



## wwPDB EM Validation Summary Report ⓘ

Mar 7, 2026 – 04:07 AM UTC

PDB ID : 6TRC / pdb\_00006trc  
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](mailto: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>.

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

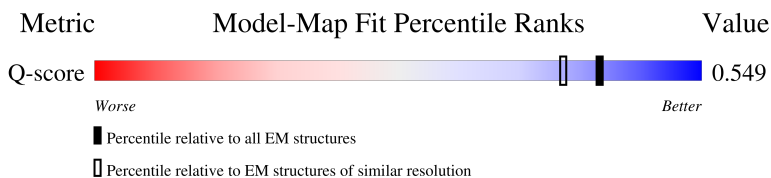
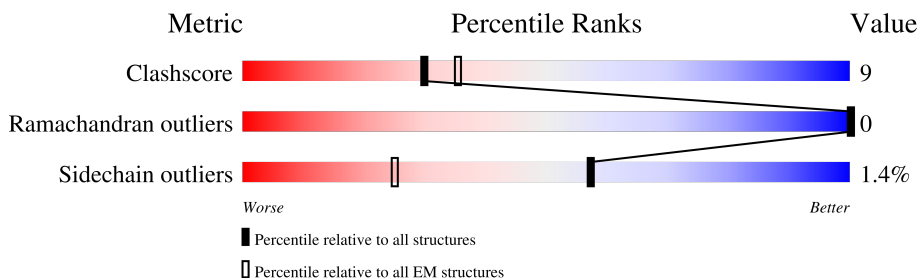
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance i

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13236 ( 2.48 - 3.48 )

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  $\geq 3$ , 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 style="display: flex; justify-content: space-between; align-items: center;"> <span>25%</span> <span>79%</span> <span>20%</span> <span>.</span> </div>
1	A	755	<div style="display: flex; justify-content: space-between; align-items: center;"> <span>25%</span> <span>79%</span> <span>20%</span> <span>.</span> </div>
1	a	755	<div style="display: flex; justify-content: space-between; align-items: center;"> <span>24%</span> <span>79%</span> <span>19%</span> <span>.</span> </div>
2	2	741	<div style="display: flex; justify-content: space-between; align-items: center;"> <span>18%</span> <span>80%</span> <span>19%</span> </div>

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Mol	Chain	Length	Quality of chain
2	B	741	17% 81% 19%
2	b	741	18% 80% 20%
3	3	81	78% 19% ..
3	C	81	78% 19% ..
3	c	81	75% 21% ..
4	4	139	19% 84% 15% .
4	D	139	18% 86% 14% .
4	d	139	18% 86% 13% .
5	5	76	39% 72% 16% . 8%
5	E	76	41% 74% 14% . 8%
5	e	76	41% 74% 14% . 8%
6	6	141	82% 72% 26% ..
6	F	141	83% 72% 26% ..
6	f	141	82% 74% 25% ..
7	7	38	5% 84% 16%
7	I	38	5% 82% 18%
7	i	38	5% 84% 16%
8	8	41	85% 66% 32% .
8	J	41	88% 59% 39% .
8	j	41	90% 61% 37% .
9	9	83	88% 64% 30% . 5%
9	K	83	87% 63% 31% . 5%
9	k	83	90% 64% 30% . 5%
10	0	155	6% 79% 19% .
10	L	155	7% 79% 19% .

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Mol	Chain	Length	Quality of chain
10	l	155	
11	M	31	
11	m	31	
11	y	31	
12	X	36	
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
14	CLA	1	819	X	-	-	-
14	CLA	1	820	X	-	-	-
14	CLA	1	821	X	-	-	-
14	CLA	1	822	X	-	-	-
14	CLA	1	823	X	-	-	-
14	CLA	1	824	X	-	-	-
14	CLA	1	825	X	-	-	-
14	CLA	1	826	X	-	-	-
14	CLA	1	827	X	-	-	-
14	CLA	1	828	X	-	-	-
14	CLA	1	829	X	-	-	-
14	CLA	1	830	X	-	-	-
14	CLA	1	831	X	-	-	-
14	CLA	1	832	X	-	-	-
14	CLA	1	833	X	-	-	-
14	CLA	1	834	X	-	-	-
14	CLA	1	835	X	-	-	-
14	CLA	1	836	X	-	-	-
14	CLA	1	837	X	-	-	-
14	CLA	1	838	X	-	-	-
14	CLA	1	839	X	-	-	-
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	-	-	-

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

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

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

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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
			Total	C	N	O	S		
1	A	746	5826	3823	995	982	26	0	0
1	a	746	5826	3823	995	982	26	0	0
1	1	746	5826	3823	995	982	26	0	0

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

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

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

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

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

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

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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

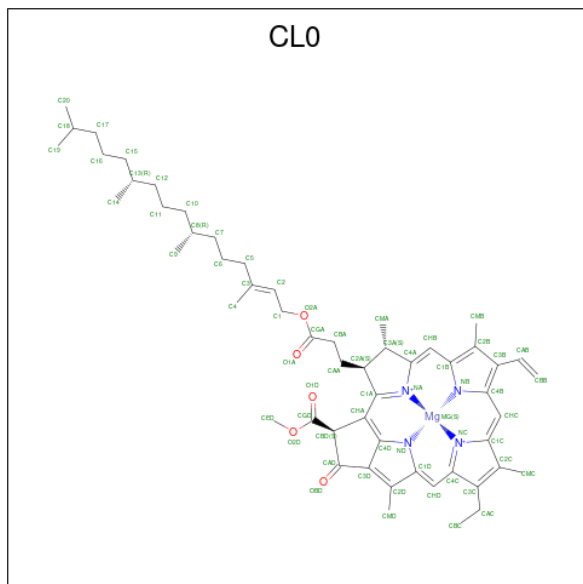
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

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.

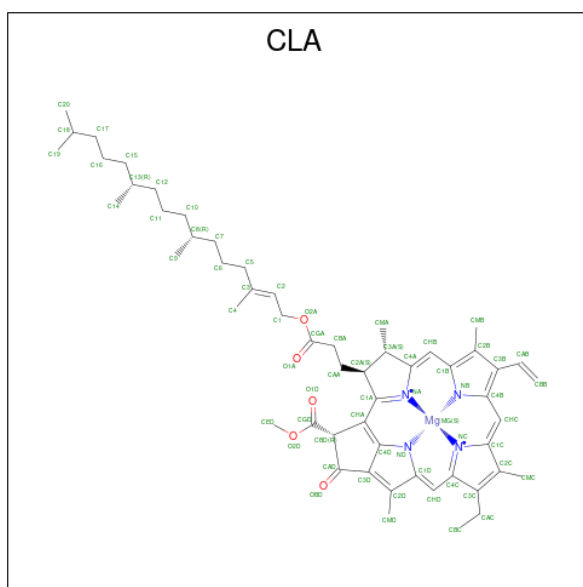
Mol	Chain	Residues	Atoms				AltConf	Trace
12	X	27	Total	C	N	O	0	0
			228	163	33	32		
12	x	27	Total	C	N	O	0	0
			228	163	33	32		
12	z	27	Total	C	N	O	0	0
			228	163	33	32		

- Molecule 13 is CHLOROPHYLL A ISOMER (CCD ID: 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 (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



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

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

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

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

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

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

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

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

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

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

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

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

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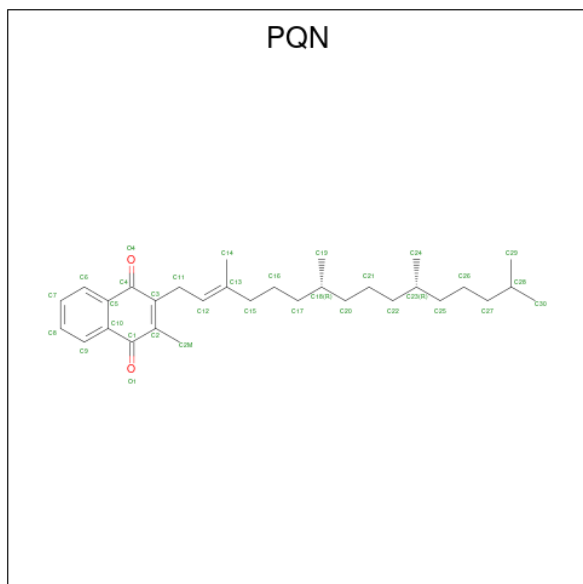
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	2	1	65	55	1	4	5	0
14	2	1	65	55	1	4	5	0
14	2	1	50	40	1	4	5	0
14	2	1	45	35	1	4	5	0
14	2	1	60	50	1	4	5	0
14	2	1	65	55	1	4	5	0
14	2	1	47	37	1	4	5	0
14	2	1	65	55	1	4	5	0
14	2	1	65	55	1	4	5	0
14	6	1	58	48	1	4	5	0
14	6	1	45	35	1	4	5	0
14	6	1	50	40	1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

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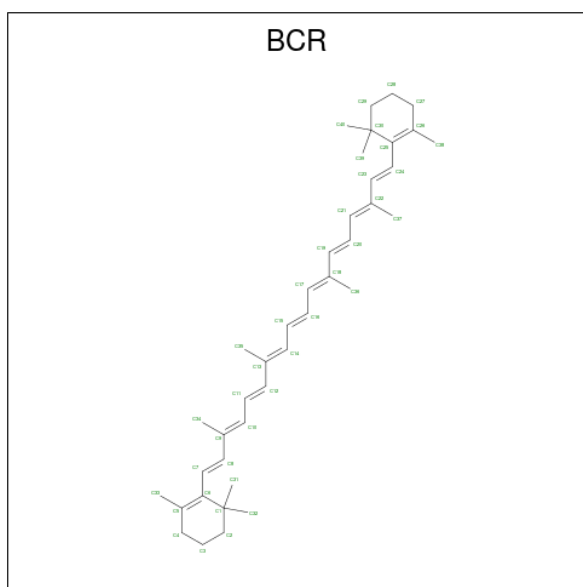
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
14	z	1	45	35	1	4	5	0

- Molecule 15 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



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

- Molecule 16 is BETA-CAROTENE (CCD ID: BCR) (formula:  $C_{40}H_{56}$ ).



Mol	Chain	Residues	Atoms	AltConf
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
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	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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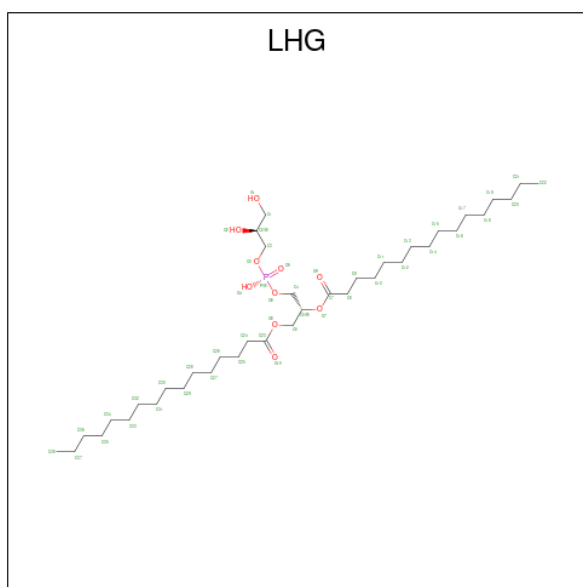
Mol	Chain	Residues	Atoms	AltConf
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16	b	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	f	1	Total C 40 40	0
16	i	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	j	1	Total C 40 40	0
16	k	1	Total C 25 25	0
16	l	1	Total C 40 40	0
16	l	1	Total 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 (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



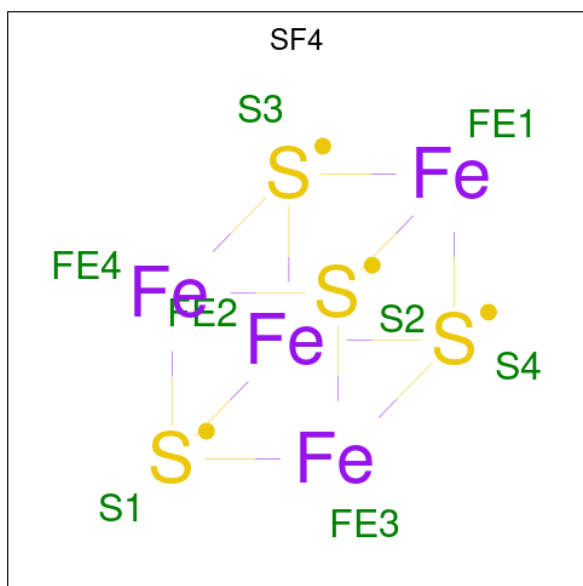
Mol	Chain	Residues	Atoms			AltConf	
			Total	C	O		P
17	A	1	49	38	10	1	0
17	A	1	41	30	10	1	0
17	B	1	49	38	10	1	0
17	L	1	49	38	10	1	0
17	L	1	39	28	10	1	0
17	a	1	49	38	10	1	0
17	a	1	41	30	10	1	0
17	b	1	49	38	10	1	0
17	l	1	49	38	10	1	0
17	l	1	39	28	10	1	0
17	1	1	49	38	10	1	0
17	1	1	41	30	10	1	0
17	2	1	49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

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

- Molecule 18 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).

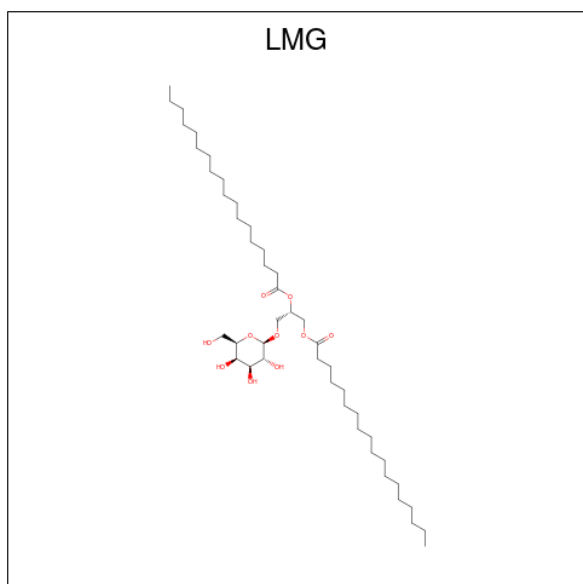


Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
18	B	1	8	4	4	0
18	C	1	8	4	4	0
18	C	1	8	4	4	0
18	b	1	8	4	4	0
18	c	1	8	4	4	0
18	c	1	8	4	4	0
18	2	1	8	4	4	0
18	3	1	8	4	4	0
18	3	1	8	4	4	0

- Molecule 19 is CALCIUM ION (CCD ID: 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 (CCD ID: 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 O 65 65	0
21	B	77	Total O 77 77	0
21	C	28	Total O 28 28	0
21	D	22	Total O 22 22	0
21	E	7	Total O 7 7	0
21	F	4	Total O 4 4	0
21	I	1	Total O 1 1	0
21	J	1	Total O 1 1	0
21	K	1	Total O 1 1	0
21	L	10	Total O 10 10	0
21	M	1	Total O 1 1	0
21	a	65	Total O 65 65	0
21	b	74	Total O 74 74	0
21	c	28	Total O 28 28	0
21	d	19	Total O 19 19	0
21	e	9	Total O 9 9	0
21	f	5	Total O 5 5	0
21	i	2	Total O 2 2	0
21	j	1	Total O 1 1	0
21	k	1	Total O 1 1	0
21	l	11	Total O 11 11	0
21	m	2	Total O 2 2	0

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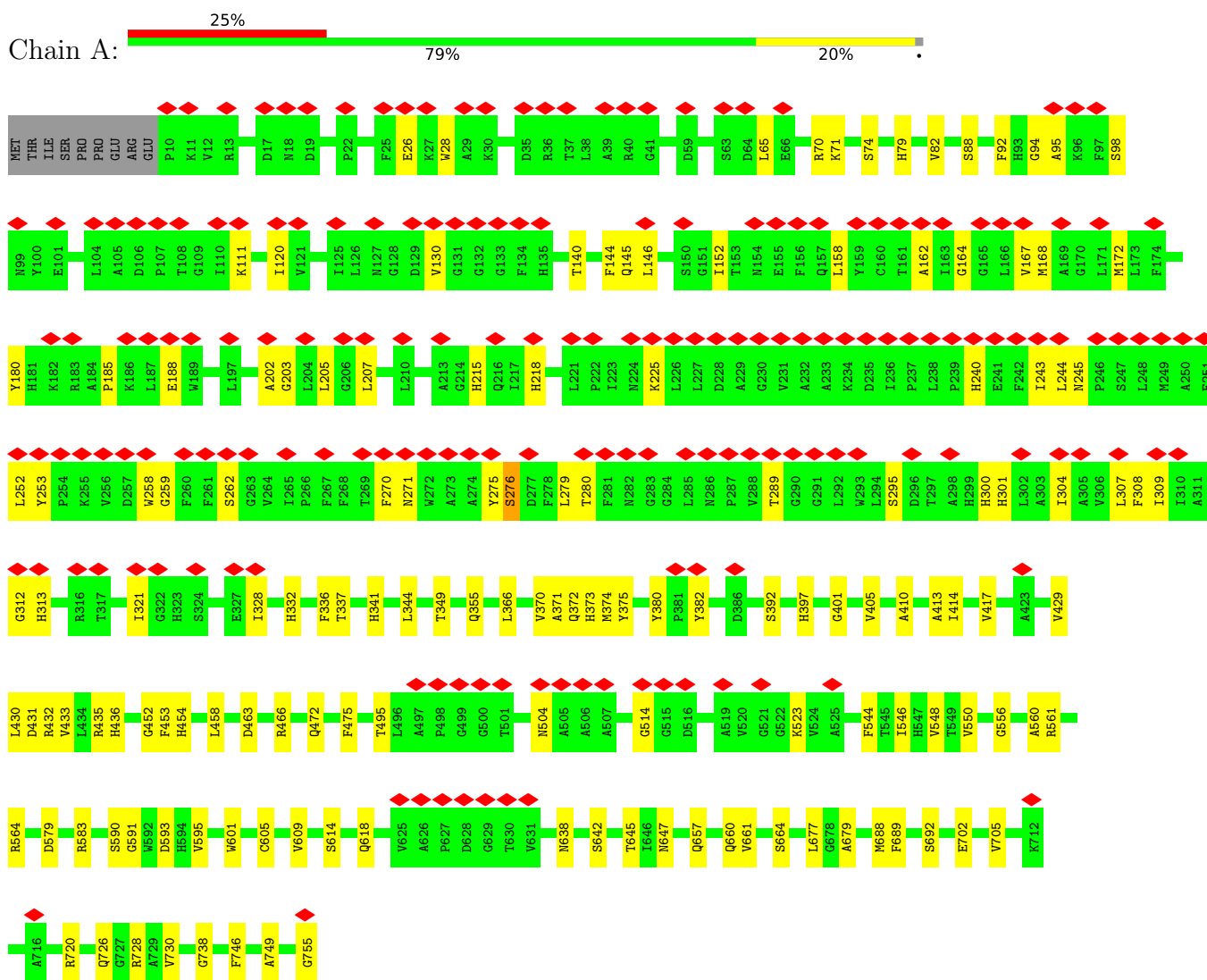
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Mol	Chain	Residues	Atoms		AltConf
21	1	65	Total 65	O 65	0
21	2	75	Total 75	O 75	0
21	3	27	Total 27	O 27	0
21	4	22	Total 22	O 22	0
21	5	8	Total 8	O 8	0
21	6	4	Total 4	O 4	0
21	7	2	Total 2	O 2	0
21	8	1	Total 1	O 1	0
21	9	1	Total 1	O 1	0
21	0	10	Total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

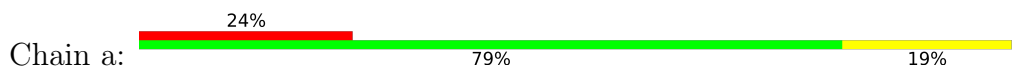
### 3 Residue-property plots

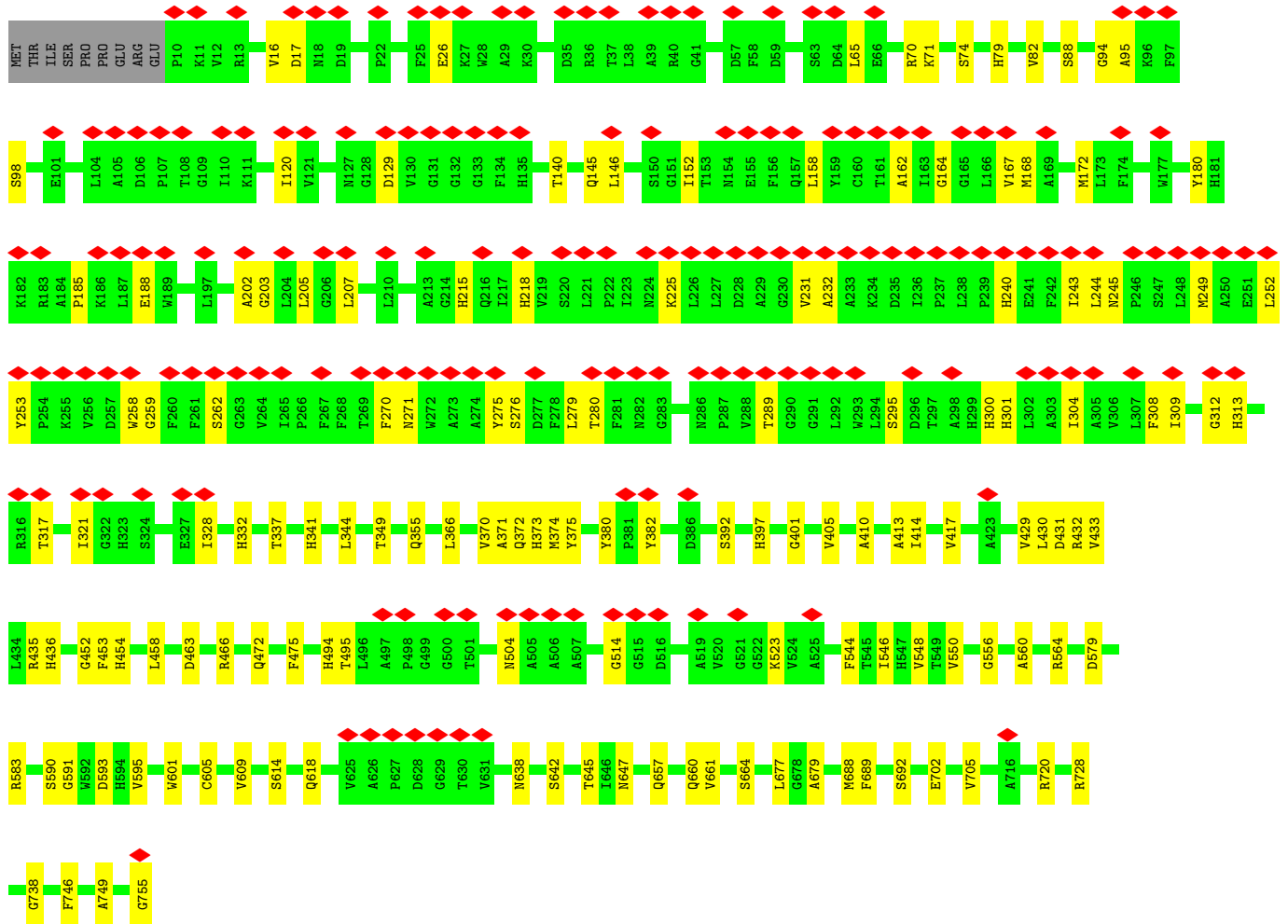
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

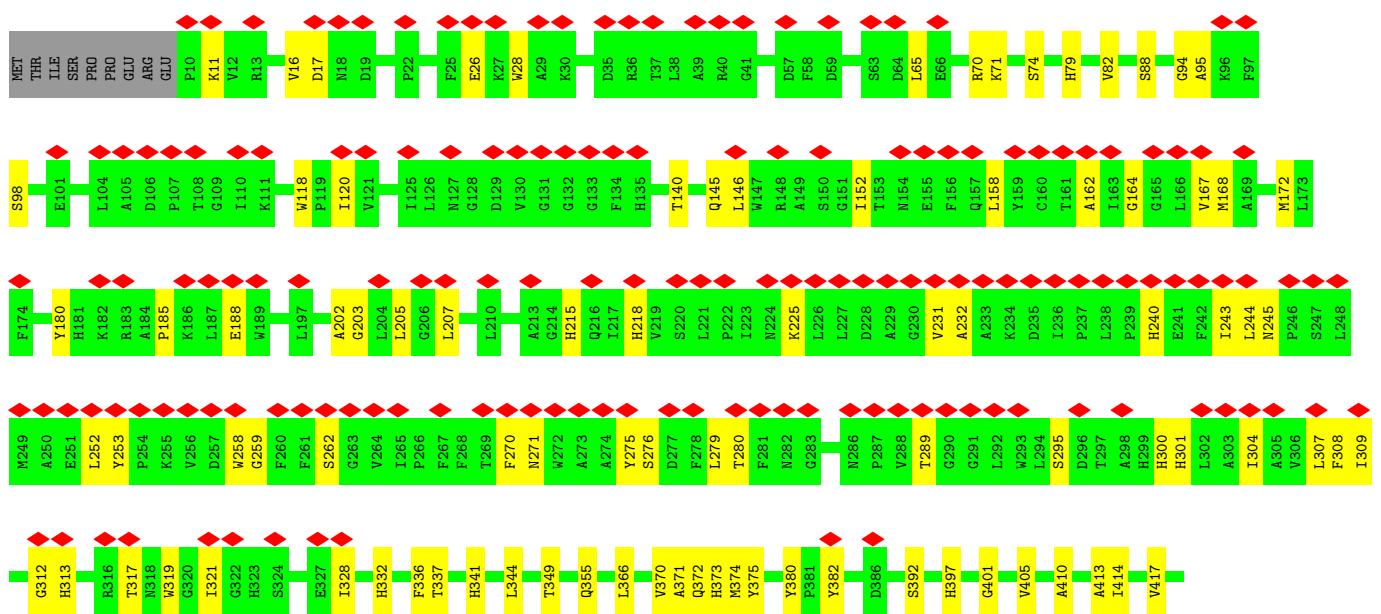
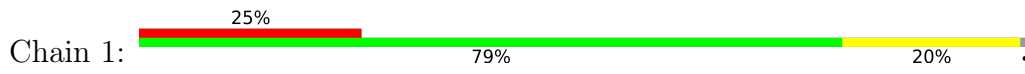


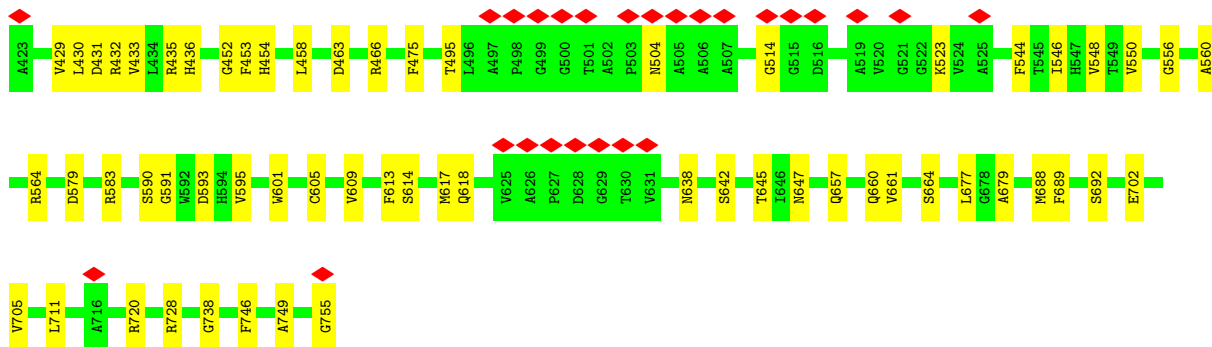
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



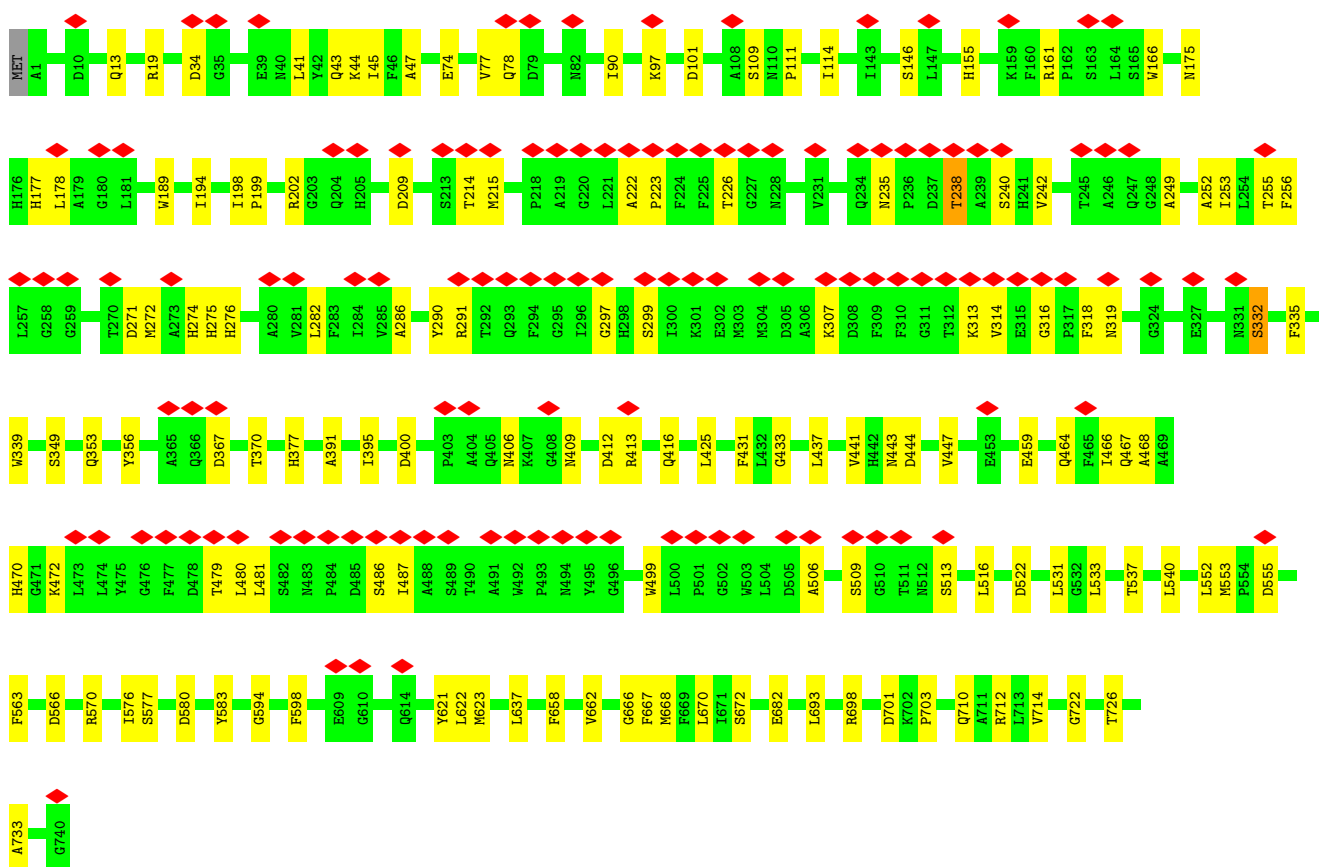
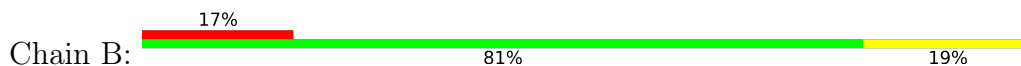


● Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

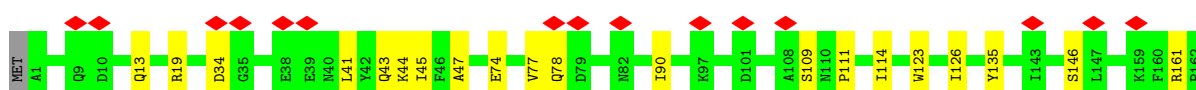


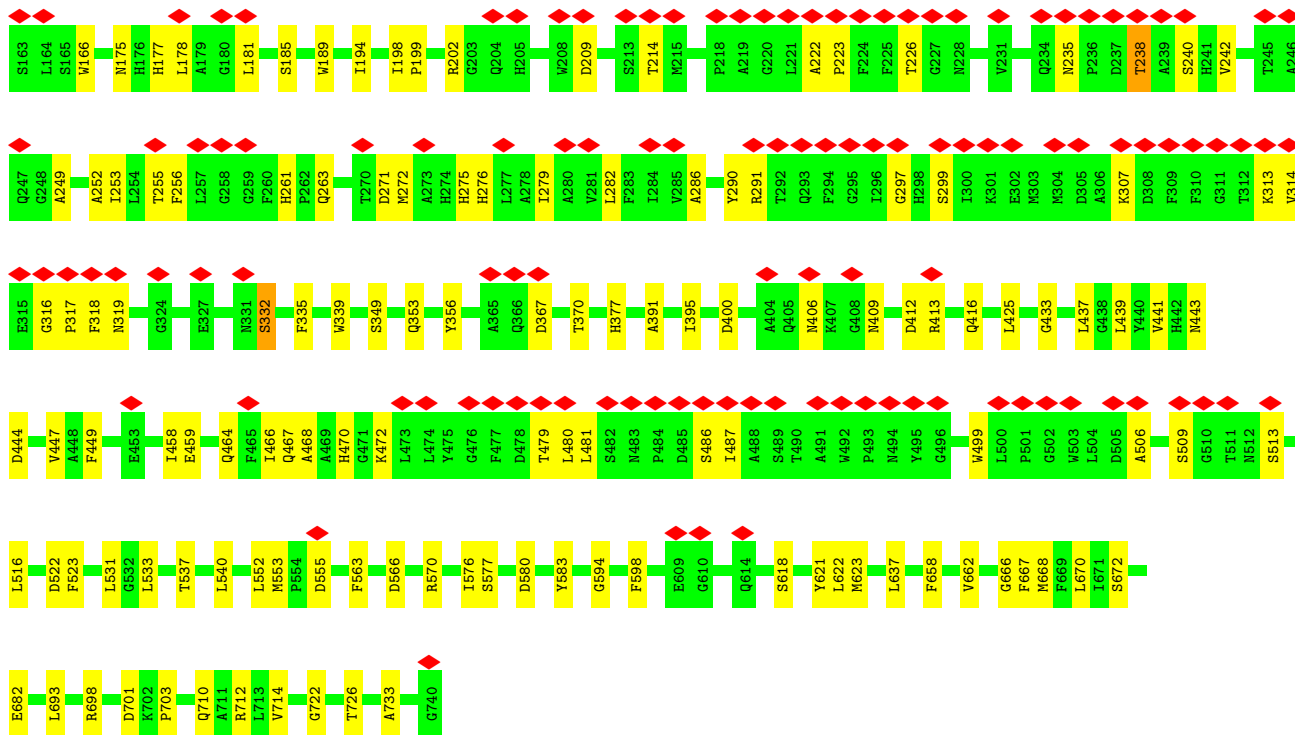


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

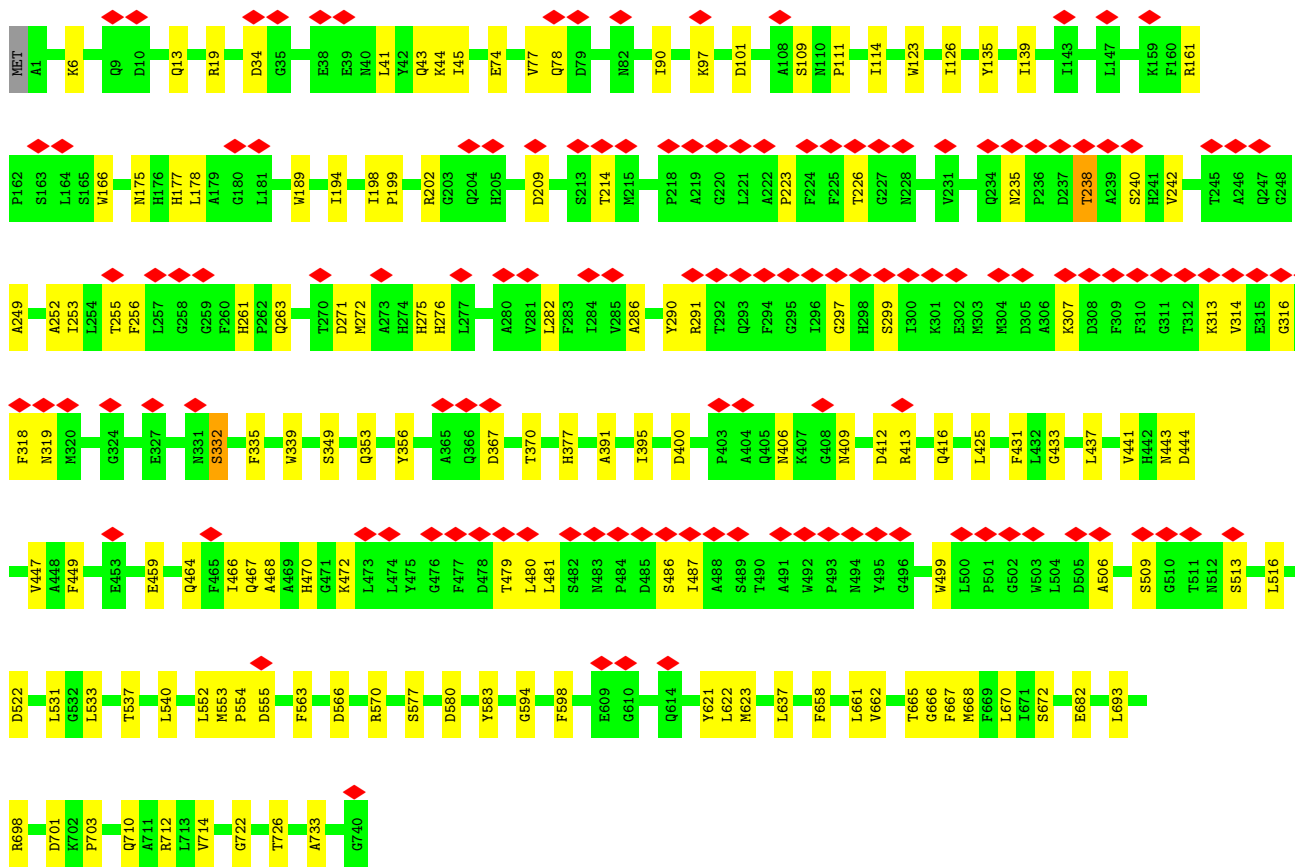
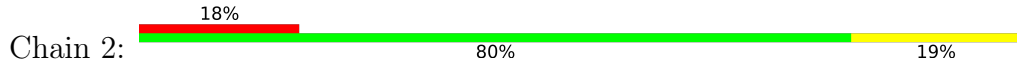


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

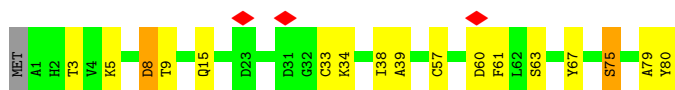
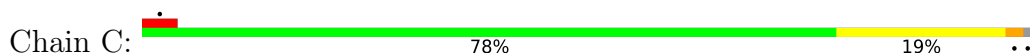




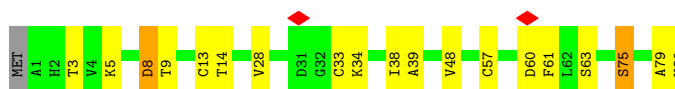
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



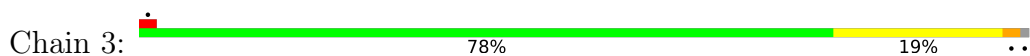
• Molecule 3: Photosystem I iron-sulfur center



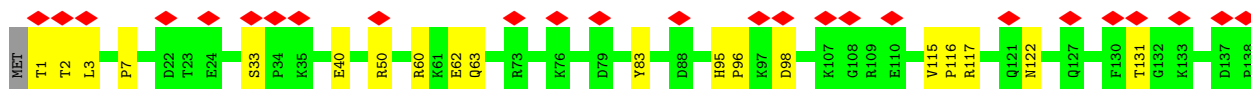
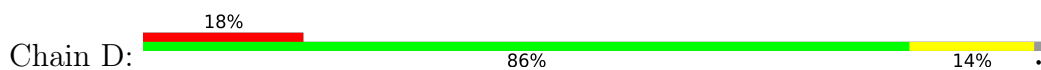
• Molecule 3: Photosystem I iron-sulfur center



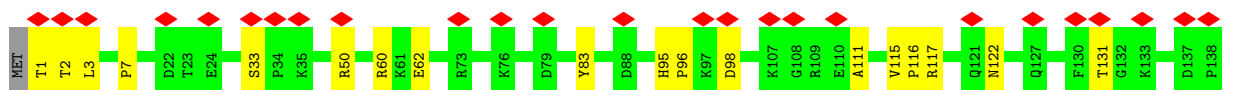
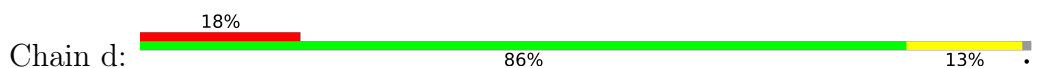
• Molecule 3: Photosystem I iron-sulfur center



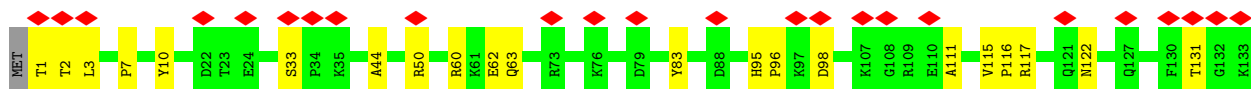
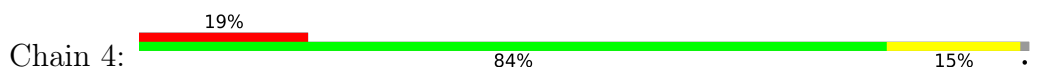
• Molecule 4: Photosystem I reaction center subunit II



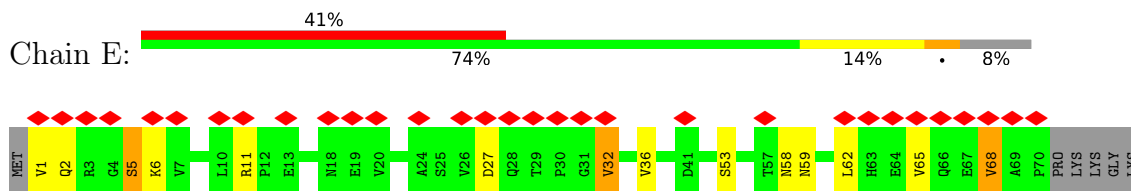
• Molecule 4: Photosystem I reaction center subunit II



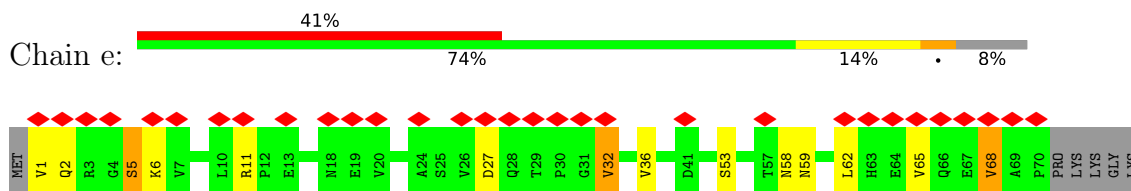
• Molecule 4: Photosystem I reaction center subunit II



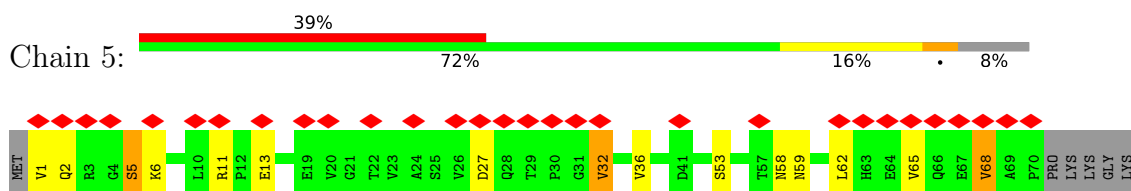
• Molecule 5: Photosystem I reaction center subunit IV



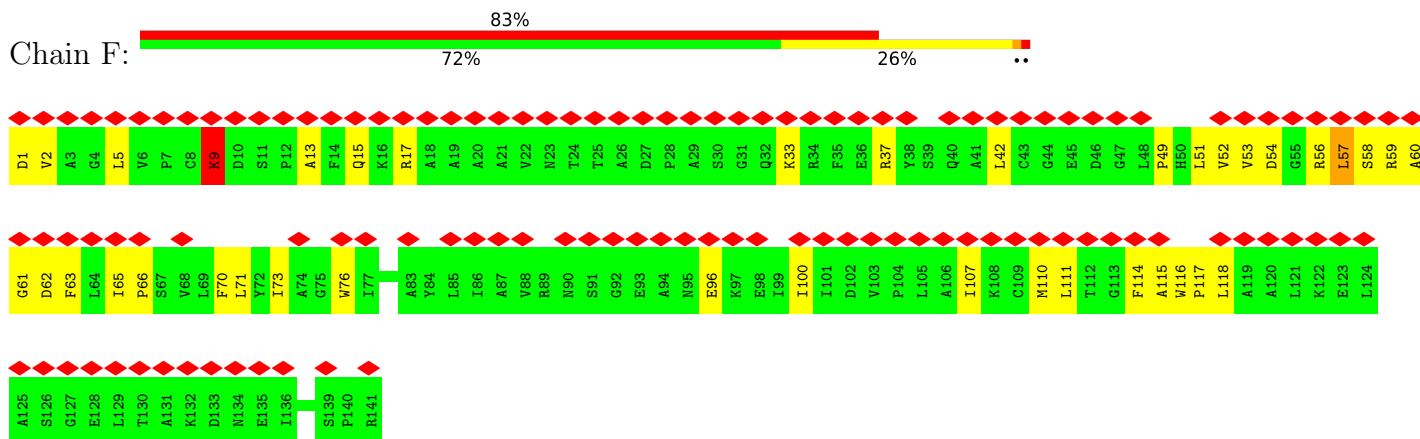
• Molecule 5: Photosystem I reaction center subunit IV



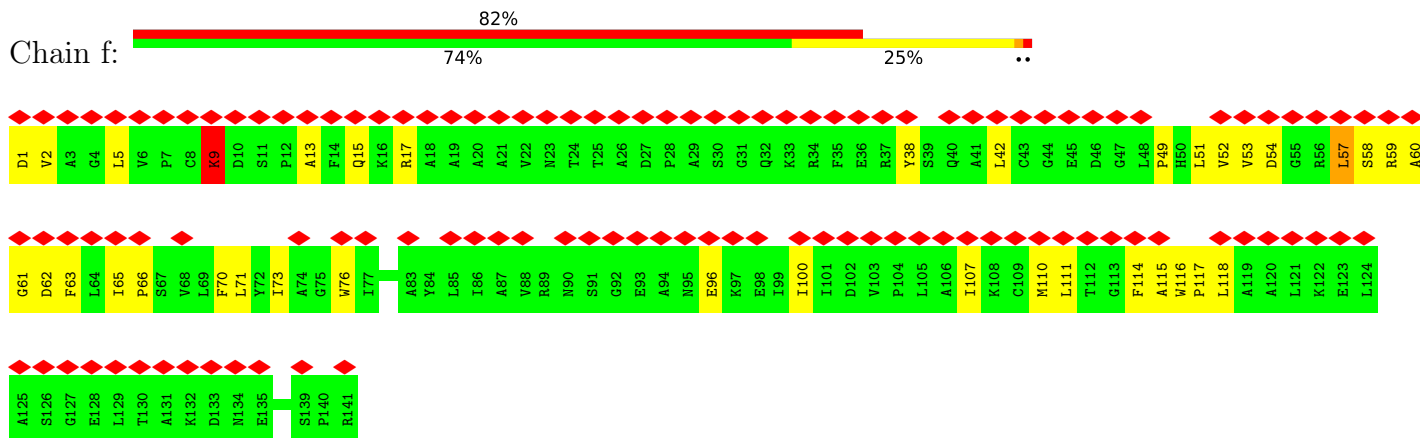
• Molecule 5: Photosystem I reaction center subunit IV



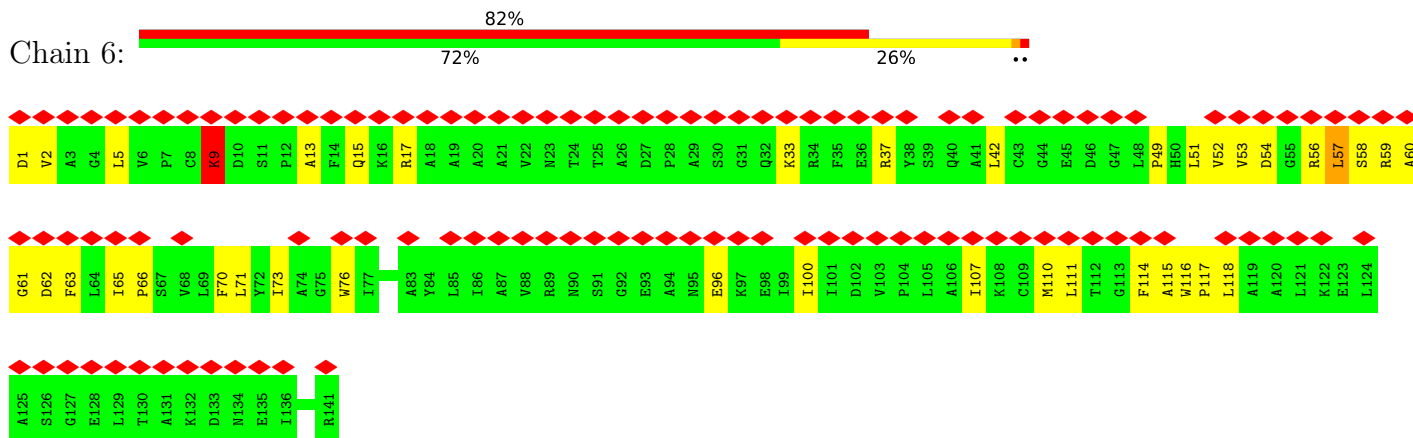
• Molecule 6: Photosystem I reaction center subunit III



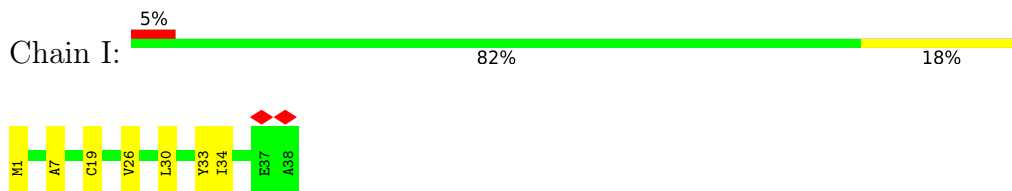
• Molecule 6: Photosystem I reaction center subunit III



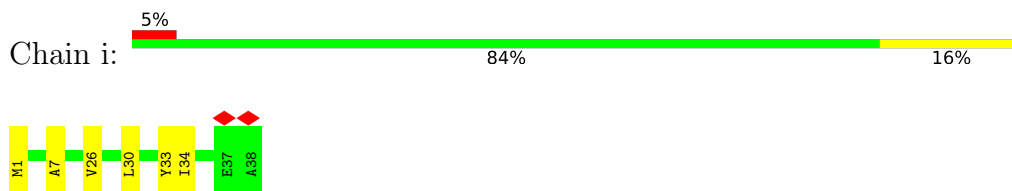
• Molecule 6: Photosystem I reaction center subunit III



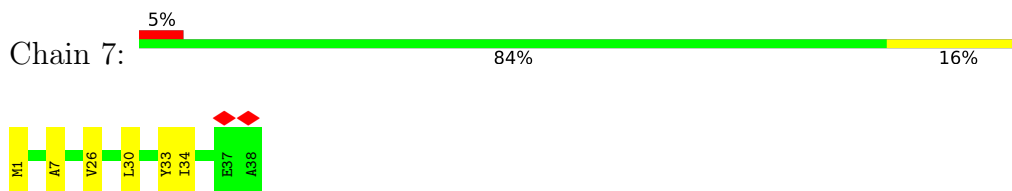
• Molecule 7: Photosystem I reaction center subunit VIII



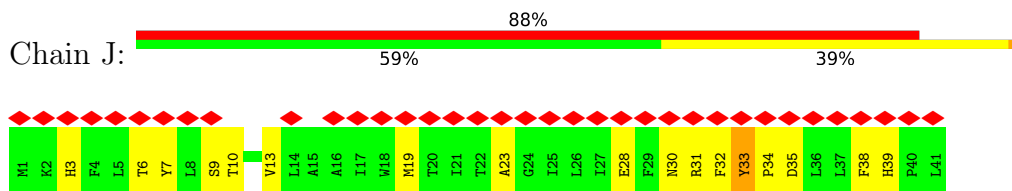
• Molecule 7: Photosystem I reaction center subunit VIII



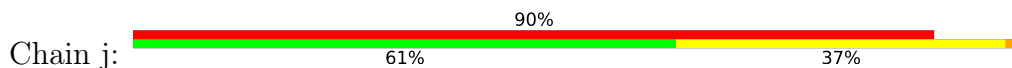
• Molecule 7: Photosystem I reaction center subunit VIII

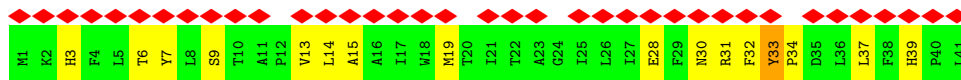


• Molecule 8: Photosystem I reaction center subunit IX

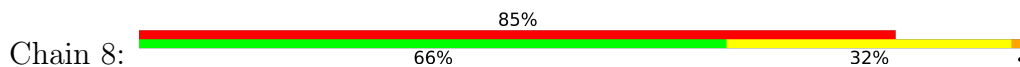


• Molecule 8: Photosystem I reaction center subunit IX

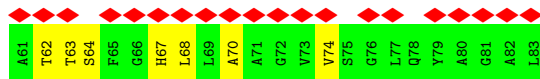
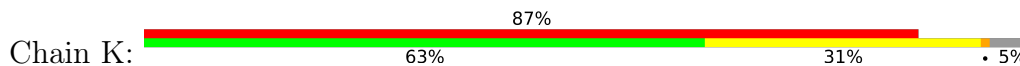




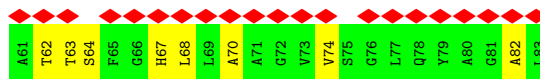
• Molecule 8: Photosystem I reaction center subunit IX



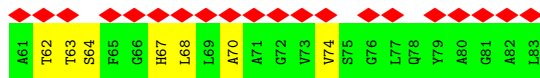
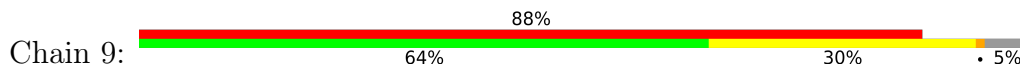
• Molecule 9: Photosystem I reaction center subunit PsaK



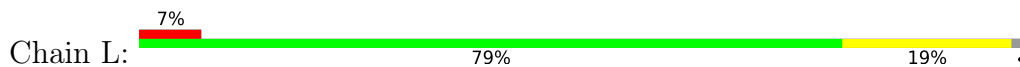
• Molecule 9: Photosystem I reaction center subunit PsaK



• Molecule 9: Photosystem I reaction center subunit PsaK

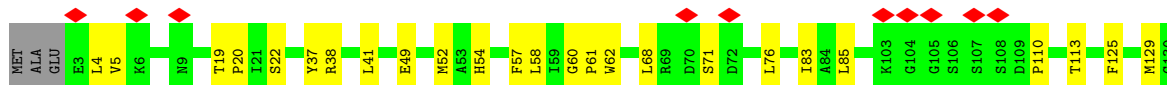
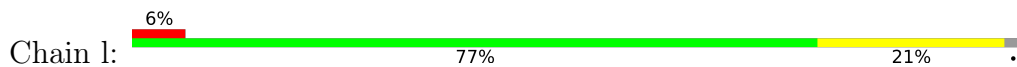


• Molecule 10: Photosystem I reaction center subunit XI

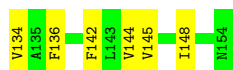
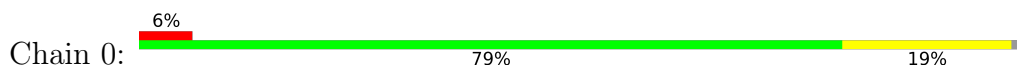




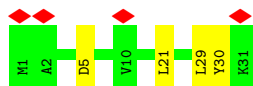
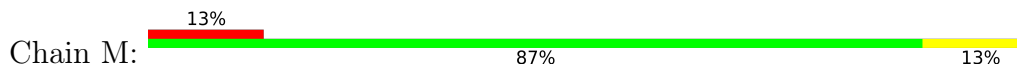
- Molecule 10: Photosystem I reaction center subunit XI



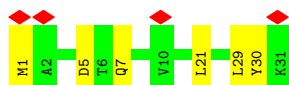
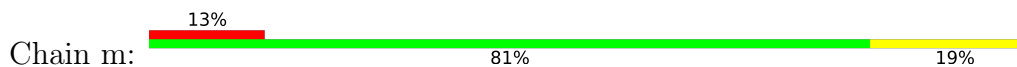
- Molecule 10: Photosystem I reaction center subunit XI



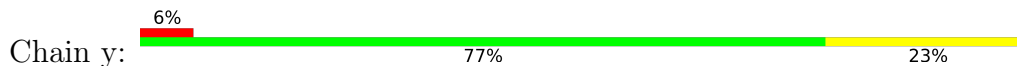
- Molecule 11: Photosystem I reaction center subunit XII



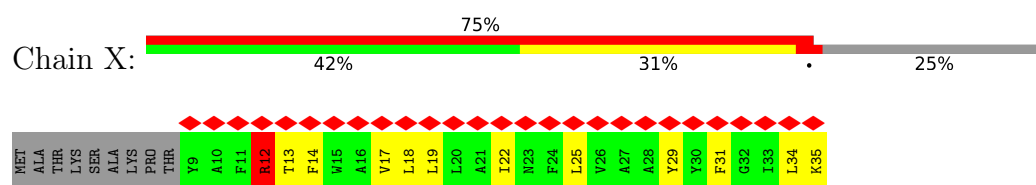
- Molecule 11: Photosystem I reaction center subunit XII



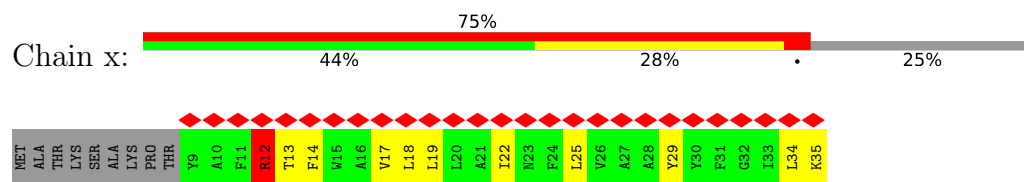
- Molecule 11: Photosystem I reaction center subunit XII



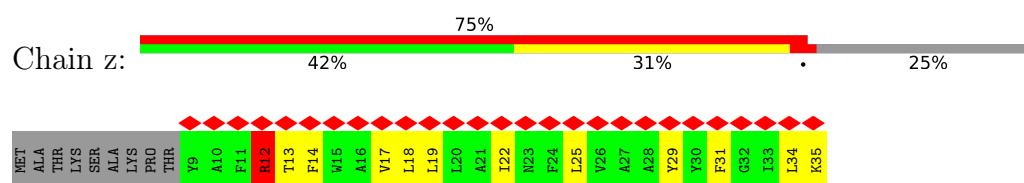
- Molecule 12: Photosystem I 4.8K protein



- 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 ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	0.628, 0.628, 0.628	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	0.37	0/6027	0.45	0/8220
1	A	0.37	0/6027	0.45	0/8220
1	a	0.37	0/6027	0.45	0/8220
2	2	0.38	0/6112	0.45	0/8350
2	B	0.38	0/6112	0.45	0/8350
2	b	0.38	0/6112	0.45	0/8350
3	3	0.42	0/608	0.52	0/824
3	C	0.42	0/608	0.53	0/824
3	c	0.42	0/608	0.52	0/824
4	4	0.36	0/1101	0.44	0/1492
4	D	0.36	0/1101	0.44	0/1492
4	d	0.36	0/1101	0.44	0/1492
5	5	0.27	0/559	0.39	0/762
5	E	0.27	0/559	0.39	0/762
5	e	0.27	0/559	0.39	0/762
6	6	0.25	0/1087	0.53	1/1476 (0.1%)
6	F	0.25	0/1087	0.53	1/1476 (0.1%)
6	f	0.25	0/1087	0.53	1/1476 (0.1%)
7	7	0.39	0/304	0.42	0/415
7	I	0.39	0/304	0.42	0/415
7	i	0.39	0/304	0.42	0/415
8	8	0.30	0/342	0.49	0/467
8	J	0.30	0/342	0.49	0/467
8	j	0.30	0/342	0.49	0/467
9	9	0.22	0/585	0.56	0/800
9	K	0.23	0/585	0.56	0/800
9	k	0.22	0/585	0.56	0/800
10	0	0.41	0/1153	0.43	0/1565
10	L	0.41	0/1153	0.43	0/1565
10	l	0.41	0/1153	0.43	0/1565
11	M	0.35	0/244	0.41	0/332
11	m	0.35	0/244	0.41	0/332

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
11	y	0.35	0/244	0.41	0/332
12	X	0.29	0/236	0.82	1/321 (0.3%)
12	x	0.28	0/236	0.82	1/321 (0.3%)
12	z	0.29	0/236	0.82	1/321 (0.3%)
All	All	0.36	0/55074	0.46	6/75072 (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 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
6	F	9	LYS	CD-CE-NZ	5.22	128.60	111.90
6	f	9	LYS	CD-CE-NZ	5.21	128.58	111.90
6	6	9	LYS	CD-CE-NZ	5.20	128.55	111.90
12	x	12	ARG	CA-CB-CG	5.20	124.50	114.10
12	z	12	ARG	CA-CB-CG	5.20	124.50	114.10

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	5826	0	5692	119	0
1	A	5826	0	5692	122	0
1	a	5826	0	5692	117	0
2	2	5894	0	5653	113	0
2	B	5894	0	5653	110	0
2	b	5894	0	5653	123	0
3	3	598	0	580	17	0
3	C	598	0	580	17	0
3	c	598	0	580	18	0
4	4	1075	0	1077	18	0
4	D	1075	0	1077	16	0
4	d	1075	0	1077	16	0
5	5	546	0	535	11	0
5	E	546	0	535	10	0
5	e	546	0	535	9	0
6	6	1065	0	1077	31	0
6	F	1065	0	1077	32	0
6	f	1065	0	1077	28	0
7	7	303	0	305	4	0
7	I	303	0	305	5	0
7	i	303	0	305	4	0
8	8	340	0	346	11	0
8	J	340	0	346	16	0
8	j	340	0	346	16	0
9	9	571	0	593	23	0
9	K	571	0	593	25	0
9	k	571	0	593	23	0
10	0	1124	0	1127	22	0
10	L	1124	0	1127	22	0
10	l	1124	0	1127	23	0
11	M	241	0	264	6	0
11	m	241	0	264	7	0
11	y	241	0	264	11	0
12	X	228	0	234	18	0
12	x	228	0	234	14	0
12	z	228	0	234	15	0
13	1	65	0	72	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	A	65	0	72	1	0
13	a	65	0	72	1	0
14	0	296	0	312	6	0
14	1	2674	0	2849	55	0
14	2	2446	0	2562	73	0
14	6	153	0	127	6	0
14	8	82	0	58	0	0
14	9	104	0	88	0	0
14	A	2710	0	2873	53	0
14	B	2446	0	2562	71	0
14	F	153	0	127	7	0
14	J	82	0	58	0	0
14	K	104	0	88	2	0
14	L	260	0	288	7	0
14	M	36	0	24	0	0
14	X	45	0	33	0	0
14	a	2609	0	2777	54	0
14	b	2446	0	2562	69	0
14	f	153	0	127	7	0
14	j	147	0	130	4	0
14	k	104	0	88	0	0
14	l	260	0	288	5	0
14	x	45	0	33	0	0
14	z	45	0	33	2	0
15	1	33	0	46	1	0
15	2	33	0	46	0	0
15	A	33	0	46	1	0
15	B	33	0	46	0	0
15	a	33	0	46	3	0
15	b	33	0	46	0	0
16	0	120	0	168	1	0
16	1	225	0	313	11	0
16	2	280	0	392	11	0
16	6	80	0	112	0	0
16	7	40	0	56	0	0
16	8	80	0	112	6	0
16	9	65	0	89	3	0
16	A	265	0	369	13	0
16	B	320	0	448	10	0
16	F	80	0	112	0	0
16	I	80	0	112	1	0
16	J	80	0	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	K	25	0	33	2	0
16	L	40	0	56	0	0
16	M	40	0	56	1	0
16	a	265	0	369	12	0
16	b	240	0	336	8	0
16	f	80	0	112	0	0
16	i	40	0	56	0	0
16	j	120	0	168	13	0
16	k	25	0	33	2	0
16	l	120	0	168	1	0
16	m	40	0	56	1	0
16	y	40	0	56	4	0
17	0	88	0	125	1	0
17	1	90	0	129	2	0
17	2	49	0	74	3	0
17	A	90	0	129	2	0
17	B	49	0	74	5	0
17	L	88	0	125	2	0
17	a	90	0	129	2	0
17	b	49	0	74	3	0
17	l	88	0	125	2	0
18	2	8	0	0	0	0
18	3	16	0	0	0	0
18	B	8	0	0	0	0
18	C	16	0	0	0	0
18	b	8	0	0	0	0
18	c	16	0	0	0	0
19	0	1	0	0	0	0
19	2	1	0	0	0	0
19	B	1	0	0	0	0
19	L	1	0	0	0	0
19	b	1	0	0	0	0
19	l	1	0	0	0	0
20	2	55	0	86	1	0
20	B	55	0	86	0	0
20	b	55	0	86	0	0
21	0	10	0	0	0	0
21	1	65	0	0	12	0
21	2	75	0	0	11	0
21	3	27	0	0	4	0
21	4	22	0	0	2	0
21	5	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	6	4	0	0	0	0
21	7	2	0	0	0	0
21	8	1	0	0	0	0
21	9	1	0	0	0	0
21	A	65	0	0	14	0
21	B	77	0	0	11	0
21	C	28	0	0	4	0
21	D	22	0	0	2	0
21	E	7	0	0	0	0
21	F	4	0	0	0	0
21	I	1	0	0	0	0
21	J	1	0	0	0	0
21	K	1	0	0	0	0
21	L	10	0	0	0	0
21	M	1	0	0	0	0
21	a	65	0	0	14	0
21	b	74	0	0	9	0
21	c	28	0	0	4	0
21	d	19	0	0	1	0
21	e	9	0	0	0	0
21	f	5	0	0	0	0
21	i	2	0	0	0	0
21	j	1	0	0	0	0
21	k	1	0	0	0	0
21	l	11	0	0	0	0
21	m	2	0	0	0	0
21	y	2	0	0	0	0
All	All	75591	0	76164	1368	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

The worst 5 of 1368 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:4:33:SER:OG	4:4:50:ARG:O	1.83	0.96
4:D:33:SER:OG	4:D:50:ARG:O	1.83	0.96
4:d:33:SER:OG	4:d:50:ARG:O	1.83	0.95
1:1:657:GLN:O	21:1:901:HOH:O	1.88	0.92
1:A:657:GLN:O	21:A:901:HOH:O	1.88	0.92

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	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
8	8	39/41 (95%)	37 (95%)	2 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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 [i](#)

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%)	592 (100%)	2 (0%)	86	91
1	A	594/603 (98%)	592 (100%)	2 (0%)	86	91
1	a	594/603 (98%)	592 (100%)	2 (0%)	86	91
2	2	597/598 (100%)	591 (99%)	6 (1%)	68	83
2	B	597/598 (100%)	591 (99%)	6 (1%)	68	83
2	b	597/598 (100%)	591 (99%)	6 (1%)	68	83
3	3	67/68 (98%)	65 (97%)	2 (3%)	36	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	C	67/68 (98%)	65 (97%)	2 (3%)	36	67
3	c	67/68 (98%)	65 (97%)	2 (3%)	36	67
4	4	115/116 (99%)	113 (98%)	2 (2%)	53	77
4	D	115/116 (99%)	113 (98%)	2 (2%)	53	77
4	d	115/116 (99%)	113 (98%)	2 (2%)	53	77
5	5	60/65 (92%)	56 (93%)	4 (7%)	15	44
5	E	60/65 (92%)	56 (93%)	4 (7%)	15	44
5	e	60/65 (92%)	56 (93%)	4 (7%)	15	44
6	6	109/109 (100%)	108 (99%)	1 (1%)	70	85
6	F	109/109 (100%)	108 (99%)	1 (1%)	70	85
6	f	109/109 (100%)	108 (99%)	1 (1%)	70	85
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%)	10	34
8	J	35/35 (100%)	32 (91%)	3 (9%)	10	34
8	j	35/35 (100%)	32 (91%)	3 (9%)	10	34
9	9	58/61 (95%)	55 (95%)	3 (5%)	21	53
9	K	58/61 (95%)	55 (95%)	3 (5%)	21	53
9	k	58/61 (95%)	55 (95%)	3 (5%)	21	53
10	0	117/120 (98%)	116 (99%)	1 (1%)	70	85
10	L	117/120 (98%)	116 (99%)	1 (1%)	70	85
10	l	117/120 (98%)	116 (99%)	1 (1%)	70	85
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%)	8	29
12	x	21/28 (75%)	19 (90%)	2 (10%)	8	29
12	z	21/28 (75%)	19 (90%)	2 (10%)	8	29
All	All	5490/5580 (98%)	5412 (99%)	78 (1%)	57	80

5 of 78 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	2	332	SER
8	8	33	TYR
2	2	486	SER
5	5	32	VAL
10	0	22	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
10	1	16	HIS
1	1	718	GLN
1	1	93	HIS
1	1	353	HIS
2	2	405	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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
7	FME	I	1	7	8,9,10	1.04	1 (12%)	8,9,11	1.22	1 (12%)
8	FME	8	1	8	8,9,10	0.98	0	8,9,11	0.97	0
8	FME	j	1	8	8,9,10	0.98	0	8,9,11	0.97	0
8	FME	J	1	8	8,9,10	0.98	0	8,9,11	0.97	0
7	FME	i	1	7	8,9,10	1.04	0	8,9,11	1.23	1 (12%)
7	FME	7	1	7	8,9,10	1.04	1 (12%)	8,9,11	1.23	1 (12%)

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
7	FME	I	1	7	-	3/7/9/11	-
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	i	1	7	-	3/7/9/11	-
7	FME	7	1	7	-	3/7/9/11	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	7	1	FME	CA-N	-2.03	1.43	1.46
7	I	1	FME	CA-N	-2.01	1.43	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	i	1	FME	C-CA-N	2.63	114.58	109.50
7	7	1	FME	C-CA-N	2.63	114.57	109.50
7	I	1	FME	C-CA-N	2.62	114.56	109.50

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
7	I	1	FME	N-CA-CB-CG
7	i	1	FME	N-CA-CB-CG

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

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	1	802	-	69,73,73	1.16	11 (15%)	82,113,113	1.48	10 (12%)
14	CLA	b	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	a	838	-	69,73,73	1.17	8 (11%)	82,113,113	1.36	6 (7%)
14	CLA	B	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
14	CLA	1	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	2	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	B	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	a	823	-	69,73,73	1.17	9 (13%)	82,113,113	1.34	4 (4%)
16	BCR	0	210	-	41,41,41	1.24	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	a	826	21	69,73,73	1.16	10 (14%)	82,113,113	1.40	9 (10%)
14	CLA	b	3023	21	59,63,73	1.26	8 (13%)	70,101,113	1.38	6 (8%)
14	CLA	a	815	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	A	827	21	69,73,73	1.15	9 (13%)	82,113,113	1.40	10 (12%)
14	CLA	L	204	-	69,73,73	1.15	8 (11%)	82,113,113	1.43	8 (9%)
14	CLA	A	831	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	5 (6%)
14	CLA	1	811	-	53,57,73	1.31	9 (16%)	61,93,113	1.36	5 (8%)
14	CLA	b	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	817	21	69,73,73	1.18	8 (11%)	82,113,113	1.38	8 (9%)
14	CLA	A	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.38	7 (8%)
16	BCR	9	102	-	41,41,41	1.21	3 (7%)	56,56,56	1.36	10 (17%)
14	CLA	A	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	6 (7%)
16	BCR	F	205	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	1	813	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	4 (6%)
14	CLA	f	203	21	49,53,73	1.38	9 (18%)	58,89,113	1.47	6 (10%)
14	CLA	8	102	-	41,45,73	1.48	8 (19%)	50,78,113	1.39	4 (8%)
14	CLA	a	817	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	LHG	2	3051	-	48,48,48	0.69	2 (4%)	51,54,54	1.20	5 (9%)
20	LMG	b	3050	-	55,55,55	0.91	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	a	809	1	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	f	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	1	839	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	1	817	21	69,73,73	1.17	9 (13%)	82,113,113	1.38	8 (9%)
16	BCR	6	205	-	41,41,41	1.19	2 (4%)	56,56,56	1.36	8 (14%)
14	CLA	b	3036	21	54,58,73	1.36	8 (14%)	64,95,113	1.41	7 (10%)
16	BCR	A	850	-	41,41,41	1.36	4 (9%)	56,56,56	1.32	7 (12%)
16	BCR	j	1106	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	2	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.50	10 (12%)
14	CLA	A	813	-	49,53,73	1.37	9 (18%)	58,89,113	1.48	4 (6%)
16	BCR	A	848	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	l	203	2	69,73,73	1.17	9 (13%)	82,113,113	1.37	9 (10%)
16	BCR	b	3045	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	2	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	2	3005	-	69,73,73	1.15	6 (8%)	82,113,113	1.47	7 (8%)
14	CLA	A	837	1	49,53,73	1.39	8 (16%)	58,89,113	1.37	6 (10%)
14	CLA	B	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.33	8 (9%)
14	CLA	2	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.38	8 (9%)
14	CLA	b	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.52	10 (12%)
14	CLA	2	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
16	BCR	b	3044	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	2	3004	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	5 (6%)
18	SF4	B	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	1	821	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
14	CLA	B	3042	-	69,73,73	1.18	8 (11%)	82,113,113	1.39	7 (8%)
14	CLA	2	3041	21	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	b	3047	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
17	LHG	a	853	14	40,40,48	0.79	2 (5%)	43,46,54	1.19	3 (6%)
14	CLA	2	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
14	CLA	b	3008	-	69,73,73	1.18	8 (11%)	82,113,113	1.34	6 (7%)
14	CLA	x	1701	-	49,53,73	1.41	7 (14%)	58,89,113	1.41	4 (6%)
16	BCR	1	847	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	a	808	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	F	204	-	54,58,73	1.33	7 (12%)	64,95,113	1.45	7 (10%)
14	CLA	A	821	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
16	BCR	k	103	-	25,25,41	1.11	1 (4%)	33,33,56	1.25	3 (9%)
16	BCR	L	206	-	41,41,41	1.19	4 (9%)	56,56,56	1.20	4 (7%)
16	BCR	0	205	-	41,41,41	1.45	5 (12%)	56,56,56	1.31	6 (10%)
14	CLA	b	3004	-	69,73,73	1.16	8 (11%)	82,113,113	1.34	5 (6%)
14	CLA	b	3006	-	69,73,73	1.17	9 (13%)	82,113,113	1.38	7 (8%)
16	BCR	l	209	-	41,41,41	1.23	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	b	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	8 (11%)
14	CLA	a	835	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	5 (6%)
16	BCR	6	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
15	PQN	a	844	-	34,34,34	0.44	0	43,45,45	0.50	1 (2%)
14	CLA	a	833	-	69,73,73	1.15	10 (14%)	82,113,113	1.40	9 (10%)
16	BCR	1	851	-	25,25,41	1.16	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	2	3036	21	54,58,73	1.36	8 (14%)	64,95,113	1.41	8 (12%)
14	CLA	b	3012	-	69,73,73	1.16	7 (10%)	82,113,113	1.43	8 (9%)
15	PQN	1	845	-	34,34,34	0.44	0	43,45,45	0.49	1 (2%)
14	CLA	1	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	1	840	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	A	823	-	49,53,73	1.37	8 (16%)	58,89,113	1.46	6 (10%)
14	CLA	2	3038	-	64,68,73	1.22	9 (14%)	76,107,113	1.35	5 (6%)
14	CLA	1	803	21	69,73,73	1.21	9 (13%)	82,113,113	1.22	3 (3%)
14	CLA	A	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.41	6 (9%)
14	CLA	2	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.43	8 (9%)
14	CLA	B	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	A	815	-	69,73,73	1.17	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	A	834	-	69,73,73	1.16	10 (14%)	82,113,113	1.41	9 (10%)
14	CLA	b	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	5 (6%)
13	CL0	a	801	-	58,73,73	2.17	13 (22%)	60,113,113	1.78	14 (23%)
14	CLA	A	814	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	1	826	21	69,73,73	1.17	9 (13%)	82,113,113	1.39	10 (12%)
14	CLA	1	815	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	5 (6%)
14	CLA	b	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	2	3029	-	69,73,73	1.18	8 (11%)	82,113,113	1.19	5 (6%)
16	BCR	A	847	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	A	803	21	69,73,73	1.22	8 (11%)	82,113,113	1.23	3 (3%)
14	CLA	2	3020	21	69,73,73	1.17	8 (11%)	82,113,113	1.31	5 (6%)
14	CLA	2	3040	-	51,55,73	1.34	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	L	201	2	69,73,73	1.16	10 (14%)	82,113,113	1.38	9 (10%)
14	CLA	1	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.47	7 (8%)
14	CLA	2	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	l	206	10	69,73,73	1.18	9 (13%)	82,113,113	1.35	9 (10%)
17	LHG	L	207	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
14	CLA	B	3035	-	69,73,73	1.16	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	A	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	9 (10%)
14	CLA	1	809	1	69,73,73	1.14	9 (13%)	82,113,113	1.34	7 (8%)
14	CLA	b	3040	-	51,55,73	1.35	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	1	828	-	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
16	BCR	b	3046	-	41,41,41	1.28	3 (7%)	56,56,56	1.22	5 (8%)
14	CLA	a	842	21	69,73,73	1.19	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	b	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	6 (7%)
14	CLA	A	812	-	69,73,73	1.16	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	A	833	-	69,73,73	1.15	9 (13%)	82,113,113	1.27	5 (6%)
14	CLA	1	831	-	69,73,73	1.19	8 (11%)	82,113,113	1.34	6 (7%)
14	CLA	8	101	-	49,53,73	1.39	9 (18%)	58,89,113	1.44	5 (8%)
16	BCR	B	3044	-	41,41,41	1.17	2 (4%)	56,56,56	1.21	4 (7%)
14	CLA	L	203	10	69,73,73	1.19	9 (13%)	82,113,113	1.35	9 (10%)
14	CLA	6	203	21	49,53,73	1.38	9 (18%)	58,89,113	1.46	6 (10%)
14	CLA	j	1102	-	49,53,73	1.39	6 (12%)	58,89,113	1.45	5 (8%)
14	CLA	2	3006	-	69,73,73	1.17	9 (13%)	82,113,113	1.39	7 (8%)
18	SF4	c	102	3	0,12,12	-	-	-	-	-
14	CLA	1	812	-	69,73,73	1.16	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	A	816	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	a	837	-	69,73,73	1.18	9 (13%)	82,113,113	1.44	9 (10%)
17	LHG	B	3051	-	48,48,48	0.69	2 (4%)	51,54,54	1.21	5 (9%)
14	CLA	b	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	9 (10%)
16	BCR	B	3053	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	A	842	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	9 (10%)
14	CLA	X	1701	-	49,53,73	1.41	8 (16%)	58,89,113	1.41	4 (6%)
18	SF4	C	102	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
17	LHG	1	853	14	40,40,48	0.79	2 (5%)	43,46,54	1.19	3 (6%)
16	BCR	9	104	-	25,25,41	1.10	1 (4%)	33,33,56	1.25	2 (6%)
16	BCR	A	851	-	41,41,41	1.34	4 (9%)	56,56,56	1.32	6 (10%)
16	BCR	B	3045	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	a	807	-	55,59,73	1.30	8 (14%)	64,96,113	1.41	6 (9%)
15	PQN	A	845	-	34,34,34	0.44	0	43,45,45	0.49	1 (2%)
16	BCR	j	1105	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	2	3035	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	A	840	-	69,73,73	1.15	8 (11%)	82,113,113	1.28	6 (7%)
16	BCR	a	849	-	41,41,41	1.36	4 (9%)	56,56,56	1.32	7 (12%)
14	CLA	l	208	21	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
14	CLA	B	3004	-	69,73,73	1.16	7 (10%)	82,113,113	1.34	5 (6%)
14	CLA	2	3034	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	K	103	-	25,25,41	1.11	1 (4%)	33,33,56	1.25	2 (6%)
16	BCR	8	103	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	a	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.39	5 (6%)
16	BCR	j	1104	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	1	843	21	69,73,73	1.18	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	2	3022	-	49,53,73	1.37	7 (14%)	58,89,113	1.53	6 (10%)
16	BCR	2	3045	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	1	833	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	4 (4%)
14	CLA	a	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
14	CLA	B	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	6 (7%)
14	CLA	A	820	-	69,73,73	1.18	9 (13%)	82,113,113	1.41	9 (10%)
17	LHG	b	3051	-	48,48,48	0.68	2 (4%)	51,54,54	1.20	5 (9%)
14	CLA	1	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	5 (6%)
14	CLA	B	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	a	841	-	69,73,73	1.17	9 (13%)	82,113,113	1.31	8 (9%)
16	BCR	J	103	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	5 (8%)
14	CLA	9	101	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	4 (6%)
14	CLA	1	825	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
14	CLA	a	813	-	69,73,73	1.16	9 (13%)	82,113,113	1.31	4 (4%)
14	CLA	a	822	-	49,53,73	1.37	9 (18%)	58,89,113	1.48	6 (10%)
14	CLA	j	1103	-	41,45,73	1.48	10 (24%)	50,78,113	1.40	5 (10%)
14	CLA	B	3015	-	69,73,73	1.16	7 (10%)	82,113,113	1.31	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	820	-	69,73,73	1.17	6 (8%)	82,113,113	1.31	7 (8%)
13	CL0	1	801	-	58,73,73	2.18	13 (22%)	60,113,113	1.79	14 (23%)
18	SF4	C	101	3	0,12,12	-	-	-	-	-
14	CLA	F	203	21	49,53,73	1.39	9 (18%)	58,89,113	1.46	6 (10%)
14	CLA	L	205	21	69,73,73	1.16	8 (11%)	82,113,113	1.33	8 (9%)
16	BCR	I	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	4 (7%)
16	BCR	a	847	-	41,41,41	1.26	3 (7%)	56,56,56	1.38	7 (12%)
14	CLA	b	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.48	6 (10%)
16	BCR	a	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.33	6 (10%)
14	CLA	2	3037	21	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
14	CLA	B	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.21	6 (7%)
16	BCR	y	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	b	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.51	10 (12%)
14	CLA	a	827	-	69,73,73	1.17	9 (13%)	82,113,113	1.28	6 (7%)
14	CLA	A	822	21	69,73,73	1.16	9 (13%)	82,113,113	1.35	7 (8%)
16	BCR	l	210	-	41,41,41	1.19	3 (7%)	56,56,56	1.21	4 (7%)
14	CLA	1	838	-	69,73,73	1.17	9 (13%)	82,113,113	1.44	9 (10%)
14	CLA	b	3038	-	64,68,73	1.22	9 (14%)	76,107,113	1.34	5 (6%)
14	CLA	0	209	21	69,73,73	1.16	8 (11%)	82,113,113	1.34	8 (9%)
15	PQN	b	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	z	1701	-	49,53,73	1.41	8 (16%)	58,89,113	1.42	4 (6%)
14	CLA	B	3008	-	69,73,73	1.17	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	B	3046	-	41,41,41	1.28	3 (7%)	56,56,56	1.22	5 (8%)
16	BCR	m	101	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	B	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.31	6 (7%)
16	BCR	I	102	-	41,41,41	1.23	5 (12%)	56,56,56	1.33	6 (10%)
14	CLA	2	3011	2	69,73,73	1.18	8 (11%)	82,113,113	1.45	9 (10%)
17	LHG	A	853	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	b	3029	-	69,73,73	1.18	9 (13%)	82,113,113	1.20	5 (6%)
14	CLA	b	3022	-	49,53,73	1.38	7 (14%)	58,89,113	1.55	6 (10%)
14	CLA	b	3026	21	69,73,73	1.18	9 (13%)	82,113,113	1.53	14 (17%)
16	BCR	f	205	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	8 (14%)
17	LHG	0	201	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
17	LHG	l	202	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	j	1101	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	a	824	-	69,73,73	1.16	9 (13%)	82,113,113	1.36	8 (9%)
14	CLA	1	834	-	69,73,73	1.16	10 (14%)	82,113,113	1.41	9 (10%)
14	CLA	A	843	21	69,73,73	1.19	10 (14%)	82,113,113	1.37	6 (7%)
14	CLA	b	3032	-	53,57,73	1.30	9 (16%)	61,93,113	1.44	7 (11%)
14	CLA	a	810	-	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
14	CLA	2	3009	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	7 (8%)
14	CLA	b	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	2	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	A	832	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)
14	CLA	1	819	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	4 (4%)
14	CLA	9	103	21	62,66,73	1.24	8 (12%)	73,104,113	1.32	6 (8%)
14	CLA	B	3011	2	69,73,73	1.17	8 (11%)	82,113,113	1.44	9 (10%)
14	CLA	b	3005	-	69,73,73	1.16	6 (8%)	82,113,113	1.47	7 (8%)
16	BCR	b	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
14	CLA	A	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	A	805	-	63,67,73	1.21	10 (15%)	74,105,113	1.41	7 (9%)
14	CLA	2	3023	21	59,63,73	1.27	8 (13%)	70,101,113	1.37	6 (8%)
16	BCR	B	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
14	CLA	A	836	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	5 (6%)
14	CLA	1	823	-	49,53,73	1.37	8 (16%)	58,89,113	1.47	6 (10%)
16	BCR	l	204	-	41,41,41	1.44	5 (12%)	56,56,56	1.31	7 (12%)
14	CLA	a	840	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	6 (7%)
13	CL0	A	801	-	58,73,73	2.17	13 (22%)	60,113,113	1.79	14 (23%)
14	CLA	1	820	-	69,73,73	1.18	9 (13%)	82,113,113	1.41	9 (10%)
18	SF4	3	101	3	0,12,12	-	-	-	-	-
18	SF4	c	101	3	0,12,12	-	-	-	-	-
14	CLA	A	825	-	69,73,73	1.16	9 (13%)	82,113,113	1.35	8 (9%)
14	CLA	a	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.48	7 (8%)
14	CLA	A	819	-	69,73,73	1.15	8 (11%)	82,113,113	1.31	4 (4%)
14	CLA	b	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	b	3014	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	1	842	-	69,73,73	1.18	9 (13%)	82,113,113	1.31	9 (10%)
14	CLA	a	829	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	1	850	-	41,41,41	1.34	4 (9%)	56,56,56	1.32	6 (10%)
14	CLA	2	3042	-	69,73,73	1.18	8 (11%)	82,113,113	1.39	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	1	824	-	69,73,73	1.18	9 (13%)	82,113,113	1.34	5 (6%)
16	BCR	J	104	-	41,41,41	1.22	3 (7%)	56,56,56	1.30	8 (14%)
14	CLA	1	827	21	69,73,73	1.15	10 (14%)	82,113,113	1.39	10 (12%)
16	BCR	M	1602	-	41,41,41	1.24	4 (9%)	56,56,56	1.24	5 (8%)
14	CLA	a	828	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	7 (8%)
14	CLA	1	841	-	69,73,73	1.16	8 (11%)	82,113,113	1.39	6 (7%)
14	CLA	2	3015	-	69,73,73	1.16	7 (10%)	82,113,113	1.32	9 (10%)
14	CLA	a	816	21	69,73,73	1.17	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	A	855	-	39,44,73	1.49	8 (20%)	47,76,113	1.46	4 (8%)
14	CLA	b	3034	-	69,73,73	1.16	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	F	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	B	3040	-	51,55,73	1.34	8 (15%)	60,91,113	1.33	5 (8%)
14	CLA	b	3015	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	10 (12%)
16	BCR	A	846	-	41,41,41	1.21	2 (4%)	56,56,56	1.37	10 (17%)
17	LHG	a	852	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	B	3003	21	69,73,73	1.16	10 (14%)	82,113,113	1.50	10 (12%)
14	CLA	B	3037	21	49,53,73	1.40	6 (12%)	58,89,113	1.43	5 (8%)
14	CLA	2	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
14	CLA	K	102	21	62,66,73	1.24	7 (11%)	73,104,113	1.32	6 (8%)
14	CLA	b	3016	-	69,73,73	1.14	8 (11%)	82,113,113	1.40	8 (9%)
14	CLA	0	203	-	39,44,73	1.50	9 (23%)	47,76,113	1.45	4 (8%)
14	CLA	b	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	1	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.40	5 (6%)
14	CLA	B	3019	-	69,73,73	1.15	8 (11%)	82,113,113	1.37	8 (9%)
14	CLA	k	102	21	62,66,73	1.24	7 (11%)	73,104,113	1.32	6 (8%)
16	BCR	A	852	-	25,25,41	1.16	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	b	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.35	8 (9%)
16	BCR	1	846	-	41,41,41	1.17	3 (7%)	56,56,56	1.29	6 (10%)
16	BCR	1	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	B	3005	-	69,73,73	1.15	6 (8%)	82,113,113	1.47	8 (9%)
14	CLA	B	3023	21	59,63,73	1.26	8 (13%)	70,101,113	1.37	6 (8%)
14	CLA	B	3036	21	54,58,73	1.37	8 (14%)	64,95,113	1.41	8 (12%)
14	CLA	A	809	1	69,73,73	1.15	9 (13%)	82,113,113	1.34	7 (8%)
14	CLA	B	3026	21	69,73,73	1.19	9 (13%)	82,113,113	1.52	14 (17%)
14	CLA	a	843	17	49,53,73	1.36	9 (18%)	58,89,113	1.52	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	2	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	10 (12%)
14	CLA	A	826	21	69,73,73	1.17	8 (11%)	82,113,113	1.40	10 (12%)
14	CLA	f	204	-	54,58,73	1.32	7 (12%)	64,95,113	1.45	7 (10%)
14	CLA	1	808	-	55,59,73	1.29	8 (14%)	64,96,113	1.40	6 (9%)
14	CLA	a	818	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	4 (4%)
14	CLA	b	3037	21	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
17	LHG	0	202	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	B	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.44	5 (8%)
14	CLA	A	830	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	b	3049	-	41,41,41	1.40	4 (9%)	56,56,56	1.29	7 (12%)
14	CLA	1	805	-	63,67,73	1.21	10 (15%)	74,105,113	1.41	7 (9%)
17	LHG	A	854	14	40,40,48	0.80	2 (5%)	43,46,54	1.19	3 (6%)
20	LMG	B	3050	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	a	831	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)
14	CLA	2	3028	-	69,73,73	1.15	8 (11%)	82,113,113	1.26	8 (9%)
14	CLA	A	806	-	69,73,73	1.16	7 (10%)	82,113,113	1.48	7 (8%)
14	CLA	l	207	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
14	CLA	A	824	-	69,73,73	1.17	8 (11%)	82,113,113	1.34	5 (6%)
14	CLA	6	201	21	62,66,73	1.23	9 (14%)	73,104,113	1.37	6 (8%)
14	CLA	M	1601	-	39,44,73	1.50	8 (20%)	47,76,113	1.45	4 (8%)
14	CLA	K	101	-	50,54,73	1.38	9 (18%)	59,90,113	1.39	4 (6%)
14	CLA	a	830	-	69,73,73	1.19	9 (13%)	82,113,113	1.33	6 (7%)
14	CLA	a	821	21	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
14	CLA	B	3017	-	69,73,73	1.15	8 (11%)	82,113,113	1.51	10 (12%)
14	CLA	B	3041	21	69,73,73	1.16	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	A	841	-	69,73,73	1.15	8 (11%)	82,113,113	1.39	6 (7%)
14	CLA	b	3035	-	69,73,73	1.17	7 (10%)	82,113,113	1.34	5 (6%)
18	SF4	3	102	3	0,12,12	-	-	-	-	-
14	CLA	a	825	21	69,73,73	1.17	9 (13%)	82,113,113	1.39	10 (12%)
14	CLA	A	807	-	69,73,73	1.18	9 (13%)	82,113,113	1.35	7 (8%)
18	SF4	2	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	B	3024	-	49,53,73	1.38	9 (18%)	58,89,113	1.47	6 (10%)
16	BCR	A	849	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
16	BCR	2	3047	-	41,41,41	1.22	3 (7%)	56,56,56	1.25	8 (14%)
14	CLA	a	804	-	63,67,73	1.21	9 (14%)	74,105,113	1.41	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	LMG	2	3050	-	55,55,55	0.92	4 (7%)	63,63,63	1.35	9 (14%)
14	CLA	A	839	-	69,73,73	1.16	7 (10%)	82,113,113	1.35	7 (8%)
14	CLA	b	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	8 (9%)
14	CLA	J	101	-	49,53,73	1.38	8 (16%)	58,89,113	1.45	5 (8%)
14	CLA	B	3033	-	69,73,73	1.16	9 (13%)	82,113,113	1.44	8 (9%)
14	CLA	a	811	-	69,73,73	1.15	9 (13%)	82,113,113	1.24	5 (6%)
14	CLA	B	3034	-	69,73,73	1.15	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	a	851	-	25,25,41	1.15	1 (4%)	33,33,56	1.29	4 (12%)
14	CLA	B	3006	-	69,73,73	1.18	9 (13%)	82,113,113	1.38	7 (8%)
14	CLA	B	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.36	8 (11%)
15	PQN	B	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	1	816	-	69,73,73	1.17	6 (8%)	82,113,113	1.32	5 (6%)
14	CLA	A	835	-	69,73,73	1.15	7 (10%)	82,113,113	1.39	5 (6%)
14	CLA	1	844	17	49,53,73	1.37	9 (18%)	58,89,113	1.52	6 (10%)
16	BCR	7	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
14	CLA	a	832	-	69,73,73	1.16	9 (13%)	82,113,113	1.28	5 (6%)
14	CLA	A	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.34	8 (9%)
16	BCR	a	845	-	41,41,41	1.20	3 (7%)	56,56,56	1.37	11 (19%)
16	BCR	2	3044	-	41,41,41	1.16	2 (4%)	56,56,56	1.21	4 (7%)
16	BCR	B	3047	-	41,41,41	1.21	3 (7%)	56,56,56	1.24	7 (12%)
14	CLA	a	836	1	49,53,73	1.39	9 (18%)	58,89,113	1.38	6 (10%)
14	CLA	B	3029	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
14	CLA	B	3022	-	49,53,73	1.37	7 (14%)	58,89,113	1.53	6 (10%)
14	CLA	B	3038	-	64,68,73	1.21	9 (14%)	76,107,113	1.34	5 (6%)
14	CLA	B	3012	-	69,73,73	1.17	7 (10%)	82,113,113	1.43	8 (9%)
14	CLA	A	811	-	53,57,73	1.31	8 (15%)	61,93,113	1.37	5 (8%)
14	CLA	1	810	1	69,73,73	1.17	9 (13%)	82,113,113	1.33	8 (9%)
14	CLA	2	3010	-	69,73,73	1.16	8 (11%)	82,113,113	1.52	11 (13%)
14	CLA	2	3008	-	69,73,73	1.18	8 (11%)	82,113,113	1.35	6 (7%)
16	BCR	a	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.19	5 (8%)
14	CLA	a	819	-	69,73,73	1.18	9 (13%)	82,113,113	1.42	9 (10%)
17	LHG	l	201	-	48,48,48	0.70	1 (2%)	51,54,54	1.32	5 (9%)
14	CLA	b	3010	-	69,73,73	1.17	8 (11%)	82,113,113	1.51	11 (13%)
14	CLA	B	3032	-	53,57,73	1.31	9 (16%)	61,93,113	1.44	7 (11%)
14	CLA	B	3010	-	69,73,73	1.16	8 (11%)	82,113,113	1.51	11 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	b	3020	21	69,73,73	1.17	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	2	3032	-	53,57,73	1.30	9 (16%)	61,93,113	1.45	7 (11%)
14	CLA	a	814	-	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
14	CLA	b	3013	-	49,53,73	1.35	9 (18%)	58,89,113	1.45	5 (8%)
14	CLA	k	101	-	50,54,73	1.37	9 (18%)	59,90,113	1.39	5 (8%)
14	CLA	B	3020	21	69,73,73	1.17	9 (13%)	82,113,113	1.31	5 (6%)
14	CLA	2	3027	-	69,73,73	1.19	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	2	3021	-	69,73,73	1.16	8 (11%)	82,113,113	1.20	5 (6%)
14	CLA	b	3011	2	69,73,73	1.17	8 (11%)	82,113,113	1.44	9 (10%)
14	CLA	B	3025	2	69,73,73	1.18	9 (13%)	82,113,113	1.25	5 (6%)
14	CLA	2	3031	-	59,63,73	1.27	9 (15%)	70,101,113	1.37	7 (10%)
15	PQN	2	3043	-	34,34,34	0.46	0	43,45,45	0.48	0
14	CLA	2	3026	21	69,73,73	1.18	9 (13%)	82,113,113	1.52	14 (17%)
14	CLA	A	818	-	69,73,73	1.17	9 (13%)	82,113,113	1.29	6 (7%)
16	BCR	8	104	-	41,41,41	1.23	3 (7%)	56,56,56	1.29	7 (12%)
14	CLA	A	844	17	49,53,73	1.36	9 (18%)	58,89,113	1.53	6 (10%)
14	CLA	0	208	-	69,73,73	1.15	8 (11%)	82,113,113	1.44	8 (9%)
14	CLA	1	830	-	69,73,73	1.16	9 (13%)	82,113,113	1.34	8 (9%)
14	CLA	2	3018	-	69,73,73	1.17	7 (10%)	82,113,113	1.32	8 (9%)
18	SF4	b	3001	2,1	0,12,12	-	-	-	-	-
14	CLA	a	802	-	69,73,73	1.16	11 (15%)	82,113,113	1.48	10 (12%)
14	CLA	2	3012	-	69,73,73	1.16	7 (10%)	82,113,113	1.42	7 (8%)
14	CLA	0	204	2	69,73,73	1.16	9 (13%)	82,113,113	1.37	9 (10%)
14	CLA	b	3041	21	69,73,73	1.15	8 (11%)	82,113,113	1.35	6 (7%)
14	CLA	a	803	21	69,73,73	1.22	8 (11%)	82,113,113	1.23	3 (3%)
14	CLA	1	818	-	69,73,73	1.17	9 (13%)	82,113,113	1.30	6 (7%)
14	CLA	b	3042	-	69,73,73	1.17	7 (10%)	82,113,113	1.39	7 (8%)
16	BCR	f	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
16	BCR	2	3048	-	41,41,41	1.32	4 (9%)	56,56,56	1.25	6 (10%)
16	BCR	B	3052	-	41,41,41	1.44	5 (12%)	56,56,56	1.31	6 (10%)
14	CLA	J	102	-	41,45,73	1.48	9 (21%)	50,78,113	1.39	5 (10%)
16	BCR	2	3052	-	41,41,41	1.29	2 (4%)	56,56,56	1.44	11 (19%)
14	CLA	1	837	1	49,53,73	1.39	9 (18%)	58,89,113	1.39	6 (10%)
14	CLA	B	3039	-	69,73,73	1.17	10 (14%)	82,113,113	1.45	9 (10%)
14	CLA	2	3030	-	69,73,73	1.16	8 (11%)	82,113,113	1.32	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
14	CLA	B	3007	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	8 (9%)
16	BCR	B	3049	-	41,41,41	1.39	4 (9%)	56,56,56	1.30	7 (12%)
14	CLA	1	829	-	69,73,73	1.16	8 (11%)	82,113,113	1.36	6 (7%)
16	BCR	2	3049	-	41,41,41	1.40	4 (9%)	56,56,56	1.30	7 (12%)
14	CLA	6	204	-	54,58,73	1.33	6 (11%)	64,95,113	1.45	7 (10%)
17	LHG	1	852	-	48,48,48	0.81	2 (4%)	51,54,54	1.25	4 (7%)
14	CLA	a	806	-	69,73,73	1.17	9 (13%)	82,113,113	1.35	7 (8%)
14	CLA	a	812	-	49,53,73	1.38	9 (18%)	58,89,113	1.49	5 (8%)
14	CLA	A	802	-	69,73,73	1.15	11 (15%)	82,113,113	1.48	10 (12%)
16	BCR	i	101	-	41,41,41	1.29	4 (9%)	56,56,56	1.27	5 (8%)
14	CLA	1	807	-	69,73,73	1.17	10 (14%)	82,113,113	1.34	7 (8%)
16	BCR	0	211	-	41,41,41	1.18	3 (7%)	56,56,56	1.21	4 (7%)
16	BCR	2	3046	-	41,41,41	1.29	3 (7%)	56,56,56	1.22	5 (8%)
16	BCR	1	849	-	41,41,41	1.36	4 (9%)	56,56,56	1.33	7 (12%)
14	CLA	1	822	21	69,73,73	1.16	9 (13%)	82,113,113	1.36	7 (8%)
14	CLA	0	207	10	69,73,73	1.19	9 (13%)	82,113,113	1.35	9 (10%)
16	BCR	F	202	-	41,41,41	1.18	3 (7%)	56,56,56	1.25	7 (12%)
16	BCR	a	846	-	41,41,41	1.18	3 (7%)	56,56,56	1.28	6 (10%)
17	LHG	L	208	-	38,38,48	0.78	0	41,44,54	1.30	4 (9%)
14	CLA	1	832	-	64,68,73	1.22	10 (15%)	76,107,113	1.35	5 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	802	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	a	838	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	1	804	-	1/1/15/20	14/39/115/115	-
14	CLA	2	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3016	-	1/1/15/20	11/39/115/115	-
14	CLA	a	823	-	1/1/15/20	18/39/115/115	-
16	BCR	0	210	-	-	9/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	826	21	1/1/15/20	13/39/115/115	-
14	CLA	b	3023	21	1/1/13/20	9/27/103/115	-
14	CLA	a	815	-	1/1/15/20	18/39/115/115	-
14	CLA	A	827	21	1/1/15/20	13/39/115/115	-
14	CLA	L	204	-	1/1/15/20	10/39/115/115	-
14	CLA	A	831	-	1/1/15/20	8/39/115/115	-
14	CLA	1	811	-	1/1/11/20	6/20/96/115	-
14	CLA	b	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	A	817	21	1/1/15/20	17/39/115/115	-
14	CLA	A	804	-	1/1/15/20	14/39/115/115	-
16	BCR	9	102	-	-	5/29/63/63	0/2/2/2
14	CLA	A	828	-	1/1/15/20	5/39/115/115	-
16	BCR	F	205	-	-	8/29/63/63	0/2/2/2
14	CLA	1	813	-	1/1/11/20	6/15/91/115	-
14	CLA	f	203	21	1/1/11/20	5/15/91/115	-
14	CLA	8	102	-	1/1/8/20	0/4/76/115	-
14	CLA	a	817	-	1/1/15/20	13/39/115/115	-
17	LHG	2	3051	-	-	24/53/53/53	-
20	LMG	b	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	a	809	1	1/1/15/20	14/39/115/115	-
14	CLA	f	201	21	1/1/13/20	5/31/107/115	-
14	CLA	1	839	-	1/1/15/20	14/39/115/115	-
14	CLA	1	817	21	1/1/15/20	17/39/115/115	-
16	BCR	6	205	-	-	8/29/63/63	0/2/2/2
14	CLA	b	3036	21	1/1/12/20	9/21/97/115	-
16	BCR	A	850	-	-	4/29/63/63	0/2/2/2
16	BCR	j	1106	-	-	16/29/63/63	0/2/2/2
14	CLA	2	3003	21	1/1/15/20	17/39/115/115	-
14	CLA	A	813	-	1/1/11/20	6/15/91/115	-
16	BCR	A	848	-	-	17/29/63/63	0/2/2/2
14	CLA	1	203	2	1/1/15/20	8/39/115/115	-
16	BCR	b	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	2	3013	-	-	4/15/91/115	-
14	CLA	2	3005	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	A	837	1	1/1/11/20	2/15/91/115	-
14	CLA	2	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3018	-	-	16/39/115/115	-
14	CLA	b	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	2	3025	2	1/1/15/20	13/39/115/115	-
16	BCR	b	3044	-	-	7/29/63/63	0/2/2/2
14	CLA	2	3004	-	1/1/15/20	13/39/115/115	-
18	SF4	B	3001	2,1	-	-	0/6/5/5
14	CLA	1	821	-	1/1/15/20	18/39/115/115	-
14	CLA	B	3042	-	1/1/15/20	14/39/115/115	-
14	CLA	2	3041	21	1/1/15/20	7/39/115/115	-
16	BCR	b	3047	-	-	13/29/63/63	0/2/2/2
17	LHG	a	853	14	-	21/45/45/53	-
14	CLA	2	3024	-	-	5/15/91/115	-
14	CLA	b	3008	-	1/1/15/20	12/39/115/115	-
14	CLA	x	1701	-	1/1/11/20	4/15/91/115	-
16	BCR	1	847	-	-	17/29/63/63	0/2/2/2
14	CLA	a	808	1	1/1/15/20	16/39/115/115	-
14	CLA	F	204	-	1/1/12/20	7/21/97/115	-
14	CLA	A	821	-	1/1/15/20	18/39/115/115	-
16	BCR	k	103	-	-	2/18/35/63	0/1/1/2
16	BCR	L	206	-	-	6/29/63/63	0/2/2/2
16	BCR	0	205	-	-	13/29/63/63	0/2/2/2
14	CLA	b	3004	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3006	-	1/1/15/20	17/39/115/115	-
16	BCR	l	209	-	-	9/29/63/63	0/2/2/2
14	CLA	b	3031	-	1/1/13/20	11/27/103/115	-
14	CLA	a	835	-	1/1/15/20	14/39/115/115	-
16	BCR	6	202	-	-	11/29/63/63	0/2/2/2
15	PQN	a	844	-	-	2/23/43/43	0/2/2/2
14	CLA	a	833	-	1/1/15/20	13/39/115/115	-
16	BCR	1	851	-	-	15/18/35/63	0/1/1/2
14	CLA	2	3036	21	1/1/12/20	9/21/97/115	-
14	CLA	b	3012	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	PQN	1	845	-	-	2/23/43/43	0/2/2/2
14	CLA	1	814	-	1/1/15/20	13/39/115/115	-
14	CLA	1	840	-	1/1/15/20	12/39/115/115	-
14	CLA	A	823	-	1/1/11/20	3/15/91/115	-
14	CLA	2	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	1	803	21	1/1/15/20	7/39/115/115	-
14	CLA	A	808	-	1/1/12/20	2/23/99/115	-
14	CLA	2	3033	-	1/1/15/20	13/39/115/115	-
14	CLA	B	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	A	815	-	1/1/15/20	15/39/115/115	-
14	CLA	A	834	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3021	-	1/1/15/20	10/39/115/115	-
13	CL0	a	801	-	3/3/20/25	9/37/135/135	-
14	CLA	A	814	-	1/1/15/20	13/39/115/115	-
14	CLA	1	826	21	1/1/15/20	15/39/115/115	-
14	CLA	1	815	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3025	2	1/1/15/20	13/39/115/115	-
14	CLA	2	3029	-	1/1/15/20	6/39/115/115	-
16	BCR	A	847	-	-	17/29/63/63	0/2/2/2
14	CLA	A	803	21	1/1/15/20	7/39/115/115	-
14	CLA	2	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3040	-	-	2/18/94/115	-
14	CLA	L	201	2	1/1/15/20	8/39/115/115	-
14	CLA	1	806	-	1/1/15/20	21/39/115/115	-
14	CLA	2	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	l	206	10	1/1/15/20	15/39/115/115	-
17	LHG	L	207	-	-	24/53/53/53	-
14	CLA	B	3035	-	1/1/15/20	13/39/115/115	-
14	CLA	A	838	-	1/1/15/20	16/39/115/115	-
14	CLA	1	809	1	1/1/15/20	16/39/115/115	-
14	CLA	b	3040	-	-	2/18/94/115	-
14	CLA	1	828	-	1/1/15/20	5/39/115/115	-
16	BCR	b	3046	-	-	11/29/63/63	0/2/2/2
14	CLA	a	842	21	1/1/15/20	14/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3027	-	1/1/15/20	11/39/115/115	-
14	CLA	A	812	-	1/1/15/20	10/39/115/115	-
14	CLA	A	833	-	1/1/15/20	14/39/115/115	-
14	CLA	1	831	-	1/1/15/20	8/39/115/115	-
14	CLA	8	101	-	1/1/11/20	4/15/91/115	-
16	BCR	B	3044	-	-	7/29/63/63	0/2/2/2
14	CLA	L	203	10	1/1/15/20	15/39/115/115	-
14	CLA	6	203	21	1/1/11/20	5/15/91/115	-
14	CLA	j	1102	-	1/1/11/20	4/15/91/115	-
14	CLA	2	3006	-	1/1/15/20	17/39/115/115	-
18	SF4	c	102	3	-	-	0/6/5/5
14	CLA	1	812	-	1/1/15/20	11/39/115/115	-
14	CLA	A	816	-	1/1/15/20	18/39/115/115	-
14	CLA	a	837	-	1/1/15/20	16/39/115/115	-
17	LHG	B	3051	-	-	24/53/53/53	-
14	CLA	b	3033	-	1/1/15/20	13/39/115/115	-
16	BCR	B	3053	-	-	16/29/63/63	0/2/2/2
14	CLA	A	842	-	1/1/15/20	7/39/115/115	-
14	CLA	X	1701	-	1/1/11/20	4/15/91/115	-
18	SF4	C	102	3	-	-	0/6/5/5
17	LHG	1	853	14	-	21/45/45/53	-
16	BCR	9	104	-	-	2/18/35/63	0/1/1/2
16	BCR	A	851	-	-	21/29/63/63	0/2/2/2
16	BCR	B	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	a	807	-	1/1/12/20	2/23/99/115	-
15	PQN	A	845	-	-	2/23/43/43	0/2/2/2
16	BCR	j	1105	-	-	14/29/63/63	0/2/2/2
14	CLA	2	3035	-	1/1/15/20	13/39/115/115	-
14	CLA	A	840	-	1/1/15/20	12/39/115/115	-
16	BCR	a	849	-	-	4/29/63/63	0/2/2/2
14	CLA	l	208	21	1/1/15/20	12/39/115/115	-
14	CLA	B	3004	-	1/1/15/20	13/39/115/115	-
14	CLA	2	3034	-	1/1/15/20	13/39/115/115	-
16	BCR	K	103	-	-	2/18/35/63	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	8	103	-	-	9/29/63/63	0/2/2/2
14	CLA	a	834	-	1/1/15/20	11/39/115/115	-
16	BCR	j	1104	-	-	9/29/63/63	0/2/2/2
14	CLA	1	843	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3022	-	1/1/11/20	4/15/91/115	-
16	BCR	2	3045	-	-	8/29/63/63	0/2/2/2
14	CLA	1	833	-	1/1/15/20	14/39/115/115	-
14	CLA	a	839	-	1/1/15/20	12/39/115/115	-
14	CLA	B	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	A	820	-	1/1/15/20	9/39/115/115	-
17	LHG	b	3051	-	-	24/53/53/53	-
14	CLA	1	836	-	1/1/15/20	14/39/115/115	-
14	CLA	B	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	a	841	-	1/1/15/20	7/39/115/115	-
16	BCR	J	103	-	-	9/29/63/63	0/2/2/2
14	CLA	9	101	-	1/1/11/20	9/17/93/115	-
14	CLA	1	825	-	1/1/15/20	15/39/115/115	-
14	CLA	a	813	-	1/1/15/20	13/39/115/115	-
14	CLA	a	822	-	1/1/11/20	3/15/91/115	-
14	CLA	j	1103	-	1/1/8/20	0/4/76/115	-
14	CLA	B	3015	-	1/1/15/20	16/39/115/115	-
14	CLA	a	820	-	1/1/15/20	18/39/115/115	-
13	CL0	1	801	-	3/3/20/25	9/37/135/135	-
18	SF4	C	101	3	-	-	0/6/5/5
14	CLA	F	203	21	1/1/11/20	5/15/91/115	-
14	CLA	L	205	21	1/1/15/20	12/39/115/115	-
16	BCR	I	101	-	-	7/29/63/63	0/2/2/2
16	BCR	a	847	-	-	17/29/63/63	0/2/2/2
14	CLA	b	3024	-	-	5/15/91/115	-
16	BCR	a	850	-	-	21/29/63/63	0/2/2/2
14	CLA	2	3037	21	1/1/11/20	6/15/91/115	-
14	CLA	B	3021	-	1/1/15/20	10/39/115/115	-
16	BCR	y	101	-	-	13/29/63/63	0/2/2/2
14	CLA	b	3003	21	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	a	827	-	1/1/15/20	5/39/115/115	-
14	CLA	A	822	21	1/1/15/20	9/39/115/115	-
16	BCR	l	210	-	-	6/29/63/63	0/2/2/2
14	CLA	1	838	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	0	209	21	1/1/15/20	12/39/115/115	-
15	PQN	b	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	z	1701	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3008	-	1/1/15/20	12/39/115/115	-
16	BCR	B	3046	-	-	11/29/63/63	0/2/2/2
16	BCR	m	101	-	-	13/29/63/63	0/2/2/2
14	CLA	B	3027	-	1/1/15/20	11/39/115/115	-
16	BCR	I	102	-	-	9/29/63/63	0/2/2/2
14	CLA	2	3011	2	1/1/15/20	9/39/115/115	-
17	LHG	A	853	-	-	19/53/53/53	-
14	CLA	b	3029	-	1/1/15/20	6/39/115/115	-
14	CLA	b	3022	-	1/1/11/20	4/15/91/115	-
14	CLA	b	3026	21	1/1/15/20	12/39/115/115	-
16	BCR	f	205	-	-	8/29/63/63	0/2/2/2
17	LHG	0	201	-	-	24/53/53/53	-
17	LHG	l	202	-	-	29/43/43/53	-
14	CLA	j	1101	-	1/1/15/20	14/39/115/115	-
14	CLA	a	824	-	1/1/15/20	15/39/115/115	-
14	CLA	1	834	-	1/1/15/20	13/39/115/115	-
14	CLA	A	843	21	1/1/15/20	14/39/115/115	-
14	CLA	b	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	a	810	-	1/1/11/20	6/20/96/115	-
14	CLA	2	3009	-	1/1/15/20	8/39/115/115	-
14	CLA	b	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	2	3016	-	1/1/15/20	11/39/115/115	-
14	CLA	A	832	-	1/1/14/20	8/33/109/115	-
14	CLA	1	819	-	1/1/15/20	16/39/115/115	-
14	CLA	9	103	21	1/1/13/20	9/31/107/115	-
14	CLA	B	3011	2	1/1/15/20	9/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3005	-	1/1/15/20	12/39/115/115	-
16	BCR	b	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	A	829	-	1/1/15/20	12/39/115/115	-
14	CLA	A	805	-	1/1/13/20	11/32/108/115	-
14	CLA	2	3023	21	1/1/13/20	9/27/103/115	-
16	BCR	B	3048	-	-	10/29/63/63	0/2/2/2
14	CLA	A	836	-	1/1/15/20	14/39/115/115	-
14	CLA	1	823	-	1/1/11/20	3/15/91/115	-
16	BCR	l	204	-	-	13/29/63/63	0/2/2/2
14	CLA	a	840	-	1/1/15/20	10/39/115/115	-
13	CL0	A	801	-	3/3/20/25	9/37/135/135	-
14	CLA	1	820	-	1/1/15/20	9/39/115/115	-
18	SF4	3	101	3	-	-	0/6/5/5
18	SF4	c	101	3	-	-	0/6/5/5
14	CLA	A	825	-	1/1/15/20	15/39/115/115	-
14	CLA	a	805	-	1/1/15/20	21/39/115/115	-
14	CLA	A	819	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	b	3014	-	1/1/15/20	14/39/115/115	-
14	CLA	1	842	-	1/1/15/20	7/39/115/115	-
14	CLA	a	829	-	1/1/15/20	15/39/115/115	-
16	BCR	1	850	-	-	21/29/63/63	0/2/2/2
14	CLA	2	3042	-	1/1/15/20	13/39/115/115	-
14	CLA	1	824	-	1/1/15/20	18/39/115/115	-
16	BCR	J	104	-	-	14/29/63/63	0/2/2/2
14	CLA	1	827	21	1/1/15/20	13/39/115/115	-
16	BCR	M	1602	-	-	13/29/63/63	0/2/2/2
14	CLA	a	828	-	1/1/15/20	12/39/115/115	-
14	CLA	1	841	-	1/1/15/20	10/39/115/115	-
14	CLA	2	3015	-	1/1/15/20	16/39/115/115	-
14	CLA	a	816	21	1/1/15/20	17/39/115/115	-
14	CLA	A	855	-	1/1/7/20	1/4/72/115	-
14	CLA	b	3034	-	1/1/15/20	13/39/115/115	-
14	CLA	F	201	21	1/1/13/20	5/31/107/115	-
14	CLA	B	3040	-	-	2/18/94/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	b	3015	-	1/1/15/20	16/39/115/115	-
16	BCR	A	846	-	-	5/29/63/63	0/2/2/2
17	LHG	a	852	-	-	19/53/53/53	-
14	CLA	B	3003	21	1/1/15/20	17/39/115/115	-
14	CLA	B	3037	21	1/1/11/20	6/15/91/115	-
14	CLA	2	3007	-	1/1/15/20	12/39/115/115	-
14	CLA	K	102	21	1/1/13/20	9/31/107/115	-
14	CLA	b	3016	-	1/1/15/20	11/39/115/115	-
14	CLA	0	203	-	1/1/7/20	1/4/72/115	-
14	CLA	b	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	1	835	-	1/1/15/20	11/39/115/115	-
14	CLA	B	3019	-	1/1/15/20	14/39/115/115	-
14	CLA	k	102	21	1/1/13/20	9/31/107/115	-
16	BCR	A	852	-	-	15/18/35/63	0/1/1/2
14	CLA	b	3007	-	1/1/15/20	12/39/115/115	-
16	BCR	1	846	-	-	17/29/63/63	0/2/2/2
16	BCR	1	848	-	-	7/29/63/63	0/2/2/2
14	CLA	B	3005	-	1/1/15/20	12/39/115/115	-
14	CLA	B	3023	21	1/1/13/20	9/27/103/115	-
14	CLA	B	3036	21	1/1/12/20	9/21/97/115	-
14	CLA	A	809	1	1/1/15/20	16/39/115/115	-
14	CLA	B	3026	21	1/1/15/20	12/39/115/115	-
14	CLA	a	843	17	1/1/11/20	4/15/91/115	-
14	CLA	2	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	A	826	21	1/1/15/20	15/39/115/115	-
14	CLA	f	204	-	1/1/12/20	7/21/97/115	-
14	CLA	1	808	-	1/1/12/20	2/23/99/115	-
14	CLA	a	818	-	1/1/15/20	16/39/115/115	-
14	CLA	b	3037	21	1/1/11/20	6/15/91/115	-
17	LHG	0	202	-	-	29/43/43/53	-
14	CLA	B	3013	-	-	3/15/91/115	-
14	CLA	A	830	-	1/1/15/20	15/39/115/115	-
16	BCR	b	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	1	805	-	1/1/13/20	11/32/108/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
17	LHG	A	854	14	-	21/45/45/53	-
20	LMG	B	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	a	831	-	1/1/14/20	8/33/109/115	-
14	CLA	2	3028	-	1/1/15/20	19/39/115/115	-
14	CLA	A	806	-	1/1/15/20	21/39/115/115	-
14	CLA	l	207	-	1/1/15/20	10/39/115/115	-
14	CLA	A	824	-	1/1/15/20	18/39/115/115	-
14	CLA	6	201	21	1/1/13/20	4/31/107/115	-
14	CLA	M	1601	-	1/1/7/20	1/4/72/115	-
14	CLA	K	101	-	1/1/11/20	9/17/93/115	-
14	CLA	a	830	-	1/1/15/20	8/39/115/115	-
14	CLA	a	821	21	1/1/15/20	9/39/115/115	-
14	CLA	B	3017	-	1/1/15/20	13/39/115/115	-
14	CLA	B	3041	21	1/1/15/20	7/39/115/115	-
14	CLA	A	841	-	1/1/15/20	10/39/115/115	-
14	CLA	b	3035	-	1/1/15/20	13/39/115/115	-
18	SF4	3	102	3	-	-	0/6/5/5
14	CLA	a	825	21	1/1/15/20	15/39/115/115	-
14	CLA	A	807	-	1/1/15/20	15/39/115/115	-
18	SF4	2	3001	2,1	-	-	0/6/5/5
14	CLA	B	3024	-	-	5/15/91/115	-
16	BCR	A	849	-	-	7/29/63/63	0/2/2/2
16	BCR	2	3047	-	-	13/29/63/63	0/2/2/2
14	CLA	a	804	-	1/1/13/20	11/32/108/115	-
20	LMG	2	3050	-	-	21/50/70/70	0/1/1/1
14	CLA	A	839	-	1/1/15/20	14/39/115/115	-
14	CLA	b	3018	-	-	16/39/115/115	-
14	CLA	J	101	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3033	-	1/1/15/20	13/39/115/115	-
14	CLA	a	811	-	1/1/15/20	10/39/115/115	-
14	CLA	B	3034	-	1/1/15/20	13/39/115/115	-
16	BCR	a	851	-	-	15/18/35/63	0/1/1/2
14	CLA	B	3006	-	1/1/15/20	17/39/115/115	-
14	CLA	B	3031	-	1/1/13/20	11/27/103/115	-
15	PQN	B	3043	-	-	4/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	1	816	-	1/1/15/20	18/39/115/115	-
14	CLA	A	835	-	1/1/15/20	11/39/115/115	-
14	CLA	1	844	17	1/1/11/20	4/15/91/115	-
16	BCR	7	101	-	-	7/29/63/63	0/2/2/2
14	CLA	a	832	-	1/1/15/20	14/39/115/115	-
14	CLA	A	810	1	1/1/15/20	14/39/115/115	-
16	BCR	a	845	-	-	5/29/63/63	0/2/2/2
16	BCR	2	3044	-	-	7/29/63/63	0/2/2/2
16	BCR	B	3047	-	-	13/29/63/63	0/2/2/2
14	CLA	a	836	1	1/1/11/20	2/15/91/115	-
14	CLA	B	3029	-	1/1/15/20	6/39/115/115	-
14	CLA	B	3022	-	1/1/11/20	4/15/91/115	-
14	CLA	B	3038	-	1/1/14/20	12/33/109/115	-
14	CLA	B	3012	-	1/1/15/20	15/39/115/115	-
14	CLA	A	811	-	1/1/11/20	6/20/96/115	-
14	CLA	1	810	1	1/1/15/20	14/39/115/115	-
14	CLA	2	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	2	3008	-	1/1/15/20	12/39/115/115	-
16	BCR	a	848	-	-	7/29/63/63	0/2/2/2
14	CLA	a	819	-	1/1/15/20	9/39/115/115	-
17	LHG	l	201	-	-	24/53/53/53	-
14	CLA	b	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	B	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	B	3010	-	1/1/15/20	9/39/115/115	-
14	CLA	b	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3032	-	1/1/11/20	9/20/96/115	-
14	CLA	a	814	-	1/1/15/20	15/39/115/115	-
14	CLA	b	3013	-	-	4/15/91/115	-
14	CLA	k	101	-	1/1/11/20	9/17/93/115	-
14	CLA	B	3020	21	1/1/15/20	14/39/115/115	-
14	CLA	2	3027	-	1/1/15/20	11/39/115/115	-
14	CLA	2	3021	-	1/1/15/20	10/39/115/115	-
14	CLA	b	3011	2	1/1/15/20	9/39/115/115	-
14	CLA	B	3025	2	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	CLA	2	3031	-	1/1/13/20	11/27/103/115	-
15	PQN	2	3043	-	-	4/23/43/43	0/2/2/2
14	CLA	2	3026	21	1/1/15/20	12/39/115/115	-
14	CLA	A	818	-	1/1/15/20	13/39/115/115	-
16	BCR	8	104	-	-	14/29/63/63	0/2/2/2
14	CLA	A	844	17	1/1/11/20	4/15/91/115	-
14	CLA	0	208	-	1/1/15/20	10/39/115/115	-
14	CLA	1	830	-	1/1/15/20	15/39/115/115	-
14	CLA	2	3018	-	-	16/39/115/115	-
18	SF4	b	3001	2,1	-	-	0/6/5/5
14	CLA	a	802	-	1/1/15/20	15/39/115/115	-
14	CLA	2	3012	-	1/1/15/20	15/39/115/115	-
14	CLA	0	204	2	1/1/15/20	8/39/115/115	-
14	CLA	b	3041	21	1/1/15/20	7/39/115/115	-
14	CLA	a	803	21	1/1/15/20	7/39/115/115	-
14	CLA	1	818	-	1/1/15/20	13/39/115/115	-
14	CLA	b	3042	-	1/1/15/20	13/39/115/115	-
16	BCR	f	202	-	-	11/29/63/63	0/2/2/2
16	BCR	2	3048	-	-	10/29/63/63	0/2/2/2
16	BCR	B	3052	-	-	13/29/63/63	0/2/2/2
14	CLA	J	102	-	1/1/8/20	0/4/76/115	-
16	BCR	2	3052	-	-	16/29/63/63	0/2/2/2
14	CLA	1	837	1	1/1/11/20	2/15/91/115	-
14	CLA	B	3039	-	1/1/15/20	14/39/115/115	-
14	CLA	2	3030	-	1/1/15/20	7/39/115/115	-
14	CLA	B	3007	-	1/1/15/20	12/39/115/115	-
16	BCR	B	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	1	829	-	1/1/15/20	12/39/115/115	-
16	BCR	2	3049	-	-	2/29/63/63	0/2/2/2
14	CLA	6	204	-	1/1/12/20	7/21/97/115	-
17	LHG	1	852	-	-	19/53/53/53	-
14	CLA	a	806	-	1/1/15/20	15/39/115/115	-
14	CLA	a	812	-	1/1/11/20	6/15/91/115	-
14	CLA	A	802	-	1/1/15/20	16/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	BCR	i	101	-	-	7/29/63/63	0/2/2/2
14	CLA	1	807	-	1/1/15/20	15/39/115/115	-
16	BCR	0	211	-	-	6/29/63/63	0/2/2/2
16	BCR	2	3046	-	-	11/29/63/63	0/2/2/2
16	BCR	1	849	-	-	4/29/63/63	0/2/2/2
14	CLA	1	822	21	1/1/15/20	9/39/115/115	-
14	CLA	0	207	10	1/1/15/20	15/39/115/115	-
16	BCR	F	202	-	-	11/29/63/63	0/2/2/2
16	BCR	a	846	-	-	17/29/63/63	0/2/2/2
17	LHG	L	208	-	-	29/43/43/53	-
14	CLA	1	832	-	1/1/14/20	8/33/109/115	-

The worst 5 of 2709 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	801	CL0	C1B-C2B	8.71	1.49	1.39
13	1	801	CL0	C1B-C2B	8.68	1.49	1.39
13	a	801	CL0	C1B-C2B	8.64	1.49	1.39
13	1	801	CL0	C3B-C4B	6.92	1.48	1.41
13	a	801	CL0	C3B-C4B	6.89	1.48	1.41

The worst 5 of 2506 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	3005	CLA	C4A-NA-C1A	8.23	110.43	106.68
14	B	3005	CLA	C4A-NA-C1A	8.22	110.43	106.68
14	2	3005	CLA	C4A-NA-C1A	8.21	110.42	106.68
14	a	805	CLA	C4A-NA-C1A	8.12	110.38	106.68
14	A	806	CLA	C4A-NA-C1A	8.01	110.33	106.68

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 4318 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	804	CLA	CHA-CBD-CGD-O1D
14	A	804	CLA	CHA-CBD-CGD-O2D

There are no ring outliers.

266 monomers are involved in 501 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	1	802	CLA	3	0
14	b	3009	CLA	1	0
14	a	838	CLA	1	0
14	B	3009	CLA	1	0
14	B	3016	CLA	2	0
14	a	823	CLA	1	0
16	0	210	BCR	1	0
14	a	826	CLA	1	0
14	a	815	CLA	3	0
14	A	827	CLA	1	0
14	L	204	CLA	1	0
14	A	817	CLA	4	0
16	9	102	BCR	1	0
14	A	828	CLA	2	0
14	1	813	CLA	1	0
14	f	203	CLA	2	0
14	a	817	CLA	1	0
17	2	3051	LHG	3	0
14	f	201	CLA	2	0
14	1	839	CLA	2	0
14	1	817	CLA	2	0
14	b	3036	CLA	4	0
16	j	1106	BCR	10	0
14	2	3003	CLA	5	0
16	A	848	BCR	2	0
14	l	203	CLA	1	0
16	b	3045	BCR	1	0
14	2	3005	CLA	4	0
14	B	3018	CLA	4	0
14	2	3019	CLA	2	0
14	b	3017	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	3025	CLA	1	0
14	2	3004	CLA	1	0
14	1	821	CLA	6	0
14	B	3042	CLA	1	0
14	2	3041	CLA	1	0
16	b	3047	BCR	3	0
14	2	3024	CLA	1	0
16	1	847	BCR	2	0
14	a	808	CLA	2	0
14	F	204	CLA	3	0
14	A	821	CLA	4	0
16	k	103	BCR	2	0
14	b	3004	CLA	1	0
16	l	209	BCR	1	0
14	b	3031	CLA	6	0
15	a	844	PQN	3	0
14	2	3036	CLA	4	0
14	b	3012	CLA	3	0
15	1	845	PQN	1	0
14	1	814	CLA	1	0
14	2	3038	CLA	2	0
14	1	803	CLA	2	0
14	2	3033	CLA	3	0
14	B	3028	CLA	3	0
14	A	815	CLA	2	0
13	a	801	CL0	1	0
14	A	814	CLA	1	0
14	1	826	CLA	1	0
14	1	815	CLA	2	0
14	b	3025	CLA	2	0
16	A	847	BCR	1	0
14	A	803	CLA	2	0
14	2	3020	CLA	2	0
14	2	3040	CLA	4	0
14	L	201	CLA	2	0
14	1	806	CLA	3	0
14	2	3039	CLA	2	0
14	l	206	CLA	1	0
17	L	207	LHG	1	0
14	B	3035	CLA	3	0
14	A	838	CLA	1	0
14	1	809	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	b	3040	CLA	4	0
14	1	828	CLA	2	0
16	b	3046	BCR	1	0
14	a	842	CLA	2	0
14	A	812	CLA	1	0
14	A	833	CLA	1	0
14	L	203	CLA	1	0
14	6	203	CLA	2	0
14	2	3006	CLA	4	0
14	1	812	CLA	1	0
14	A	816	CLA	2	0
14	a	837	CLA	1	0
17	B	3051	LHG	5	0
14	b	3033	CLA	3	0
16	B	3053	BCR	3	0
14	A	842	CLA	1	0
16	9	104	BCR	2	0
16	A	851	BCR	7	0
16	B	3045	BCR	1	0
15	A	845	PQN	1	0
14	2	3035	CLA	3	0
16	a	849	BCR	1	0
14	1	208	CLA	2	0
14	B	3004	CLA	1	0
14	2	3034	CLA	4	0
16	K	103	BCR	2	0
16	8	103	BCR	4	0
16	j	1104	BCR	3	0
14	1	843	CLA	2	0
14	2	3022	CLA	1	0
16	2	3045	BCR	1	0
14	1	833	CLA	1	0
14	A	820	CLA	2	0
17	b	3051	LHG	3	0
14	a	841	CLA	1	0
16	J	103	BCR	3	0
14	1	825	CLA	2	0
14	a	813	CLA	1	0
14	B	3015	CLA	2	0
14	a	820	CLA	5	0
13	1	801	CL0	1	0
14	F	203	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	L	205	CLA	3	0
16	a	847	BCR	1	0
14	b	3024	CLA	1	0
16	a	850	BCR	6	0
14	2	3037	CLA	1	0
16	y	101	BCR	4	0
14	b	3003	CLA	6	0
14	a	827	CLA	2	0
14	1	838	CLA	1	0
14	b	3038	CLA	2	0
14	0	209	CLA	2	0
14	z	1701	CLA	2	0
16	B	3046	BCR	1	0
16	m	101	BCR	1	0
16	I	102	BCR	1	0
17	A	853	LHG	2	0
14	b	3022	CLA	1	0
14	b	3026	CLA	3	0
17	l	202	LHG	1	0
14	j	1101	CLA	4	0
14	a	824	CLA	2	0
14	A	843	CLA	2	0
14	2	3009	CLA	2	0
14	b	3028	CLA	4	0
14	2	3016	CLA	2	0
14	A	832	CLA	2	0
14	1	819	CLA	3	0
14	b	3005	CLA	4	0
16	b	3048	BCR	3	0
14	A	829	CLA	2	0
16	B	3048	BCR	2	0
14	a	840	CLA	1	0
13	A	801	CL0	1	0
14	1	820	CLA	1	0
14	A	825	CLA	2	0
14	a	805	CLA	3	0
14	A	819	CLA	3	0
14	b	3039	CLA	3	0
14	b	3014	CLA	1	0
14	1	842	CLA	1	0
14	a	829	CLA	3	0
16	1	850	BCR	7	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	2	3042	CLA	1	0
14	1	824	CLA	1	0
14	1	827	CLA	1	0
16	M	1602	BCR	1	0
14	a	828	CLA	2	0
14	1	841	CLA	1	0
14	2	3015	CLA	1	0
14	a	816	CLA	2	0
14	A	855	CLA	1	0
14	b	3034	CLA	2	0
14	F	201	CLA	1	0
14	B	3040	CLA	3	0
14	b	3015	CLA	1	0
16	A	846	BCR	1	0
17	a	852	LHG	2	0
14	B	3003	CLA	6	0
14	B	3037	CLA	1	0
14	b	3016	CLA	2	0
14	b	3019	CLA	1	0
14	B	3019	CLA	1	0
16	1	846	BCR	1	0
16	1	848	BCR	1	0
14	B	3005	CLA	4	0
14	B	3036	CLA	3	0
14	A	809	CLA	2	0
14	B	3026	CLA	2	0
14	2	3017	CLA	2	0
14	A	826	CLA	1	0
14	f	204	CLA	3	0
14	a	818	CLA	3	0
14	b	3037	CLA	1	0
17	0	202	LHG	1	0
14	A	830	CLA	3	0
14	1	805	CLA	1	0
14	a	831	CLA	2	0
14	2	3028	CLA	4	0
14	A	806	CLA	3	0
14	1	207	CLA	1	0
14	A	824	CLA	1	0
14	6	201	CLA	1	0
14	K	101	CLA	2	0
14	B	3017	CLA	2	0

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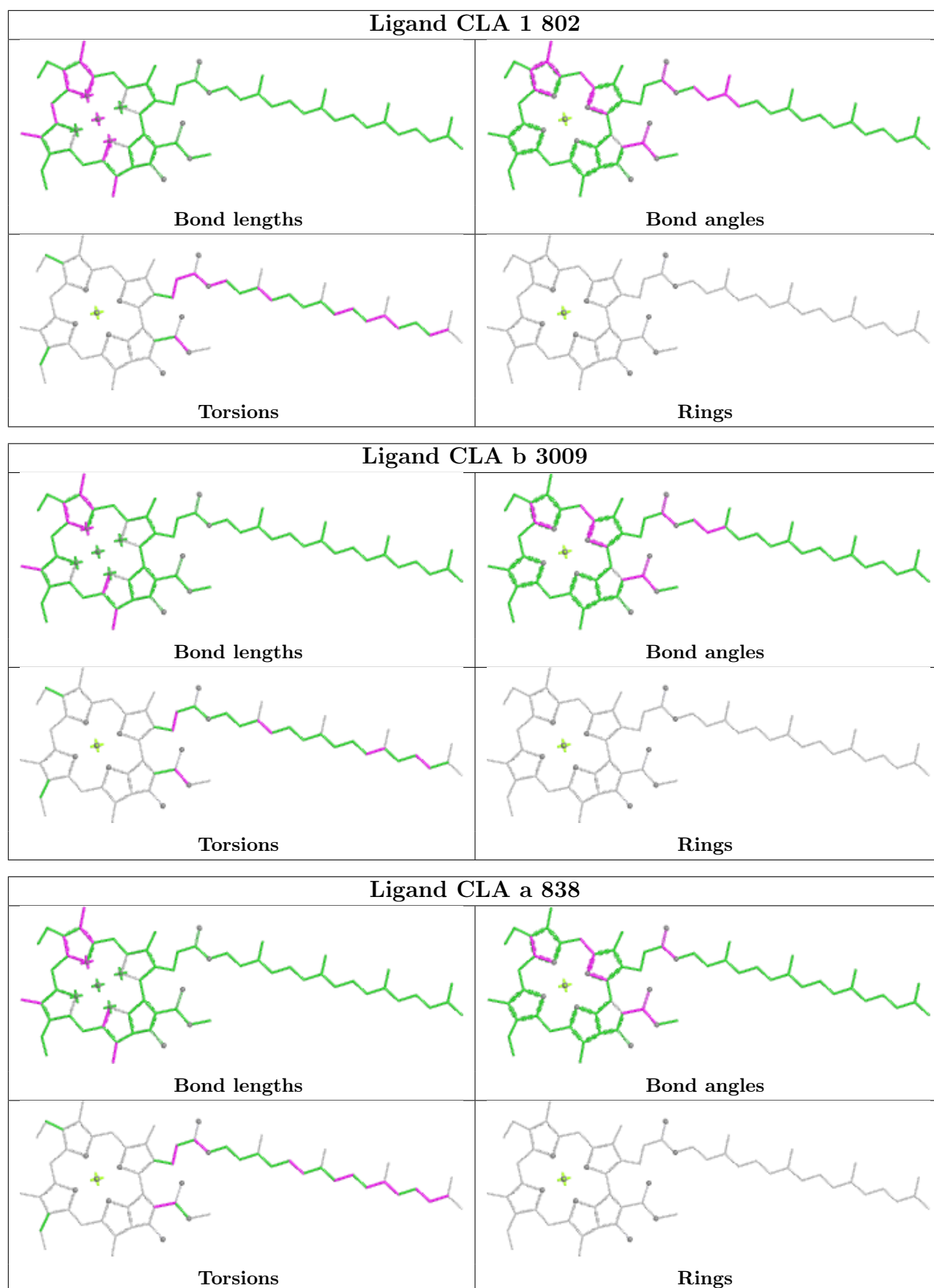
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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14	A	841	CLA	1	0
14	b	3035	CLA	3	0
14	a	825	CLA	1	0
14	A	807	CLA	3	0
14	B	3024	CLA	1	0
16	A	849	BCR	2	0
16	2	3047	BCR	2	0
14	a	804	CLA	1	0
20	2	3050	LMG	1	0
14	A	839	CLA	1	0
14	b	3018	CLA	3	0
14	B	3033	CLA	4	0
14	a	811	CLA	1	0
14	B	3034	CLA	5	0
14	B	3006	CLA	2	0
14	B	3031	CLA	6	0
14	1	816	CLA	2	0
14	a	832	CLA	2	0
14	A	810	CLA	1	0
16	a	845	BCR	1	0
16	B	3047	BCR	3	0
14	B	3022	CLA	1	0
14	B	3038	CLA	3	0
14	B	3012	CLA	3	0
14	1	810	CLA	1	0
14	2	3010	CLA	3	0
16	a	848	BCR	2	0
14	a	819	CLA	1	0
17	l	201	LHG	1	0
14	b	3010	CLA	3	0
14	B	3010	CLA	3	0
14	b	3020	CLA	2	0
14	2	3032	CLA	1	0
14	a	814	CLA	3	0
14	B	3020	CLA	2	0
14	B	3025	CLA	1	0
14	2	3031	CLA	6	0
14	2	3026	CLA	3	0
14	A	818	CLA	2	0
16	8	104	BCR	2	0
14	A	844	CLA	1	0

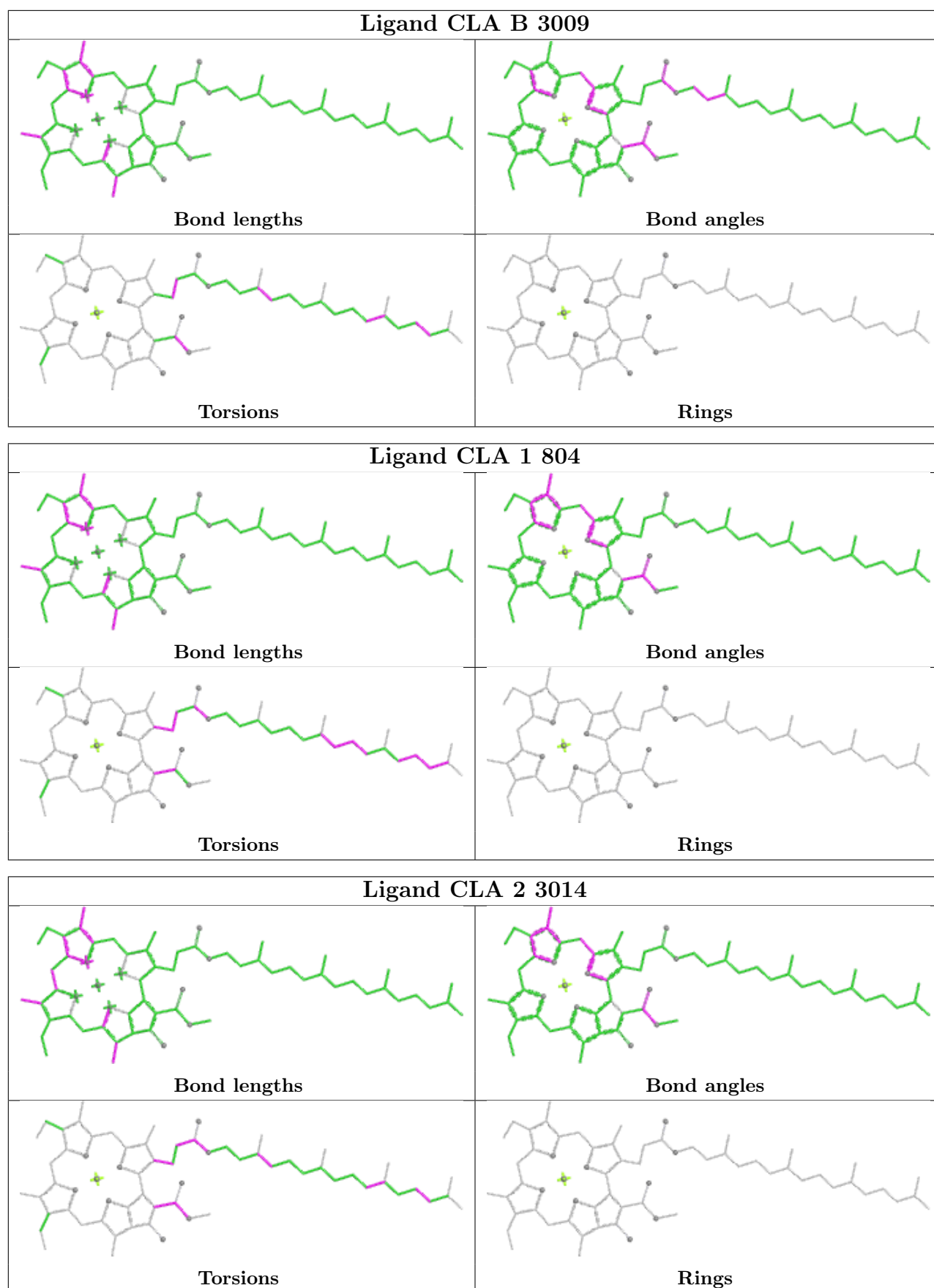
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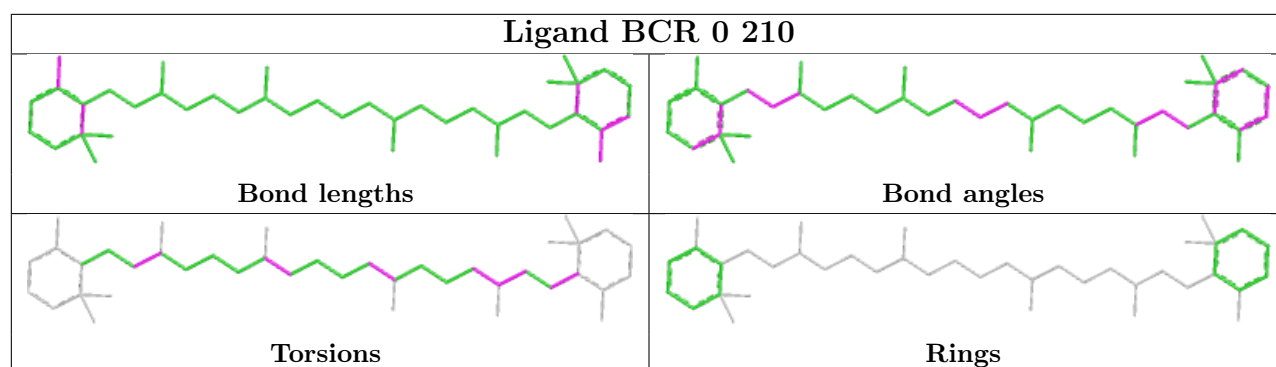
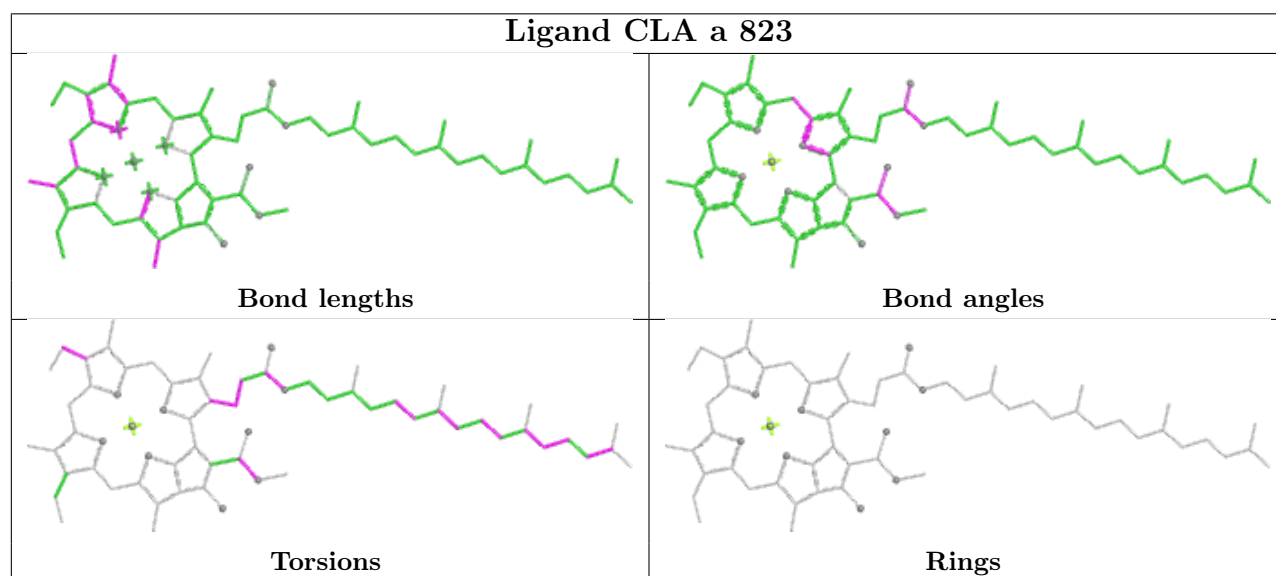
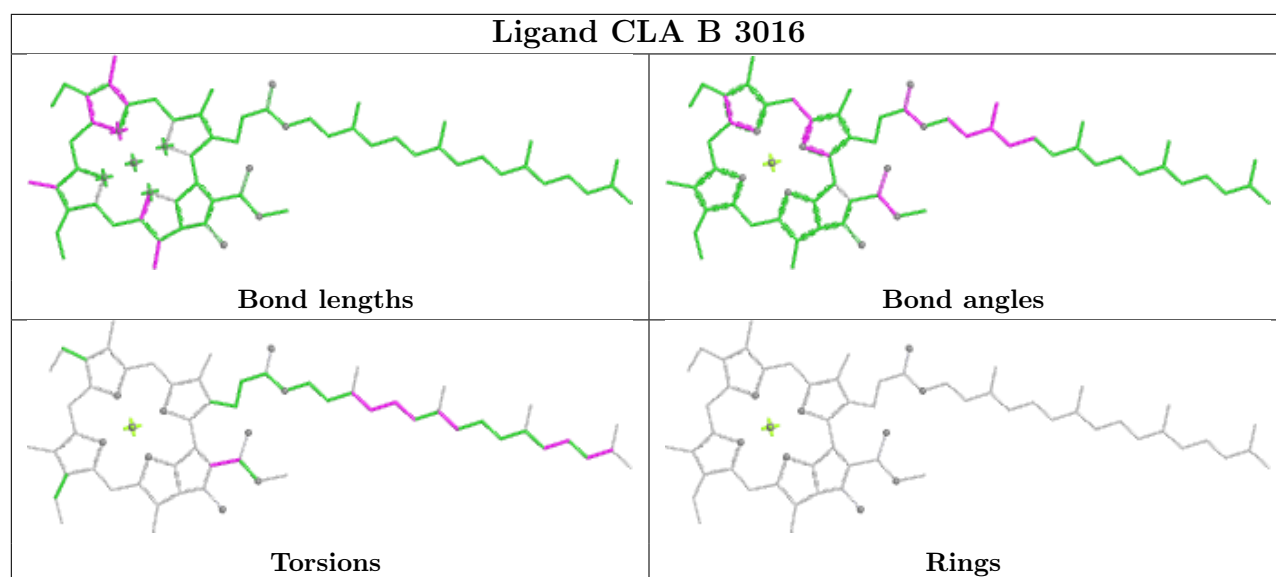
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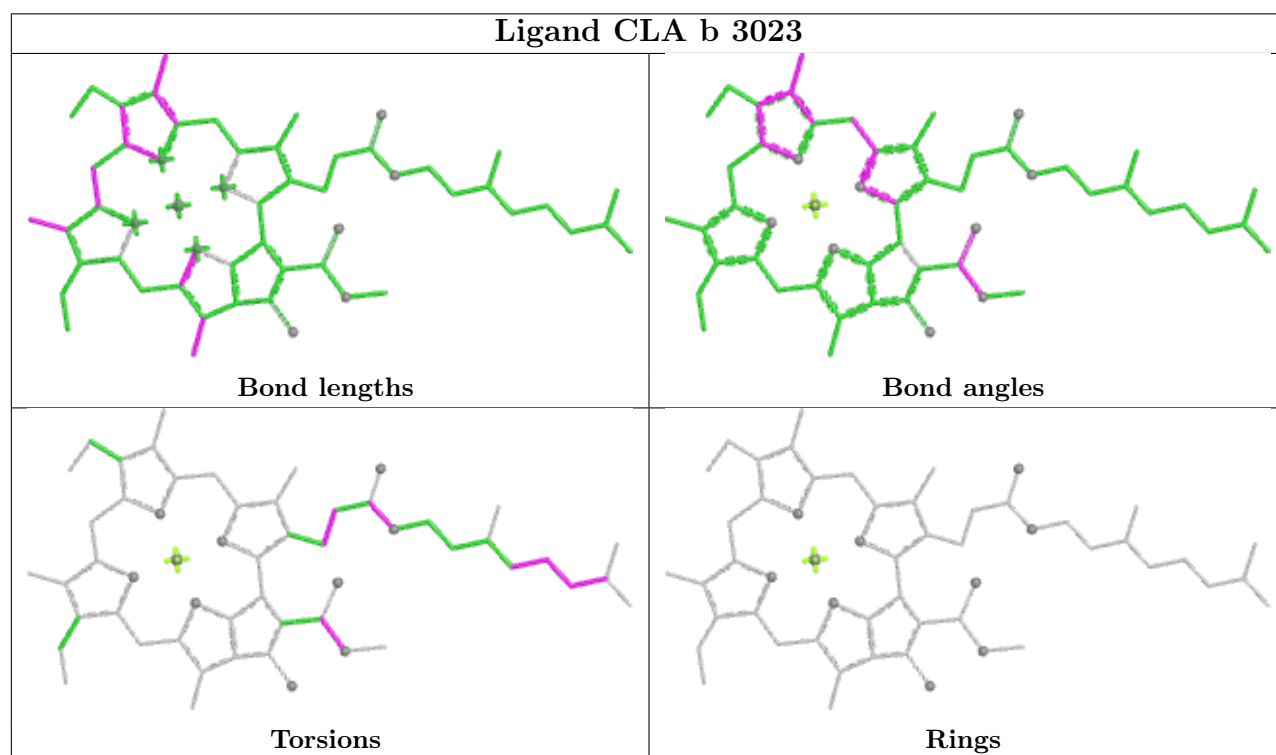
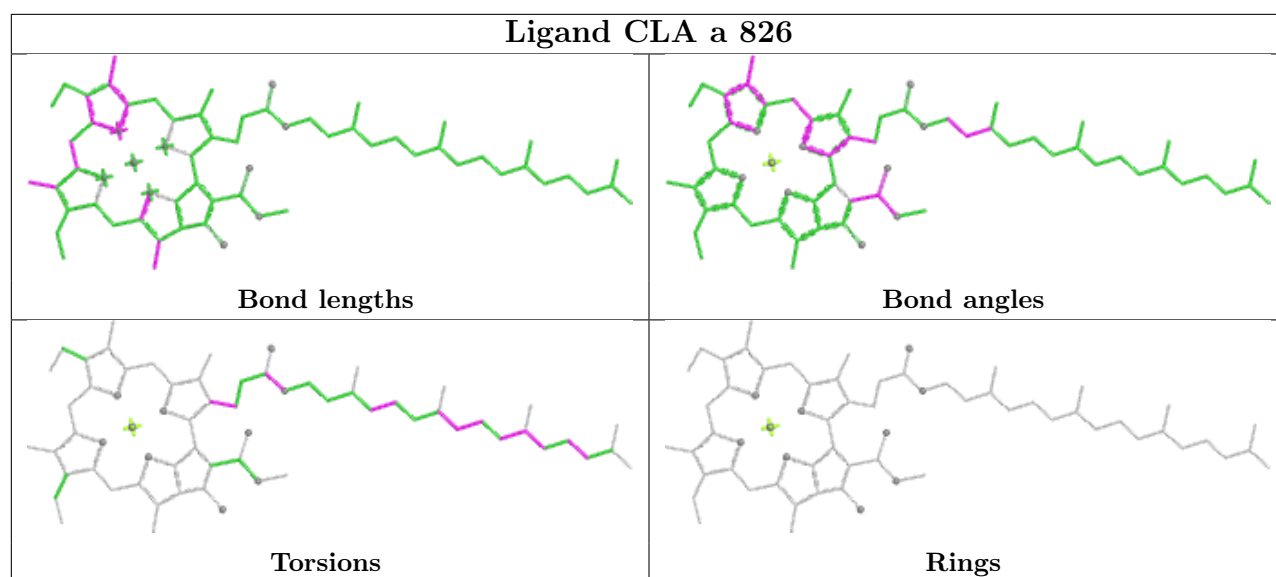
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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14	1	830	CLA	3	0
14	2	3018	CLA	3	0
14	a	802	CLA	3	0
14	2	3012	CLA	3	0
14	0	204	CLA	2	0
14	b	3041	CLA	1	0
14	a	803	CLA	2	0
14	1	818	CLA	2	0
14	b	3042	CLA	1	0
16	2	3048	BCR	4	0
16	2	3052	BCR	3	0
14	B	3039	CLA	2	0
14	1	829	CLA	3	0
14	6	204	CLA	3	0
17	1	852	LHG	2	0
14	a	806	CLA	4	0
14	a	812	CLA	1	0
14	A	802	CLA	3	0
14	1	807	CLA	3	0
16	2	3046	BCR	1	0
14	0	207	CLA	1	0
16	a	846	BCR	1	0
17	L	208	LHG	1	0
14	1	832	CLA	1	0

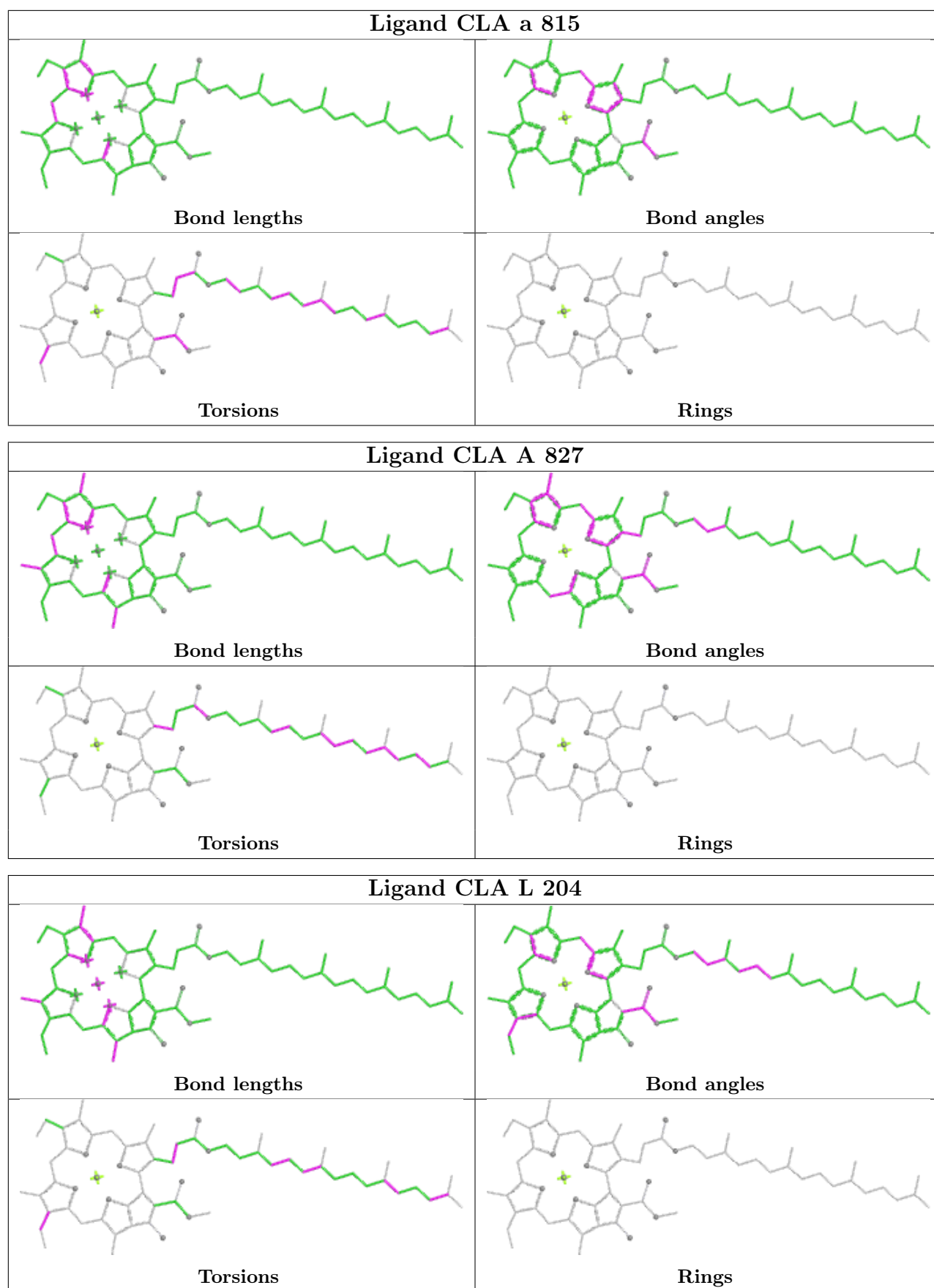
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

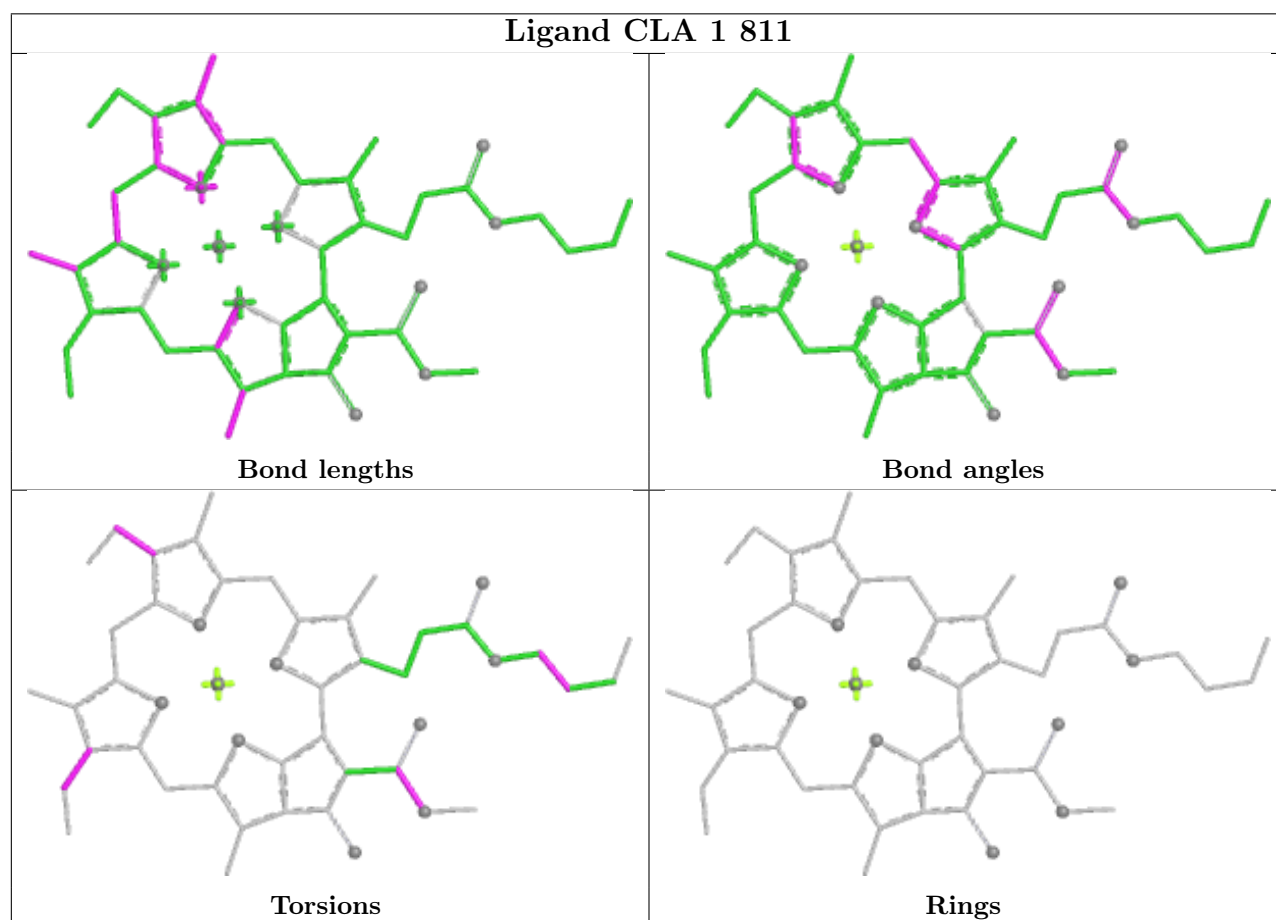
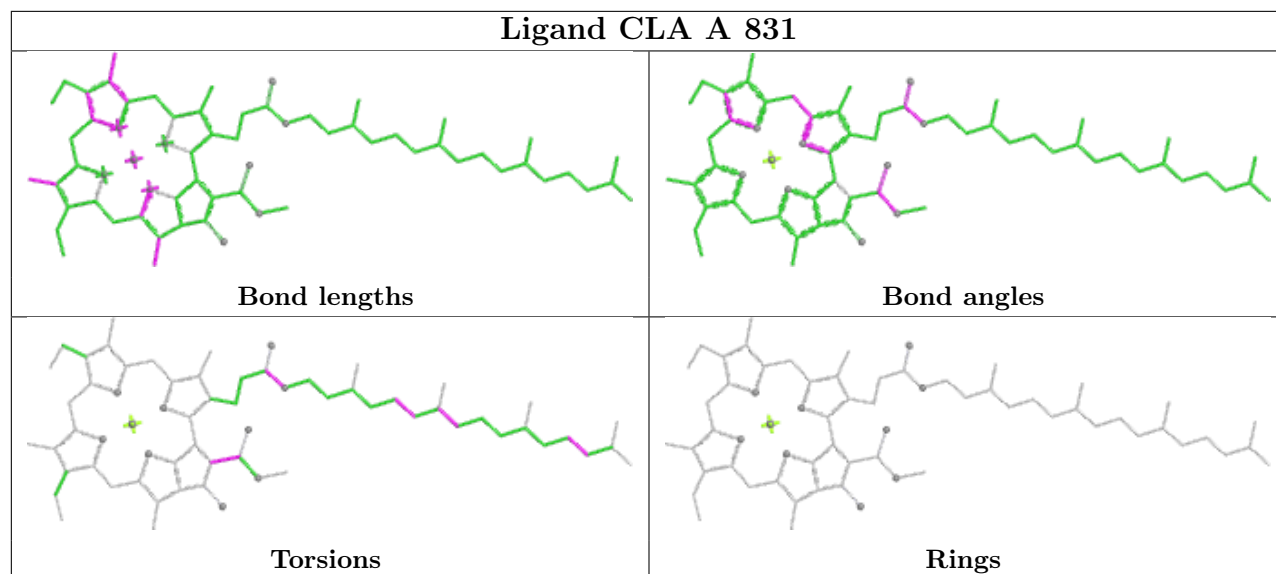


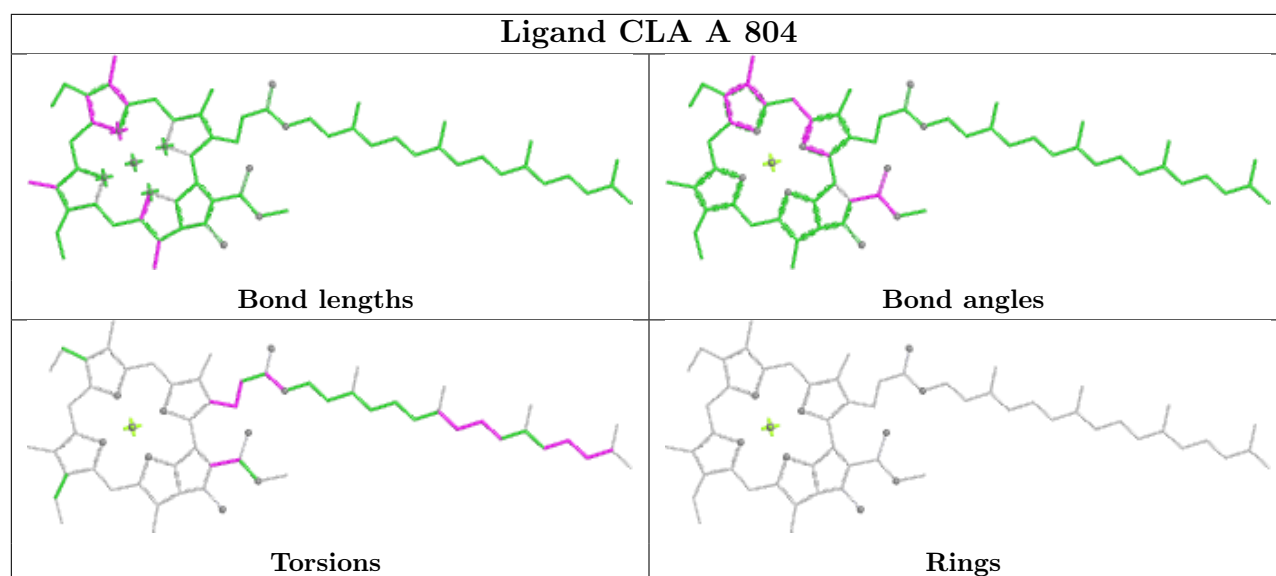
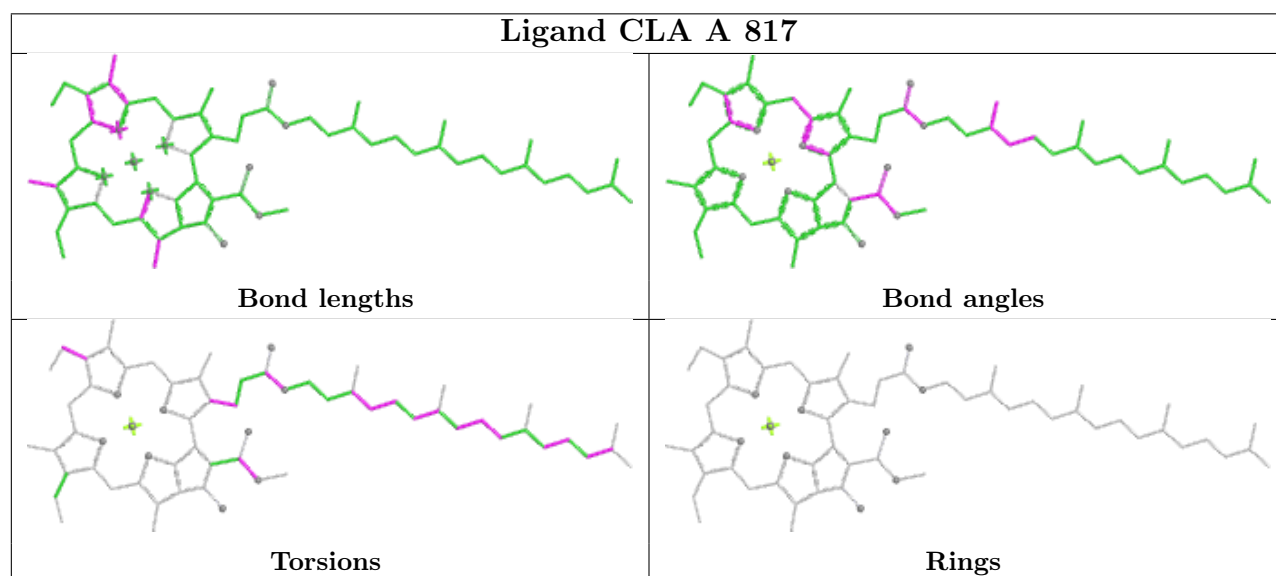
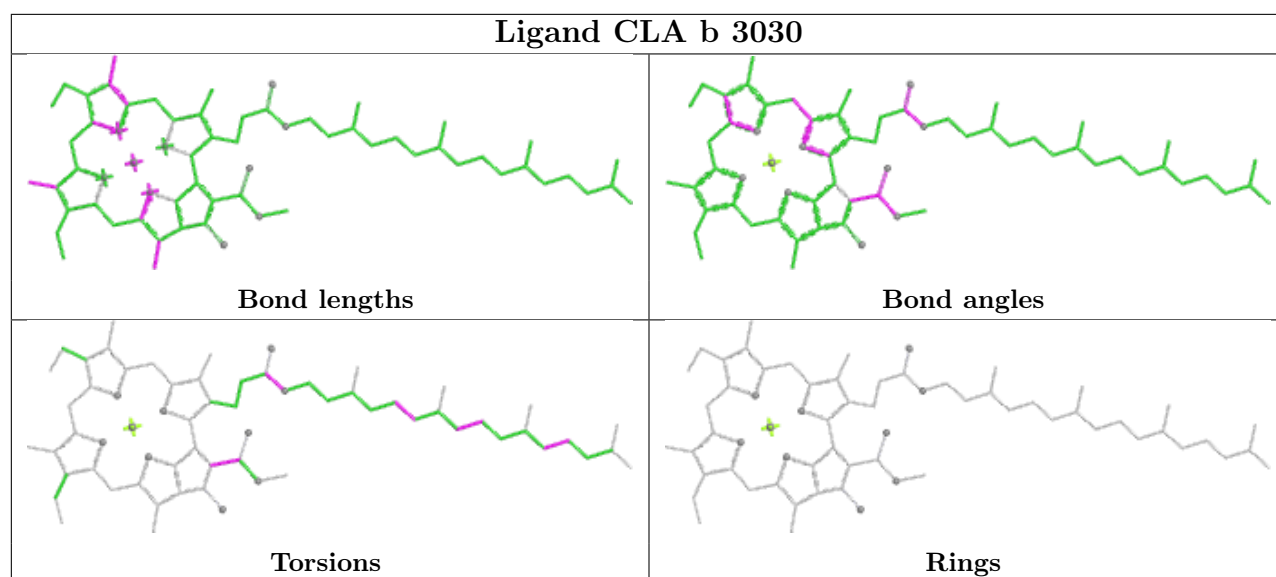


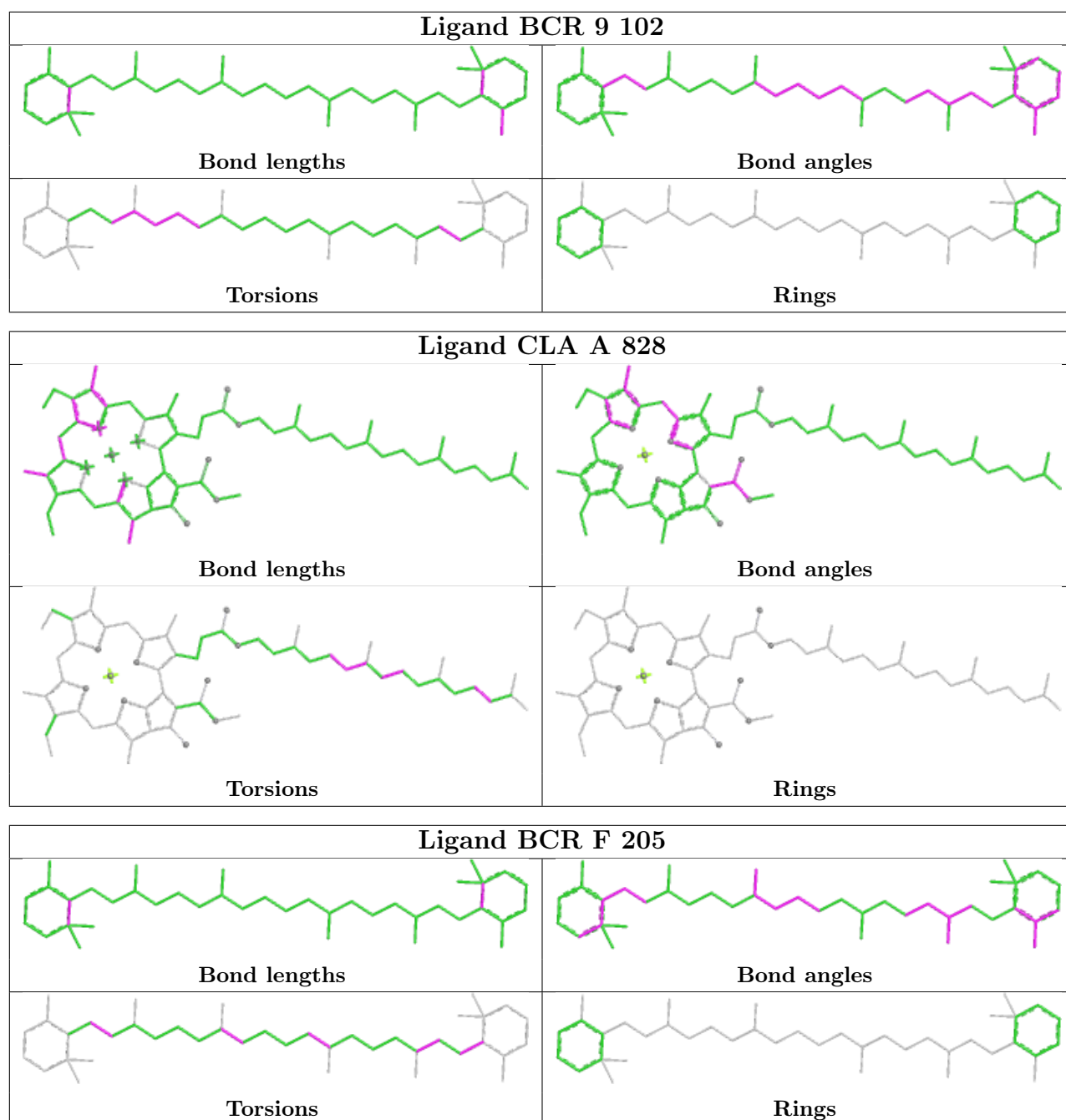


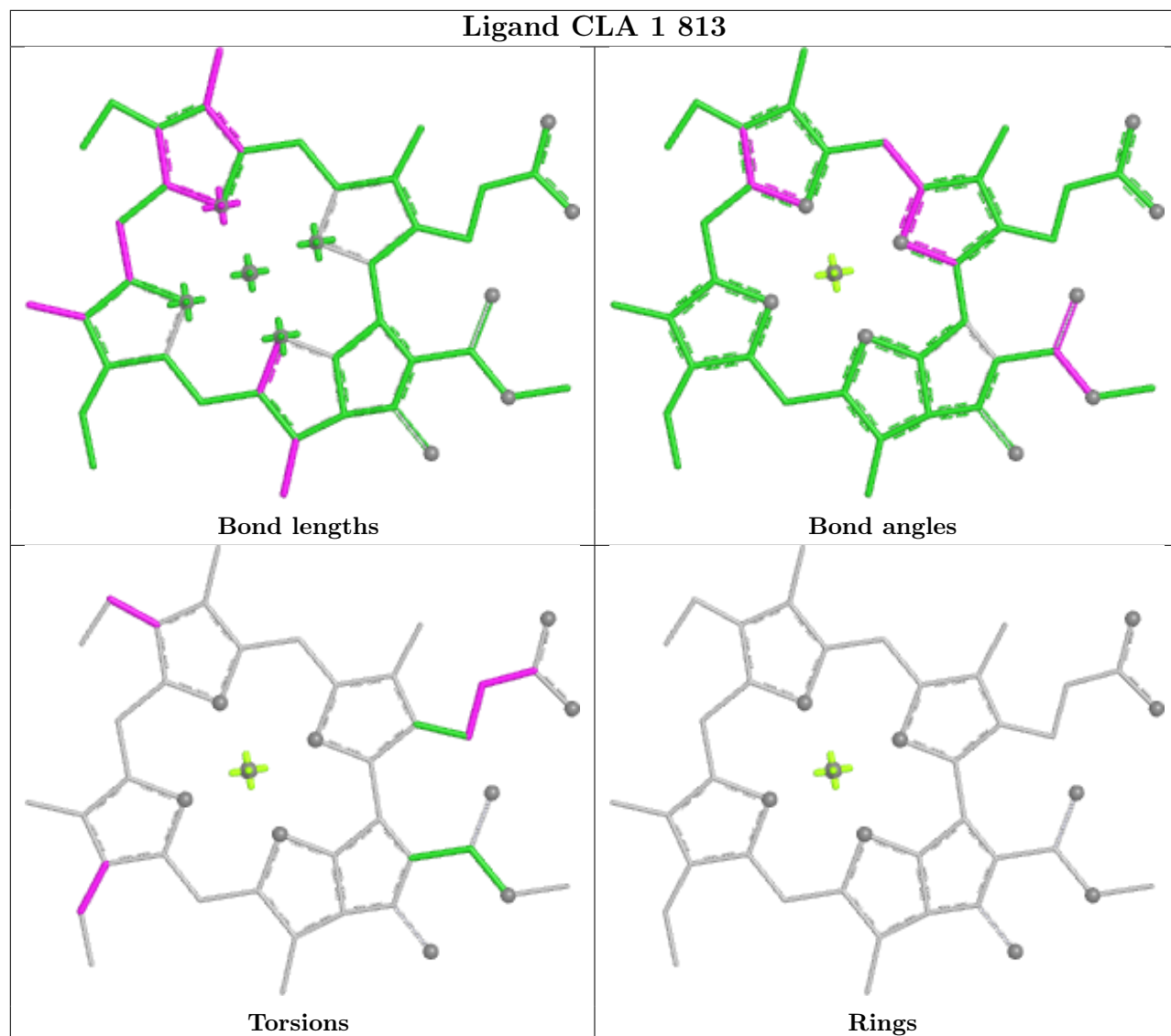


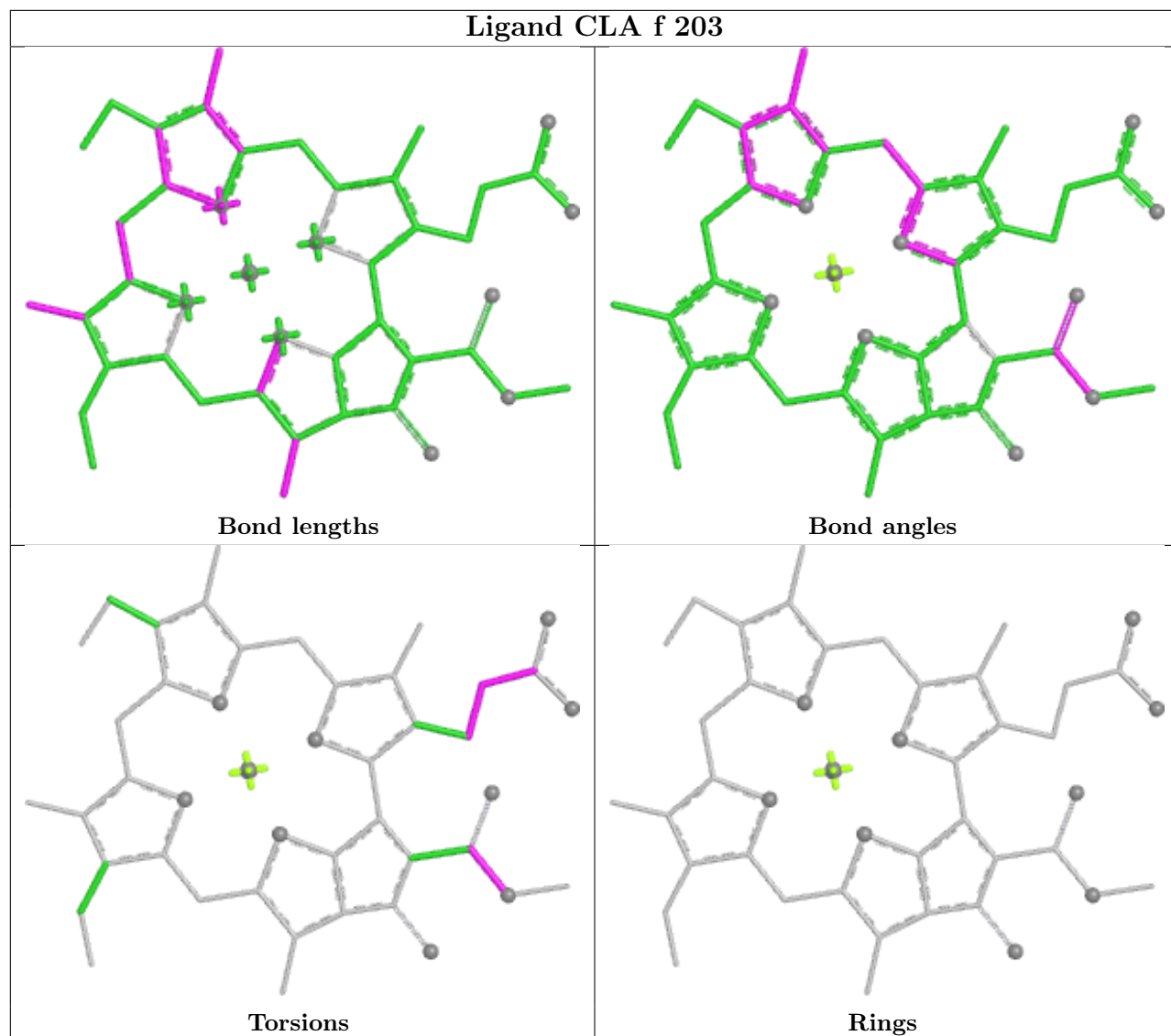




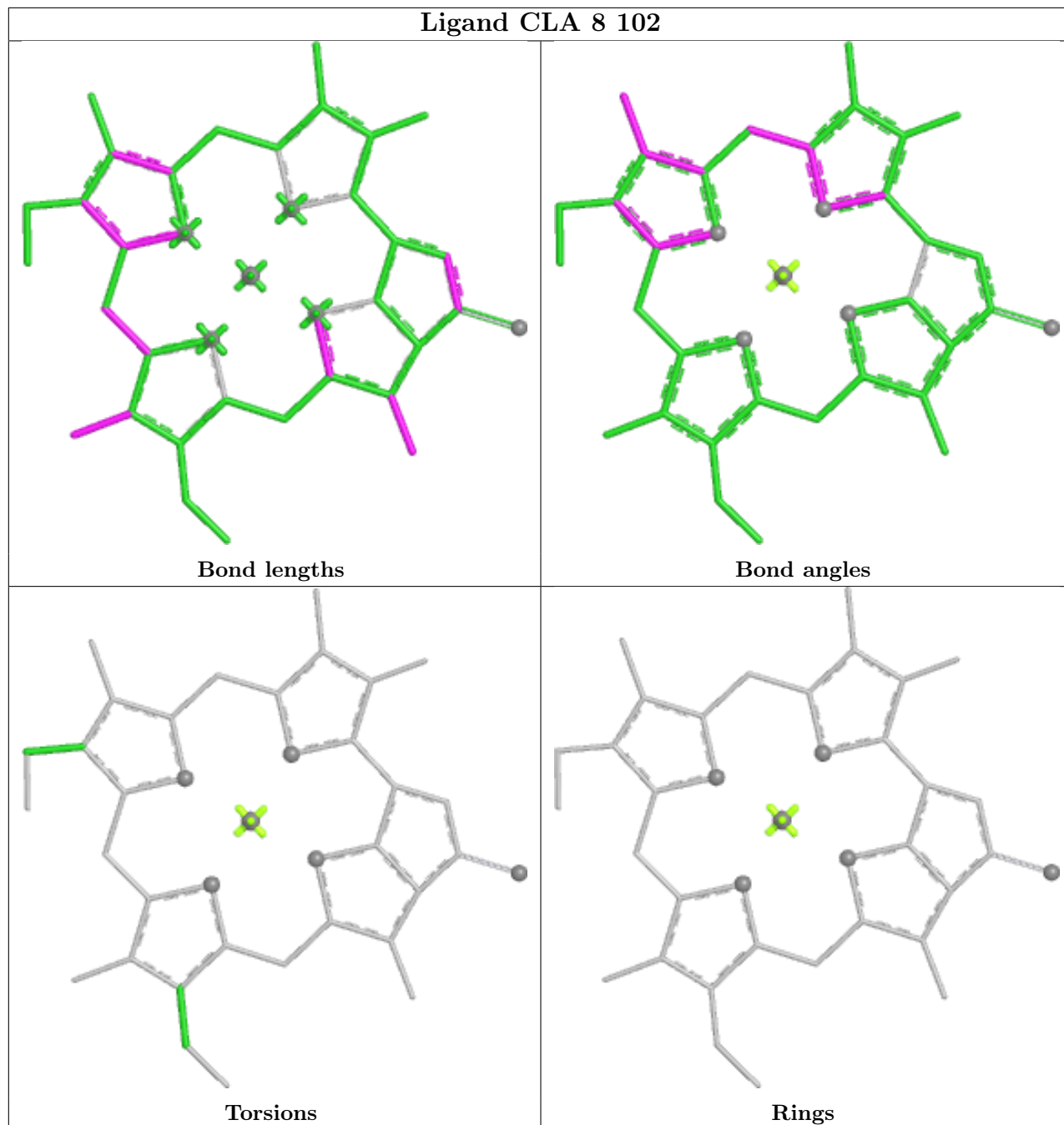


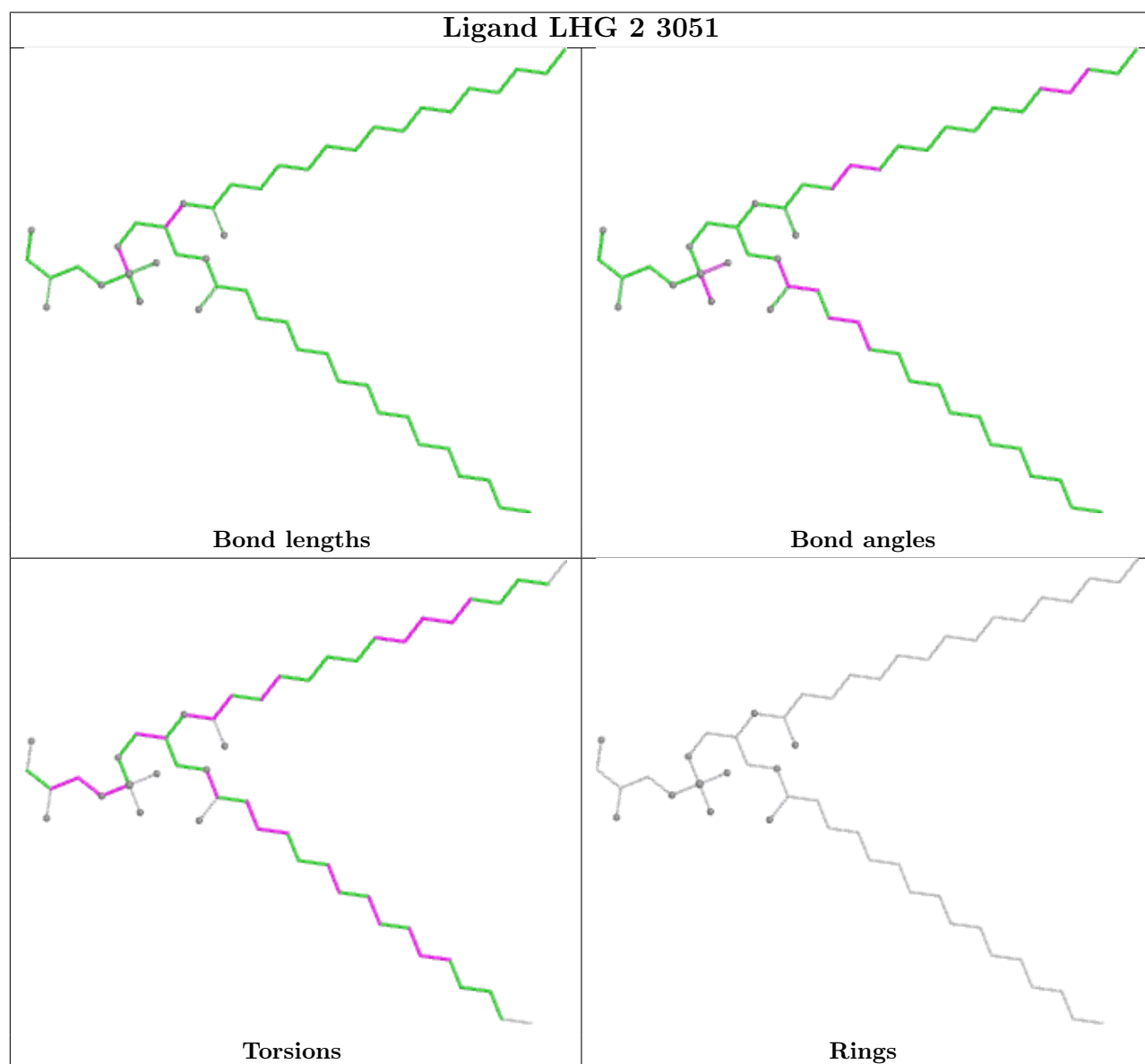
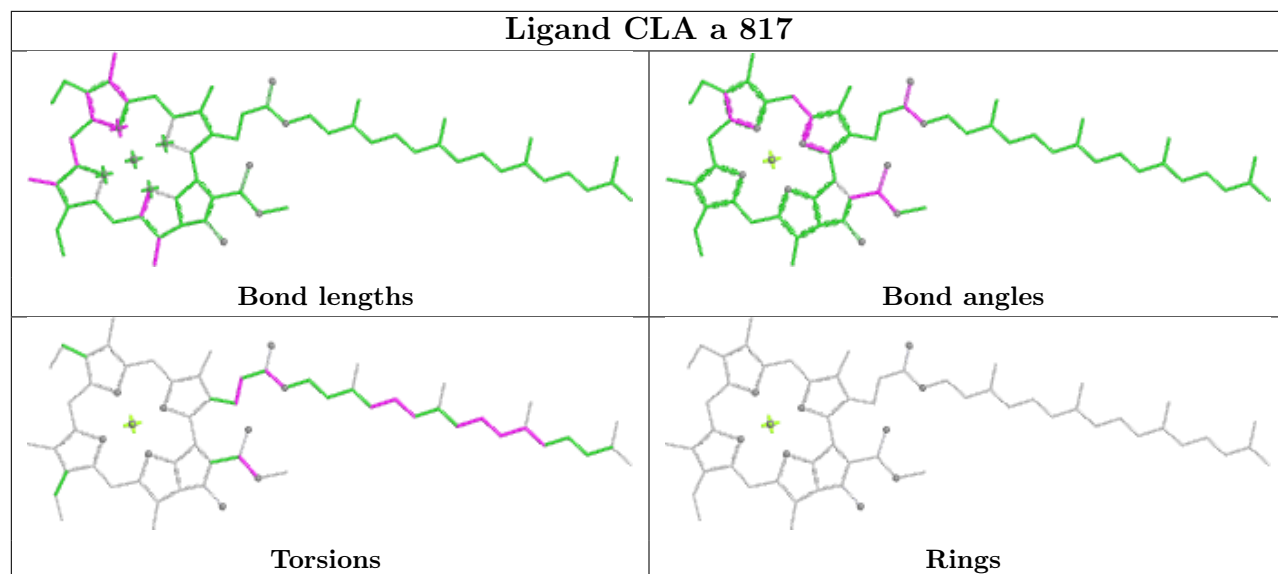


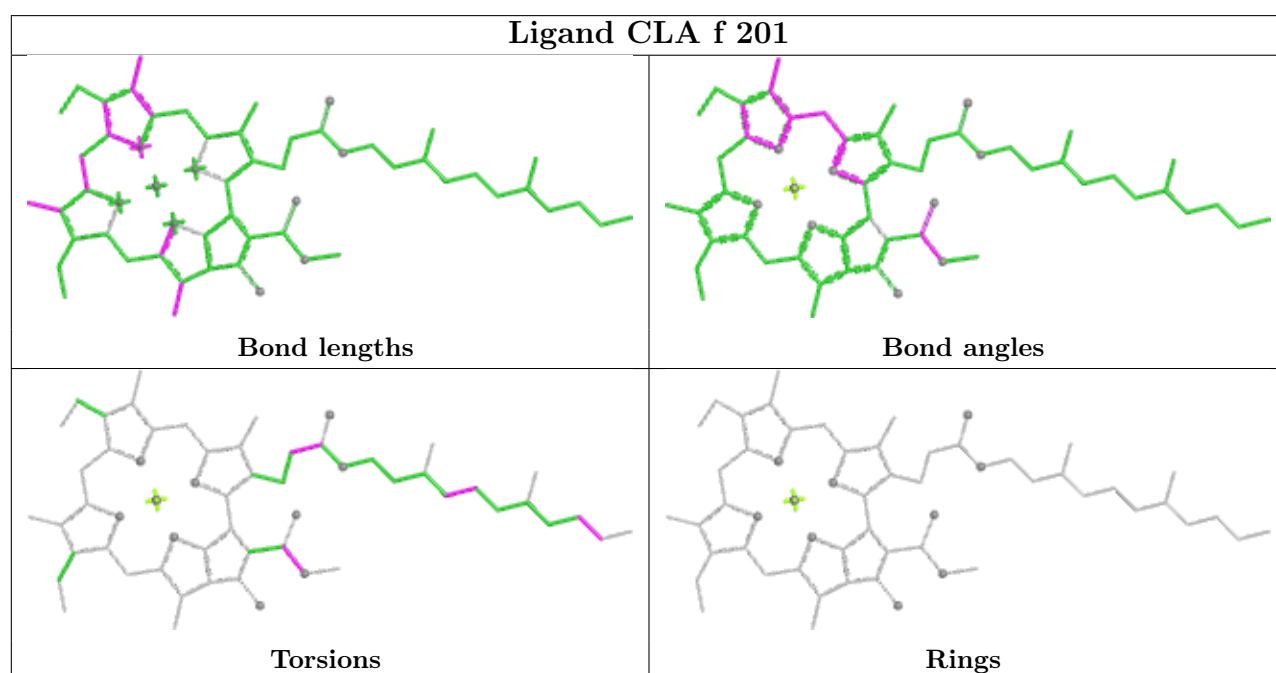
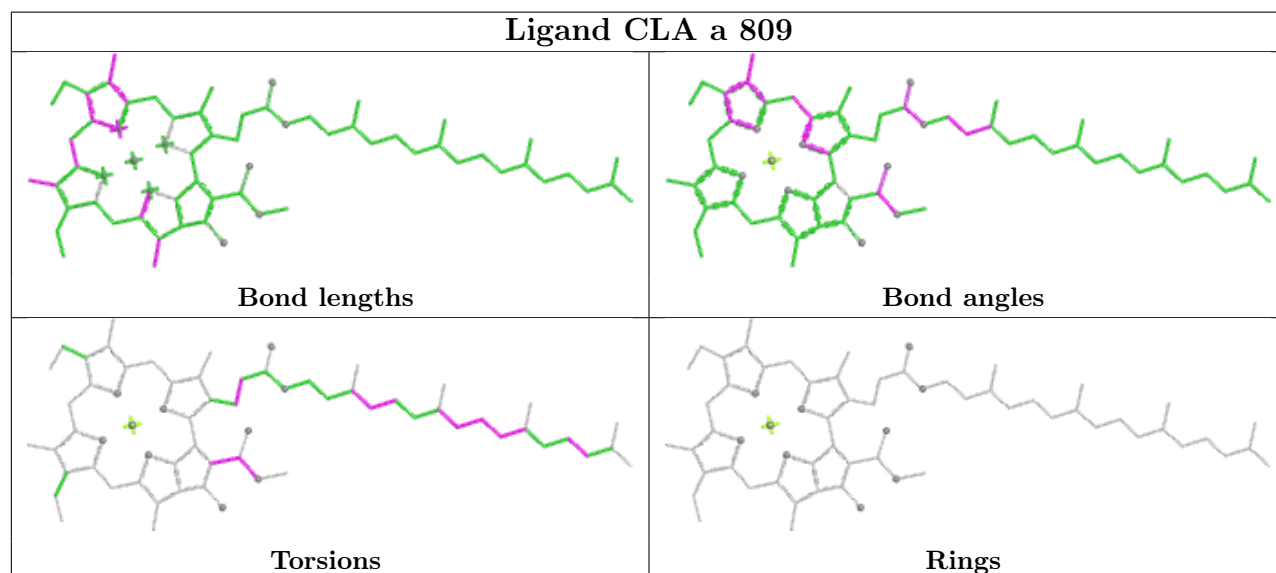
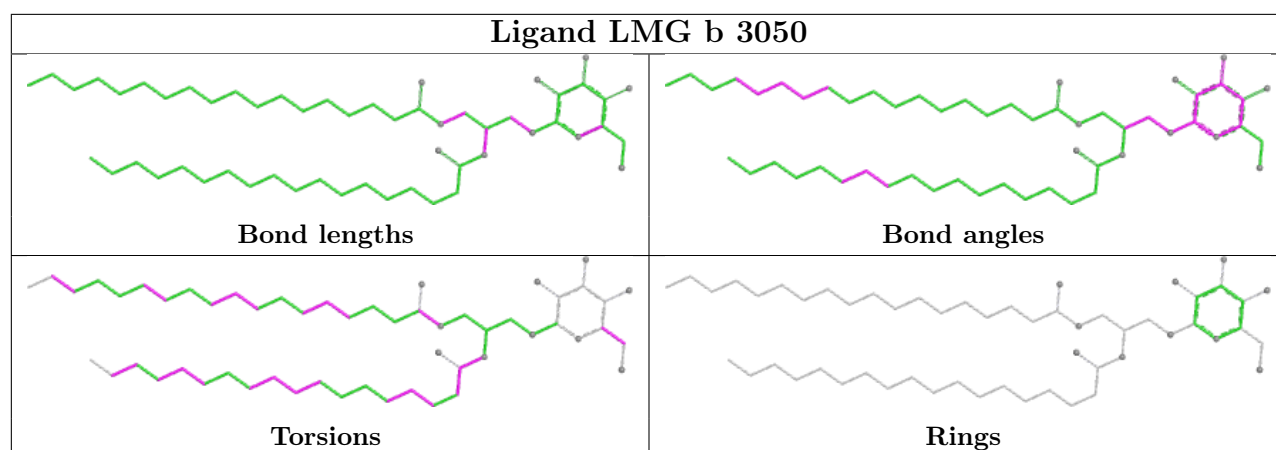


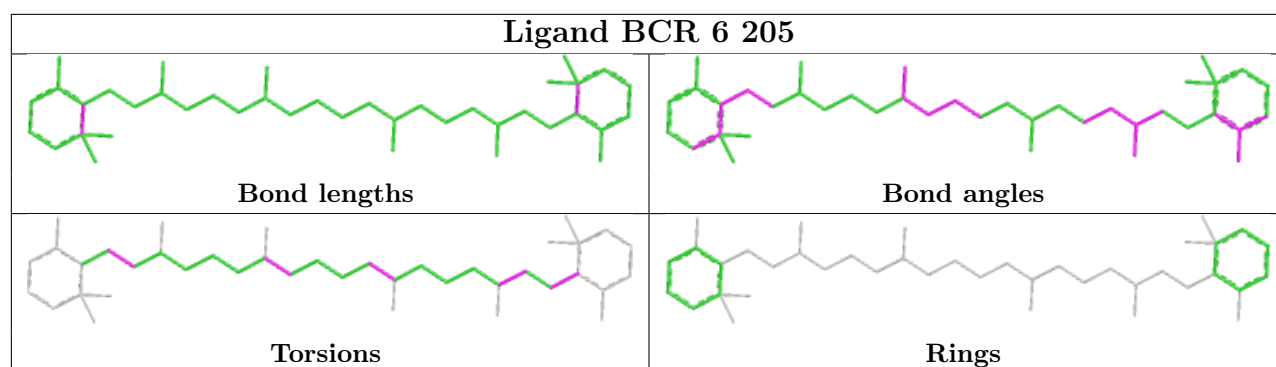
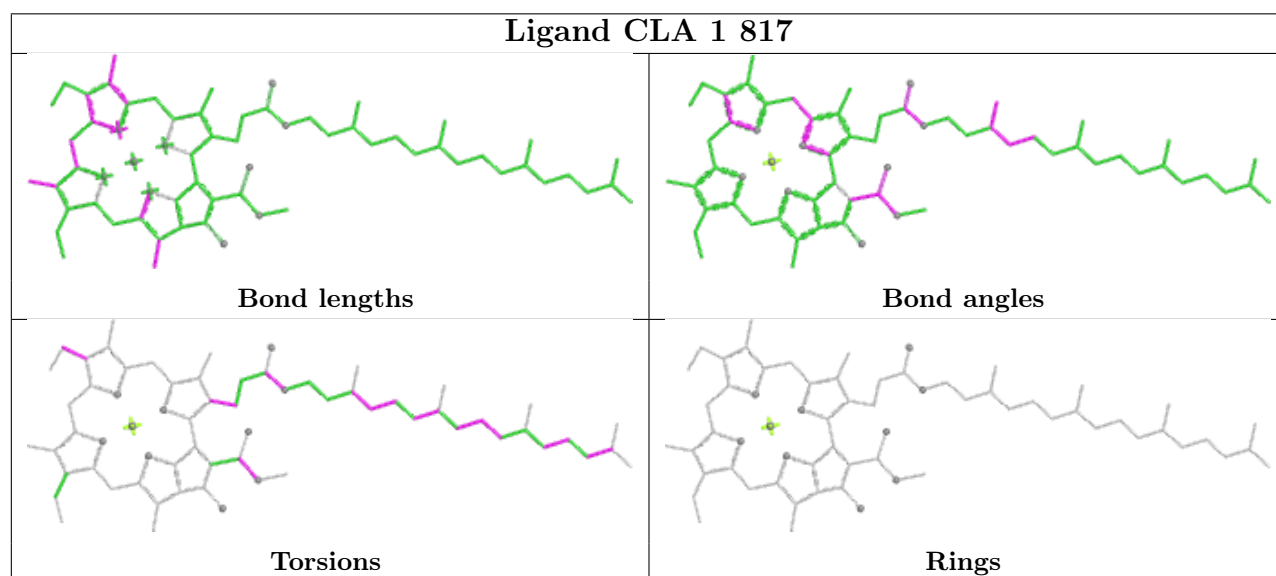
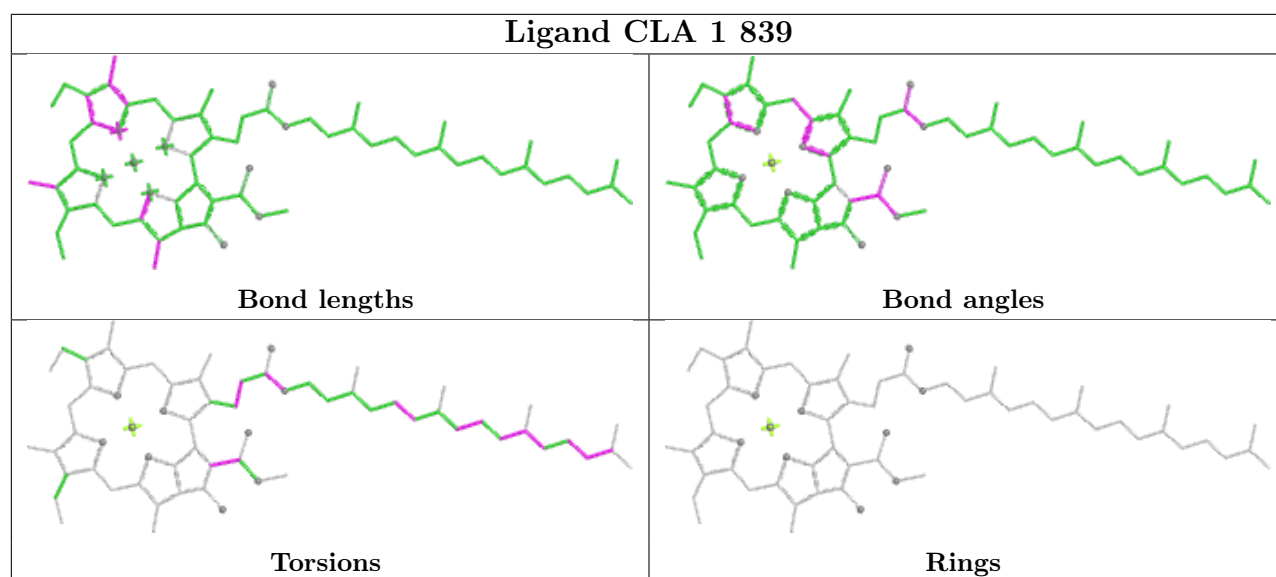


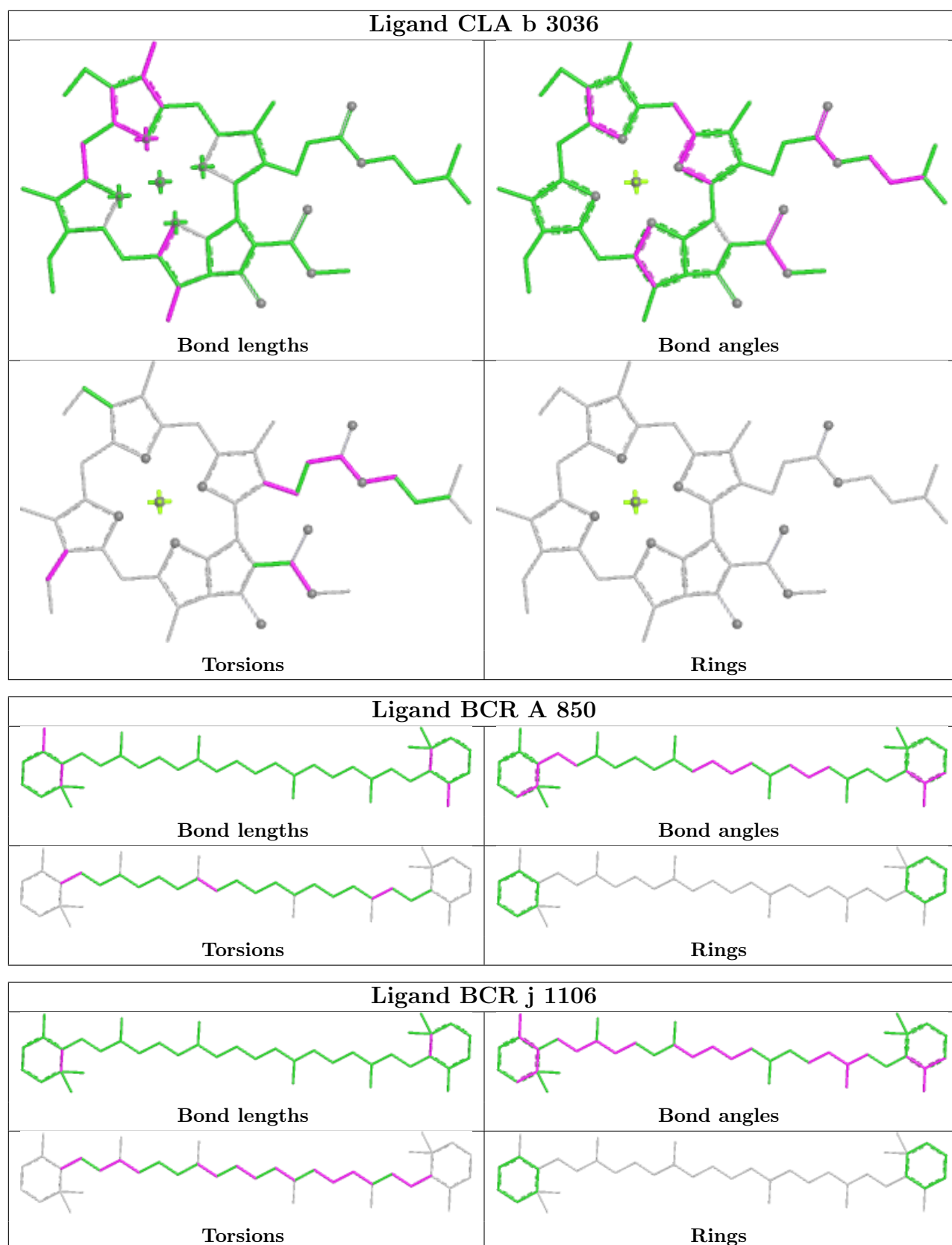
## Ligand CLA 8 102

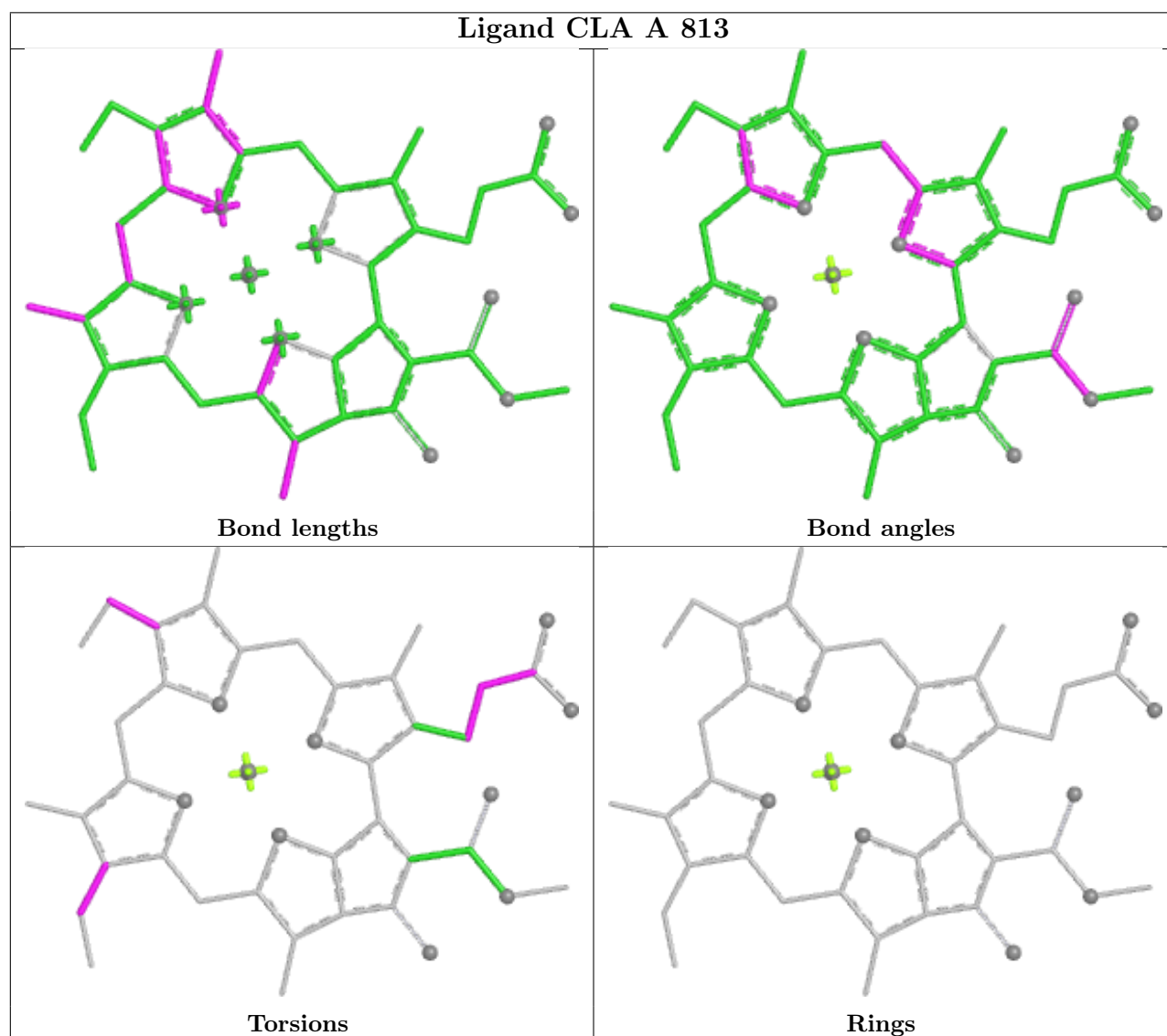
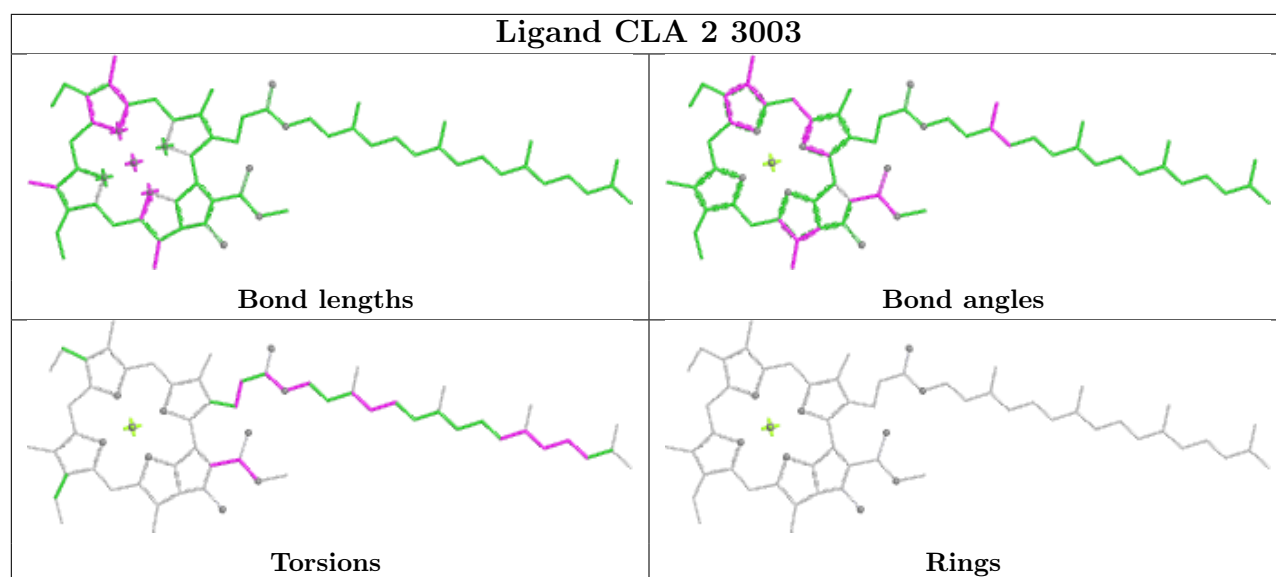


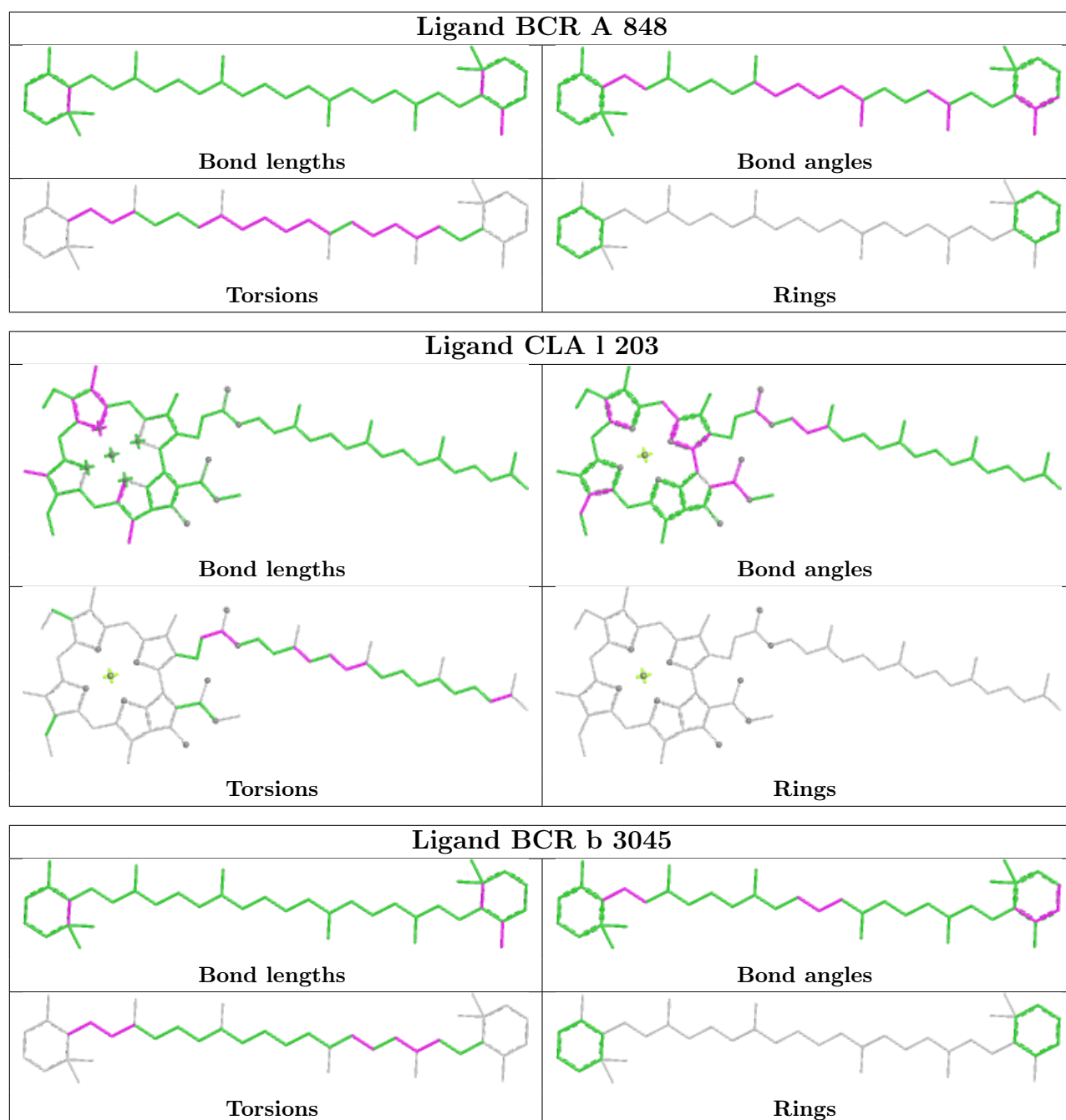


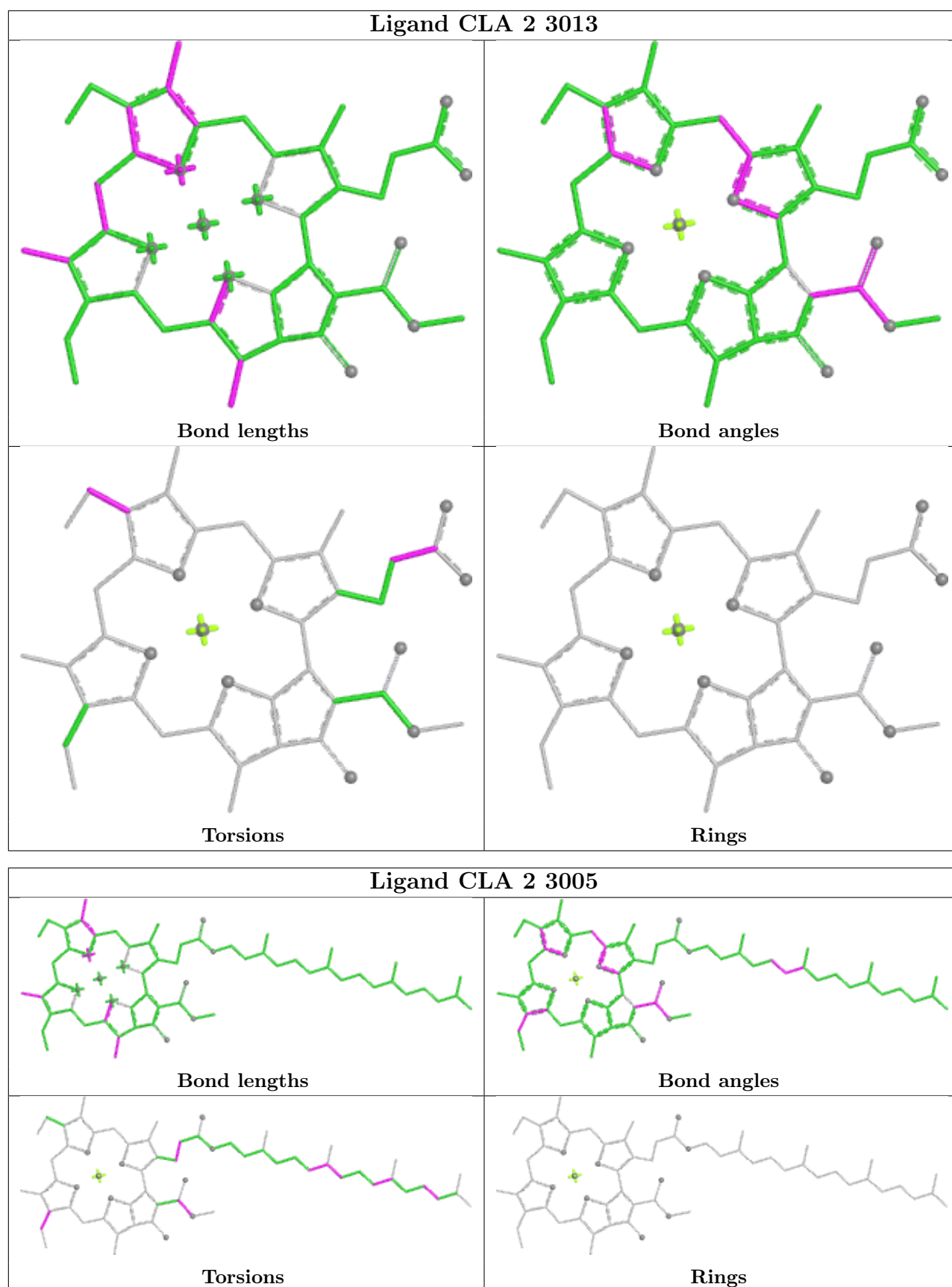


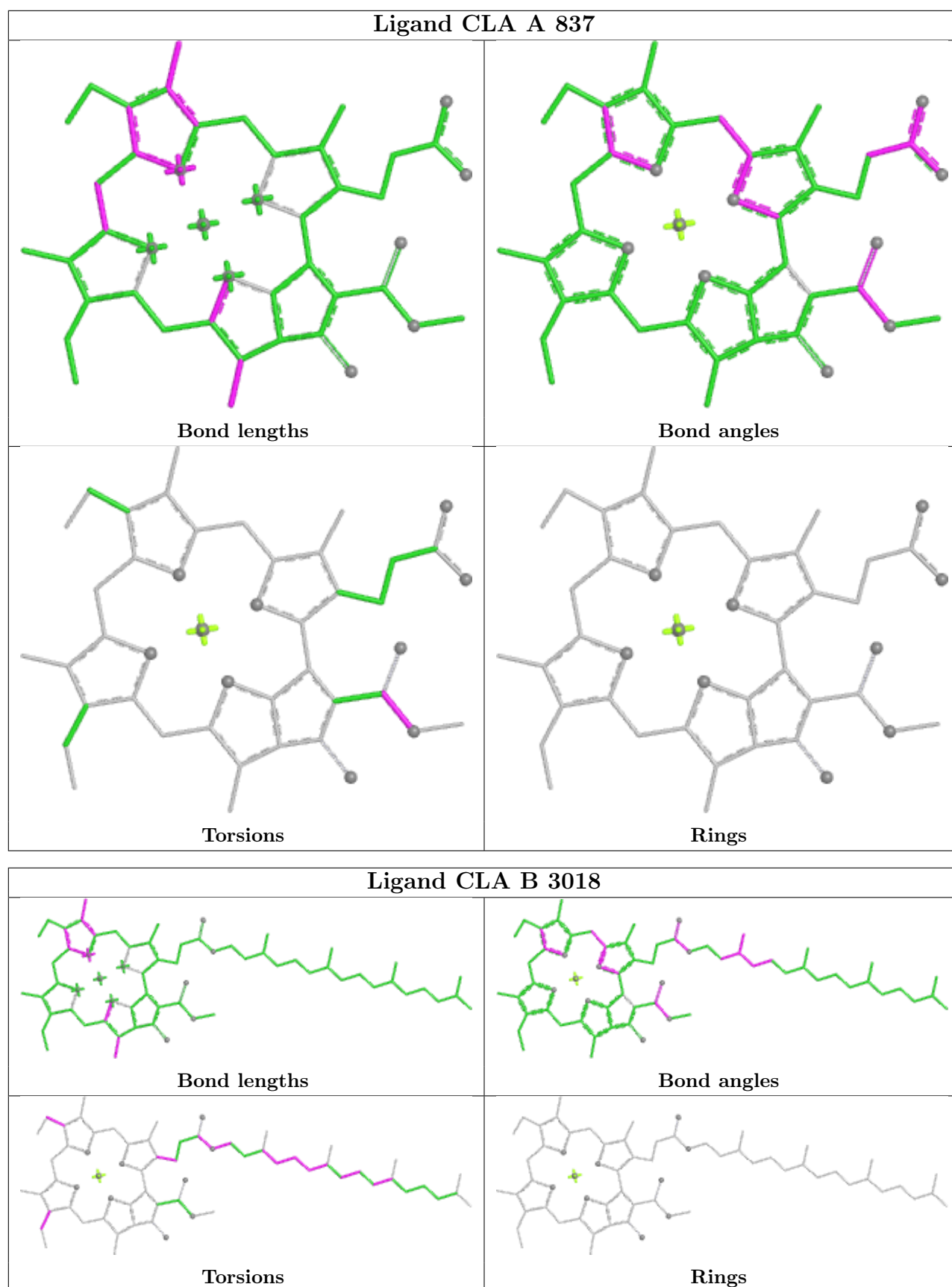


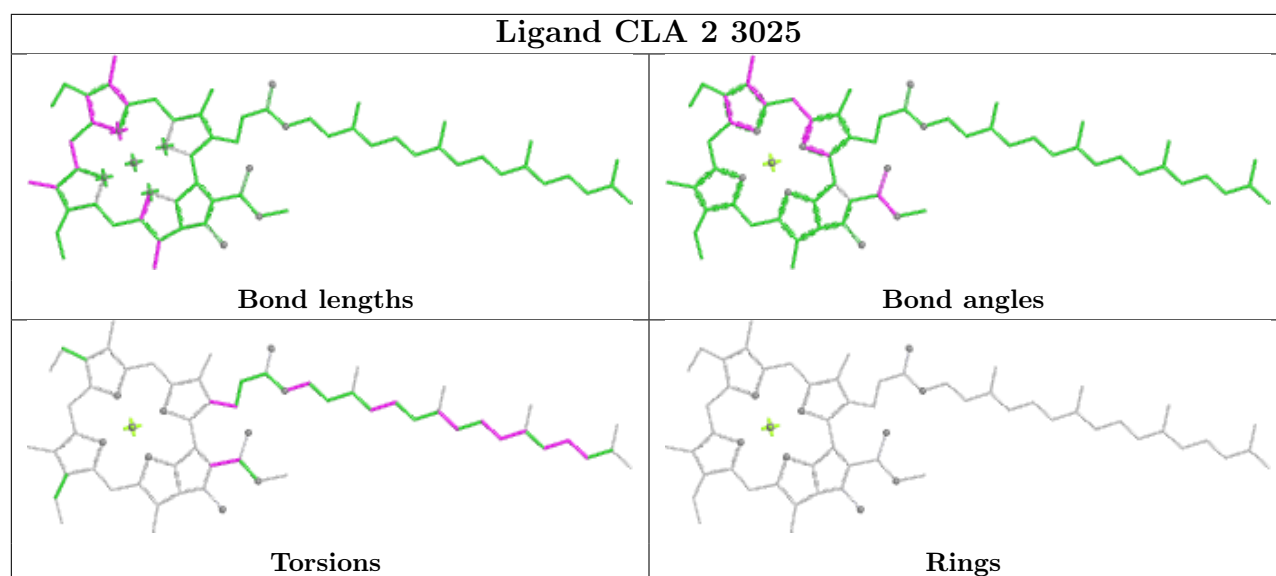
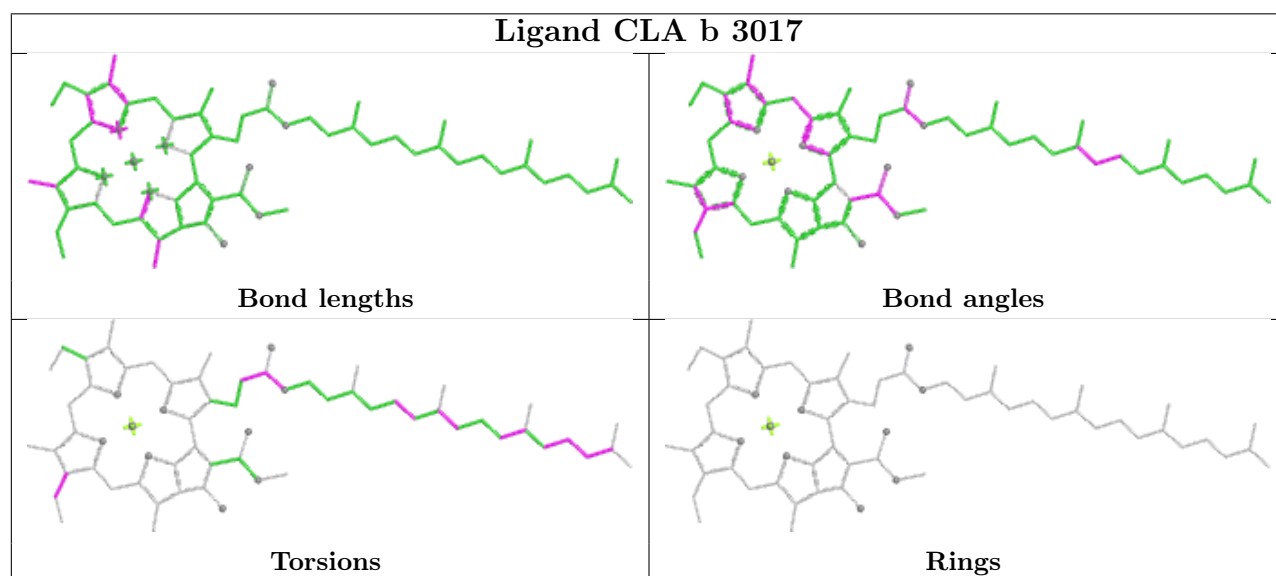
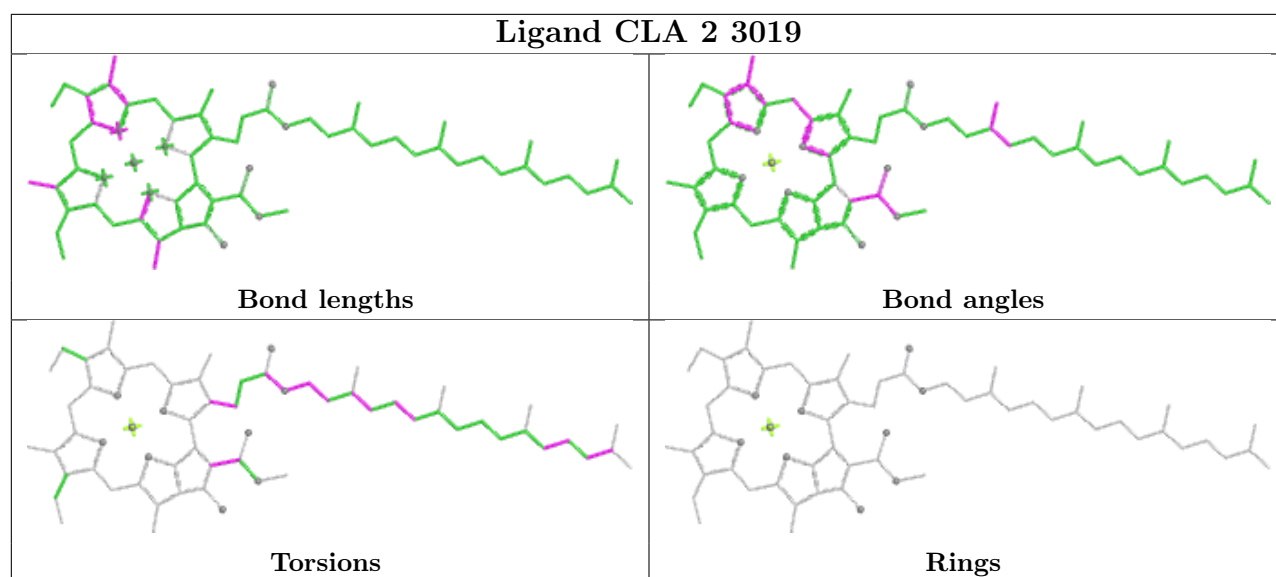


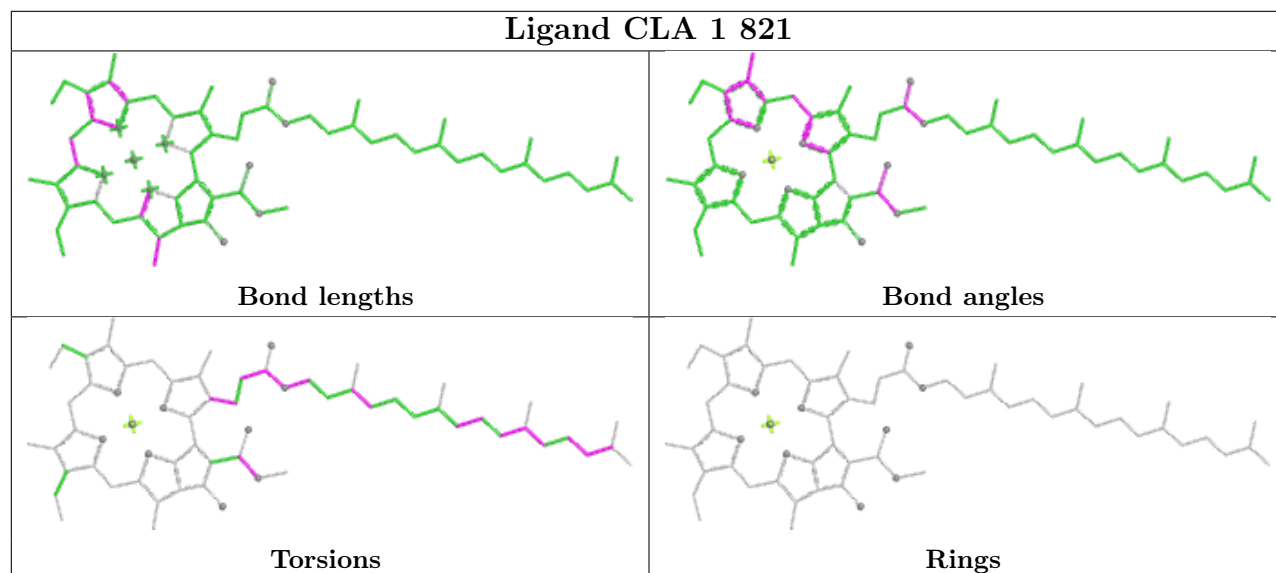
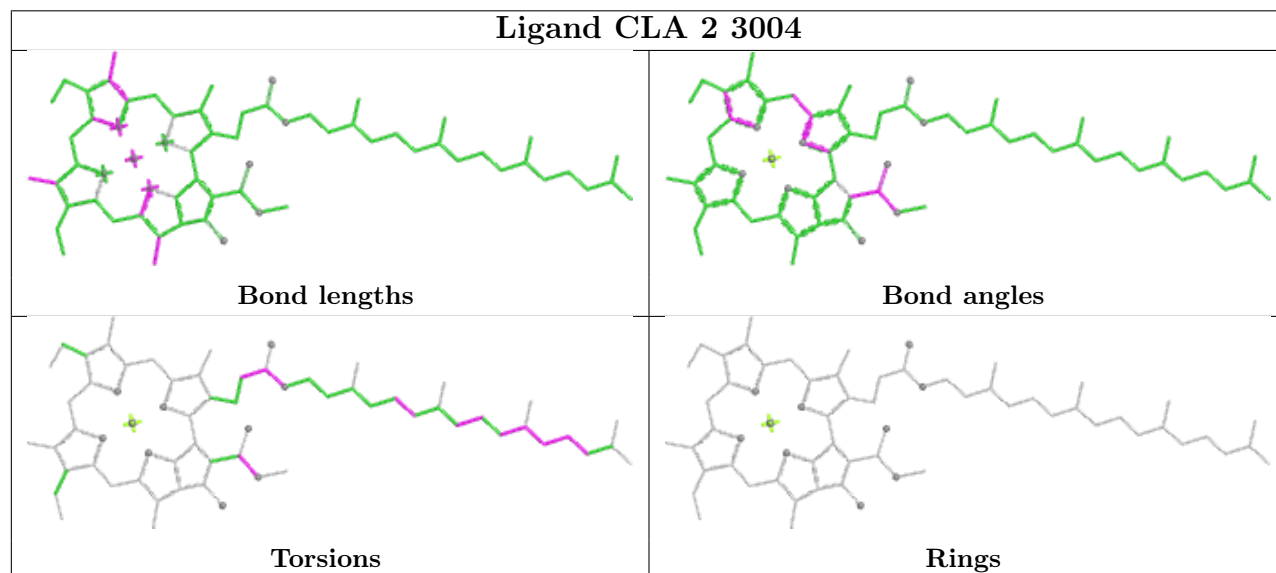
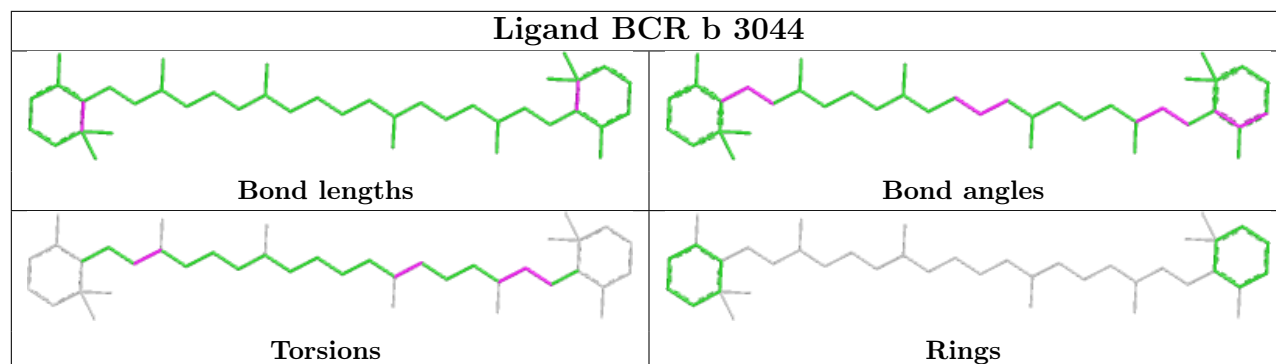


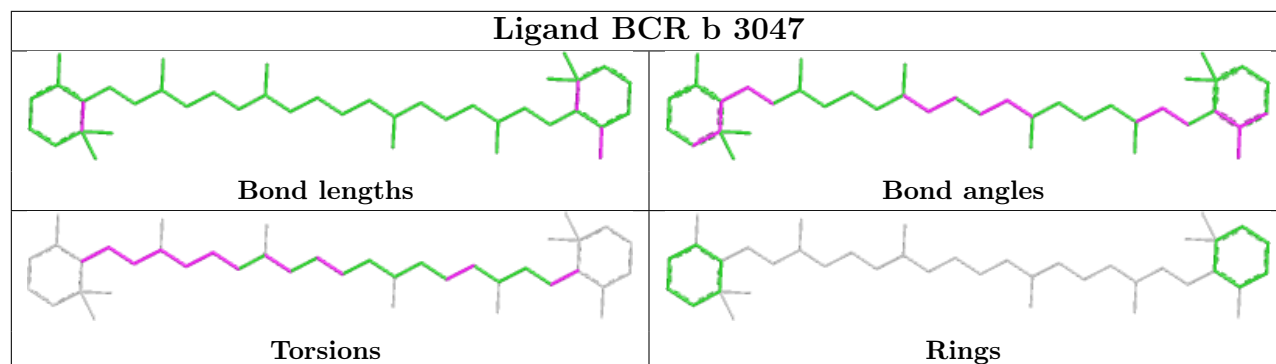
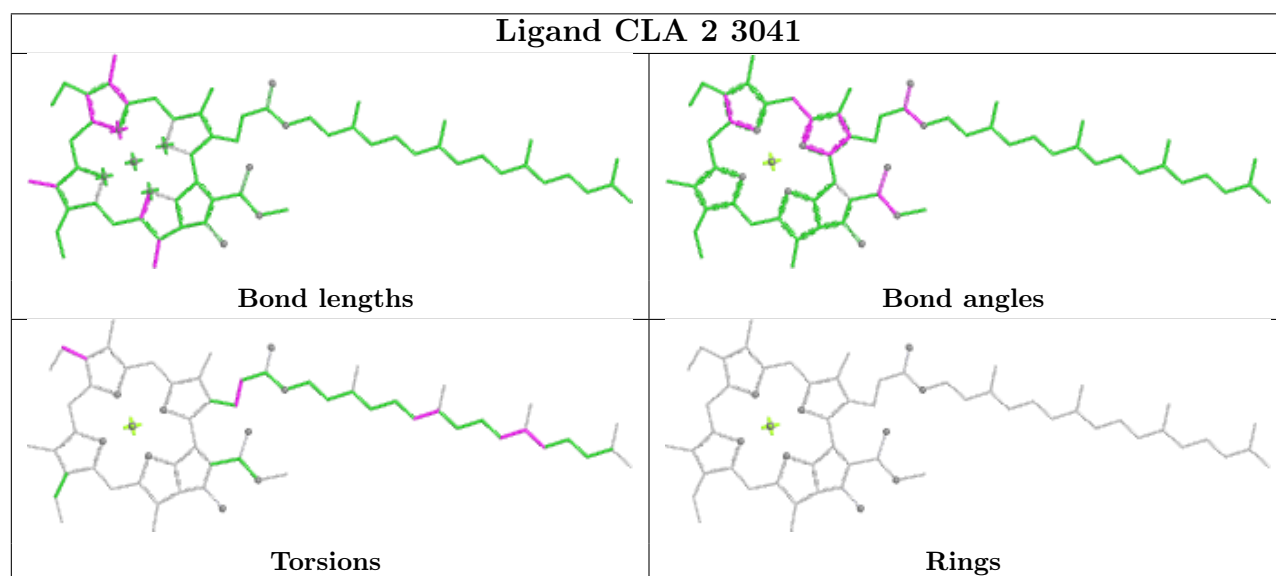
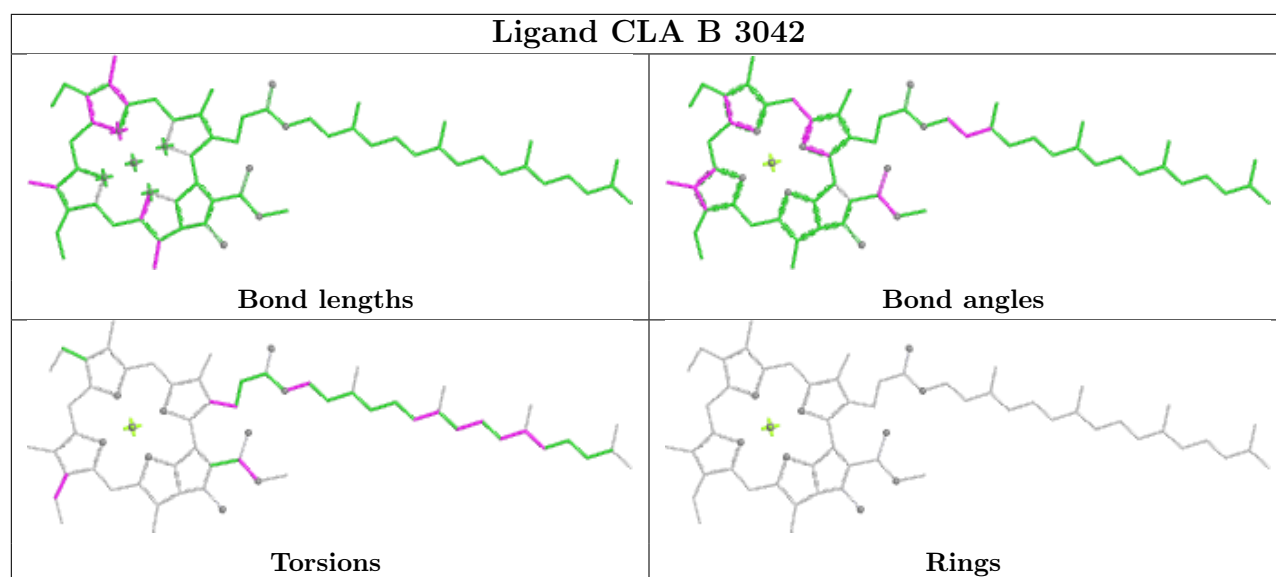


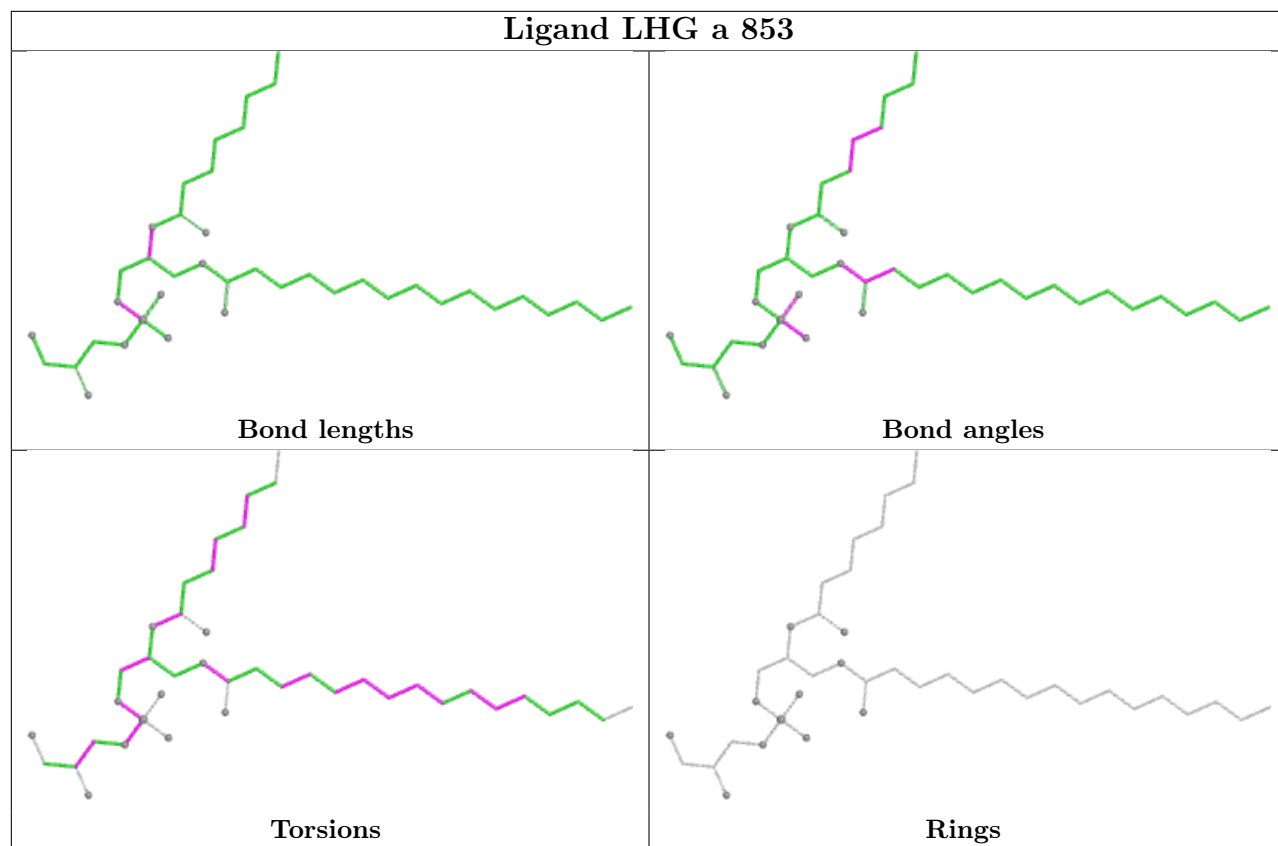


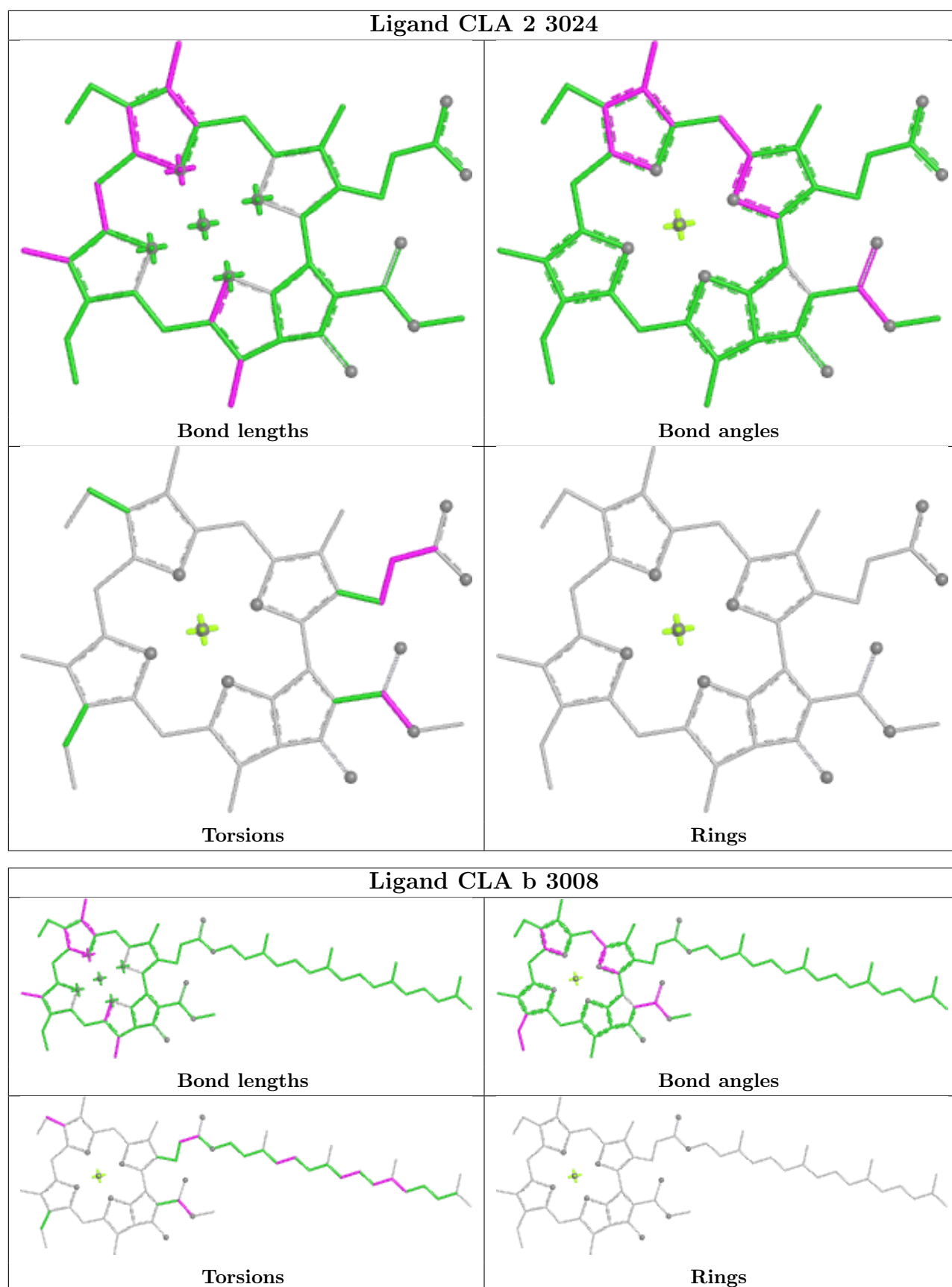


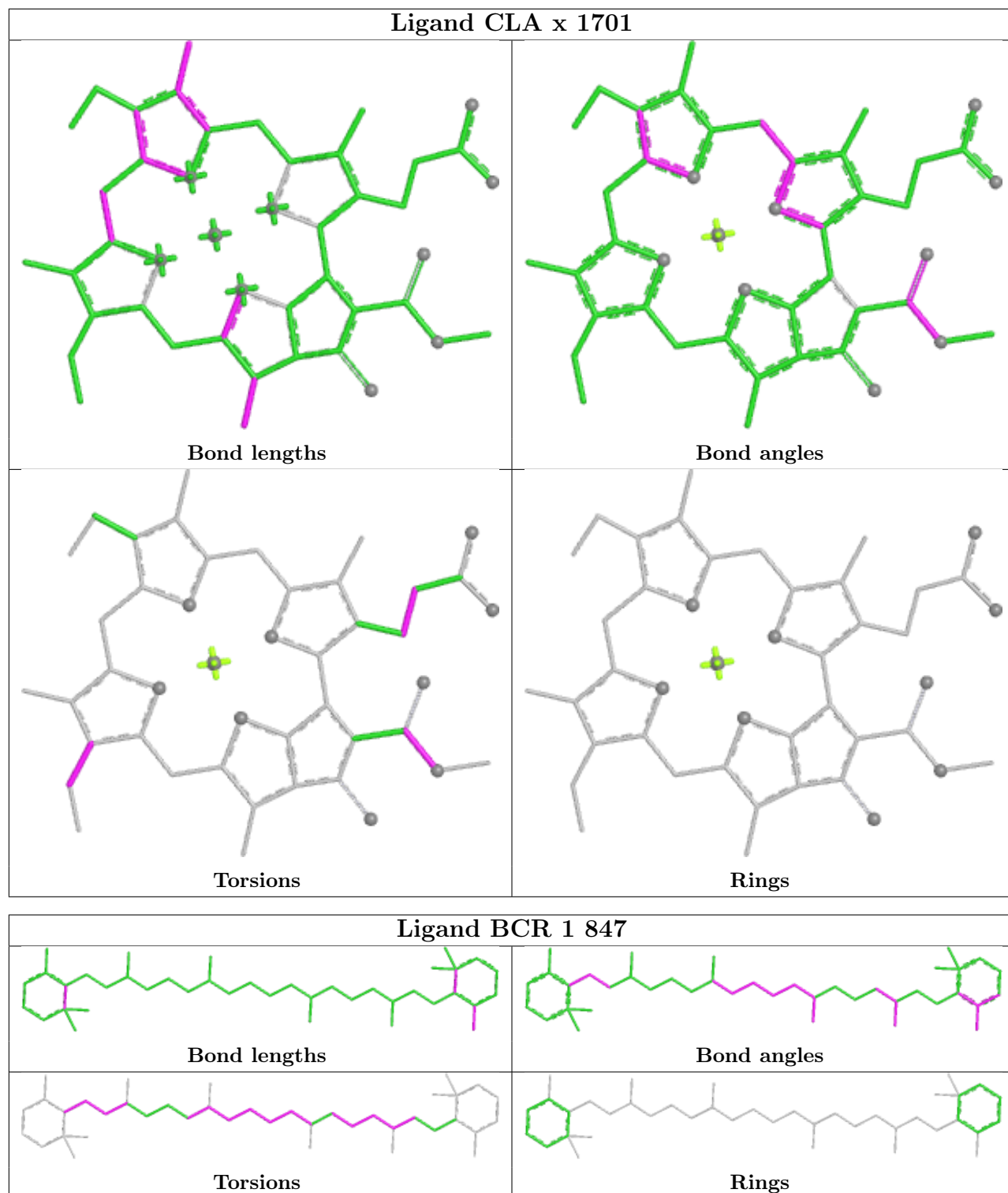


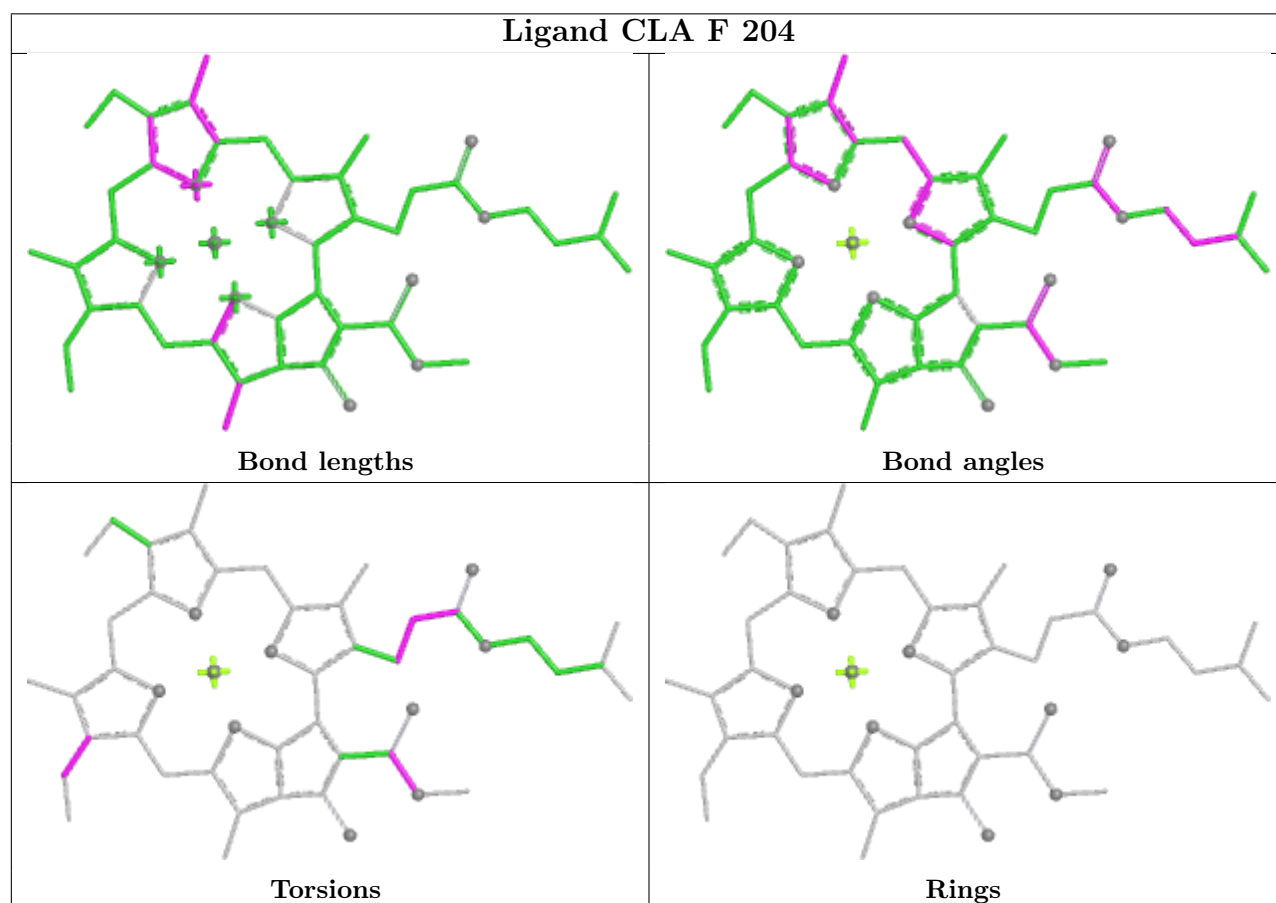
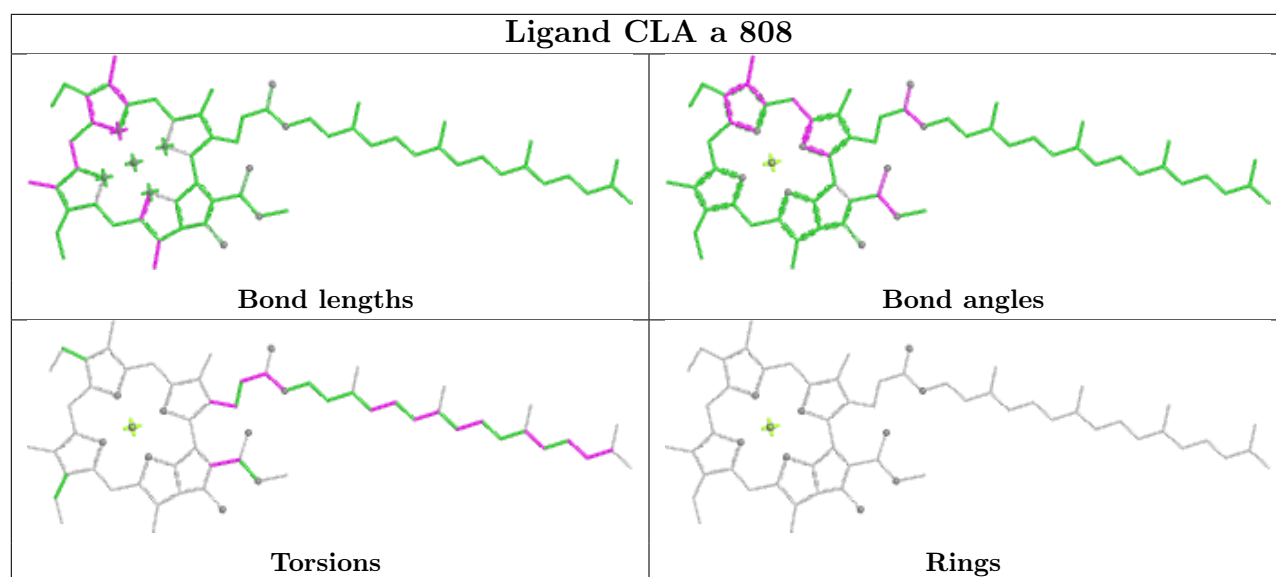


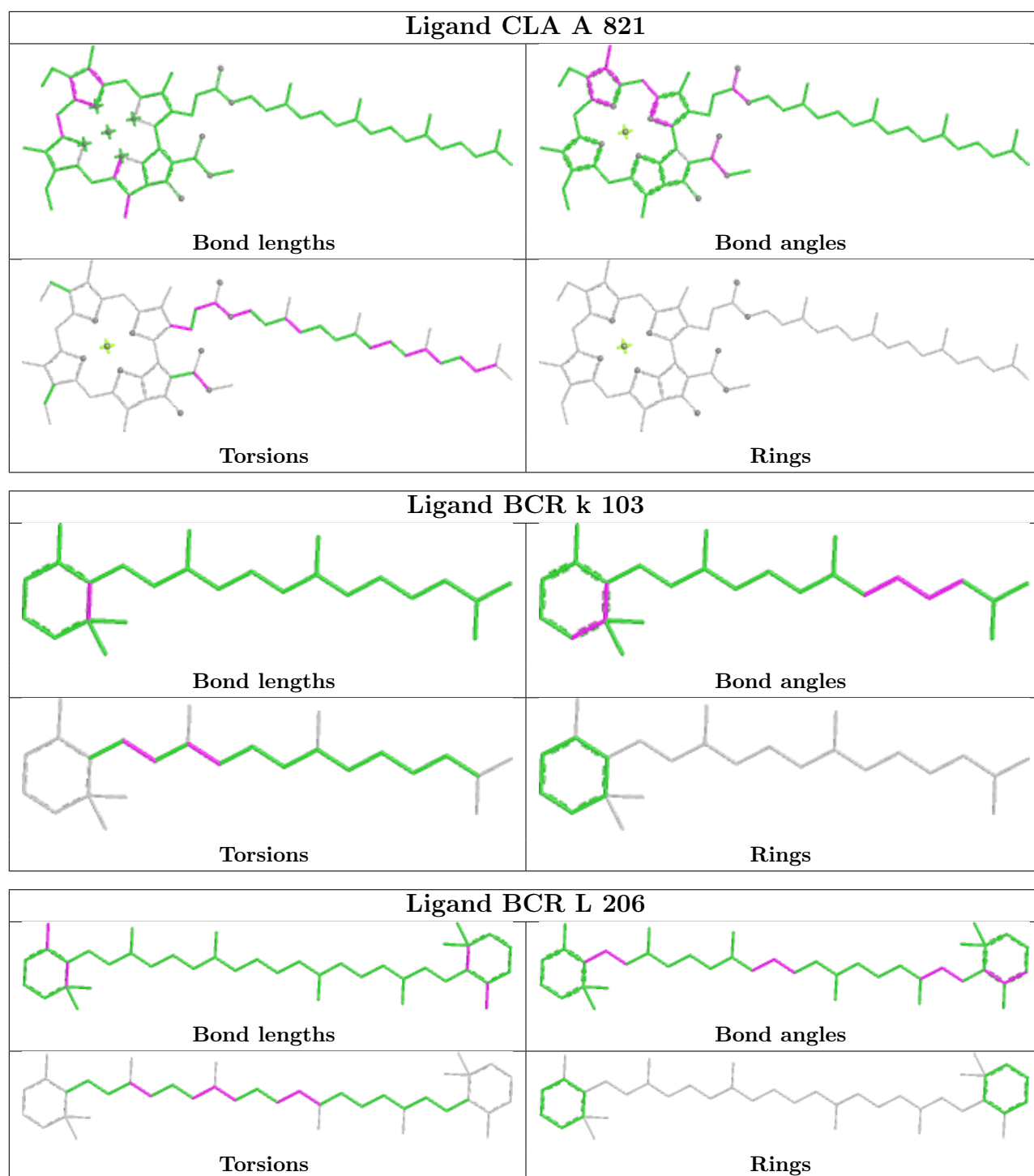


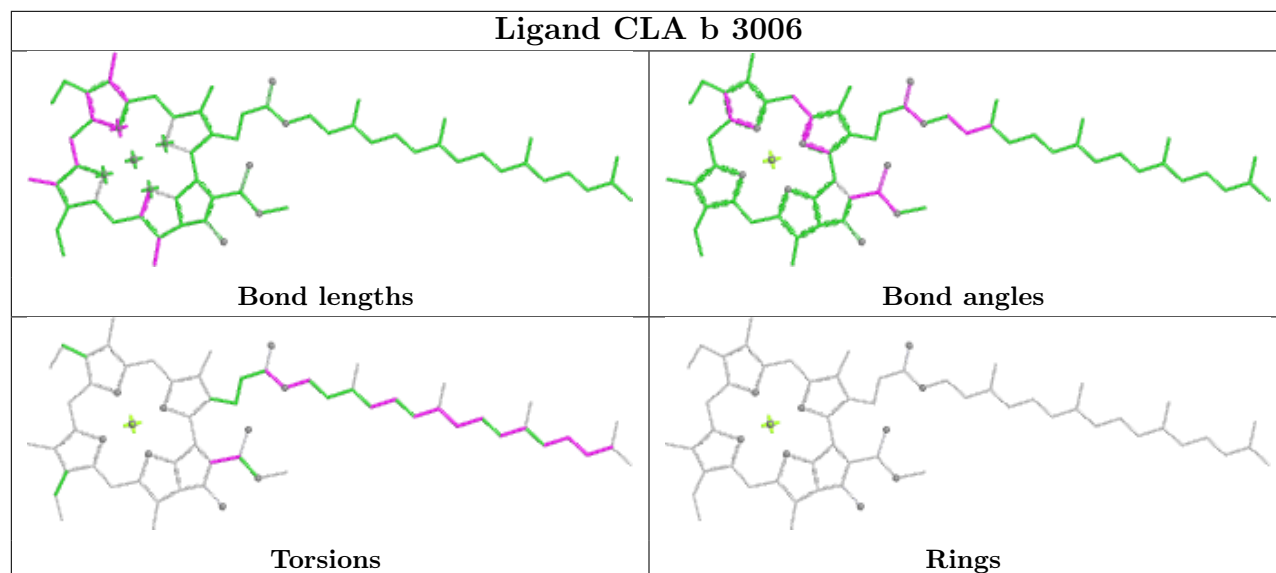
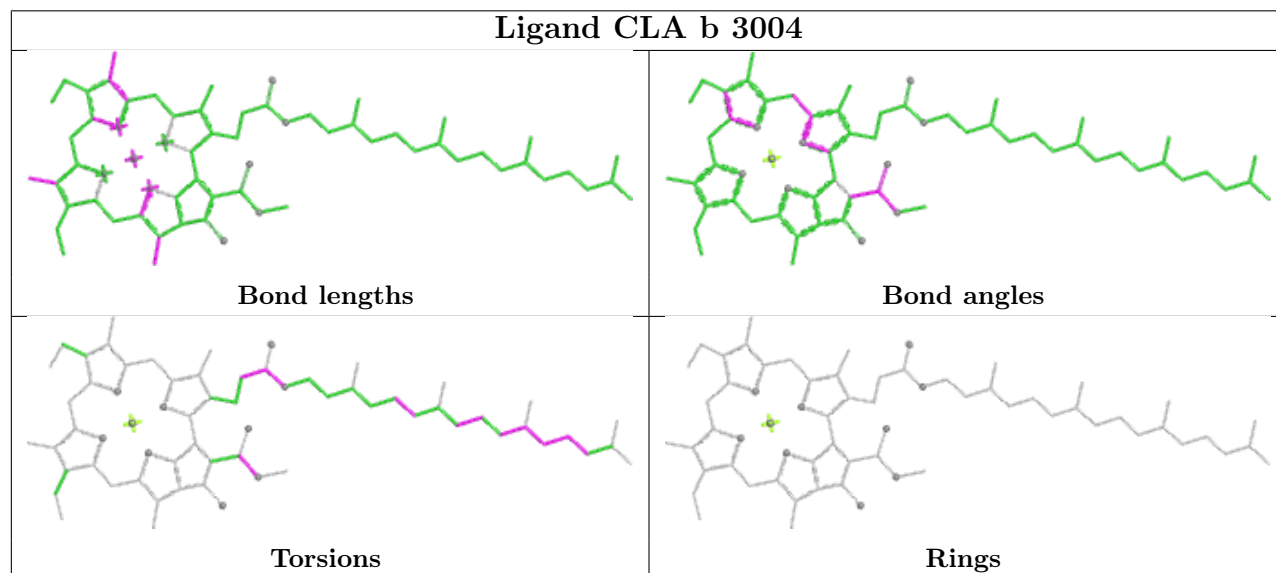
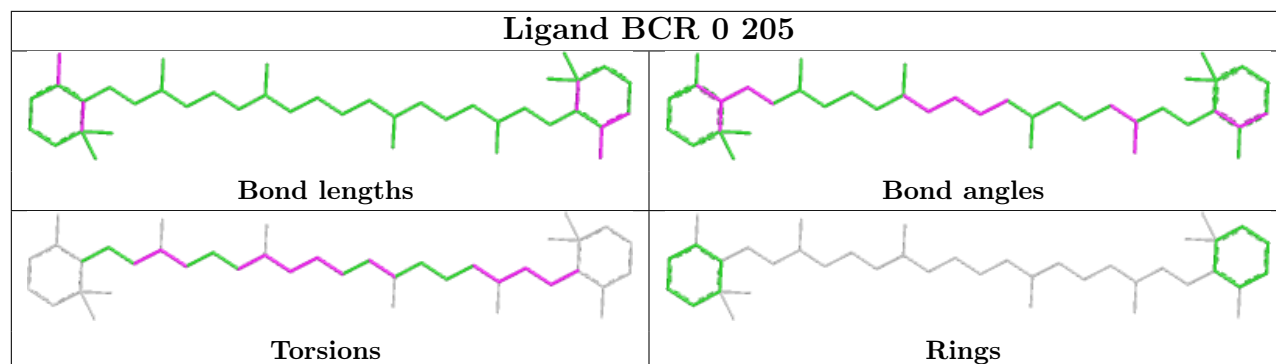


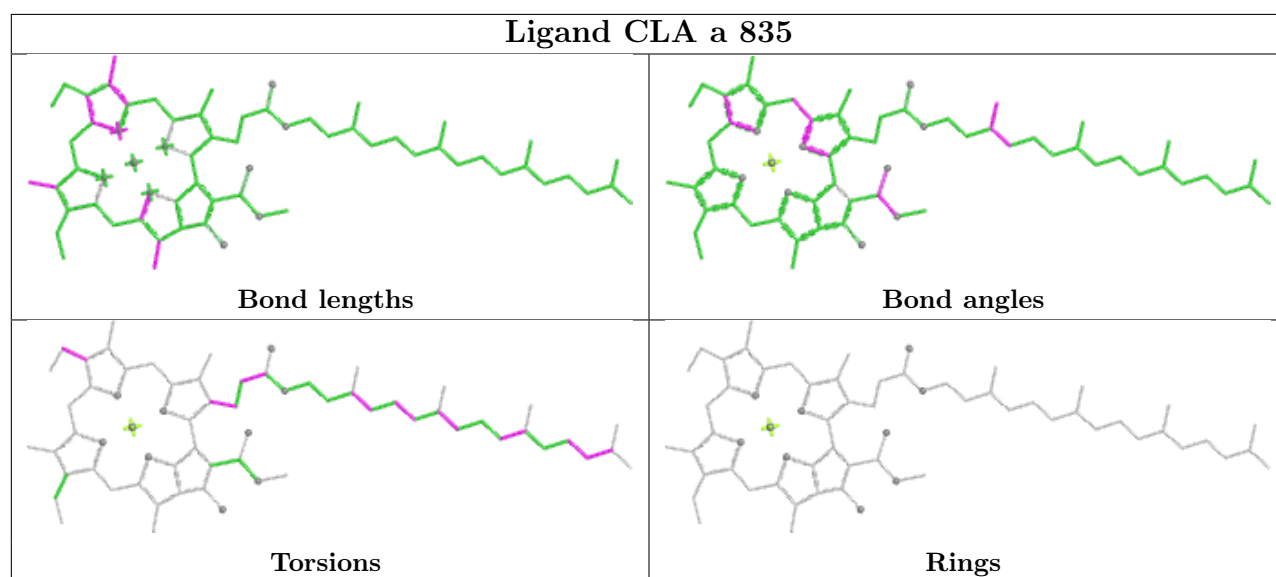
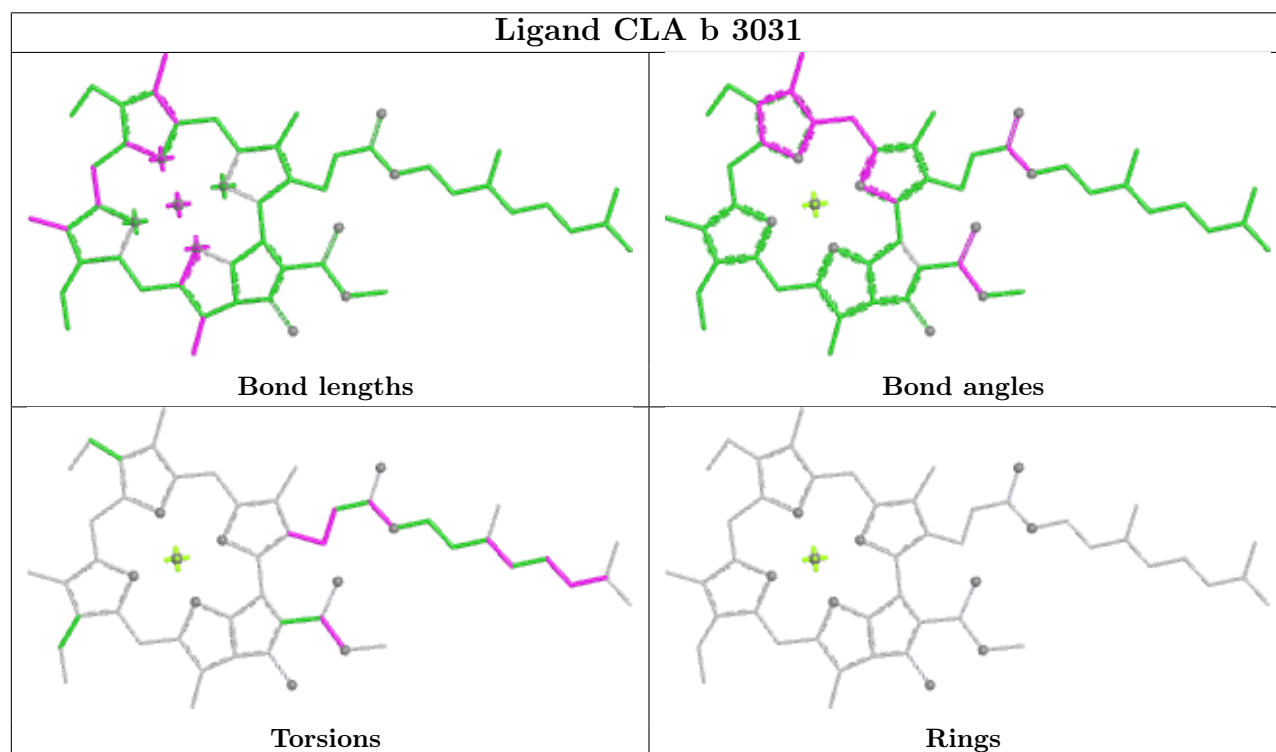
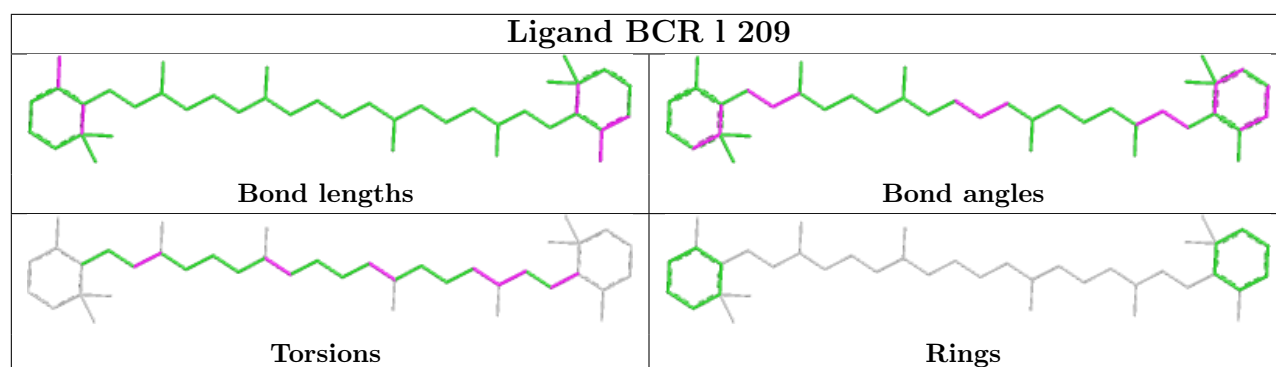


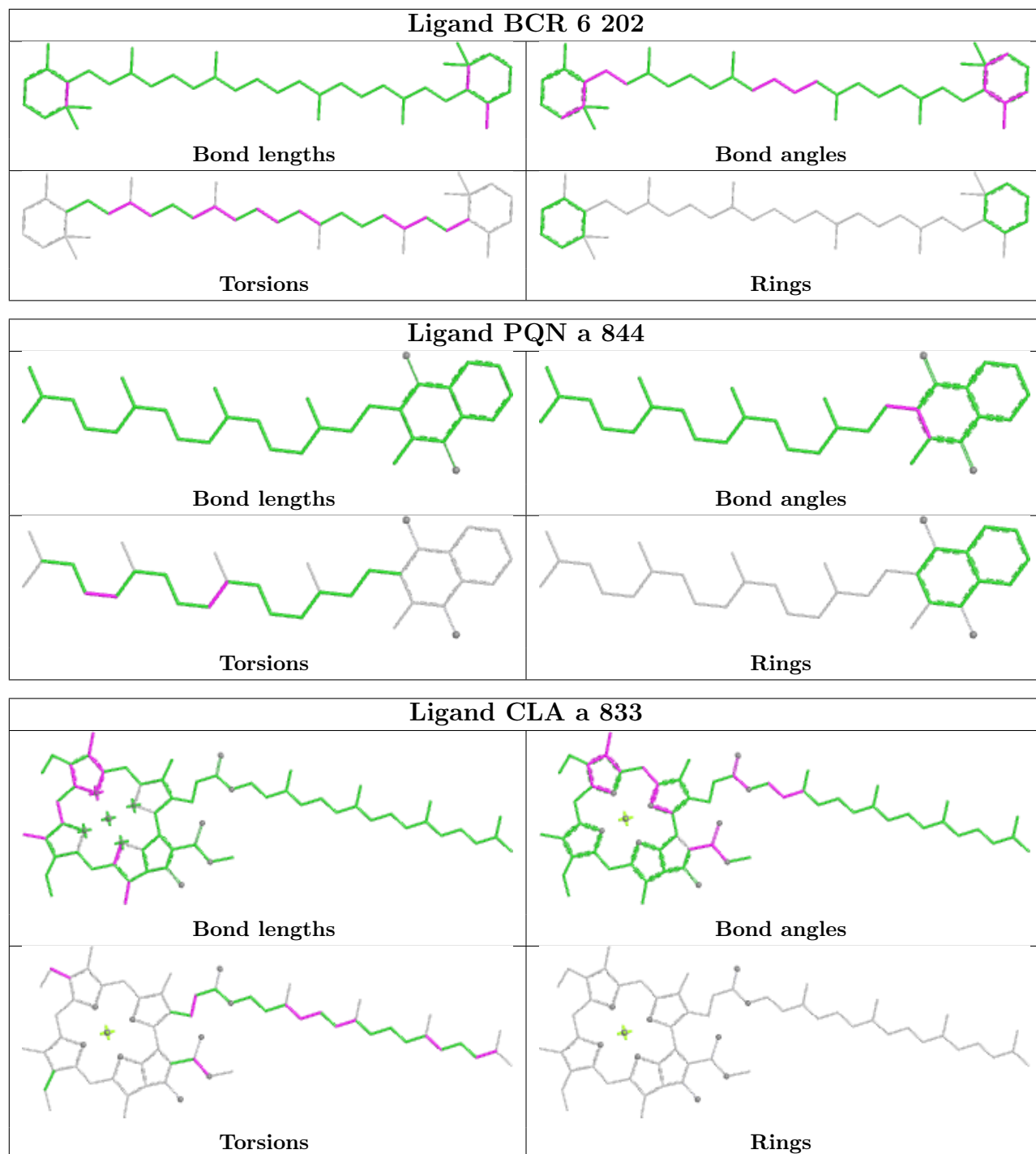


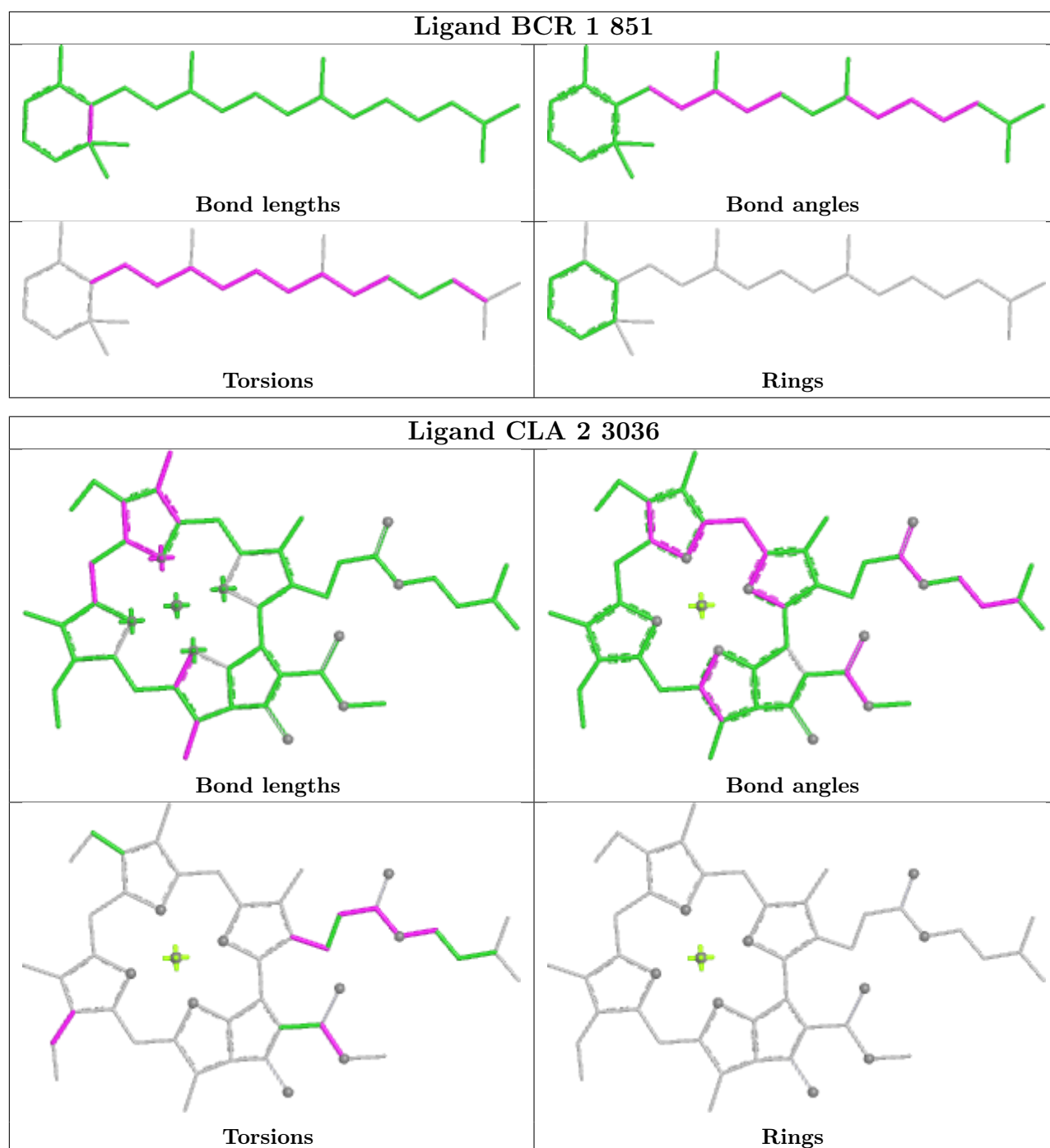


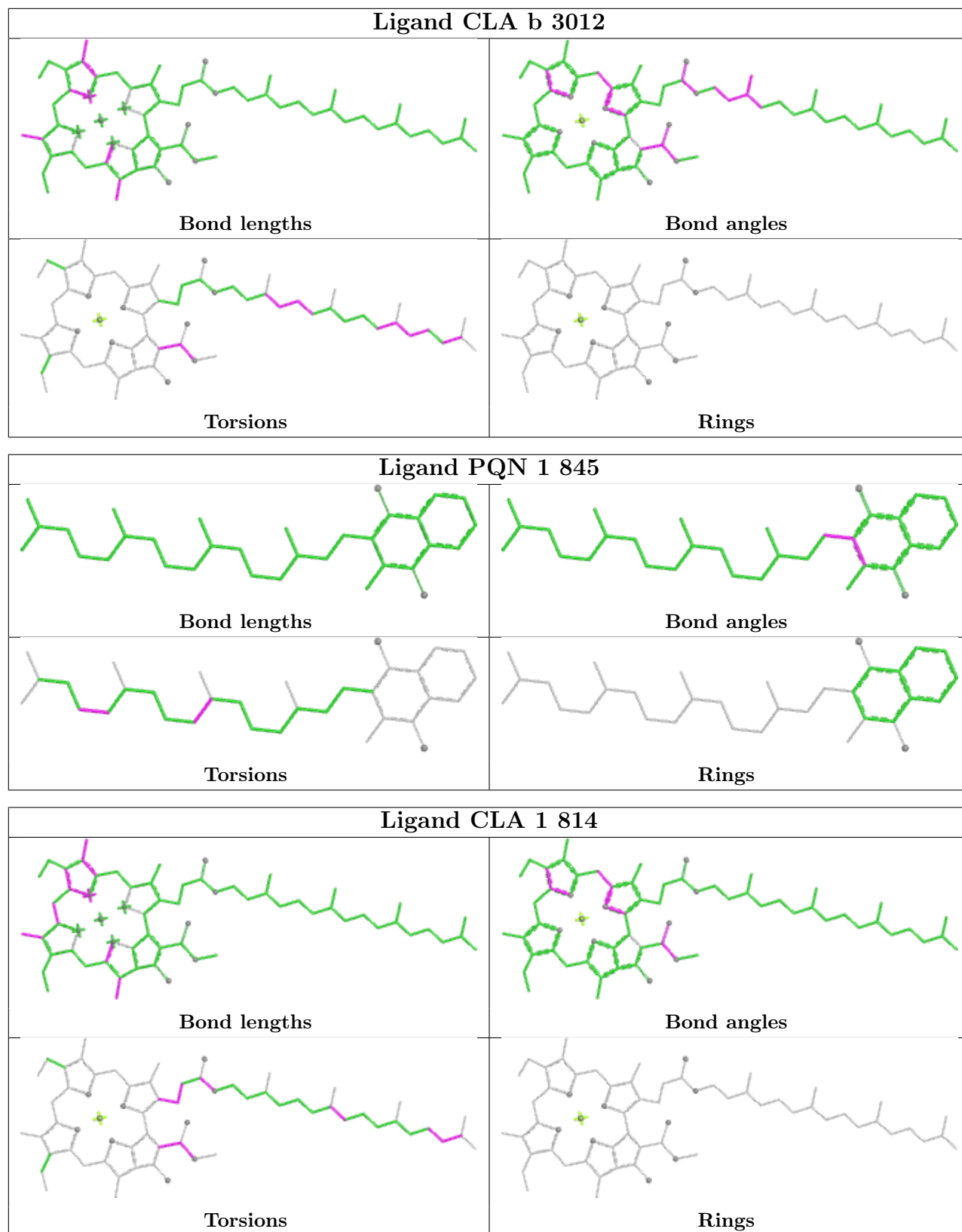


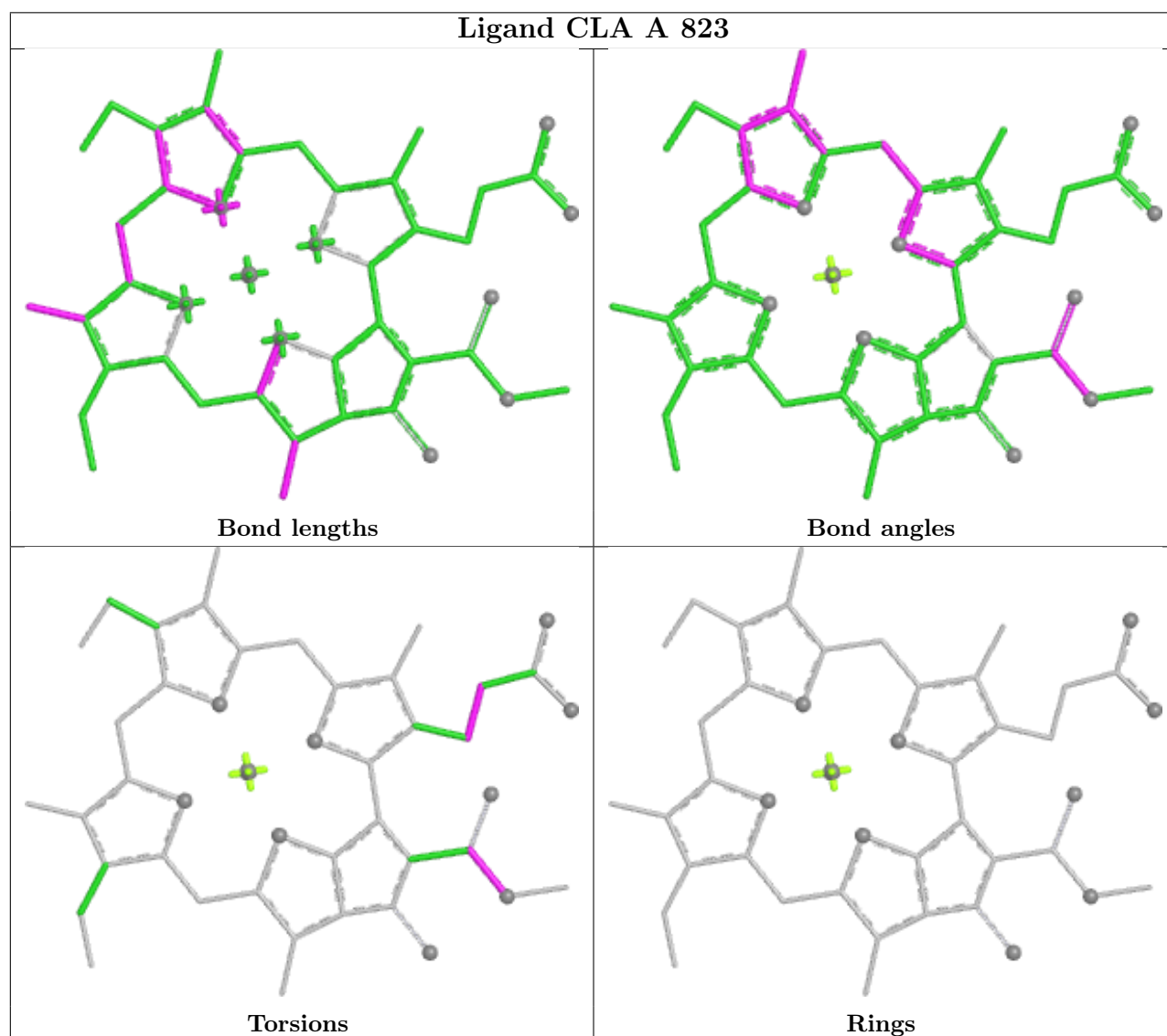
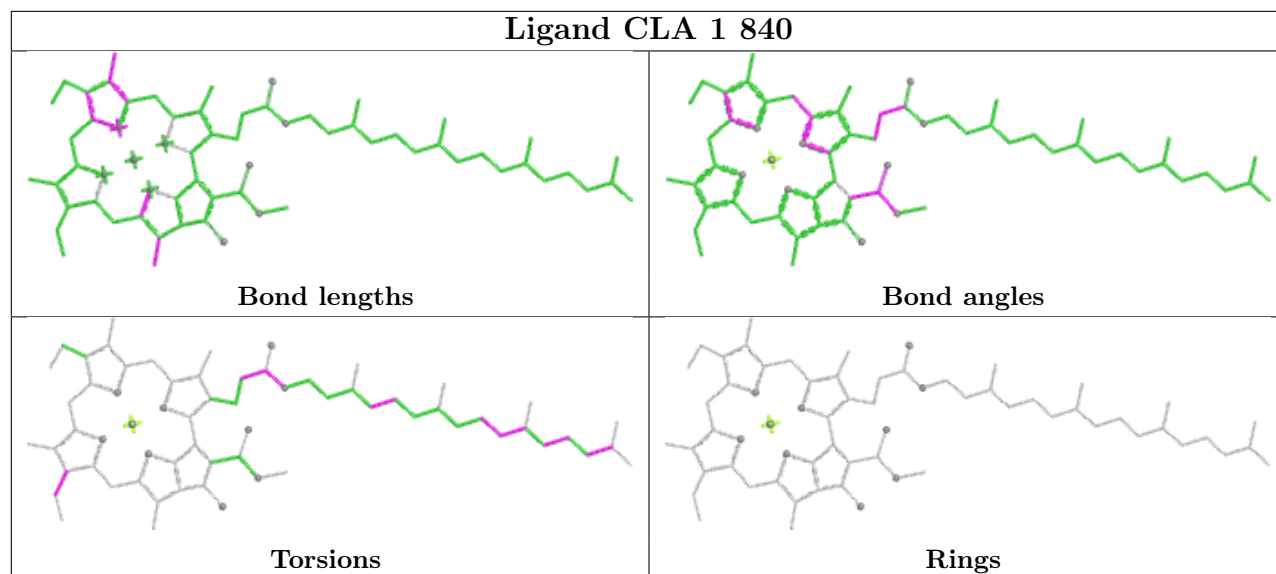


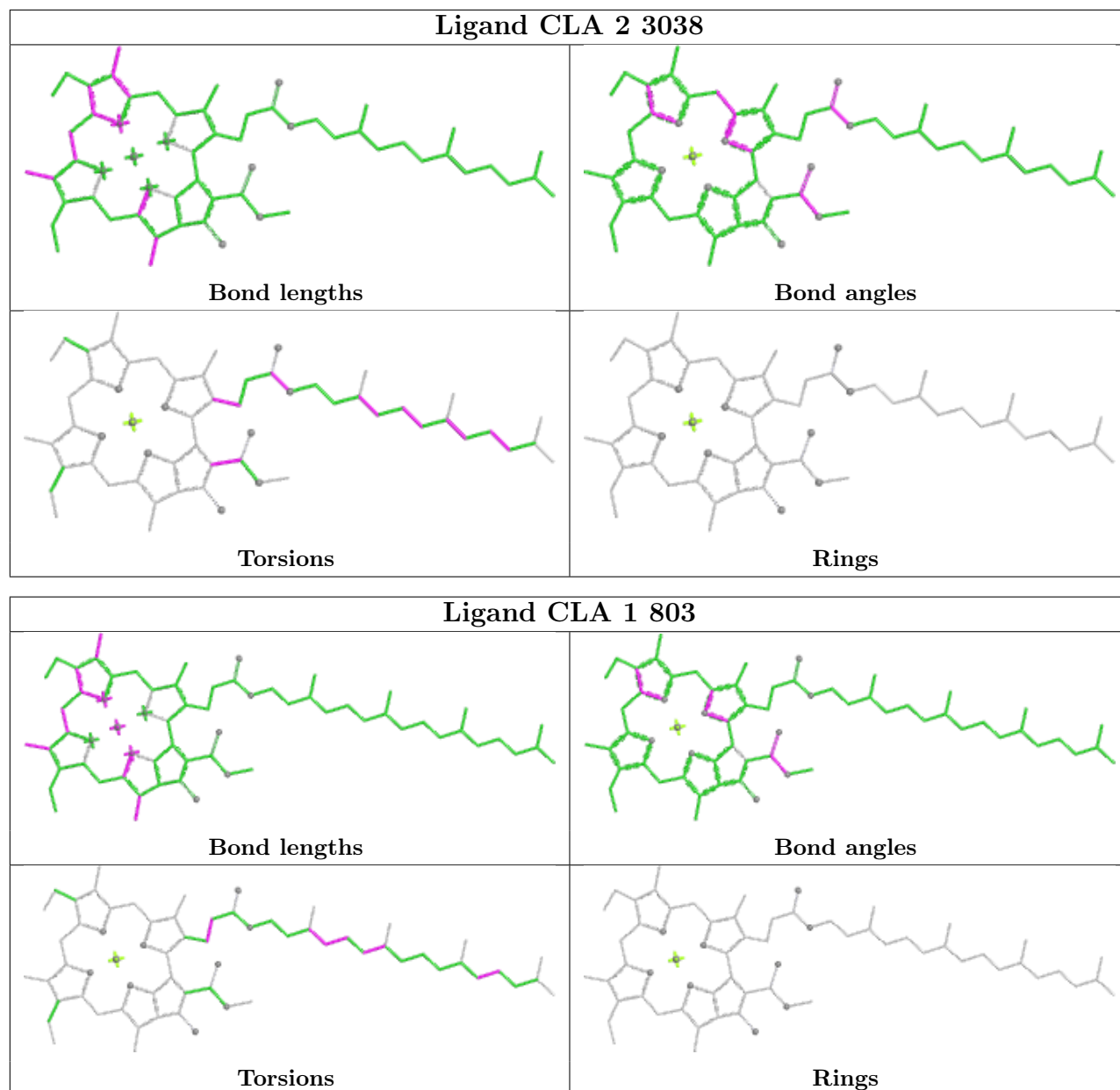


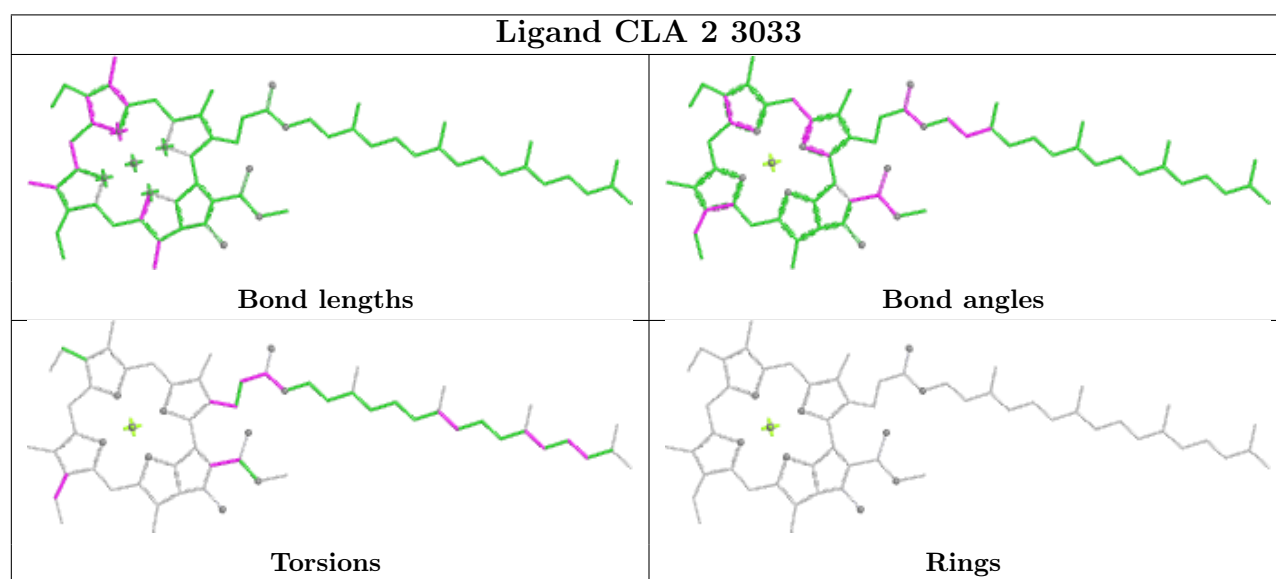
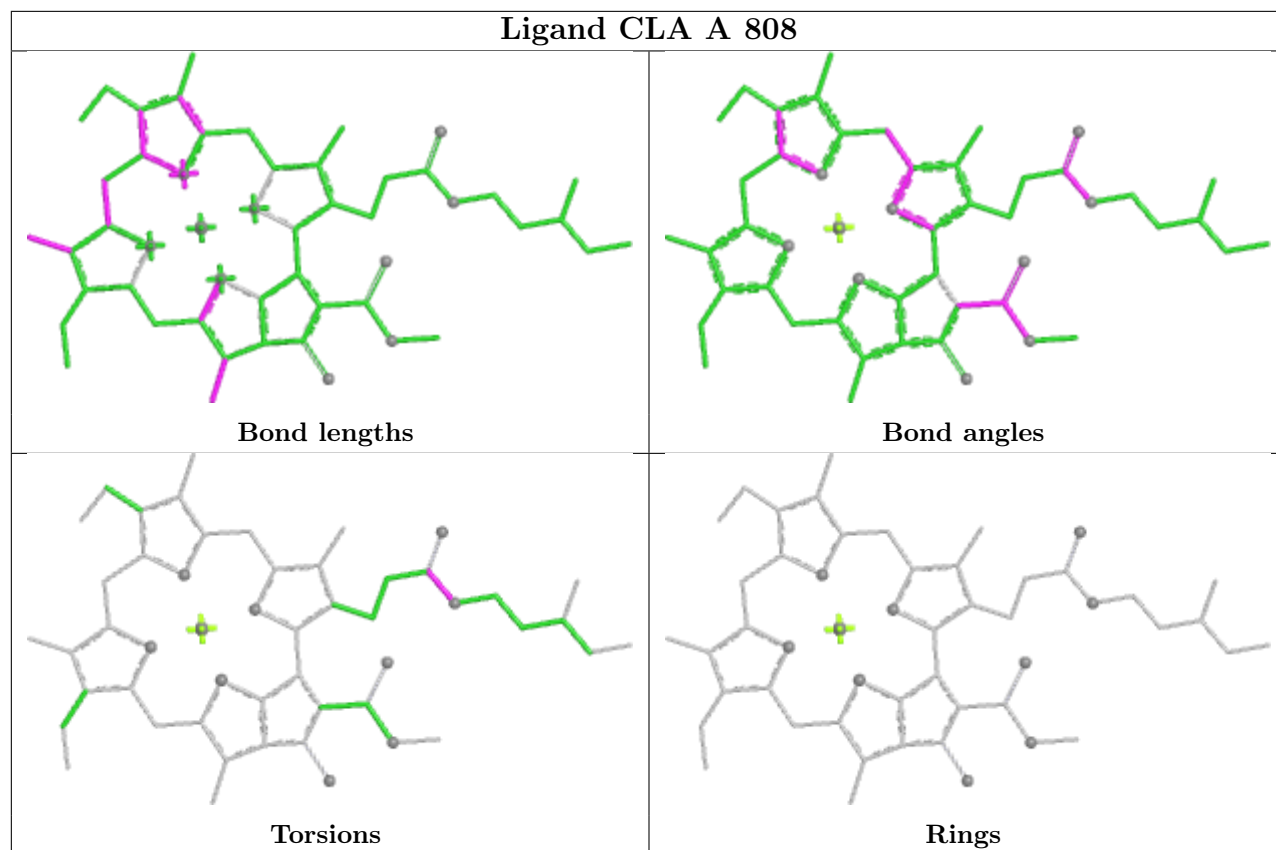


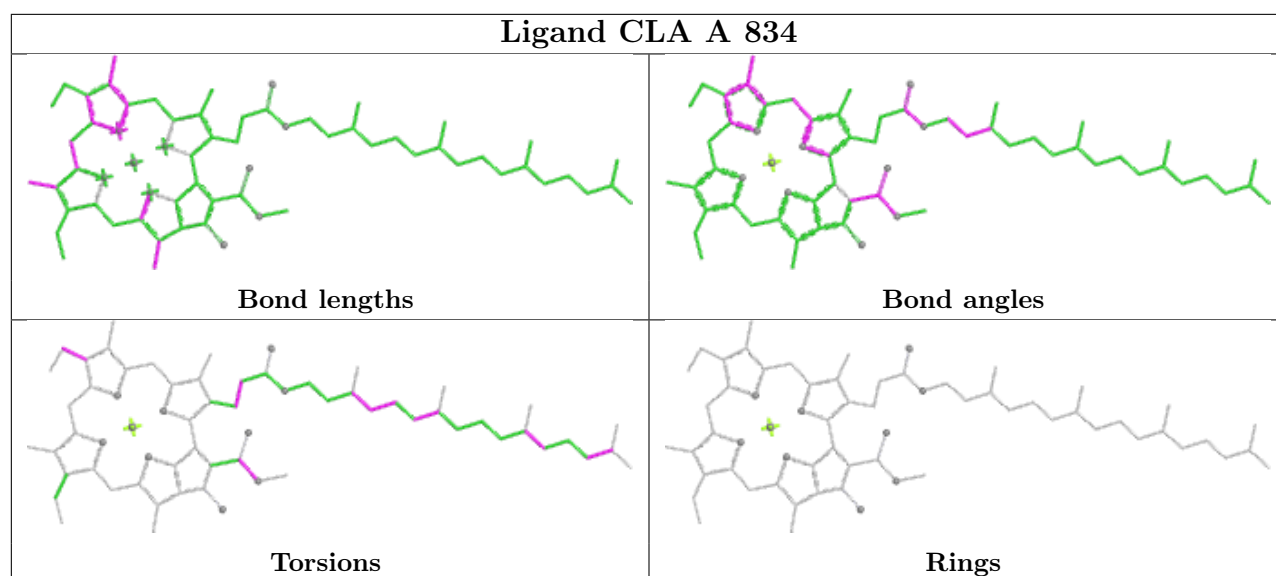
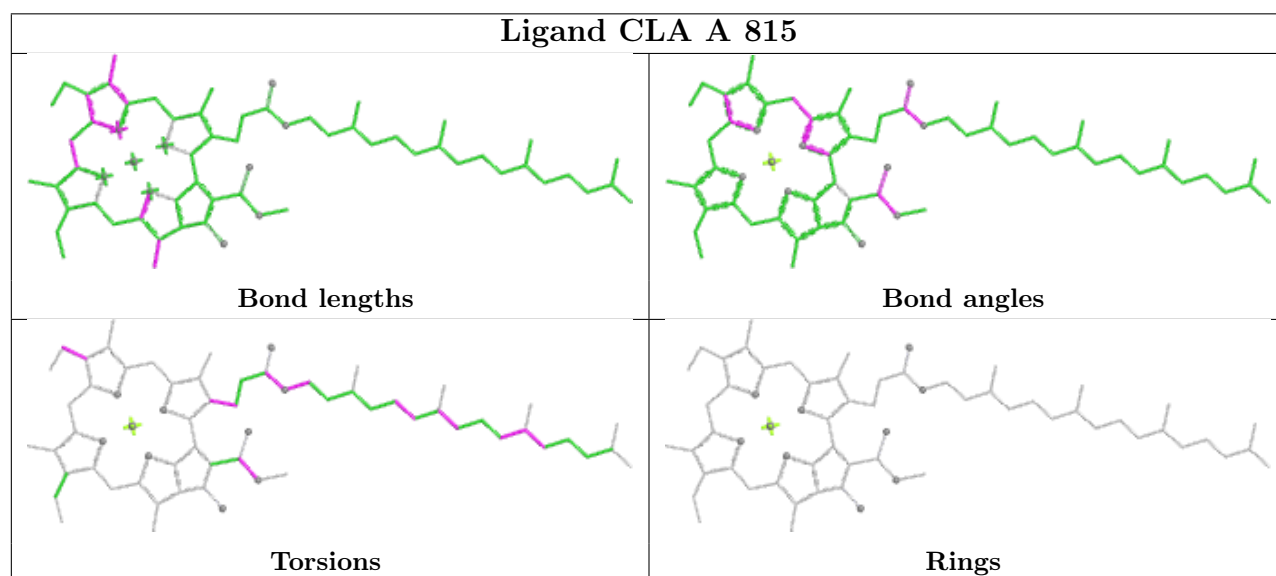
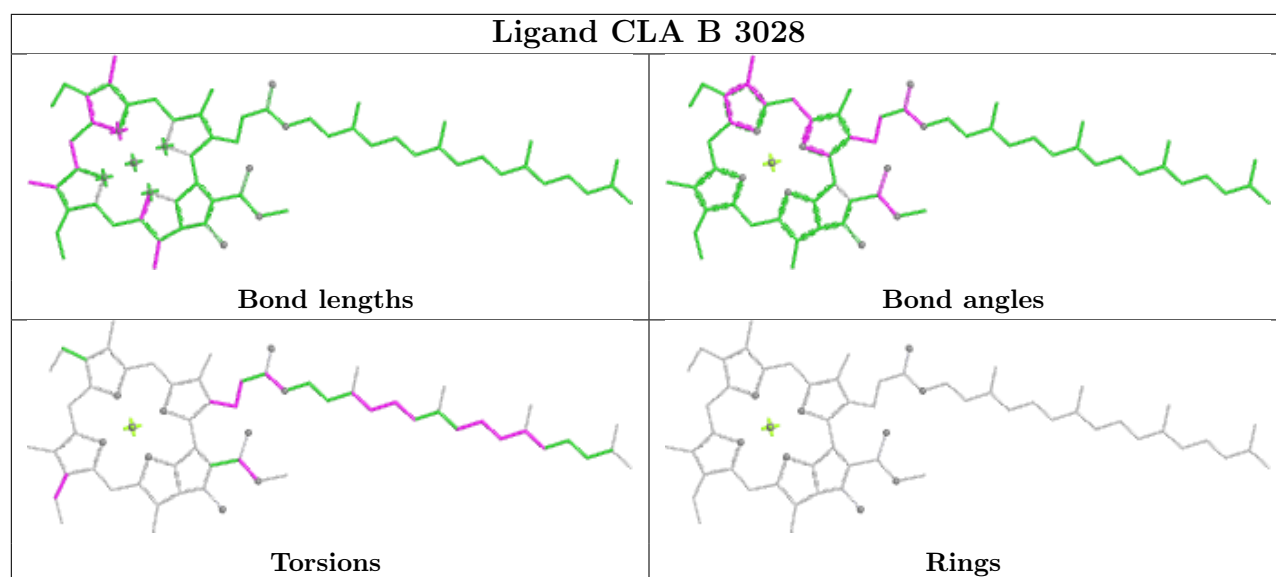


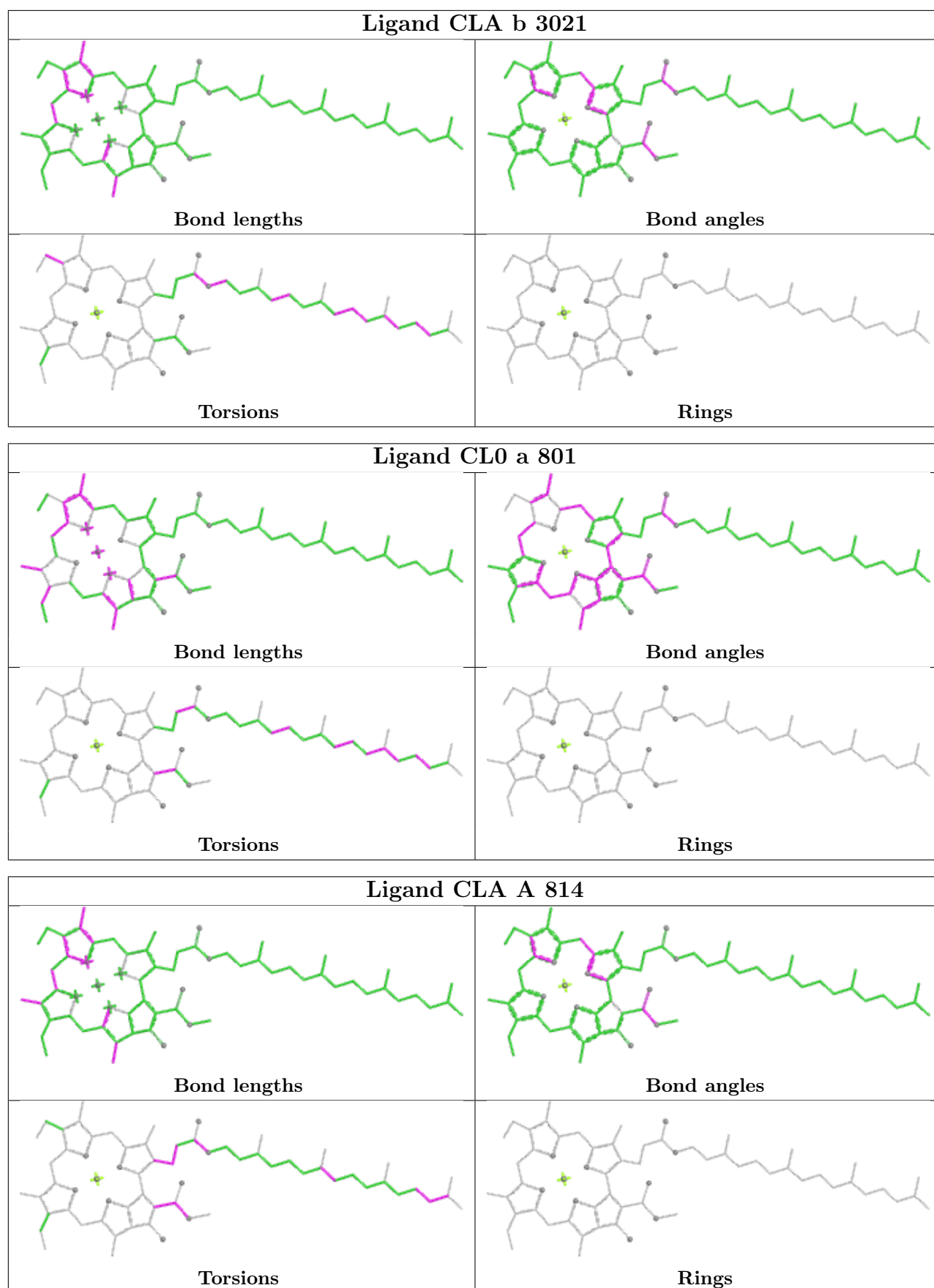


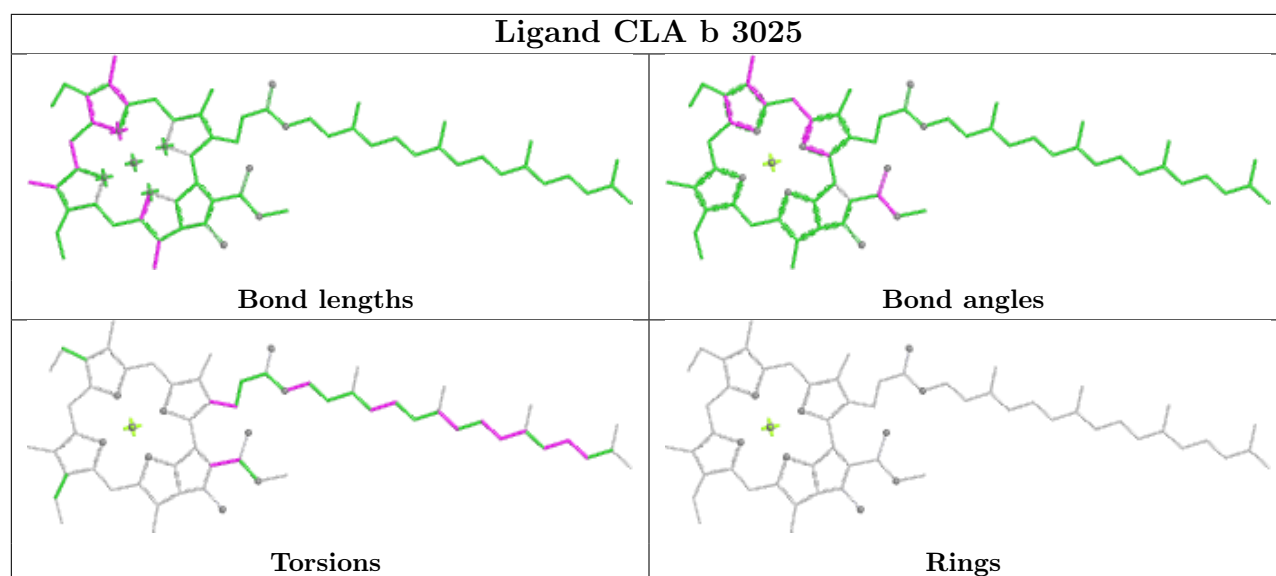
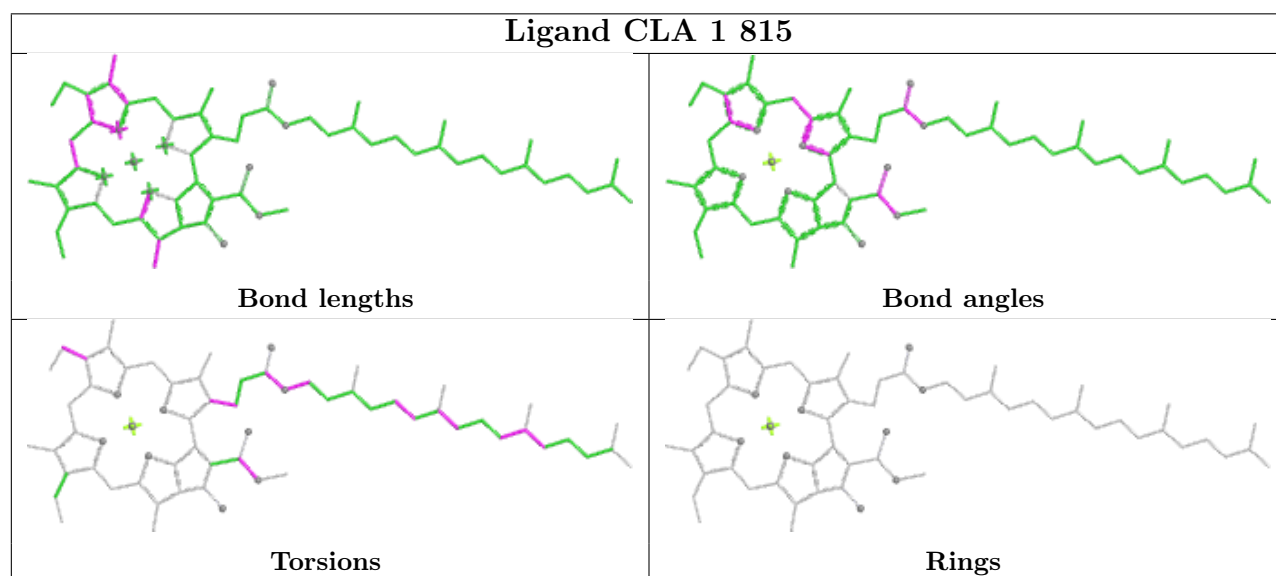
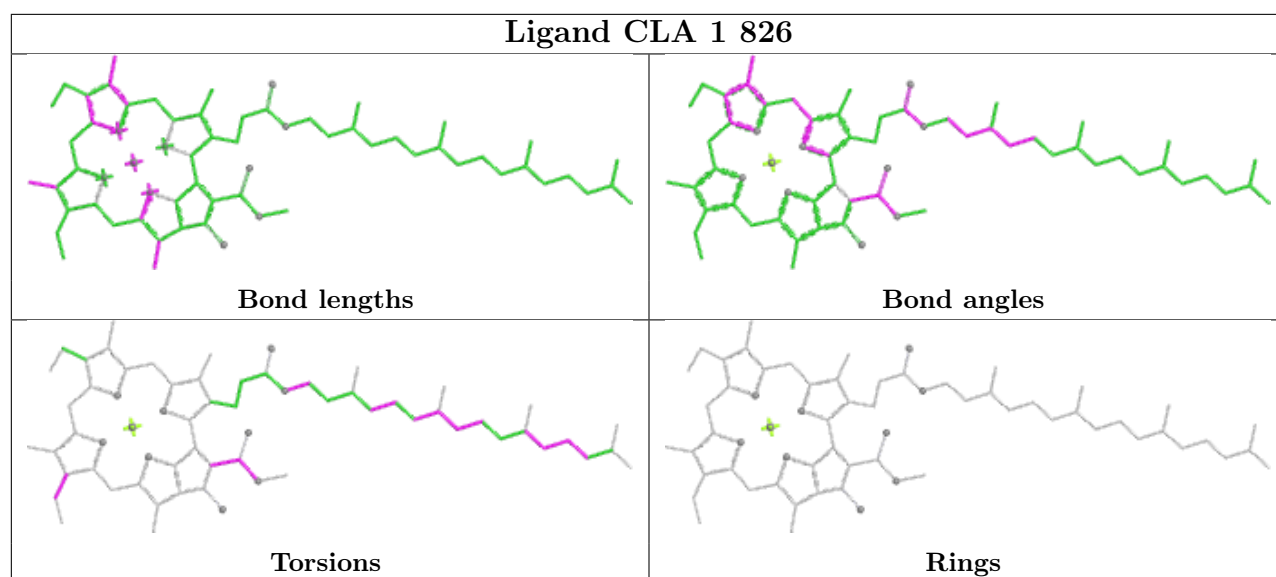


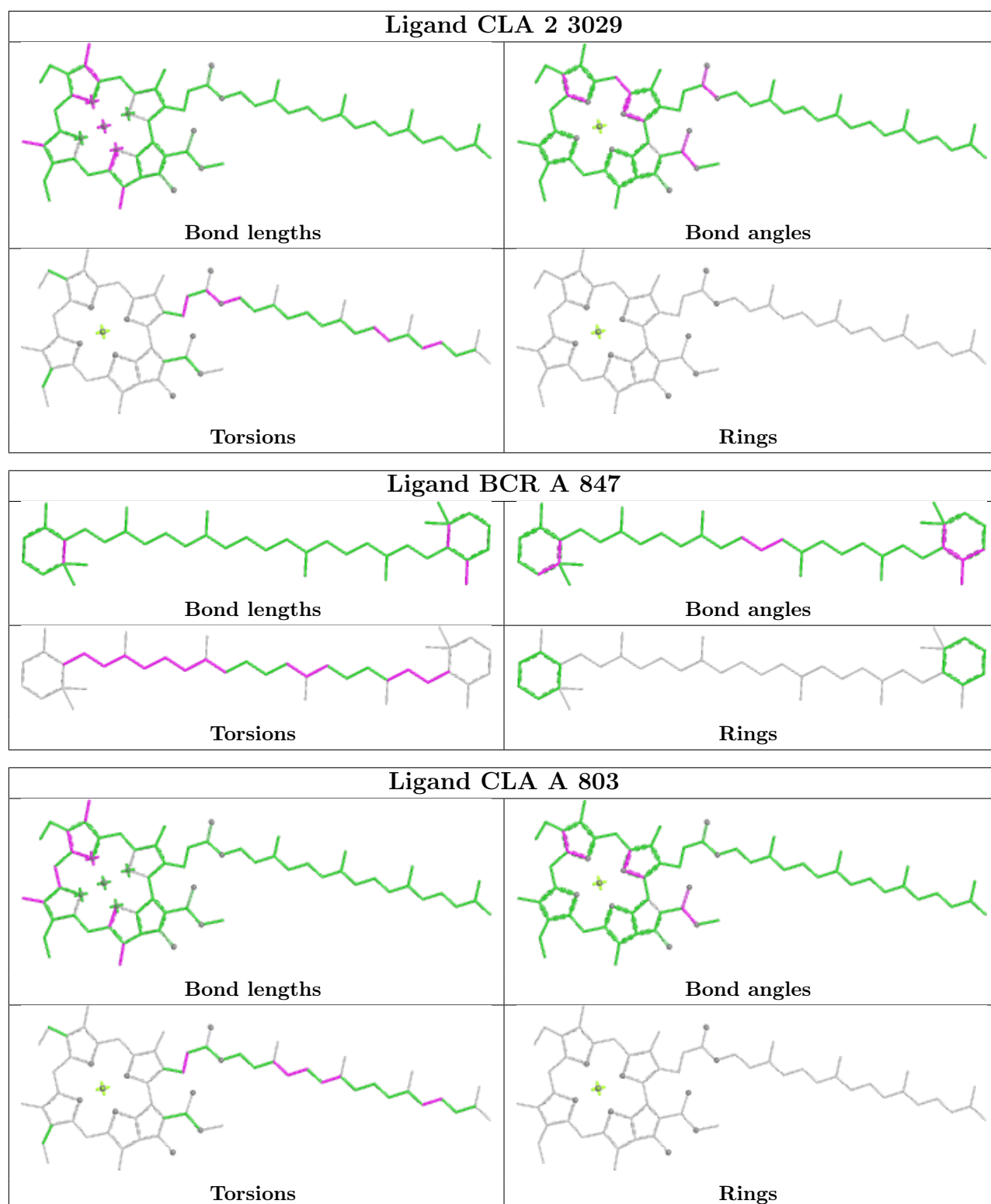


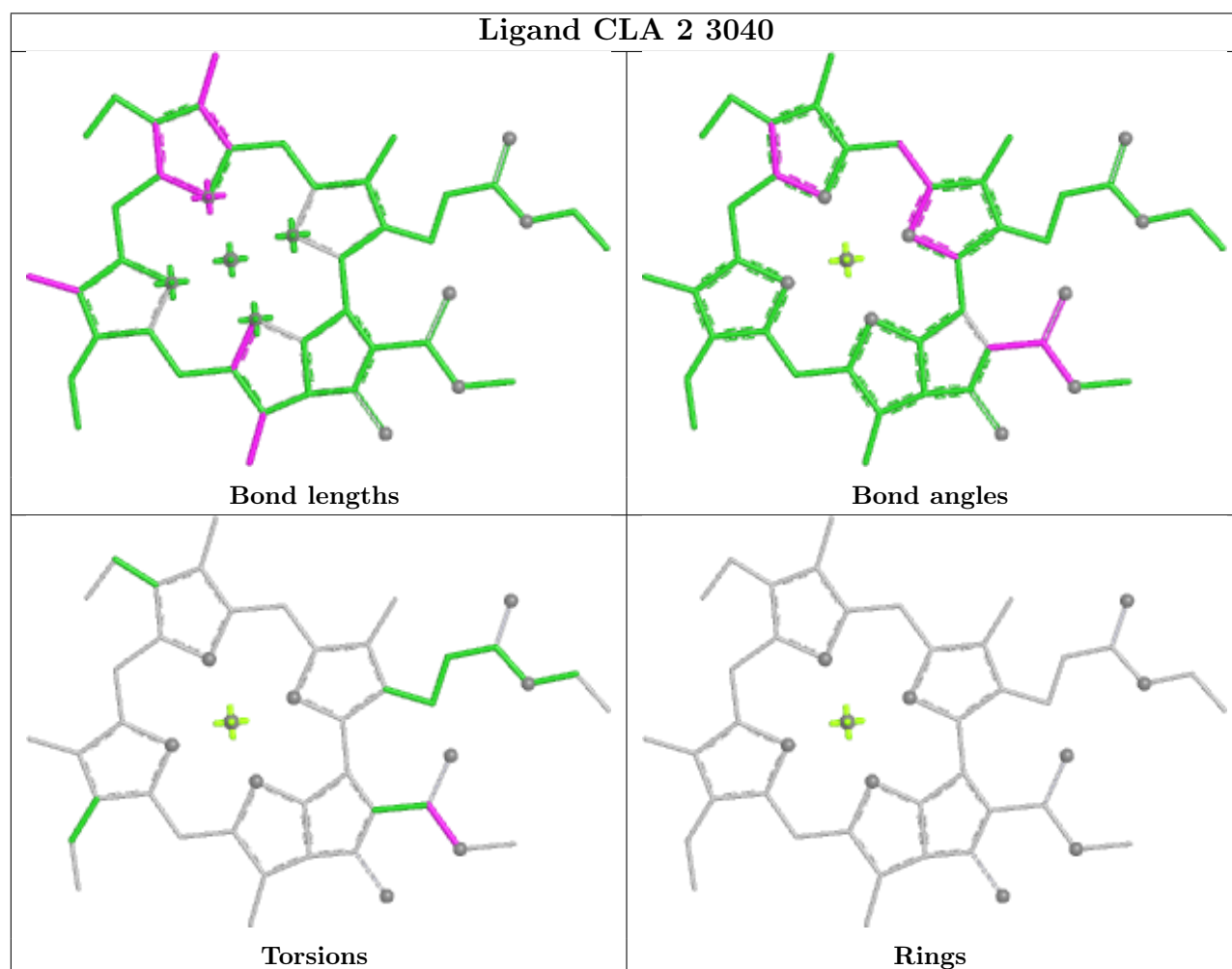
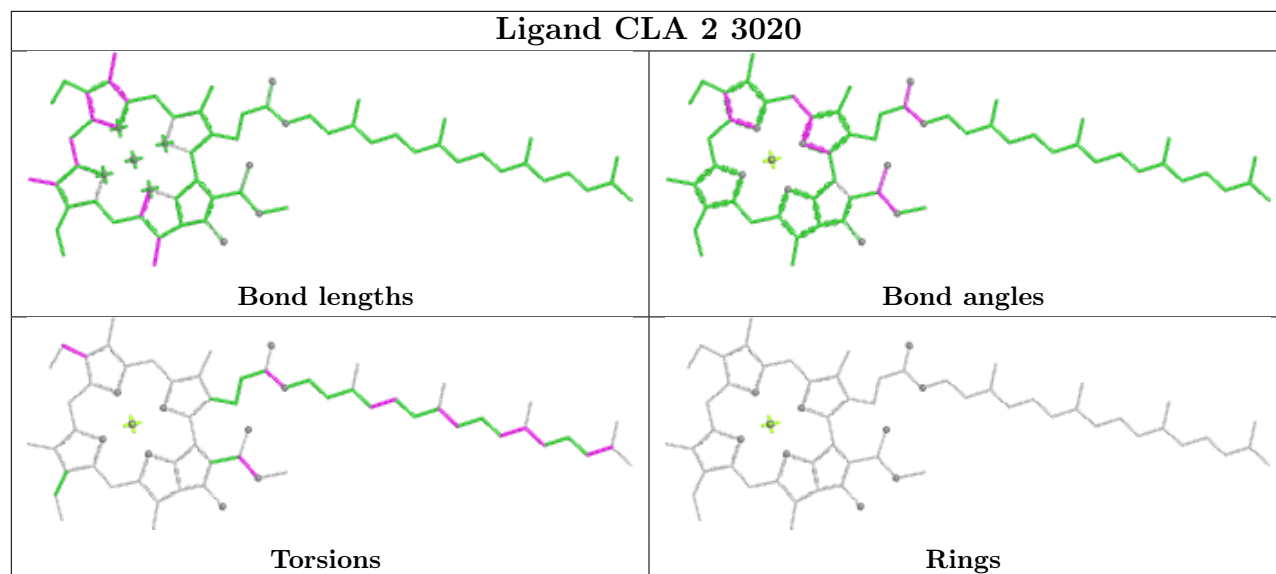


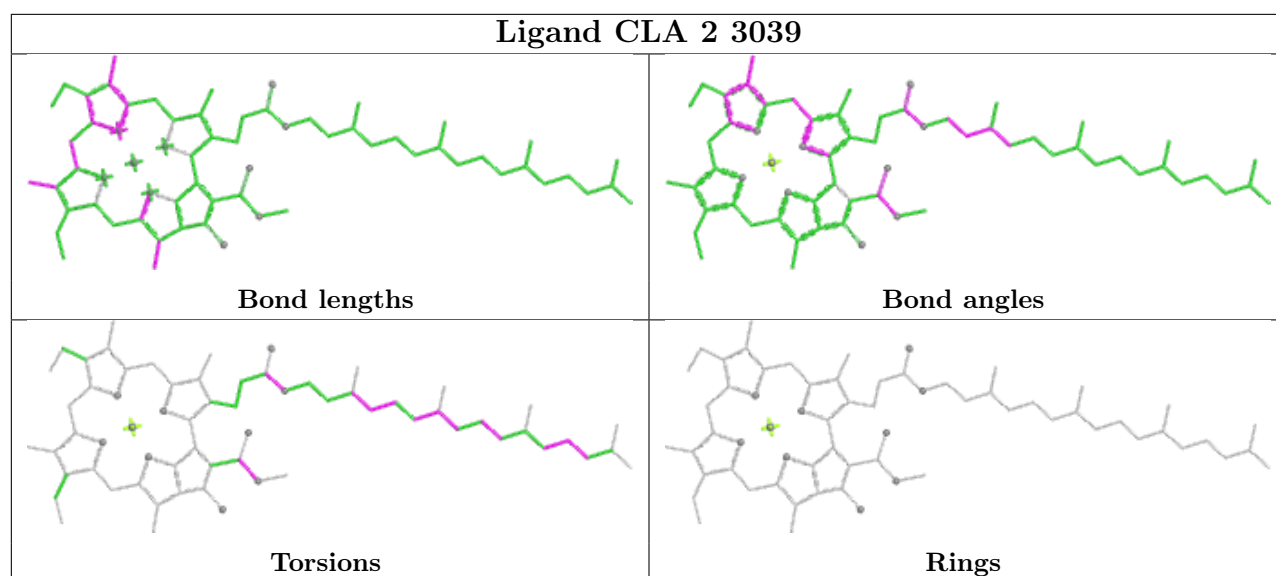
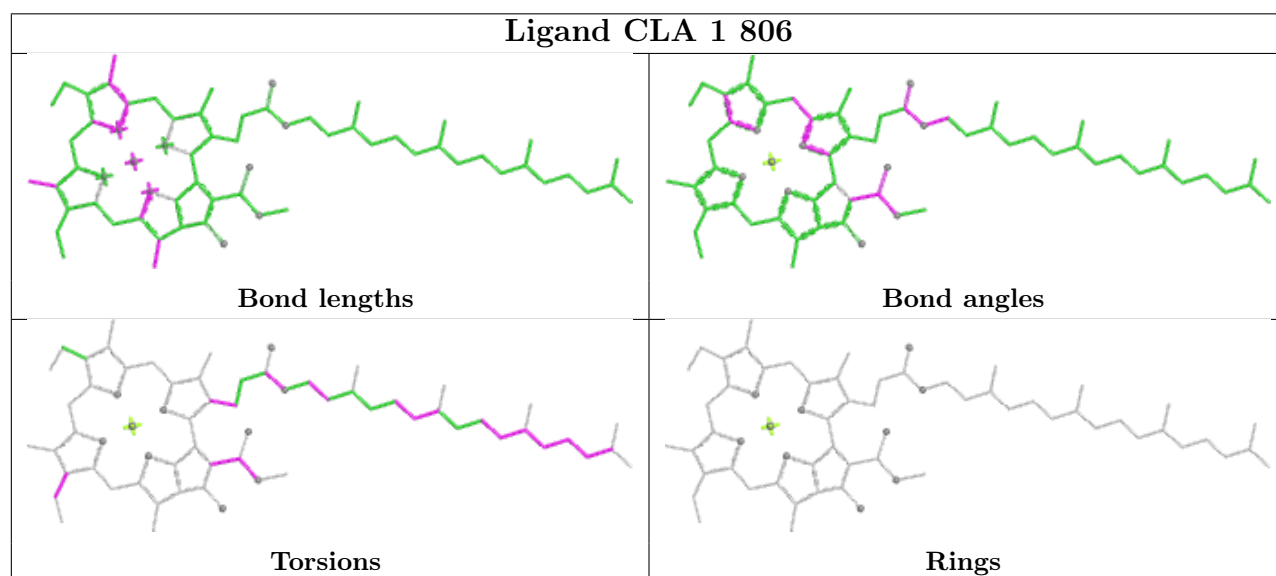
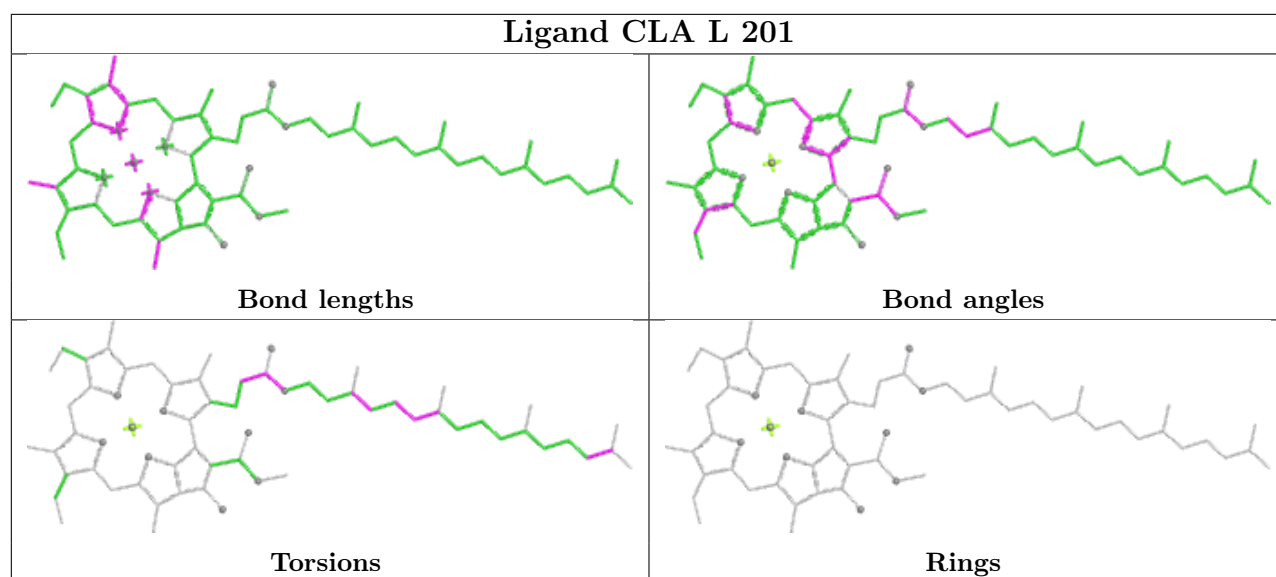


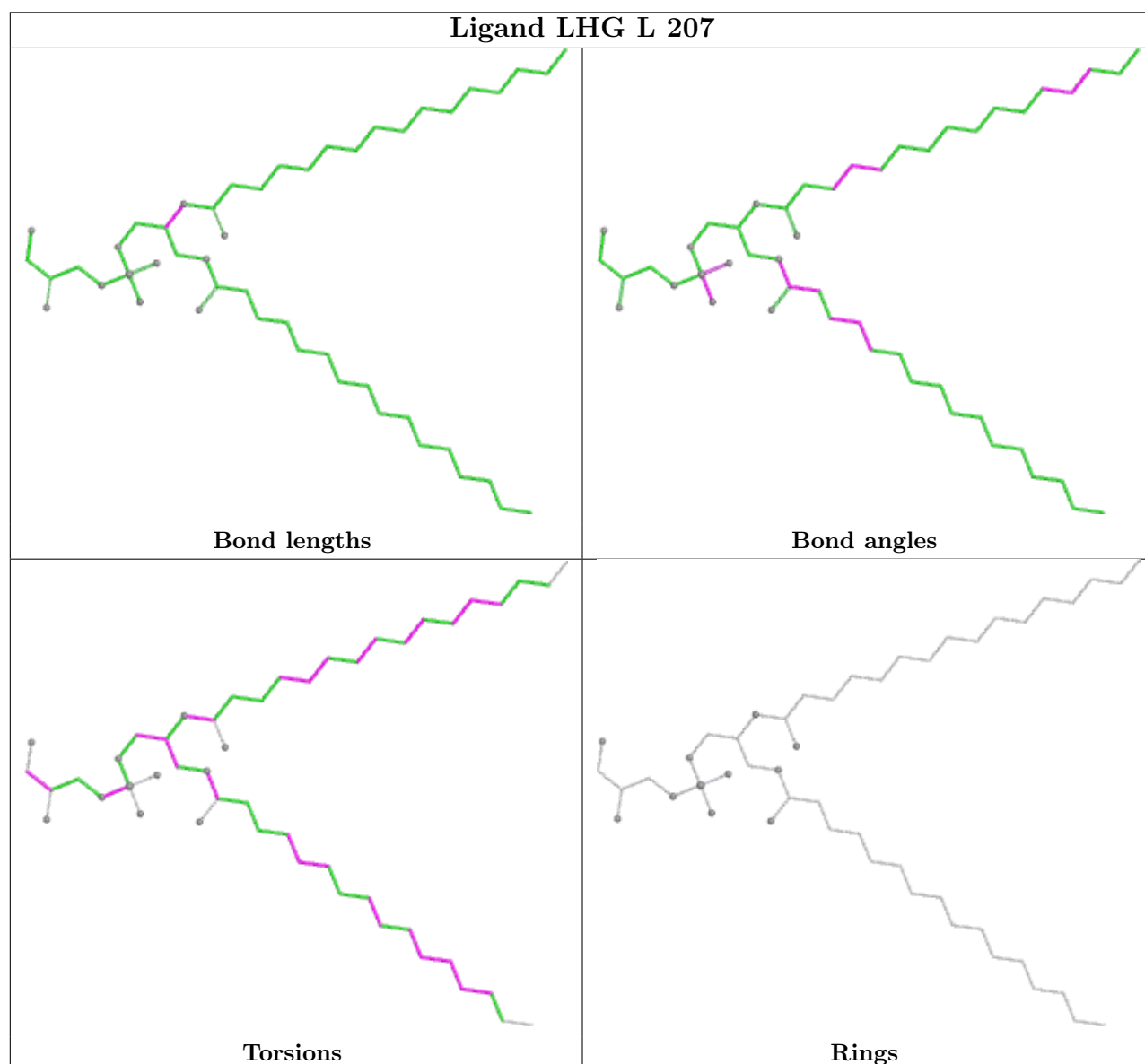
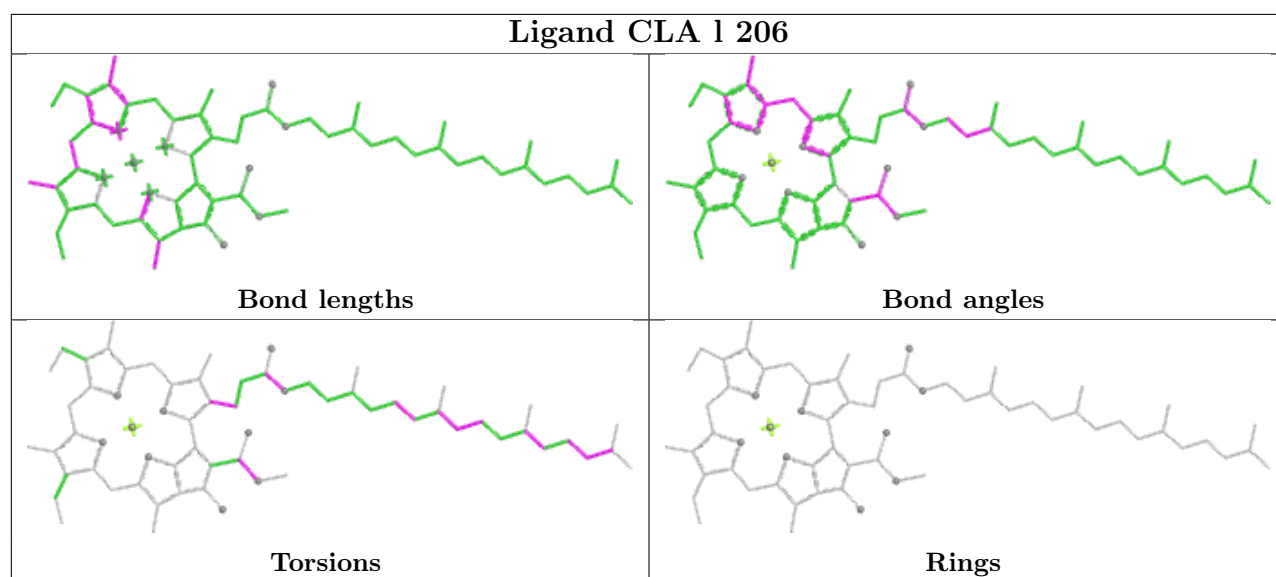


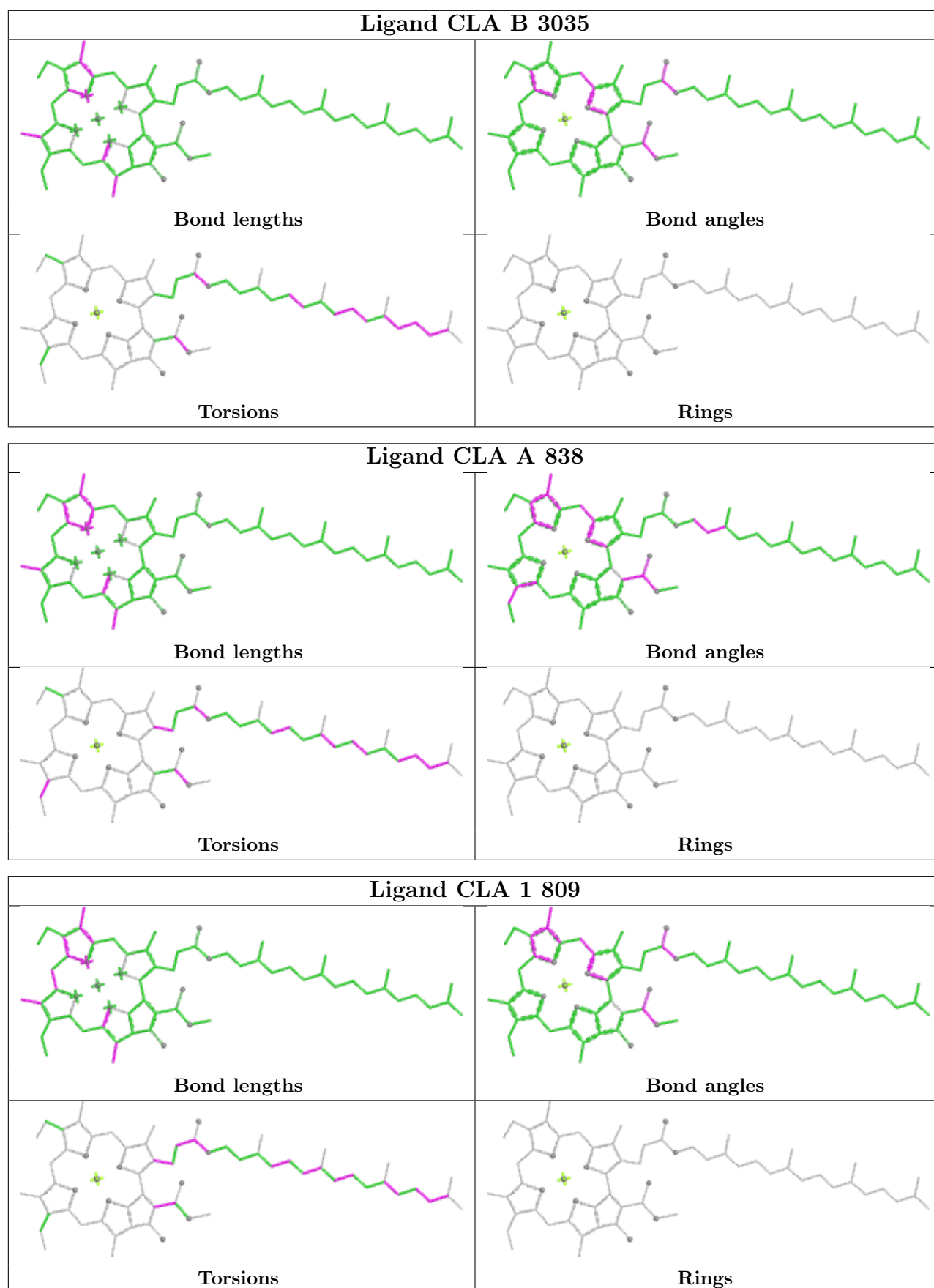


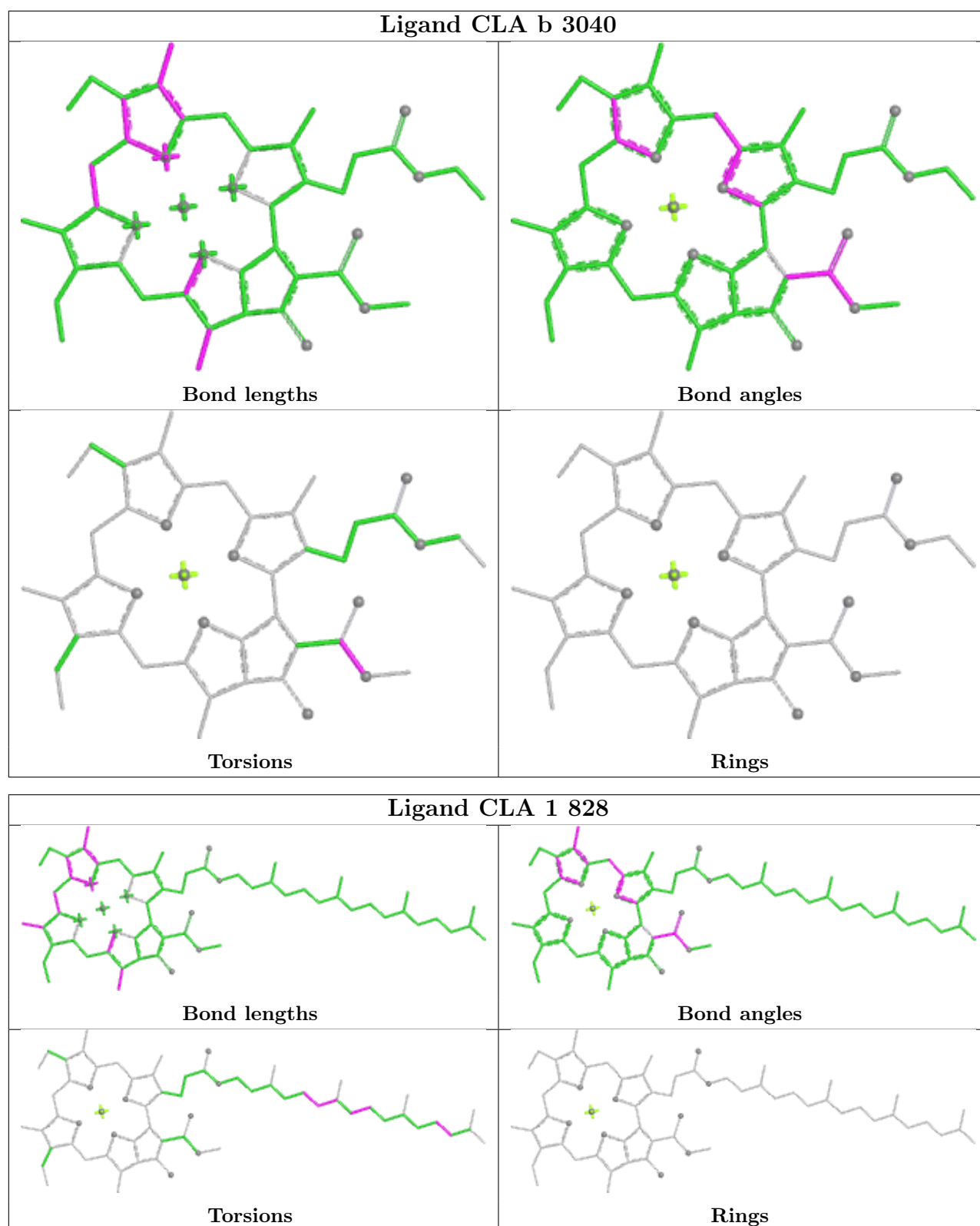


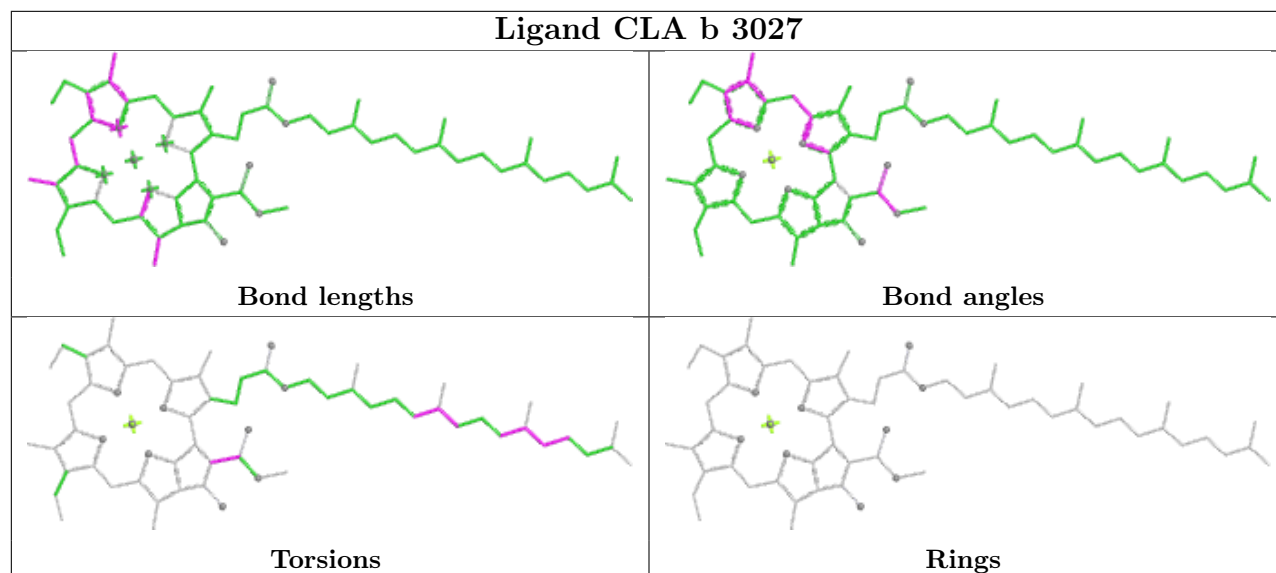
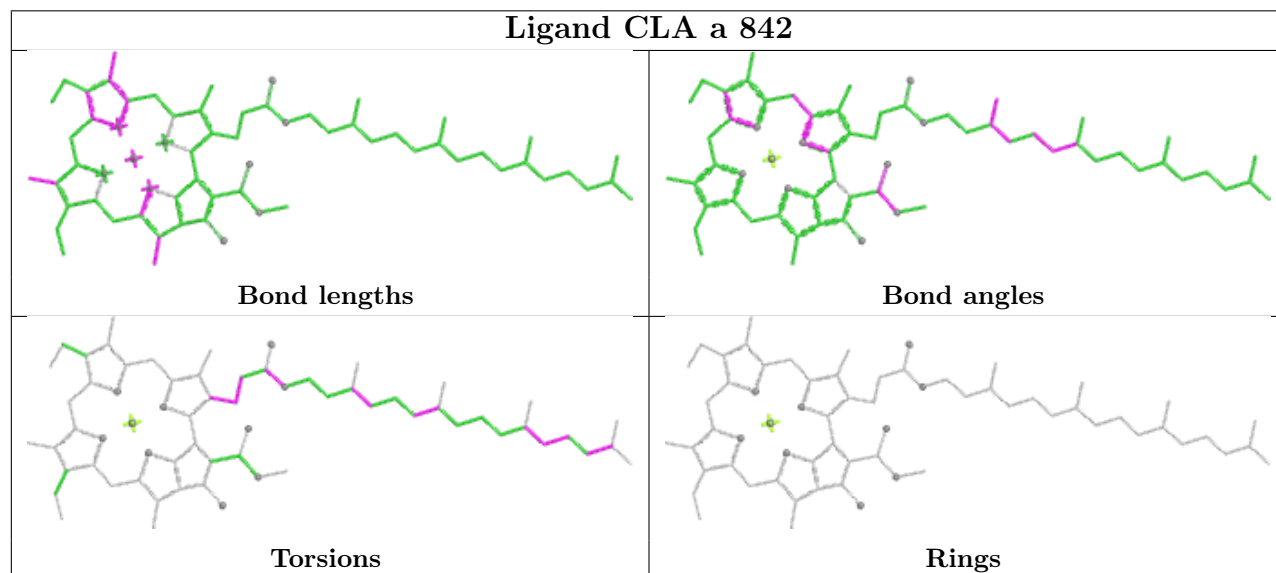
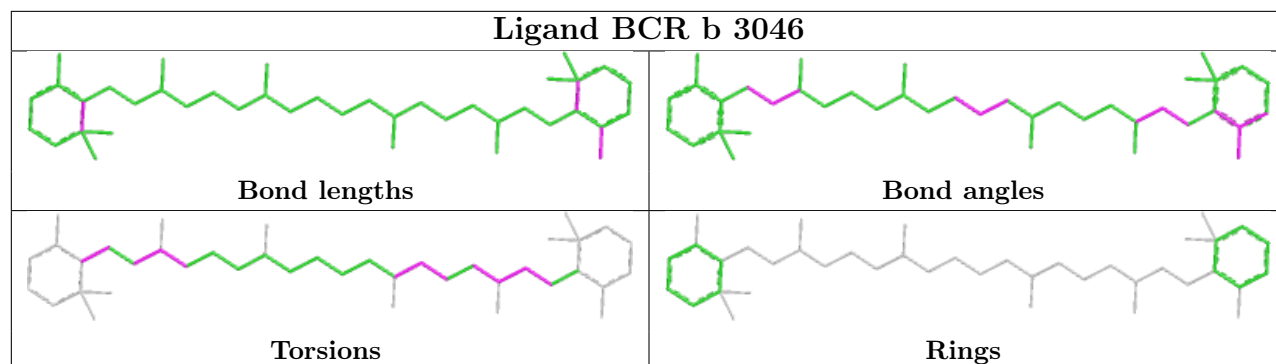


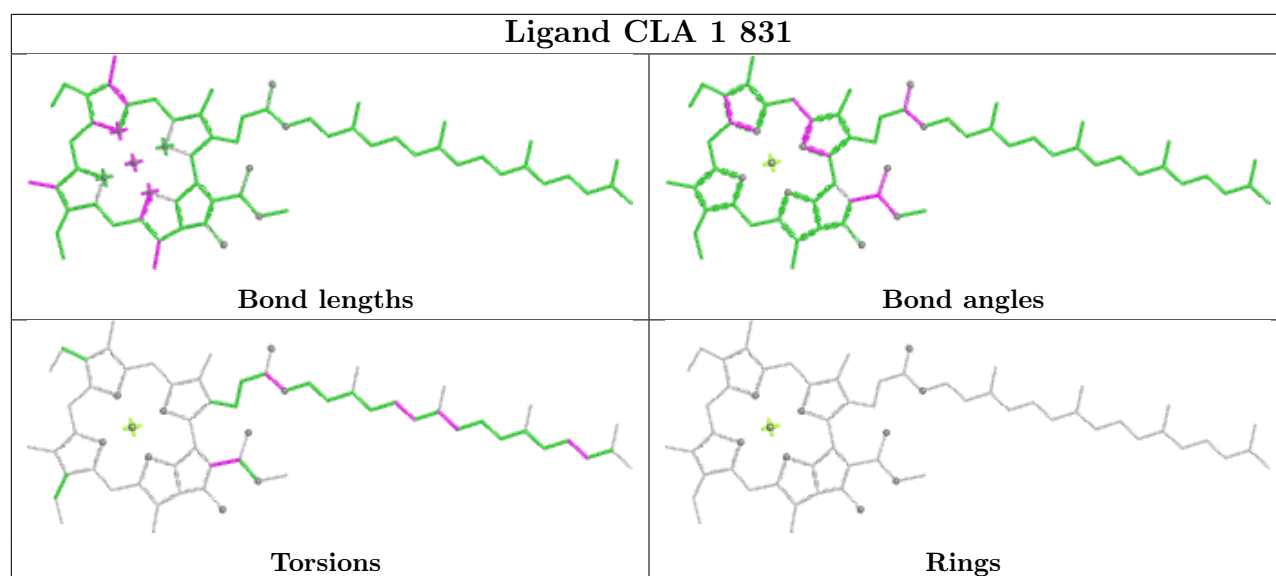
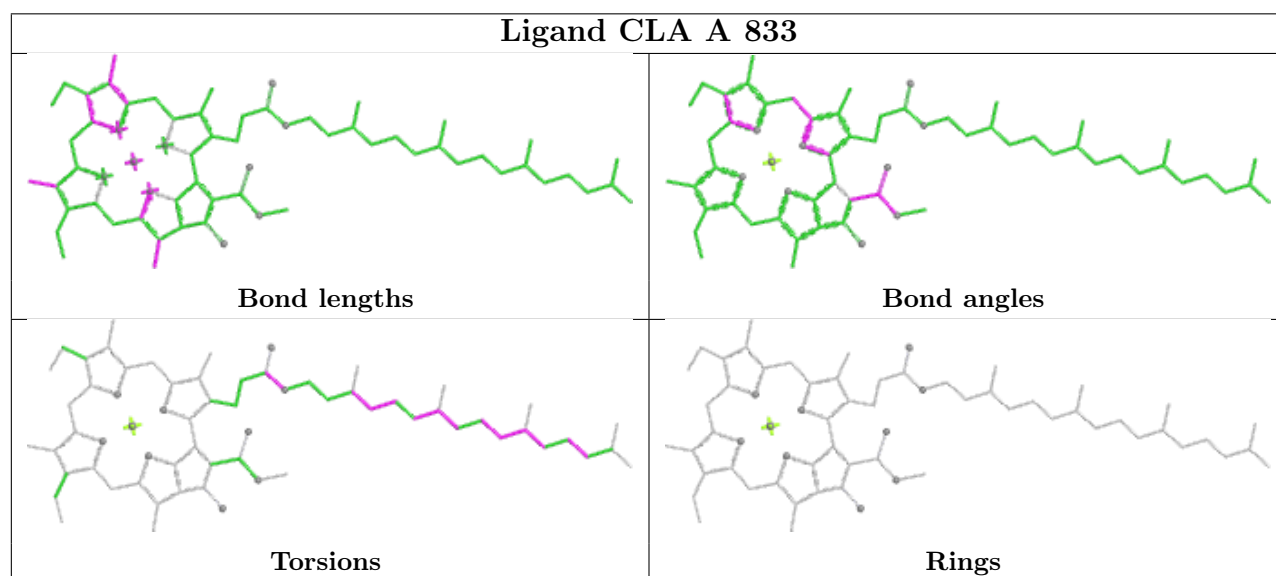
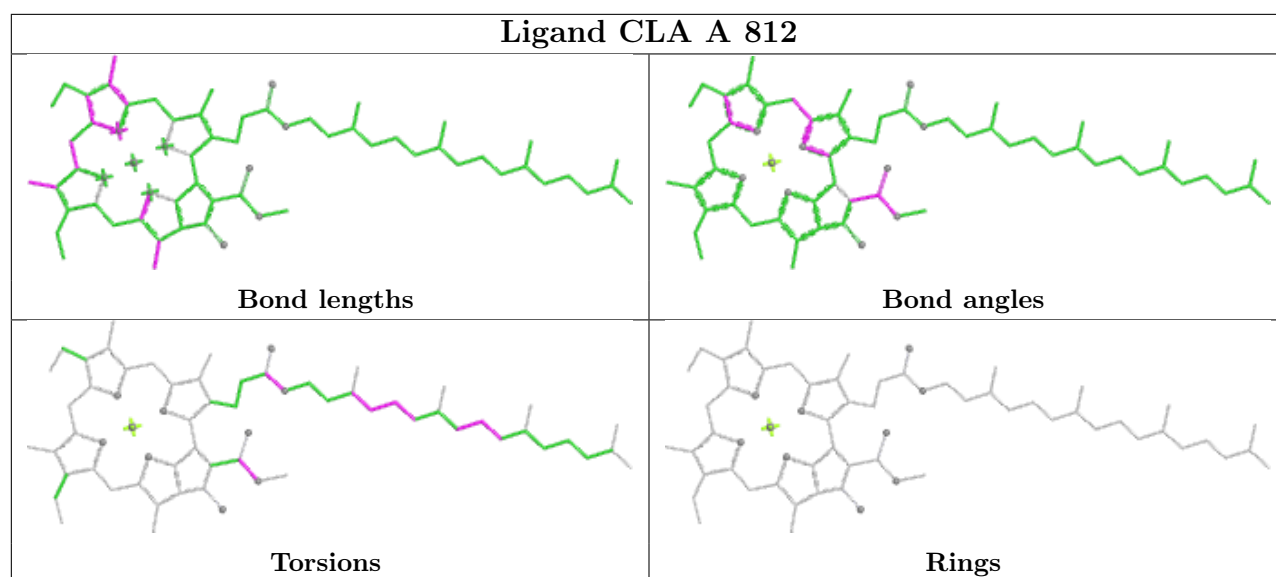


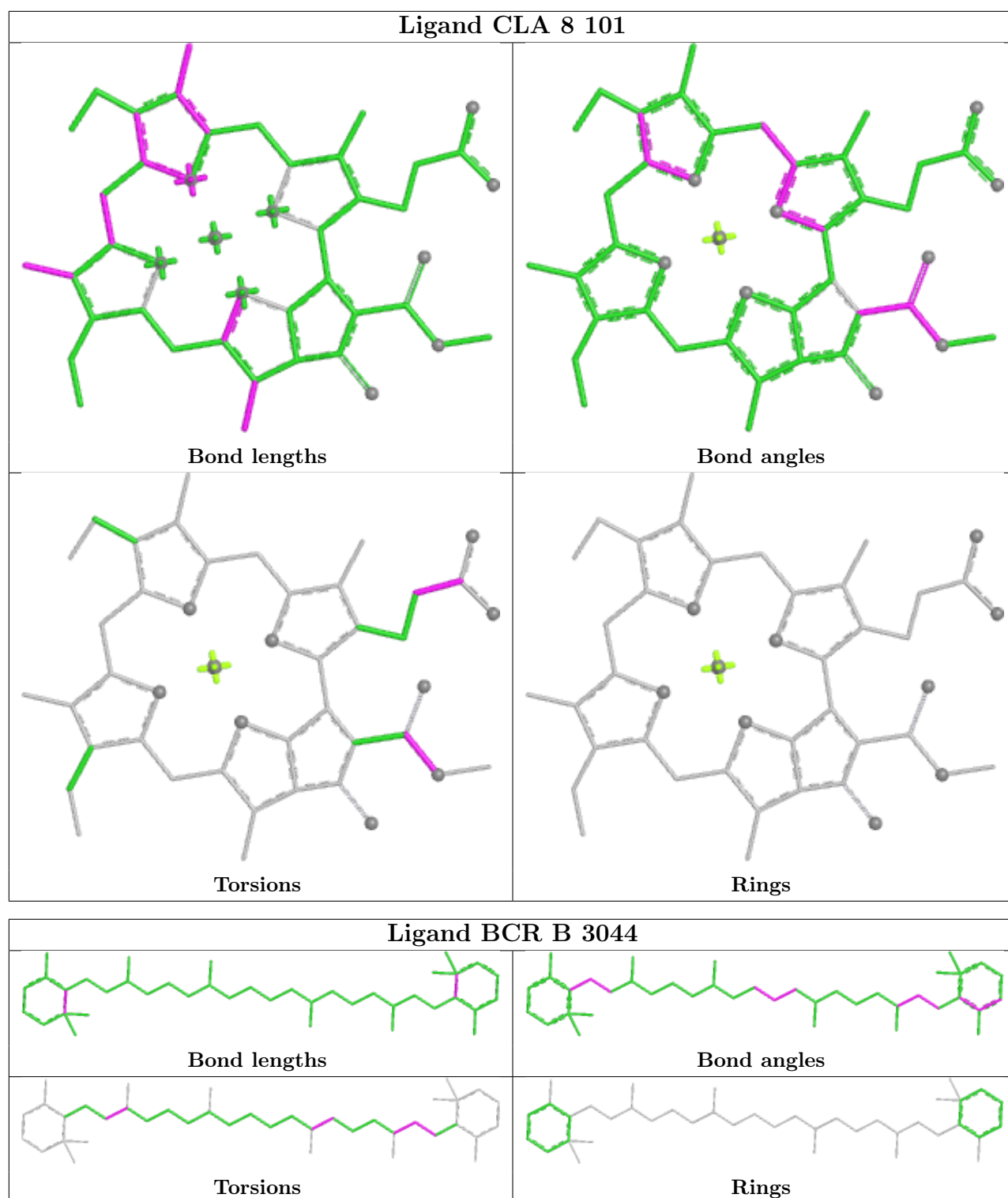


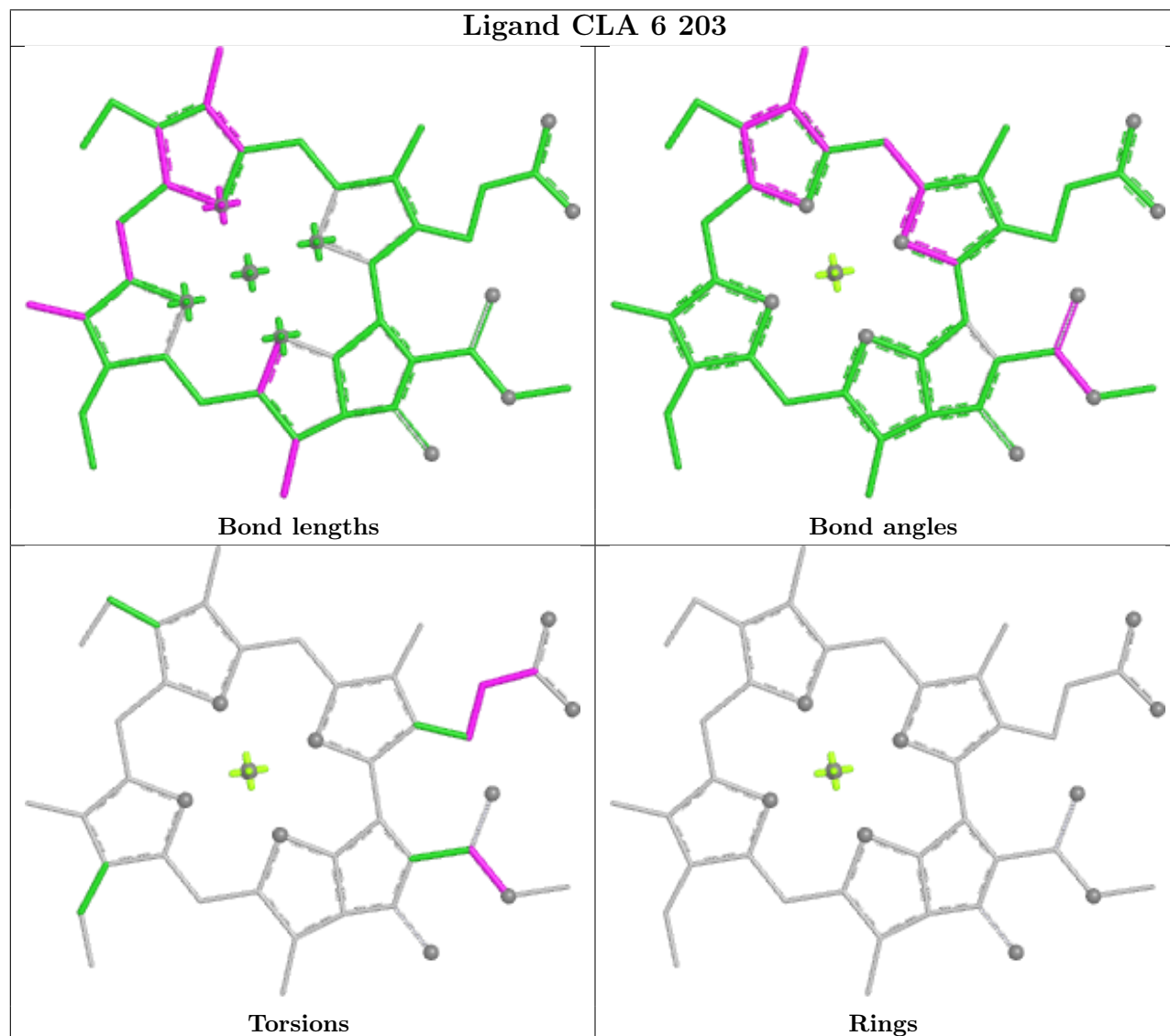
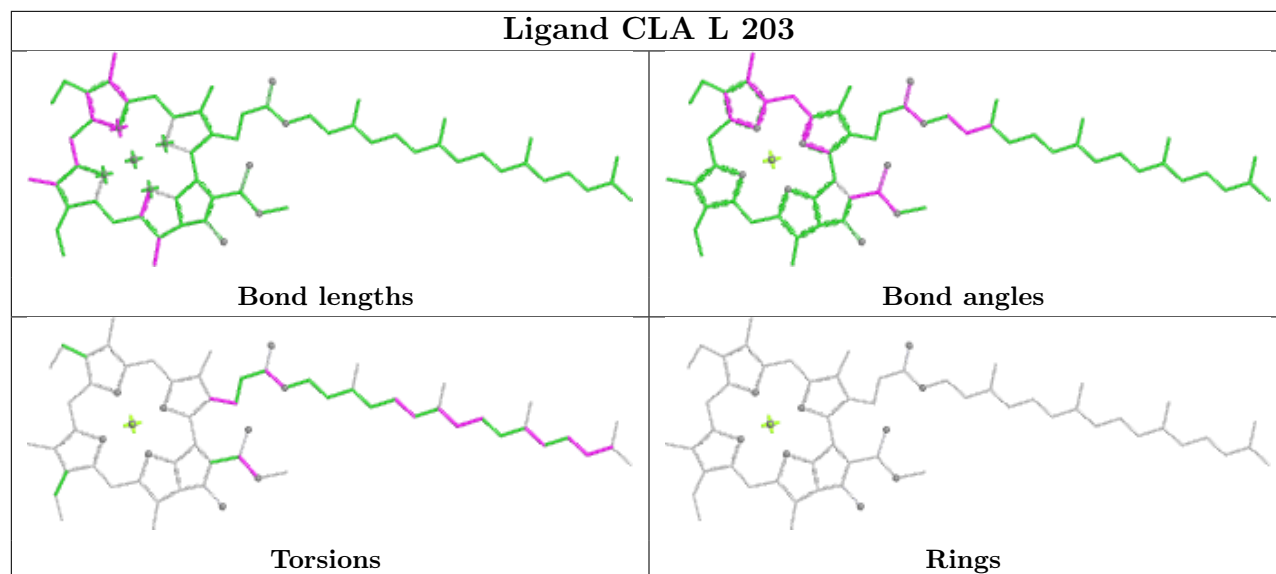


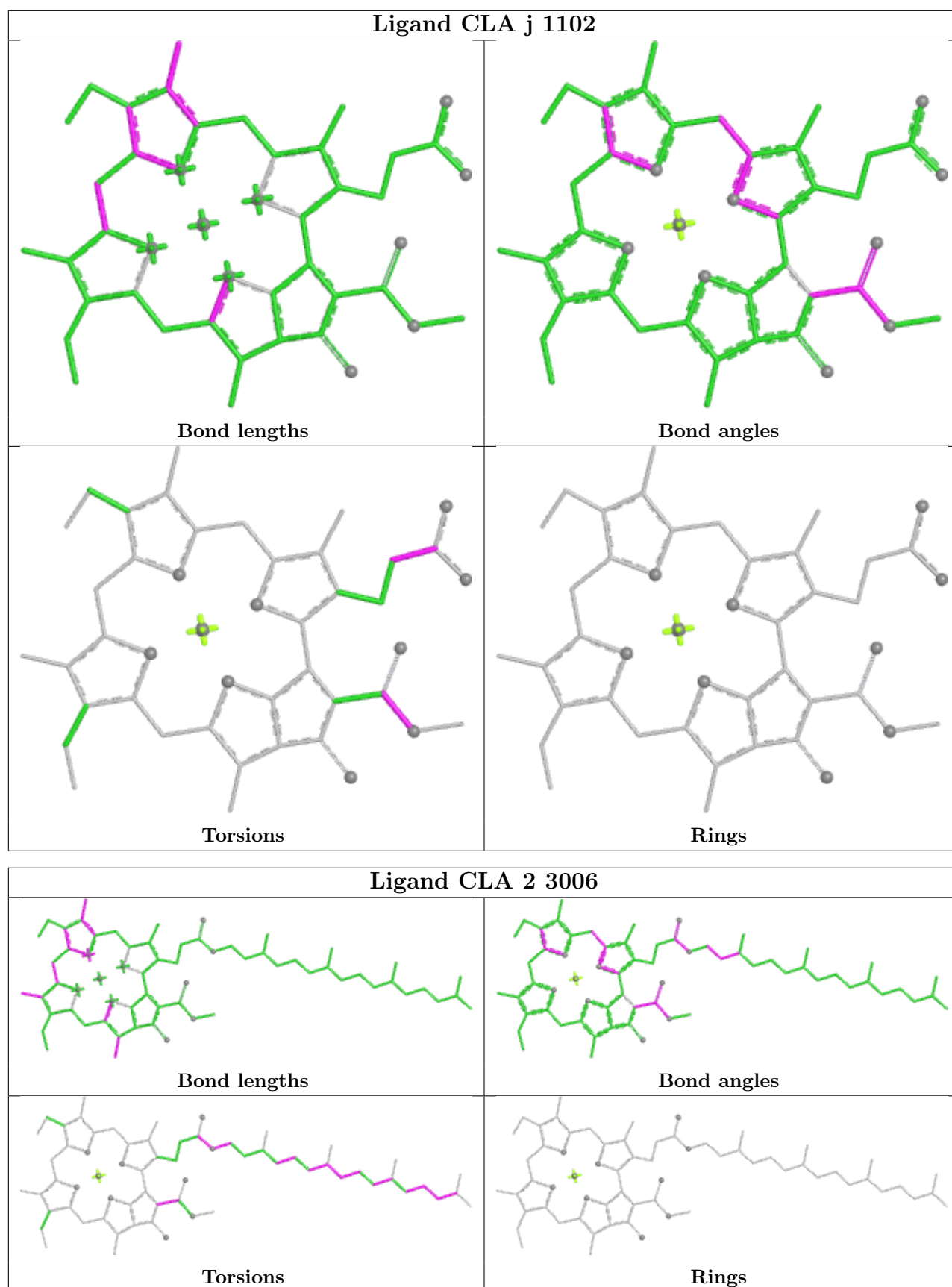


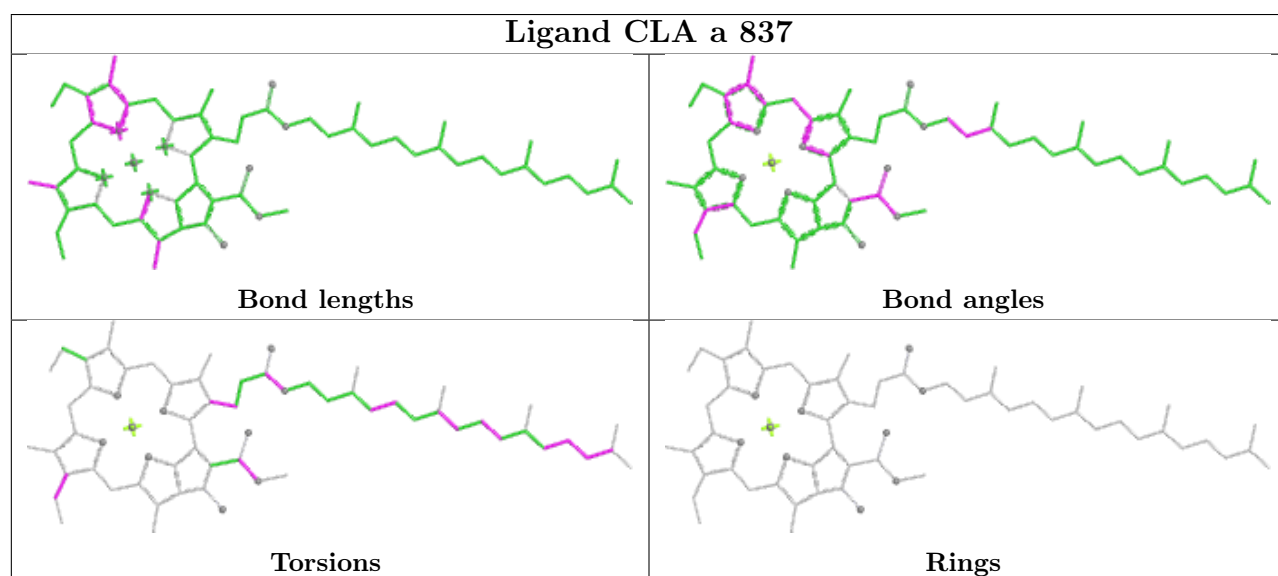
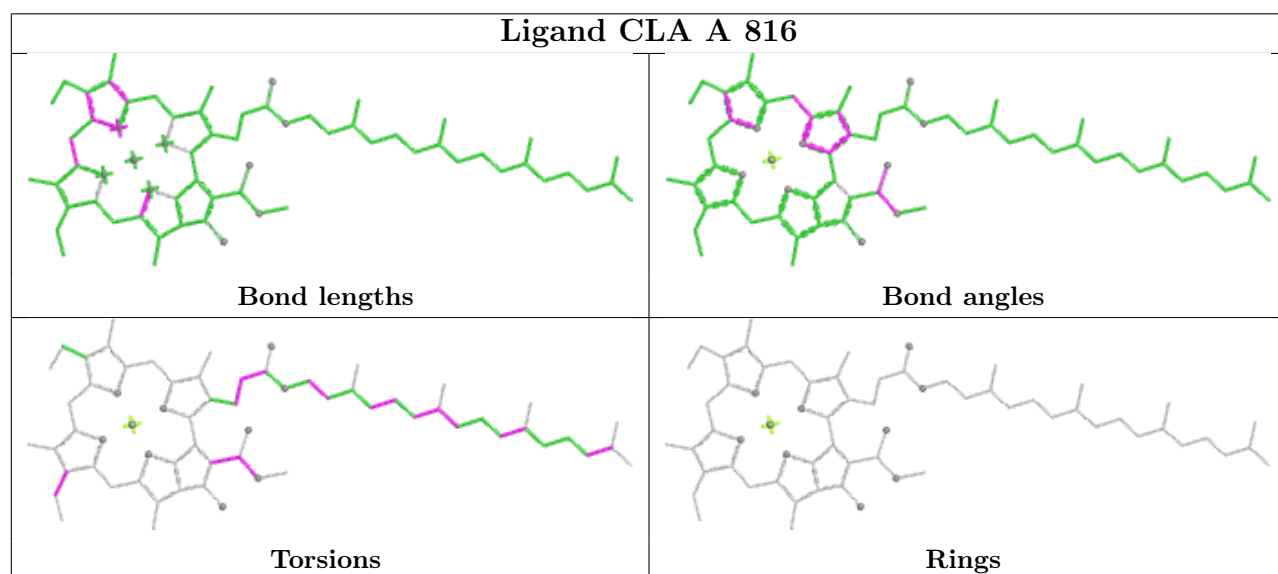
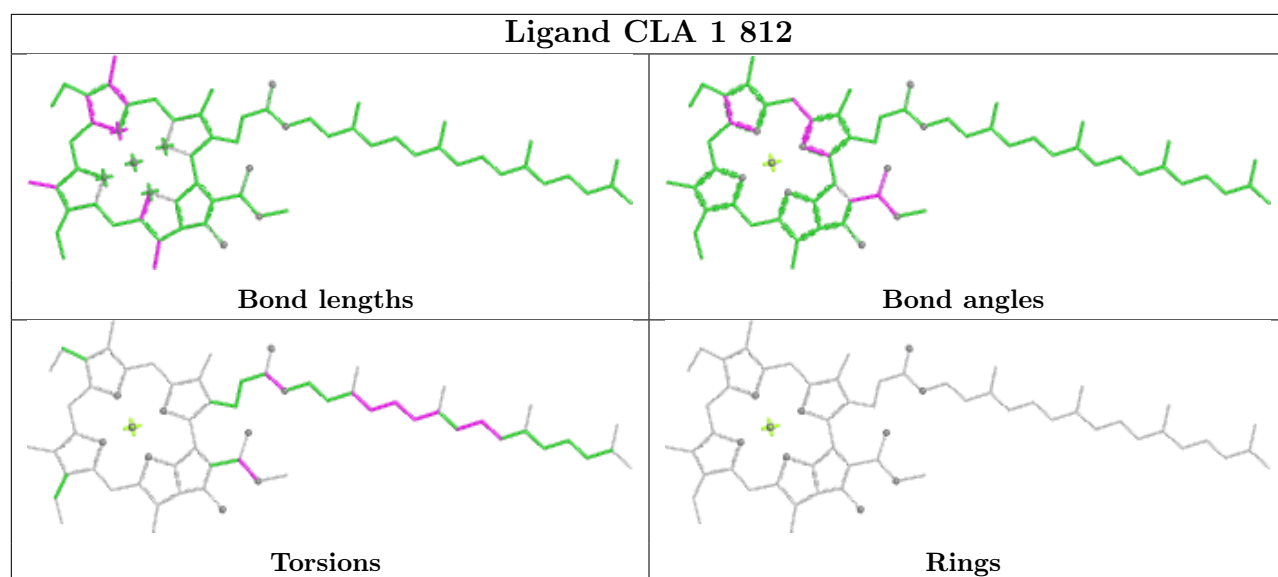


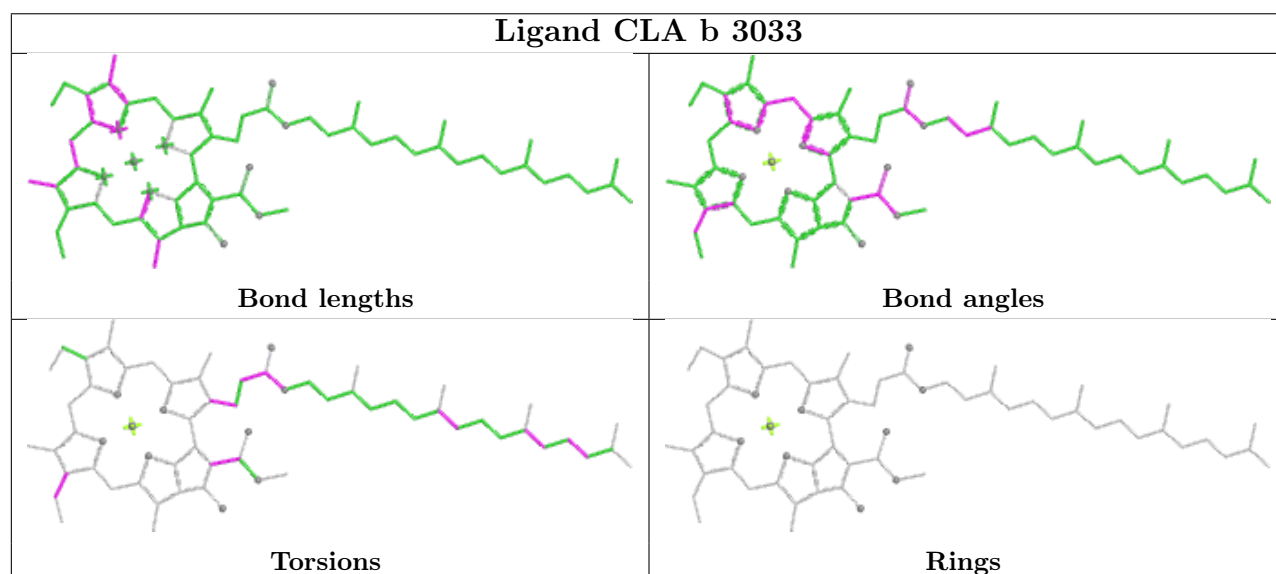
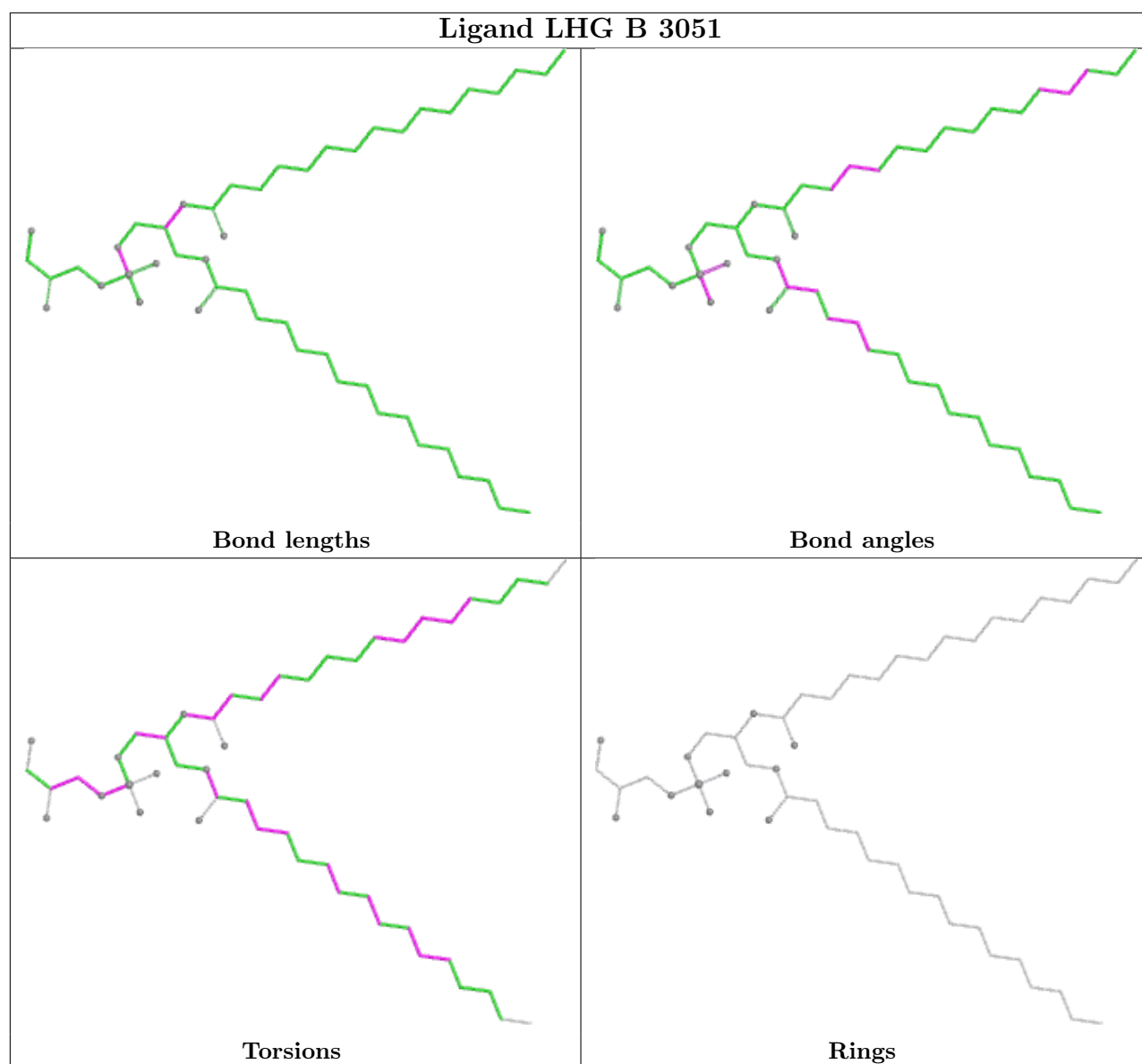


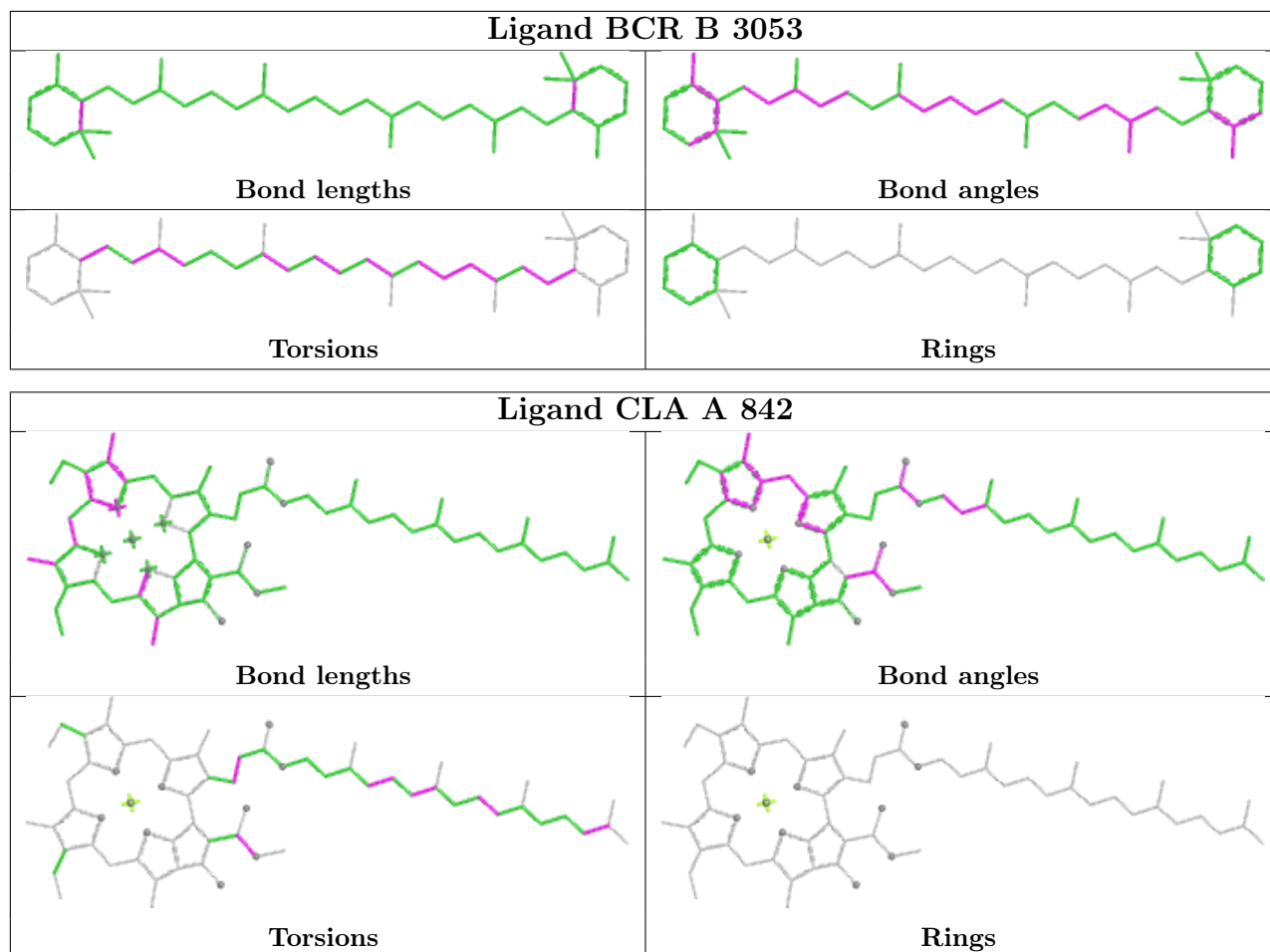


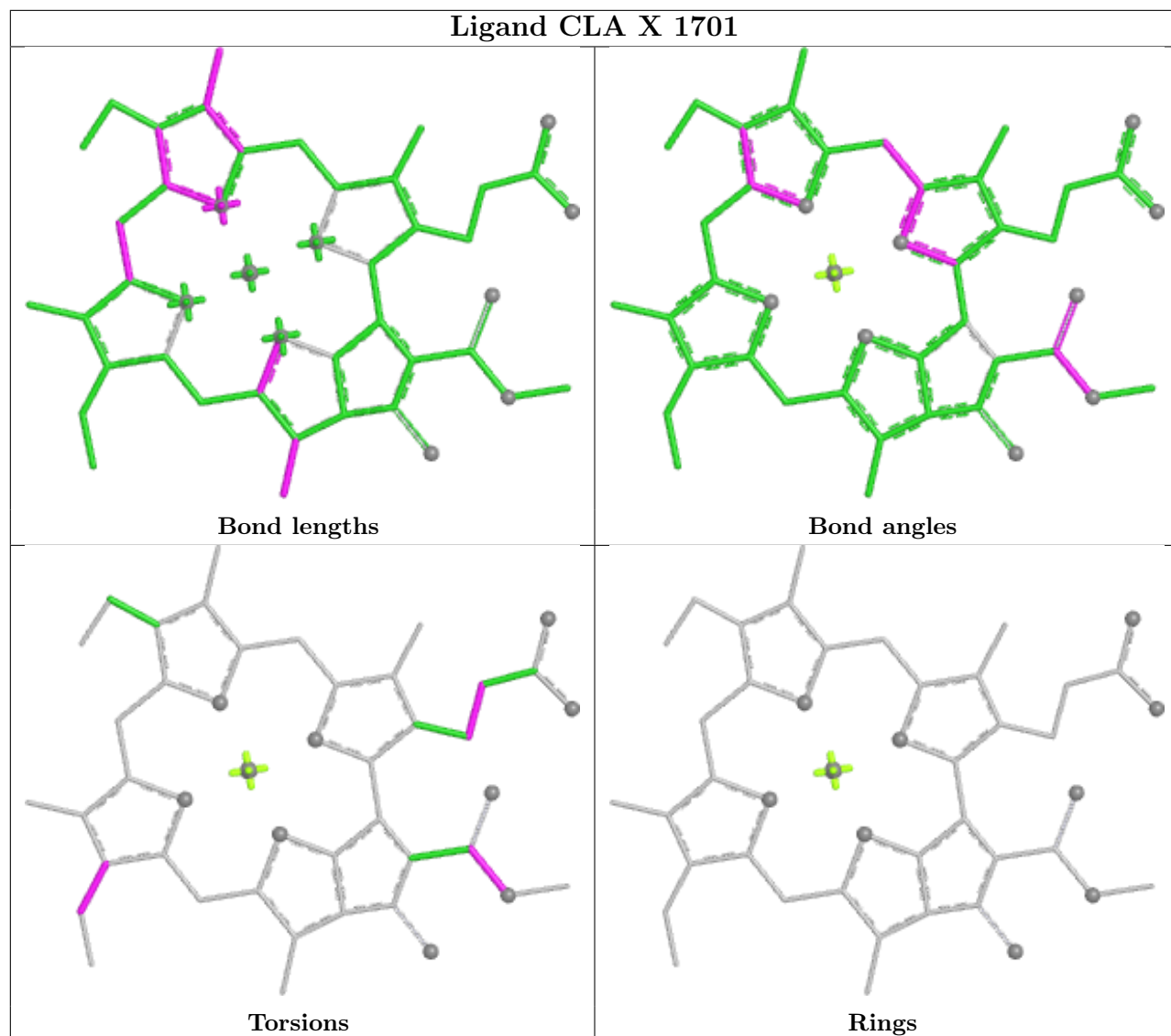


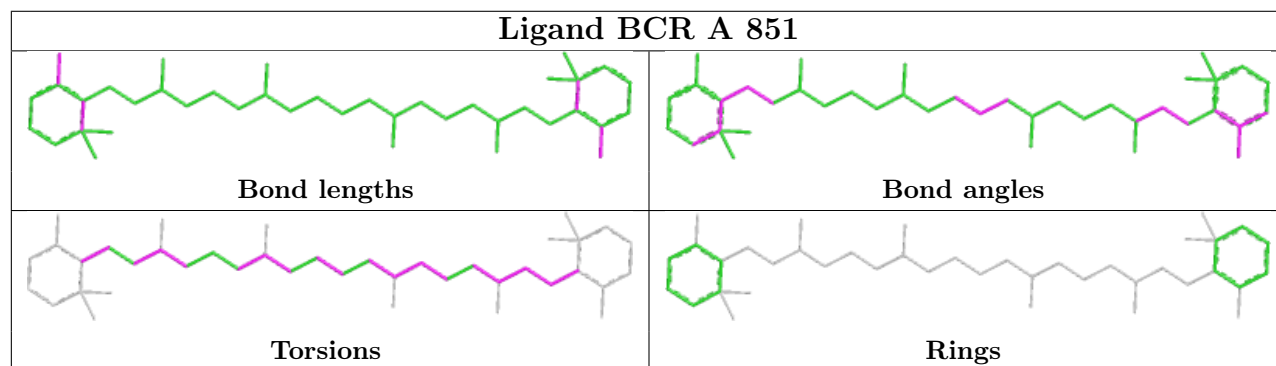
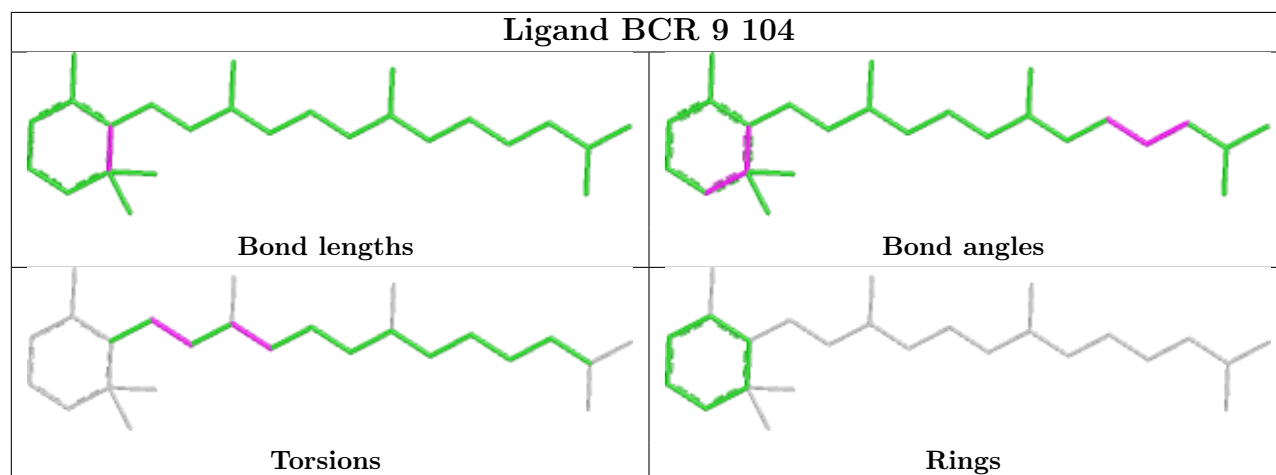
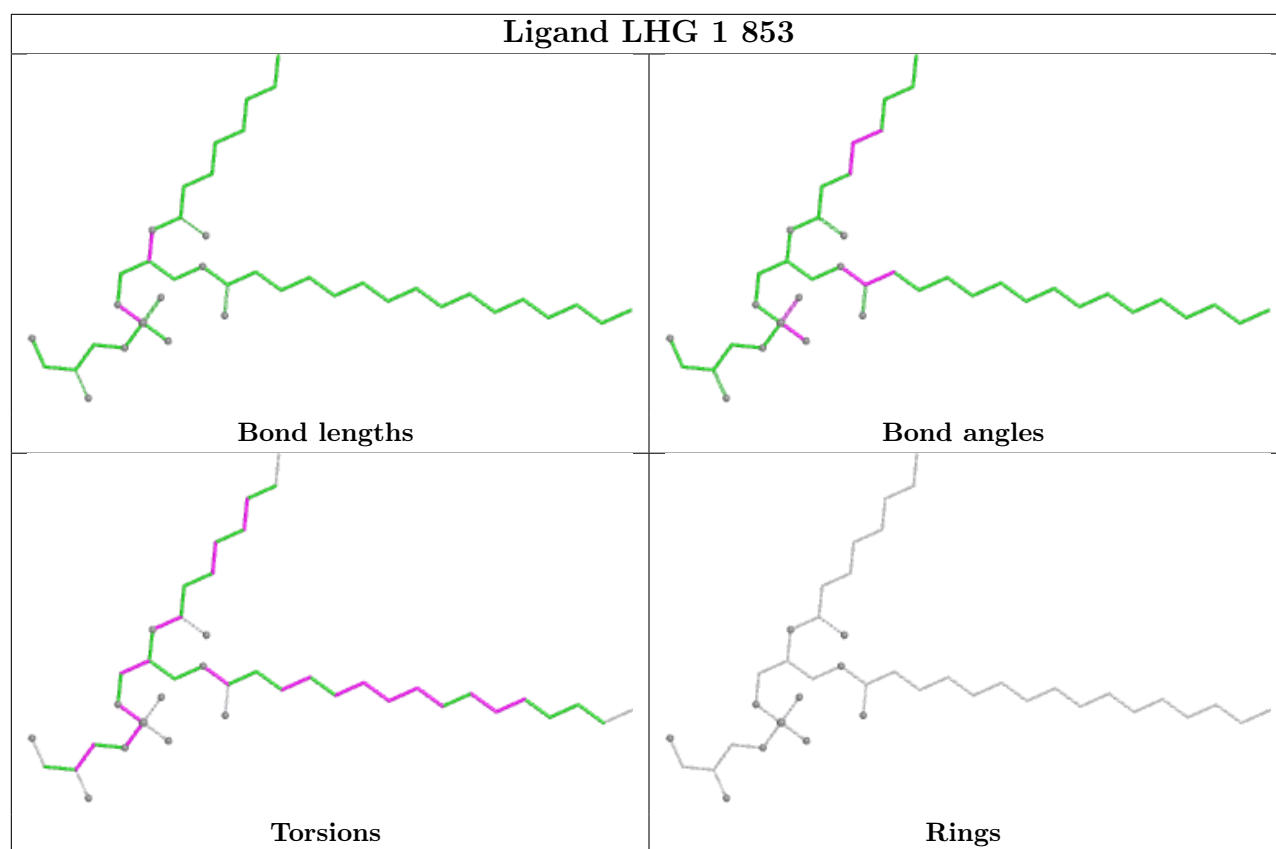


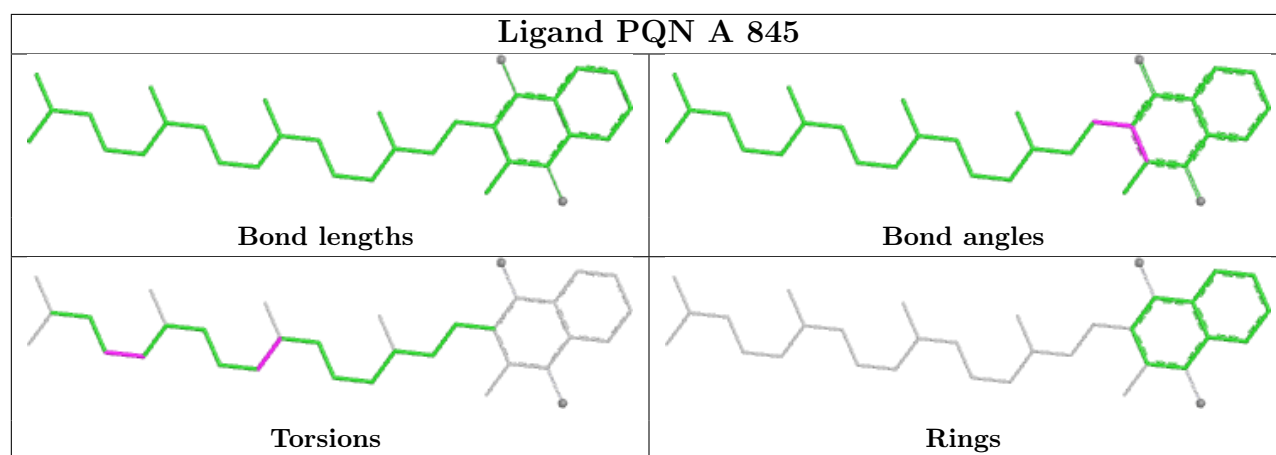
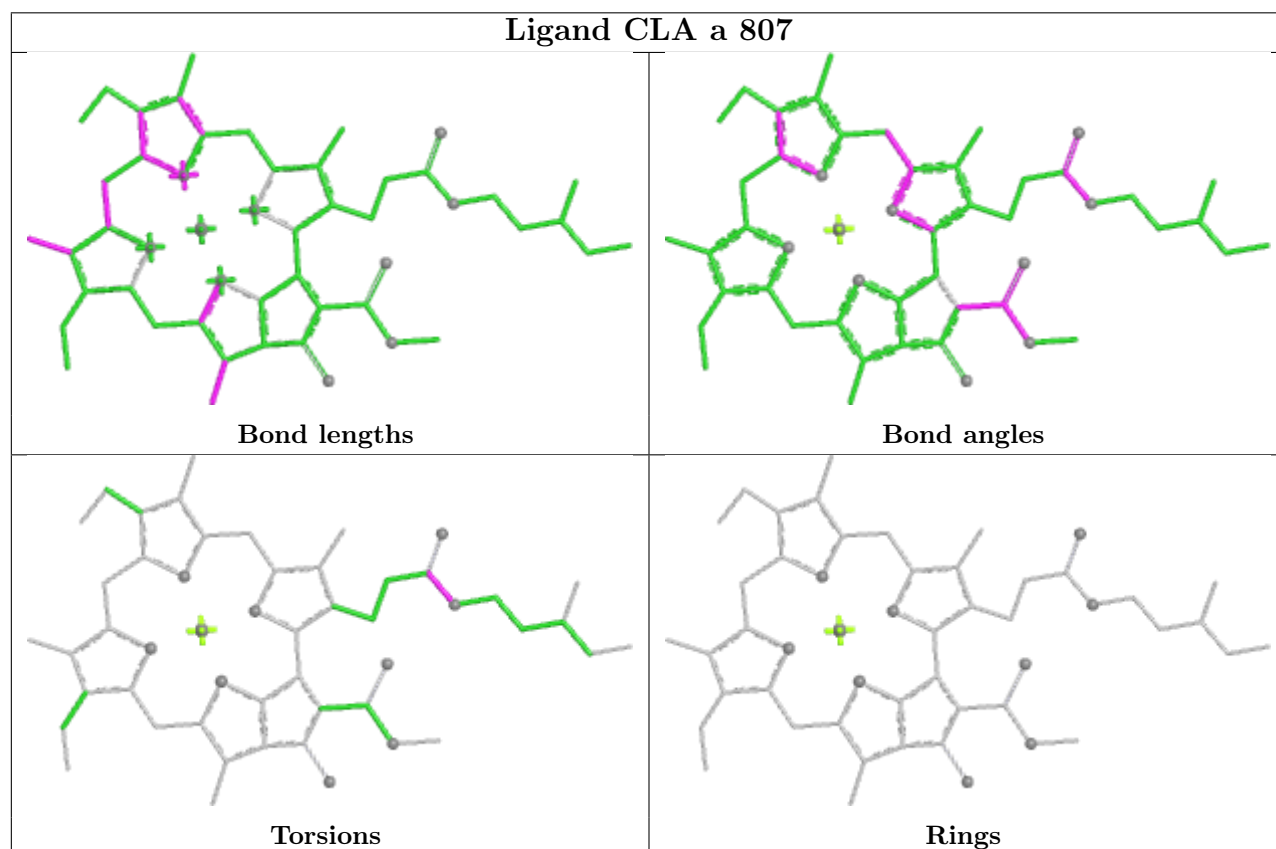
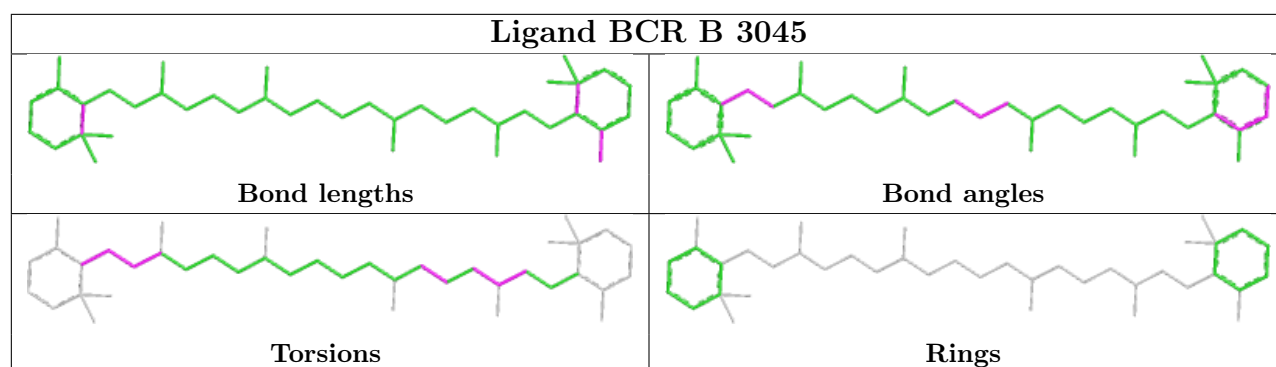


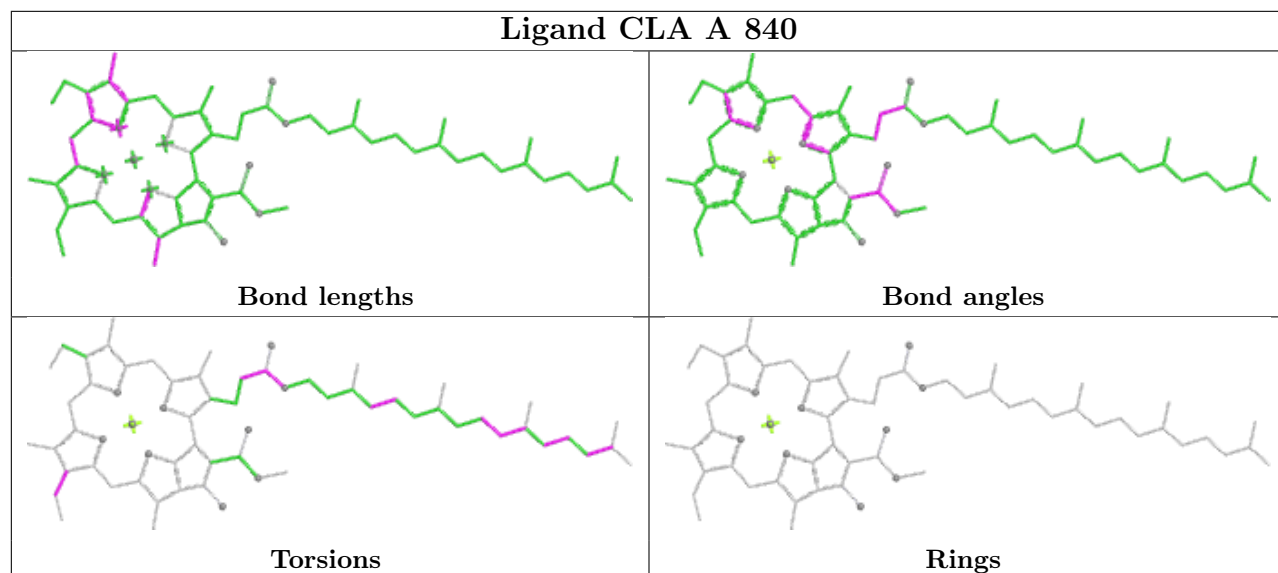
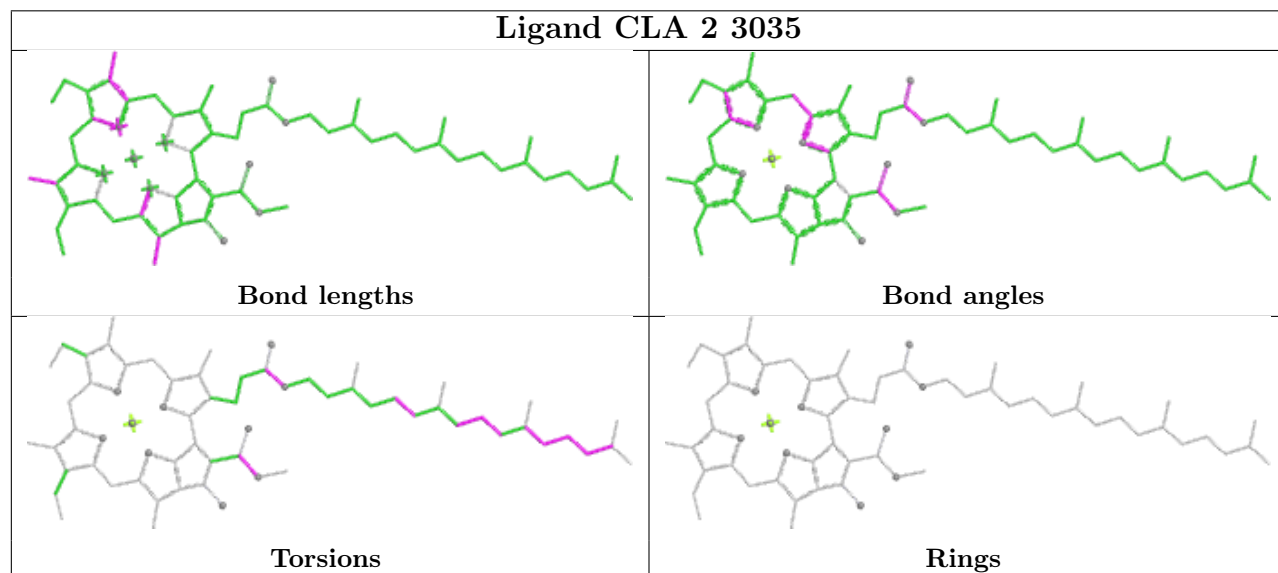
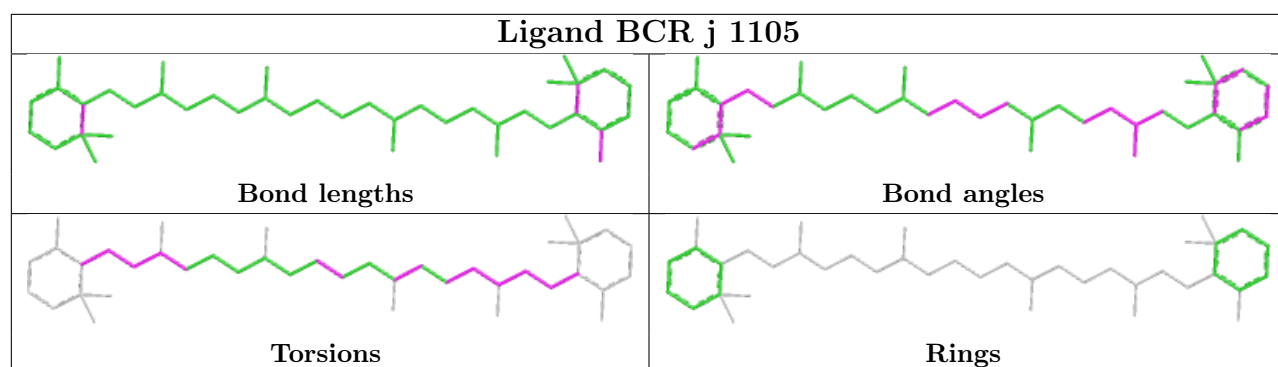


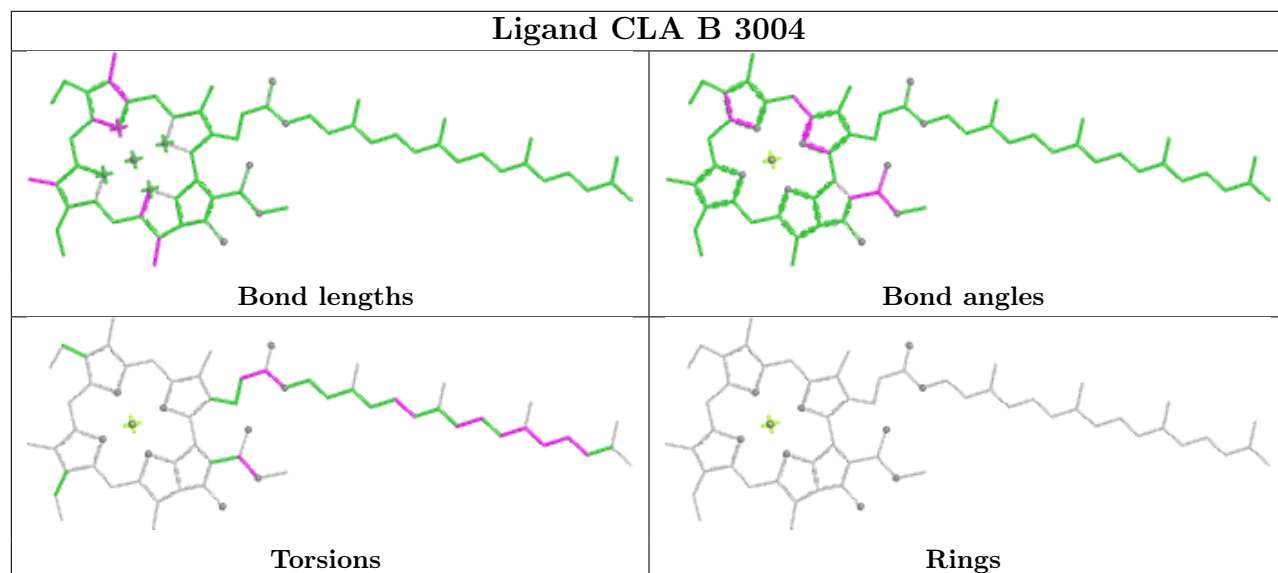
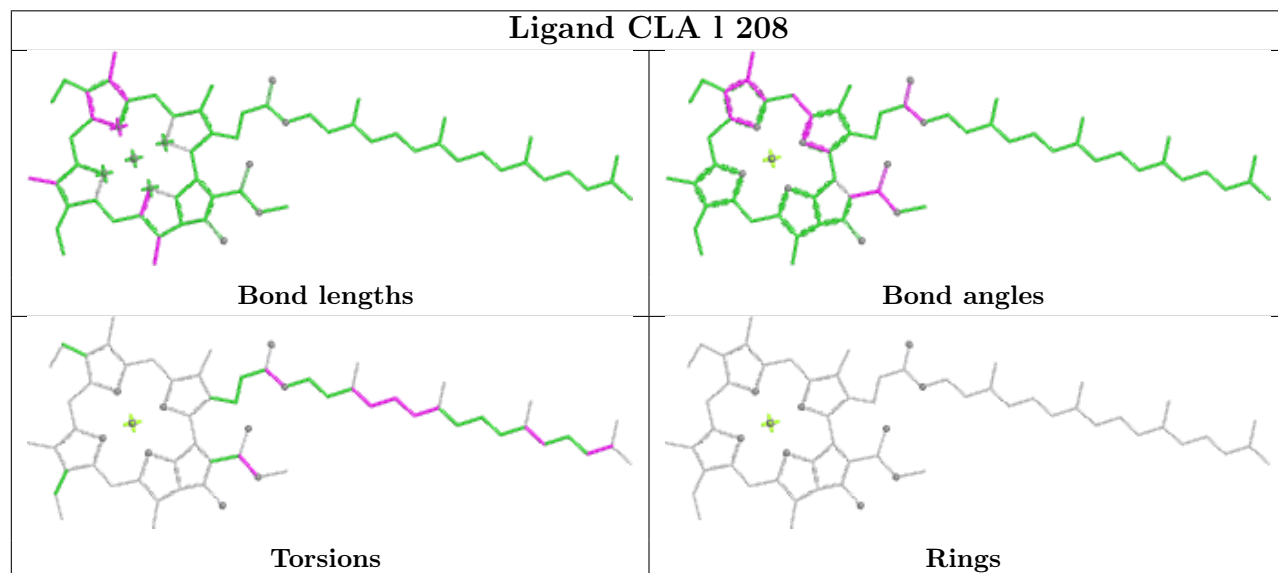
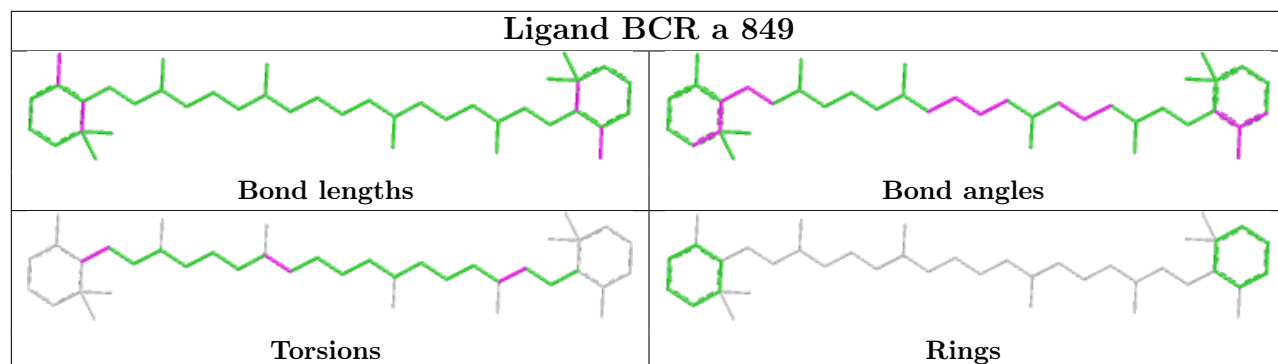


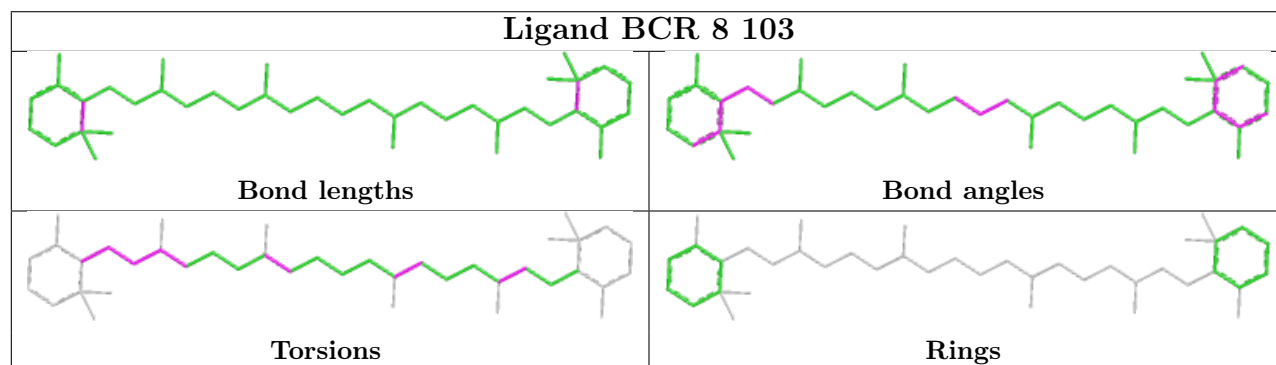
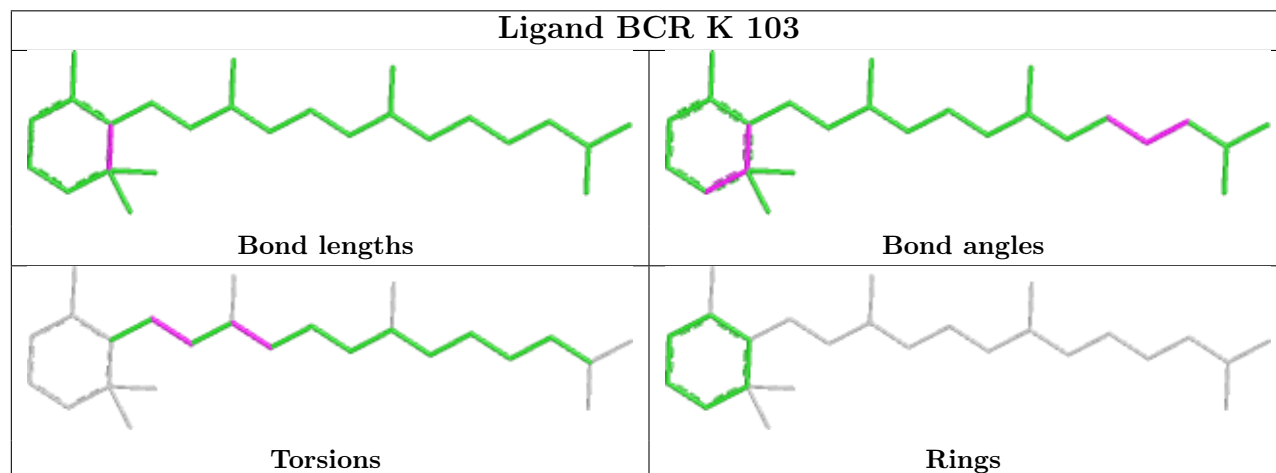
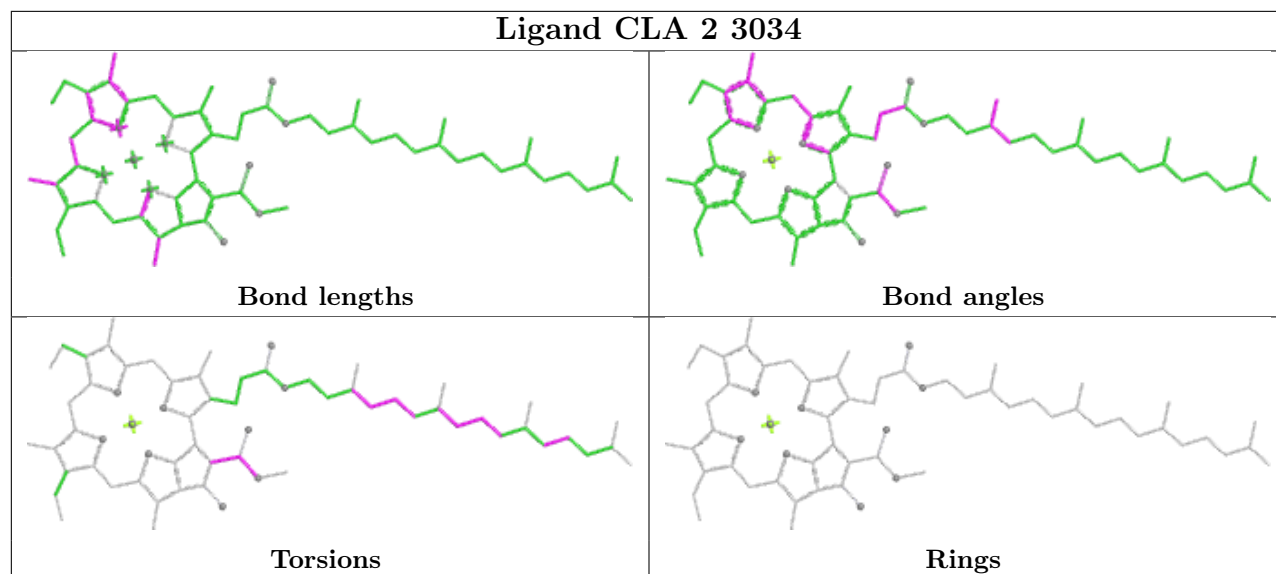


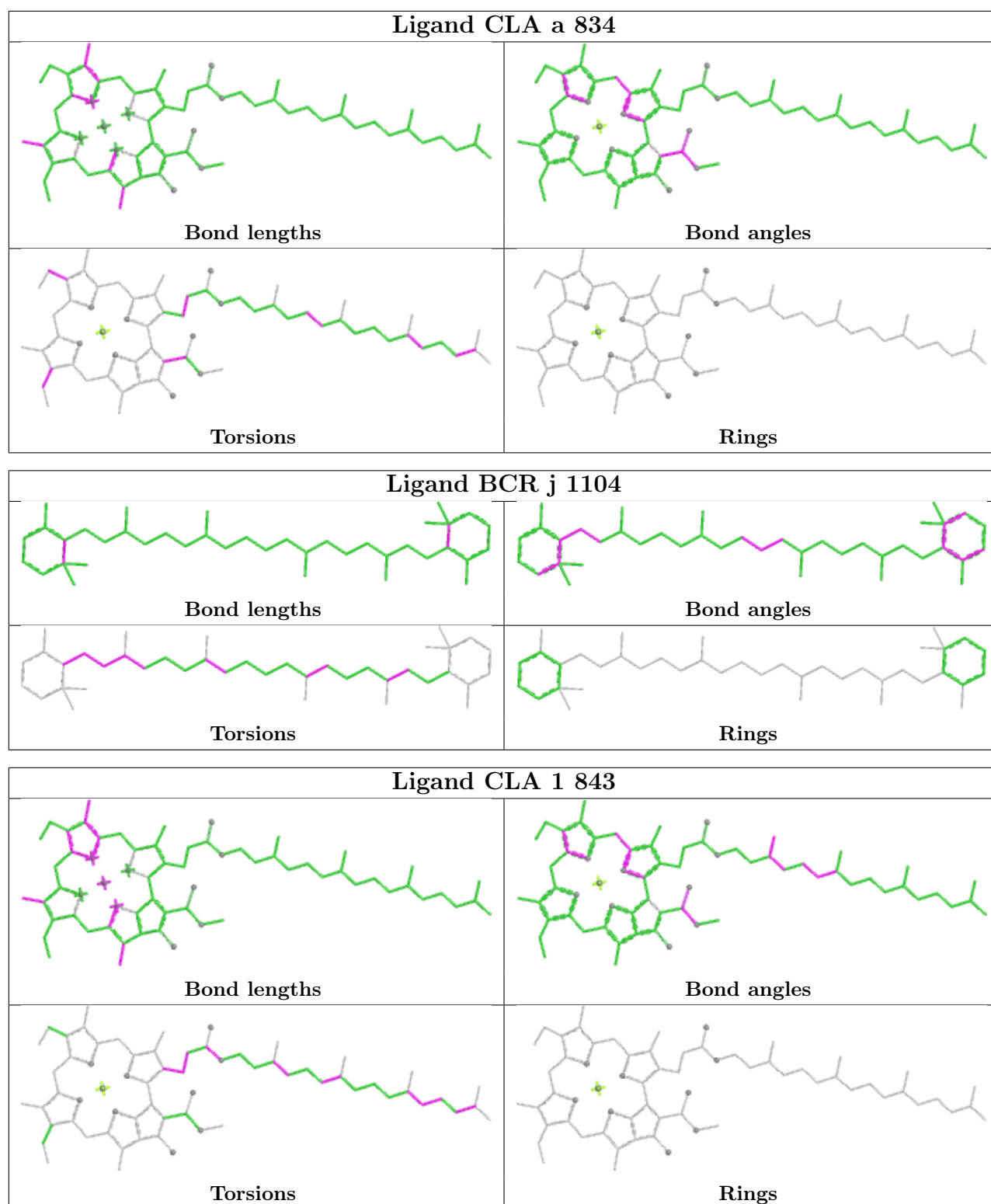


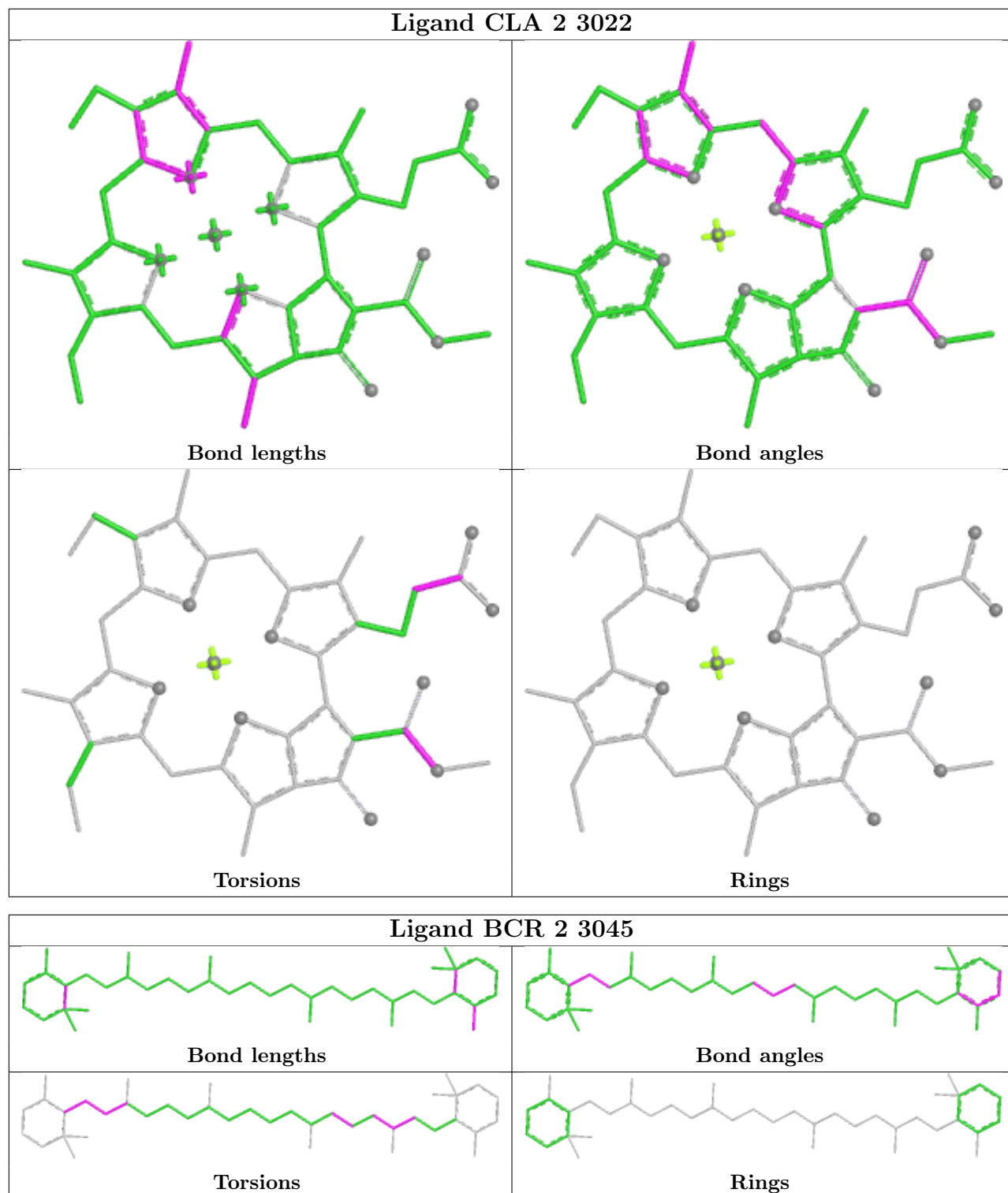


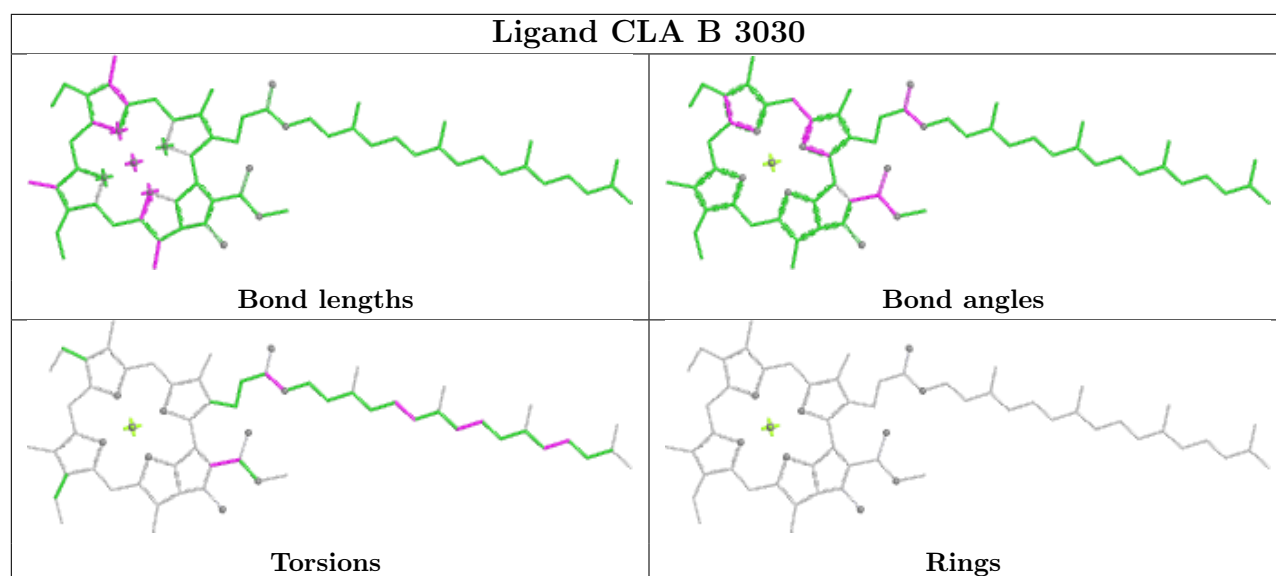
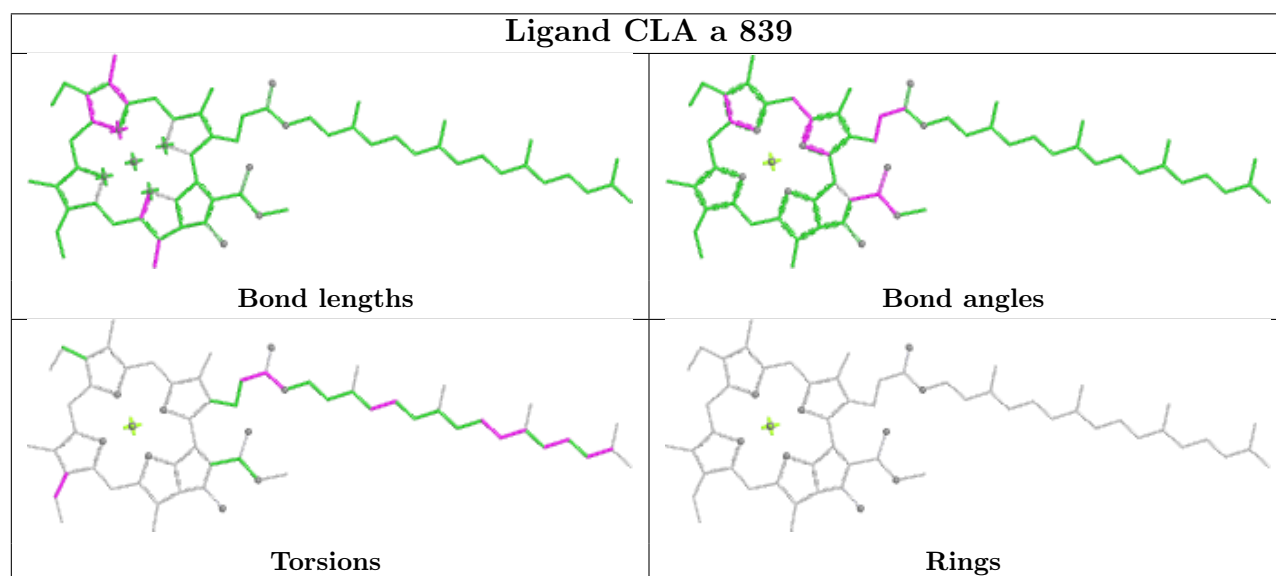
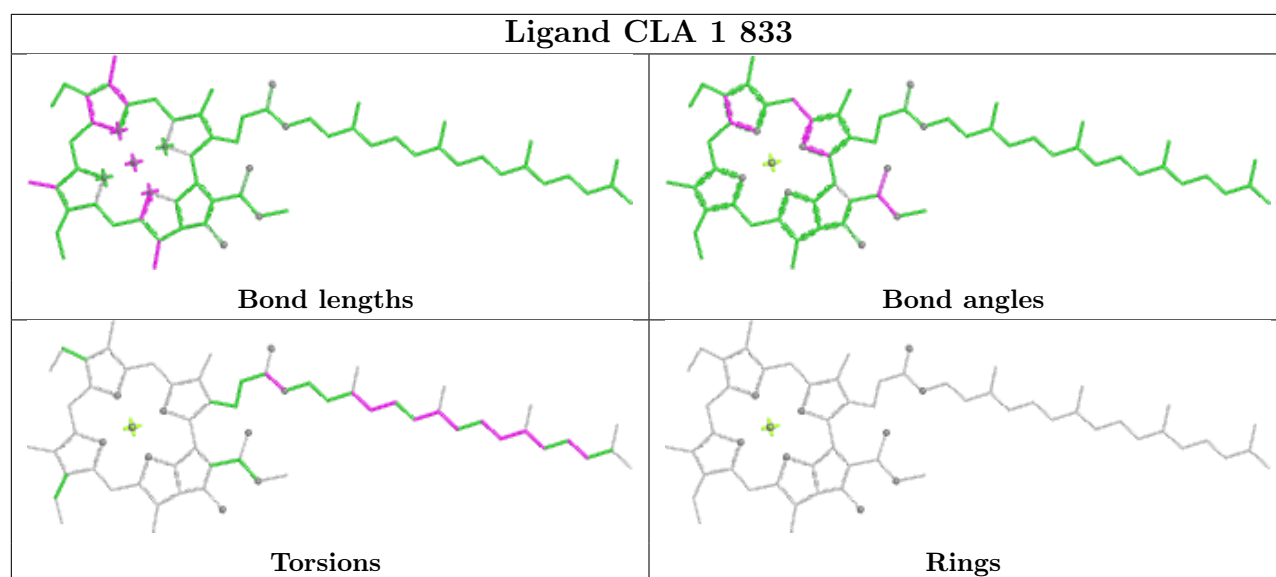


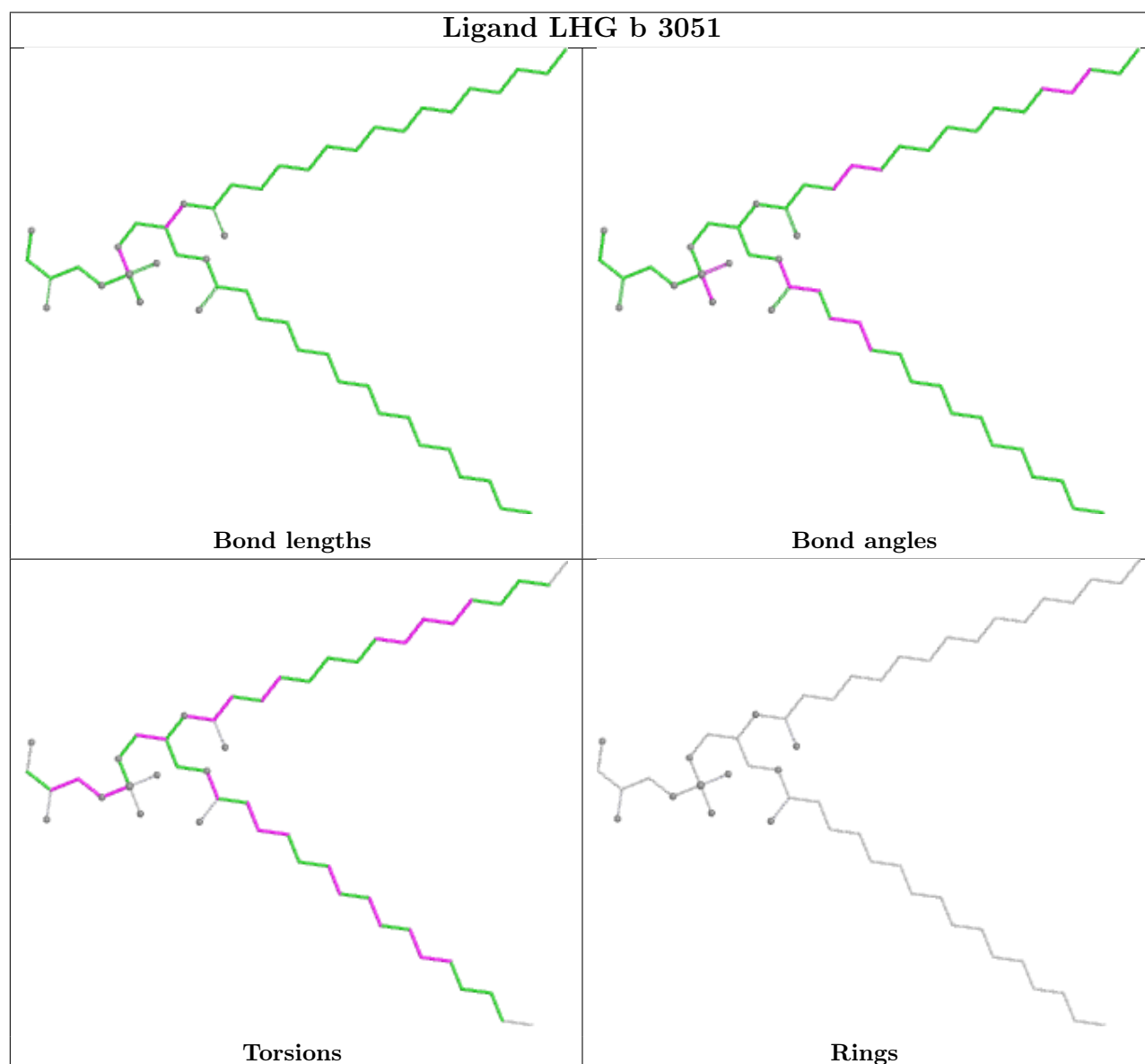
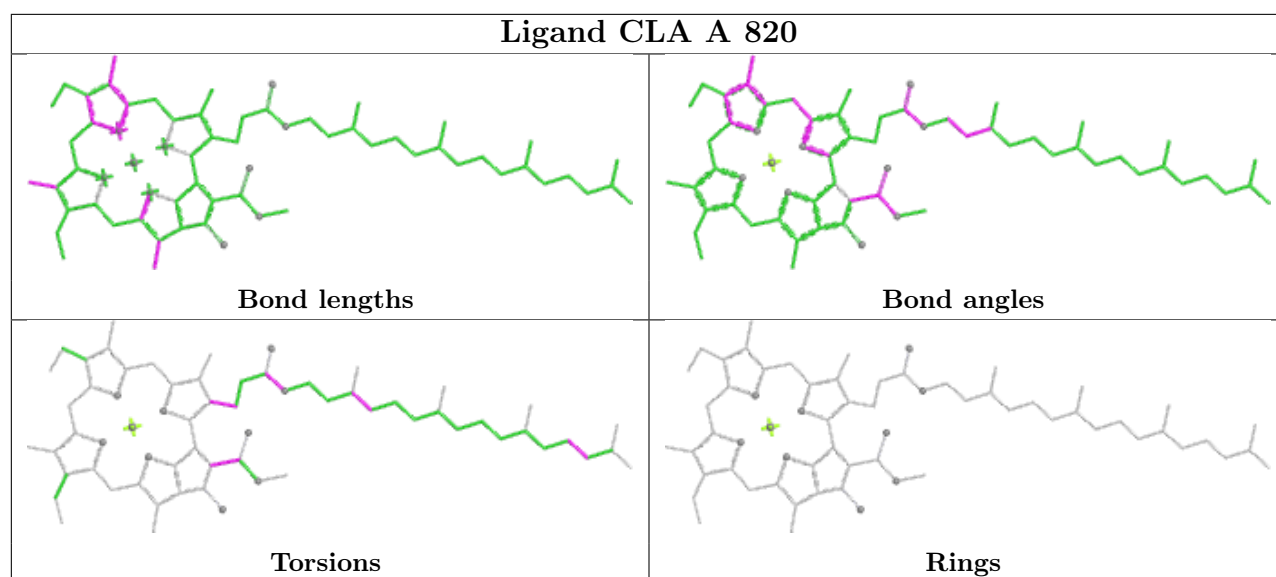


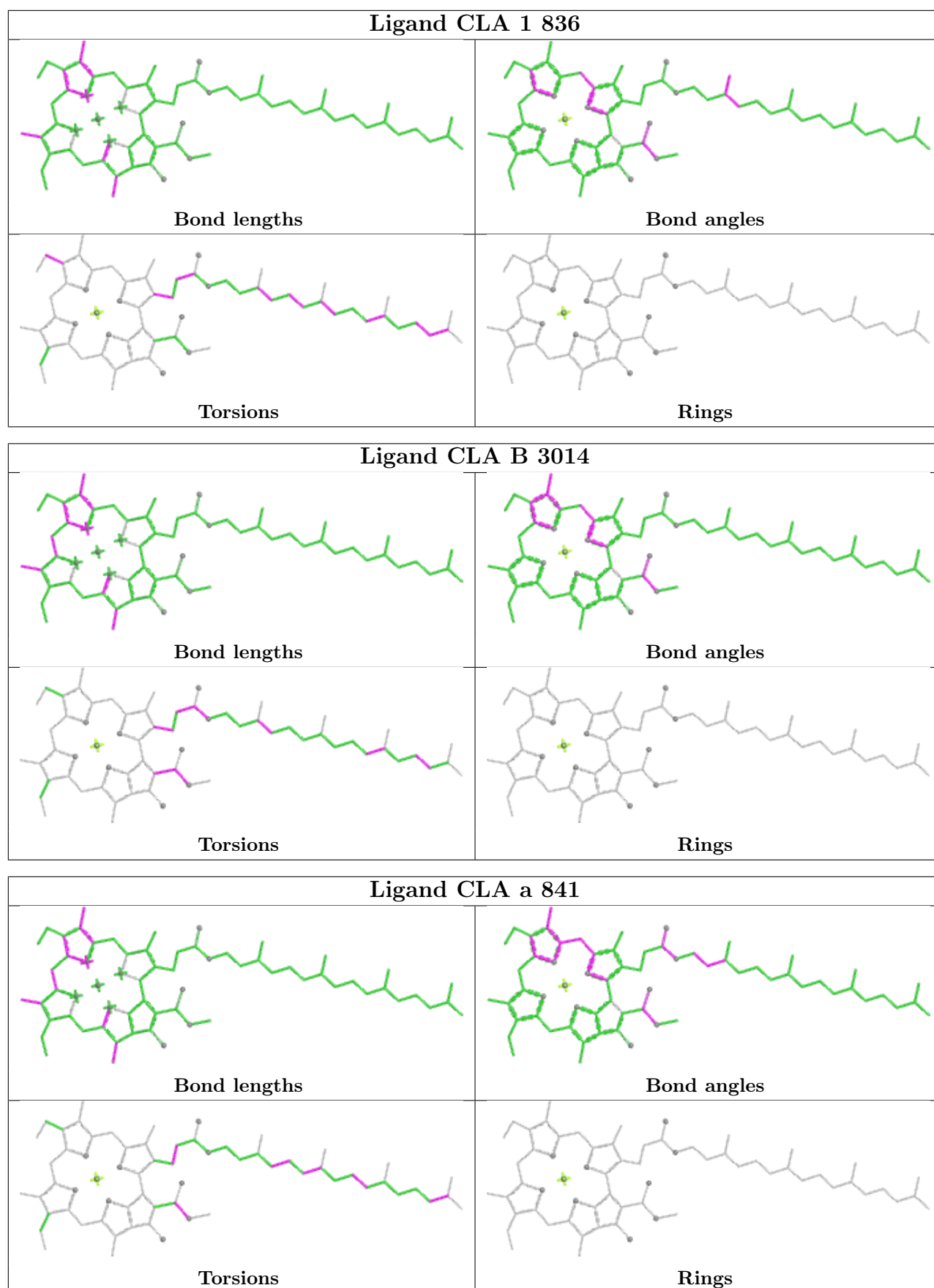


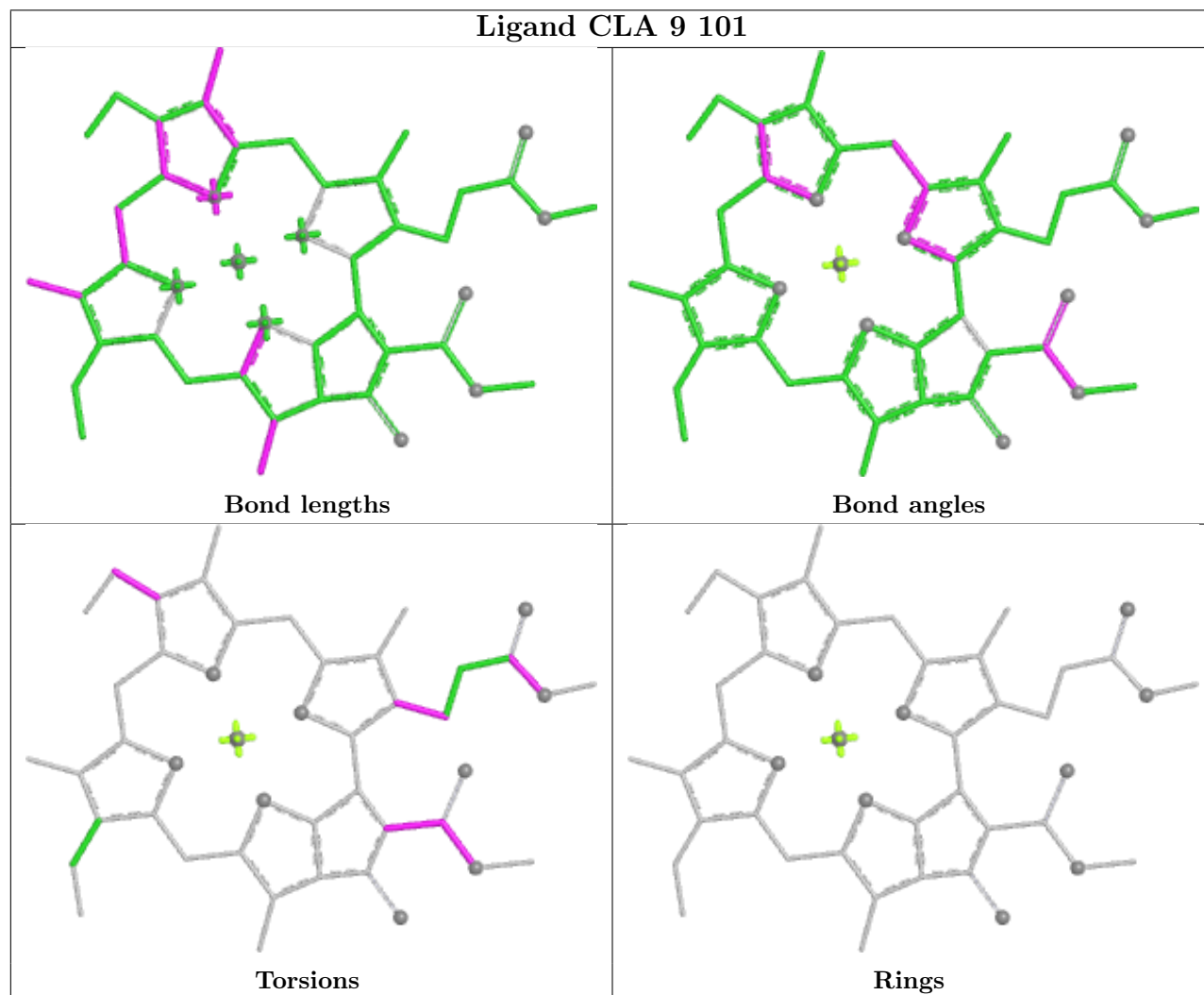
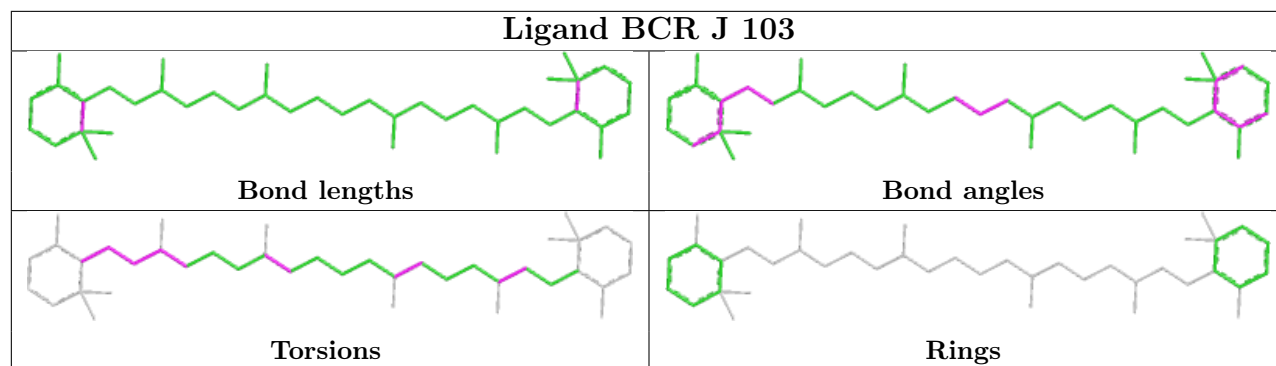


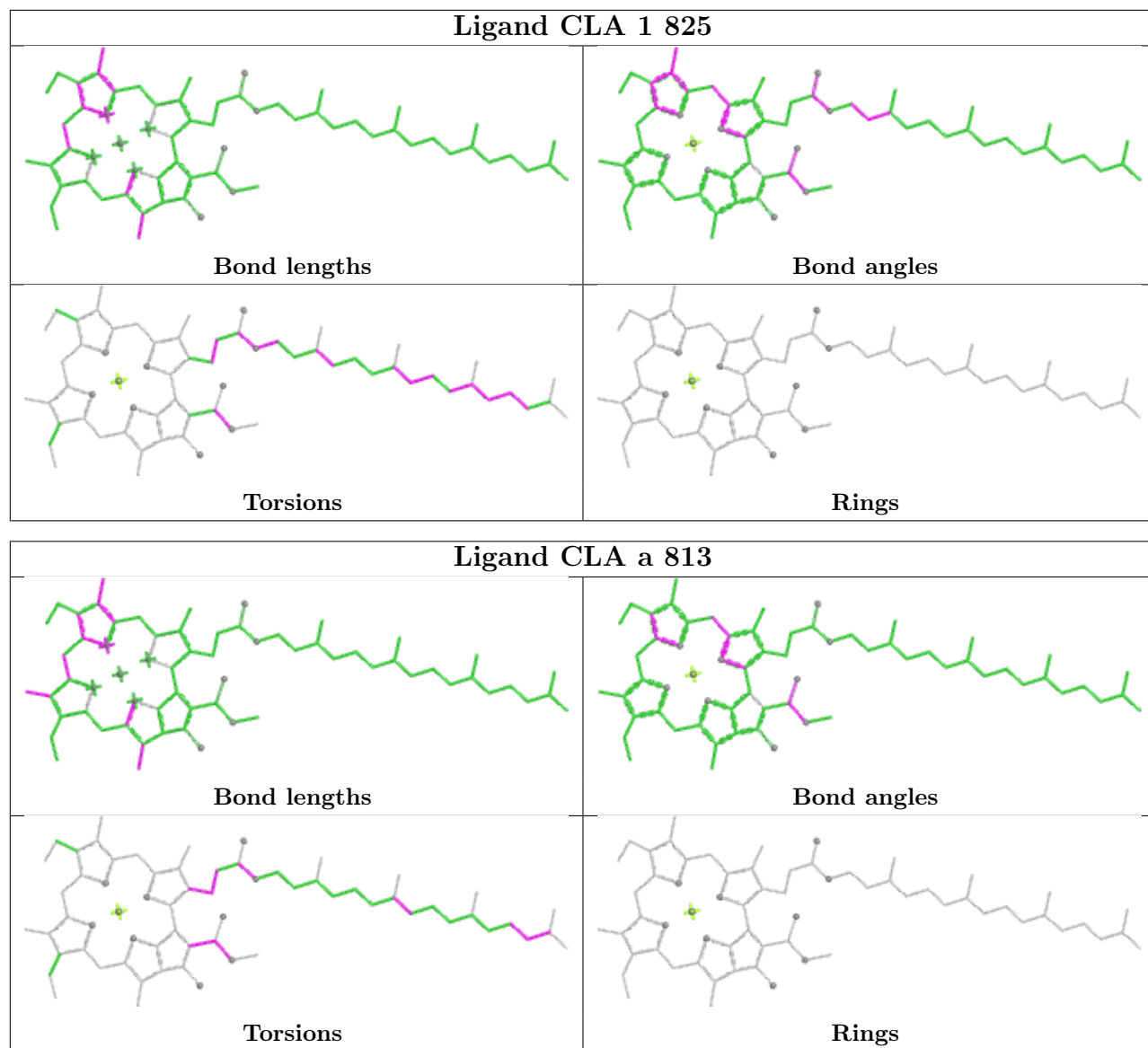


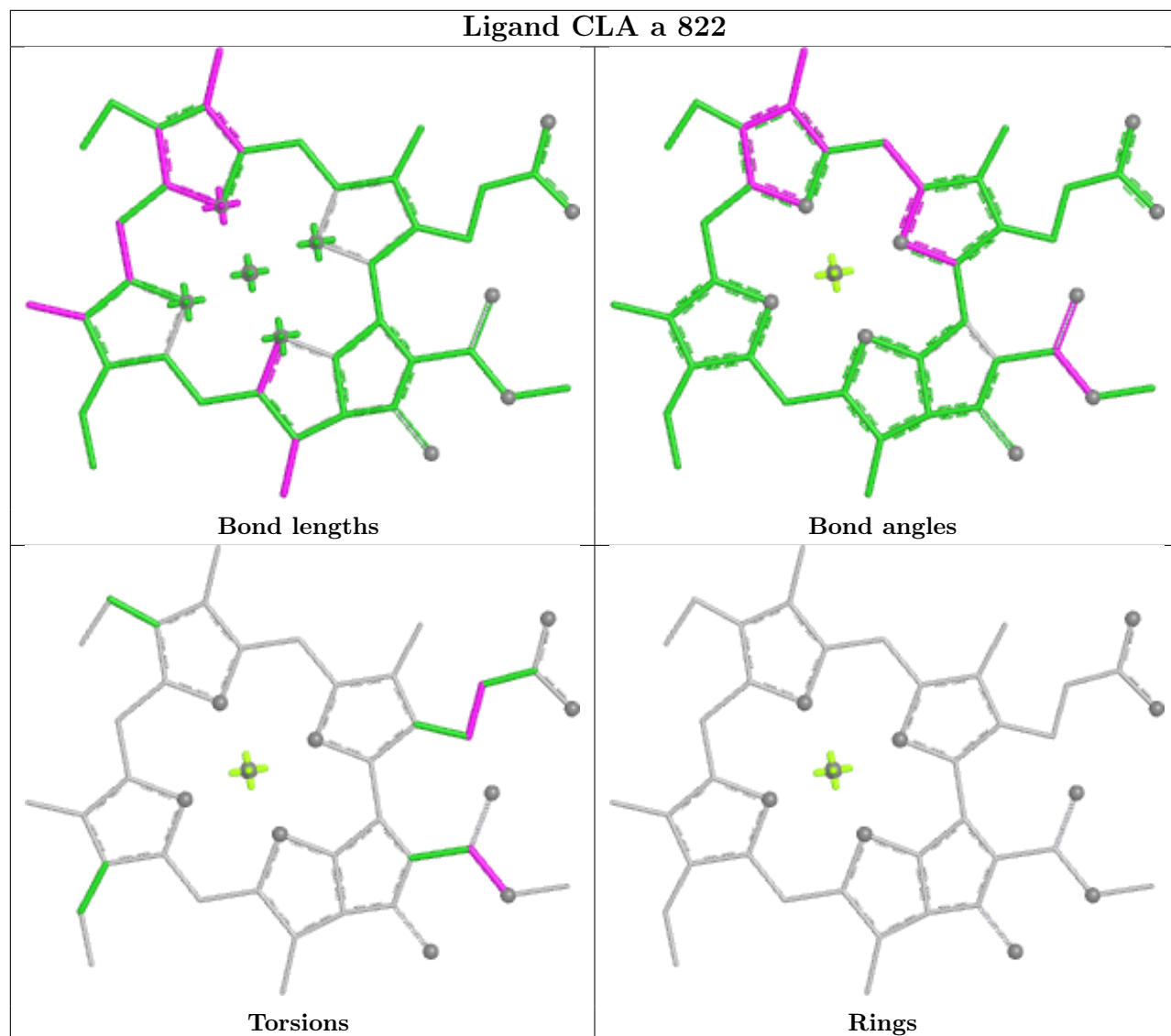


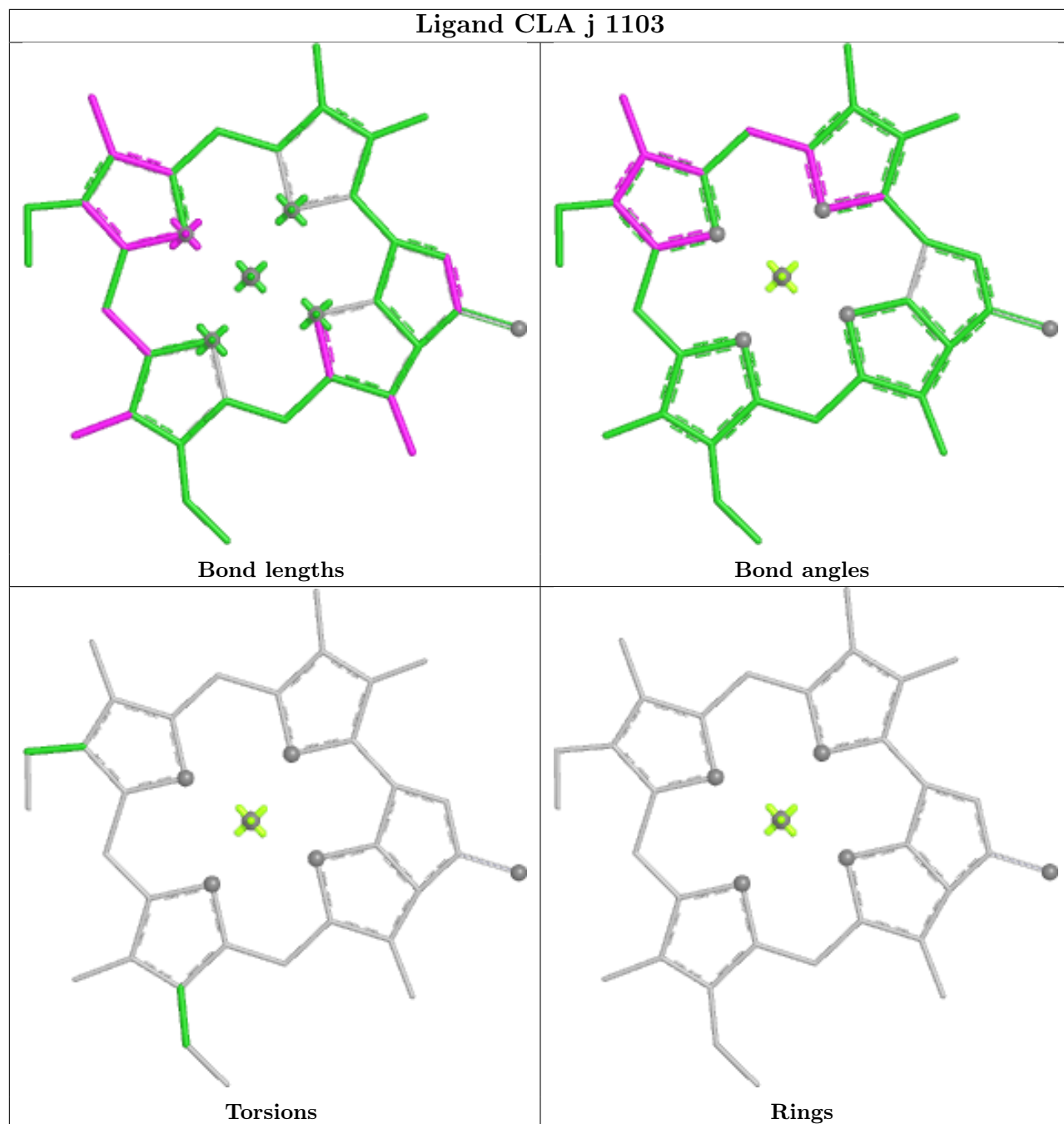


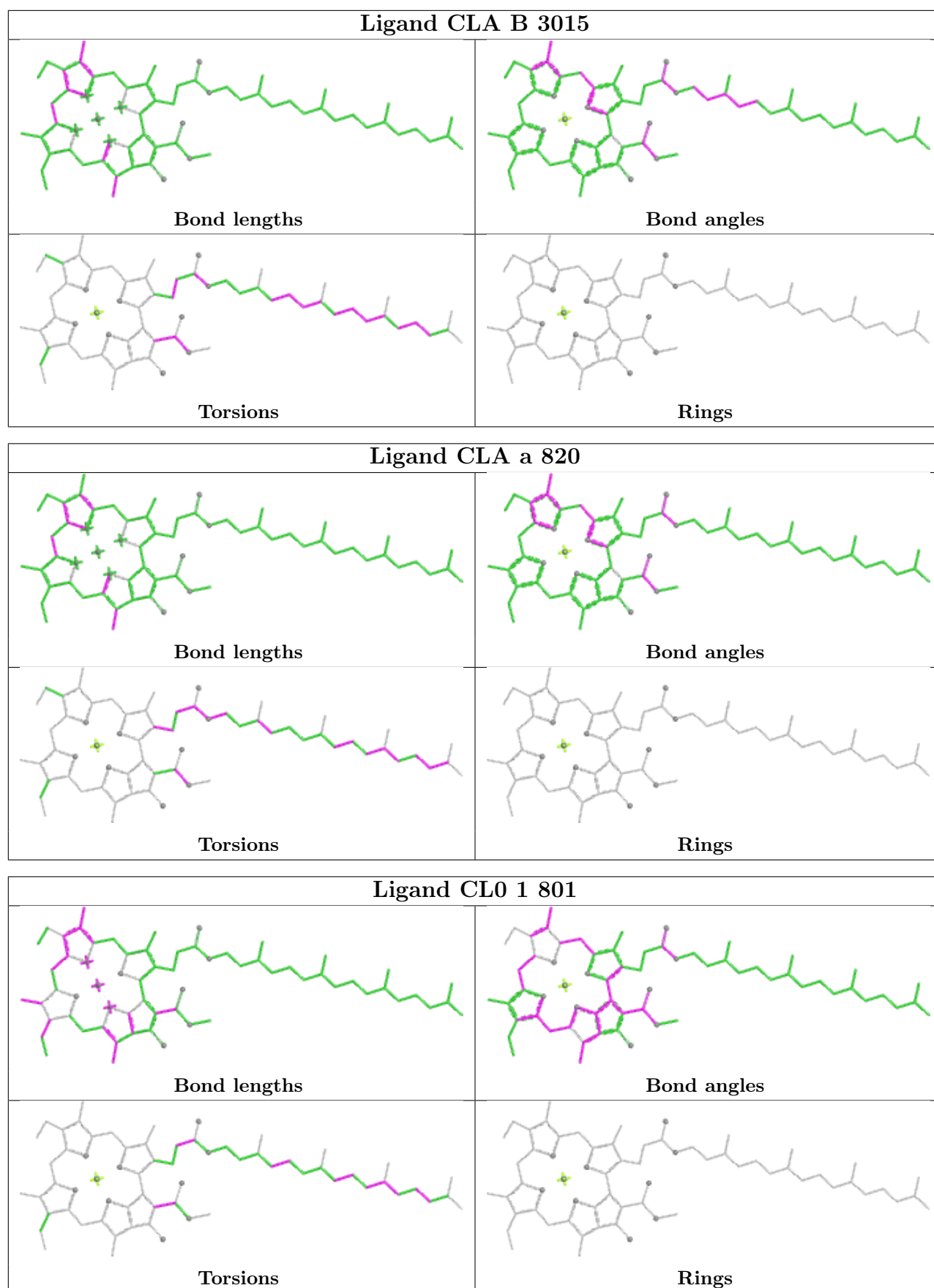


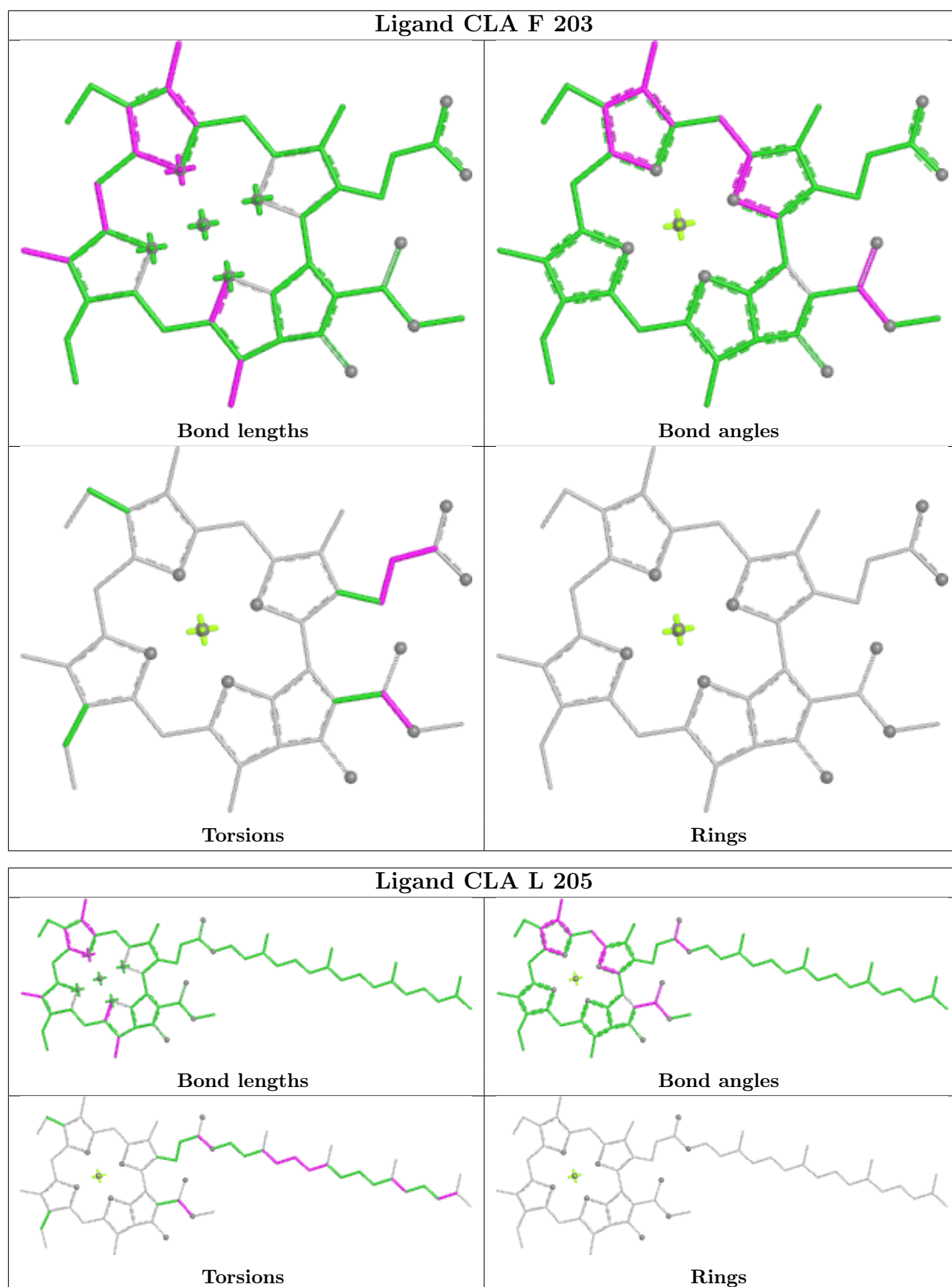


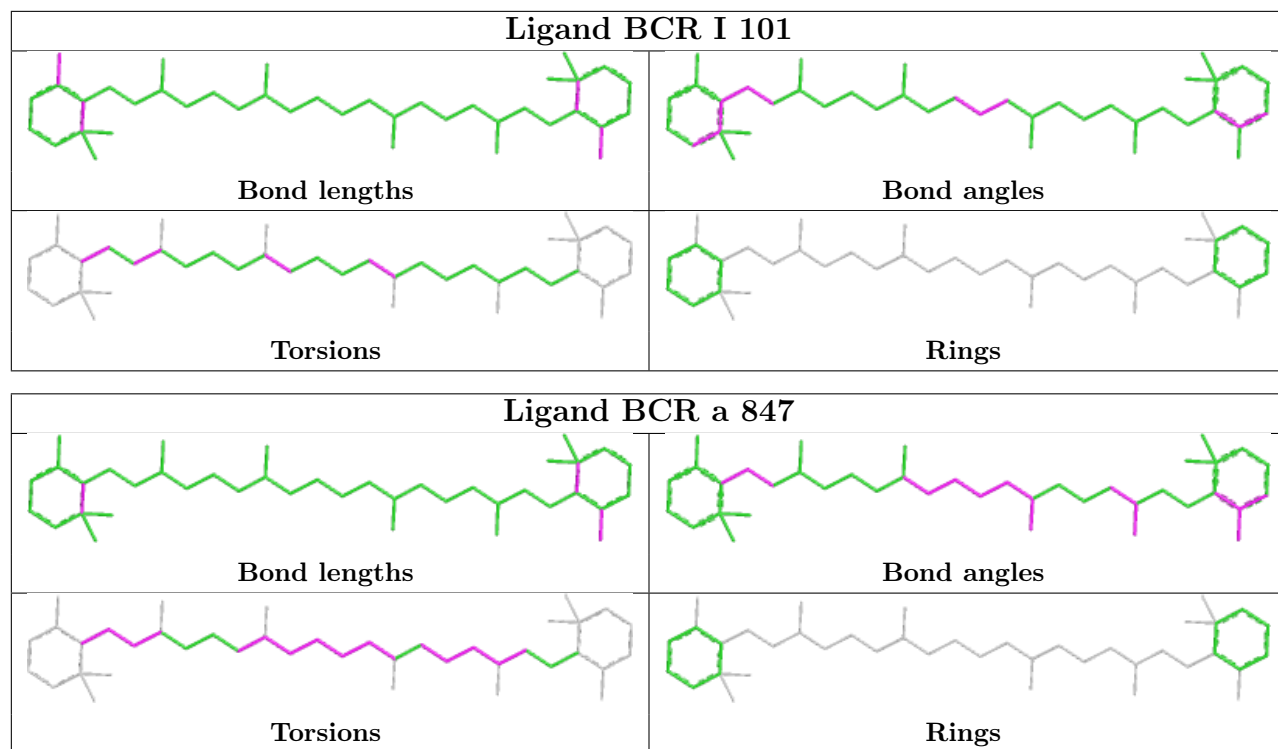


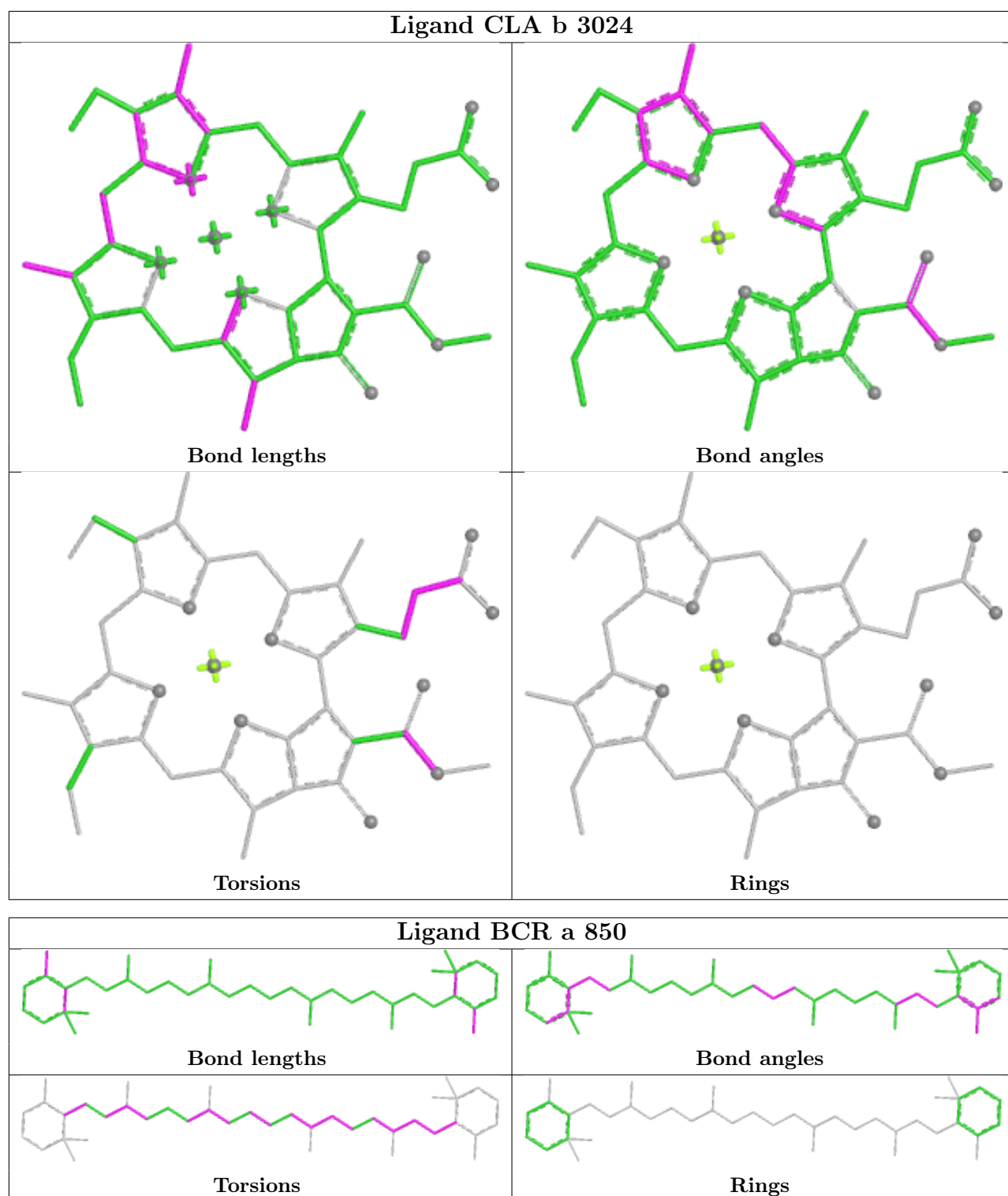


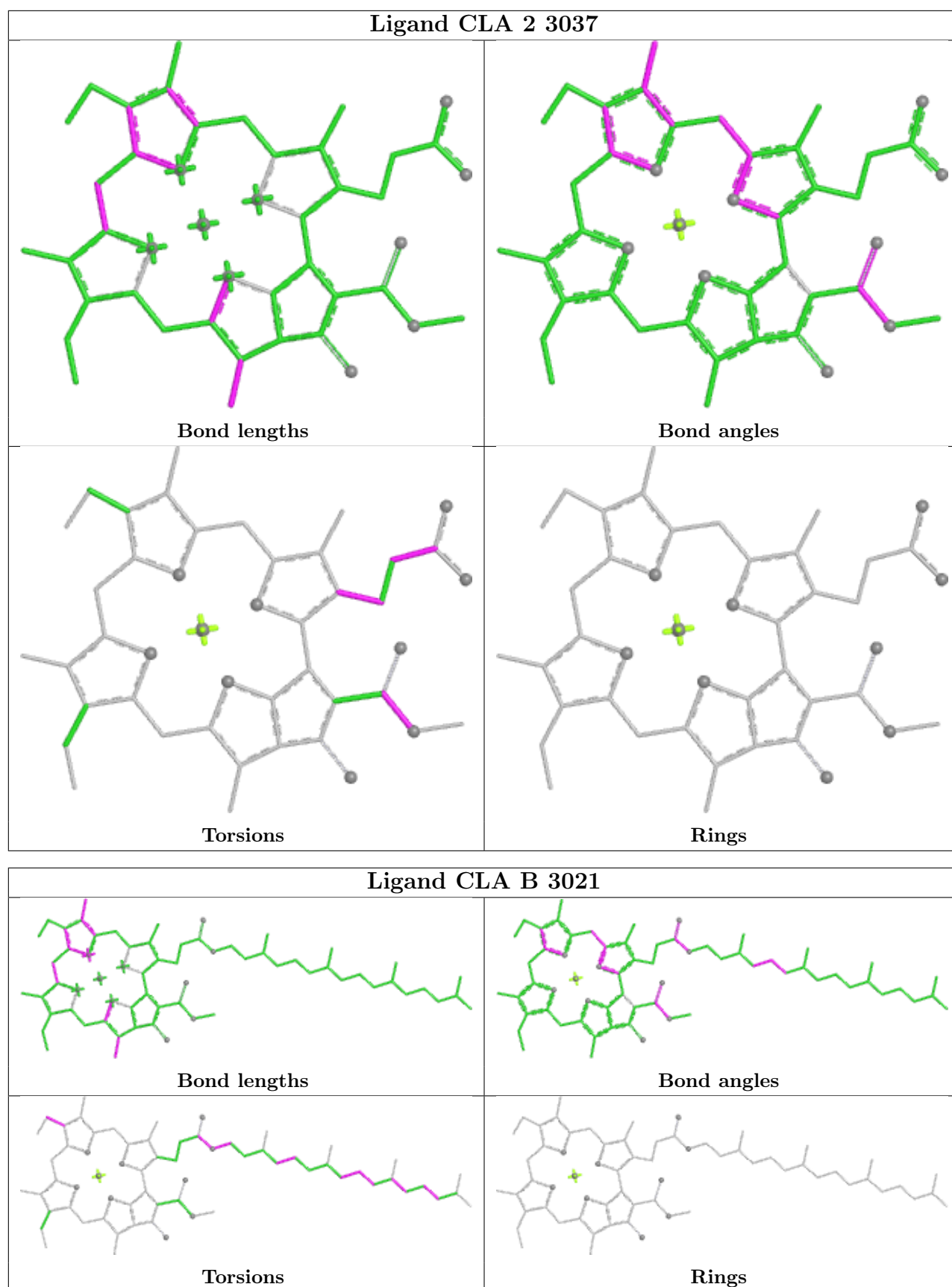


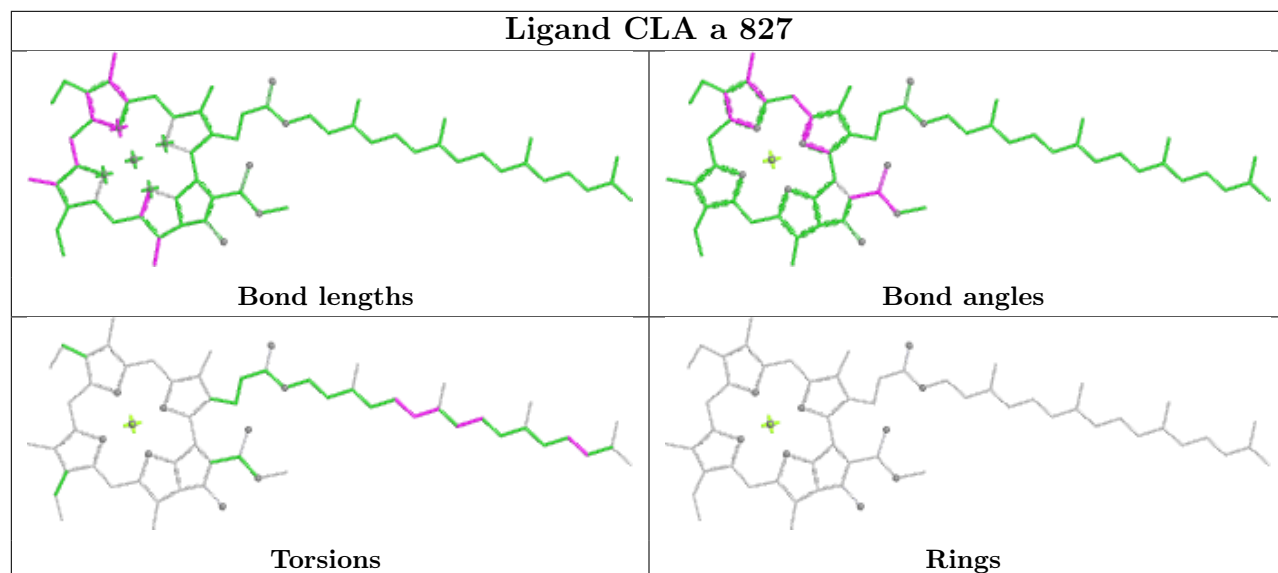
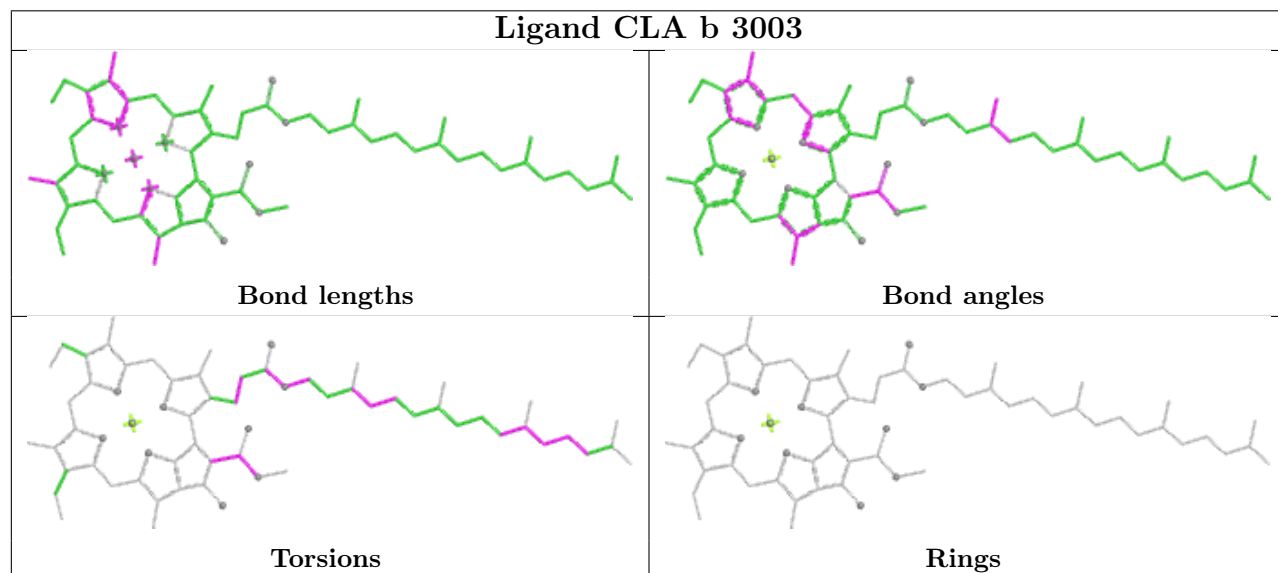
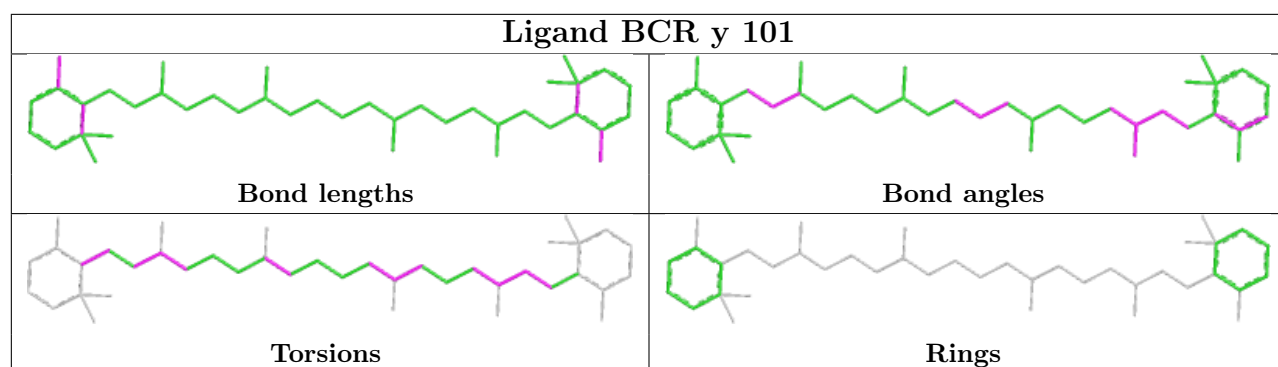


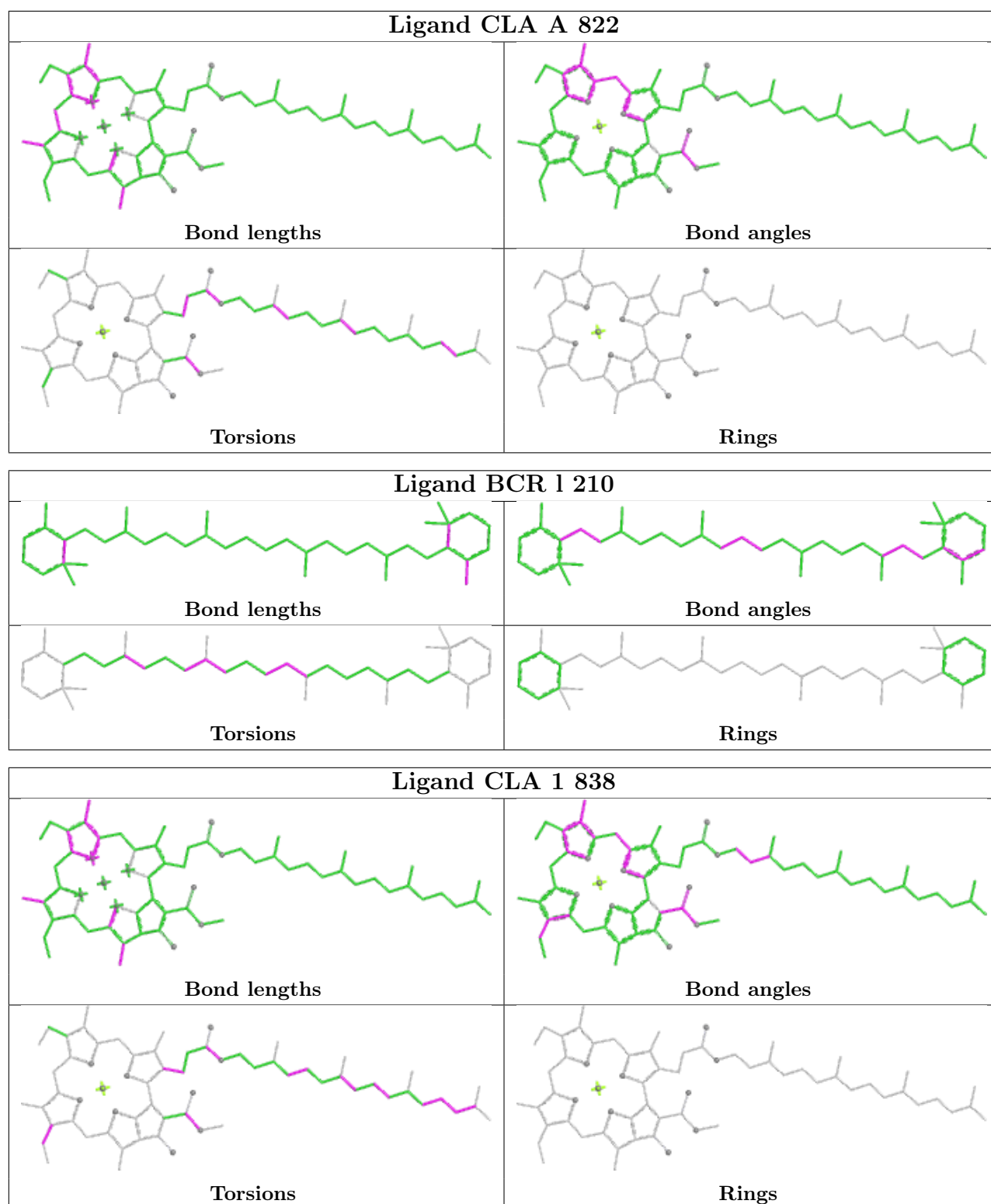


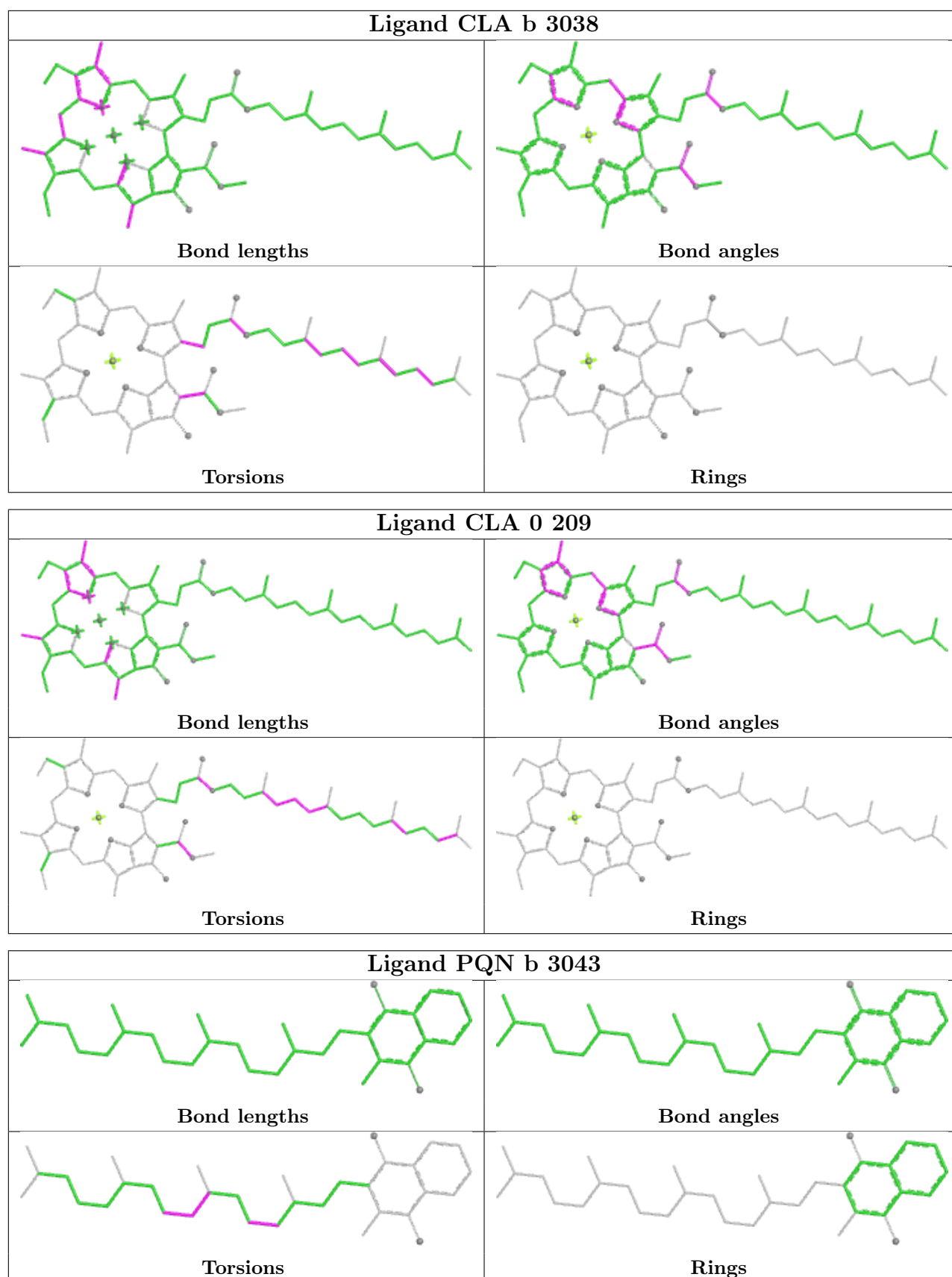


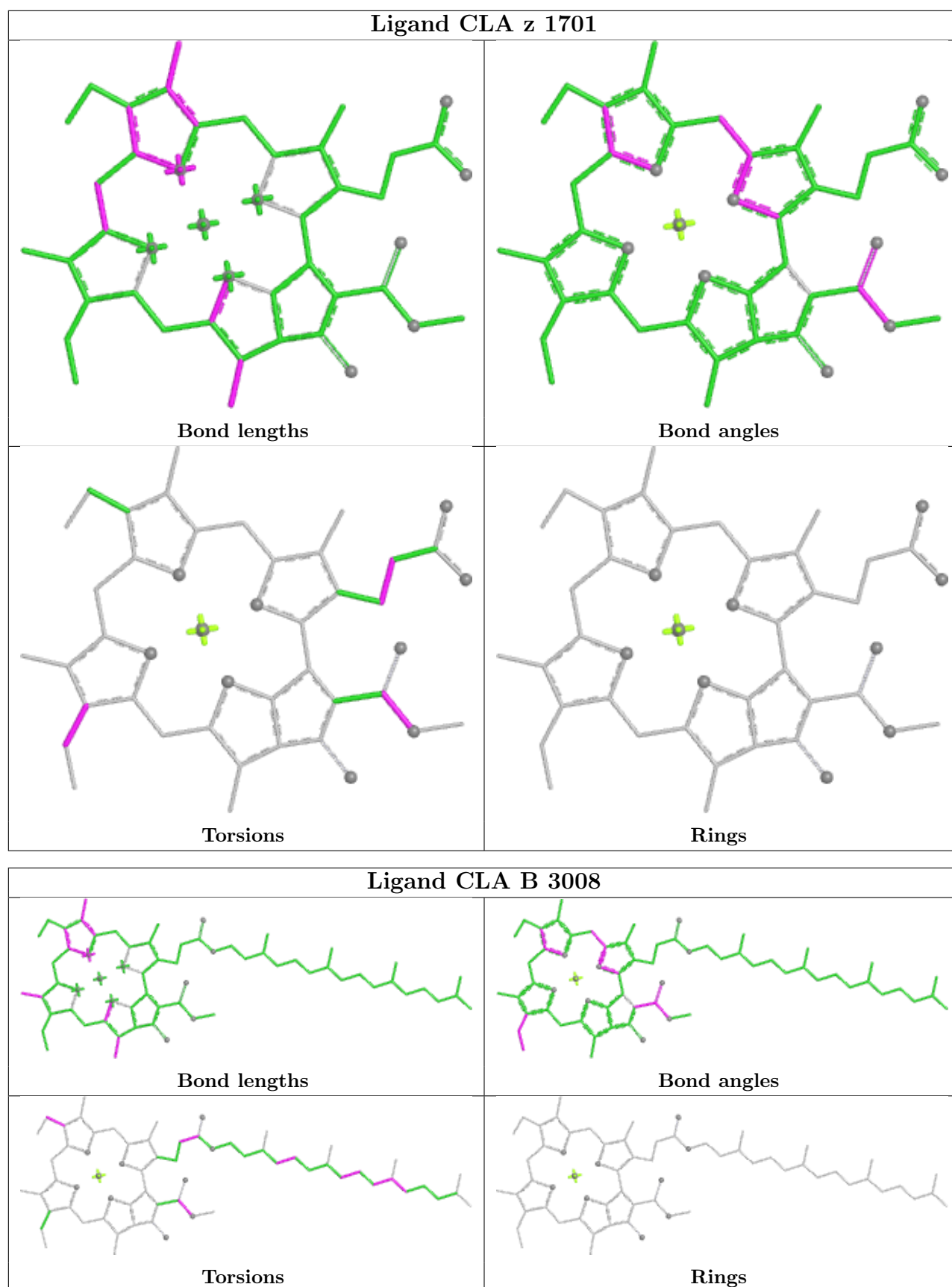


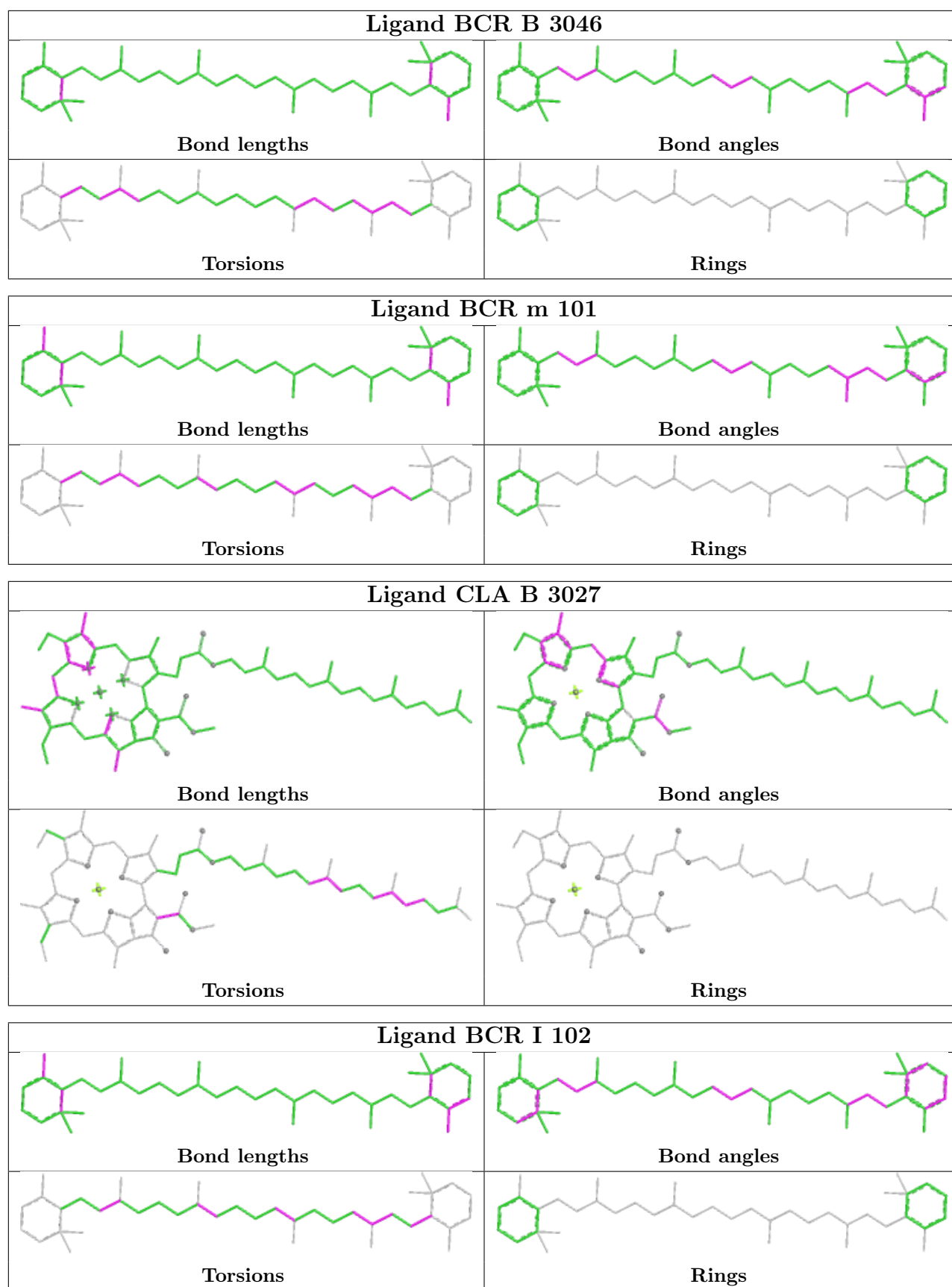


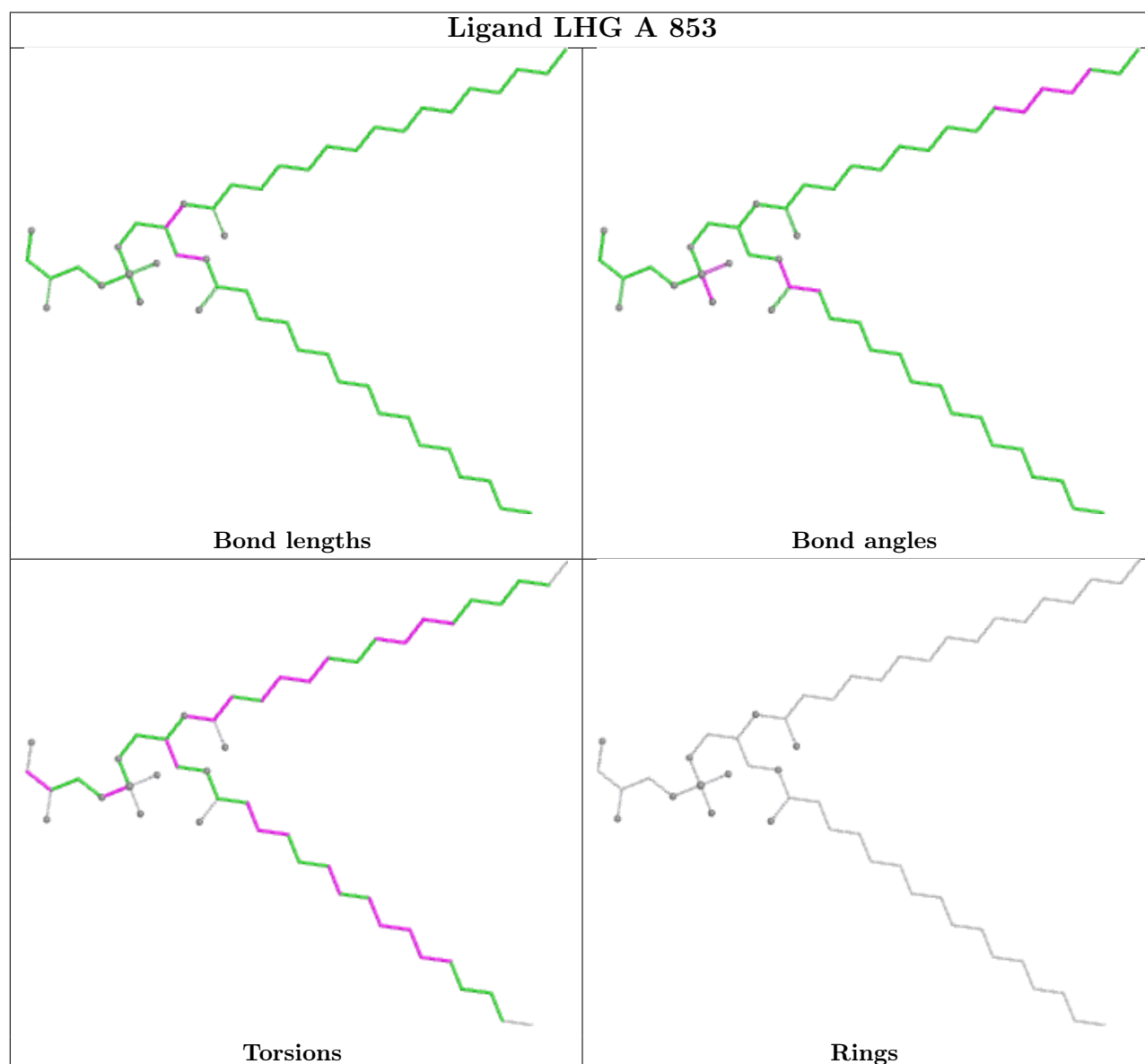
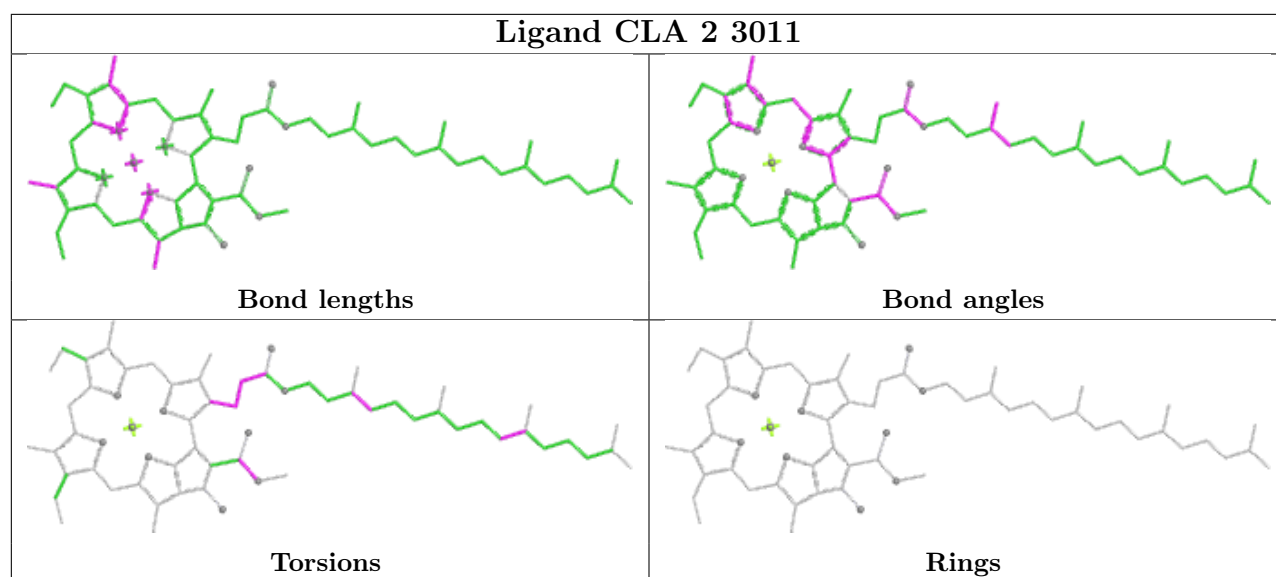


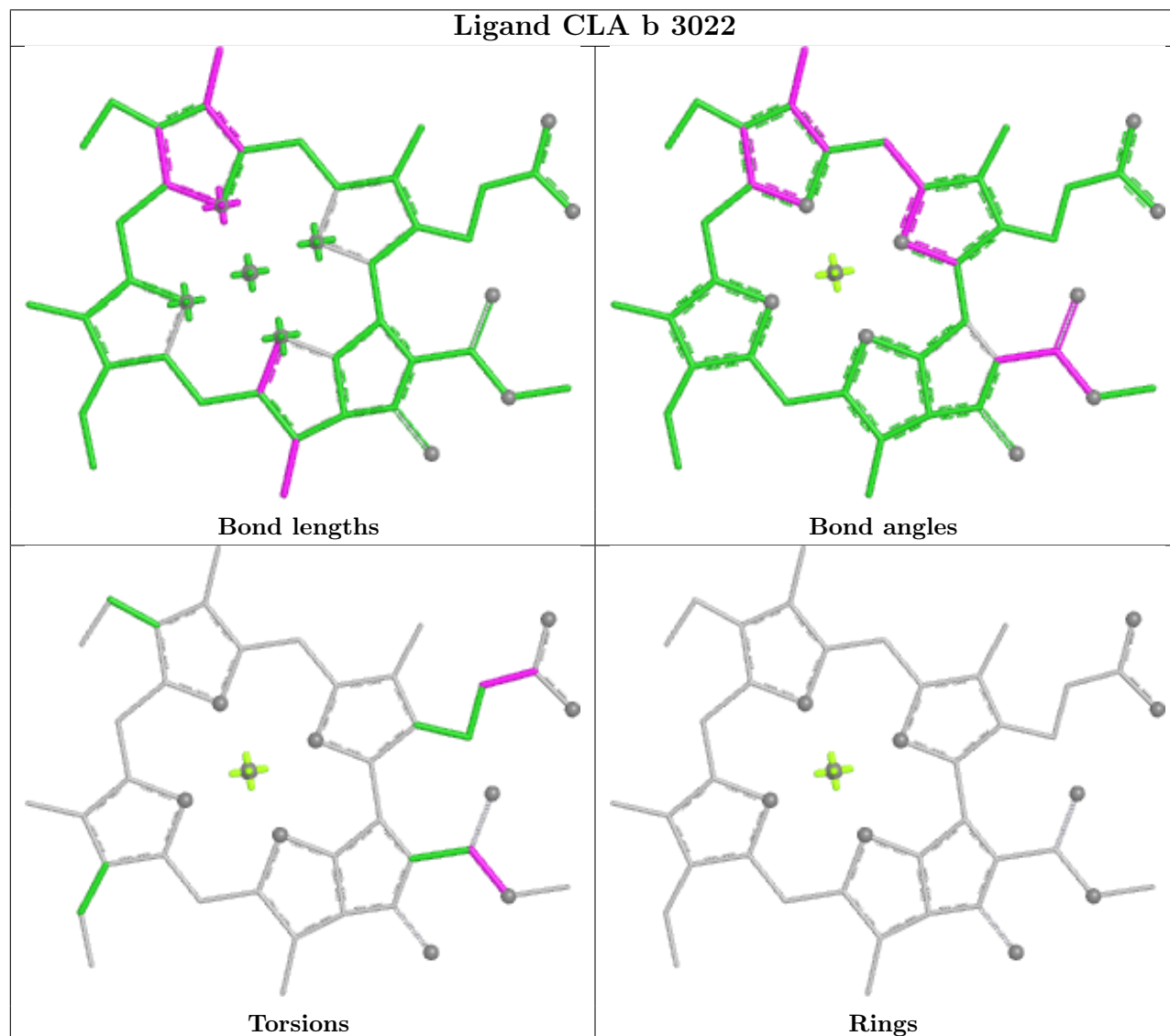
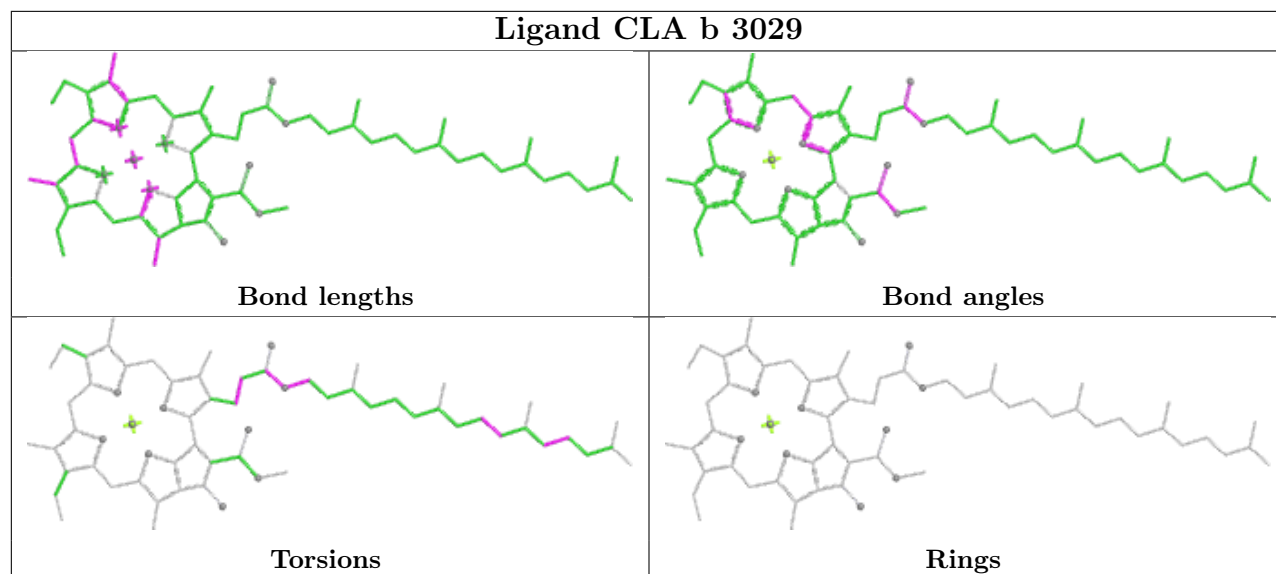


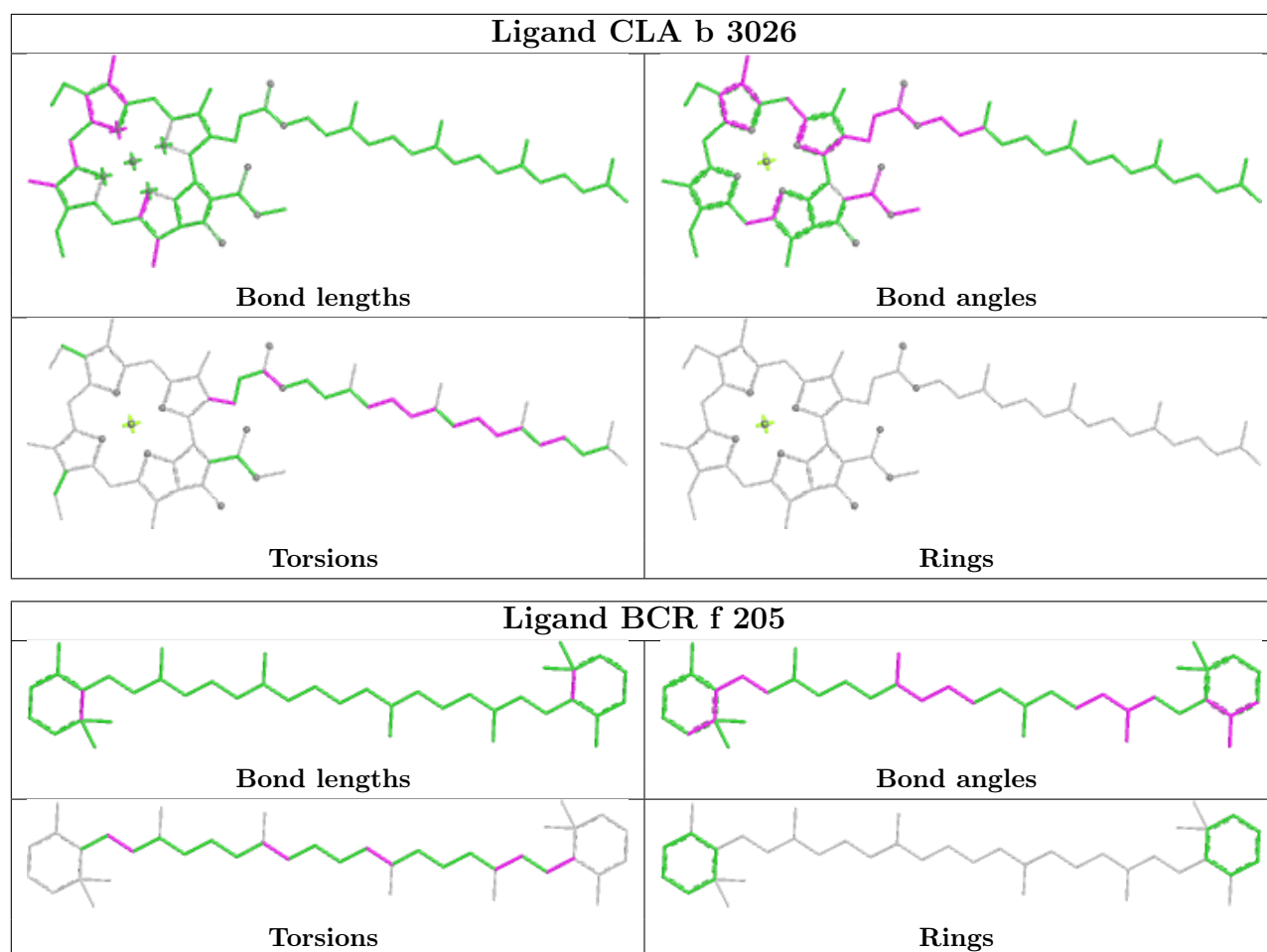


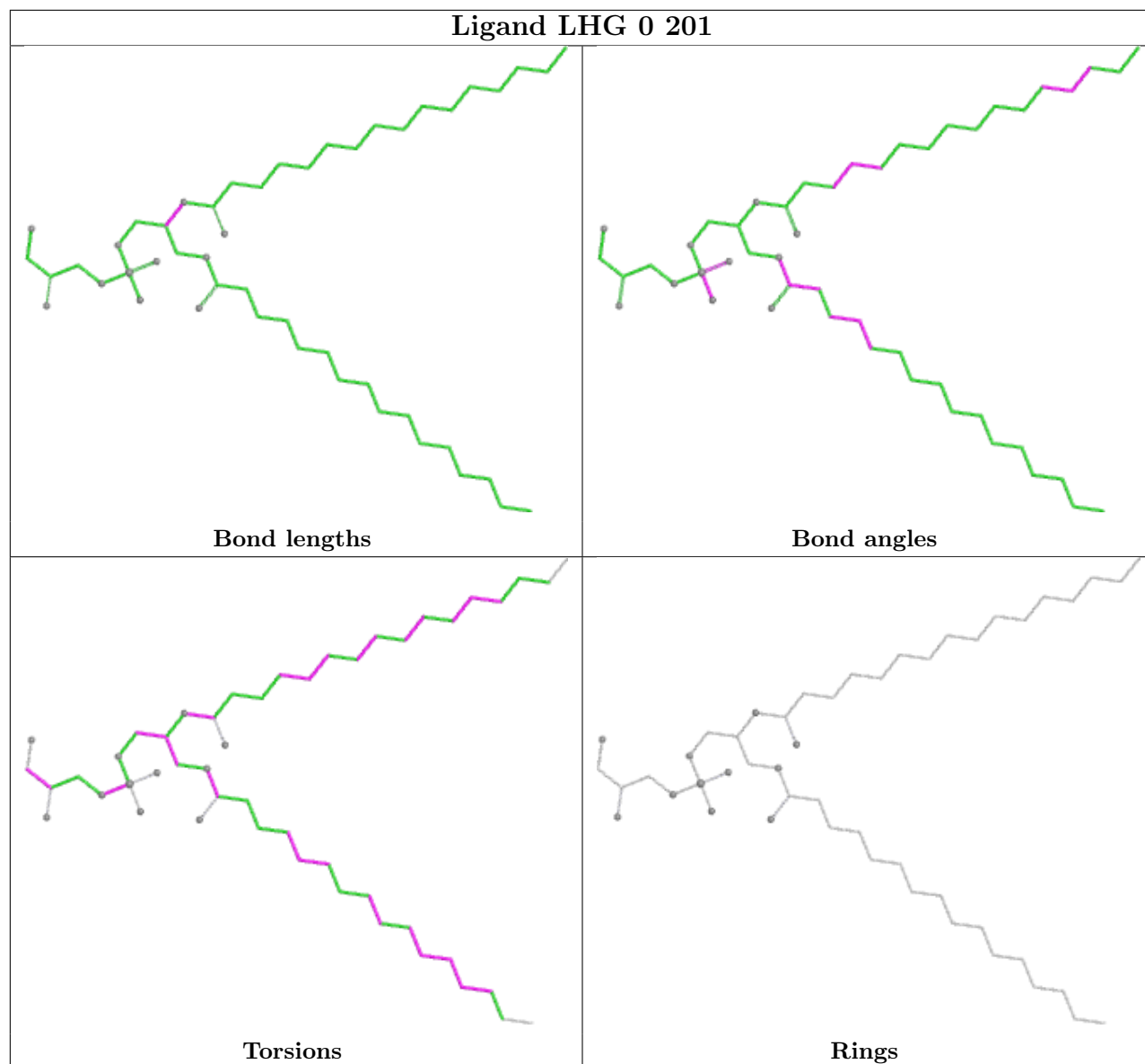


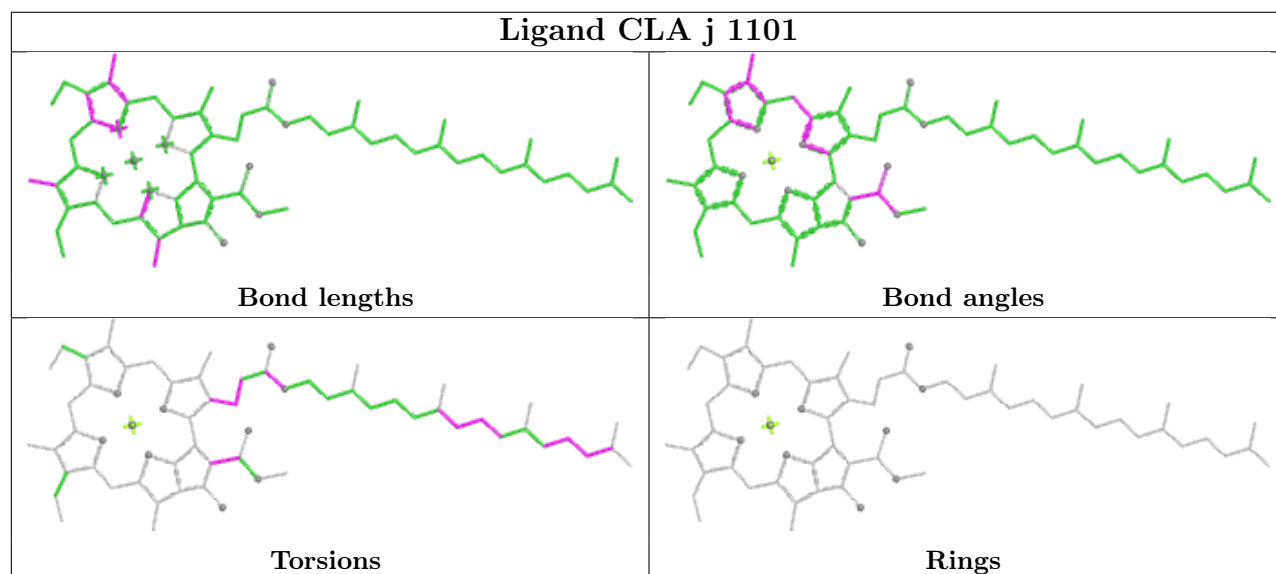
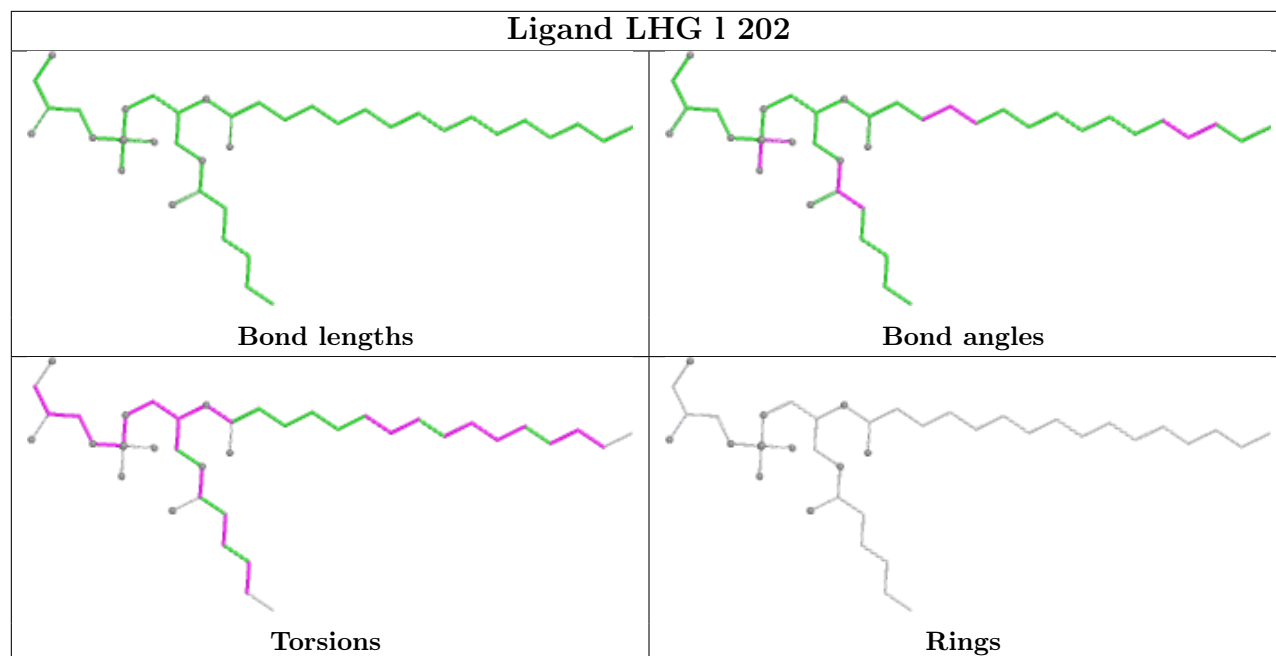


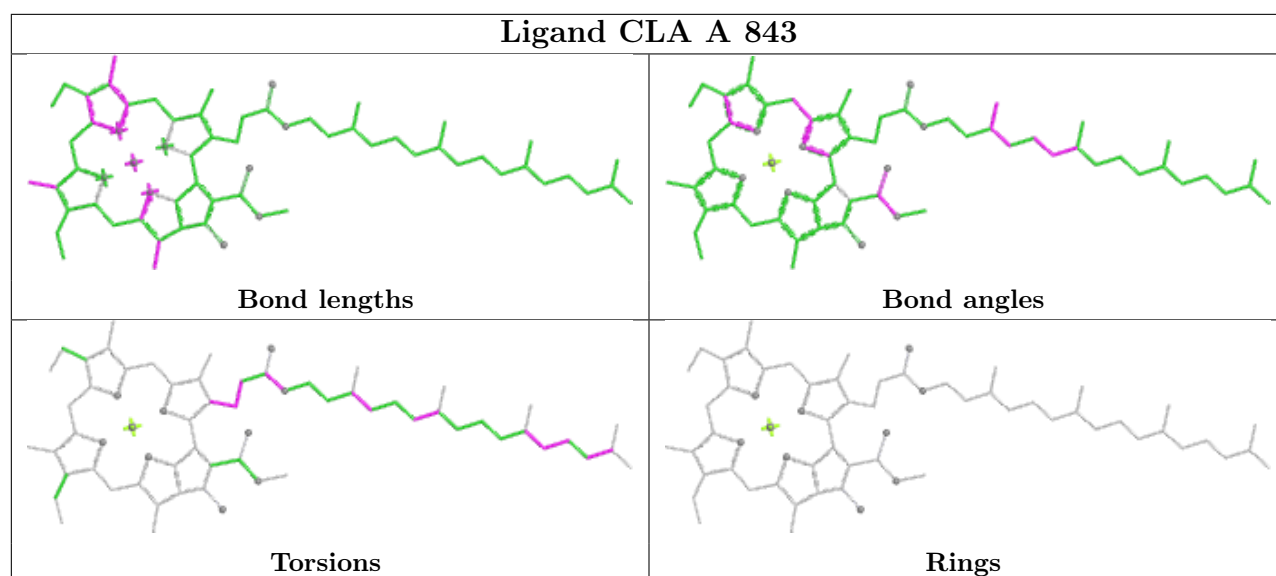
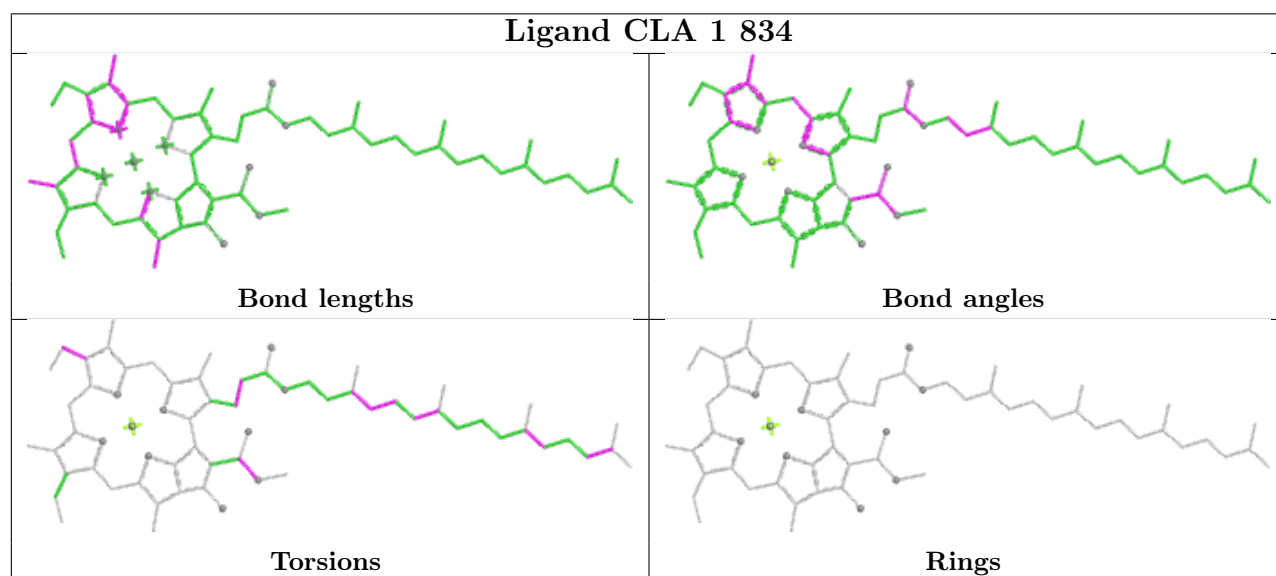
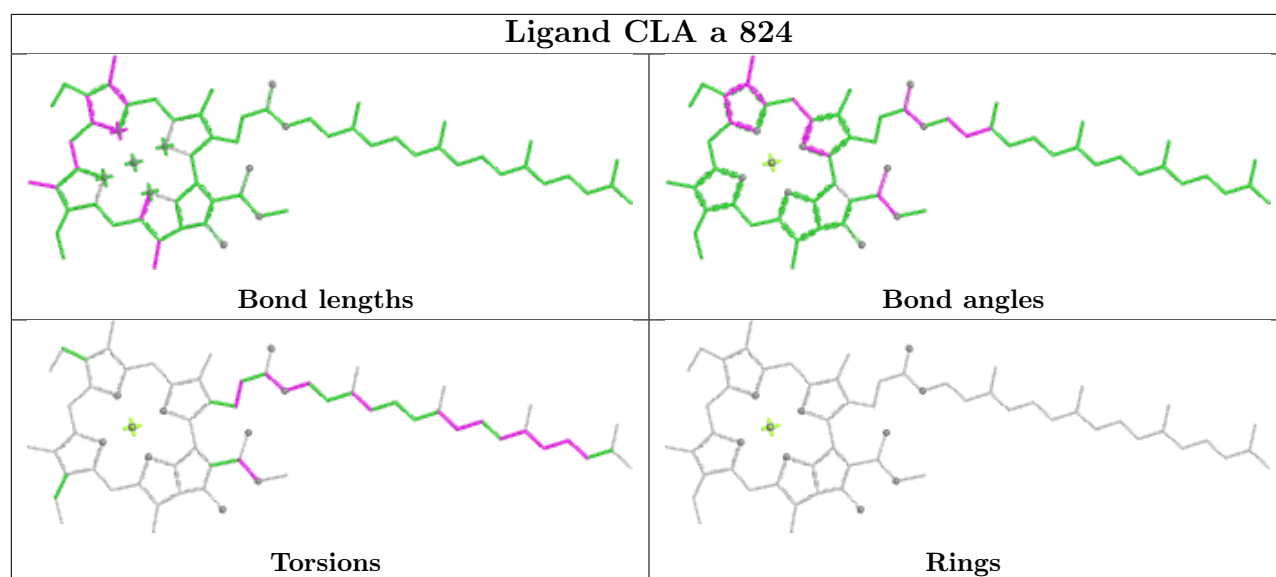


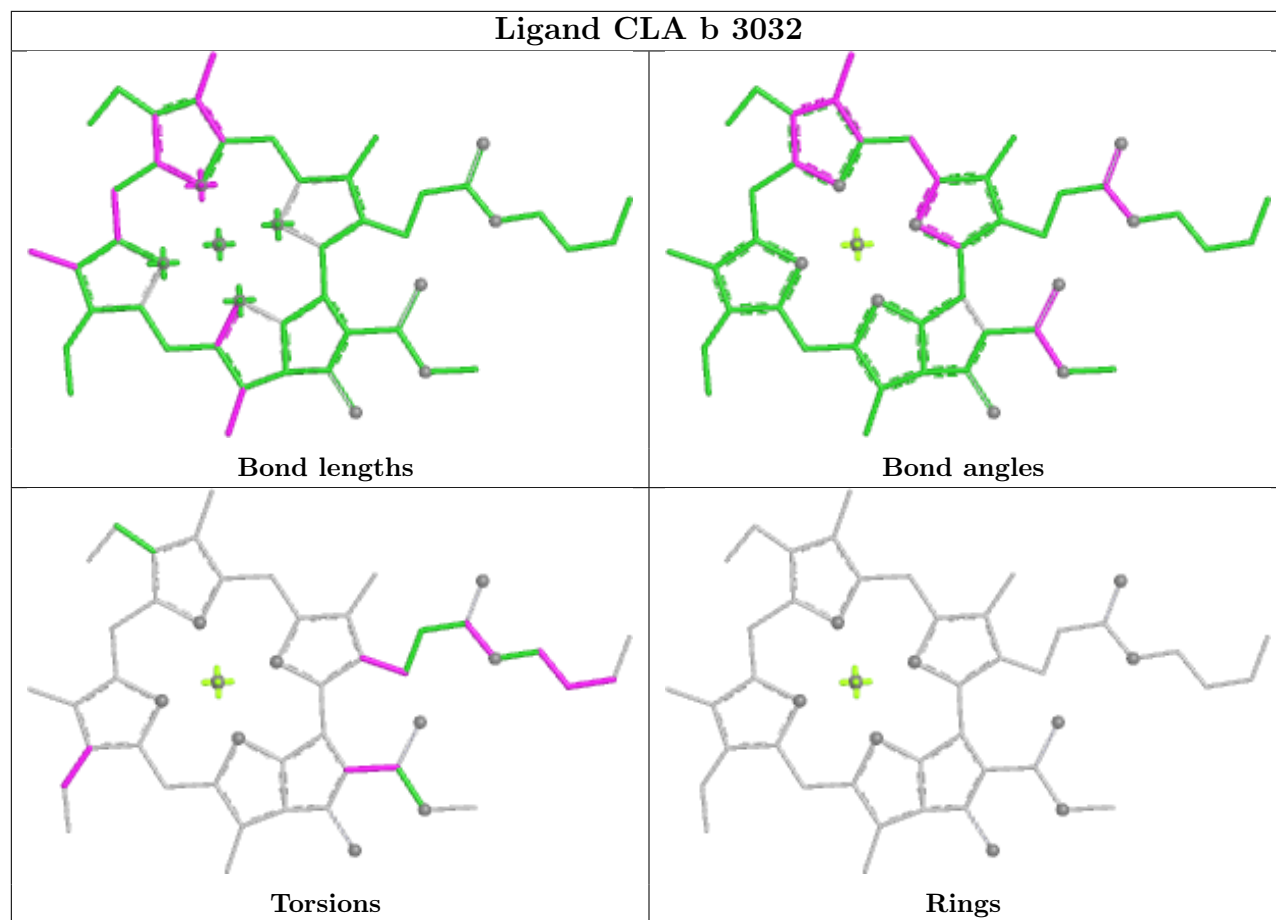


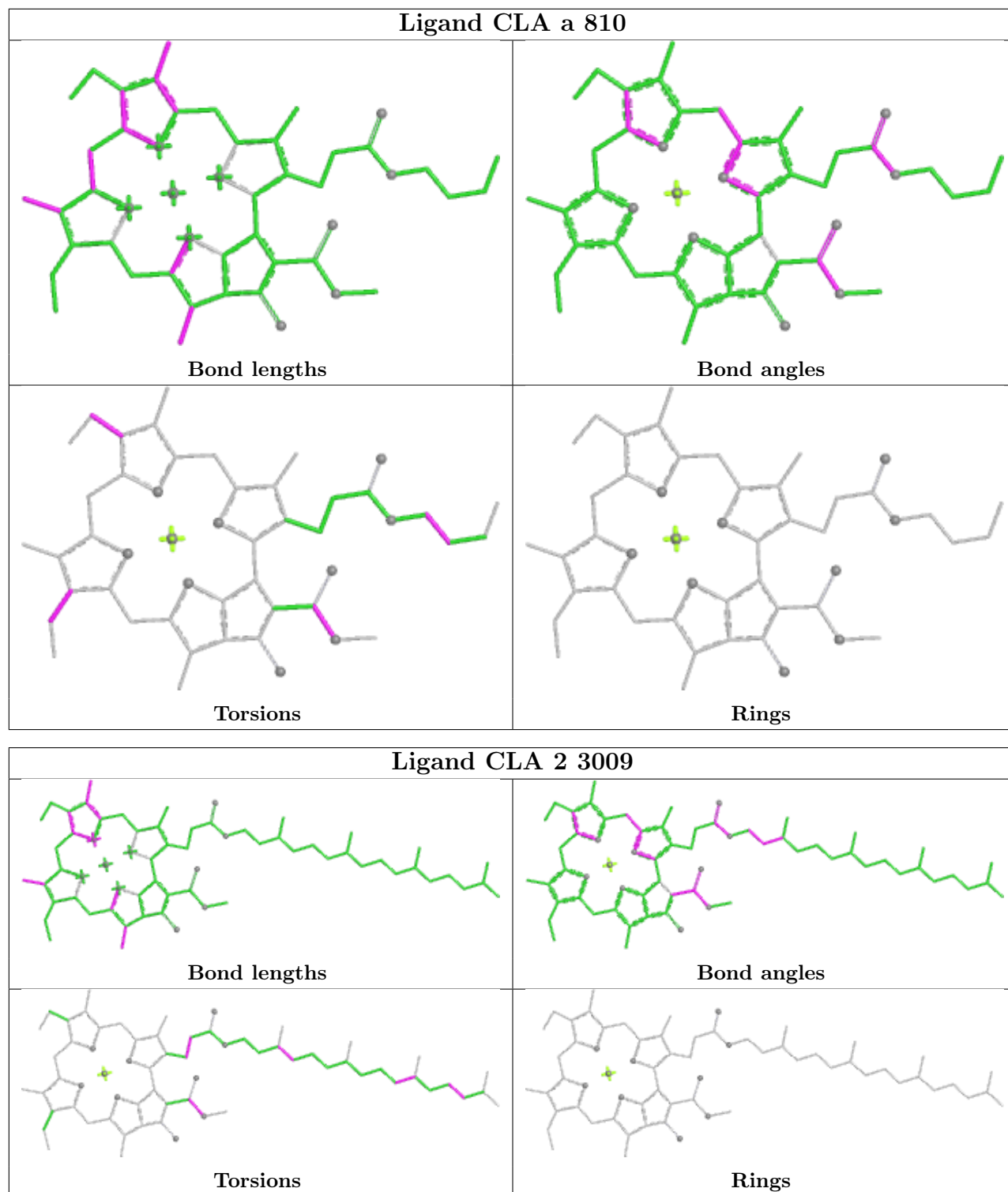


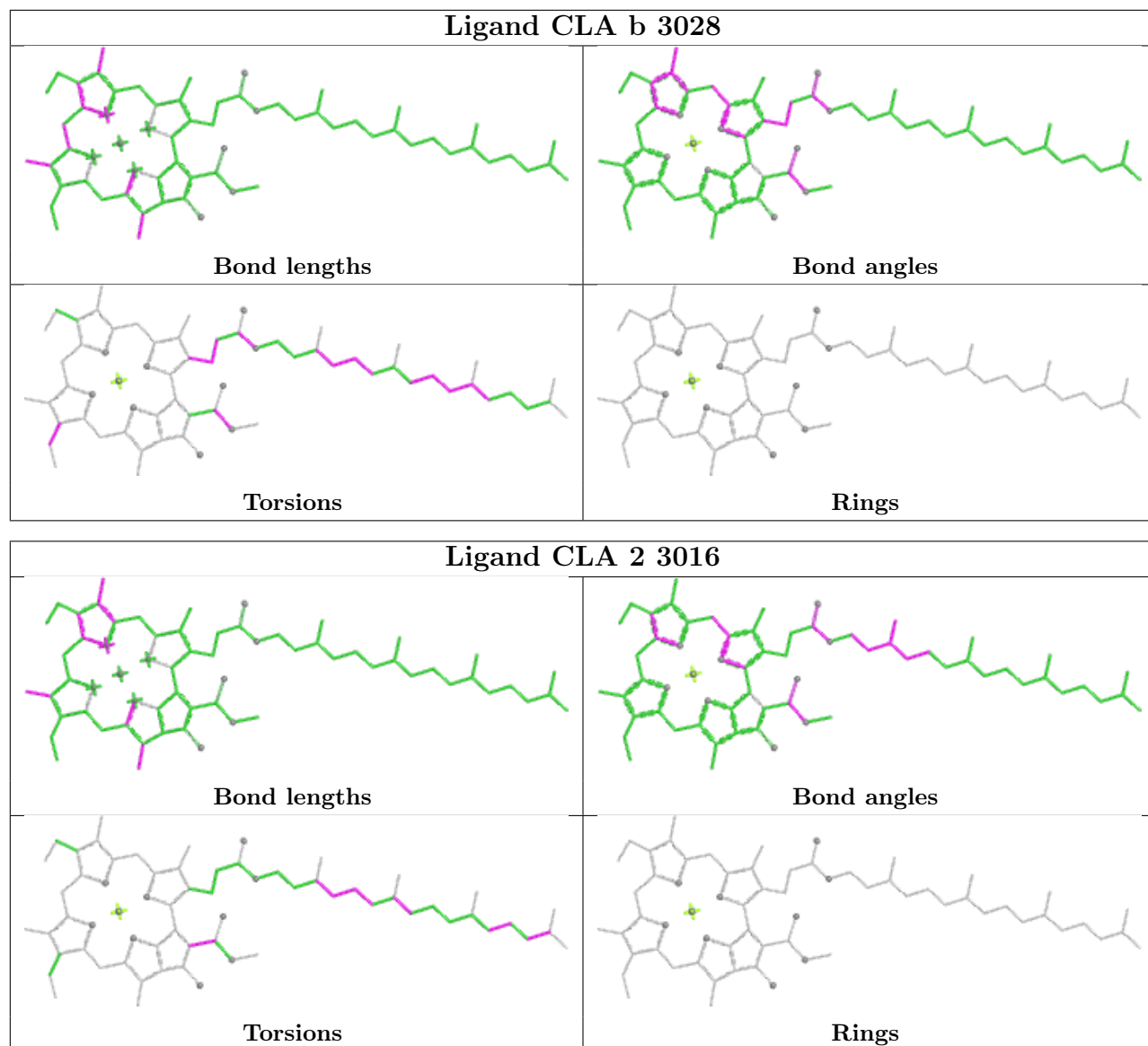


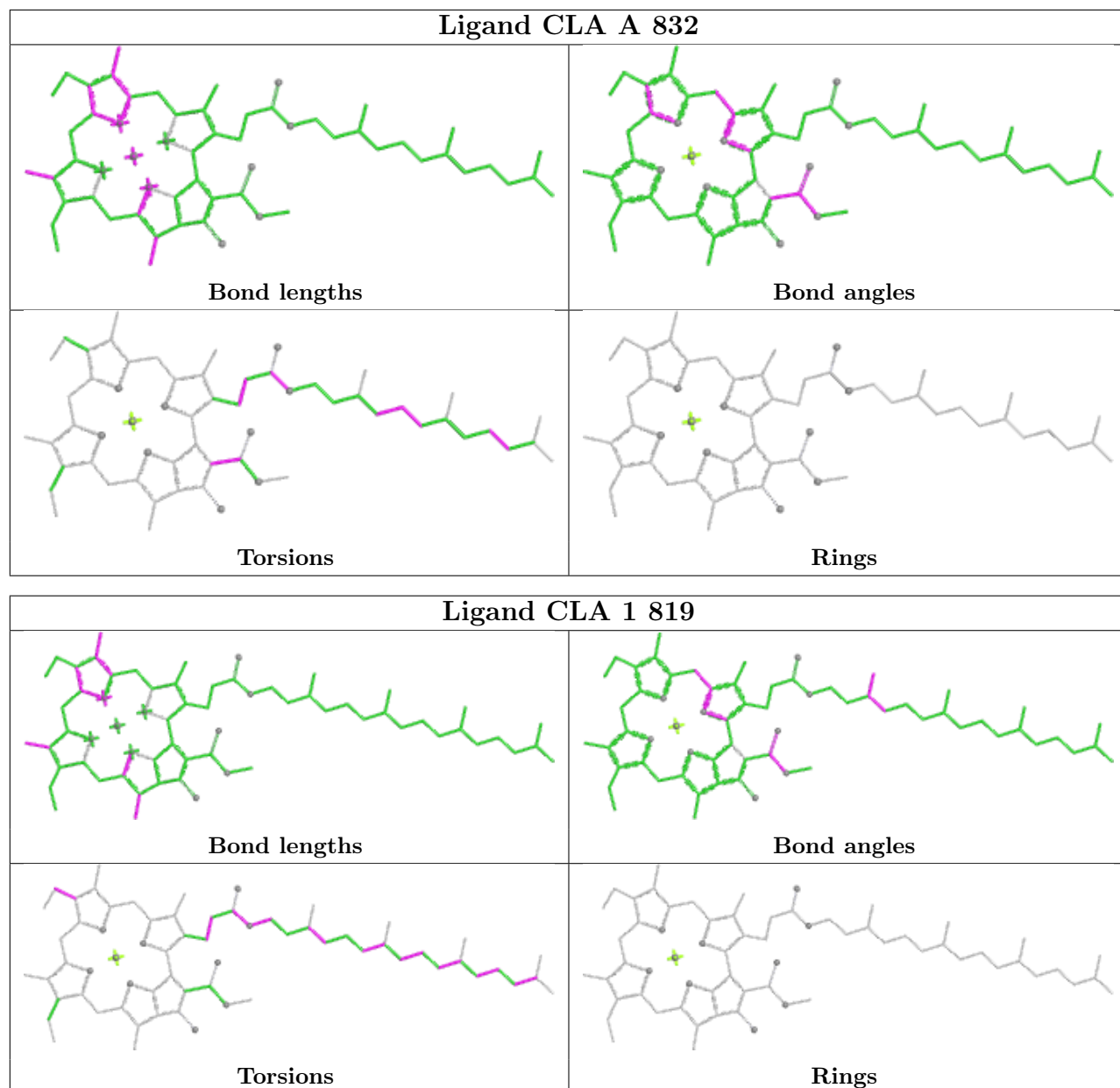


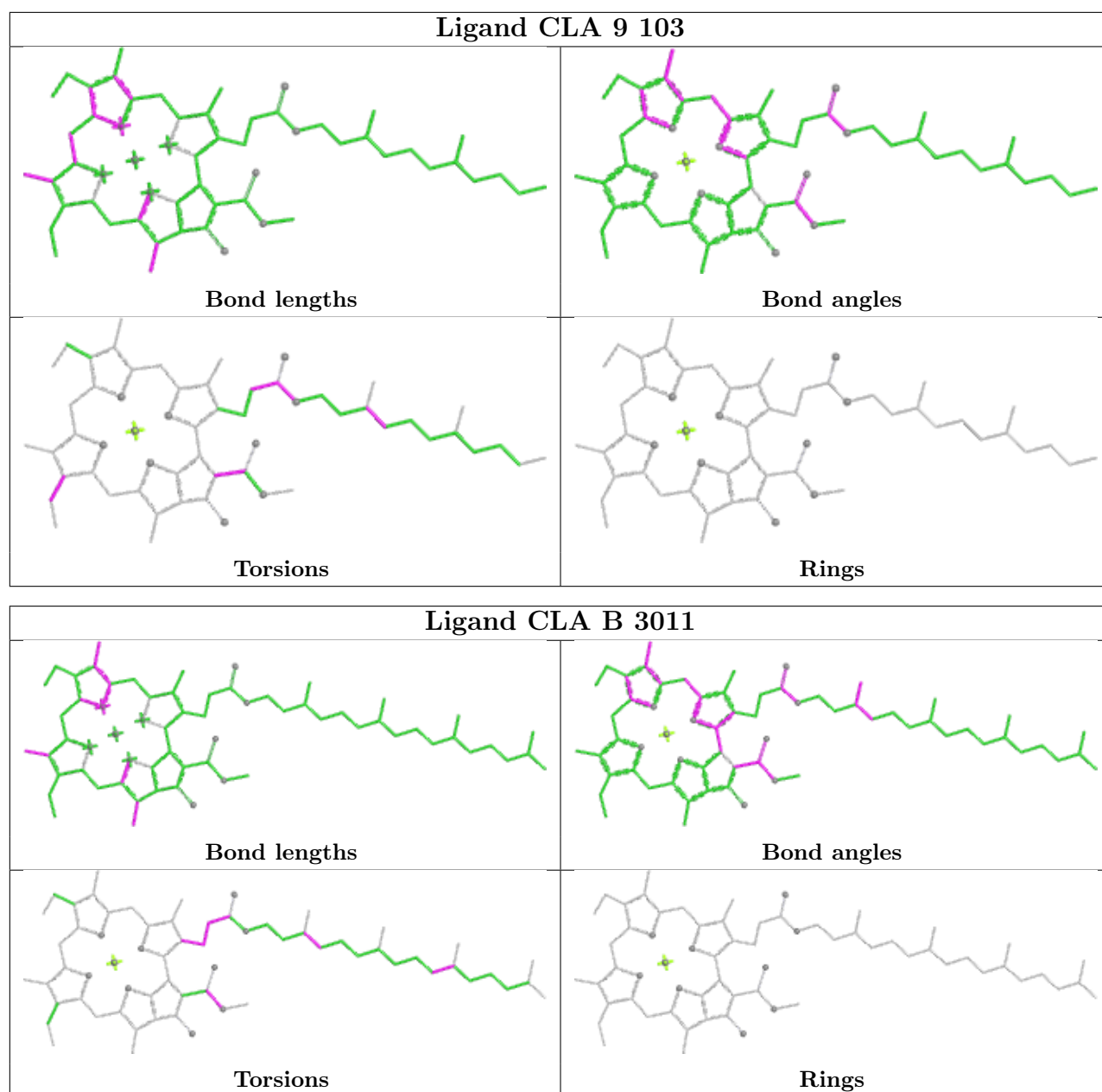


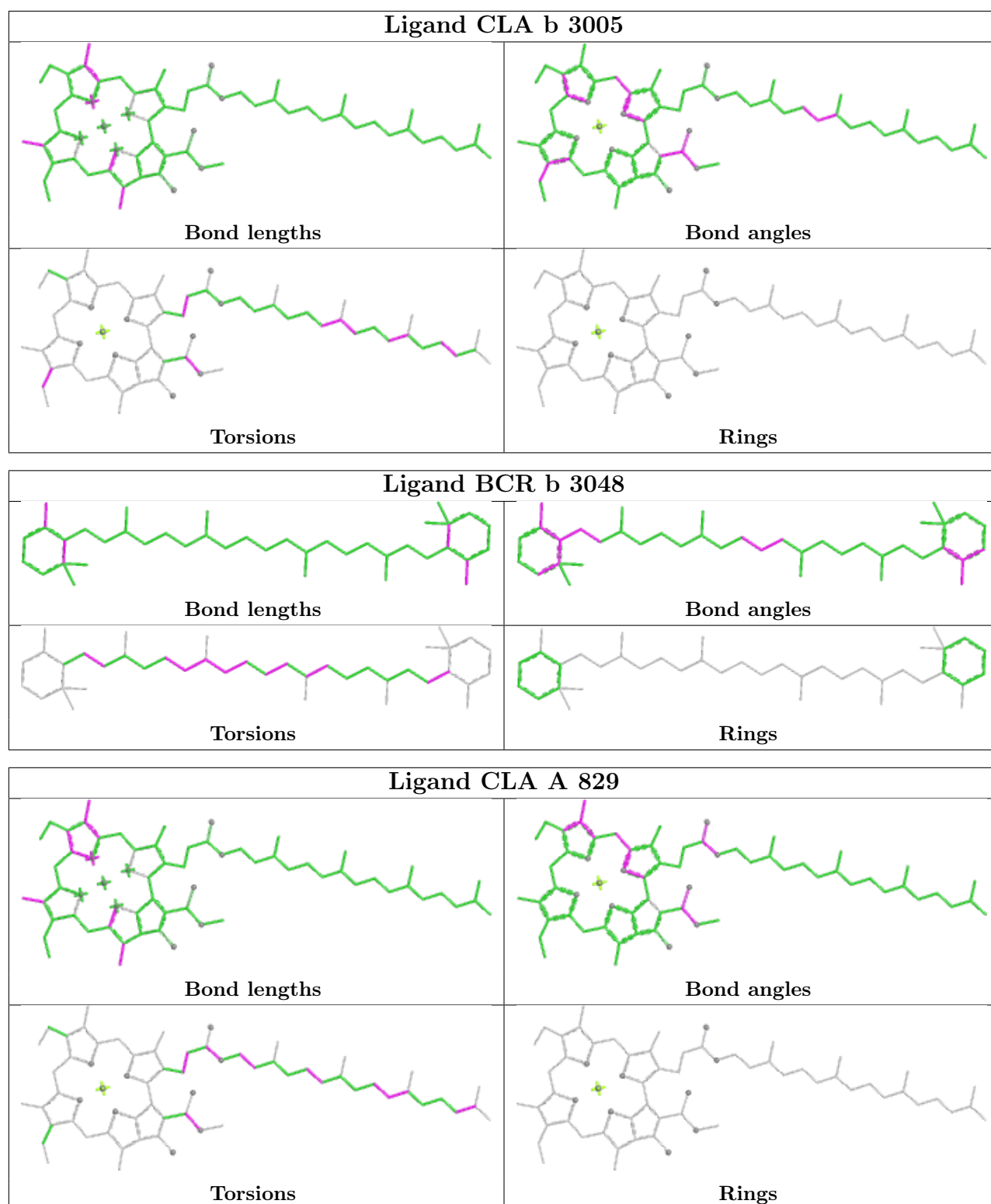


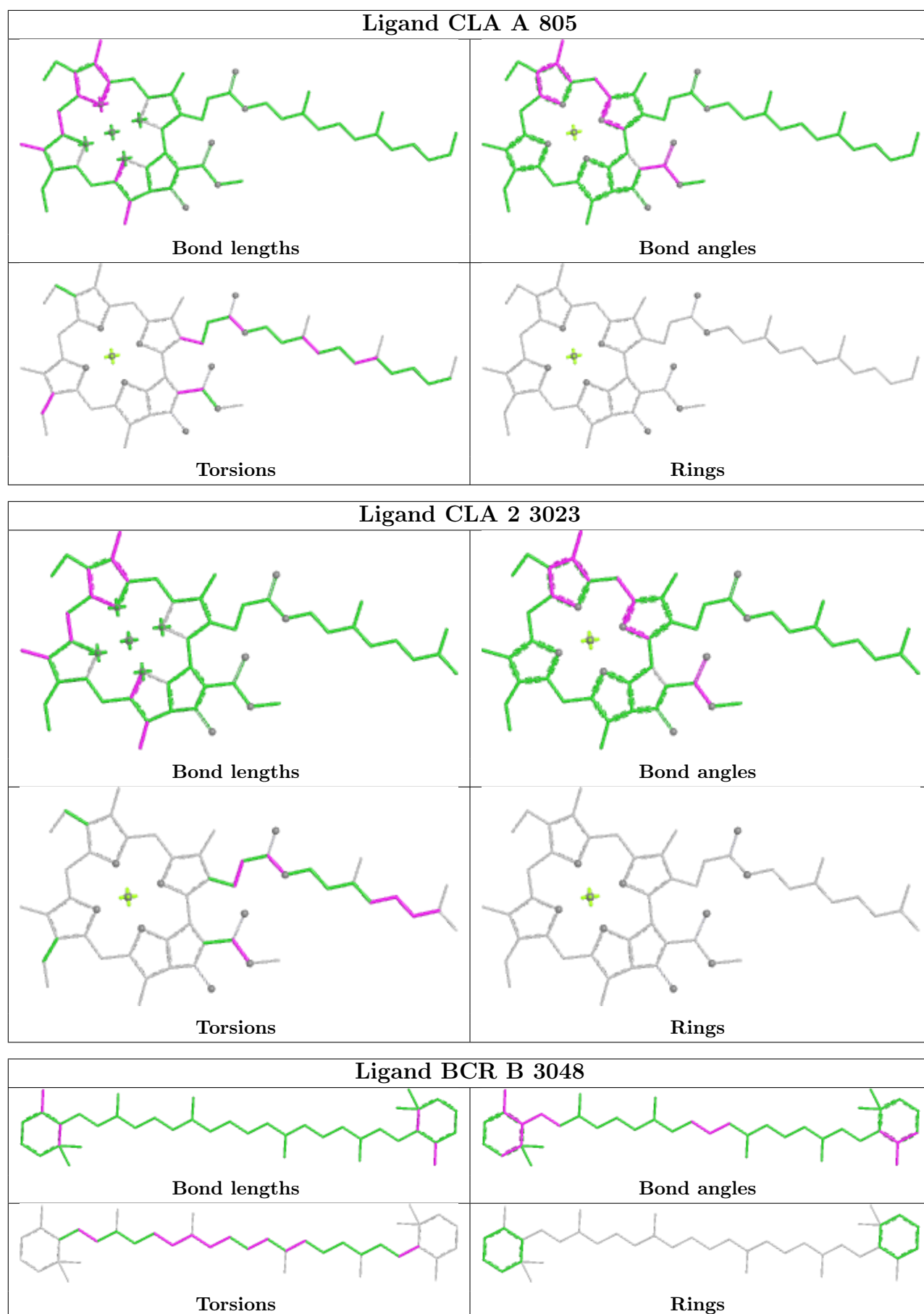


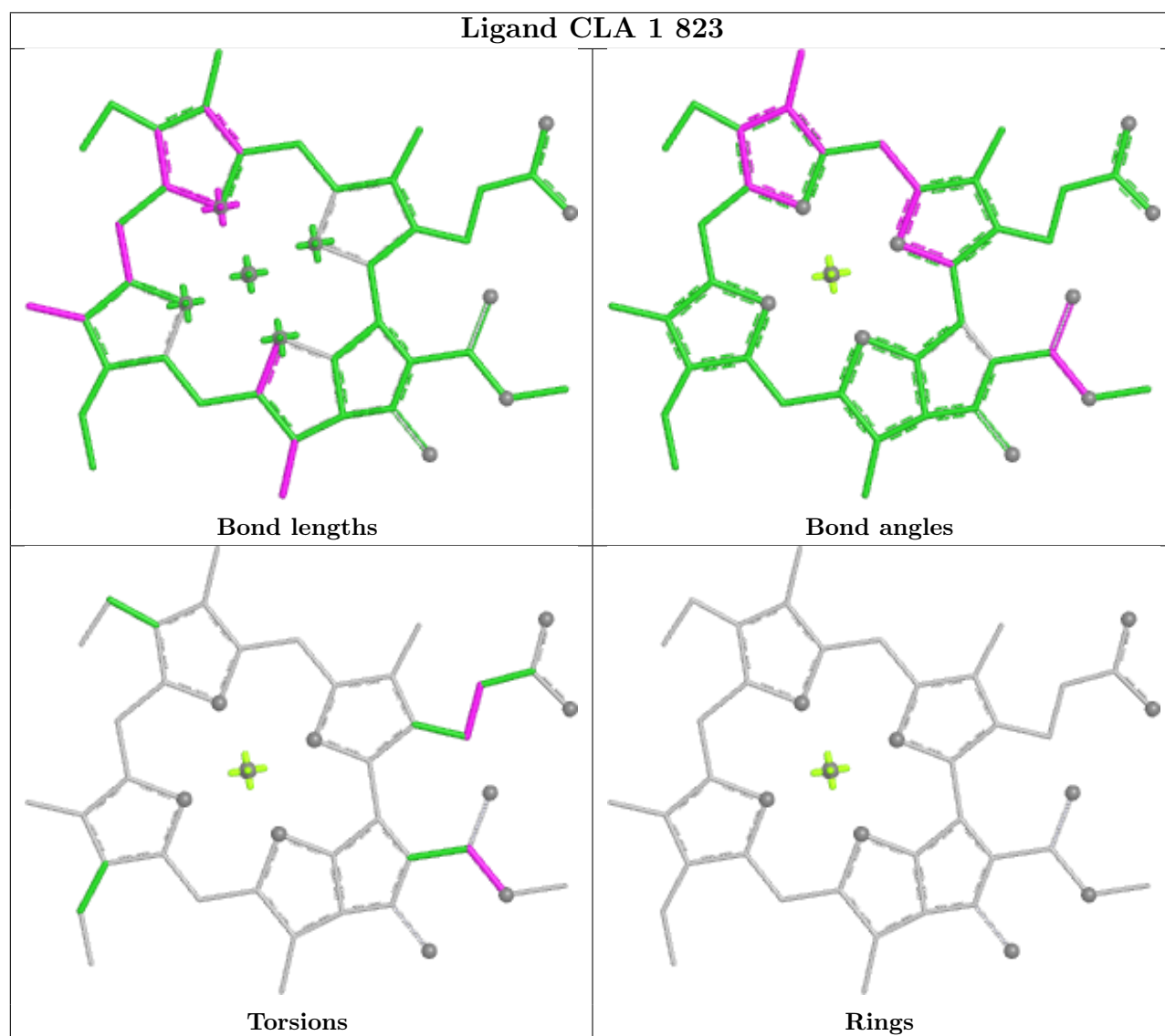
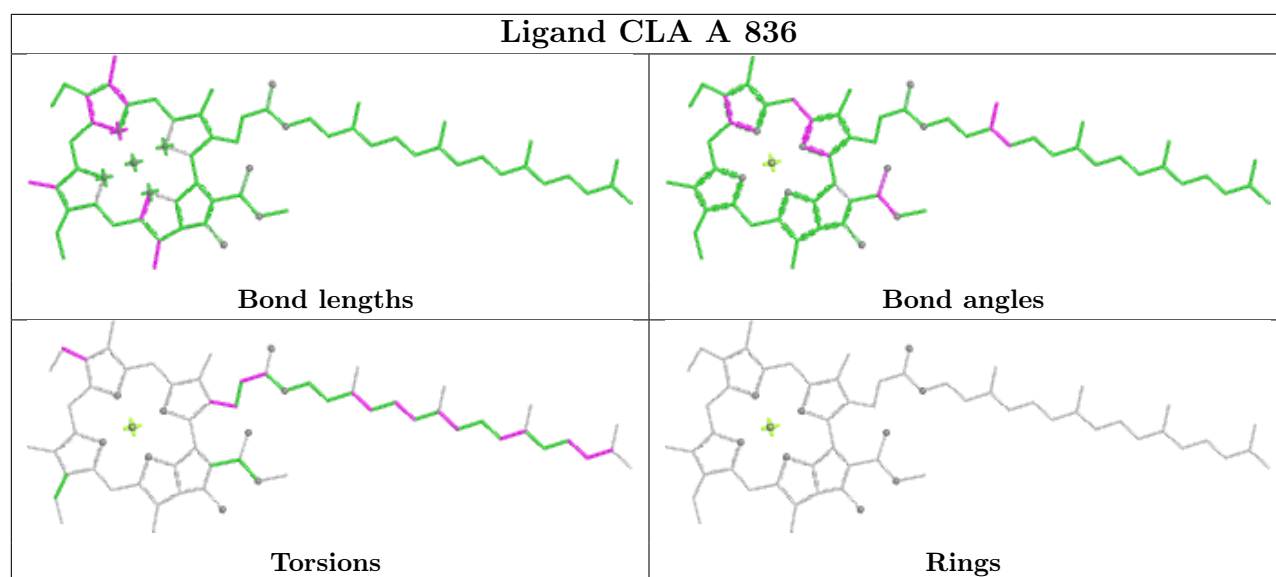


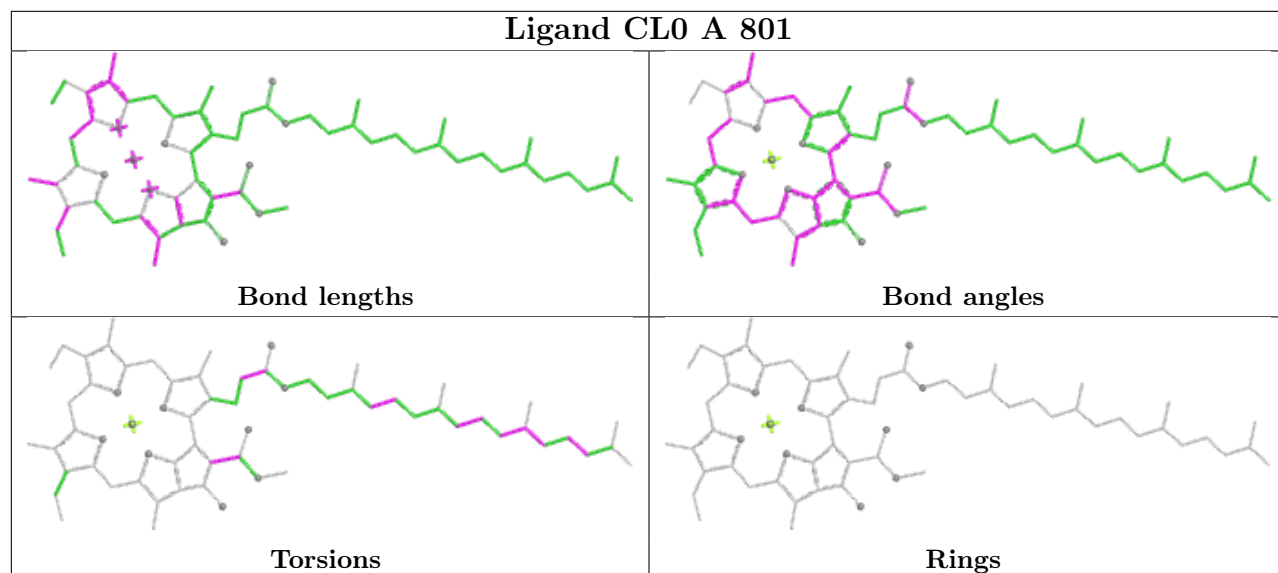
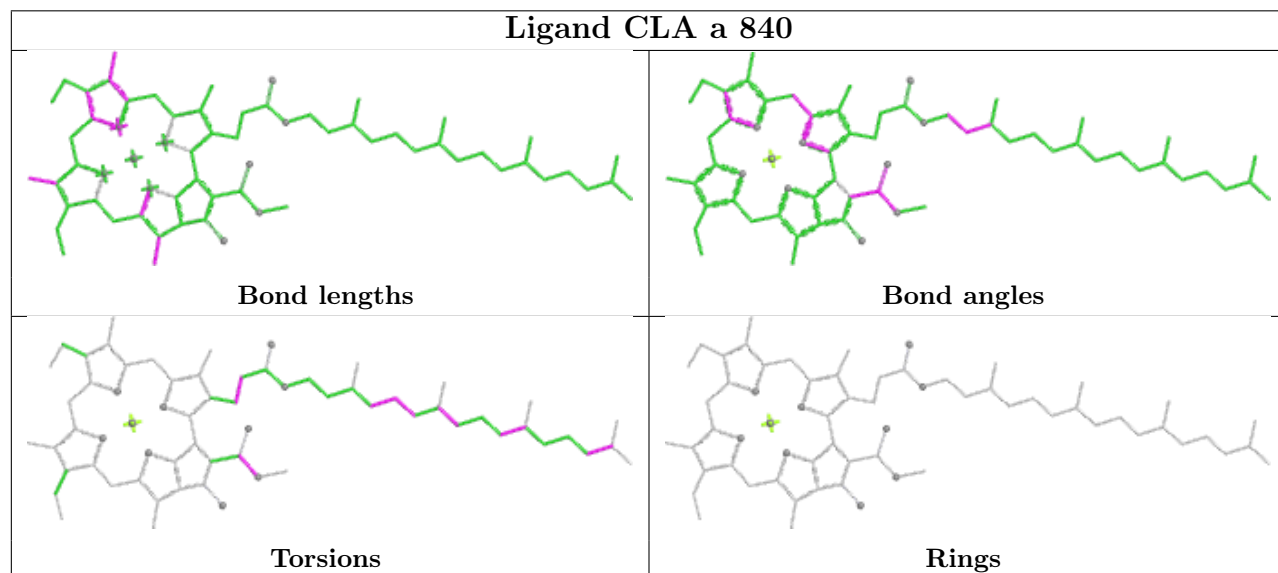
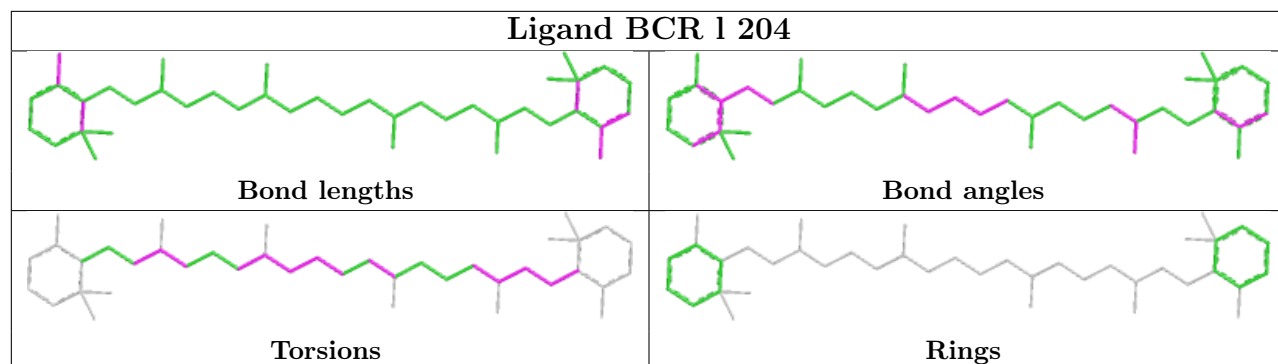


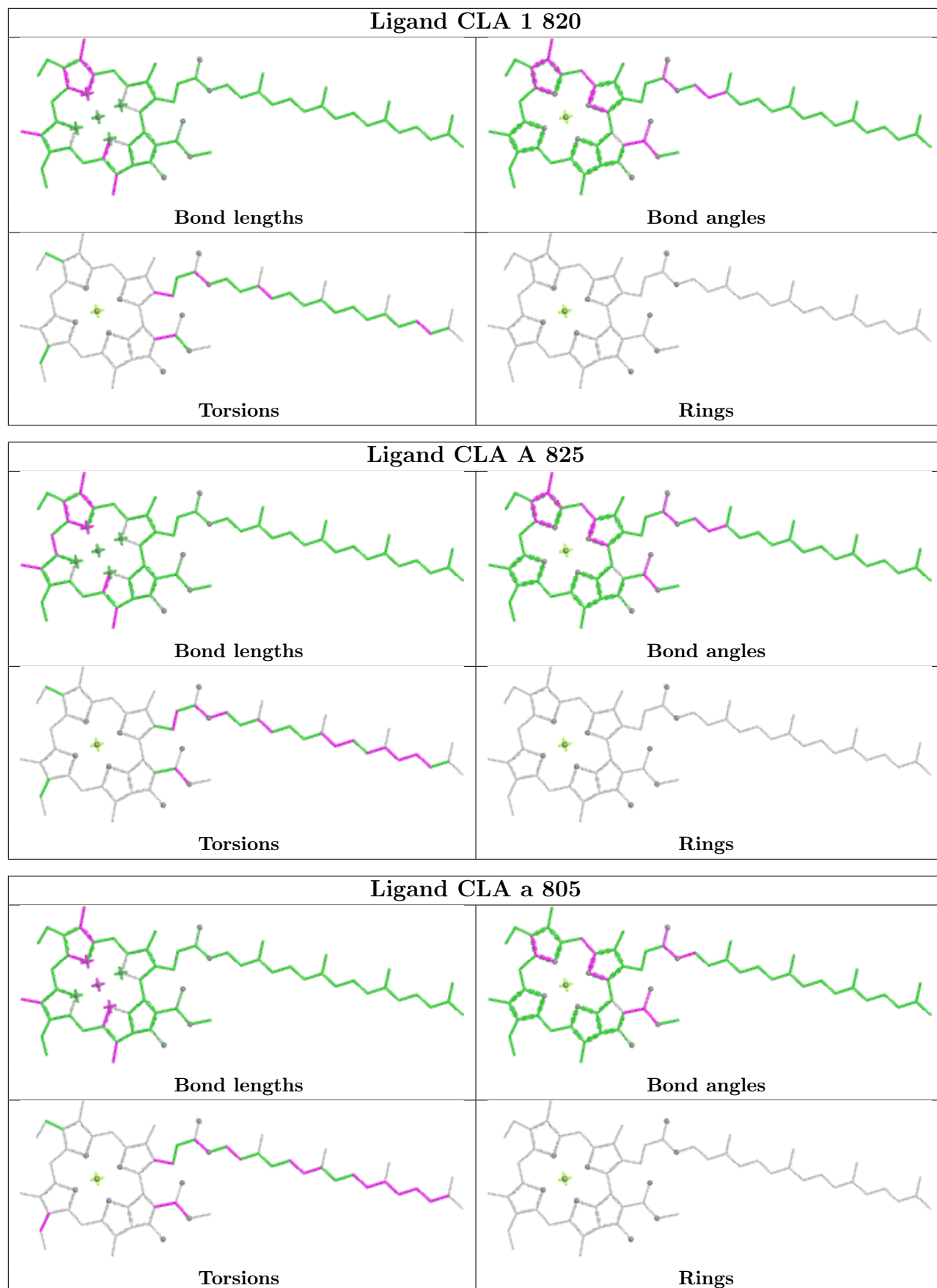


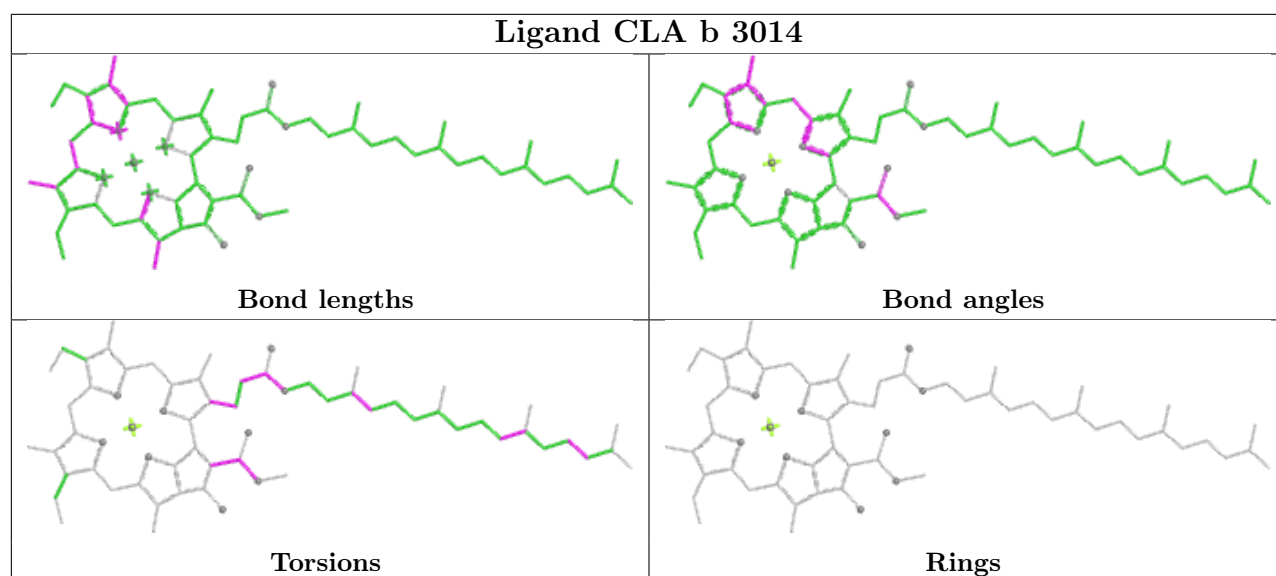
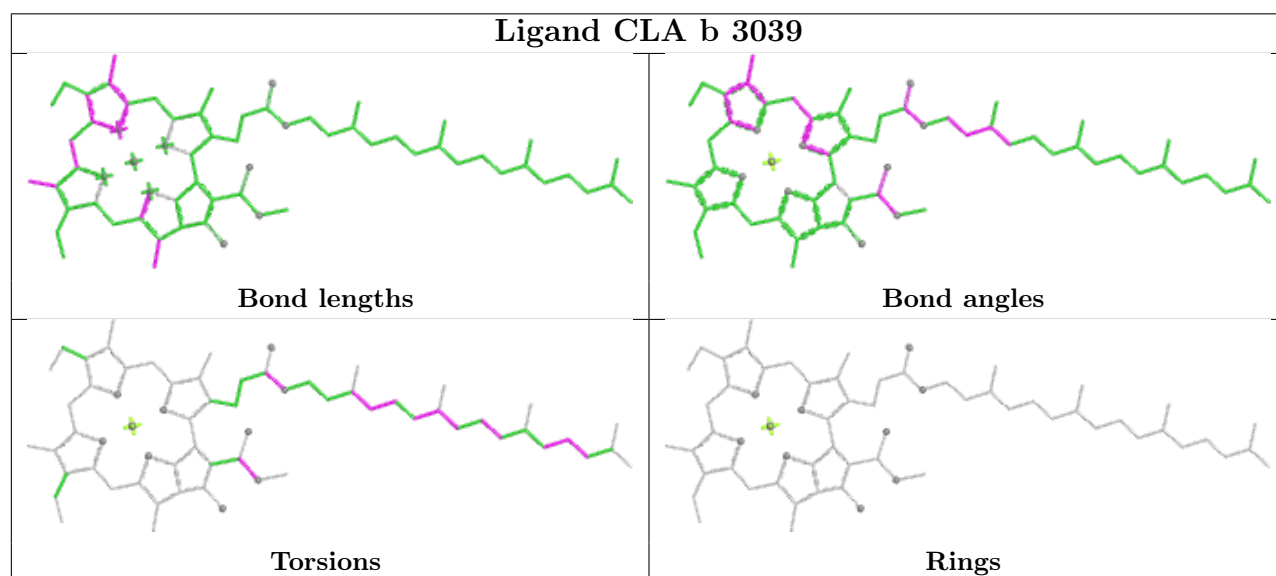
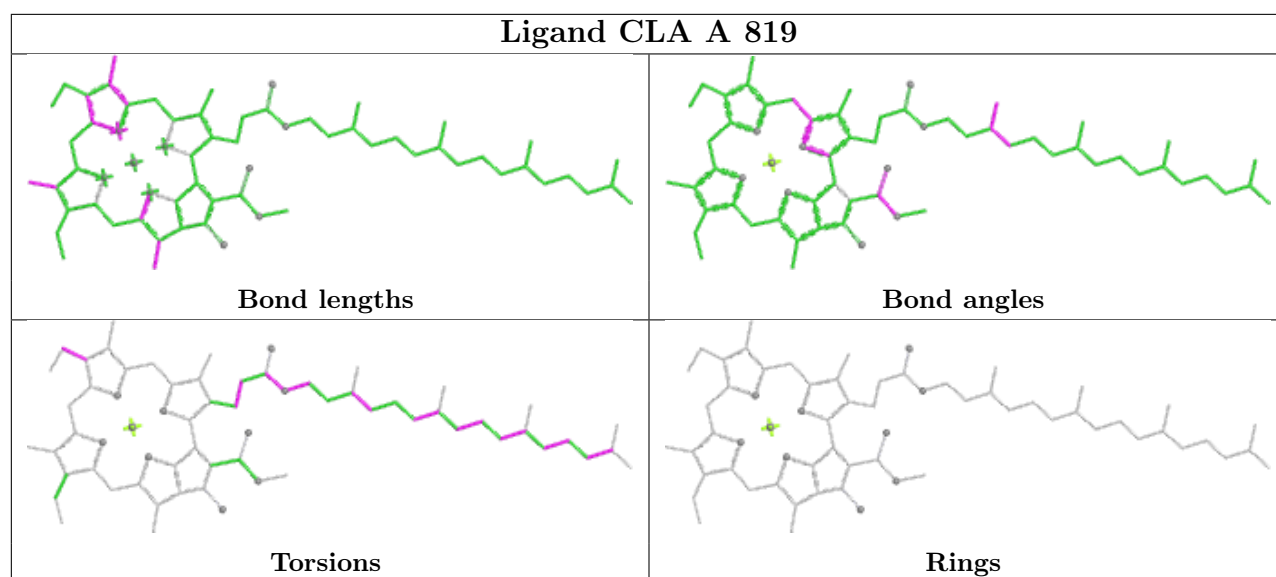


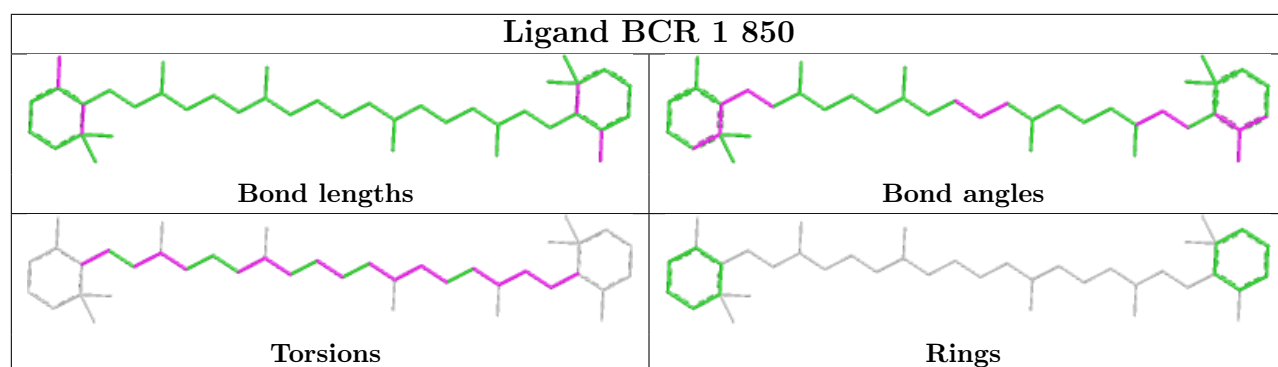
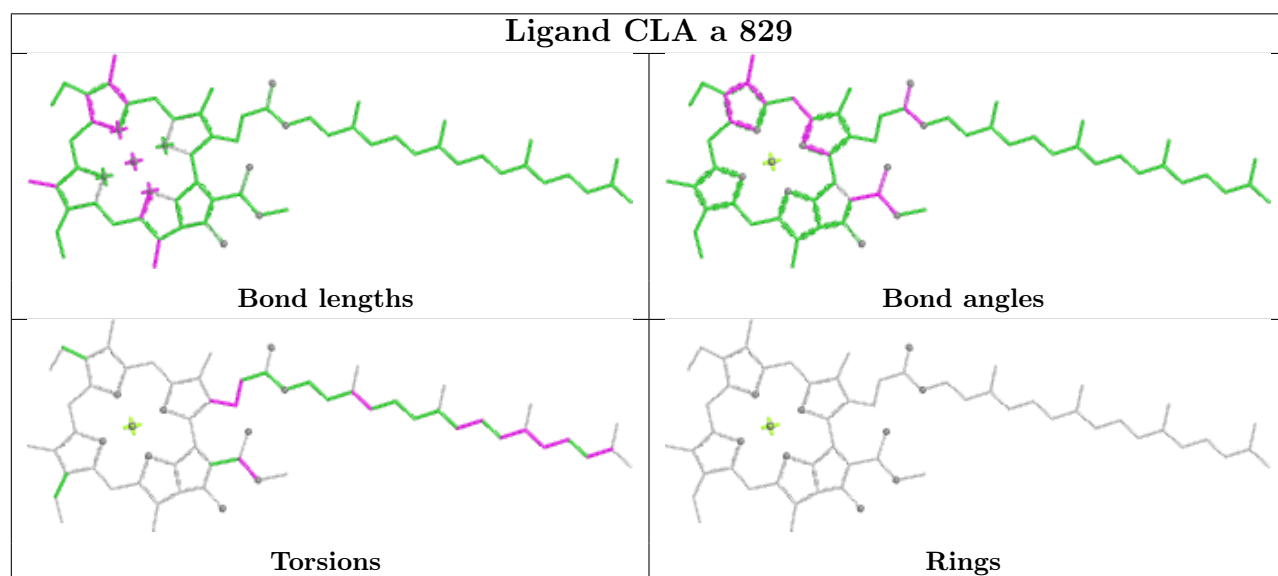
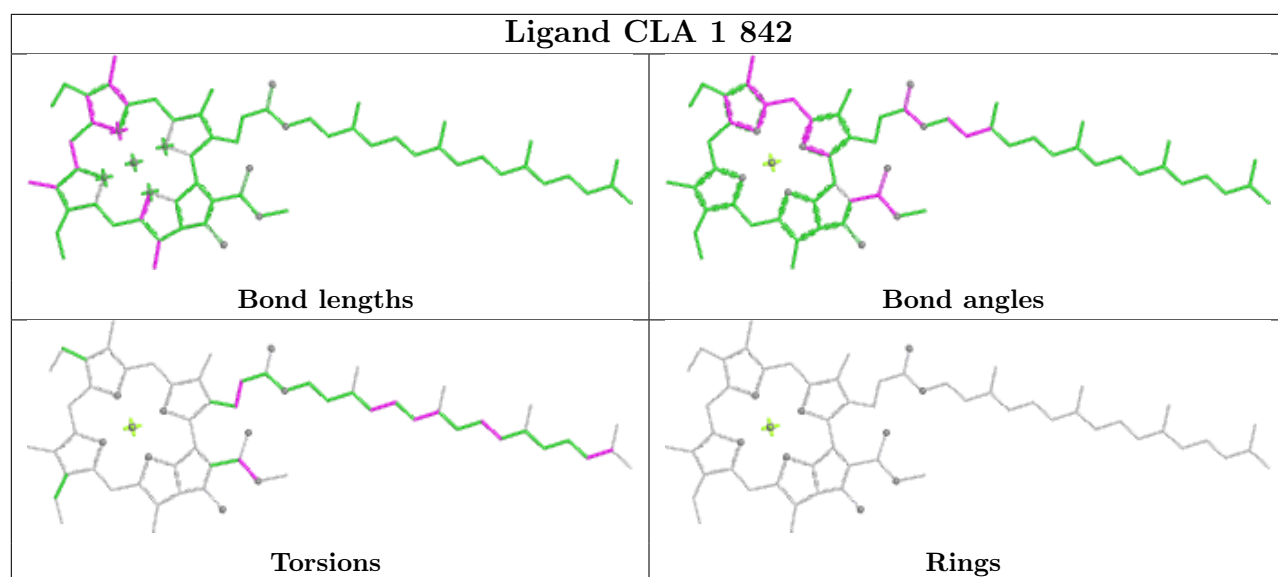


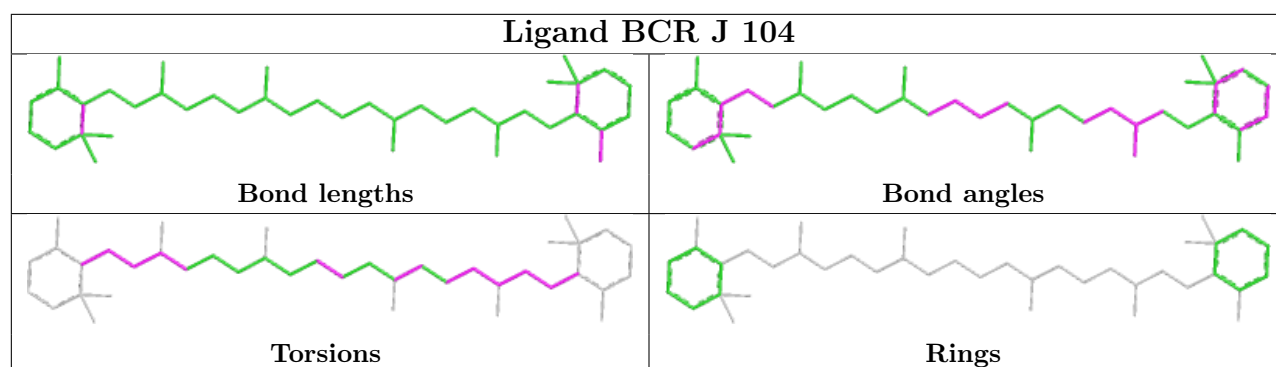
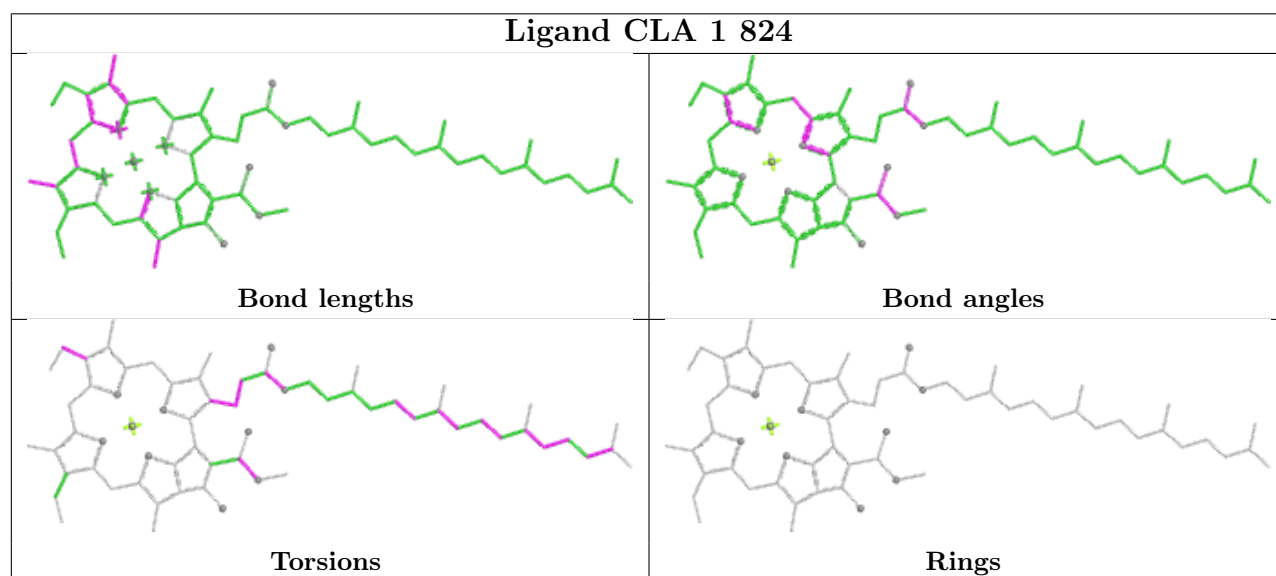
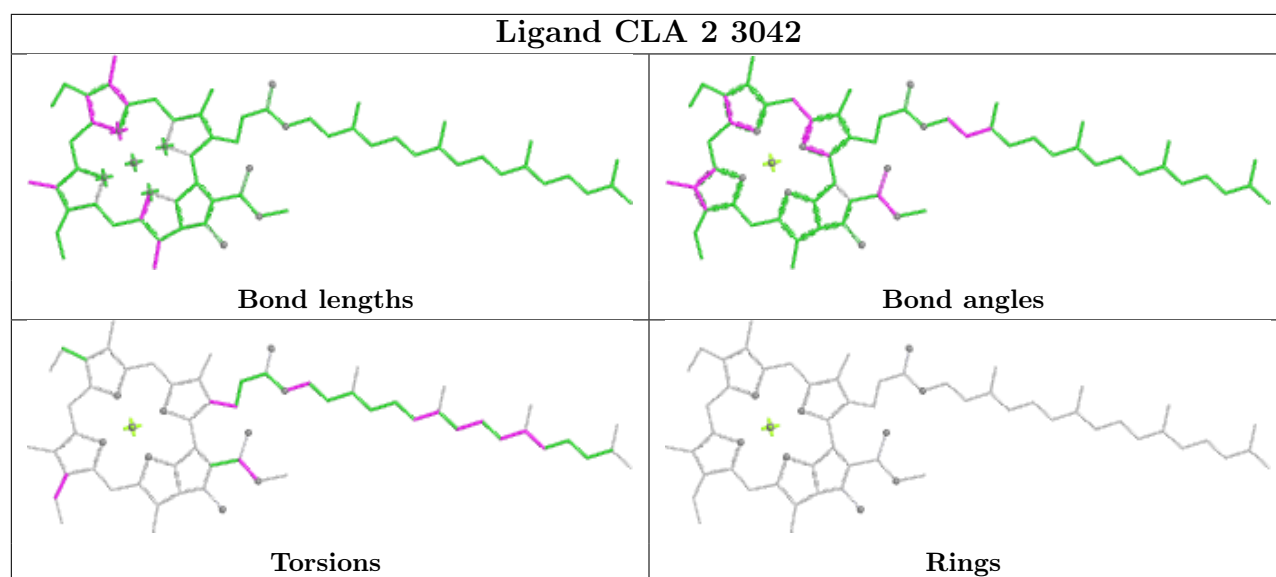


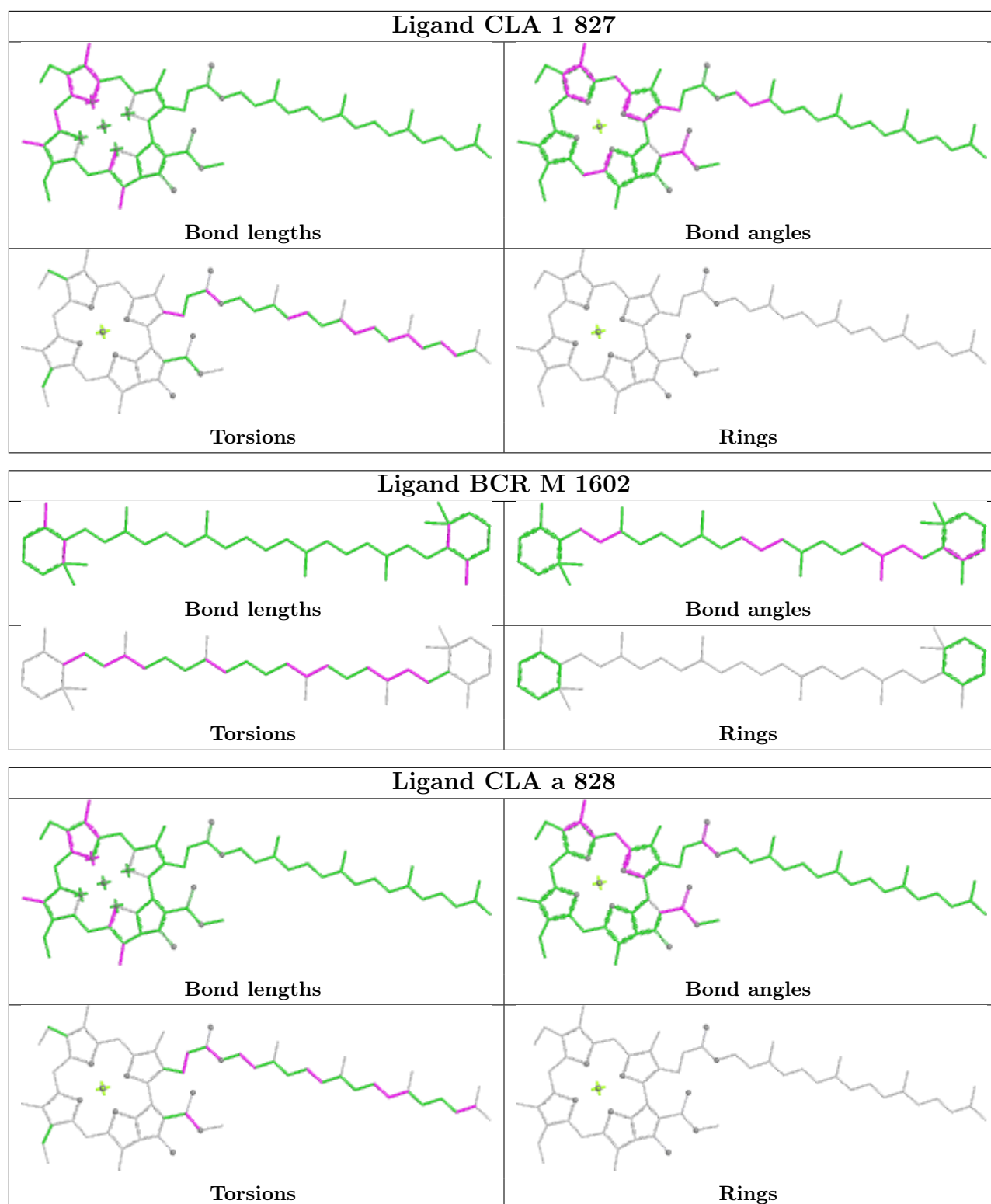


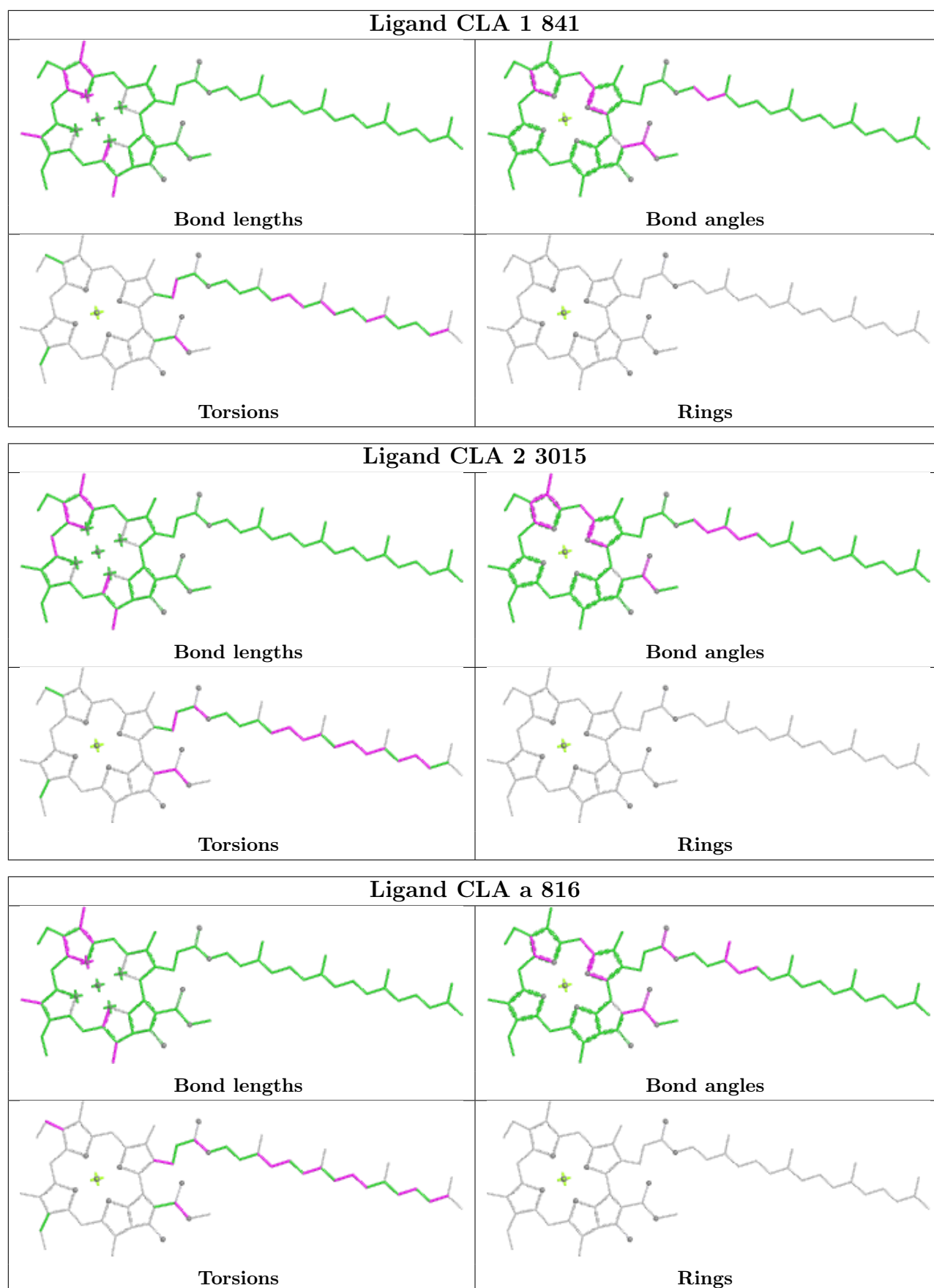


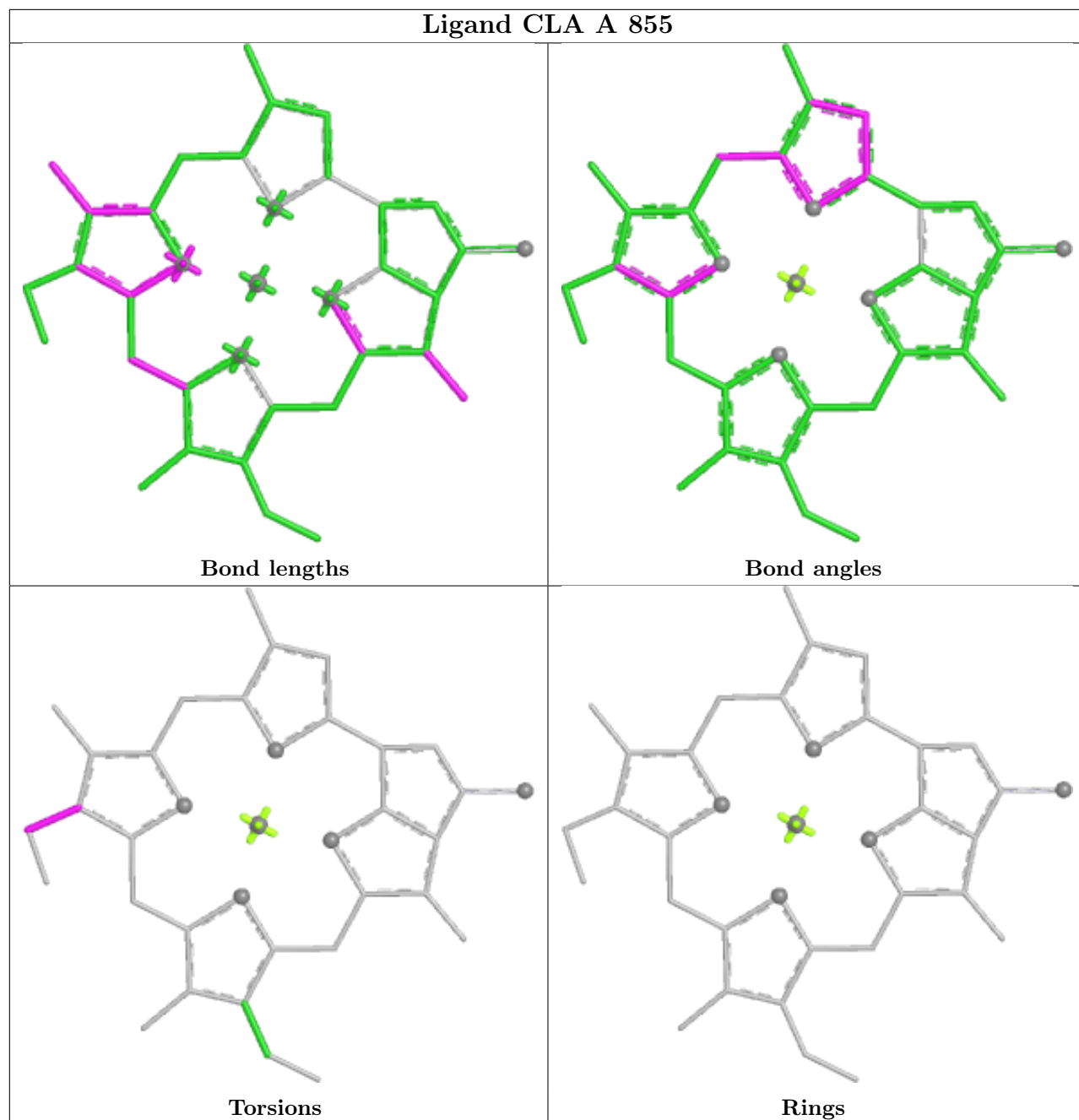


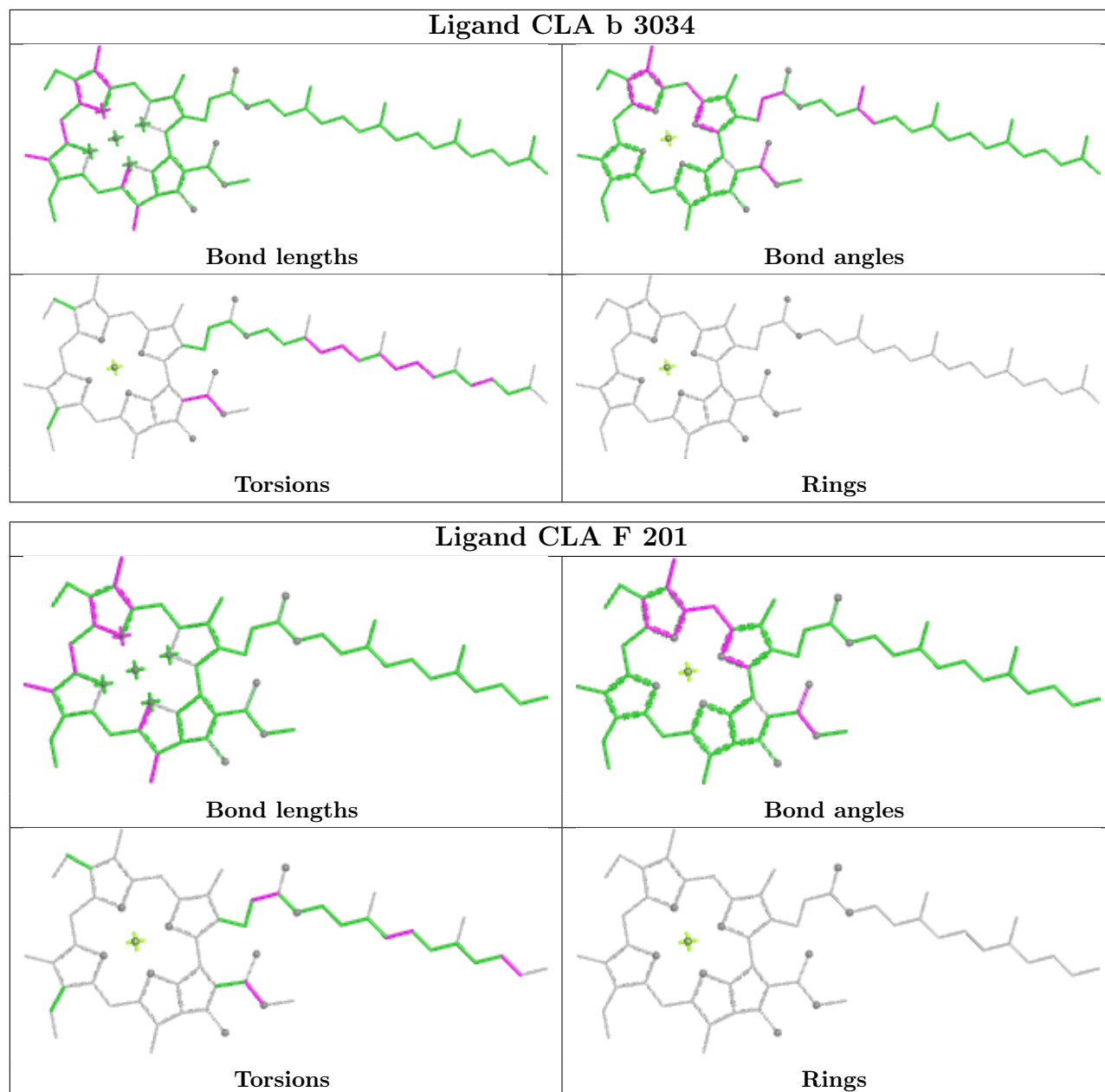


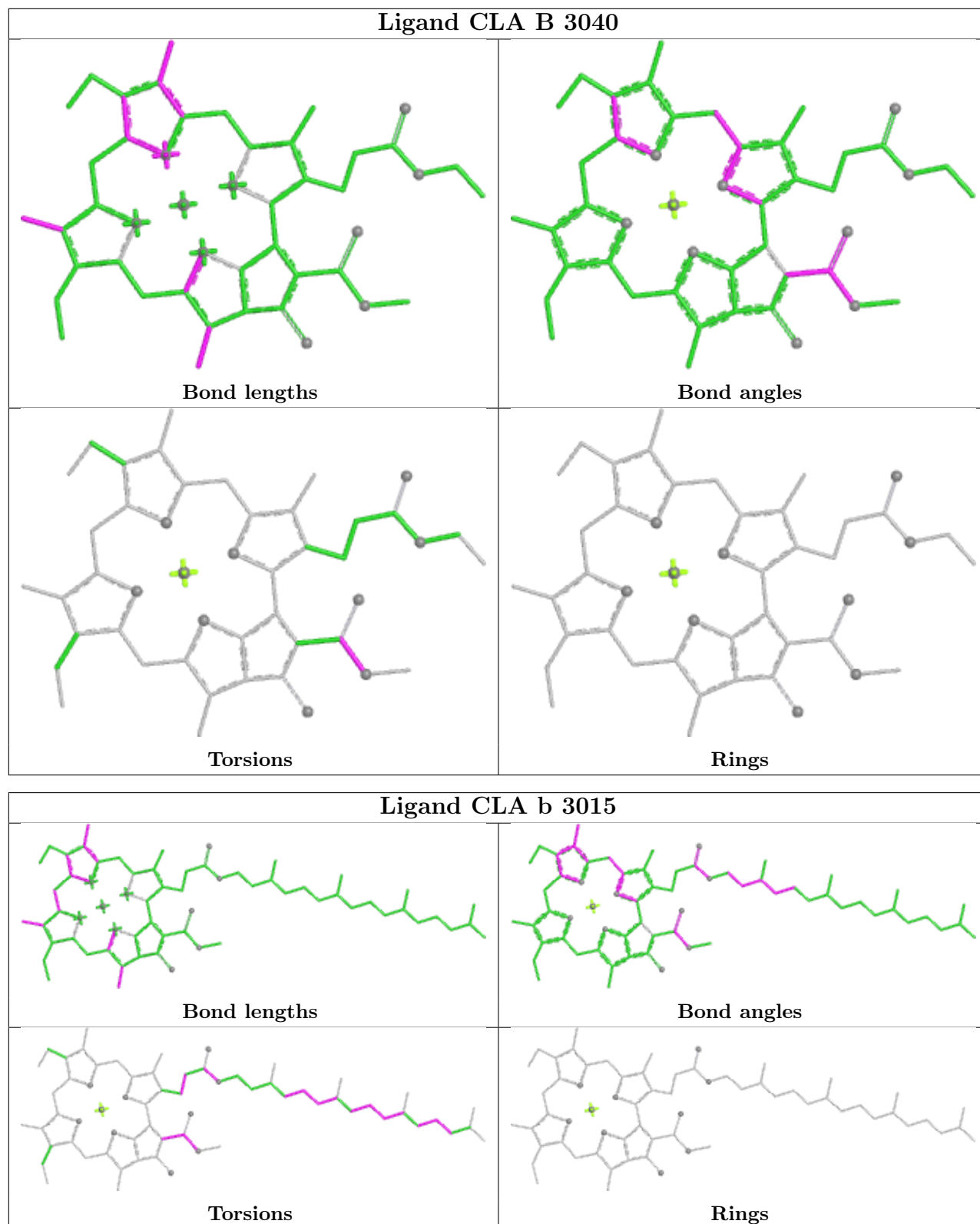


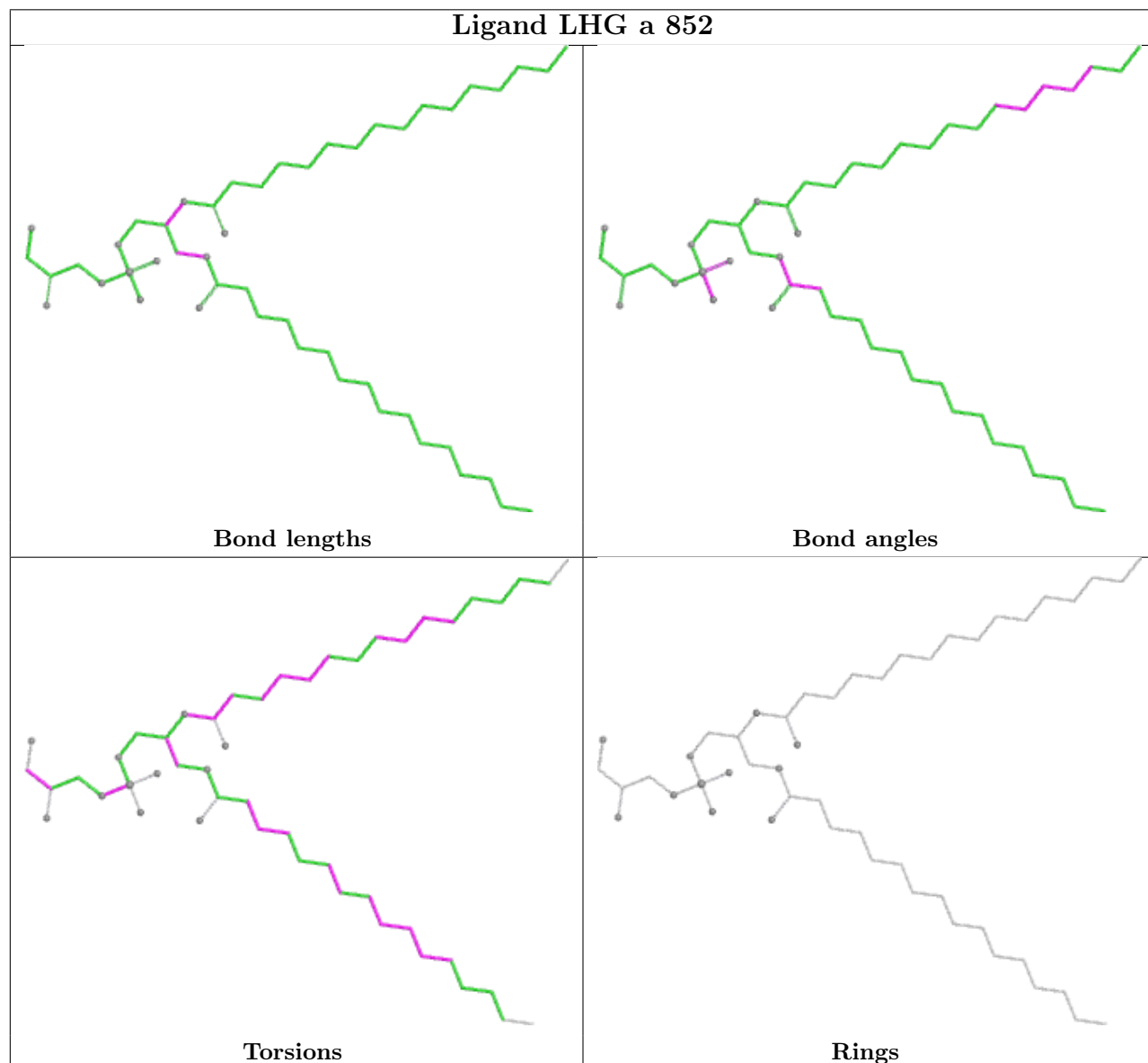
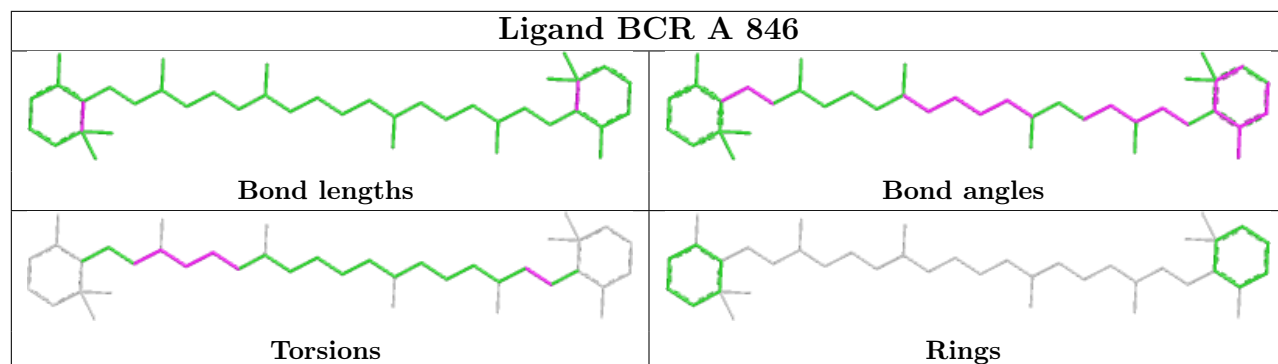


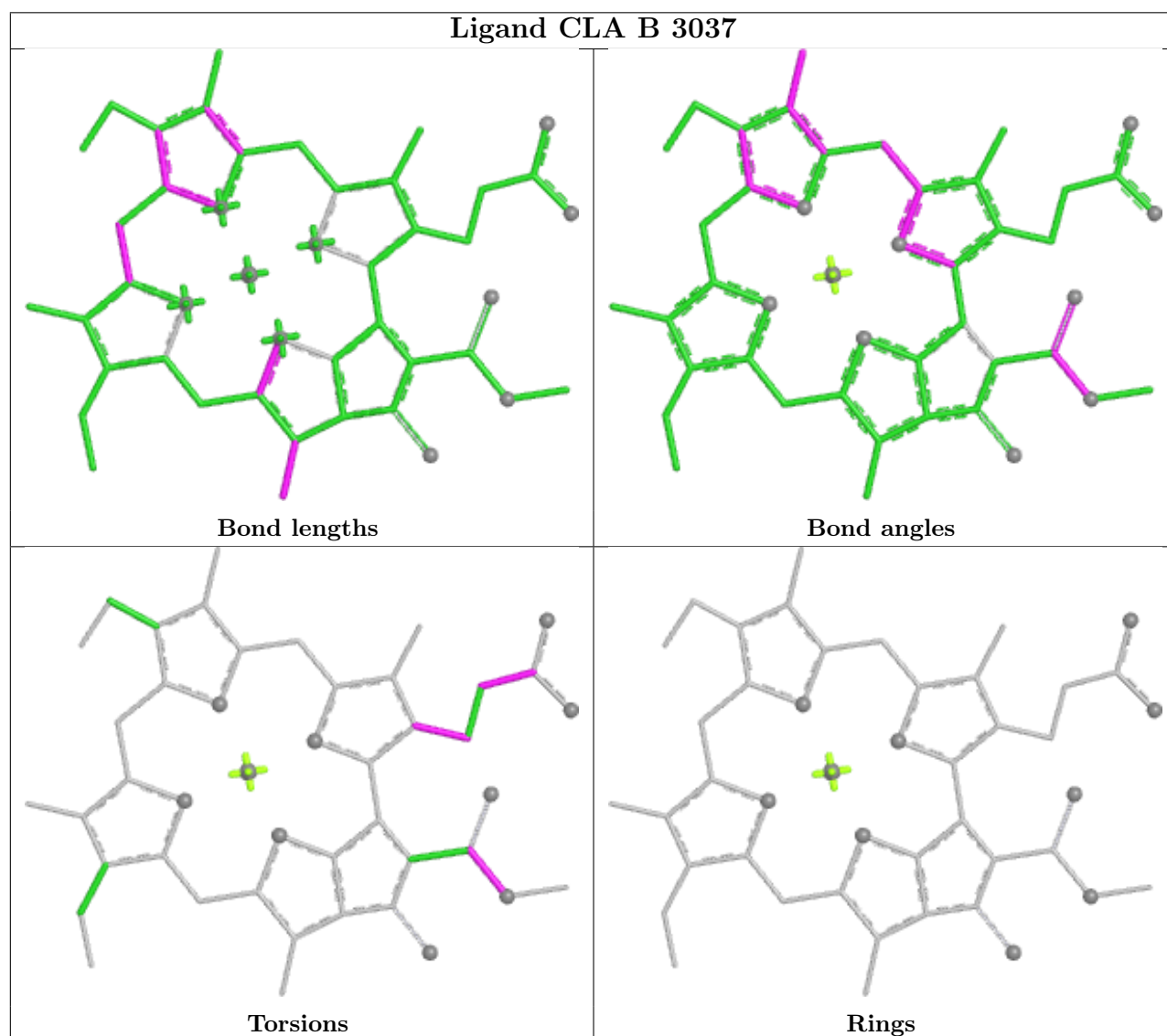
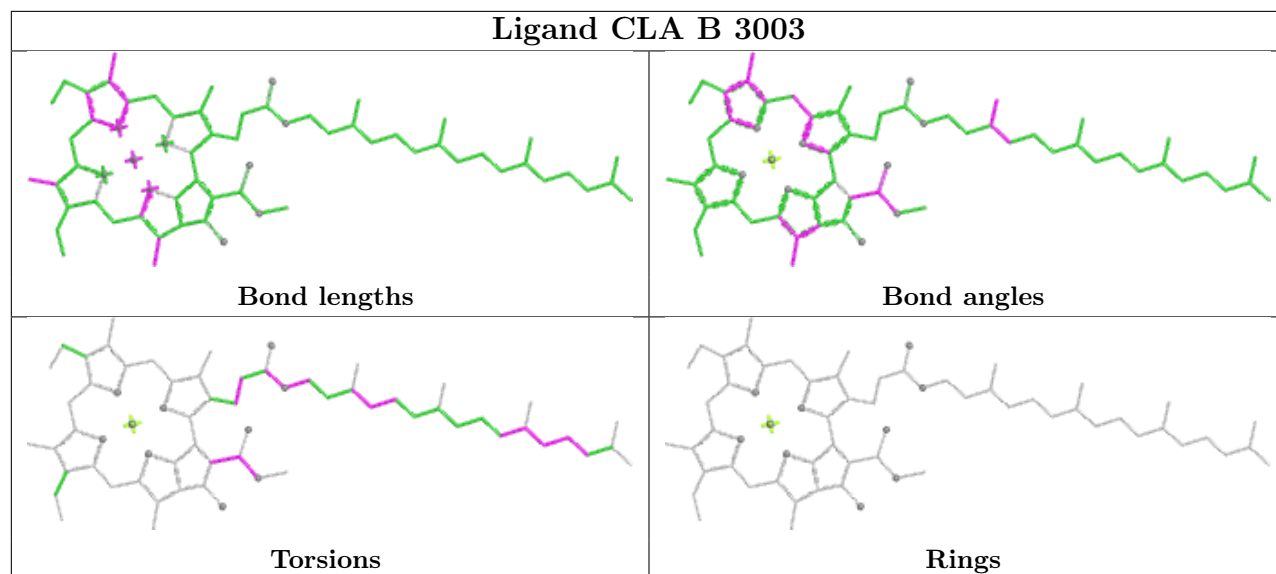


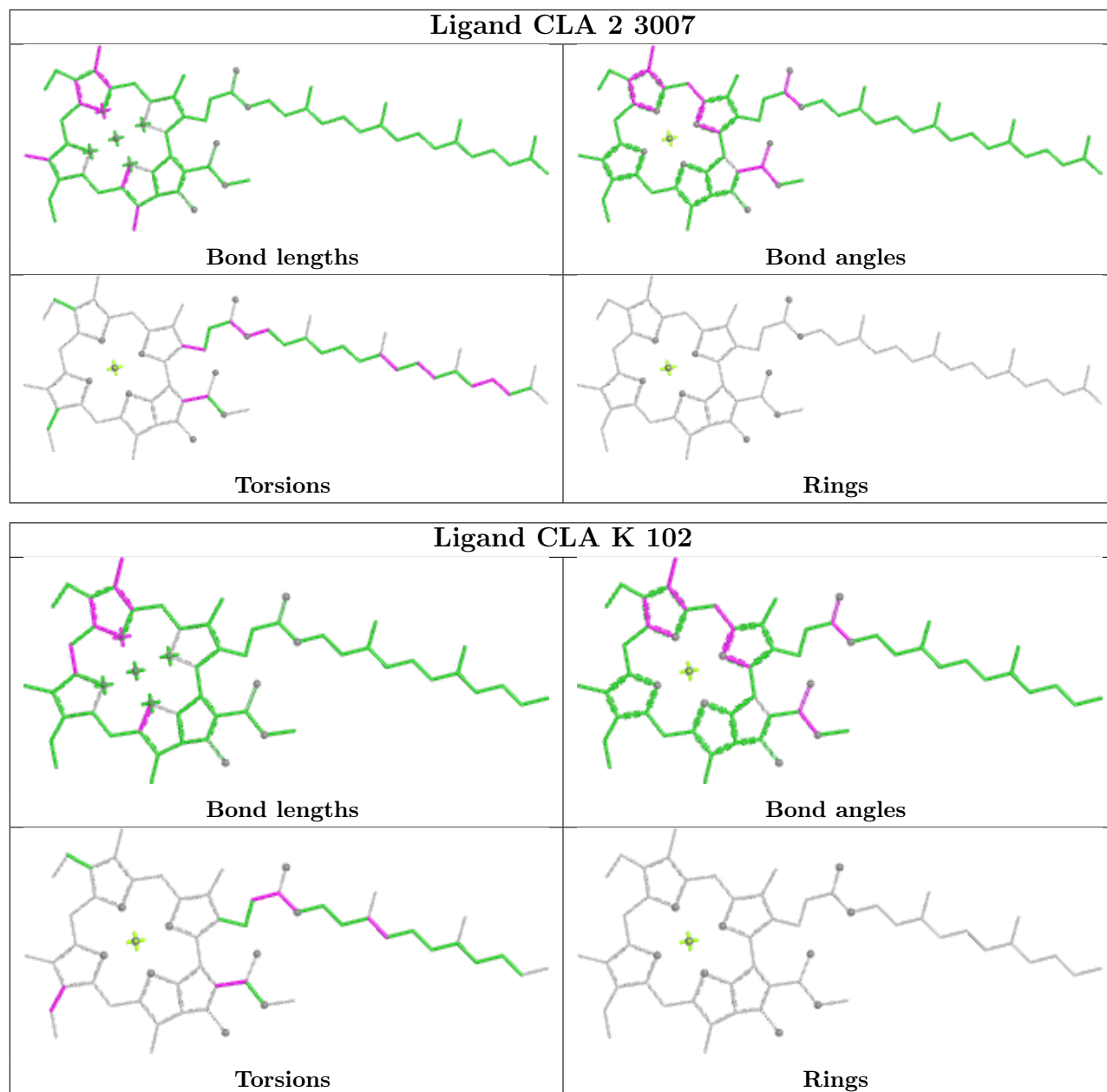


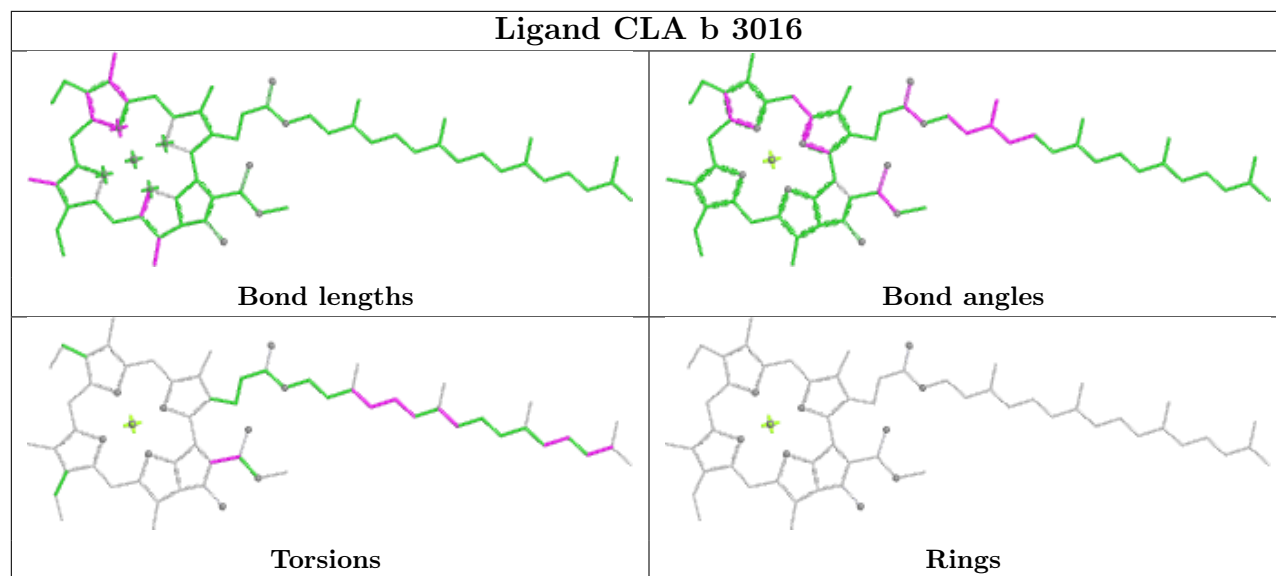


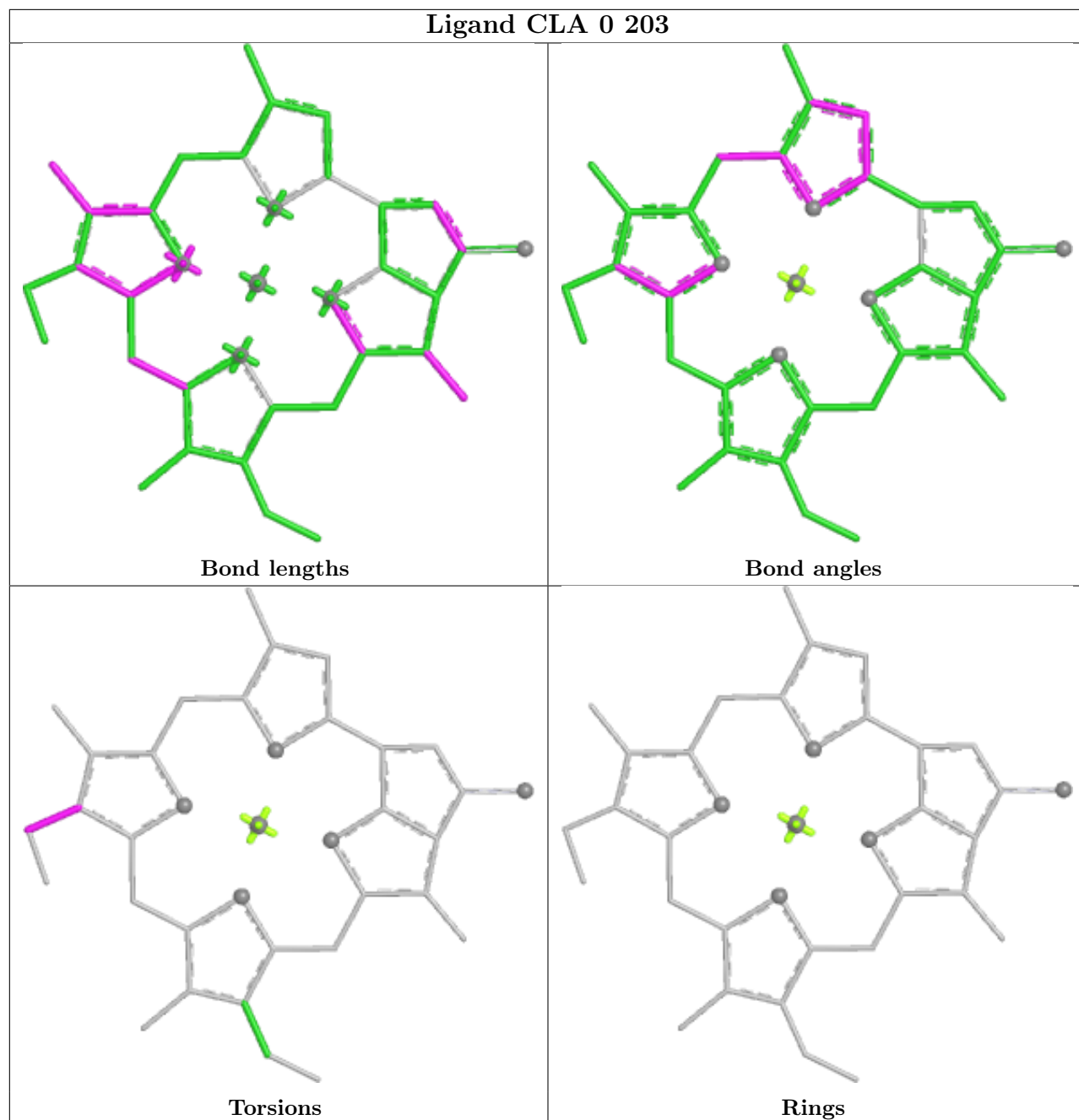


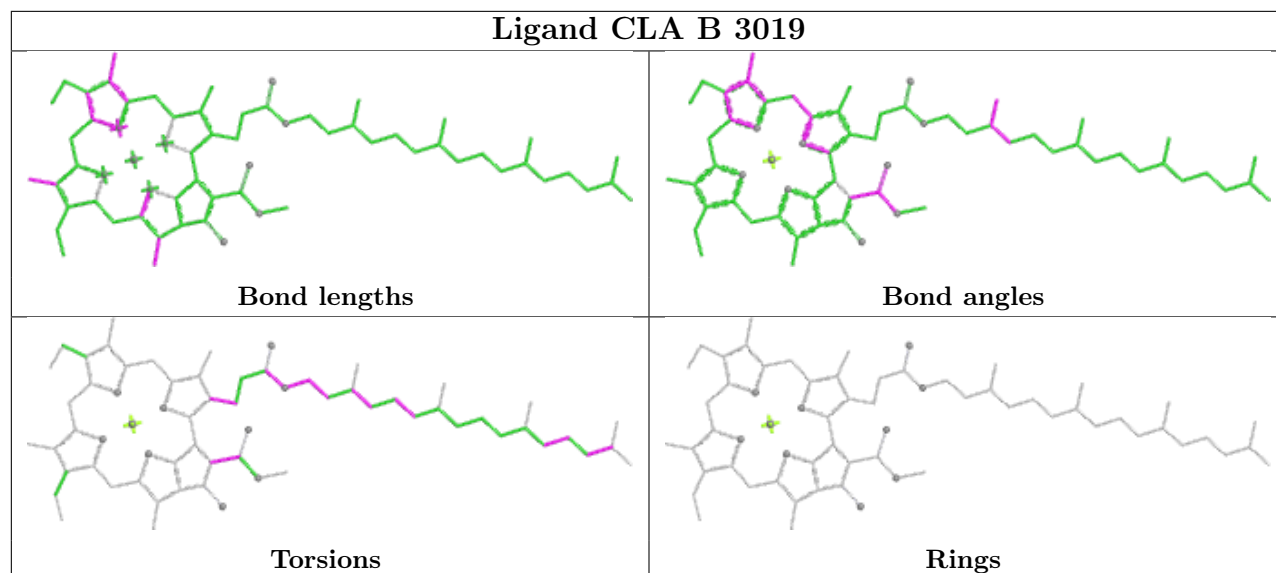
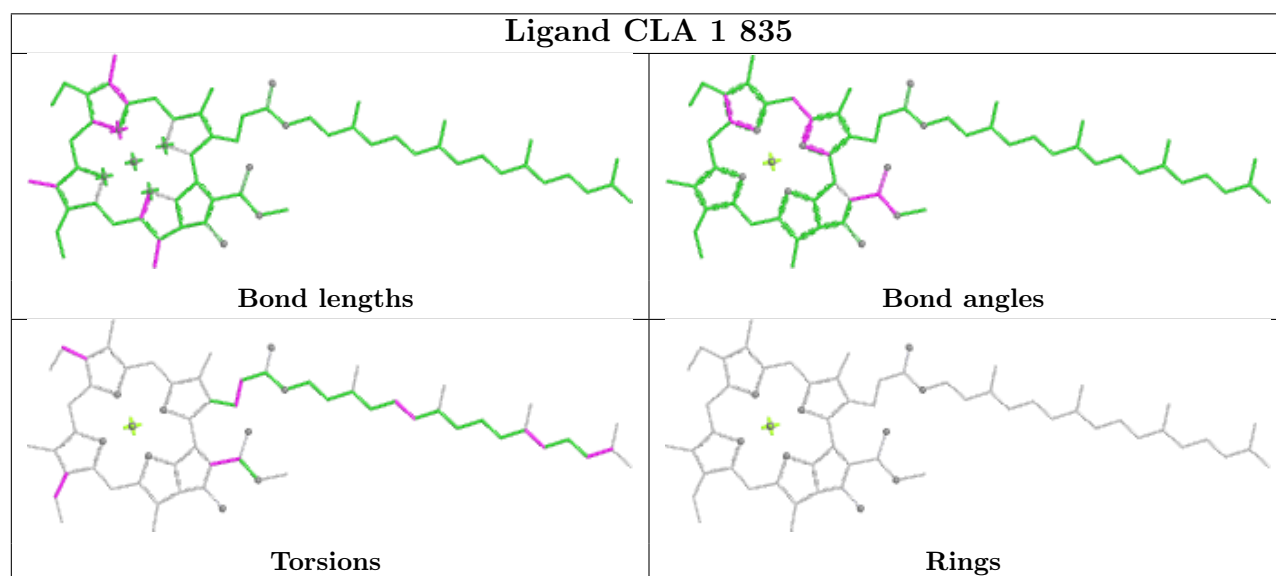
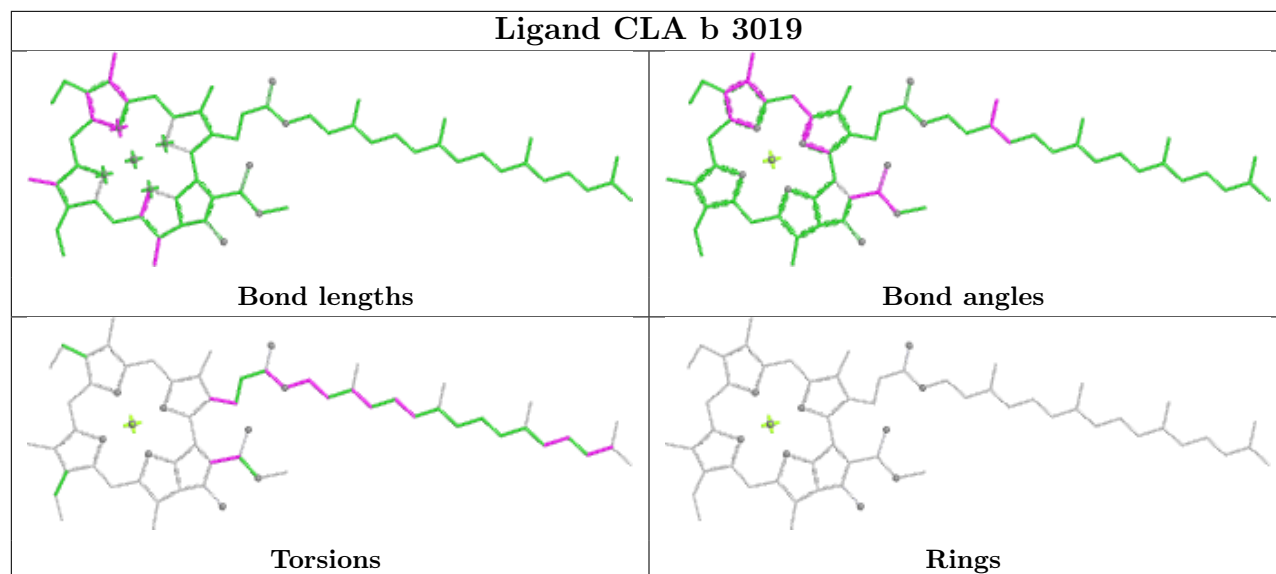


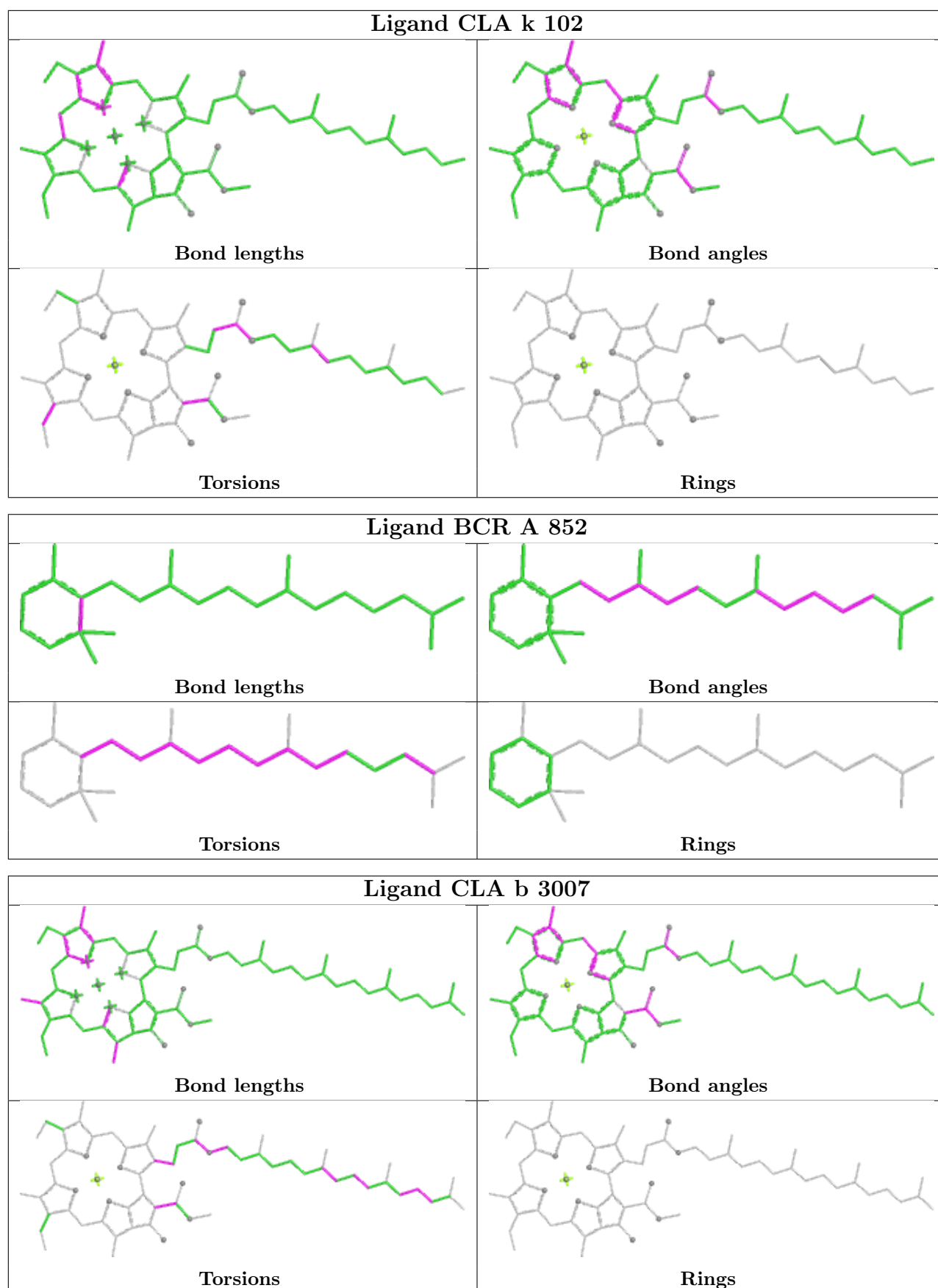


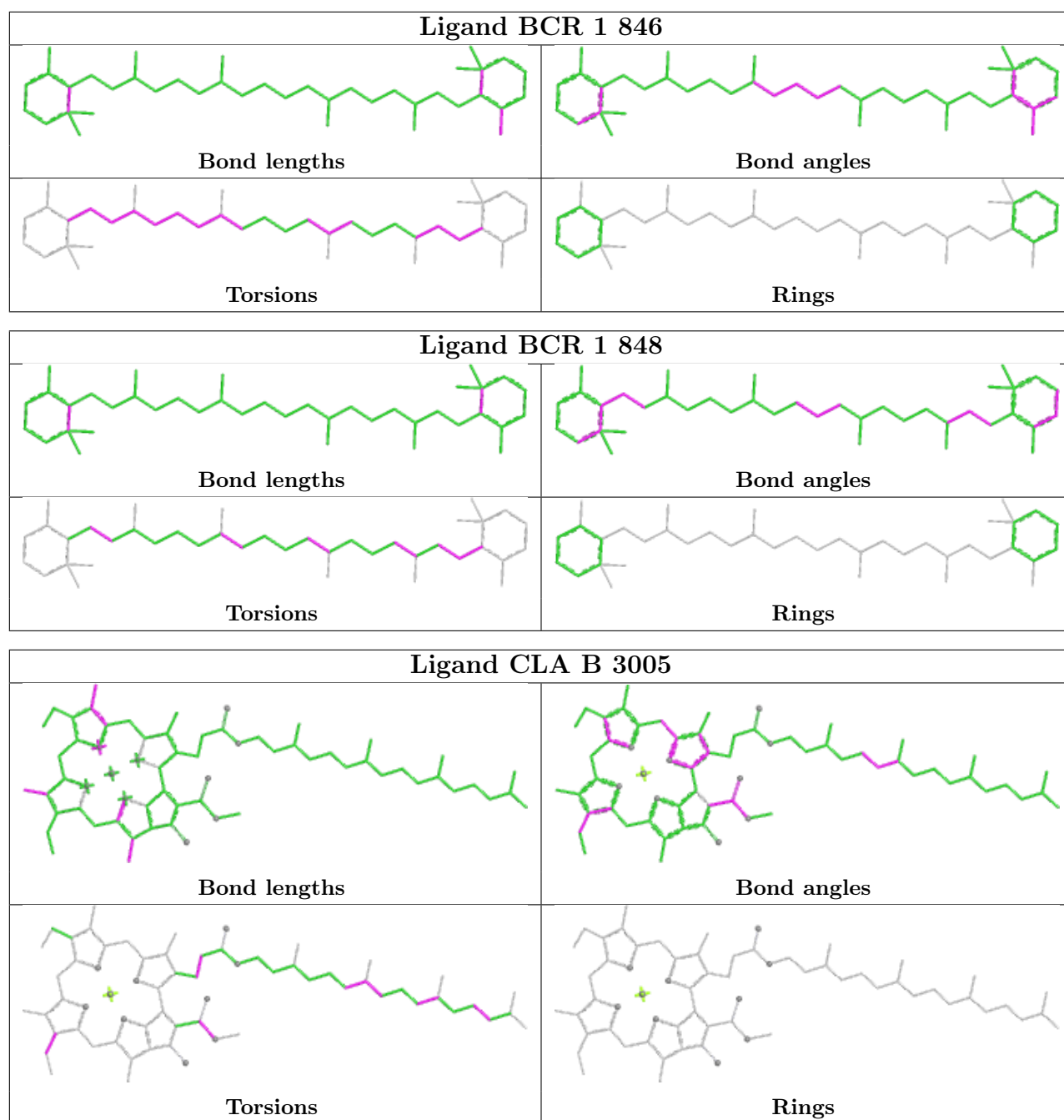


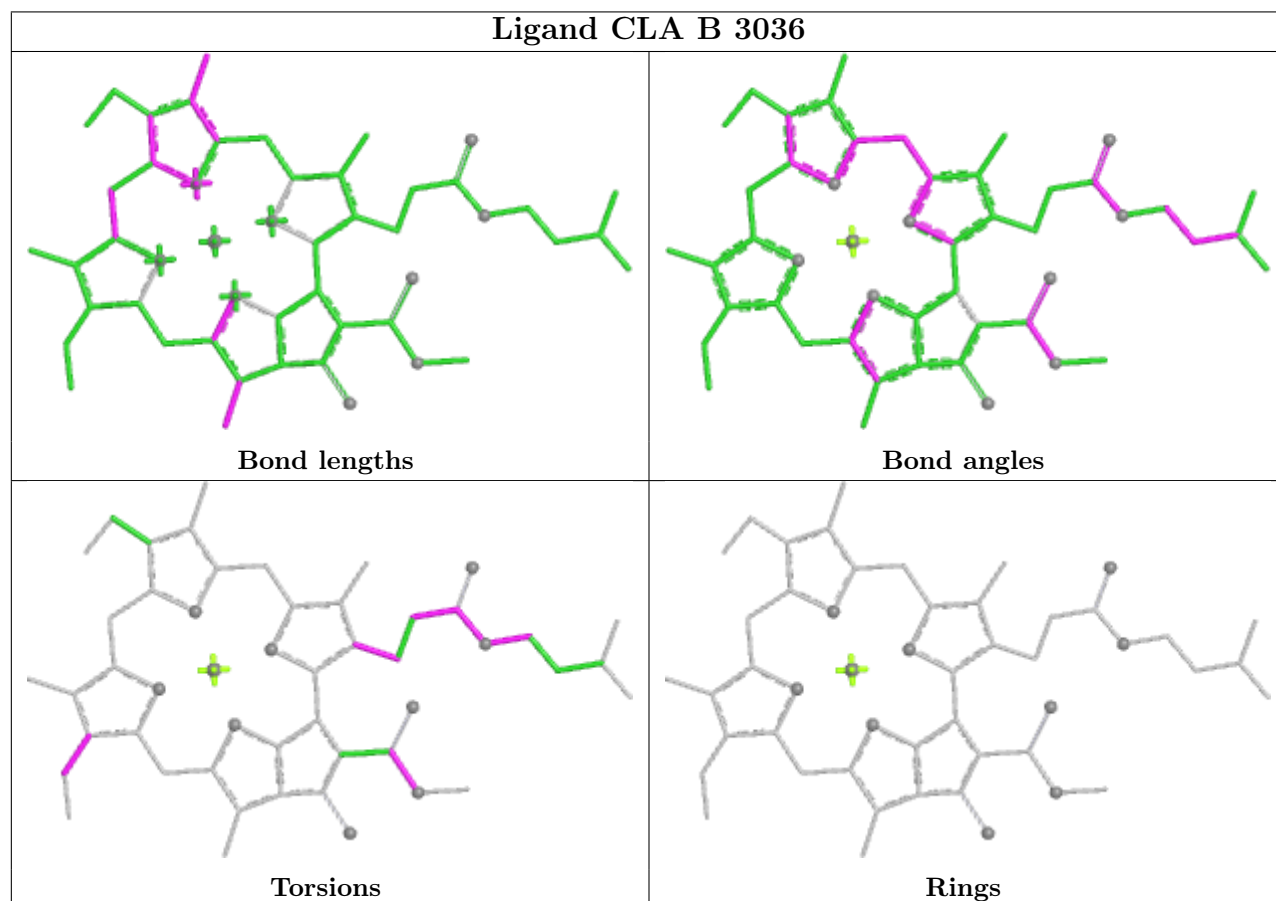
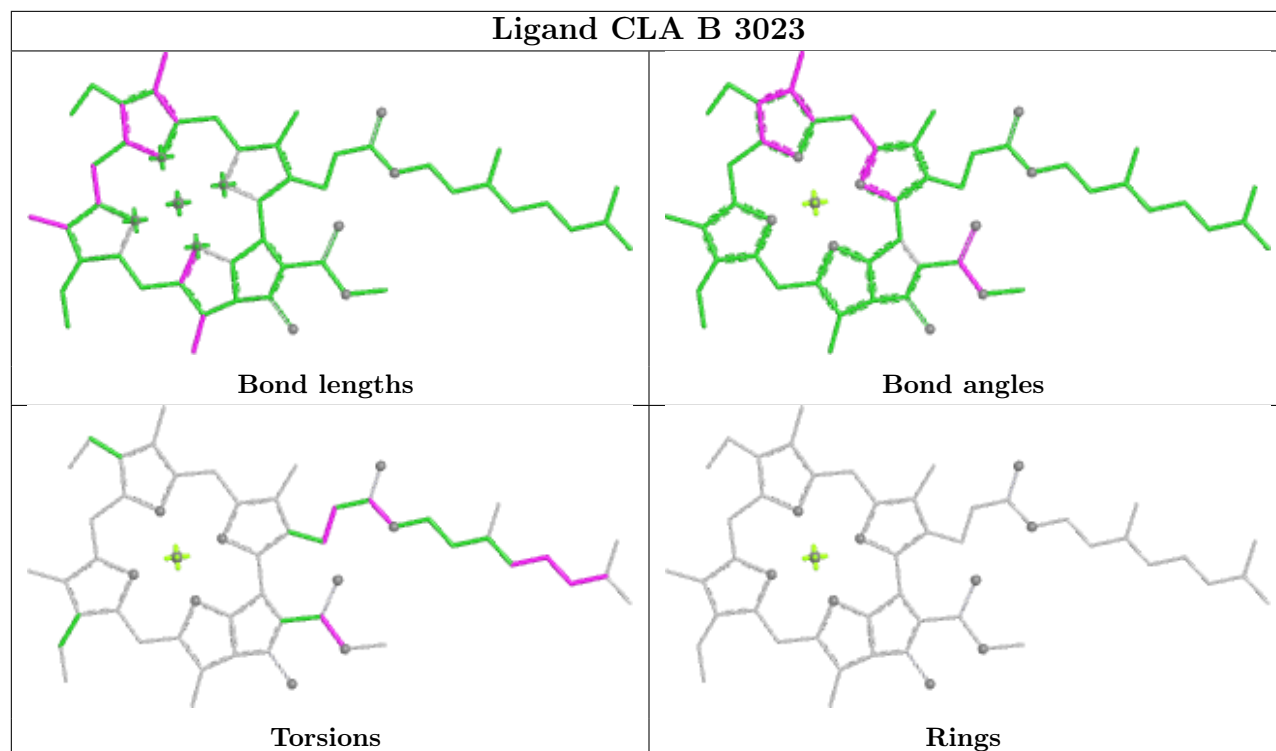


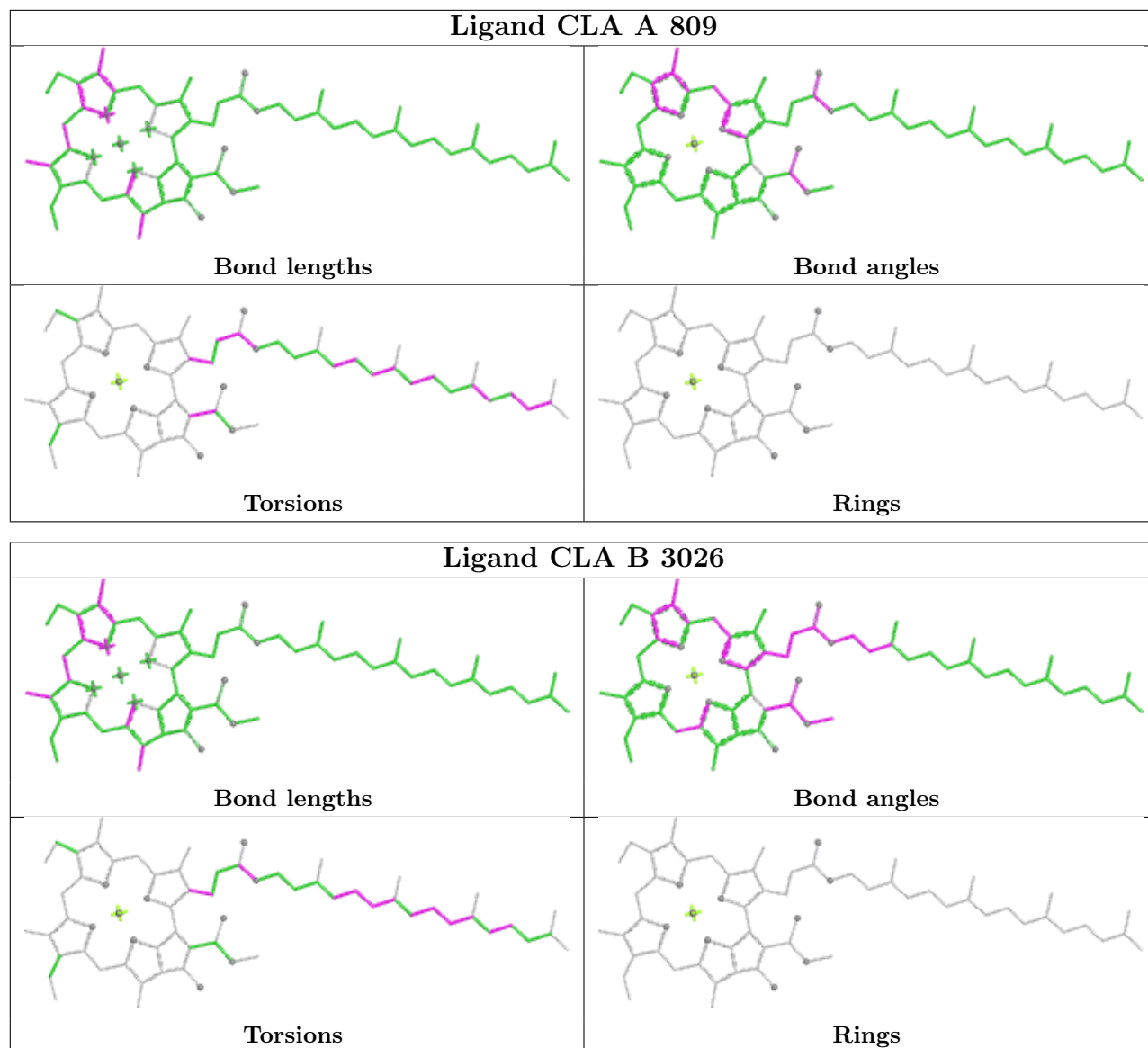


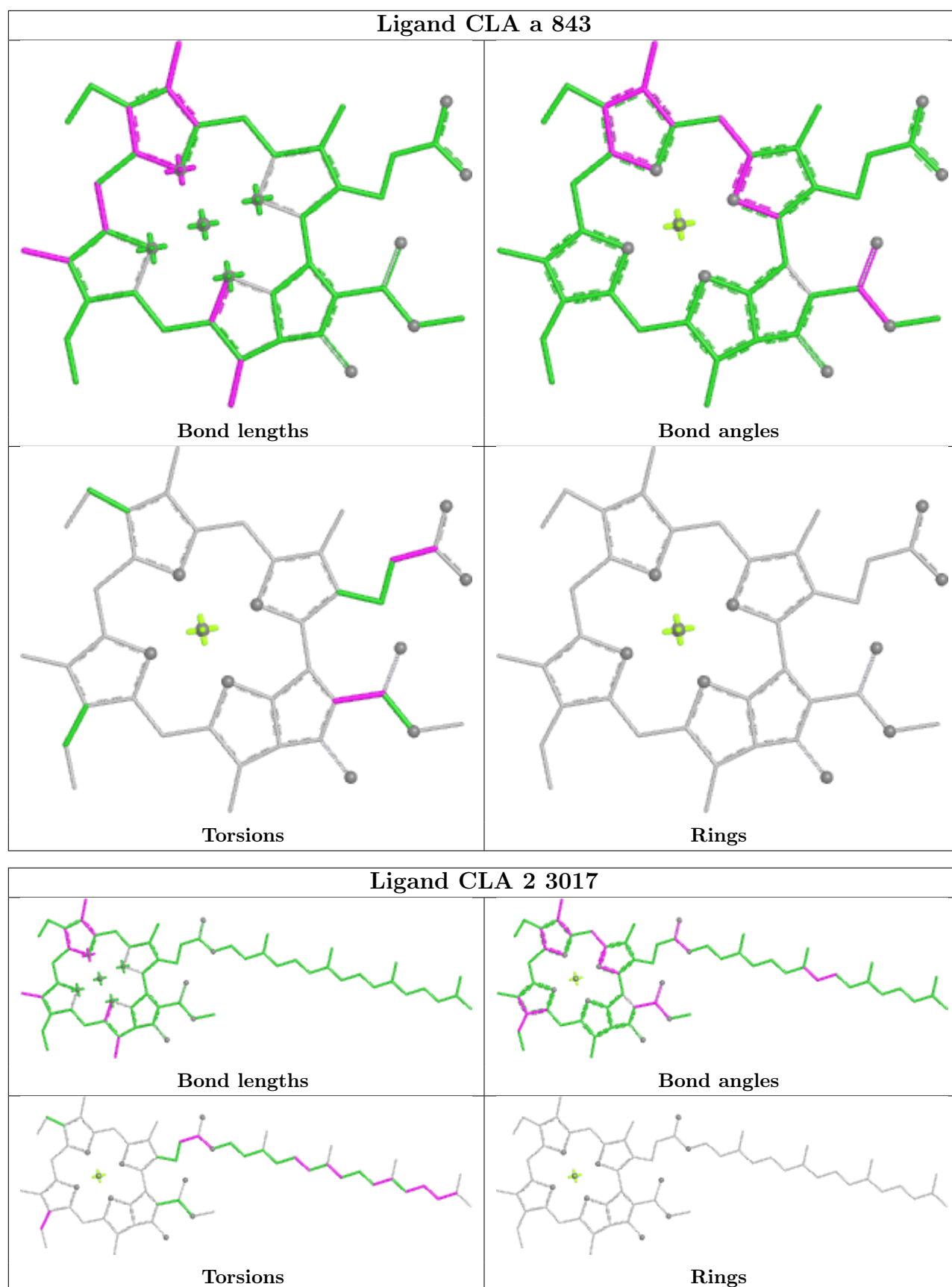


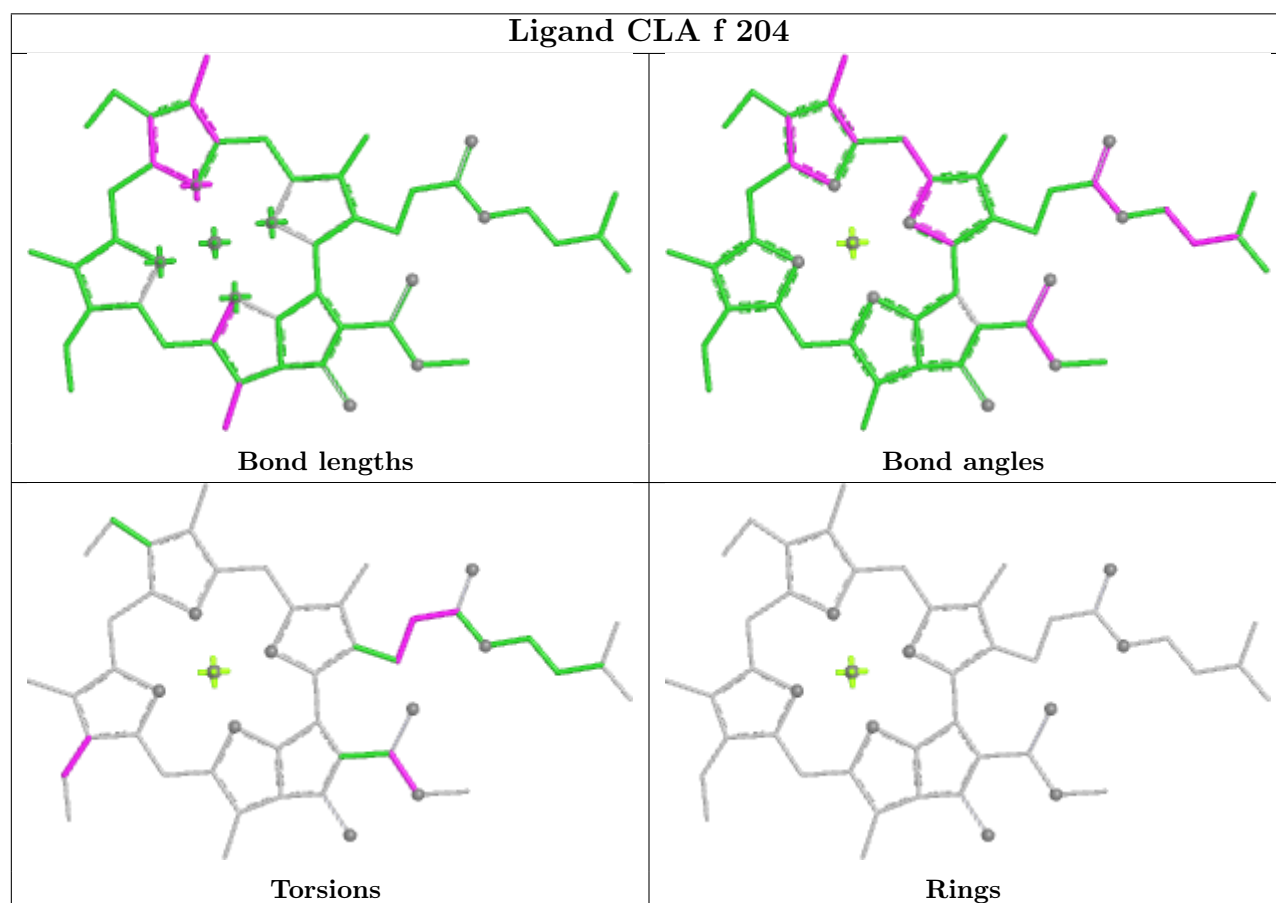
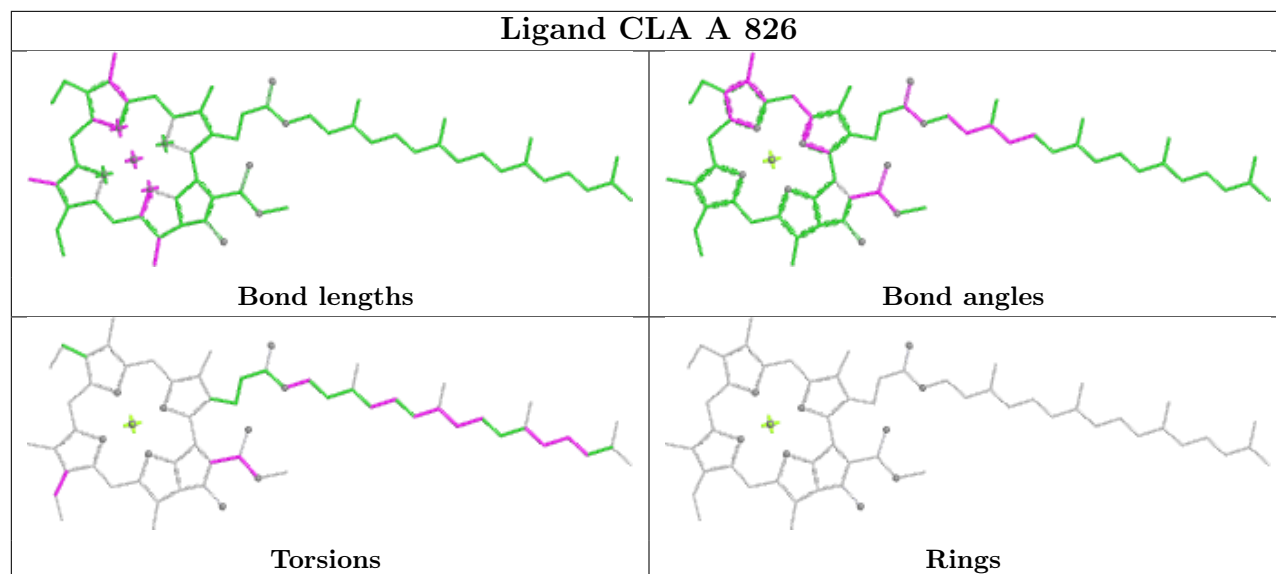


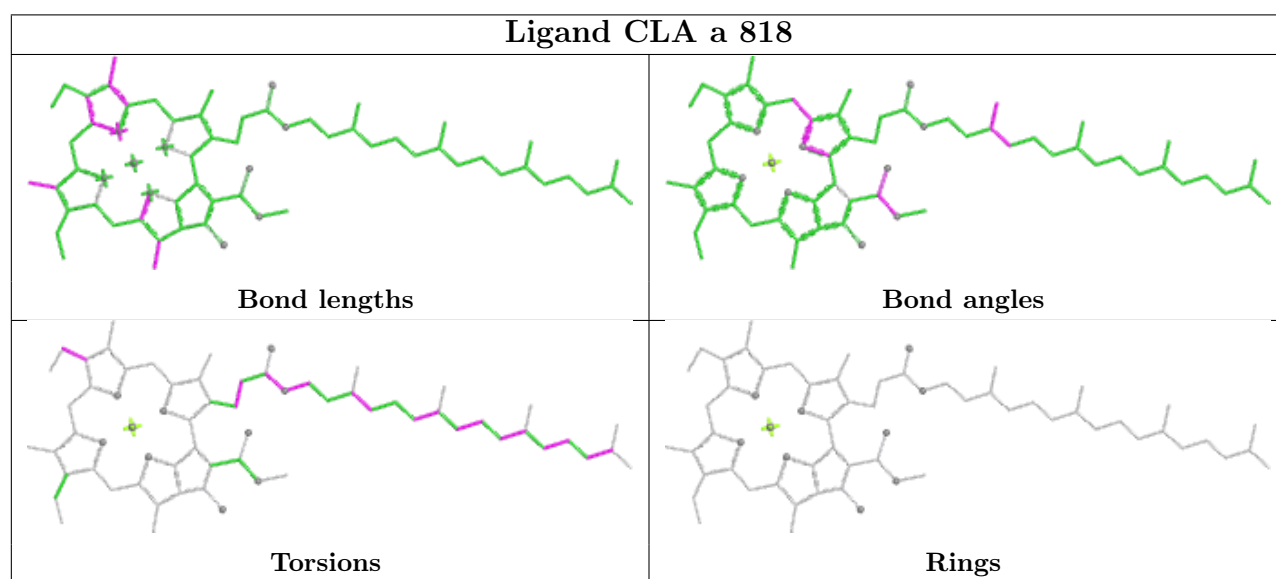
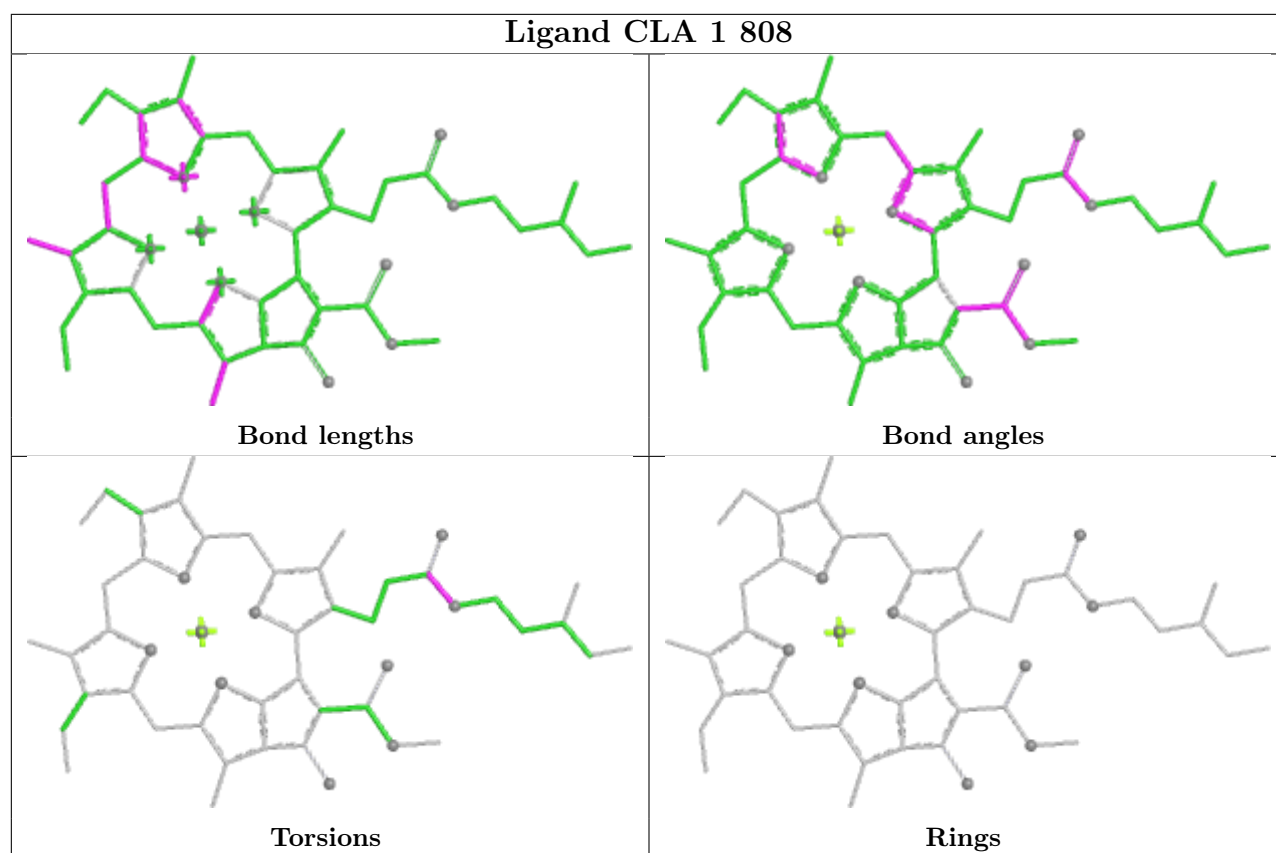


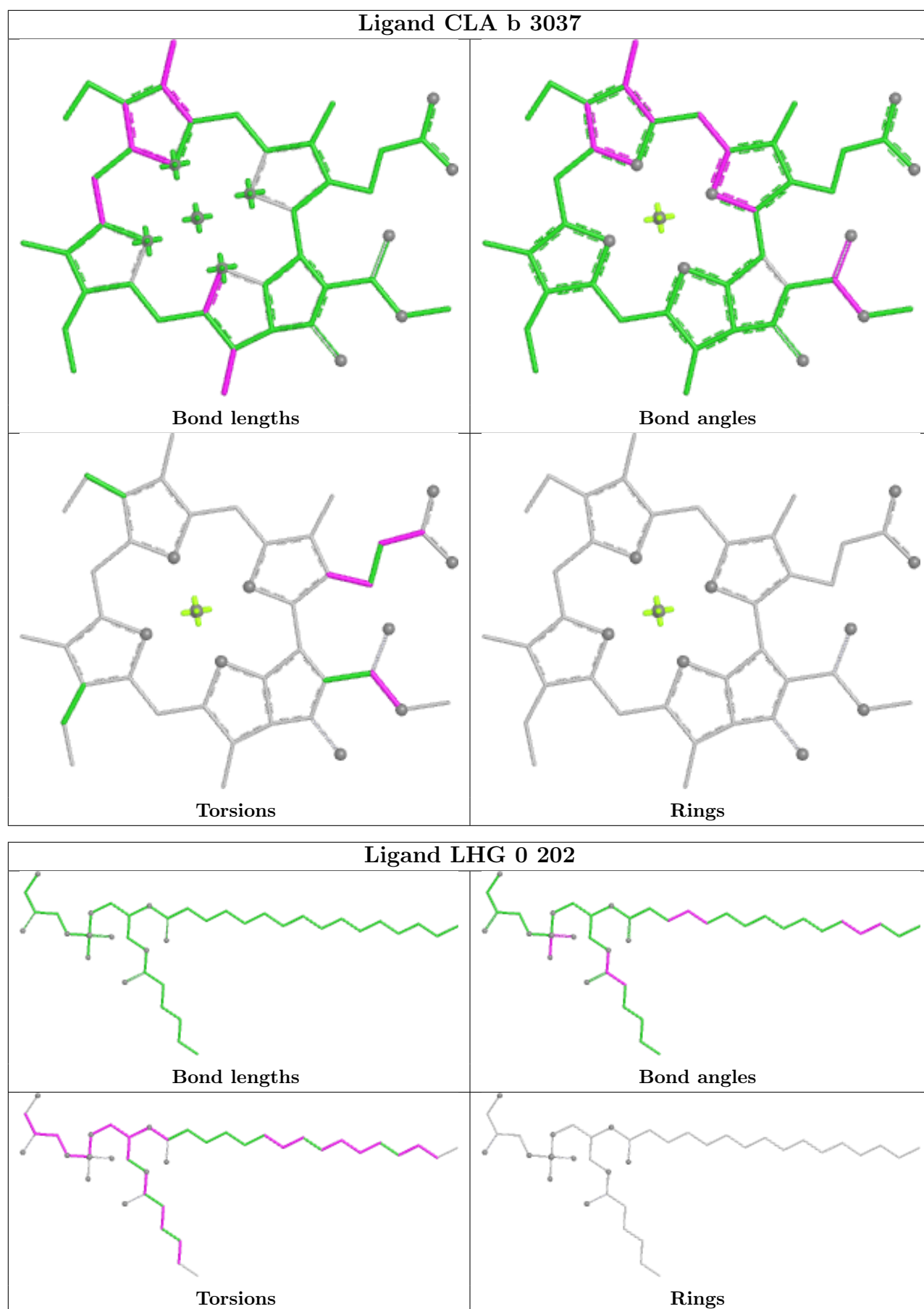


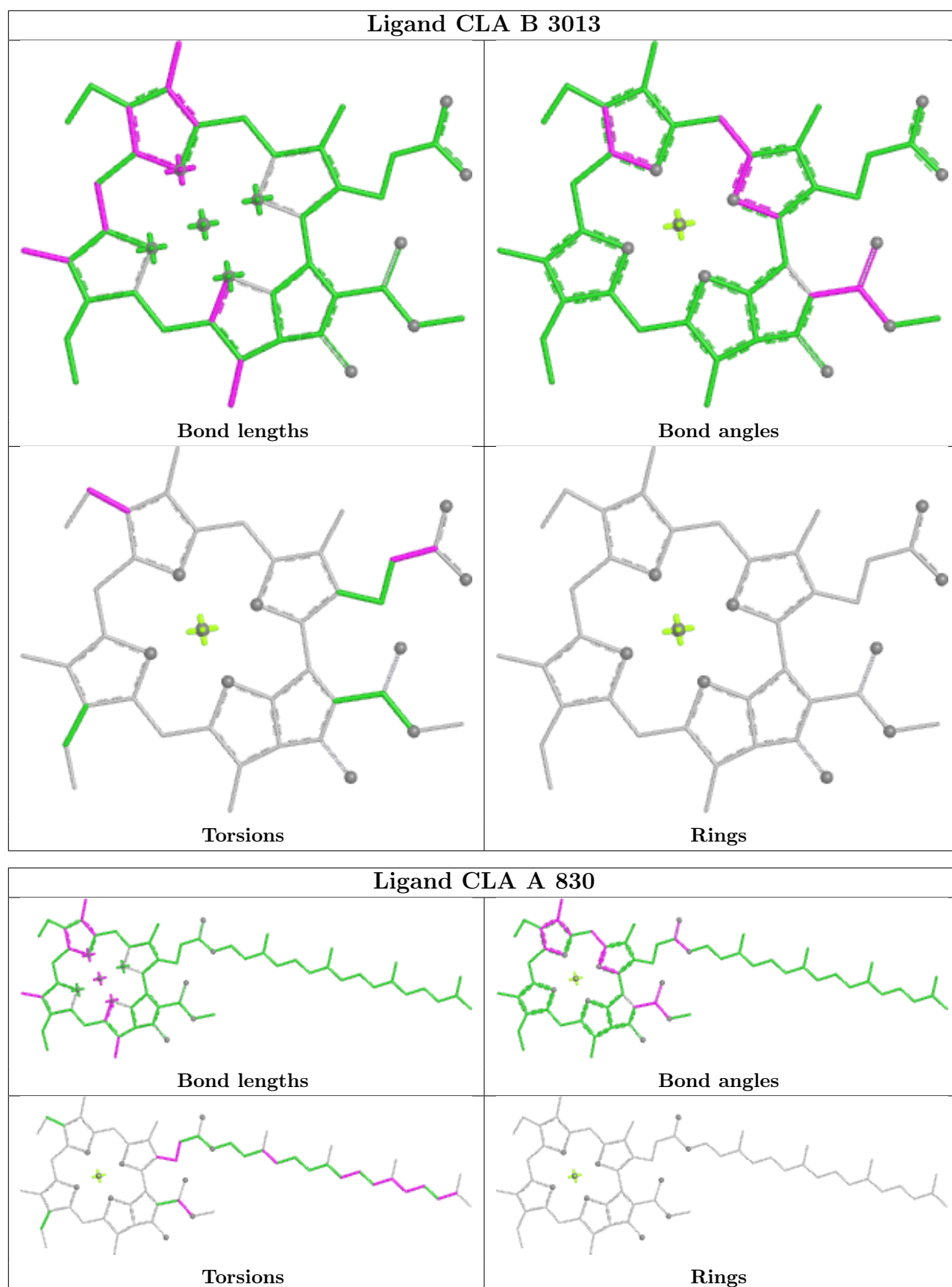


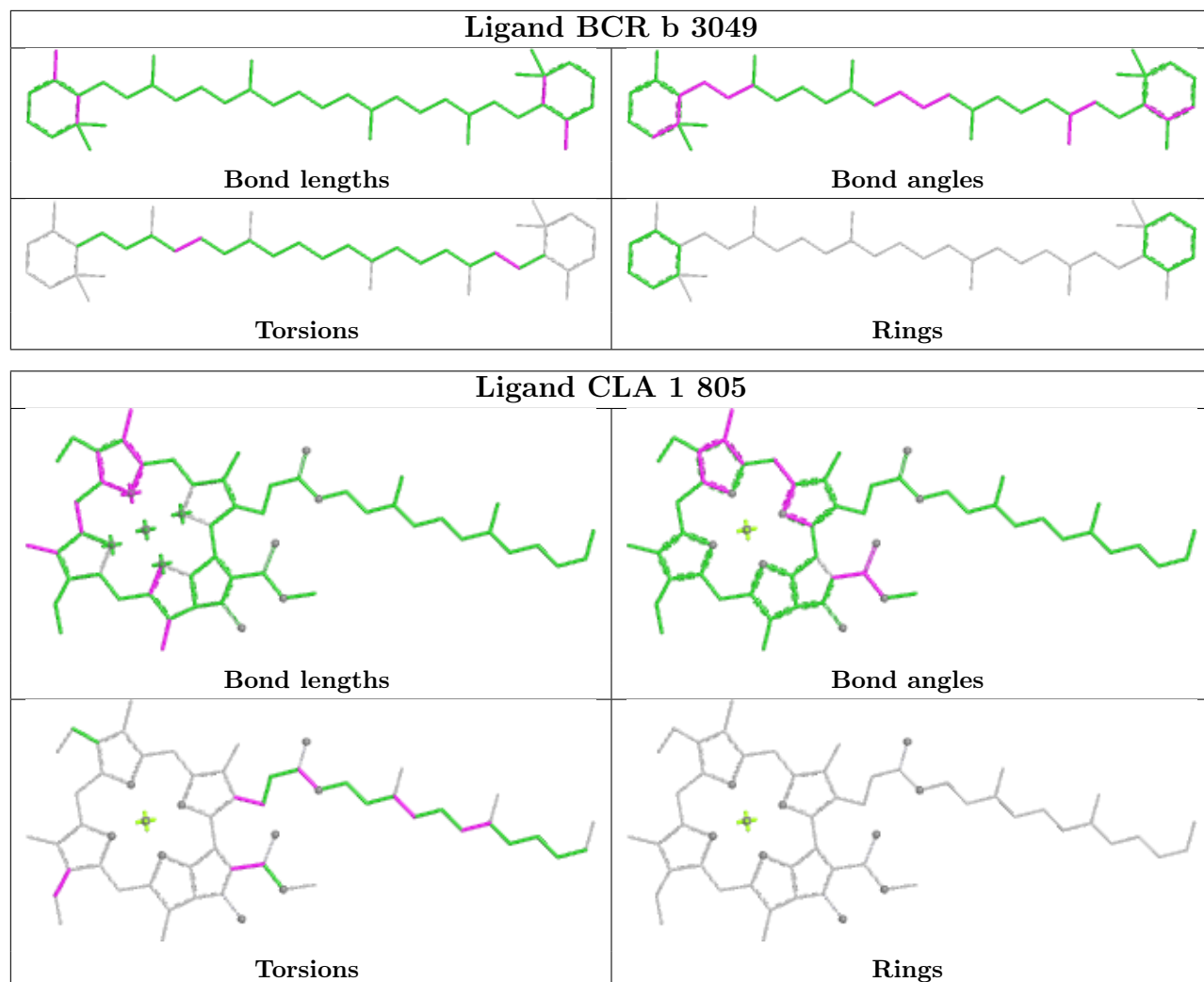


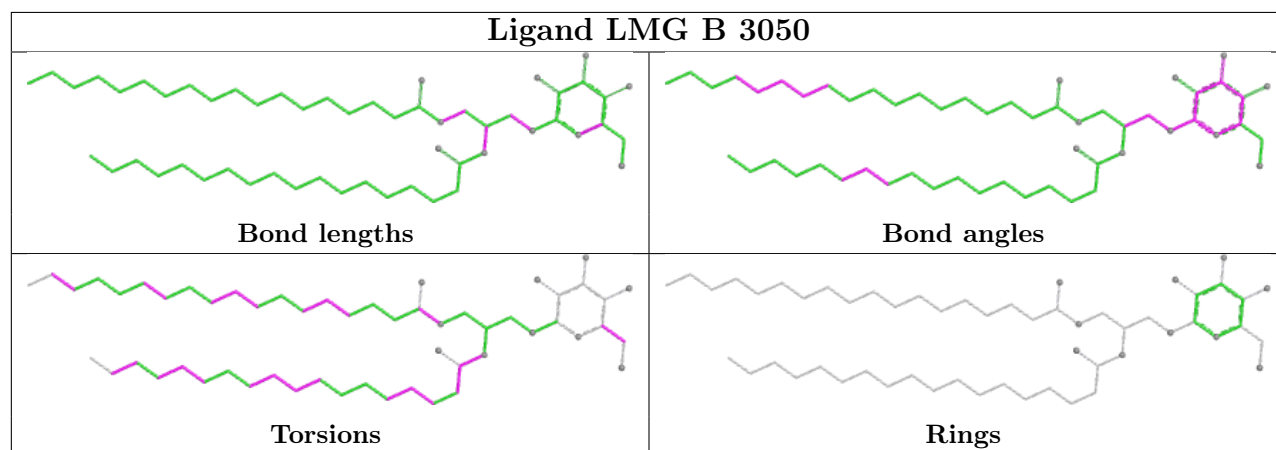
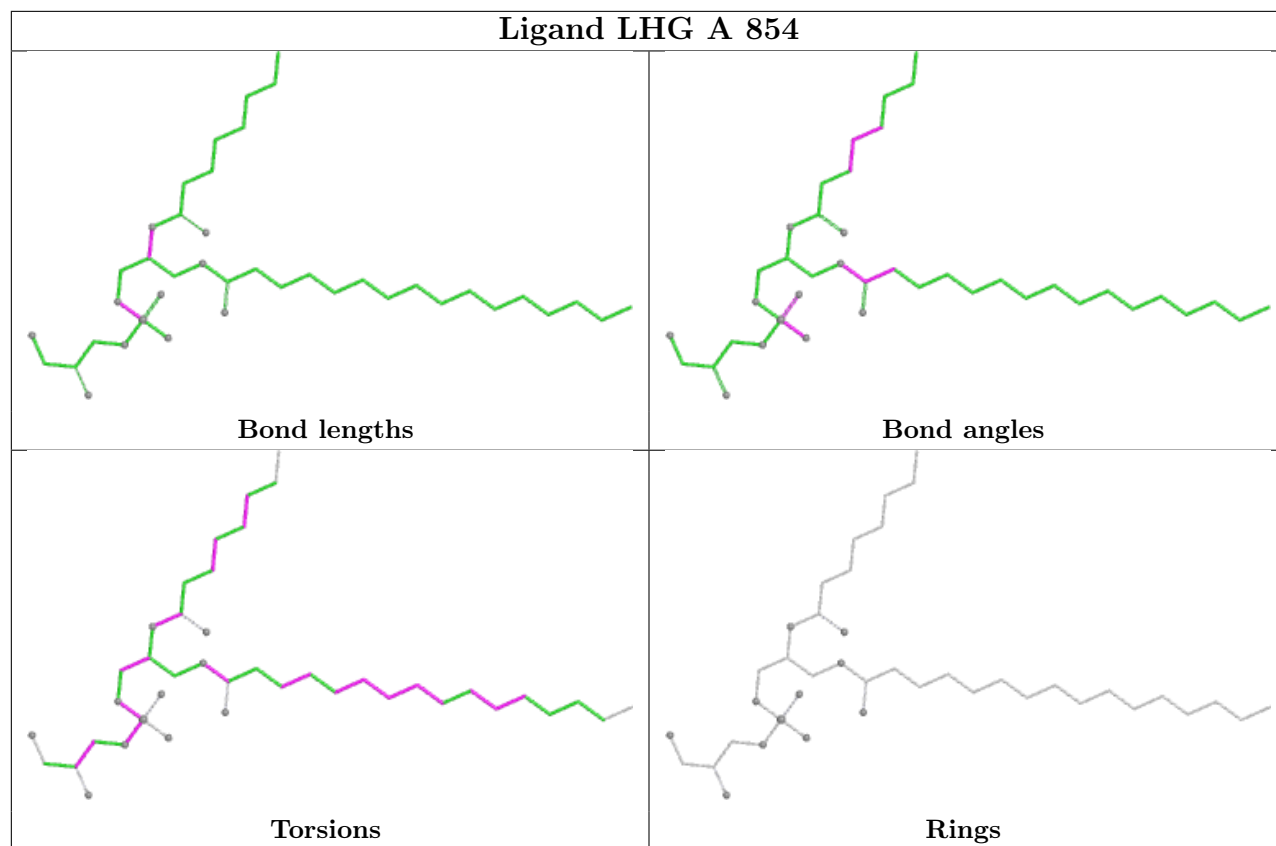


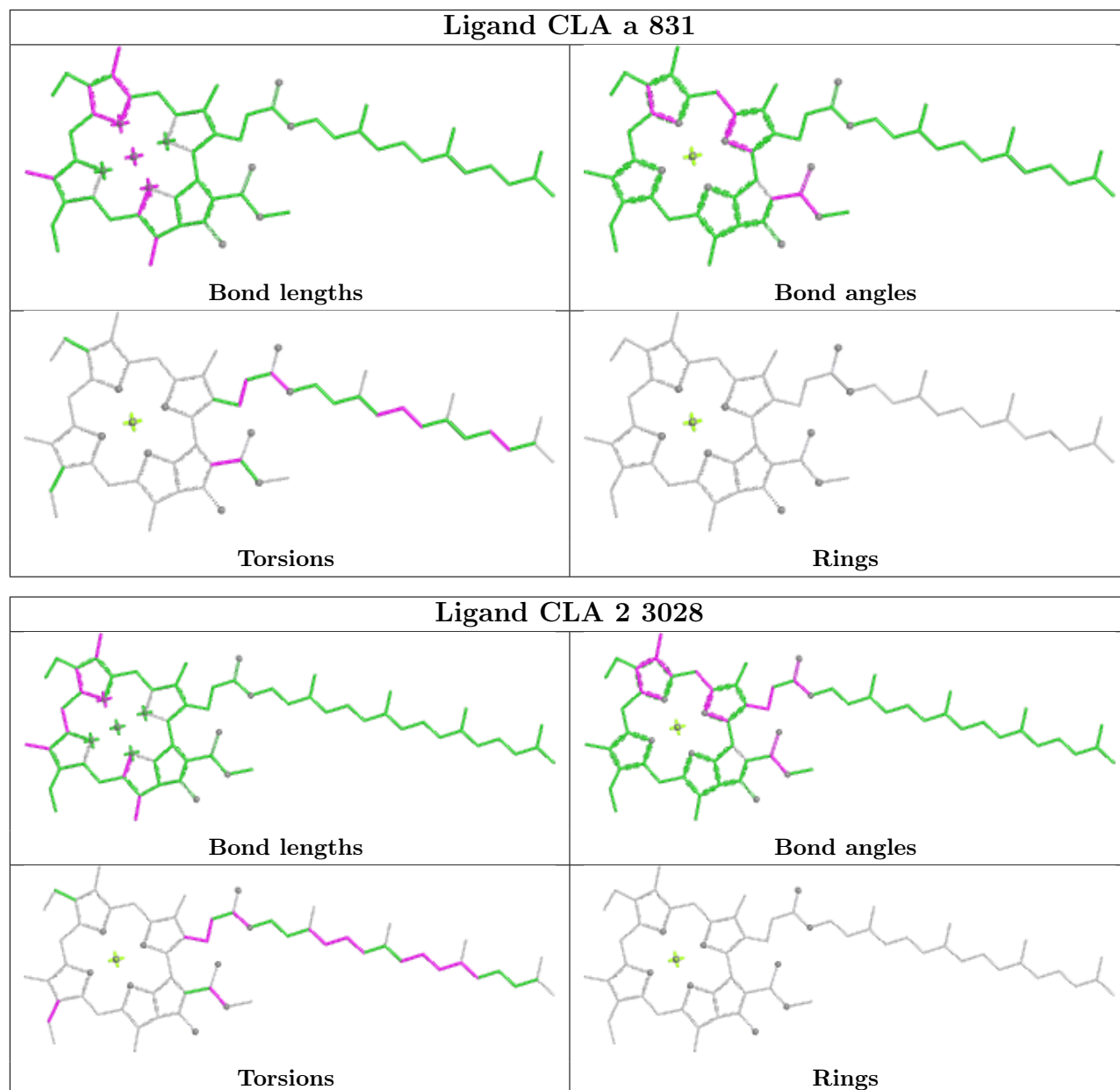


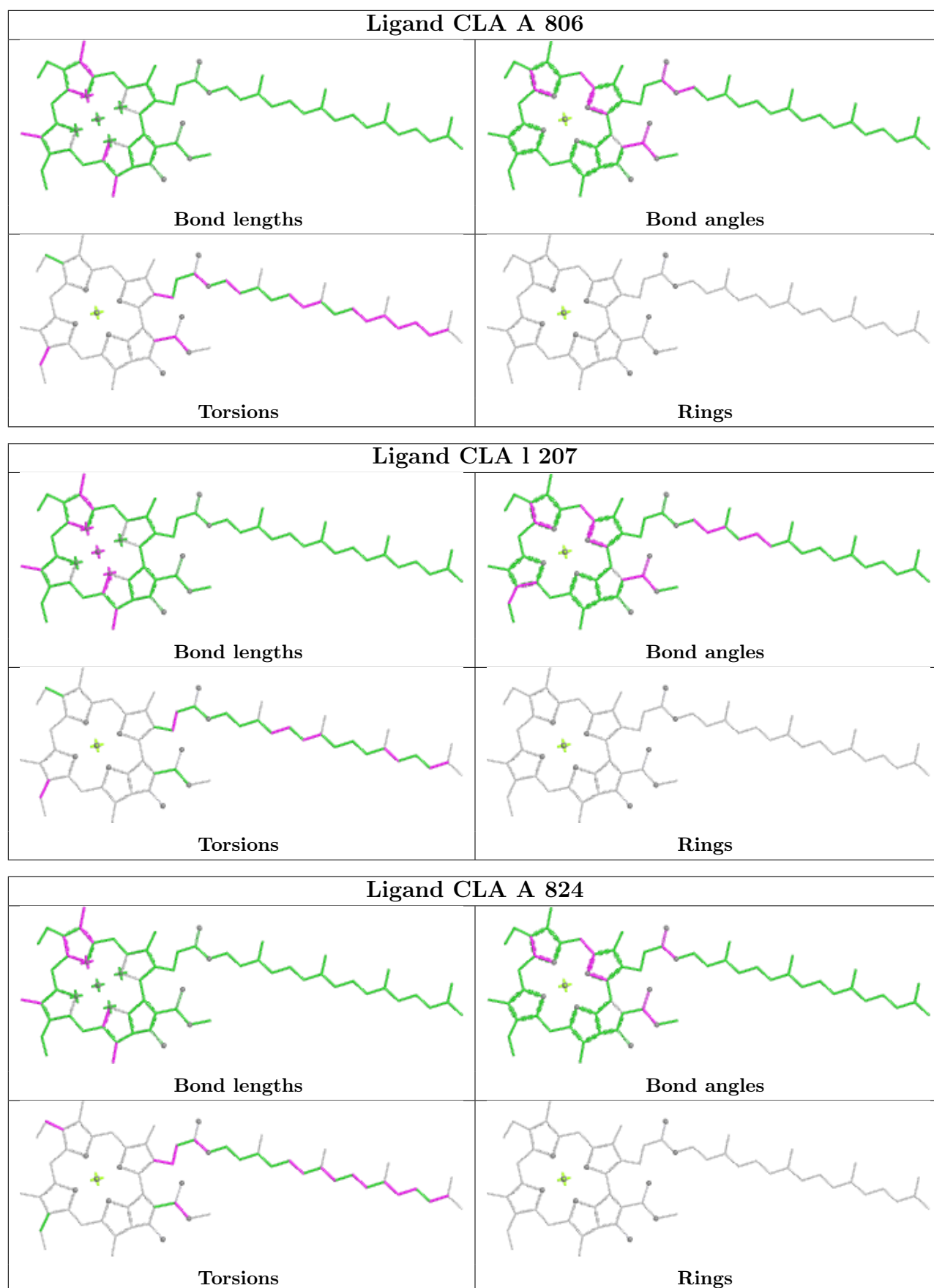


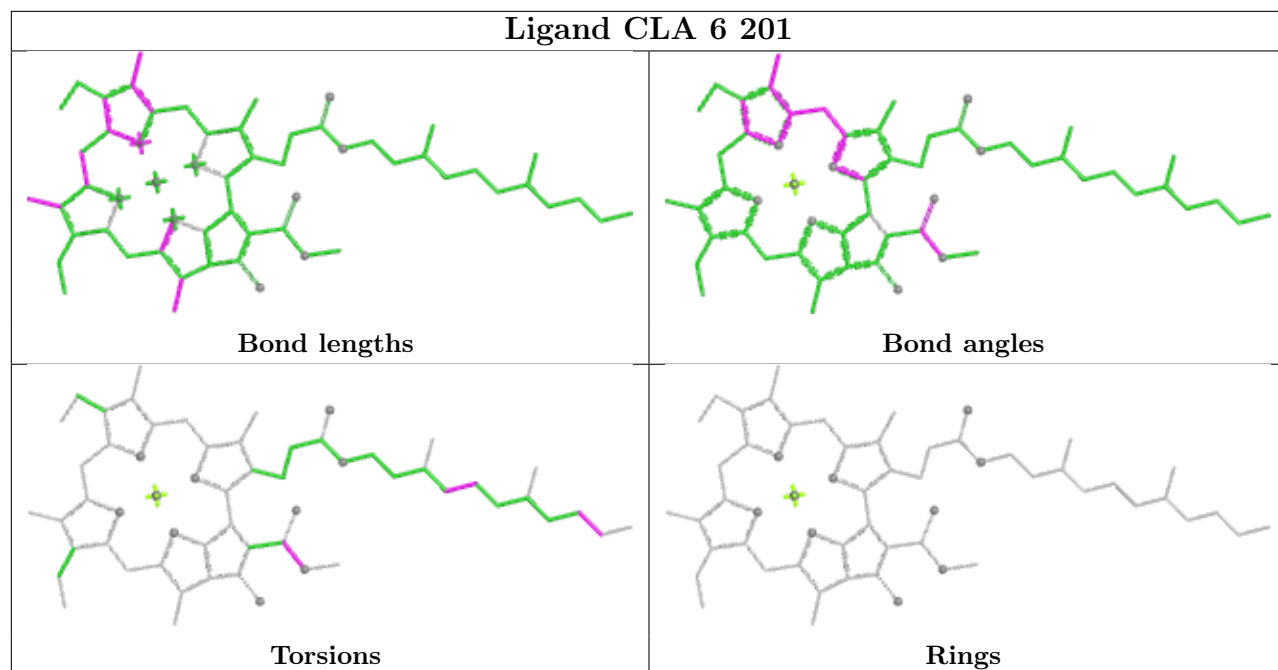


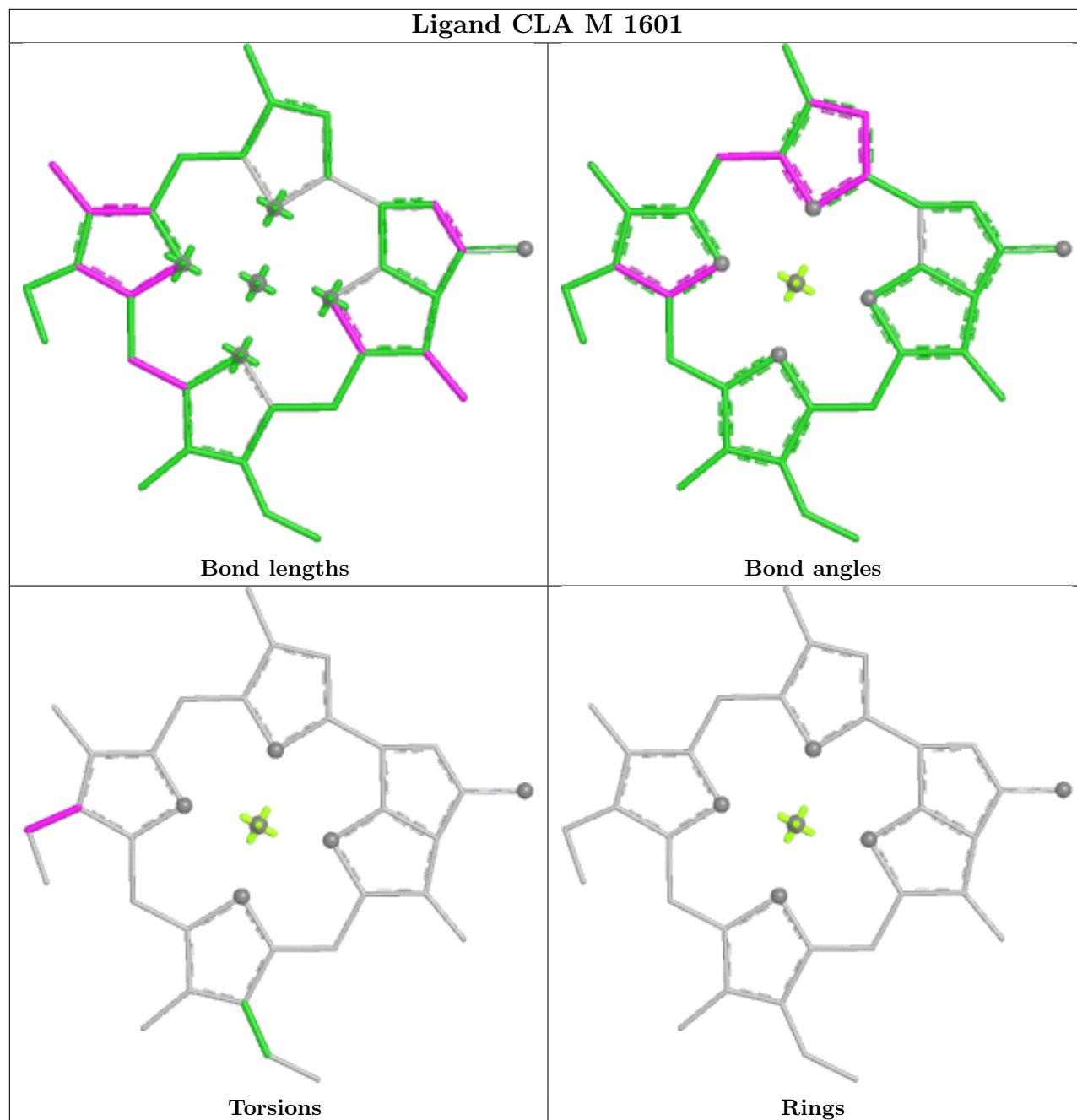


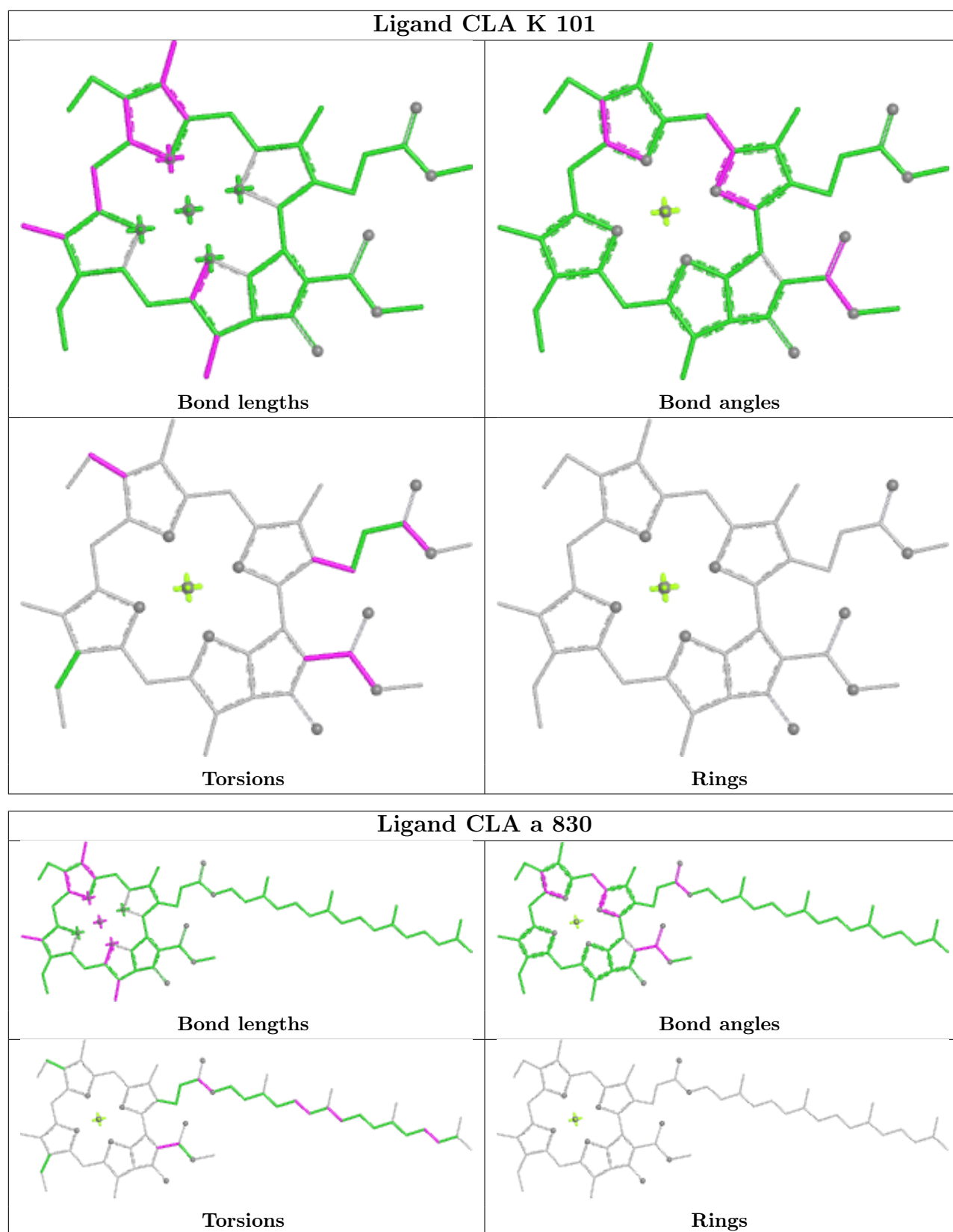


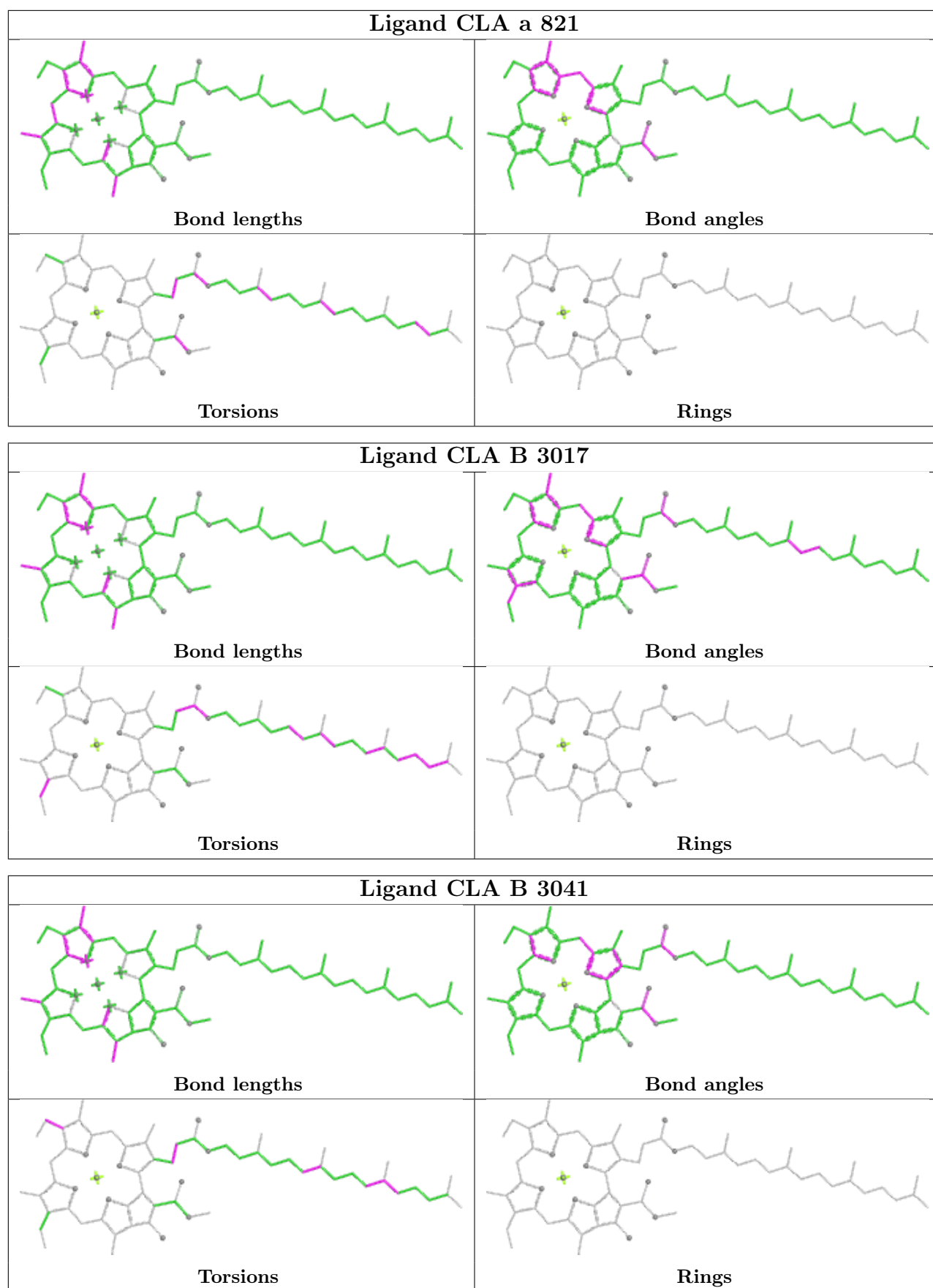


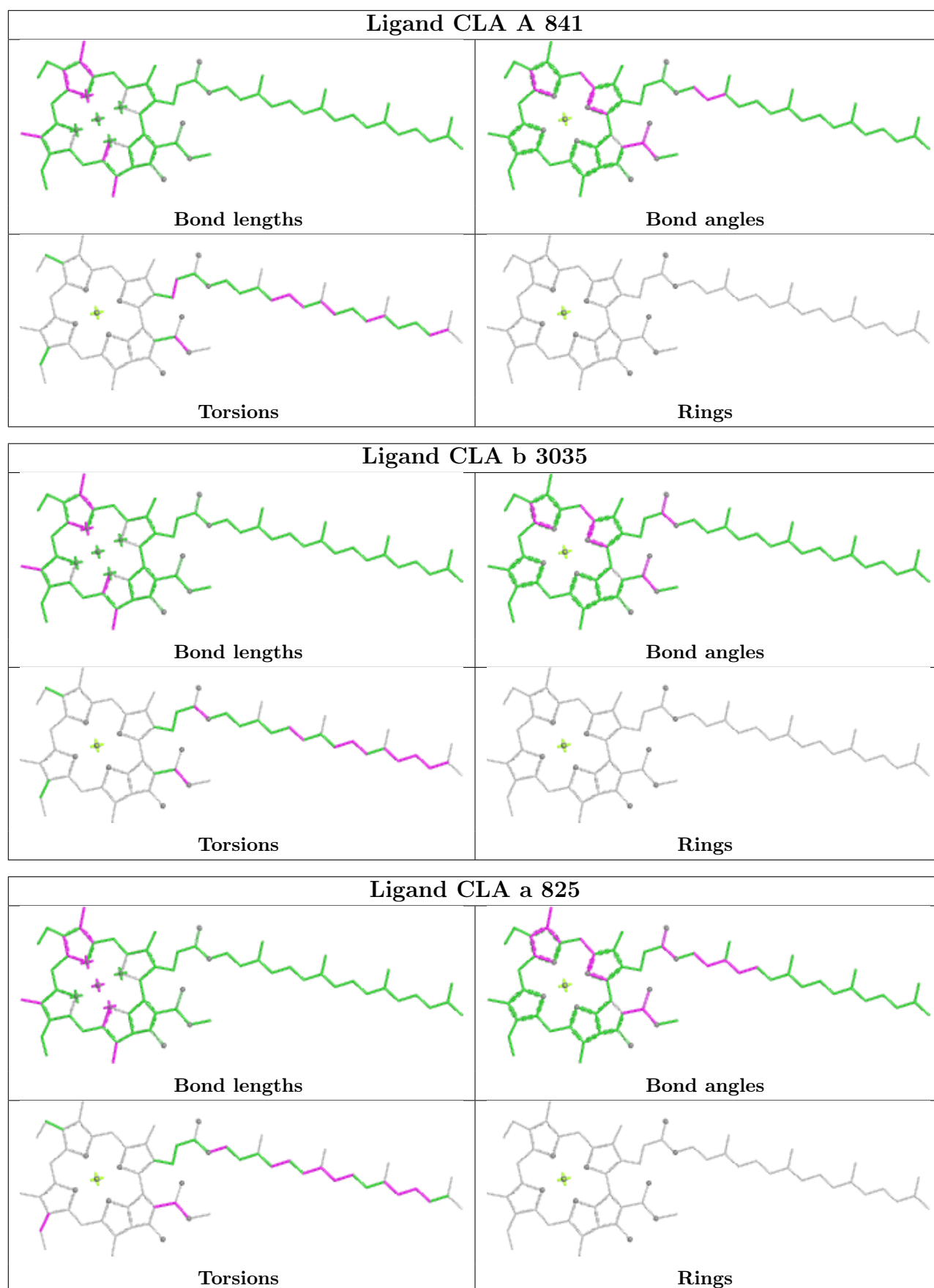


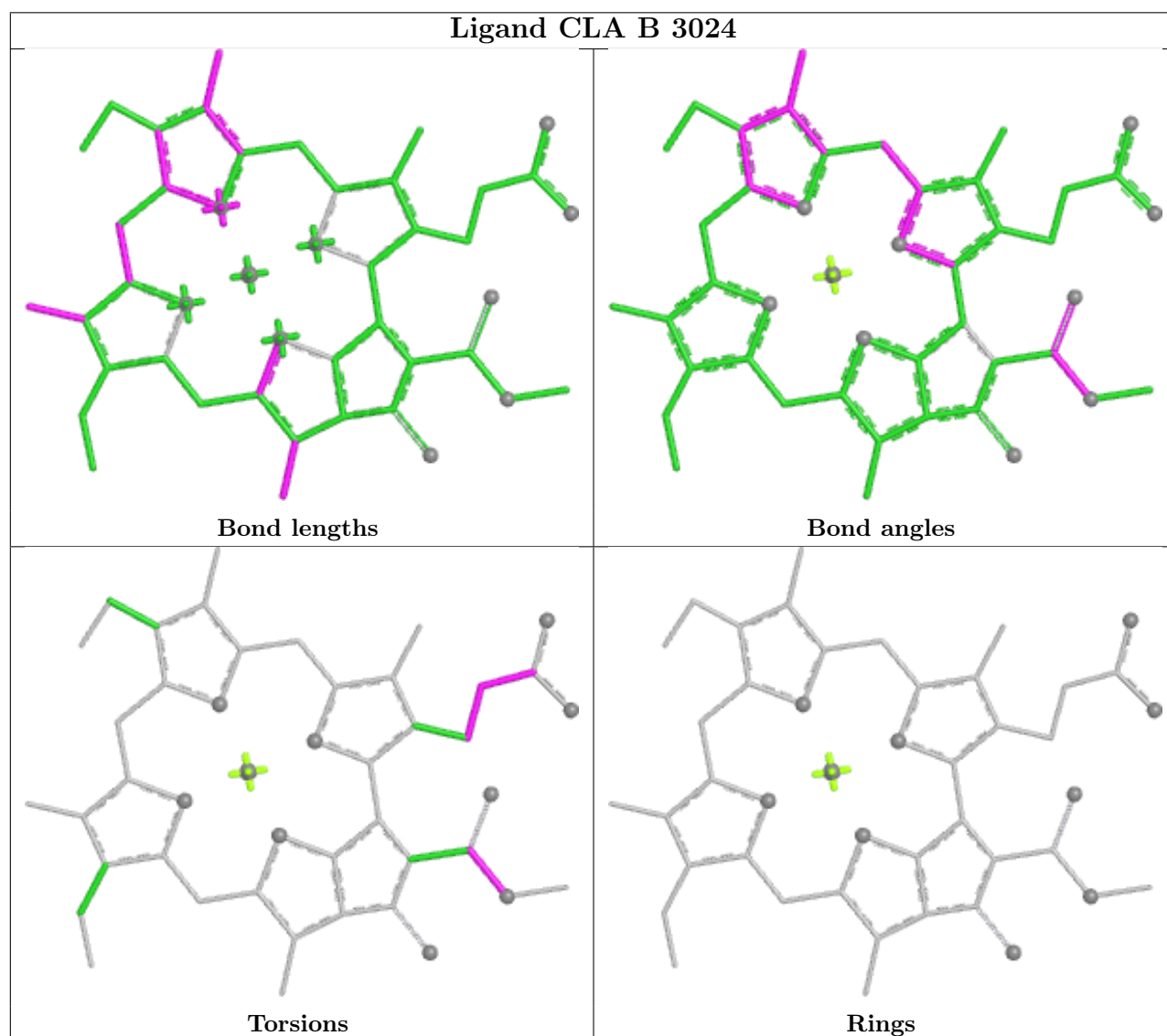
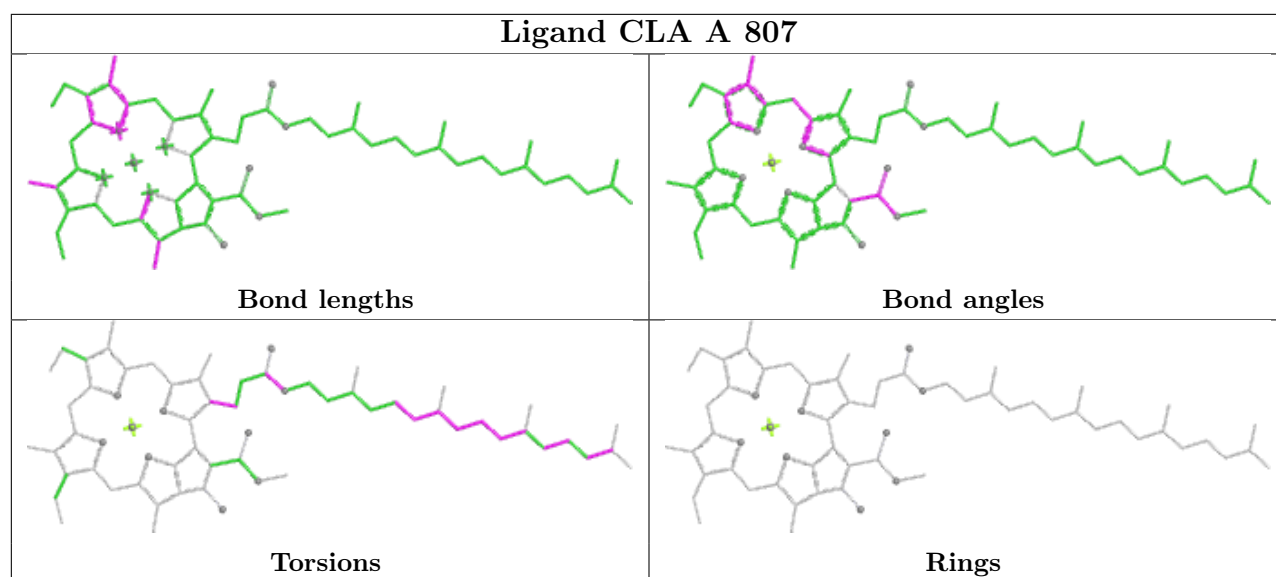


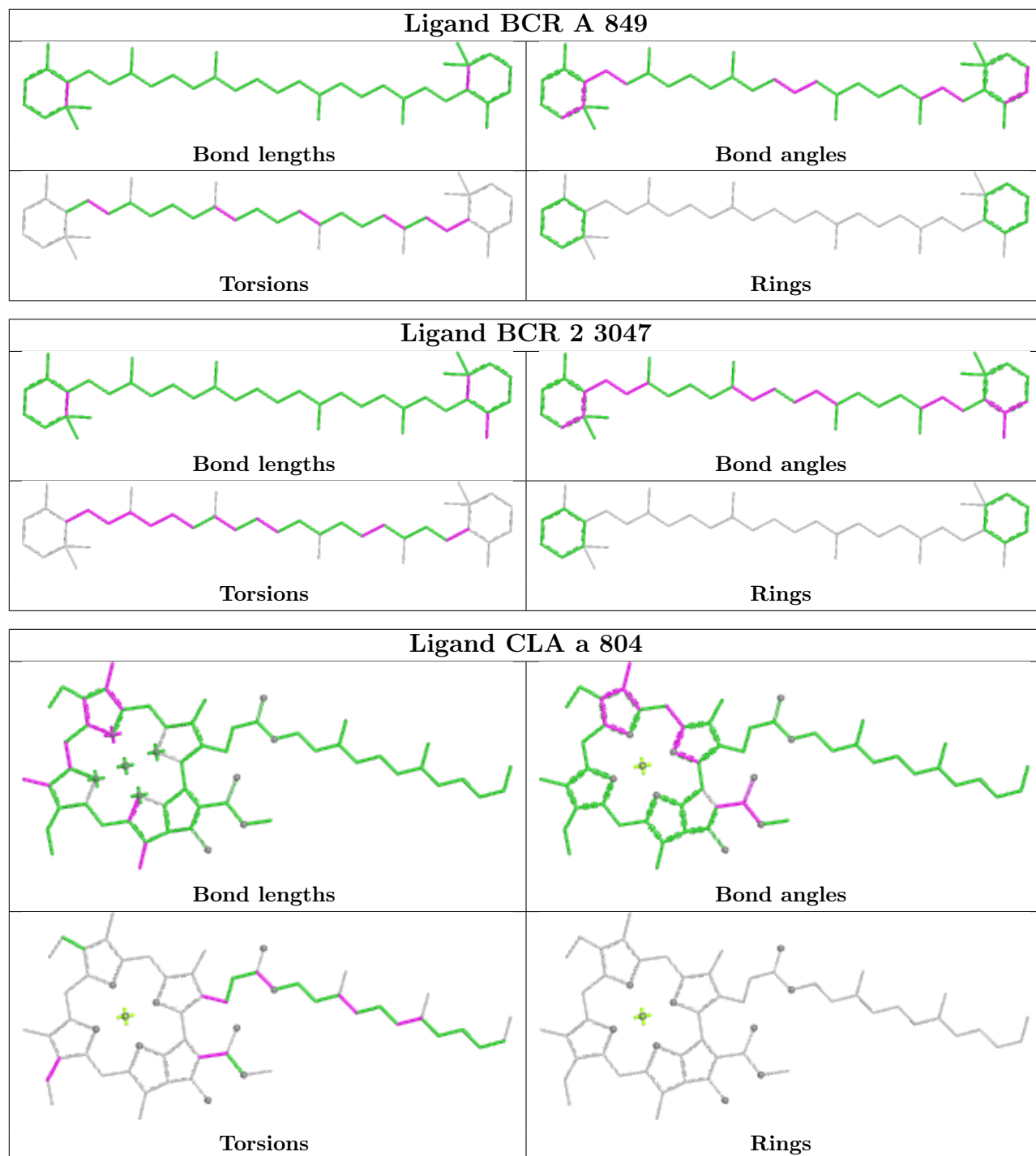


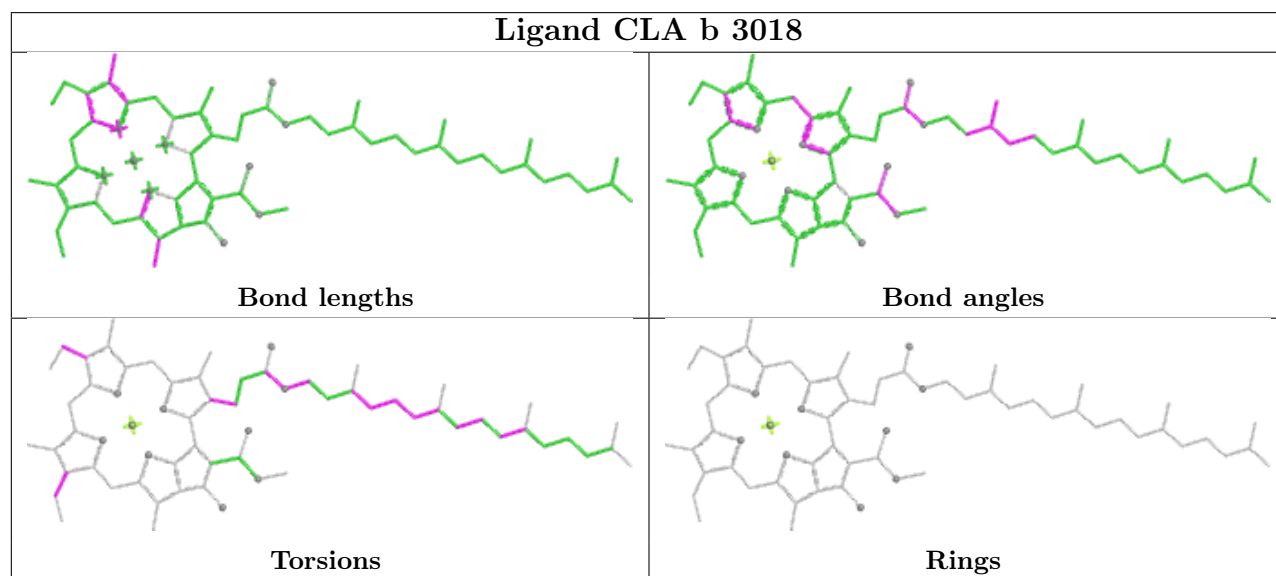
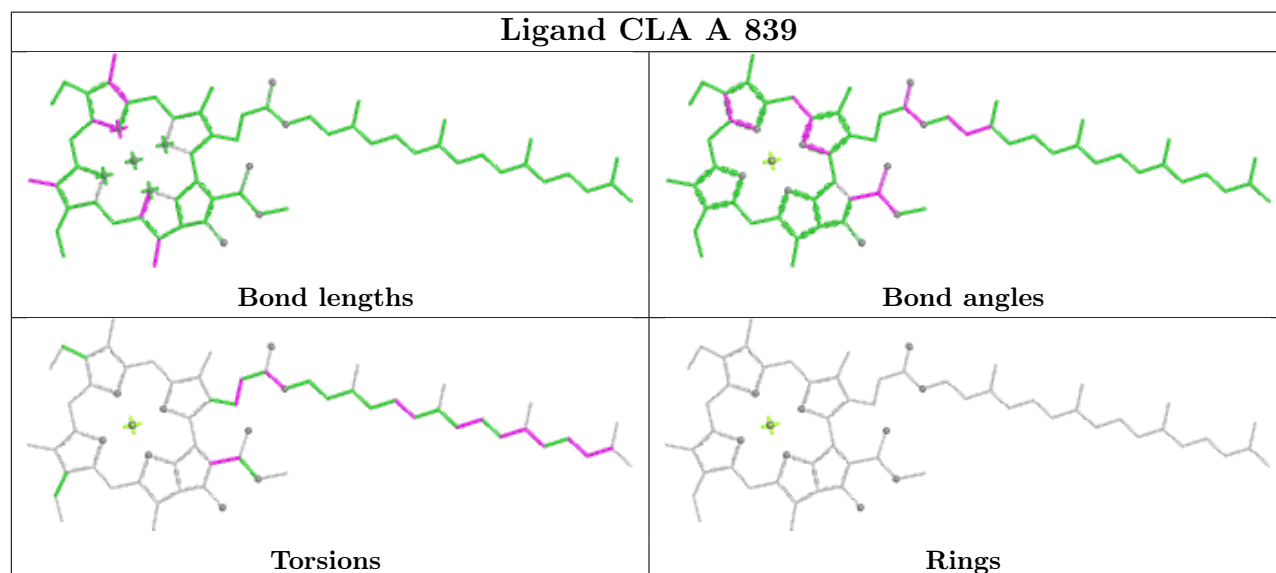
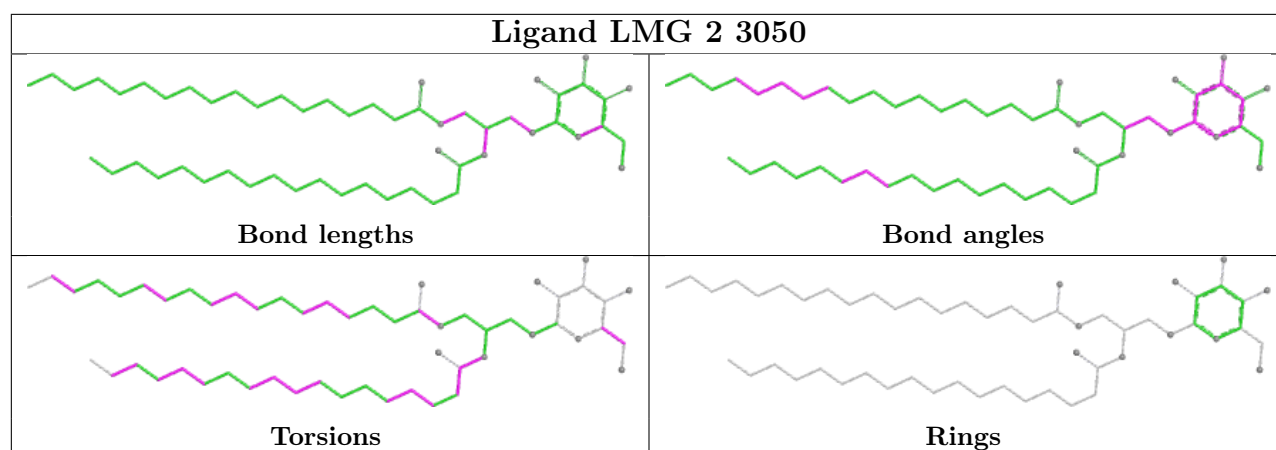


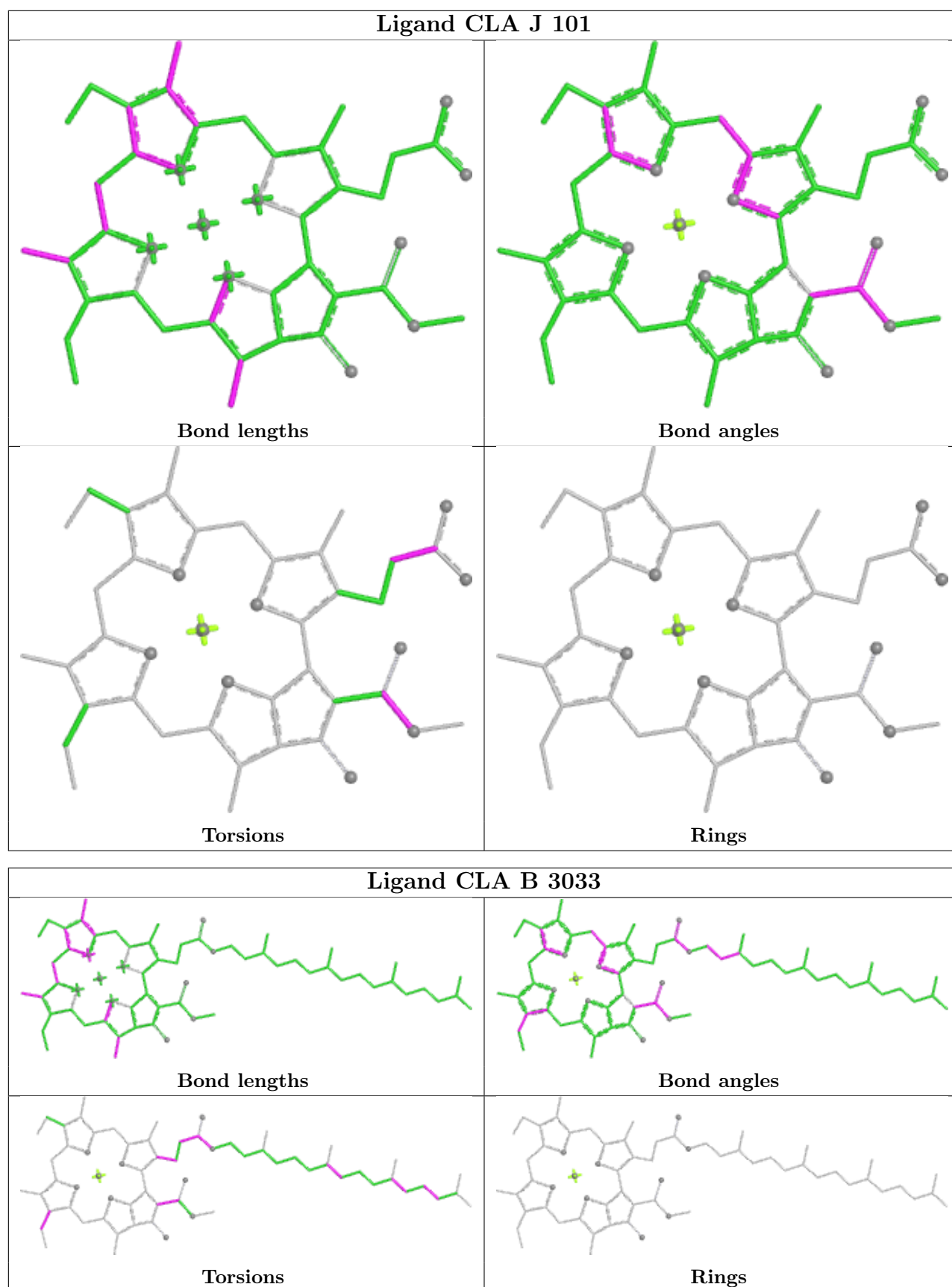


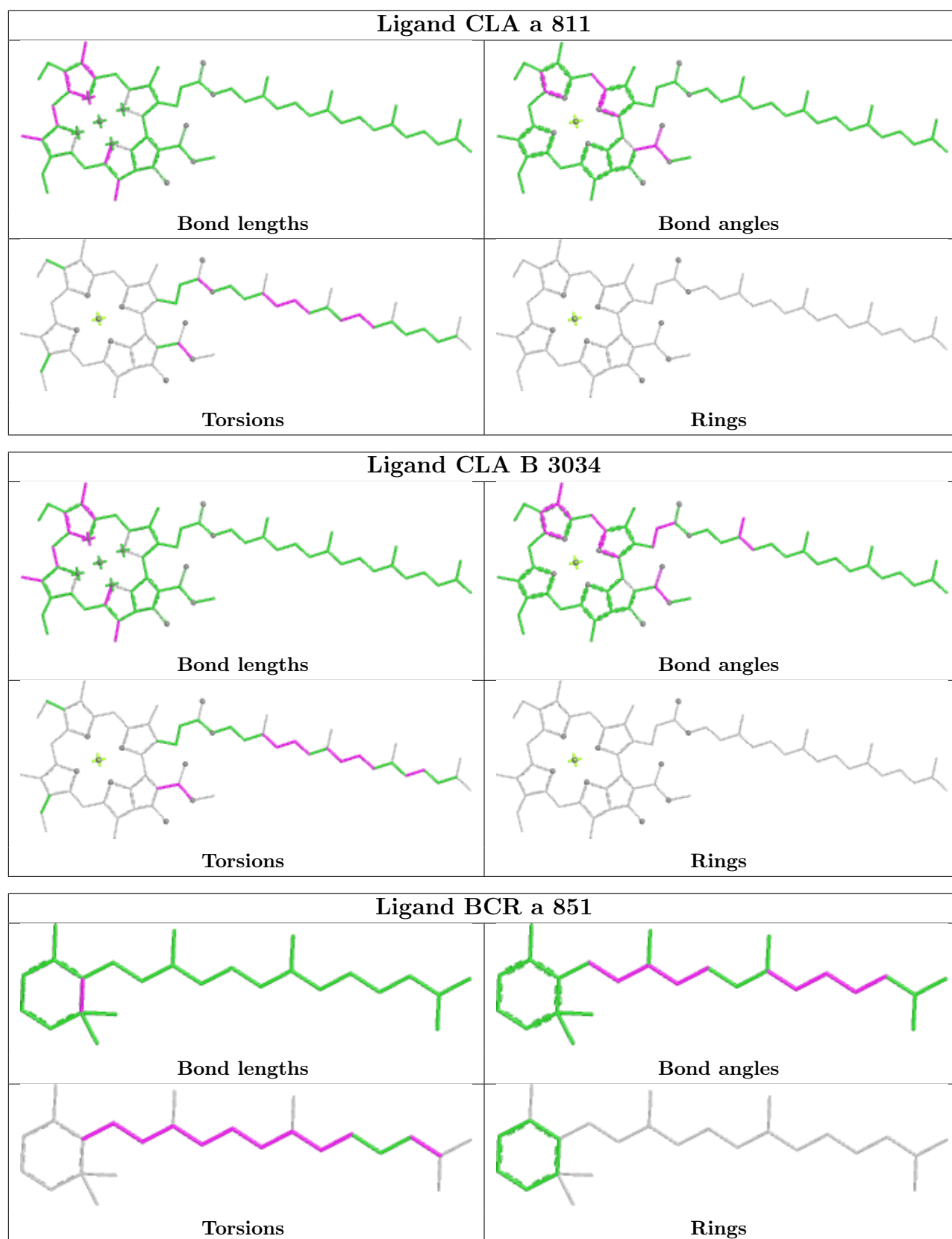


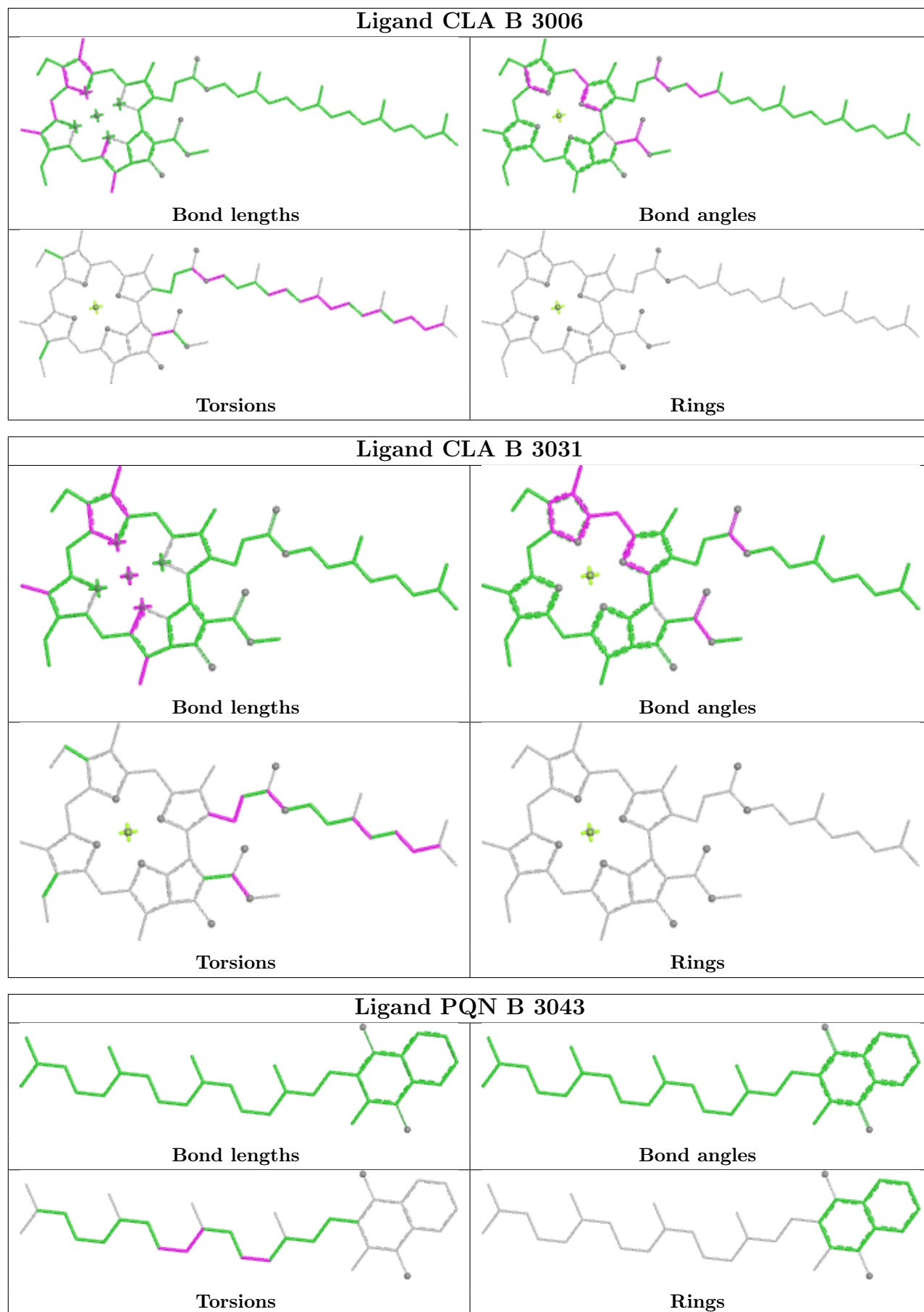


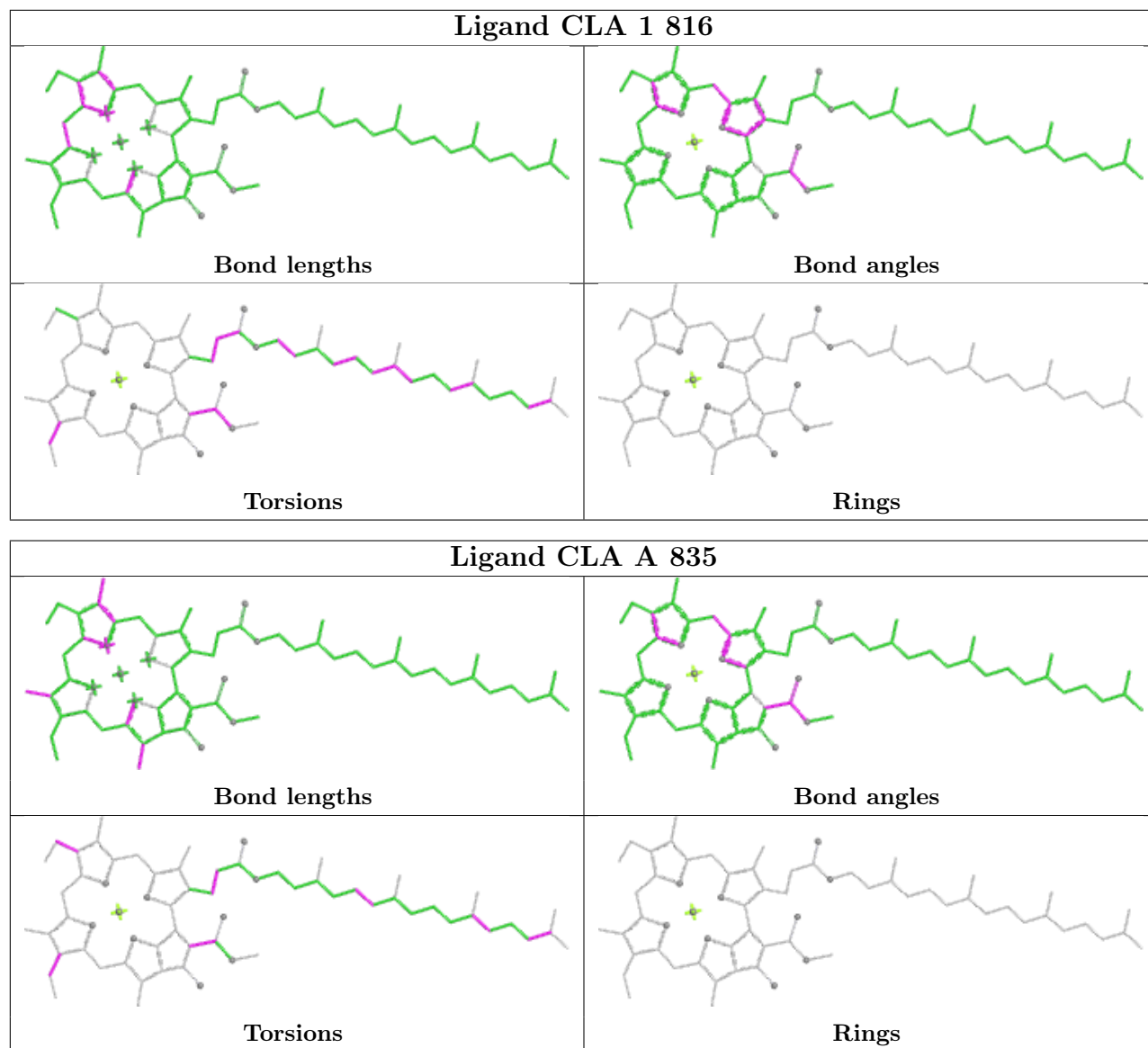


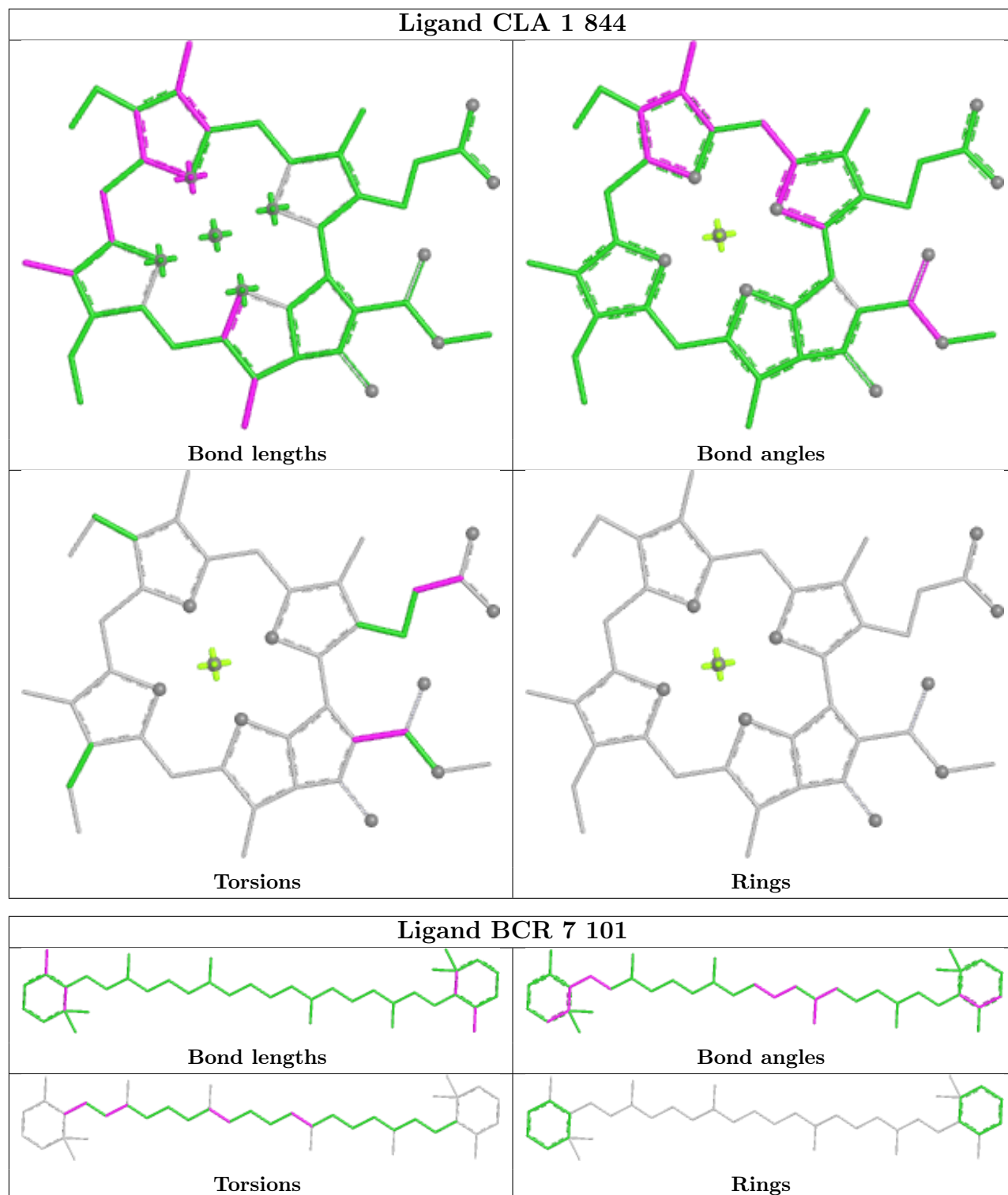


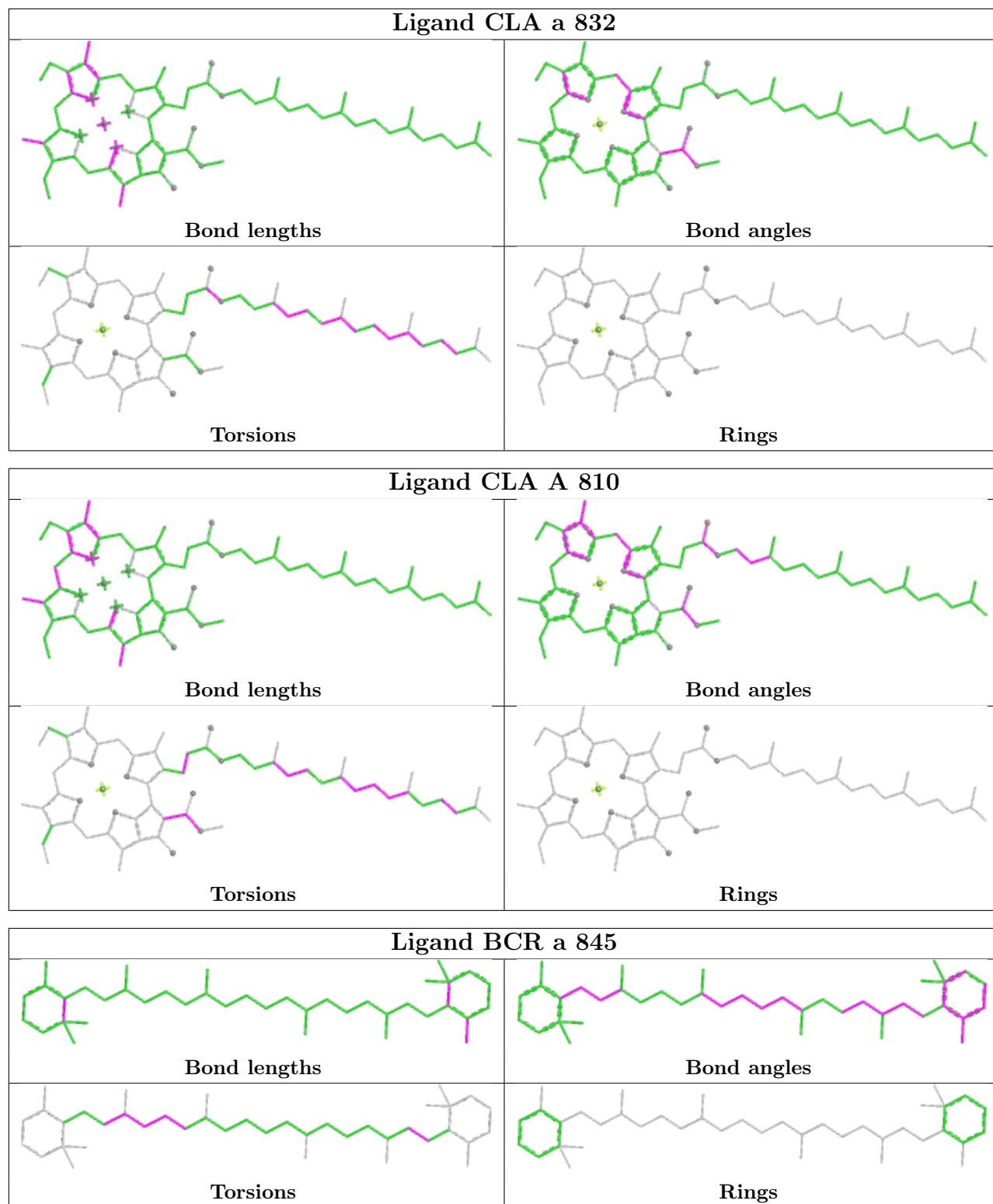


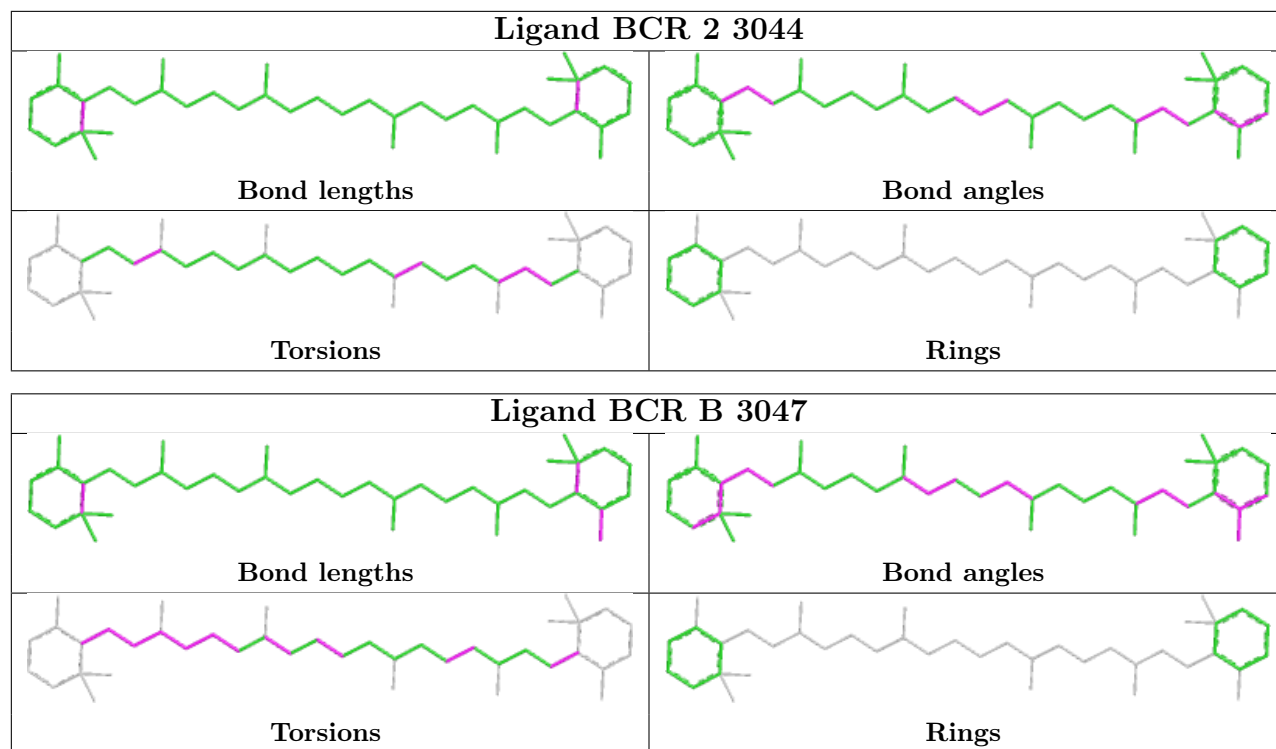


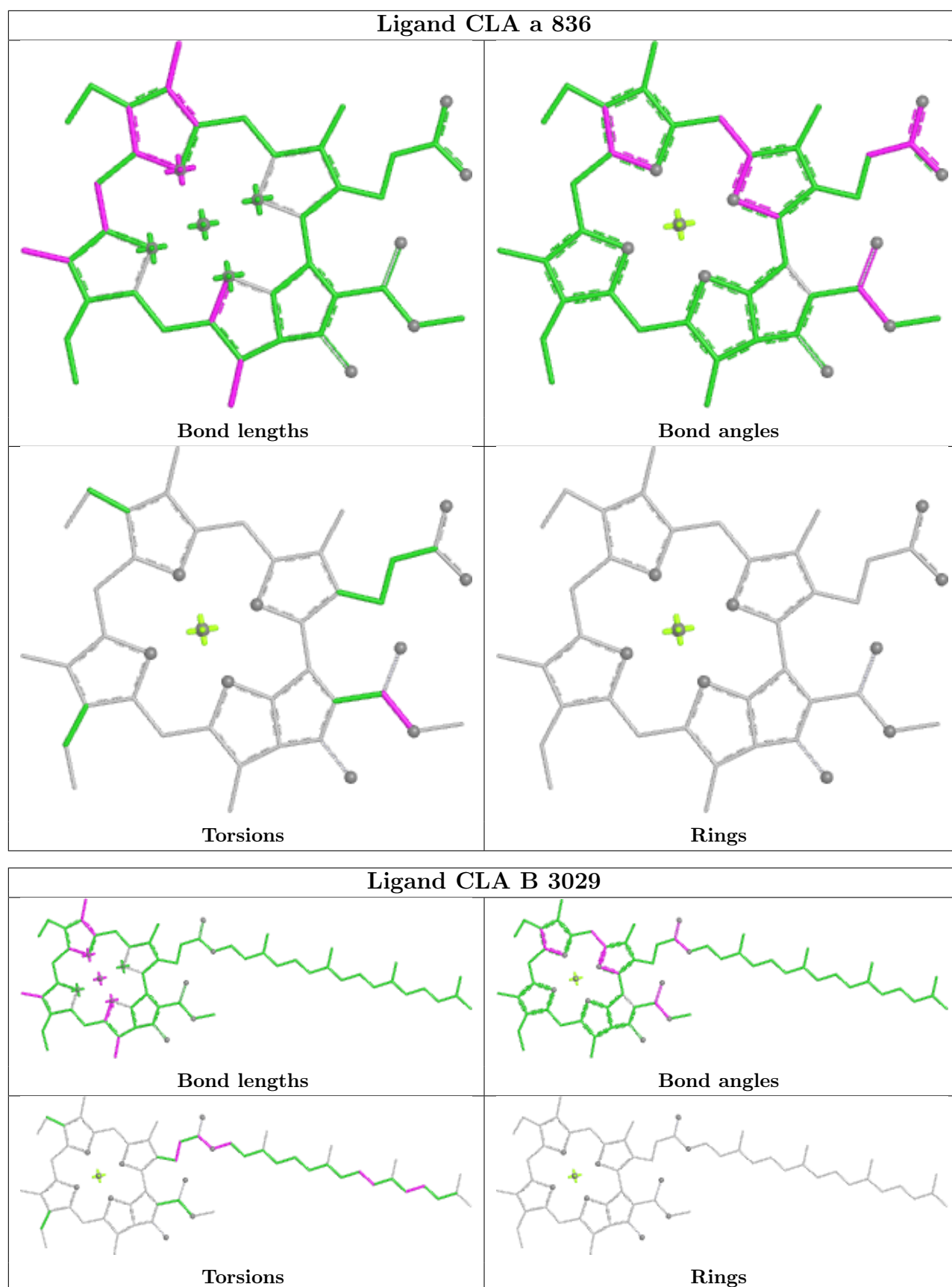


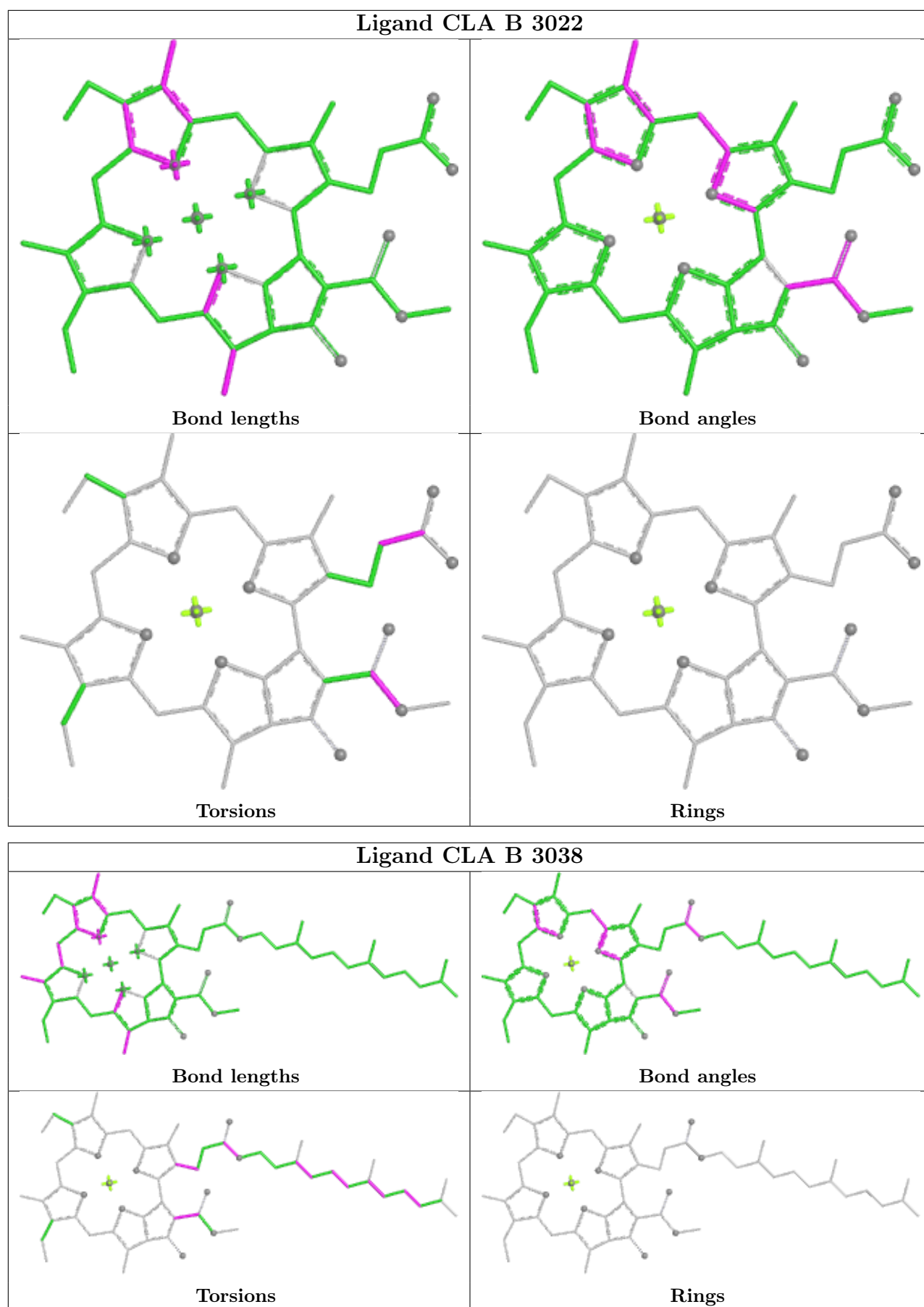


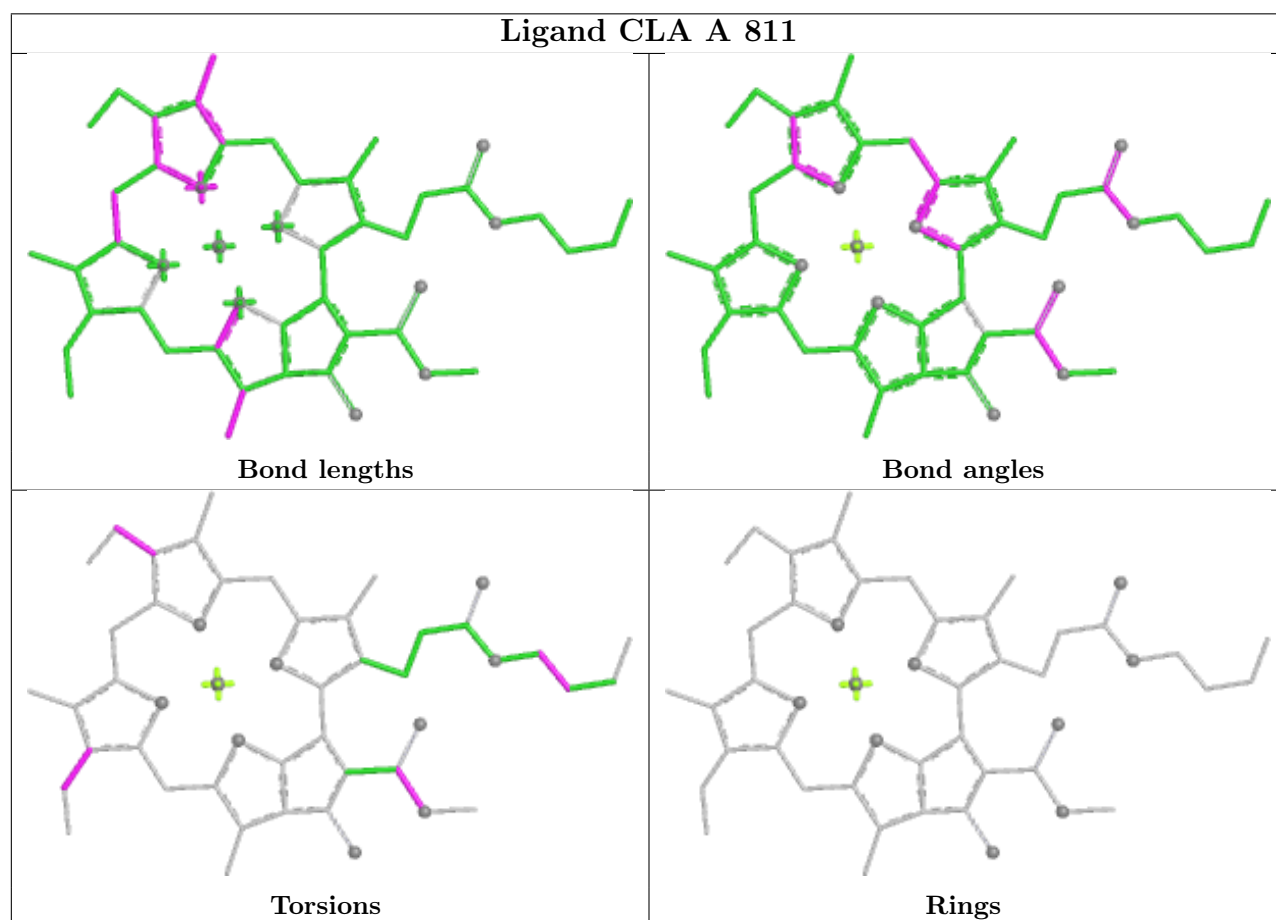
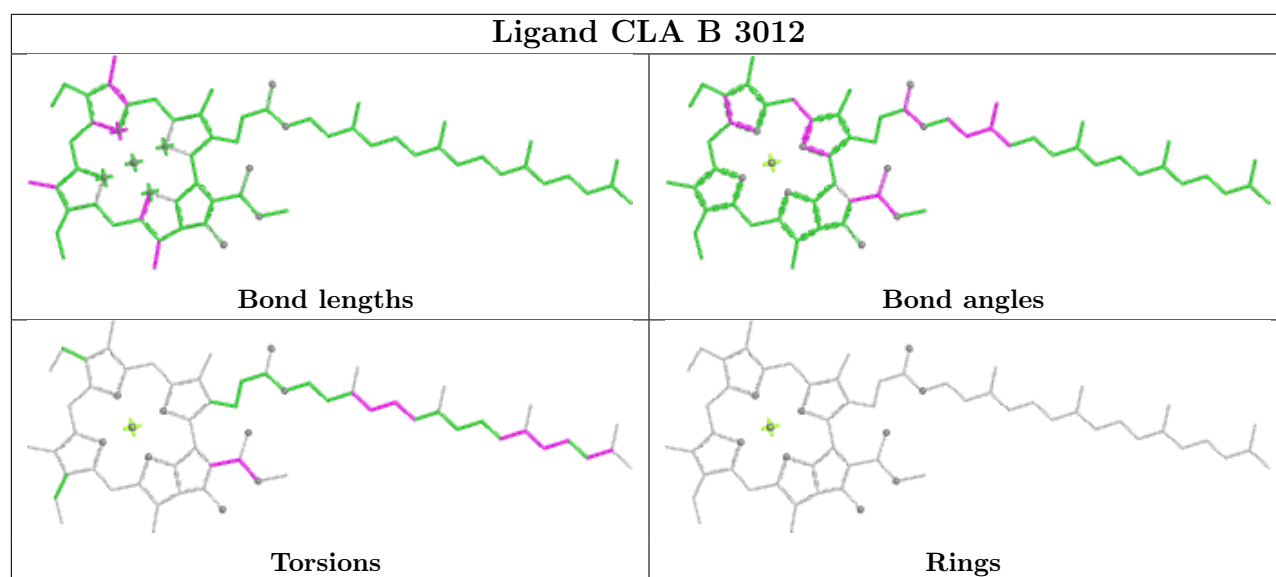


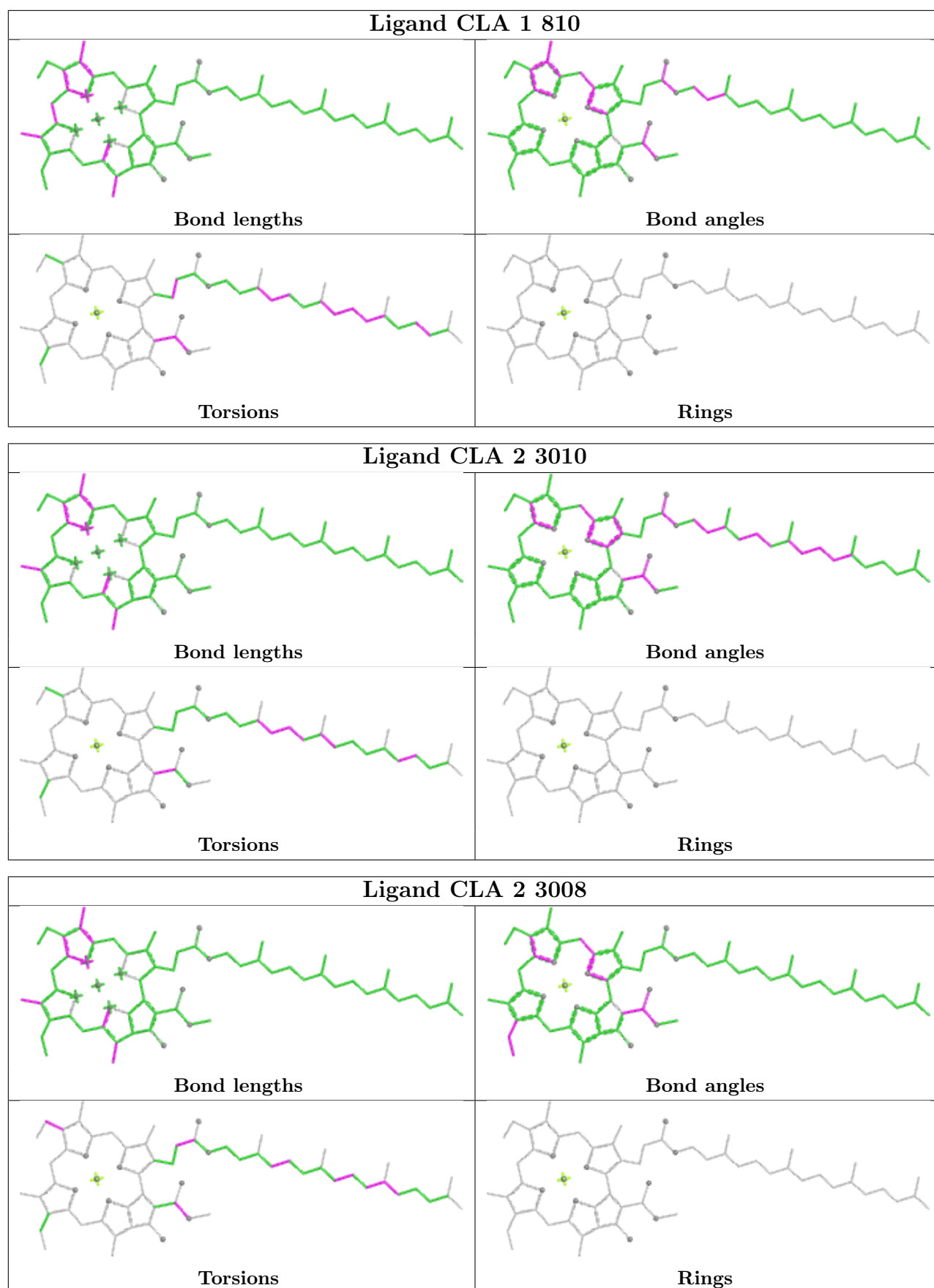


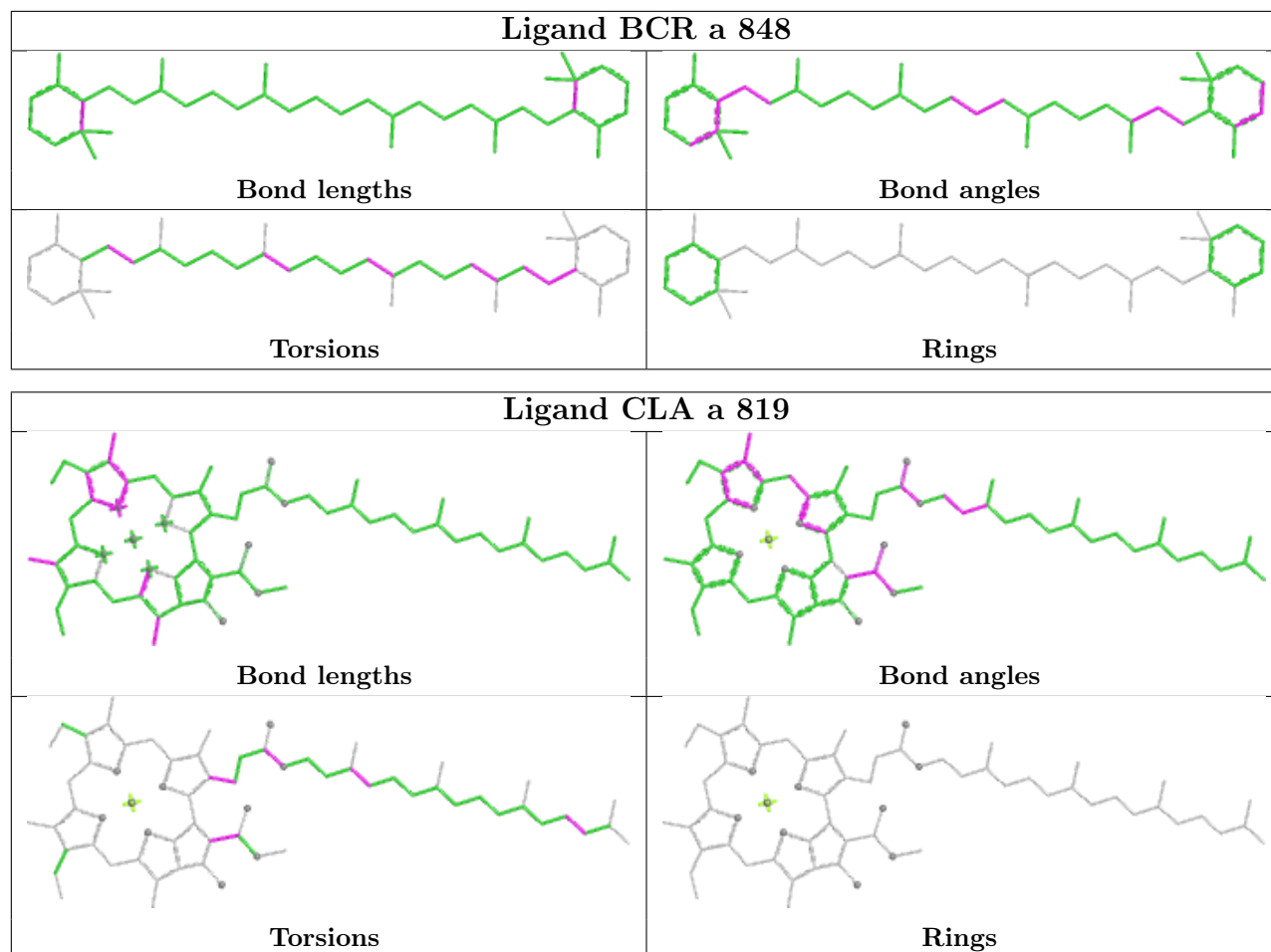


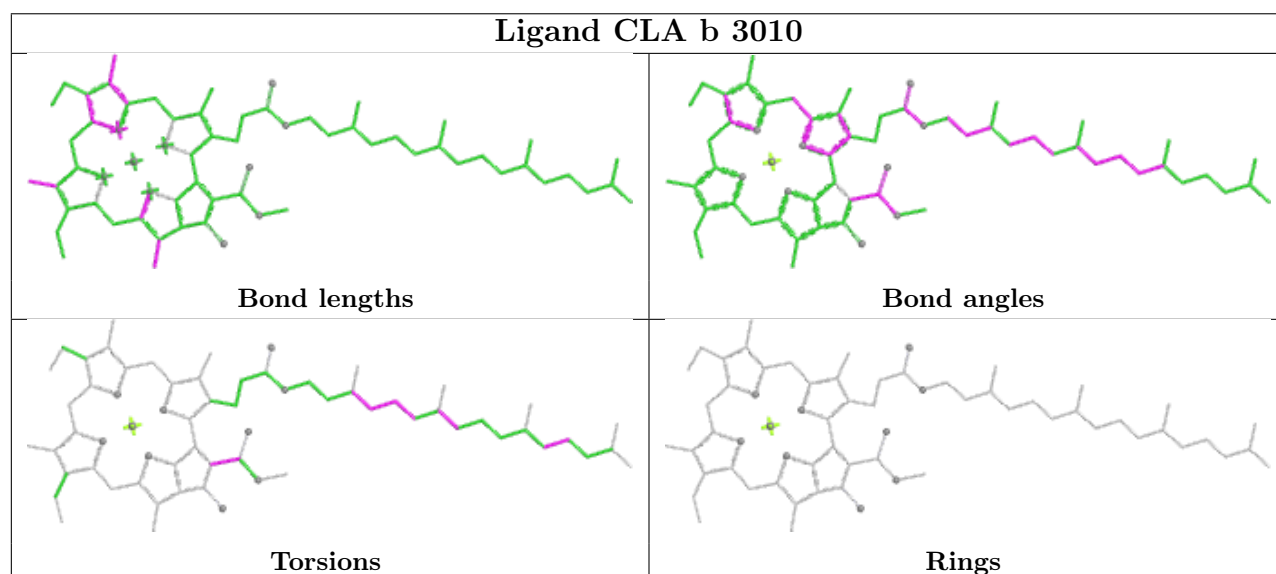
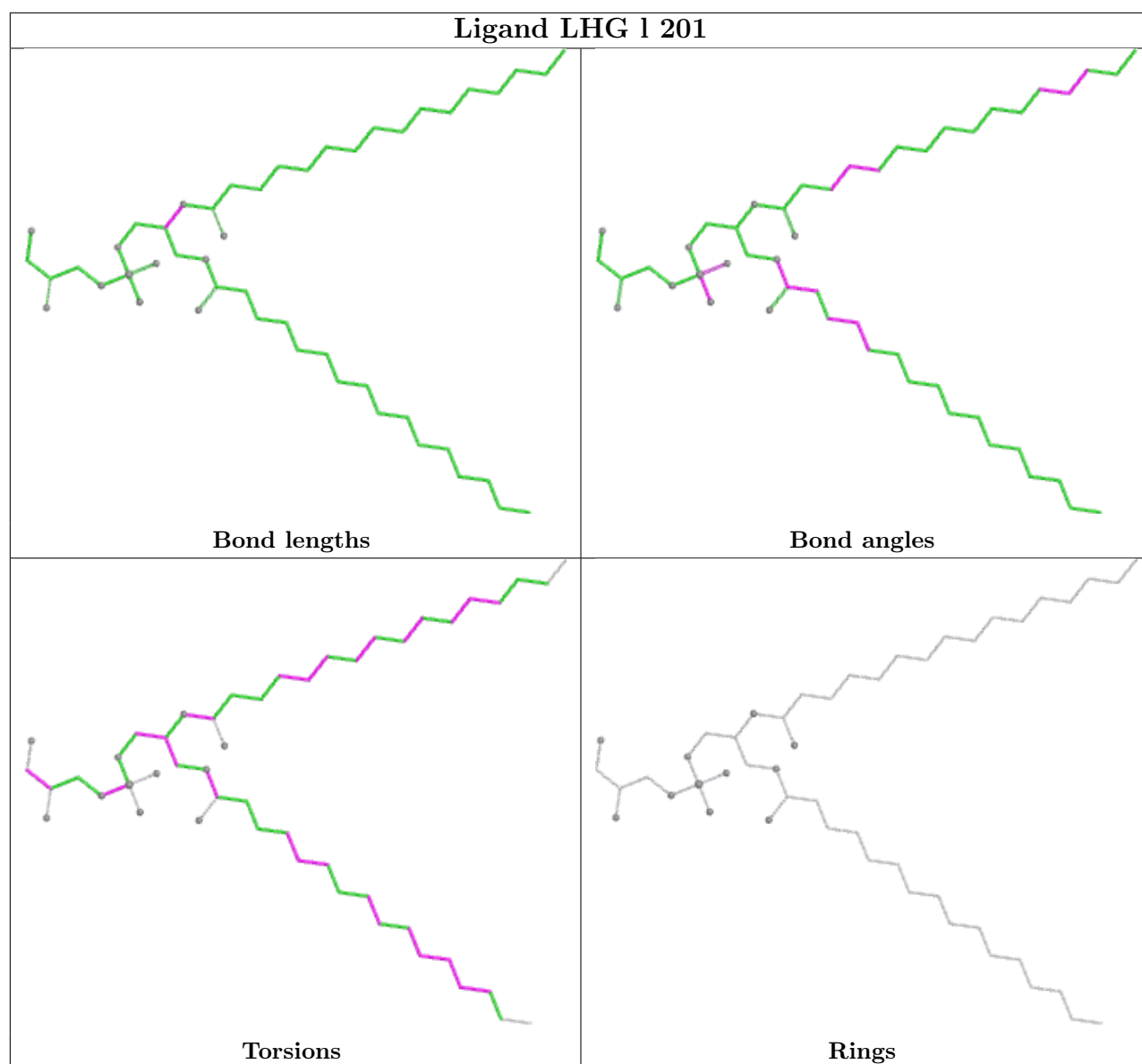


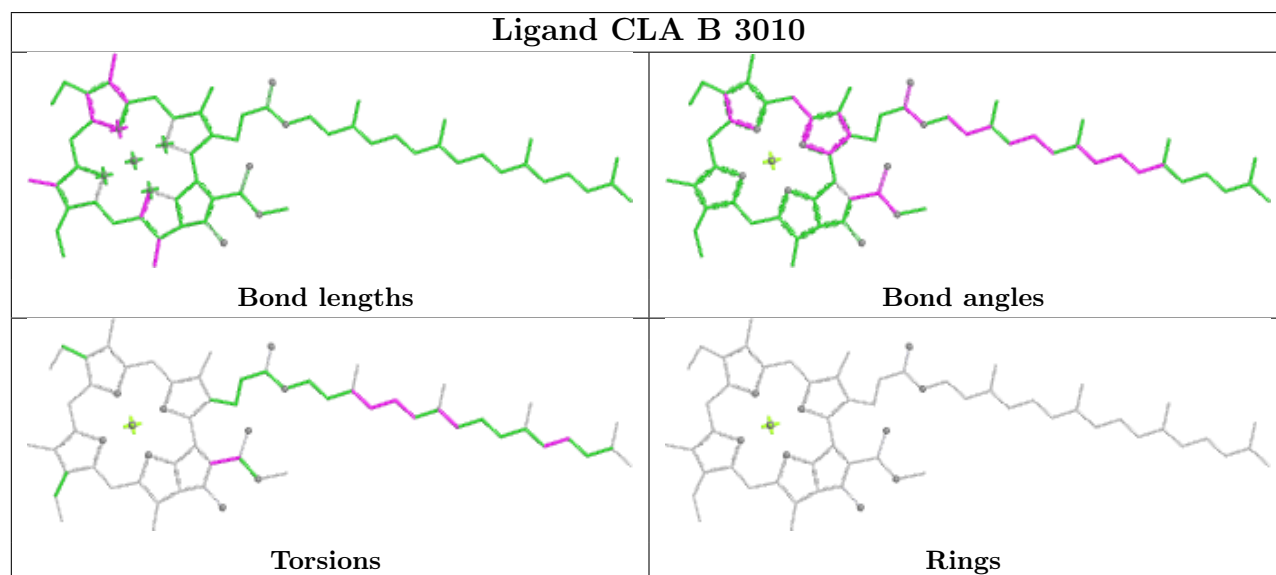
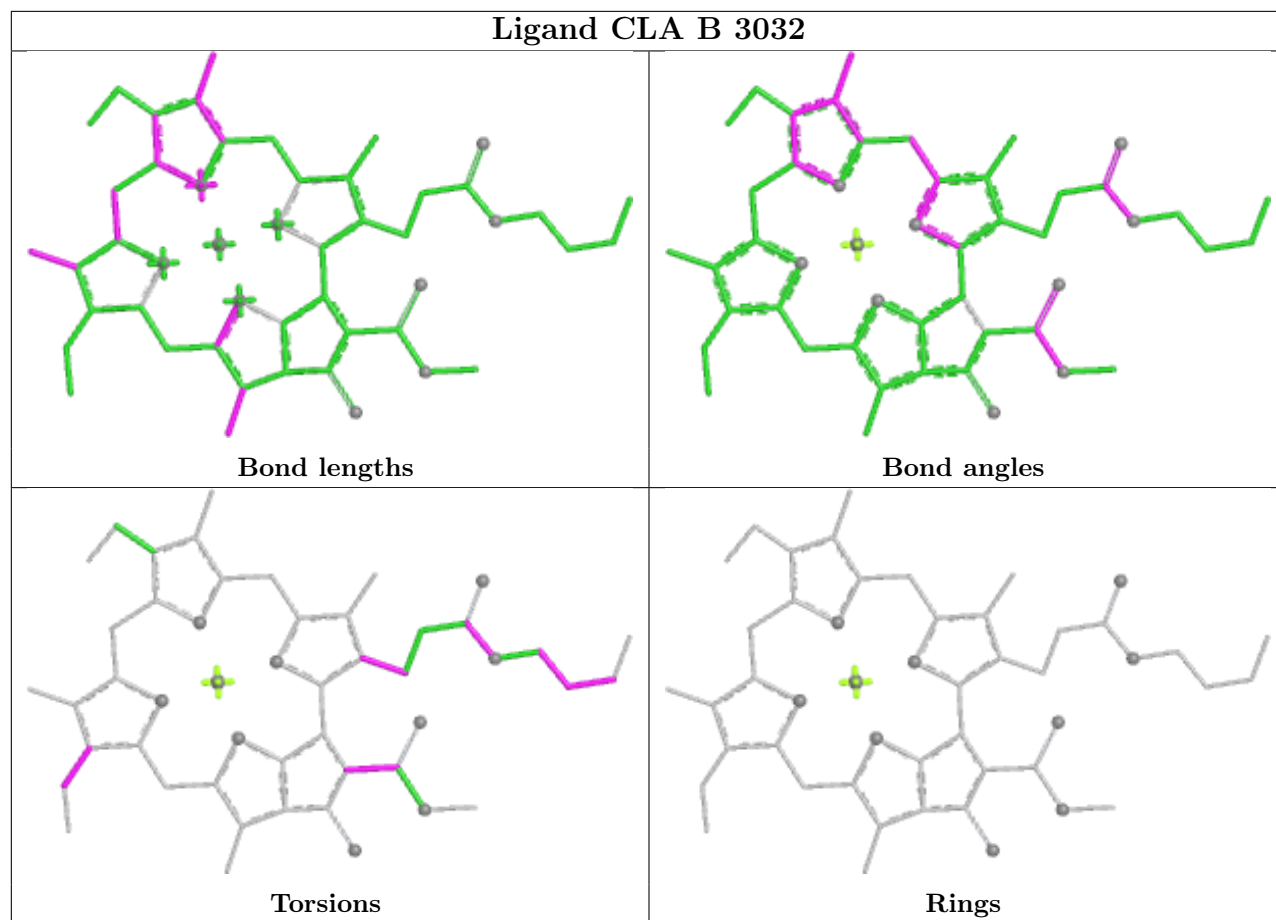


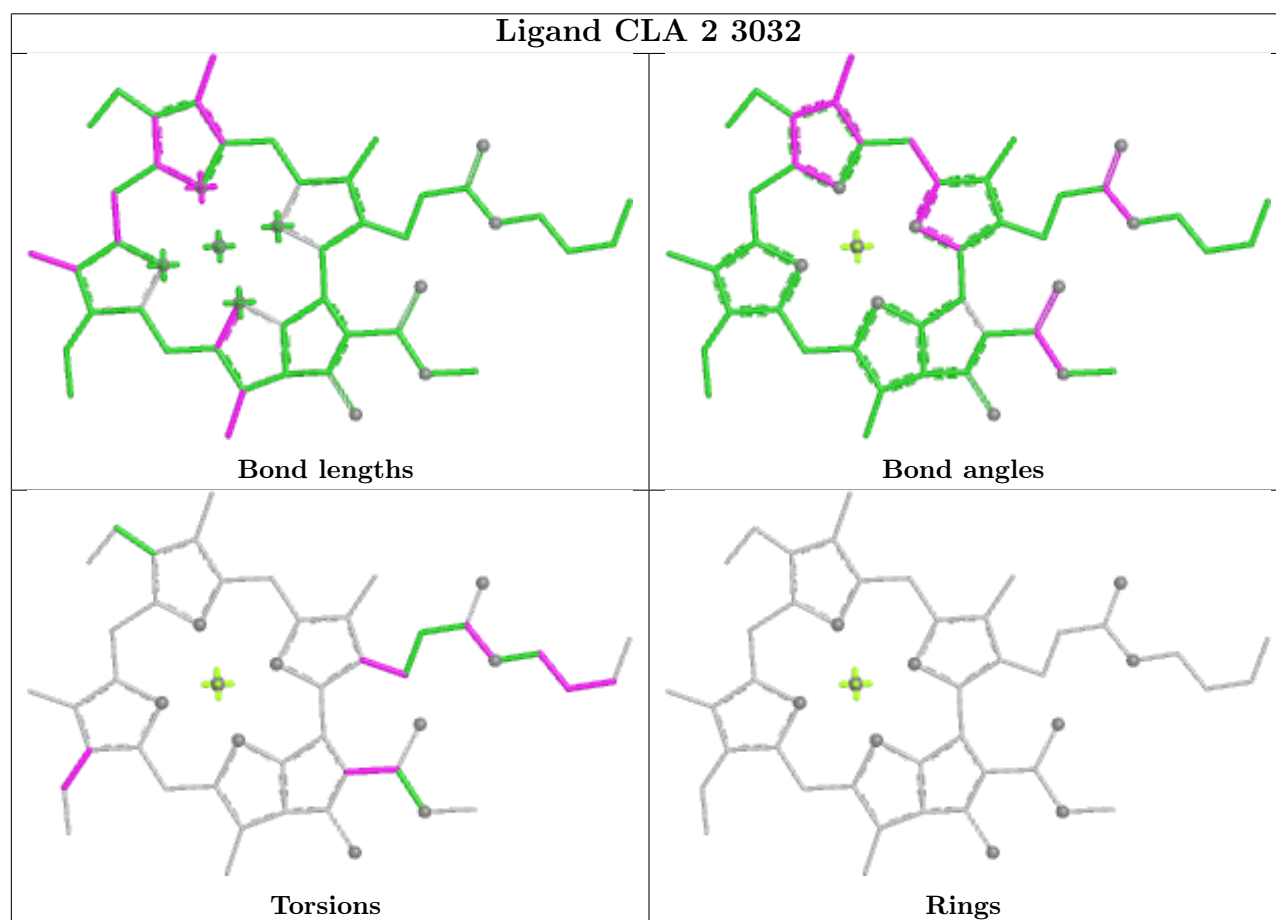
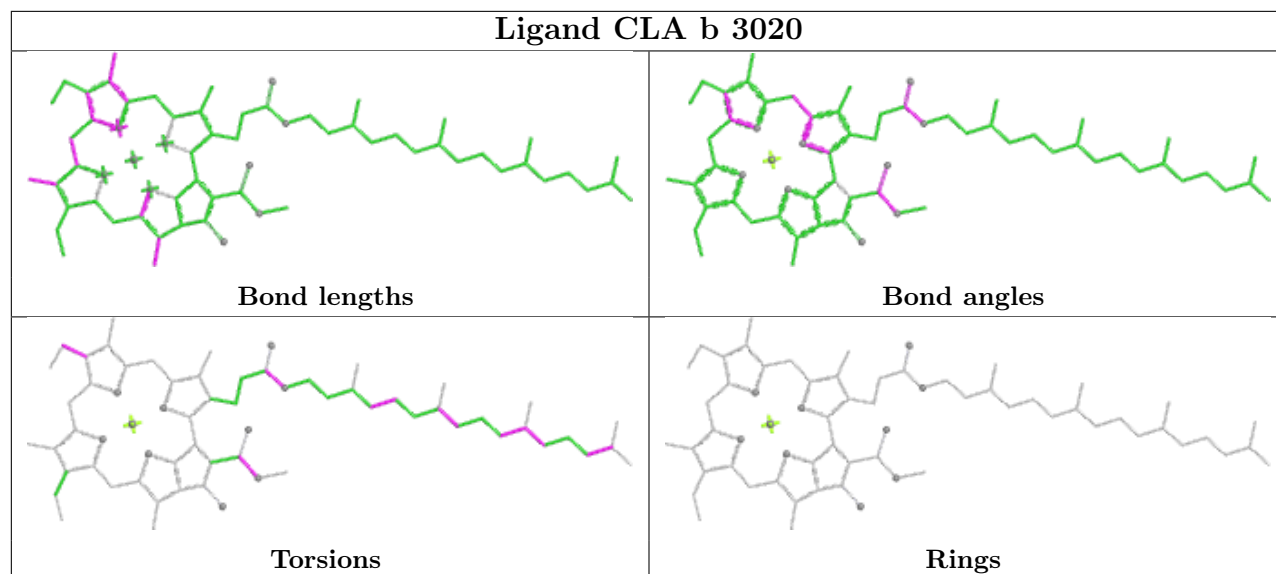


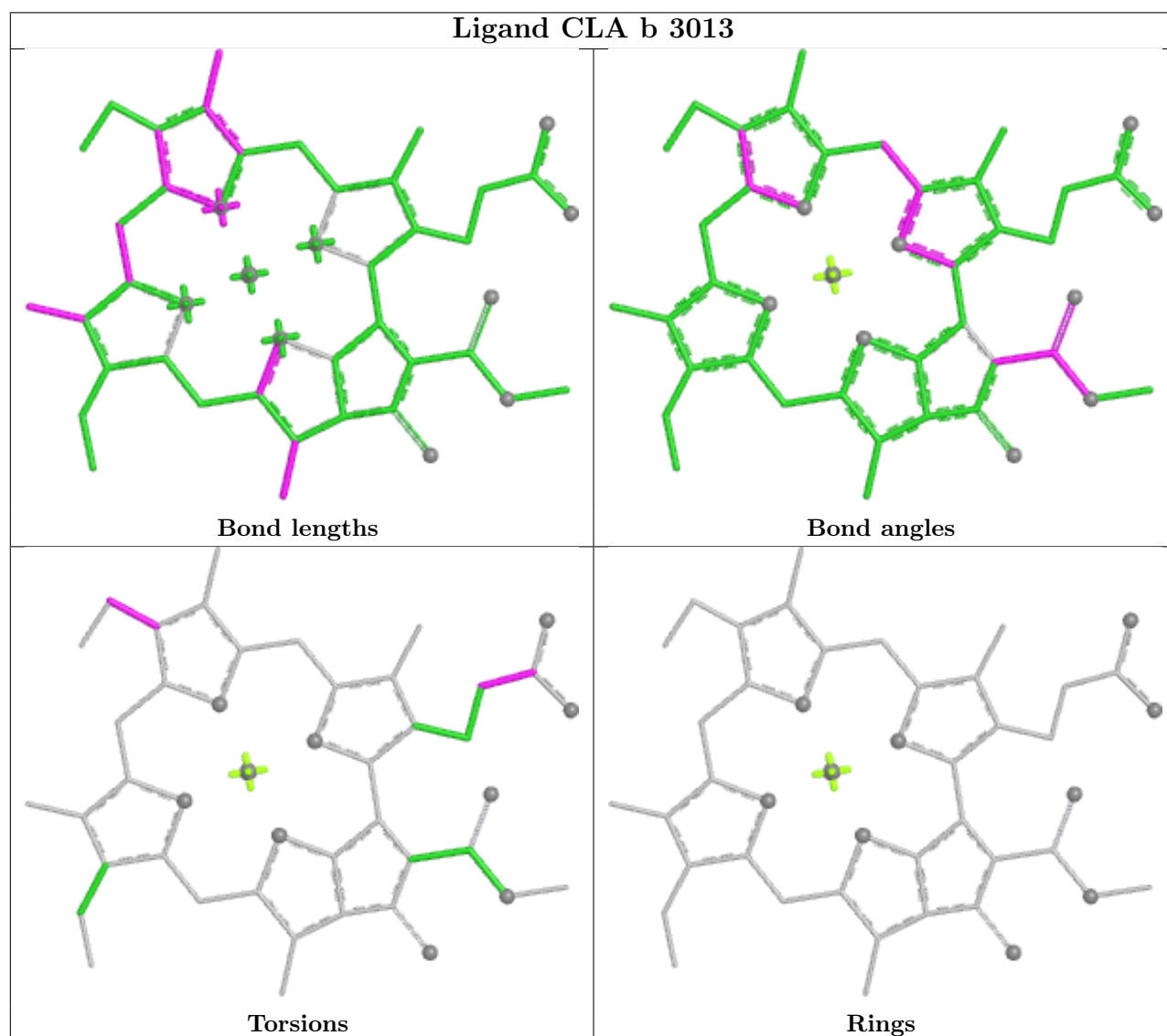
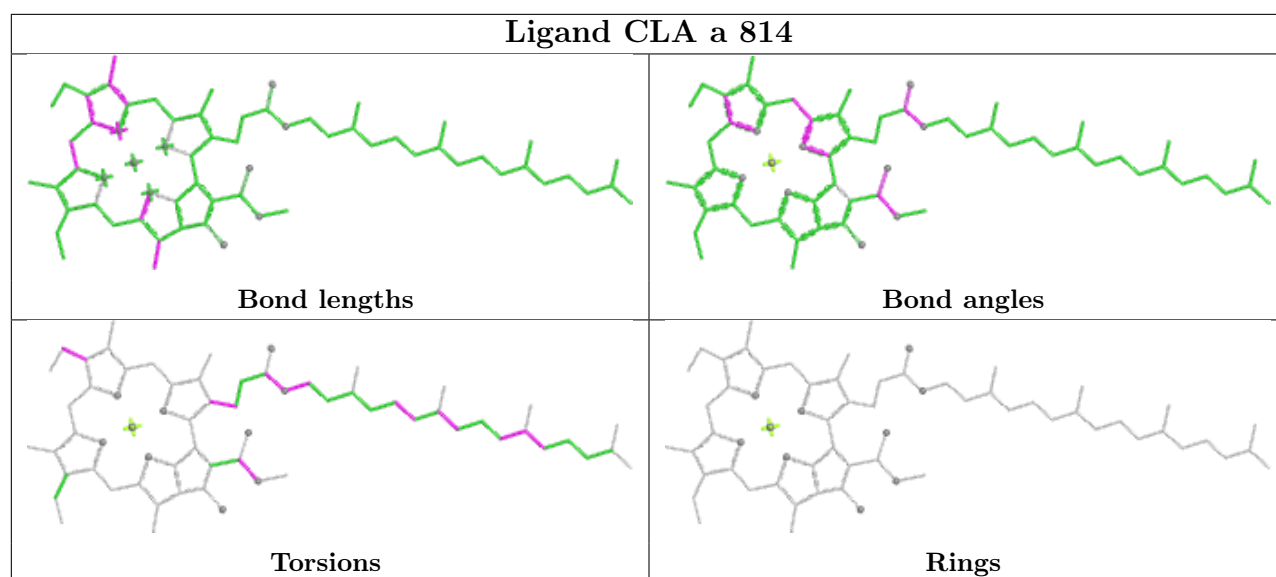


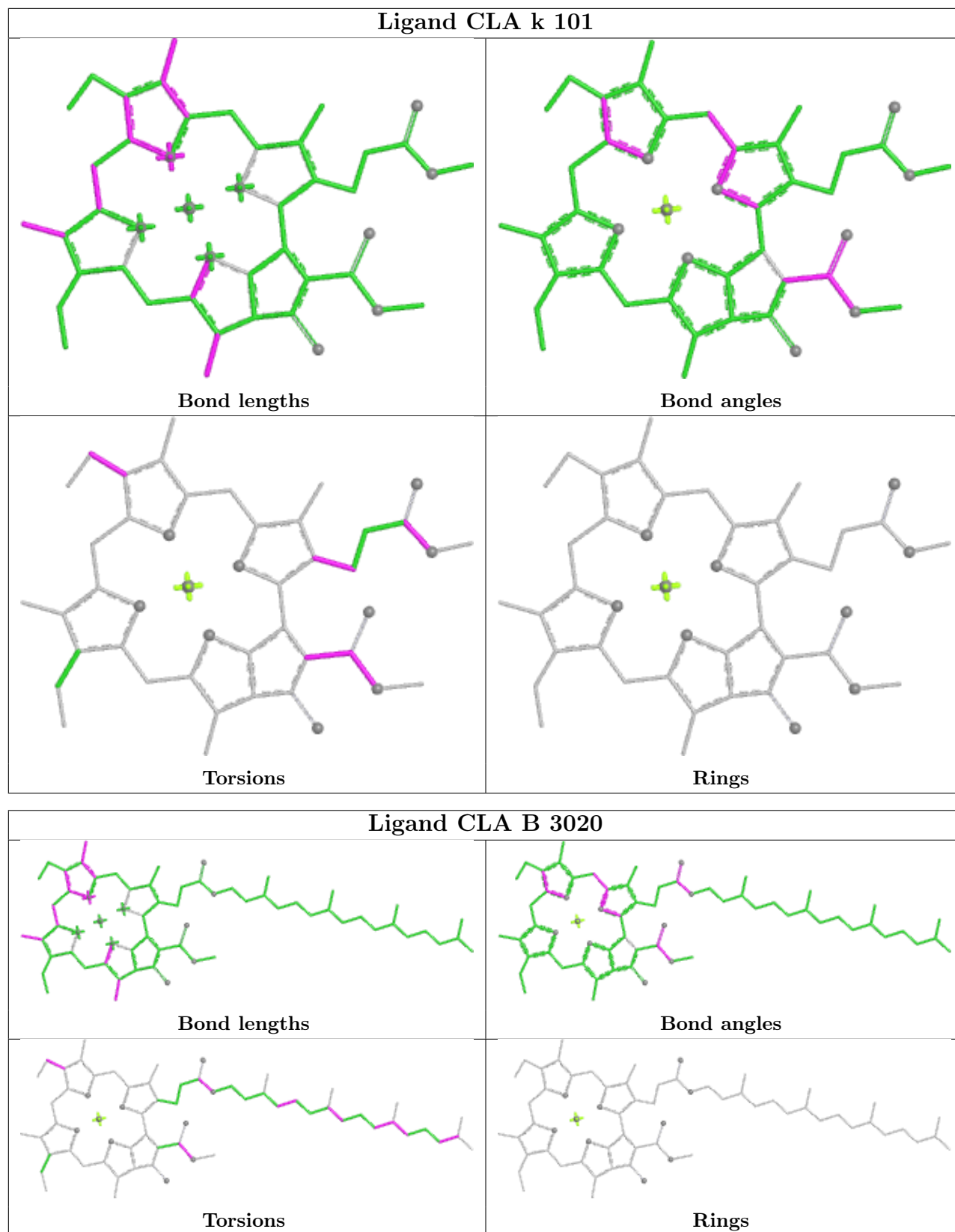


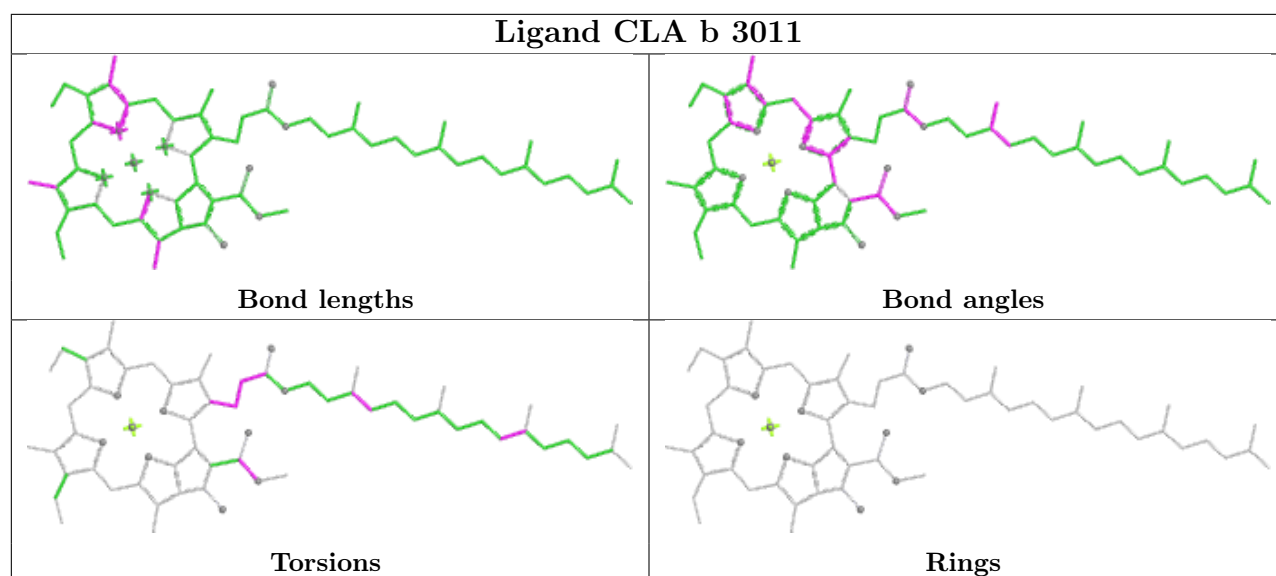
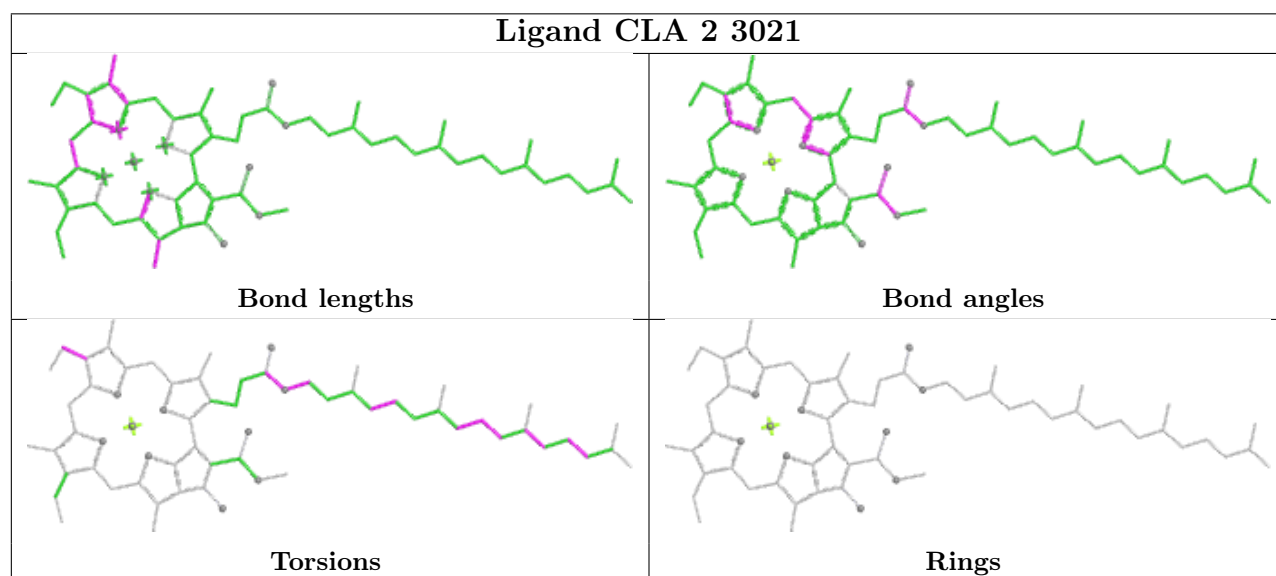
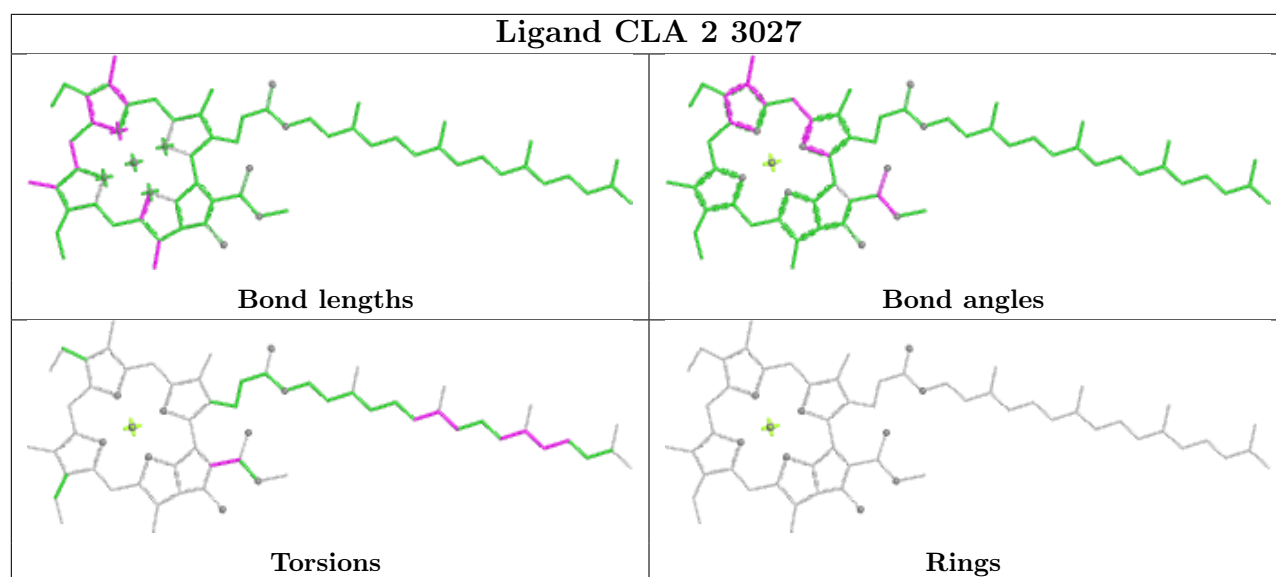


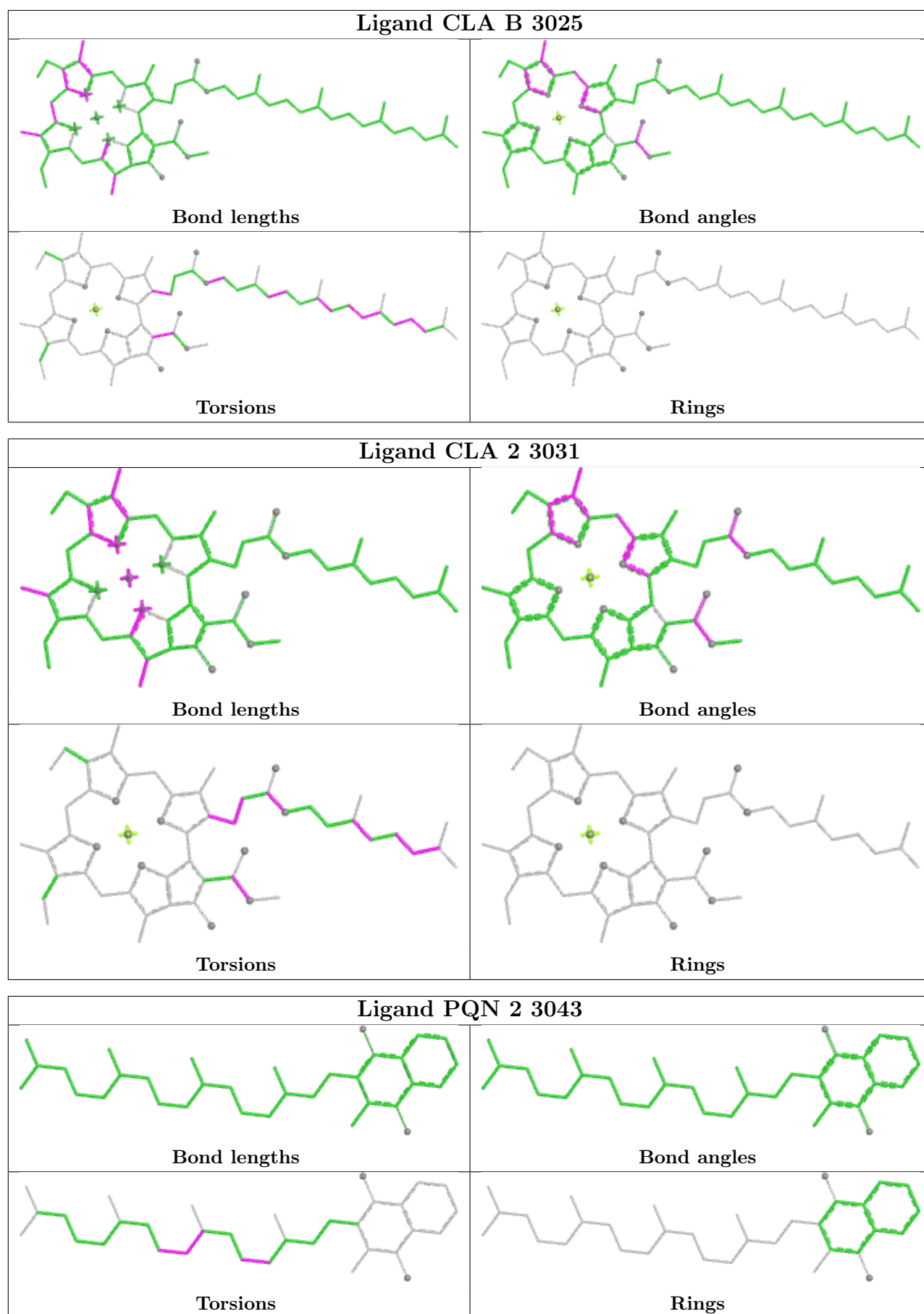


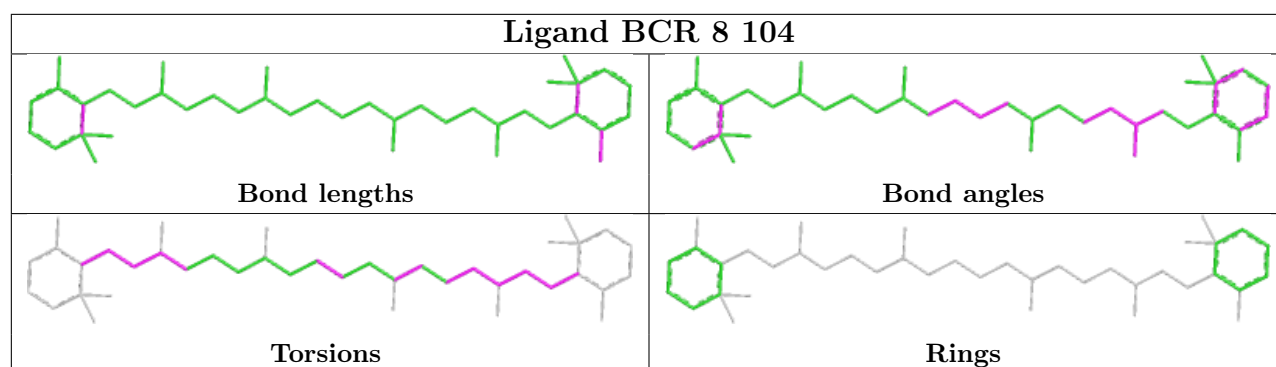
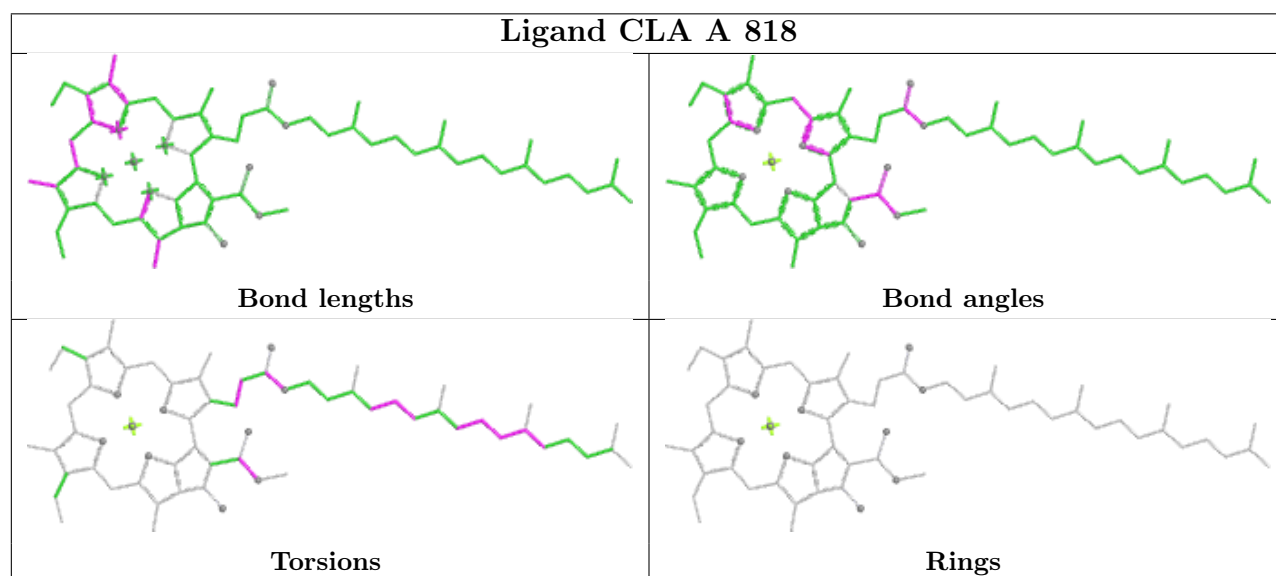
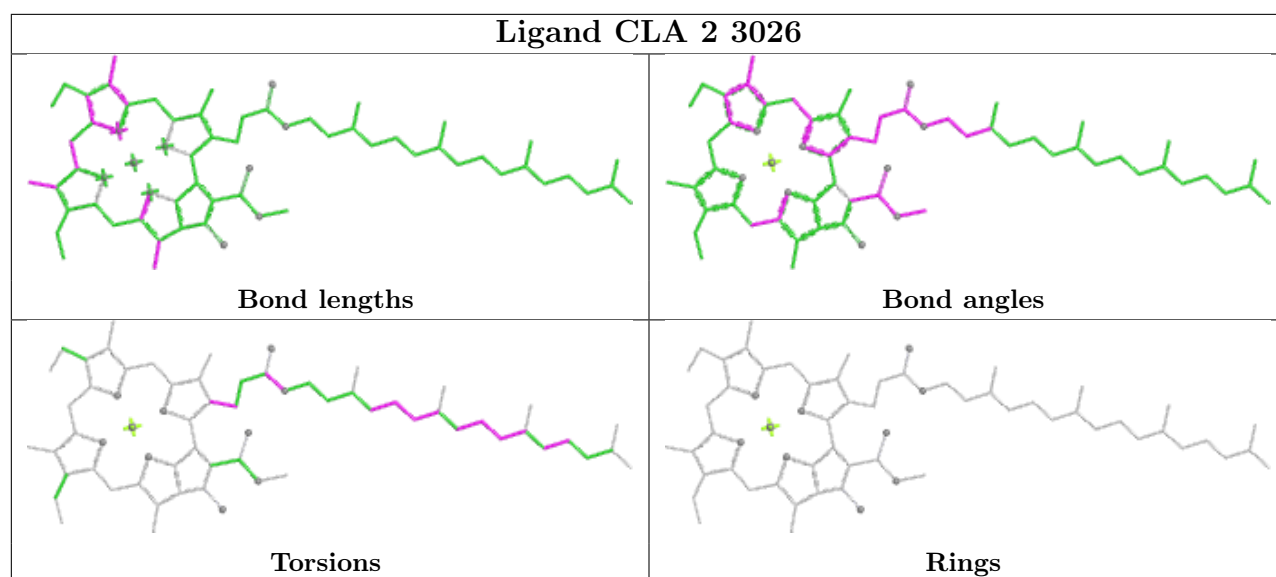


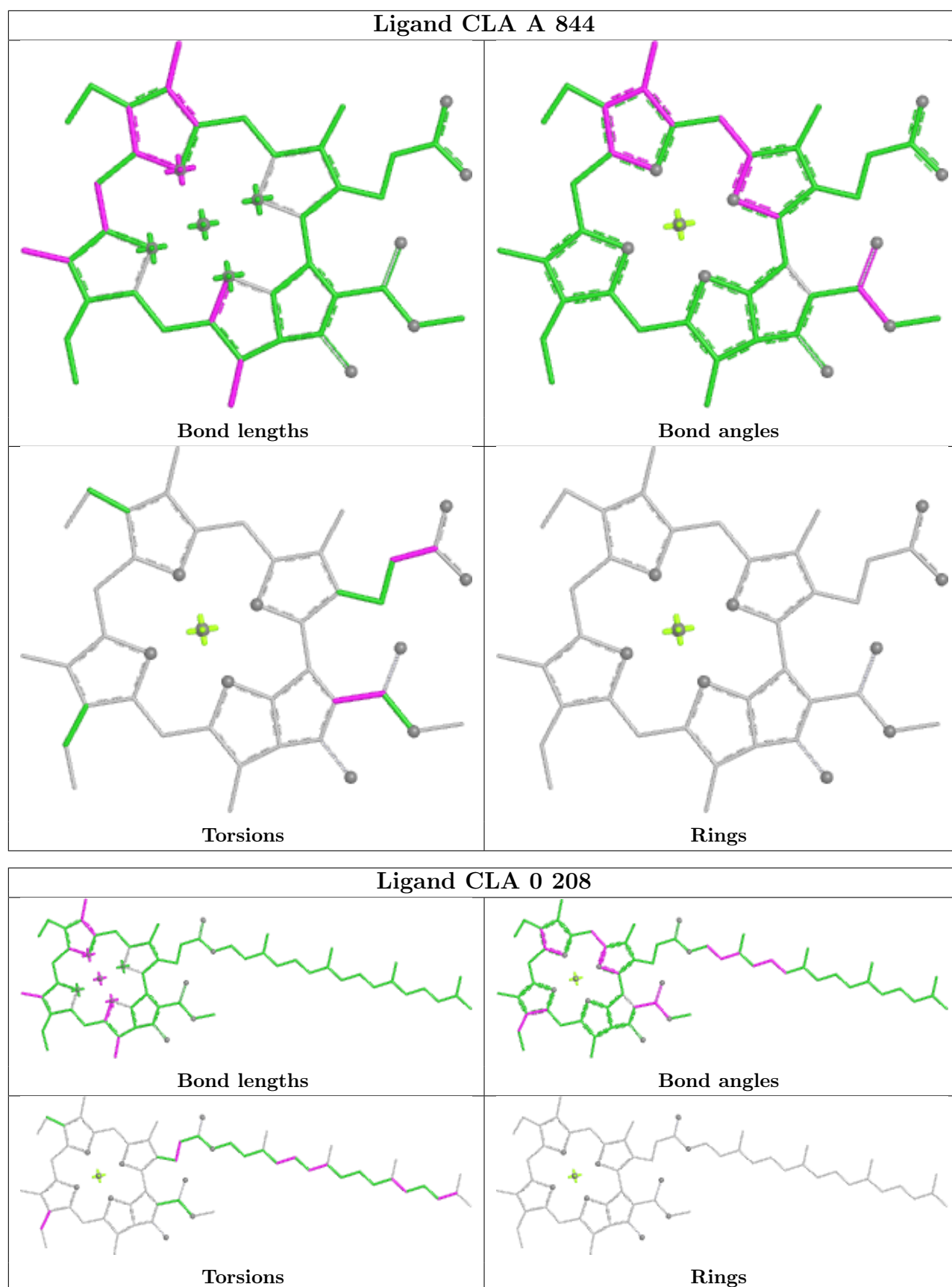


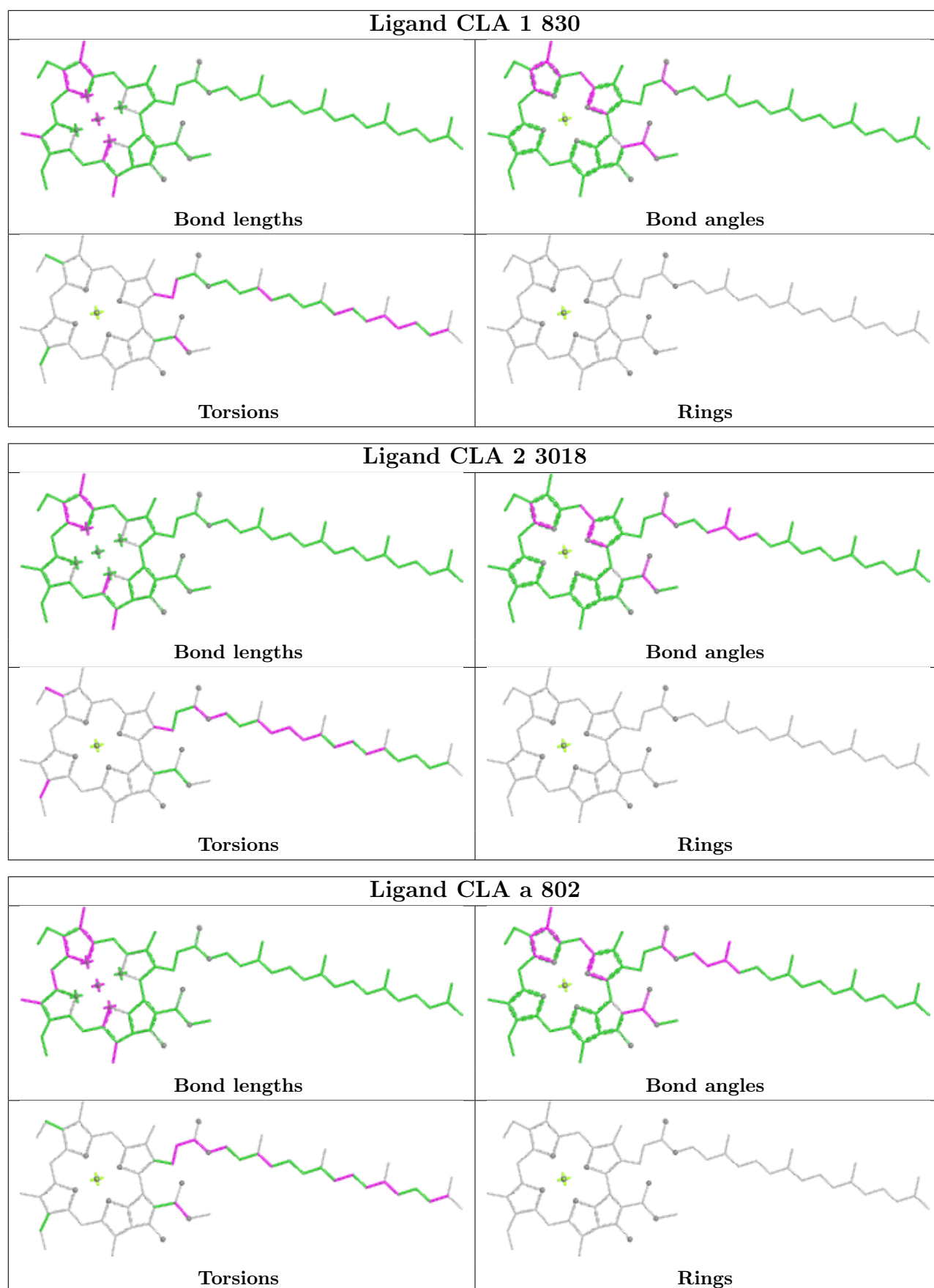


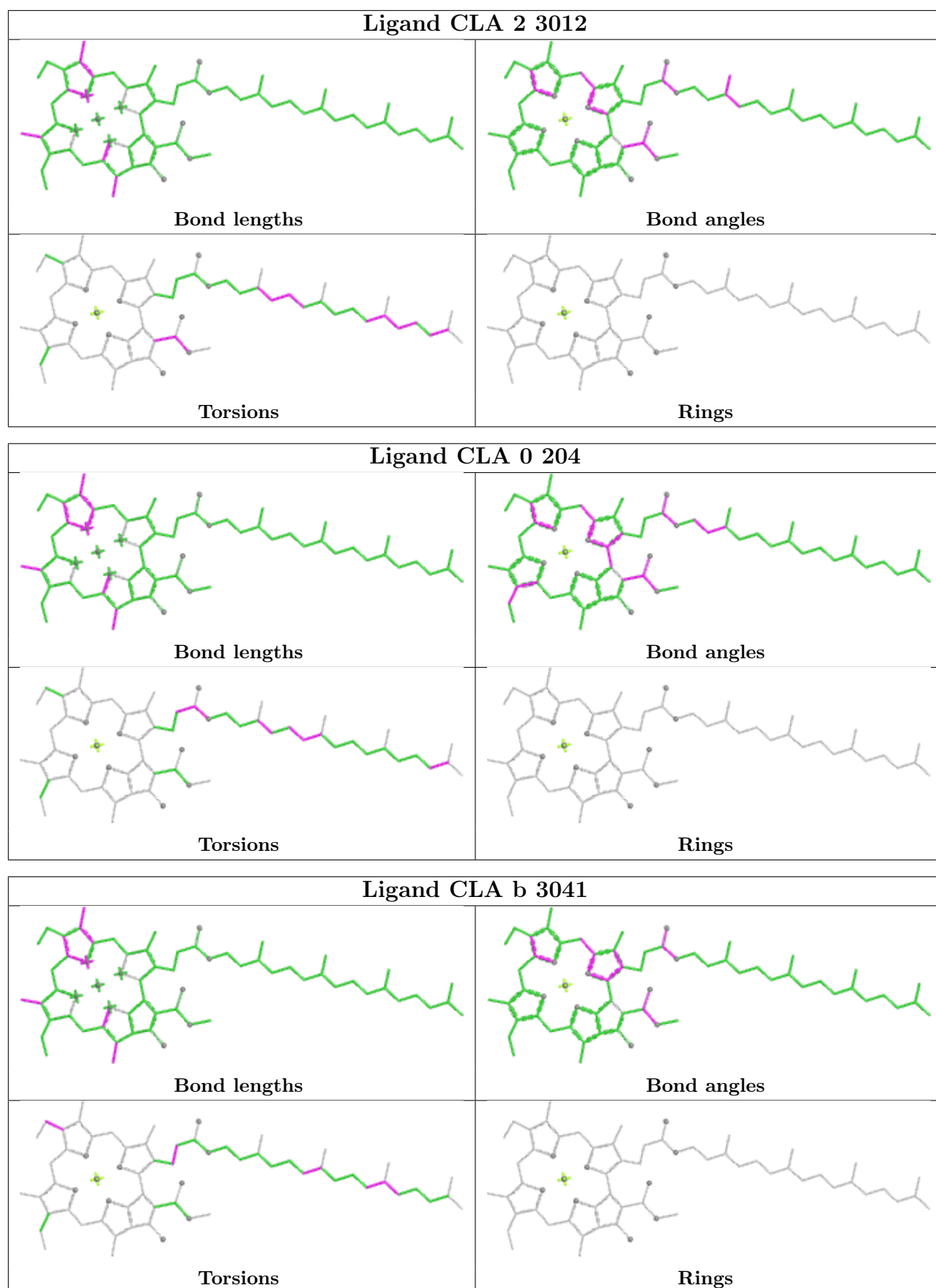


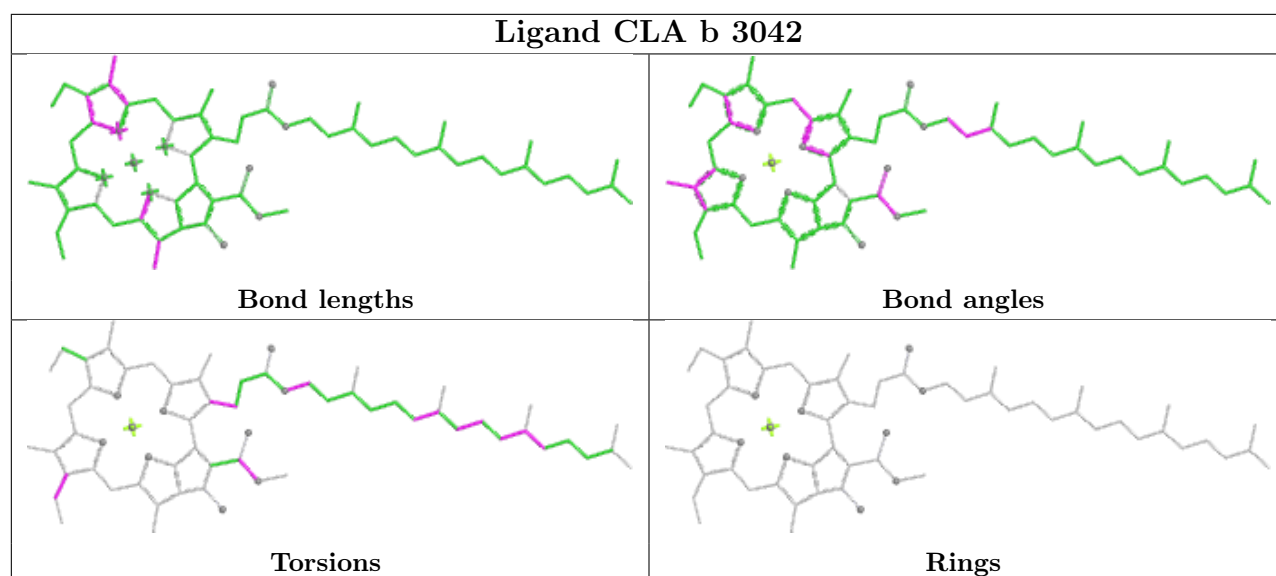
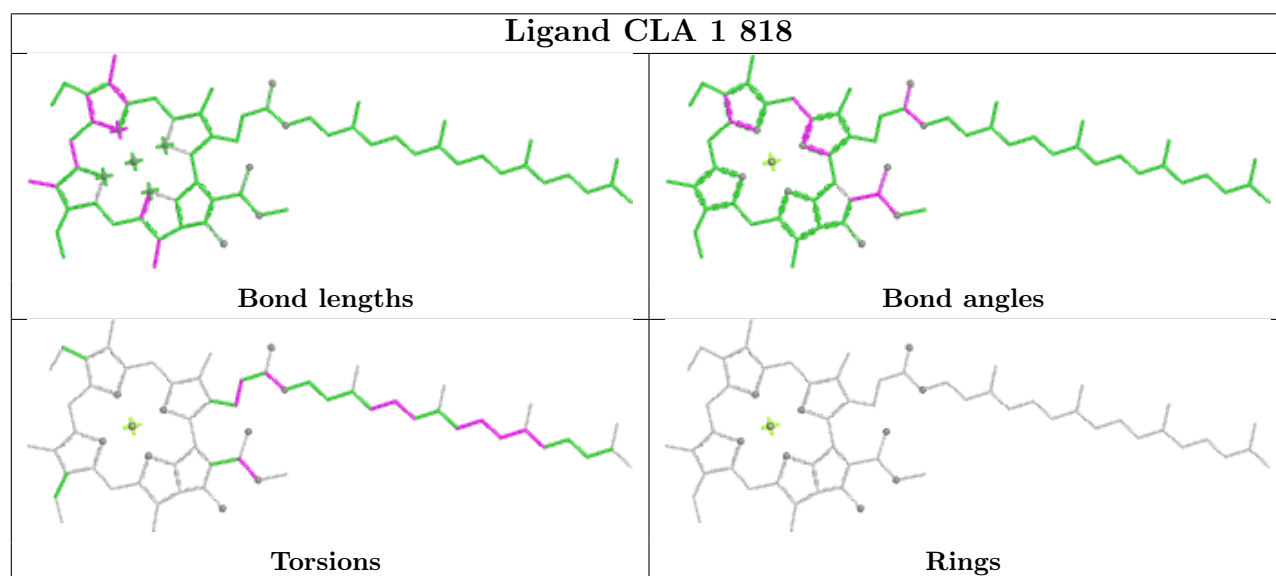
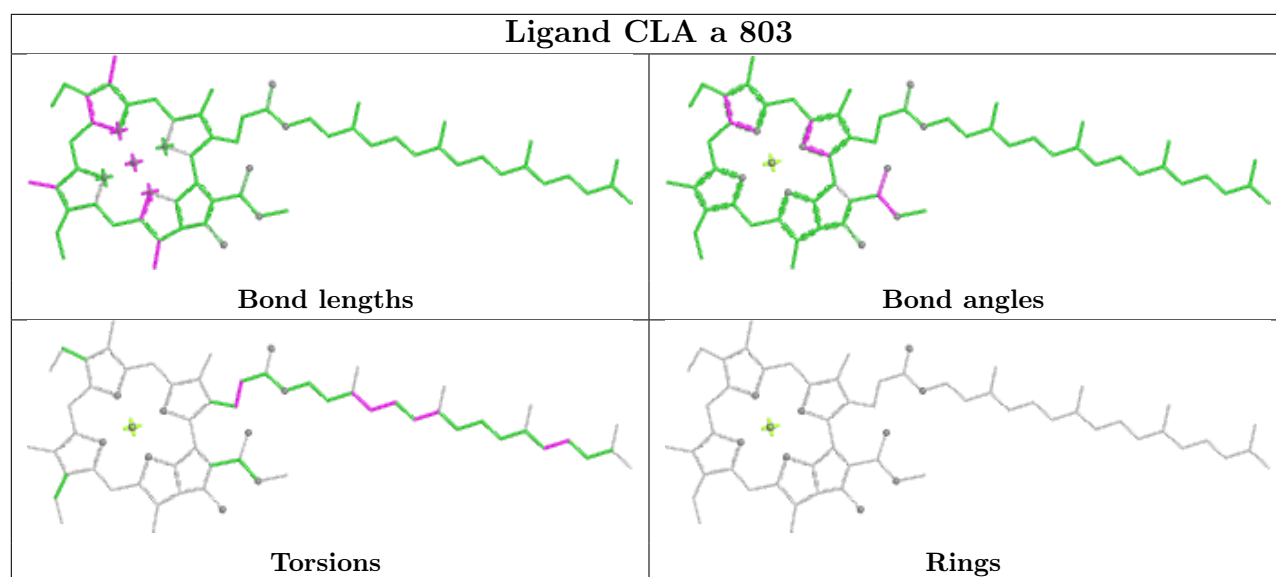


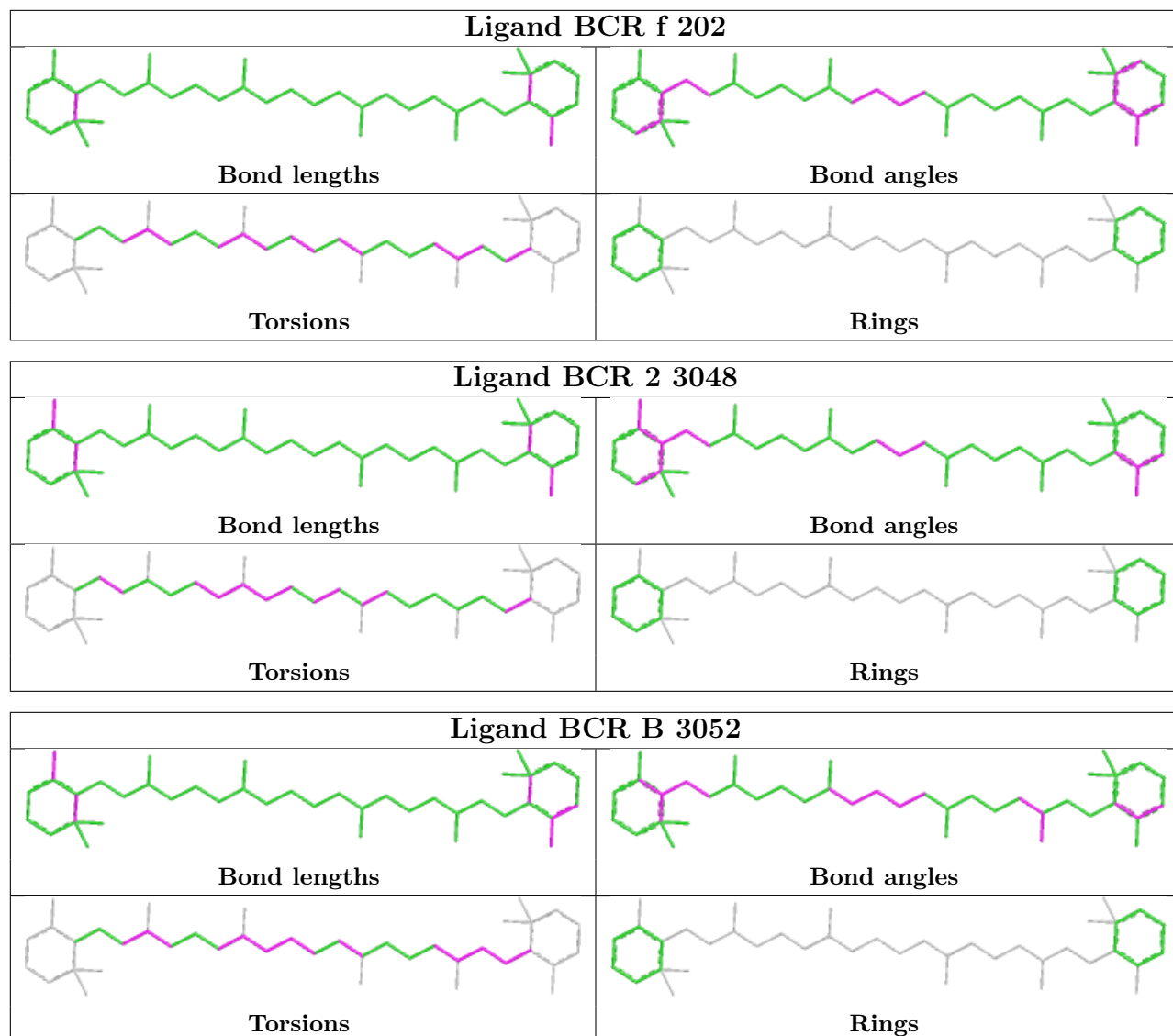


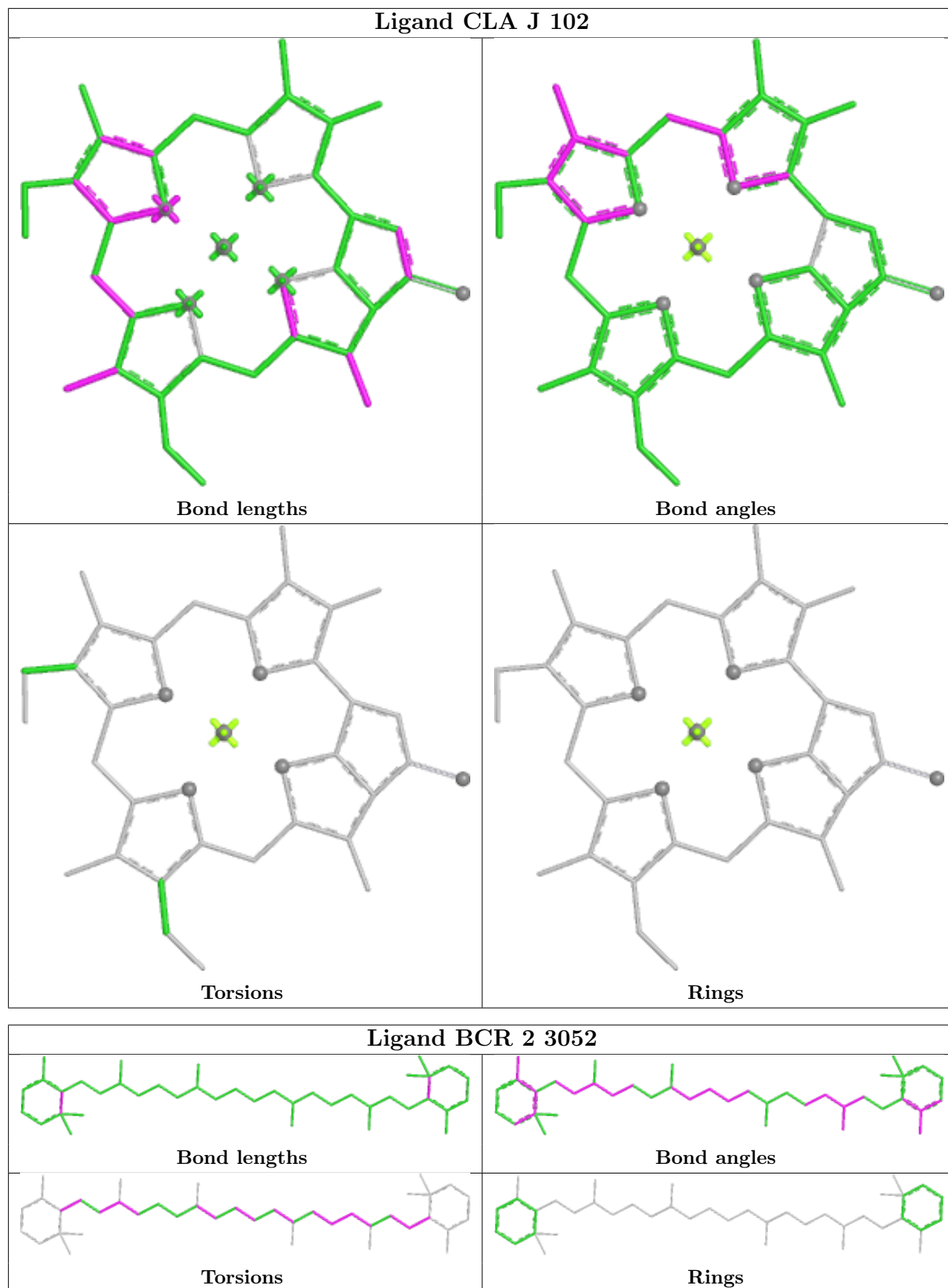


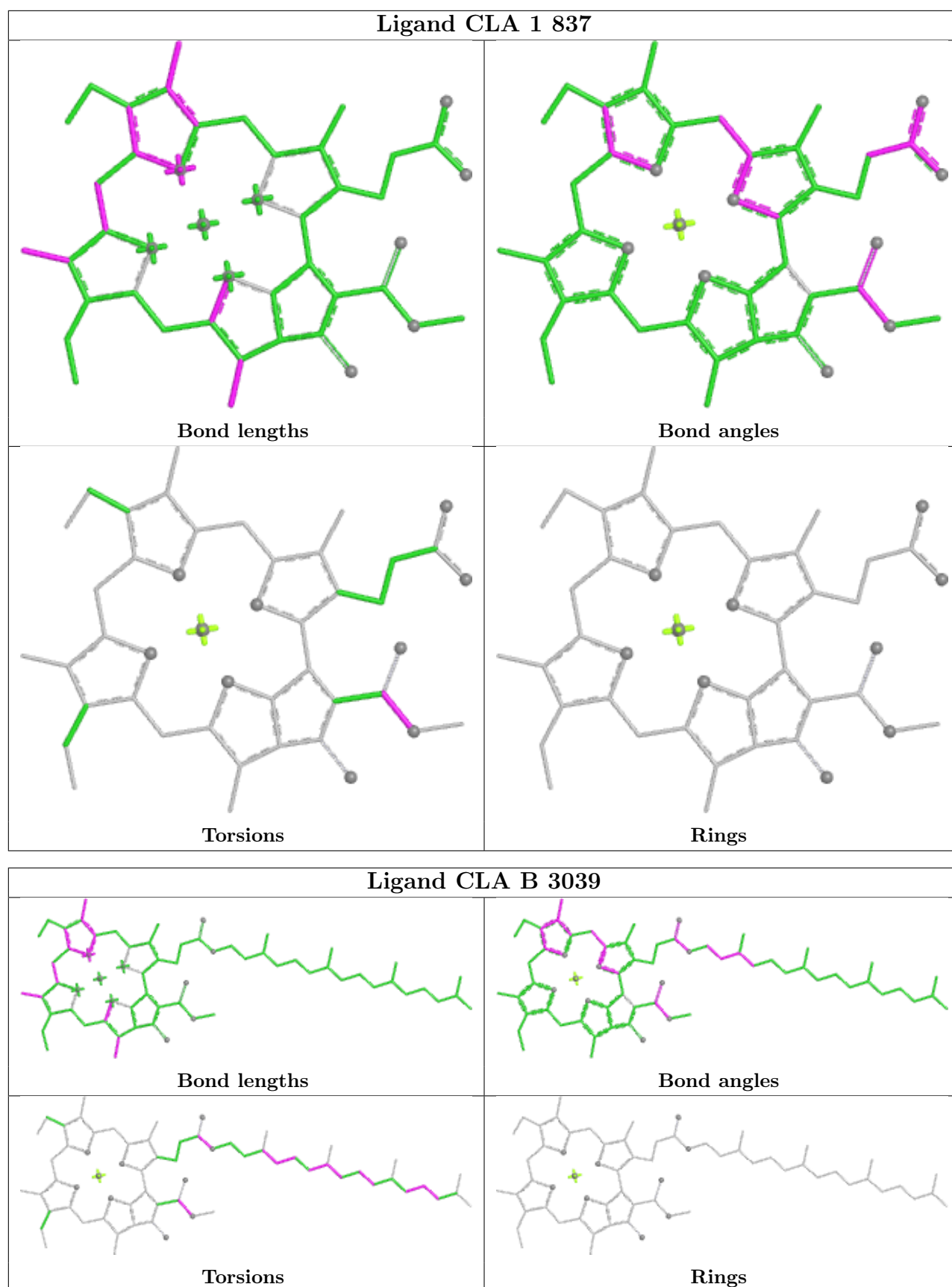


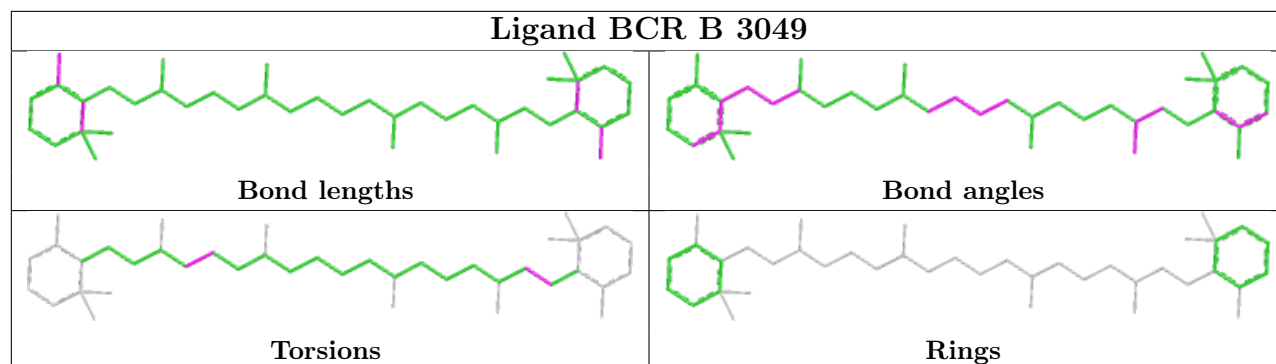
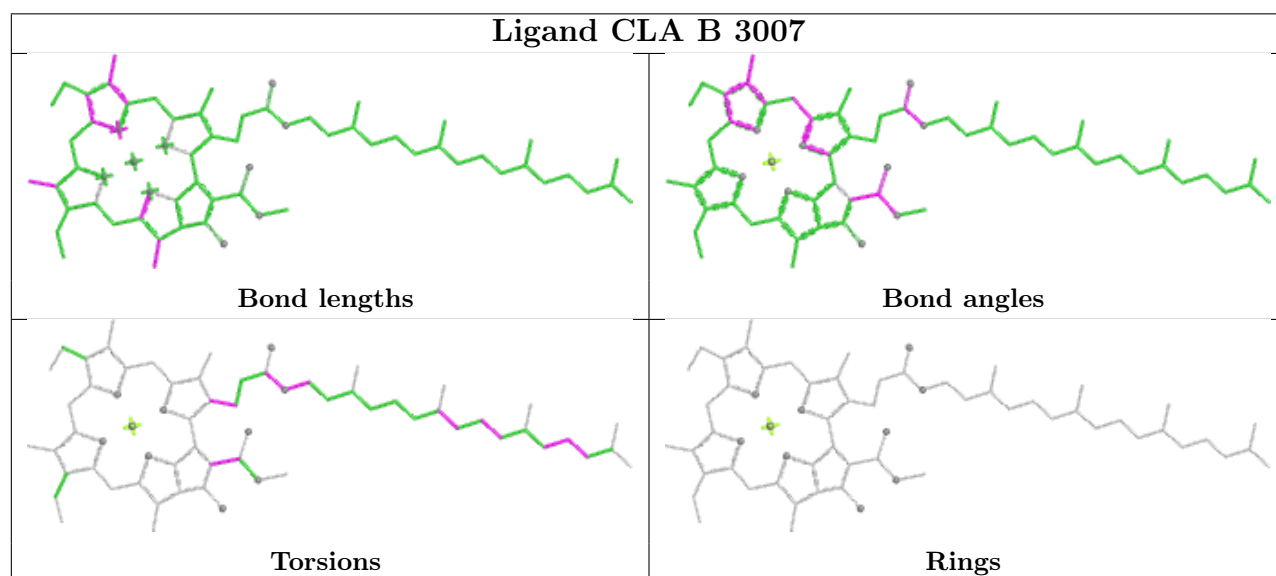
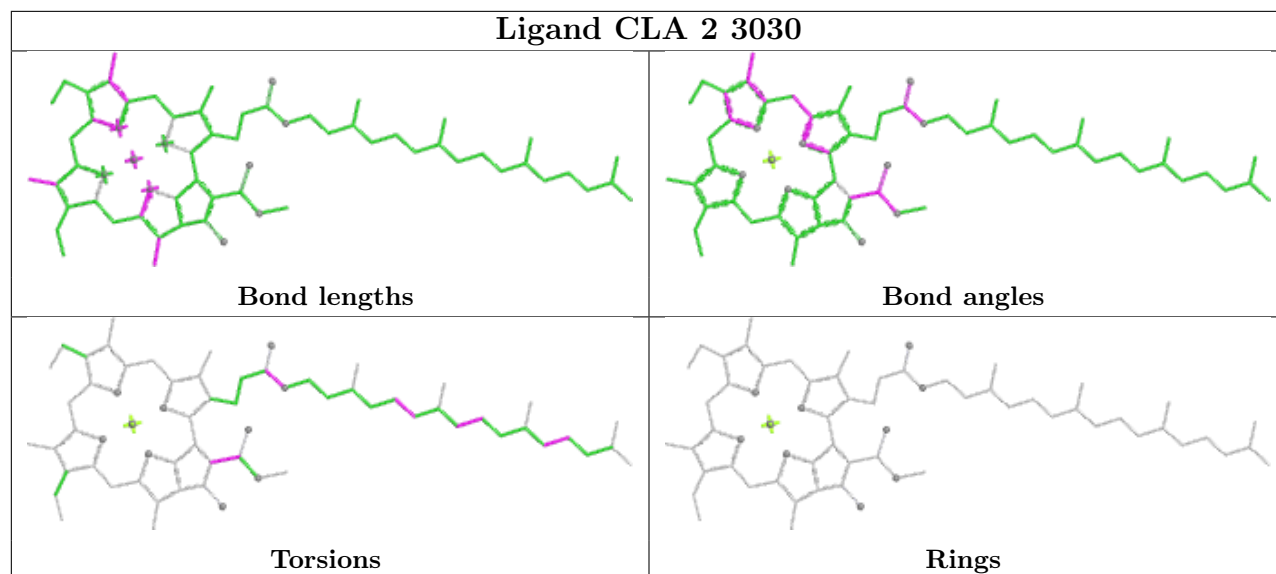


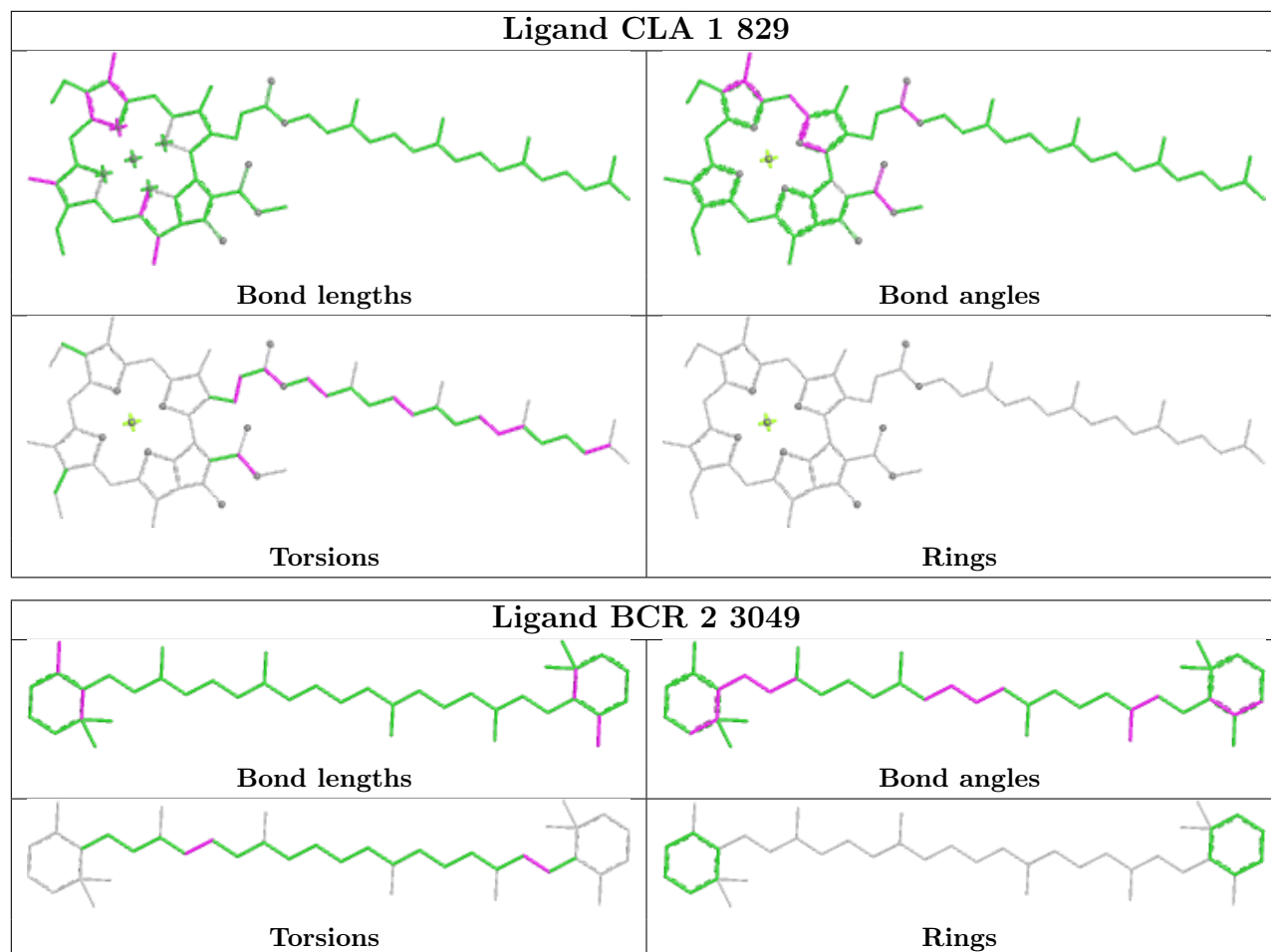


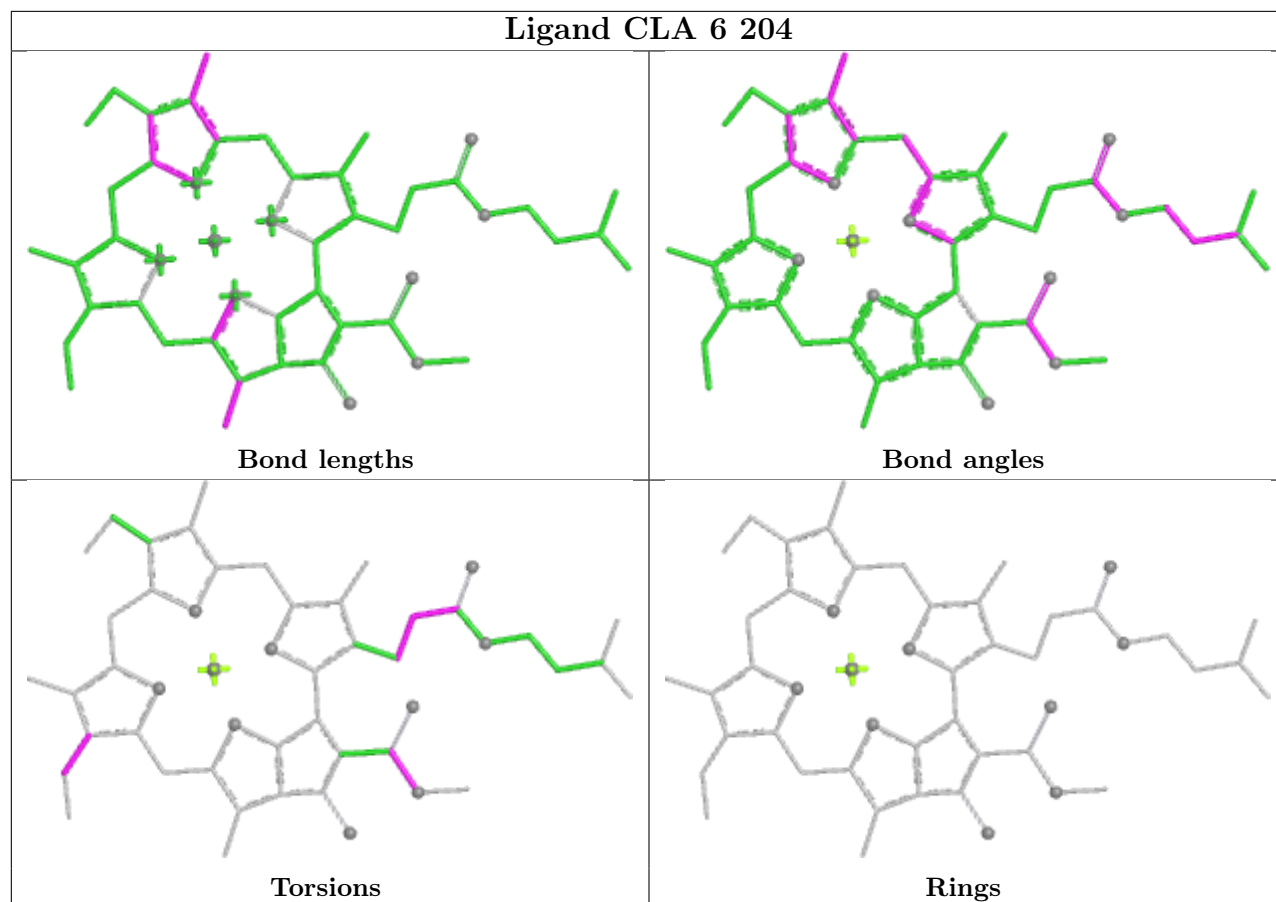


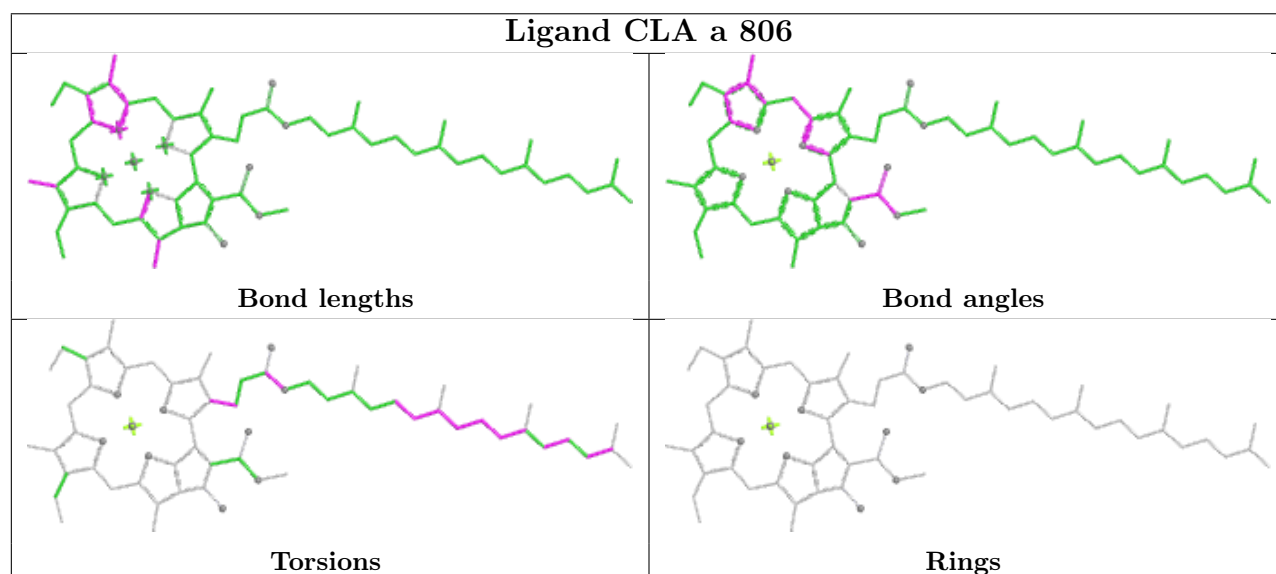
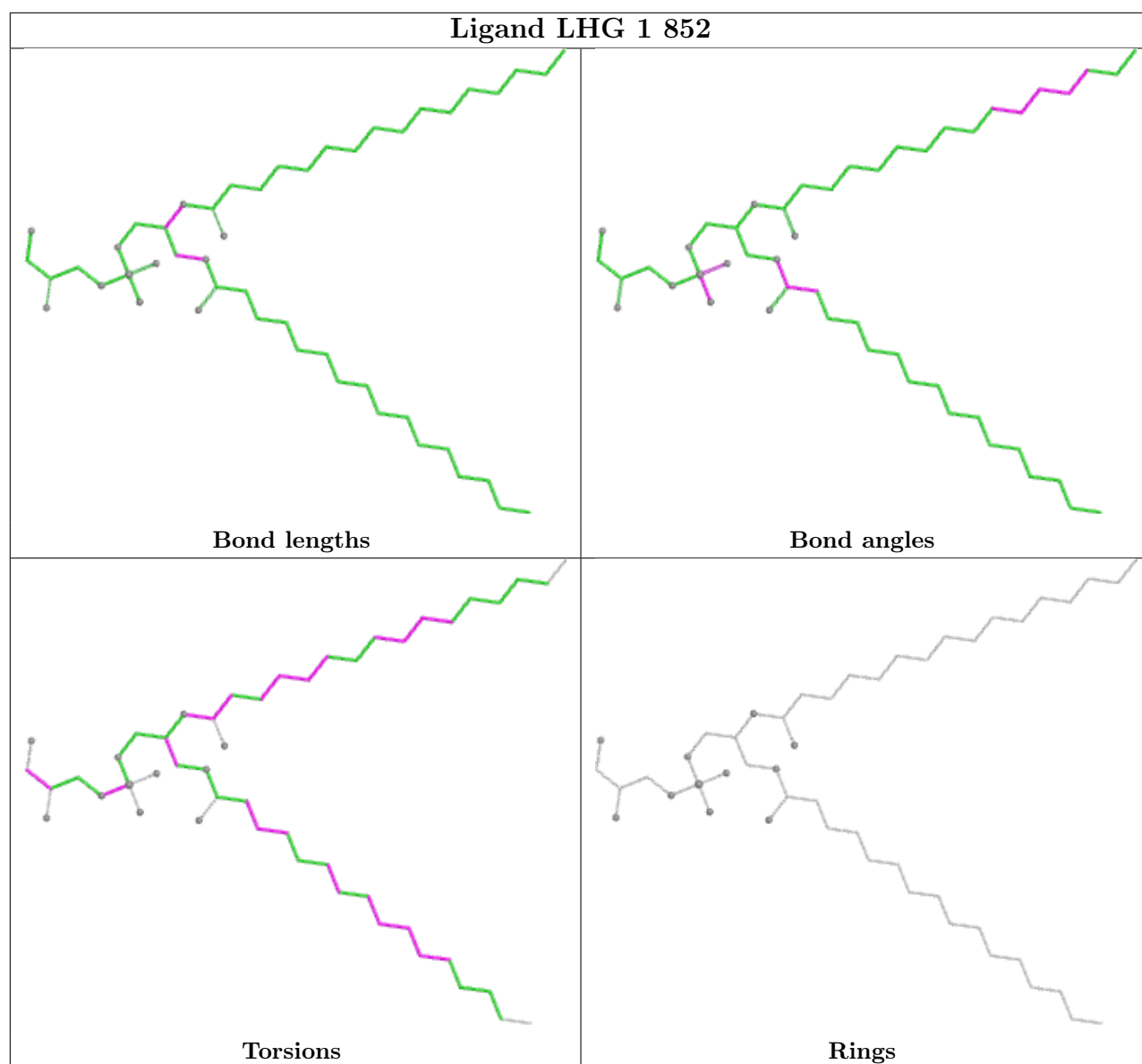


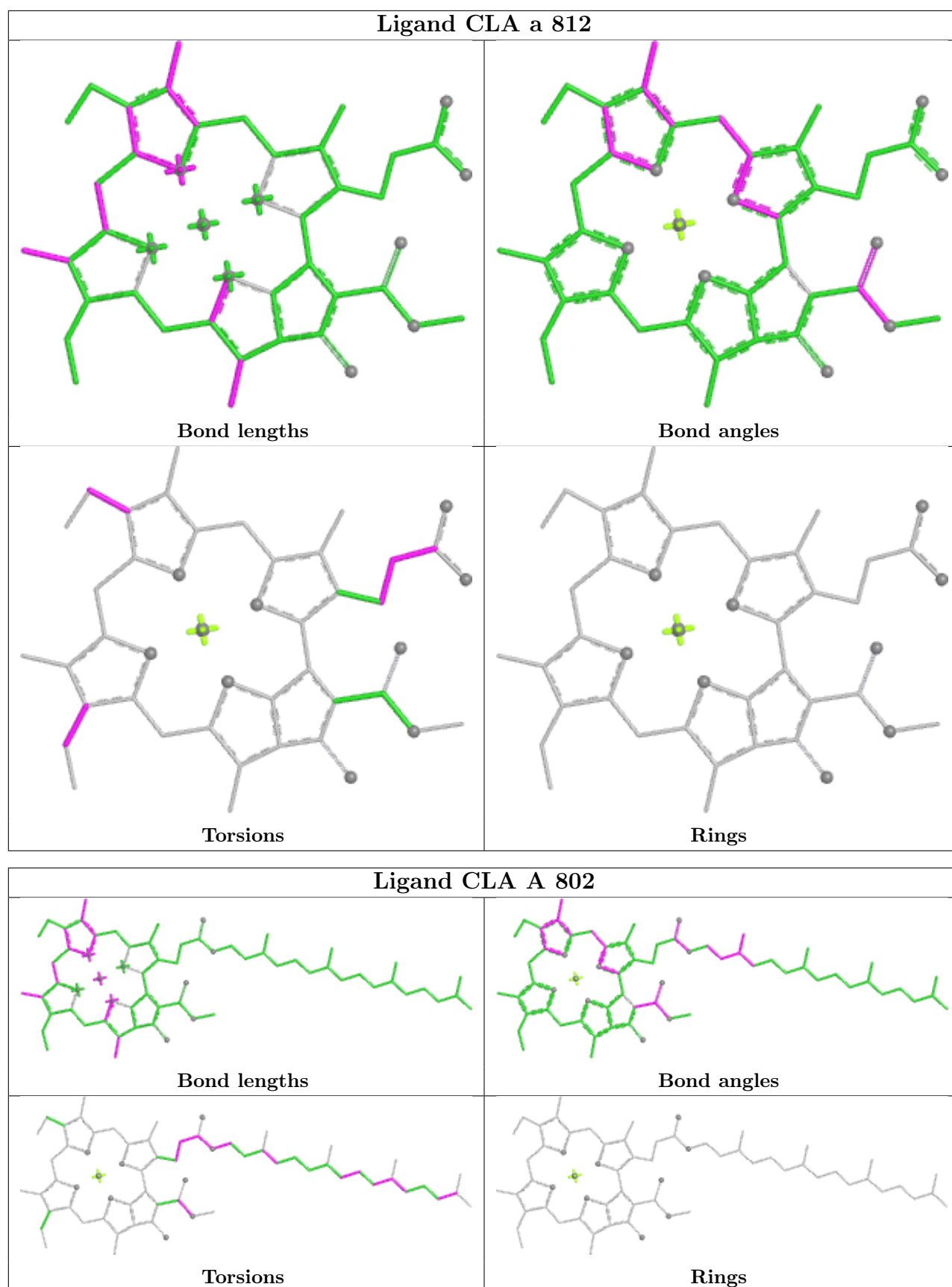


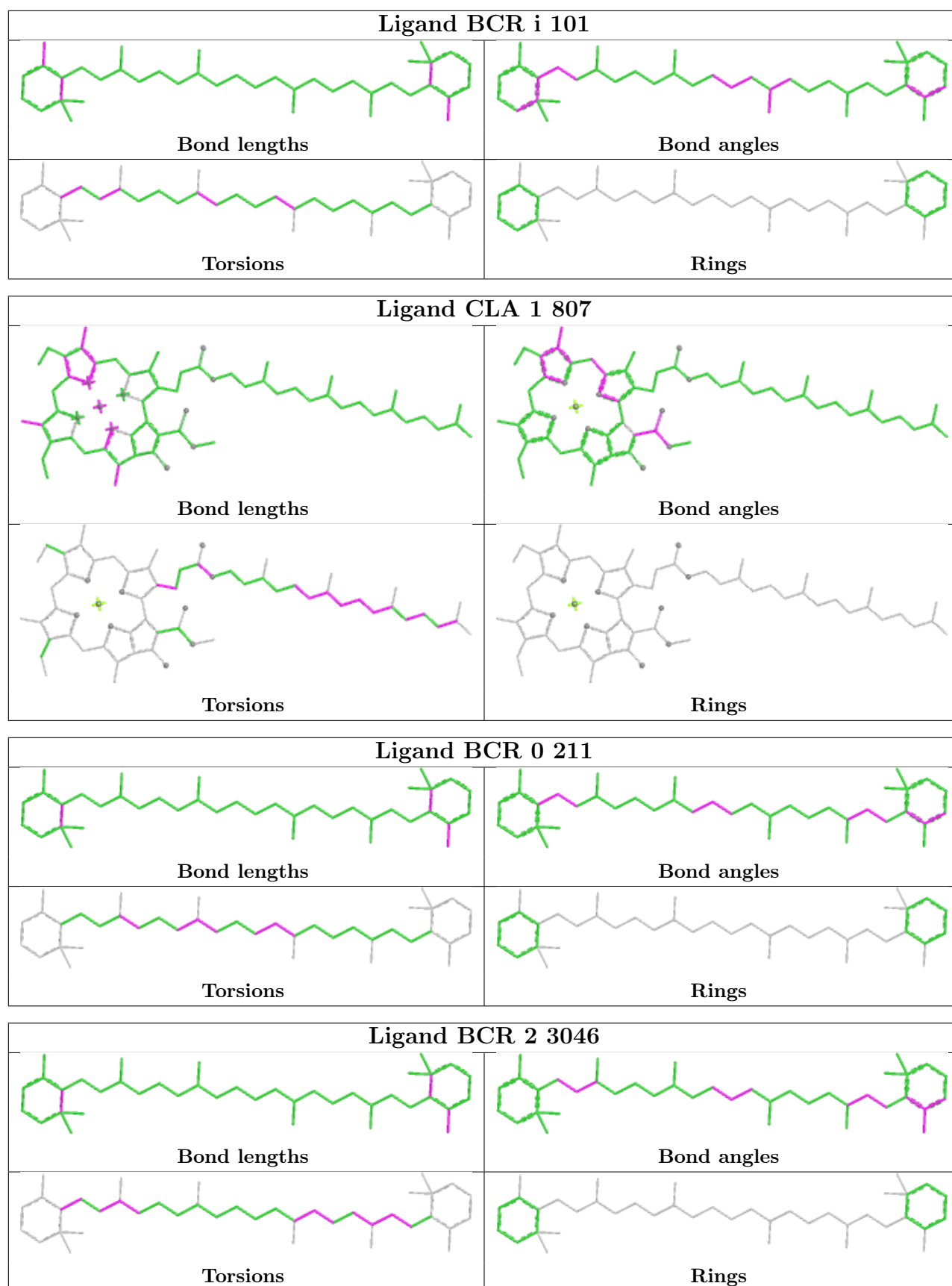


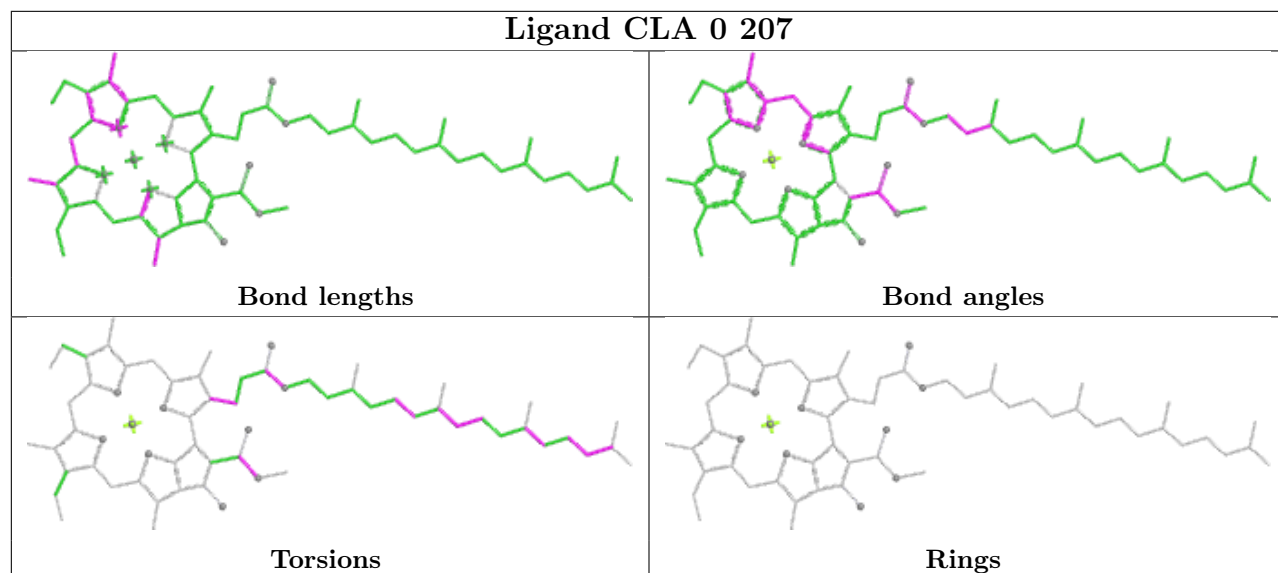
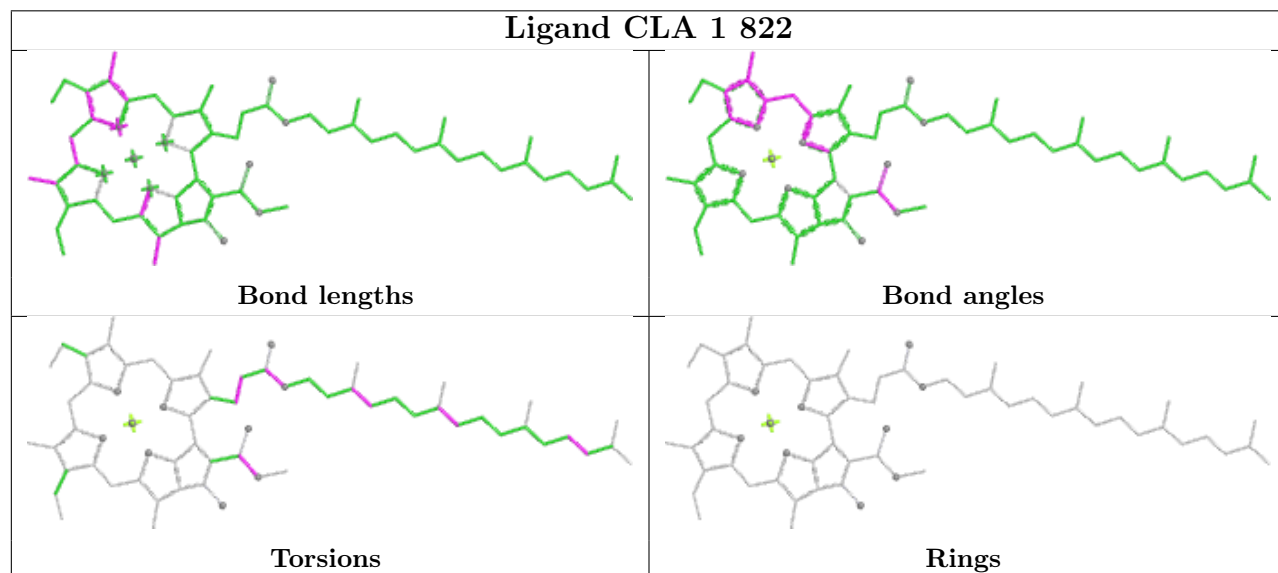
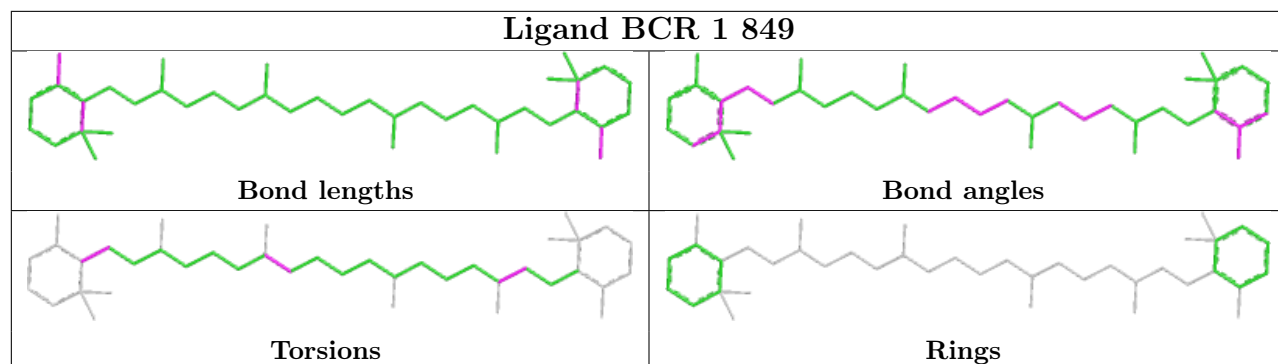


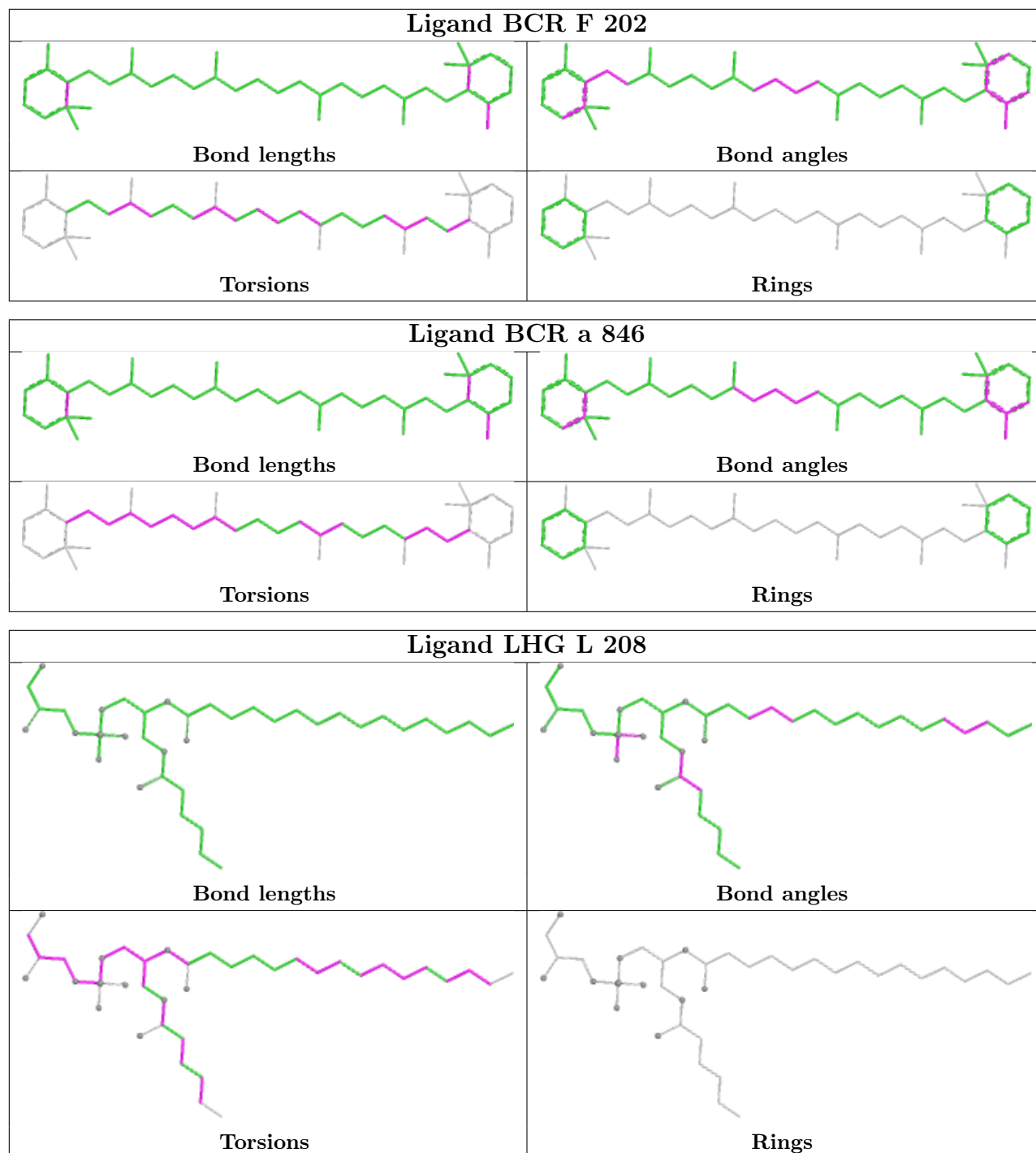


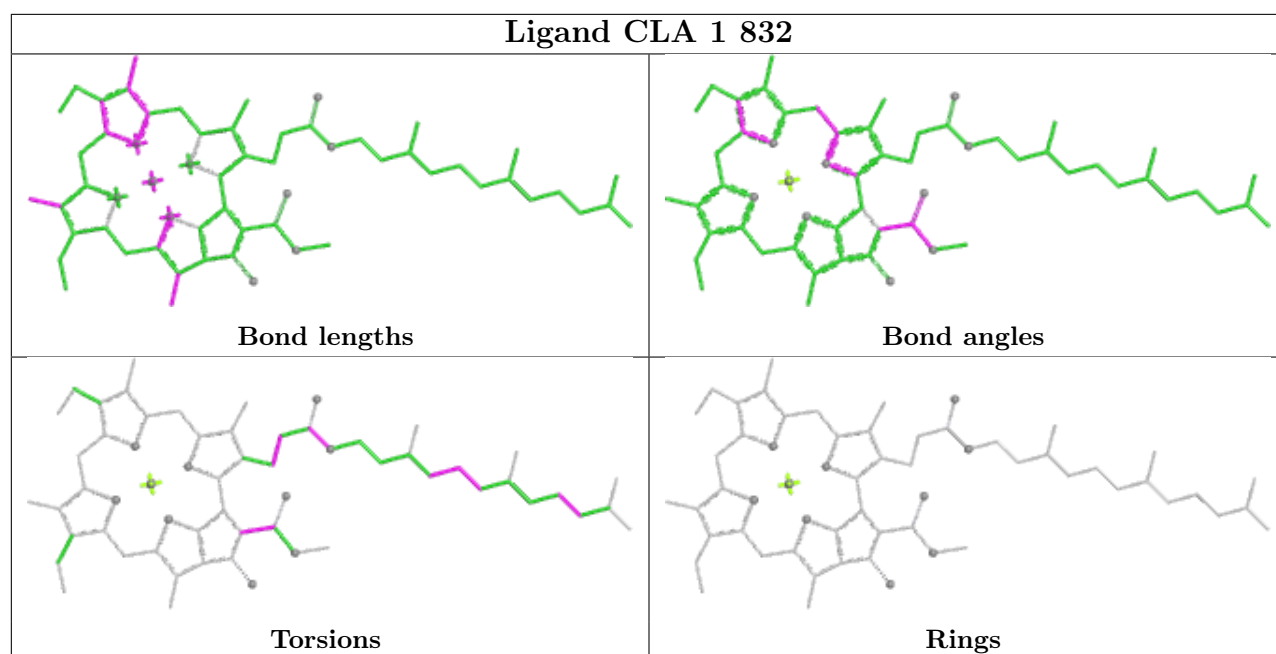












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

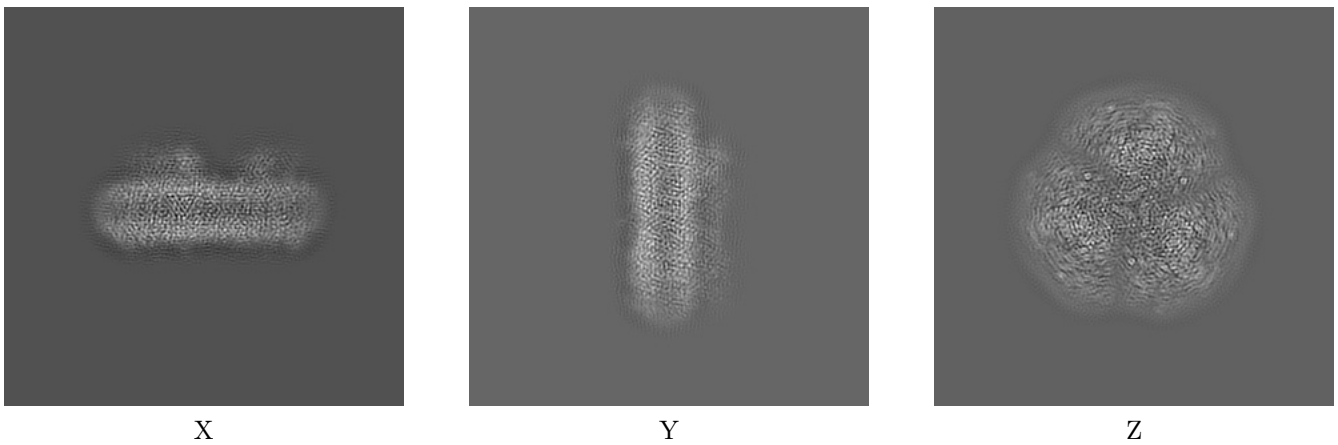
## 6 Map visualisation [i](#)

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](#)

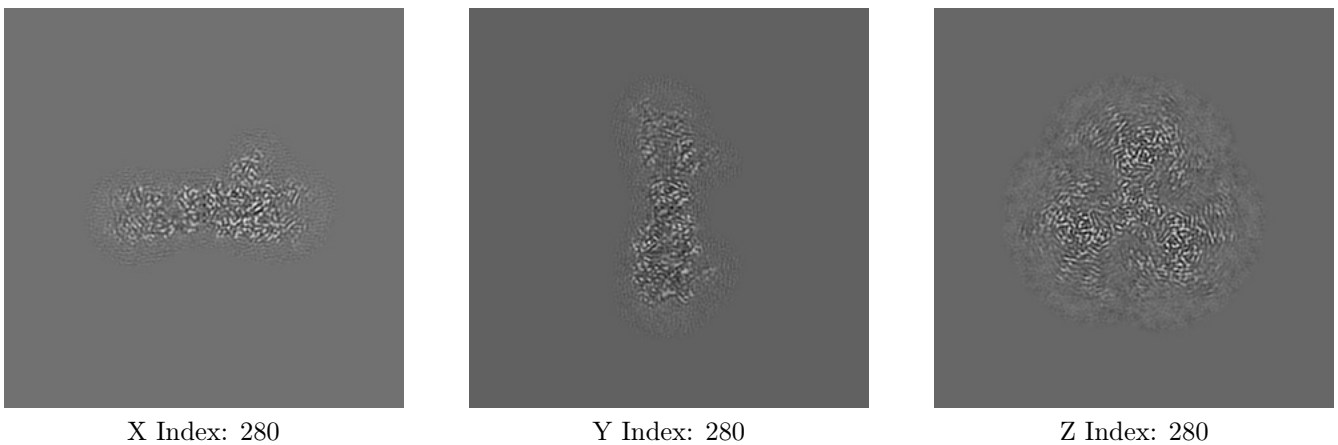
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

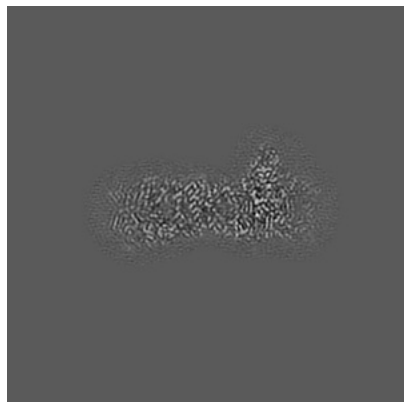
#### 6.2.1 Primary map



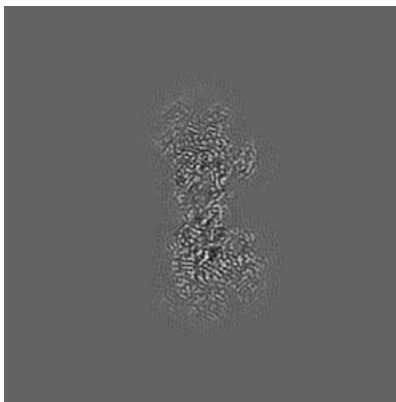
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

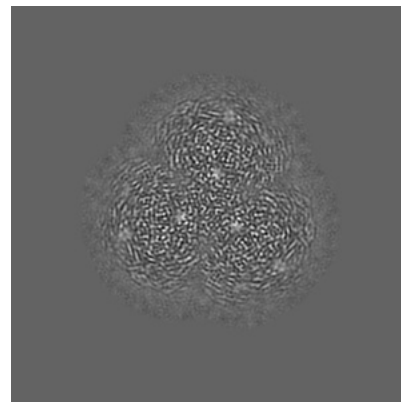
### 6.3.1 Primary map



X Index: 297



Y Index: 253

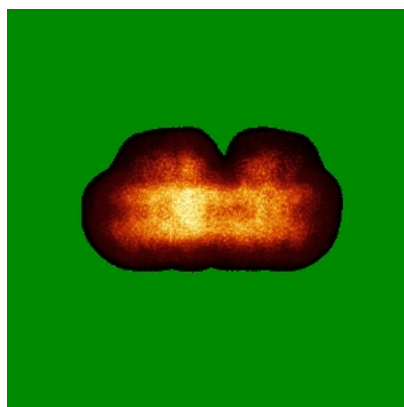


Z Index: 298

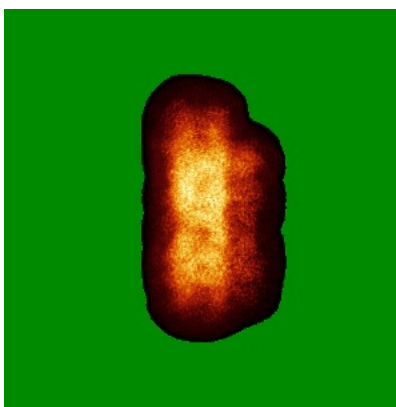
The images above show the largest variance slices of the map in three orthogonal directions.

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

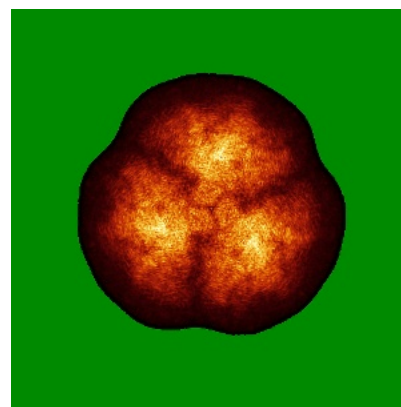
### 6.4.1 Primary map



X



Y

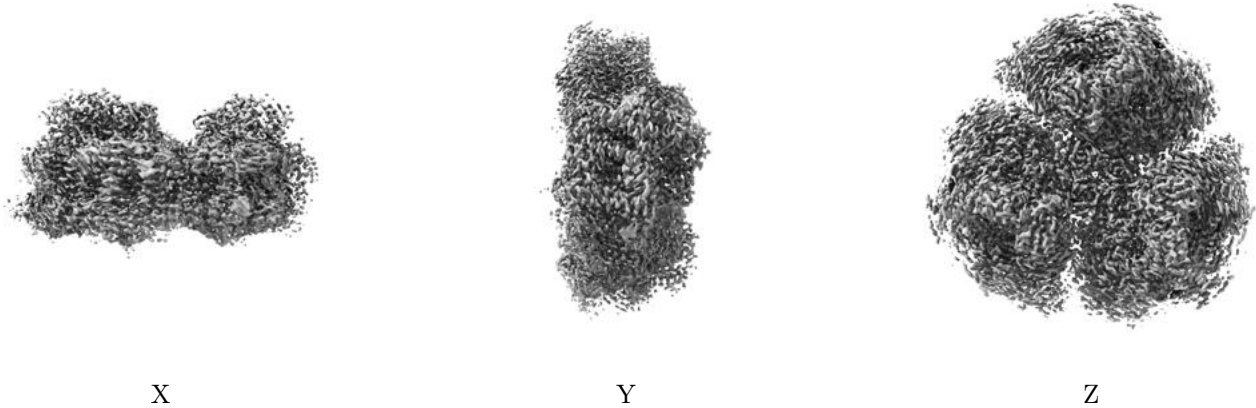


Z

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.

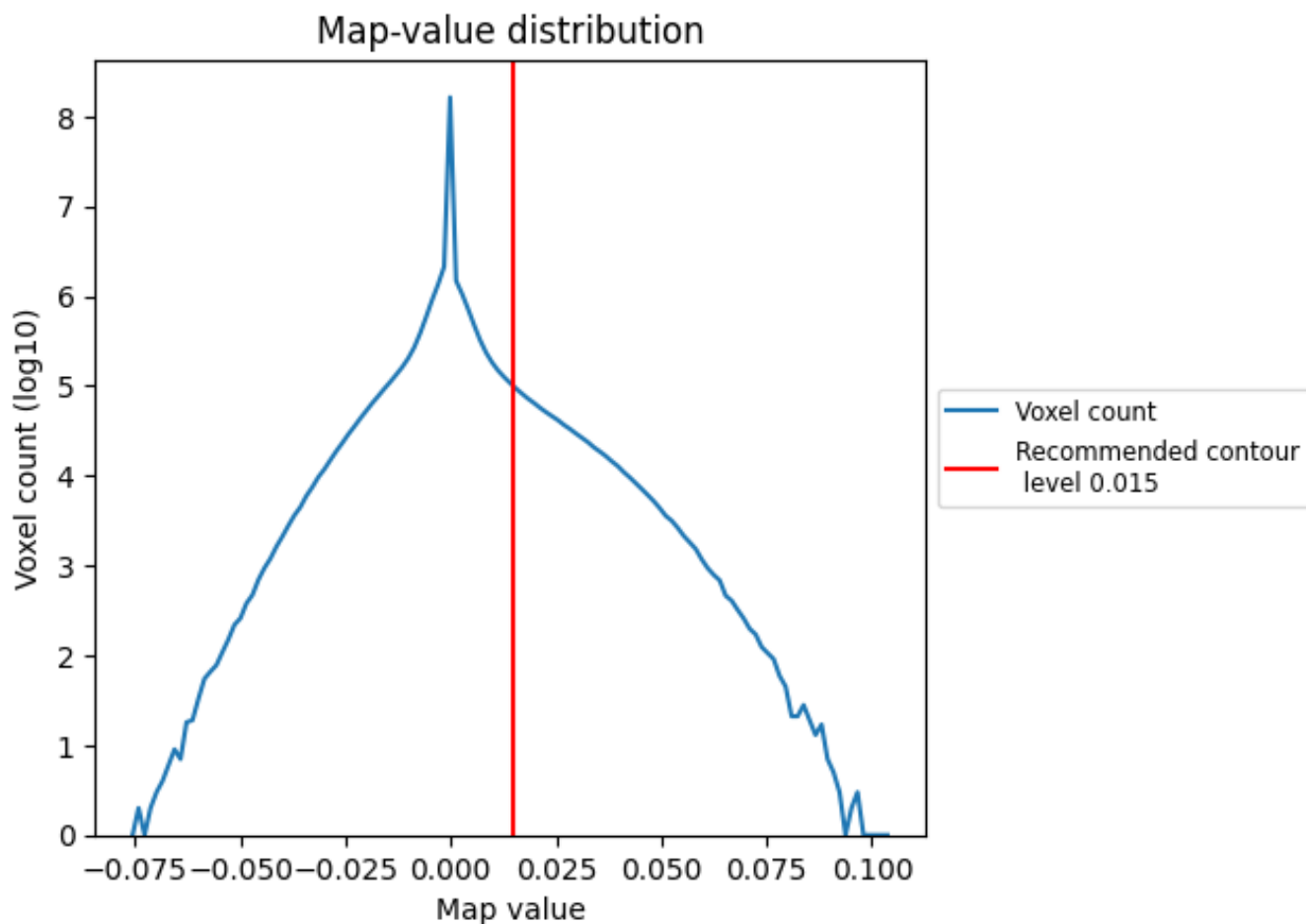
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

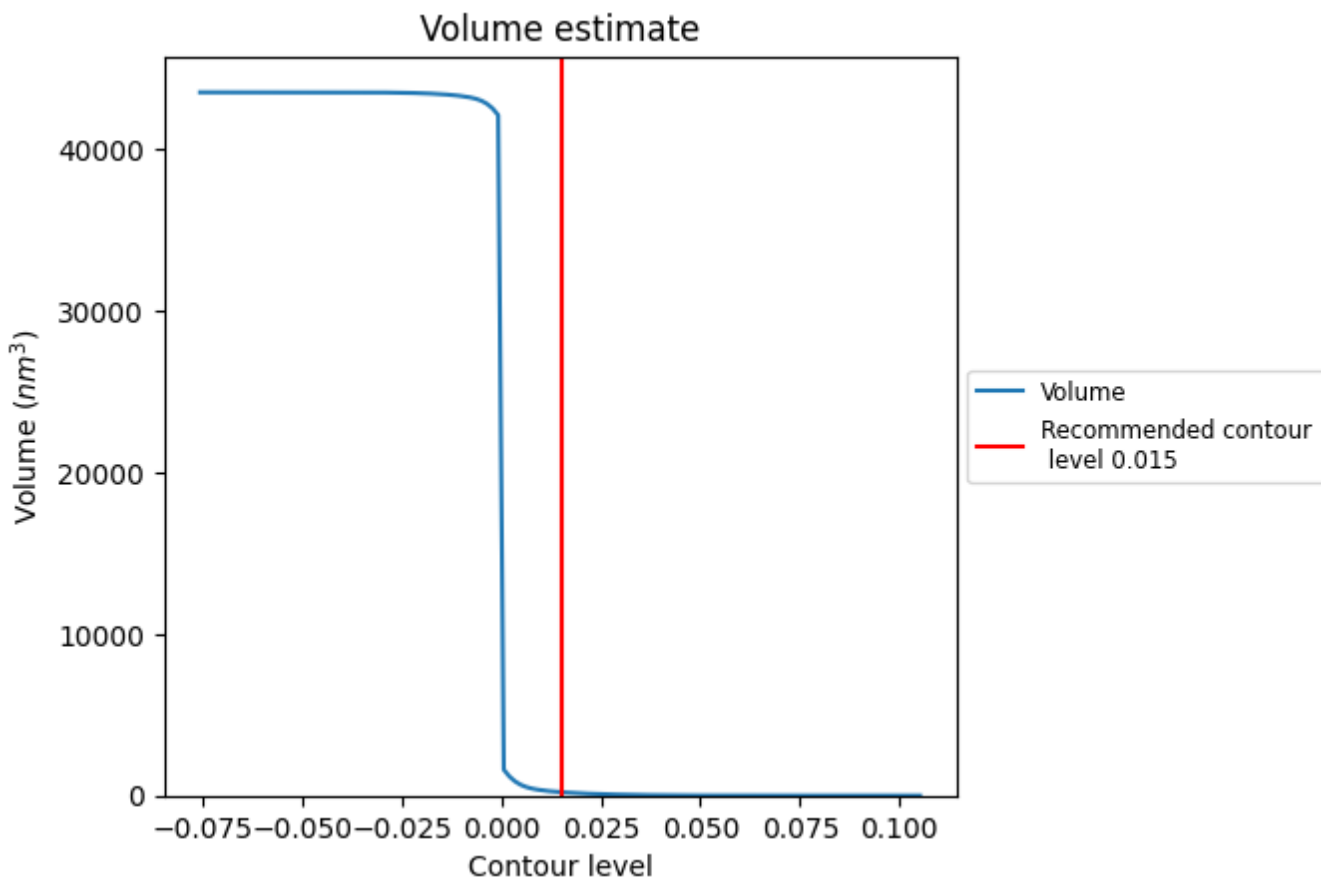
This section contains the results of statistical analysis of the map.

### 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.

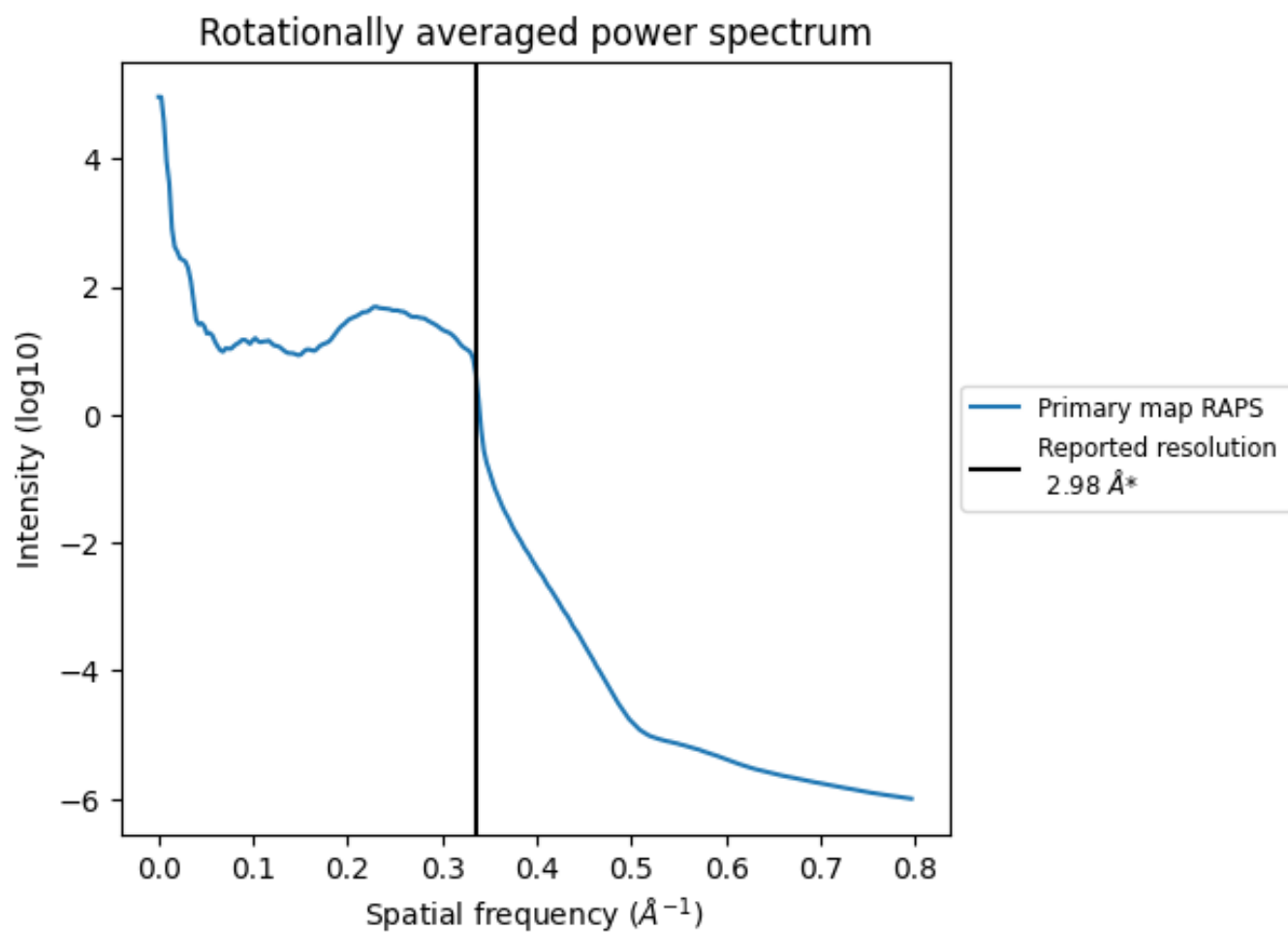
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 210 nm<sup>3</sup>; 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 [i](#)

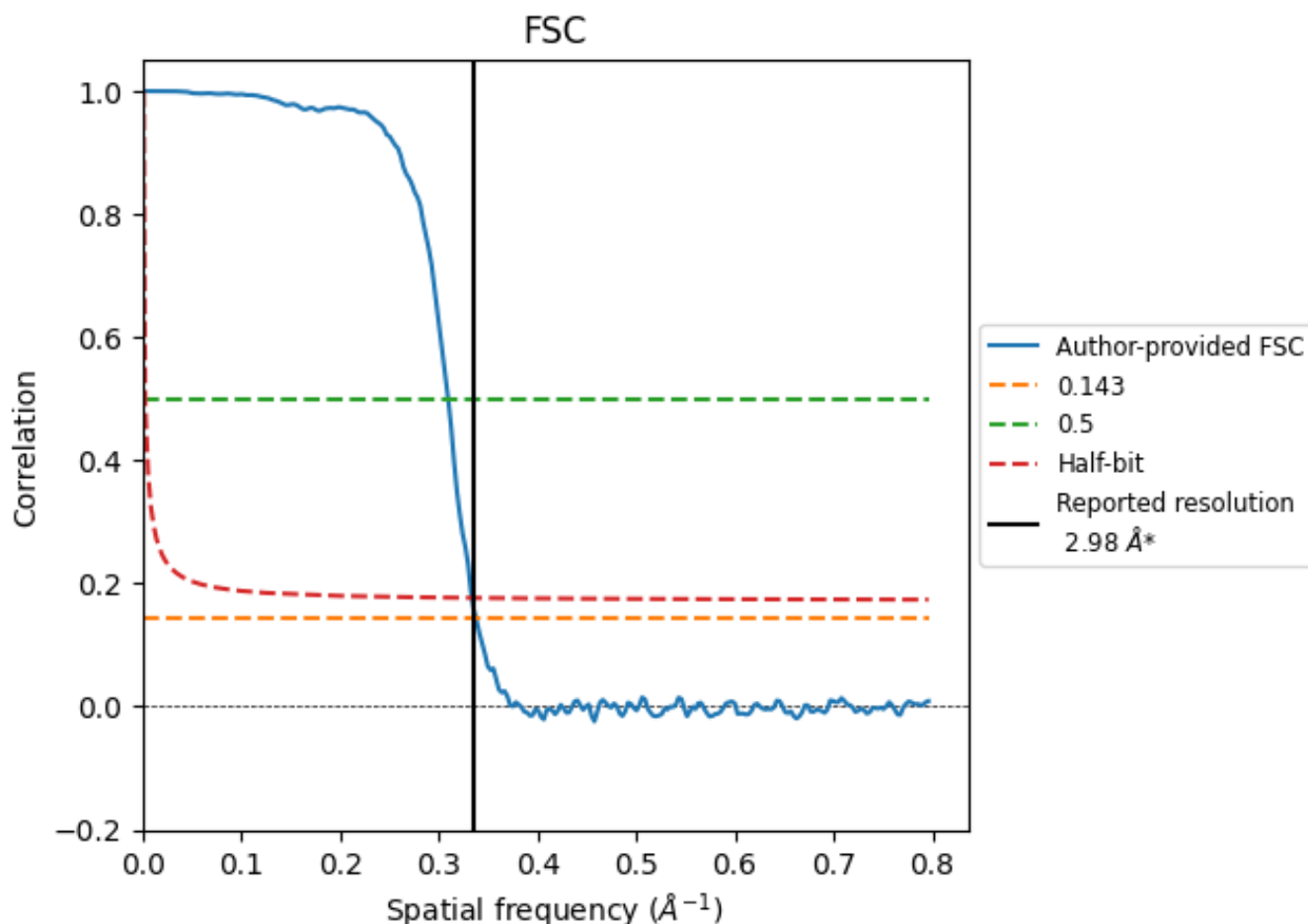


\*Reported resolution corresponds to spatial frequency of  $0.336 \text{\AA}^{-1}$

## 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<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

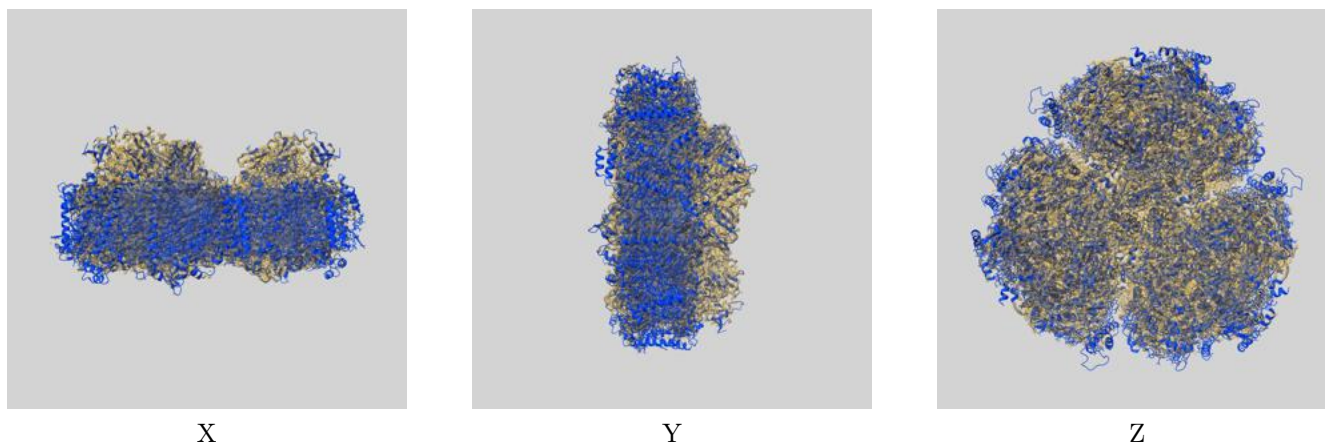
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.98	-	-
Author-provided FSC curve	2.96	3.23	3.00
Unmasked-calculated*	-	-	-

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

## 9 Map-model fit [i](#)

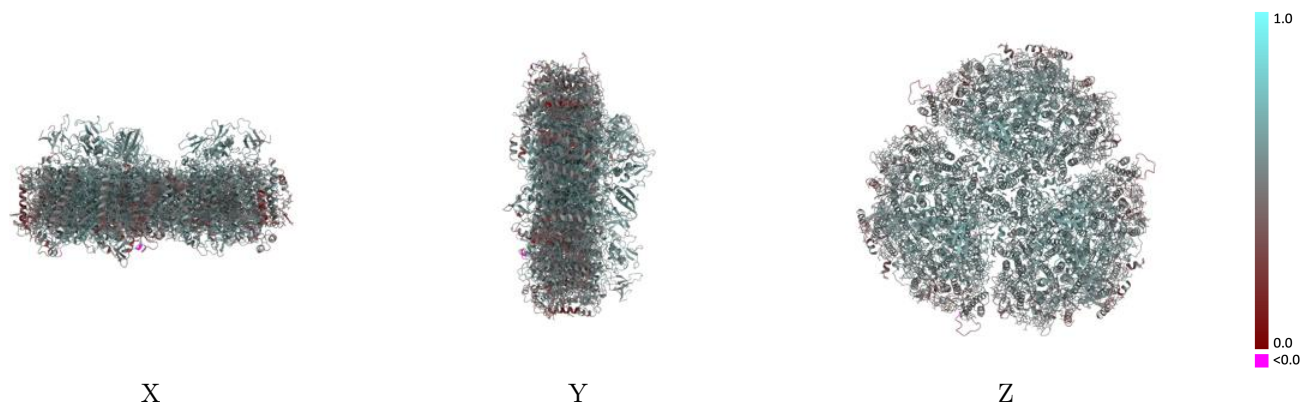
This section contains information regarding the fit between EMDB map EMD-10558 and PDB model 6TRC. Per-residue inclusion information can be found in section 3 on page 40.

### 9.1 Map-model overlay [i](#)



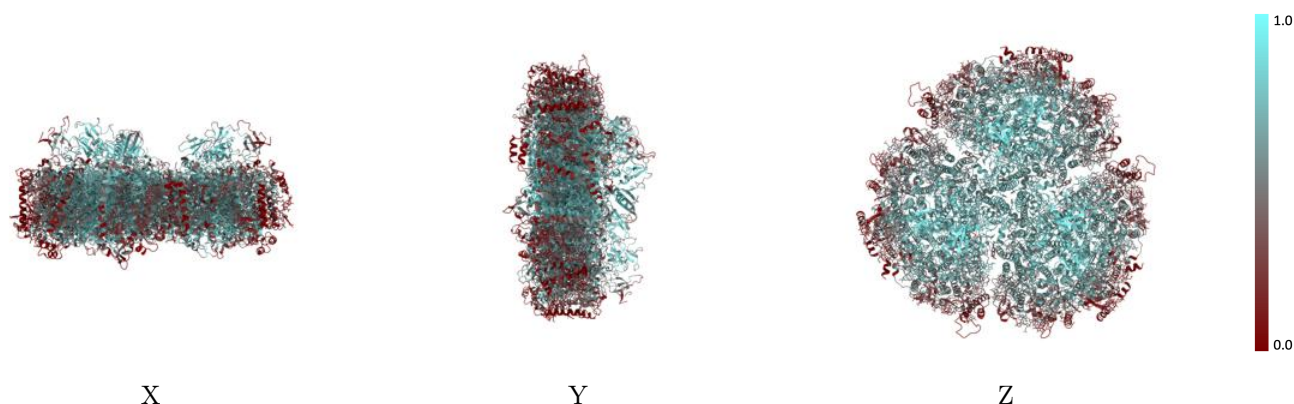
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



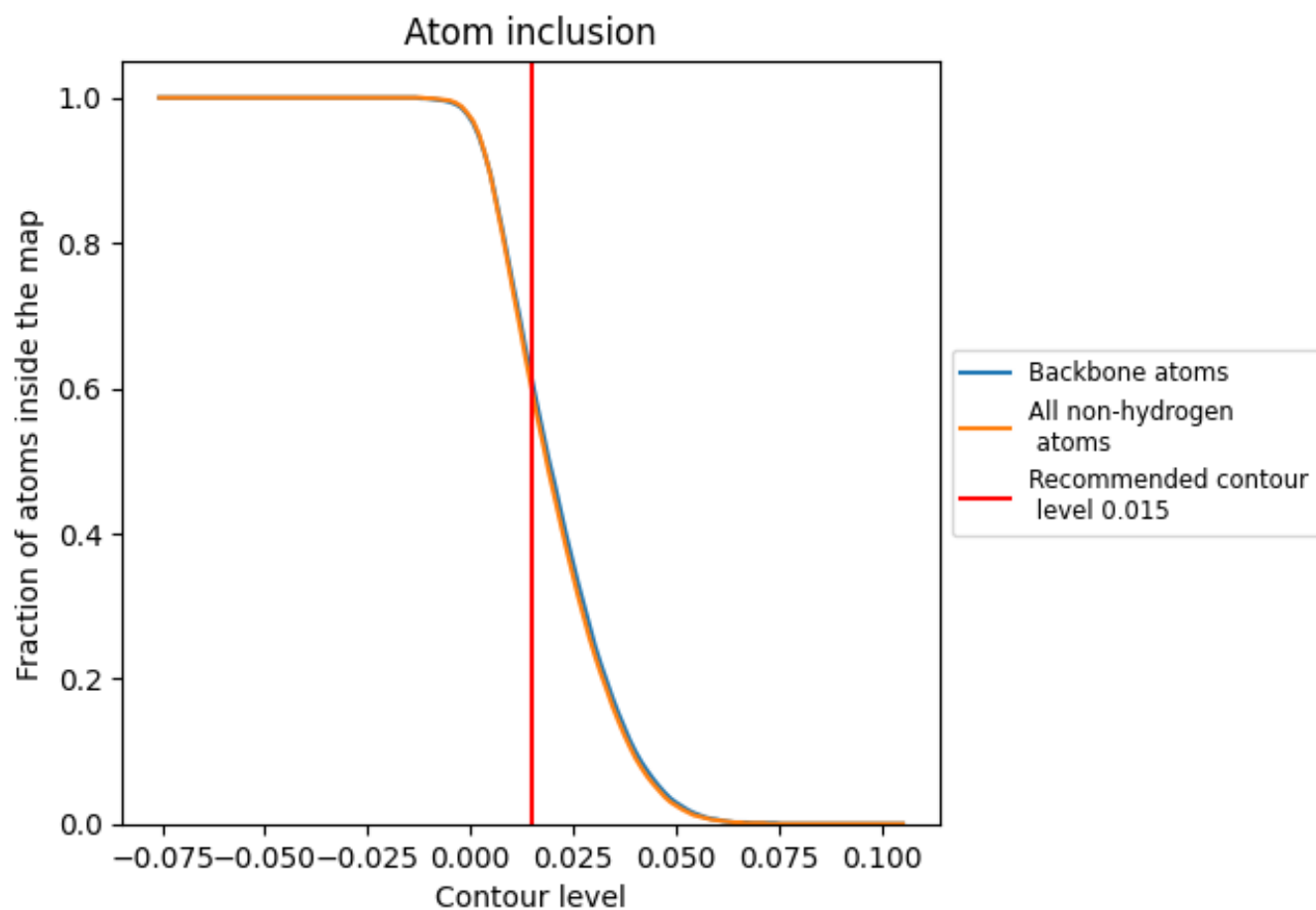
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



*Continued on next page...*

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