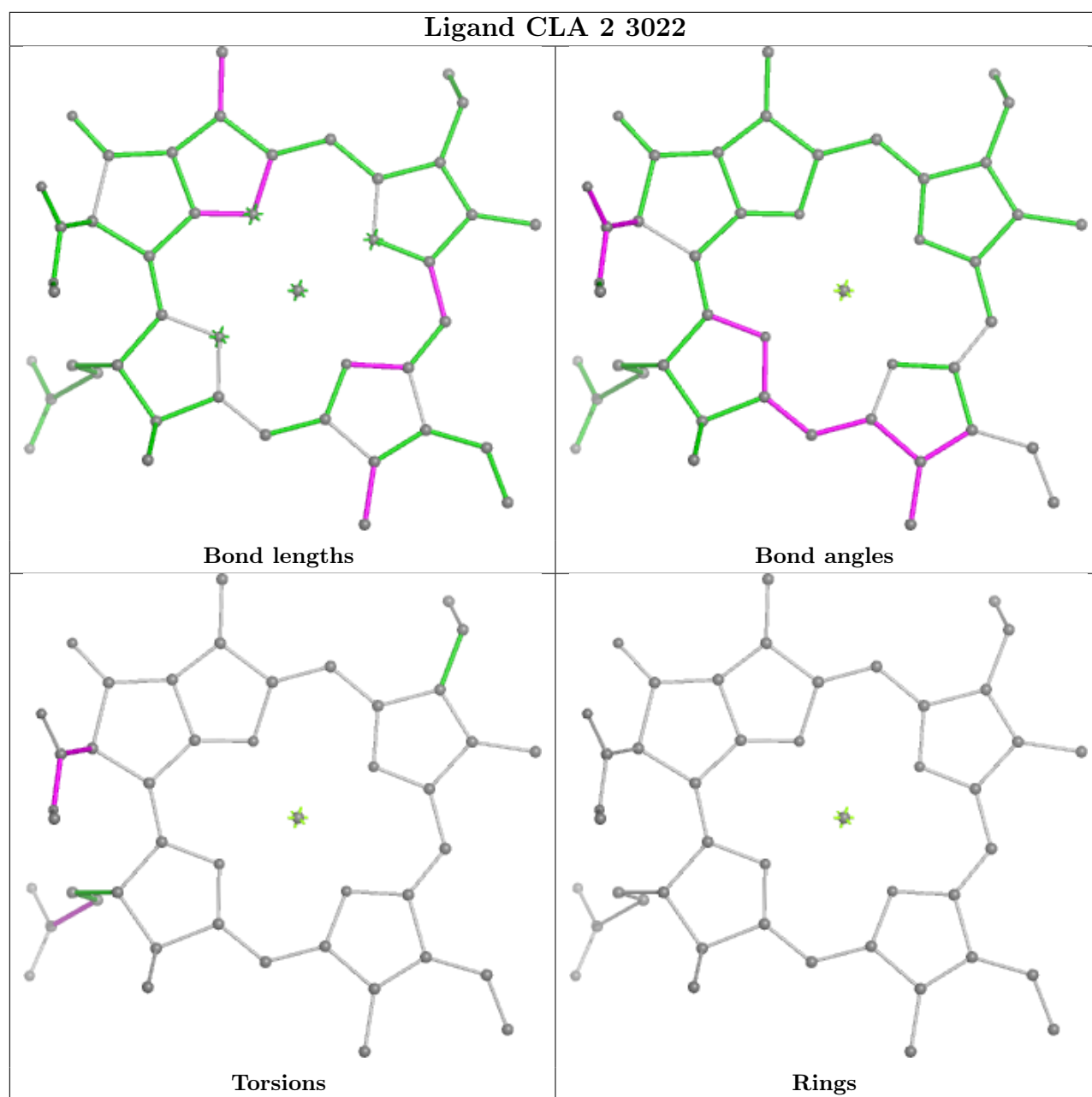


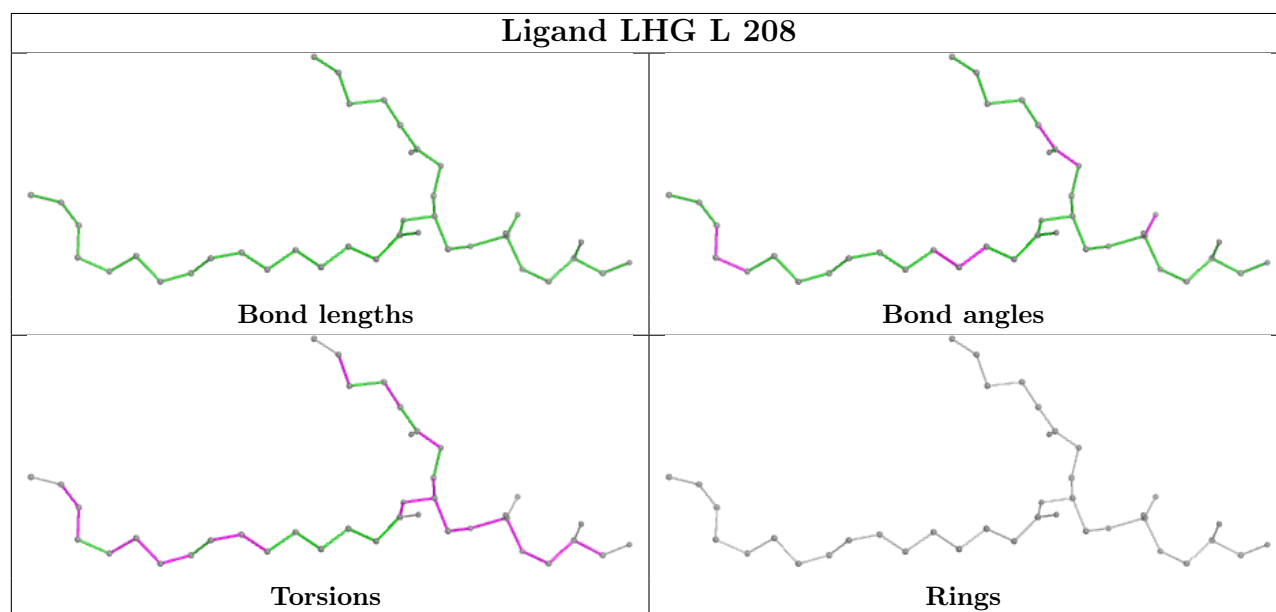
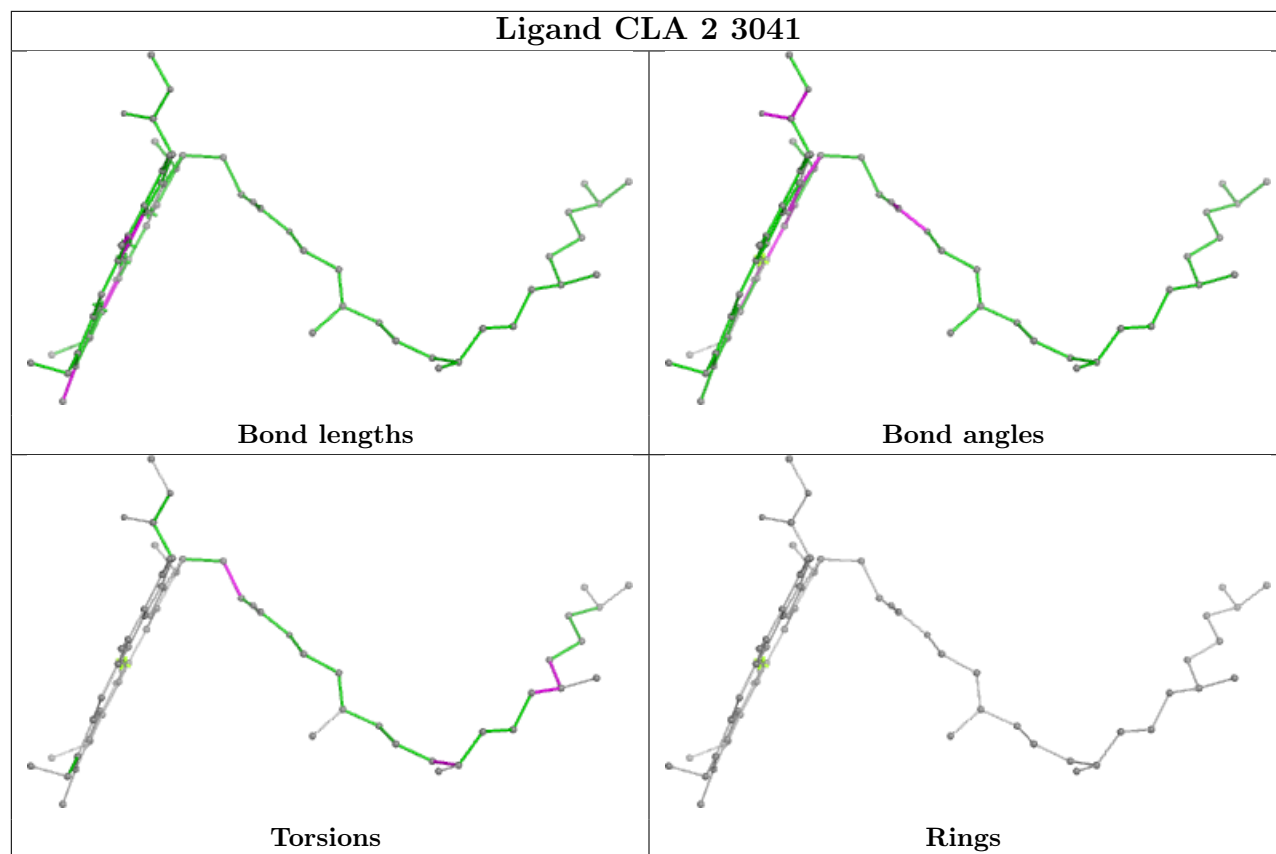
Ligand BCR B 3049

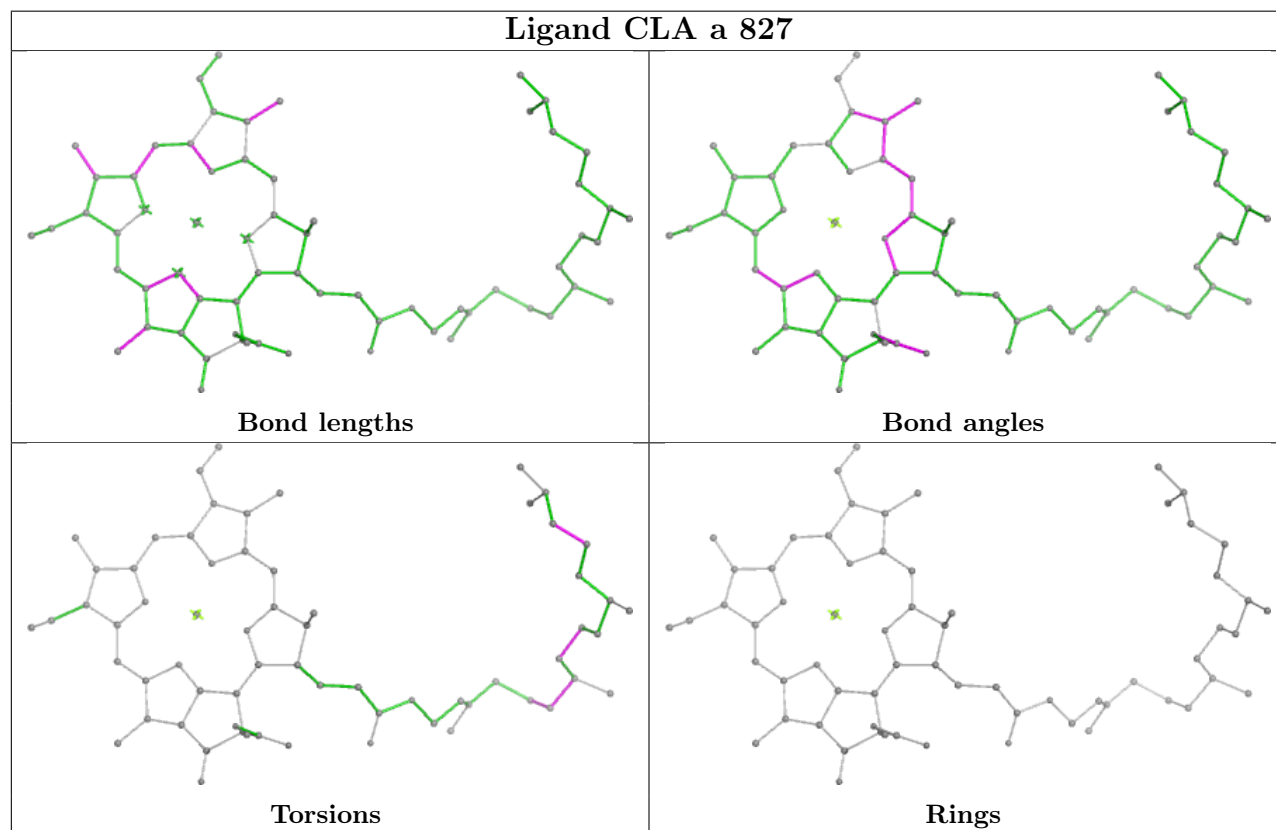
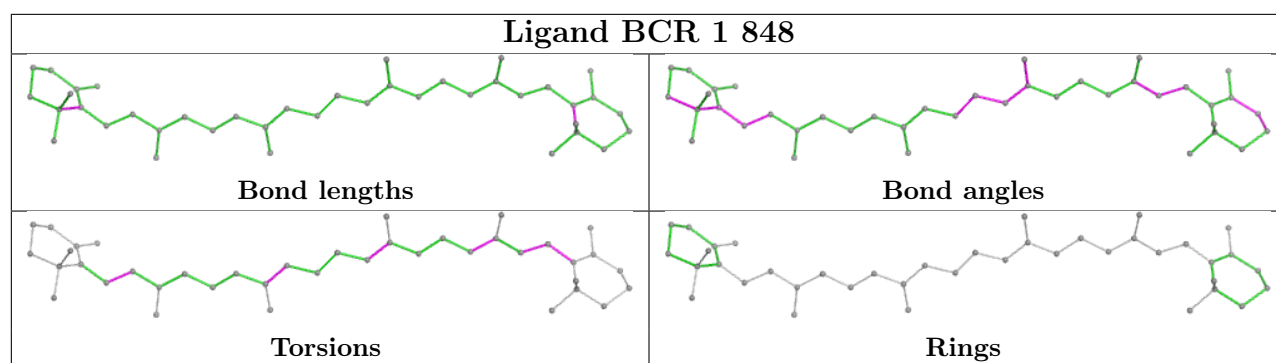


Ligand CLA 9 101

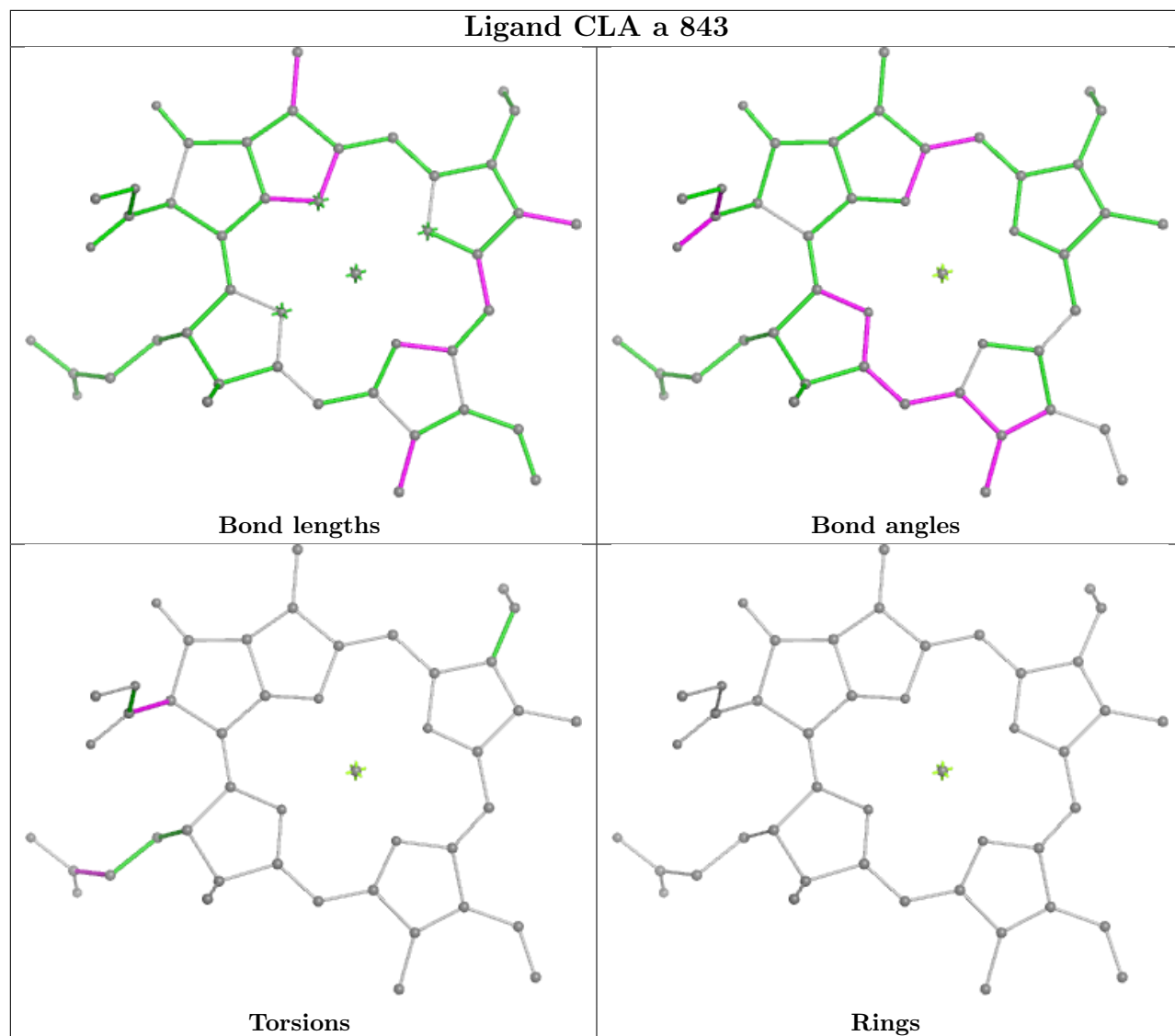


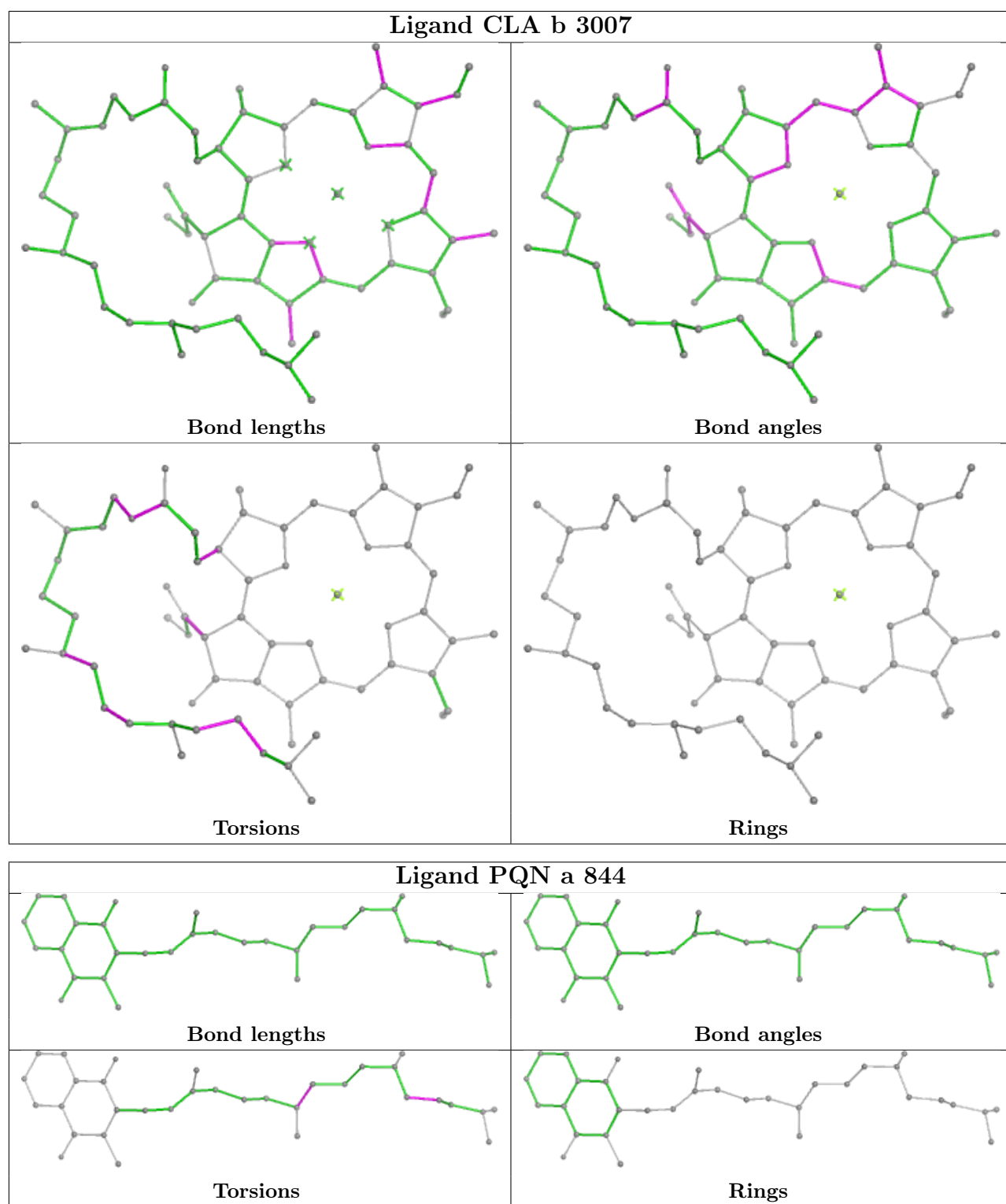




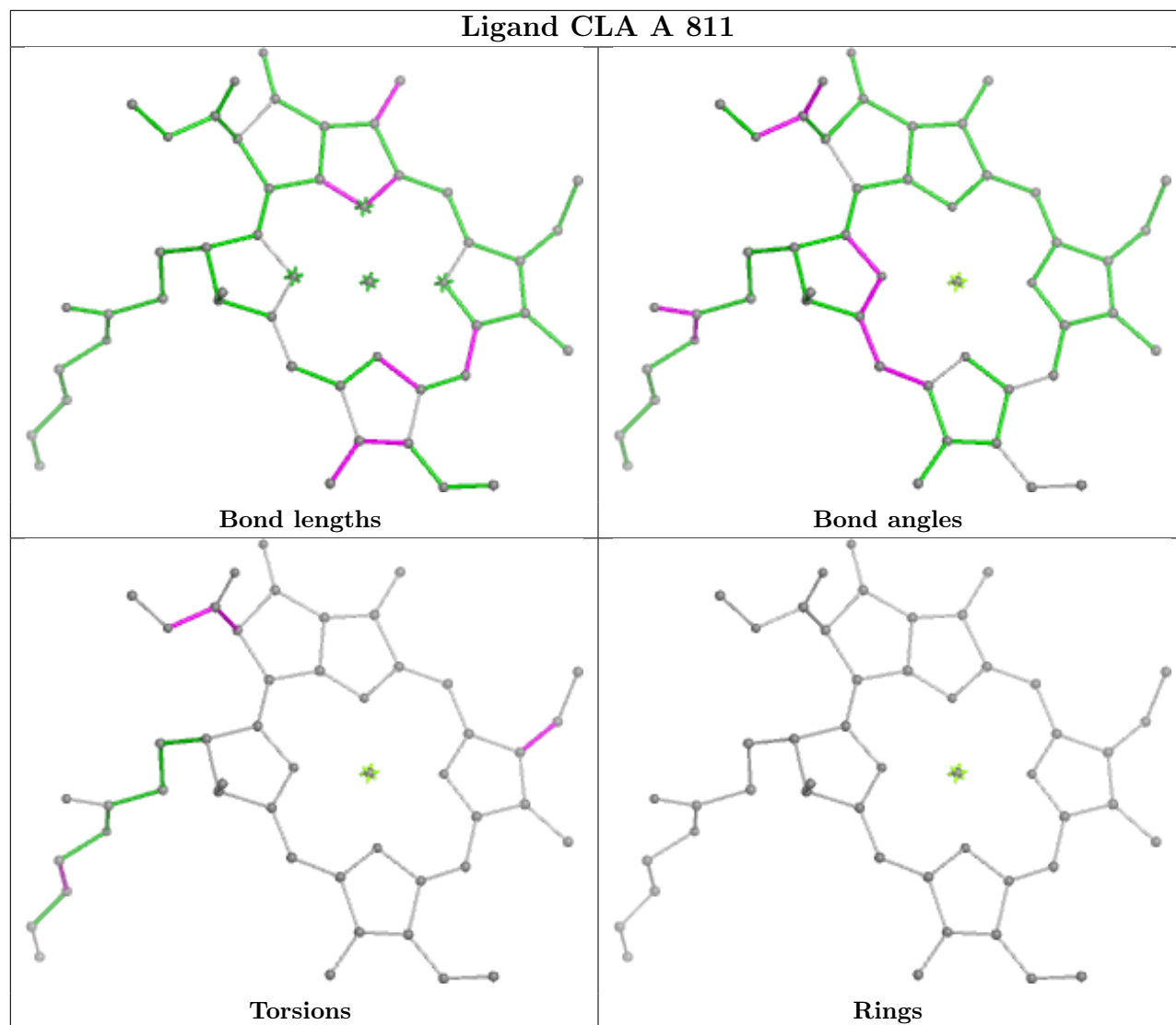


Ligand CLA a 843

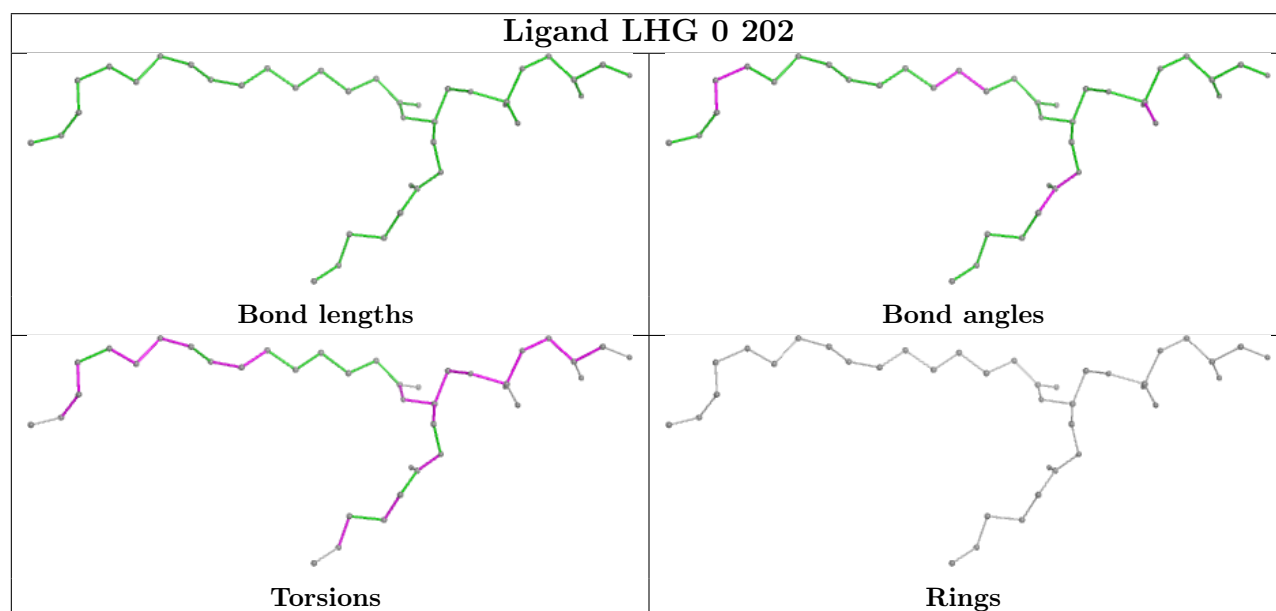




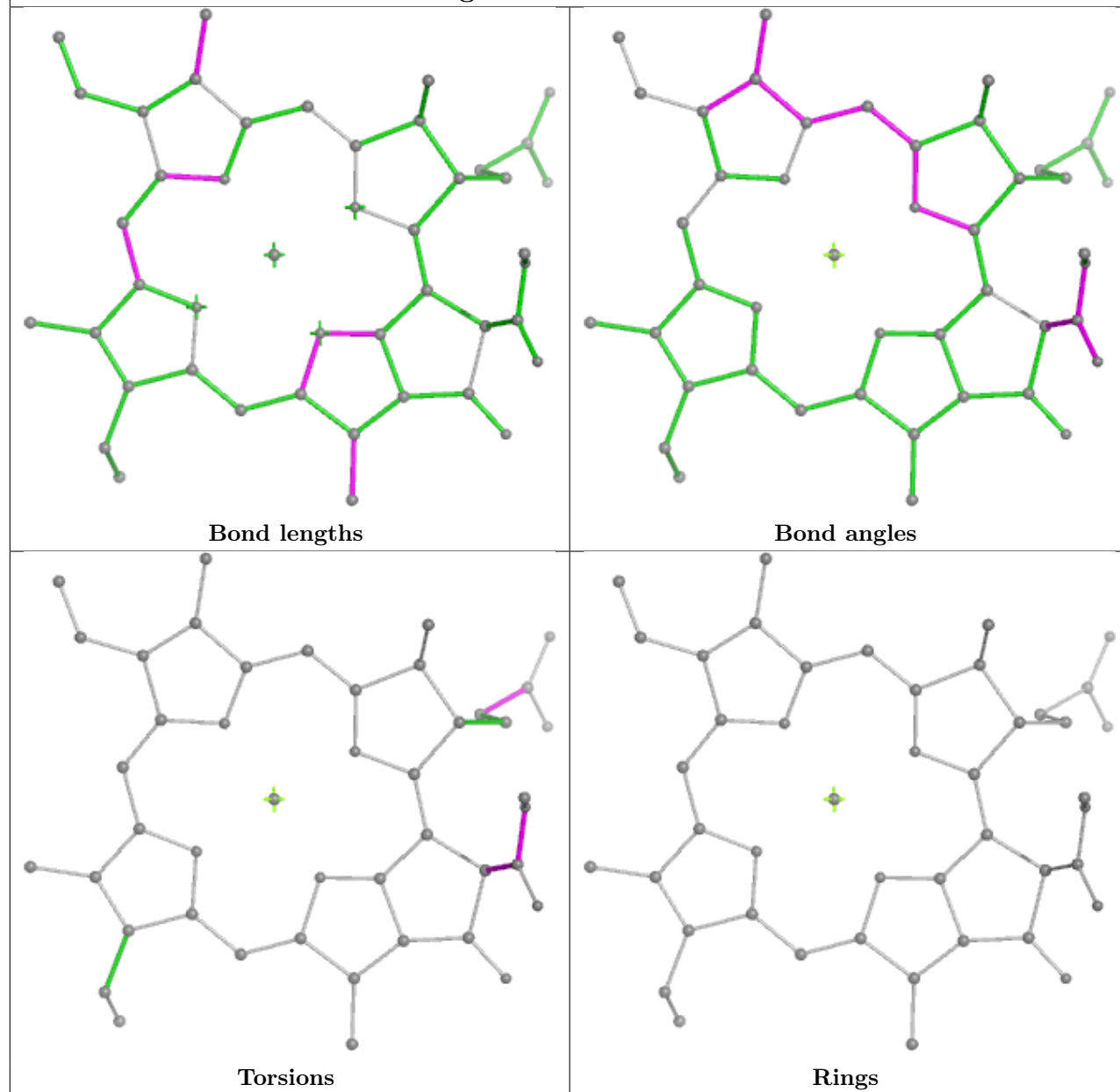
Ligand CLA A 811



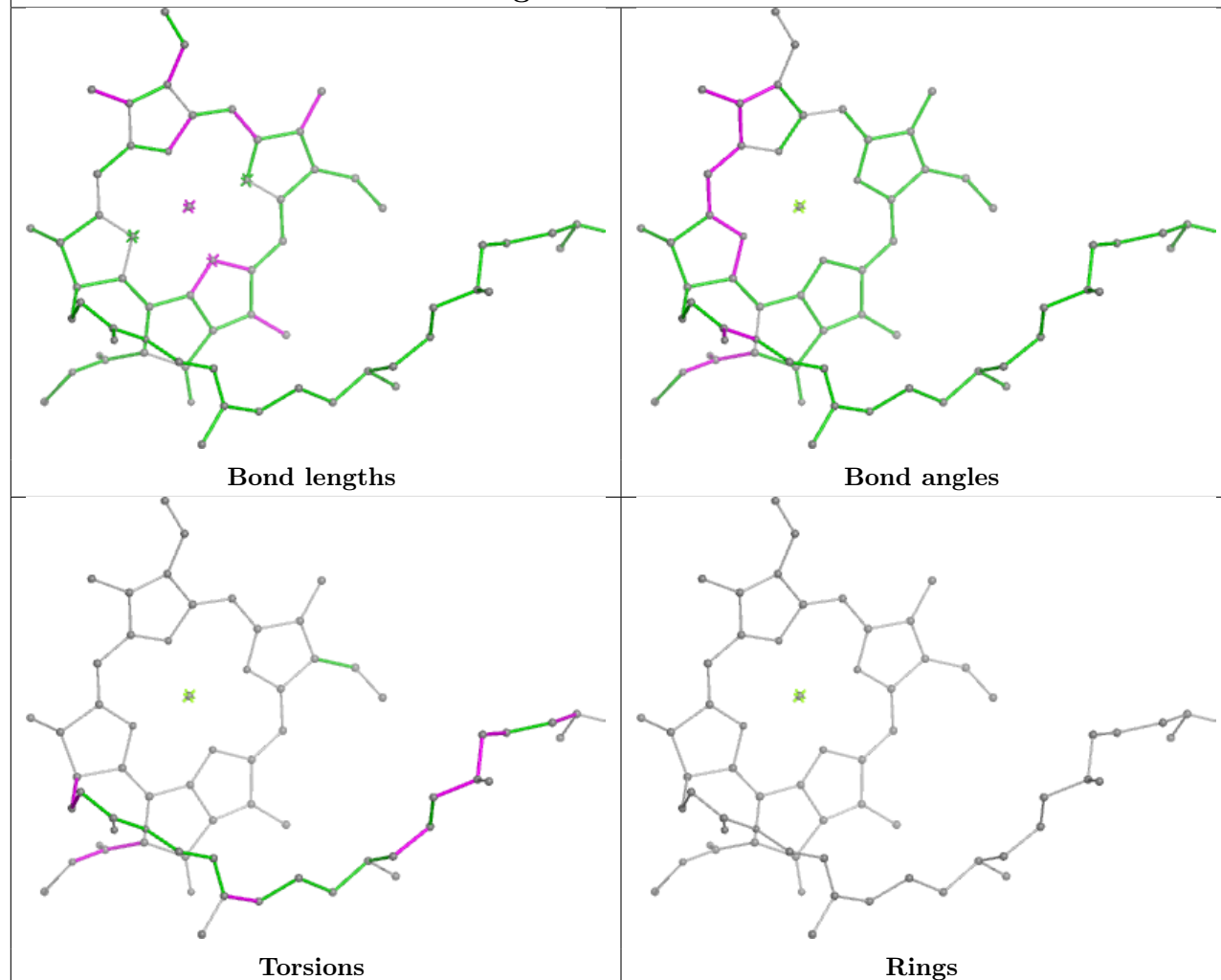
Ligand LHG 0 202



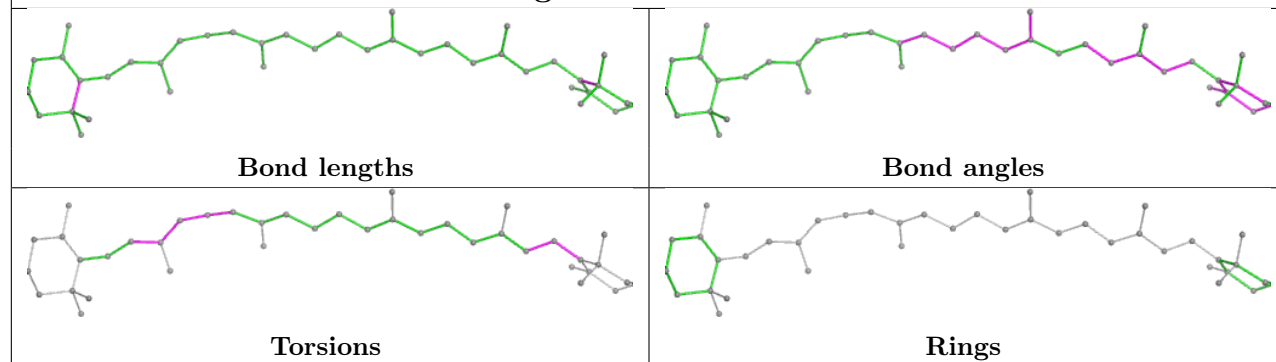
Ligand CLA B 3022

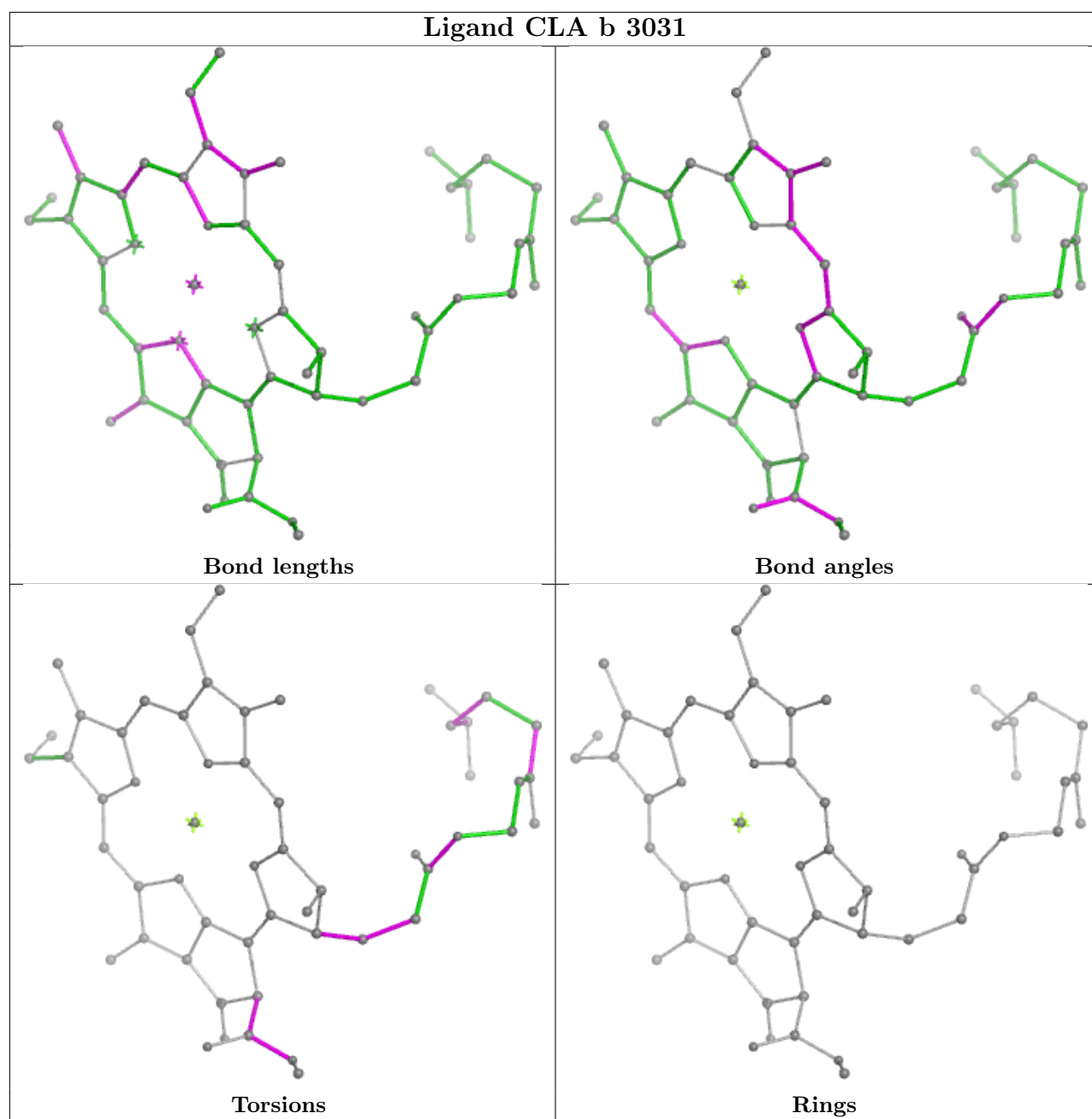


Ligand CLA 1 830

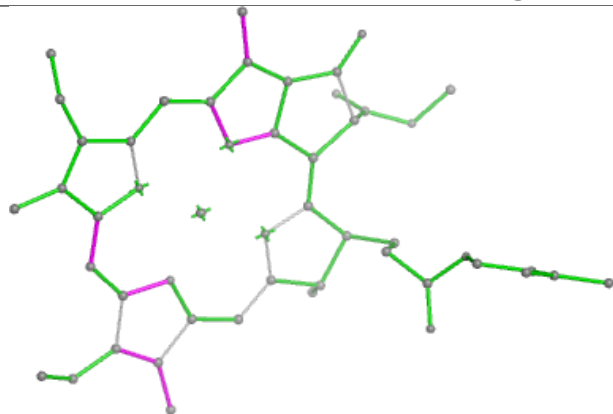


Ligand BCR 9 102

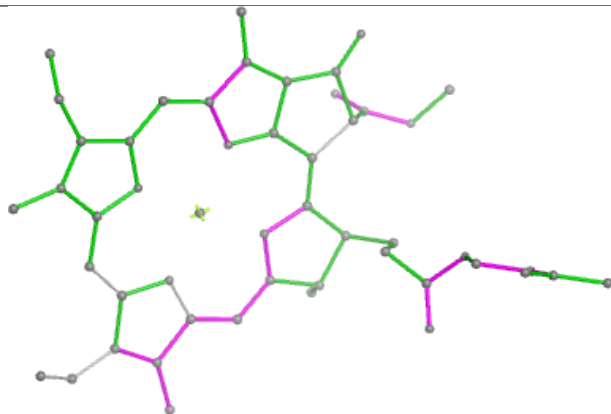




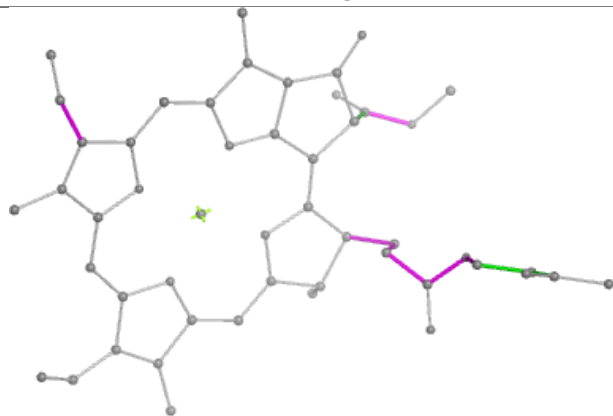
Ligand CLA 2 3036



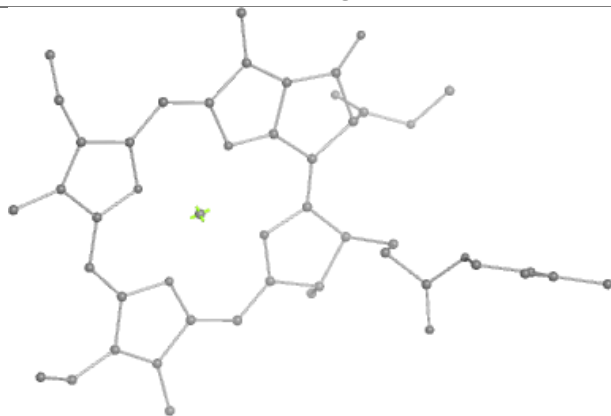
Bond lengths



Bond angles

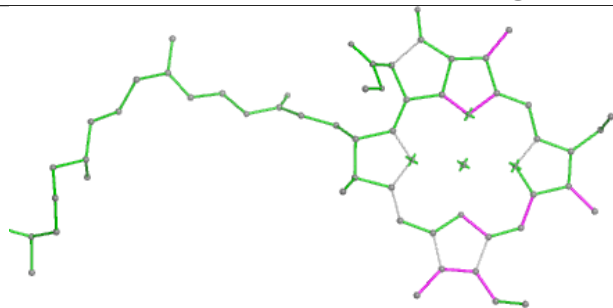


Torsions

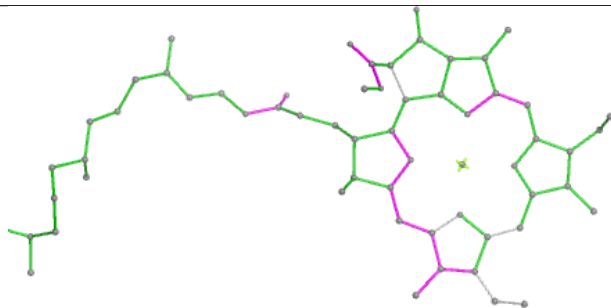


Rings

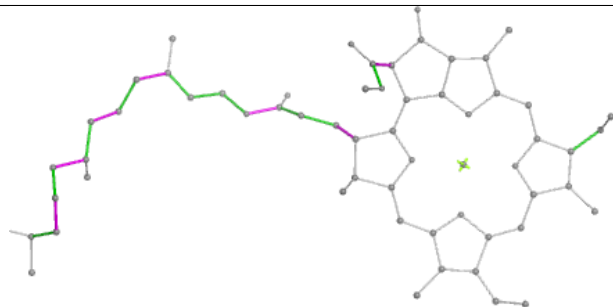
Ligand CLA 2 3038



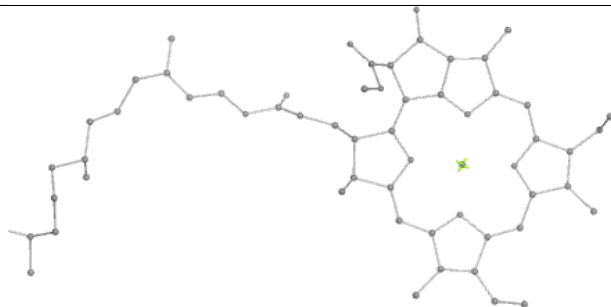
Bond lengths



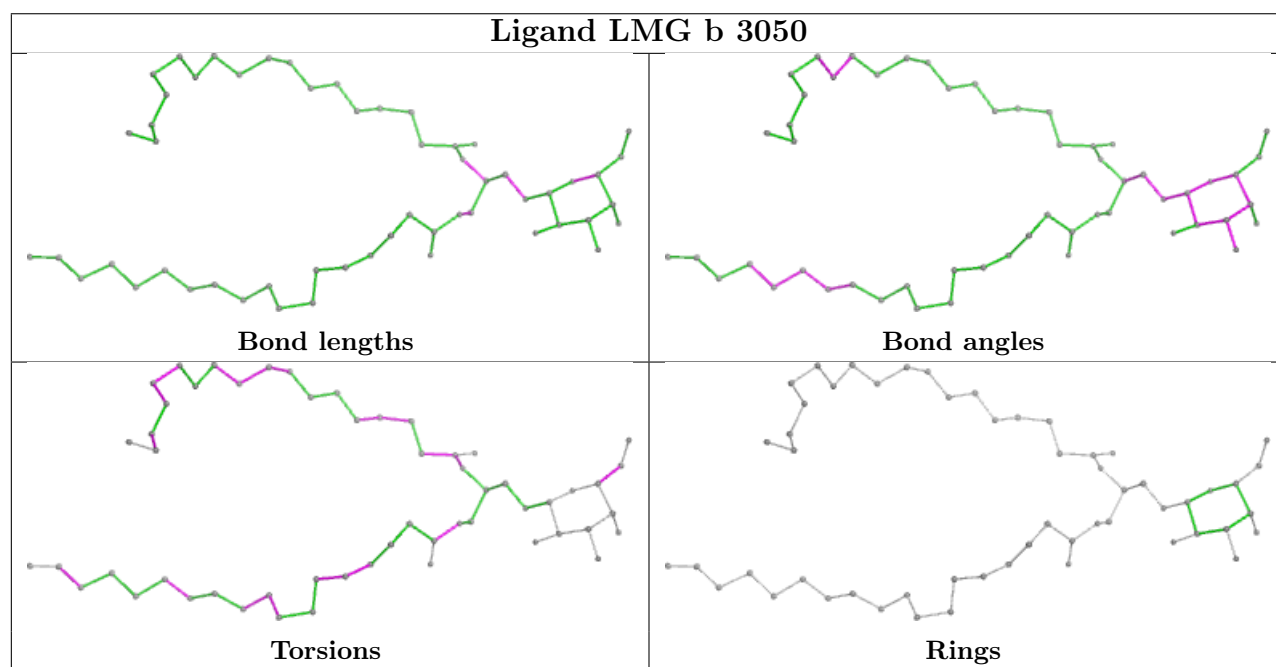
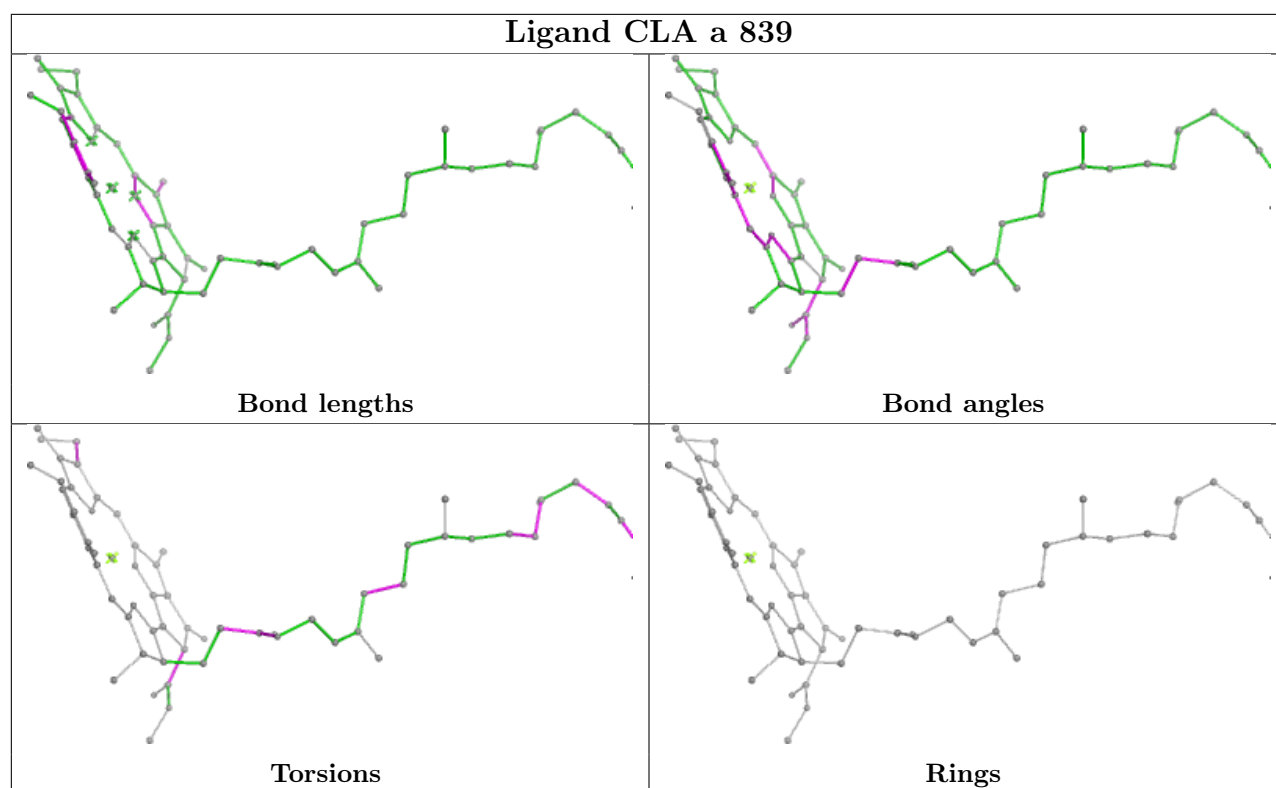
Bond angles

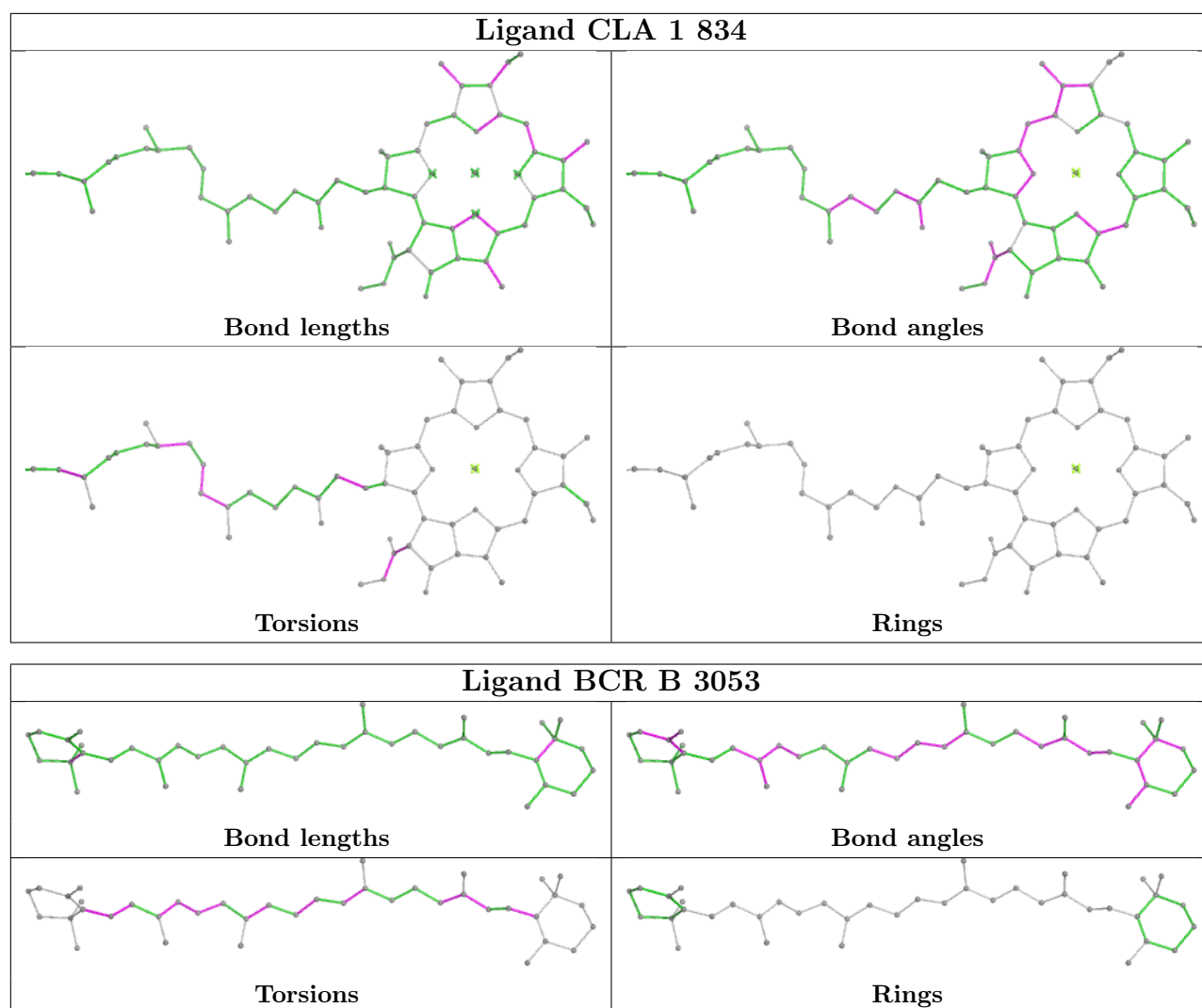


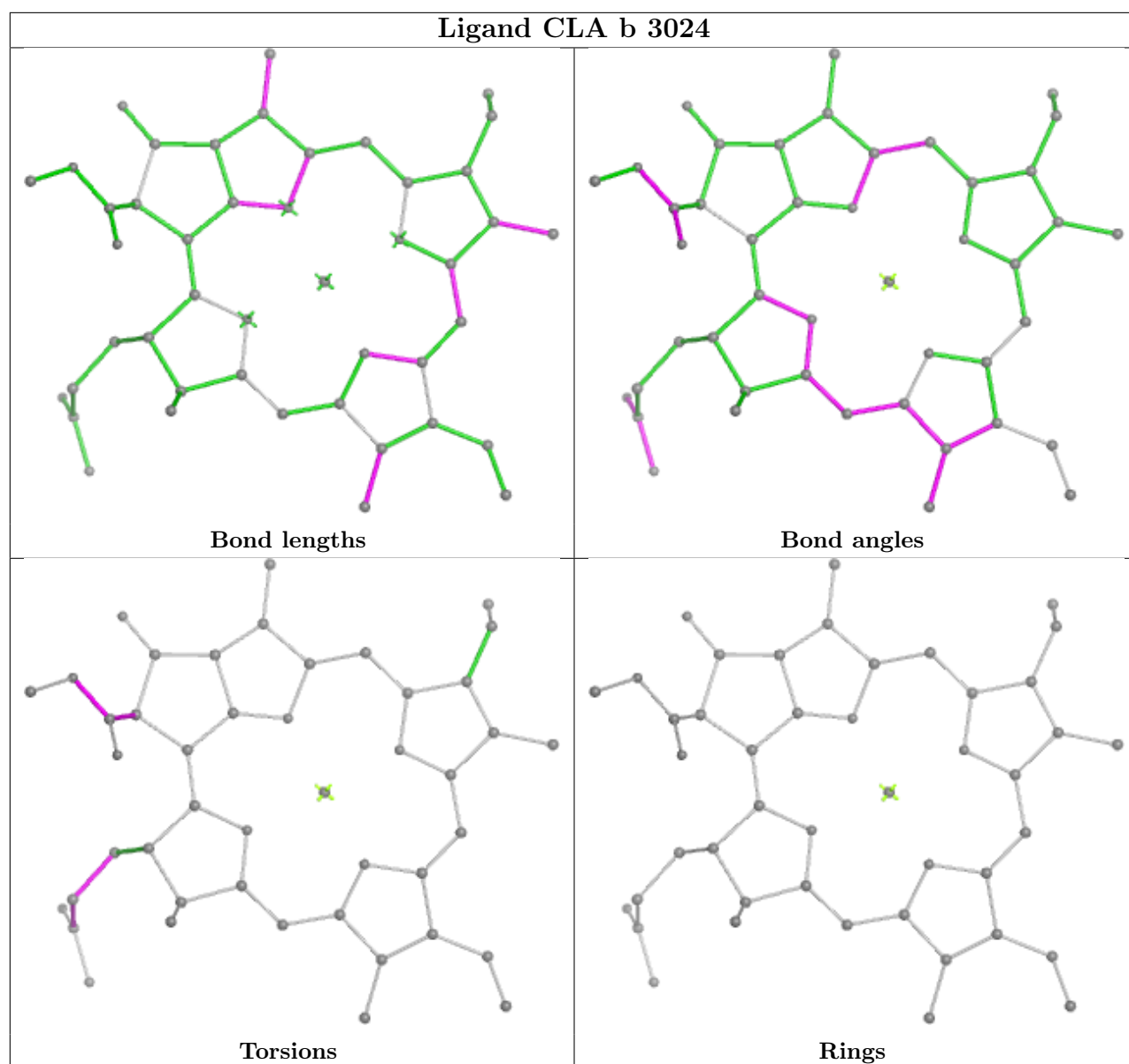
Torsions

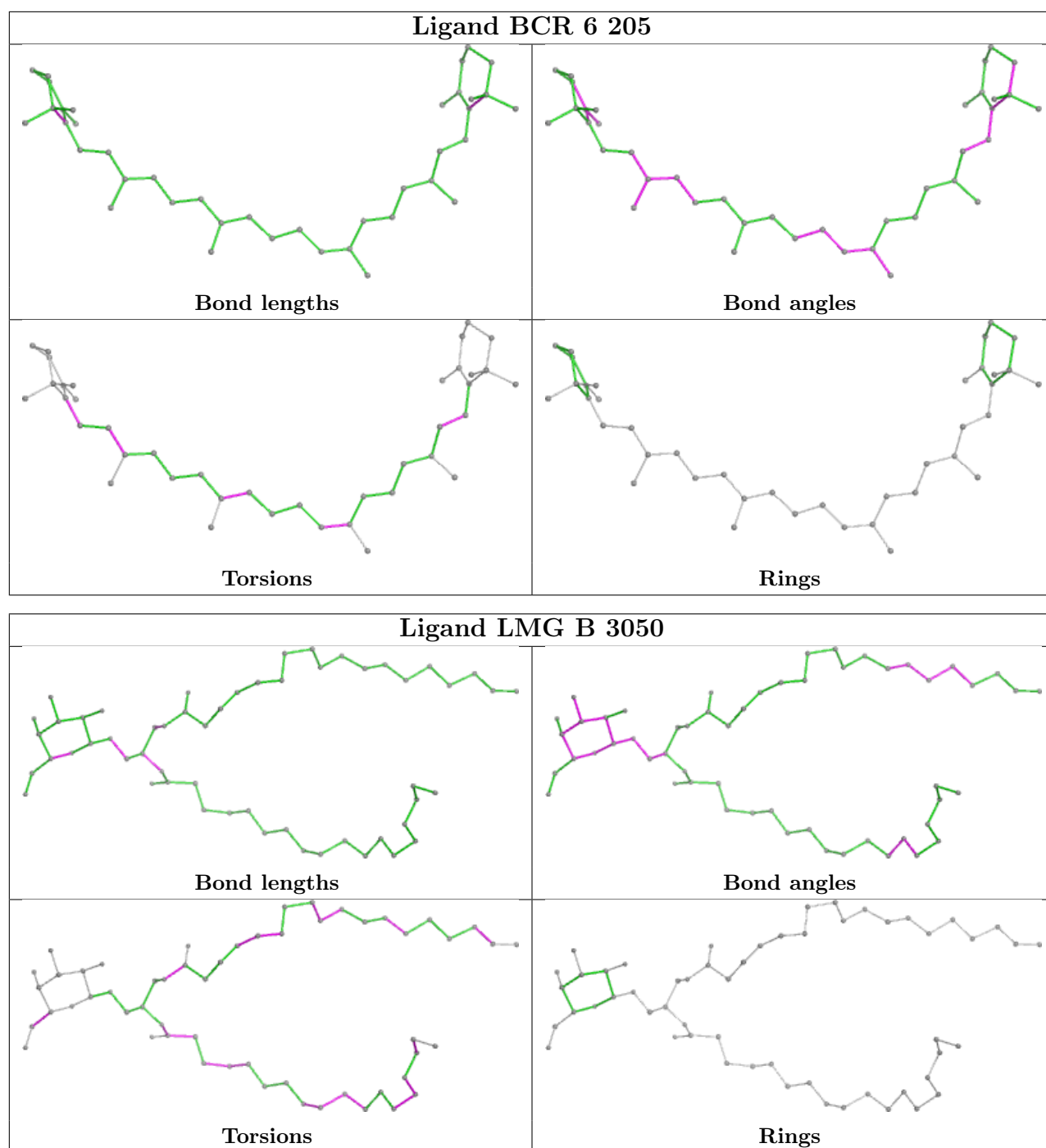


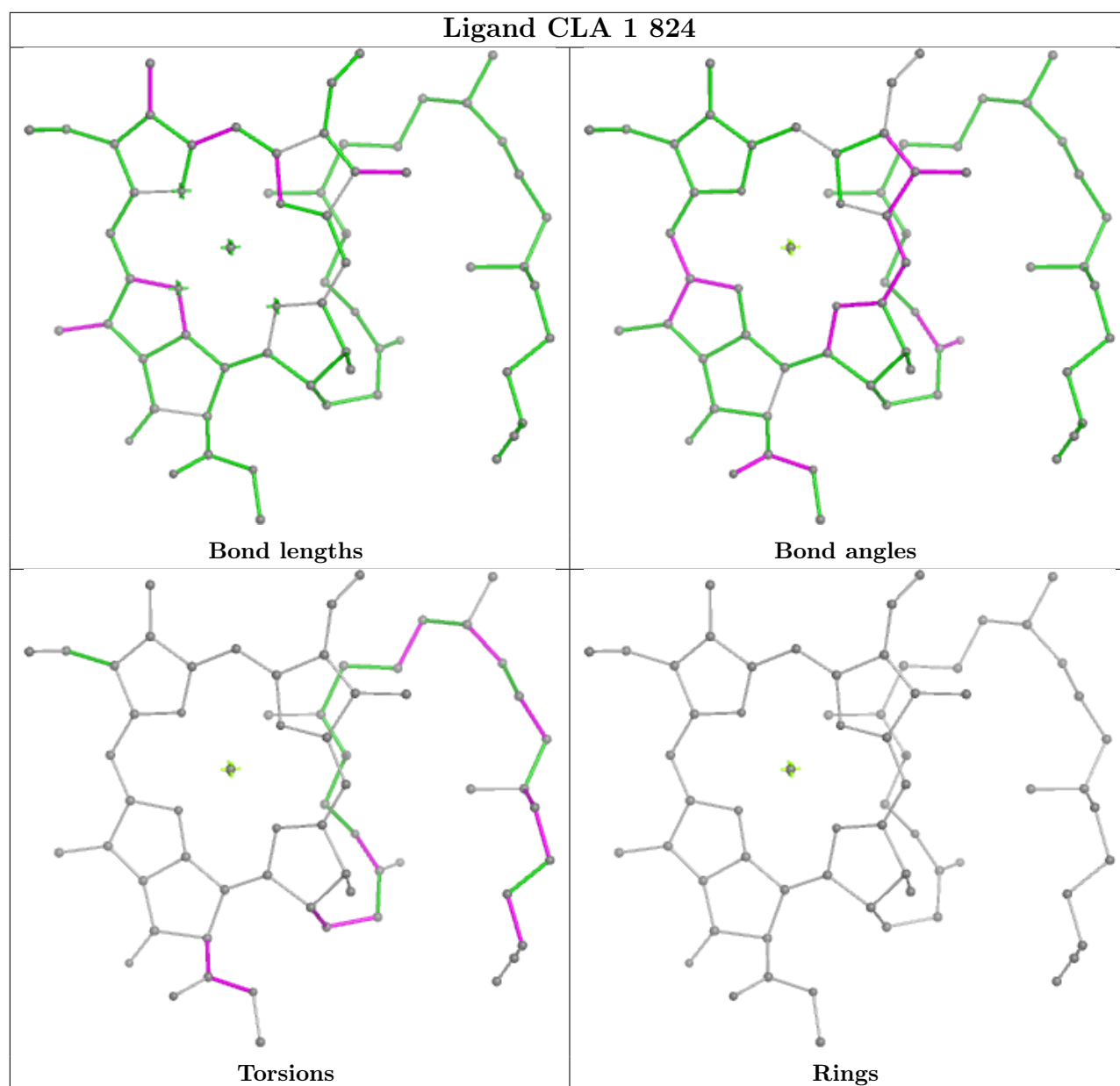
Rings



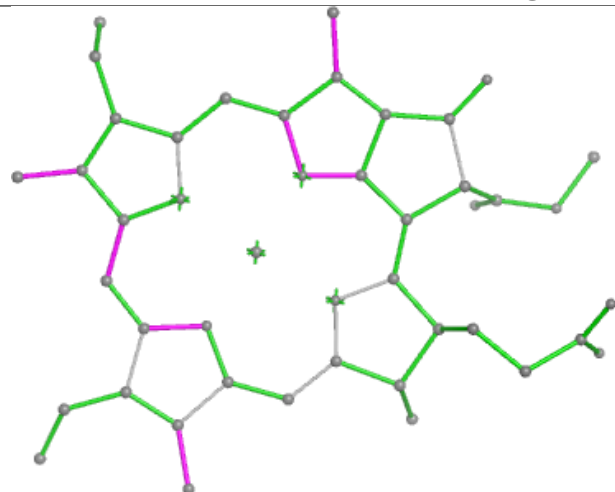




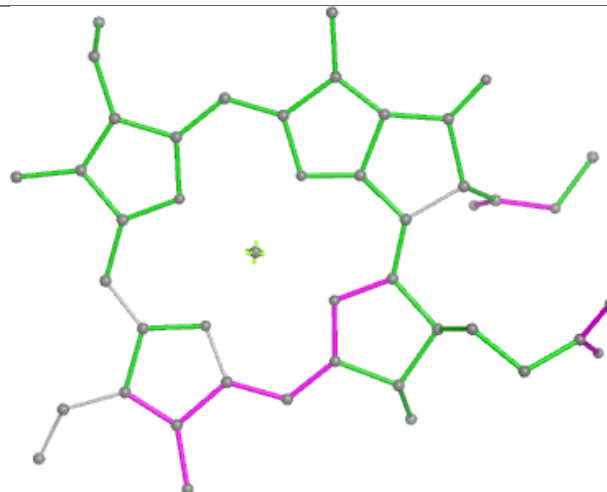




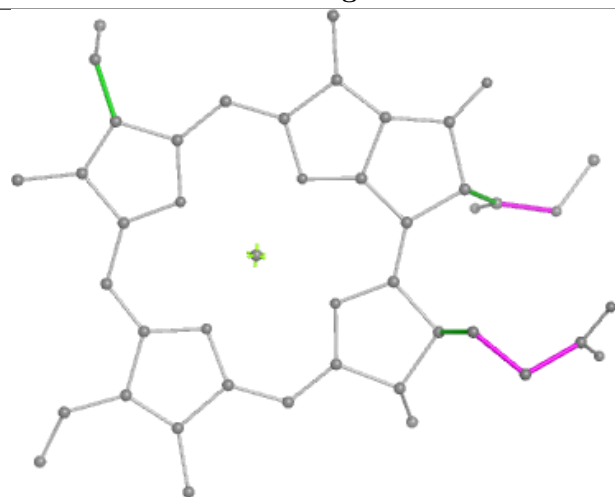
Ligand CLA f 203



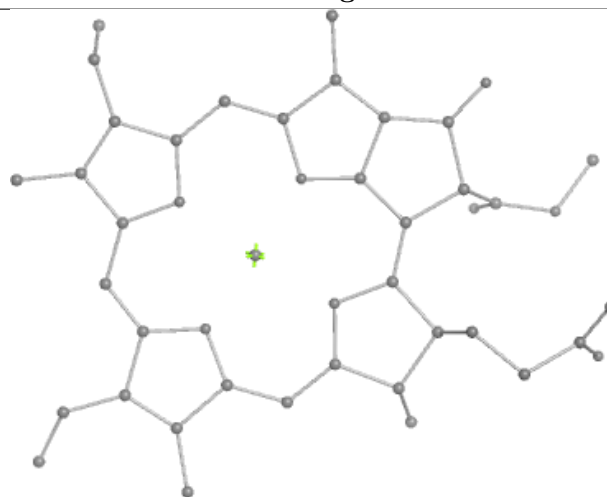
Bond lengths



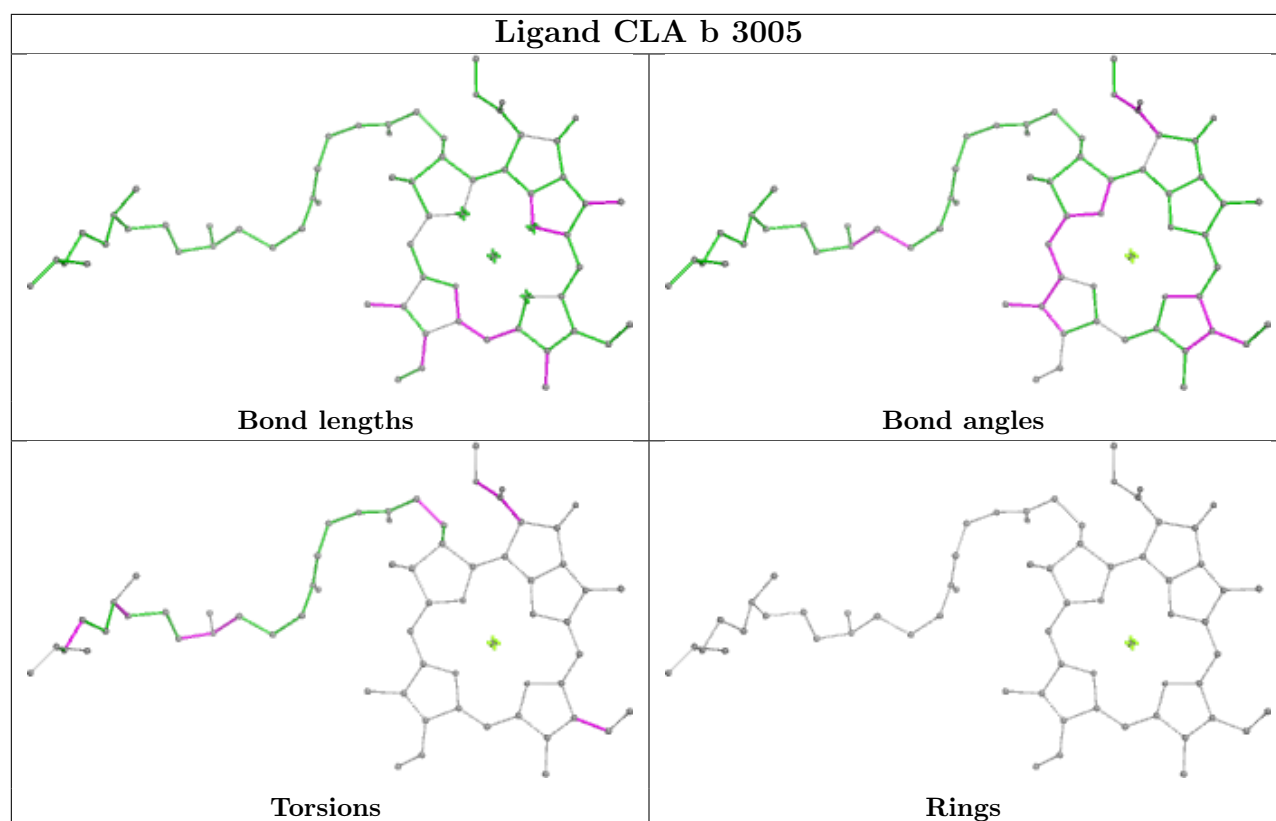
Bond angles



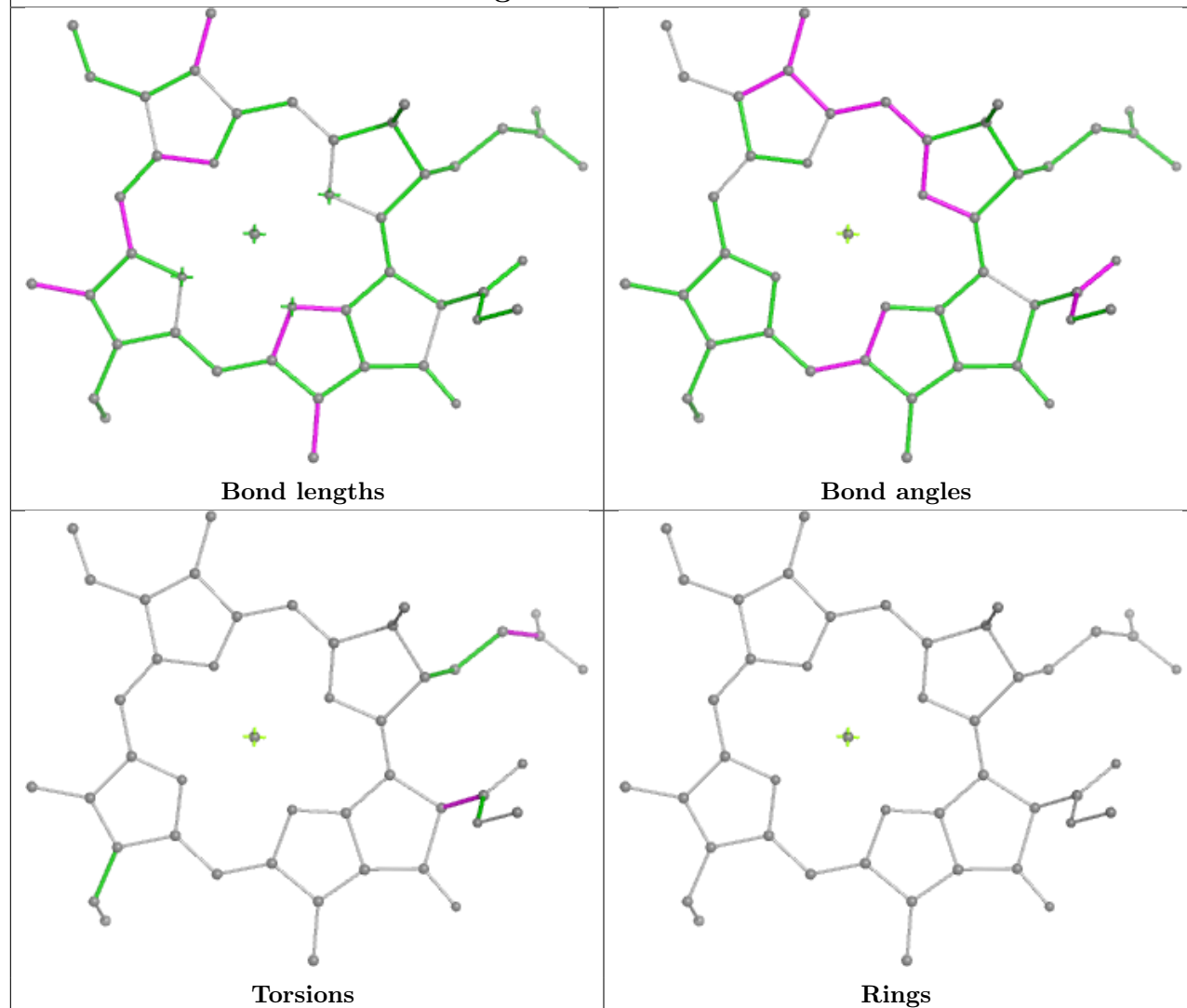
Torsions



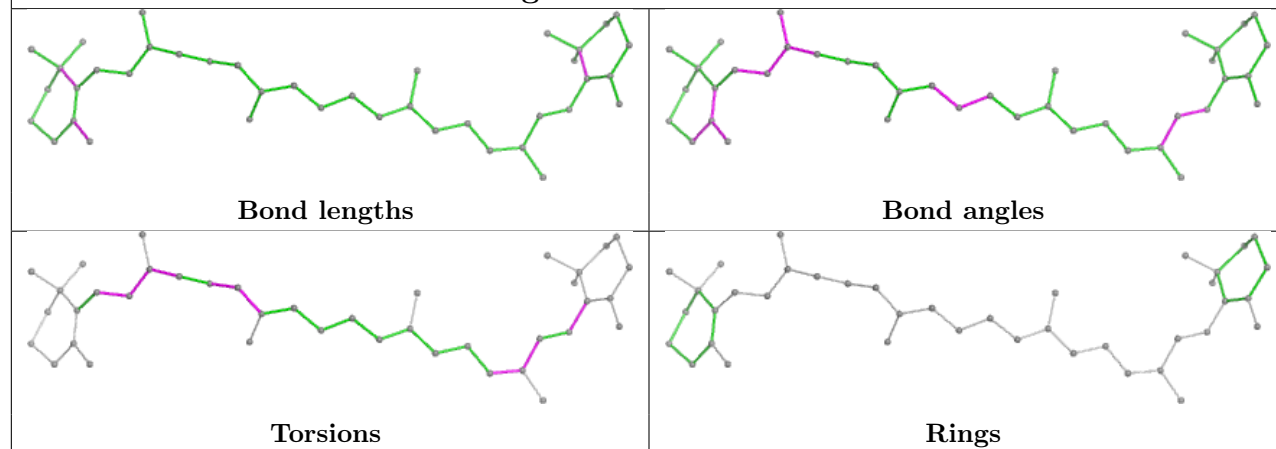
Rings

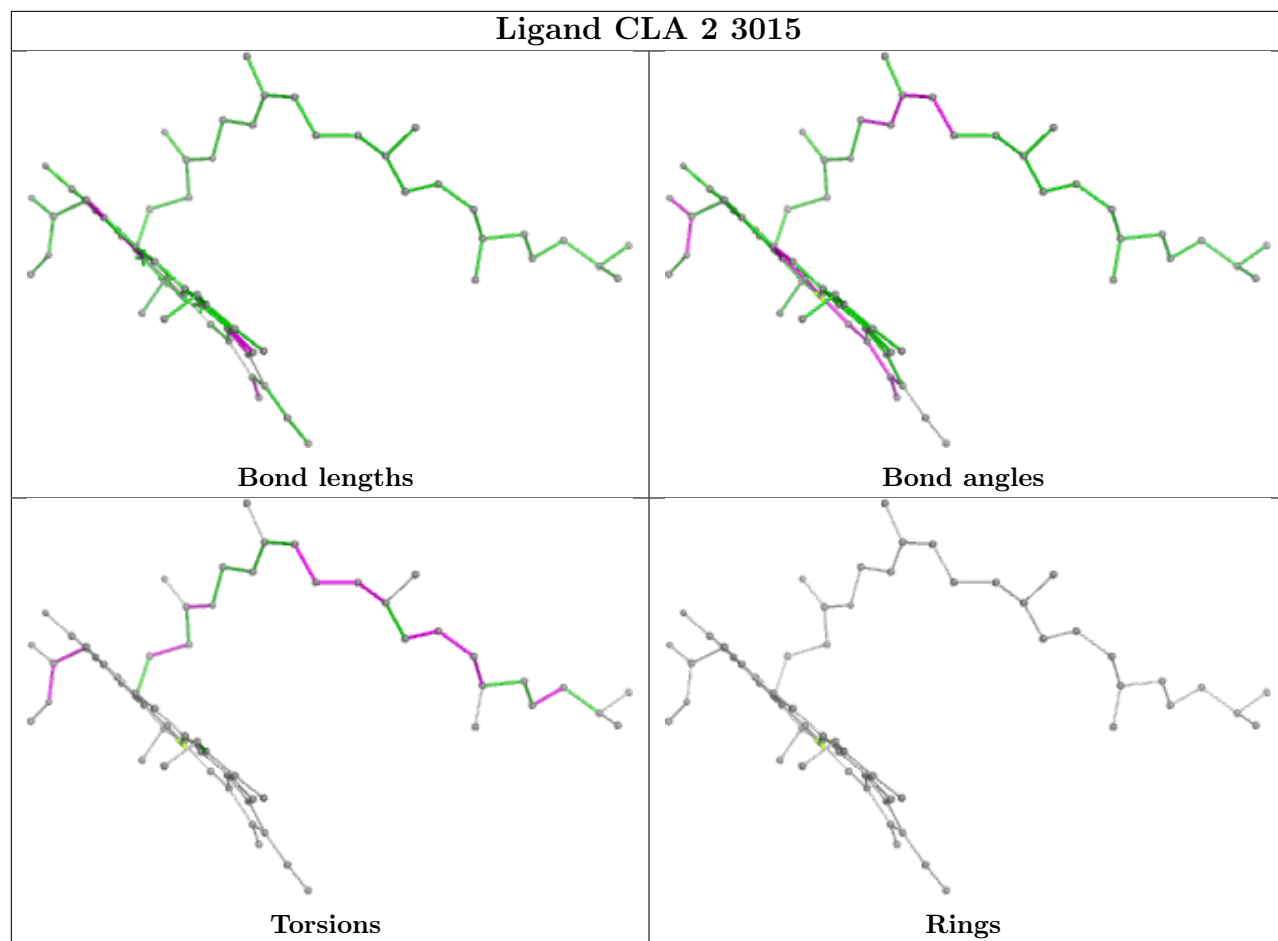


Ligand CLA A 844

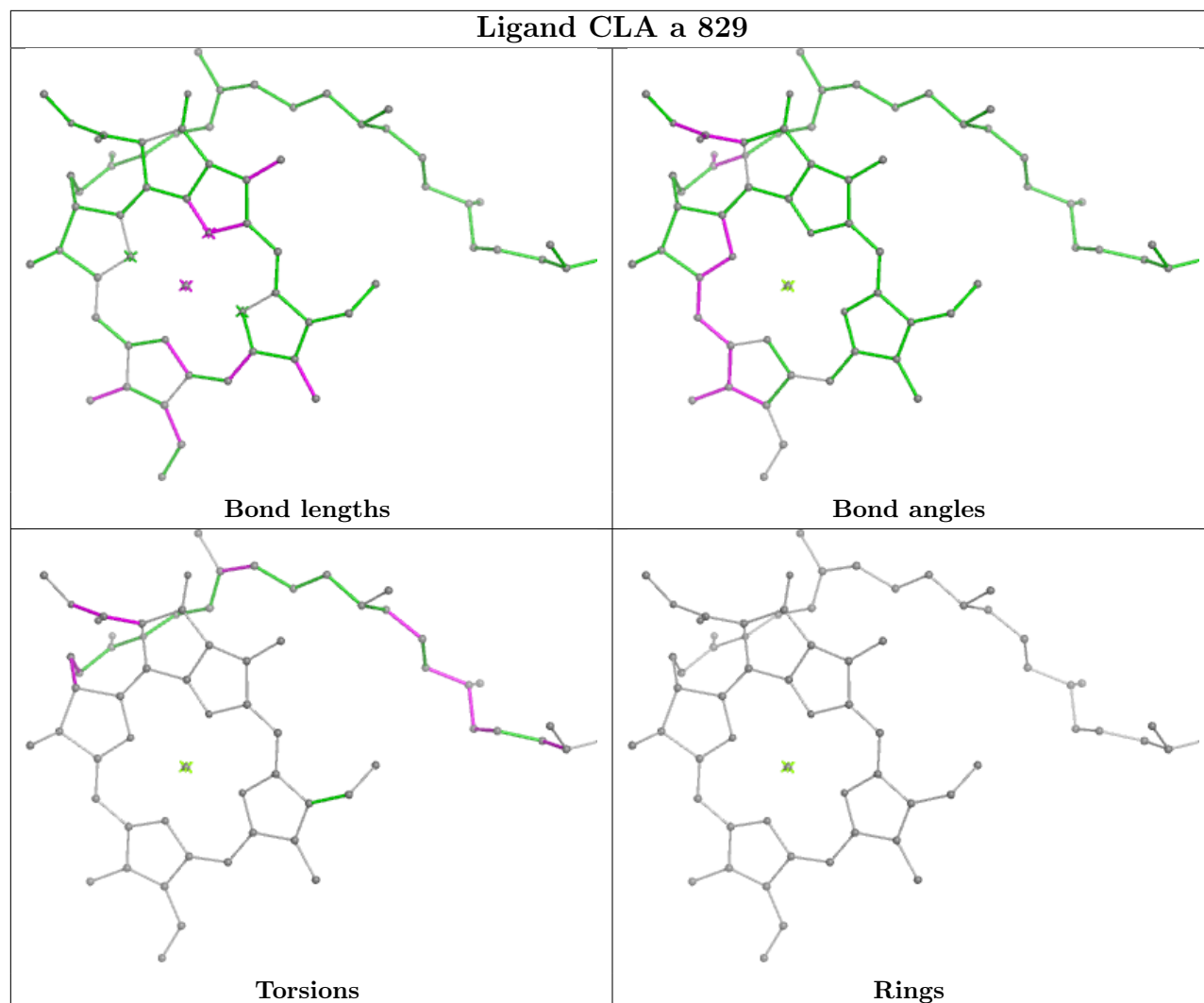


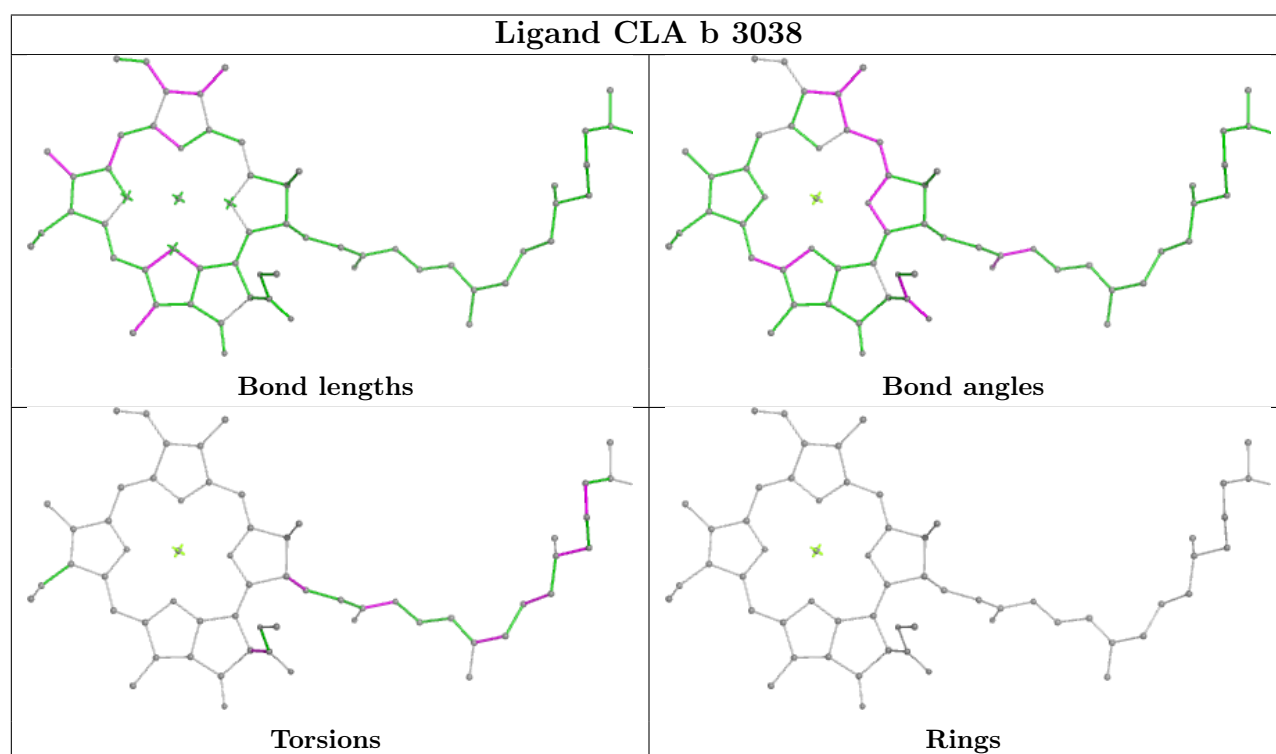
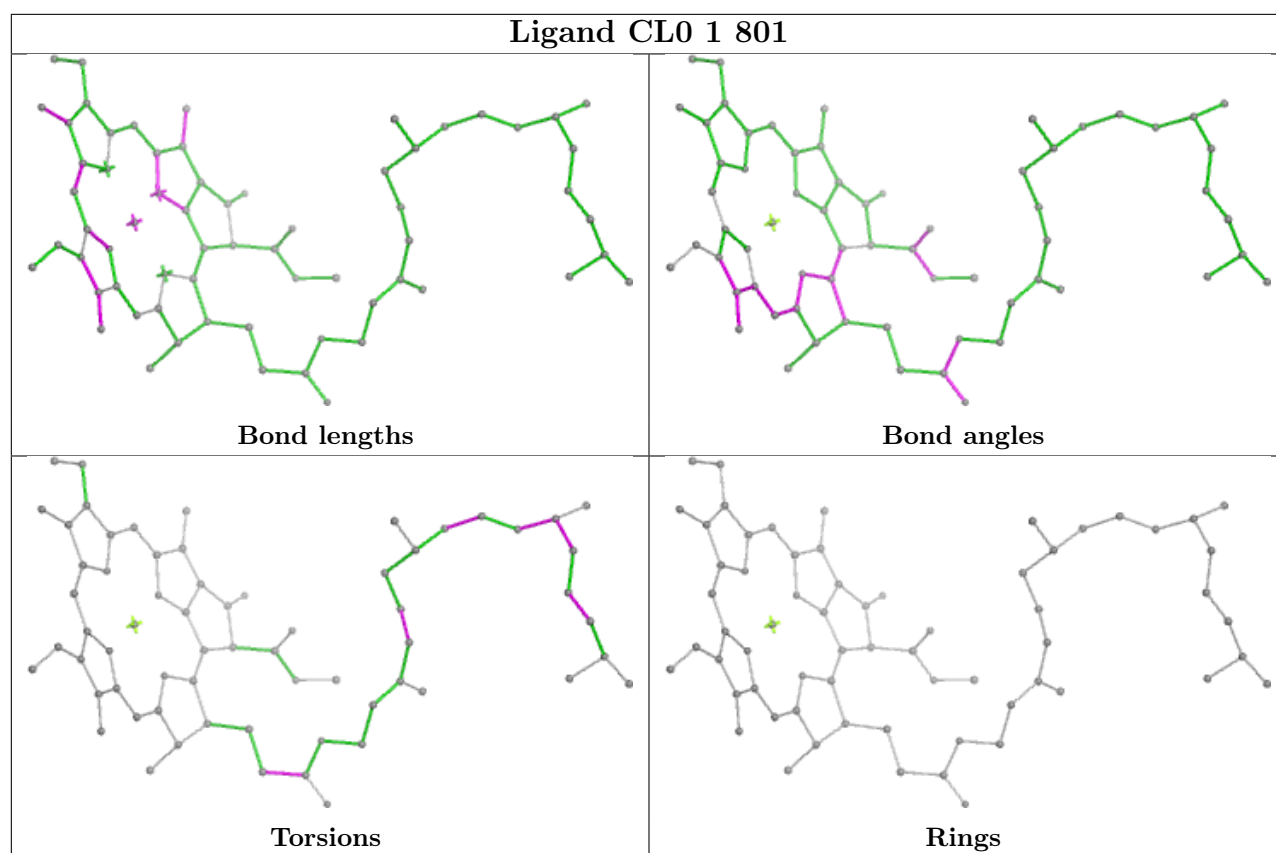
Ligand BCR B 3046

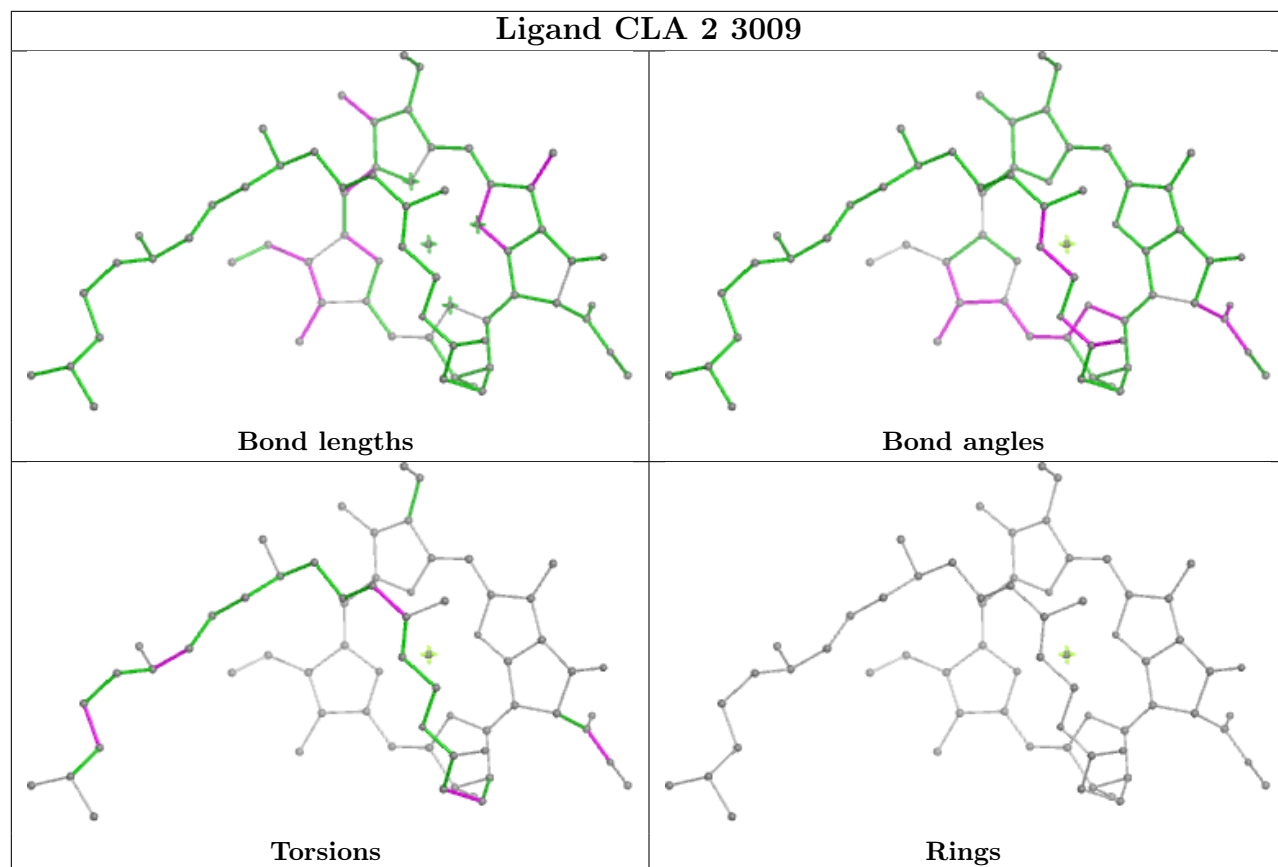


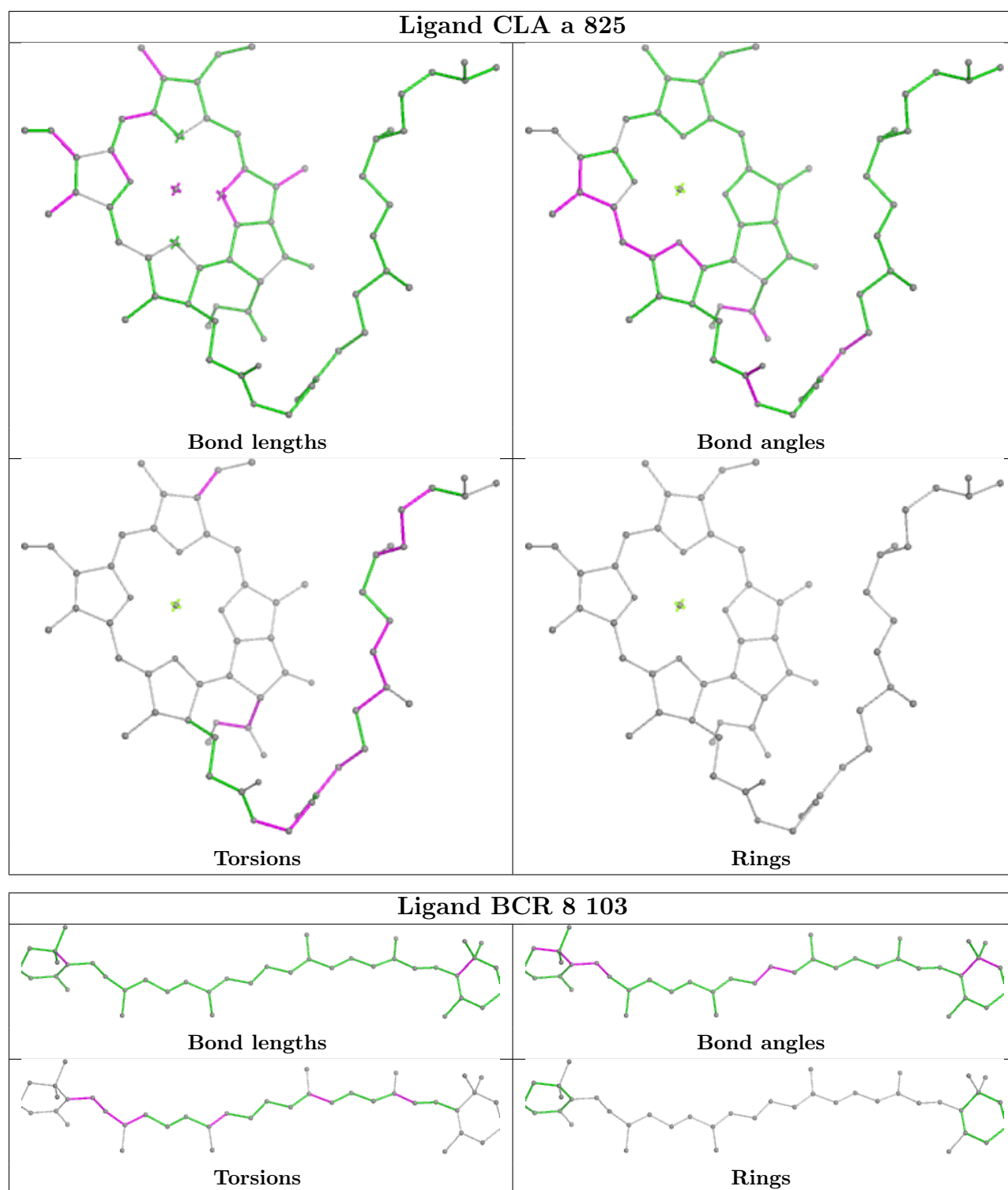


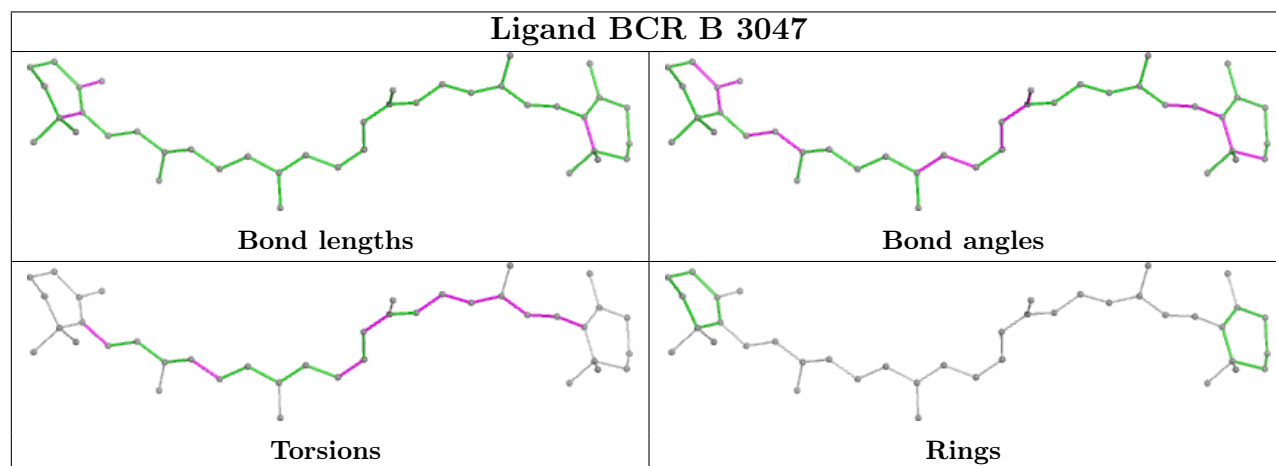
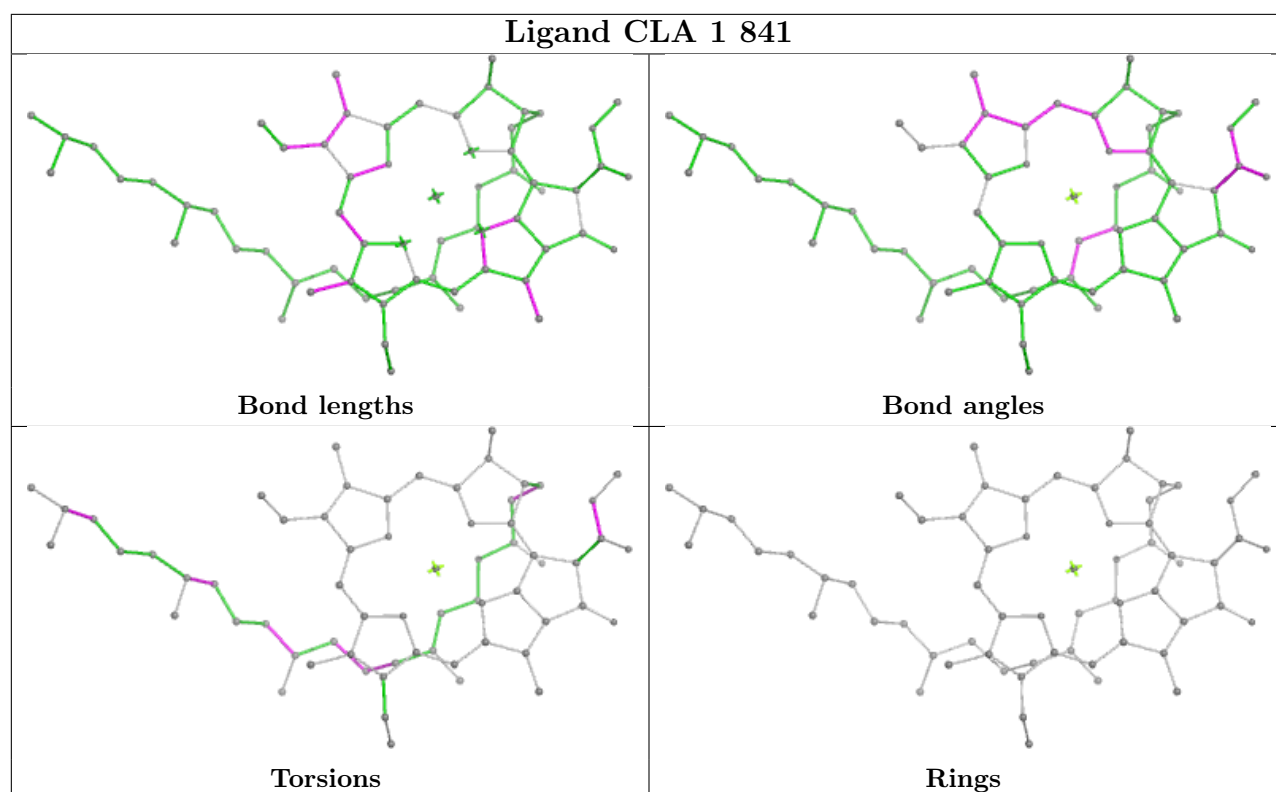
Ligand CLA a 829

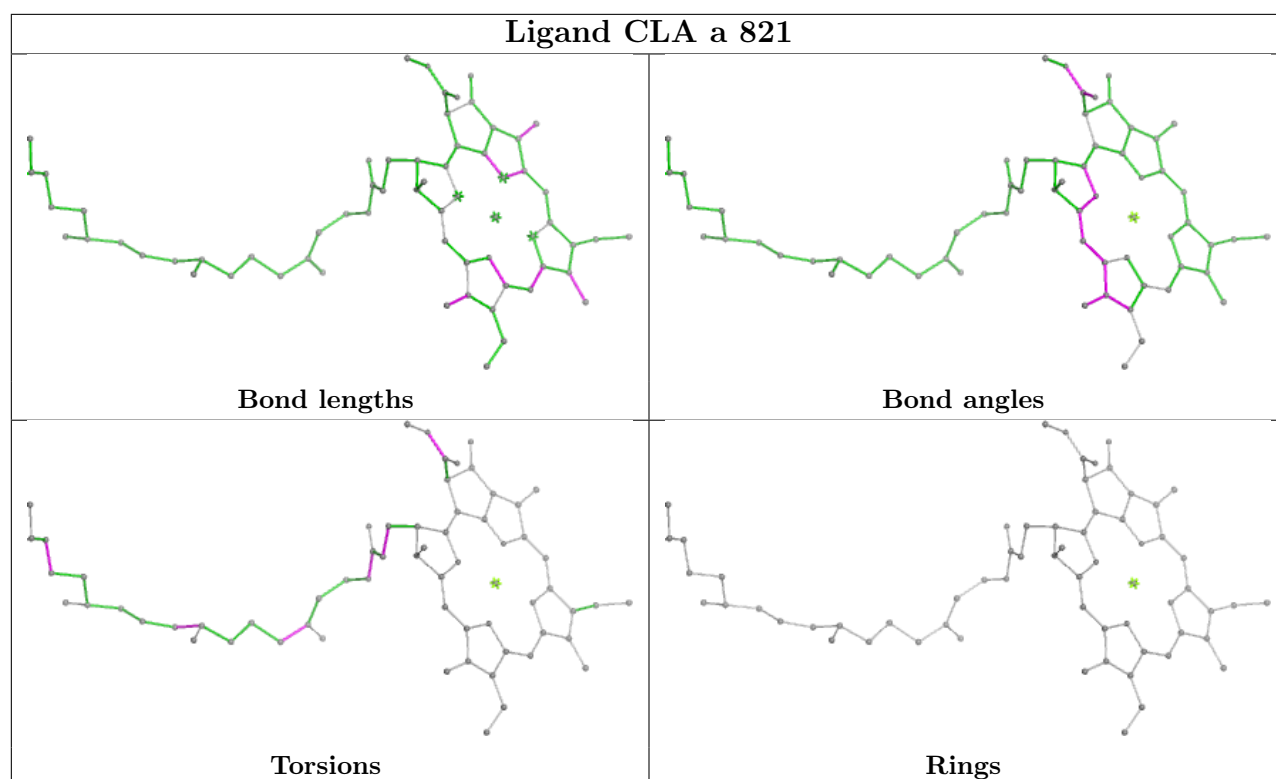


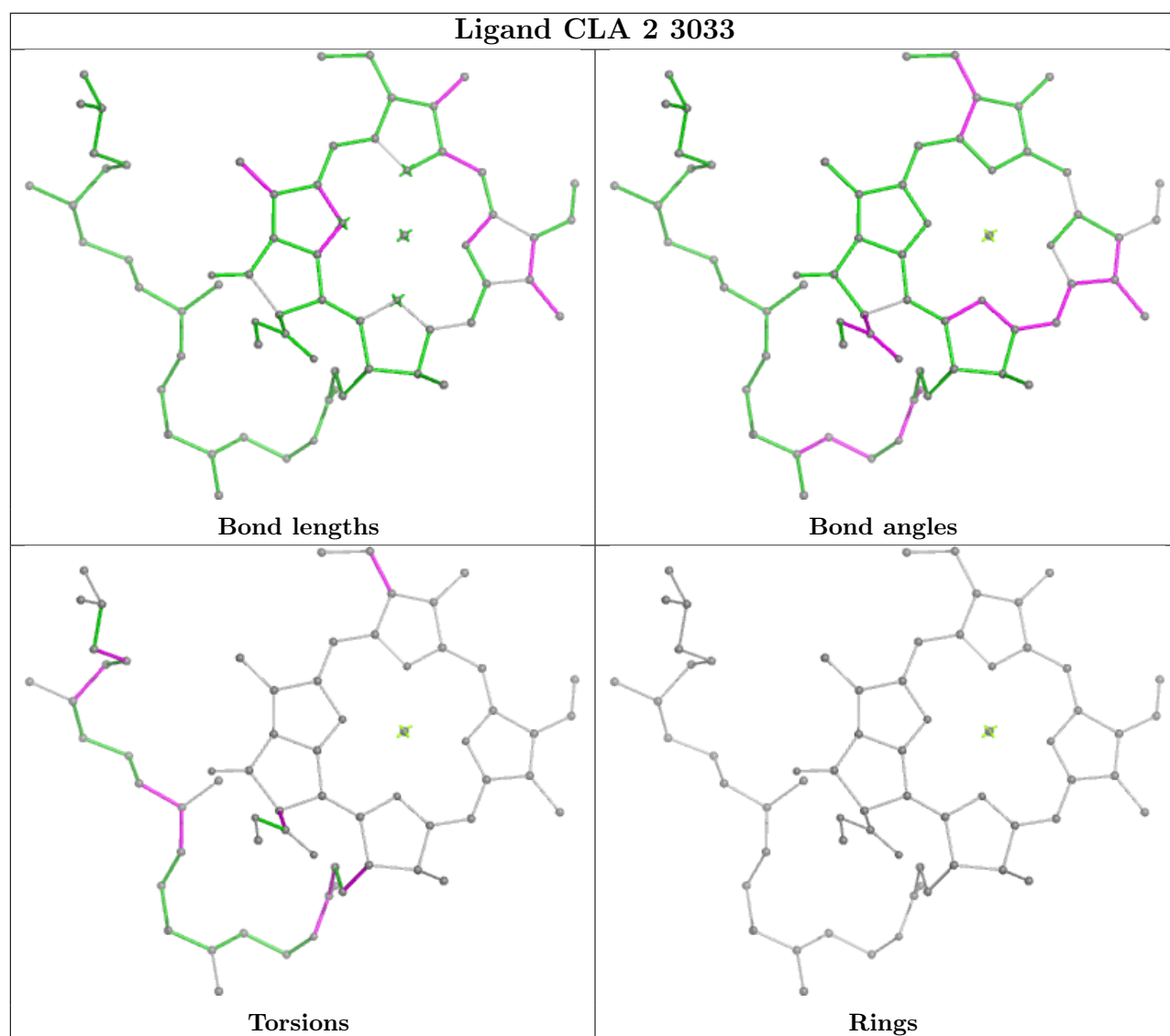


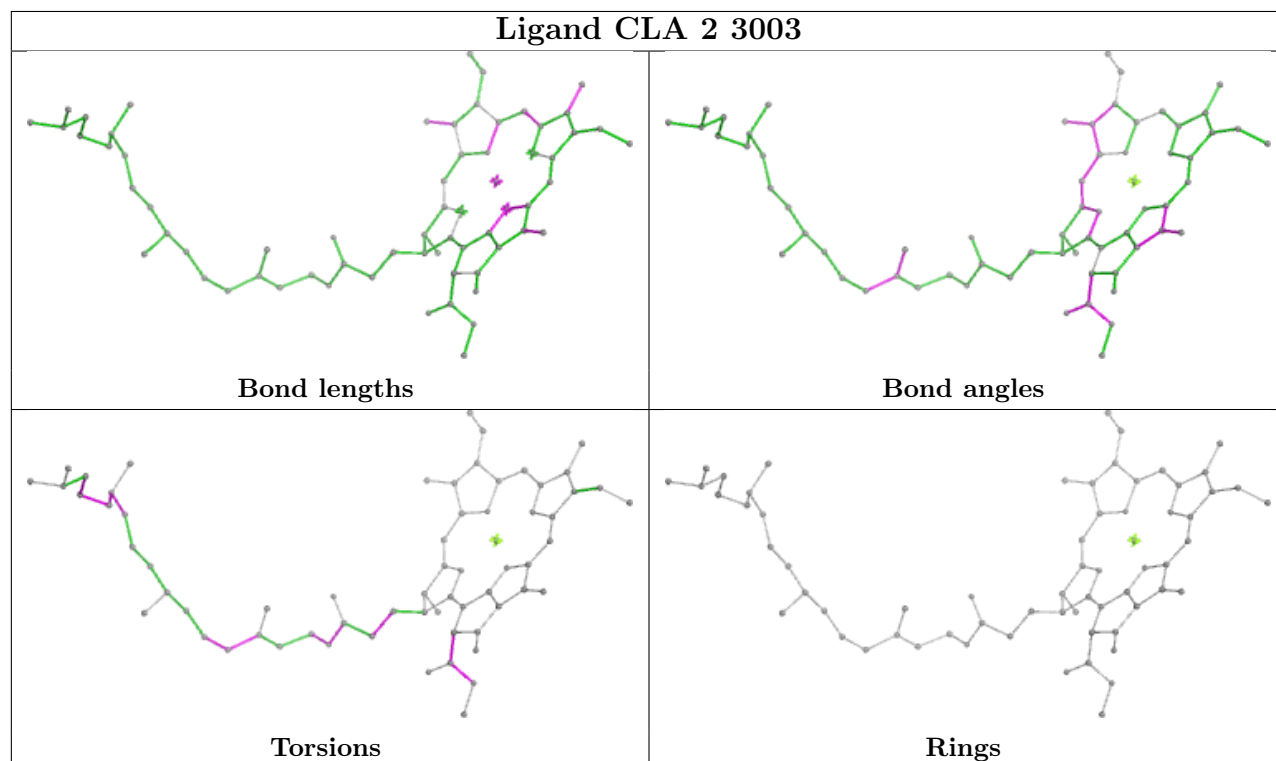
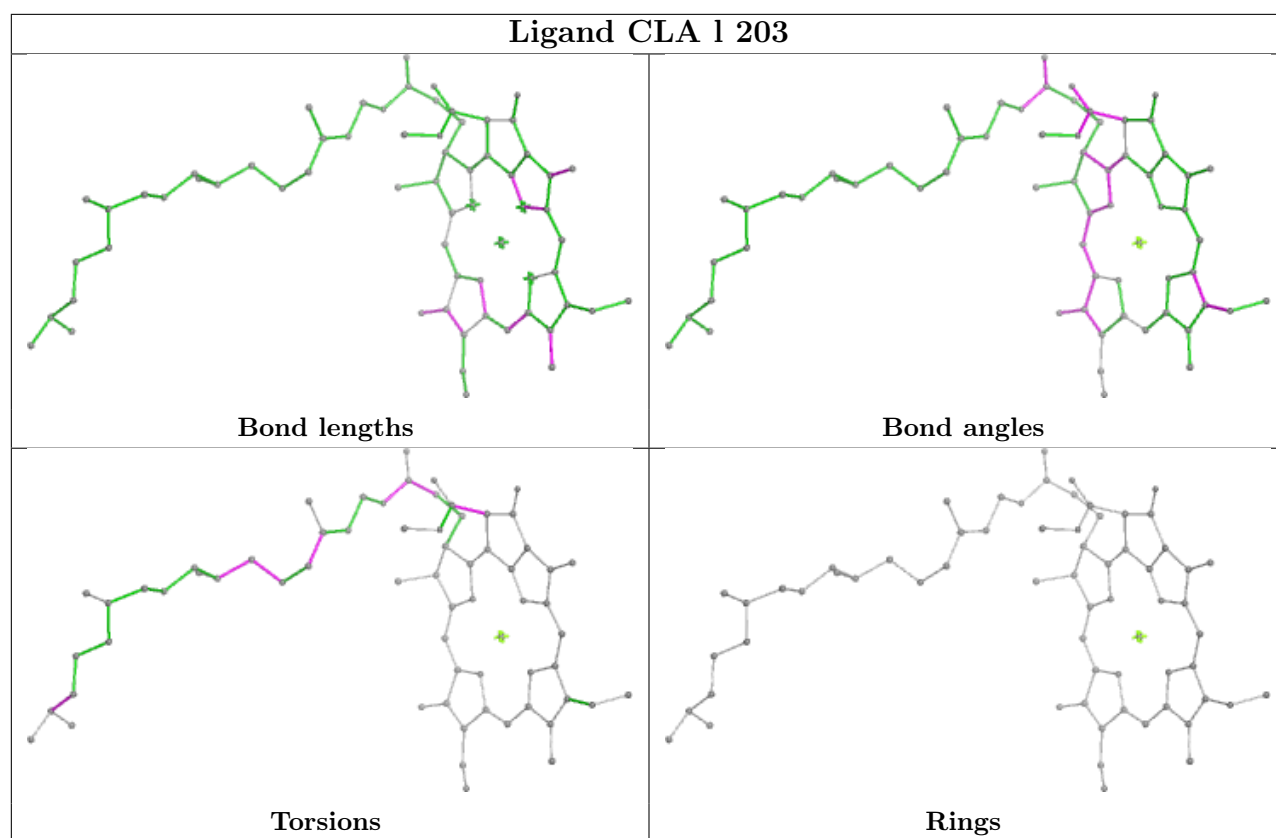




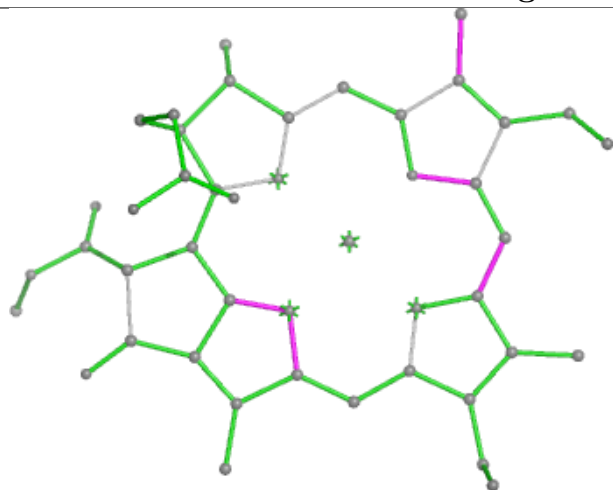




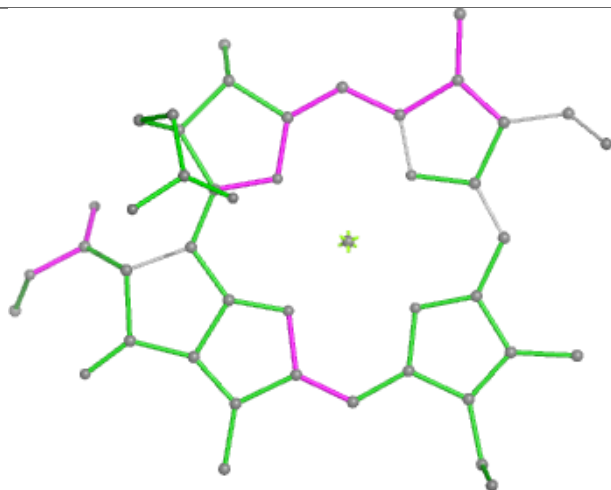




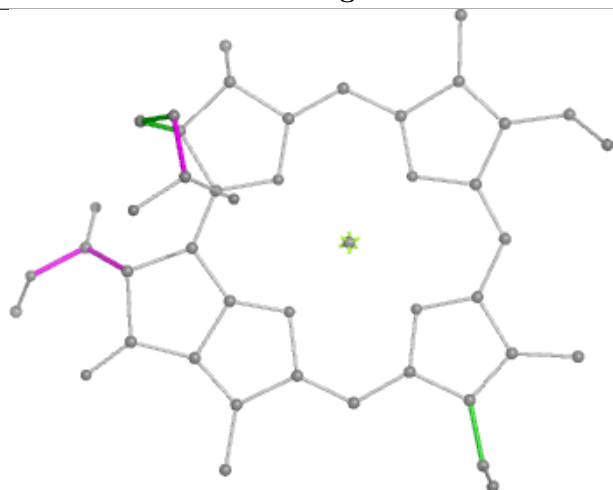
Ligand CLA J 101



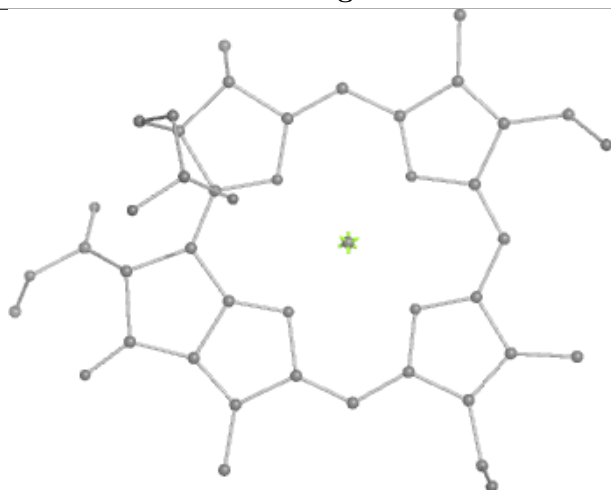
Bond lengths



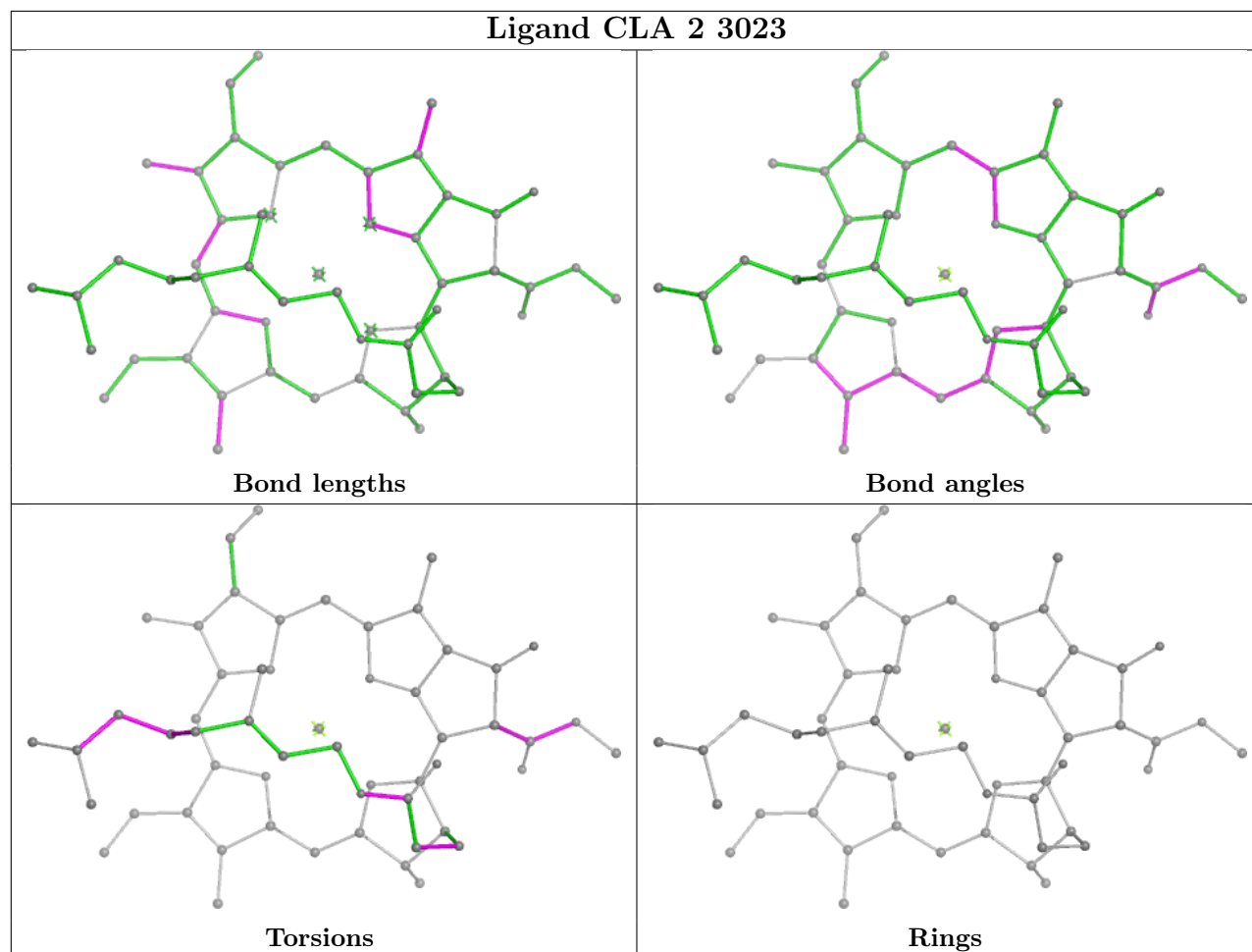
Bond angles



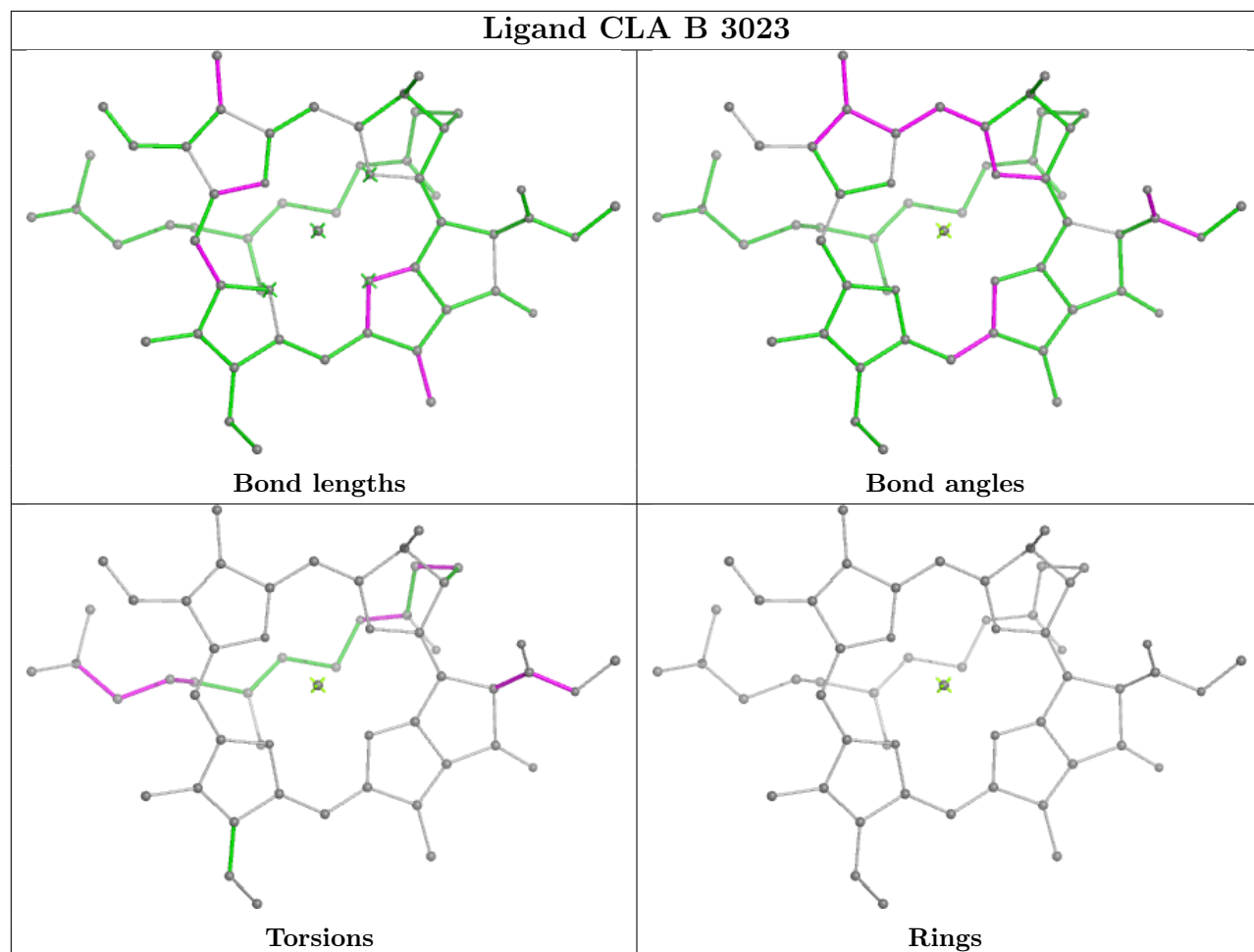
Torsions



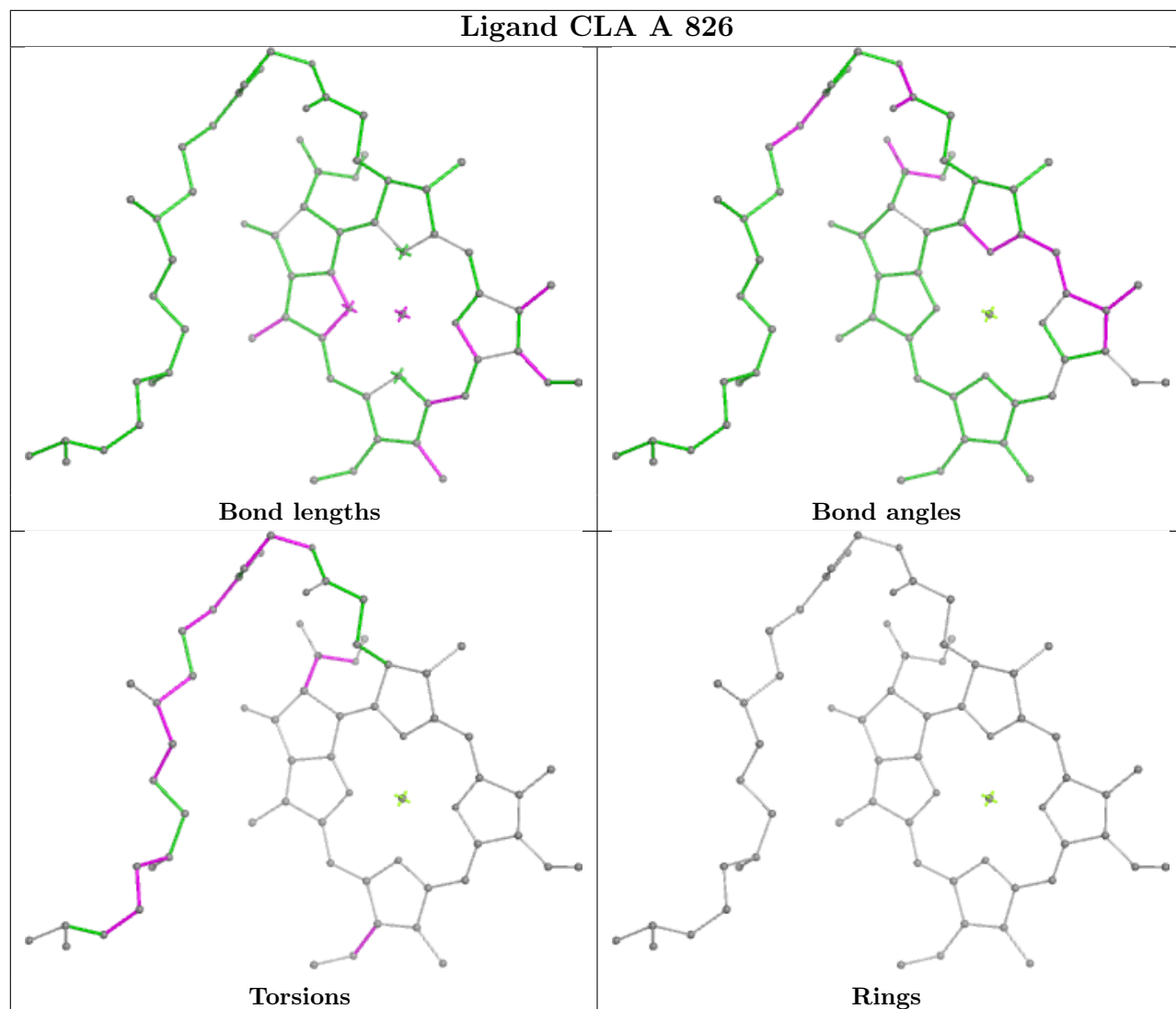
Rings

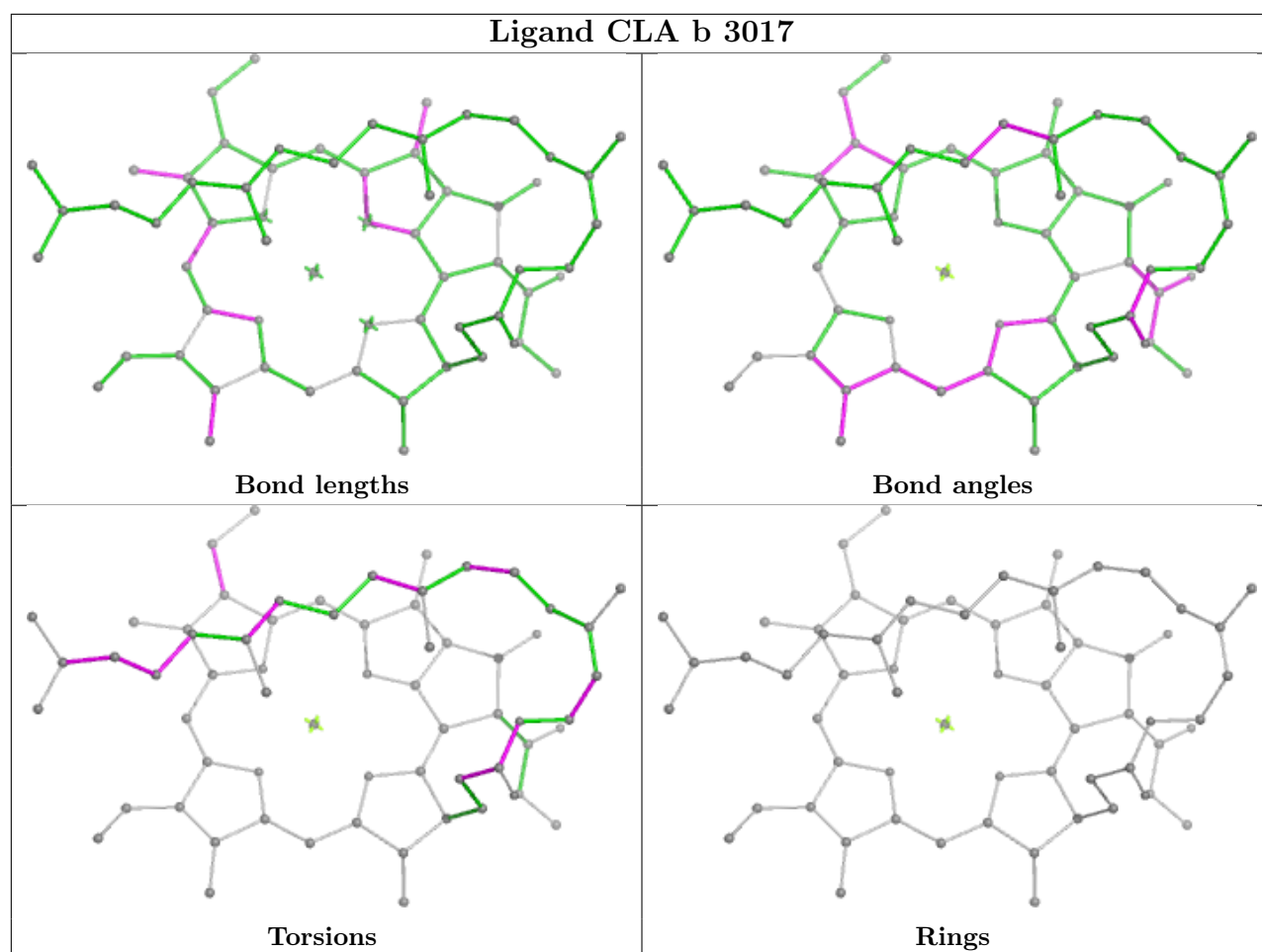


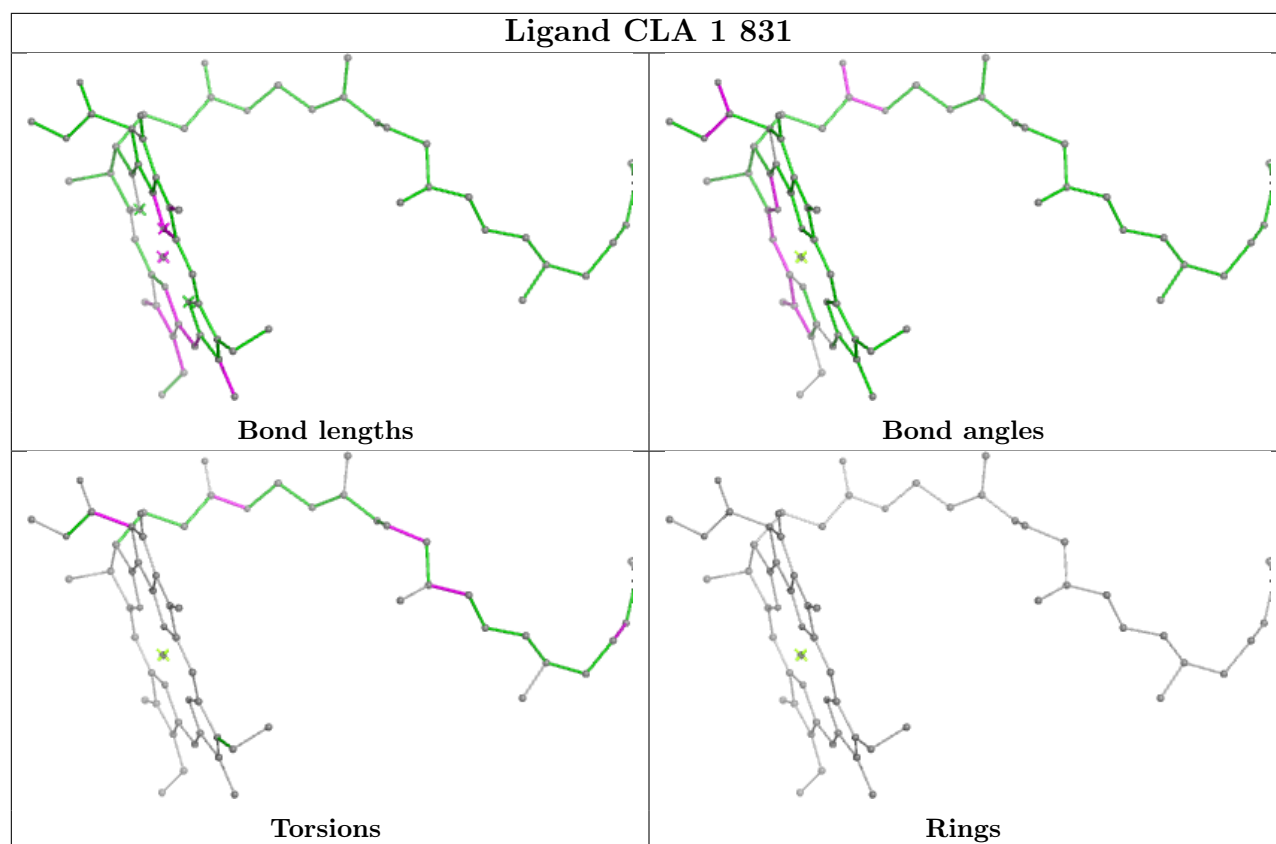
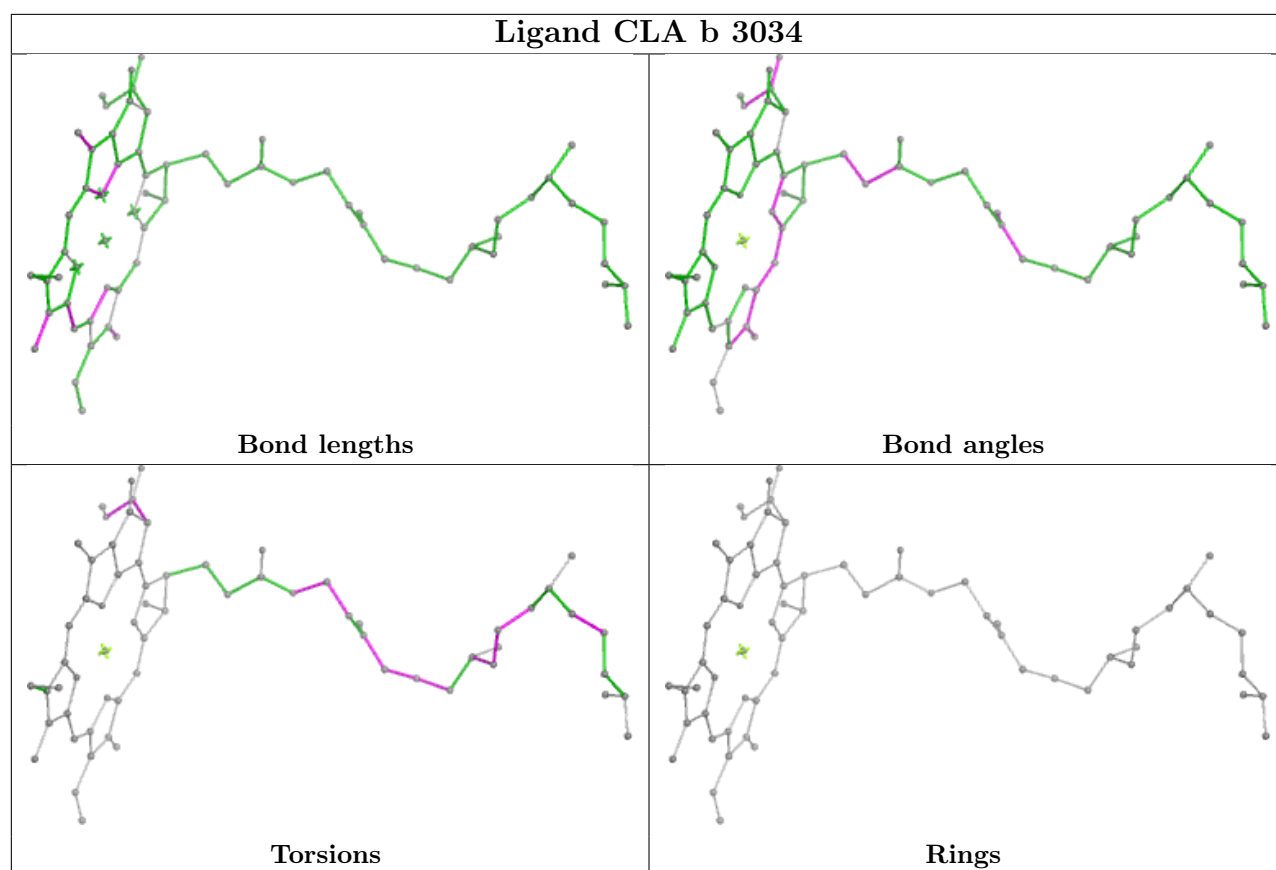
Ligand CLA B 3023

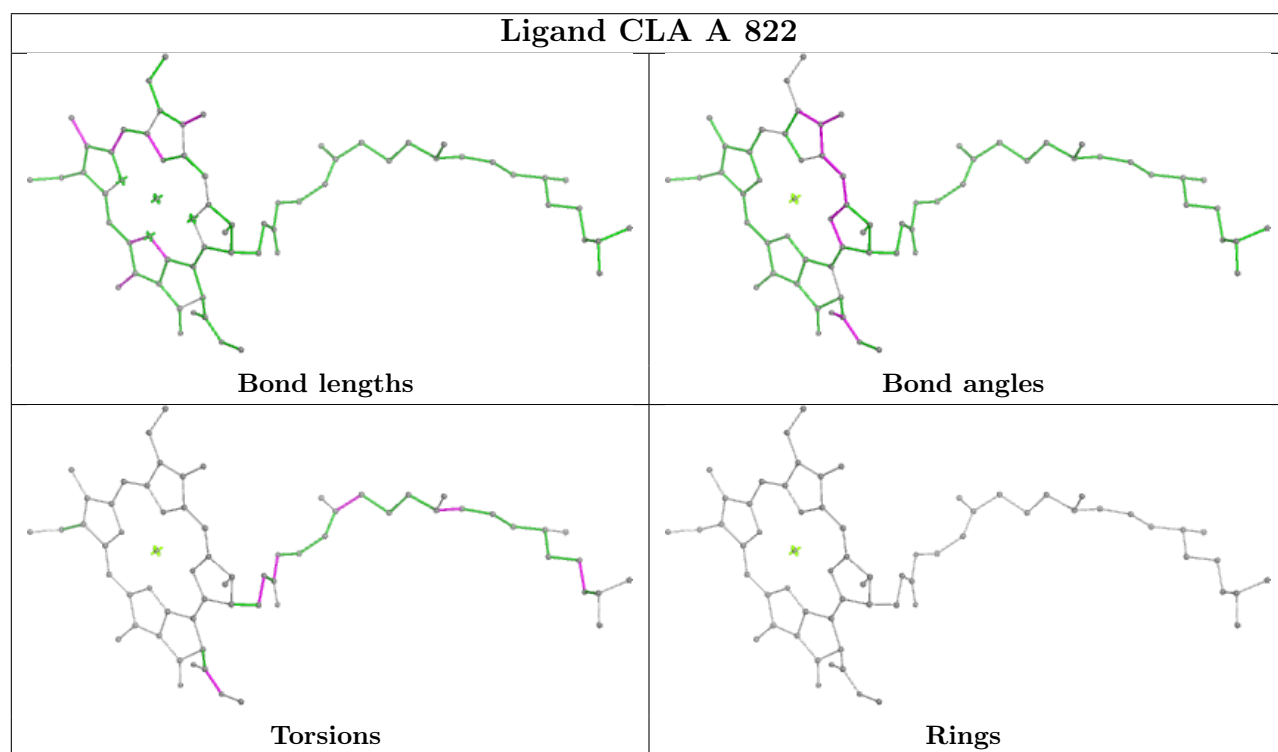
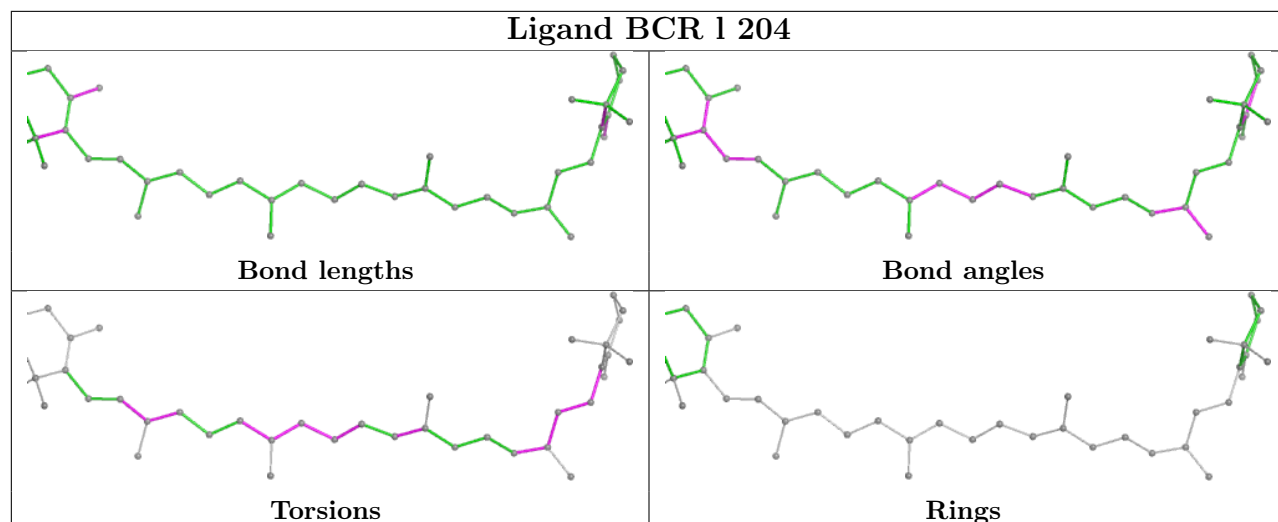


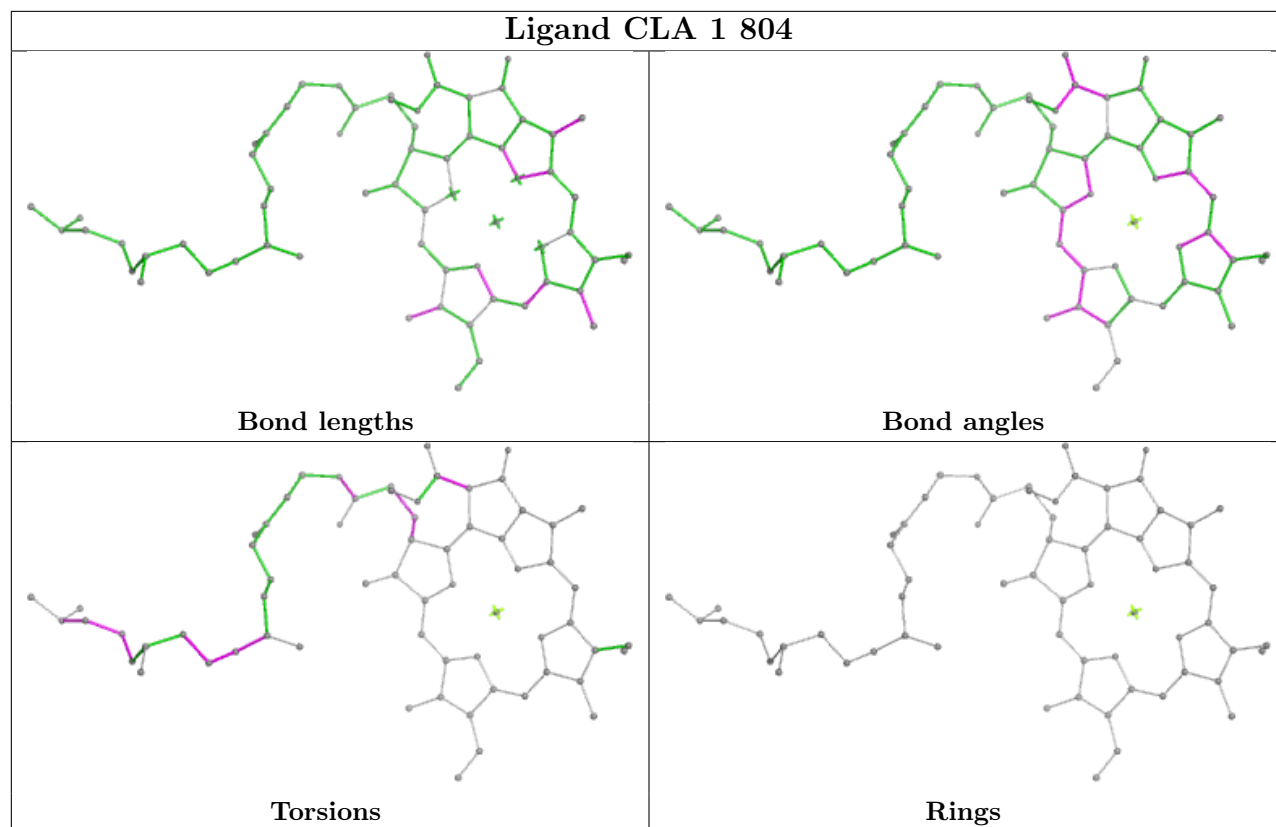
Ligand CLA A 826

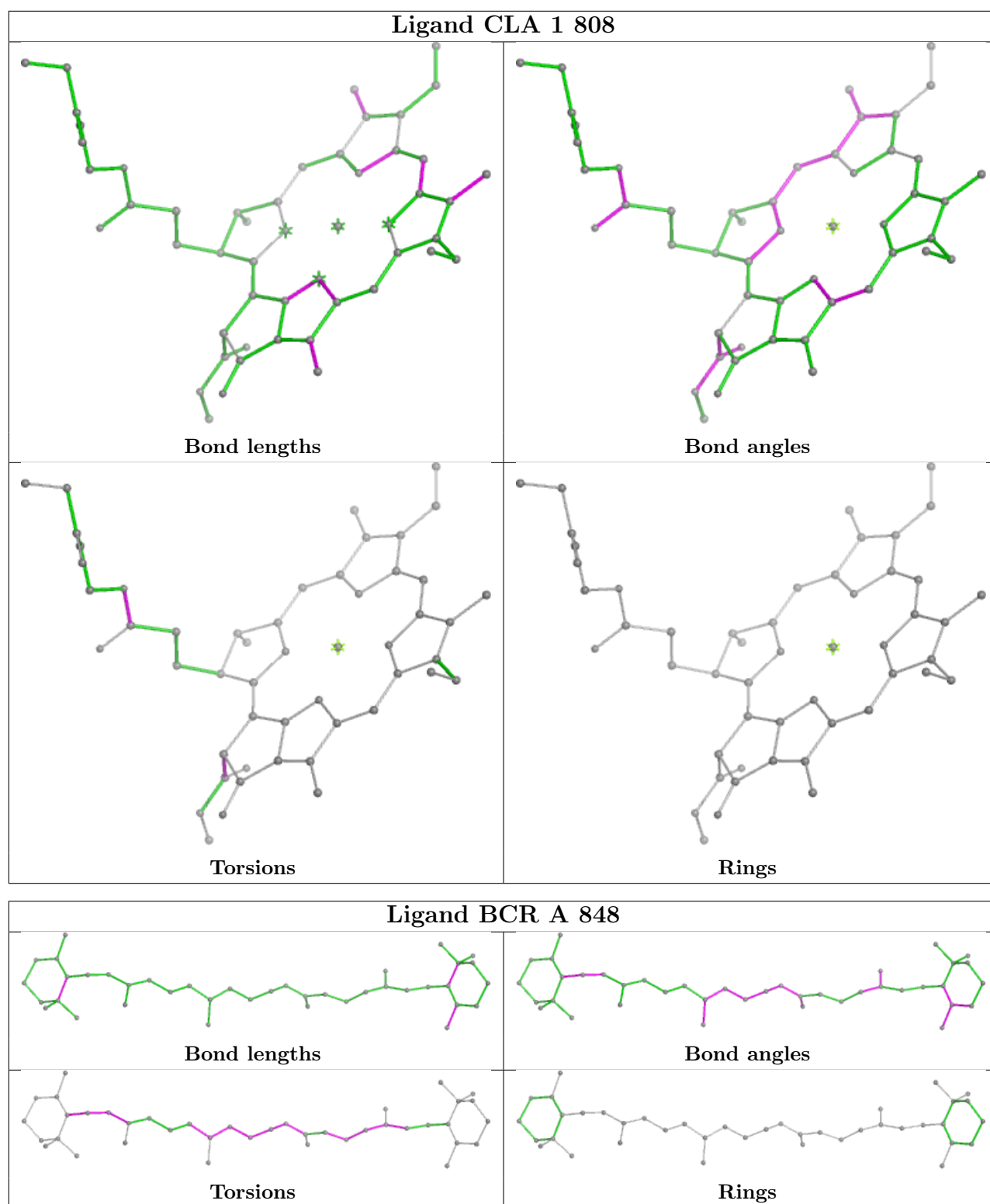


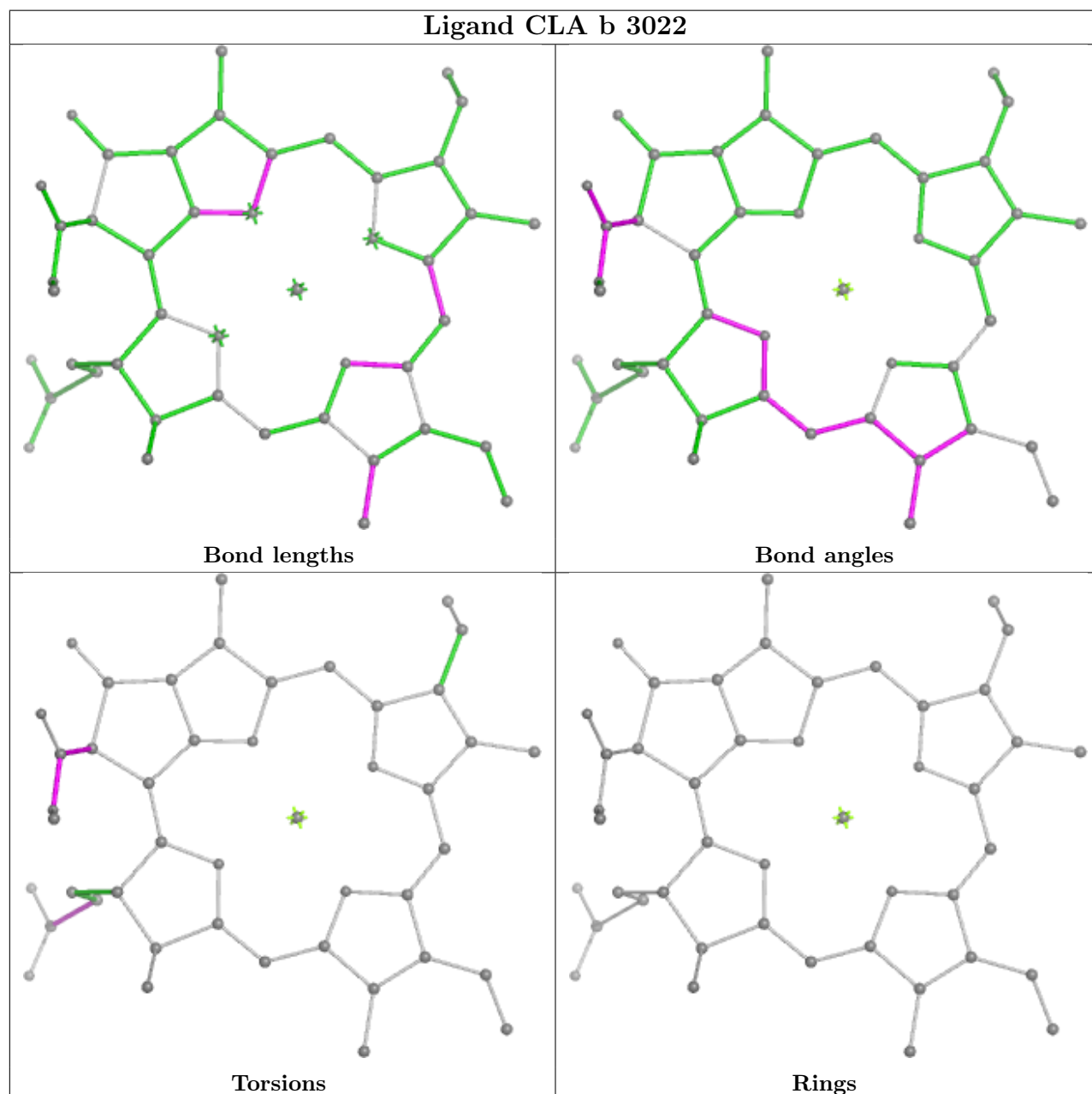
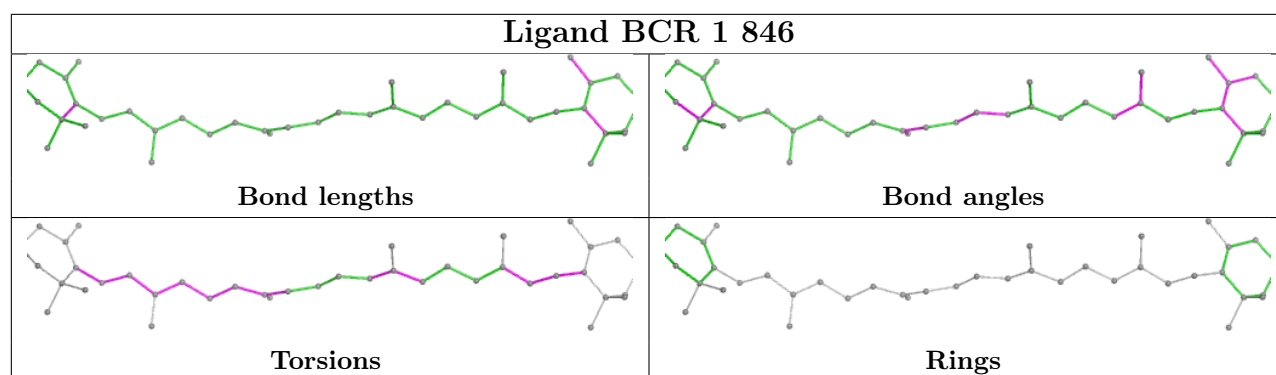




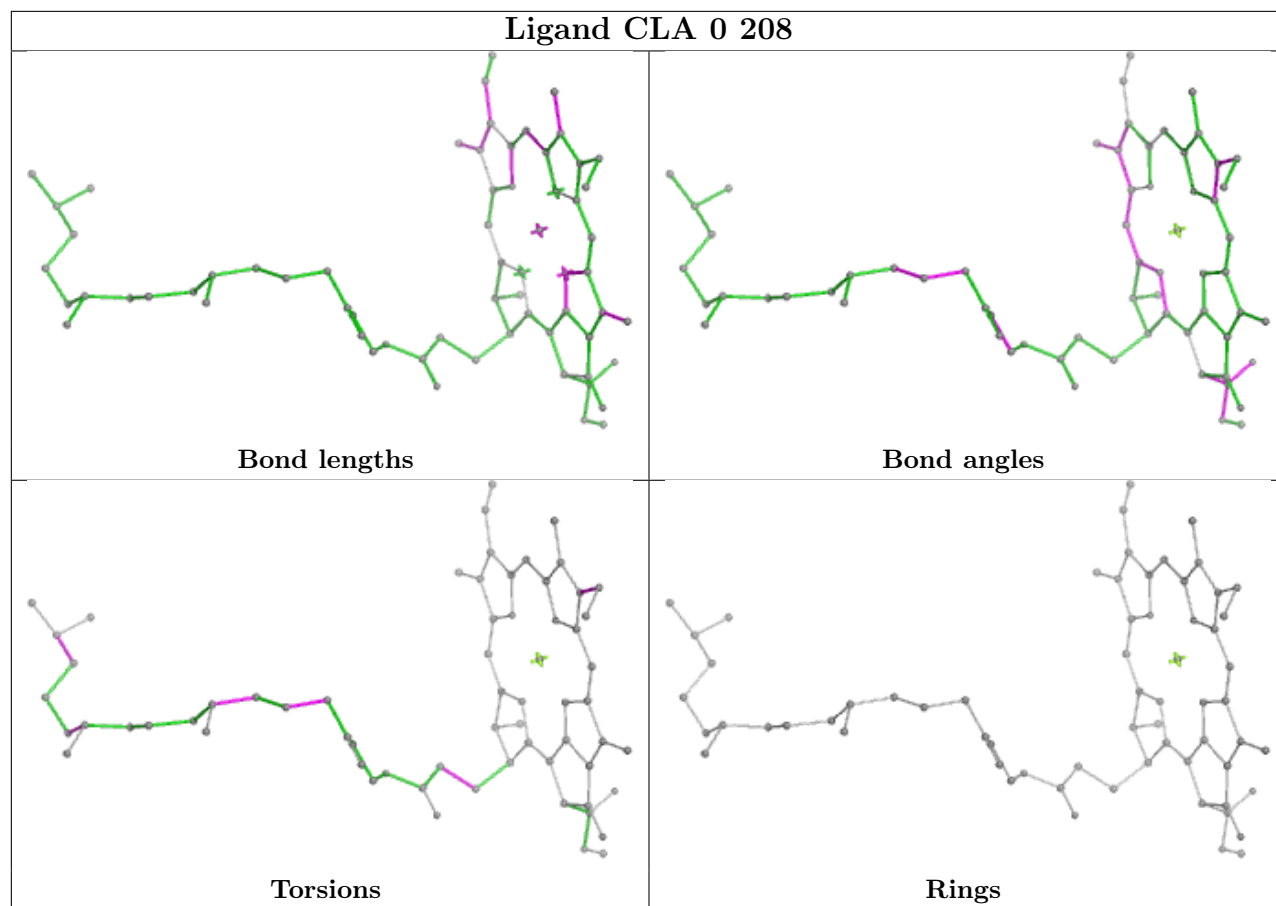




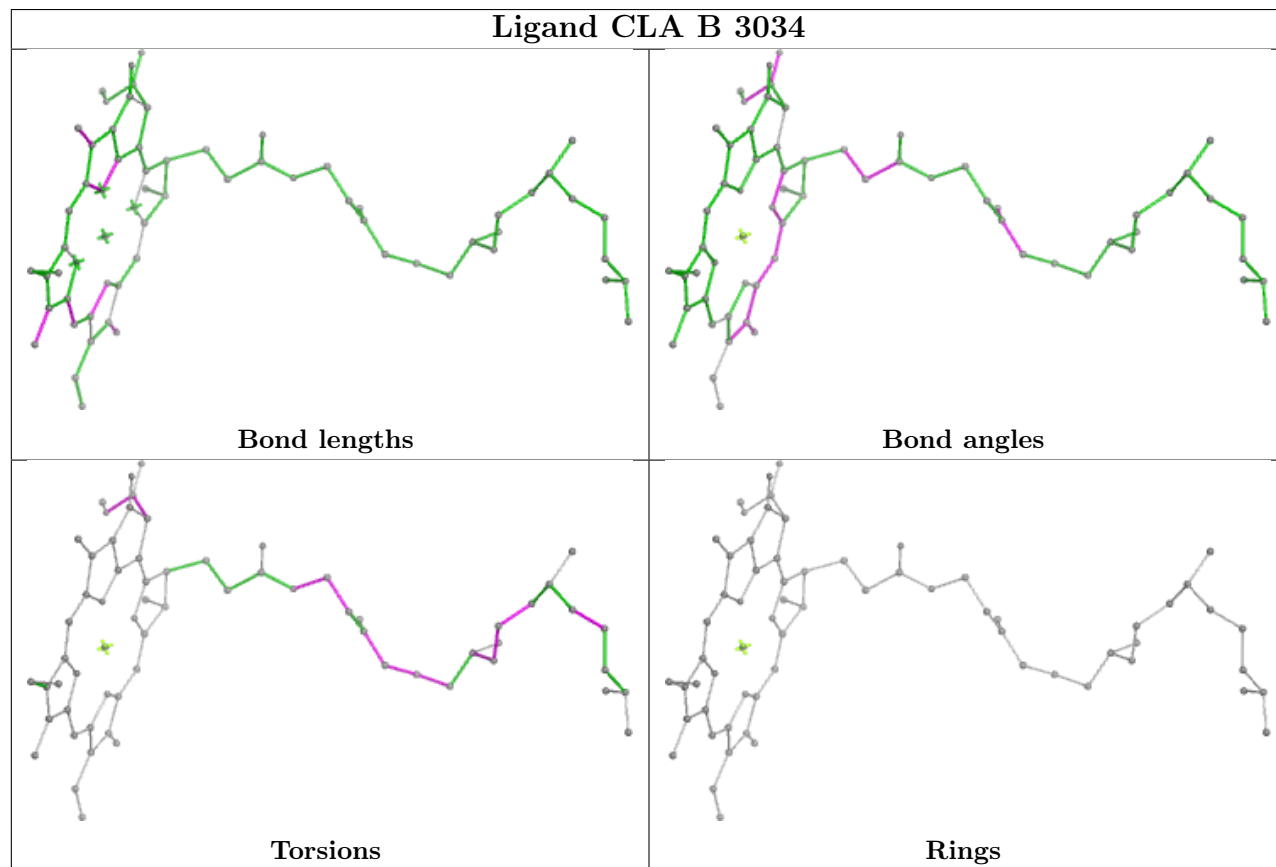




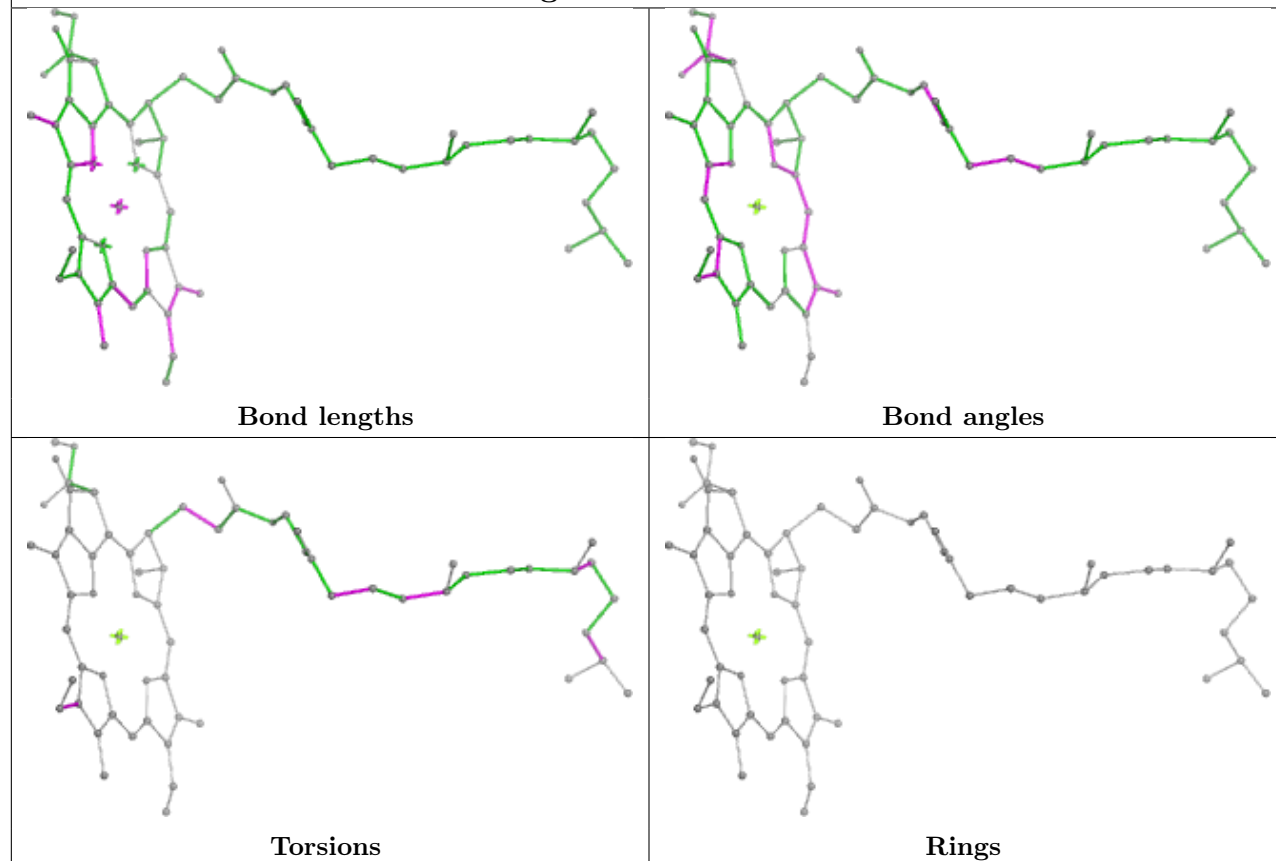
Ligand CLA 0 208



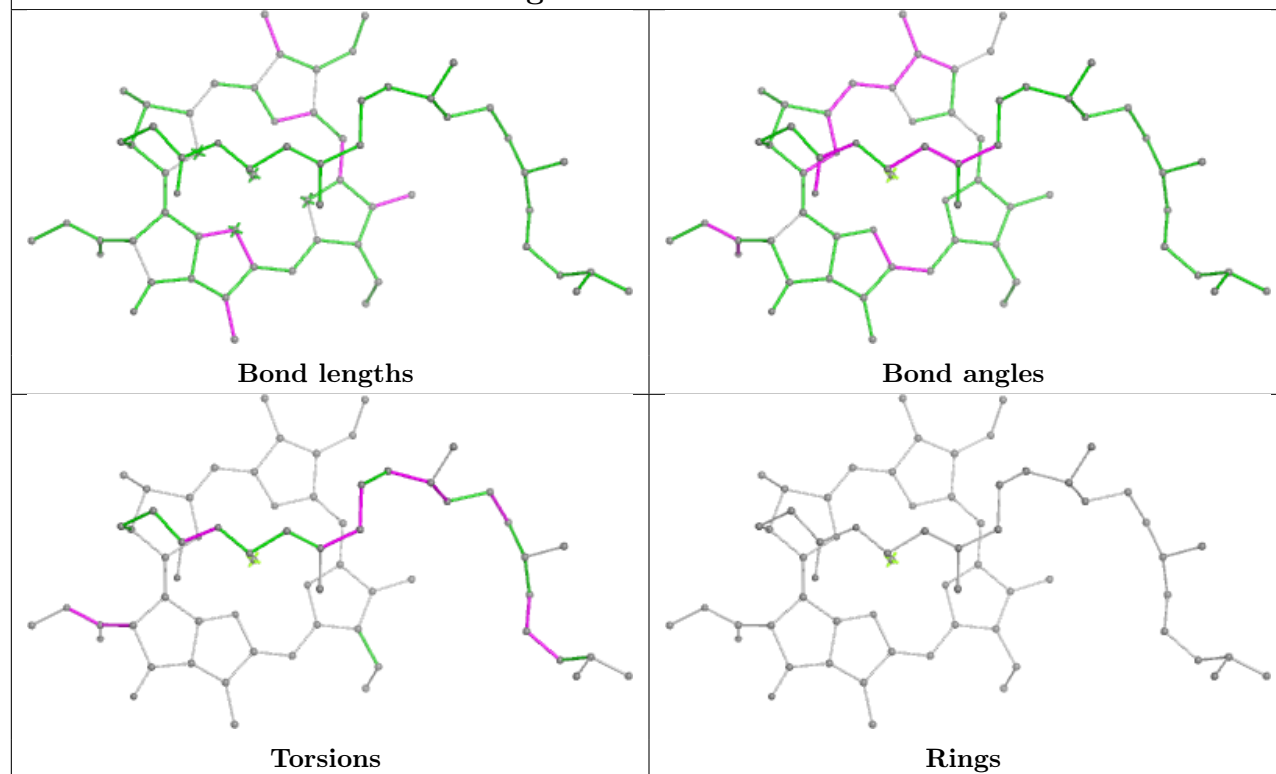
Ligand CLA B 3034

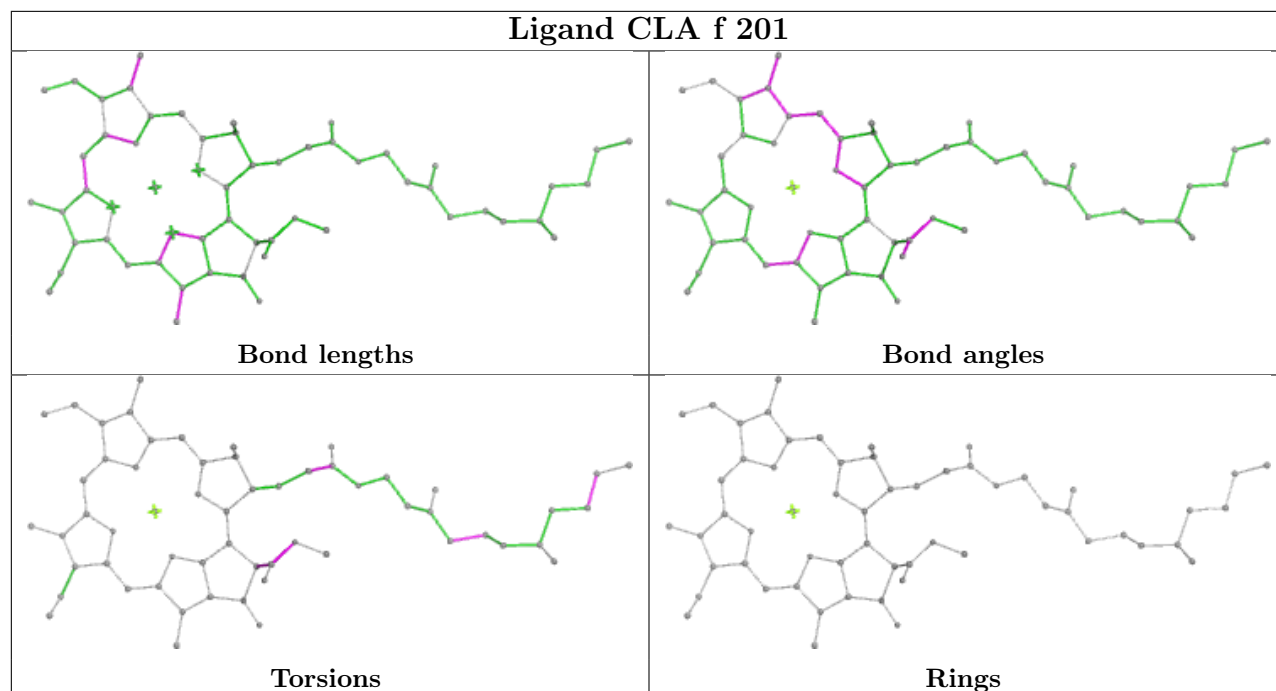
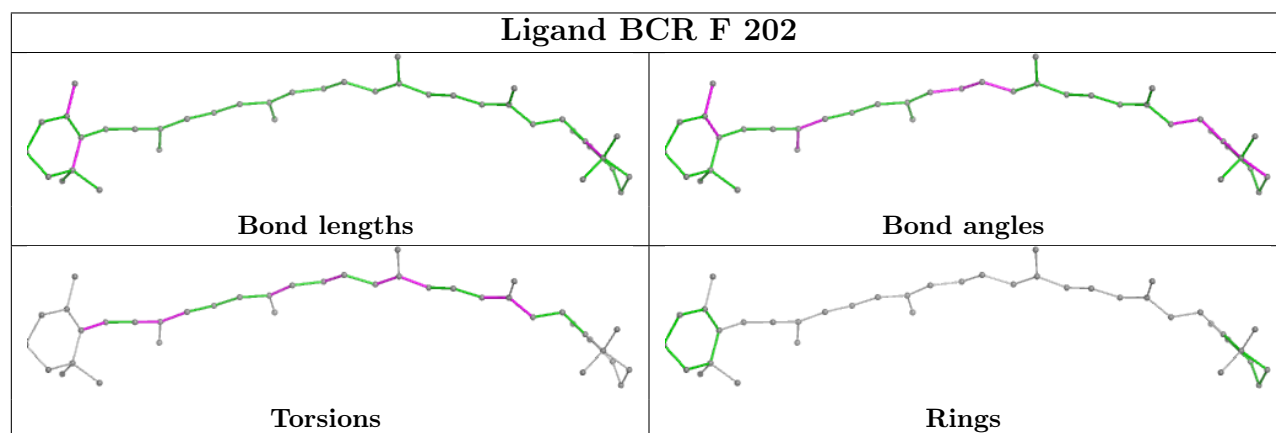


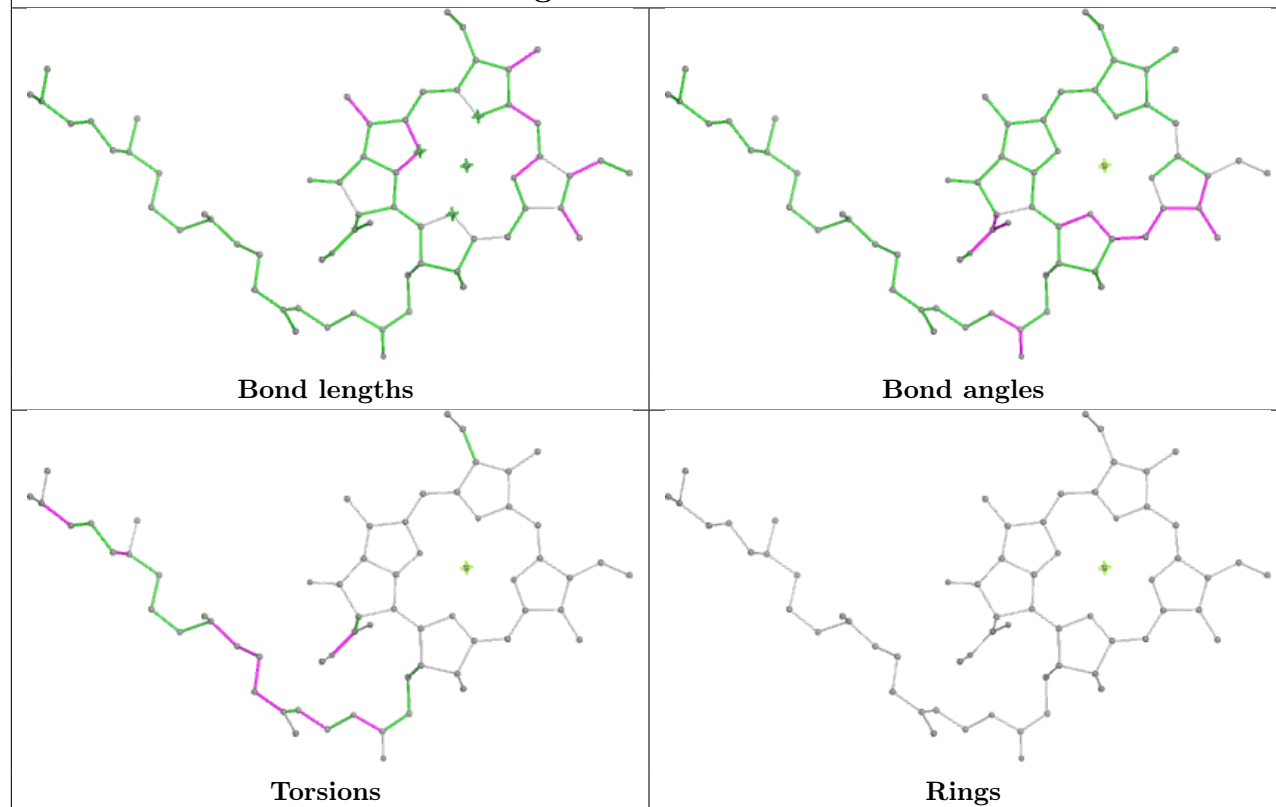
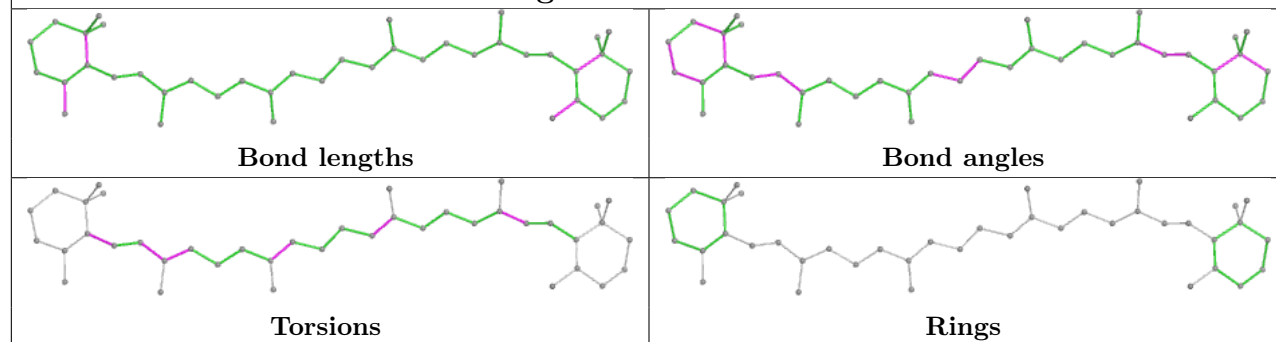
Ligand CLA l 207

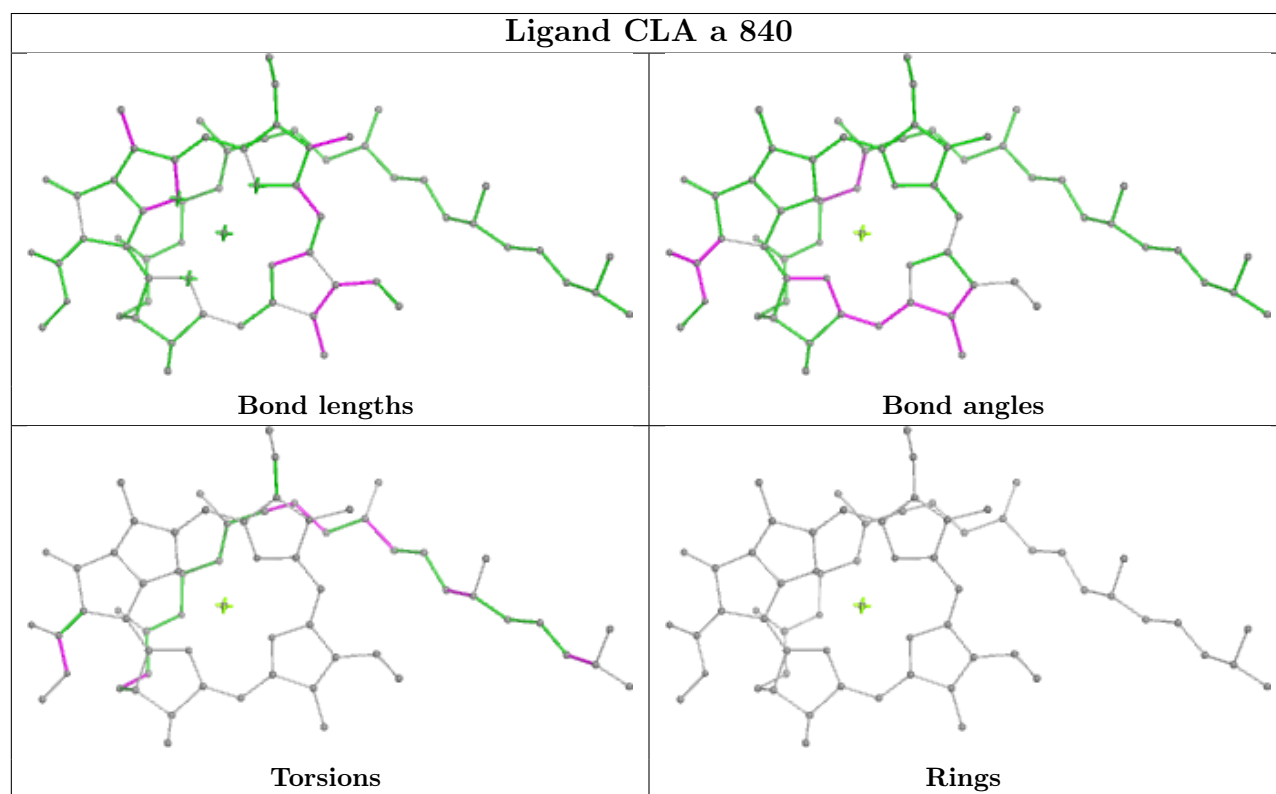
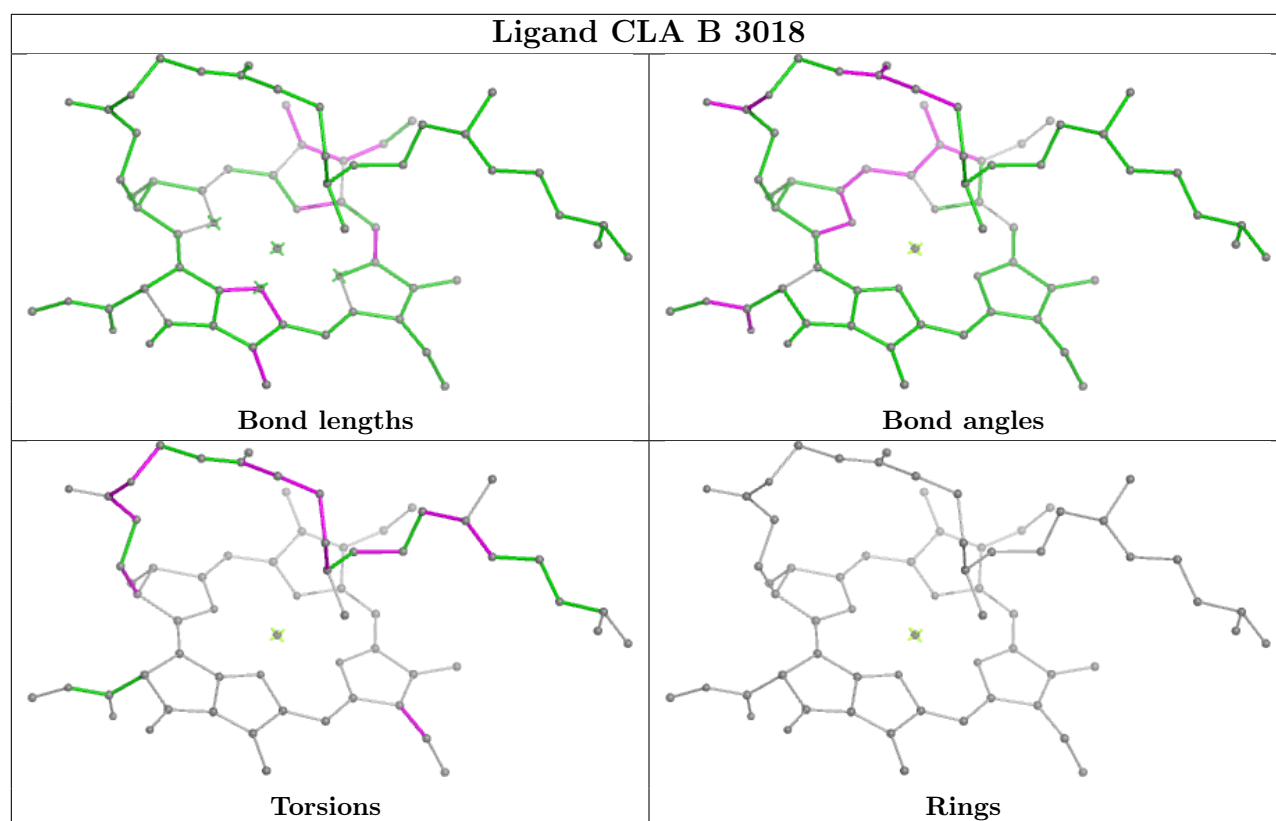


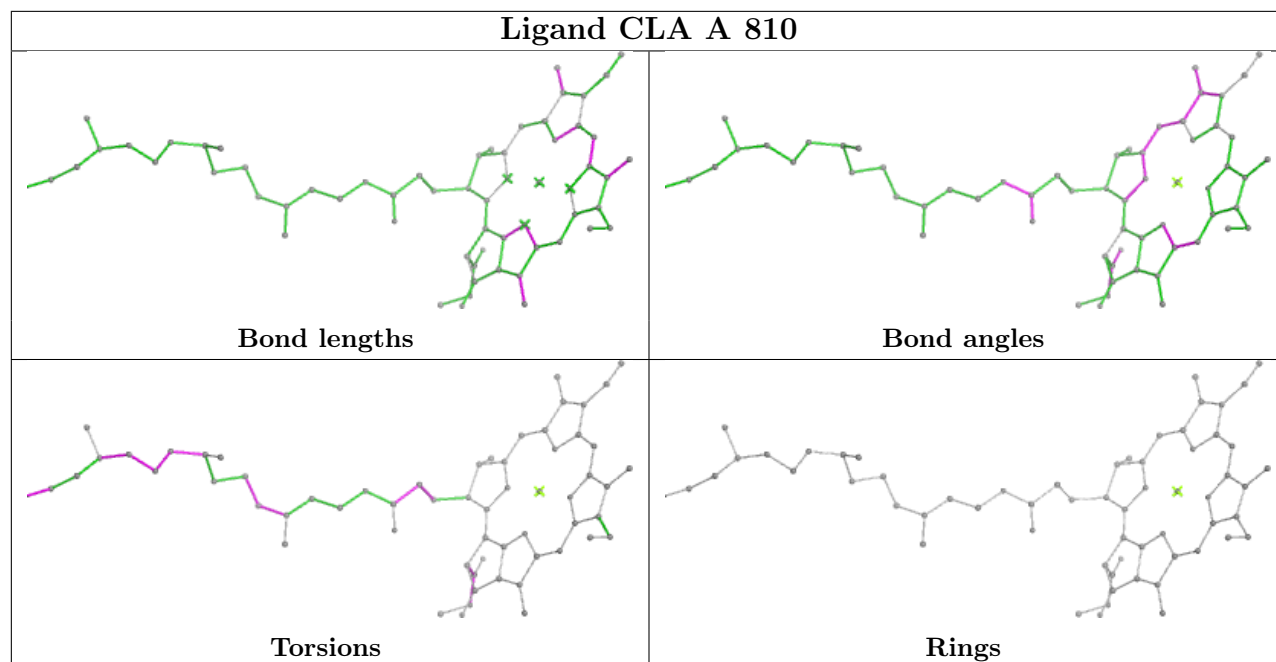
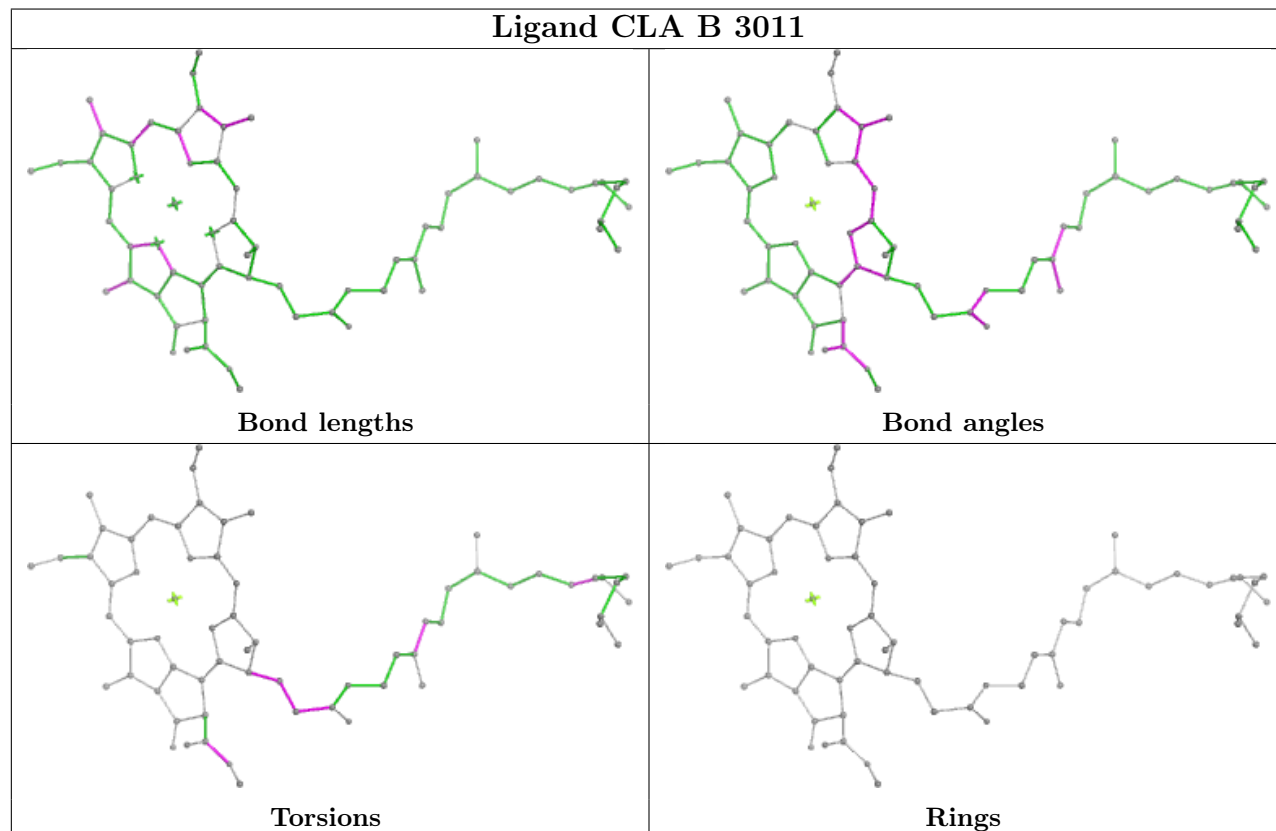
Ligand CLA b 3039

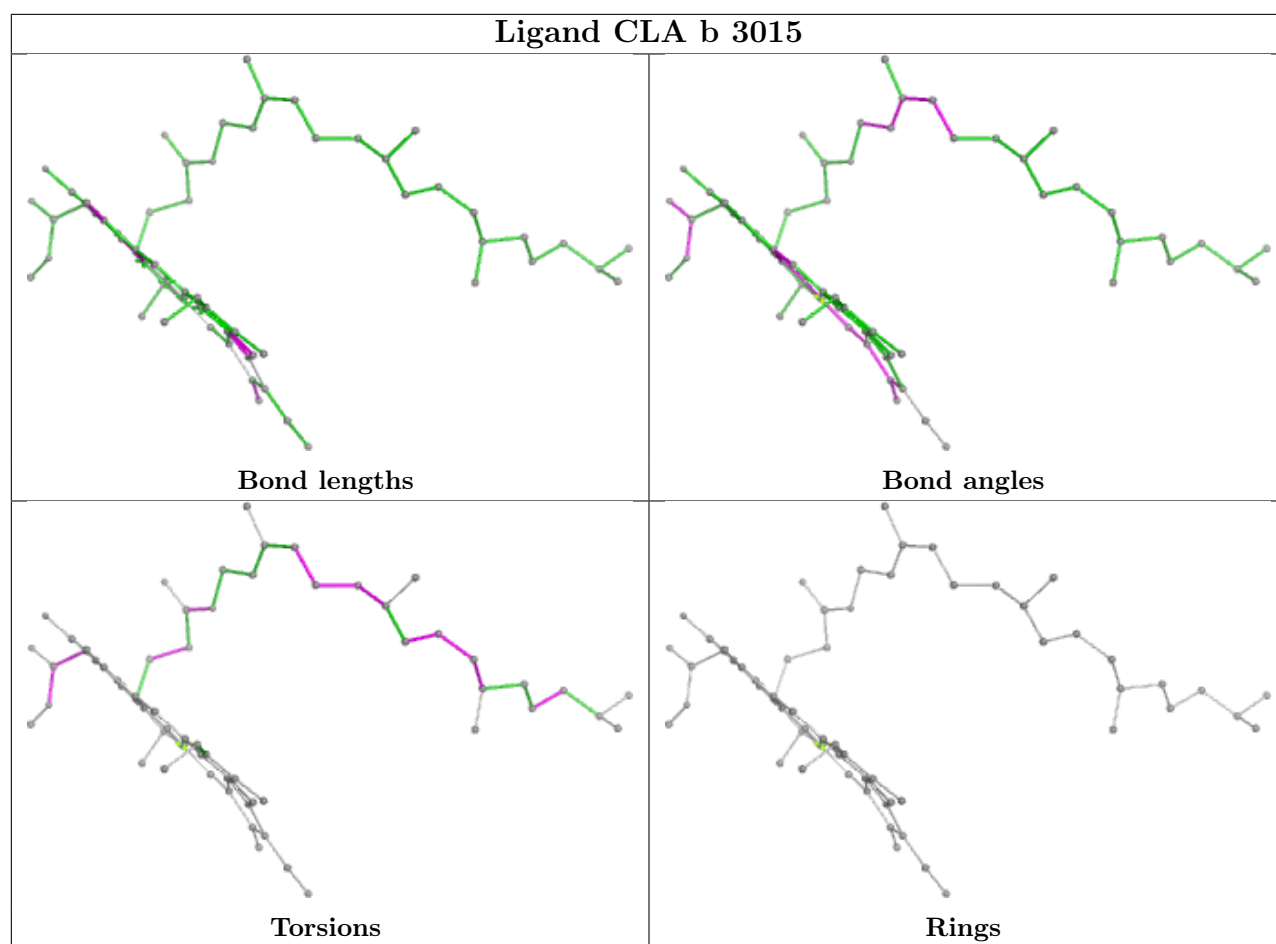


Ligand CLA f 201**Ligand BCR F 202**

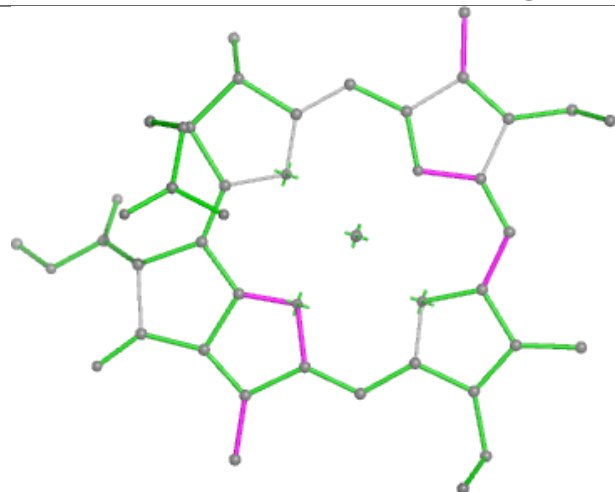
Ligand CLA L 205**Ligand BCR I 102**



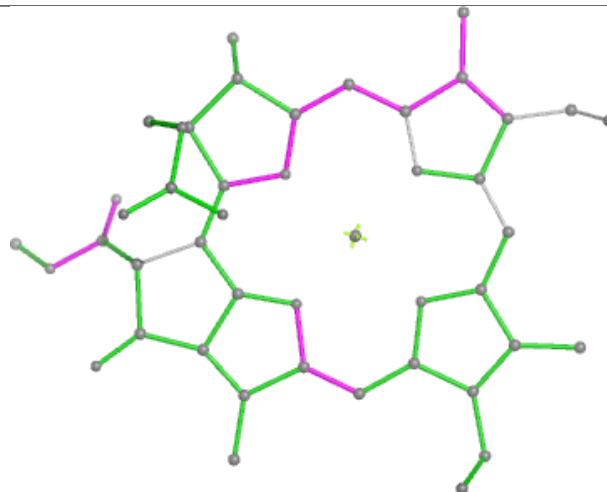
Ligand CLA A 810**Ligand CLA B 3011**



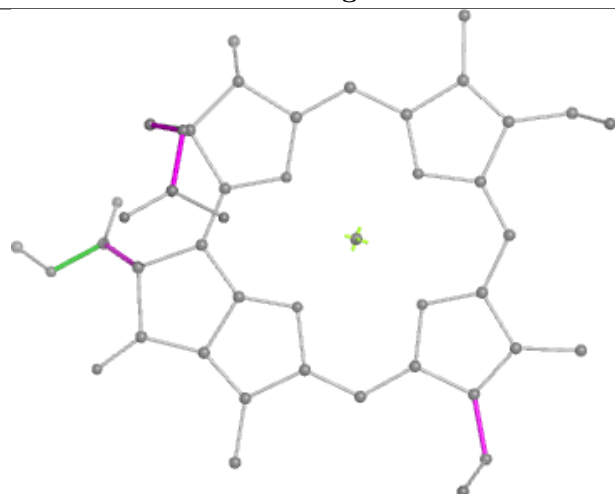
Ligand CLA a 812



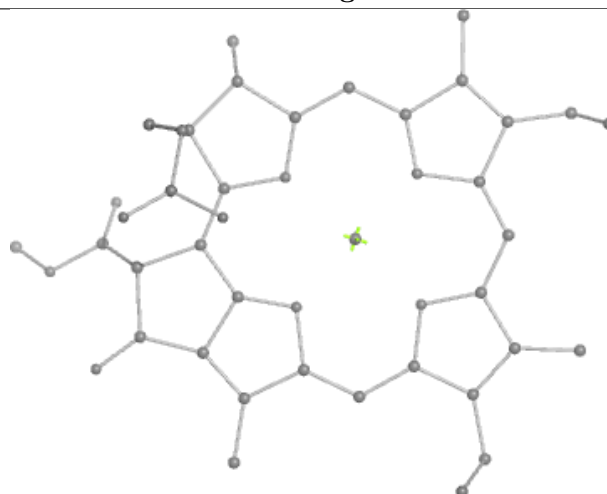
Bond lengths



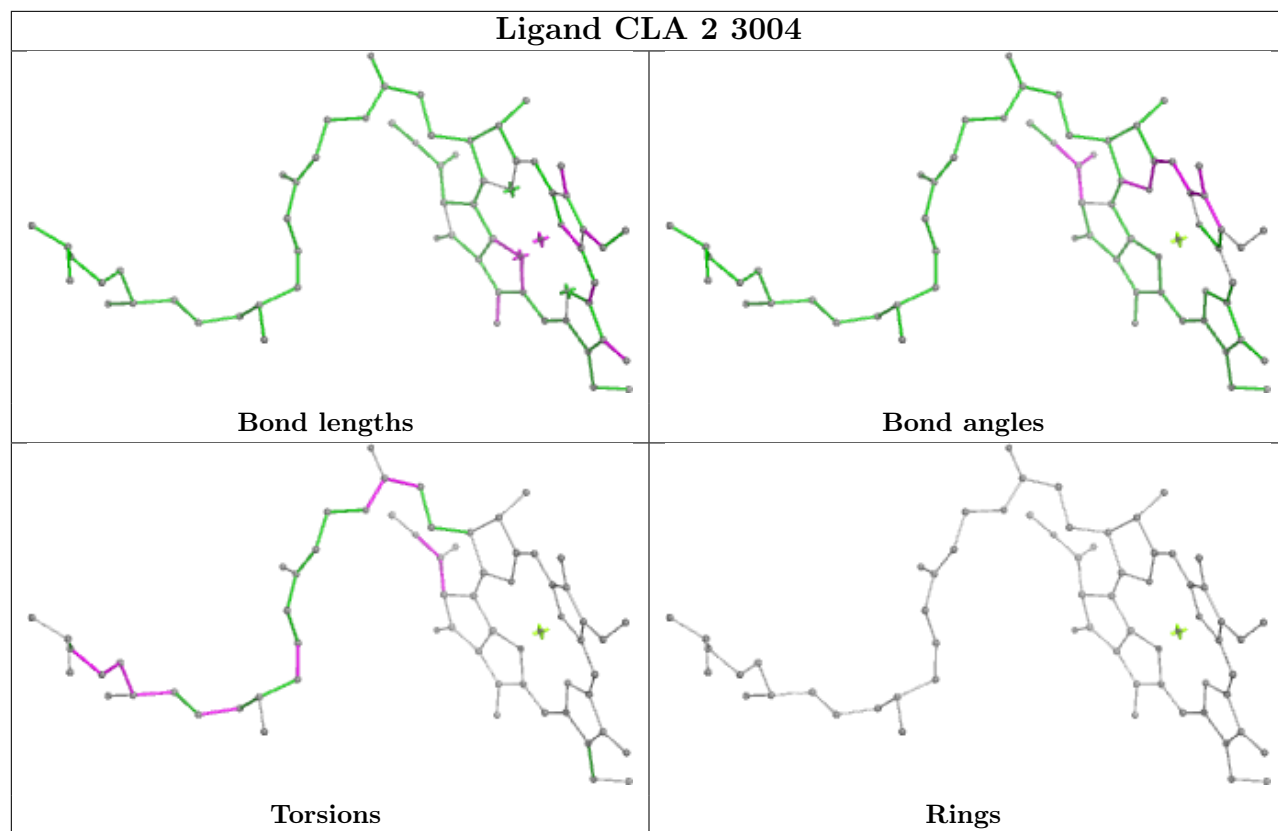
Bond angles



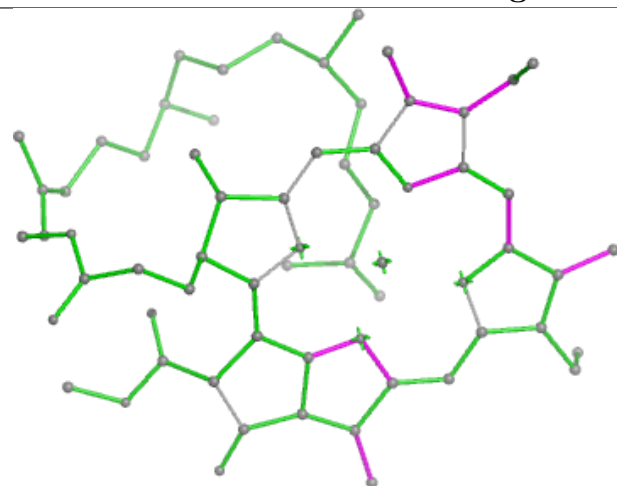
Torsions



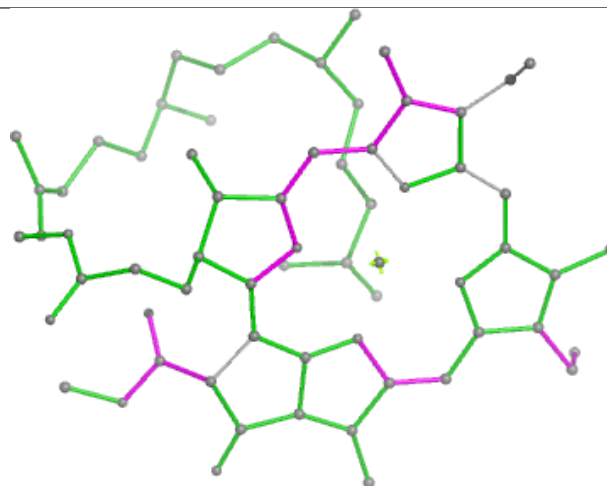
Rings



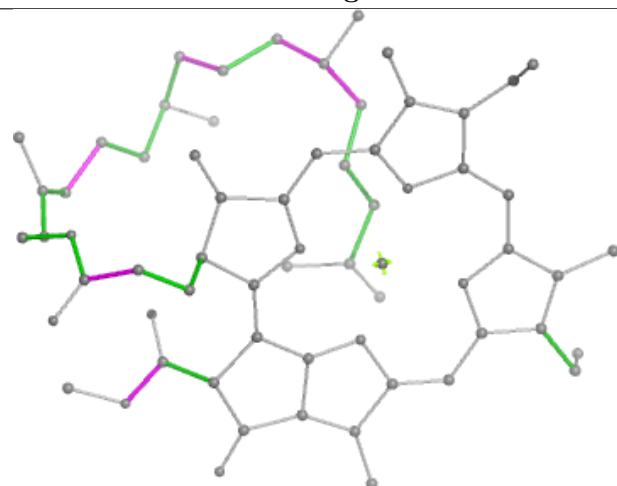
Ligand CLA B 3008



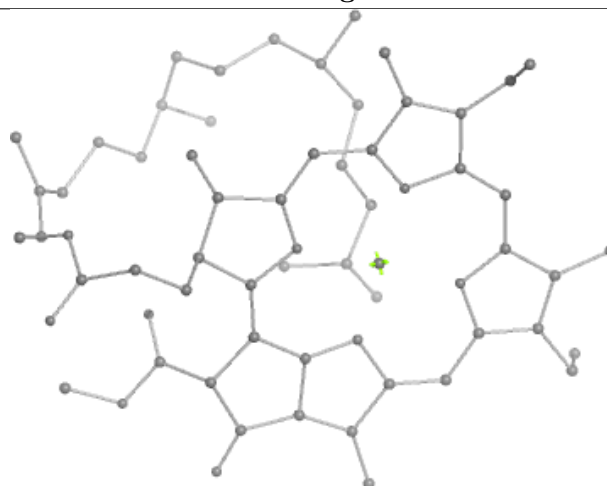
Bond lengths



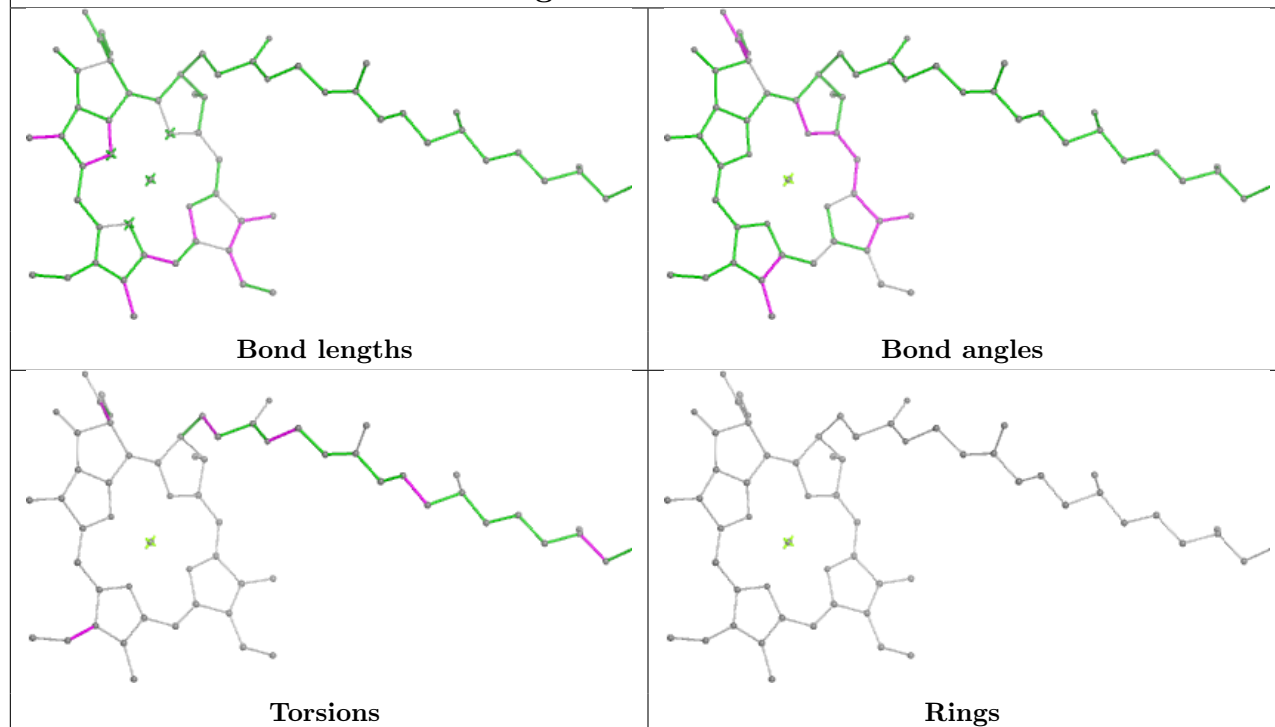
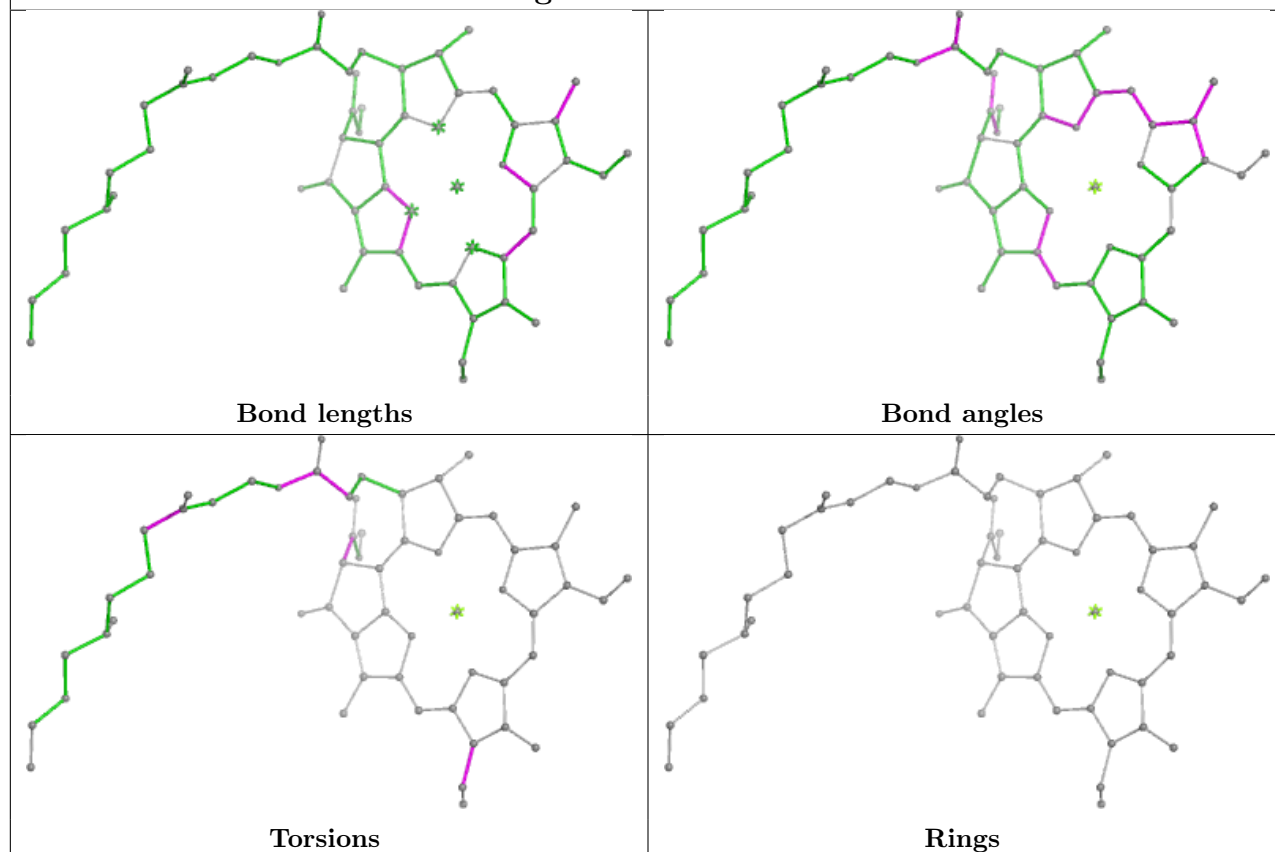
Bond angles

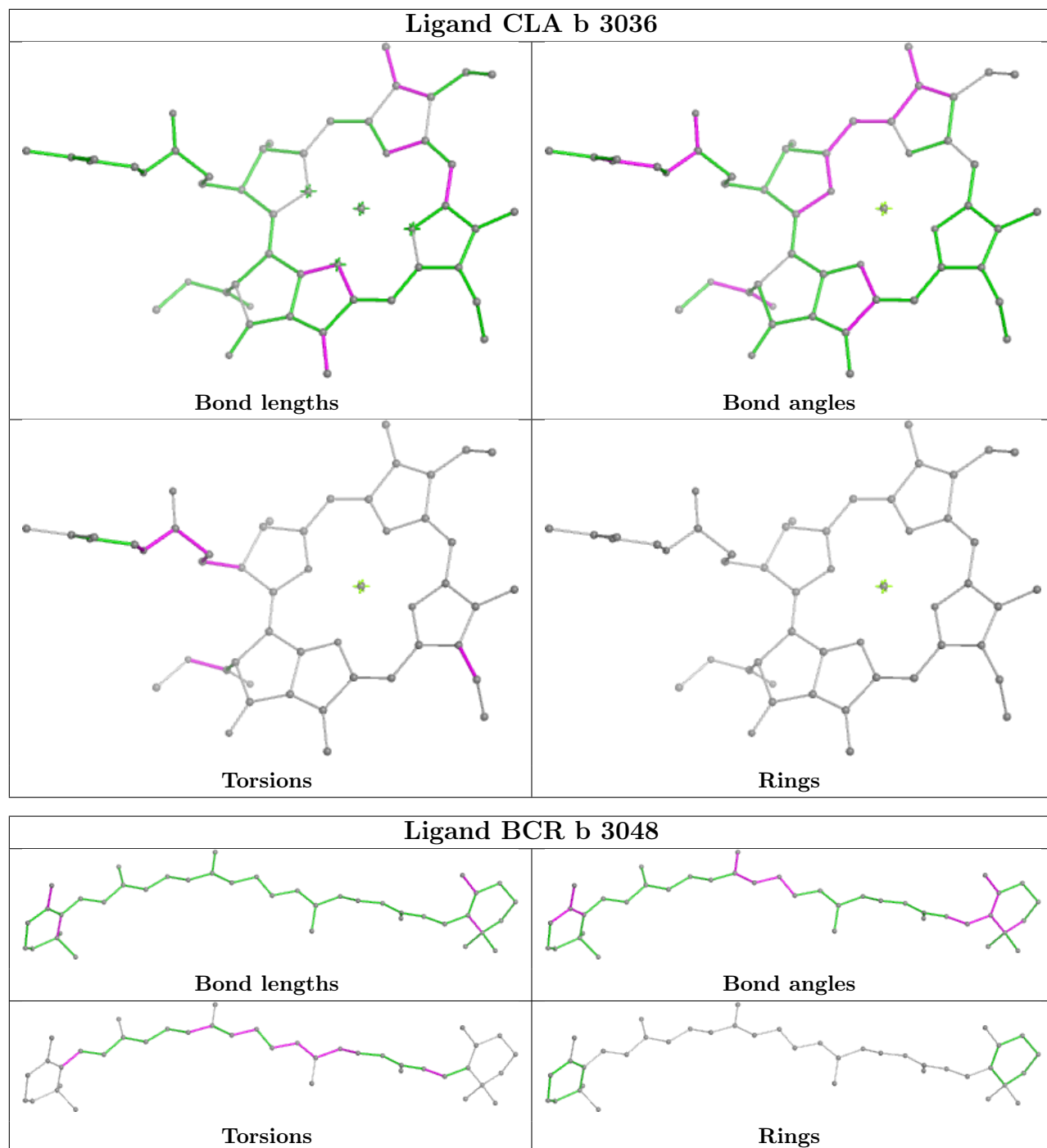


Torsions

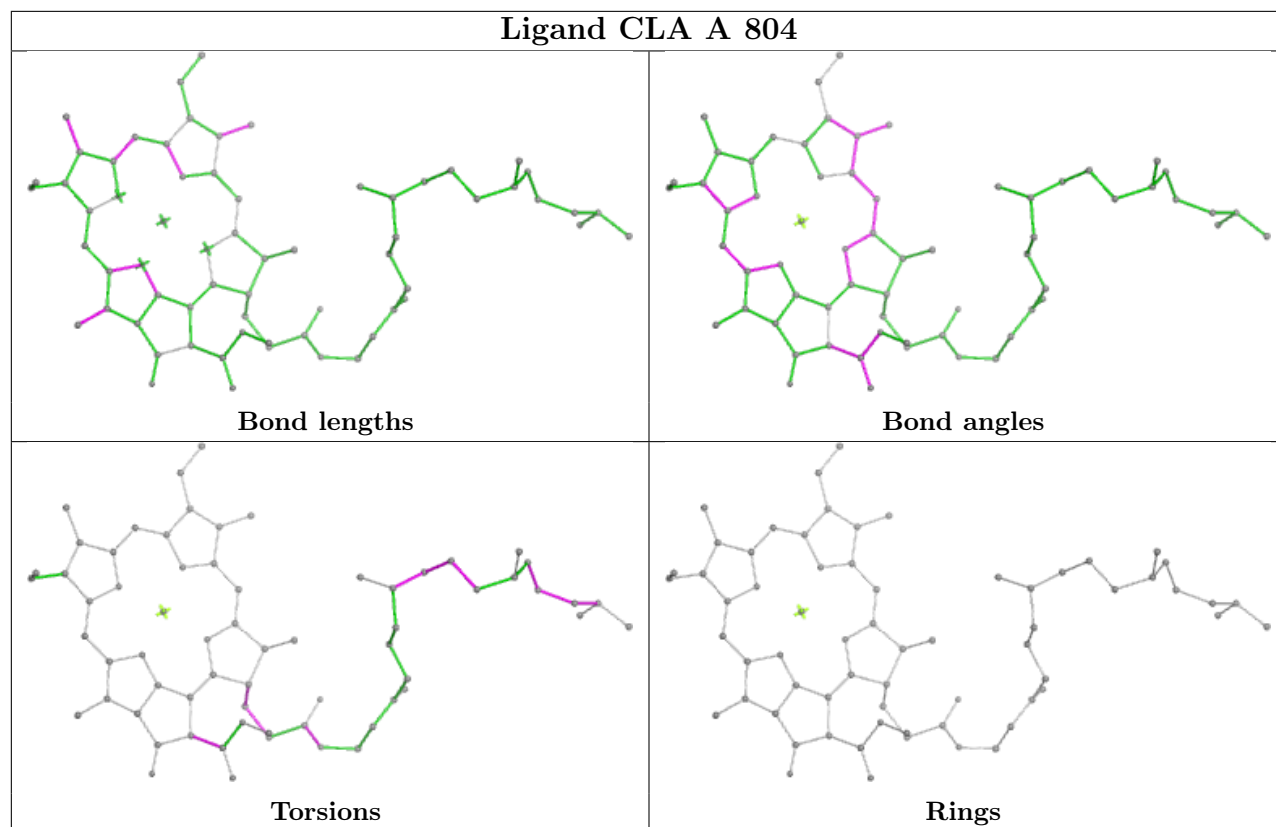


Rings

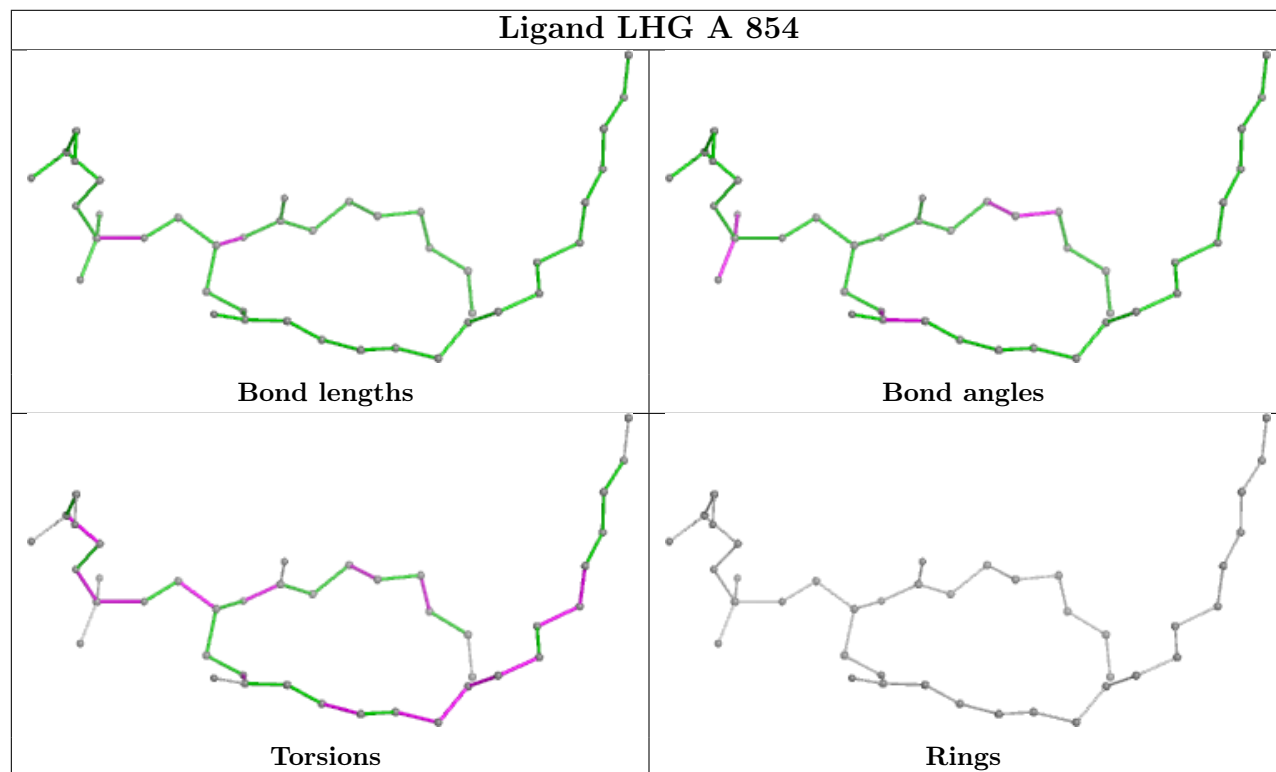
Ligand CLA 1 835**Ligand CLA k 102**

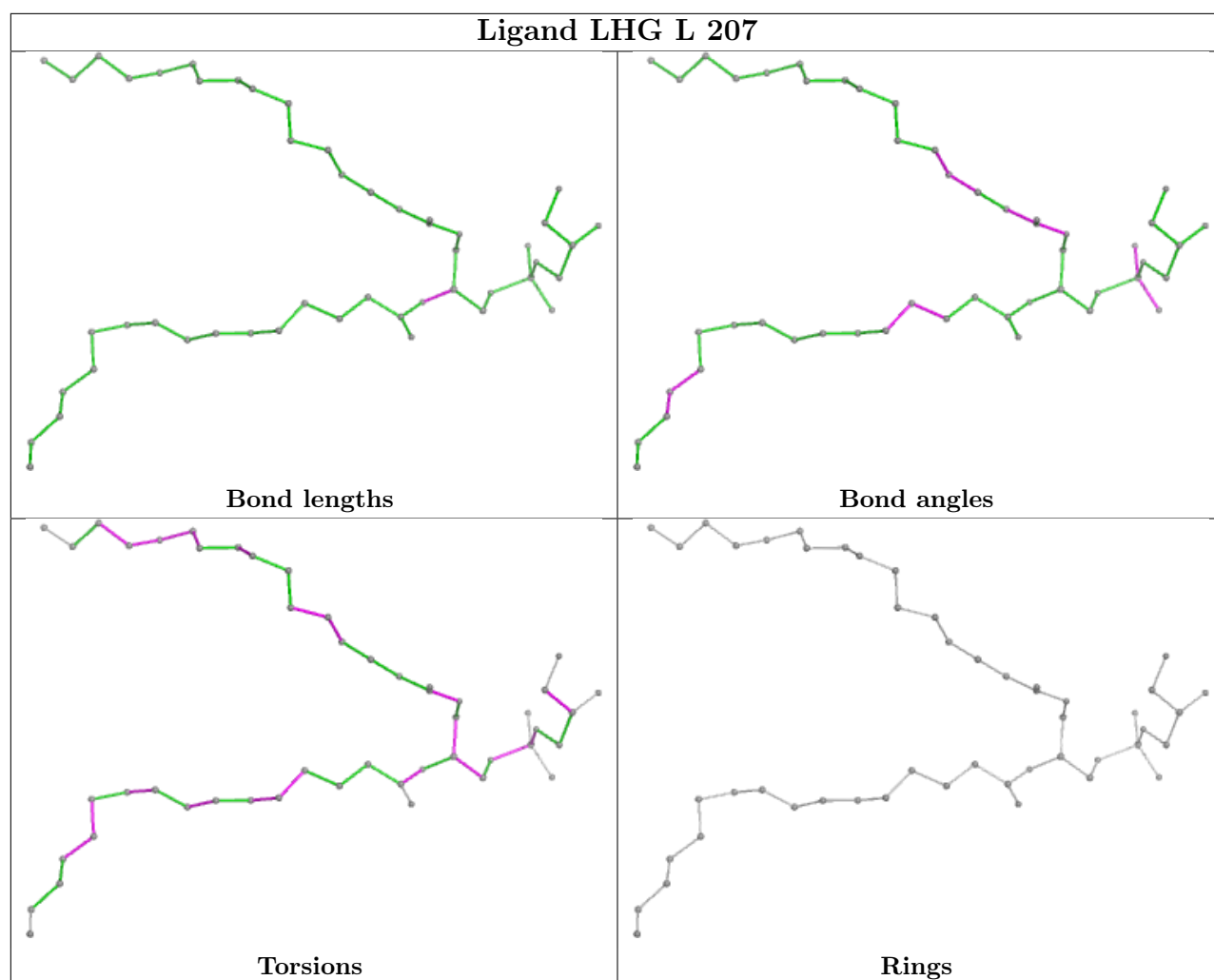


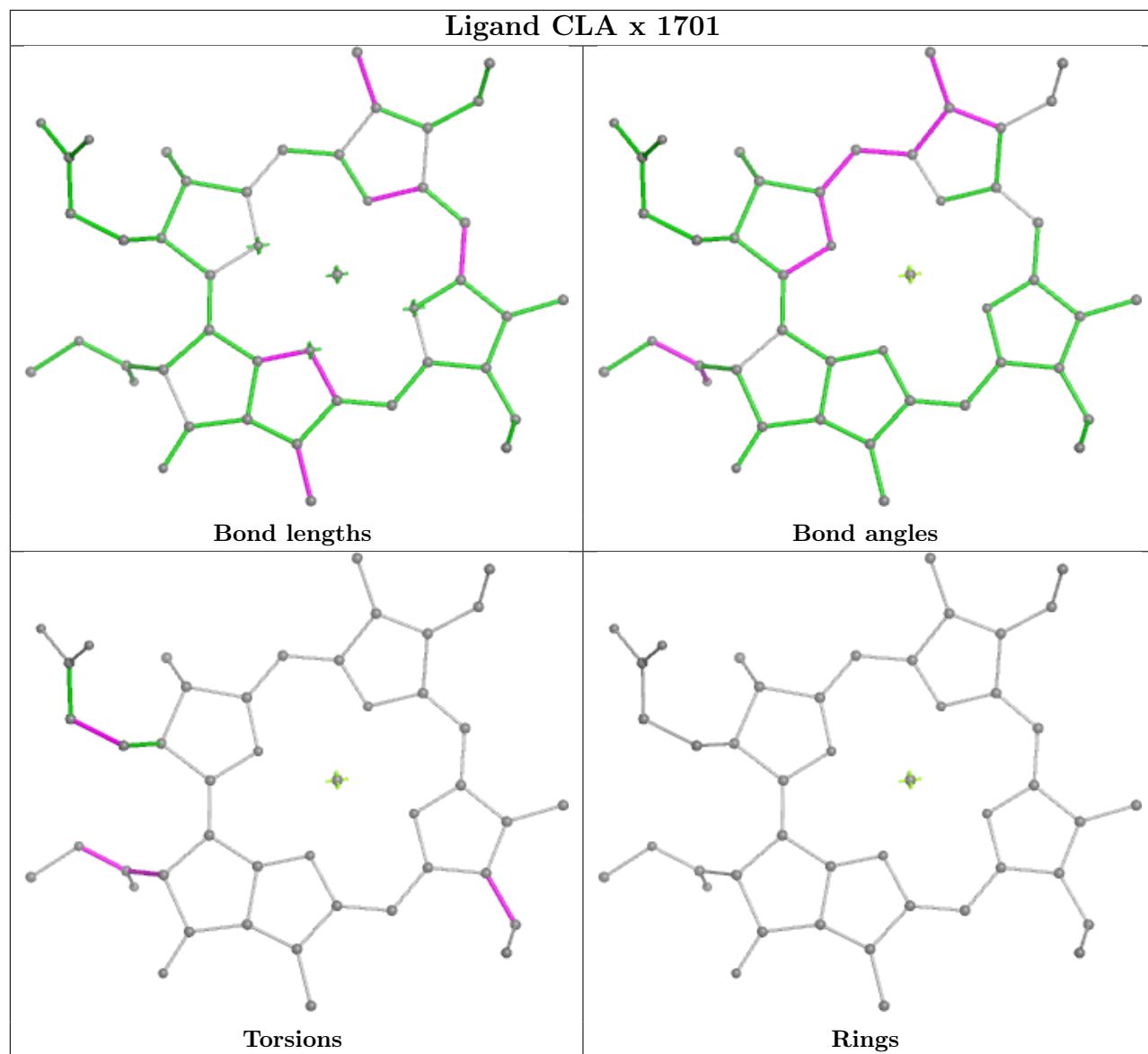
Ligand CLA A 804

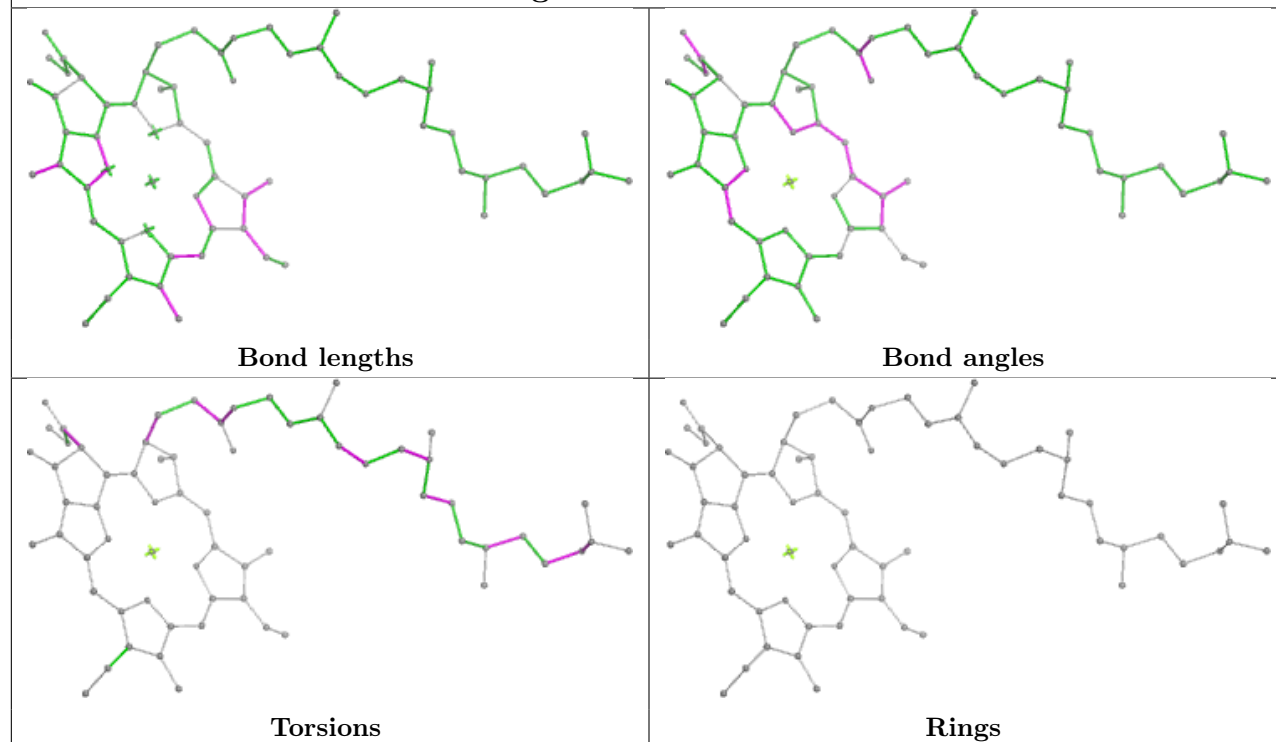
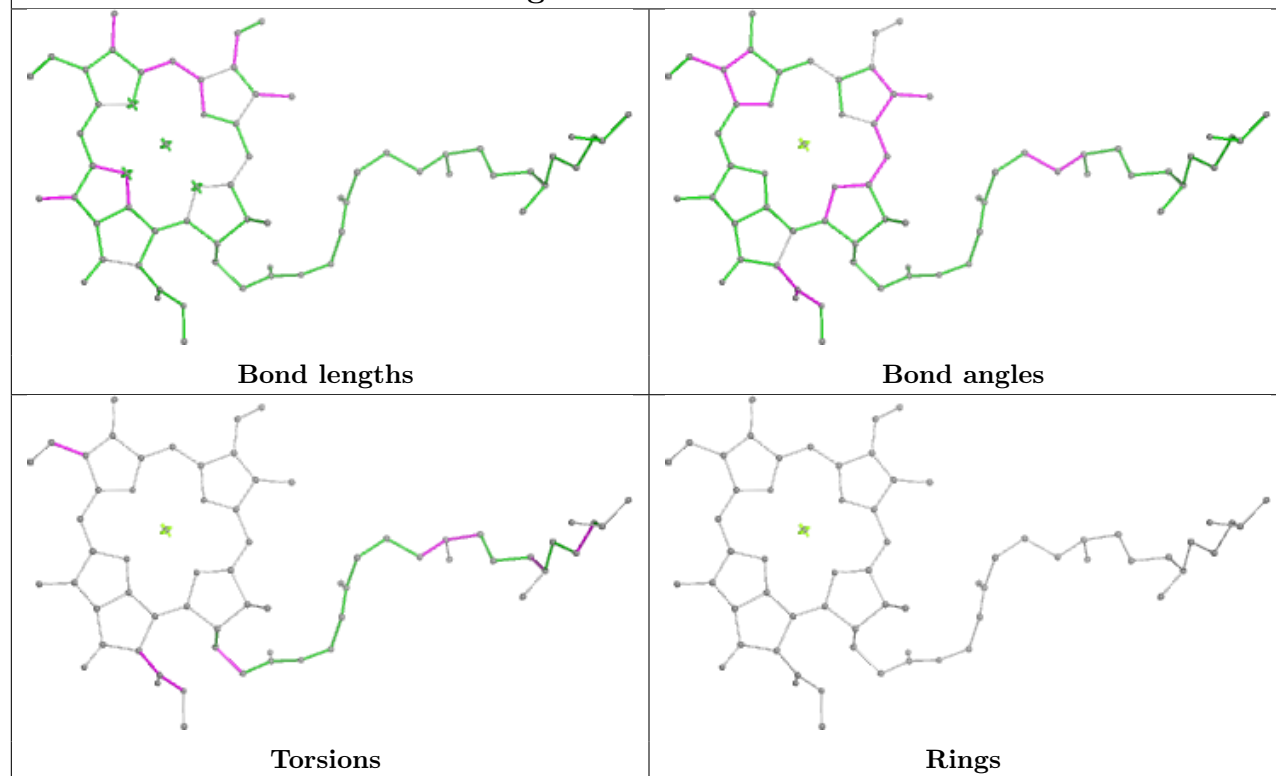


Ligand LHG A 854

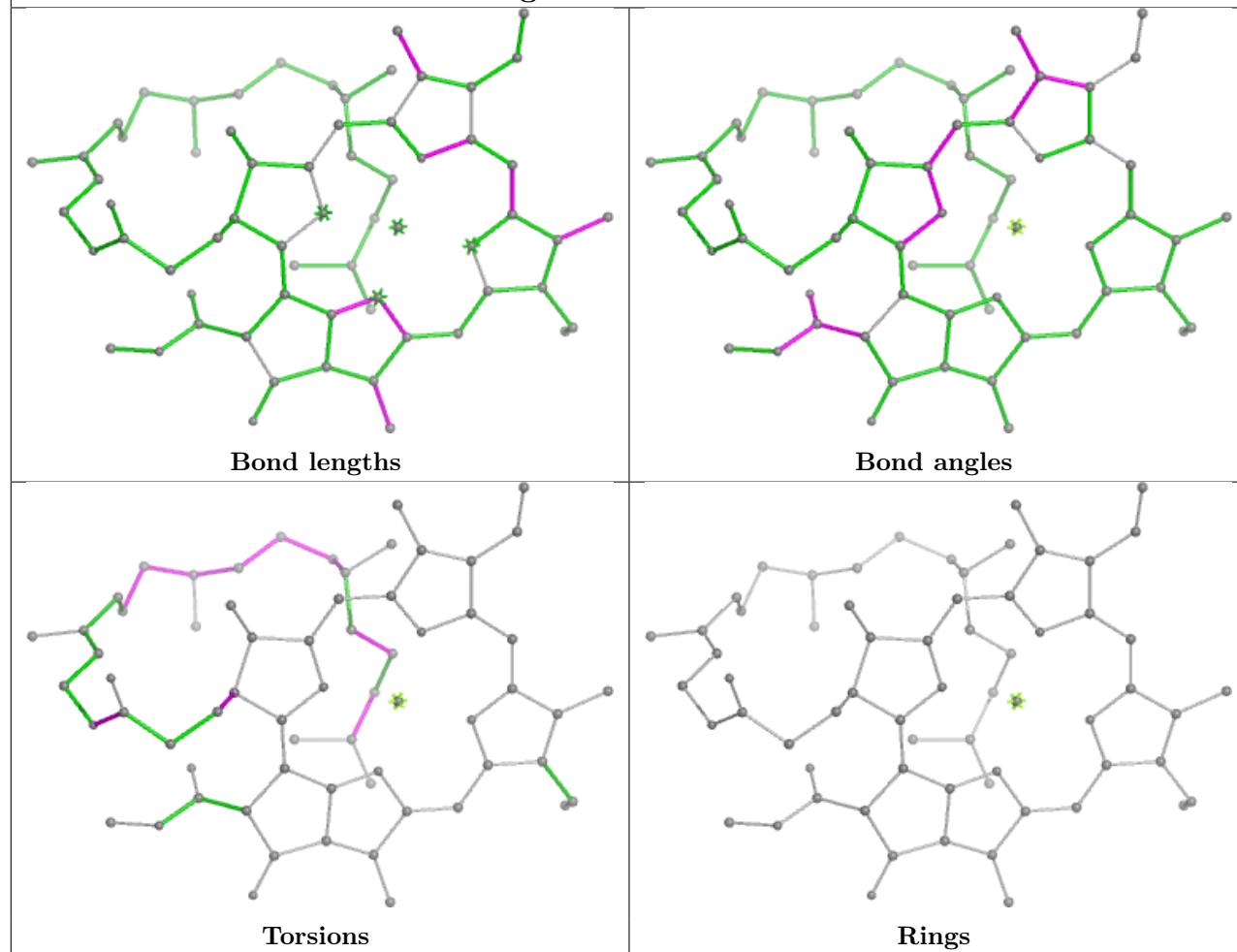




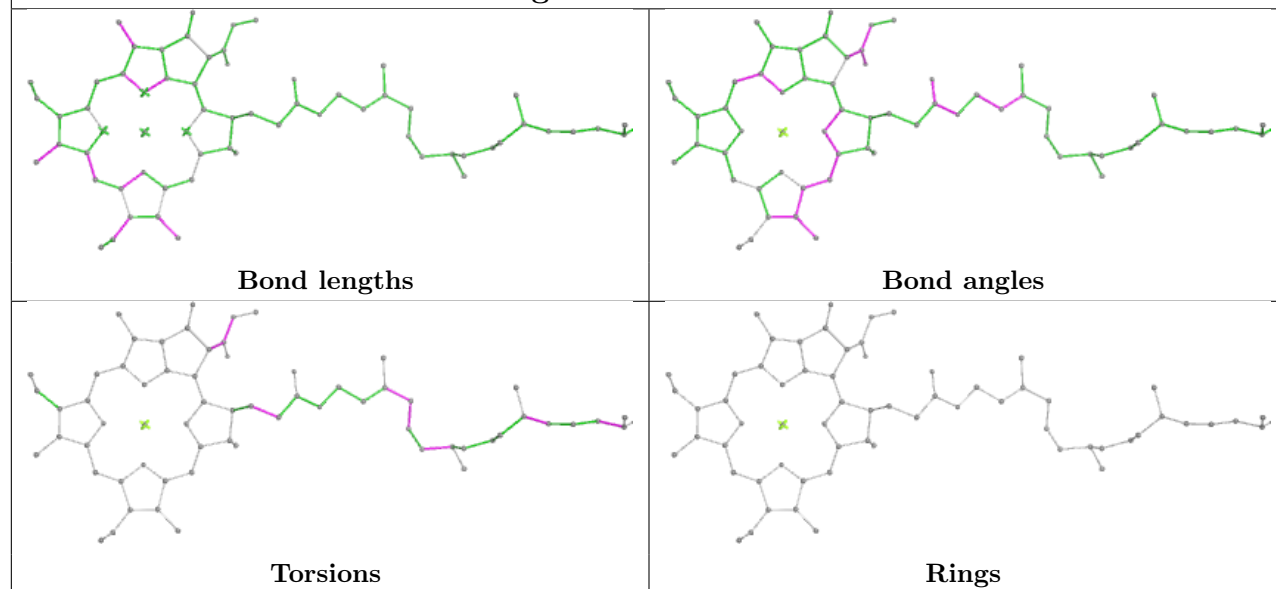


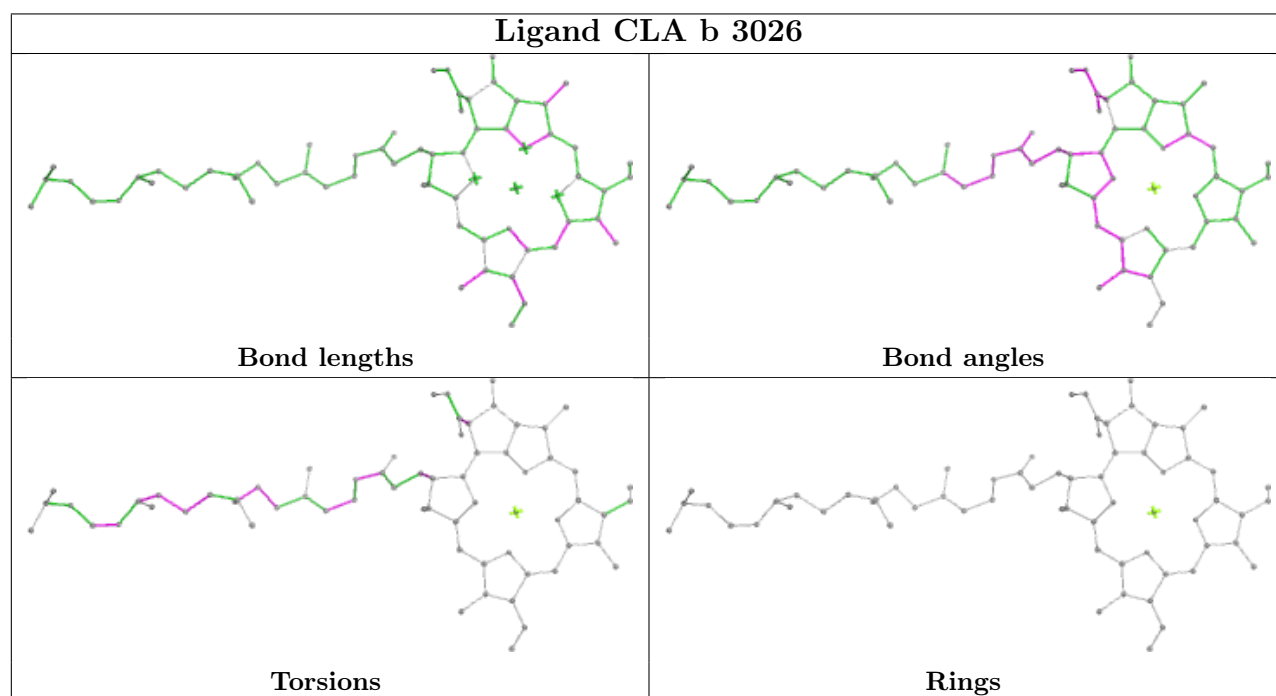
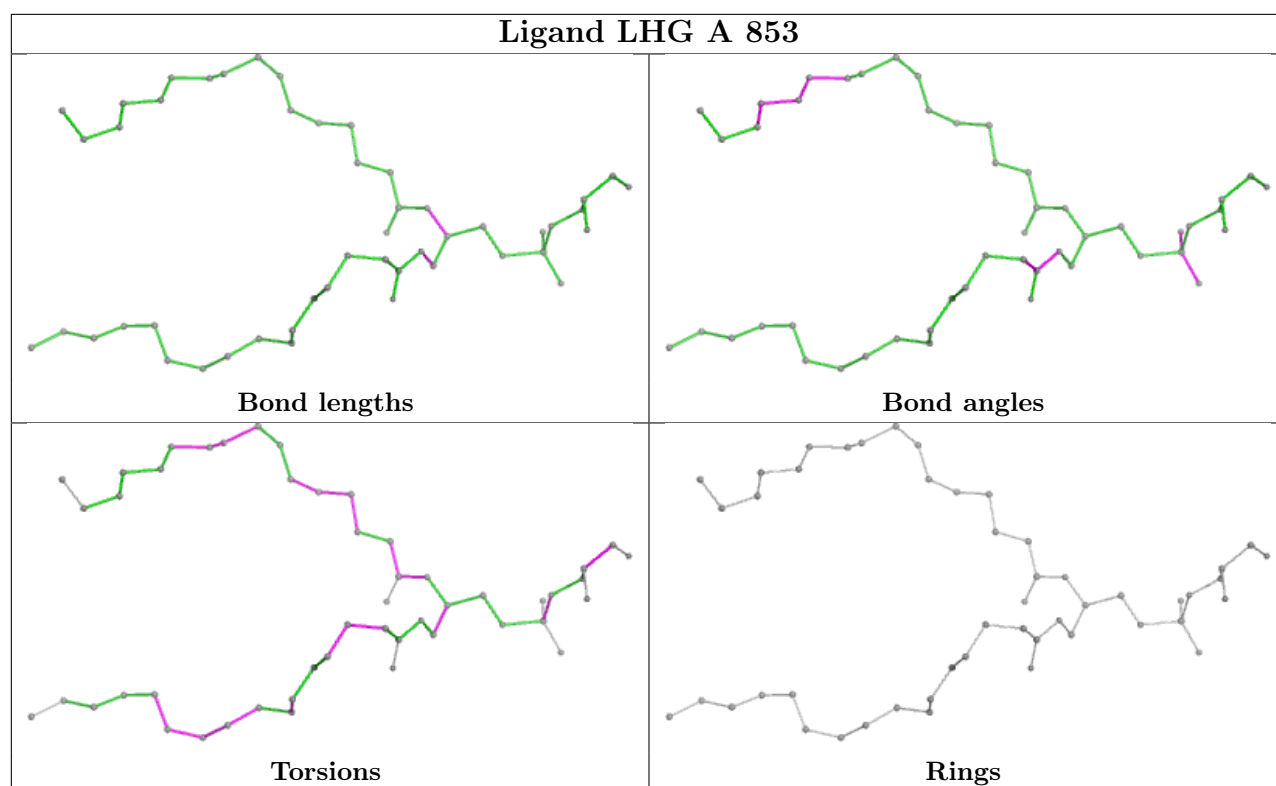
Ligand CLA A 809**Ligand CLA 2 3005**

Ligand CLA a 806

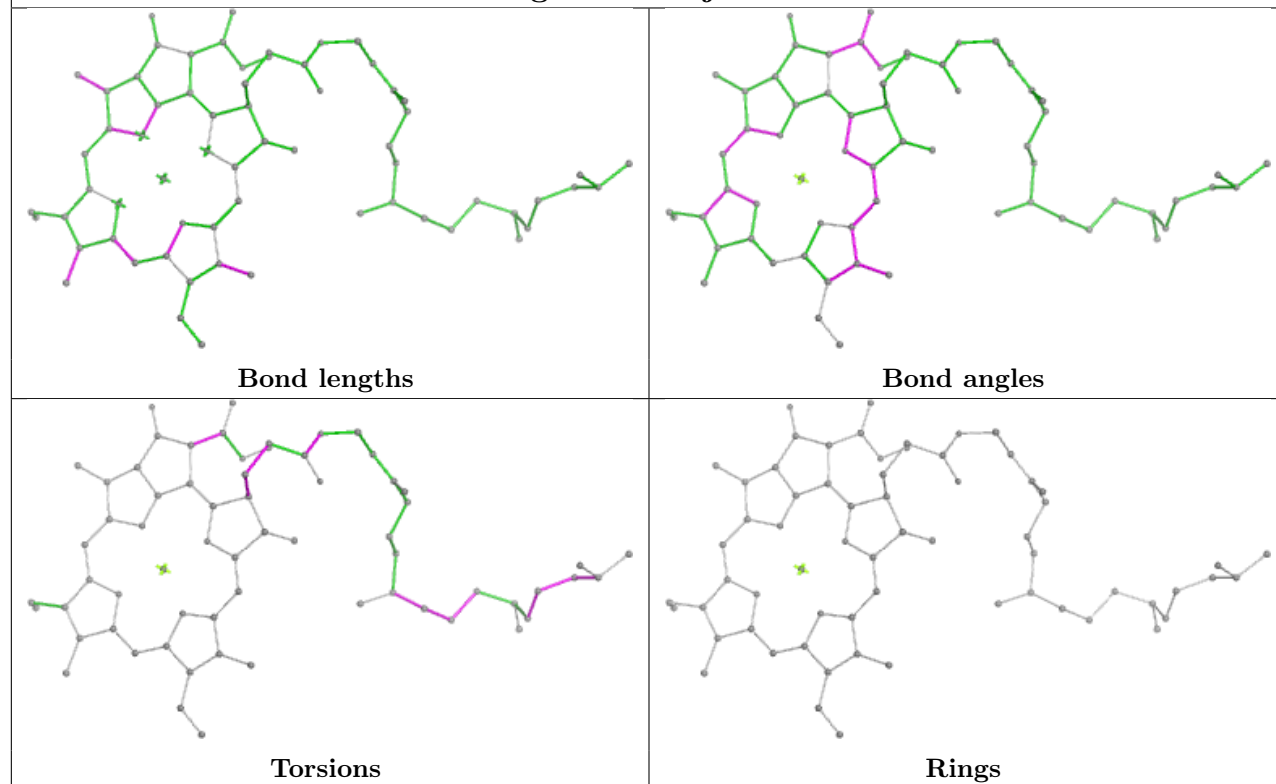


Ligand CLA A 834

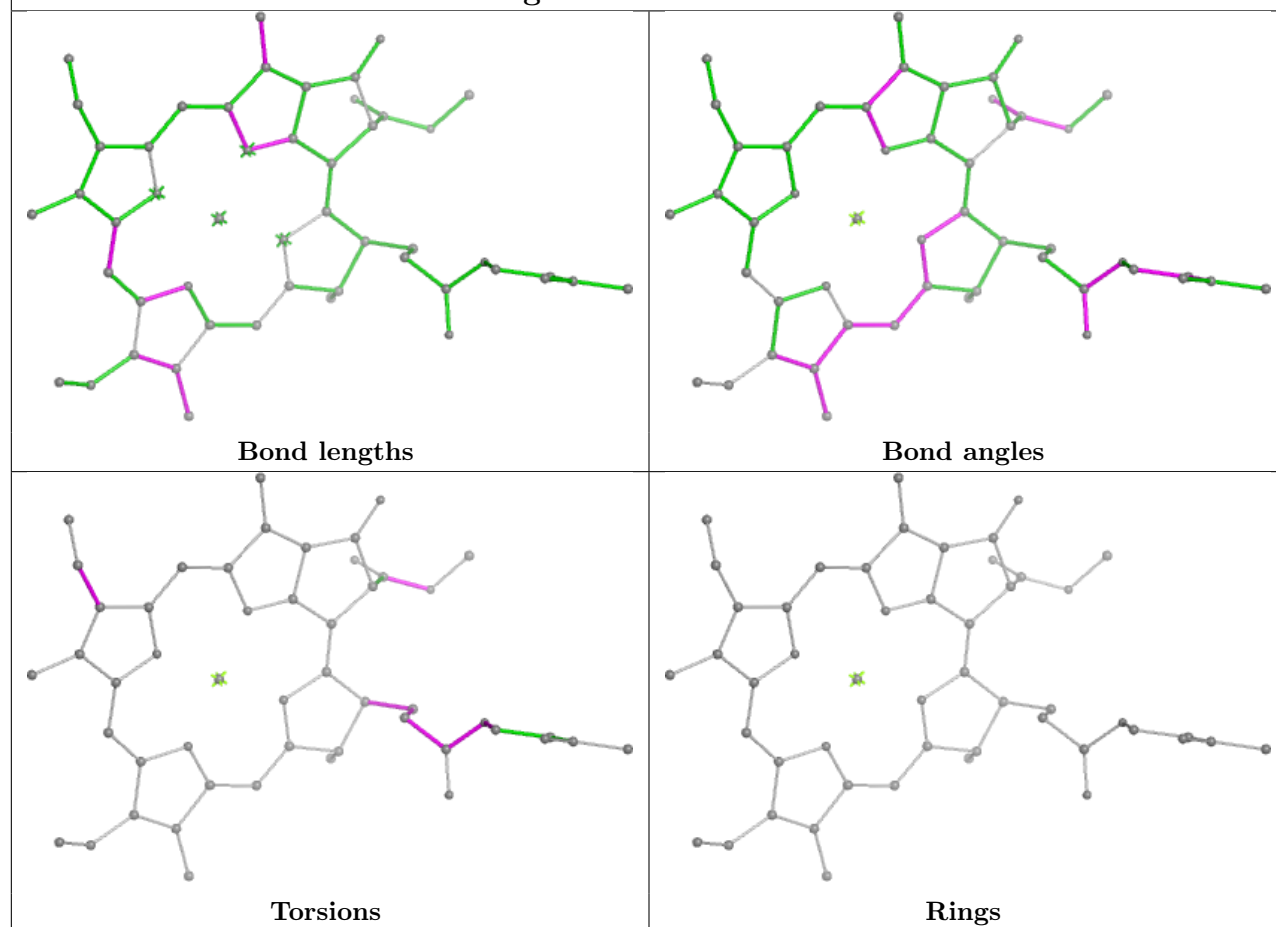


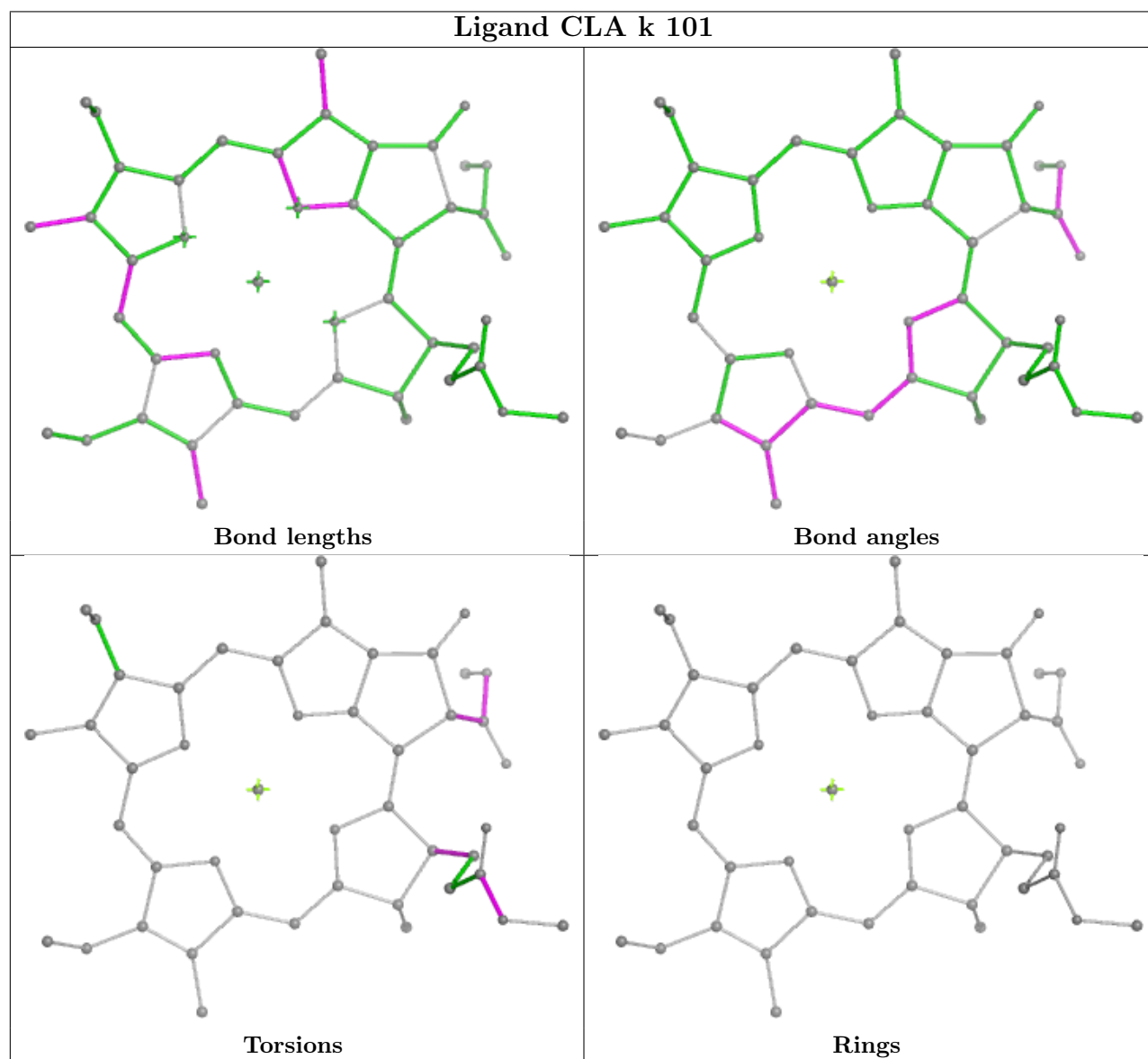
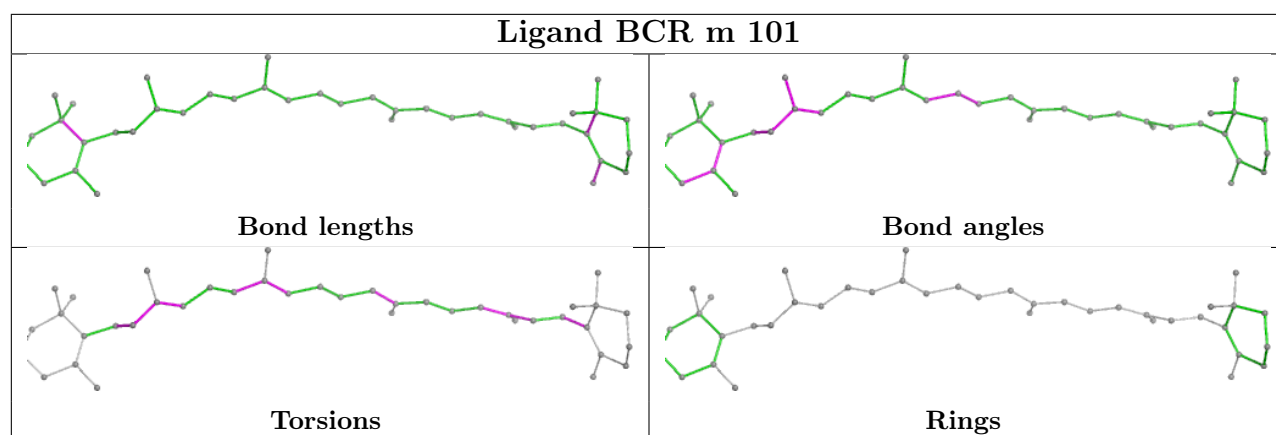


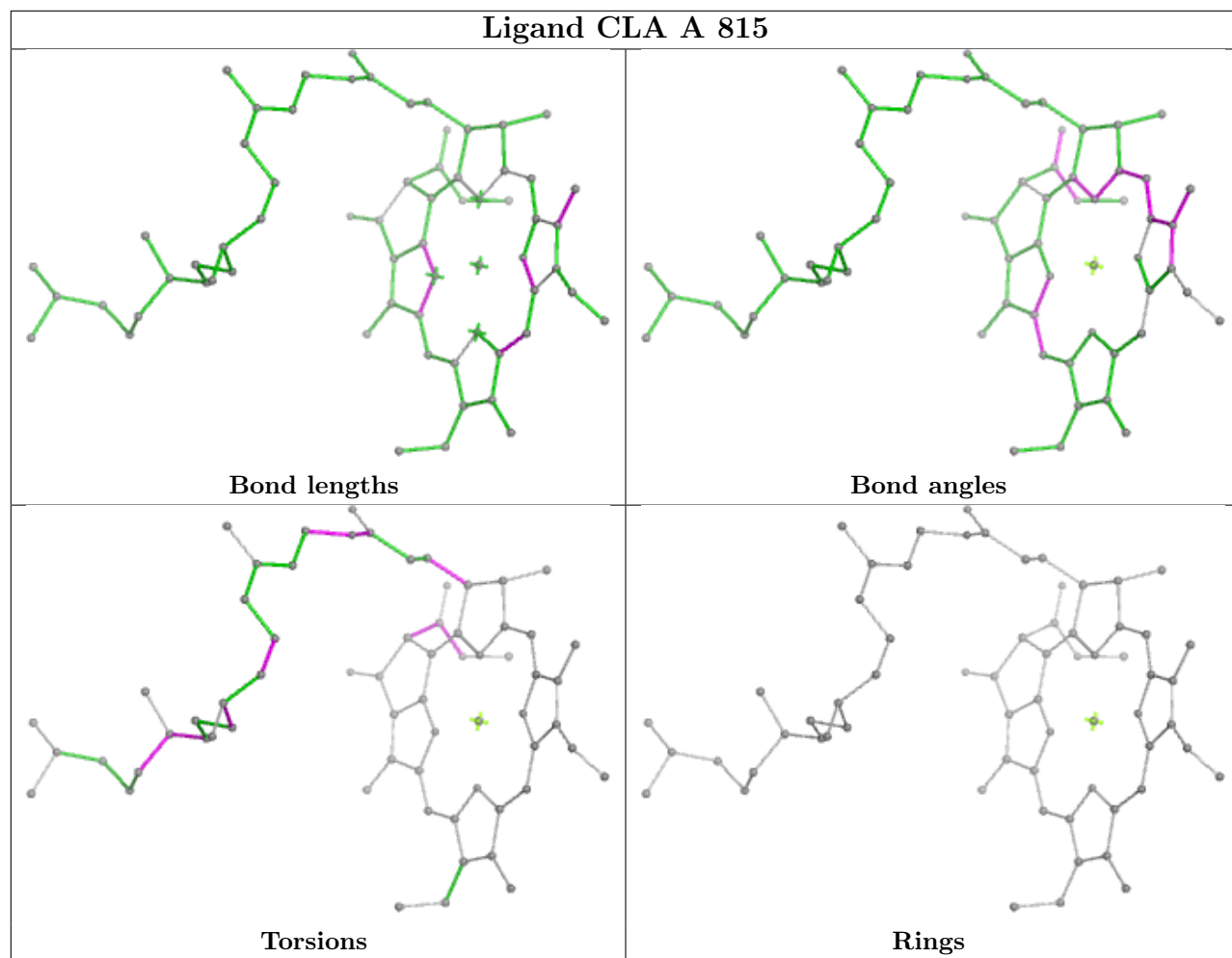
Ligand CLA j 1101



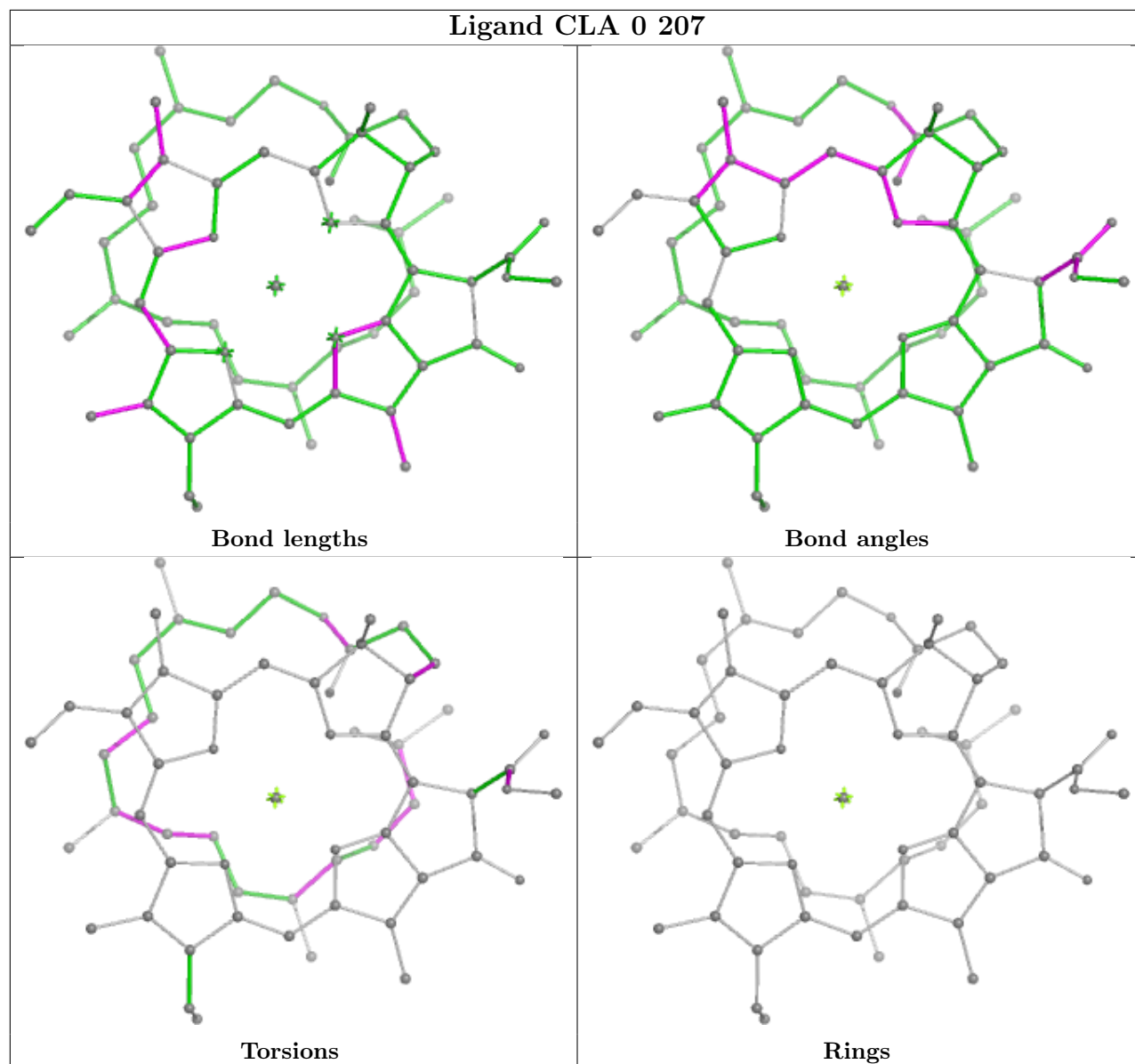
Ligand CLA B 3036

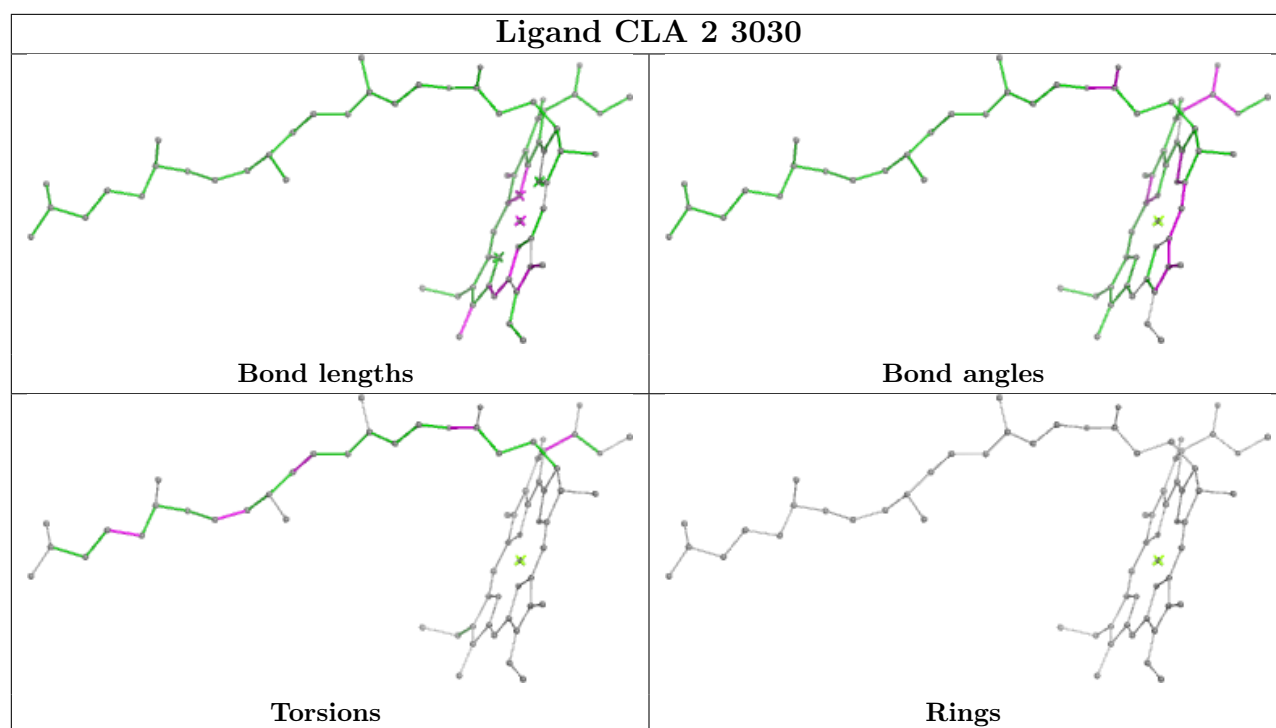




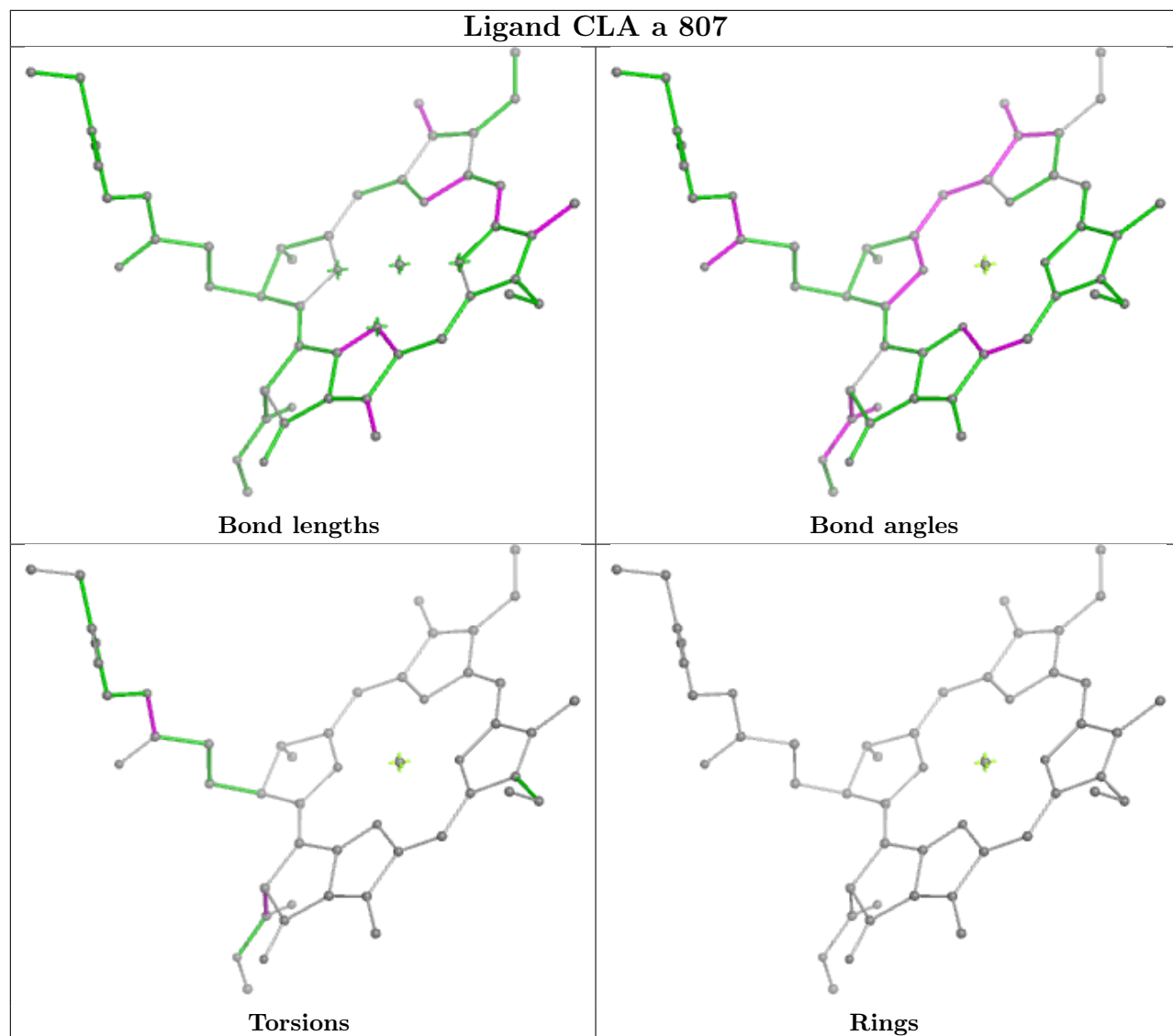


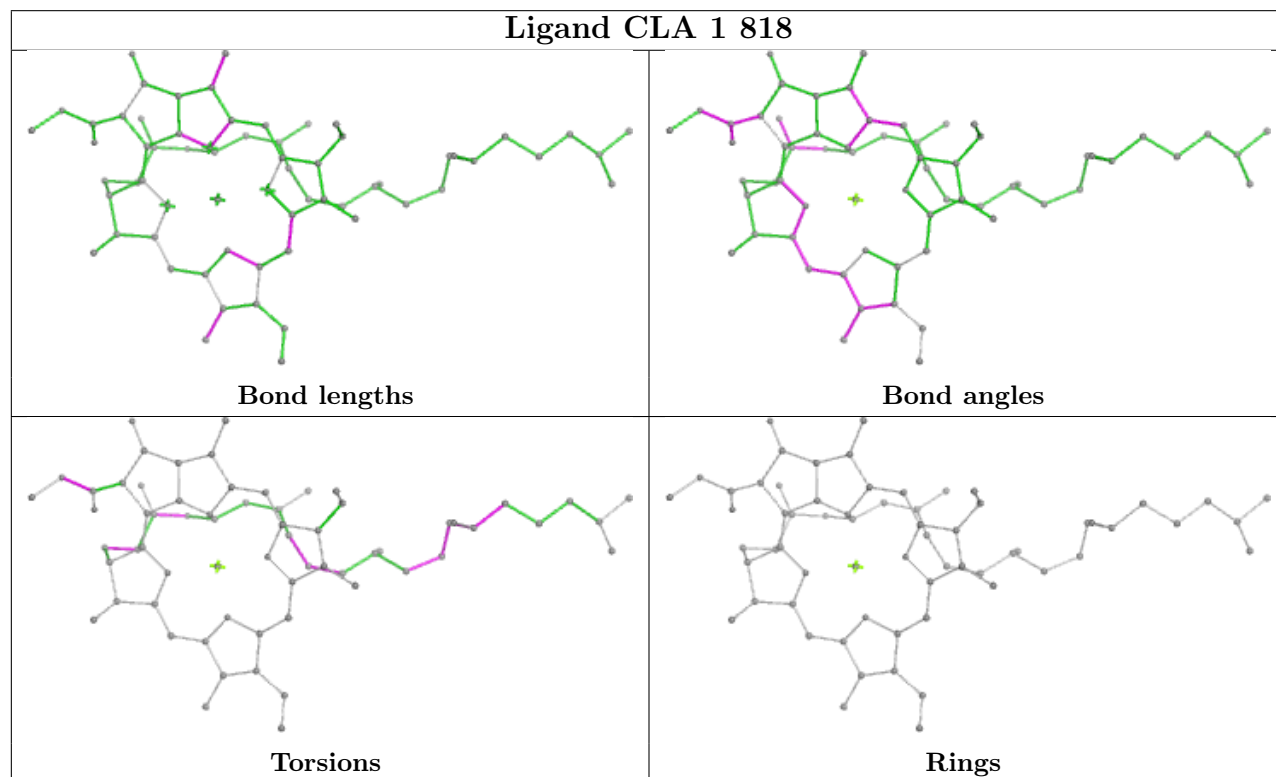
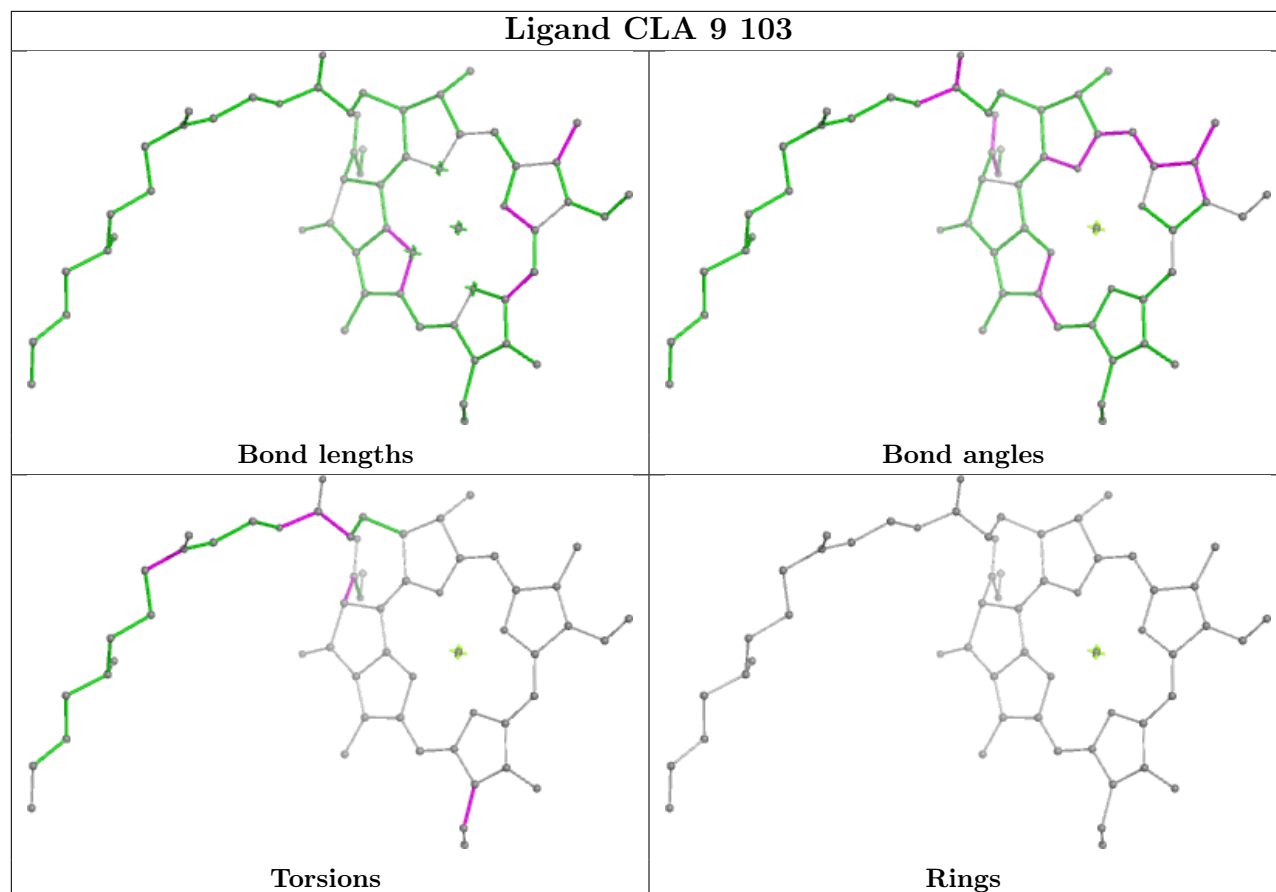
Ligand CLA 0 207



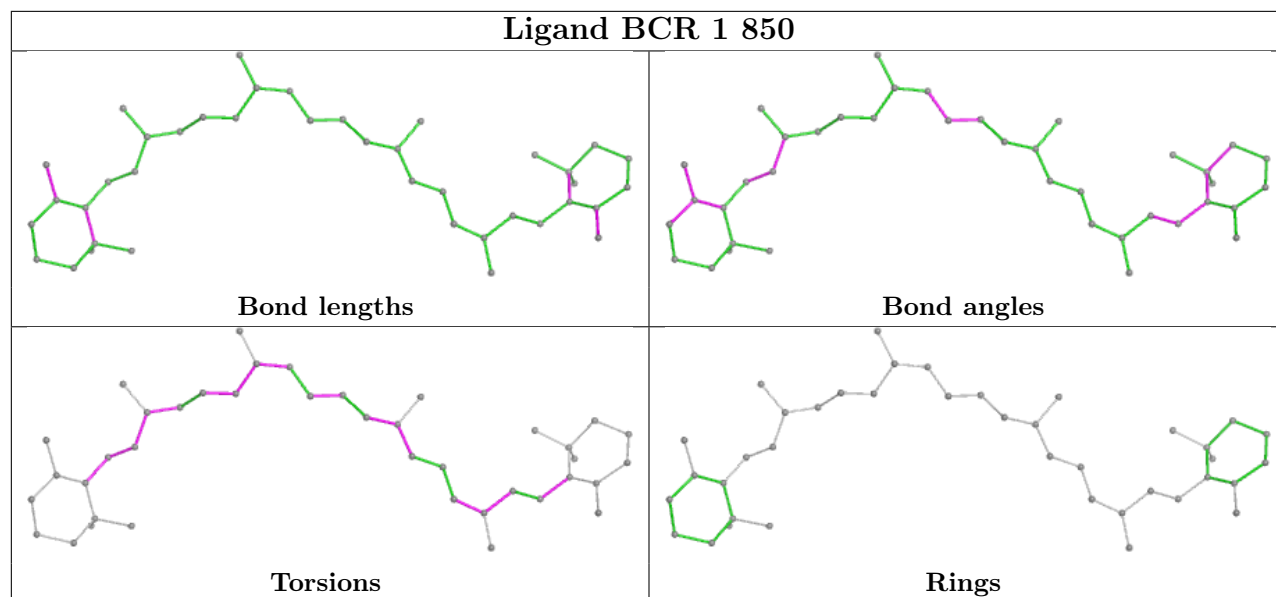


Ligand CLA a 807

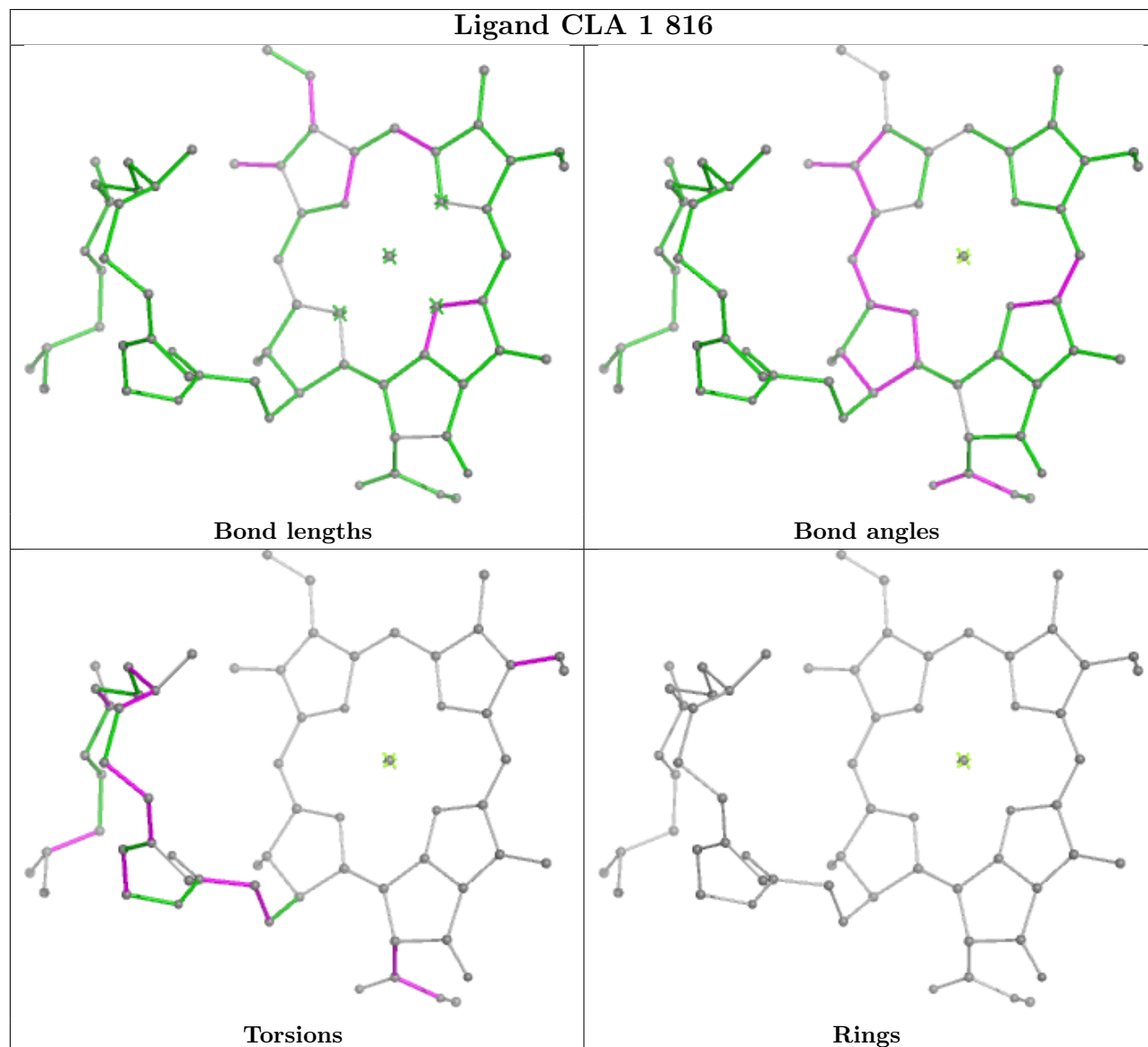




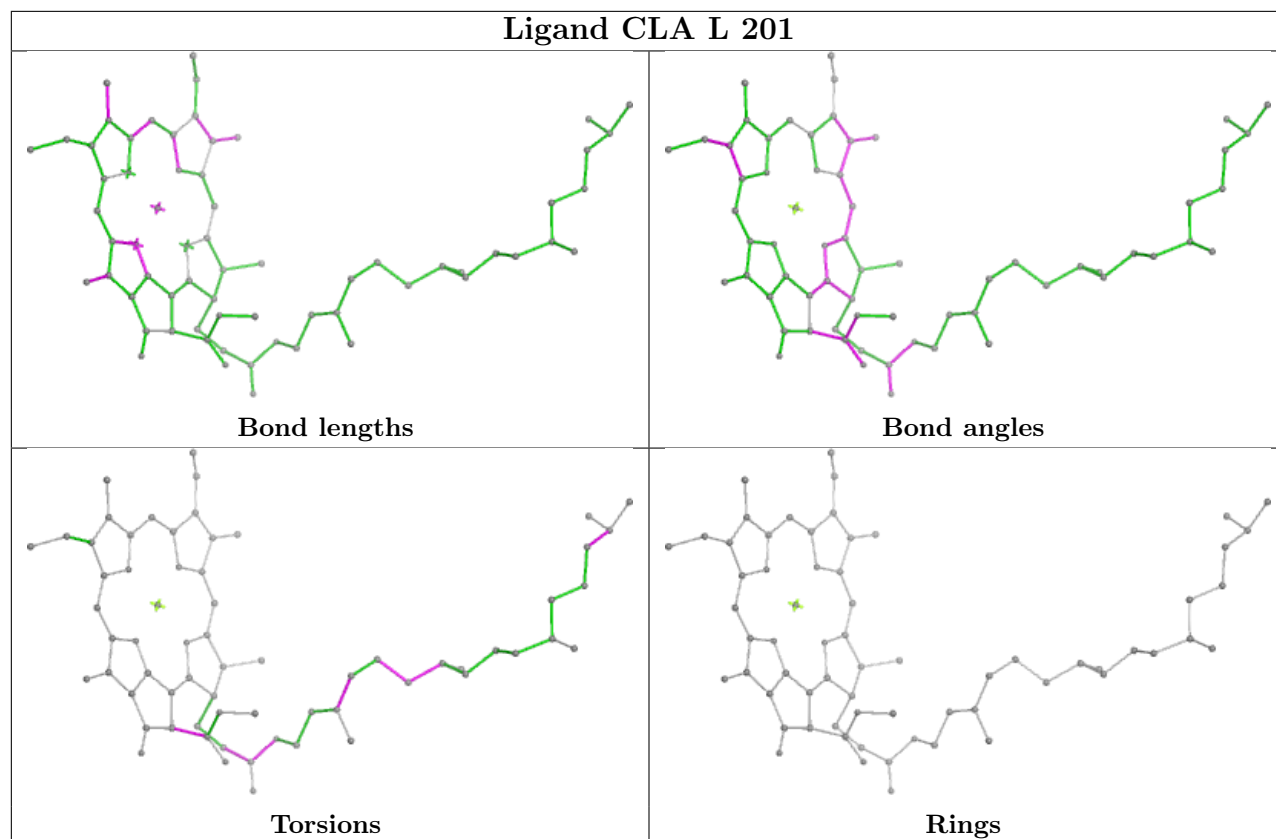
Ligand BCR 1 850



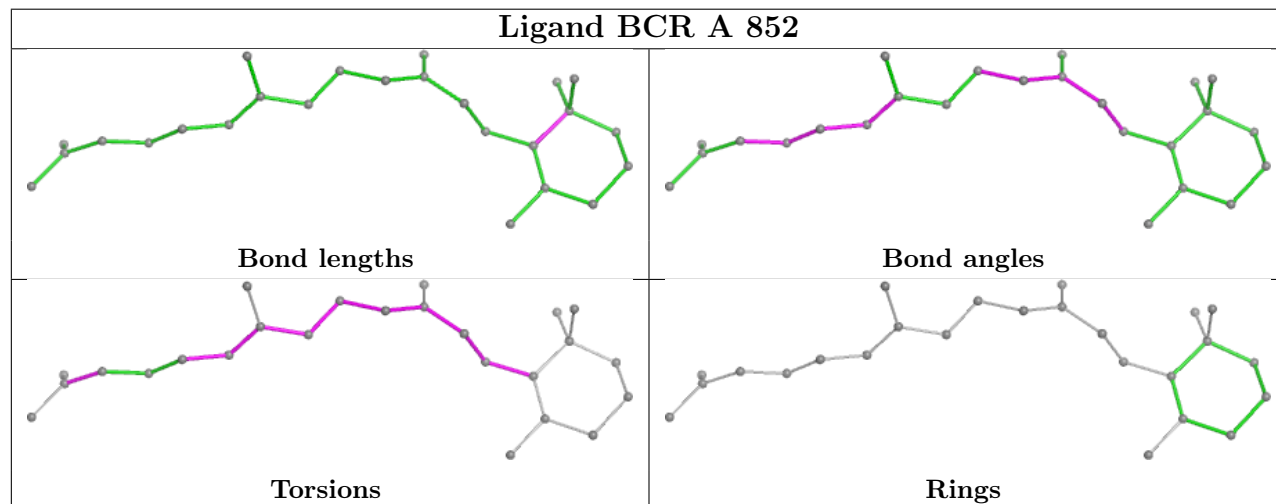
Ligand CLA 1 816



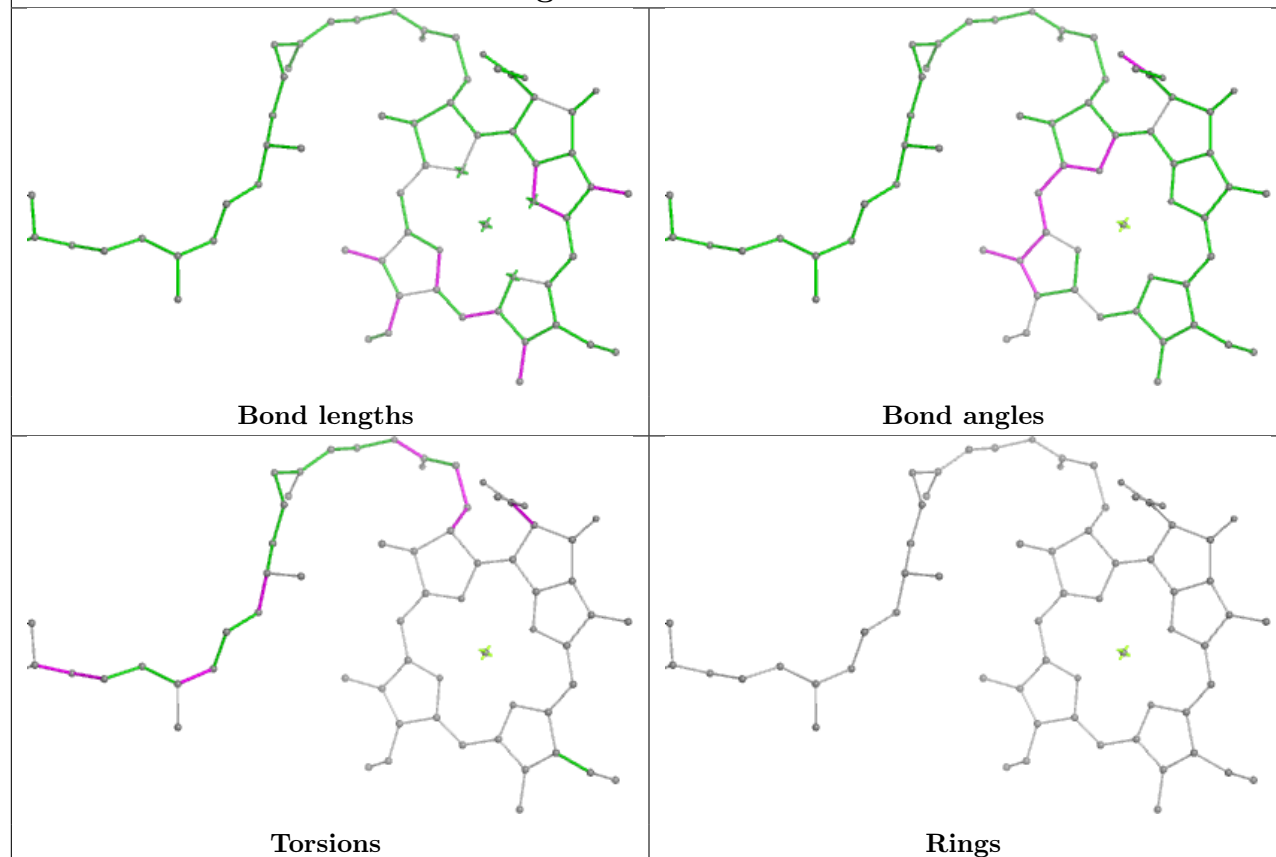
Ligand CLA L 201



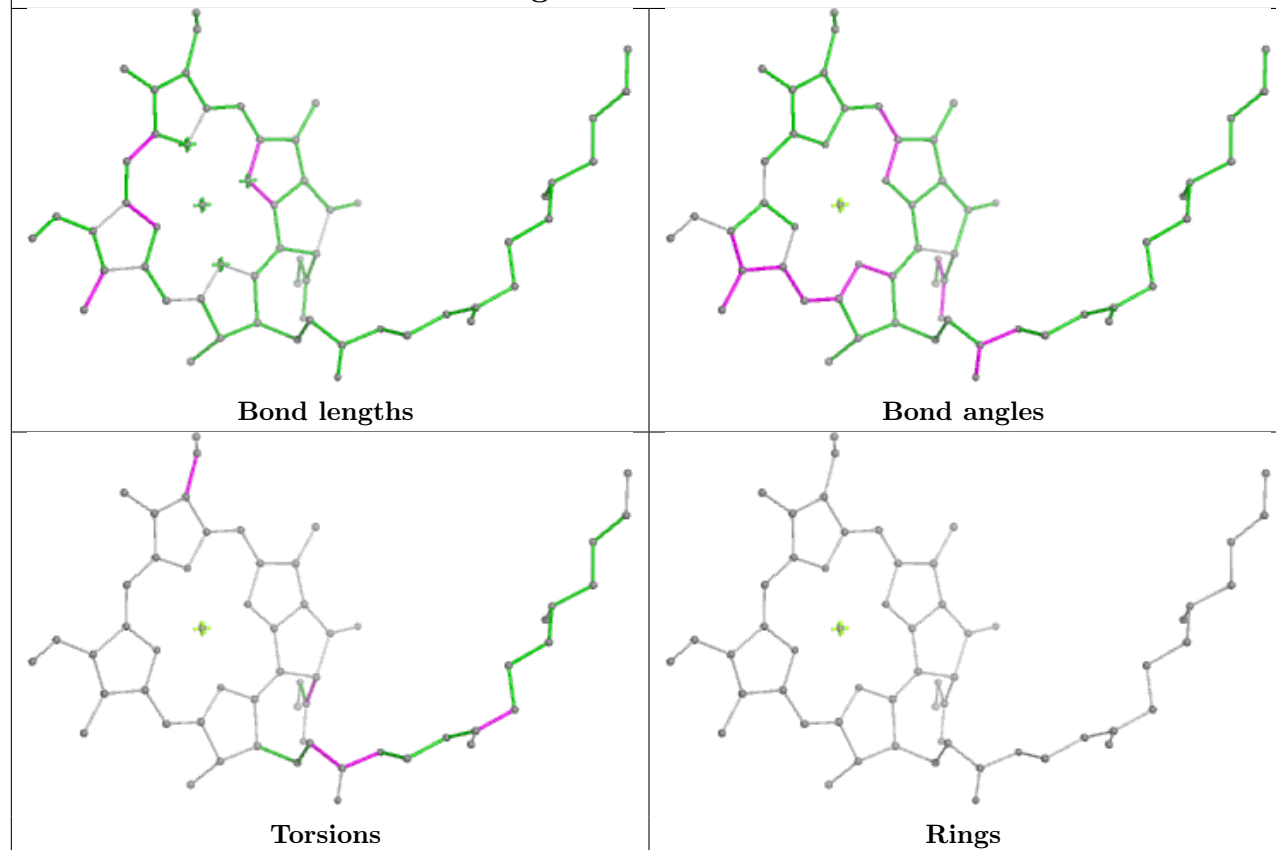
Ligand BCR A 852

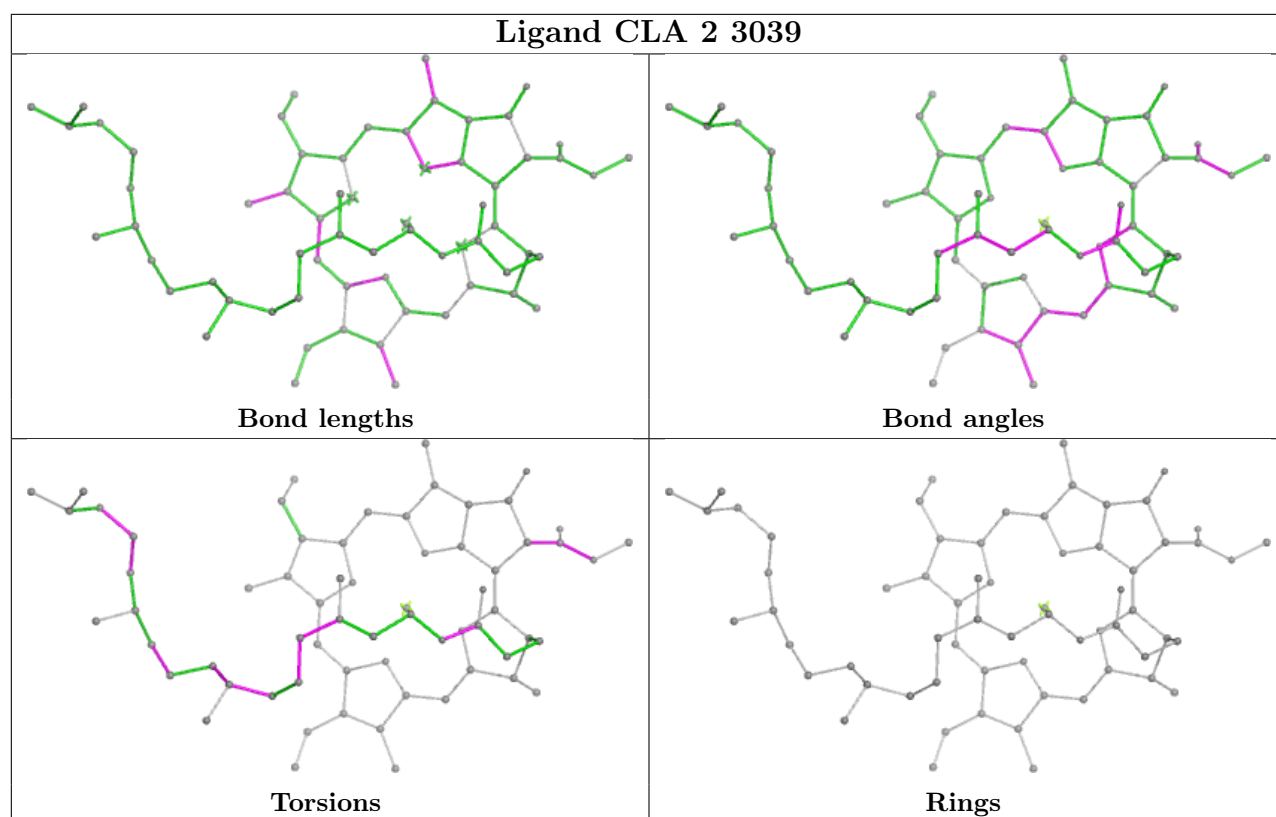


Ligand CLA 1 814



Ligand CLA K 102





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

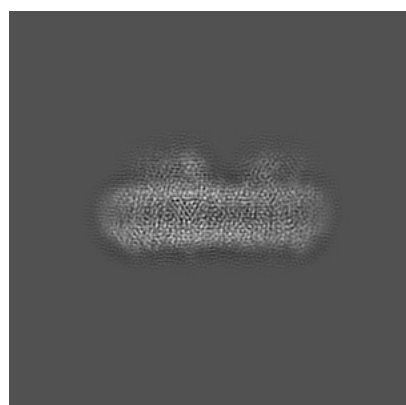
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-10558. These allow visual inspection of the internal detail of the map and identification of artifacts.

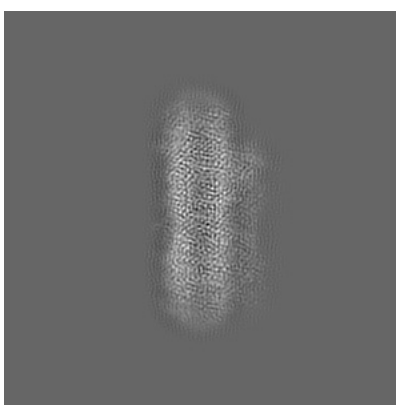
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

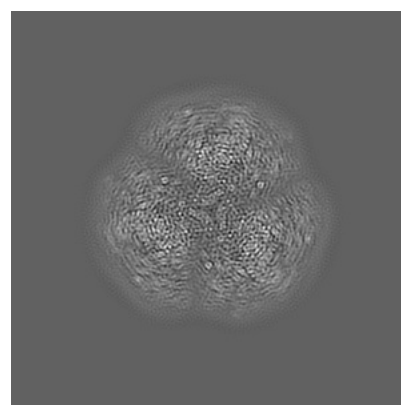
6.1.1 Primary map



X



Y

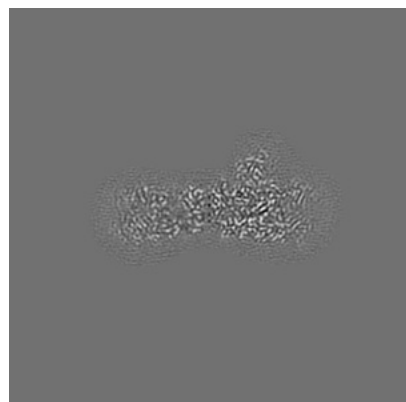


Z

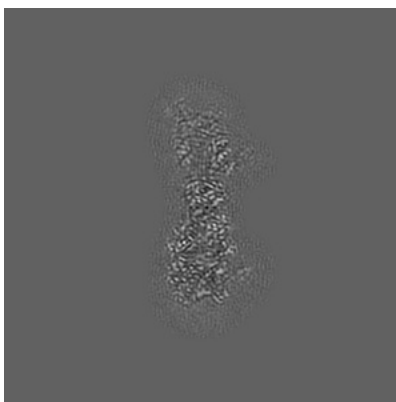
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

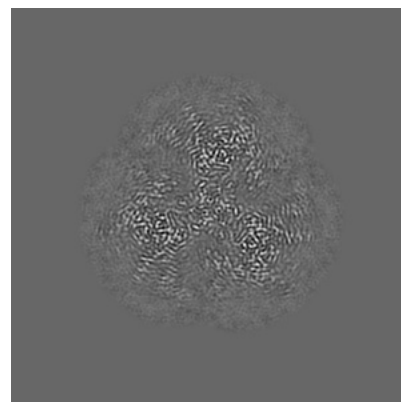
6.2.1 Primary map



X Index: 280



Y Index: 280



Z Index: 280

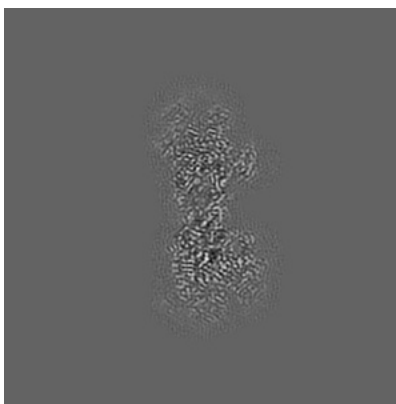
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

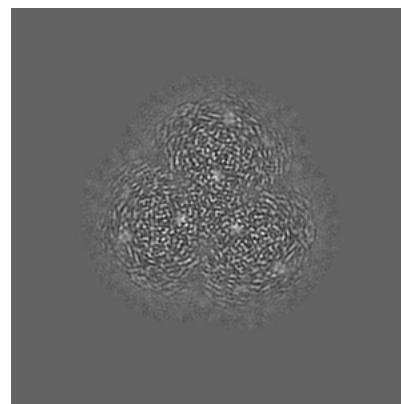
6.3.1 Primary map



X Index: 297



Y Index: 253

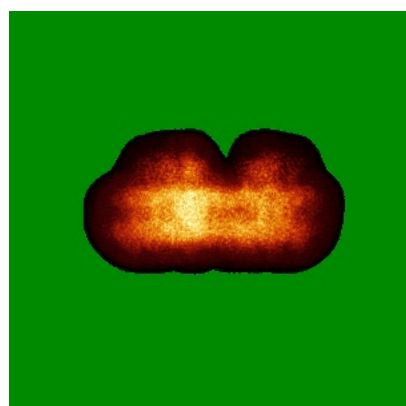


Z Index: 298

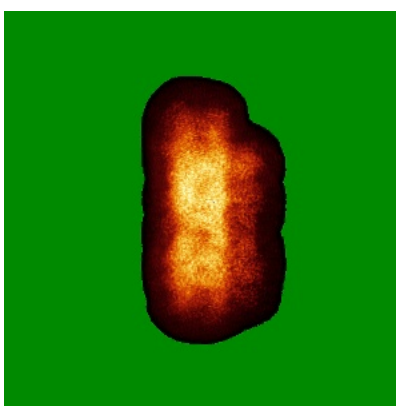
The images above show the largest variance slices of the map in three orthogonal directions.

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

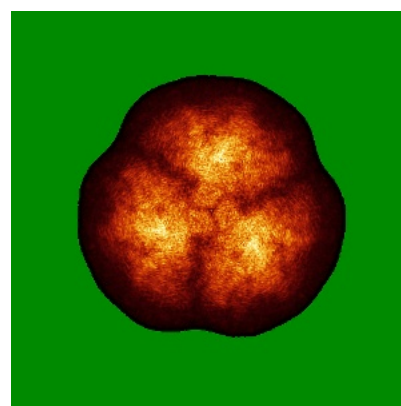
6.4.1 Primary map



X



Y

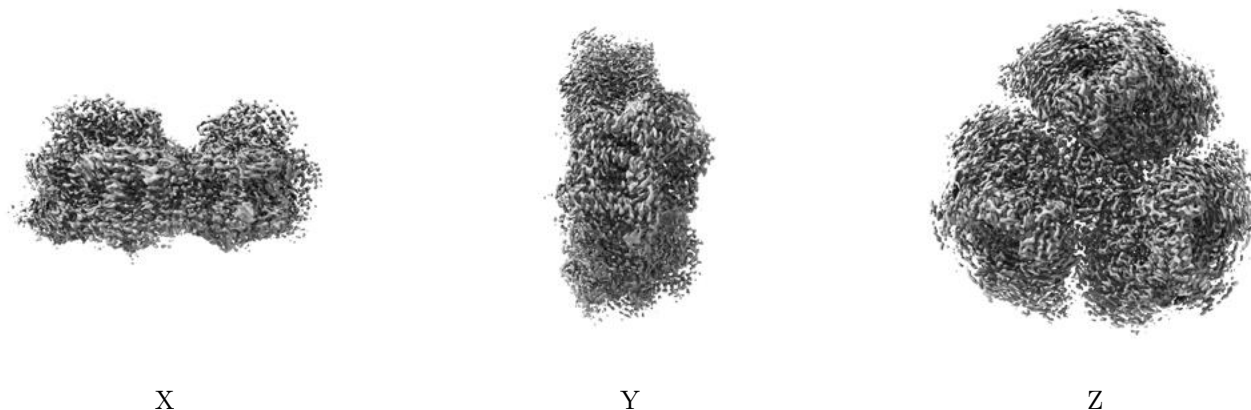


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

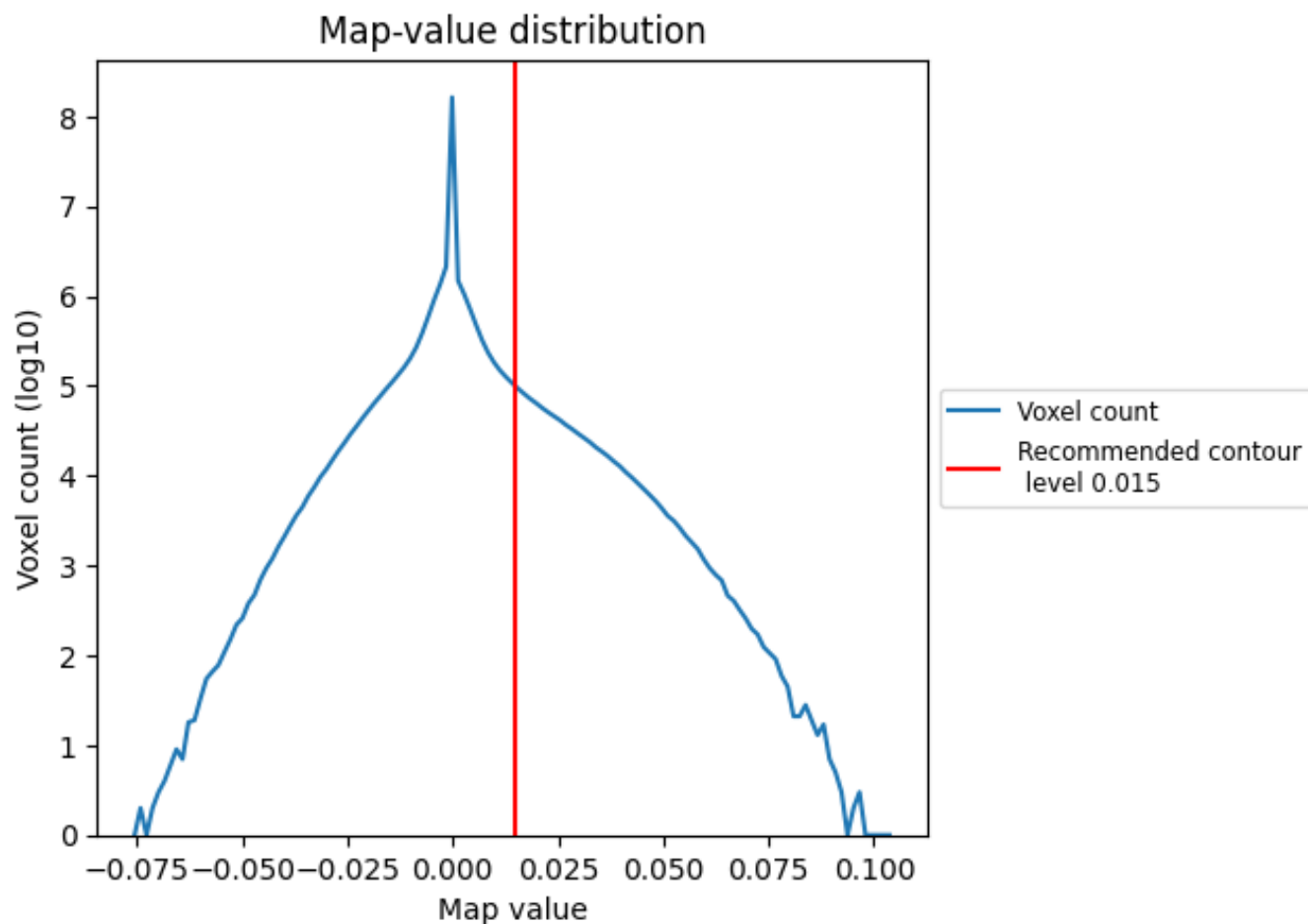
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

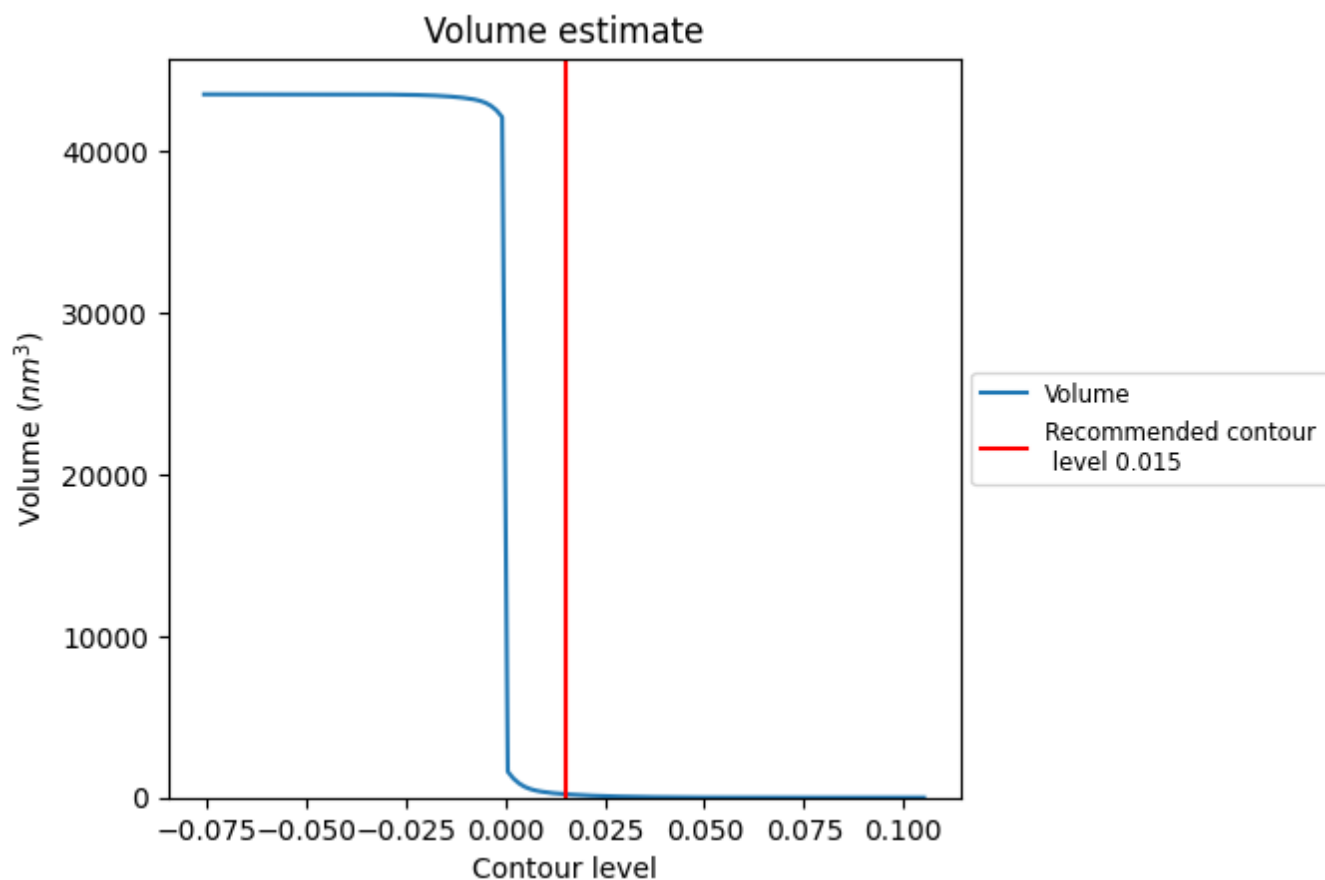
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

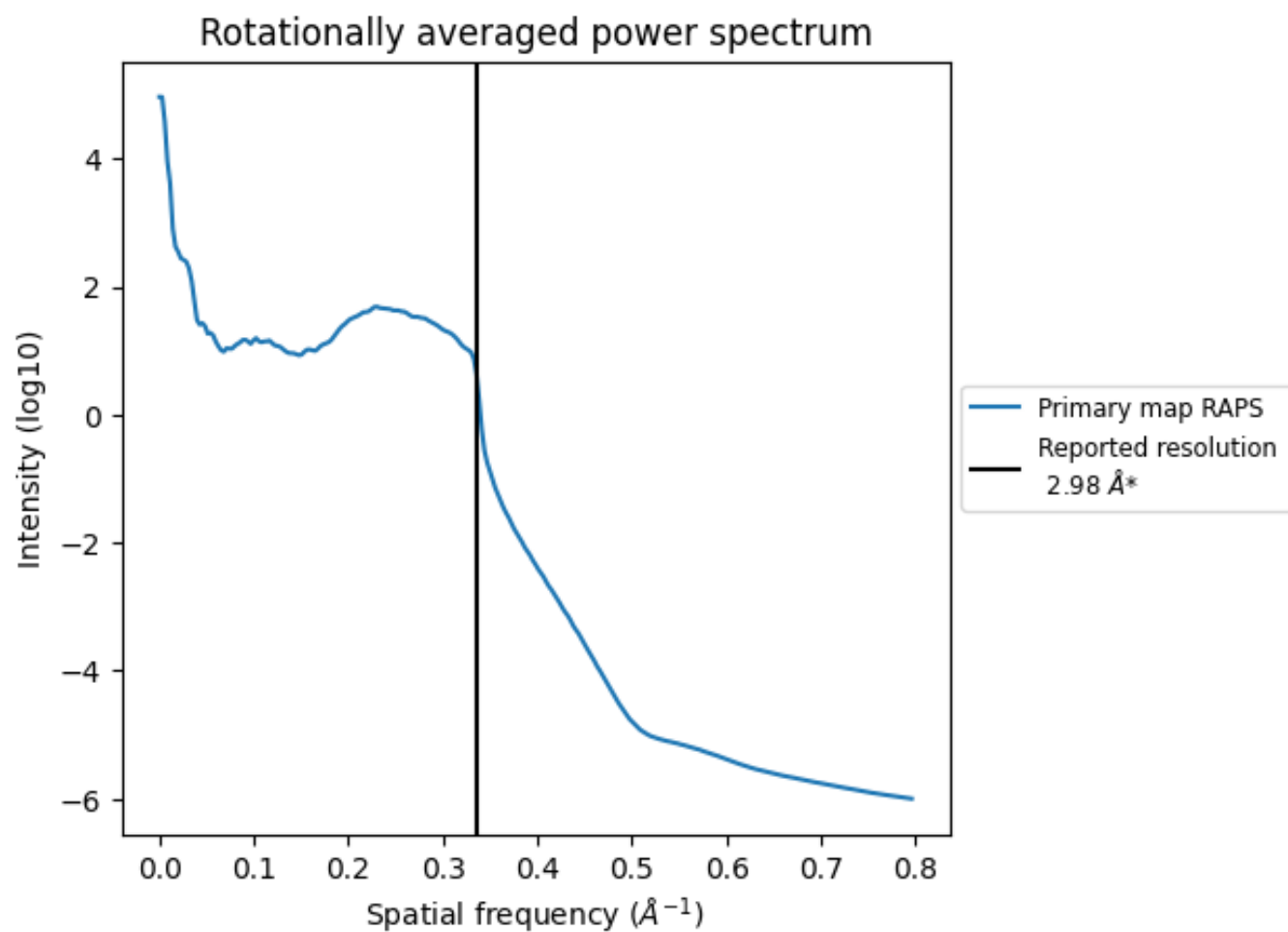
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm^3 ; this corresponds to an approximate mass of 190 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

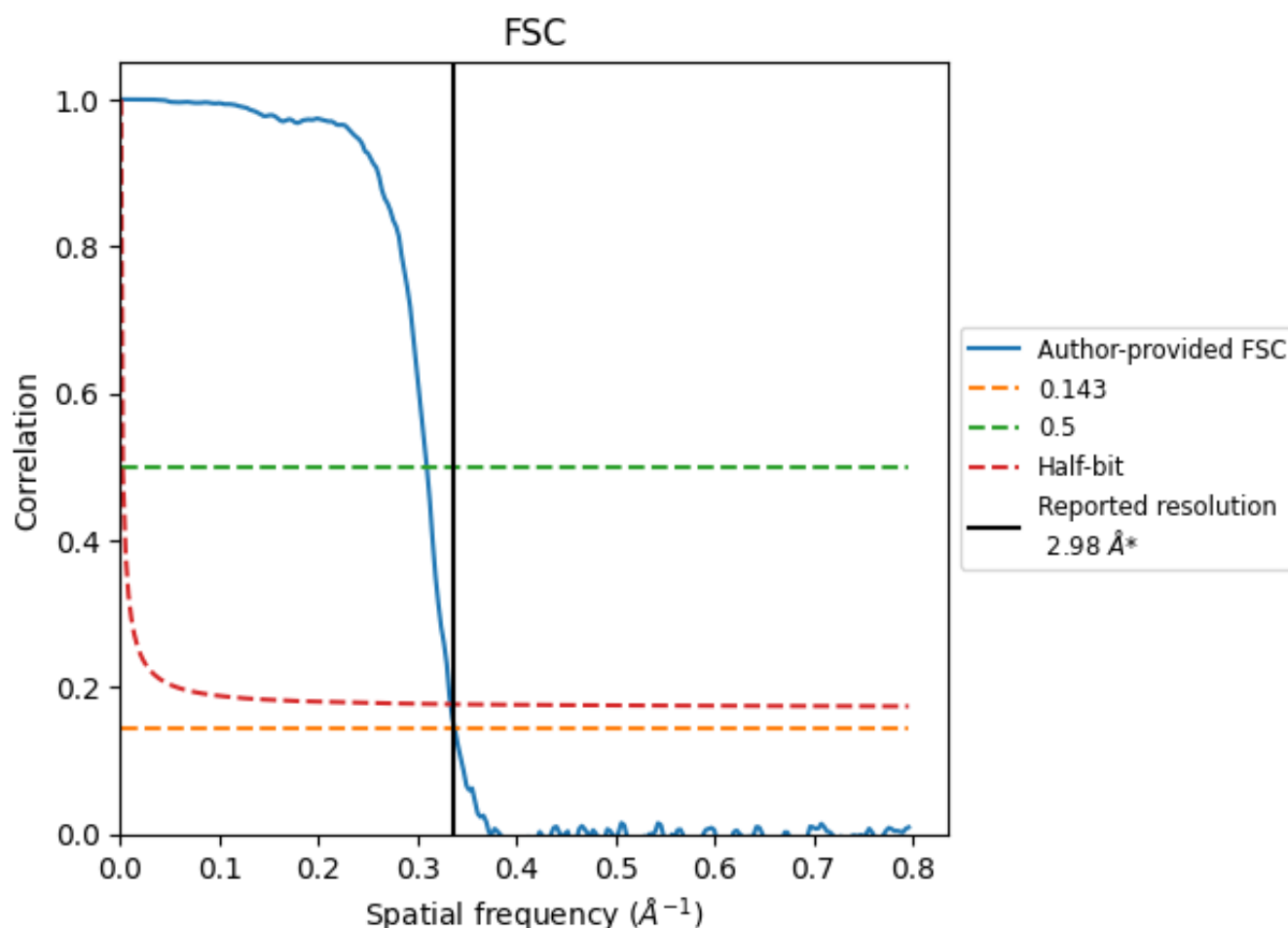


*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.336 Å⁻¹

8.2 Resolution estimates [i](#)

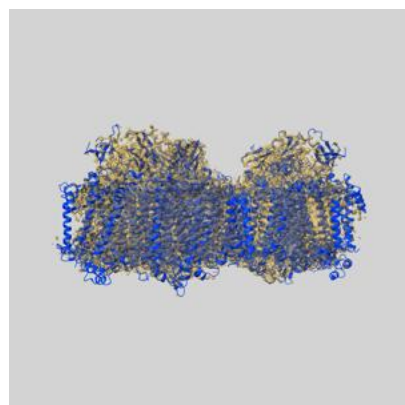
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.96	3.23	3.00
Unmasked-calculated*	-	-	-

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

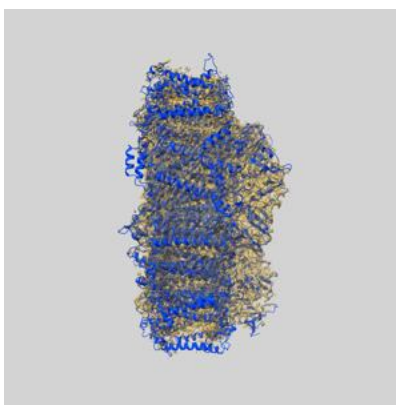
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-10558 and PDB model 6TRC. Per-residue inclusion information can be found in section 3 on page 39.

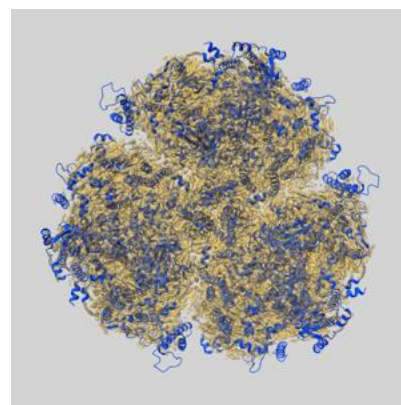
9.1 Map-model overlay [i](#)



X



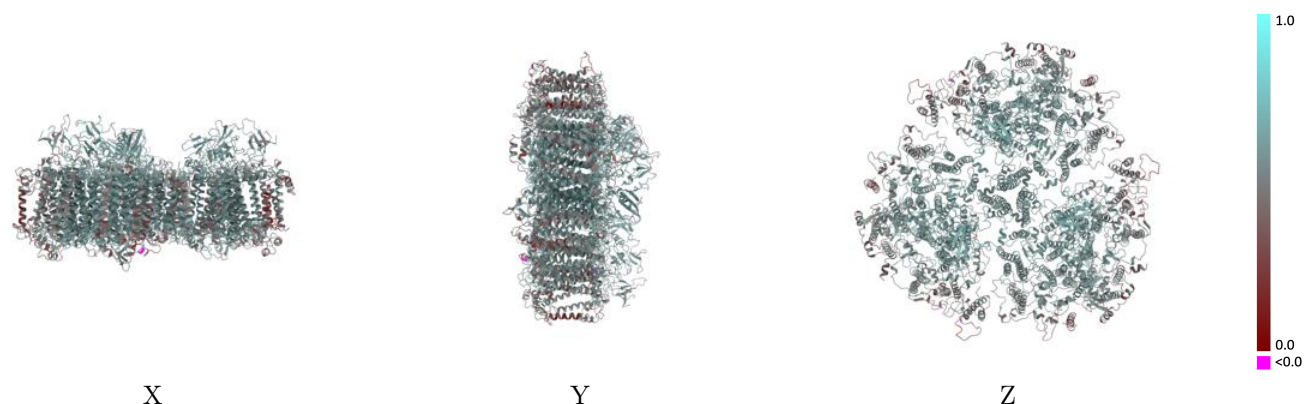
Y



Z

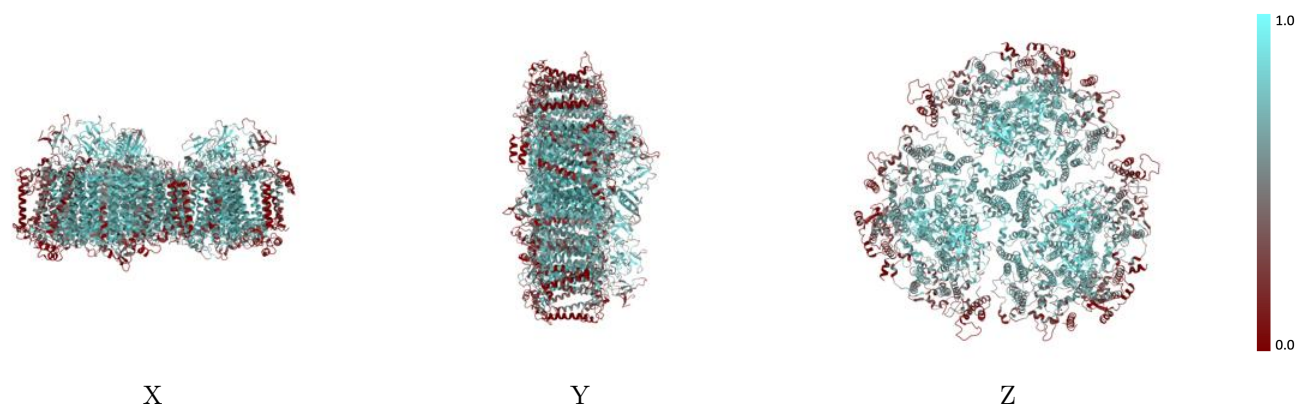
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



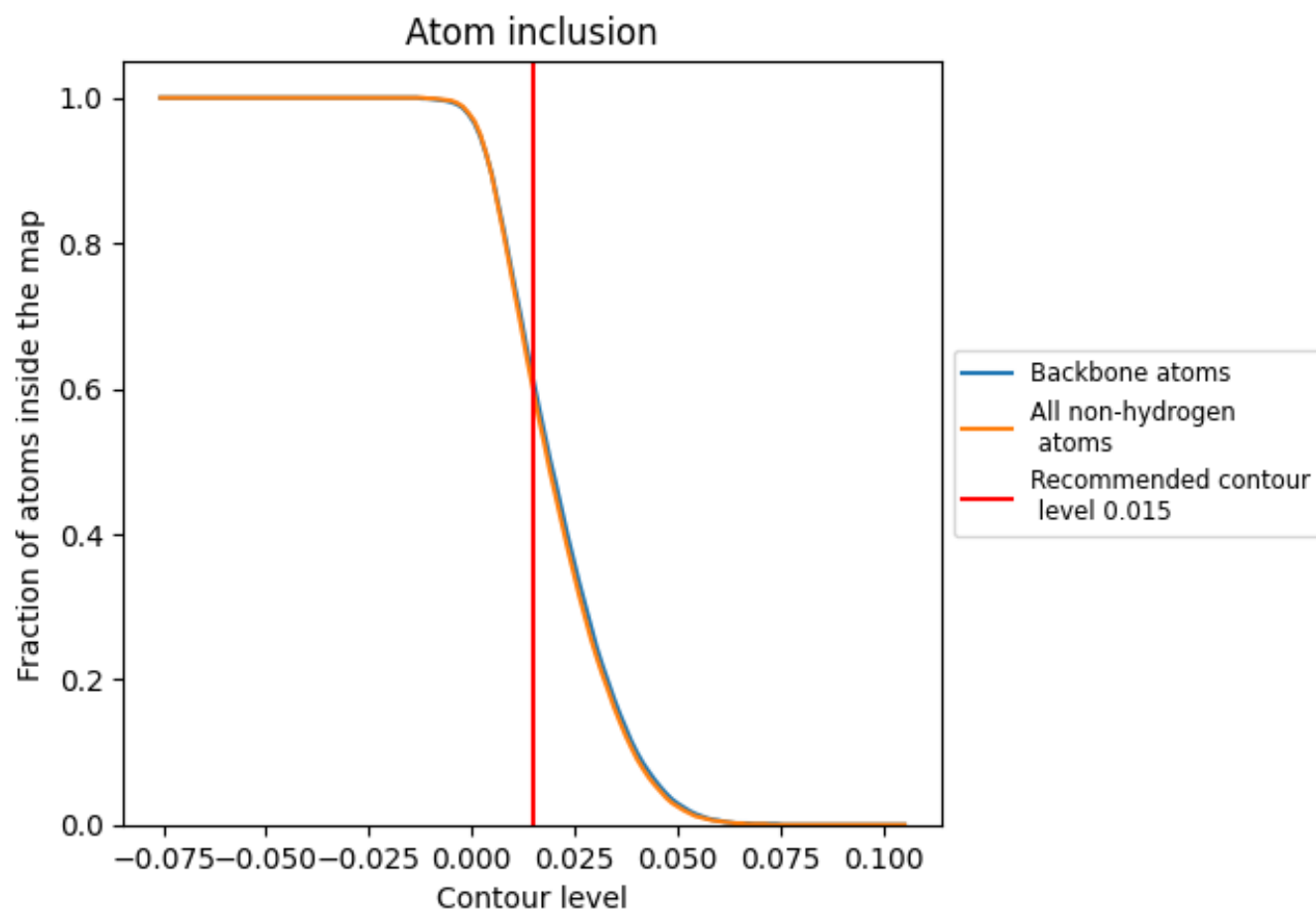
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.015).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 61% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5950	 0.5490
0	 0.7680	 0.6070
1	 0.6210	 0.5490
2	 0.6490	 0.5630
3	 0.7950	 0.6000
4	 0.6730	 0.5830
5	 0.4570	 0.5410
6	 0.2080	 0.4670
7	 0.7960	 0.6020
8	 0.1840	 0.4360
9	 0.1320	 0.4570
A	 0.6180	 0.5480
B	 0.6500	 0.5630
C	 0.7900	 0.6000
D	 0.6720	 0.5830
E	 0.4530	 0.5430
F	 0.2040	 0.4630
I	 0.8180	 0.6090
J	 0.1740	 0.4340
K	 0.1140	 0.4490
L	 0.7650	 0.6070
M	 0.6310	 0.5810
X	 0.0000	 0.3130
a	 0.6200	 0.5470
b	 0.6520	 0.5650
c	 0.7930	 0.6000
d	 0.6750	 0.5830
e	 0.4610	 0.5420
f	 0.2050	 0.4670
i	 0.7930	 0.6050
j	 0.2120	 0.4530
k	 0.1110	 0.4450
l	 0.7780	 0.6080
m	 0.6610	 0.5880
x	 0.0110	 0.3160



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Chain	Atom inclusion	Q-score
y	 0.6530	 0.5740
z	 0.0040	 0.3140