



wwPDB EM Validation Summary Report ⓘ

Mar 6, 2026 – 11:12 PM UTC

PDB ID : 7ZQD / pdb_00007zqd
EMDB ID : EMD-14871
Title : Dimeric PSI of Chlamydomonas reinhardtii at 2.97 Å resolution
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.97 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

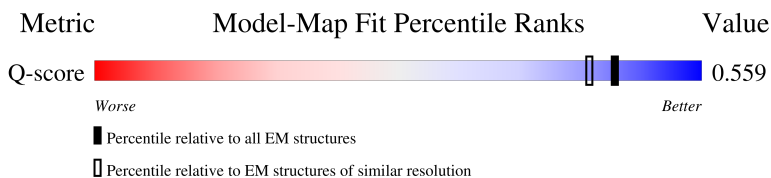
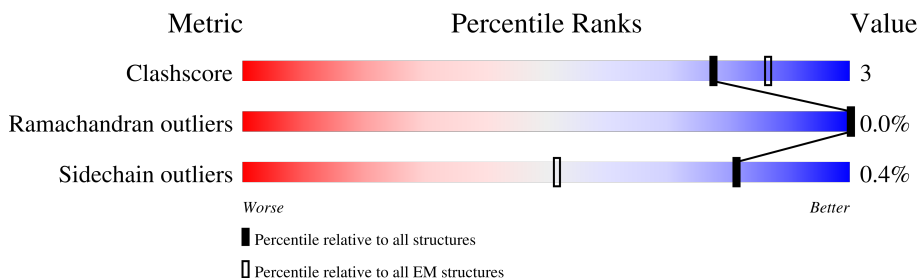
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

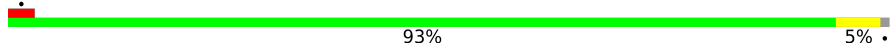
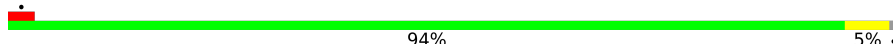
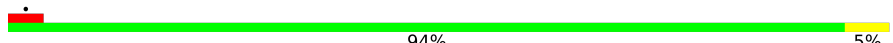
The reported resolution of this entry is 2.97 Å.

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	13205 (2.47 - 3.47)

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

Mol	Chain	Length	Quality of chain
1	A	751	 93% 5% .
1	A2	751	 94% 5% .
2	B	735	 94% 5%
2	B2	735	 93% 6%

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Mol	Chain	Length	Quality of chain
3	C	81	
3	C2	81	
4	D	196	
4	D2	196	
5	E	97	
5	E2	97	
6	F	227	
6	F2	227	
7	G	126	
7	G2	126	
8	I	106	
8	I2	106	
9	J	40	
9	J2	40	
10	L	196	
10	L2	196	
11	K	113	
11	K2	113	
12	1	228	
12	12	228	
12	Z	228	
12	Z2	228	
13	3	298	
13	32	298	
14	7	241	

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Mol	Chain	Length	Quality of chain
14	72	241	
15	8	243	
15	82	243	
16	4	264	
16	42	264	
17	5	257	
17	52	257	
18	6	257	
18	62	257	
19	9	213	
19	92	213	

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
20	CL0	A	801	X	-	-	-
20	CL0	A2	801	X	-	-	-
21	CLA	1	602	X	-	-	-
21	CLA	1	603	X	-	-	-
21	CLA	1	604	X	-	-	-
21	CLA	1	608	X	-	-	-
21	CLA	1	609	X	-	-	-
21	CLA	1	610	X	-	-	-
21	CLA	1	611	X	-	-	-
21	CLA	1	612	X	-	-	-
21	CLA	1	613	X	-	-	-
21	CLA	1	614	X	-	-	-
21	CLA	1	616	X	-	-	-
21	CLA	12	602	X	-	-	-
21	CLA	12	603	X	-	-	-
21	CLA	12	604	X	-	-	-
21	CLA	12	608	X	-	-	-
21	CLA	12	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	12	610	X	-	-	-
21	CLA	12	611	X	-	-	-
21	CLA	12	612	X	-	-	-
21	CLA	12	613	X	-	-	-
21	CLA	12	614	X	-	-	-
21	CLA	12	616	X	-	-	-
21	CLA	3	602	X	-	-	-
21	CLA	3	603	X	-	-	-
21	CLA	3	604	X	-	-	-
21	CLA	3	606	X	-	-	-
21	CLA	3	607	X	-	-	-
21	CLA	3	609	X	-	-	-
21	CLA	3	610	X	-	-	-
21	CLA	3	611	X	-	-	-
21	CLA	3	612	X	-	-	-
21	CLA	3	613	X	-	-	-
21	CLA	3	614	X	-	-	-
21	CLA	3	615	X	-	-	-
21	CLA	3	617	X	-	-	-
21	CLA	32	602	X	-	-	-
21	CLA	32	603	X	-	-	-
21	CLA	32	604	X	-	-	-
21	CLA	32	606	X	-	-	-
21	CLA	32	607	X	-	-	-
21	CLA	32	609	X	-	-	-
21	CLA	32	610	X	-	-	-
21	CLA	32	611	X	-	-	-
21	CLA	32	612	X	-	-	-
21	CLA	32	613	X	-	-	-
21	CLA	32	614	X	-	-	-
21	CLA	32	615	X	-	-	-
21	CLA	32	617	X	-	-	-
21	CLA	4	602	X	-	-	-
21	CLA	4	603	X	-	-	-
21	CLA	4	604	X	-	-	-
21	CLA	4	609	X	-	-	-
21	CLA	4	610	X	-	-	-
21	CLA	4	611	X	-	-	-
21	CLA	4	612	X	-	-	-
21	CLA	4	613	X	-	-	-
21	CLA	4	614	X	-	-	-
21	CLA	4	616	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	42	602	X	-	-	-
21	CLA	42	603	X	-	-	-
21	CLA	42	604	X	-	-	-
21	CLA	42	609	X	-	-	-
21	CLA	42	610	X	-	-	-
21	CLA	42	611	X	-	-	-
21	CLA	42	612	X	-	-	-
21	CLA	42	613	X	-	-	-
21	CLA	42	614	X	-	-	-
21	CLA	42	616	X	-	-	-
21	CLA	5	601	X	-	-	-
21	CLA	5	602	X	-	-	-
21	CLA	5	603	X	-	-	-
21	CLA	5	604	X	-	-	-
21	CLA	5	609	X	-	-	-
21	CLA	5	610	X	-	-	-
21	CLA	5	611	X	-	-	-
21	CLA	5	612	X	-	-	-
21	CLA	5	613	X	-	-	-
21	CLA	5	614	X	-	-	-
21	CLA	5	616	X	-	-	-
21	CLA	5	617	X	-	-	-
21	CLA	5	621	X	-	-	-
21	CLA	52	601	X	-	-	-
21	CLA	52	602	X	-	-	-
21	CLA	52	603	X	-	-	-
21	CLA	52	604	X	-	-	-
21	CLA	52	609	X	-	-	-
21	CLA	52	610	X	-	-	-
21	CLA	52	611	X	-	-	-
21	CLA	52	612	X	-	-	-
21	CLA	52	613	X	-	-	-
21	CLA	52	614	X	-	-	-
21	CLA	52	616	X	-	-	-
21	CLA	52	617	X	-	-	-
21	CLA	52	621	X	-	-	-
21	CLA	6	602	X	-	-	-
21	CLA	6	603	X	-	-	-
21	CLA	6	604	X	-	-	-
21	CLA	6	609	X	-	-	-
21	CLA	6	610	X	-	-	-
21	CLA	6	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	6	612	X	-	-	-
21	CLA	6	613	X	-	-	-
21	CLA	6	614	X	-	-	-
21	CLA	6	617	X	-	-	-
21	CLA	6	622	X	-	-	-
21	CLA	62	602	X	-	-	-
21	CLA	62	603	X	-	-	-
21	CLA	62	604	X	-	-	-
21	CLA	62	609	X	-	-	-
21	CLA	62	610	X	-	-	-
21	CLA	62	611	X	-	-	-
21	CLA	62	612	X	-	-	-
21	CLA	62	613	X	-	-	-
21	CLA	62	614	X	-	-	-
21	CLA	62	617	X	-	-	-
21	CLA	62	622	X	-	-	-
21	CLA	7	602	X	-	-	-
21	CLA	7	603	X	-	-	-
21	CLA	7	604	X	-	-	-
21	CLA	7	608	X	-	-	-
21	CLA	7	609	X	-	-	-
21	CLA	7	610	X	-	-	-
21	CLA	7	611	X	-	-	-
21	CLA	7	612	X	-	-	-
21	CLA	7	613	X	-	-	-
21	CLA	7	614	X	-	-	-
21	CLA	7	616	X	-	-	-
21	CLA	7	620	X	-	-	-
21	CLA	72	602	X	-	-	-
21	CLA	72	603	X	-	-	-
21	CLA	72	604	X	-	-	-
21	CLA	72	608	X	-	-	-
21	CLA	72	609	X	-	-	-
21	CLA	72	610	X	-	-	-
21	CLA	72	611	X	-	-	-
21	CLA	72	612	X	-	-	-
21	CLA	72	613	X	-	-	-
21	CLA	72	614	X	-	-	-
21	CLA	72	616	X	-	-	-
21	CLA	72	620	X	-	-	-
21	CLA	8	602	X	-	-	-
21	CLA	8	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	8	604	X	-	-	-
21	CLA	8	608	X	-	-	-
21	CLA	8	609	X	-	-	-
21	CLA	8	610	X	-	-	-
21	CLA	8	611	X	-	-	-
21	CLA	8	612	X	-	-	-
21	CLA	8	613	X	-	-	-
21	CLA	8	614	X	-	-	-
21	CLA	8	616	X	-	-	-
21	CLA	82	602	X	-	-	-
21	CLA	82	603	X	-	-	-
21	CLA	82	604	X	-	-	-
21	CLA	82	608	X	-	-	-
21	CLA	82	609	X	-	-	-
21	CLA	82	610	X	-	-	-
21	CLA	82	611	X	-	-	-
21	CLA	82	612	X	-	-	-
21	CLA	82	613	X	-	-	-
21	CLA	82	614	X	-	-	-
21	CLA	82	616	X	-	-	-
21	CLA	9	601	X	-	-	-
21	CLA	9	602	X	-	-	-
21	CLA	9	603	X	-	-	-
21	CLA	9	604	X	-	-	-
21	CLA	9	609	X	-	-	-
21	CLA	9	610	X	-	-	-
21	CLA	9	611	X	-	-	-
21	CLA	9	612	X	-	-	-
21	CLA	9	613	X	-	-	-
21	CLA	9	614	X	-	-	-
21	CLA	92	601	X	-	-	-
21	CLA	92	602	X	-	-	-
21	CLA	92	603	X	-	-	-
21	CLA	92	604	X	-	-	-
21	CLA	92	609	X	-	-	-
21	CLA	92	610	X	-	-	-
21	CLA	92	611	X	-	-	-
21	CLA	92	612	X	-	-	-
21	CLA	92	613	X	-	-	-
21	CLA	92	614	X	-	-	-
21	CLA	A	802	X	-	-	-
21	CLA	A	803	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A	804	X	-	-	-
21	CLA	A	805	X	-	-	-
21	CLA	A	806	X	-	-	-
21	CLA	A	807	X	-	-	-
21	CLA	A	808	X	-	-	-
21	CLA	A	809	X	-	-	-
21	CLA	A	810	X	-	-	-
21	CLA	A	811	X	-	-	-
21	CLA	A	812	X	-	-	-
21	CLA	A	813	X	-	-	-
21	CLA	A	814	X	-	-	-
21	CLA	A	815	X	-	-	-
21	CLA	A	816	X	-	-	-
21	CLA	A	817	X	-	-	-
21	CLA	A	818	X	-	-	-
21	CLA	A	819	X	-	-	-
21	CLA	A	820	X	-	-	-
21	CLA	A	821	X	-	-	-
21	CLA	A	822	X	-	-	-
21	CLA	A	823	X	-	-	-
21	CLA	A	824	X	-	-	-
21	CLA	A	825	X	-	-	-
21	CLA	A	826	X	-	-	-
21	CLA	A	827	X	-	-	-
21	CLA	A	828	X	-	-	-
21	CLA	A	829	X	-	-	-
21	CLA	A	830	X	-	-	-
21	CLA	A	831	X	-	-	-
21	CLA	A	832	X	-	-	-
21	CLA	A	833	X	-	-	-
21	CLA	A	834	X	-	-	-
21	CLA	A	835	X	-	-	-
21	CLA	A	836	X	-	-	-
21	CLA	A	837	X	-	-	-
21	CLA	A	838	X	-	-	-
21	CLA	A	839	X	-	-	-
21	CLA	A	840	X	-	-	-
21	CLA	A	841	X	-	-	-
21	CLA	A	842	X	-	-	-
21	CLA	A	843	X	-	-	-
21	CLA	A	845	X	-	-	-
21	CLA	A	854	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A2	802	X	-	-	-
21	CLA	A2	803	X	-	-	-
21	CLA	A2	804	X	-	-	-
21	CLA	A2	805	X	-	-	-
21	CLA	A2	806	X	-	-	-
21	CLA	A2	807	X	-	-	-
21	CLA	A2	808	X	-	-	-
21	CLA	A2	809	X	-	-	-
21	CLA	A2	810	X	-	-	-
21	CLA	A2	811	X	-	-	-
21	CLA	A2	812	X	-	-	-
21	CLA	A2	813	X	-	-	-
21	CLA	A2	814	X	-	-	-
21	CLA	A2	815	X	-	-	-
21	CLA	A2	816	X	-	-	-
21	CLA	A2	817	X	-	-	-
21	CLA	A2	818	X	-	-	-
21	CLA	A2	819	X	-	-	-
21	CLA	A2	820	X	-	-	-
21	CLA	A2	821	X	-	-	-
21	CLA	A2	822	X	-	-	-
21	CLA	A2	823	X	-	-	-
21	CLA	A2	824	X	-	-	-
21	CLA	A2	825	X	-	-	-
21	CLA	A2	826	X	-	-	-
21	CLA	A2	827	X	-	-	-
21	CLA	A2	828	X	-	-	-
21	CLA	A2	829	X	-	-	-
21	CLA	A2	830	X	-	-	-
21	CLA	A2	831	X	-	-	-
21	CLA	A2	832	X	-	-	-
21	CLA	A2	833	X	-	-	-
21	CLA	A2	834	X	-	-	-
21	CLA	A2	835	X	-	-	-
21	CLA	A2	836	X	-	-	-
21	CLA	A2	837	X	-	-	-
21	CLA	A2	838	X	-	-	-
21	CLA	A2	839	X	-	-	-
21	CLA	A2	840	X	-	-	-
21	CLA	A2	841	X	-	-	-
21	CLA	A2	842	X	-	-	-
21	CLA	A2	843	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	A2	845	X	-	-	-
21	CLA	A2	854	X	-	-	-
21	CLA	B	802	X	-	-	-
21	CLA	B	803	X	-	-	-
21	CLA	B	804	X	-	-	-
21	CLA	B	805	X	-	-	-
21	CLA	B	806	X	-	-	-
21	CLA	B	807	X	-	-	-
21	CLA	B	808	X	-	-	-
21	CLA	B	809	X	-	-	-
21	CLA	B	810	X	-	-	-
21	CLA	B	811	X	-	-	-
21	CLA	B	812	X	-	-	-
21	CLA	B	813	X	-	-	-
21	CLA	B	814	X	-	-	-
21	CLA	B	815	X	-	-	-
21	CLA	B	816	X	-	-	-
21	CLA	B	817	X	-	-	-
21	CLA	B	818	X	-	-	-
21	CLA	B	819	X	-	-	-
21	CLA	B	820	X	-	-	-
21	CLA	B	821	X	-	-	-
21	CLA	B	822	X	-	-	-
21	CLA	B	823	X	-	-	-
21	CLA	B	824	X	-	-	-
21	CLA	B	825	X	-	-	-
21	CLA	B	826	X	-	-	-
21	CLA	B	827	X	-	-	-
21	CLA	B	828	X	-	-	-
21	CLA	B	829	X	-	-	-
21	CLA	B	830	X	-	-	-
21	CLA	B	831	X	-	-	-
21	CLA	B	832	X	-	-	-
21	CLA	B	833	X	-	-	-
21	CLA	B	834	X	-	-	-
21	CLA	B	835	X	-	-	-
21	CLA	B	836	X	-	-	-
21	CLA	B	837	X	-	-	-
21	CLA	B	838	X	-	-	-
21	CLA	B	839	X	-	-	-
21	CLA	B	840	X	-	-	-
21	CLA	B	841	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	B2	802	X	-	-	-
21	CLA	B2	803	X	-	-	-
21	CLA	B2	804	X	-	-	-
21	CLA	B2	805	X	-	-	-
21	CLA	B2	806	X	-	-	-
21	CLA	B2	807	X	-	-	-
21	CLA	B2	808	X	-	-	-
21	CLA	B2	809	X	-	-	-
21	CLA	B2	810	X	-	-	-
21	CLA	B2	811	X	-	-	-
21	CLA	B2	812	X	-	-	-
21	CLA	B2	813	X	-	-	-
21	CLA	B2	814	X	-	-	-
21	CLA	B2	815	X	-	-	-
21	CLA	B2	816	X	-	-	-
21	CLA	B2	817	X	-	-	-
21	CLA	B2	818	X	-	-	-
21	CLA	B2	819	X	-	-	-
21	CLA	B2	820	X	-	-	-
21	CLA	B2	821	X	-	-	-
21	CLA	B2	822	X	-	-	-
21	CLA	B2	823	X	-	-	-
21	CLA	B2	824	X	-	-	-
21	CLA	B2	825	X	-	-	-
21	CLA	B2	826	X	-	-	-
21	CLA	B2	827	X	-	-	-
21	CLA	B2	828	X	-	-	-
21	CLA	B2	829	X	-	-	-
21	CLA	B2	830	X	-	-	-
21	CLA	B2	831	X	-	-	-
21	CLA	B2	832	X	-	-	-
21	CLA	B2	833	X	-	-	-
21	CLA	B2	834	X	-	-	-
21	CLA	B2	835	X	-	-	-
21	CLA	B2	836	X	-	-	-
21	CLA	B2	837	X	-	-	-
21	CLA	B2	838	X	-	-	-
21	CLA	B2	839	X	-	-	-
21	CLA	B2	840	X	-	-	-
21	CLA	B2	841	X	-	-	-
21	CLA	F	301	X	-	-	-
21	CLA	F	303	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	F	304	X	-	-	-
21	CLA	F2	301	X	-	-	-
21	CLA	F2	303	X	-	-	-
21	CLA	F2	304	X	-	-	-
21	CLA	G	203	X	-	-	-
21	CLA	G	204	X	-	-	-
21	CLA	G2	203	X	-	-	-
21	CLA	G2	204	X	-	-	-
21	CLA	J	101	X	-	-	-
21	CLA	J2	101	X	-	-	-
21	CLA	K	201	X	-	-	-
21	CLA	K	203	X	-	-	-
21	CLA	K	204	X	-	-	-
21	CLA	K	206	X	-	-	-
21	CLA	K2	201	X	-	-	-
21	CLA	K2	203	X	-	-	-
21	CLA	K2	204	X	-	-	-
21	CLA	K2	206	X	-	-	-
21	CLA	L	203	X	-	-	-
21	CLA	L	204	X	-	-	-
21	CLA	L2	203	X	-	-	-
21	CLA	L2	204	X	-	-	-
21	CLA	Z	602	X	-	-	-
21	CLA	Z	603	X	-	-	-
21	CLA	Z	604	X	-	-	-
21	CLA	Z	608	X	-	-	-
21	CLA	Z	609	X	-	-	-
21	CLA	Z	610	X	-	-	-
21	CLA	Z	611	X	-	-	-
21	CLA	Z	612	X	-	-	-
21	CLA	Z	613	X	-	-	-
21	CLA	Z	614	X	-	-	-
21	CLA	Z	616	X	-	-	-
21	CLA	Z2	602	X	-	-	-
21	CLA	Z2	603	X	-	-	-
21	CLA	Z2	604	X	-	-	-
21	CLA	Z2	608	X	-	-	-
21	CLA	Z2	609	X	-	-	-
21	CLA	Z2	610	X	-	-	-
21	CLA	Z2	611	X	-	-	-
21	CLA	Z2	612	X	-	-	-
21	CLA	Z2	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	CLA	Z2	614	X	-	-	-
21	CLA	Z2	616	X	-	-	-
30	CHL	1	601	X	-	-	-
30	CHL	1	606	X	-	-	-
30	CHL	1	607	X	-	-	-
30	CHL	12	601	X	-	-	-
30	CHL	12	606	X	-	-	-
30	CHL	12	607	X	-	-	-
30	CHL	3	608	X	-	-	-
30	CHL	32	608	X	-	-	-
30	CHL	4	601	X	-	-	-
30	CHL	4	606	X	-	-	-
30	CHL	4	607	X	-	-	-
30	CHL	4	608	X	-	-	-
30	CHL	4	618	X	-	-	-
30	CHL	42	601	X	-	-	-
30	CHL	42	606	X	-	-	-
30	CHL	42	607	X	-	-	-
30	CHL	42	608	X	-	-	-
30	CHL	42	618	X	-	-	-
30	CHL	5	606	X	-	-	-
30	CHL	5	607	X	-	-	-
30	CHL	5	608	X	-	-	-
30	CHL	5	618	X	-	-	-
30	CHL	52	606	X	-	-	-
30	CHL	52	607	X	-	-	-
30	CHL	52	608	X	-	-	-
30	CHL	52	618	X	-	-	-
30	CHL	6	601	X	-	-	-
30	CHL	6	606	X	-	-	-
30	CHL	6	607	X	-	-	-
30	CHL	6	608	X	-	-	-
30	CHL	6	616	X	-	-	-
30	CHL	6	618	X	-	-	-
30	CHL	62	601	X	-	-	-
30	CHL	62	606	X	-	-	-
30	CHL	62	607	X	-	-	-
30	CHL	62	608	X	-	-	-
30	CHL	62	616	X	-	-	-
30	CHL	62	618	X	-	-	-
30	CHL	7	601	X	-	-	-
30	CHL	7	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
30	CHL	7	607	X	-	-	-
30	CHL	72	601	X	-	-	-
30	CHL	72	606	X	-	-	-
30	CHL	72	607	X	-	-	-
30	CHL	8	601	X	-	-	-
30	CHL	8	606	X	-	-	-
30	CHL	8	607	X	-	-	-
30	CHL	82	601	X	-	-	-
30	CHL	82	606	X	-	-	-
30	CHL	82	607	X	-	-	-
30	CHL	9	606	X	-	-	-
30	CHL	9	607	X	-	-	-
30	CHL	92	606	X	-	-	-
30	CHL	92	607	X	-	-	-
30	CHL	Z	601	X	-	-	-
30	CHL	Z	606	X	-	-	-
30	CHL	Z	607	X	-	-	-
30	CHL	Z2	601	X	-	-	-
30	CHL	Z2	606	X	-	-	-
30	CHL	Z2	607	X	-	-	-
31	XAT	5	624	X	-	-	-
31	XAT	52	624	X	-	-	-

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 202818 atoms, of which 101988 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		
1	A2	742	Total	C	H	N	O	S	0	0
			11500	3808	5675	994	1001	22		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		
2	B2	733	Total	C	H	N	O	S	0	0
			11400	3824	5576	977	1005	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		
3	C2	80	Total	C	H	N	O	S	0	0
			1183	369	582	103	117	12		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		
4	D2	144	Total	C	H	N	O	S	0	0
			2284	725	1151	200	201	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		
5	E2	64	Total	C	H	N	O	0	0
			1011	322	505	89	95		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		
6	F2	165	Total	C	H	N	O	S	0	0
			2568	817	1302	213	233	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		
7	G2	95	Total	C	H	N	O	0	0
			1393	452	687	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
8	I	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		
8	I2	37	Total	C	H	N	O	S	0	0
			573	195	292	39	46	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
9	J	40	Total 657	C 224	H 328	N 46	O 58	S 1	0	0
9	J2	40	Total 657	C 224	H 328	N 46	O 58	S 1	0	0

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		

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Mol	Chain	Residues	Atoms						AltConf	Trace
10	L2	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
11	K	86	Total	C	H	N	O	S	0	0
			1203	370	620	100	111	2		
11	K2	86	Total	C	H	N	O	S	0	0
			1203	370	620	100	111	2		

- Molecule 12 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	1	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	Z	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	12	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		
12	Z2	194	Total	C	H	N	O	S	0	0
			2842	941	1397	240	261	3		

- Molecule 13 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	3	227	Total	C	H	N	O	S	0	0
			3431	1128	1695	283	317	8		
13	32	227	Total	C	H	N	O	S	0	0
			3431	1128	1695	283	317	8		

- Molecule 14 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
14	7	213	Total	C	H	N	O	S	0	0
			3240	1072	1590	274	298	6		
14	72	213	Total	C	H	N	O	S	0	0
			3240	1072	1590	274	298	6		

- Molecule 15 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	8	217	Total	C	H	N	O	S	0	0
			3280	1073	1630	280	293	4		
15	82	217	Total	C	H	N	O	S	0	0
			3280	1073	1630	280	293	4		

- Molecule 16 is a protein called Chlorophyll a-b binding protein, chloroplastic (Lhca4).

Mol	Chain	Residues	Atoms						AltConf	Trace
16	4	212	Total	C	H	N	O	S	0	0
			3251	1080	1603	268	295	5		
16	42	212	Total	C	H	N	O	S	0	0
			3251	1080	1603	268	295	5		

- Molecule 17 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
17	5	227	Total	C	H	N	O	S	0	0
			3522	1154	1747	297	316	8		
17	52	227	Total	C	H	N	O	S	0	0
			3522	1154	1747	297	316	8		

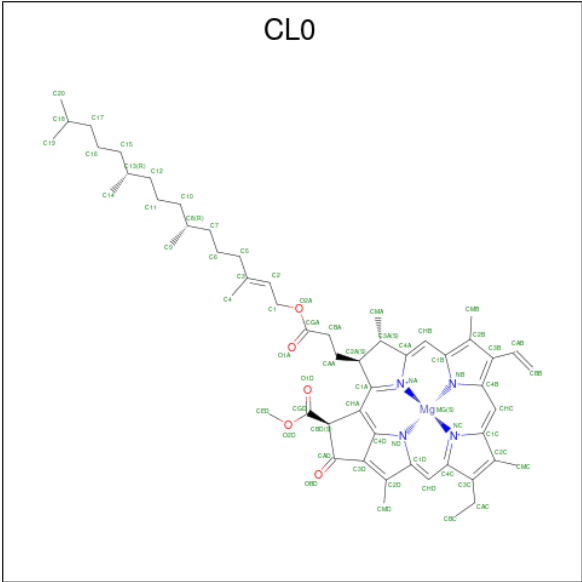
- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	6	230	Total	C	H	N	O	S	0	0
			3542	1167	1770	293	306	6		
18	62	230	Total	C	H	N	O	S	0	0
			3542	1167	1770	293	306	6		

- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

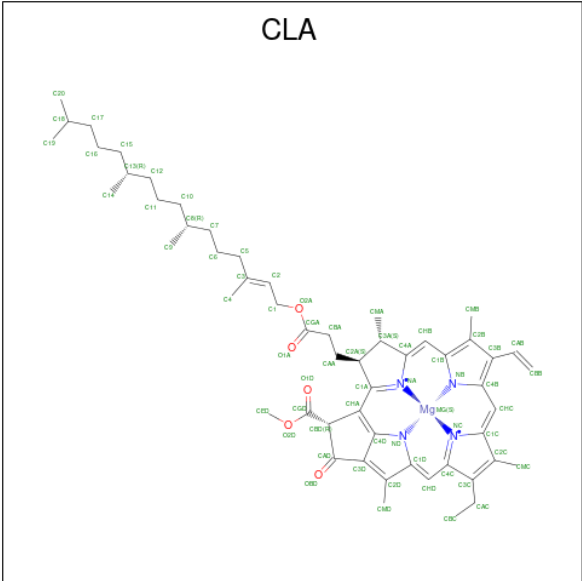
Mol	Chain	Residues	Atoms						AltConf	Trace
19	9	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		
19	92	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		

- Molecule 20 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 89	C 40	H 39	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	B	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
21	B	1	Total 107	C 46	H 51	Mg 1	N 4	O 5	0
21	B	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
21	B	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	G	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	J	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
21	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
21	7	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	7	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	4	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	5	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	5	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	9	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	9	1	Total 98	C 43	H 45	Mg 1	N 4	O 5	0
21	9	1	Total 92	C 41	H 41	Mg 1	N 4	O 5	0
21	9	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
21	9	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	9	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	9	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	9	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 89	C 40	H 39	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
21	A2	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			117	49	58	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	F2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	G2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	G2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	J2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	L2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	K2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	12	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	12	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
21	32	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	32	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	32	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
21	72	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	72	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
21	82	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	82	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	Z2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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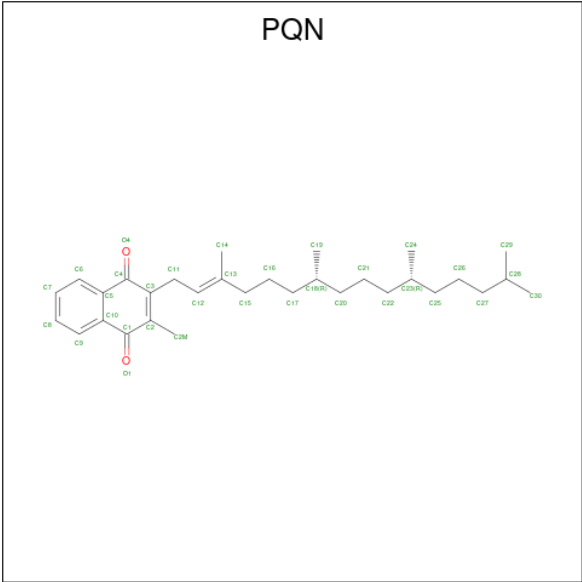
Mol	Chain	Residues	Atoms						AltConf
21	42	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	42	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	52	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	

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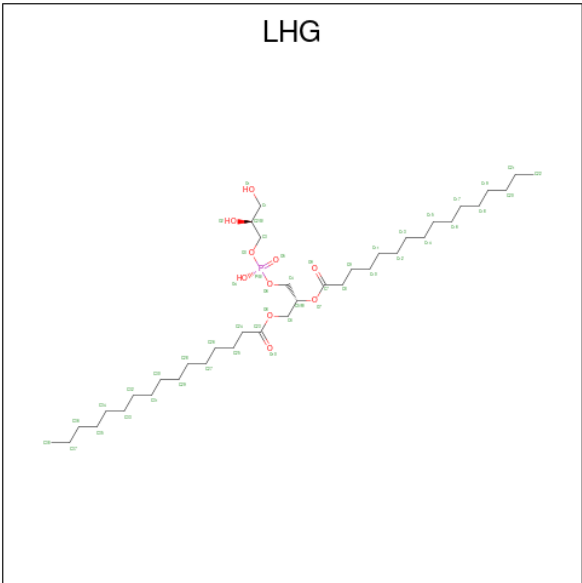
Mol	Chain	Residues	Atoms						AltConf
21	62	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
21	62	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
21	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 22 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
22	A	1	Total	C	H	O	0
			79	31	46	2	
22	B	1	Total	C	H	O	0
			79	31	46	2	
22	A2	1	Total	C	H	O	0
			79	31	46	2	
22	B2	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 23 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



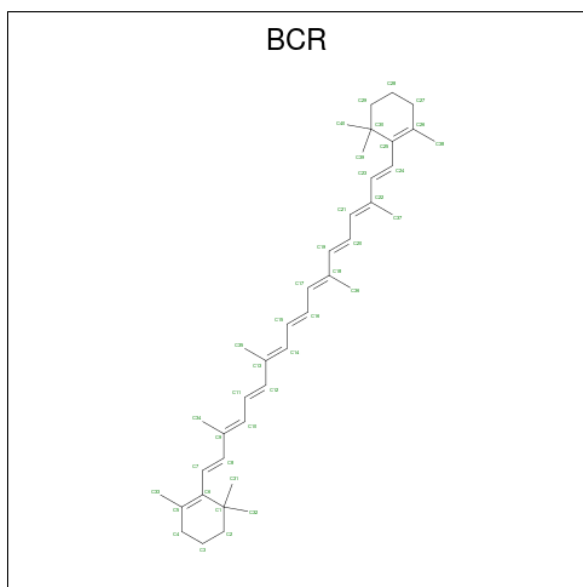
Mol	Chain	Residues	Atoms					AltConf
23	A	1	Total 123	C 38	H 74	O 10	P 1	0
23	A	1	Total 87	C 27	H 49	O 10	P 1	0
23	B	1	Total 108	C 34	H 63	O 10	P 1	0
23	1	1	Total 87	C 28	H 48	O 10	P 1	0
23	3	1	Total 63	C 20	H 32	O 10	P 1	0
23	3	1	Total 114	C 36	H 67	O 10	P 1	0
23	7	1	Total 123	C 38	H 74	O 10	P 1	0
23	8	1	Total 105	C 33	H 61	O 10	P 1	0
23	Z	1	Total 87	C 28	H 48	O 10	P 1	0
23	4	1	Total 123	C 38	H 74	O 10	P 1	0
23	4	1	Total 87	C 27	H 49	O 10	P 1	0
23	5	1	Total 81	C 26	H 44	O 10	P 1	0
23	6	1	Total 123	C 38	H 74	O 10	P 1	0
23	6	1	Total 78	C 25	H 42	O 10	P 1	0
23	9	1	Total 96	C 30	H 55	O 10	P 1	0
23	A2	1	Total 123	C 38	H 74	O 10	P 1	0
23	A2	1	Total 87	C 27	H 49	O 10	P 1	0
23	B2	1	Total 108	C 34	H 63	O 10	P 1	0
23	12	1	Total 87	C 28	H 48	O 10	P 1	0
23	32	1	Total 63	C 20	H 32	O 10	P 1	0
23	32	1	Total 114	C 36	H 67	O 10	P 1	0
23	72	1	Total 123	C 38	H 74	O 10	P 1	0

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Mol	Chain	Residues	Atoms					AltConf
23	82	1	Total	C	H	O	P	0
			105	33	61	10	1	
23	Z2	1	Total	C	H	O	P	0
			87	28	48	10	1	
23	42	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	42	1	Total	C	H	O	P	0
			87	27	49	10	1	
23	52	1	Total	C	H	O	P	0
			81	26	44	10	1	
23	62	1	Total	C	H	O	P	0
			123	38	74	10	1	
23	62	1	Total	C	H	O	P	0
			78	25	42	10	1	
23	92	1	Total	C	H	O	P	0
			96	30	55	10	1	

- Molecule 24 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	
24	A	1	Total	C	H	0
			96	40	56	

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Mol	Chain	Residues	Atoms			AltConf
24	A	1	Total 96	C 40	H 56	0
24	A	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	B	1	Total 96	C 40	H 56	0
24	G	1	Total 96	C 40	H 56	0
24	I	1	Total 96	C 40	H 56	0
24	J	1	Total 96	C 40	H 56	0
24	L	1	Total 96	C 40	H 56	0
24	L	1	Total 96	C 40	H 56	0
24	K	1	Total 96	C 40	H 56	0
24	K	1	Total 96	C 40	H 56	0
24	3	1	Total 96	C 40	H 56	0
24	3	1	Total 96	C 40	H 56	0
24	3	1	Total 96	C 40	H 56	0
24	7	1	Total 96	C 40	H 56	0
24	8	1	Total 96	C 40	H 56	0

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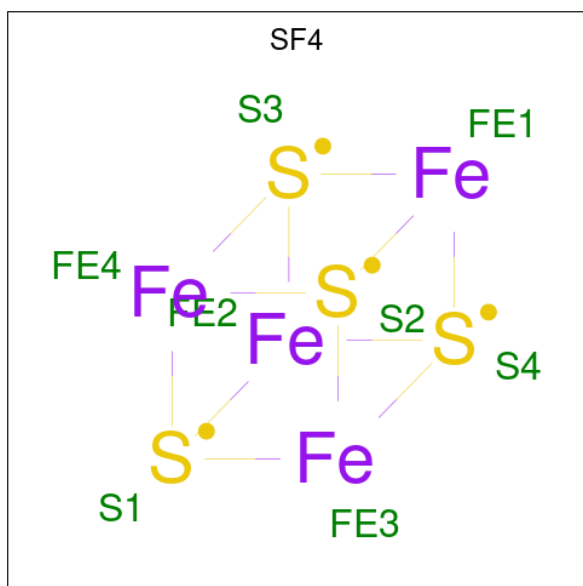
Mol	Chain	Residues	Atoms			AltConf
24	4	1	Total 96	C 40	H 56	0
24	5	1	Total 96	C 40	H 56	0
24	6	1	Total 96	C 40	H 56	0
24	9	1	Total 96	C 40	H 56	0
24	A2	1	Total 96	C 40	H 56	0
24	A2	1	Total 96	C 40	H 56	0
24	A2	1	Total 96	C 40	H 56	0
24	A2	1	Total 96	C 40	H 56	0
24	A2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	B2	1	Total 96	C 40	H 56	0
24	G2	1	Total 96	C 40	H 56	0
24	I2	1	Total 96	C 40	H 56	0
24	J2	1	Total 96	C 40	H 56	0
24	L2	1	Total 96	C 40	H 56	0
24	L2	1	Total 96	C 40	H 56	0

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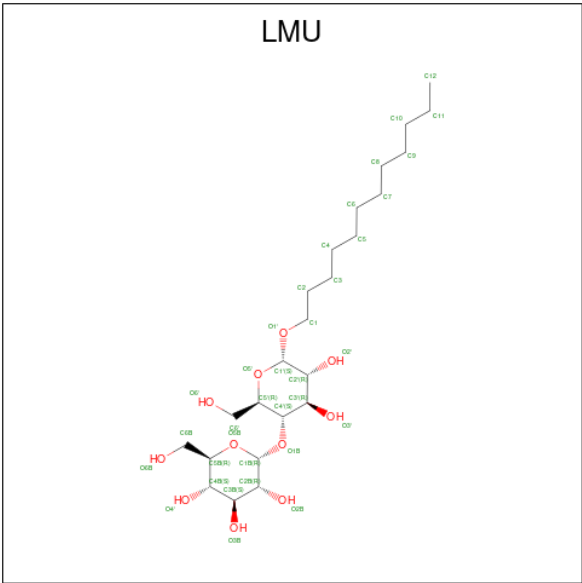
Mol	Chain	Residues	Atoms			AltConf
24	K2	1	Total	C	H	0
			96	40	56	
24	K2	1	Total	C	H	0
			96	40	56	
24	32	1	Total	C	H	0
			96	40	56	
24	32	1	Total	C	H	0
			96	40	56	
24	32	1	Total	C	H	0
			96	40	56	
24	72	1	Total	C	H	0
			96	40	56	
24	82	1	Total	C	H	0
			96	40	56	
24	42	1	Total	C	H	0
			96	40	56	
24	52	1	Total	C	H	0
			96	40	56	
24	62	1	Total	C	H	0
			96	40	56	
24	92	1	Total	C	H	0
			96	40	56	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	C	1	Total	Fe	S	0
			8	4	4	
25	A2	1	Total	Fe	S	0
			8	4	4	
25	C2	1	Total	Fe	S	0
			8	4	4	
25	C2	1	Total	Fe	S	0
			8	4	4	

- Molecule 26 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C₂₄H₄₆O₁₁) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			75	23	41	11	
26	A	1	Total	C	H	O	0
			81	24	46	11	
26	A	1	Total	C	H	O	0
			44	14	24	6	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	A	1	Total	C	H	O	0
			81	24	46	11	

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Mol	Chain	Residues	Atoms				AltConf
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	A	1	Total	C	H	O	0
			59	18	35	6	
26	B	1	Total	C	H	O	0
			81	24	46	11	
26	G	1	Total	C	H	O	0
			59	18	35	6	
26	K	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			81	24	46	11	
26	1	1	Total	C	H	O	0
			41	13	22	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			50	16	28	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	1	1	Total	C	H	O	0
			59	18	35	6	
26	7	1	Total	C	H	O	0
			69	21	37	11	
26	7	1	Total	C	H	O	0
			50	16	28	6	
26	7	1	Total	C	H	O	0
			54	16	27	11	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	8	1	Total	C	H	O	0
			81	24	46	11	
26	8	1	Total	C	H	O	0
			59	18	35	6	
26	Z	1	Total	C	H	O	0
			66	20	35	11	
26	Z	1	Total	C	H	O	0
			50	16	28	6	
26	4	1	Total	C	H	O	0
			72	22	39	11	

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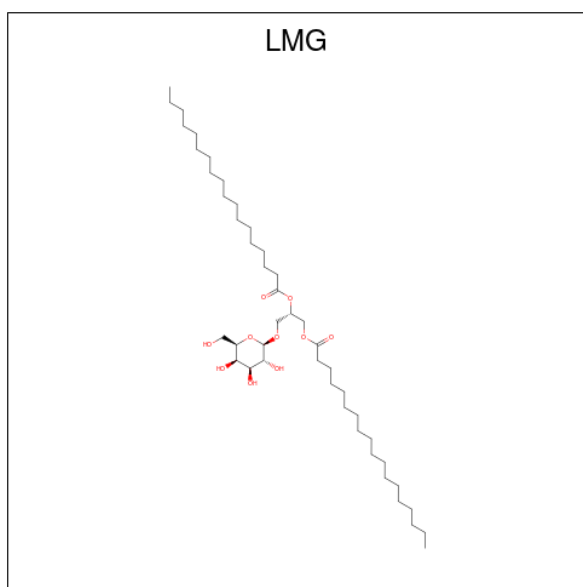
Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	H	O	0
			44	14	24	6	
26	5	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			44	14	24	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	6	1	Total	C	H	O	0
			59	18	35	6	
26	9	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			75	23	41	11	
26	A2	1	Total	C	H	O	0
			81	24	46	11	
26	A2	1	Total	C	H	O	0
			44	14	24	6	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			81	24	46	11	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	A2	1	Total	C	H	O	0
			59	18	35	6	
26	B2	1	Total	C	H	O	0
			81	24	46	11	
26	G2	1	Total	C	H	O	0
			59	18	35	6	
26	K2	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			81	24	46	11	
26	12	1	Total	C	H	O	0
			41	13	22	6	
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			50	16	28	6	

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Mol	Chain	Residues	Atoms				AltConf
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	12	1	Total	C	H	O	0
			59	18	35	6	
26	72	1	Total	C	H	O	0
			69	21	37	11	
26	72	1	Total	C	H	O	0
			50	16	28	6	
26	72	1	Total	C	H	O	0
			54	16	27	11	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	82	1	Total	C	H	O	0
			81	24	46	11	
26	82	1	Total	C	H	O	0
			59	18	35	6	
26	Z2	1	Total	C	H	O	0
			66	20	35	11	
26	Z2	1	Total	C	H	O	0
			50	16	28	6	
26	42	1	Total	C	H	O	0
			72	22	39	11	
26	42	1	Total	C	H	O	0
			44	14	24	6	
26	52	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			44	14	24	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	62	1	Total	C	H	O	0
			59	18	35	6	
26	92	1	Total	C	H	O	0
			59	18	35	6	

- Molecule 27 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



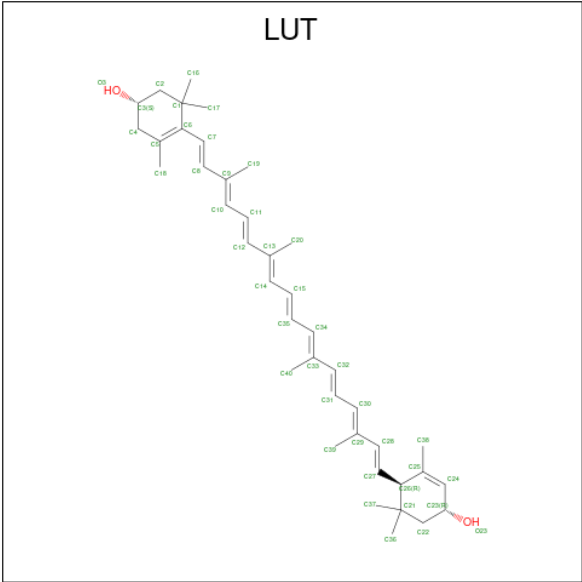
Mol	Chain	Residues	Atoms				AltConf
27	A	1	Total	C	H	O	0
			117	38	69	10	
27	A	1	Total	C	H	O	0
			78	26	42	10	
27	B	1	Total	C	H	O	0
			99	33	56	10	
27	B	1	Total	C	H	O	0
			78	26	42	10	
27	J	1	Total	C	H	O	0
			99	32	57	10	
27	J	1	Total	C	H	O	0
			75	25	40	10	
27	1	1	Total	C	H	O	0
			78	26	42	10	
27	1	1	Total	C	H	O	0
			96	32	54	10	
27	3	1	Total	C	H	O	0
			120	40	75	5	
27	7	1	Total	C	H	O	0
			81	27	44	10	
27	8	1	Total	C	H	O	0
			66	22	34	10	
27	8	1	Total	C	H	O	0
			99	32	57	10	
27	4	1	Total	C	H	O	0
			96	31	55	10	
27	6	1	Total	C	H	O	0
			55	18	35	2	

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Mol	Chain	Residues	Atoms				AltConf
27	9	1	Total	C	H	O	0
			105	34	61	10	
27	A2	1	Total	C	H	O	0
			117	38	69	10	
27	A2	1	Total	C	H	O	0
			78	26	42	10	
27	B2	1	Total	C	H	O	0
			99	33	56	10	
27	B2	1	Total	C	H	O	0
			78	26	42	10	
27	J2	1	Total	C	H	O	0
			99	32	57	10	
27	J2	1	Total	C	H	O	0
			75	25	40	10	
27	12	1	Total	C	H	O	0
			78	26	42	10	
27	12	1	Total	C	H	O	0
			96	32	54	10	
27	32	1	Total	C	H	O	0
			120	40	75	5	
27	72	1	Total	C	H	O	0
			81	27	44	10	
27	82	1	Total	C	H	O	0
			66	22	34	10	
27	82	1	Total	C	H	O	0
			99	32	57	10	
27	42	1	Total	C	H	O	0
			96	31	55	10	
27	62	1	Total	C	H	O	0
			55	18	35	2	
27	92	1	Total	C	H	O	0
			105	34	61	10	

- Molecule 28 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C₄₀H₅₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			98	40	56	2	
28	F	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	1	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	3	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	7	1	Total	C	H	O	0
			98	40	56	2	
28	8	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			98	40	56	2	
28	Z	1	Total	C	H	O	0
			59	25	33	1	
28	4	1	Total	C	H	O	0
			98	40	56	2	
28	5	1	Total	C	H	O	0
			98	40	56	2	

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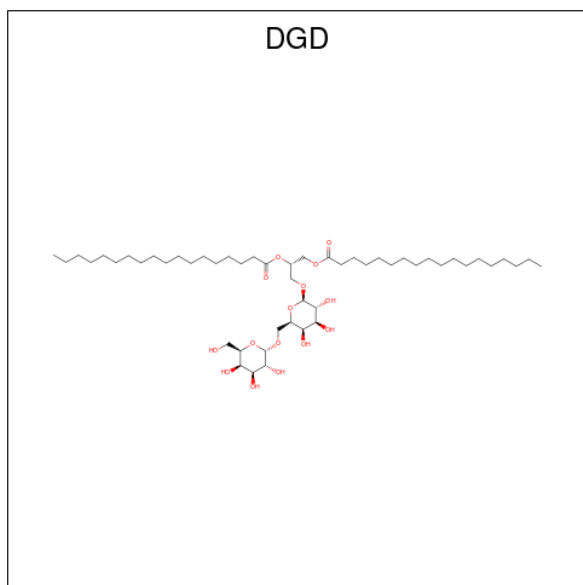
Mol	Chain	Residues	Atoms				AltConf
28	5	1	Total	C	H	O	0
			98	40	56	2	
28	6	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	
28	9	1	Total	C	H	O	0
			98	40	56	2	
28	A2	1	Total	C	H	O	0
			98	40	56	2	
28	F2	1	Total	C	H	O	0
			98	40	56	2	
28	12	1	Total	C	H	O	0
			98	40	56	2	
28	12	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	32	1	Total	C	H	O	0
			98	40	56	2	
28	72	1	Total	C	H	O	0
			98	40	56	2	
28	72	1	Total	C	H	O	0
			98	40	56	2	
28	82	1	Total	C	H	O	0
			98	40	56	2	
28	Z2	1	Total	C	H	O	0
			98	40	56	2	
28	Z2	1	Total	C	H	O	0
			59	25	33	1	
28	42	1	Total	C	H	O	0
			98	40	56	2	
28	52	1	Total	C	H	O	0
			98	40	56	2	
28	52	1	Total	C	H	O	0
			98	40	56	2	
28	62	1	Total	C	H	O	0
			98	40	56	2	
28	92	1	Total	C	H	O	0
			98	40	56	2	

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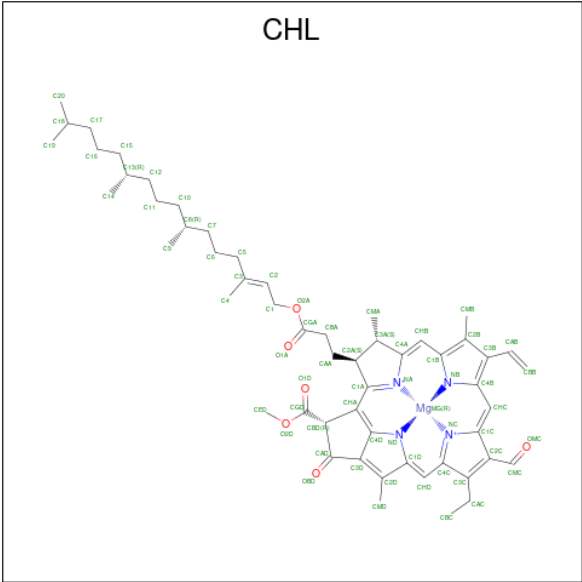
Mol	Chain	Residues	Atoms				AltConf
28	92	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 29 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
29	B	1	Total	C	H	O	0
			138	44	79	15	
29	B2	1	Total	C	H	O	0
			138	44	79	15	

- Molecule 30 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
30	1	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	1	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	3	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	7	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	8	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	Z	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
30	4	1	Total	C	H	Mg	N	O	0
			103	45	47	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	4	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	5	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			109	47	51	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	6	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
30	9	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	12	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	32	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	72	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	

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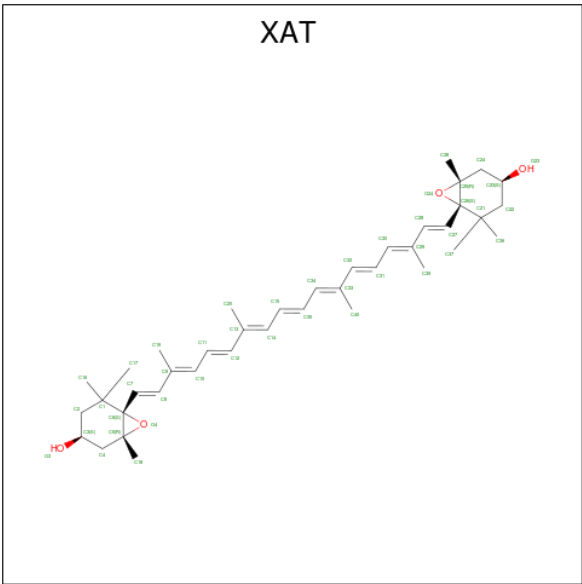
Mol	Chain	Residues	Atoms						AltConf
30	72	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	72	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	82	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	Z2	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			103	45	47	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	42	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
30	52	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			109	47	51	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	

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Mol	Chain	Residues	Atoms						AltConf
30	62	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
30	62	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
30	92	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
30	92	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	

- Molecule 31 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



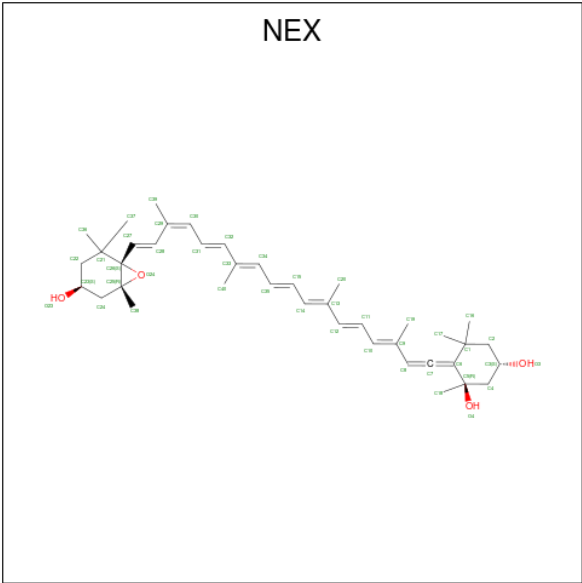
Mol	Chain	Residues	Atoms				AltConf
31	1	1	Total	C	H	O	0
			100	40	56	4	
31	7	1	Total	C	H	O	0
			100	40	56	4	
31	8	1	Total	C	H	O	0
			100	40	56	4	
31	Z	1	Total	C	H	O	0
			100	40	56	4	
31	4	1	Total	C	H	O	0
			100	40	56	4	
31	5	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
31	6	1	Total	C	H	O	0
			100	40	56	4	
31	12	1	Total	C	H	O	0
			100	40	56	4	
31	72	1	Total	C	H	O	0
			100	40	56	4	
31	82	1	Total	C	H	O	0
			100	40	56	4	
31	Z2	1	Total	C	H	O	0
			100	40	56	4	
31	42	1	Total	C	H	O	0
			100	40	56	4	
31	52	1	Total	C	H	O	0
			100	40	56	4	
31	62	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 32 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
32	5	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
32	6	1	Total	C	H	O	0
			100	40	56	4	
32	52	1	Total	C	H	O	0
			100	40	56	4	
32	62	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 33 is water.

Mol	Chain	Residues	Atoms		AltConf
33	H	10	Total	O	0
			10	10	
33	H	19	Total	O	0
			19	19	
33	H	1	Total	O	0
			1	1	
33	H	1	Total	O	0
			1	1	
33	H	4	Total	O	0
			4	4	
33	H	1	Total	O	0
			1	1	
33	H	1	Total	O	0
			1	1	
33	H	7	Total	O	0
			7	7	
33	H	6	Total	O	0
			6	6	
33	H	6	Total	O	0
			6	6	
33	H	6	Total	O	0
			6	6	
33	H	5	Total	O	0
			5	5	
33	H	3	Total	O	0
			3	3	
33	H	5	Total	O	0
			5	5	
33	H	5	Total	O	0
			5	5	
33	H	1	Total	O	0
			1	1	

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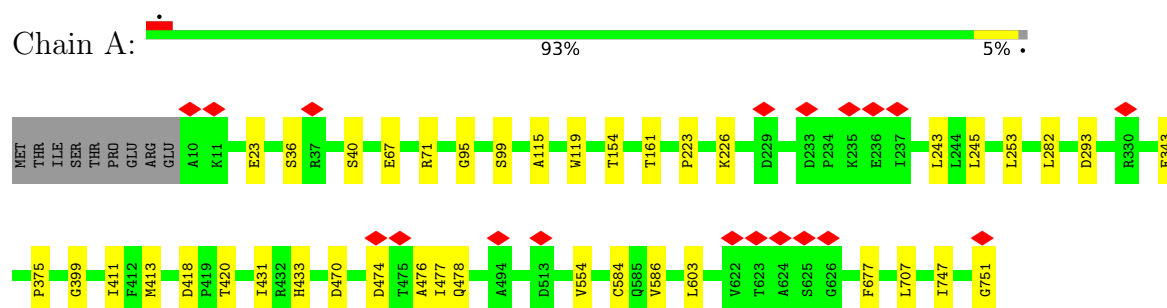
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Mol	Chain	Residues	Atoms		AltConf
33	H	11	Total 11	O 11	0
33	H	18	Total 18	O 18	0
33	H	1	Total 1	O 1	0
33	H	1	Total 1	O 1	0
33	H	4	Total 4	O 4	0
33	H	1	Total 1	O 1	0
33	H	1	Total 1	O 1	0
33	H	7	Total 7	O 7	0
33	H	5	Total 5	O 5	0
33	H	6	Total 6	O 6	0
33	H	5	Total 5	O 5	0
33	H	5	Total 5	O 5	0
33	H	3	Total 3	O 3	0
33	H	5	Total 5	O 5	0
33	H	5	Total 5	O 5	0
33	H	1	Total 1	O 1	0

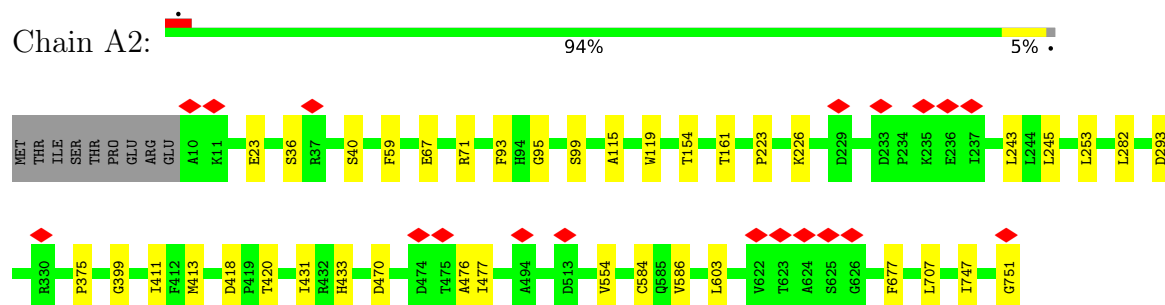
3 Residue-property plots [i](#)

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

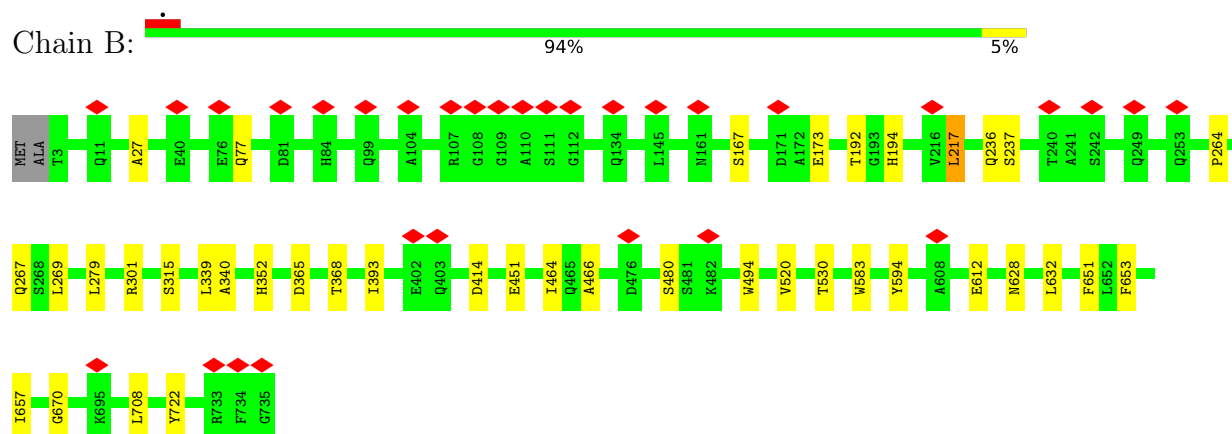
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



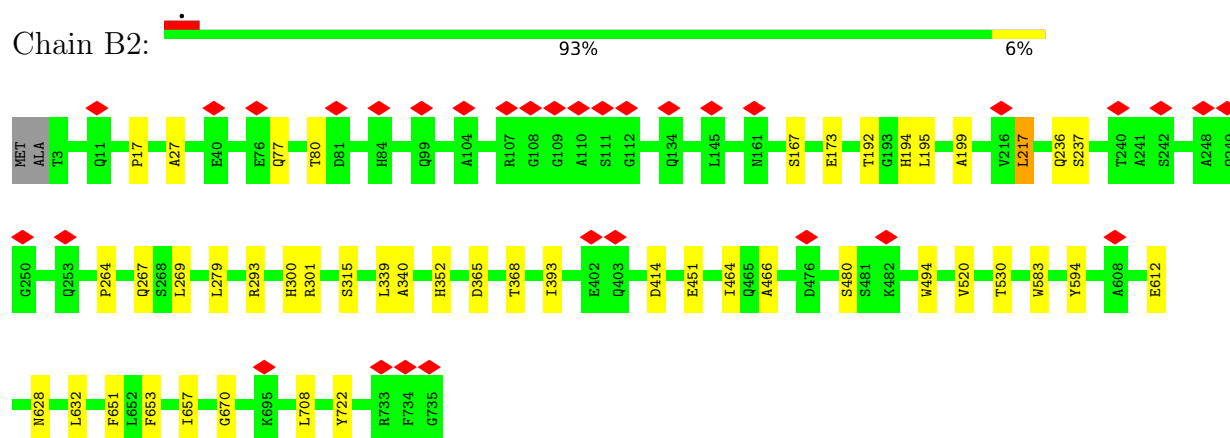
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



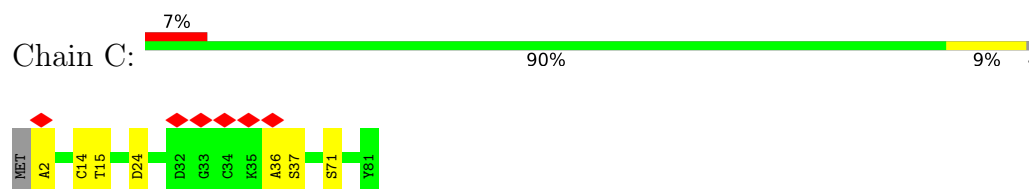
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



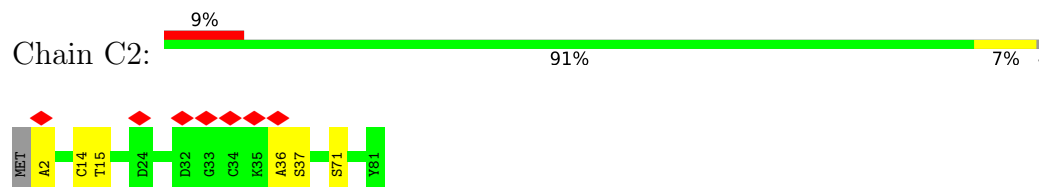
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



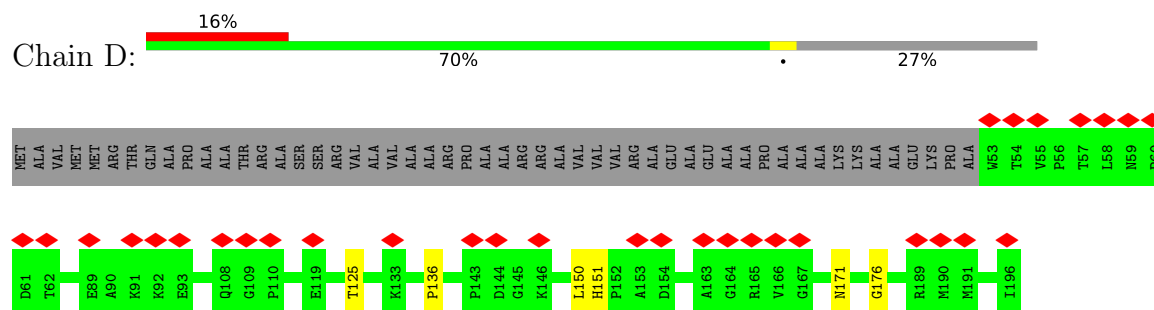
- Molecule 3: Photosystem I iron-sulfur center



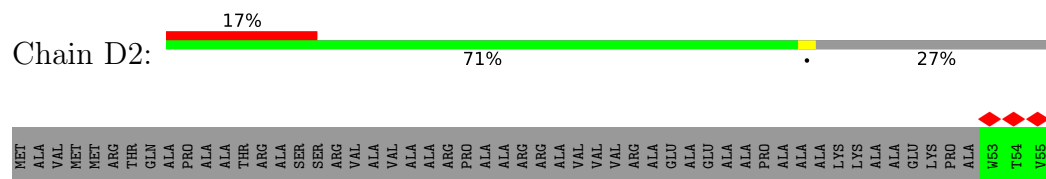
- Molecule 3: Photosystem I iron-sulfur center

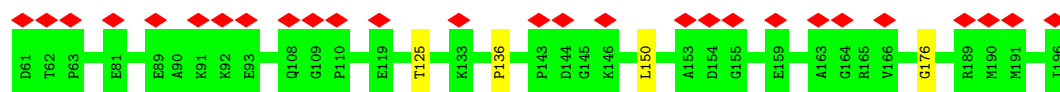


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

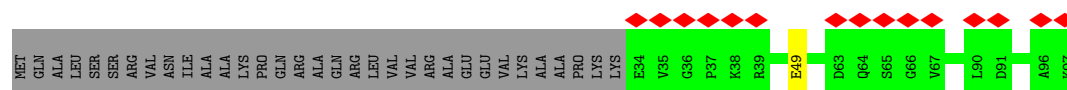


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

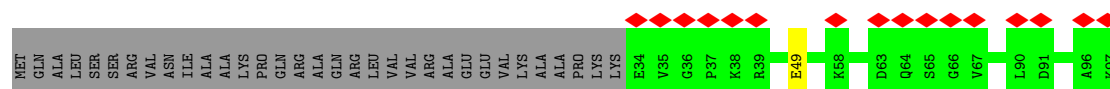




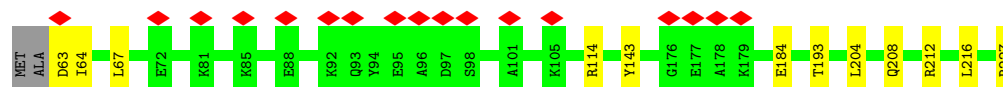
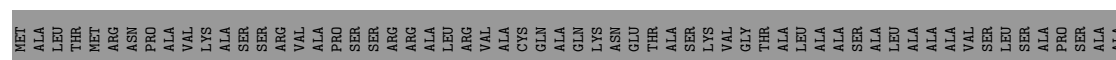
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



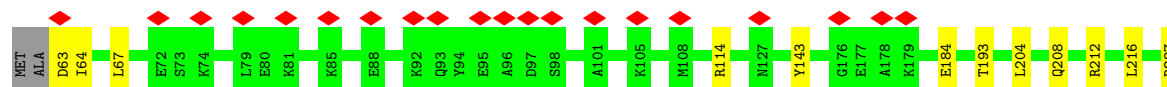
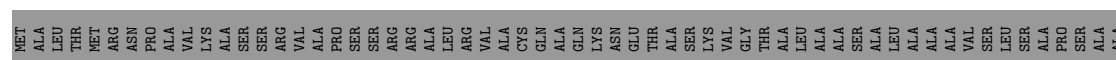
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



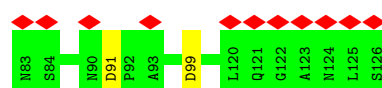
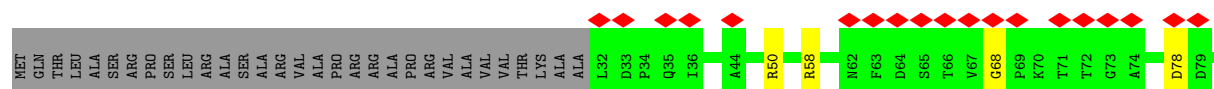
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



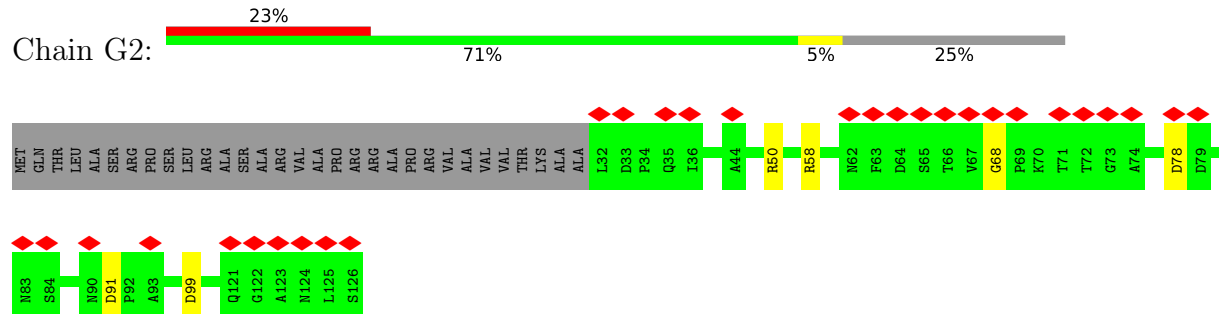
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



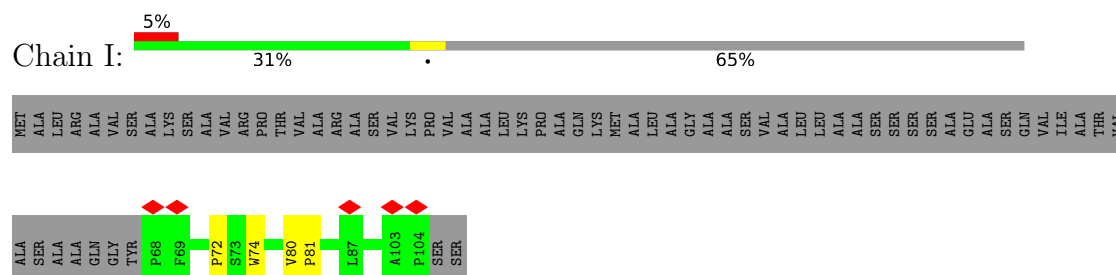
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



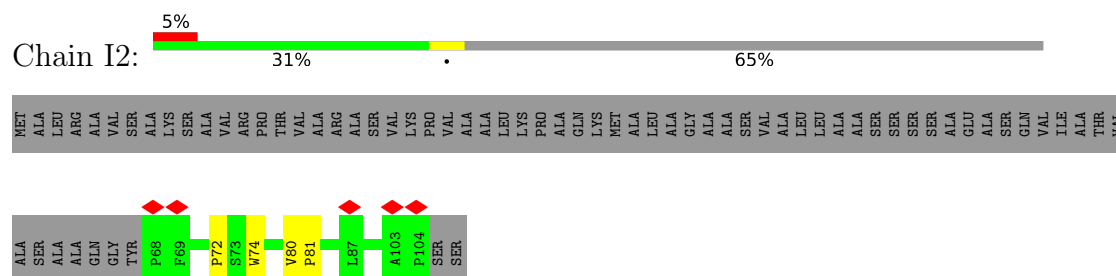
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



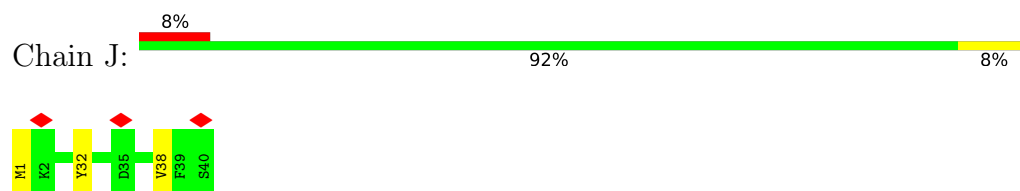
- Molecule 8: Photosystem I reaction center subunit VIII



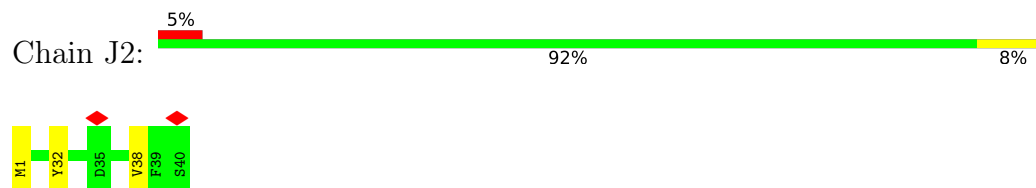
- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 9: Photosystem I reaction center subunit IX

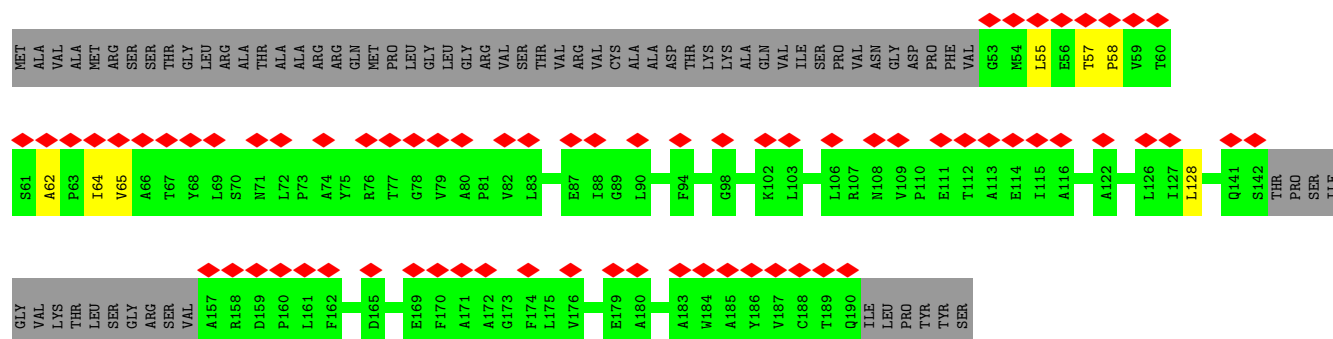


- Molecule 9: Photosystem I reaction center subunit IX

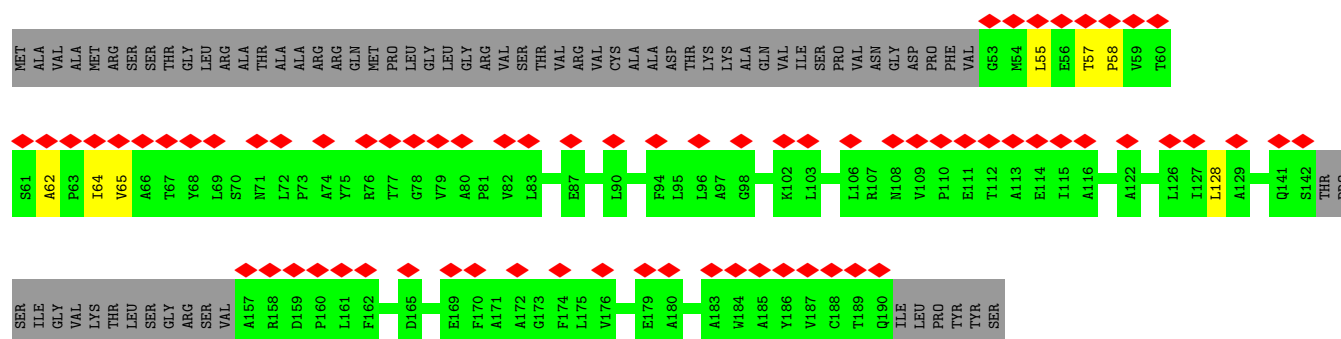


- Molecule 10: PSI subunit V

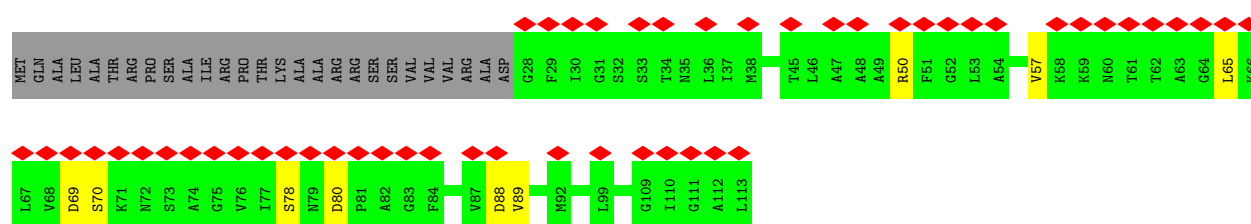




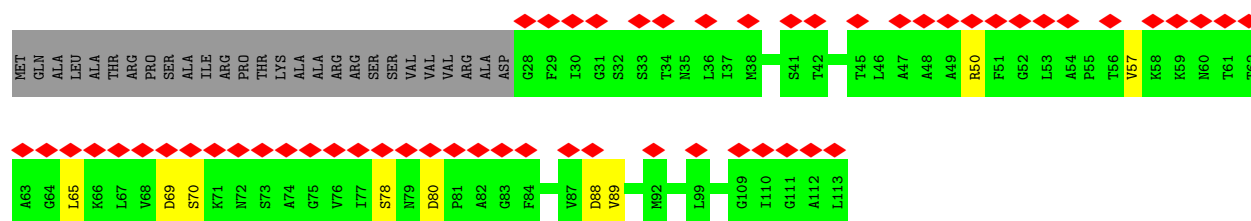
• Molecule 10: PSI subunit V



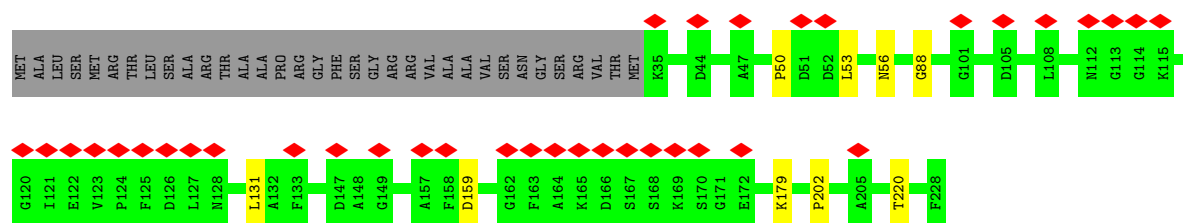
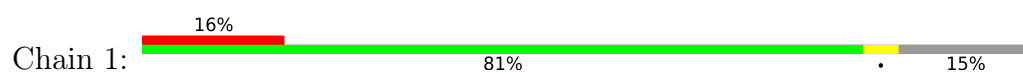
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



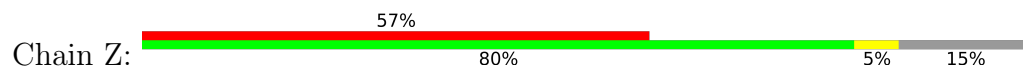
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



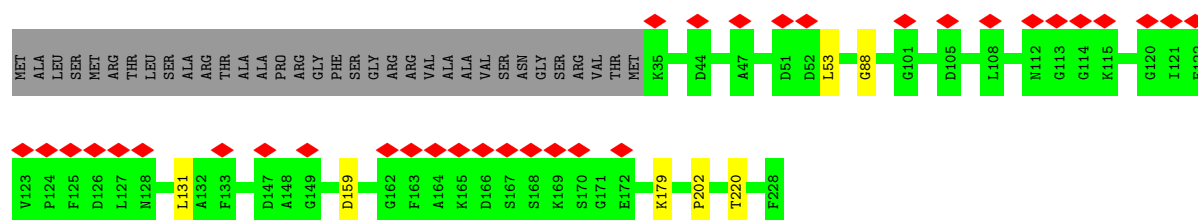
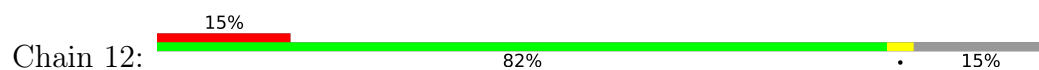
• Molecule 12: Chlorophyll a-b binding protein, chloroplastic



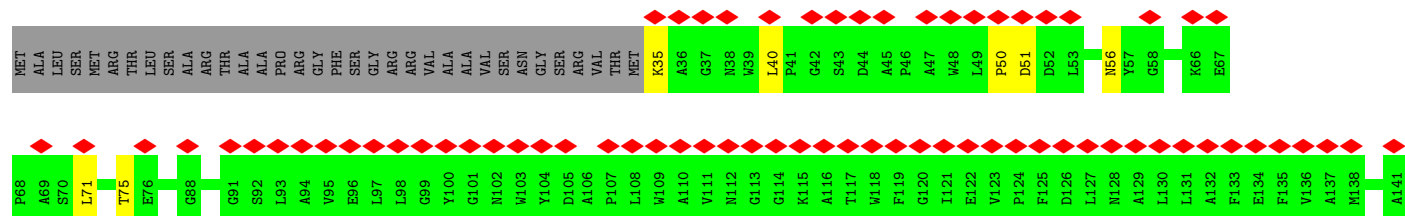
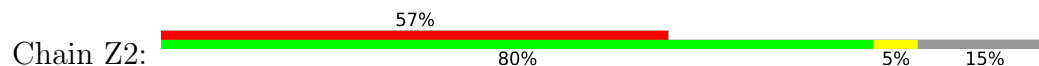
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

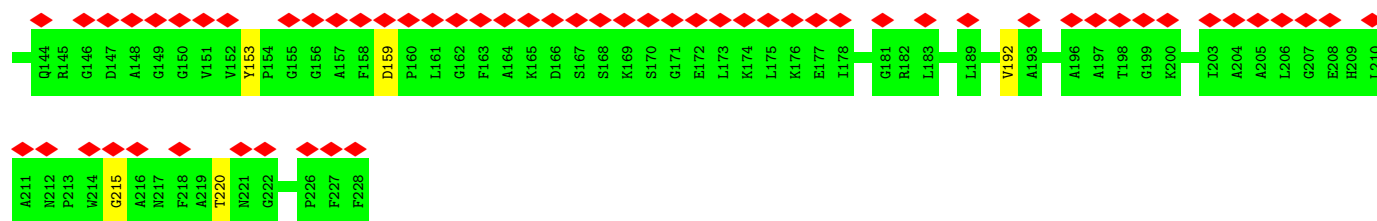


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

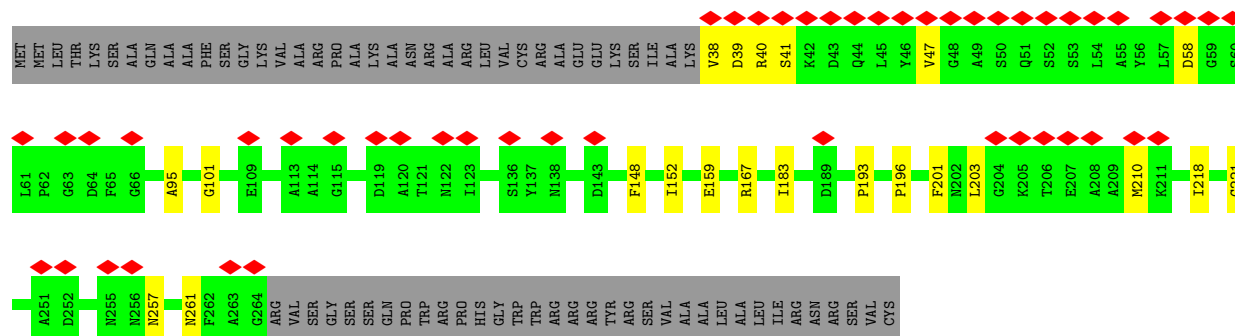


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

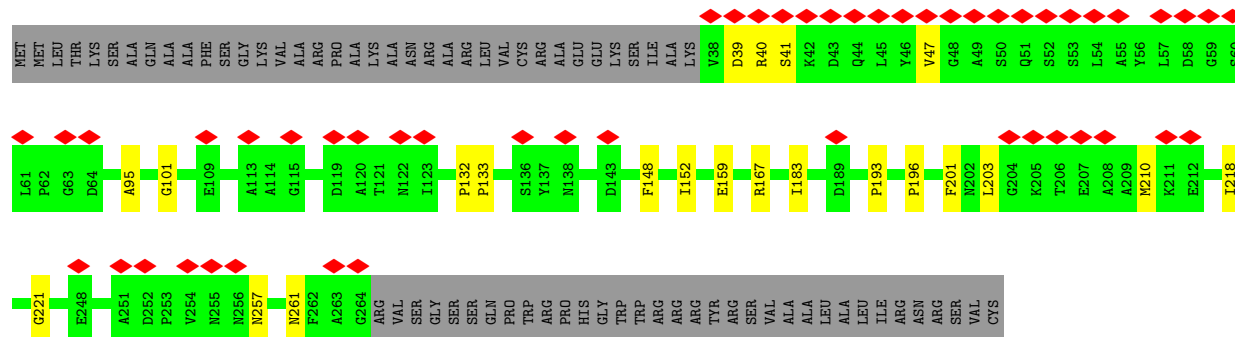




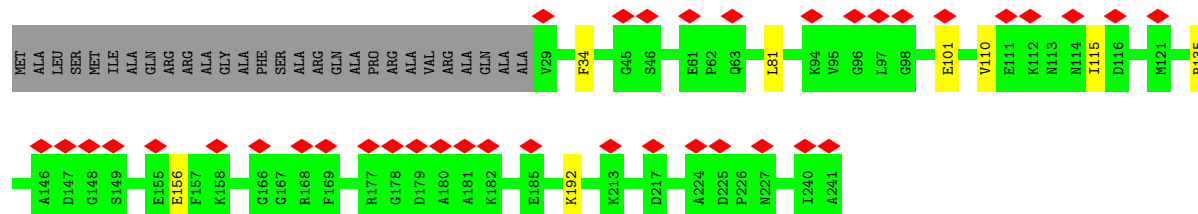
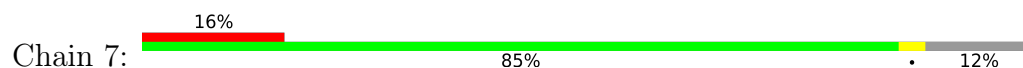
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



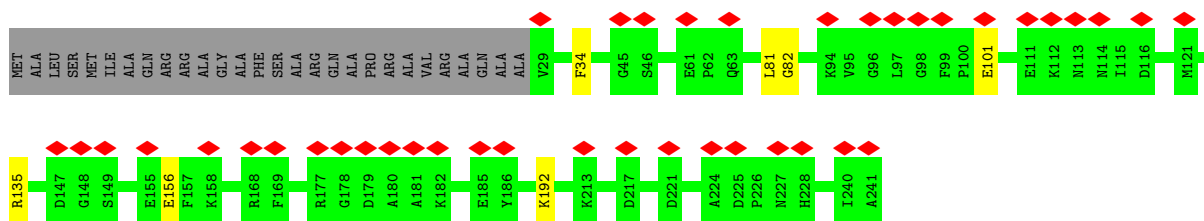
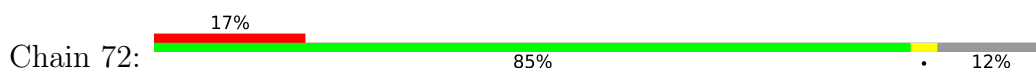
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



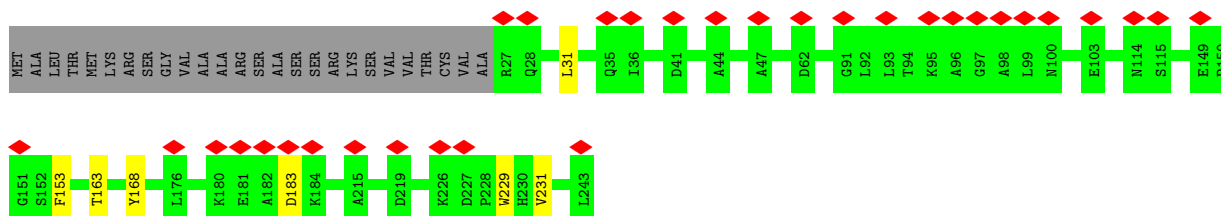
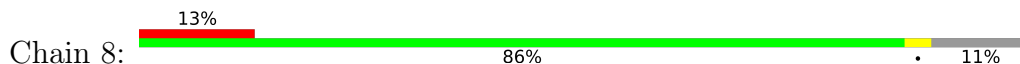
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



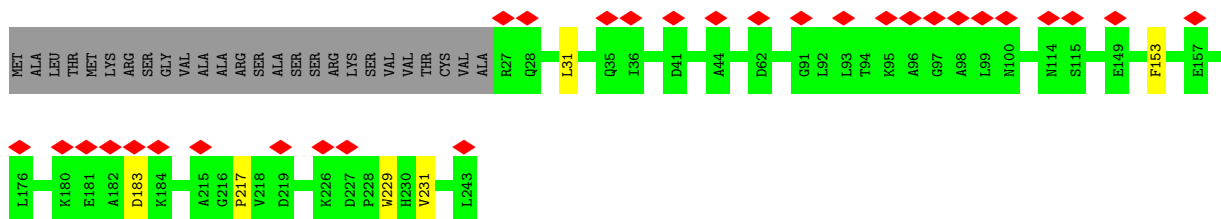
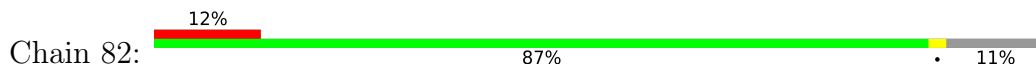
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



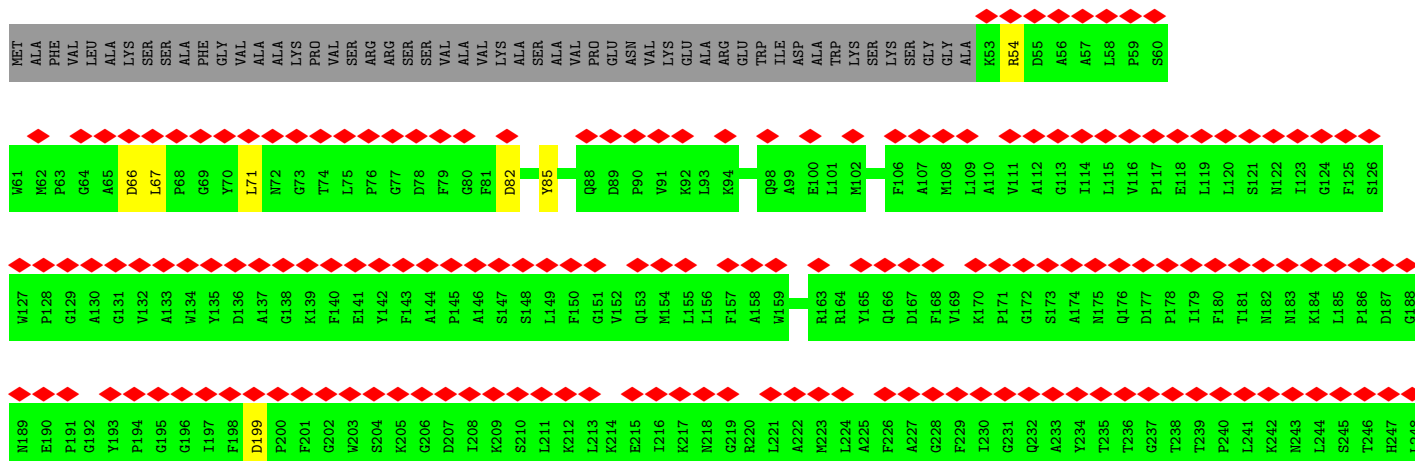
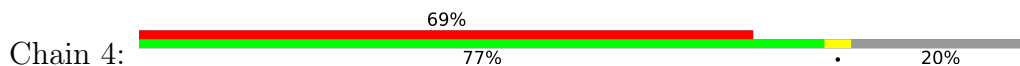
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic

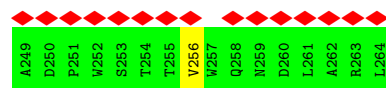


- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



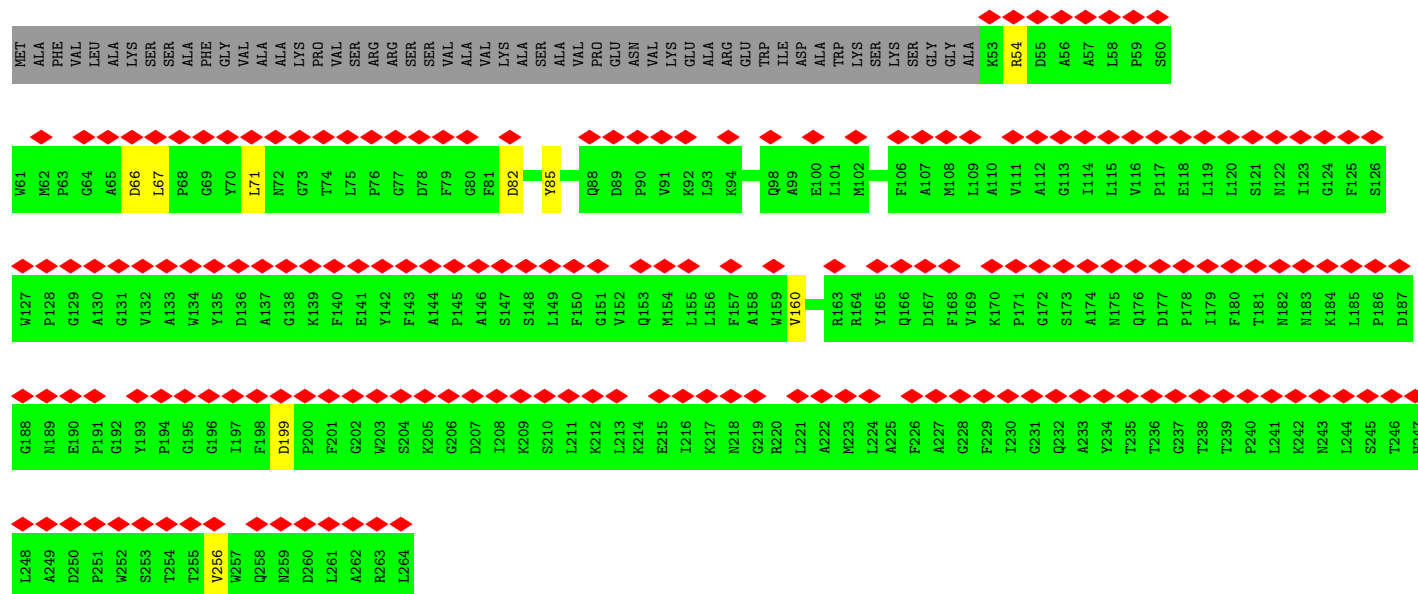
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)





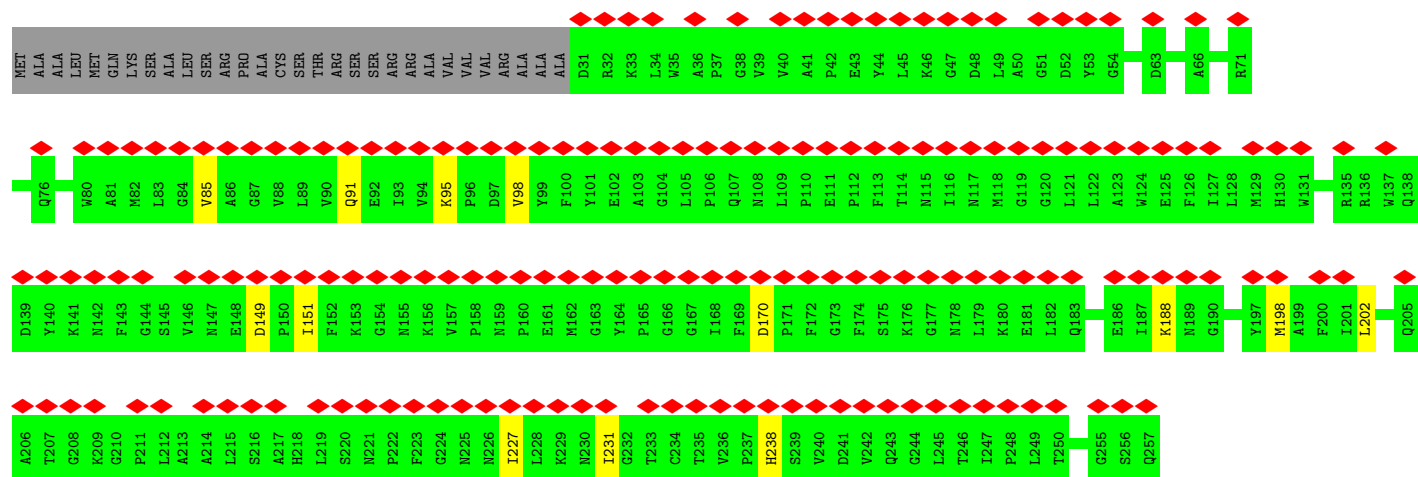
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)

Chain 42:



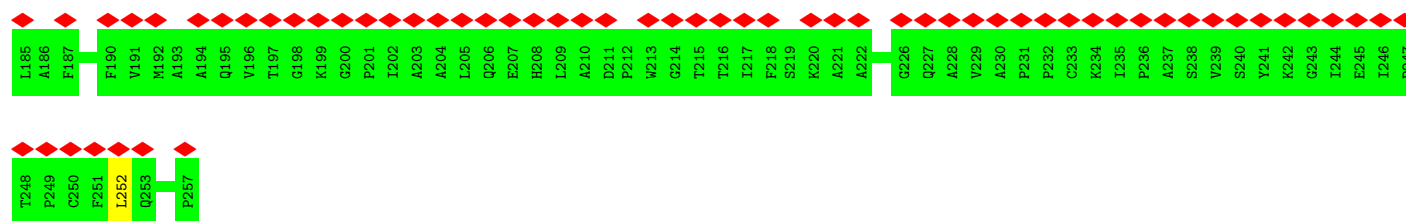
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

Chain 5:

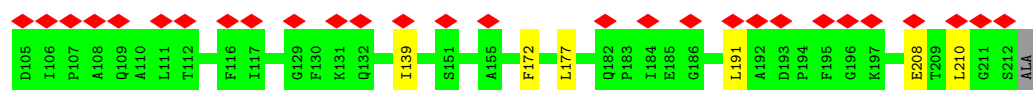
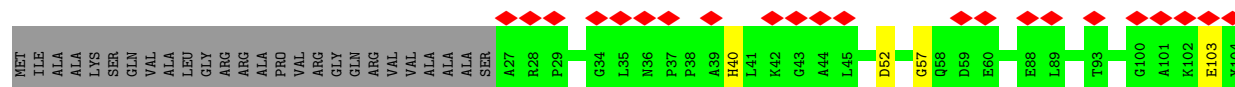
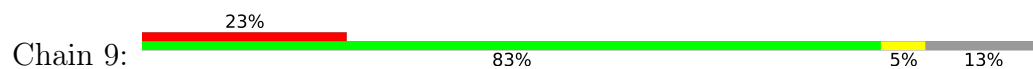


- Molecule 17: Chlorophyll a-b binding protein, chloroplastic

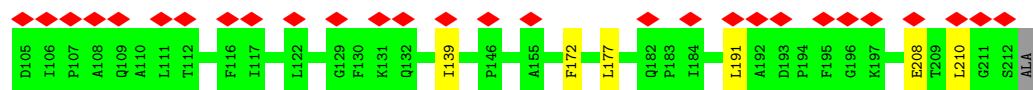
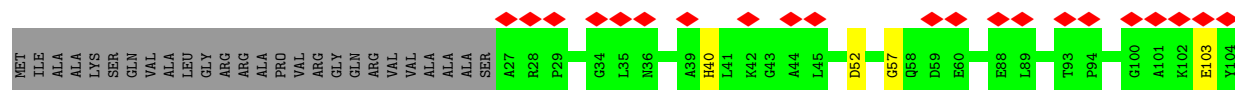
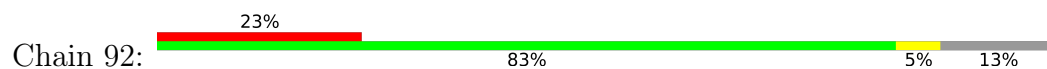
Chain 52:



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Chlorophyll a-b binding protein, chloroplastic



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17439	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.183	Depositor
Minimum map value	-0.090	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.036	Depositor
Map size ($\text{\AA}$)	588.0, 588.0, 588.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL0, CLA, SF4, LMU, DGD, PQN, NEX, LMG, AME, LUT, XAT, BCR, CHL, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.14	0/6021	0.22	0/8208
1	A2	0.15	0/6021	0.23	0/8208
2	B	0.15	0/6036	0.23	0/8240
2	B2	0.15	0/6036	0.22	0/8240
3	C	0.14	0/611	0.28	0/826
3	C2	0.14	0/611	0.27	0/826
4	D	0.13	0/1161	0.24	0/1567
4	D2	0.13	0/1161	0.24	0/1567
5	E	0.13	0/516	0.18	0/700
5	E2	0.13	0/516	0.18	0/700
6	F	0.13	0/1292	0.21	0/1747
6	F2	0.13	0/1292	0.21	0/1747
7	G	0.12	0/721	0.19	0/980
7	G2	0.12	0/721	0.19	0/980
8	I	0.13	0/293	0.26	0/406
8	I2	0.13	0/293	0.26	0/406
9	J	0.14	0/329	0.22	0/452
9	J2	0.14	0/329	0.22	0/452
10	L	0.12	0/920	0.19	0/1257
10	L2	0.12	0/920	0.19	0/1257
11	K	0.13	0/588	0.17	0/795
11	K2	0.13	0/588	0.17	0/795
12	1	0.12	0/1491	0.20	0/2028
12	12	0.12	0/1491	0.20	0/2028
12	Z	0.09	0/1491	0.18	0/2028
12	Z2	0.10	0/1491	0.18	0/2028
13	3	0.12	0/1784	0.23	0/2420
13	32	0.12	0/1784	0.23	0/2420
14	7	0.12	0/1702	0.20	0/2310
14	72	0.12	0/1702	0.20	0/2310
15	8	0.12	0/1701	0.21	0/2315
15	82	0.12	0/1701	0.20	0/2315

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	4	0.09	0/1703	0.19	0/2321
16	42	0.09	0/1703	0.19	0/2321
17	5	0.09	0/1830	0.21	0/2492
17	52	0.09	0/1830	0.21	0/2492
18	6	0.09	0/1834	0.20	0/2505
18	62	0.09	0/1834	0.20	0/2505
19	9	0.12	0/1461	0.20	0/1987
19	92	0.12	0/1461	0.21	0/1987
All	All	0.13	0/66970	0.21	0/91168

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	5675	5675	27	0
1	A2	5825	5675	5675	25	0
2	B	5824	5576	5577	35	0
2	B2	5824	5576	5577	38	0
3	C	601	582	581	4	0
3	C2	601	582	581	3	0
4	D	1133	1151	1150	4	0
4	D2	1133	1151	1150	2	0
5	E	506	505	504	1	0
5	E2	506	505	504	1	0
6	F	1266	1302	1301	10	0
6	F2	1266	1302	1301	9	0
7	G	706	687	686	4	0
7	G2	706	687	686	4	0
8	I	281	292	292	3	0
8	I2	281	292	292	3	0
9	J	329	328	328	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	J2	329	328	328	1	0
10	L	899	907	905	7	0
10	L2	899	907	905	8	0
11	K	583	620	620	6	0
11	K2	583	620	620	6	0
12	1	1445	1397	1396	8	0
12	12	1445	1397	1396	7	0
12	Z	1445	1397	1396	9	0
12	Z2	1445	1397	1396	9	0
13	3	1736	1695	1694	15	0
13	32	1736	1695	1694	15	0
14	7	1650	1590	1589	8	0
14	72	1650	1590	1589	8	0
15	8	1650	1630	1629	6	0
15	82	1650	1630	1629	6	0
16	4	1648	1603	1602	6	0
16	42	1648	1603	1602	7	0
17	5	1775	1747	1746	11	0
17	52	1775	1747	1746	11	0
18	6	1772	1770	1770	9	0
18	62	1772	1770	1770	9	0
19	9	1420	1400	1399	9	0
19	92	1420	1400	1399	9	0
20	A	65	72	72	0	0
20	A2	65	72	72	0	0
21	1	639	625	625	5	0
21	12	639	625	625	5	0
21	3	740	718	718	12	0
21	32	740	718	718	14	0
21	4	565	534	534	3	0
21	42	565	534	534	4	0
21	5	740	712	712	9	0
21	52	740	712	712	9	0
21	6	628	605	605	2	0
21	62	628	605	605	2	0
21	7	652	598	598	5	0
21	72	652	598	598	5	0
21	8	614	578	578	4	0
21	82	614	578	578	3	0
21	9	565	535	535	1	0
21	92	565	535	535	1	0
21	A	2718	2856	2856	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	A2	2718	2856	2856	26	0
21	B	2463	2580	2580	28	0
21	B2	2463	2580	2580	29	0
21	F	175	177	177	1	0
21	F2	175	177	177	1	0
21	G	106	92	92	0	0
21	G2	106	92	92	0	0
21	J	55	49	49	1	0
21	J2	55	49	49	1	0
21	K	196	158	158	2	0
21	K2	196	158	158	2	0
21	L	110	105	105	1	0
21	L2	110	105	105	0	0
21	Z	627	593	593	7	0
21	Z2	627	593	593	9	0
22	A	33	46	46	0	0
22	A2	33	46	46	0	0
22	B	33	46	46	0	0
22	B2	33	46	46	0	0
23	1	39	48	48	1	0
23	12	39	48	48	1	0
23	3	78	99	99	1	0
23	32	78	99	99	1	0
23	4	87	123	123	1	0
23	42	87	123	123	1	0
23	5	37	44	44	1	0
23	52	37	44	44	1	0
23	6	85	116	116	0	0
23	62	85	116	116	0	0
23	7	49	74	74	1	0
23	72	49	74	74	1	0
23	8	44	61	61	0	0
23	82	44	61	61	0	0
23	9	41	55	55	0	0
23	92	41	55	55	0	0
23	A	87	123	123	0	0
23	A2	87	123	123	0	0
23	B	45	63	63	0	0
23	B2	45	63	63	0	0
23	Z	39	48	48	0	0
23	Z2	39	48	48	1	0
24	3	120	168	168	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	32	120	168	168	4	0
24	4	40	56	56	0	0
24	42	40	56	56	1	0
24	5	40	56	56	0	0
24	52	40	56	56	0	0
24	6	40	56	56	2	0
24	62	40	56	56	1	0
24	7	40	56	56	0	0
24	72	40	56	56	0	0
24	8	40	56	56	2	0
24	82	40	56	56	2	0
24	9	40	56	56	1	0
24	92	40	56	56	2	0
24	A	200	280	280	12	0
24	A2	200	280	280	9	0
24	B	280	392	392	11	0
24	B2	280	392	392	11	0
24	G	40	56	56	0	0
24	G2	40	56	56	2	0
24	I	40	56	56	1	0
24	I2	40	56	56	1	0
24	J	40	56	56	1	0
24	J2	40	56	56	1	0
24	K	80	112	112	5	0
24	K2	80	112	112	6	0
24	L	80	112	112	5	0
24	L2	80	112	112	5	0
25	A	8	0	0	0	0
25	A2	8	0	0	0	0
25	C	16	0	0	0	0
25	C2	16	0	0	0	0
26	1	148	201	201	0	0
26	12	148	201	201	0	0
26	4	53	63	63	1	0
26	42	53	63	63	1	0
26	5	24	35	35	0	0
26	52	24	35	35	0	0
26	6	92	129	129	0	0
26	62	92	129	129	0	0
26	7	81	92	92	1	0
26	72	81	92	92	1	0
26	8	107	151	151	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
26	82	107	151	151	0	0
26	9	24	35	35	1	0
26	92	24	35	35	1	0
26	A	196	262	262	5	0
26	A2	196	262	262	2	0
26	B	35	46	46	3	0
26	B2	35	46	46	2	0
26	G	24	35	35	0	0
26	G2	24	35	35	0	0
26	K	24	35	35	0	0
26	K2	24	35	35	0	0
26	Z	53	63	63	1	0
26	Z2	53	63	63	1	0
27	1	78	96	96	0	0
27	12	78	96	96	0	0
27	3	45	75	75	1	0
27	32	45	75	75	1	0
27	4	41	55	55	0	0
27	42	41	55	55	0	0
27	6	20	35	35	0	0
27	62	20	35	35	0	0
27	7	37	44	44	0	0
27	72	37	44	44	0	0
27	8	74	91	91	1	0
27	82	74	91	91	0	0
27	9	44	61	61	1	0
27	92	44	61	61	1	0
27	A	84	111	111	1	0
27	A2	84	111	111	1	0
27	B	79	98	98	1	0
27	B2	79	98	98	1	0
27	J	77	97	97	2	0
27	J2	77	97	97	2	0
28	1	84	112	112	2	0
28	12	84	112	112	2	0
28	3	126	168	168	2	0
28	32	126	168	168	2	0
28	4	42	56	56	1	0
28	42	42	56	56	1	0
28	5	84	112	112	3	0
28	52	84	112	112	3	0
28	6	42	56	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
28	62	42	56	56	1	0
28	7	84	112	112	4	0
28	72	84	112	112	4	0
28	8	42	56	56	0	0
28	82	42	56	56	1	0
28	9	84	112	112	3	0
28	92	84	112	112	3	0
28	A	42	56	56	1	0
28	A2	42	56	56	2	0
28	F	42	56	56	3	0
28	F2	42	56	56	2	0
28	Z	68	89	89	2	0
28	Z2	68	89	89	2	0
29	B	59	79	79	1	0
29	B2	59	79	79	1	0
30	1	158	132	132	1	0
30	12	158	132	132	0	0
30	3	66	70	70	2	0
30	32	66	70	70	3	0
30	4	300	288	288	4	0
30	42	300	288	288	2	0
30	5	206	167	167	1	0
30	52	206	167	167	1	0
30	6	350	327	327	7	0
30	62	350	327	327	7	0
30	7	158	132	132	3	0
30	72	158	132	132	2	0
30	8	198	210	210	2	0
30	82	198	210	210	2	0
30	9	93	64	64	0	0
30	92	93	64	64	0	0
30	Z	178	171	171	1	0
30	Z2	178	171	171	1	0
31	1	44	56	56	1	0
31	12	44	56	56	1	0
31	4	44	56	56	0	0
31	42	44	56	56	0	0
31	5	44	56	56	0	0
31	52	44	56	56	0	0
31	6	44	56	56	1	0
31	62	44	56	56	1	0
31	7	44	56	56	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	72	44	56	56	1	0
31	8	44	56	56	0	0
31	82	44	56	56	0	0
31	Z	44	56	56	0	0
31	Z2	44	56	56	0	0
32	5	44	56	56	0	0
32	52	44	56	56	0	0
32	6	44	56	56	1	0
32	62	44	56	56	1	0
33	H	160	0	0	17	0
All	All	100830	101988	101960	579	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 3.

The worst 5 of 579 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)
28:7:624:LUT:H381	28:7:624:LUT:H28	1.51	0.93
28:72:624:LUT:H381	28:72:624:LUT:H28	1.51	0.91
1:A2:95:GLY:O	1:A2:99:SER:OG	1.95	0.83
17:5:170:ASP:OD1	28:5:620:LUT:O23	1.96	0.82
1:A:95:GLY:O	1:A:99:SER:OG	1.96	0.82

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	727 (98%)	13 (2%)	0	100	100
1	A2	740/751 (98%)	727 (98%)	13 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
2	B2	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
4	D2	142/196 (72%)	139 (98%)	3 (2%)	0	100	100
5	E	62/97 (64%)	62 (100%)	0	0	100	100
5	E2	62/97 (64%)	62 (100%)	0	0	100	100
6	F	163/227 (72%)	163 (100%)	0	0	100	100
6	F2	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
7	G2	93/126 (74%)	92 (99%)	1 (1%)	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	35 (100%)	0	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
9	J2	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
10	L2	120/196 (61%)	118 (98%)	2 (2%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
11	K2	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	12	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
12	Z2	192/228 (84%)	190 (99%)	2 (1%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
13	32	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
14	72	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
15	8	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
15	82	215/243 (88%)	212 (99%)	3 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
16	42	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
17	52	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
18	62	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	58
19	92	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	58
All	All	8336/9794 (85%)	8203 (98%)	131 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
19	9	139	ILE
19	92	139	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	599 (100%)	2 (0%)	86	91
1	A2	601/610 (98%)	598 (100%)	3 (0%)	81	89
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	91
2	B2	596/597 (100%)	593 (100%)	3 (0%)	81	89
3	C	69/70 (99%)	69 (100%)	0	100	100
3	C2	69/70 (99%)	69 (100%)	0	100	100
4	D	121/152 (80%)	120 (99%)	1 (1%)	73	86
4	D2	121/152 (80%)	120 (99%)	1 (1%)	73	86
5	E	55/81 (68%)	55 (100%)	0	100	100
5	E2	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	F2	127/169 (75%)	127 (100%)	0	100	100
7	G	71/94 (76%)	71 (100%)	0	100	100
7	G2	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	68
9	J2	35/35 (100%)	34 (97%)	1 (3%)	37	68
10	L	90/148 (61%)	89 (99%)	1 (1%)	65	82
10	L2	90/148 (61%)	89 (99%)	1 (1%)	65	82
11	K	59/80 (74%)	59 (100%)	0	100	100
11	K2	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	12	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
12	Z2	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	172 (99%)	2 (1%)	65	82
13	32	174/230 (76%)	173 (99%)	1 (1%)	78	88
14	7	164/181 (91%)	164 (100%)	0	100	100
14	72	164/181 (91%)	164 (100%)	0	100	100
15	8	163/183 (89%)	162 (99%)	1 (1%)	78	88
15	82	163/183 (89%)	162 (99%)	1 (1%)	78	88
16	4	166/205 (81%)	166 (100%)	0	100	100
16	42	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	181 (98%)	3 (2%)	55	78
17	52	184/206 (89%)	181 (98%)	3 (2%)	55	78
18	6	184/203 (91%)	184 (100%)	0	100	100
18	62	184/203 (91%)	184 (100%)	0	100	100
19	9	142/159 (89%)	142 (100%)	0	100	100
19	92	142/159 (89%)	142 (100%)	0	100	100
All	All	6612/7606 (87%)	6585 (100%)	27 (0%)	81	90

5 of 27 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A2	154	THR
2	B2	217	LEU
17	52	91	GLN
2	B2	17	PRO
2	B2	612	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
12	12	195	HIS
15	82	220	ASN
17	52	72	GLN
16	4	166	GLN
12	Z	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	$\# Z > 2$
9	AME	J2	1	9	9,10,11	0.54	0	9,11,13	0.88	1 (11%)
9	AME	J	1	9	9,10,11	0.54	0	9,11,13	0.87	1 (11%)

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
9	AME	J2	1	9	-	3/9/10/12	-
9	AME	J	1	9	-	3/9/10/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J2	1	AME	O-C-CA	-2.56	118.17	124.77
9	J	1	AME	O-C-CA	-2.55	118.20	124.77

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	1	AME	C-CA-CB-CG
9	J	1	AME	N-CA-CB-CG
9	J2	1	AME	C-CA-CB-CG
9	J2	1	AME	N-CA-CB-CG
9	J	1	AME	CB-CA-N-CT1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

706 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CL0	A2	801	-	58,73,73	1.48	6 (10%)	60,113,113	1.57	3 (5%)
21	CLA	9	603	19,27	59,63,73	1.26	5 (8%)	70,101,113	0.89	4 (5%)
24	BCR	L	201	-	41,41,41	0.17	0	56,56,56	0.35	0
21	CLA	B	802	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	B2	828	-	69,73,73	1.15	4 (5%)	82,113,113	0.80	3 (3%)
21	CLA	72	603	-	56,60,73	1.30	5 (8%)	65,97,113	0.93	3 (4%)
23	LHG	42	623	-	37,37,48	0.24	0	40,43,54	0.29	0
27	LMG	A	860	-	36,36,55	0.19	0	44,44,63	0.25	0
26	LMU	Z	621	-	22,22,36	0.14	0	27,27,47	0.26	0
30	CHL	72	601	14	60,74,74	1.95	10 (16%)	58,114,114	1.04	5 (8%)
21	CLA	Z	616	12	64,68,73	1.23	4 (6%)	76,107,113	0.86	3 (3%)
27	LMG	12	624	-	36,36,55	0.19	0	44,44,63	0.18	0
21	CLA	A	845	23	49,53,73	1.39	4 (8%)	58,89,113	0.95	2 (3%)
21	CLA	K2	204	-	50,54,73	1.37	4 (8%)	59,90,113	0.98	3 (5%)
30	CHL	6	606	33	52,66,74	2.10	10 (19%)	48,104,114	1.18	5 (10%)
21	CLA	1	613	33	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	B	823	-	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
28	LUT	F	305	-	42,43,43	0.38	0	51,60,60	0.89	2 (3%)
21	CLA	A2	809	1	69,73,73	1.17	5 (7%)	82,113,113	0.89	4 (4%)
21	CLA	A2	834	-	69,73,73	1.20	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	Z2	612	12	49,53,73	1.35	4 (8%)	58,89,113	0.95	2 (3%)
25	SF4	C2	102	3	0,12,12	-	-	-	-	-
21	CLA	A	831	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
26	LMU	72	629	-	28,28,36	0.10	0	39,39,47	0.28	0
21	CLA	B	821	-	69,73,73	1.20	5 (7%)	82,113,113	0.83	2 (2%)
30	CHL	82	601	15	60,74,74	1.93	10 (16%)	58,114,114	1.09	4 (6%)
23	LHG	A2	847	21	37,37,48	0.26	0	40,43,54	0.30	0
23	LHG	8	620	21	43,43,48	0.24	0	46,49,54	0.27	0
21	CLA	52	617	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
21	CLA	5	609	17	69,73,73	1.15	4 (5%)	82,113,113	0.82	3 (3%)
30	CHL	5	606	33	40,54,74	2.38	10 (25%)	34,90,114	1.41	5 (14%)
24	BCR	B	845	-	41,41,41	0.14	0	56,56,56	0.36	0
21	CLA	A	820	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	62	614	-	54,58,73	1.32	4 (7%)	64,95,113	0.94	3 (4%)
21	CLA	6	611	23	62,66,73	1.25	4 (6%)	73,104,113	0.87	3 (4%)
21	CLA	K2	201	11	49,53,73	1.41	4 (8%)	58,89,113	0.97	1 (1%)
24	BCR	3	620	-	41,41,41	0.19	0	56,56,56	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LMU	8	628	-	24,24,36	0.15	0	29,29,47	0.32	0
21	CLA	A	819	-	64,68,73	1.26	4 (6%)	76,107,113	0.87	2 (2%)
21	CLA	A2	811	-	69,73,73	1.15	5 (7%)	82,113,113	0.81	3 (3%)
26	LMU	A2	861	-	24,24,36	0.12	0	29,29,47	0.30	0
21	CLA	B2	834	-	64,68,73	1.23	4 (6%)	76,107,113	0.86	3 (3%)
30	CHL	5	618	17	37,51,74	2.45	10 (27%)	30,86,114	1.48	5 (16%)
24	BCR	A	849	-	41,41,41	0.16	0	56,56,56	0.31	0
21	CLA	B	841	23	69,73,73	1.18	4 (5%)	82,113,113	0.85	4 (4%)
31	XAT	72	622	-	41,47,47	0.13	0	54,74,74	0.59	0
21	CLA	82	613	15	69,73,73	1.17	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	B	809	2	69,73,73	1.19	4 (5%)	82,113,113	0.80	2 (2%)
24	BCR	B2	847	-	41,41,41	0.19	0	56,56,56	0.41	0
21	CLA	K	203	33	64,68,73	1.23	4 (6%)	76,107,113	0.86	2 (2%)
26	LMU	A2	858	-	36,36,36	0.08	0	47,47,47	0.19	0
30	CHL	42	608	-	60,74,74	1.96	10 (16%)	58,114,114	1.05	5 (8%)
21	CLA	6	613	33	69,73,73	1.17	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	A2	841	-	69,73,73	1.17	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	5	614	-	49,53,73	1.40	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	4	609	16	64,68,73	1.25	4 (6%)	76,107,113	0.87	2 (2%)
24	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.46	0
21	CLA	B	833	-	62,66,73	1.21	5 (8%)	73,104,113	0.89	3 (4%)
30	CHL	Z	601	12	60,74,74	1.93	10 (16%)	58,114,114	1.11	5 (8%)
24	BCR	B	843	-	41,41,41	0.16	0	56,56,56	0.31	0
28	LUT	52	626	-	42,43,43	0.24	0	51,60,60	0.40	0
28	LUT	7	624	-	42,43,43	0.22	0	51,60,60	0.44	0
26	LMU	K	208	-	24,24,36	0.11	0	29,29,47	0.30	0
21	CLA	1	612	12	49,53,73	1.39	4 (8%)	58,89,113	0.96	3 (5%)
21	CLA	32	602	13	64,68,73	1.22	4 (6%)	76,107,113	0.85	3 (3%)
25	SF4	A2	853	1,2	0,12,12	-	-	-	-	-
21	CLA	3	609	13	65,69,73	1.23	4 (6%)	77,108,113	0.84	2 (2%)
21	CLA	52	602	17	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	5	604	33	59,63,73	1.28	4 (6%)	70,101,113	0.88	3 (4%)
21	CLA	A2	816	-	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
23	LHG	B2	851	21	44,44,48	0.25	0	47,50,54	0.32	0
24	BCR	5	622	-	41,41,41	0.17	0	56,56,56	0.33	0
26	LMU	42	626	-	20,20,36	0.15	0	25,25,47	0.28	0
30	CHL	8	607	33	60,74,74	1.91	10 (16%)	58,114,114	1.10	5 (8%)
21	CLA	72	613	14	69,73,73	1.18	4 (5%)	82,113,113	0.84	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	5	623	21	36,36,48	0.25	0	39,42,54	0.28	0
22	PQN	B2	842	-	34,34,34	0.31	0	43,45,45	0.43	0
30	CHL	9	606	-	36,50,74	2.54	10 (27%)	29,85,114	1.40	4 (13%)
21	CLA	52	614	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
28	LUT	Z	617	-	42,43,43	0.26	0	51,60,60	0.44	0
21	CLA	B2	814	-	64,68,73	1.20	4 (6%)	76,107,113	0.86	3 (3%)
21	CLA	42	616	16	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
22	PQN	A	844	-	34,34,34	0.32	0	43,45,45	0.43	0
21	CLA	1	609	12	69,73,73	1.19	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	B	811	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	A2	813	-	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
26	LMU	72	628	-	22,22,36	0.14	0	27,27,47	0.33	0
21	CLA	B	837	-	69,73,73	1.19	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	8	612	15	59,63,73	1.24	4 (6%)	70,101,113	0.87	3 (4%)
21	CLA	4	616	16	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	4	612	16	49,53,73	1.39	4 (8%)	58,89,113	0.96	3 (5%)
24	BCR	9	623	-	41,41,41	0.14	0	56,56,56	0.34	0
21	CLA	4	604	33	54,58,73	1.32	4 (7%)	64,95,113	0.93	3 (4%)
28	LUT	32	622	-	42,43,43	0.32	0	51,60,60	0.47	0
26	LMU	Z2	622	-	32,32,36	0.10	0	43,43,47	0.18	0
21	CLA	B2	804	-	49,53,73	1.40	4 (8%)	58,89,113	0.94	2 (3%)
21	CLA	72	608	33	54,58,73	1.34	4 (7%)	64,95,113	0.91	3 (4%)
30	CHL	62	601	18	60,74,74	1.97	10 (16%)	58,114,114	0.99	4 (6%)
21	CLA	A	824	-	49,53,73	1.39	4 (8%)	58,89,113	0.99	3 (5%)
21	CLA	8	610	15	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	B2	832	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
23	LHG	A2	846	-	48,48,48	0.24	0	51,54,54	0.29	0
24	BCR	8	619	-	41,41,41	0.15	0	56,56,56	0.32	0
30	CHL	8	606	33	60,74,74	1.97	10 (16%)	58,114,114	1.09	5 (8%)
21	CLA	Z2	614	-	54,58,73	1.31	4 (7%)	64,95,113	0.93	3 (4%)
28	LUT	6	621	-	42,43,43	0.24	0	51,60,60	0.40	0
24	BCR	A	852	-	41,41,41	0.13	0	56,56,56	0.38	0
30	CHL	7	607	33	40,54,74	2.39	10 (25%)	34,90,114	1.43	5 (14%)
21	CLA	6	610	18	64,68,73	1.22	4 (6%)	76,107,113	0.85	3 (3%)
21	CLA	8	614	-	61,65,73	1.25	4 (6%)	72,103,113	0.85	2 (2%)
27	LMG	6	633	-	19,19,55	0.30	0	19,19,63	0.29	0
21	CLA	B2	824	33	69,73,73	1.20	4 (5%)	82,113,113	0.84	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	LHG	3	721	-	30,30,48	0.27	0	33,36,54	0.36	0
26	LMU	8	625	-	24,24,36	0.11	0	29,29,47	0.27	0
24	BCR	A2	852	-	41,41,41	0.13	0	56,56,56	0.37	0
21	CLA	8	608	33	54,58,73	1.35	4 (7%)	64,95,113	0.92	2 (3%)
21	CLA	F2	301	33	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
26	LMU	A2	863	-	36,36,36	0.09	0	47,47,47	0.27	0
21	CLA	A	805	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
26	LMU	6	632	-	20,20,36	0.15	0	25,25,47	0.26	0
27	LMG	8	626	-	32,32,55	0.19	0	40,40,63	0.19	0
27	LMG	4	624	-	41,41,55	0.18	0	49,49,63	0.26	0
21	CLA	Z	602	12	64,68,73	1.23	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	B2	823	-	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
21	CLA	5	611	23	59,63,73	1.27	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	72	609	14	49,53,73	1.42	4 (8%)	58,89,113	0.96	3 (5%)
21	CLA	82	602	15	66,70,73	1.23	5 (7%)	78,109,113	0.84	2 (2%)
30	CHL	62	608	33	45,59,74	2.27	10 (22%)	40,96,114	1.28	5 (12%)
23	LHG	12	620	21	38,38,48	0.25	0	41,44,54	0.30	0
21	CLA	8	611	23	49,53,73	1.40	5 (10%)	58,89,113	1.01	3 (5%)
21	CLA	L	204	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	3 (5%)
21	CLA	Z	609	12	69,73,73	1.20	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	A	822	33	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	B2	838	-	54,58,73	1.36	4 (7%)	64,95,113	0.91	2 (3%)
21	CLA	A	838	-	55,59,73	1.30	4 (7%)	64,96,113	0.93	2 (3%)
24	BCR	32	620	-	41,41,41	0.19	0	56,56,56	0.37	0
21	CLA	B	820	-	60,64,73	1.28	4 (6%)	71,102,113	0.87	2 (2%)
21	CLA	5	621	33	50,54,73	1.41	4 (8%)	59,90,113	1.07	5 (8%)
24	BCR	42	621	-	41,41,41	0.14	0	56,56,56	0.36	0
21	CLA	A	803	33	69,73,73	1.23	5 (7%)	82,113,113	0.83	4 (4%)
21	CLA	3	604	33	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	B2	825	33	69,73,73	1.17	5 (7%)	82,113,113	0.79	3 (3%)
21	CLA	82	604	33	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
27	LMG	J2	104	-	35,35,55	0.19	0	43,43,63	0.20	0
27	LMG	1	624	-	36,36,55	0.19	0	44,44,63	0.19	0
21	CLA	B	817	-	69,73,73	1.18	4 (5%)	82,113,113	0.83	3 (3%)
24	BCR	A	848	-	41,41,41	0.14	0	56,56,56	0.30	0
21	CLA	B2	809	2	69,73,73	1.20	4 (5%)	82,113,113	0.80	2 (2%)
26	LMU	7	628	-	22,22,36	0.14	0	27,27,47	0.33	0
23	LHG	62	619	21	48,48,48	0.22	0	51,54,54	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	BCR	K2	207	-	41,41,41	0.14	0	56,56,56	0.28	0
21	CLA	A	834	-	69,73,73	1.20	5 (7%)	82,113,113	0.84	3 (3%)
28	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.40	0
21	CLA	B2	833	-	62,66,73	1.21	5 (8%)	73,104,113	0.89	3 (4%)
21	CLA	7	608	33	54,58,73	1.33	4 (7%)	64,95,113	0.92	3 (4%)
30	CHL	72	607	33	40,54,74	2.39	10 (25%)	34,90,114	1.44	5 (14%)
29	DGD	B2	850	-	60,60,67	0.16	0	74,74,81	0.33	0
24	BCR	82	619	-	41,41,41	0.14	0	56,56,56	0.32	0
26	LMU	6	631	-	24,24,36	0.14	0	29,29,47	0.27	0
21	CLA	B	810	-	69,73,73	1.18	4 (5%)	82,113,113	0.83	3 (3%)
30	CHL	Z2	607	33	60,74,74	1.96	10 (16%)	58,114,114	1.09	6 (10%)
21	CLA	B	834	-	64,68,73	1.23	5 (7%)	76,107,113	0.86	3 (3%)
23	LHG	52	623	21	36,36,48	0.25	0	39,42,54	0.28	0
30	CHL	42	607	33	60,74,74	1.95	10 (16%)	58,114,114	1.03	4 (6%)
21	CLA	A2	804	-	69,73,73	1.17	5 (7%)	82,113,113	0.80	3 (3%)
21	CLA	Z2	611	23	64,68,73	1.20	4 (6%)	76,107,113	0.87	3 (3%)
24	BCR	32	719	-	41,41,41	0.11	0	56,56,56	0.41	0
21	CLA	F	304	6	69,73,73	1.17	4 (5%)	82,113,113	0.90	3 (3%)
26	LMU	A	863	-	36,36,36	0.09	0	47,47,47	0.27	0
21	CLA	B	818	-	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
26	LMU	Z	622	-	32,32,36	0.10	0	43,43,47	0.17	0
21	CLA	9	610	19	64,68,73	1.22	5 (7%)	76,107,113	0.88	3 (3%)
30	CHL	42	606	33	50,64,74	2.13	10 (20%)	46,102,114	1.26	6 (13%)
21	CLA	A	839	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	4 (4%)
21	CLA	B2	817	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	7	609	14	49,53,73	1.43	4 (8%)	58,89,113	0.95	3 (5%)
21	CLA	B	831	-	59,63,73	1.26	5 (8%)	70,101,113	0.88	3 (4%)
23	LHG	A	847	21	37,37,48	0.26	0	40,43,54	0.30	0
21	CLA	3	611	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
24	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.46	0
31	XAT	5	624	-	41,47,47	0.12	0	54,74,74	0.64	0
21	CLA	B	838	-	54,58,73	1.36	4 (7%)	64,95,113	0.91	2 (3%)
21	CLA	A	832	-	59,63,73	1.26	5 (8%)	70,101,113	0.90	3 (4%)
24	BCR	62	623	-	41,41,41	0.15	0	56,56,56	0.35	0
24	BCR	72	623	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	42	610	16	64,68,73	1.22	4 (6%)	76,107,113	0.83	3 (3%)
27	LMG	42	624	-	41,41,55	0.18	0	49,49,63	0.26	0
21	CLA	92	601	19	50,54,73	1.40	4 (8%)	59,90,113	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	LUT	12	619	-	42,43,43	0.21	0	51,60,60	0.42	0
30	CHL	4	606	33	50,64,74	2.13	10 (20%)	46,102,114	1.27	6 (13%)
26	LMU	9	624	-	24,24,36	0.14	0	29,29,47	0.37	0
21	CLA	F	301	33	69,73,73	1.15	4 (5%)	82,113,113	0.81	2 (2%)
26	LMU	Z2	621	-	22,22,36	0.14	0	27,27,47	0.27	0
27	LMG	8	629	-	42,42,55	0.18	0	50,50,63	0.15	0
30	CHL	4	607	33	60,74,74	1.95	10 (16%)	58,114,114	1.03	4 (6%)
26	LMU	1	623	-	24,24,36	0.13	0	29,29,47	0.27	0
21	CLA	52	610	17	64,68,73	1.21	4 (6%)	76,107,113	0.83	3 (3%)
21	CLA	B	812	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	B2	826	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
24	BCR	3	718	-	41,41,41	0.15	0	56,56,56	0.34	0
21	CLA	7	611	23	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
24	BCR	6	623	-	41,41,41	0.15	0	56,56,56	0.35	0
21	CLA	A2	835	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)
26	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0
21	CLA	A	840	-	69,73,73	1.19	4 (5%)	82,113,113	0.82	2 (2%)
28	LUT	1	617	-	42,43,43	0.26	0	51,60,60	0.42	0
26	LMU	52	627	-	24,24,36	0.12	0	29,29,47	0.26	0
21	CLA	6	602	18	69,73,73	1.18	4 (5%)	82,113,113	0.83	3 (3%)
21	CLA	1	614	-	64,68,73	1.22	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	12	612	12	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
21	CLA	3	602	13	64,68,73	1.23	5 (7%)	76,107,113	0.85	3 (3%)
30	CHL	62	606	33	52,66,74	2.10	10 (19%)	48,104,114	1.18	5 (10%)
24	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.39	0
21	CLA	6	604	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)
27	LMG	A2	860	-	36,36,55	0.19	0	44,44,63	0.26	0
21	CLA	B	816	-	69,73,73	1.16	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	72	620	33	57,61,73	1.29	4 (7%)	67,98,113	0.89	2 (2%)
21	CLA	G2	204	7	50,54,73	1.38	4 (8%)	59,90,113	0.96	3 (5%)
30	CHL	3	608	33	60,74,74	1.99	10 (16%)	58,114,114	1.10	5 (8%)
23	LHG	62	629	-	35,35,48	0.26	0	38,41,54	0.29	0
28	LUT	F2	305	-	42,43,43	0.37	0	51,60,60	0.89	2 (3%)
31	XAT	82	618	-	41,47,47	0.15	0	54,74,74	0.61	0
23	LHG	72	625	21	48,48,48	0.23	0	51,54,54	0.23	0
21	CLA	1	604	33	54,58,73	1.32	4 (7%)	64,95,113	0.94	3 (4%)
26	LMU	K2	208	-	24,24,36	0.10	0	29,29,47	0.30	0
30	CHL	6	608	33	45,59,74	2.25	10 (22%)	40,96,114	1.28	5 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	835	33	49,53,73	1.41	4 (8%)	58,89,113	0.97	2 (3%)
21	CLA	4	614	-	59,63,73	1.28	4 (6%)	70,101,113	0.88	3 (4%)
21	CLA	82	610	15	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
24	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
21	CLA	A	813	-	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
26	LMU	12	627	-	22,22,36	0.13	0	27,27,47	0.30	0
23	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.29	0
26	LMU	5	627	-	24,24,36	0.12	0	29,29,47	0.26	0
26	LMU	7	627	-	33,33,36	0.10	0	44,44,47	0.17	0
21	CLA	82	614	-	61,65,73	1.26	4 (6%)	72,103,113	0.86	2 (2%)
21	CLA	Z2	603	-	59,63,73	1.28	5 (8%)	70,101,113	0.87	2 (2%)
21	CLA	72	616	14	50,54,73	1.37	4 (8%)	59,90,113	0.95	3 (5%)
21	CLA	7	603	-	56,60,73	1.31	5 (8%)	65,97,113	0.93	3 (4%)
32	NEX	52	625	-	40,46,46	0.45	1 (2%)	50,70,70	0.80	3 (6%)
21	CLA	9	614	-	49,53,73	1.43	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	F2	304	6	69,73,73	1.17	4 (5%)	82,113,113	0.90	3 (3%)
27	LMG	82	626	-	32,32,55	0.20	0	40,40,63	0.19	0
21	CLA	9	609	19	55,59,73	1.31	4 (7%)	64,96,113	0.92	3 (4%)
21	CLA	A2	812	-	69,73,73	1.15	5 (7%)	82,113,113	0.80	4 (4%)
21	CLA	Z	612	12	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
25	SF4	C2	101	3	0,12,12	-	-	-	-	-
21	CLA	7	602	14	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	72	610	14	69,73,73	1.21	4 (5%)	82,113,113	0.86	3 (3%)
21	CLA	B	805	-	69,73,73	1.14	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	5	603	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	A	815	-	59,63,73	1.28	4 (6%)	70,101,113	0.87	2 (2%)
21	CLA	B2	806	2	69,73,73	1.19	5 (7%)	82,113,113	0.77	2 (2%)
21	CLA	12	603	-	61,65,73	1.25	4 (6%)	72,103,113	0.86	2 (2%)
28	LUT	Z2	619	-	26,26,43	0.38	0	33,35,60	0.37	0
23	LHG	32	721	-	30,30,48	0.26	0	33,36,54	0.36	0
25	SF4	C	102	3	0,12,12	-	-	-	-	-
21	CLA	Z	610	12	64,68,73	1.20	4 (6%)	76,107,113	0.84	3 (3%)
21	CLA	L2	204	-	49,53,73	1.40	4 (8%)	58,89,113	0.98	3 (5%)
21	CLA	62	609	18	59,63,73	1.26	4 (6%)	70,101,113	0.93	4 (5%)
24	BCR	L2	205	-	41,41,41	0.15	0	56,56,56	0.39	0
24	BCR	A2	850	-	41,41,41	0.15	0	56,56,56	0.24	0
32	NEX	62	625	-	40,46,46	0.28	0	50,70,70	0.88	3 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	32	604	33	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	82	603	-	69,73,73	1.20	5 (7%)	82,113,113	0.81	3 (3%)
21	CLA	B2	812	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	82	616	15	49,53,73	1.38	5 (10%)	58,89,113	0.99	3 (5%)
26	LMU	A	865	-	24,24,36	0.12	0	29,29,47	0.46	0
21	CLA	52	604	33	59,63,73	1.28	4 (6%)	70,101,113	0.89	3 (4%)
30	CHL	62	607	33	60,74,74	1.94	10 (16%)	58,114,114	1.12	6 (10%)
21	CLA	32	613	13	64,68,73	1.22	4 (6%)	76,107,113	0.86	3 (3%)
23	LHG	32	623	-	46,46,48	0.22	0	49,52,54	0.27	0
28	LUT	42	619	-	42,43,43	0.24	0	51,60,60	0.49	0
21	CLA	32	603	-	69,73,73	1.19	4 (5%)	82,113,113	0.81	2 (2%)
26	LMU	G2	206	-	24,24,36	0.13	0	29,29,47	0.24	0
21	CLA	A	808	-	54,58,73	1.33	5 (9%)	64,95,113	0.91	2 (3%)
21	CLA	B2	829	-	69,73,73	1.16	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	A	804	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	3 (3%)
21	CLA	7	620	33	57,61,73	1.29	4 (7%)	67,98,113	0.89	2 (2%)
21	CLA	62	604	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
21	CLA	9	604	19	57,61,73	1.27	5 (8%)	67,98,113	0.91	3 (4%)
21	CLA	B2	830	-	49,53,73	1.36	5 (10%)	58,89,113	0.99	3 (5%)
30	CHL	82	606	33	60,74,74	1.96	10 (16%)	58,114,114	1.08	5 (8%)
30	CHL	7	601	14	60,74,74	1.94	10 (16%)	58,114,114	1.05	5 (8%)
30	CHL	52	618	17	37,51,74	2.45	10 (27%)	30,86,114	1.48	5 (16%)
24	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.27	0
24	BCR	B2	801	-	41,41,41	0.16	0	56,56,56	0.38	0
21	CLA	32	609	13	65,69,73	1.22	4 (6%)	77,108,113	0.84	2 (2%)
28	LUT	9	616	-	42,43,43	0.26	0	51,60,60	0.39	0
26	LMU	A	858	-	36,36,36	0.08	0	47,47,47	0.19	0
21	CLA	62	611	23	62,66,73	1.24	4 (6%)	73,104,113	0.87	3 (4%)
21	CLA	A2	815	-	59,63,73	1.29	4 (6%)	70,101,113	0.86	2 (2%)
21	CLA	52	609	17	69,73,73	1.16	4 (5%)	82,113,113	0.82	3 (3%)
30	CHL	5	607	33	60,74,74	1.99	10 (16%)	58,114,114	0.98	4 (6%)
28	LUT	3	720	-	42,43,43	0.23	0	51,60,60	0.34	0
21	CLA	F2	303	33	49,53,73	1.38	4 (8%)	58,89,113	0.96	3 (5%)
21	CLA	Z2	616	12	64,68,73	1.23	4 (6%)	76,107,113	0.86	3 (3%)
21	CLA	A	826	33	69,73,73	1.20	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	A	842	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	8	603	-	69,73,73	1.19	4 (5%)	82,113,113	0.80	2 (2%)
21	CLA	62	613	33	69,73,73	1.16	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	42	602	16	64,68,73	1.23	4 (6%)	76,107,113	0.85	3 (3%)
31	XAT	8	618	-	41,47,47	0.16	0	54,74,74	0.60	0
28	LUT	62	621	-	42,43,43	0.23	0	51,60,60	0.40	0
21	CLA	B2	841	23	69,73,73	1.18	4 (5%)	82,113,113	0.84	4 (4%)
21	CLA	42	612	16	49,53,73	1.38	4 (8%)	58,89,113	0.95	2 (3%)
23	LHG	4	622	21	48,48,48	0.23	0	51,54,54	0.27	0
21	CLA	B2	822	-	63,67,73	1.22	4 (6%)	74,105,113	0.87	3 (4%)
30	CHL	Z2	606	33	40,54,74	2.35	10 (25%)	34,90,114	1.43	5 (14%)
21	CLA	32	614	-	49,53,73	1.40	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	B2	820	-	60,64,73	1.28	4 (6%)	71,102,113	0.87	2 (2%)
27	LMG	62	633	-	19,19,55	0.30	0	19,19,63	0.29	0
21	CLA	B2	819	33	64,68,73	1.24	5 (7%)	76,107,113	0.84	3 (3%)
26	LMU	12	623	-	24,24,36	0.13	0	29,29,47	0.27	0
21	CLA	Z	608	33	54,58,73	1.34	4 (7%)	64,95,113	0.95	3 (4%)
26	LMU	62	632	-	20,20,36	0.15	0	25,25,47	0.25	0
24	BCR	52	622	-	41,41,41	0.17	0	56,56,56	0.32	0
28	LUT	3	621	-	42,43,43	0.29	0	51,60,60	0.40	0
21	CLA	5	613	17	60,64,73	1.24	4 (6%)	71,102,113	0.88	3 (4%)
31	XAT	7	622	-	41,47,47	0.13	0	54,74,74	0.59	0
21	CLA	7	610	14	69,73,73	1.21	4 (5%)	82,113,113	0.86	3 (3%)
21	CLA	B2	836	-	64,68,73	1.21	4 (6%)	76,107,113	0.86	3 (3%)
26	LMU	1	626	-	24,24,36	0.11	0	29,29,47	0.27	0
21	CLA	B2	802	-	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	32	611	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	92	604	19	57,61,73	1.27	5 (8%)	67,98,113	0.91	3 (4%)
21	CLA	5	617	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
26	LMU	A2	862	-	20,20,36	0.12	0	25,25,47	0.28	0
21	CLA	A2	838	-	55,59,73	1.30	4 (7%)	64,96,113	0.93	2 (3%)
21	CLA	12	609	12	69,73,73	1.18	4 (5%)	82,113,113	0.83	3 (3%)
30	CHL	12	606	33	40,54,74	2.40	10 (25%)	34,90,114	1.38	5 (14%)
21	CLA	B2	803	-	69,73,73	1.20	4 (5%)	82,113,113	0.78	2 (2%)
21	CLA	52	601	17	69,73,73	1.16	4 (5%)	82,113,113	0.83	2 (2%)
30	CHL	52	606	33	40,54,74	2.39	10 (25%)	34,90,114	1.41	5 (14%)
21	CLA	K	201	11	49,53,73	1.41	4 (8%)	58,89,113	0.97	2 (3%)
30	CHL	7	606	33	40,54,74	2.38	10 (25%)	34,90,114	1.40	5 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	B	813	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	6	617	-	49,53,73	1.41	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	A2	840	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	3	617	13	50,54,73	1.38	4 (8%)	59,90,113	0.98	2 (3%)
21	CLA	B2	821	-	69,73,73	1.21	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	B2	805	-	69,73,73	1.14	5 (7%)	82,113,113	0.84	3 (3%)
24	BCR	A2	848	-	41,41,41	0.13	0	56,56,56	0.30	0
30	CHL	1	606	33	40,54,74	2.40	10 (25%)	34,90,114	1.39	5 (14%)
31	XAT	6	624	-	41,47,47	0.13	0	54,74,74	0.64	0
24	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.34	0
28	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.40	0
28	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.40	0
31	XAT	1	618	-	41,47,47	0.13	0	54,74,74	0.70	1 (1%)
21	CLA	7	613	14	69,73,73	1.18	4 (5%)	82,113,113	0.84	2 (2%)
28	LUT	72	621	-	42,43,43	0.25	0	51,60,60	0.39	0
21	CLA	A2	825	-	59,63,73	1.28	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	62	603	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
21	CLA	32	617	13	50,54,73	1.38	4 (8%)	59,90,113	0.98	2 (3%)
21	CLA	12	614	-	64,68,73	1.22	4 (6%)	76,107,113	0.88	3 (3%)
21	CLA	A2	808	-	54,58,73	1.33	4 (7%)	64,95,113	0.91	2 (3%)
21	CLA	B2	827	-	69,73,73	1.19	4 (5%)	82,113,113	0.83	2 (2%)
21	CLA	A2	805	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
21	CLA	A2	826	33	69,73,73	1.20	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	B	839	33	69,73,73	1.18	4 (5%)	82,113,113	0.85	3 (3%)
26	LMU	1	621	-	36,36,36	0.09	0	47,47,47	0.29	0
21	CLA	8	604	33	64,68,73	1.23	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	A2	824	-	49,53,73	1.39	5 (10%)	58,89,113	0.99	3 (5%)
28	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.42	0
21	CLA	3	603	-	69,73,73	1.19	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	12	613	33	69,73,73	1.17	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	A	830	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
27	LMG	A2	859	-	48,48,55	0.18	0	56,56,63	0.17	0
21	CLA	B	807	-	59,63,73	1.29	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	92	614	-	49,53,73	1.43	4 (8%)	58,89,113	0.97	3 (5%)
30	CHL	1	601	12	60,74,74	1.94	10 (16%)	58,114,114	1.05	4 (6%)
21	CLA	Z2	609	12	69,73,73	1.20	4 (5%)	82,113,113	0.82	2 (2%)
24	BCR	K2	202	-	41,41,41	0.15	0	56,56,56	0.37	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LMG	92	620	21	44,44,55	0.17	0	52,52,63	0.36	0
21	CLA	B2	835	33	49,53,73	1.40	5 (10%)	58,89,113	0.97	3 (5%)
21	CLA	52	603	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	52	612	17	49,53,73	1.37	4 (8%)	58,89,113	0.96	2 (3%)
26	LMU	62	631	-	24,24,36	0.14	0	29,29,47	0.28	0
24	BCR	B	847	-	41,41,41	0.19	0	56,56,56	0.41	0
27	LMG	B	852	-	43,43,55	0.17	0	51,51,63	0.23	0
21	CLA	9	601	19	50,54,73	1.39	4 (8%)	59,90,113	0.98	3 (5%)
21	CLA	K	206	11	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
26	LMU	62	630	-	24,24,36	0.14	0	29,29,47	0.28	0
21	CLA	Z	611	23	64,68,73	1.20	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	5	610	17	64,68,73	1.21	4 (6%)	76,107,113	0.84	3 (3%)
21	CLA	92	611	23	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
21	CLA	82	612	15	59,63,73	1.25	4 (6%)	70,101,113	0.87	2 (2%)
31	XAT	42	620	-	41,47,47	0.12	0	54,74,74	0.68	0
21	CLA	A	825	-	59,63,73	1.28	5 (8%)	70,101,113	0.89	3 (4%)
24	BCR	B2	846	-	41,41,41	0.13	0	56,56,56	0.35	0
21	CLA	A	829	-	69,73,73	1.23	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	9	612	19	69,73,73	1.15	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	32	607	13	59,63,73	1.27	4 (6%)	70,101,113	0.89	3 (4%)
24	BCR	7	623	-	41,41,41	0.15	0	56,56,56	0.38	0
21	CLA	12	608	33	69,73,73	1.19	4 (5%)	82,113,113	0.83	3 (3%)
21	CLA	4	603	16	69,73,73	1.18	5 (7%)	82,113,113	0.80	2 (2%)
21	CLA	A	814	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)
28	LUT	32	621	-	42,43,43	0.28	0	51,60,60	0.40	0
21	CLA	3	615	33	69,73,73	1.20	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	Z2	608	33	54,58,73	1.34	4 (7%)	64,95,113	0.94	3 (4%)
23	LHG	82	620	21	43,43,48	0.24	0	46,49,54	0.27	0
31	XAT	52	624	-	41,47,47	0.11	0	54,74,74	0.64	0
21	CLA	B2	811	-	69,73,73	1.17	4 (5%)	82,113,113	0.83	2 (2%)
21	CLA	A2	820	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	A2	836	-	69,73,73	1.20	5 (7%)	82,113,113	0.82	2 (2%)
21	CLA	A2	837	1	61,65,73	1.31	4 (6%)	72,103,113	0.91	3 (4%)
23	LHG	B	851	21	44,44,48	0.25	0	47,50,54	0.32	0
21	CLA	5	616	17	57,61,73	1.29	4 (7%)	67,98,113	0.91	2 (2%)
21	CLA	72	602	14	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	7	604	33	55,59,73	1.30	4 (7%)	64,96,113	0.93	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	4	602	16	64,68,73	1.23	4 (6%)	76,107,113	0.85	3 (3%)
21	CLA	Z	614	-	54,58,73	1.31	4 (7%)	64,95,113	0.93	3 (4%)
21	CLA	Z2	604	33	61,65,73	1.24	4 (6%)	72,103,113	0.87	3 (4%)
30	CHL	6	616	18	60,74,74	1.95	10 (16%)	58,114,114	1.09	6 (10%)
21	CLA	42	604	33	54,58,73	1.32	4 (7%)	64,95,113	0.94	3 (4%)
30	CHL	5	608	33	45,59,74	2.26	10 (22%)	40,96,114	1.33	5 (12%)
21	CLA	A2	823	-	69,73,73	1.19	5 (7%)	82,113,113	0.81	3 (3%)
27	LMG	12	628	-	42,42,55	0.18	0	50,50,63	0.28	0
21	CLA	42	613	16	69,73,73	1.17	4 (5%)	82,113,113	0.83	2 (2%)
26	LMU	82	625	-	24,24,36	0.11	0	29,29,47	0.28	0
21	CLA	F	303	33	49,53,73	1.38	4 (8%)	58,89,113	0.97	3 (5%)
23	LHG	9	622	21	40,40,48	0.24	0	43,46,54	0.29	0
26	LMU	82	624	-	24,24,36	0.14	0	29,29,47	0.26	0
24	BCR	92	623	-	41,41,41	0.15	0	56,56,56	0.35	0
21	CLA	12	611	23	65,69,73	1.21	4 (6%)	77,108,113	0.83	3 (3%)
31	XAT	4	620	-	41,47,47	0.11	0	54,74,74	0.68	0
27	LMG	7	626	-	37,37,55	0.19	0	45,45,63	0.27	0
21	CLA	B	808	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	3	613	13	64,68,73	1.22	4 (6%)	76,107,113	0.86	3 (3%)
21	CLA	12	610	12	69,73,73	1.17	5 (7%)	82,113,113	0.81	3 (3%)
21	CLA	B	815	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	A2	827	33	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	K2	206	11	49,53,73	1.40	4 (8%)	58,89,113	0.98	3 (5%)
21	CLA	B	832	-	69,73,73	1.14	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	A	854	33	69,73,73	1.24	5 (7%)	82,113,113	0.79	2 (2%)
21	CLA	A2	839	-	69,73,73	1.18	5 (7%)	82,113,113	0.84	4 (4%)
23	LHG	Z	620	21	38,38,48	0.25	0	41,44,54	0.29	0
21	CLA	A2	806	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
24	BCR	J2	102	-	41,41,41	0.16	0	56,56,56	0.30	0
30	CHL	52	608	33	45,59,74	2.27	10 (22%)	40,96,114	1.33	5 (12%)
21	CLA	A2	819	-	64,68,73	1.25	4 (6%)	76,107,113	0.86	2 (2%)
21	CLA	8	616	15	49,53,73	1.38	5 (10%)	58,89,113	0.99	3 (5%)
24	BCR	A2	849	-	41,41,41	0.17	0	56,56,56	0.31	0
24	BCR	A2	851	-	41,41,41	0.13	0	56,56,56	0.34	0
21	CLA	J	101	9	59,63,73	1.28	4 (6%)	70,101,113	0.88	2 (2%)
26	LMU	42	625	-	34,34,36	0.10	0	45,45,47	0.20	0
23	LHG	42	622	21	48,48,48	0.23	0	51,54,54	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	12	607	33	40,54,74	2.41	10 (25%)	34,90,114	1.27	4 (11%)
21	CLA	1	608	33	69,73,73	1.19	5 (7%)	82,113,113	0.83	2 (2%)
21	CLA	4	613	16	69,73,73	1.18	4 (5%)	82,113,113	0.84	2 (2%)
26	LMU	G	206	-	24,24,36	0.13	0	29,29,47	0.25	0
21	CLA	A2	828	-	69,73,73	1.18	4 (5%)	82,113,113	0.78	2 (2%)
21	CLA	B2	831	-	59,63,73	1.26	5 (8%)	70,101,113	0.88	3 (4%)
21	CLA	8	602	15	66,70,73	1.23	5 (7%)	78,109,113	0.84	2 (2%)
21	CLA	A2	832	-	59,63,73	1.26	5 (8%)	70,101,113	0.90	2 (2%)
26	LMU	4	625	-	34,34,36	0.11	0	45,45,47	0.20	0
28	LUT	5	626	-	42,43,43	0.25	0	51,60,60	0.40	0
26	LMU	A	857	-	35,35,36	0.09	0	46,46,47	0.18	0
21	CLA	92	609	19	55,59,73	1.32	5 (9%)	64,96,113	0.93	3 (4%)
30	CHL	92	606	-	36,50,74	2.53	10 (27%)	29,85,114	1.39	4 (13%)
27	LMG	3	722	-	44,44,55	0.20	0	46,46,63	0.25	0
27	LMG	J2	103	-	42,42,55	0.17	0	50,50,63	0.39	0
21	CLA	42	611	23	64,68,73	1.22	4 (6%)	76,107,113	0.85	3 (3%)
26	LMU	12	626	-	24,24,36	0.11	0	29,29,47	0.27	0
21	CLA	B	814	-	64,68,73	1.21	4 (6%)	76,107,113	0.85	3 (3%)
30	CHL	92	607	33	45,59,74	2.20	10 (22%)	40,96,114	1.24	7 (17%)
21	CLA	A	817	33	59,63,73	1.30	4 (6%)	70,101,113	0.88	2 (2%)
21	CLA	A	835	-	69,73,73	1.17	4 (5%)	82,113,113	0.83	3 (3%)
25	SF4	A	853	1,2	0,12,12	-	-	-	-	-
27	LMG	J	103	-	42,42,55	0.17	0	50,50,63	0.38	0
21	CLA	A	833	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	3 (3%)
26	LMU	6	628	-	24,24,36	0.12	0	29,29,47	0.29	0
21	CLA	A2	818	-	69,73,73	1.15	4 (5%)	82,113,113	0.82	3 (3%)
30	CHL	1	607	33	40,54,74	2.42	10 (25%)	34,90,114	1.28	4 (11%)
21	CLA	B	804	-	49,53,73	1.40	4 (8%)	58,89,113	0.94	2 (3%)
27	LMG	B2	854	-	36,36,55	0.20	0	44,44,63	0.17	0
21	CLA	72	612	14	56,60,73	1.28	4 (7%)	65,97,113	0.89	2 (3%)
21	CLA	6	614	-	54,58,73	1.32	4 (7%)	64,95,113	0.93	3 (4%)
32	NEX	6	625	-	40,46,46	0.20	0	50,70,70	0.84	3 (6%)
28	LUT	A	856	-	42,43,43	0.27	0	51,60,60	0.41	0
24	BCR	32	718	-	41,41,41	0.16	0	56,56,56	0.34	0
21	CLA	B	803	-	69,73,73	1.20	4 (5%)	82,113,113	0.78	2 (2%)
21	CLA	A	828	-	69,73,73	1.18	4 (5%)	82,113,113	0.78	2 (2%)
21	CLA	62	602	18	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	830	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
24	BCR	G	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	92	613	19	69,73,73	1.16	4 (5%)	82,113,113	0.85	4 (4%)
21	CLA	A2	803	33	69,73,73	1.23	5 (7%)	82,113,113	0.83	4 (4%)
31	XAT	Z	618	-	41,47,47	0.14	0	54,74,74	0.61	0
26	LMU	1	622	-	19,19,36	0.13	0	24,24,47	0.31	0
21	CLA	B	824	33	69,73,73	1.21	4 (5%)	82,113,113	0.83	2 (2%)
26	LMU	12	621	-	36,36,36	0.09	0	47,47,47	0.29	0
21	CLA	B2	818	-	69,73,73	1.18	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	A2	810	1	69,73,73	1.20	4 (5%)	82,113,113	0.85	2 (2%)
30	CHL	8	601	15	60,74,74	1.93	10 (16%)	58,114,114	1.09	4 (6%)
26	LMU	72	627	-	33,33,36	0.10	0	44,44,47	0.17	0
21	CLA	6	622	33	59,63,73	1.29	4 (6%)	70,101,113	0.87	2 (2%)
30	CHL	82	607	33	60,74,74	1.92	10 (16%)	58,114,114	1.11	5 (8%)
23	LHG	4	623	-	37,37,48	0.24	0	40,43,54	0.29	0
26	LMU	8	627	-	36,36,36	0.10	0	47,47,47	0.37	0
21	CLA	5	602	17	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
30	CHL	42	618	16	40,54,74	2.36	10 (25%)	34,90,114	1.37	5 (14%)
26	LMU	A	864	-	24,24,36	0.11	0	29,29,47	0.28	0
21	CLA	32	606	33	46,50,73	1.46	4 (8%)	53,85,113	1.00	2 (3%)
30	CHL	6	607	33	60,74,74	1.95	10 (16%)	58,114,114	1.11	6 (10%)
21	CLA	A	827	33	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
30	CHL	9	607	33	45,59,74	2.25	10 (22%)	40,96,114	1.20	6 (15%)
24	BCR	G2	205	-	41,41,41	0.14	0	56,56,56	0.32	0
21	CLA	5	612	17	49,53,73	1.38	4 (8%)	58,89,113	0.96	2 (3%)
24	BCR	L2	201	-	41,41,41	0.17	0	56,56,56	0.35	0
21	CLA	A2	829	-	69,73,73	1.23	4 (5%)	82,113,113	0.83	3 (3%)
28	LUT	Z	619	-	26,26,43	0.38	0	33,35,60	0.37	0
21	CLA	B	840	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
30	CHL	Z	606	33	40,54,74	2.34	10 (25%)	34,90,114	1.43	5 (14%)
30	CHL	4	618	16	40,54,74	2.36	10 (25%)	34,90,114	1.37	5 (14%)
26	LMU	1	625	-	24,24,36	0.10	0	29,29,47	0.30	0
21	CLA	K2	203	33	64,68,73	1.23	4 (6%)	76,107,113	0.86	2 (2%)
21	CLA	B2	810	-	69,73,73	1.17	4 (5%)	82,113,113	0.83	3 (3%)
24	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.47	0
23	LHG	7	625	21	48,48,48	0.23	0	51,54,54	0.23	0
21	CLA	B	825	33	69,73,73	1.16	5 (7%)	82,113,113	0.80	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	52	613	17	60,64,73	1.24	4 (6%)	71,102,113	0.88	3 (4%)
21	CLA	A	841	-	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
24	BCR	I2	172	-	41,41,41	0.19	0	56,56,56	0.37	0
24	BCR	B2	848	-	41,41,41	0.13	0	56,56,56	0.47	0
21	CLA	1	611	23	65,69,73	1.21	4 (6%)	77,108,113	0.83	3 (3%)
21	CLA	A	836	-	69,73,73	1.20	5 (7%)	82,113,113	0.82	2 (2%)
21	CLA	A2	842	-	69,73,73	1.15	5 (7%)	82,113,113	0.84	2 (2%)
27	LMG	B2	852	-	43,43,55	0.17	0	51,51,63	0.23	0
21	CLA	3	607	13	59,63,73	1.27	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	9	613	19	69,73,73	1.16	4 (5%)	82,113,113	0.85	3 (3%)
24	BCR	J	102	-	41,41,41	0.14	0	56,56,56	0.31	0
21	CLA	A2	814	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
21	CLA	9	611	23	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
30	CHL	12	601	12	60,74,74	1.94	10 (16%)	58,114,114	1.05	4 (6%)
21	CLA	92	603	19,27	59,63,73	1.26	5 (8%)	70,101,113	0.90	4 (5%)
21	CLA	92	612	19	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
21	CLA	A	823	-	69,73,73	1.19	5 (7%)	82,113,113	0.81	3 (3%)
28	LUT	52	620	-	42,43,43	0.24	0	51,60,60	0.48	0
29	DGD	B	850	-	60,60,67	0.17	0	74,74,81	0.50	0
21	CLA	A	811	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	3 (3%)
30	CHL	Z2	601	12	60,74,74	1.93	10 (16%)	58,114,114	1.10	5 (8%)
30	CHL	42	601	16	60,74,74	1.95	10 (16%)	58,114,114	1.11	5 (8%)
21	CLA	A	821	-	59,63,73	1.27	5 (8%)	70,101,113	0.86	2 (2%)
21	CLA	B	826	-	69,73,73	1.16	4 (5%)	82,113,113	0.82	3 (3%)
28	LUT	7	621	-	42,43,43	0.25	0	51,60,60	0.39	0
21	CLA	92	610	19	64,68,73	1.22	5 (7%)	76,107,113	0.89	3 (3%)
26	LMU	6	630	-	24,24,36	0.14	0	29,29,47	0.28	0
28	LUT	72	624	-	42,43,43	0.22	0	51,60,60	0.44	0
21	CLA	4	611	23	64,68,73	1.22	4 (6%)	76,107,113	0.85	3 (3%)
21	CLA	G	203	-	64,68,73	1.22	4 (6%)	76,107,113	0.81	2 (2%)
21	CLA	5	601	17	69,73,73	1.16	4 (5%)	82,113,113	0.83	2 (2%)
21	CLA	Z2	610	12	64,68,73	1.21	4 (6%)	76,107,113	0.84	3 (3%)
21	CLA	B2	816	-	69,73,73	1.15	4 (5%)	82,113,113	0.84	3 (3%)
21	CLA	62	617	-	49,53,73	1.40	4 (8%)	58,89,113	0.96	3 (5%)
27	LMG	32	722	-	44,44,55	0.21	0	46,46,63	0.25	0
21	CLA	12	604	33	54,58,73	1.33	4 (7%)	64,95,113	0.94	3 (4%)
21	CLA	B2	815	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	1	610	12	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	B	822	-	63,67,73	1.21	4 (6%)	74,105,113	0.87	3 (4%)
21	CLA	7	614	-	47,51,73	1.44	4 (8%)	55,86,113	1.01	3 (5%)
31	XAT	12	618	-	41,47,47	0.13	0	54,74,74	0.71	2 (3%)
21	CLA	B2	839	33	69,73,73	1.18	4 (5%)	82,113,113	0.85	3 (3%)
28	LUT	Z2	617	-	42,43,43	0.26	0	51,60,60	0.44	0
26	LMU	A	862	-	20,20,36	0.13	0	25,25,47	0.28	0
28	LUT	82	617	-	42,43,43	0.28	0	51,60,60	0.45	0
26	LMU	92	624	-	24,24,36	0.14	0	29,29,47	0.36	0
24	BCR	A	851	-	41,41,41	0.13	0	56,56,56	0.34	0
24	BCR	K	202	-	41,41,41	0.15	0	56,56,56	0.37	0
21	CLA	1	616	12	50,54,73	1.39	4 (8%)	59,90,113	0.98	3 (5%)
27	LMG	J	104	-	35,35,55	0.19	0	43,43,63	0.20	0
21	CLA	6	609	18	59,63,73	1.26	4 (6%)	70,101,113	0.93	4 (5%)
26	LMU	82	628	-	24,24,36	0.15	0	29,29,47	0.31	0
21	CLA	A	802	-	69,73,73	1.16	5 (7%)	82,113,113	0.77	2 (2%)
26	LMU	A2	865	-	24,24,36	0.12	0	29,29,47	0.46	0
21	CLA	A	818	-	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
21	CLA	Z	603	-	59,63,73	1.29	5 (8%)	70,101,113	0.87	2 (2%)
21	CLA	72	604	33	55,59,73	1.31	4 (7%)	64,96,113	0.93	3 (4%)
28	LUT	4	619	-	42,43,43	0.24	0	51,60,60	0.49	0
21	CLA	82	608	33	54,58,73	1.35	4 (7%)	64,95,113	0.94	2 (3%)
30	CHL	72	606	33	40,54,74	2.40	10 (25%)	34,90,114	1.40	5 (14%)
21	CLA	3	606	33	46,50,73	1.47	4 (8%)	53,85,113	1.00	2 (3%)
21	CLA	A2	833	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	3 (3%)
24	BCR	B	801	-	41,41,41	0.16	0	56,56,56	0.38	0
24	BCR	B2	845	-	41,41,41	0.13	0	56,56,56	0.36	0
26	LMU	12	625	-	24,24,36	0.11	0	29,29,47	0.31	0
21	CLA	12	602	12	64,68,73	1.23	5 (7%)	76,107,113	0.86	3 (3%)
21	CLA	Z2	613	33	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
21	CLA	42	603	16	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
21	CLA	G2	203	-	64,68,73	1.22	4 (6%)	76,107,113	0.81	2 (2%)
21	CLA	62	612	18	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	A	812	-	69,73,73	1.15	5 (7%)	82,113,113	0.80	4 (4%)
28	LUT	A2	856	-	42,43,43	0.27	0	51,60,60	0.41	0
21	CLA	B	827	-	69,73,73	1.20	4 (5%)	82,113,113	0.82	2 (2%)
21	CLA	8	613	15	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A	806	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	J2	101	9	59,63,73	1.28	4 (6%)	70,101,113	0.89	2 (2%)
21	CLA	A	810	1	69,73,73	1.21	4 (5%)	82,113,113	0.85	2 (2%)
31	XAT	62	624	-	41,47,47	0.13	0	54,74,74	0.64	0
21	CLA	B2	840	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
30	CHL	52	607	33	60,74,74	1.99	10 (16%)	58,114,114	0.98	4 (6%)
28	LUT	12	617	-	42,43,43	0.26	0	51,60,60	0.42	0
26	LMU	B	853	-	36,36,36	0.12	0	47,47,47	0.68	2 (4%)
21	CLA	72	614	-	47,51,73	1.43	4 (8%)	55,86,113	1.01	4 (7%)
21	CLA	6	612	18	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
21	CLA	62	610	18	64,68,73	1.22	4 (6%)	76,107,113	0.85	3 (3%)
24	BCR	B2	843	-	41,41,41	0.16	0	56,56,56	0.31	0
26	LMU	A2	864	-	24,24,36	0.11	0	29,29,47	0.28	0
21	CLA	82	609	15	49,53,73	1.41	4 (8%)	58,89,113	0.95	2 (3%)
21	CLA	A	809	1	69,73,73	1.16	5 (7%)	82,113,113	0.89	4 (4%)
26	LMU	12	622	-	19,19,36	0.13	0	24,24,47	0.31	0
30	CHL	Z	607	33	60,74,74	1.95	10 (16%)	58,114,114	1.09	6 (10%)
25	SF4	C	101	3	0,12,12	-	-	-	-	-
21	CLA	32	612	13	50,54,73	1.36	4 (8%)	59,90,113	0.94	3 (5%)
30	CHL	4	608	-	60,74,74	1.96	10 (16%)	58,114,114	1.06	5 (8%)
23	LHG	Z2	620	21	38,38,48	0.25	0	41,44,54	0.29	0
21	CLA	B	828	-	69,73,73	1.15	4 (5%)	82,113,113	0.80	3 (3%)
30	CHL	62	616	18	60,74,74	1.95	10 (16%)	58,114,114	1.10	6 (10%)
21	CLA	52	611	23	59,63,73	1.26	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	52	621	33	50,54,73	1.41	4 (8%)	59,90,113	1.07	5 (8%)
21	CLA	3	610	13	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
27	LMG	82	629	-	42,42,55	0.18	0	50,50,63	0.16	0
30	CHL	32	608	33	60,74,74	1.99	10 (16%)	58,114,114	1.10	5 (8%)
27	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.17	0
24	BCR	A	850	-	41,41,41	0.15	0	56,56,56	0.24	0
21	CLA	Z	604	33	61,65,73	1.24	4 (6%)	72,103,113	0.87	3 (4%)
30	CHL	6	601	18	60,74,74	1.96	10 (16%)	58,114,114	0.98	4 (6%)
23	LHG	6	619	21	48,48,48	0.22	0	51,54,54	0.24	0
21	CLA	L2	203	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	3 (3%)
21	CLA	Z2	602	12	64,68,73	1.23	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	3	614	-	49,53,73	1.40	4 (8%)	58,89,113	0.98	3 (5%)
24	BCR	4	621	-	41,41,41	0.13	0	56,56,56	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
21	CLA	A2	843	33	69,73,73	1.17	5 (7%)	82,113,113	0.84	3 (3%)
31	XAT	Z2	618	-	41,47,47	0.14	0	54,74,74	0.61	0
28	LUT	8	617	-	42,43,43	0.28	0	51,60,60	0.45	0
21	CLA	7	612	14	56,60,73	1.29	4 (7%)	65,97,113	0.90	2 (3%)
21	CLA	Z	613	33	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
26	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.29	0
21	CLA	42	609	16	64,68,73	1.25	4 (6%)	76,107,113	0.87	2 (2%)
21	CLA	32	610	13	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	A	816	-	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
26	LMU	82	627	-	36,36,36	0.10	0	47,47,47	0.37	0
21	CLA	82	611	23	49,53,73	1.40	4 (8%)	58,89,113	1.00	3 (5%)
21	CLA	A	837	1	61,65,73	1.31	5 (8%)	72,103,113	0.90	3 (4%)
32	NEX	5	625	-	40,46,46	0.52	1 (2%)	50,70,70	0.81	3 (6%)
21	CLA	B	819	33	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
22	PQN	A2	844	-	34,34,34	0.32	0	43,45,45	0.43	0
27	LMG	1	628	-	42,42,55	0.18	0	50,50,63	0.28	0
27	LMG	9	620	21	44,44,55	0.17	0	52,52,63	0.35	0
21	CLA	1	603	-	61,65,73	1.26	4 (6%)	72,103,113	0.86	2 (2%)
21	CLA	B2	837	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	92	602	19	64,68,73	1.24	4 (6%)	76,107,113	0.85	3 (3%)
21	CLA	42	614	-	59,63,73	1.28	4 (6%)	70,101,113	0.88	3 (4%)
21	CLA	A2	831	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	3 (3%)
21	CLA	52	616	17	57,61,73	1.29	4 (7%)	67,98,113	0.91	2 (2%)
23	LHG	A	846	-	48,48,48	0.23	0	51,54,54	0.29	0
27	LMG	A	859	-	48,48,55	0.17	0	56,56,63	0.17	0
28	LUT	5	620	-	42,43,43	0.24	0	51,60,60	0.48	0
21	CLA	K	204	-	50,54,73	1.38	5 (10%)	59,90,113	0.99	3 (5%)
21	CLA	62	622	33	59,63,73	1.29	4 (6%)	70,101,113	0.87	2 (2%)
21	CLA	L	203	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	3 (3%)
21	CLA	72	611	23	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
21	CLA	B	829	-	69,73,73	1.17	5 (7%)	82,113,113	0.84	2 (2%)
21	CLA	B2	808	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	1	602	12	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
22	PQN	B	842	-	34,34,34	0.32	0	43,45,45	0.43	0
28	LUT	32	720	-	42,43,43	0.22	0	51,60,60	0.33	0
21	CLA	A	807	1	69,73,73	1.19	5 (7%)	82,113,113	0.77	2 (2%)
21	CLA	A2	817	33	59,63,73	1.30	4 (6%)	70,101,113	0.88	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	CHL	62	618	18	37,51,74	2.45	10 (27%)	30,86,114	1.51	5 (16%)
21	CLA	B	830	-	49,53,73	1.35	5 (10%)	58,89,113	0.98	3 (5%)
26	LMU	7	629	-	28,28,36	0.10	0	39,39,47	0.27	0
23	LHG	92	622	21	40,40,48	0.24	0	43,46,54	0.29	0
24	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.41	0
30	CHL	4	601	16	60,74,74	1.95	10 (16%)	58,114,114	1.10	5 (8%)
21	CLA	A2	854	33	69,73,73	1.24	4 (5%)	82,113,113	0.80	2 (2%)
23	LHG	3	623	-	46,46,48	0.22	0	49,52,54	0.27	0
21	CLA	G	204	7	50,54,73	1.38	4 (8%)	59,90,113	0.96	2 (3%)
20	CL0	A	801	-	58,73,73	1.48	6 (10%)	60,113,113	1.57	3 (5%)
21	CLA	B2	807	-	59,63,73	1.29	4 (6%)	70,101,113	0.89	3 (4%)
21	CLA	7	616	14	50,54,73	1.37	5 (10%)	59,90,113	0.95	3 (5%)
21	CLA	A2	802	-	69,73,73	1.16	5 (7%)	82,113,113	0.77	2 (2%)
21	CLA	32	615	33	69,73,73	1.19	4 (5%)	82,113,113	0.84	2 (2%)
27	LMG	72	626	-	37,37,55	0.18	0	45,45,63	0.27	0
21	CLA	6	603	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
26	LMU	62	628	-	24,24,36	0.12	0	29,29,47	0.29	0
28	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.47	0
21	CLA	B	806	2	69,73,73	1.19	5 (7%)	82,113,113	0.76	2 (2%)
21	CLA	A2	845	23	49,53,73	1.40	4 (8%)	58,89,113	0.95	2 (3%)
21	CLA	A2	821	-	59,63,73	1.27	5 (8%)	70,101,113	0.86	2 (2%)
26	LMU	8	624	-	24,24,36	0.13	0	29,29,47	0.26	0
30	CHL	6	618	18	37,51,74	2.44	10 (27%)	30,86,114	1.51	5 (16%)
21	CLA	9	602	19	64,68,73	1.24	5 (7%)	76,107,113	0.85	3 (3%)
21	CLA	A2	807	1	69,73,73	1.18	5 (7%)	82,113,113	0.78	2 (2%)
21	CLA	A2	822	33	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
21	CLA	12	616	12	50,54,73	1.39	4 (8%)	59,90,113	0.97	3 (5%)
26	LMU	B2	853	-	36,36,36	0.12	0	47,47,47	0.68	2 (4%)
21	CLA	A	843	33	69,73,73	1.17	5 (7%)	82,113,113	0.84	3 (3%)
21	CLA	8	609	15	49,53,73	1.41	4 (8%)	58,89,113	0.95	3 (5%)
23	LHG	1	620	21	38,38,48	0.25	0	41,44,54	0.30	0
21	CLA	B2	813	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	2 (2%)
26	LMU	A	861	-	24,24,36	0.12	0	29,29,47	0.30	0
26	LMU	A2	857	-	35,35,36	0.09	0	46,46,47	0.18	0
21	CLA	B	836	-	64,68,73	1.20	4 (6%)	76,107,113	0.87	3 (3%)
21	CLA	4	610	16	64,68,73	1.22	4 (6%)	76,107,113	0.83	3 (3%)
21	CLA	3	612	13	50,54,73	1.37	4 (8%)	59,90,113	0.94	3 (5%)

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
20	CL0	A2	801	-	3/3/25/25	3/37/135/135	-
21	CLA	9	603	19,27	1/1/18/20	6/27/103/115	-
24	BCR	L	201	-	-	4/29/63/63	0/2/2/2
21	CLA	B	802	-	1/1/20/20	5/39/115/115	-
21	CLA	B2	828	-	1/1/20/20	4/39/115/115	-
21	CLA	72	603	-	1/1/17/20	4/24/100/115	-
30	CHL	72	601	14	3/3/26/26	5/39/137/137	-
23	LHG	42	623	-	-	15/42/42/53	-
26	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
27	LMG	A	860	-	-	6/31/51/70	0/1/1/1
21	CLA	Z	616	12	1/1/19/20	4/33/109/115	-
27	LMG	12	624	-	-	4/31/51/70	0/1/1/1
21	CLA	A	845	23	1/1/15/20	2/15/91/115	-
21	CLA	K2	204	-	1/1/15/20	4/17/93/115	-
30	CHL	6	606	33	3/3/24/26	2/30/128/137	-
21	CLA	1	613	33	1/1/20/20	5/39/115/115	-
21	CLA	B	823	-	1/1/20/20	4/39/115/115	-
28	LUT	F	305	-	-	5/29/67/67	0/2/2/2
21	CLA	A2	809	1	1/1/20/20	7/39/115/115	-
21	CLA	A2	834	-	1/1/20/20	6/39/115/115	-
21	CLA	Z2	612	12	1/1/15/20	5/15/91/115	-
25	SF4	C2	102	3	-	-	0/6/5/5
21	CLA	A	831	-	1/1/20/20	2/39/115/115	-
26	LMU	72	629	-	-	4/13/53/61	0/2/2/2
21	CLA	B	821	-	1/1/20/20	5/39/115/115	-
30	CHL	82	601	15	3/3/26/26	7/39/137/137	-
23	LHG	A2	847	21	-	4/42/42/53	-
23	LHG	8	620	21	-	15/48/48/53	-
21	CLA	52	617	-	1/1/20/20	6/39/115/115	-
21	CLA	5	609	17	1/1/20/20	2/39/115/115	-
30	CHL	5	606	33	3/3/21/26	2/15/113/137	-
24	BCR	B	845	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	820	-	1/1/20/20	6/39/115/115	-
21	CLA	62	614	-	1/1/17/20	2/21/97/115	-
21	CLA	6	611	23	1/1/18/20	4/31/107/115	-
21	CLA	K2	201	11	1/1/15/20	2/15/91/115	-
24	BCR	3	620	-	-	4/29/63/63	0/2/2/2
26	LMU	8	628	-	-	4/15/35/61	0/1/1/2
21	CLA	A	819	-	1/1/19/20	3/33/109/115	-
21	CLA	A2	811	-	1/1/20/20	4/39/115/115	-
30	CHL	5	618	17	3/3/20/26	2/12/110/137	-
21	CLA	B2	834	-	1/1/19/20	8/33/109/115	-
26	LMU	A2	861	-	-	2/15/35/61	0/1/1/2
24	BCR	A	849	-	-	0/29/63/63	0/2/2/2
21	CLA	B	841	23	1/1/20/20	8/39/115/115	-
31	XAT	72	622	-	-	0/31/93/93	0/4/4/4
21	CLA	82	613	15	1/1/20/20	7/39/115/115	-
21	CLA	B	809	2	1/1/20/20	5/39/115/115	-
24	BCR	B2	847	-	-	2/29/63/63	0/2/2/2
21	CLA	K	203	33	1/1/19/20	1/33/109/115	-
30	CHL	42	608	-	3/3/26/26	5/39/137/137	-
26	LMU	A2	858	-	-	6/21/61/61	0/2/2/2
21	CLA	6	613	33	1/1/20/20	4/39/115/115	-
21	CLA	A2	841	-	1/1/20/20	7/39/115/115	-
21	CLA	5	614	-	1/1/15/20	4/15/91/115	-
21	CLA	4	609	16	1/1/19/20	6/33/109/115	-
30	CHL	Z	601	12	3/3/26/26	7/39/137/137	-
21	CLA	B	833	-	1/1/18/20	4/31/107/115	-
24	BCR	B	844	-	-	0/29/63/63	0/2/2/2
24	BCR	B	843	-	-	0/29/63/63	0/2/2/2
28	LUT	52	626	-	-	4/29/67/67	0/2/2/2
28	LUT	7	624	-	-	4/29/67/67	0/2/2/2
26	LMU	K	208	-	-	3/15/35/61	0/1/1/2
21	CLA	1	612	12	1/1/15/20	7/15/91/115	-
21	CLA	32	602	13	1/1/19/20	2/33/109/115	-
25	SF4	A2	853	1,2	-	-	0/6/5/5
21	CLA	3	609	13	1/1/19/20	2/35/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	52	602	17	1/1/20/20	2/39/115/115	-
21	CLA	5	604	33	1/1/18/20	4/27/103/115	-
21	CLA	A2	816	-	1/1/20/20	4/39/115/115	-
23	LHG	B2	851	21	-	11/49/49/53	-
30	CHL	8	607	33	3/3/26/26	8/39/137/137	-
24	BCR	5	622	-	-	2/29/63/63	0/2/2/2
26	LMU	42	626	-	-	0/11/31/61	0/1/1/2
21	CLA	72	613	14	1/1/20/20	0/39/115/115	-
23	LHG	5	623	21	-	11/41/41/53	-
22	PQN	B2	842	-	-	1/23/43/43	0/2/2/2
30	CHL	9	606	-	3/3/20/26	0/10/108/137	-
21	CLA	52	614	-	1/1/15/20	4/15/91/115	-
28	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
21	CLA	B2	814	-	1/1/19/20	2/33/109/115	-
21	CLA	42	616	16	1/1/15/20	0/15/91/115	-
22	PQN	A	844	-	-	3/23/43/43	0/2/2/2
21	CLA	1	609	12	1/1/20/20	5/39/115/115	-
21	CLA	B	811	-	1/1/20/20	7/39/115/115	-
21	CLA	A2	813	-	1/1/20/20	4/39/115/115	-
26	LMU	72	628	-	-	3/13/33/61	0/1/1/2
21	CLA	B	837	-	1/1/20/20	0/39/115/115	-
21	CLA	8	612	15	1/1/18/20	5/27/103/115	-
21	CLA	4	616	16	1/1/15/20	0/15/91/115	-
21	CLA	4	612	16	1/1/15/20	4/15/91/115	-
24	BCR	9	623	-	-	2/29/63/63	0/2/2/2
21	CLA	4	604	33	1/1/17/20	1/21/97/115	-
28	LUT	32	622	-	-	2/29/67/67	0/2/2/2
26	LMU	Z2	622	-	-	3/17/57/61	0/2/2/2
21	CLA	B2	804	-	1/1/15/20	4/15/91/115	-
21	CLA	72	608	33	1/1/17/20	0/21/97/115	-
30	CHL	62	601	18	3/3/26/26	5/39/137/137	-
21	CLA	A	824	-	1/1/15/20	4/15/91/115	-
21	CLA	8	610	15	1/1/20/20	2/39/115/115	-
21	CLA	B2	832	-	1/1/20/20	4/39/115/115	-
23	LHG	A2	846	-	-	9/53/53/53	-
24	BCR	8	619	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	8	606	33	3/3/26/26	1/39/137/137	-
21	CLA	Z2	614	-	1/1/17/20	0/21/97/115	-
28	LUT	6	621	-	-	2/29/67/67	0/2/2/2
24	BCR	A	852	-	-	4/29/63/63	0/2/2/2
30	CHL	7	607	33	3/3/21/26	1/15/113/137	-
21	CLA	6	610	18	1/1/19/20	0/33/109/115	-
21	CLA	8	614	-	1/1/18/20	6/30/106/115	-
27	LMG	6	633	-	-	1/17/17/70	-
21	CLA	B2	824	33	1/1/20/20	3/39/115/115	-
23	LHG	3	721	-	-	12/35/35/53	-
26	LMU	8	625	-	-	2/15/35/61	0/1/1/2
24	BCR	A2	852	-	-	4/29/63/63	0/2/2/2
21	CLA	8	608	33	1/1/17/20	2/21/97/115	-
21	CLA	F2	301	33	1/1/20/20	3/39/115/115	-
26	LMU	A2	863	-	-	7/21/61/61	0/2/2/2
21	CLA	A	805	-	1/1/18/20	1/27/103/115	-
26	LMU	6	632	-	-	3/11/31/61	0/1/1/2
27	LMG	8	626	-	-	6/27/47/70	0/1/1/1
27	LMG	4	624	-	-	6/36/56/70	0/1/1/1
21	CLA	Z	602	12	1/1/19/20	2/33/109/115	-
21	CLA	B2	823	-	1/1/20/20	4/39/115/115	-
21	CLA	5	611	23	1/1/18/20	4/27/103/115	-
21	CLA	72	609	14	1/1/15/20	1/15/91/115	-
21	CLA	82	602	15	1/1/19/20	3/36/112/115	-
30	CHL	62	608	33	3/3/23/26	0/21/119/137	-
23	LHG	12	620	21	-	7/43/43/53	-
21	CLA	8	611	23	1/1/15/20	2/15/91/115	-
21	CLA	L	204	-	1/1/15/20	2/15/91/115	-
21	CLA	Z	609	12	1/1/20/20	9/39/115/115	-
21	CLA	A	822	33	1/1/20/20	0/39/115/115	-
21	CLA	B2	838	-	1/1/17/20	1/21/97/115	-
21	CLA	A	838	-	1/1/17/20	0/23/99/115	-
24	BCR	32	620	-	-	4/29/63/63	0/2/2/2
21	CLA	B	820	-	1/1/18/20	5/29/105/115	-
21	CLA	5	621	33	1/1/15/20	10/17/93/115	-
24	BCR	42	621	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A	803	33	1/1/20/20	2/39/115/115	-
21	CLA	3	604	33	1/1/20/20	1/39/115/115	-
21	CLA	B2	825	33	1/1/20/20	2/39/115/115	-
21	CLA	82	604	33	1/1/19/20	2/33/109/115	-
27	LMG	J2	104	-	-	8/30/50/70	0/1/1/1
27	LMG	1	624	-	-	4/31/51/70	0/1/1/1
21	CLA	B	817	-	1/1/20/20	8/39/115/115	-
24	BCR	A	848	-	-	2/29/63/63	0/2/2/2
21	CLA	B2	809	2	1/1/20/20	5/39/115/115	-
26	LMU	7	628	-	-	3/13/33/61	0/1/1/2
23	LHG	62	619	21	-	3/53/53/53	-
24	BCR	K2	207	-	-	4/29/63/63	0/2/2/2
21	CLA	A	834	-	1/1/20/20	6/39/115/115	-
28	LUT	92	616	-	-	2/29/67/67	0/2/2/2
21	CLA	B2	833	-	1/1/18/20	4/31/107/115	-
21	CLA	7	608	33	1/1/17/20	0/21/97/115	-
30	CHL	72	607	33	3/3/21/26	1/15/113/137	-
29	DGD	B2	850	-	-	10/48/88/95	0/2/2/2
24	BCR	82	619	-	-	4/29/63/63	0/2/2/2
26	LMU	6	631	-	-	4/15/35/61	0/1/1/2
21	CLA	B	810	-	1/1/20/20	2/39/115/115	-
30	CHL	Z2	607	33	3/3/26/26	4/39/137/137	-
21	CLA	B	834	-	1/1/19/20	8/33/109/115	-
23	LHG	52	623	21	-	11/41/41/53	-
30	CHL	42	607	33	3/3/26/26	1/39/137/137	-
21	CLA	A2	804	-	1/1/20/20	4/39/115/115	-
21	CLA	Z2	611	23	1/1/19/20	6/33/109/115	-
24	BCR	32	719	-	-	2/29/63/63	0/2/2/2
21	CLA	F	304	6	1/1/20/20	7/39/115/115	-
26	LMU	A	863	-	-	7/21/61/61	0/2/2/2
21	CLA	B	818	-	1/1/20/20	4/39/115/115	-
26	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
21	CLA	9	610	19	1/1/19/20	0/33/109/115	-
30	CHL	42	606	33	3/3/24/26	1/27/125/137	-
21	CLA	A	839	-	1/1/20/20	2/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	817	-	1/1/20/20	8/39/115/115	-
21	CLA	7	609	14	1/1/15/20	1/15/91/115	-
21	CLA	B	831	-	1/1/18/20	1/27/103/115	-
23	LHG	A	847	21	-	4/42/42/53	-
21	CLA	3	611	-	1/1/20/20	6/39/115/115	-
24	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
31	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
21	CLA	B	838	-	1/1/17/20	1/21/97/115	-
21	CLA	A	832	-	1/1/18/20	0/27/103/115	-
24	BCR	62	623	-	-	2/29/63/63	0/2/2/2
24	BCR	72	623	-	-	2/29/63/63	0/2/2/2
21	CLA	42	610	16	1/1/19/20	3/33/109/115	-
27	LMG	42	624	-	-	6/36/56/70	0/1/1/1
21	CLA	92	601	19	1/1/15/20	2/17/93/115	-
28	LUT	12	619	-	-	2/29/67/67	0/2/2/2
30	CHL	4	606	33	3/3/24/26	1/27/125/137	-
26	LMU	9	624	-	-	4/15/35/61	0/1/1/2
21	CLA	F	301	33	1/1/20/20	3/39/115/115	-
26	LMU	Z2	621	-	-	2/13/33/61	0/1/1/2
27	LMG	8	629	-	-	9/37/57/70	0/1/1/1
30	CHL	4	607	33	3/3/26/26	1/39/137/137	-
26	LMU	1	623	-	-	1/15/35/61	0/1/1/2
21	CLA	52	610	17	1/1/19/20	2/33/109/115	-
21	CLA	B	812	-	1/1/20/20	2/39/115/115	-
21	CLA	B2	826	-	1/1/20/20	4/39/115/115	-
24	BCR	3	718	-	-	2/29/63/63	0/2/2/2
21	CLA	7	611	23	1/1/20/20	7/39/115/115	-
24	BCR	6	623	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	835	-	1/1/20/20	6/39/115/115	-
26	LMU	4	626	-	-	0/11/31/61	0/1/1/2
21	CLA	A	840	-	1/1/20/20	7/39/115/115	-
28	LUT	1	617	-	-	2/29/67/67	0/2/2/2
26	LMU	52	627	-	-	1/15/35/61	0/1/1/2
21	CLA	6	602	18	1/1/20/20	2/39/115/115	-
21	CLA	1	614	-	1/1/19/20	7/33/109/115	-
21	CLA	12	612	12	1/1/15/20	7/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	3	602	13	1/1/19/20	2/33/109/115	-
30	CHL	62	606	33	3/3/24/26	2/30/128/137	-
24	BCR	L	205	-	-	2/29/63/63	0/2/2/2
21	CLA	6	604	-	1/1/20/20	2/39/115/115	-
27	LMG	A2	860	-	-	6/31/51/70	0/1/1/1
21	CLA	B	816	-	1/1/20/20	0/39/115/115	-
21	CLA	72	620	33	1/1/17/20	6/25/101/115	-
21	CLA	G2	204	7	1/1/15/20	4/17/93/115	-
30	CHL	3	608	33	3/3/26/26	3/39/137/137	-
23	LHG	62	629	-	-	10/40/40/53	-
28	LUT	F2	305	-	-	5/29/67/67	0/2/2/2
31	XAT	82	618	-	-	0/31/93/93	0/4/4/4
23	LHG	72	625	21	-	12/53/53/53	-
21	CLA	1	604	33	1/1/17/20	0/21/97/115	-
26	LMU	K2	208	-	-	3/15/35/61	0/1/1/2
30	CHL	6	608	33	3/3/23/26	0/21/119/137	-
21	CLA	B	835	33	1/1/15/20	0/15/91/115	-
21	CLA	4	614	-	1/1/18/20	5/27/103/115	-
21	CLA	82	610	15	1/1/20/20	2/39/115/115	-
24	BCR	I	172	-	-	0/29/63/63	0/2/2/2
21	CLA	A	813	-	1/1/20/20	4/39/115/115	-
26	LMU	12	627	-	-	3/13/33/61	0/1/1/2
23	LHG	6	629	-	-	10/40/40/53	-
26	LMU	5	627	-	-	1/15/35/61	0/1/1/2
26	LMU	7	627	-	-	2/18/58/61	0/2/2/2
21	CLA	82	614	-	1/1/18/20	6/30/106/115	-
21	CLA	Z2	603	-	1/1/18/20	6/27/103/115	-
21	CLA	72	616	14	1/1/15/20	3/17/93/115	-
21	CLA	7	603	-	1/1/17/20	4/24/100/115	-
32	NEX	52	625	-	-	2/27/83/83	1/3/3/3
21	CLA	9	614	-	1/1/15/20	4/15/91/115	-
21	CLA	F2	304	6	1/1/20/20	7/39/115/115	-
27	LMG	82	626	-	-	6/27/47/70	0/1/1/1
21	CLA	9	609	19	1/1/17/20	4/23/99/115	-
21	CLA	A2	812	-	1/1/20/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	Z	612	12	1/1/15/20	5/15/91/115	-
25	SF4	C2	101	3	-	-	0/6/5/5
21	CLA	7	602	14	1/1/20/20	2/39/115/115	-
21	CLA	72	610	14	1/1/20/20	6/39/115/115	-
21	CLA	B	805	-	1/1/20/20	8/39/115/115	-
21	CLA	5	603	-	1/1/20/20	15/39/115/115	-
21	CLA	A	815	-	1/1/18/20	2/27/103/115	-
21	CLA	B2	806	2	1/1/20/20	2/39/115/115	-
21	CLA	12	603	-	1/1/18/20	6/30/106/115	-
28	LUT	Z2	619	-	-	2/18/37/67	0/1/1/2
23	LHG	32	721	-	-	12/35/35/53	-
25	SF4	C	102	3	-	-	0/6/5/5
21	CLA	Z	610	12	1/1/19/20	0/33/109/115	-
21	CLA	L2	204	-	1/1/15/20	2/15/91/115	-
21	CLA	62	609	18	1/1/18/20	4/27/103/115	-
24	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
24	BCR	A2	850	-	-	0/29/63/63	0/2/2/2
32	NEX	62	625	-	-	5/27/83/83	0/3/3/3
21	CLA	32	604	33	1/1/20/20	1/39/115/115	-
21	CLA	82	603	-	1/1/20/20	4/39/115/115	-
21	CLA	B2	812	-	1/1/20/20	2/39/115/115	-
21	CLA	82	616	15	1/1/15/20	0/15/91/115	-
26	LMU	A	865	-	-	3/15/35/61	0/1/1/2
21	CLA	52	604	33	1/1/18/20	4/27/103/115	-
30	CHL	62	607	33	3/3/26/26	10/39/137/137	-
21	CLA	32	613	13	1/1/19/20	5/33/109/115	-
23	LHG	32	623	-	-	13/51/51/53	-
28	LUT	42	619	-	-	1/29/67/67	0/2/2/2
21	CLA	32	603	-	1/1/20/20	5/39/115/115	-
26	LMU	G2	206	-	-	4/15/35/61	0/1/1/2
21	CLA	A	808	-	1/1/17/20	0/21/97/115	-
21	CLA	B2	829	-	1/1/20/20	3/39/115/115	-
21	CLA	A	804	-	1/1/20/20	4/39/115/115	-
21	CLA	7	620	33	1/1/17/20	6/25/101/115	-
21	CLA	62	604	-	1/1/20/20	2/39/115/115	-
21	CLA	9	604	19	1/1/17/20	0/25/101/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	B2	830	-	1/1/15/20	0/15/91/115	-
30	CHL	82	606	33	3/3/26/26	1/39/137/137	-
30	CHL	7	601	14	3/3/26/26	4/39/137/137	-
30	CHL	52	618	17	3/3/20/26	2/12/110/137	-
24	BCR	K	207	-	-	4/29/63/63	0/2/2/2
24	BCR	B2	801	-	-	0/29/63/63	0/2/2/2
21	CLA	32	609	13	1/1/19/20	2/35/111/115	-
28	LUT	9	616	-	-	2/29/67/67	0/2/2/2
26	LMU	A	858	-	-	6/21/61/61	0/2/2/2
21	CLA	62	611	23	1/1/18/20	4/31/107/115	-
21	CLA	A2	815	-	1/1/18/20	2/27/103/115	-
21	CLA	52	609	17	1/1/20/20	2/39/115/115	-
30	CHL	5	607	33	3/3/26/26	11/39/137/137	-
28	LUT	3	720	-	-	0/29/67/67	0/2/2/2
21	CLA	F2	303	33	1/1/15/20	1/15/91/115	-
21	CLA	Z2	616	12	1/1/19/20	4/33/109/115	-
21	CLA	A	826	33	1/1/20/20	8/39/115/115	-
21	CLA	A	842	-	1/1/20/20	3/39/115/115	-
21	CLA	8	603	-	1/1/20/20	4/39/115/115	-
21	CLA	62	613	33	1/1/20/20	4/39/115/115	-
21	CLA	42	602	16	1/1/19/20	2/33/109/115	-
31	XAT	8	618	-	-	0/31/93/93	0/4/4/4
28	LUT	62	621	-	-	2/29/67/67	0/2/2/2
21	CLA	B2	841	23	1/1/20/20	8/39/115/115	-
21	CLA	42	612	16	1/1/15/20	4/15/91/115	-
23	LHG	4	622	21	-	14/53/53/53	-
21	CLA	B2	822	-	1/1/18/20	3/32/108/115	-
30	CHL	Z2	606	33	3/3/21/26	4/15/113/137	-
21	CLA	32	614	-	1/1/15/20	2/15/91/115	-
21	CLA	B2	820	-	1/1/18/20	5/29/105/115	-
27	LMG	62	633	-	-	1/17/17/70	-
21	CLA	B2	819	33	1/1/19/20	5/33/109/115	-
26	LMU	12	623	-	-	1/15/35/61	0/1/1/2
21	CLA	Z	608	33	1/1/17/20	2/21/97/115	-
26	LMU	62	632	-	-	3/11/31/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	52	622	-	-	2/29/63/63	0/2/2/2
28	LUT	3	621	-	-	2/29/67/67	0/2/2/2
21	CLA	5	613	17	1/1/18/20	4/29/105/115	-
31	XAT	7	622	-	-	0/31/93/93	0/4/4/4
21	CLA	7	610	14	1/1/20/20	6/39/115/115	-
21	CLA	B2	836	-	1/1/19/20	4/33/109/115	-
26	LMU	1	626	-	-	0/15/35/61	0/1/1/2
21	CLA	B2	802	-	1/1/20/20	5/39/115/115	-
21	CLA	32	611	-	1/1/20/20	6/39/115/115	-
21	CLA	92	604	19	1/1/17/20	0/25/101/115	-
21	CLA	5	617	-	1/1/20/20	6/39/115/115	-
26	LMU	A2	862	-	-	2/11/31/61	0/1/1/2
21	CLA	A2	838	-	1/1/17/20	0/23/99/115	-
21	CLA	12	609	12	1/1/20/20	5/39/115/115	-
30	CHL	12	606	33	3/3/21/26	0/15/113/137	-
21	CLA	B2	803	-	1/1/20/20	2/39/115/115	-
21	CLA	52	601	17	1/1/20/20	5/39/115/115	-
30	CHL	52	606	33	3/3/21/26	2/15/113/137	-
21	CLA	K	201	11	1/1/15/20	2/15/91/115	-
30	CHL	7	606	33	3/3/21/26	2/15/113/137	-
21	CLA	B	813	-	1/1/20/20	3/39/115/115	-
21	CLA	6	617	-	1/1/15/20	2/15/91/115	-
21	CLA	A2	840	-	1/1/20/20	7/39/115/115	-
21	CLA	3	617	13	1/1/15/20	2/17/93/115	-
21	CLA	B2	821	-	1/1/20/20	5/39/115/115	-
21	CLA	B2	805	-	1/1/20/20	8/39/115/115	-
24	BCR	A2	848	-	-	2/29/63/63	0/2/2/2
30	CHL	1	606	33	3/3/21/26	0/15/113/137	-
31	XAT	6	624	-	-	0/31/93/93	0/4/4/4
24	BCR	B	846	-	-	2/29/63/63	0/2/2/2
28	LUT	9	617	-	-	0/29/67/67	0/2/2/2
28	LUT	92	617	-	-	0/29/67/67	0/2/2/2
31	XAT	1	618	-	-	0/31/93/93	0/4/4/4
21	CLA	7	613	14	1/1/20/20	1/39/115/115	-
28	LUT	72	621	-	-	2/29/67/67	0/2/2/2
21	CLA	A2	825	-	1/1/18/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	62	603	-	1/1/20/20	7/39/115/115	-
21	CLA	32	617	13	1/1/15/20	2/17/93/115	-
21	CLA	12	614	-	1/1/19/20	7/33/109/115	-
21	CLA	A2	808	-	1/1/17/20	0/21/97/115	-
21	CLA	B2	827	-	1/1/20/20	5/39/115/115	-
21	CLA	A2	805	-	1/1/18/20	1/27/103/115	-
21	CLA	A2	826	33	1/1/20/20	8/39/115/115	-
21	CLA	B	839	33	1/1/20/20	6/39/115/115	-
26	LMU	1	621	-	-	6/21/61/61	0/2/2/2
21	CLA	8	604	33	1/1/19/20	2/33/109/115	-
21	CLA	A2	824	-	1/1/15/20	4/15/91/115	-
28	LUT	1	619	-	-	2/29/67/67	0/2/2/2
21	CLA	3	603	-	1/1/20/20	5/39/115/115	-
21	CLA	12	613	33	1/1/20/20	5/39/115/115	-
21	CLA	A	830	-	1/1/20/20	4/39/115/115	-
27	LMG	A2	859	-	-	9/43/63/70	0/1/1/1
21	CLA	B	807	-	1/1/18/20	4/27/103/115	-
21	CLA	92	614	-	1/1/15/20	4/15/91/115	-
30	CHL	1	601	12	3/3/26/26	9/39/137/137	-
21	CLA	Z2	609	12	1/1/20/20	9/39/115/115	-
24	BCR	K2	202	-	-	2/29/63/63	0/2/2/2
27	LMG	92	620	21	-	6/39/59/70	0/1/1/1
21	CLA	B2	835	33	1/1/15/20	1/15/91/115	-
21	CLA	52	603	-	1/1/20/20	15/39/115/115	-
21	CLA	52	612	17	1/1/15/20	6/15/91/115	-
26	LMU	62	631	-	-	4/15/35/61	0/1/1/2
24	BCR	B	847	-	-	2/29/63/63	0/2/2/2
27	LMG	B	852	-	-	5/38/58/70	0/1/1/1
21	CLA	9	601	19	1/1/15/20	2/17/93/115	-
21	CLA	K	206	11	1/1/15/20	4/15/91/115	-
26	LMU	62	630	-	-	1/15/35/61	0/1/1/2
21	CLA	Z	611	23	1/1/19/20	6/33/109/115	-
21	CLA	5	610	17	1/1/19/20	2/33/109/115	-
21	CLA	92	611	23	1/1/20/20	6/39/115/115	-
21	CLA	82	612	15	1/1/18/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	XAT	42	620	-	-	0/31/93/93	0/4/4/4
21	CLA	A	825	-	1/1/18/20	6/27/103/115	-
24	BCR	B2	846	-	-	2/29/63/63	0/2/2/2
21	CLA	A	829	-	1/1/20/20	8/39/115/115	-
21	CLA	9	612	19	1/1/20/20	5/39/115/115	-
21	CLA	32	607	13	1/1/18/20	5/27/103/115	-
24	BCR	7	623	-	-	2/29/63/63	0/2/2/2
21	CLA	12	608	33	1/1/20/20	2/39/115/115	-
21	CLA	4	603	16	1/1/20/20	6/39/115/115	-
21	CLA	A	814	-	1/1/20/20	4/39/115/115	-
28	LUT	32	621	-	-	2/29/67/67	0/2/2/2
21	CLA	3	615	33	1/1/20/20	6/39/115/115	-
21	CLA	Z2	608	33	1/1/17/20	2/21/97/115	-
31	XAT	52	624	-	1/1/26/26	0/31/93/93	0/4/4/4
23	LHG	82	620	21	-	15/48/48/53	-
21	CLA	B2	811	-	1/1/20/20	7/39/115/115	-
21	CLA	A2	820	-	1/1/20/20	6/39/115/115	-
21	CLA	A2	836	-	1/1/20/20	5/39/115/115	-
21	CLA	A2	837	1	1/1/18/20	0/30/106/115	-
23	LHG	B	851	21	-	11/49/49/53	-
21	CLA	5	616	17	1/1/17/20	7/25/101/115	-
21	CLA	72	602	14	1/1/20/20	2/39/115/115	-
21	CLA	7	604	33	1/1/17/20	1/23/99/115	-
21	CLA	4	602	16	1/1/19/20	2/33/109/115	-
21	CLA	Z	614	-	1/1/17/20	0/21/97/115	-
21	CLA	Z2	604	33	1/1/18/20	3/30/106/115	-
30	CHL	6	616	18	3/3/26/26	3/39/137/137	-
21	CLA	42	604	33	1/1/17/20	1/21/97/115	-
30	CHL	5	608	33	3/3/23/26	0/21/119/137	-
21	CLA	A2	823	-	1/1/20/20	7/39/115/115	-
27	LMG	12	628	-	-	6/37/57/70	0/1/1/1
21	CLA	42	613	16	1/1/20/20	6/39/115/115	-
26	LMU	82	625	-	-	2/15/35/61	0/1/1/2
21	CLA	F	303	33	1/1/15/20	1/15/91/115	-
23	LHG	9	622	21	-	13/45/45/53	-
26	LMU	82	624	-	-	1/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	BCR	92	623	-	-	2/29/63/63	0/2/2/2
21	CLA	12	611	23	1/1/19/20	4/35/111/115	-
31	XAT	4	620	-	-	0/31/93/93	0/4/4/4
27	LMG	7	626	-	-	7/32/52/70	0/1/1/1
21	CLA	B	808	-	1/1/20/20	9/39/115/115	-
21	CLA	3	613	13	1/1/19/20	5/33/109/115	-
21	CLA	12	610	12	1/1/20/20	2/39/115/115	-
21	CLA	B	815	-	1/1/20/20	4/39/115/115	-
21	CLA	A2	827	33	1/1/20/20	2/39/115/115	-
21	CLA	K2	206	11	1/1/15/20	4/15/91/115	-
21	CLA	B	832	-	1/1/20/20	4/39/115/115	-
21	CLA	A	854	33	1/1/20/20	1/39/115/115	-
21	CLA	A2	839	-	1/1/20/20	2/39/115/115	-
23	LHG	Z	620	21	-	6/43/43/53	-
21	CLA	A2	806	-	1/1/20/20	10/39/115/115	-
24	BCR	J2	102	-	-	2/29/63/63	0/2/2/2
30	CHL	52	608	33	3/3/23/26	0/21/119/137	-
21	CLA	A2	819	-	1/1/19/20	3/33/109/115	-
21	CLA	8	616	15	1/1/15/20	0/15/91/115	-
24	BCR	A2	849	-	-	0/29/63/63	0/2/2/2
24	BCR	A2	851	-	-	2/29/63/63	0/2/2/2
21	CLA	J	101	9	1/1/18/20	3/27/103/115	-
26	LMU	42	625	-	-	3/19/59/61	0/2/2/2
23	LHG	42	622	21	-	14/53/53/53	-
30	CHL	12	607	33	3/3/21/26	2/15/113/137	-
21	CLA	1	608	33	1/1/20/20	2/39/115/115	-
21	CLA	4	613	16	1/1/20/20	6/39/115/115	-
26	LMU	G	206	-	-	4/15/35/61	0/1/1/2
21	CLA	A2	828	-	1/1/20/20	5/39/115/115	-
21	CLA	B2	831	-	1/1/18/20	1/27/103/115	-
21	CLA	8	602	15	1/1/19/20	3/36/112/115	-
21	CLA	A2	832	-	1/1/18/20	0/27/103/115	-
26	LMU	4	625	-	-	3/19/59/61	0/2/2/2
28	LUT	5	626	-	-	4/29/67/67	0/2/2/2
26	LMU	A	857	-	-	3/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	92	609	19	1/1/17/20	4/23/99/115	-
30	CHL	92	606	-	3/3/20/26	0/10/108/137	-
27	LMG	3	722	-	-	5/46/46/70	-
27	LMG	J2	103	-	-	3/37/57/70	0/1/1/1
21	CLA	42	611	23	1/1/19/20	5/33/109/115	-
26	LMU	12	626	-	-	0/15/35/61	0/1/1/2
21	CLA	B	814	-	1/1/19/20	2/33/109/115	-
30	CHL	92	607	33	3/3/23/26	9/21/119/137	-
21	CLA	A	817	33	1/1/18/20	4/27/103/115	-
21	CLA	A	835	-	1/1/20/20	6/39/115/115	-
25	SF4	A	853	1,2	-	-	0/6/5/5
27	LMG	J	103	-	-	3/37/57/70	0/1/1/1
21	CLA	A	833	-	1/1/20/20	1/39/115/115	-
30	CHL	1	607	33	3/3/21/26	2/15/113/137	-
21	CLA	A2	818	-	1/1/20/20	2/39/115/115	-
26	LMU	6	628	-	-	2/15/35/61	0/1/1/2
21	CLA	B	804	-	1/1/15/20	4/15/91/115	-
27	LMG	B2	854	-	-	2/31/51/70	0/1/1/1
21	CLA	72	612	14	1/1/17/20	3/24/100/115	-
21	CLA	6	614	-	1/1/17/20	2/21/97/115	-
32	NEX	6	625	-	-	5/27/83/83	0/3/3/3
28	LUT	A	856	-	-	4/29/67/67	0/2/2/2
24	BCR	32	718	-	-	2/29/63/63	0/2/2/2
21	CLA	B	803	-	1/1/20/20	2/39/115/115	-
21	CLA	A	828	-	1/1/20/20	5/39/115/115	-
21	CLA	62	602	18	1/1/20/20	2/39/115/115	-
21	CLA	A2	830	-	1/1/20/20	5/39/115/115	-
24	BCR	G	205	-	-	1/29/63/63	0/2/2/2
21	CLA	92	613	19	1/1/20/20	5/39/115/115	-
21	CLA	A2	803	33	1/1/20/20	2/39/115/115	-
31	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
26	LMU	1	622	-	-	4/10/30/61	0/1/1/2
21	CLA	B	824	33	1/1/20/20	3/39/115/115	-
26	LMU	12	621	-	-	6/21/61/61	0/2/2/2
21	CLA	B2	818	-	1/1/20/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	A2	810	1	1/1/20/20	8/39/115/115	-
30	CHL	8	601	15	3/3/26/26	7/39/137/137	-
26	LMU	72	627	-	-	2/18/58/61	0/2/2/2
21	CLA	6	622	33	1/1/18/20	2/27/103/115	-
30	CHL	82	607	33	3/3/26/26	8/39/137/137	-
30	CHL	42	618	16	3/3/21/26	0/15/113/137	-
23	LHG	4	623	-	-	15/42/42/53	-
21	CLA	5	602	17	1/1/20/20	2/39/115/115	-
26	LMU	8	627	-	-	9/21/61/61	0/2/2/2
26	LMU	A	864	-	-	3/15/35/61	0/1/1/2
21	CLA	32	606	33	1/1/14/20	0/12/88/115	-
30	CHL	6	607	33	3/3/26/26	10/39/137/137	-
21	CLA	A	827	33	1/1/20/20	2/39/115/115	-
30	CHL	9	607	33	3/3/23/26	10/21/119/137	-
24	BCR	G2	205	-	-	1/29/63/63	0/2/2/2
21	CLA	5	612	17	1/1/15/20	6/15/91/115	-
24	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
21	CLA	A2	829	-	1/1/20/20	7/39/115/115	-
28	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
21	CLA	B	840	-	1/1/20/20	7/39/115/115	-
30	CHL	Z	606	33	3/3/21/26	4/15/113/137	-
30	CHL	4	618	16	3/3/21/26	0/15/113/137	-
26	LMU	1	625	-	-	4/15/35/61	0/1/1/2
21	CLA	K2	203	33	1/1/19/20	1/33/109/115	-
21	CLA	B2	810	-	1/1/20/20	2/39/115/115	-
24	BCR	B	848	-	-	2/29/63/63	0/2/2/2
23	LHG	7	625	21	-	12/53/53/53	-
21	CLA	B	825	33	1/1/20/20	2/39/115/115	-
21	CLA	52	613	17	1/1/18/20	4/29/105/115	-
21	CLA	A	841	-	1/1/20/20	7/39/115/115	-
24	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
24	BCR	B2	848	-	-	2/29/63/63	0/2/2/2
21	CLA	1	611	23	1/1/19/20	4/35/111/115	-
21	CLA	A	836	-	1/1/20/20	5/39/115/115	-
21	CLA	A2	842	-	1/1/20/20	3/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMG	B2	852	-	-	5/38/58/70	0/1/1/1
21	CLA	3	607	13	1/1/18/20	4/27/103/115	-
21	CLA	9	613	19	1/1/20/20	5/39/115/115	-
24	BCR	J	102	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	814	-	1/1/20/20	4/39/115/115	-
21	CLA	9	611	23	1/1/20/20	6/39/115/115	-
30	CHL	12	601	12	3/3/26/26	9/39/137/137	-
21	CLA	92	603	19,27	1/1/18/20	6/27/103/115	-
21	CLA	92	612	19	1/1/20/20	5/39/115/115	-
21	CLA	A	823	-	1/1/20/20	7/39/115/115	-
28	LUT	52	620	-	-	2/29/67/67	0/2/2/2
29	DGD	B	850	-	-	14/48/88/95	0/2/2/2
21	CLA	A	811	-	1/1/20/20	4/39/115/115	-
30	CHL	Z2	601	12	3/3/26/26	7/39/137/137	-
30	CHL	42	601	16	3/3/26/26	6/39/137/137	-
21	CLA	A	821	-	1/1/18/20	4/27/103/115	-
21	CLA	B	826	-	1/1/20/20	4/39/115/115	-
28	LUT	7	621	-	-	2/29/67/67	0/2/2/2
21	CLA	92	610	19	1/1/19/20	0/33/109/115	-
26	LMU	6	630	-	-	1/15/35/61	0/1/1/2
28	LUT	72	624	-	-	4/29/67/67	0/2/2/2
21	CLA	4	611	23	1/1/19/20	5/33/109/115	-
21	CLA	G	203	-	1/1/19/20	2/33/109/115	-
21	CLA	5	601	17	1/1/20/20	5/39/115/115	-
21	CLA	Z2	610	12	1/1/19/20	0/33/109/115	-
21	CLA	B2	816	-	1/1/20/20	0/39/115/115	-
21	CLA	62	617	-	1/1/15/20	2/15/91/115	-
27	LMG	32	722	-	-	5/46/46/70	-
21	CLA	12	604	33	1/1/17/20	0/21/97/115	-
21	CLA	B2	815	-	1/1/20/20	4/39/115/115	-
21	CLA	1	610	12	1/1/20/20	2/39/115/115	-
21	CLA	B	822	-	1/1/18/20	3/32/108/115	-
21	CLA	7	614	-	1/1/14/20	5/13/89/115	-
31	XAT	12	618	-	-	0/31/93/93	0/4/4/4
21	CLA	B2	839	33	1/1/20/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	Z2	617	-	-	2/29/67/67	0/2/2/2
26	LMU	A	862	-	-	2/11/31/61	0/1/1/2
28	LUT	82	617	-	-	2/29/67/67	0/2/2/2
26	LMU	92	624	-	-	4/15/35/61	0/1/1/2
24	BCR	A	851	-	-	2/29/63/63	0/2/2/2
24	BCR	K	202	-	-	2/29/63/63	0/2/2/2
21	CLA	1	616	12	1/1/15/20	2/17/93/115	-
27	LMG	J	104	-	-	8/30/50/70	0/1/1/1
21	CLA	6	609	18	1/1/18/20	4/27/103/115	-
26	LMU	82	628	-	-	4/15/35/61	0/1/1/2
21	CLA	A	802	-	1/1/20/20	0/39/115/115	-
26	LMU	A2	865	-	-	3/15/35/61	0/1/1/2
21	CLA	A	818	-	1/1/20/20	2/39/115/115	-
21	CLA	Z	603	-	1/1/18/20	6/27/103/115	-
21	CLA	72	604	33	1/1/17/20	1/23/99/115	-
28	LUT	4	619	-	-	1/29/67/67	0/2/2/2
21	CLA	82	608	33	1/1/17/20	2/21/97/115	-
30	CHL	72	606	33	3/3/21/26	2/15/113/137	-
21	CLA	3	606	33	1/1/14/20	0/12/88/115	-
21	CLA	A2	833	-	1/1/20/20	1/39/115/115	-
24	BCR	B	801	-	-	0/29/63/63	0/2/2/2
24	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
26	LMU	12	625	-	-	4/15/35/61	0/1/1/2
21	CLA	12	602	12	1/1/19/20	2/33/109/115	-
21	CLA	Z2	613	33	1/1/20/20	2/39/115/115	-
21	CLA	42	603	16	1/1/20/20	6/39/115/115	-
21	CLA	G2	203	-	1/1/19/20	2/33/109/115	-
21	CLA	62	612	18	1/1/15/20	2/15/91/115	-
21	CLA	A	812	-	1/1/20/20	6/39/115/115	-
28	LUT	A2	856	-	-	4/29/67/67	0/2/2/2
21	CLA	B	827	-	1/1/20/20	5/39/115/115	-
21	CLA	8	613	15	1/1/20/20	7/39/115/115	-
21	CLA	A	806	-	1/1/20/20	10/39/115/115	-
21	CLA	J2	101	9	1/1/18/20	3/27/103/115	-
21	CLA	A	810	1	1/1/20/20	7/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	XAT	62	624	-	-	0/31/93/93	0/4/4/4
21	CLA	B2	840	-	1/1/20/20	7/39/115/115	-
30	CHL	52	607	33	3/3/26/26	11/39/137/137	-
28	LUT	12	617	-	-	2/29/67/67	0/2/2/2
26	LMU	B	853	-	-	7/21/61/61	0/2/2/2
21	CLA	72	614	-	1/1/14/20	5/13/89/115	-
21	CLA	6	612	18	1/1/15/20	2/15/91/115	-
21	CLA	62	610	18	1/1/19/20	0/33/109/115	-
24	BCR	B2	843	-	-	0/29/63/63	0/2/2/2
26	LMU	A2	864	-	-	2/15/35/61	0/1/1/2
21	CLA	82	609	15	1/1/15/20	0/15/91/115	-
21	CLA	A	809	1	1/1/20/20	7/39/115/115	-
30	CHL	Z	607	33	3/3/26/26	4/39/137/137	-
26	LMU	12	622	-	-	4/10/30/61	0/1/1/2
25	SF4	C	101	3	-	-	0/6/5/5
21	CLA	32	612	13	1/1/15/20	2/17/93/115	-
30	CHL	4	608	-	3/3/26/26	5/39/137/137	-
30	CHL	62	616	18	3/3/26/26	3/39/137/137	-
21	CLA	B	828	-	1/1/20/20	4/39/115/115	-
23	LHG	Z2	620	21	-	6/43/43/53	-
21	CLA	52	611	23	1/1/18/20	4/27/103/115	-
21	CLA	52	621	33	1/1/15/20	10/17/93/115	-
21	CLA	3	610	13	1/1/20/20	0/39/115/115	-
27	LMG	82	629	-	-	9/37/57/70	0/1/1/1
30	CHL	32	608	33	3/3/26/26	3/39/137/137	-
27	LMG	B	854	-	-	2/31/51/70	0/1/1/1
24	BCR	A	850	-	-	0/29/63/63	0/2/2/2
21	CLA	Z	604	33	1/1/18/20	3/30/106/115	-
30	CHL	6	601	18	3/3/26/26	5/39/137/137	-
23	LHG	6	619	21	-	4/53/53/53	-
21	CLA	L2	203	-	1/1/20/20	6/39/115/115	-
21	CLA	Z2	602	12	1/1/19/20	2/33/109/115	-
21	CLA	3	614	-	1/1/15/20	2/15/91/115	-
24	BCR	4	621	-	-	2/29/63/63	0/2/2/2
21	CLA	A2	843	33	1/1/20/20	4/39/115/115	-
31	XAT	Z2	618	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	LUT	8	617	-	-	2/29/67/67	0/2/2/2
21	CLA	7	612	14	1/1/17/20	2/24/100/115	-
21	CLA	Z	613	33	1/1/20/20	2/39/115/115	-
26	LMU	1	627	-	-	3/13/33/61	0/1/1/2
21	CLA	42	609	16	1/1/19/20	6/33/109/115	-
21	CLA	32	610	13	1/1/20/20	0/39/115/115	-
21	CLA	A	816	-	1/1/20/20	4/39/115/115	-
26	LMU	82	627	-	-	9/21/61/61	0/2/2/2
21	CLA	82	611	23	1/1/15/20	2/15/91/115	-
21	CLA	A	837	1	1/1/18/20	0/30/106/115	-
32	NEX	5	625	-	-	2/27/83/83	1/3/3/3
21	CLA	B	819	33	1/1/19/20	5/33/109/115	-
22	PQN	A2	844	-	-	3/23/43/43	0/2/2/2
27	LMG	1	628	-	-	6/37/57/70	0/1/1/1
27	LMG	9	620	21	-	6/39/59/70	0/1/1/1
21	CLA	1	603	-	1/1/18/20	6/30/106/115	-
21	CLA	B2	837	-	1/1/20/20	0/39/115/115	-
21	CLA	92	602	19	1/1/19/20	2/33/109/115	-
21	CLA	42	614	-	1/1/18/20	5/27/103/115	-
21	CLA	A2	831	-	1/1/20/20	2/39/115/115	-
21	CLA	52	616	17	1/1/17/20	7/25/101/115	-
23	LHG	A	846	-	-	9/53/53/53	-
27	LMG	A	859	-	-	9/43/63/70	0/1/1/1
28	LUT	5	620	-	-	2/29/67/67	0/2/2/2
21	CLA	K	204	-	1/1/15/20	4/17/93/115	-
21	CLA	62	622	33	1/1/18/20	2/27/103/115	-
21	CLA	L	203	-	1/1/20/20	6/39/115/115	-
21	CLA	72	611	23	1/1/20/20	7/39/115/115	-
21	CLA	B	829	-	1/1/20/20	3/39/115/115	-
21	CLA	B2	808	-	1/1/20/20	9/39/115/115	-
21	CLA	1	602	12	1/1/19/20	2/33/109/115	-
22	PQN	B	842	-	-	1/23/43/43	0/2/2/2
28	LUT	32	720	-	-	0/29/67/67	0/2/2/2
21	CLA	A	807	1	1/1/20/20	3/39/115/115	-
21	CLA	A2	817	33	1/1/18/20	4/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	CHL	62	618	18	3/3/20/26	0/12/110/137	-
21	CLA	B	830	-	1/1/15/20	0/15/91/115	-
26	LMU	7	629	-	-	4/13/53/61	0/2/2/2
23	LHG	92	622	21	-	13/45/45/53	-
24	BCR	3	719	-	-	2/29/63/63	0/2/2/2
30	CHL	4	601	16	3/3/26/26	6/39/137/137	-
21	CLA	A2	854	33	1/1/20/20	1/39/115/115	-
23	LHG	3	623	-	-	13/51/51/53	-
21	CLA	G	204	7	1/1/15/20	4/17/93/115	-
20	CL0	A	801	-	3/3/25/25	3/37/135/135	-
21	CLA	B2	807	-	1/1/18/20	4/27/103/115	-
21	CLA	7	616	14	1/1/15/20	3/17/93/115	-
21	CLA	A2	802	-	1/1/20/20	0/39/115/115	-
21	CLA	32	615	33	1/1/20/20	6/39/115/115	-
27	LMG	72	626	-	-	7/32/52/70	0/1/1/1
21	CLA	6	603	-	1/1/20/20	7/39/115/115	-
26	LMU	62	628	-	-	2/15/35/61	0/1/1/2
28	LUT	3	622	-	-	2/29/67/67	0/2/2/2
21	CLA	B	806	2	1/1/20/20	2/39/115/115	-
21	CLA	A2	845	23	1/1/15/20	2/15/91/115	-
21	CLA	A2	821	-	1/1/18/20	4/27/103/115	-
30	CHL	6	618	18	3/3/20/26	0/12/110/137	-
26	LMU	8	624	-	-	1/15/35/61	0/1/1/2
21	CLA	9	602	19	1/1/19/20	2/33/109/115	-
21	CLA	A2	807	1	1/1/20/20	3/39/115/115	-
21	CLA	A2	822	33	1/1/20/20	0/39/115/115	-
21	CLA	12	616	12	1/1/15/20	2/17/93/115	-
26	LMU	B2	853	-	-	7/21/61/61	0/2/2/2
21	CLA	A	843	33	1/1/20/20	5/39/115/115	-
21	CLA	8	609	15	1/1/15/20	0/15/91/115	-
23	LHG	1	620	21	-	7/43/43/53	-
21	CLA	B2	813	-	1/1/20/20	3/39/115/115	-
26	LMU	A	861	-	-	2/15/35/61	0/1/1/2
26	LMU	A2	857	-	-	3/20/60/61	0/2/2/2
21	CLA	B	836	-	1/1/19/20	4/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	CLA	4	610	16	1/1/19/20	3/33/109/115	-
21	CLA	3	612	13	1/1/15/20	2/17/93/115	-

The worst 5 of 2327 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	9	607	CHL	C1B-C2B	7.62	1.48	1.39
30	62	601	CHL	MG-NB	-7.46	1.91	2.05
30	6	601	CHL	MG-NB	-7.43	1.91	2.05
30	Z	601	CHL	MG-NB	-7.41	1.91	2.05
30	Z2	601	CHL	MG-NB	-7.41	1.91	2.05

The worst 5 of 1399 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A2	801	CL0	C1B-CHB-C4A	10.02	127.77	121.32
20	A	801	CL0	C1B-CHB-C4A	10.01	127.76	121.32
30	8	601	CHL	C1B-CHB-C4A	4.95	124.51	121.32
30	82	601	CHL	C1B-CHB-C4A	4.92	124.49	121.32
30	82	607	CHL	C1B-CHB-C4A	4.79	124.41	121.32

5 of 584 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	A	801	CL0	NC
20	A	801	CL0	ND
20	A	801	CL0	NA
20	A2	801	CL0	NC
20	A2	801	CL0	ND

5 of 2606 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
21	A	806	CLA	CAD-CBD-CGD-O1D
21	A	806	CLA	CAD-CBD-CGD-O2D
21	A	806	CLA	C4-C3-C5-C6
21	A	809	CLA	CHA-CBD-CGD-O1D
21	A	809	CLA	CHA-CBD-CGD-O2D

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
32	52	625	NEX	C1-C2-C3-C4-C5-C6
32	5	625	NEX	C1-C2-C3-C4-C5-C6

300 monomers are involved in 403 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	L	201	BCR	1	0
21	B	802	CLA	2	0
23	42	623	LHG	1	0
27	A	860	LMG	1	0
30	72	601	CHL	2	0
21	Z	616	CLA	2	0
30	6	606	CHL	1	0
21	1	613	CLA	1	0
21	B	823	CLA	1	0
28	F	305	LUT	3	0
21	A2	809	CLA	2	0
21	A	831	CLA	2	0
21	B	821	CLA	1	0
30	82	601	CHL	1	0
21	52	617	CLA	1	0
24	B	845	BCR	3	0
21	K2	201	CLA	2	0
24	3	620	BCR	1	0
21	A2	811	CLA	2	0
21	B2	834	CLA	1	0
24	A	849	BCR	2	0
21	B	841	CLA	2	0
31	72	622	XAT	1	0
21	82	613	CLA	1	0
24	B2	847	BCR	1	0
26	A2	858	LMU	1	0
21	4	609	CLA	1	0
24	B	844	BCR	3	0
21	B	833	CLA	1	0
30	Z	601	CHL	1	0
24	B	843	BCR	2	0
28	7	624	LUT	4	0
21	32	602	CLA	1	0
21	3	609	CLA	1	0
21	52	602	CLA	1	0
23	5	623	LHG	1	0
28	Z	617	LUT	2	0
21	B2	814	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A2	813	CLA	2	0
26	72	628	LMU	1	0
21	B	837	CLA	2	0
21	8	612	CLA	1	0
24	9	623	BCR	1	0
28	32	622	LUT	2	0
26	Z2	622	LMU	1	0
21	72	608	CLA	1	0
30	62	601	CHL	3	0
21	B2	832	CLA	1	0
24	8	619	BCR	2	0
30	8	606	CHL	1	0
28	6	621	LUT	1	0
24	A	852	BCR	4	0
24	A2	852	BCR	2	0
27	8	626	LMG	1	0
21	B2	823	CLA	1	0
21	72	609	CLA	1	0
30	62	608	CHL	2	0
23	12	620	LHG	1	0
21	A	822	CLA	1	0
21	5	621	CLA	3	0
24	42	621	BCR	1	0
21	A	803	CLA	1	0
21	82	604	CLA	1	0
27	J2	104	LMG	1	0
21	B	817	CLA	1	0
24	A	848	BCR	3	0
26	7	628	LMU	1	0
24	K2	207	BCR	2	0
28	92	616	LUT	1	0
21	7	608	CLA	1	0
29	B2	850	DGD	1	0
24	82	619	BCR	2	0
21	B	834	CLA	1	0
23	52	623	LHG	1	0
30	42	607	CHL	1	0
21	A2	804	CLA	1	0
21	Z2	611	CLA	1	0
24	32	719	BCR	4	0
21	F	304	CLA	1	0
26	A	863	LMU	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
26	Z	622	LMU	1	0
21	B2	817	CLA	1	0
21	7	609	CLA	1	0
21	3	611	CLA	1	0
24	B2	844	BCR	2	0
24	62	623	BCR	1	0
21	42	610	CLA	1	0
30	4	606	CHL	2	0
26	9	624	LMU	1	0
30	4	607	CHL	1	0
21	52	610	CLA	1	0
21	B2	826	CLA	1	0
24	3	718	BCR	1	0
24	6	623	BCR	2	0
21	A2	835	CLA	1	0
21	A	840	CLA	1	0
28	1	617	LUT	2	0
21	6	602	CLA	1	0
21	3	602	CLA	1	0
30	62	606	CHL	1	0
24	L	205	BCR	4	0
27	A2	860	LMG	1	0
21	B	816	CLA	2	0
21	72	620	CLA	1	0
30	3	608	CHL	2	0
28	F2	305	LUT	2	0
23	72	625	LHG	1	0
30	6	608	CHL	2	0
21	B	835	CLA	1	0
21	4	614	CLA	1	0
24	I	172	BCR	1	0
21	A	813	CLA	3	0
21	Z2	603	CLA	3	0
21	9	614	CLA	1	0
21	F2	304	CLA	1	0
21	A2	812	CLA	1	0
21	72	610	CLA	3	0
21	5	603	CLA	3	0
21	B2	806	CLA	1	0
21	12	603	CLA	3	0
21	Z	610	CLA	1	0
24	L2	205	BCR	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	A2	850	BCR	3	0
32	62	625	NEX	1	0
21	82	603	CLA	1	0
30	62	607	CHL	1	0
23	32	623	LHG	1	0
28	42	619	LUT	1	0
21	32	603	CLA	2	0
21	B2	829	CLA	6	0
21	A	804	CLA	1	0
21	7	620	CLA	1	0
30	82	606	CHL	1	0
30	7	601	CHL	3	0
24	K	207	BCR	2	0
24	B2	801	BCR	3	0
21	32	609	CLA	1	0
28	9	616	LUT	1	0
26	A	858	LMU	2	0
21	Z2	616	CLA	2	0
21	8	603	CLA	1	0
28	62	621	LUT	1	0
21	B2	841	CLA	2	0
21	B2	822	CLA	1	0
21	Z	608	CLA	1	0
21	7	610	CLA	3	0
21	B2	836	CLA	1	0
21	B2	802	CLA	3	0
21	32	611	CLA	1	0
21	K	201	CLA	2	0
21	A2	840	CLA	1	0
21	B2	821	CLA	1	0
24	A2	848	BCR	2	0
31	6	624	XAT	1	0
28	9	617	LUT	2	0
28	92	617	LUT	2	0
31	1	618	XAT	1	0
21	62	603	CLA	1	0
21	B2	827	CLA	1	0
21	B	839	CLA	1	0
21	8	604	CLA	1	0
21	3	603	CLA	2	0
21	12	613	CLA	1	0
21	92	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
30	1	601	CHL	1	0
24	K2	202	BCR	4	0
27	92	620	LMG	1	0
21	B2	835	CLA	1	0
21	52	603	CLA	3	0
24	B	847	BCR	1	0
21	A	829	CLA	3	0
21	32	607	CLA	1	0
21	3	615	CLA	5	0
21	Z2	608	CLA	1	0
21	A2	820	CLA	1	0
21	5	616	CLA	3	0
30	5	608	CHL	1	0
21	42	613	CLA	3	0
24	92	623	BCR	2	0
21	B	808	CLA	1	0
21	A	854	CLA	2	0
21	A2	806	CLA	1	0
24	J2	102	BCR	1	0
30	52	608	CHL	1	0
24	A2	849	BCR	2	0
24	A2	851	BCR	1	0
21	J	101	CLA	1	0
26	42	625	LMU	1	0
21	4	613	CLA	2	0
21	A2	832	CLA	1	0
26	4	625	LMU	1	0
26	A	857	LMU	1	0
27	3	722	LMG	1	0
27	J2	103	LMG	1	0
21	B	814	CLA	1	0
21	A	817	CLA	1	0
21	A	835	CLA	1	0
27	J	103	LMG	1	0
21	A	833	CLA	3	0
21	A2	818	CLA	1	0
27	B2	854	LMG	1	0
32	6	625	NEX	1	0
28	A	856	LUT	1	0
21	62	602	CLA	1	0
21	A2	830	CLA	1	0
21	A2	803	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
21	A2	810	CLA	1	0
30	8	601	CHL	1	0
23	4	623	LHG	1	0
26	8	627	LMU	1	0
21	5	602	CLA	1	0
30	6	607	CHL	1	0
24	G2	205	BCR	2	0
24	L2	201	BCR	1	0
21	A2	829	CLA	2	0
21	B	840	CLA	2	0
24	B	848	BCR	1	0
23	7	625	LHG	1	0
24	I2	172	BCR	1	0
24	B2	848	BCR	1	0
21	3	607	CLA	1	0
24	J	102	BCR	1	0
28	52	620	LUT	3	0
29	B	850	DGD	1	0
21	A	811	CLA	3	0
30	Z2	601	CHL	1	0
30	42	601	CHL	1	0
21	B	826	CLA	1	0
28	72	624	LUT	4	0
21	Z2	610	CLA	1	0
21	B2	816	CLA	2	0
27	32	722	LMG	1	0
21	B	822	CLA	1	0
31	12	618	XAT	1	0
21	B2	839	CLA	1	0
28	Z2	617	LUT	2	0
26	A	862	LMU	2	0
28	82	617	LUT	1	0
26	92	624	LMU	1	0
24	A	851	BCR	3	0
24	K	202	BCR	3	0
27	J	104	LMG	1	0
21	A	802	CLA	2	0
21	A	818	CLA	1	0
21	Z	603	CLA	2	0
28	4	619	LUT	1	0
21	A2	833	CLA	3	0
24	B	801	BCR	1	0

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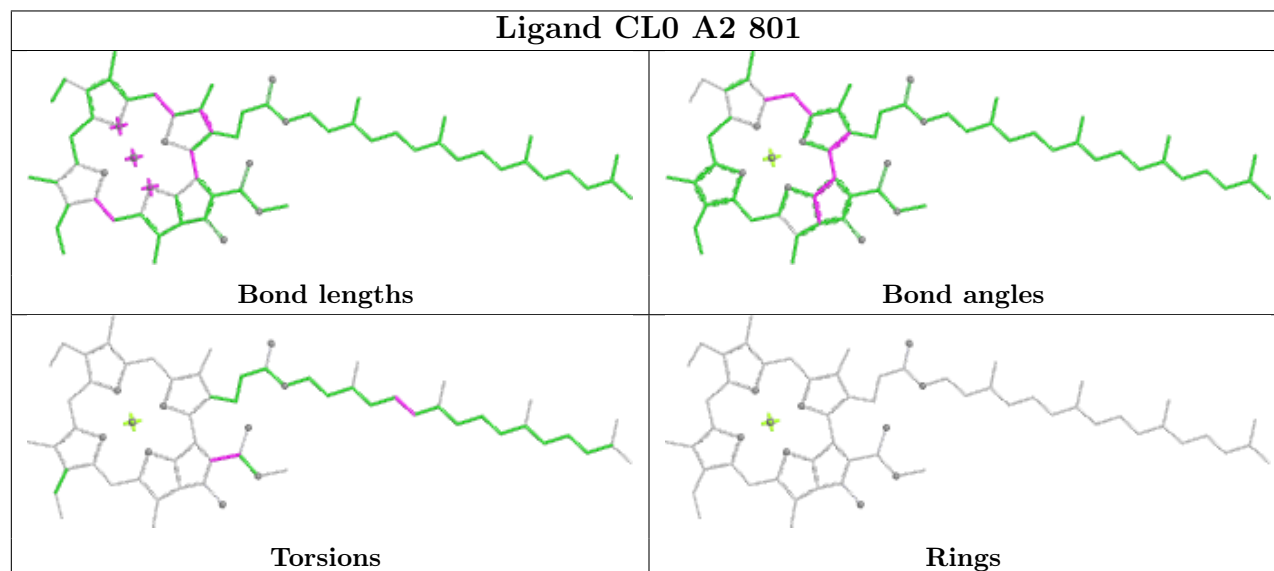
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21	12	602	CLA	1	0
21	Z2	613	CLA	1	0
21	A	812	CLA	1	0
28	A2	856	LUT	2	0
21	B	827	CLA	1	0
21	8	613	CLA	1	0
21	J2	101	CLA	1	0
21	A	810	CLA	2	0
31	62	624	XAT	1	0
21	B2	840	CLA	3	0
28	12	617	LUT	2	0
26	B	853	LMU	3	0
24	B2	843	BCR	2	0
21	A	809	CLA	2	0
23	Z2	620	LHG	1	0
21	52	621	CLA	2	0
21	3	610	CLA	2	0
30	32	608	CHL	3	0
27	B	854	LMG	1	0
24	A	850	BCR	1	0
30	6	601	CHL	3	0
21	A2	843	CLA	1	0
21	Z	613	CLA	1	0
21	32	610	CLA	3	0
27	9	620	LMG	1	0
21	1	603	CLA	3	0
21	B2	837	CLA	1	0
21	42	614	CLA	1	0
21	A2	831	CLA	1	0
21	52	616	CLA	2	0
28	5	620	LUT	3	0
21	L	203	CLA	1	0
21	B	829	CLA	6	0
21	B2	808	CLA	1	0
21	1	602	CLA	1	0
21	A2	817	CLA	1	0
24	3	719	BCR	5	0
30	4	601	CHL	1	0
21	A2	854	CLA	3	0
23	3	623	LHG	1	0
21	A2	802	CLA	2	0

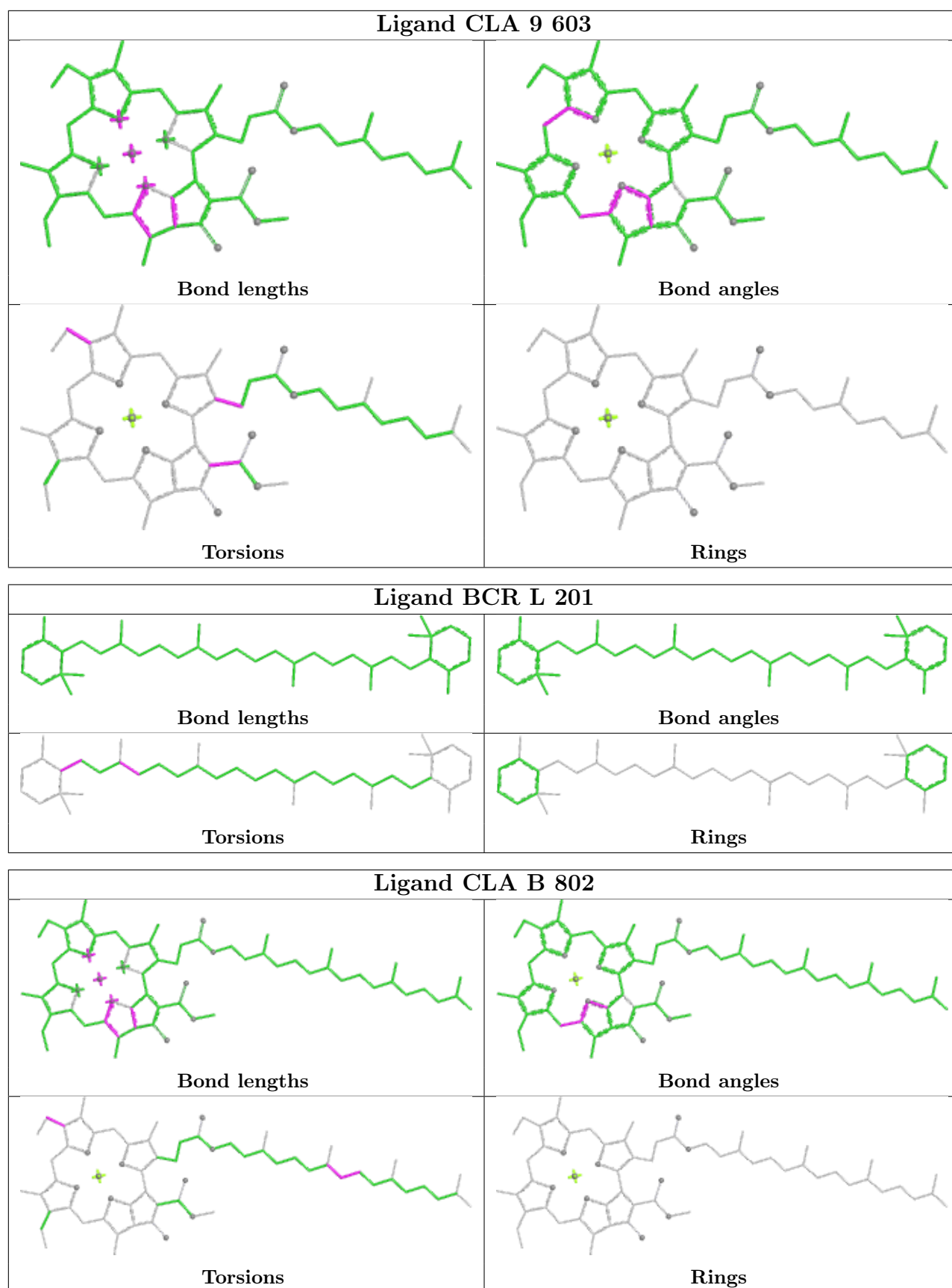
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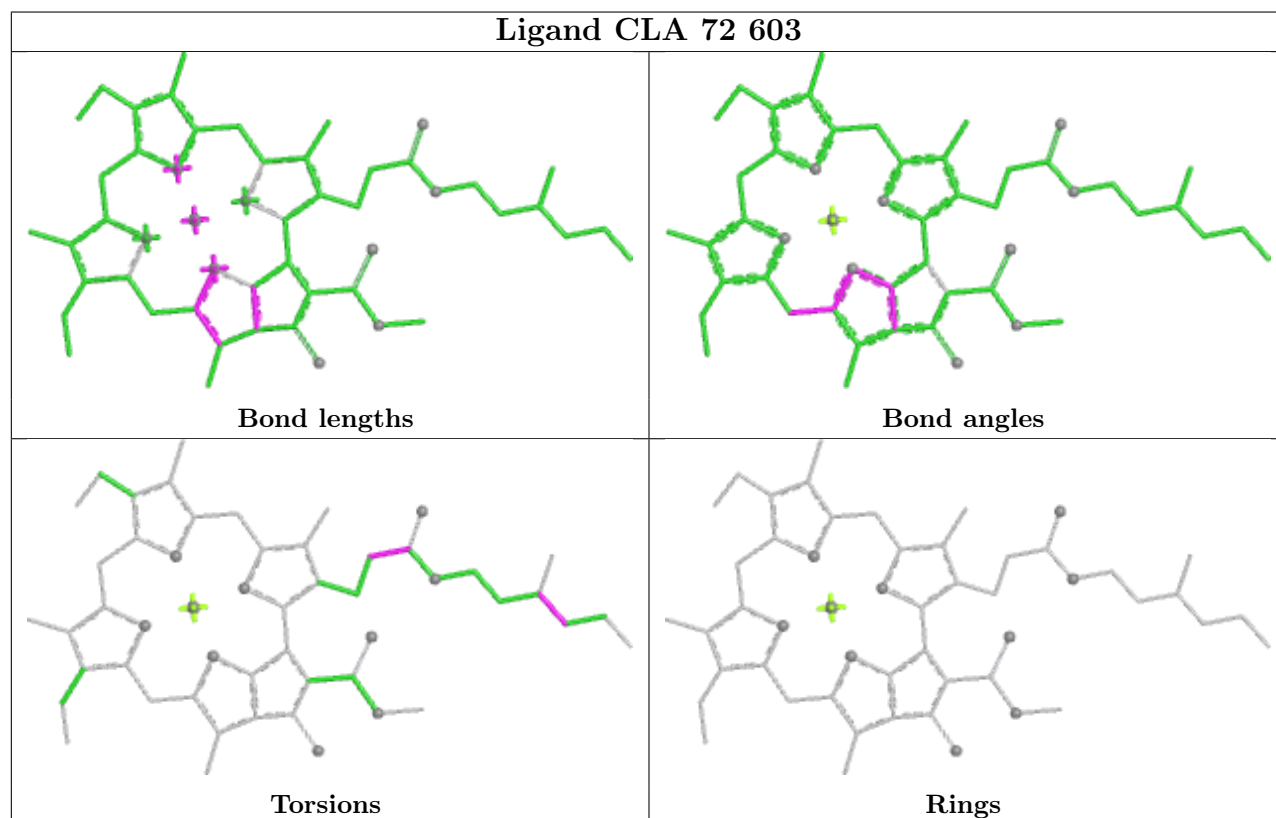
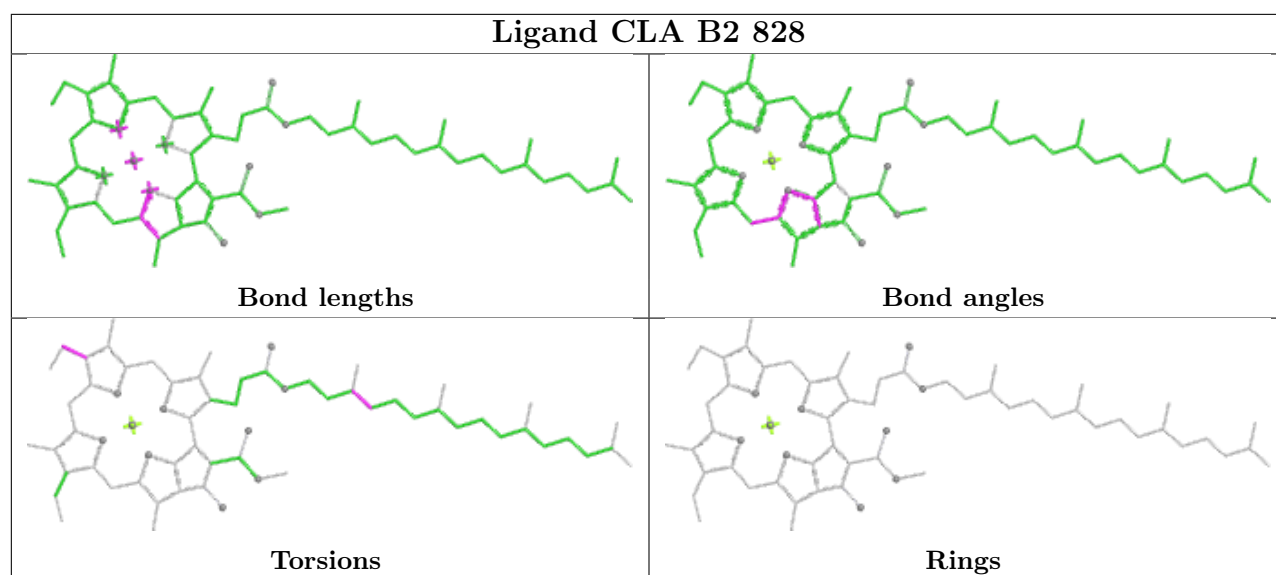
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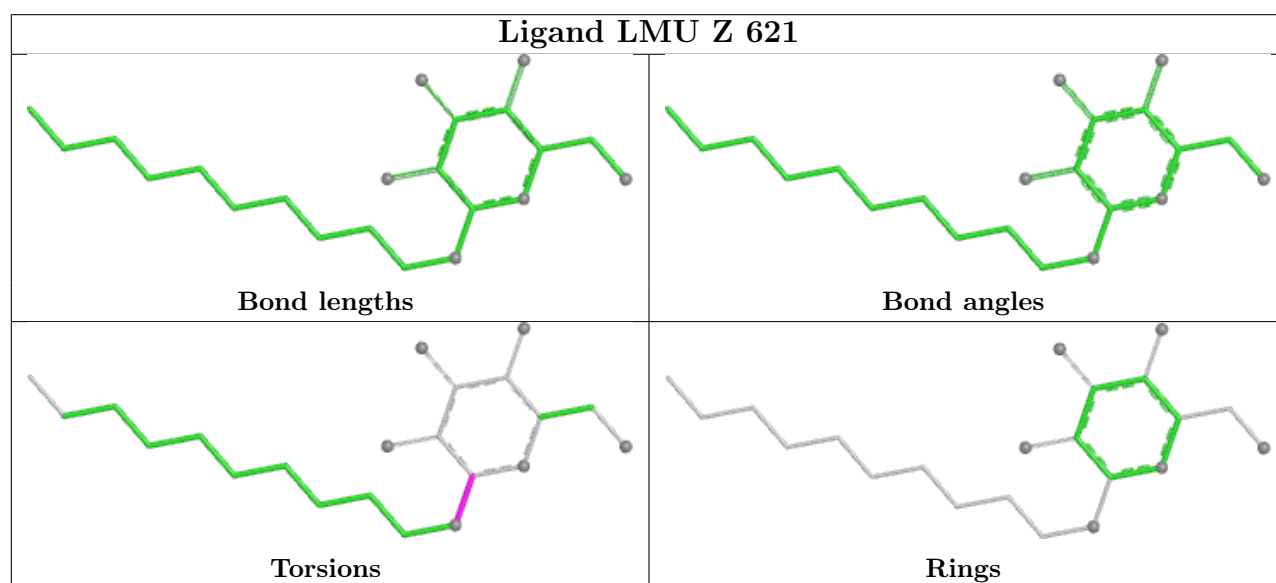
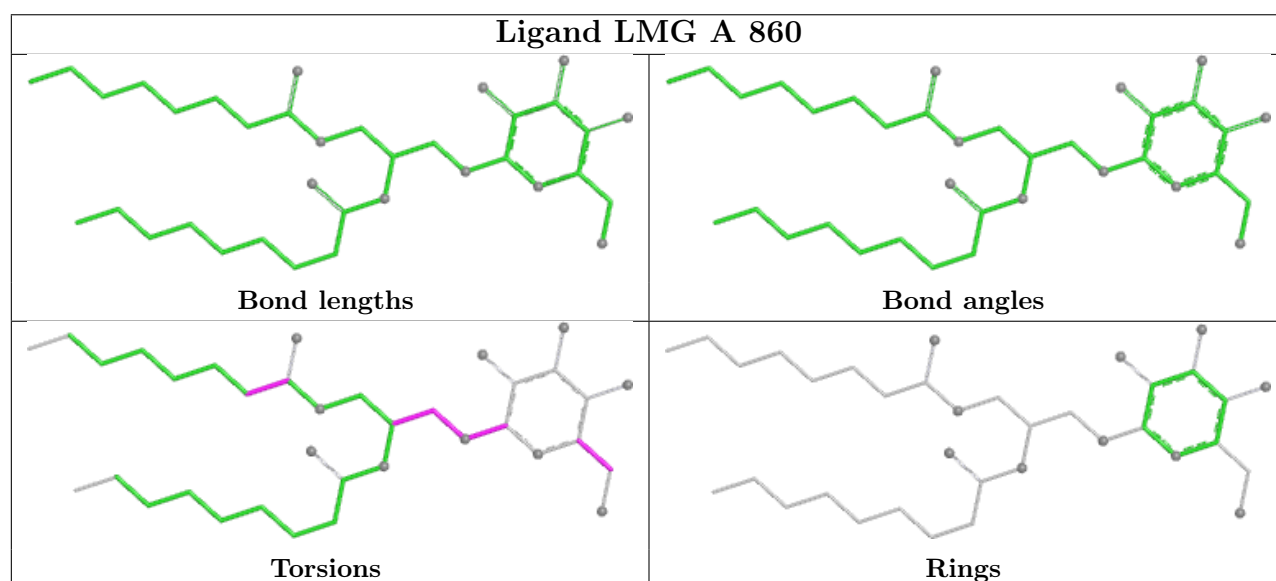
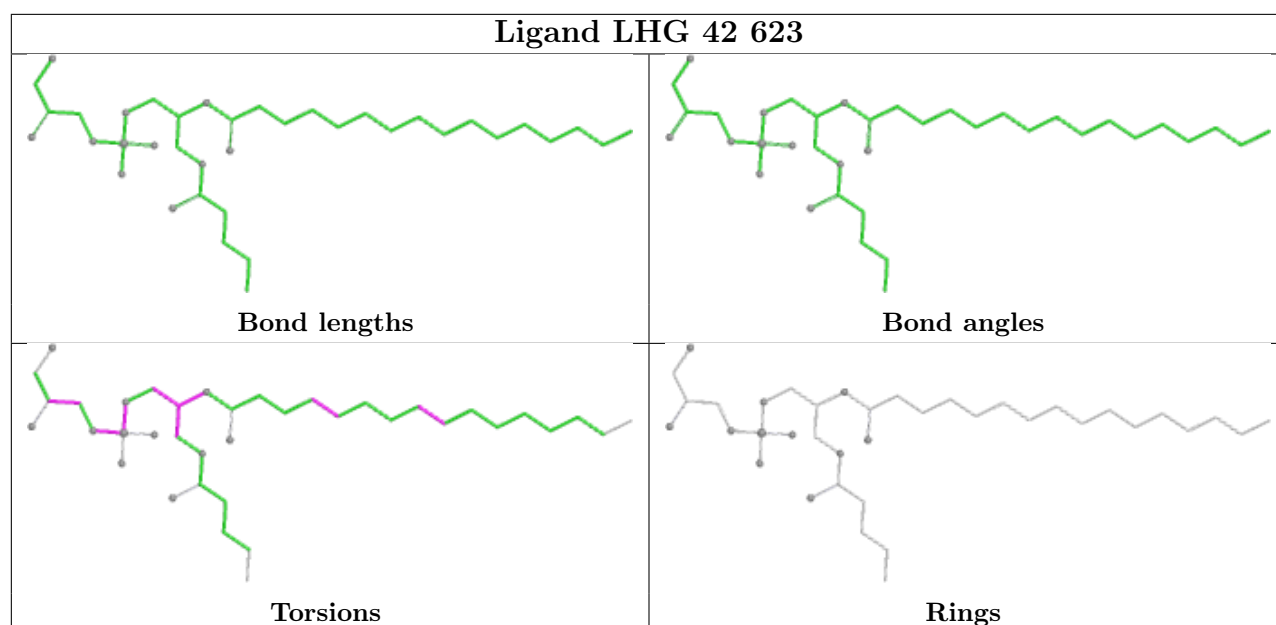
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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21	6	603	CLA	1	0
28	3	622	LUT	2	0
21	B	806	CLA	1	0
21	A2	822	CLA	1	0
26	B2	853	LMU	2	0
21	A	843	CLA	1	0
23	1	620	LHG	1	0
26	A2	857	LMU	1	0
21	B	836	CLA	1	0

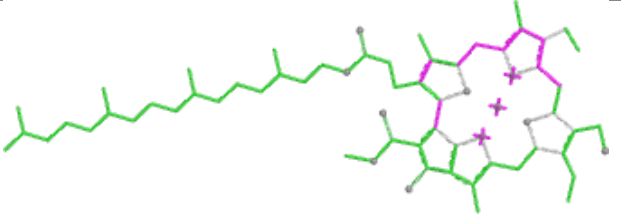
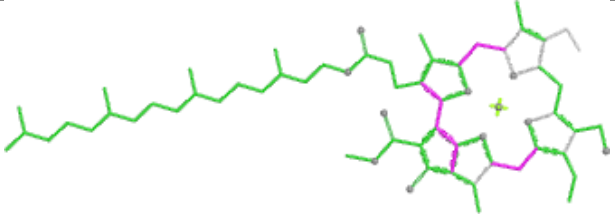
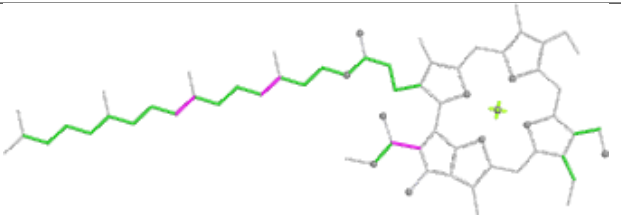
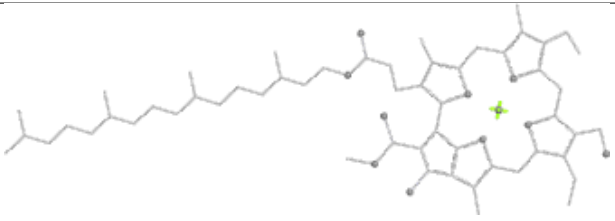
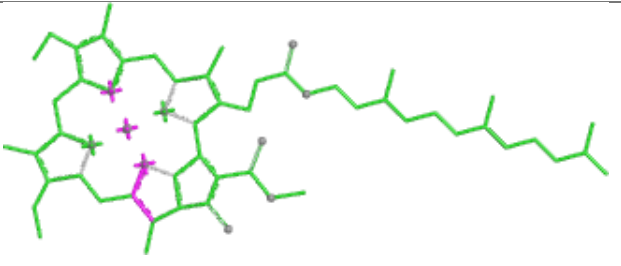
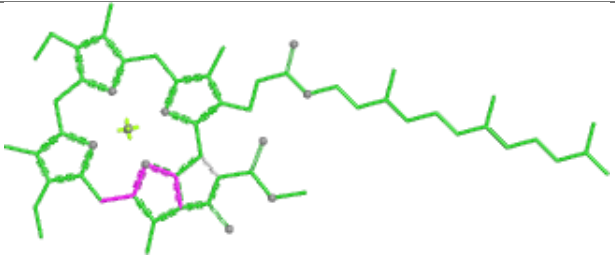
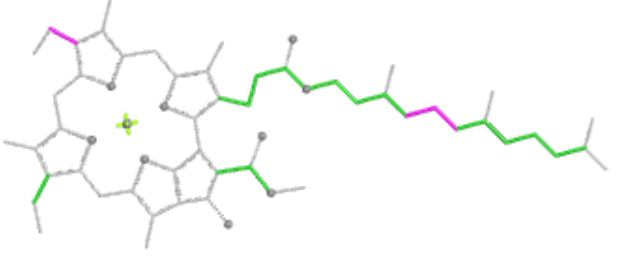
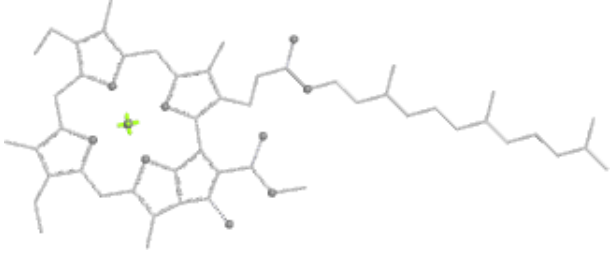
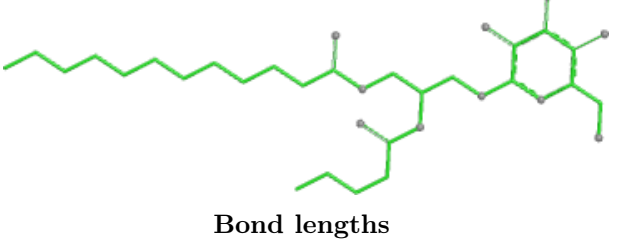
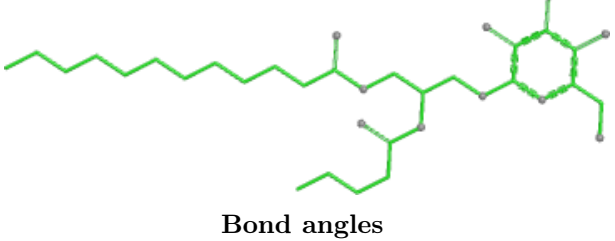
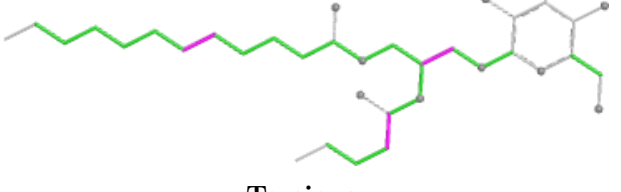
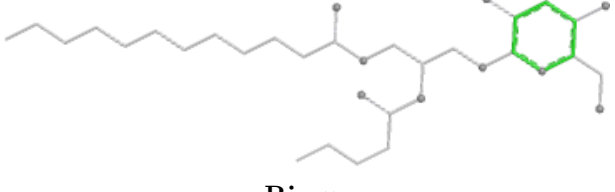
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



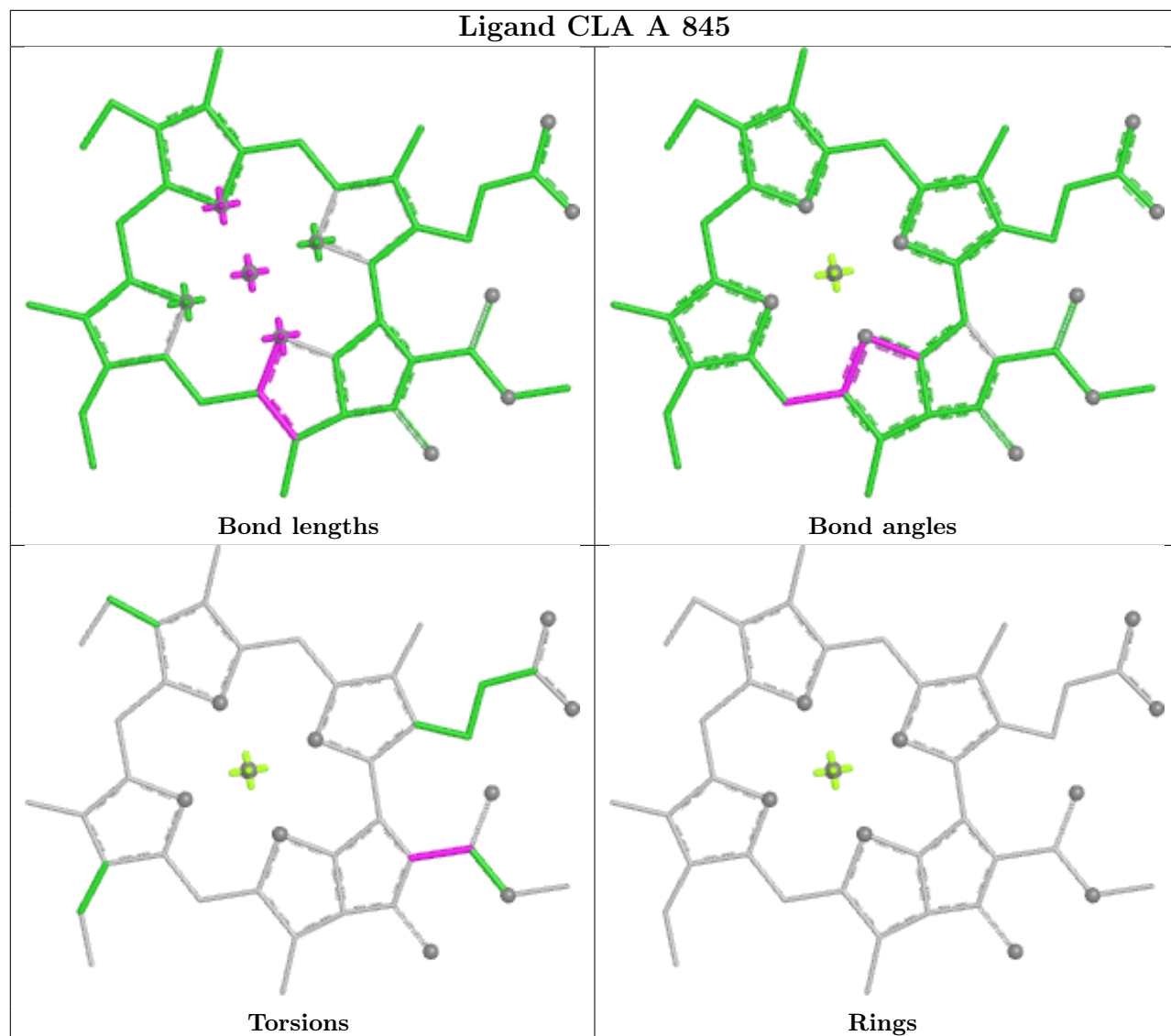




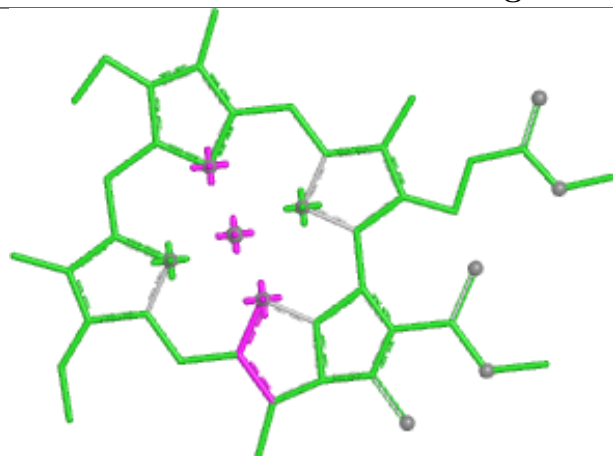


Ligand CHL 72 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA Z 616	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 12 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

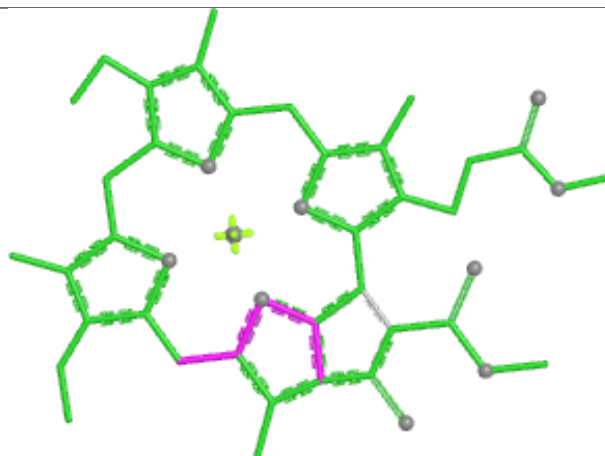
Ligand CLA A 845



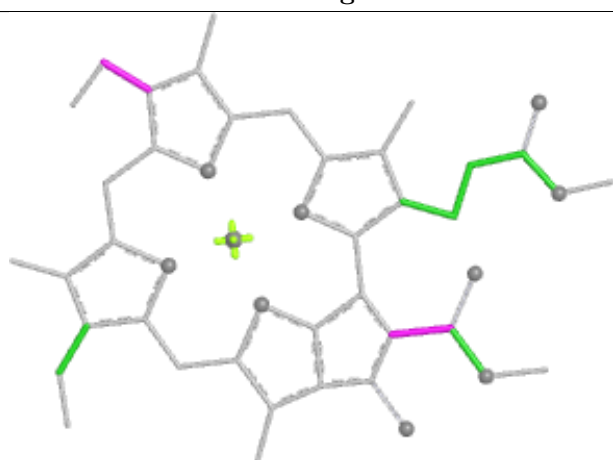
Ligand CLA K2 204



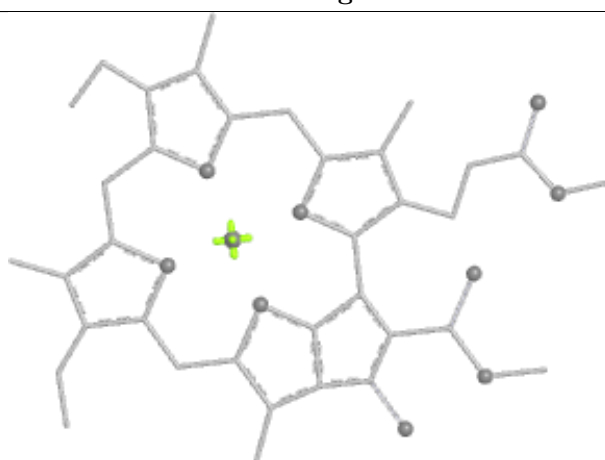
Bond lengths



Bond angles

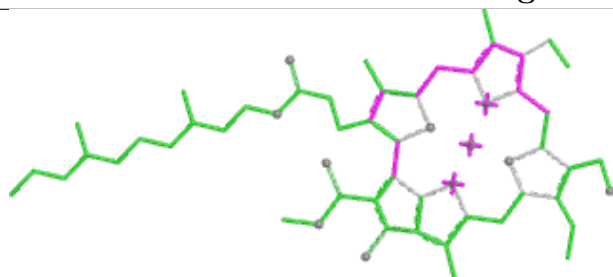


Torsions

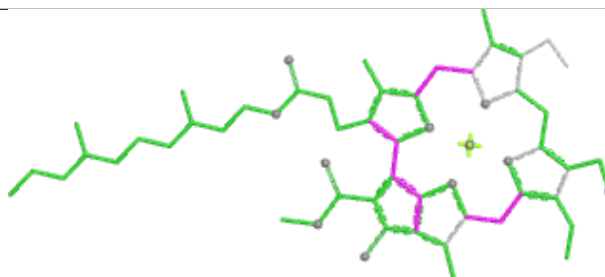


Rings

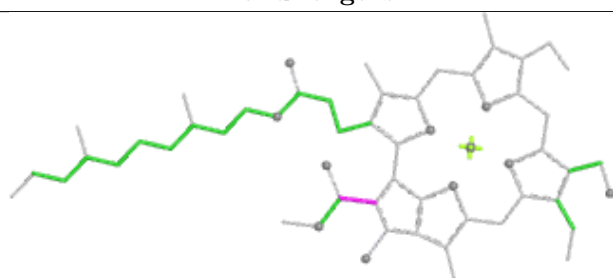
Ligand CHL 6 606



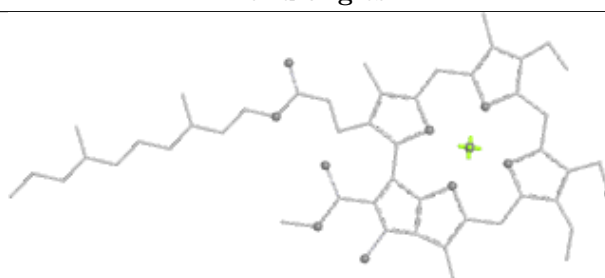
Bond lengths



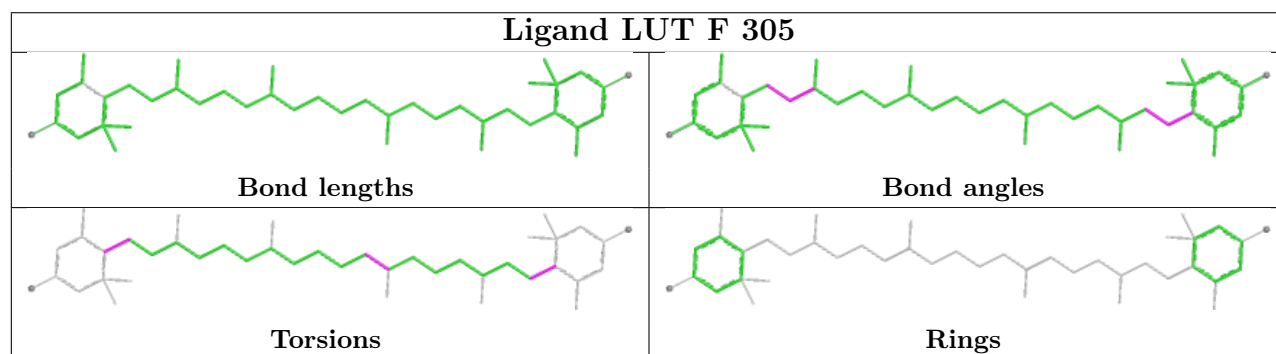
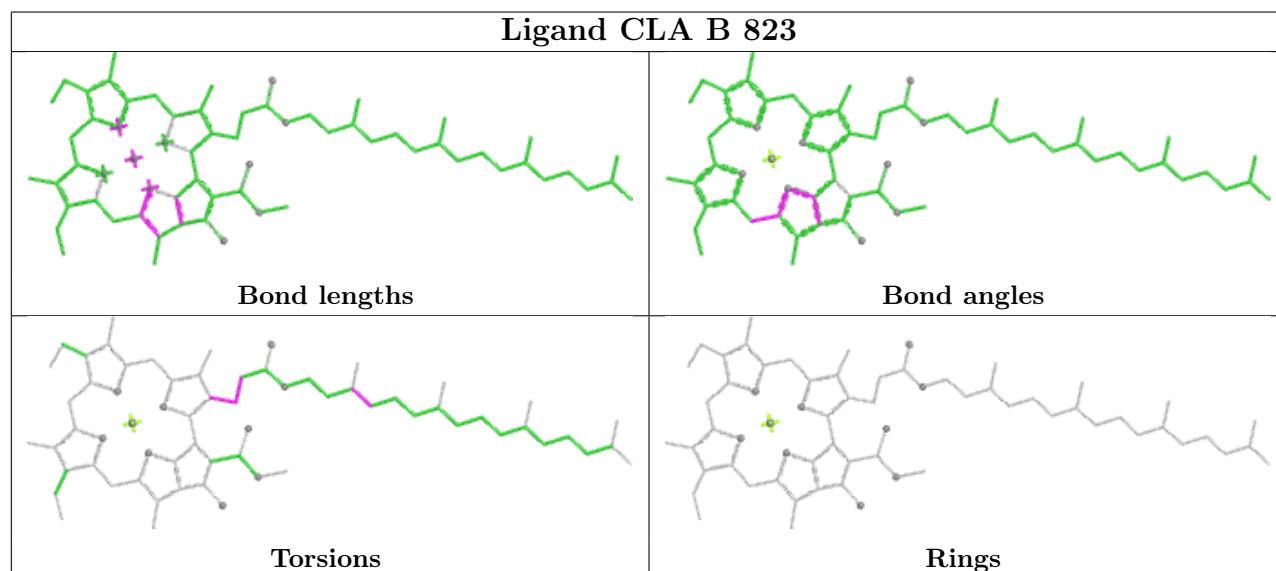
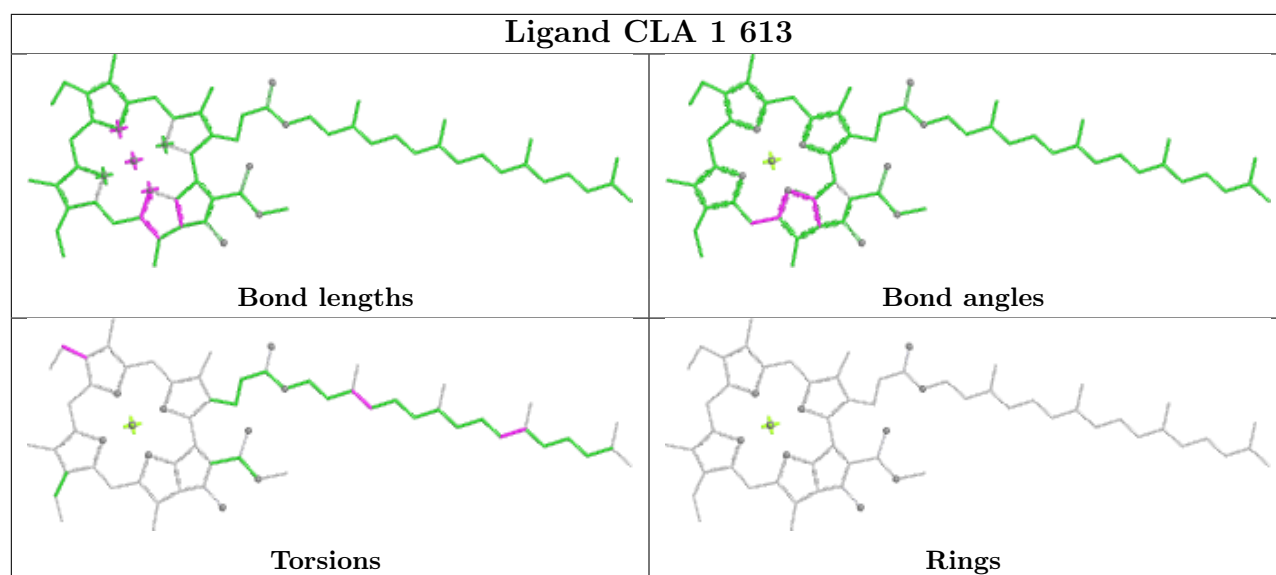
Bond angles

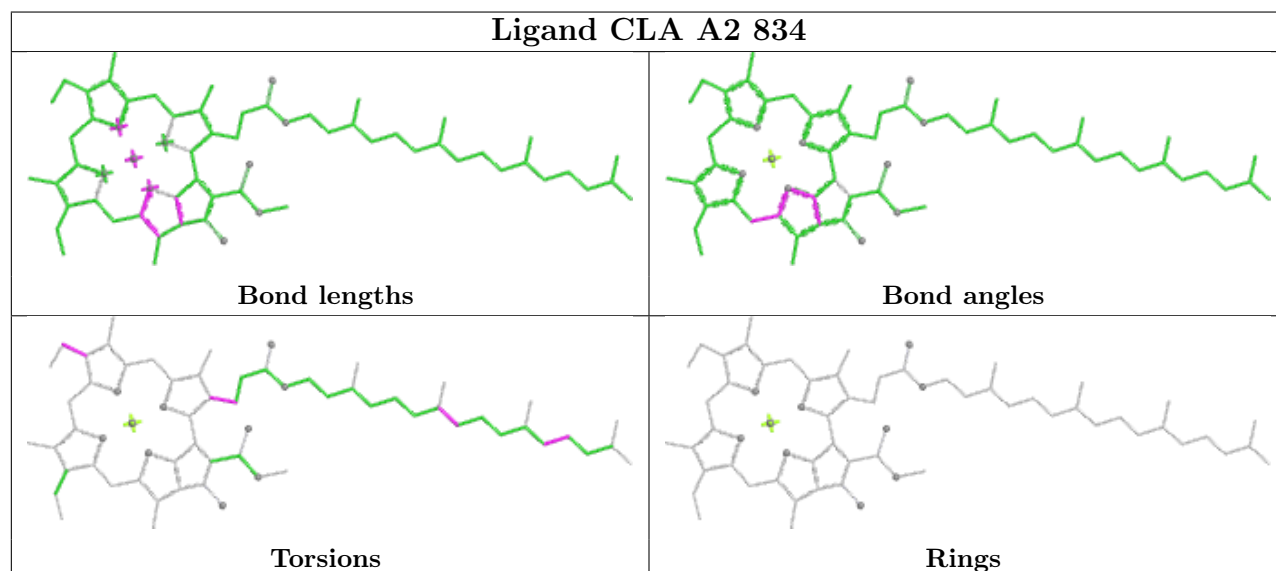
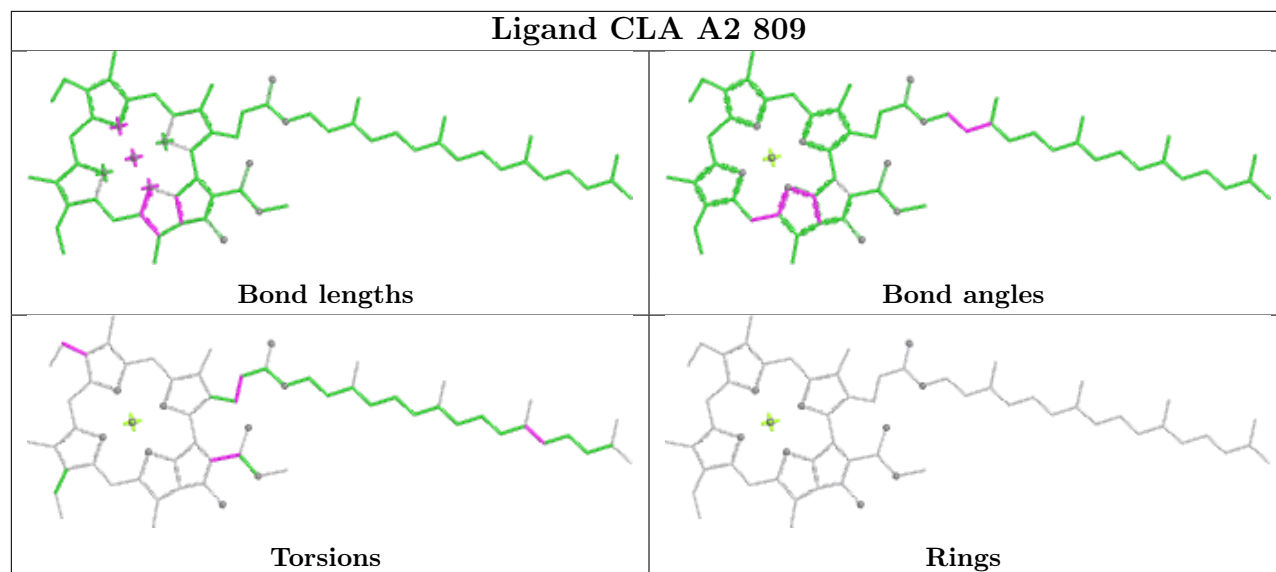


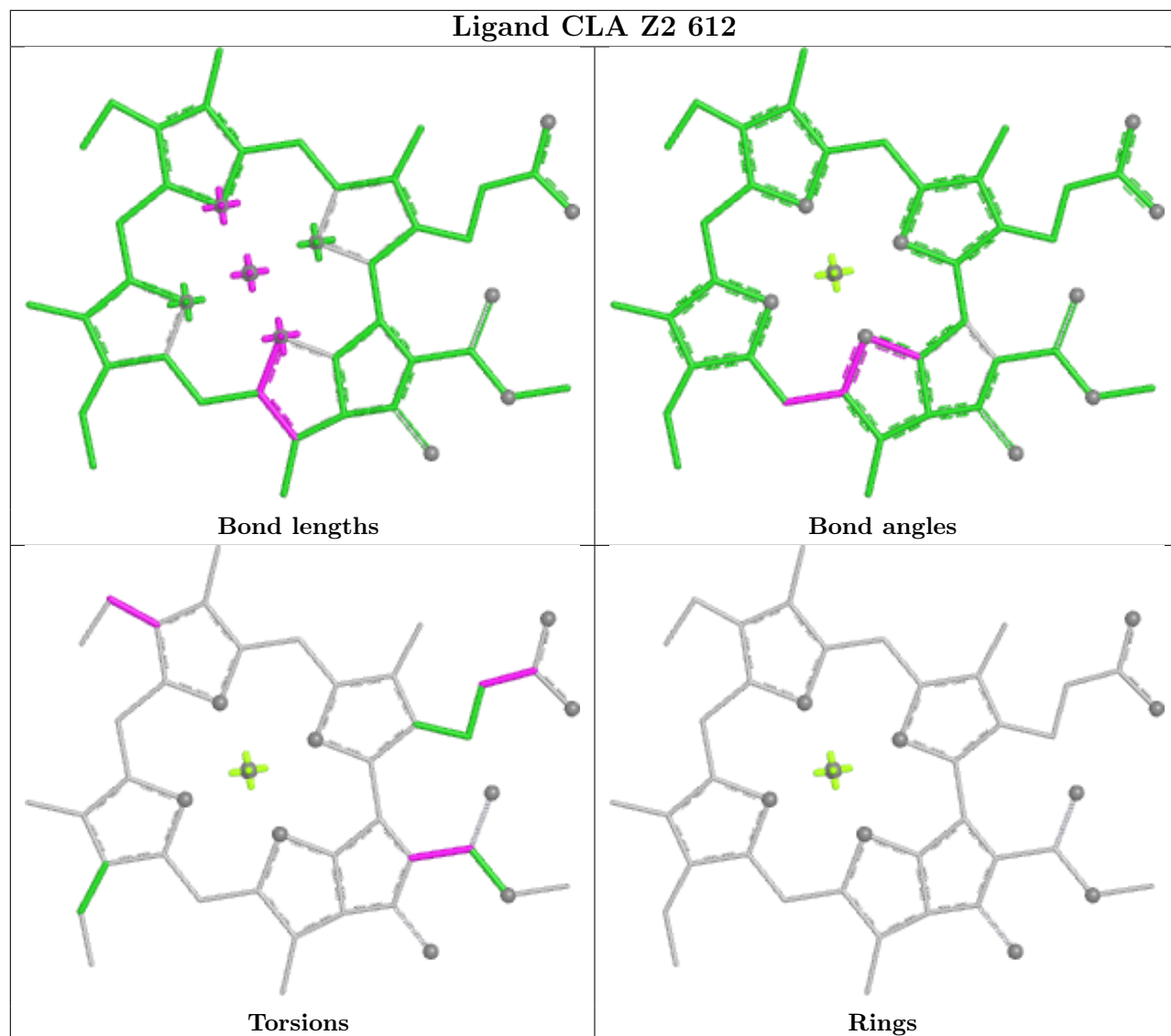
Torsions

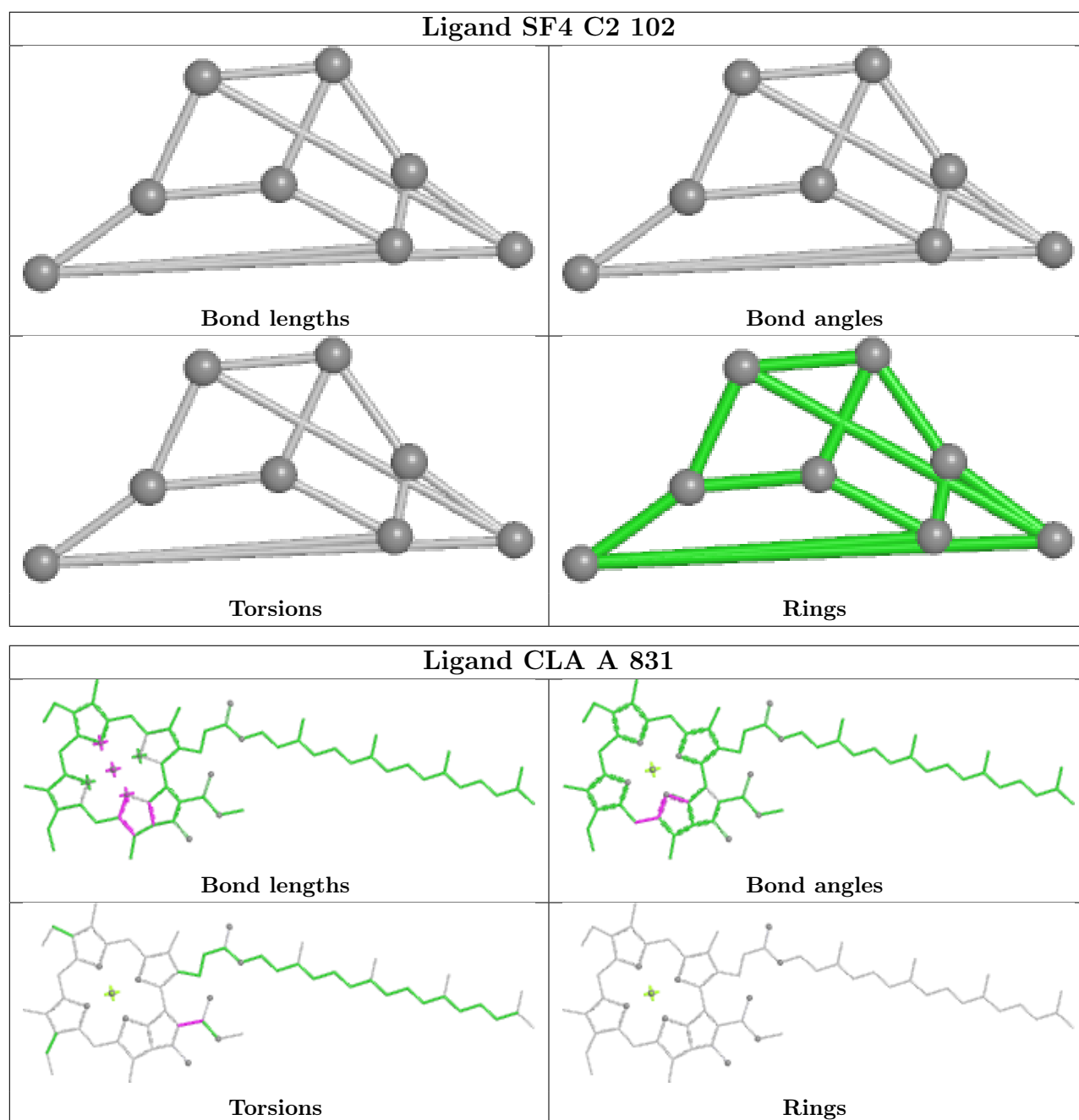


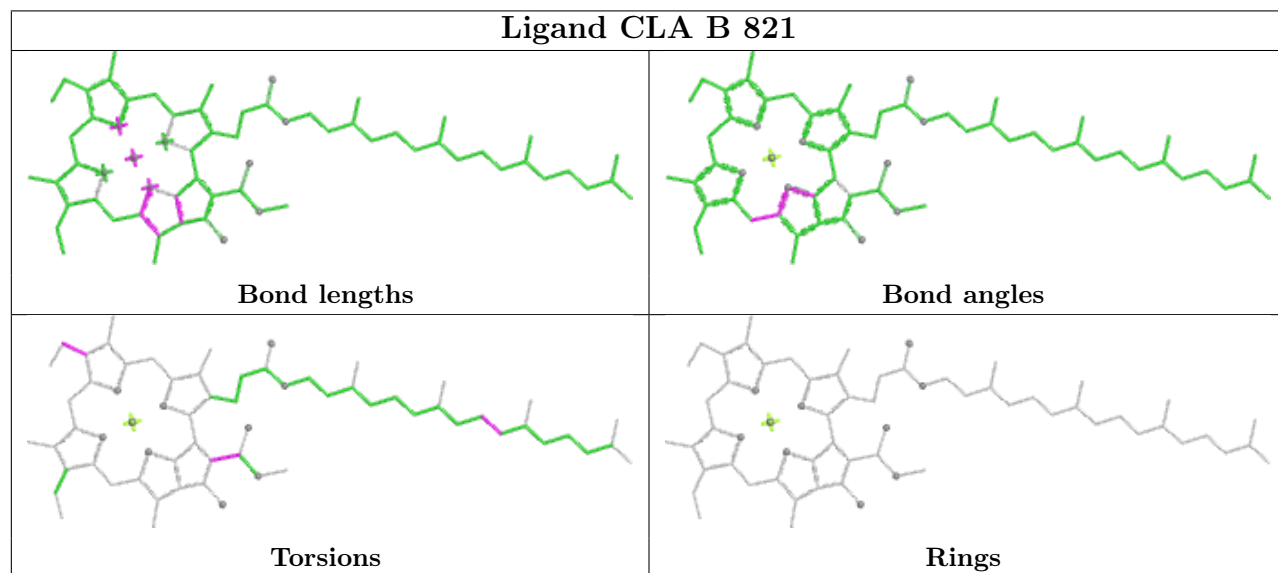
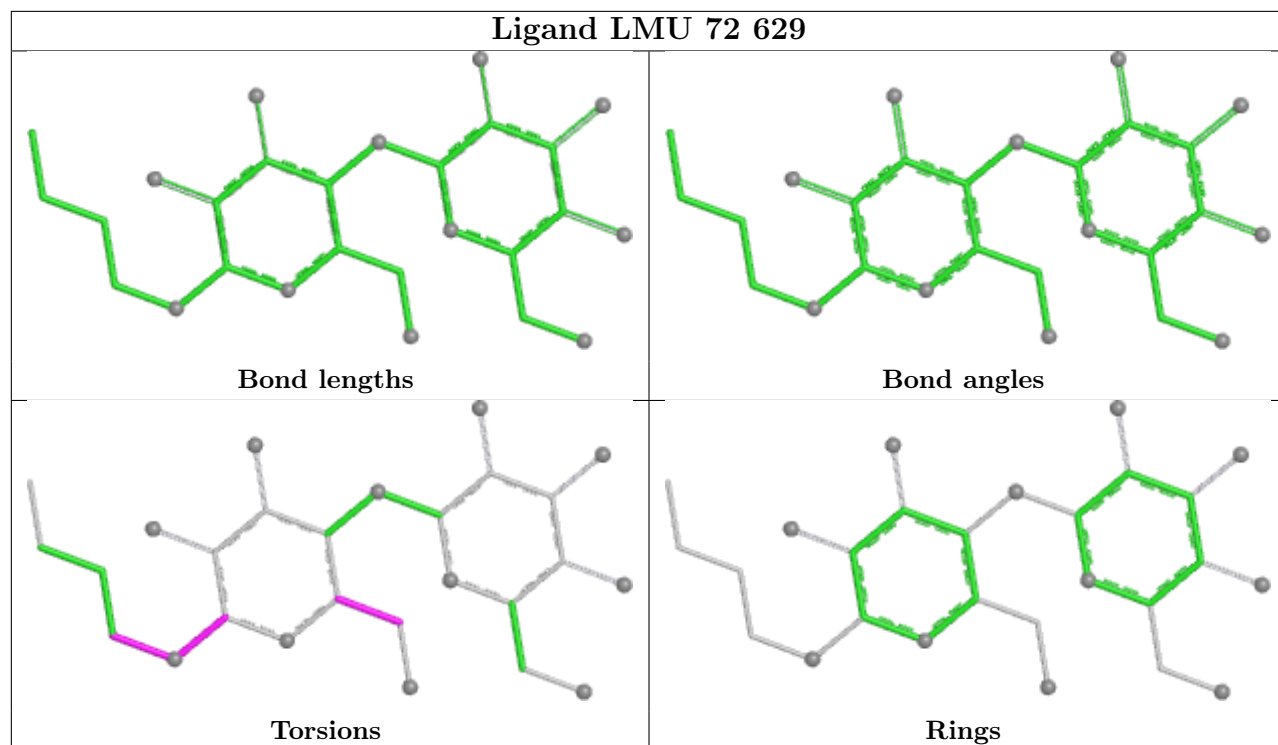
Rings

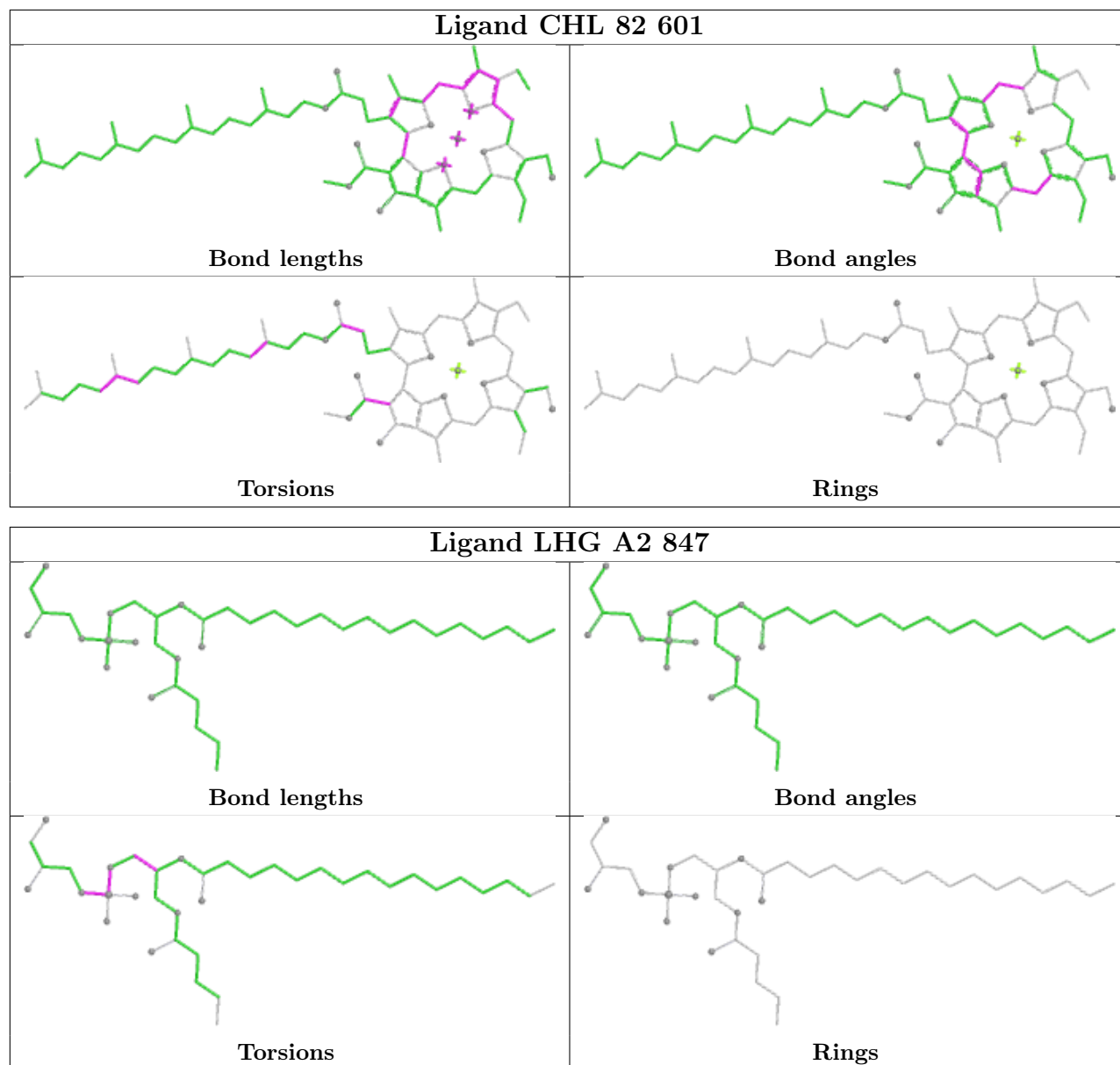


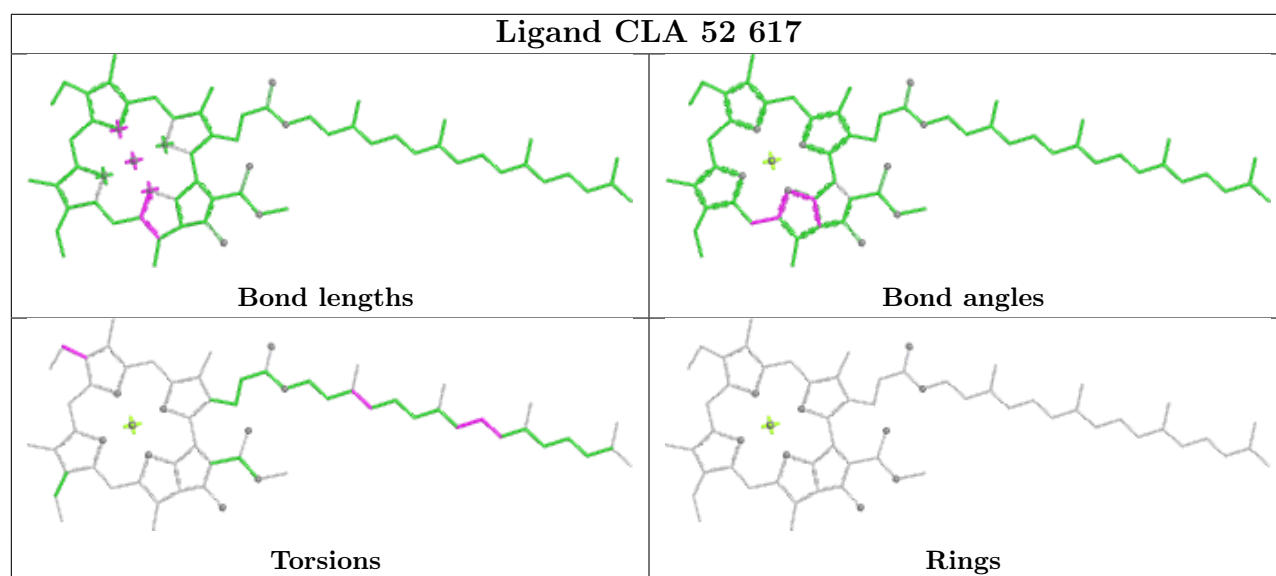
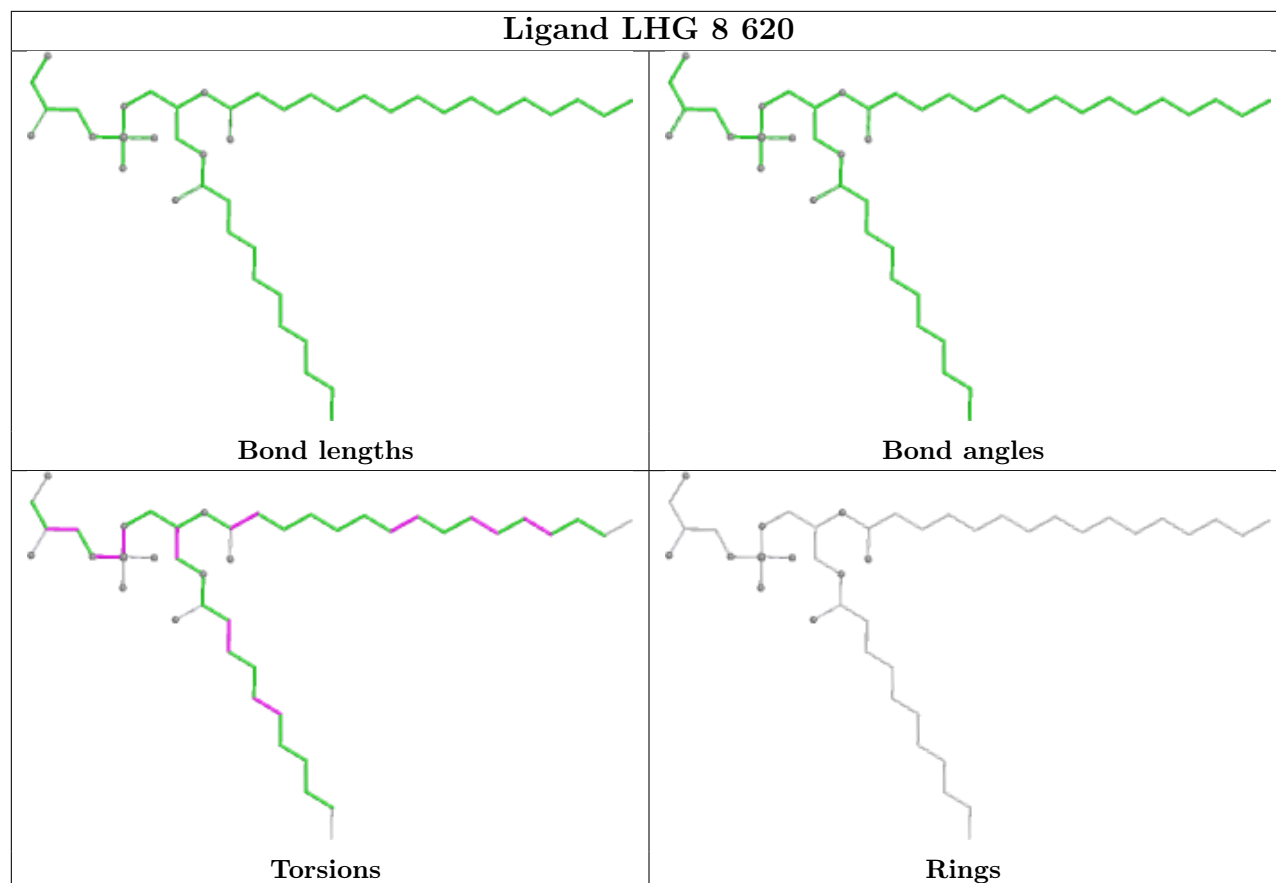


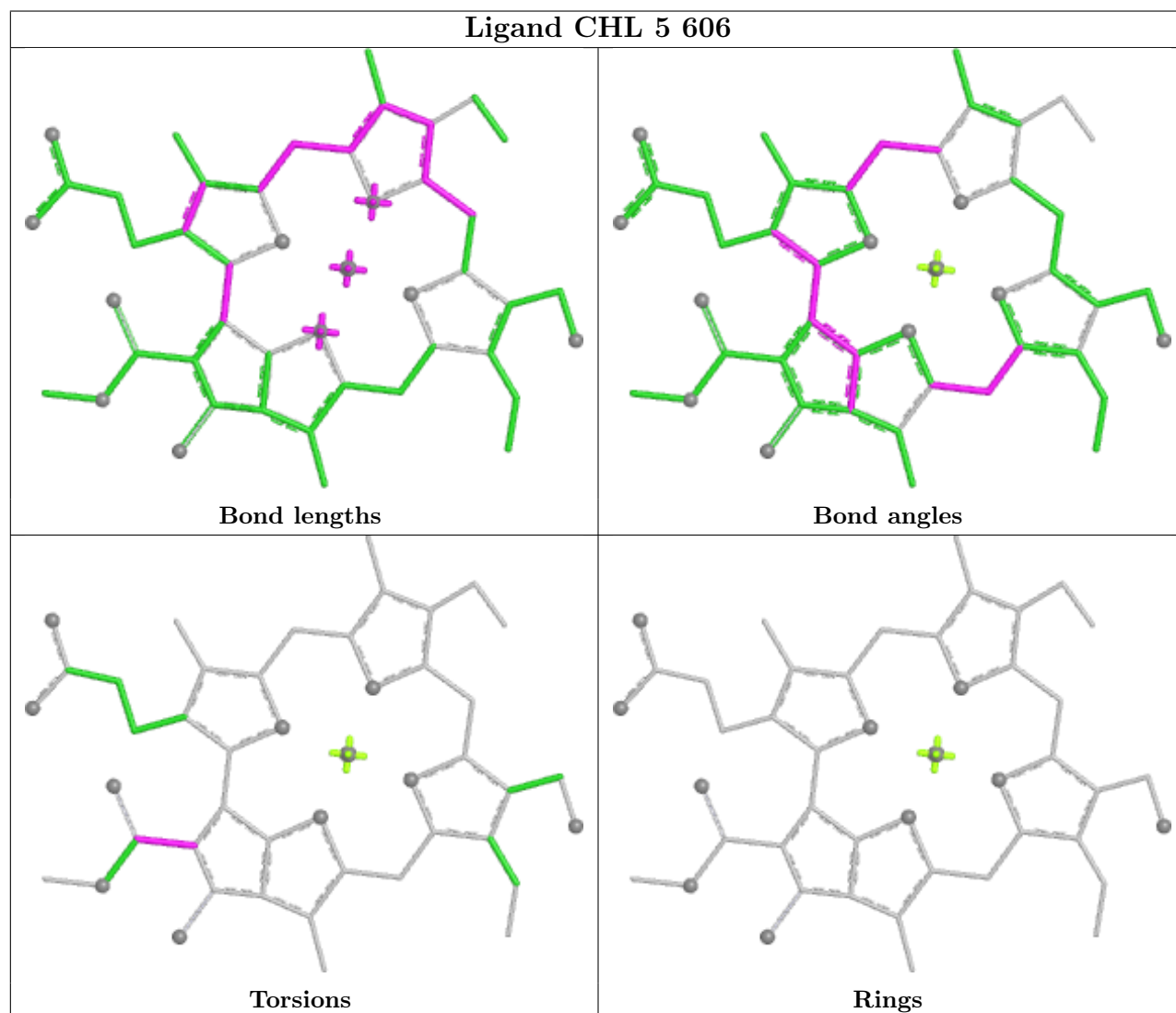
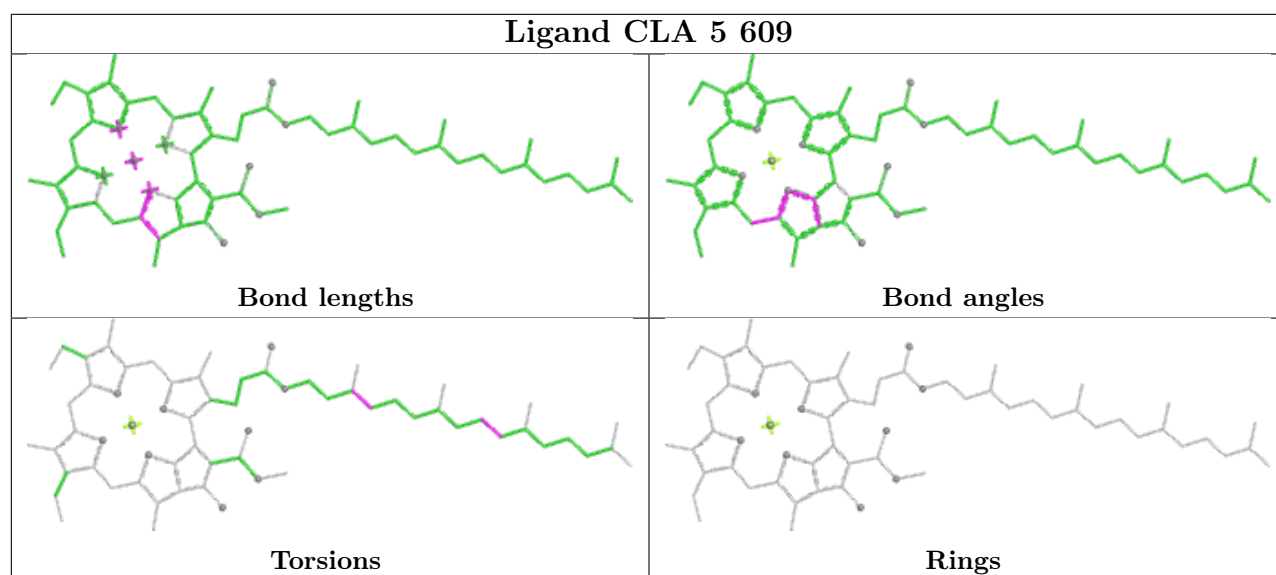


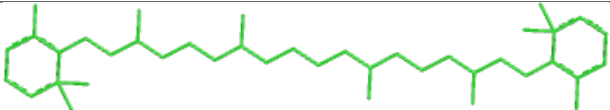
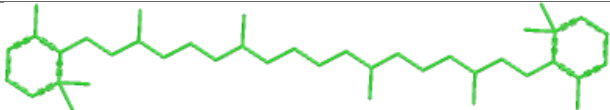
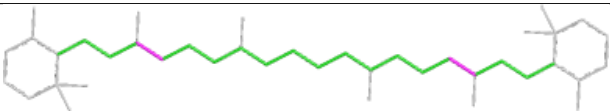
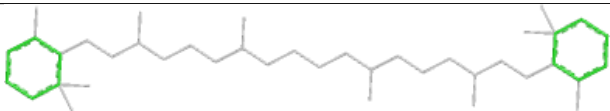


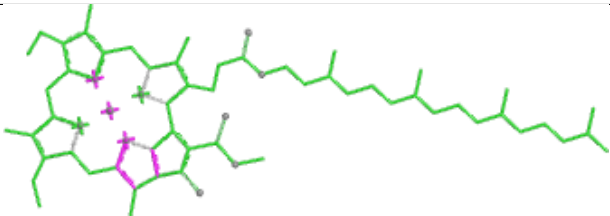
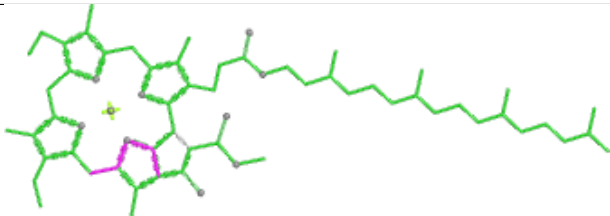
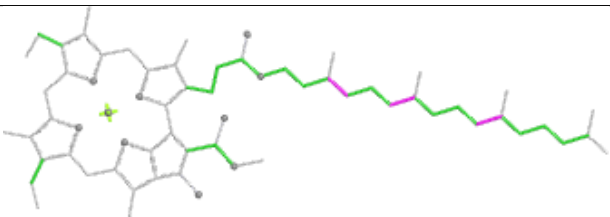
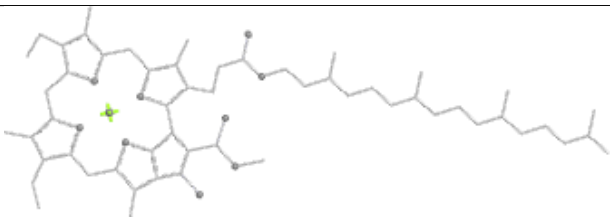


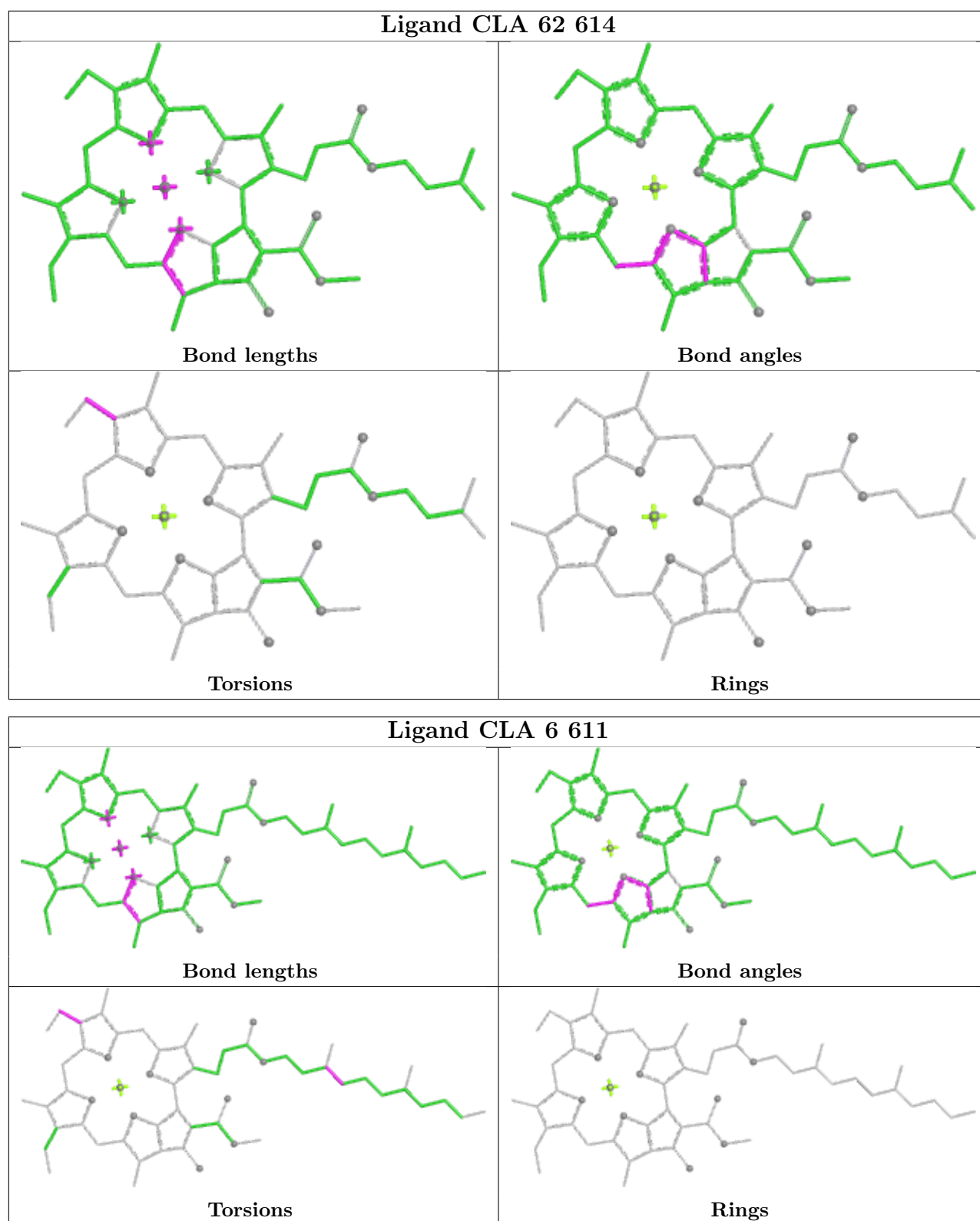




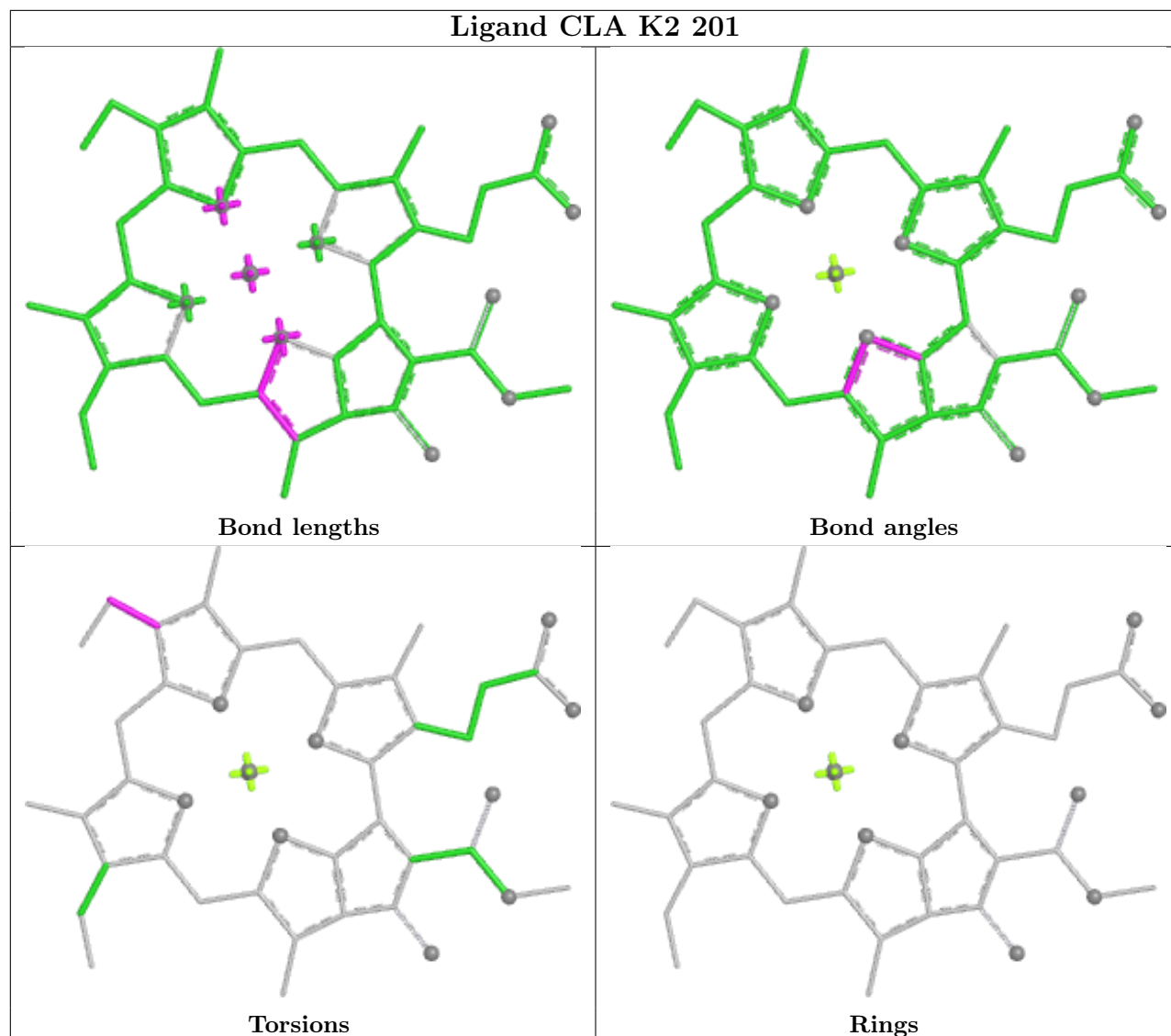


Ligand BCR B 845			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

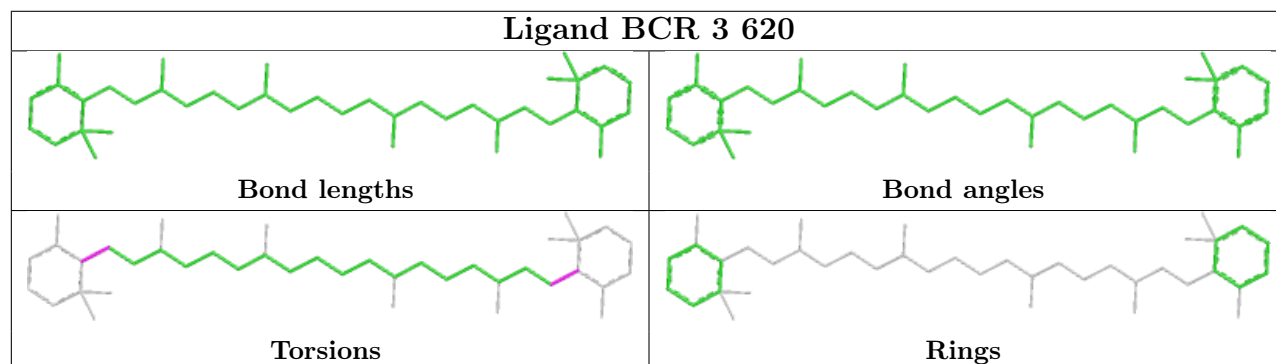
Ligand CLA A 820			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

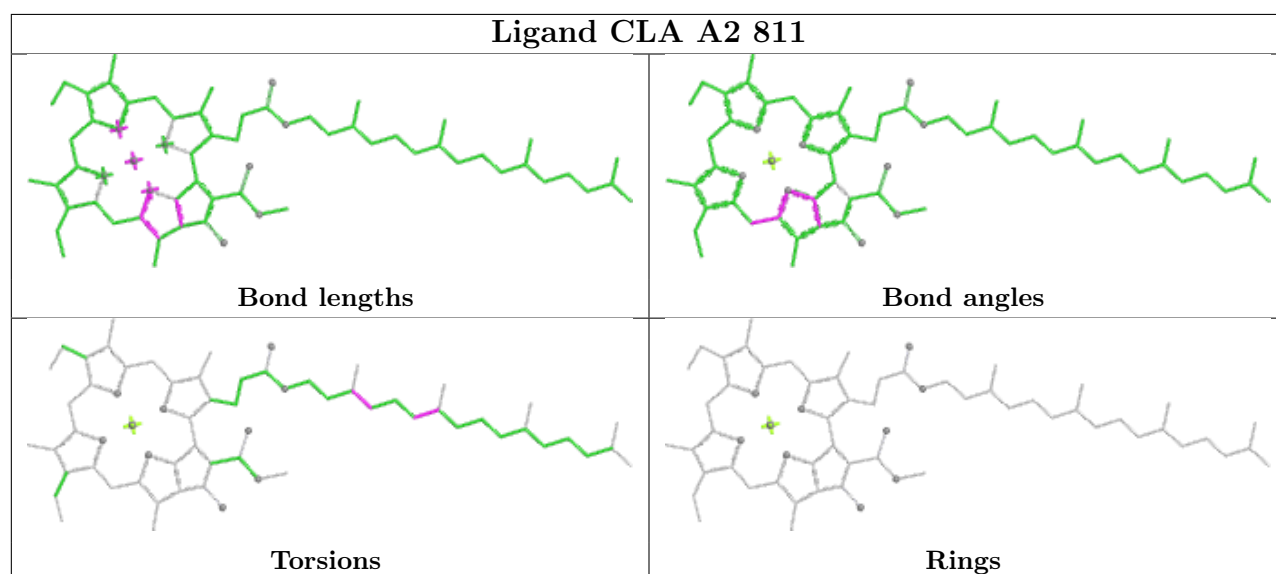
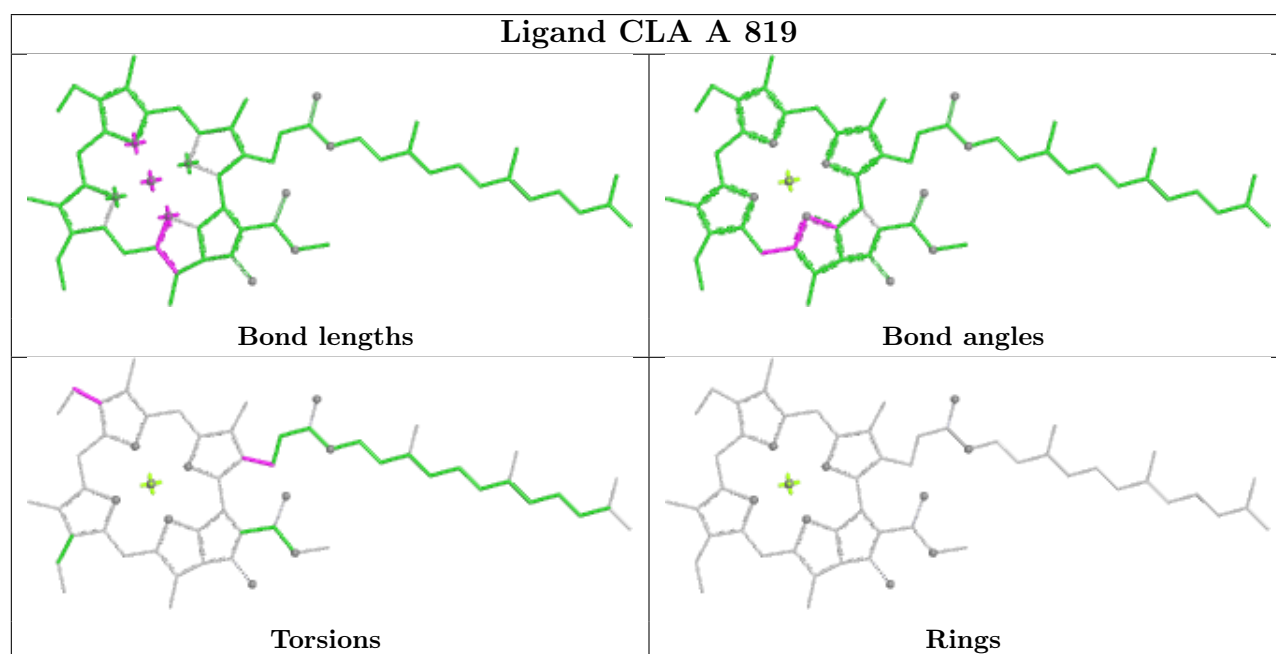
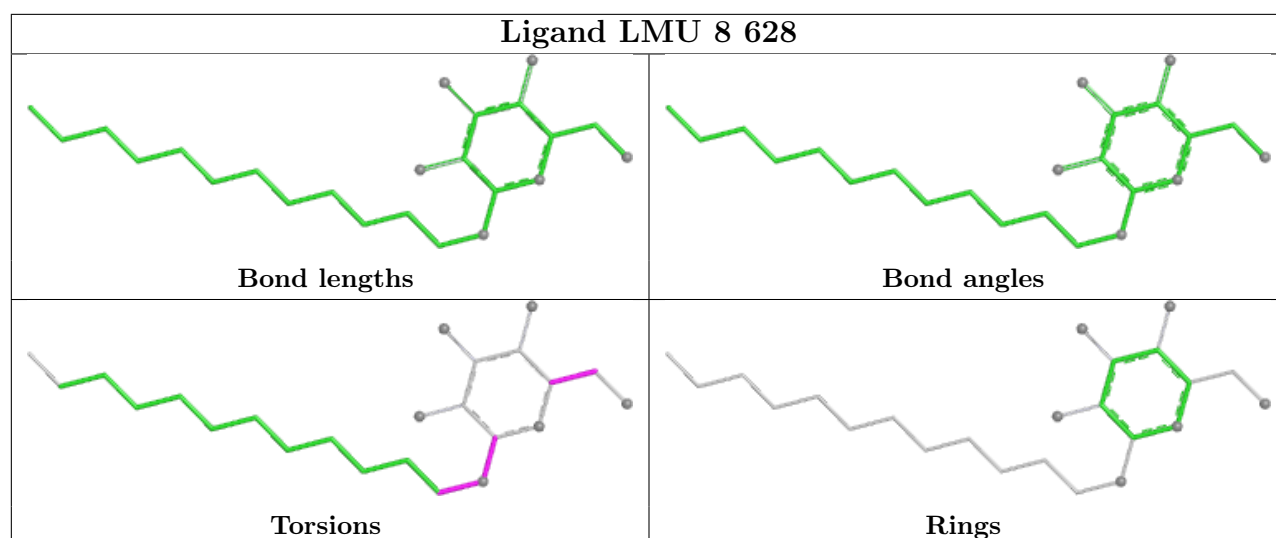


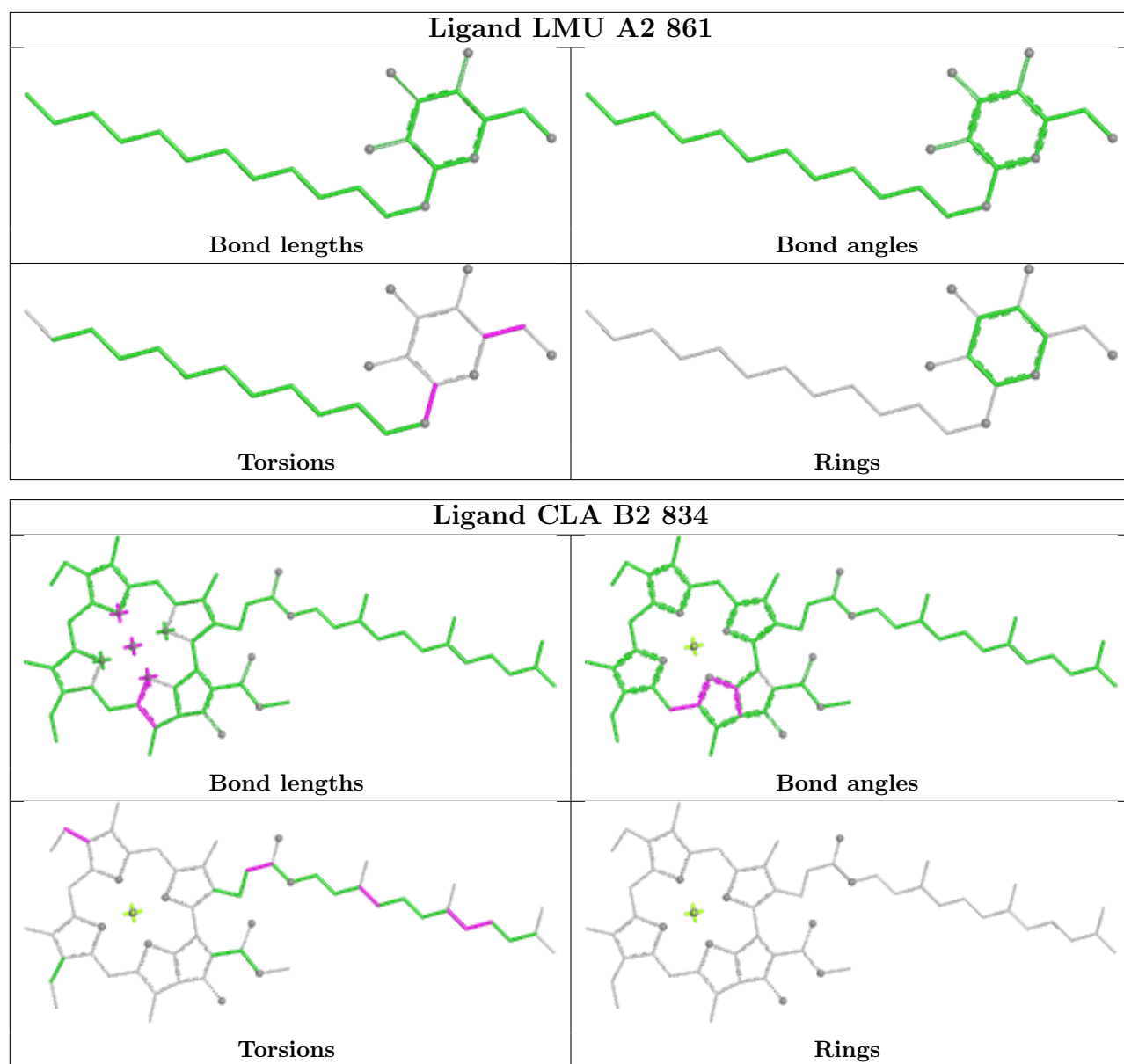
Ligand CLA K2 201



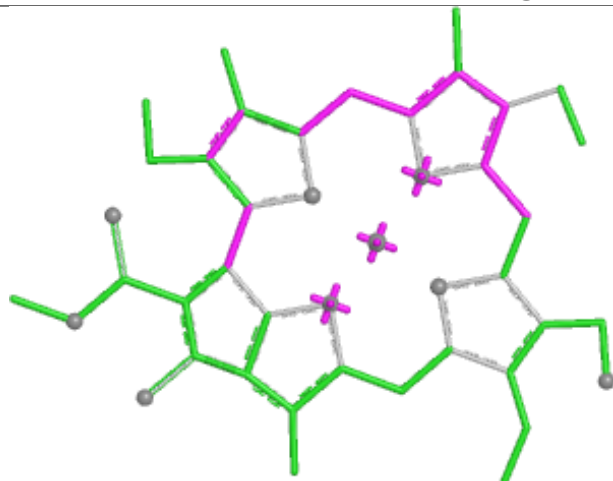
Ligand BCR 3 620



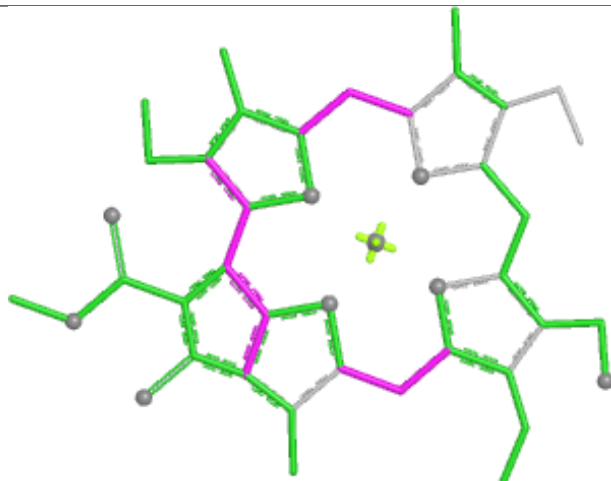




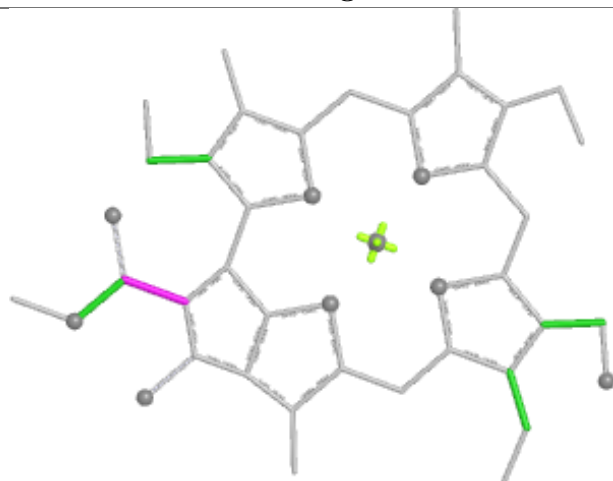
Ligand CHL 5 618



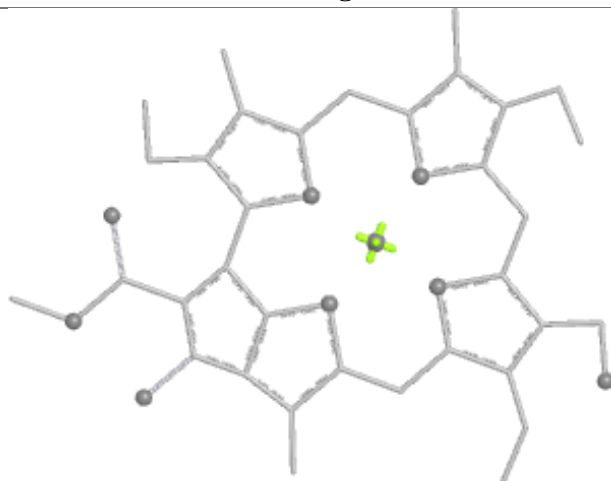
Bond lengths



Bond angles

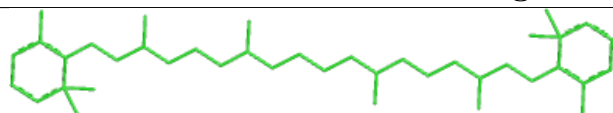


Torsions

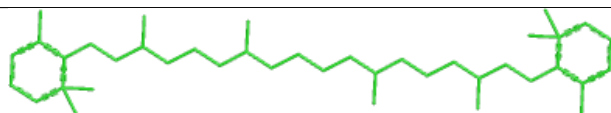


Rings

Ligand BCR A 849



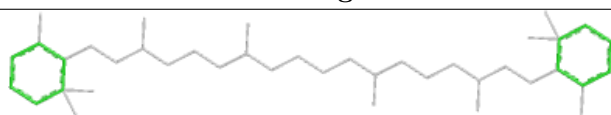
Bond lengths



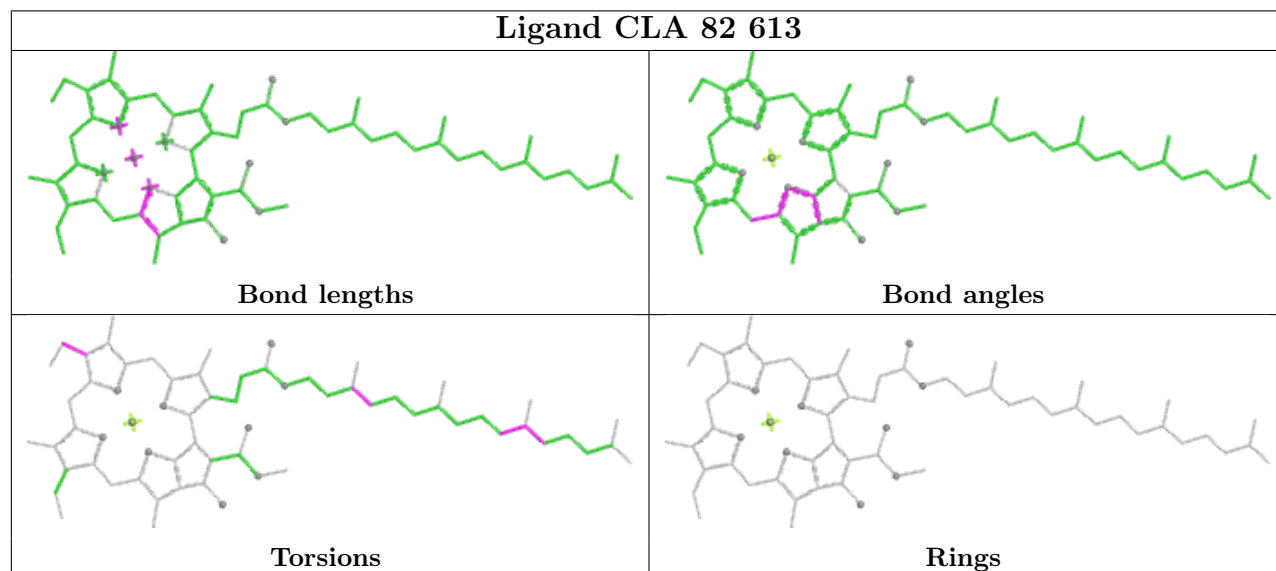
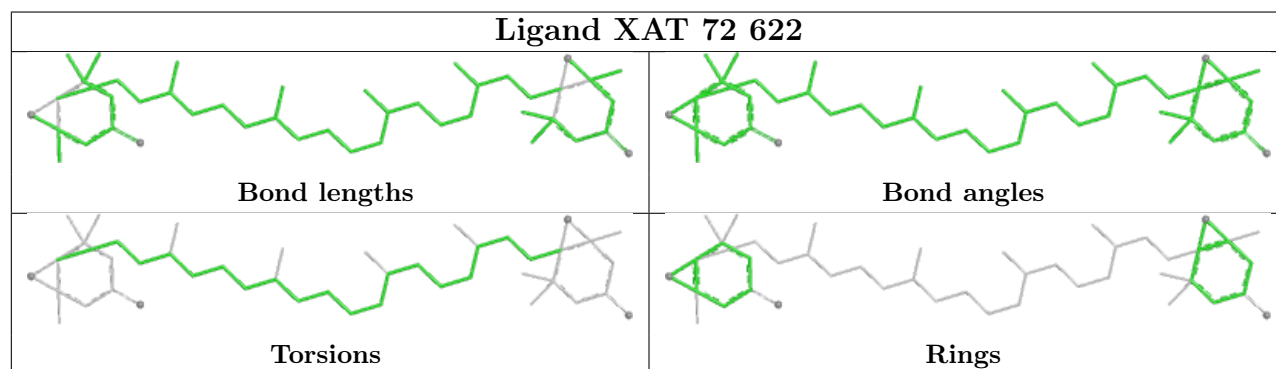
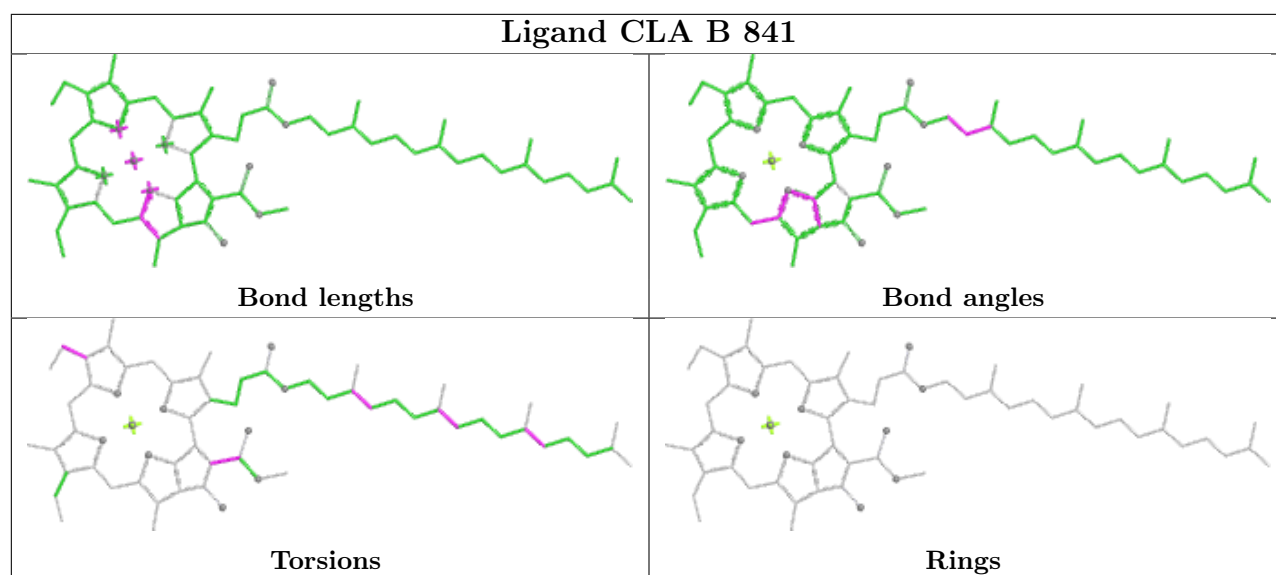
Bond angles

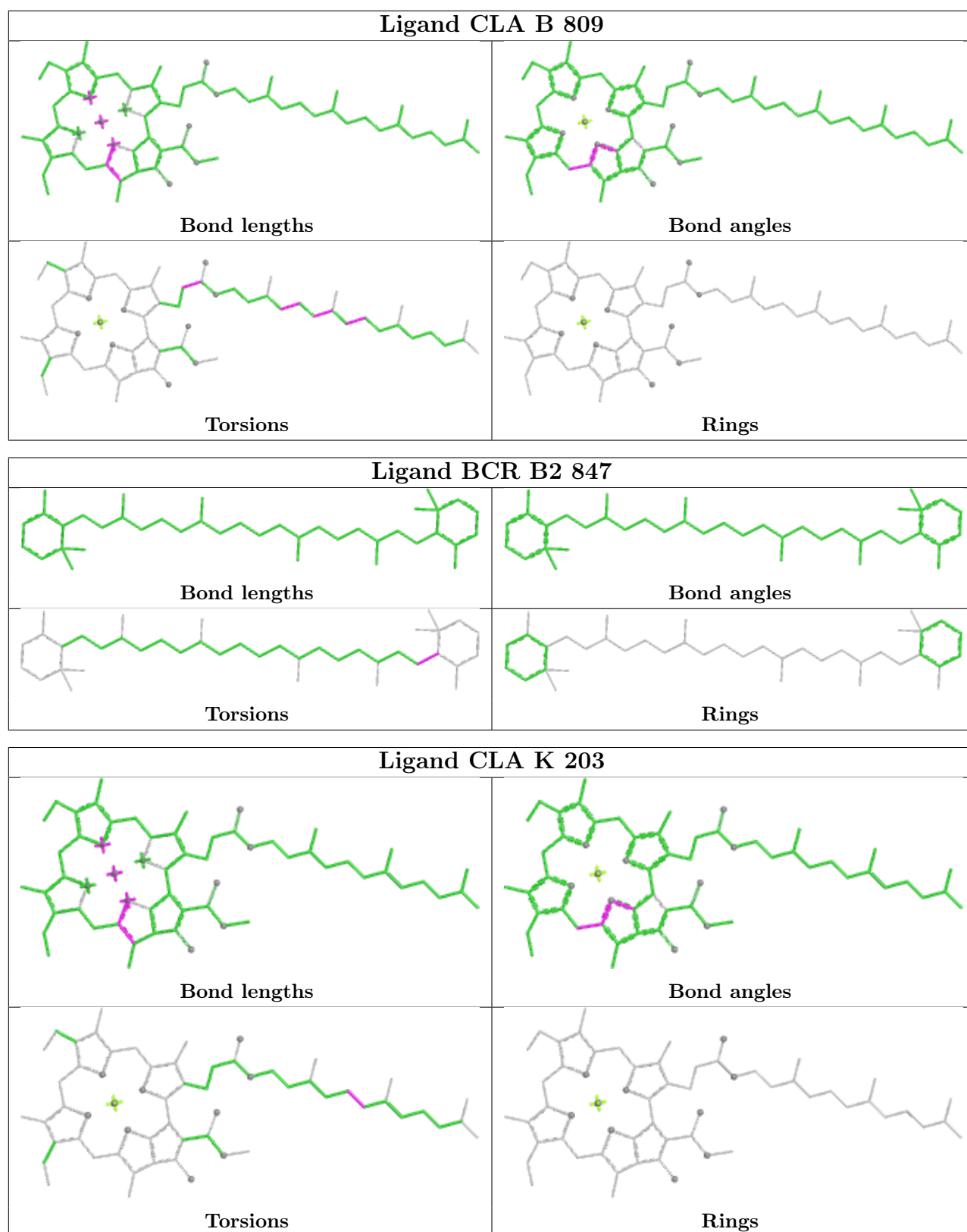


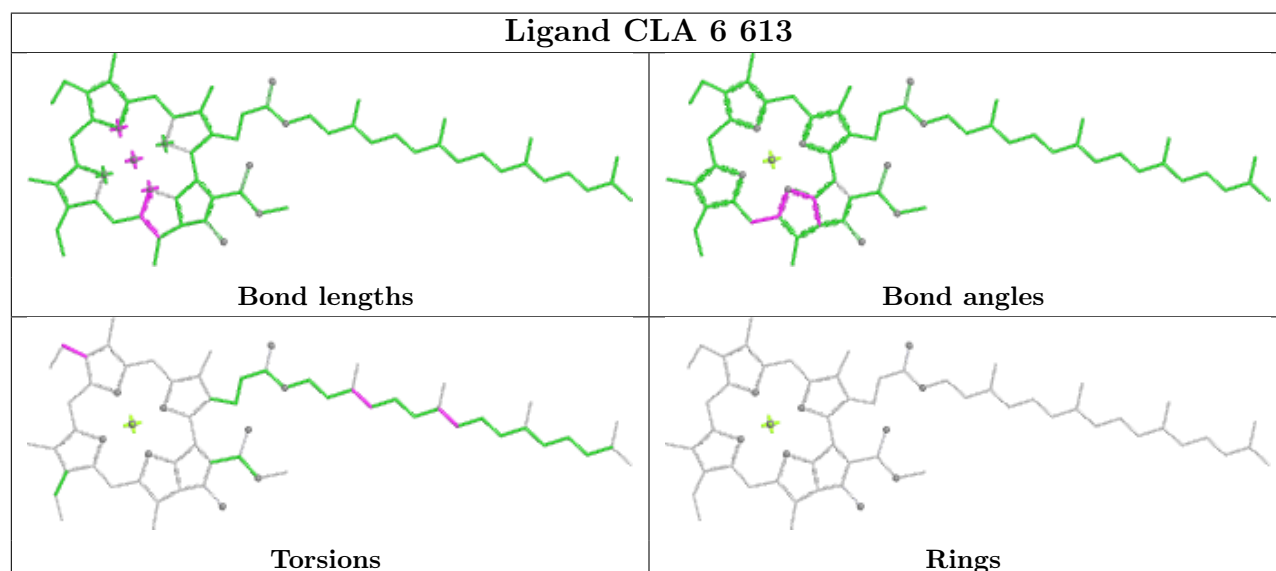
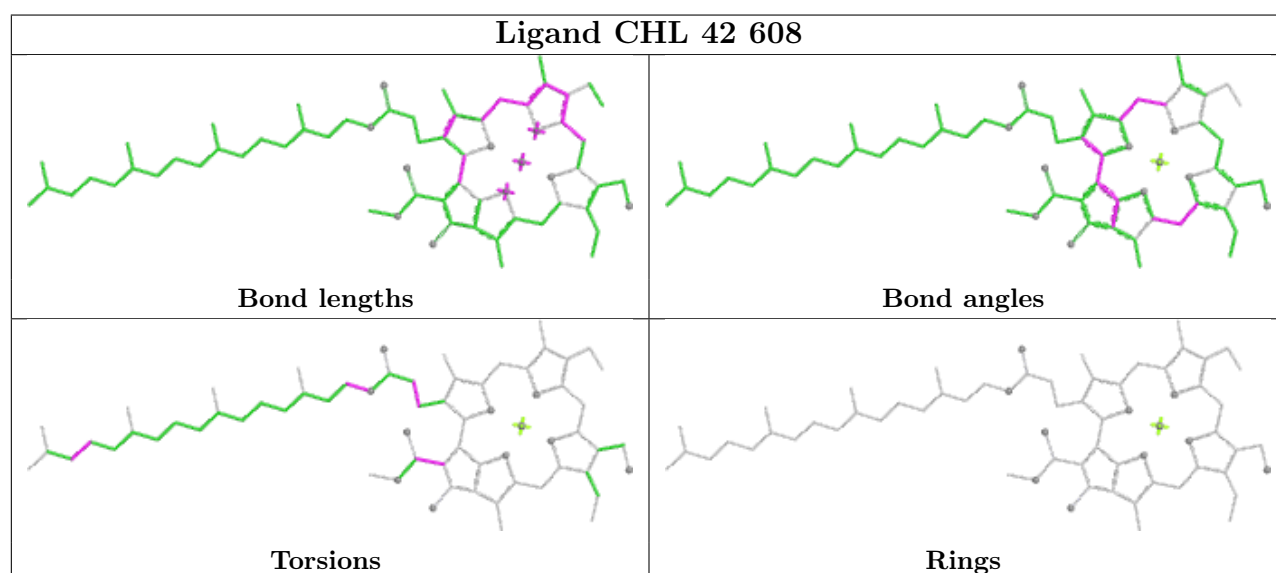
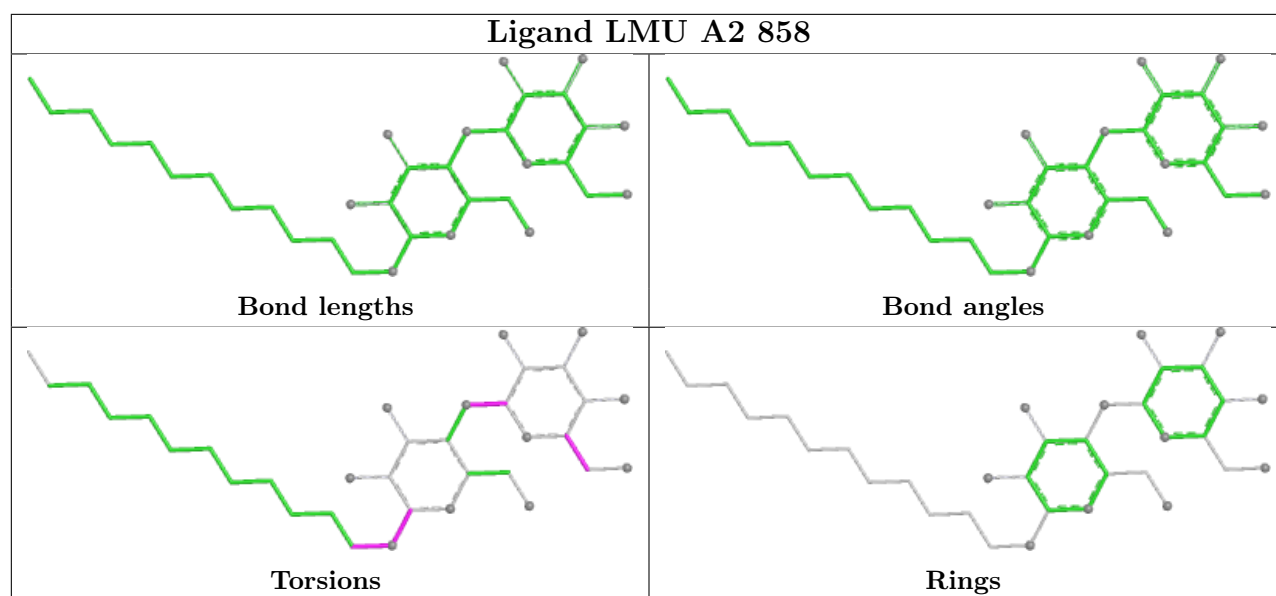
Torsions

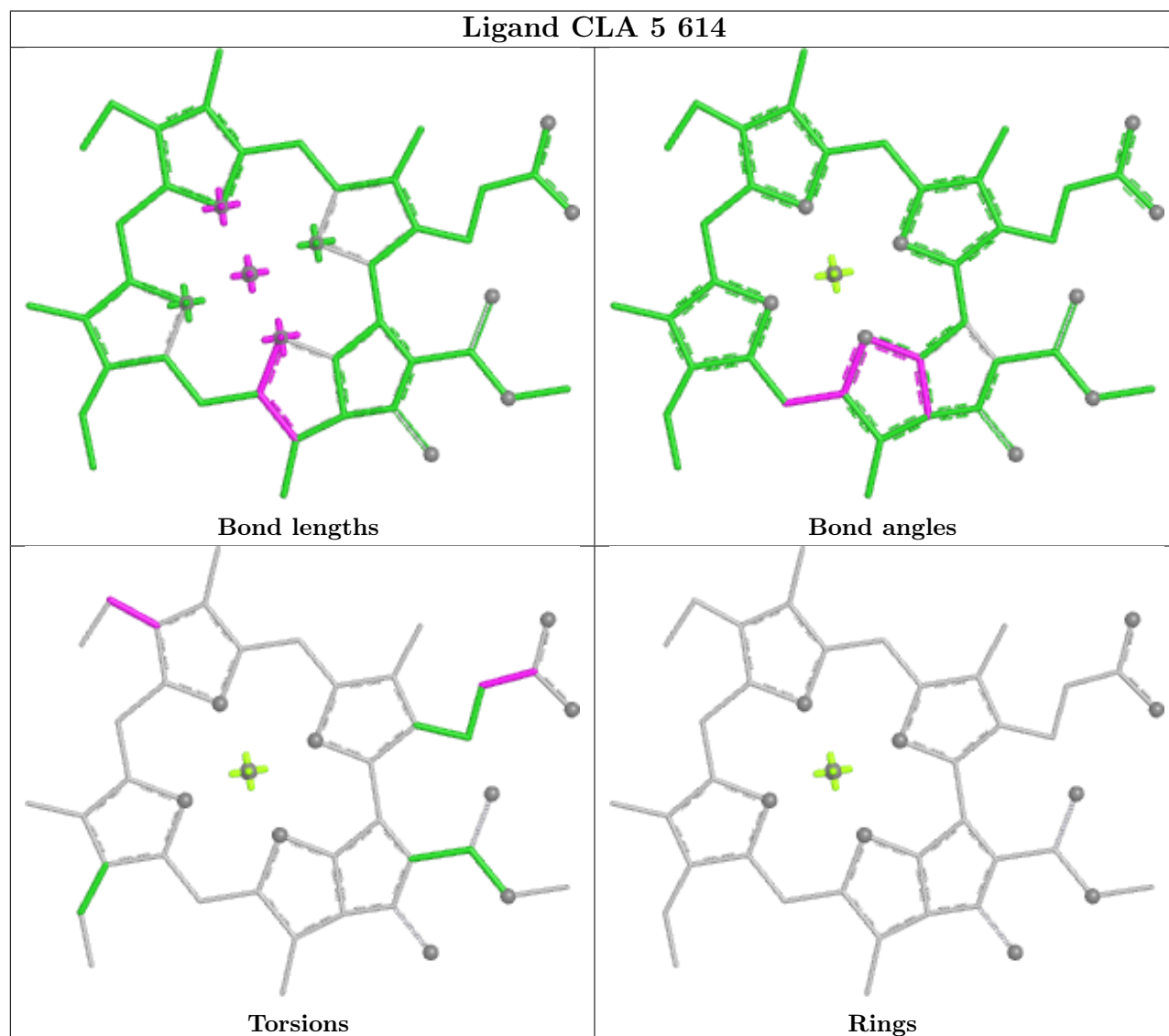
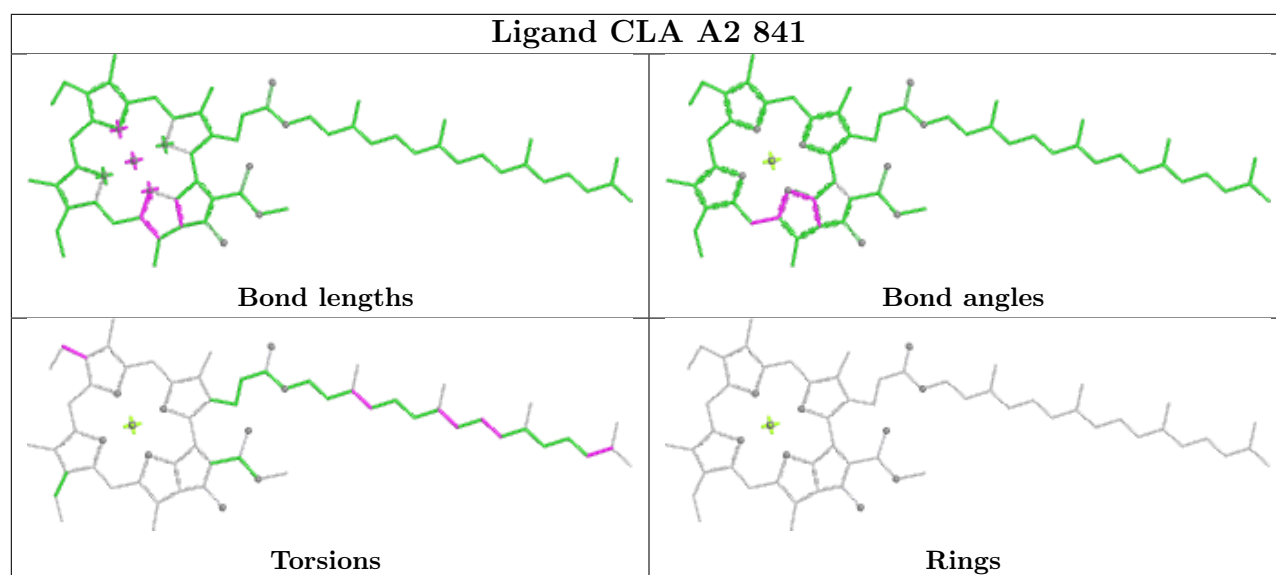


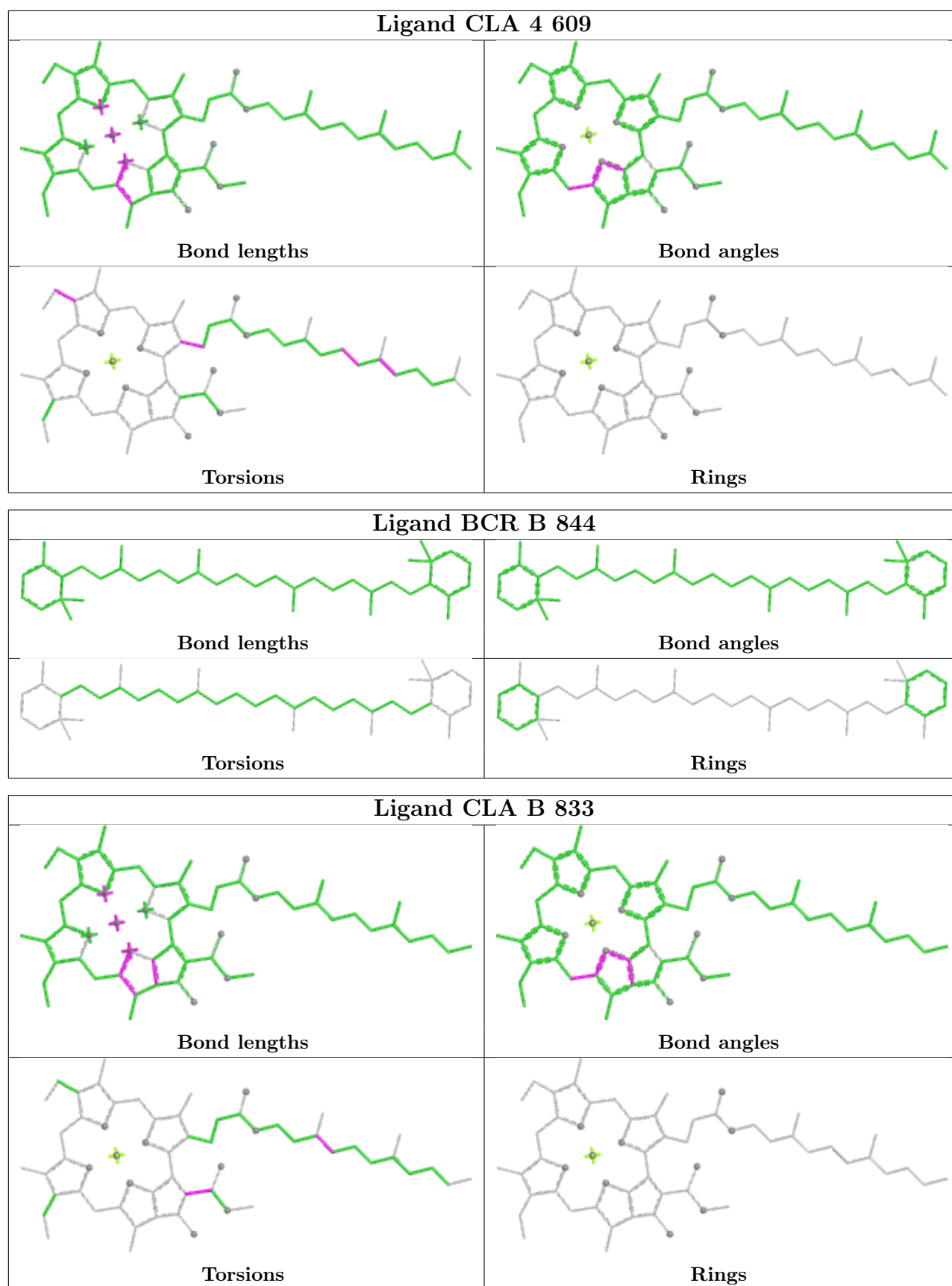
Rings

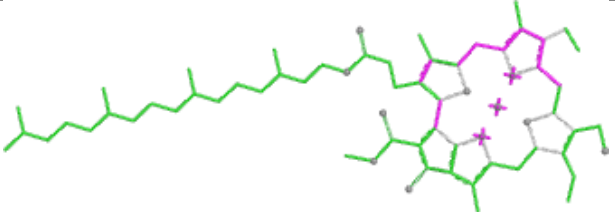
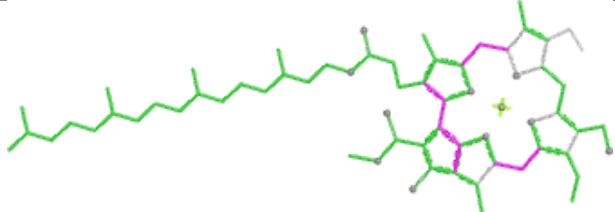
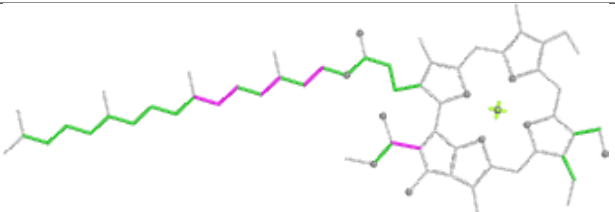
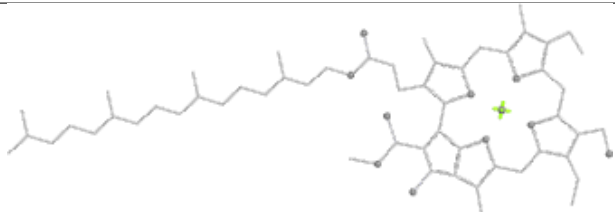
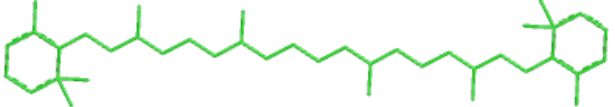
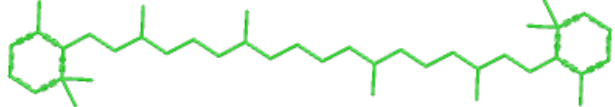
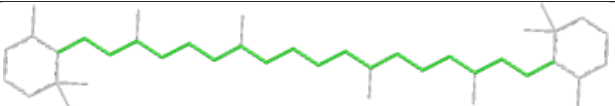
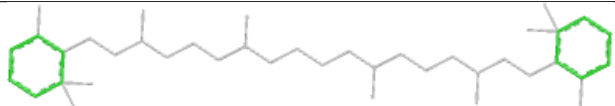
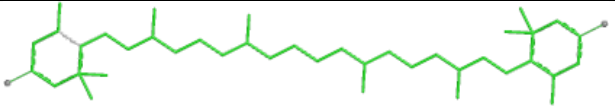
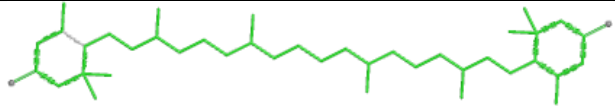
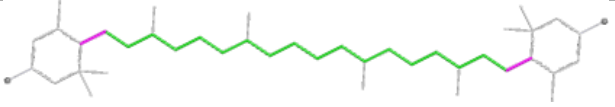
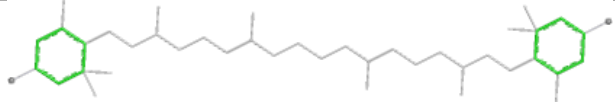
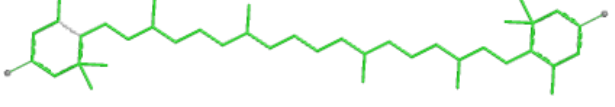
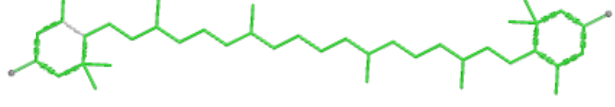
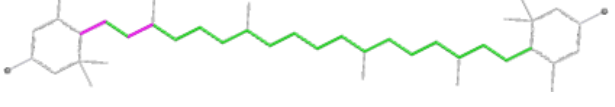
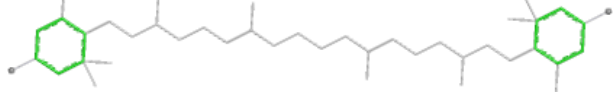


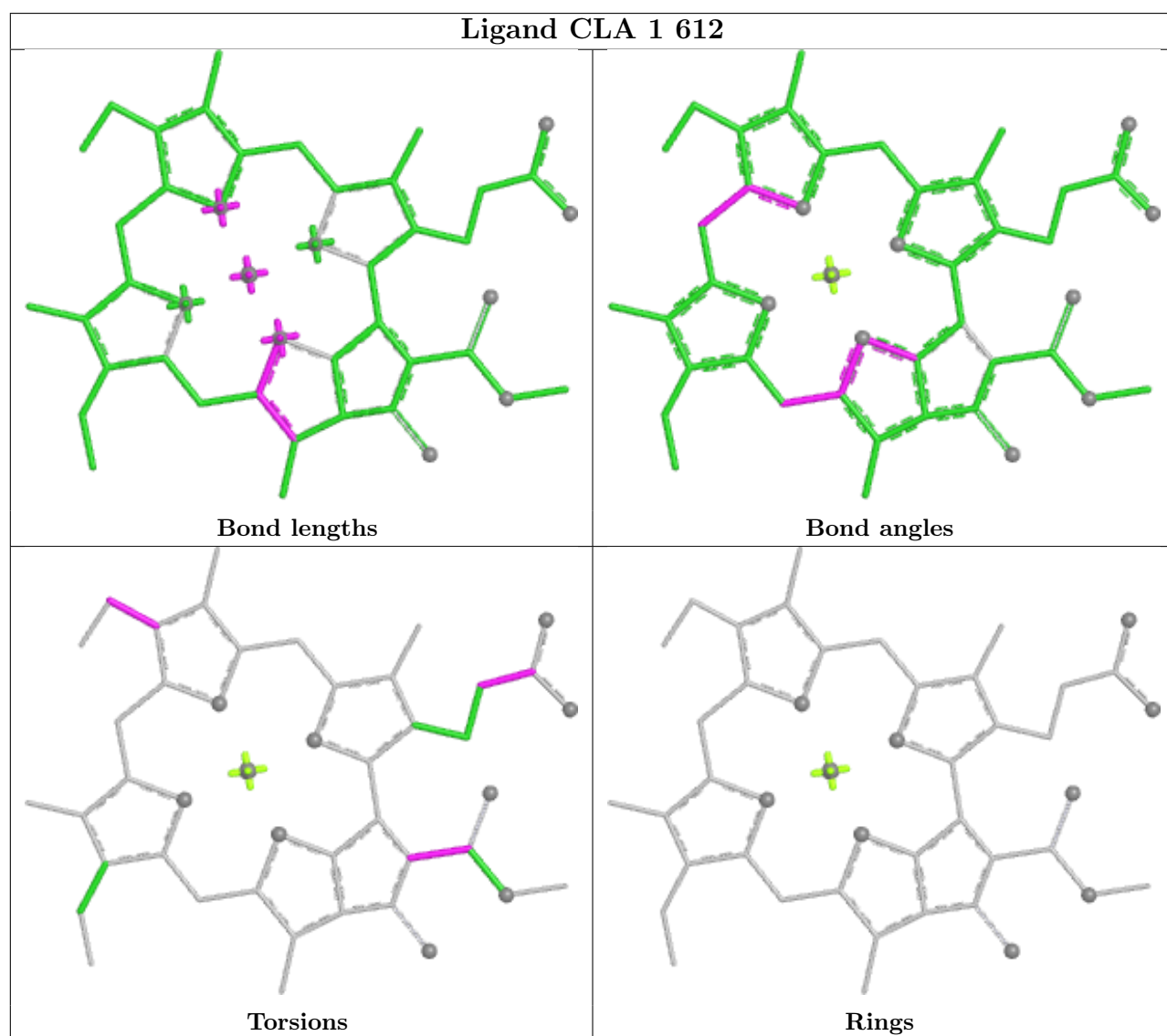
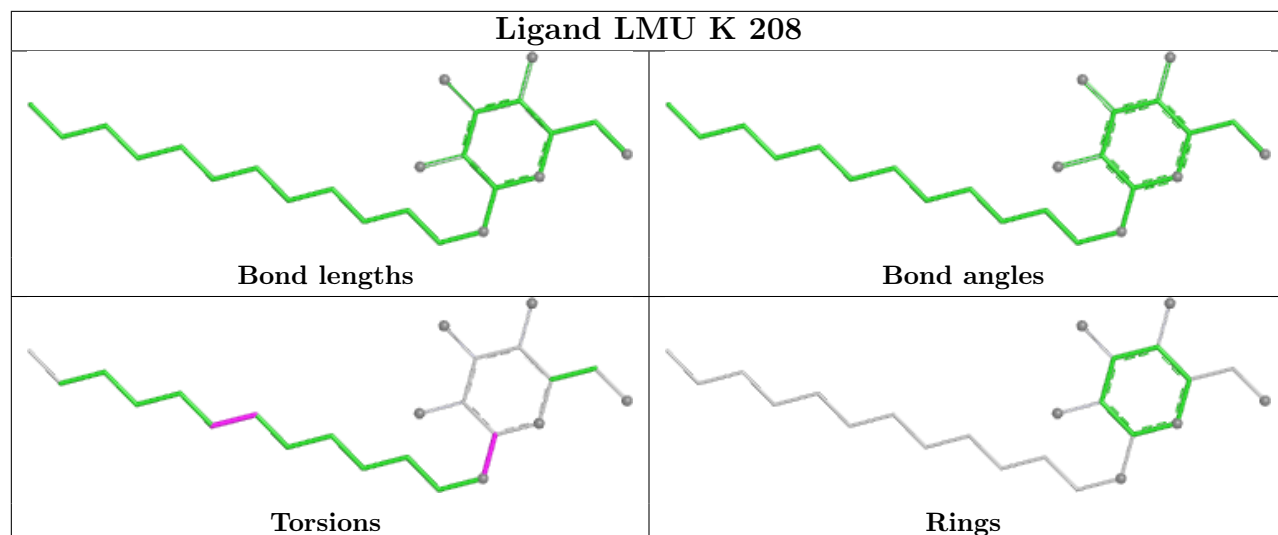


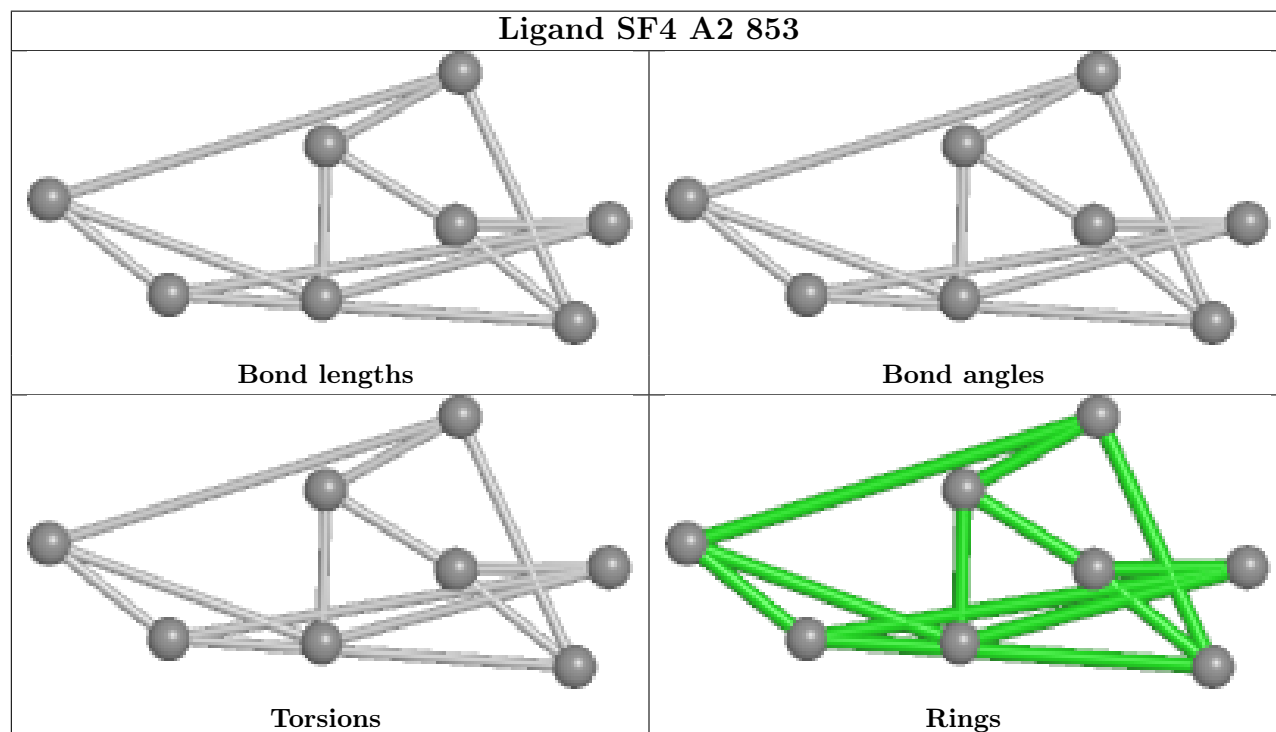
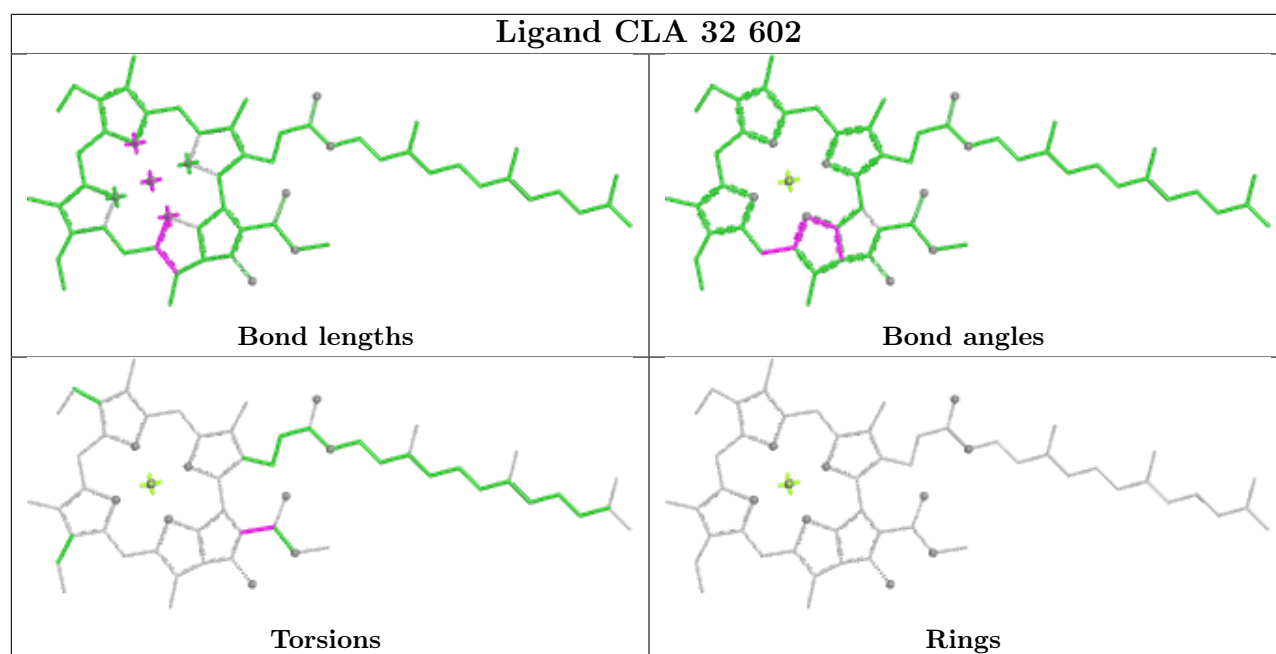


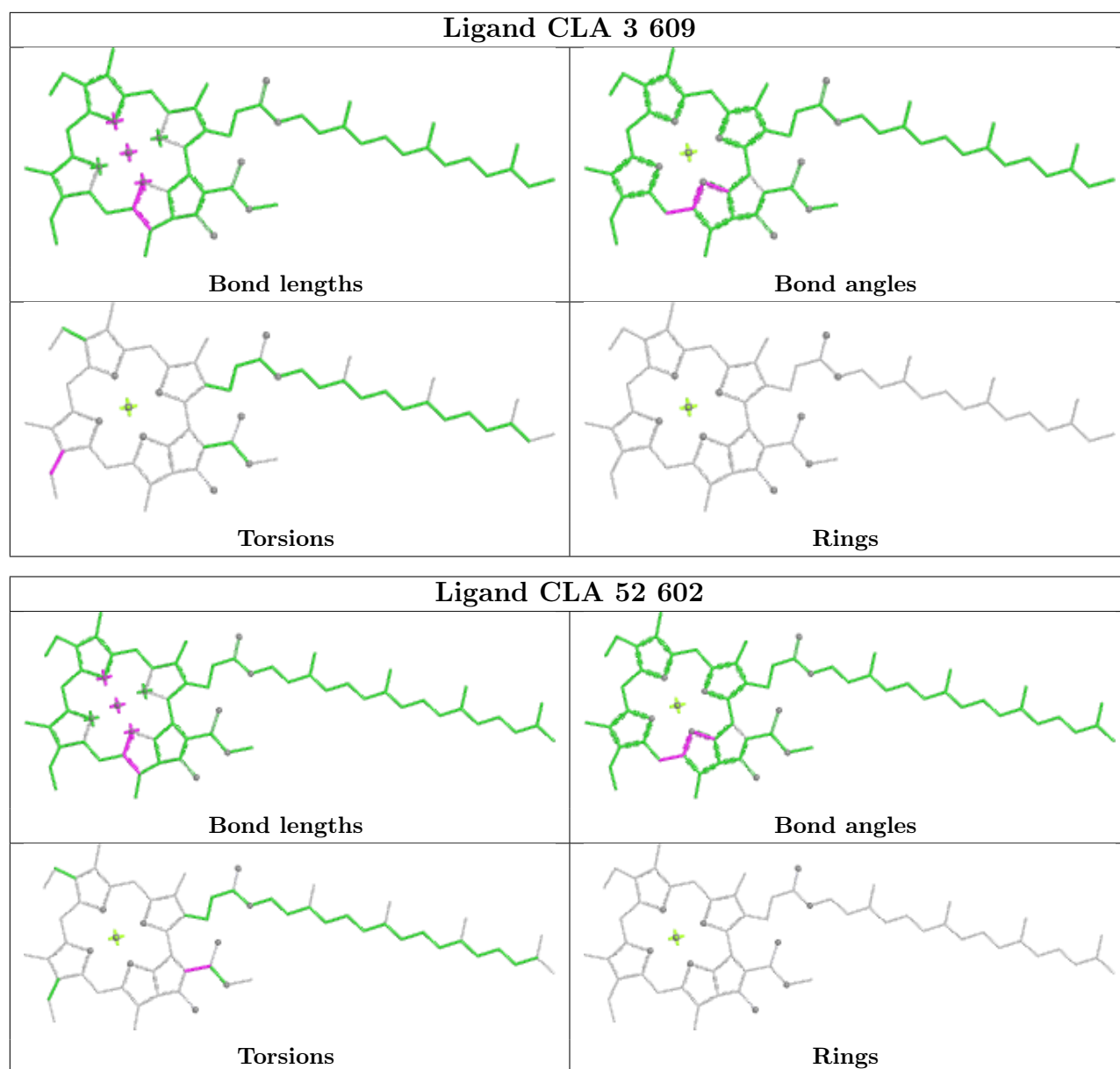




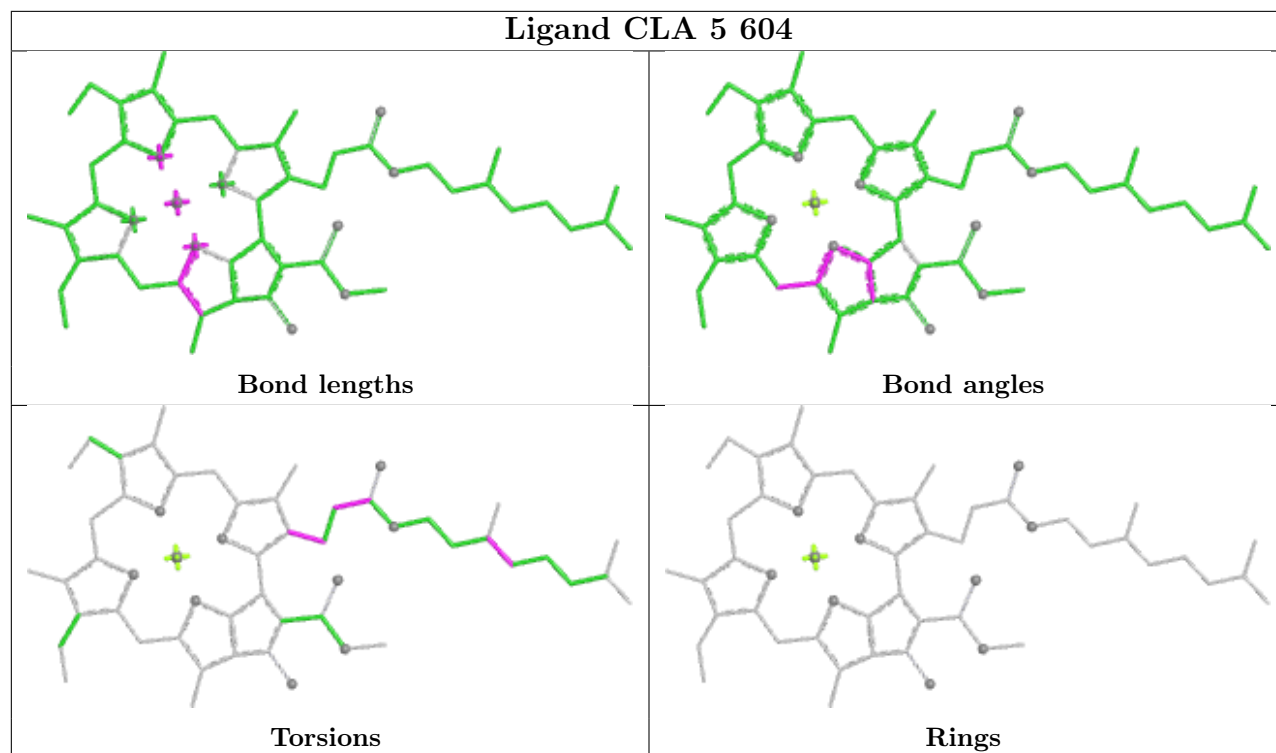
Ligand CHL Z 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B 843	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 52 626	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 7 624	
 Bond lengths	 Bond angles
 Torsions	 Rings



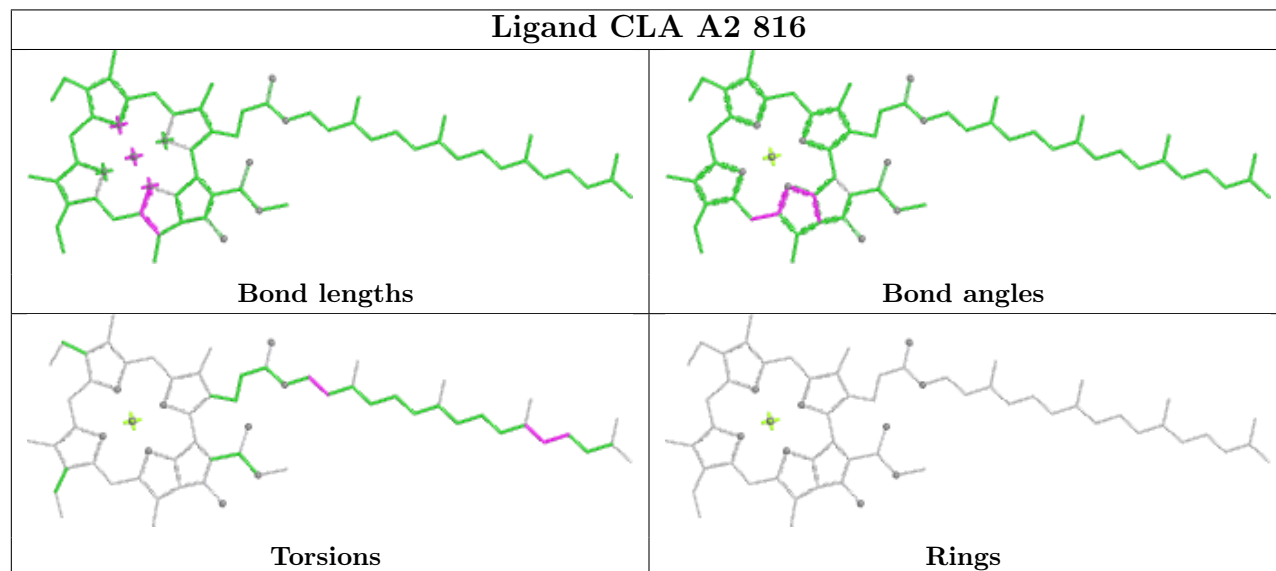


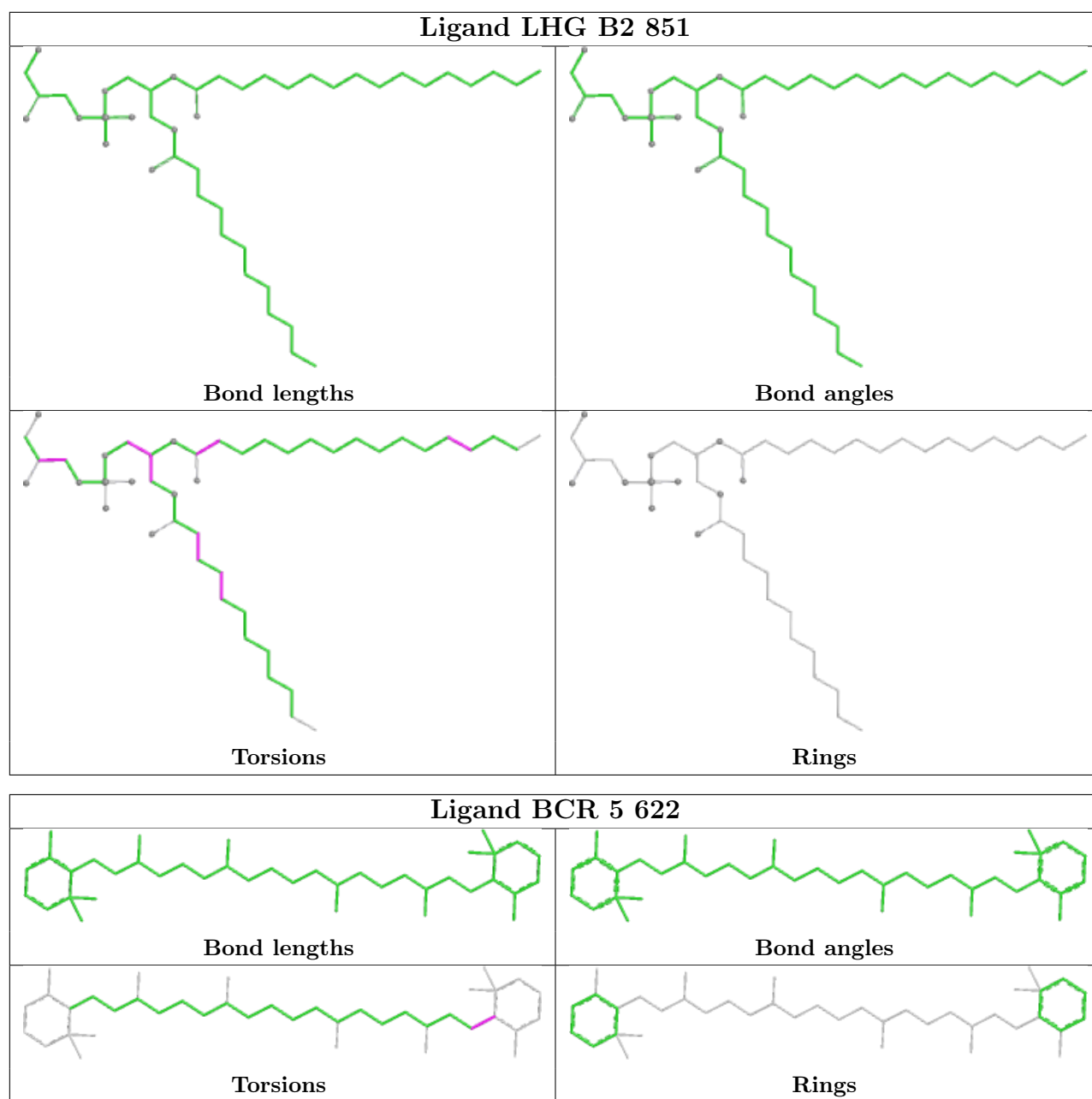


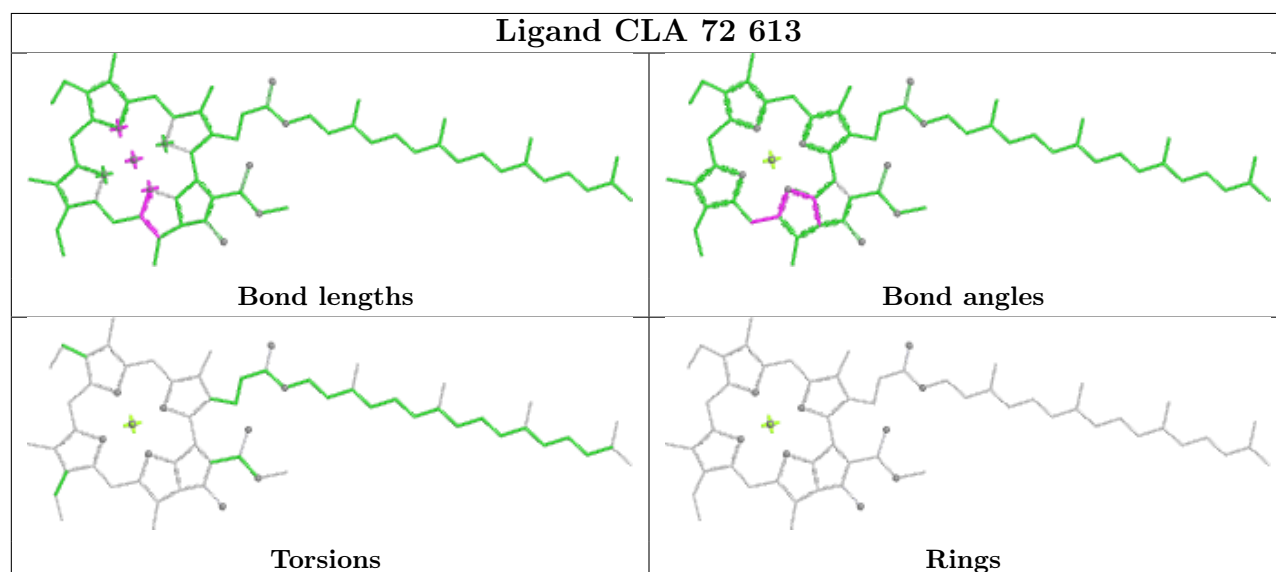
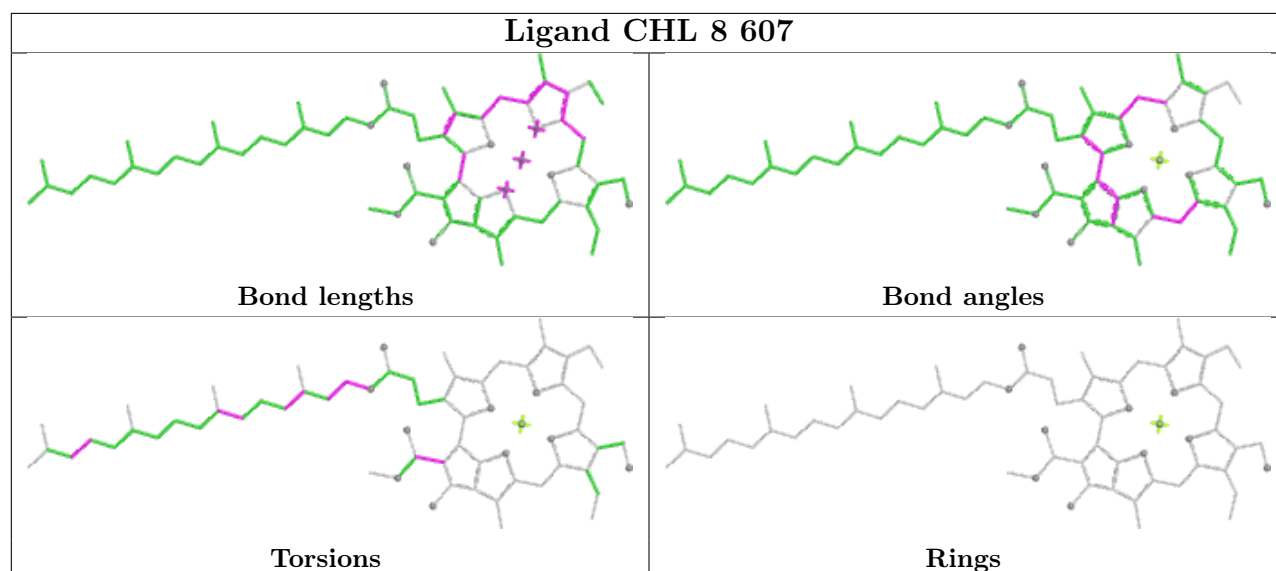
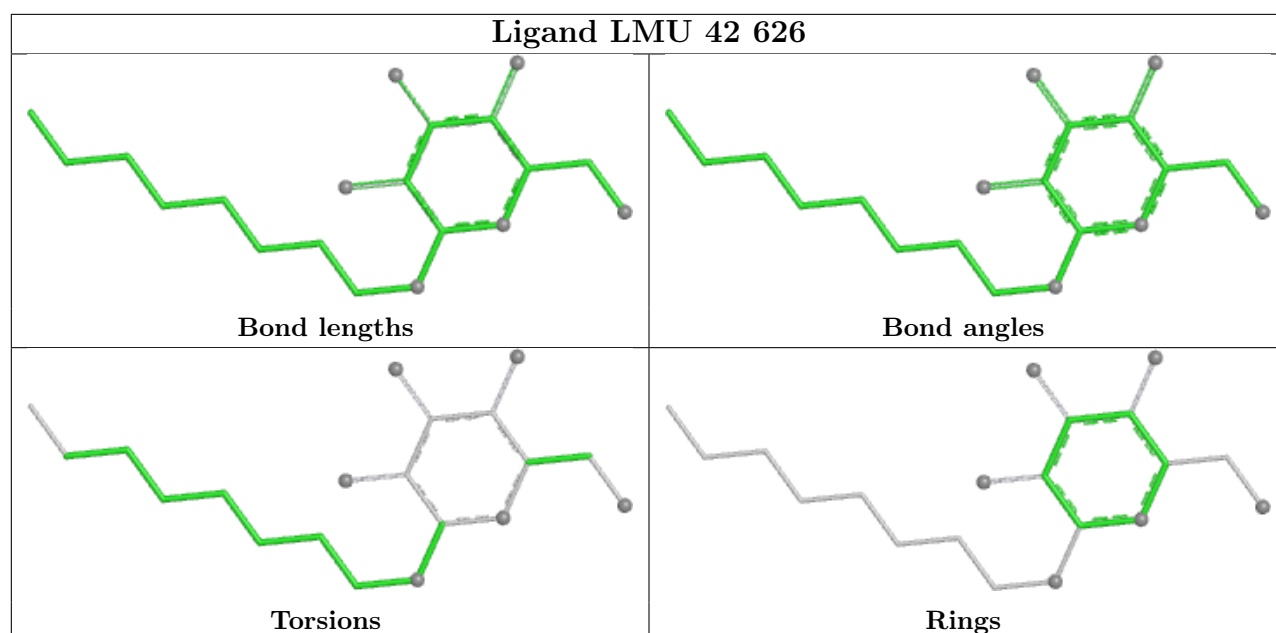
Ligand CLA 5 604

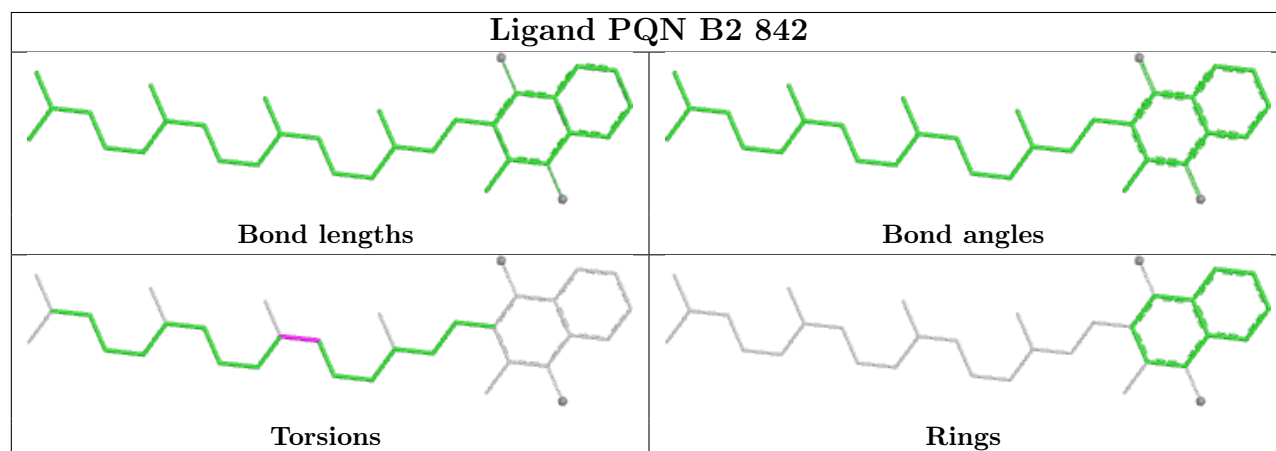
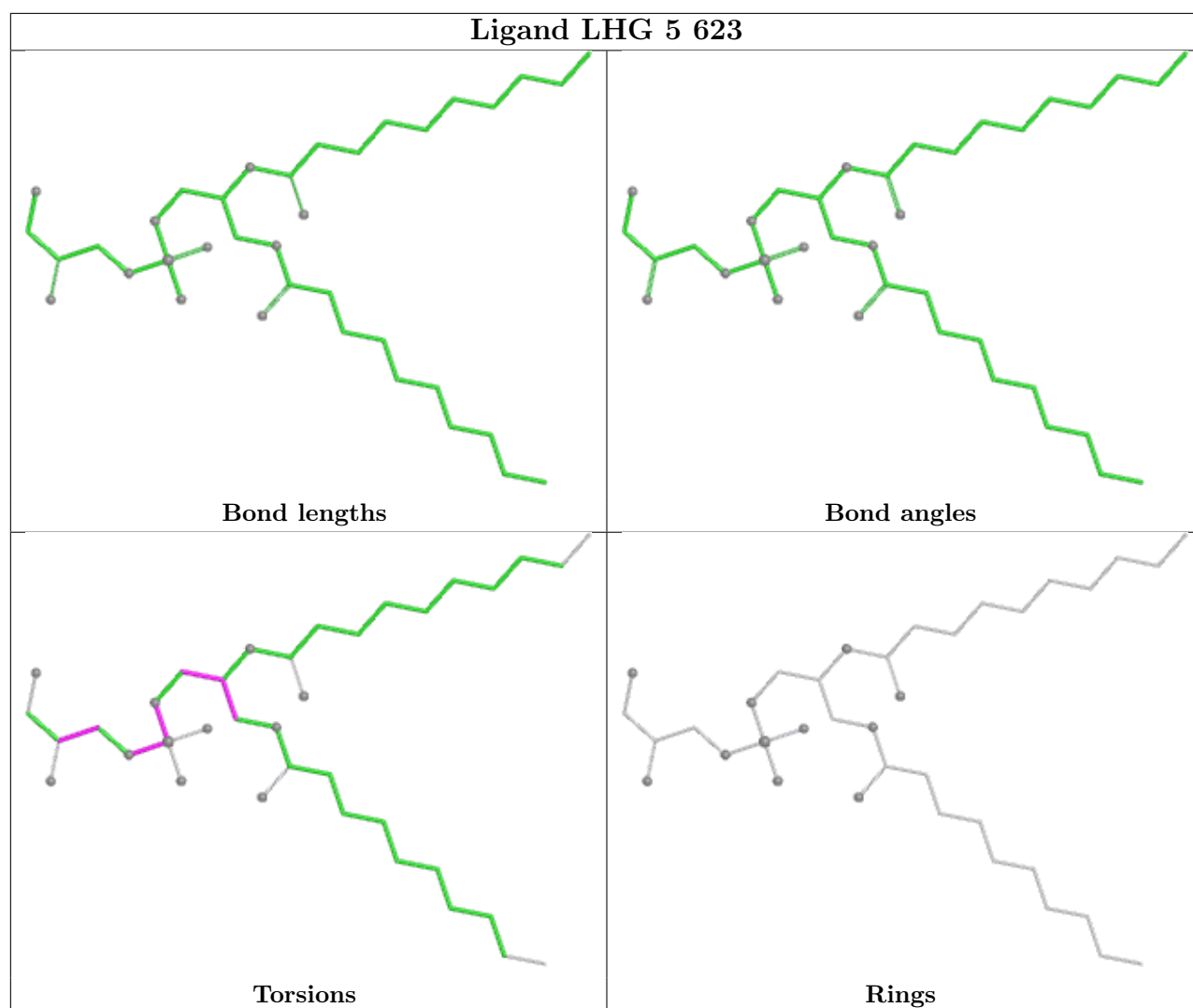


Ligand CLA A2 816

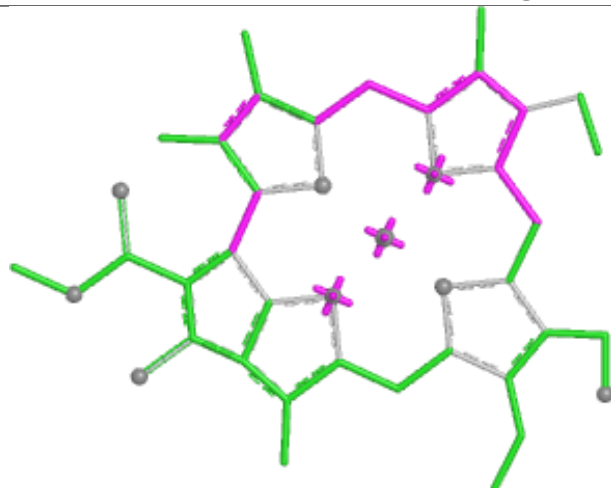




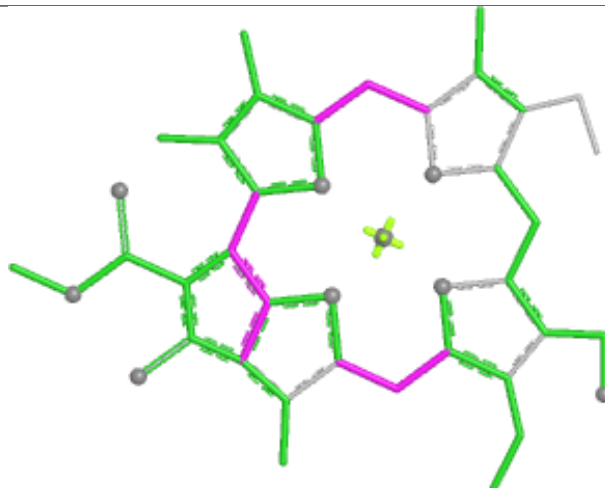




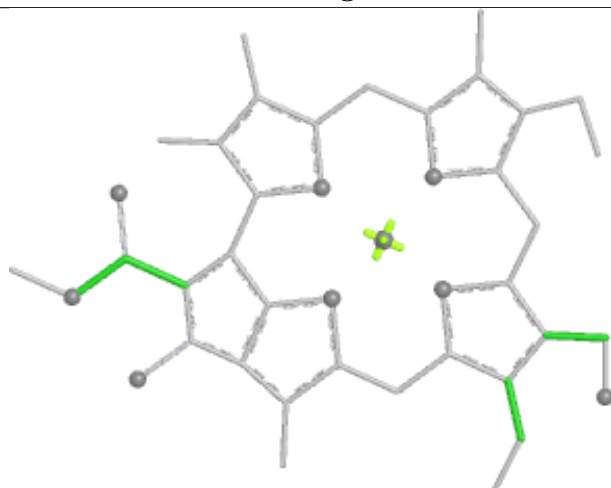
Ligand CHL 9 606



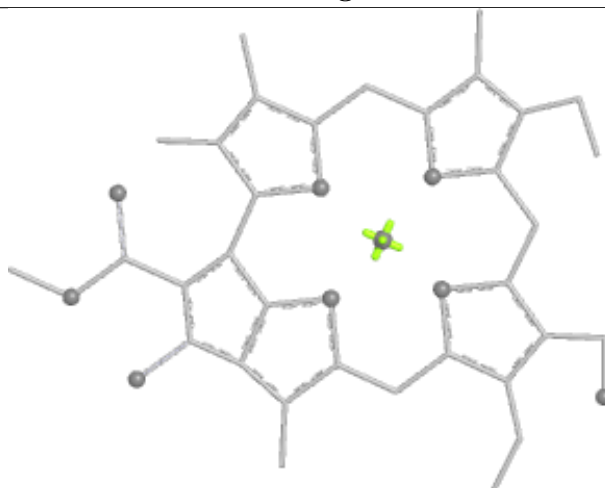
Bond lengths



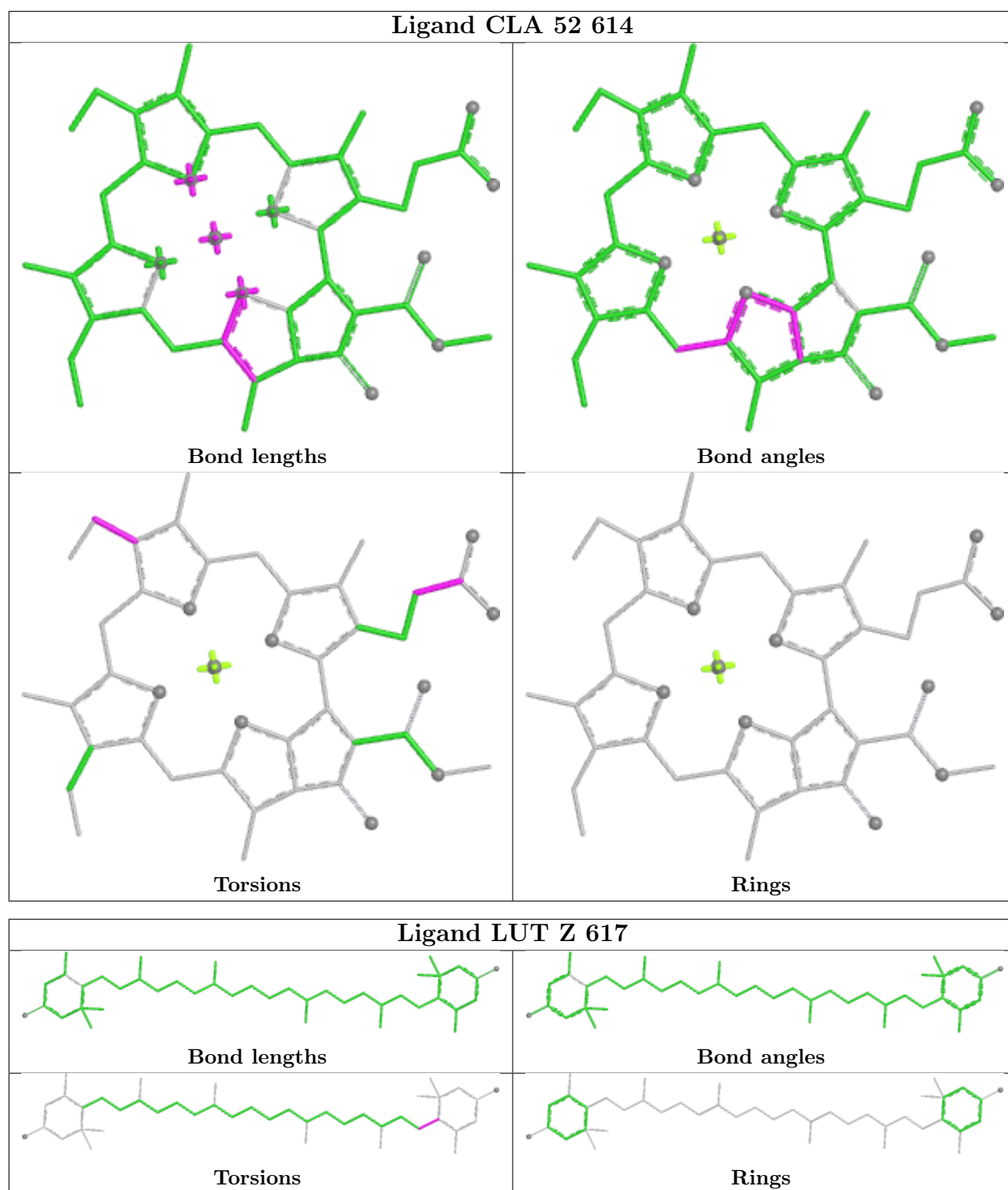
Bond angles

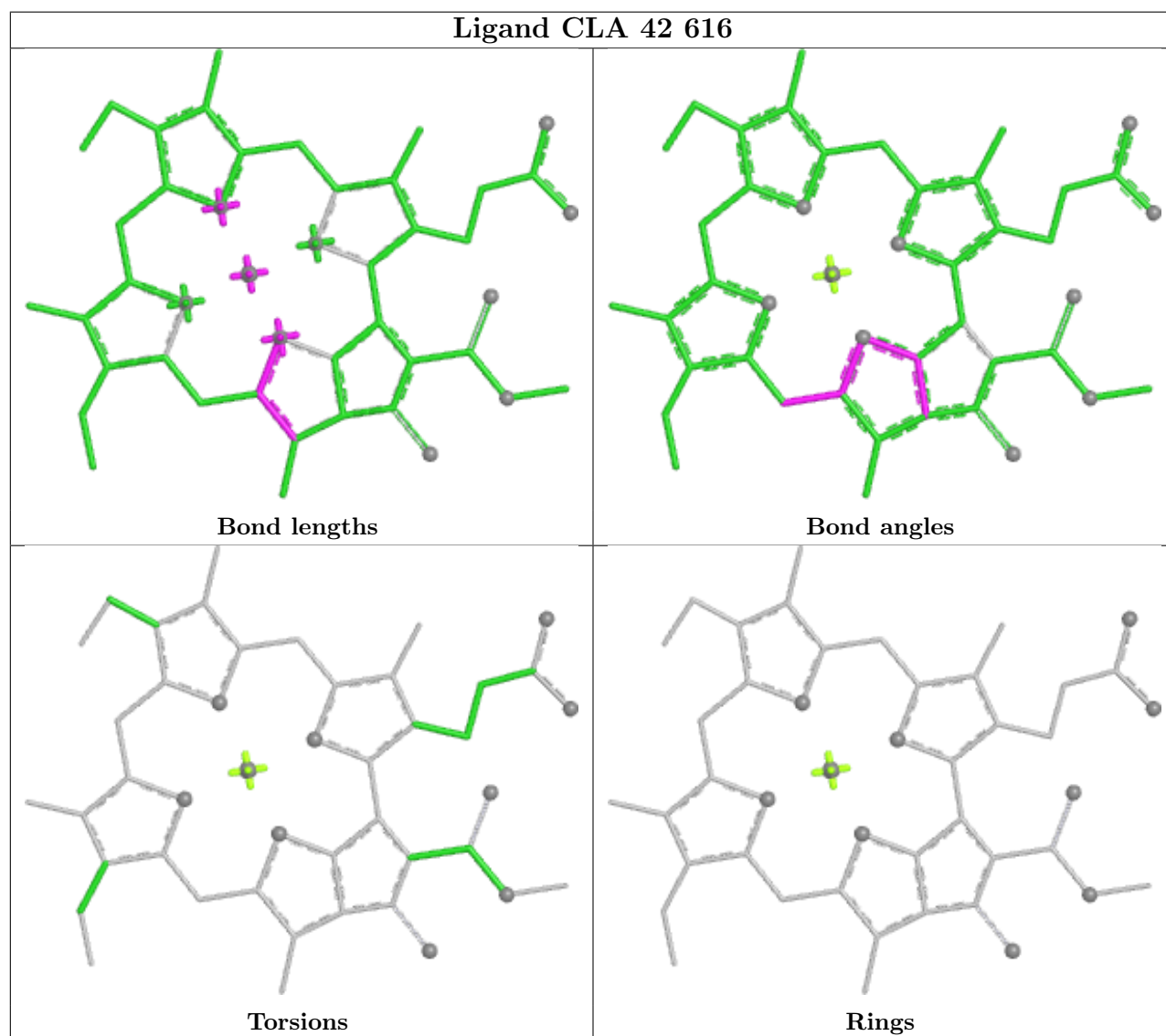
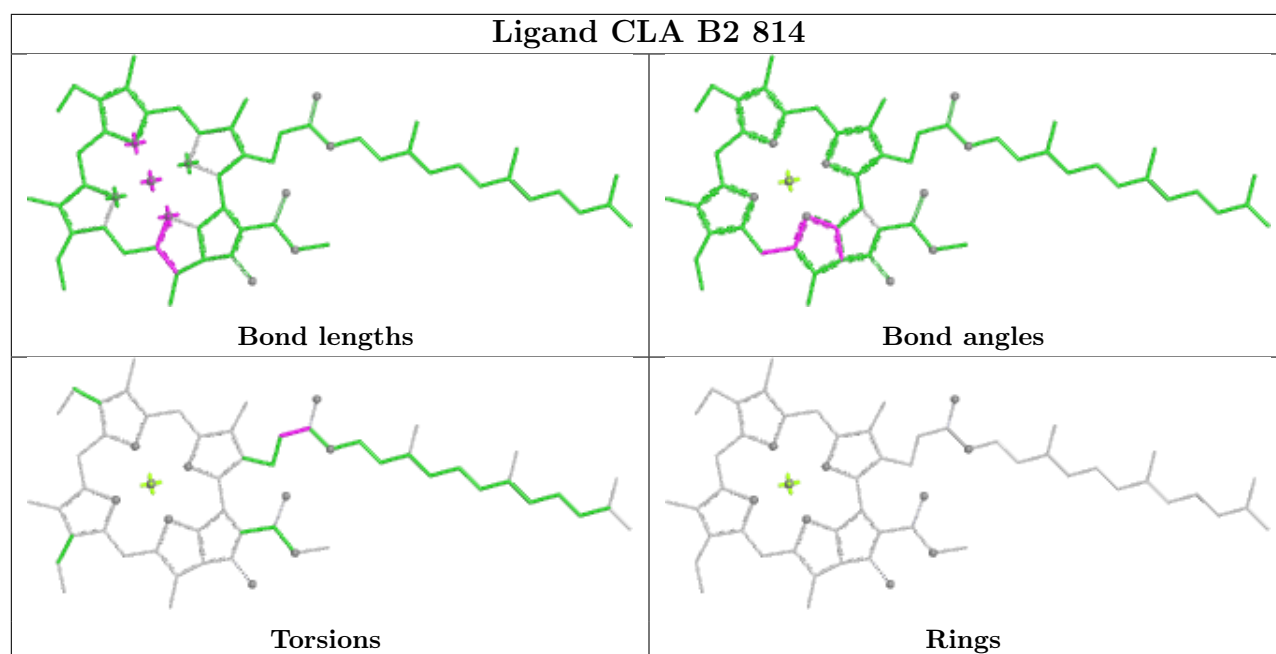


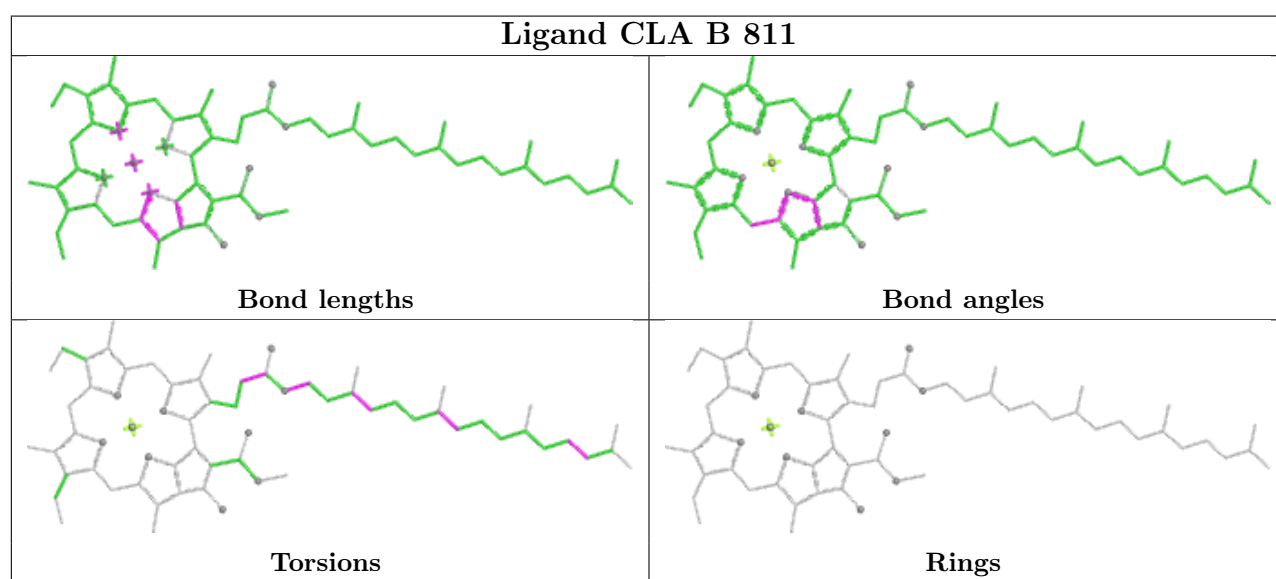
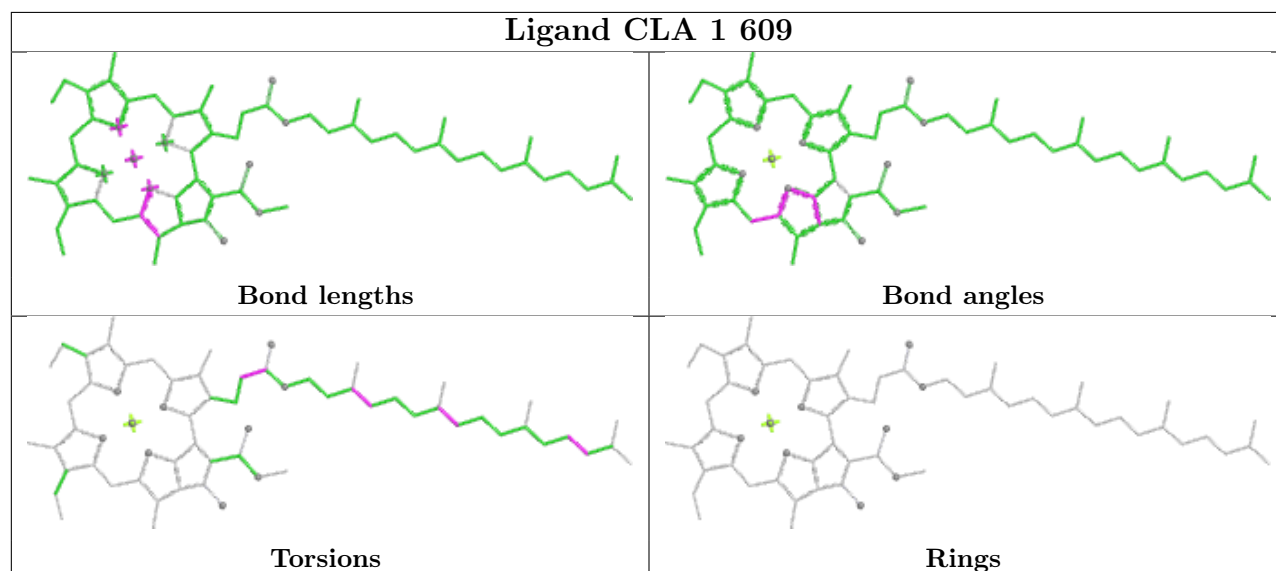
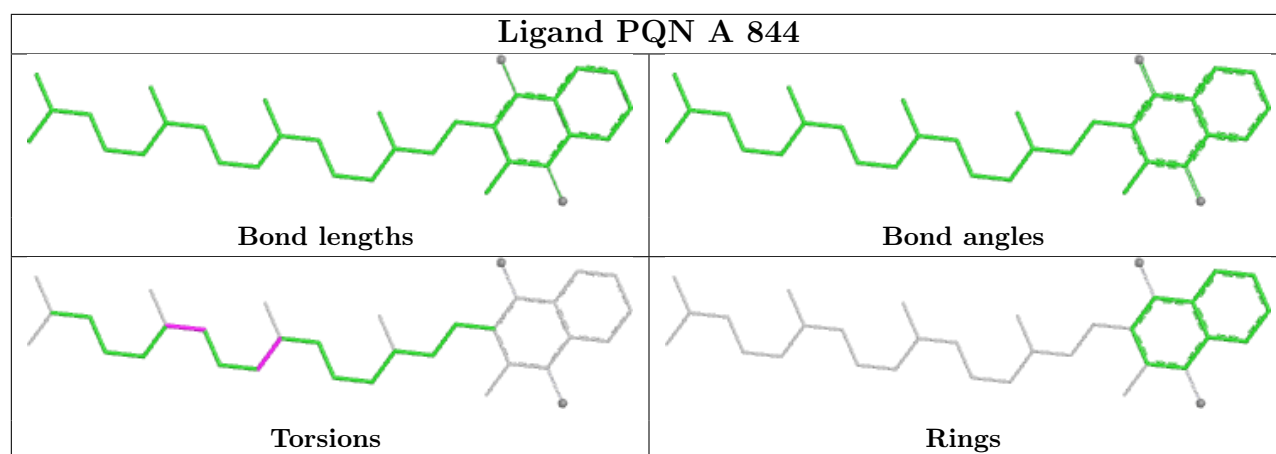
Torsions

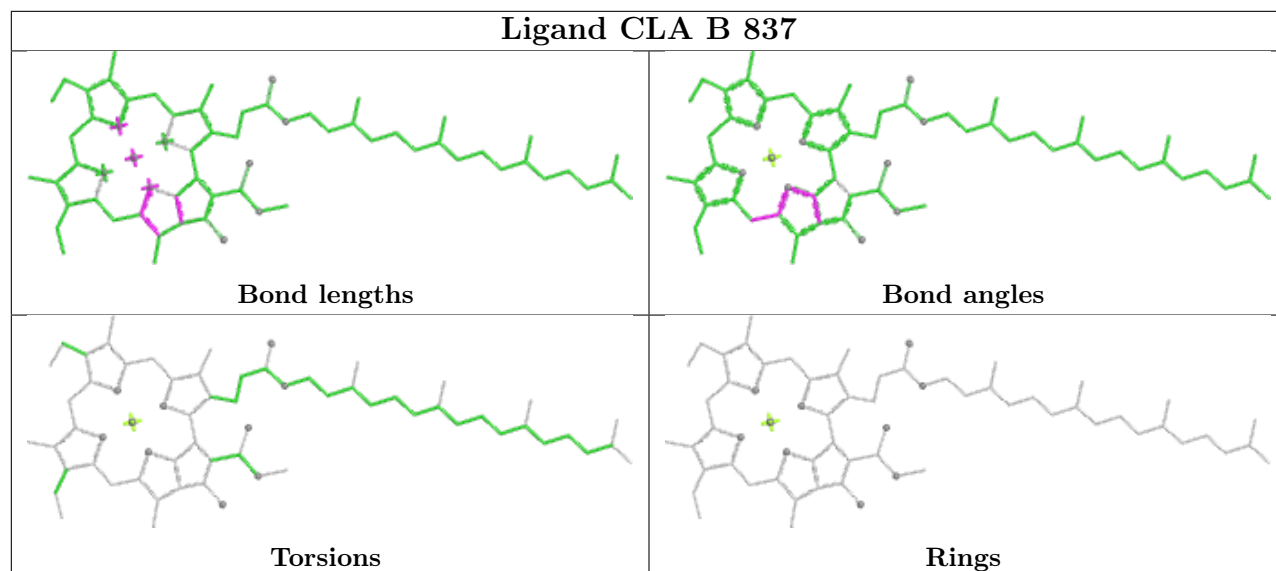
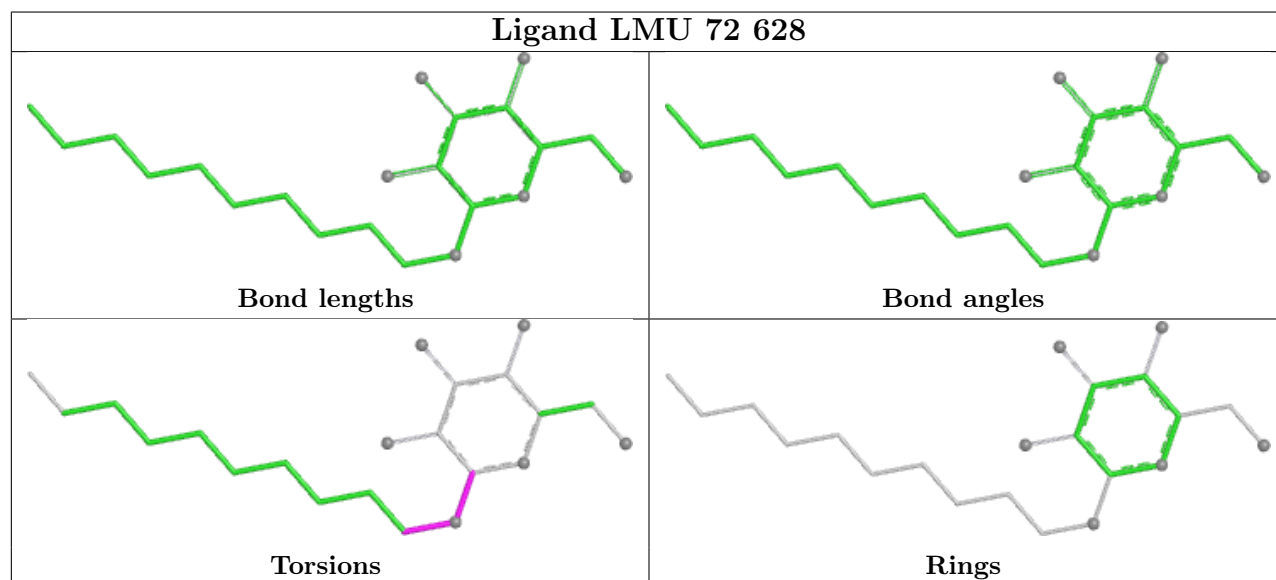
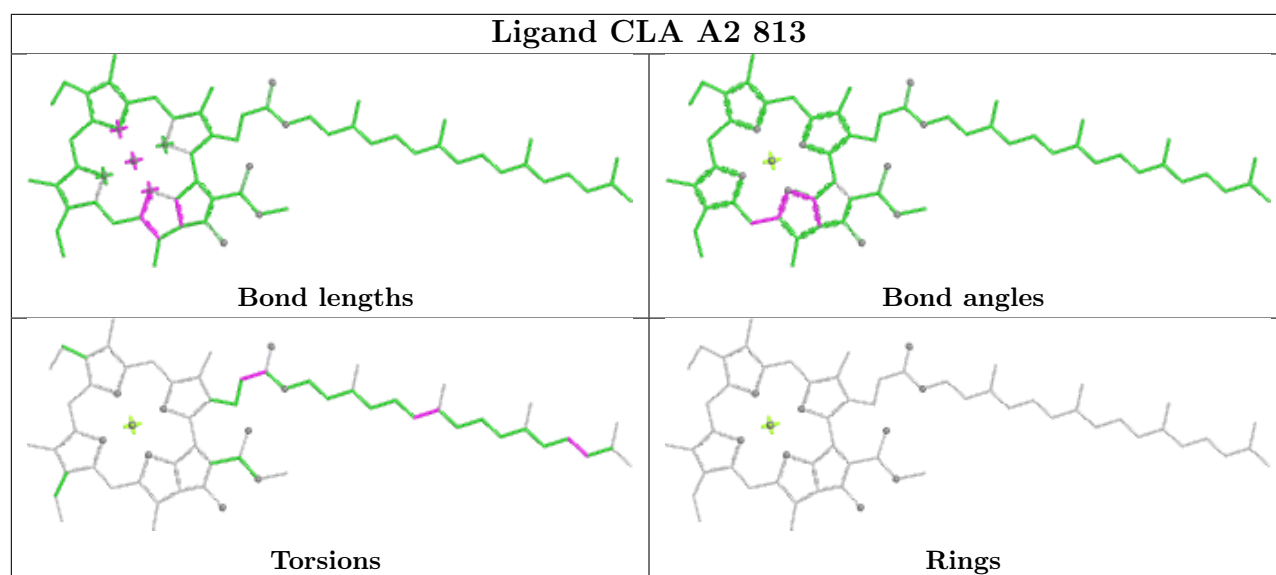


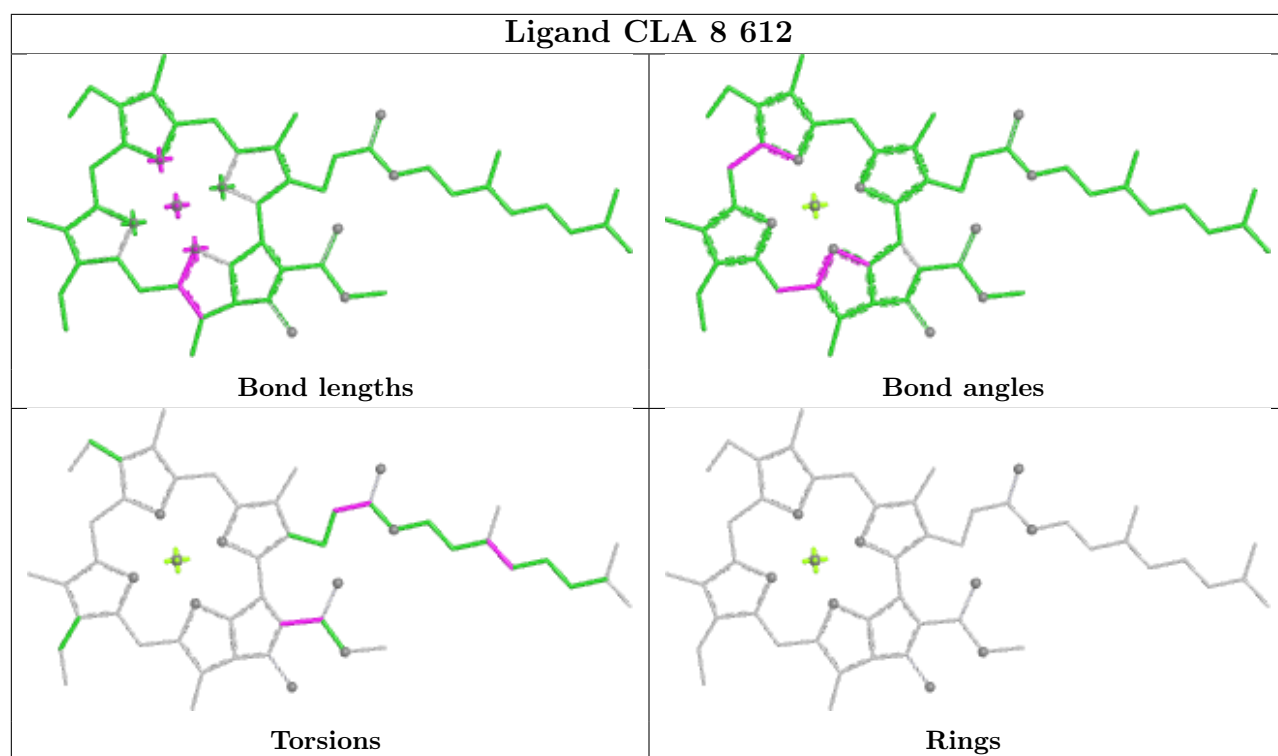
Rings



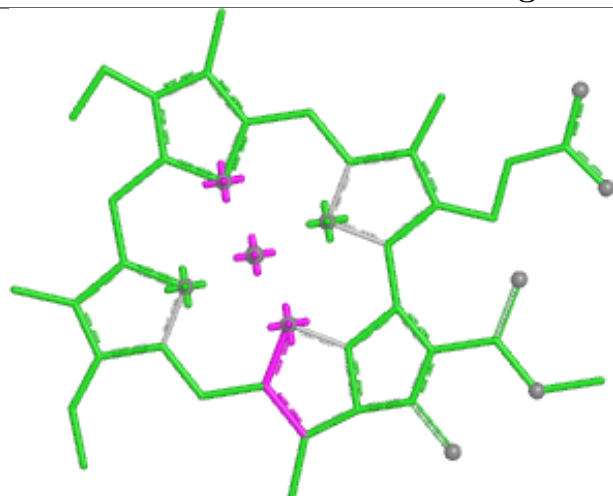




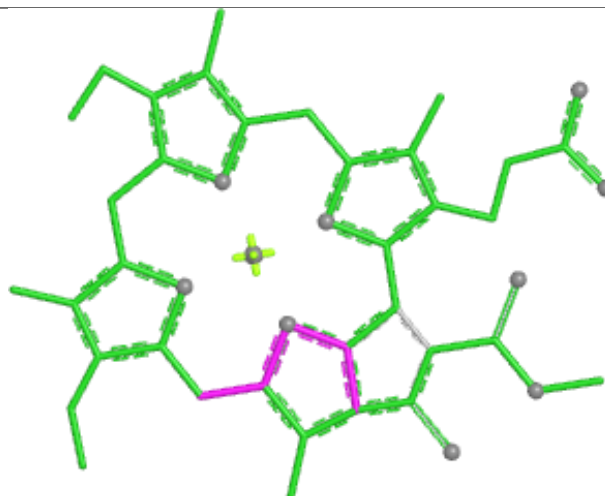




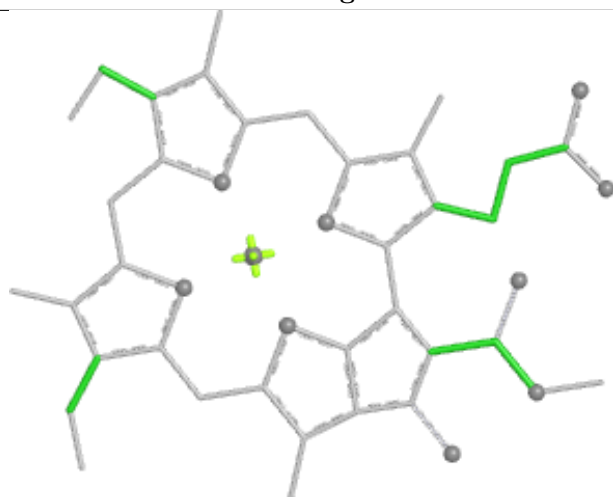
Ligand CLA 4 616



Bond lengths



Bond angles

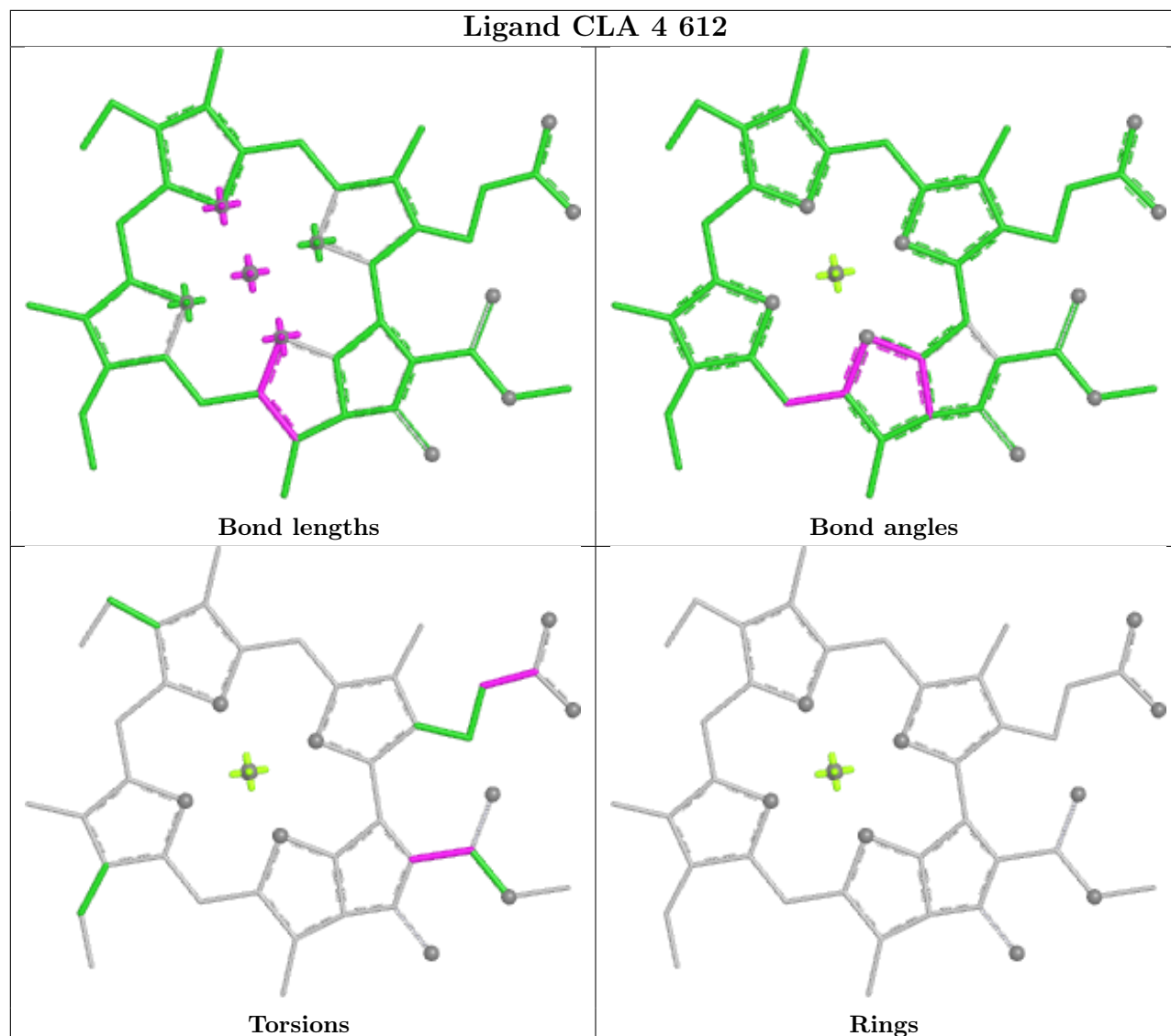


Torsions

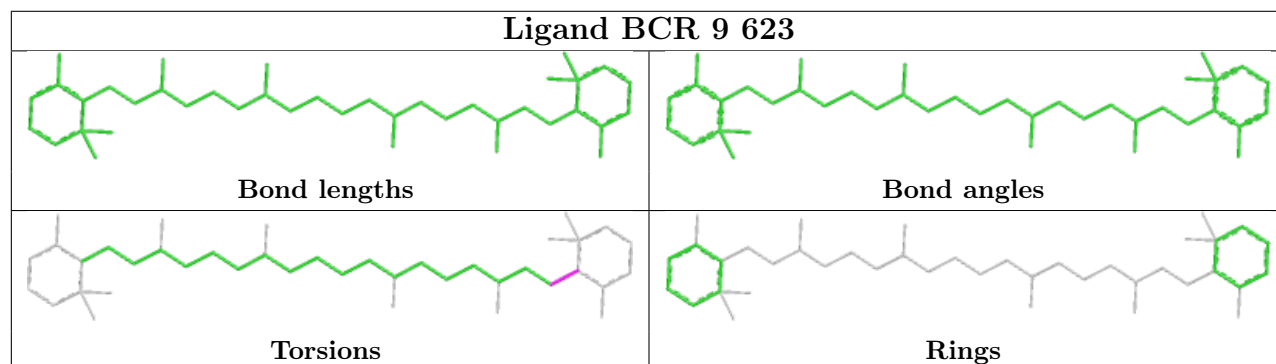


Rings

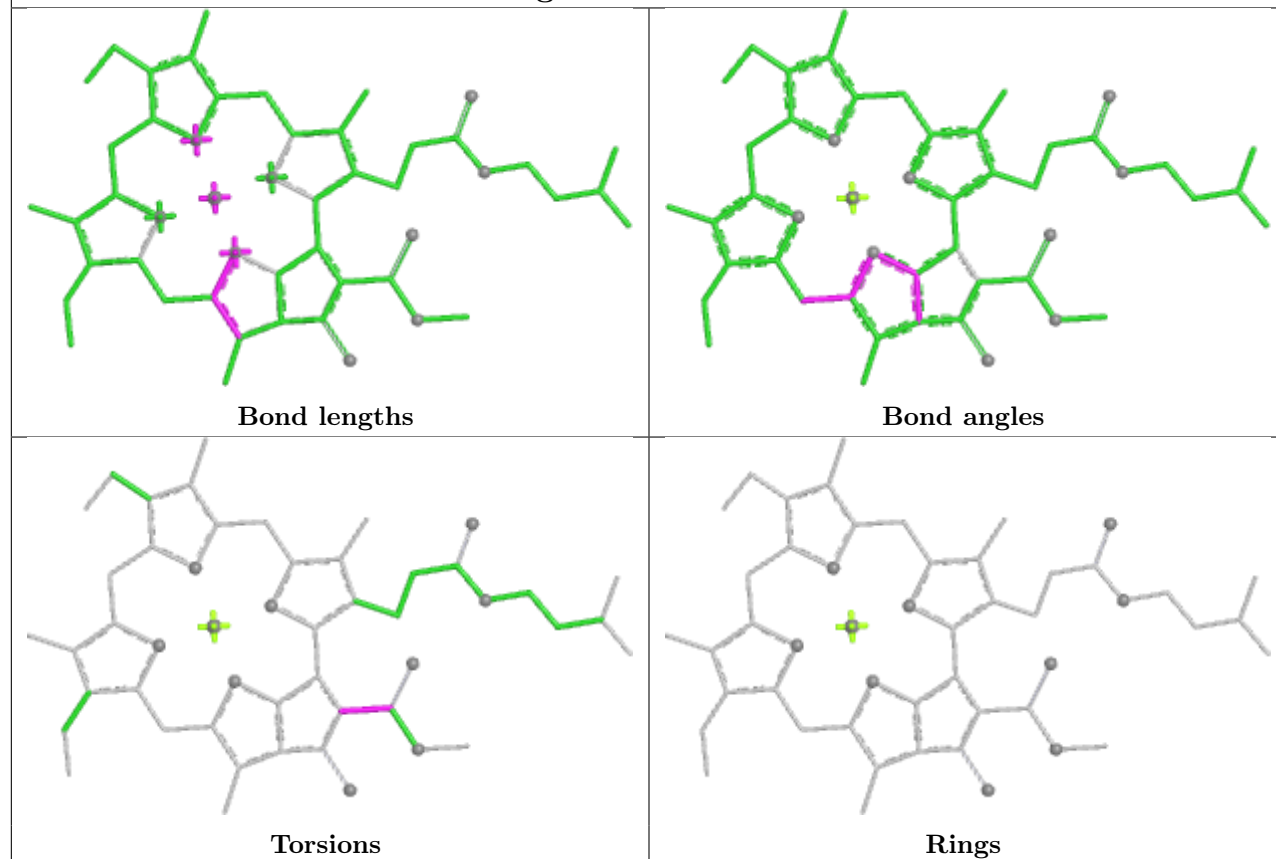
Ligand CLA 4 612



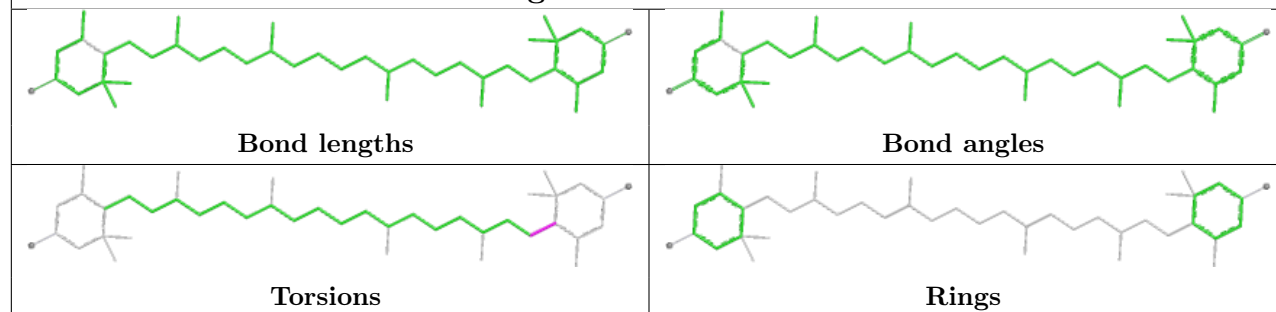
Ligand BCR 9 623

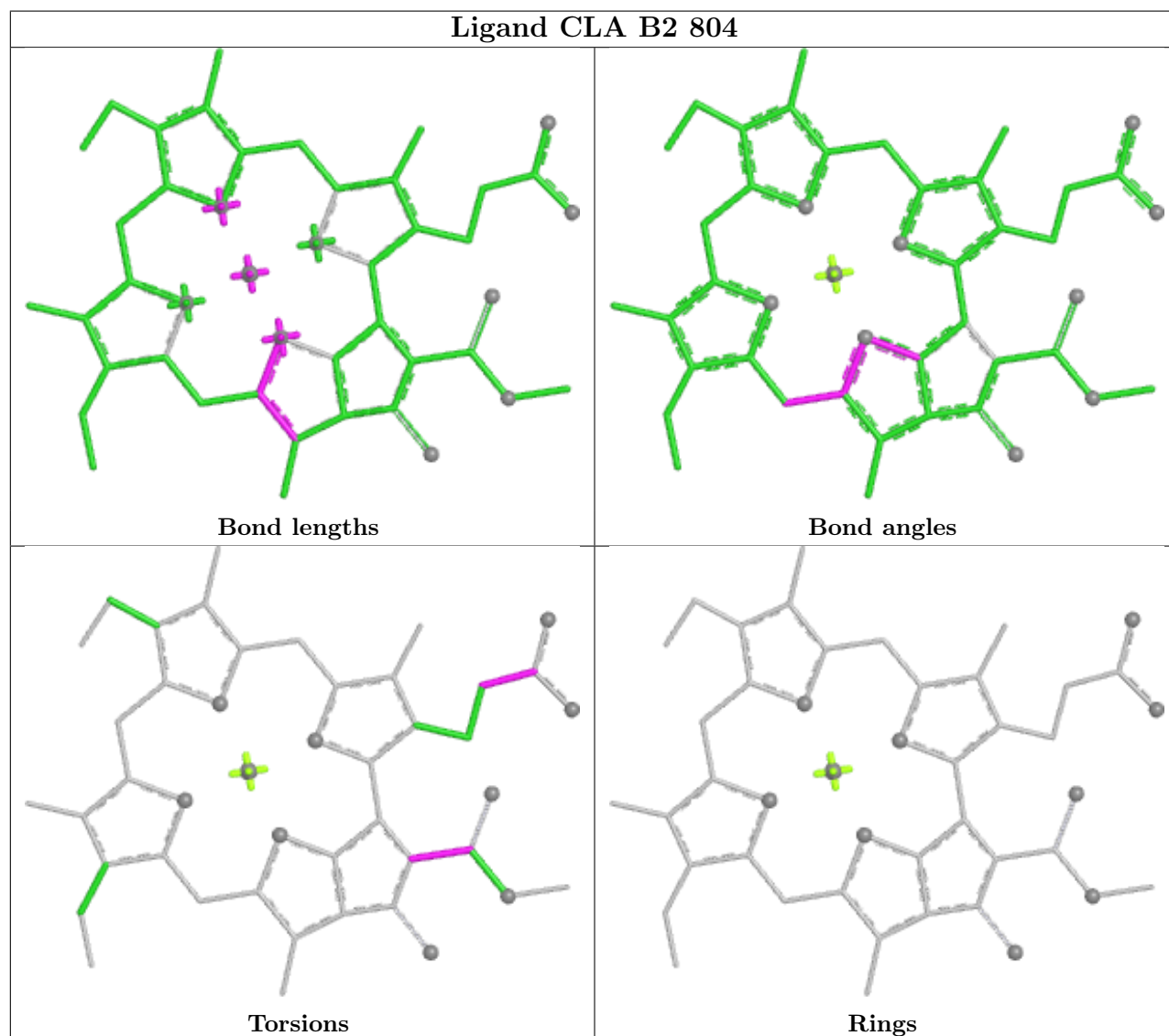
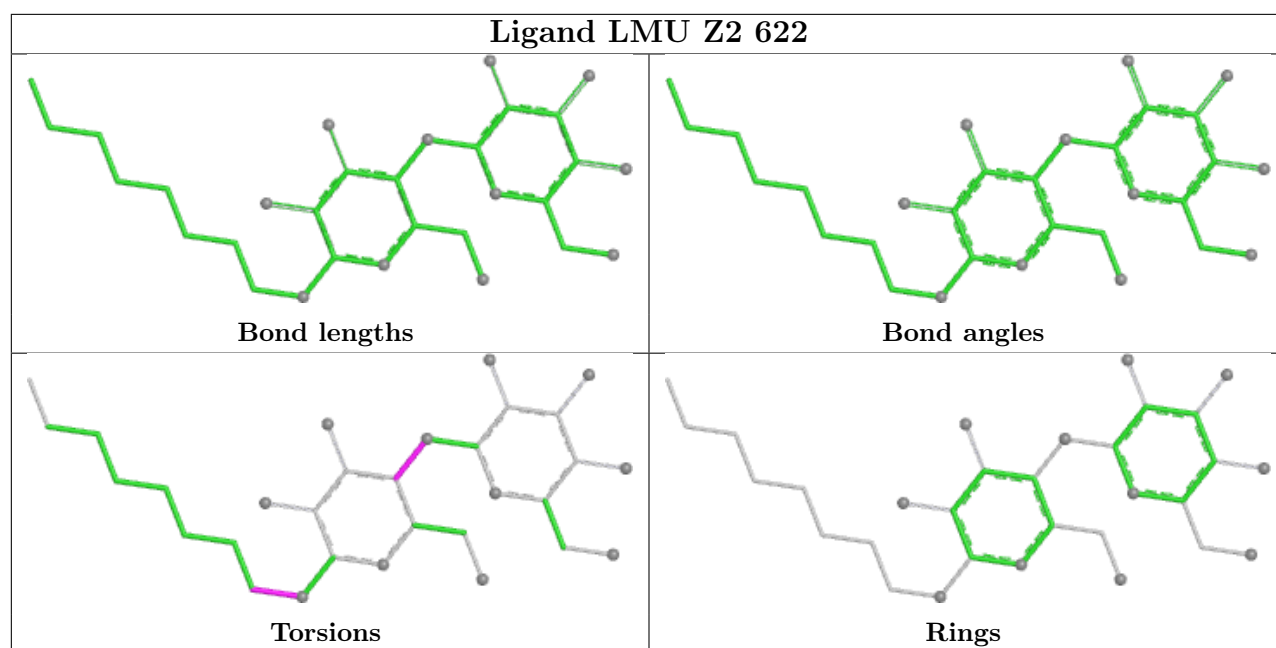


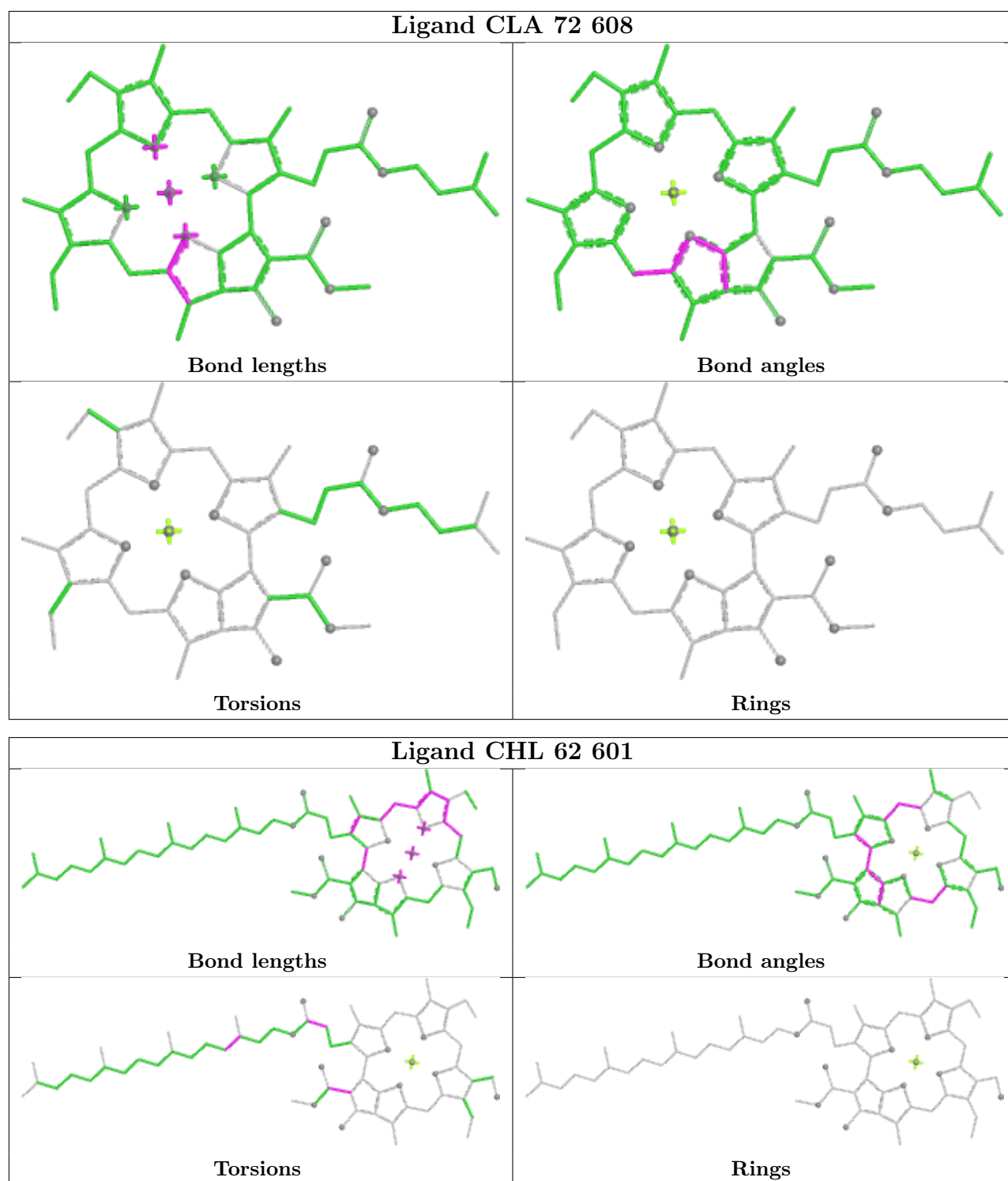
Ligand CLA 4 604



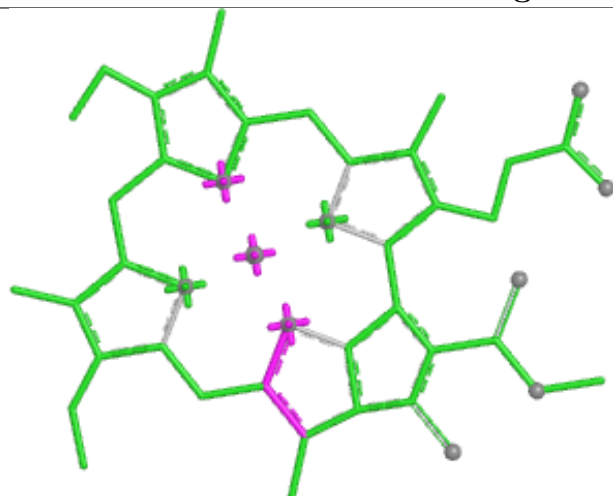
Ligand LUT 32 622



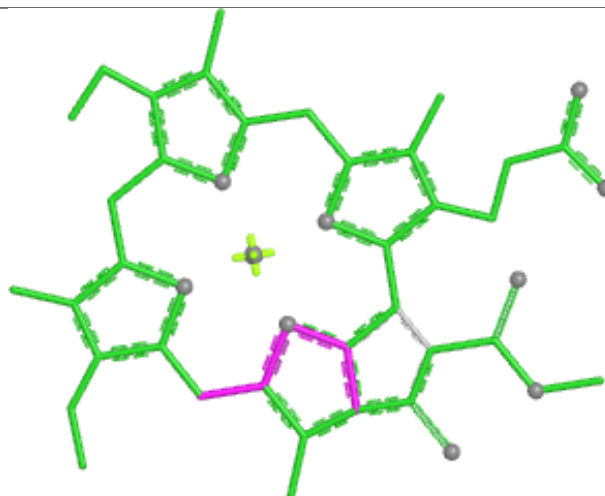




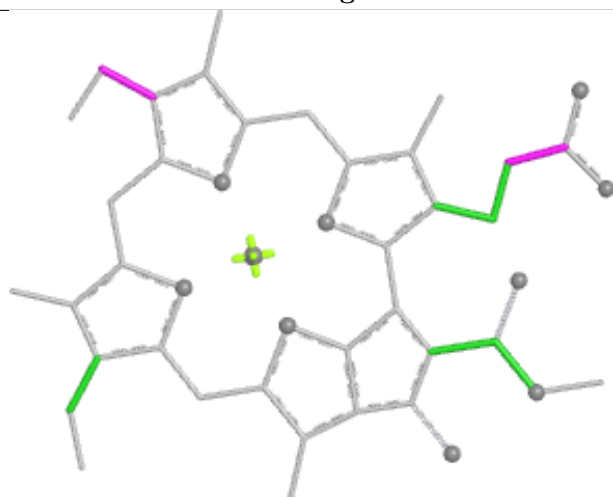
Ligand CLA A 824



Bond lengths



Bond angles

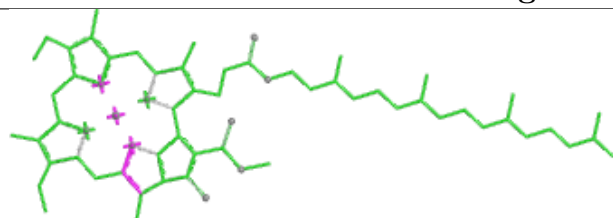


Torsions

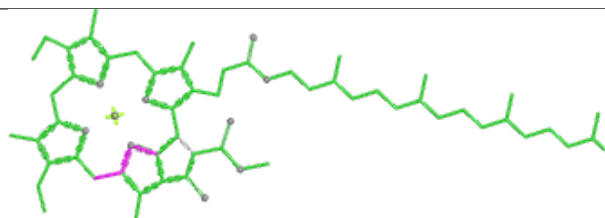


Rings

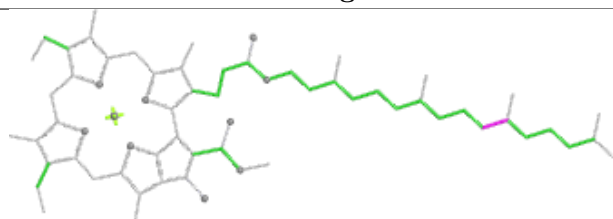
Ligand CLA 8 610



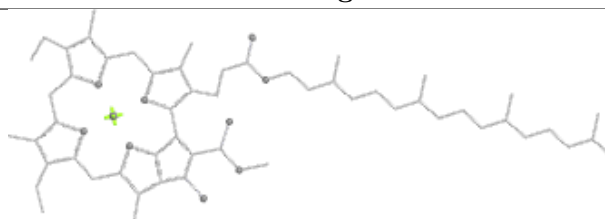
Bond lengths



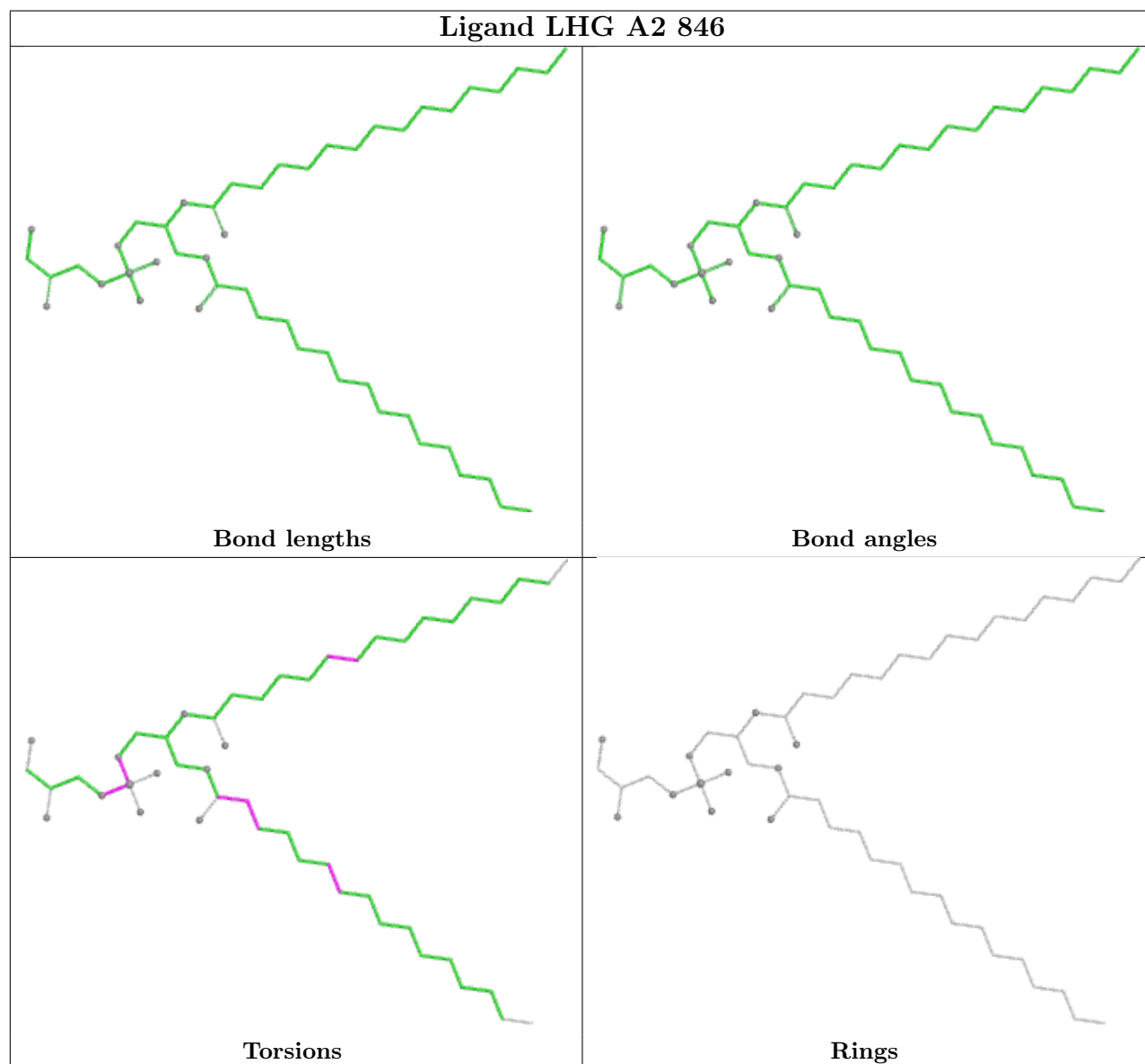
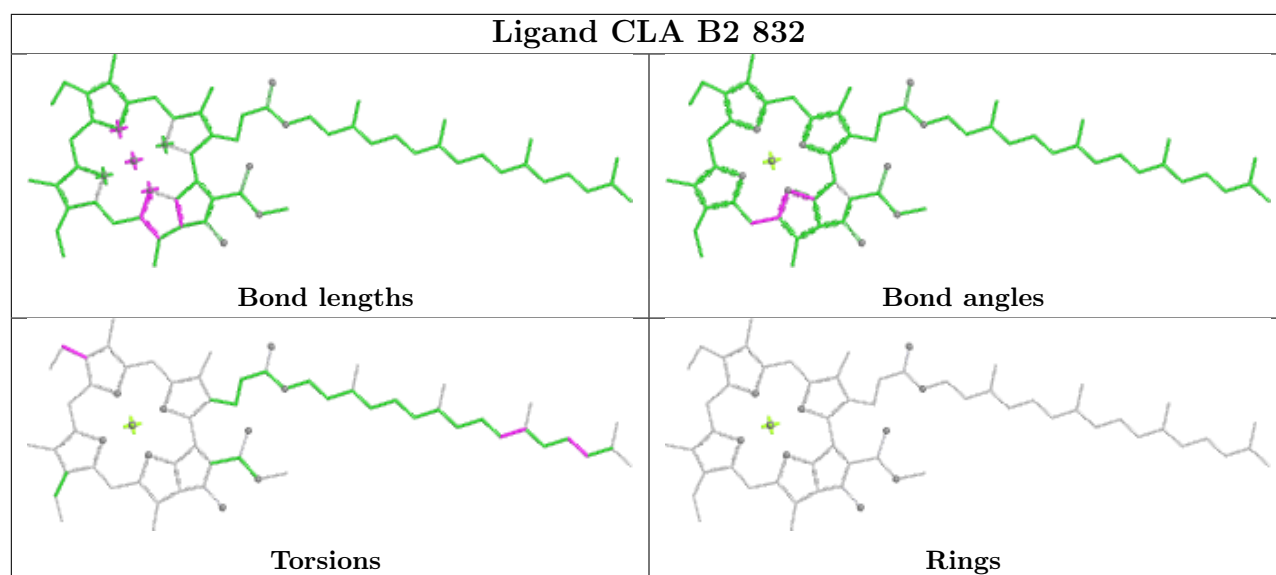
Bond angles

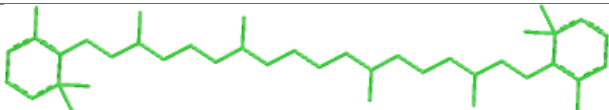
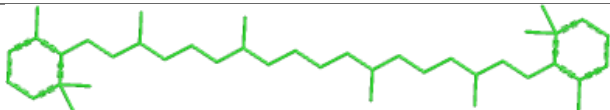
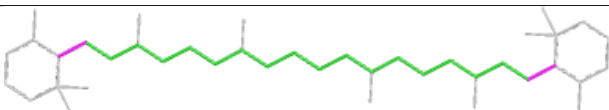
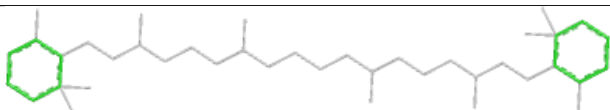


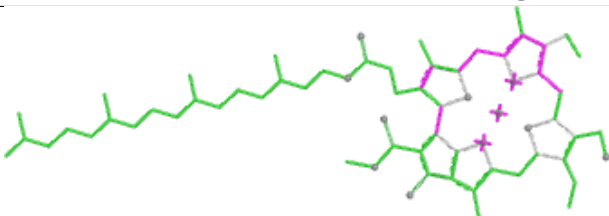
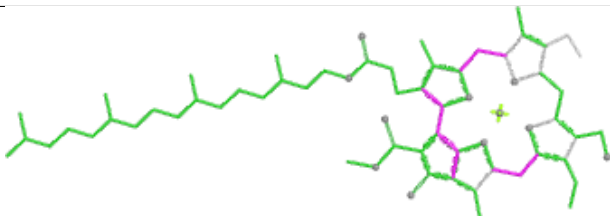
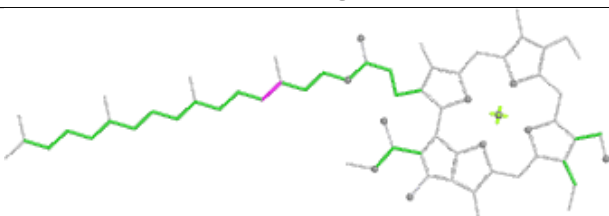
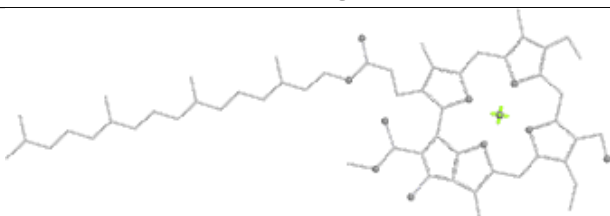
Torsions

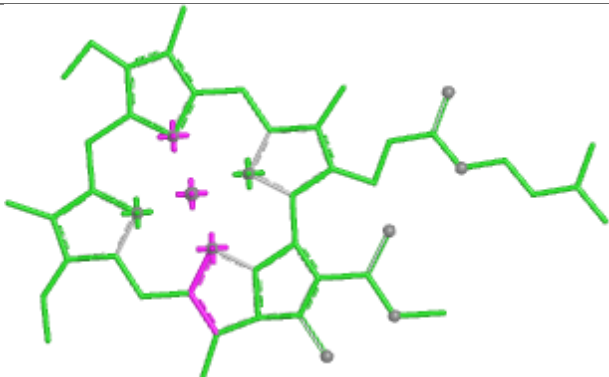
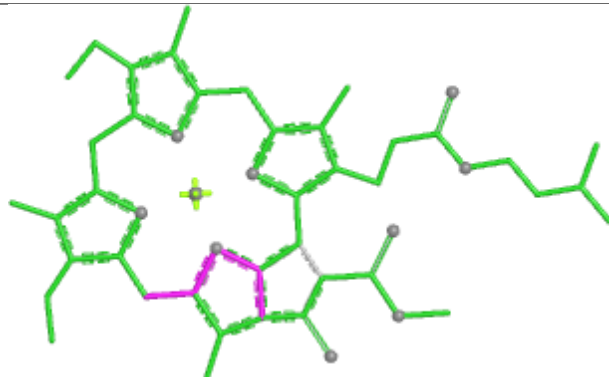
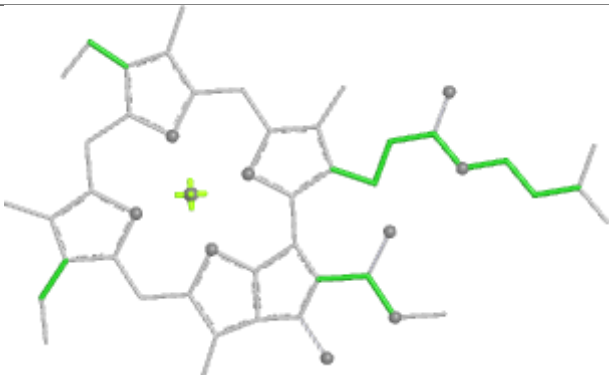
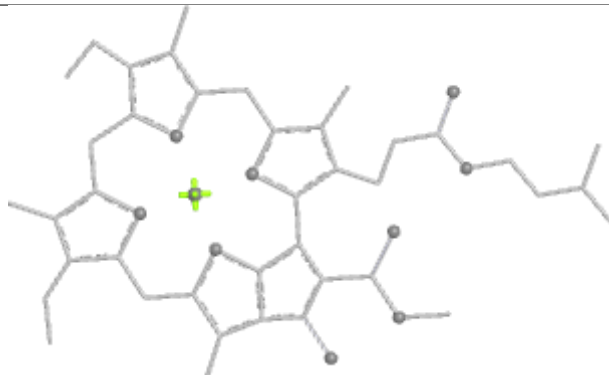


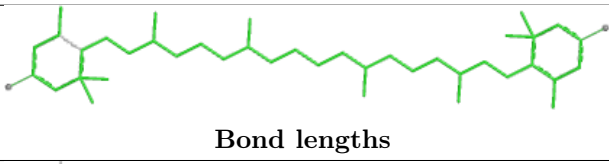
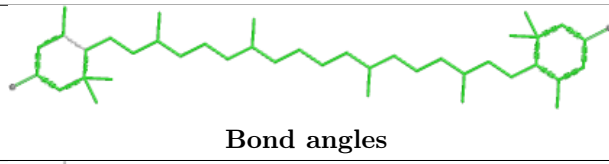
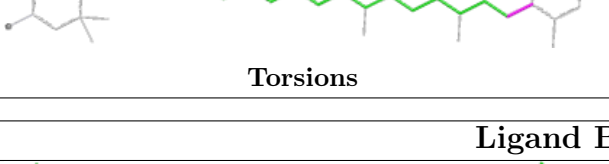
Rings

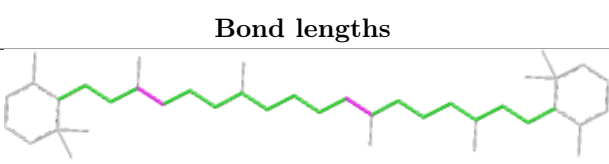
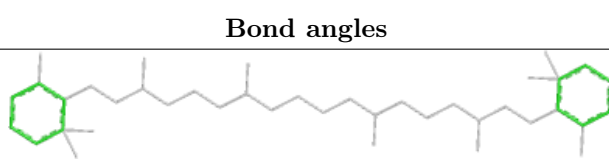


Ligand BCR 8 619	
	
Bond lengths	Bond angles
	
Torsions	Rings

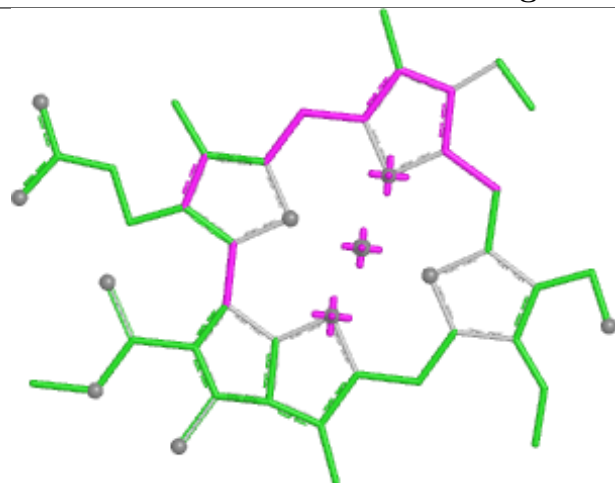
Ligand CHL 8 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Z2 614	
	
Bond lengths	Bond angles
	
Torsions	Rings

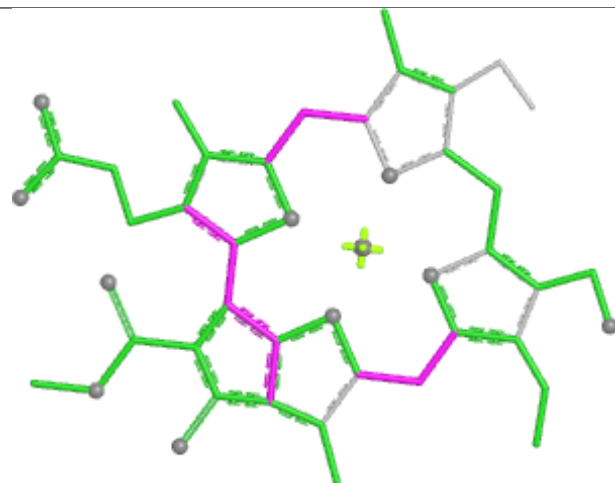
Ligand LUT 6 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 852	
	
Bond lengths	Bond angles
Torsions	Rings

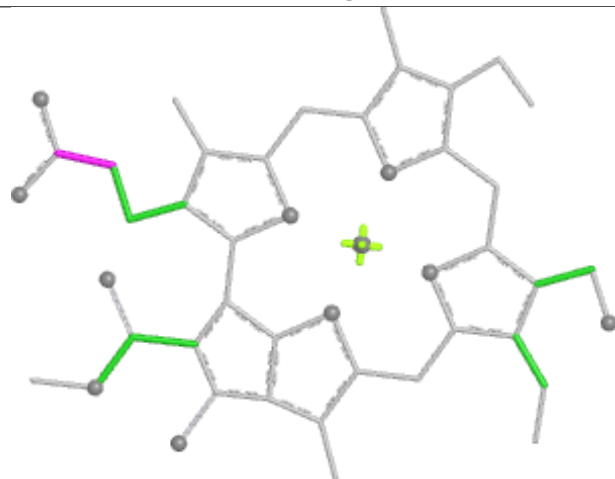
Ligand CHL 7 607



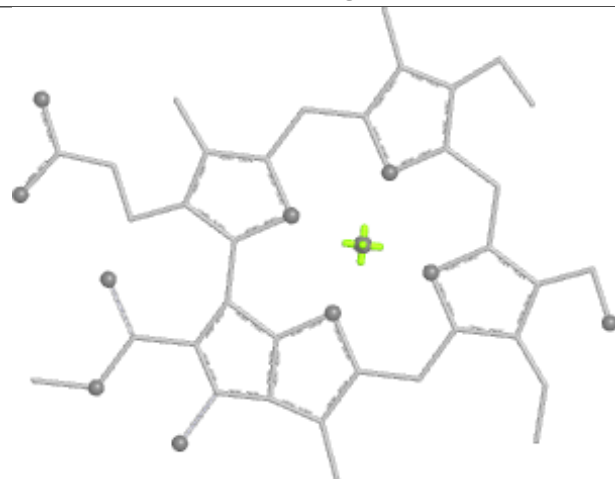
Bond lengths



Bond angles

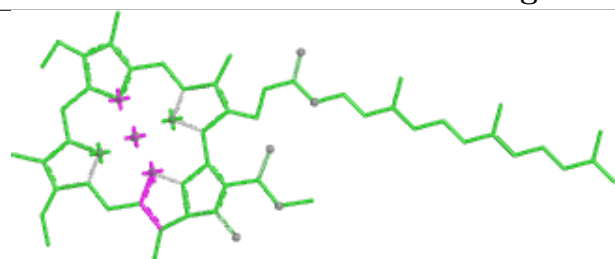


Torsions

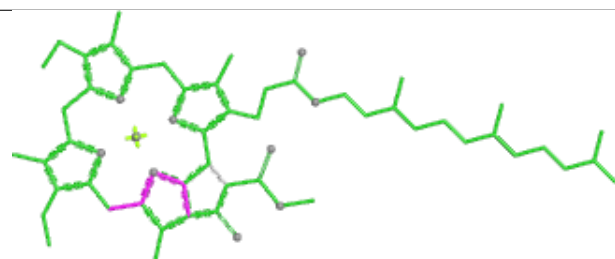


Rings

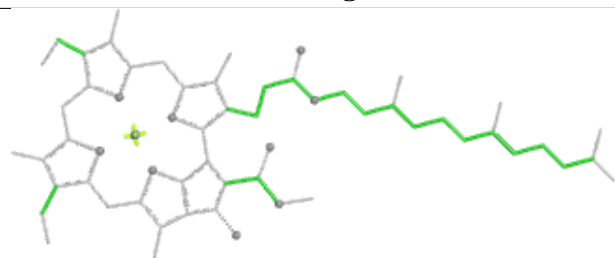
Ligand CLA 6 610



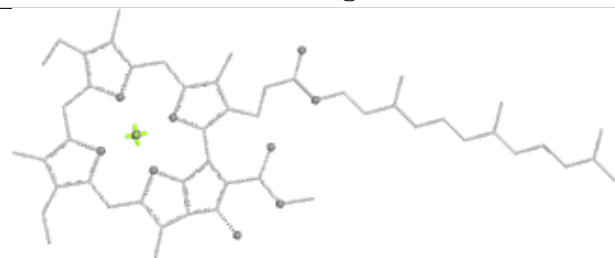
Bond lengths



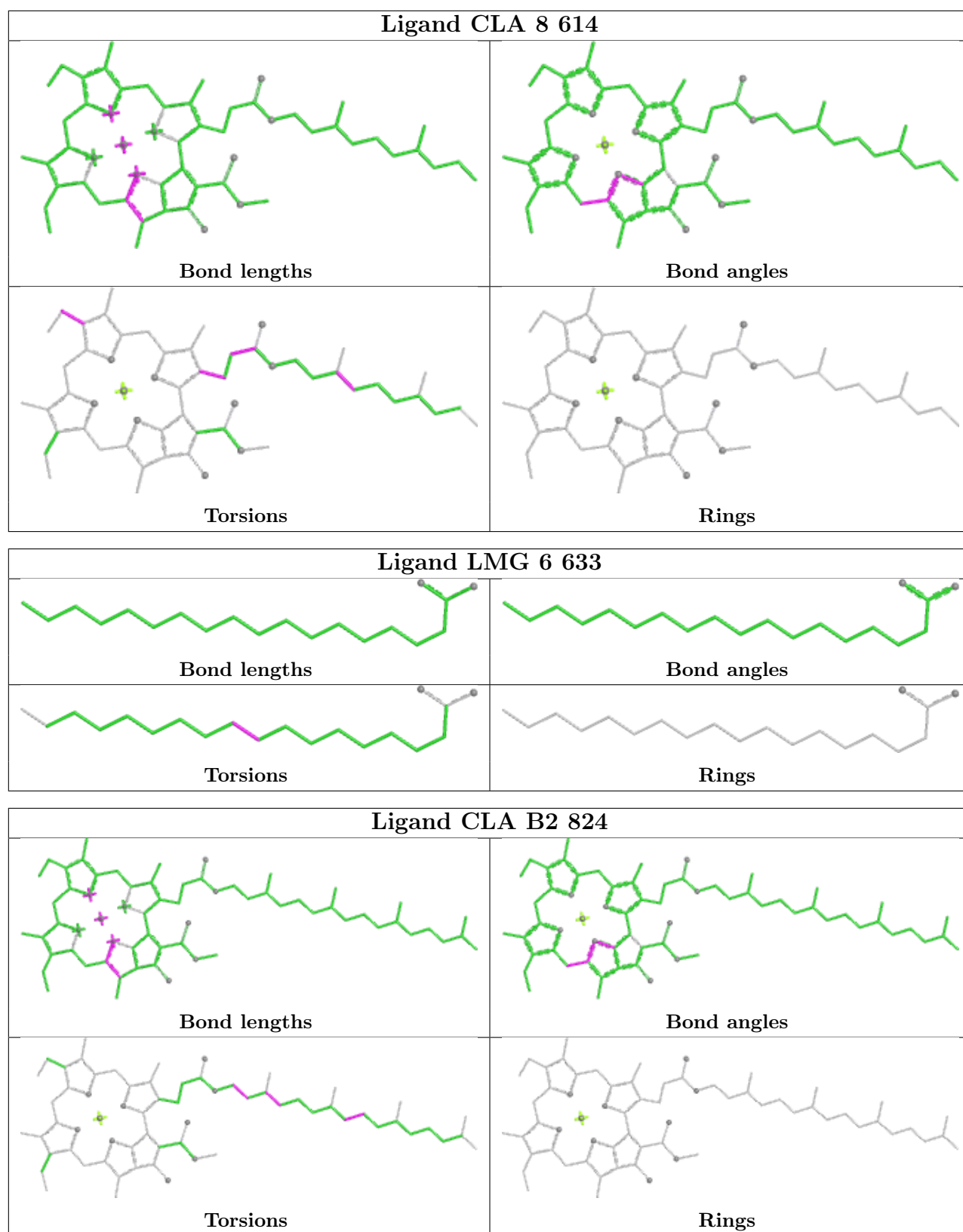
Bond angles

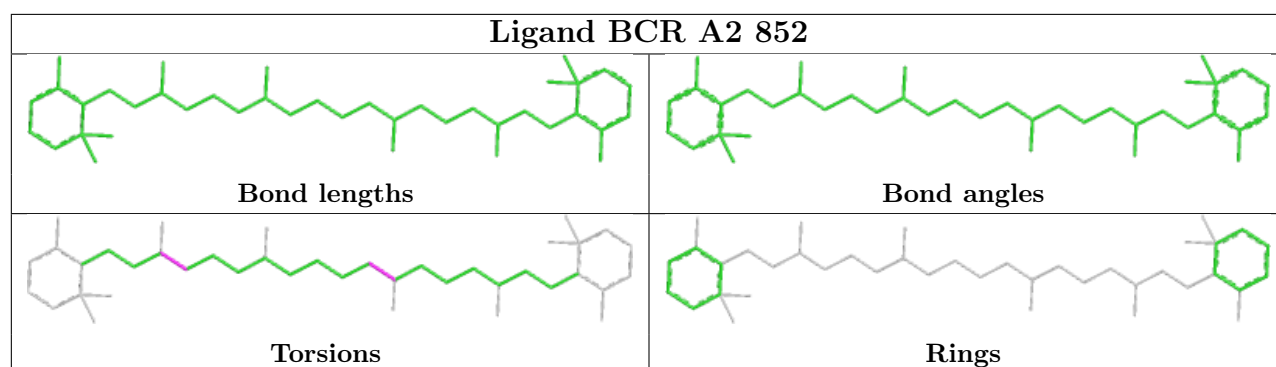
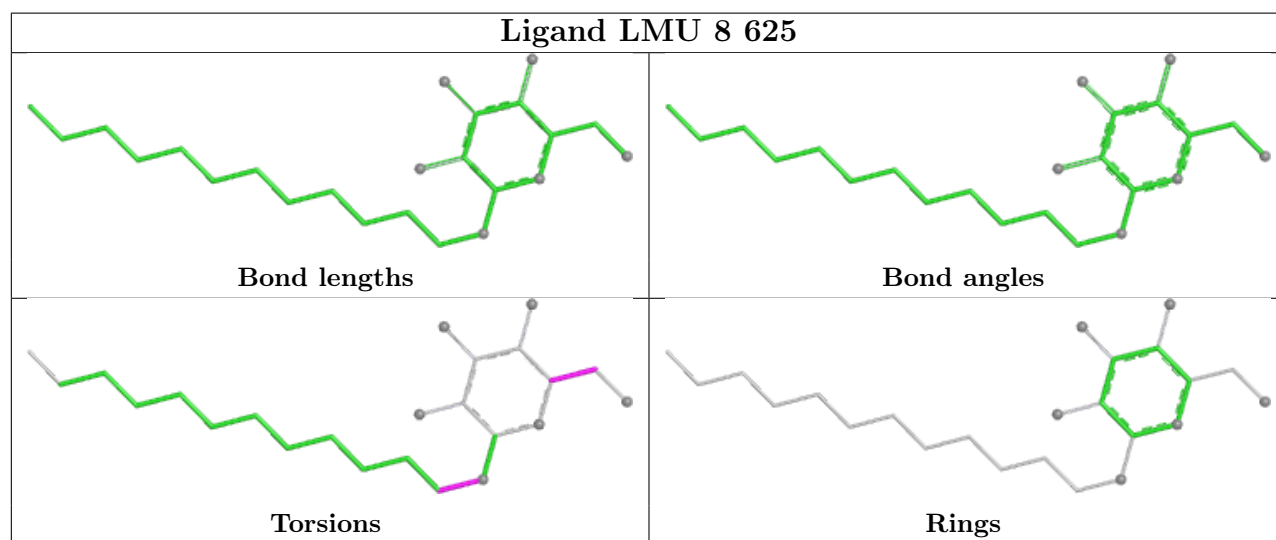
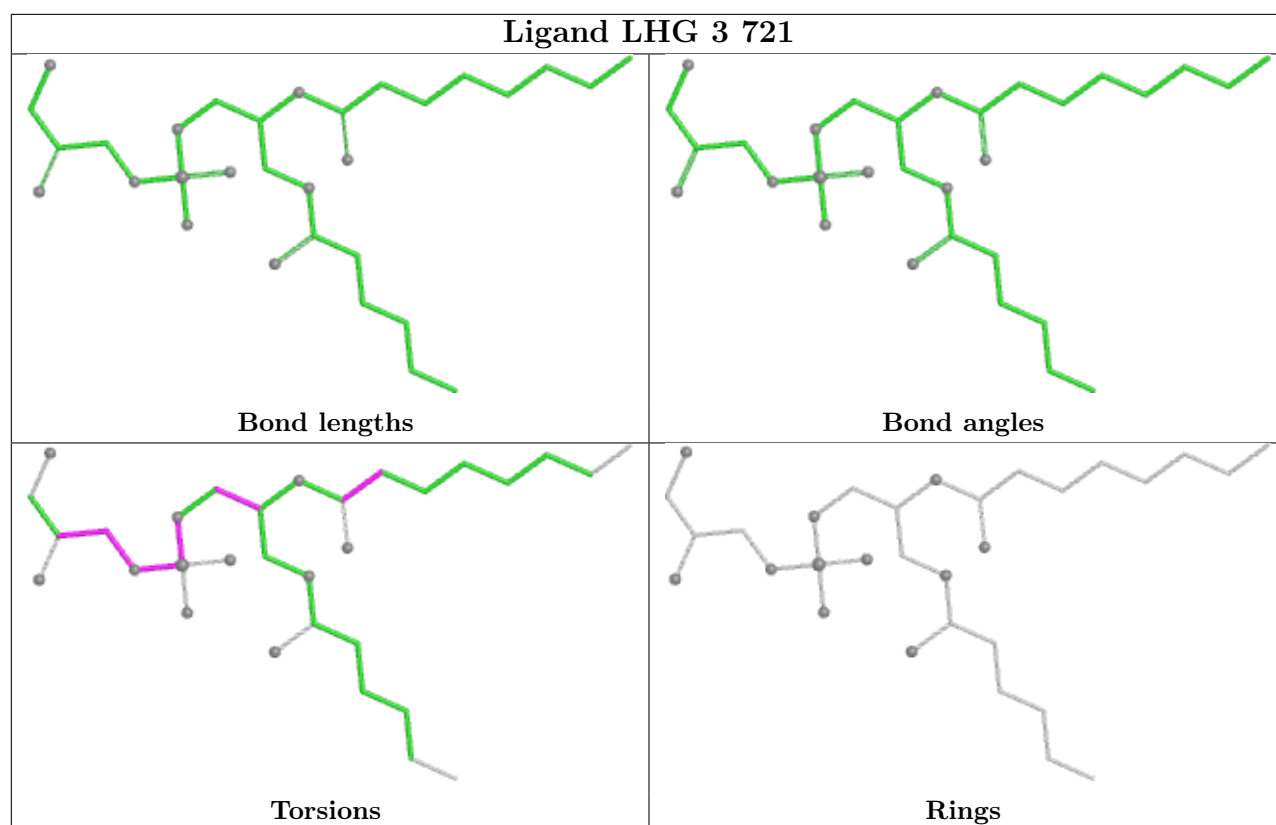


Torsions

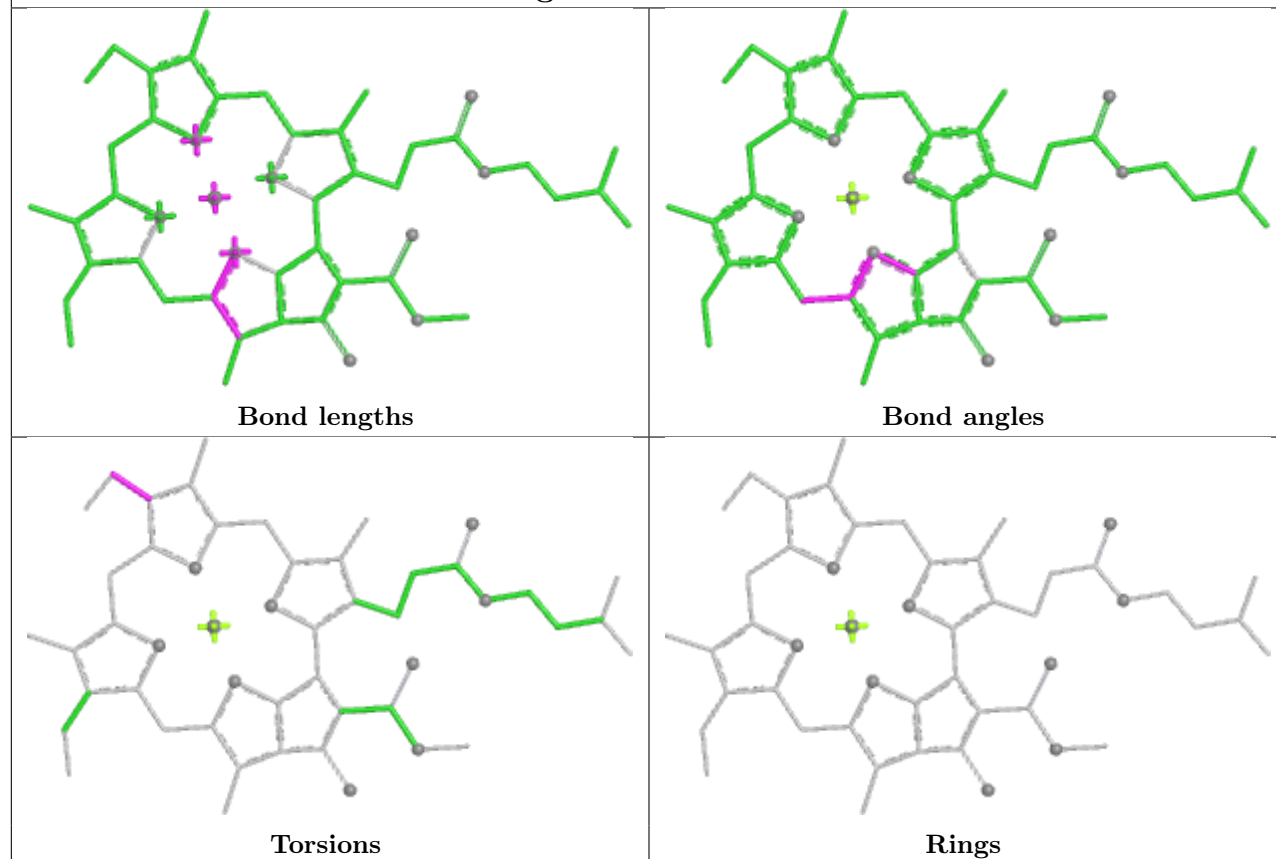


Rings

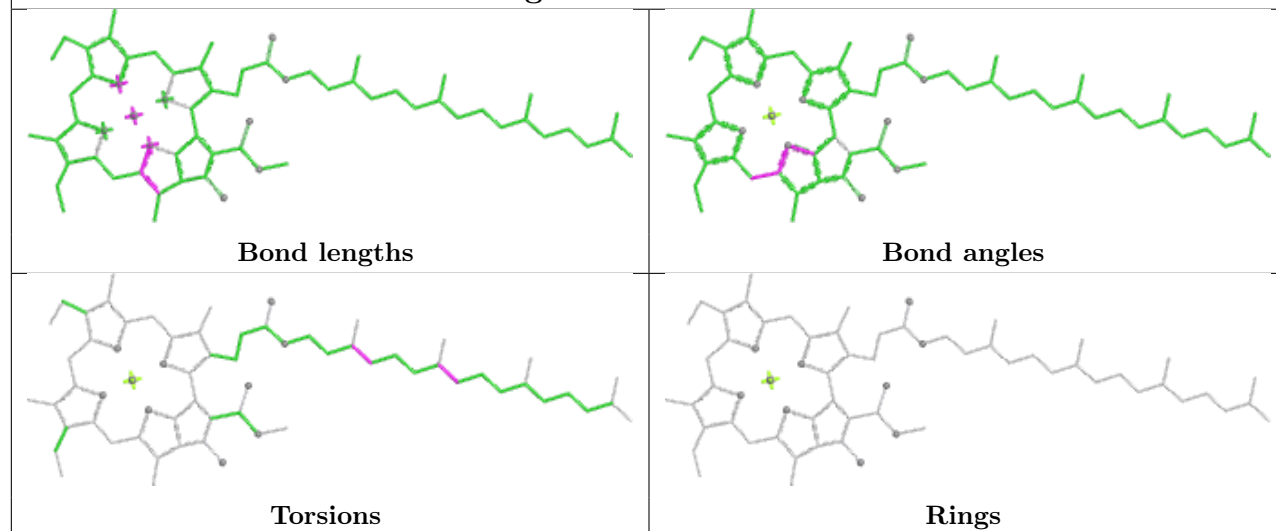


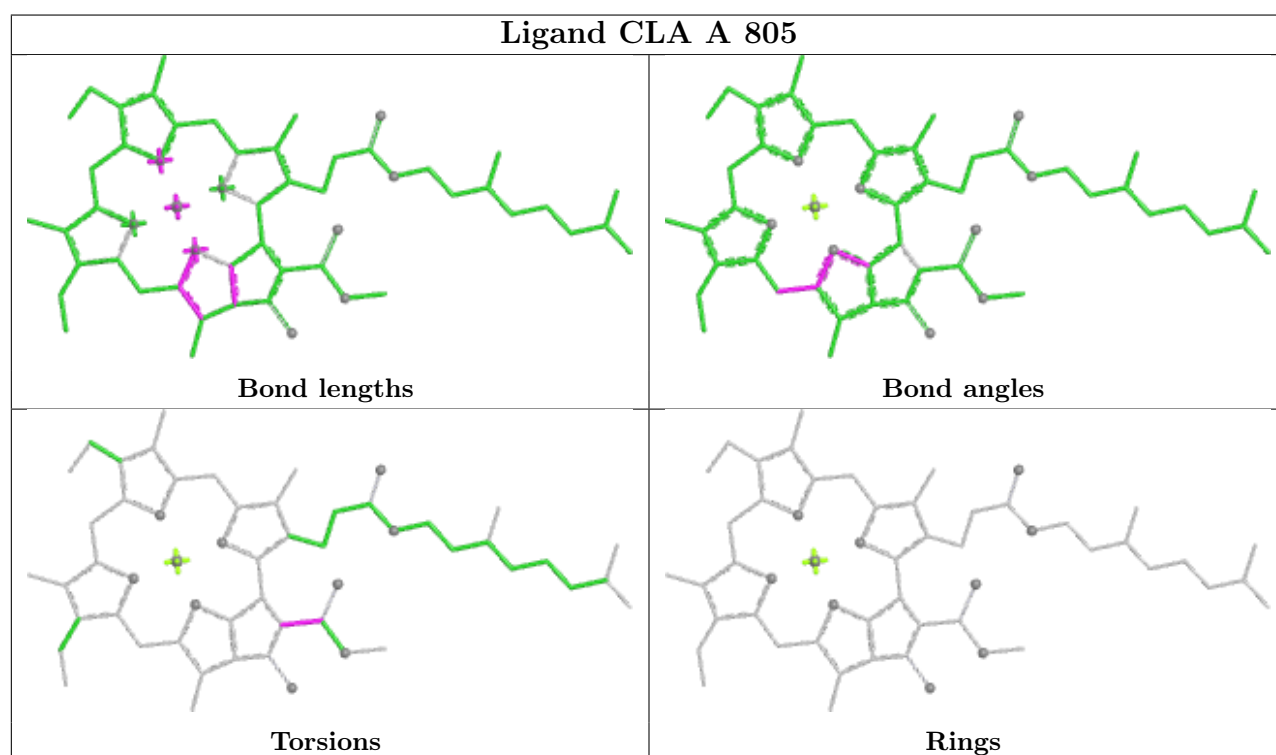
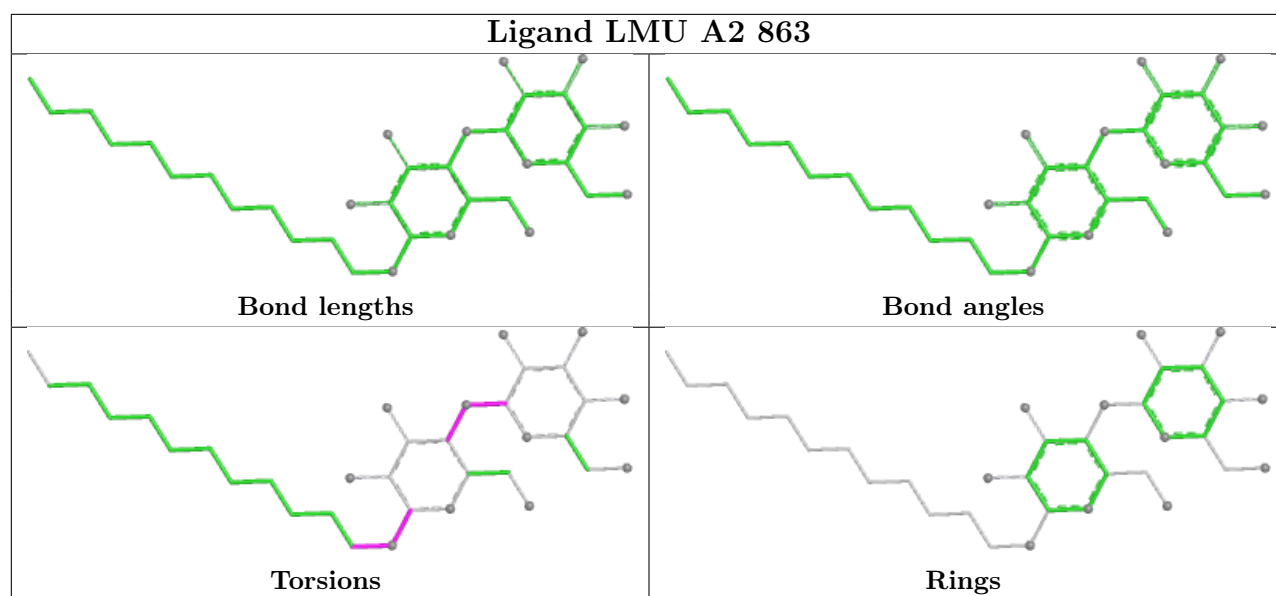


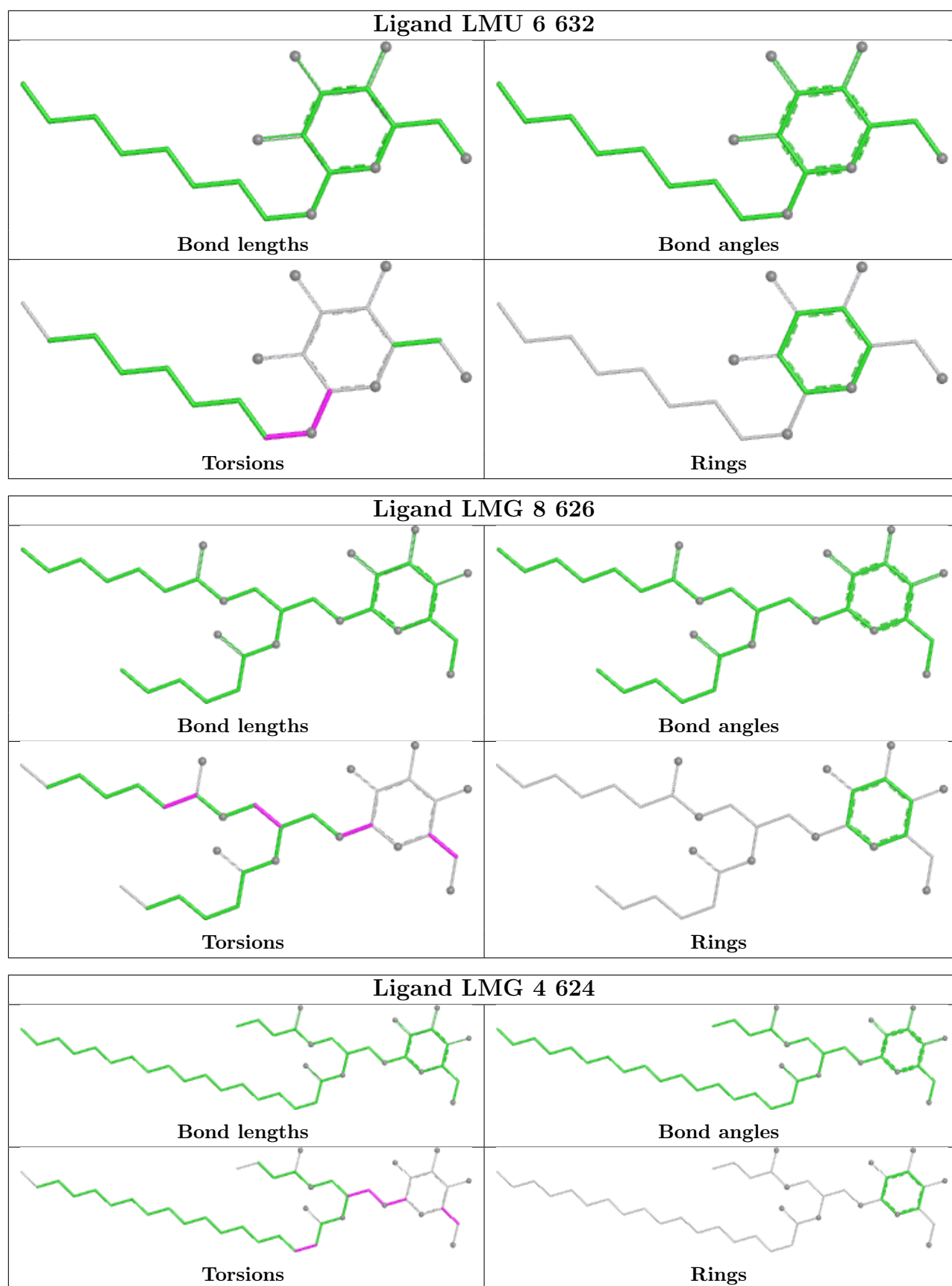
Ligand CLA 8 608

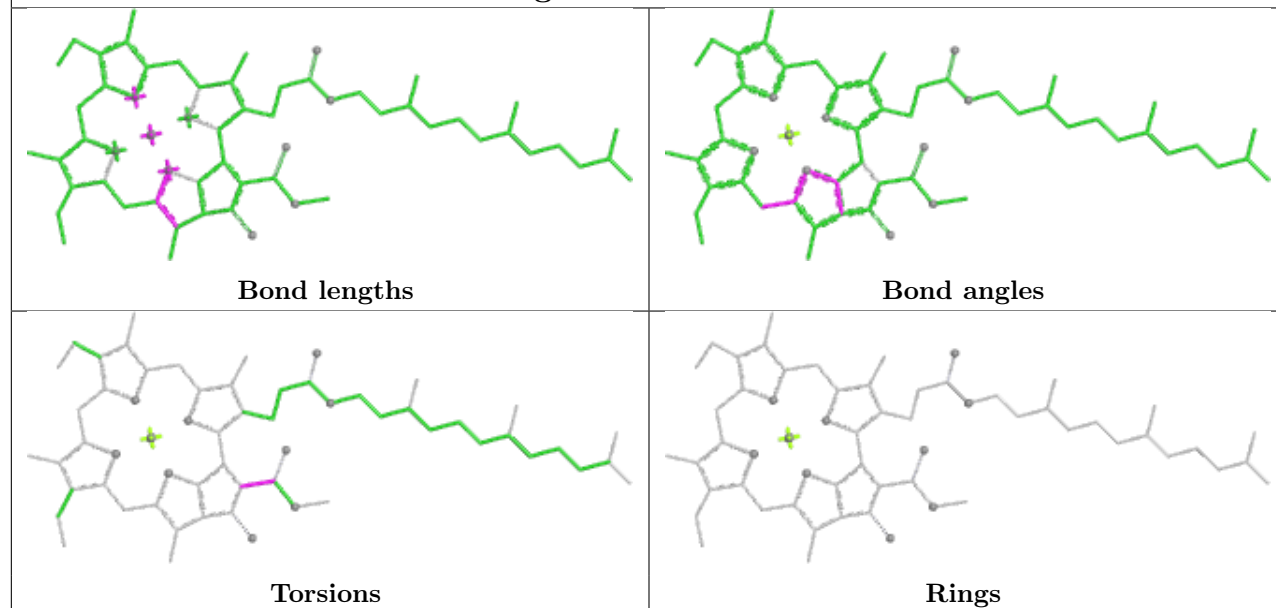
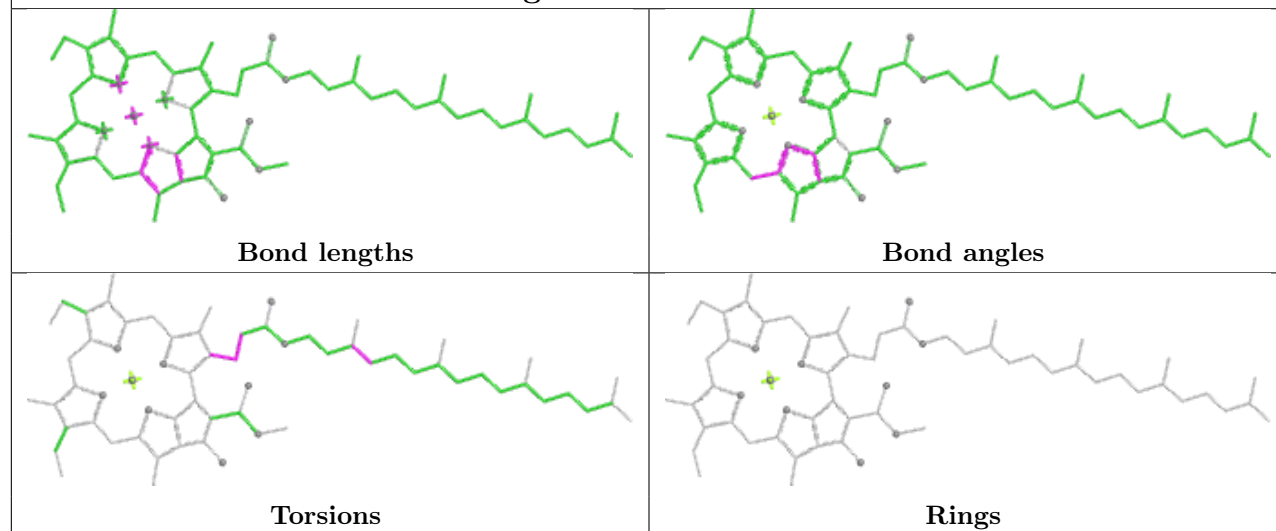


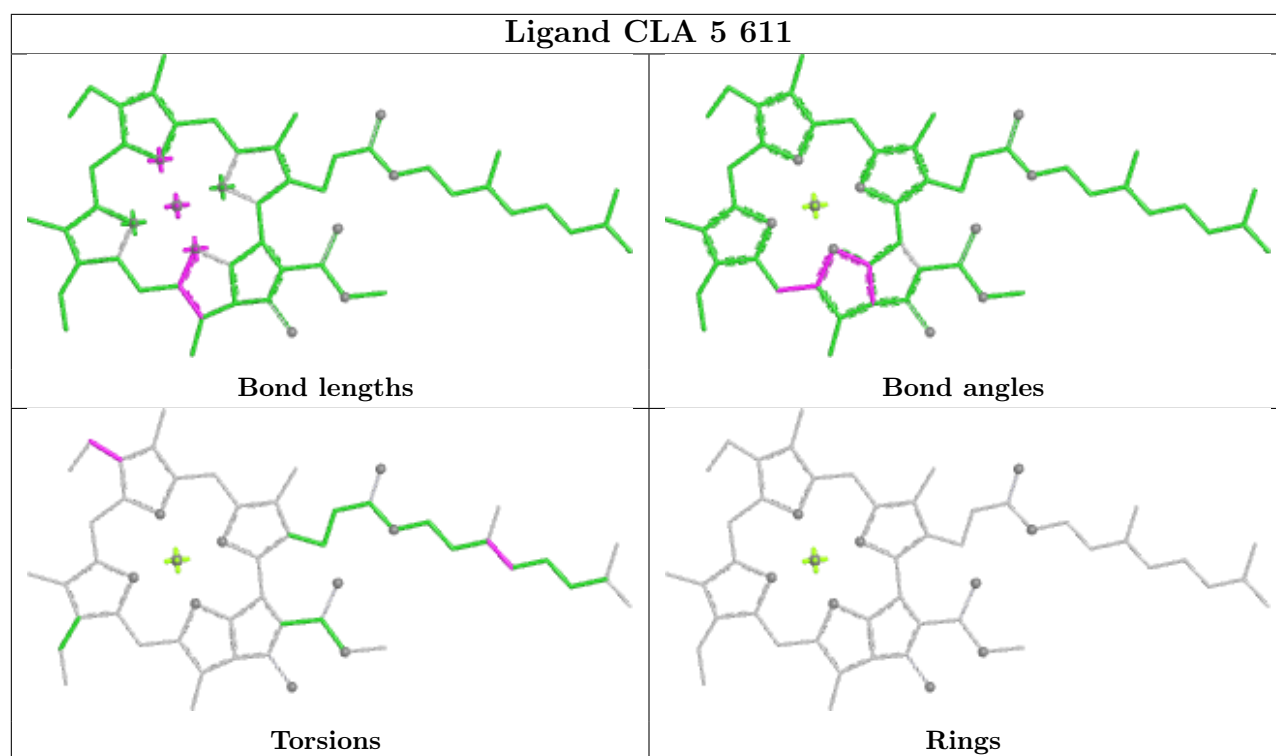
Ligand CLA F2 301

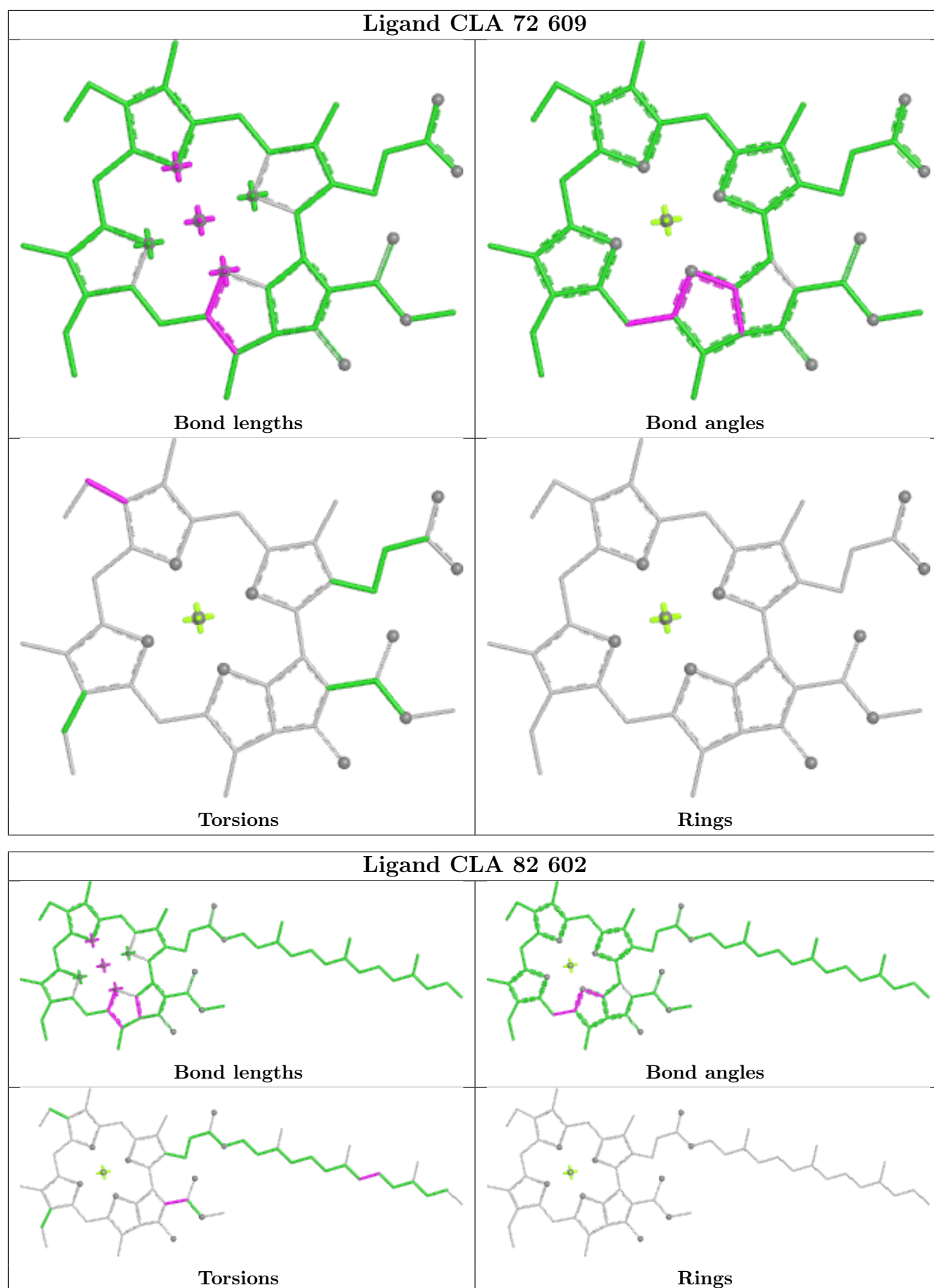


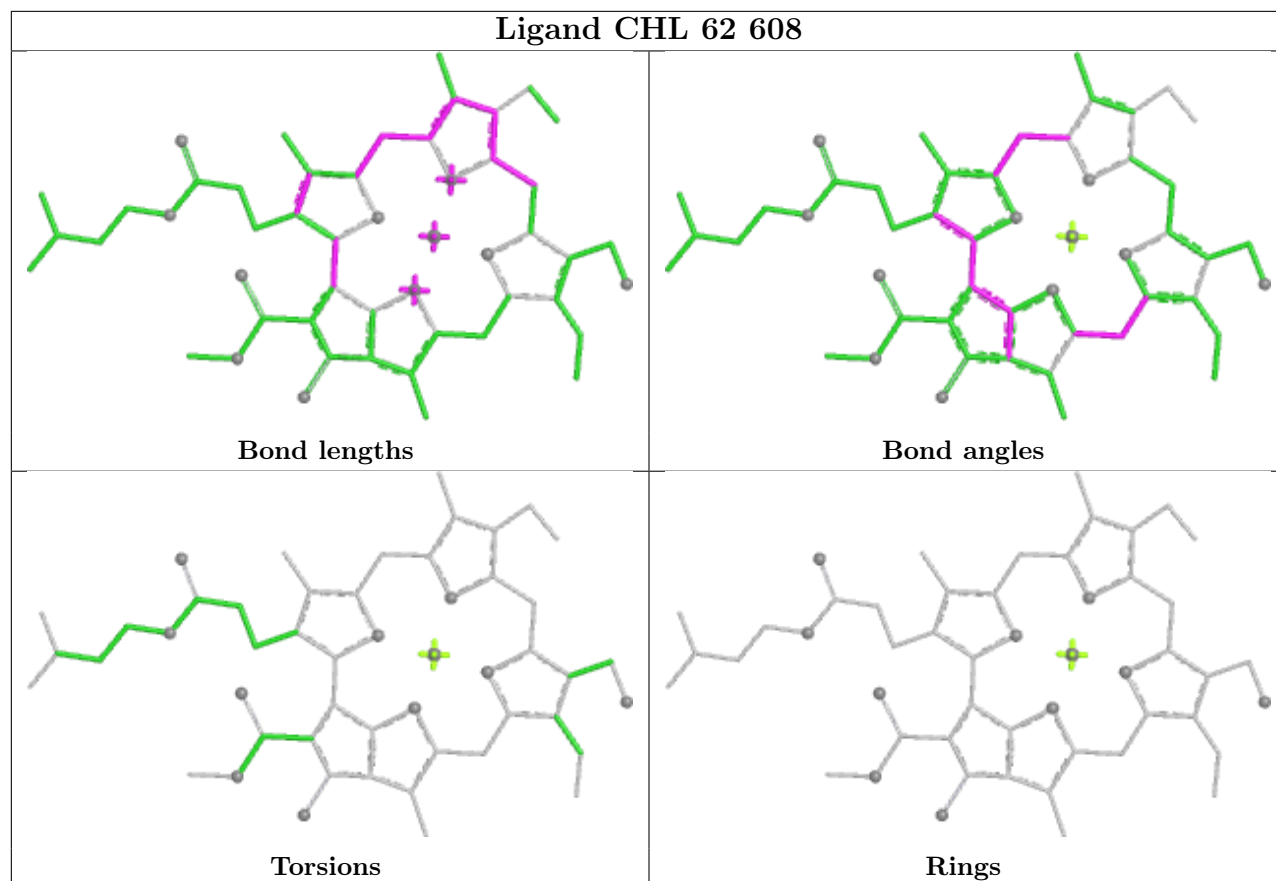


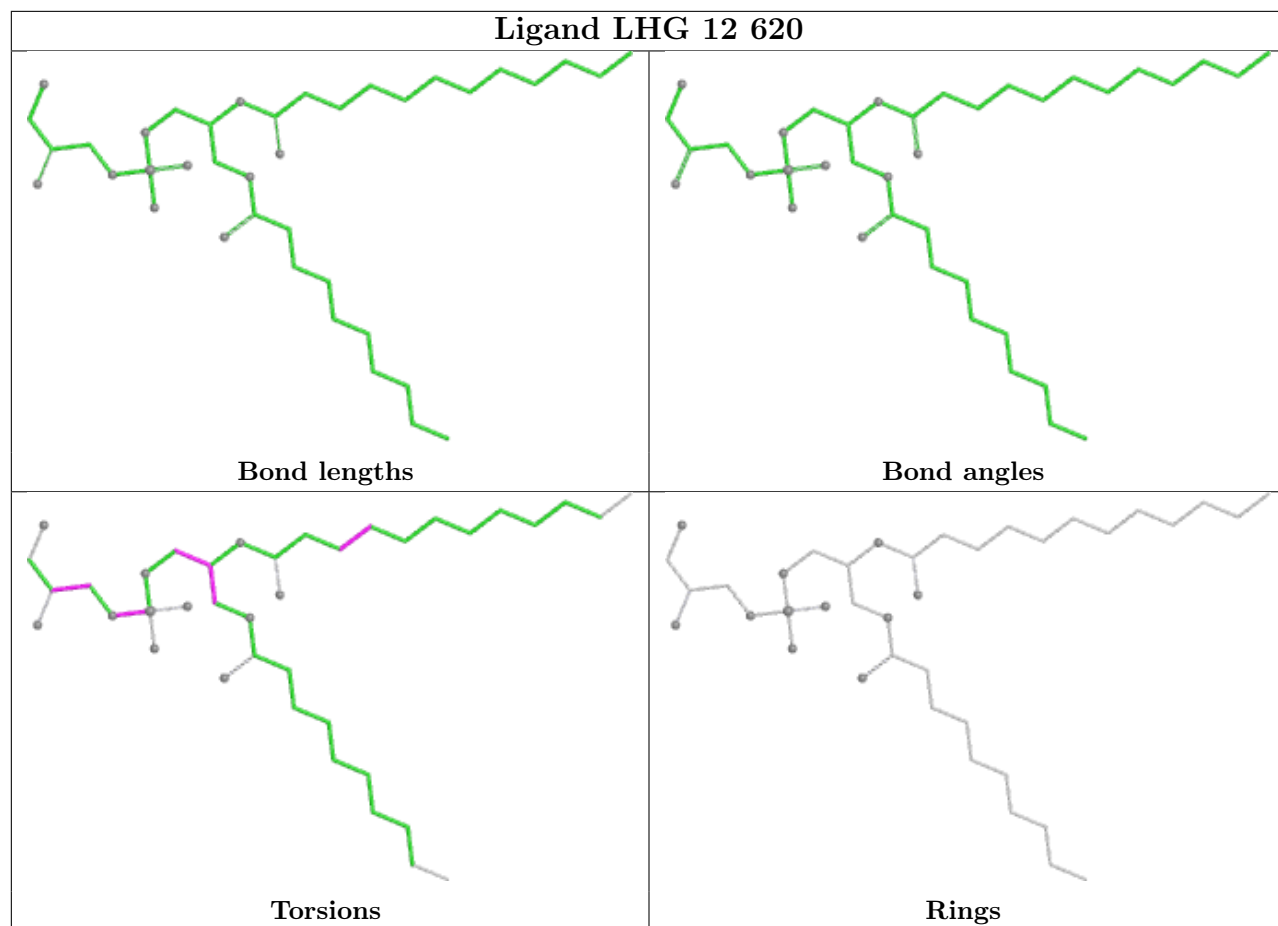


Ligand CLA Z 602**Ligand CLA B2 823**

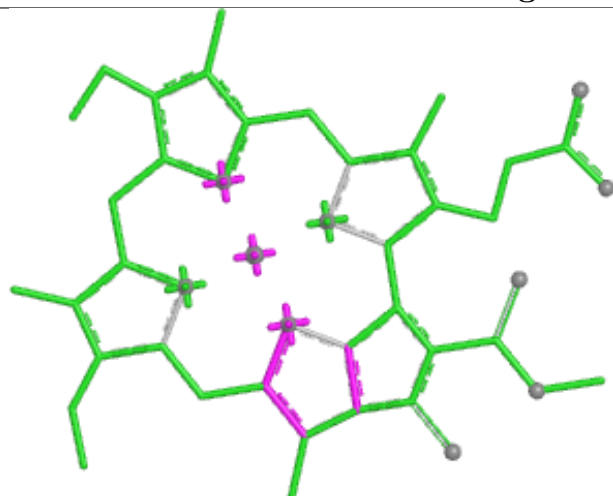




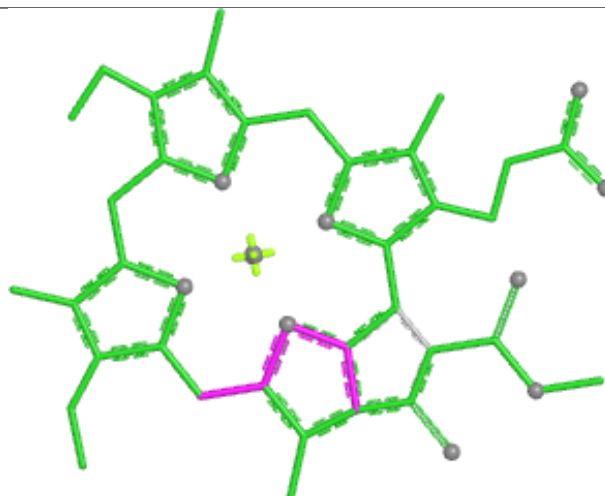




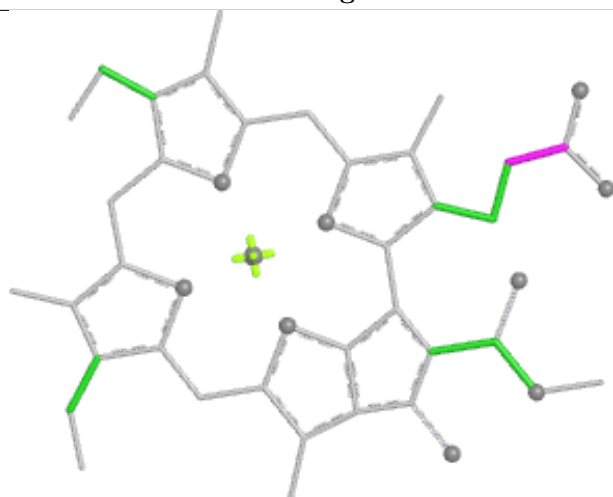
Ligand CLA 8 611



Bond lengths



Bond angles

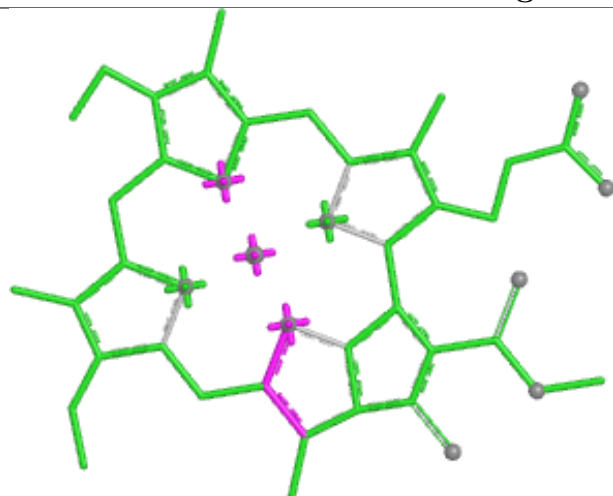


Torsions

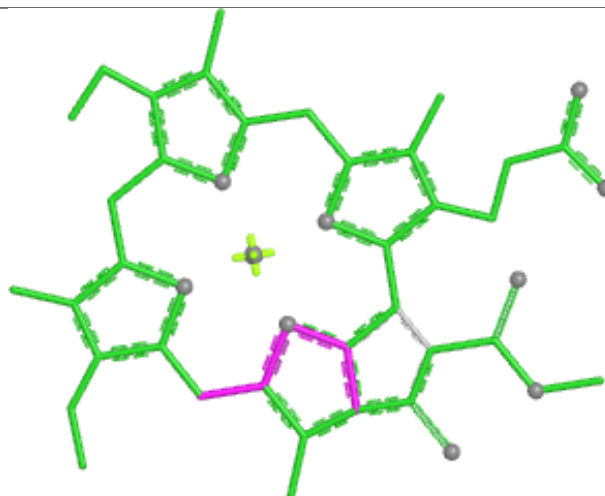


Rings

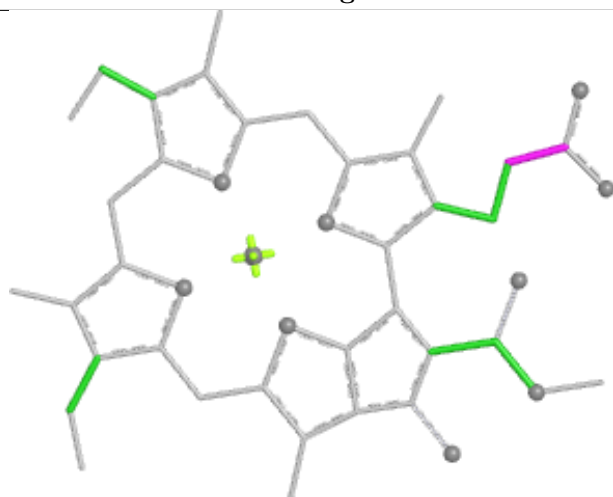
Ligand CLA L 204



Bond lengths



Bond angles

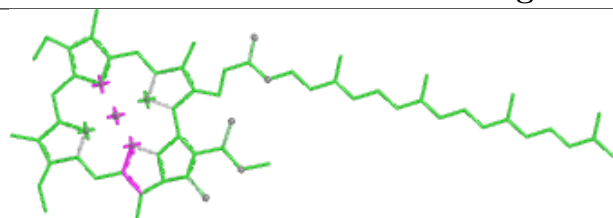


Torsions

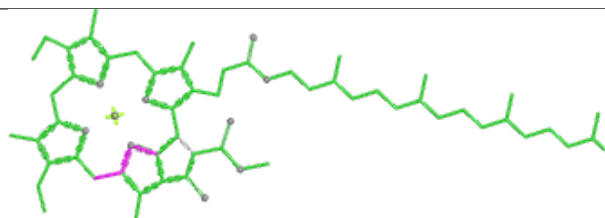


Rings

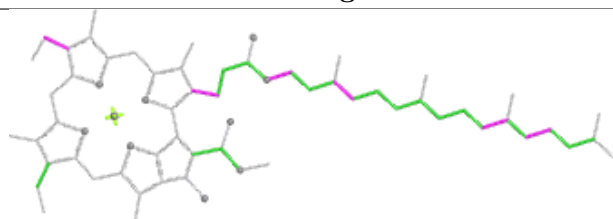
Ligand CLA Z 609



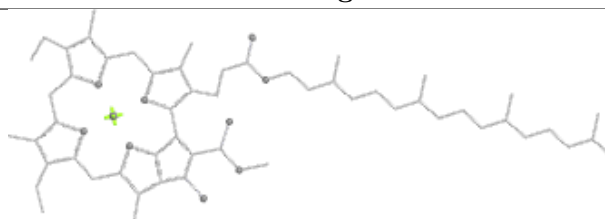
Bond lengths



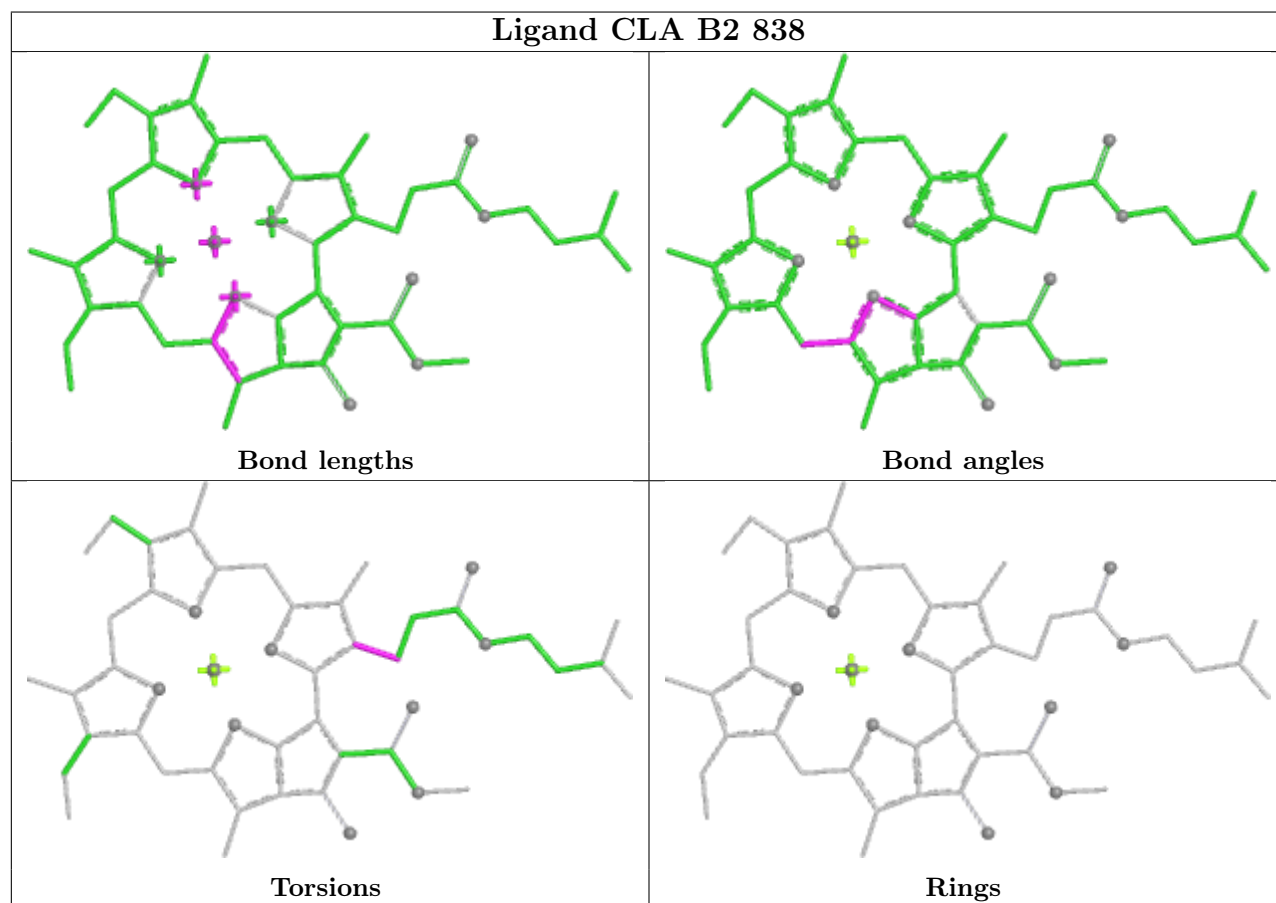
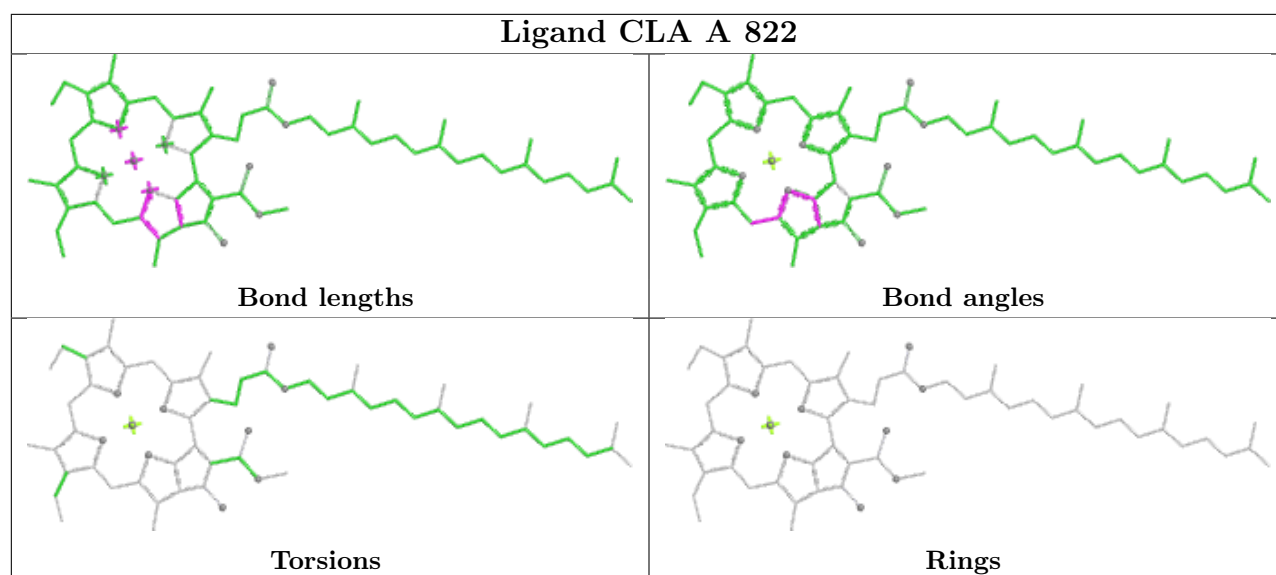
Bond angles

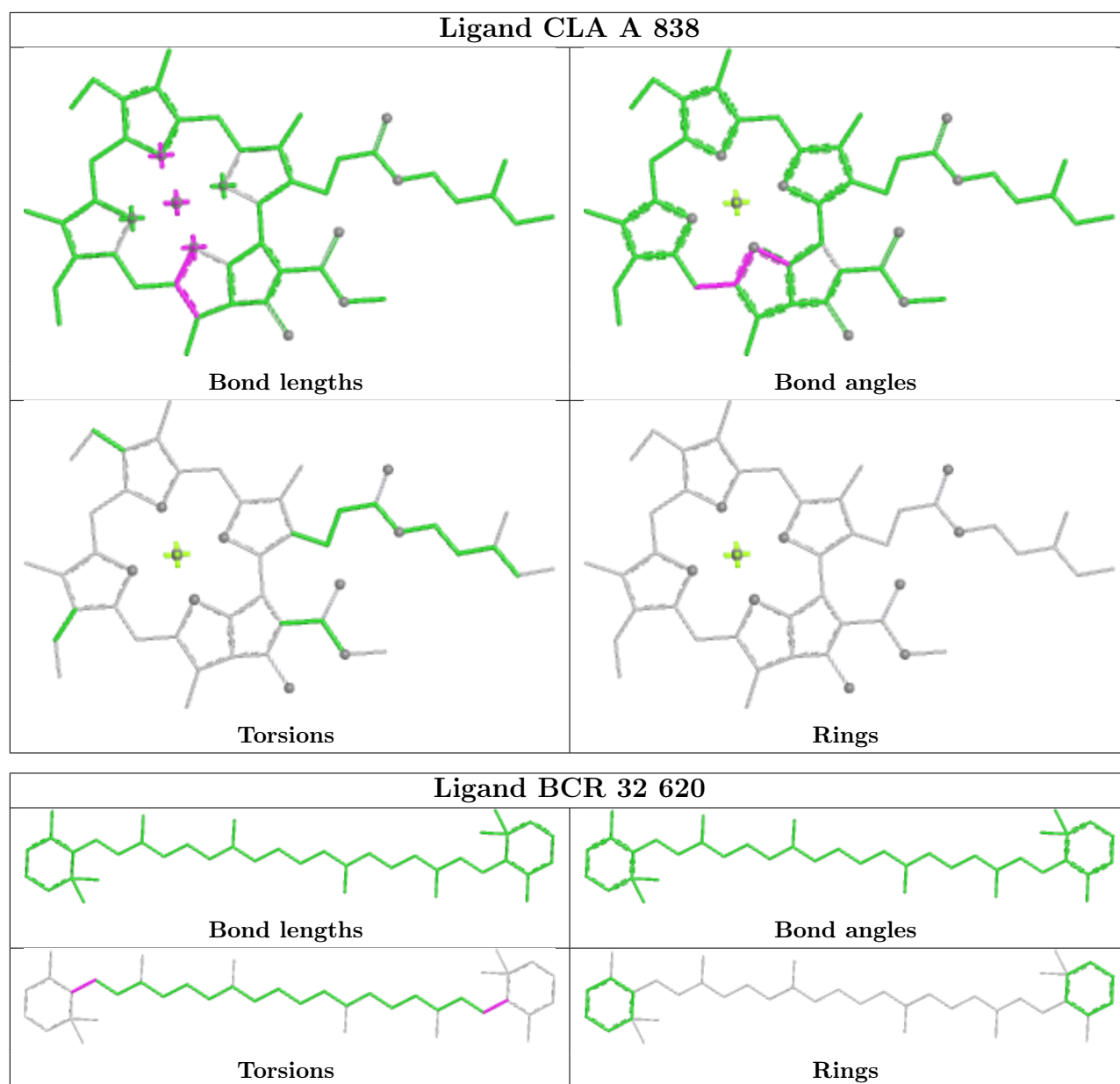


Torsions

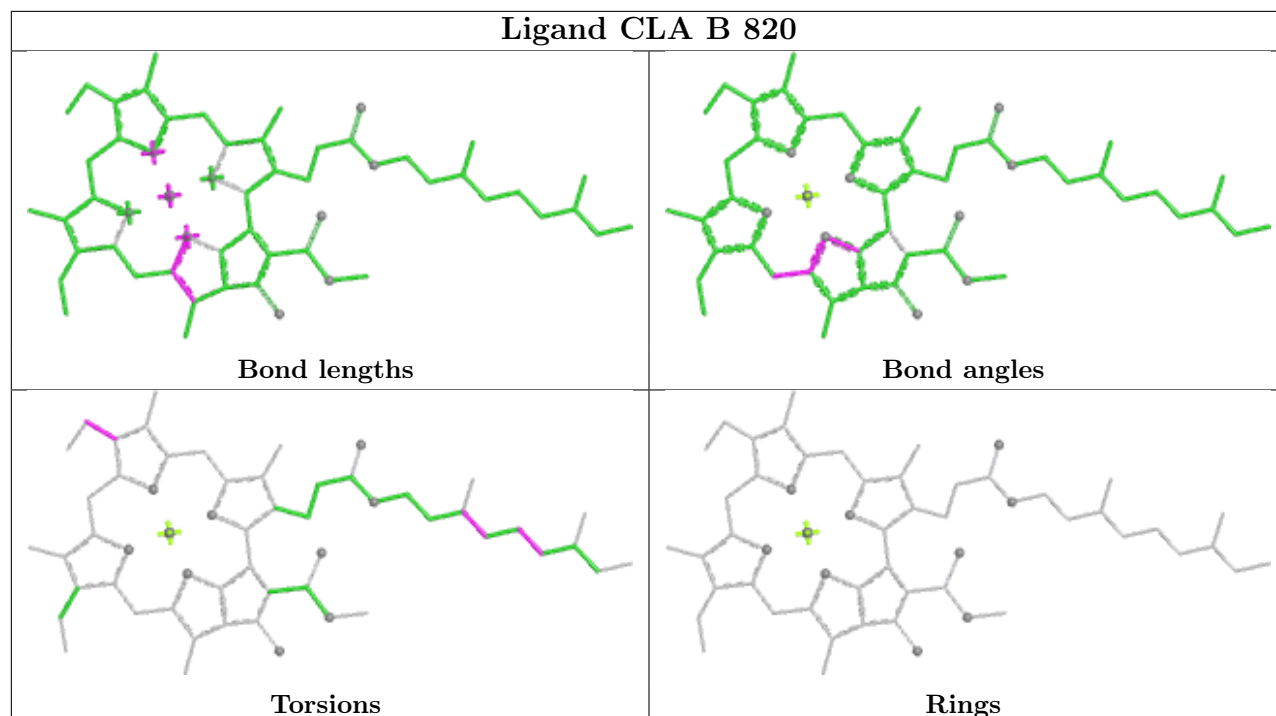


Rings

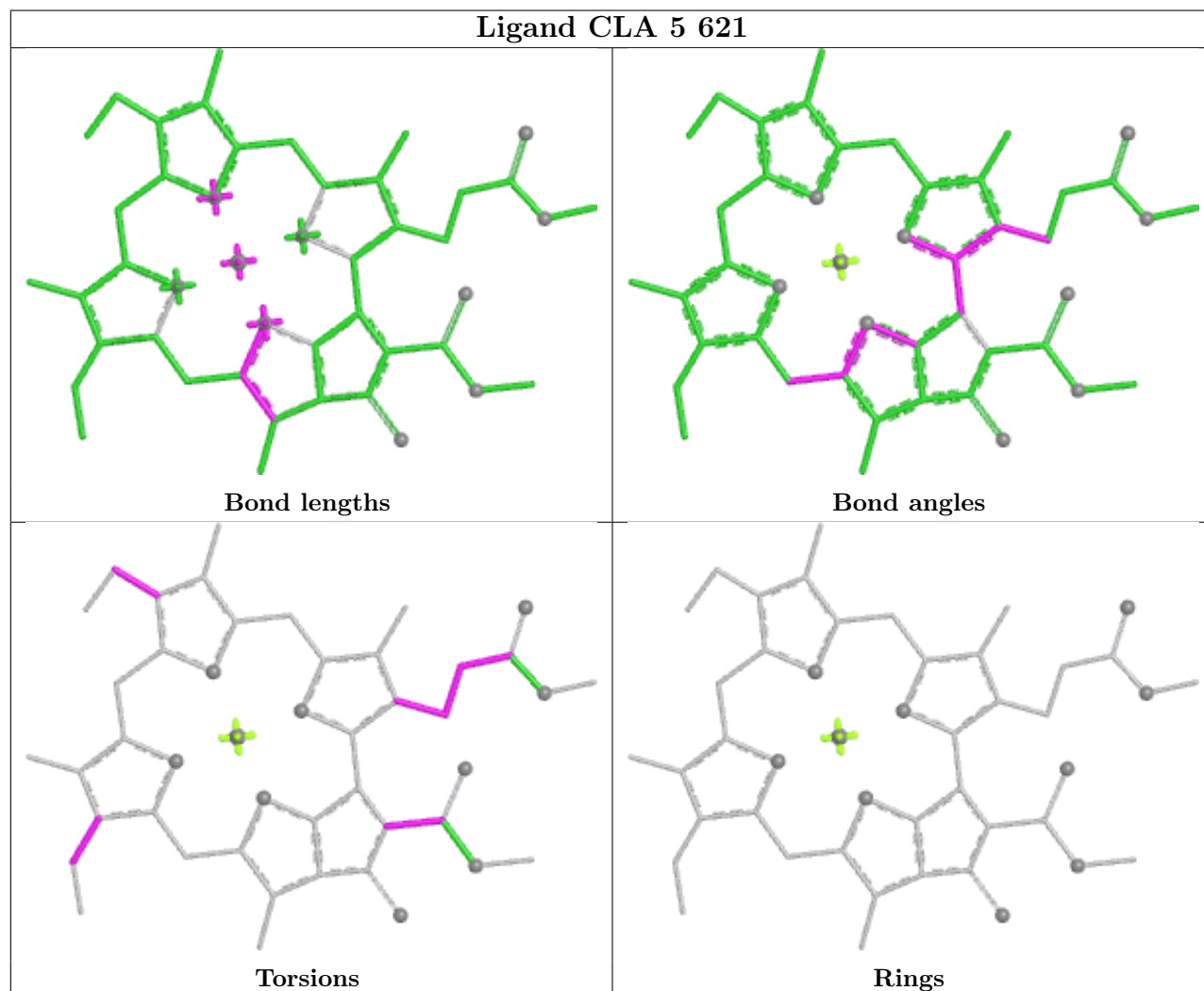


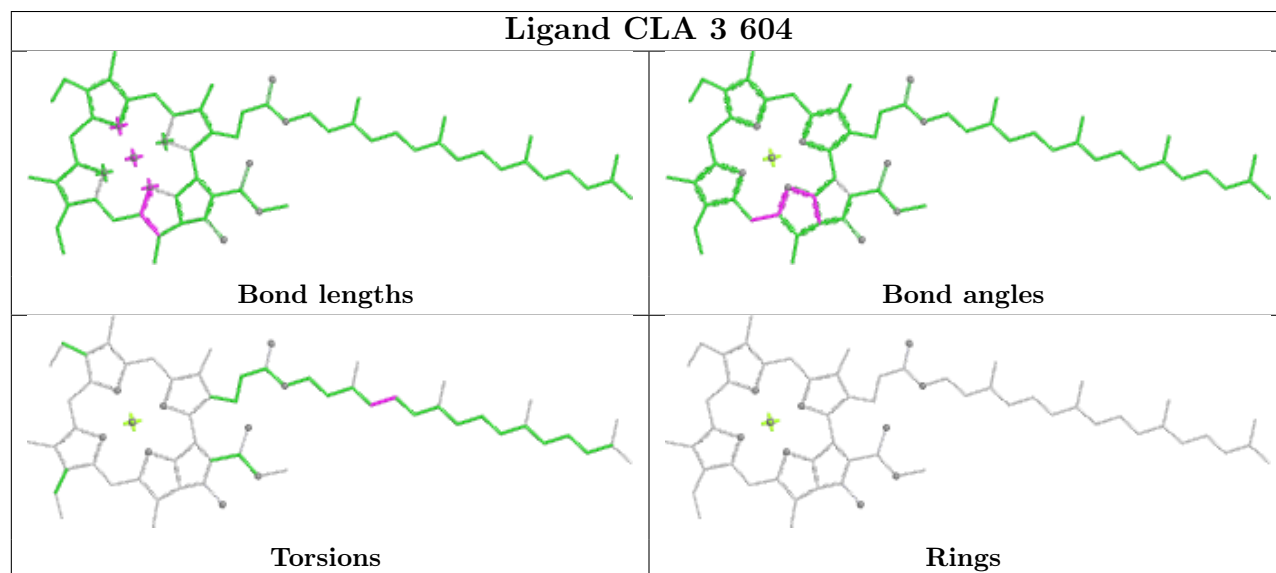
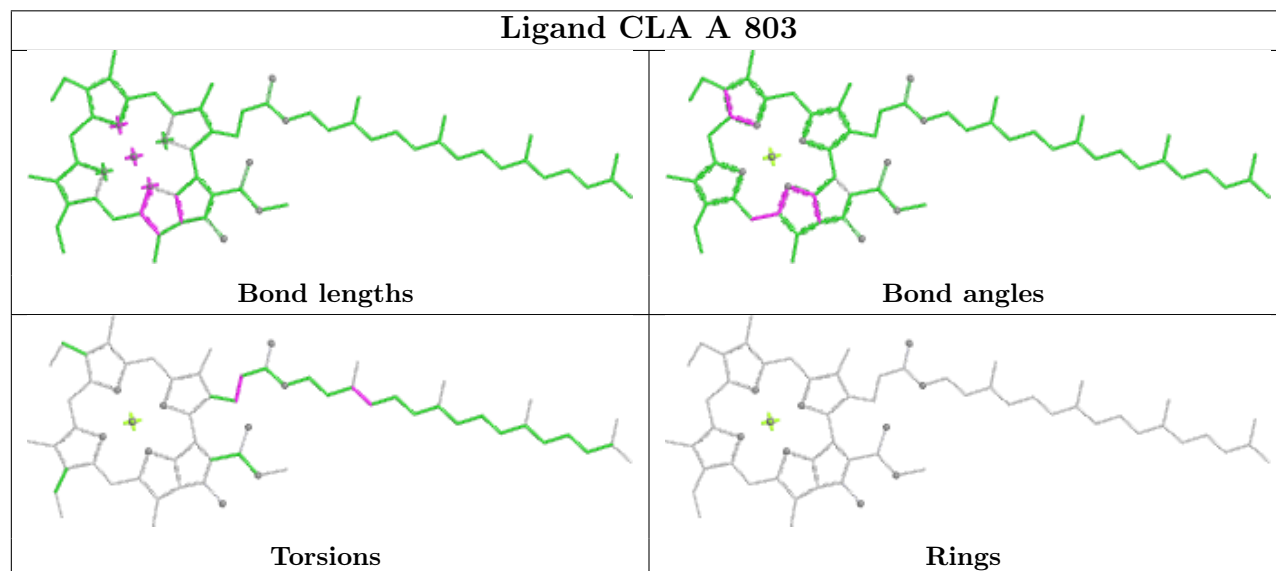
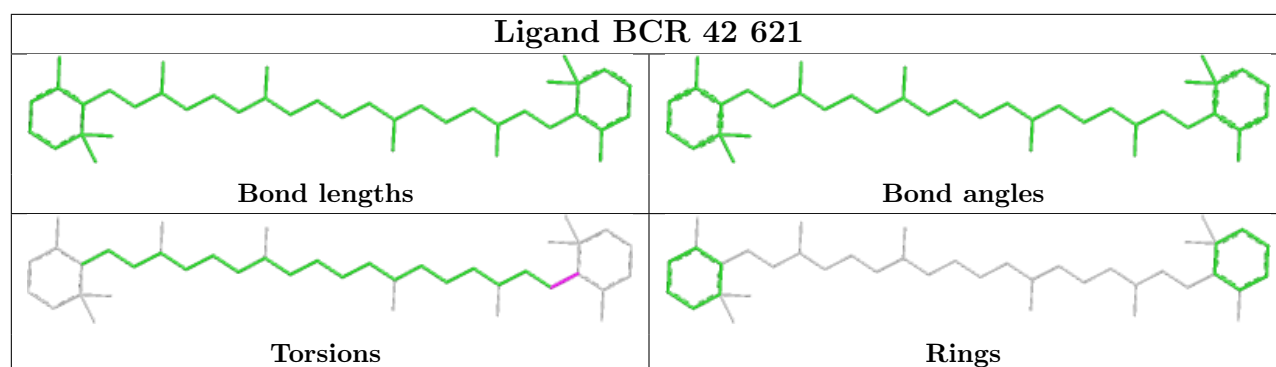


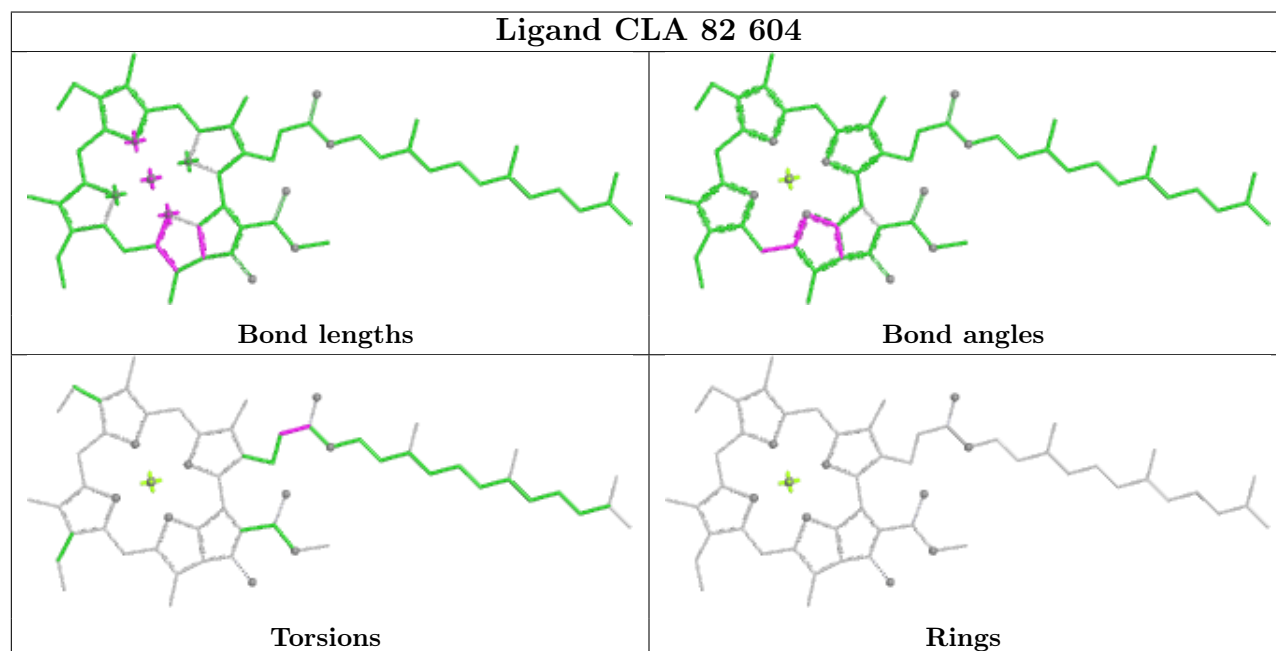
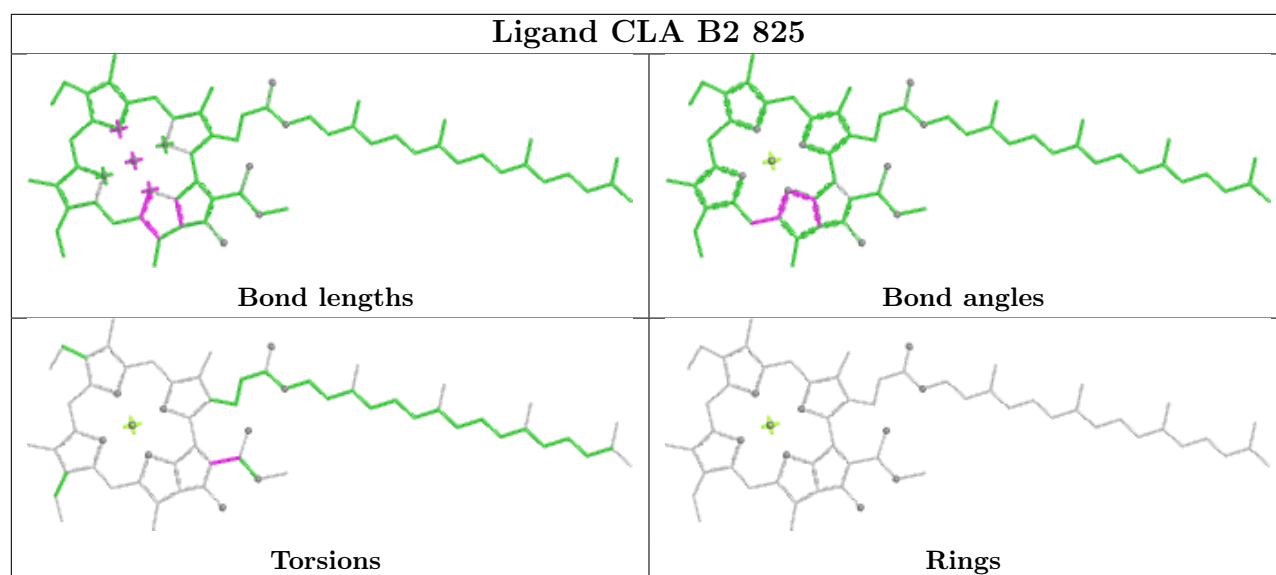
Ligand CLA B 820

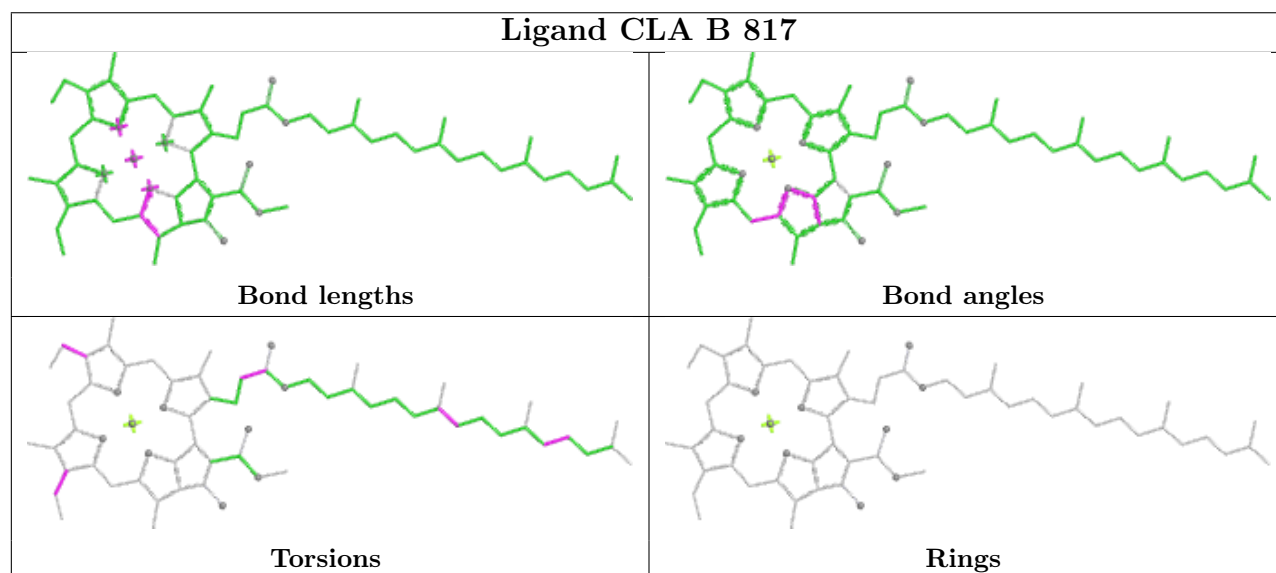
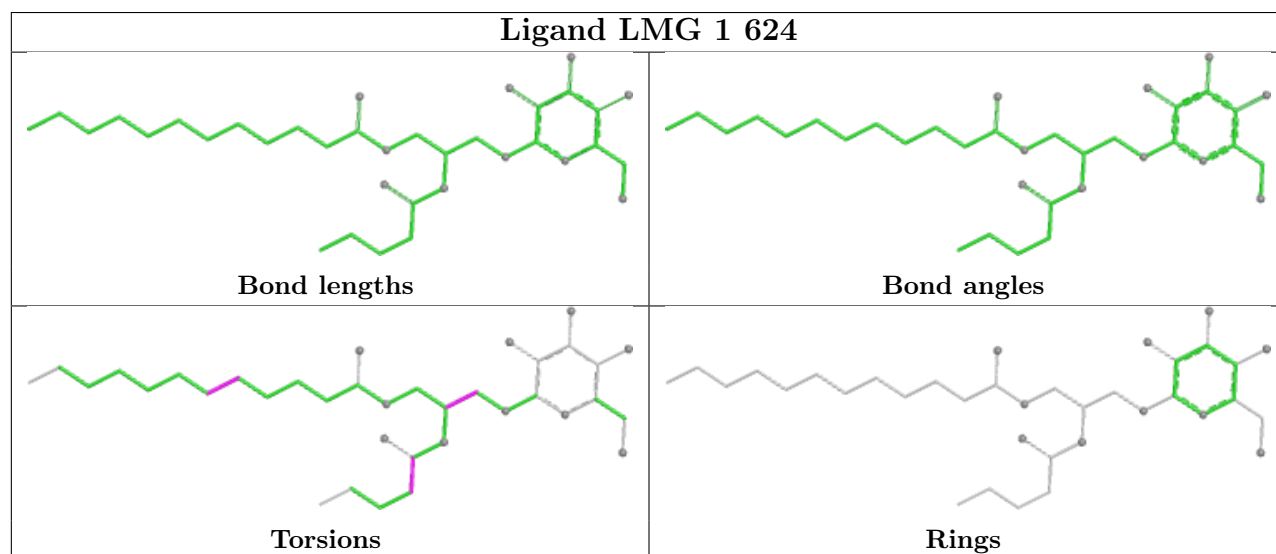
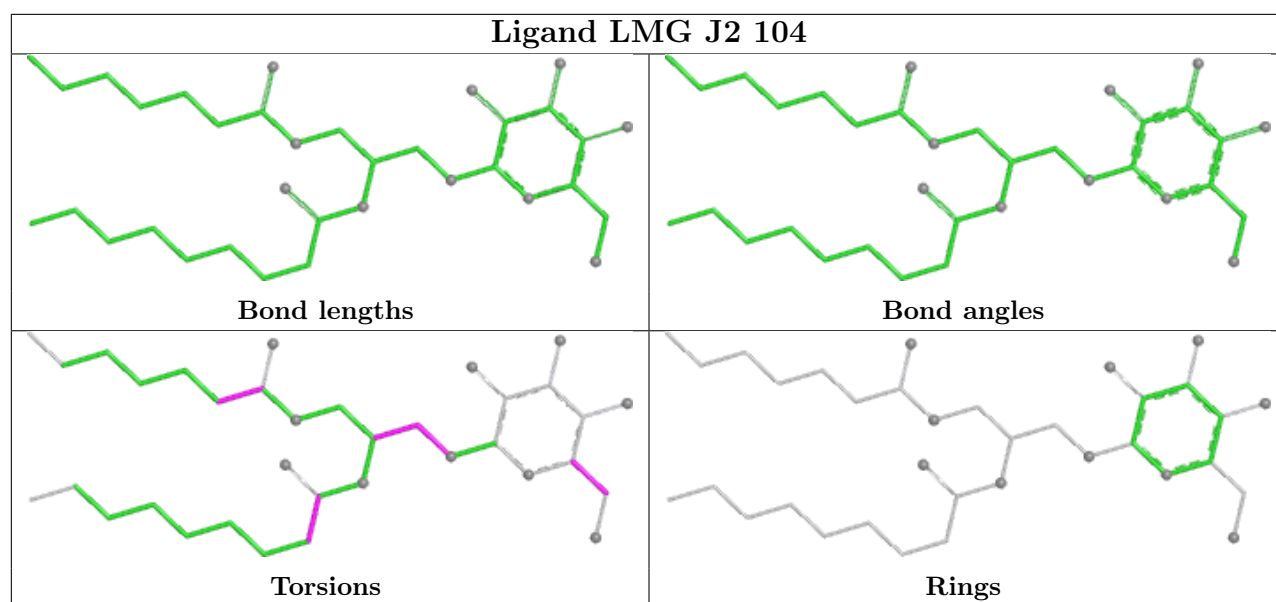


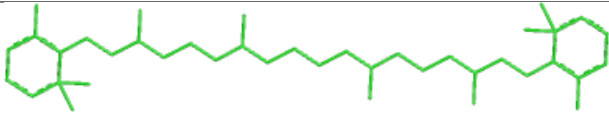
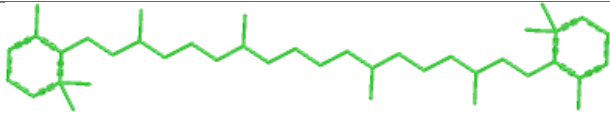
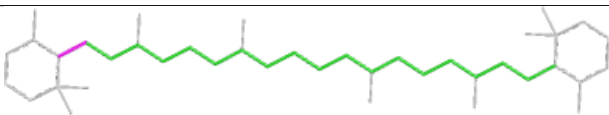
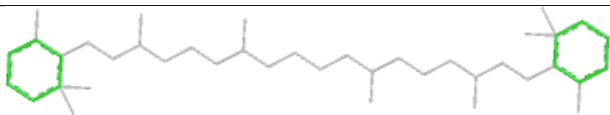
Ligand CLA 5 621

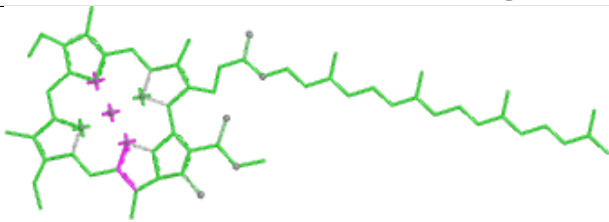
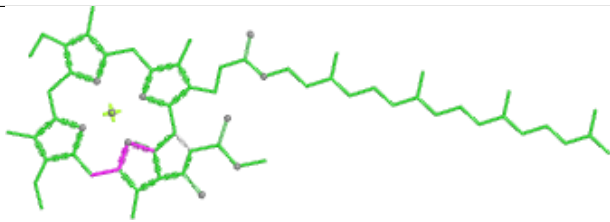
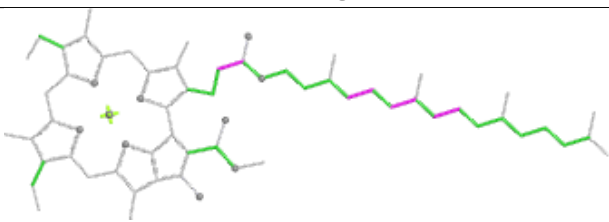
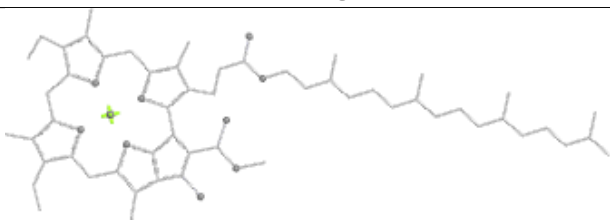


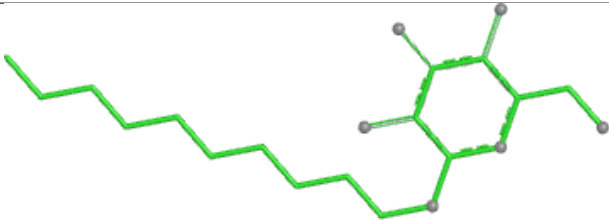
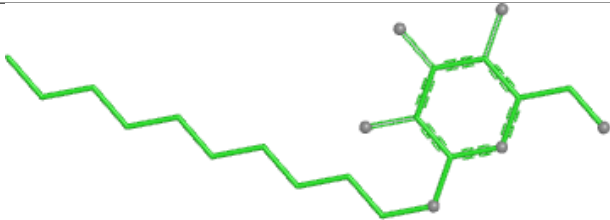
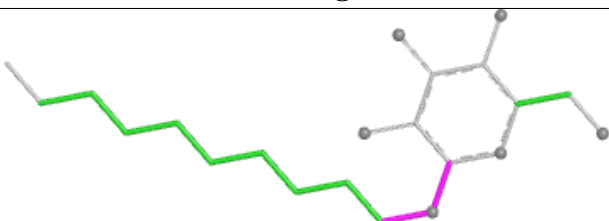
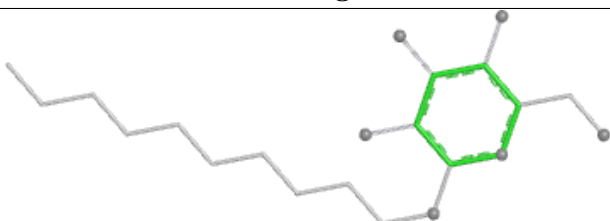


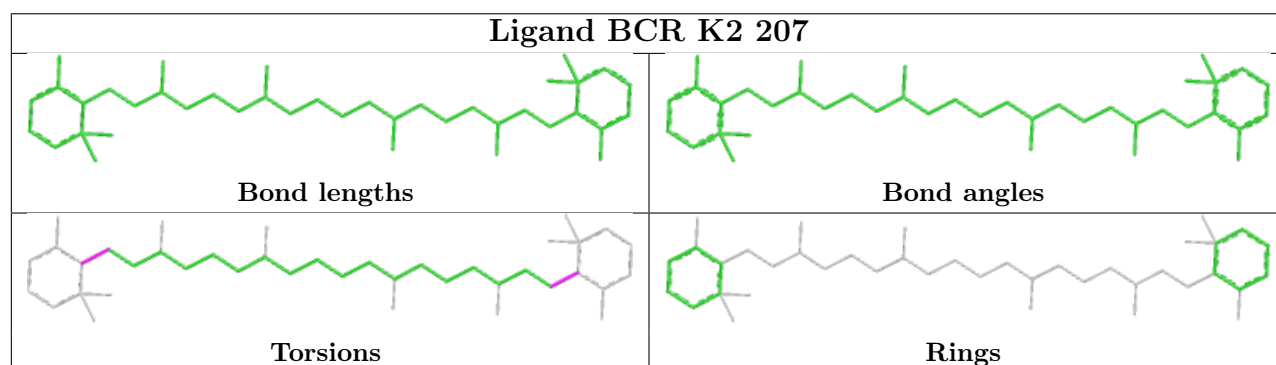
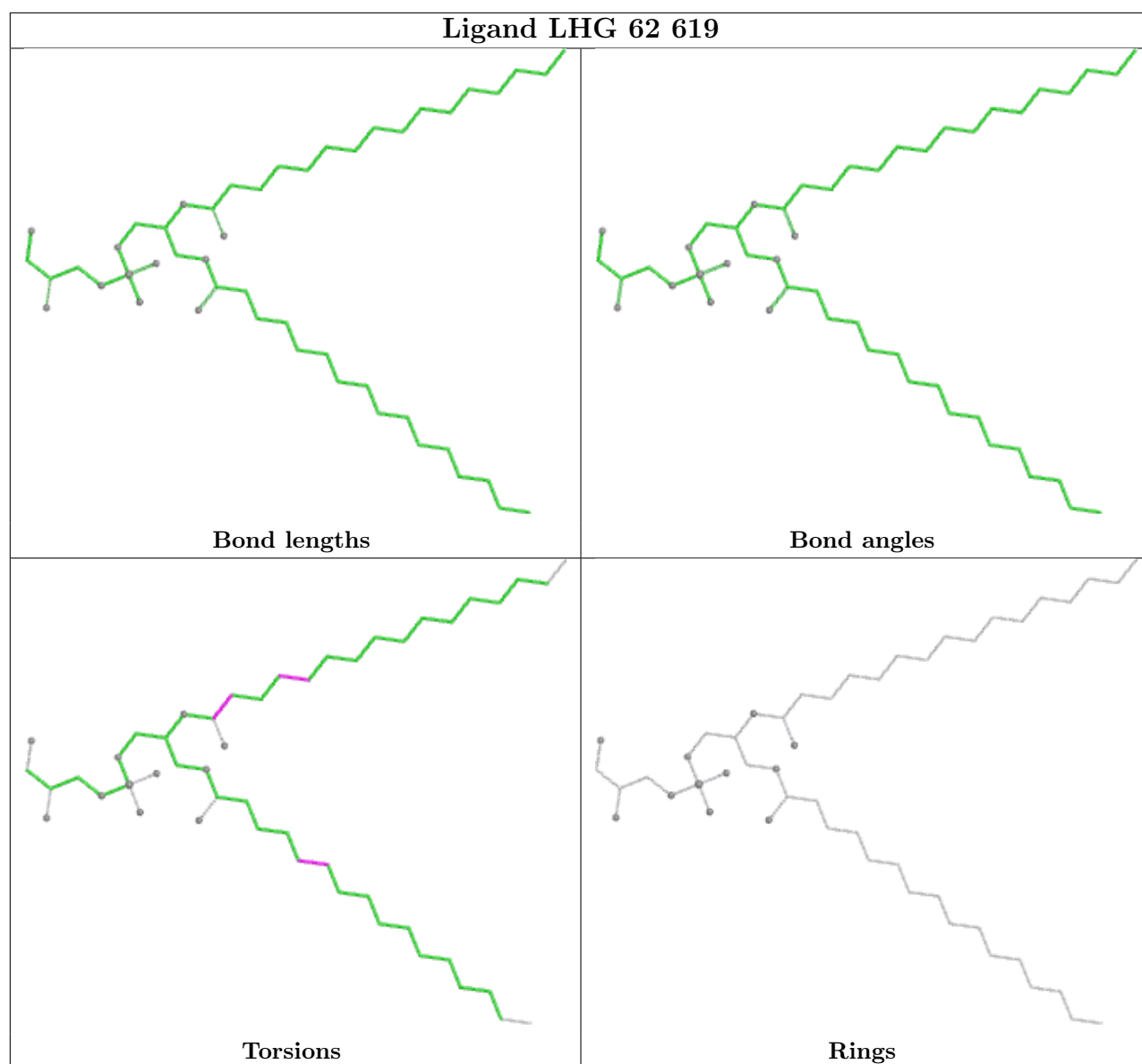


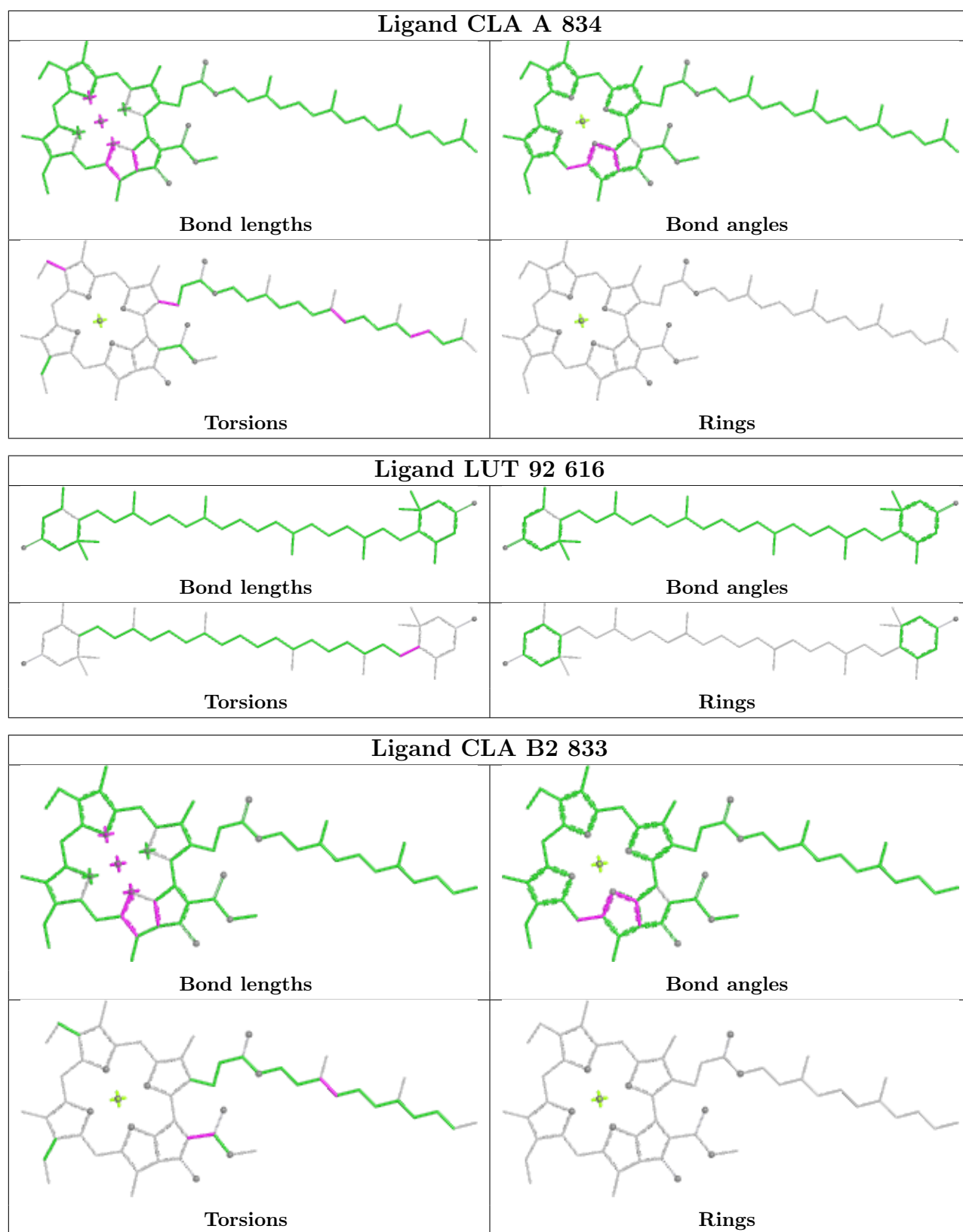


Ligand BCR A 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

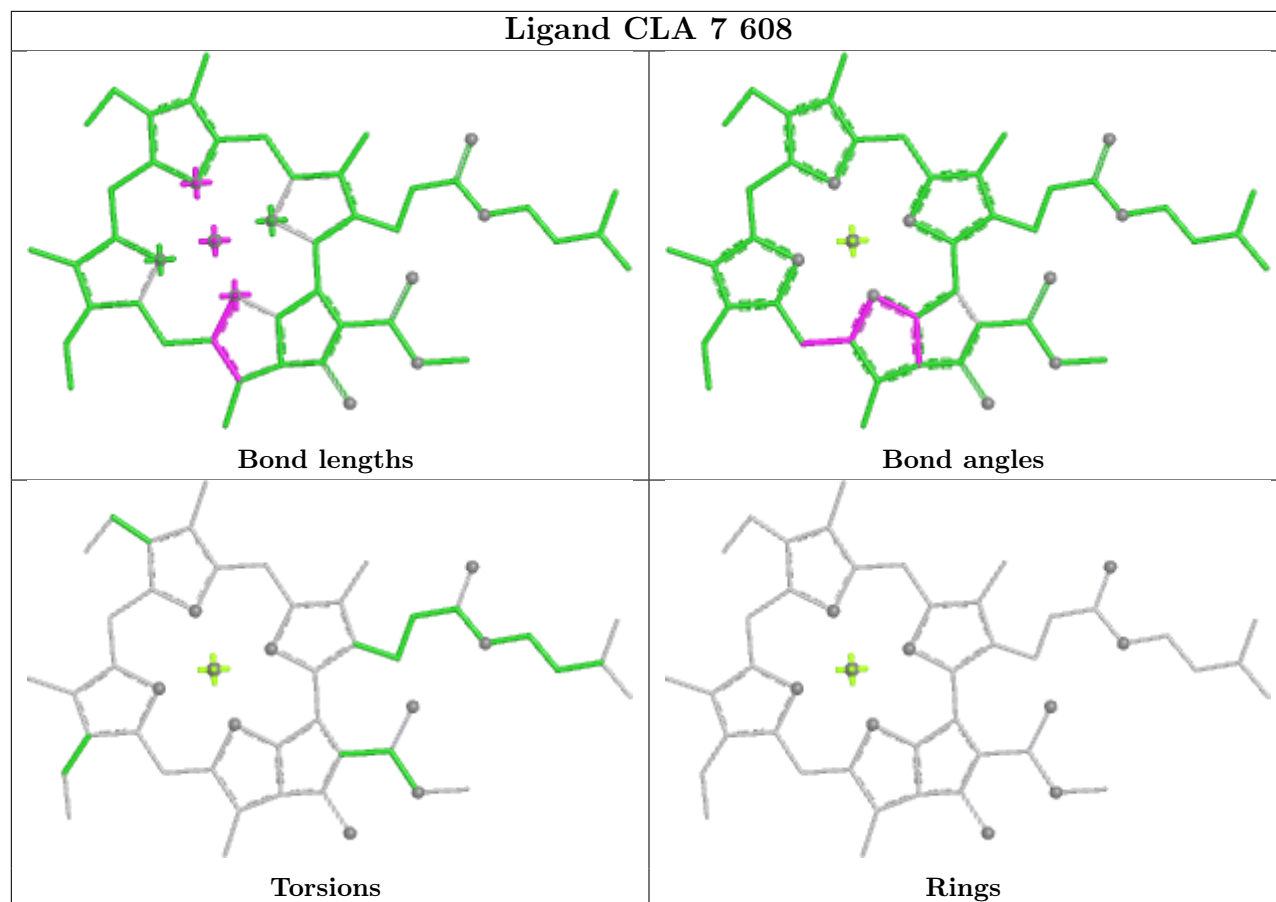
Ligand CLA B2 809	
	
Bond lengths	Bond angles
	
Torsions	Rings

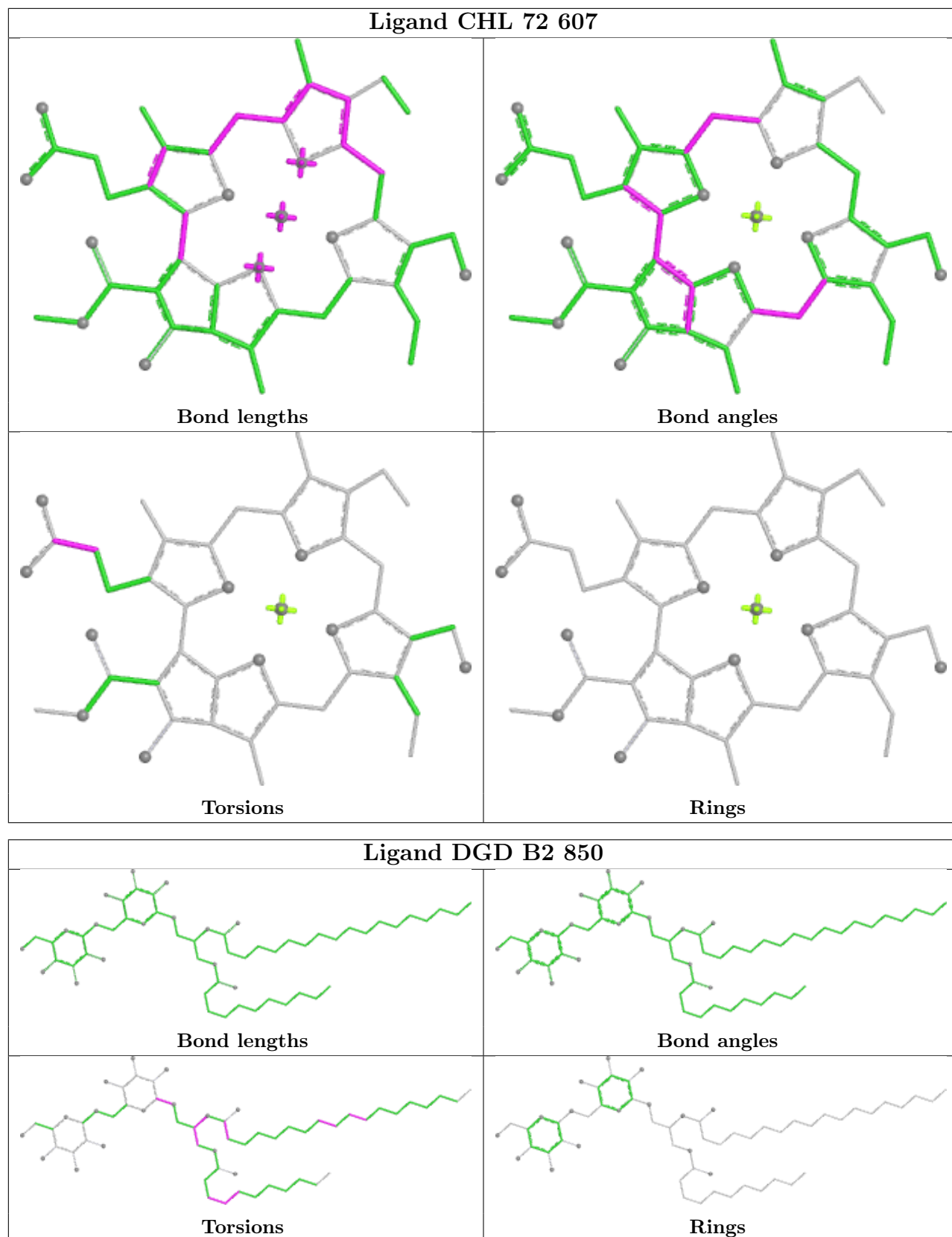
Ligand LMU 7 628	
	
Bond lengths	Bond angles
	
Torsions	Rings

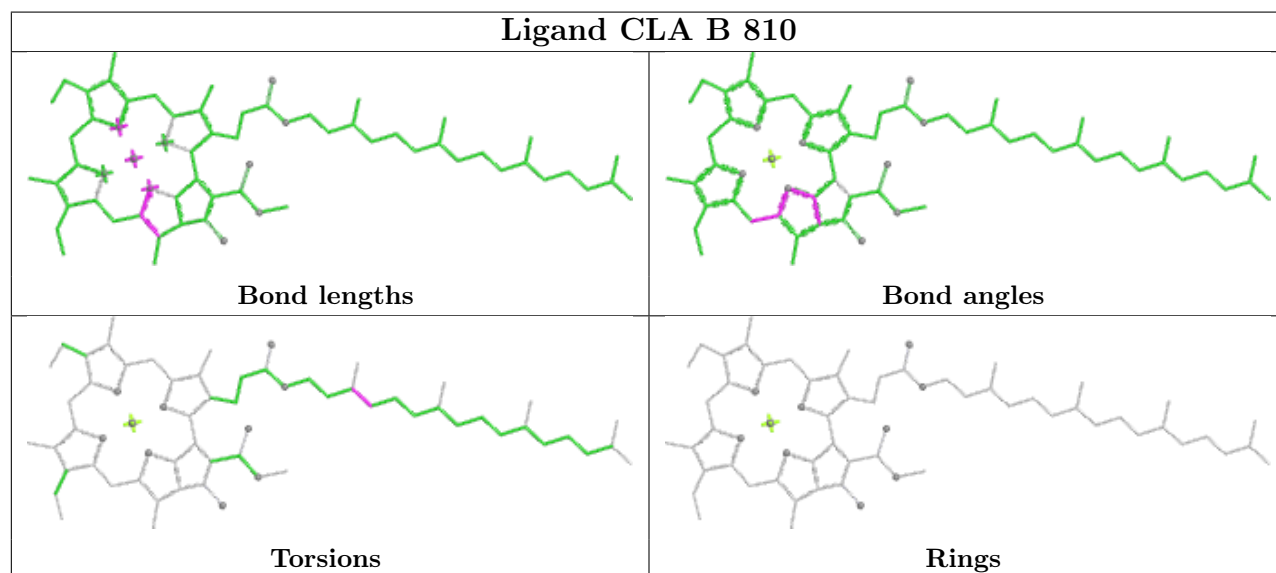
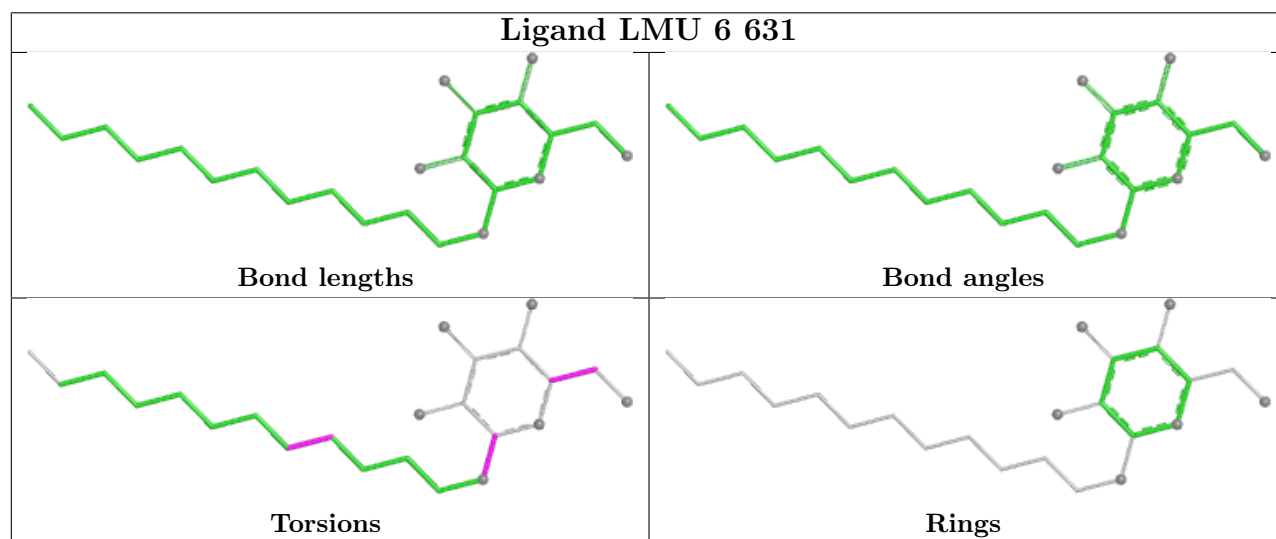
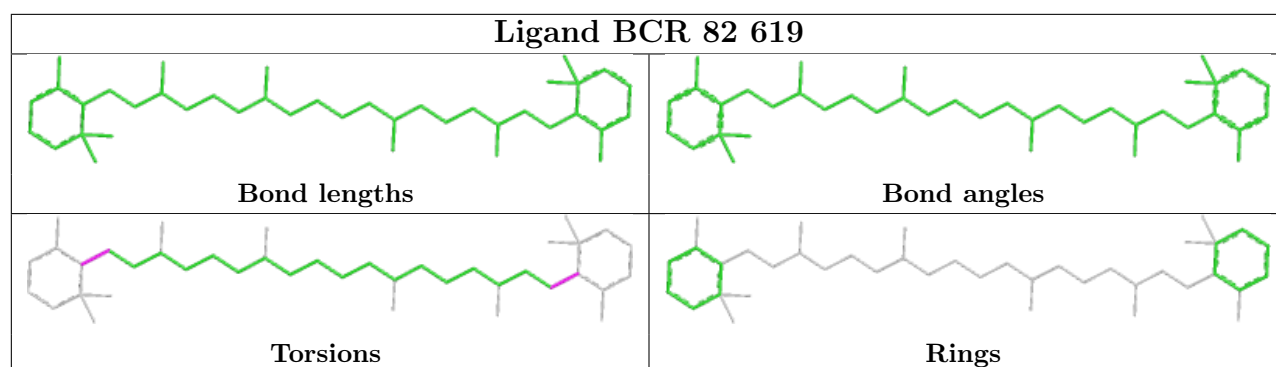


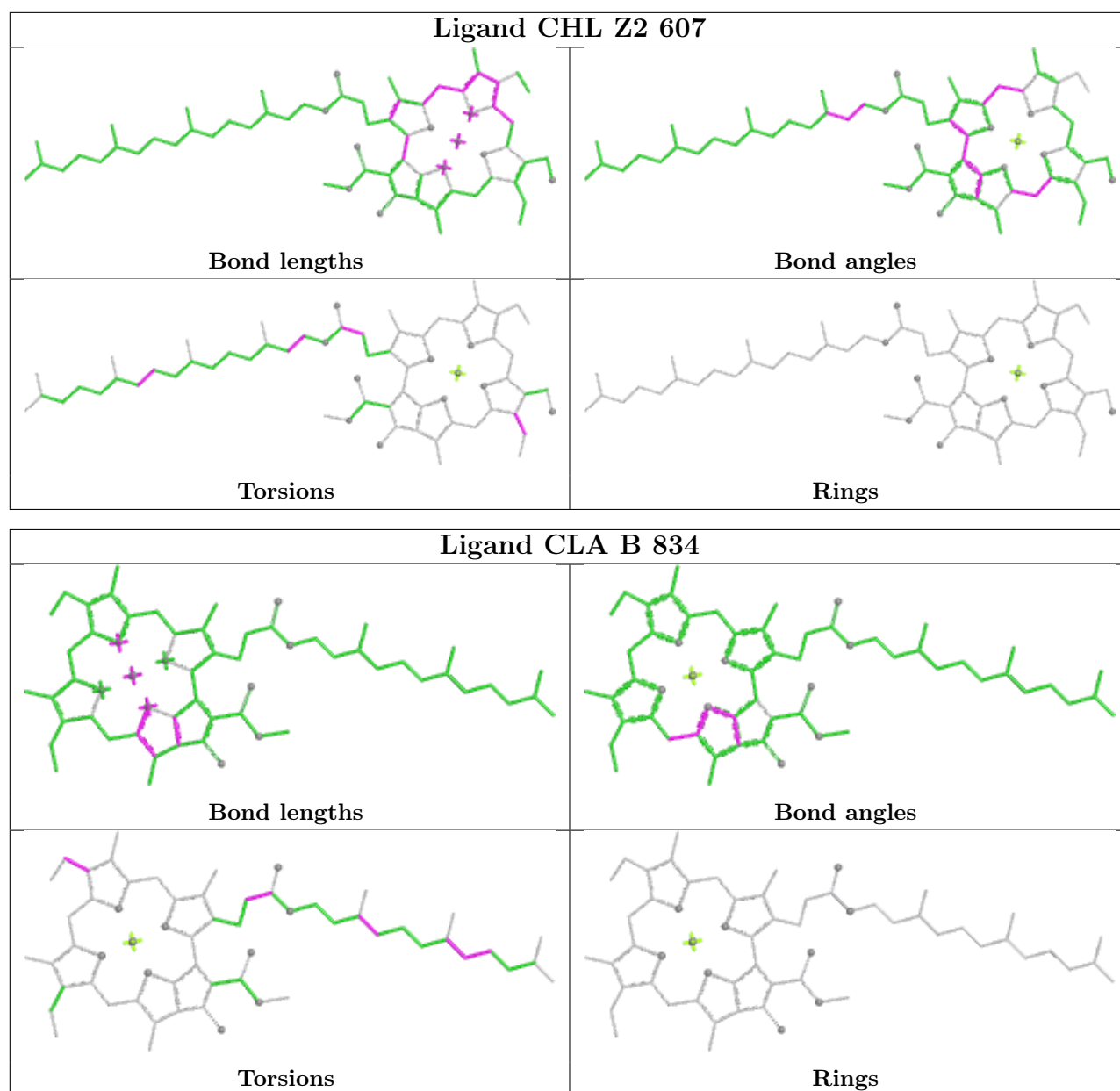


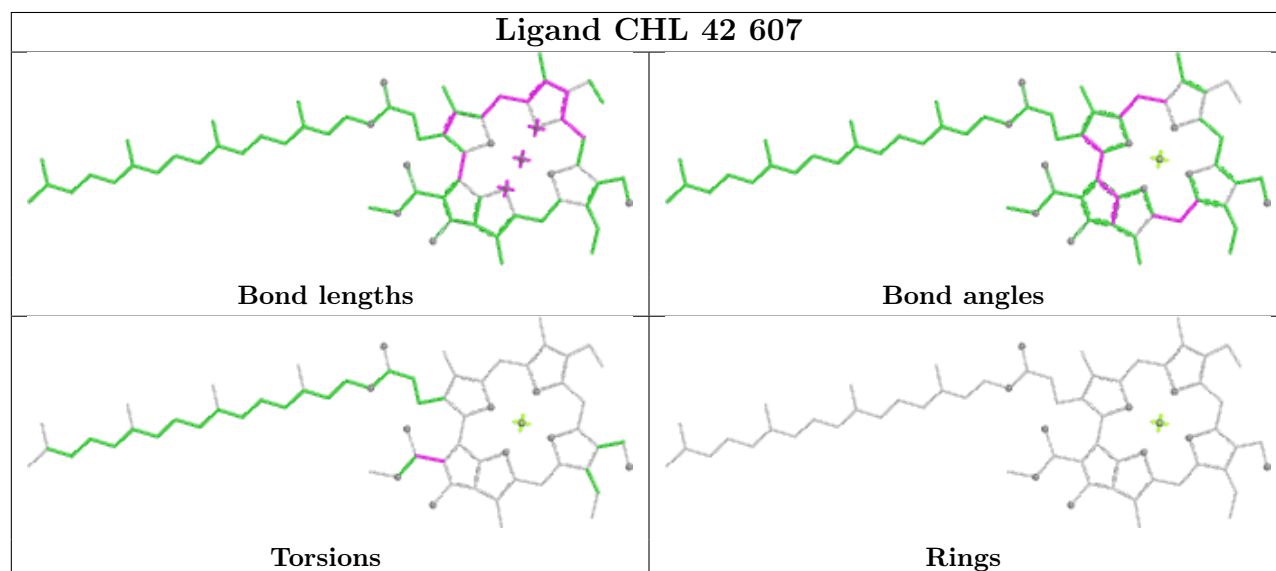
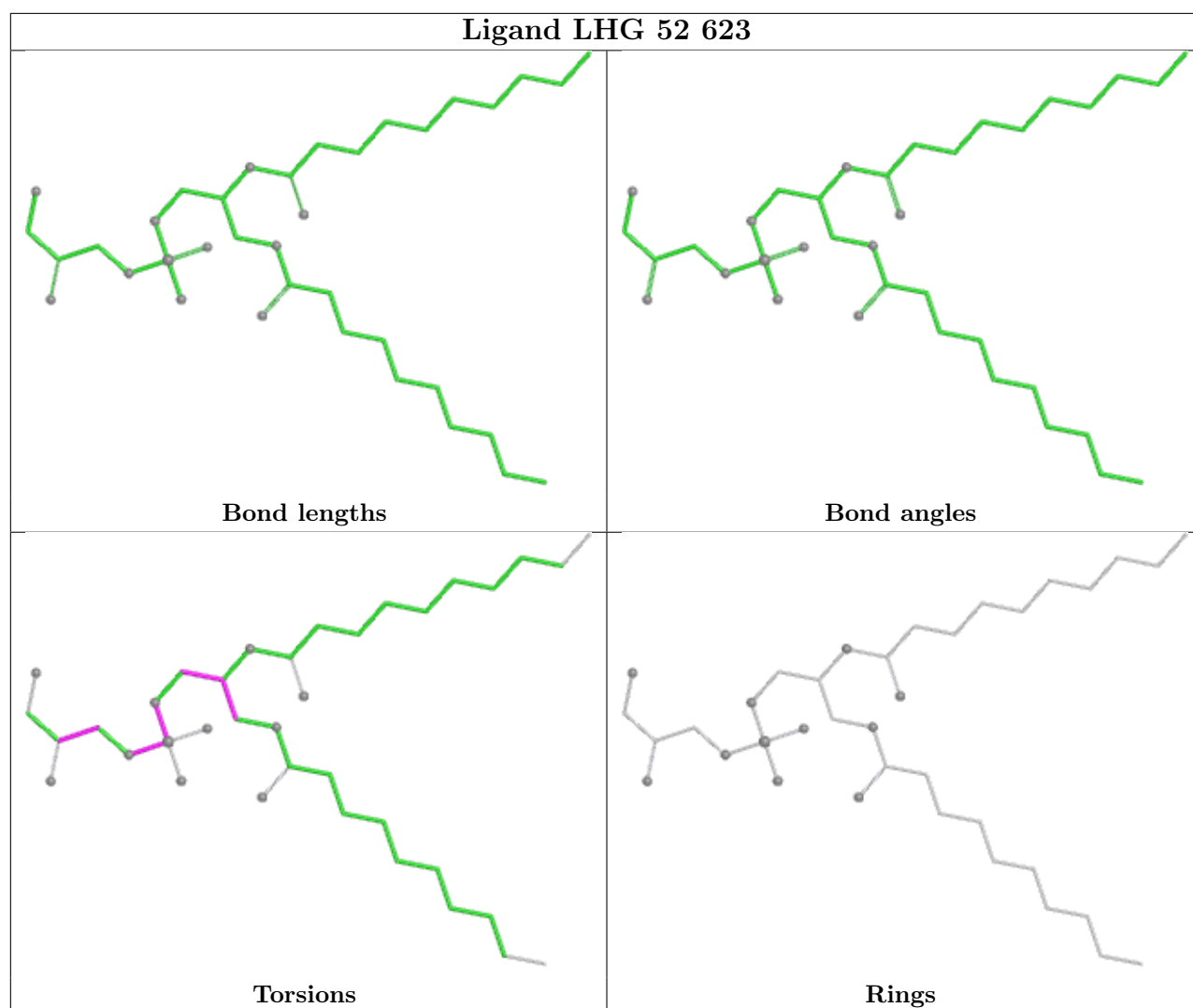
Ligand CLA 7 608

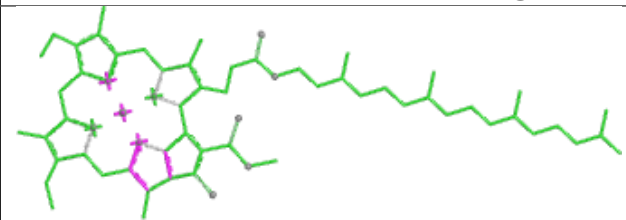
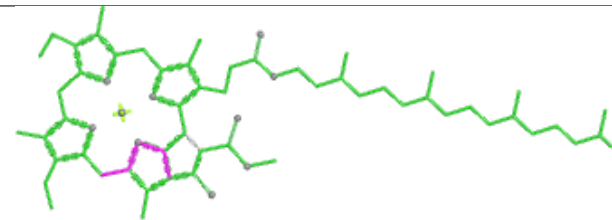
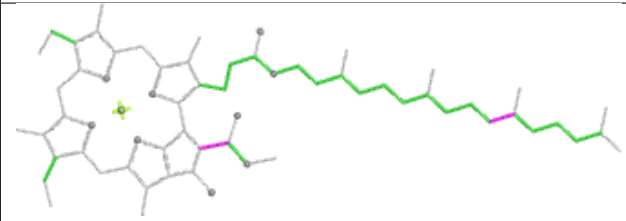
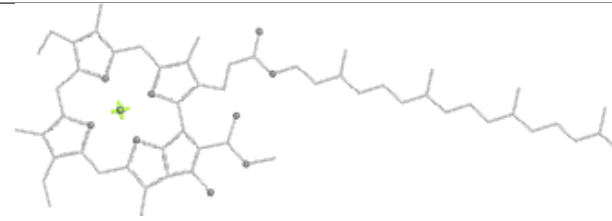


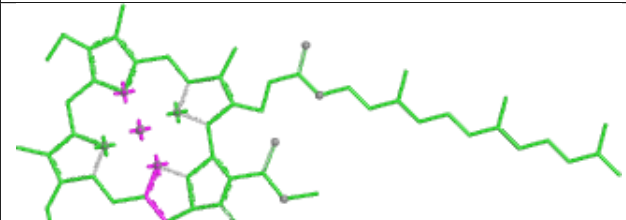
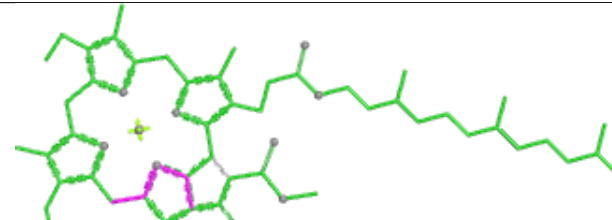
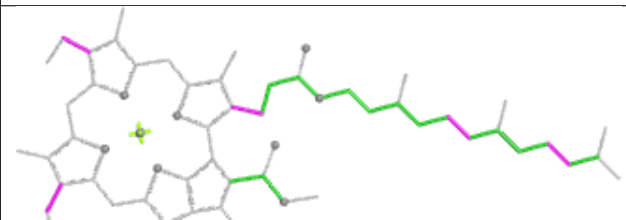
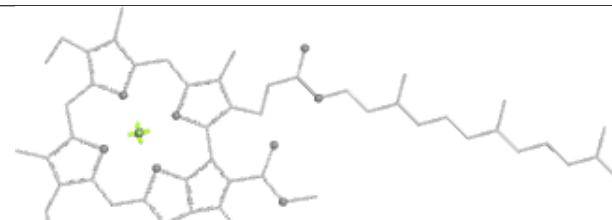


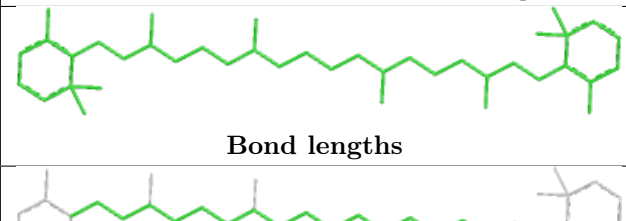
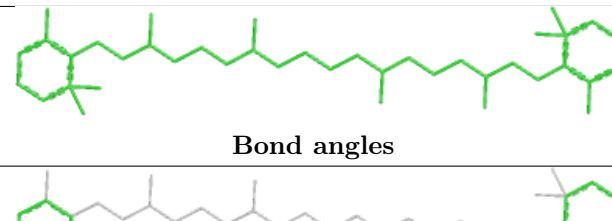


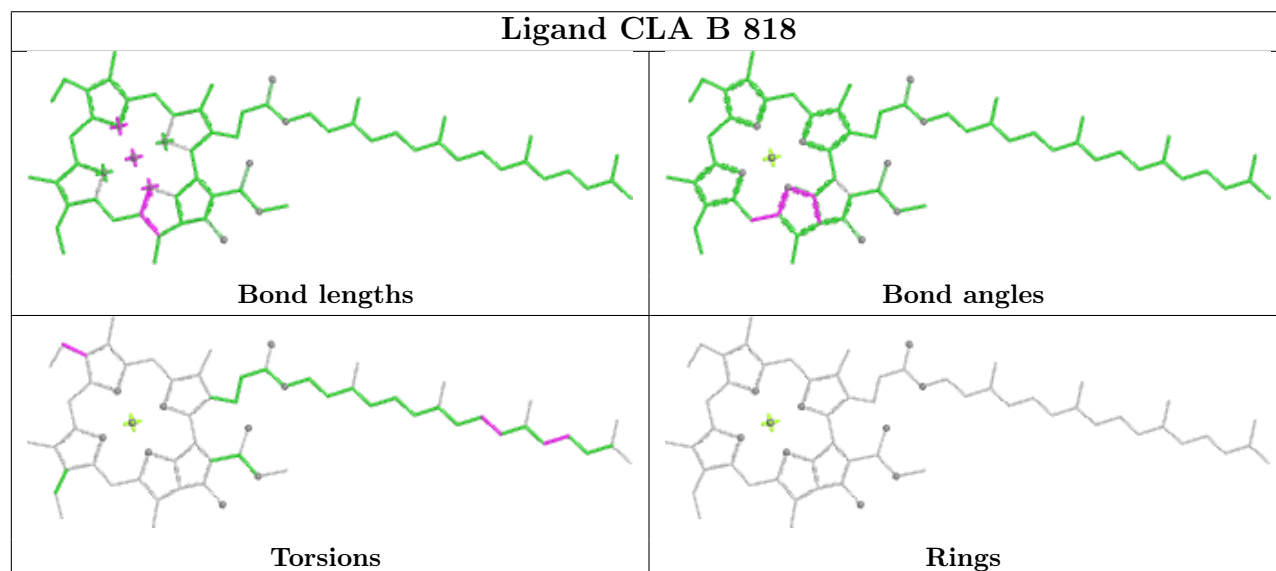
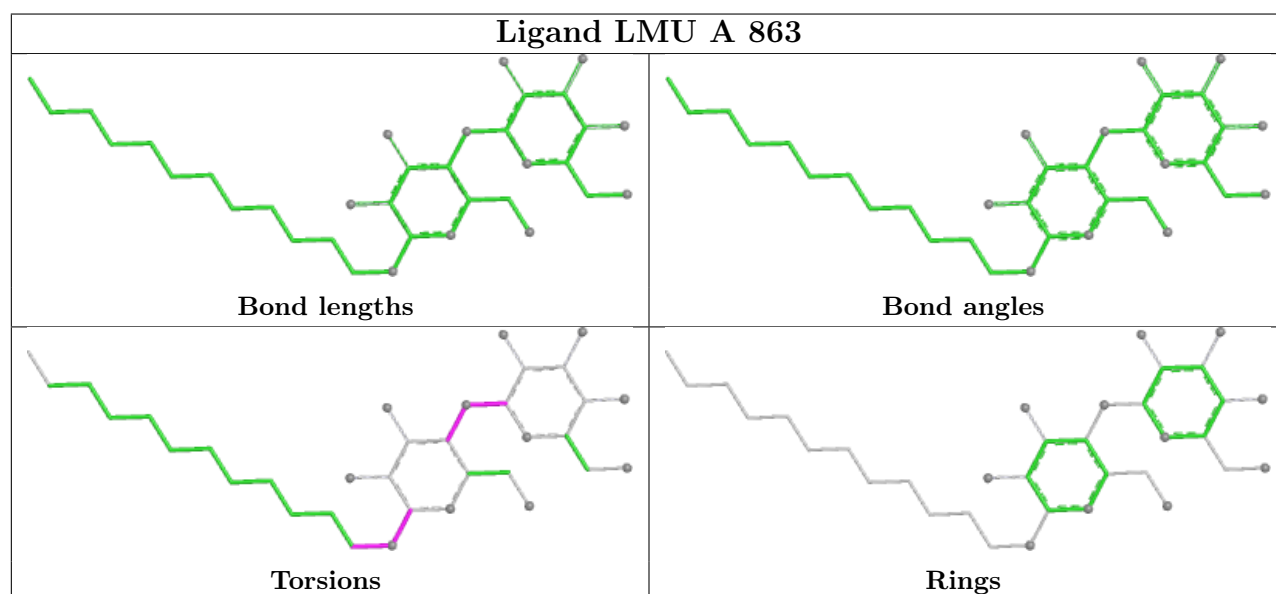
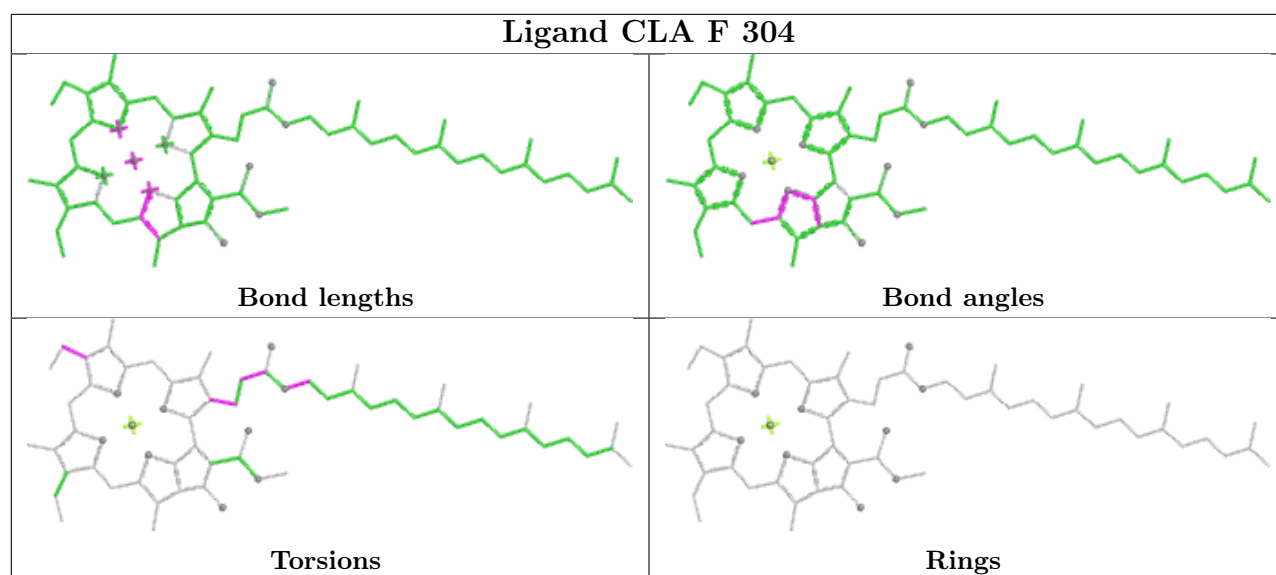


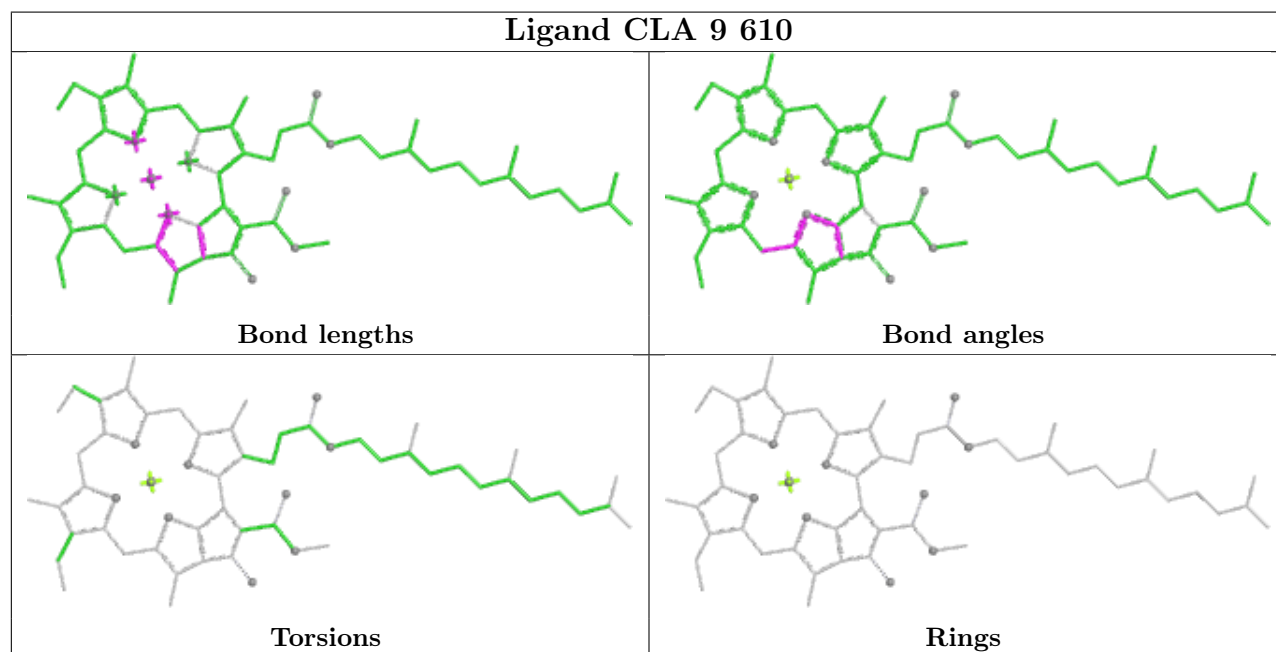
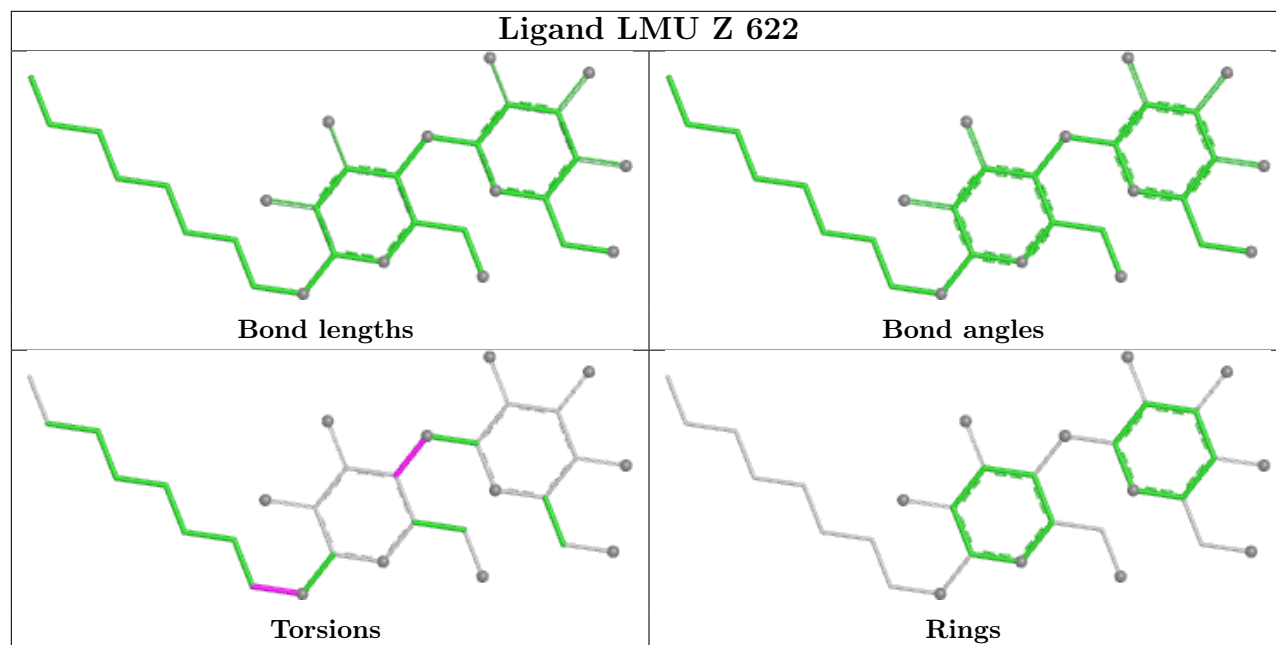


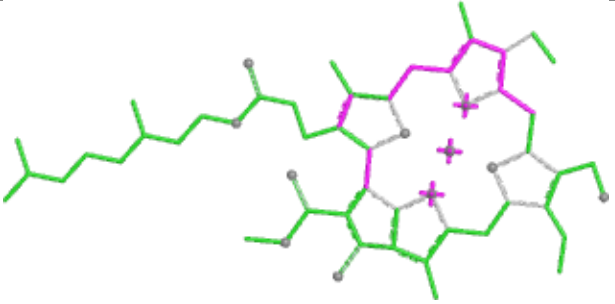
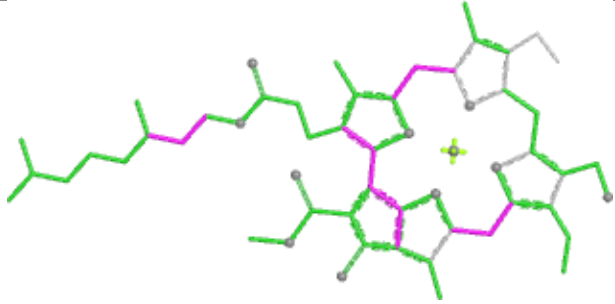
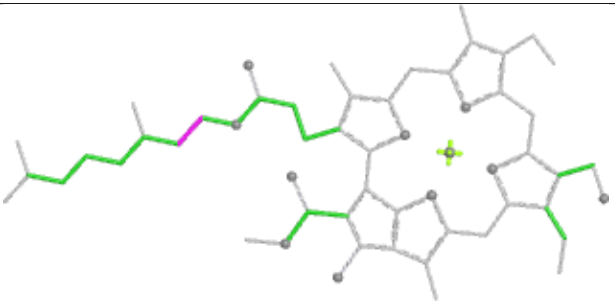
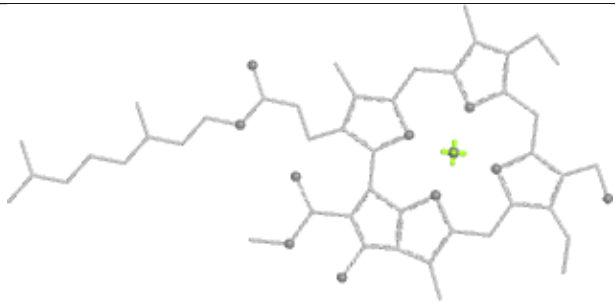
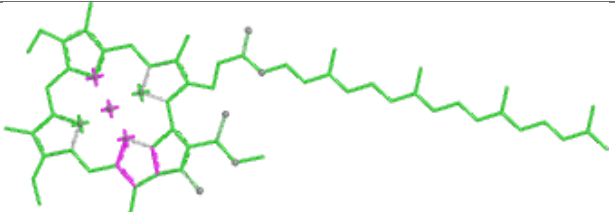
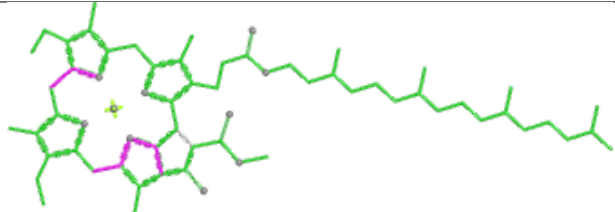
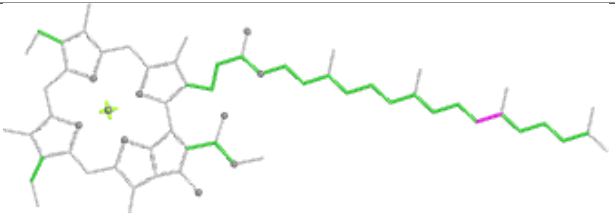
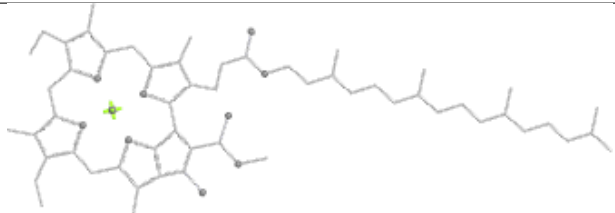
Ligand CLA A2 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

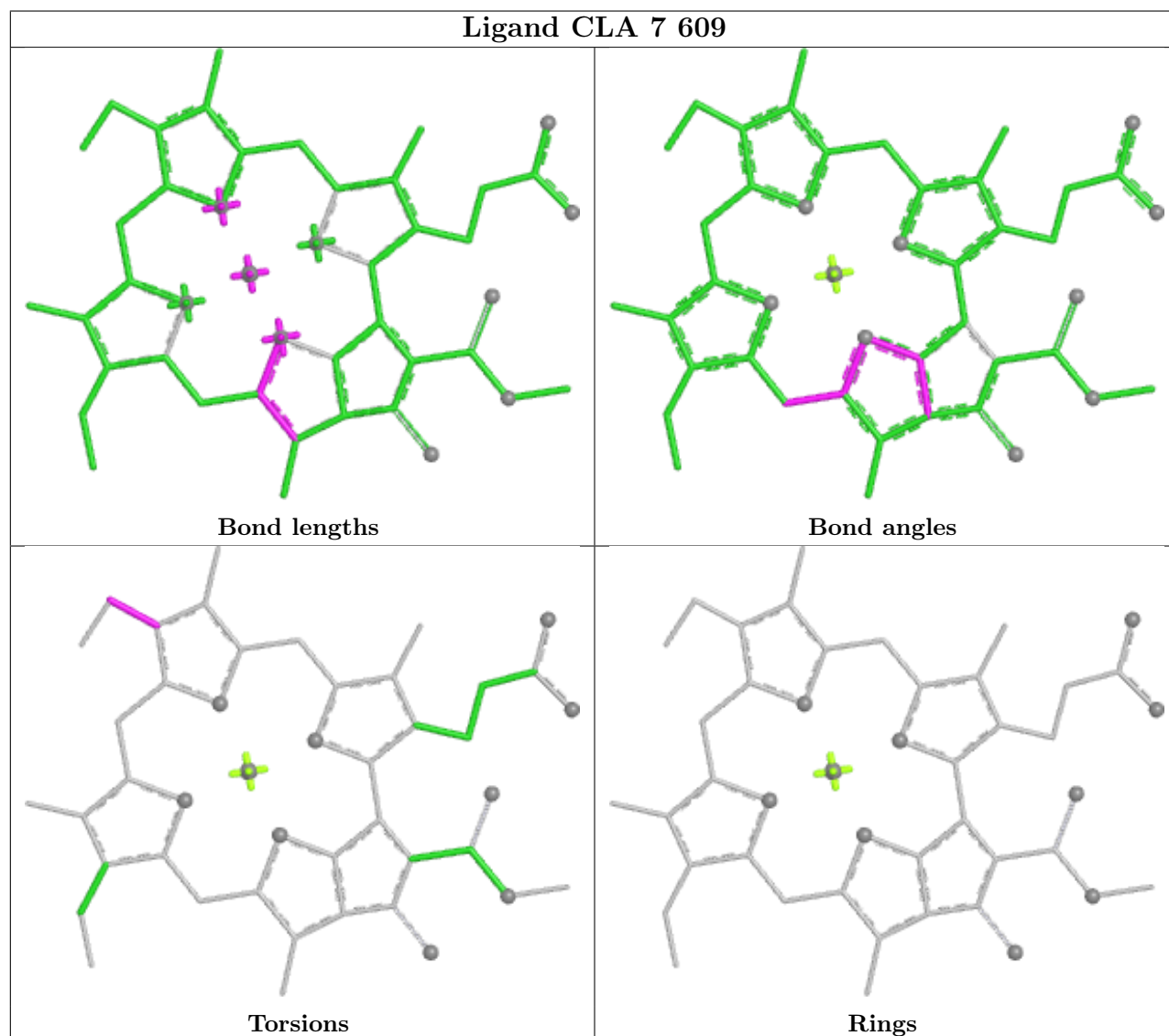
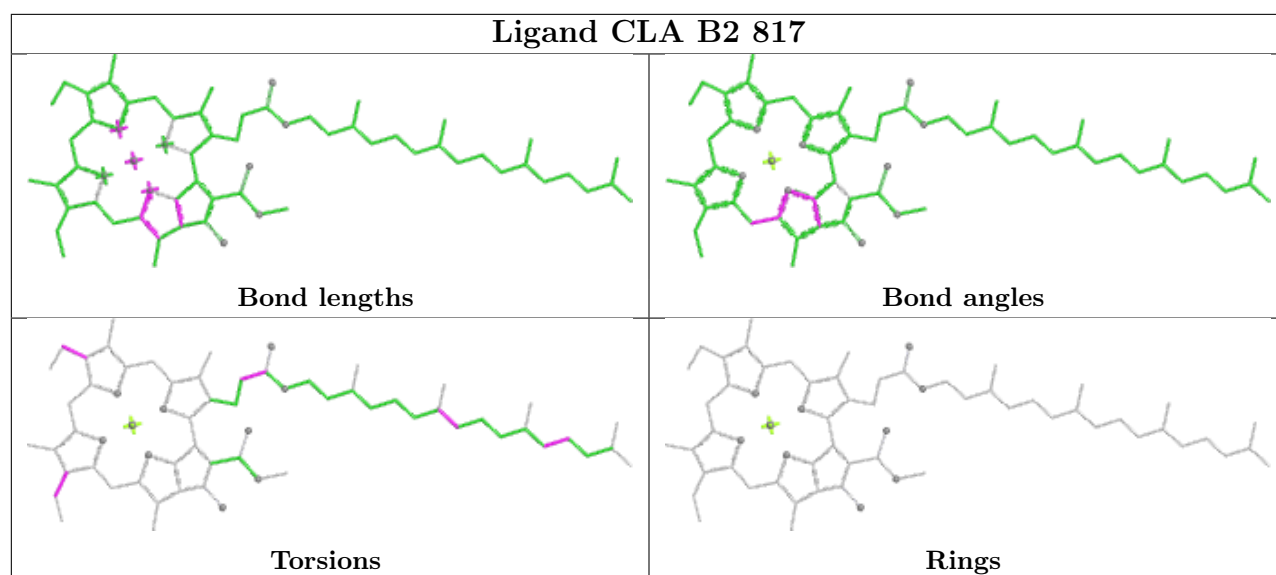
Ligand CLA Z2 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

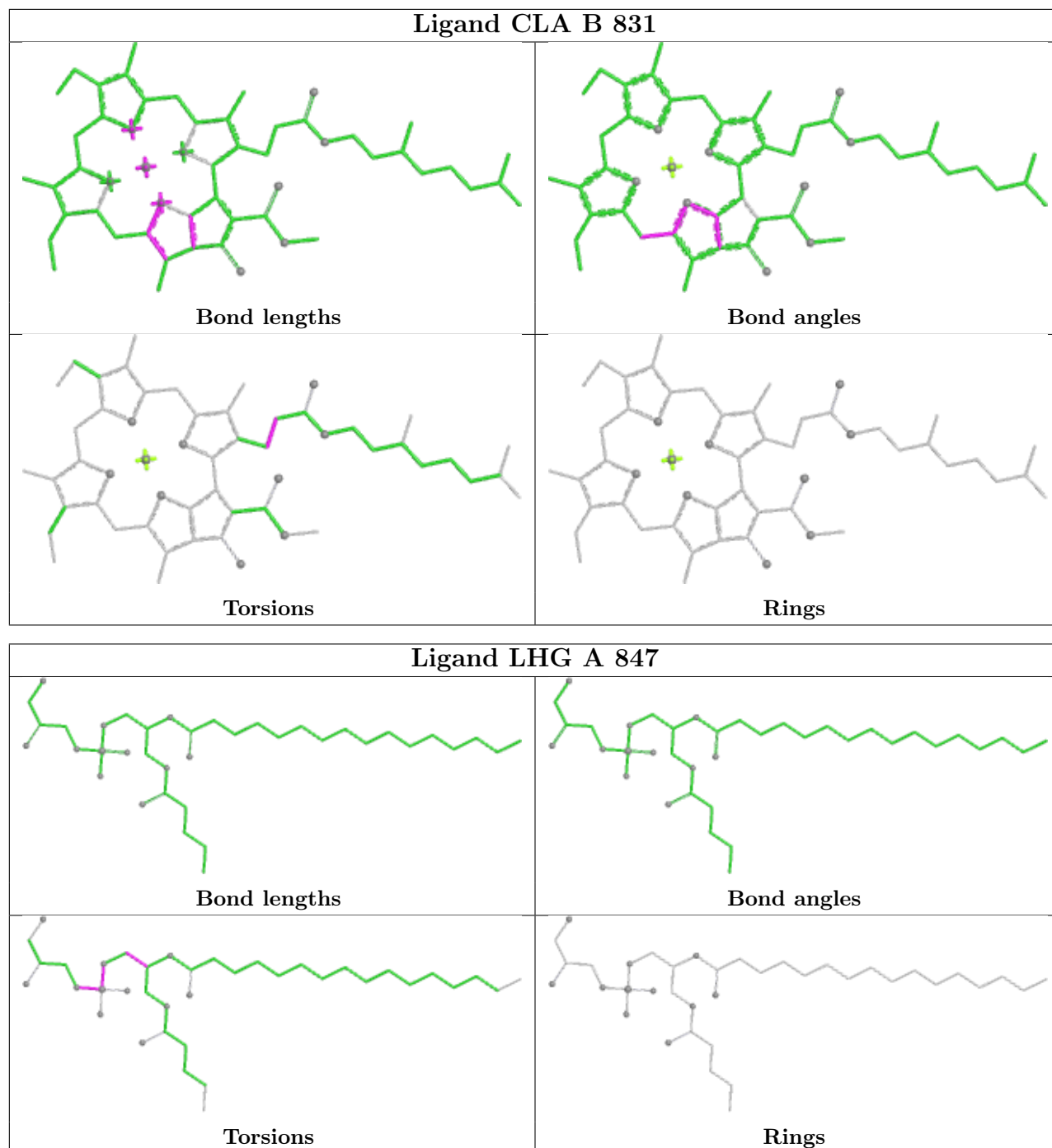
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Bond lengths	Bond angles
	
Torsions	Rings

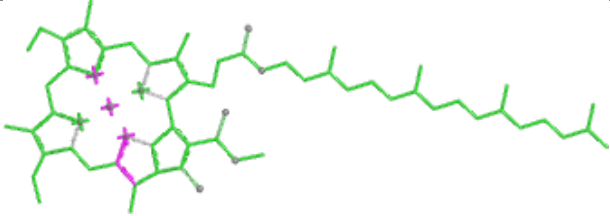
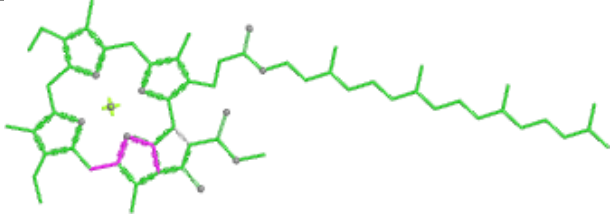
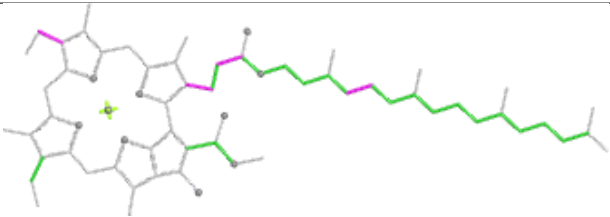
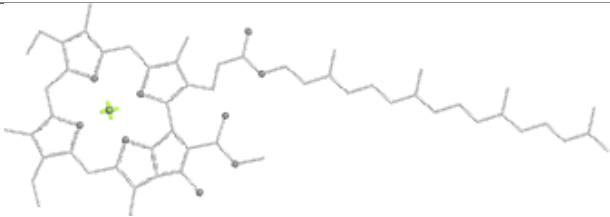
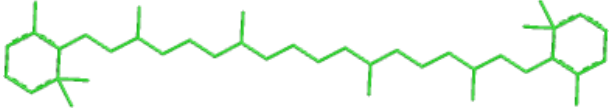
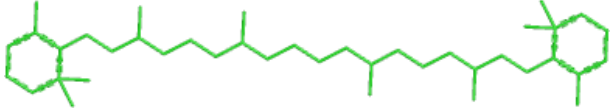
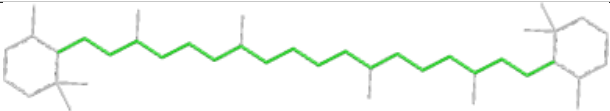
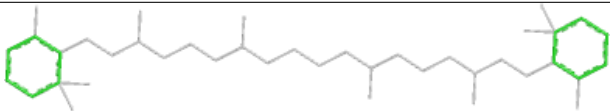
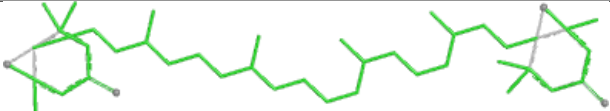
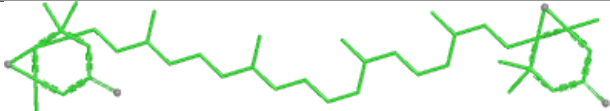
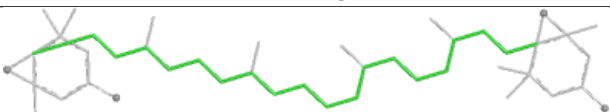
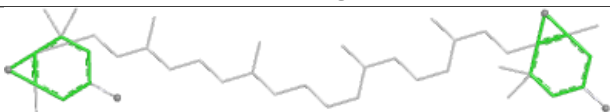




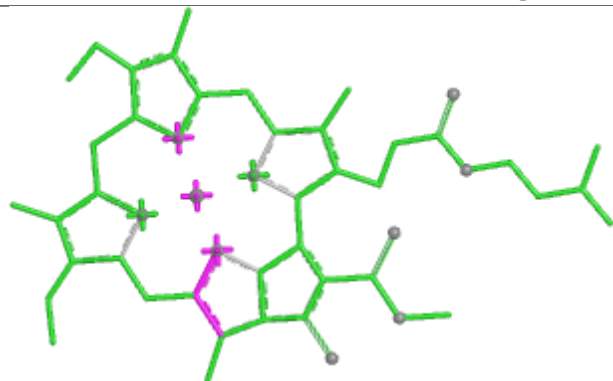
Ligand CHL 42 606	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 839	
 Bond lengths	 Bond angles
 Torsions	 Rings



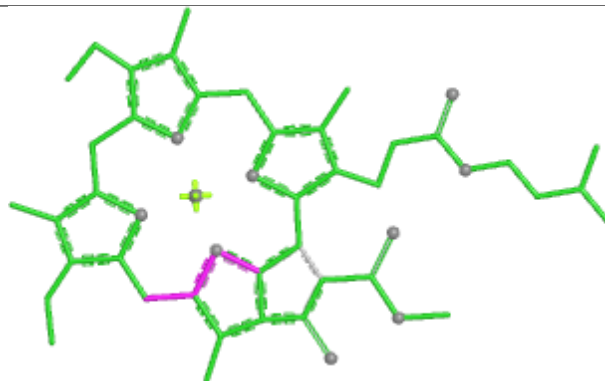


Ligand CLA 3 611	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR B2 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand XAT 5 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

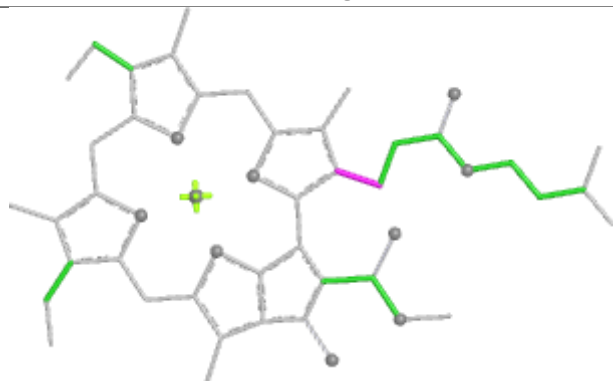
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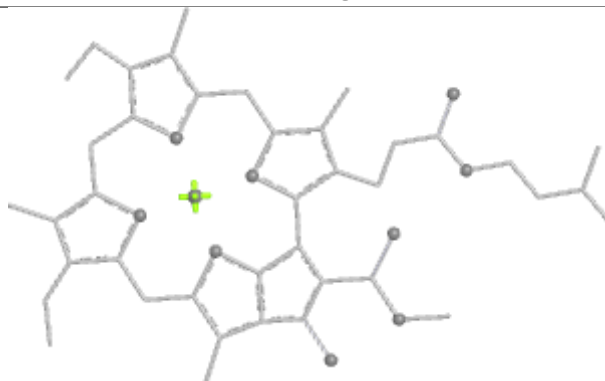
Bond lengths



Bond angles

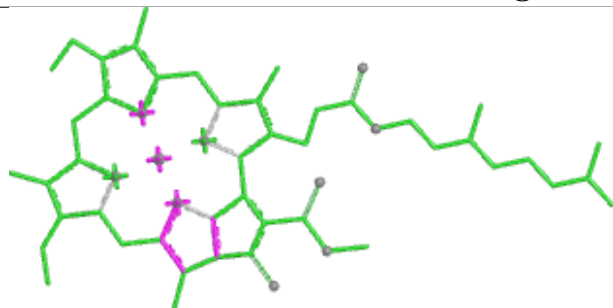


Torsions

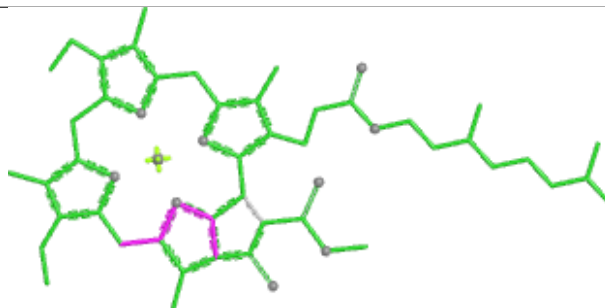


Rings

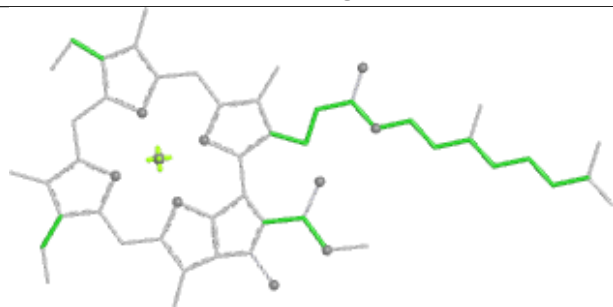
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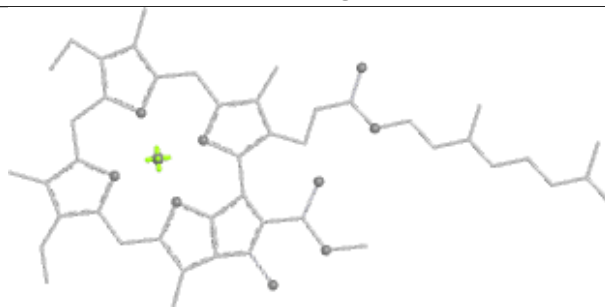
Bond lengths



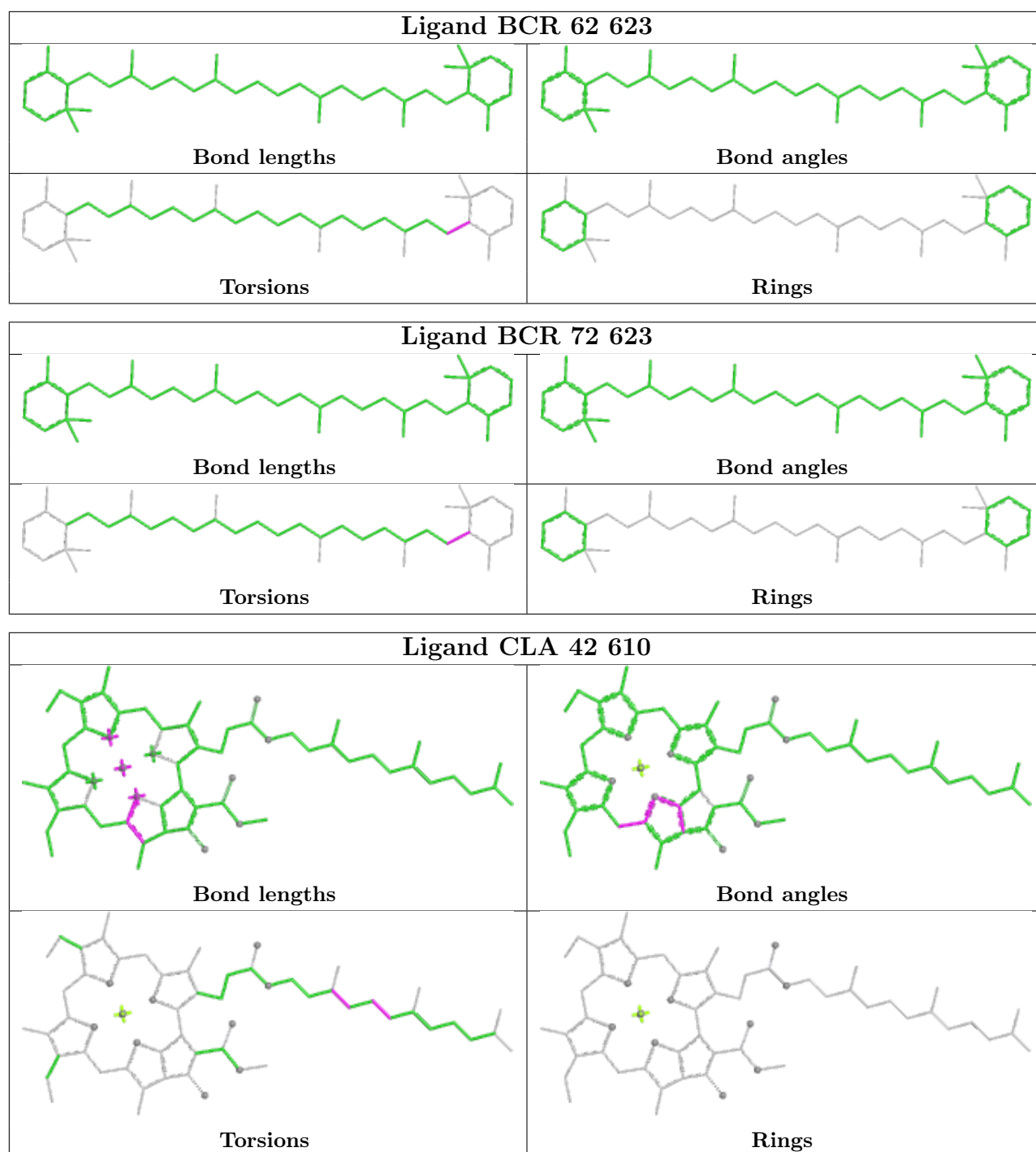
Bond angles

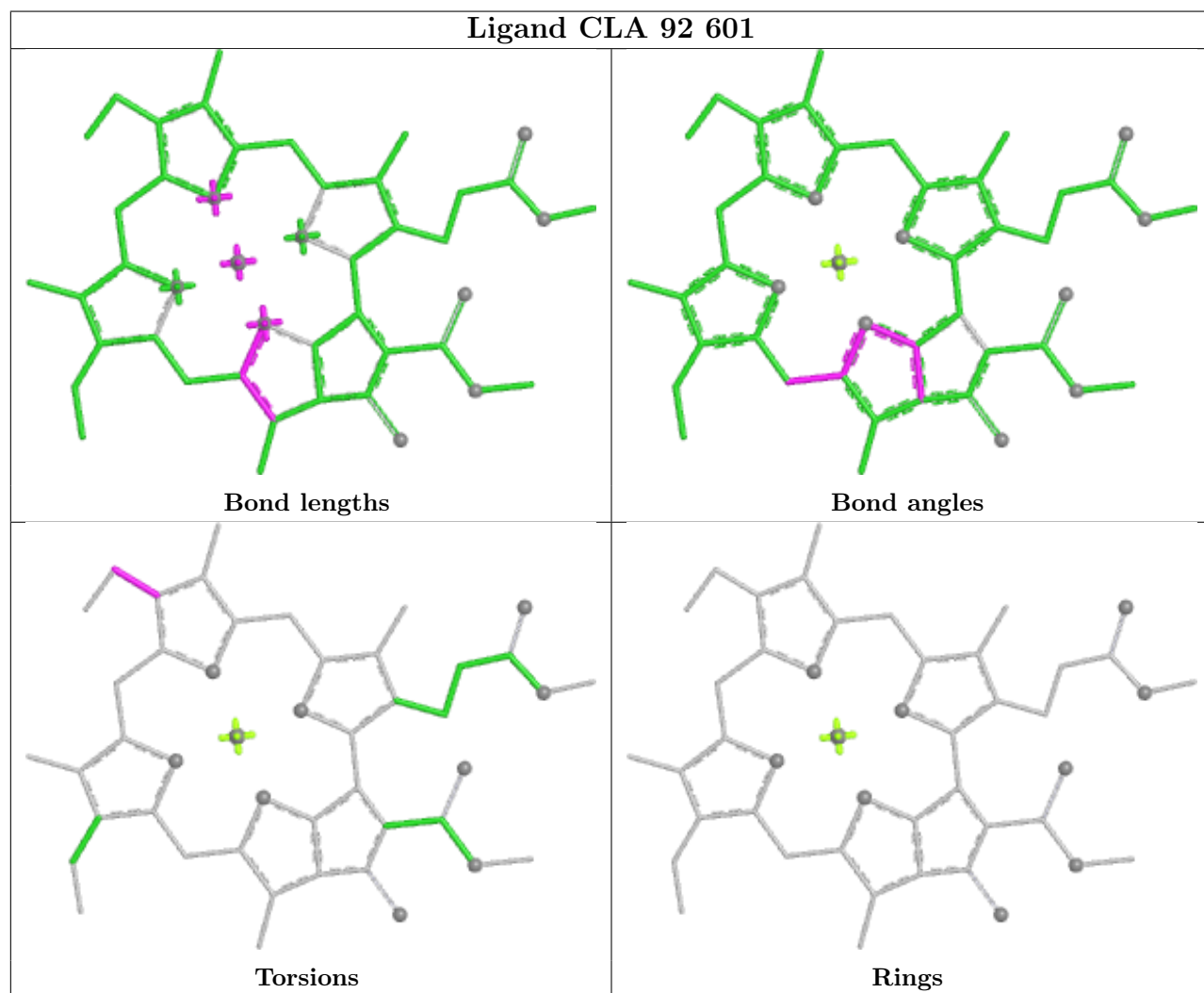
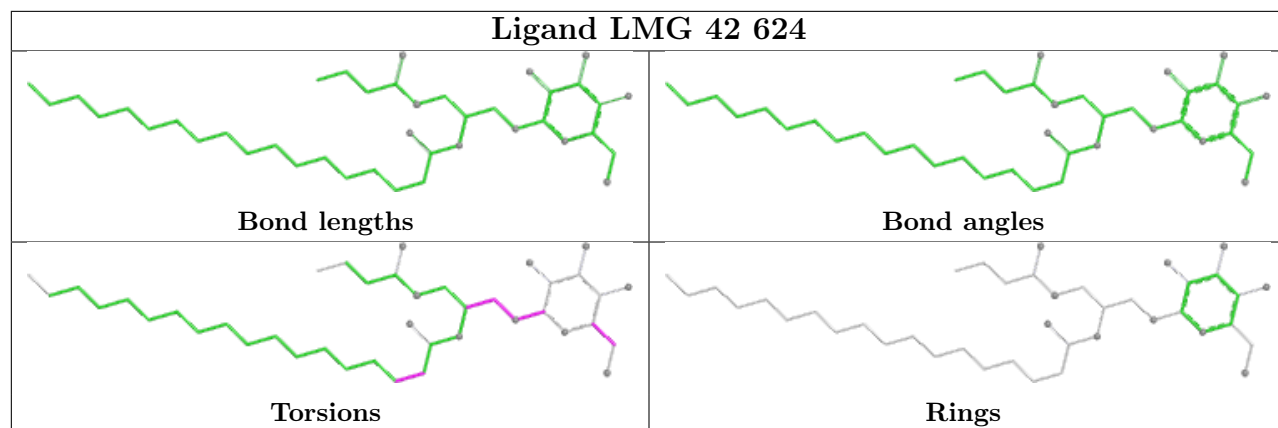


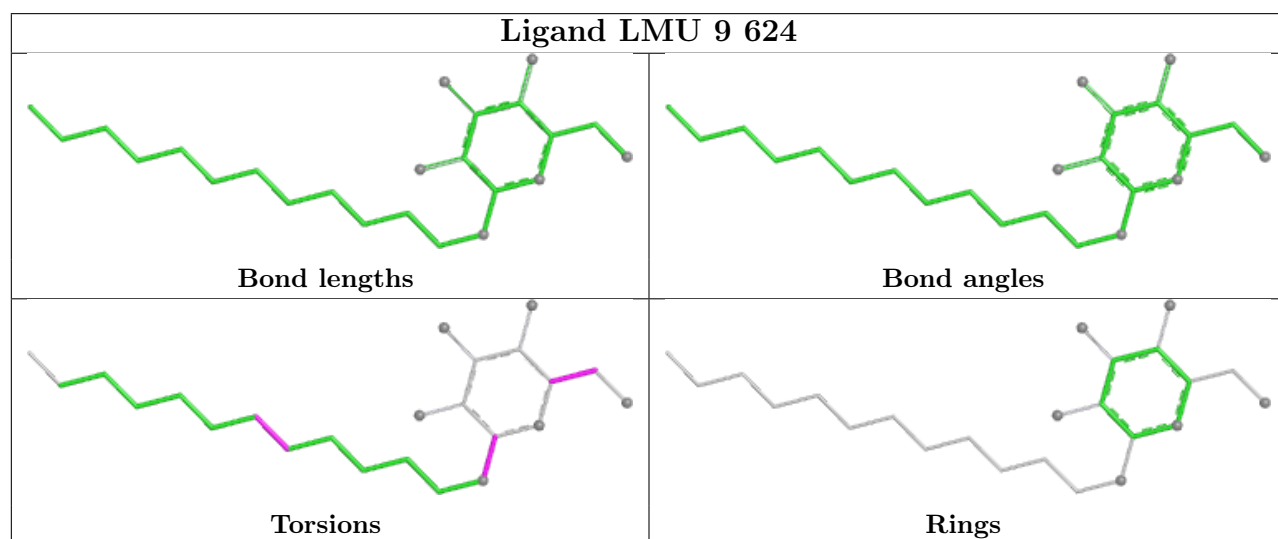
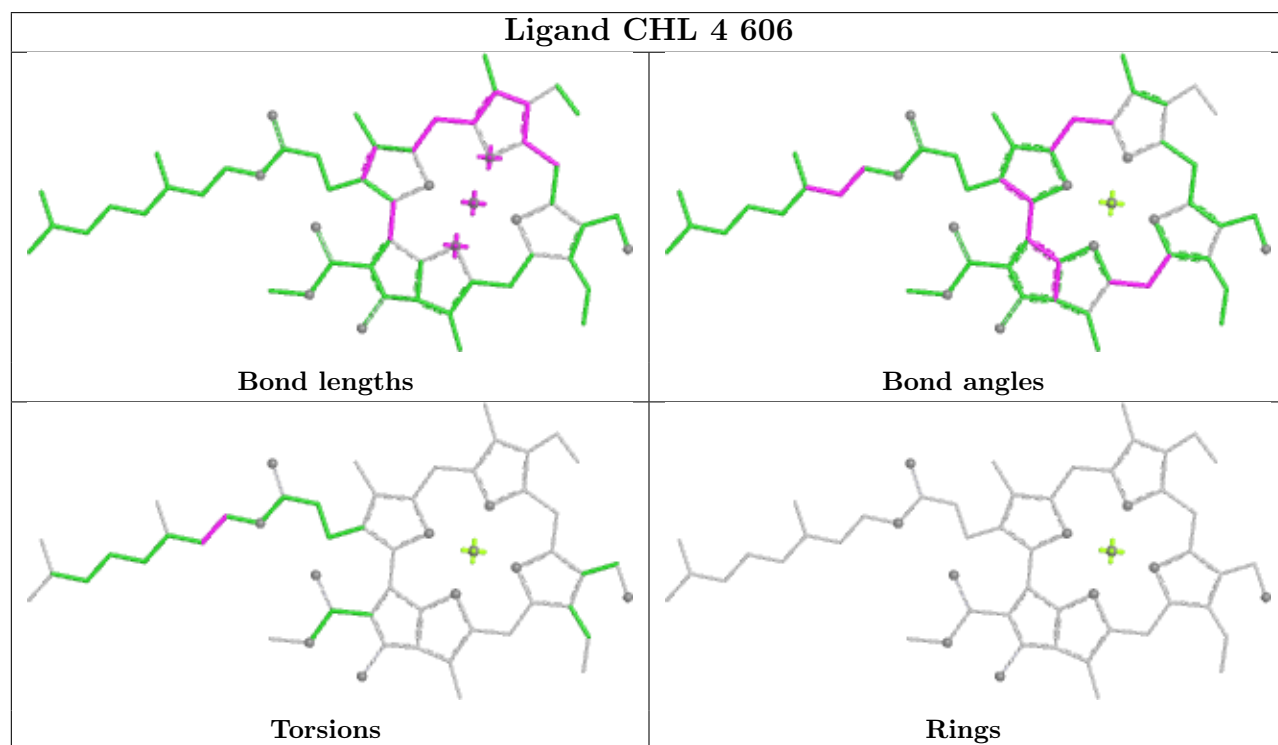
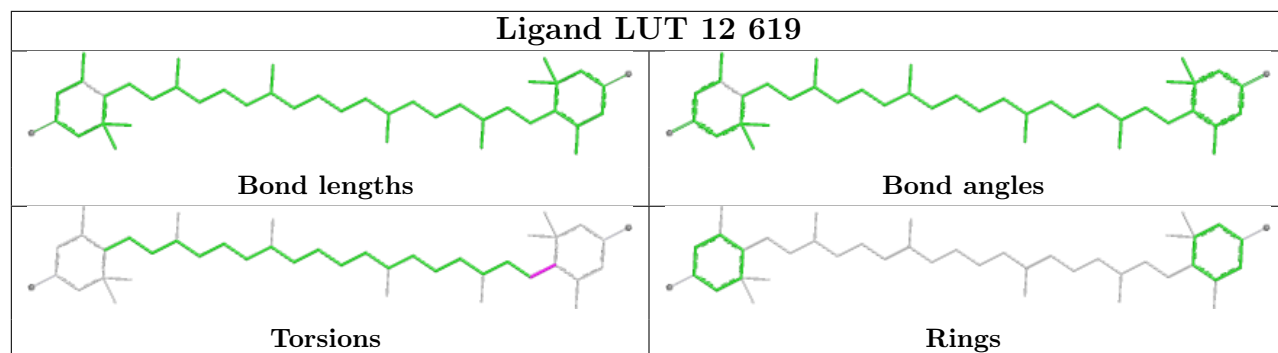
Torsions

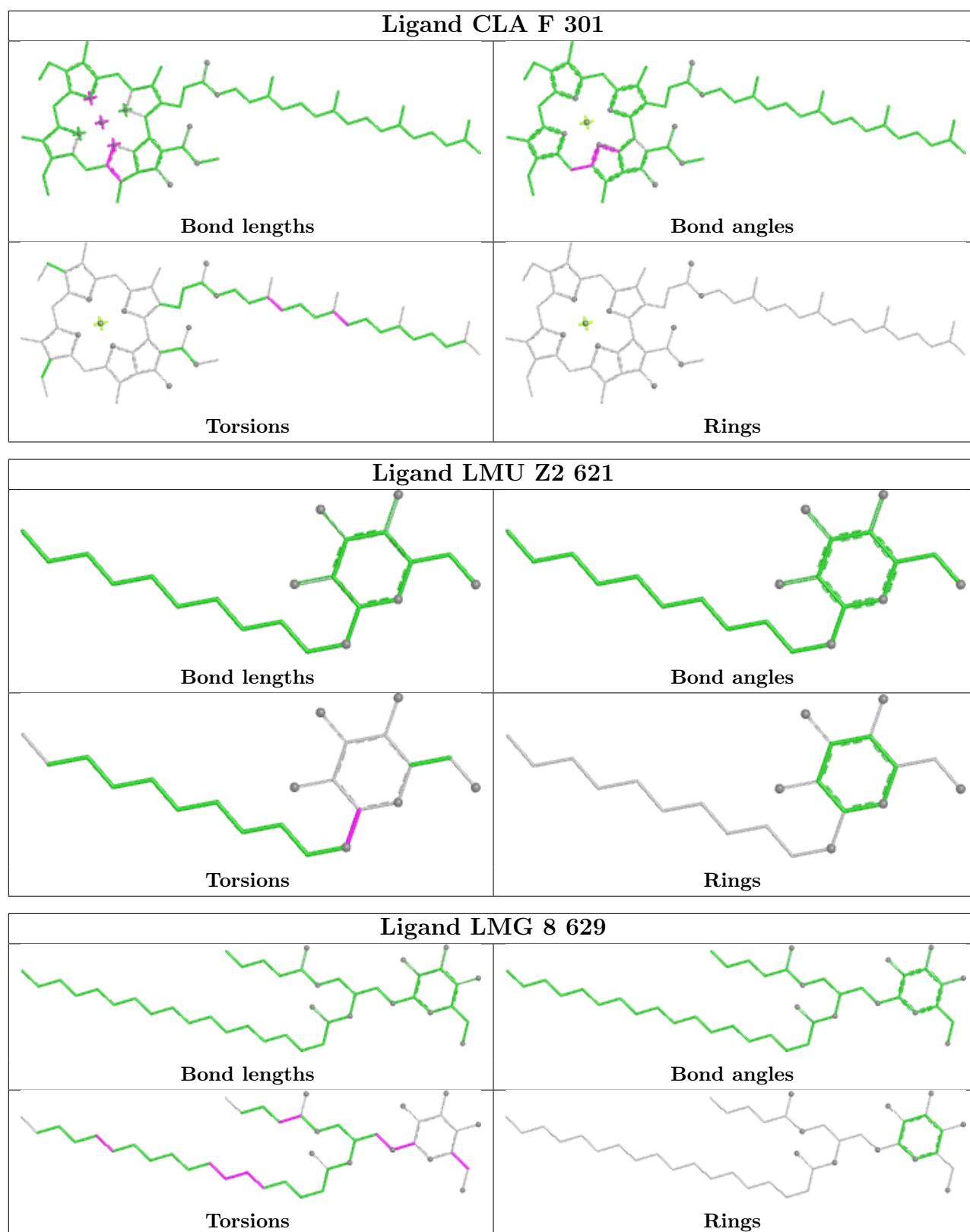


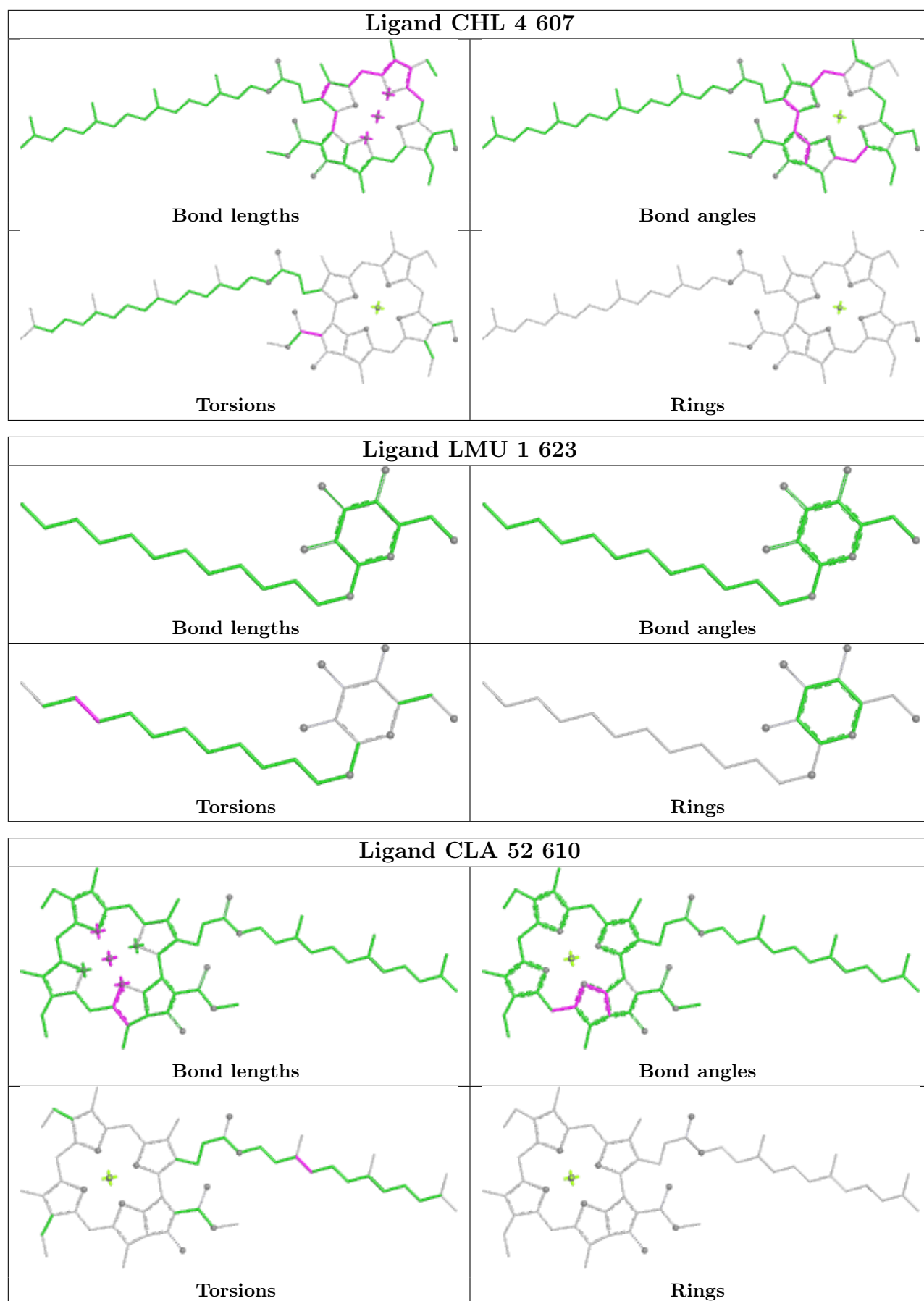
Rings

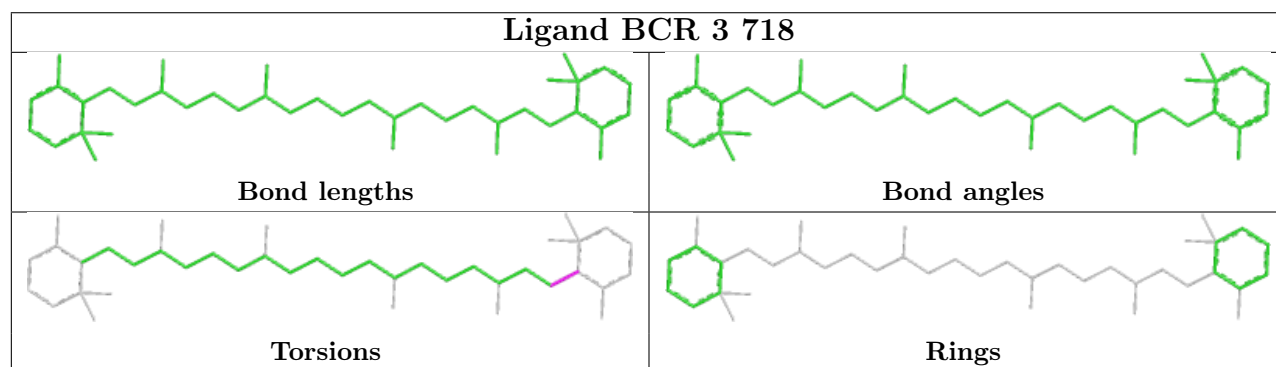
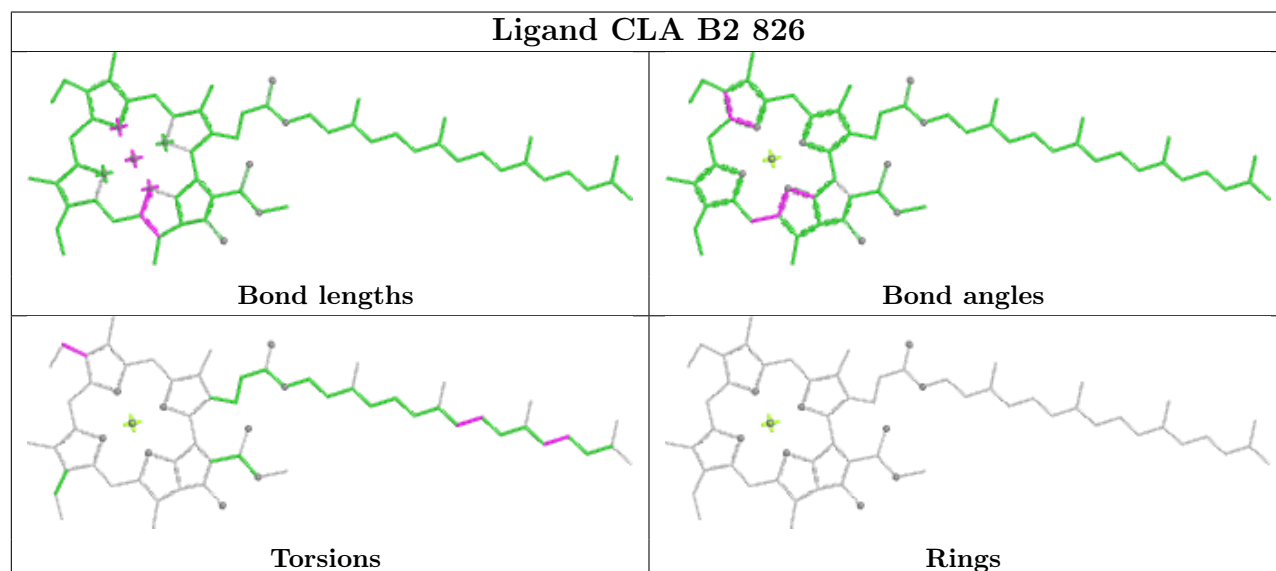
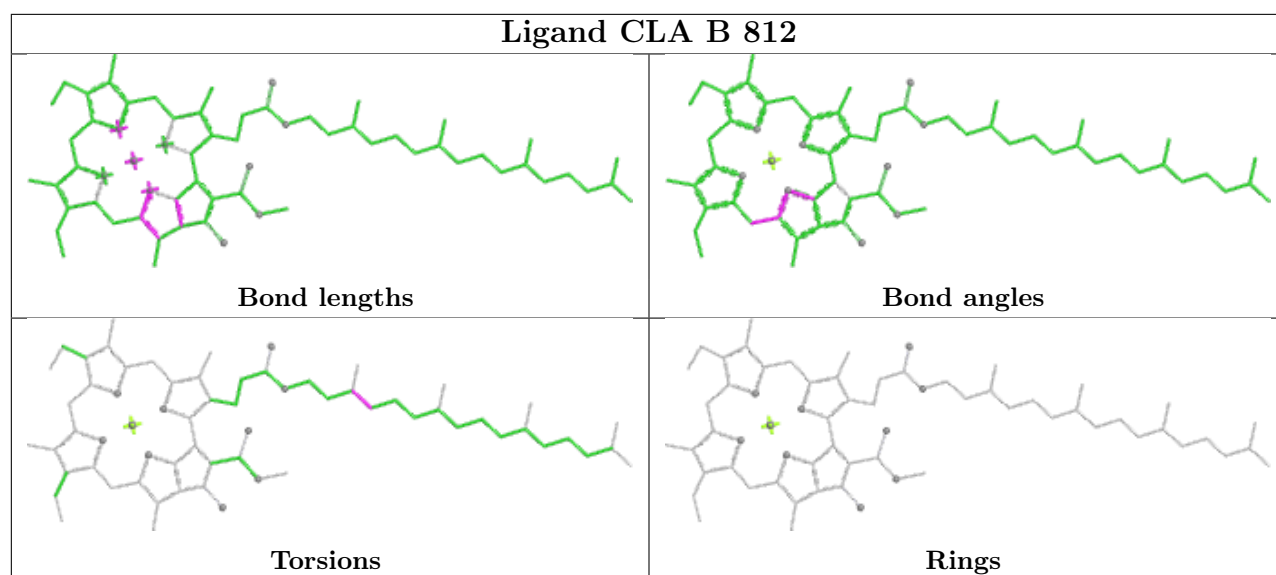


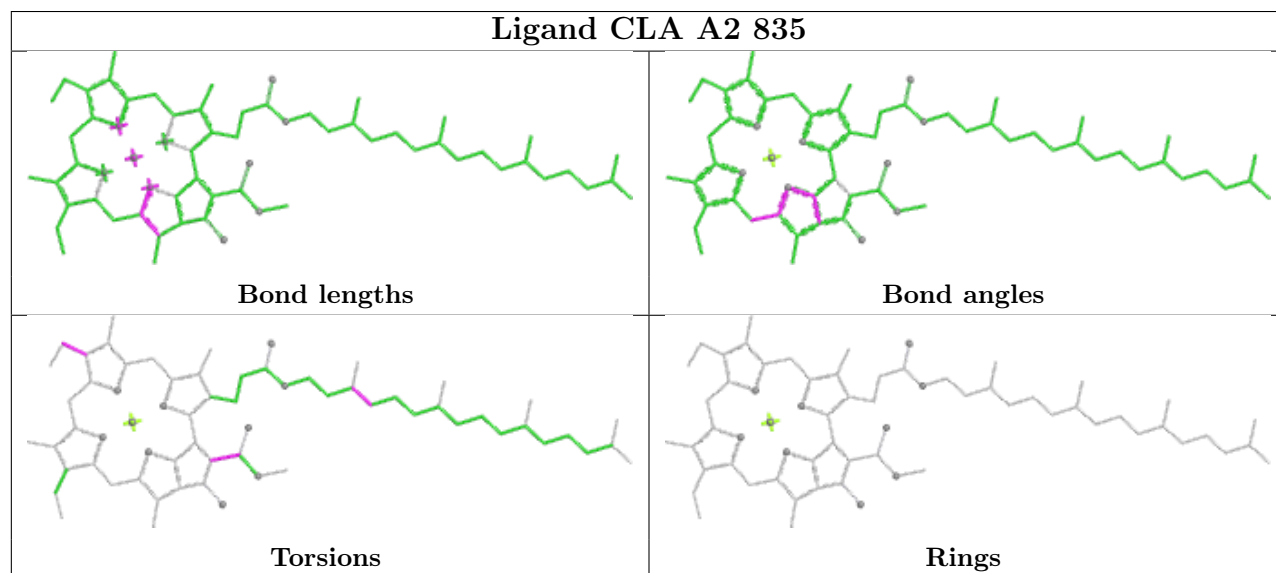
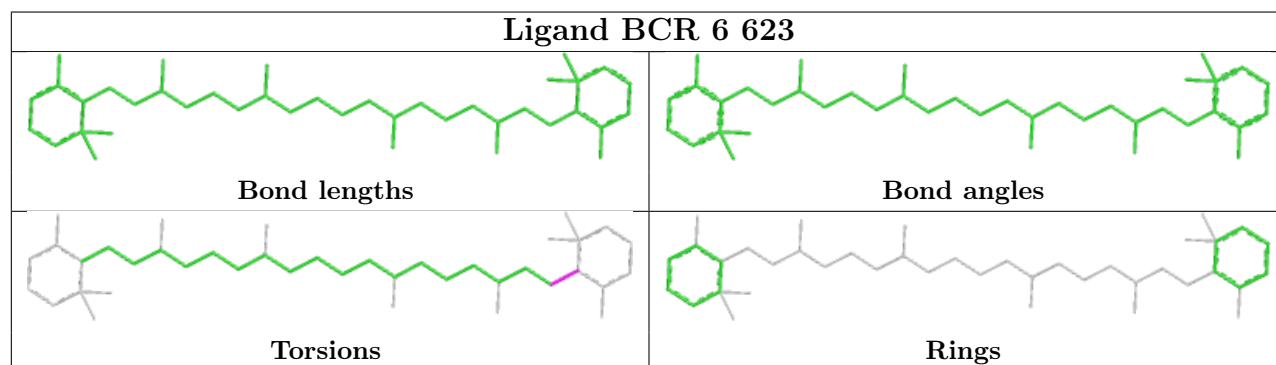
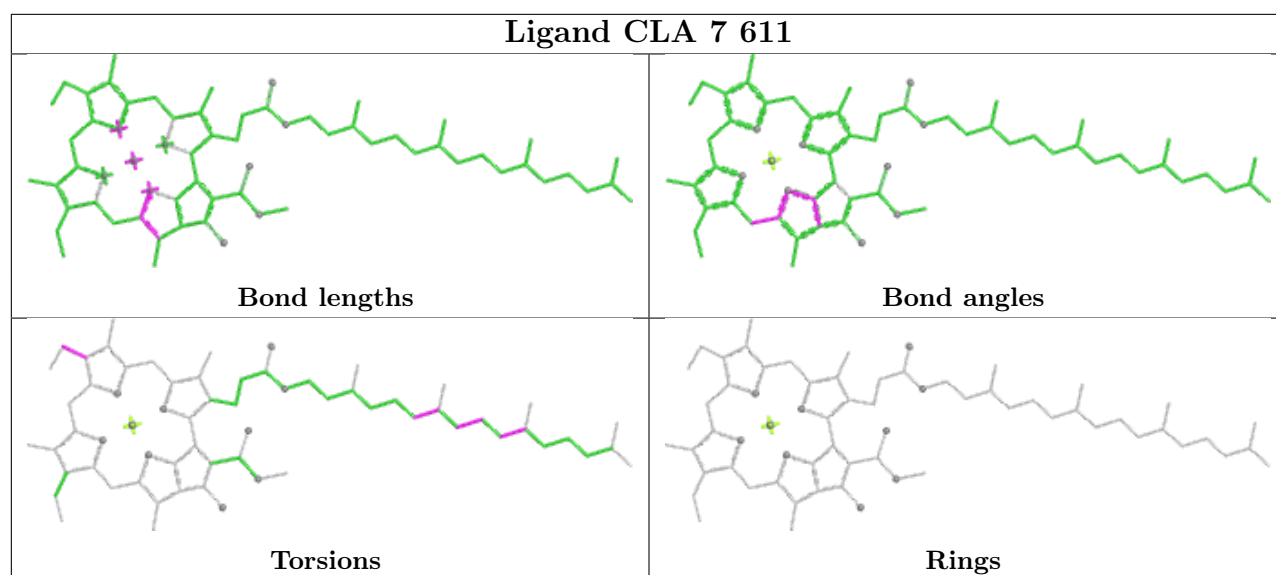


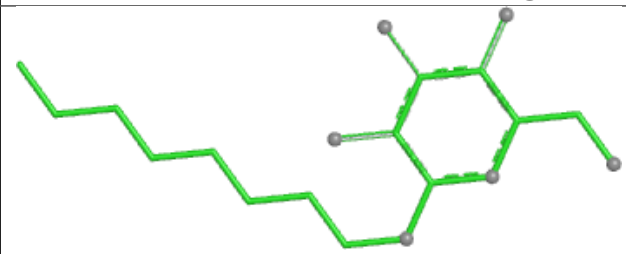
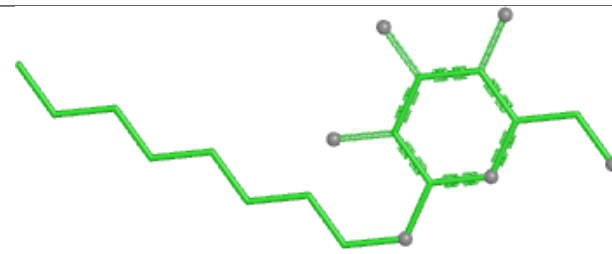
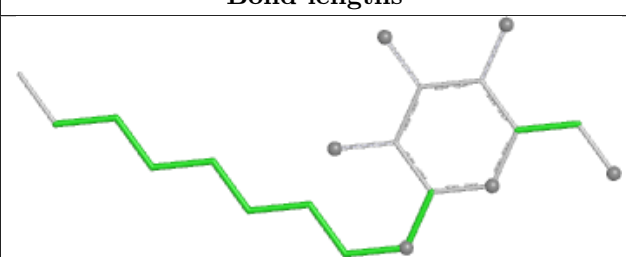
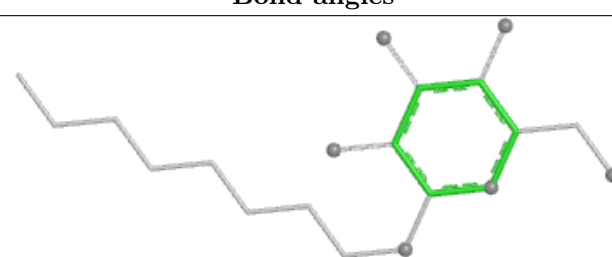
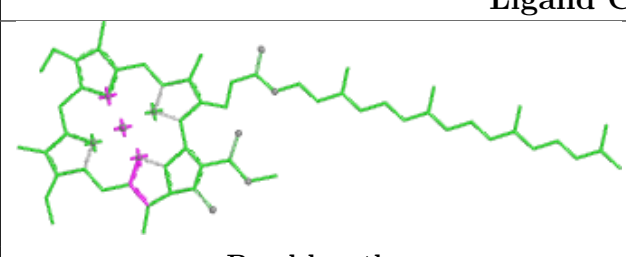
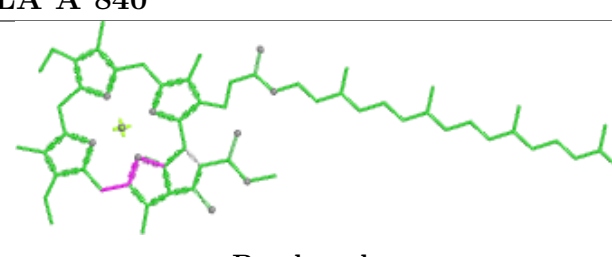
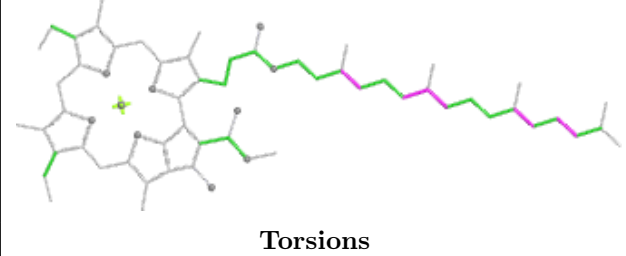
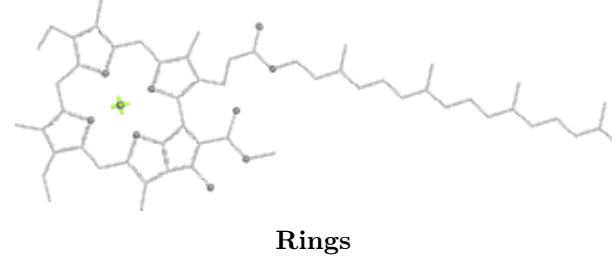
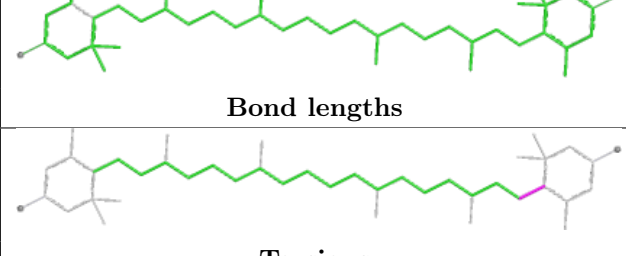
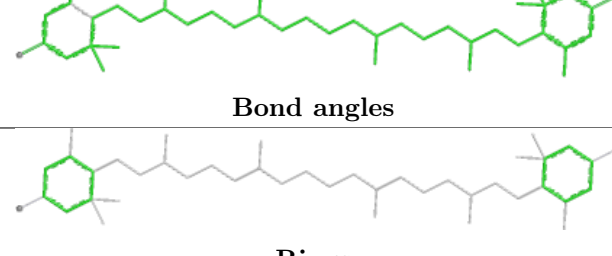


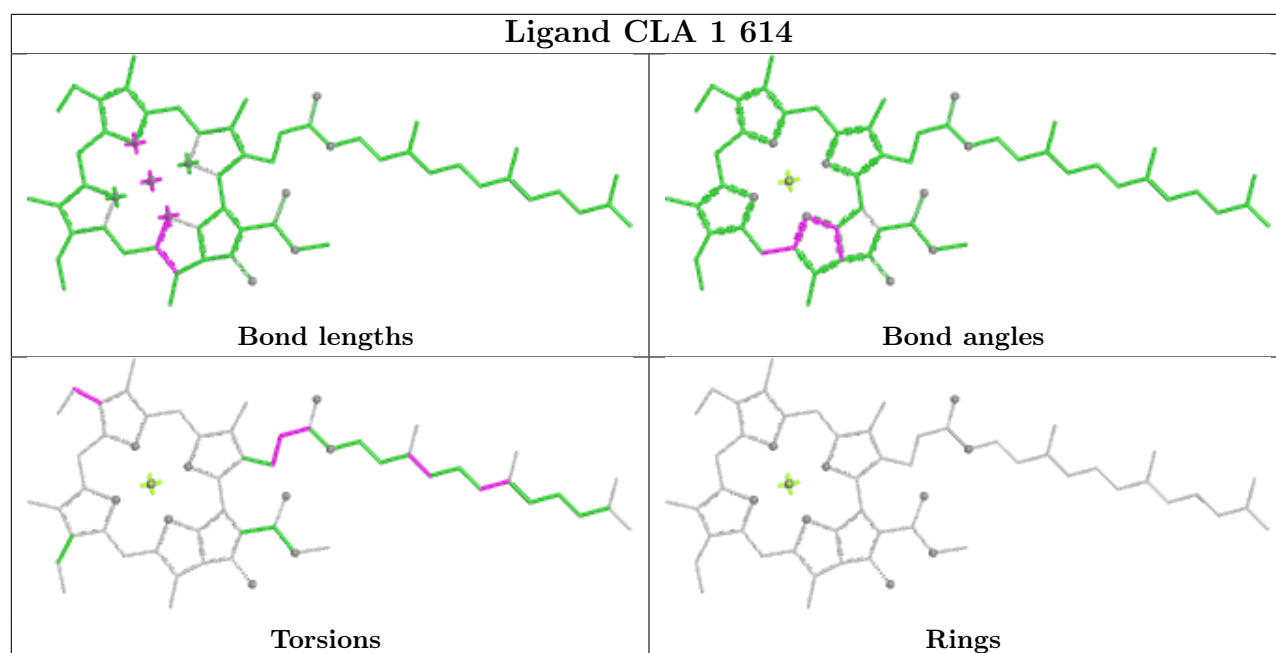
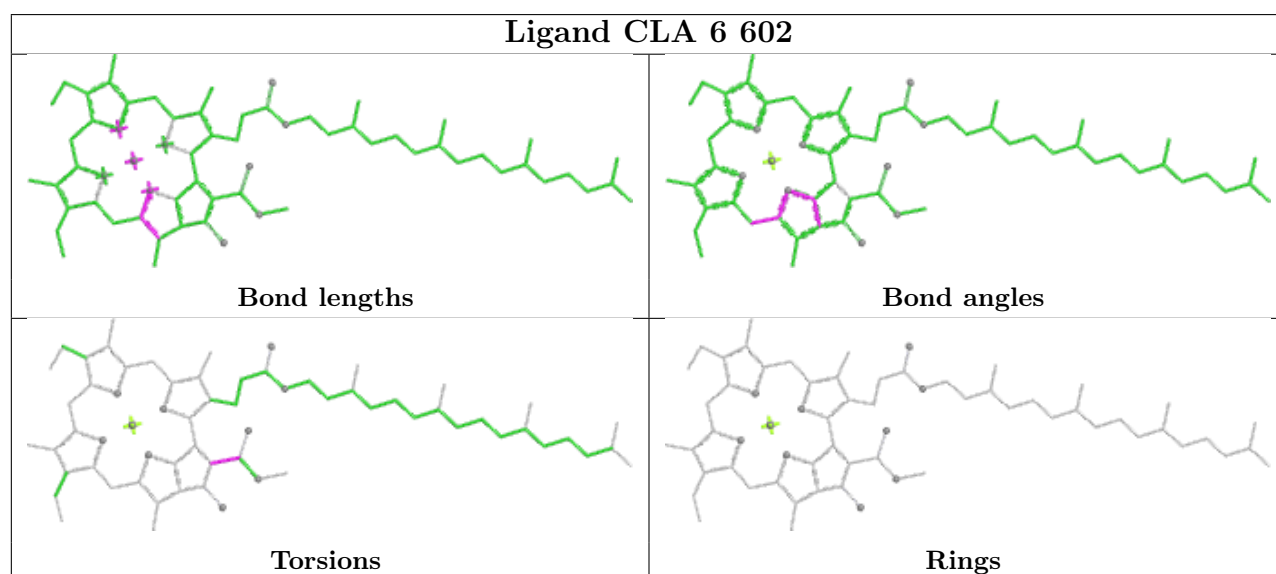
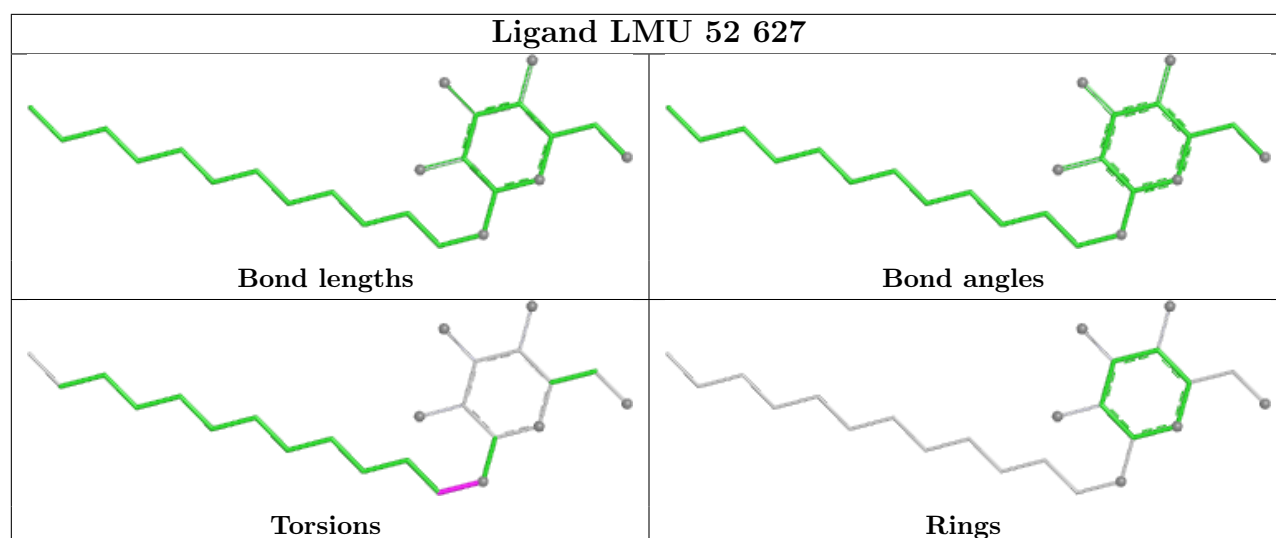


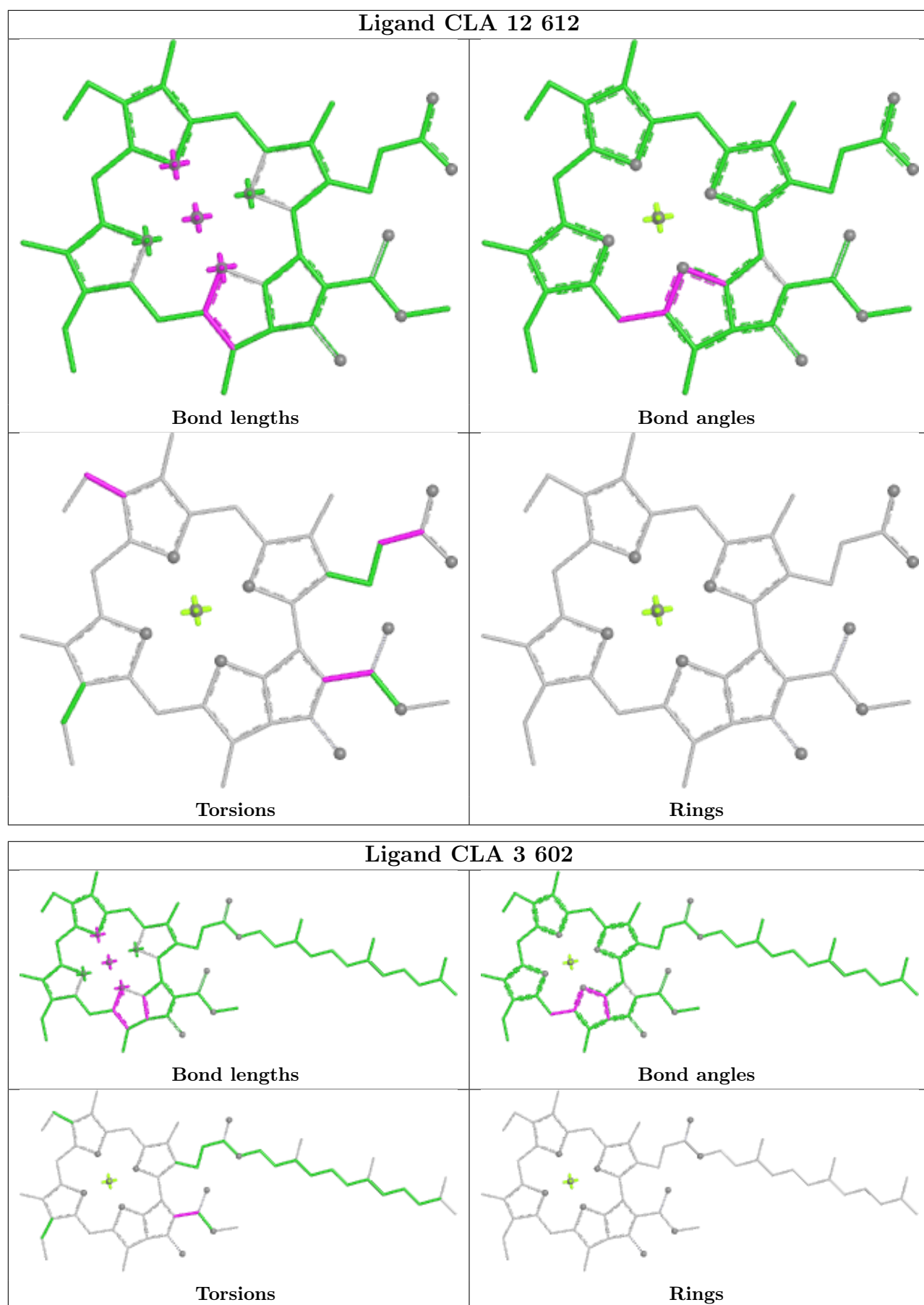


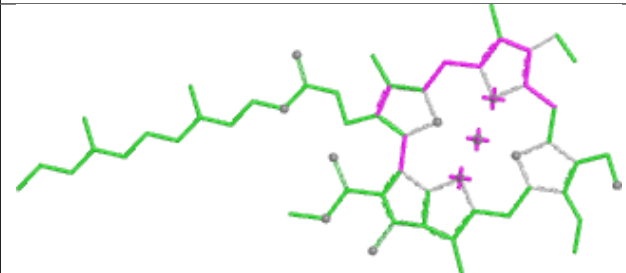
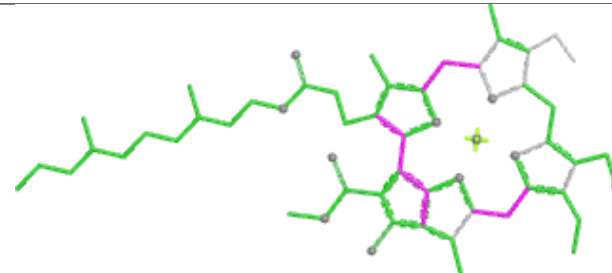
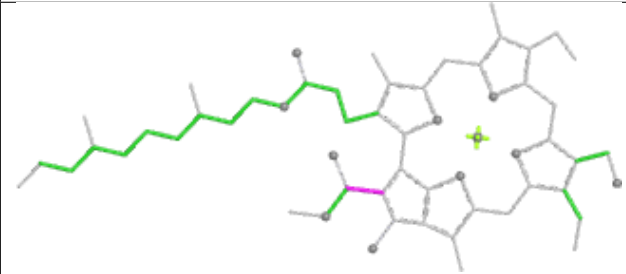
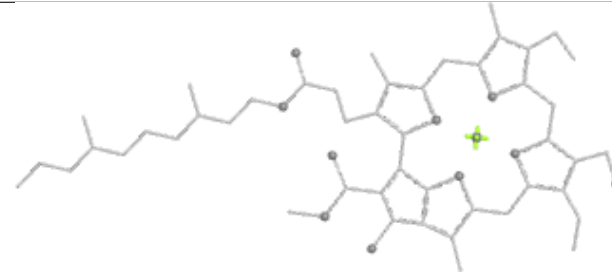


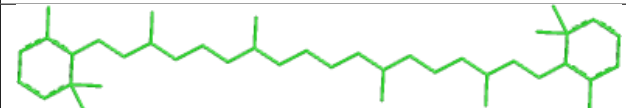
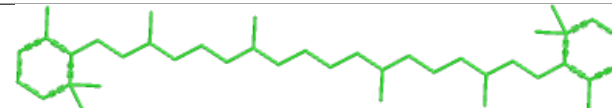
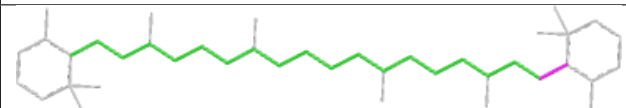
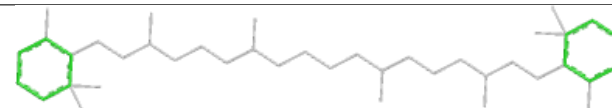


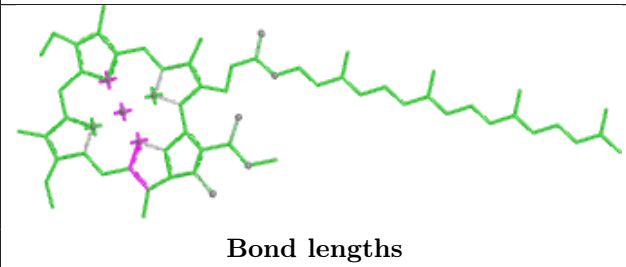
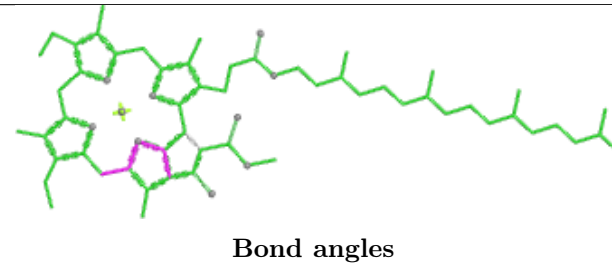
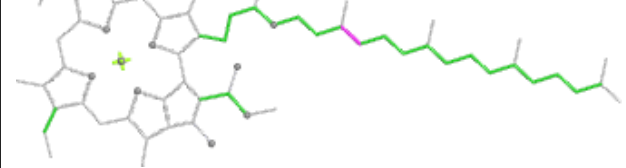
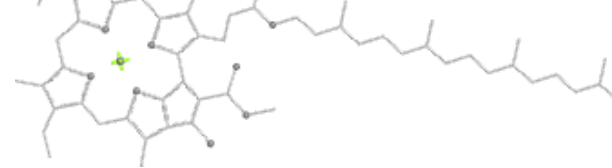
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 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA A 840	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 1 617	
 Bond lengths	 Bond angles
 Torsions	 Rings

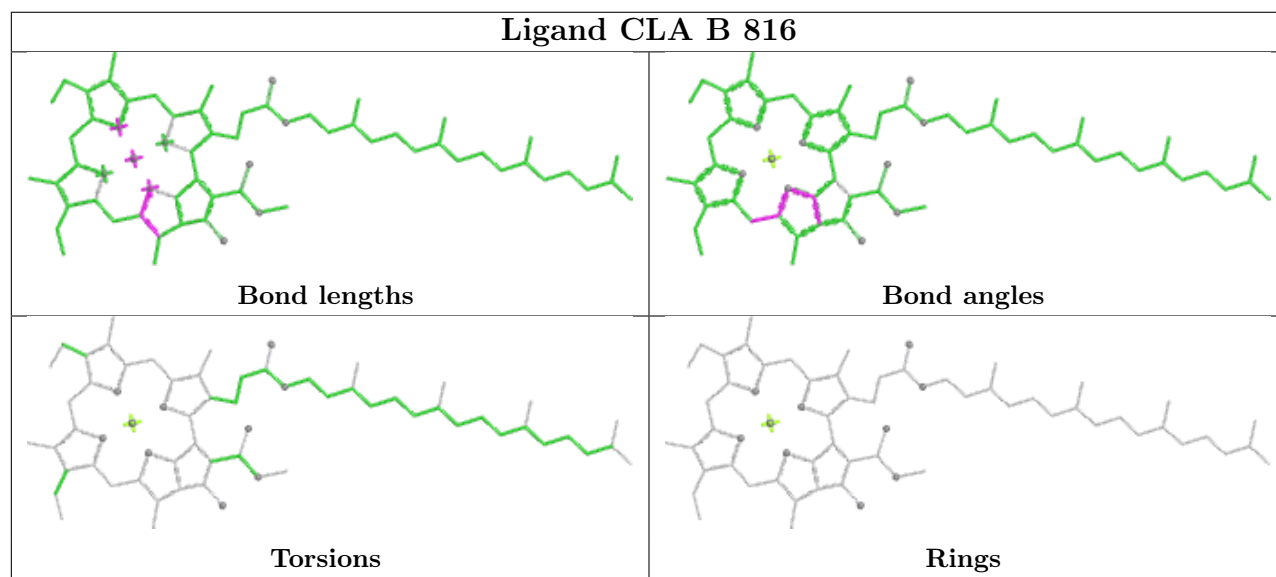
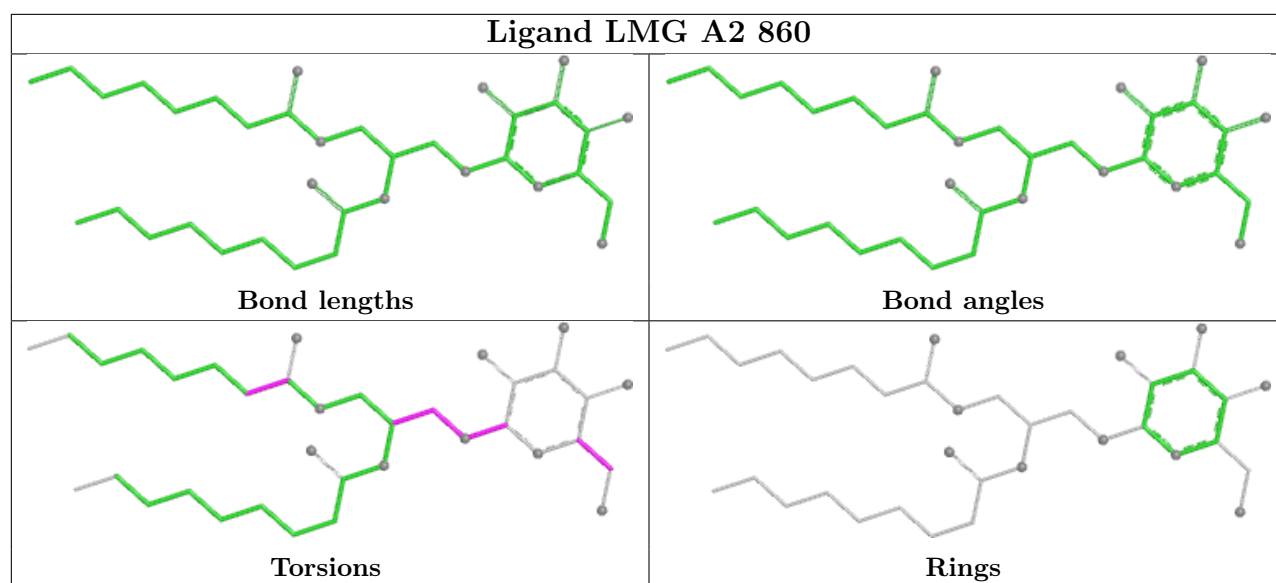


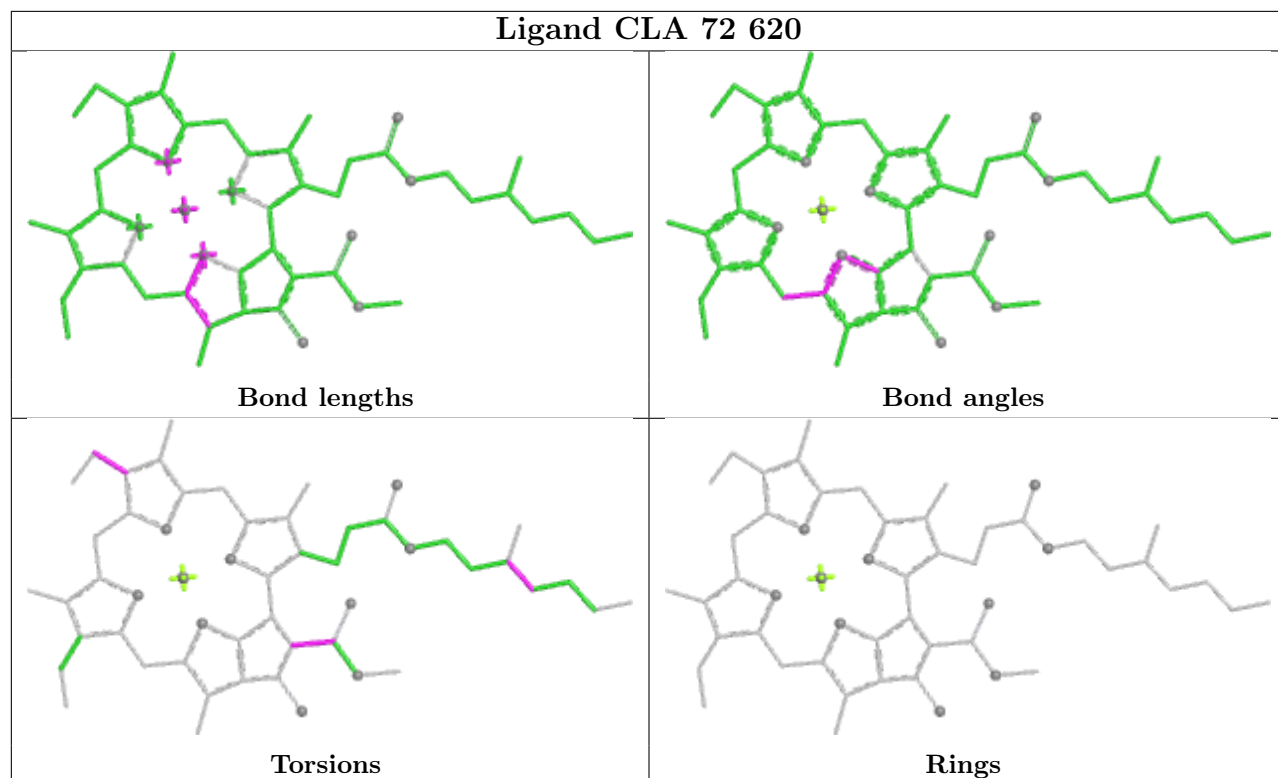


Ligand CHL 62 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

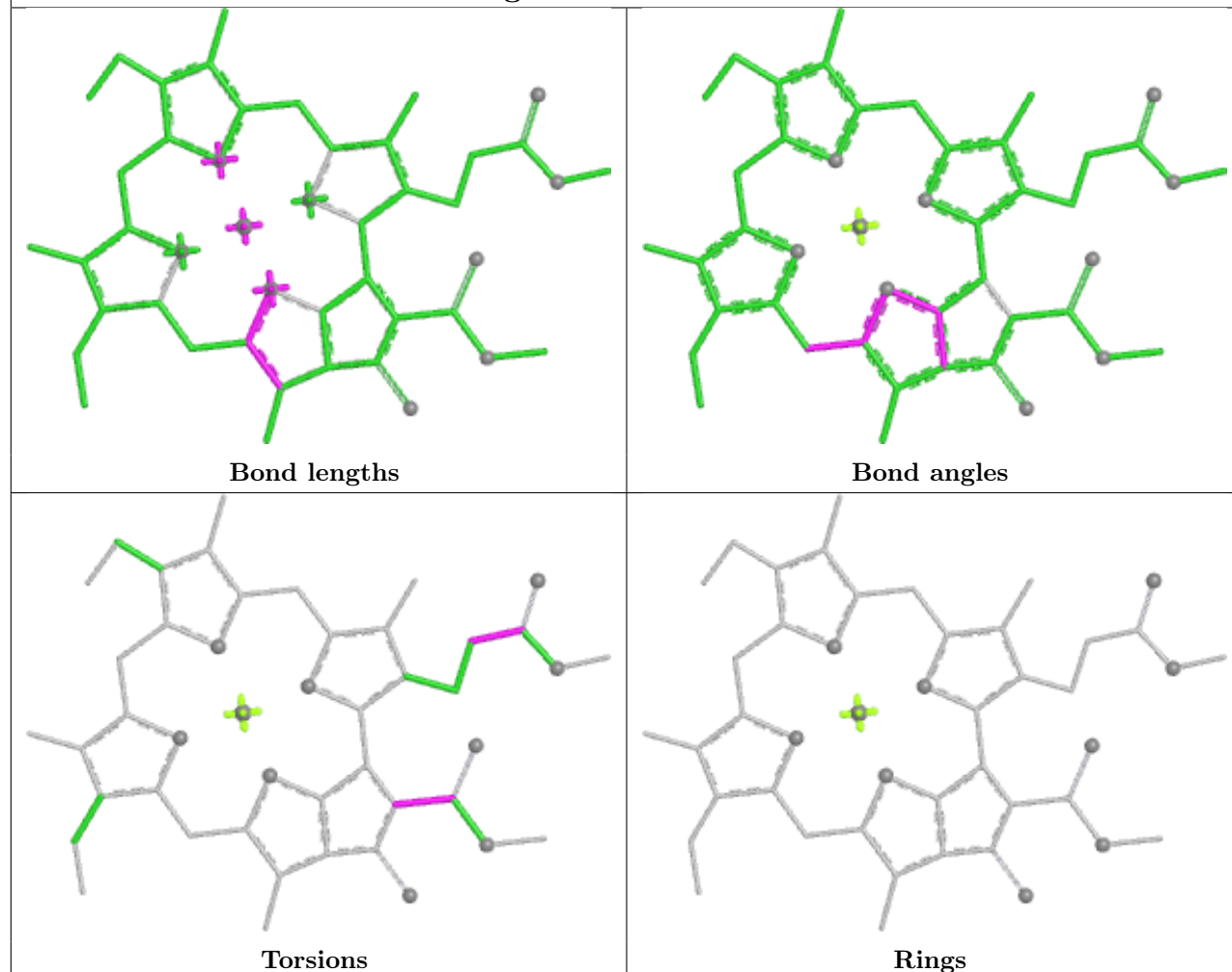
Ligand BCR L 205	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 6 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

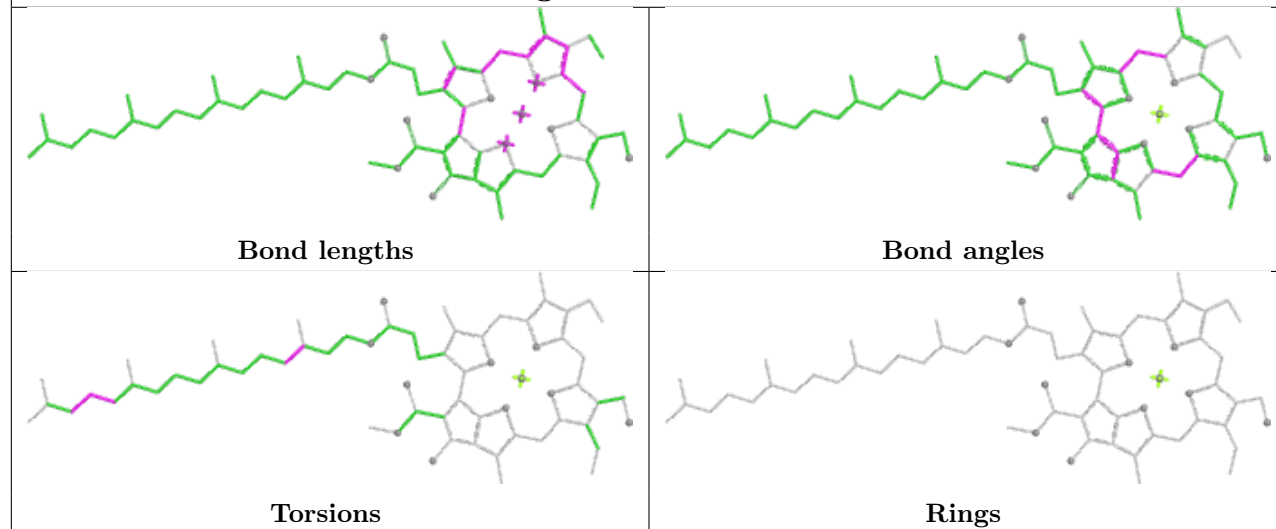


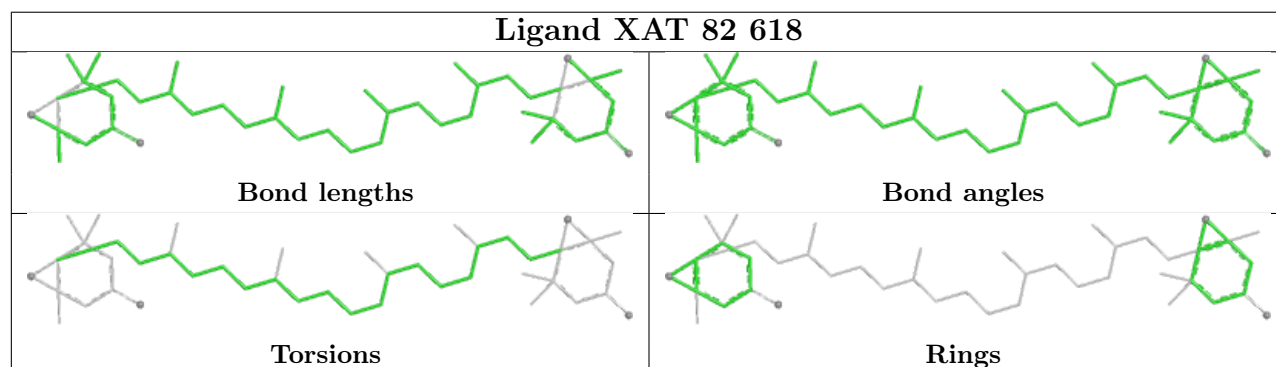
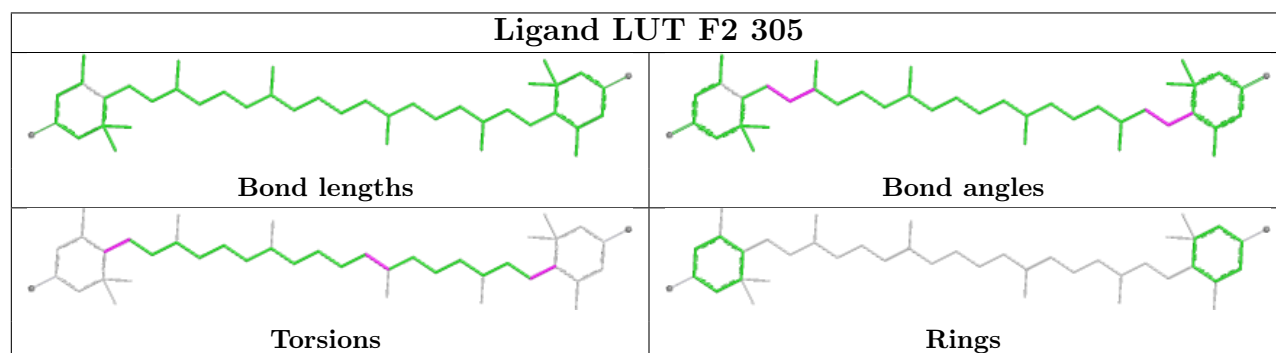
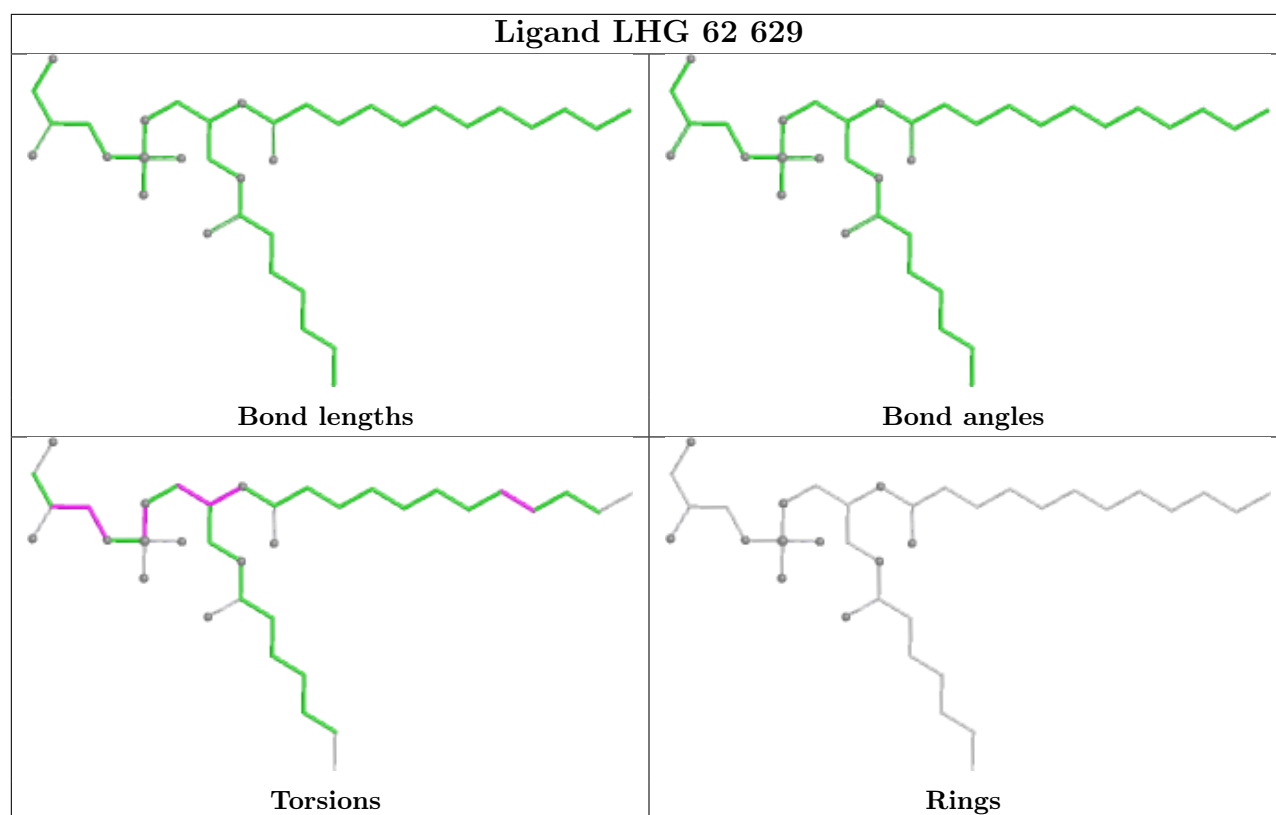


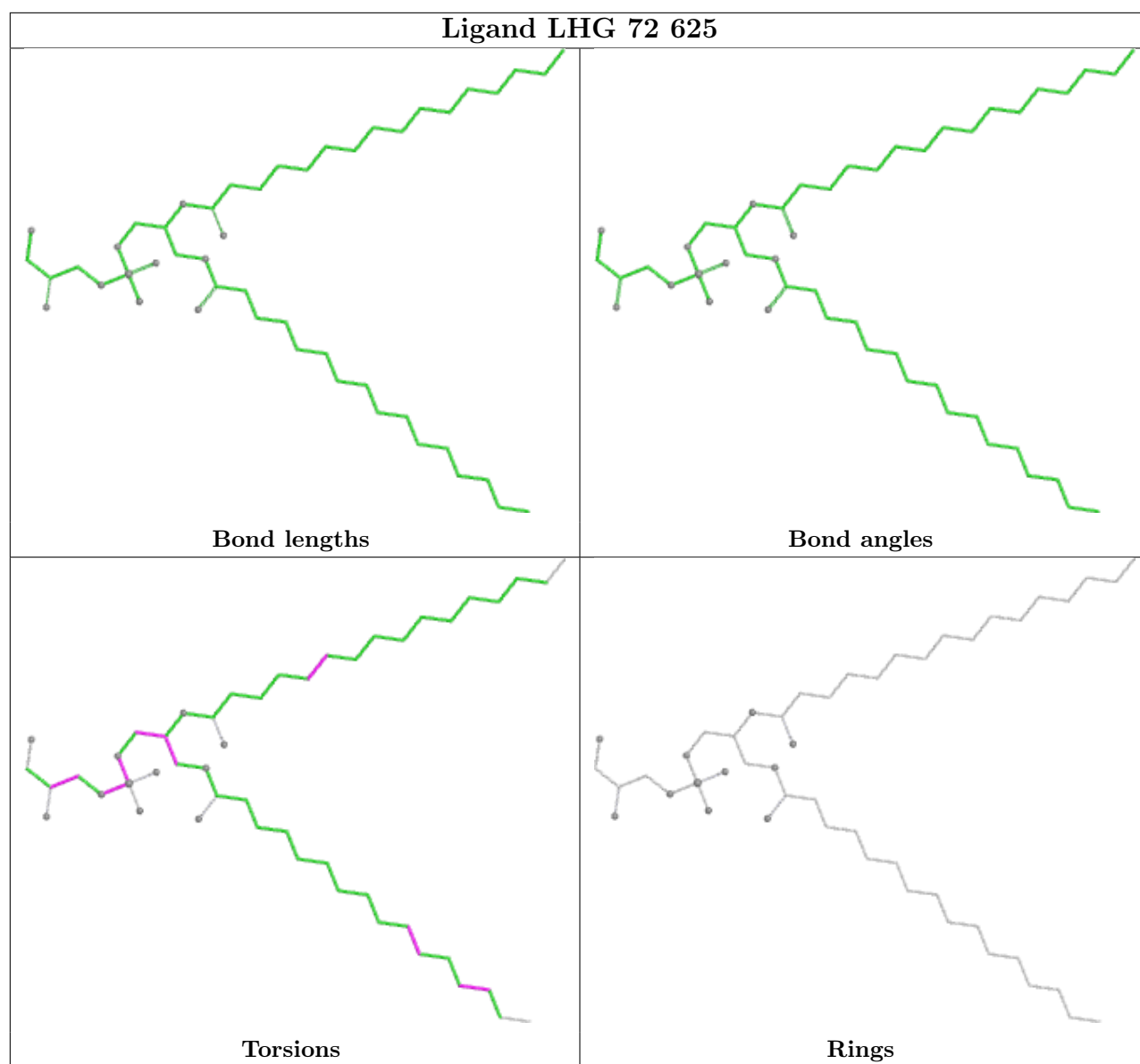
Ligand CLA G2 204



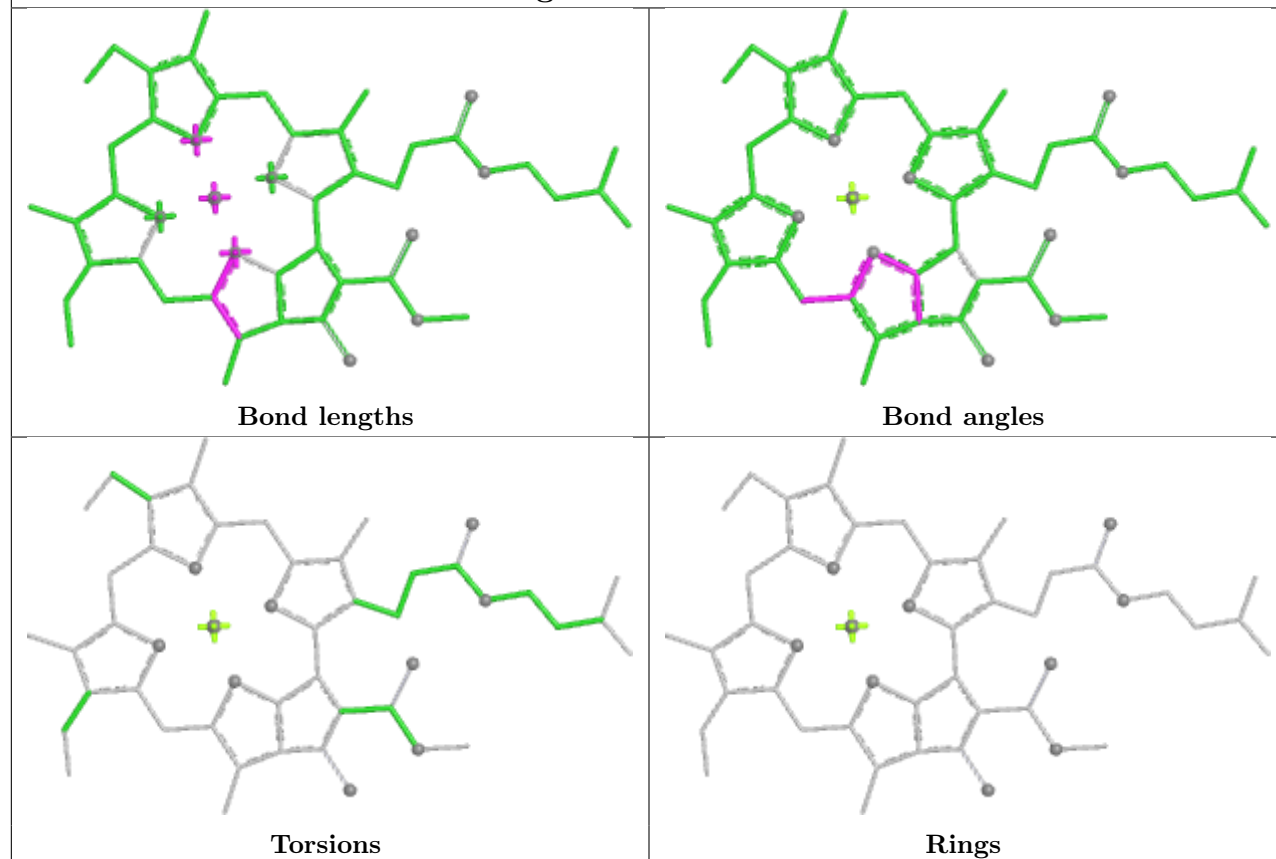
Ligand CHL 3 608



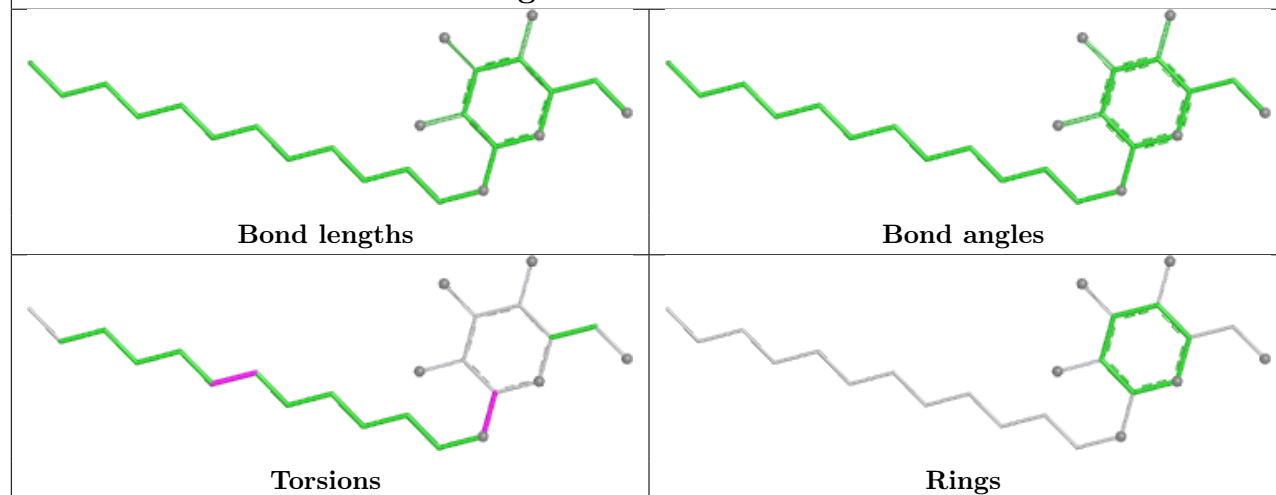


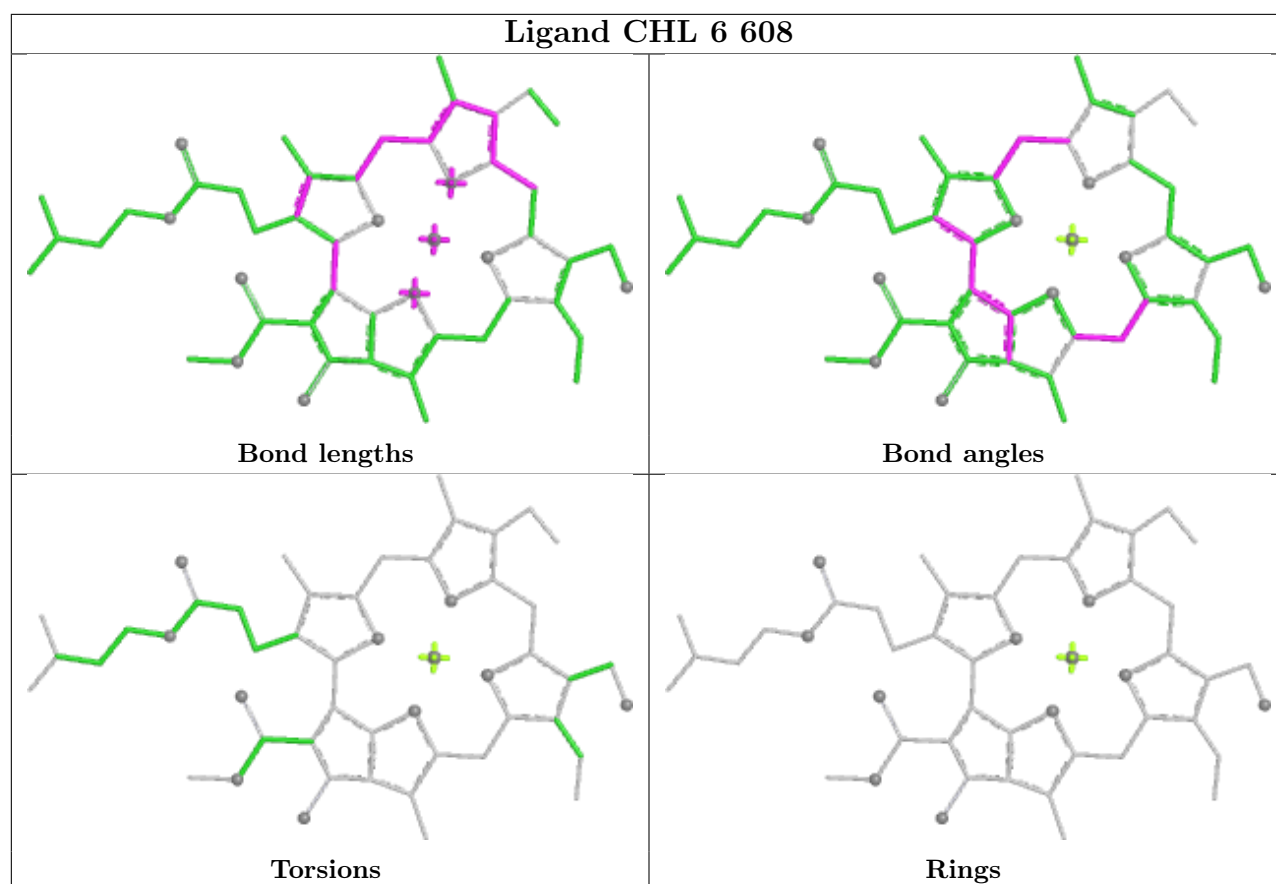


Ligand CLA 1 604

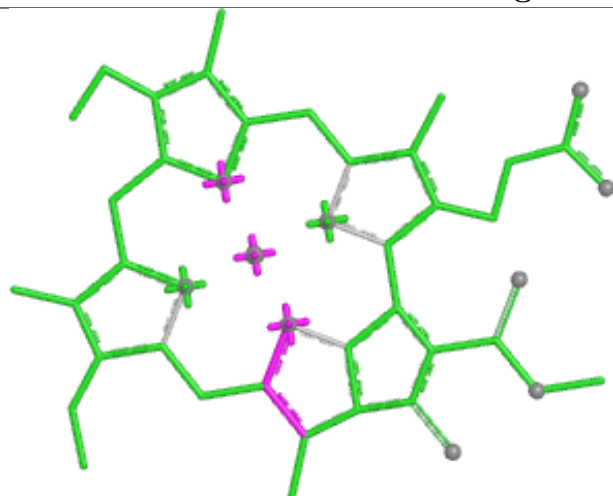


Ligand LMU K2 208

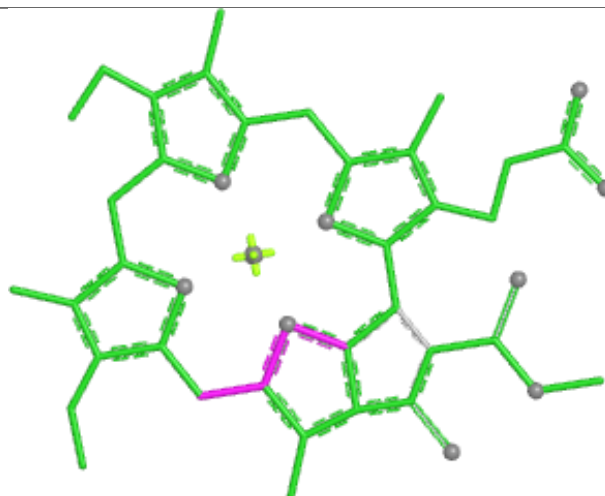




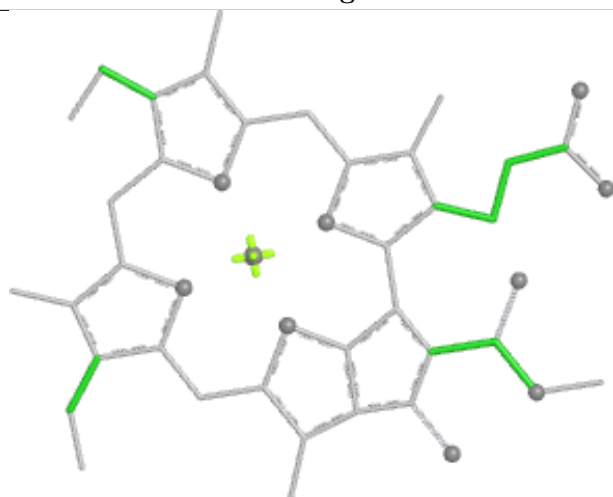
Ligand CLA B 835



Bond lengths



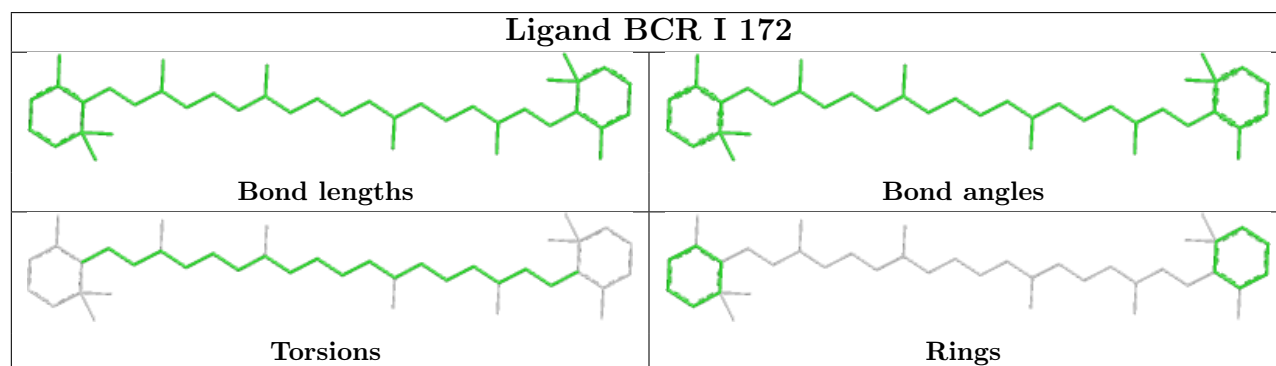
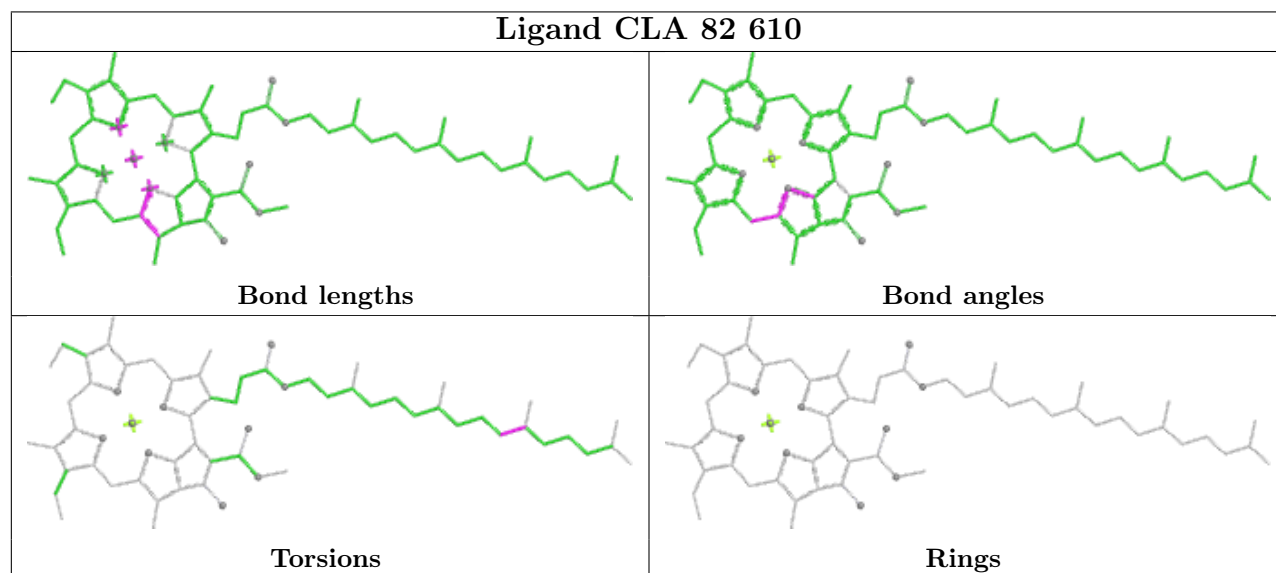
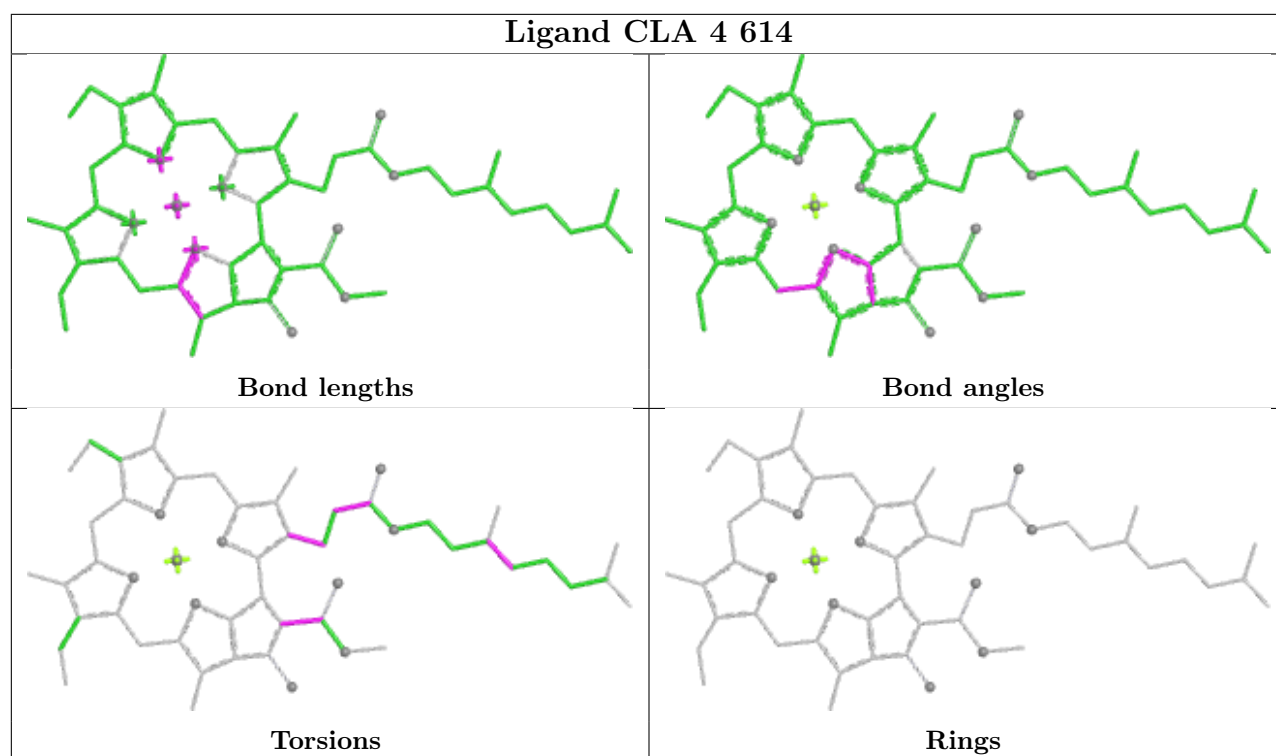
Bond angles

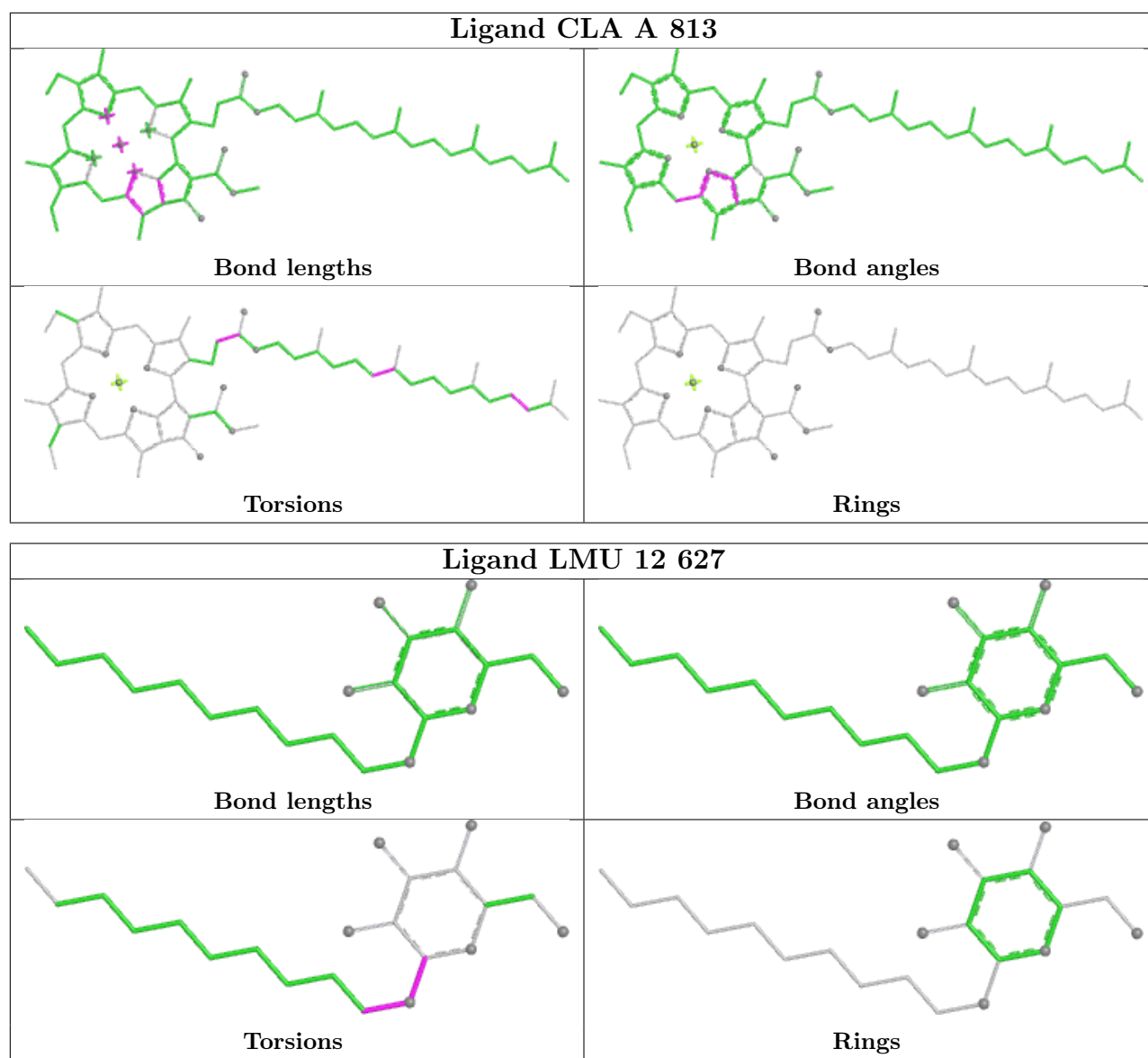


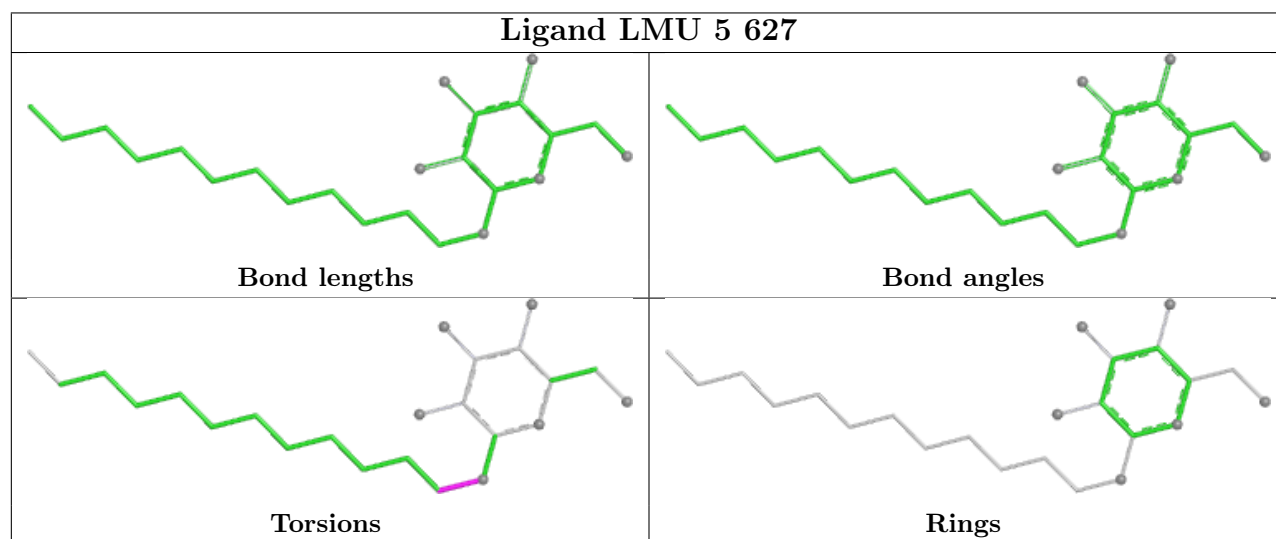
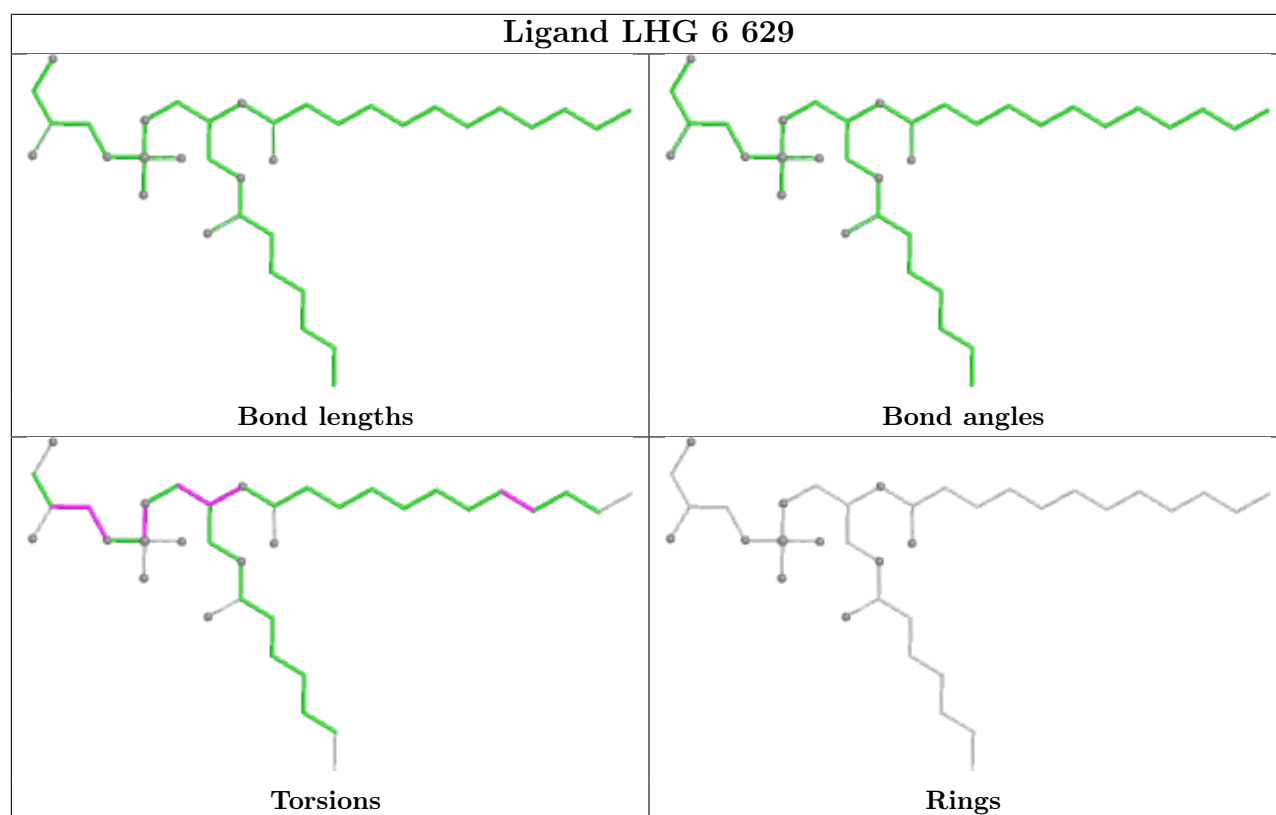
Torsions

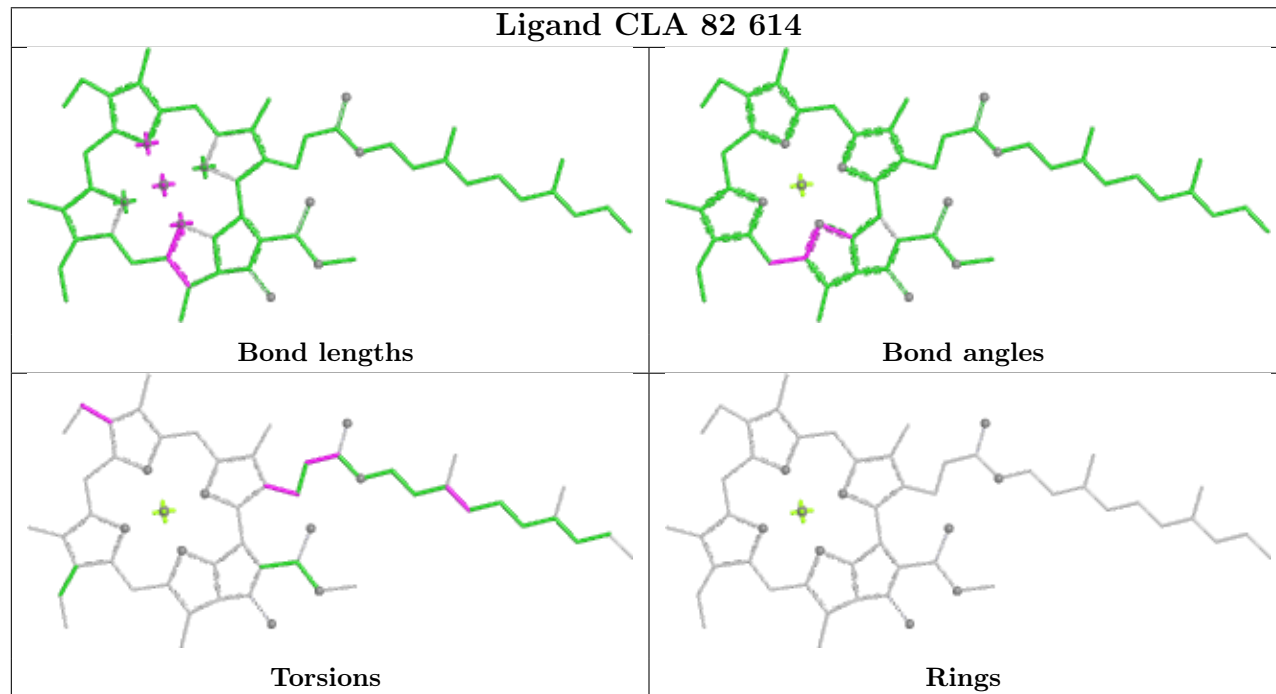
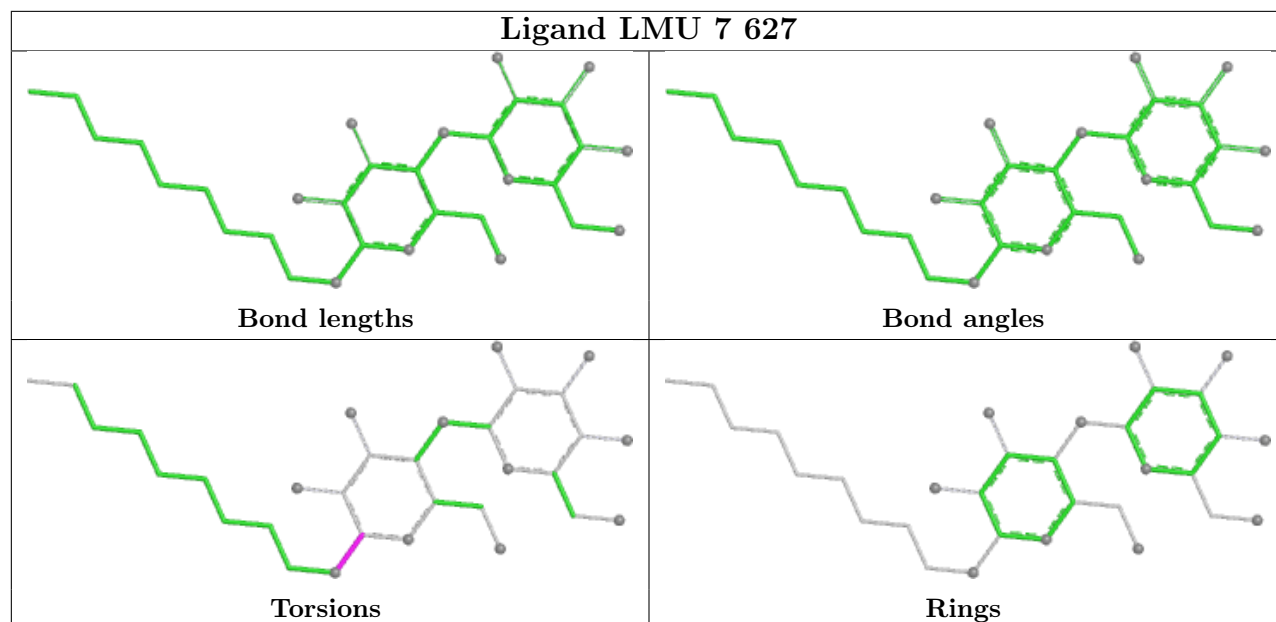


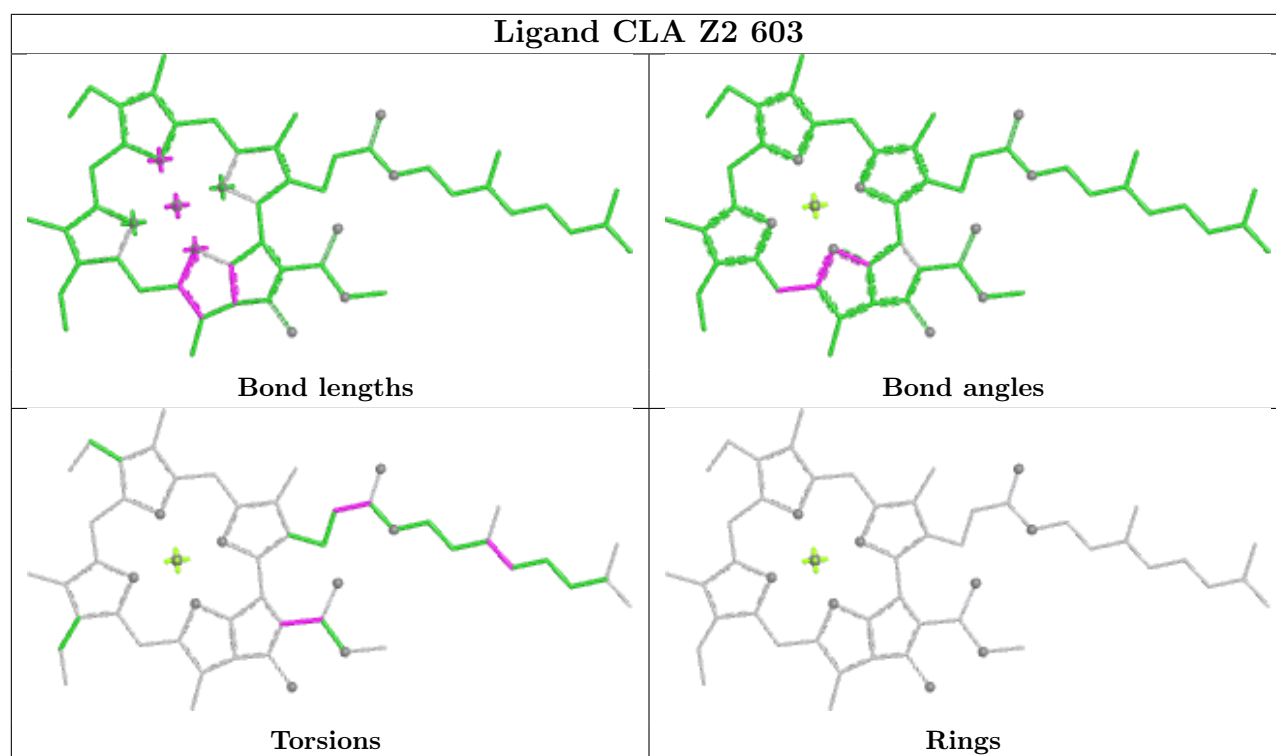
Rings

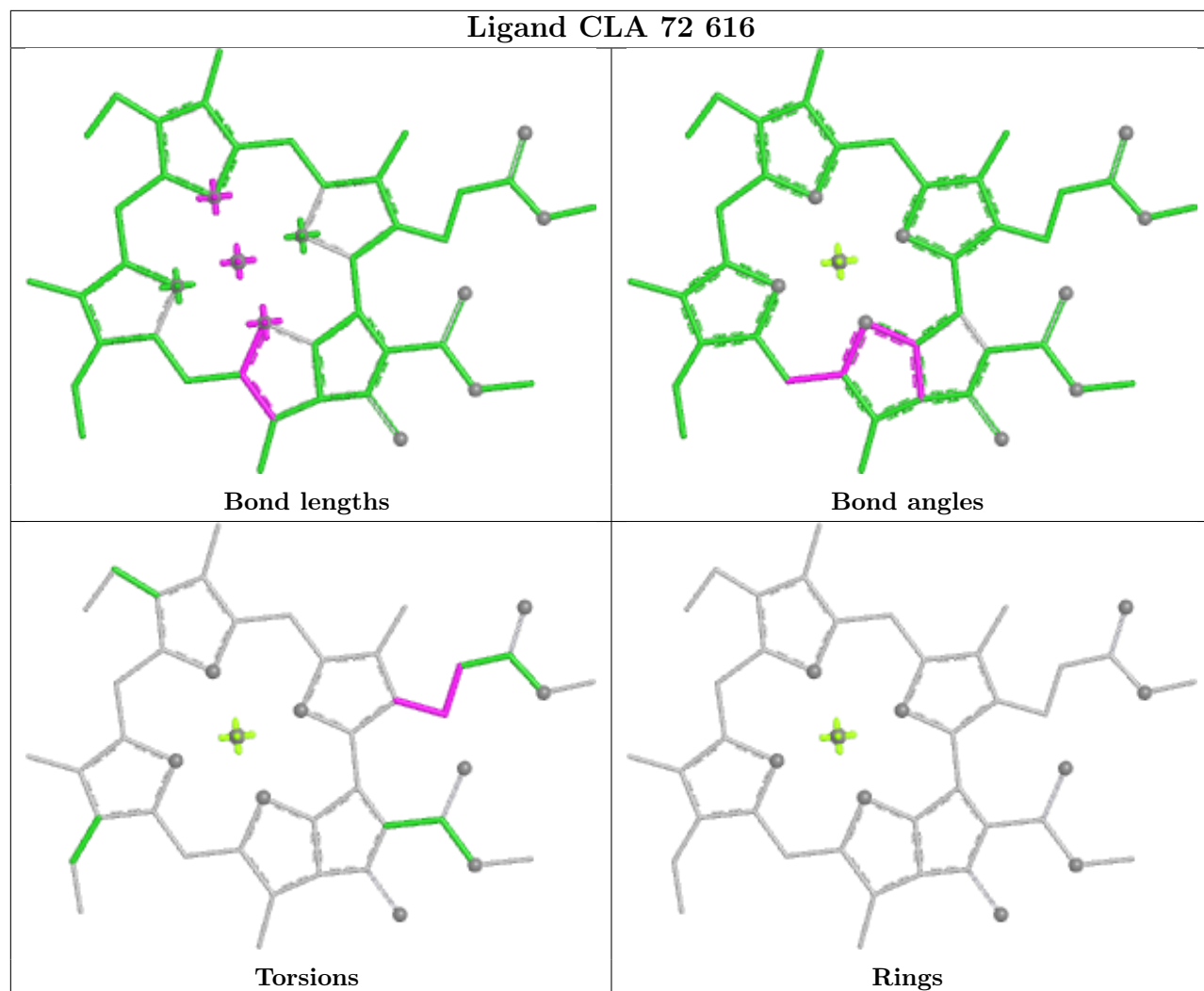


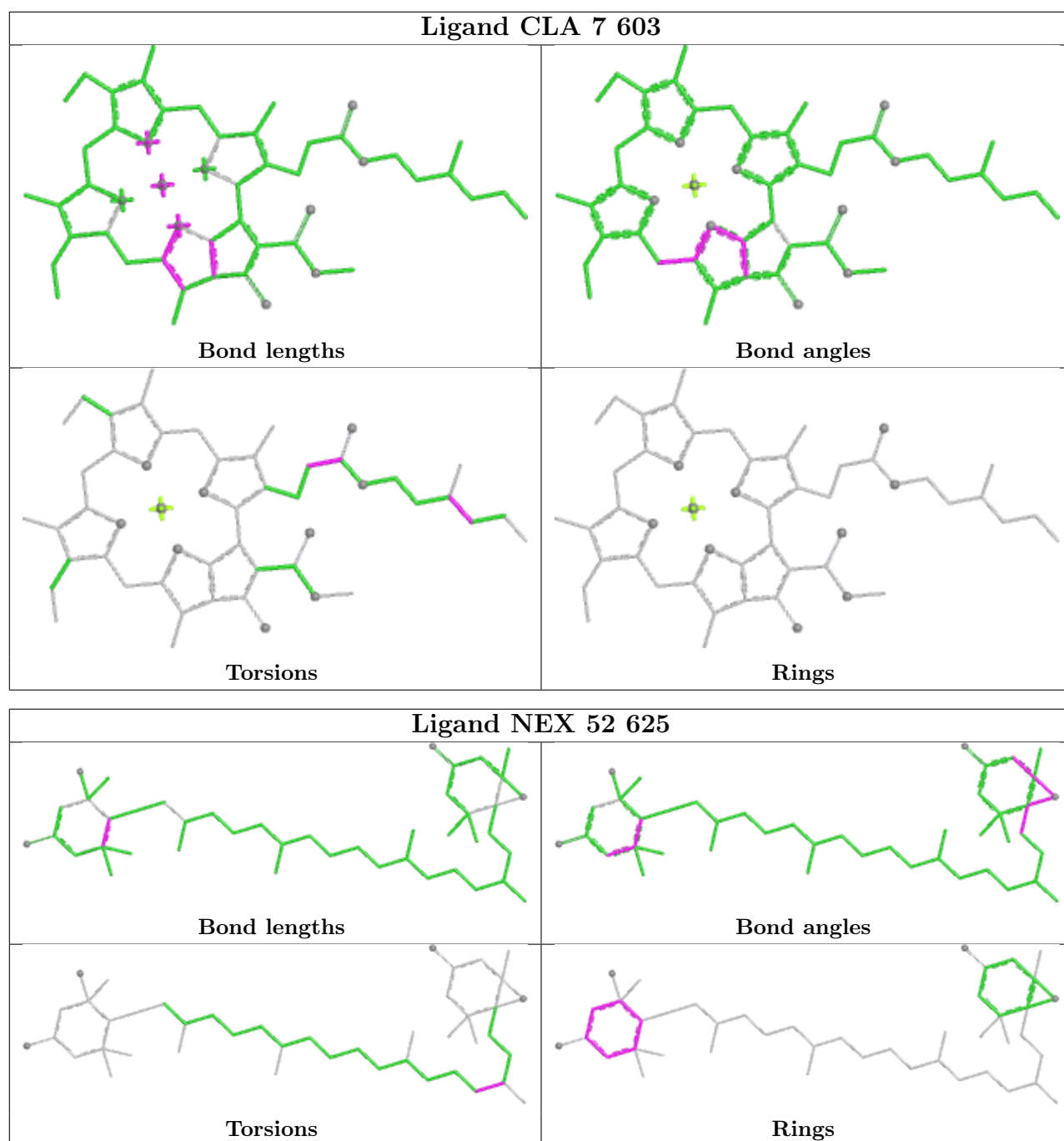




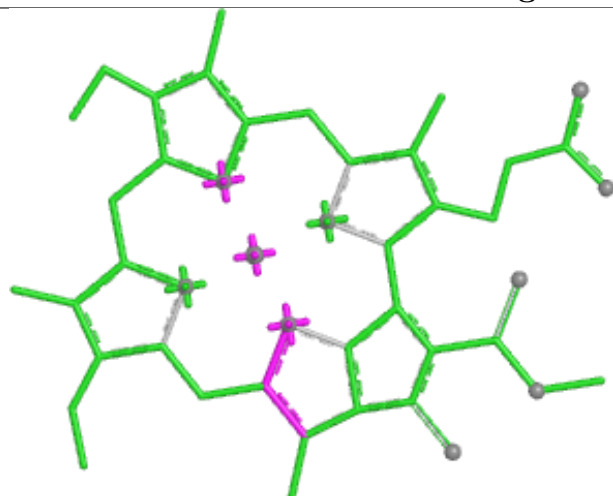




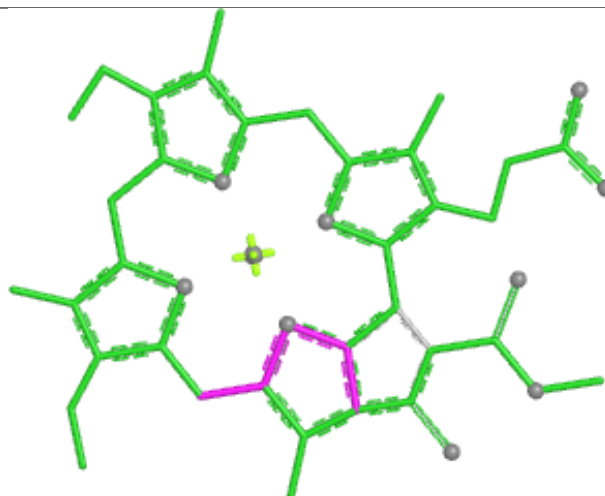




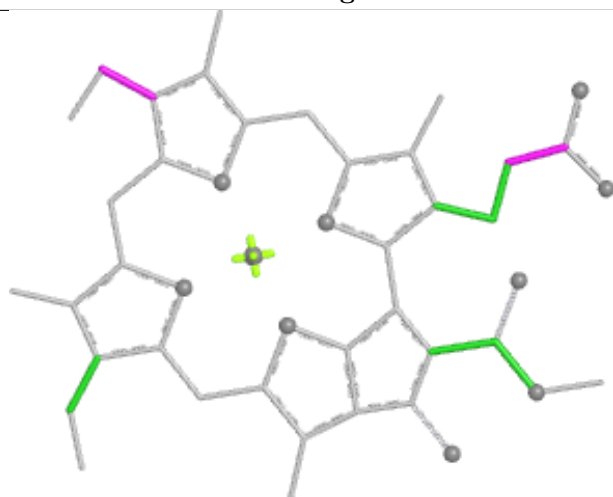
Ligand CLA 9 614



Bond lengths



Bond angles

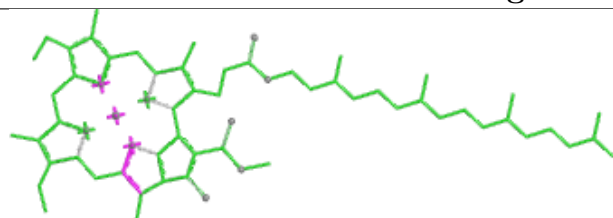


Torsions

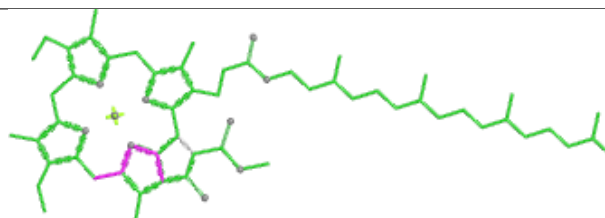


Rings

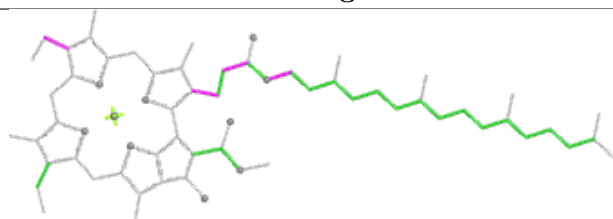
Ligand CLA F2 304



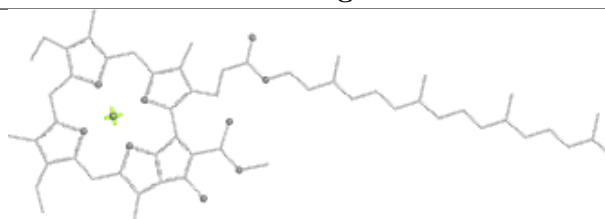
Bond lengths



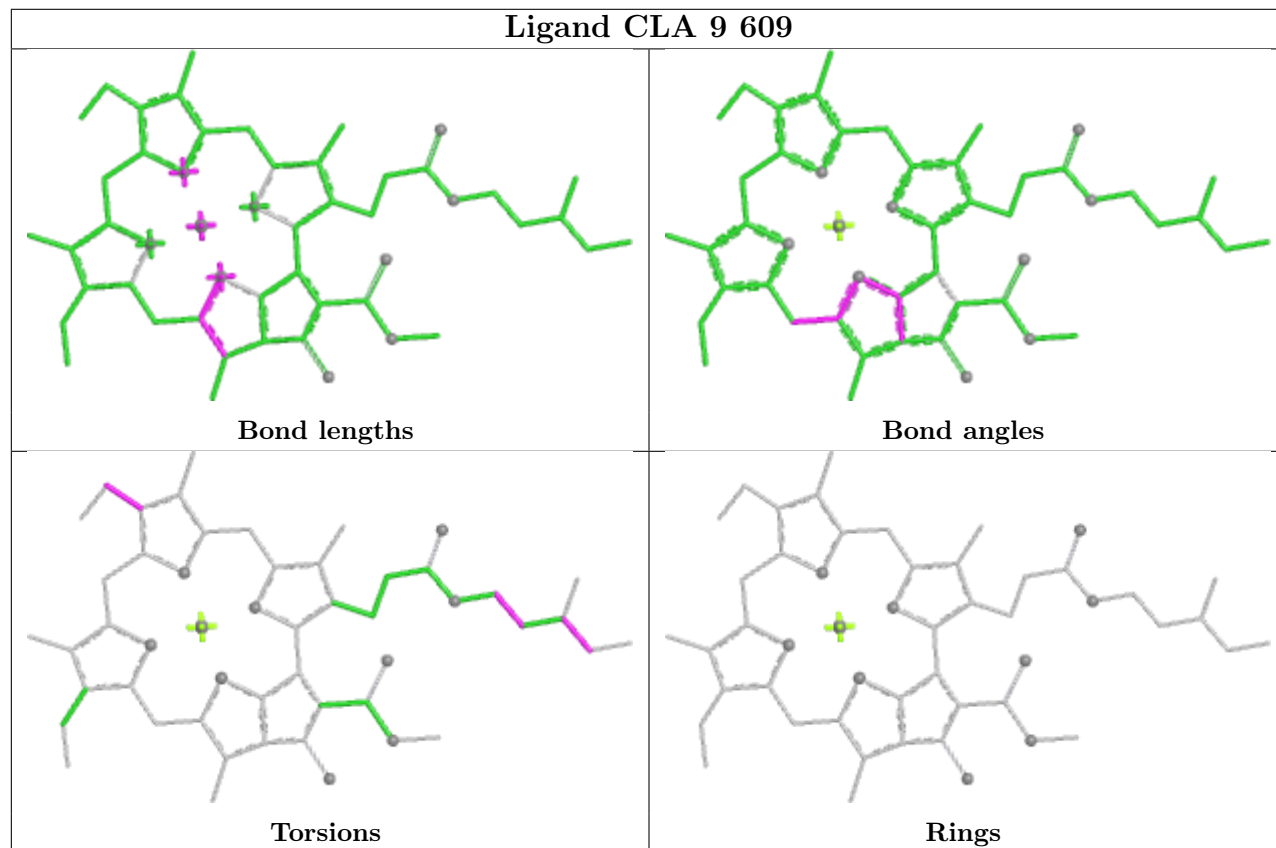
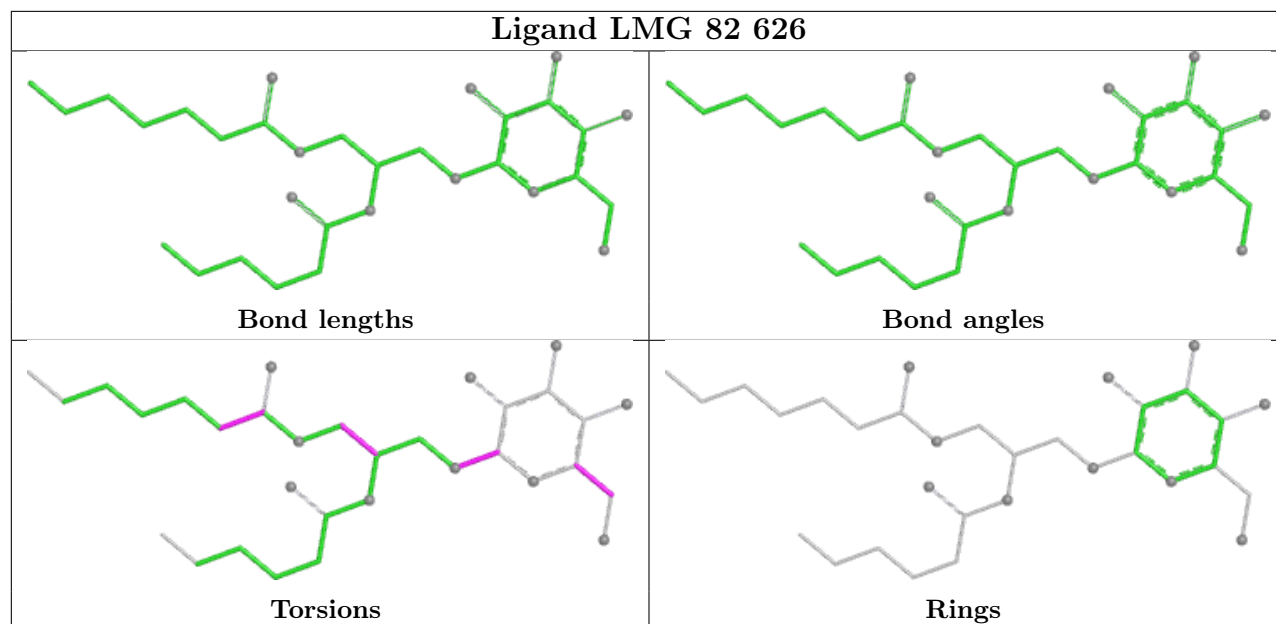
Bond angles

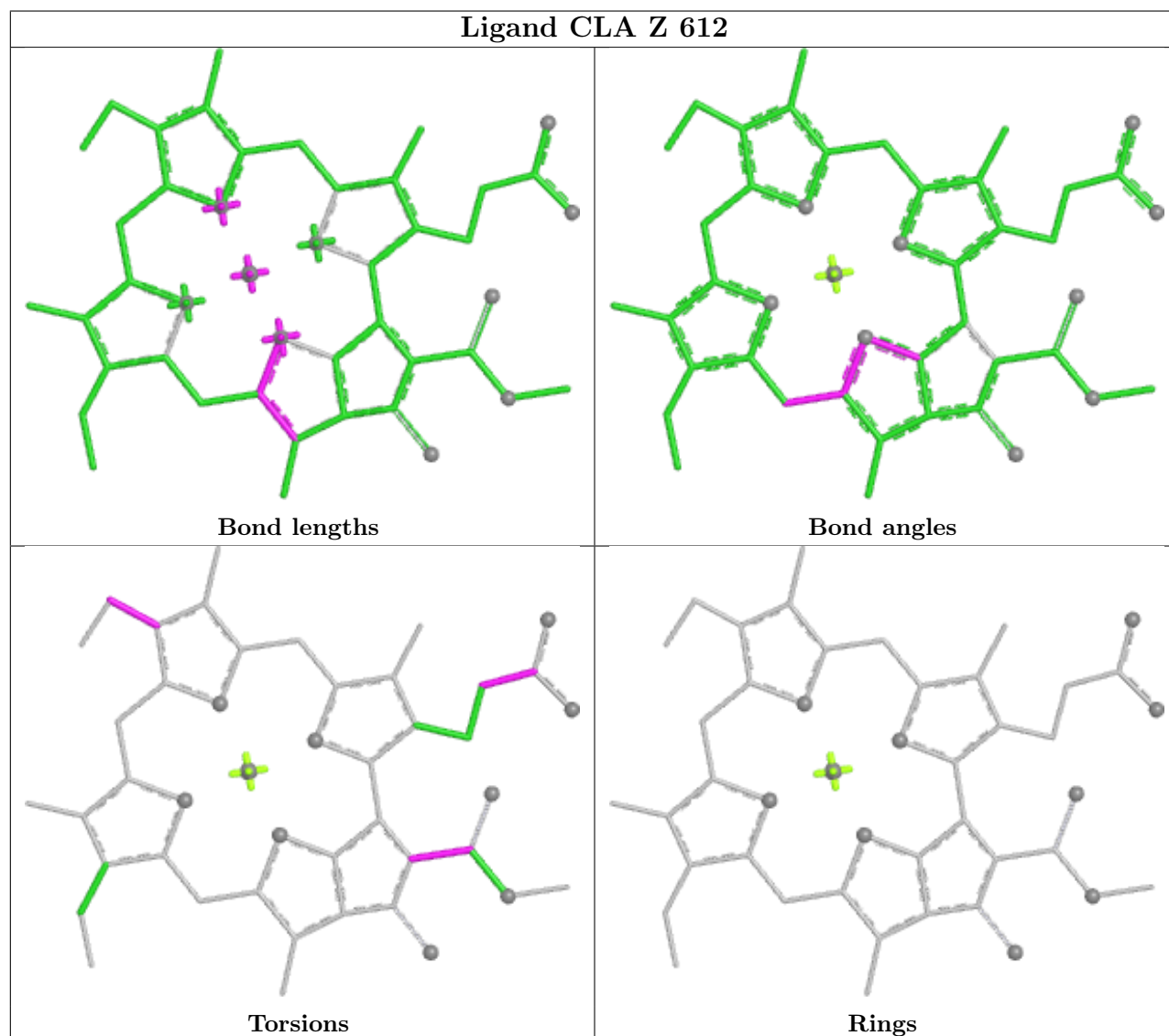
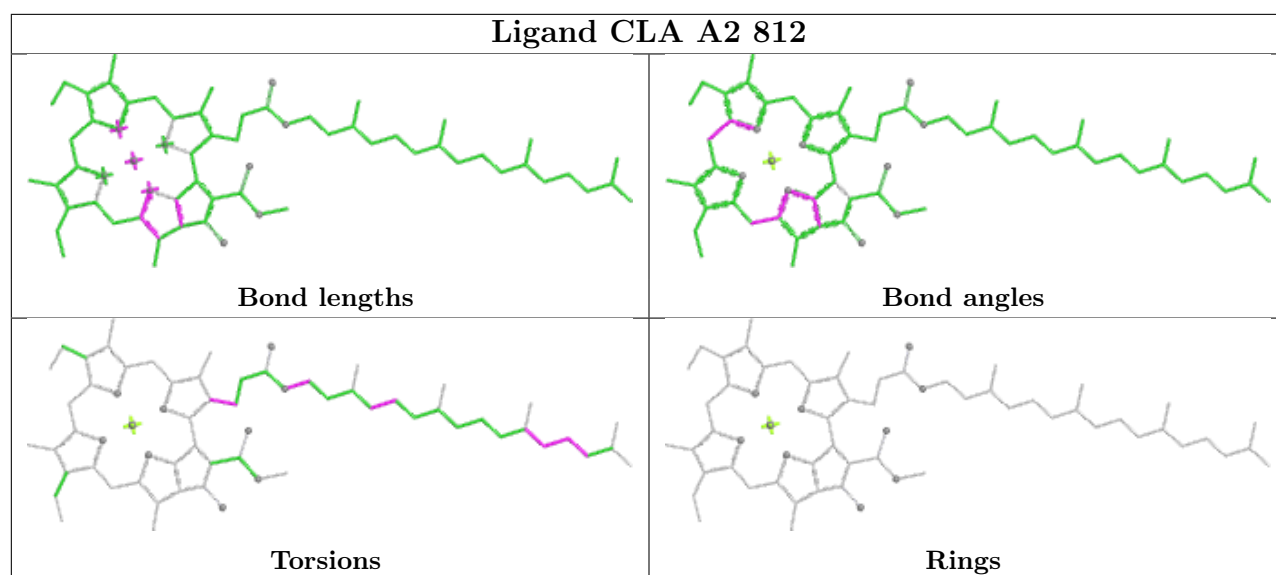


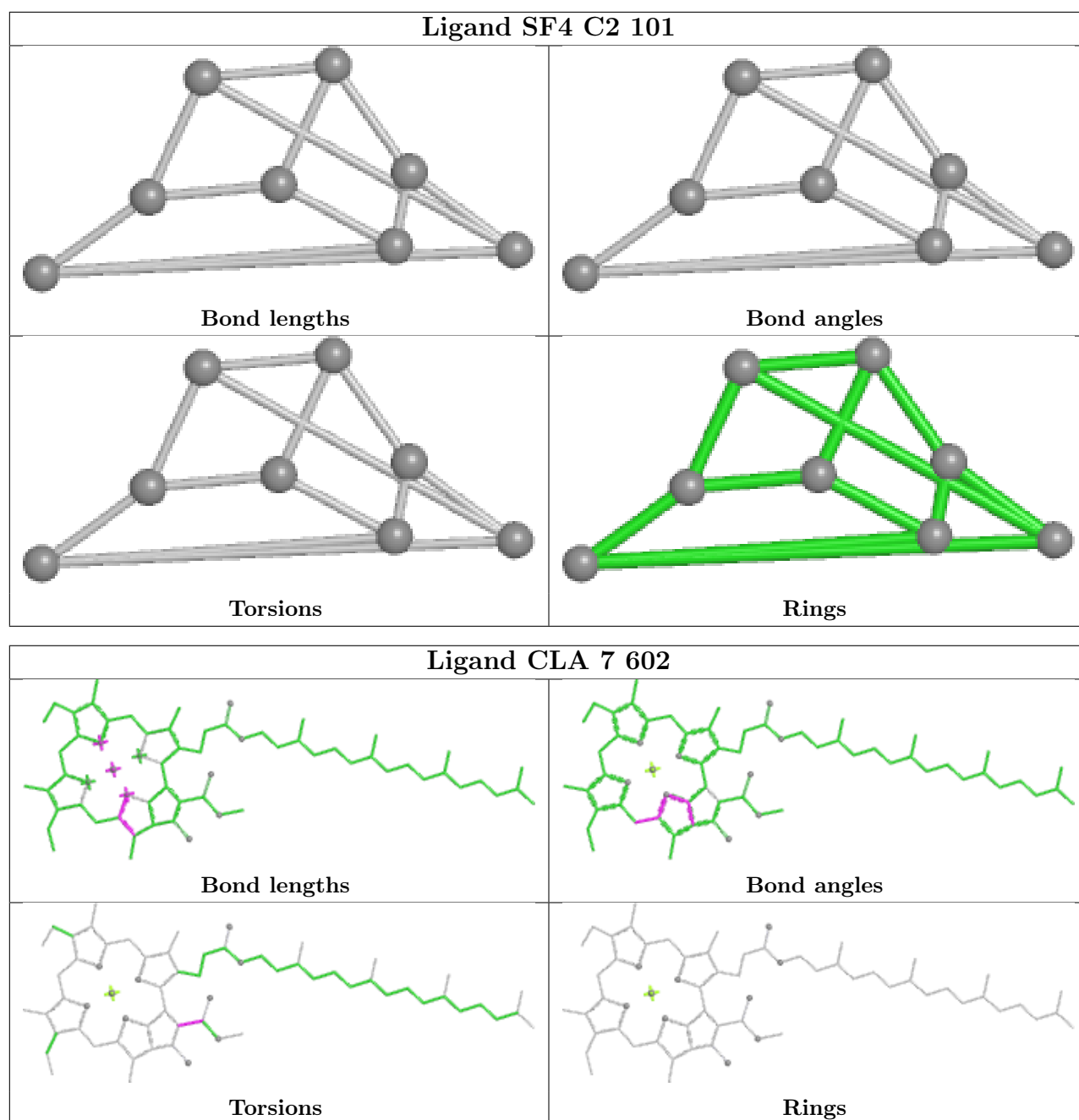
Torsions

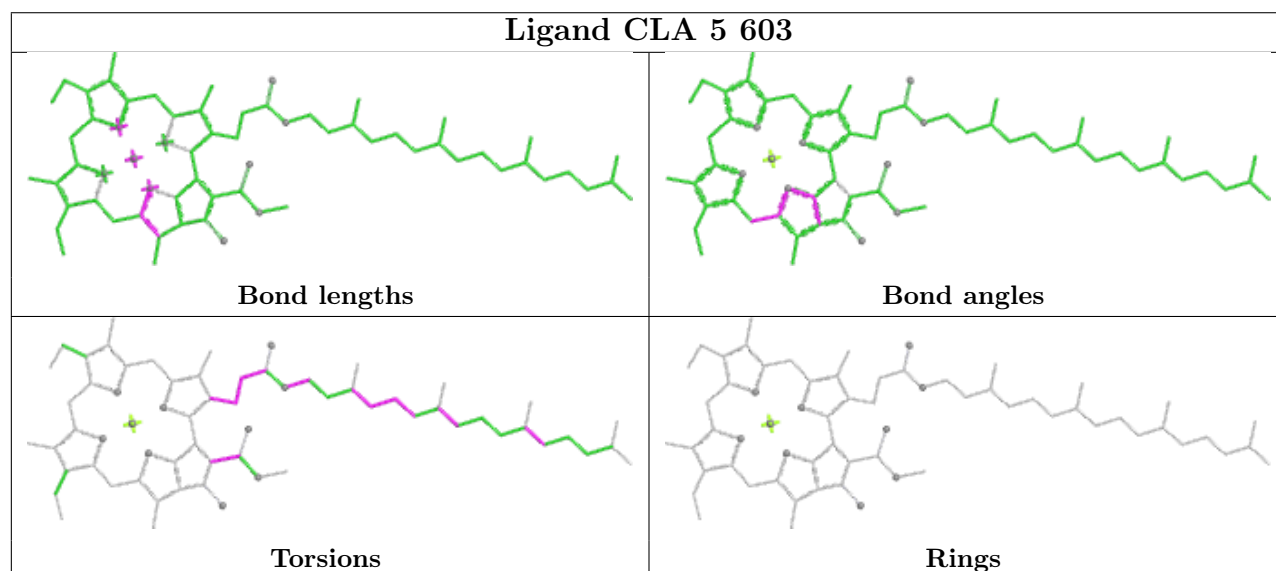
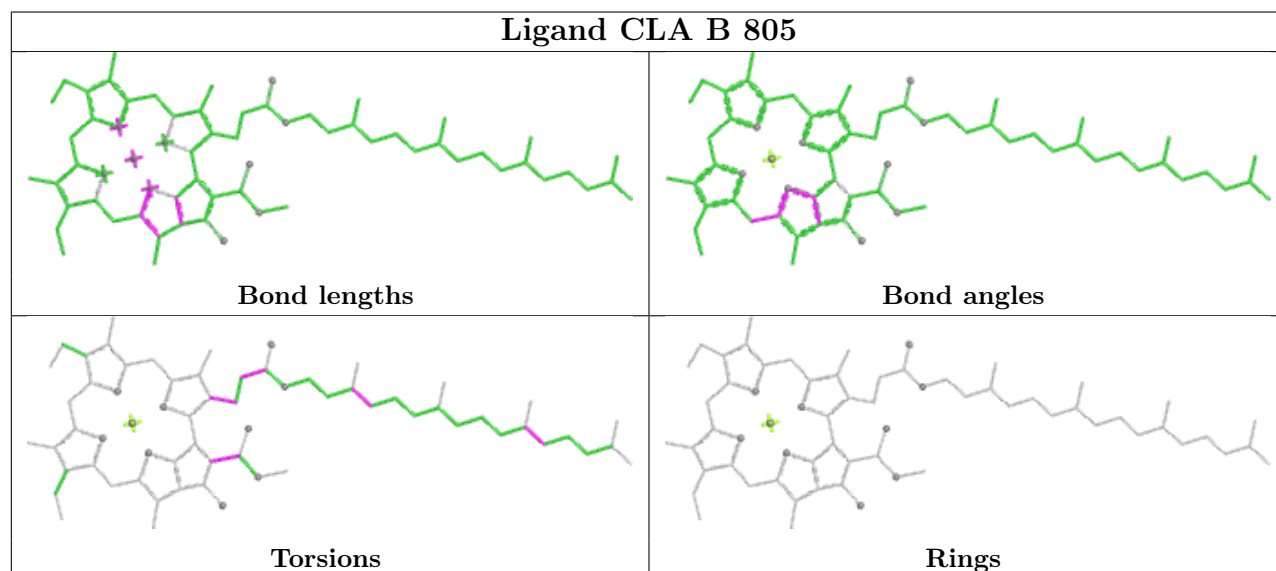
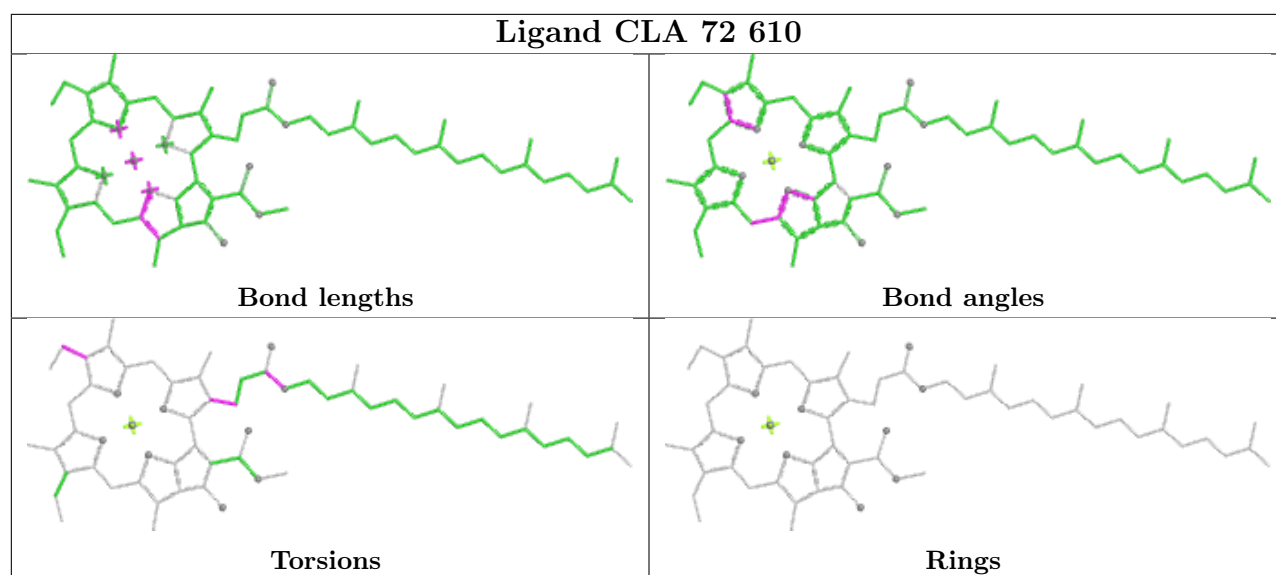


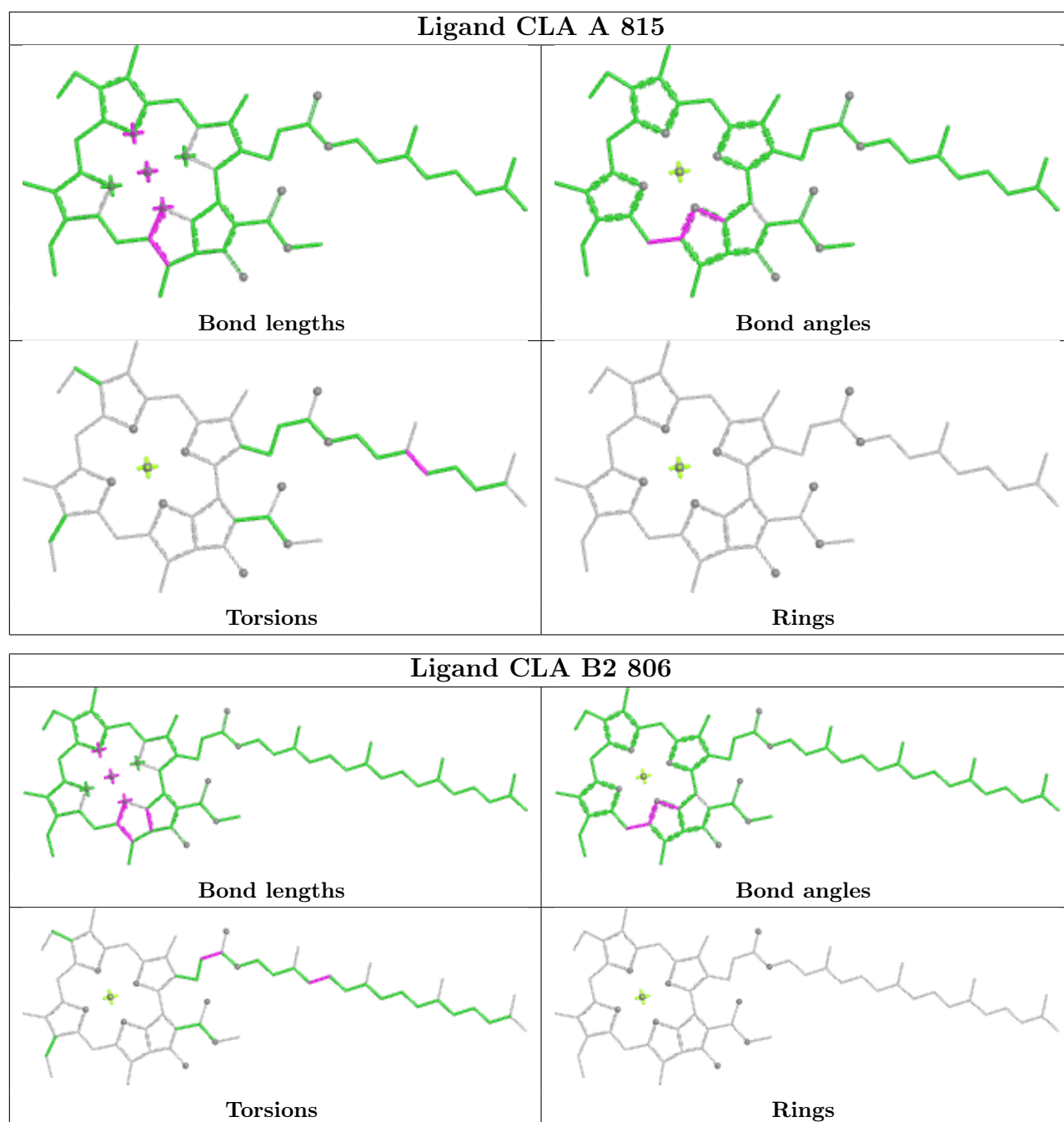
Rings

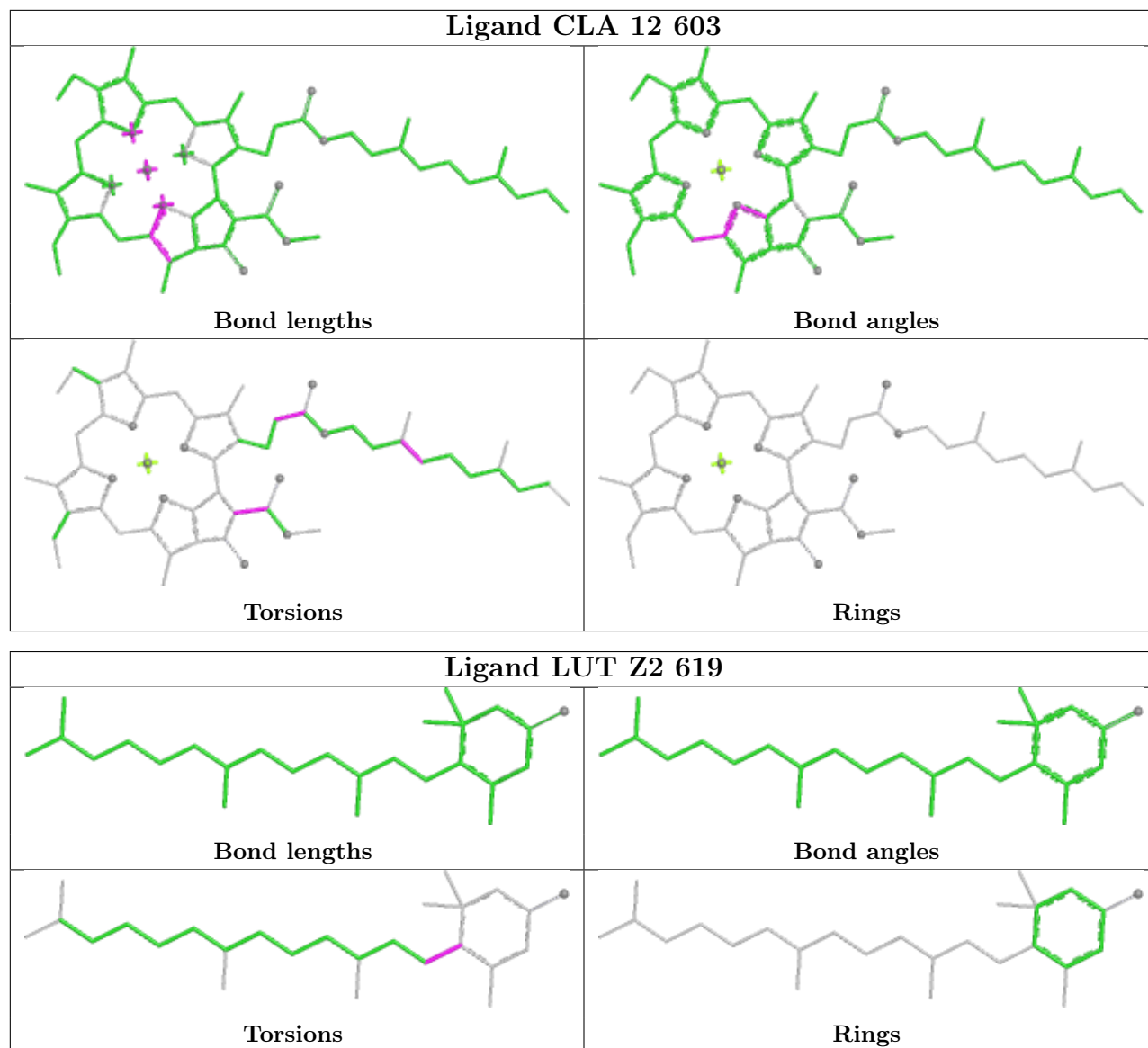


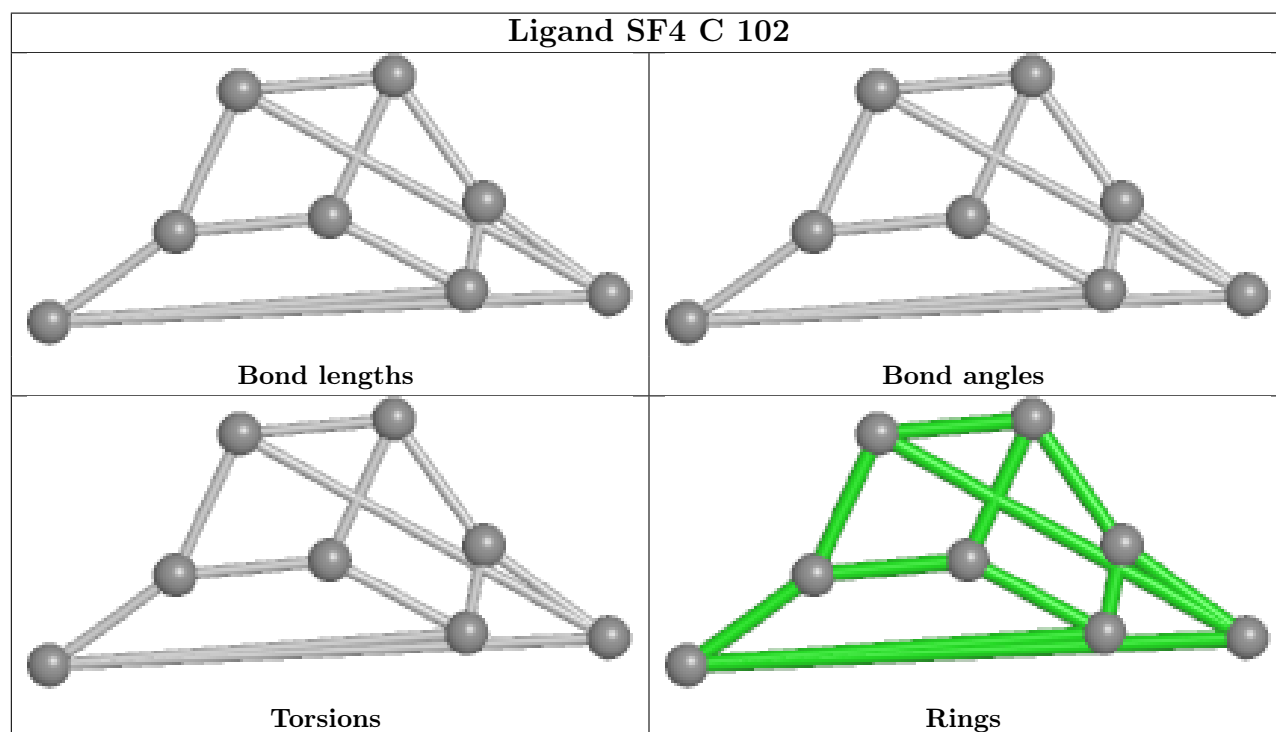
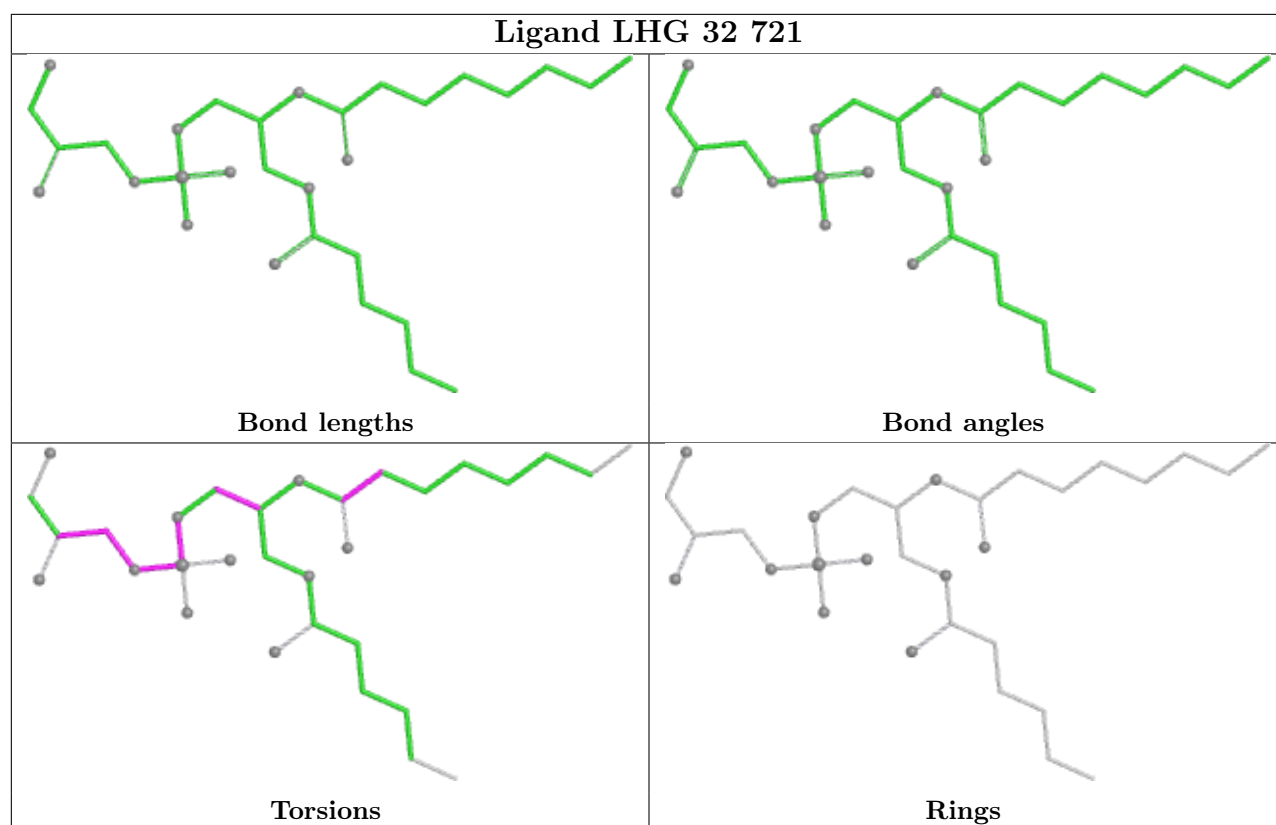




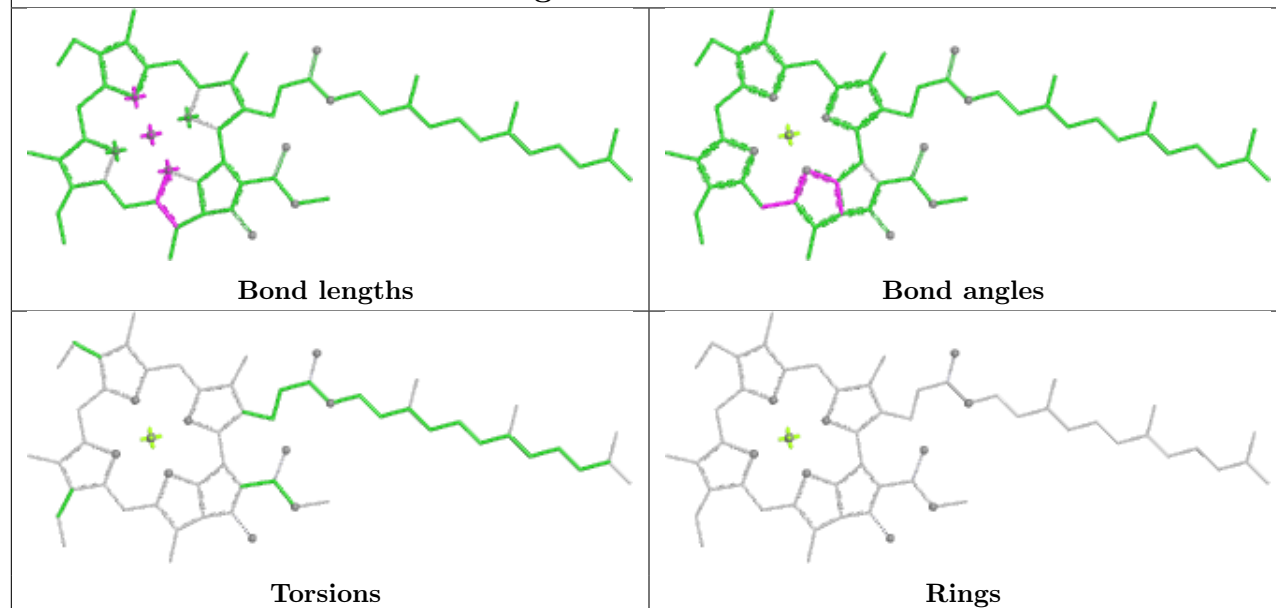




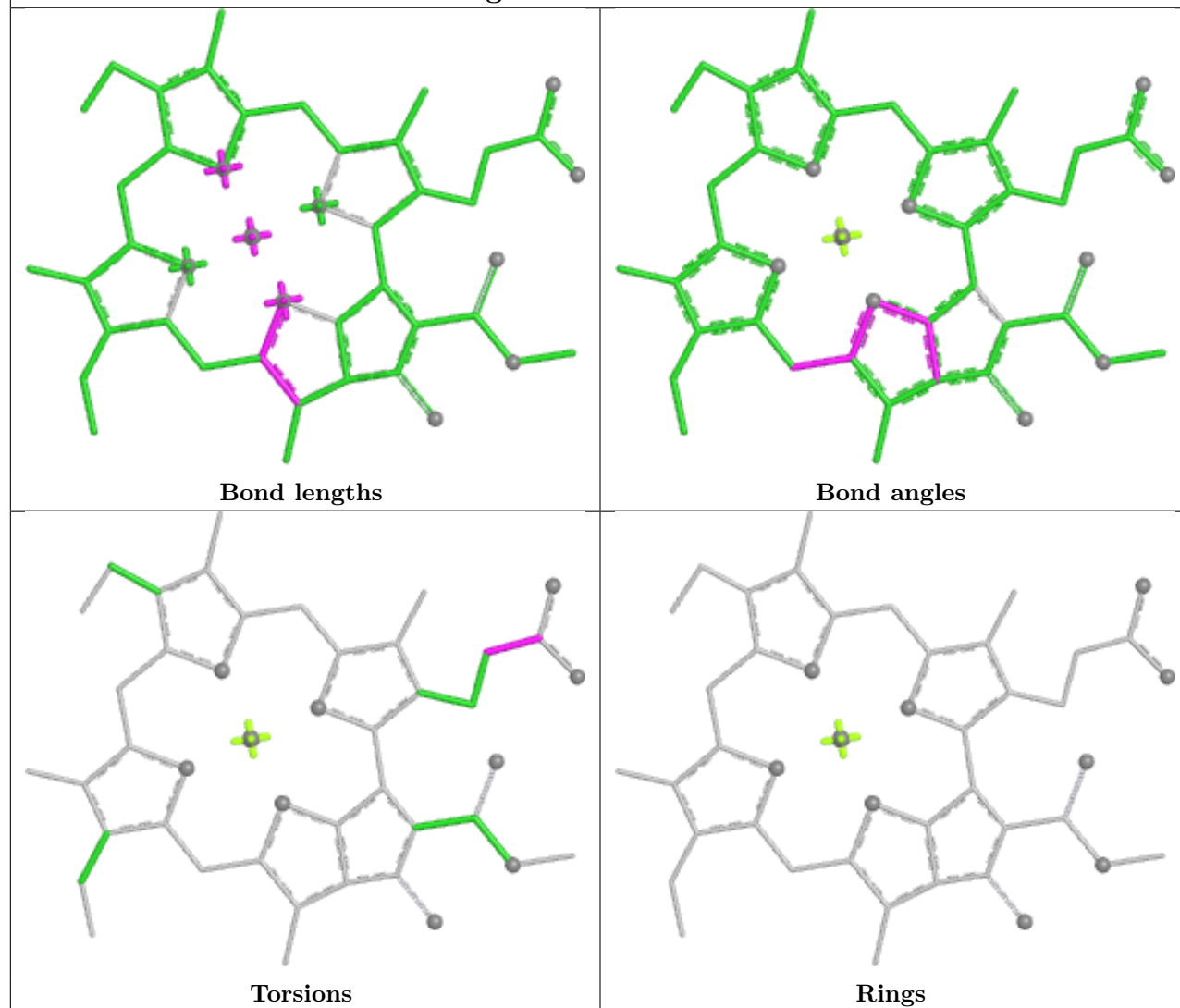


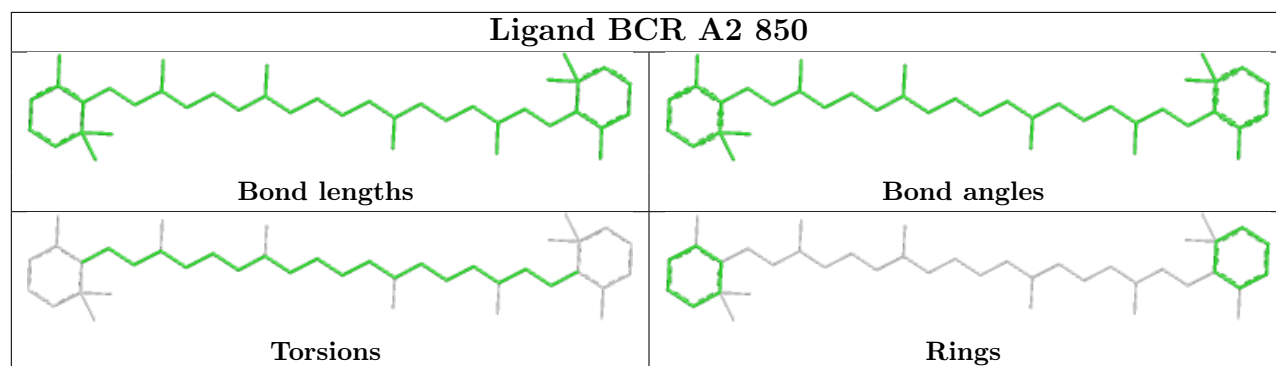
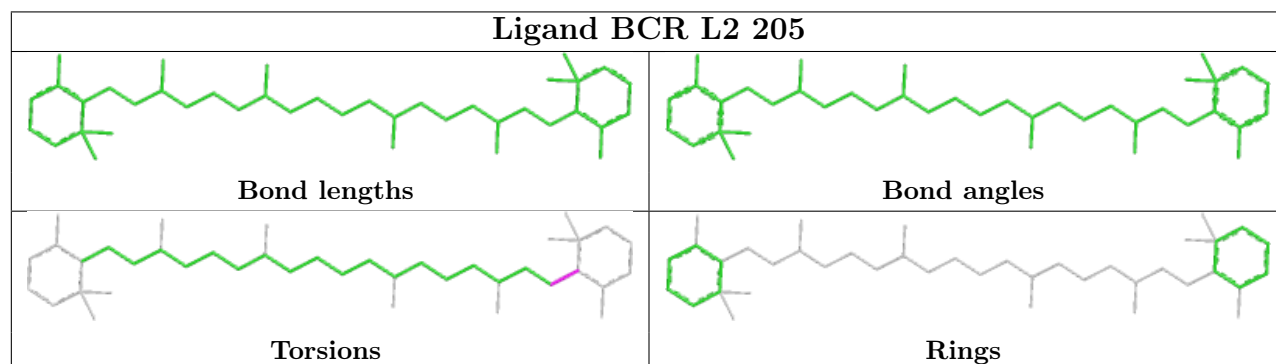
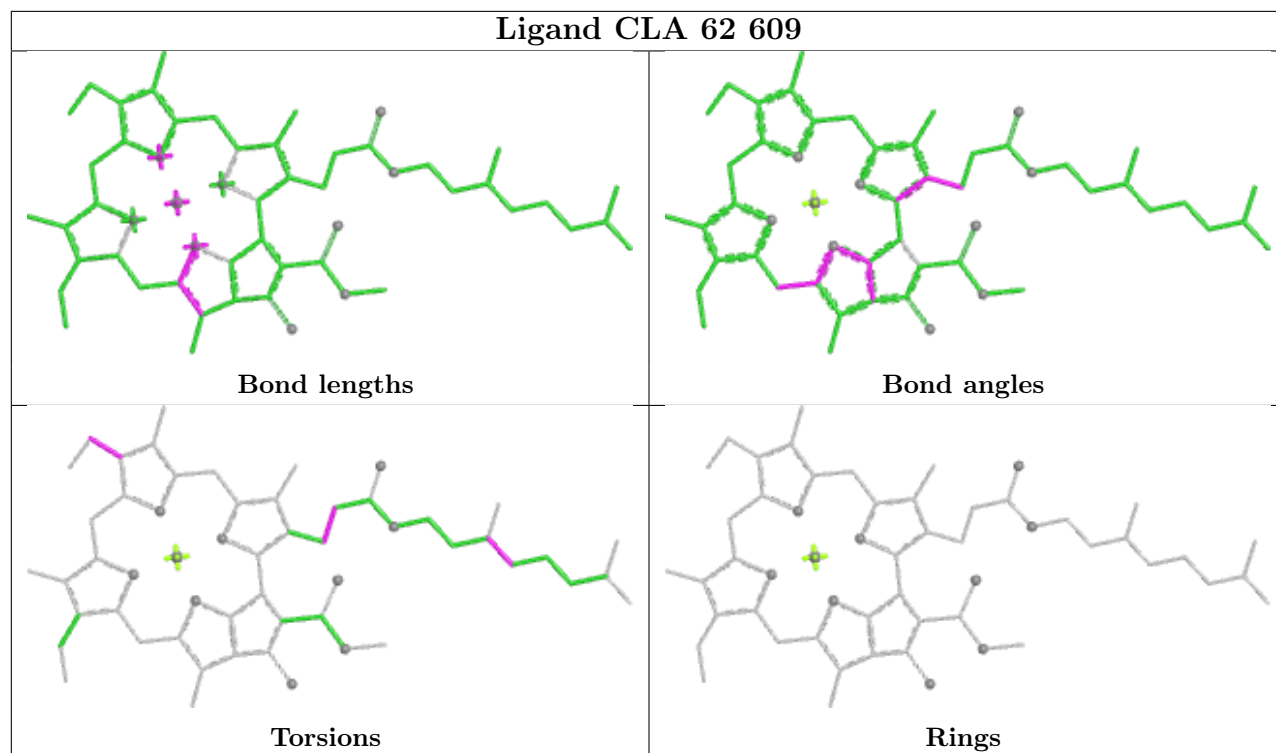


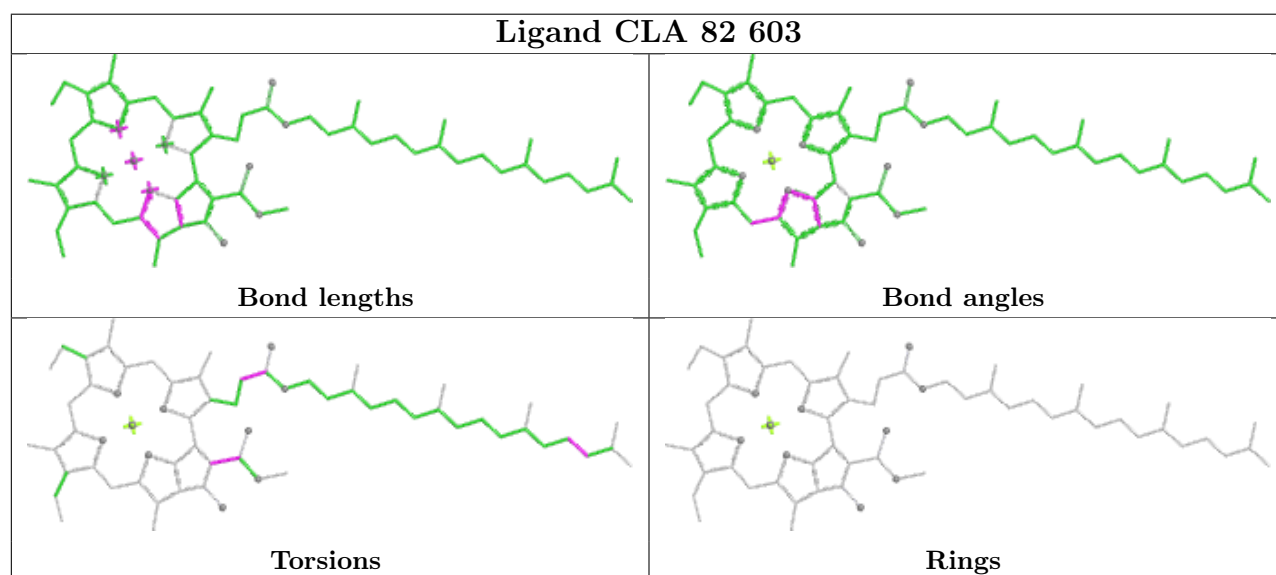
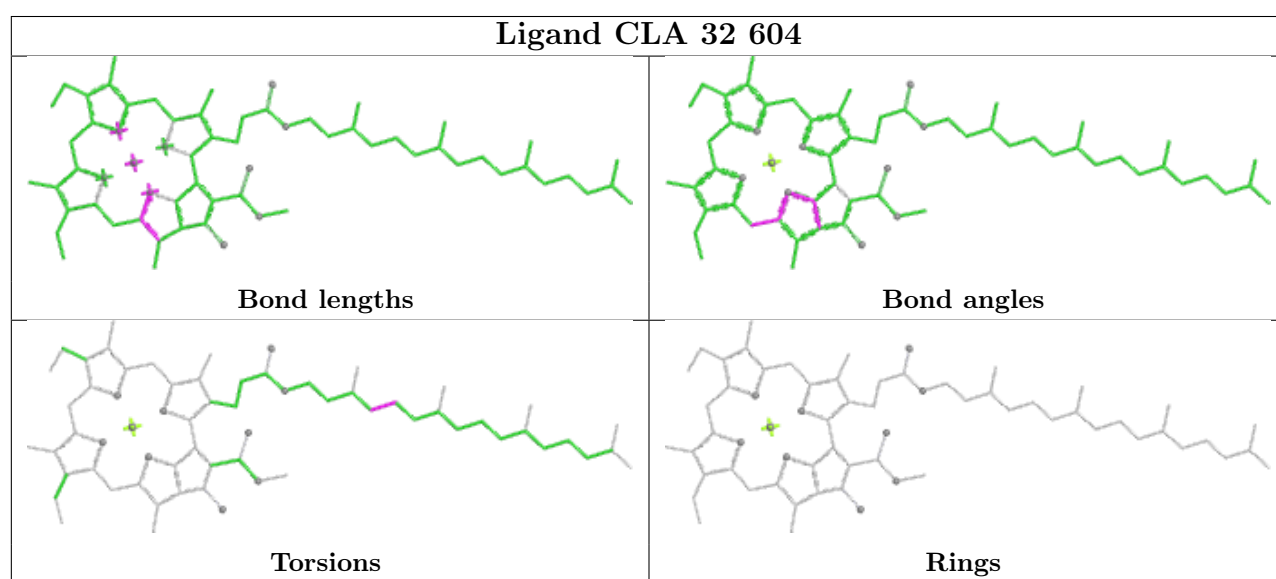
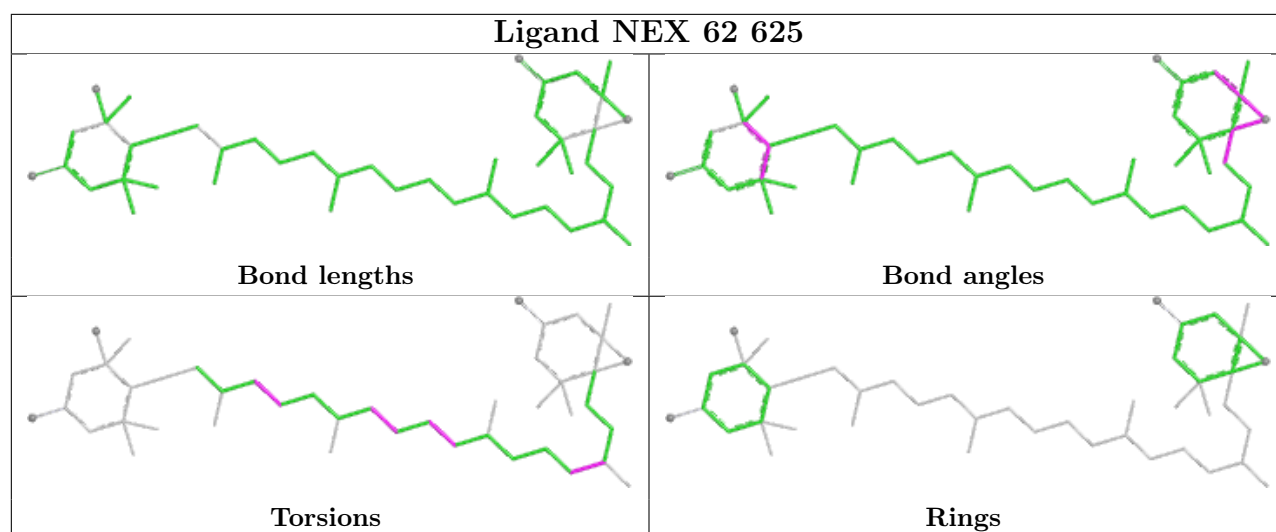
Ligand CLA Z 610

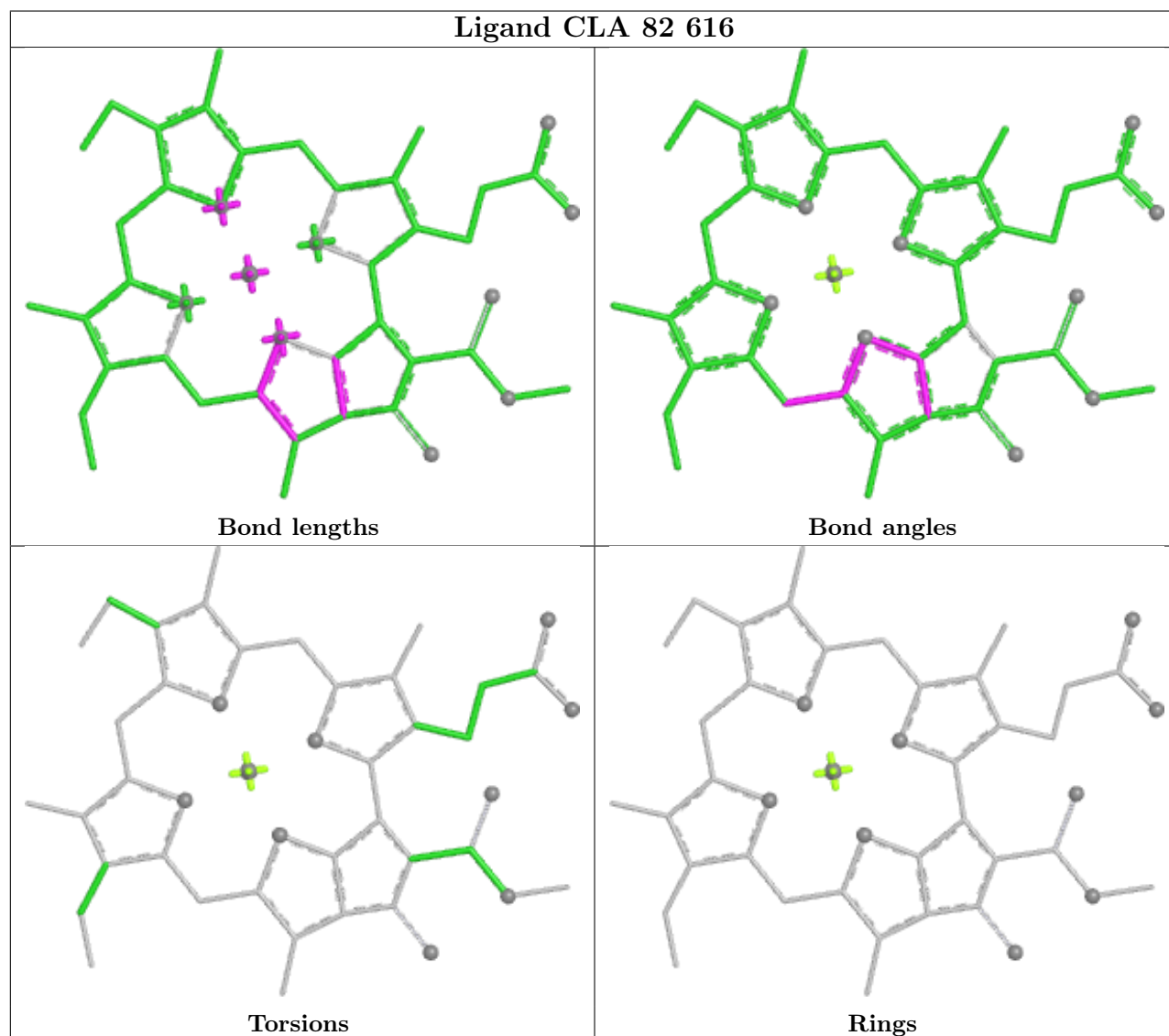
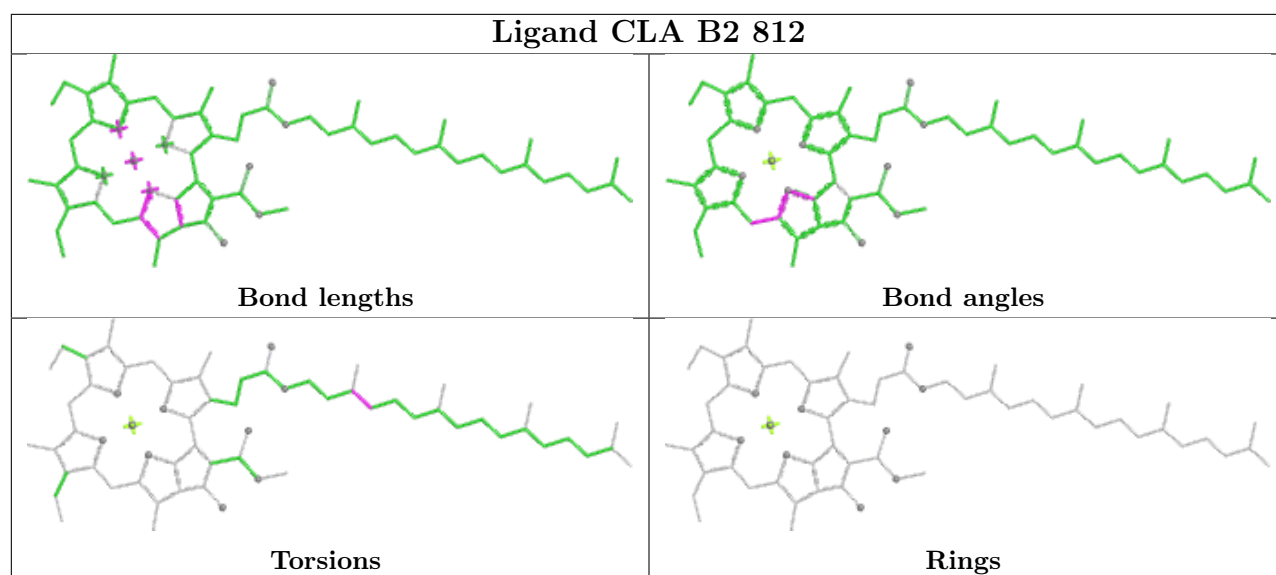


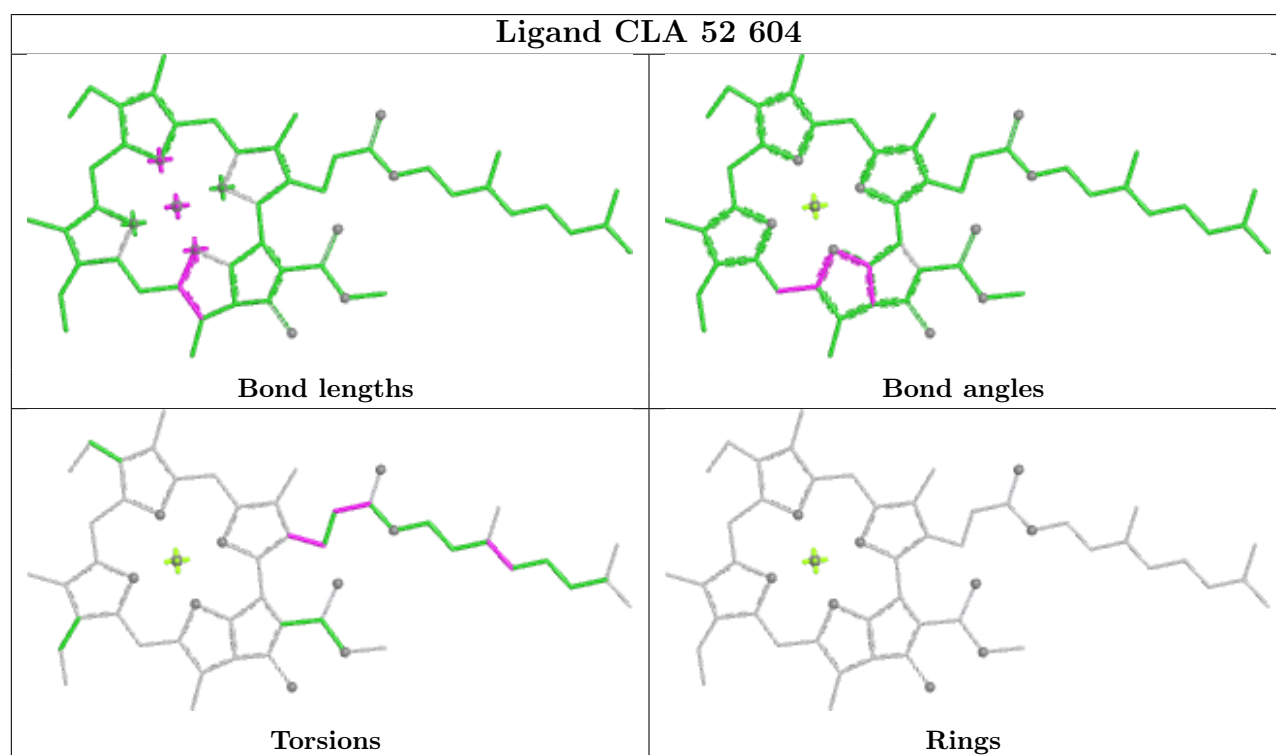
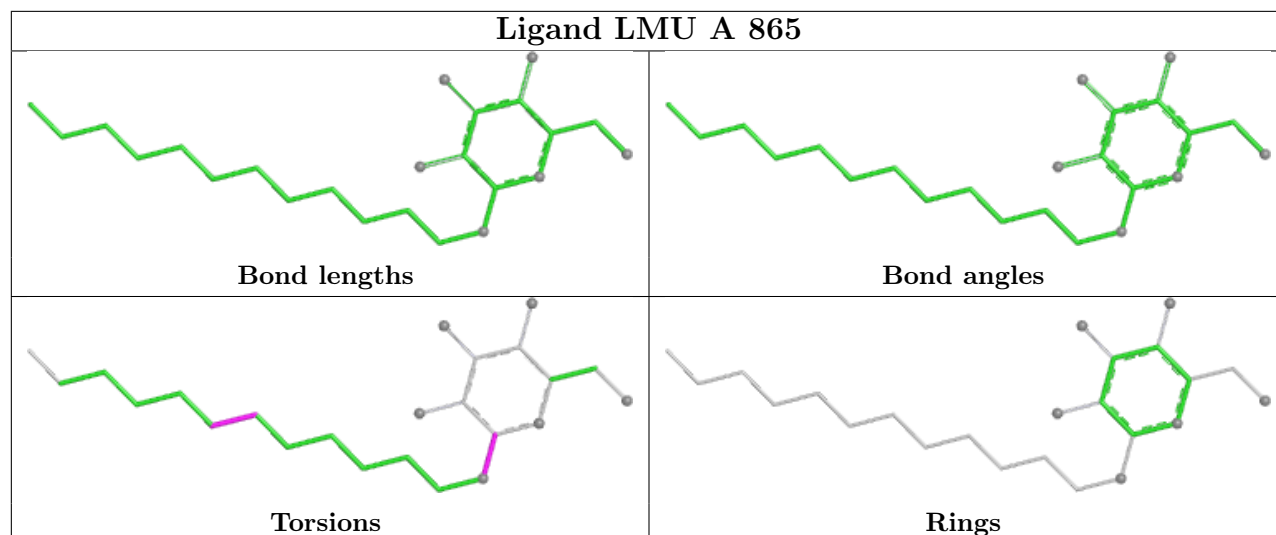
Ligand CLA L2 204

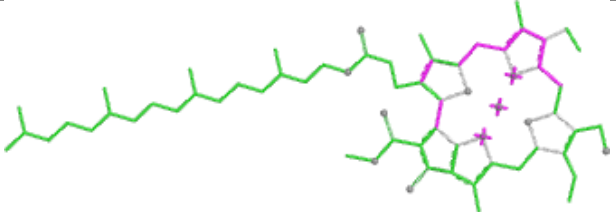
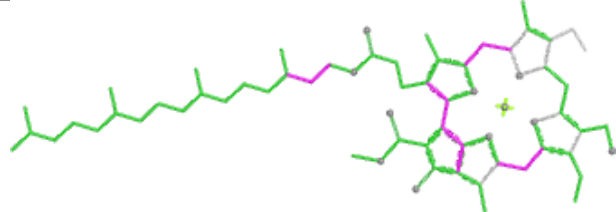
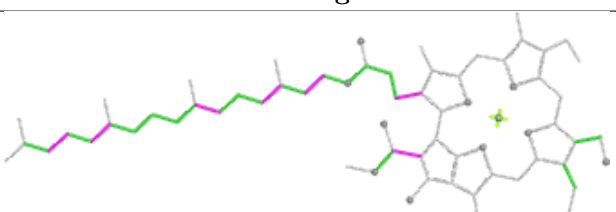
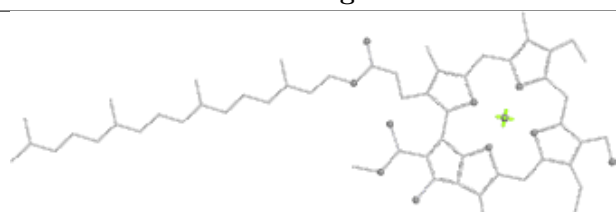


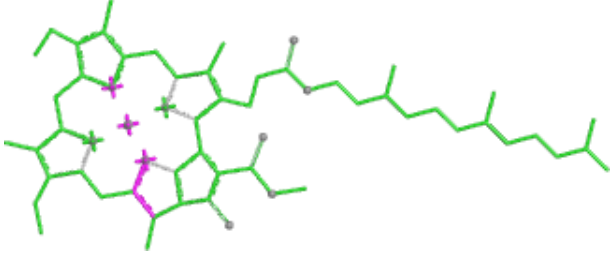
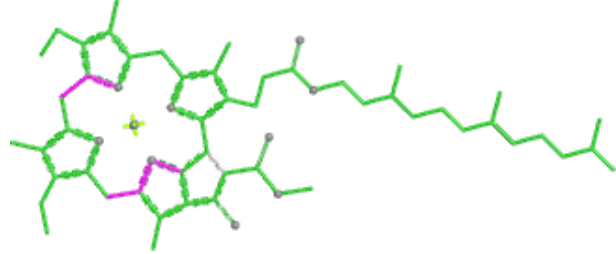
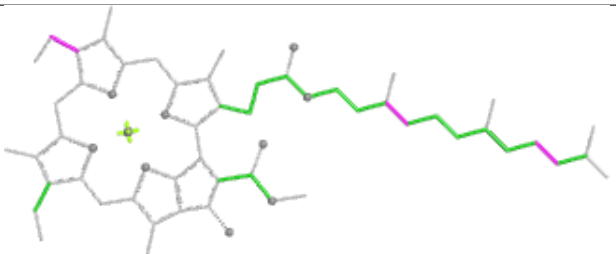
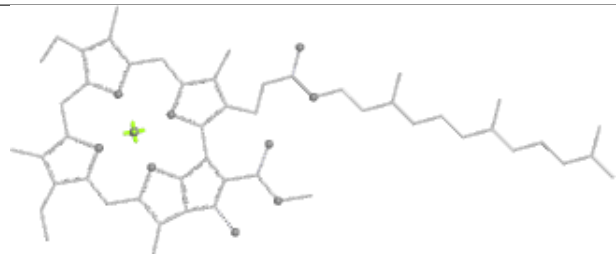


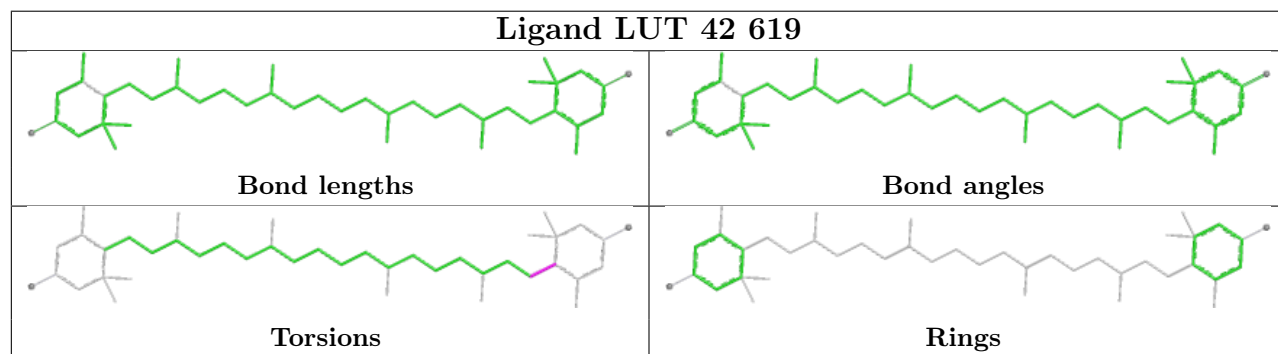
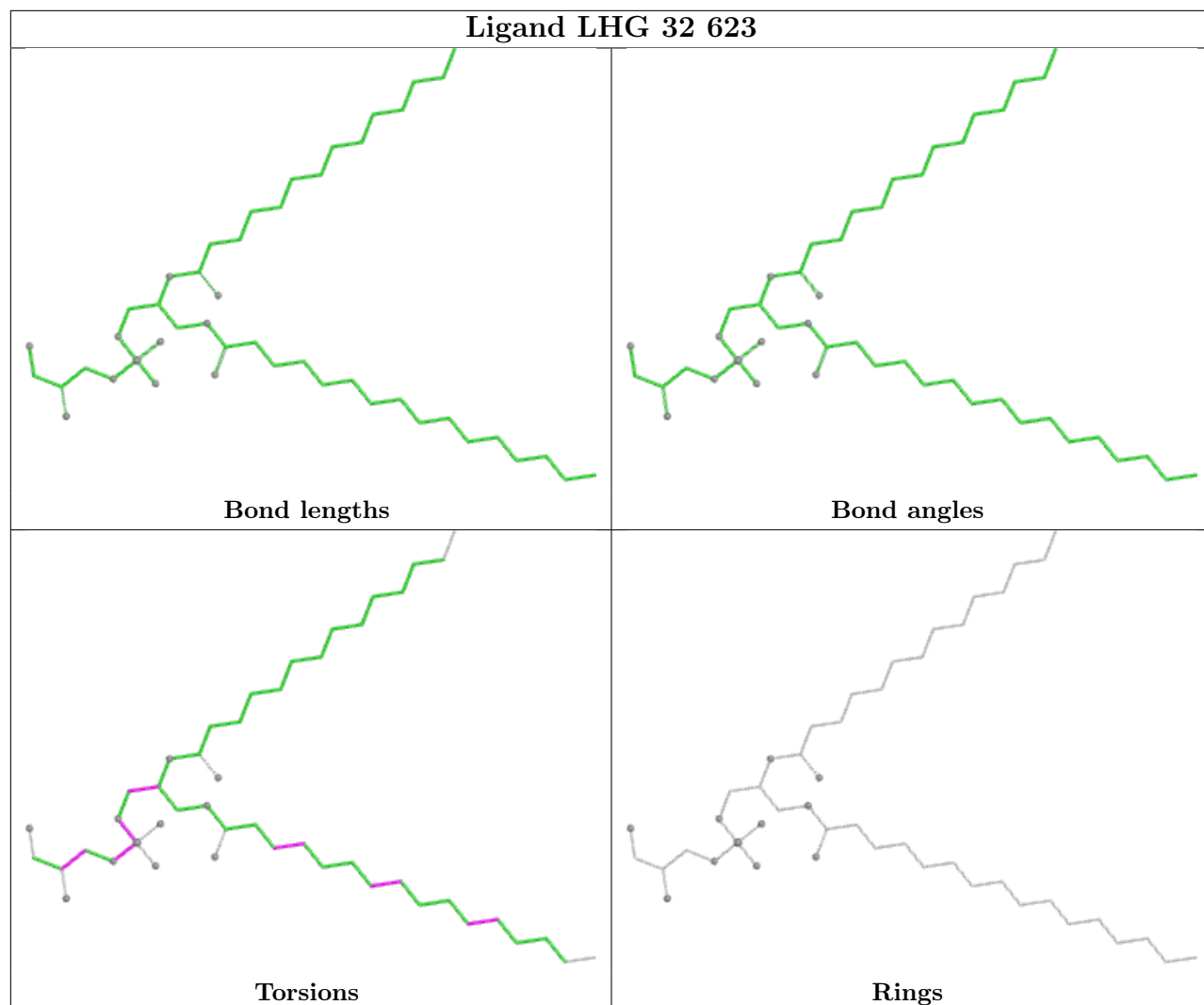


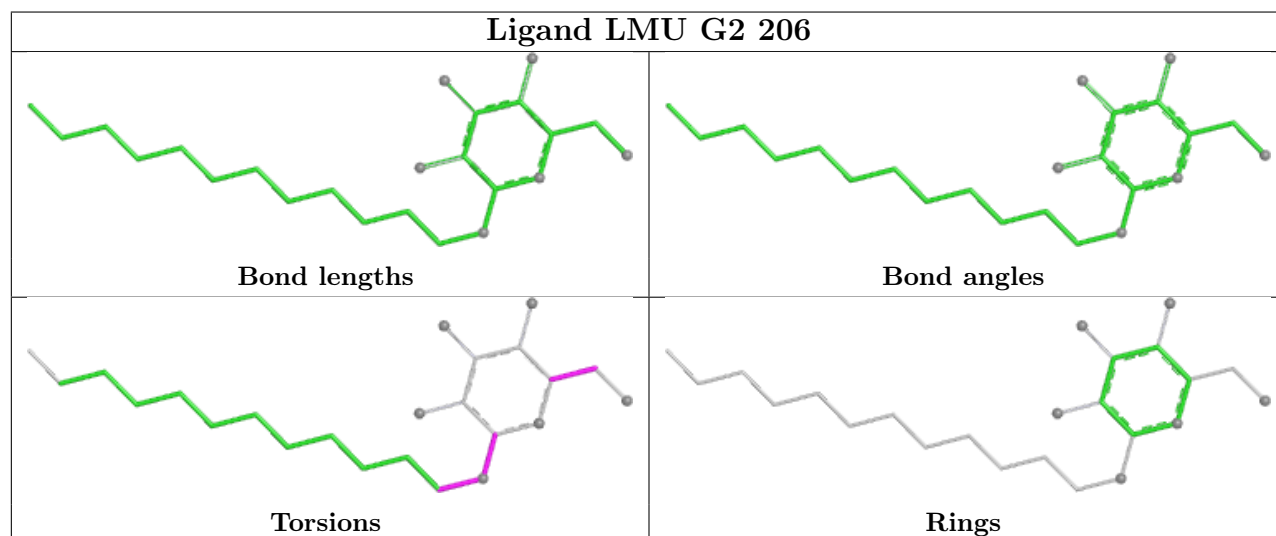
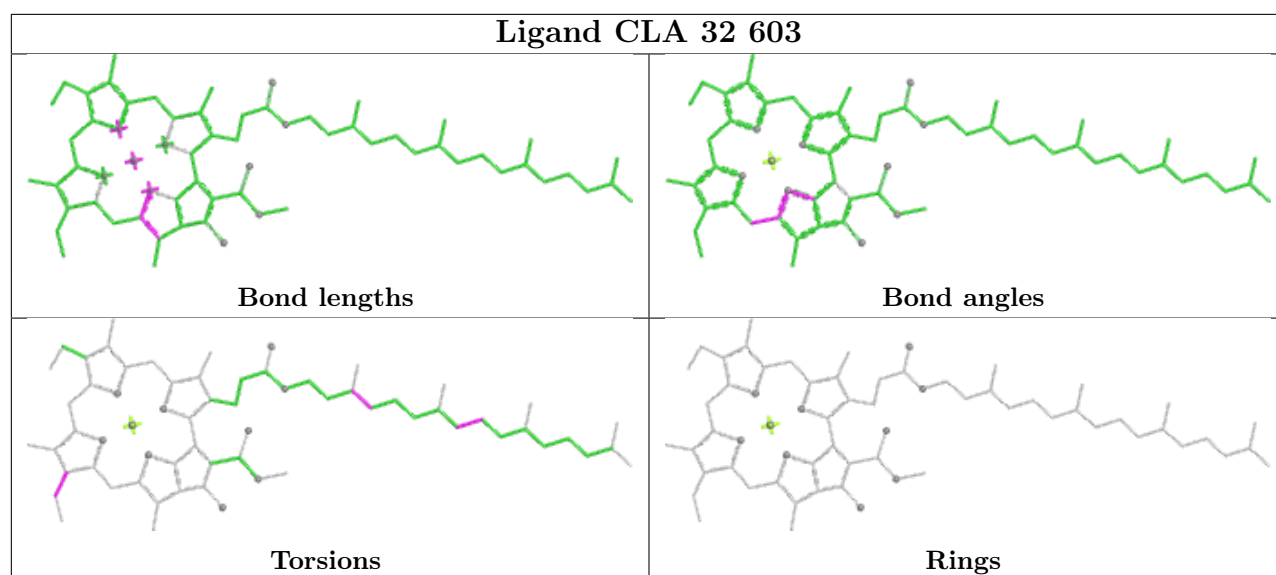




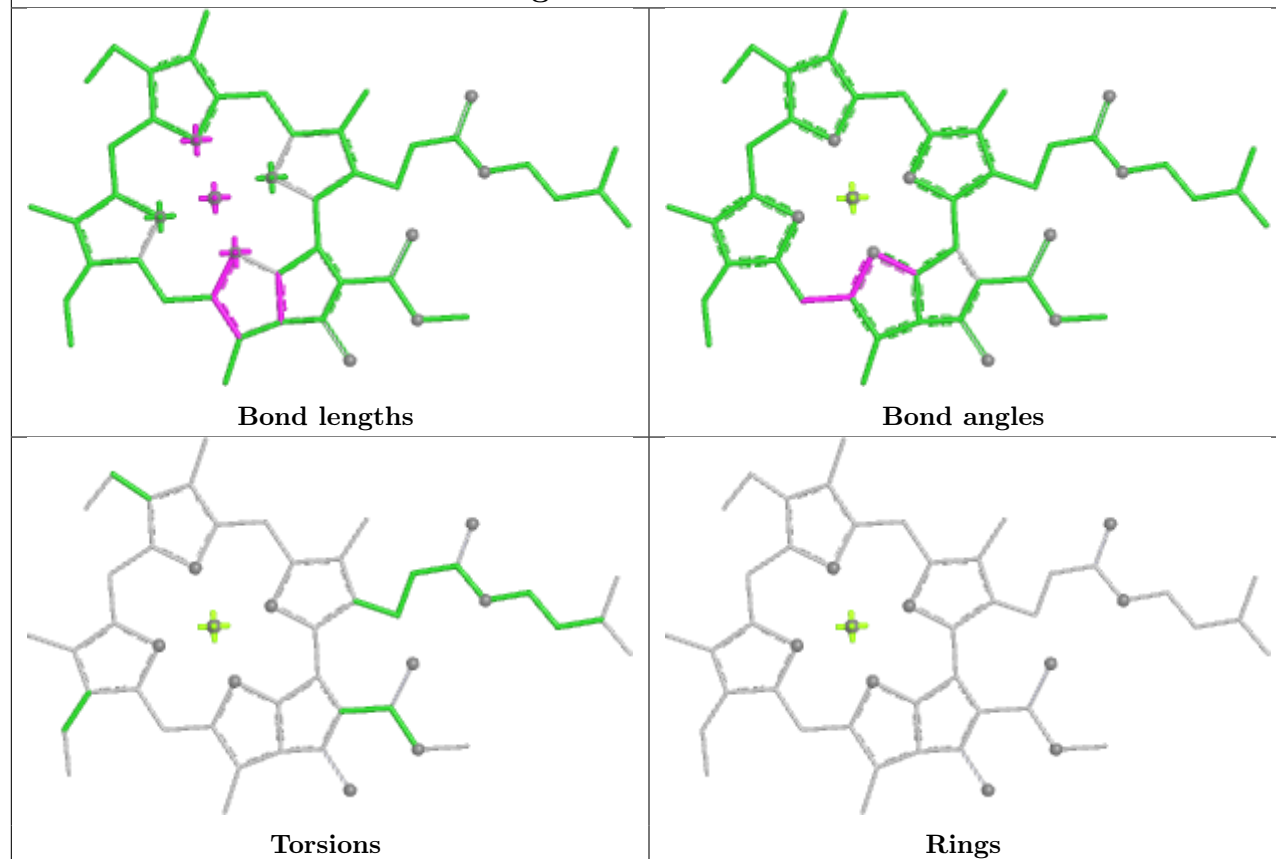
Ligand CHL 62 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 32 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

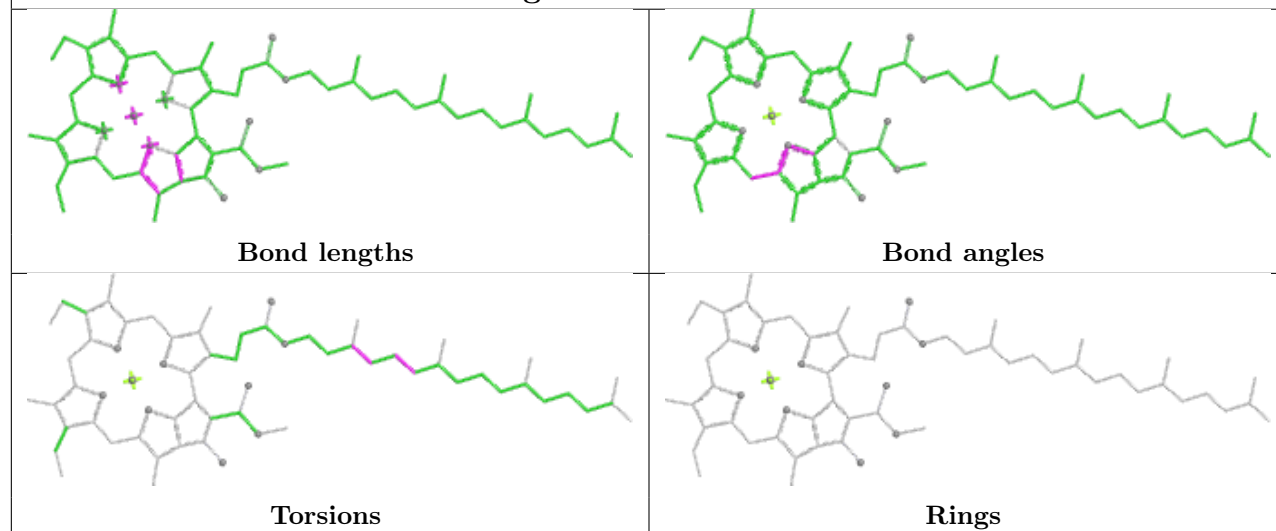


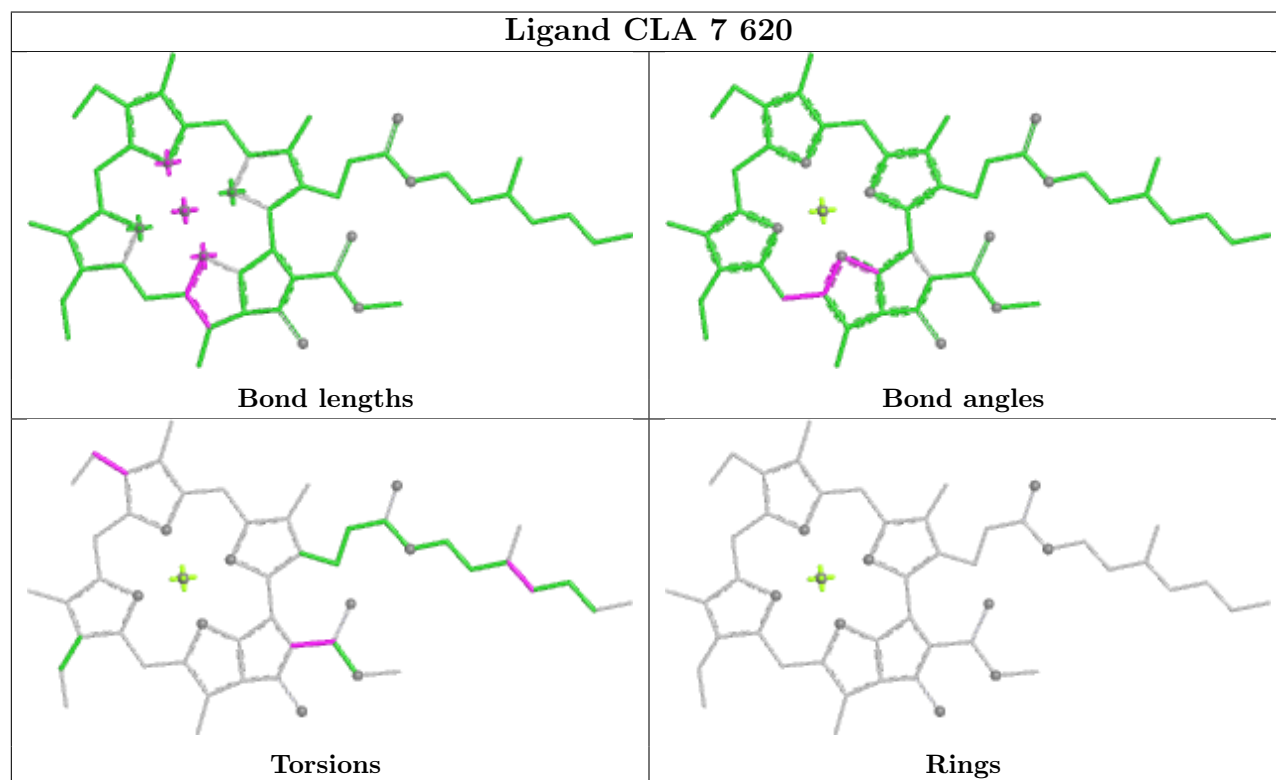
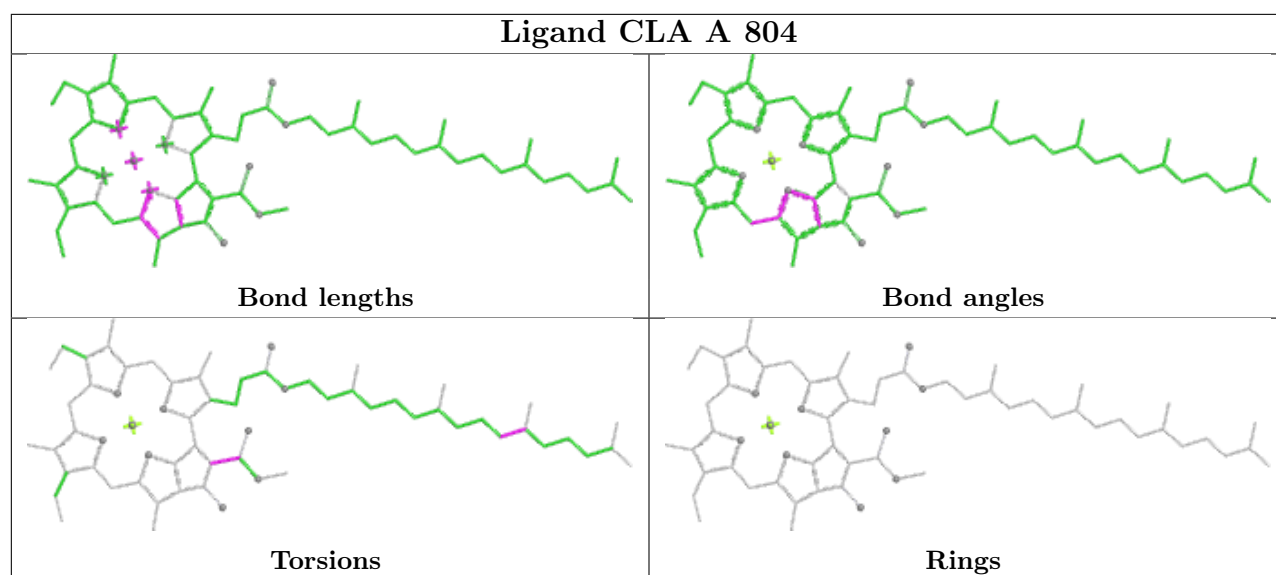


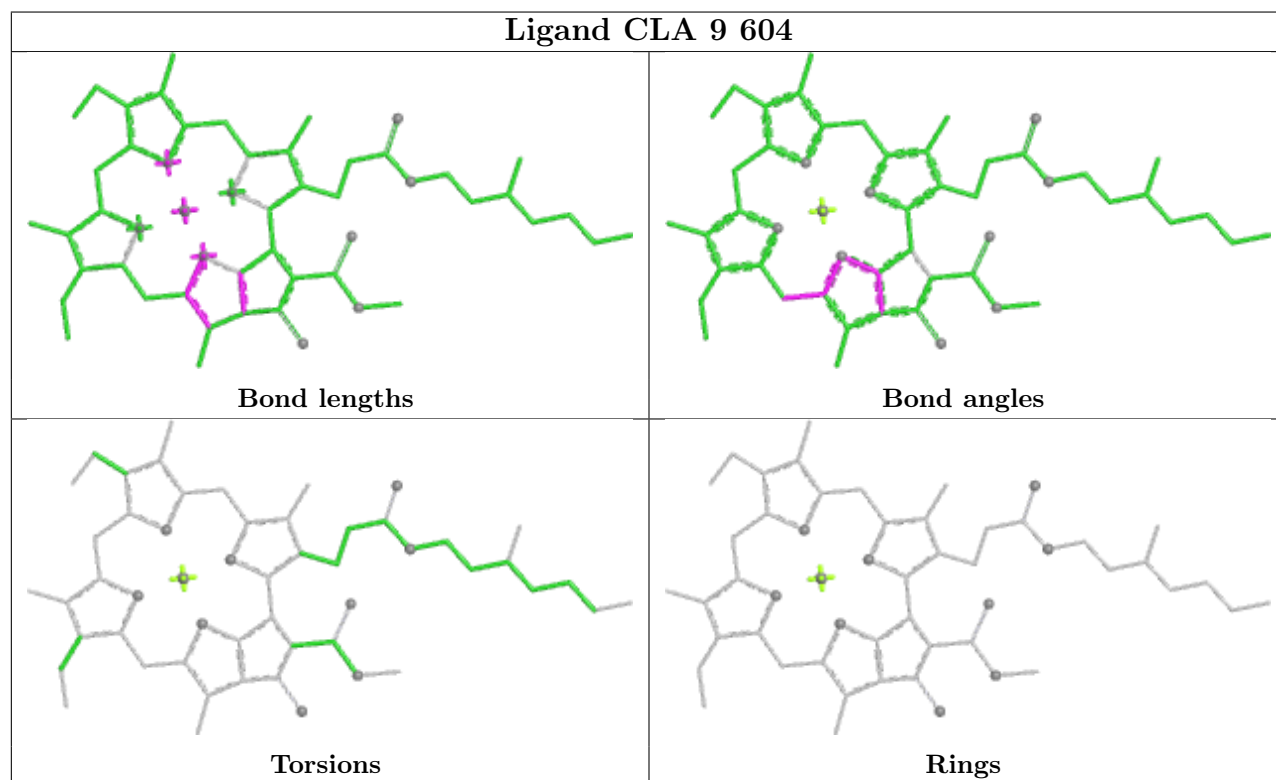
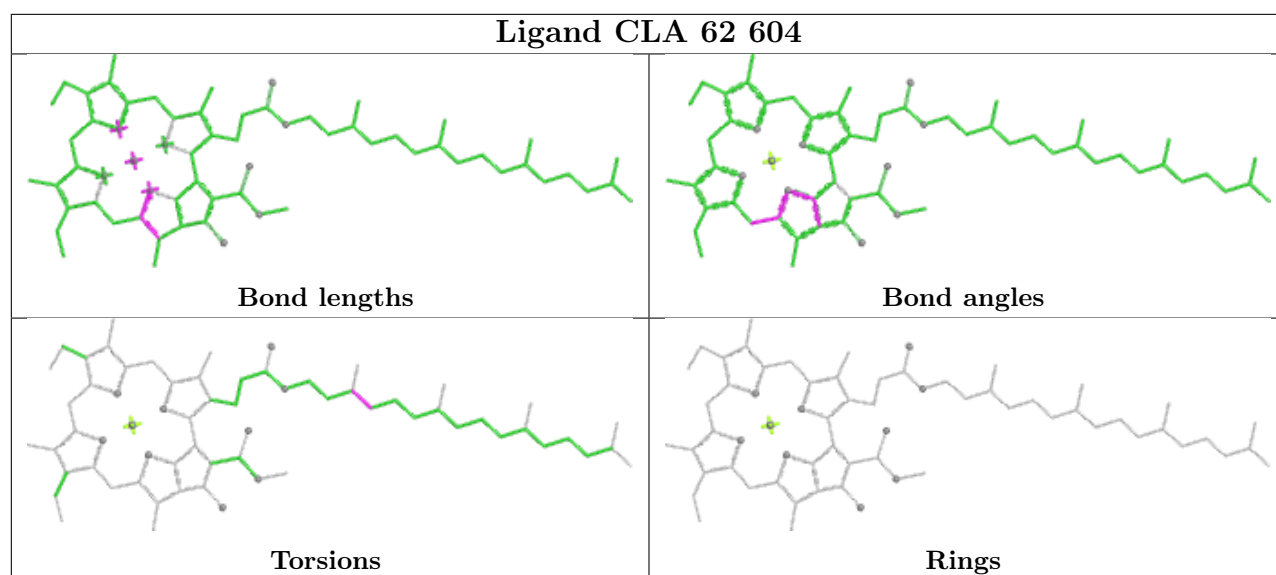
Ligand CLA A 808

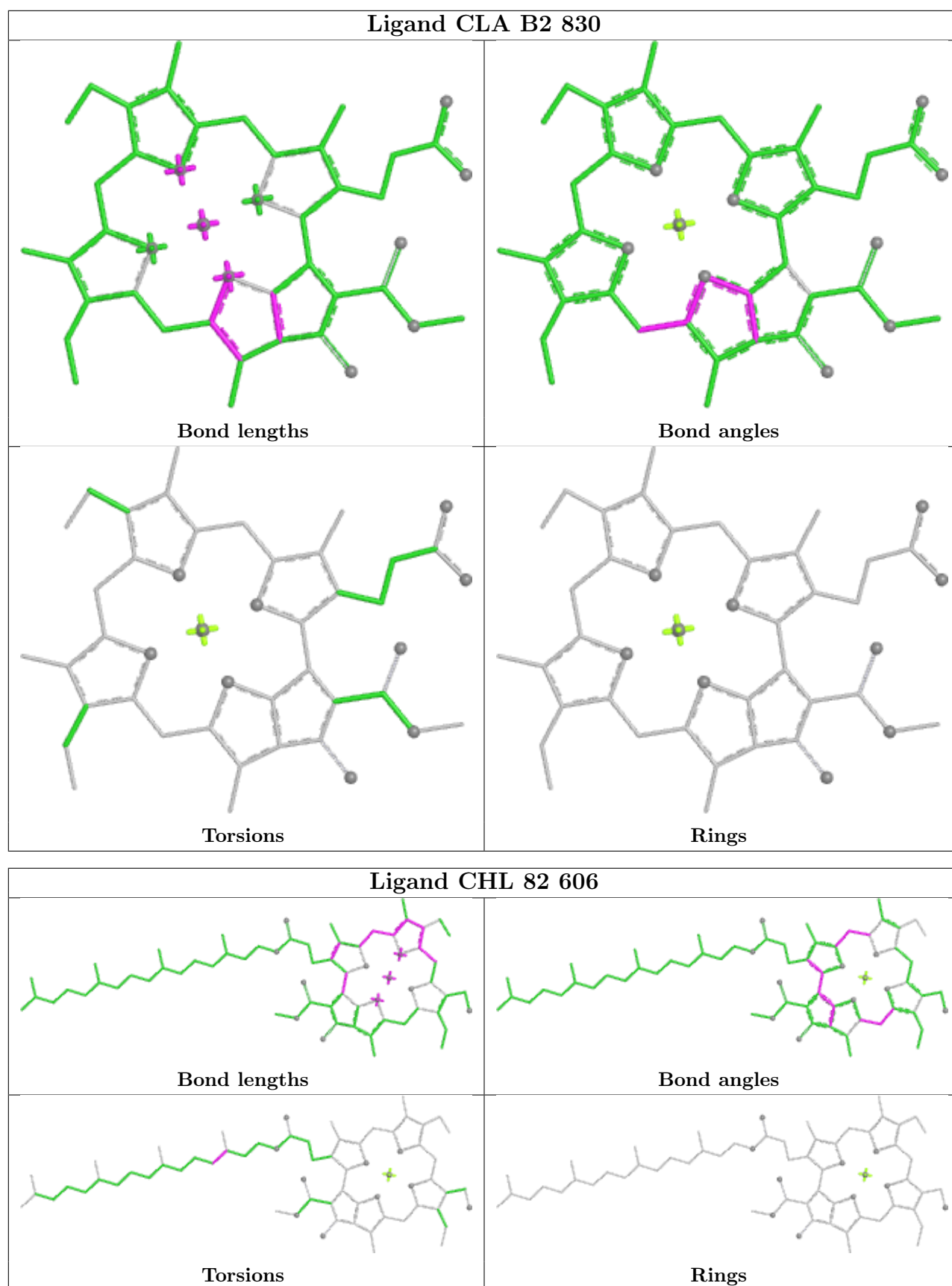


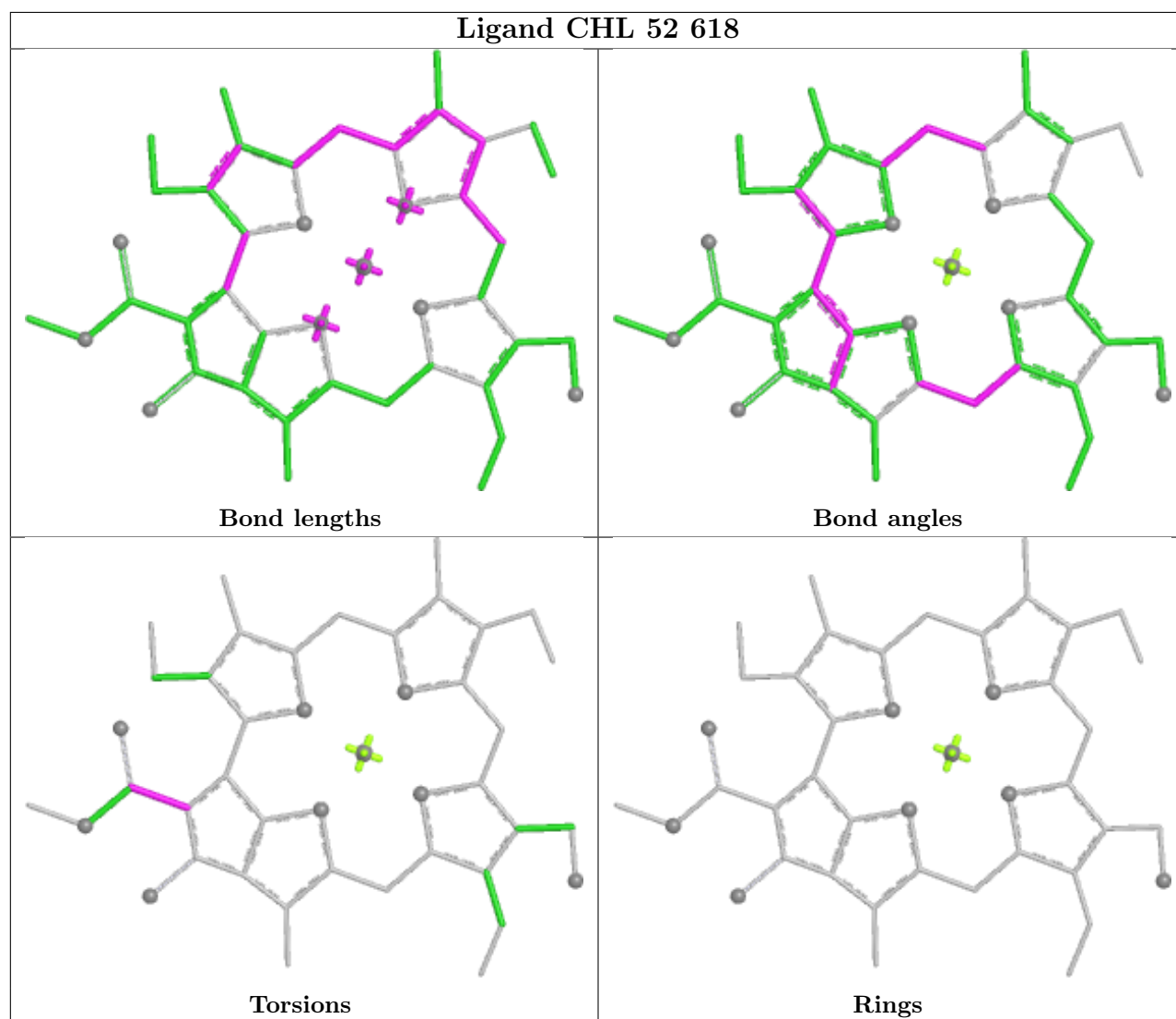
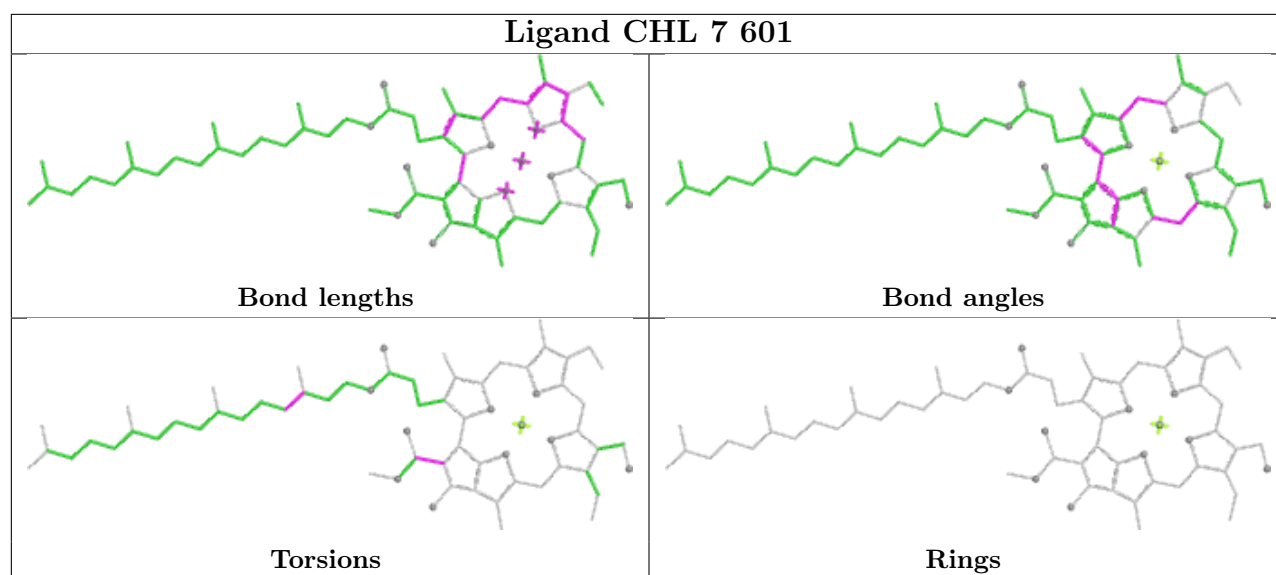
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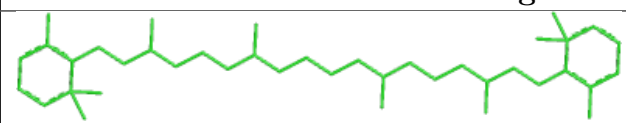
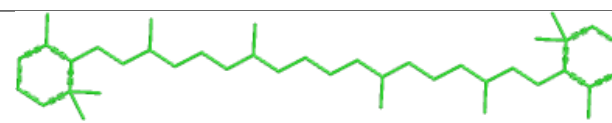
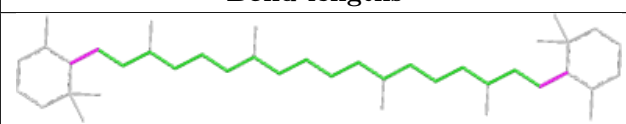
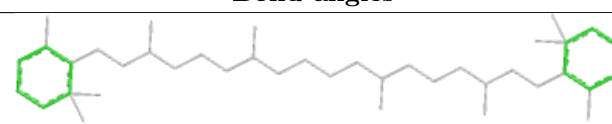


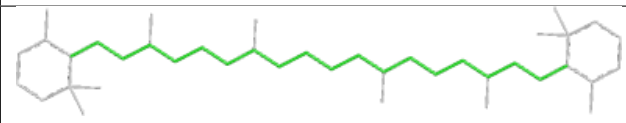
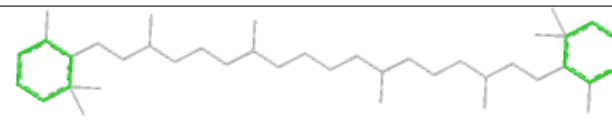


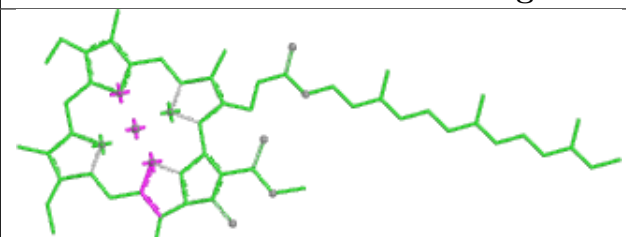
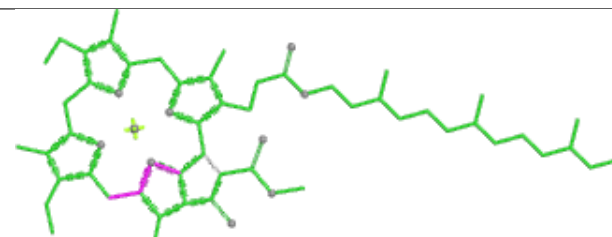
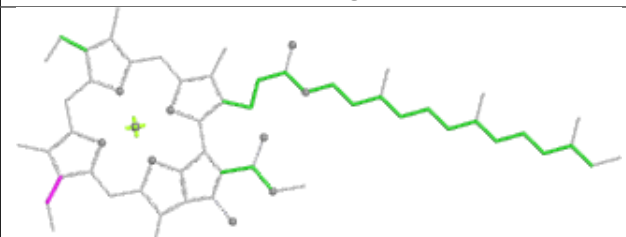
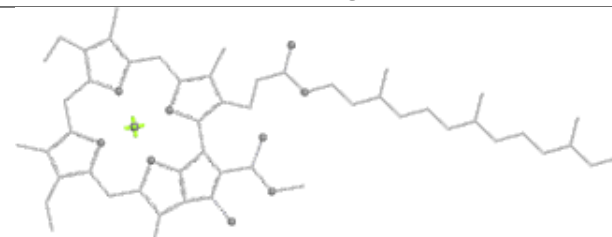


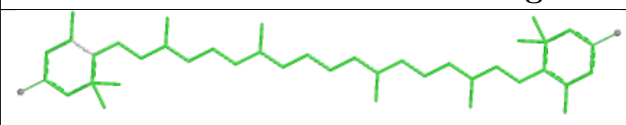
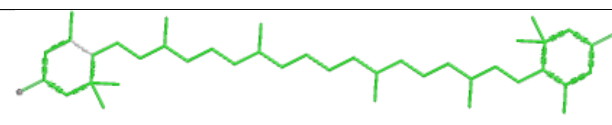
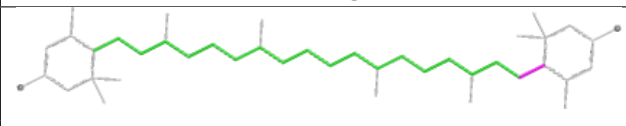
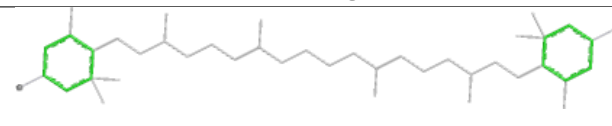


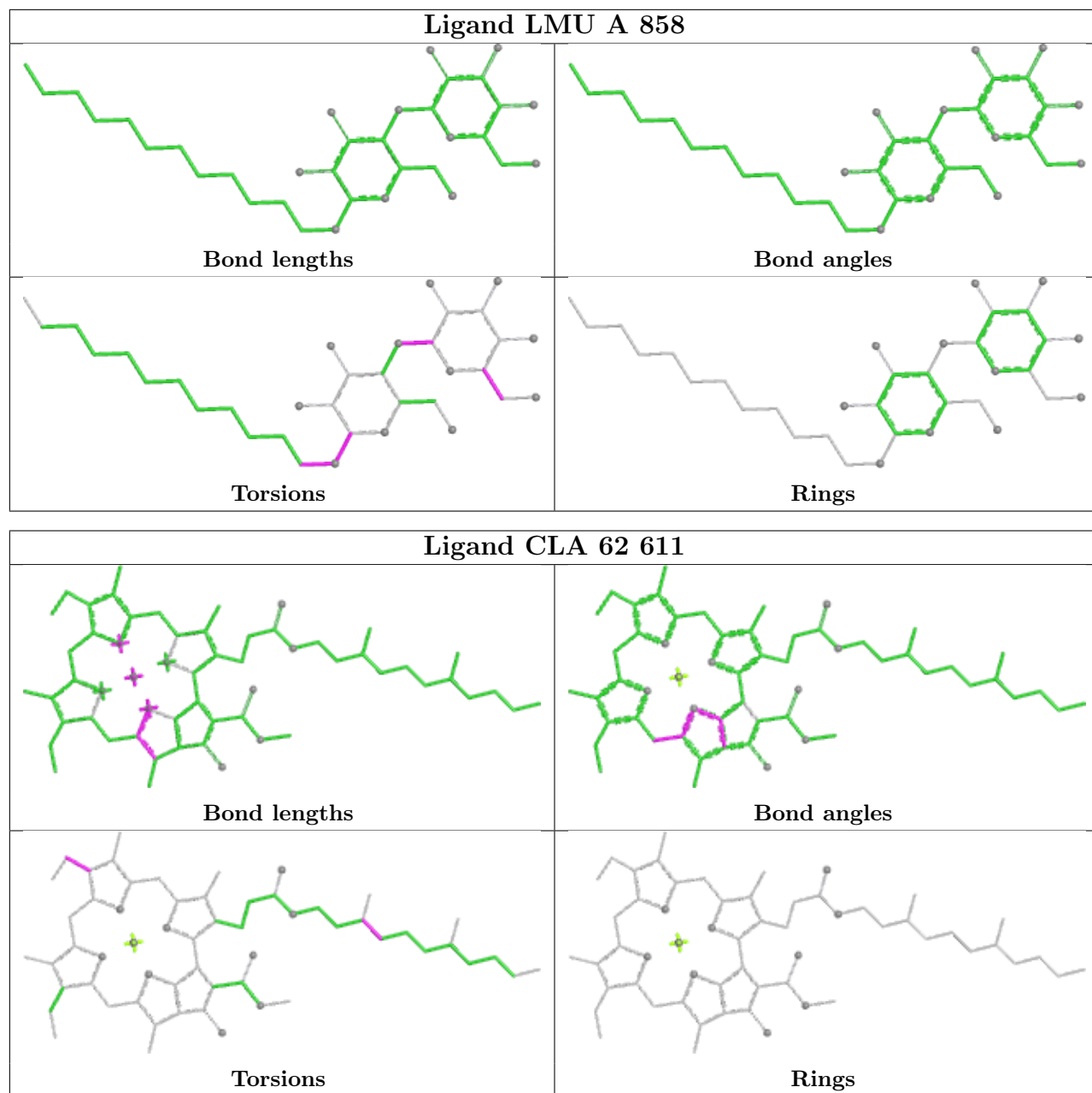


Ligand BCR K 207	
	
Bond lengths	Bond angles
	
Torsions	Rings

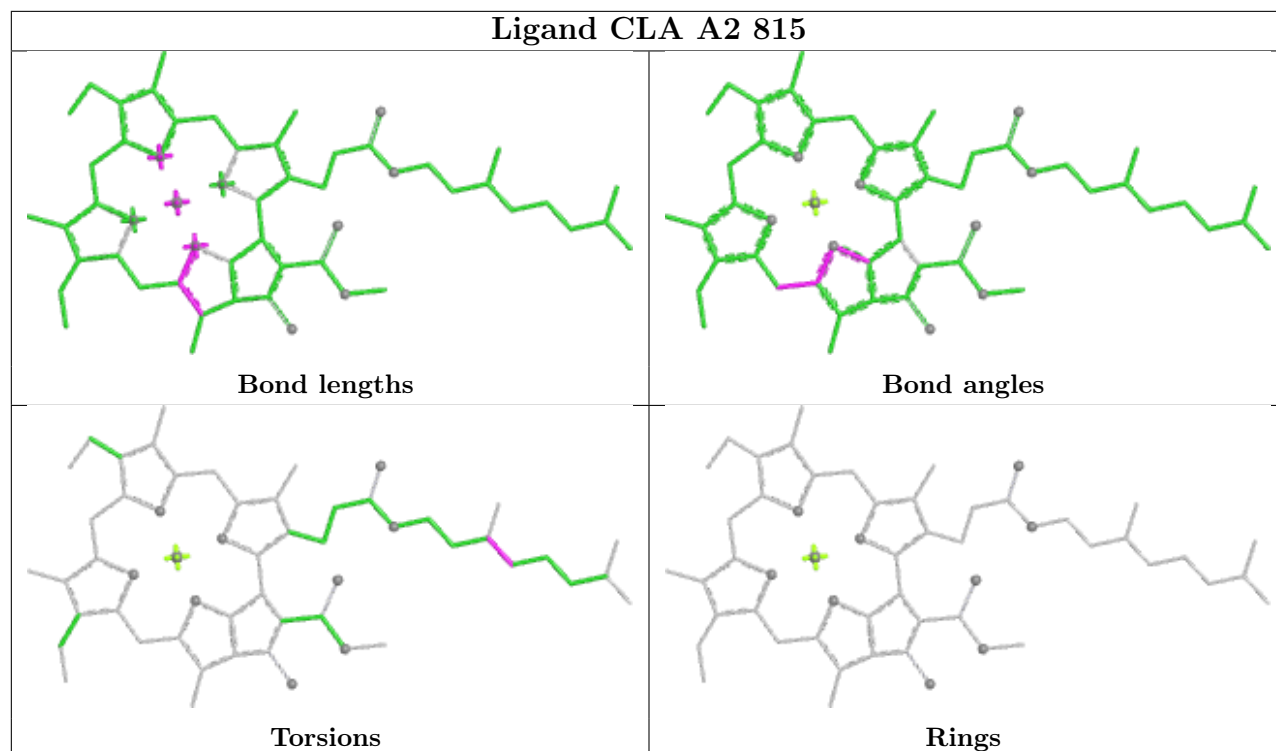
Ligand BCR B2 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 32 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

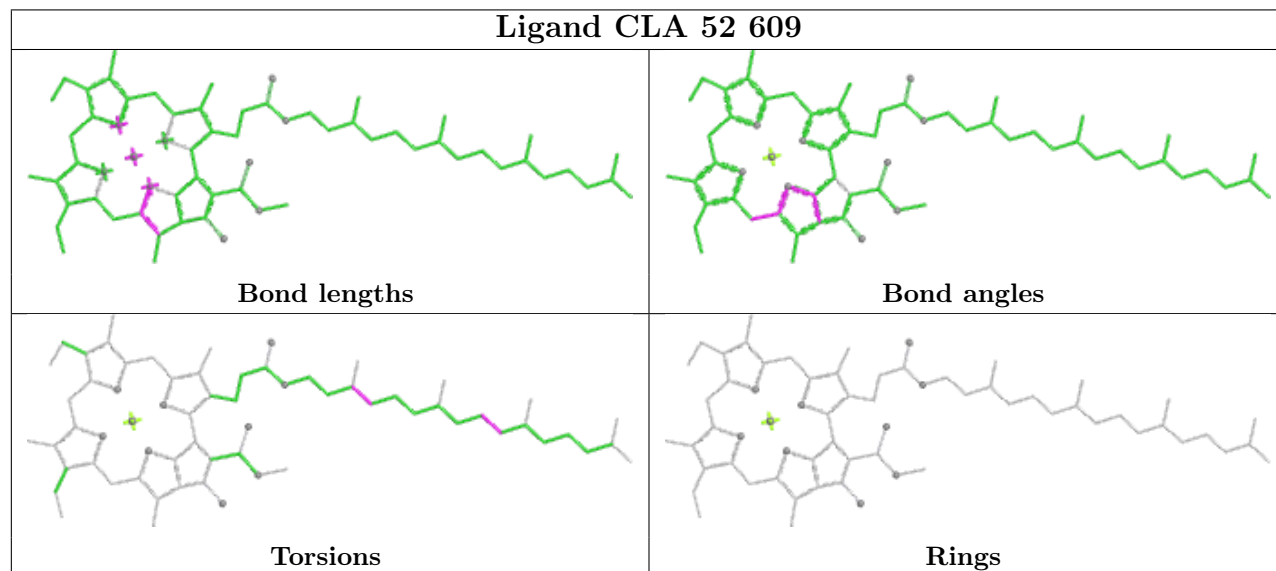
Ligand LUT 9 616	
	
Bond lengths	Bond angles
	
Torsions	Rings

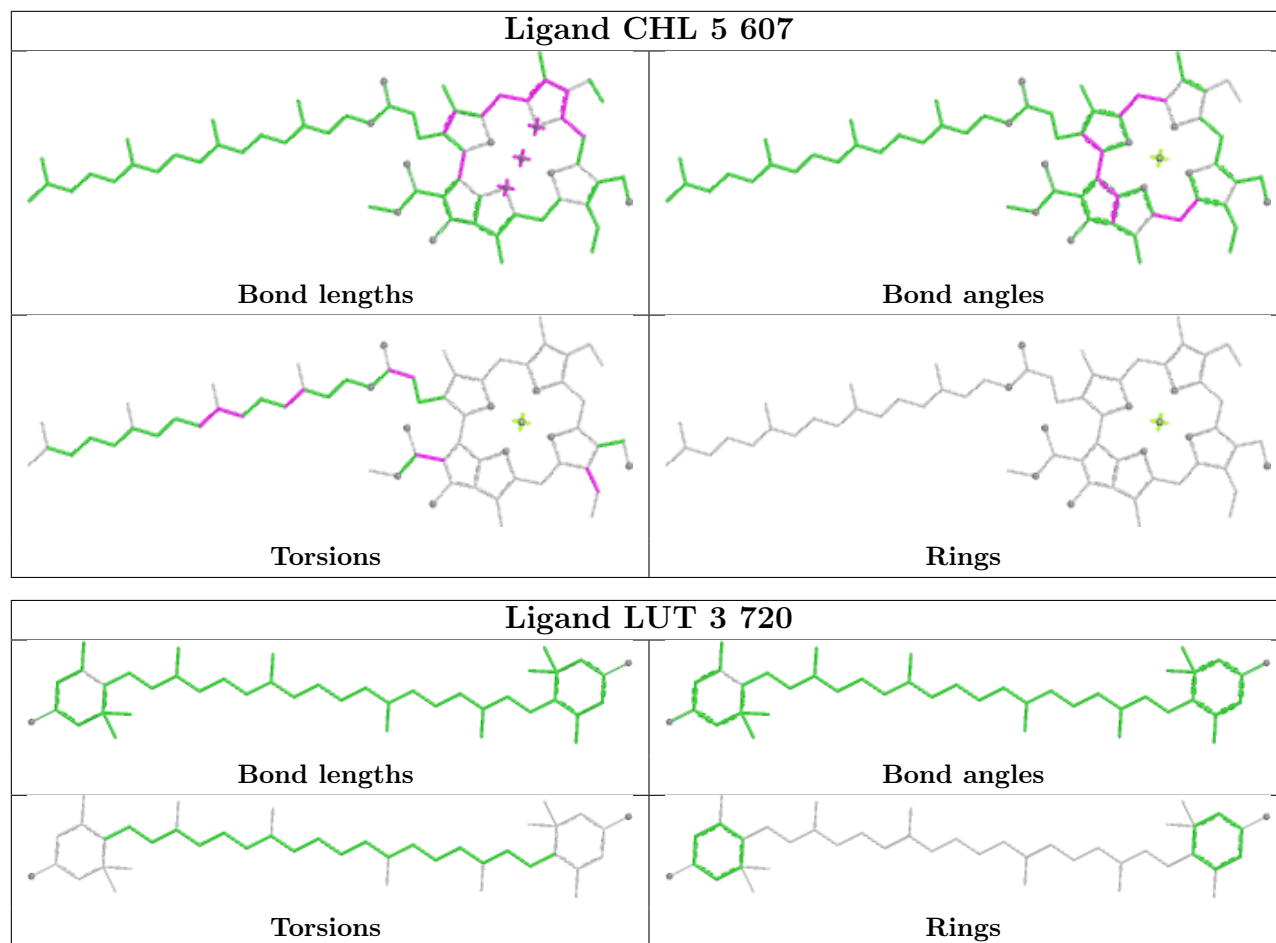


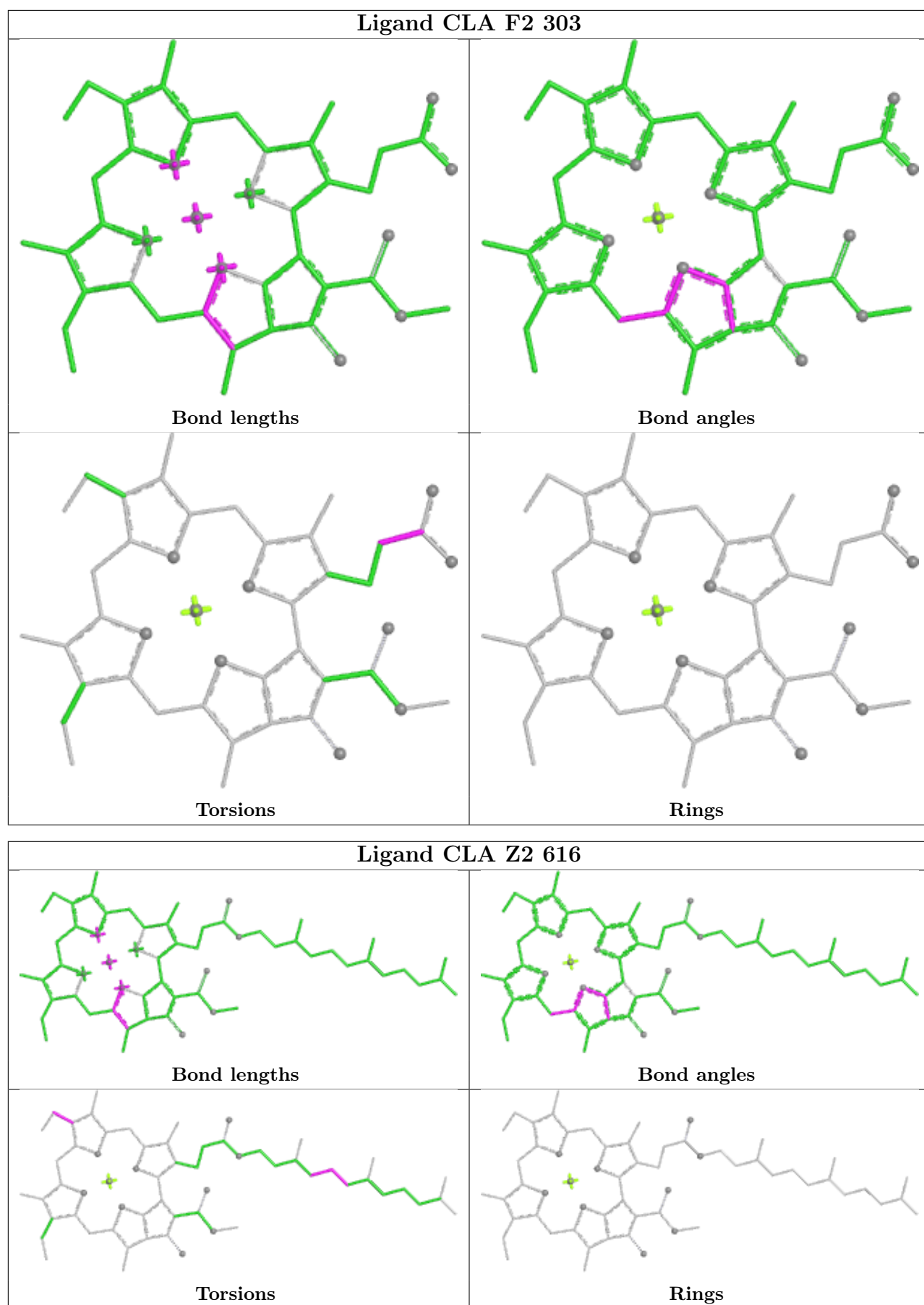
Ligand CLA A2 815

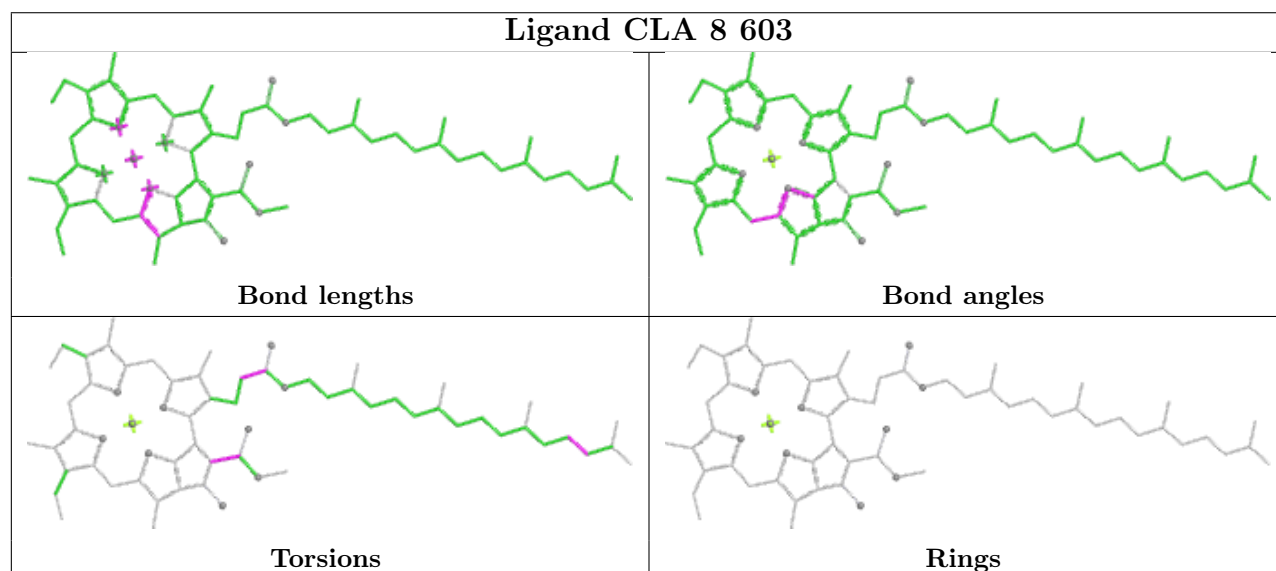
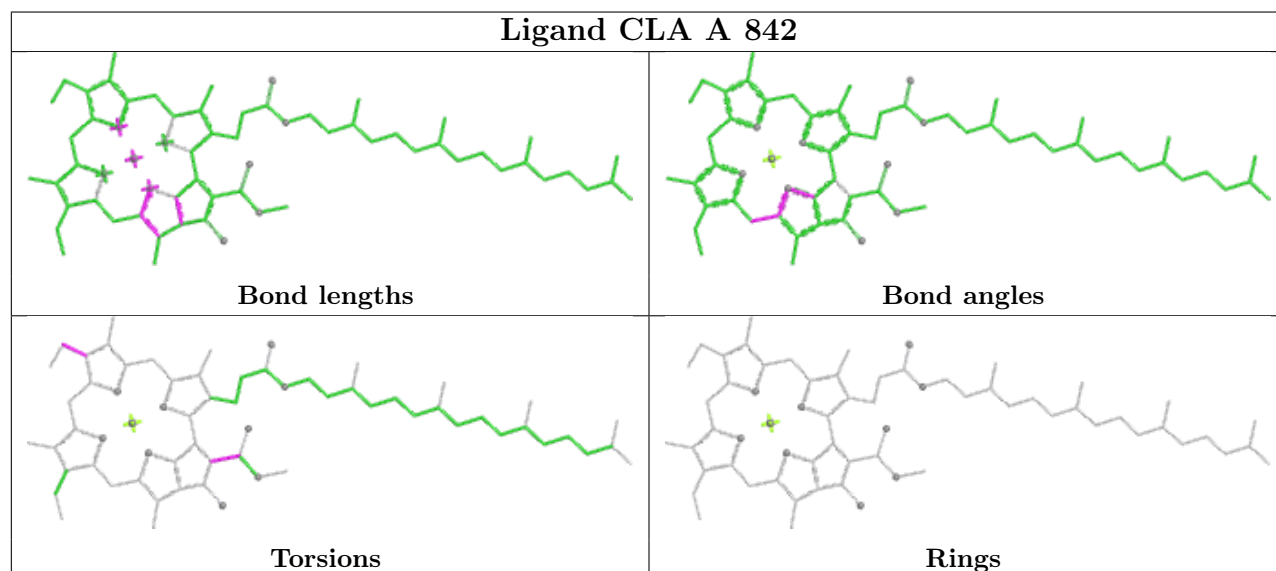
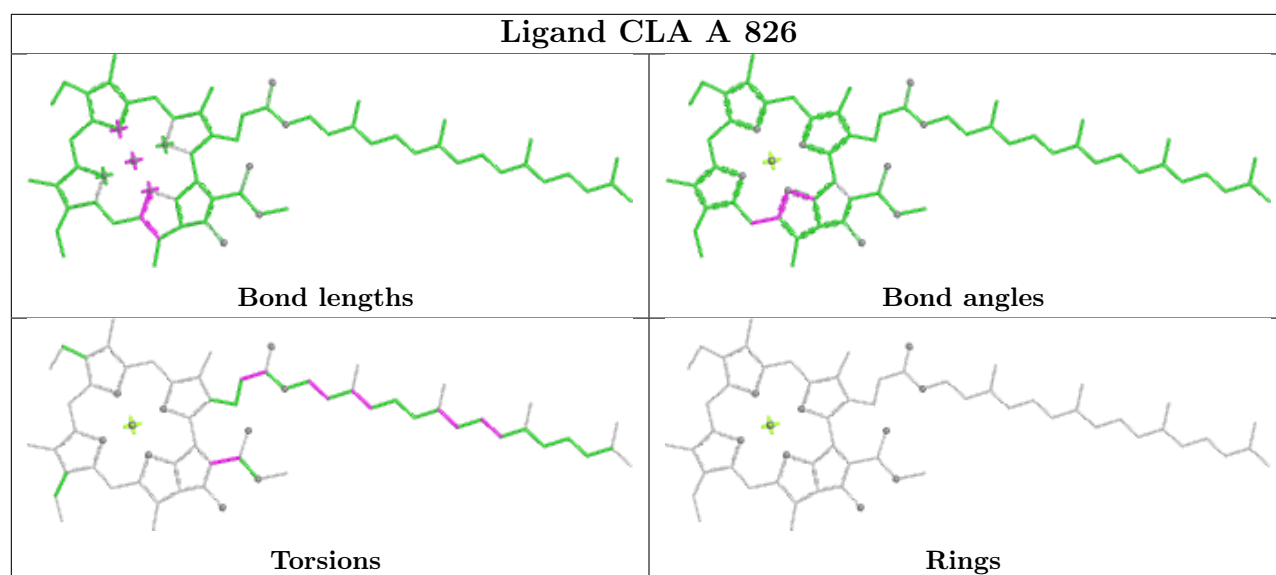


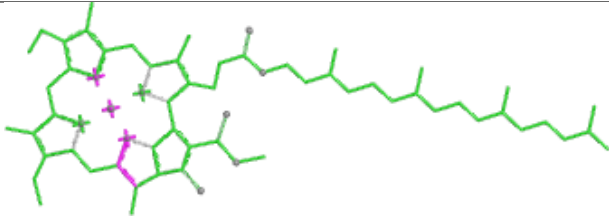
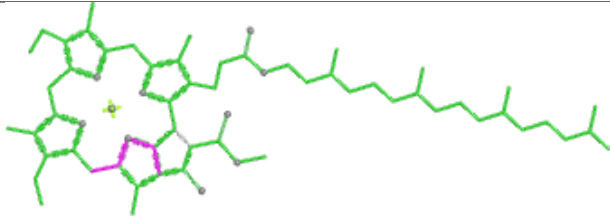
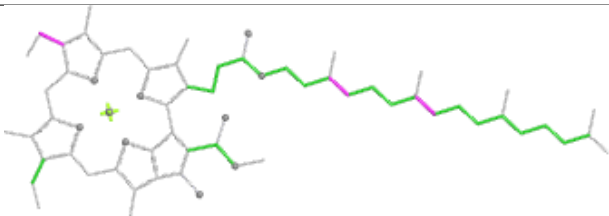
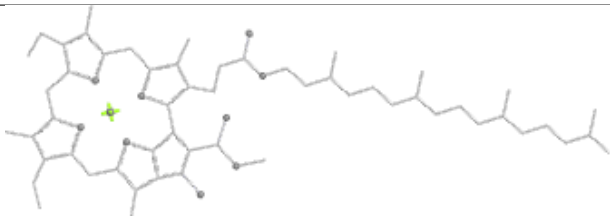
Ligand CLA 52 609

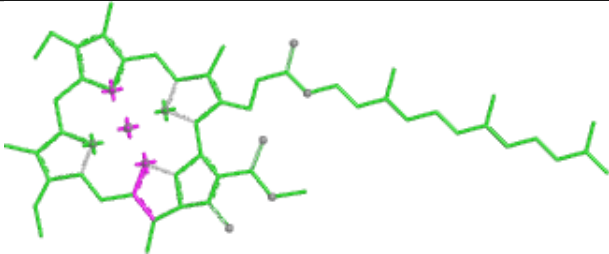
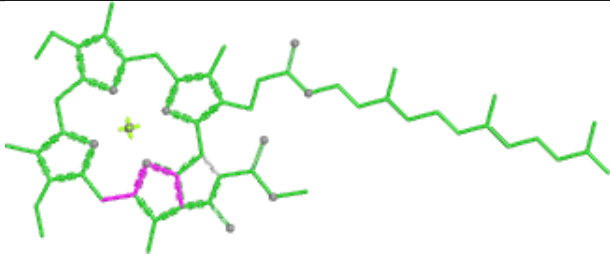
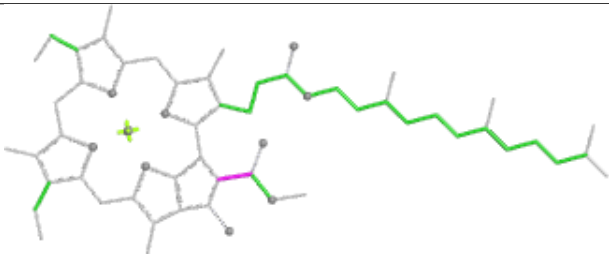
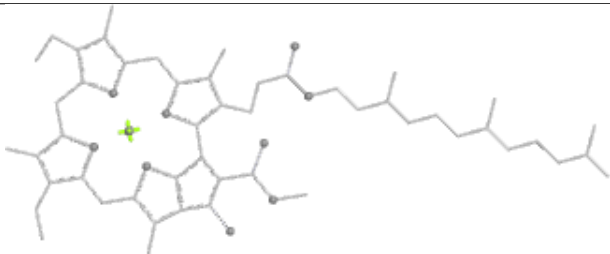


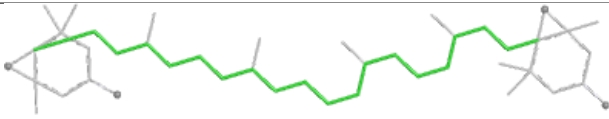
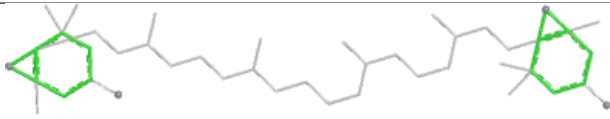


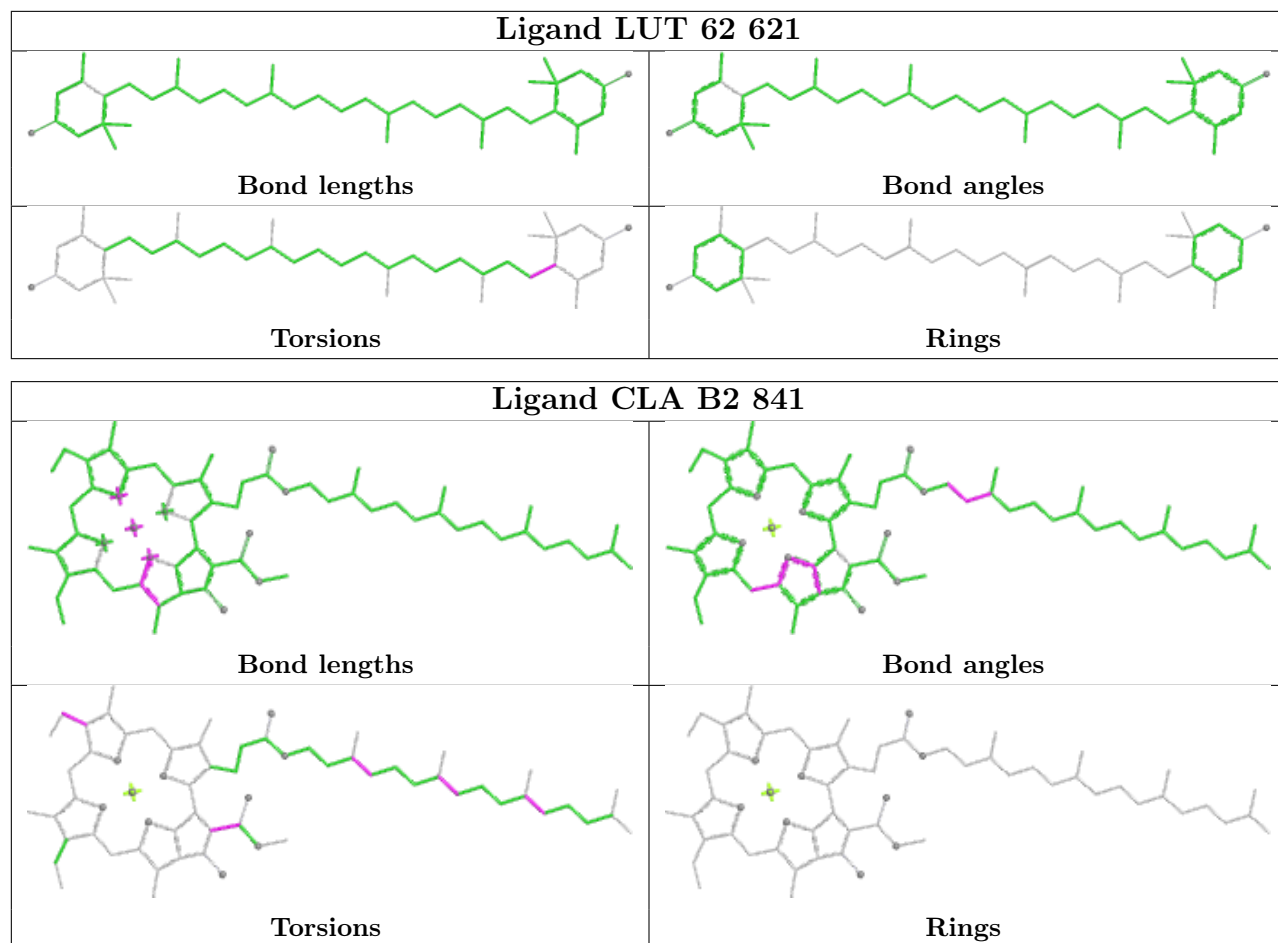


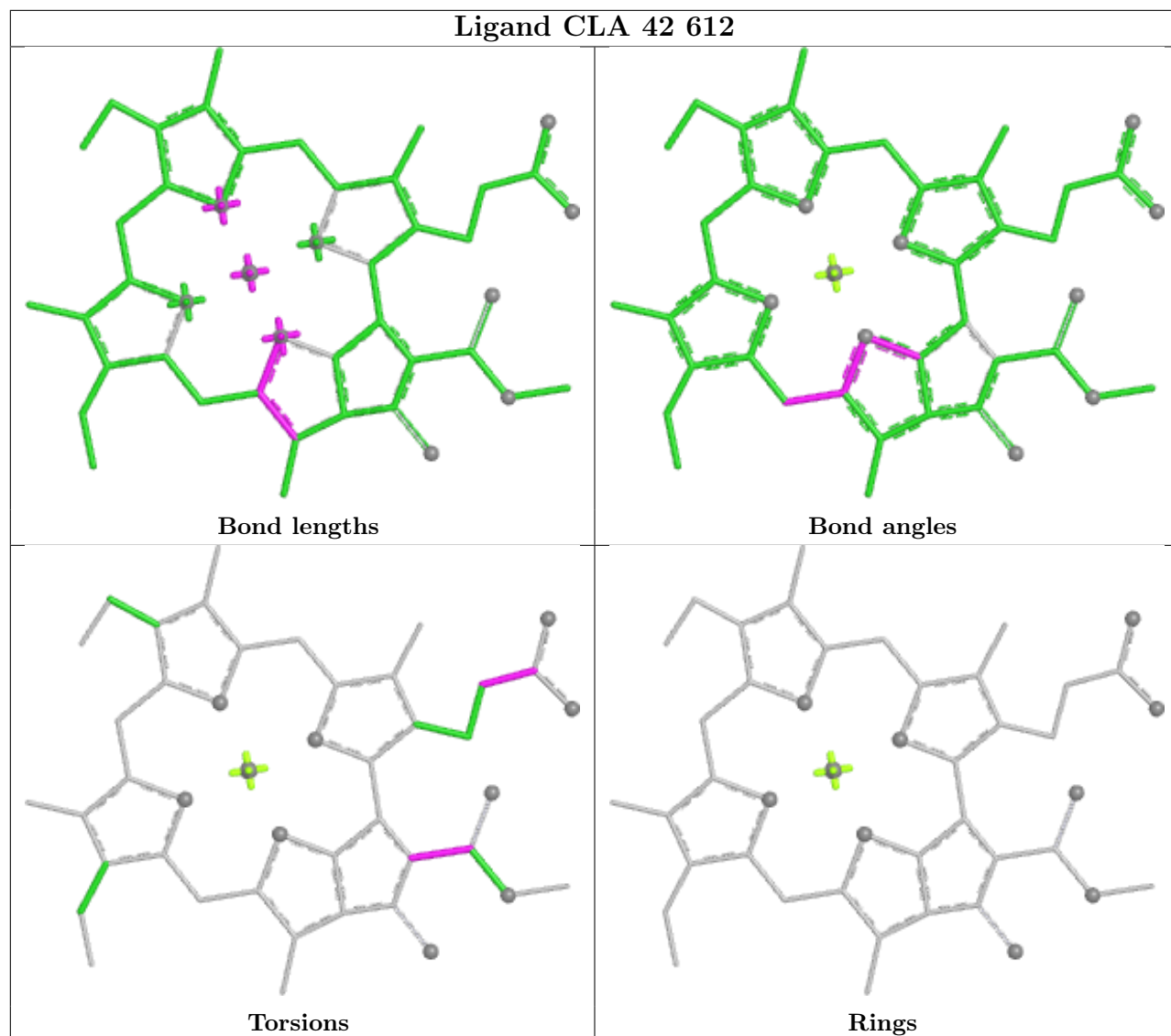


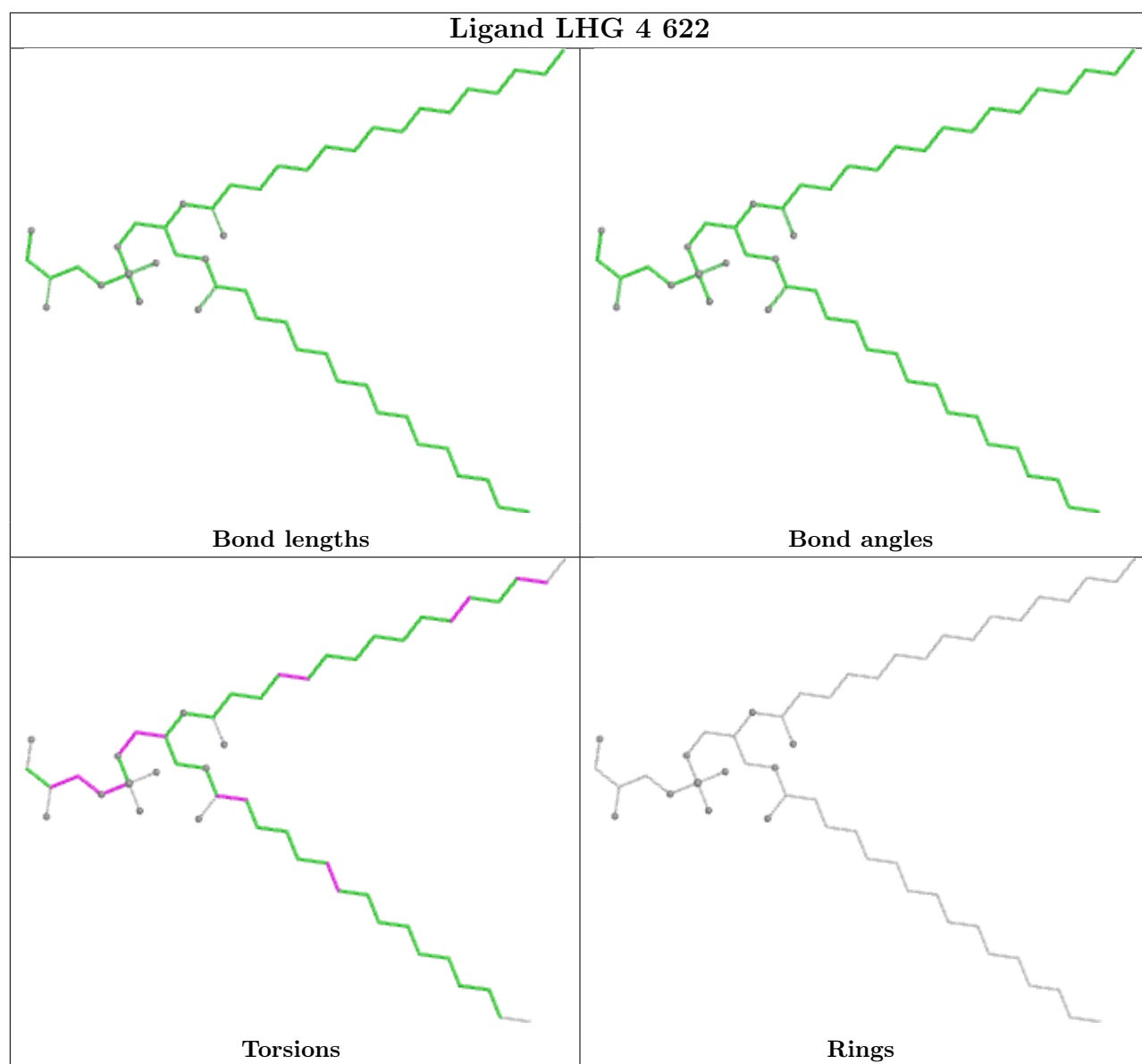
Ligand CLA 62 613	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 42 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

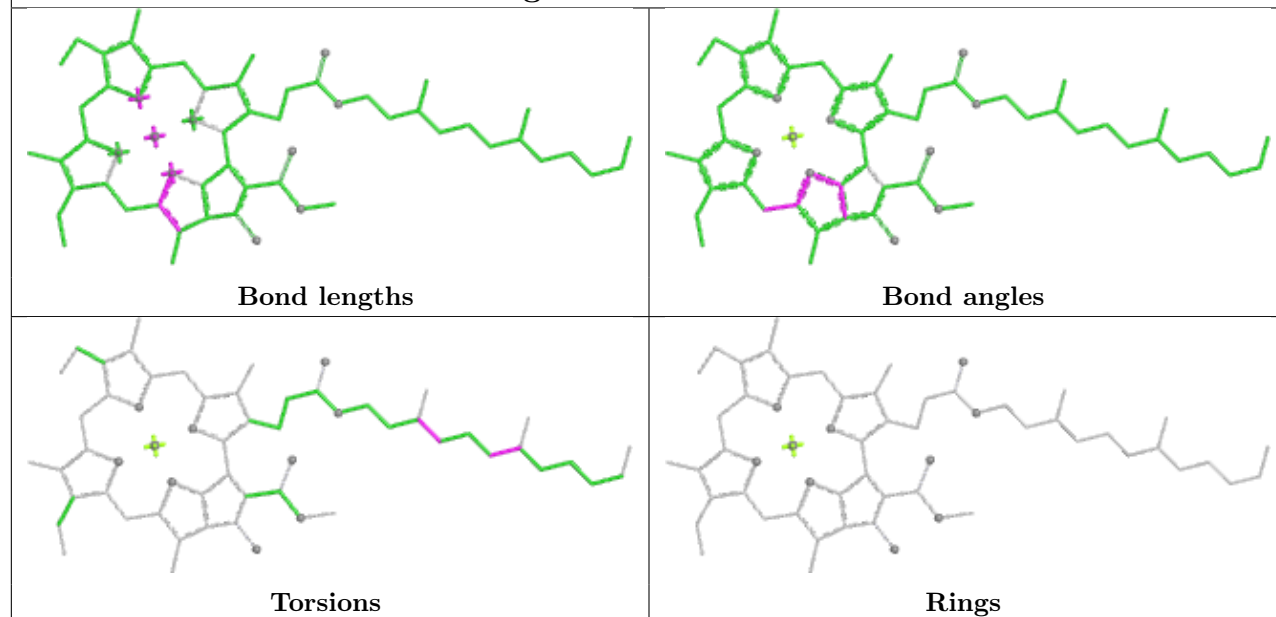
Ligand XAT 8 618	
	
Bond lengths	Bond angles
	
Torsions	Rings



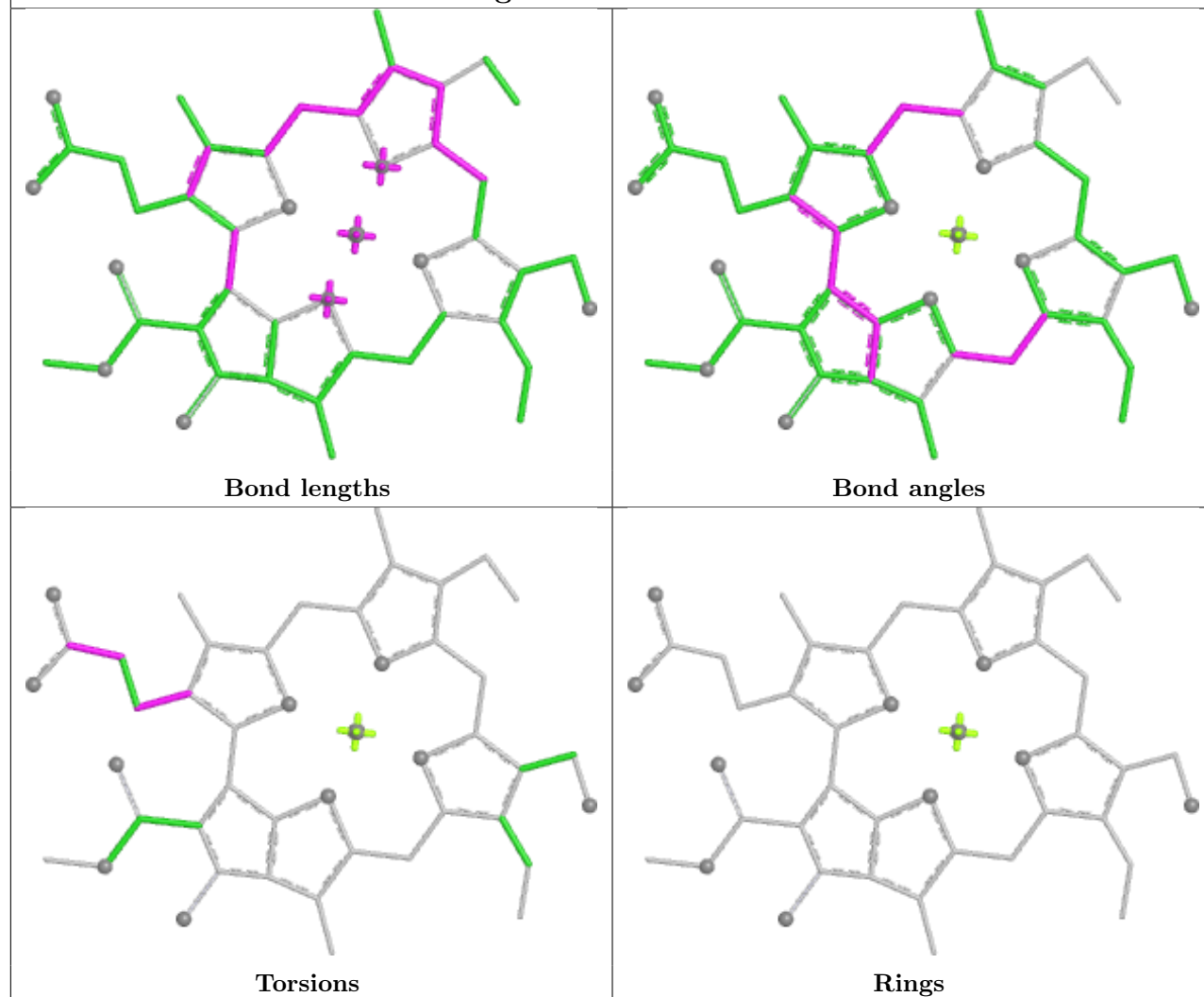


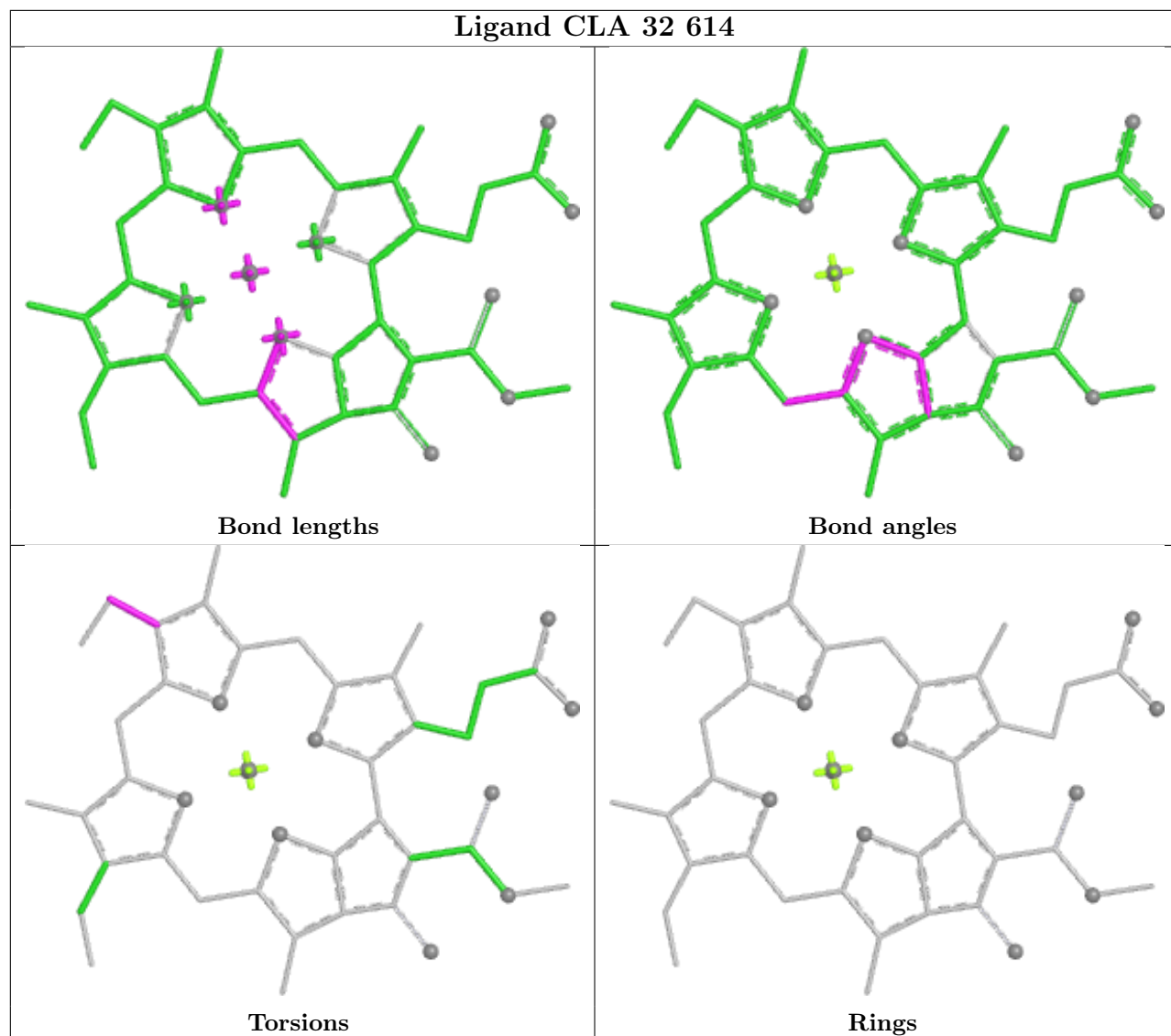


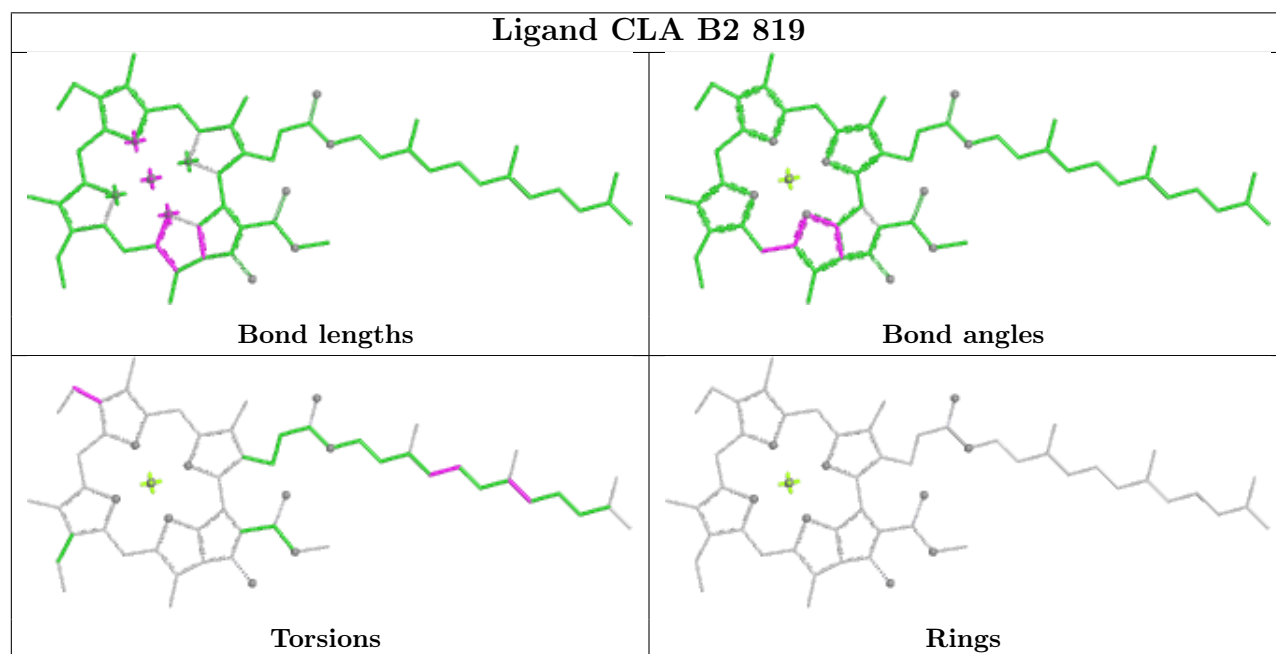
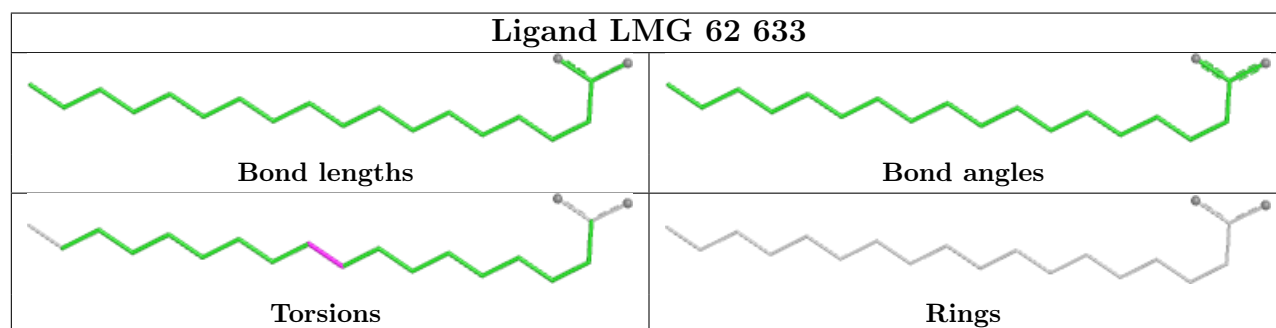
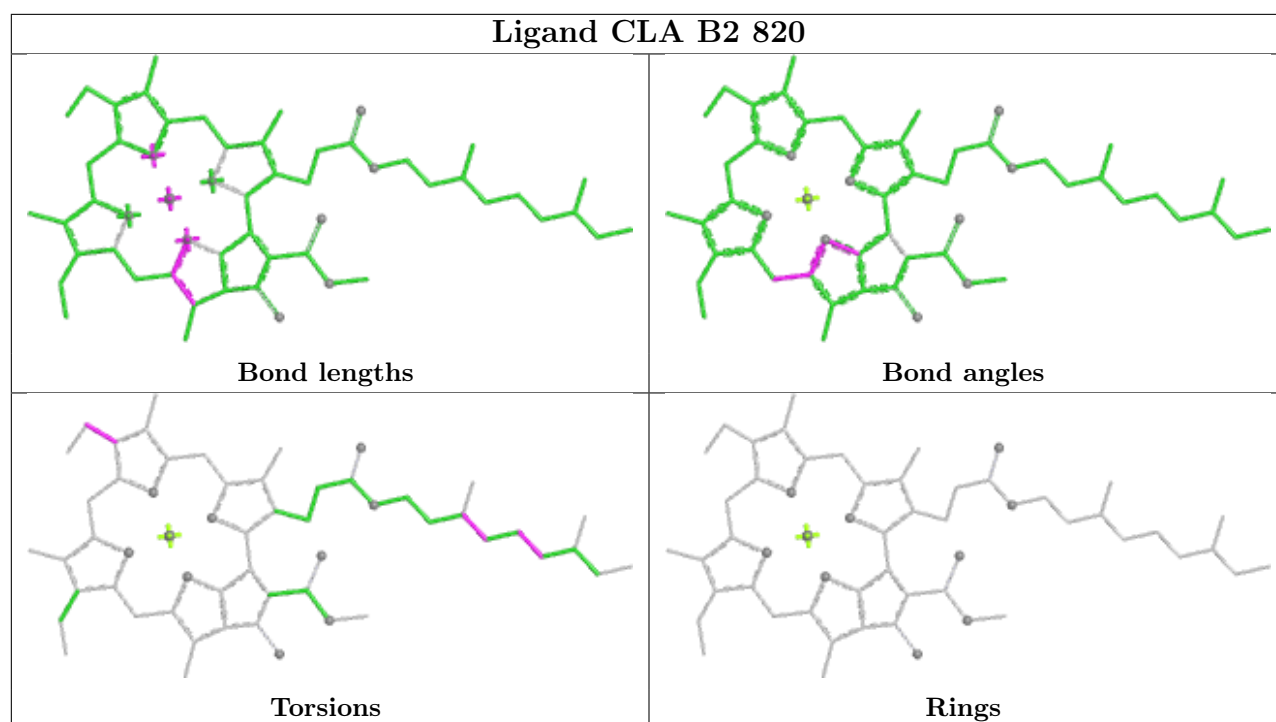
Ligand CLA B2 822

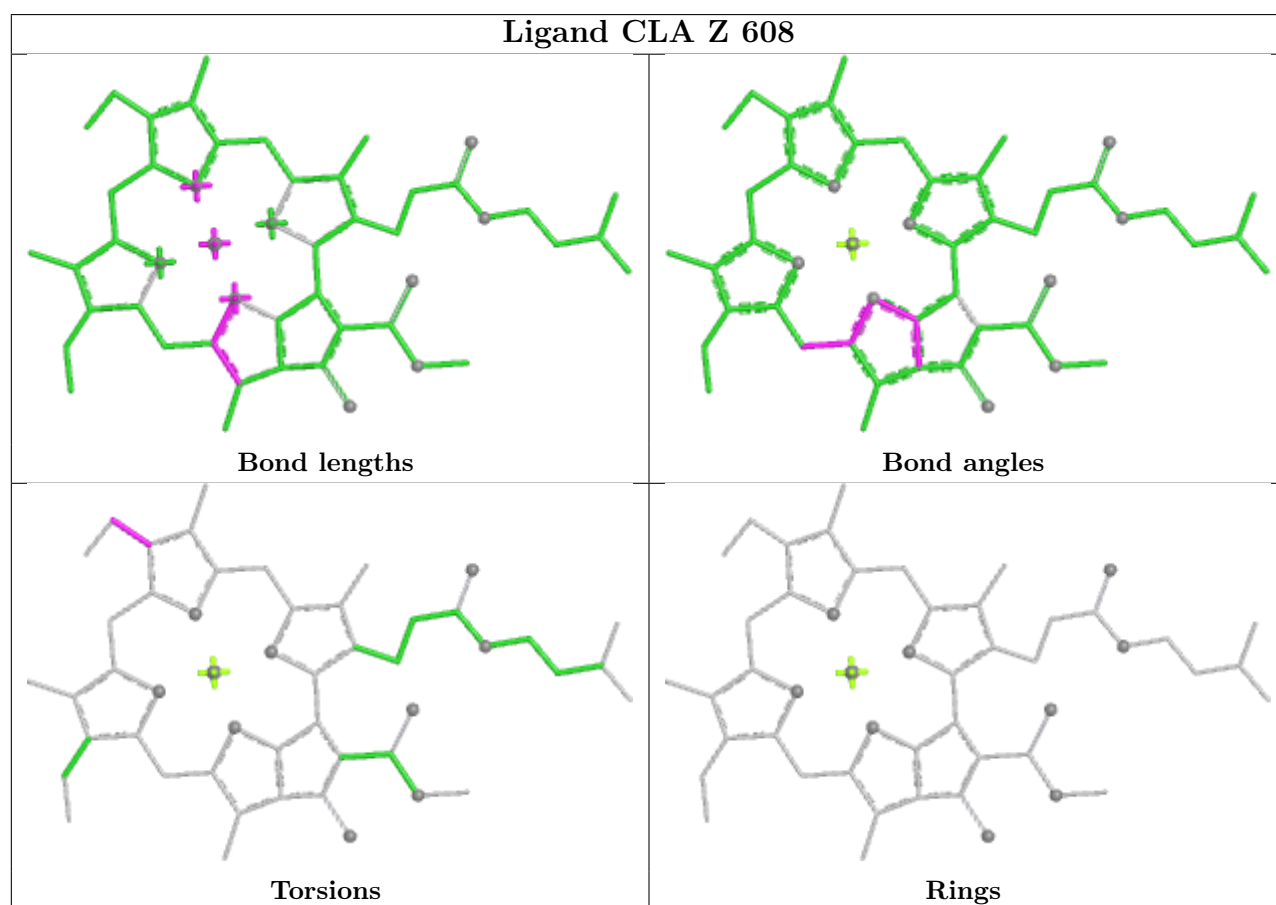
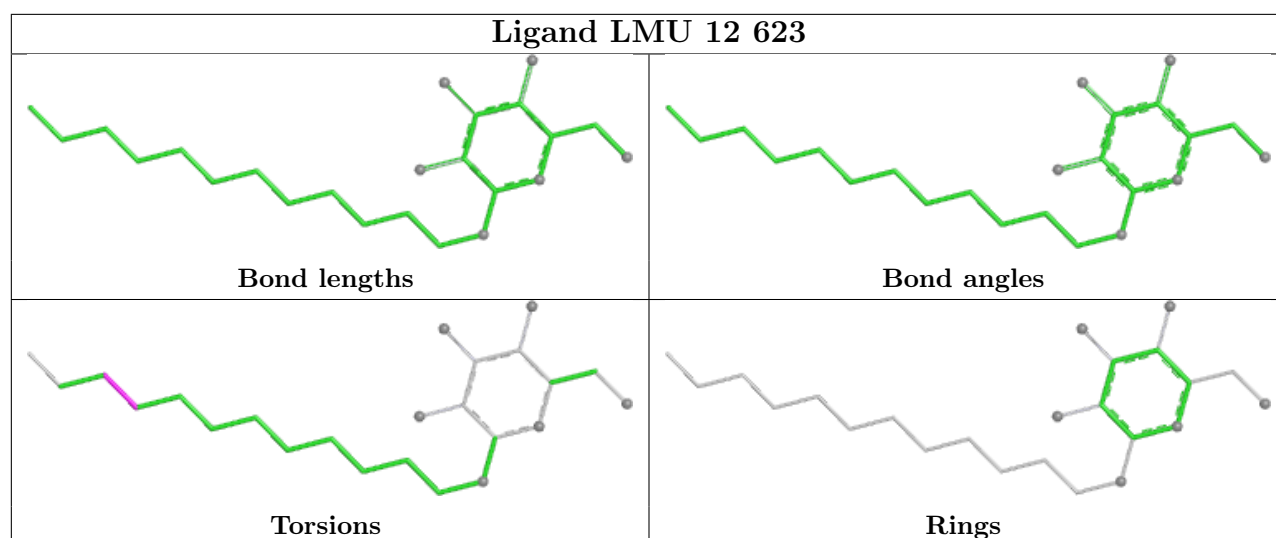


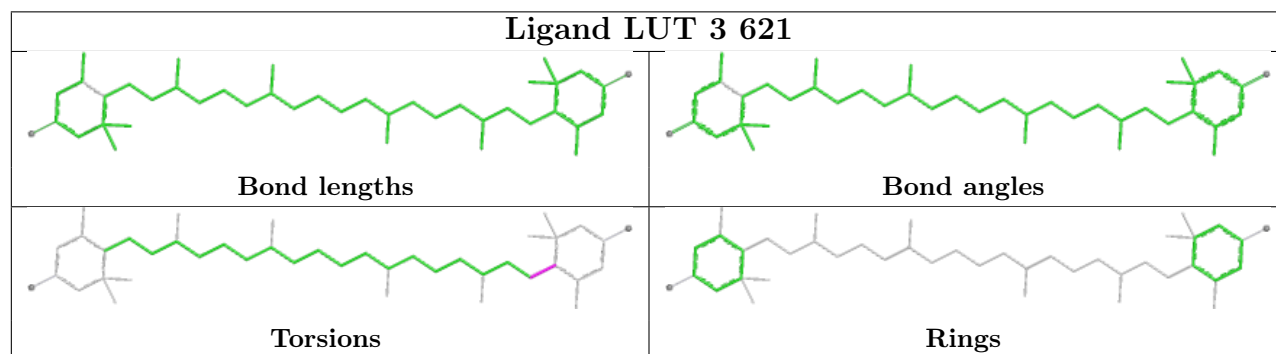
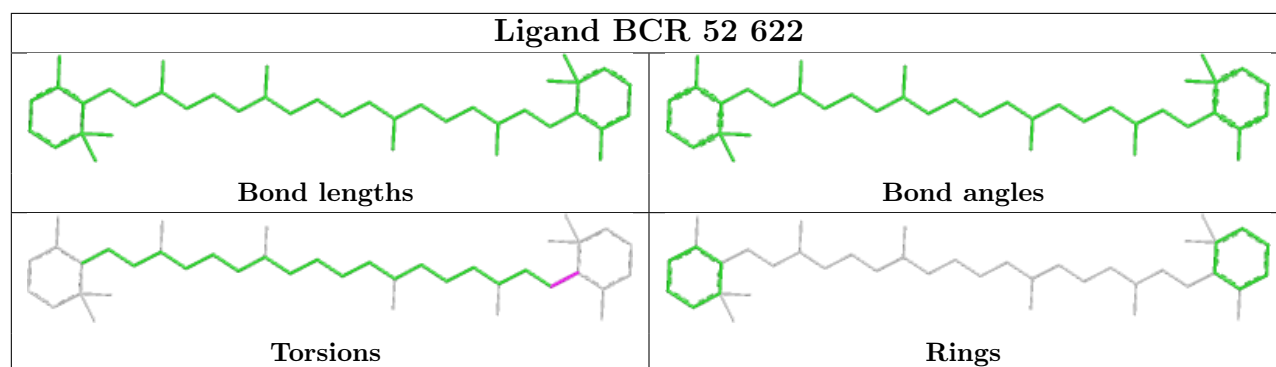
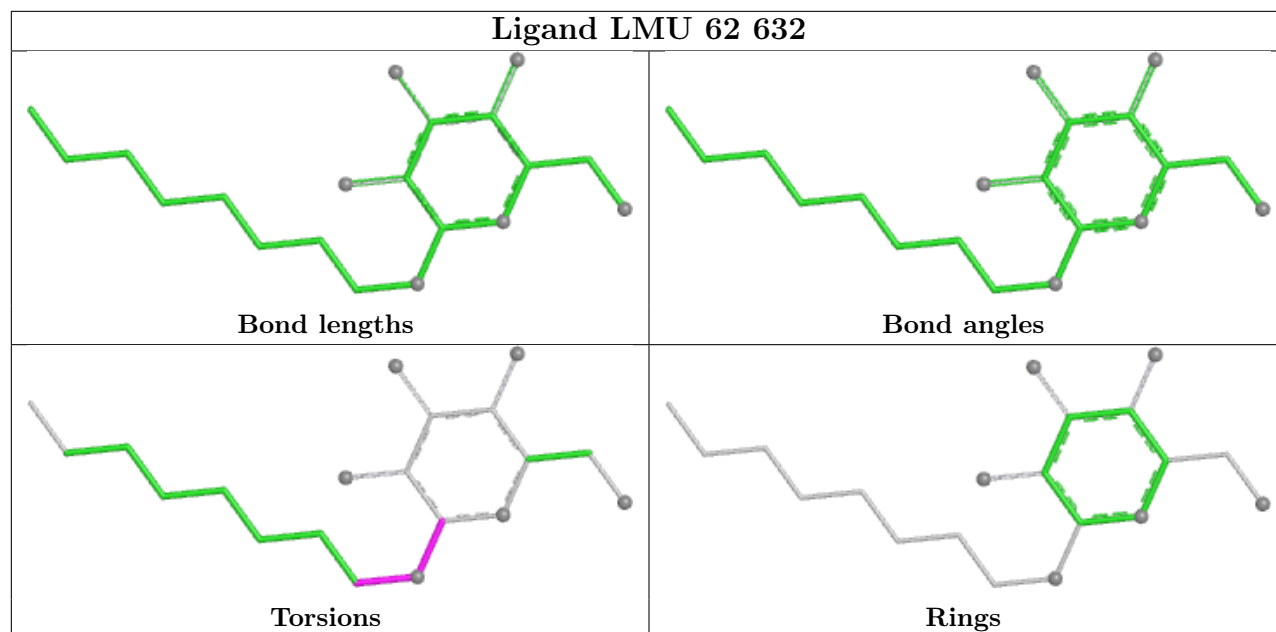
Ligand CHL Z2 606

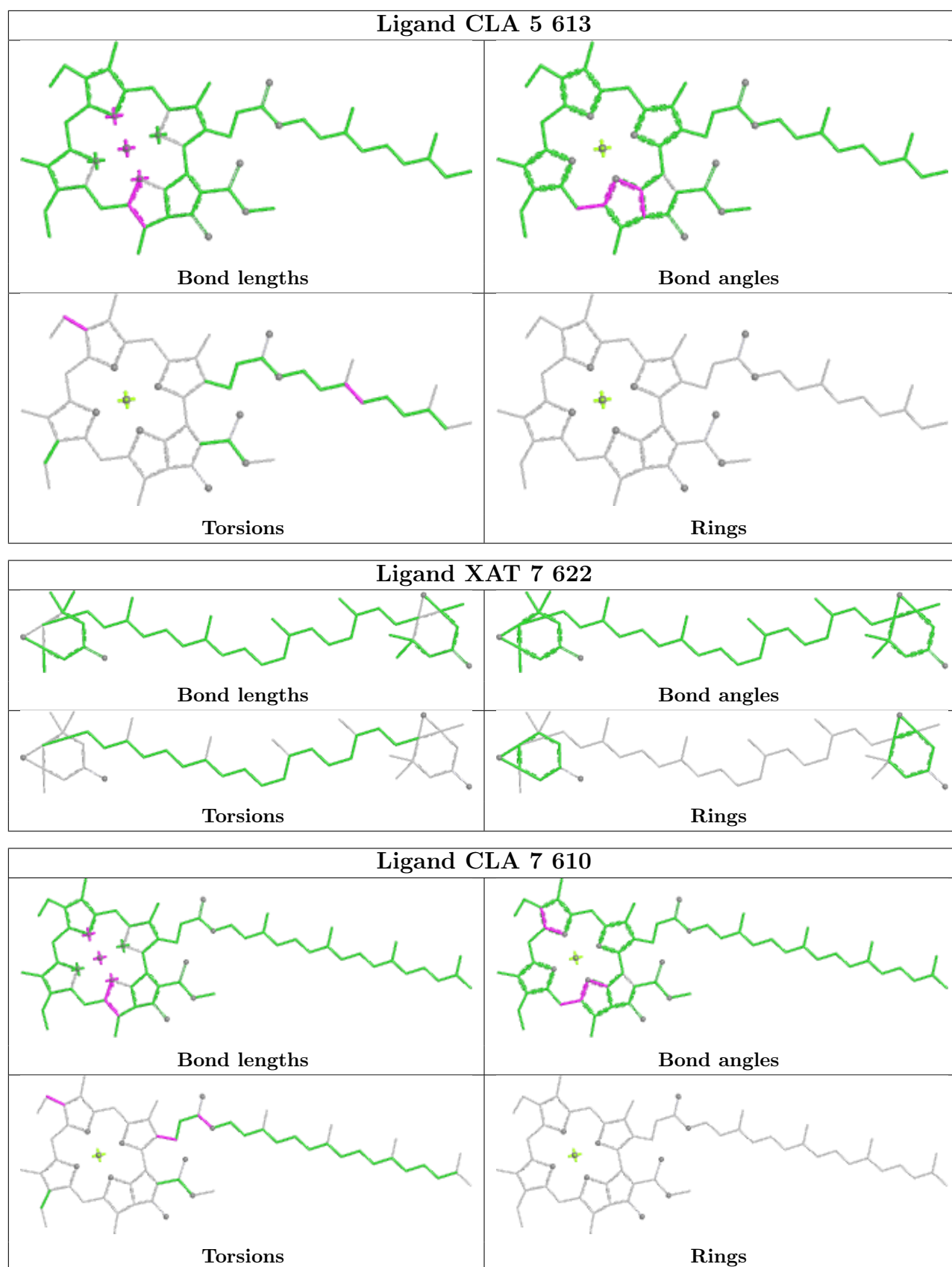


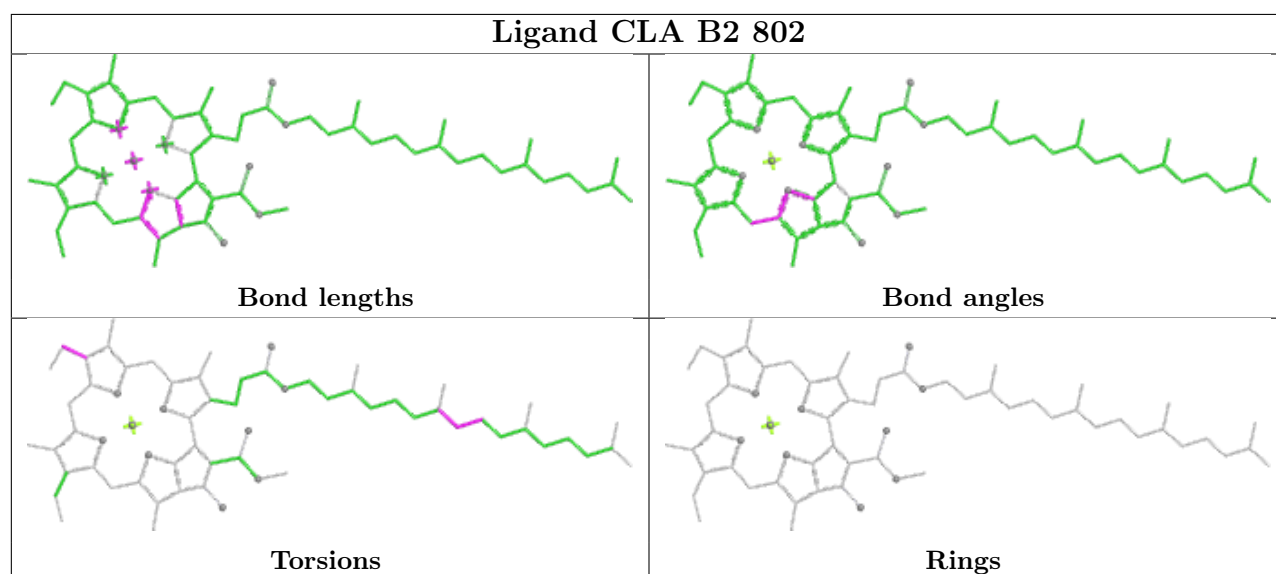
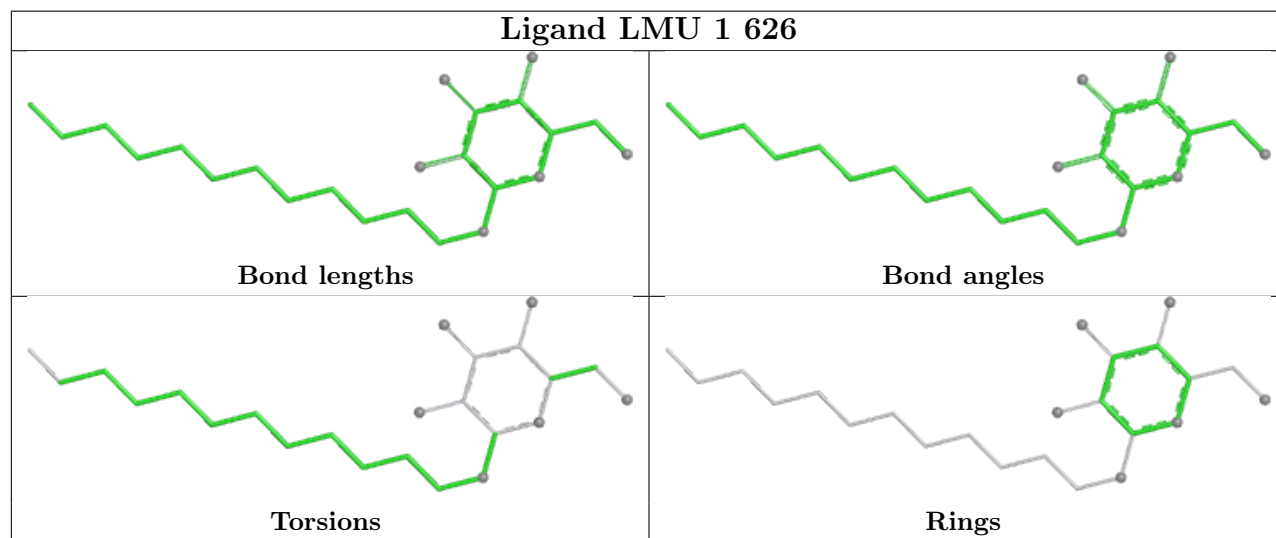
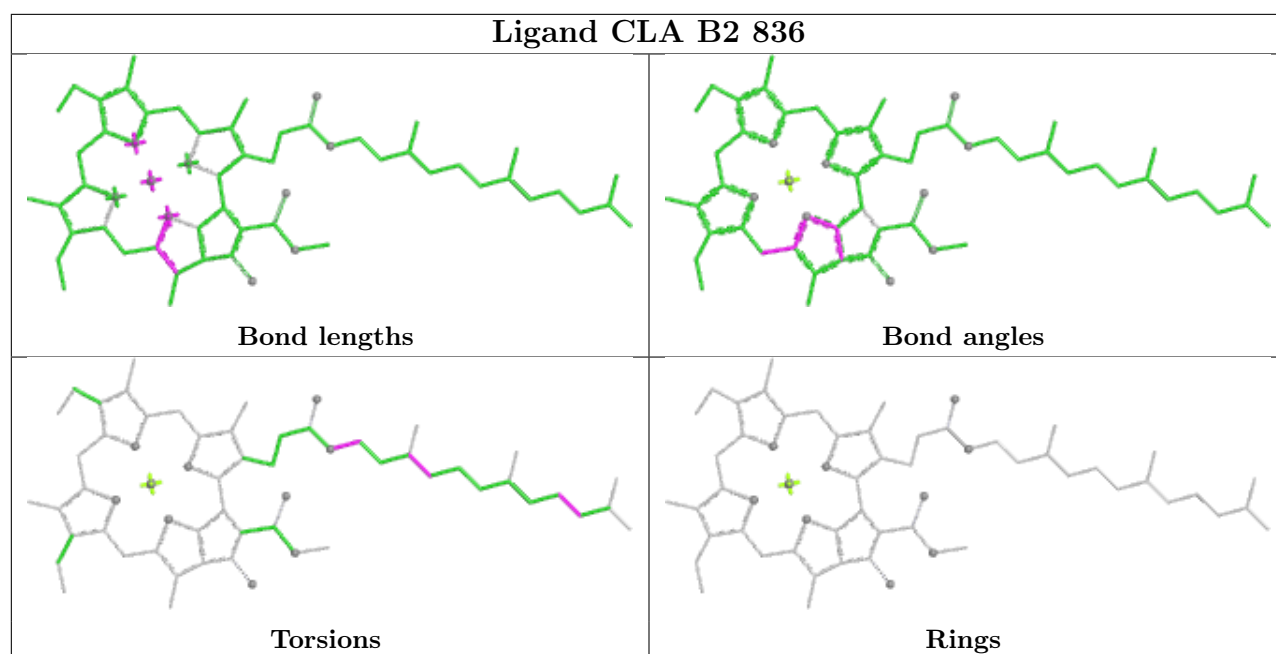


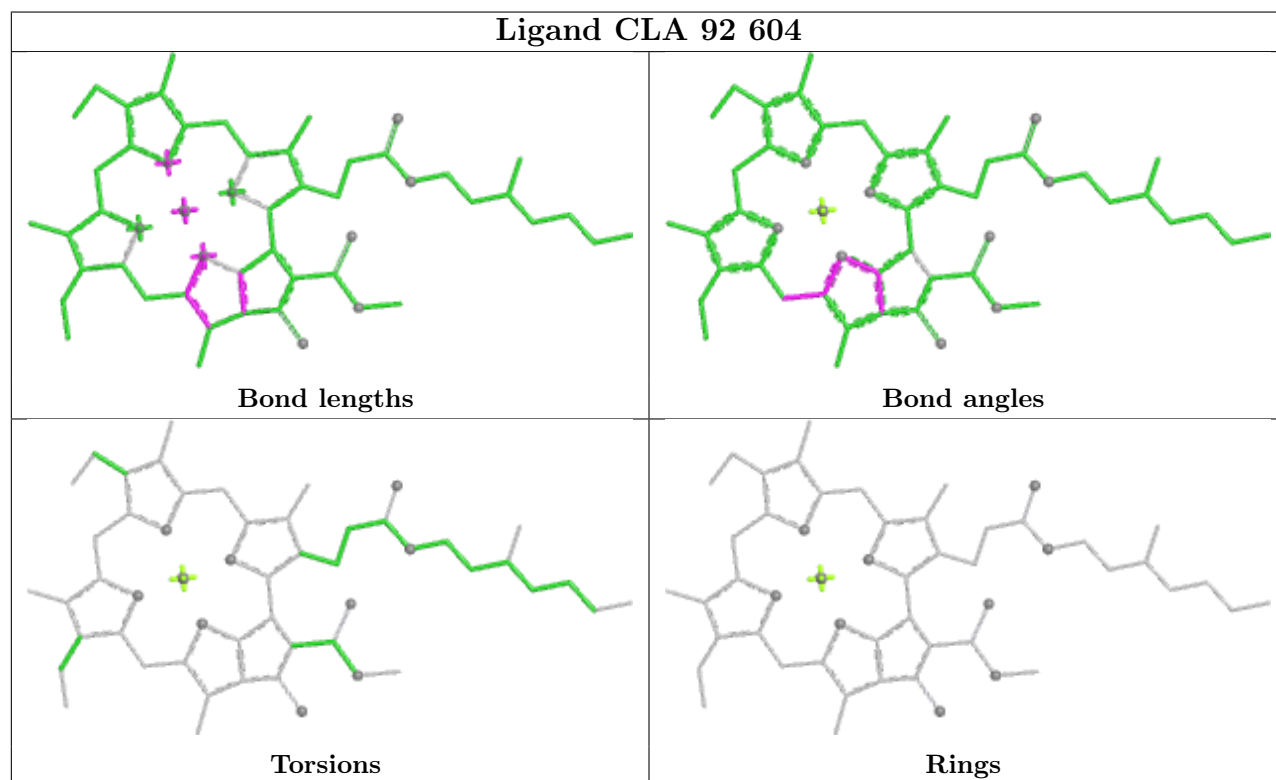
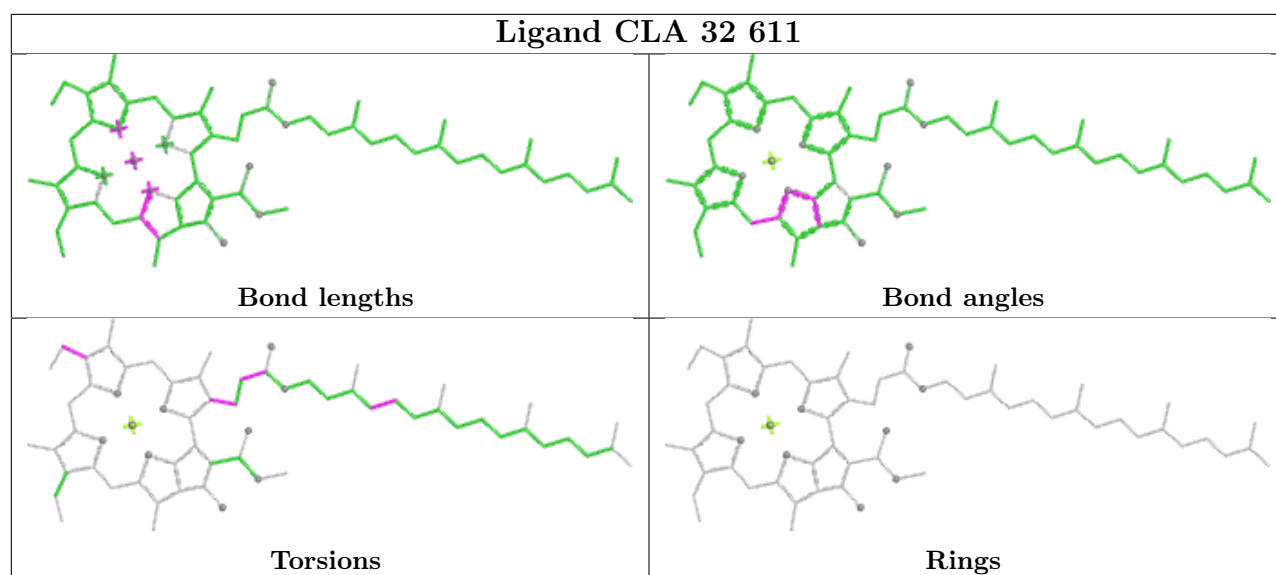


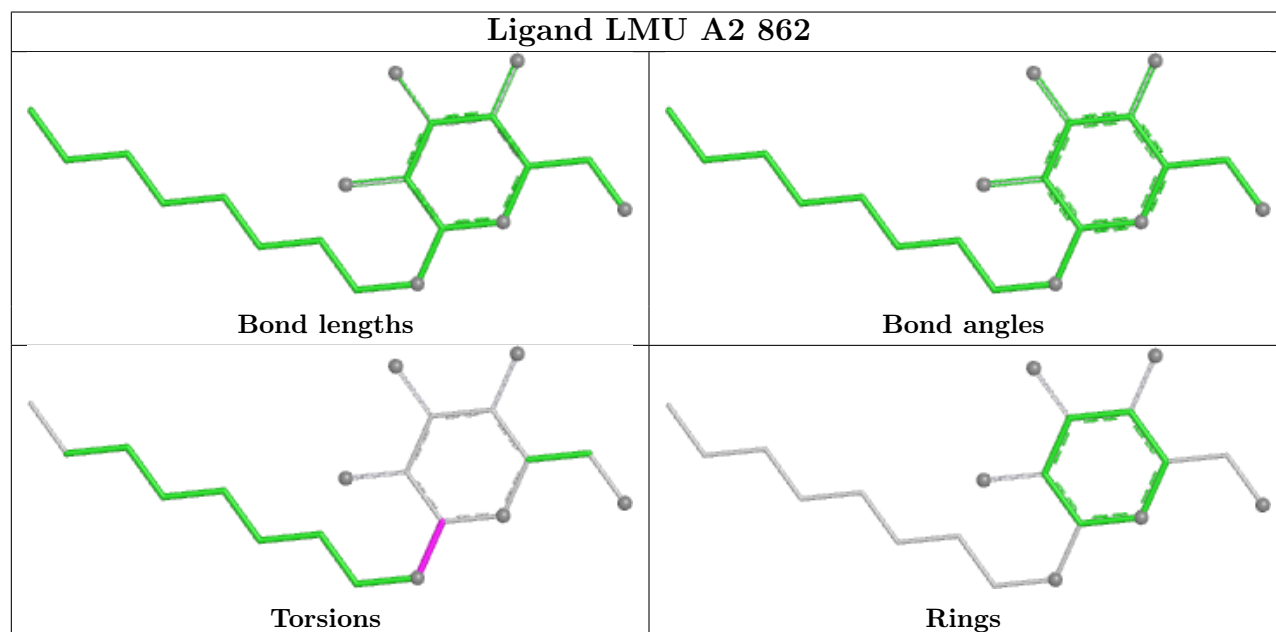
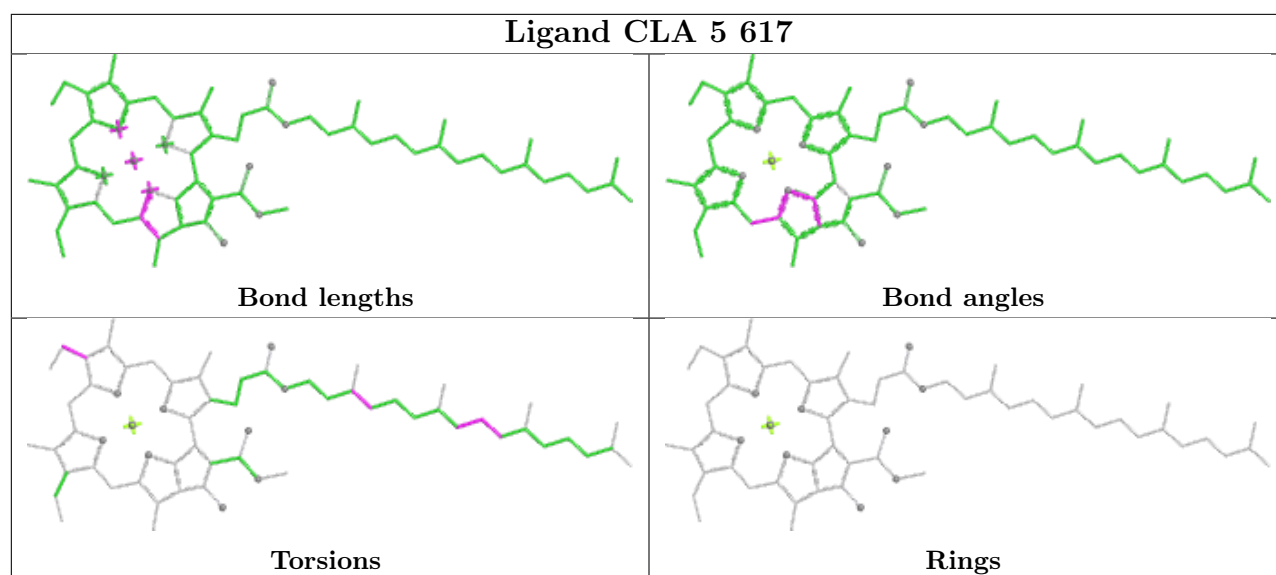




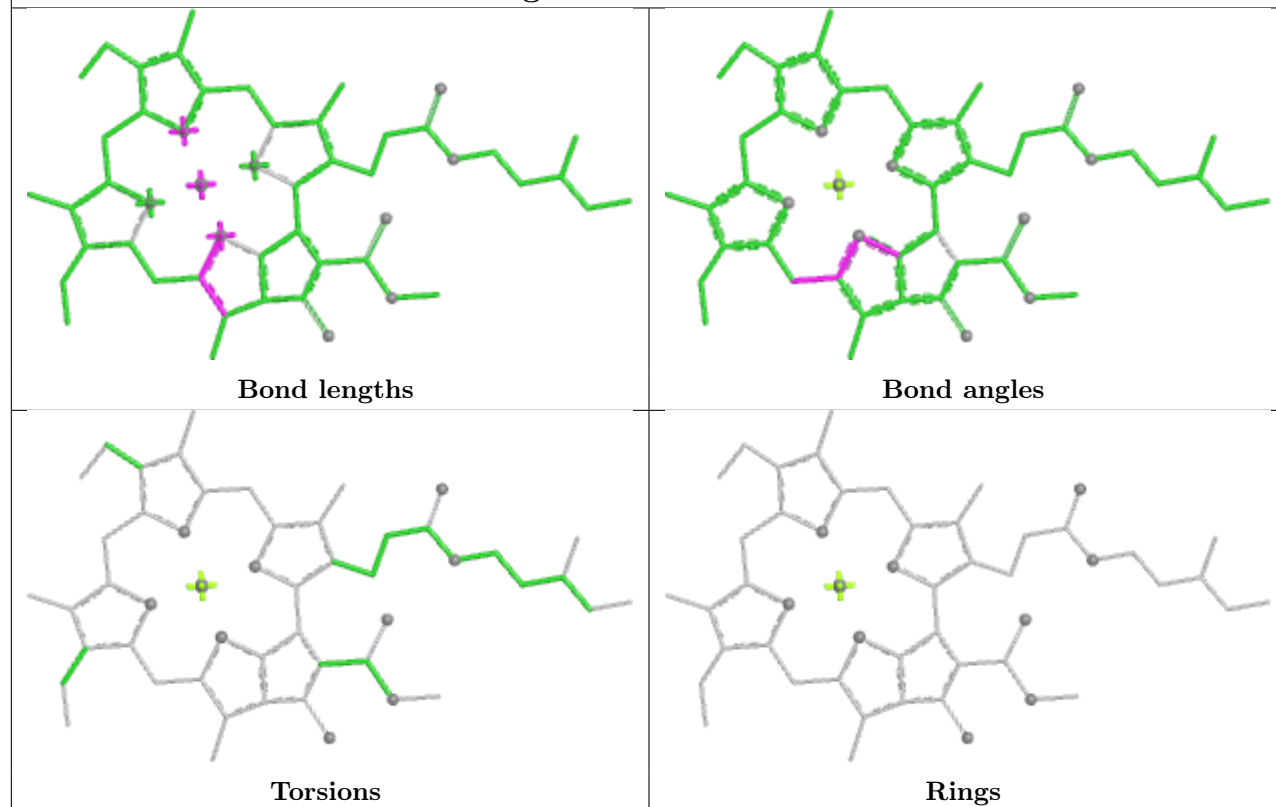




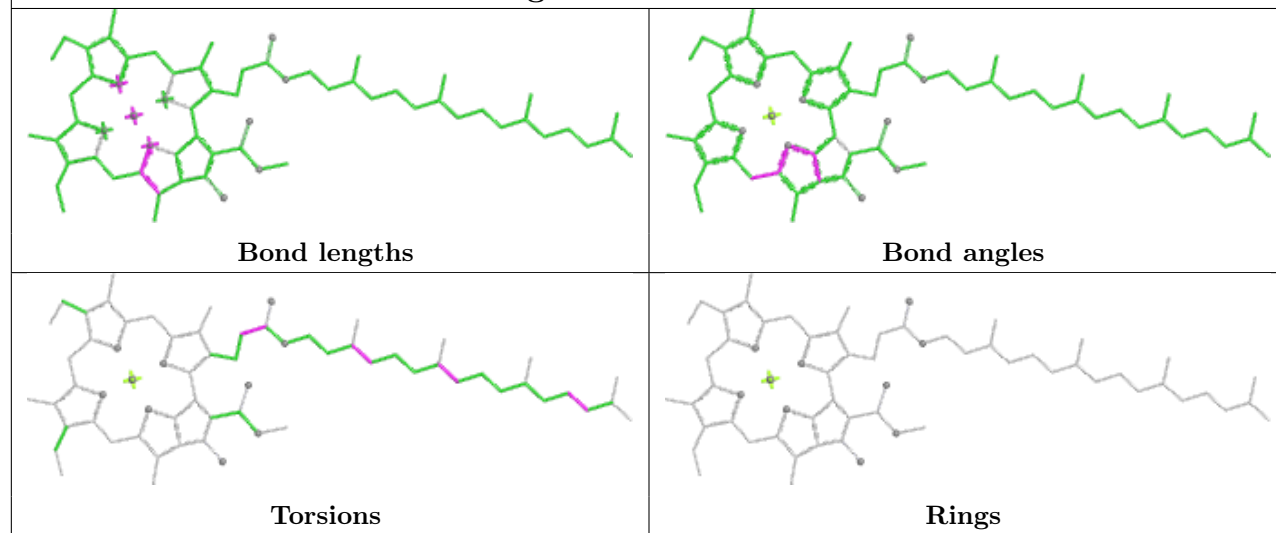


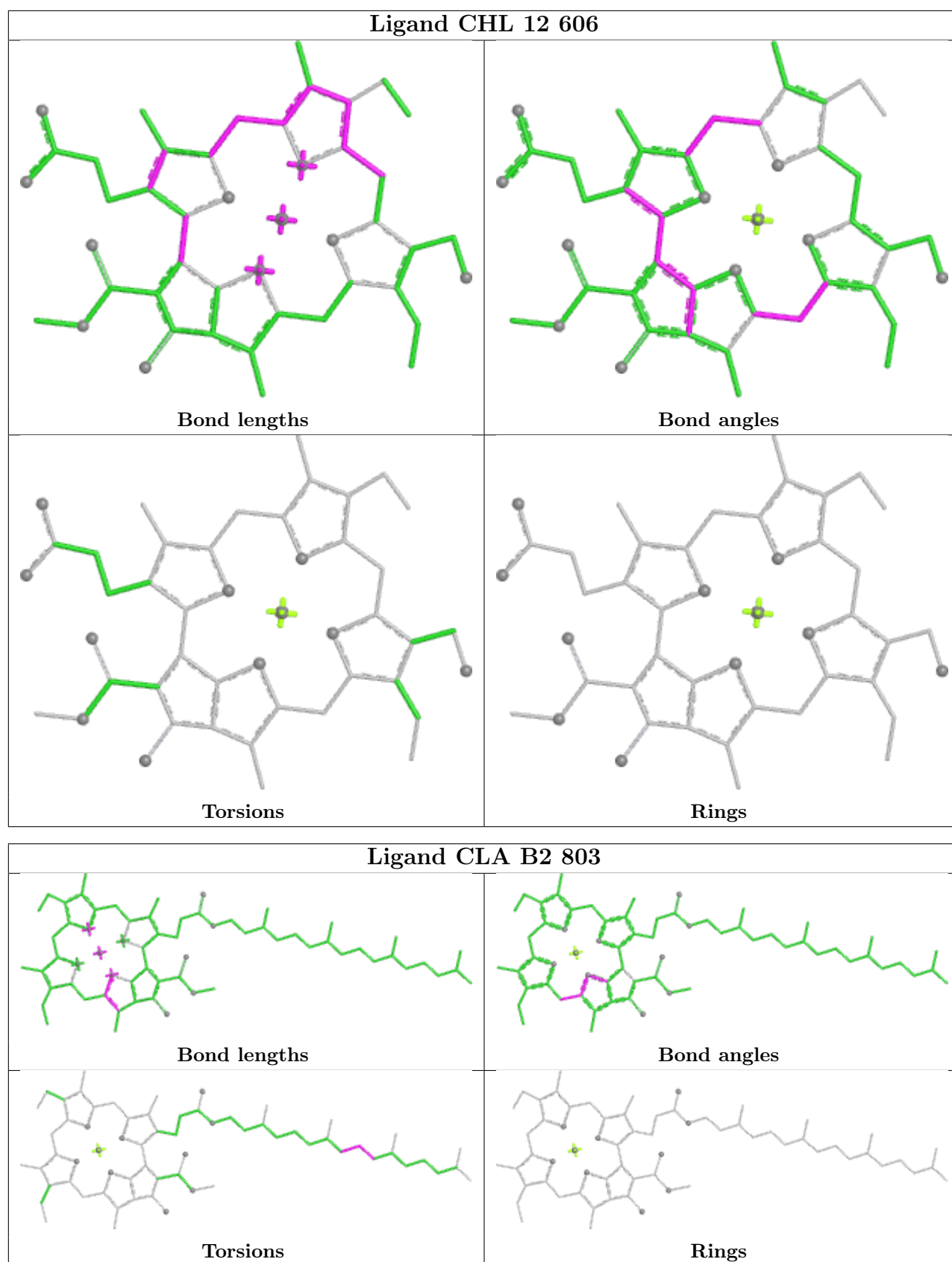


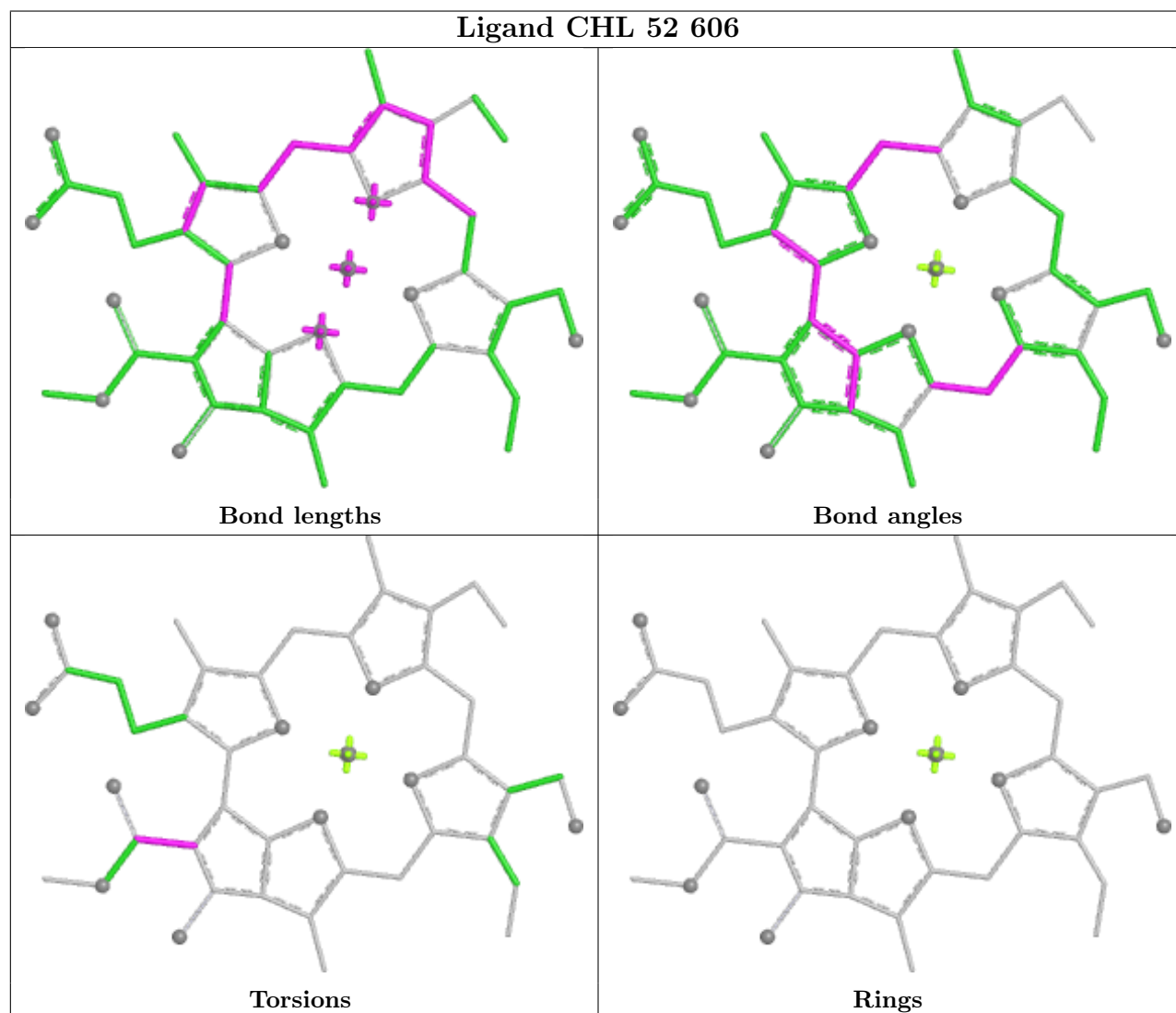
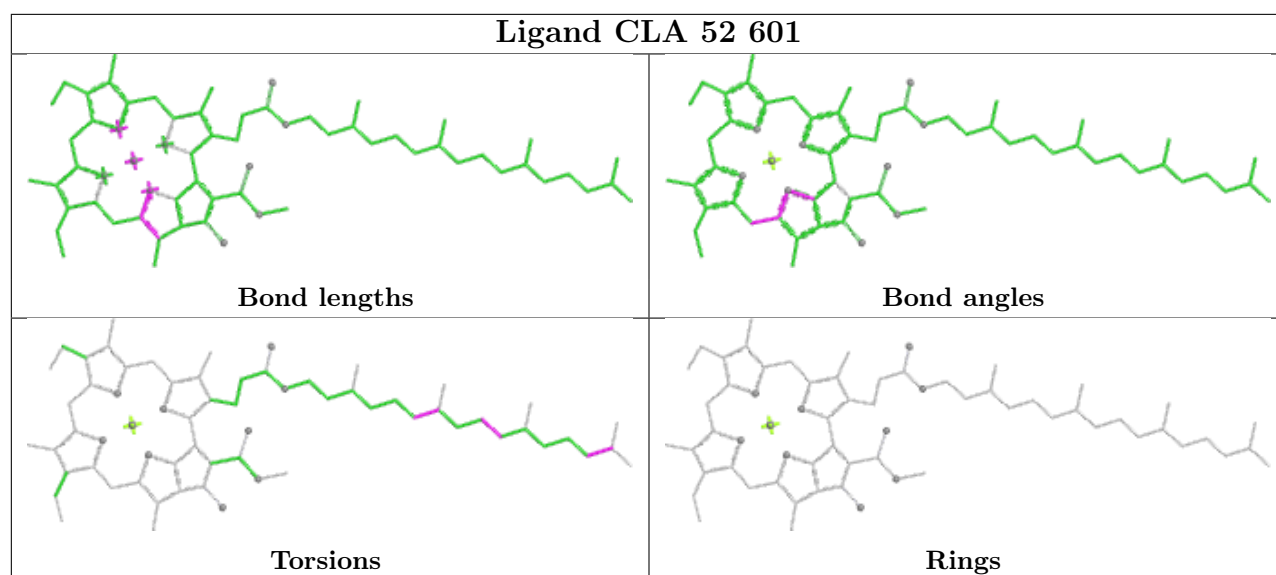
Ligand CLA A2 838

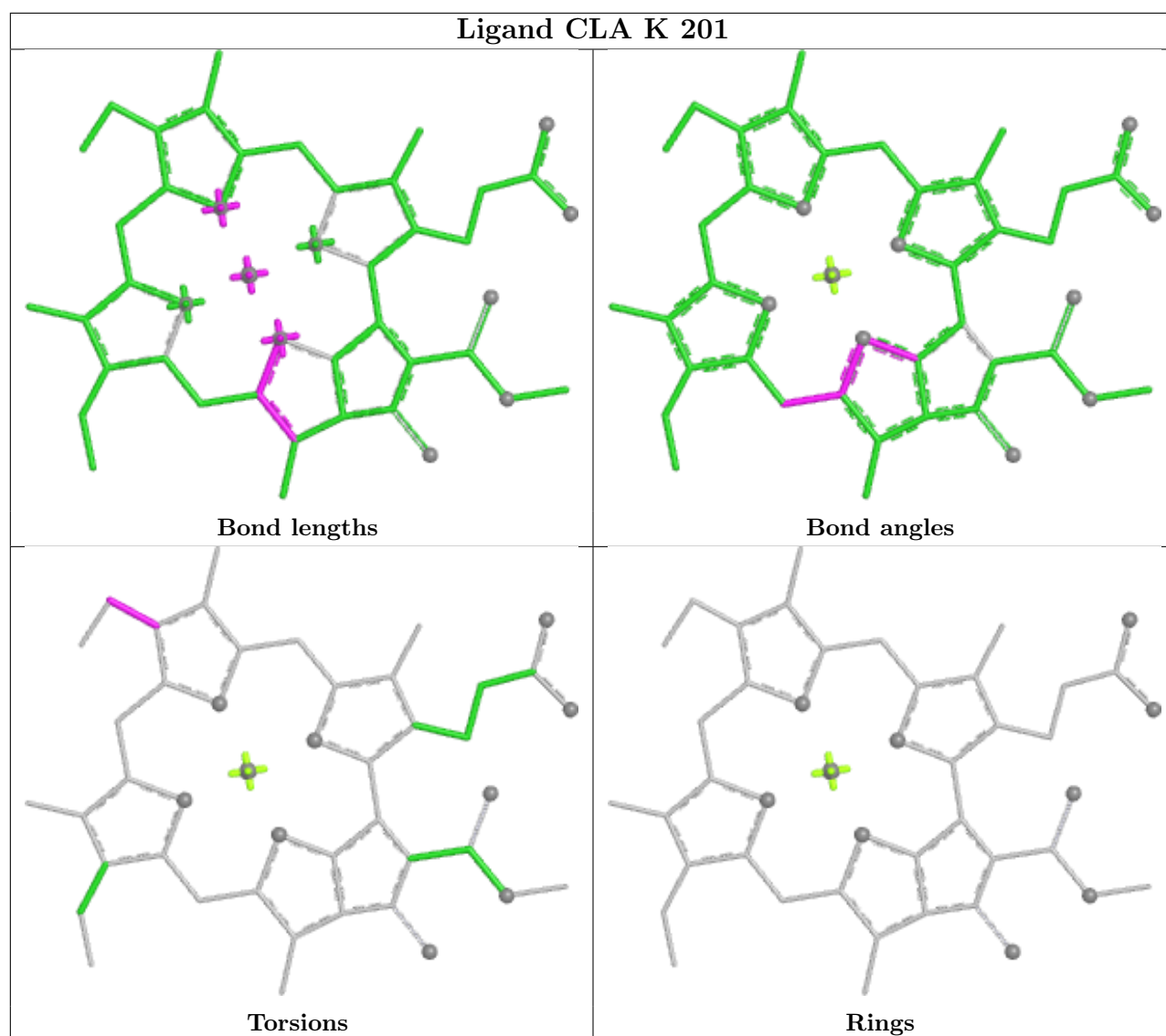


Ligand CLA 12 609

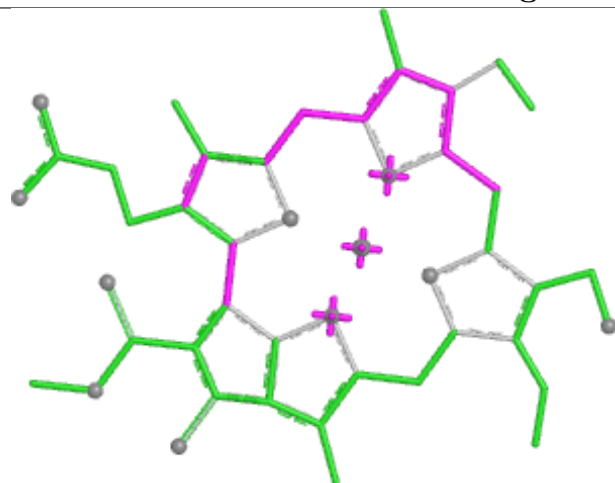




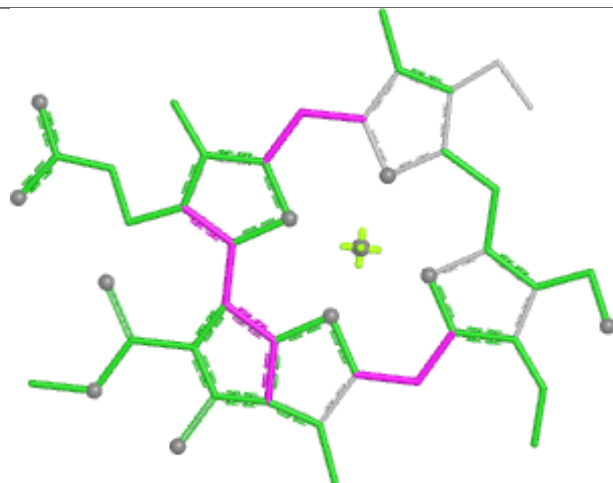




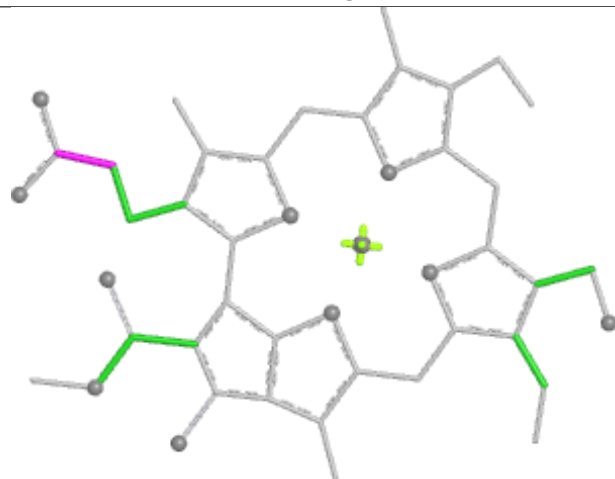
Ligand CHL 7 606



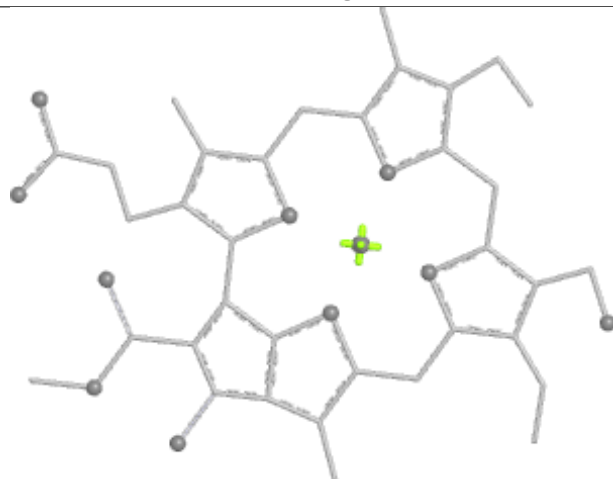
Bond lengths



Bond angles

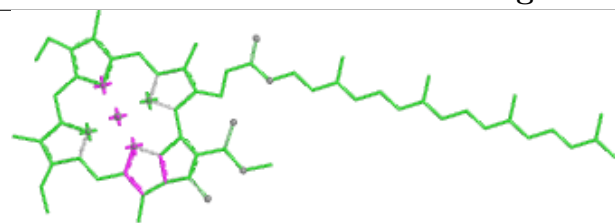


Torsions

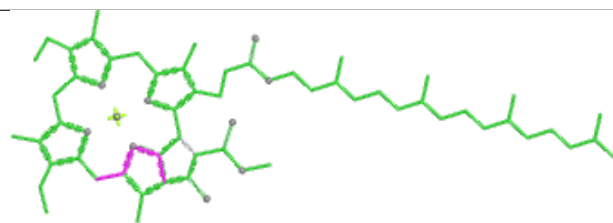


Rings

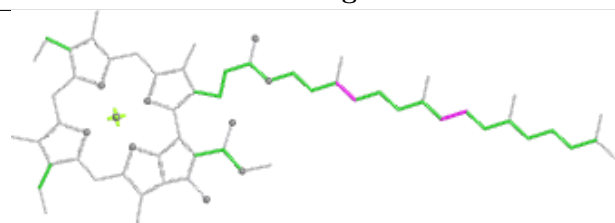
Ligand CLA B 813



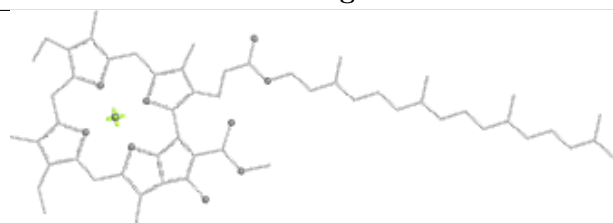
Bond lengths



Bond angles

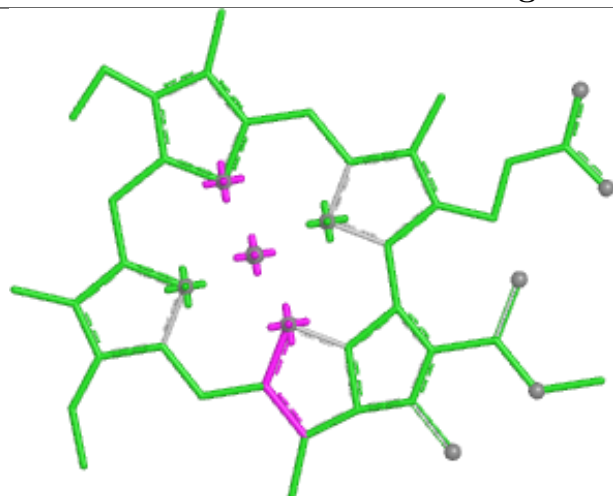


Torsions

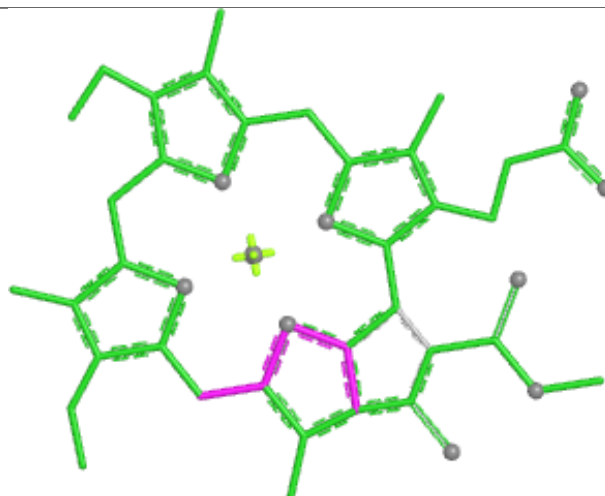


Rings

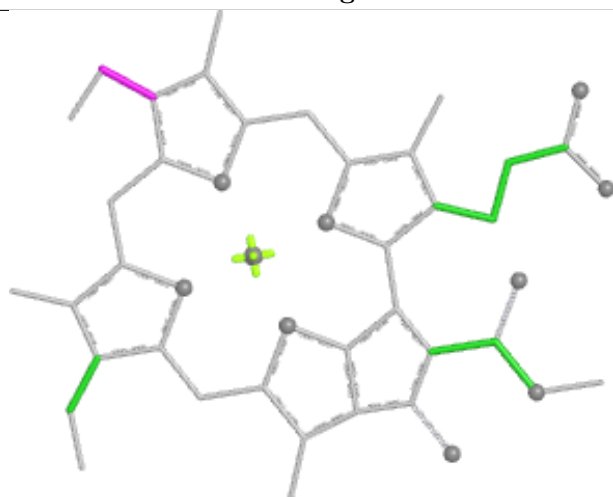
Ligand CLA 6 617



Bond lengths



Bond angles

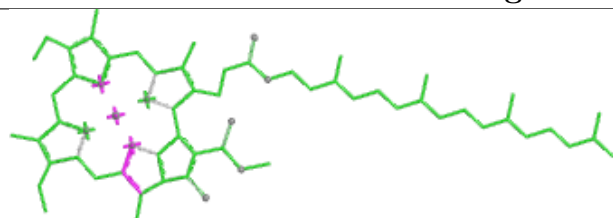


Torsions

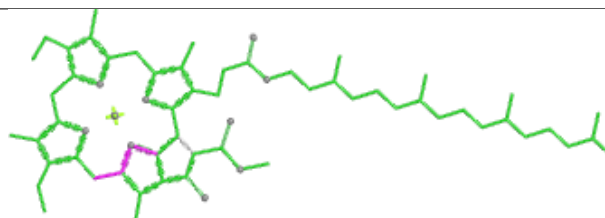


Rings

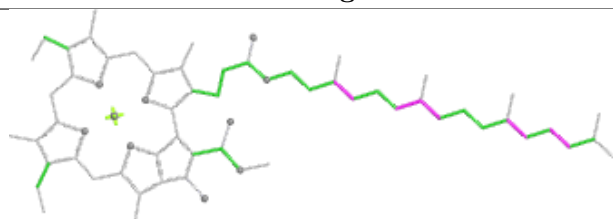
Ligand CLA A2 840



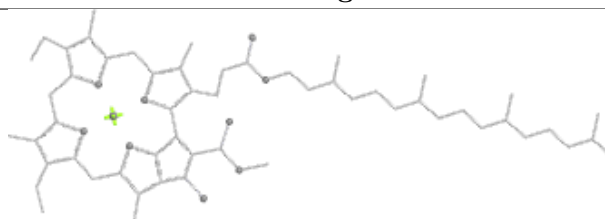
Bond lengths



Bond angles

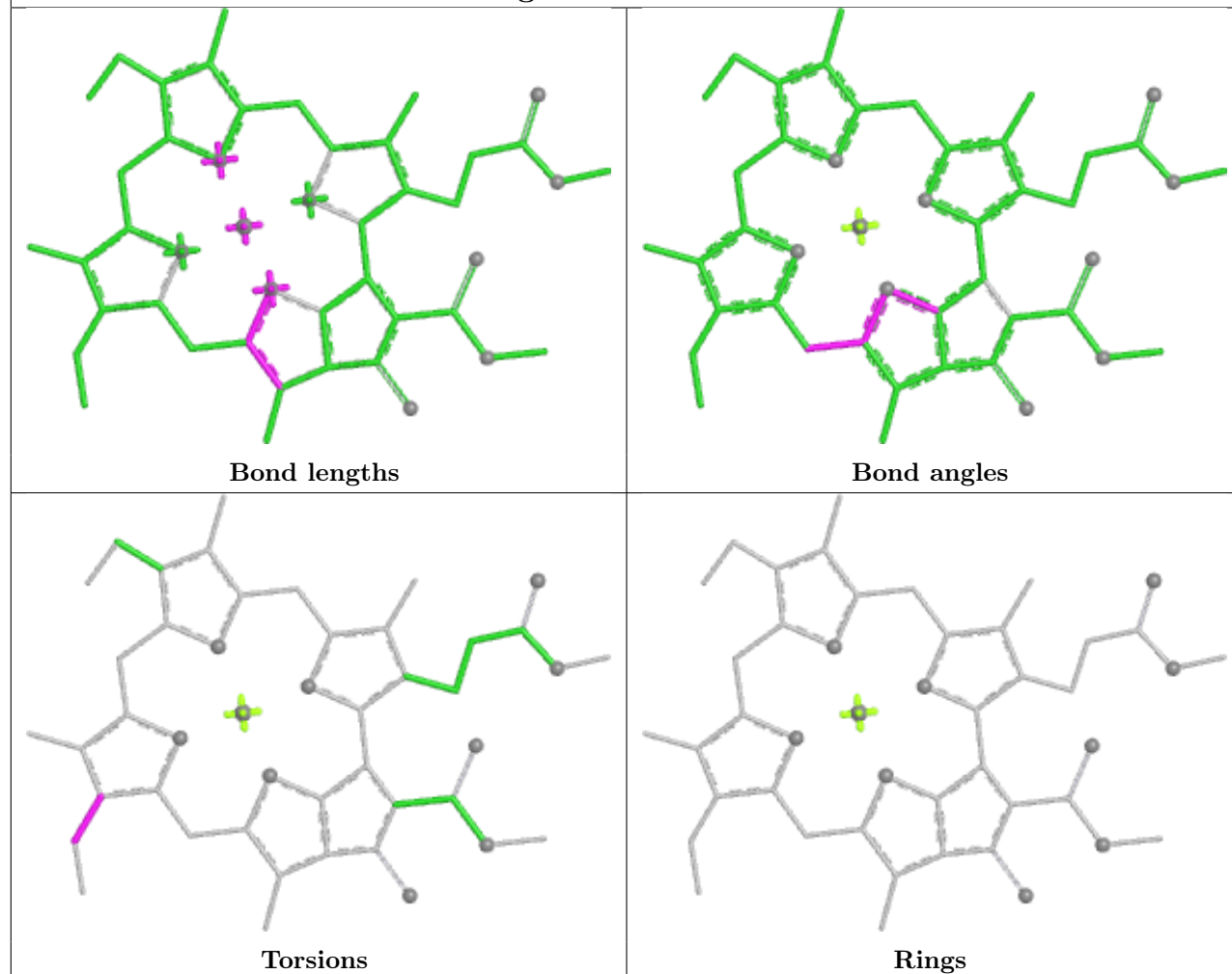


Torsions

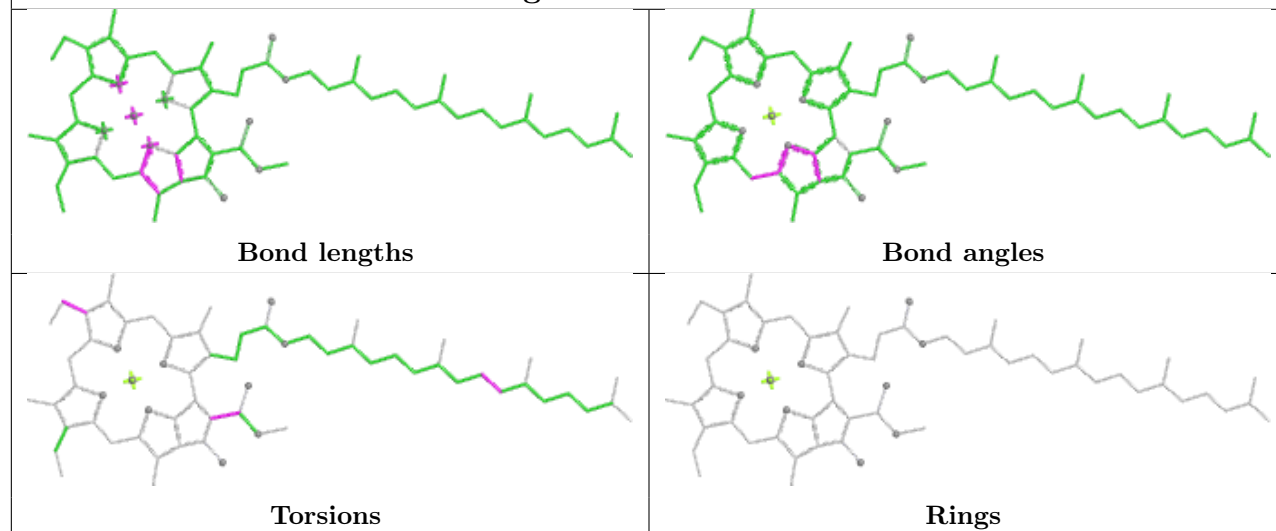


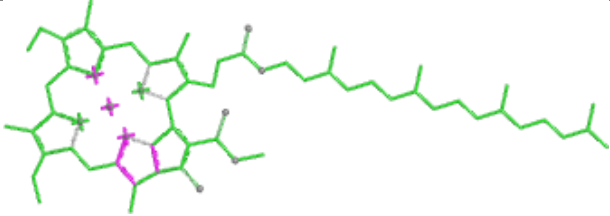
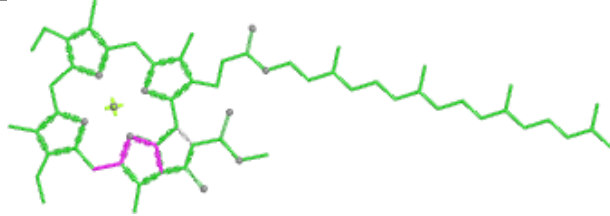
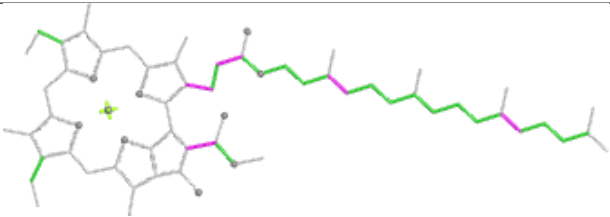
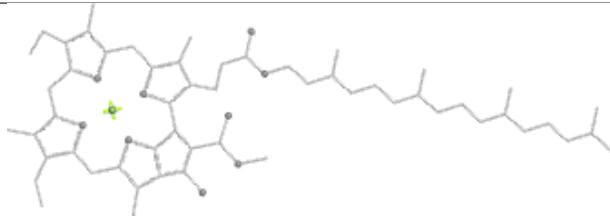
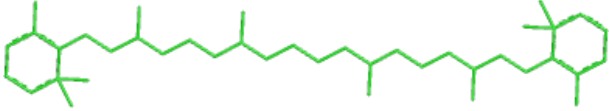
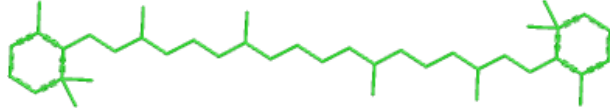
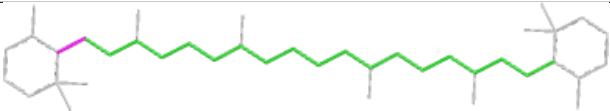
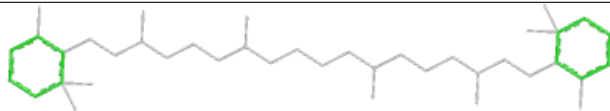
Rings

Ligand CLA 3 617

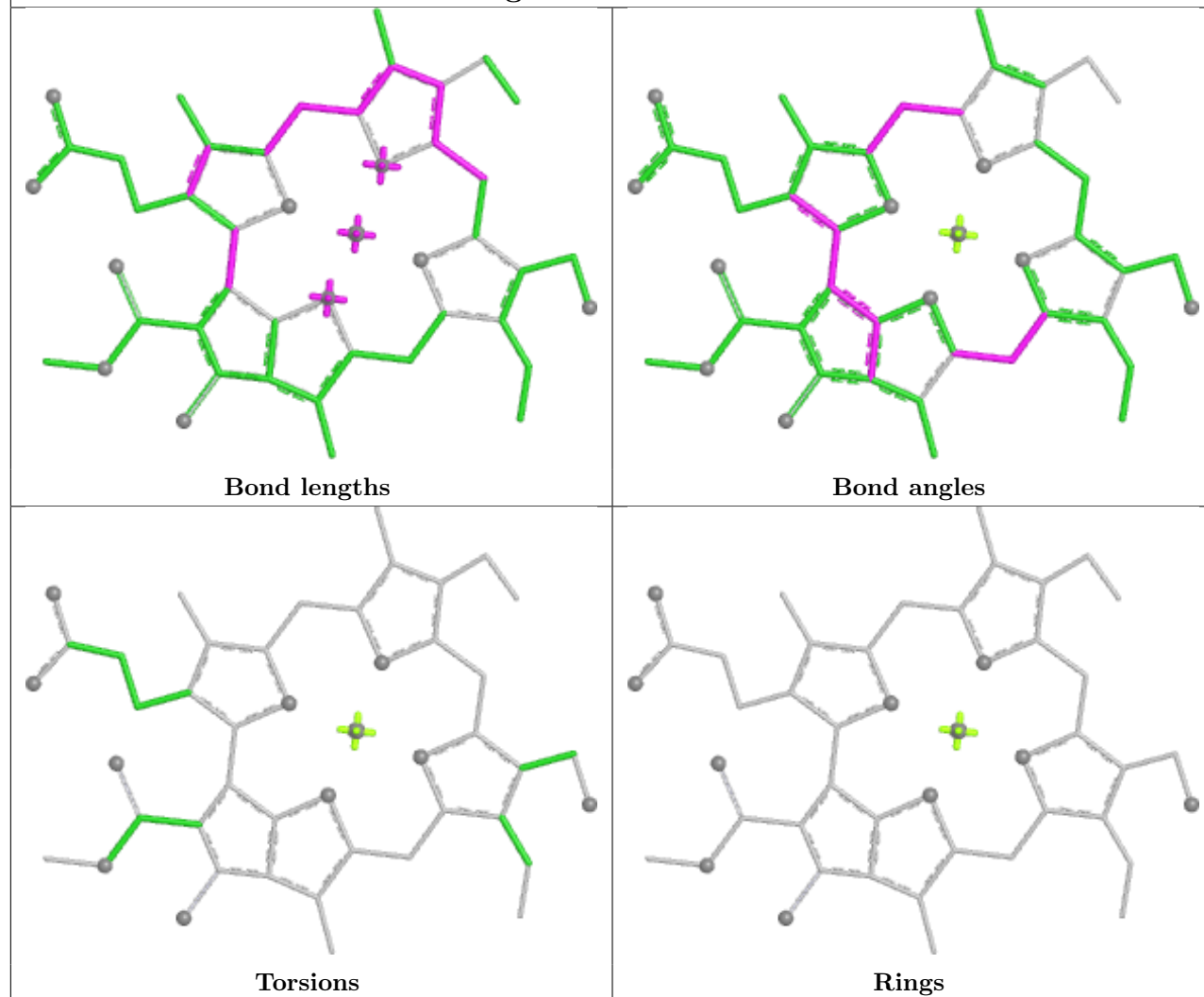


Ligand CLA B2 821

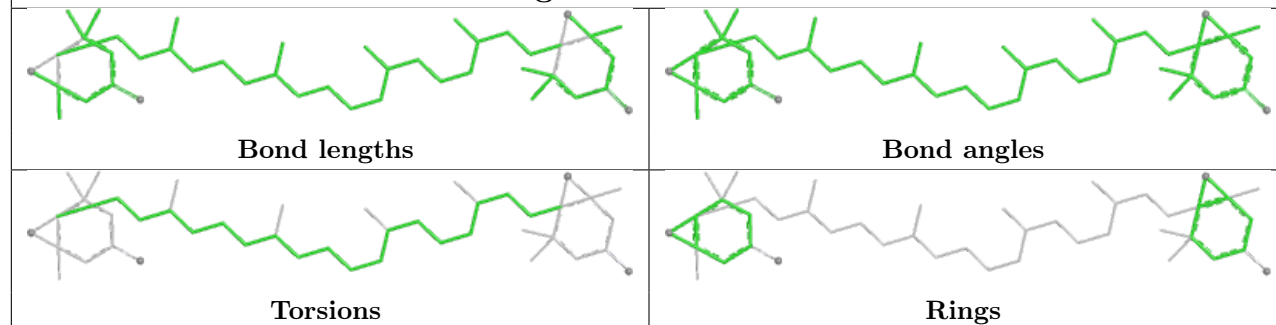


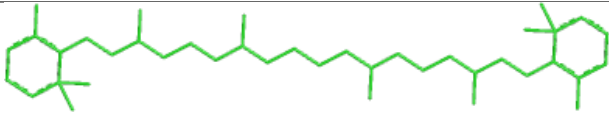
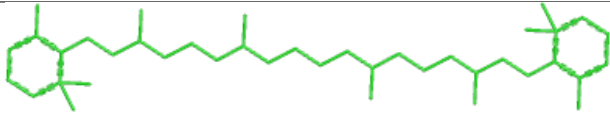
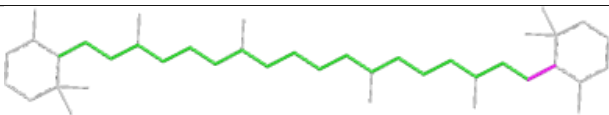
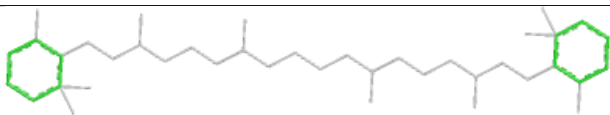
Ligand CLA B2 805	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A2 848	
 Bond lengths	 Bond angles
 Torsions	 Rings

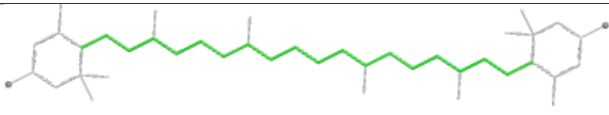
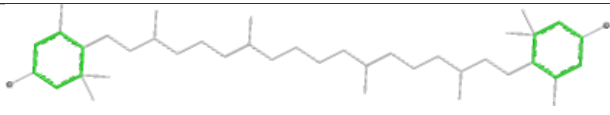
Ligand CHL 1 606

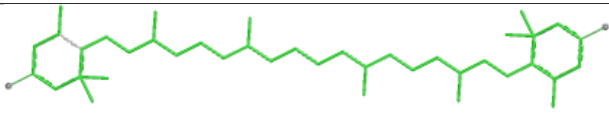
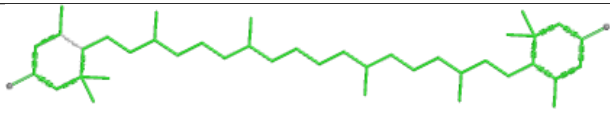
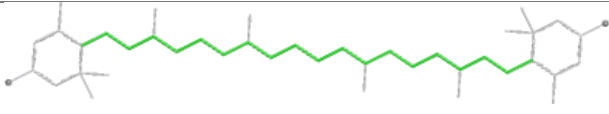
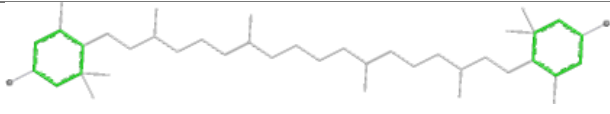


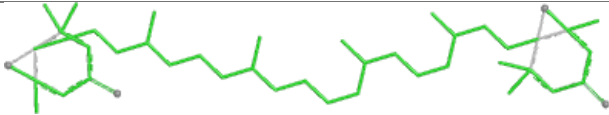
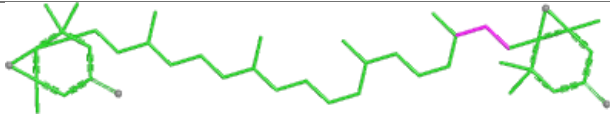
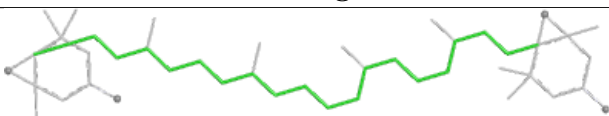
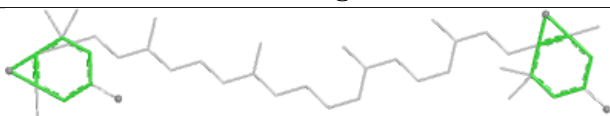
Ligand XAT 6 624

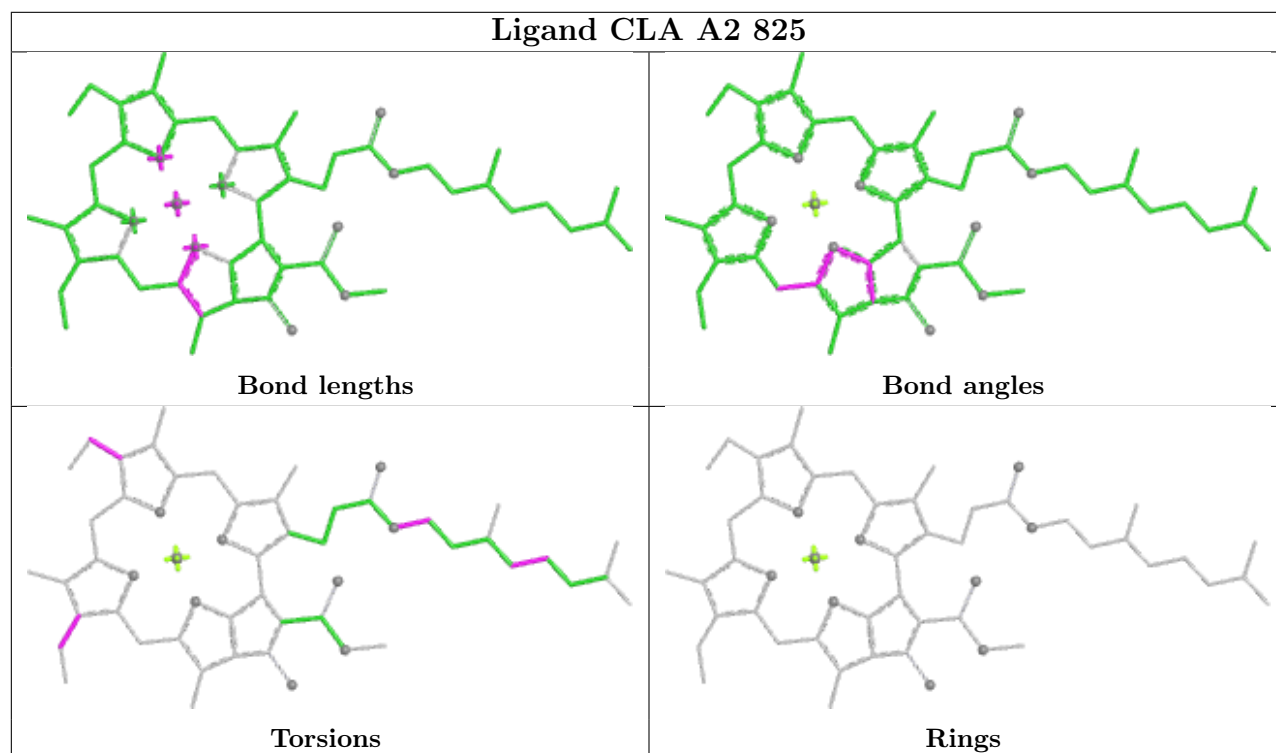
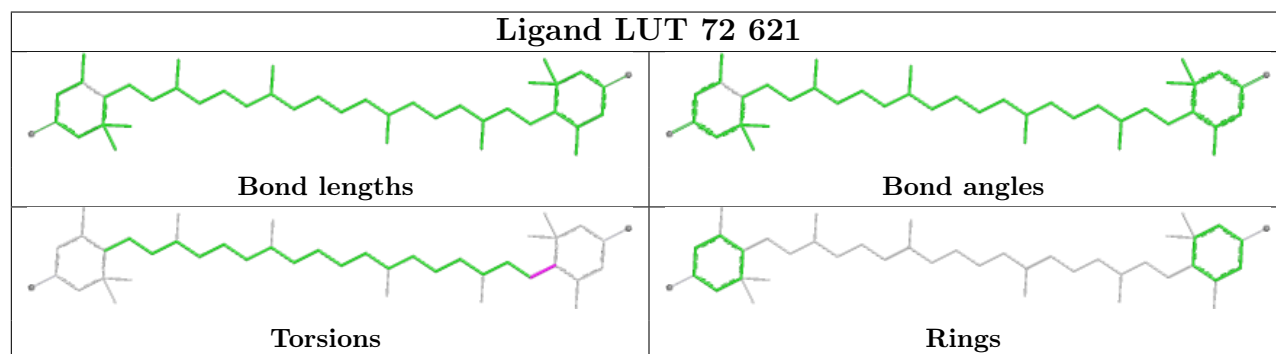
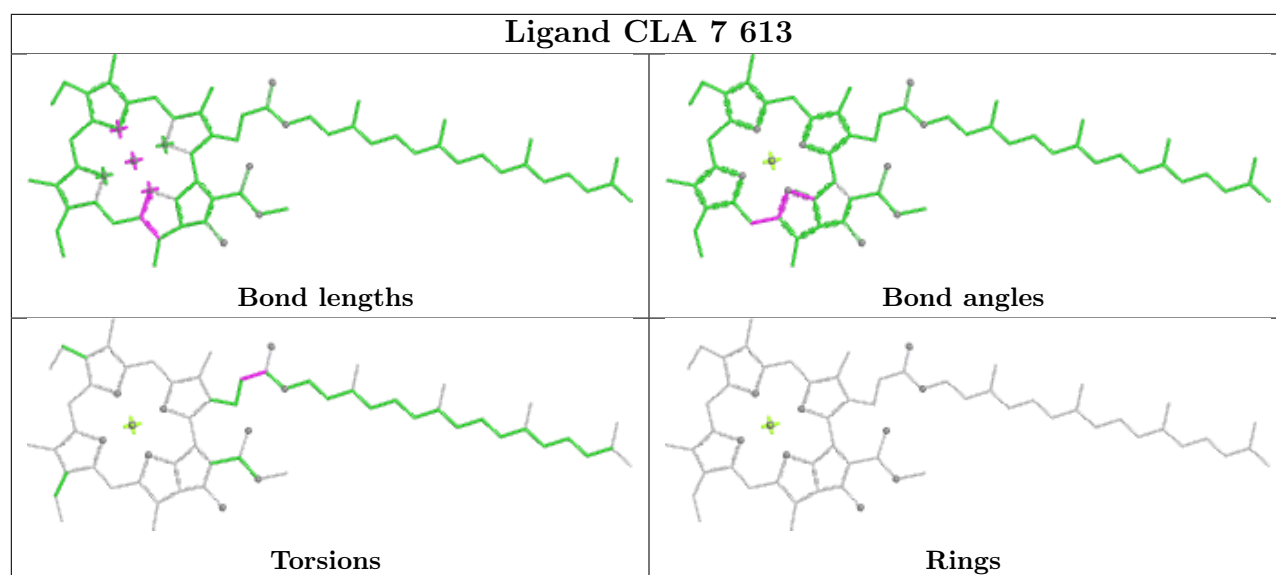


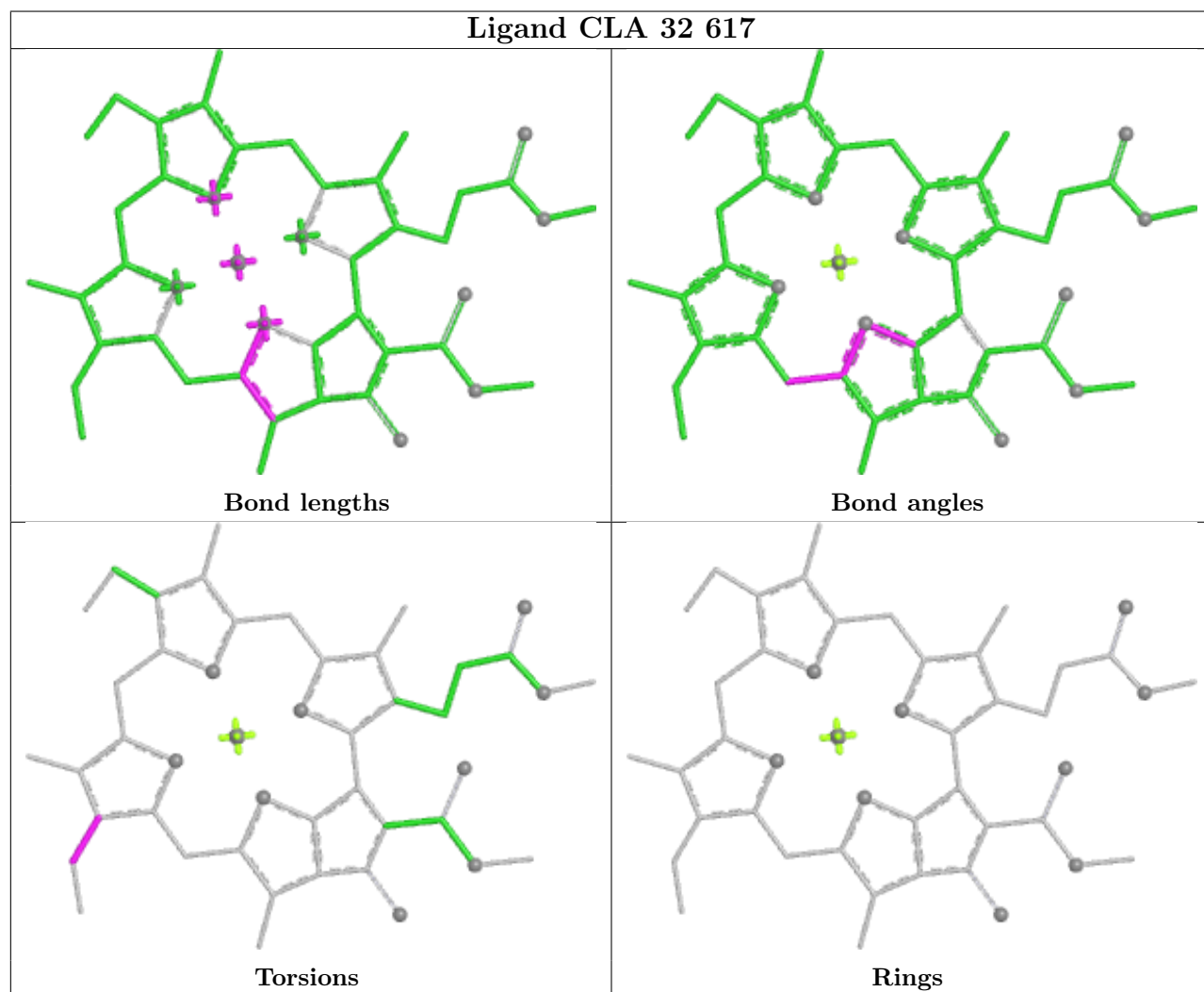
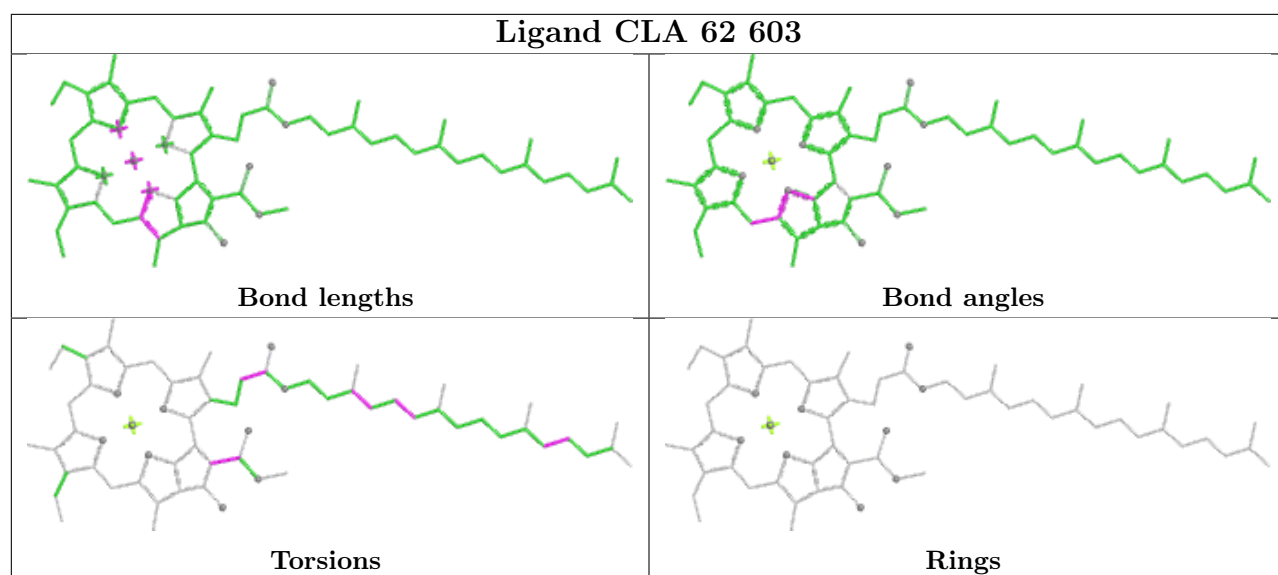
Ligand BCR B 846	
	
Bond lengths	Bond angles
	
Torsions	Rings

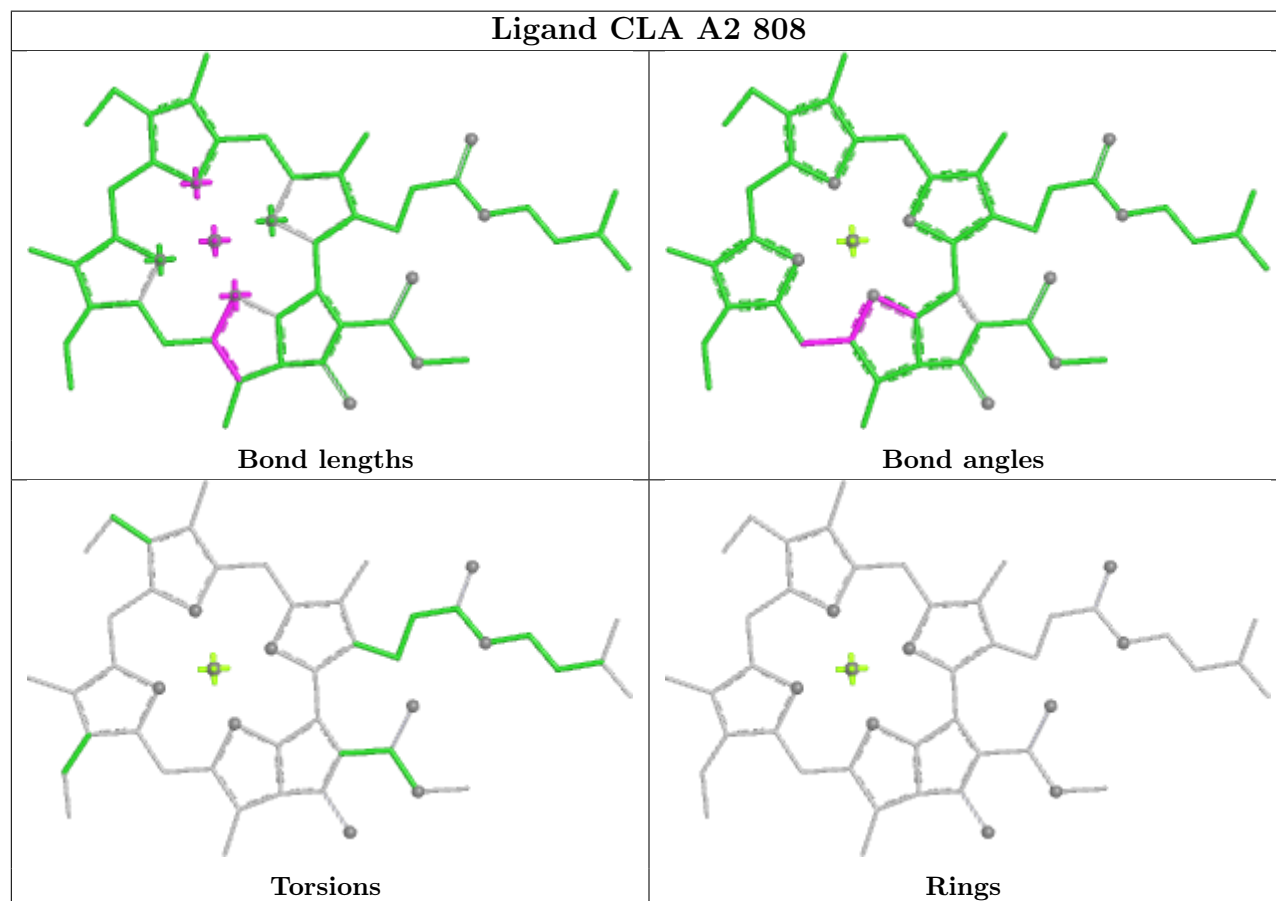
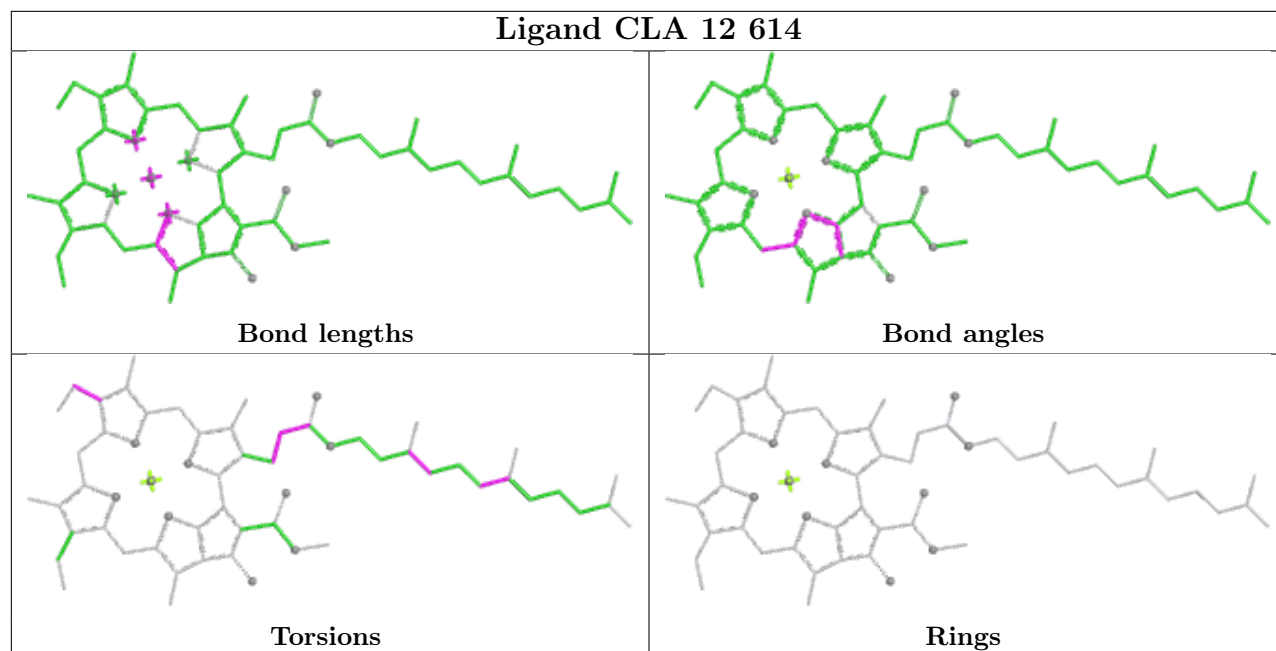
Ligand LUT 9 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

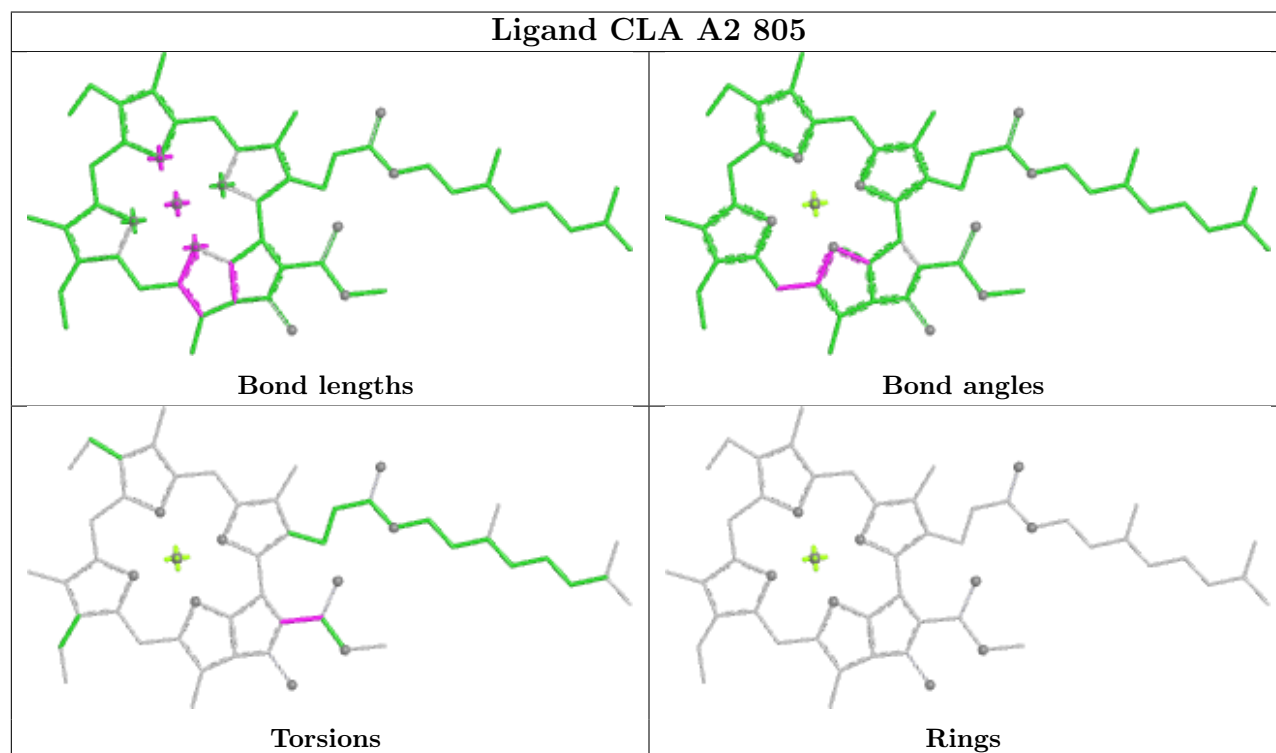
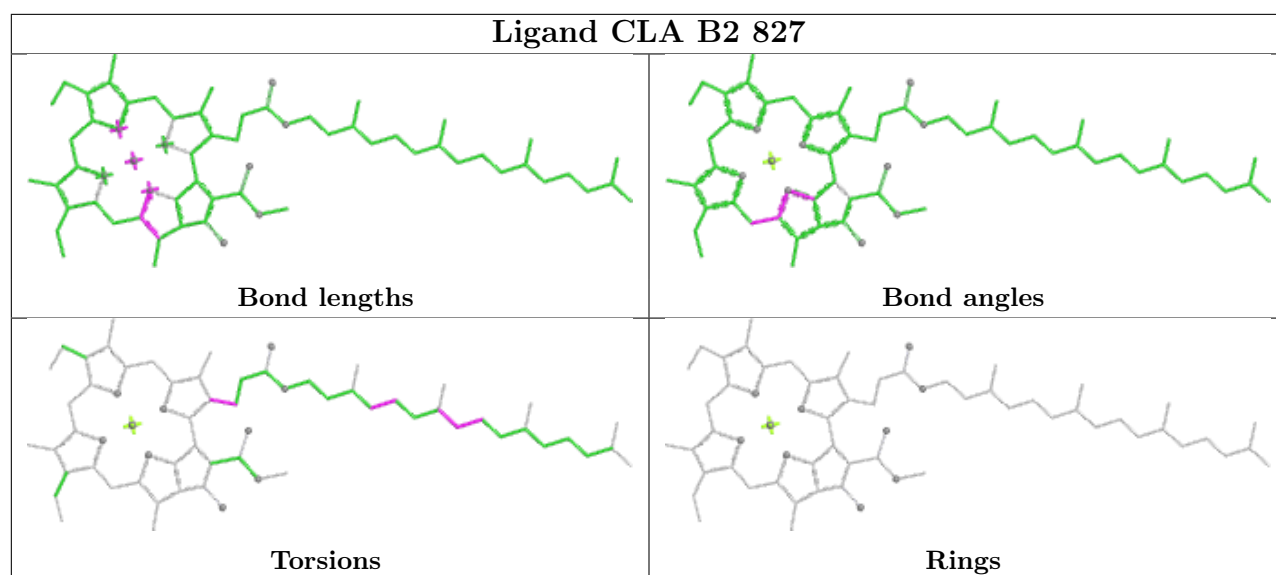
Ligand LUT 92 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

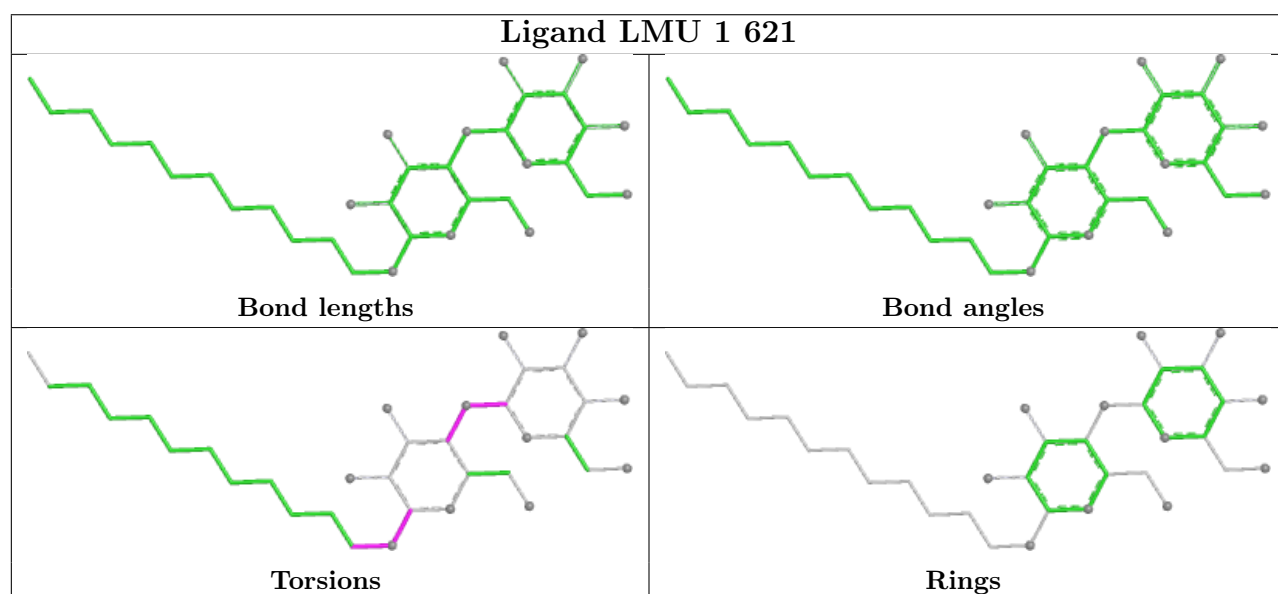
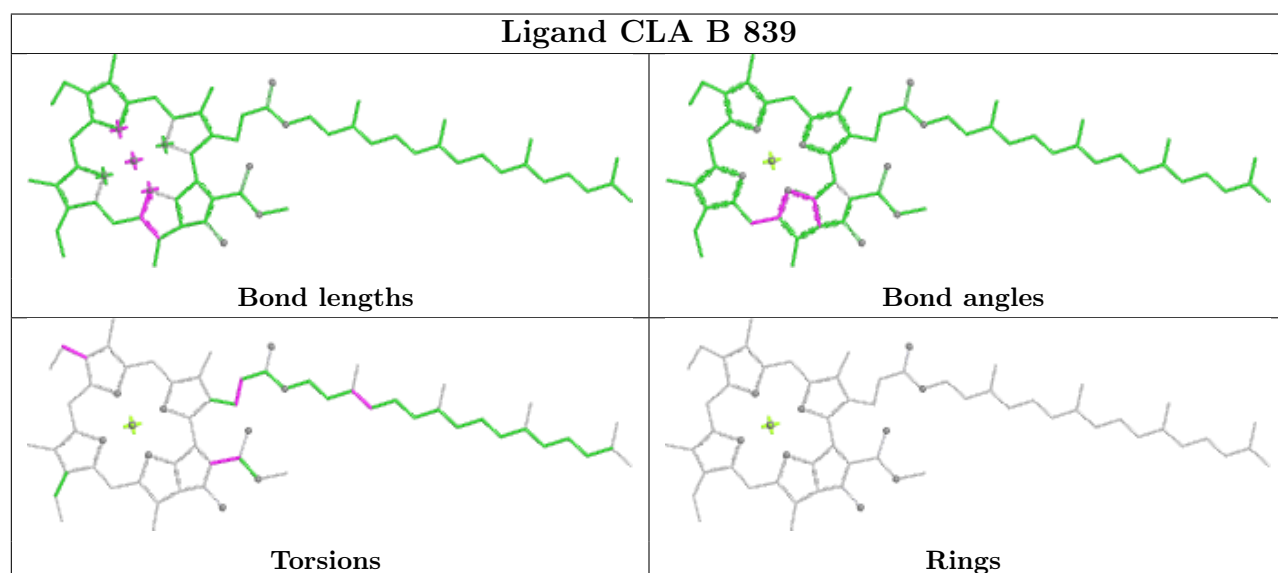
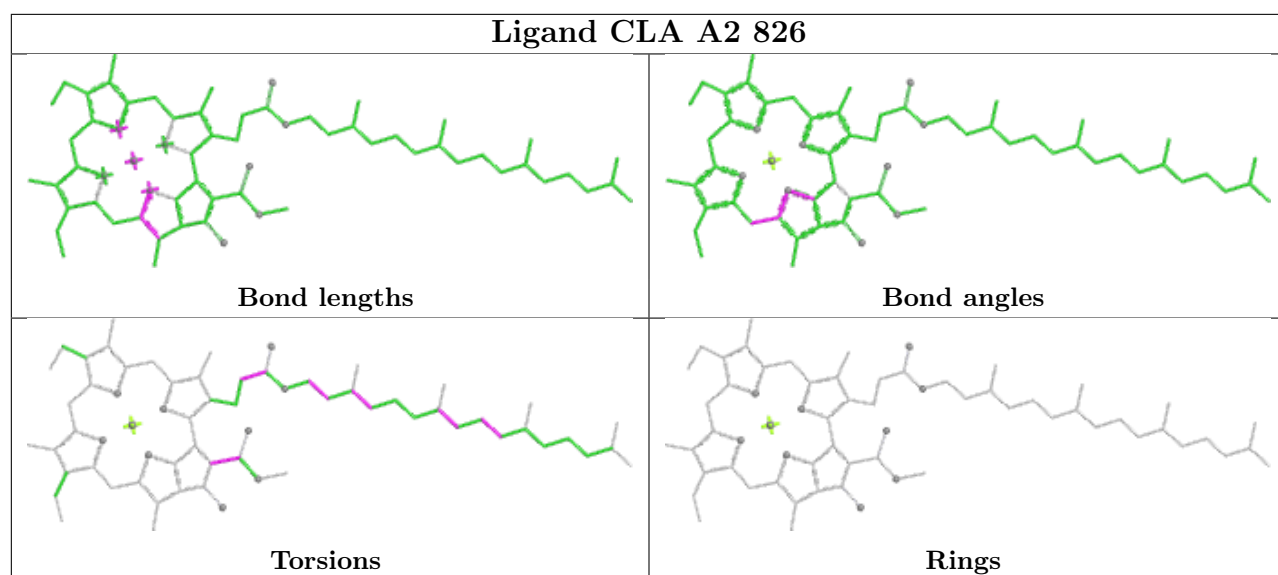
Ligand XAT 1 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

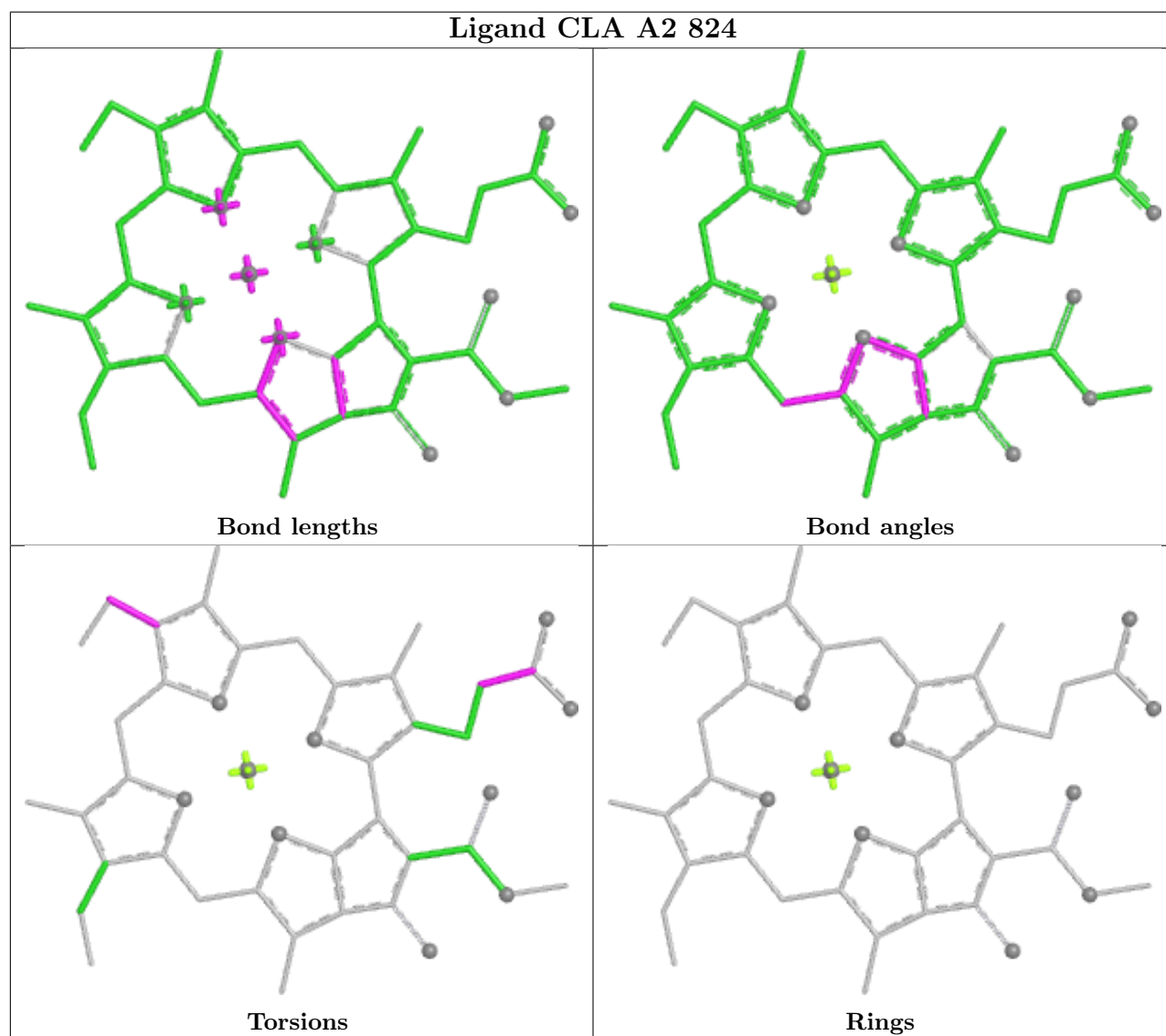
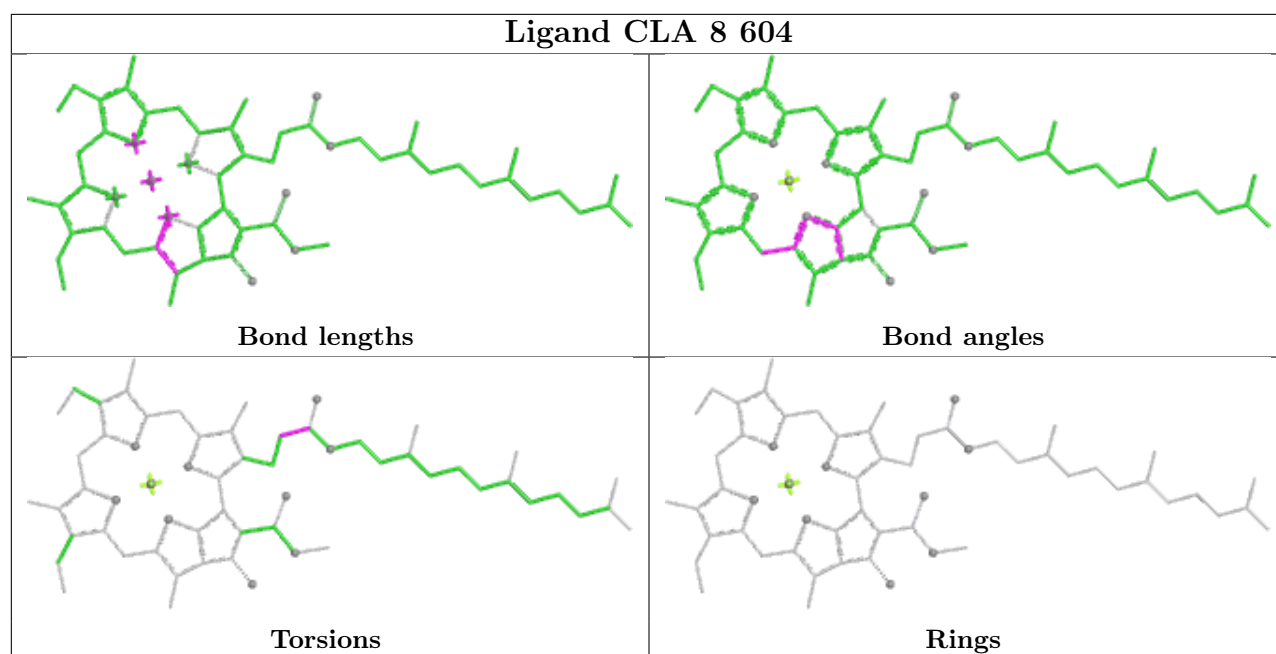


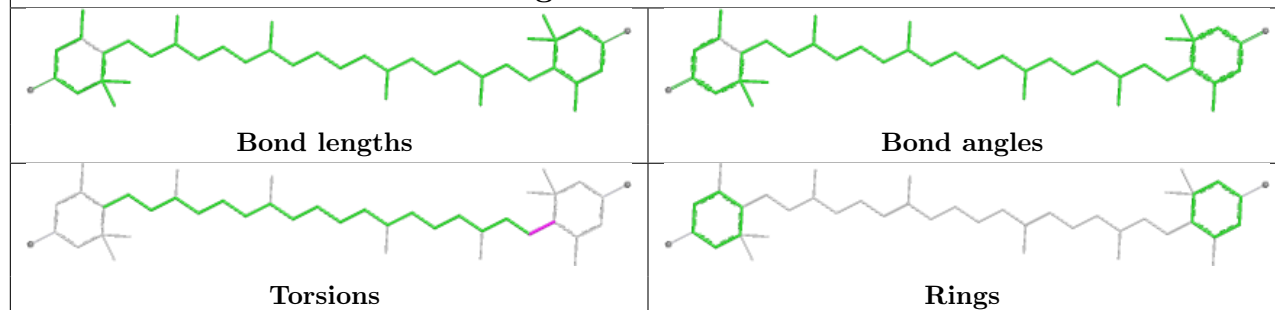
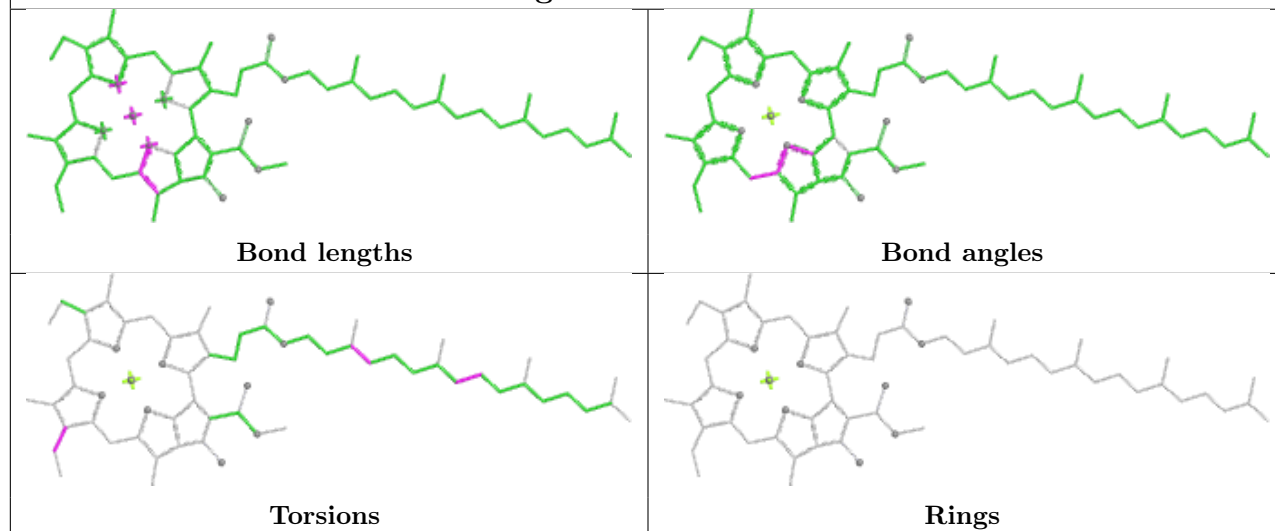
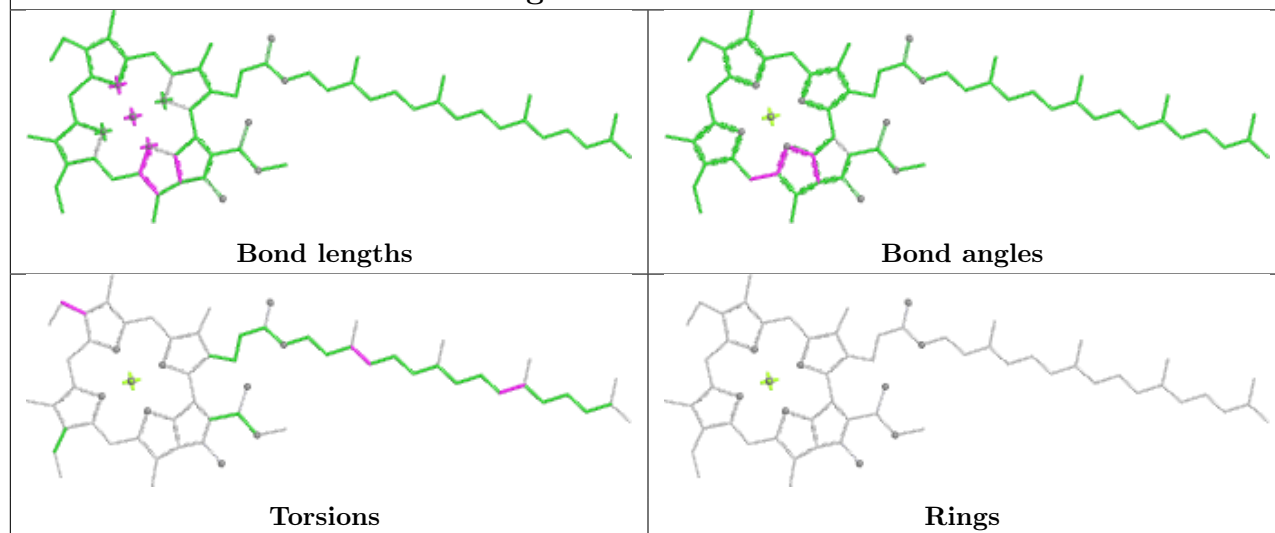


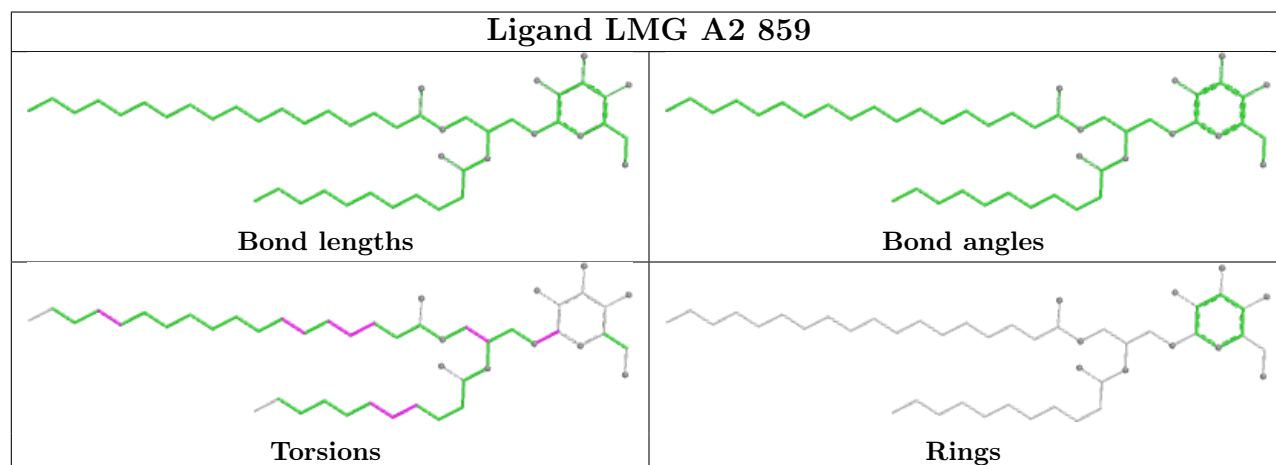
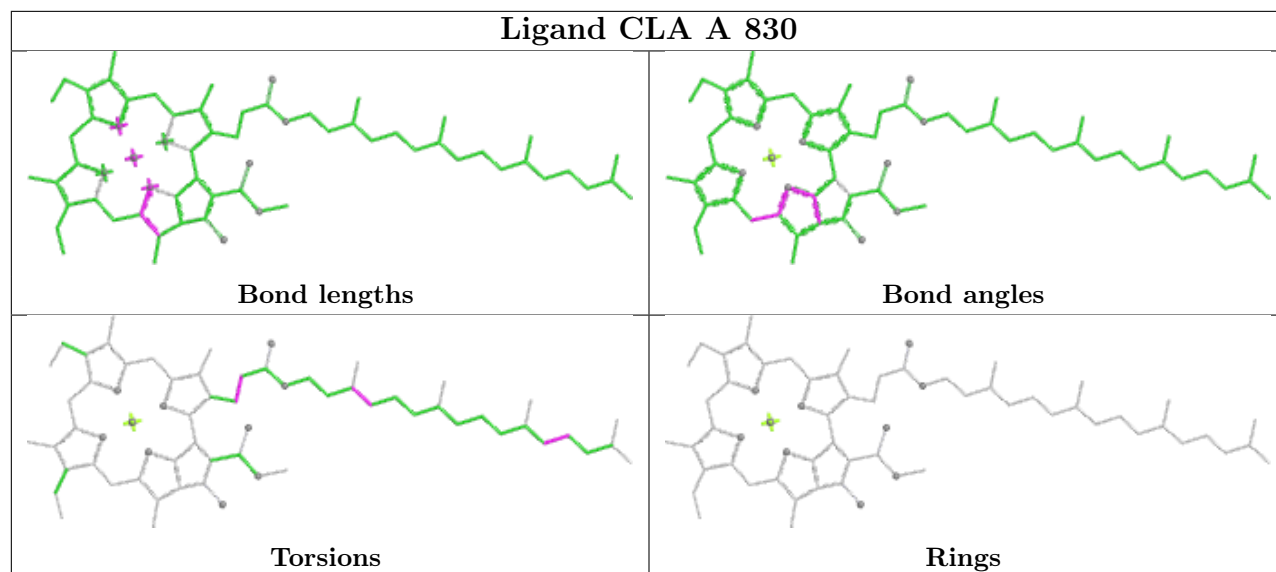


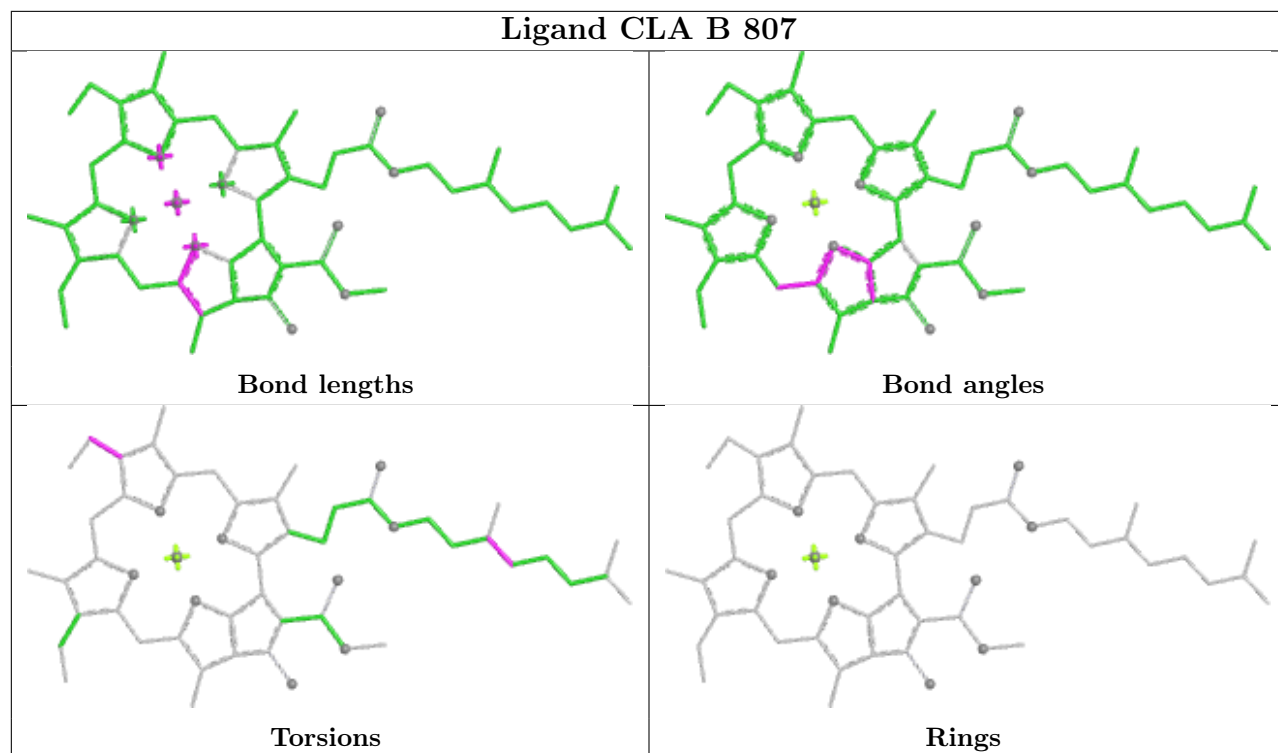


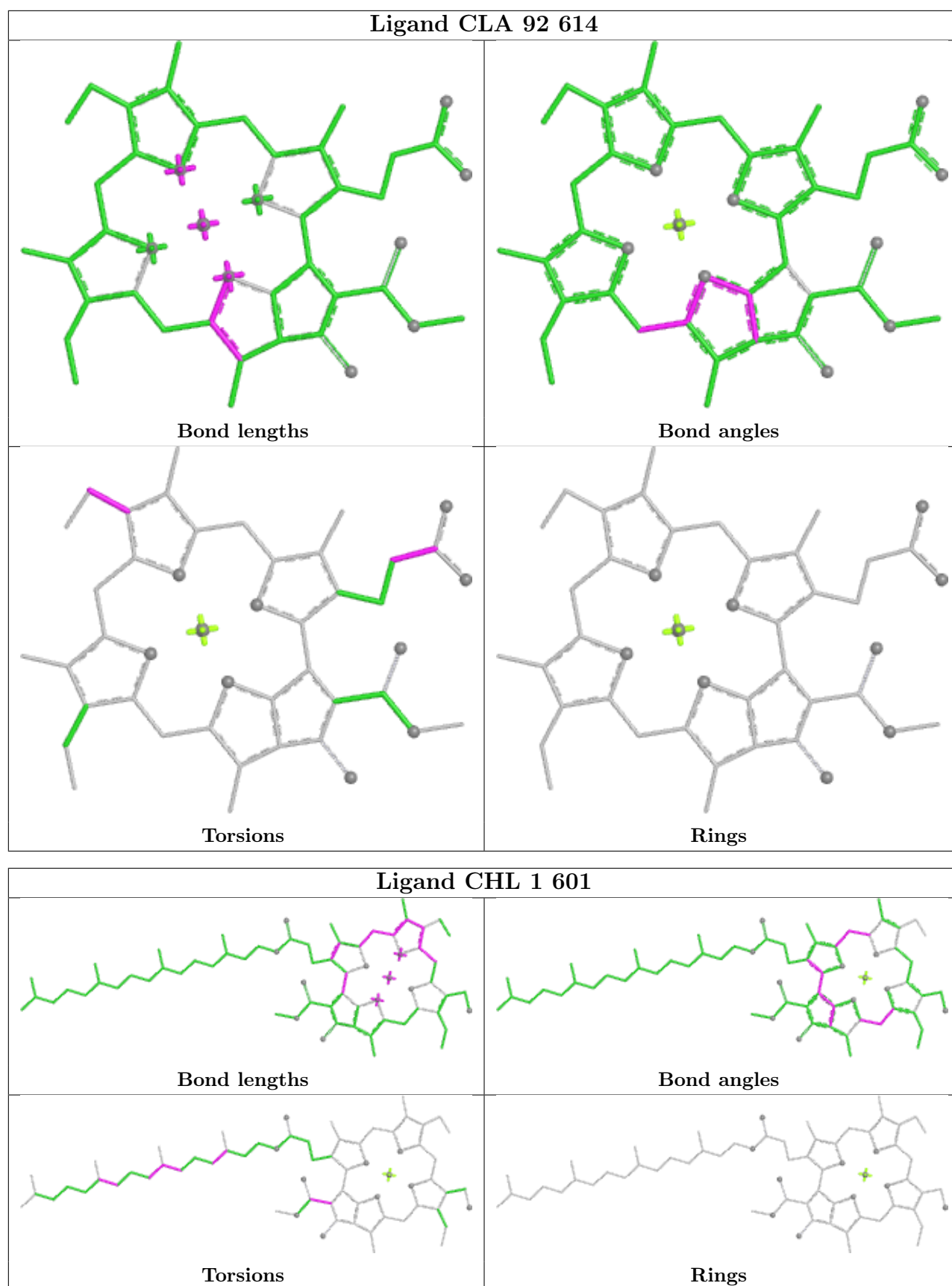


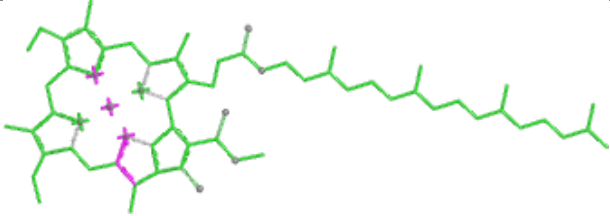
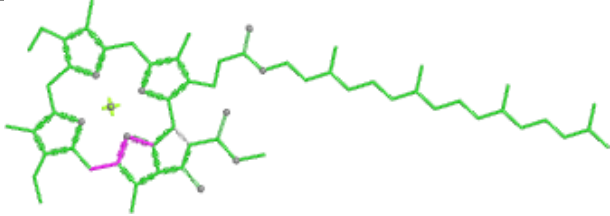
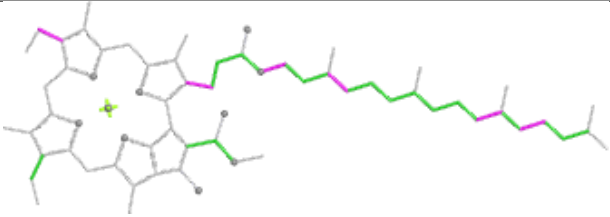
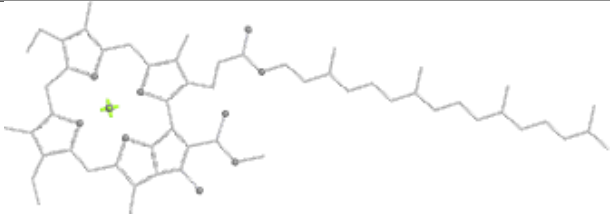
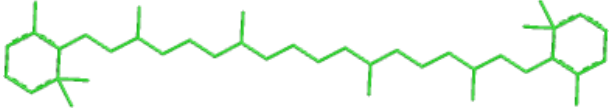
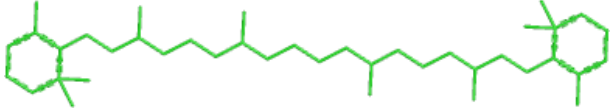
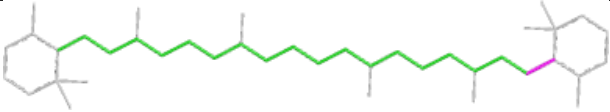
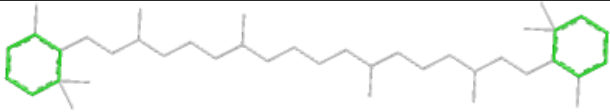
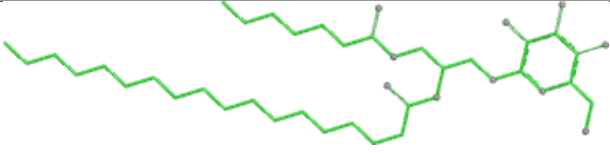
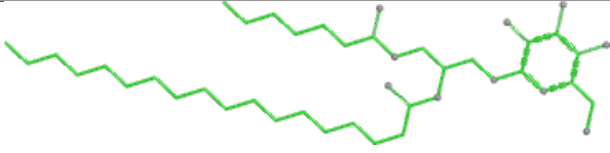
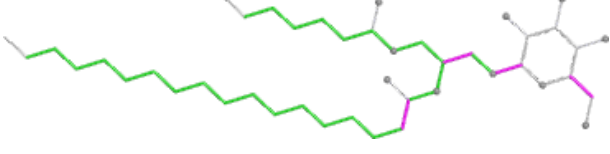


Ligand LUT 1 619**Ligand CLA 3 603****Ligand CLA 12 613**

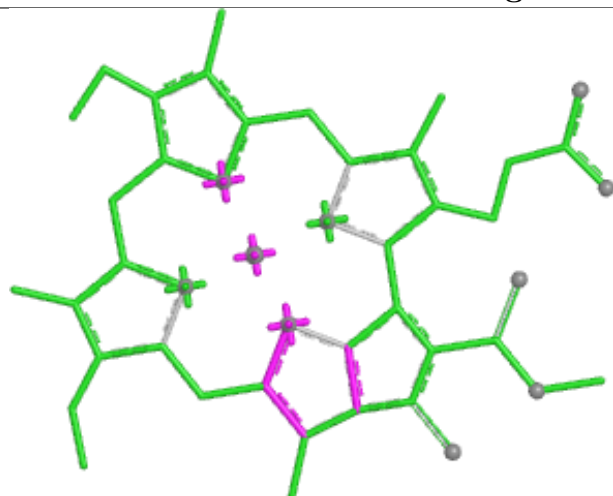




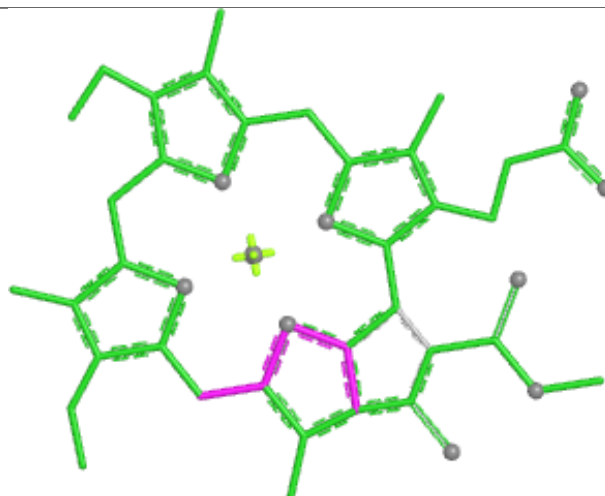


Ligand CLA Z2 609	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR K2 202	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 92 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

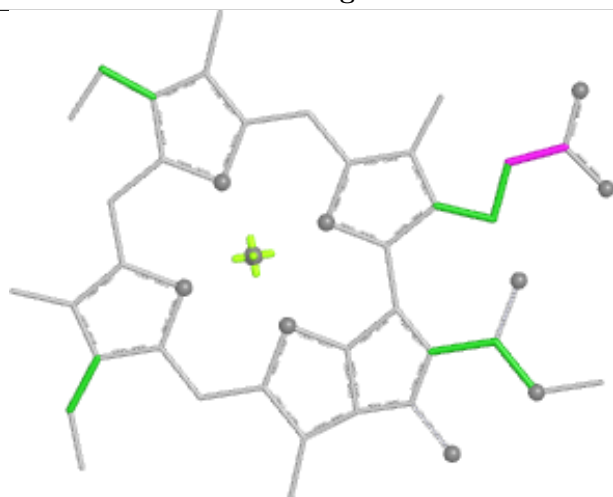
Ligand CLA B2 835



Bond lengths



Bond angles

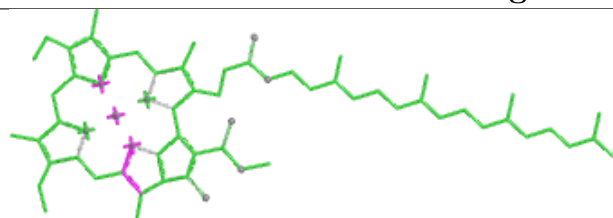


Torsions

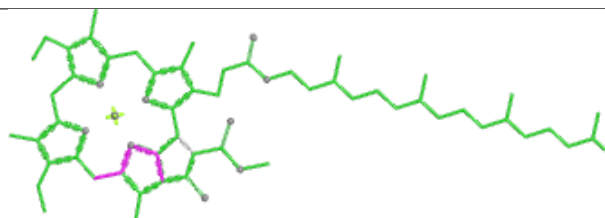


Rings

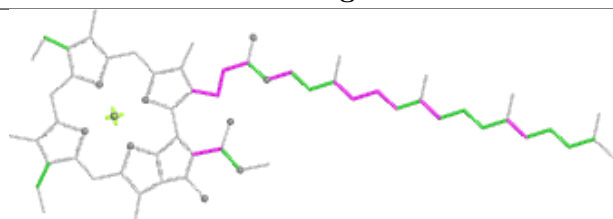
Ligand CLA 52 603



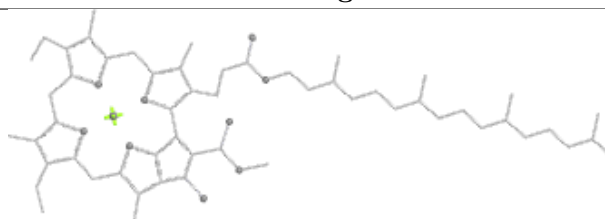
Bond lengths



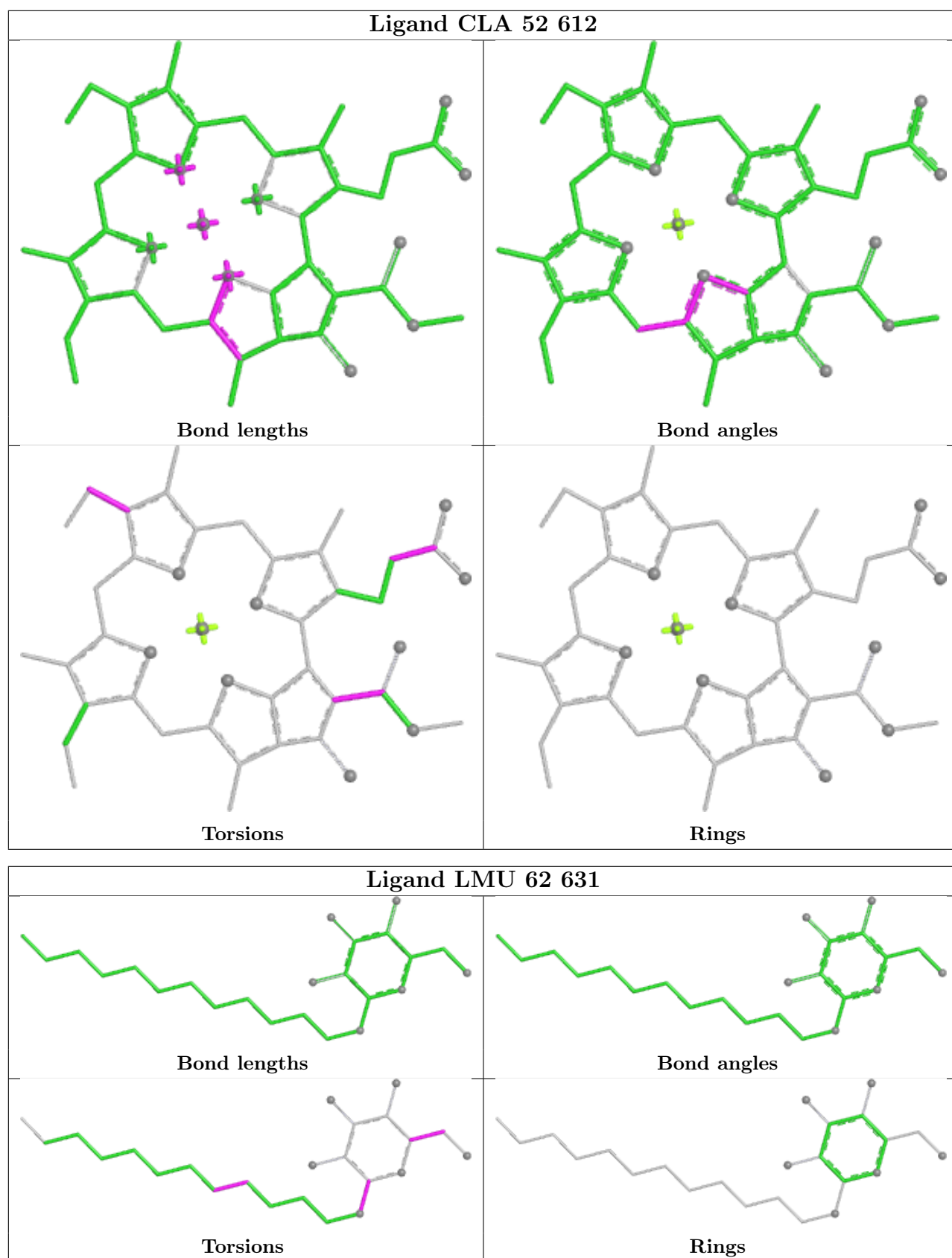
Bond angles

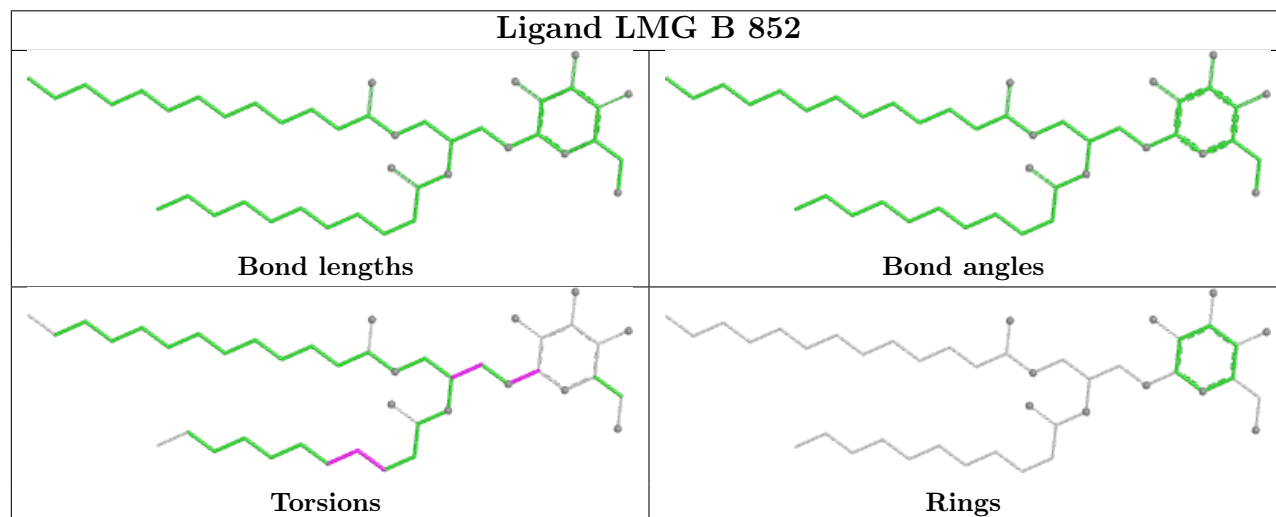
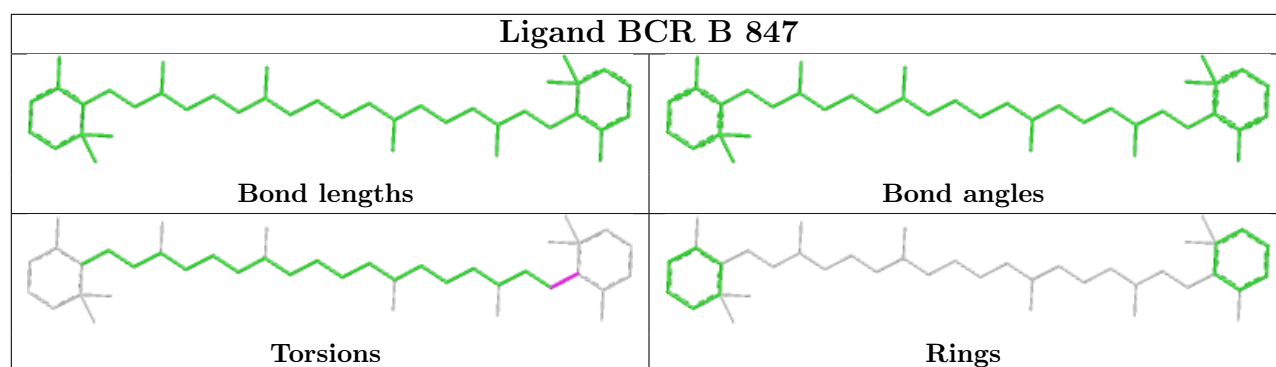


Torsions

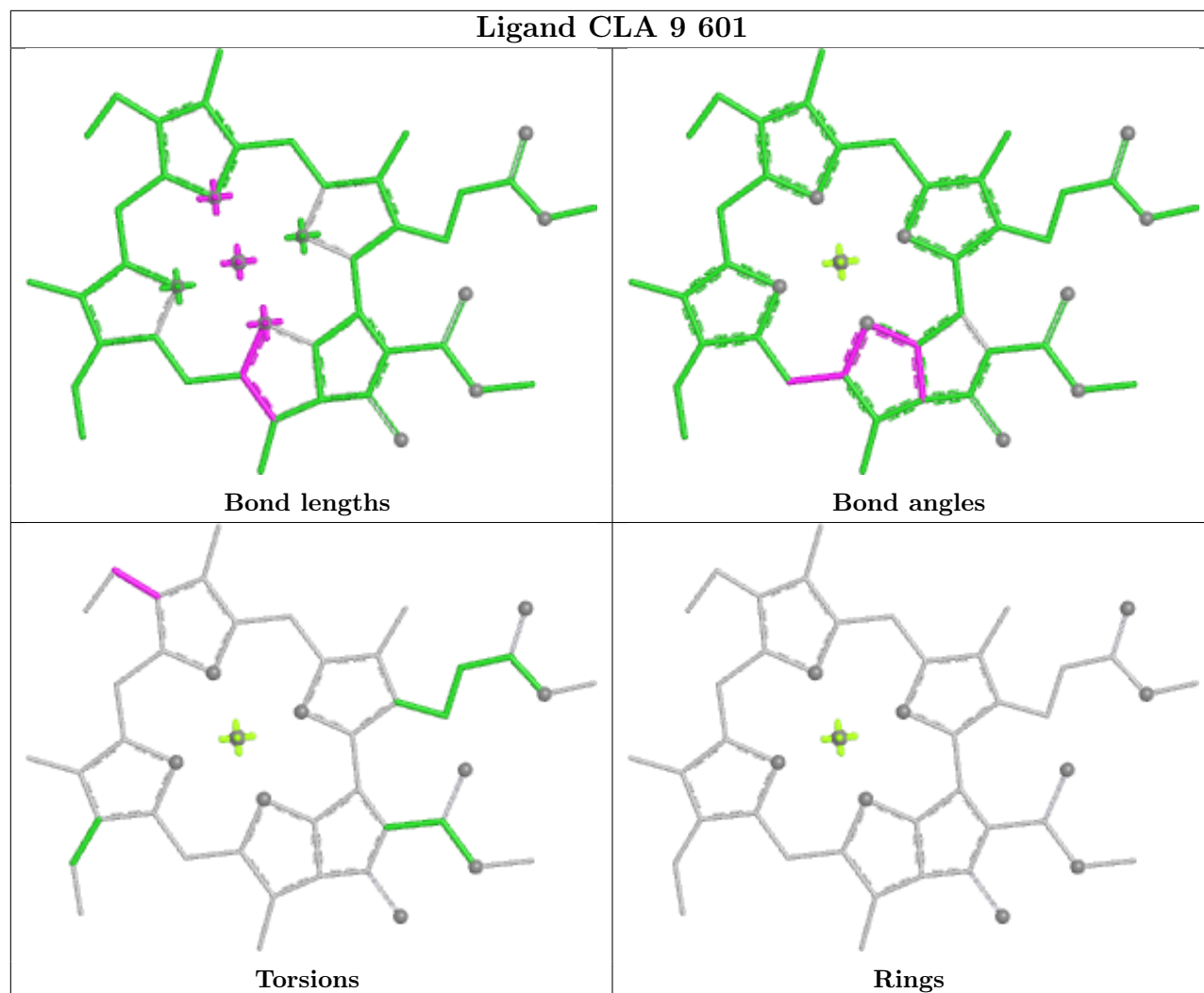


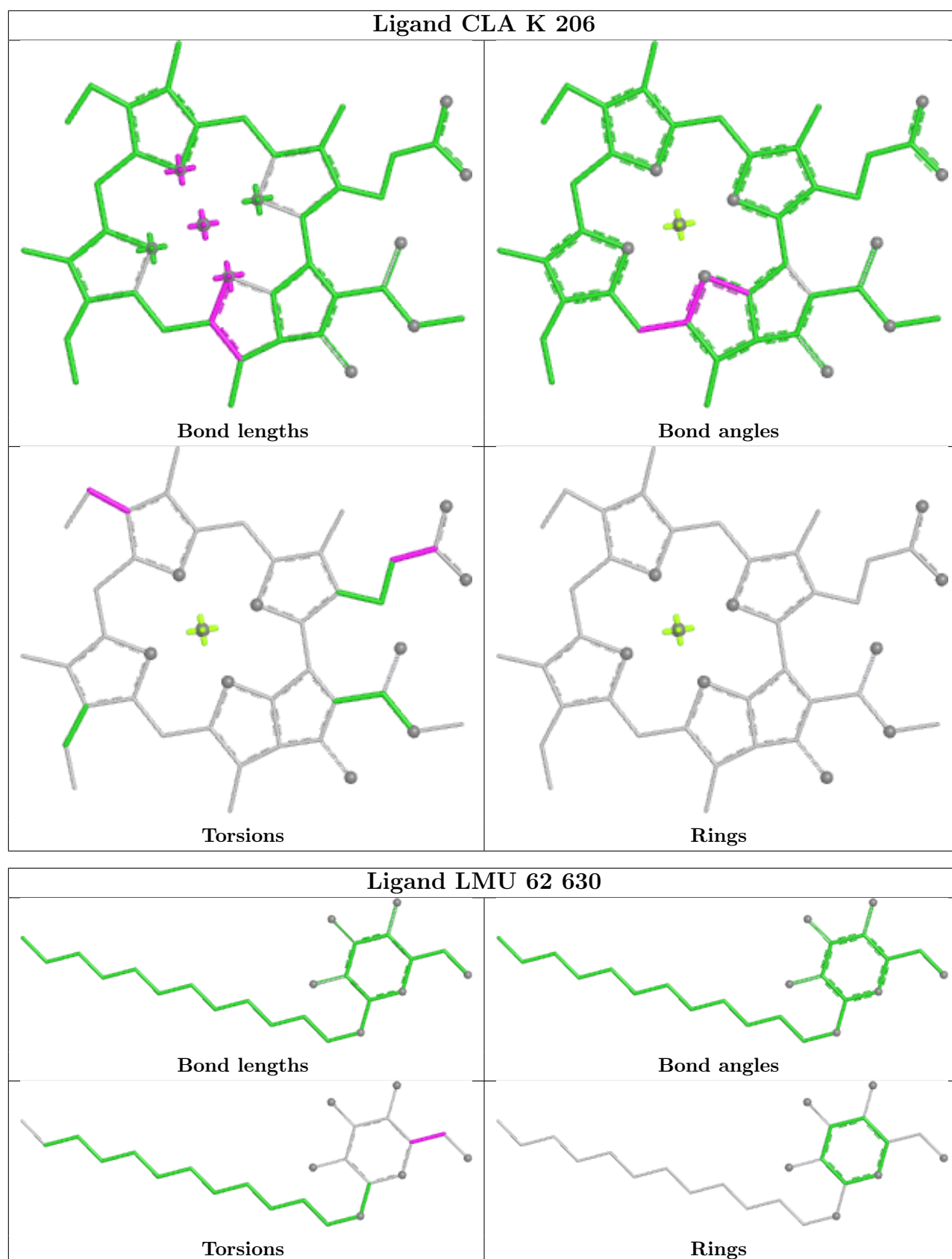
Rings

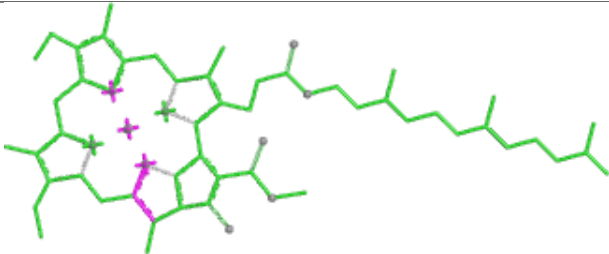
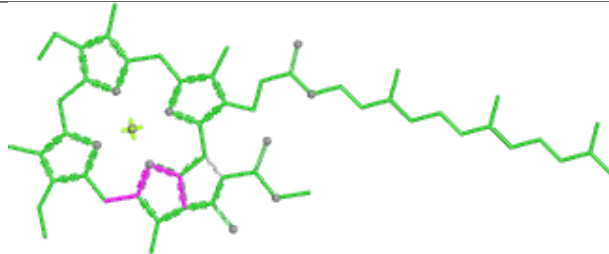
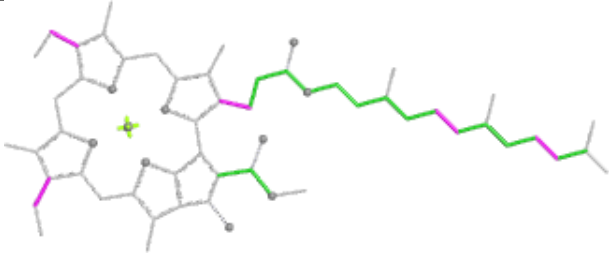
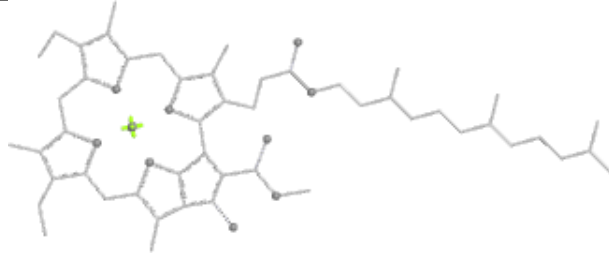


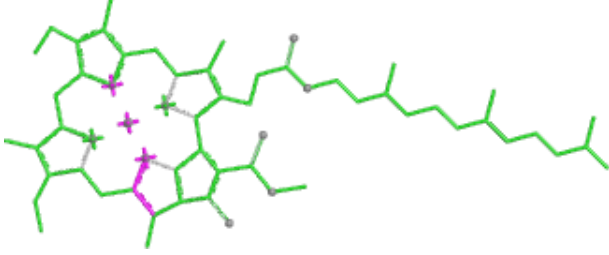
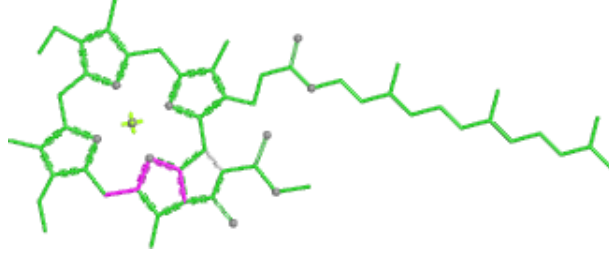
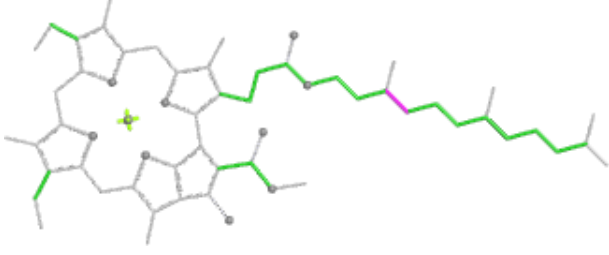
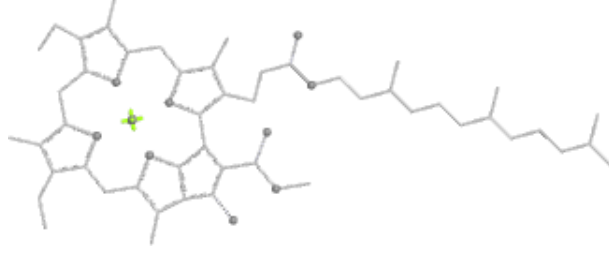


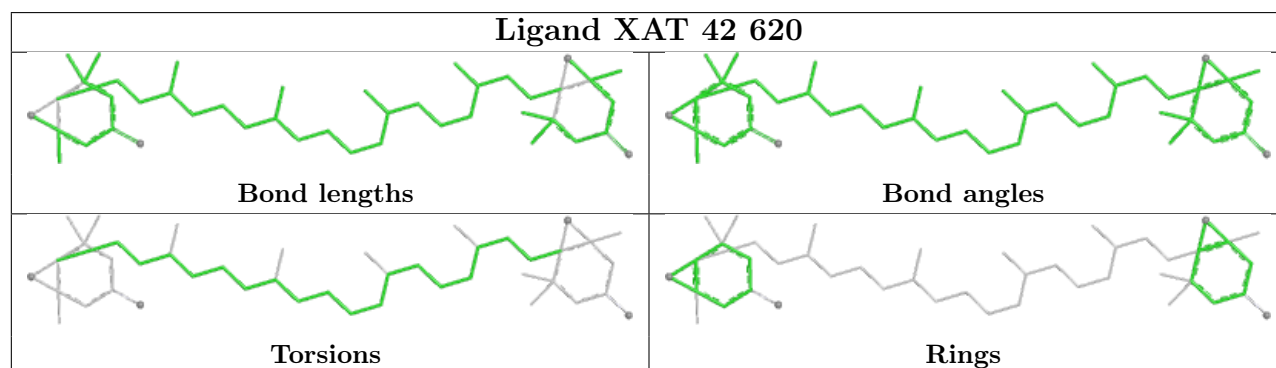
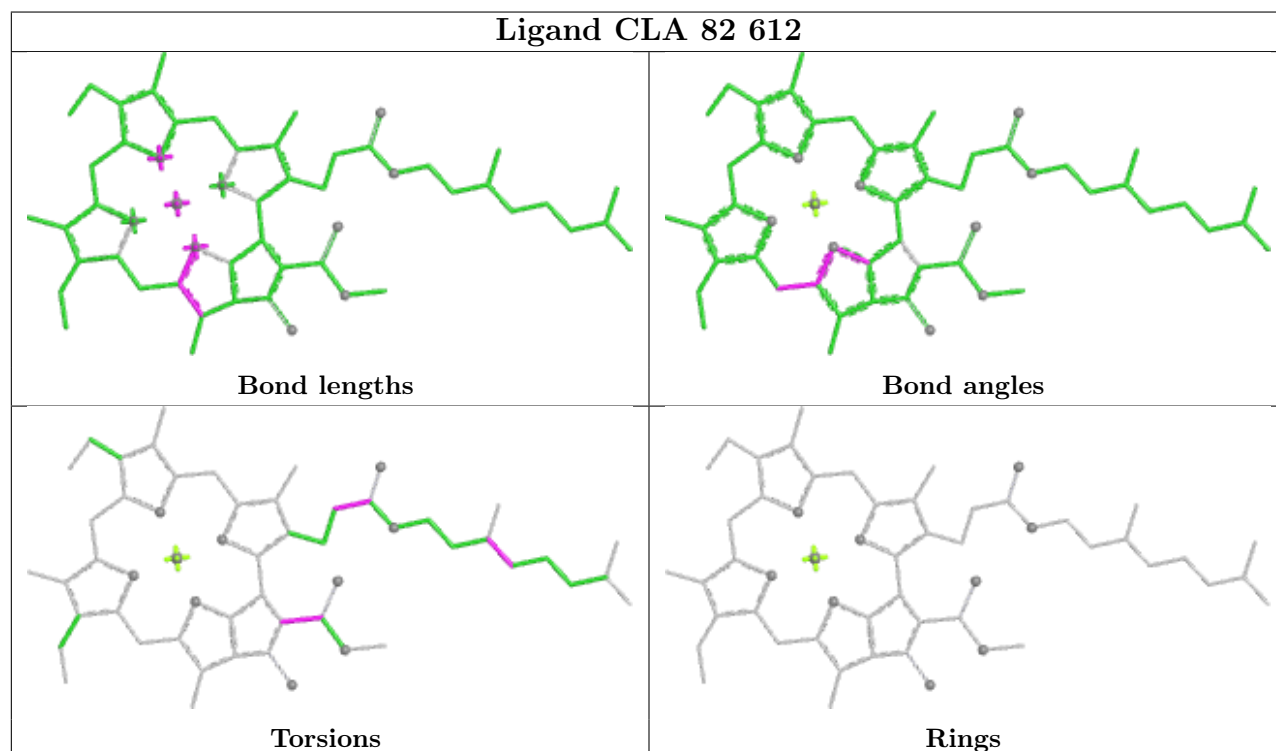
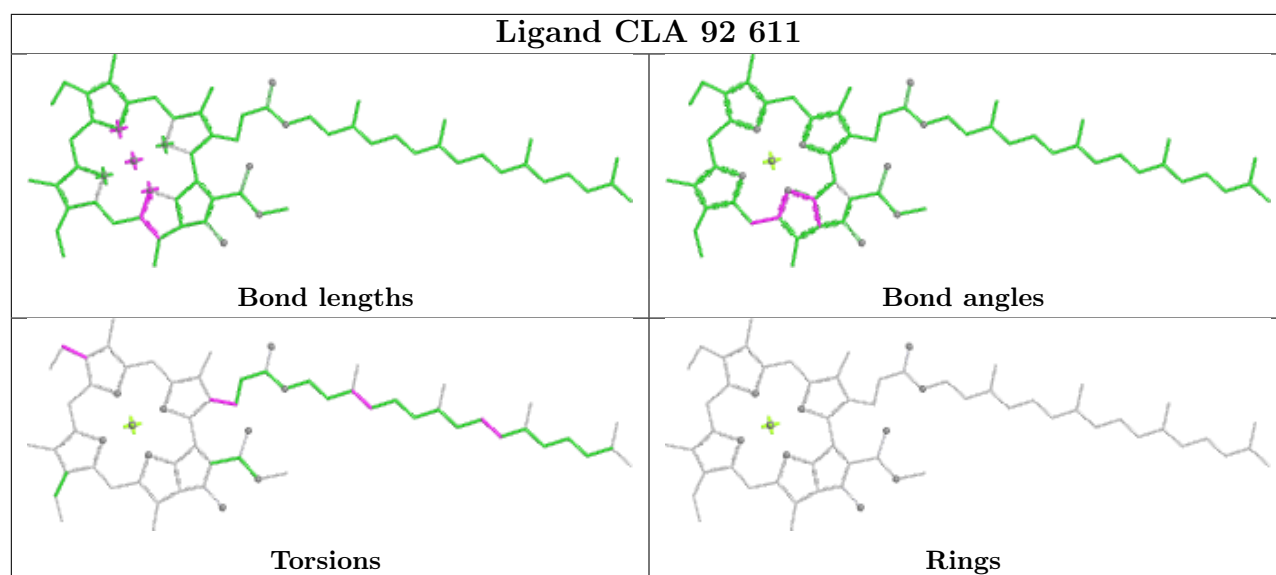
Ligand CLA 9 601

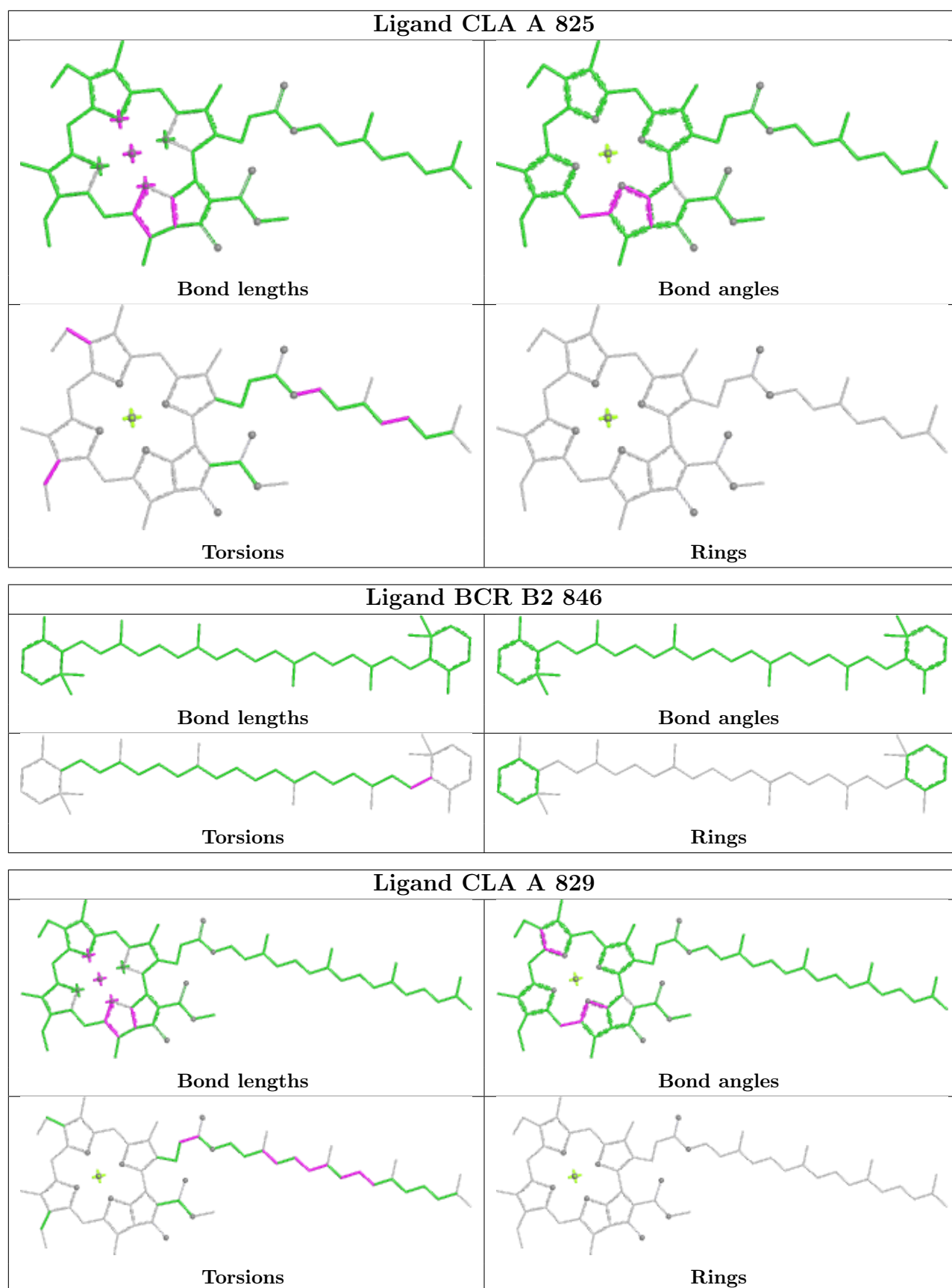


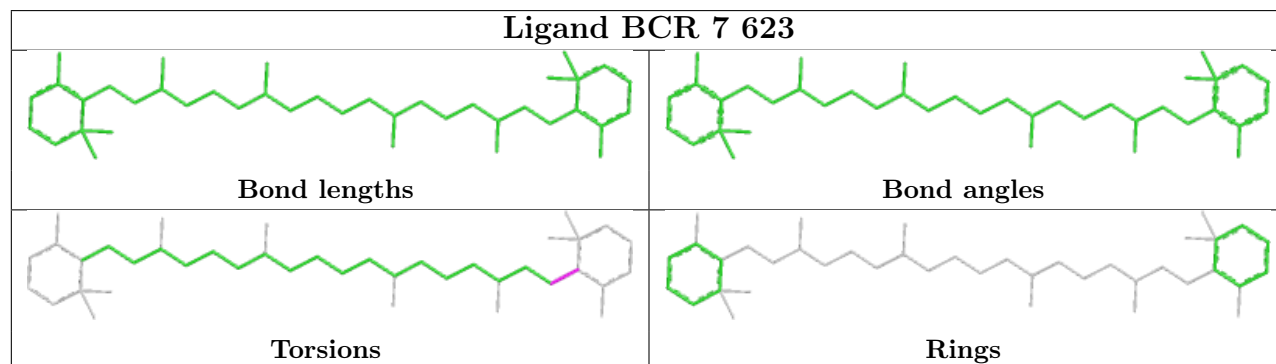
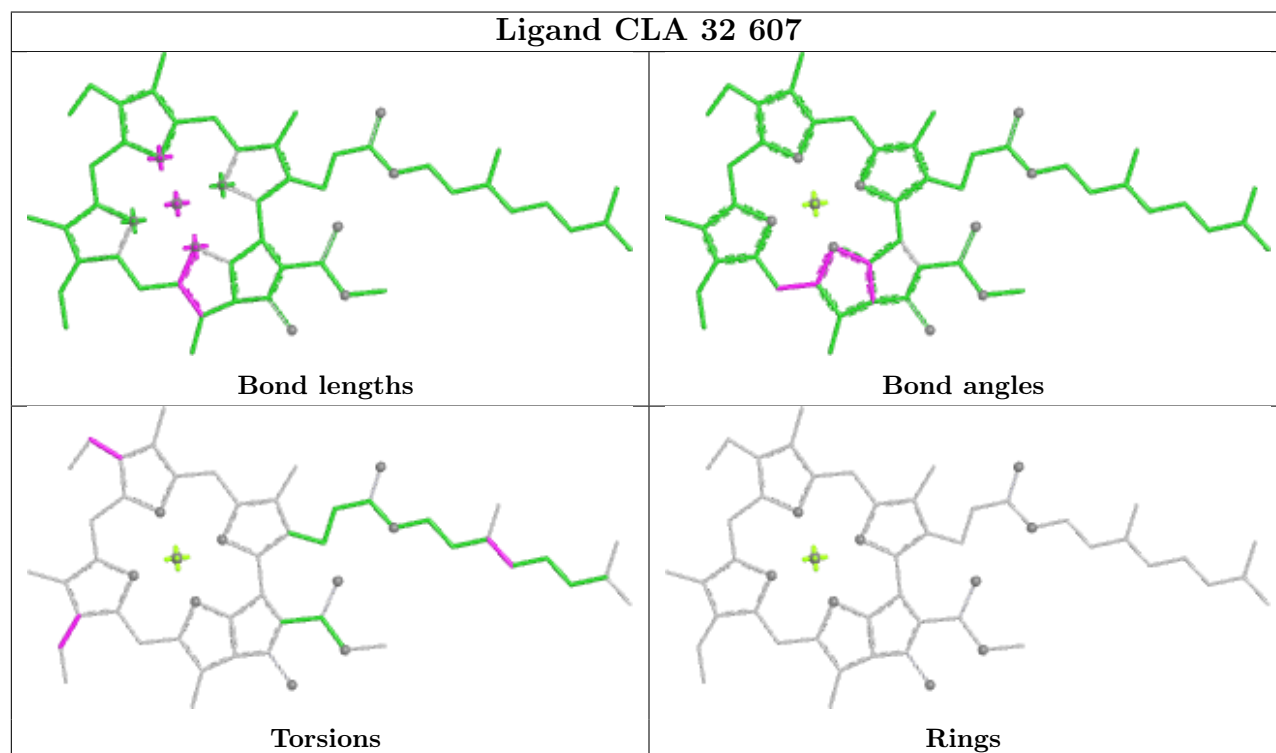
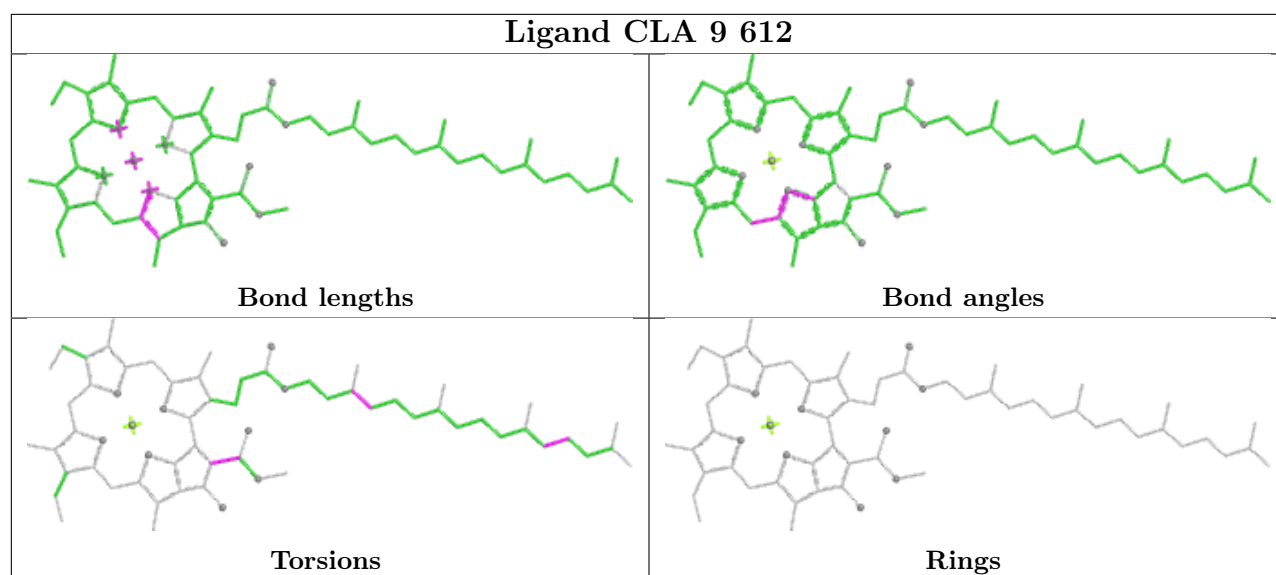


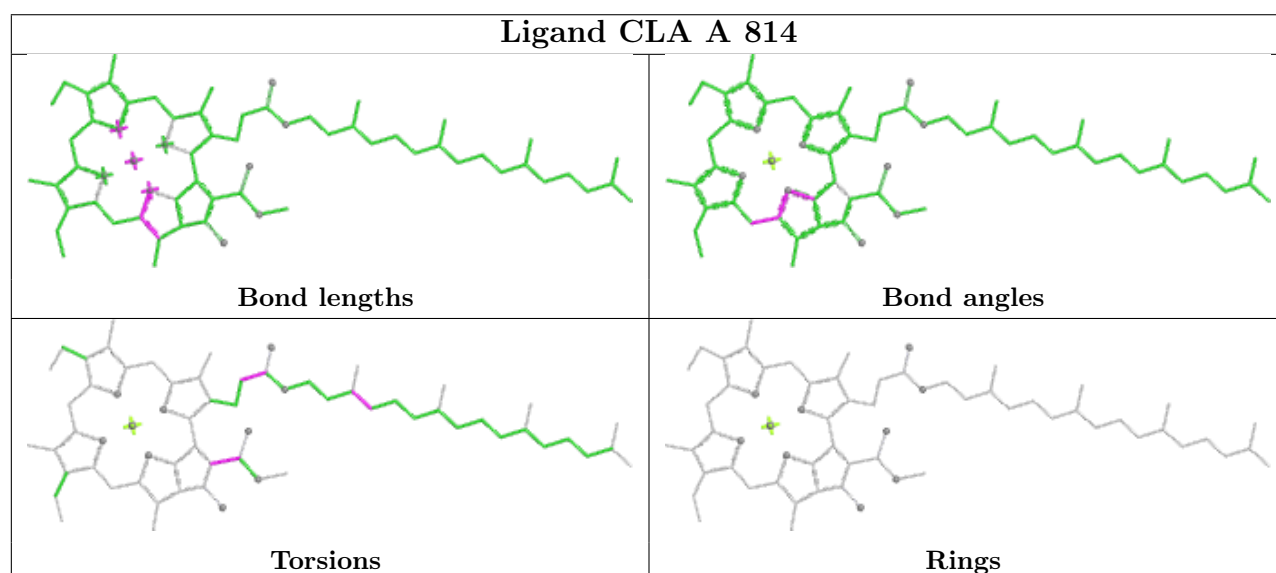
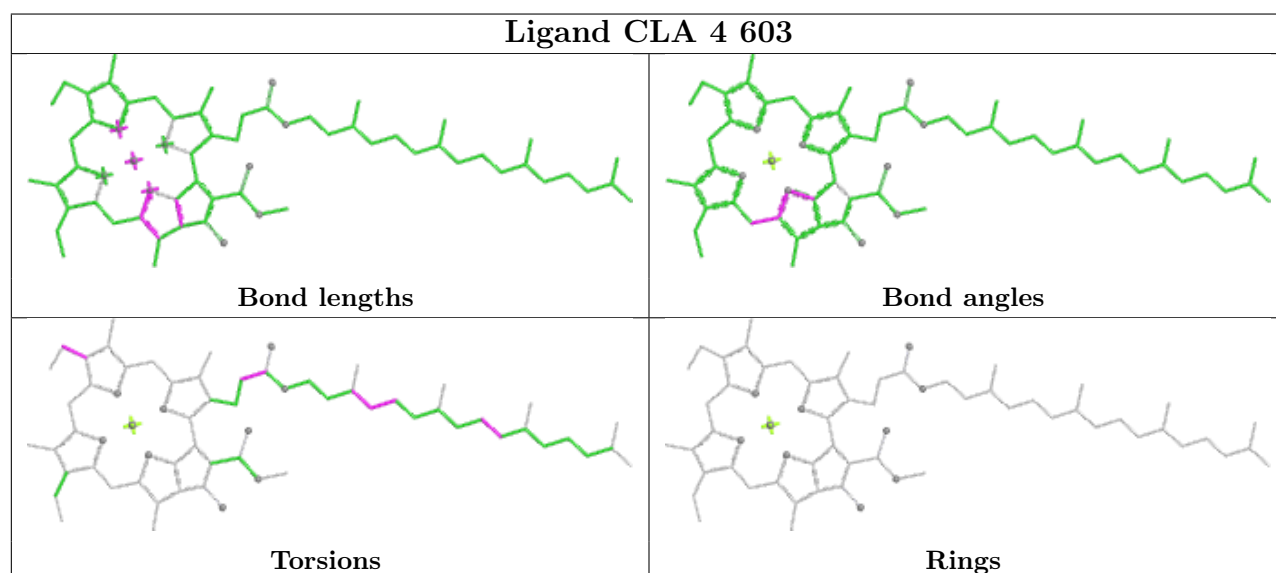
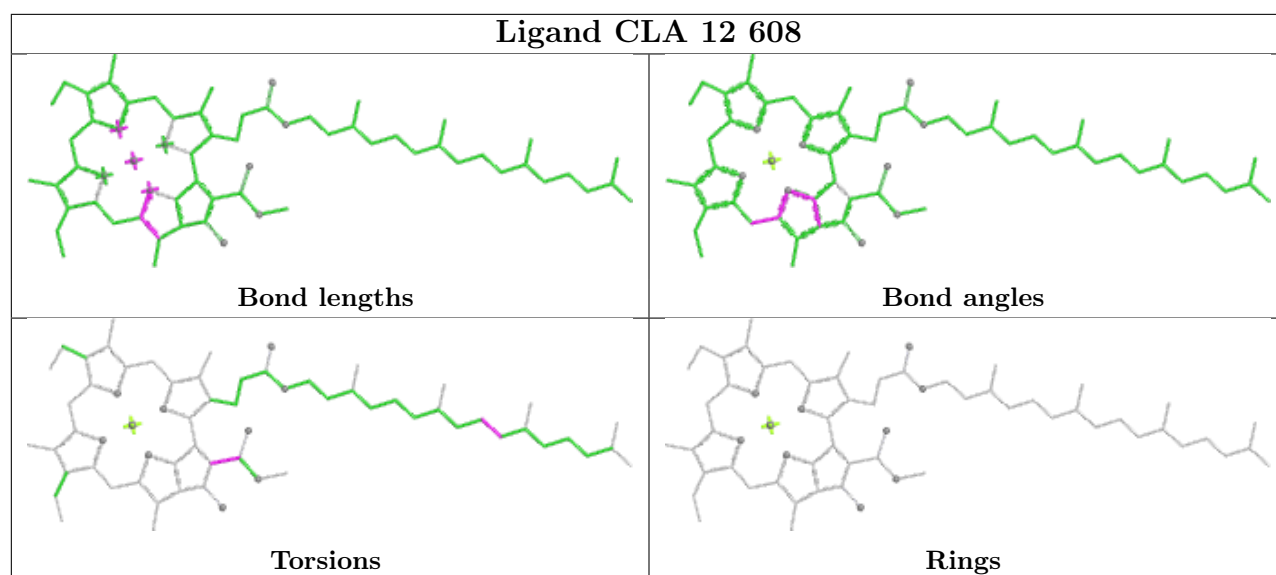
Ligand CLA Z 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

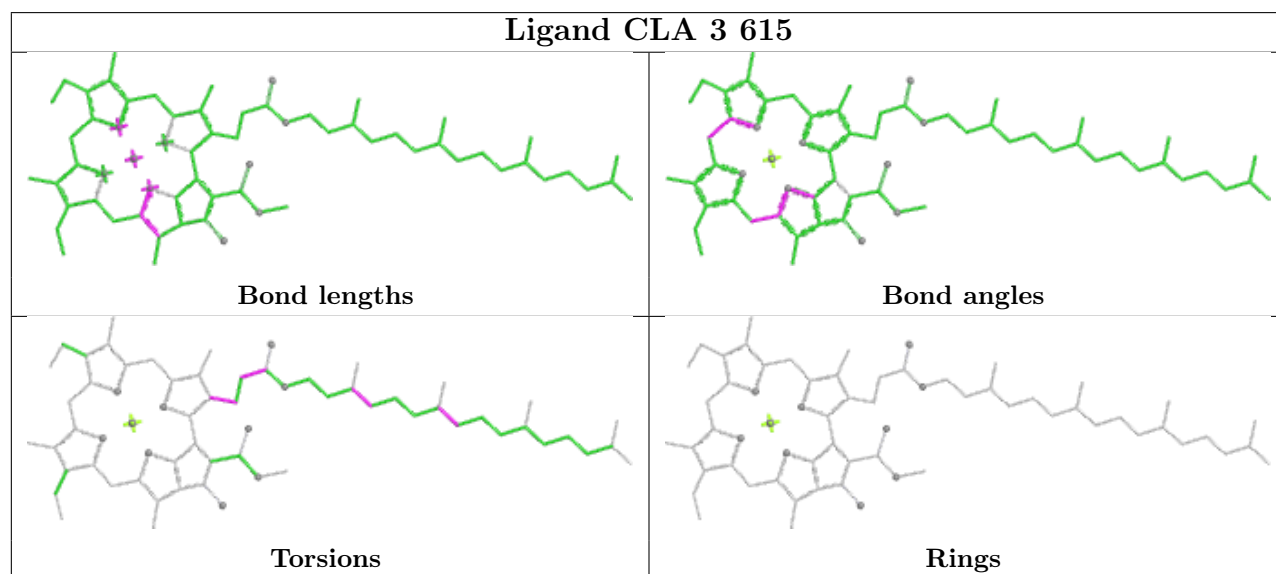
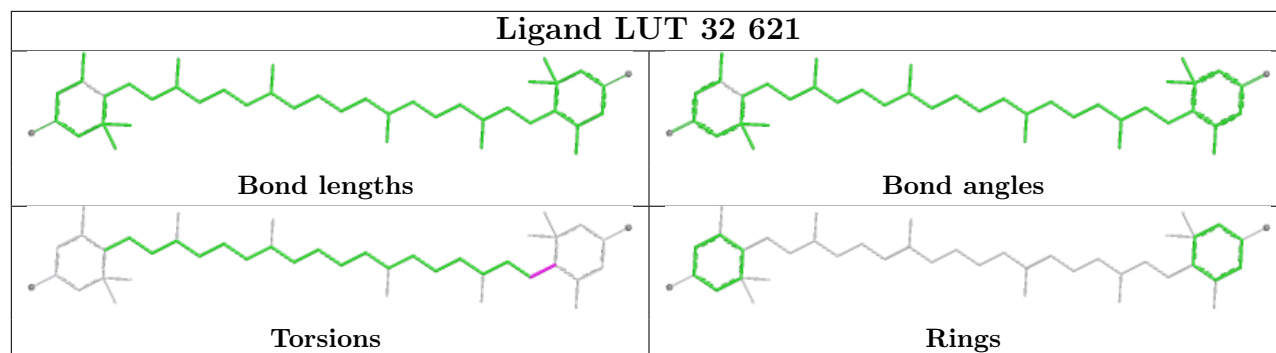
Ligand CLA 5 610	
	
Bond lengths	Bond angles
	
Torsions	Rings



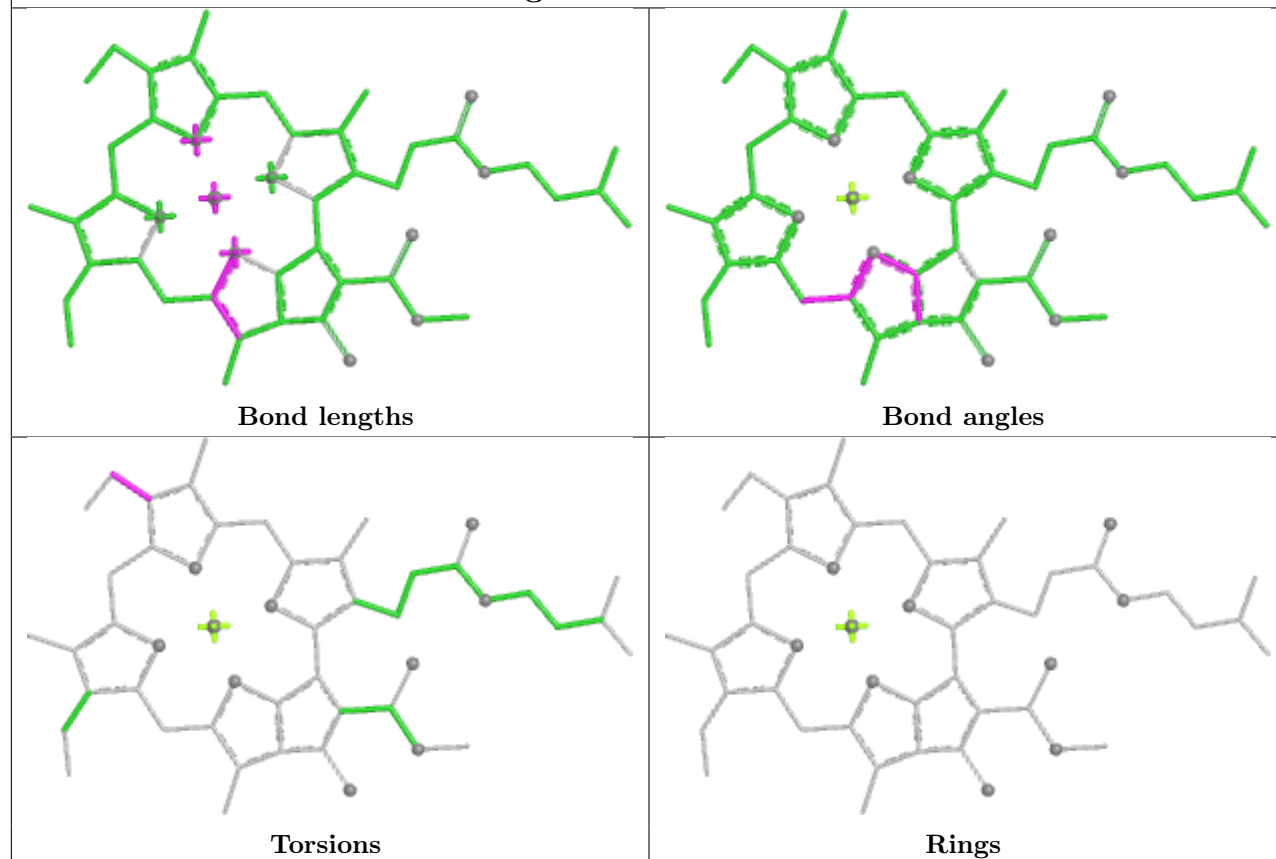




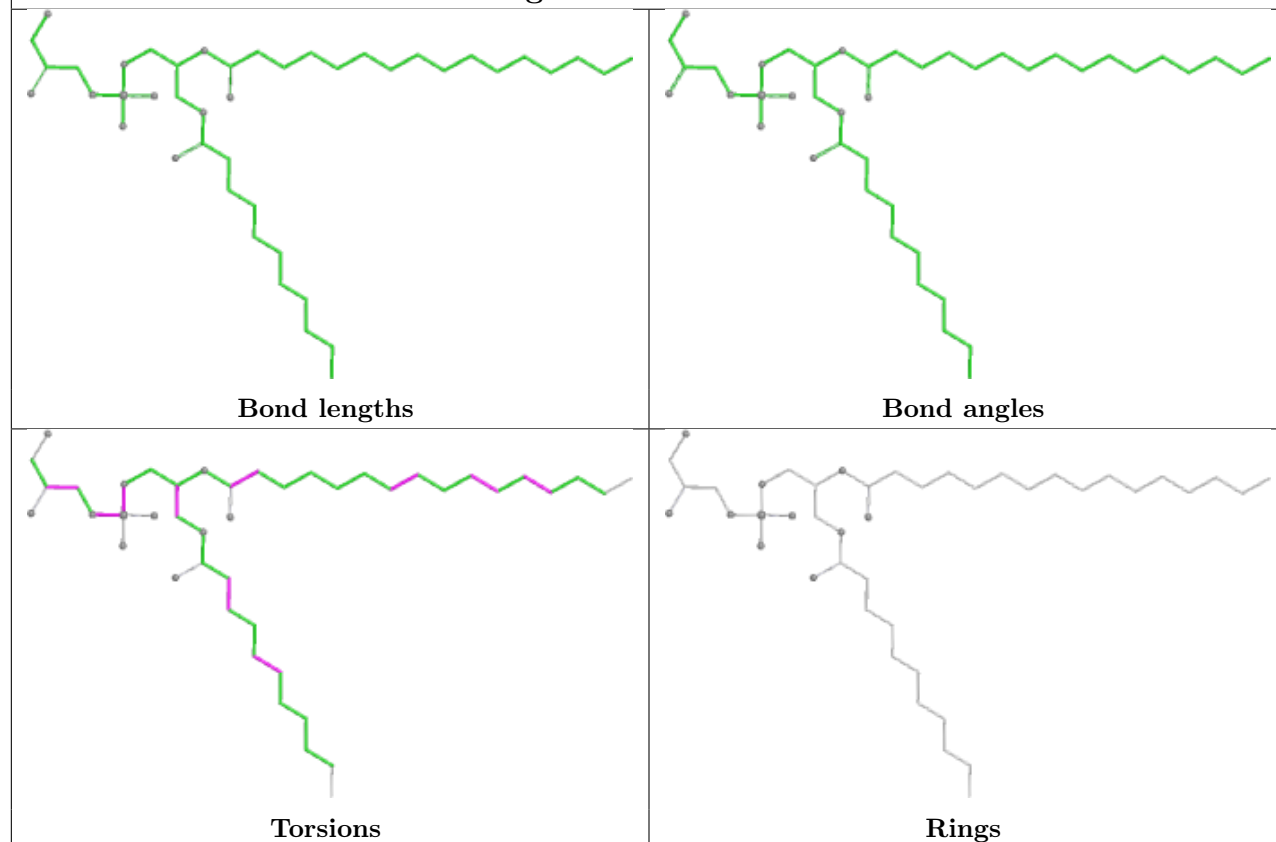


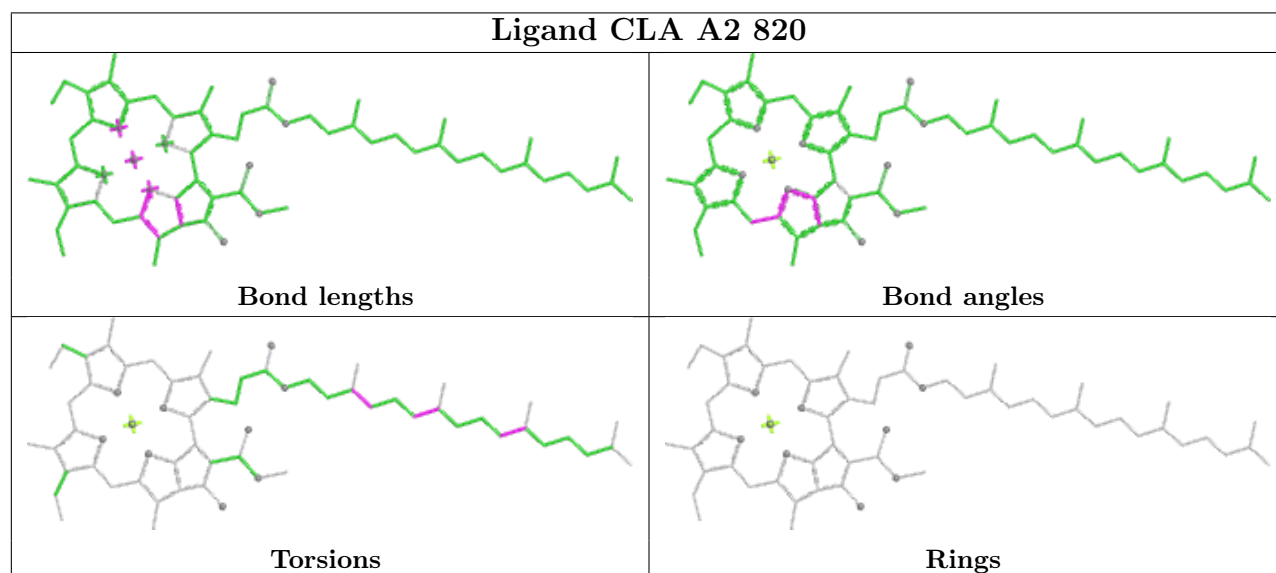
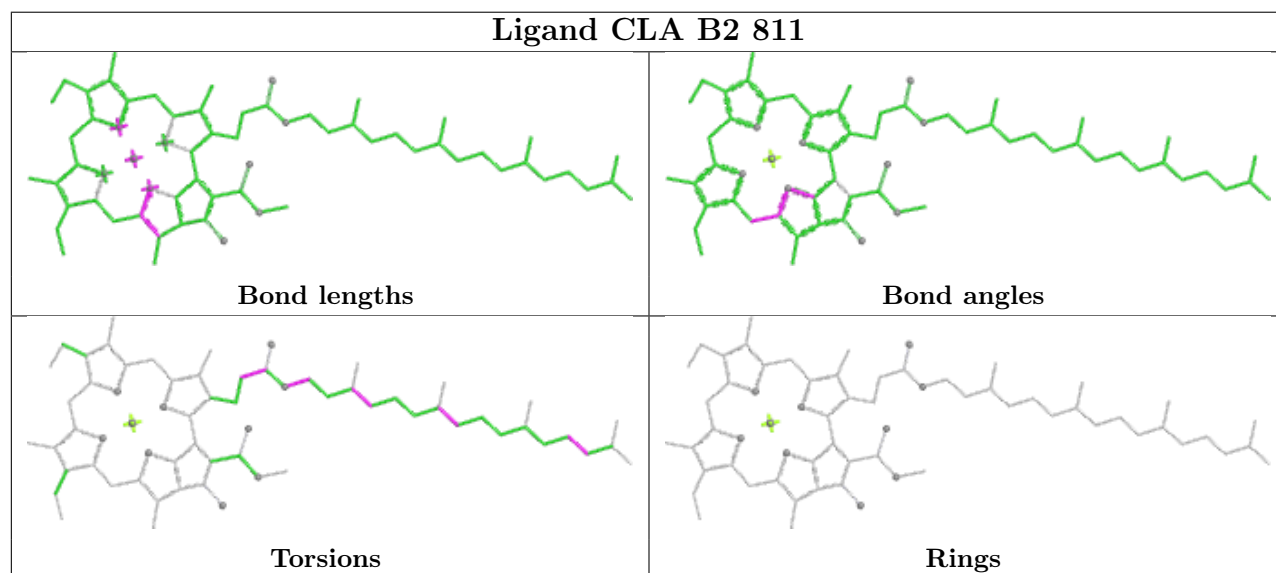
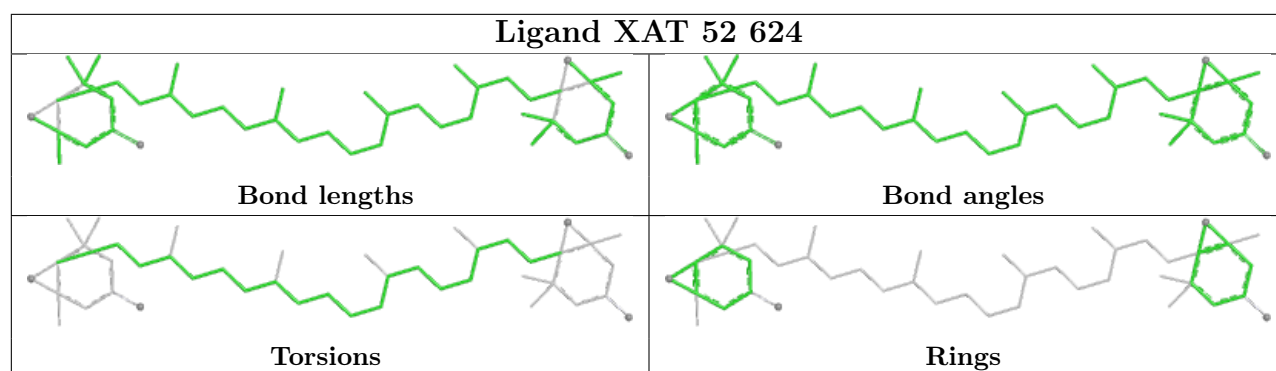


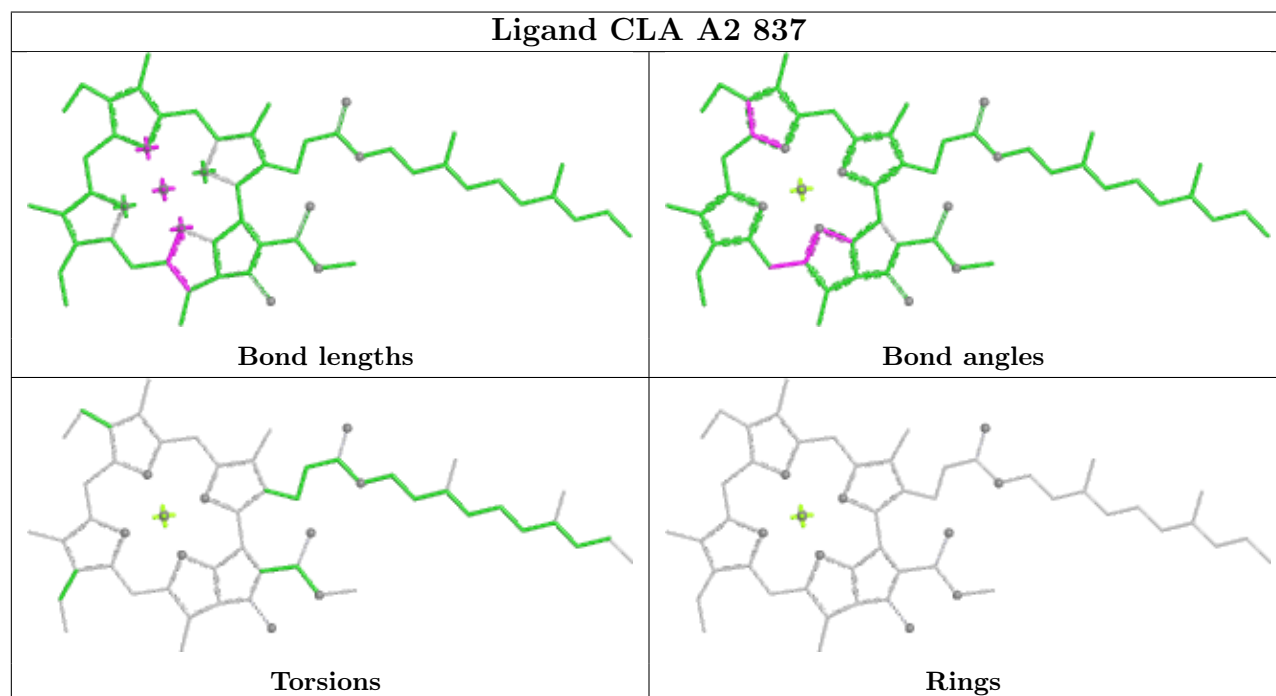
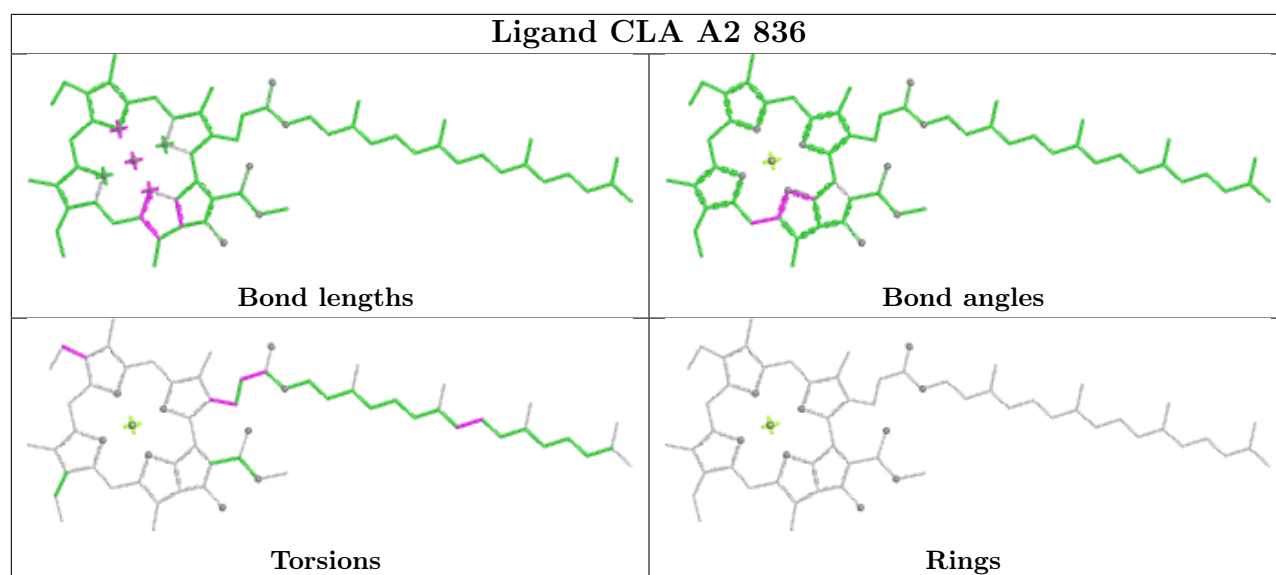
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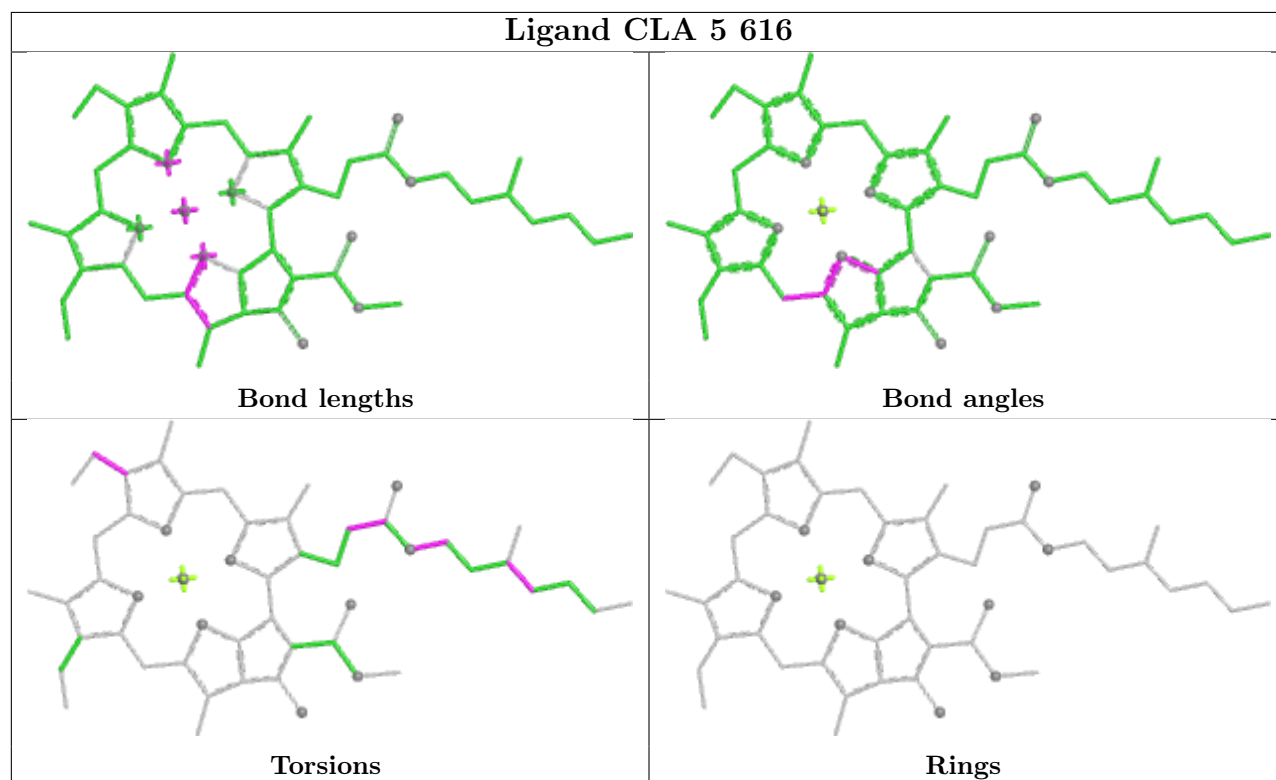
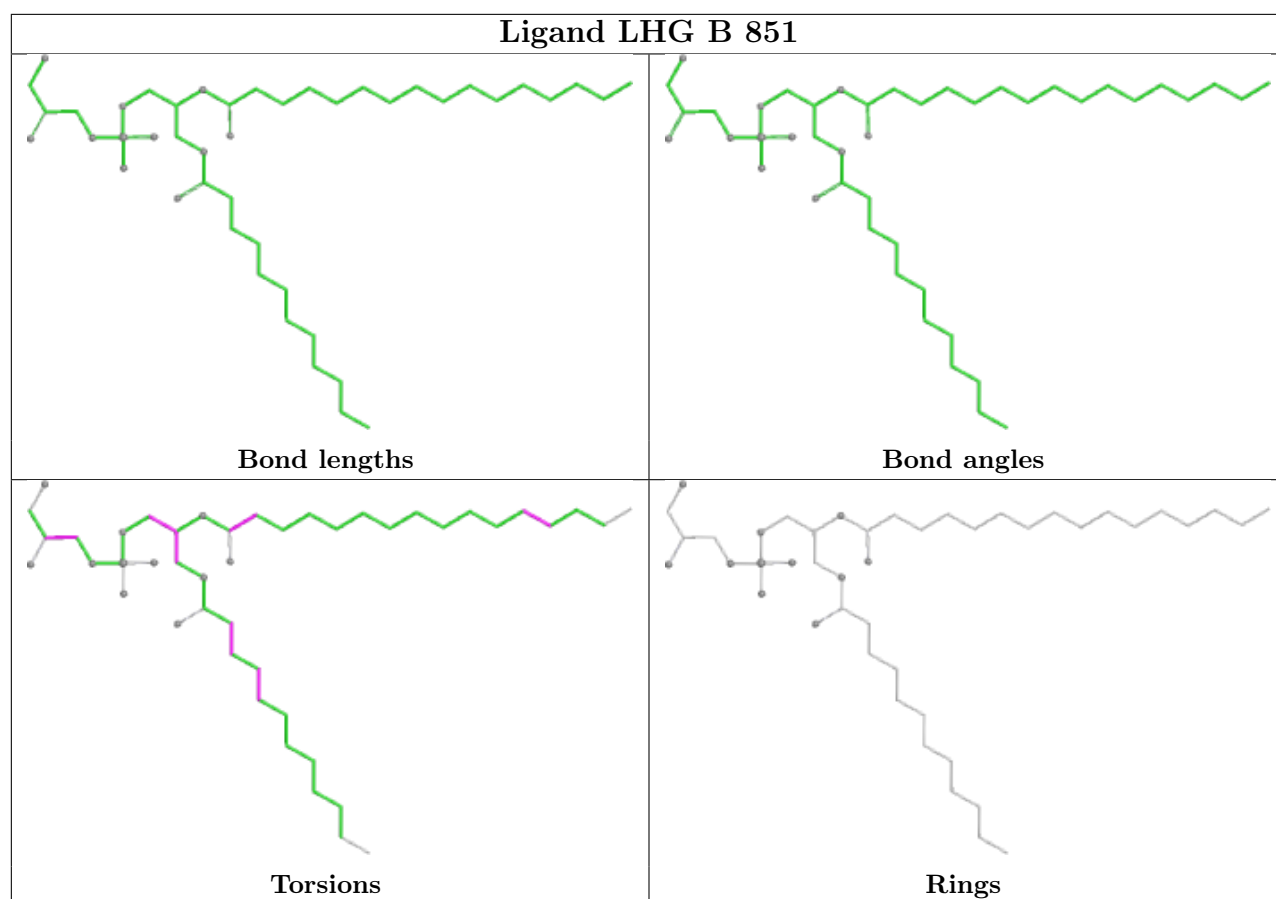


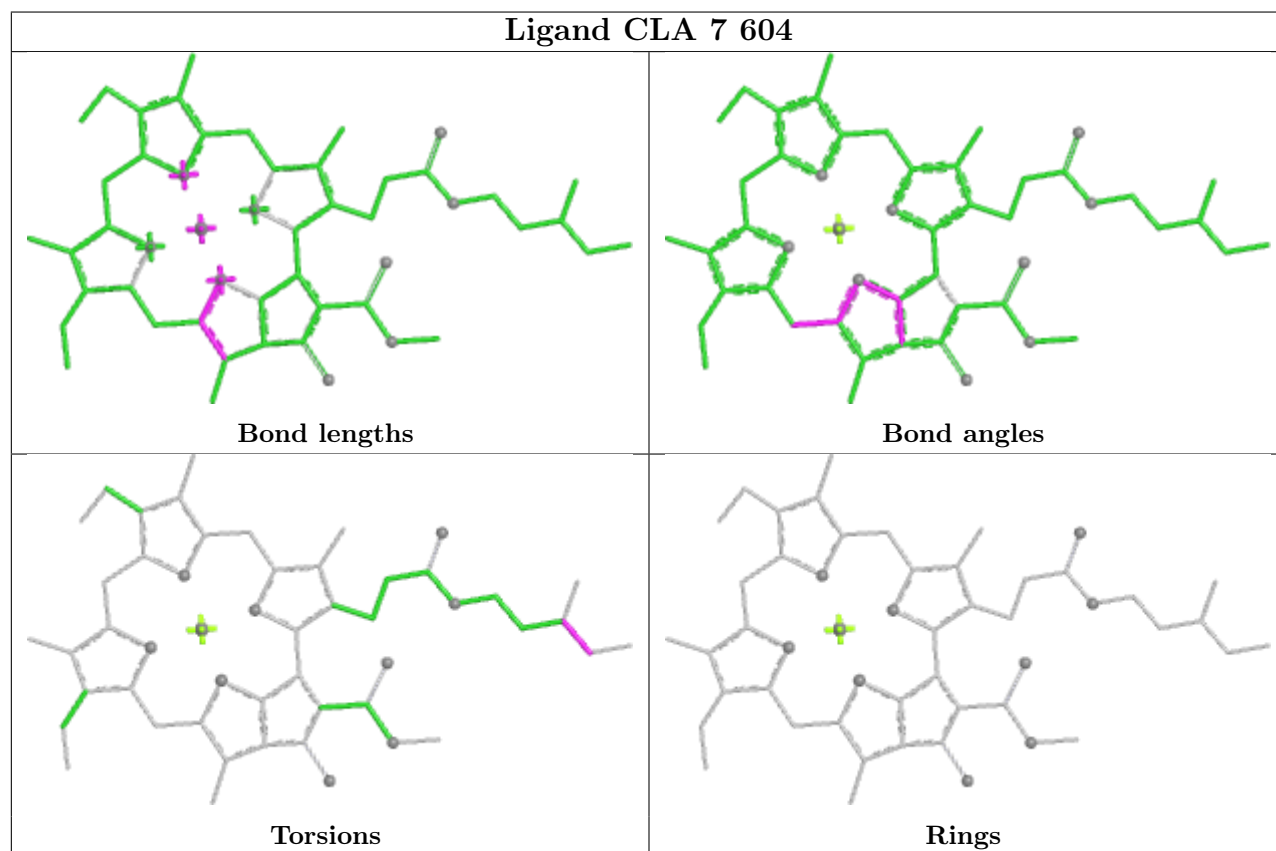
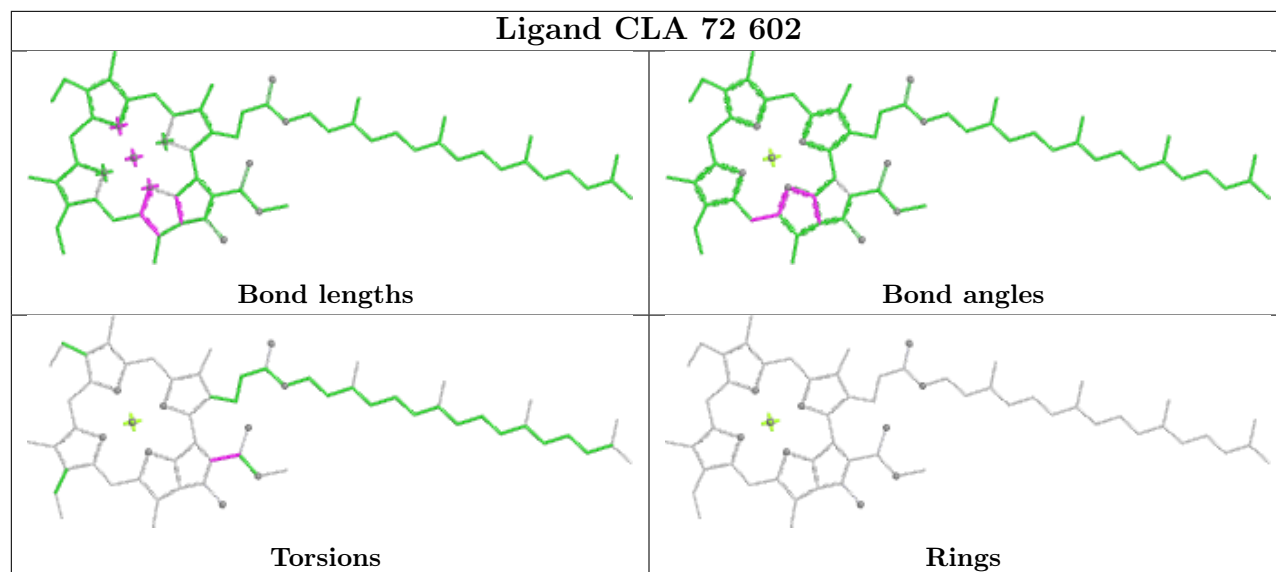
Ligand LHG 82 620

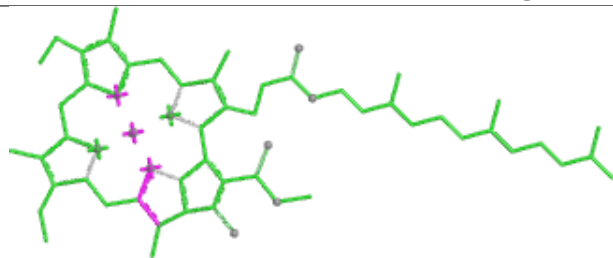
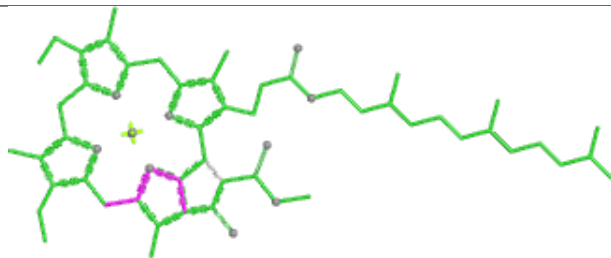
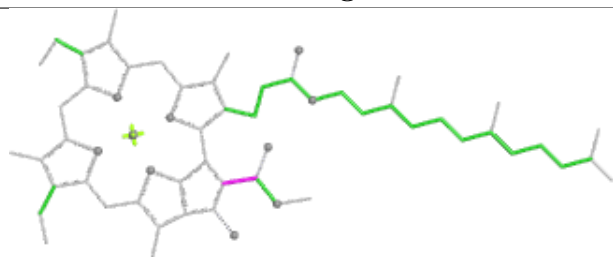
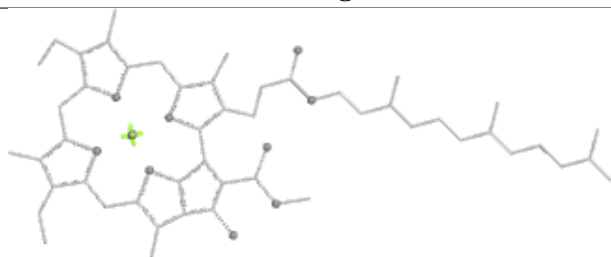
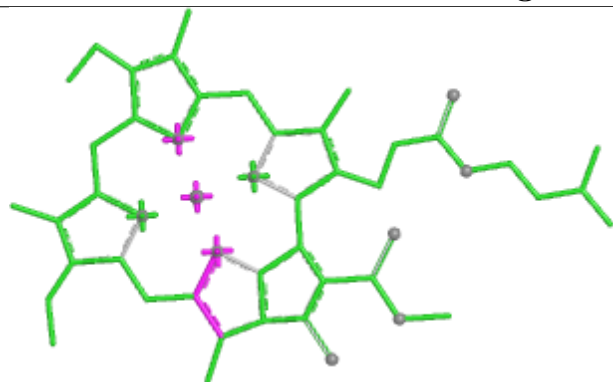
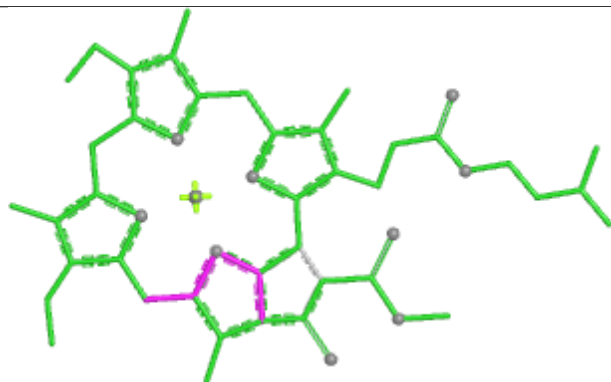
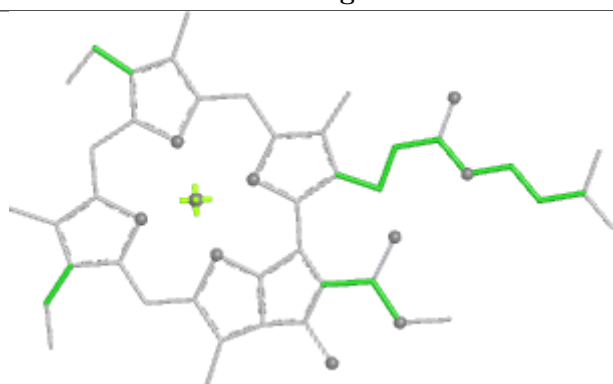
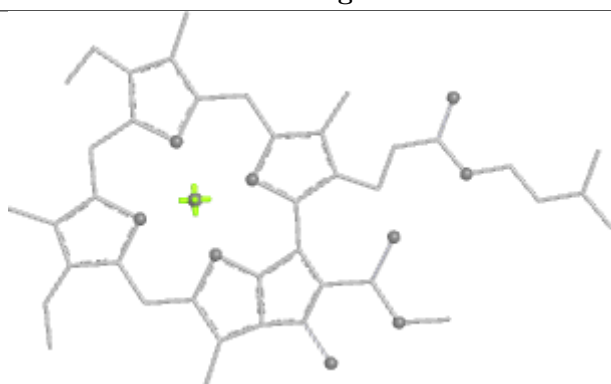


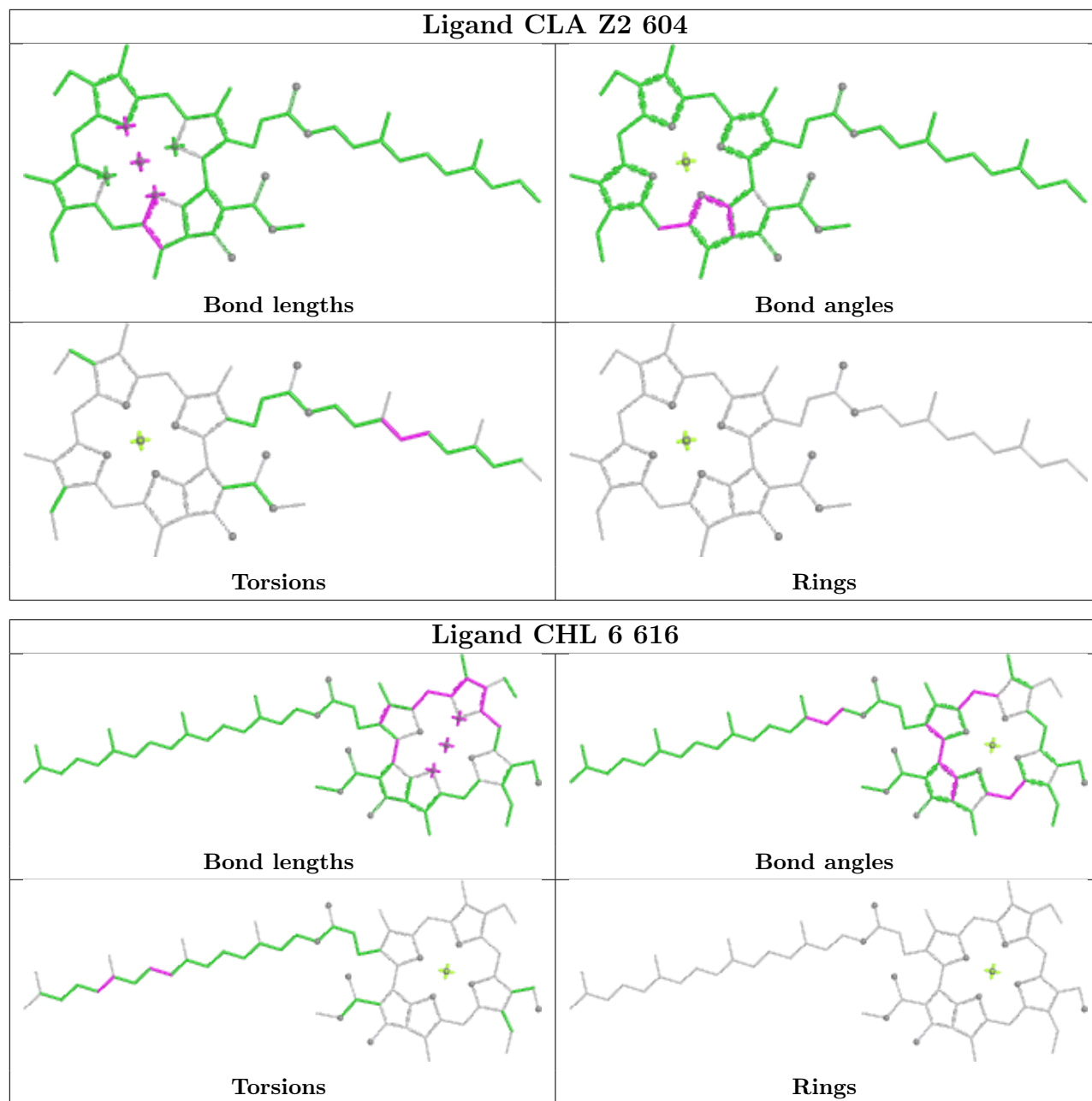


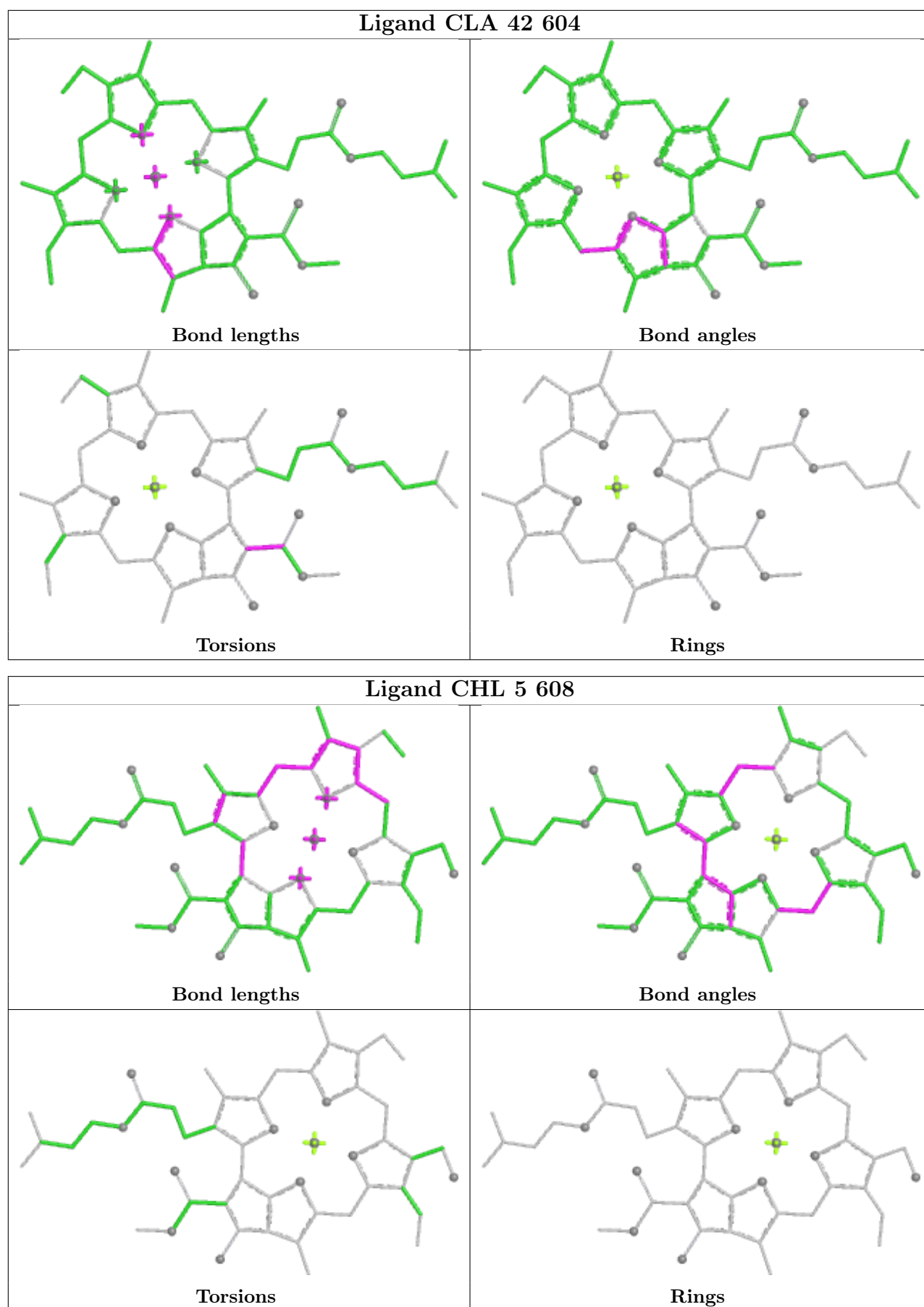


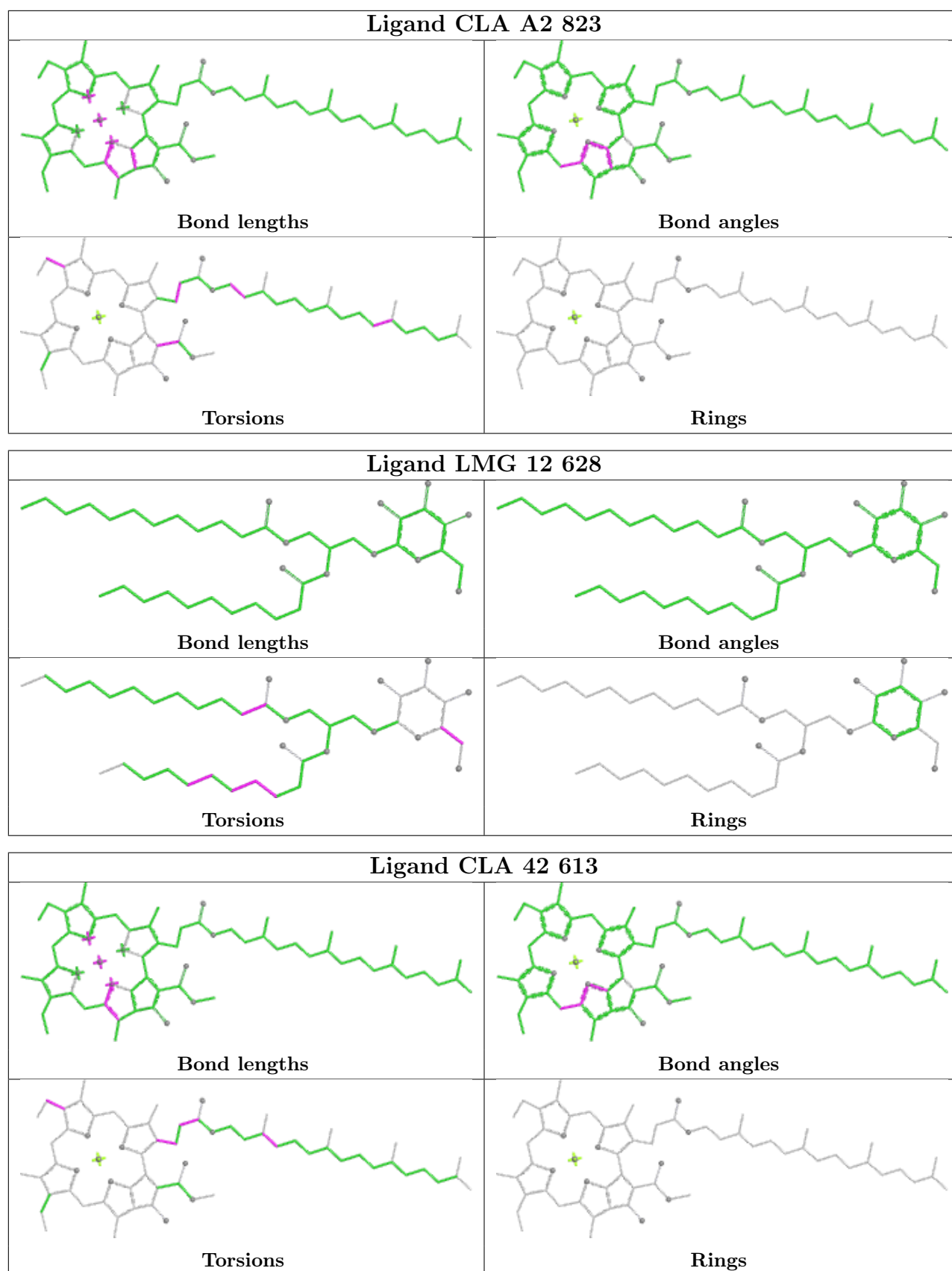


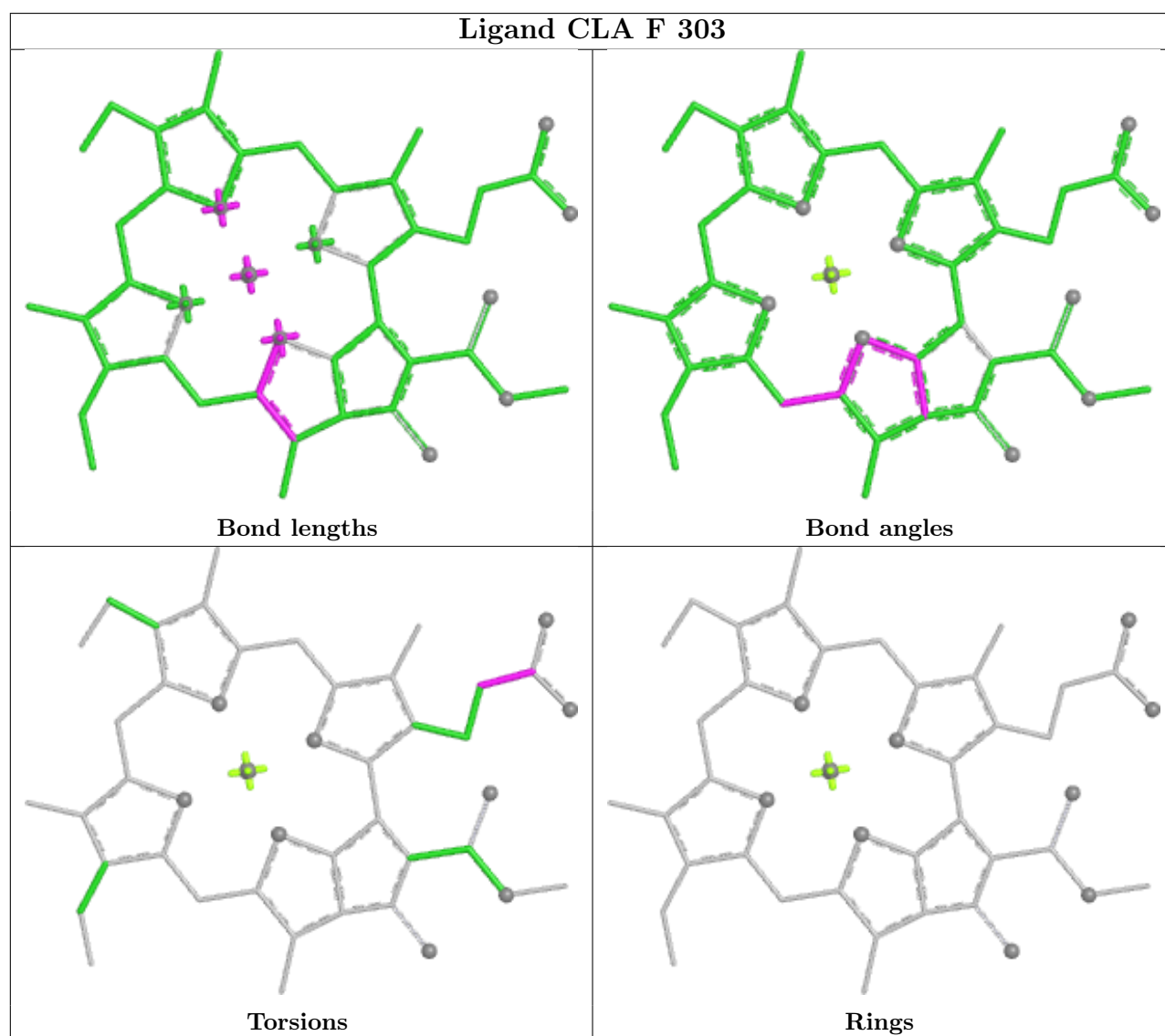
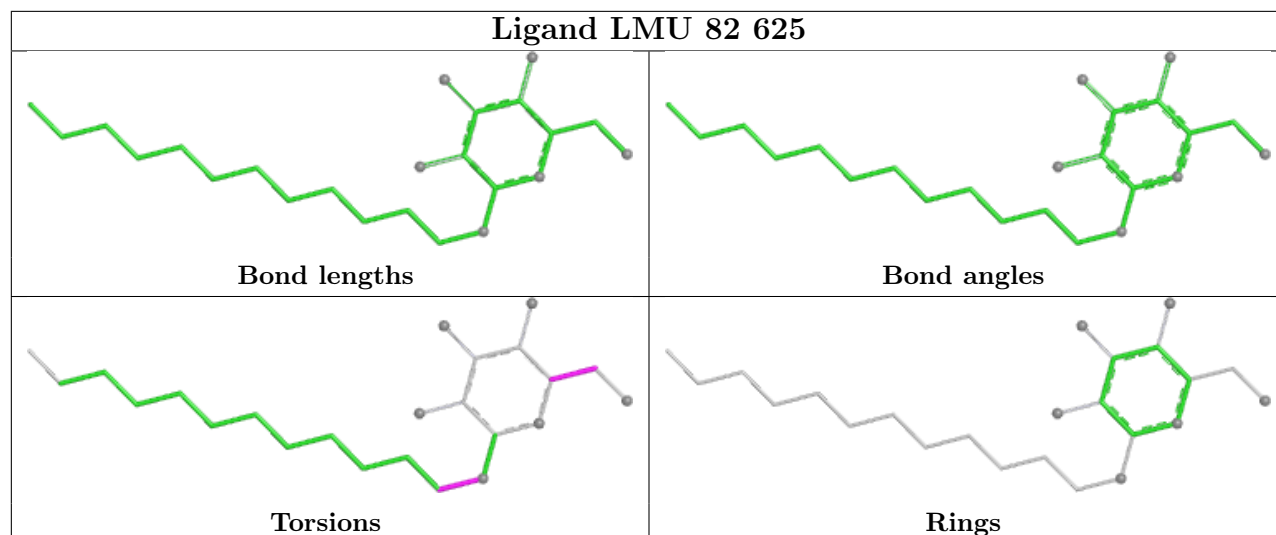


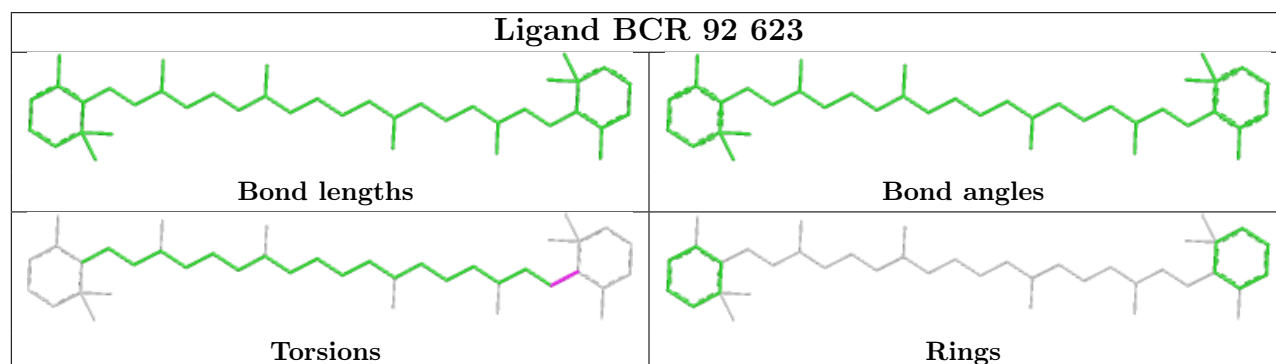
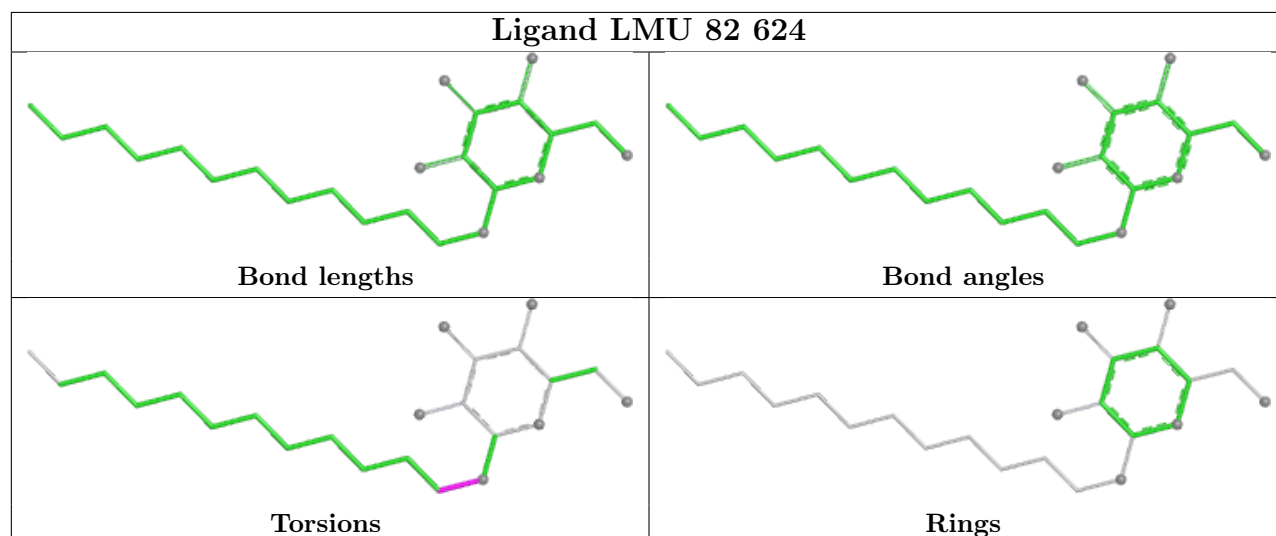
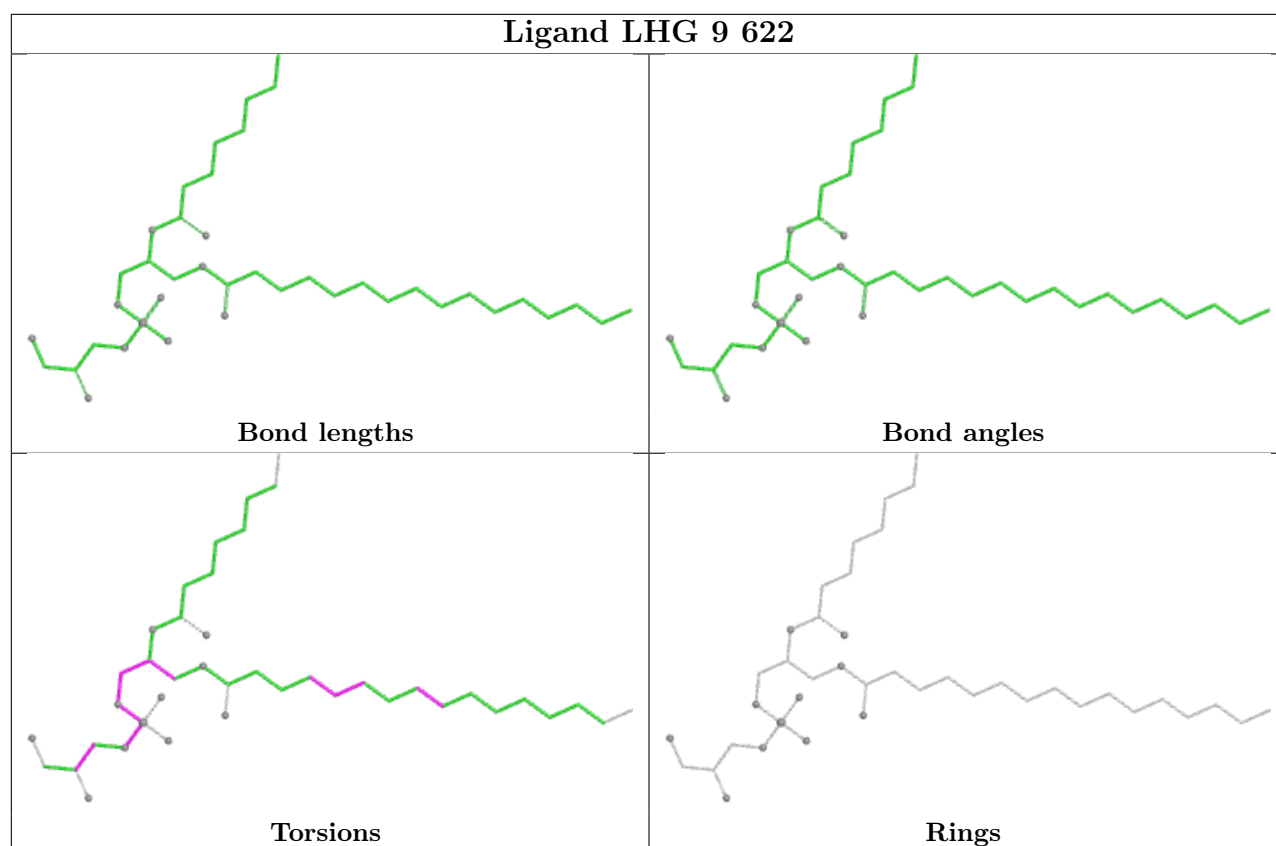
Ligand CLA 4 602**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA Z 614****Bond lengths****Bond angles****Torsions****Rings**

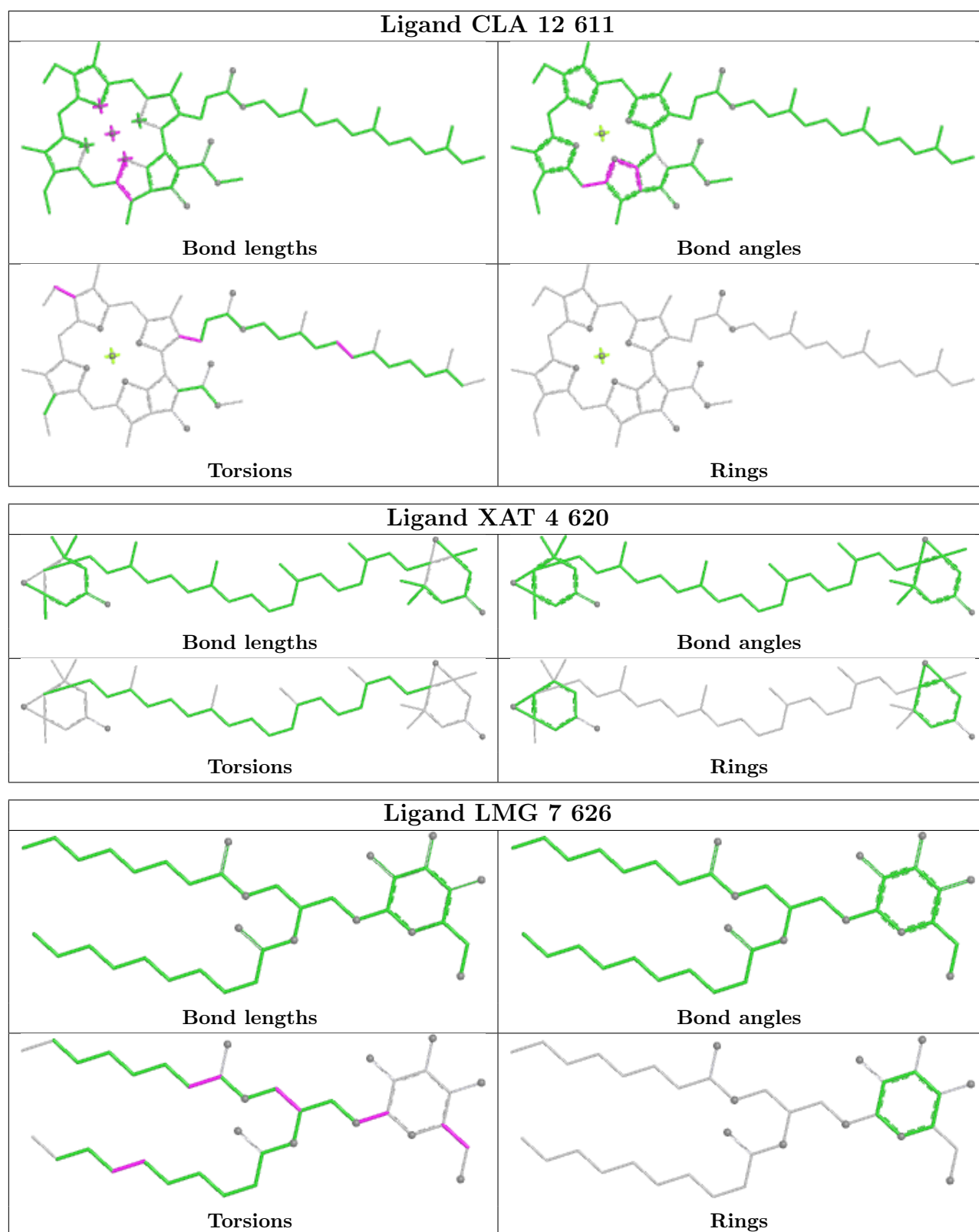


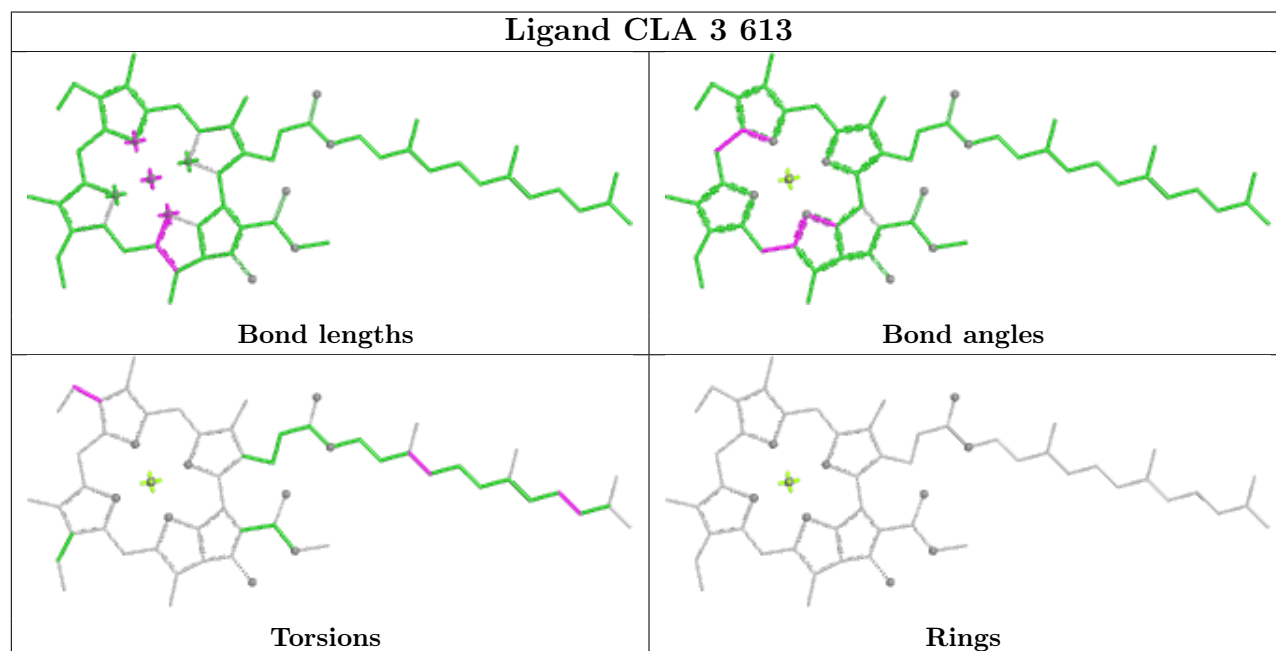
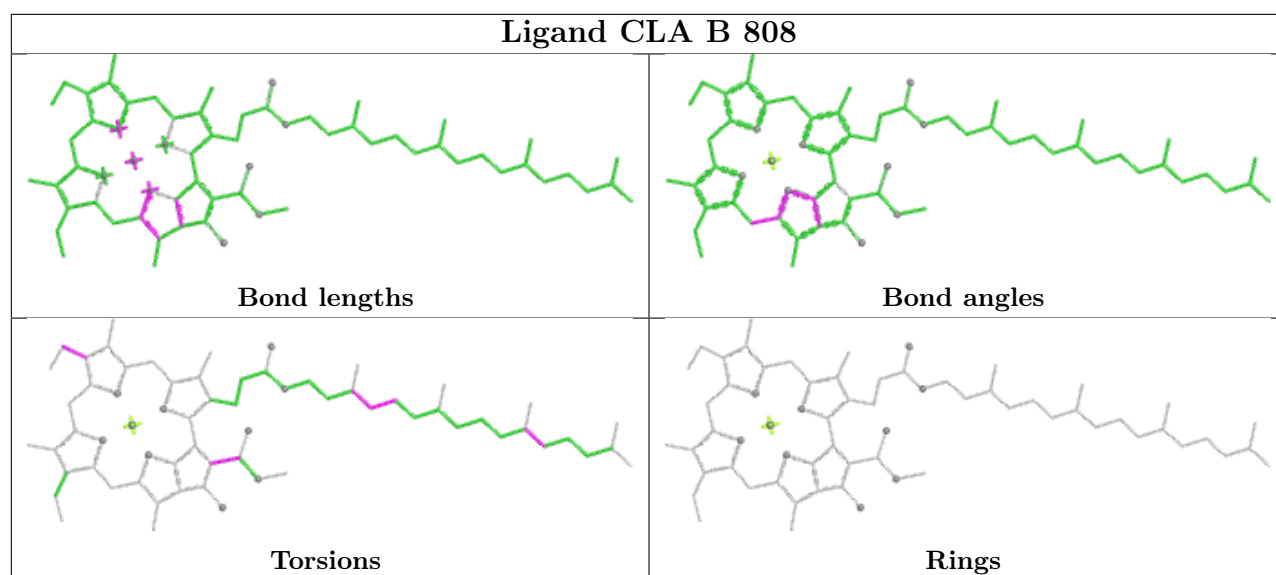


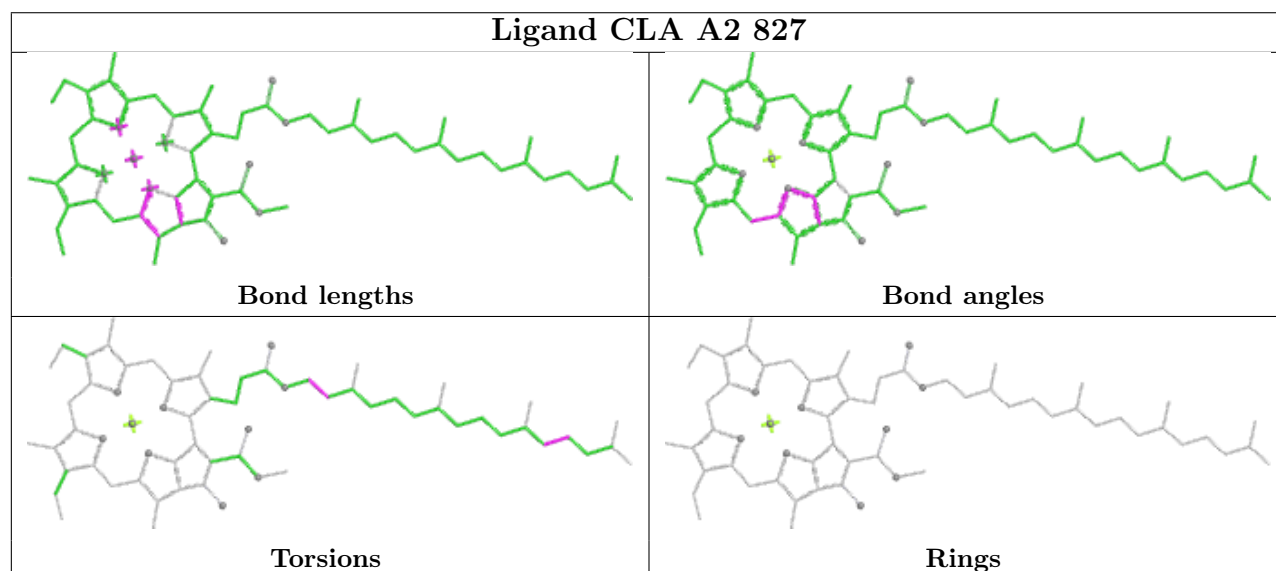
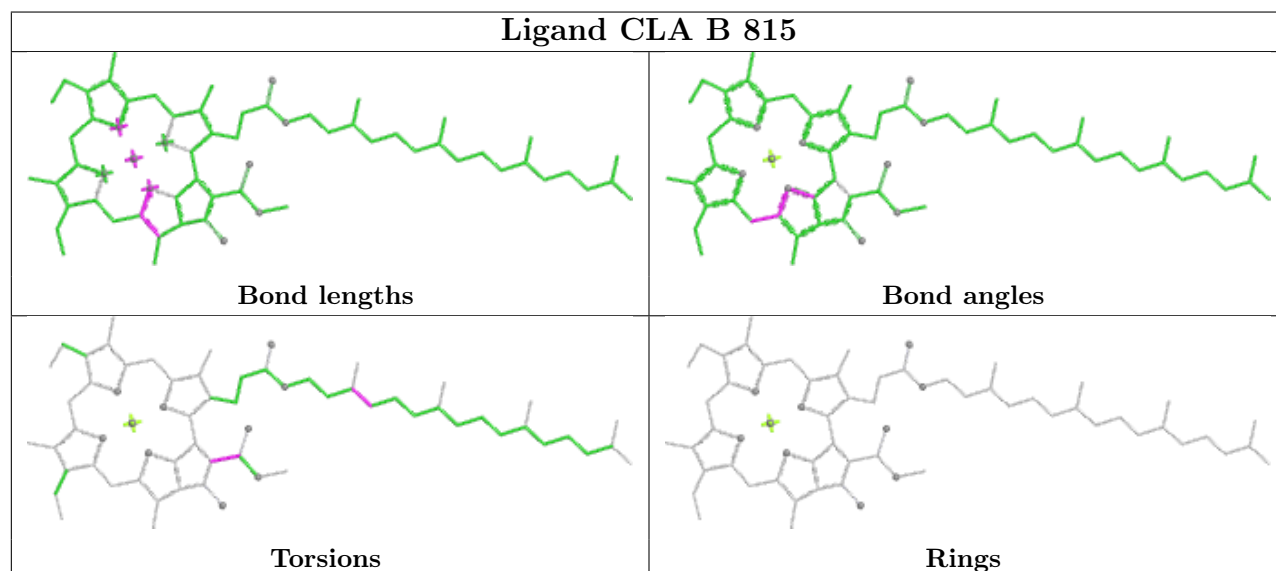
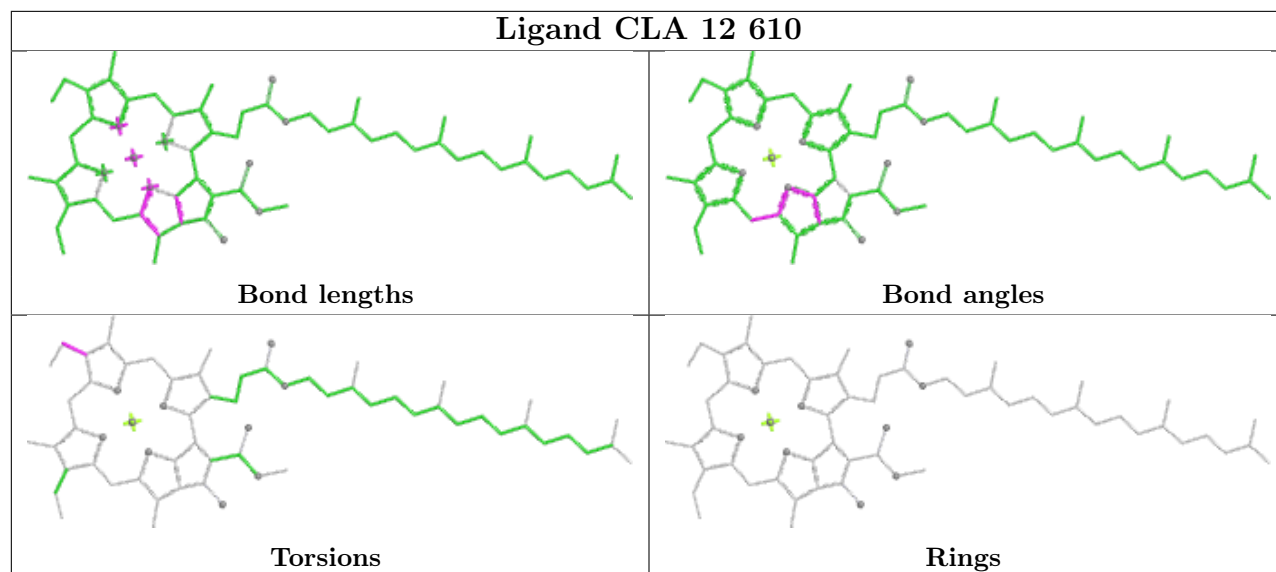




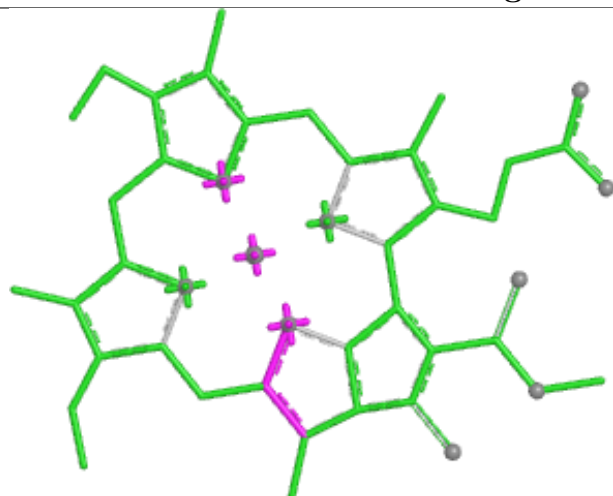




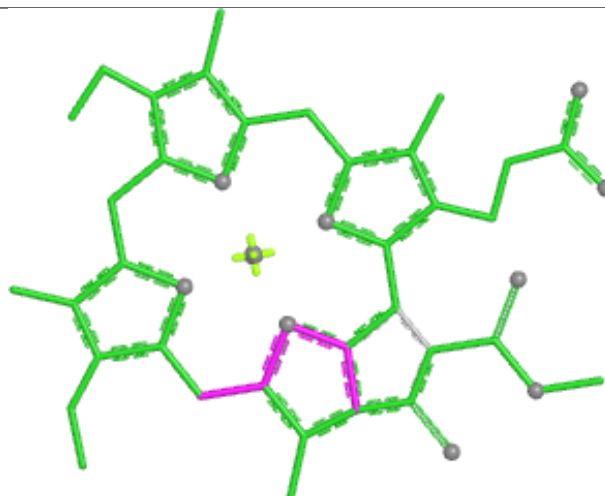




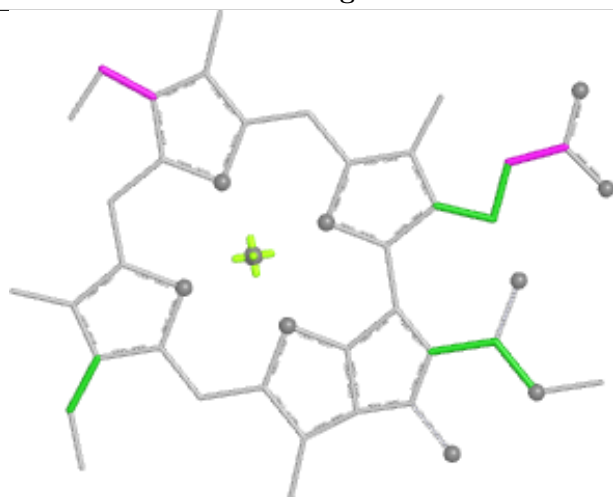
Ligand CLA K2 206



Bond lengths



Bond angles

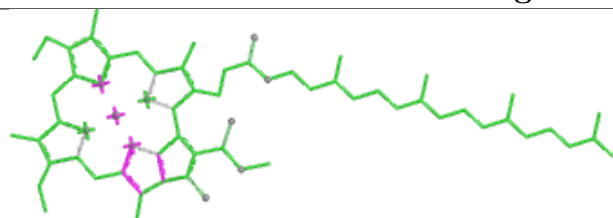


Torsions

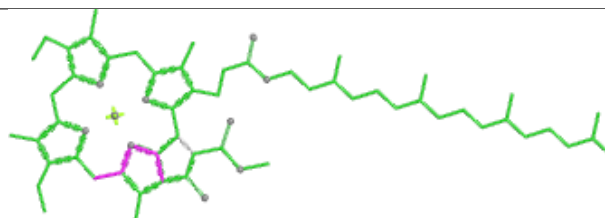


Rings

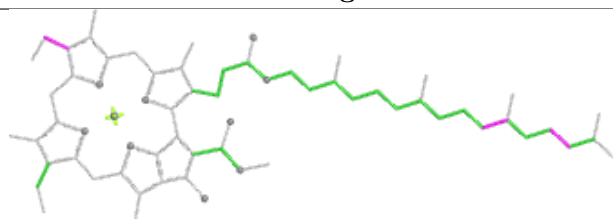
Ligand CLA B 832



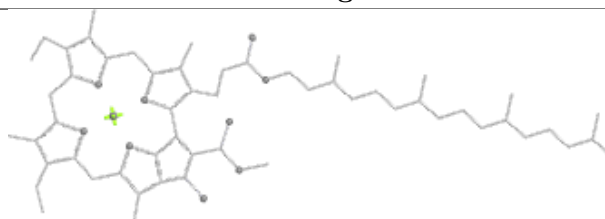
Bond lengths



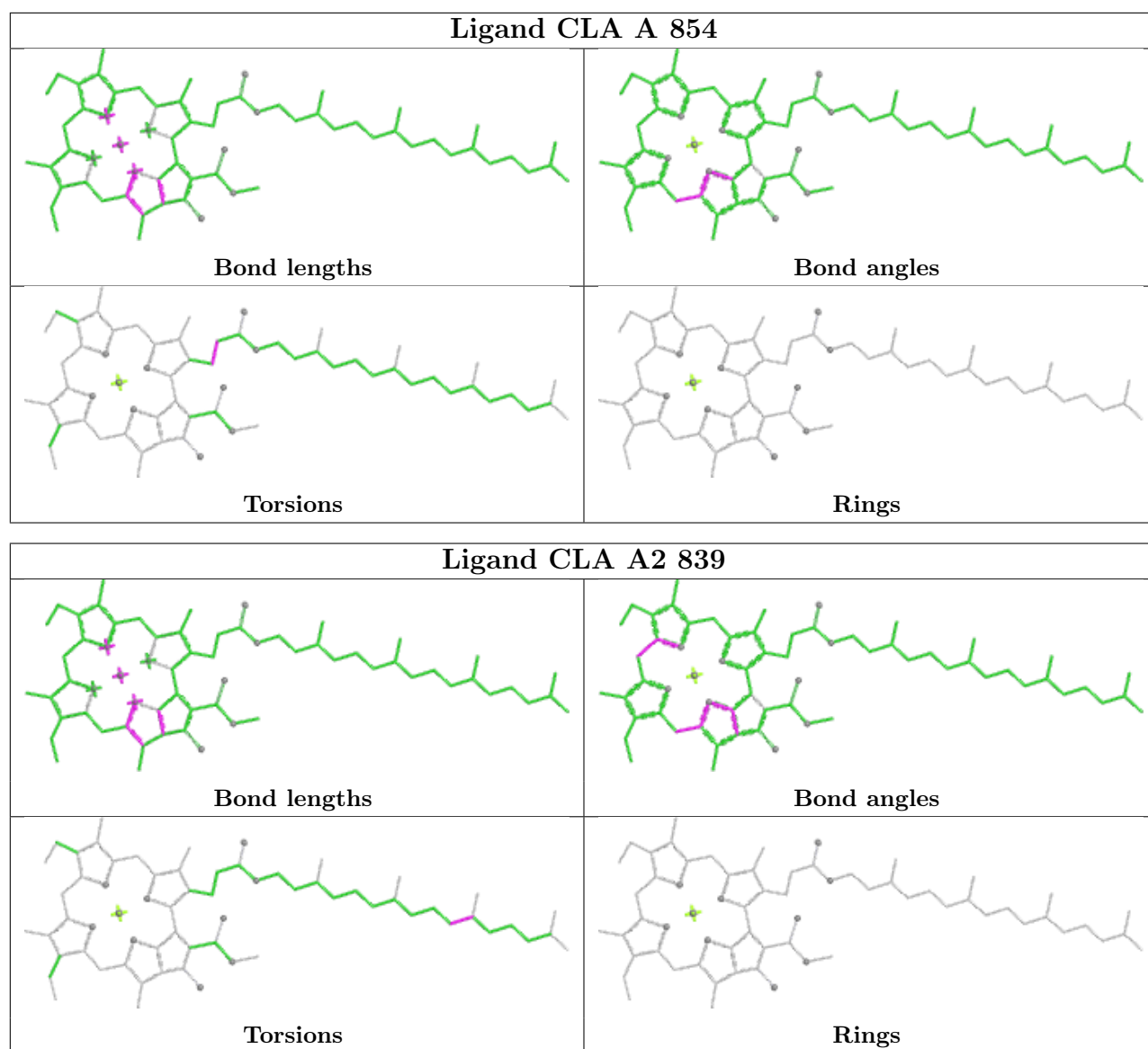
Bond angles

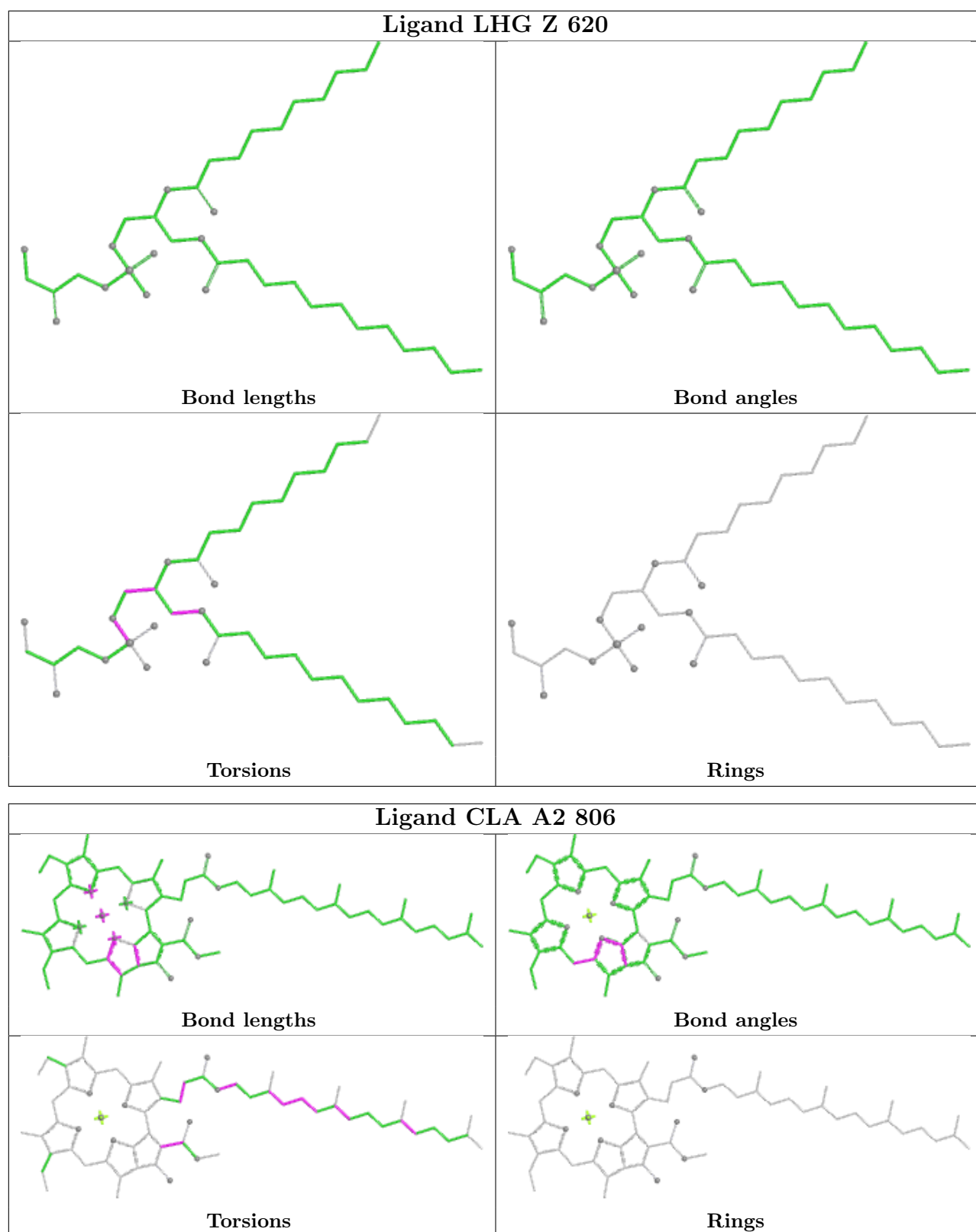


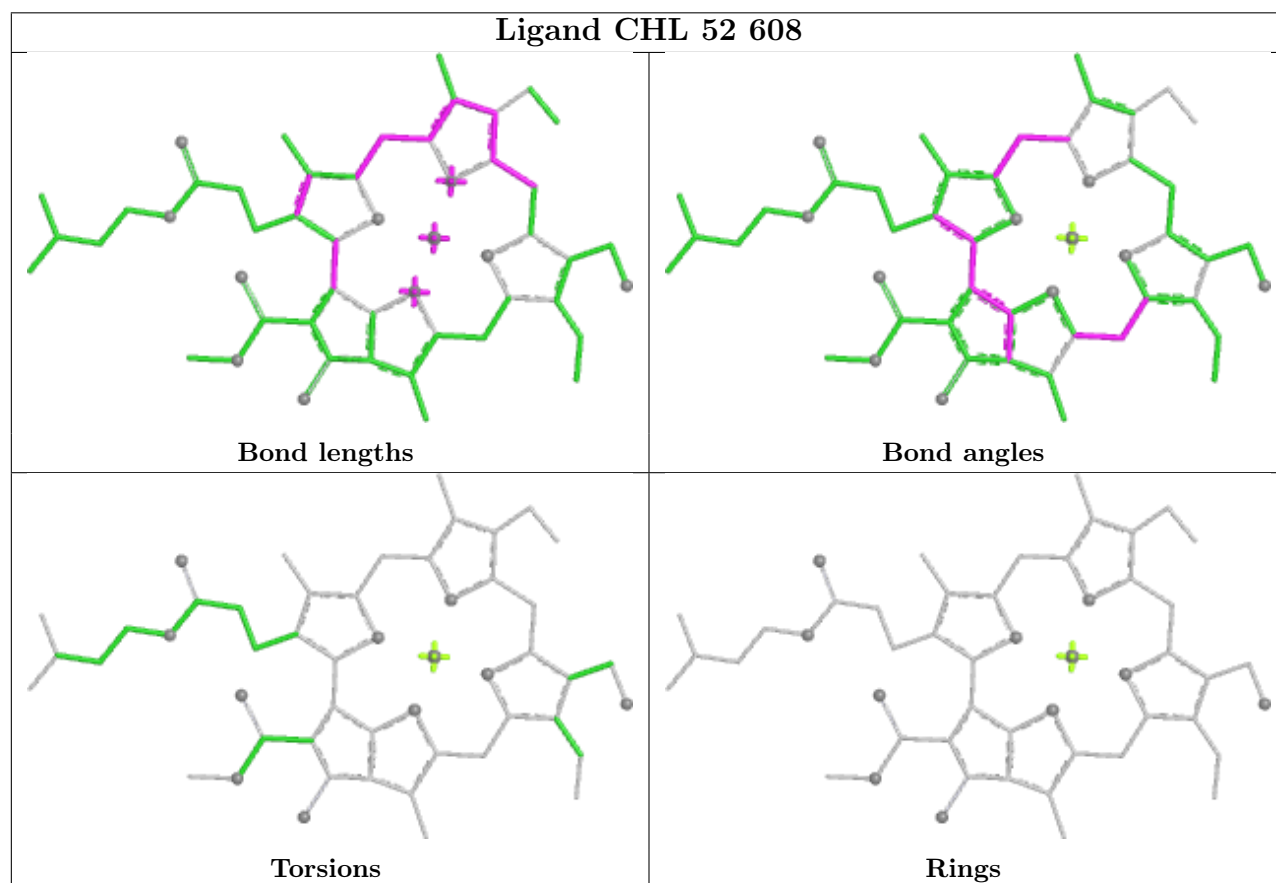
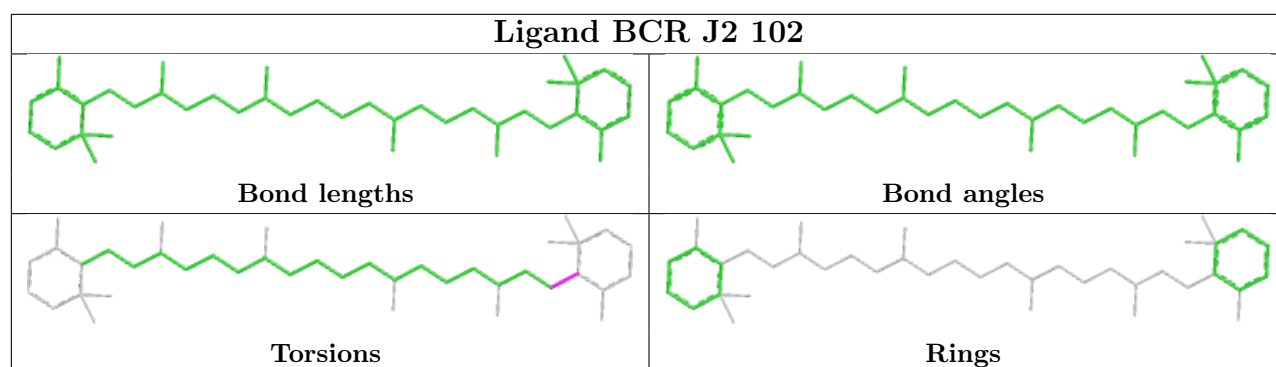
Torsions



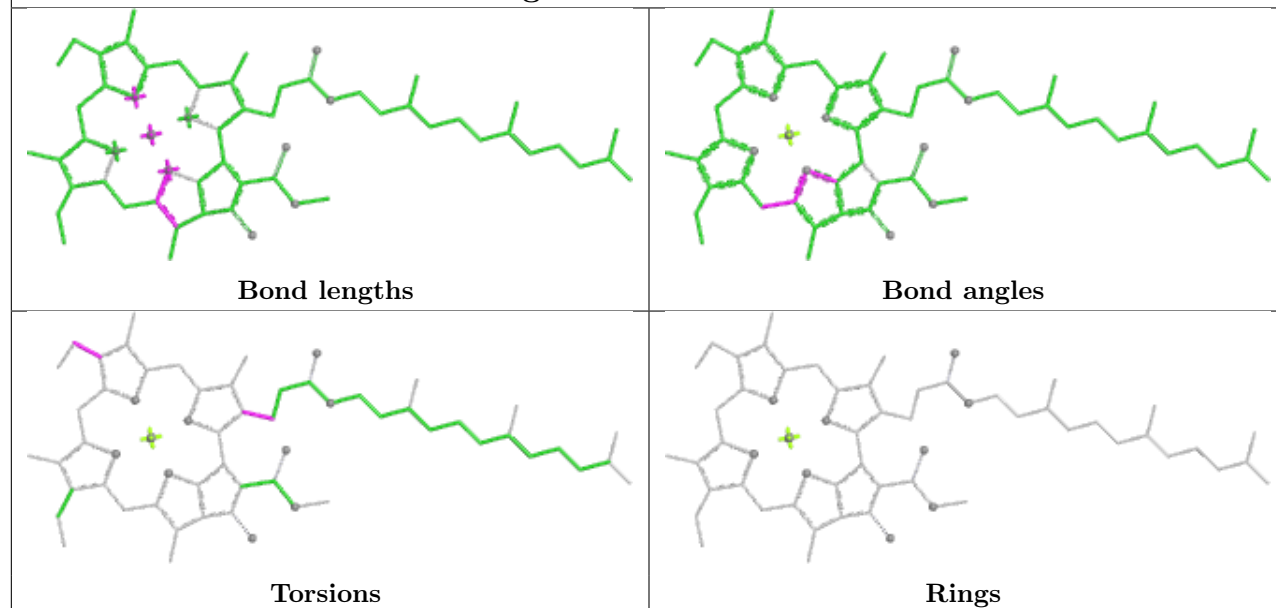
Rings



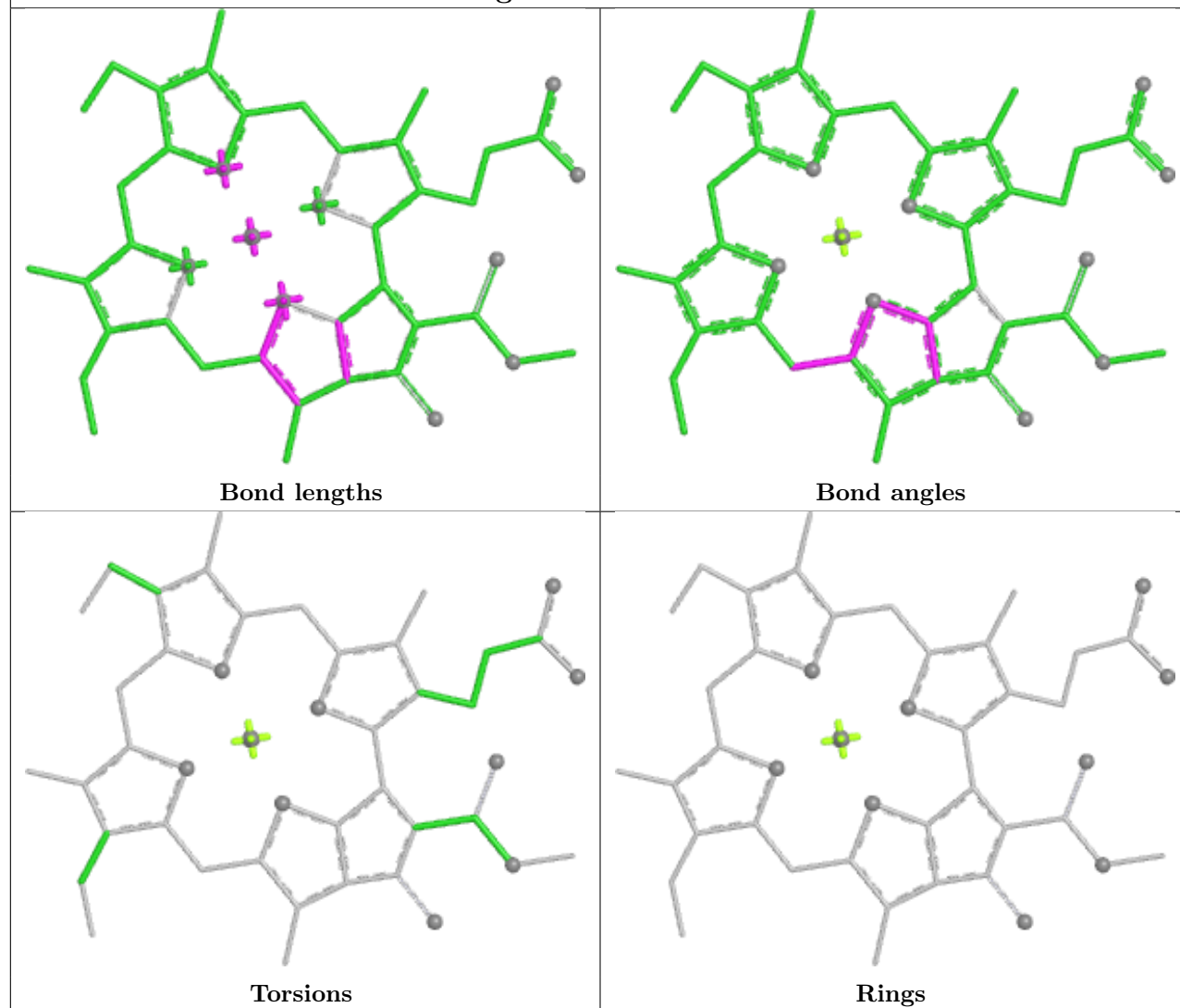


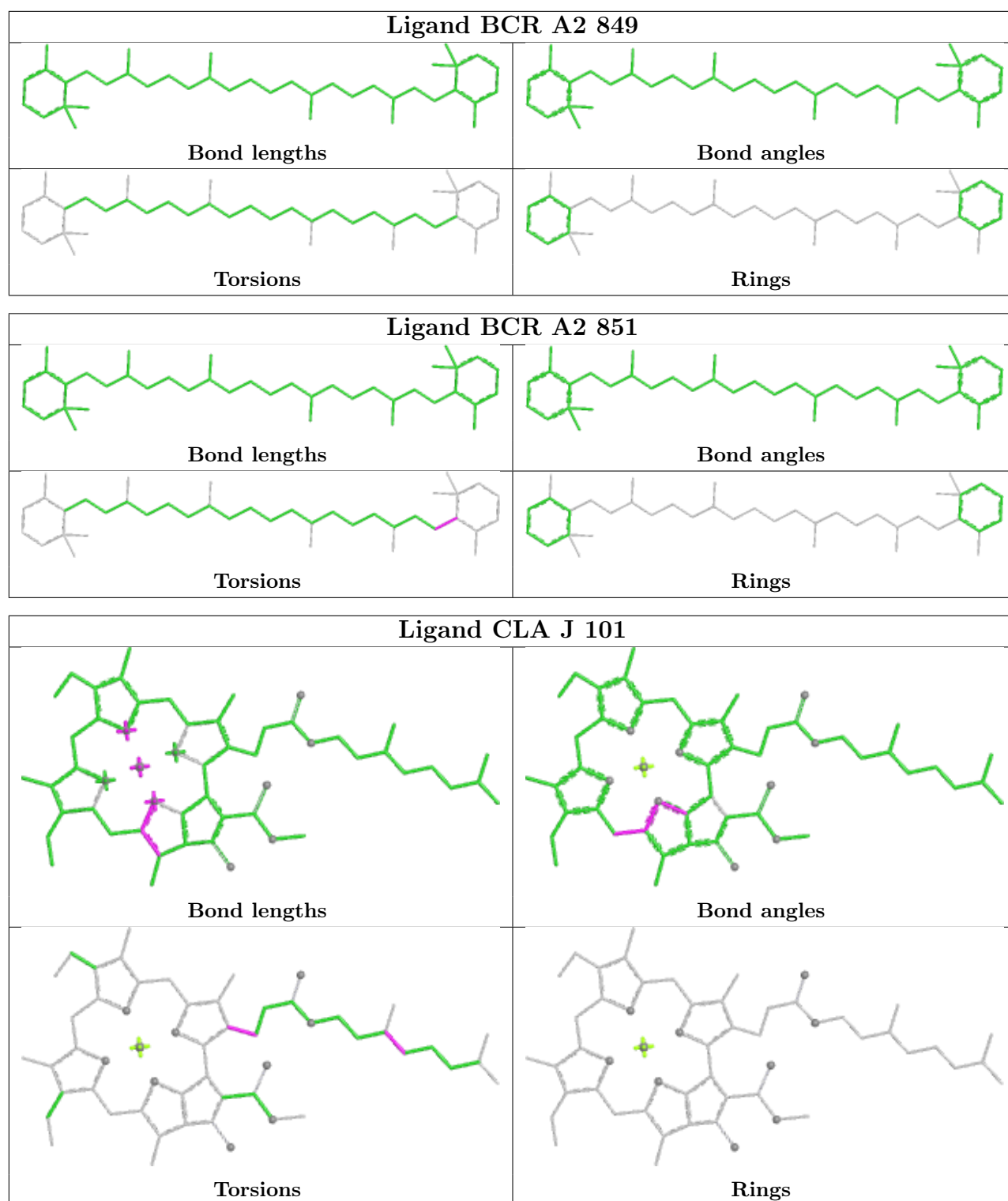


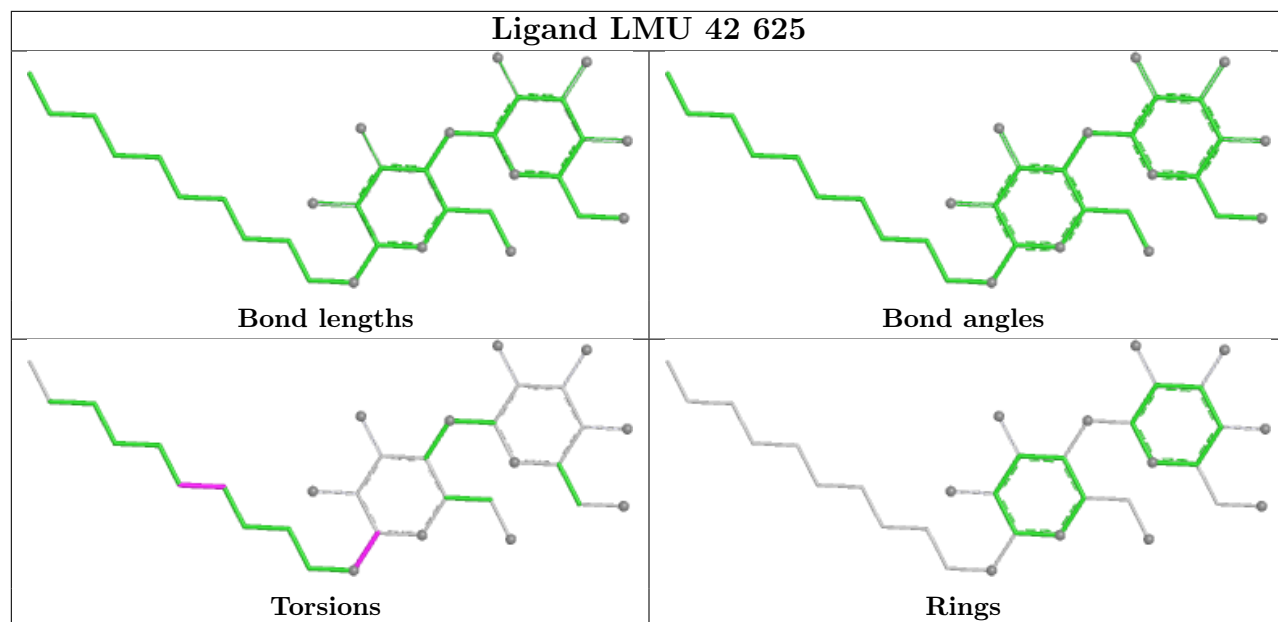
Ligand CLA A2 819

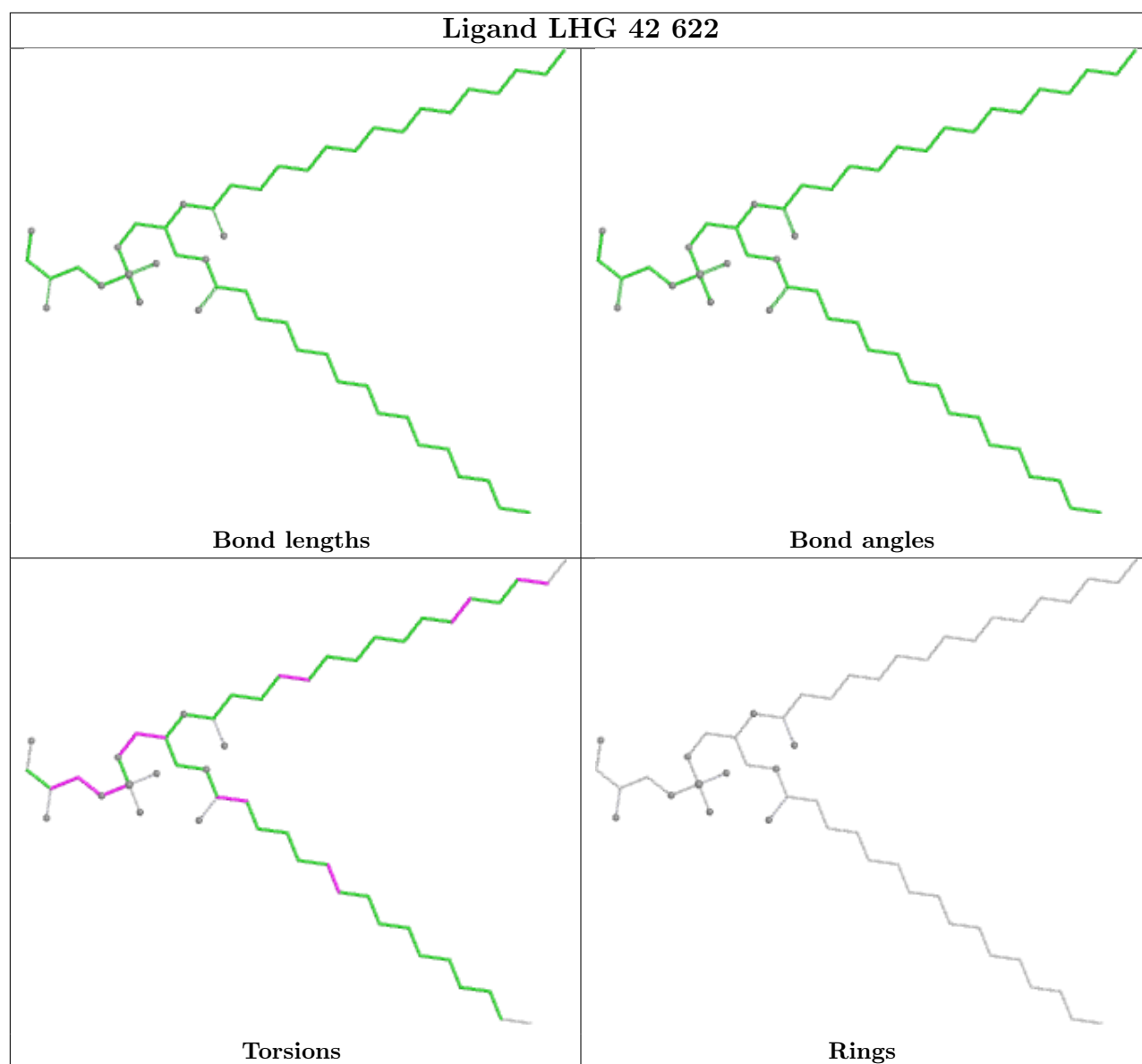


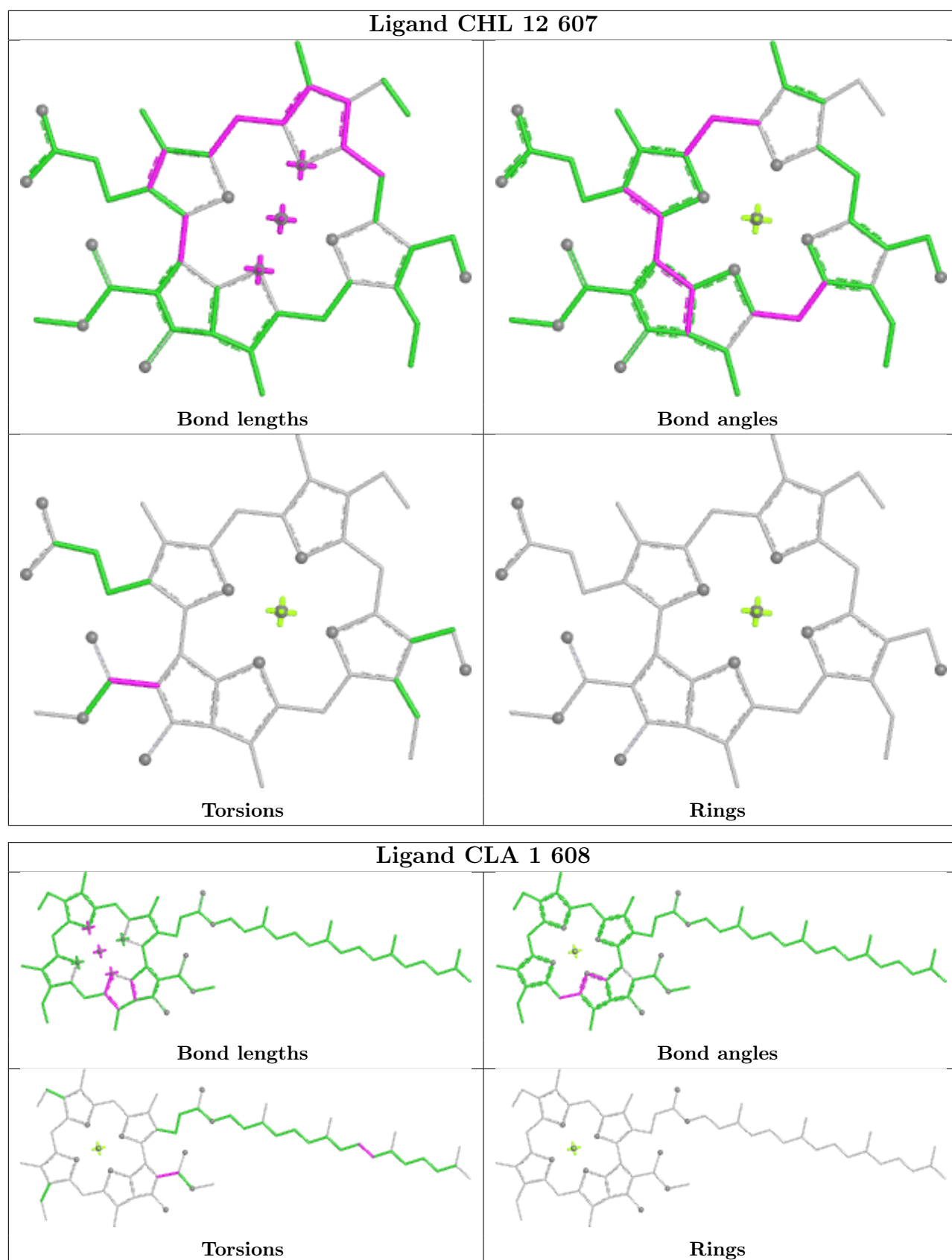
Ligand CLA 8 616

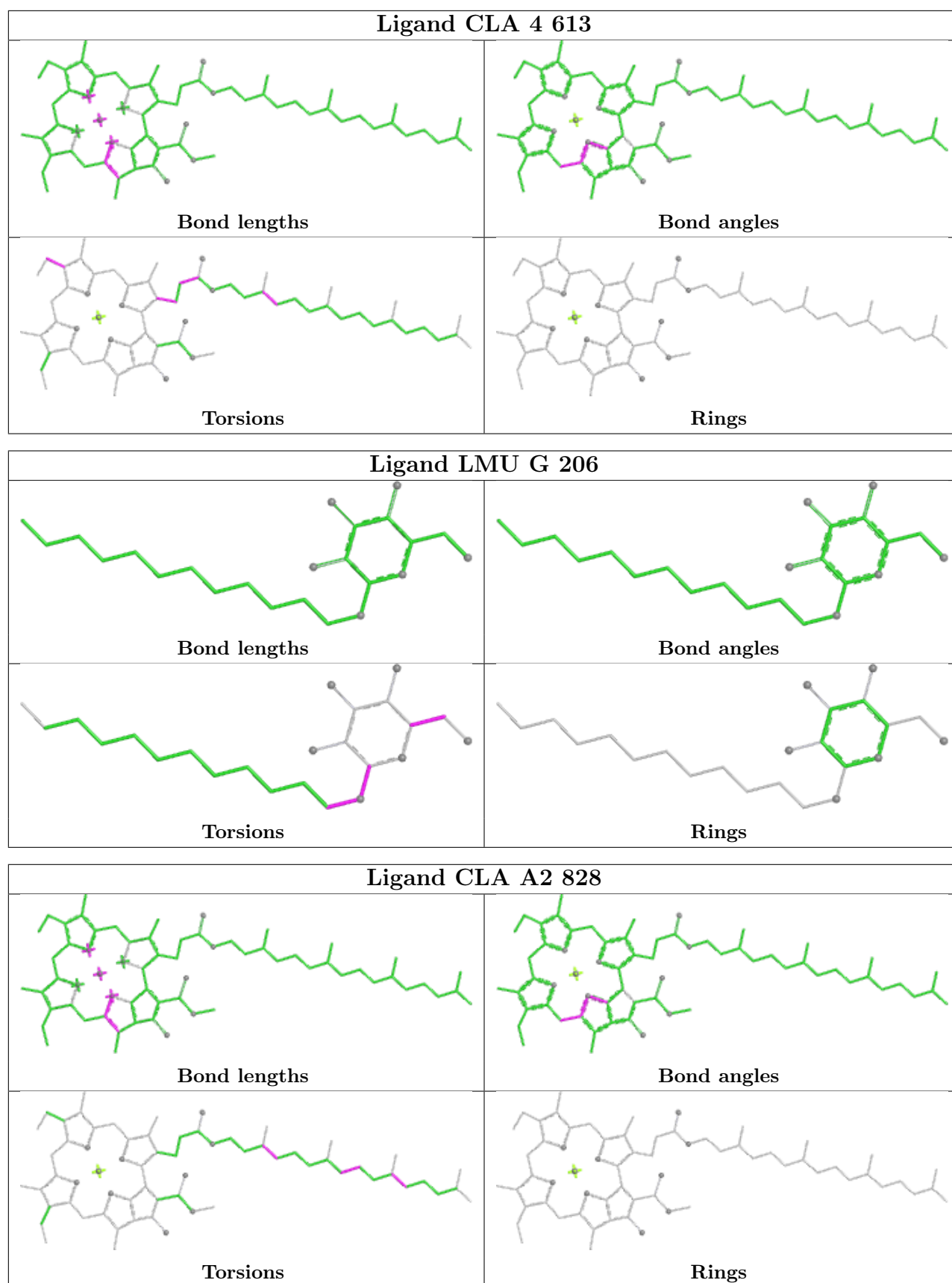




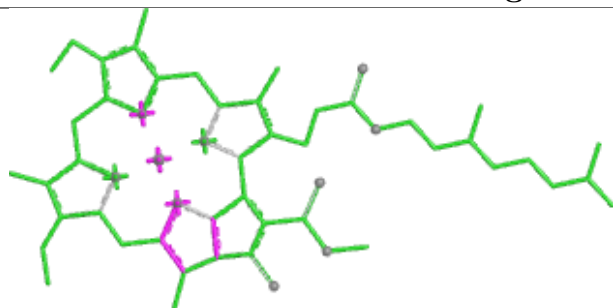




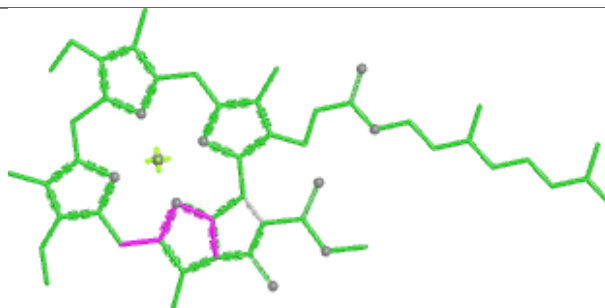




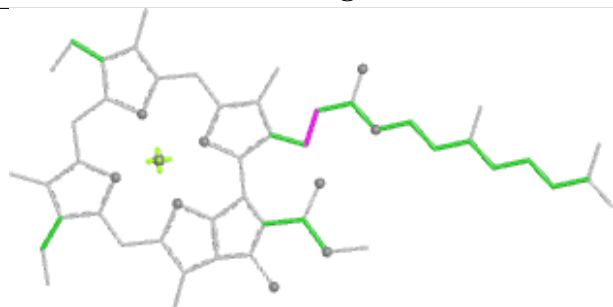
Ligand CLA B2 831



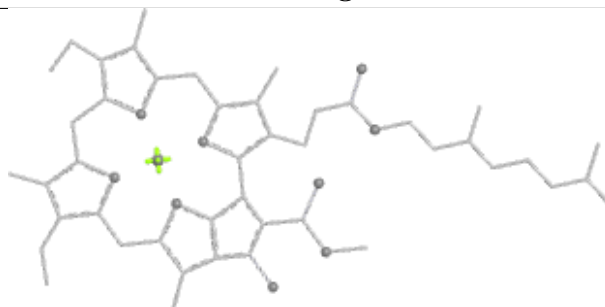
Bond lengths



Bond angles

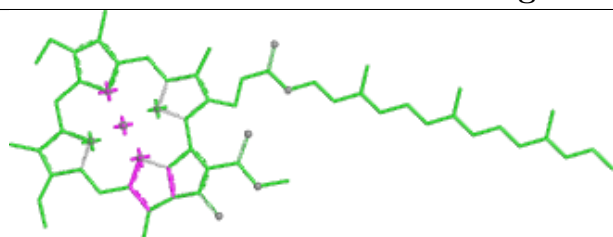


Torsions

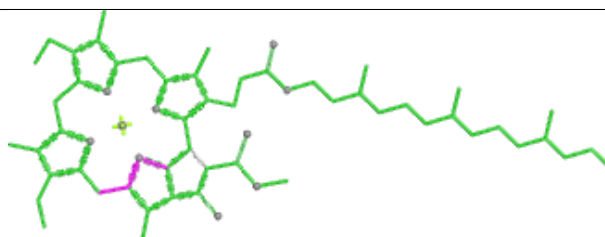


Rings

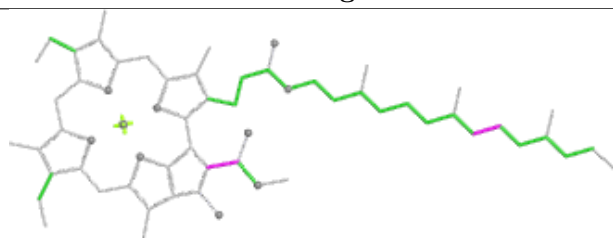
Ligand CLA 8 602



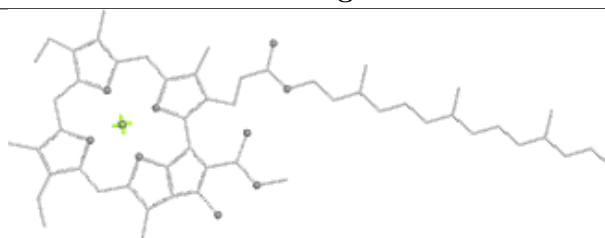
Bond lengths



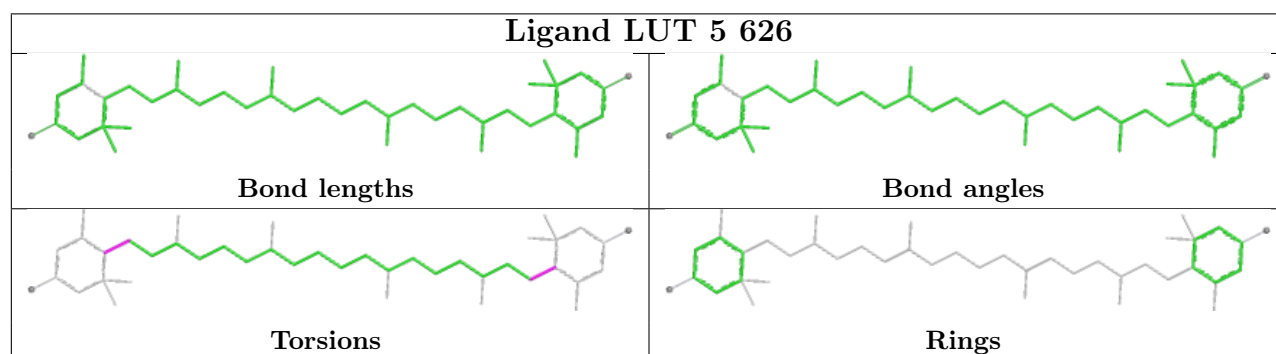
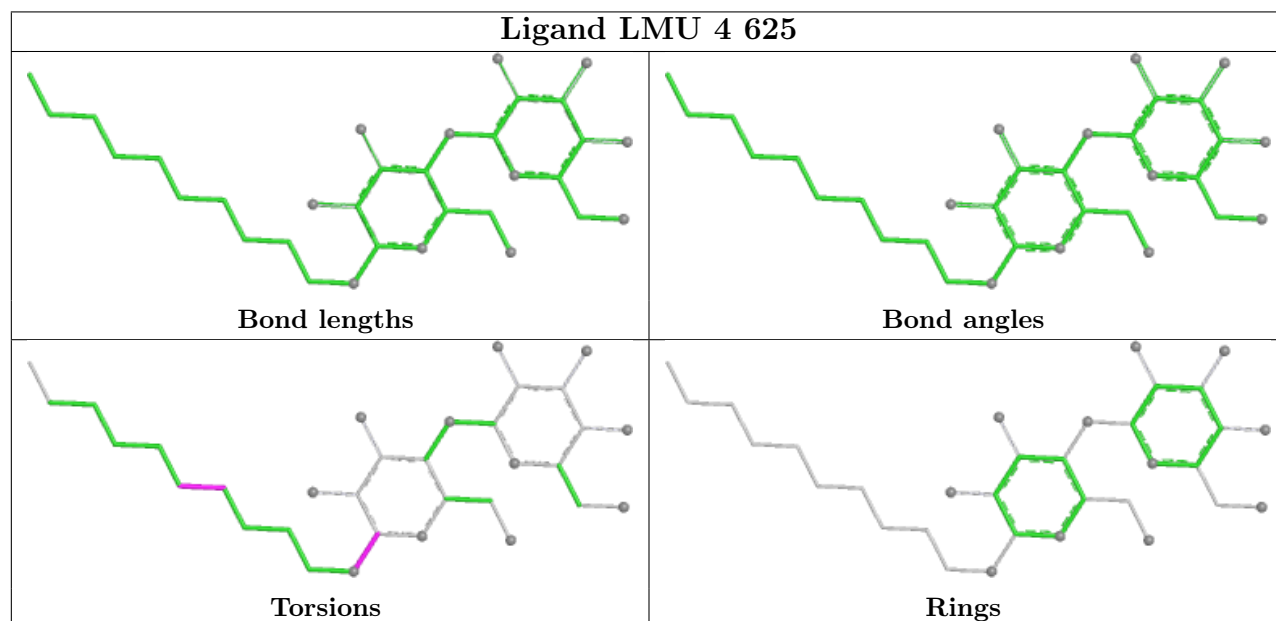
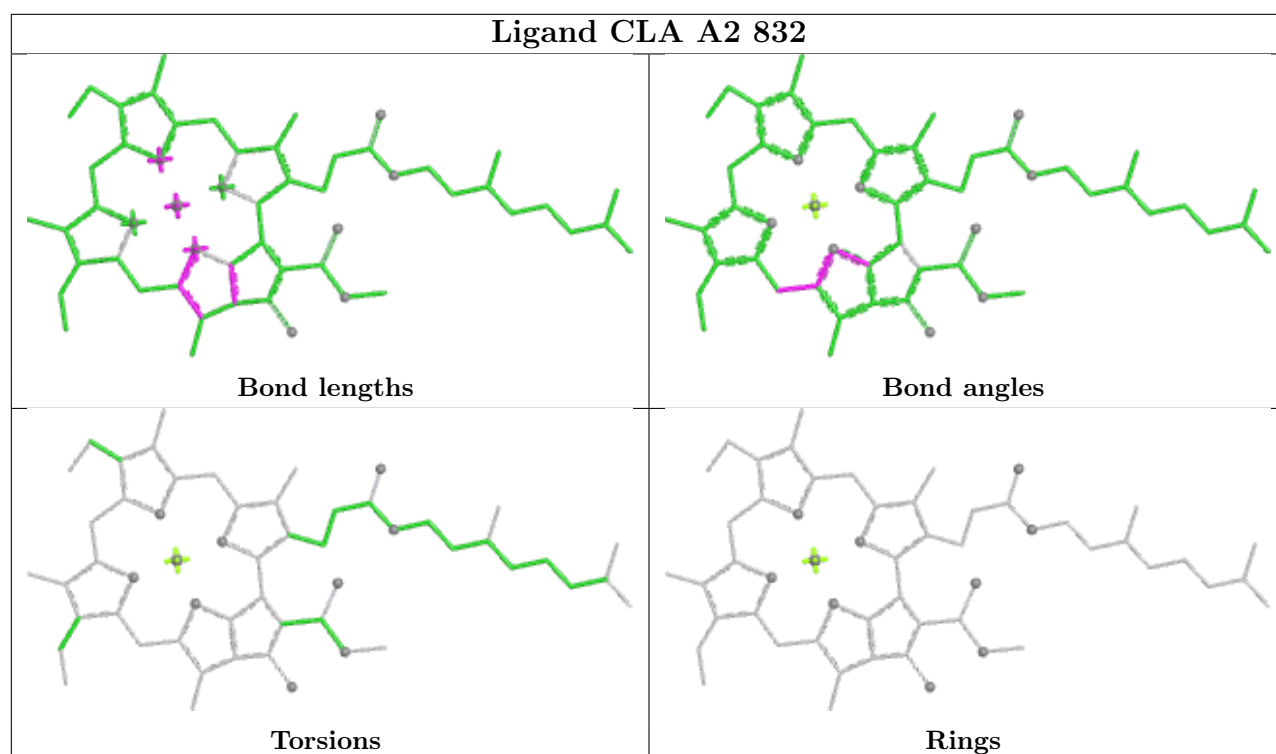
Bond angles

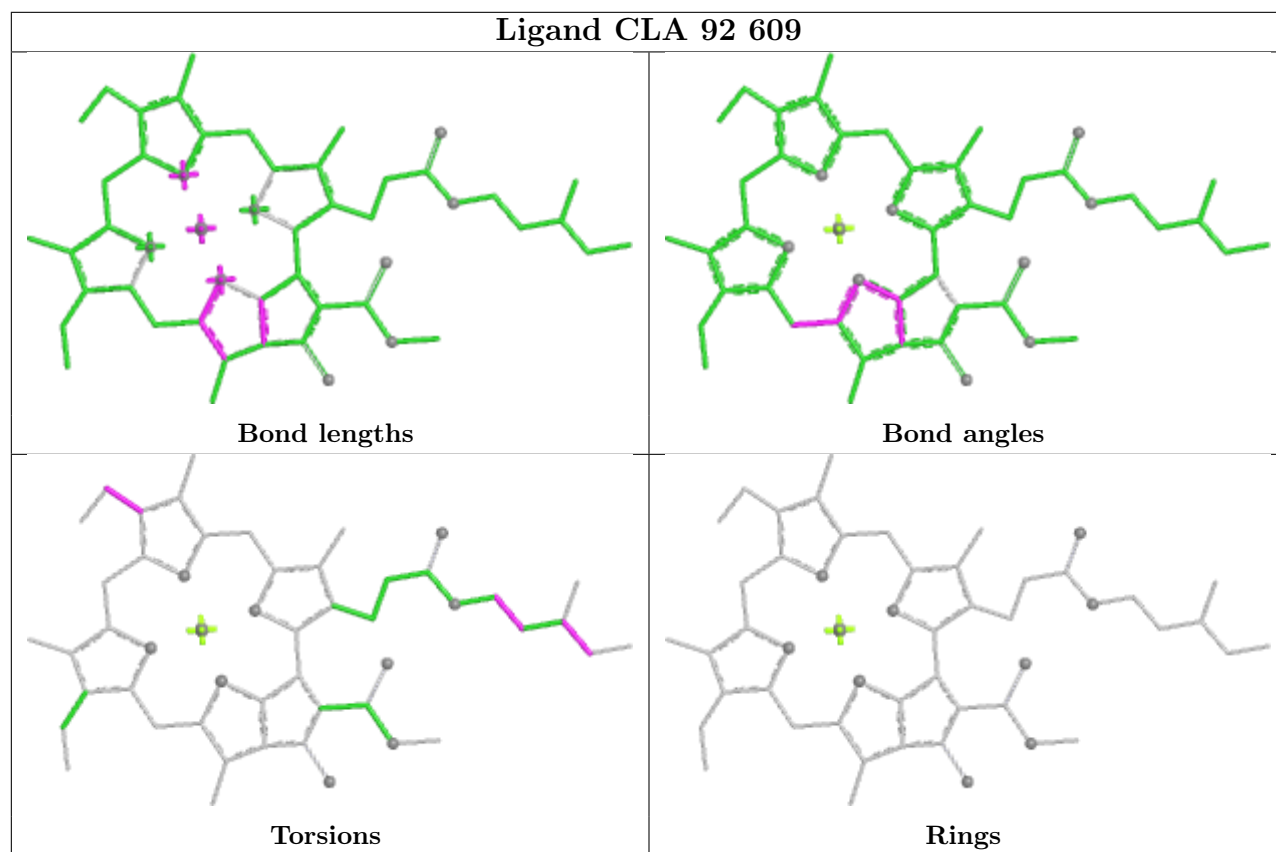
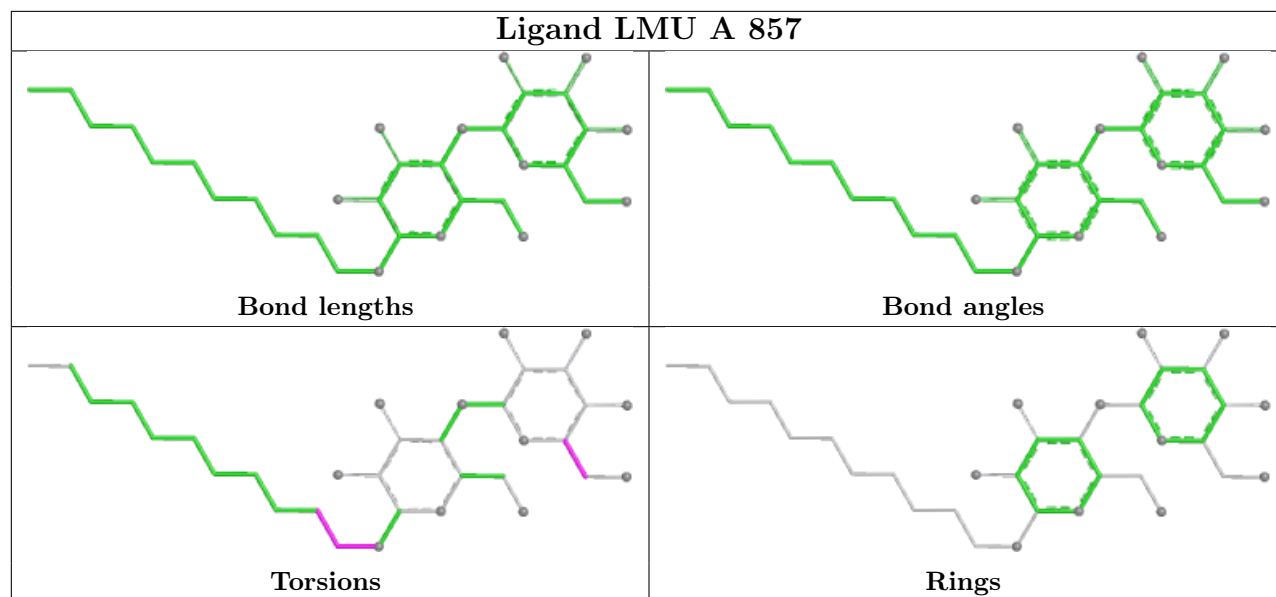


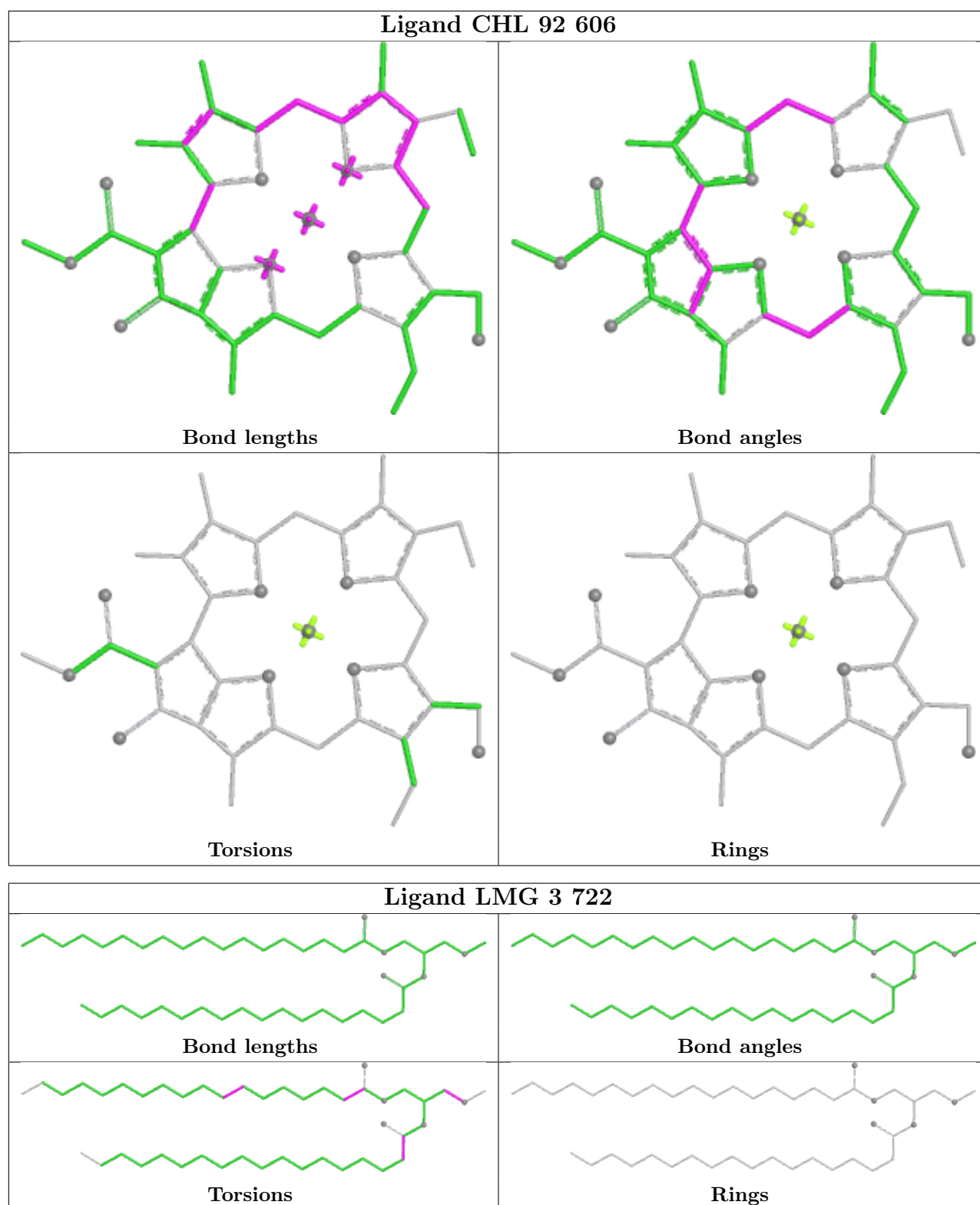
Torsions

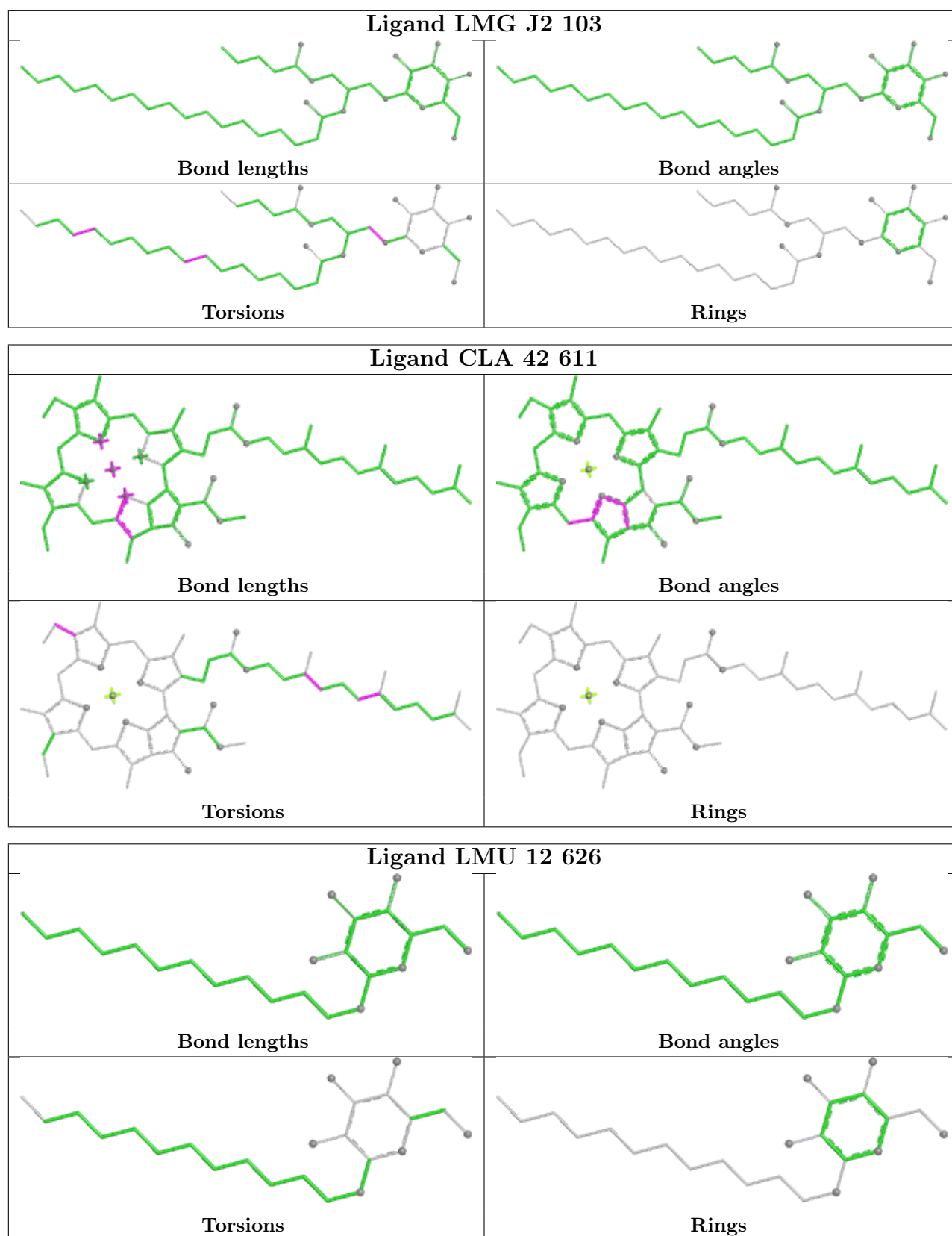


Rings

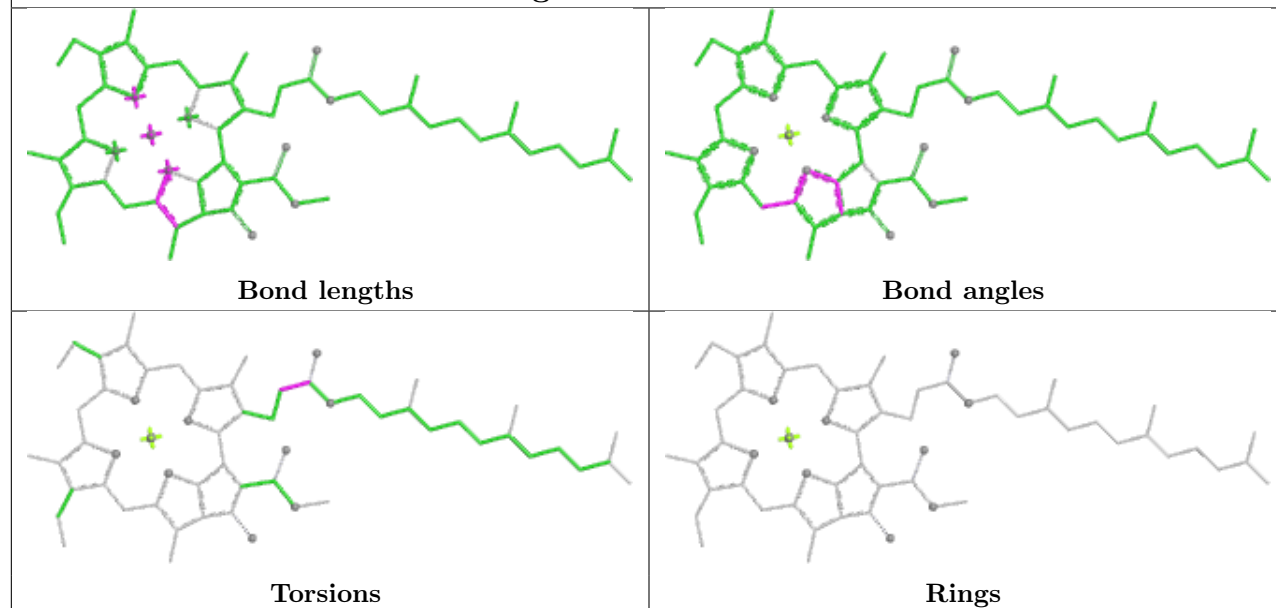




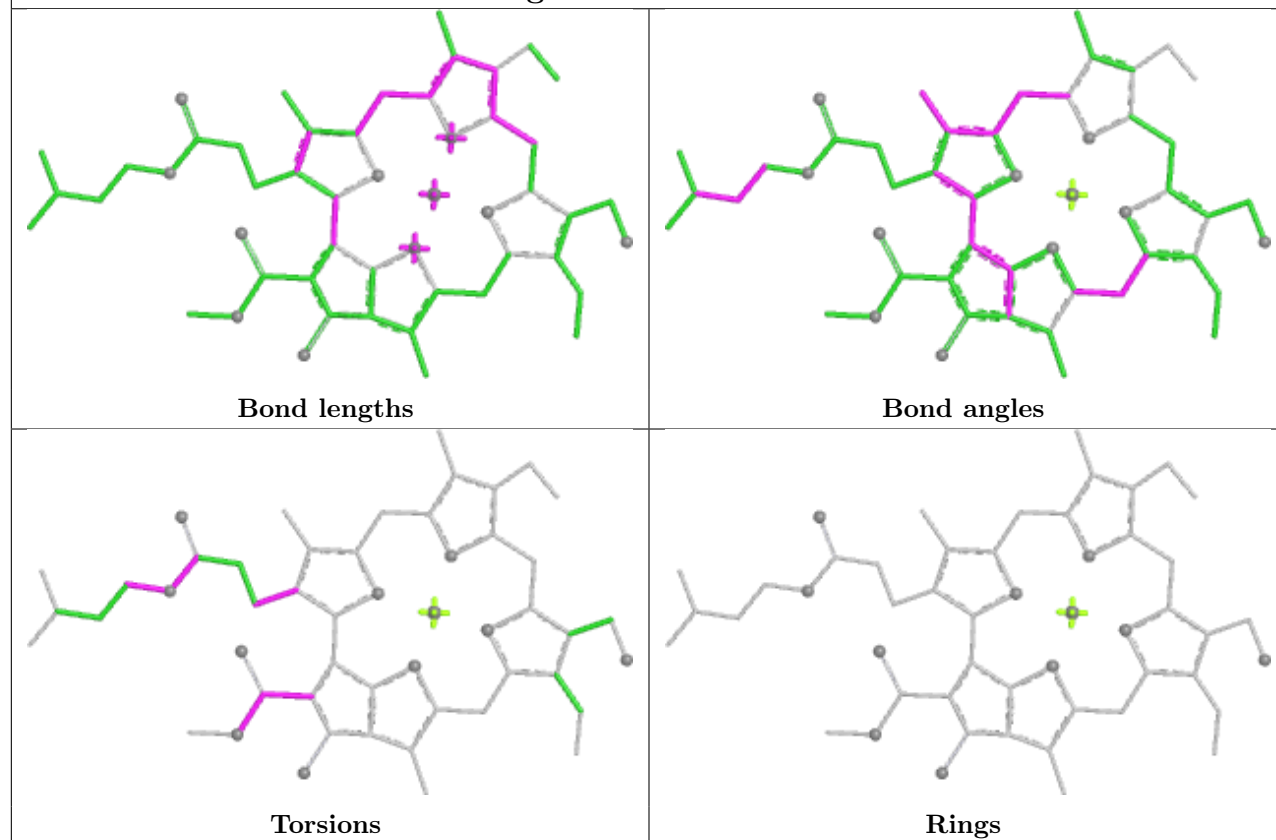




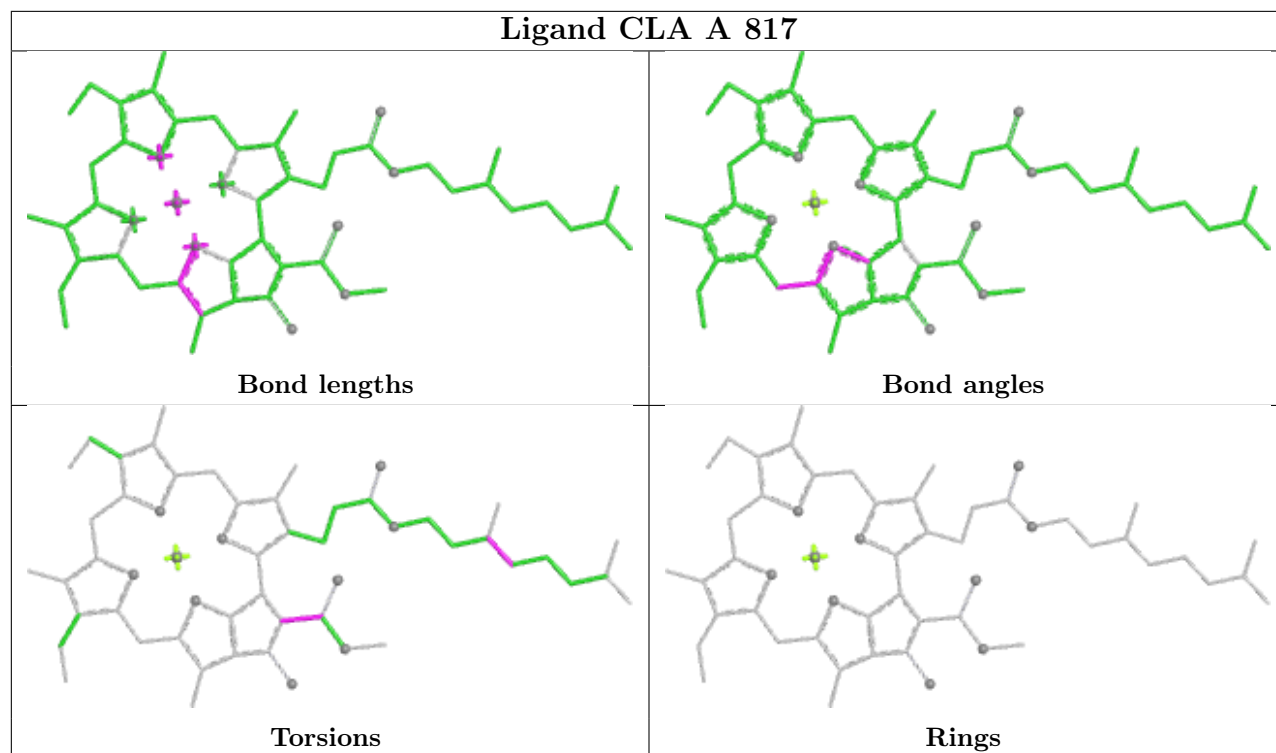
Ligand CLA B 814



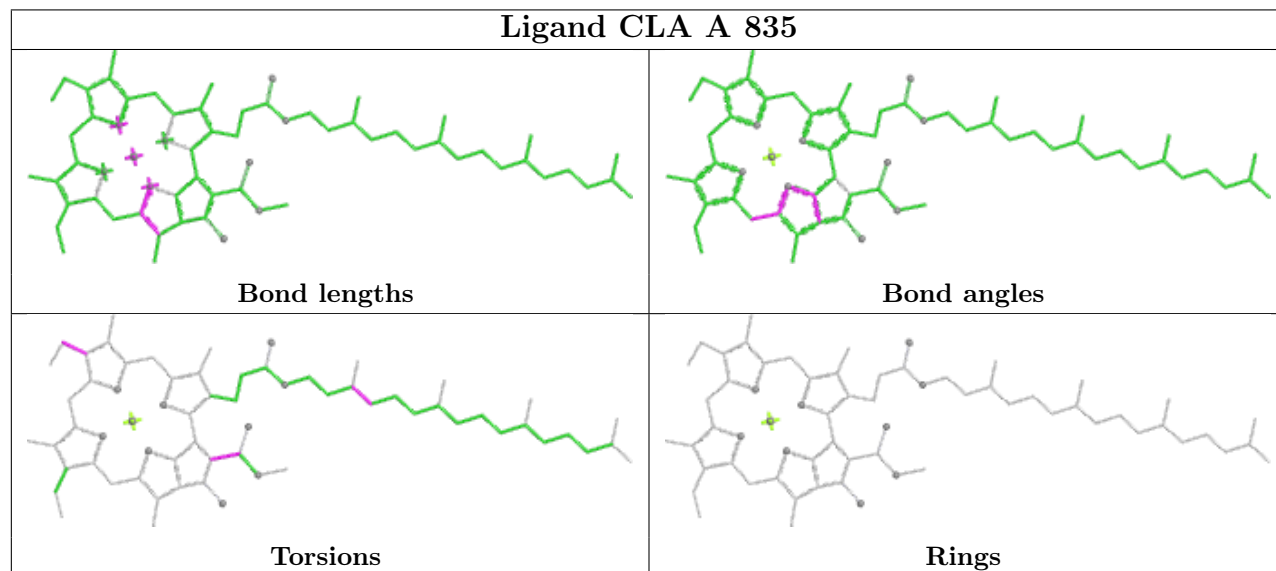
Ligand CHL 92 607

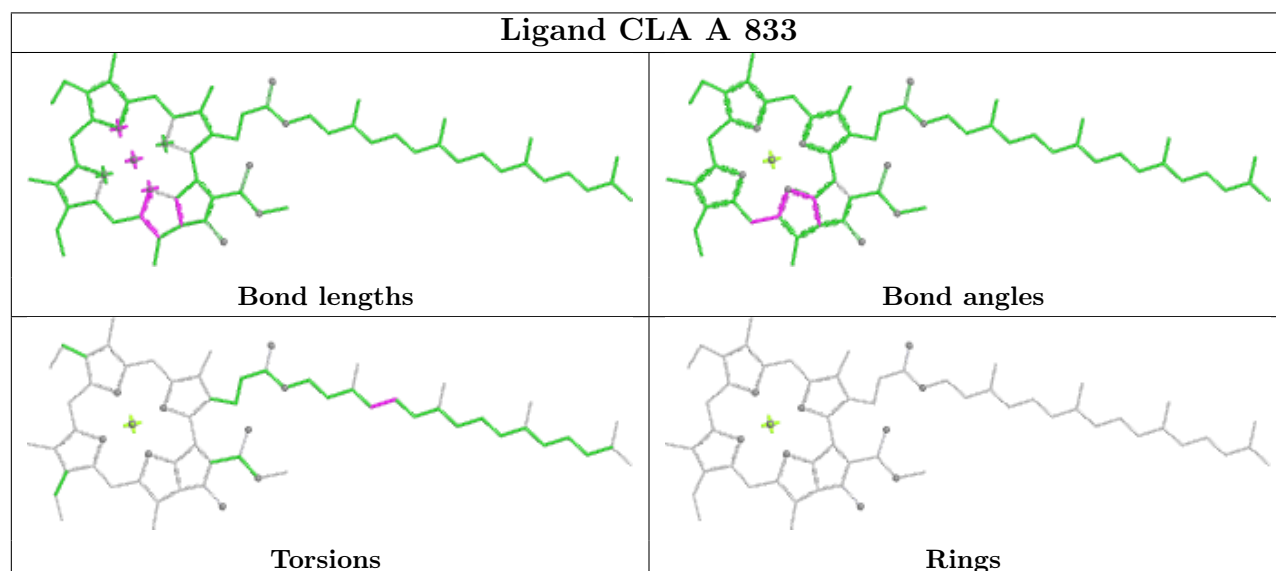
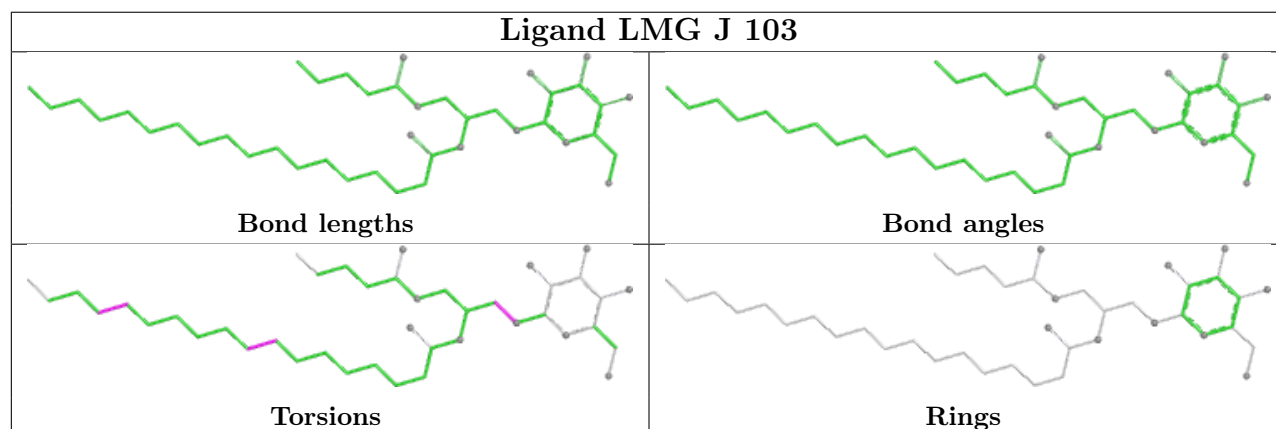
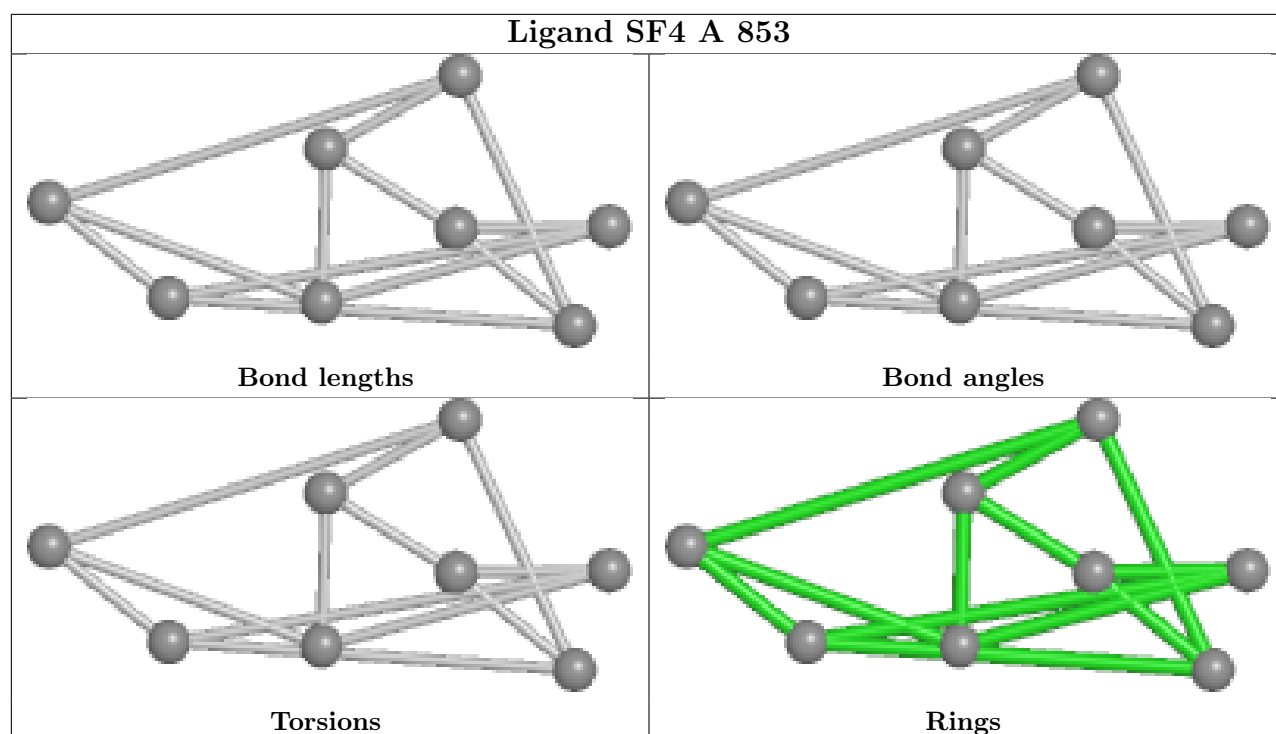


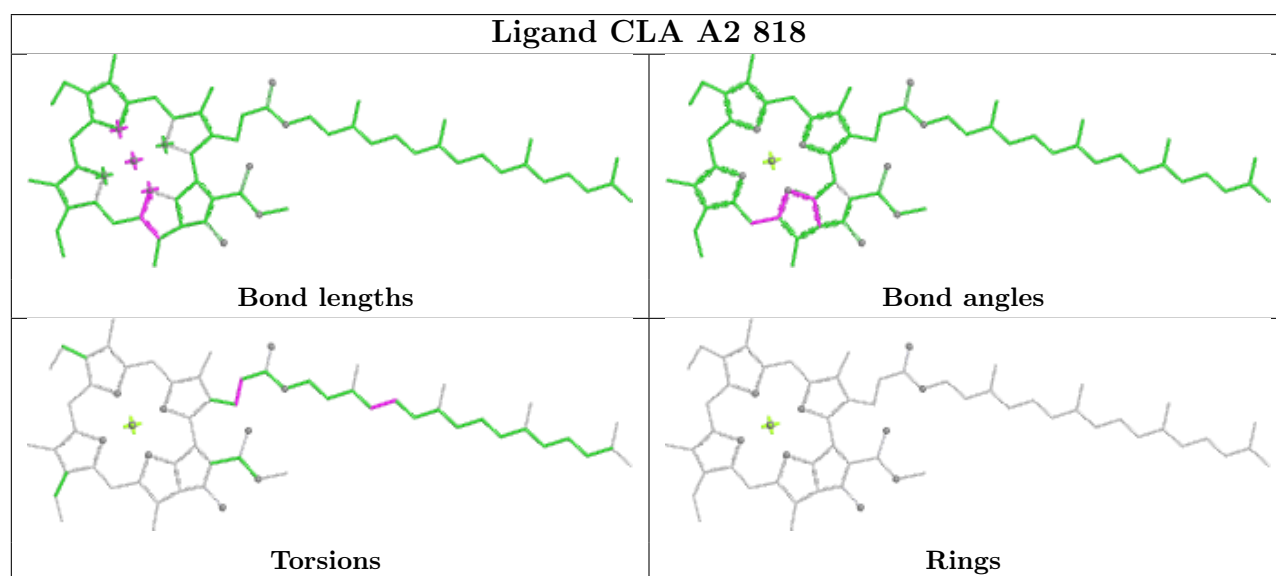
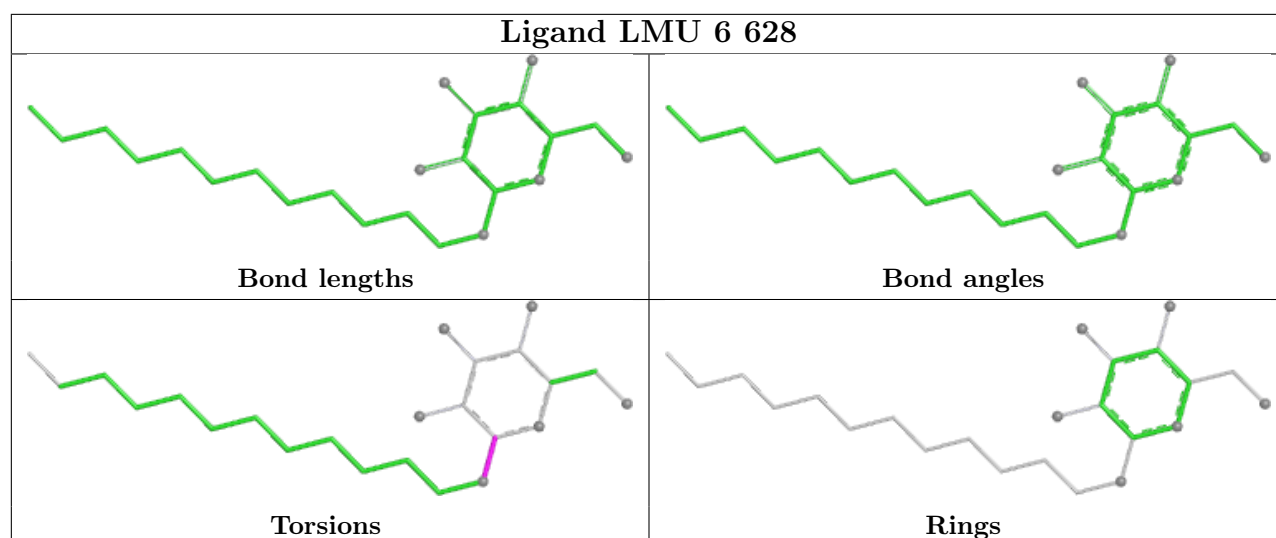
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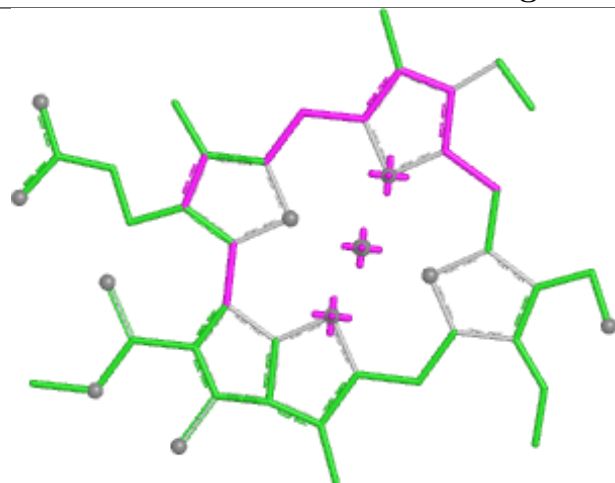
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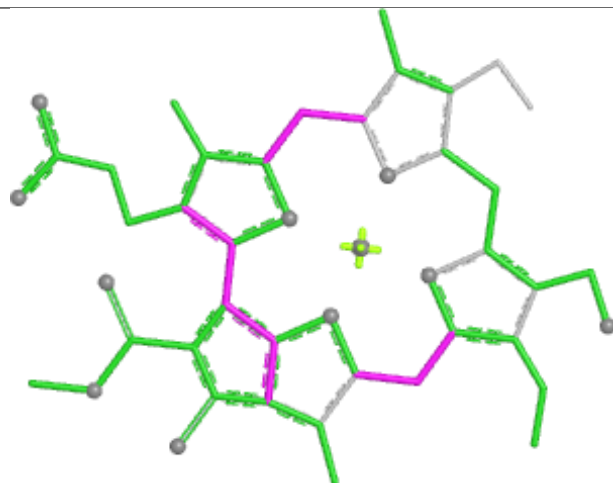




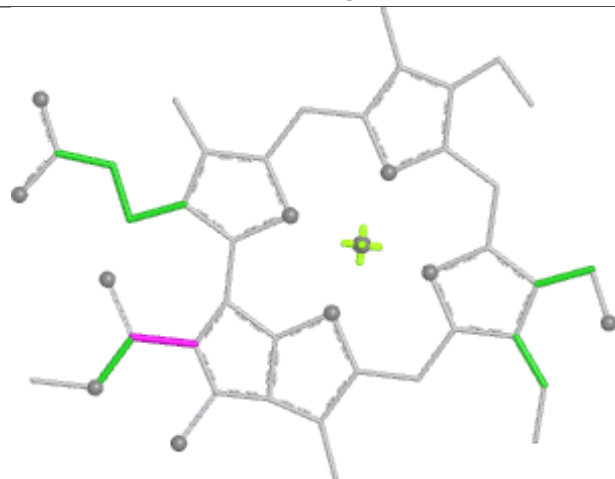
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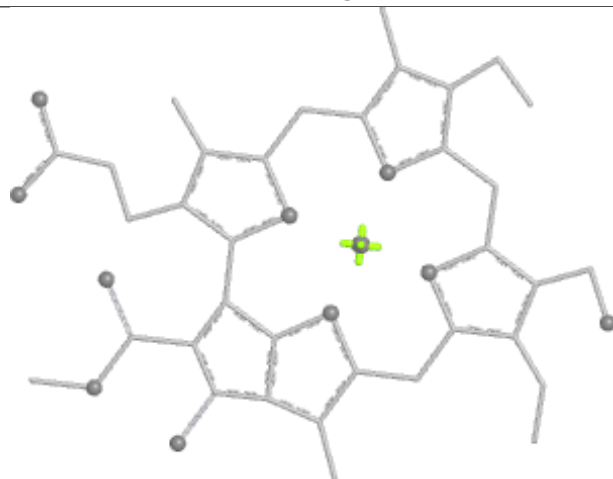
Bond lengths



Bond angles

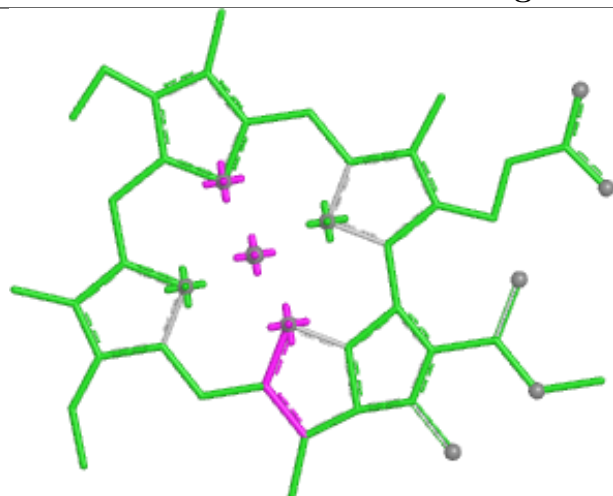


Torsions

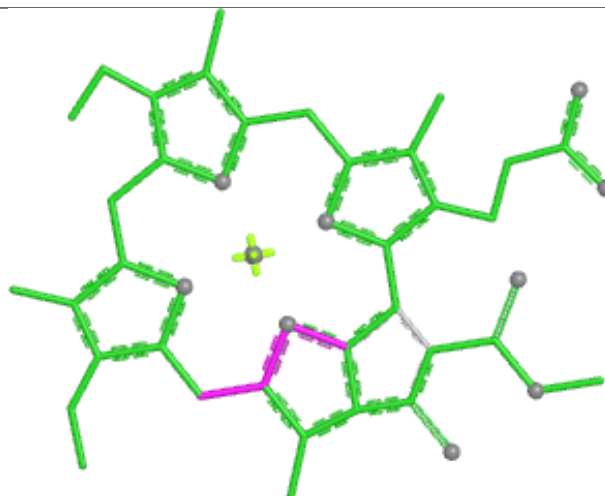


Rings

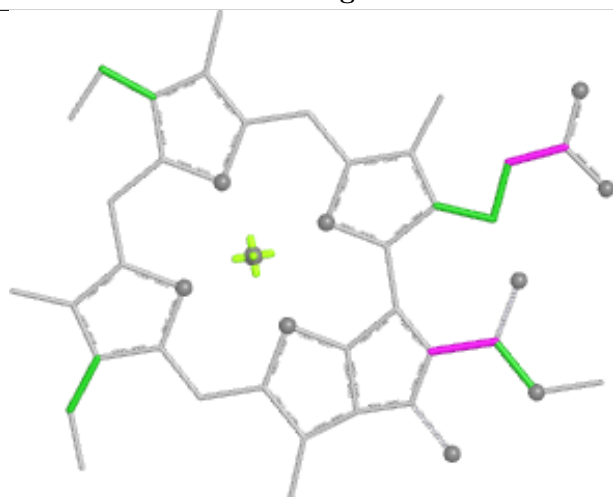
Ligand CLA B 804



Bond lengths



Bond angles

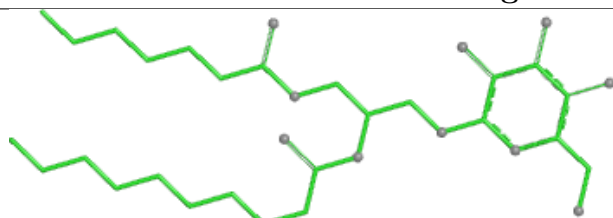


Torsions

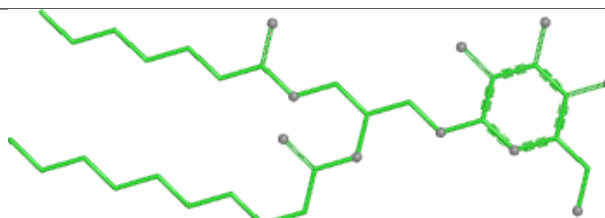


Rings

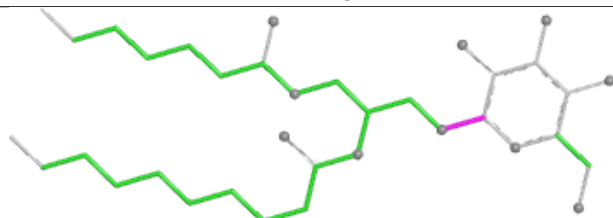
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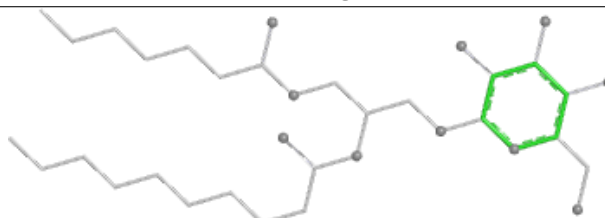
Bond lengths



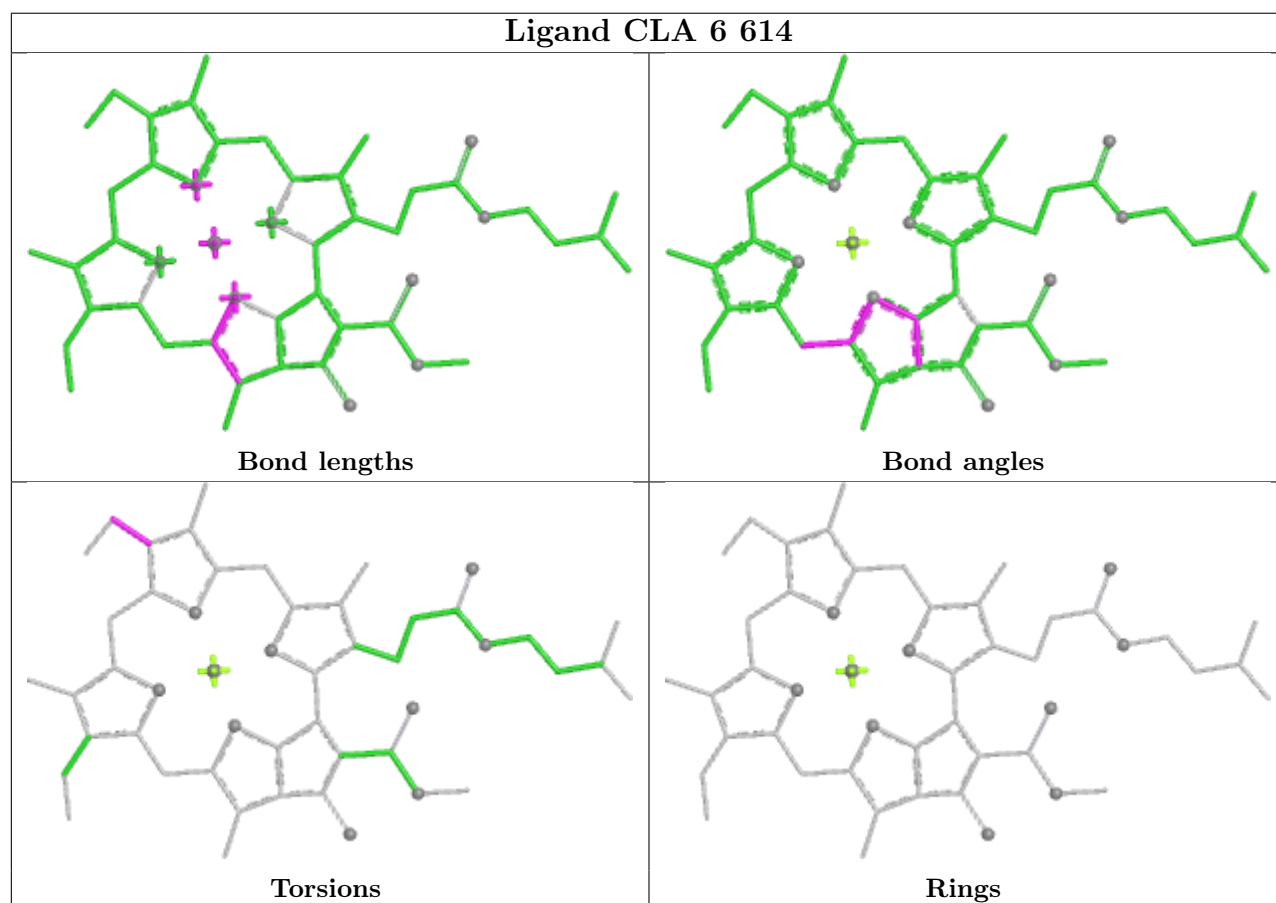
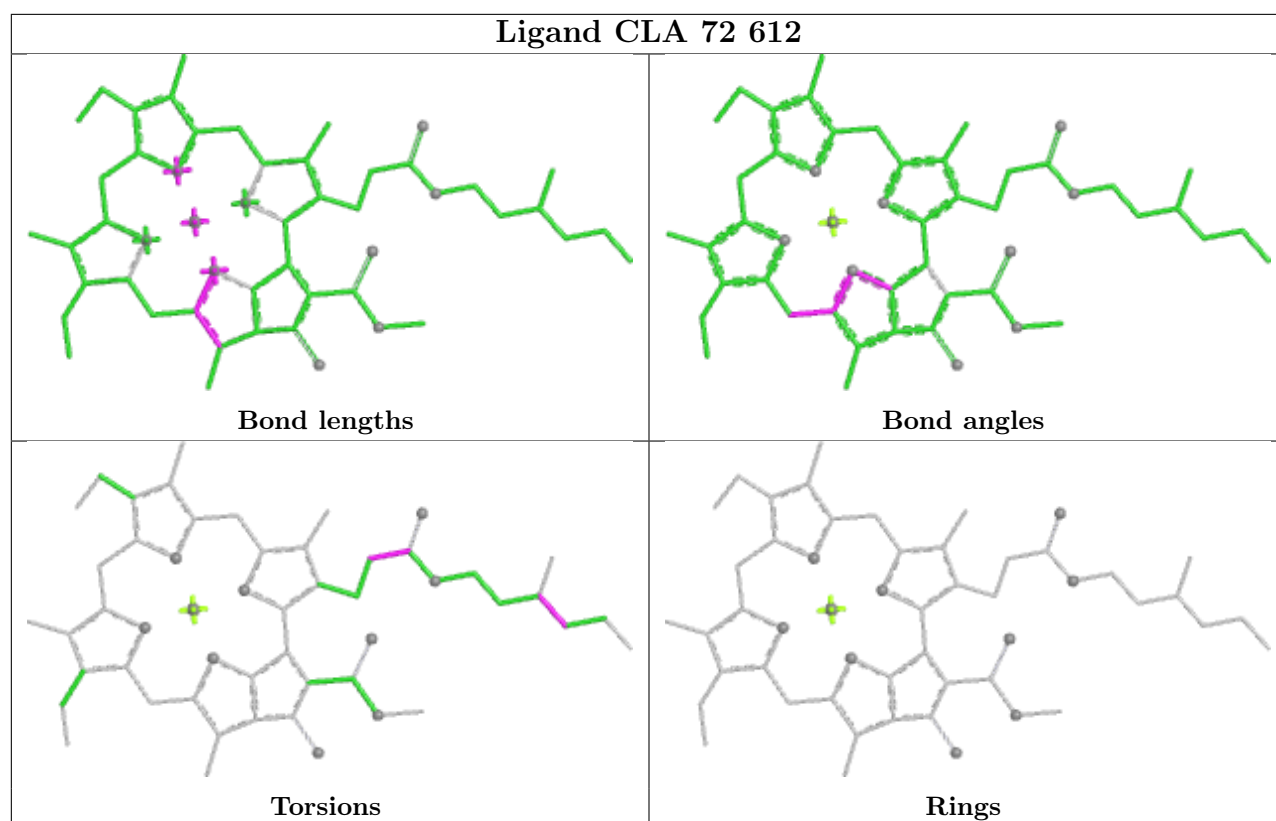
Bond angles

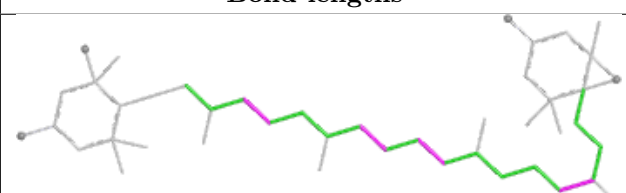
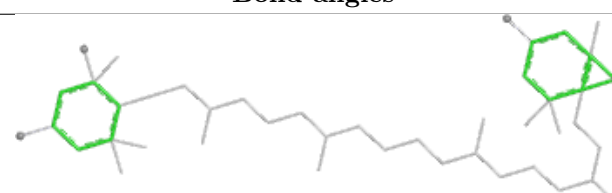


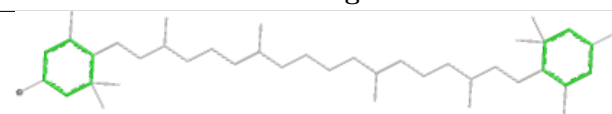
Torsions

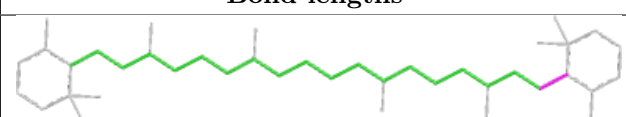
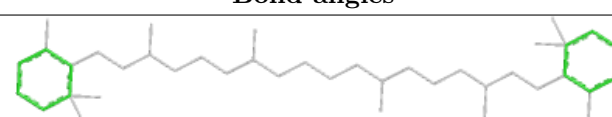


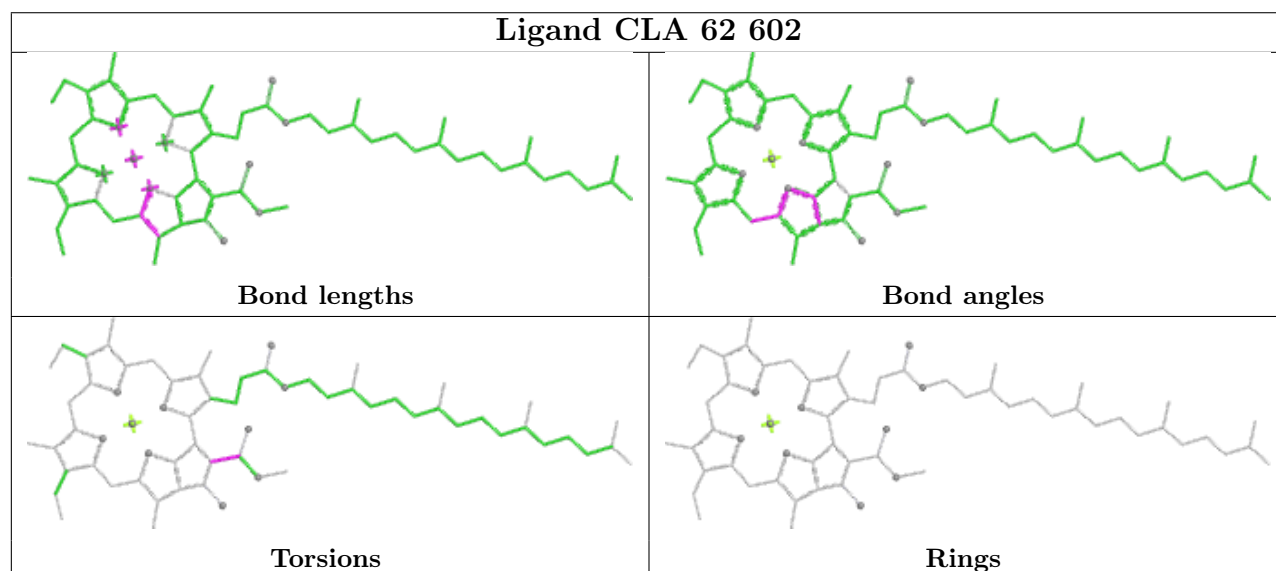
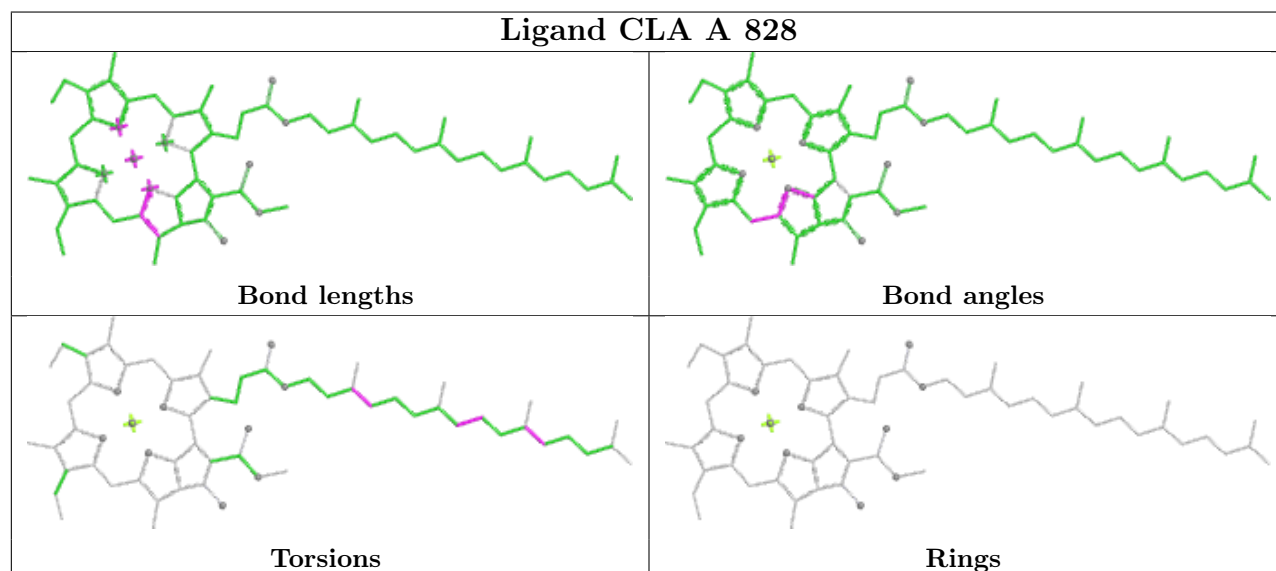
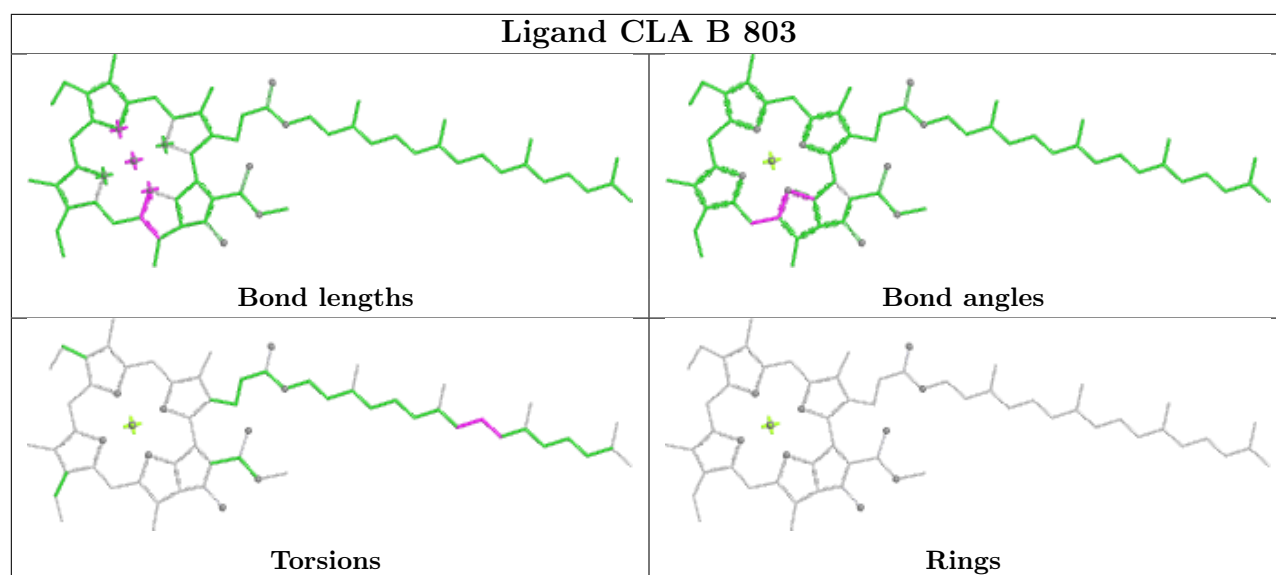
Rings

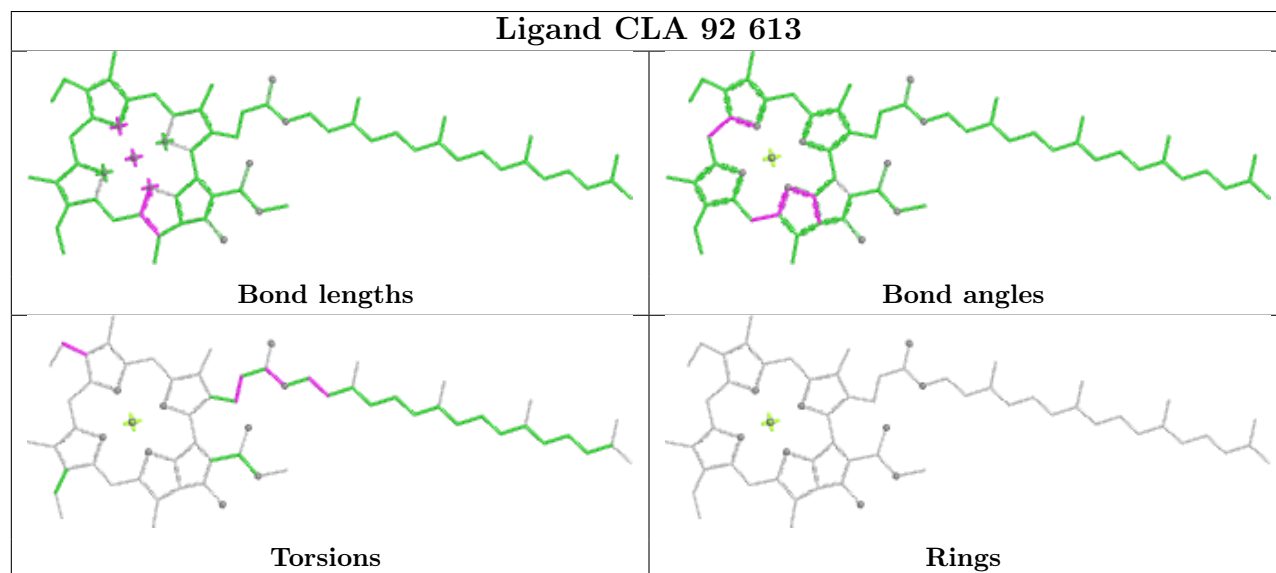
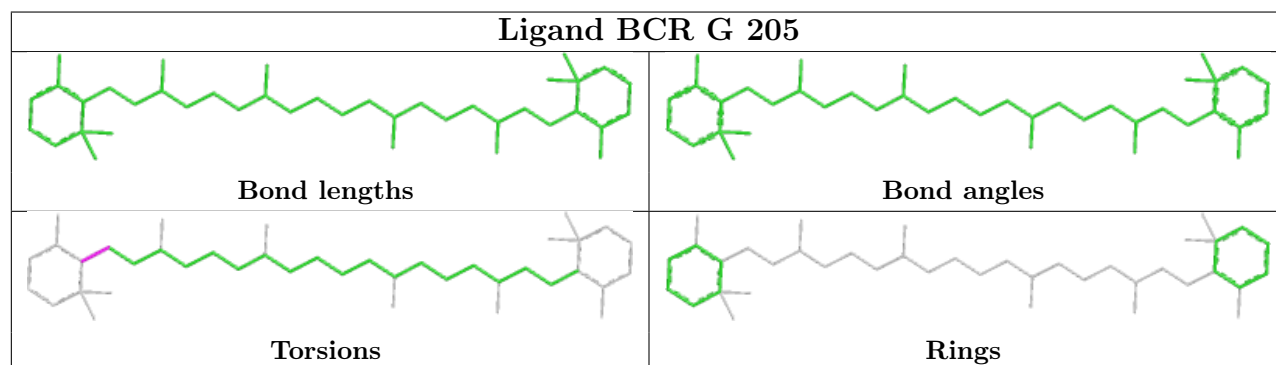
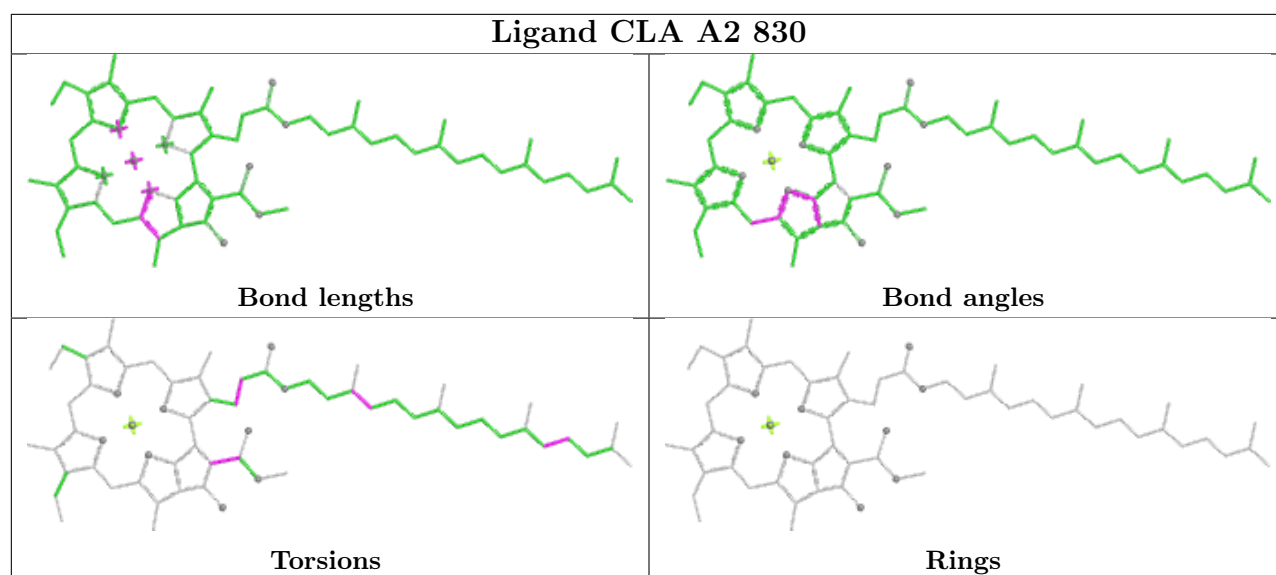


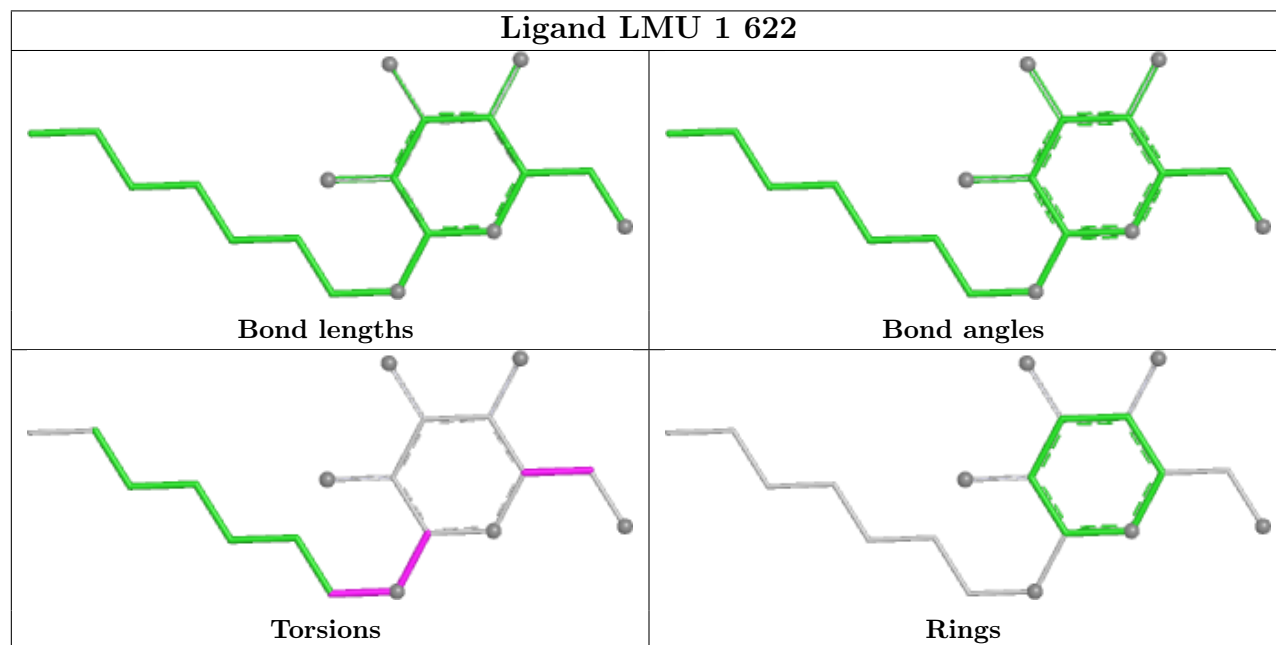
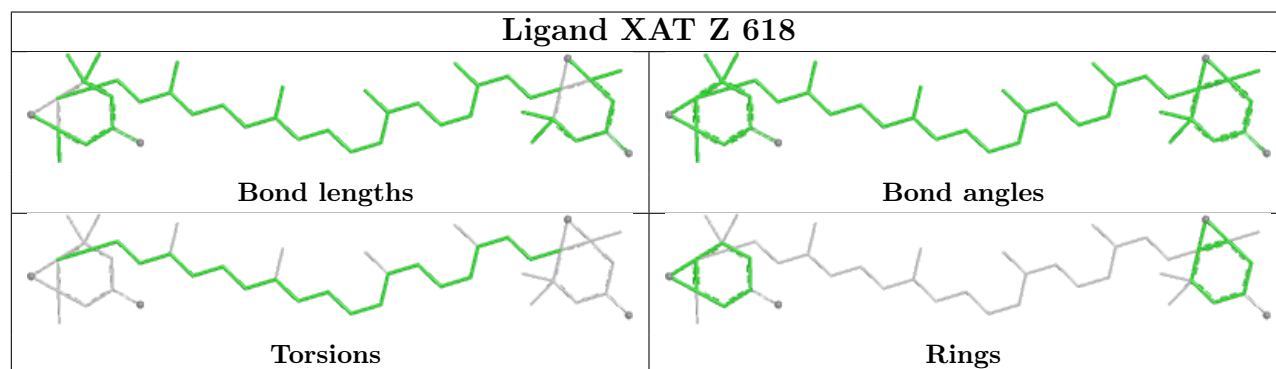
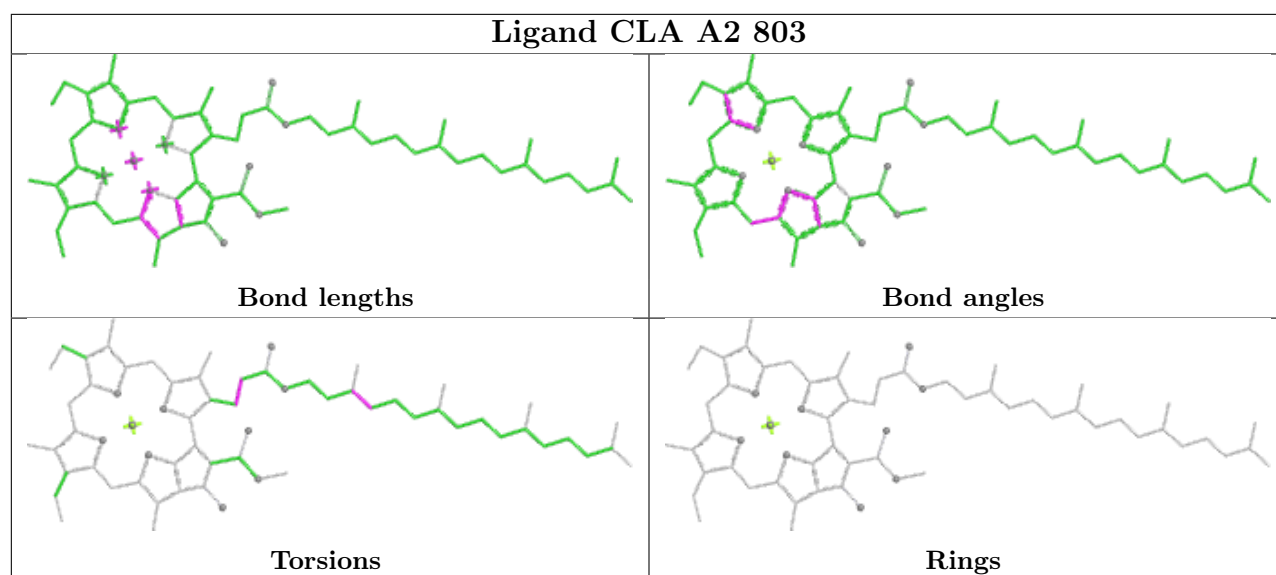
Ligand NEX 6 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

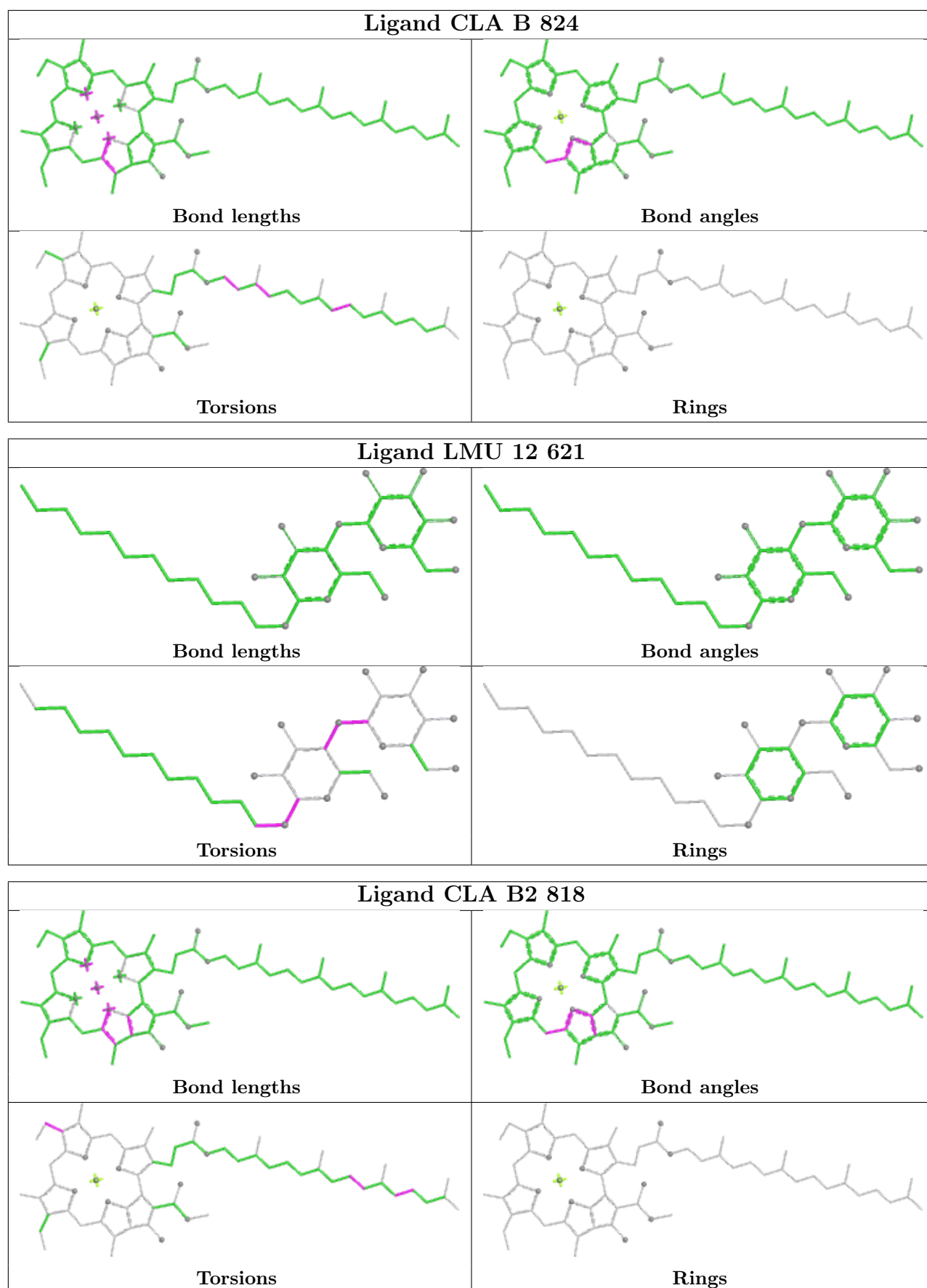
Ligand LUT A 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

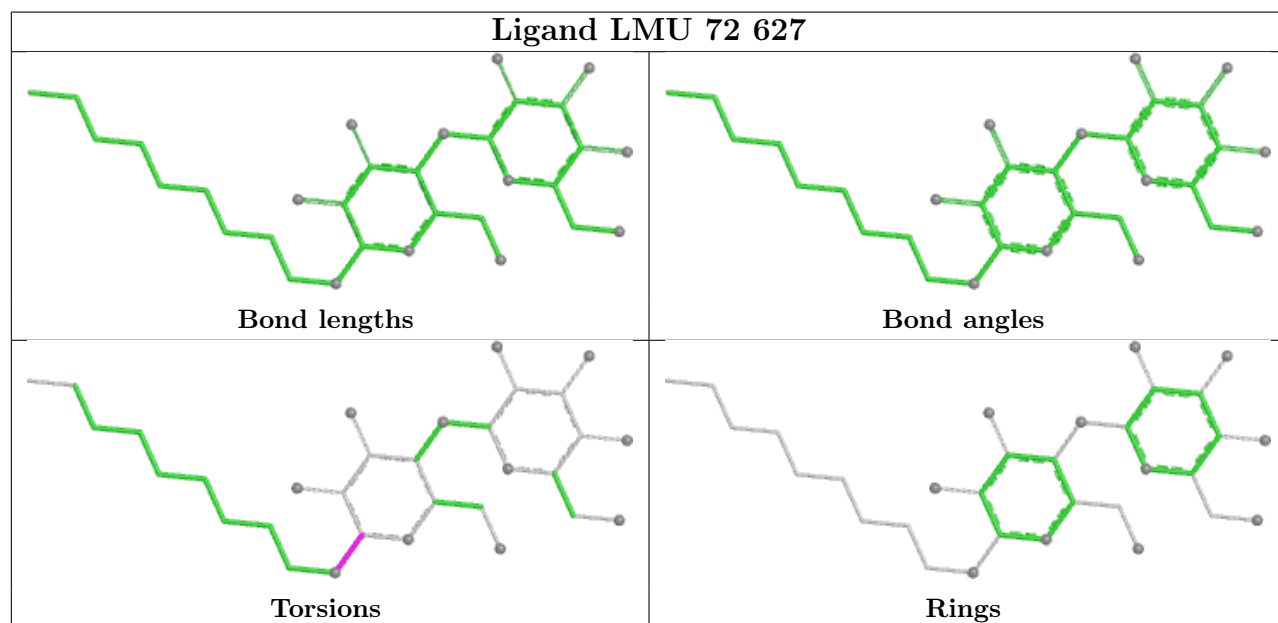
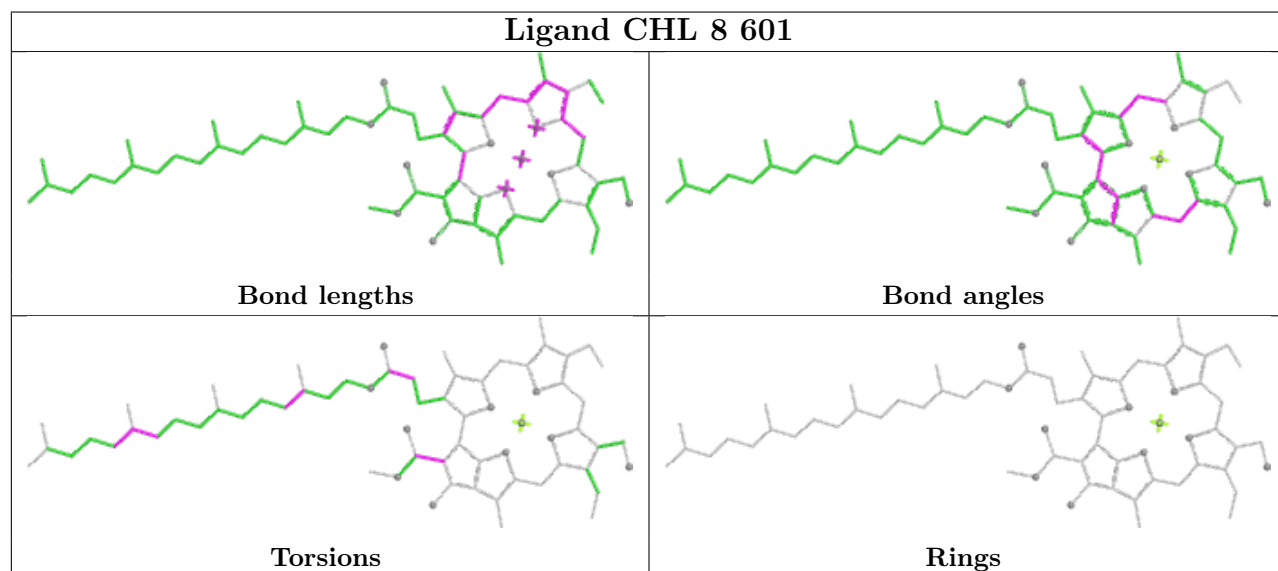
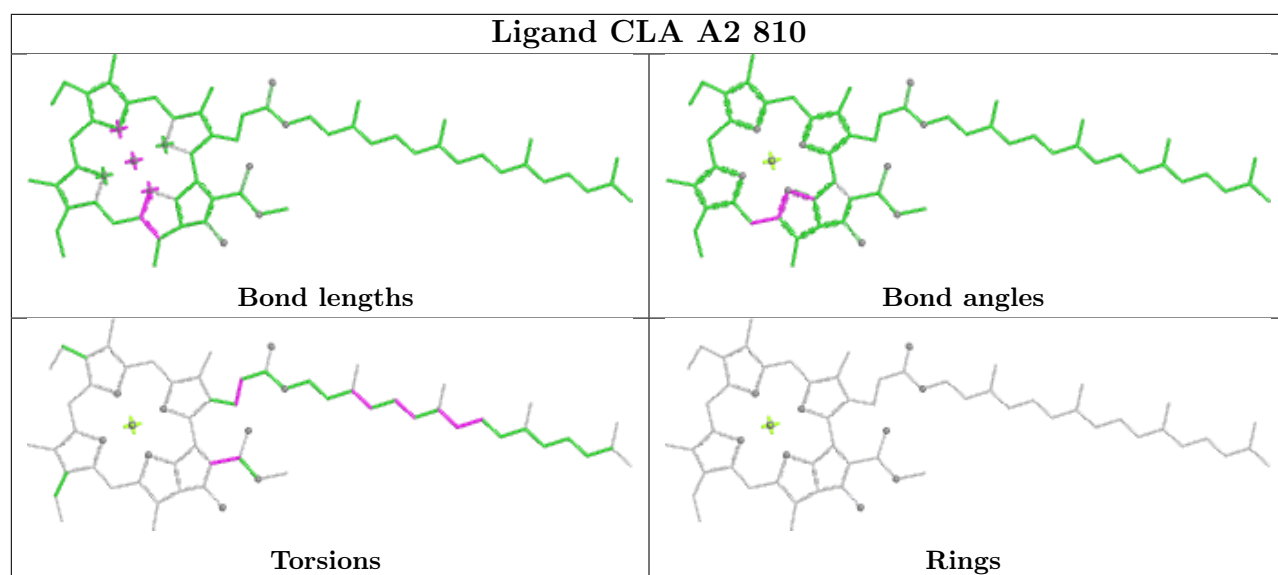
Ligand BCR 32 718	
	
Bond lengths	Bond angles
	
Torsions	Rings

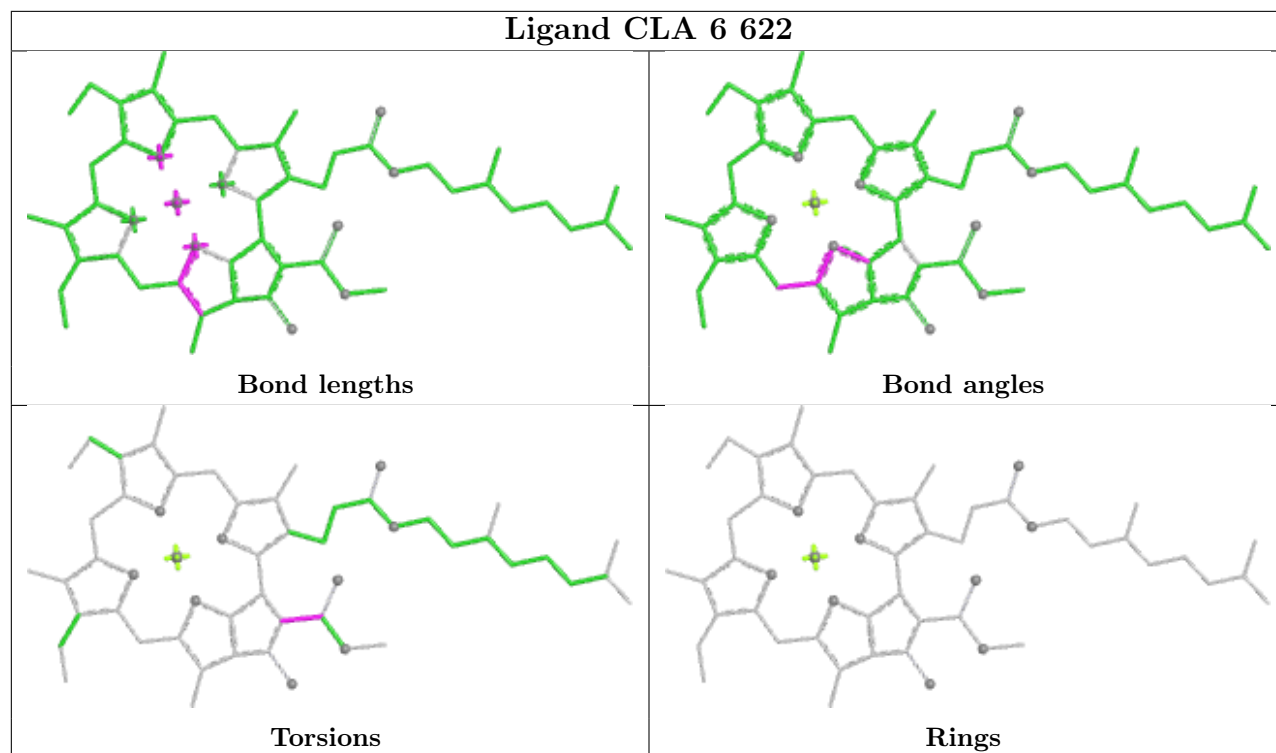
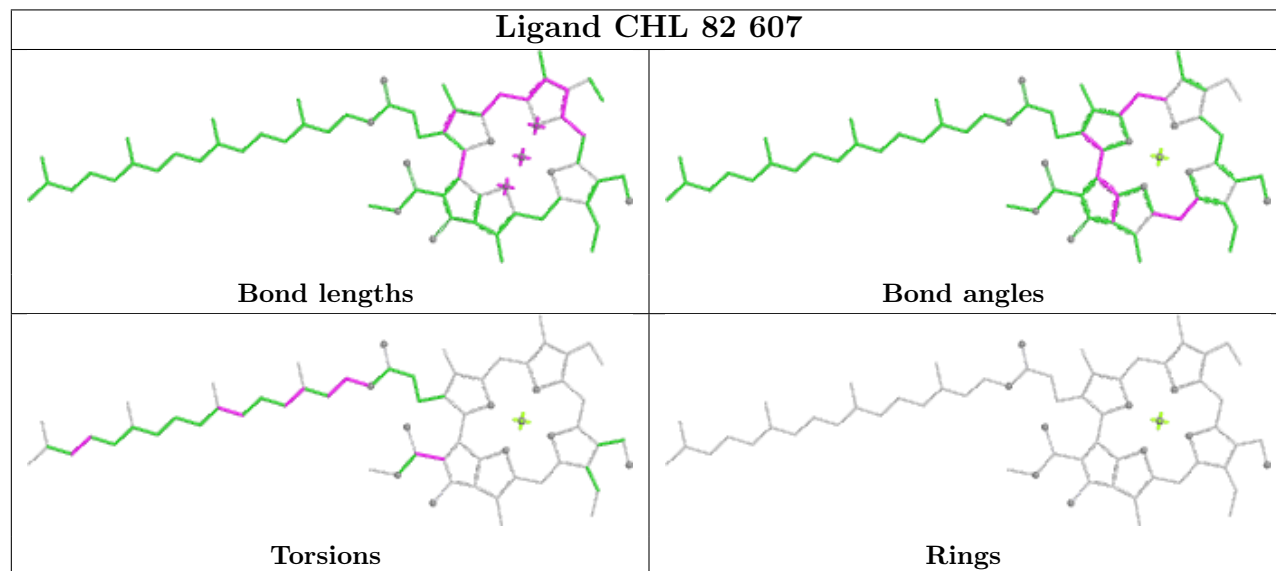


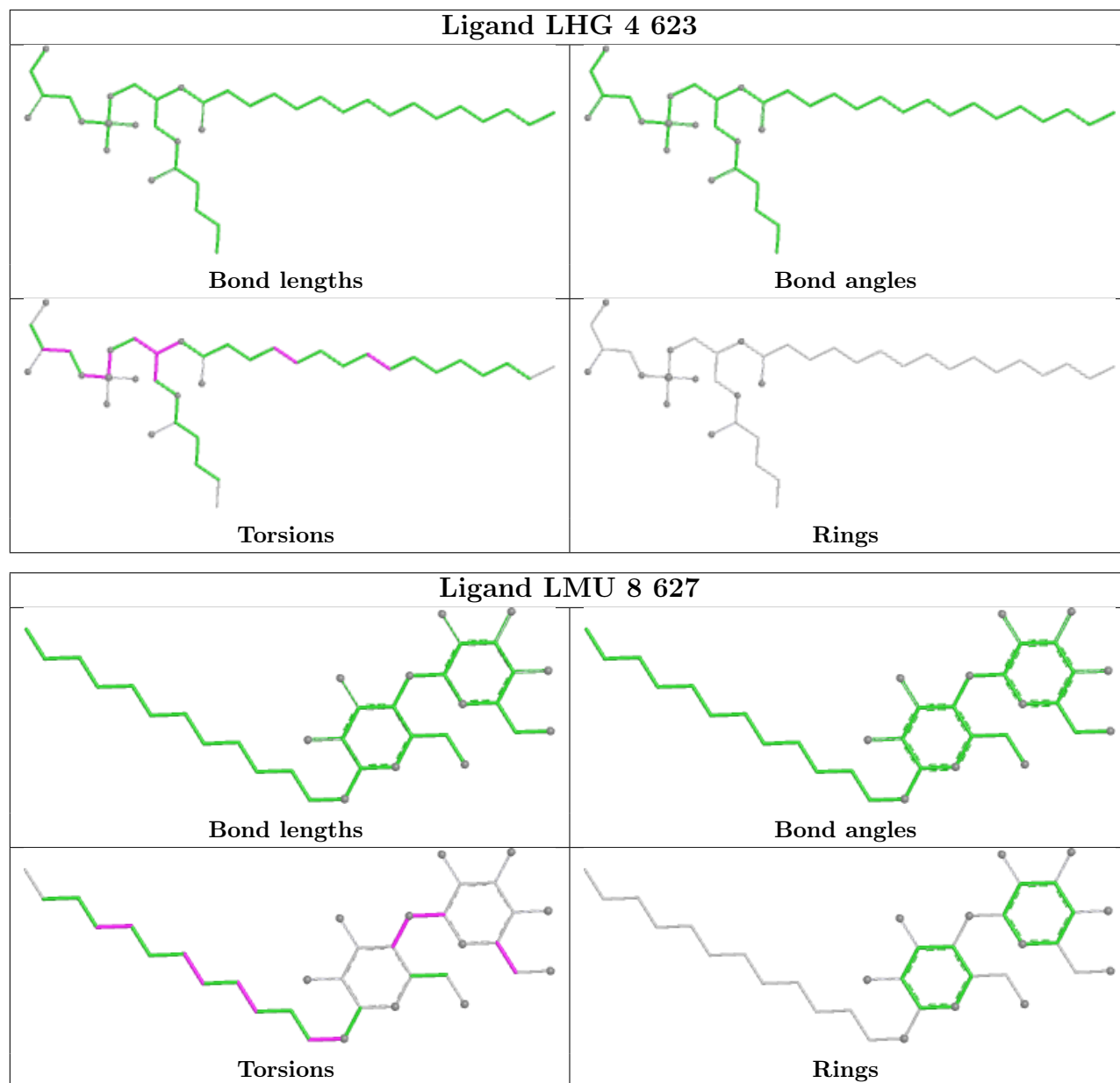


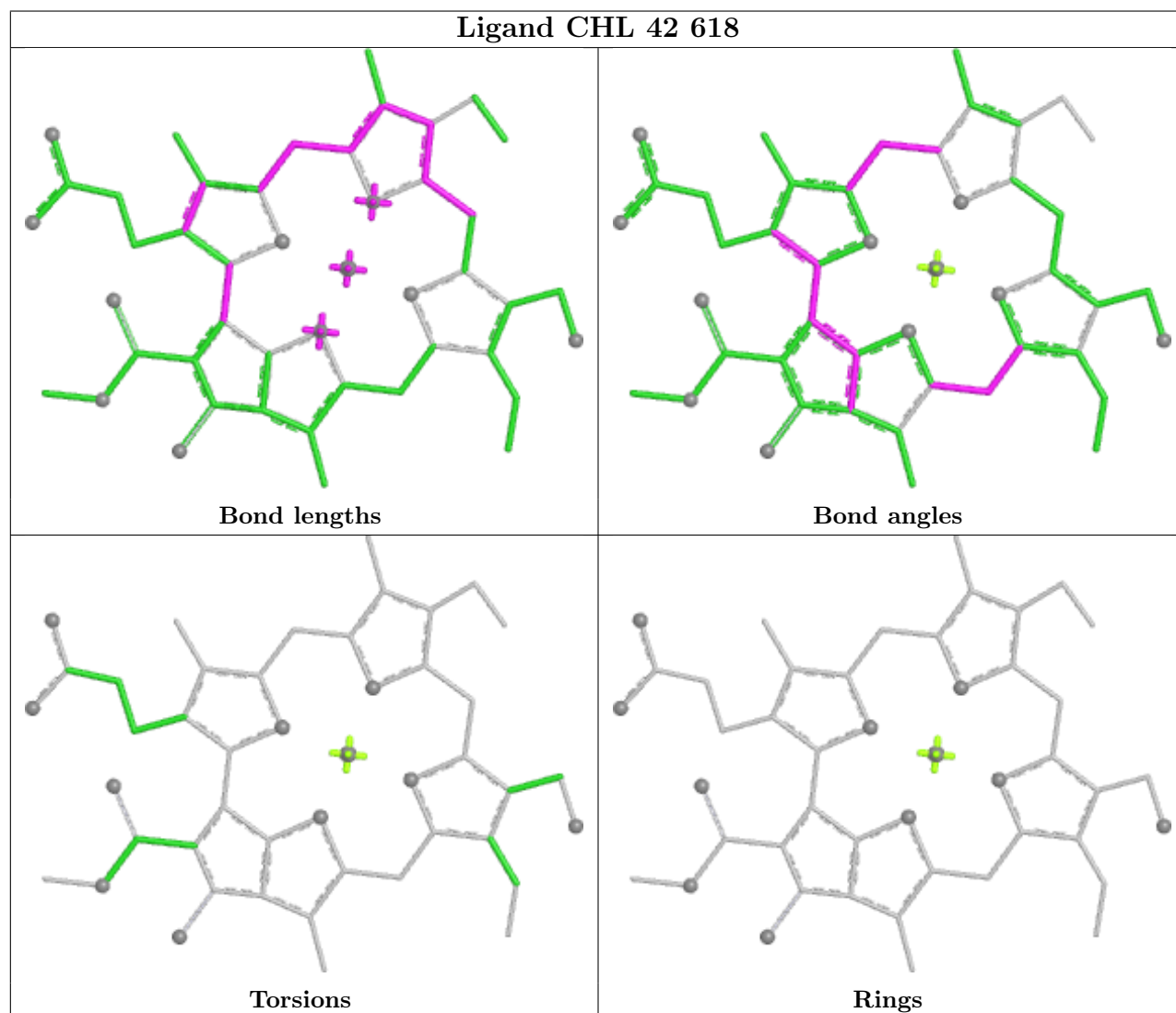
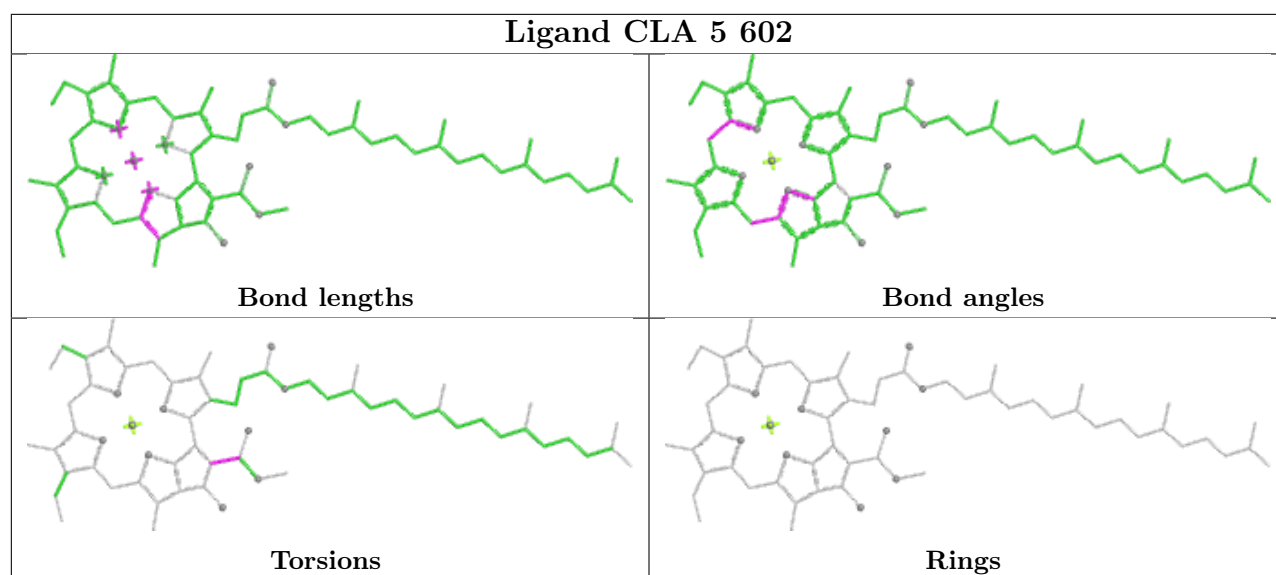


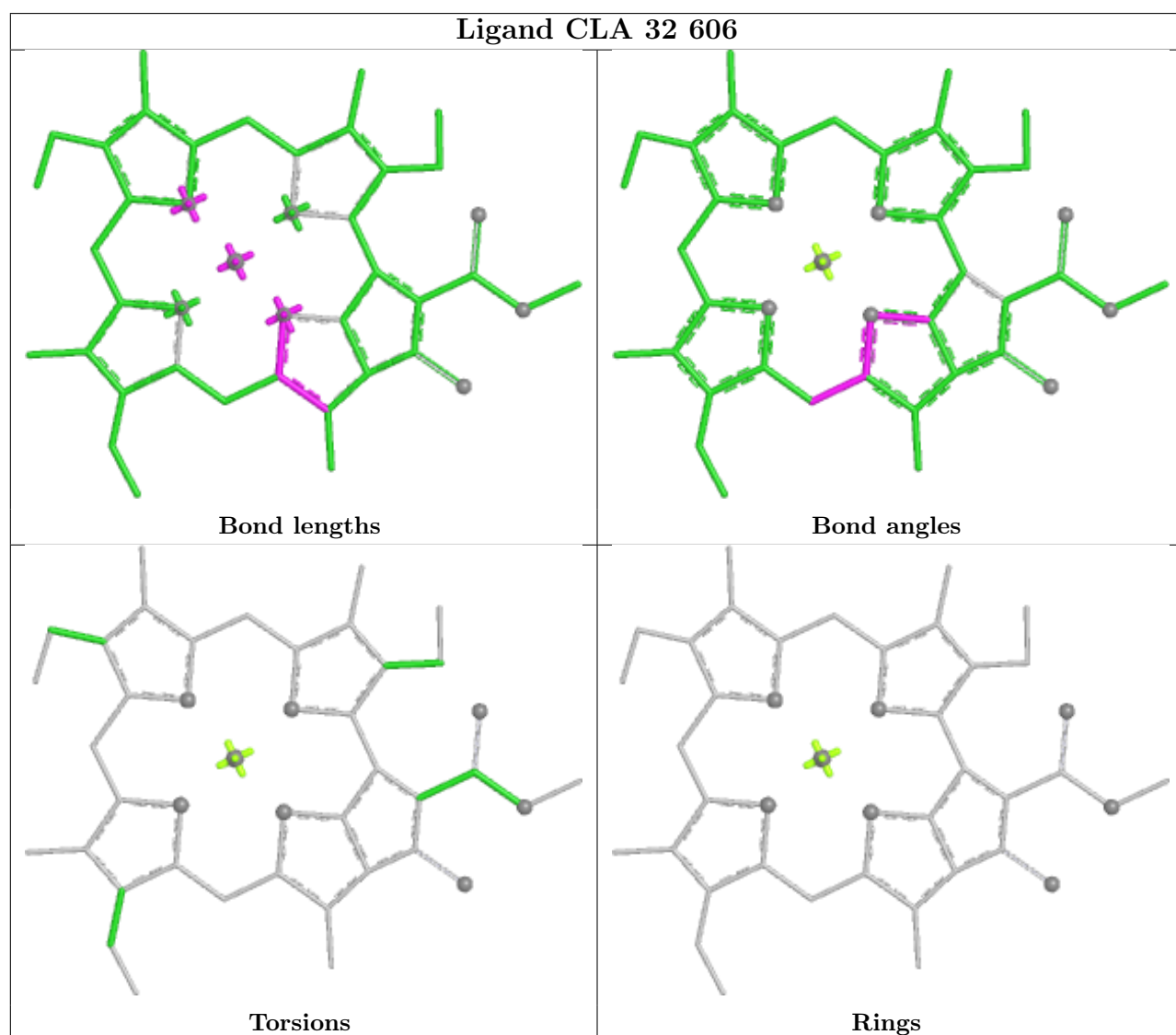
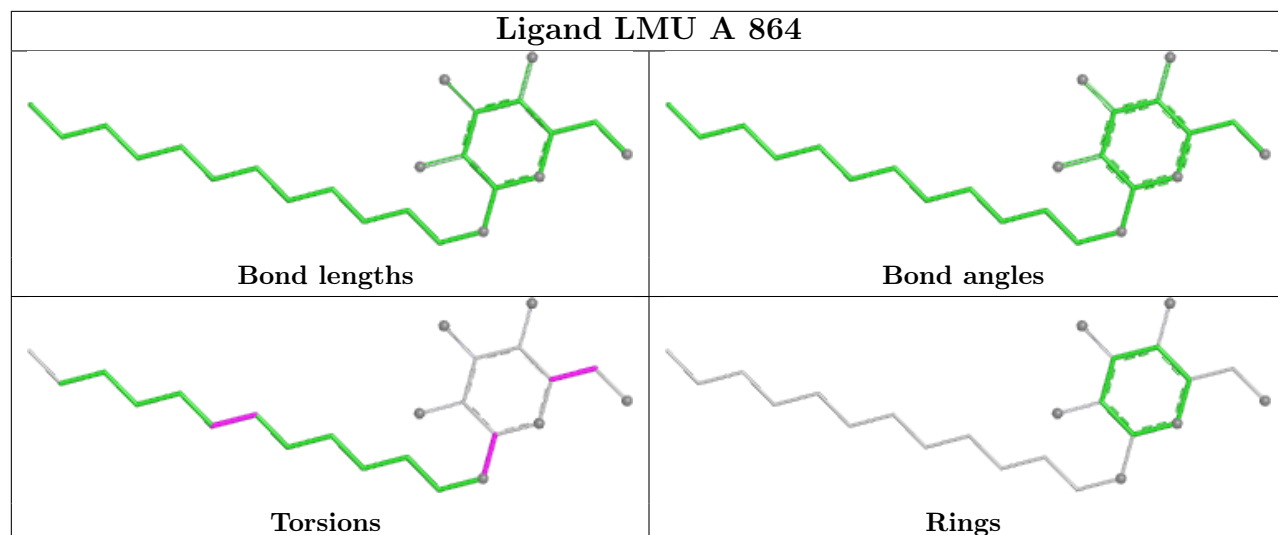


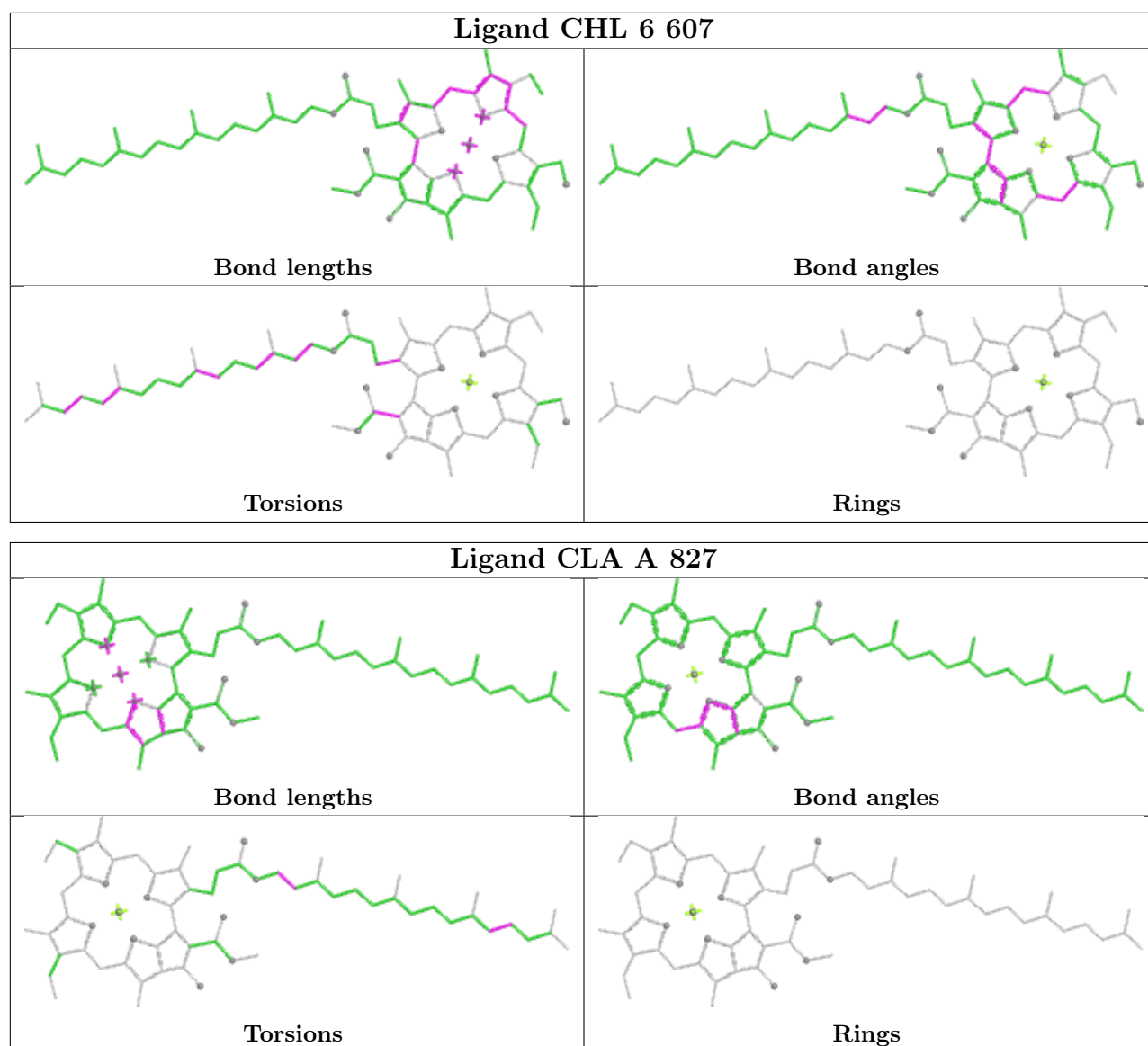


Ligand CLA 6 622**Ligand CHL 82 607**

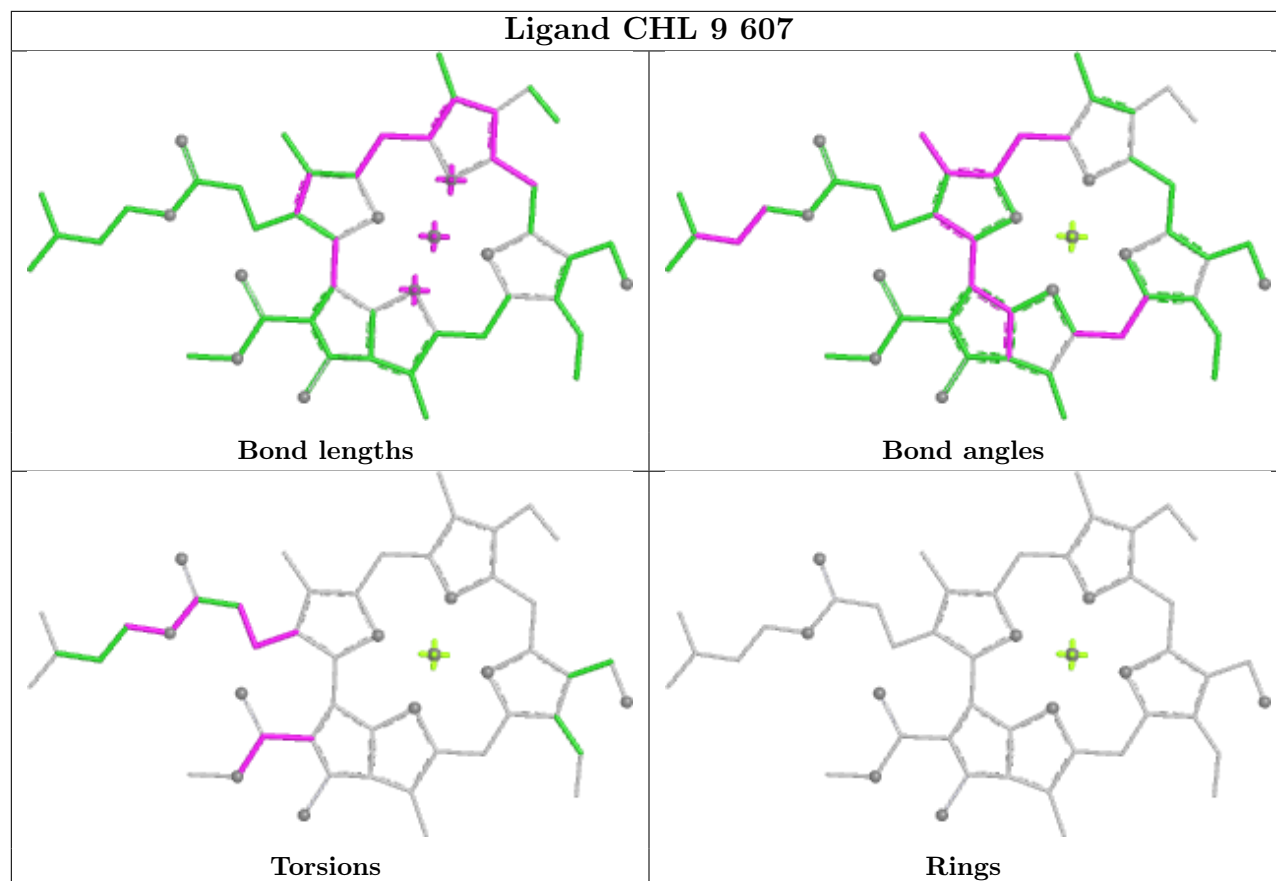




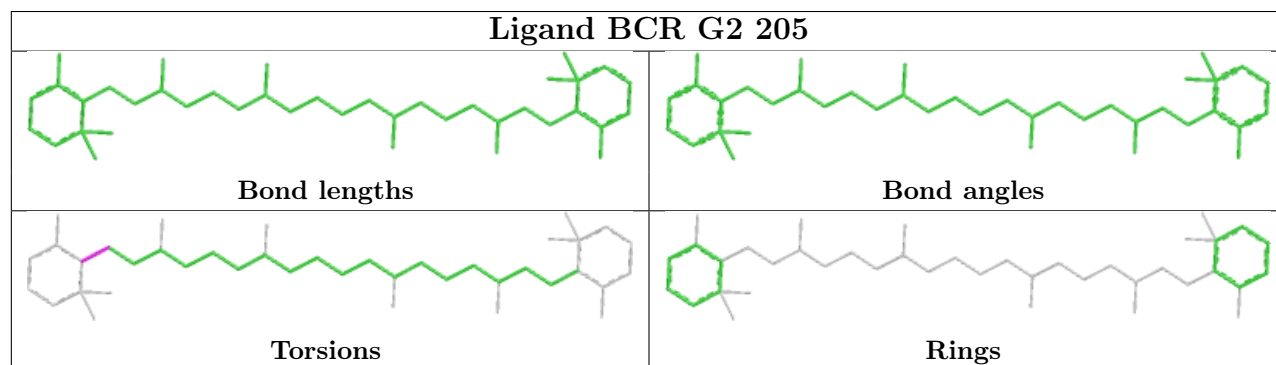




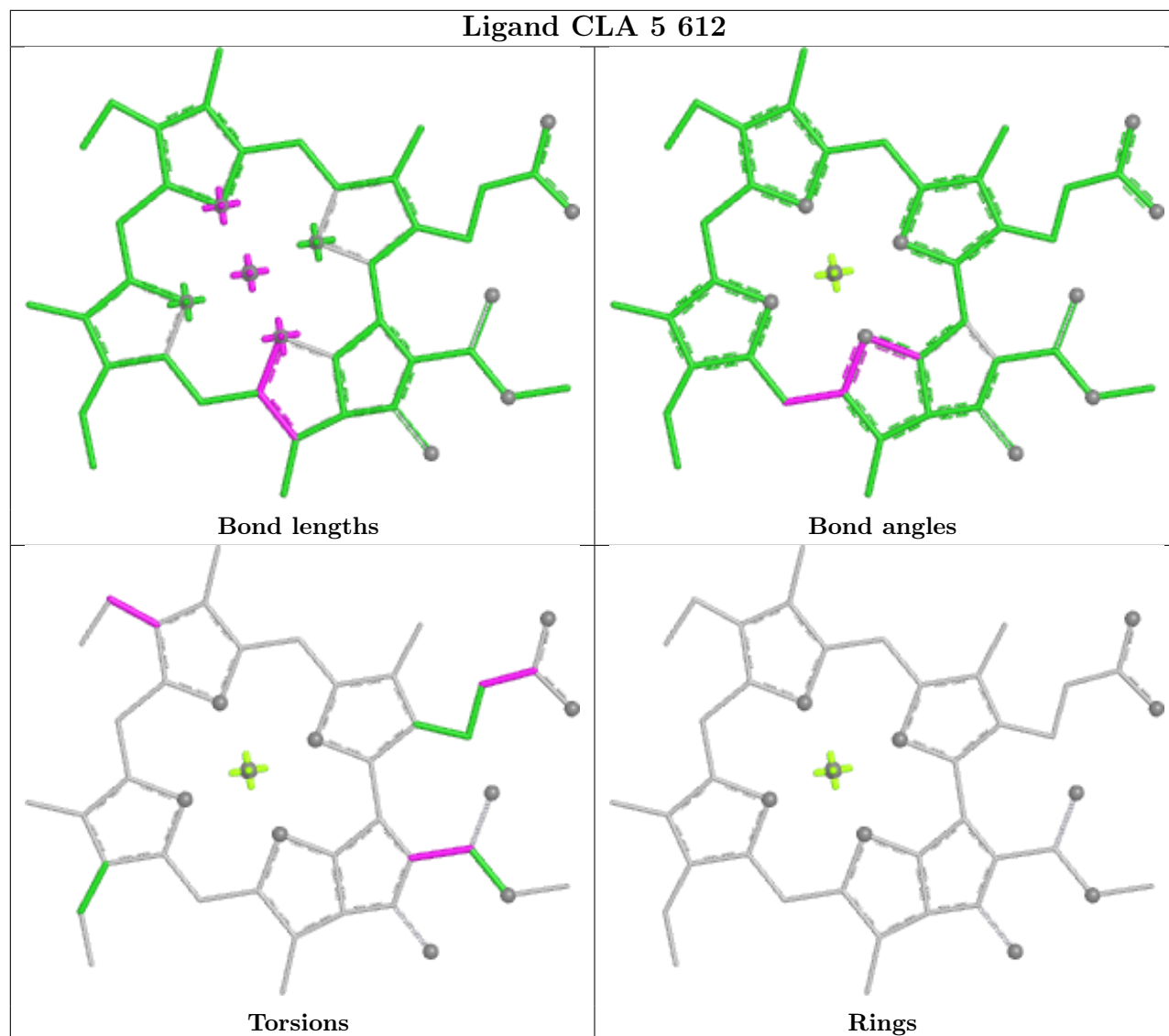
Ligand CHL 9 607



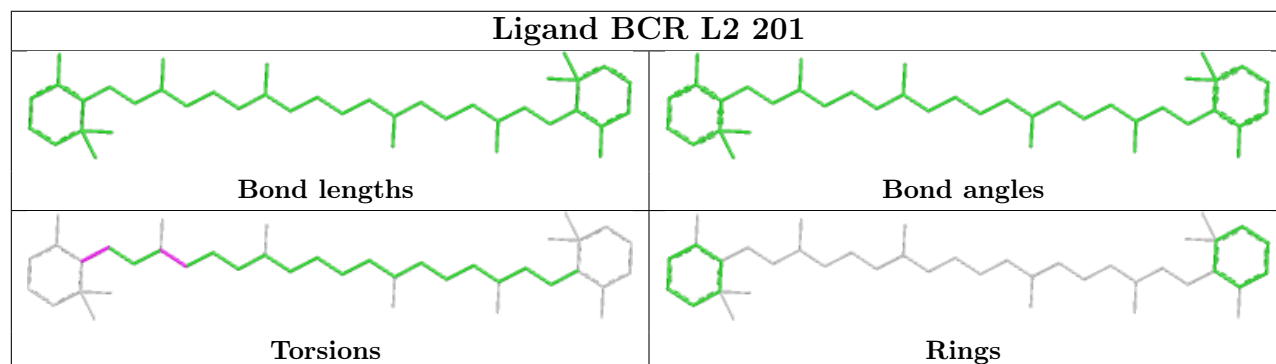
Ligand BCR G2 205

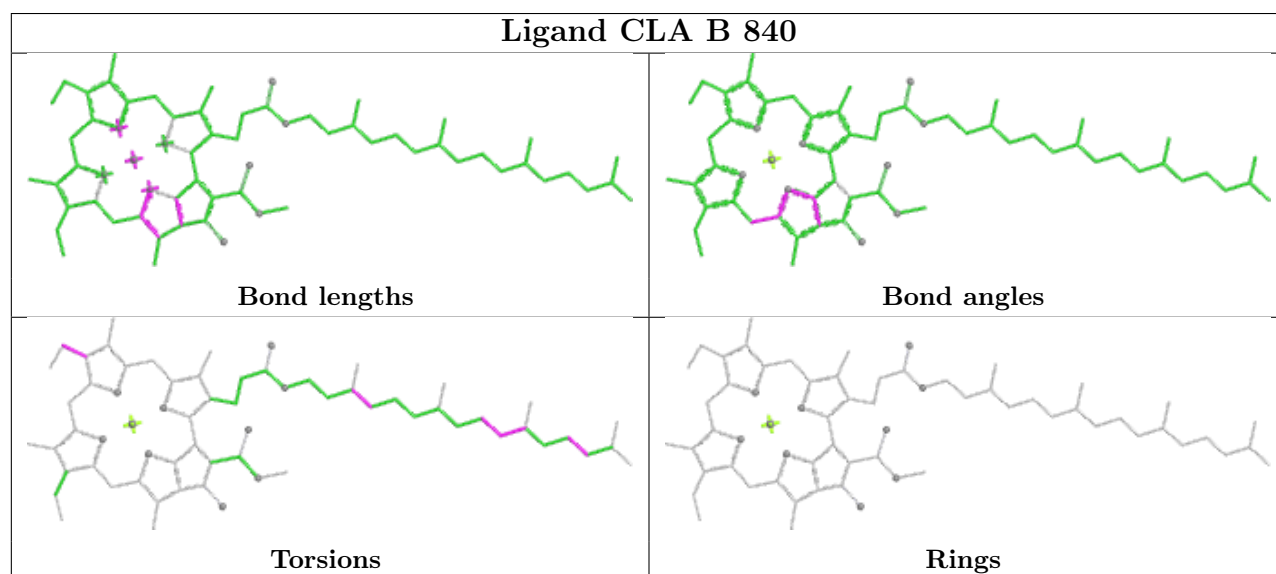
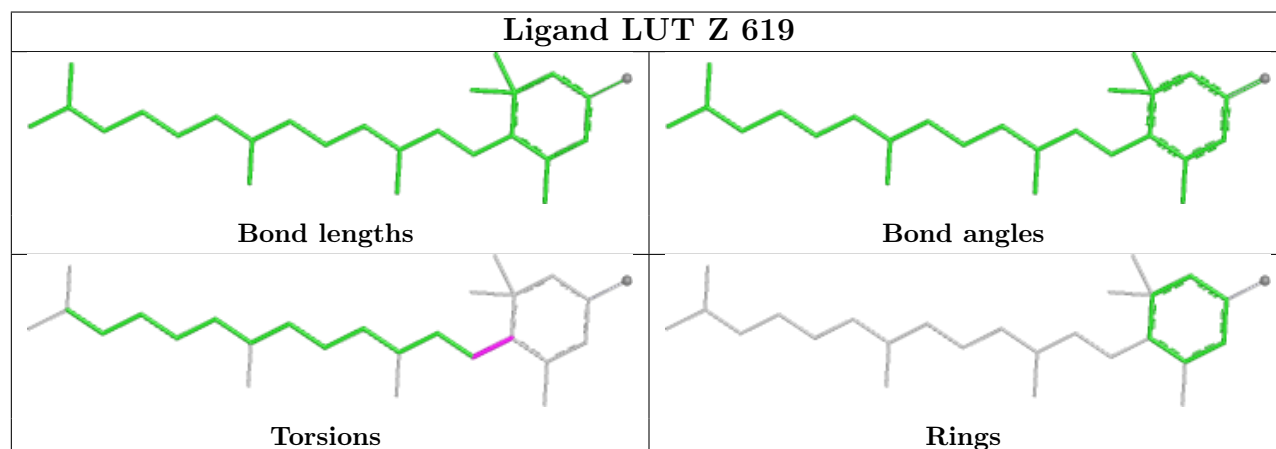
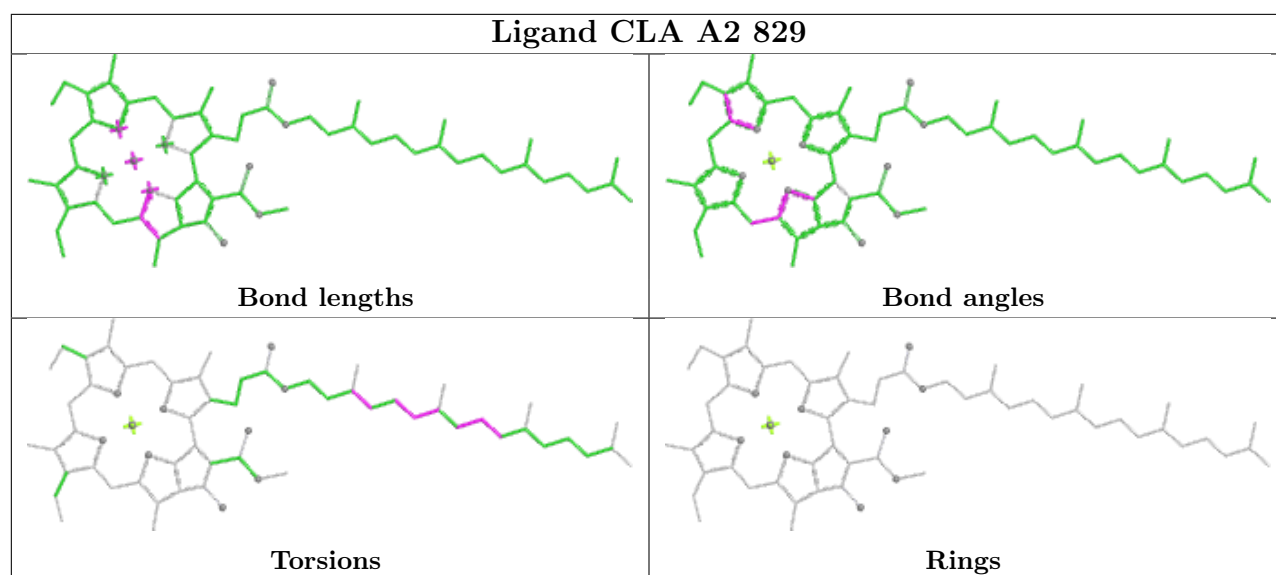


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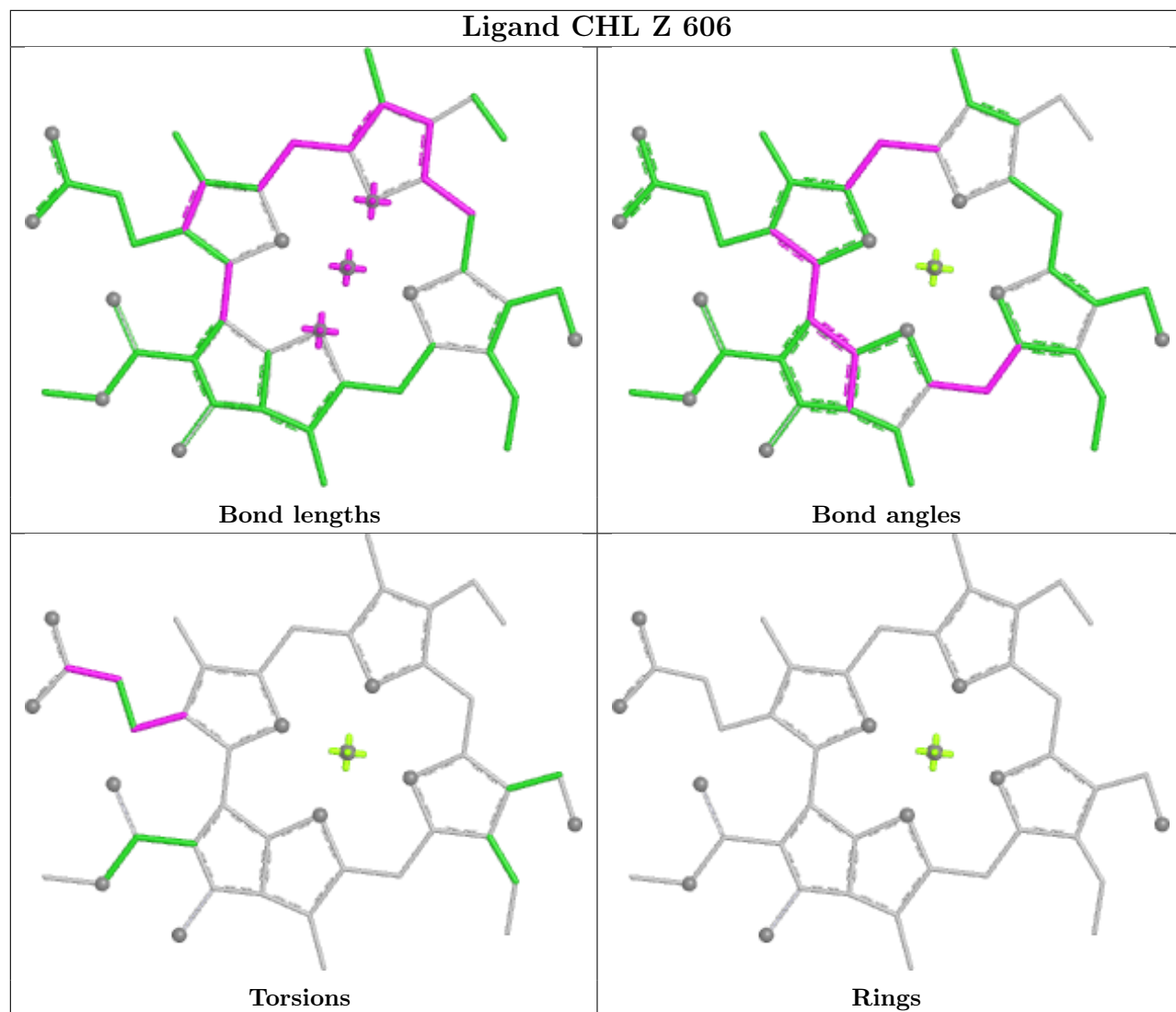


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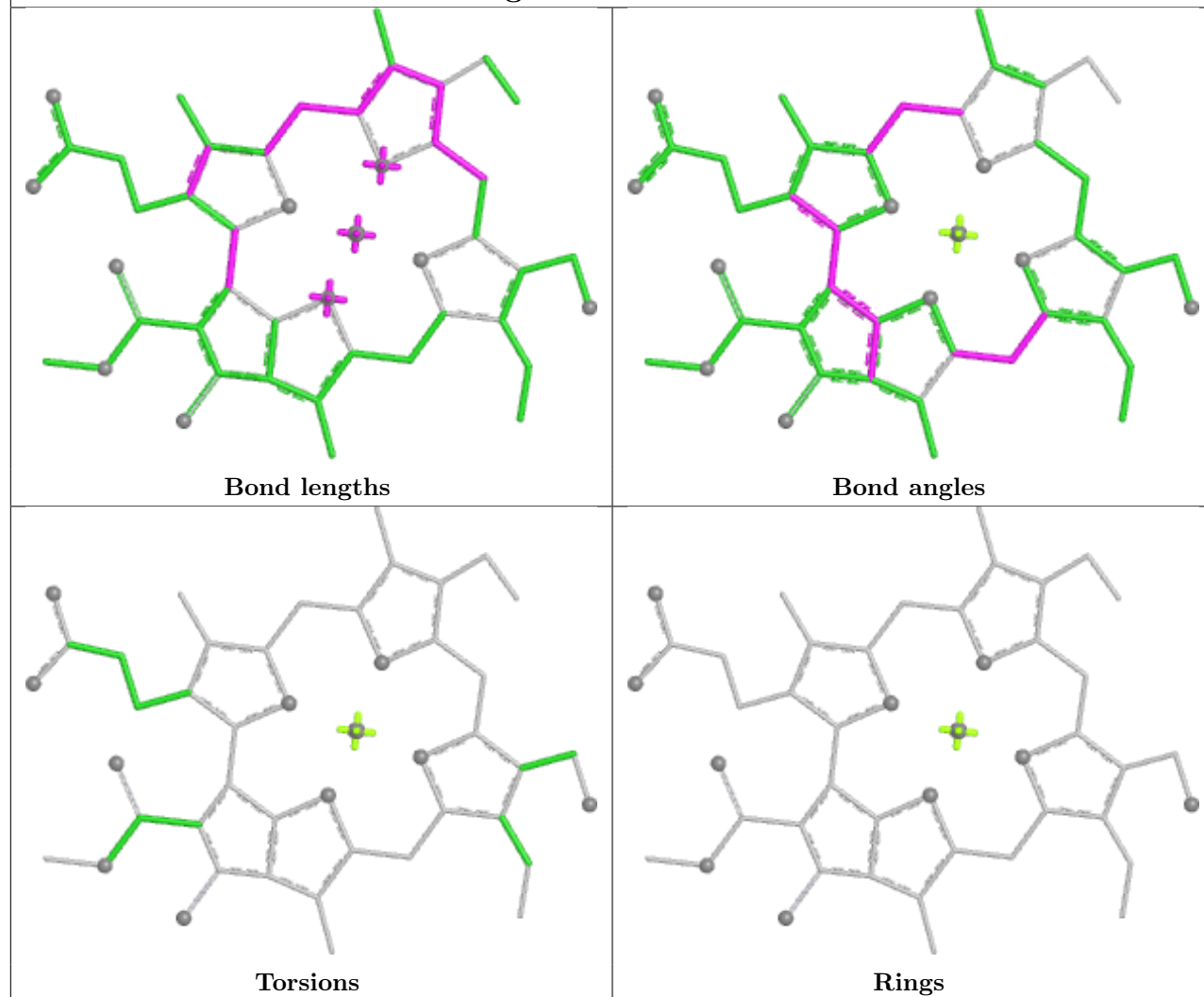




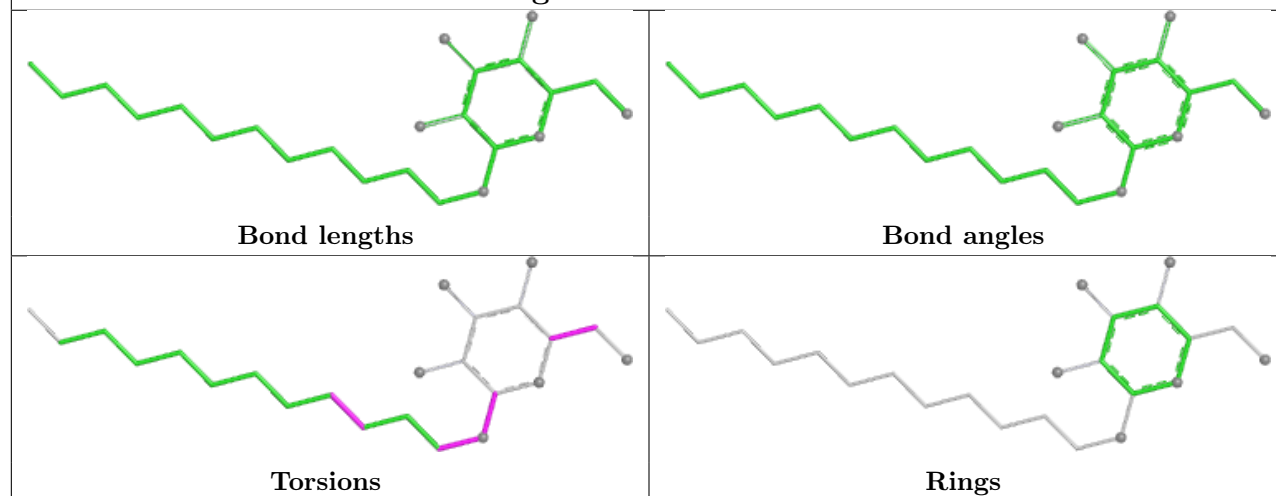
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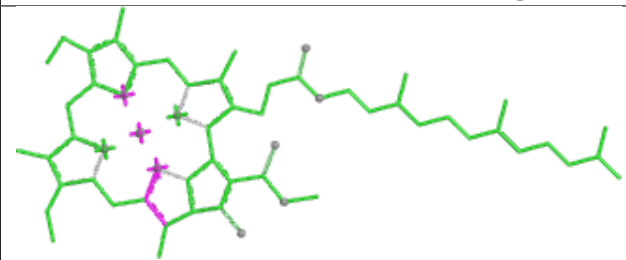
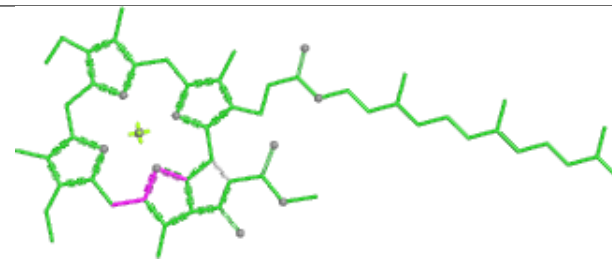
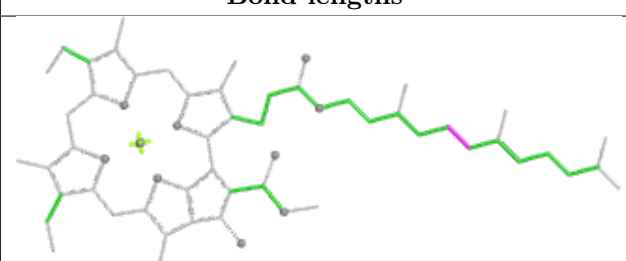
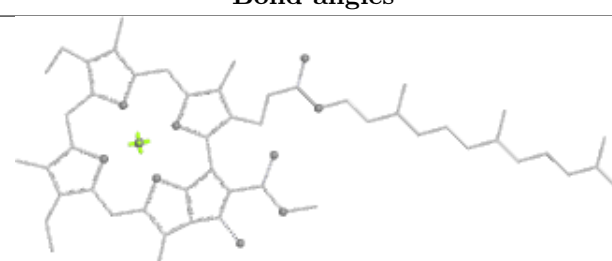
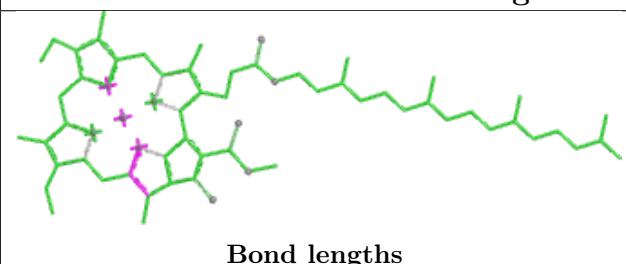
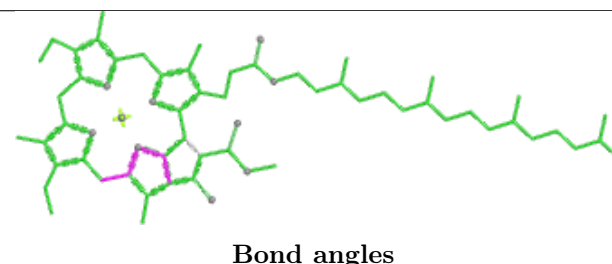
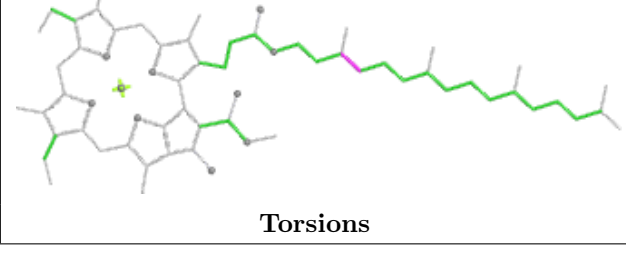
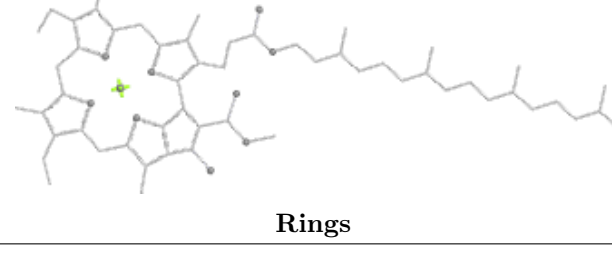
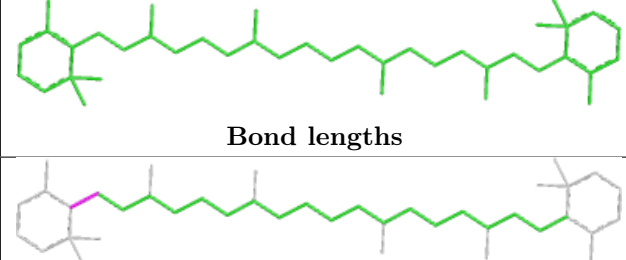
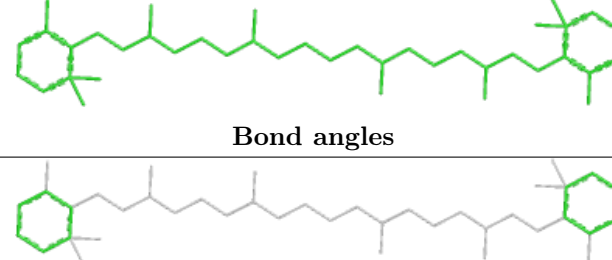
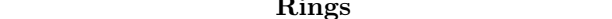


Ligand CHL 4 618

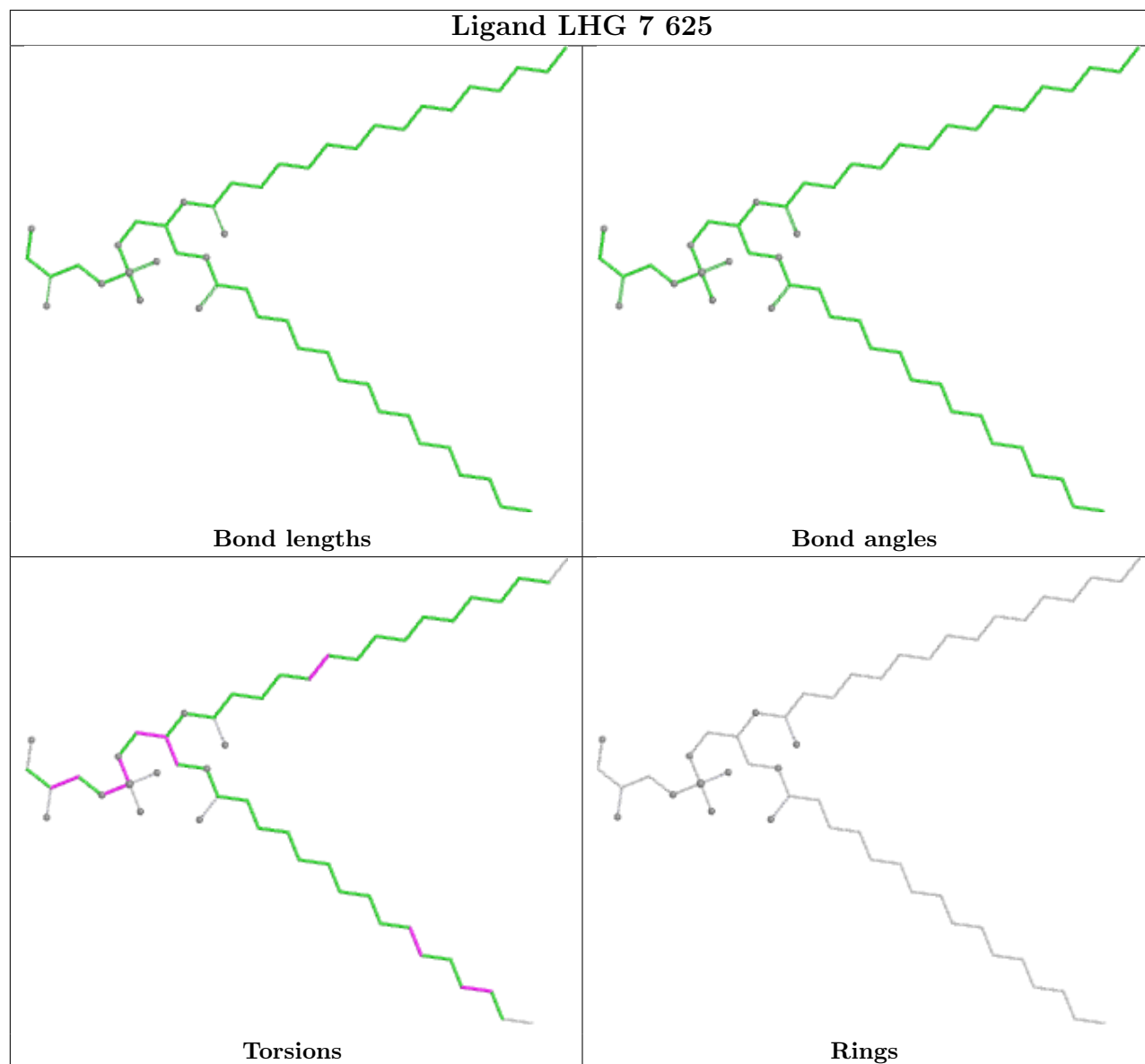


Ligand LMU 1 625

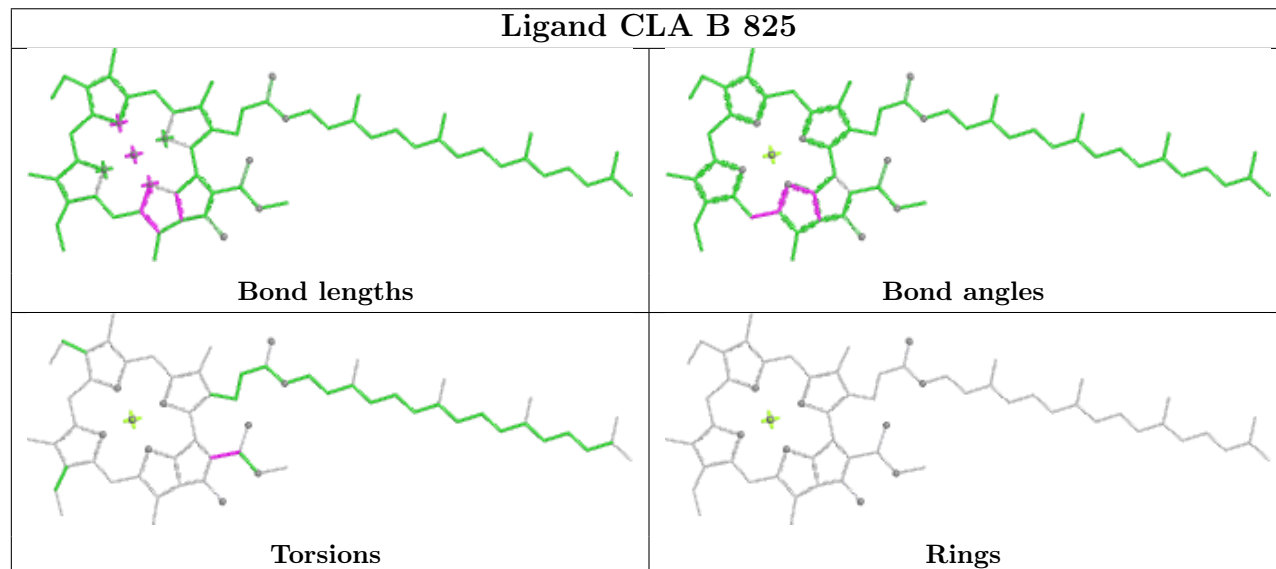


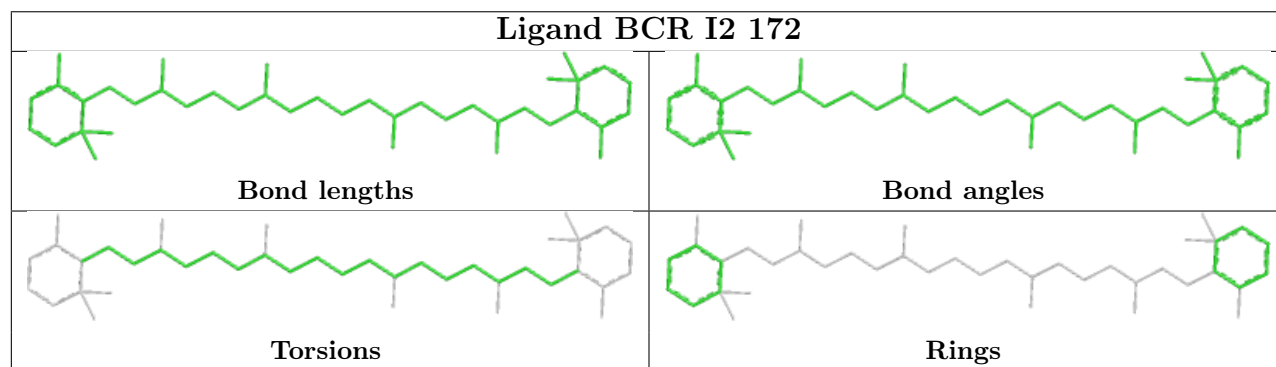
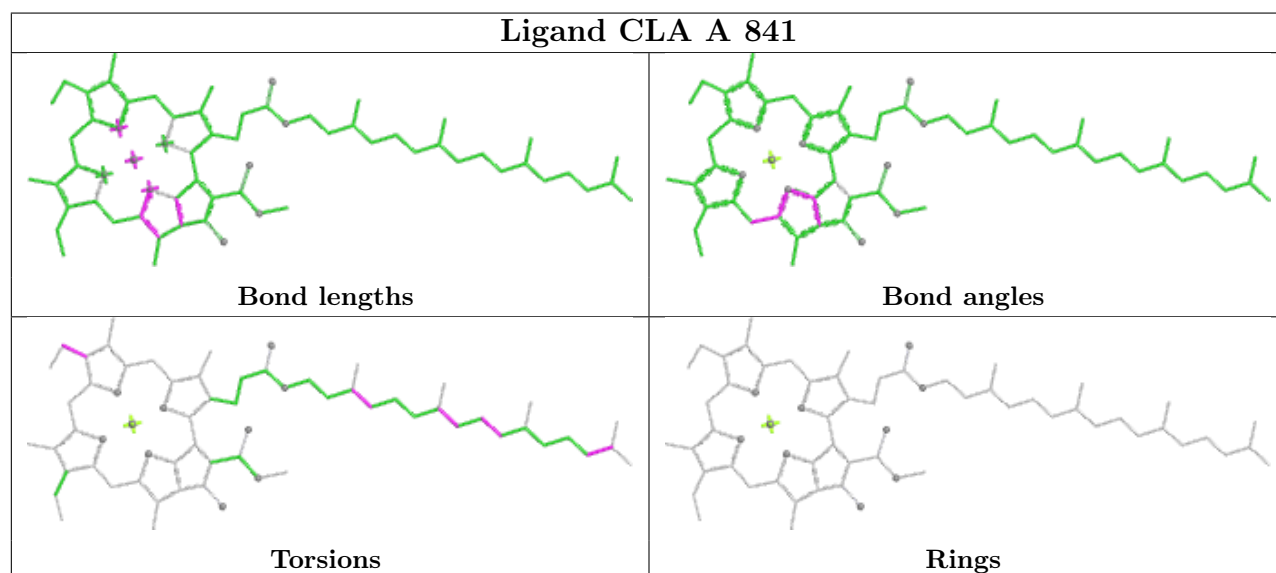
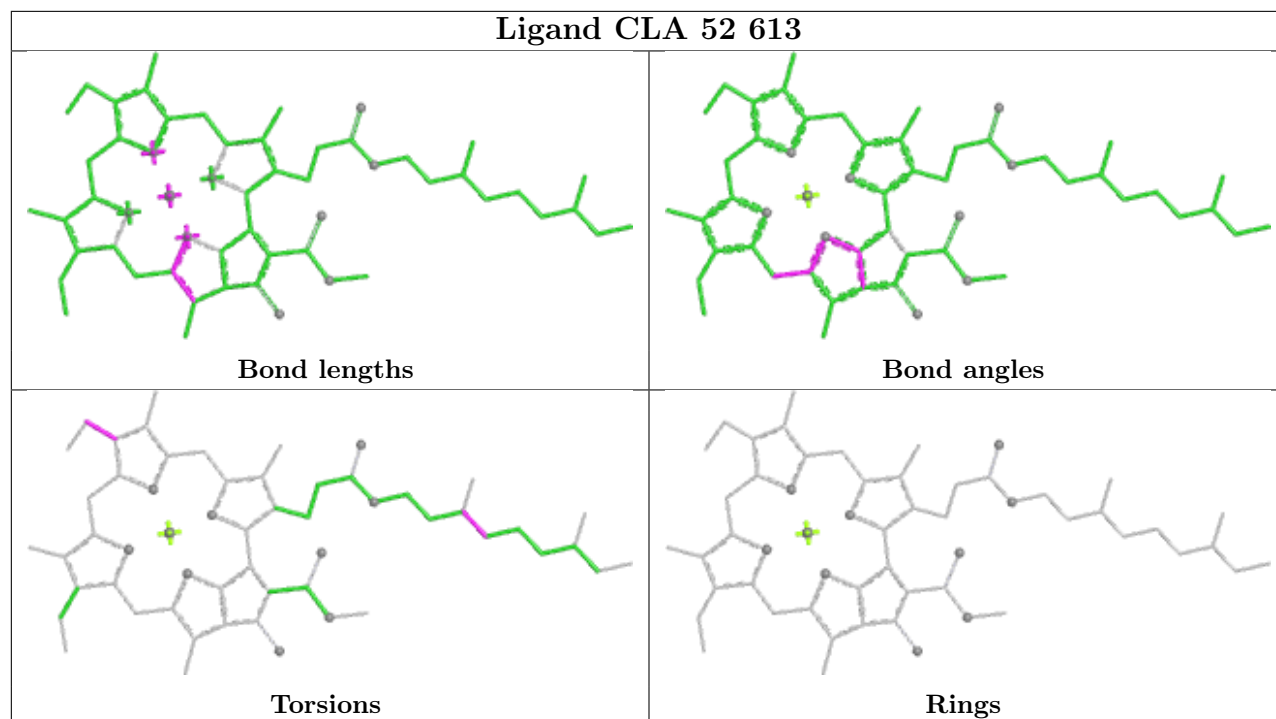
Ligand CLA K2 203	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CLA B2 810	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

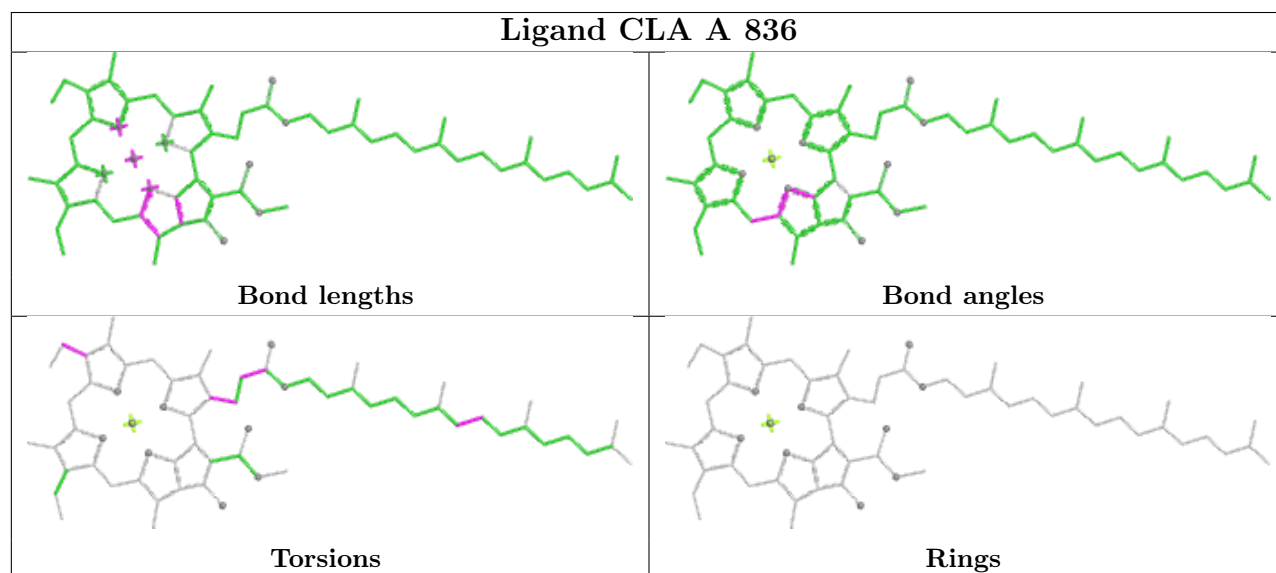
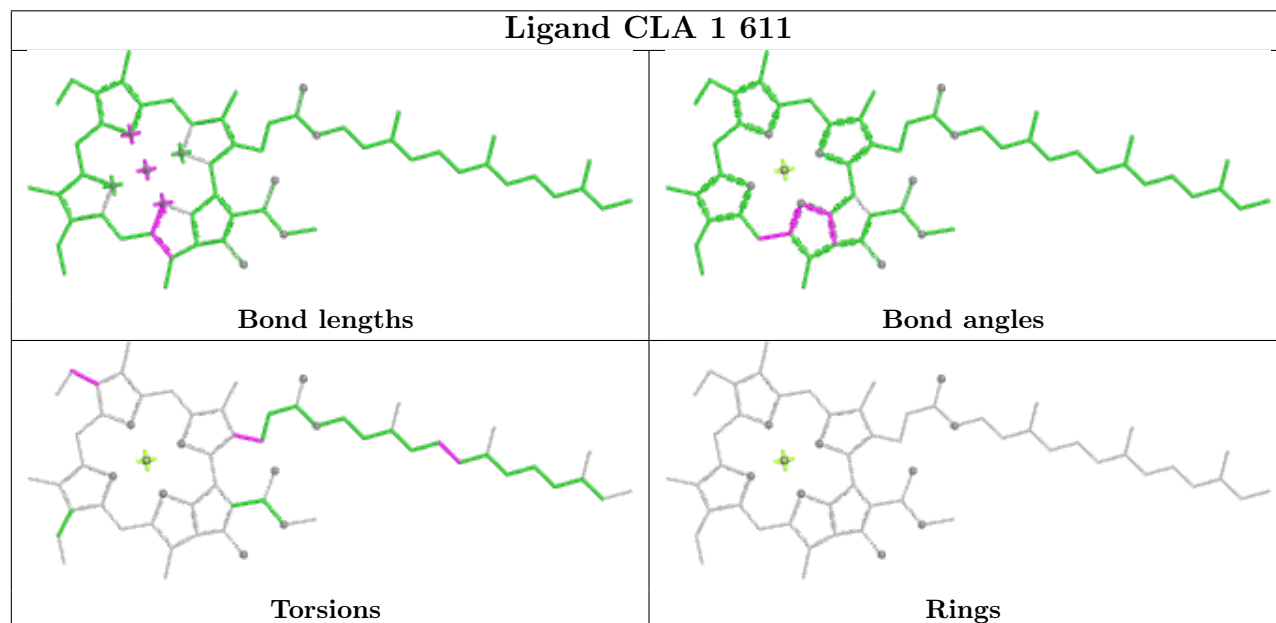
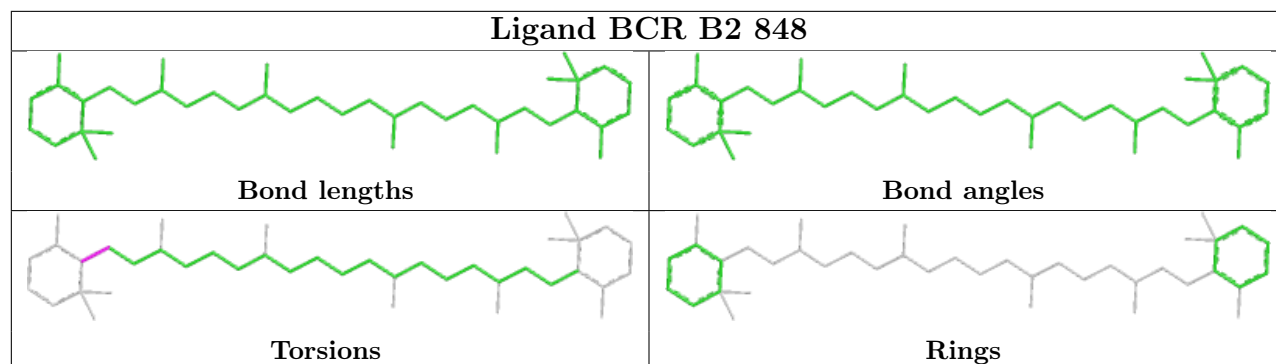
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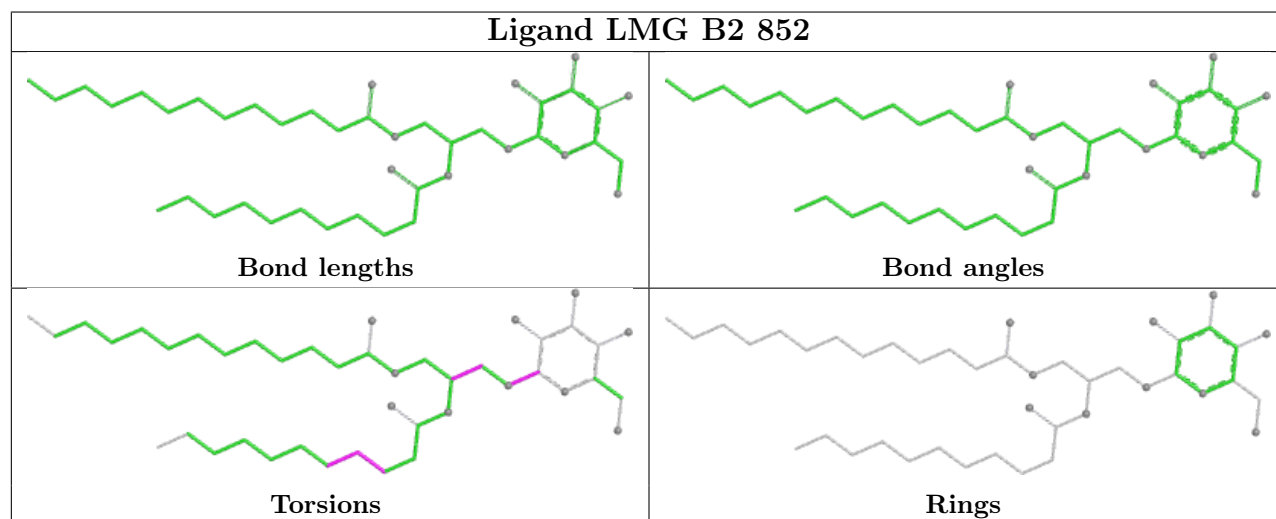
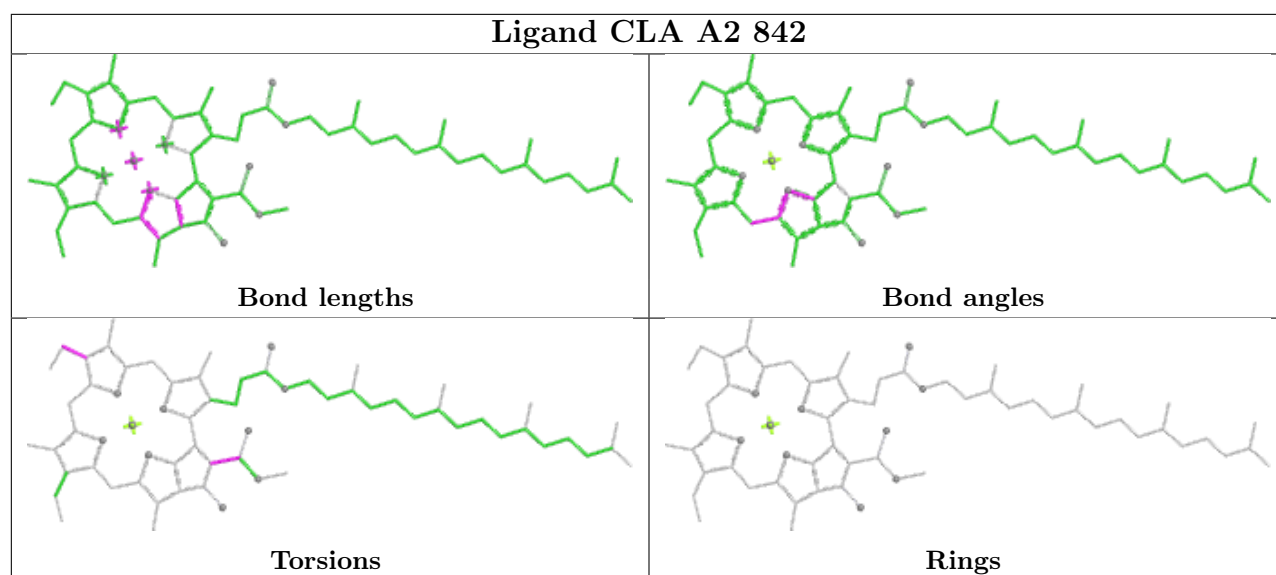


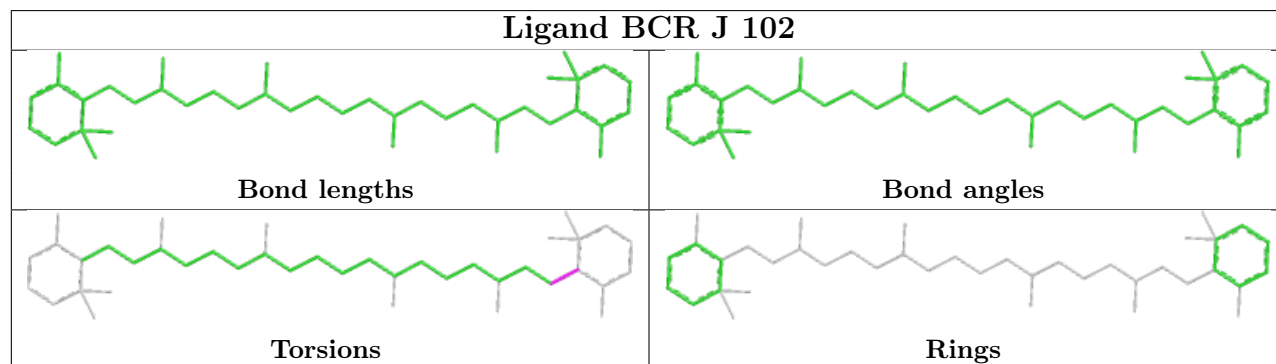
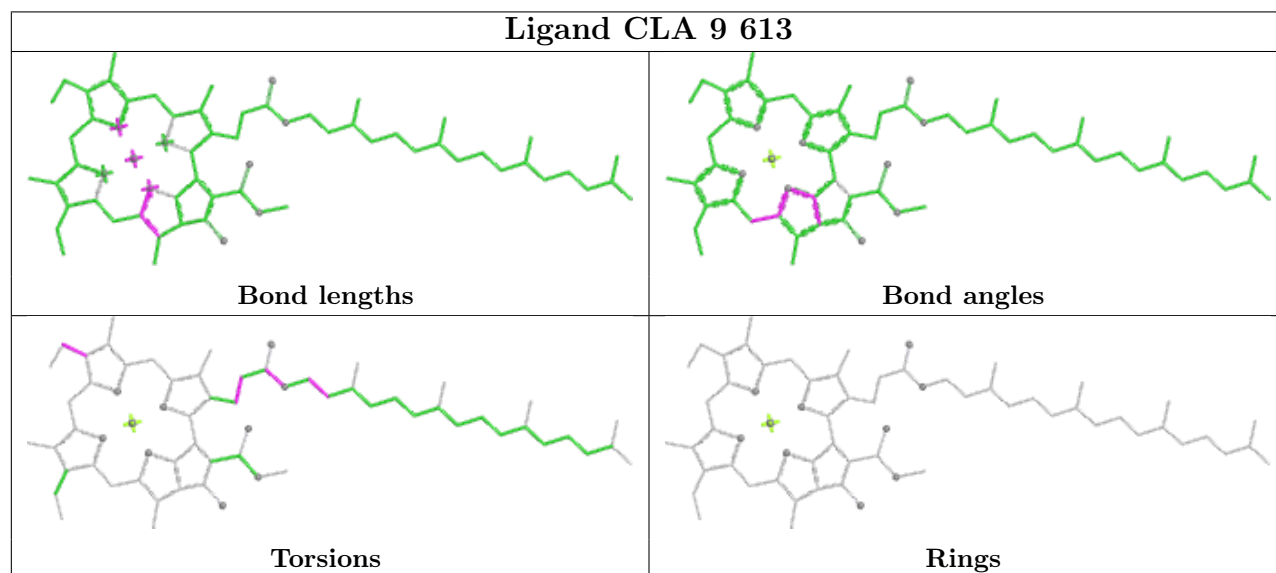
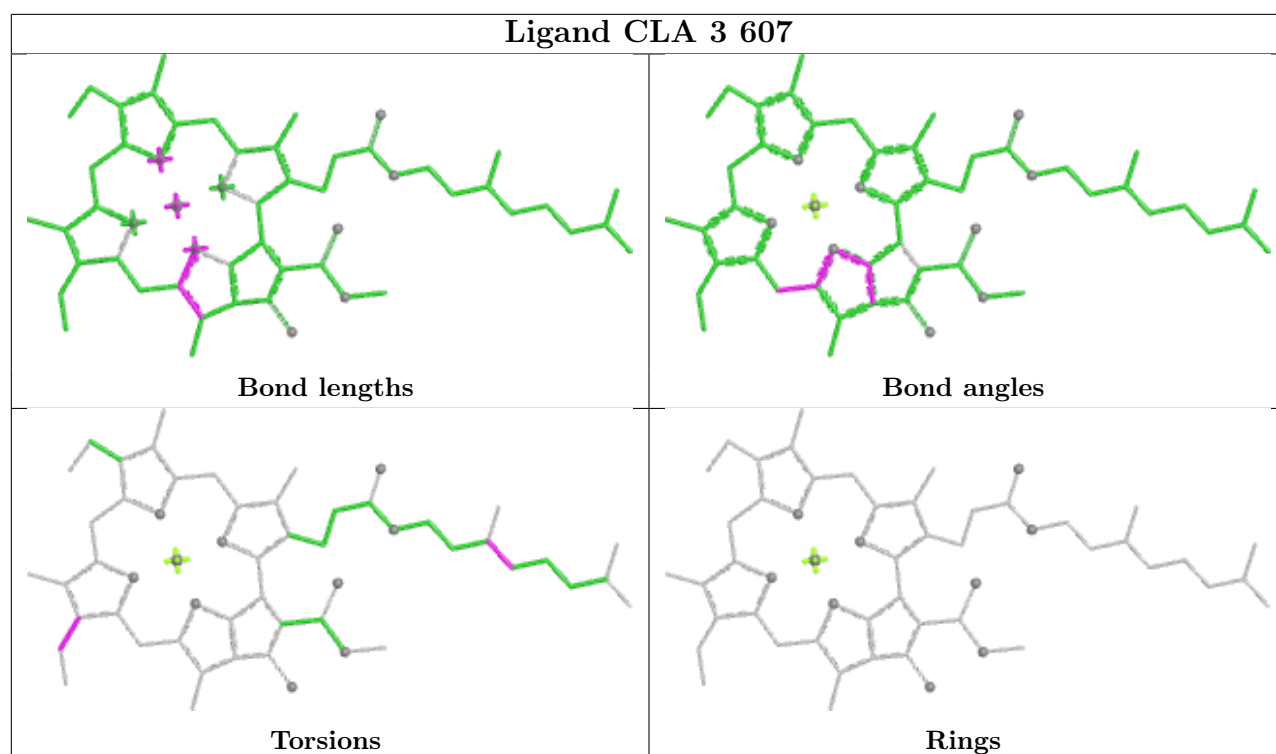
Ligand CLA B 825

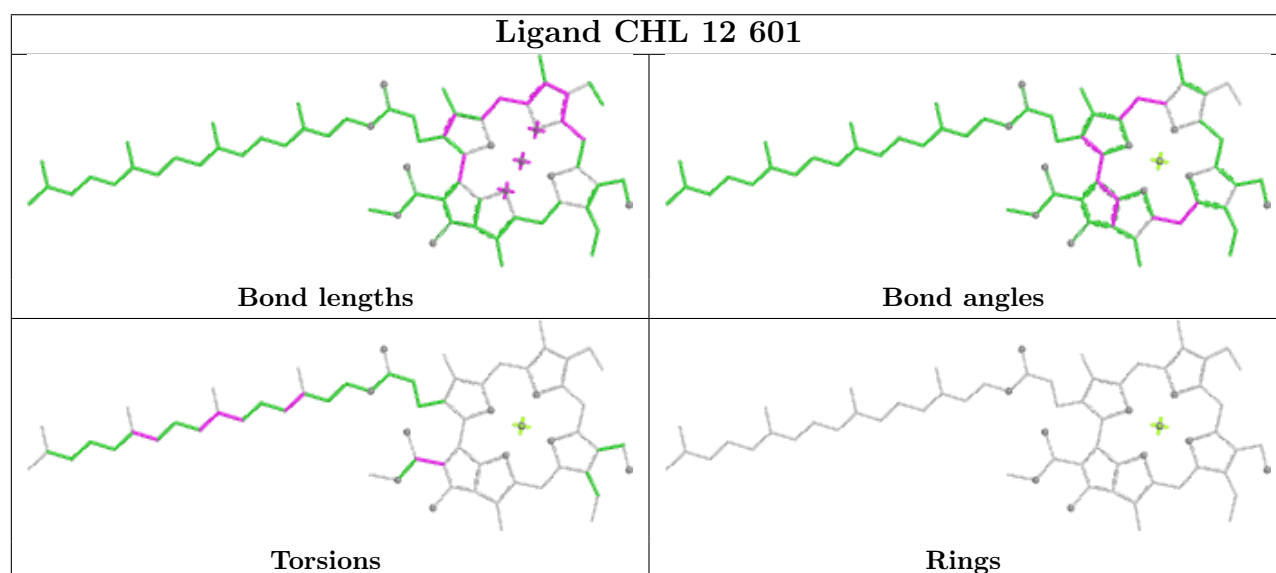
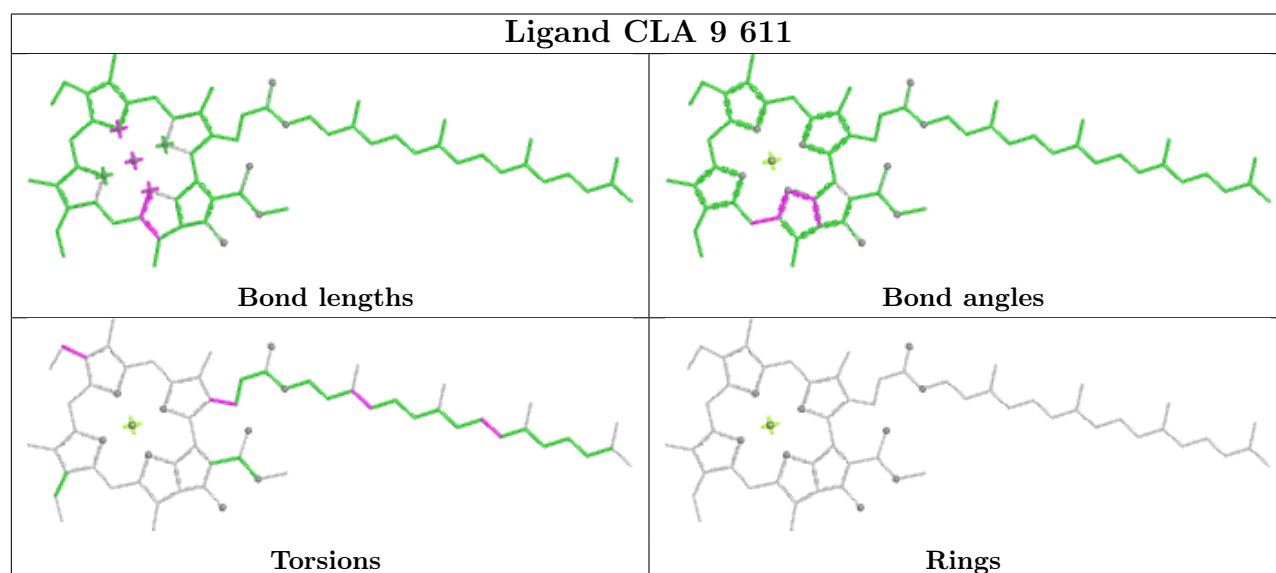
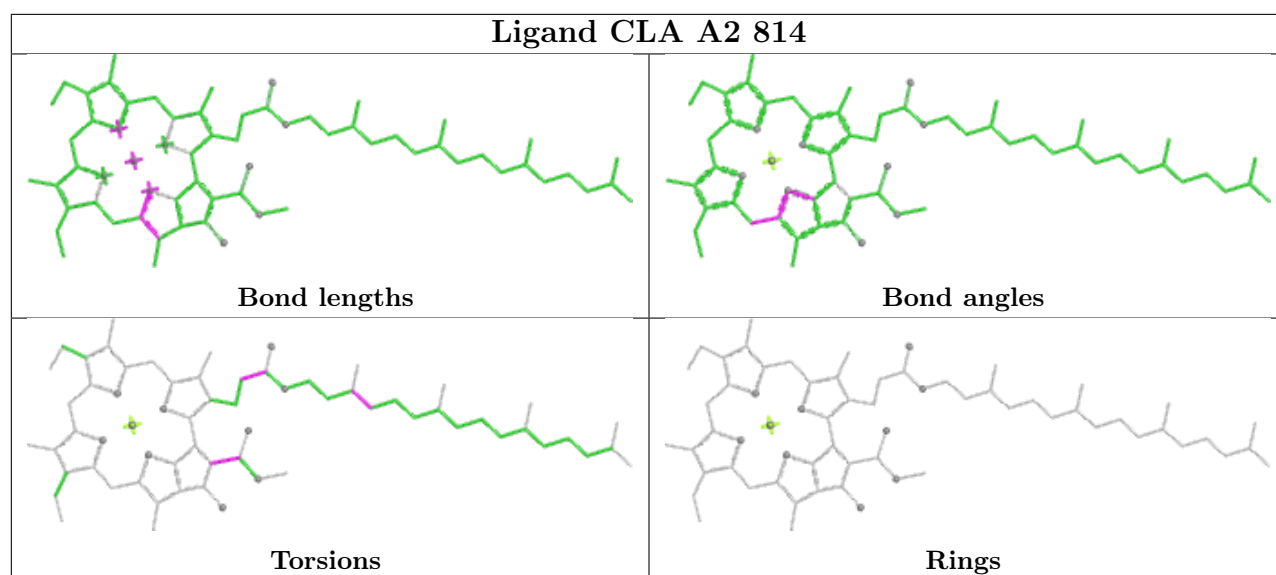


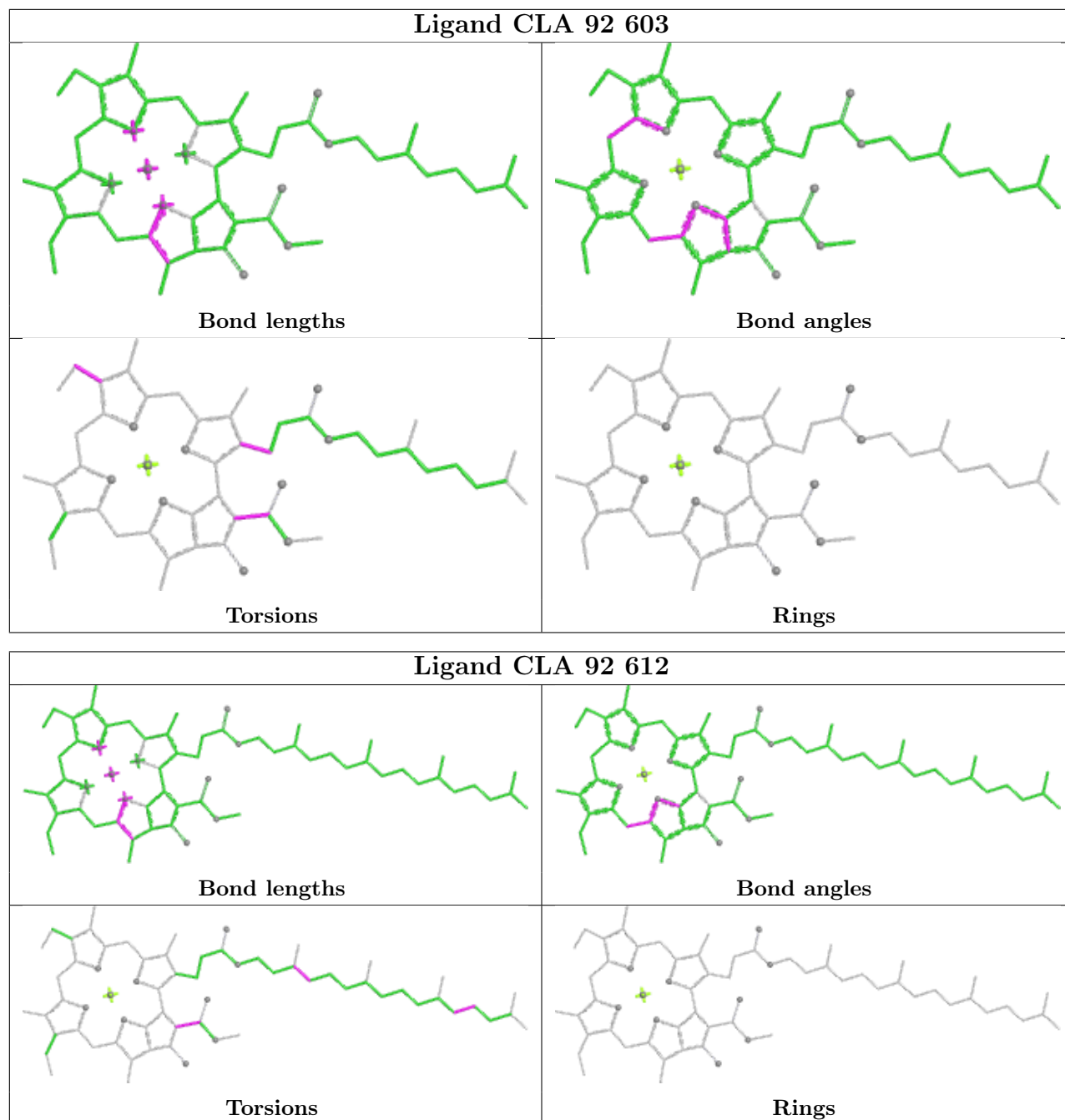


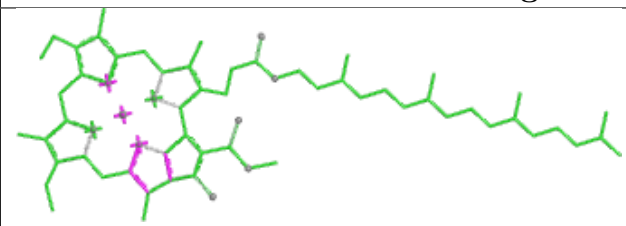
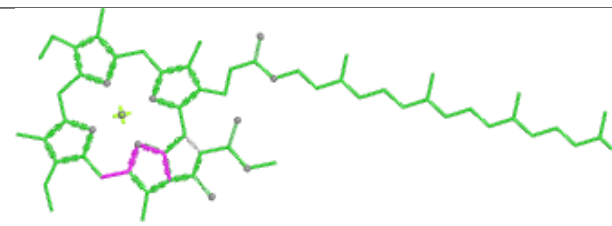
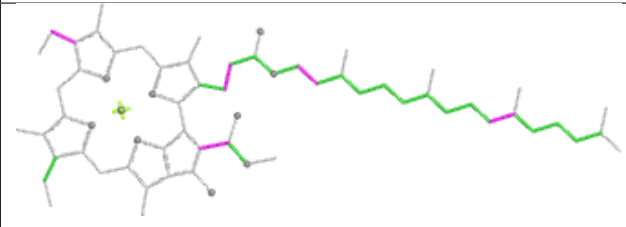
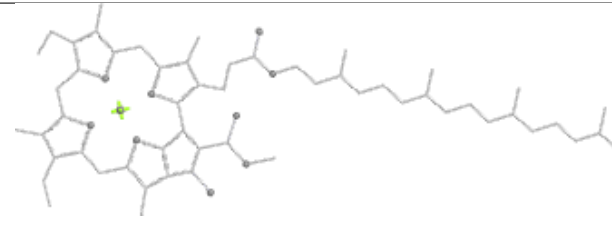


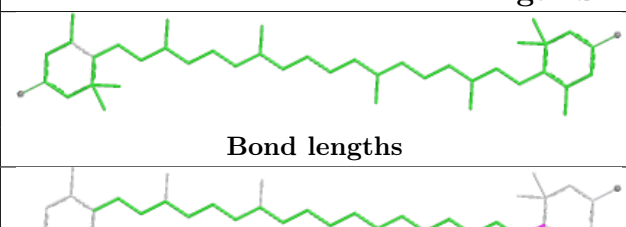
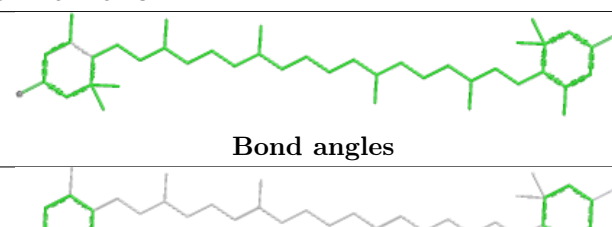
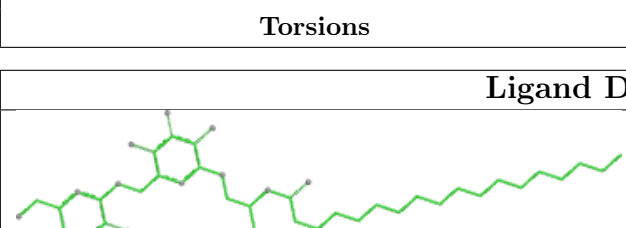
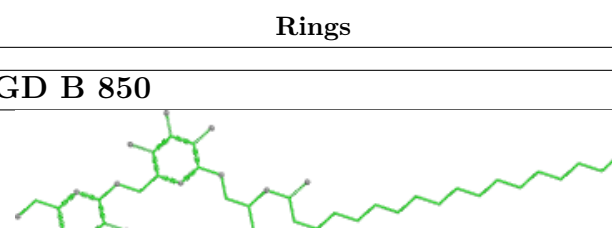


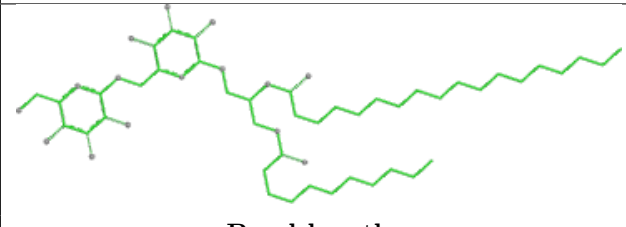
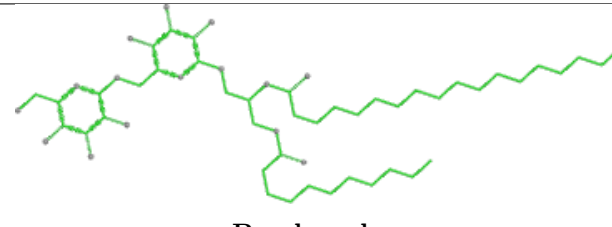
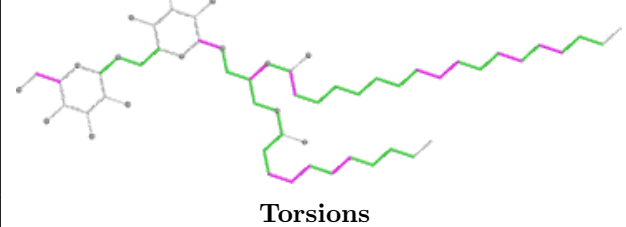
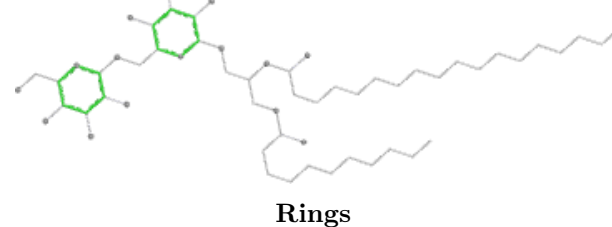


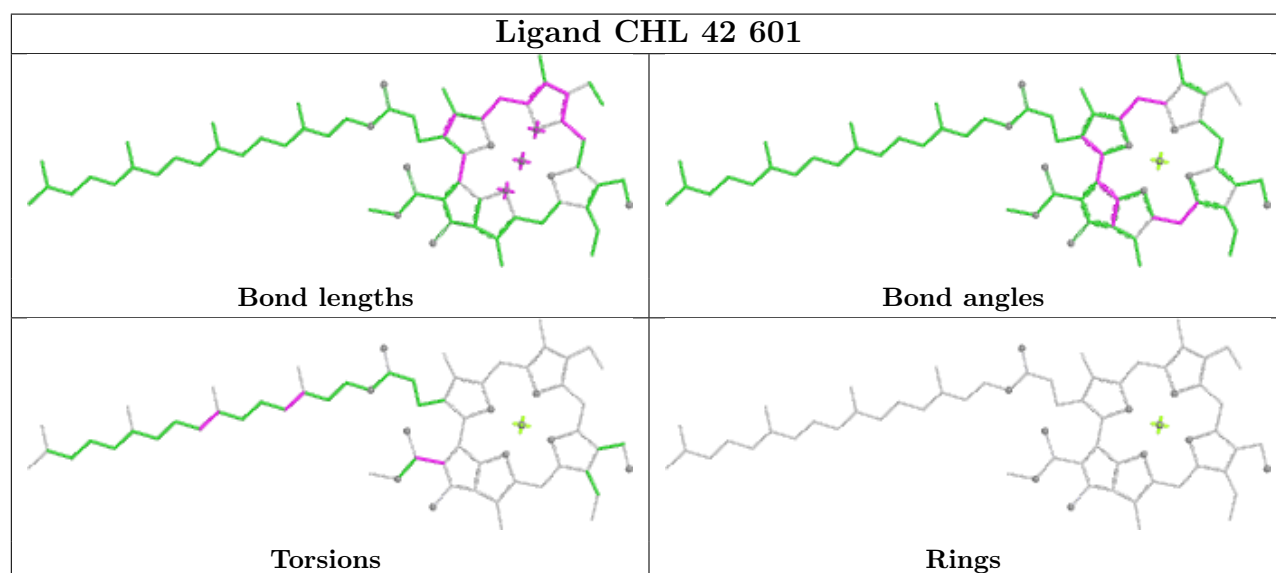
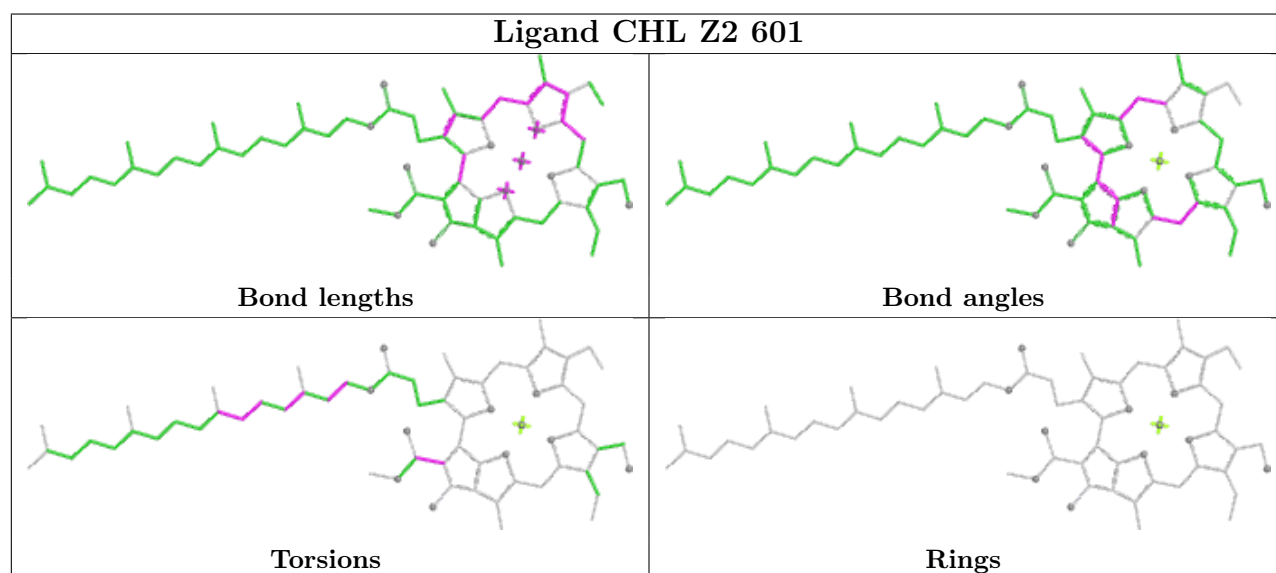
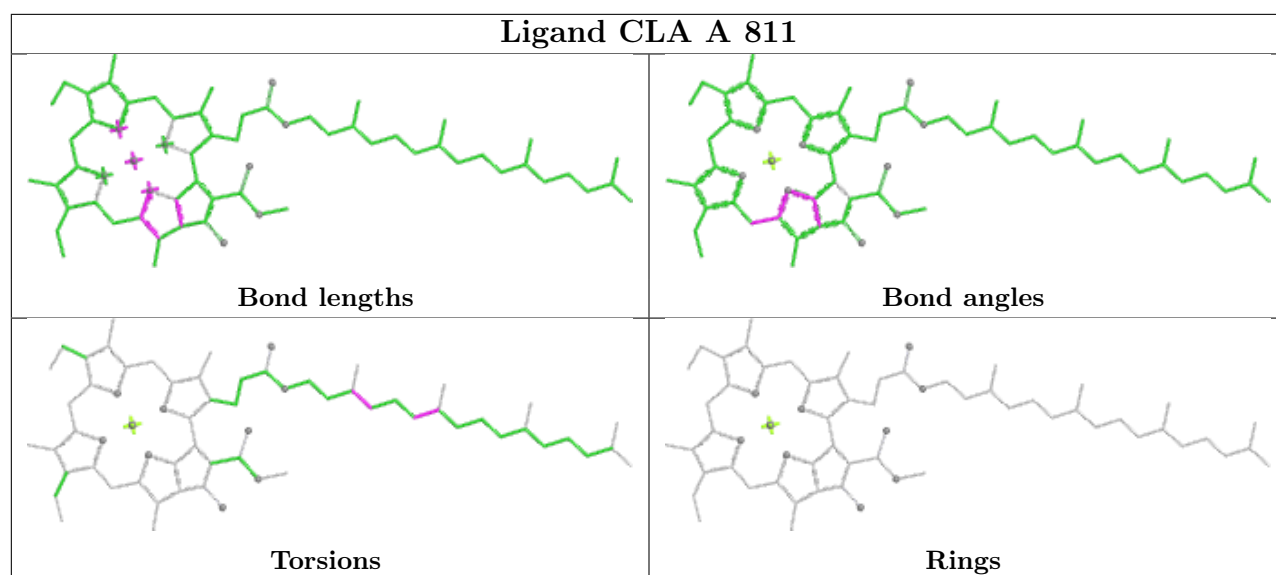


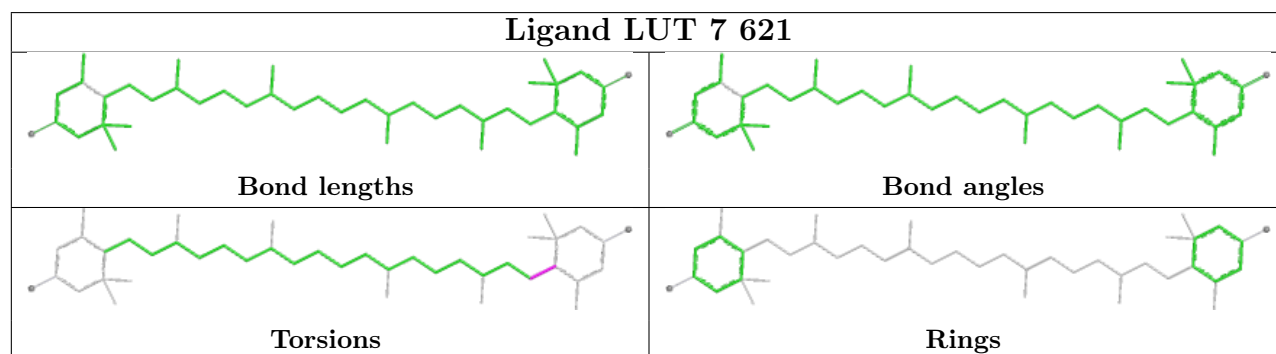
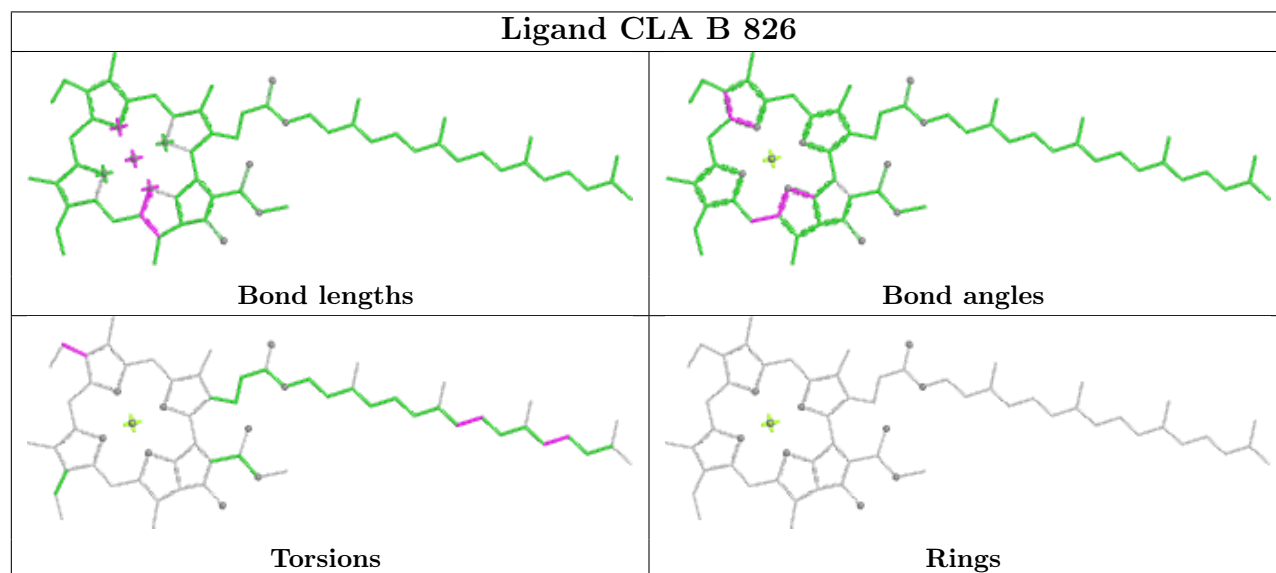
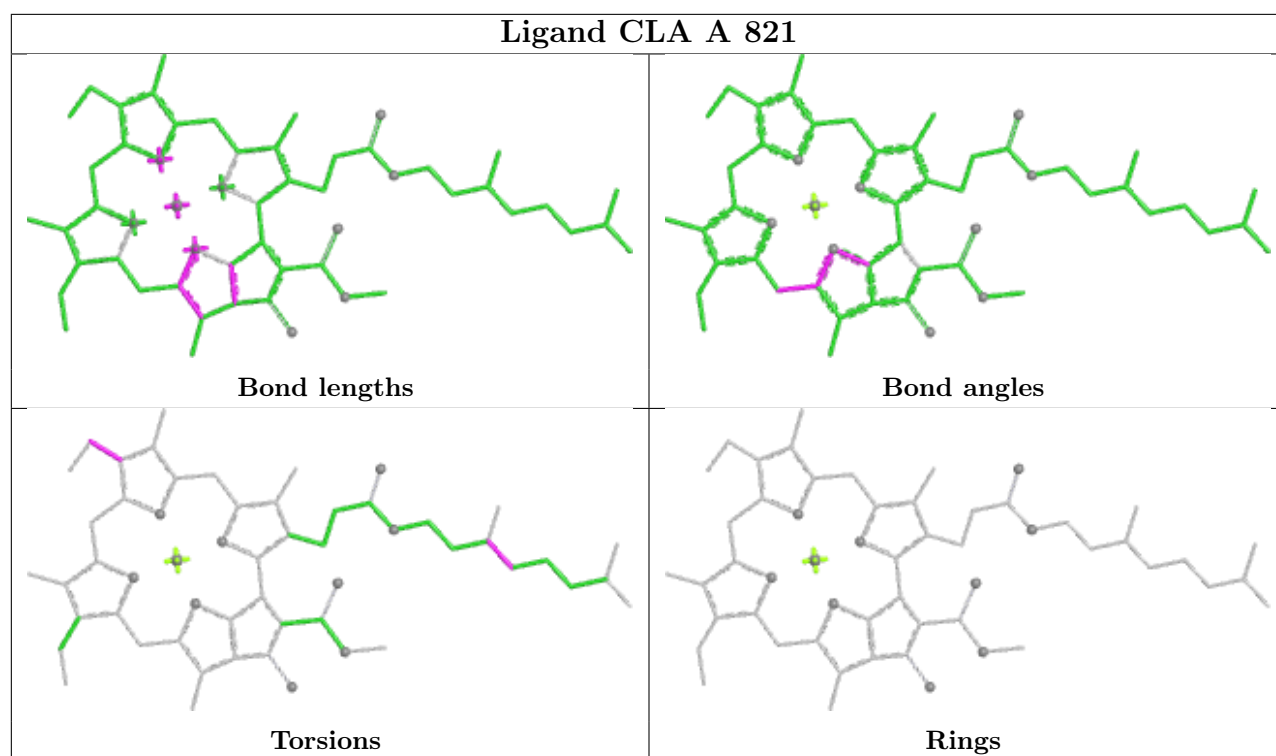


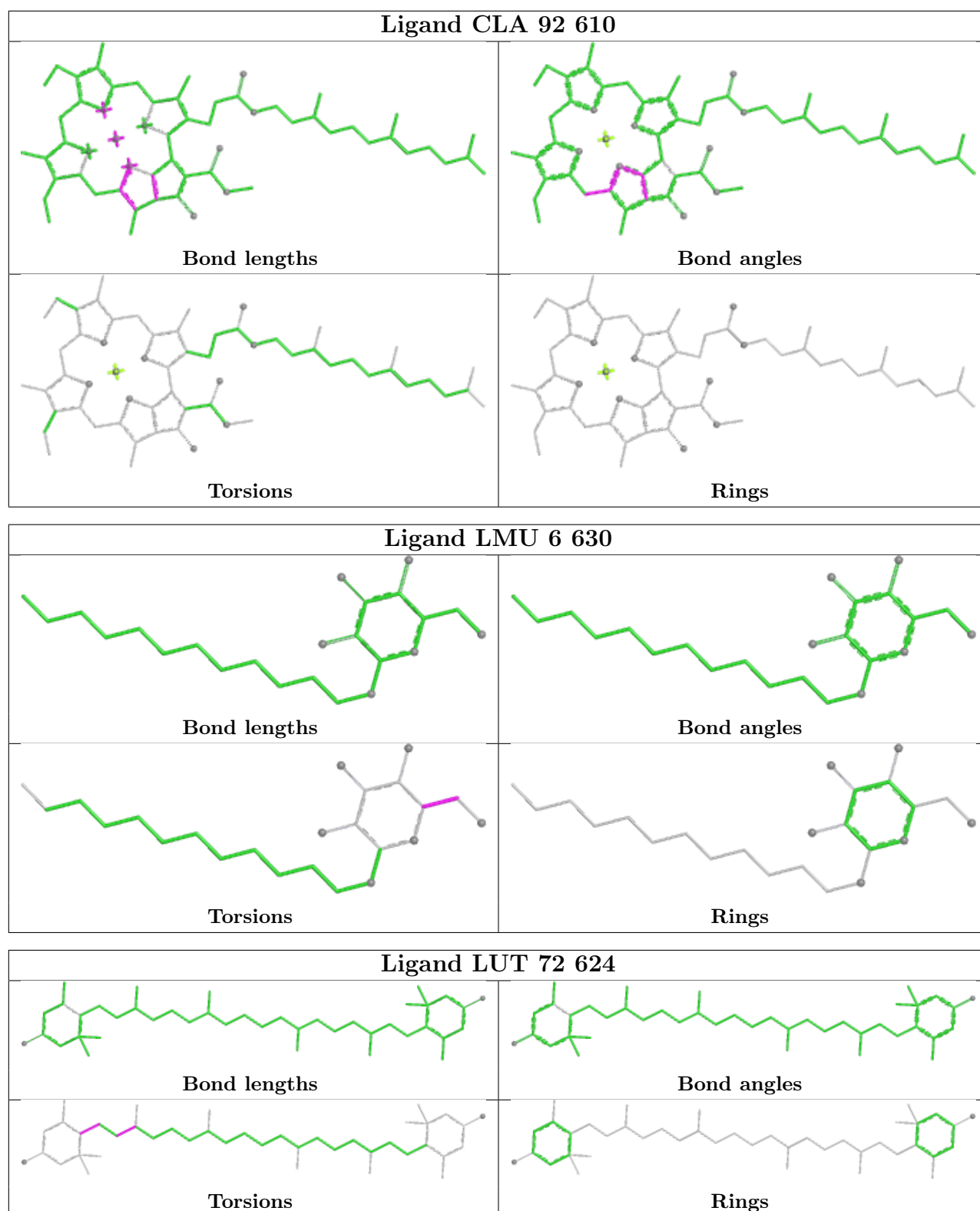
Ligand CLA A 823	
	
Bond lengths	Bond angles
	
Torsions	Rings

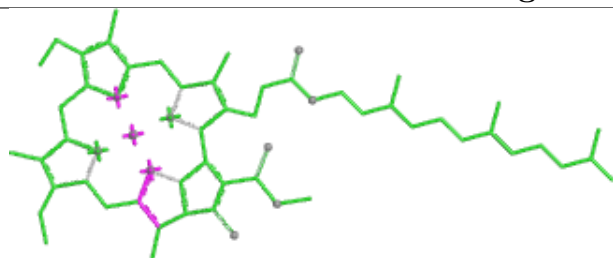
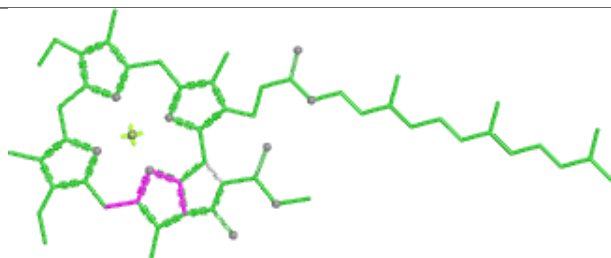
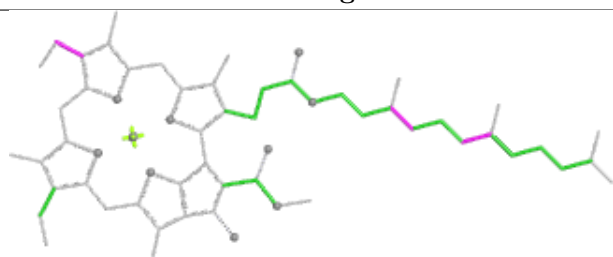
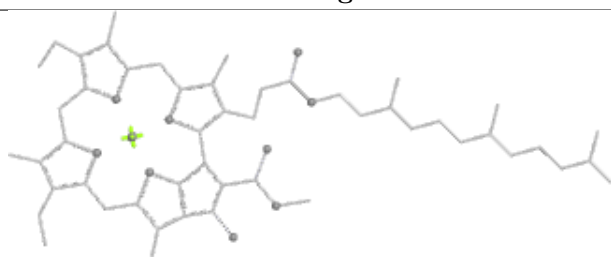
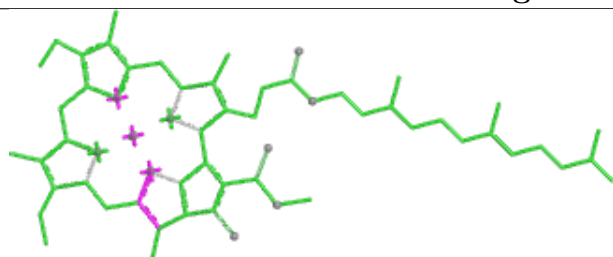
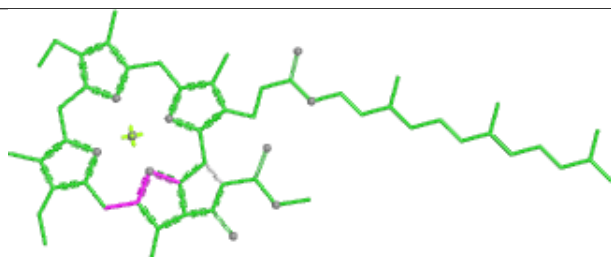
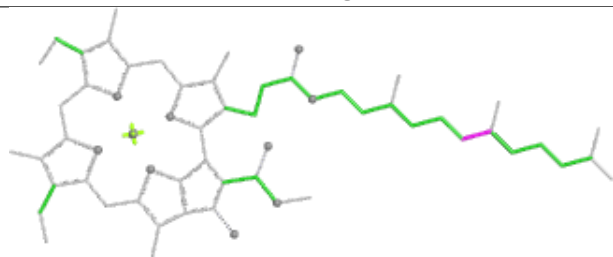
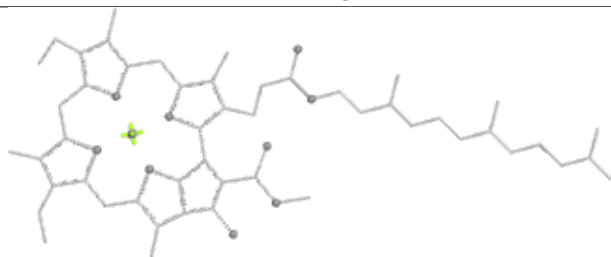
Ligand LUT 52 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

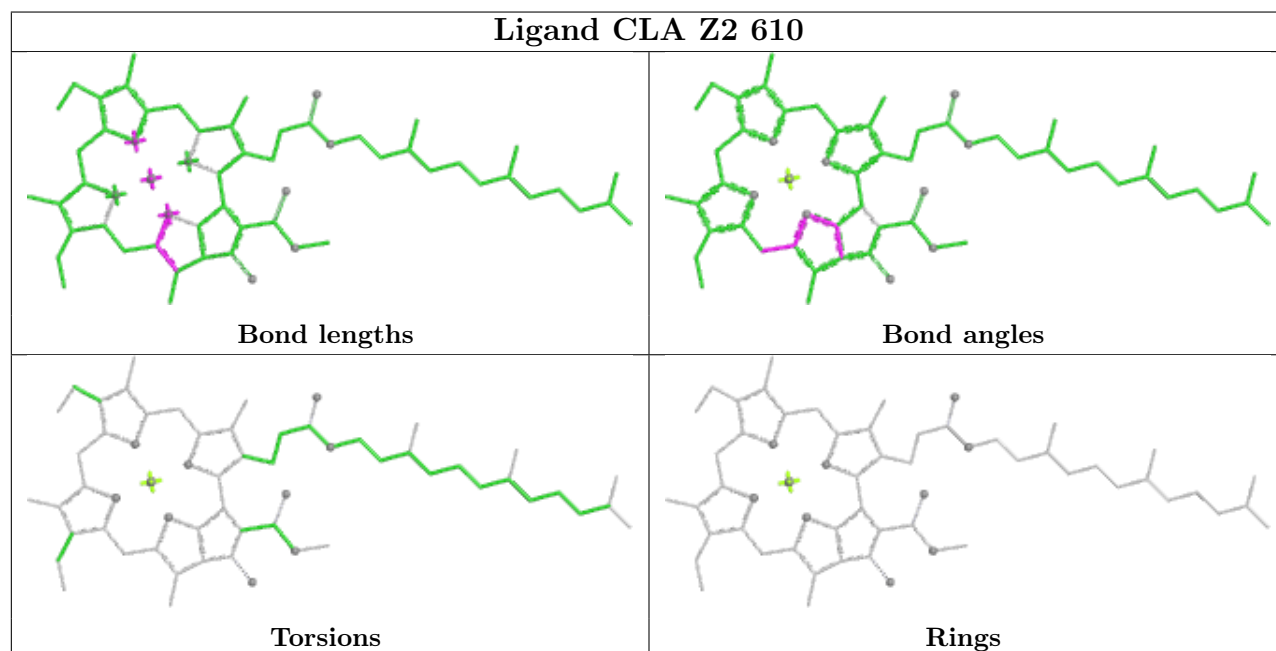
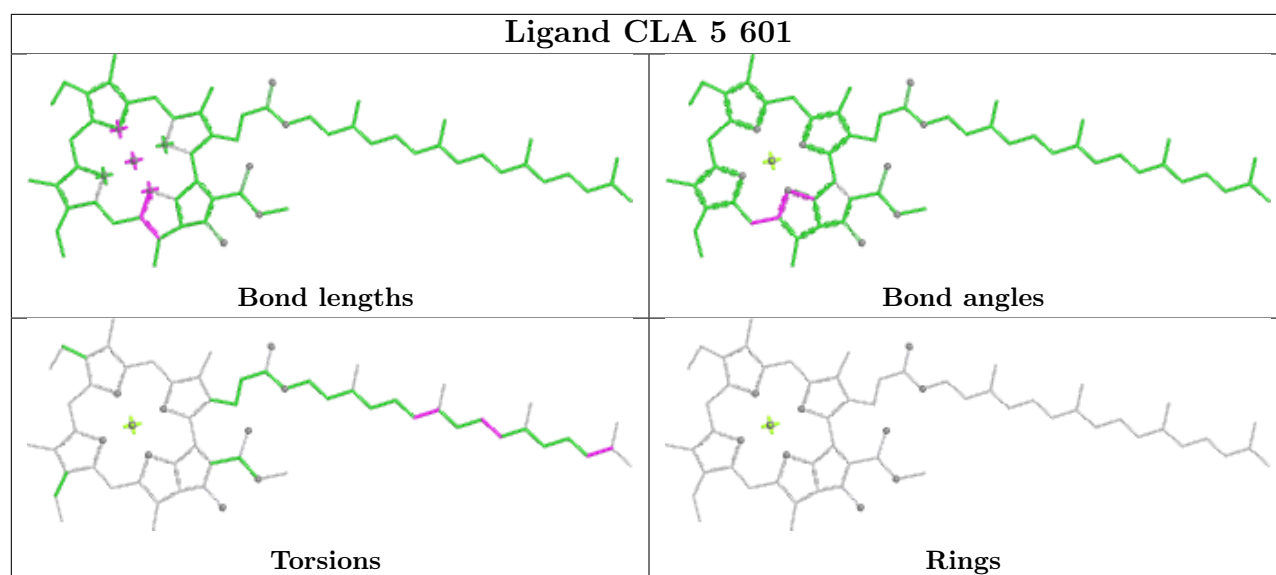
Ligand DGD B 850	
	
Bond lengths	Bond angles
	
Torsions	Rings

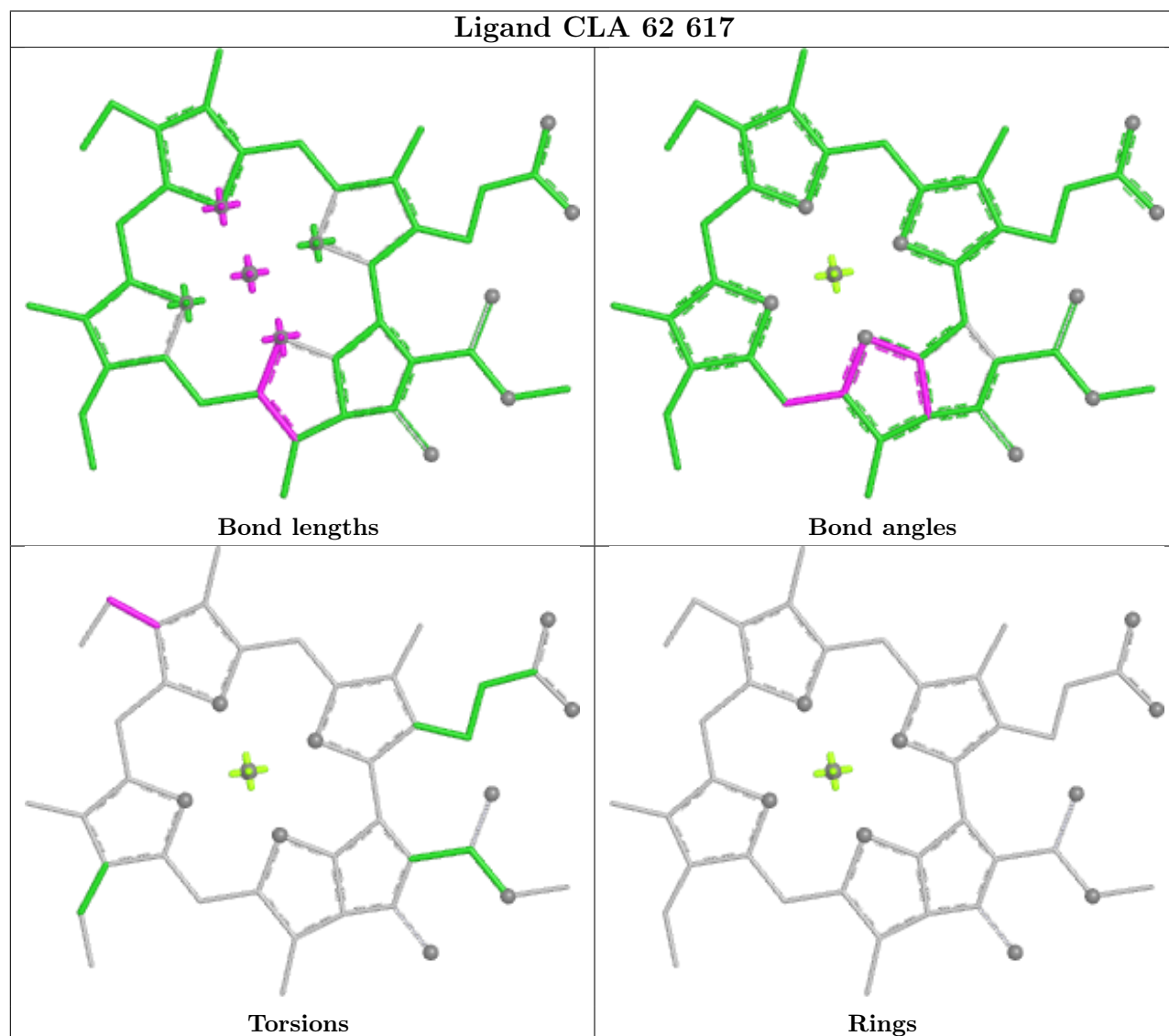
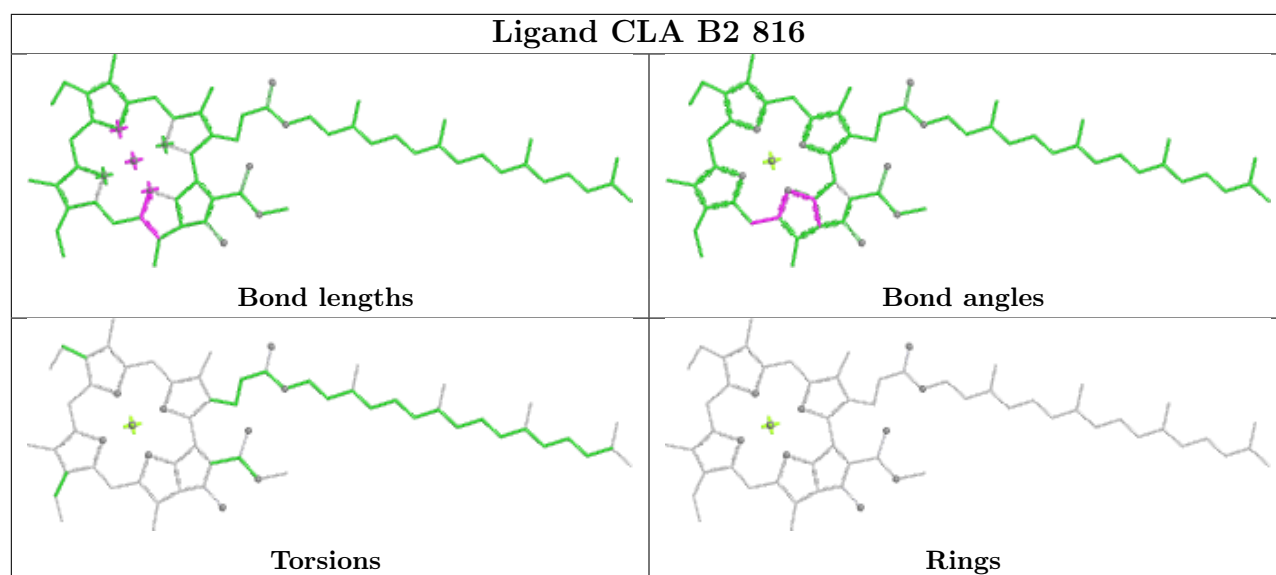


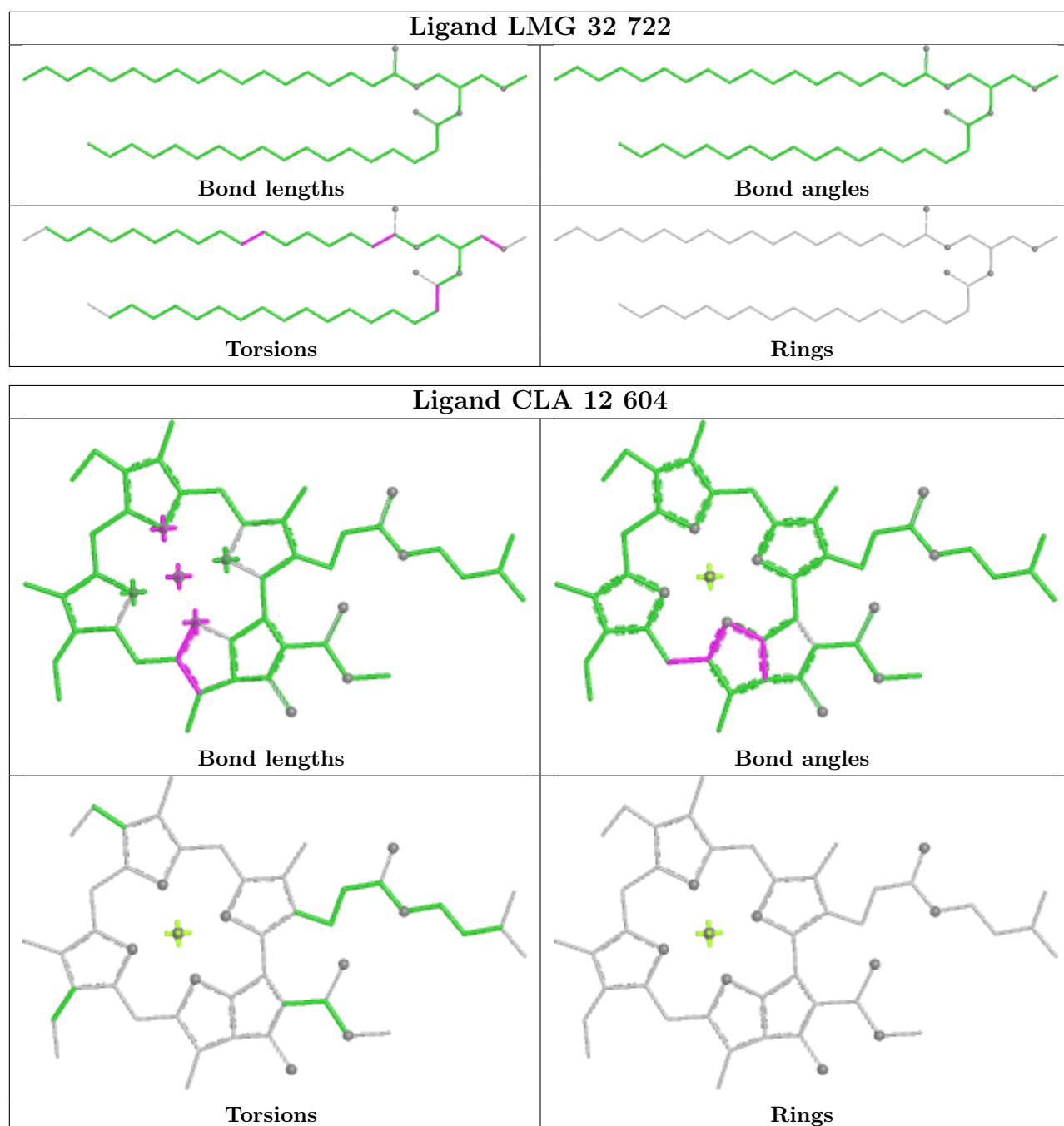


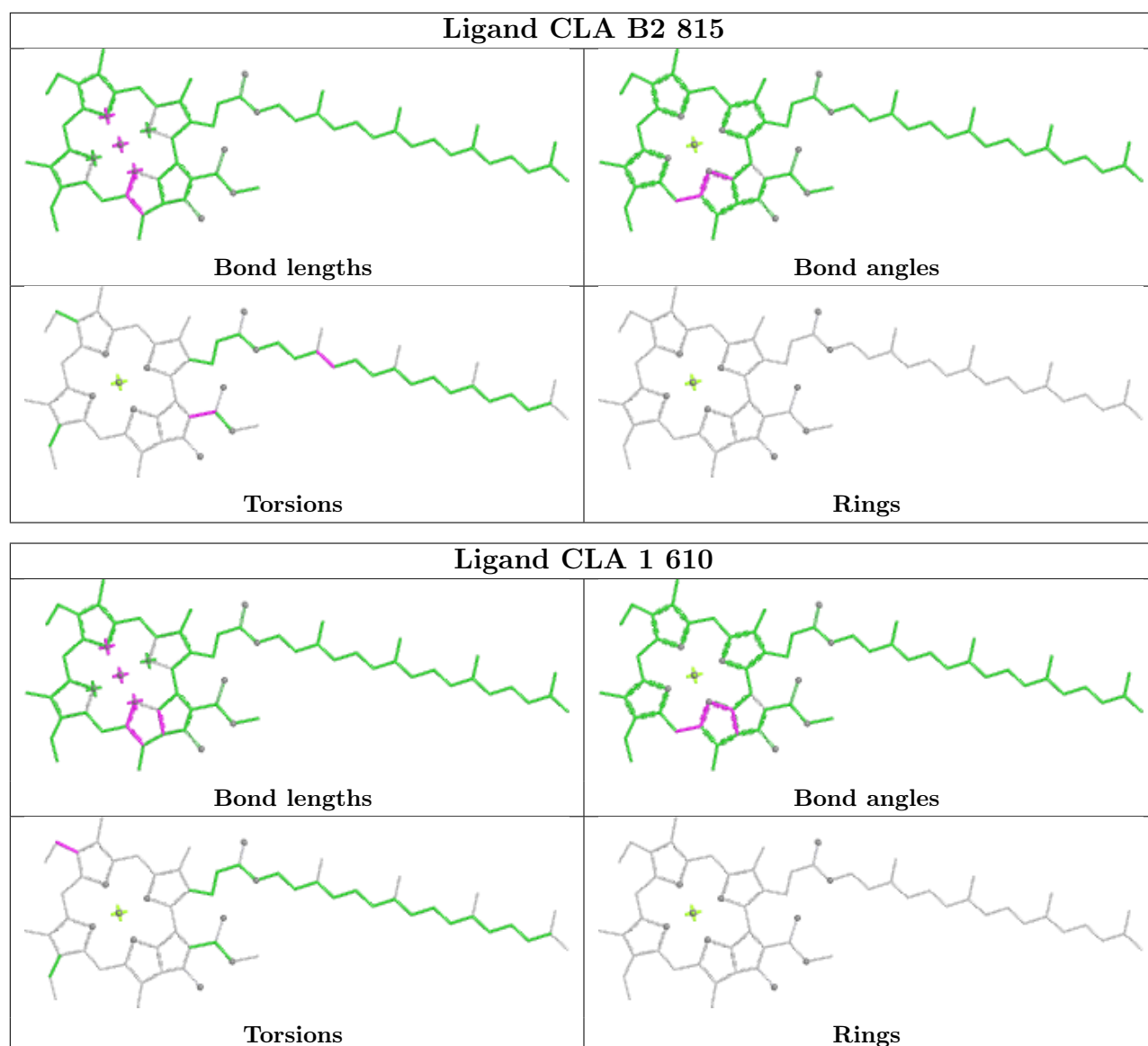


Ligand CLA 4 611**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA G 203****Bond lengths****Bond angles****Torsions****Rings**

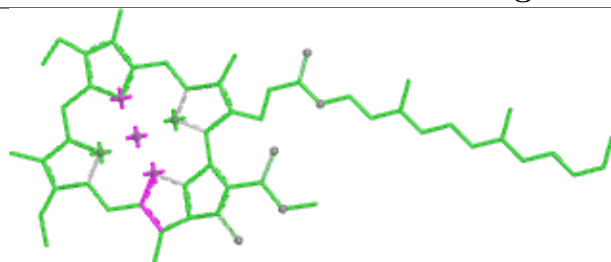




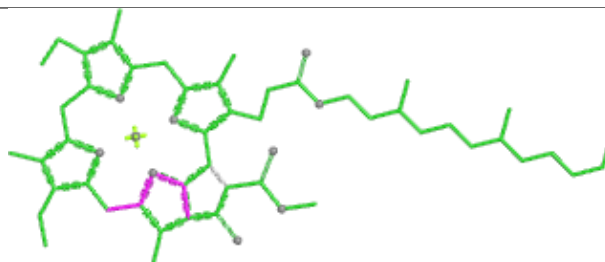




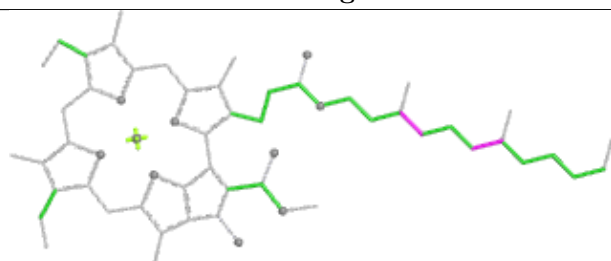
Ligand CLA B 822



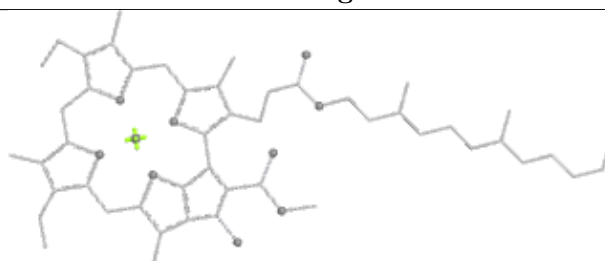
Bond lengths



Bond angles

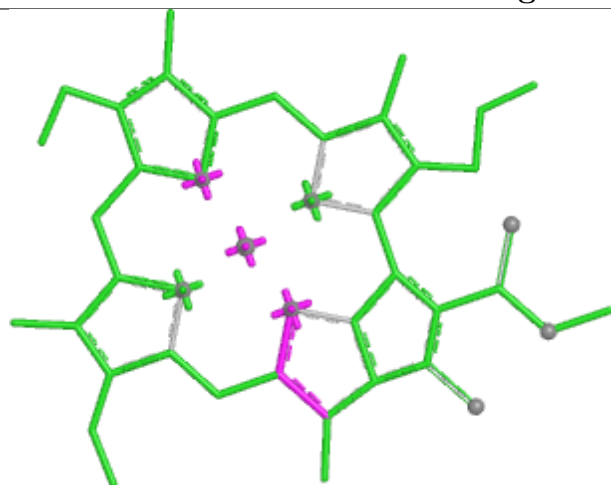


Torsions

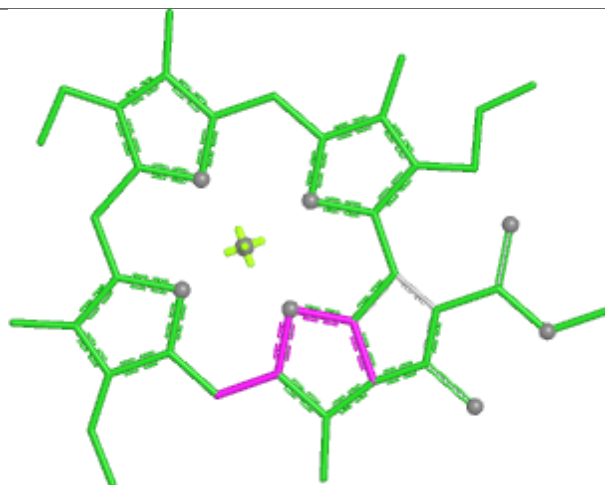


Rings

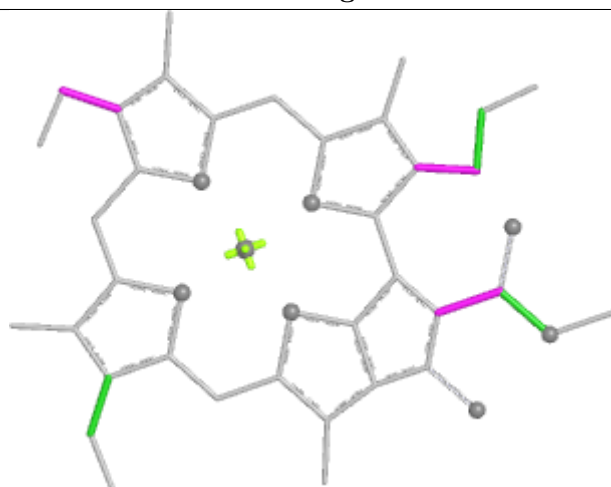
Ligand CLA 7 614



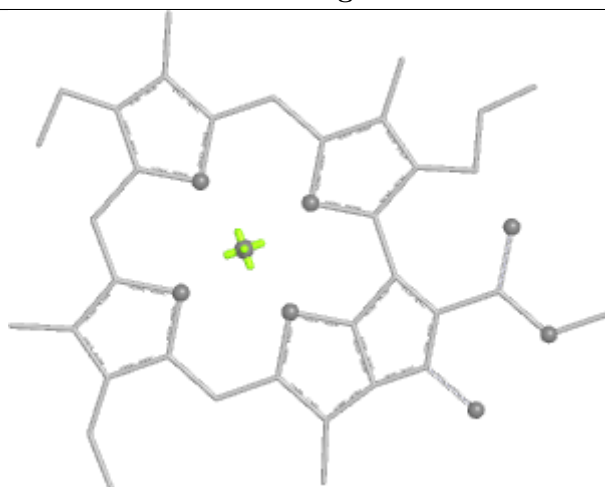
Bond lengths



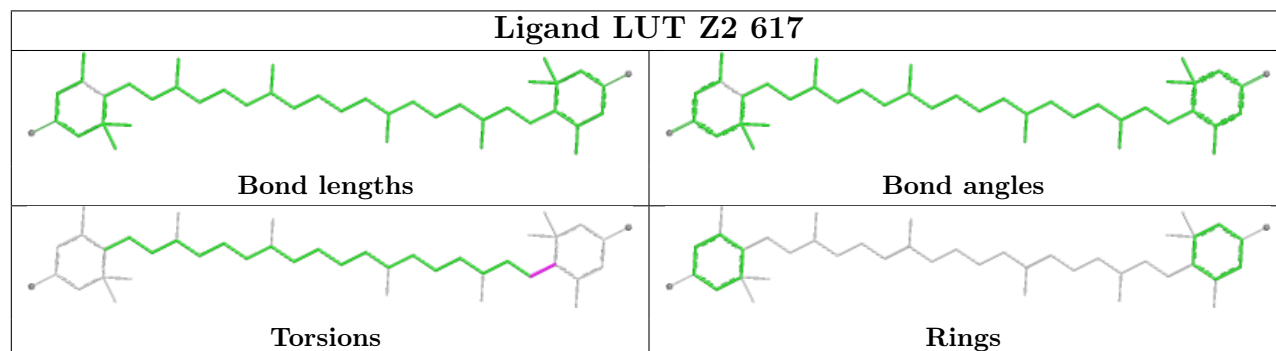
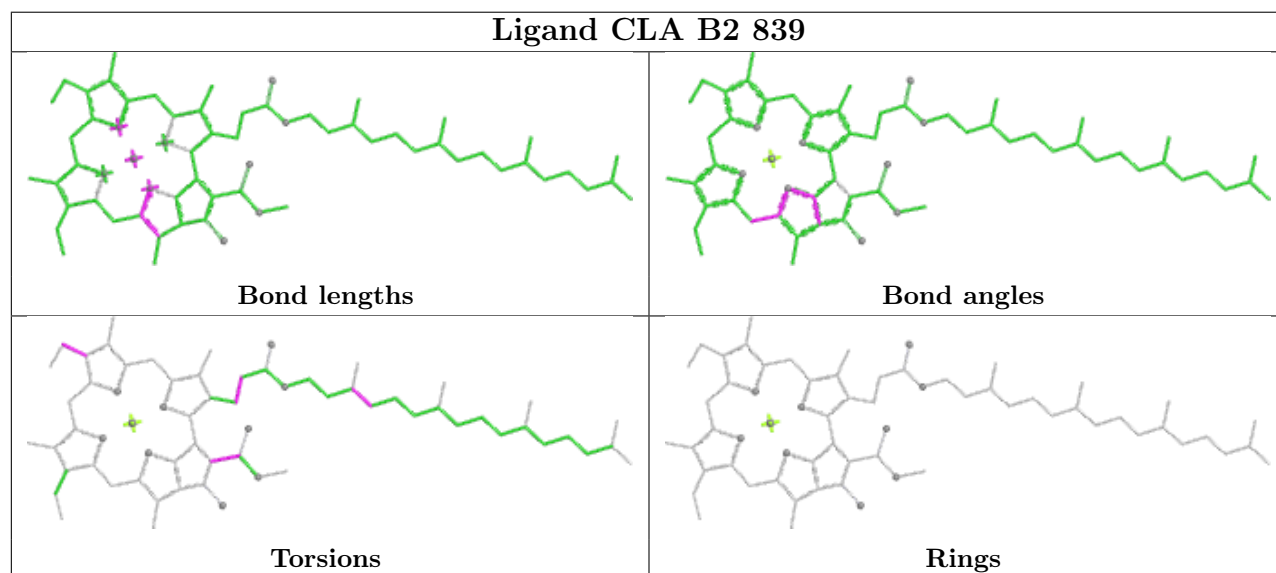
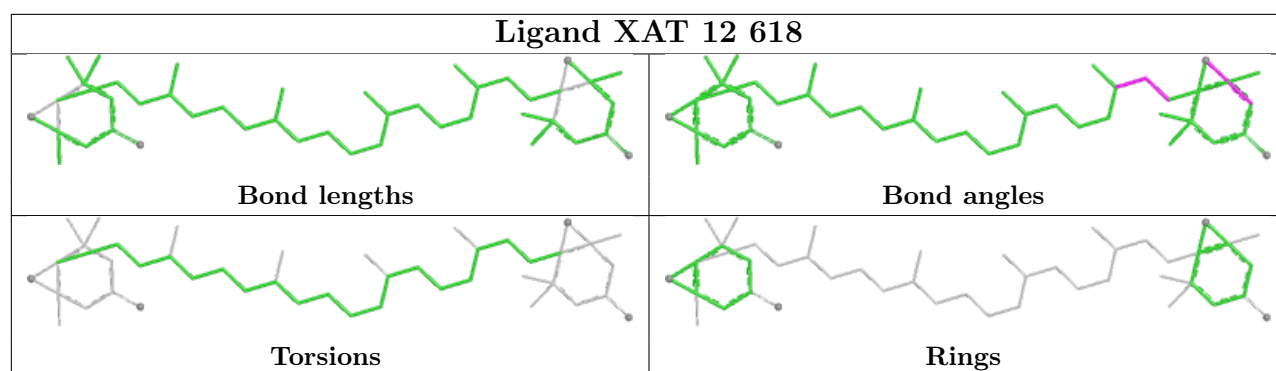
Bond angles

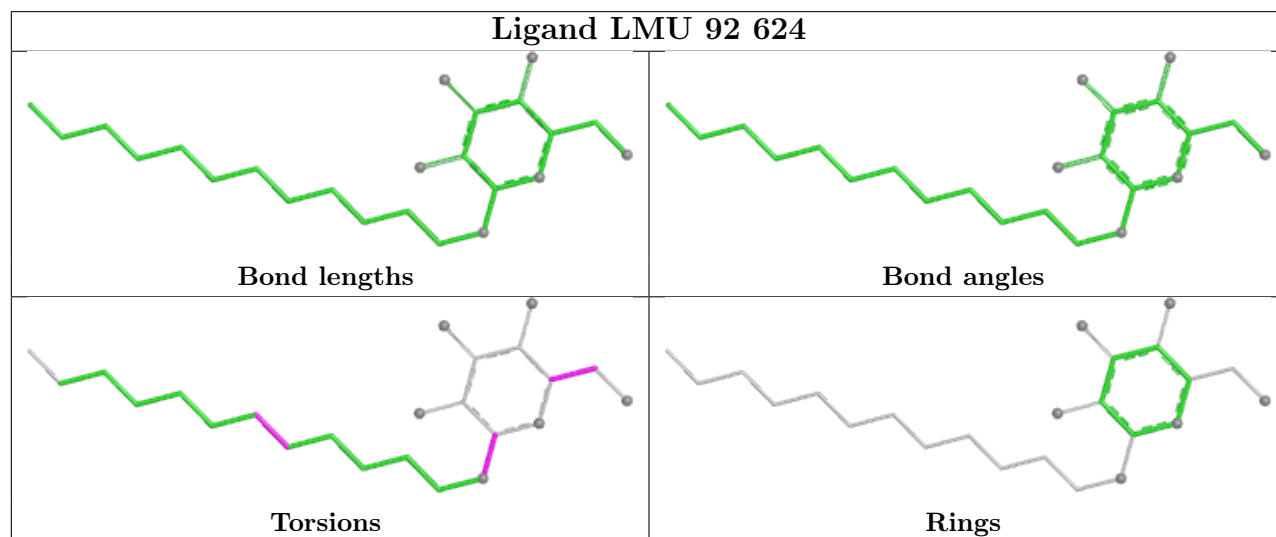
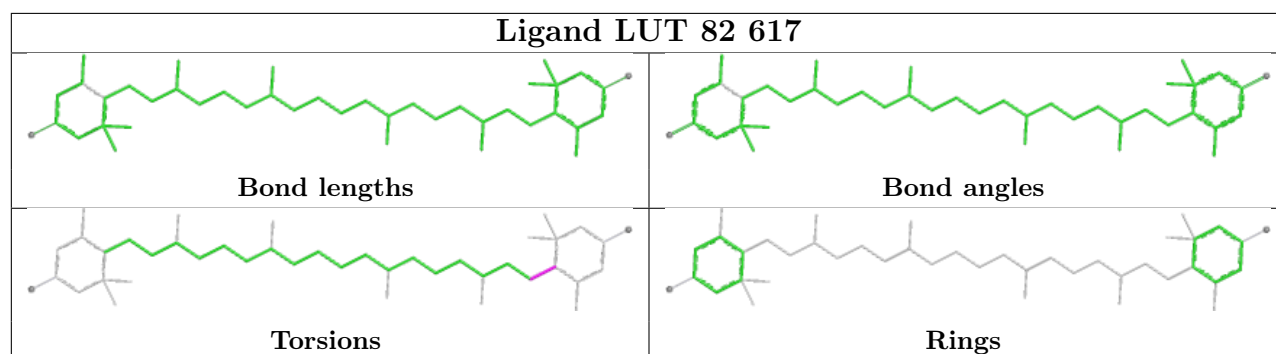
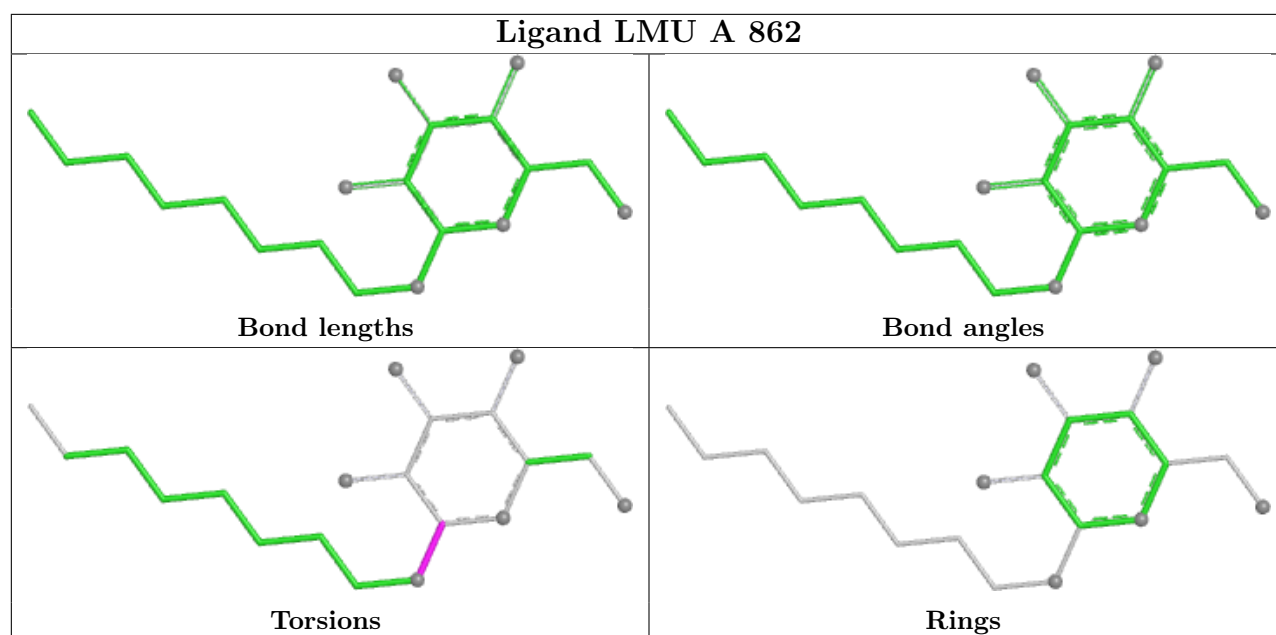


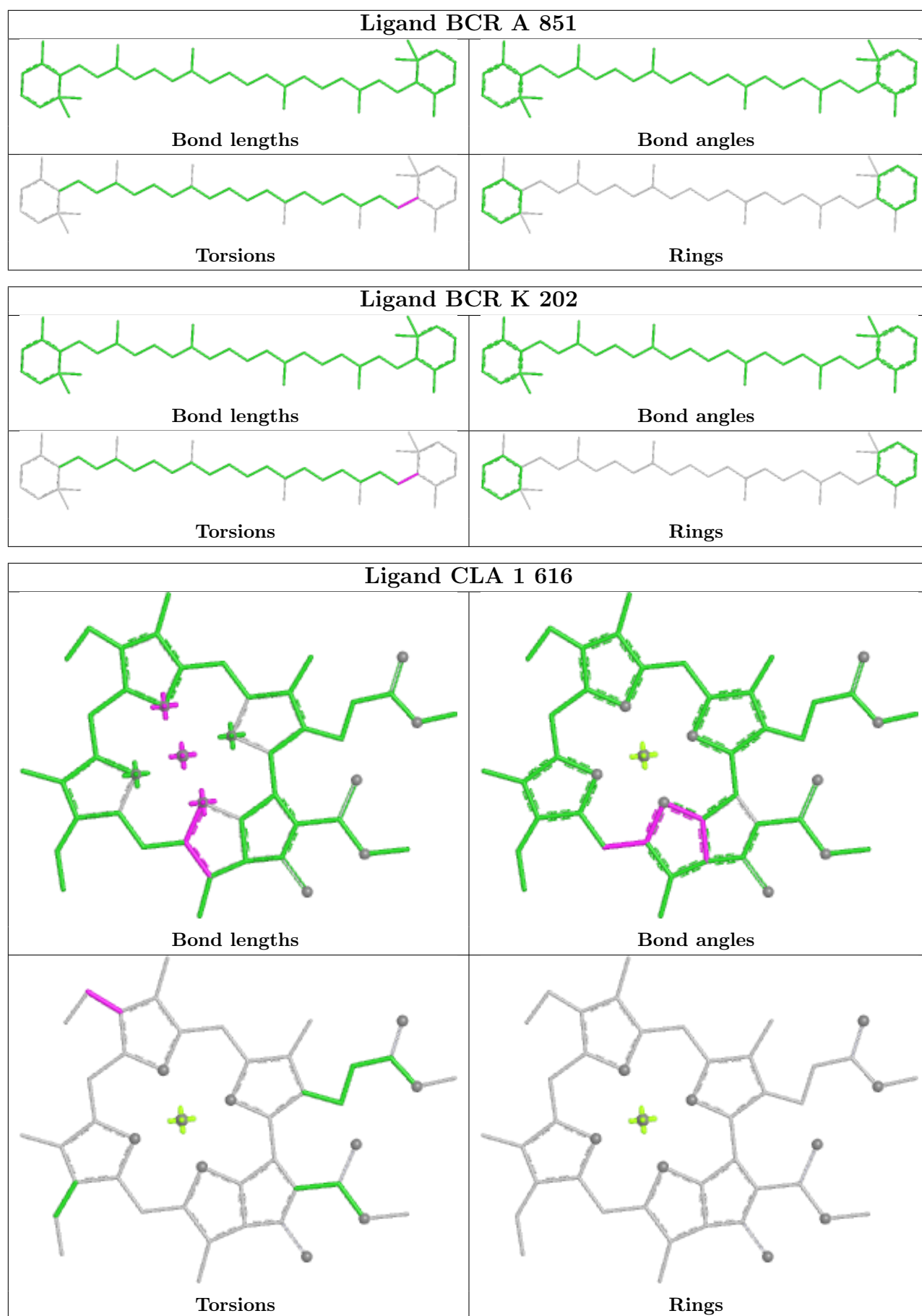
Torsions

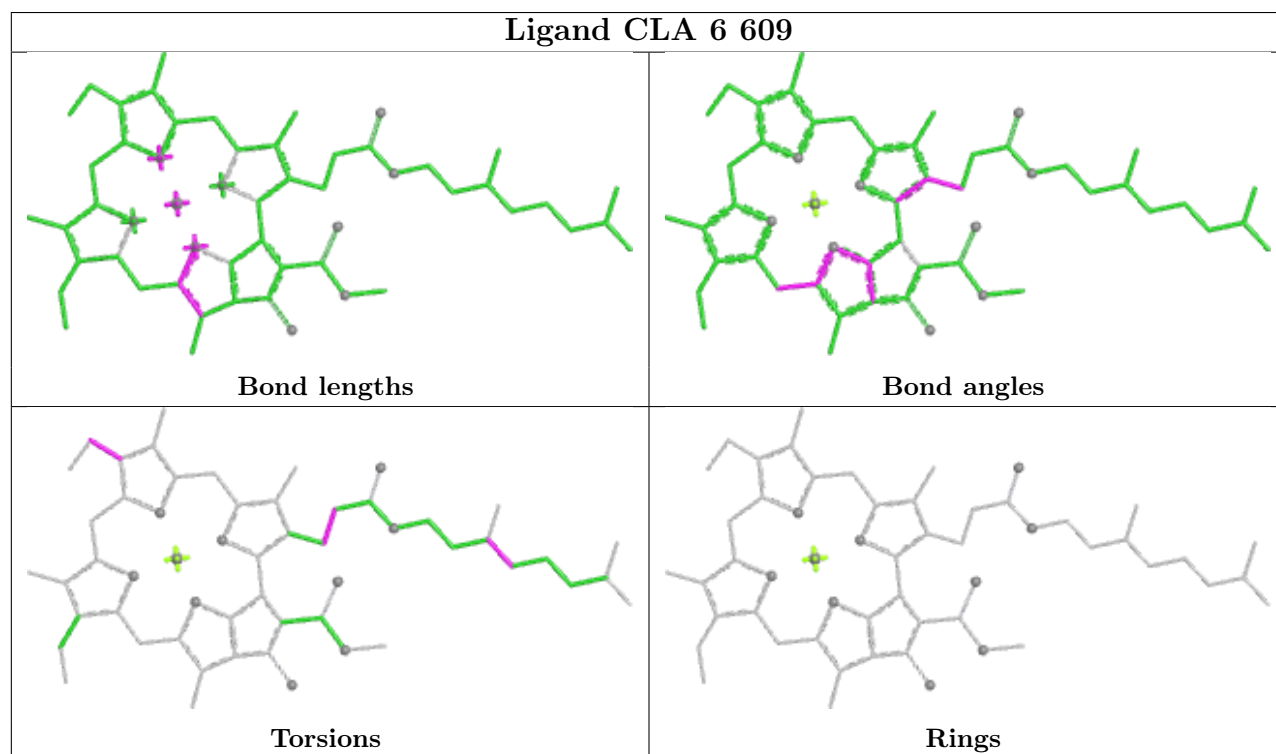
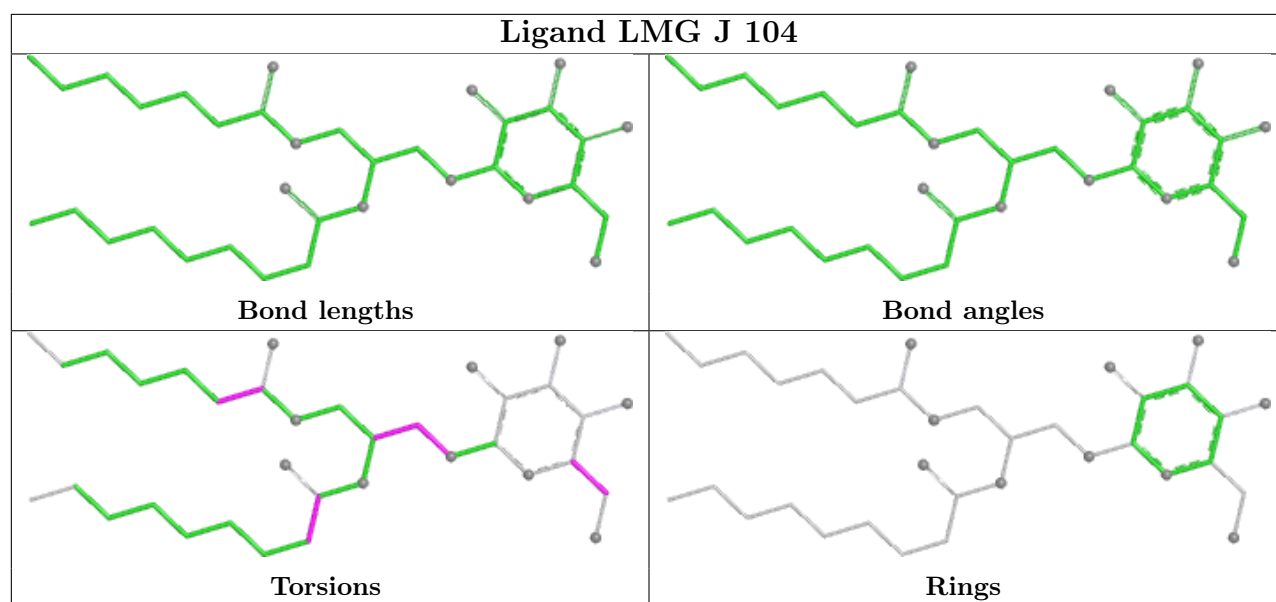


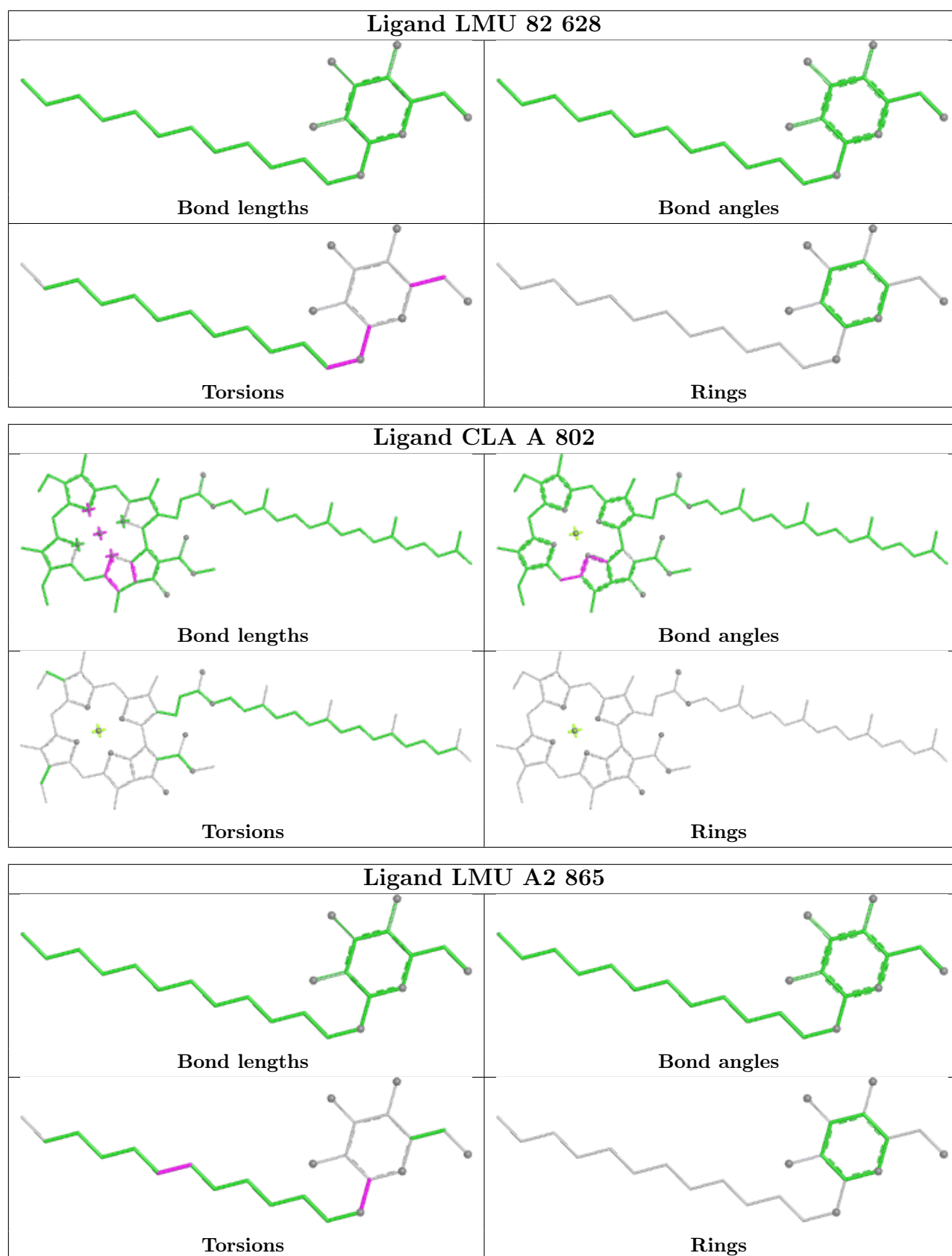
Rings

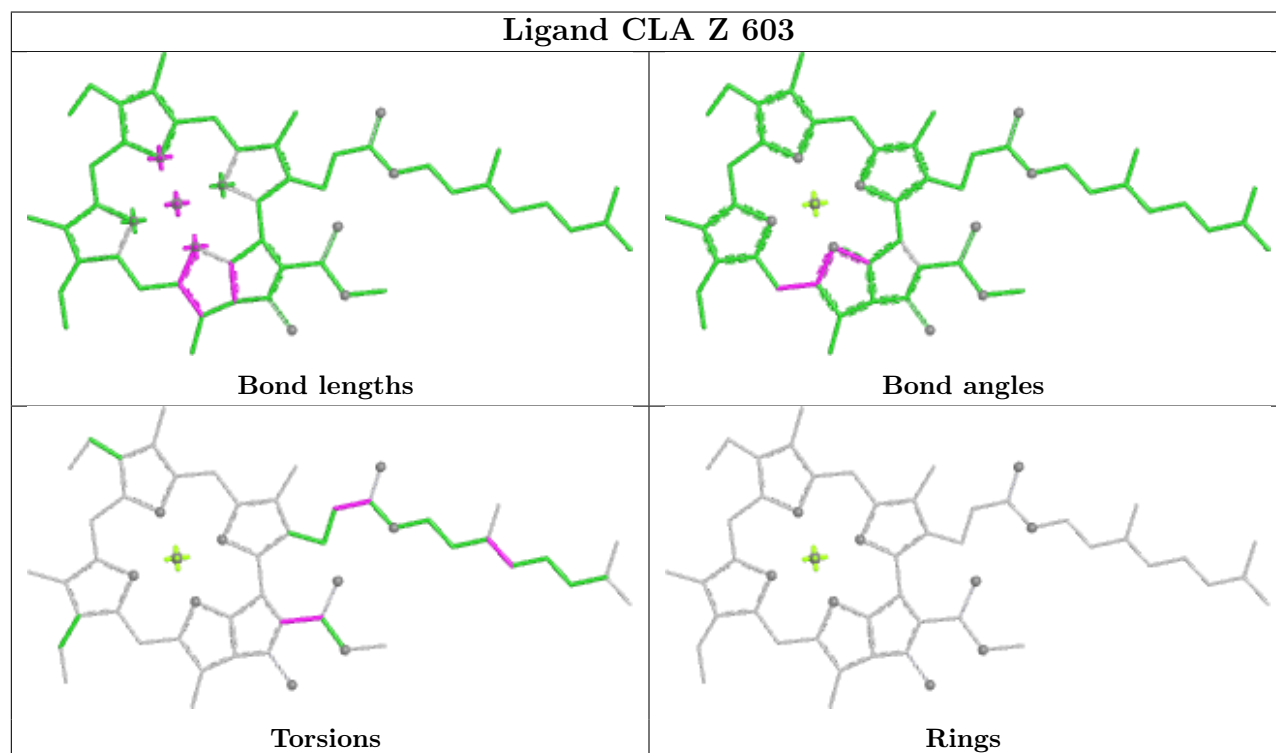
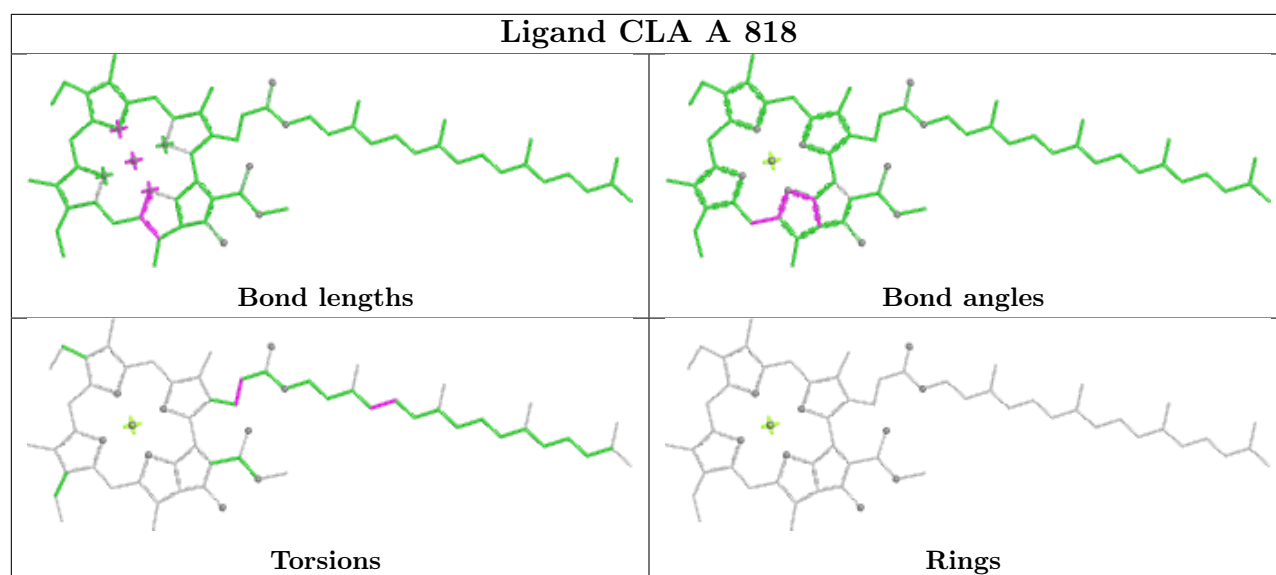


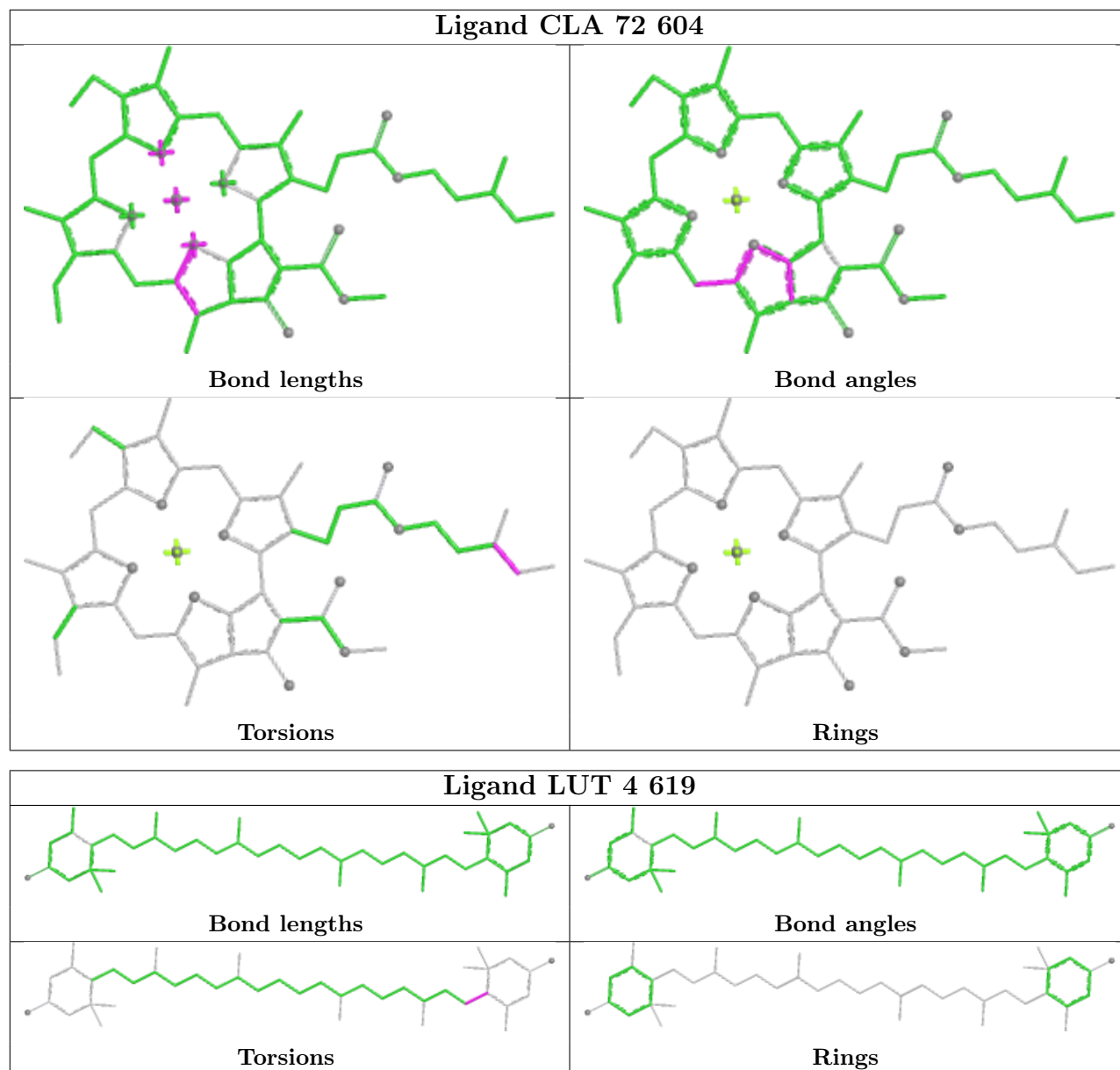


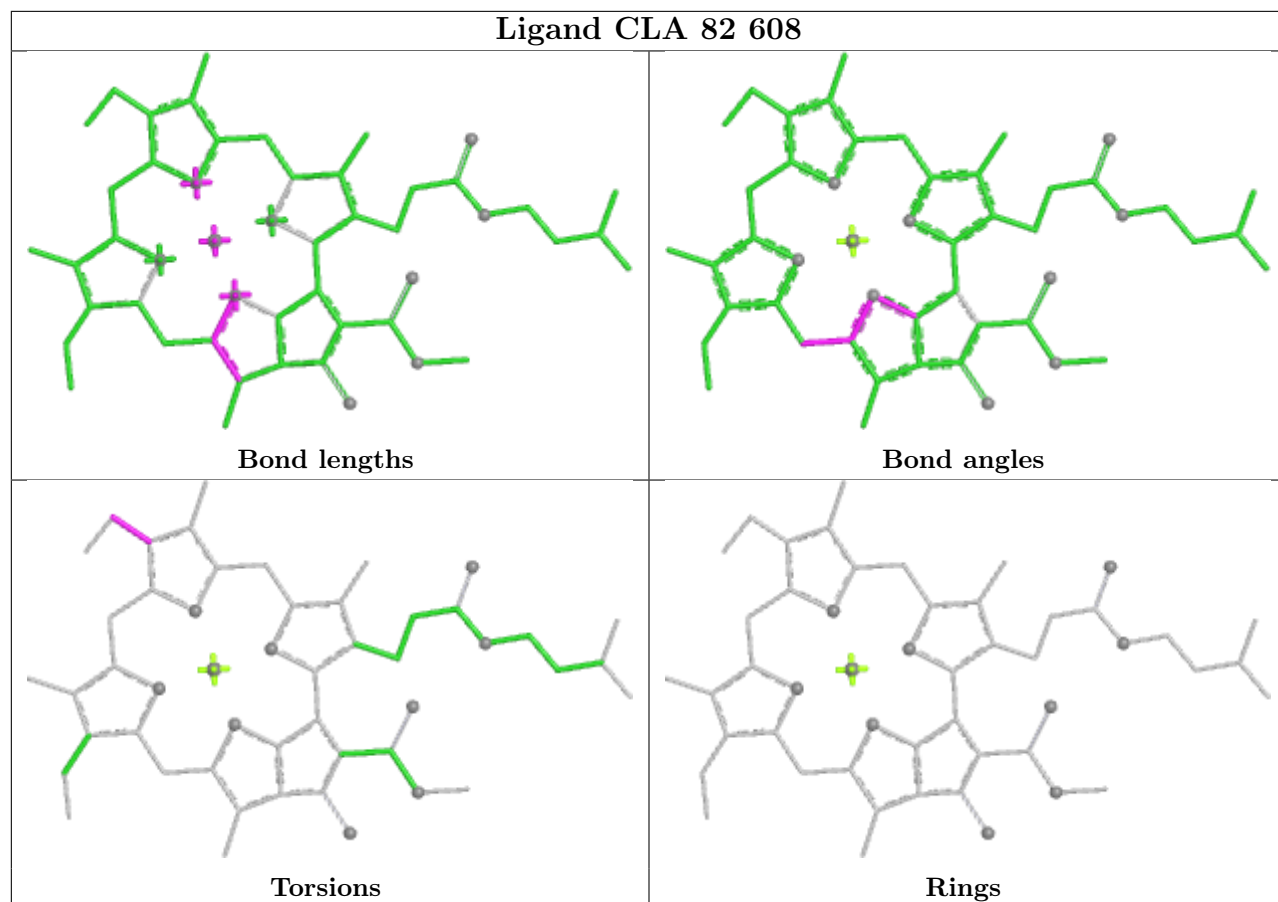


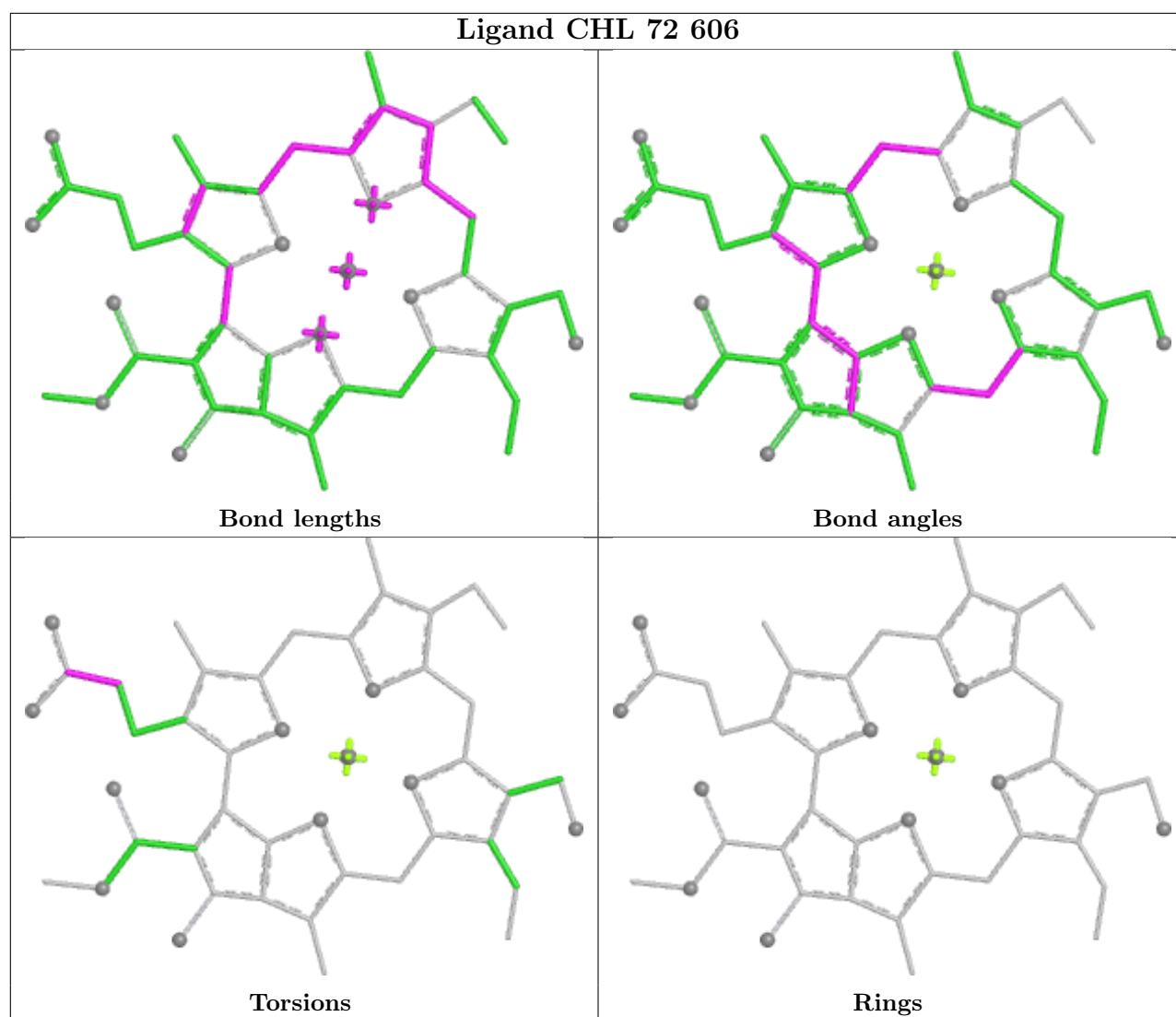




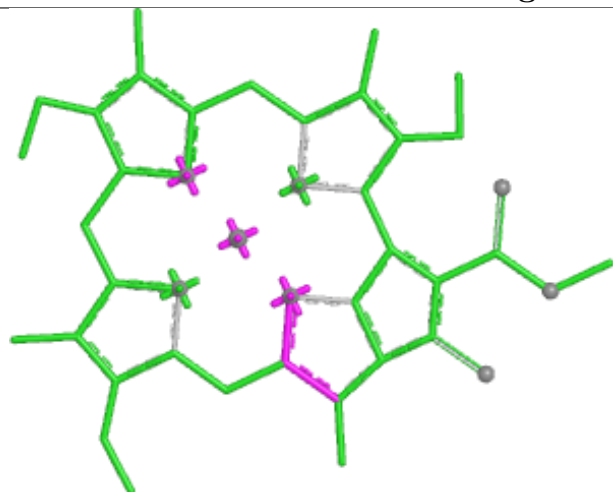








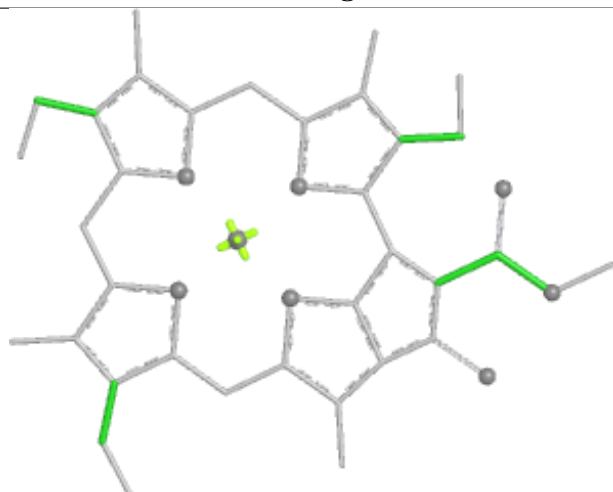
Ligand CLA 3 606



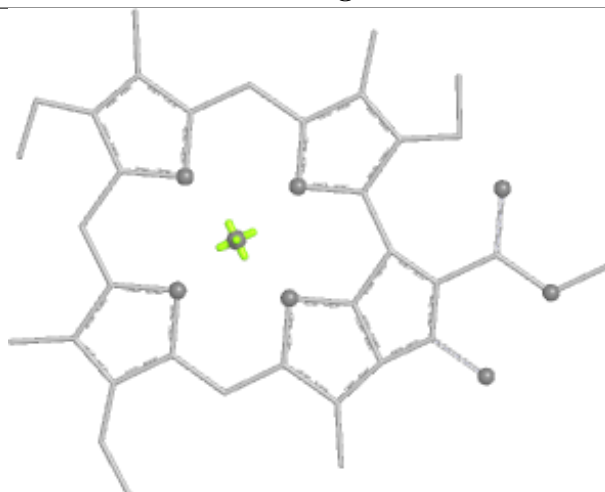
Bond lengths



Bond angles

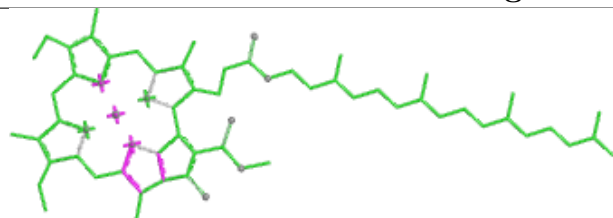


Torsions

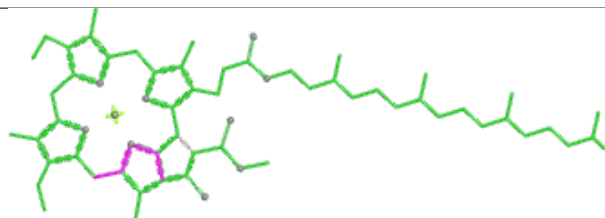


Rings

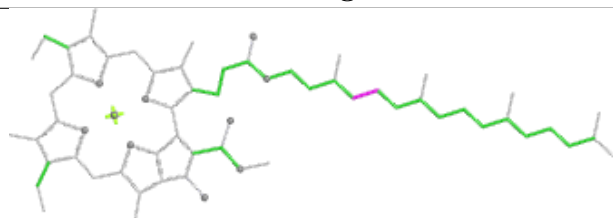
Ligand CLA A2 833



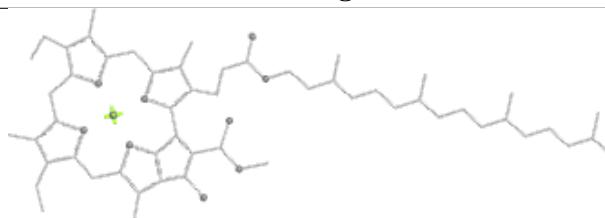
Bond lengths



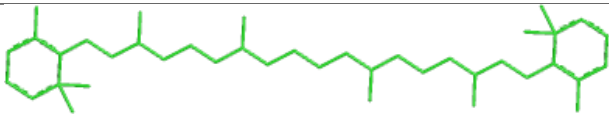
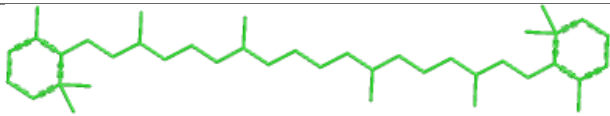
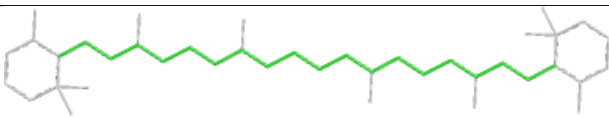
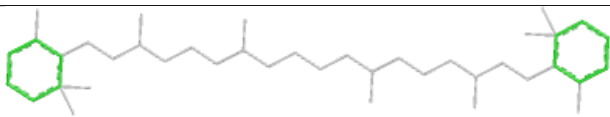
Bond angles

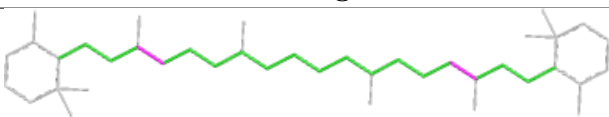
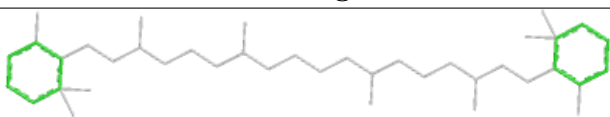


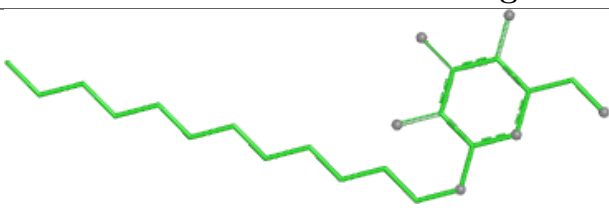
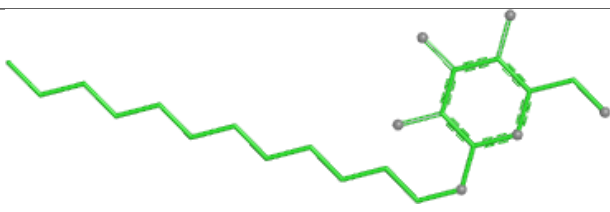
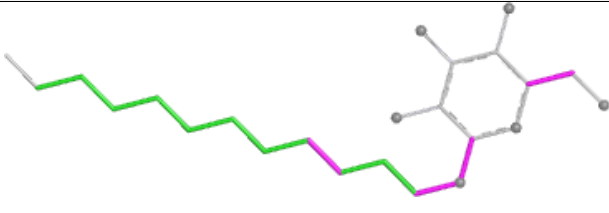
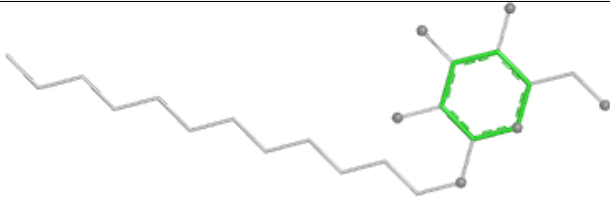
Torsions

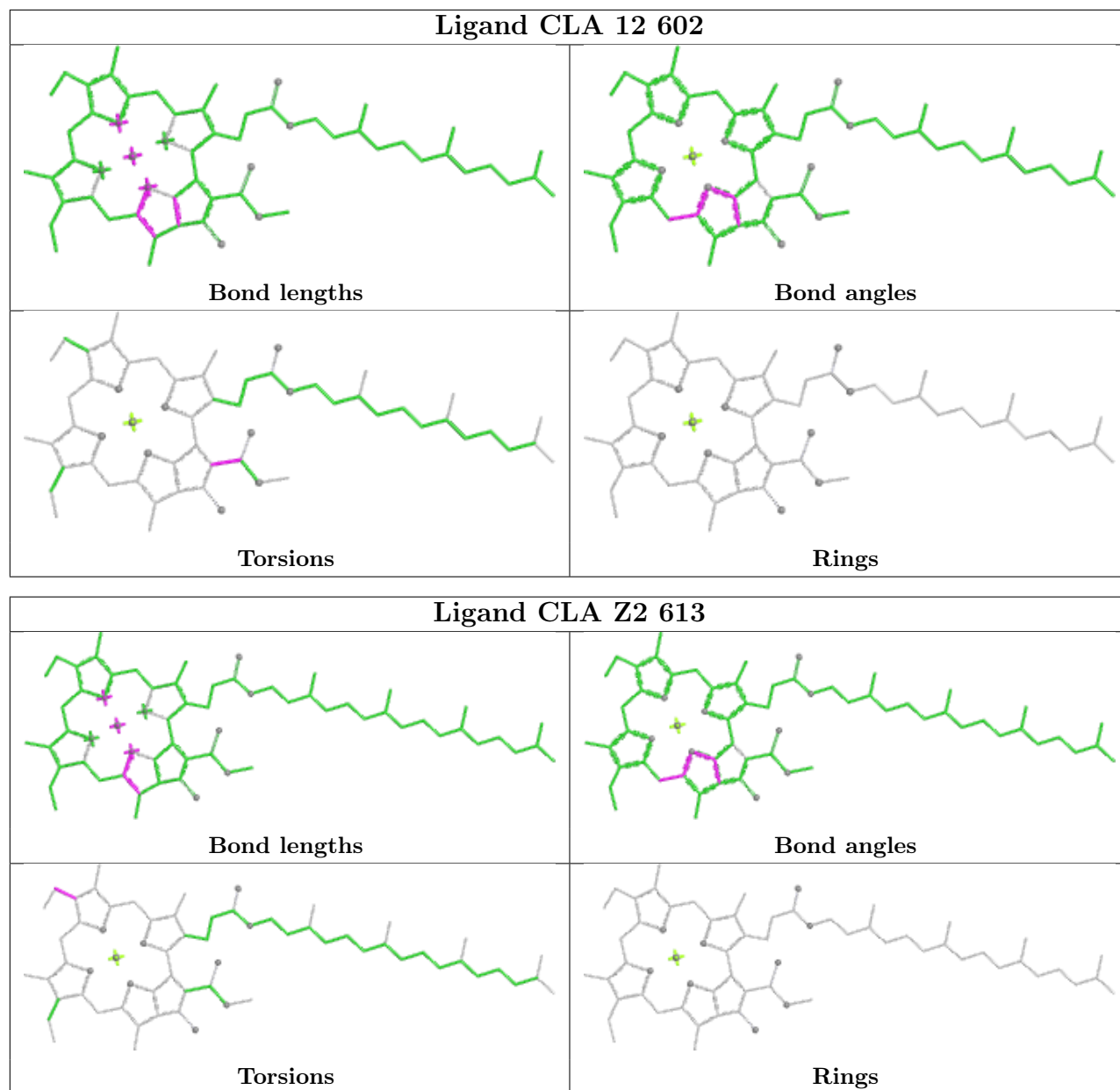


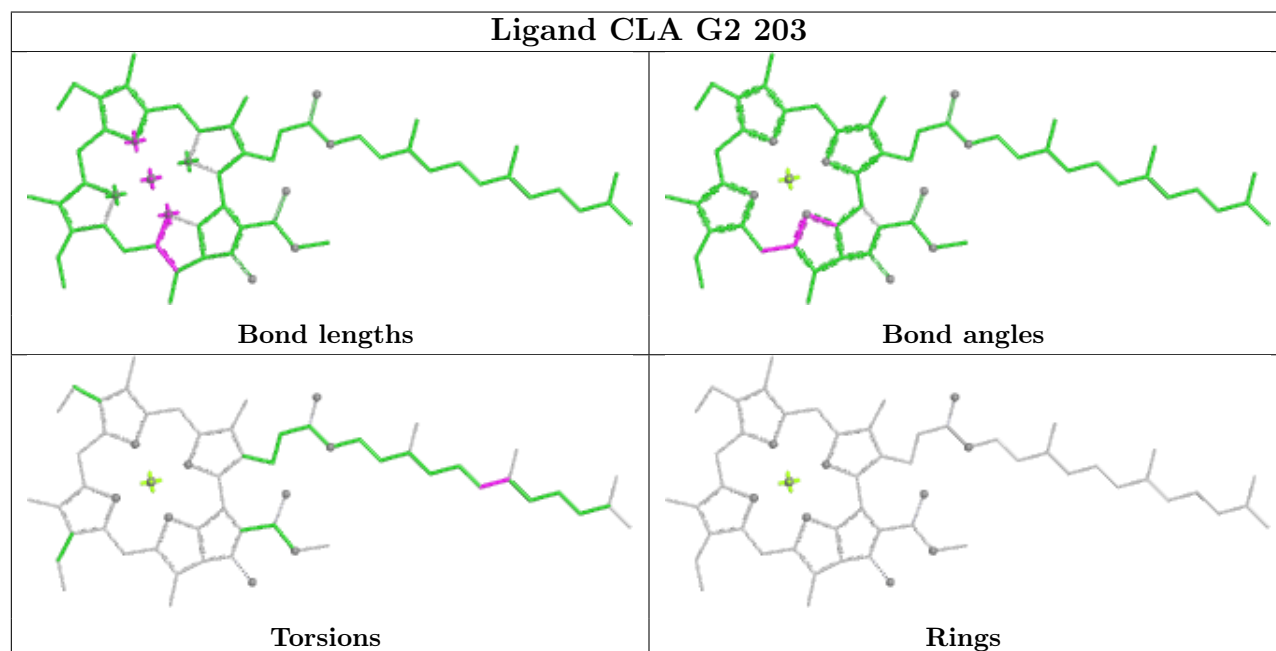
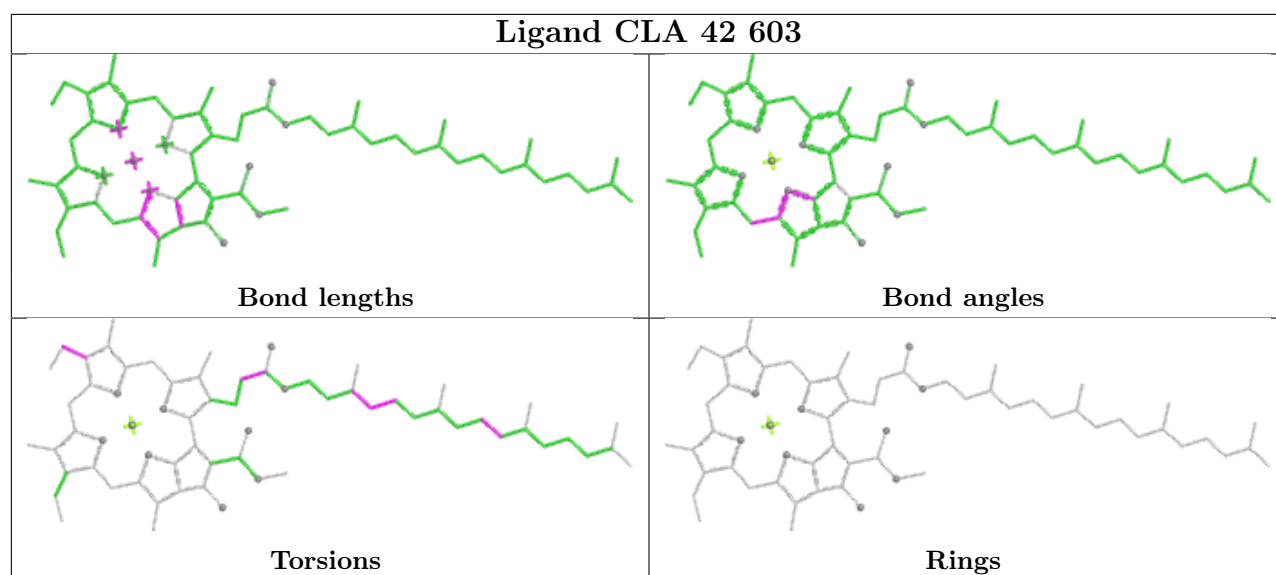
Rings

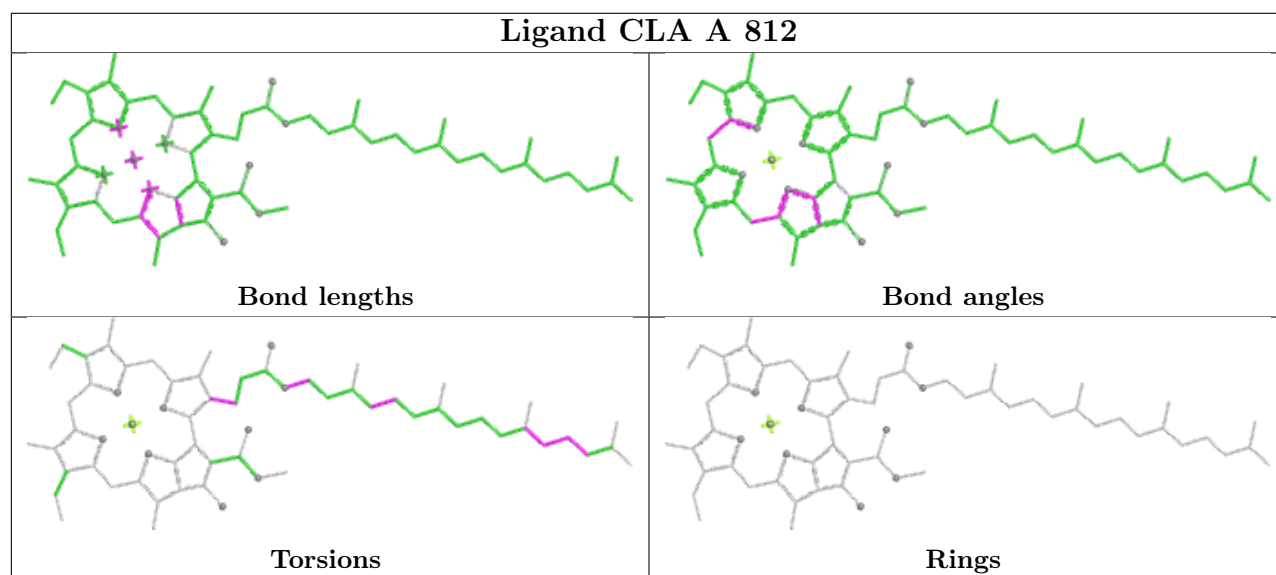
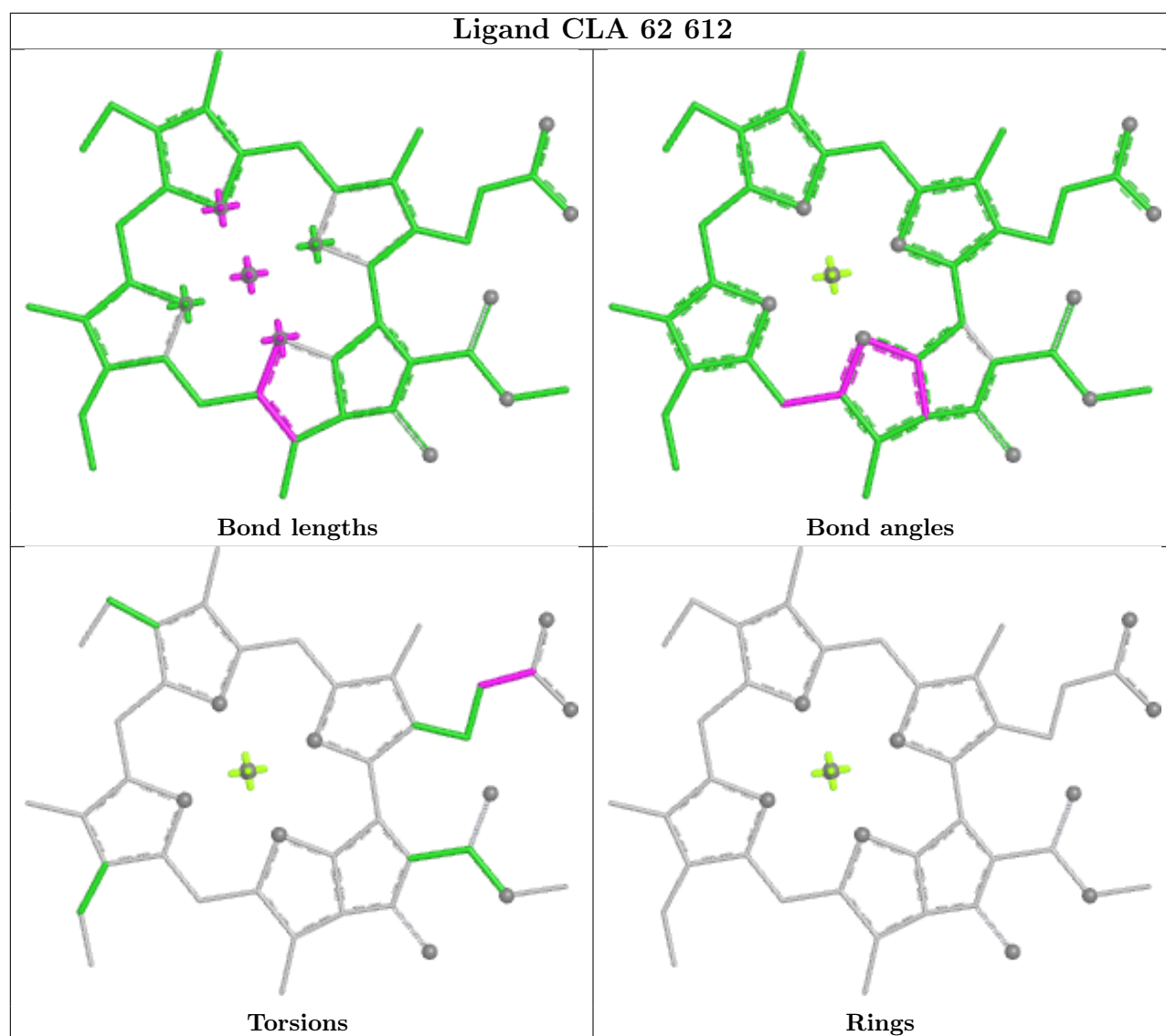
Ligand BCR B 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

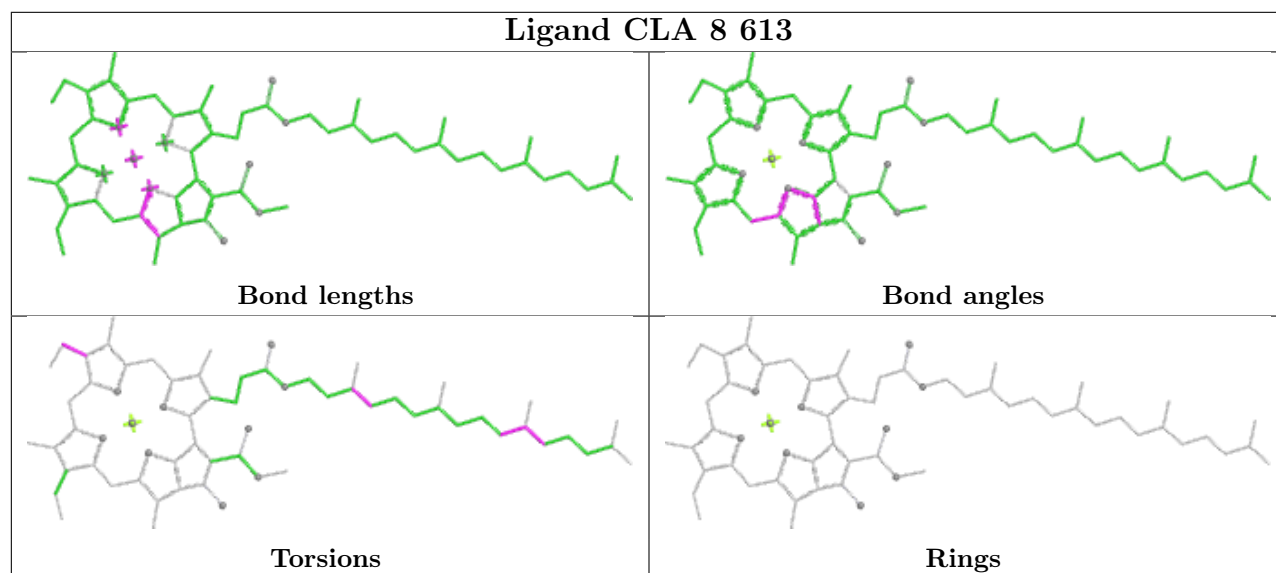
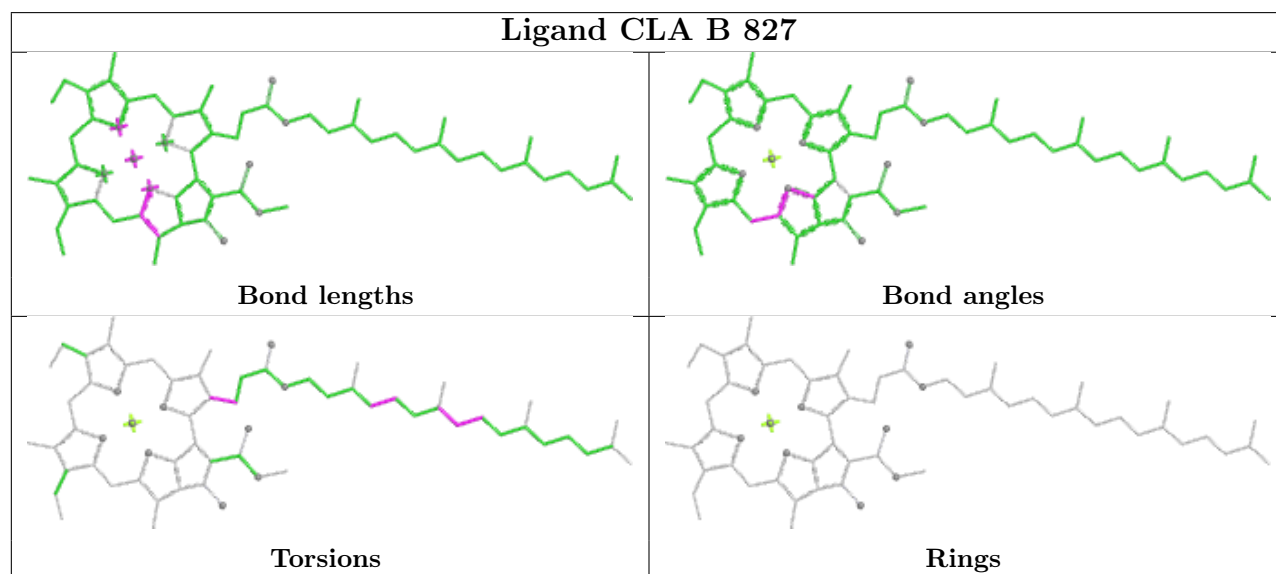
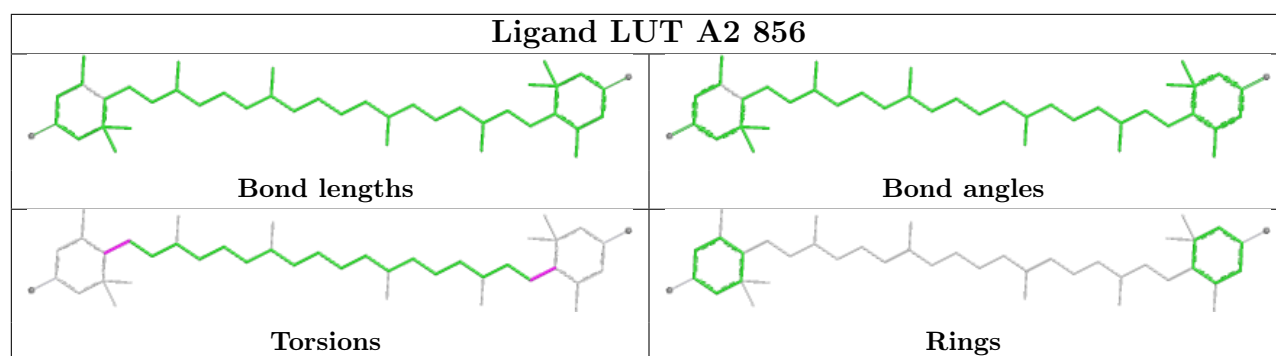
Ligand BCR B2 845	
	
Bond lengths	Bond angles
	
Torsions	Rings

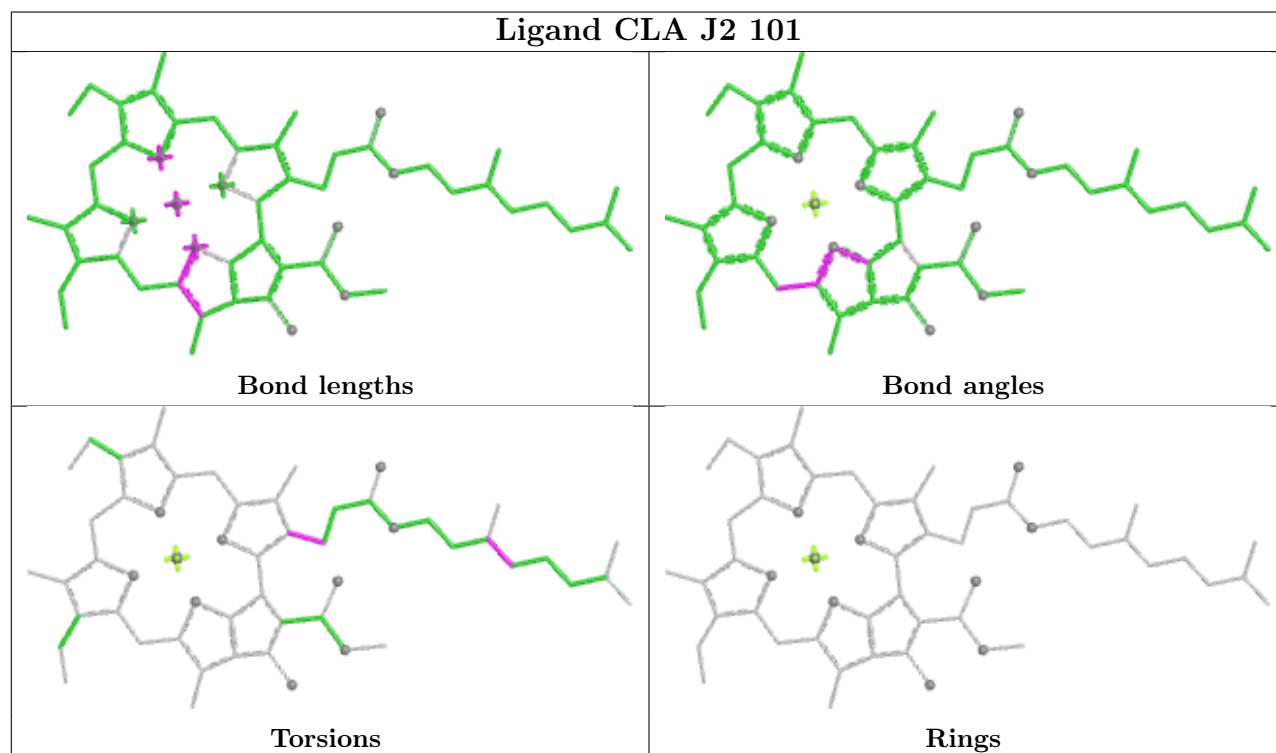
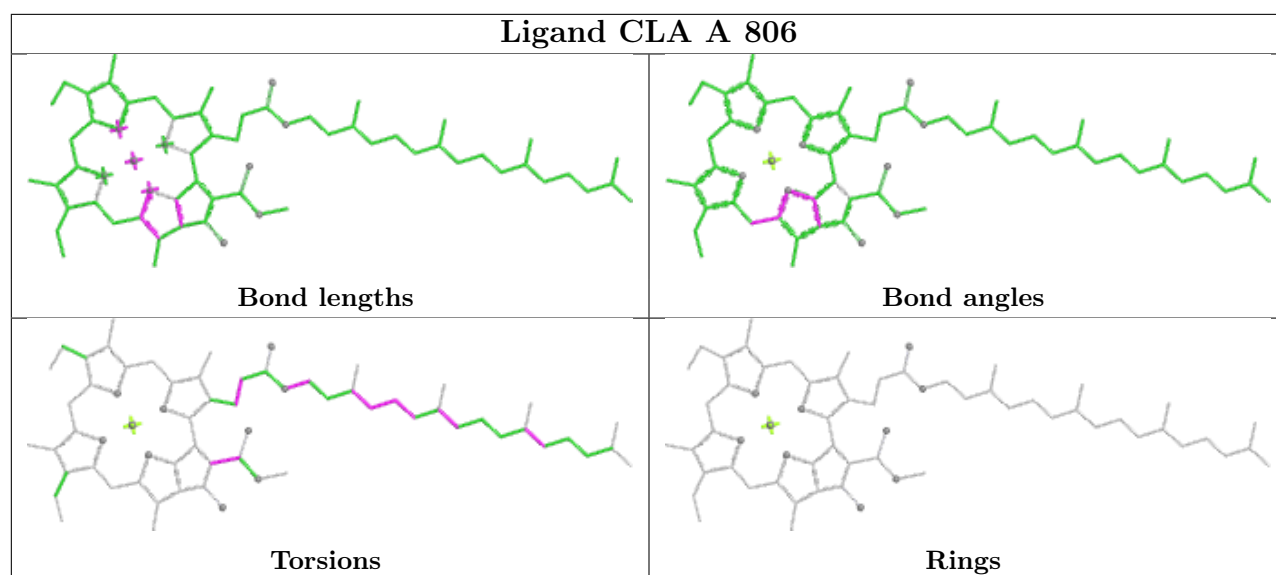
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Bond lengths	Bond angles
	
Torsions	Rings

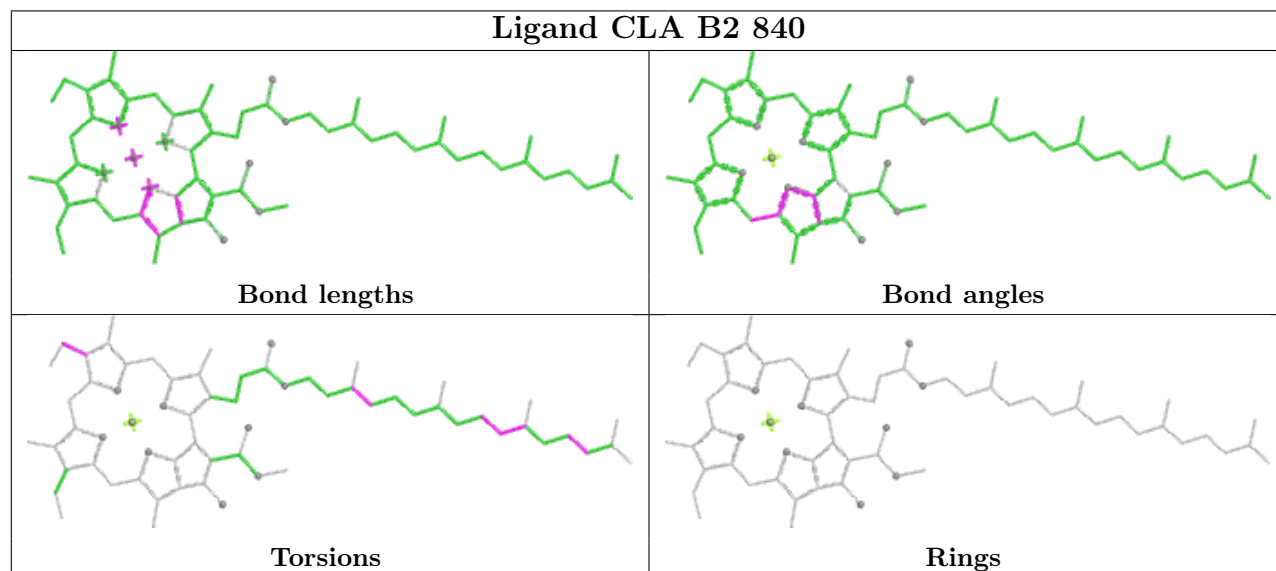
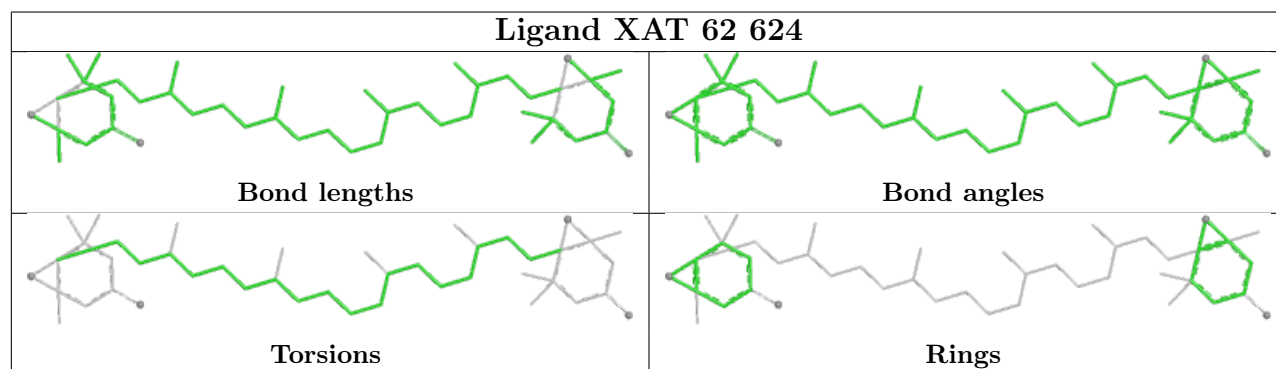
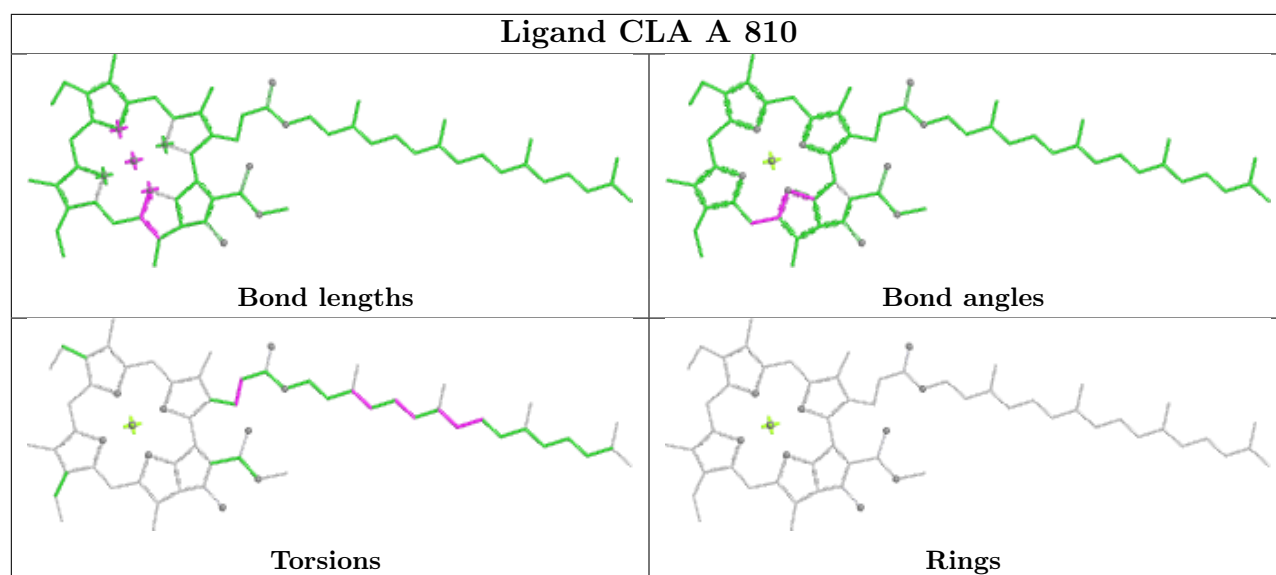


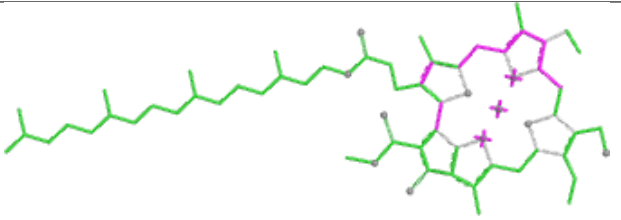
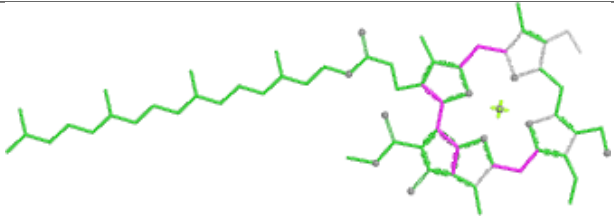
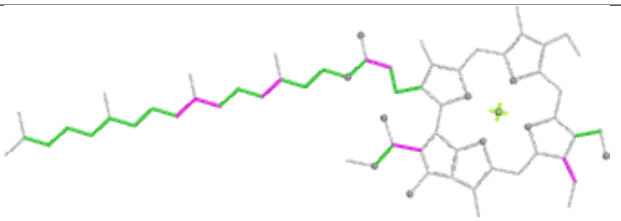
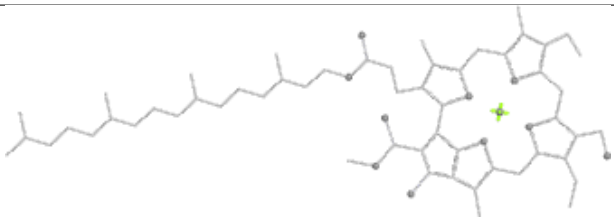


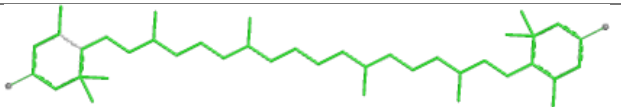
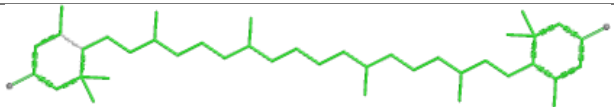
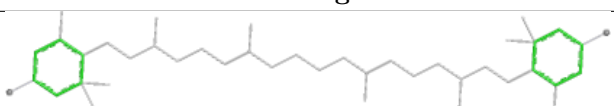


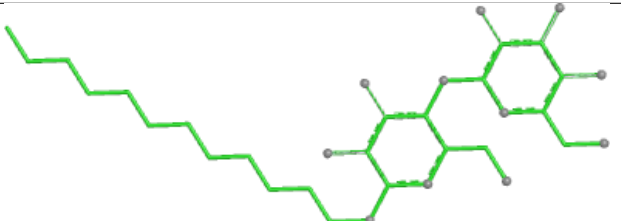
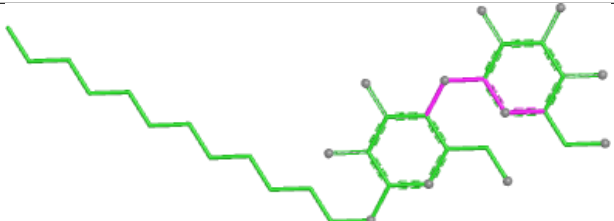
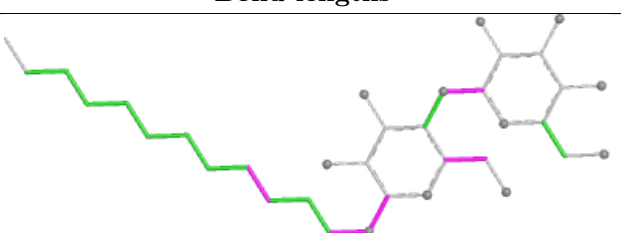
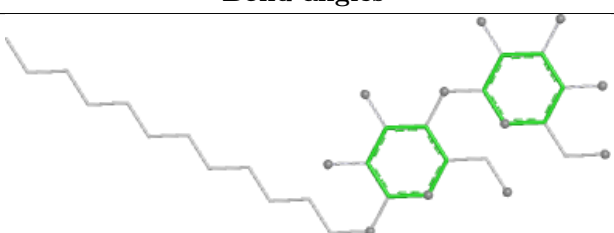


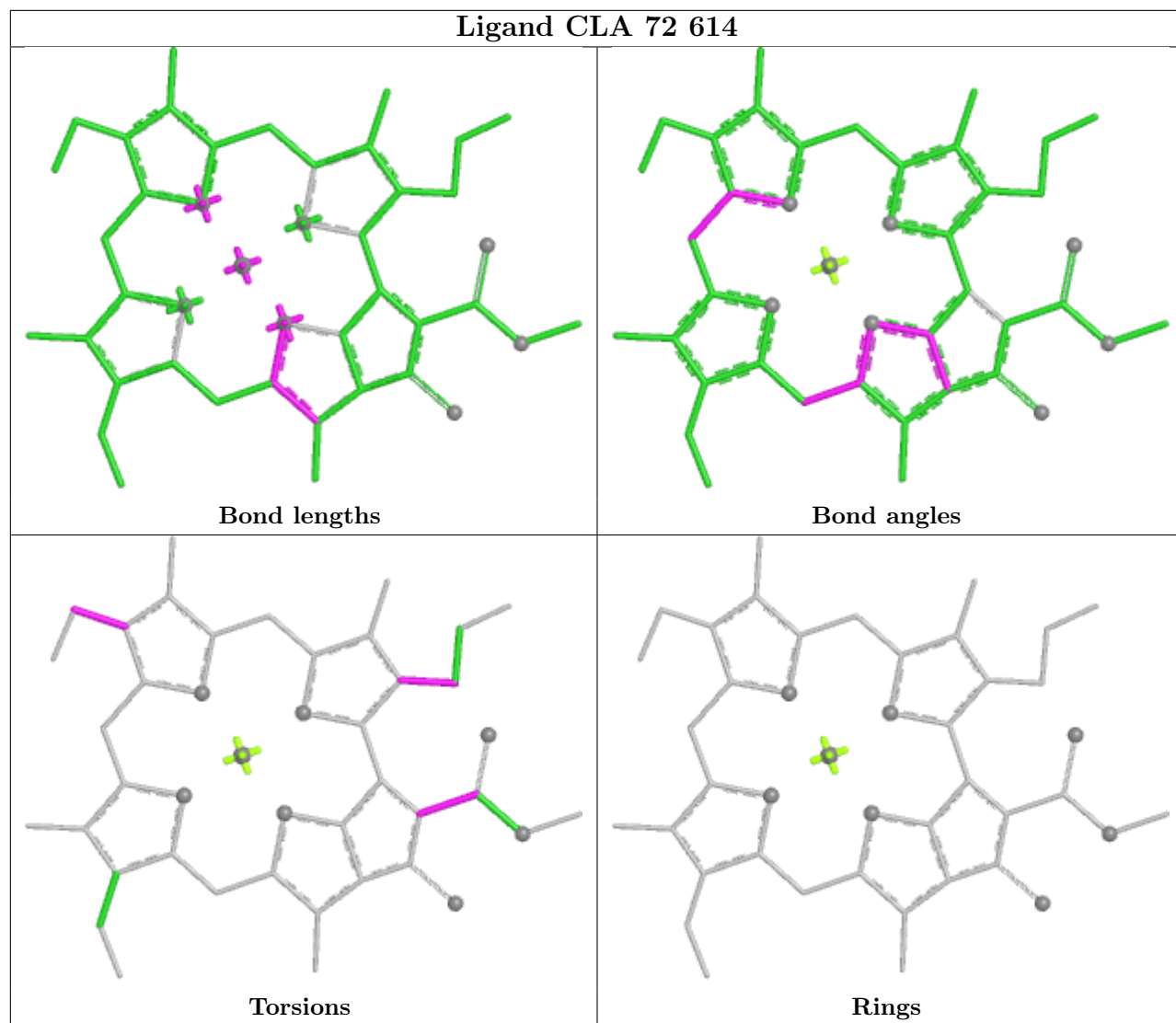




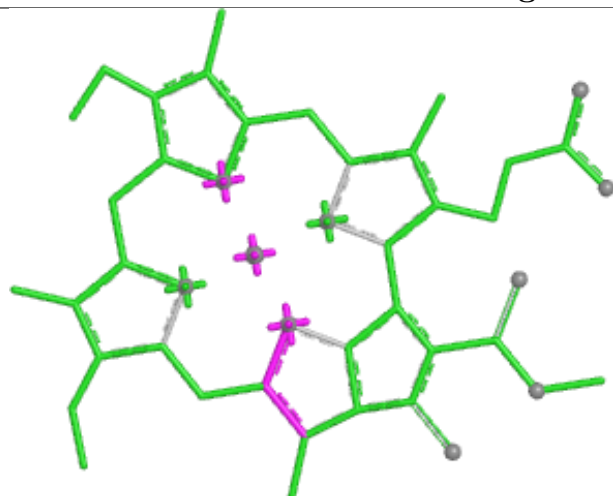
Ligand CHL 52 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 12 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

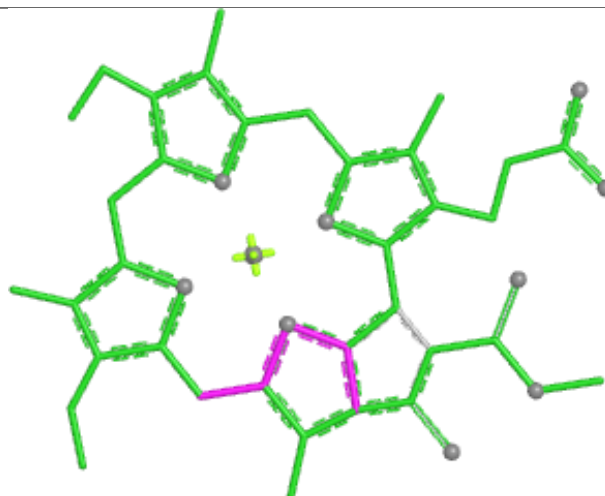
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Bond lengths	Bond angles
	
Torsions	Rings



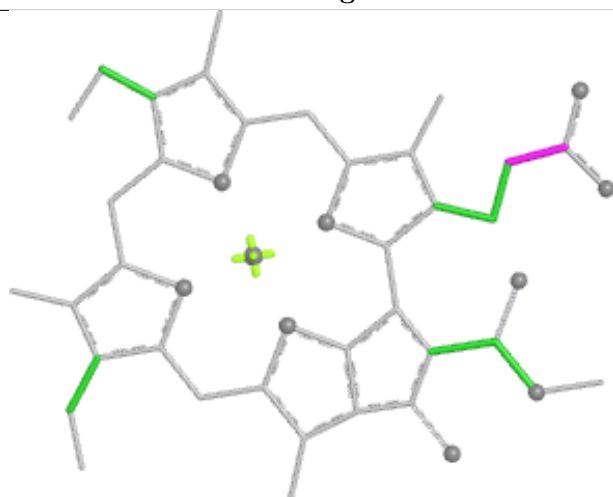
Ligand CLA 6 612



Bond lengths



Bond angles

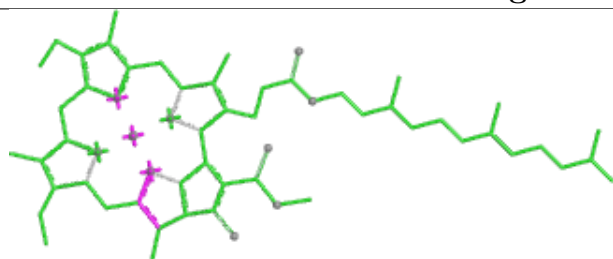


Torsions

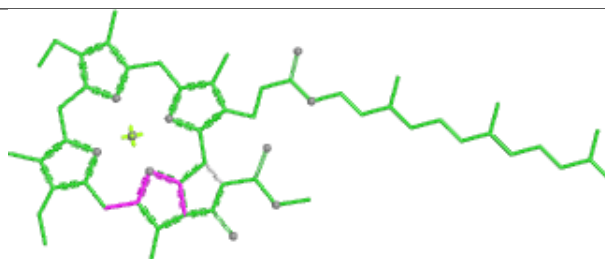


Rings

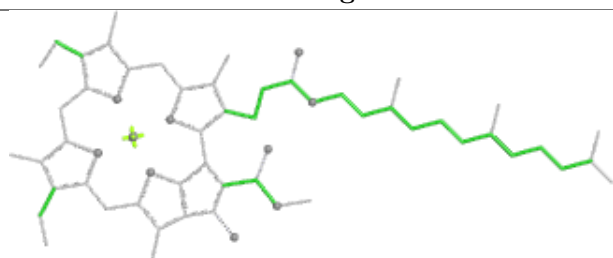
Ligand CLA 62 610



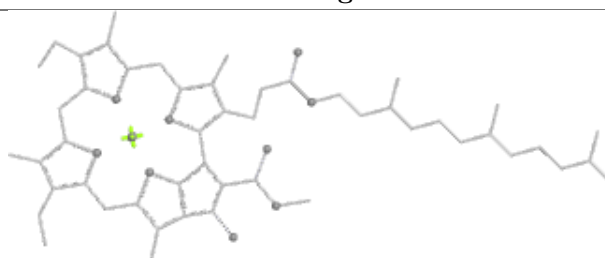
Bond lengths



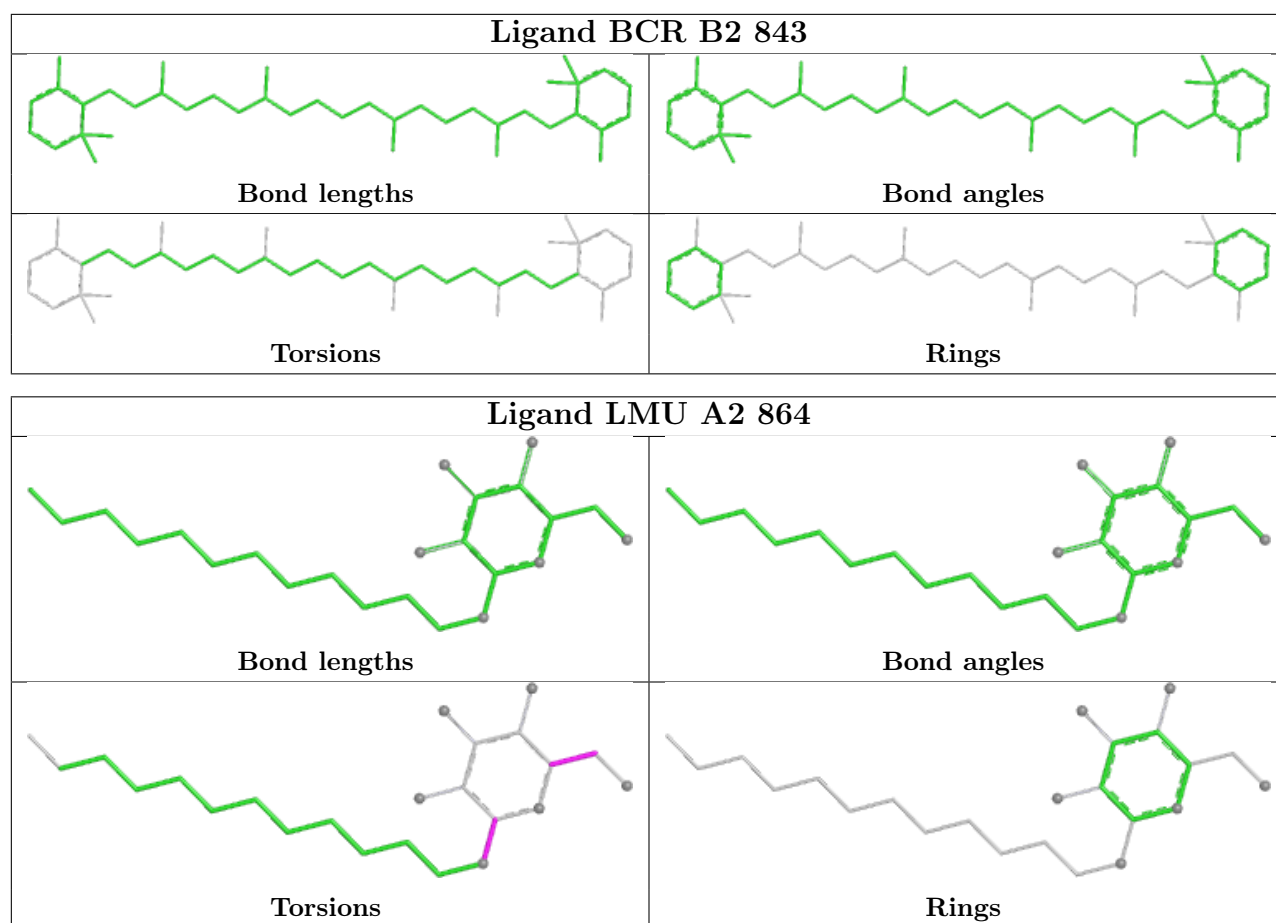
Bond angles

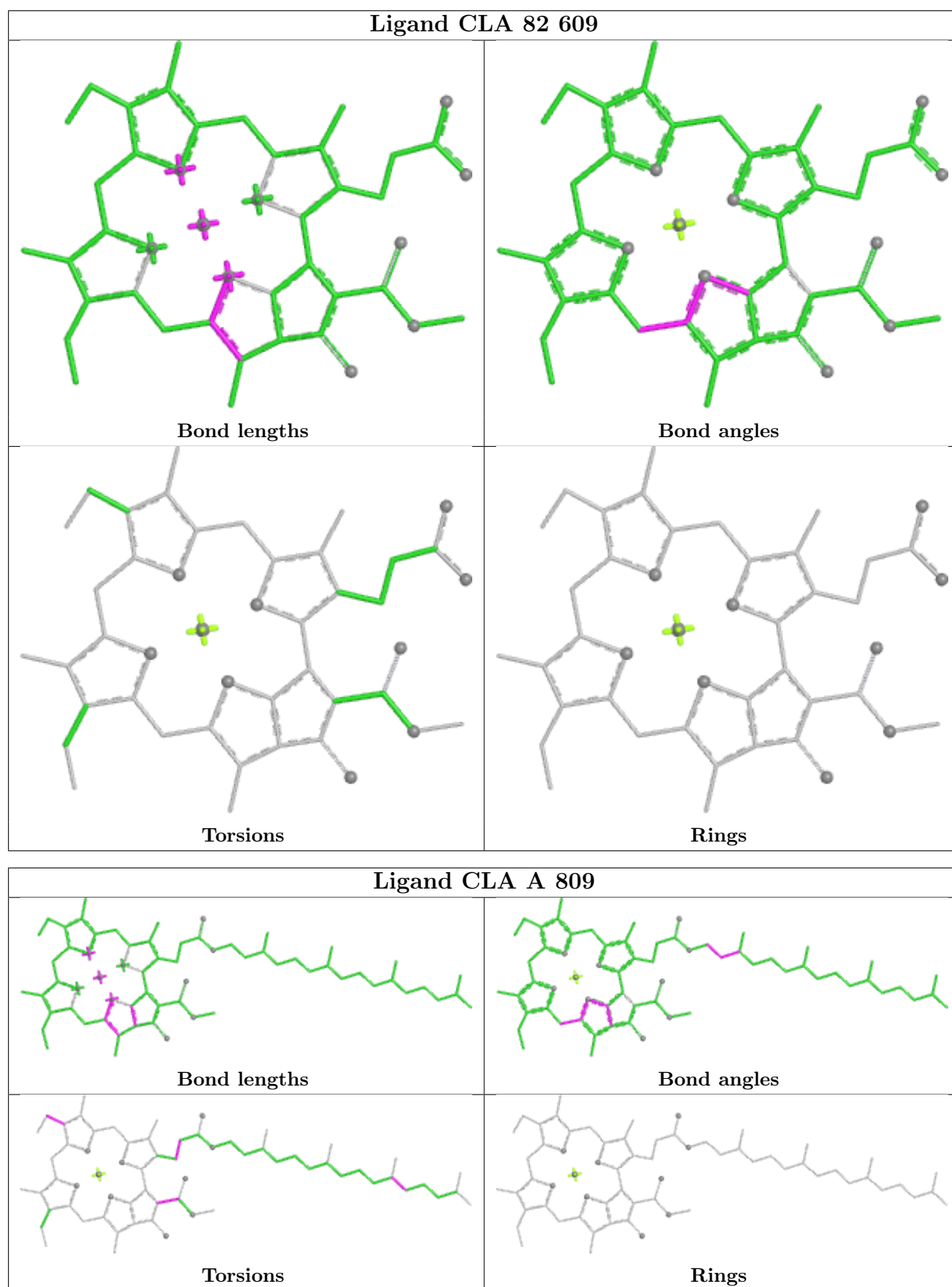


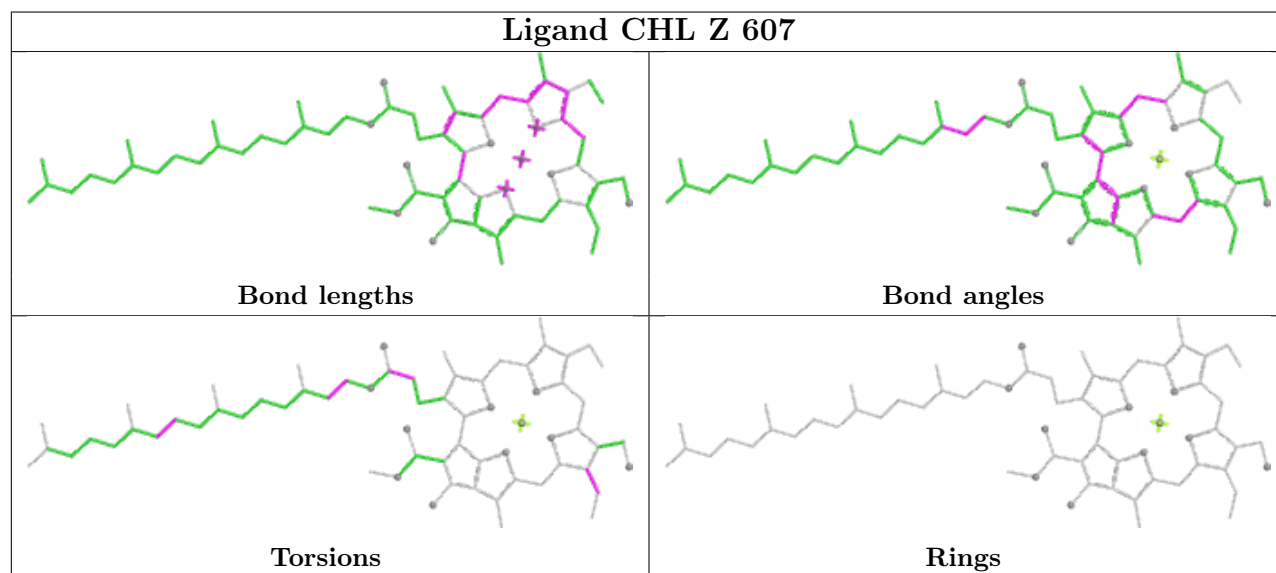
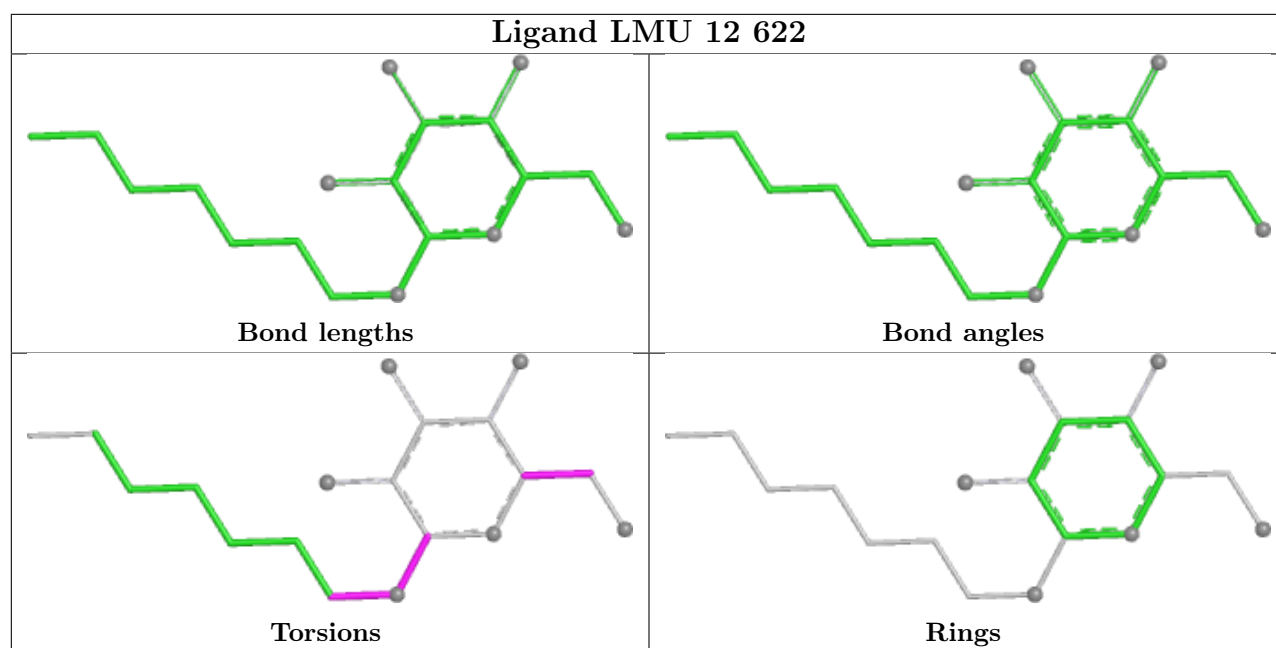
Torsions

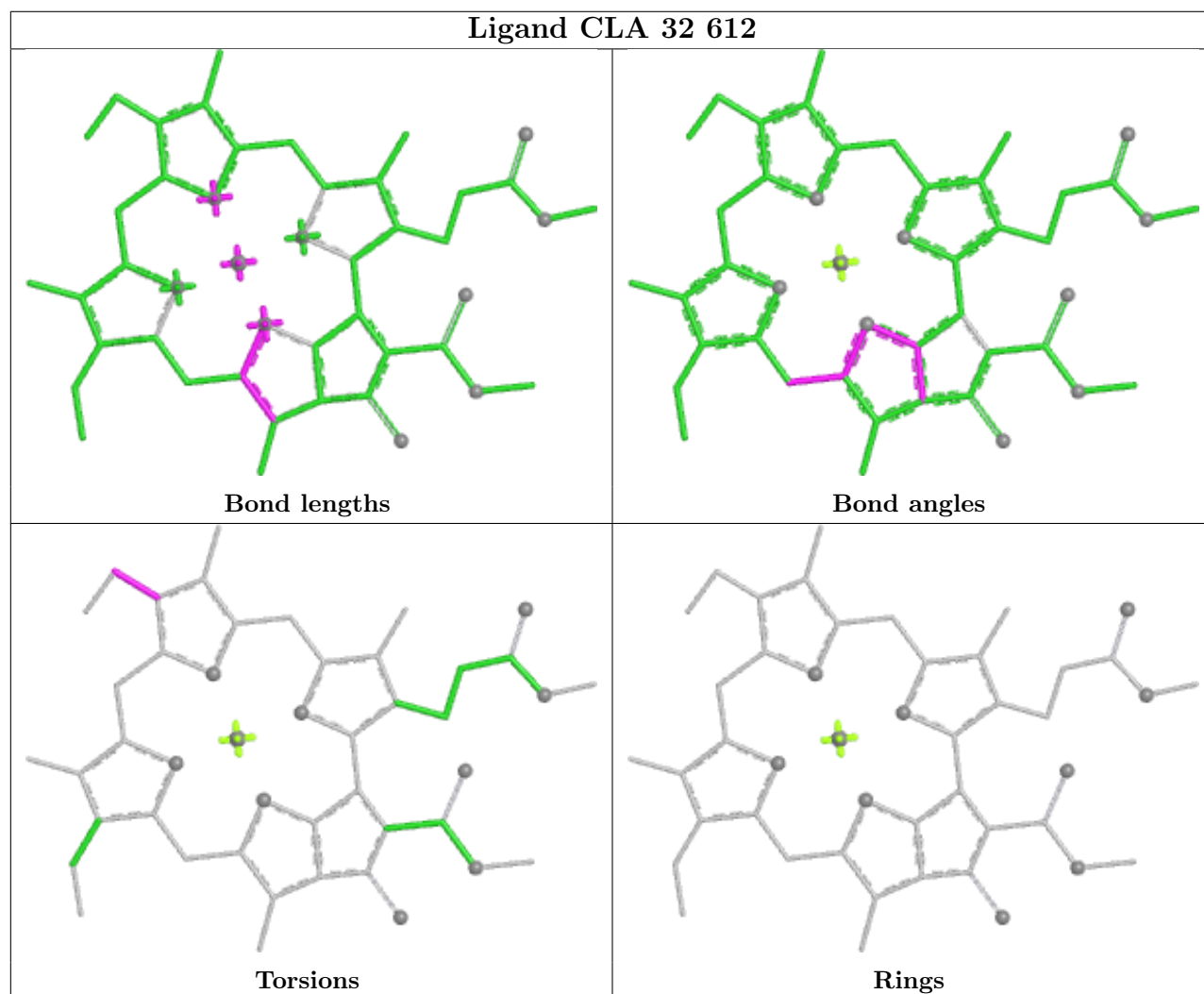
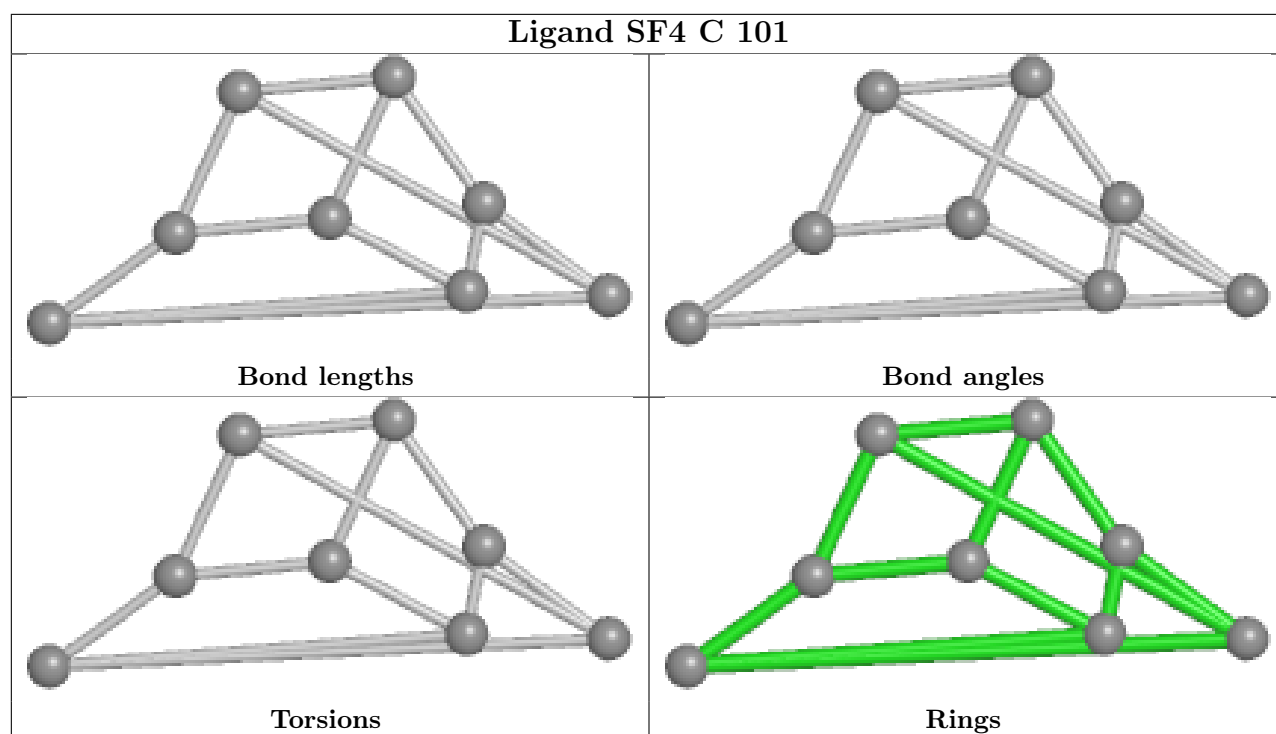


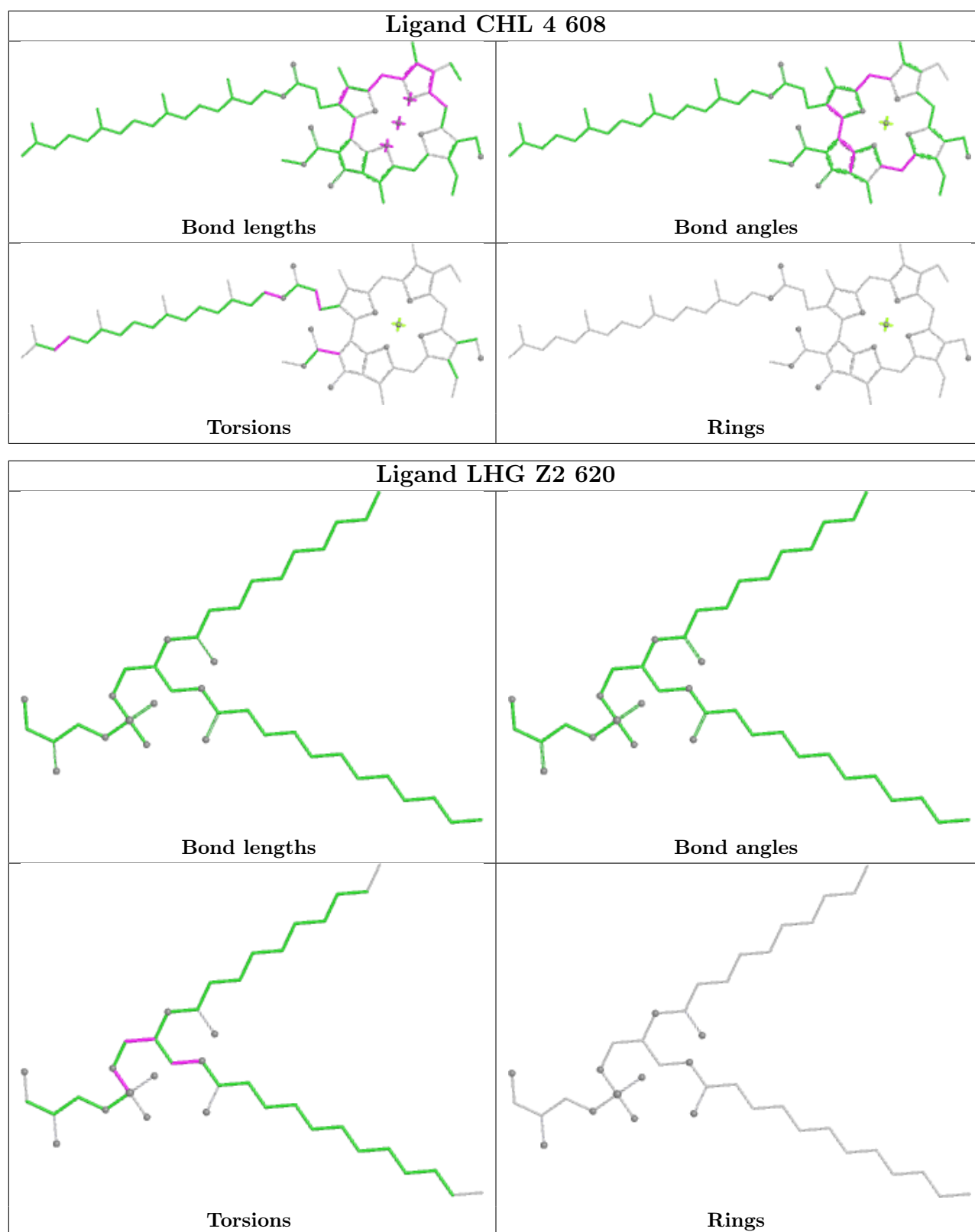
Rings

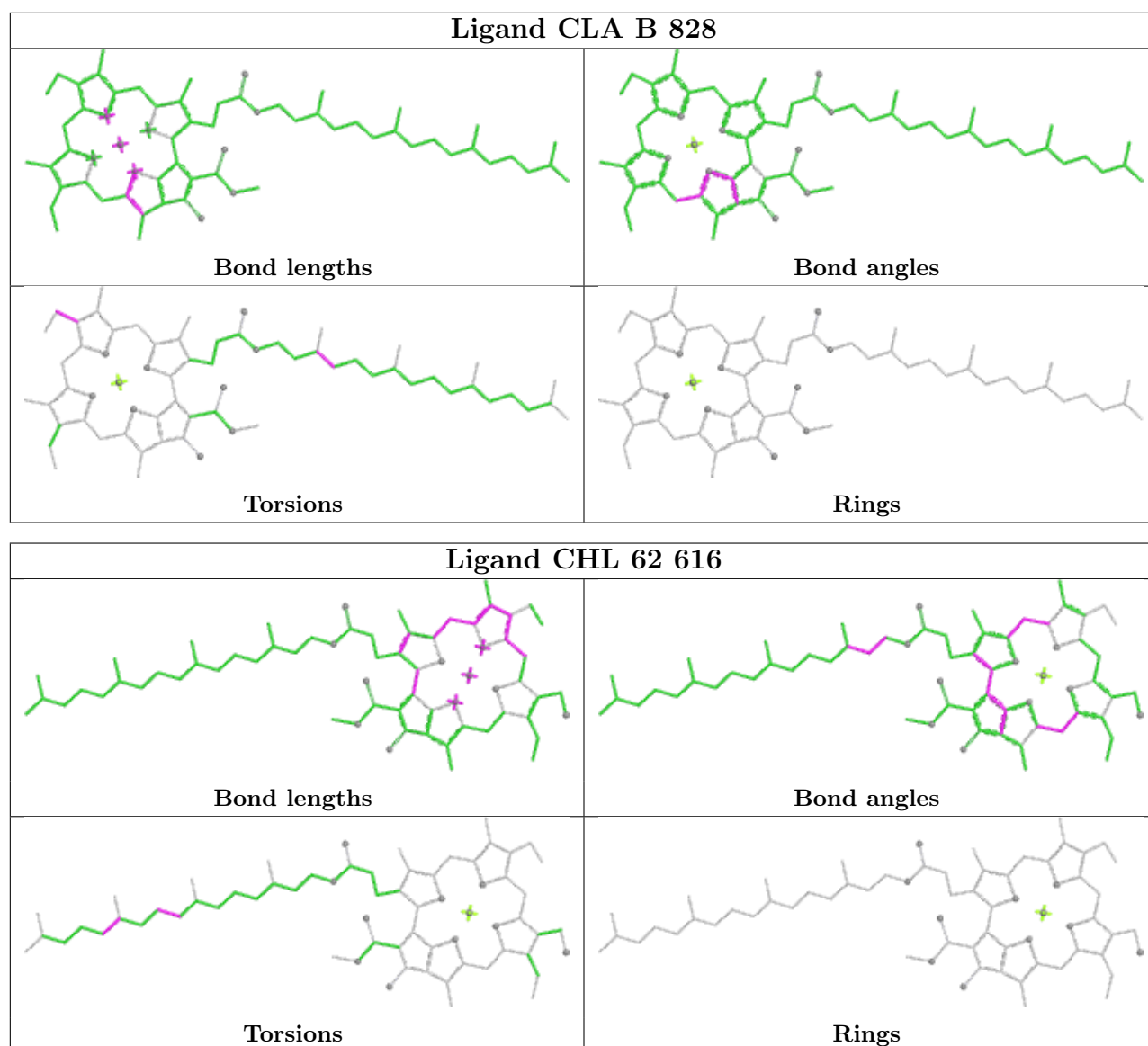


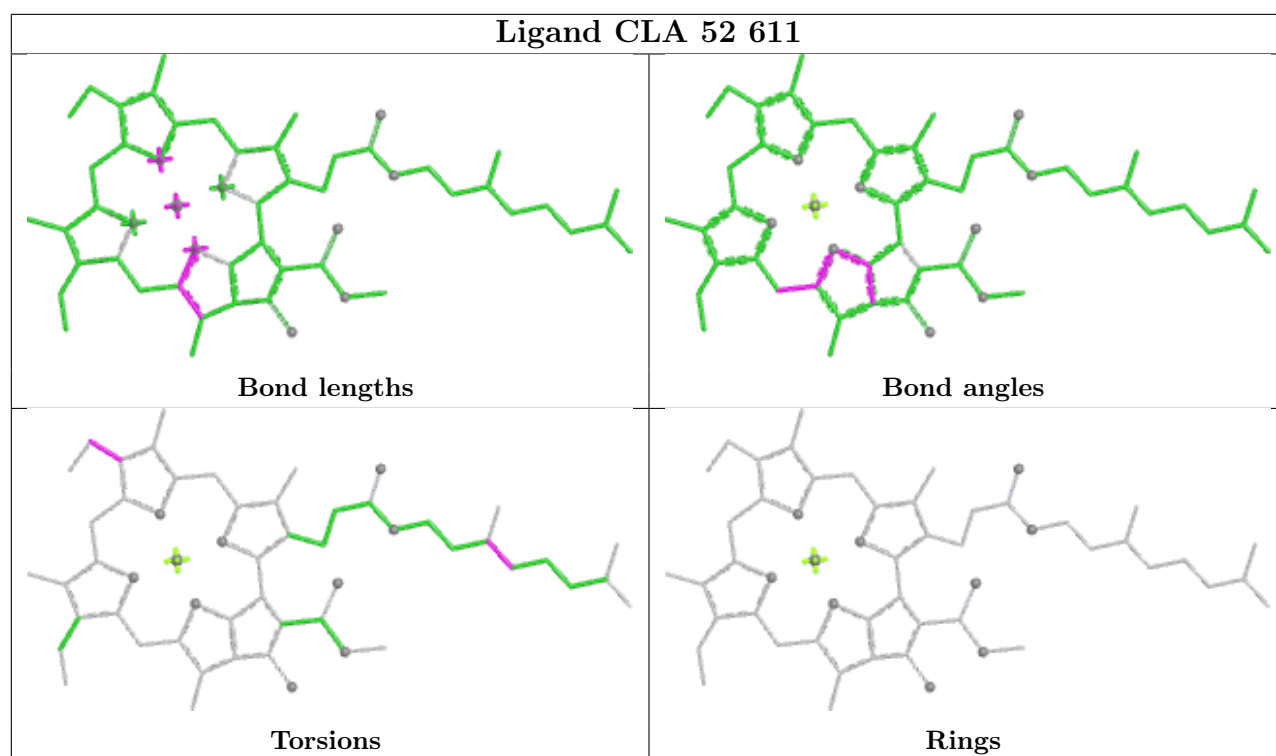


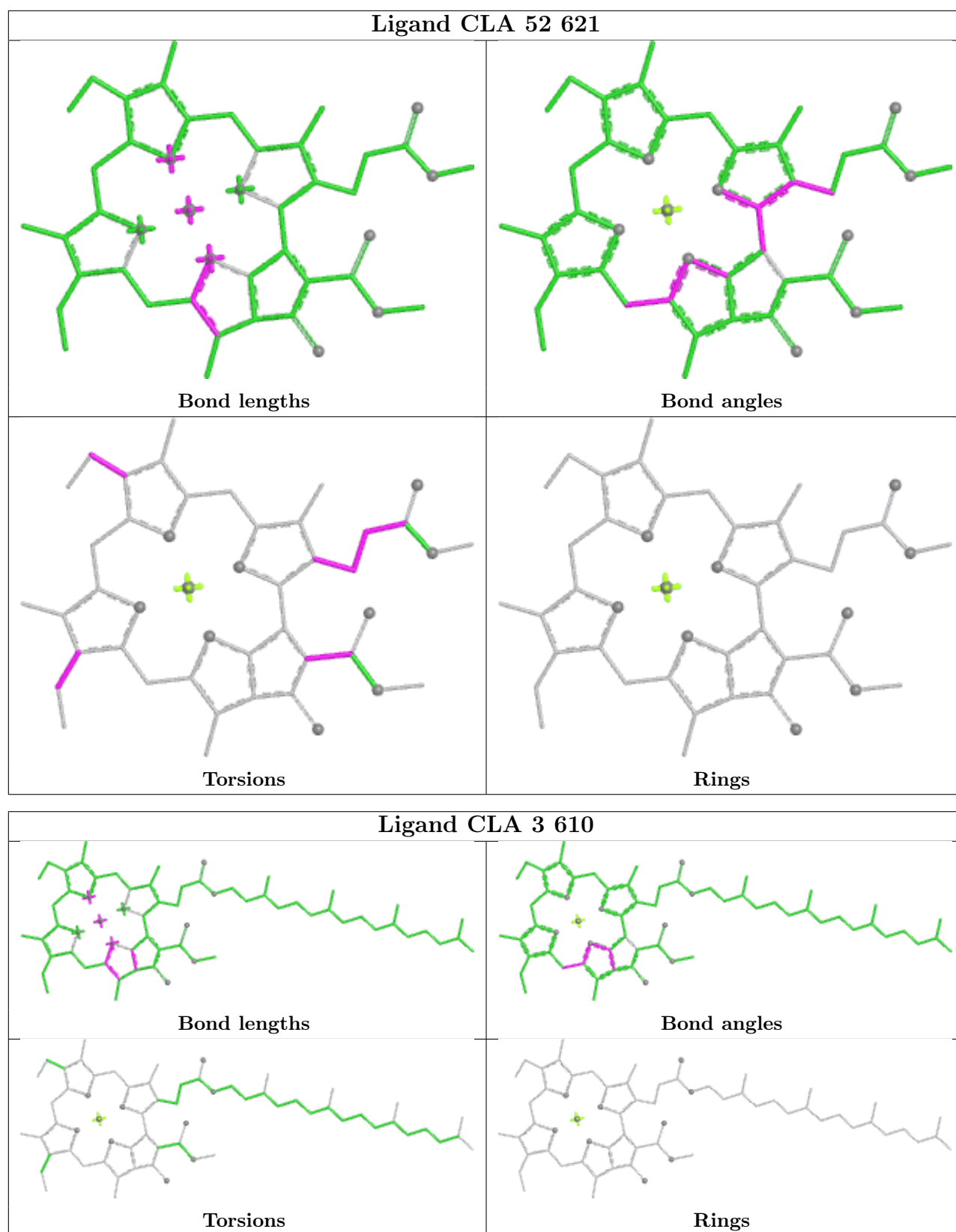


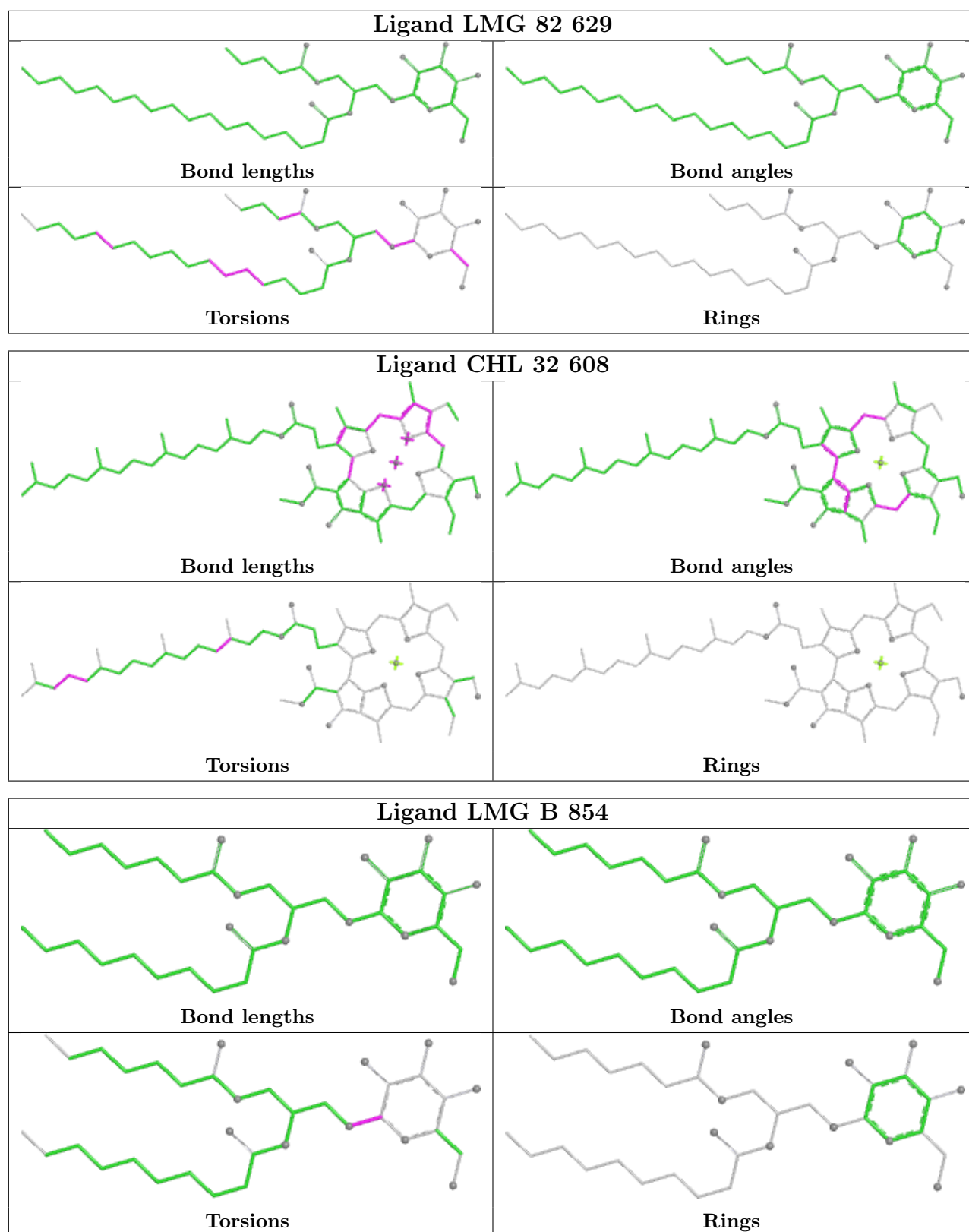


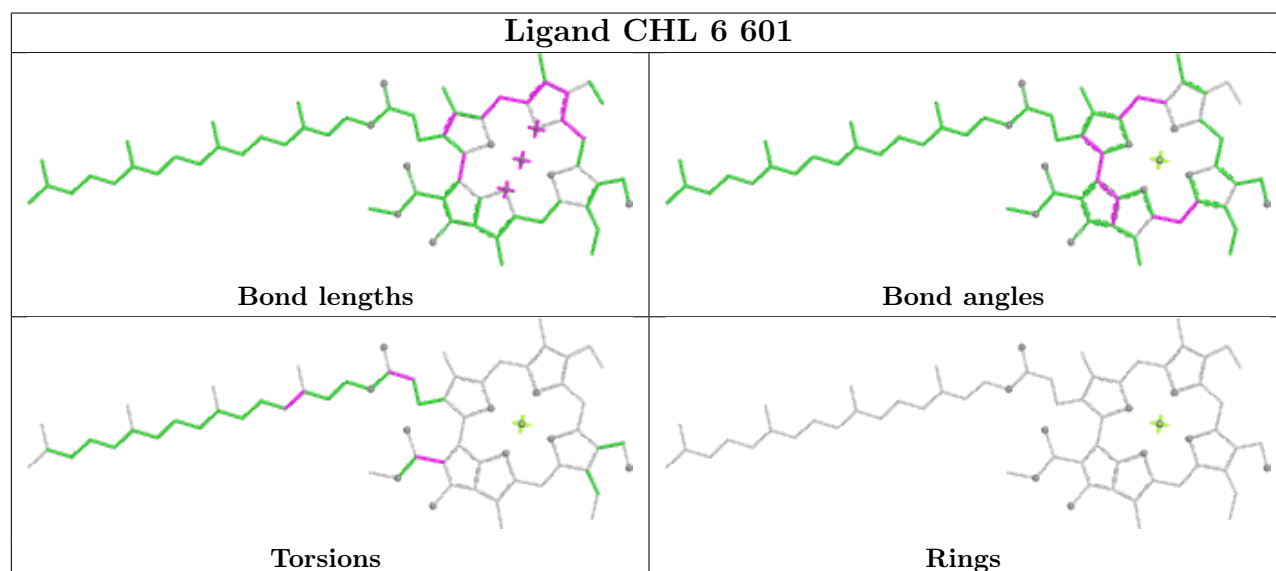
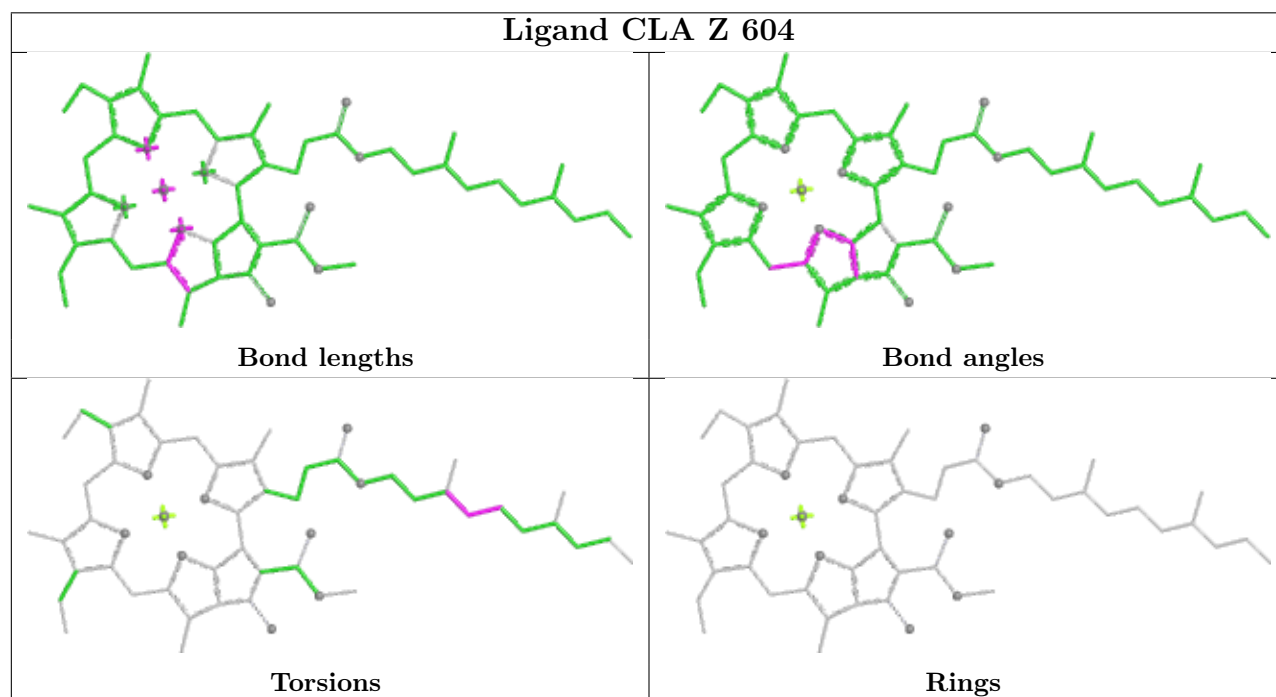
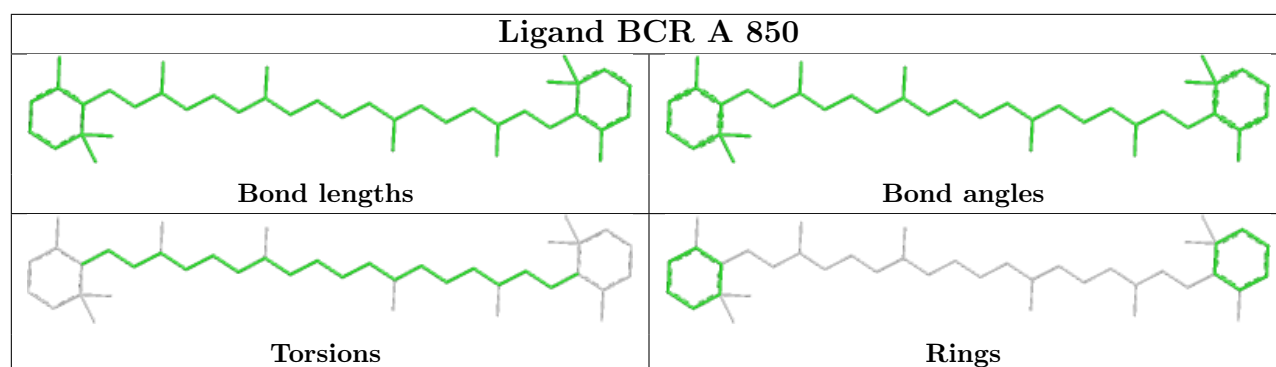


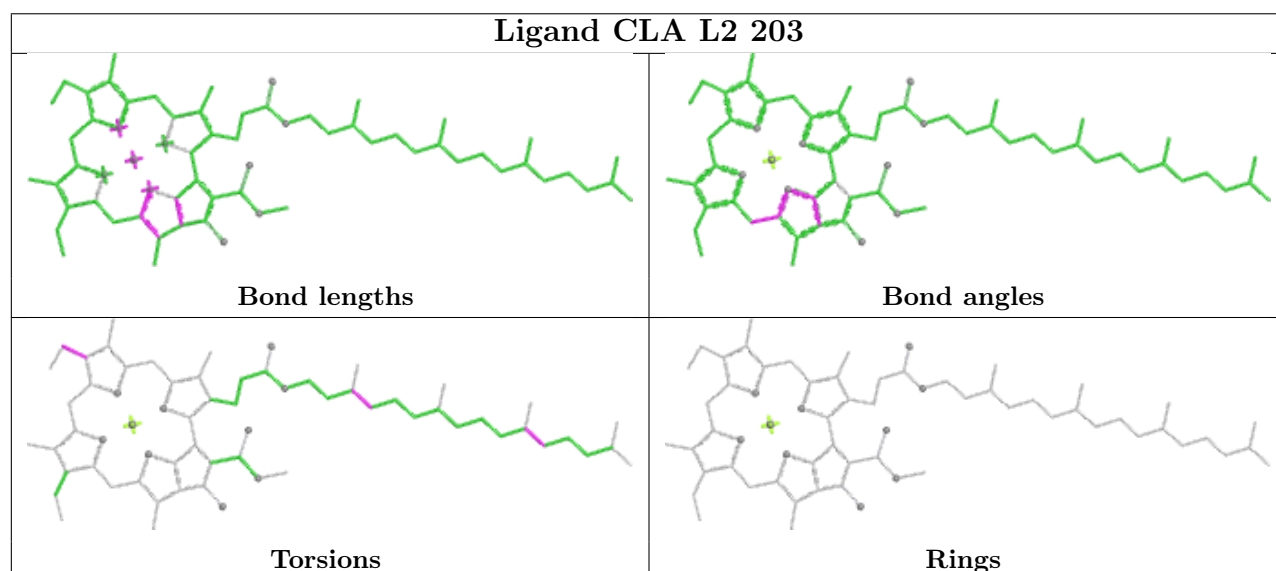
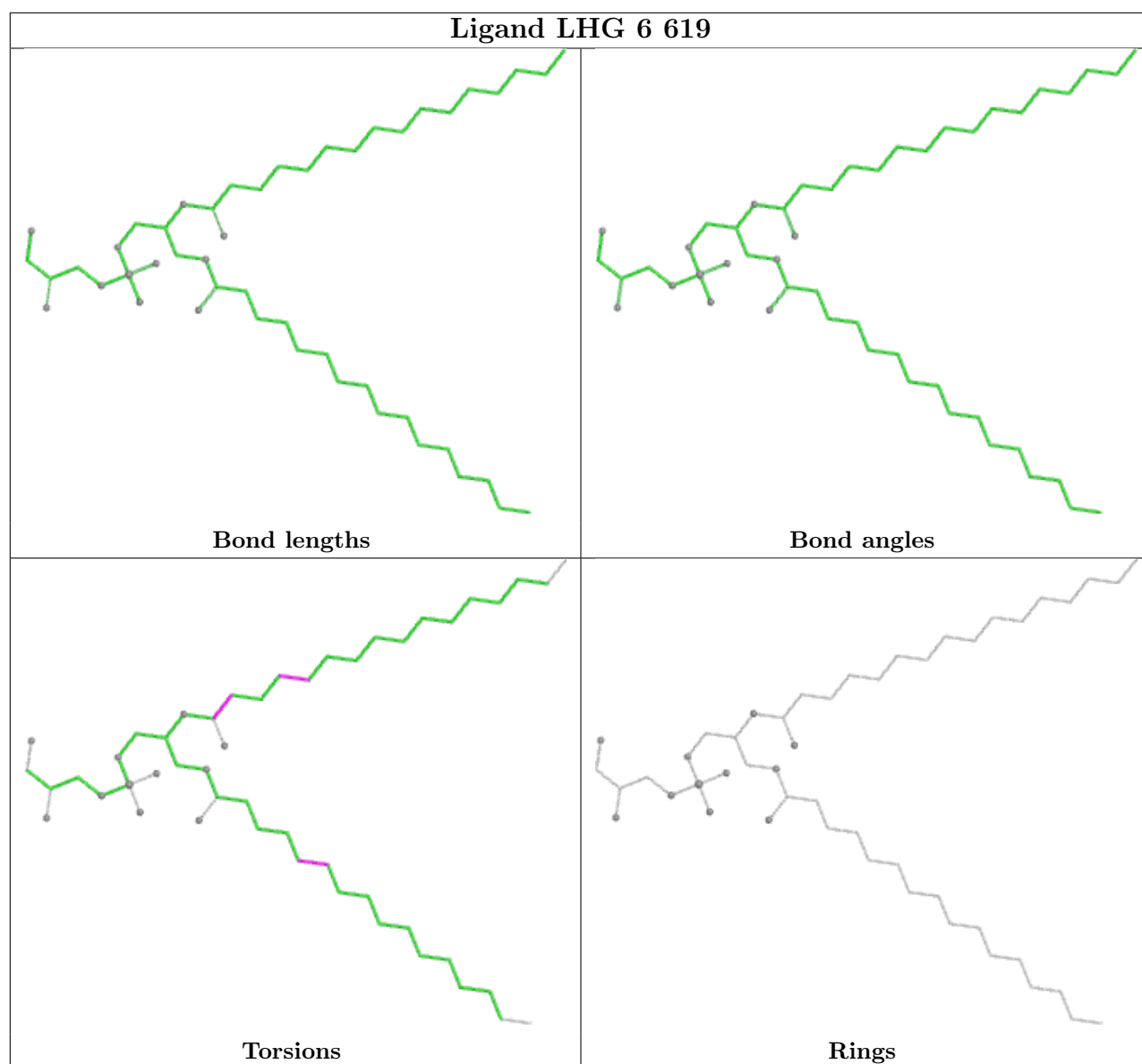


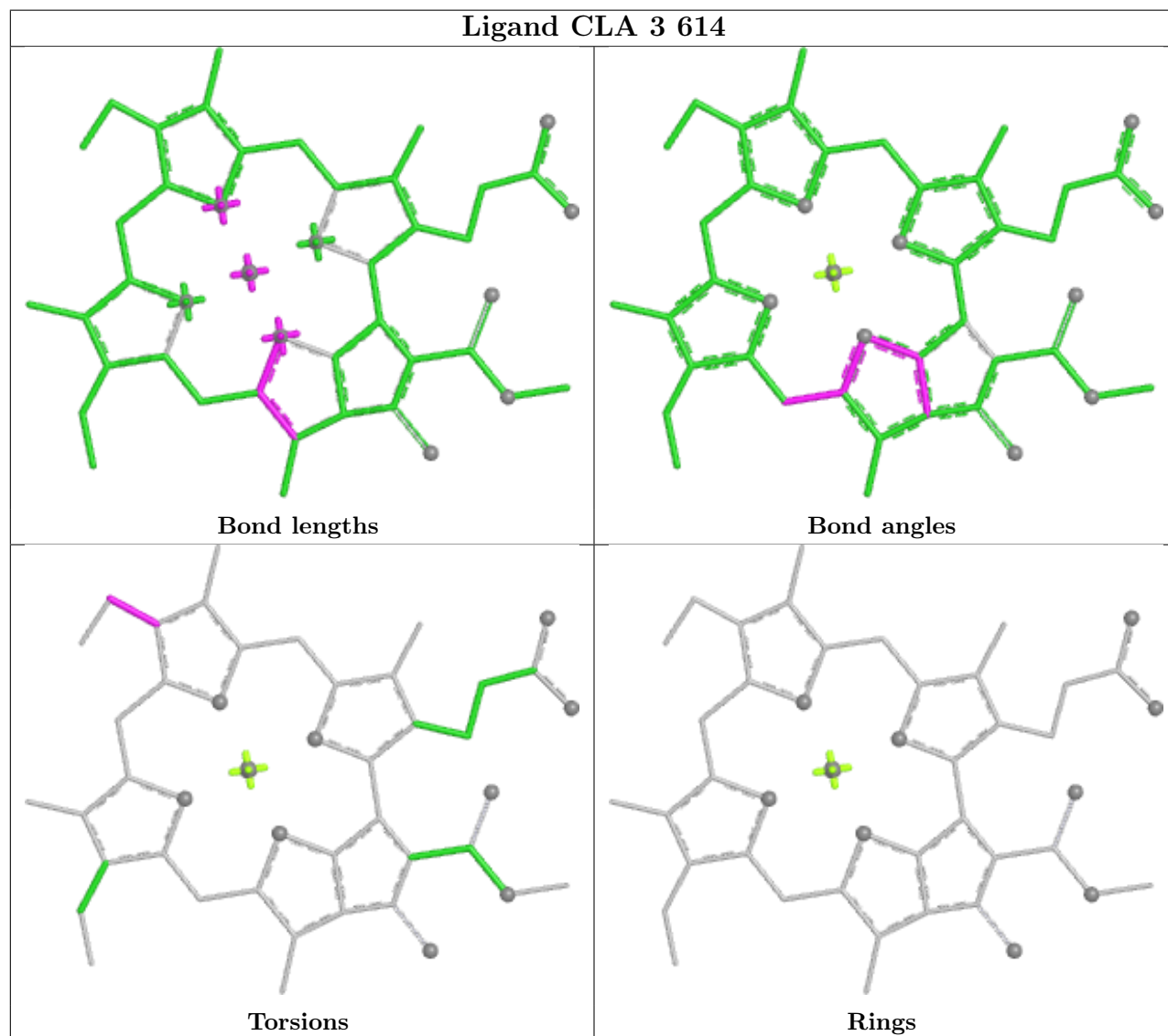
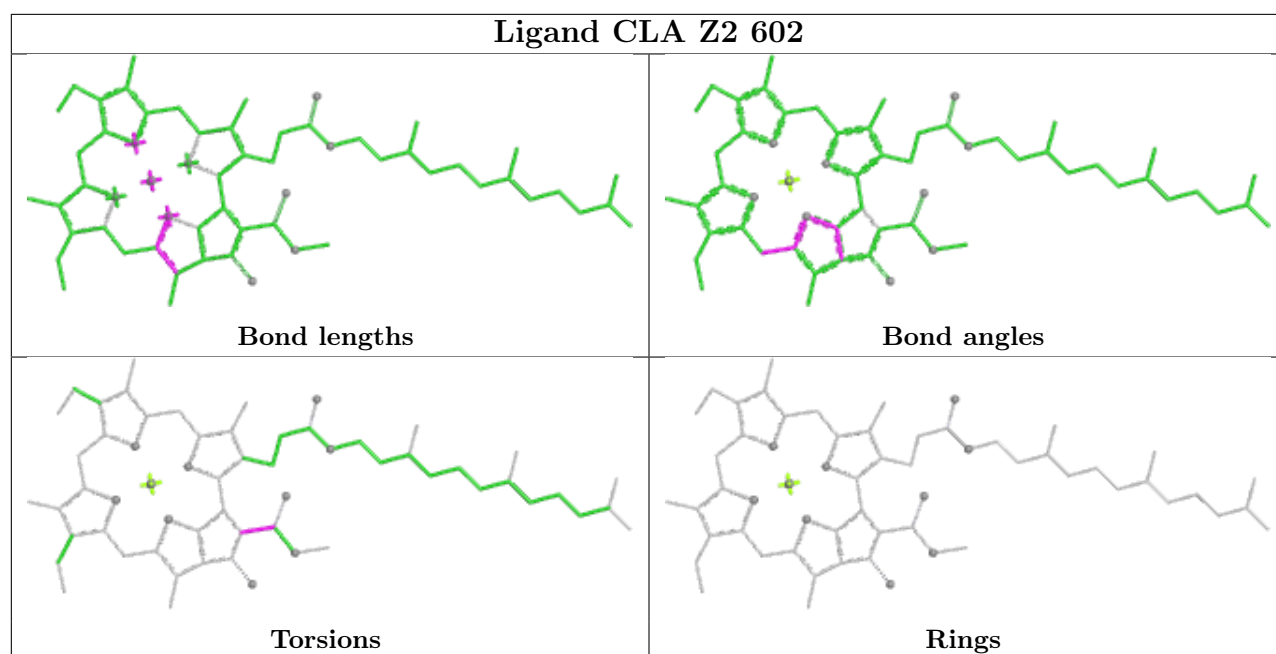


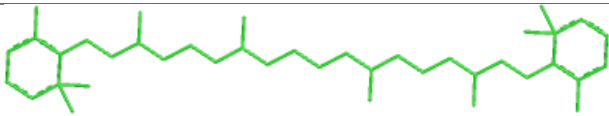
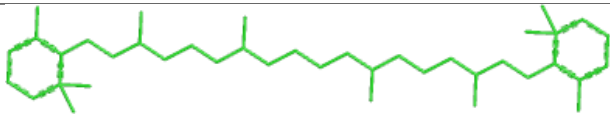
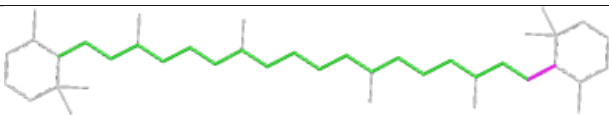
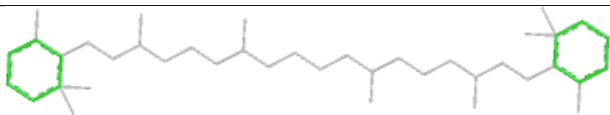


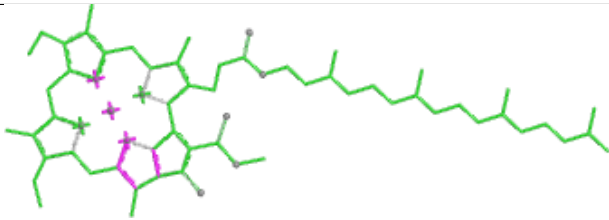
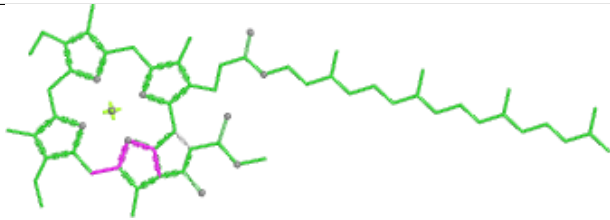
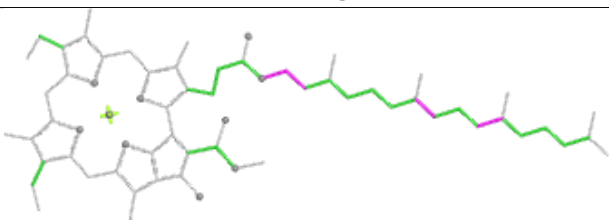
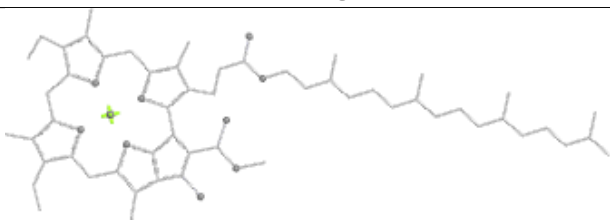


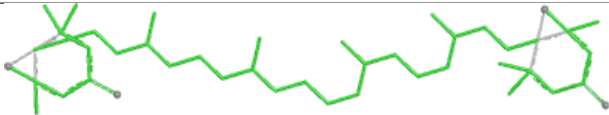
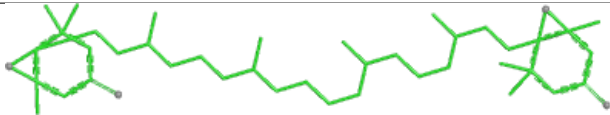
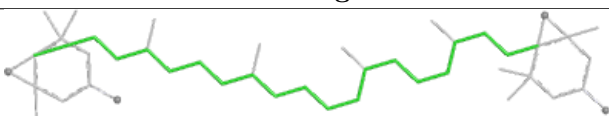
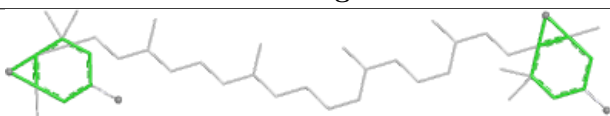


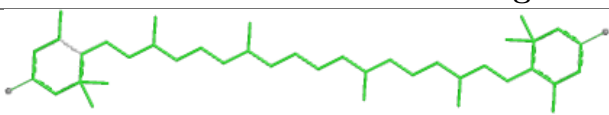
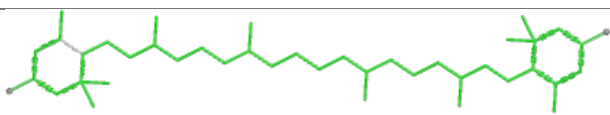
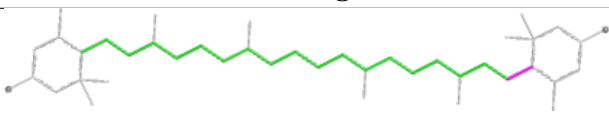
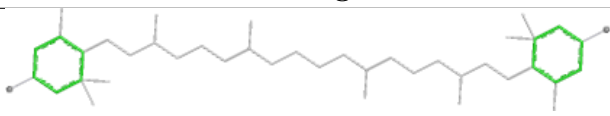


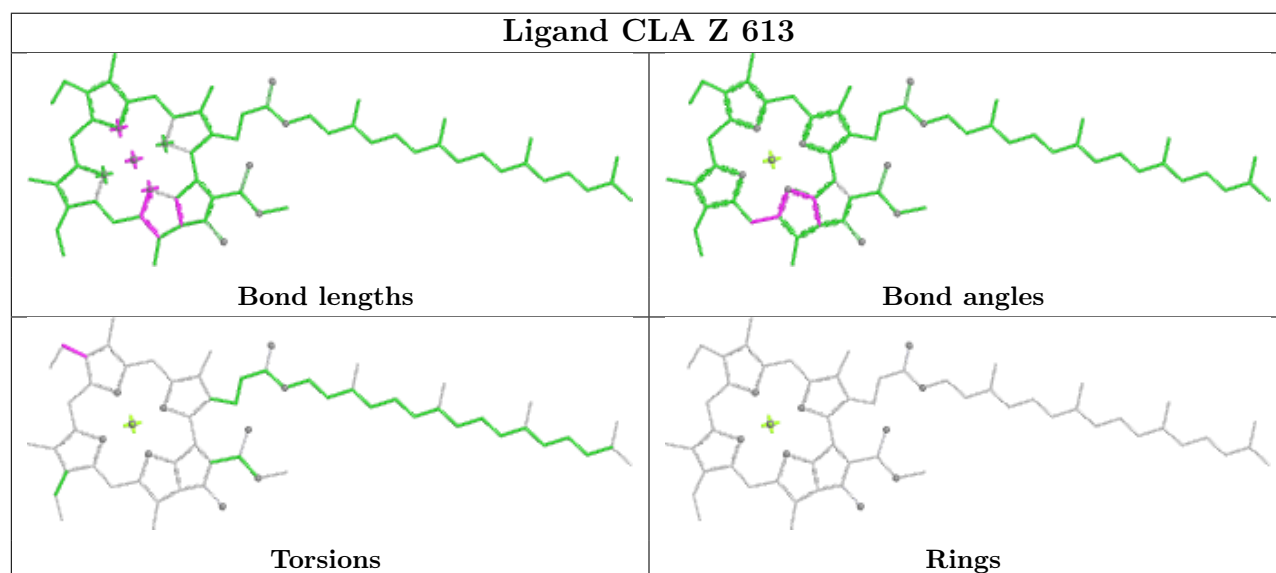
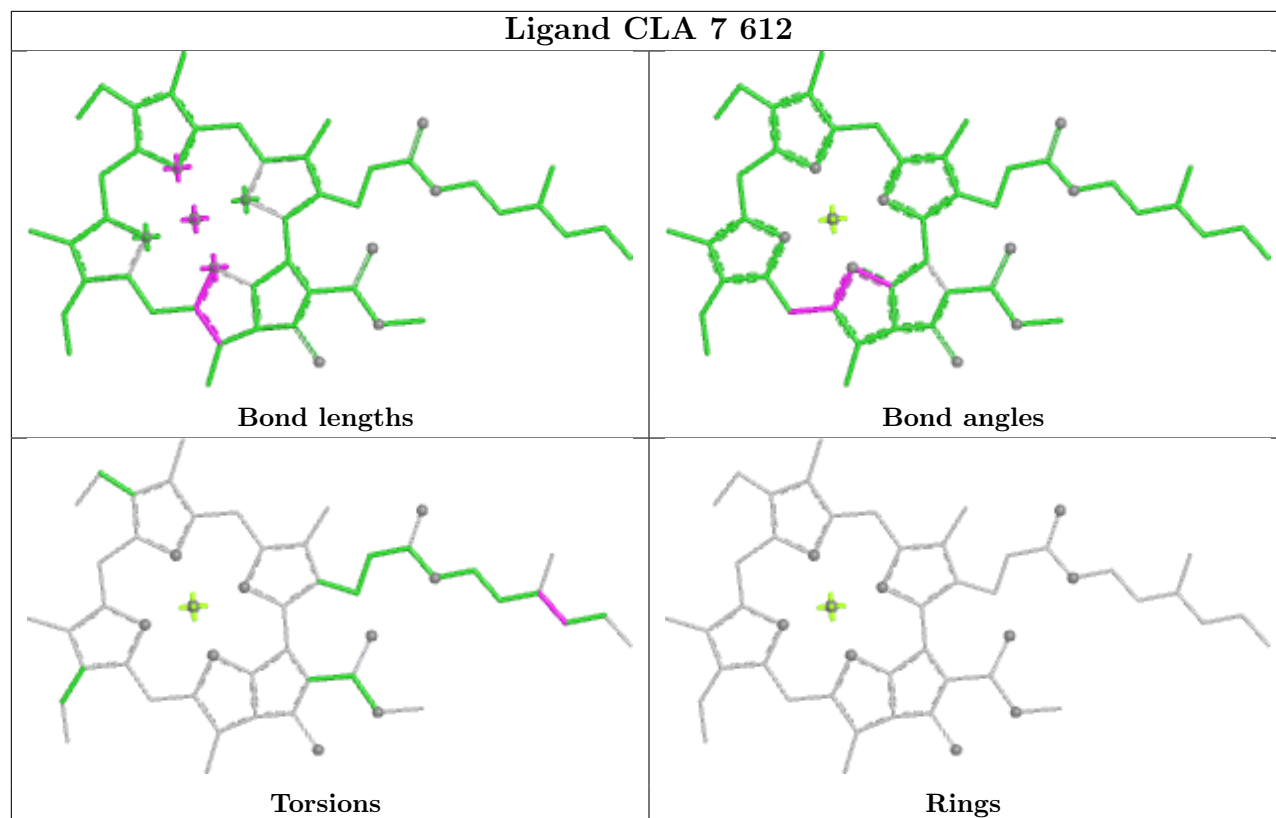


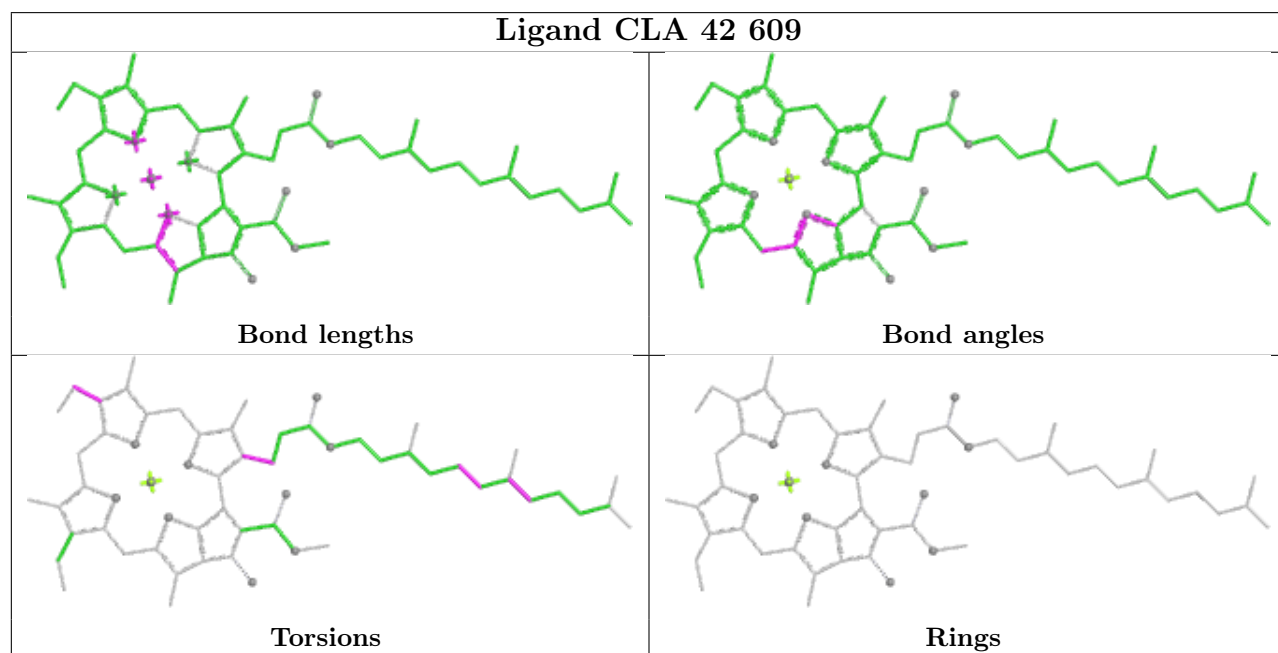
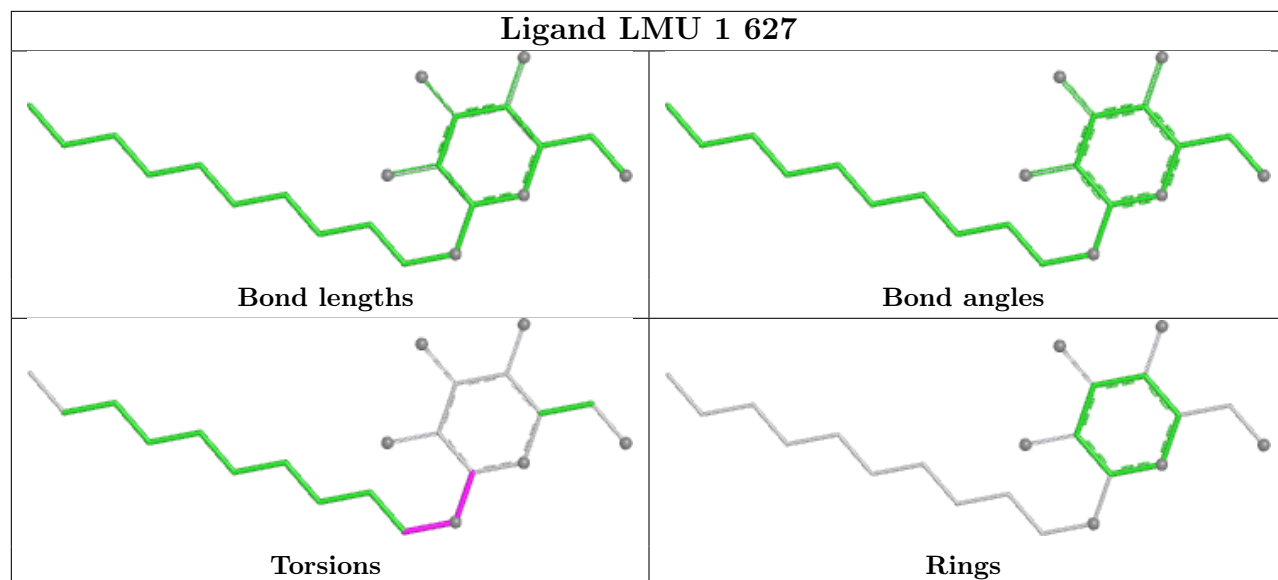
Ligand BCR 4 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

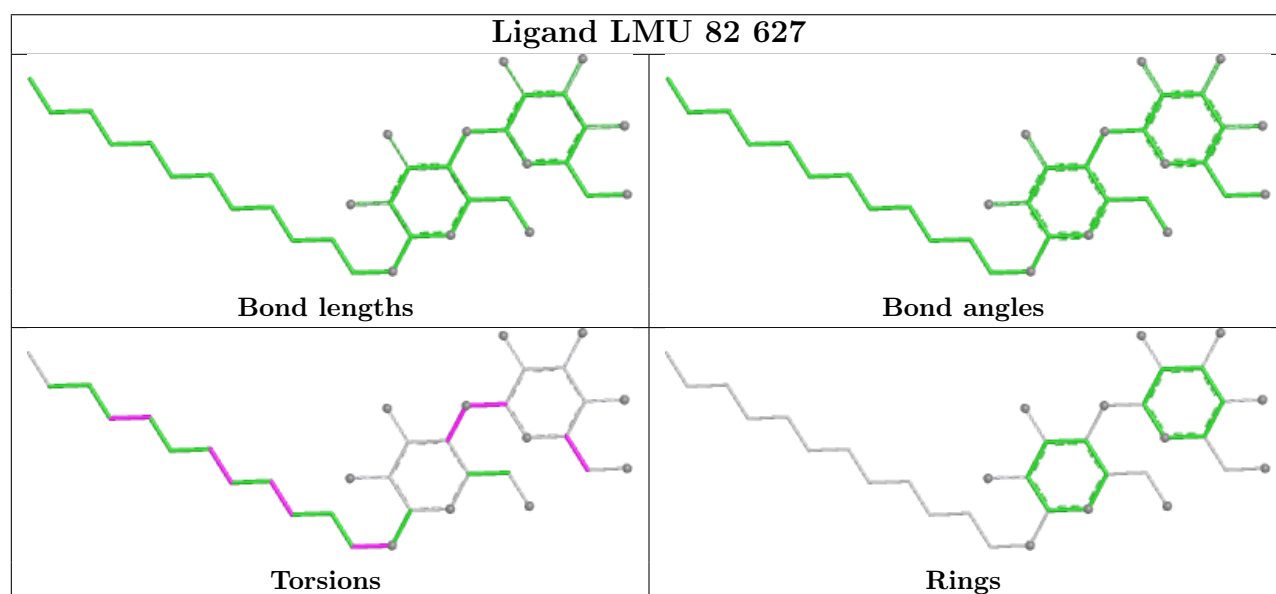
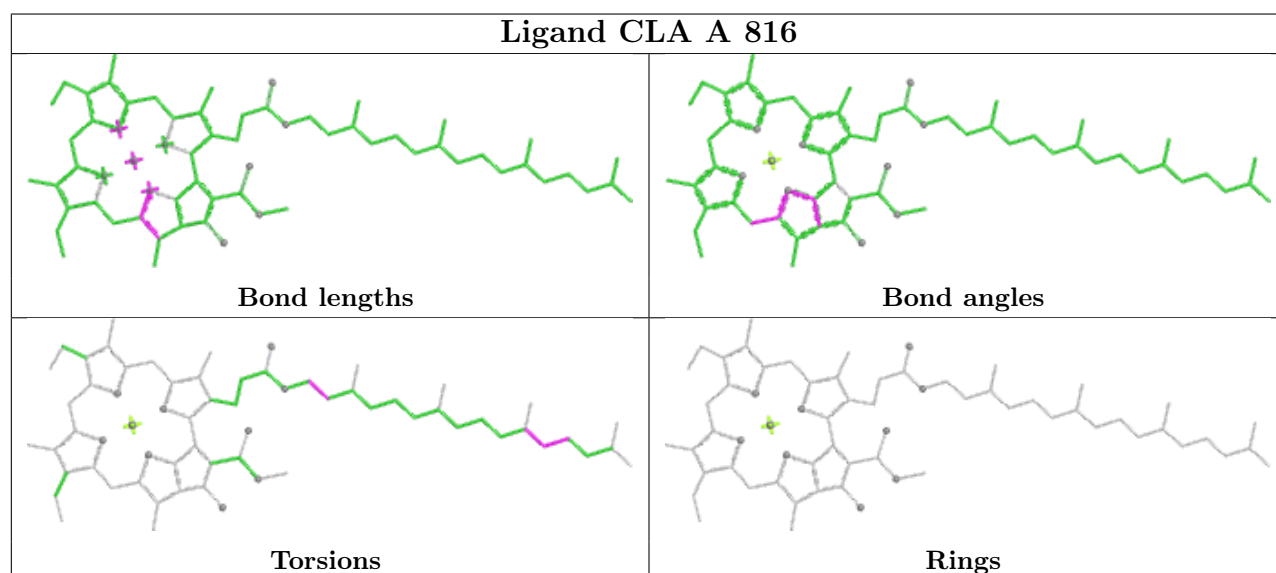
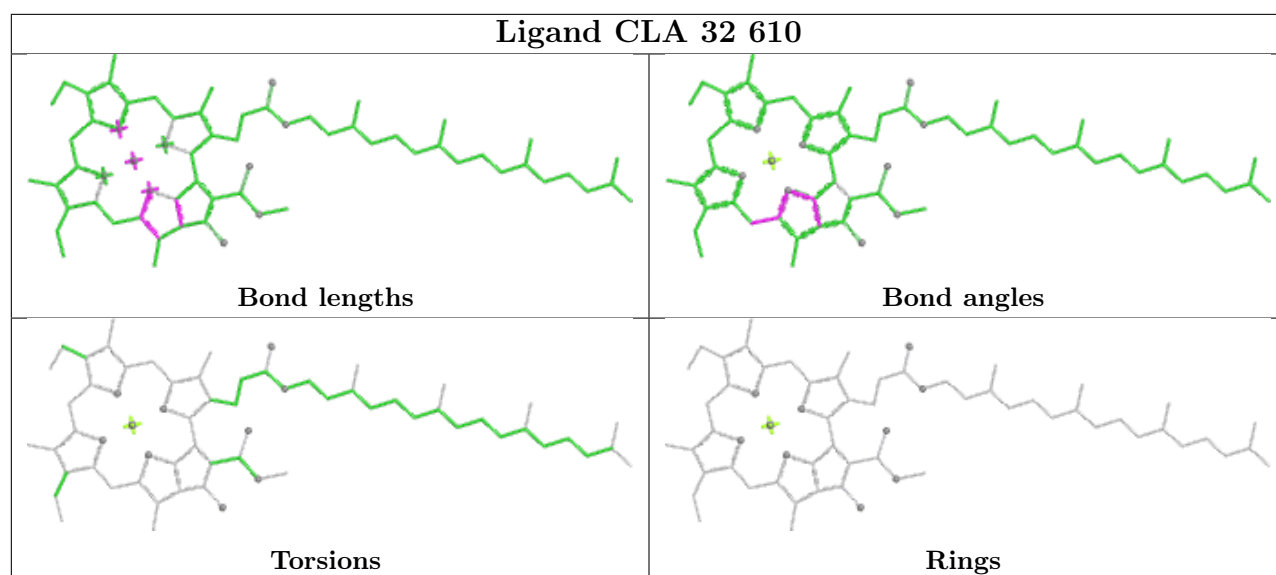
Ligand CLA A2 843	
	
Bond lengths	Bond angles
	
Torsions	Rings

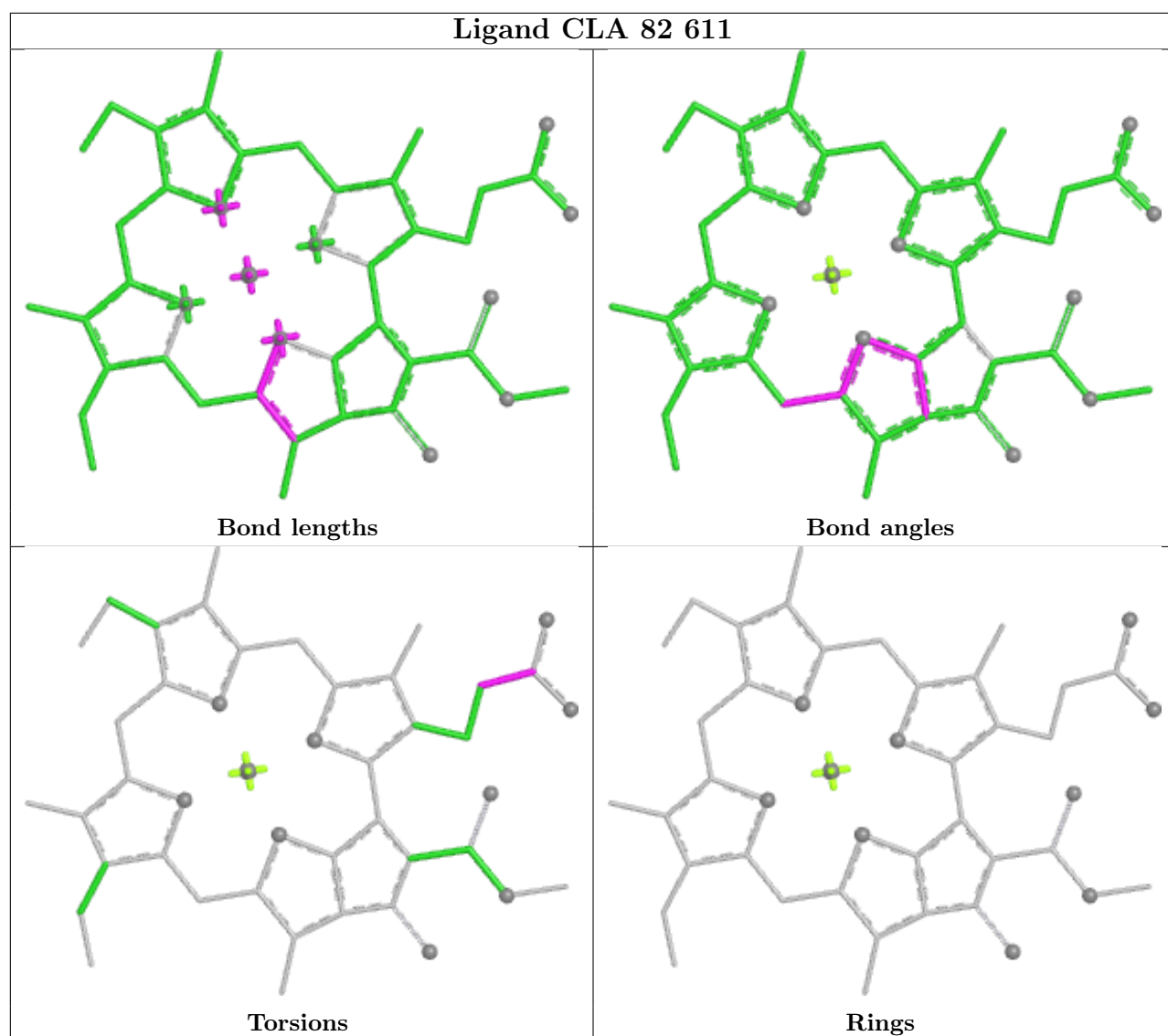
Ligand XAT Z2 618	
	
Bond lengths	Bond angles
	
Torsions	Rings

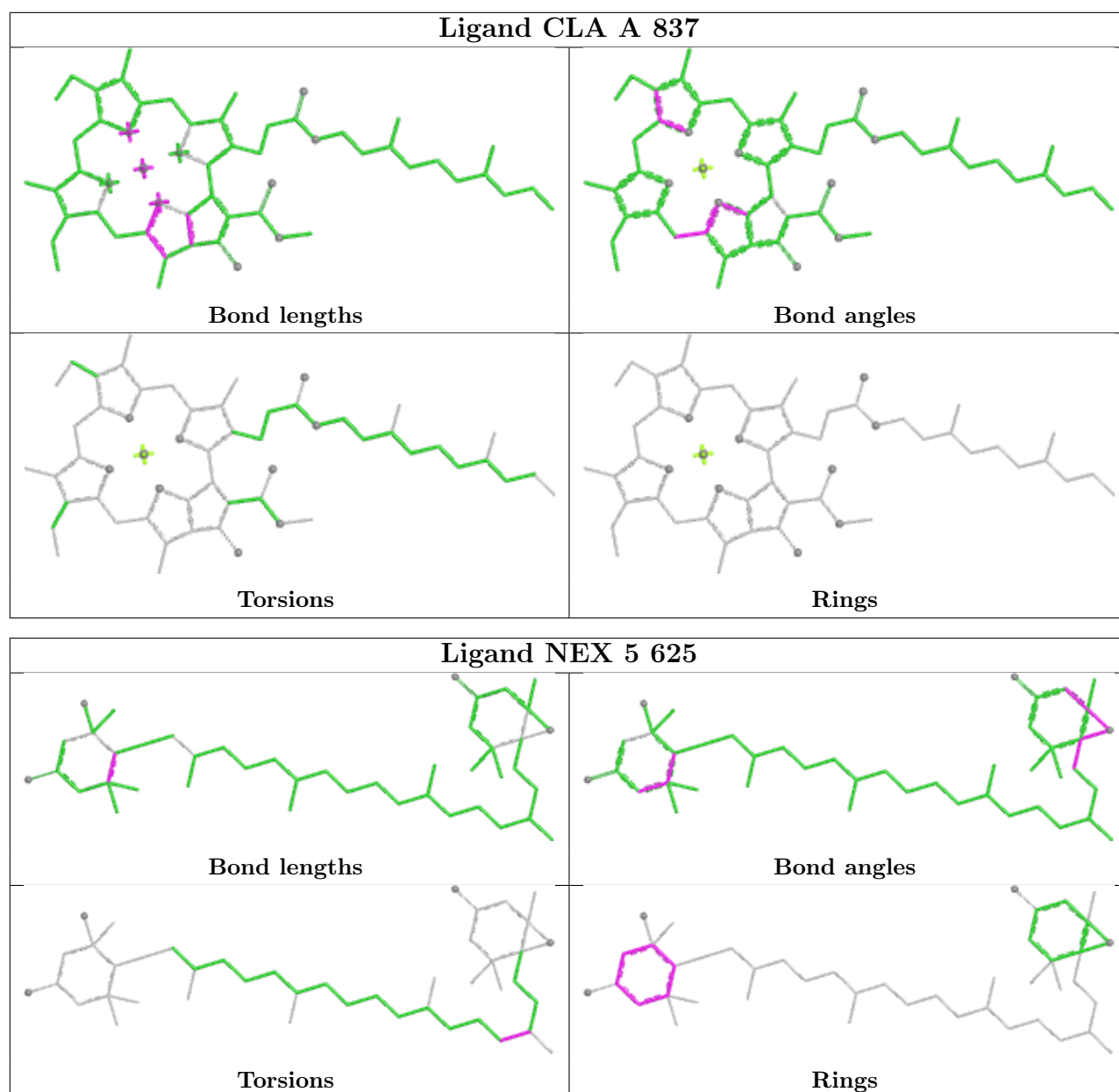
Ligand LUT 8 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

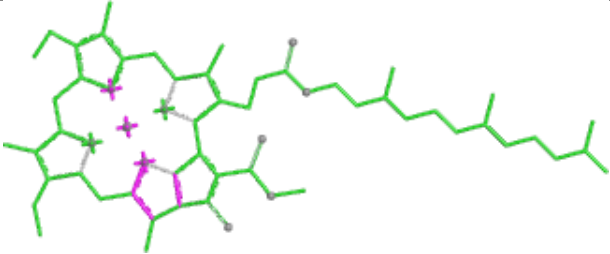
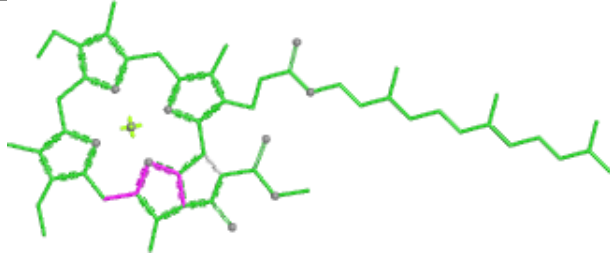
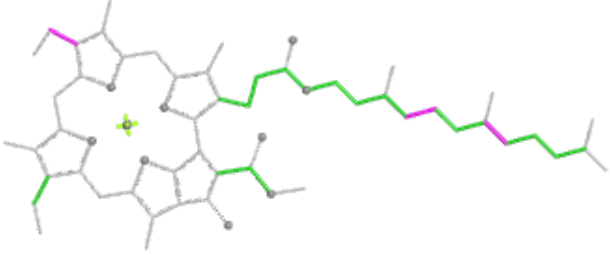
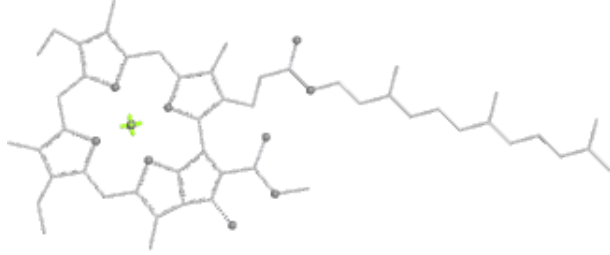
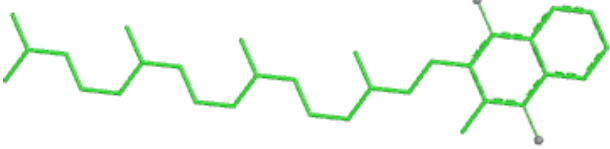
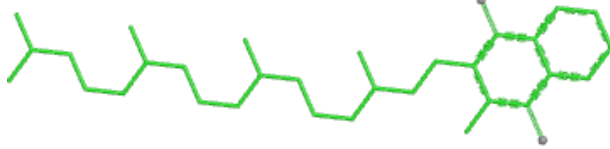
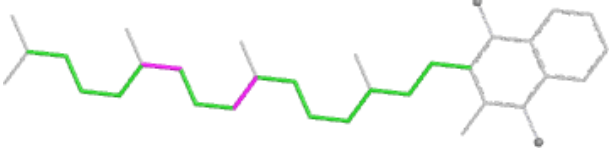
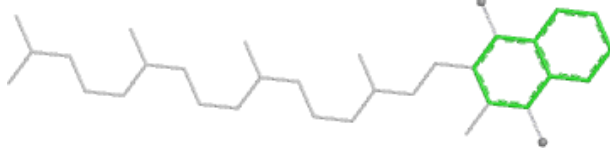
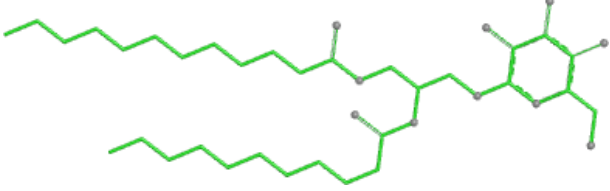
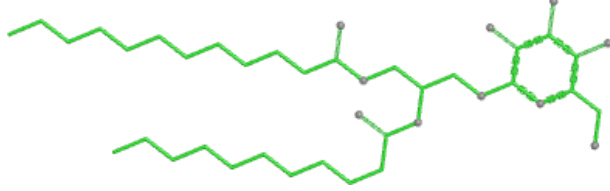
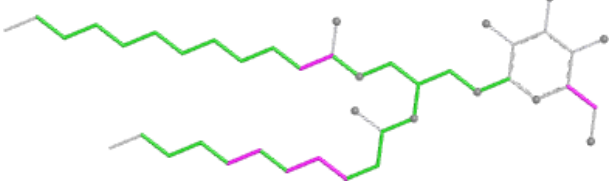
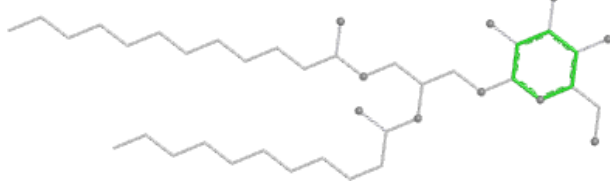


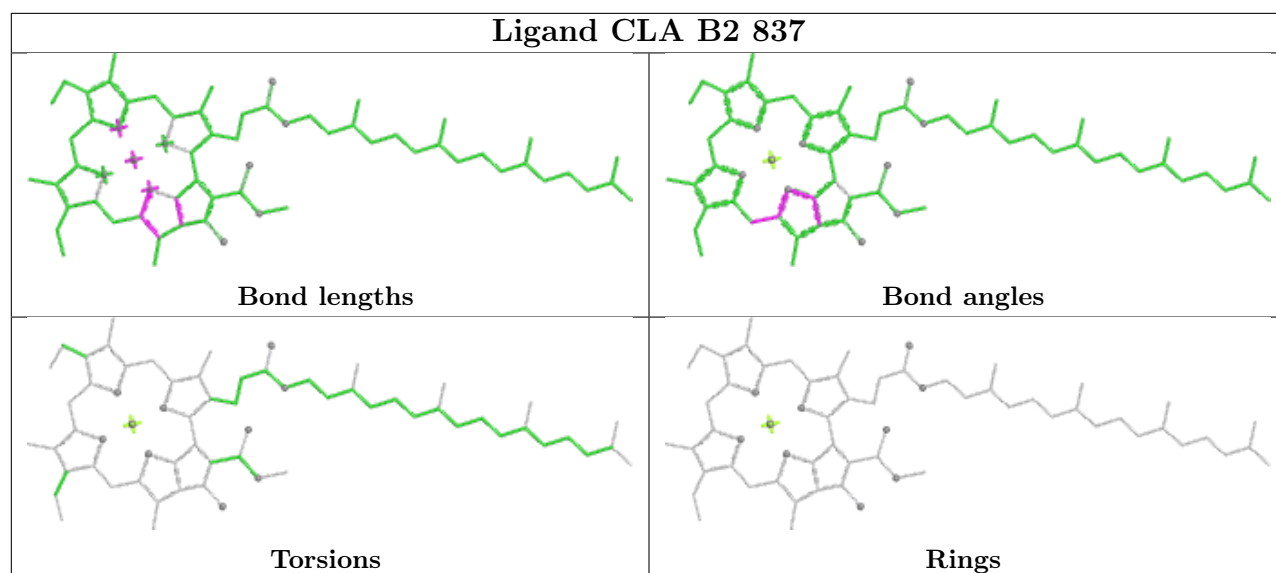
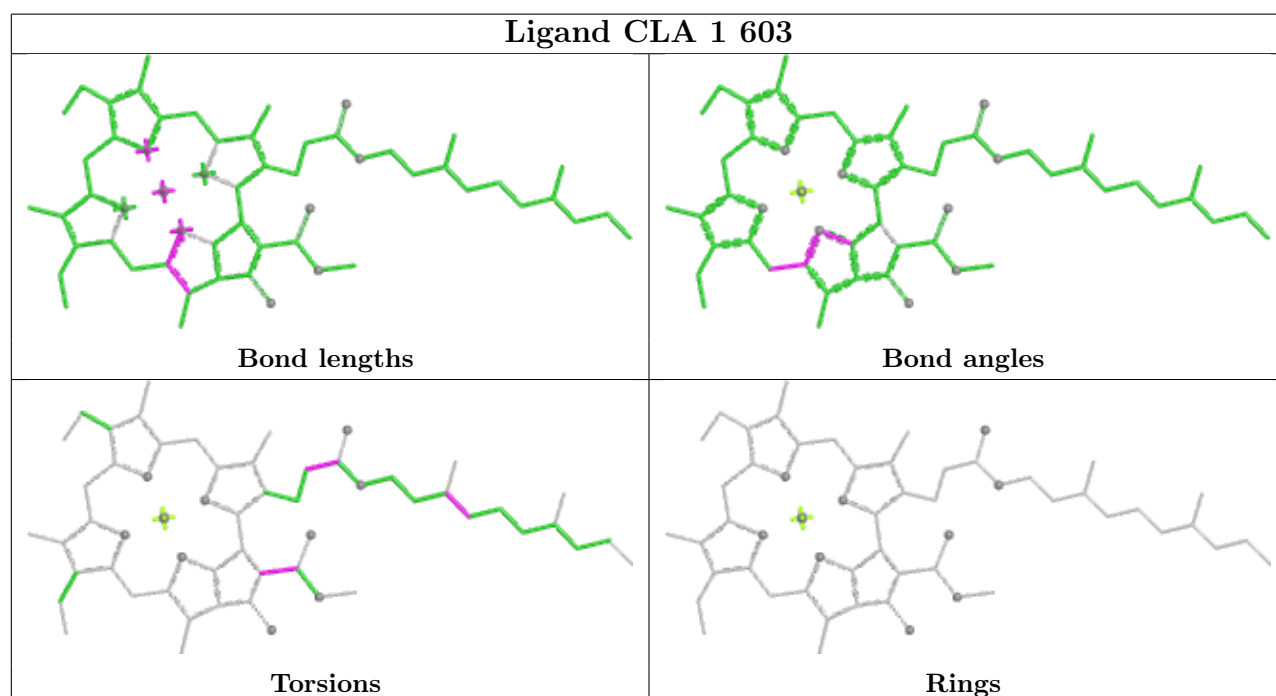
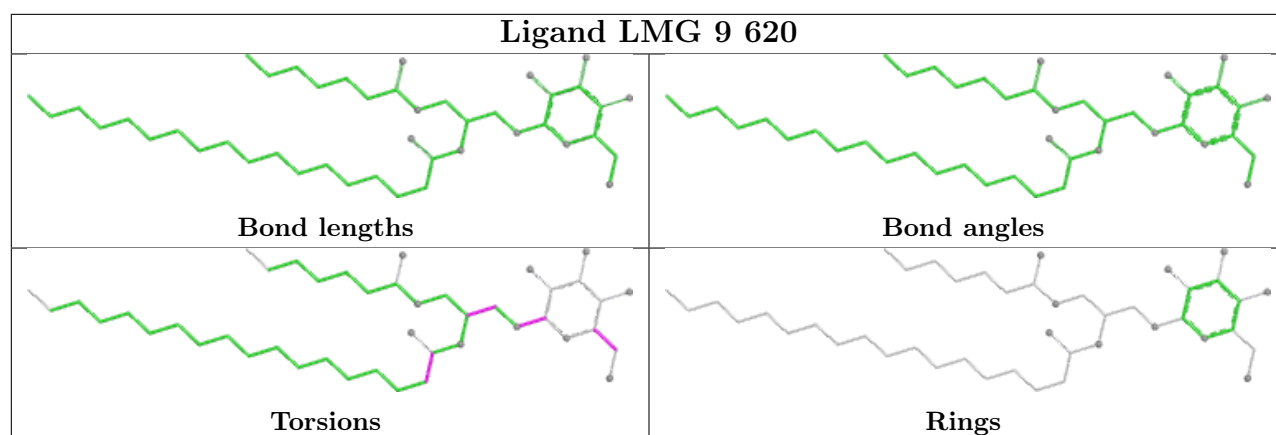


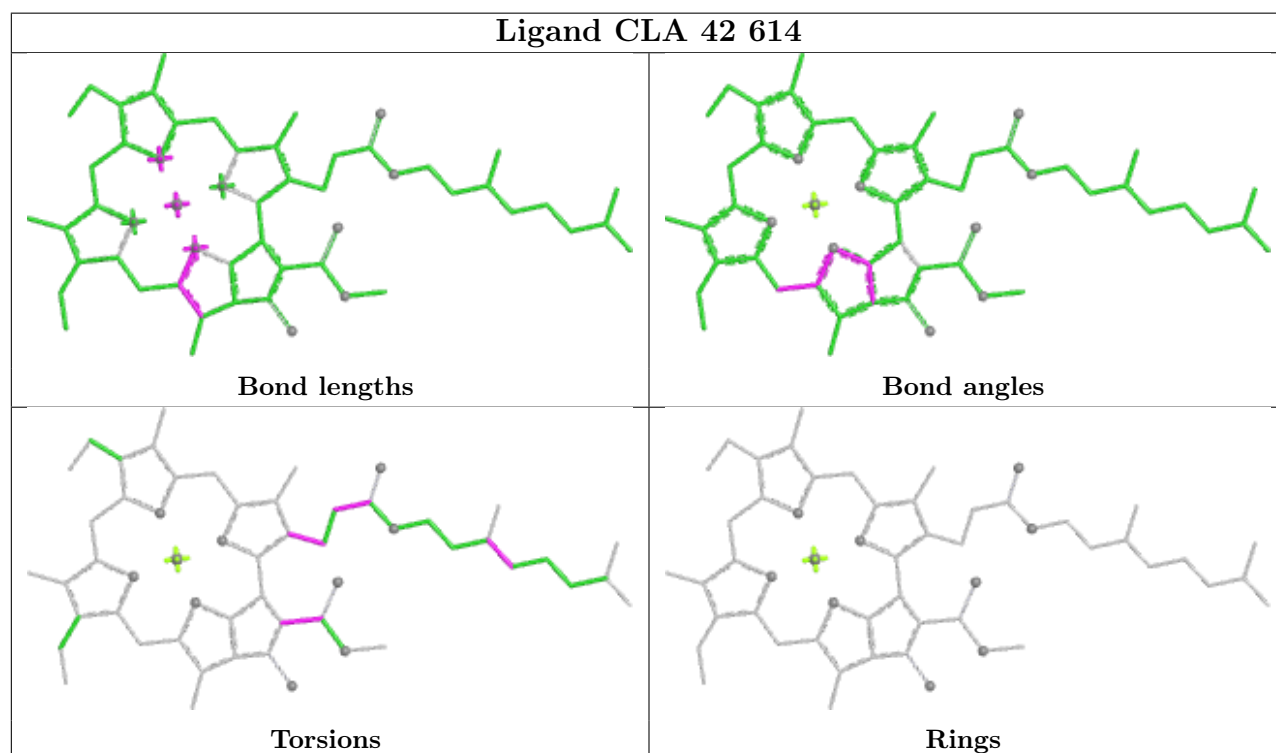
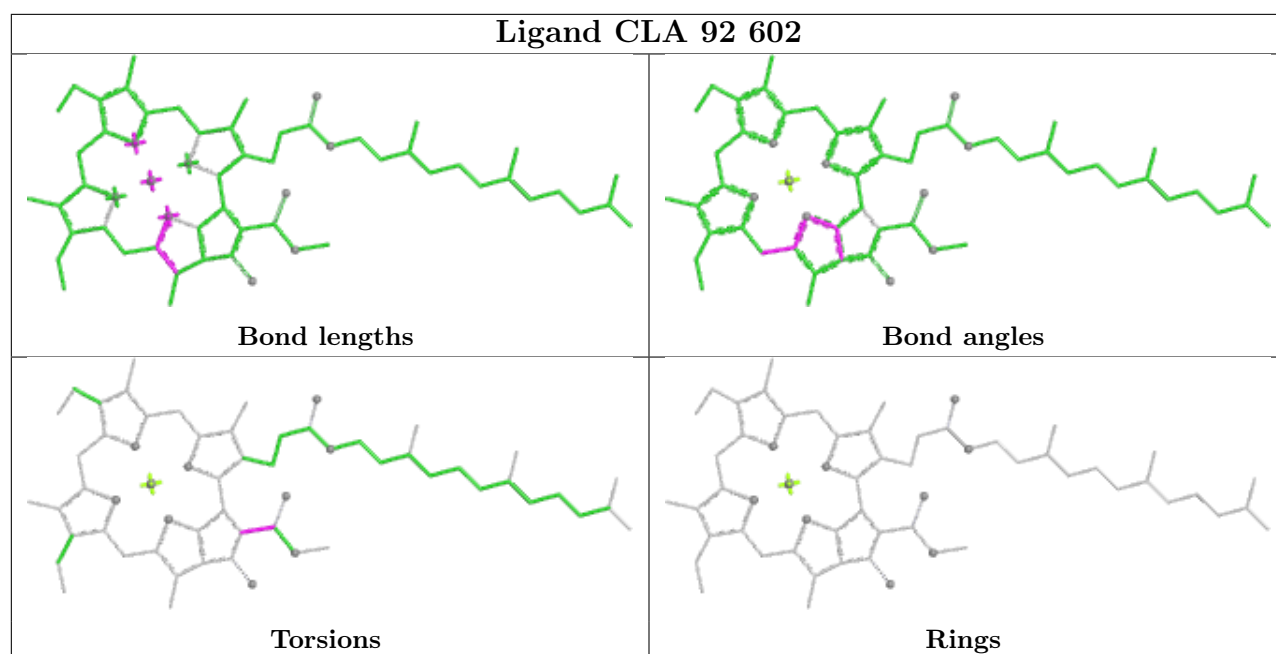


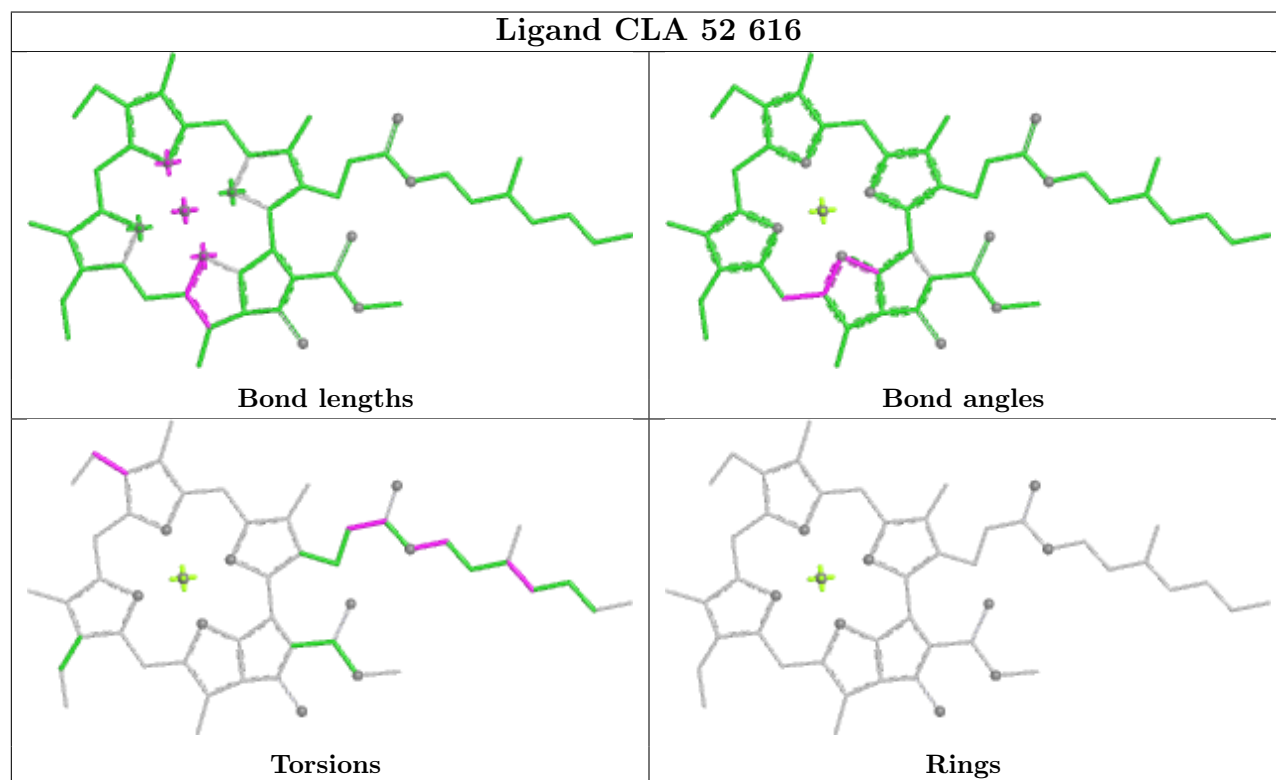
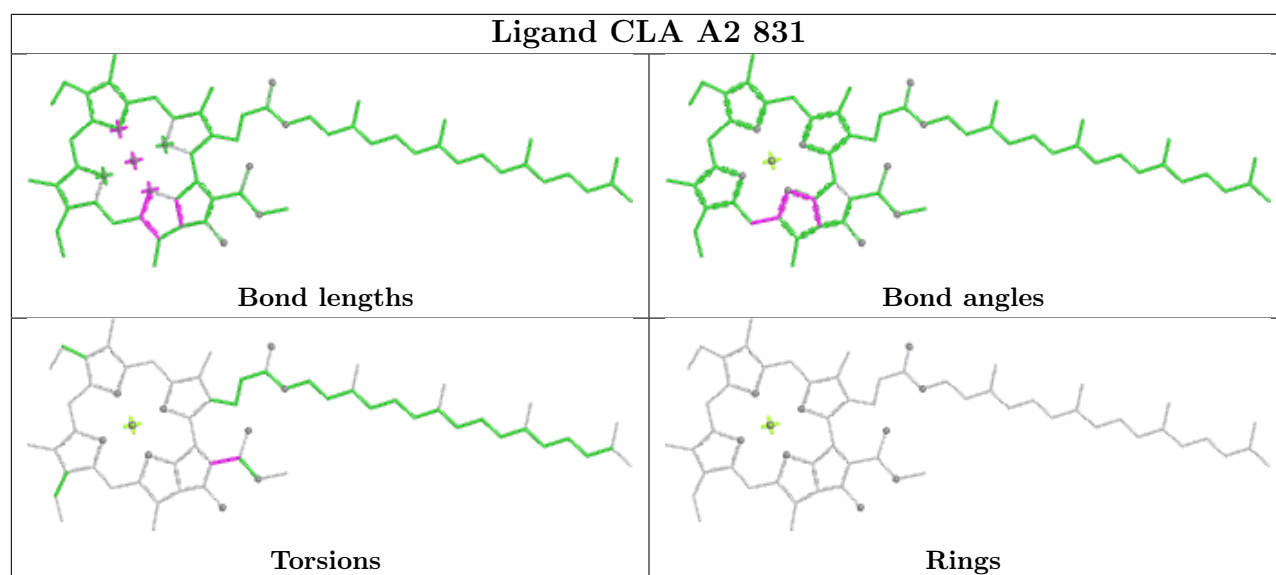


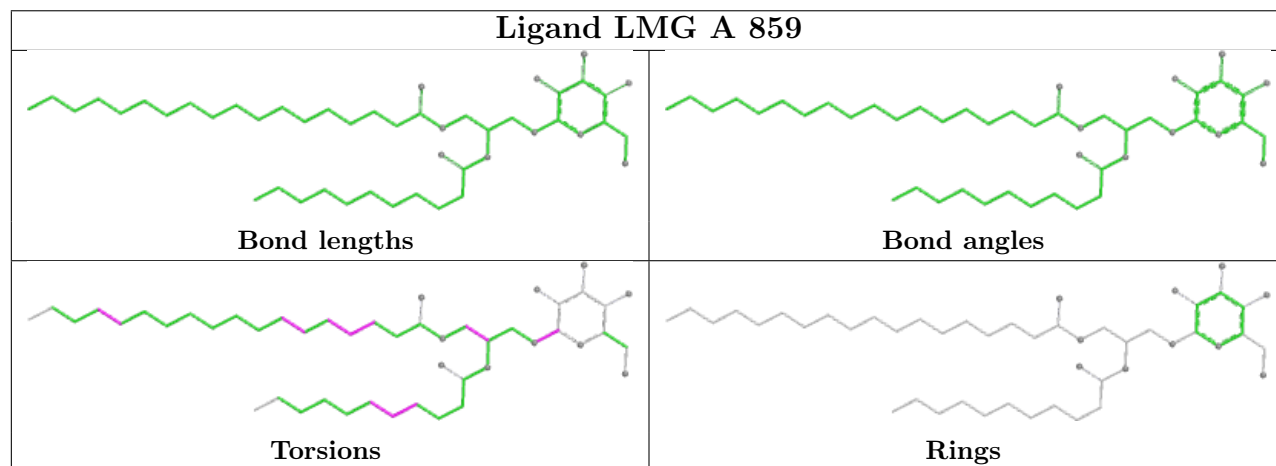
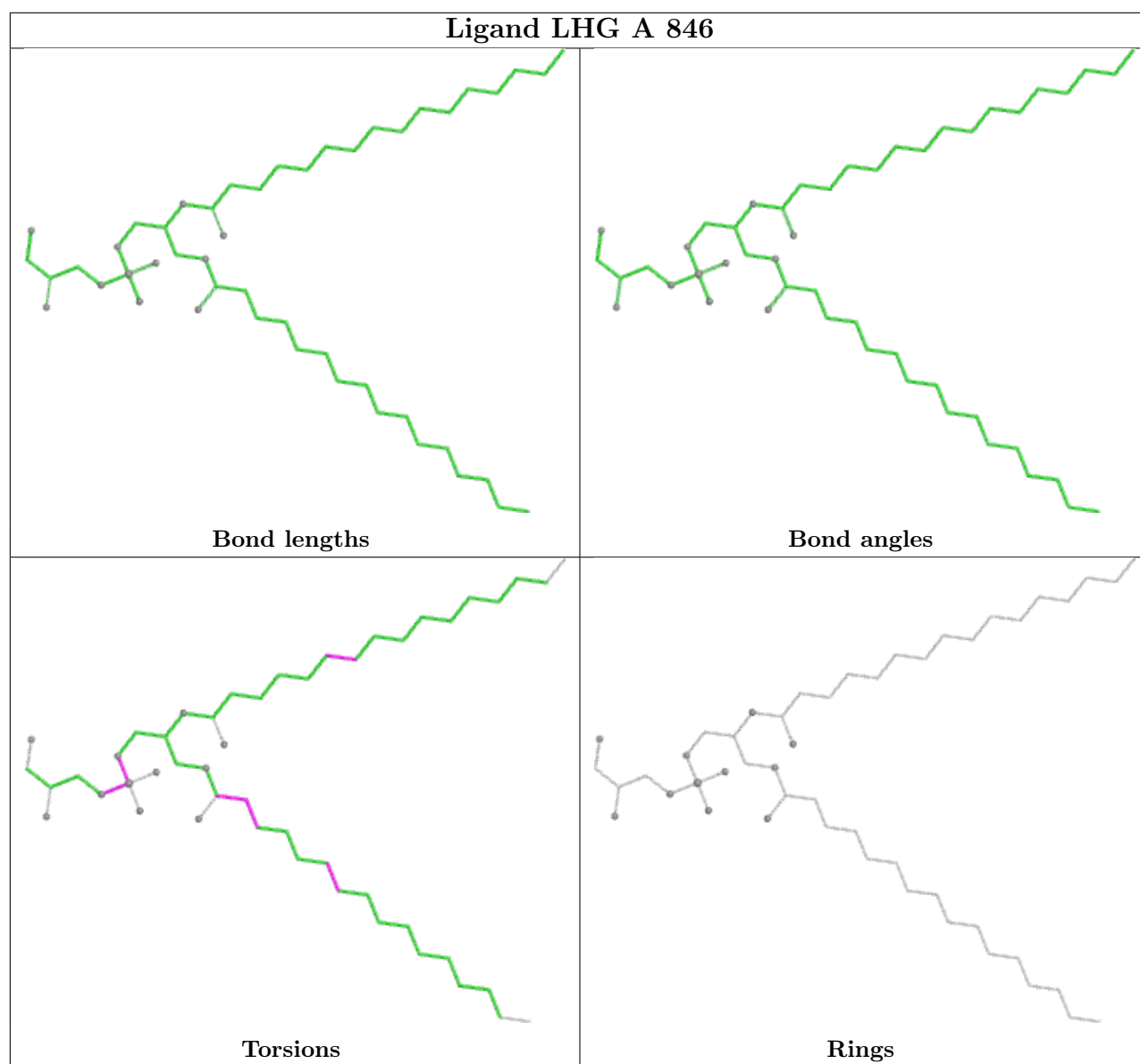


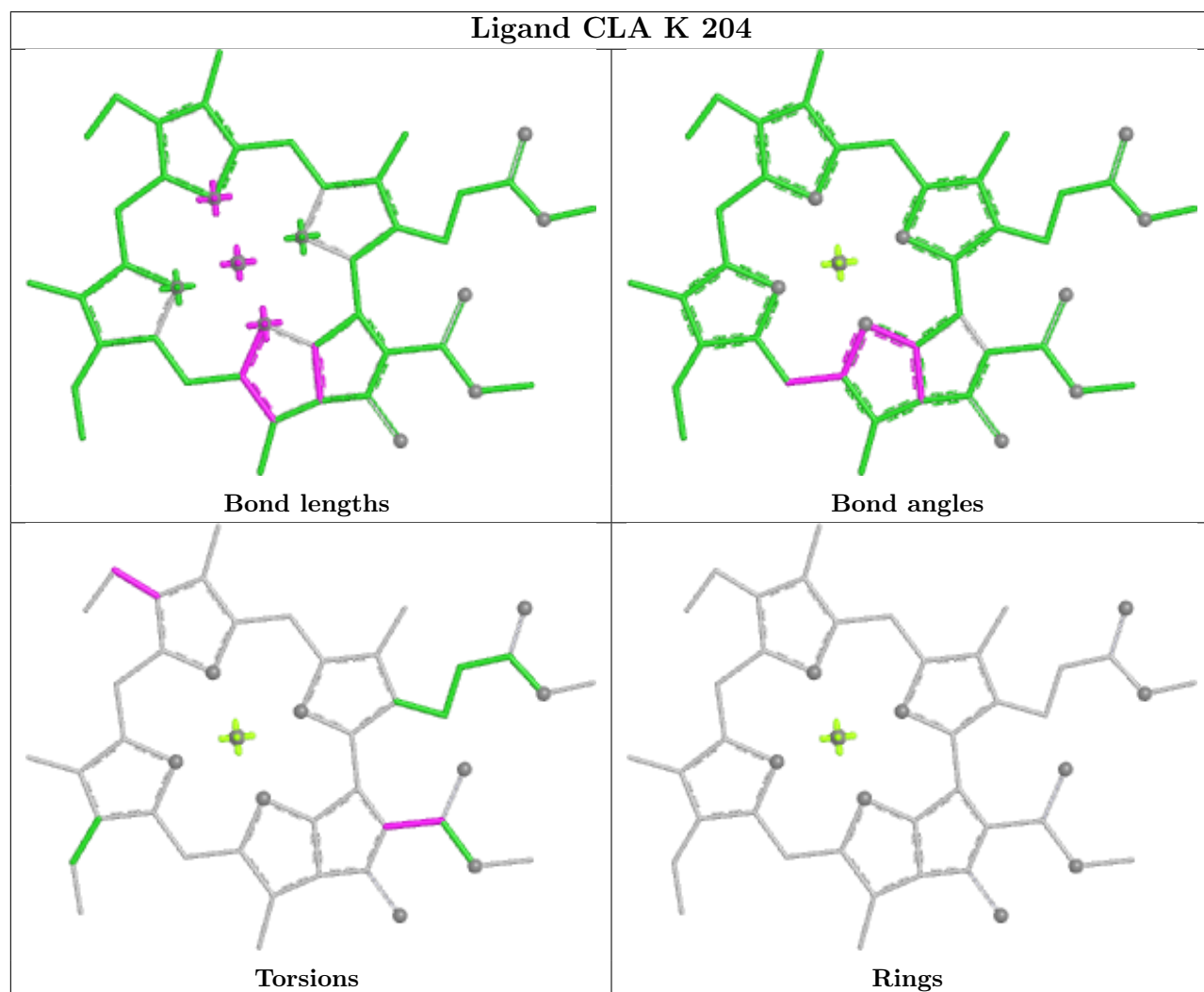
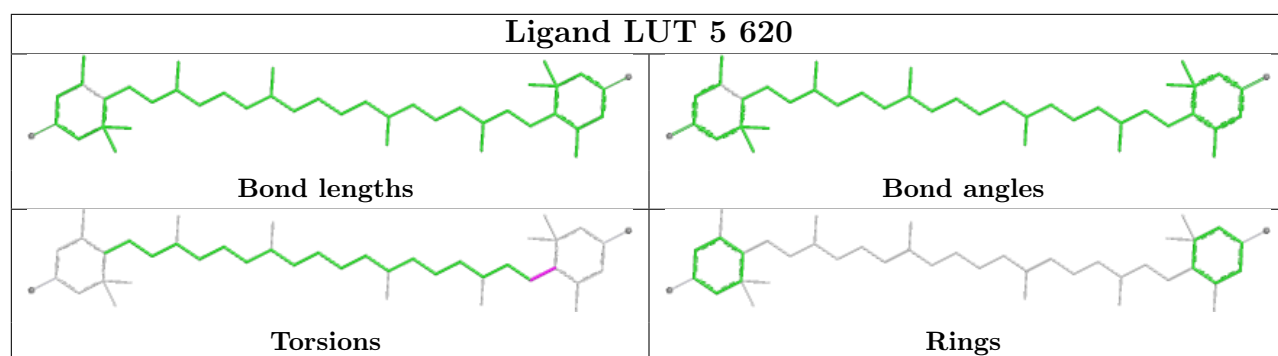
Ligand CLA B 819	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand PQN A2 844	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG 1 628	
 Bond lengths	 Bond angles
 Torsions	 Rings

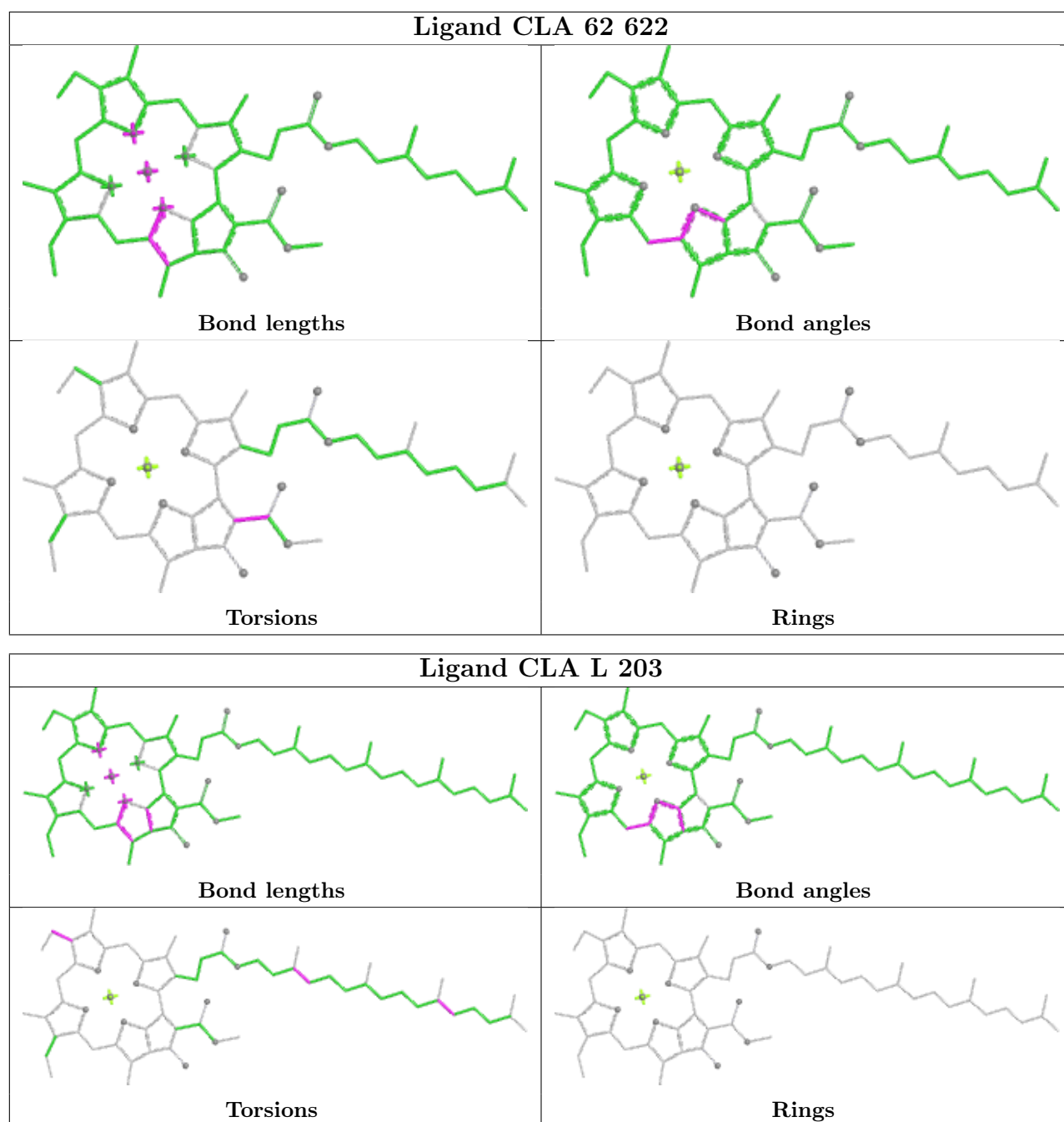


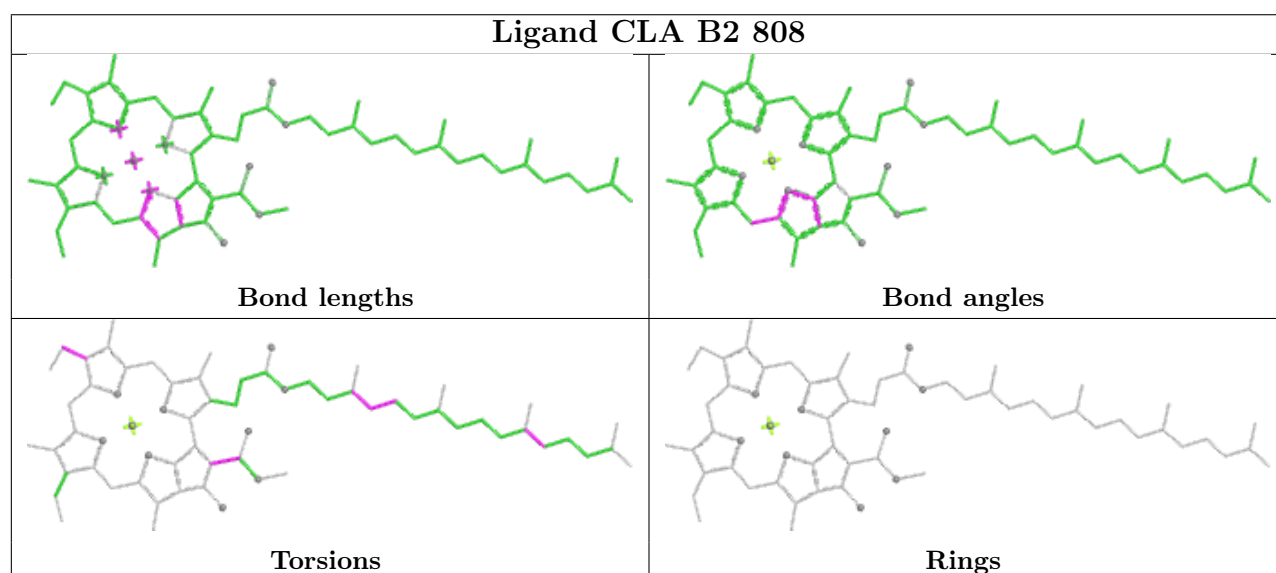
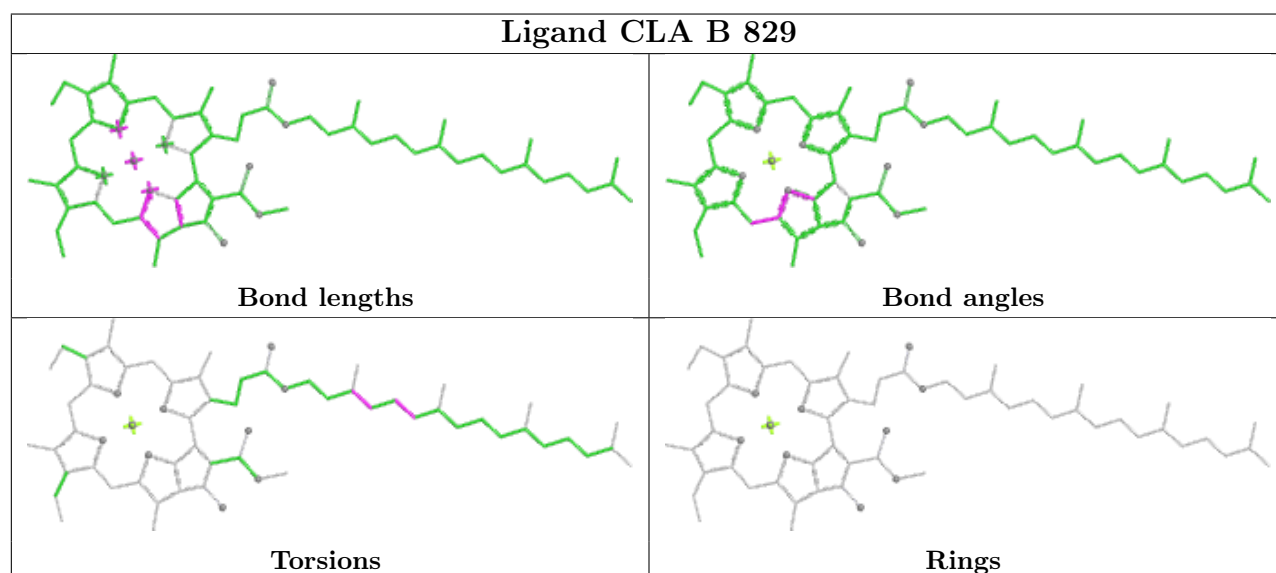
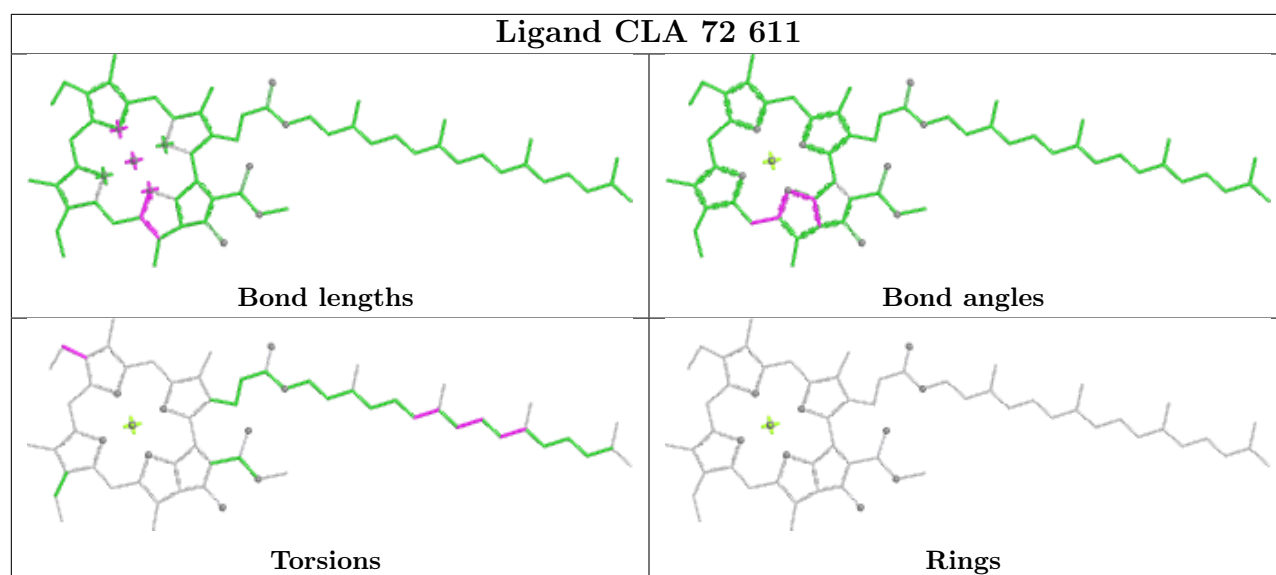


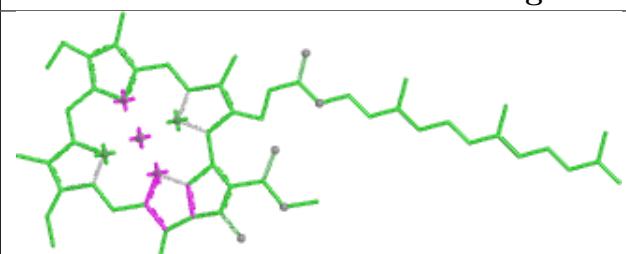
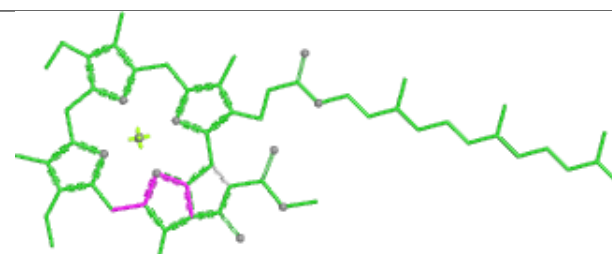
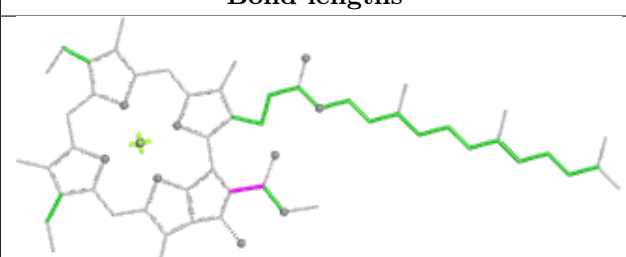
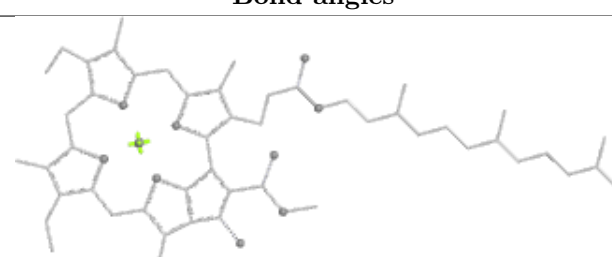


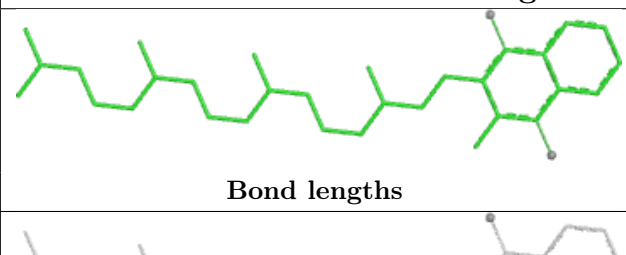
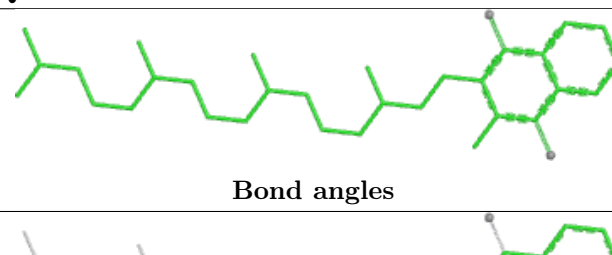
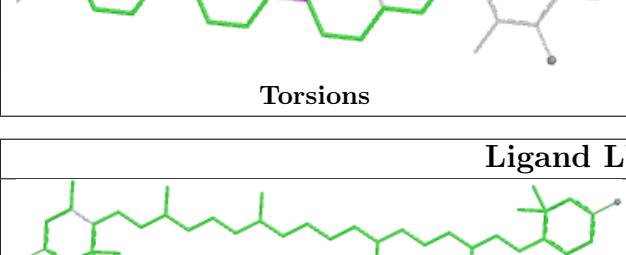


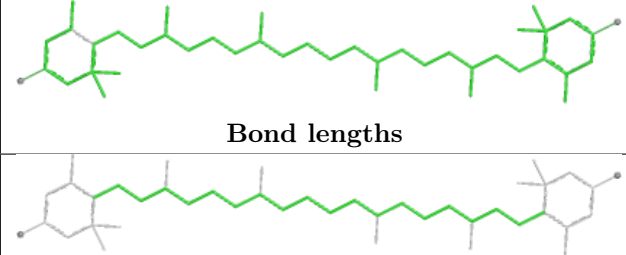
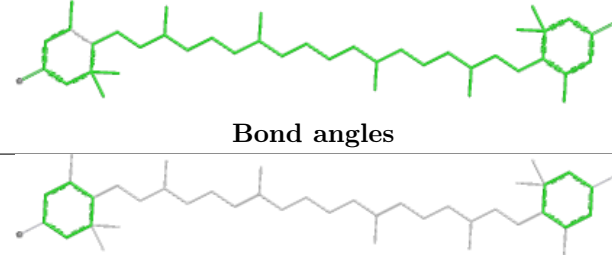


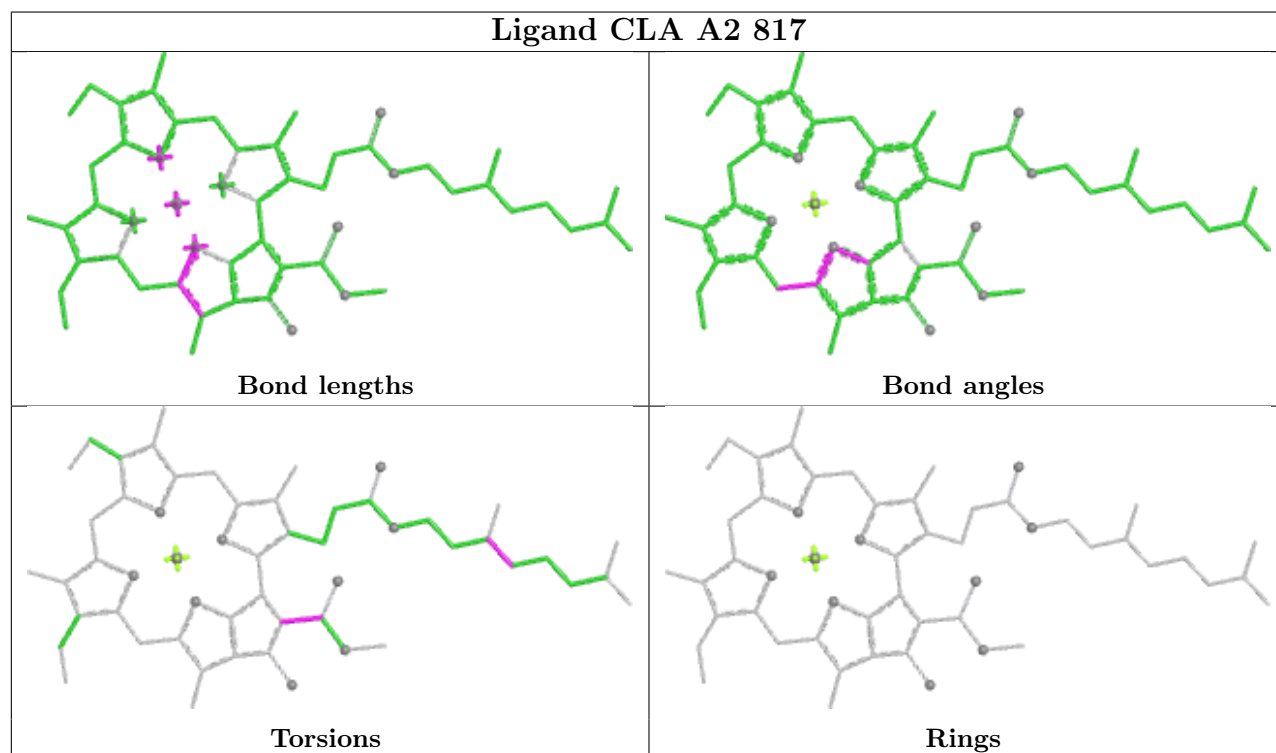
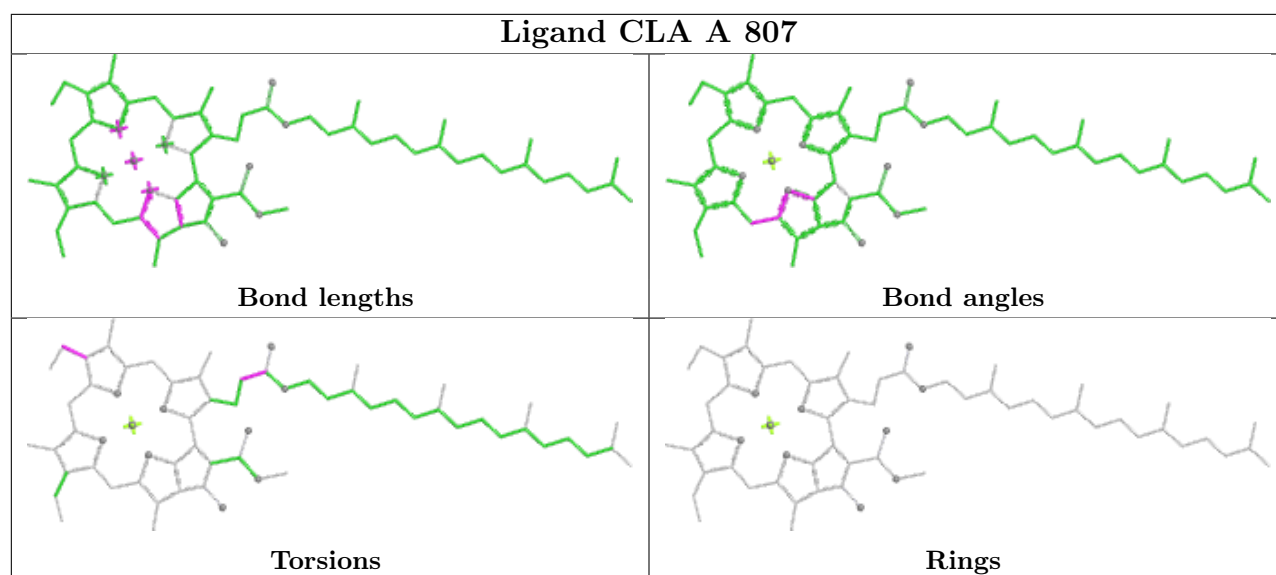


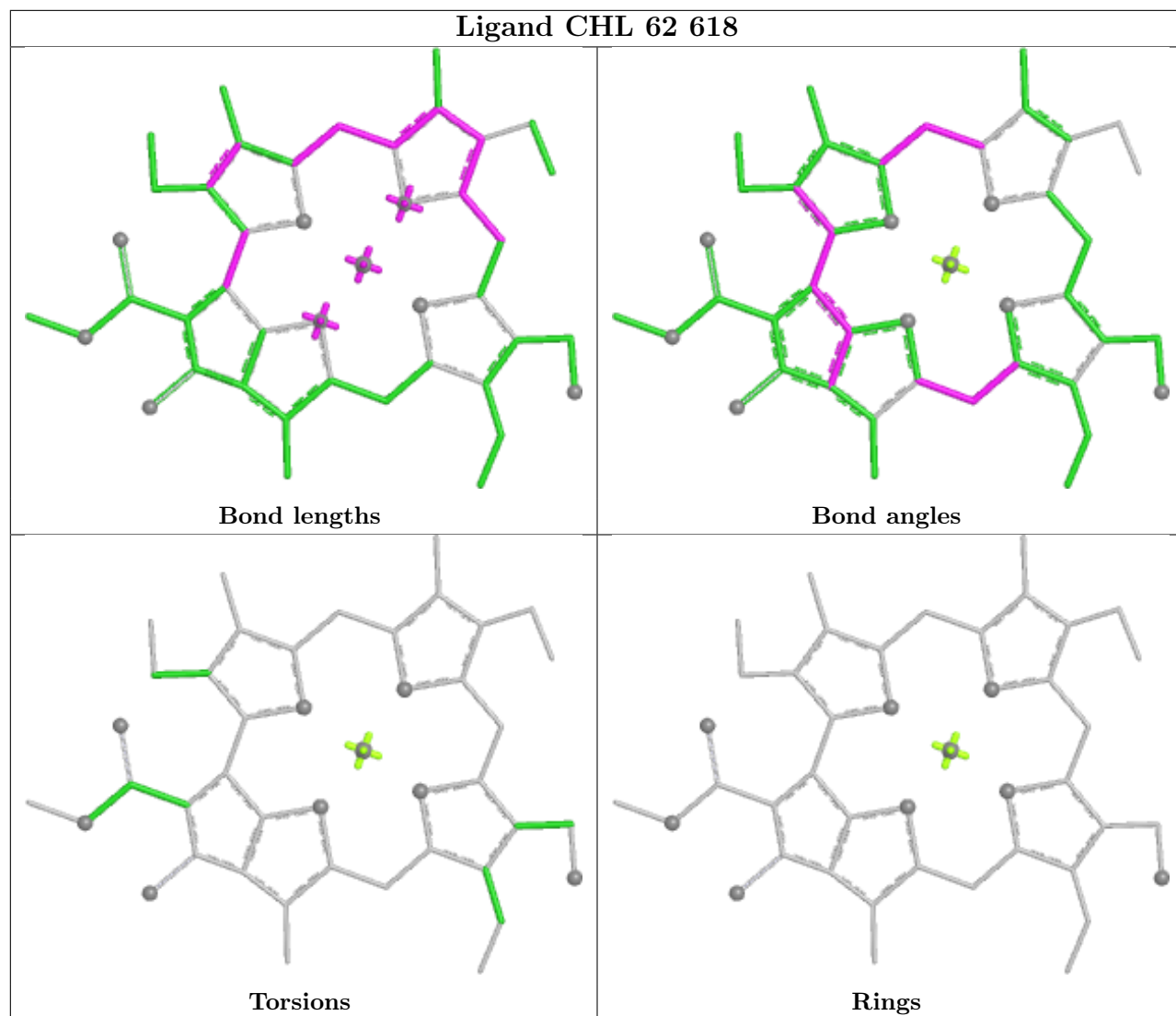


Ligand CLA 1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

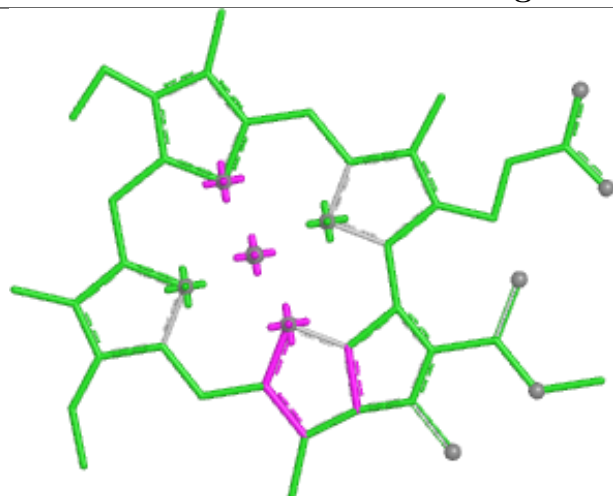
Ligand PQN B 842	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 32 720	
	
Bond lengths	Bond angles
	
Torsions	Rings

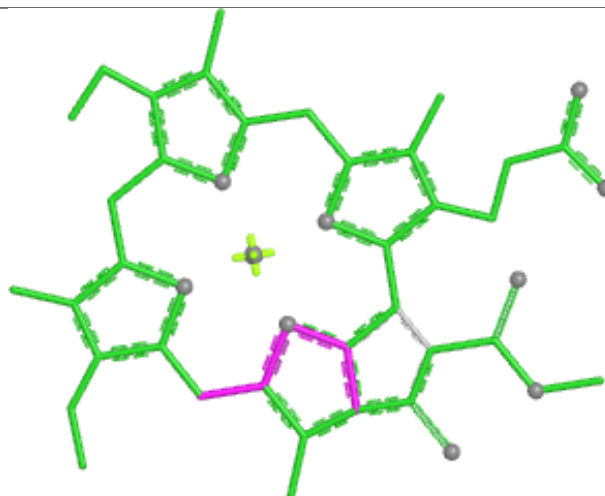




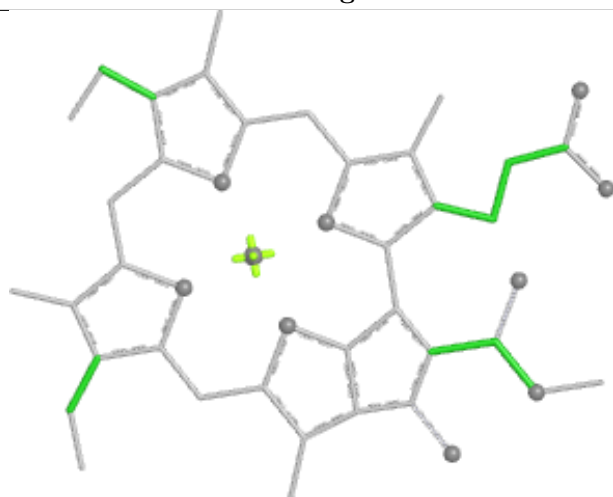
Ligand CLA B 830



Bond lengths



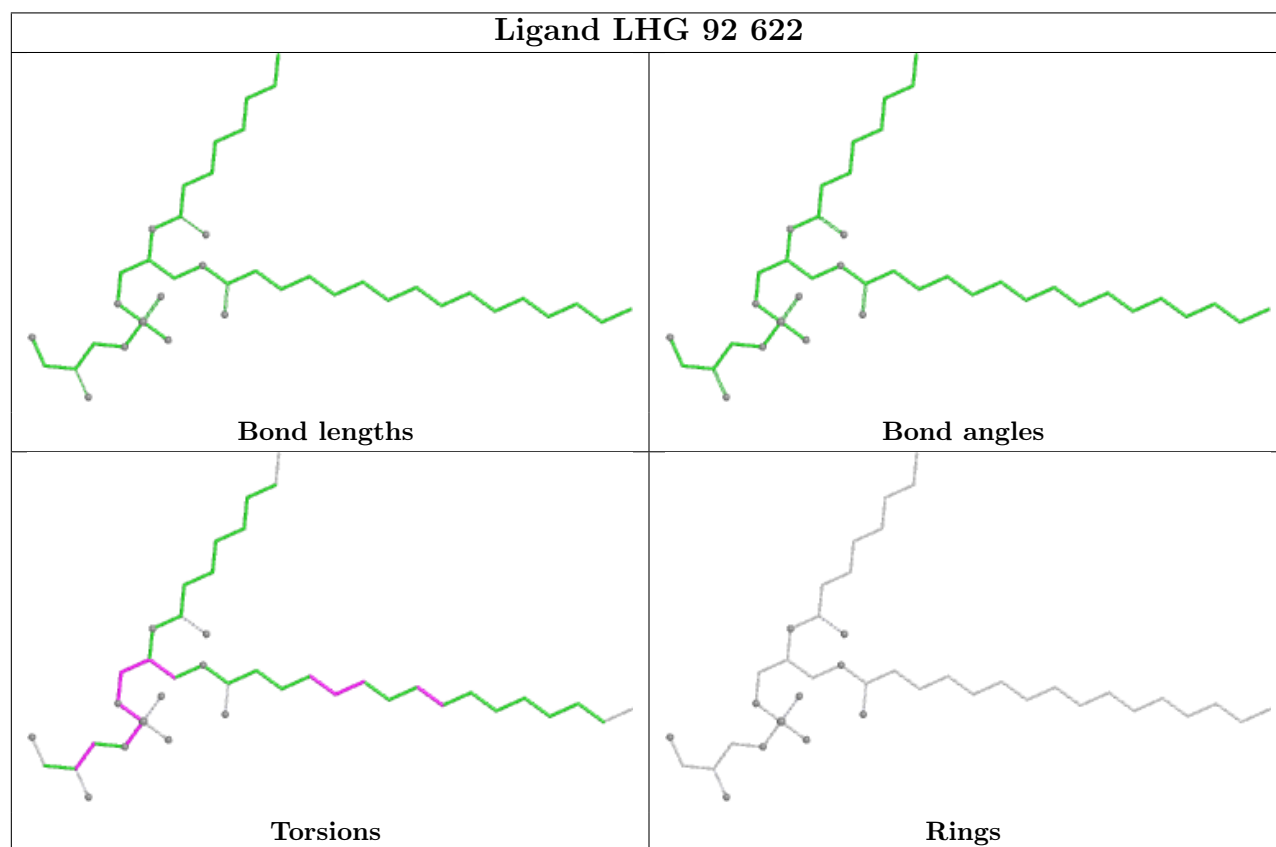
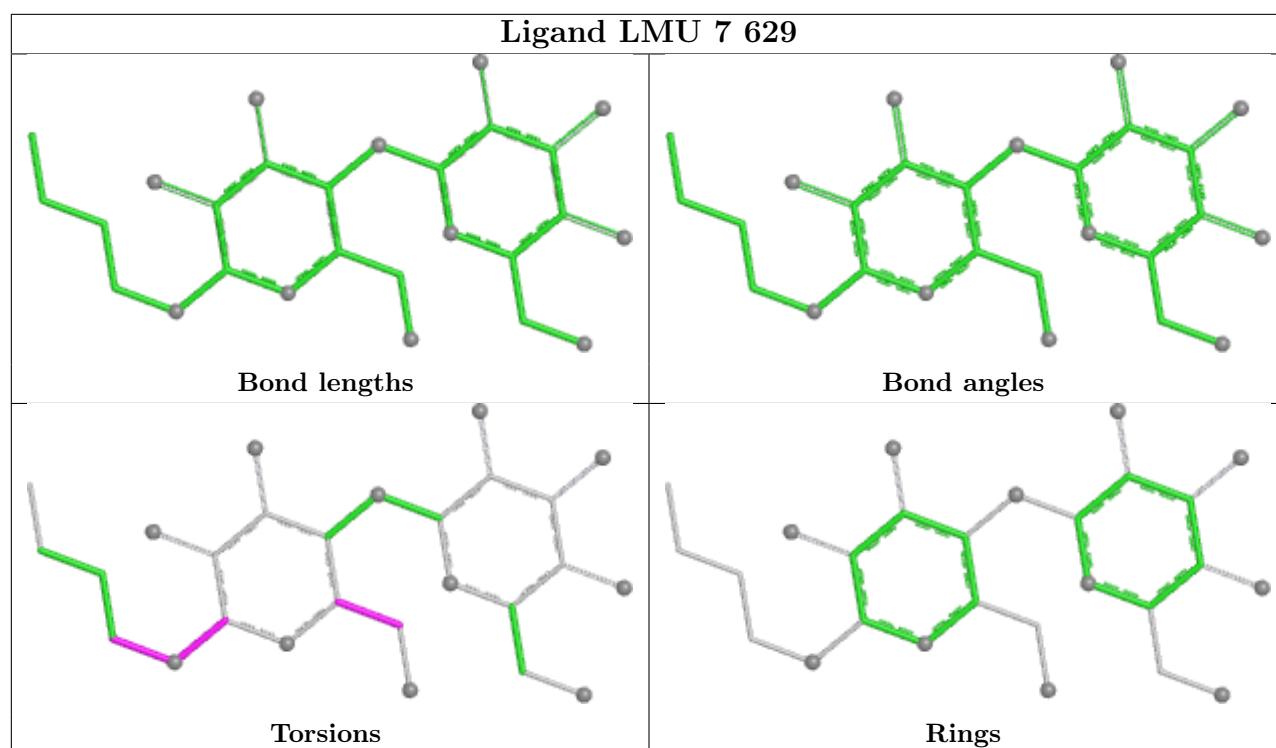
Bond angles

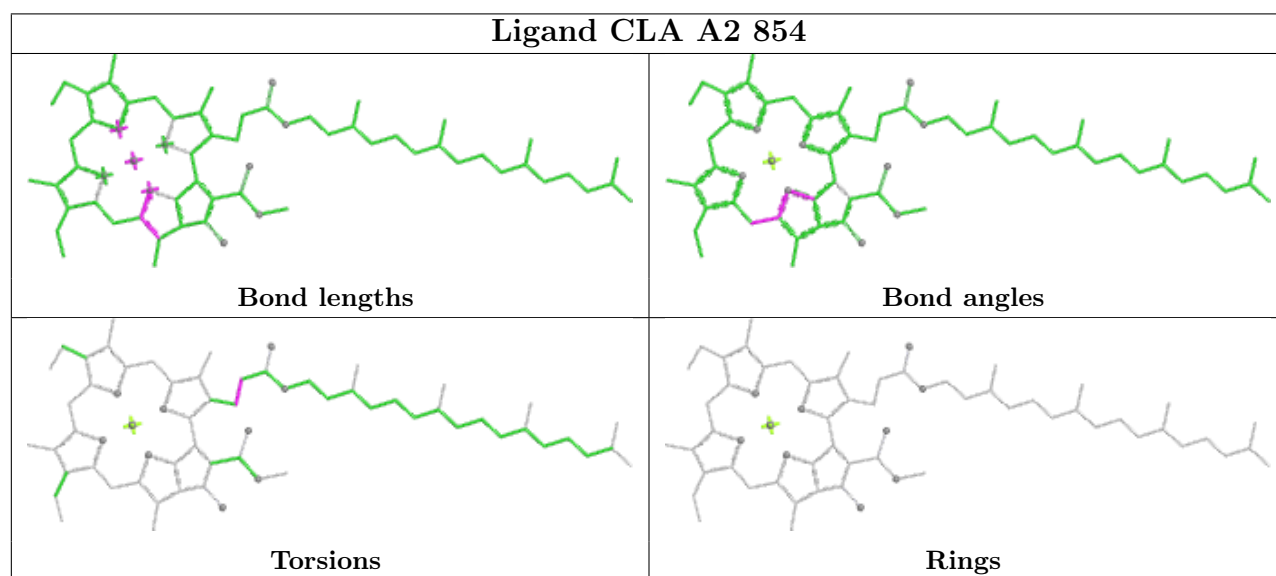
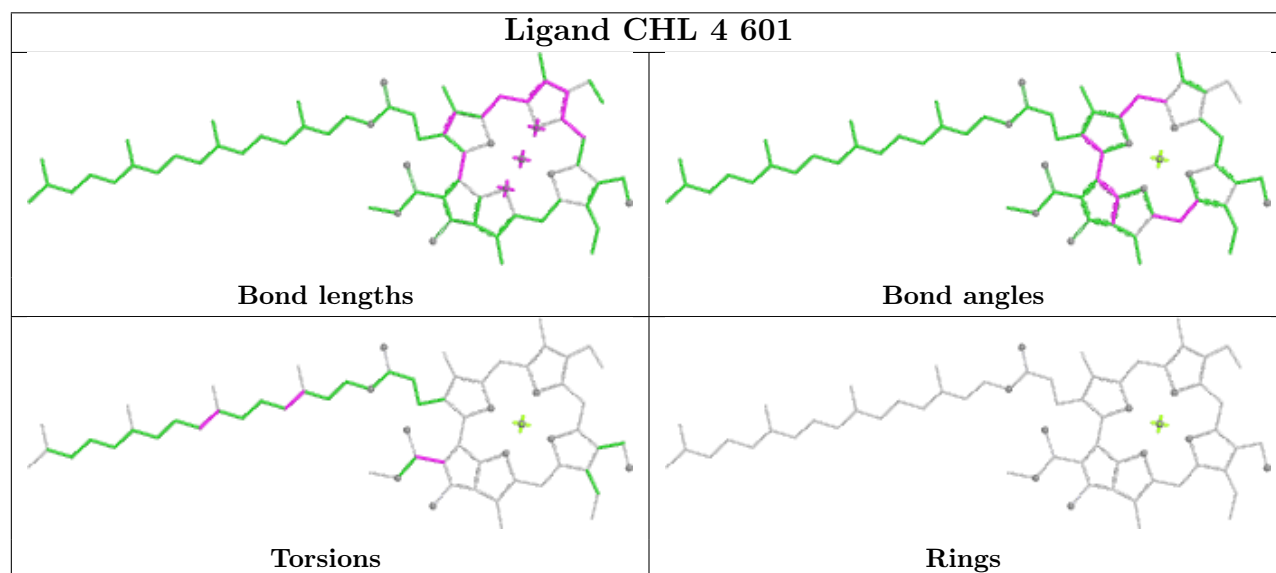
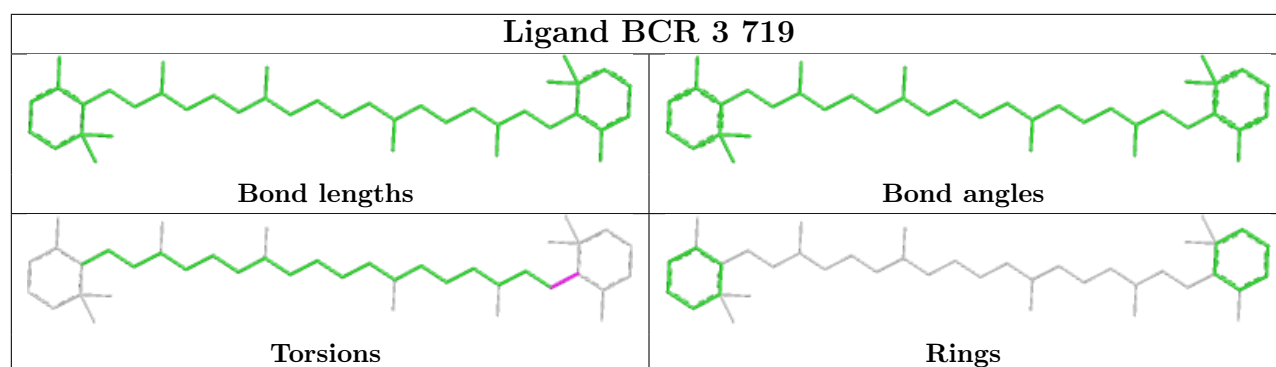


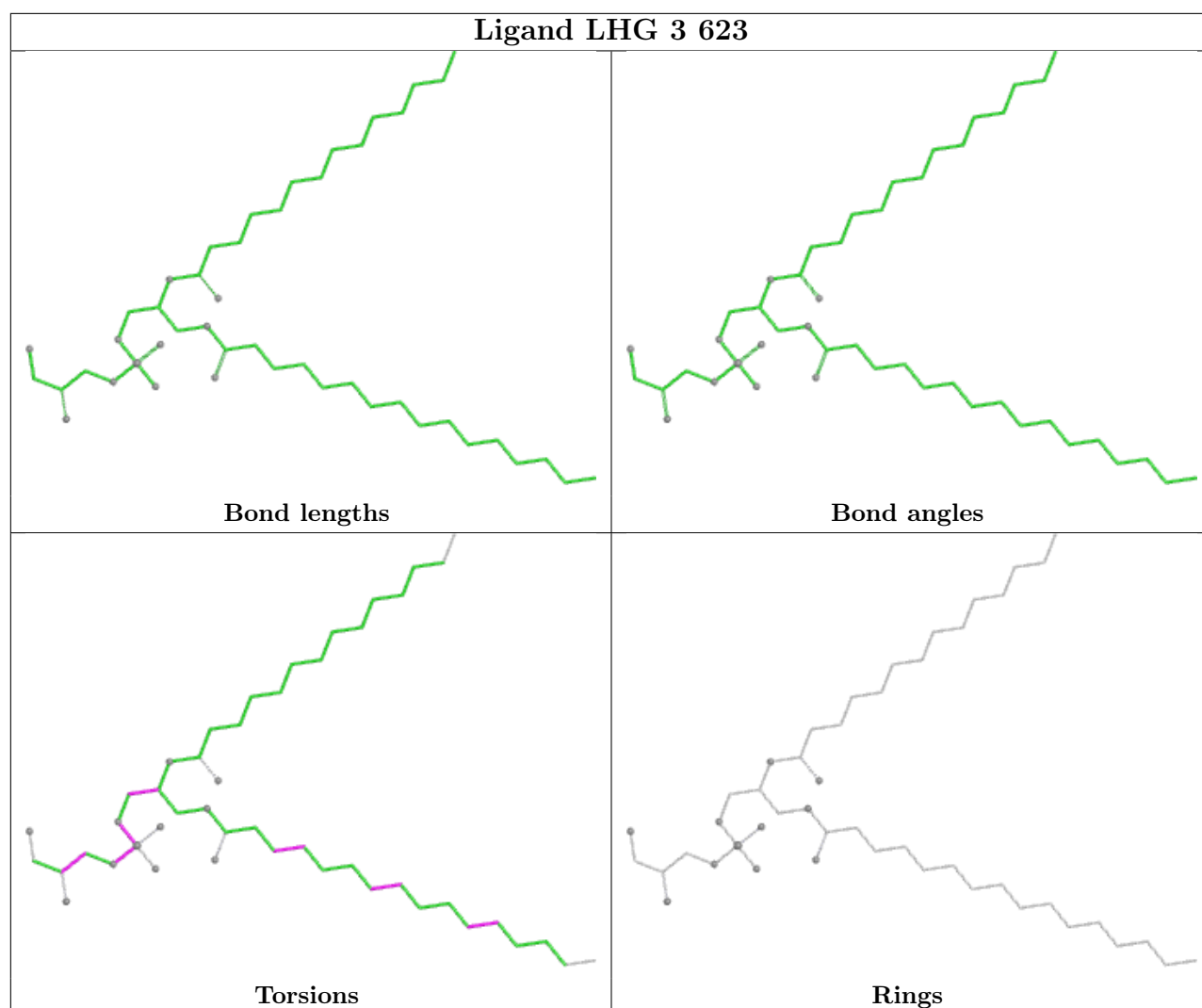
Torsions



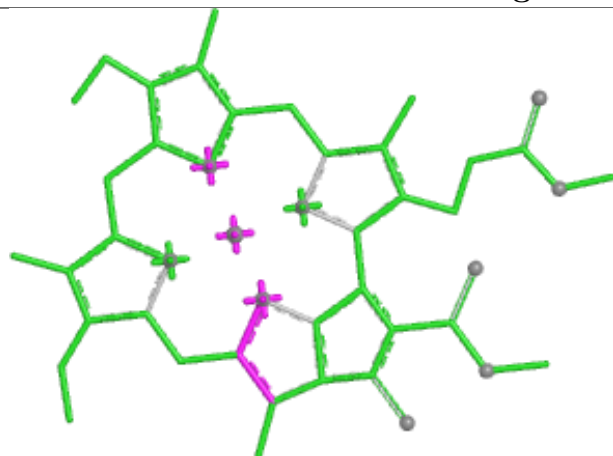
Rings



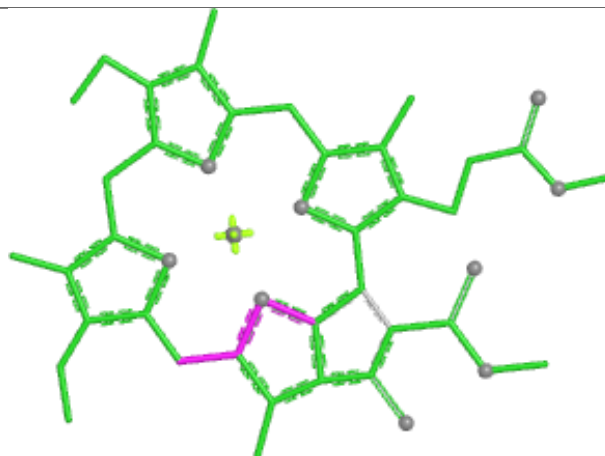




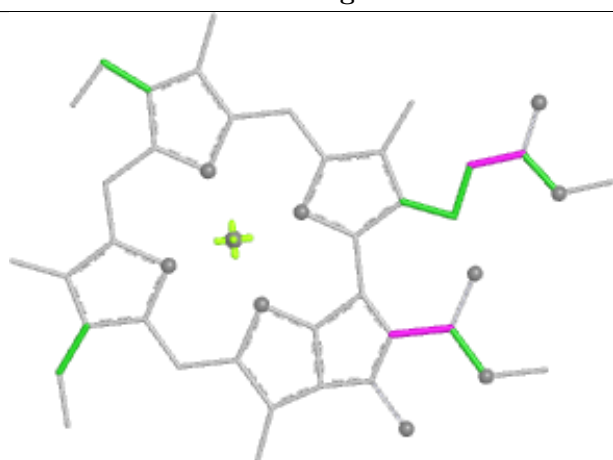
Ligand CLA G 204



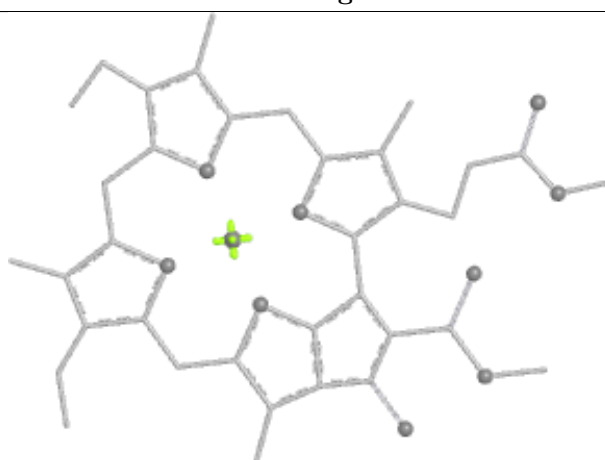
Bond lengths



Bond angles

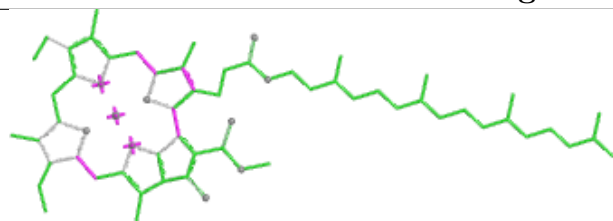


Torsions

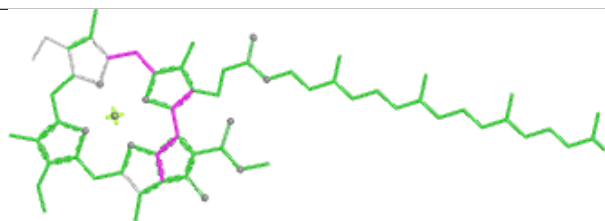


Rings

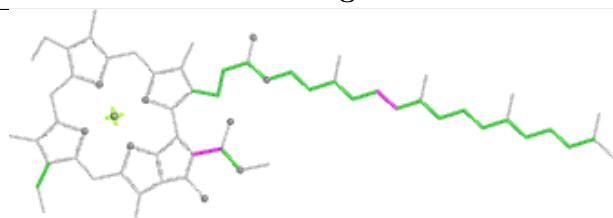
Ligand CL0 A 801



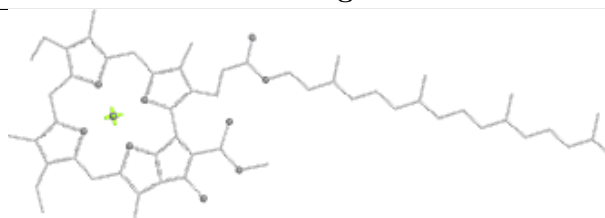
Bond lengths



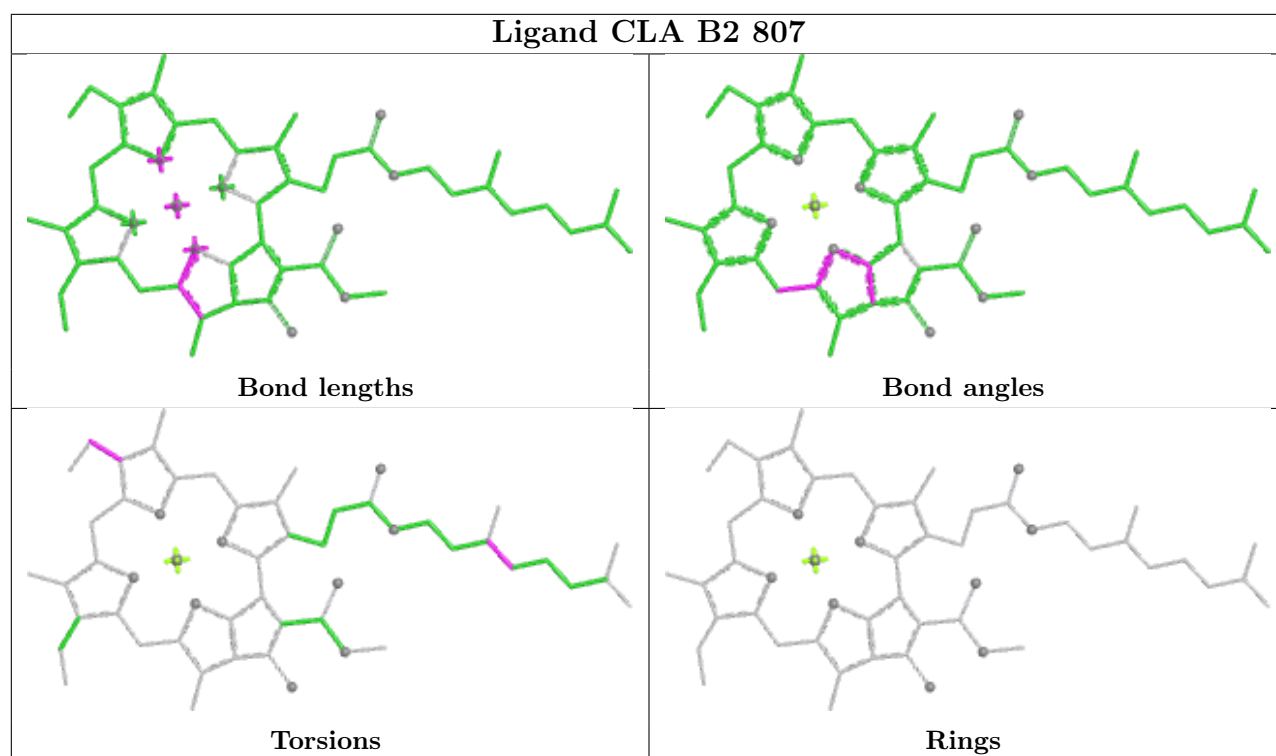
Bond angles



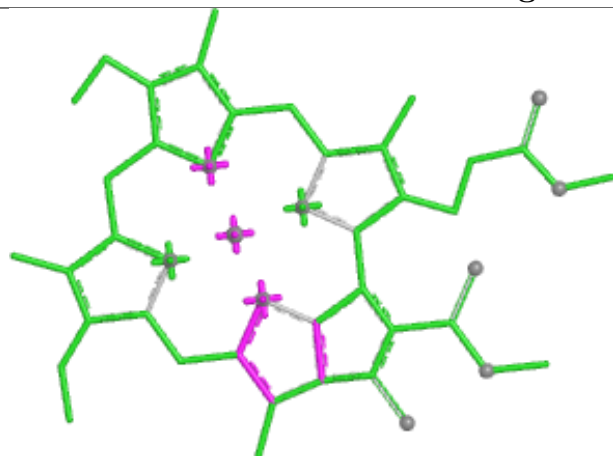
Torsions



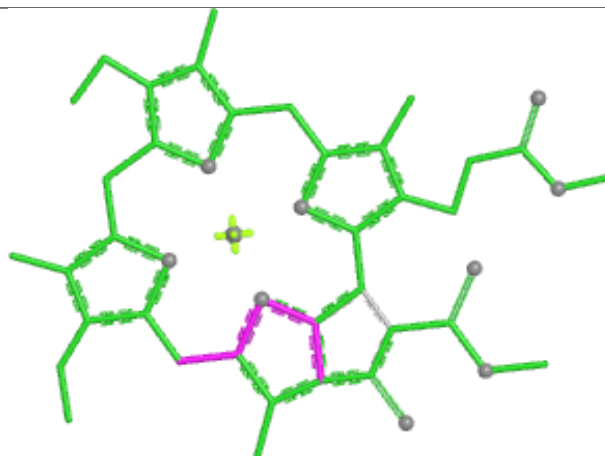
Rings



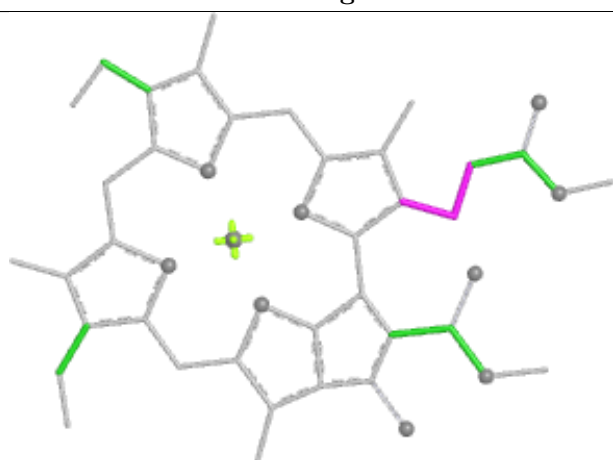
Ligand CLA 7 616



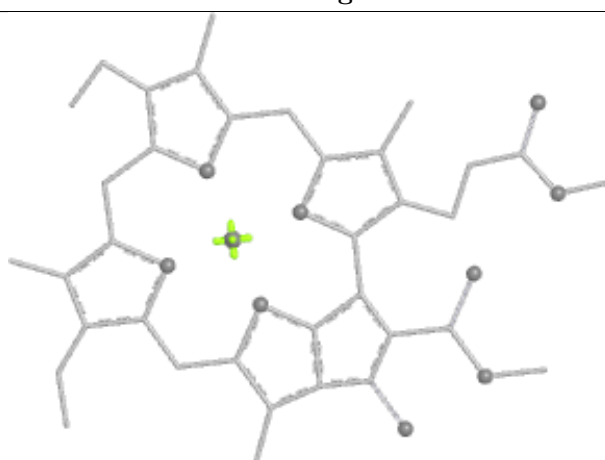
Bond lengths



Bond angles

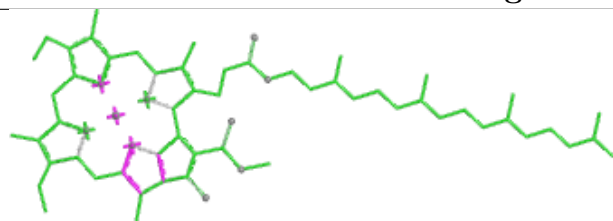


Torsions

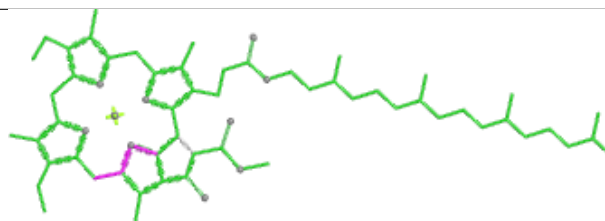


Rings

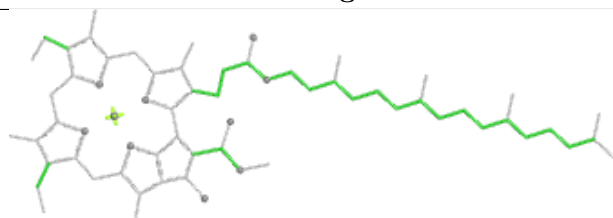
Ligand CLA A2 802



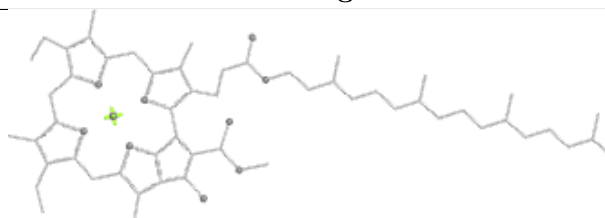
Bond lengths



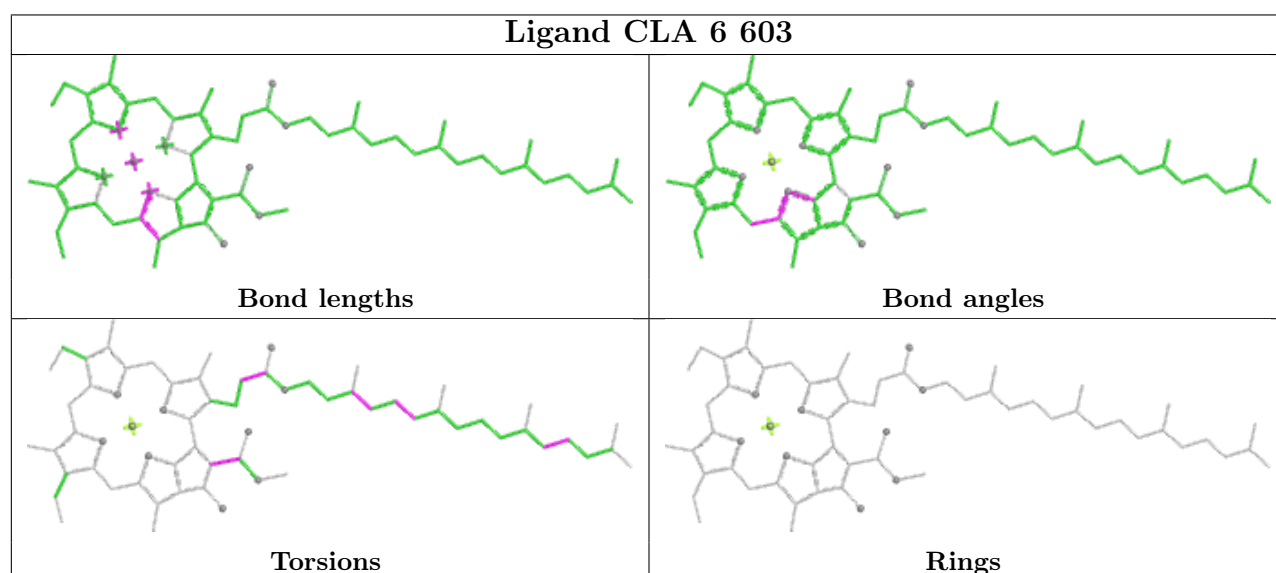
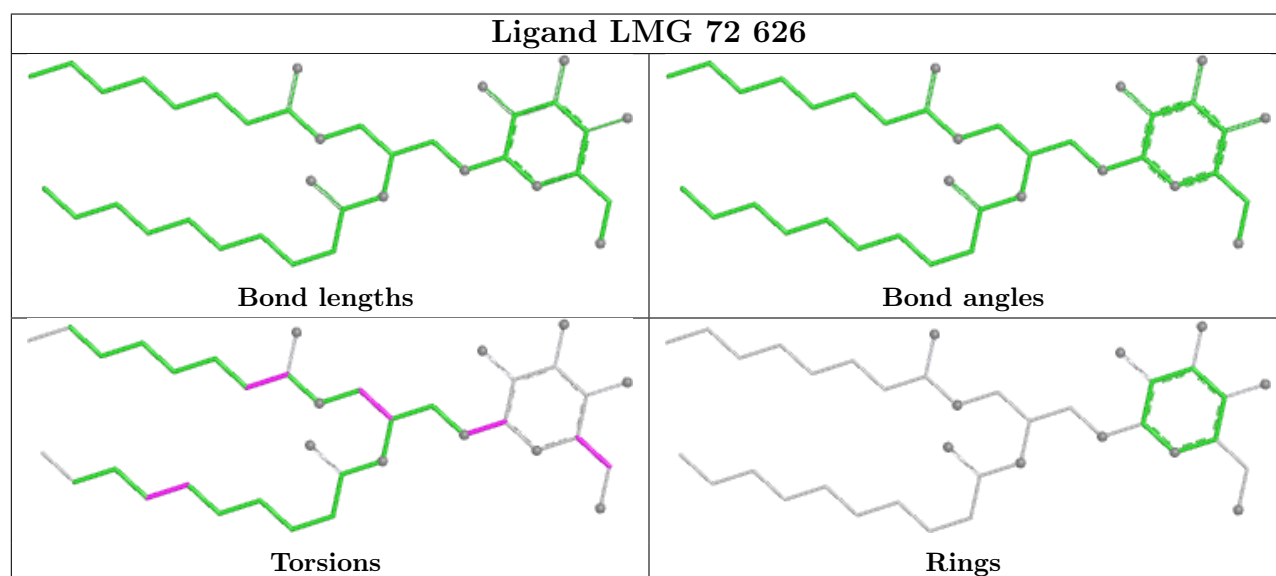
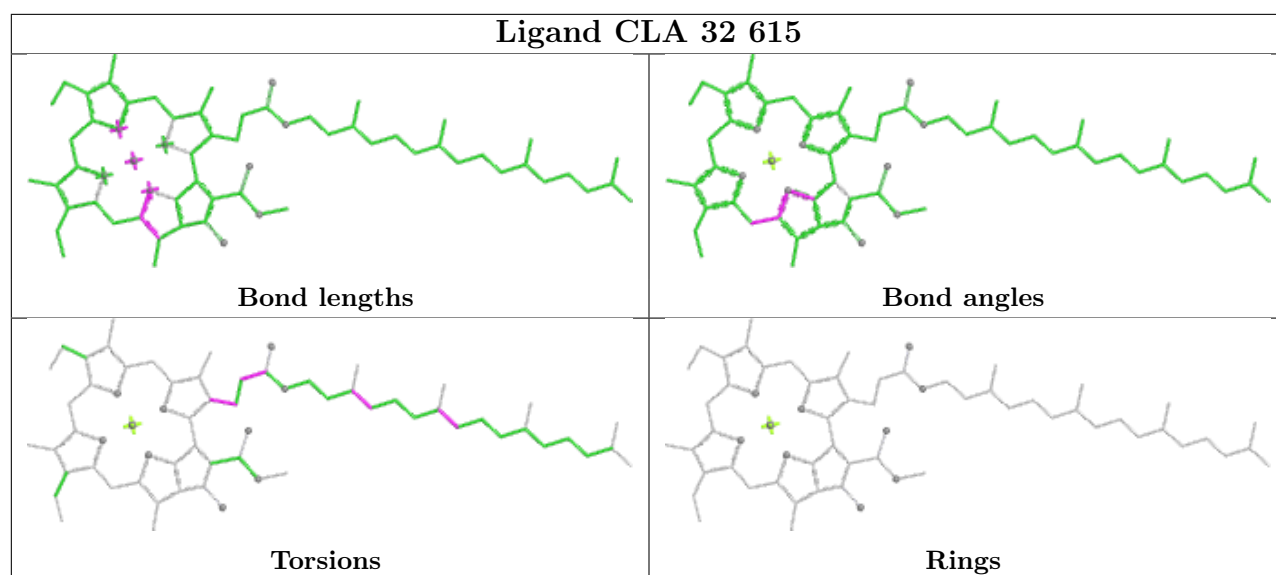
Bond angles

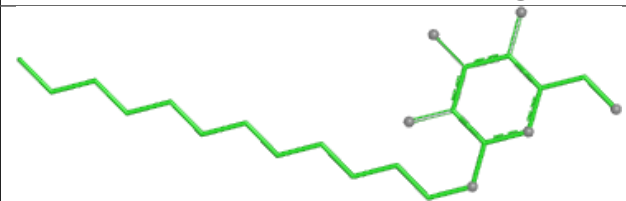
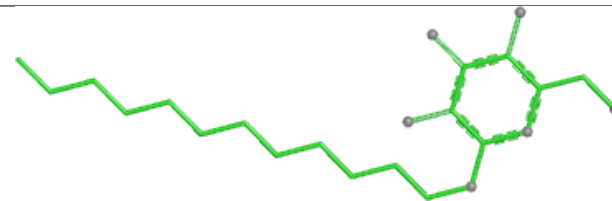
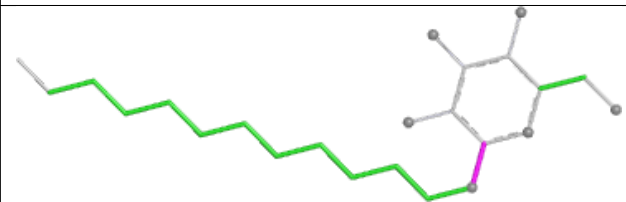
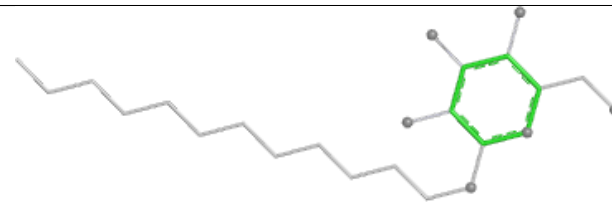
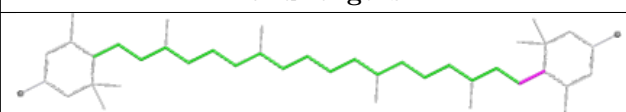
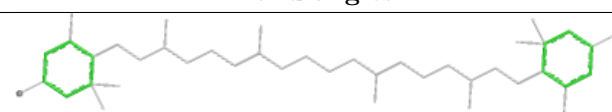
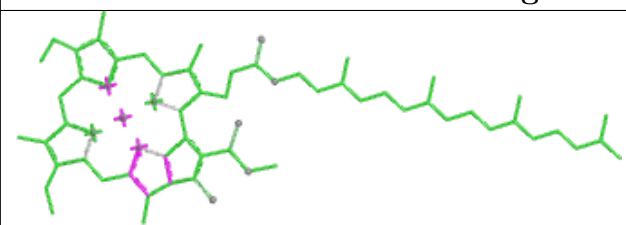
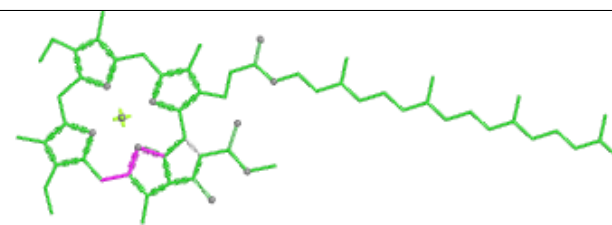
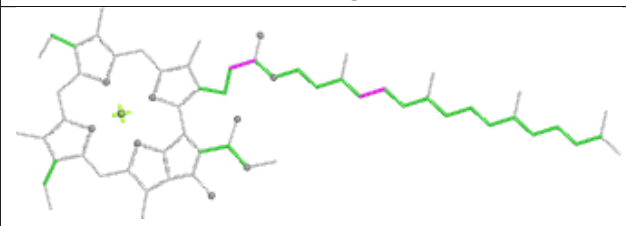
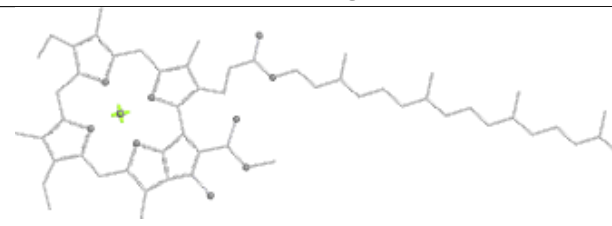


Torsions

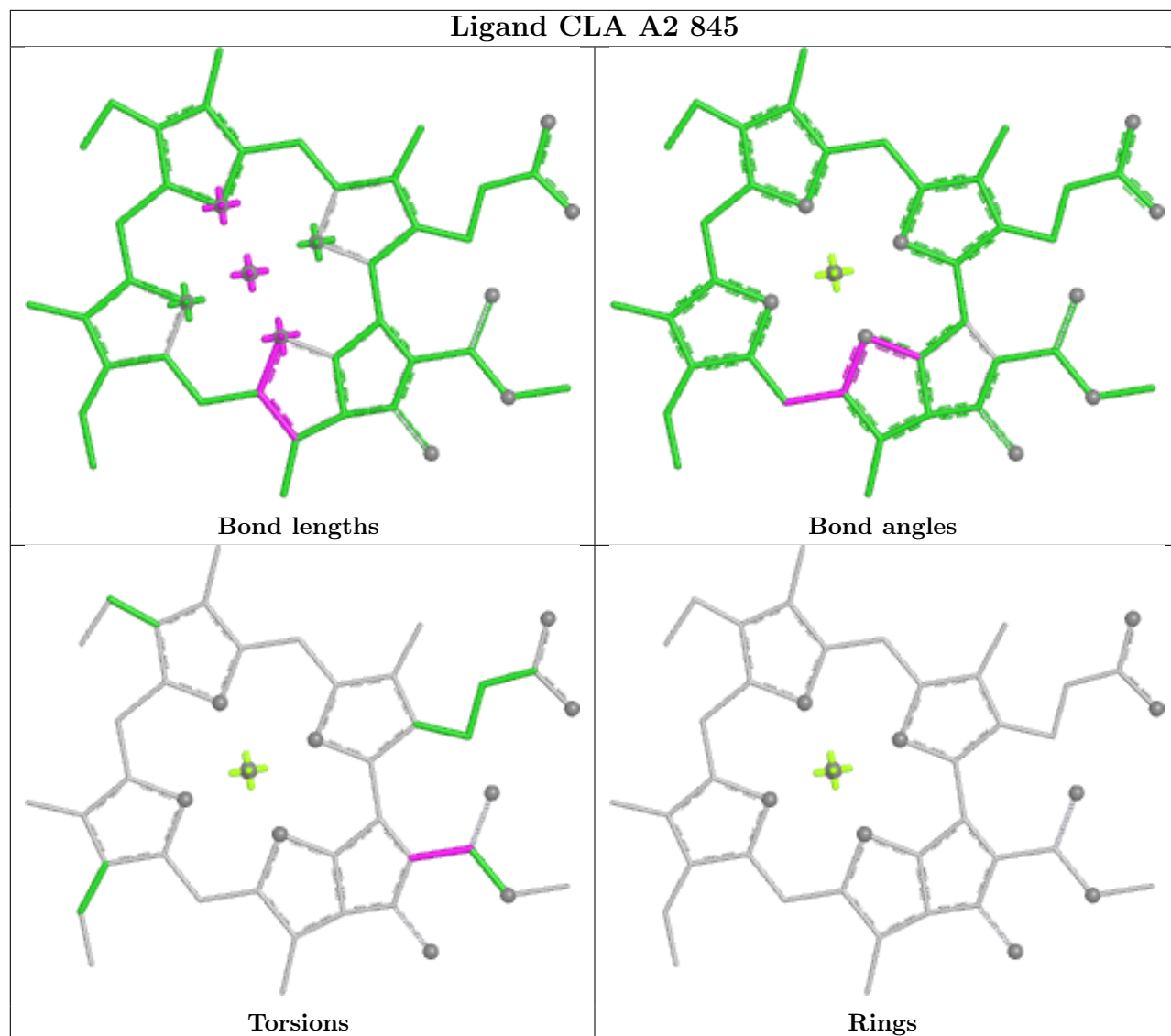


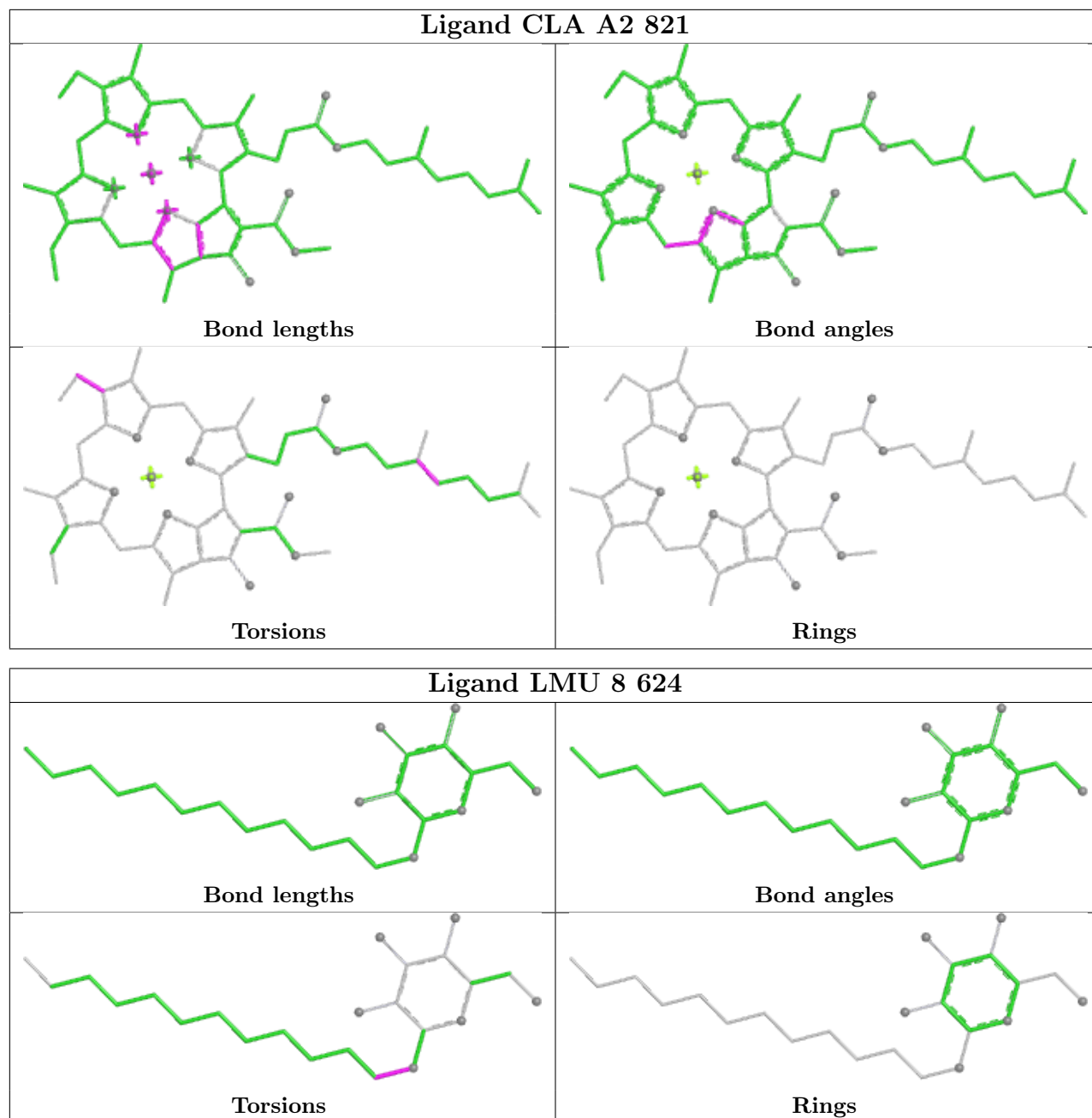
Rings



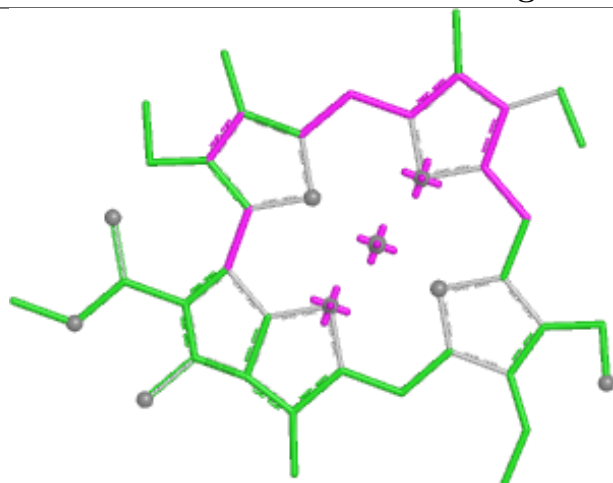
Ligand LMU 62 628	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LUT 3 622	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA B 806	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA A2 845

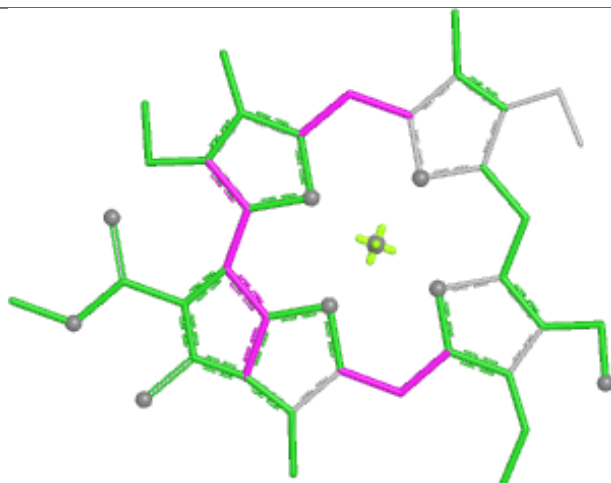




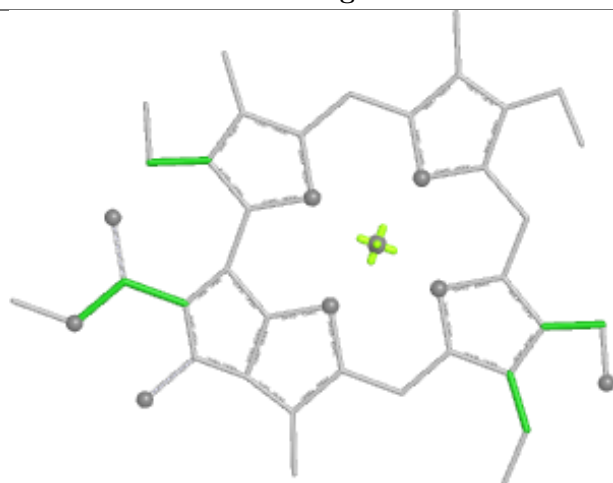
Ligand CHL 6 618



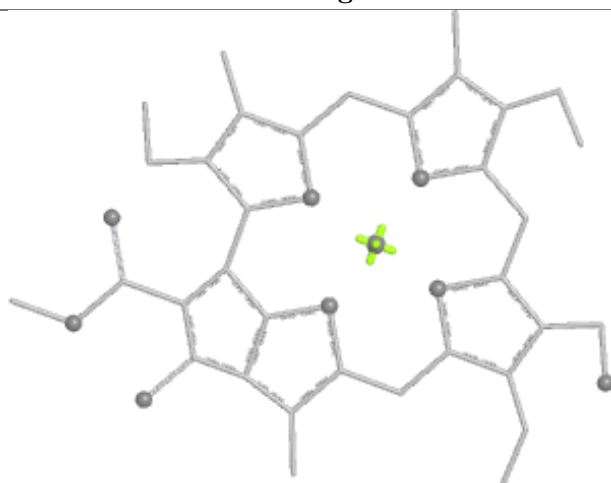
Bond lengths



Bond angles

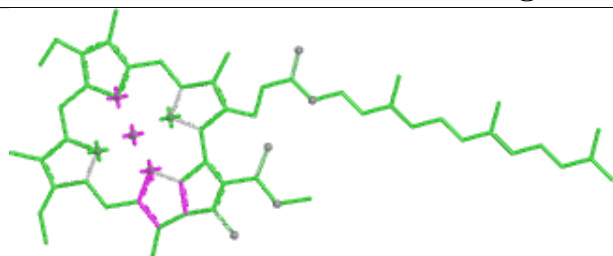


Torsions

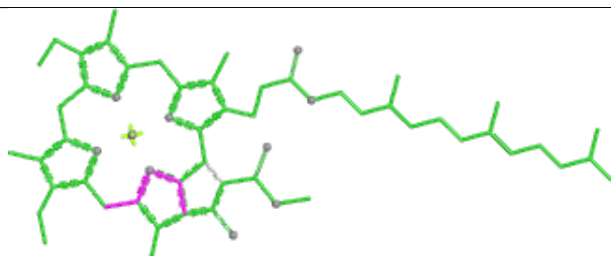


Rings

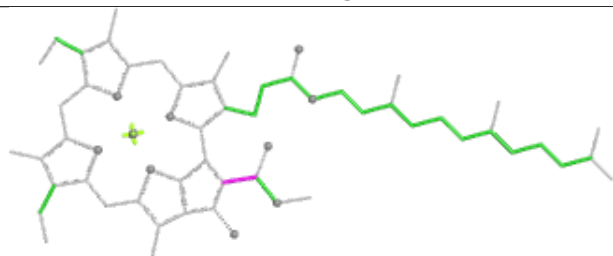
Ligand CLA 9 602



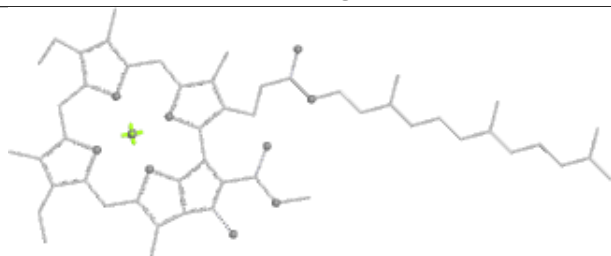
Bond lengths



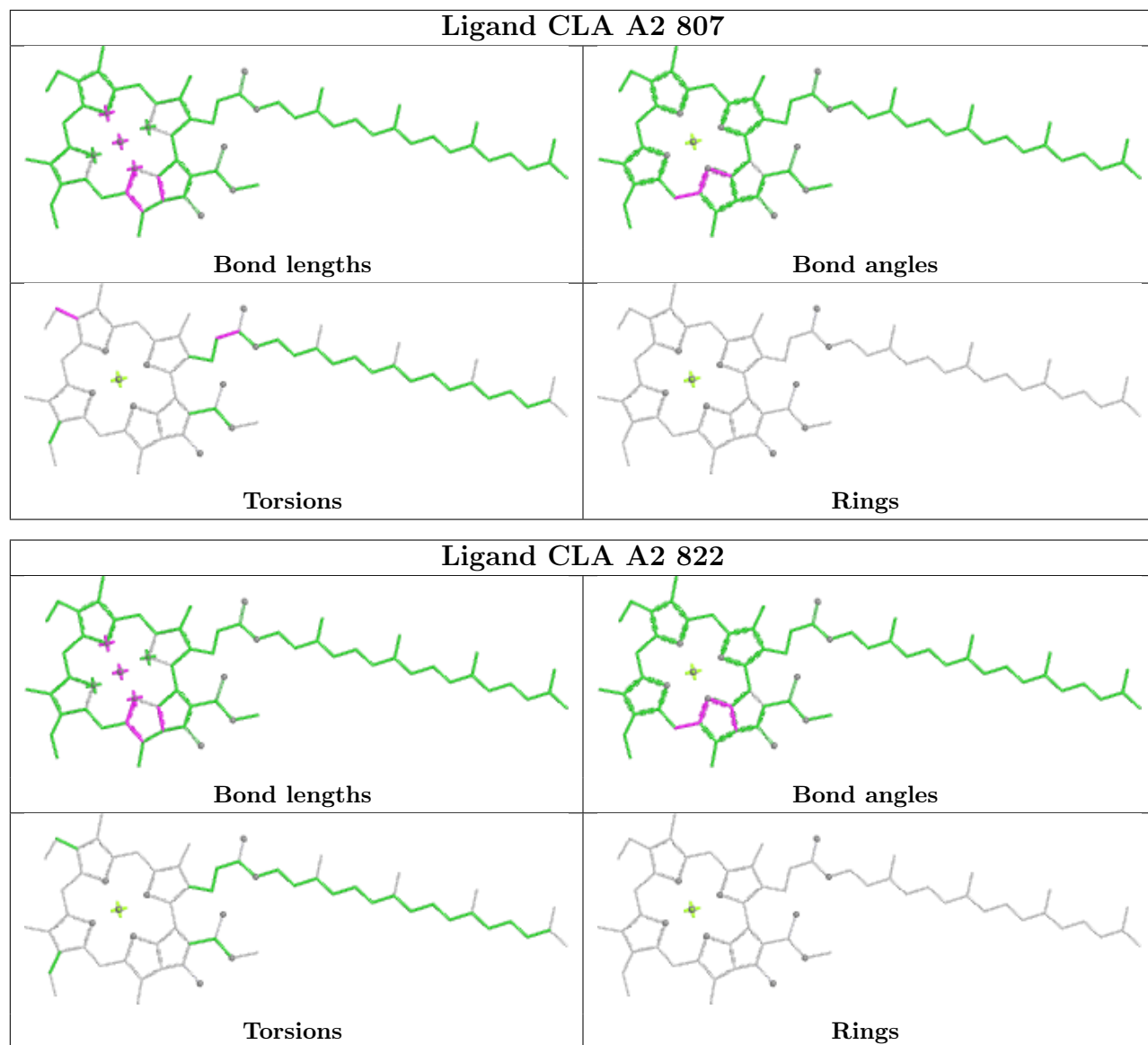
Bond angles

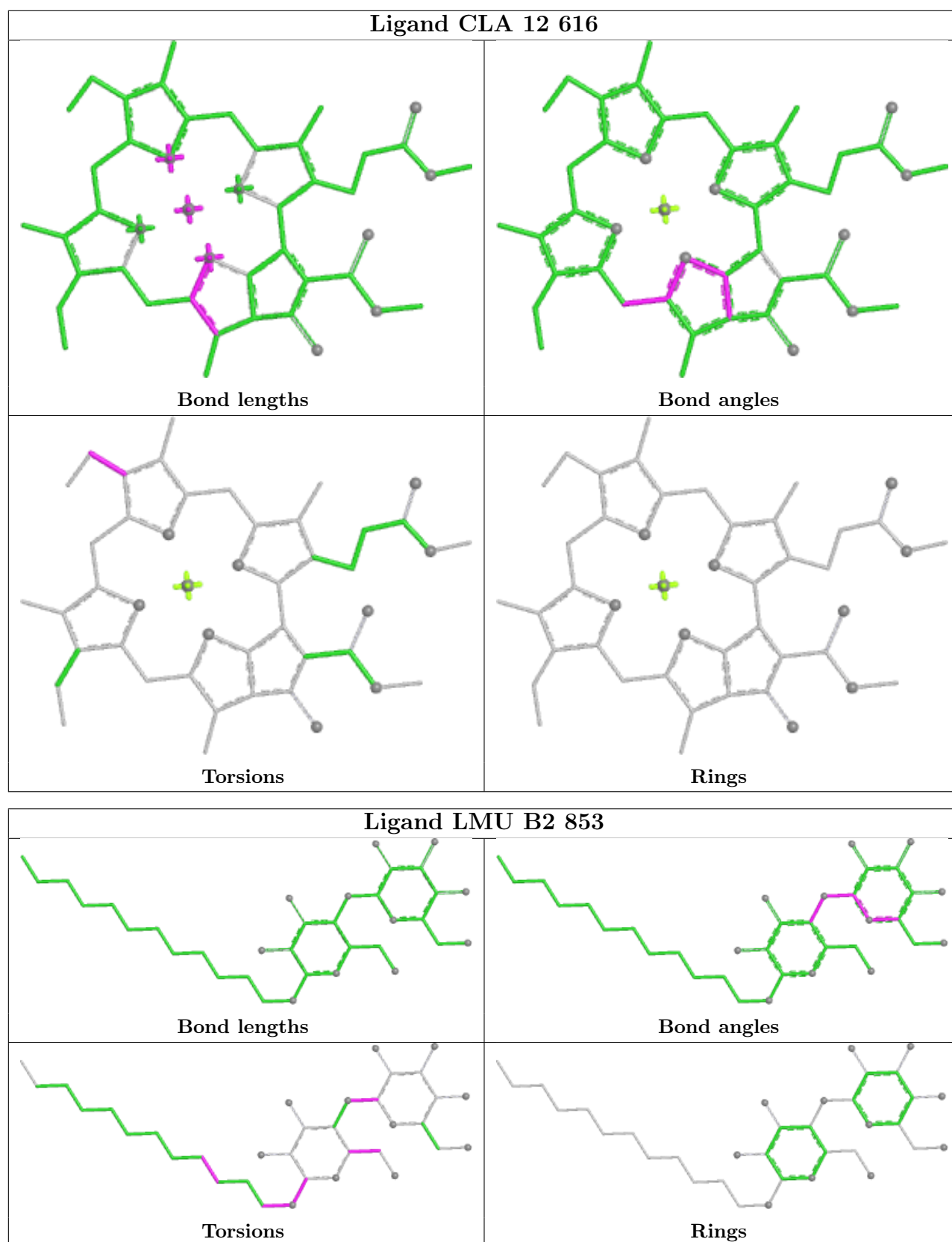


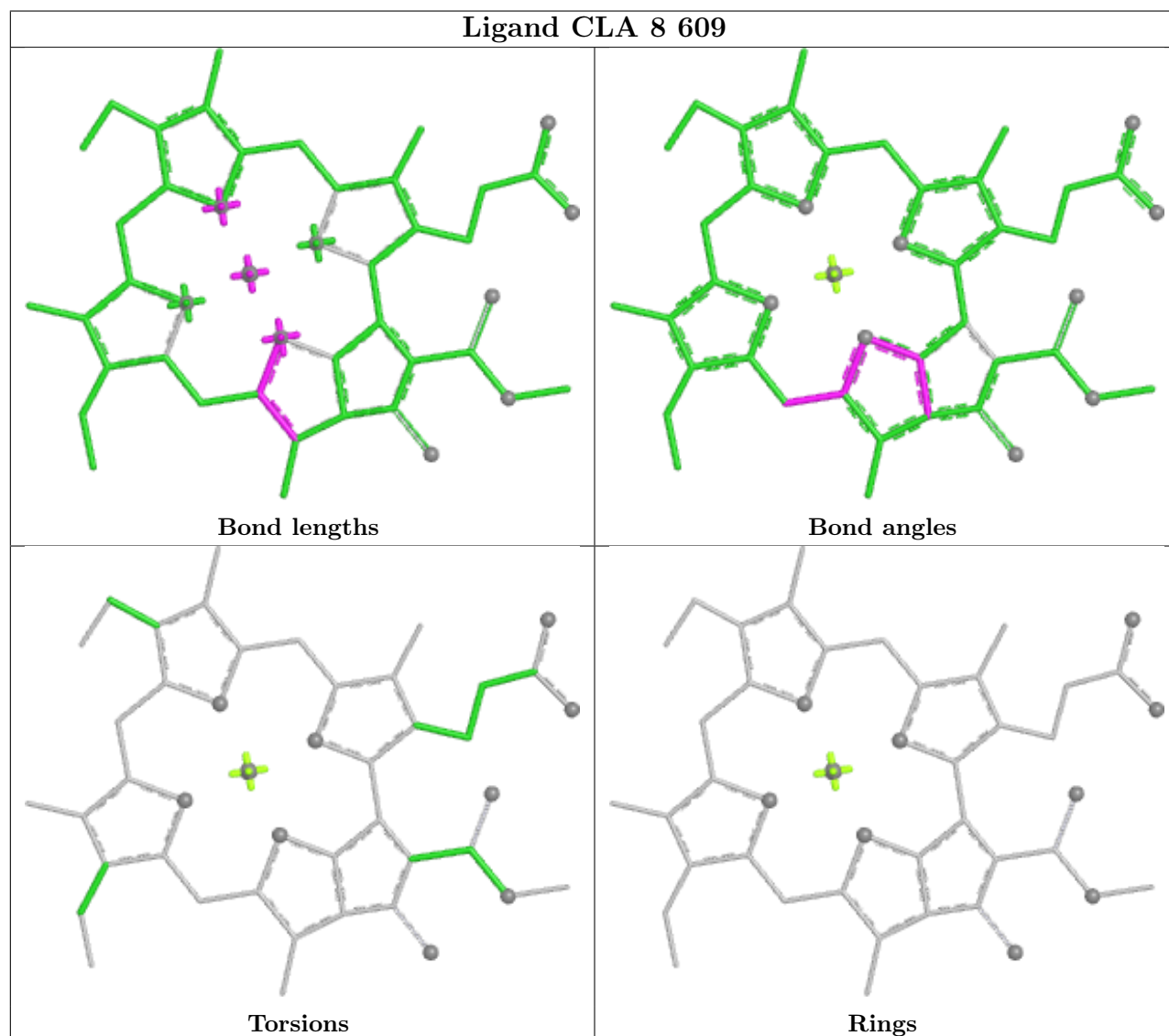
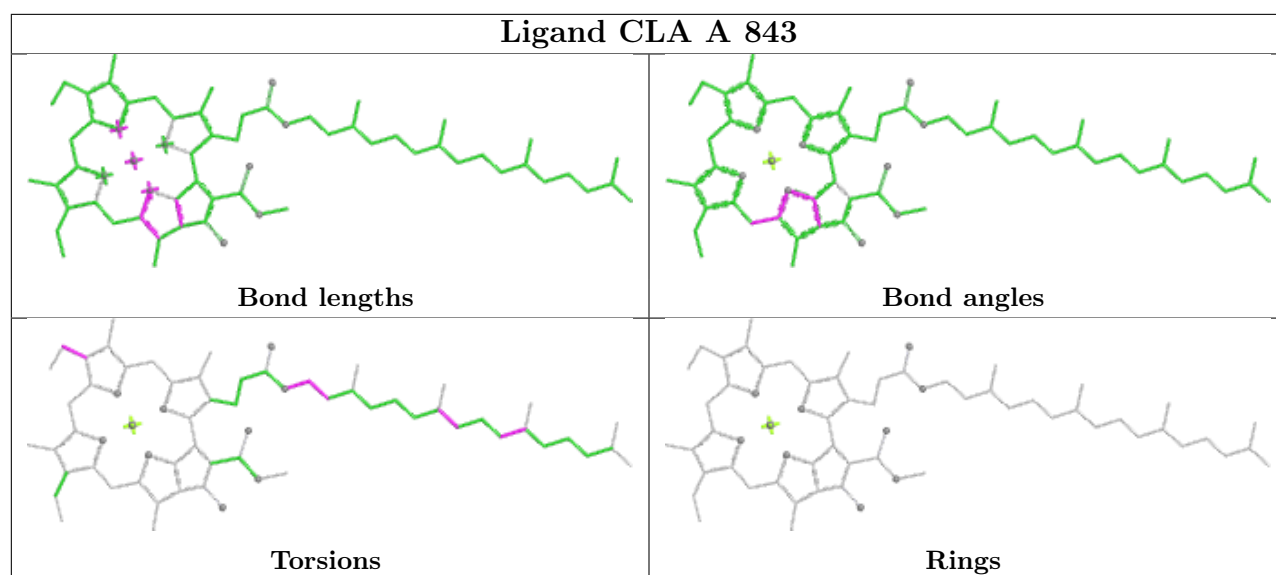
Torsions

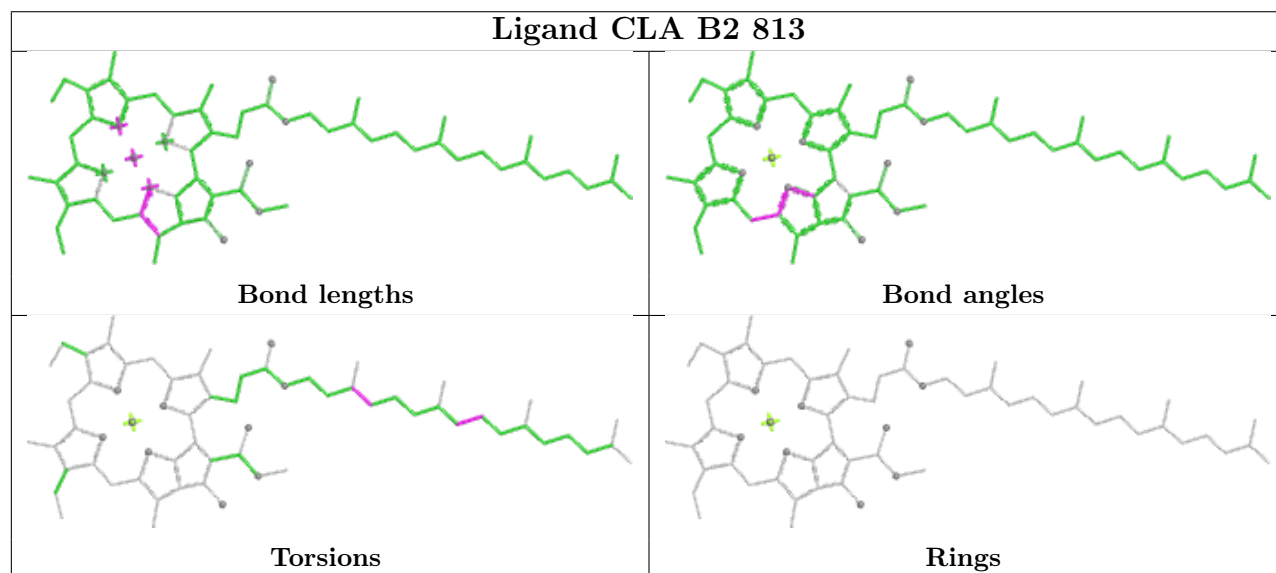
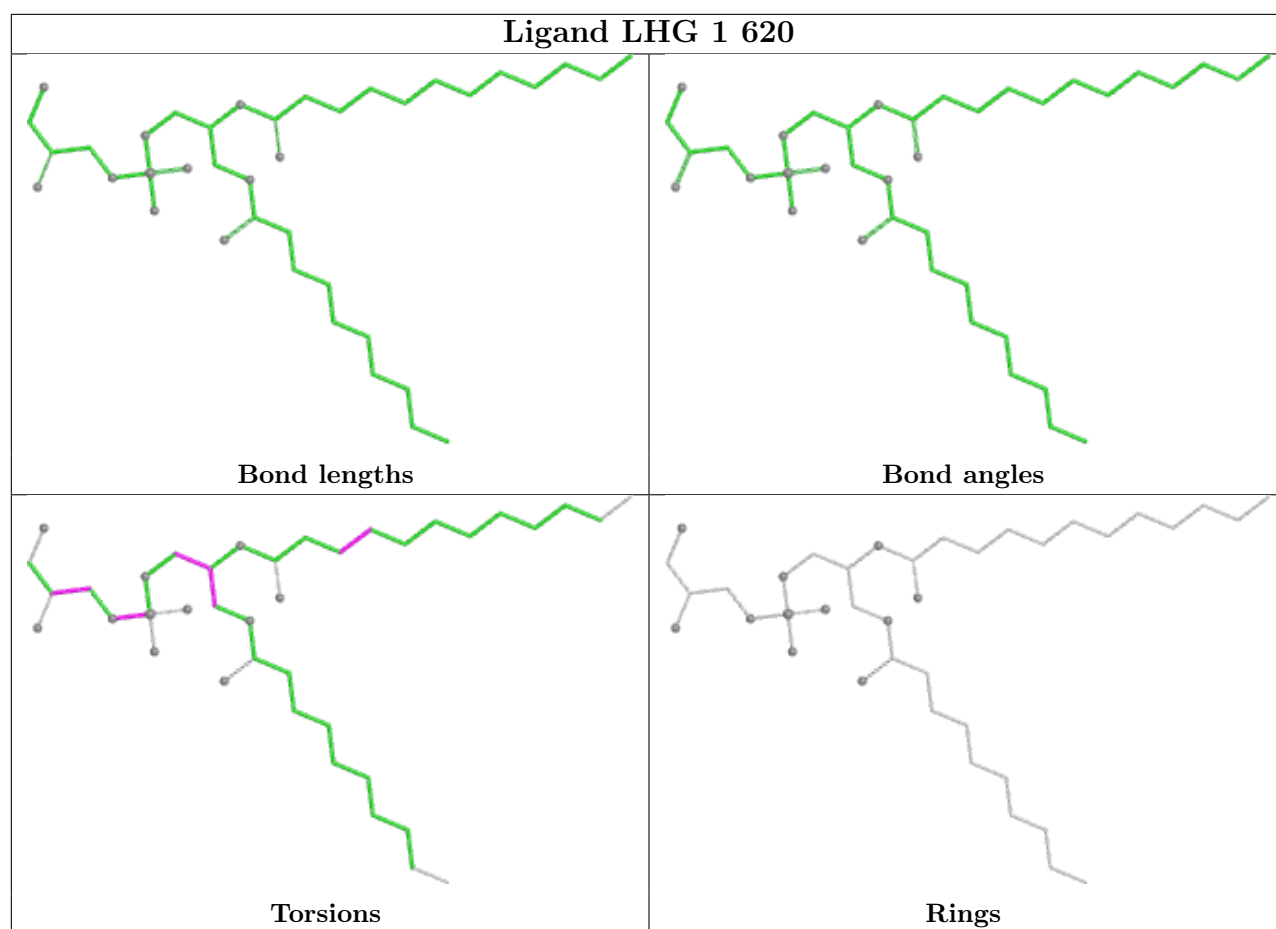


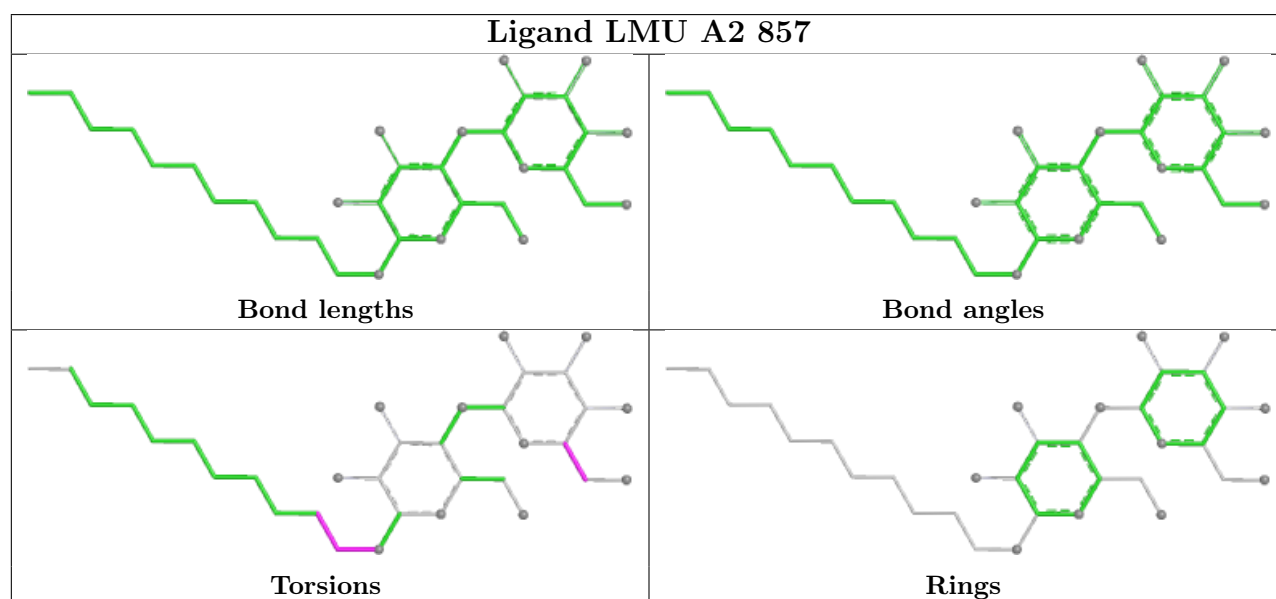
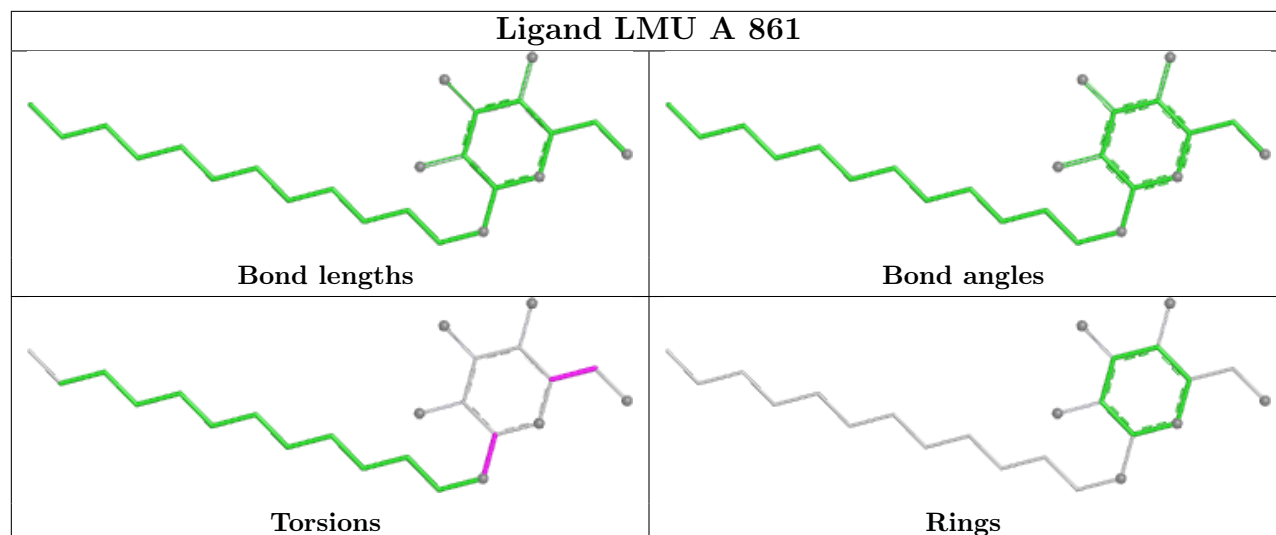
Rings

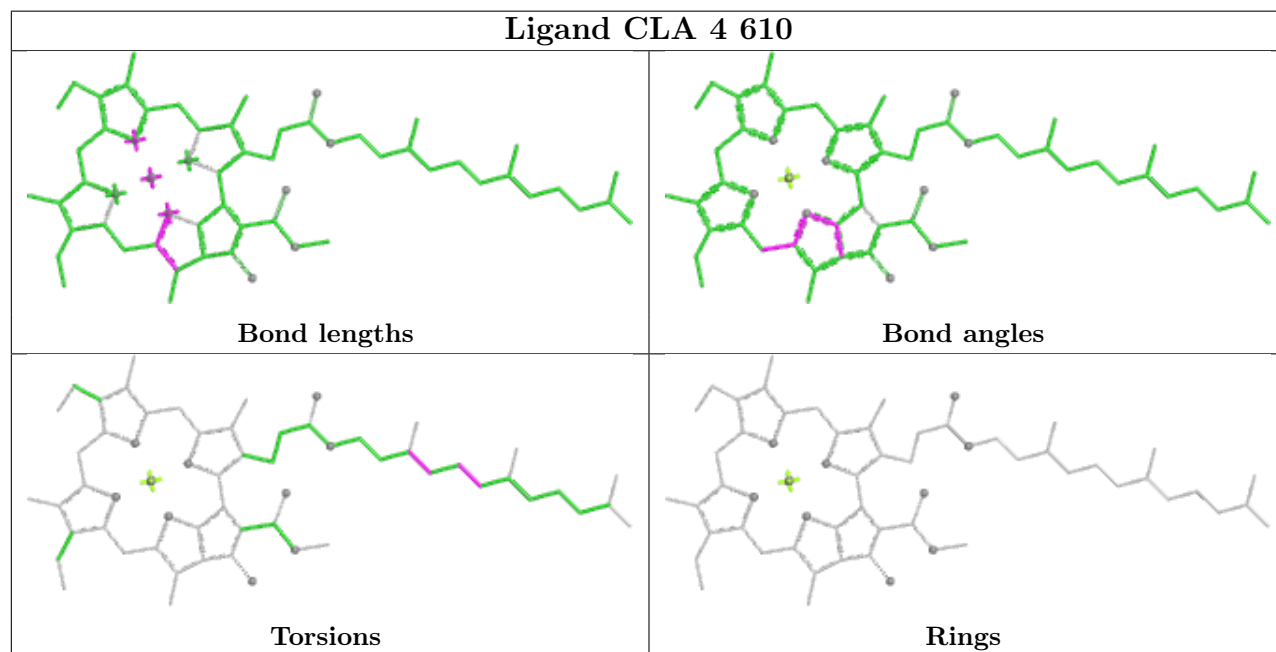
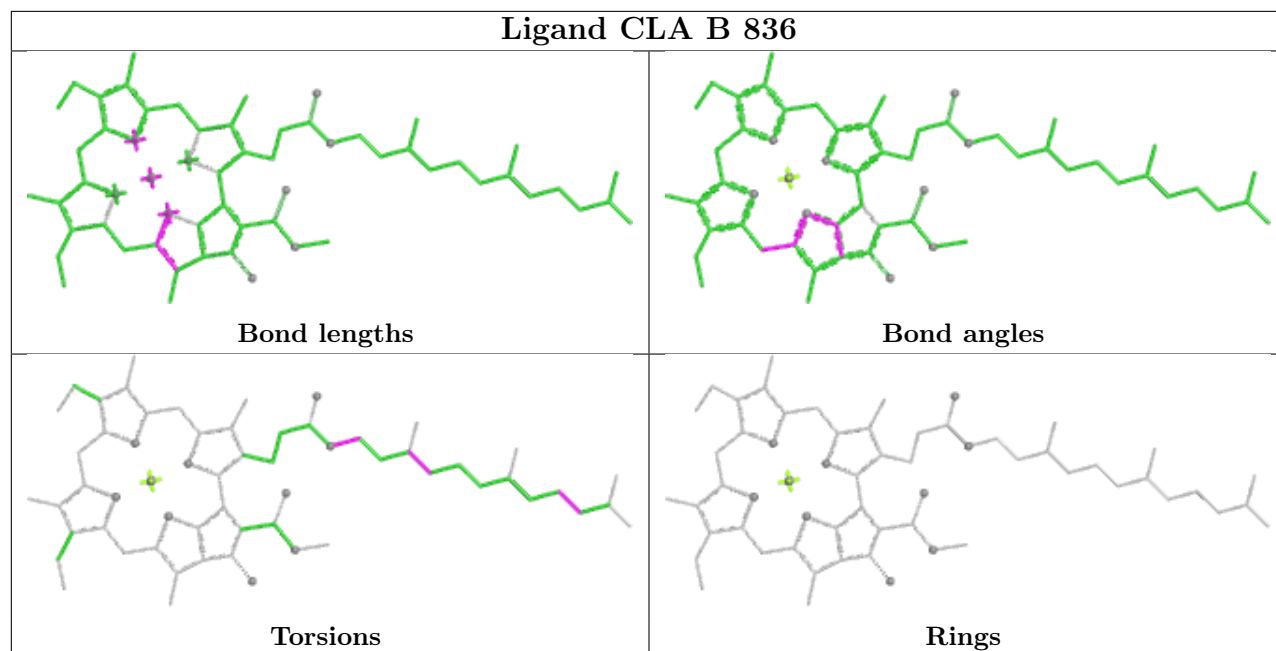


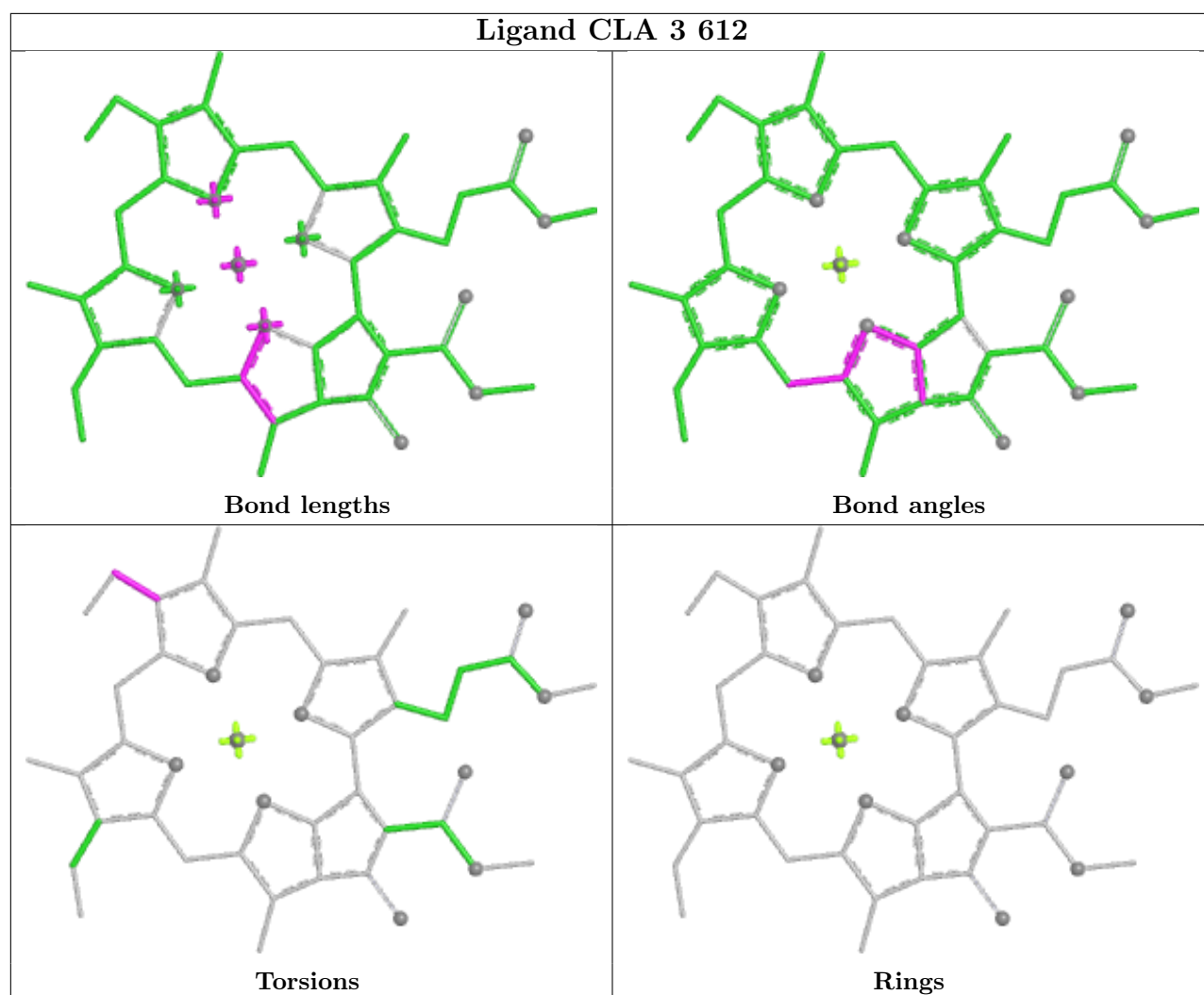












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

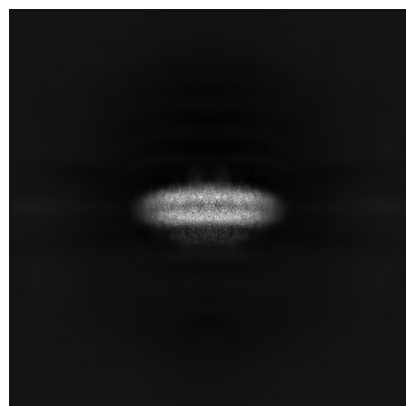
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14871. These allow visual inspection of the internal detail of the map and identification of artifacts.

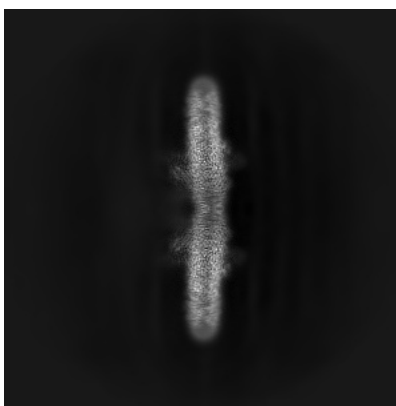
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

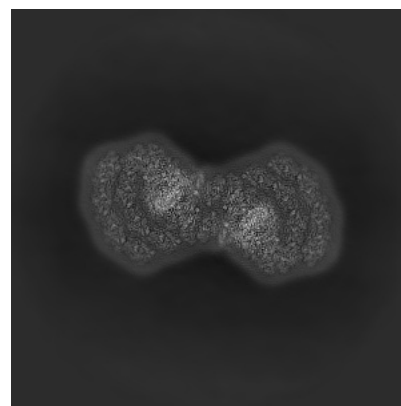
6.1.1 Primary map



X

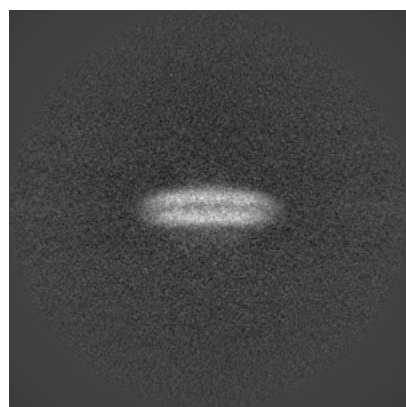


Y

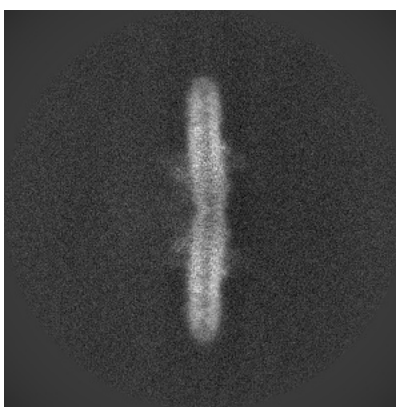


Z

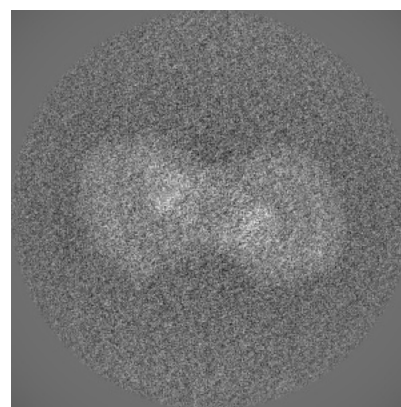
6.1.2 Raw map



X



Y



Z

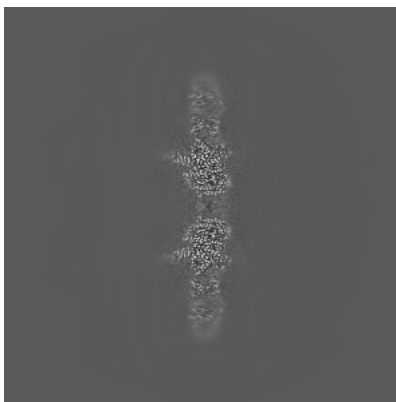
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

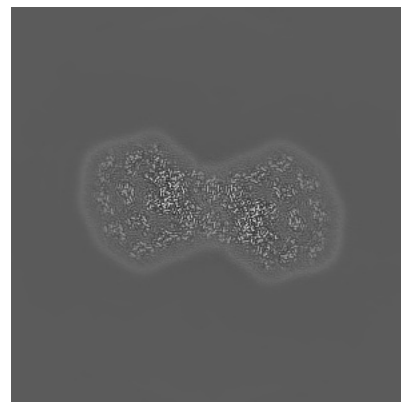
6.2.1 Primary map



X Index: 350

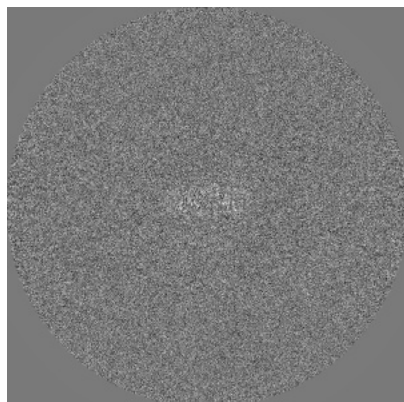


Y Index: 350

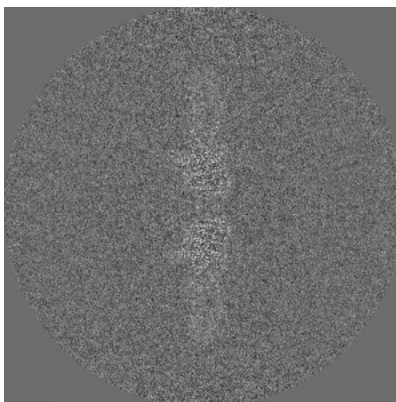


Z Index: 350

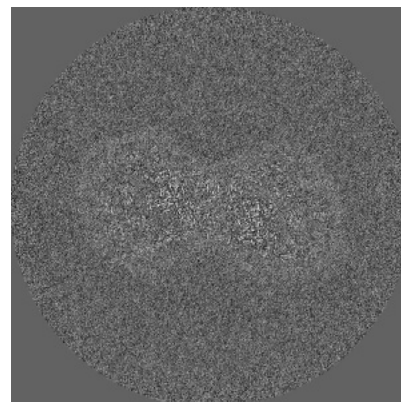
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

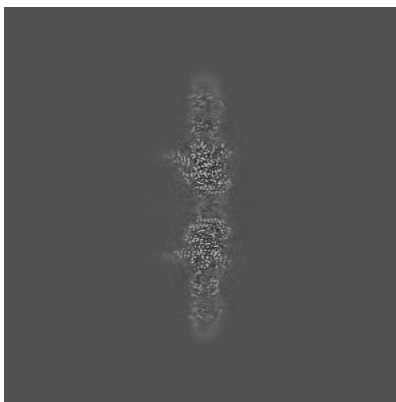
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

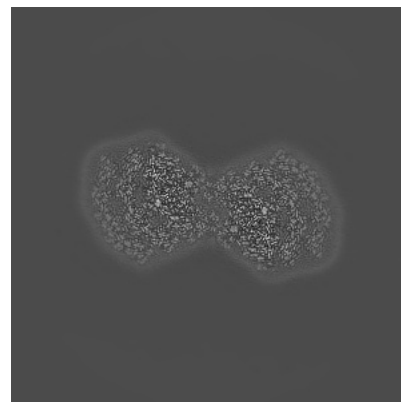
6.3.1 Primary map



X Index: 422

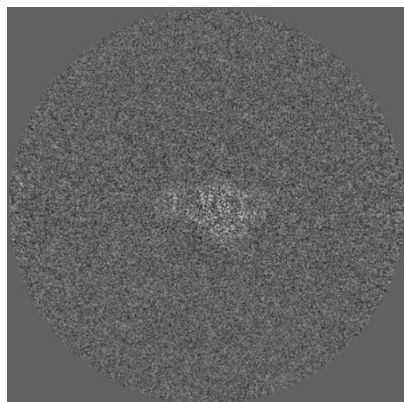


Y Index: 349

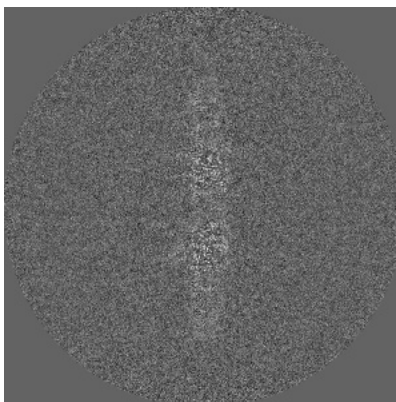


Z Index: 340

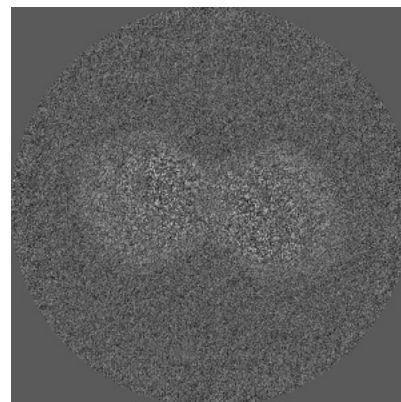
6.3.2 Raw map



X Index: 292



Y Index: 355

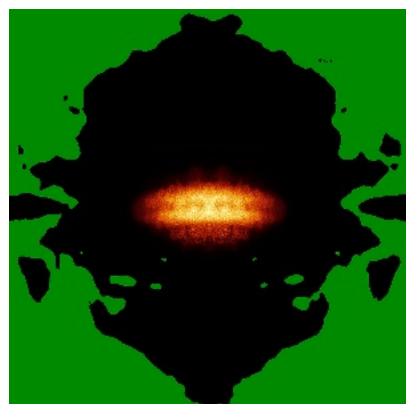


Z Index: 339

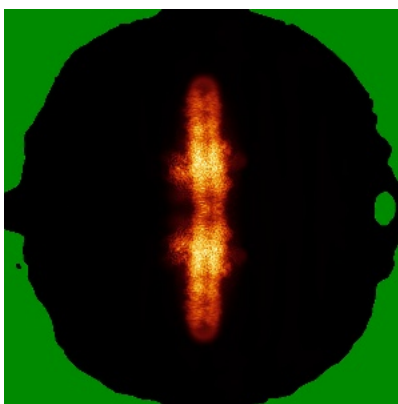
The images above show the largest variance slices of the map in three orthogonal directions.

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

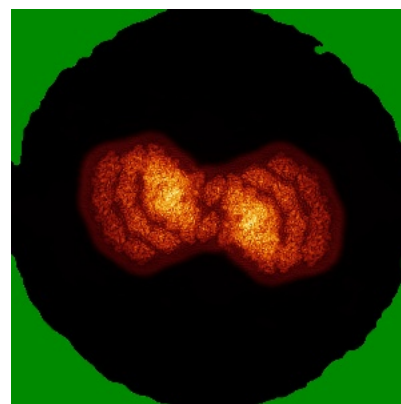
6.4.1 Primary map



X

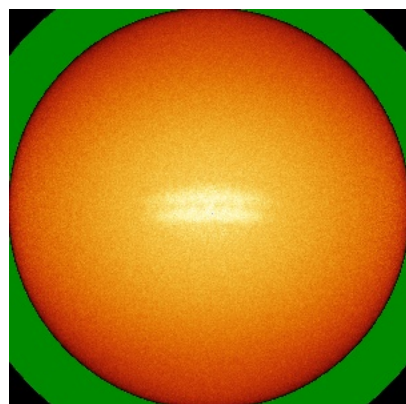


Y

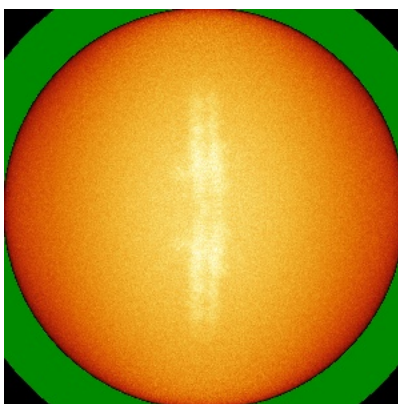


Z

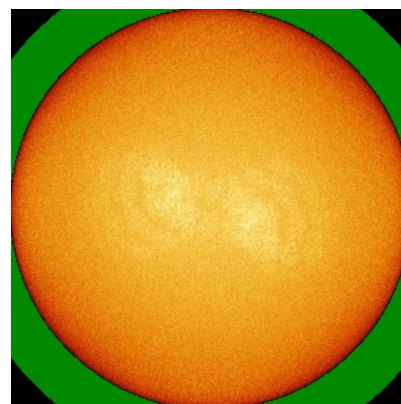
6.4.2 Raw map



X



Y

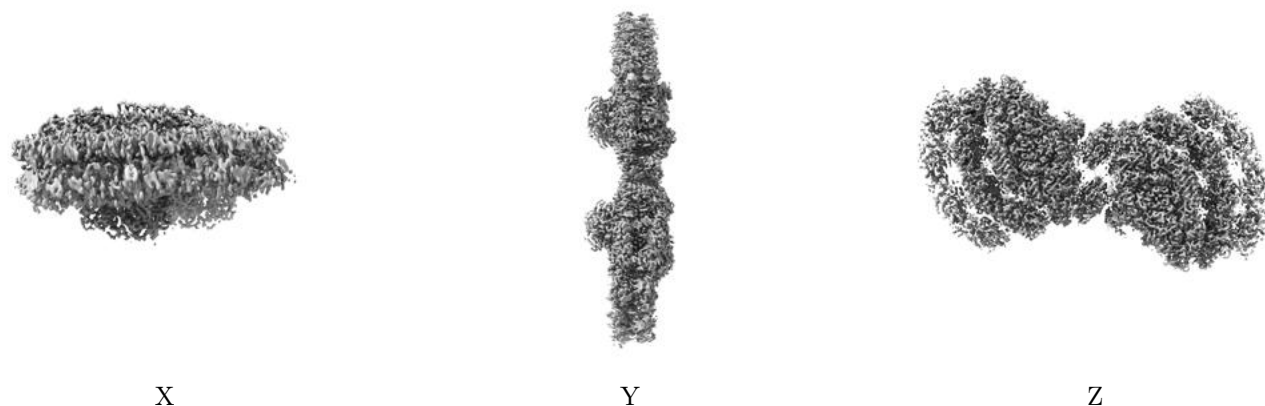


Z

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.

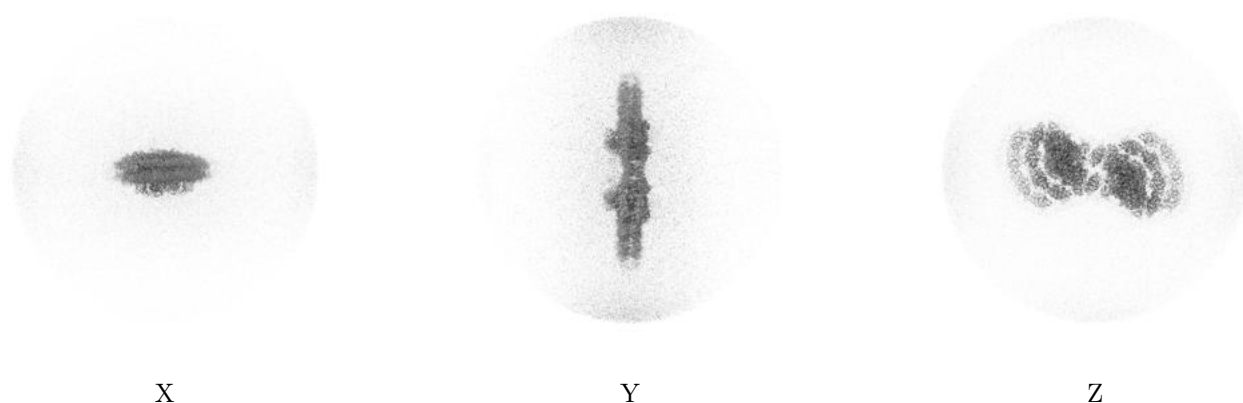
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.036. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

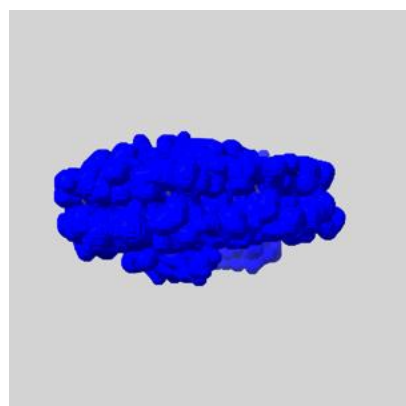
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

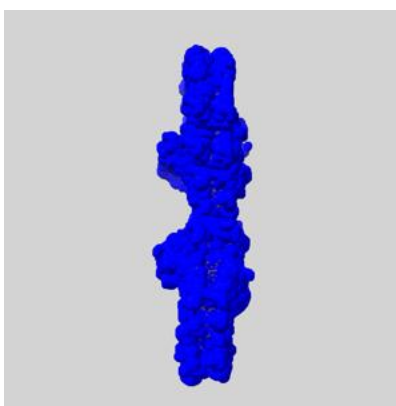
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

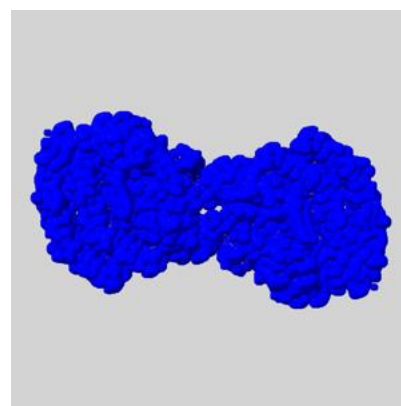
6.6.1 emd_14871_msk_1.map [i](#)



X



Y

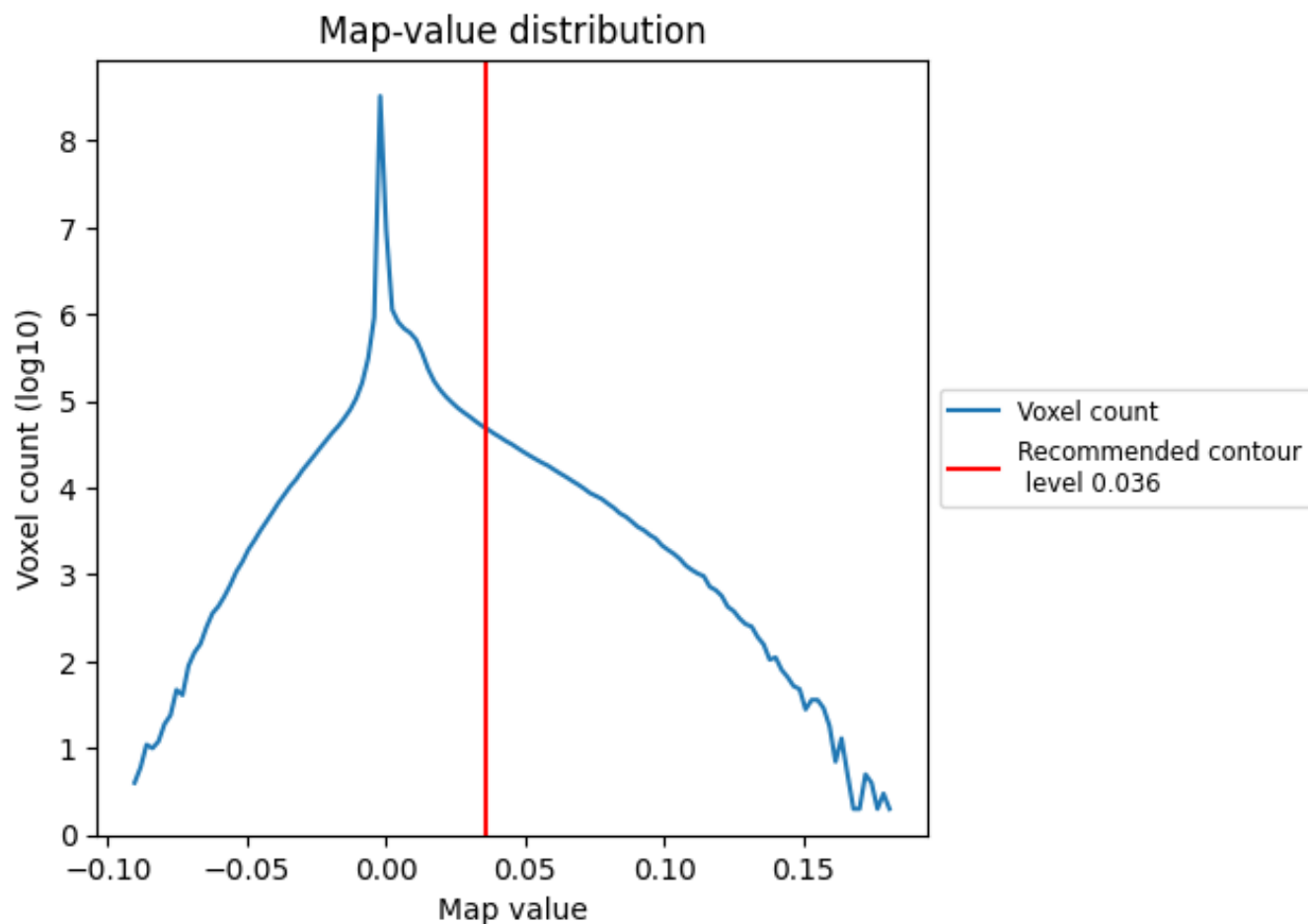


Z

7 Map analysis [i](#)

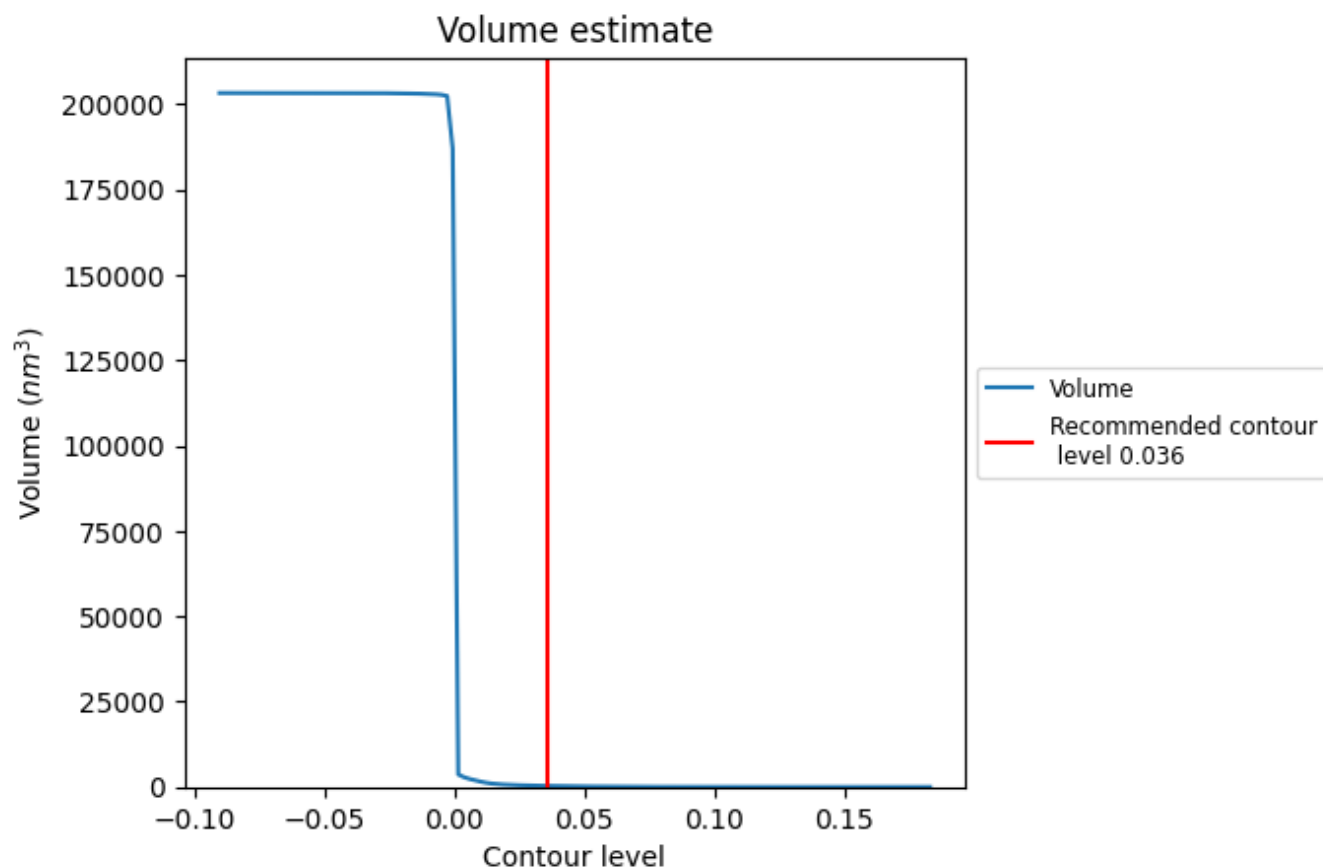
This section contains the results of statistical analysis of the map.

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.

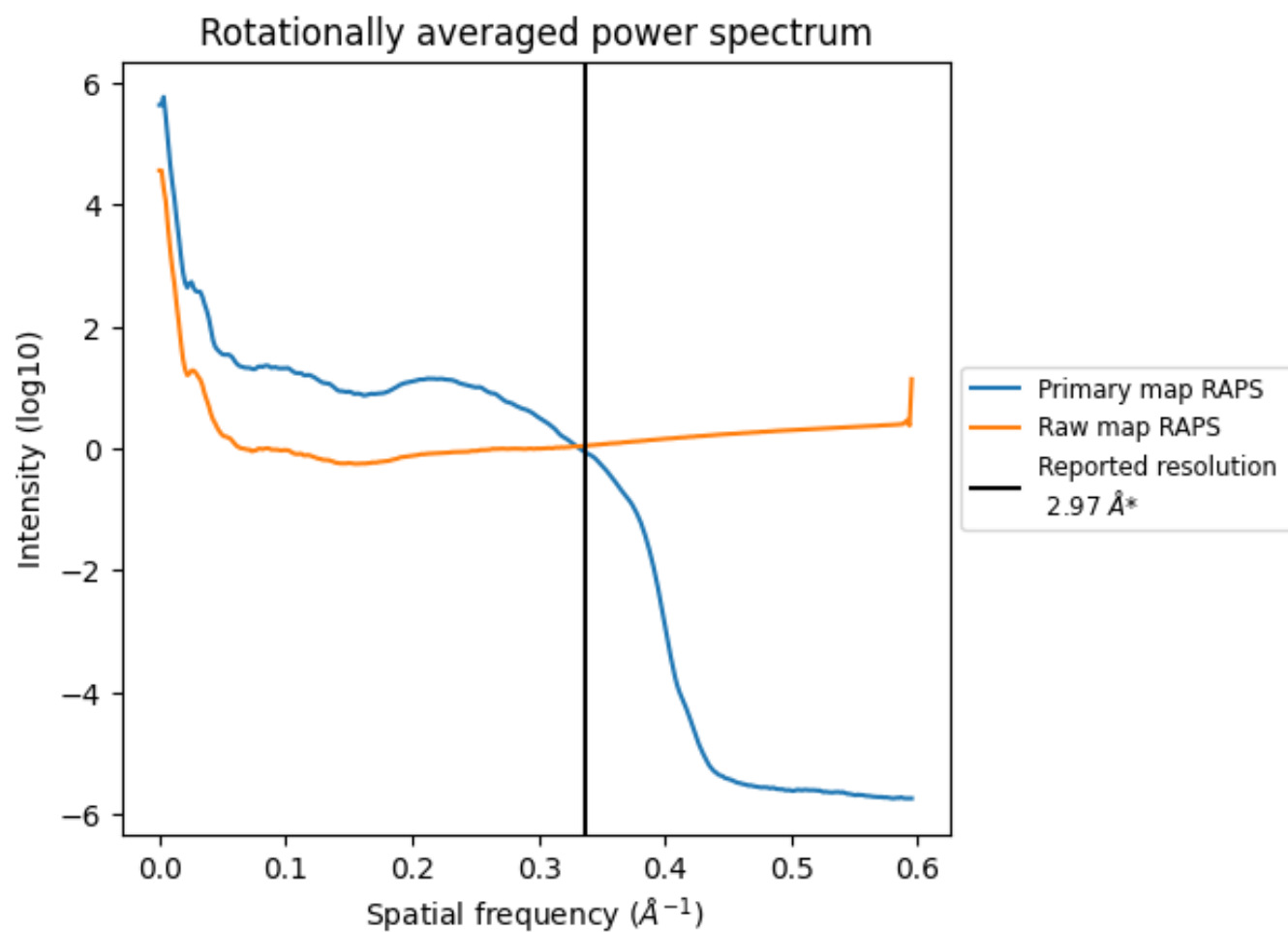
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 297 nm³; this corresponds to an approximate mass of 268 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

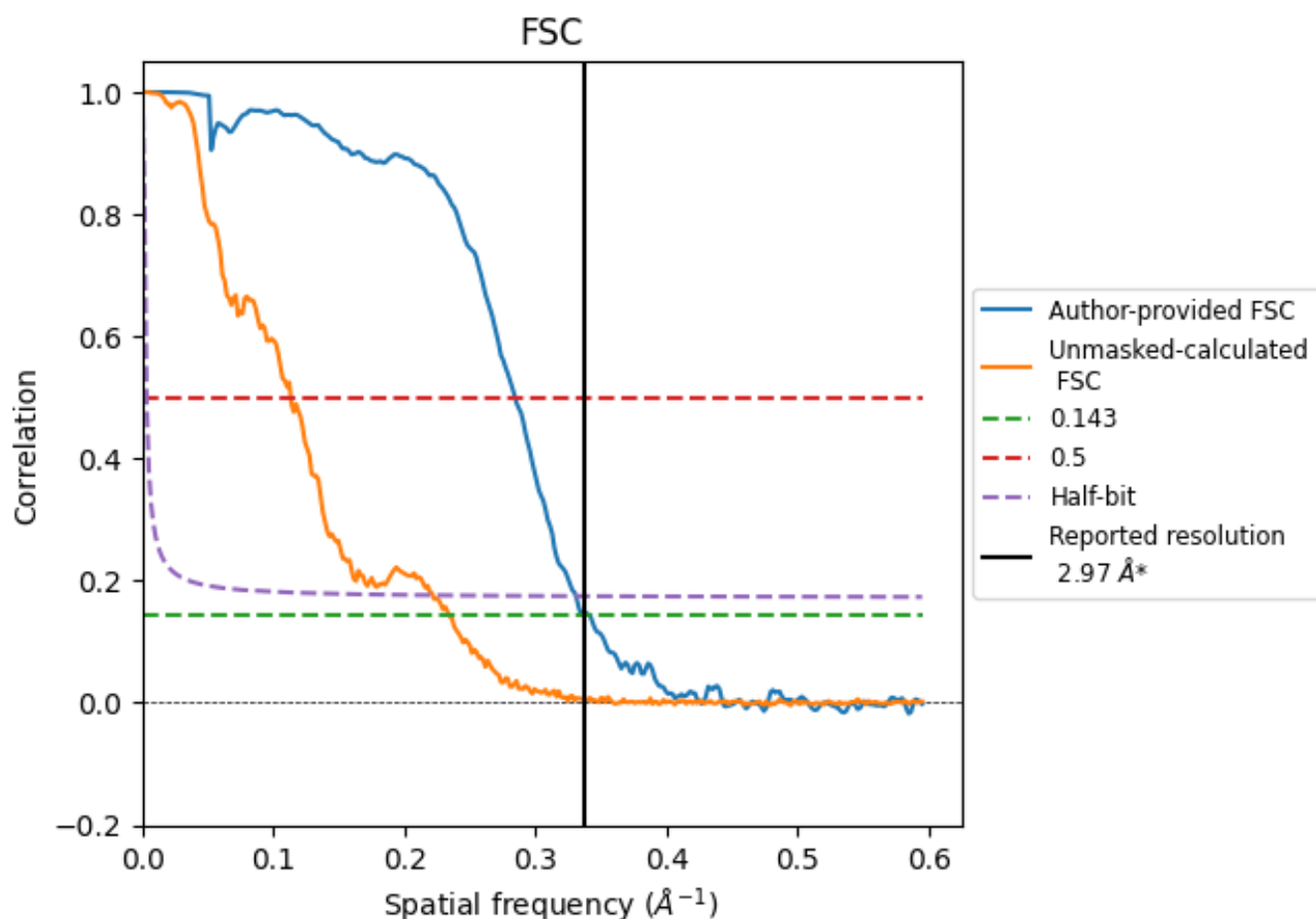


*Reported resolution corresponds to spatial frequency of 0.337 $\text{\AA}^{-1}$

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 0.337 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

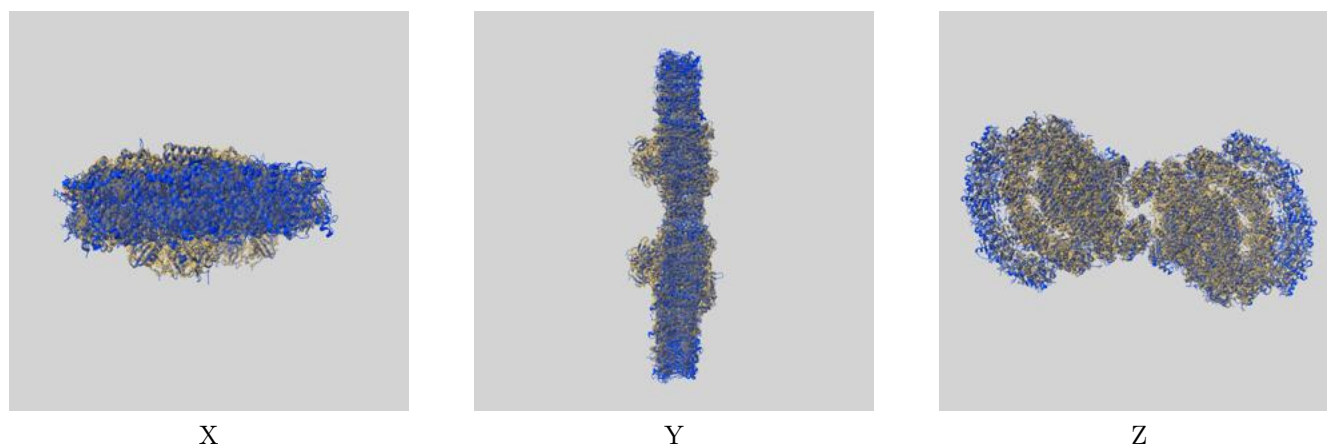
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.97	-	-
Author-provided FSC curve	2.92	3.51	3.02
Unmasked-calculated*	4.27	8.82	4.51

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.27 differs from the reported value 2.97 by more than 10 %

9 Map-model fit [i](#)

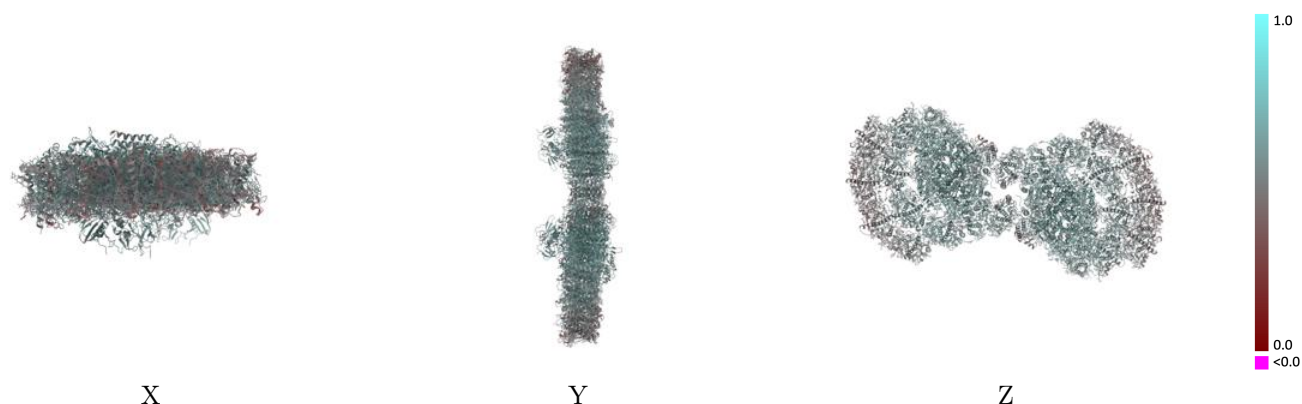
This section contains information regarding the fit between EMDB map EMD-14871 and PDB model 7ZQD. Per-residue inclusion information can be found in section [3](#) on page [62](#).

9.1 Map-model overlay [i](#)



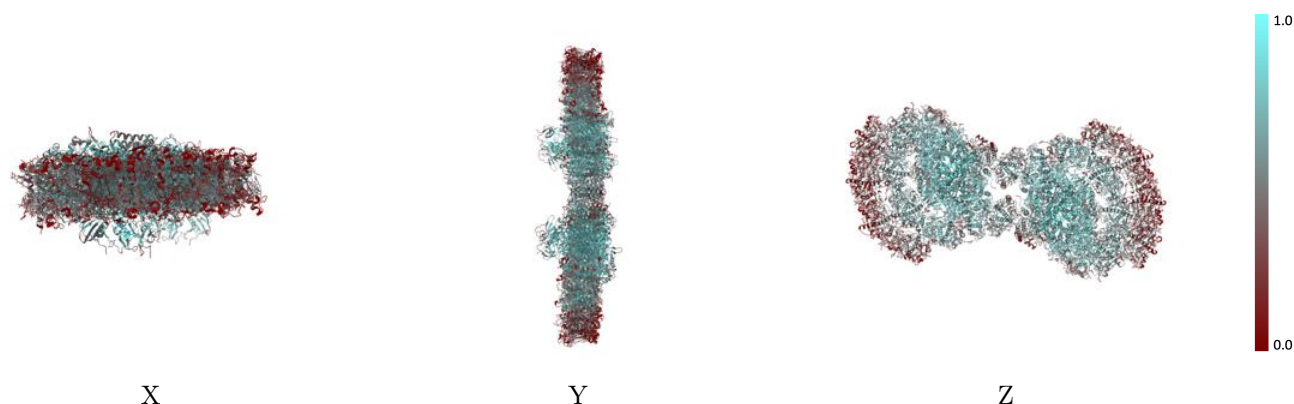
The images above show the 3D surface view of the map at the recommended contour level 0.036 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



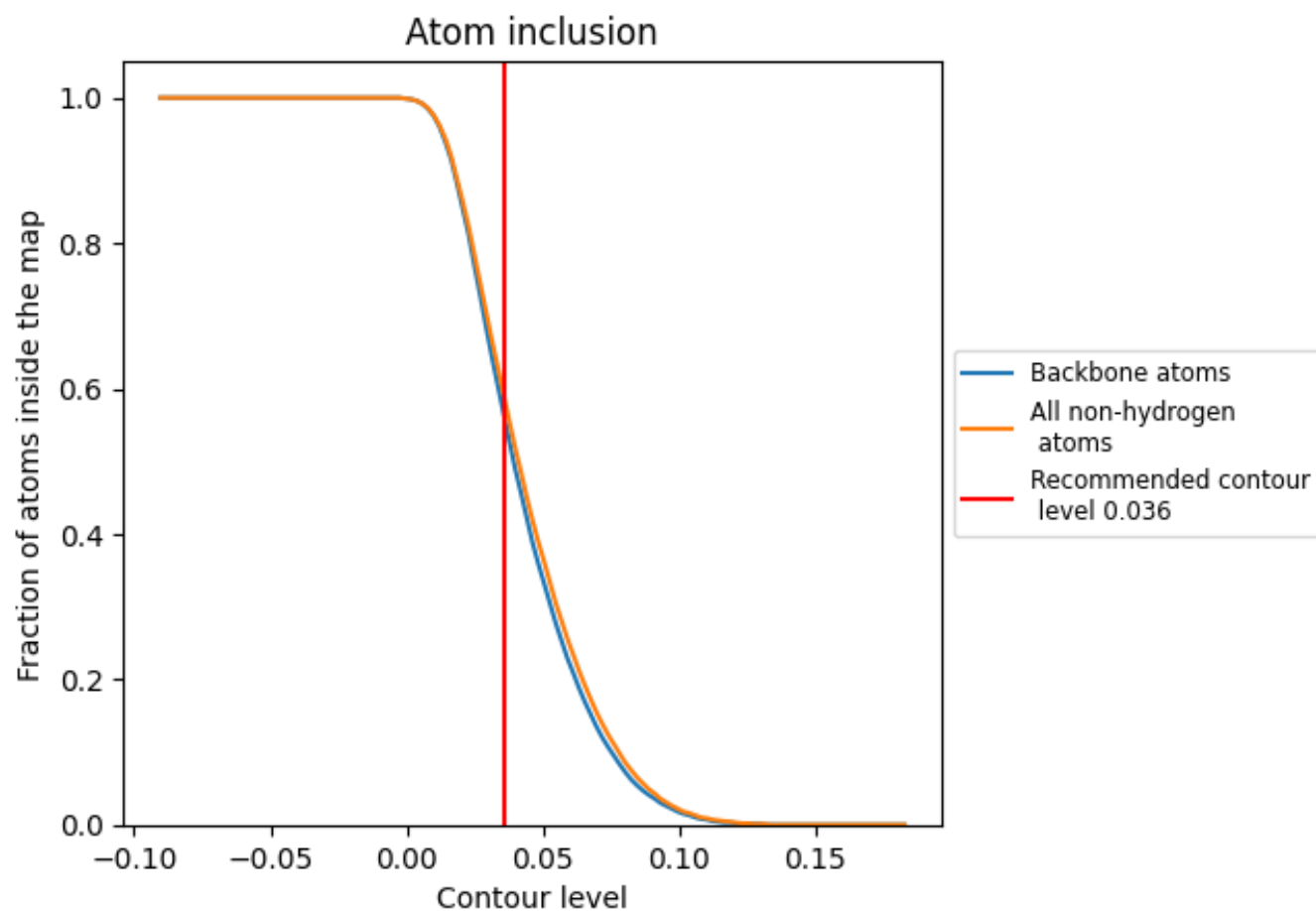
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.036).

9.4 Atom inclusion [i](#)



At the recommended contour level, 56% of all backbone atoms, 59% 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 (0.036) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5860	 0.5590
1	 0.5840	 0.5670
12	 0.5940	 0.5700
3	 0.5550	 0.5510
32	 0.5540	 0.5520
4	 0.2170	 0.4530
42	 0.2180	 0.4540
5	 0.2790	 0.4730
52	 0.2720	 0.4740
6	 0.1970	 0.4450
62	 0.2040	 0.4470
7	 0.5830	 0.5540
72	 0.5770	 0.5510
8	 0.6230	 0.5710
82	 0.6220	 0.5700
9	 0.5400	 0.5400
92	 0.5430	 0.5420
A	 0.7970	 0.6210
A2	 0.7980	 0.6200
B	 0.8060	 0.6190
B2	 0.8070	 0.6190
C	 0.7500	 0.6000
C2	 0.7510	 0.5950
D	 0.5600	 0.5630
D2	 0.5610	 0.5590
E	 0.6130	 0.5730
E2	 0.6050	 0.5720
F	 0.6940	 0.5900
F2	 0.6890	 0.5870
G	 0.5060	 0.5480
G2	 0.5050	 0.5490
I	 0.5740	 0.5470
I2	 0.5740	 0.5440
J	 0.7280	 0.5920
J2	 0.7340	 0.5950



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Chain	Atom inclusion	Q-score
K	 0.3470	 0.5380
K2	 0.3190	 0.5390
L	 0.3930	 0.5010
L2	 0.3890	 0.5010
Z	 0.3190	 0.4950
Z2	 0.3190	 0.4960