



## wwPDB EM Validation Summary Report ⓘ

Apr 6, 2026 – 01:48 AM UTC

PDB ID : 9SE6 / pdb\_00009se6  
EMDB ID : EMD-54803  
Title : Structure of Photosystem I from *Chlamydomonas reinhardtii* at 1.83 Å resolution  
Authors : Mahapatra, G.P.; Schuller, J.M.  
Deposited on : 2025-08-15  
Resolution : 1.83 Å (reported)  
Based on initial model : 7ZQC

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

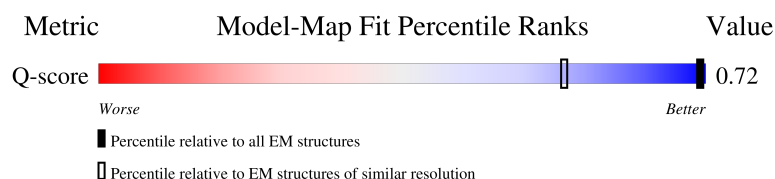
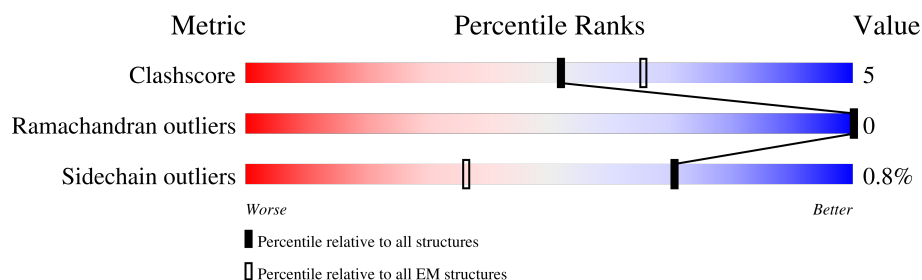
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 1.83 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	903 ( 1.33 - 2.33 )

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

Mol	Chain	Length	Quality of chain
1	3	221	
2	4	212	
3	5	227	
4	6	230	

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Mol	Chain	Length	Quality of chain
5	7	213	
6	8	217	
7	A	742	
8	B	733	
9	C	80	
10	D	144	
11	E	64	
12	I	37	
13	J	41	
14	K	86	
15	1	194	
15	Z	194	
16	F	165	
17	G	95	
18	L	124	

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
19	CLA	1	302	X	-	-	-
19	CLA	1	303	X	-	-	-
19	CLA	1	304	X	-	-	-
19	CLA	1	307	X	-	-	-
19	CLA	1	308	X	-	-	-
19	CLA	1	309	X	-	-	-
19	CLA	1	310	X	-	-	-
19	CLA	1	311	X	-	-	-
19	CLA	1	312	X	-	-	-
19	CLA	1	313	X	-	-	-
19	CLA	1	314	X	-	-	-
19	CLA	3	301	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	3	302	X	-	-	-
19	CLA	3	303	X	-	-	-
19	CLA	3	304	X	-	-	-
19	CLA	3	305	X	-	-	-
19	CLA	3	307	X	-	-	-
19	CLA	3	308	X	-	-	-
19	CLA	3	309	X	-	-	-
19	CLA	3	310	X	-	-	-
19	CLA	3	311	X	-	-	-
19	CLA	3	312	X	-	-	-
19	CLA	3	313	X	-	-	-
19	CLA	3	314	X	-	-	-
19	CLA	4	602	X	-	-	-
19	CLA	4	603	X	-	-	-
19	CLA	4	604	X	-	-	-
19	CLA	4	608	X	-	-	-
19	CLA	4	609	X	-	-	-
19	CLA	4	610	X	-	-	-
19	CLA	4	611	X	-	-	-
19	CLA	4	612	X	-	-	-
19	CLA	4	613	X	-	-	-
19	CLA	4	614	X	-	-	-
19	CLA	5	302	X	-	-	-
19	CLA	5	303	X	-	-	-
19	CLA	5	304	X	-	-	-
19	CLA	5	305	X	-	-	-
19	CLA	5	309	X	-	-	-
19	CLA	5	310	X	-	-	-
19	CLA	5	311	X	-	-	-
19	CLA	5	312	X	-	-	-
19	CLA	5	313	X	-	-	-
19	CLA	5	314	X	-	-	-
19	CLA	5	315	X	-	-	-
19	CLA	5	316	X	-	-	-
19	CLA	5	319	X	-	-	-
19	CLA	6	303	X	-	-	-
19	CLA	6	304	X	-	-	-
19	CLA	6	305	X	-	-	-
19	CLA	6	309	X	-	-	-
19	CLA	6	310	X	-	-	-
19	CLA	6	311	X	-	-	-
19	CLA	6	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	6	313	X	-	-	-
19	CLA	6	314	X	-	-	-
19	CLA	6	316	X	-	-	-
19	CLA	6	320	X	-	-	-
19	CLA	6	327	X	-	-	-
19	CLA	7	602	X	-	-	-
19	CLA	7	603	X	-	-	-
19	CLA	7	604	X	-	-	-
19	CLA	7	607	X	-	-	-
19	CLA	7	608	X	-	-	-
19	CLA	7	609	X	-	-	-
19	CLA	7	610	X	-	-	-
19	CLA	7	611	X	-	-	-
19	CLA	7	612	X	-	-	-
19	CLA	7	613	X	-	-	-
19	CLA	7	614	X	-	-	-
19	CLA	8	302	X	-	-	-
19	CLA	8	303	X	-	-	-
19	CLA	8	304	X	-	-	-
19	CLA	8	307	X	-	-	-
19	CLA	8	308	X	-	-	-
19	CLA	8	309	X	-	-	-
19	CLA	8	310	X	-	-	-
19	CLA	8	311	X	-	-	-
19	CLA	8	312	X	-	-	-
19	CLA	8	313	X	-	-	-
19	CLA	8	314	X	-	-	-
19	CLA	A	803	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	843	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	846	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	838	X	-	-	-
19	CLA	B	839	X	-	-	-
19	CLA	B	840	X	-	-	-
19	CLA	B	841	X	-	-	-
19	CLA	B	842	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F	303	X	-	-	-
19	CLA	F	304	X	-	-	-
19	CLA	G	202	X	-	-	-
19	CLA	G	203	X	-	-	-
19	CLA	J	102	X	-	-	-
19	CLA	K	202	X	-	-	-
19	CLA	K	203	X	-	-	-
19	CLA	K	204	X	-	-	-
19	CLA	K	205	X	-	-	-
19	CLA	L	203	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	Z	602	X	-	-	-
19	CLA	Z	603	X	-	-	-
19	CLA	Z	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	Z	607	X	-	-	-
19	CLA	Z	608	X	-	-	-
19	CLA	Z	609	X	-	-	-
19	CLA	Z	610	X	-	-	-
19	CLA	Z	611	X	-	-	-
19	CLA	Z	612	X	-	-	-
19	CLA	Z	613	X	-	-	-
19	CLA	Z	614	X	-	-	-
20	CHL	1	305	X	-	-	-
20	CHL	1	306	X	-	-	-
20	CHL	3	306	X	-	-	-
20	CHL	4	601	X	-	-	-
20	CHL	4	605	X	-	-	-
20	CHL	4	606	X	-	-	-
20	CHL	4	607	X	-	-	-
20	CHL	4	615	X	-	-	-
20	CHL	5	306	X	-	-	-
20	CHL	5	307	X	-	-	-
20	CHL	5	308	X	-	-	-
20	CHL	5	317	X	-	-	-
20	CHL	6	302	X	-	-	-
20	CHL	6	306	X	-	-	-
20	CHL	6	307	X	-	-	-
20	CHL	6	308	X	-	-	-
20	CHL	6	315	X	-	-	-
20	CHL	6	317	X	-	-	-
20	CHL	7	601	X	-	-	-
20	CHL	7	605	X	-	-	-
20	CHL	7	606	X	-	-	-
20	CHL	7	621	X	-	-	-
20	CHL	8	305	X	-	-	-
20	CHL	8	306	X	-	-	-
20	CHL	8	320	X	-	-	-
20	CHL	Z	601	X	-	-	-
20	CHL	Z	605	X	-	-	-
20	CHL	Z	606	X	-	-	-
27	NEX	5	323	X	-	-	-
28	CL0	A	802	X	-	-	-

## 2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 48478 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Light-harvesting chlorophyll-a/b protein of photosystem I, type III.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	221	Total	C	N	O	S	0	0
			1687	1100	273	306	8		

- Molecule 2 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	4	212	Total	C	N	O	S	0	0
			1652	1083	269	295	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	5	227	Total	C	N	O	S	0	0
			1775	1154	297	316	8		

- Molecule 4 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	230	Total	C	N	O	S	0	0
			1772	1167	293	306	6		

- Molecule 5 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	7	213	Total	C	N	O	S	0	0
			1650	1072	274	298	6		

- Molecule 6 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	8	217	Total	C	N	O	S	0	0
			1650	1073	280	293	4		

- Molecule 7 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	742	Total	C	N	O	S	0	0
			5825	3808	994	1001	22		

- Molecule 8 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	B	733	Total	C	N	O	S	0	0
			5824	3824	977	1005	18		

- Molecule 9 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	80	Total	C	N	O	S	0	0
			601	369	103	117	12		

- Molecule 10 is a protein called Photosystem I reaction center subunit II, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D	144	Total	C	N	O	S	0	0
			1133	725	200	201	7		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	E	64	Total	C	N	O	0	0
			506	322	89	95		

- Molecule 12 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	I	37	Total	C	N	O	S	0	0
			281	195	39	46	1		

- Molecule 13 is a protein called Photosystem I reaction center subunit IX.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	J	41	Total	C	N	O	S	0	0
			329	224	46	58	1		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	0	ACE	-	acetylation	UNP P59777

- Molecule 14 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	86	Total	C	N	O	S	0	0
			583	370	100	111	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Z	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		
15	1	194	Total	C	N	O	S	0	0
			1445	941	240	261	3		

- Molecule 16 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	F	165	Total	C	N	O	S	0	0
			1266	817	213	233	3		

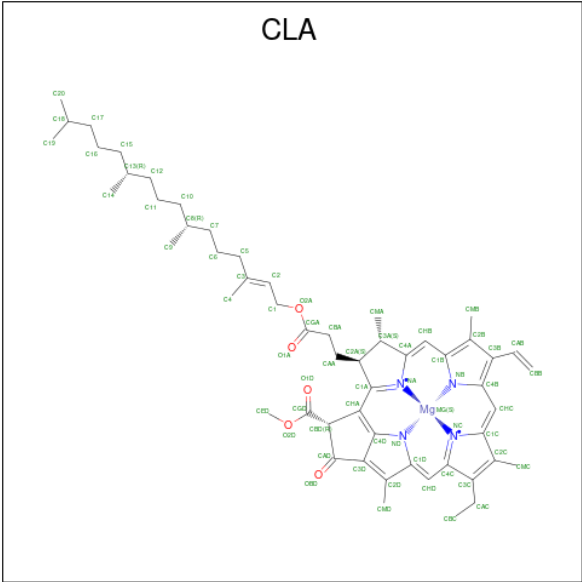
- Molecule 17 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	G	70	Total	C	N	O	0	0
			512	328	90	94		

- Molecule 18 is a protein called Chains: L.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	124	Total	C	N	O	S	0	0
			899	586	146	164	3		

- Molecule 19 is CHLOROPHYLL A (CCD ID: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
19	3	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 56	C 46	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	5	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	5	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	6	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	6	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	6	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	6	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	6	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	6	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	6	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	6	1	Total 53	C 43	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 52	C 42	Mg 1	N 4	O 5	0
19	7	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	7	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	7	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	7	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	7	1	Total 43	C 35	Mg 1	N 4	O 3	0
19	7	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	8	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	8	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	8	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	8	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	8	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	8	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 50	C 40	Mg 1	N 4	O 5	0

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

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Mol	Chain	Residues	Atoms					AltConf
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	A	1	Total 51	C 41	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	A	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 58	C 48	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	J	1	Total 55	C 45	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	K	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	K	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	K	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
19	Z	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	Z	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	Z	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	Z	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	Z	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 57	C 47	Mg 1	N 4	O 5	0
19	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 61	C 51	Mg 1	N 4	O 5	0
19	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
19	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
19	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
19	1	1	Total 46	C 36	Mg 1	N 4	O 5	0
19	F	1	Total 65	C 55	Mg 1	N 4	O 5	0

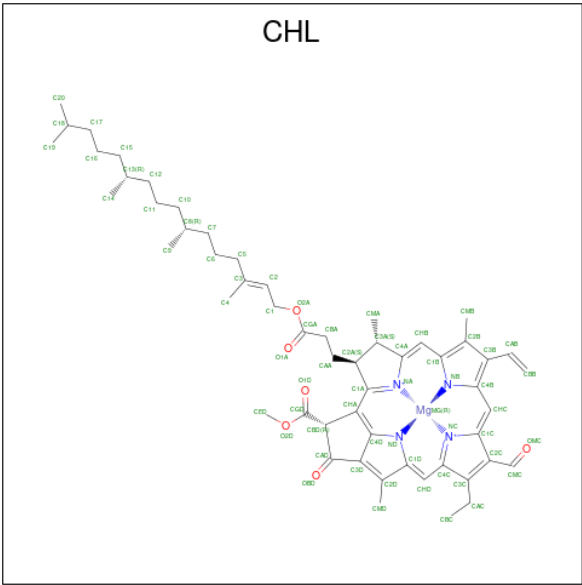
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Mol	Chain	Residues	Atoms					AltConf
19	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
19	F	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
19	G	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
19	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 20 is CHLOROPHYLL B (CCD ID: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
20	3	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
20	4	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
20	4	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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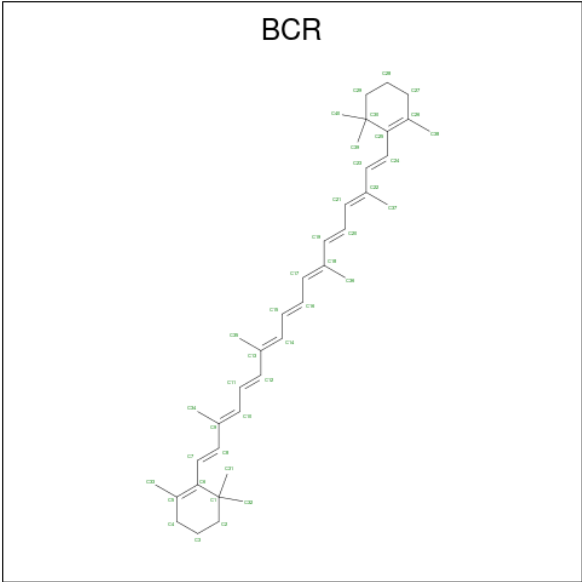
Mol	Chain	Residues	Atoms					AltConf
20	4	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	5	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	5	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	5	1	Total 51	C 40	Mg 1	N 4	O 6	0
20	5	1	Total 43	C 34	Mg 1	N 4	O 4	0
20	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	6	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	6	1	Total 51	C 40	Mg 1	N 4	O 6	0
20	6	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	6	1	Total 43	C 34	Mg 1	N 4	O 4	0
20	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	7	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	7	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	8	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0
20	Z	1	Total 46	C 35	Mg 1	N 4	O 6	0
20	Z	1	Total 66	C 55	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms					AltConf
20	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
20	1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

- Molecule 21 is BETA-CAROTENE (CCD ID: BCR) (formula: C<sub>40</sub>H<sub>56</sub>) (labeled as "Ligand of Interest" by depositor).



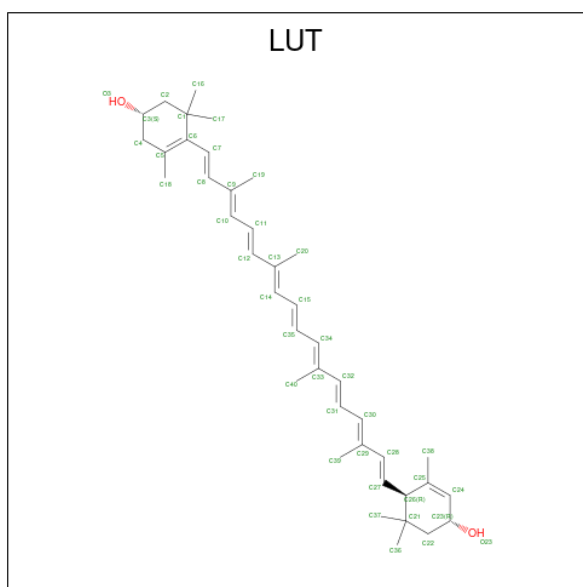
Mol	Chain	Residues	Atoms		AltConf
21	3	1	Total	C	0
			40	40	
21	3	1	Total	C	0
			40	40	
21	3	1	Total	C	0
			40	40	
21	4	1	Total	C	0
			40	40	
21	5	1	Total	C	0
			40	40	
21	6	1	Total	C	0
			40	40	
21	7	1	Total	C	0
			40	40	
21	8	1	Total	C	0
			40	40	
21	A	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	A	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	B	1	Total C 40 40	0
21	I	1	Total C 40 40	0
21	J	1	Total C 40 40	0
21	K	1	Total C 40 40	0
21	G	1	Total C 40 40	0
21	L	1	Total C 40 40	0
21	L	1	Total C 40 40	0

- Molecule 22 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



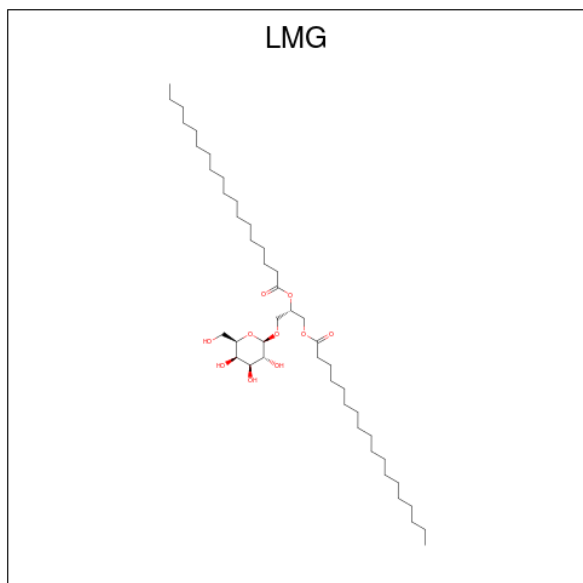
Mol	Chain	Residues	Atoms			AltConf
22	3	1	Total 42	C 40	O 2	0
22	3	1	Total 42	C 40	O 2	0
22	3	1	Total 20	C 19	O 1	0
22	4	1	Total 42	C 40	O 2	0
22	5	1	Total 42	C 40	O 2	0
22	5	1	Total 42	C 40	O 2	0
22	6	1	Total 42	C 40	O 2	0
22	7	1	Total 42	C 40	O 2	0
22	8	1	Total 42	C 40	O 2	0
22	8	1	Total 42	C 40	O 2	0
22	J	1	Total 42	C 40	O 2	0
22	Z	1	Total 42	C 40	O 2	0
22	Z	1	Total 26	C 25	O 1	0
22	1	1	Total 42	C 40	O 2	0

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Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			42	40	2	
22	F	1	Total	C	O	0
			42	40	2	

- Molecule 23 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula:  $C_{45}H_{86}O_{10}$ ).



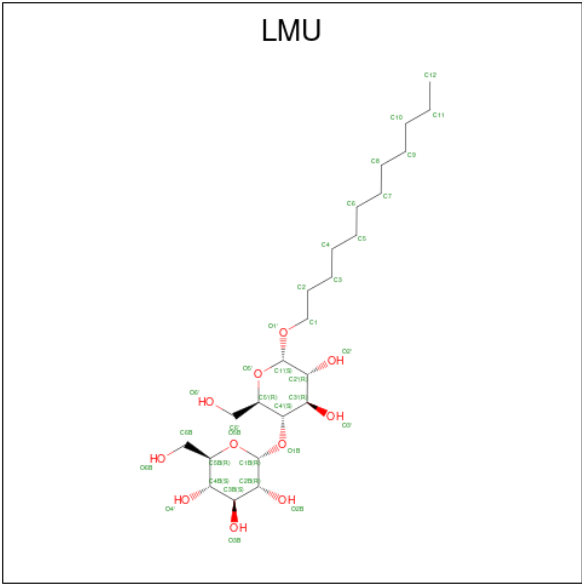
Mol	Chain	Residues	Atoms			AltConf
23	3	1	Total	C	O	0
			37	27	10	
23	4	1	Total	C	O	0
			41	31	10	
23	6	1	Total	C	O	0
			27	22	5	
23	6	1	Total	C	O	0
			20	18	2	
23	7	1	Total	C	O	0
			32	22	10	
23	8	1	Total	C	O	0
			49	39	10	
23	B	1	Total	C	O	0
			43	33	10	
23	J	1	Total	C	O	0
			42	32	10	
23	J	1	Total	C	O	0
			35	25	10	

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Mol	Chain	Residues	Atoms			AltConf
23	F	1	Total	C	O	0
			32	22	10	
23	G	1	Total	C	O	0
			36	26	10	
23	L	1	Total	C	O	0
			40	30	10	

- Molecule 24 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: C<sub>24</sub>H<sub>46</sub>O<sub>11</sub>).



Mol	Chain	Residues	Atoms			AltConf
24	3	1	Total	C	O	0
			34	23	11	
24	3	1	Total	C	O	0
			24	18	6	
24	3	1	Total	C	O	0
			35	24	11	
24	3	1	Total	C	O	0
			24	18	6	
24	4	1	Total	C	O	0
			22	16	6	
24	4	1	Total	C	O	0
			20	14	6	
24	4	1	Total	C	O	0
			24	18	6	
24	4	1	Total	C	O	0
			22	16	6	

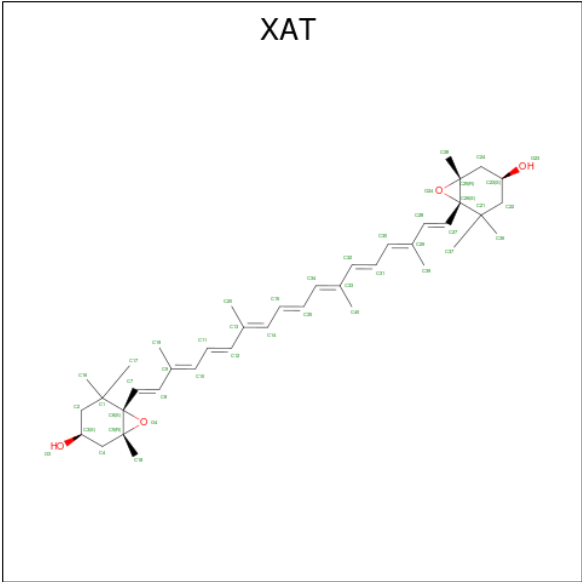
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Mol	Chain	Residues	Atoms			AltConf
24	6	1	Total	C	O	0
			24	18	6	
24	6	1	Total	C	O	0
			24	18	6	
24	7	1	Total	C	O	0
			21	15	6	
24	7	1	Total	C	O	0
			22	16	6	
24	8	1	Total	C	O	0
			24	18	6	
24	A	1	Total	C	O	0
			35	24	11	
24	A	1	Total	C	O	0
			20	14	6	
24	A	1	Total	C	O	0
			24	18	6	
24	B	1	Total	C	O	0
			35	24	11	
24	K	1	Total	C	O	0
			24	18	6	
24	Z	1	Total	C	O	0
			31	20	11	
24	Z	1	Total	C	O	0
			24	18	6	
24	Z	1	Total	C	O	0
			24	18	6	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			35	24	11	
24	1	1	Total	C	O	0
			19	13	6	
24	1	1	Total	C	O	0
			24	18	6	
24	1	1	Total	C	O	0
			22	16	6	
24	F	1	Total	C	O	0
			35	24	11	

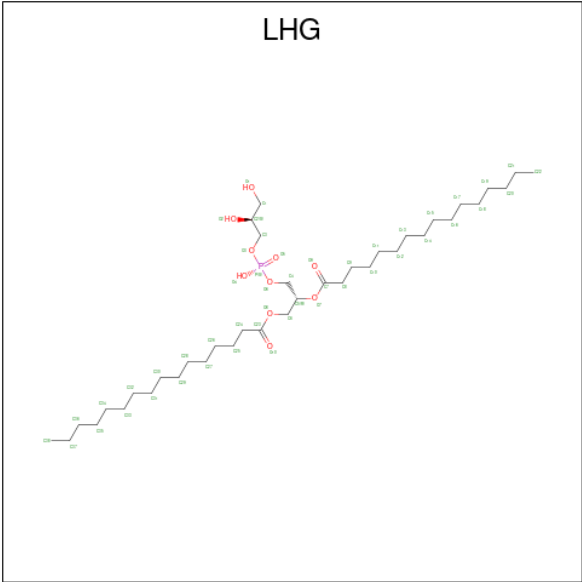
- Molecule 25 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>) (labeled as "Ligand of Interest" by depositor).





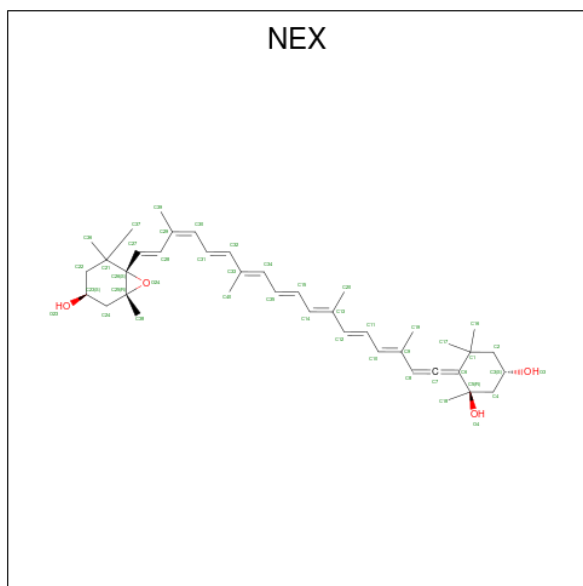
Mol	Chain	Residues	Atoms			AltConf
25	4	1	Total	C	O	0
			44	40	4	
25	5	1	Total	C	O	0
			44	40	4	
25	6	1	Total	C	O	0
			44	40	4	
25	7	1	Total	C	O	0
			44	40	4	
25	8	1	Total	C	O	0
			44	40	4	
25	Z	1	Total	C	O	0
			44	40	4	
25	1	1	Total	C	O	0
			44	40	4	

- Molecule 26 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



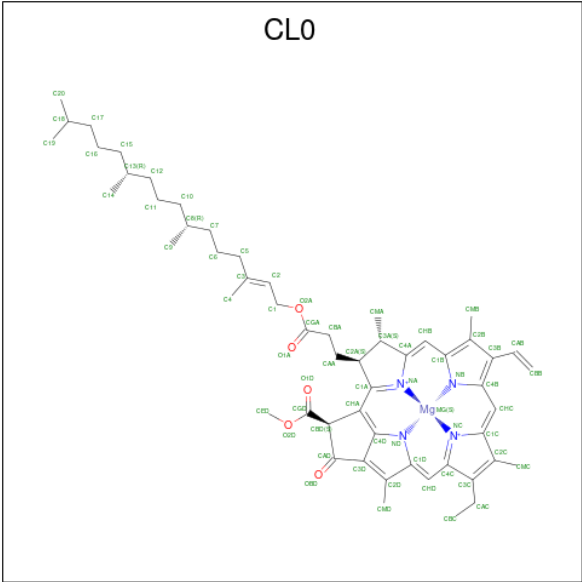
Mol	Chain	Residues	Atoms				AltConf
26	4	1	Total	C	O	P	0
			49	38	10	1	
26	4	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			38	27	10	1	
26	5	1	Total	C	O	P	0
			37	26	10	1	
26	6	1	Total	C	O	P	0
			49	38	10	1	
26	6	1	Total	C	O	P	0
			36	25	10	1	
26	7	1	Total	C	O	P	0
			49	38	10	1	
26	8	1	Total	C	O	P	0
			44	33	10	1	
26	A	1	Total	C	O	P	0
			31	20	10	1	
26	A	1	Total	C	O	P	0
			49	38	10	1	
26	A	1	Total	C	O	P	0
			38	27	10	1	
26	B	1	Total	C	O	P	0
			45	34	10	1	
26	Z	1	Total	C	O	P	0
			39	28	10	1	
26	1	1	Total	C	O	P	0
			44	33	10	1	

- Molecule 27 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:  $C_{40}H_{56}O_4$ ) (labeled as "Ligand of Interest" by depositor).



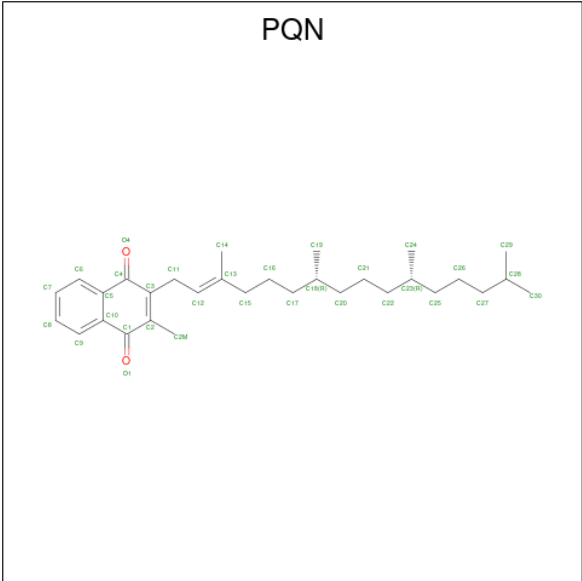
Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	

- Molecule 28 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula:  $C_{55}H_{72}MgN_4O_5$ ) (labeled as "Ligand of Interest" by depositor).



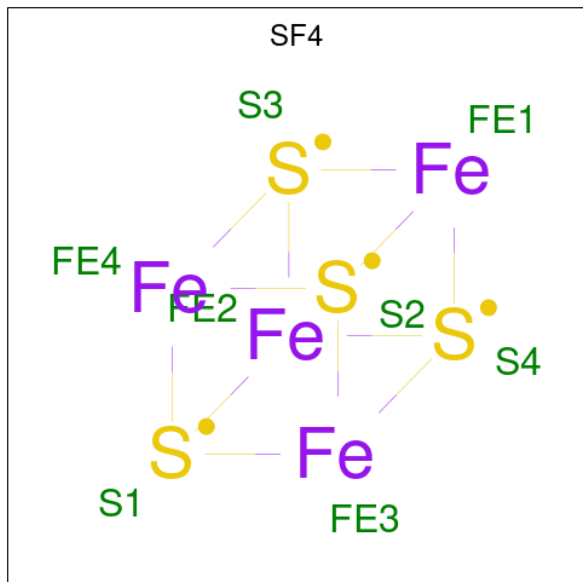
Mol	Chain	Residues	Atoms					AltConf
28	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 29 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ) (labeled as "Lig- and of Interest" by depositor).



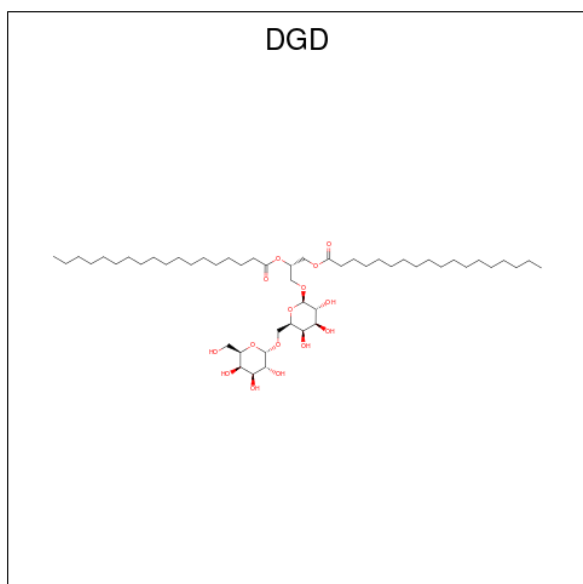
Mol	Chain	Residues	Atoms			AltConf
29	A	1	Total	C	O	0
			33	31	2	
29	B	1	Total	C	O	0
			33	31	2	

- Molecule 30 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula:  $\text{Fe}_4\text{S}_4$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	A	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	
30	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 31 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula:  $\text{C}_{51}\text{H}_{96}\text{O}_{15}$ ).



Mol	Chain	Residues	Atoms			AltConf
31	B	1	Total	C	O	0
			59	44	15	

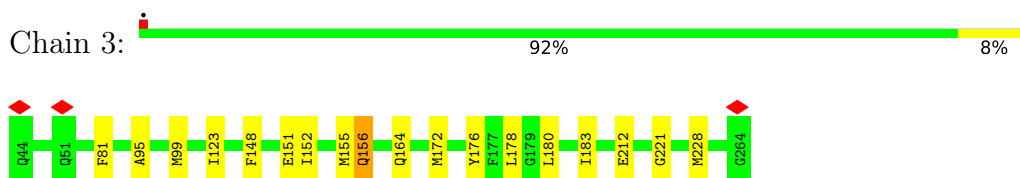
- Molecule 32 is water.

Mol	Chain	Residues	Atoms			AltConf
32	3	55	Total	O		0
			55	55		
32	4	17	Total	O		0
			17	17		
32	5	36	Total	O		0
			36	36		
32	6	21	Total	O		0
			21	21		
32	7	74	Total	O		0
			74	74		
32	8	61	Total	O		0
			61	61		
32	A	288	Total	O		0
			288	288		
32	B	237	Total	O		0
			237	237		
32	C	50	Total	O		0
			50	50		
32	D	49	Total	O		0
			49	49		
32	E	21	Total	O		0
			21	21		
32	I	2	Total	O		0
			2	2		
32	J	9	Total	O		0
			9	9		
32	K	3	Total	O		0
			3	3		
32	Z	11	Total	O		0
			11	11		
32	1	32	Total	O		0
			32	32		
32	F	47	Total	O		0
			47	47		
32	L	6	Total	O		0
			6	6		

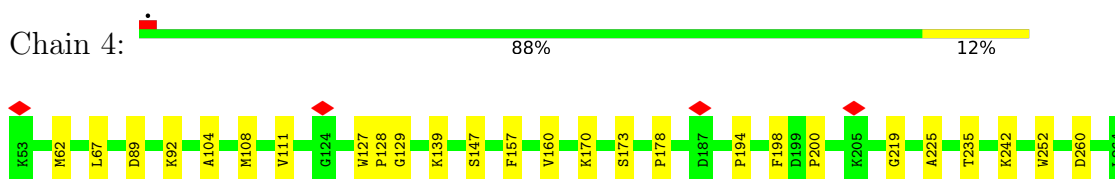
### 3 Residue-property plots [i](#)

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.

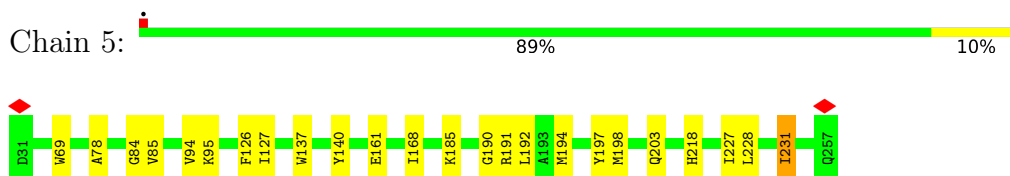
- Molecule 1: Light-harvesting chlorophyll-a/b protein of photosystem I, type III



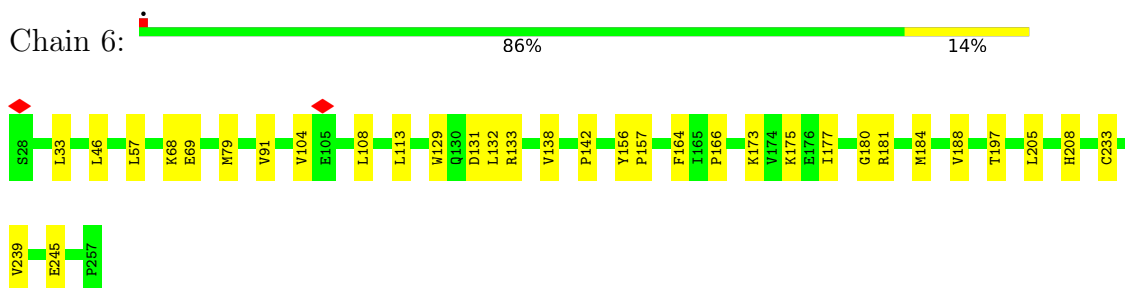
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic



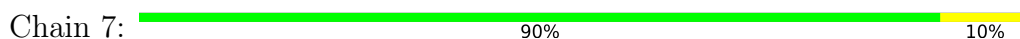
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



- Molecule 4: Chlorophyll a-b binding protein, chloroplastic



- Molecule 5: Chlorophyll a-b binding protein, chloroplastic





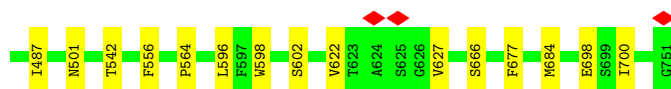
- Molecule 6: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 87% 13%



- Molecule 7: Photosystem I P700 chlorophyll a apoprotein A1

Chain A: 94% 6%



- Molecule 8: Photosystem I P700 chlorophyll a apoprotein A2

Chain B: 93% 7%



- Molecule 9: Photosystem I iron-sulfur center

Chain C: 94% 6%



- Molecule 10: Photosystem I reaction center subunit II, chloroplastic

Chain D: 94% 6%



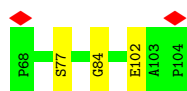
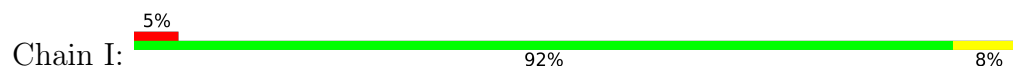
- Molecule 11: Photosystem I reaction center subunit IV, chloroplastic

Chain E: 95% 5%





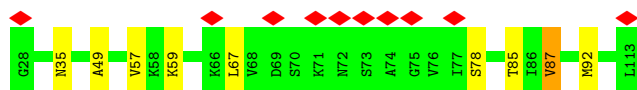
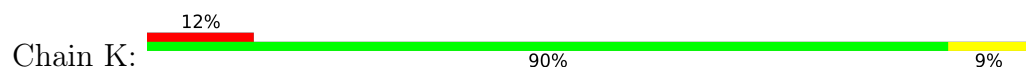
- Molecule 12: Photosystem I reaction center subunit VIII



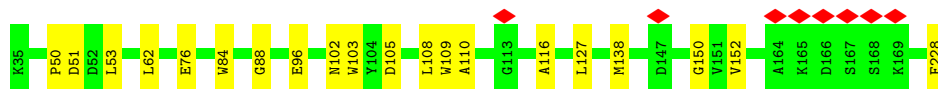
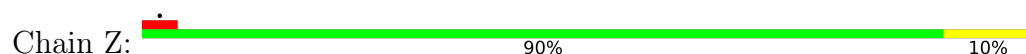
- Molecule 13: Photosystem I reaction center subunit IX



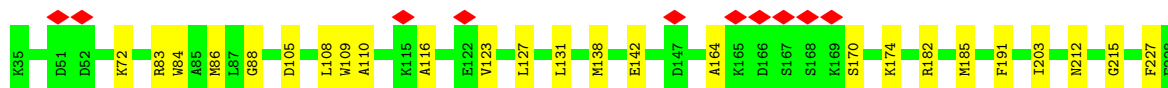
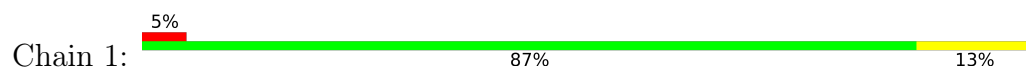
- Molecule 14: Photosystem I reaction center subunit psaK, chloroplastic



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



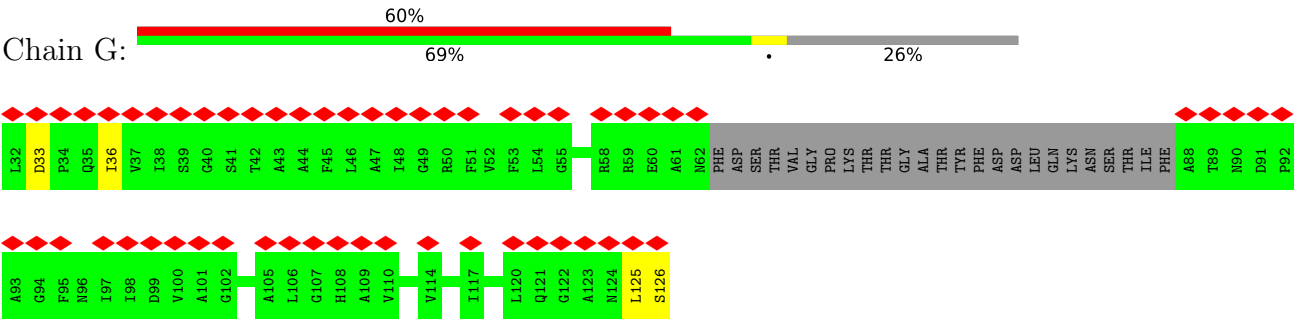
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



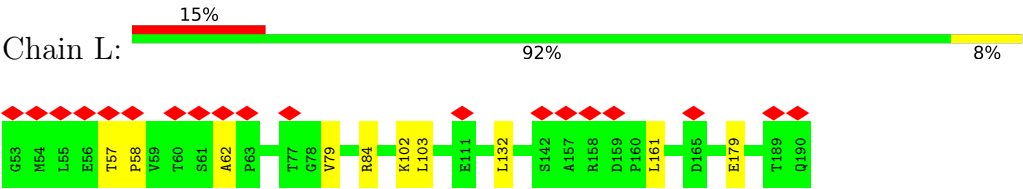
- Molecule 16: Photosystem I reaction center subunit III, chloroplastic



- Molecule 17: Photosystem I reaction center subunit V, chloroplastic



• Molecule 18: Chains: L



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	246159	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.108	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size ( $\text{\AA}$ )	373.76, 373.76, 373.76	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	0.73, 0.73, 0.73	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	3	0.16	0/1735	0.39	1/2355 (0.0%)
2	4	0.13	0/1707	0.28	0/2325
3	5	0.14	0/1830	0.30	0/2492
4	6	0.13	0/1834	0.30	0/2505
5	7	0.14	0/1702	0.30	0/2310
6	8	0.14	0/1701	0.29	0/2315
7	A	0.15	0/6021	0.32	0/8208
8	B	0.15	0/6036	0.34	0/8240
9	C	0.12	0/611	0.34	0/826
10	D	0.12	0/1161	0.34	0/1567
11	E	0.11	0/516	0.29	0/700
12	I	0.13	0/293	0.29	0/406
13	J	0.17	0/338	0.33	0/464
14	K	0.12	0/588	0.26	0/795
15	1	0.15	0/1491	0.32	0/2028
15	Z	0.13	0/1491	0.27	0/2028
16	F	0.13	0/1292	0.31	0/1747
17	G	0.09	0/521	0.20	0/706
18	L	0.13	0/920	0.27	0/1257
All	All	0.14	0/31788	0.32	1/43274 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	3	156	GLN	CA-CB-CG	7.14	128.39	114.10

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	3	1687	0	1646	16	0
2	4	1652	0	1613	19	0
3	5	1775	0	1746	19	0
4	6	1772	0	1770	29	0
5	7	1650	0	1589	16	0
6	8	1650	0	1629	19	0
7	A	5825	0	5675	40	0
8	B	5824	0	5577	41	0
9	C	601	0	581	3	0
10	D	1133	0	1150	6	0
11	E	506	0	504	2	0
12	I	281	0	292	2	0
13	J	329	0	328	3	0
14	K	583	0	620	7	0
15	1	1445	0	1396	20	0
15	Z	1445	0	1396	14	0
16	F	1266	0	1301	8	0
17	G	512	0	503	3	0
18	L	899	0	905	8	0
19	1	639	0	625	16	0
19	3	720	0	674	22	0
19	4	565	0	534	15	0
19	5	717	0	667	26	0
19	6	667	0	619	19	0
19	7	599	0	553	14	0
19	8	617	0	587	16	0
19	A	2653	0	2784	68	0
19	B	2528	0	2652	79	0
19	F	175	0	177	7	0
19	G	106	0	92	0	0
19	J	55	0	49	1	0
19	K	196	0	158	5	0
19	L	110	0	105	3	0
19	Z	637	0	616	10	0
20	1	92	0	62	2	0
20	3	66	0	70	0	0
20	4	287	0	270	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
20	5	206	0	167	5	0
20	6	338	0	307	15	0
20	7	224	0	202	3	0
20	8	198	0	210	5	0
20	Z	178	0	171	1	0
21	3	120	0	168	6	0
21	4	40	0	56	1	0
21	5	40	0	56	4	0
21	6	40	0	56	2	0
21	7	40	0	56	3	0
21	8	40	0	56	1	0
21	A	240	0	336	9	0
21	B	280	0	392	10	0
21	G	40	0	56	0	0
21	I	40	0	56	1	0
21	J	40	0	56	1	0
21	K	40	0	56	1	0
21	L	80	0	112	4	0
22	1	84	0	112	3	0
22	3	104	0	138	1	0
22	4	42	0	56	3	0
22	5	84	0	112	4	0
22	6	42	0	56	0	0
22	7	42	0	56	0	0
22	8	84	0	112	0	0
22	F	42	0	56	1	0
22	J	42	0	56	3	0
22	Z	68	0	89	1	0
23	3	37	0	44	4	0
23	4	41	0	55	0	0
23	6	47	0	68	3	0
23	7	32	0	34	0	0
23	8	49	0	71	1	0
23	B	43	0	56	1	0
23	F	32	0	34	1	0
23	G	36	0	42	0	0
23	J	77	0	97	4	0
23	L	40	0	50	2	0
24	1	135	0	177	5	0
24	3	117	0	157	3	0
24	4	88	0	115	2	0
24	6	48	0	70	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	7	43	0	54	1	0
24	8	24	0	35	1	0
24	A	79	0	105	1	0
24	B	35	0	46	2	0
24	F	35	0	46	2	0
24	K	24	0	35	0	0
24	Z	79	0	105	0	0
25	1	44	0	56	1	0
25	4	44	0	56	1	0
25	5	44	0	56	3	0
25	6	44	0	56	2	0
25	7	44	0	56	1	0
25	8	44	0	56	0	0
25	Z	44	0	56	2	0
26	1	44	0	58	0	0
26	4	87	0	123	5	0
26	5	75	0	90	2	0
26	6	85	0	116	7	0
26	7	49	0	74	1	0
26	8	44	0	61	3	0
26	A	118	0	155	3	0
26	B	45	0	63	6	0
26	Z	39	0	48	0	0
27	5	44	0	56	0	0
27	6	44	0	56	2	0
28	A	65	0	72	0	0
29	A	33	0	46	0	0
29	B	33	0	46	0	0
30	A	8	0	0	0	0
30	C	16	0	0	0	0
31	B	59	0	79	2	0
32	1	32	0	0	0	0
32	3	55	0	0	0	0
32	4	17	0	0	0	0
32	5	36	0	0	0	0
32	6	21	0	0	0	0
32	7	74	0	0	0	0
32	8	61	0	0	0	0
32	A	288	0	0	0	0
32	B	237	0	0	1	0
32	C	50	0	0	0	0
32	D	49	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
32	E	21	0	0	0	0
32	F	47	0	0	0	0
32	I	2	0	0	0	0
32	J	9	0	0	0	0
32	K	3	0	0	0	0
32	L	6	0	0	0	0
32	Z	11	0	0	0	0
All	All	48478	0	47958	518	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 5.

The worst 5 of 518 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)
8:B:663:MET:HB2	19:B:804:CLA:C1C	2.07	0.83
20:5:308:CHL:HBB2	20:5:317:CHL:HHC	1.60	0.81
20:4:607:CHL:HBB2	20:4:615:CHL:HHC	1.65	0.77
21:5:320:BCR:HC42	26:6:318:LHG:H102	1.70	0.73
15:1:142:GLU:HG3	19:1:308:CLA:C4B	2.18	0.73

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	3	219/221 (99%)	216 (99%)	3 (1%)	0	100	100
2	4	210/212 (99%)	209 (100%)	1 (0%)	0	100	100
3	5	225/227 (99%)	222 (99%)	3 (1%)	0	100	100
4	6	228/230 (99%)	224 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	7	211/213 (99%)	207 (98%)	4 (2%)	0	100	100
6	8	215/217 (99%)	214 (100%)	1 (0%)	0	100	100
7	A	740/742 (100%)	728 (98%)	12 (2%)	0	100	100
8	B	731/733 (100%)	714 (98%)	17 (2%)	0	100	100
9	C	78/80 (98%)	78 (100%)	0	0	100	100
10	D	142/144 (99%)	138 (97%)	4 (3%)	0	100	100
11	E	62/64 (97%)	61 (98%)	1 (2%)	0	100	100
12	I	35/37 (95%)	35 (100%)	0	0	100	100
13	J	39/41 (95%)	39 (100%)	0	0	100	100
14	K	84/86 (98%)	83 (99%)	1 (1%)	0	100	100
15	1	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
15	Z	192/194 (99%)	191 (100%)	1 (0%)	0	100	100
16	F	163/165 (99%)	161 (99%)	2 (1%)	0	100	100
17	G	66/95 (70%)	66 (100%)	0	0	100	100
18	L	120/124 (97%)	120 (100%)	0	0	100	100
All	All	3952/4019 (98%)	3897 (99%)	55 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	3	168/168 (100%)	168 (100%)	0	100	100
2	4	167/167 (100%)	165 (99%)	2 (1%)	63	51
3	5	184/184 (100%)	180 (98%)	4 (2%)	45	29
4	6	184/184 (100%)	182 (99%)	2 (1%)	65	54
5	7	164/164 (100%)	164 (100%)	0	100	100
6	8	163/163 (100%)	162 (99%)	1 (1%)	78	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	A	601/601 (100%)	600 (100%)	1 (0%)	87	84
8	B	596/596 (100%)	592 (99%)	4 (1%)	76	68
9	C	69/69 (100%)	69 (100%)	0	100	100
10	D	121/121 (100%)	117 (97%)	4 (3%)	33	15
11	E	55/55 (100%)	55 (100%)	0	100	100
12	I	31/31 (100%)	30 (97%)	1 (3%)	34	17
13	J	36/36 (100%)	36 (100%)	0	100	100
14	K	59/59 (100%)	58 (98%)	1 (2%)	53	37
15	1	137/137 (100%)	136 (99%)	1 (1%)	76	68
15	Z	137/137 (100%)	136 (99%)	1 (1%)	76	68
16	F	127/127 (100%)	125 (98%)	2 (2%)	55	39
17	G	49/71 (69%)	49 (100%)	0	100	100
18	L	90/90 (100%)	90 (100%)	0	100	100
All	All	3138/3160 (99%)	3114 (99%)	24 (1%)	70	65

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
10	D	57	THR
10	D	191	MET
10	D	175	ILE
12	I	102	GLU
4	6	233	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
7	A	387	GLN
15	1	212	ASN
8	B	84	HIS
15	1	128	ASN
8	B	77	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

328 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$
19	CLA	A	839	7	55,59,73	1.31	8 (14%)	64,96,113	1.40	6 (9%)
19	CLA	6	314	4	54,58,73	1.32	8 (14%)	64,95,113	1.36	6 (9%)
22	LUT	F	305	-	42,43,43	0.28	0	51,60,60	0.75	1 (1%)
21	BCR	7	617	-	41,41,41	0.31	0	56,56,56	0.65	0
19	CLA	A	821	7	69,73,73	1.17	8 (11%)	82,113,113	1.25	8 (9%)
24	LMU	1	322	-	22,22,36	0.37	0	27,27,47	0.72	0
19	CLA	8	303	6	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
19	CLA	3	313	32	64,68,73	1.20	7 (10%)	76,107,113	1.46	8 (10%)
19	CLA	8	302	6	69,73,73	1.16	6 (8%)	82,113,113	1.27	6 (7%)
21	BCR	6	321	-	41,41,41	0.30	0	56,56,56	0.56	0
19	CLA	B	833	8	69,73,73	1.17	7 (10%)	82,113,113	1.29	7 (8%)
21	BCR	A	850	-	41,41,41	0.31	0	56,56,56	0.63	1 (1%)
22	LUT	Z	617	-	26,26,43	0.43	0	33,35,60	0.61	0
19	CLA	L	204	32	49,53,73	1.40	7 (14%)	58,89,113	1.41	4 (6%)
19	CLA	B	805	8	49,53,73	1.38	6 (12%)	58,89,113	1.43	4 (6%)
19	CLA	A	840	7	69,73,73	1.16	8 (11%)	82,113,113	1.28	7 (8%)
19	CLA	A	810	7	69,73,73	1.16	7 (10%)	82,113,113	1.29	6 (7%)
21	BCR	A	849	-	41,41,41	0.31	0	56,56,56	0.53	0
22	LUT	8	315	-	42,43,43	0.29	0	51,60,60	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	4	608	2	64,68,73	1.21	6 (9%)	76,107,113	1.33	5 (6%)
19	CLA	A	841	7	69,73,73	1.17	7 (10%)	82,113,113	1.30	6 (7%)
19	CLA	1	310	26	65,69,73	1.20	6 (9%)	77,108,113	1.28	5 (6%)
19	CLA	8	304	32	64,68,73	1.21	7 (10%)	76,107,113	1.28	5 (6%)
19	CLA	7	612	5	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
19	CLA	B	829	8	69,73,73	1.15	6 (8%)	82,113,113	1.20	6 (7%)
20	CHL	4	601	2	60,74,74	0.94	3 (5%)	58,114,114	1.83	6 (10%)
22	LUT	3	320	-	19,20,43	0.47	0	21,28,60	0.45	0
21	BCR	3	318	-	41,41,41	0.31	0	56,56,56	0.58	0
20	CHL	6	315	4	60,74,74	0.89	3 (5%)	58,114,114	1.74	7 (12%)
19	CLA	A	803	-	69,73,73	1.16	7 (10%)	82,113,113	1.20	6 (7%)
30	SF4	C	101	9	0,12,12	-	-	-		
20	CHL	Z	606	32	60,74,74	0.90	3 (5%)	58,114,114	1.82	7 (12%)
19	CLA	8	313	6	61,65,73	1.24	7 (11%)	72,103,113	1.27	6 (8%)
21	BCR	A	853	-	41,41,41	0.33	0	56,56,56	0.63	0
19	CLA	B	832	8	59,63,73	1.26	7 (11%)	70,101,113	1.34	7 (10%)
19	CLA	6	316	4	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
24	LMU	4	622	-	22,22,36	0.40	0	27,27,47	0.70	0
24	LMU	3	324	-	36,36,36	0.44	0	47,47,47	1.08	5 (10%)
19	CLA	1	304	32	54,58,73	1.31	7 (12%)	64,95,113	1.40	7 (10%)
19	CLA	4	609	2	64,68,73	1.20	7 (10%)	76,107,113	1.29	7 (9%)
20	CHL	8	306	32	60,74,74	0.95	3 (5%)	58,114,114	2.17	6 (10%)
19	CLA	F	304	16	69,73,73	1.17	9 (13%)	82,113,113	1.18	4 (4%)
19	CLA	B	823	8	63,67,73	1.23	8 (12%)	74,105,113	1.31	6 (8%)
19	CLA	K	203	32	64,68,73	1.21	6 (9%)	76,107,113	1.37	9 (11%)
19	CLA	6	309	4	59,63,73	1.26	6 (10%)	70,101,113	1.31	6 (8%)
19	CLA	B	816	8	69,73,73	1.16	8 (11%)	82,113,113	1.28	6 (7%)
19	CLA	7	611	5	56,60,73	1.29	9 (16%)	65,97,113	1.38	5 (7%)
24	LMU	3	322	-	35,35,36	0.47	0	46,46,47	0.65	0
28	CLO	A	802	7	58,73,73	0.84	2 (3%)	60,113,113	2.08	6 (10%)
21	BCR	B	845	-	41,41,41	0.34	0	56,56,56	0.74	0
23	LMG	3	321	-	37,37,55	0.57	0	45,45,63	0.71	0
25	XAT	8	316	-	41,47,47	0.73	2 (4%)	54,74,74	0.74	0
19	CLA	5	311	26	59,63,73	1.26	6 (10%)	70,101,113	1.35	7 (10%)
20	CHL	5	317	3	37,51,74	1.21	3 (8%)	30,86,114	2.73	7 (23%)
19	CLA	A	842	7	69,73,73	1.15	7 (10%)	82,113,113	1.26	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	Z	607	32	54,58,73	1.33	8 (14%)	64,95,113	1.39	5 (7%)
21	BCR	B	802	-	41,41,41	0.36	0	56,56,56	1.09	4 (7%)
20	CHL	5	306	32	40,54,74	1.14	3 (7%)	34,90,114	2.79	6 (17%)
19	CLA	1	314	15	50,54,73	1.36	7 (14%)	59,90,113	1.42	4 (6%)
19	CLA	5	305	32	59,63,73	1.27	8 (13%)	70,101,113	1.33	5 (7%)
19	CLA	A	831	7	69,73,73	1.18	7 (10%)	82,113,113	1.23	5 (6%)
20	CHL	6	307	32	60,74,74	0.84	3 (5%)	58,114,114	2.22	6 (10%)
19	CLA	4	612	2	69,73,73	1.17	8 (11%)	82,113,113	1.41	7 (8%)
21	BCR	L	205	-	41,41,41	0.34	0	56,56,56	0.57	0
20	CHL	1	306	32	40,54,74	1.17	3 (7%)	34,90,114	2.49	5 (14%)
19	CLA	A	813	19,7	69,73,73	1.14	6 (8%)	82,113,113	1.20	5 (6%)
20	CHL	Z	605	32	40,54,74	1.09	2 (5%)	34,90,114	2.81	5 (14%)
19	CLA	B	809	8	69,73,73	1.16	7 (10%)	82,113,113	1.30	7 (8%)
19	CLA	B	835	8	64,68,73	1.21	7 (10%)	76,107,113	1.32	6 (7%)
19	CLA	A	816	7	59,63,73	1.28	7 (11%)	70,101,113	1.31	5 (7%)
19	CLA	A	812	7	69,73,73	1.16	7 (10%)	82,113,113	1.23	6 (7%)
25	XAT	Z	616	-	41,47,47	0.72	2 (4%)	54,74,74	0.82	0
19	CLA	3	302	1	69,73,73	1.16	7 (10%)	82,113,113	1.33	7 (8%)
19	CLA	B	808	8	59,63,73	1.26	7 (11%)	70,101,113	1.33	6 (8%)
19	CLA	Z	614	15	64,68,73	1.23	8 (12%)	76,107,113	1.29	6 (7%)
30	SF4	C	102	9	0,12,12	-	-	-	-	-
19	CLA	B	811	8	69,73,73	1.17	7 (10%)	82,113,113	1.28	5 (6%)
19	CLA	A	825	7	49,53,73	1.39	8 (16%)	58,89,113	1.39	5 (8%)
25	XAT	6	322	-	41,47,47	0.73	2 (4%)	54,74,74	0.85	0
19	CLA	F	302	32	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
19	CLA	8	312	6	69,73,73	1.18	7 (10%)	82,113,113	1.24	5 (6%)
19	CLA	B	819	8	69,73,73	1.17	8 (11%)	82,113,113	1.26	8 (9%)
22	LUT	7	615	-	42,43,43	0.29	0	51,60,60	0.54	0
19	CLA	B	836	32	49,53,73	1.38	7 (14%)	58,89,113	1.45	6 (10%)
19	CLA	1	309	15	69,73,73	1.16	7 (10%)	82,113,113	1.25	7 (8%)
30	SF4	A	854	8,7	0,12,12	-	-	-	-	-
21	BCR	A	851	-	41,41,41	0.32	0	56,56,56	0.70	0
19	CLA	B	806	8	69,73,73	1.17	6 (8%)	82,113,113	1.27	5 (6%)
19	CLA	A	822	7	59,63,73	1.25	6 (10%)	70,101,113	1.32	6 (8%)
19	CLA	F	303	32	49,53,73	1.39	7 (14%)	58,89,113	1.42	6 (10%)
19	CLA	3	305	1	55,59,73	1.31	7 (12%)	64,96,113	1.36	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	Z	613	15	54,58,73	1.32	7 (12%)	64,95,113	1.39	6 (9%)
21	BCR	I	201	-	41,41,41	0.33	0	56,56,56	0.76	0
19	CLA	4	614	2	49,53,73	1.39	6 (12%)	58,89,113	1.42	4 (6%)
19	CLA	A	830	7	69,73,73	1.16	7 (10%)	82,113,113	1.24	7 (8%)
24	LMU	1	320	-	19,19,36	0.41	0	24,24,47	0.65	0
19	CLA	1	313	15	64,68,73	1.21	7 (10%)	76,107,113	1.28	7 (9%)
19	CLA	7	602	5	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
24	LMU	7	620	-	22,22,36	0.40	0	27,27,47	0.68	0
19	CLA	B	840	32	69,73,73	1.18	7 (10%)	82,113,113	1.28	6 (7%)
19	CLA	B	815	8	64,68,73	1.21	6 (9%)	76,107,113	1.28	5 (6%)
19	CLA	B	820	32	64,68,73	1.23	6 (9%)	76,107,113	1.28	6 (7%)
19	CLA	B	804	-	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
19	CLA	B	838	8	69,73,73	1.16	8 (11%)	82,113,113	1.26	5 (6%)
22	LUT	Z	615	-	42,43,43	0.30	0	51,60,60	0.65	0
21	BCR	B	848	-	41,41,41	0.29	0	56,56,56	0.81	1 (1%)
23	LMG	7	622	-	32,32,55	0.57	0	40,40,63	0.72	0
19	CLA	8	308	6	49,53,73	1.37	6 (12%)	58,89,113	1.42	4 (6%)
24	LMU	4	624	-	24,24,36	0.38	0	29,29,47	0.64	0
24	LMU	A	855	-	36,36,36	0.44	0	47,47,47	1.09	2 (4%)
19	CLA	A	807	7	69,73,73	1.17	9 (13%)	82,113,113	1.28	8 (9%)
21	BCR	A	858	-	41,41,41	0.32	0	56,56,56	0.84	3 (5%)
19	CLA	5	313	3	60,64,73	1.24	8 (13%)	71,102,113	1.37	6 (8%)
19	CLA	A	834	7	69,73,73	1.16	6 (8%)	82,113,113	1.29	5 (6%)
19	CLA	4	611	2	49,53,73	1.39	8 (16%)	58,89,113	1.44	5 (8%)
19	CLA	3	304	32	46,50,73	1.40	9 (19%)	53,85,113	1.41	4 (7%)
19	CLA	B	826	32	69,73,73	1.16	6 (8%)	82,113,113	1.26	8 (9%)
22	LUT	J	101	-	42,43,43	0.29	0	51,60,60	0.82	2 (3%)
19	CLA	L	203	18	69,73,73	1.16	7 (10%)	82,113,113	1.30	8 (9%)
19	CLA	A	815	7	69,73,73	1.18	6 (8%)	82,113,113	1.27	7 (8%)
19	CLA	J	102	13	59,63,73	1.26	7 (11%)	70,101,113	1.36	6 (8%)
19	CLA	B	814	8	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
22	LUT	3	317	-	42,43,43	0.26	0	51,60,60	0.56	0
19	CLA	K	204	14	50,54,73	1.36	8 (16%)	59,90,113	1.41	4 (6%)
21	BCR	B	844	-	41,41,41	0.36	0	56,56,56	0.91	3 (5%)
19	CLA	A	846	26	49,53,73	1.38	7 (14%)	58,89,113	1.43	5 (8%)
20	CHL	8	305	32	60,74,74	0.94	3 (5%)	58,114,114	2.20	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	6	311	26	62,66,73	1.24	7 (11%)	73,104,113	1.27	5 (6%)
22	LUT	1	317	-	42,43,43	0.28	0	51,60,60	0.69	0
24	LMU	3	323	-	24,24,36	0.36	0	29,29,47	0.67	0
19	CLA	1	311	15	49,53,73	1.38	9 (18%)	58,89,113	1.42	4 (6%)
19	CLA	Z	609	15	64,68,73	1.21	8 (12%)	76,107,113	1.29	7 (9%)
19	CLA	1	307	32	69,73,73	1.17	8 (11%)	82,113,113	1.29	6 (7%)
20	CHL	5	307	32	60,74,74	0.93	3 (5%)	58,114,114	2.21	7 (12%)
24	LMU	A	857	-	24,24,36	0.36	0	29,29,47	0.61	0
26	LHG	6	318	19	48,48,48	0.51	0	51,54,54	0.51	0
20	CHL	7	606	32	40,54,74	1.12	3 (7%)	34,90,114	2.68	5 (14%)
20	CHL	3	306	32	60,74,74	0.90	3 (5%)	58,114,114	2.01	6 (10%)
19	CLA	5	304	3	54,58,73	1.30	7 (12%)	64,95,113	1.42	7 (10%)
19	CLA	5	319	32	50,54,73	1.37	7 (14%)	59,90,113	1.48	5 (8%)
19	CLA	A	814	7	69,73,73	1.16	6 (8%)	82,113,113	1.28	6 (7%)
21	BCR	J	103	-	41,41,41	0.32	0	56,56,56	0.53	0
19	CLA	A	805	7	69,73,73	1.16	8 (11%)	82,113,113	1.34	8 (9%)
23	LMG	6	326	-	19,19,55	0.34	0	19,19,63	0.46	0
19	CLA	B	841	8	69,73,73	1.16	7 (10%)	82,113,113	1.28	5 (6%)
20	CHL	4	607	32	60,74,74	0.95	3 (5%)	58,114,114	2.03	4 (6%)
19	CLA	B	825	32	69,73,73	1.17	6 (8%)	82,113,113	1.27	7 (8%)
29	PQN	B	843	-	34,34,34	0.36	0	43,45,45	0.63	1 (2%)
20	CHL	5	308	32	45,59,74	1.08	3 (6%)	40,96,114	2.49	6 (15%)
19	CLA	3	311	1	64,68,73	1.22	7 (10%)	76,107,113	1.27	6 (7%)
19	CLA	8	310	26	49,53,73	1.38	8 (16%)	58,89,113	1.39	4 (6%)
19	CLA	A	836	7	69,73,73	1.16	9 (13%)	82,113,113	1.27	6 (7%)
19	CLA	7	610	26	69,73,73	1.16	7 (10%)	82,113,113	1.26	5 (6%)
21	BCR	B	849	-	41,41,41	0.31	0	56,56,56	0.71	0
19	CLA	7	613	5	47,51,73	1.39	7 (14%)	55,86,113	1.42	5 (9%)
24	LMU	1	301	-	36,36,36	0.43	0	47,47,47	1.09	2 (4%)
22	LUT	3	316	-	42,43,43	0.25	0	51,60,60	0.56	0
24	LMU	4	625	-	22,22,36	0.39	0	27,27,47	0.60	0
19	CLA	3	303	32	69,73,73	1.17	8 (11%)	82,113,113	1.28	8 (9%)
24	LMU	3	325	-	24,24,36	0.36	0	29,29,47	0.65	0
19	CLA	Z	604	32	61,65,73	1.24	7 (11%)	72,103,113	1.33	6 (8%)
21	BCR	8	317	-	41,41,41	0.30	0	56,56,56	0.54	0
19	CLA	B	803	8	69,73,73	1.17	7 (10%)	82,113,113	1.23	5 (6%)
19	CLA	7	607	32	54,58,73	1.30	7 (12%)	64,95,113	1.44	7 (10%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
23	LMG	6	301	-	26,26,55	0.46	0	28,28,63	0.49	0
19	CLA	A	818	32	59,63,73	1.26	8 (13%)	70,101,113	1.36	6 (8%)
20	CHL	6	308	32	45,59,74	1.03	3 (6%)	40,96,114	2.11	6 (15%)
26	LHG	6	325	-	35,35,48	0.57	0	38,41,54	0.75	1 (2%)
26	LHG	5	321	19	36,36,48	0.58	0	39,42,54	0.55	0
24	LMU	8	319	-	24,24,36	0.38	0	29,29,47	0.61	0
21	BCR	B	846	-	41,41,41	0.31	0	56,56,56	0.57	0
19	CLA	B	828	8	69,73,73	1.17	6 (8%)	82,113,113	1.22	6 (7%)
20	CHL	6	306	32	40,54,74	1.11	3 (7%)	34,90,114	2.59	6 (17%)
19	CLA	3	301	1	64,68,73	1.20	7 (10%)	76,107,113	1.33	7 (9%)
19	CLA	5	315	3	49,53,73	1.38	7 (14%)	58,89,113	1.40	6 (10%)
25	XAT	5	322	-	41,47,47	0.73	2 (4%)	54,74,74	0.83	0
26	LHG	B	851	19	44,44,48	0.53	0	47,50,54	0.53	0
19	CLA	A	827	32	69,73,73	1.17	7 (10%)	82,113,113	1.29	6 (7%)
19	CLA	1	302	15	64,68,73	1.22	7 (10%)	76,107,113	1.28	5 (6%)
19	CLA	6	305	4	69,73,73	1.17	8 (11%)	82,113,113	1.27	6 (7%)
24	LMU	F	306	-	36,36,36	0.45	0	47,47,47	0.77	1 (2%)
21	BCR	4	618	-	41,41,41	0.30	0	56,56,56	0.59	0
19	CLA	A	824	7	69,73,73	1.17	6 (8%)	82,113,113	1.27	5 (6%)
20	CHL	6	302	4	60,74,74	0.94	3 (5%)	58,114,114	2.14	6 (10%)
19	CLA	3	312	1	49,53,73	1.39	8 (16%)	58,89,113	1.39	4 (6%)
26	LHG	Z	618	19	38,38,48	0.57	0	41,44,54	0.54	0
20	CHL	8	320	15	60,74,74	0.91	3 (5%)	58,114,114	2.23	7 (12%)
23	LMG	L	201	-	40,40,55	0.54	0	48,48,63	0.59	0
19	CLA	A	832	7	69,73,73	1.16	8 (11%)	82,113,113	1.26	7 (8%)
19	CLA	B	842	26	69,73,73	1.17	8 (11%)	82,113,113	1.28	6 (7%)
25	XAT	1	316	-	41,47,47	0.73	2 (4%)	54,74,74	0.85	0
19	CLA	Z	603	15	69,73,73	1.17	9 (13%)	82,113,113	1.27	4 (4%)
19	CLA	Z	610	26	64,68,73	1.20	7 (10%)	76,107,113	1.28	7 (9%)
19	CLA	G	203	17	50,54,73	1.37	6 (12%)	59,90,113	1.41	4 (6%)
24	LMU	1	321	-	24,24,36	0.37	0	29,29,47	0.63	0
19	CLA	4	602	2	64,68,73	1.21	7 (10%)	76,107,113	1.29	7 (9%)
20	CHL	7	621	6	60,74,74	0.94	3 (5%)	58,114,114	2.27	6 (10%)
19	CLA	3	309	32	59,63,73	1.26	8 (13%)	70,101,113	1.37	6 (8%)
19	CLA	B	801	32	69,73,73	1.18	8 (11%)	82,113,113	1.20	6 (7%)
23	LMG	B	852	-	43,43,55	0.53	0	51,51,63	0.68	0
19	CLA	B	813	8	69,73,73	1.18	6 (8%)	82,113,113	1.26	7 (8%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	8	314	6	49,53,73	1.39	7 (14%)	58,89,113	1.40	5 (8%)
21	BCR	G	204	-	41,41,41	0.33	0	56,56,56	0.59	0
22	LUT	1	315	-	42,43,43	0.30	0	51,60,60	0.62	0
24	LMU	Z	621	-	24,24,36	0.38	0	29,29,47	0.60	0
22	LUT	6	319	-	42,43,43	0.30	0	51,60,60	0.68	0
19	CLA	A	844	32	69,73,73	1.18	8 (11%)	82,113,113	1.28	6 (7%)
31	DGD	B	850	-	60,60,67	0.58	0	74,74,81	0.80	2 (2%)
19	CLA	B	812	8	69,73,73	1.17	7 (10%)	82,113,113	1.22	5 (6%)
22	LUT	4	616	-	42,43,43	0.29	0	51,60,60	0.72	0
19	CLA	B	817	8	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
21	BCR	B	847	-	41,41,41	0.30	0	56,56,56	0.58	0
26	LHG	4	619	19	48,48,48	0.52	0	51,54,54	0.49	0
23	LMG	F	301	-	32,32,55	0.60	0	40,40,63	0.74	0
19	CLA	8	311	6	59,63,73	1.26	8 (13%)	70,101,113	1.34	5 (7%)
22	LUT	5	318	-	42,43,43	0.30	0	51,60,60	0.69	1 (1%)
20	CHL	7	601	5	60,74,74	0.85	3 (5%)	58,114,114	2.23	6 (10%)
24	LMU	6	324	-	24,24,36	0.39	0	29,29,47	0.61	0
19	CLA	5	309	3	69,73,73	1.16	7 (10%)	82,113,113	1.27	4 (4%)
26	LHG	8	318	19	43,43,48	0.54	0	46,49,54	0.54	0
19	CLA	5	316	3	69,73,73	1.16	8 (11%)	82,113,113	1.25	6 (7%)
19	CLA	3	310	1	50,54,73	1.36	7 (14%)	59,90,113	1.38	5 (8%)
19	CLA	5	314	3	49,53,73	1.39	8 (16%)	58,89,113	1.42	4 (6%)
19	CLA	A	837	7	69,73,73	1.18	8 (11%)	82,113,113	1.24	4 (4%)
24	LMU	B	853	-	36,36,36	0.45	0	47,47,47	0.67	0
19	CLA	7	609	5	69,73,73	1.16	7 (10%)	82,113,113	1.24	6 (7%)
19	CLA	A	809	7	54,58,73	1.30	7 (12%)	64,95,113	1.41	8 (12%)
20	CHL	Z	601	15	60,74,74	1.04	3 (5%)	58,114,114	1.93	6 (10%)
19	CLA	6	303	4	69,73,73	1.17	6 (8%)	82,113,113	1.26	5 (6%)
19	CLA	6	320	32	59,63,73	1.26	7 (11%)	70,101,113	1.34	9 (12%)
26	LHG	A	847	-	48,48,48	0.51	0	51,54,54	0.47	0
19	CLA	A	838	7	61,65,73	1.24	6 (9%)	72,103,113	1.31	7 (9%)
19	CLA	Z	608	15	69,73,73	1.18	8 (11%)	82,113,113	1.22	4 (4%)
19	CLA	A	833	7	59,63,73	1.26	7 (11%)	70,101,113	1.35	5 (7%)
21	BCR	3	319	-	41,41,41	0.30	0	56,56,56	0.61	0
19	CLA	B	821	8	60,64,73	1.26	7 (11%)	71,102,113	1.34	6 (8%)
19	CLA	B	831	8	49,53,73	1.37	7 (14%)	58,89,113	1.46	4 (6%)
19	CLA	A	823	32	69,73,73	1.17	8 (11%)	82,113,113	1.25	8 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
21	BCR	3	315	-	41,41,41	0.31	0	56,56,56	0.55	0
19	CLA	6	304	4	55,59,73	1.31	6 (10%)	64,96,113	1.40	6 (9%)
24	LMU	Z	619	-	32,32,36	0.46	0	43,43,47	0.86	1 (2%)
19	CLA	A	817	7	69,73,73	1.17	6 (8%)	82,113,113	1.27	5 (6%)
19	CLA	A	829	7	69,73,73	1.16	8 (11%)	82,113,113	1.25	6 (7%)
19	CLA	Z	612	32	69,73,73	1.16	7 (10%)	82,113,113	1.28	6 (7%)
26	LHG	4	620	-	37,37,48	0.57	0	40,43,54	0.52	0
19	CLA	8	307	32	54,58,73	1.32	8 (14%)	64,95,113	1.41	6 (9%)
22	LUT	8	301	-	42,43,43	0.30	0	51,60,60	0.62	0
19	CLA	5	303	3	69,73,73	1.17	7 (10%)	82,113,113	1.25	5 (6%)
19	CLA	Z	611	15	49,53,73	1.40	8 (16%)	58,89,113	1.40	4 (6%)
19	CLA	1	312	32	69,73,73	1.17	7 (10%)	82,113,113	1.28	6 (7%)
19	CLA	7	608	5	49,53,73	1.36	6 (12%)	58,89,113	1.47	5 (8%)
19	CLA	3	314	1	49,53,73	1.38	7 (14%)	58,89,113	1.37	4 (6%)
19	CLA	A	820	7	64,68,73	1.23	8 (12%)	76,107,113	1.25	5 (6%)
27	NEX	5	323	-	40,46,46	0.23	0	50,70,70	1.28	5 (10%)
27	NEX	6	323	-	40,46,46	0.21	0	50,70,70	1.30	4 (8%)
19	CLA	8	309	6	69,73,73	1.15	6 (8%)	82,113,113	1.24	6 (7%)
24	LMU	A	856	-	20,20,36	0.40	0	25,25,47	0.71	0
23	LMG	G	201	-	36,36,55	0.56	0	44,44,63	0.67	0
20	CHL	4	606	32	37,51,74	1.12	2 (5%)	30,86,114	2.70	5 (16%)
24	LMU	1	319	-	36,36,36	0.44	0	47,47,47	0.75	1 (2%)
19	CLA	B	818	8	69,73,73	1.17	8 (11%)	82,113,113	1.24	5 (6%)
19	CLA	A	828	32	69,73,73	1.17	7 (10%)	82,113,113	1.30	7 (8%)
26	LHG	A	801	-	30,30,48	0.62	0	33,36,54	0.61	0
23	LMG	4	621	-	41,41,55	0.54	0	49,49,63	0.69	0
19	CLA	6	313	32	69,73,73	1.17	8 (11%)	82,113,113	1.25	6 (7%)
26	LHG	1	318	19	43,43,48	0.54	0	46,49,54	0.52	0
19	CLA	A	843	7	69,73,73	1.18	8 (11%)	82,113,113	1.23	4 (4%)
19	CLA	B	824	8	69,73,73	1.16	7 (10%)	82,113,113	1.30	9 (10%)
19	CLA	G	202	17	64,68,73	1.23	8 (12%)	76,107,113	1.30	6 (7%)
26	LHG	5	301	-	37,37,48	0.57	0	40,43,54	0.56	0
19	CLA	7	604	32	55,59,73	1.31	8 (14%)	64,96,113	1.39	6 (9%)
19	CLA	K	202	14	49,53,73	1.39	9 (18%)	58,89,113	1.52	5 (8%)
19	CLA	A	835	7	69,73,73	1.18	8 (11%)	82,113,113	1.26	6 (7%)
20	CHL	7	605	32	40,54,74	1.16	3 (7%)	34,90,114	2.61	6 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
19	CLA	3	308	1	69,73,73	1.16	6 (8%)	82,113,113	1.26	8 (9%)
26	LHG	A	848	19	37,37,48	0.58	0	40,43,54	0.52	0
19	CLA	B	839	8	54,58,73	1.30	6 (11%)	64,95,113	1.44	8 (12%)
19	CLA	6	327	32	57,61,73	1.28	8 (14%)	67,98,113	1.36	7 (10%)
19	CLA	5	310	3	64,68,73	1.20	8 (12%)	76,107,113	1.31	8 (10%)
22	LUT	5	324	-	42,43,43	0.28	0	51,60,60	0.51	0
19	CLA	1	303	15	61,65,73	1.25	6 (9%)	72,103,113	1.35	5 (6%)
19	CLA	4	610	26	64,68,73	1.22	7 (10%)	76,107,113	1.26	4 (5%)
19	CLA	1	308	15	69,73,73	1.18	6 (8%)	82,113,113	1.26	4 (4%)
19	CLA	7	603	5	56,60,73	1.29	6 (10%)	65,97,113	1.40	6 (9%)
19	CLA	B	834	8	62,66,73	1.22	7 (11%)	73,104,113	1.38	7 (9%)
23	LMG	8	321	-	49,49,55	0.52	0	57,57,63	0.64	0
19	CLA	A	819	7	69,73,73	1.15	7 (10%)	82,113,113	1.29	6 (7%)
19	CLA	4	613	2	59,63,73	1.27	8 (13%)	70,101,113	1.32	6 (8%)
19	CLA	B	830	8	69,73,73	1.17	7 (10%)	82,113,113	1.21	7 (8%)
25	XAT	4	617	-	41,47,47	0.72	2 (4%)	54,74,74	0.90	1 (1%)
20	CHL	1	305	32	40,54,74	1.17	3 (7%)	34,90,114	2.52	5 (14%)
19	CLA	A	806	19,7	59,63,73	1.26	7 (11%)	70,101,113	1.32	4 (5%)
24	LMU	4	623	-	20,20,36	0.39	0	25,25,47	0.79	0
20	CHL	6	317	4	37,51,74	1.29	3 (8%)	30,86,114	2.48	5 (16%)
24	LMU	7	619	-	21,21,36	0.39	0	26,26,47	0.71	0
26	LHG	7	618	19	48,48,48	0.52	0	51,54,54	0.49	0
19	CLA	B	810	8	69,73,73	1.18	8 (11%)	82,113,113	1.28	5 (6%)
19	CLA	4	604	32	54,58,73	1.31	8 (14%)	64,95,113	1.39	6 (9%)
19	CLA	B	827	8	69,73,73	1.17	9 (13%)	82,113,113	1.27	7 (8%)
21	BCR	A	852	-	41,41,41	0.31	0	56,56,56	0.57	0
19	CLA	6	310	4	64,68,73	1.22	8 (12%)	76,107,113	1.27	8 (10%)
19	CLA	A	804	32	69,73,73	1.17	7 (10%)	82,113,113	1.20	4 (4%)
19	CLA	B	807	8	69,73,73	1.18	7 (10%)	82,113,113	1.26	6 (7%)
20	CHL	4	605	32	60,74,74	0.96	3 (5%)	58,114,114	1.92	6 (10%)
19	CLA	7	614	5	50,54,73	1.36	8 (16%)	59,90,113	1.38	4 (6%)
19	CLA	5	312	3	49,53,73	1.38	8 (16%)	58,89,113	1.46	7 (12%)
19	CLA	A	811	7	69,73,73	1.17	6 (8%)	82,113,113	1.31	8 (9%)
23	LMG	J	104	-	42,42,55	0.54	0	50,50,63	0.64	0
19	CLA	6	312	4	49,53,73	1.39	7 (14%)	58,89,113	1.41	4 (6%)
19	CLA	4	603	2	69,73,73	1.18	7 (10%)	82,113,113	1.24	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
20	CHL	4	615	2	40,54,74	1.17	3 (7%)	34,90,114	2.23	5 (14%)
19	CLA	A	808	7	69,73,73	1.18	7 (10%)	82,113,113	1.26	4 (4%)
21	BCR	L	202	-	41,41,41	0.33	0	56,56,56	0.54	0
19	CLA	A	826	7	59,63,73	1.27	7 (11%)	70,101,113	1.32	5 (7%)
24	LMU	K	201	-	24,24,36	0.38	0	29,29,47	0.71	0
23	LMG	J	105	-	35,35,55	0.60	0	43,43,63	0.72	0
19	CLA	3	307	1	65,69,73	1.19	8 (12%)	77,108,113	1.30	5 (6%)
19	CLA	5	302	3	69,73,73	1.18	8 (11%)	82,113,113	1.26	5 (6%)
21	BCR	5	320	-	41,41,41	0.29	0	56,56,56	0.60	0
19	CLA	K	205	14	49,53,73	1.39	8 (16%)	58,89,113	1.45	5 (8%)
25	XAT	7	616	-	41,47,47	0.72	2 (4%)	54,74,74	0.76	0
21	BCR	K	206	-	41,41,41	0.30	0	56,56,56	0.49	0
19	CLA	Z	602	15	64,68,73	1.21	7 (10%)	76,107,113	1.31	5 (6%)
24	LMU	Z	620	-	24,24,36	0.39	0	29,29,47	0.60	0
19	CLA	B	822	8	69,73,73	1.18	6 (8%)	82,113,113	1.25	6 (7%)
29	PQN	A	845	-	34,34,34	0.36	0	43,45,45	0.57	1 (2%)
19	CLA	B	837	8	64,68,73	1.22	8 (12%)	76,107,113	1.27	7 (9%)
24	LMU	6	328	-	24,24,36	0.37	0	29,29,47	0.63	0

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
19	CLA	A	839	7	1/1/12/20	1/23/99/115	-
19	CLA	6	314	4	1/1/12/20	7/21/97/115	-
22	LUT	F	305	-	-	10/29/67/67	0/2/2/2
21	BCR	7	617	-	-	4/29/63/63	0/2/2/2
19	CLA	A	821	7	1/1/15/20	1/39/115/115	-
24	LMU	1	322	-	-	5/13/33/61	0/1/1/2
19	CLA	8	303	6	1/1/15/20	17/39/115/115	-
19	CLA	3	313	32	1/1/14/20	9/33/109/115	-
19	CLA	8	302	6	1/1/15/20	5/39/115/115	-
21	BCR	6	321	-	-	2/29/63/63	0/2/2/2
19	CLA	B	833	8	1/1/15/20	6/39/115/115	-
21	BCR	A	850	-	-	0/29/63/63	0/2/2/2
22	LUT	Z	617	-	-	2/18/37/67	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	L	204	32	1/1/11/20	4/15/91/115	-
19	CLA	B	805	8	1/1/11/20	4/15/91/115	-
19	CLA	A	840	7	1/1/15/20	8/39/115/115	-
19	CLA	A	810	7	1/1/15/20	5/39/115/115	-
21	BCR	A	849	-	-	1/29/63/63	0/2/2/2
22	LUT	8	315	-	-	2/29/67/67	0/2/2/2
19	CLA	4	608	2	1/1/14/20	7/33/109/115	-
19	CLA	A	841	7	1/1/15/20	3/39/115/115	-
19	CLA	1	310	26	1/1/14/20	13/35/111/115	-
19	CLA	8	304	32	1/1/14/20	5/33/109/115	-
19	CLA	7	612	5	1/1/15/20	8/39/115/115	-
19	CLA	B	829	8	1/1/15/20	6/39/115/115	-
20	CHL	4	601	2	2/2/20/26	2/39/137/137	-
22	LUT	3	320	-	-	1/11/30/67	0/1/1/2
21	BCR	3	318	-	-	4/29/63/63	0/2/2/2
20	CHL	6	315	4	2/2/20/26	13/39/137/137	-
19	CLA	A	803	-	1/1/15/20	0/39/115/115	-
30	SF4	C	101	9	-	-	0/6/5/5
20	CHL	Z	606	32	2/2/20/26	9/39/137/137	-
19	CLA	8	313	6	1/1/13/20	6/30/106/115	-
21	BCR	A	853	-	-	4/29/63/63	0/2/2/2
19	CLA	B	832	8	1/1/13/20	2/27/103/115	-
19	CLA	6	316	4	1/1/11/20	4/15/91/115	-
24	LMU	4	622	-	-	6/13/33/61	0/1/1/2
24	LMU	3	324	-	-	9/21/61/61	0/2/2/2
19	CLA	1	304	32	1/1/12/20	2/21/97/115	-
19	CLA	4	609	2	1/1/14/20	4/33/109/115	-
20	CHL	8	306	32	2/2/20/26	12/39/137/137	-
19	CLA	F	304	16	1/1/15/20	14/39/115/115	-
19	CLA	B	823	8	1/1/13/20	5/32/108/115	-
19	CLA	K	203	32	1/1/14/20	5/33/109/115	-
19	CLA	6	309	4	1/1/13/20	5/27/103/115	-
19	CLA	B	816	8	1/1/15/20	14/39/115/115	-
19	CLA	7	611	5	1/1/12/20	6/24/100/115	-
24	LMU	3	322	-	-	2/20/60/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CL0	A	802	7	3/3/20/25	3/37/135/135	-
21	BCR	B	845	-	-	3/29/63/63	0/2/2/2
23	LMG	3	321	-	-	12/32/52/70	0/1/1/1
25	XAT	8	316	-	-	0/31/93/93	0/4/4/4
19	CLA	5	311	26	1/1/13/20	5/27/103/115	-
20	CHL	5	317	3	2/2/15/26	2/12/110/137	-
19	CLA	A	842	7	1/1/15/20	7/39/115/115	-
19	CLA	Z	607	32	1/1/12/20	4/21/97/115	-
21	BCR	B	802	-	-	6/29/63/63	0/2/2/2
20	CHL	5	306	32	2/2/16/26	5/15/113/137	-
19	CLA	1	314	15	1/1/11/20	4/17/93/115	-
19	CLA	5	305	32	1/1/13/20	8/27/103/115	-
19	CLA	A	831	7	1/1/15/20	4/39/115/115	-
20	CHL	6	307	32	3/3/20/26	13/39/137/137	-
19	CLA	4	612	2	1/1/15/20	12/39/115/115	-
21	BCR	L	205	-	-	4/29/63/63	0/2/2/2
20	CHL	1	306	32	2/2/16/26	2/15/113/137	-
19	CLA	A	813	19,7	1/1/15/20	8/39/115/115	-
20	CHL	Z	605	32	2/2/16/26	2/15/113/137	-
19	CLA	B	809	8	1/1/15/20	10/39/115/115	-
19	CLA	B	835	8	1/1/14/20	4/33/109/115	-
19	CLA	A	816	7	1/1/13/20	3/27/103/115	-
19	CLA	A	812	7	1/1/15/20	9/39/115/115	-
25	XAT	Z	616	-	-	3/31/93/93	0/4/4/4
19	CLA	3	302	1	1/1/15/20	12/39/115/115	-
19	CLA	B	808	8	1/1/13/20	5/27/103/115	-
19	CLA	Z	614	15	1/1/14/20	9/33/109/115	-
30	SF4	C	102	9	-	-	0/6/5/5
19	CLA	B	811	8	1/1/15/20	11/39/115/115	-
19	CLA	A	825	7	1/1/11/20	3/15/91/115	-
25	XAT	6	322	-	-	1/31/93/93	0/4/4/4
19	CLA	F	302	32	1/1/15/20	10/39/115/115	-
19	CLA	8	312	6	1/1/15/20	5/39/115/115	-
19	CLA	B	819	8	1/1/15/20	5/39/115/115	-
22	LUT	7	615	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	836	32	1/1/11/20	5/15/91/115	-
19	CLA	1	309	15	1/1/15/20	3/39/115/115	-
30	SF4	A	854	8,7	-	-	0/6/5/5
21	BCR	A	851	-	-	4/29/63/63	0/2/2/2
19	CLA	B	806	8	1/1/15/20	9/39/115/115	-
19	CLA	A	822	7	1/1/13/20	4/27/103/115	-
19	CLA	F	303	32	1/1/11/20	1/15/91/115	-
19	CLA	3	305	1	1/1/12/20	2/23/99/115	-
19	CLA	Z	613	15	1/1/12/20	0/21/97/115	-
21	BCR	I	201	-	-	6/29/63/63	0/2/2/2
19	CLA	4	614	2	1/1/11/20	3/15/91/115	-
19	CLA	A	830	7	1/1/15/20	11/39/115/115	-
24	LMU	1	320	-	-	6/10/30/61	0/1/1/2
19	CLA	1	313	15	1/1/14/20	10/33/109/115	-
19	CLA	7	602	5	1/1/15/20	3/39/115/115	-
24	LMU	7	620	-	-	7/13/33/61	0/1/1/2
19	CLA	B	840	32	1/1/15/20	10/39/115/115	-
19	CLA	B	815	8	1/1/14/20	6/33/109/115	-
19	CLA	B	820	32	1/1/14/20	9/33/109/115	-
19	CLA	B	804	-	1/1/15/20	13/39/115/115	-
19	CLA	B	838	8	1/1/15/20	3/39/115/115	-
22	LUT	Z	615	-	-	2/29/67/67	0/2/2/2
21	BCR	B	848	-	-	2/29/63/63	0/2/2/2
23	LMG	7	622	-	-	9/27/47/70	0/1/1/1
19	CLA	8	308	6	1/1/11/20	3/15/91/115	-
24	LMU	4	624	-	-	6/15/35/61	0/1/1/2
24	LMU	A	855	-	-	6/21/61/61	0/2/2/2
19	CLA	A	807	7	1/1/15/20	15/39/115/115	-
21	BCR	A	858	-	-	4/29/63/63	0/2/2/2
19	CLA	5	313	3	1/1/13/20	6/29/105/115	-
19	CLA	A	834	7	1/1/15/20	5/39/115/115	-
19	CLA	4	611	2	1/1/11/20	2/15/91/115	-
19	CLA	3	304	32	1/1/10/20	0/12/88/115	-
19	CLA	B	826	32	1/1/15/20	9/39/115/115	-
22	LUT	J	101	-	-	5/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	L	203	18	1/1/15/20	15/39/115/115	-
19	CLA	A	815	7	1/1/15/20	7/39/115/115	-
19	CLA	J	102	13	1/1/13/20	8/27/103/115	-
19	CLA	B	814	8	1/1/15/20	9/39/115/115	-
22	LUT	3	317	-	-	1/29/67/67	0/2/2/2
19	CLA	K	204	14	1/1/11/20	0/17/93/115	-
21	BCR	B	844	-	-	4/29/63/63	0/2/2/2
19	CLA	A	846	26	1/1/11/20	6/15/91/115	-
20	CHL	8	305	32	2/2/20/26	7/39/137/137	-
19	CLA	6	311	26	1/1/13/20	9/31/107/115	-
22	LUT	1	317	-	-	5/29/67/67	0/2/2/2
24	LMU	3	323	-	-	5/15/35/61	0/1/1/2
19	CLA	1	311	15	1/1/11/20	4/15/91/115	-
19	CLA	Z	609	15	1/1/14/20	2/33/109/115	-
19	CLA	1	307	32	1/1/15/20	13/39/115/115	-
20	CHL	5	307	32	3/3/20/26	12/39/137/137	-
24	LMU	A	857	-	-	4/15/35/61	0/1/1/2
26	LHG	6	318	19	-	15/53/53/53	-
20	CHL	7	606	32	2/2/16/26	2/15/113/137	-
20	CHL	3	306	32	2/2/20/26	5/39/137/137	-
19	CLA	5	304	3	1/1/12/20	6/21/97/115	-
19	CLA	5	319	32	1/1/11/20	11/17/93/115	-
19	CLA	A	814	7	1/1/15/20	6/39/115/115	-
21	BCR	J	103	-	-	4/29/63/63	0/2/2/2
19	CLA	A	805	7	1/1/15/20	5/39/115/115	-
23	LMG	6	326	-	-	6/17/17/70	-
19	CLA	B	841	8	1/1/15/20	11/39/115/115	-
20	CHL	4	607	32	3/3/20/26	19/39/137/137	-
19	CLA	B	825	32	1/1/15/20	8/39/115/115	-
29	PQN	B	843	-	-	1/23/43/43	0/2/2/2
20	CHL	5	308	32	2/2/17/26	4/21/119/137	-
19	CLA	3	311	1	1/1/14/20	5/33/109/115	-
19	CLA	8	310	26	1/1/11/20	4/15/91/115	-
19	CLA	A	836	7	1/1/15/20	8/39/115/115	-
19	CLA	7	610	26	1/1/15/20	5/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
21	BCR	B	849	-	-	1/29/63/63	0/2/2/2
19	CLA	7	613	5	1/1/10/20	2/13/89/115	-
24	LMU	1	301	-	-	11/21/61/61	0/2/2/2
22	LUT	3	316	-	-	2/29/67/67	0/2/2/2
24	LMU	4	625	-	-	0/13/33/61	0/1/1/2
19	CLA	3	303	32	1/1/15/20	3/39/115/115	-
24	LMU	3	325	-	-	7/15/35/61	0/1/1/2
19	CLA	Z	604	32	1/1/13/20	10/30/106/115	-
21	BCR	8	317	-	-	3/29/63/63	0/2/2/2
19	CLA	B	803	8	1/1/15/20	4/39/115/115	-
19	CLA	7	607	32	1/1/12/20	1/21/97/115	-
23	LMG	6	301	-	-	7/28/28/70	-
19	CLA	A	818	32	1/1/13/20	7/27/103/115	-
20	CHL	6	308	32	3/3/17/26	6/21/119/137	-
26	LHG	6	325	-	-	13/40/40/53	-
26	LHG	5	321	19	-	13/41/41/53	-
24	LMU	8	319	-	-	6/15/35/61	0/1/1/2
21	BCR	B	846	-	-	4/29/63/63	0/2/2/2
19	CLA	B	828	8	1/1/15/20	11/39/115/115	-
20	CHL	6	306	32	2/2/16/26	4/15/113/137	-
19	CLA	3	301	1	1/1/14/20	4/33/109/115	-
19	CLA	5	315	3	1/1/11/20	4/15/91/115	-
25	XAT	5	322	-	-	1/31/93/93	0/4/4/4
26	LHG	B	851	19	-	13/49/49/53	-
19	CLA	A	827	32	1/1/15/20	6/39/115/115	-
19	CLA	1	302	15	1/1/14/20	6/33/109/115	-
19	CLA	6	305	4	1/1/15/20	16/39/115/115	-
24	LMU	F	306	-	-	8/21/61/61	0/2/2/2
21	BCR	4	618	-	-	5/29/63/63	0/2/2/2
19	CLA	A	824	7	1/1/15/20	19/39/115/115	-
20	CHL	6	302	4	2/2/20/26	9/39/137/137	-
19	CLA	3	312	1	1/1/11/20	6/15/91/115	-
26	LHG	Z	618	19	-	5/43/43/53	-
20	CHL	8	320	15	2/2/20/26	6/39/137/137	-
23	LMG	L	201	-	-	15/35/55/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	832	7	1/1/15/20	4/39/115/115	-
19	CLA	B	842	26	1/1/15/20	6/39/115/115	-
25	XAT	1	316	-	-	0/31/93/93	0/4/4/4
19	CLA	Z	603	15	1/1/15/20	9/39/115/115	-
19	CLA	Z	610	26	1/1/14/20	7/33/109/115	-
19	CLA	G	203	17	1/1/11/20	1/17/93/115	-
24	LMU	1	321	-	-	4/15/35/61	0/1/1/2
19	CLA	4	602	2	1/1/14/20	4/33/109/115	-
20	CHL	7	621	6	2/2/20/26	9/39/137/137	-
19	CLA	3	309	32	1/1/13/20	6/27/103/115	-
19	CLA	B	801	32	1/1/15/20	11/39/115/115	-
23	LMG	B	852	-	-	9/38/58/70	0/1/1/1
19	CLA	B	813	8	1/1/15/20	17/39/115/115	-
19	CLA	8	314	6	1/1/11/20	0/15/91/115	-
21	BCR	G	204	-	-	0/29/63/63	0/2/2/2
22	LUT	1	315	-	-	3/29/67/67	0/2/2/2
24	LMU	Z	621	-	-	3/15/35/61	0/1/1/2
22	LUT	6	319	-	-	4/29/67/67	0/2/2/2
19	CLA	A	844	32	1/1/15/20	11/39/115/115	-
31	DGD	B	850	-	-	11/48/88/95	0/2/2/2
19	CLA	B	812	8	1/1/15/20	14/39/115/115	-
22	LUT	4	616	-	-	2/29/67/67	0/2/2/2
19	CLA	B	817	8	1/1/15/20	7/39/115/115	-
21	BCR	B	847	-	-	0/29/63/63	0/2/2/2
26	LHG	4	619	19	-	11/53/53/53	-
23	LMG	F	301	-	-	11/27/47/70	0/1/1/1
19	CLA	8	311	6	1/1/13/20	6/27/103/115	-
22	LUT	5	318	-	-	3/29/67/67	0/2/2/2
20	CHL	7	601	5	2/2/20/26	10/39/137/137	-
24	LMU	6	324	-	-	6/15/35/61	0/1/1/2
19	CLA	5	309	3	1/1/15/20	12/39/115/115	-
26	LHG	8	318	19	-	16/48/48/53	-
19	CLA	5	316	3	1/1/15/20	15/39/115/115	-
19	CLA	3	310	1	1/1/11/20	6/17/93/115	-
19	CLA	5	314	3	1/1/11/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	837	7	1/1/15/20	8/39/115/115	-
24	LMU	B	853	-	-	3/21/61/61	0/2/2/2
19	CLA	7	609	5	1/1/15/20	8/39/115/115	-
19	CLA	A	809	7	1/1/12/20	5/21/97/115	-
20	CHL	Z	601	15	2/2/20/26	10/39/137/137	-
19	CLA	6	303	4	1/1/15/20	3/39/115/115	-
19	CLA	6	320	32	1/1/13/20	4/27/103/115	-
26	LHG	A	847	-	-	12/53/53/53	-
19	CLA	A	838	7	1/1/13/20	6/30/106/115	-
19	CLA	Z	608	15	1/1/15/20	19/39/115/115	-
19	CLA	A	833	7	1/1/13/20	10/27/103/115	-
21	BCR	3	319	-	-	3/29/63/63	0/2/2/2
19	CLA	B	821	8	1/1/13/20	5/29/105/115	-
19	CLA	B	831	8	1/1/11/20	0/15/91/115	-
19	CLA	A	823	32	1/1/15/20	4/39/115/115	-
21	BCR	3	315	-	-	7/29/63/63	0/2/2/2
19	CLA	6	304	4	1/1/12/20	7/23/99/115	-
24	LMU	Z	619	-	-	5/17/57/61	0/2/2/2
19	CLA	A	817	7	1/1/15/20	6/39/115/115	-
19	CLA	A	829	7	1/1/15/20	2/39/115/115	-
19	CLA	Z	612	32	1/1/15/20	3/39/115/115	-
26	LHG	4	620	-	-	10/42/42/53	-
19	CLA	8	307	32	1/1/12/20	2/21/97/115	-
22	LUT	8	301	-	-	4/29/67/67	0/2/2/2
19	CLA	5	303	3	1/1/15/20	2/39/115/115	-
19	CLA	Z	611	15	1/1/11/20	6/15/91/115	-
19	CLA	1	312	32	1/1/15/20	8/39/115/115	-
19	CLA	7	608	5	1/1/11/20	1/15/91/115	-
19	CLA	3	314	1	1/1/11/20	0/15/91/115	-
19	CLA	A	820	7	1/1/14/20	14/33/109/115	-
27	NEX	5	323	-	1/1/12/25	2/27/83/83	0/3/3/3
27	NEX	6	323	-	-	3/27/83/83	0/3/3/3
19	CLA	8	309	6	1/1/15/20	6/39/115/115	-
24	LMU	A	856	-	-	3/11/31/61	0/1/1/2
23	LMG	G	201	-	-	6/31/51/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	4	606	32	2/2/15/26	2/12/110/137	-
24	LMU	1	319	-	-	7/21/61/61	0/2/2/2
19	CLA	B	818	8	1/1/15/20	8/39/115/115	-
19	CLA	A	828	32	1/1/15/20	11/39/115/115	-
26	LHG	A	801	-	-	14/35/35/53	-
23	LMG	4	621	-	-	16/36/56/70	0/1/1/1
19	CLA	6	313	32	1/1/15/20	4/39/115/115	-
26	LHG	1	318	19	-	12/48/48/53	-
19	CLA	A	843	7	1/1/15/20	6/39/115/115	-
19	CLA	B	824	8	1/1/15/20	10/39/115/115	-
19	CLA	G	202	17	1/1/14/20	8/33/109/115	-
26	LHG	5	301	-	-	12/42/42/53	-
19	CLA	7	604	32	1/1/12/20	0/23/99/115	-
19	CLA	K	202	14	1/1/11/20	4/15/91/115	-
19	CLA	A	835	7	1/1/15/20	7/39/115/115	-
20	CHL	7	605	32	2/2/16/26	0/15/113/137	-
19	CLA	3	308	1	1/1/15/20	5/39/115/115	-
26	LHG	A	848	19	-	10/42/42/53	-
19	CLA	B	839	8	1/1/12/20	1/21/97/115	-
19	CLA	6	327	32	1/1/12/20	3/25/101/115	-
19	CLA	5	310	3	1/1/14/20	5/33/109/115	-
22	LUT	5	324	-	-	11/29/67/67	0/2/2/2
19	CLA	1	303	15	1/1/13/20	8/30/106/115	-
19	CLA	4	610	26	1/1/14/20	3/33/109/115	-
19	CLA	1	308	15	1/1/15/20	13/39/115/115	-
19	CLA	7	603	5	1/1/12/20	3/24/100/115	-
19	CLA	B	834	8	1/1/13/20	5/31/107/115	-
23	LMG	8	321	-	-	22/44/64/70	0/1/1/1
19	CLA	A	819	7	1/1/15/20	6/39/115/115	-
19	CLA	4	613	2	1/1/13/20	6/27/103/115	-
19	CLA	B	830	8	1/1/15/20	10/39/115/115	-
25	XAT	4	617	-	-	0/31/93/93	0/4/4/4
20	CHL	1	305	32	2/2/16/26	0/15/113/137	-
19	CLA	A	806	19,7	1/1/13/20	1/27/103/115	-
24	LMU	4	623	-	-	4/11/31/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CHL	6	317	4	2/2/15/26	0/12/110/137	-
24	LMU	7	619	-	-	4/12/32/61	0/1/1/2
26	LHG	7	618	19	-	16/53/53/53	-
19	CLA	B	810	8	1/1/15/20	7/39/115/115	-
19	CLA	4	604	32	1/1/12/20	4/21/97/115	-
19	CLA	B	827	8	1/1/15/20	2/39/115/115	-
21	BCR	A	852	-	-	4/29/63/63	0/2/2/2
19	CLA	6	310	4	1/1/14/20	2/33/109/115	-
19	CLA	A	804	32	1/1/15/20	3/39/115/115	-
19	CLA	B	807	8	1/1/15/20	2/39/115/115	-
20	CHL	4	605	32	3/3/20/26	13/39/137/137	-
19	CLA	7	614	5	1/1/11/20	6/17/93/115	-
19	CLA	5	312	3	1/1/11/20	6/15/91/115	-
19	CLA	A	811	7	1/1/15/20	9/39/115/115	-
23	LMG	J	104	-	-	9/37/57/70	0/1/1/1
19	CLA	6	312	4	1/1/11/20	2/15/91/115	-
19	CLA	4	603	2	1/1/15/20	12/39/115/115	-
20	CHL	4	615	2	2/2/16/26	2/15/113/137	-
19	CLA	A	808	7	1/1/15/20	9/39/115/115	-
21	BCR	L	202	-	-	4/29/63/63	0/2/2/2
19	CLA	A	826	7	1/1/13/20	2/27/103/115	-
24	LMU	K	201	-	-	6/15/35/61	0/1/1/2
23	LMG	J	105	-	-	14/30/50/70	0/1/1/1
19	CLA	3	307	1	1/1/14/20	7/35/111/115	-
19	CLA	5	302	3	1/1/15/20	8/39/115/115	-
21	BCR	5	320	-	-	2/29/63/63	0/2/2/2
19	CLA	K	205	14	1/1/11/20	2/15/91/115	-
25	XAT	7	616	-	-	0/31/93/93	0/4/4/4
21	BCR	K	206	-	-	2/29/63/63	0/2/2/2
19	CLA	Z	602	15	1/1/14/20	2/33/109/115	-
24	LMU	Z	620	-	-	2/15/35/61	0/1/1/2
19	CLA	B	822	8	1/1/15/20	17/39/115/115	-
29	PQN	A	845	-	-	0/23/43/43	0/2/2/2
19	CLA	B	837	8	1/1/14/20	5/33/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LMU	6	328	-	-	7/15/35/61	0/1/1/2

The worst 5 of 1455 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	601	CHL	C1A-CHA	6.25	1.47	1.40
20	6	317	CHL	C1A-CHA	6.21	1.47	1.40
20	1	306	CHL	C1A-CHA	5.53	1.46	1.40
20	4	601	CHL	C1A-CHA	5.47	1.46	1.40
20	7	621	CHL	C1A-CHA	5.46	1.46	1.40

The worst 5 of 1302 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	7	621	CHL	C1B-CHB-C4A	15.28	131.16	121.32
20	8	320	CHL	C1B-CHB-C4A	14.92	130.92	121.32
20	7	601	CHL	C1B-CHB-C4A	14.88	130.89	121.32
20	8	305	CHL	C1B-CHB-C4A	14.71	130.79	121.32
20	5	307	CHL	C1B-CHB-C4A	14.55	130.68	121.32

5 of 253 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	3	301	CLA	ND
19	3	302	CLA	ND
19	3	303	CLA	ND
19	3	304	CLA	ND
19	3	305	CLA	ND

5 of 1992 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	3	302	CLA	C11-C12-C13-C14
19	3	305	CLA	C4-C3-C5-C6
19	3	309	CLA	CBD-CGD-O2D-CED
19	3	312	CLA	C2B-C3B-CAB-CBB
19	3	312	CLA	C4B-C3B-CAB-CBB

There are no ring outliers.

240 monomers are involved in 396 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	839	CLA	1	0
19	6	314	CLA	2	0
22	F	305	LUT	1	0
21	7	617	BCR	3	0
19	A	821	CLA	3	0
24	1	322	LMU	1	0
19	8	303	CLA	6	0
19	3	313	CLA	3	0
19	8	302	CLA	4	0
21	6	321	BCR	2	0
19	B	833	CLA	1	0
21	A	850	BCR	2	0
19	L	204	CLA	1	0
19	B	805	CLA	3	0
19	A	840	CLA	2	0
19	A	810	CLA	3	0
21	A	849	BCR	2	0
19	4	608	CLA	1	0
19	A	841	CLA	1	0
19	1	310	CLA	3	0
19	8	304	CLA	3	0
19	7	612	CLA	5	0
19	B	829	CLA	1	0
20	4	601	CHL	2	0
21	3	318	BCR	3	0
20	6	315	CHL	2	0
19	A	803	CLA	3	0
20	Z	606	CHL	1	0
19	8	313	CLA	1	0
21	A	853	BCR	3	0
19	B	832	CLA	3	0
24	3	324	LMU	2	0
19	4	609	CLA	2	0
20	8	306	CHL	2	0
19	F	304	CLA	4	0
19	B	823	CLA	2	0
19	K	203	CLA	4	0
24	3	322	LMU	1	0
21	B	845	BCR	3	0
23	3	321	LMG	4	0
19	5	311	CLA	1	0
20	5	317	CHL	1	0
19	A	842	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	Z	607	CLA	1	0
21	B	802	BCR	2	0
20	5	306	CHL	2	0
19	1	314	CLA	2	0
19	5	305	CLA	2	0
19	A	831	CLA	1	0
20	6	307	CHL	8	0
19	4	612	CLA	3	0
21	L	205	BCR	2	0
20	1	306	CHL	1	0
19	A	813	CLA	3	0
20	Z	605	CHL	1	0
19	B	809	CLA	3	0
19	B	835	CLA	1	0
19	A	816	CLA	2	0
19	A	812	CLA	1	0
25	Z	616	XAT	2	0
19	3	302	CLA	3	0
19	Z	614	CLA	1	0
19	B	811	CLA	3	0
25	6	322	XAT	2	0
19	F	302	CLA	3	0
19	8	312	CLA	1	0
19	B	819	CLA	2	0
19	1	309	CLA	2	0
21	A	851	BCR	1	0
19	B	806	CLA	2	0
19	3	305	CLA	2	0
21	I	201	BCR	1	0
19	4	614	CLA	2	0
19	A	830	CLA	2	0
19	7	602	CLA	2	0
24	7	620	LMU	1	0
19	B	815	CLA	2	0
19	B	820	CLA	1	0
19	B	804	CLA	10	0
19	B	838	CLA	3	0
22	Z	615	LUT	1	0
21	B	848	BCR	2	0
24	A	855	LMU	1	0
19	A	807	CLA	2	0
21	A	858	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	5	313	CLA	3	0
19	A	834	CLA	2	0
19	B	826	CLA	2	0
22	J	101	LUT	3	0
19	L	203	CLA	2	0
19	A	815	CLA	4	0
19	J	102	CLA	1	0
19	B	814	CLA	4	0
22	3	317	LUT	1	0
19	K	204	CLA	1	0
21	B	844	BCR	2	0
19	A	846	CLA	1	0
20	8	305	CHL	2	0
22	1	317	LUT	1	0
19	1	311	CLA	3	0
19	Z	609	CLA	1	0
19	1	307	CLA	3	0
20	5	307	CHL	3	0
26	6	318	LHG	6	0
19	5	304	CLA	4	0
19	5	319	CLA	6	0
19	A	814	CLA	2	0
21	J	103	BCR	1	0
19	A	805	CLA	1	0
23	6	326	LMG	2	0
19	B	841	CLA	2	0
20	4	607	CHL	5	0
20	5	308	CHL	1	0
19	A	836	CLA	1	0
19	7	610	CLA	4	0
19	7	613	CLA	1	0
24	1	301	LMU	2	0
19	3	303	CLA	3	0
21	8	317	BCR	1	0
19	B	803	CLA	1	0
23	6	301	LMG	1	0
19	A	818	CLA	1	0
20	6	308	CHL	1	0
26	6	325	LHG	1	0
26	5	321	LHG	1	0
24	8	319	LMU	1	0
21	B	846	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	828	CLA	3	0
20	6	306	CHL	2	0
25	5	322	XAT	3	0
26	B	851	LHG	6	0
19	A	827	CLA	3	0
19	6	305	CLA	4	0
24	F	306	LMU	2	0
21	4	618	BCR	1	0
19	A	824	CLA	2	0
20	6	302	CHL	2	0
20	8	320	CHL	1	0
23	L	201	LMG	2	0
19	A	832	CLA	3	0
19	B	842	CLA	5	0
25	1	316	XAT	1	0
19	Z	603	CLA	2	0
24	1	321	LMU	1	0
19	4	602	CLA	1	0
20	7	621	CHL	2	0
19	3	309	CLA	3	0
19	B	801	CLA	2	0
23	B	852	LMG	1	0
19	B	813	CLA	3	0
22	1	315	LUT	2	0
19	A	844	CLA	1	0
31	B	850	DGD	2	0
19	B	812	CLA	3	0
22	4	616	LUT	3	0
19	B	817	CLA	5	0
26	4	619	LHG	3	0
23	F	301	LMG	1	0
19	8	311	CLA	2	0
22	5	318	LUT	2	0
26	8	318	LHG	3	0
19	5	316	CLA	3	0
19	3	310	CLA	1	0
19	A	837	CLA	5	0
24	B	853	LMU	2	0
19	7	609	CLA	3	0
19	6	303	CLA	4	0
19	6	320	CLA	2	0
26	A	847	LHG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	838	CLA	3	0
19	Z	608	CLA	5	0
19	A	833	CLA	2	0
21	3	319	BCR	1	0
19	B	831	CLA	2	0
19	A	823	CLA	1	0
21	3	315	BCR	2	0
19	6	304	CLA	1	0
19	A	817	CLA	1	0
19	A	829	CLA	2	0
19	Z	612	CLA	1	0
26	4	620	LHG	2	0
19	8	307	CLA	1	0
19	5	303	CLA	3	0
19	Z	611	CLA	1	0
19	1	312	CLA	1	0
19	3	314	CLA	4	0
19	A	820	CLA	3	0
27	6	323	NEX	2	0
19	8	309	CLA	3	0
20	4	606	CHL	1	0
24	1	319	LMU	1	0
19	B	818	CLA	5	0
26	A	801	LHG	1	0
19	6	313	CLA	2	0
19	B	824	CLA	6	0
26	5	301	LHG	1	0
20	7	605	CHL	1	0
19	3	308	CLA	3	0
26	A	848	LHG	1	0
19	B	839	CLA	1	0
19	6	327	CLA	1	0
19	5	310	CLA	1	0
22	5	324	LUT	2	0
19	1	303	CLA	3	0
19	4	610	CLA	1	0
19	1	308	CLA	2	0
19	B	834	CLA	2	0
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19	A	819	CLA	2	0
19	4	613	CLA	1	0
19	B	830	CLA	2	0

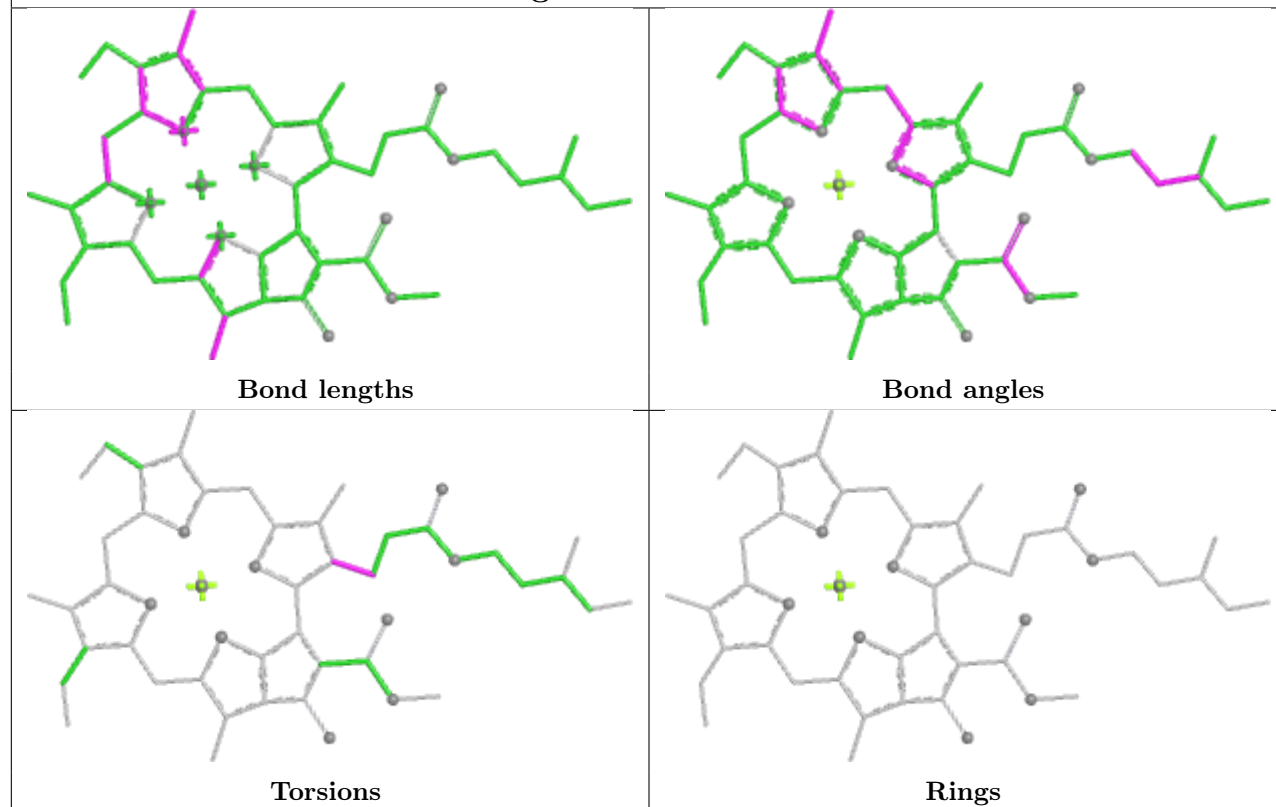
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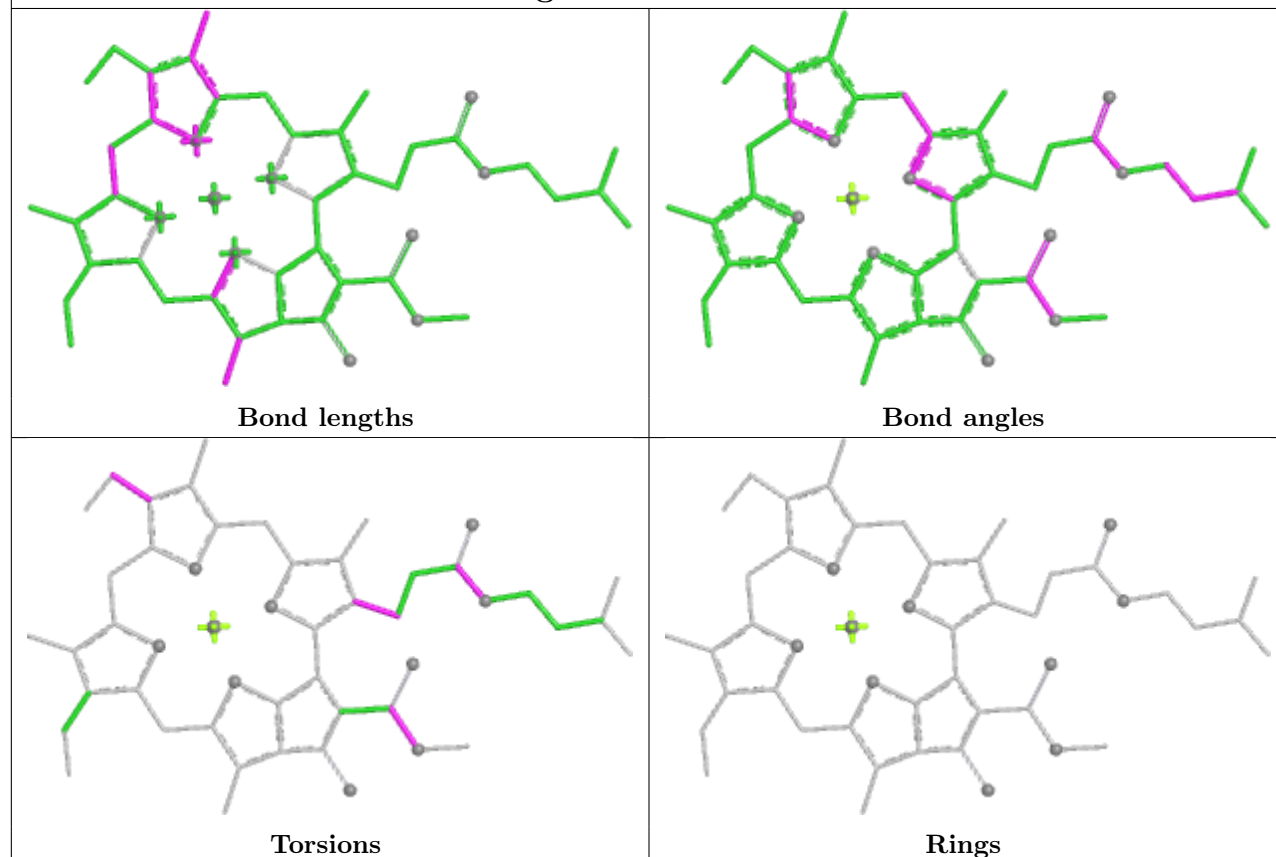
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20	1	305	CHL	2	0
24	4	623	LMU	2	0
20	6	317	CHL	1	0
26	7	618	LHG	1	0
19	B	810	CLA	1	0
19	4	604	CLA	1	0
19	B	827	CLA	1	0
21	A	852	BCR	1	0
19	6	310	CLA	3	0
19	B	807	CLA	1	0
20	4	605	CHL	3	0
19	5	312	CLA	4	0
19	A	811	CLA	6	0
23	J	104	LMG	1	0
19	6	312	CLA	2	0
19	4	603	CLA	4	0
20	4	615	CHL	2	0
19	A	808	CLA	1	0
21	L	202	BCR	2	0
19	A	826	CLA	1	0
23	J	105	LMG	3	0
19	5	302	CLA	2	0
21	5	320	BCR	4	0
25	7	616	XAT	1	0
21	K	206	BCR	1	0
19	Z	602	CLA	1	0
19	B	822	CLA	3	0
19	B	837	CLA	3	0

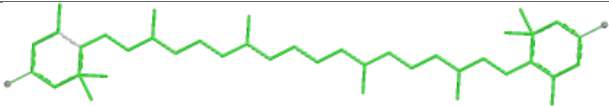
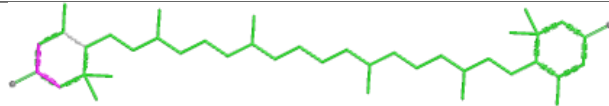
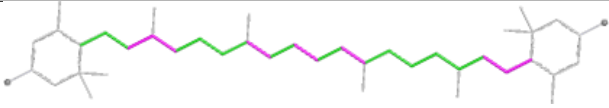
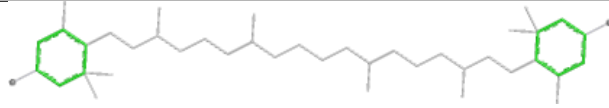
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

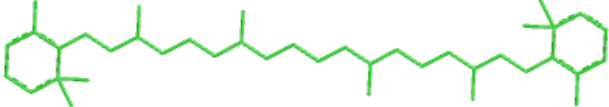
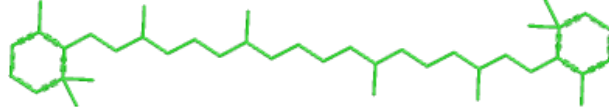
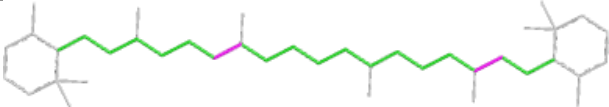
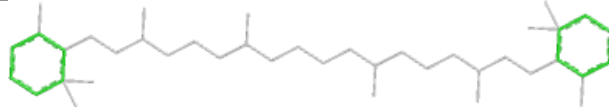
## Ligand CLA A 839

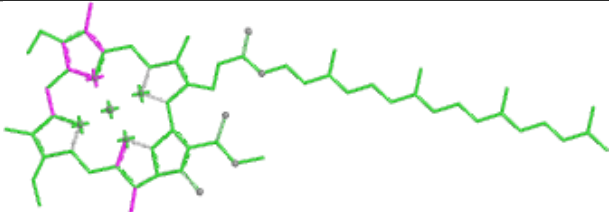
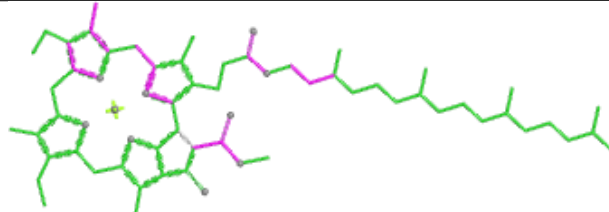
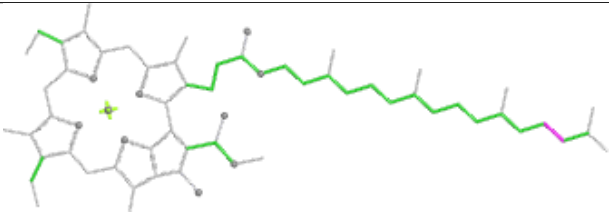
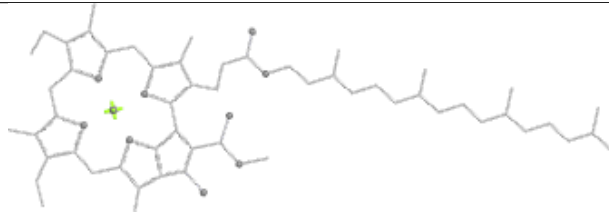


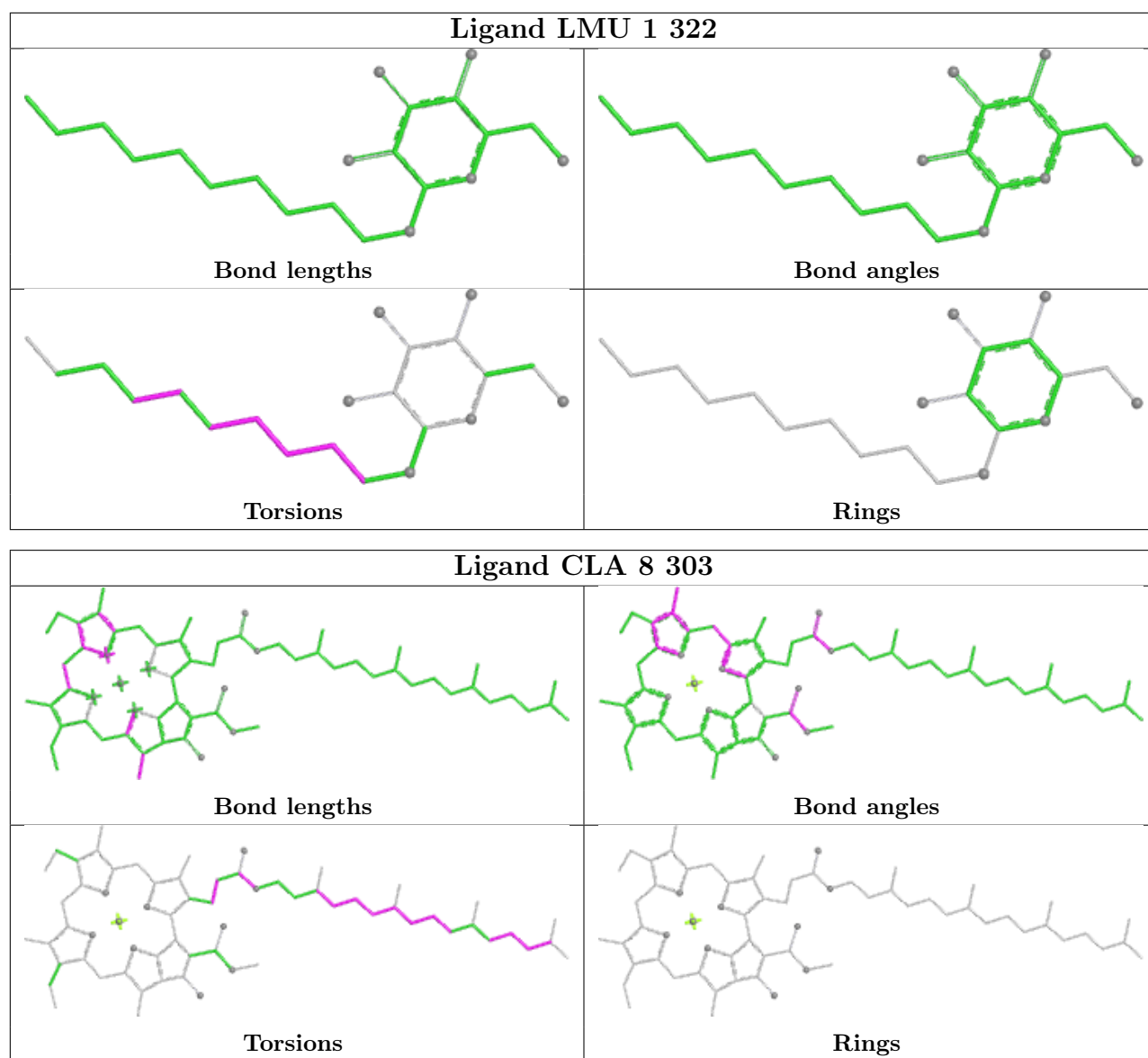
## Ligand CLA 6 314

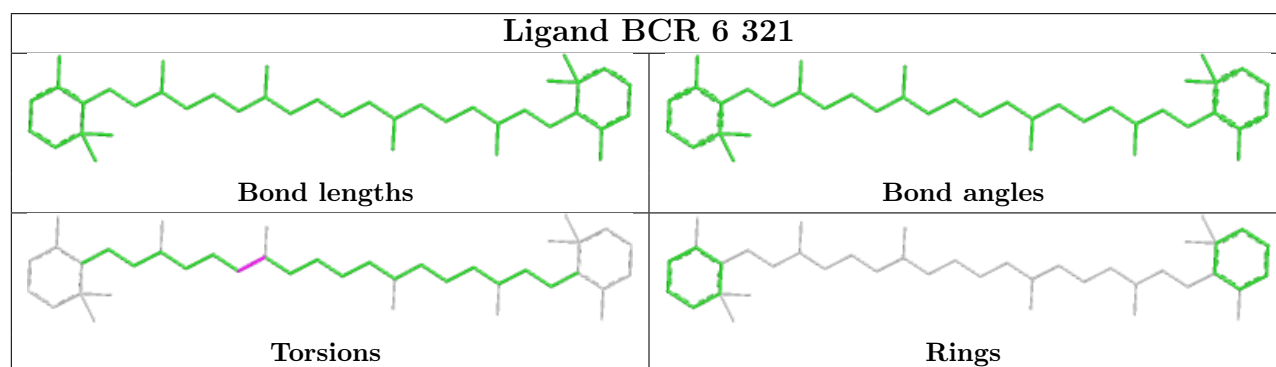
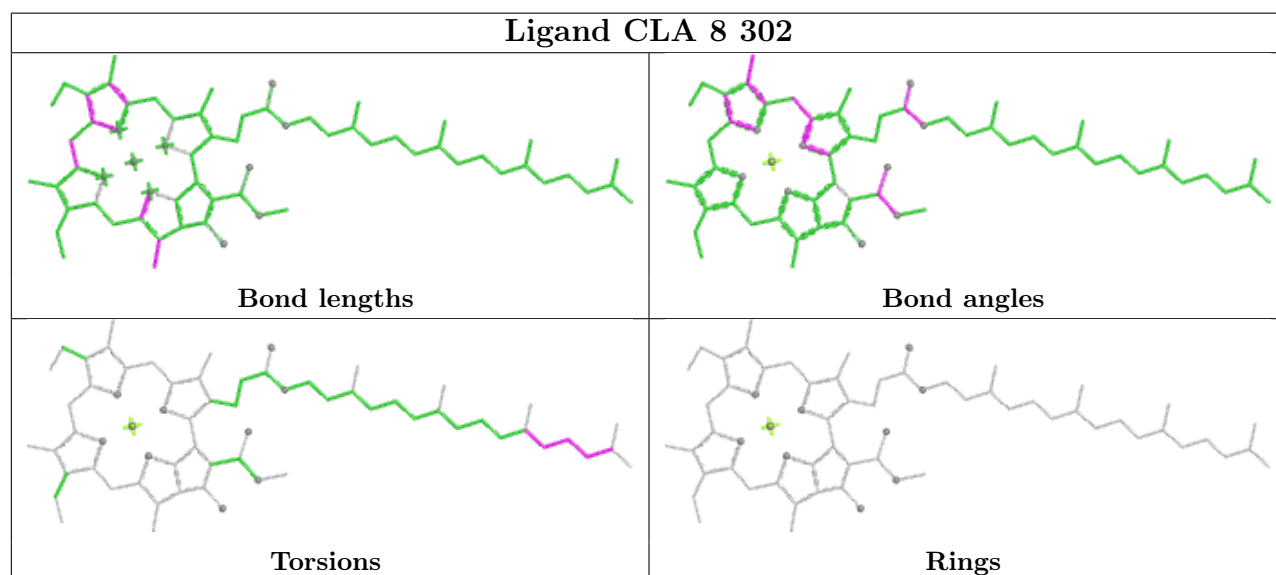
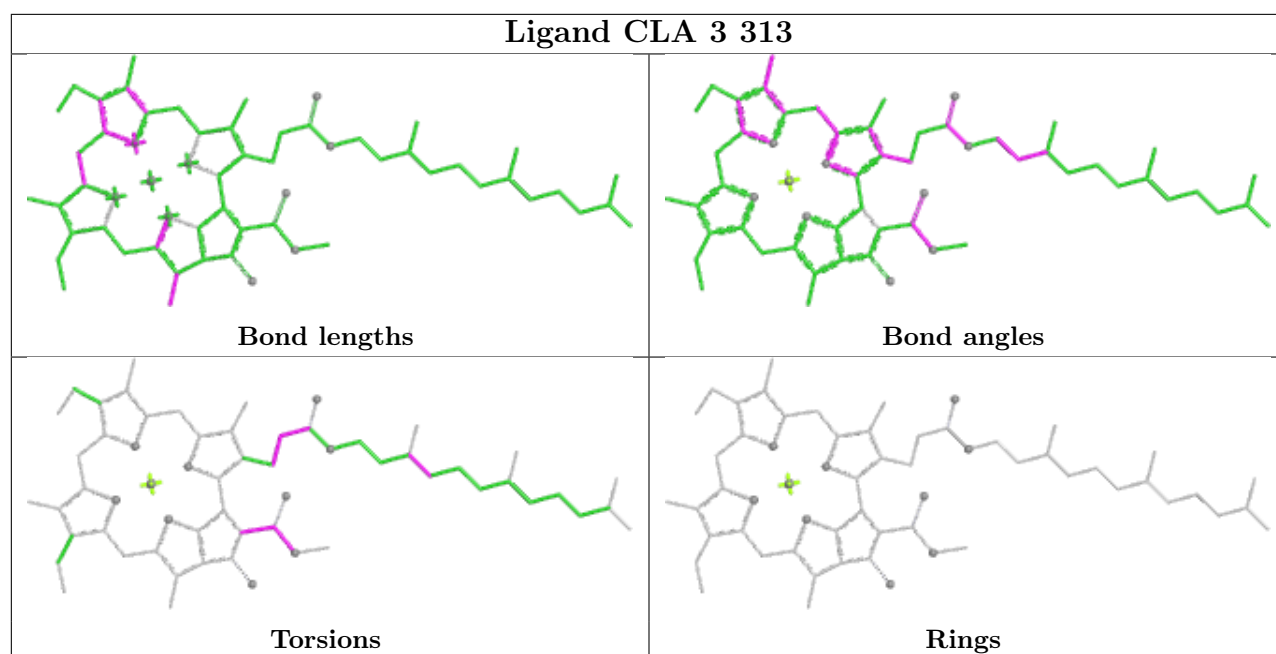


Ligand LUT F 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

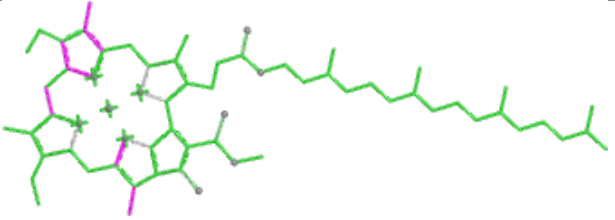
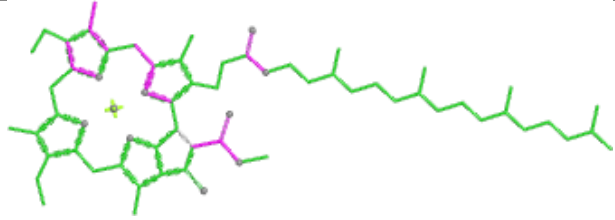
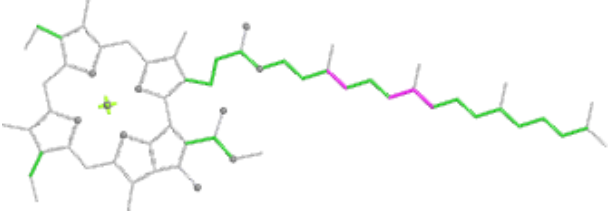
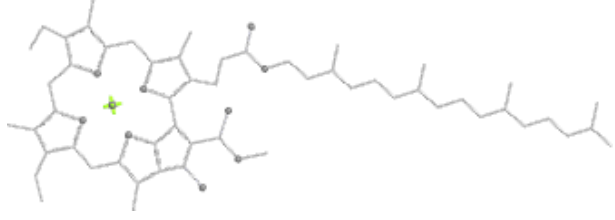
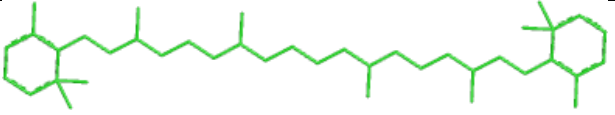

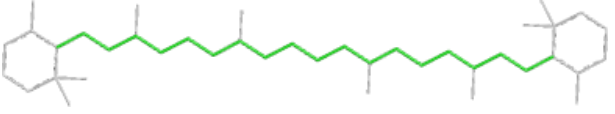
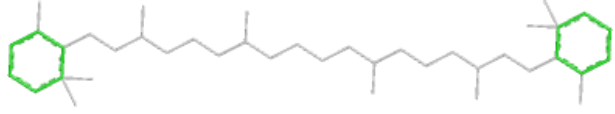
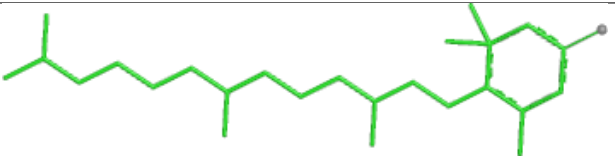
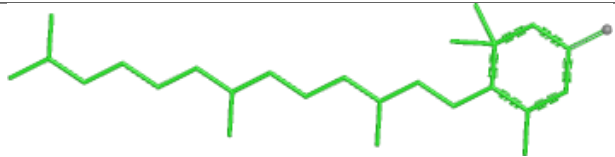

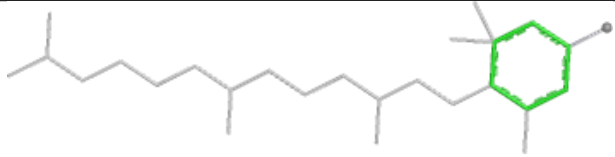
Ligand BCR 7 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 821	
	
Bond lengths	Bond angles
	
Torsions	Rings

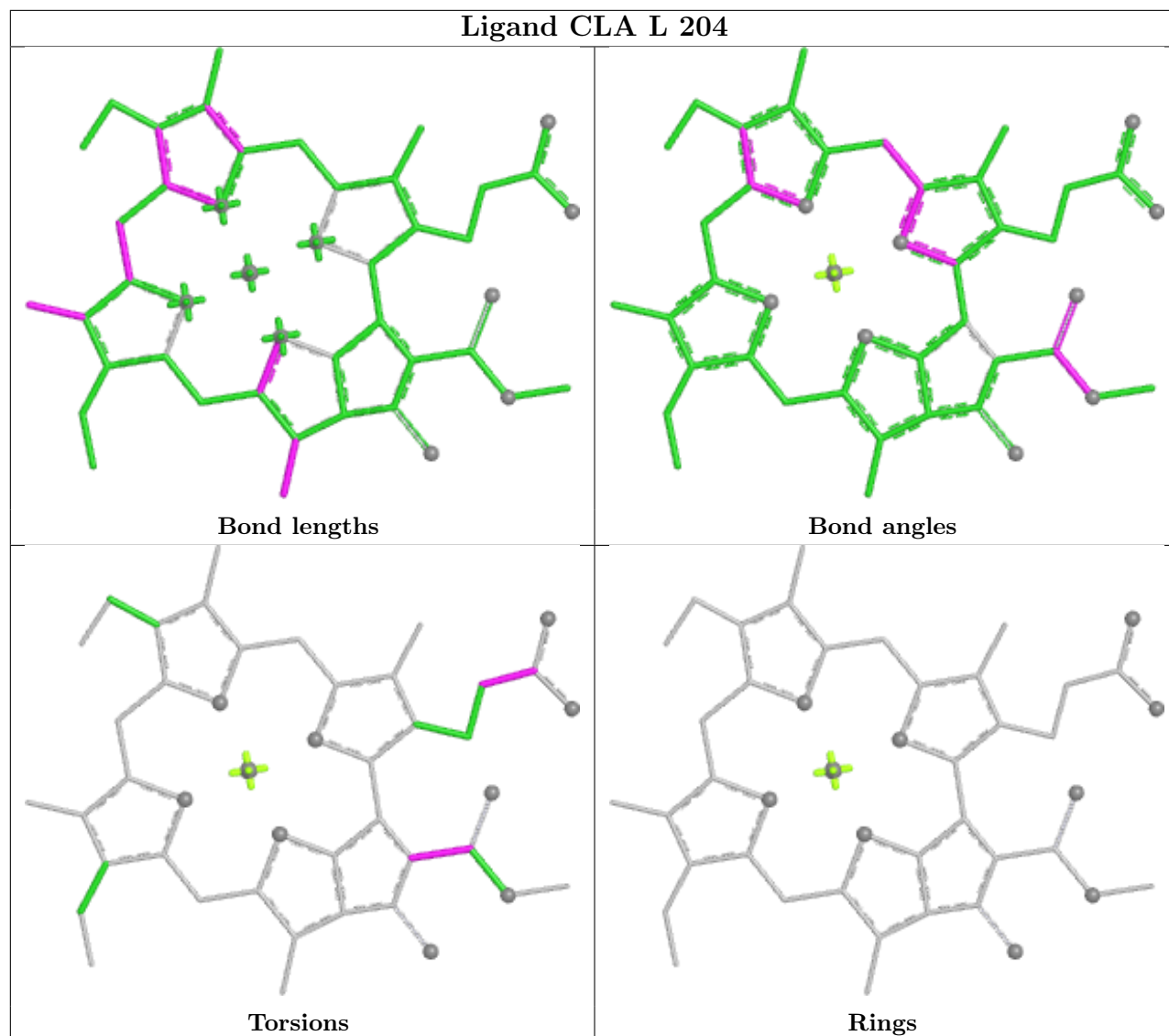


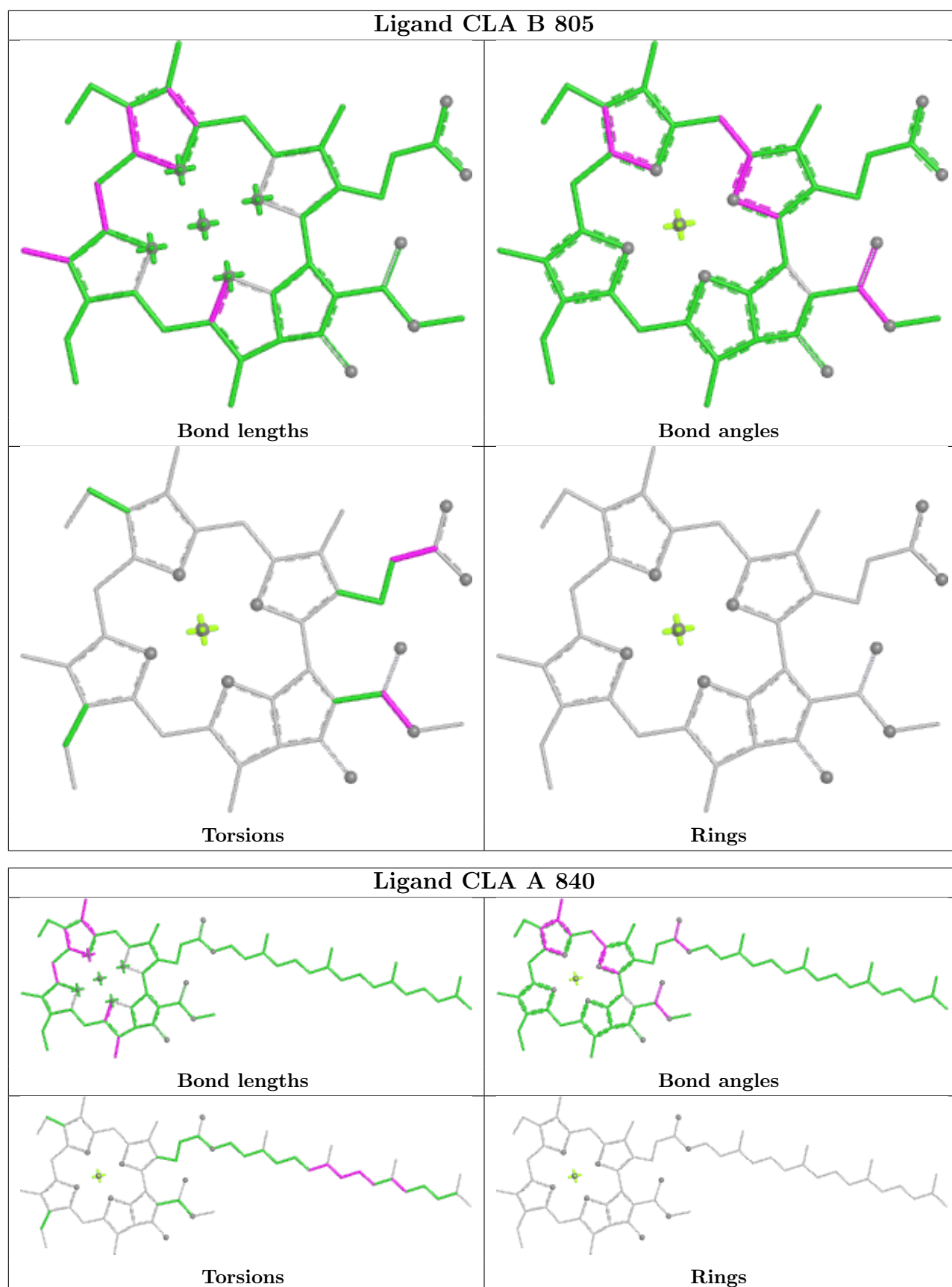


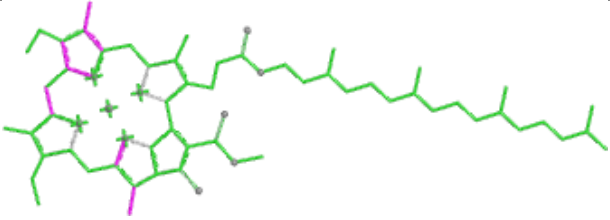
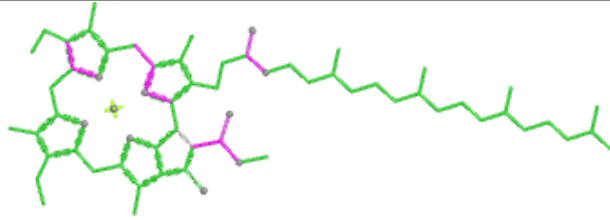
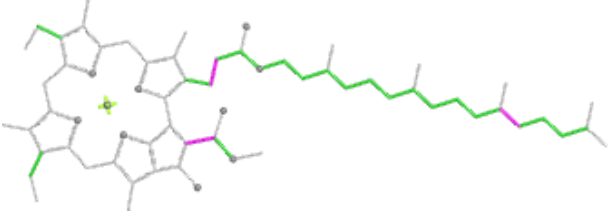
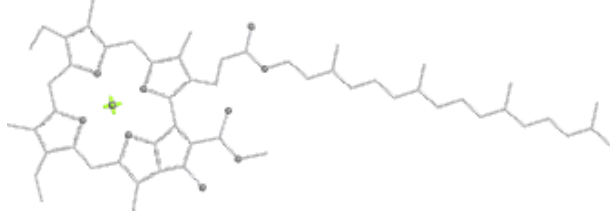
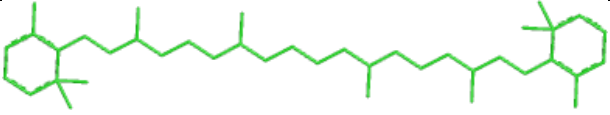
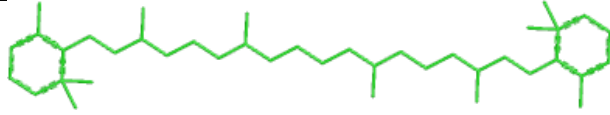
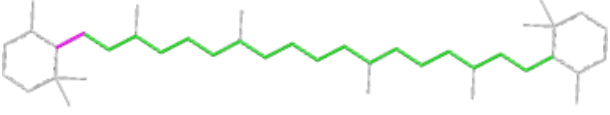
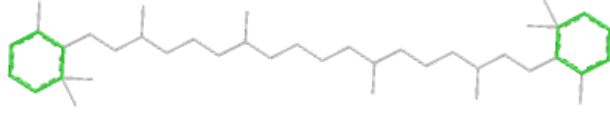
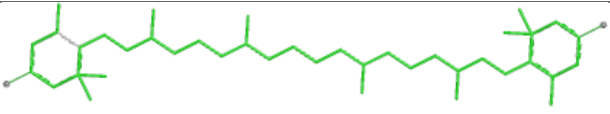
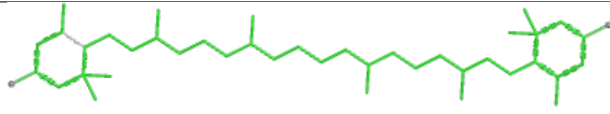
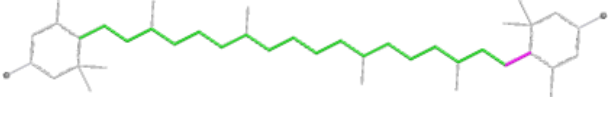
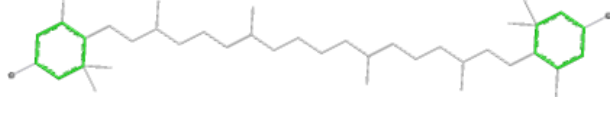


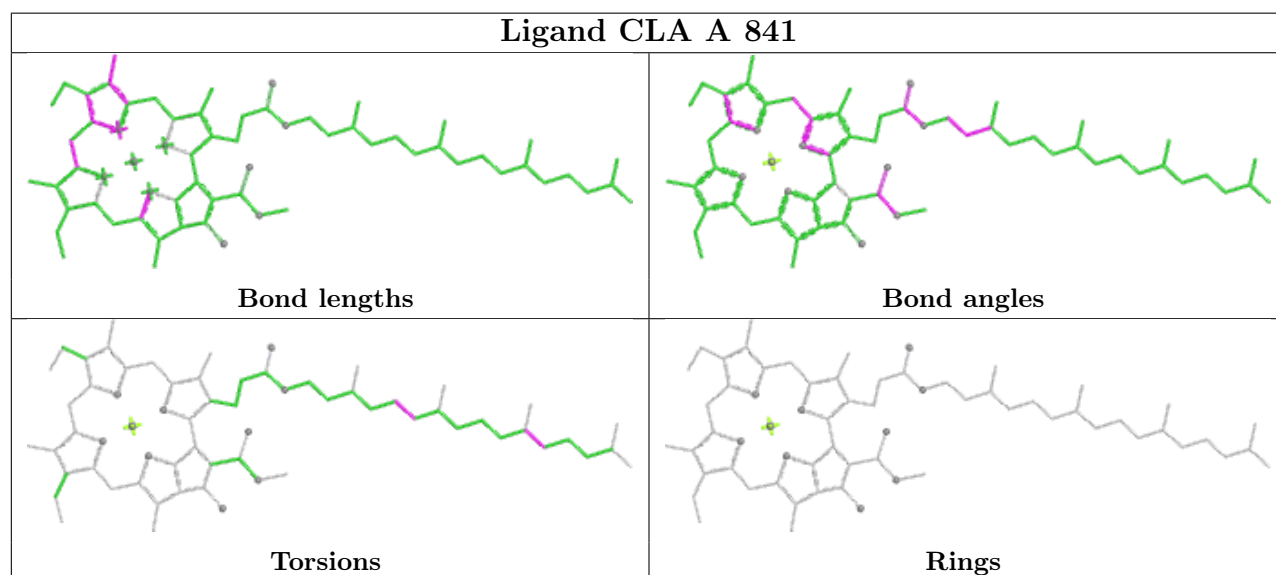
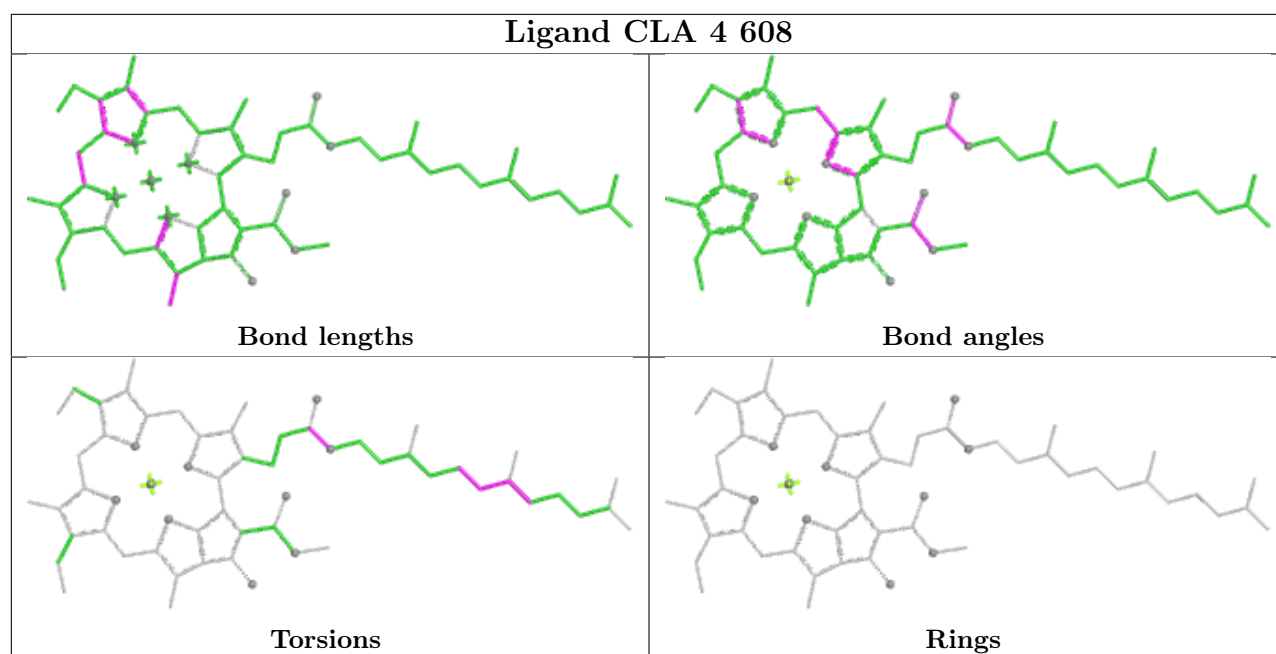
Ligand CLA B 833	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 850	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT Z 617	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

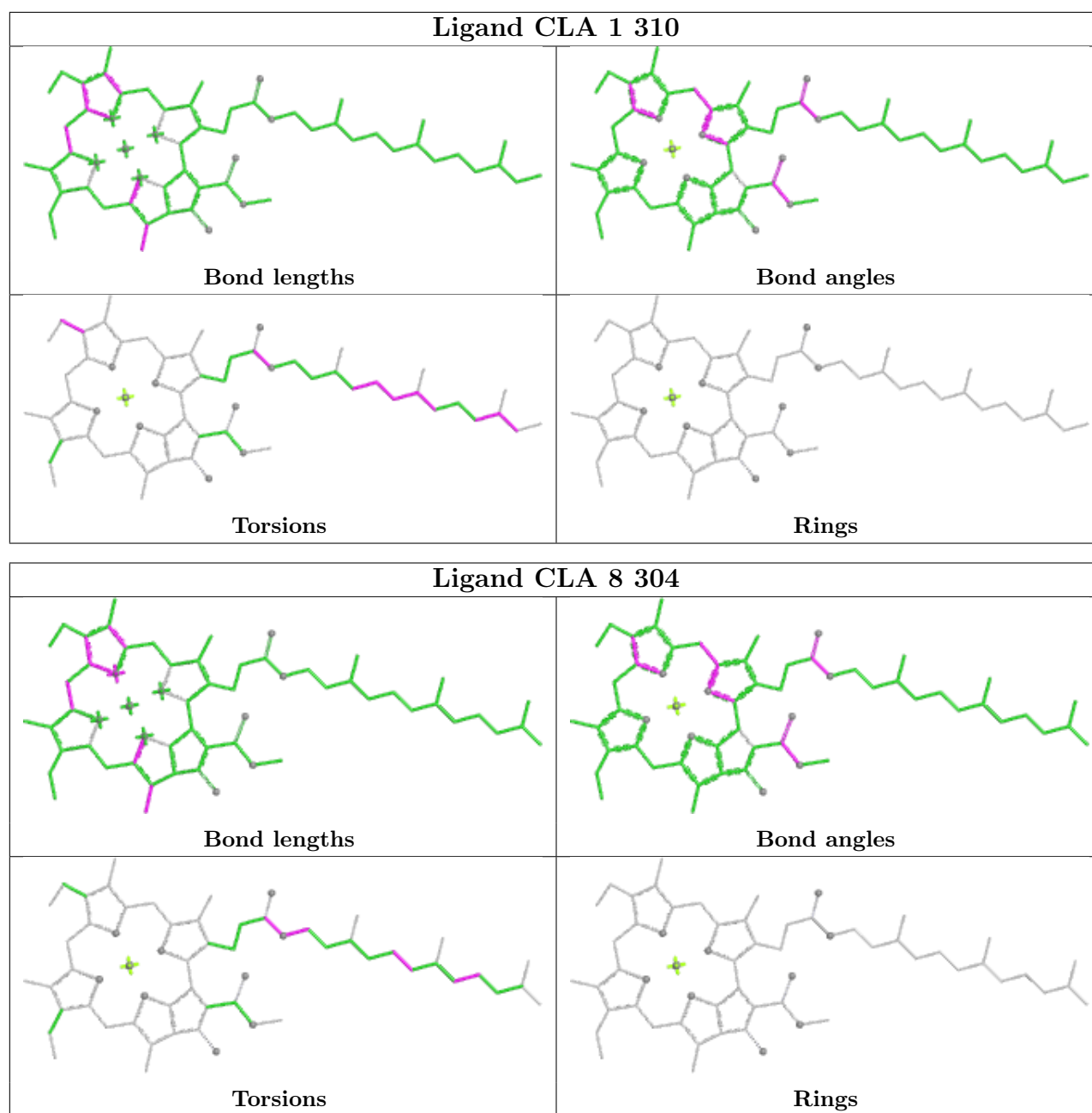
## Ligand CLA L 204

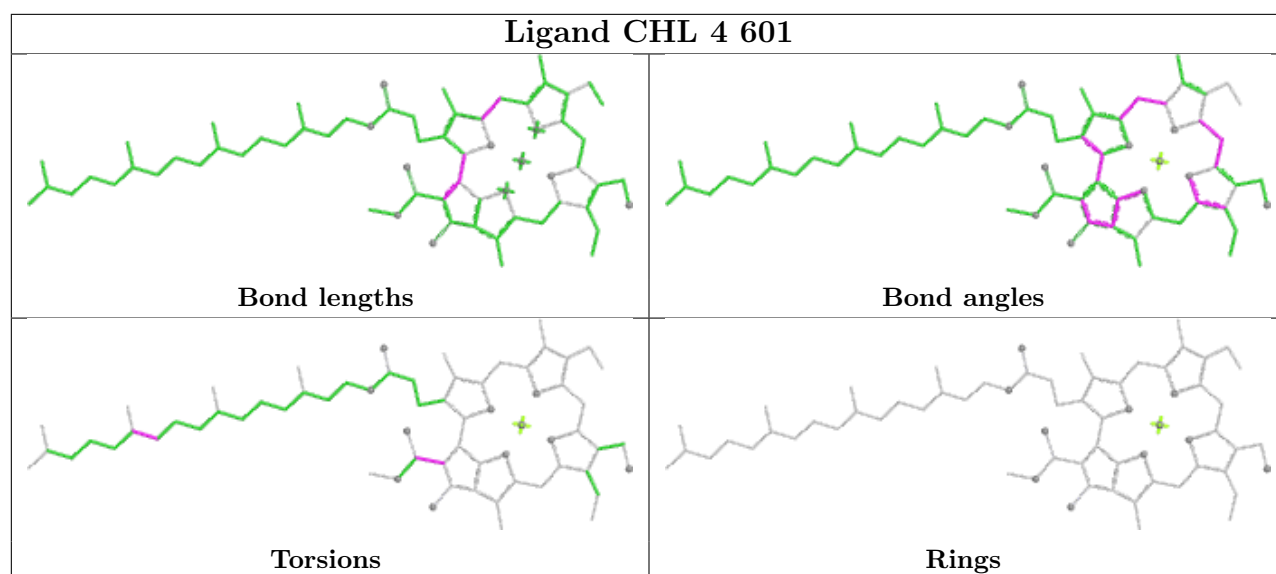
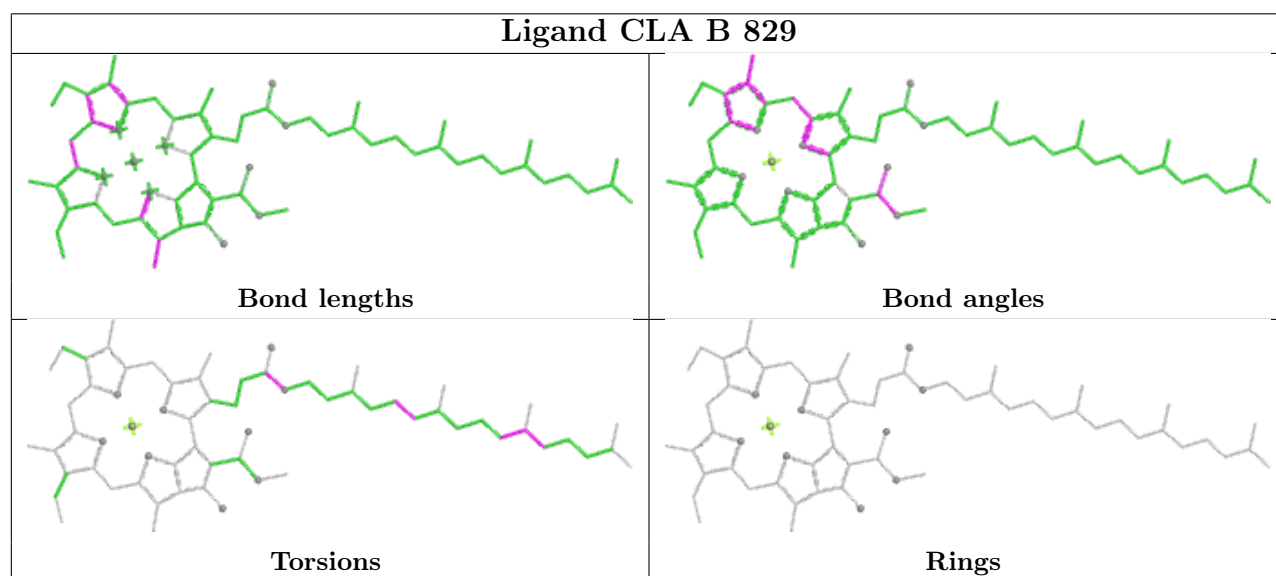
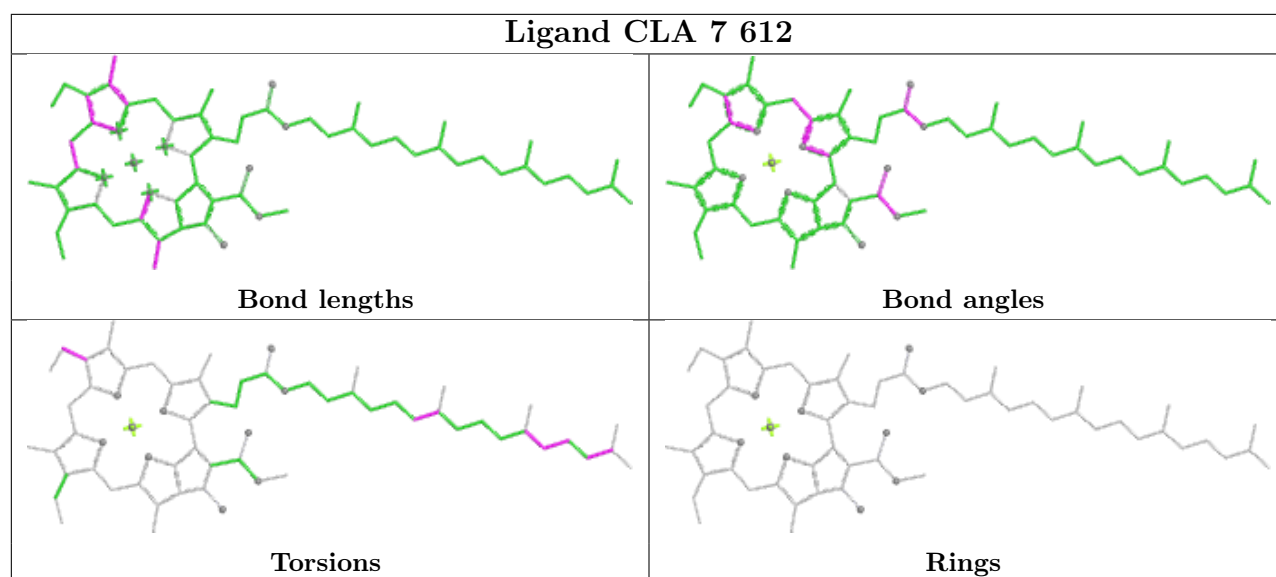


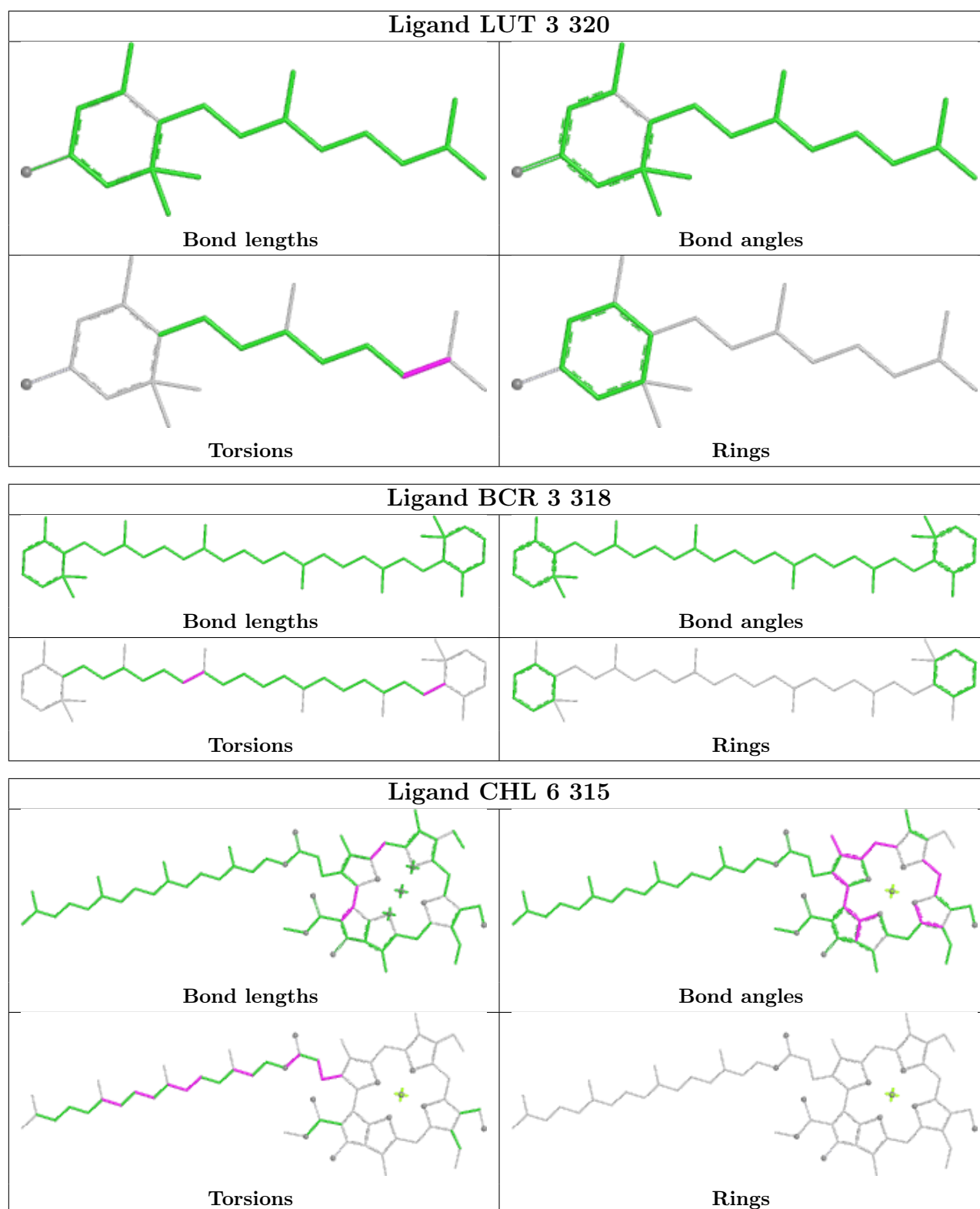


Ligand CLA A 810	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR A 849	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT 8 315	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

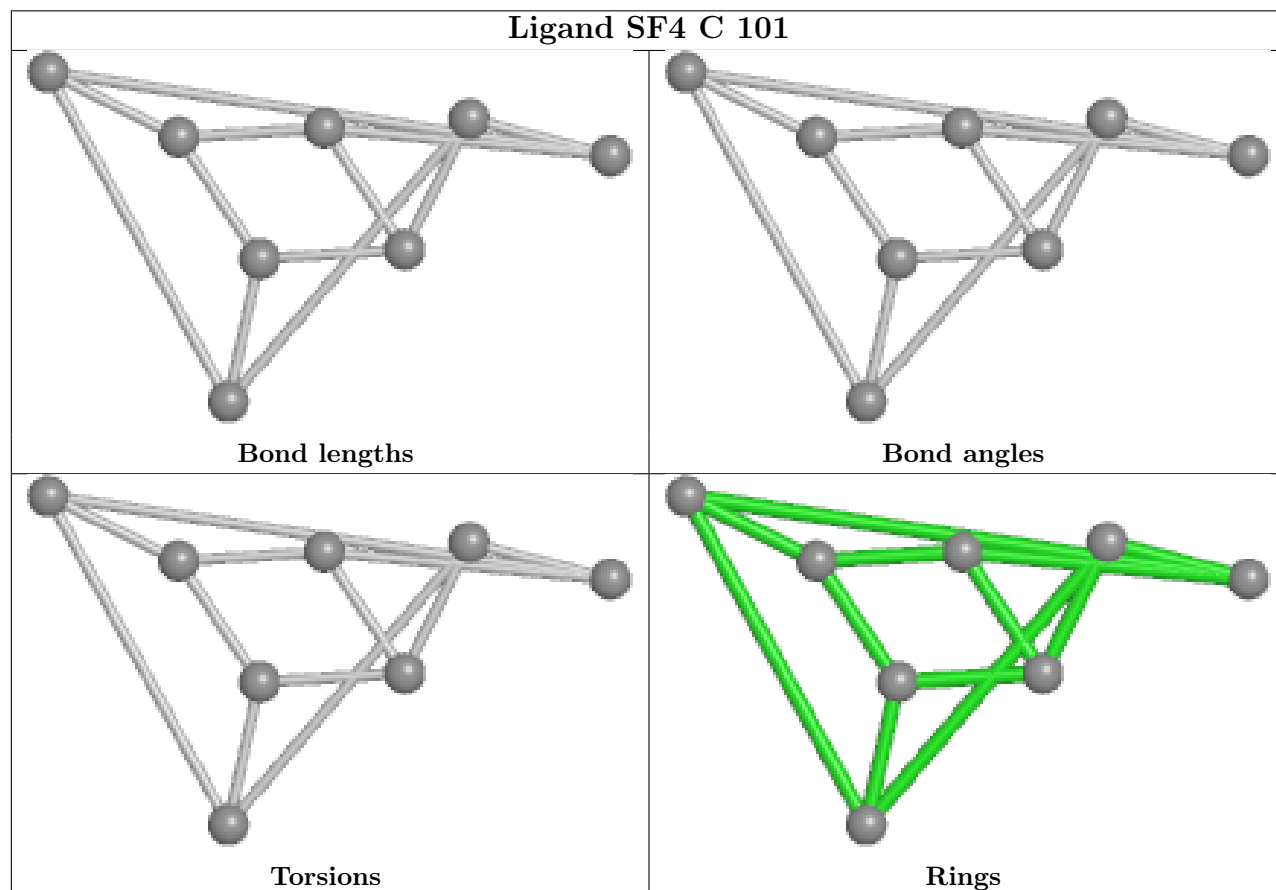
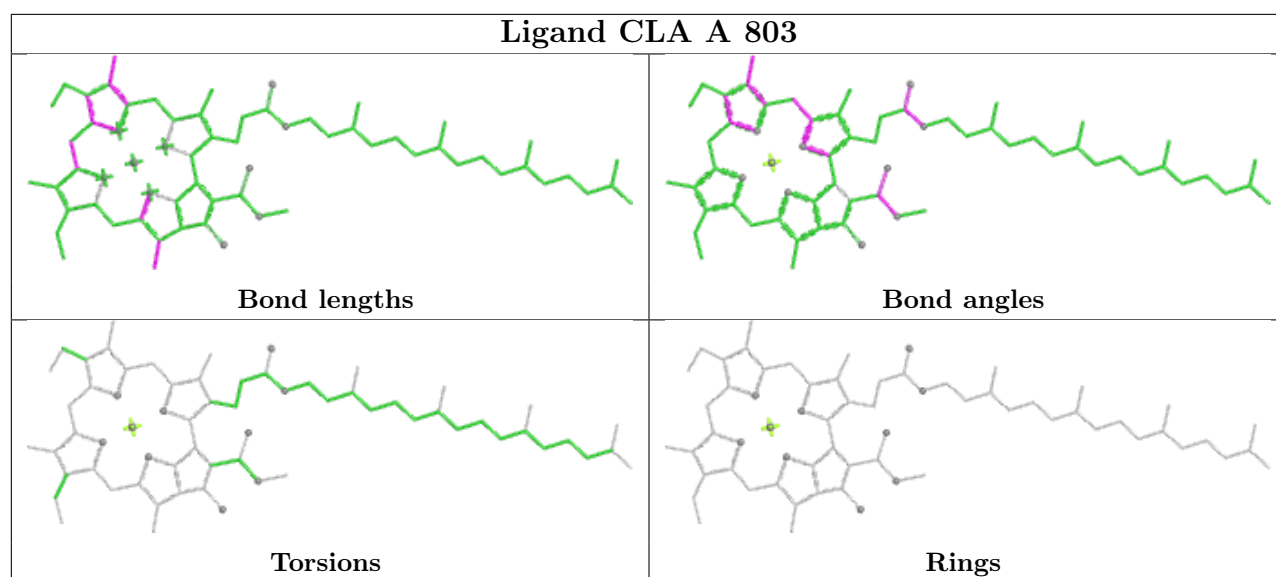


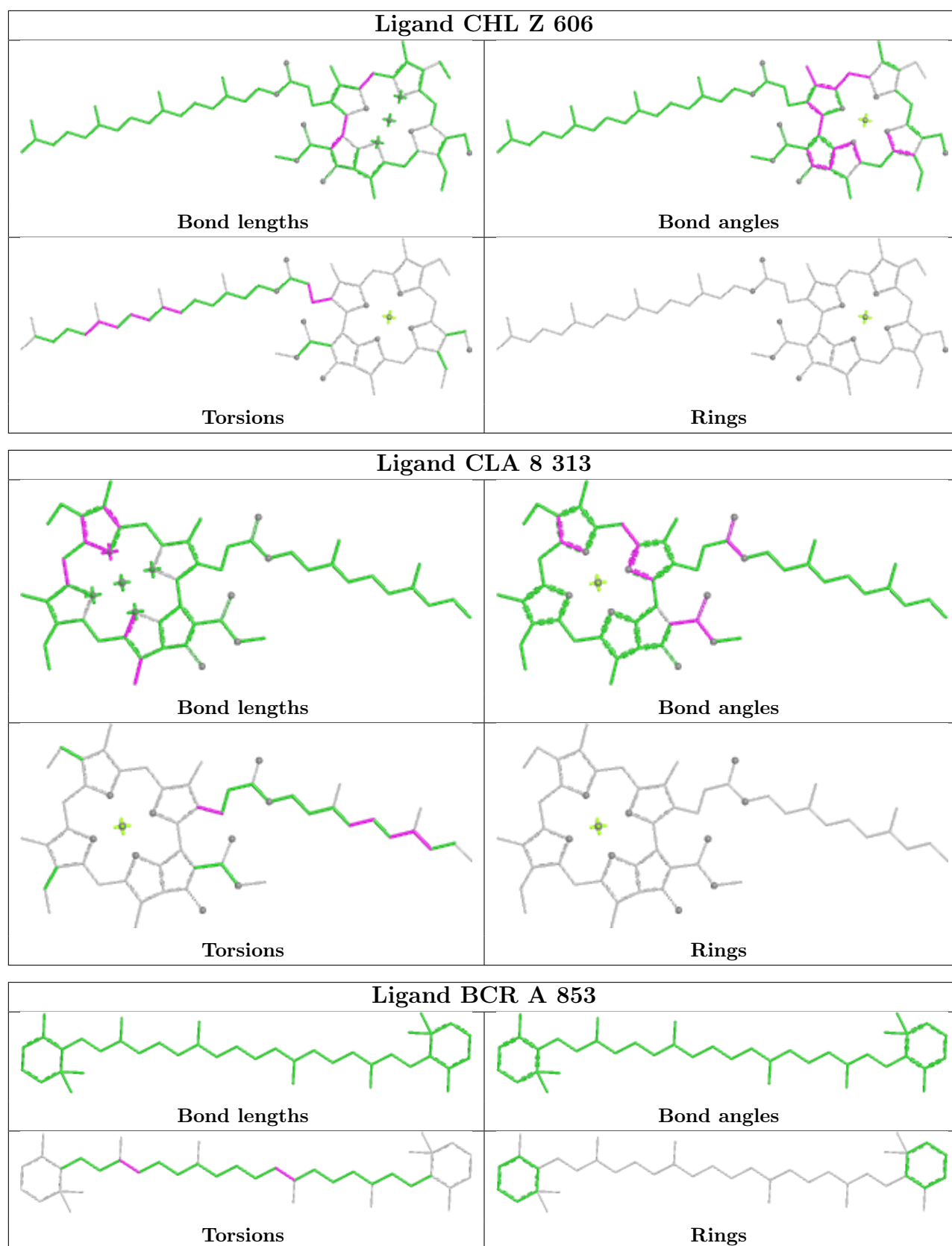


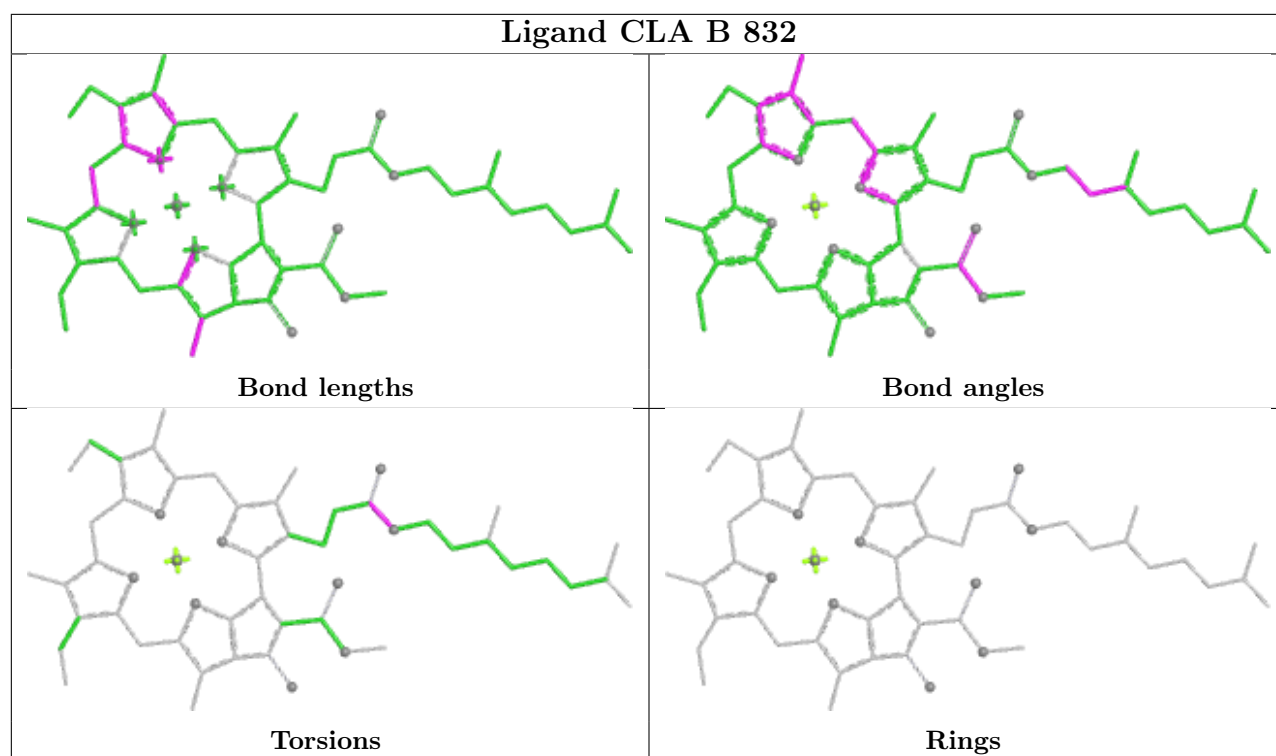




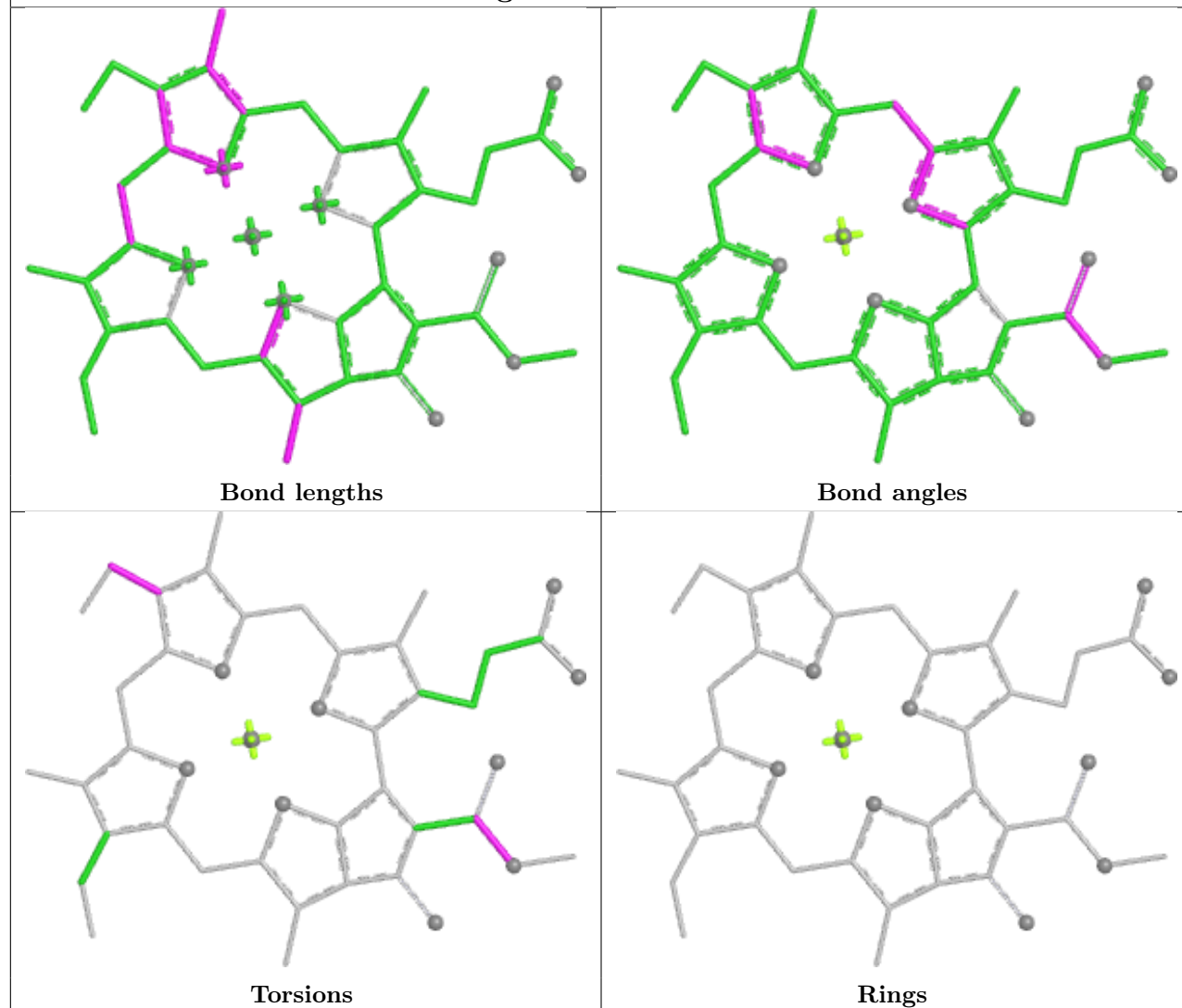




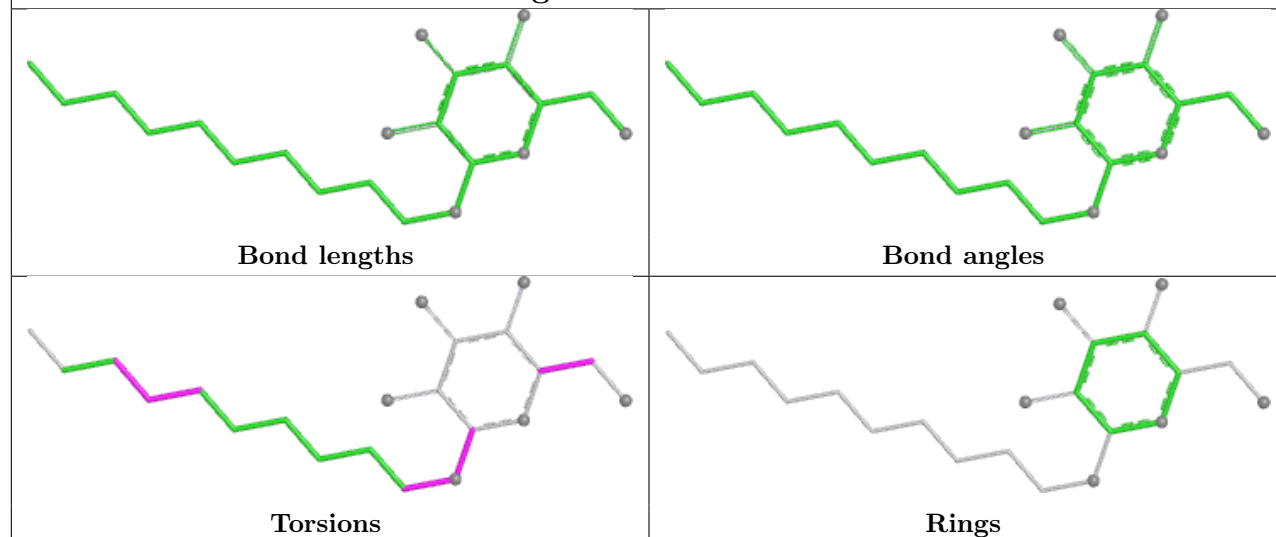


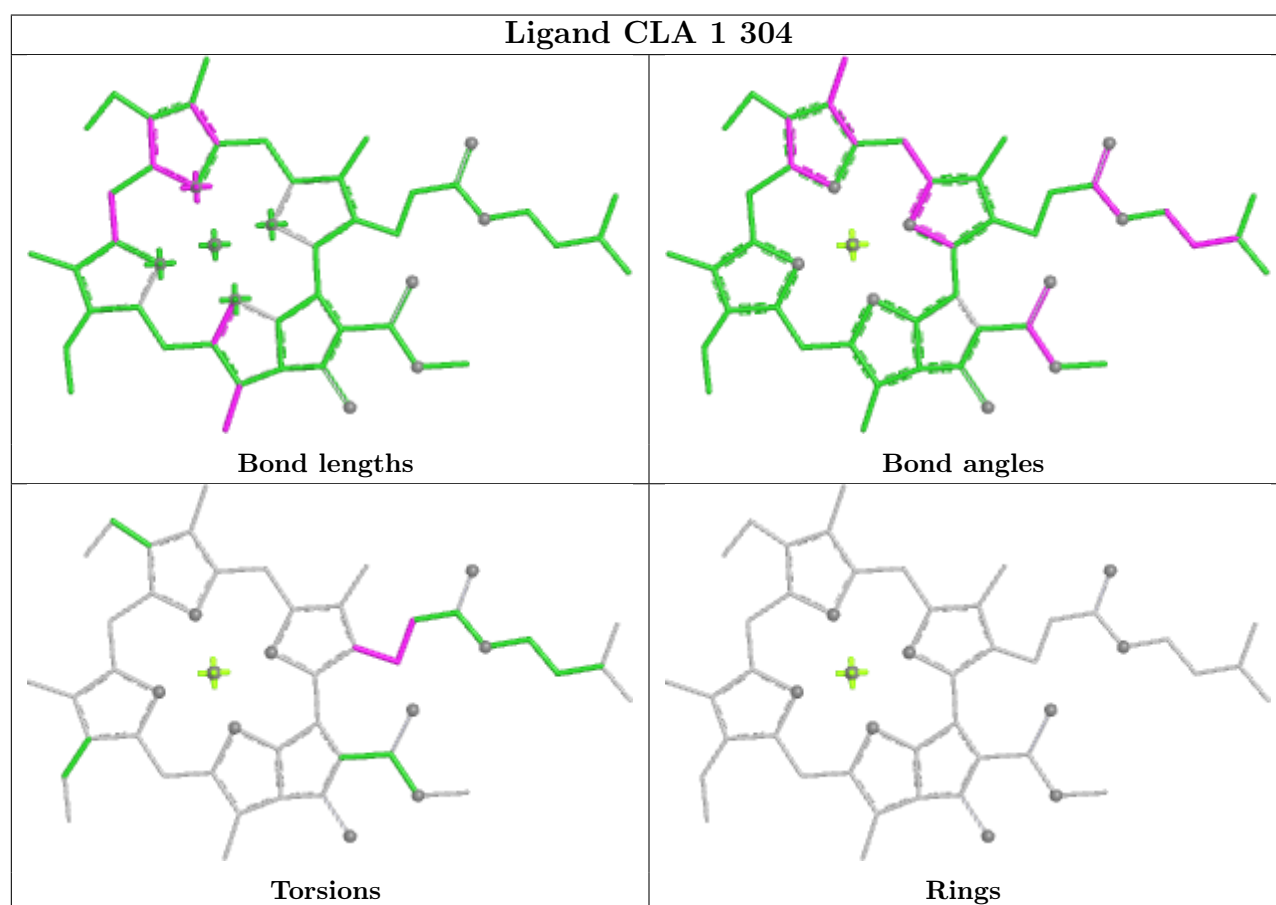
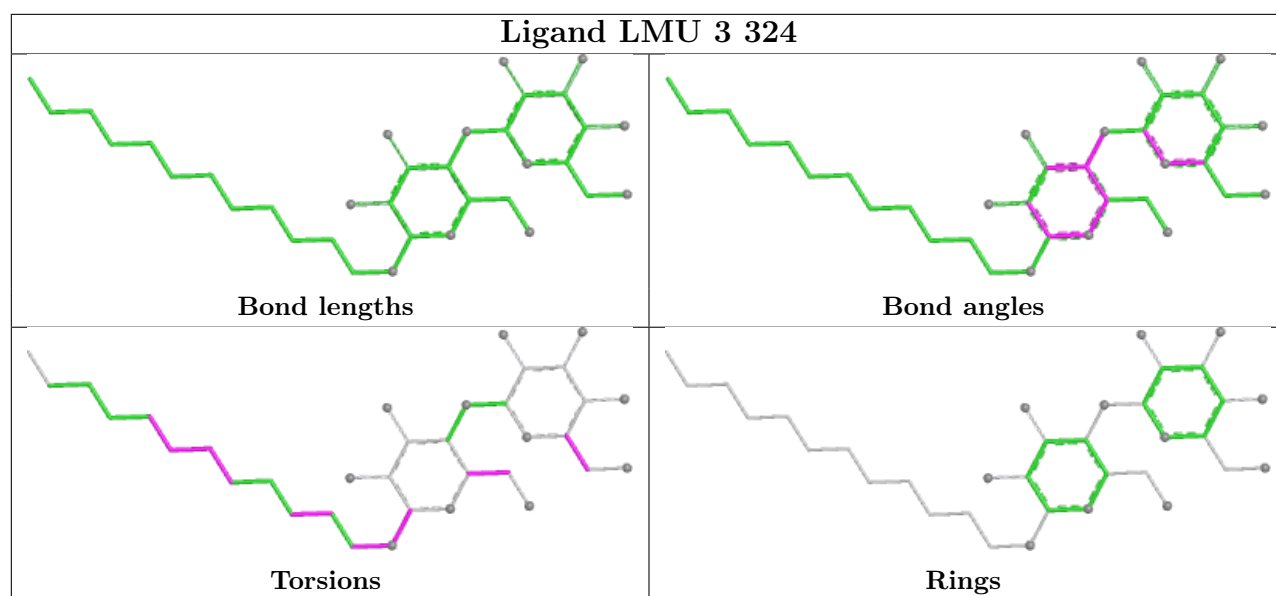


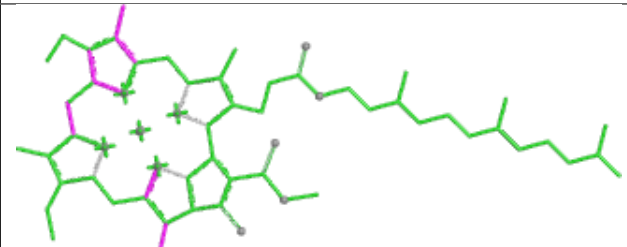
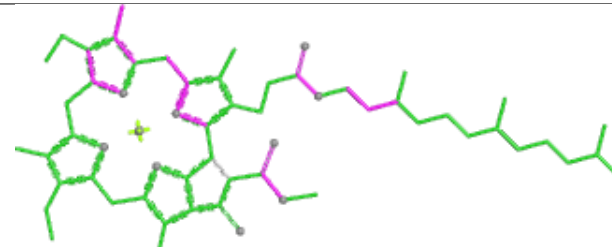
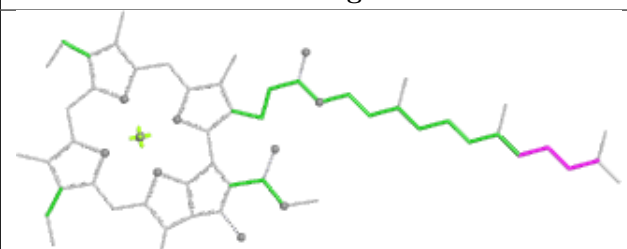
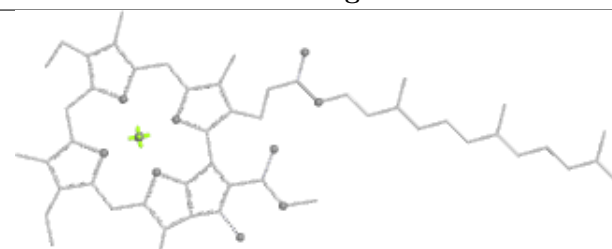
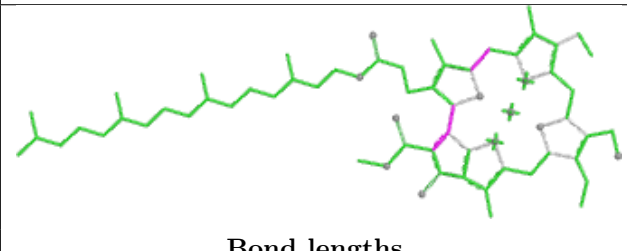
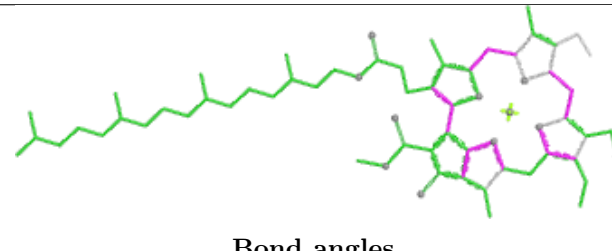
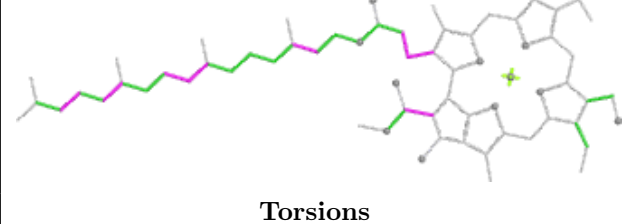
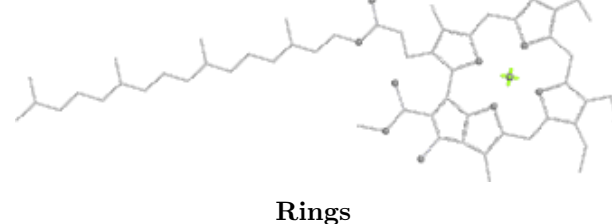
## Ligand CLA 6 316

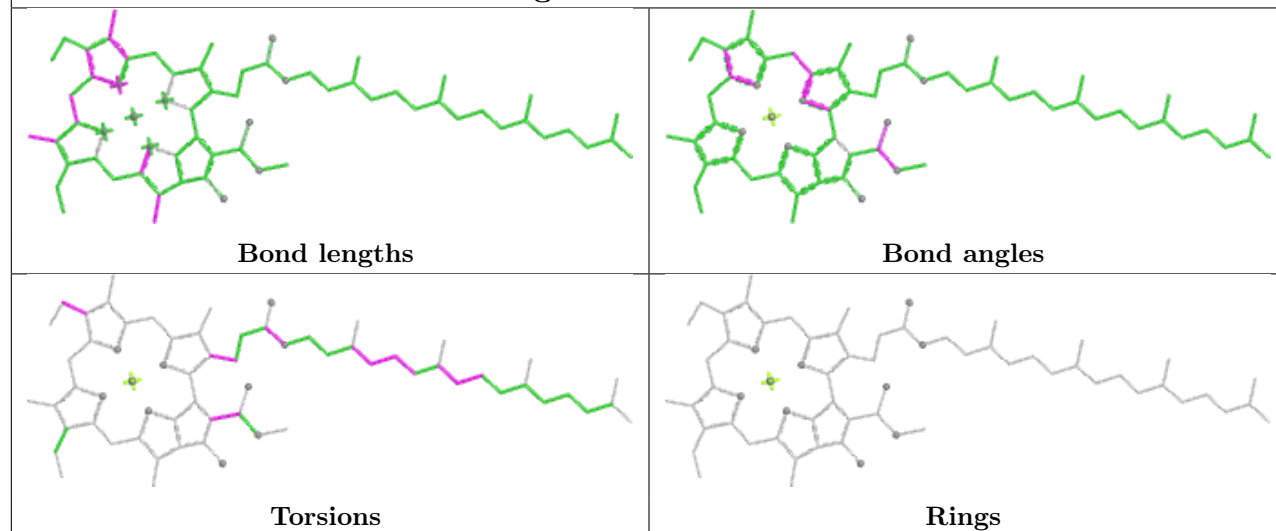
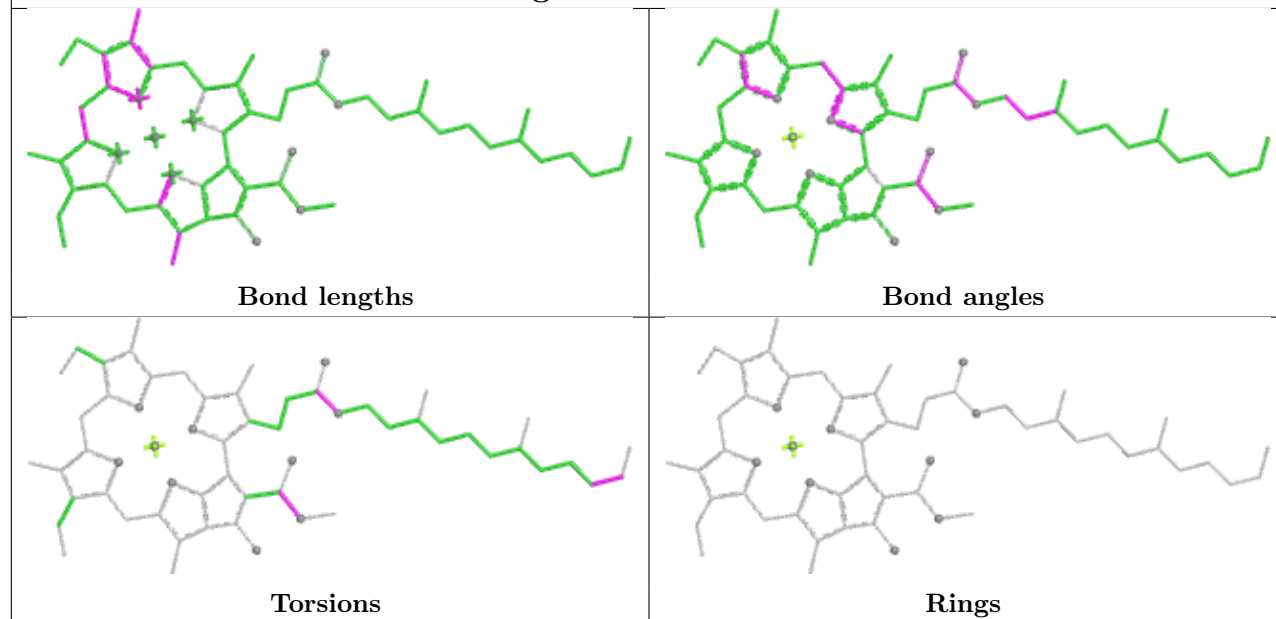


## Ligand LMU 4 622

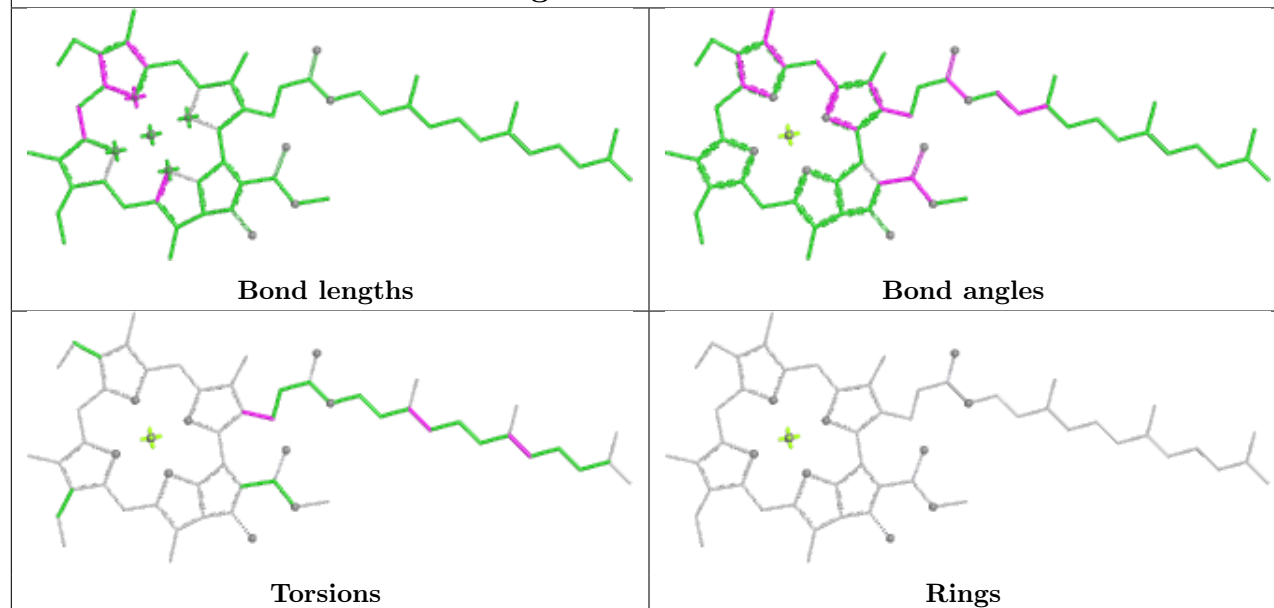




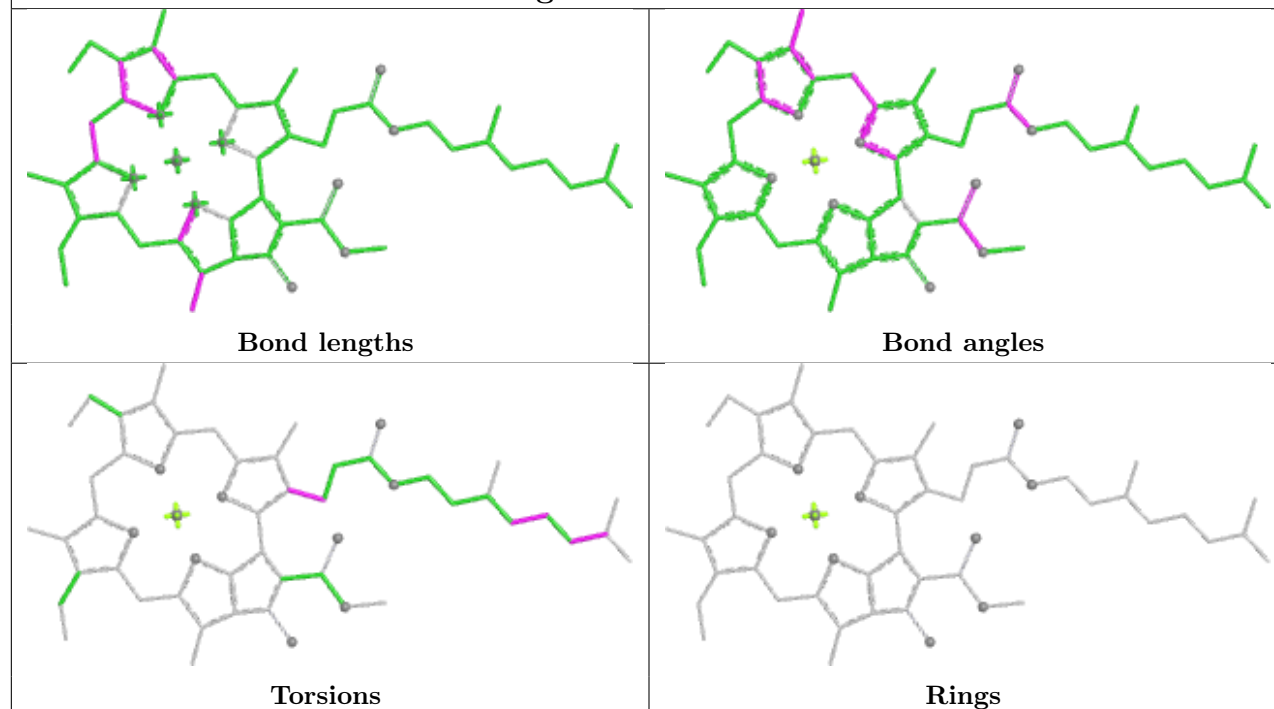
Ligand CLA 4 609	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL 8 306	
	
Bond lengths	Bond angles
	
Torsions	Rings

**Ligand CLA F 304****Ligand CLA B 823**

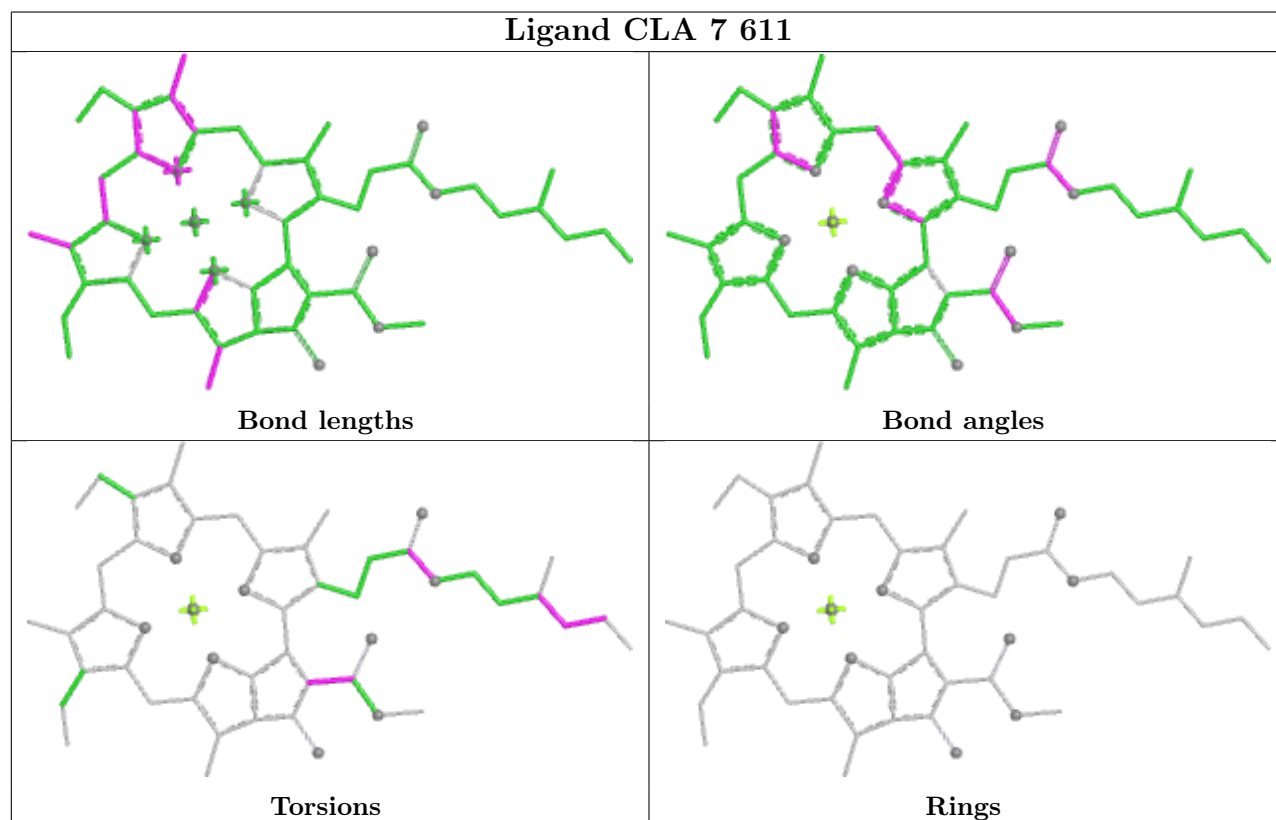
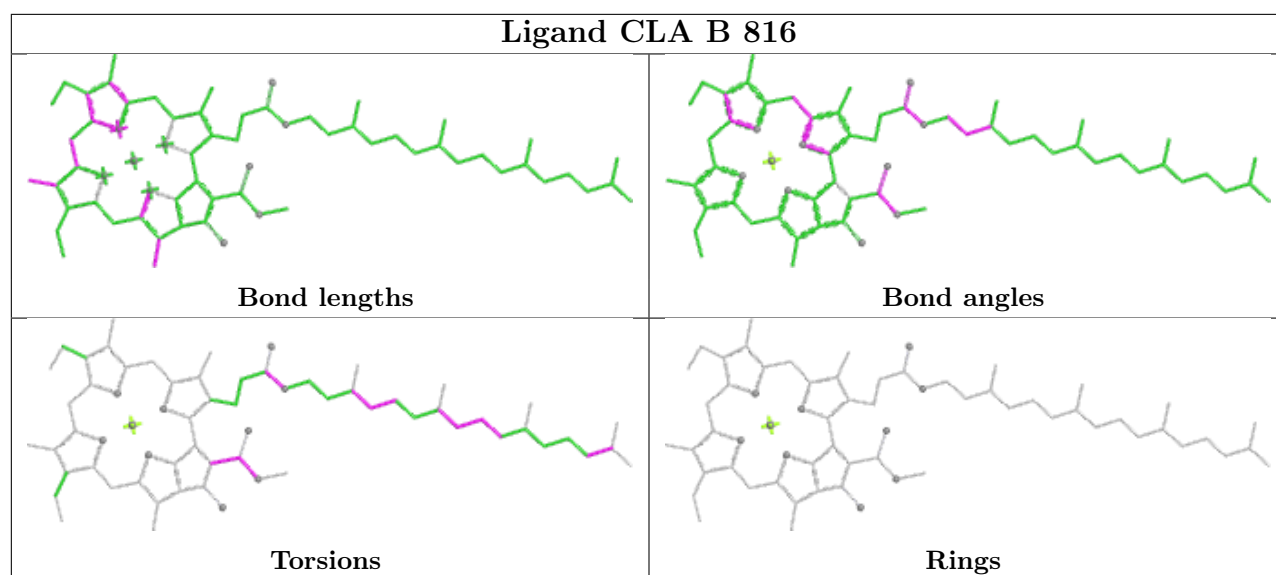
## Ligand CLA K 203

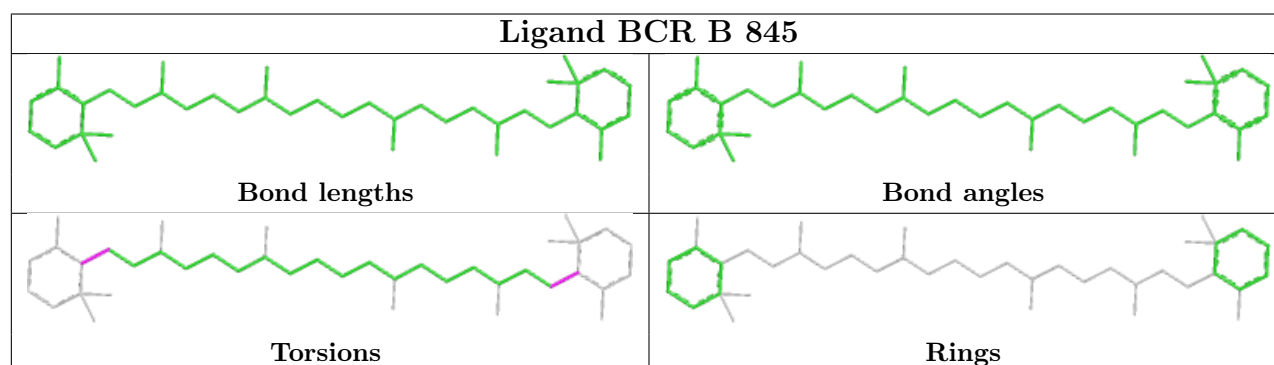
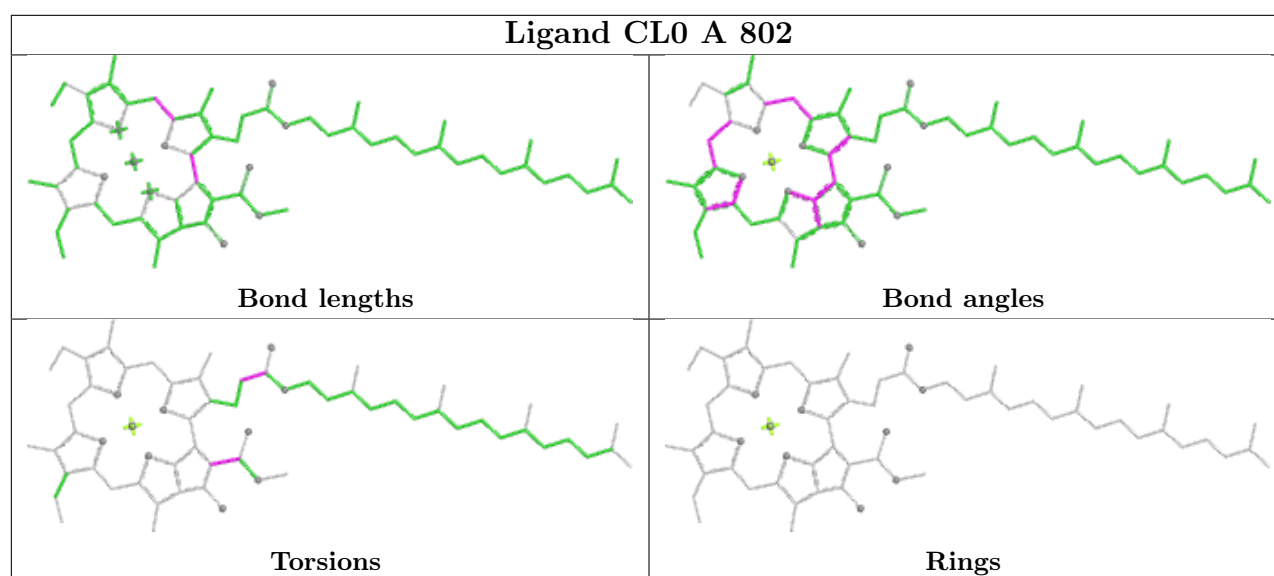
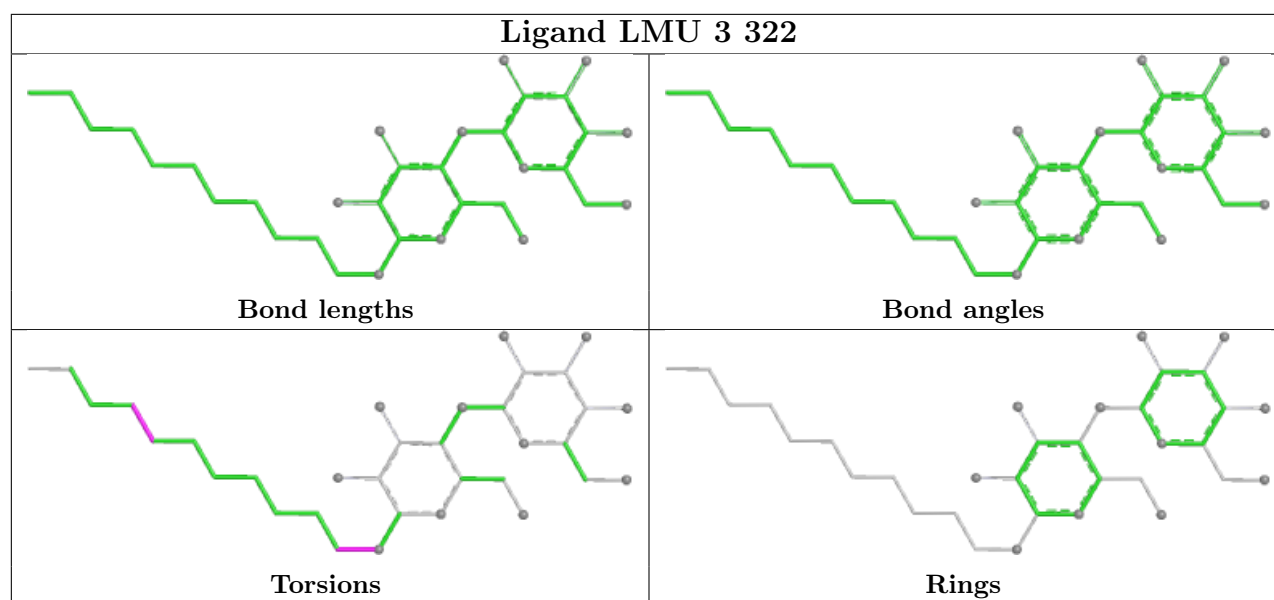


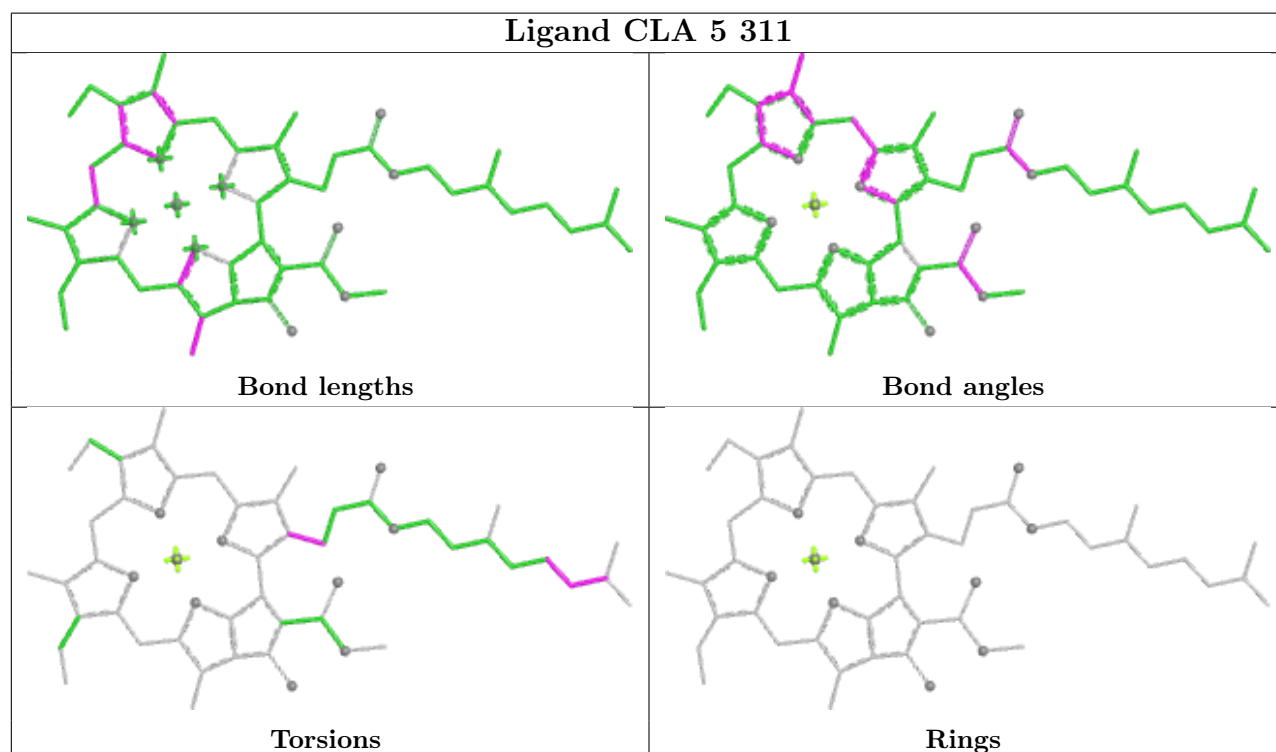
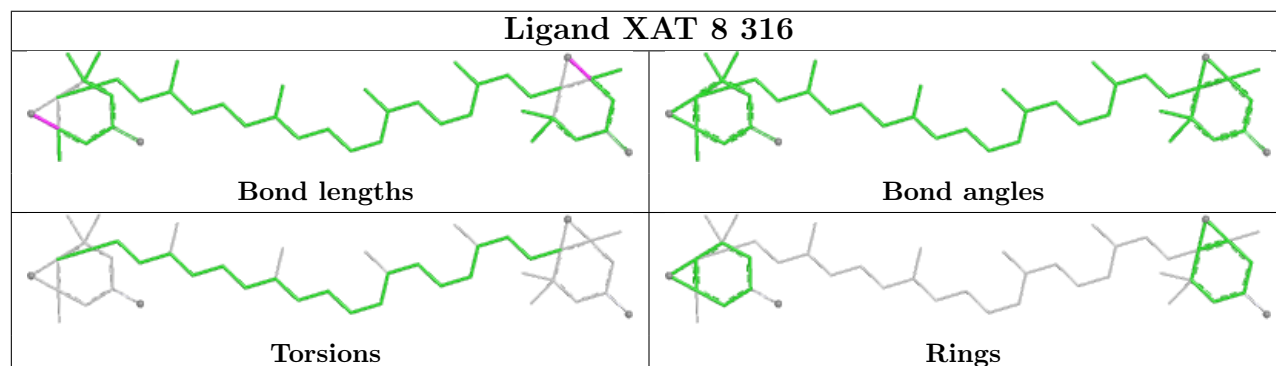
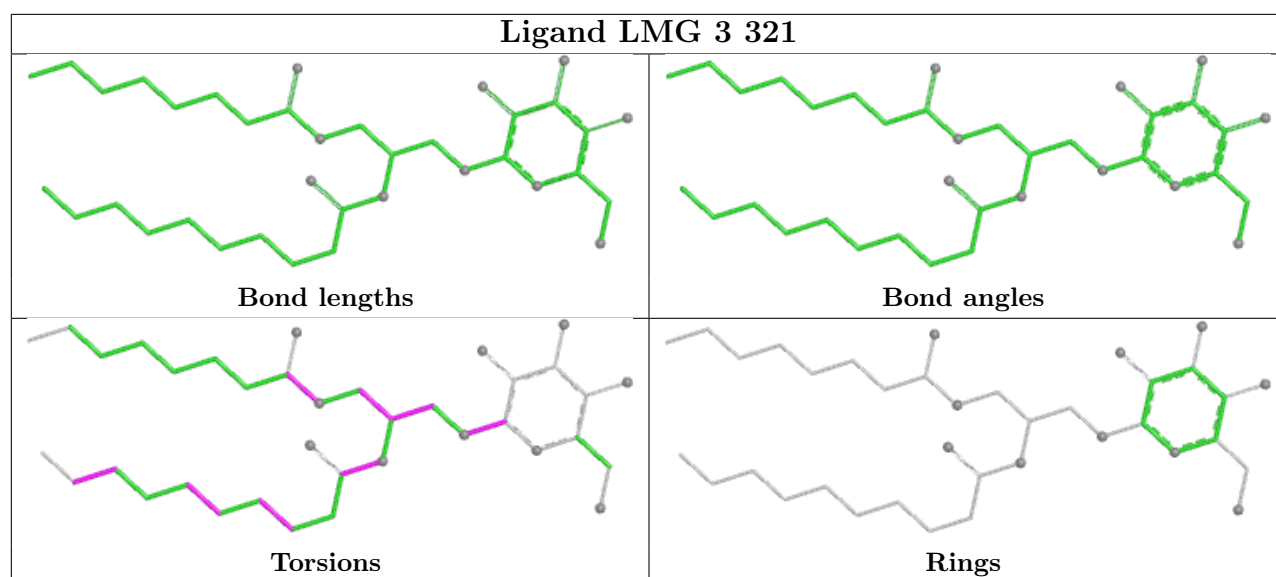
## Ligand CLA 6 309



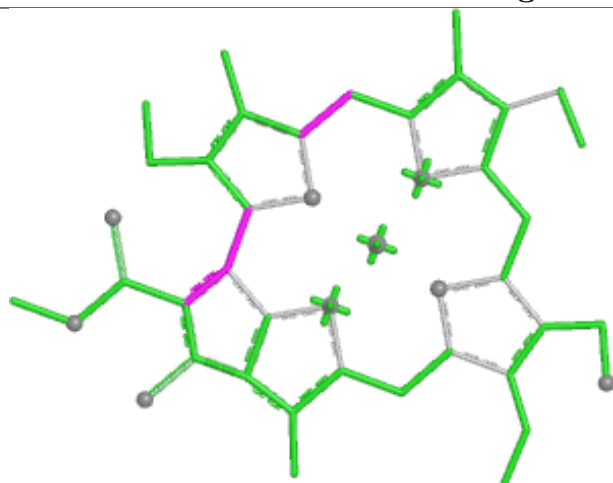




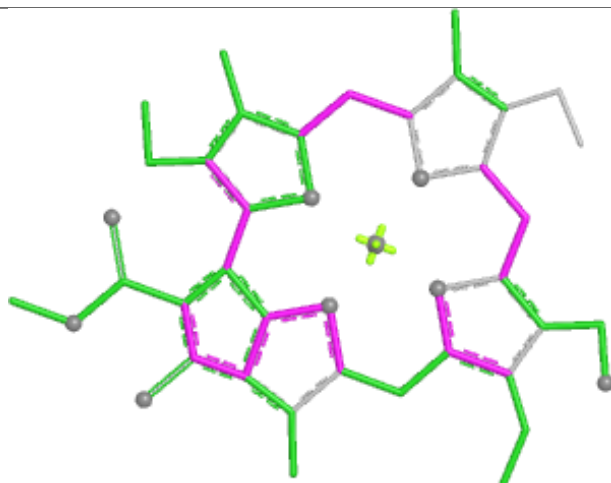




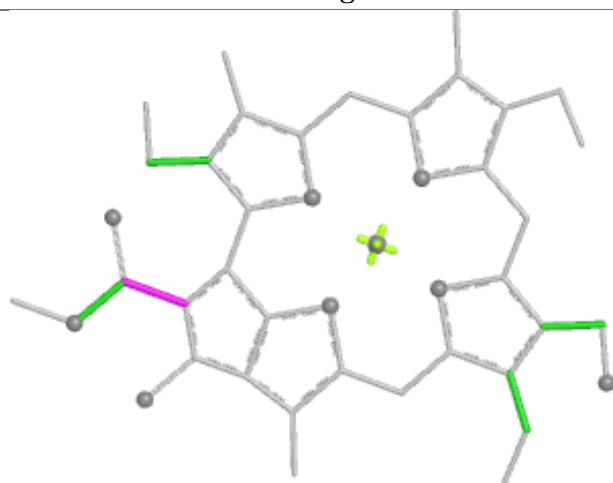
## Ligand CHL 5 317



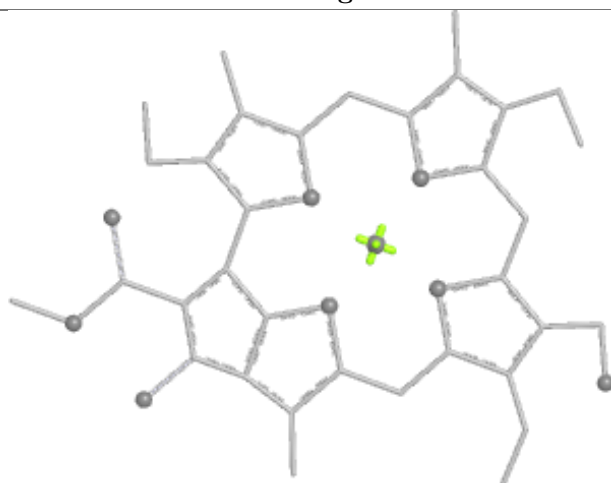
Bond lengths



Bond angles

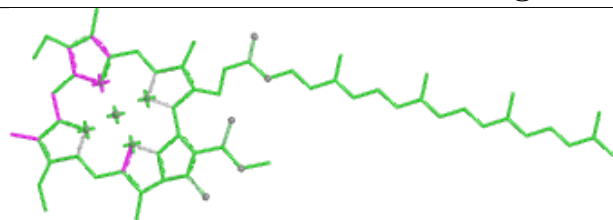


Torsions

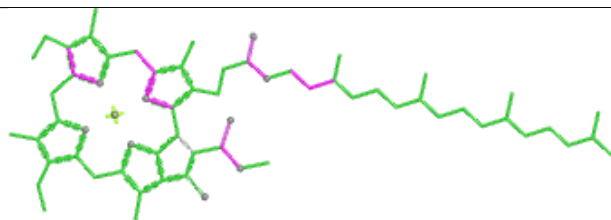


Rings

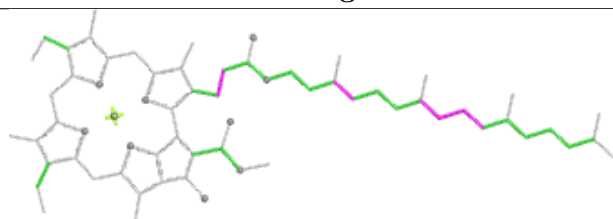
## Ligand CLA A 842



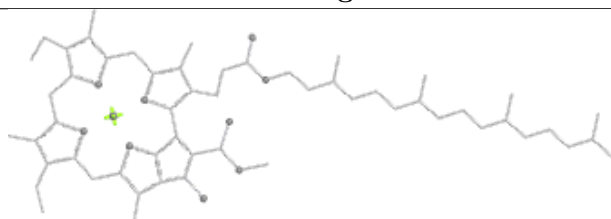
Bond lengths



Bond angles

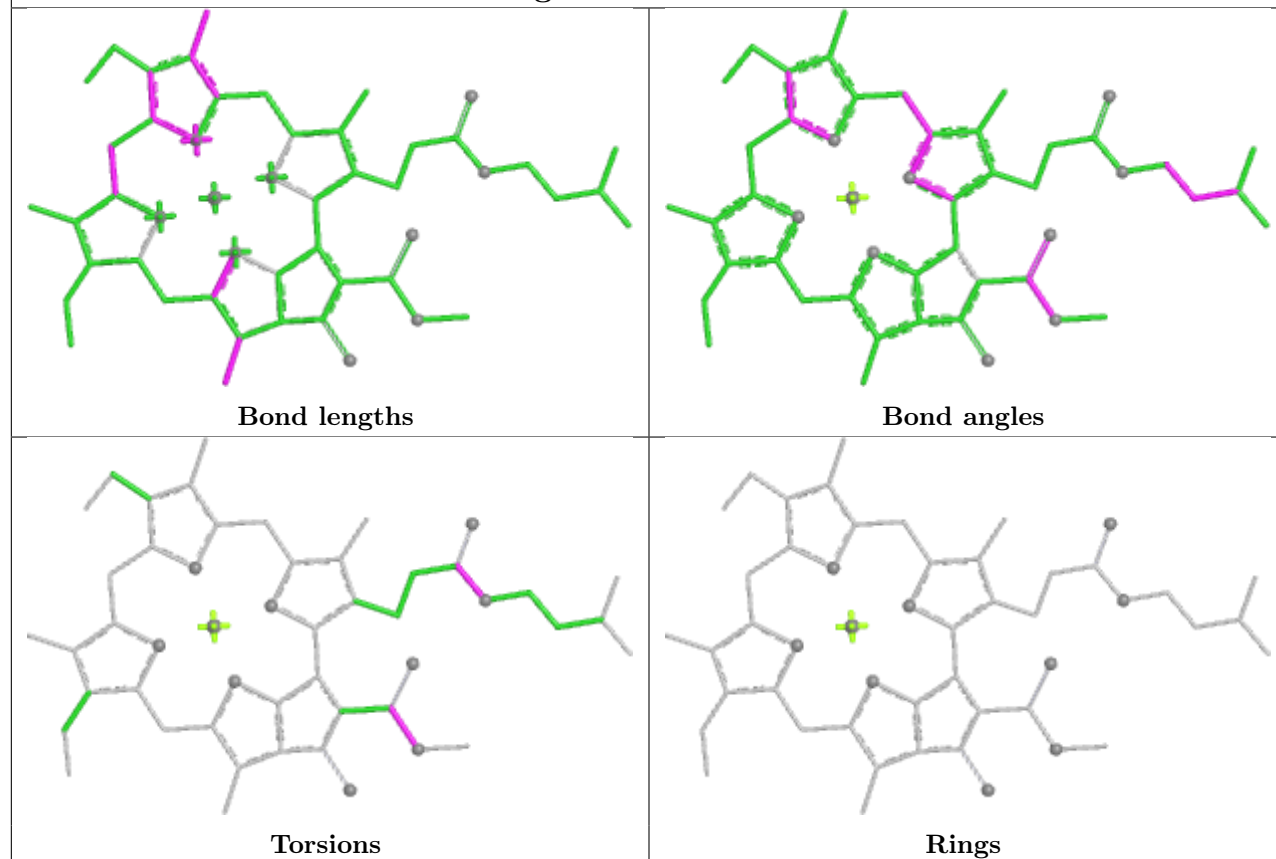


Torsions

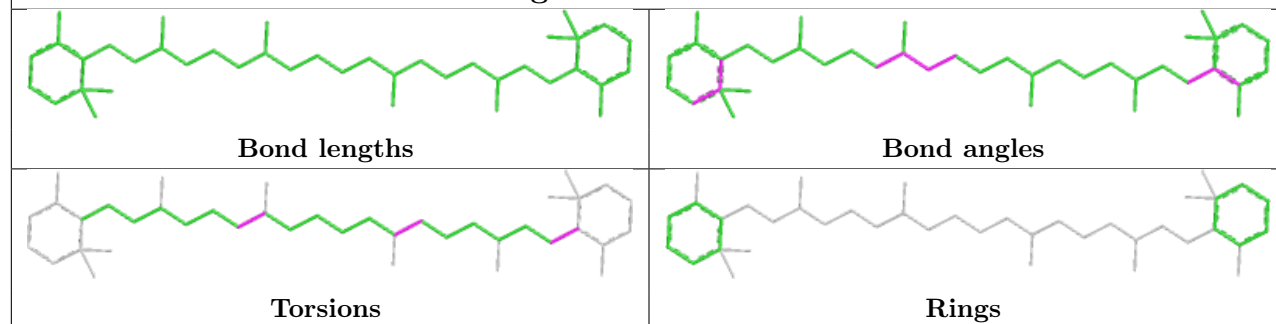


Rings

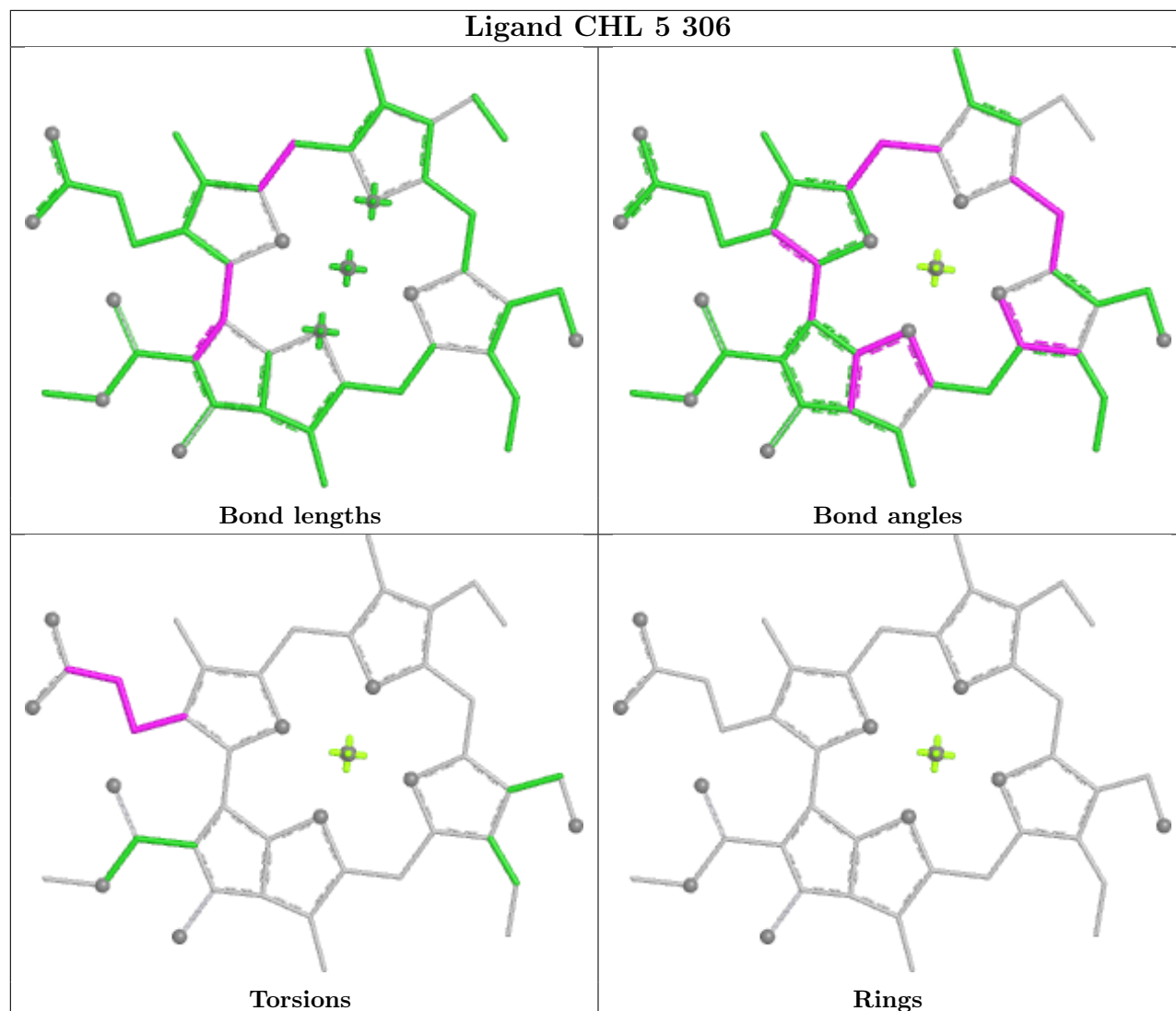
## Ligand CLA Z 607



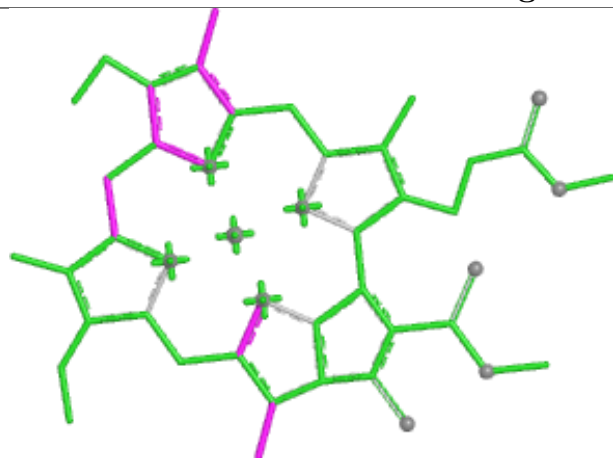
## Ligand BCR B 802



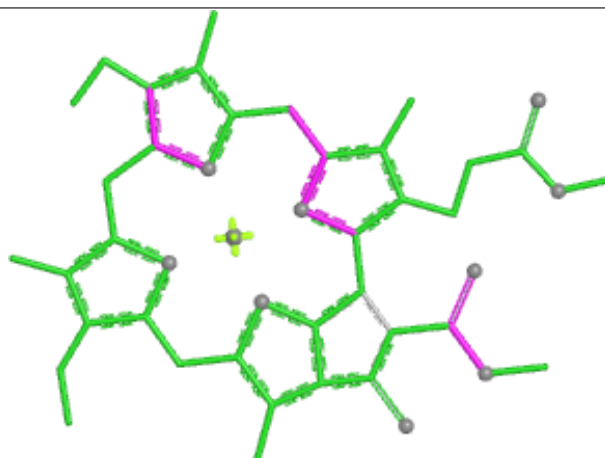
## Ligand CHL 5 306



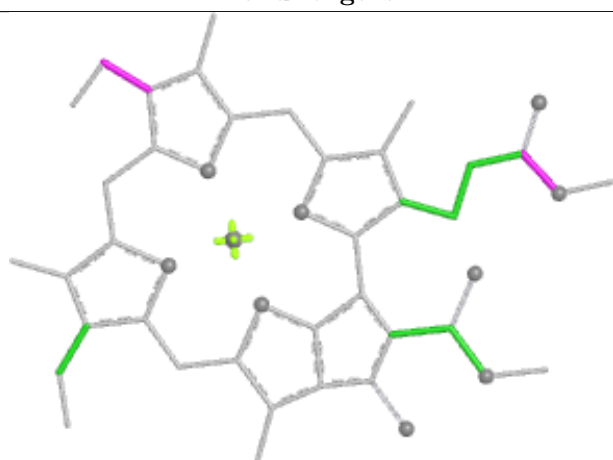
## Ligand CLA 1 314



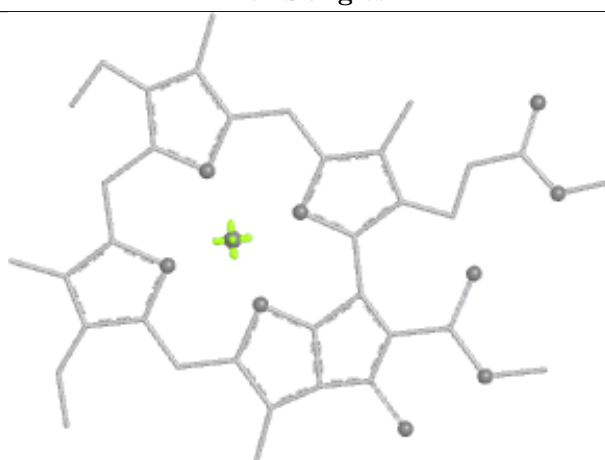
Bond lengths



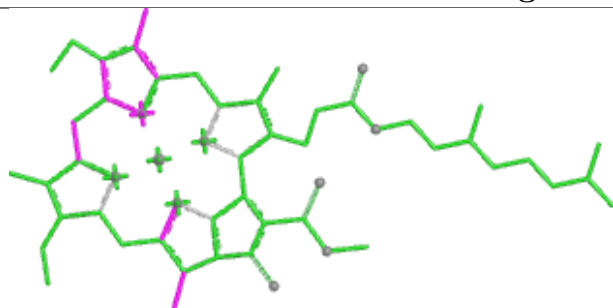
Bond angles



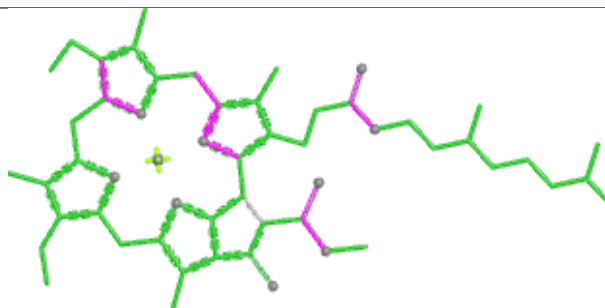
Torsions



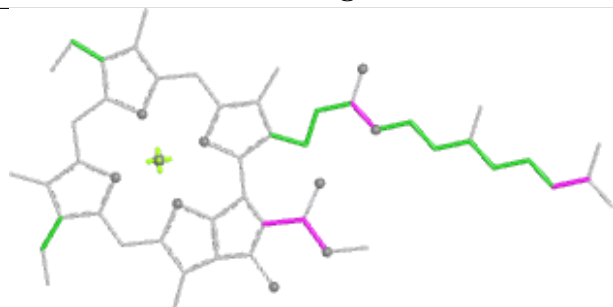
Rings

**Ligand CLA 5 305**

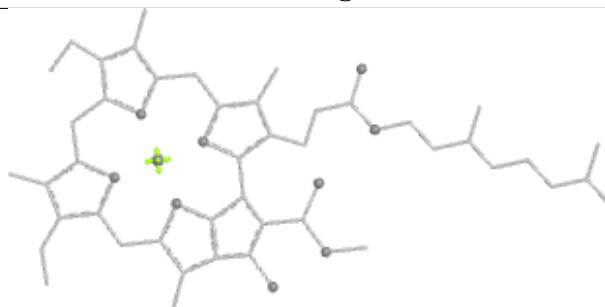
Bond lengths



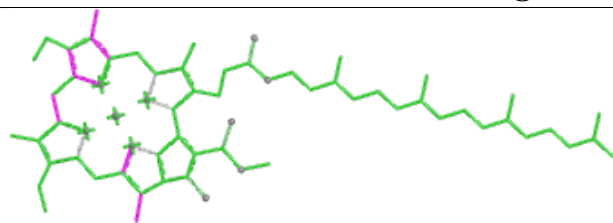
Bond angles



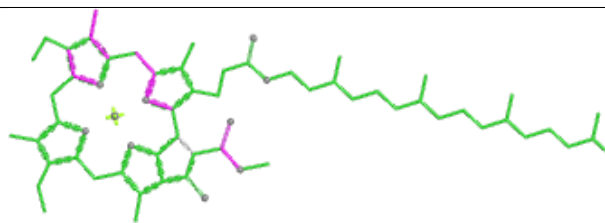
Torsions



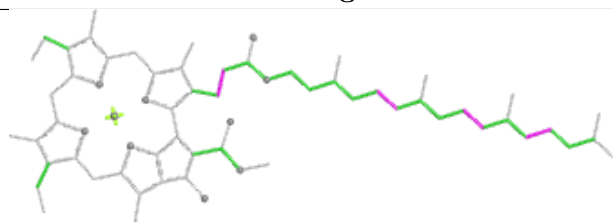
Rings

**Ligand CLA A 831**

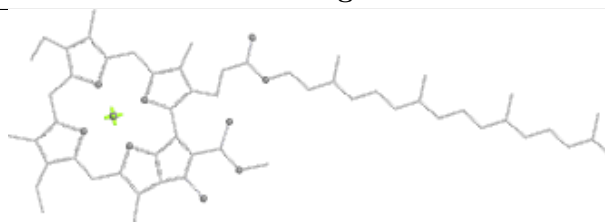
Bond lengths



Bond angles

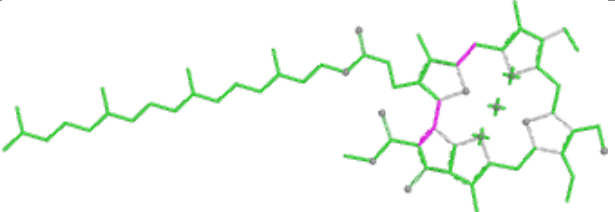
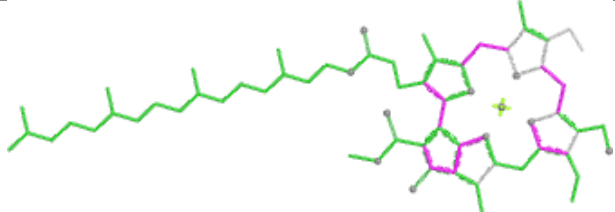
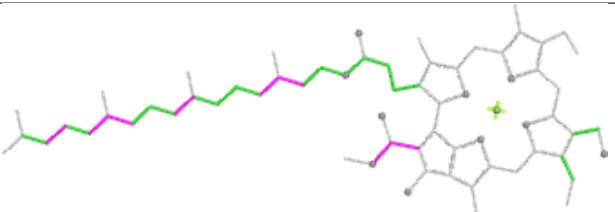
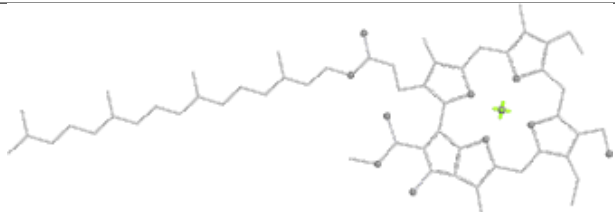
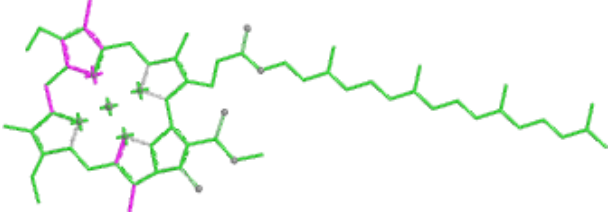
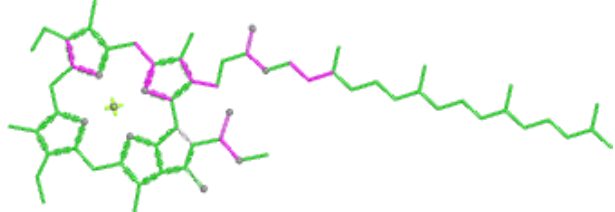
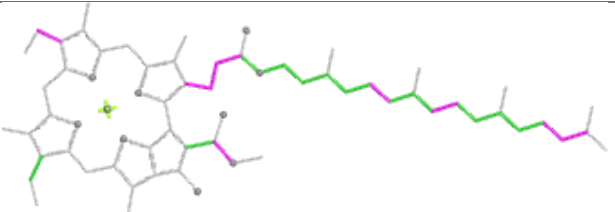
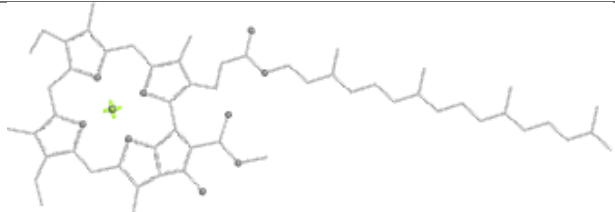
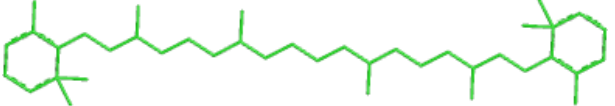
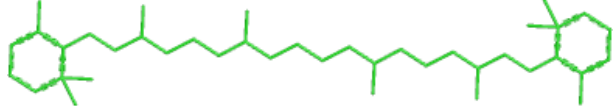
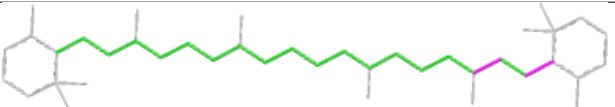
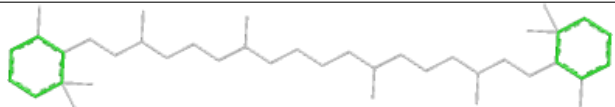


Torsions

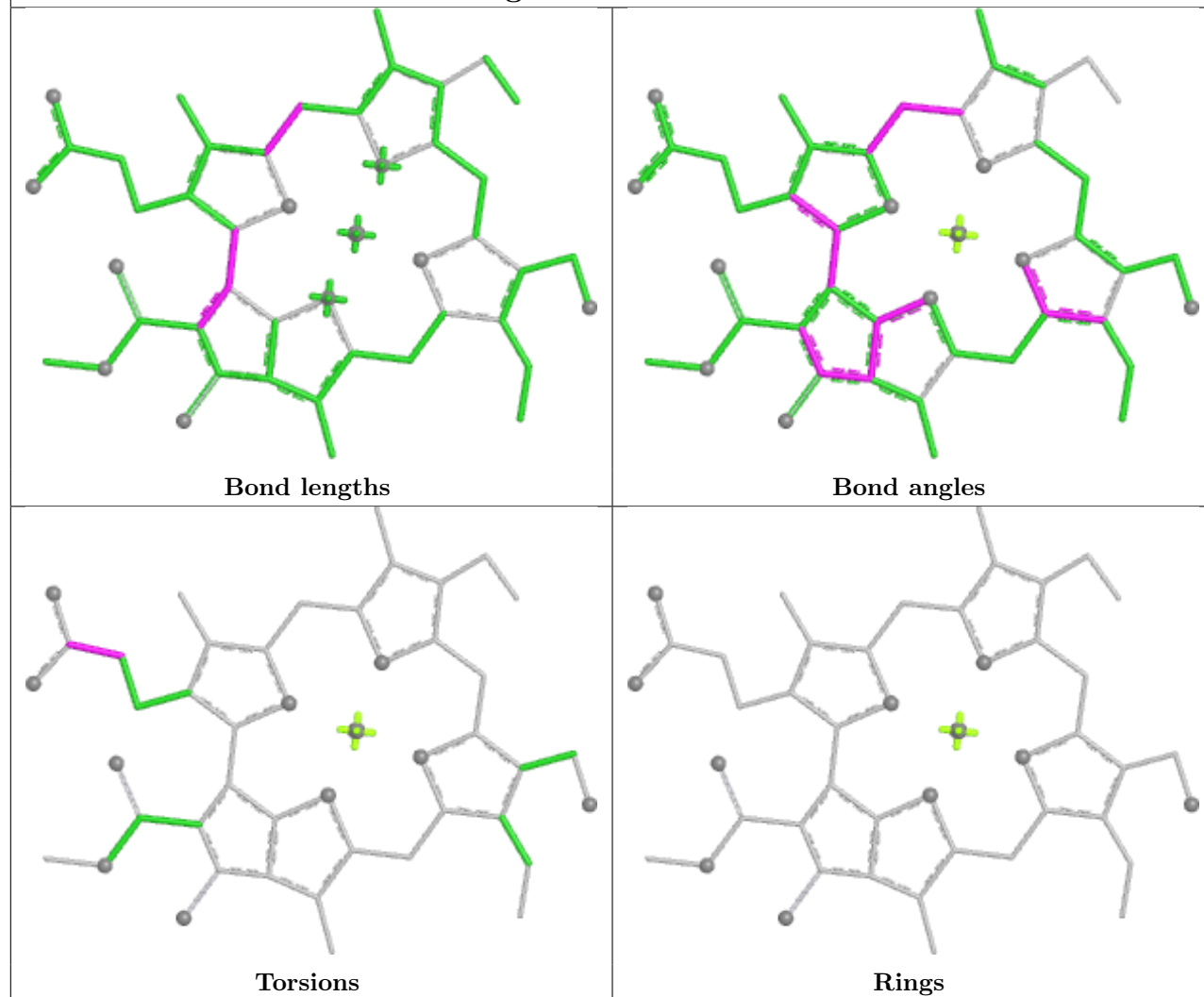


Rings

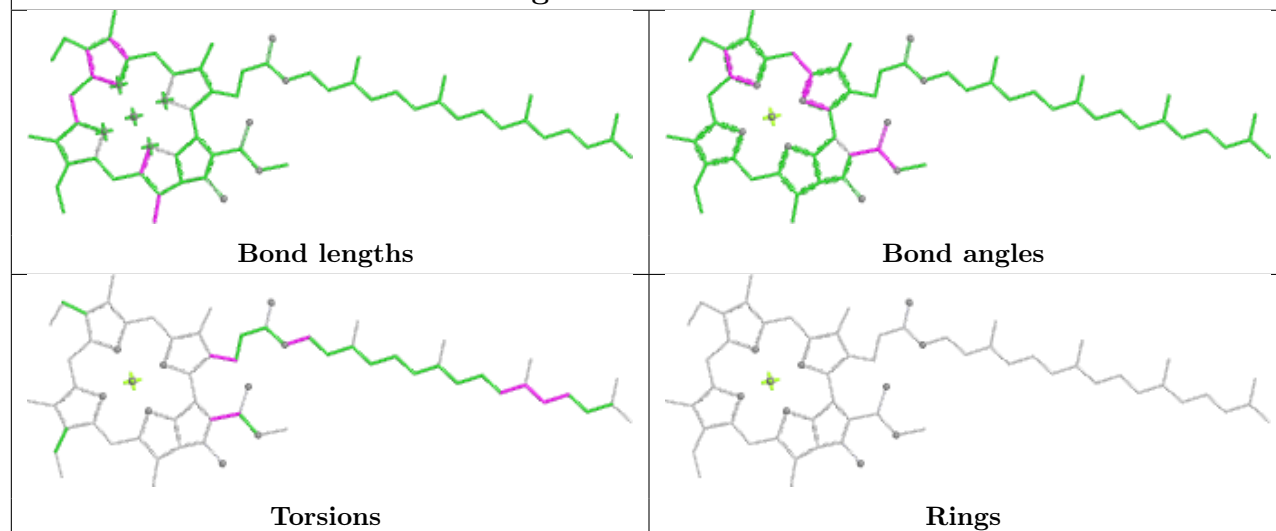


Ligand CHL 6 307	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA 4 612	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR L 205	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

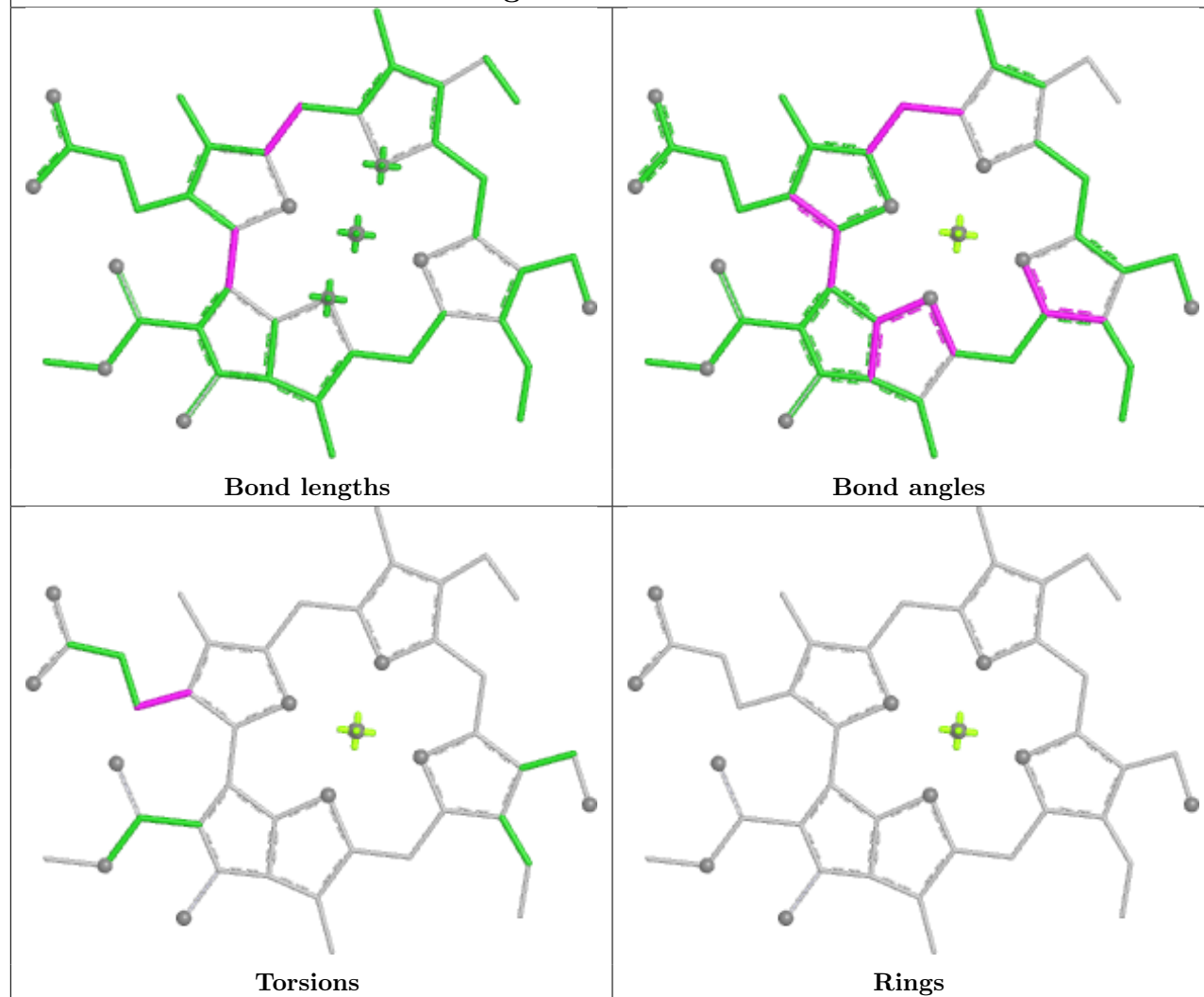
## Ligand CHL 1 306



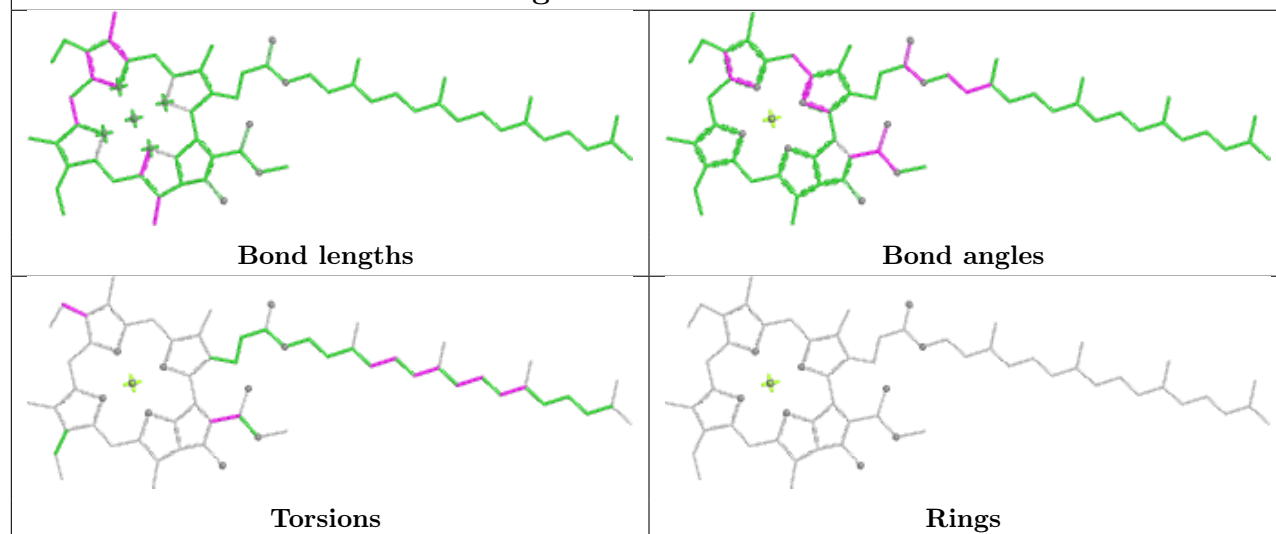
## Ligand CLA A 813

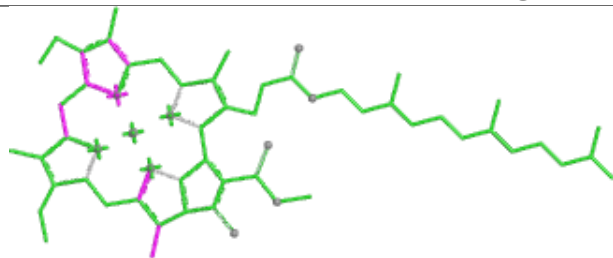
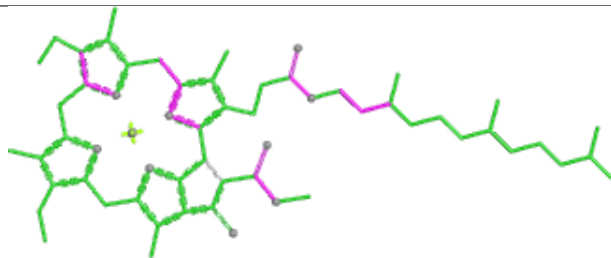
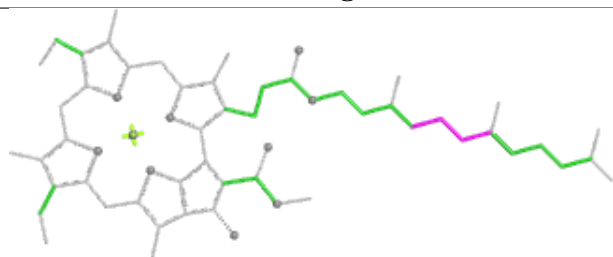
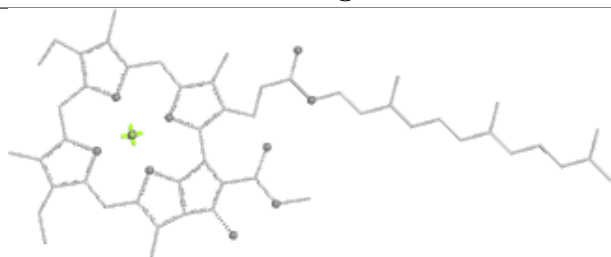
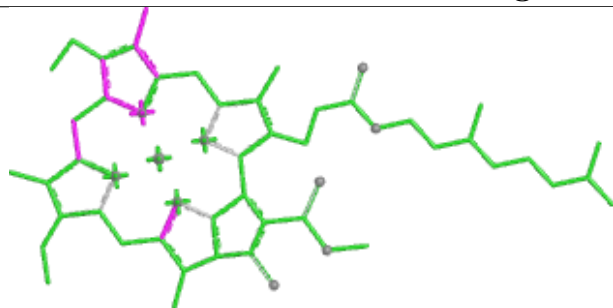
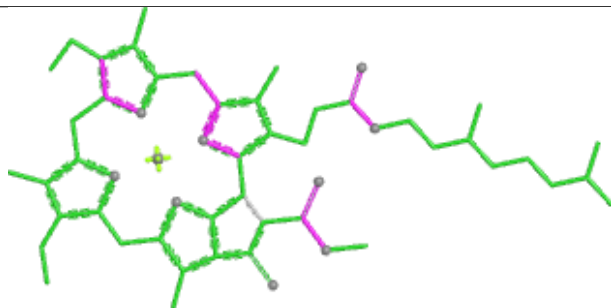
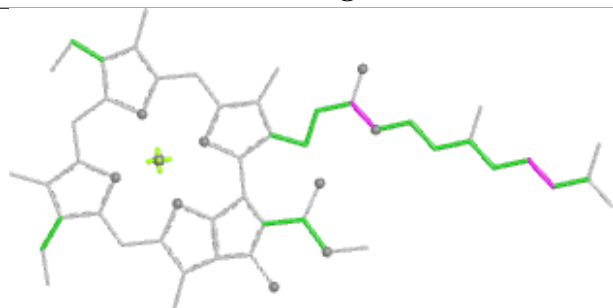
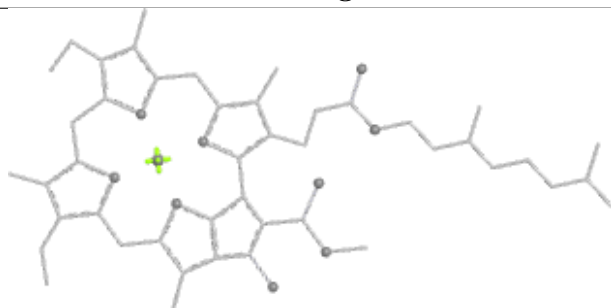


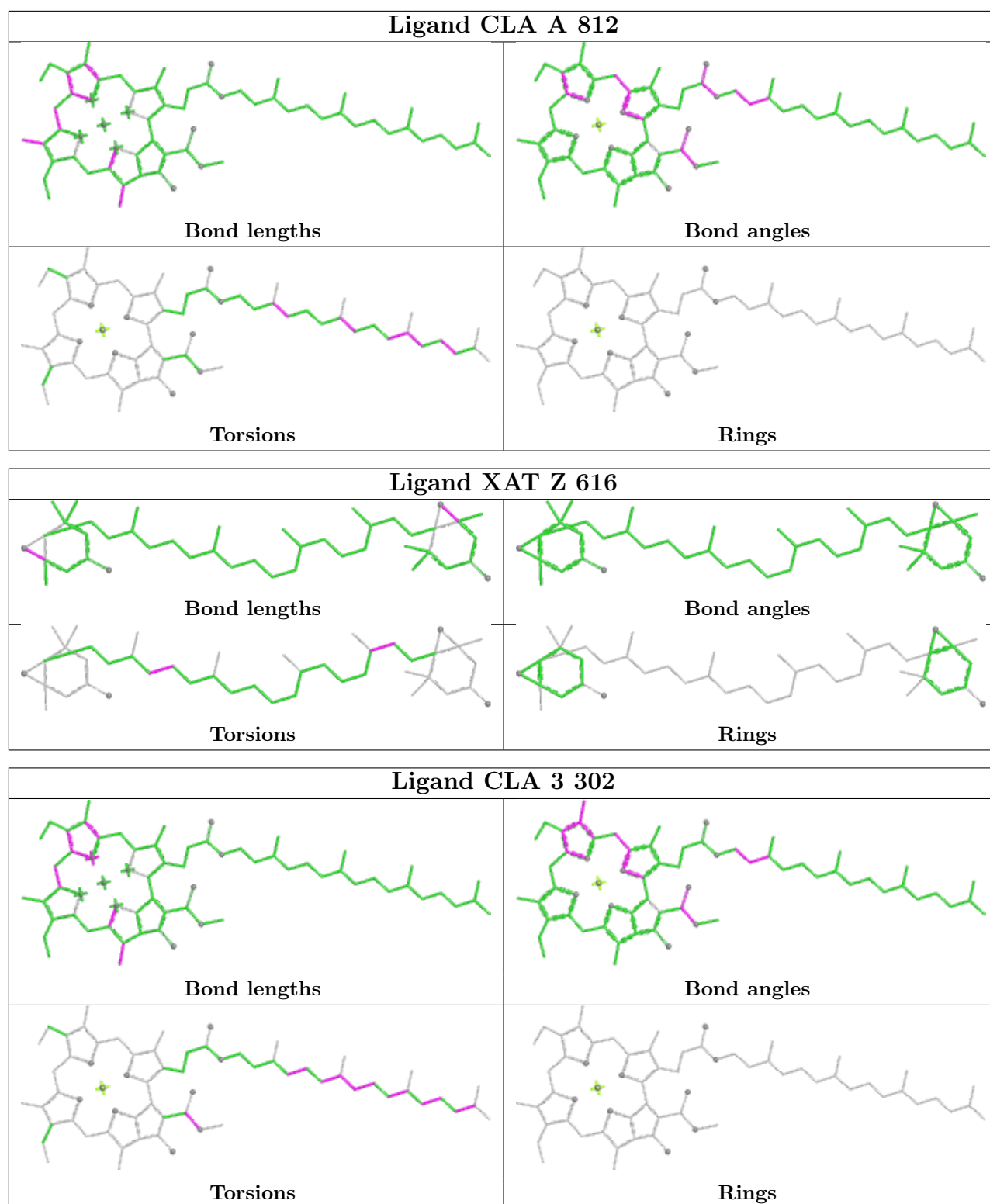
## Ligand CHL Z 605



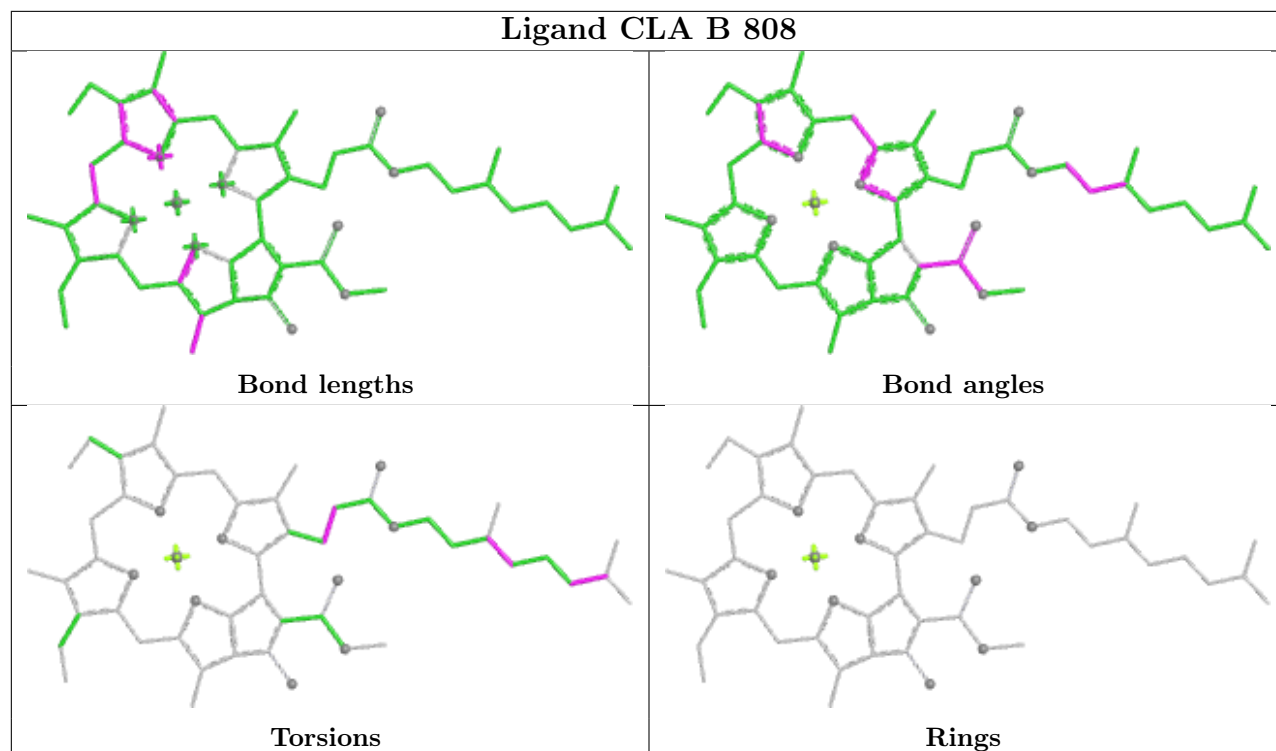
## Ligand CLA B 809



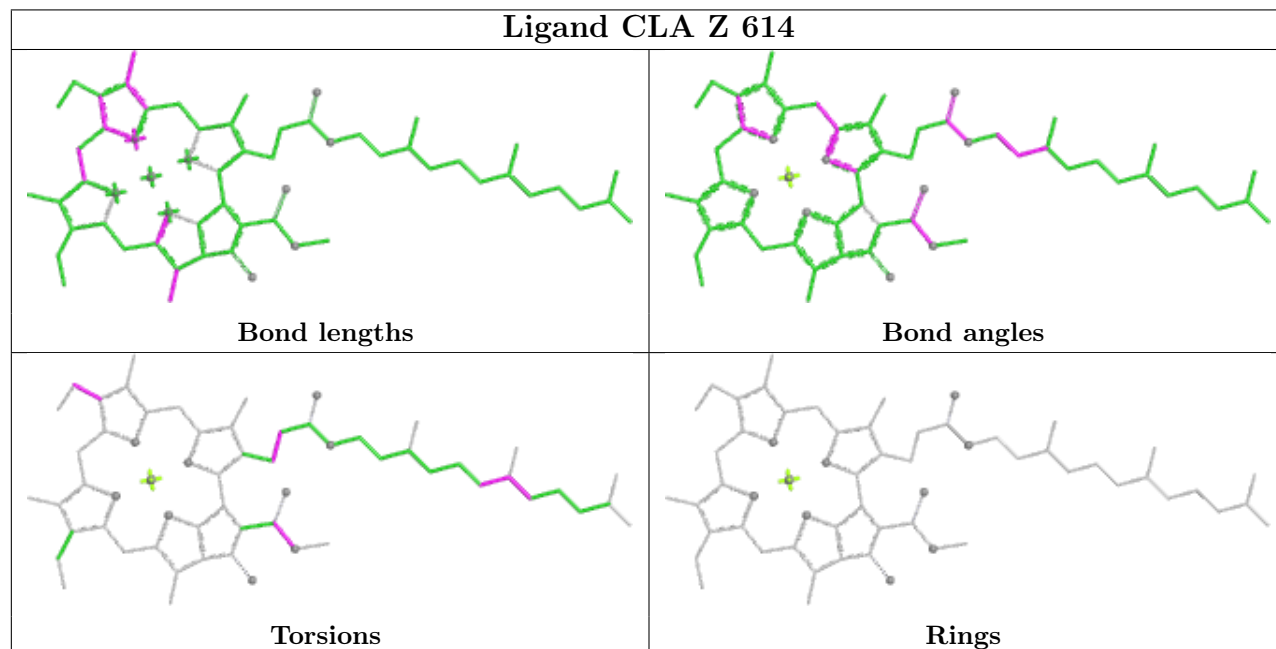
**Ligand CLA B 835****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 816****Bond lengths****Bond angles****Torsions****Rings**

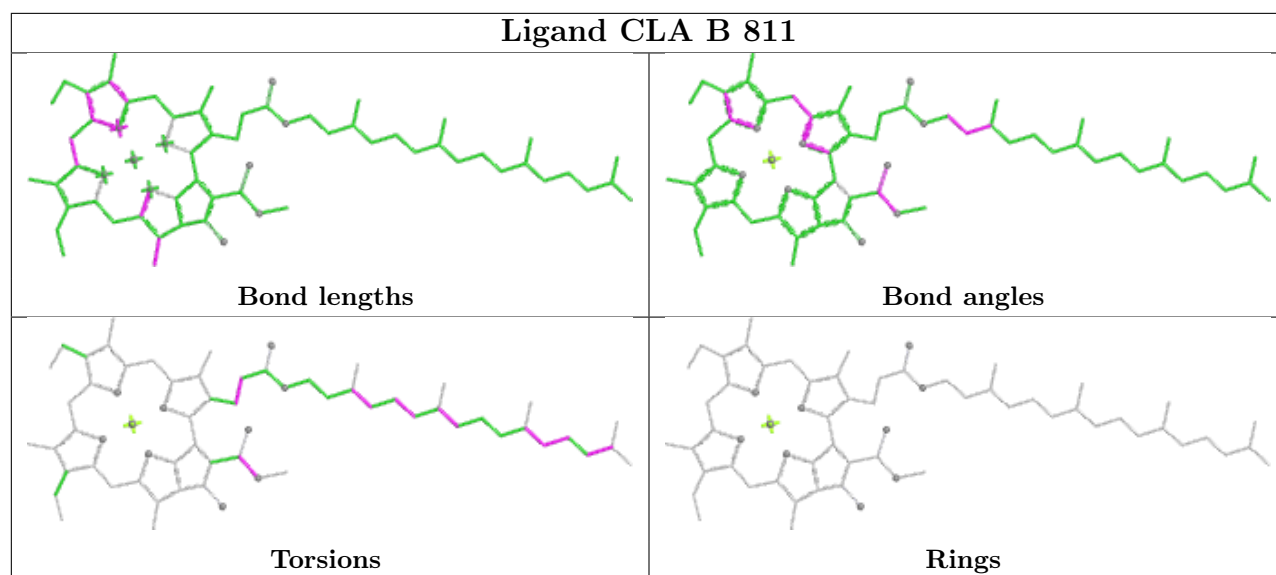
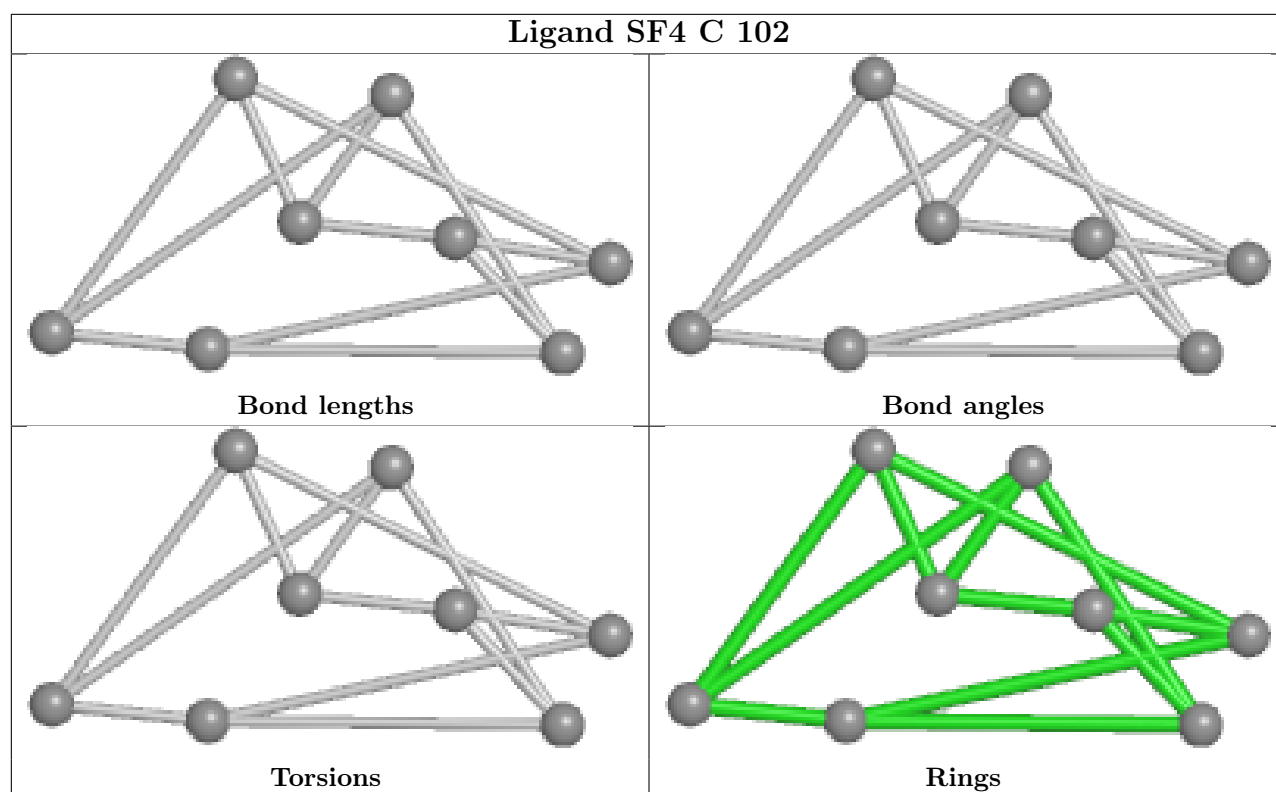


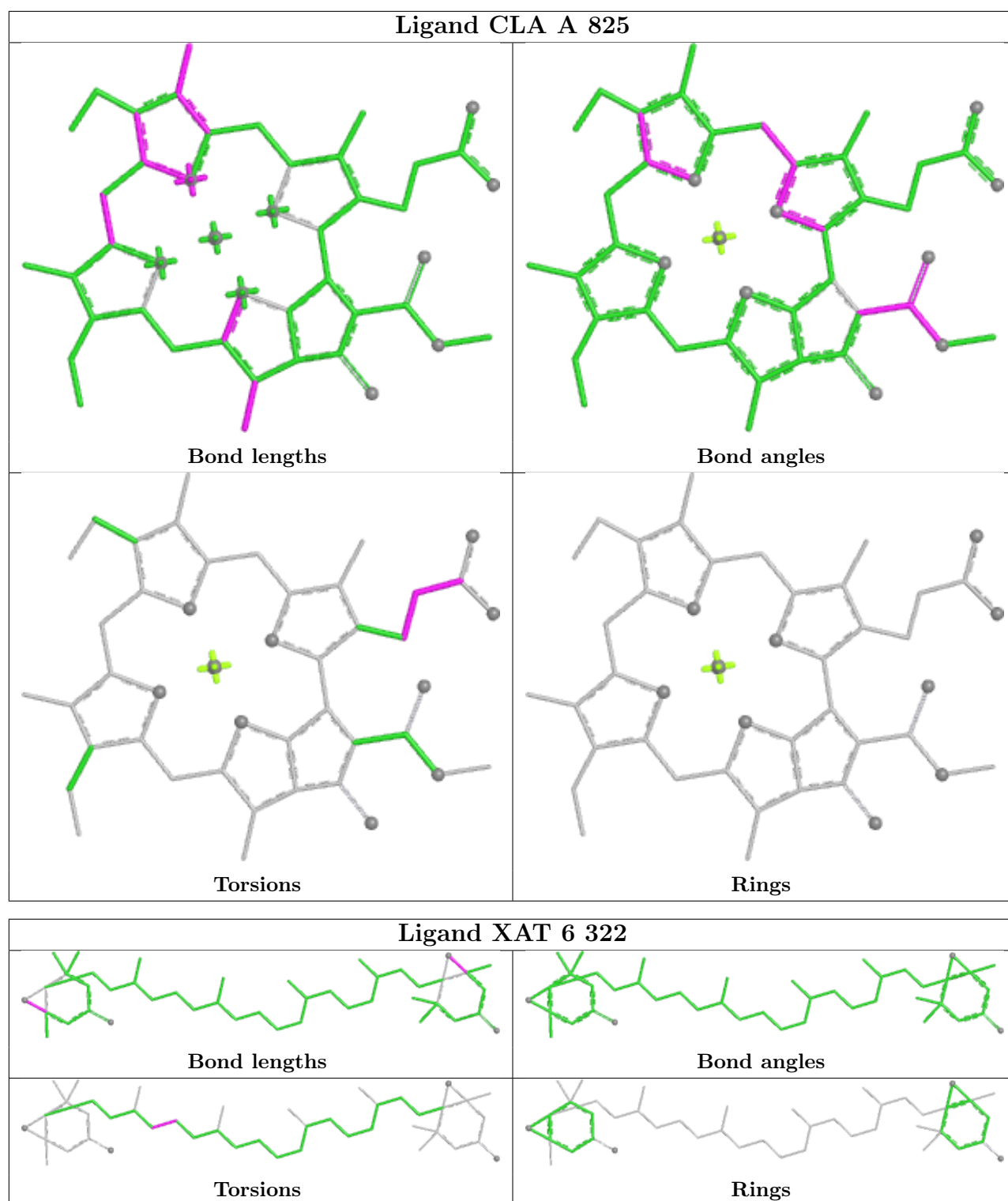
## Ligand CLA B 808



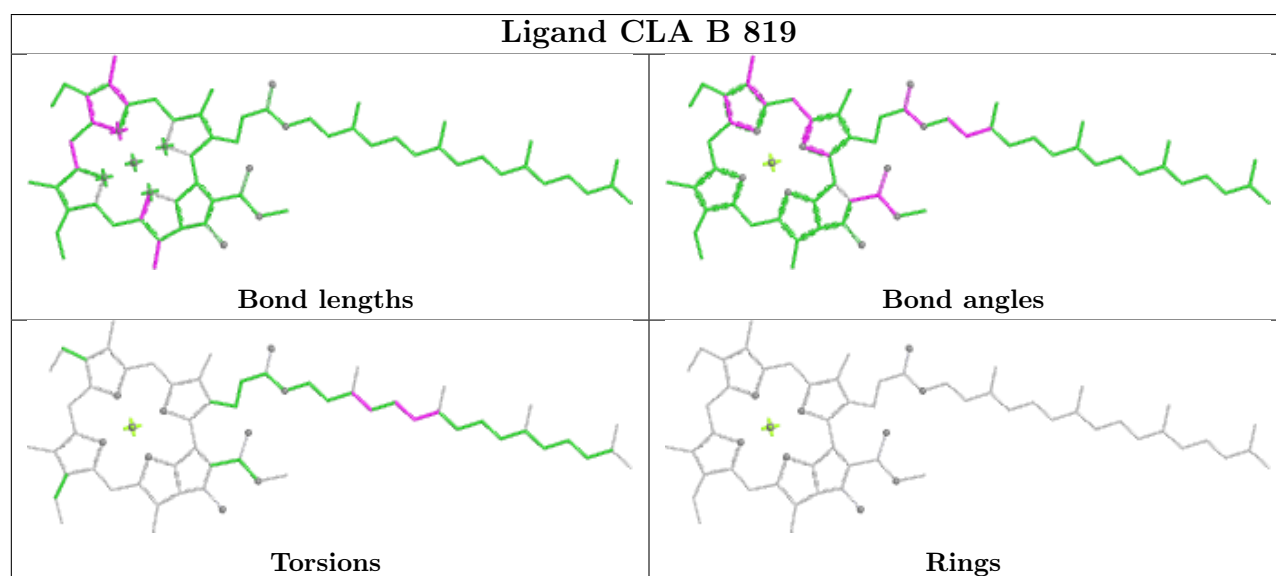
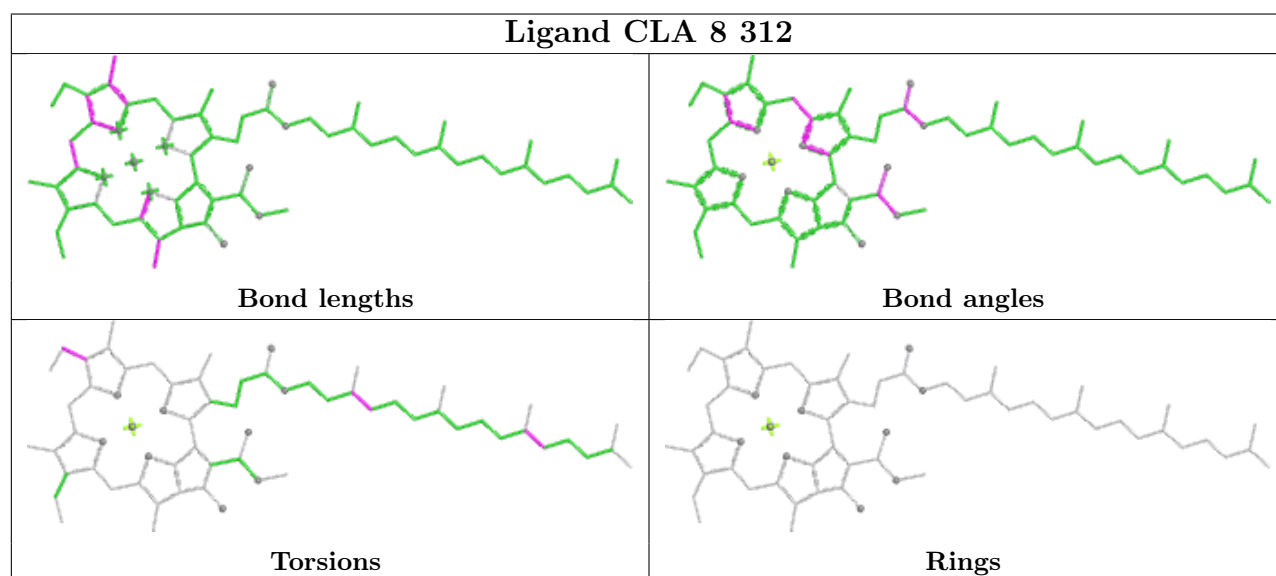
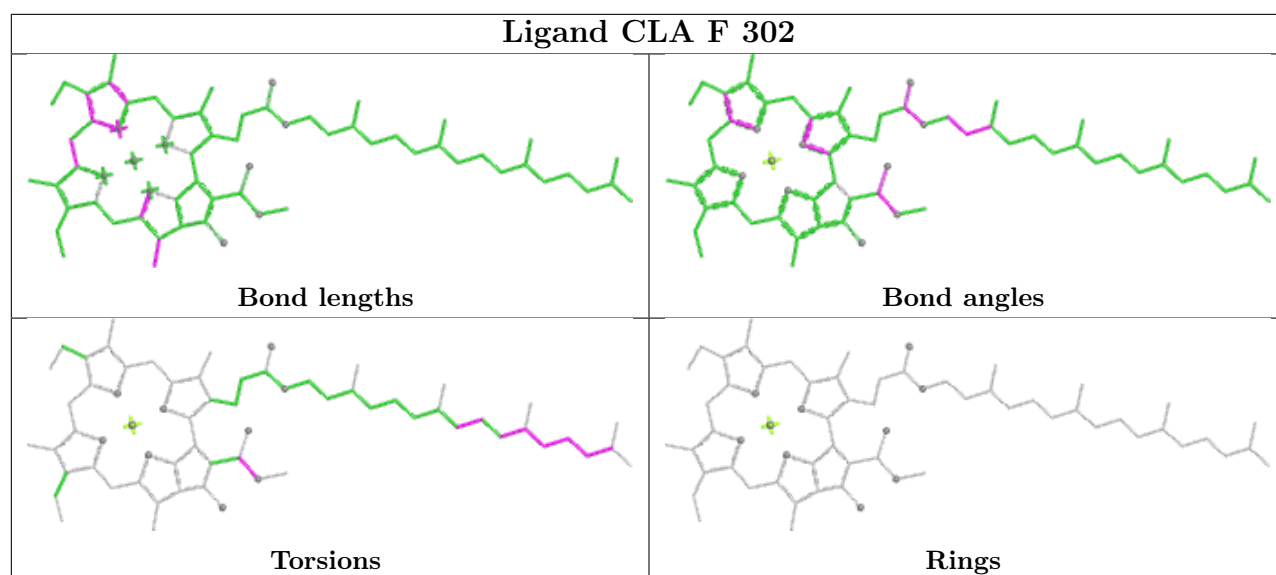
## Ligand CLA Z 614



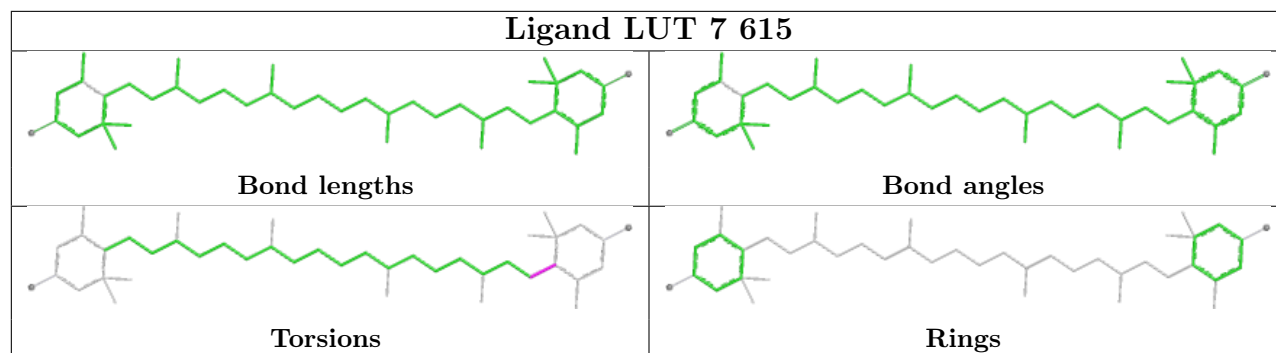




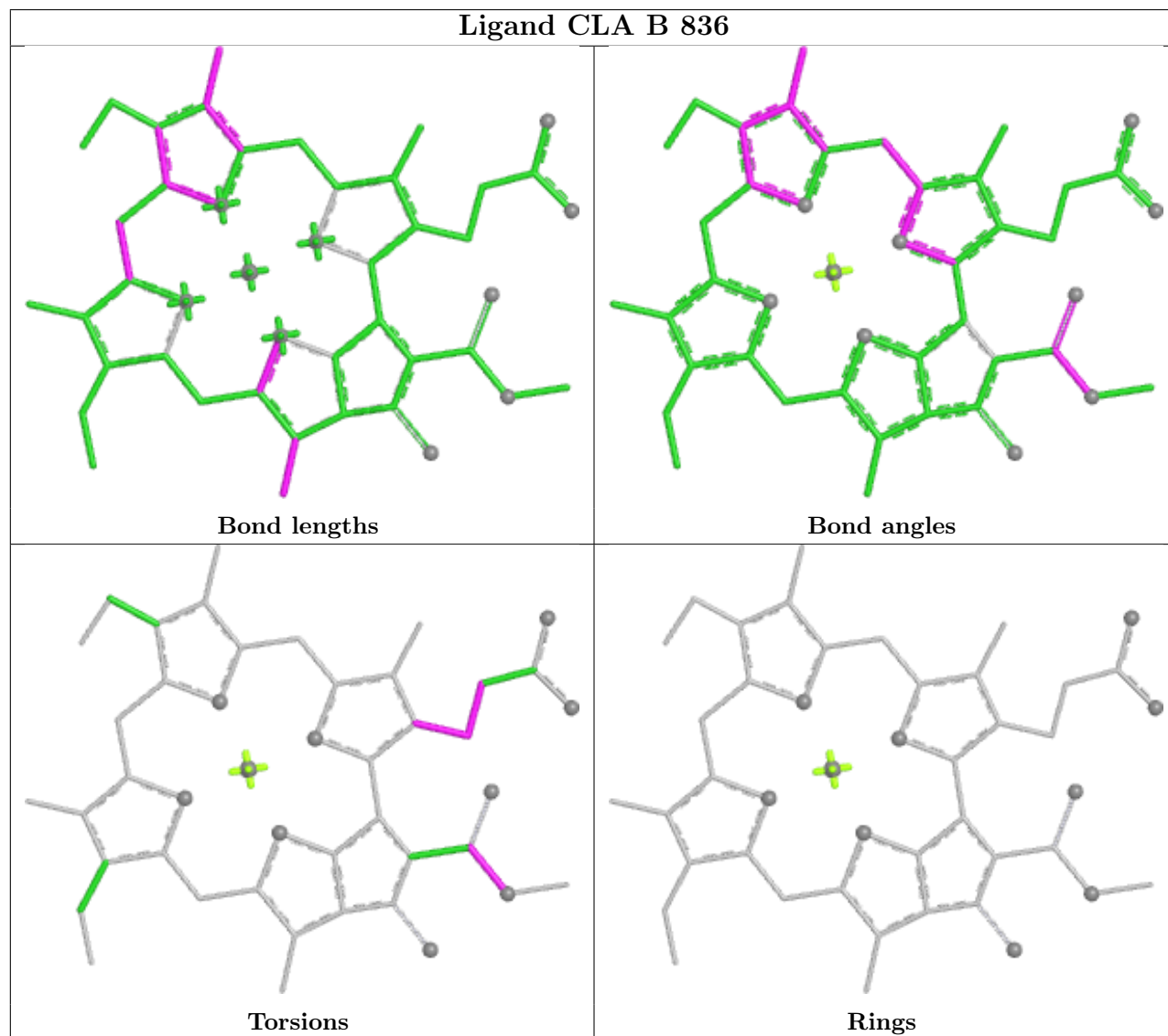


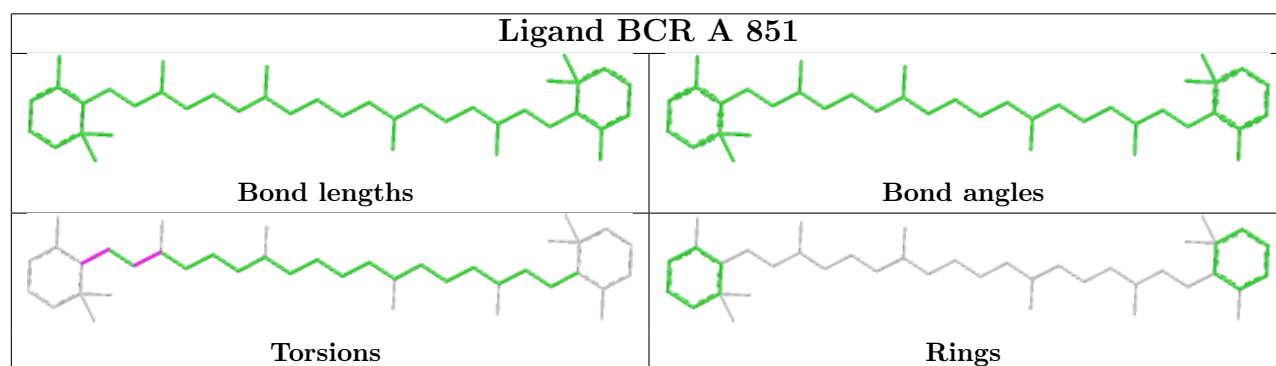
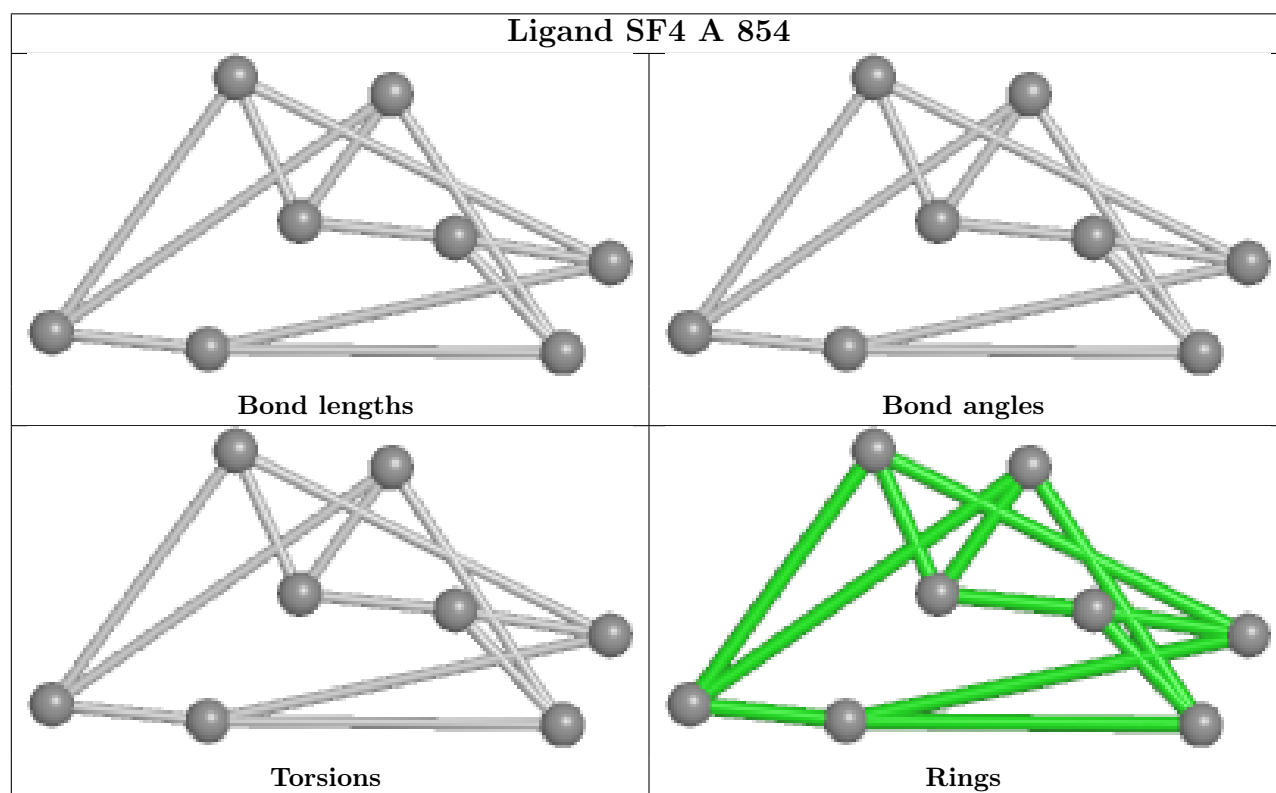
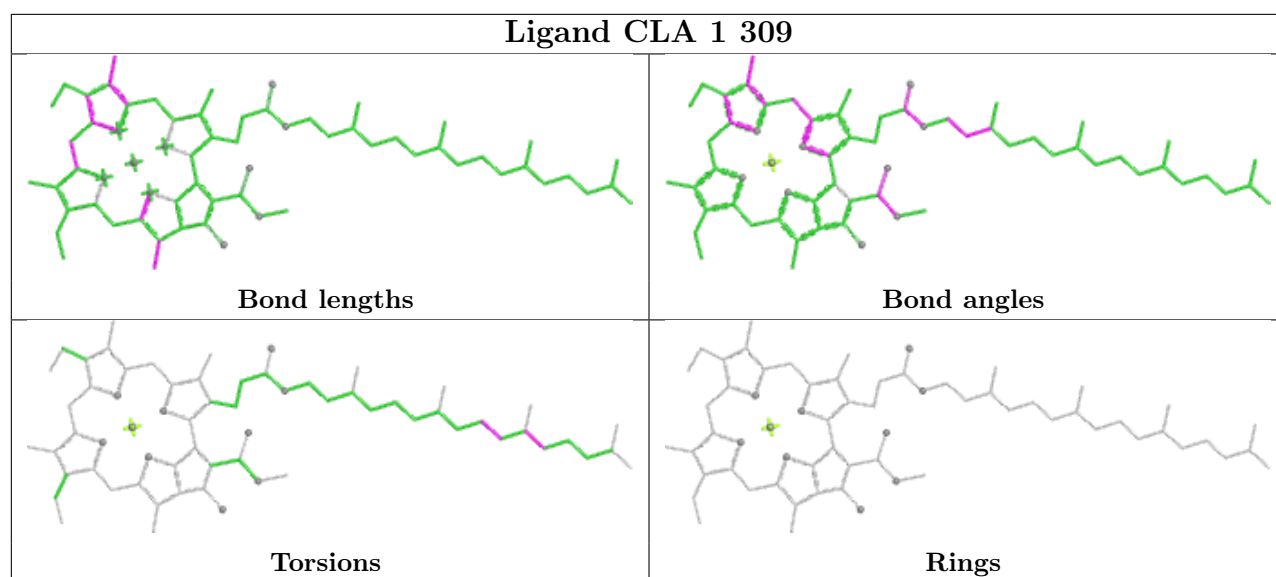


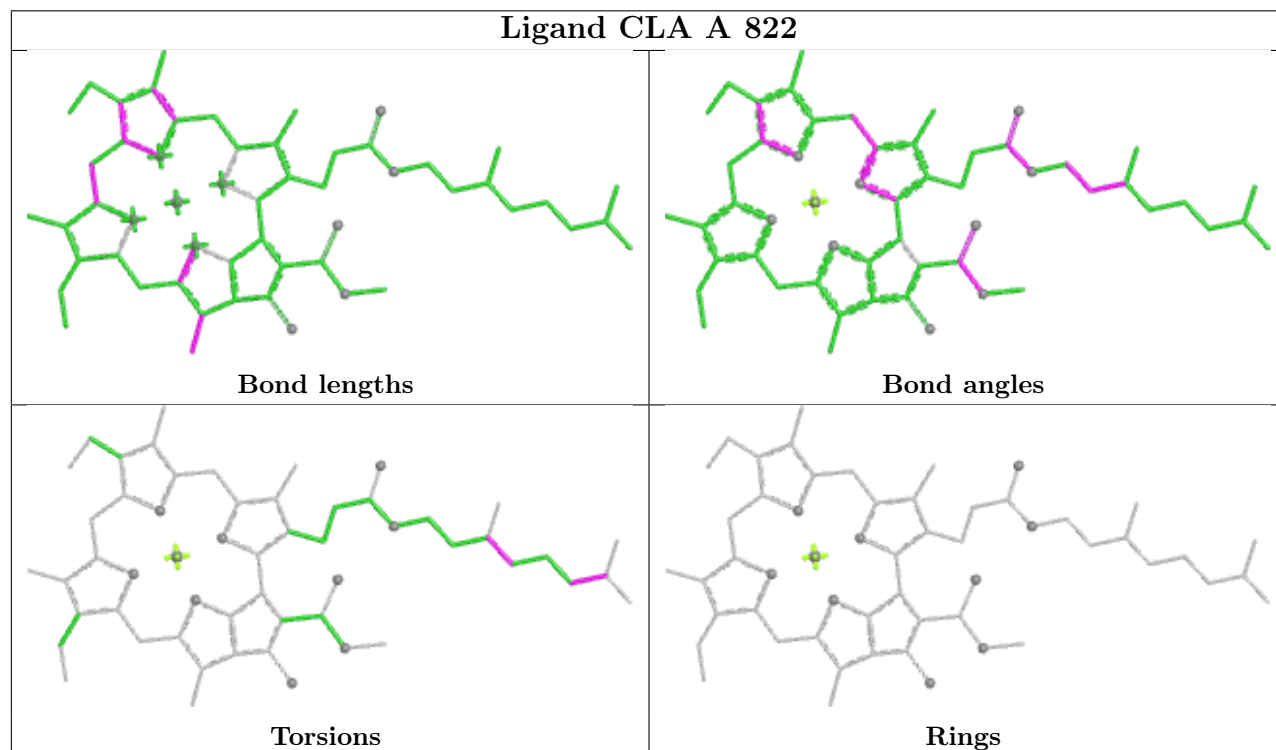
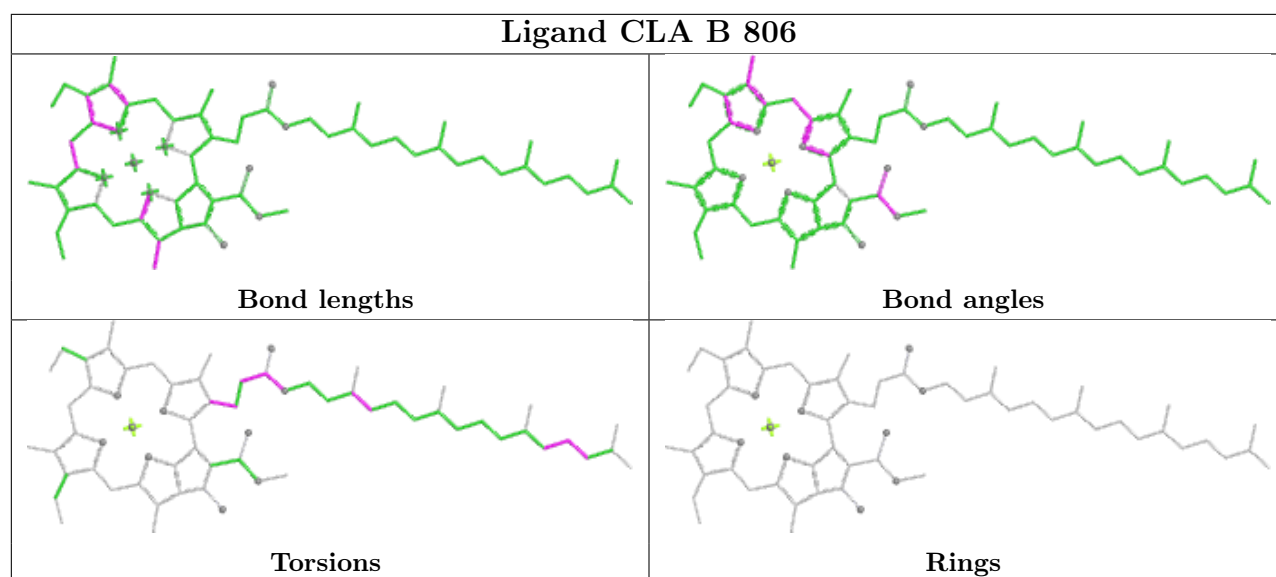
## Ligand LUT 7 615



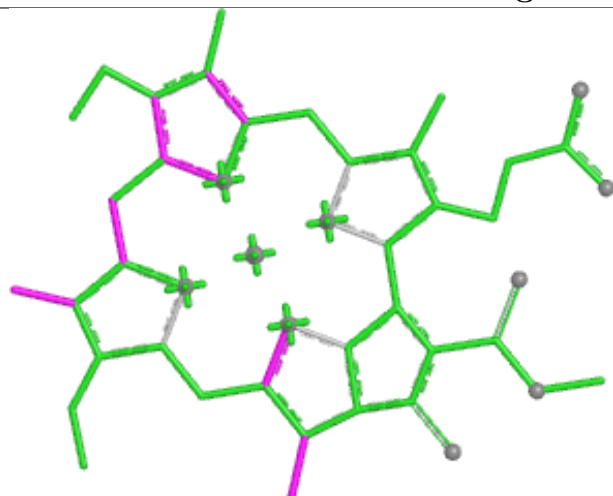
## Ligand CLA B 836



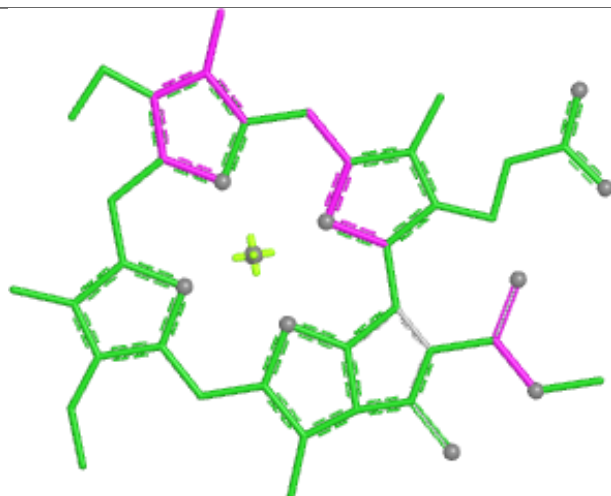




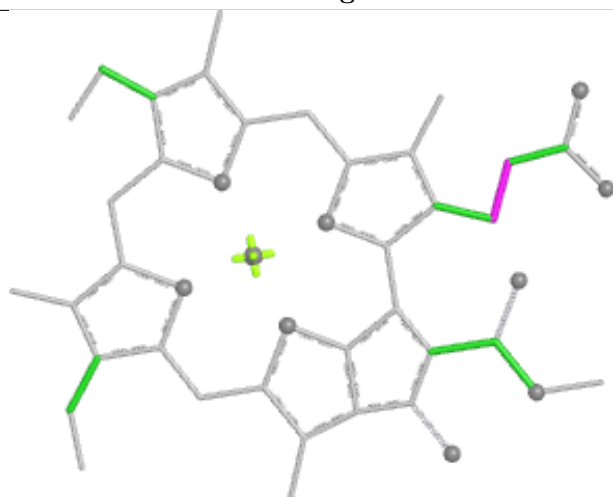
## Ligand CLA F 303



Bond lengths



Bond angles

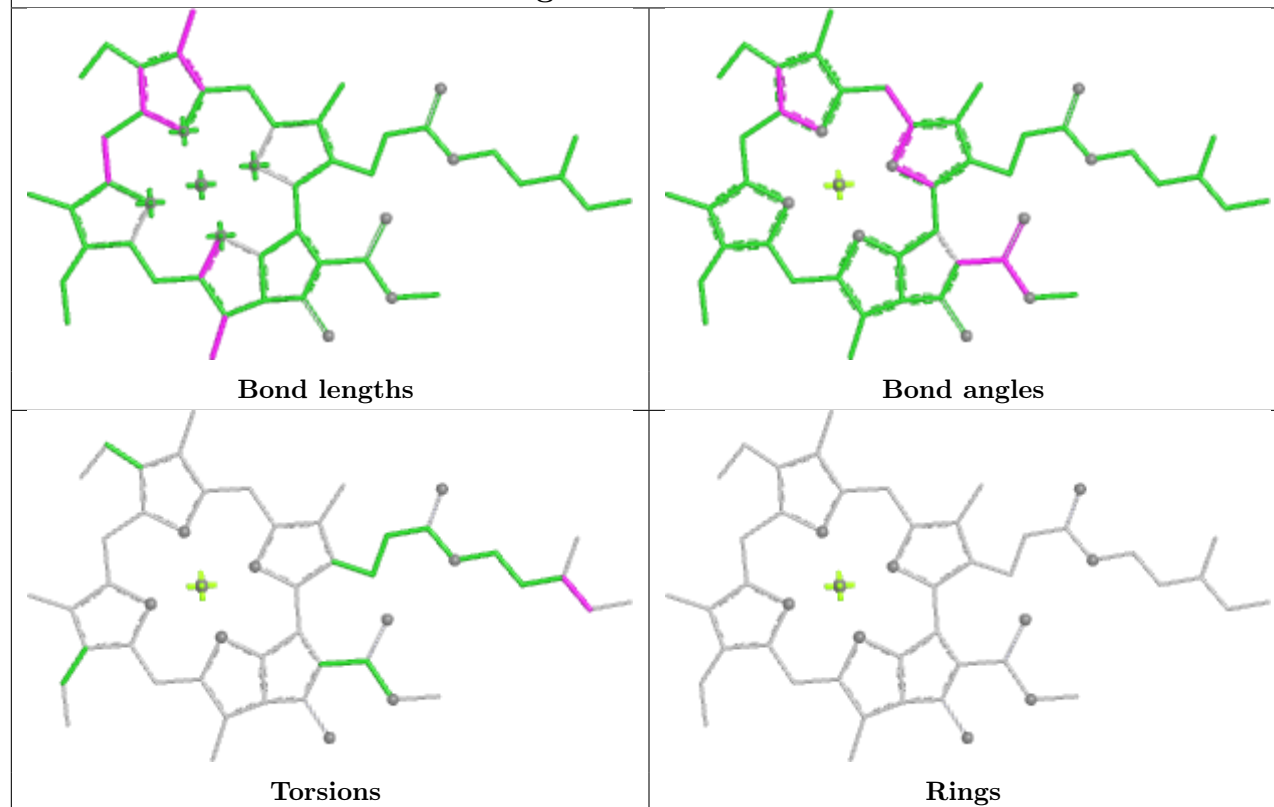


Torsions

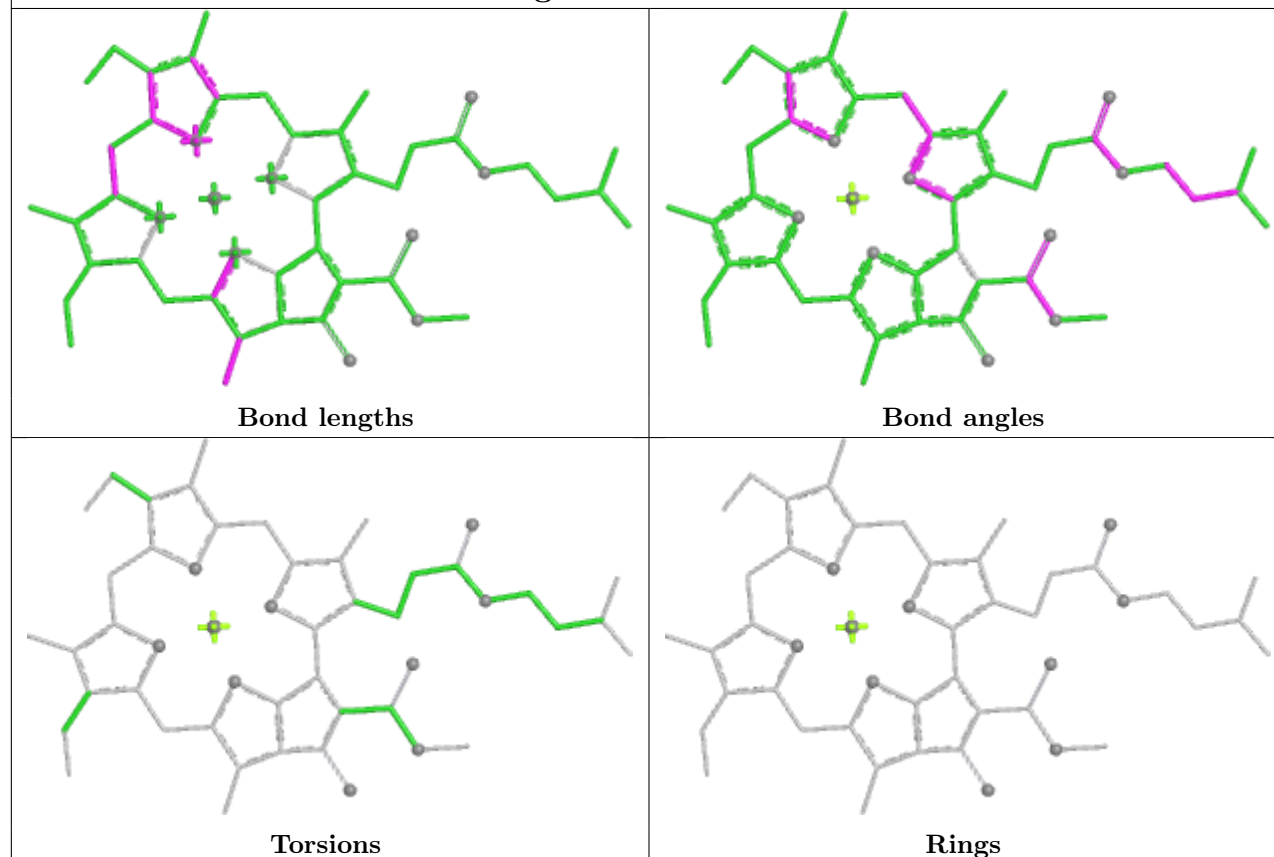


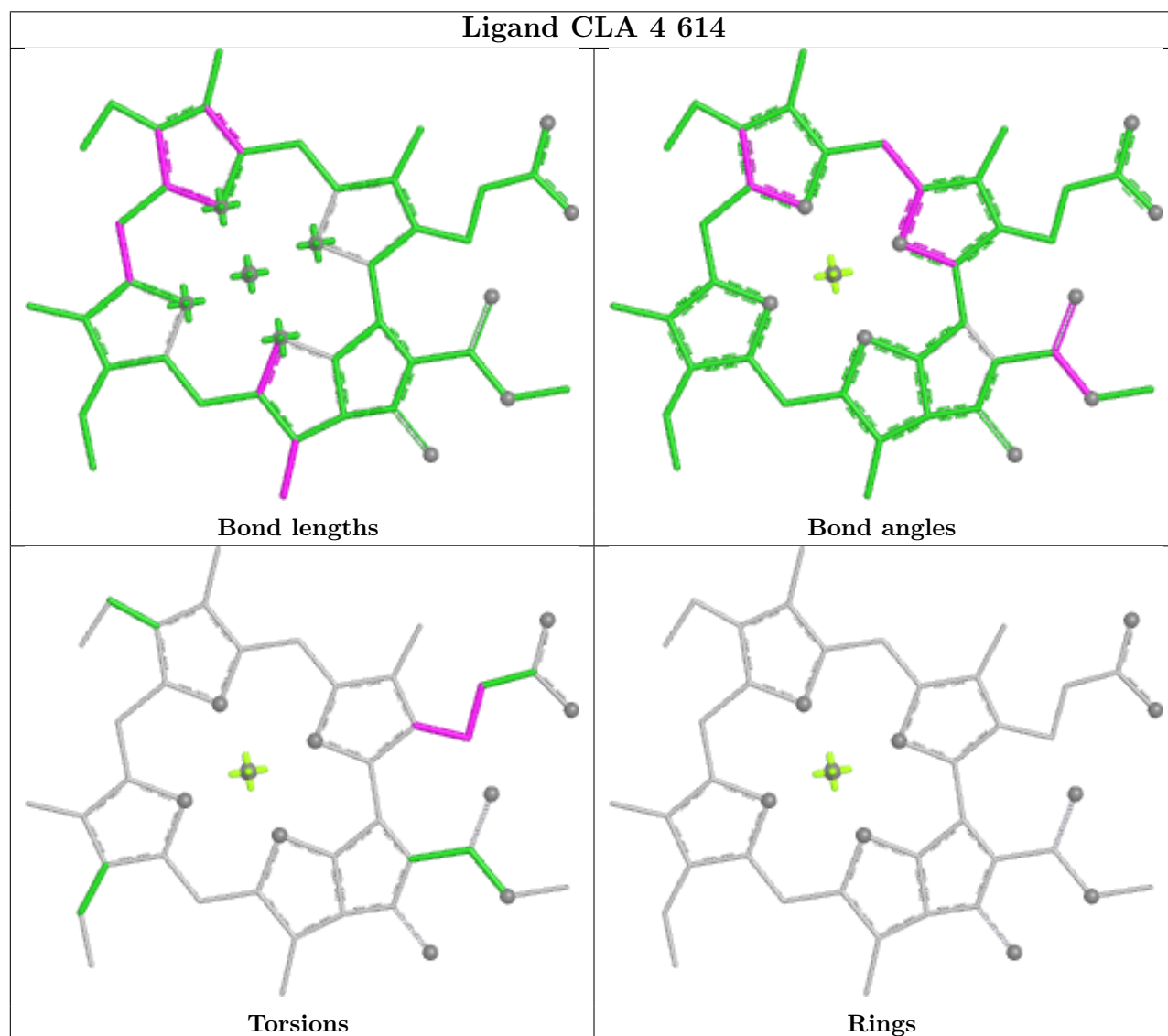
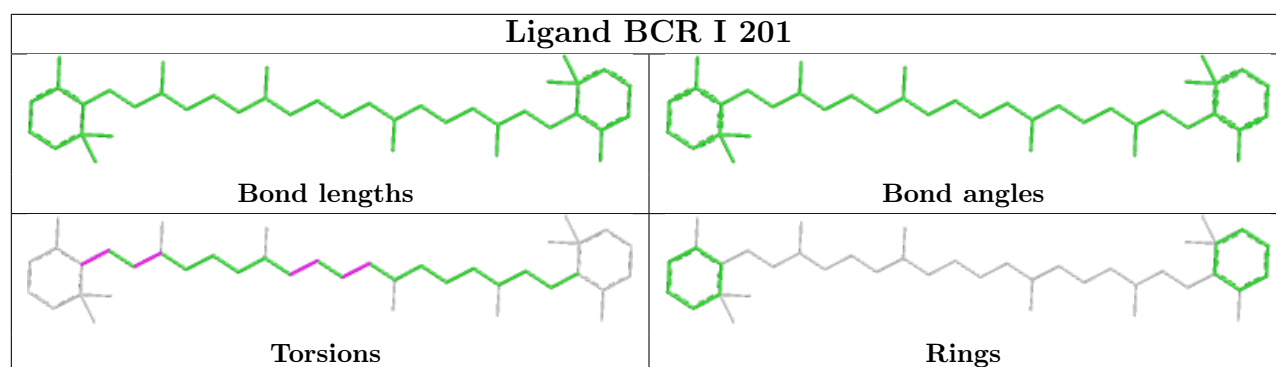
Rings

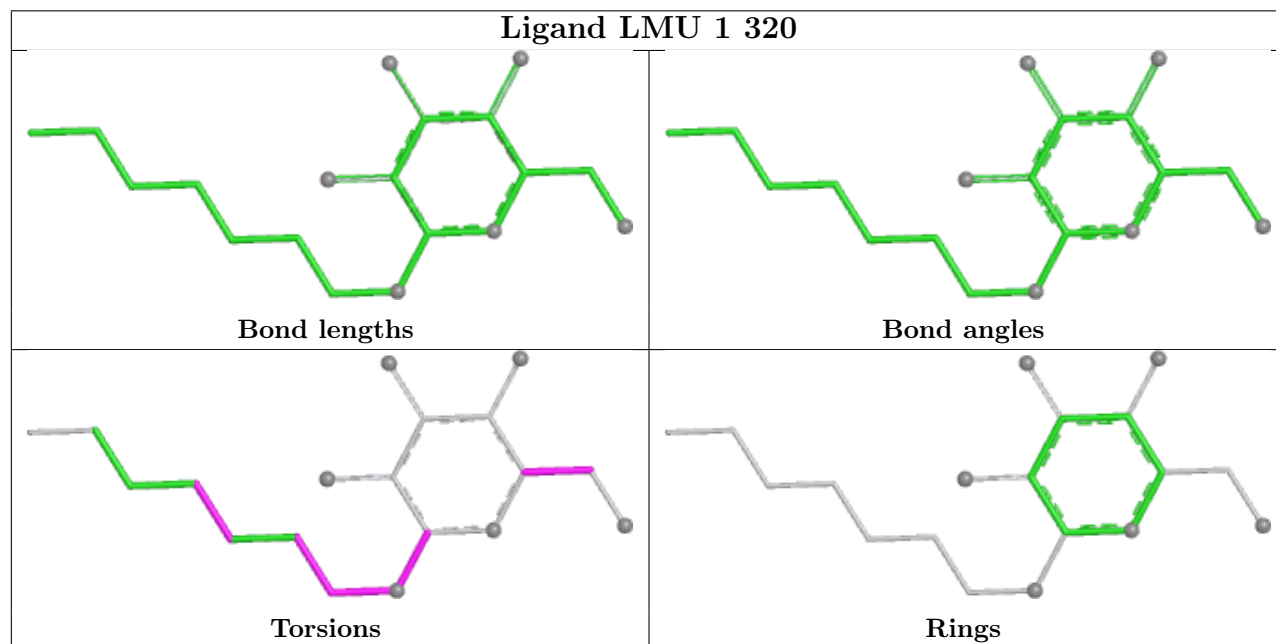
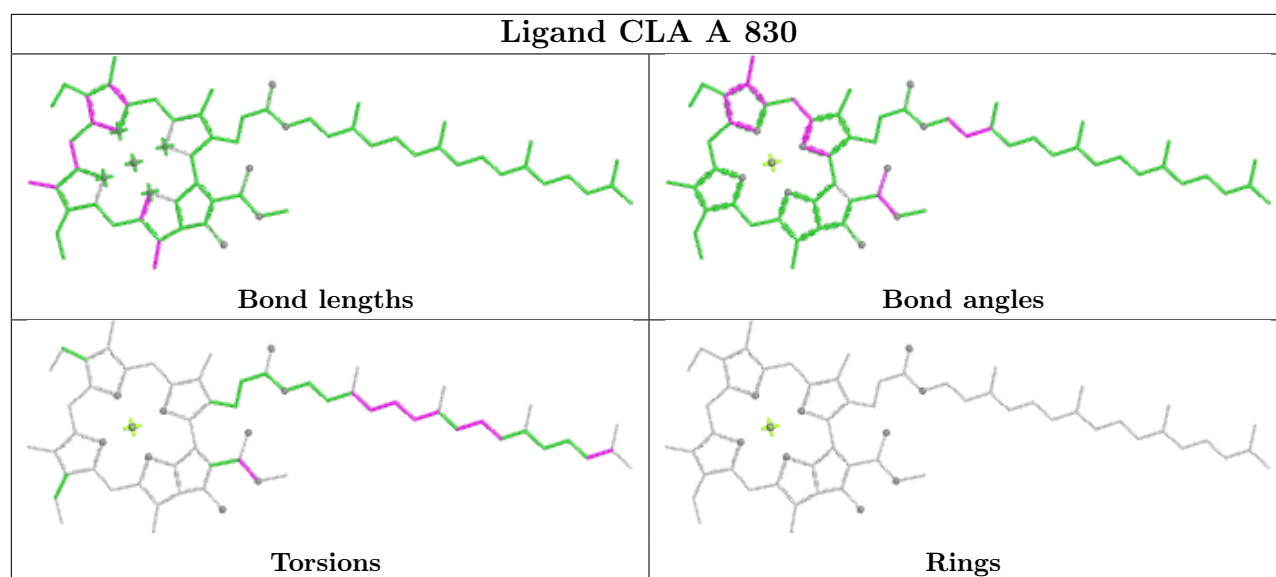
## Ligand CLA 3 305



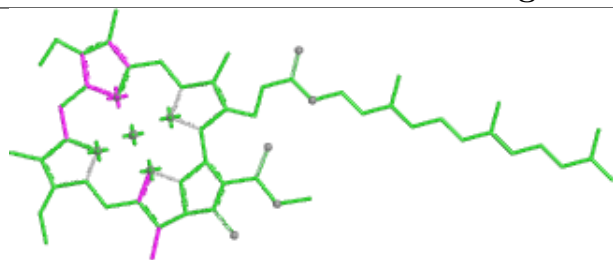
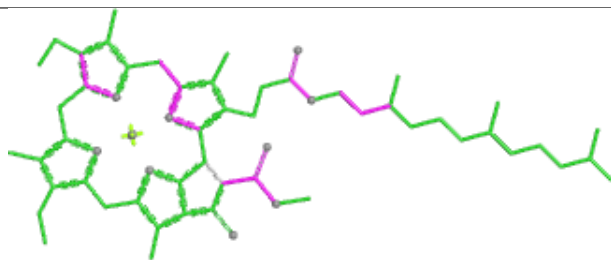
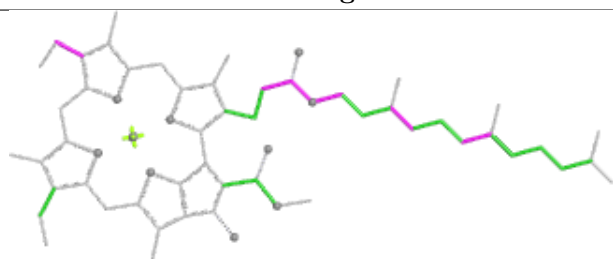
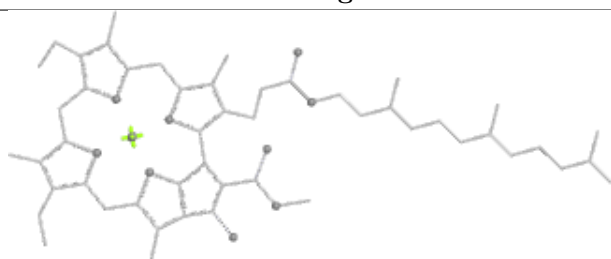
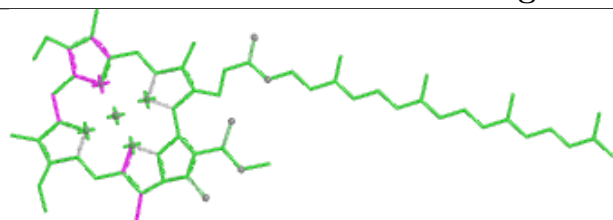
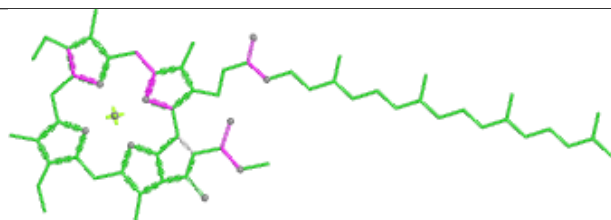
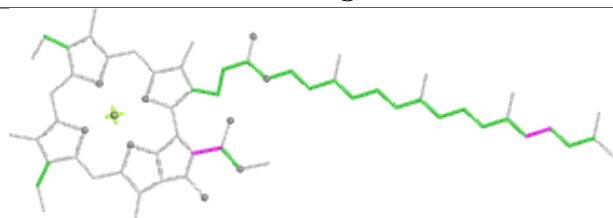
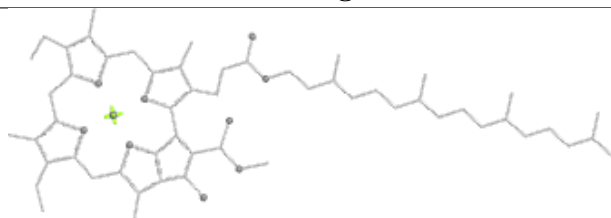
## Ligand CLA Z 613

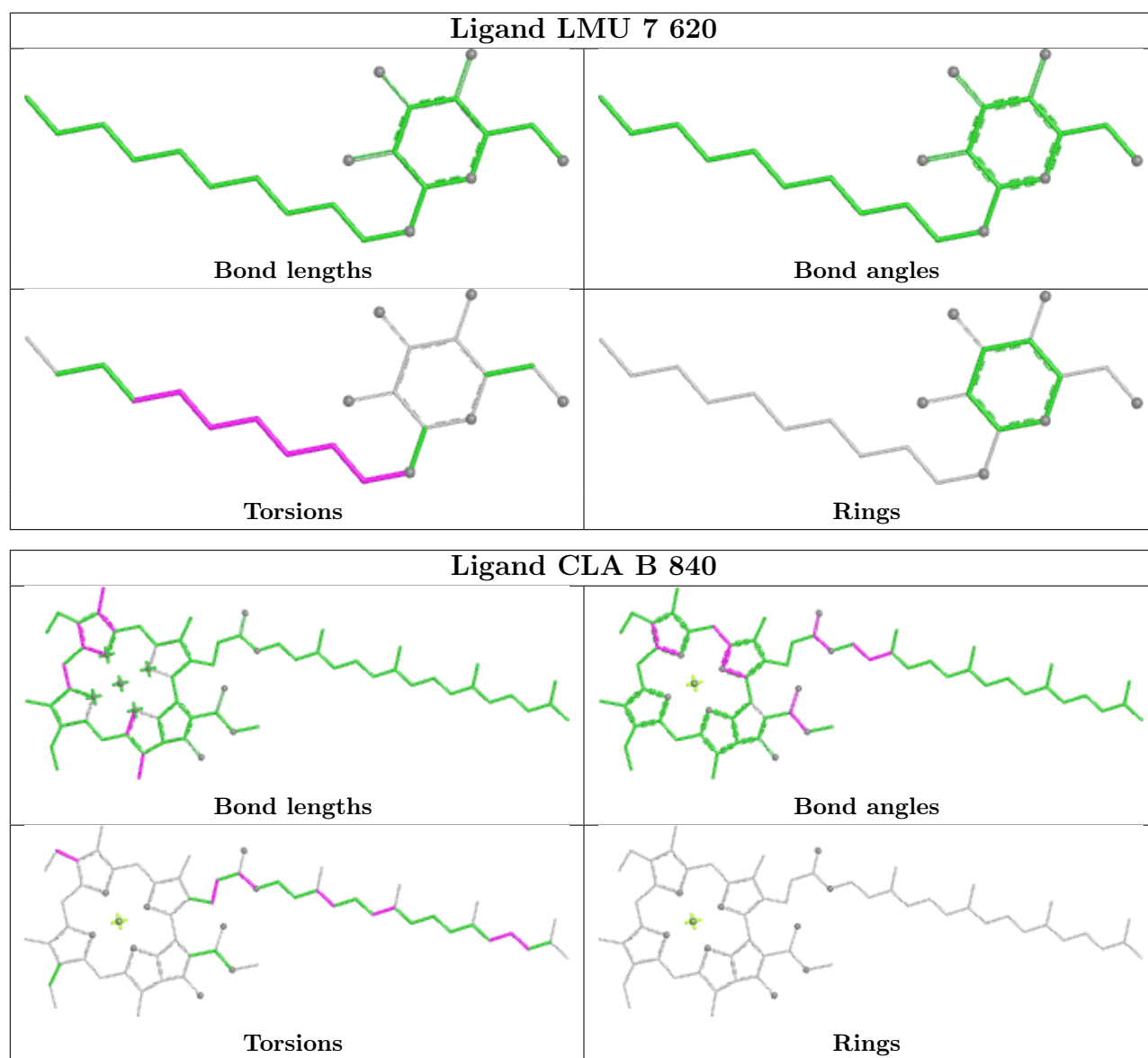


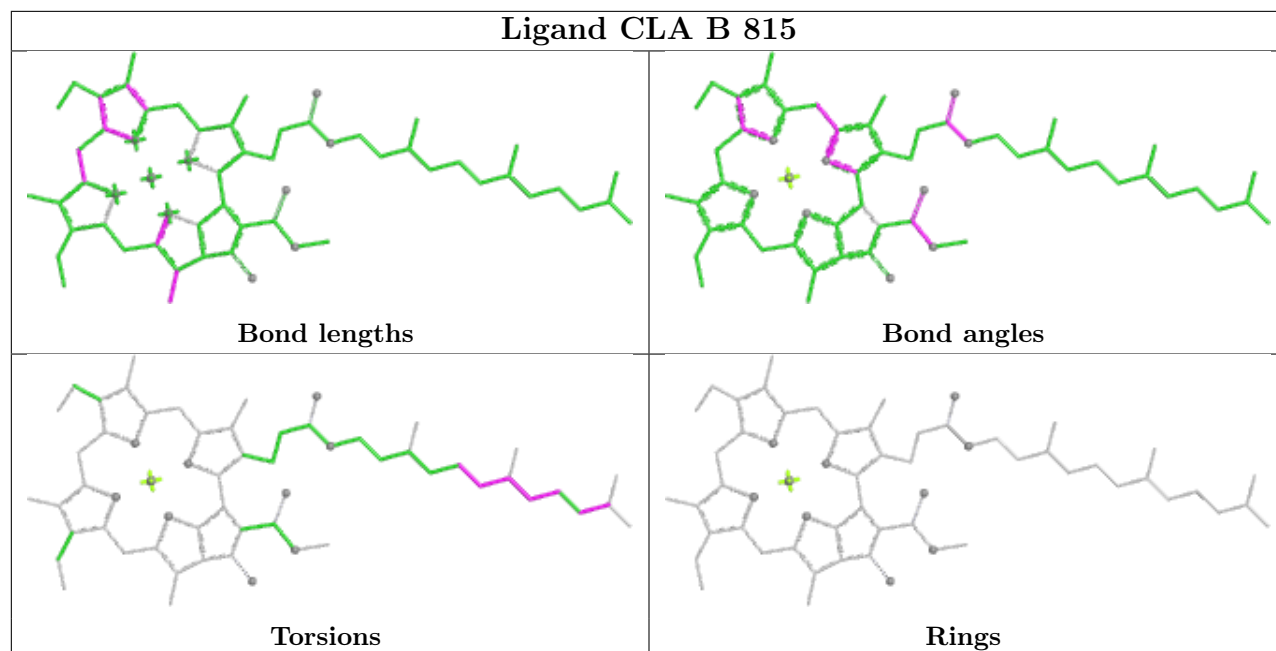
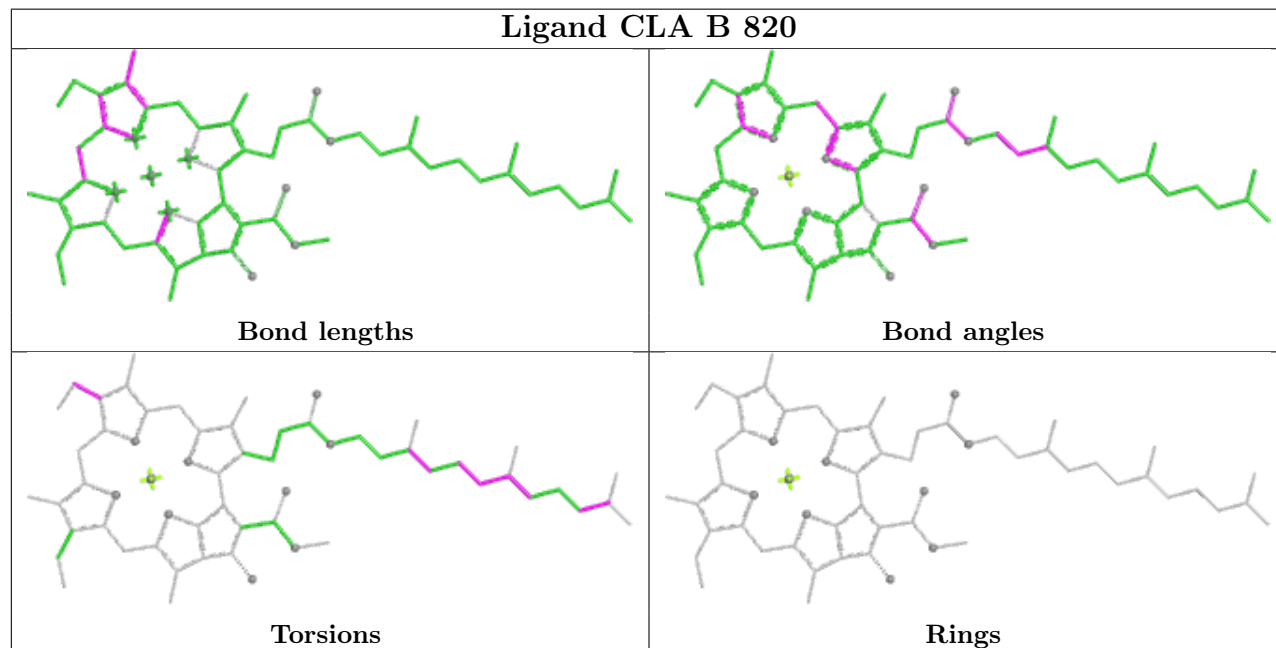


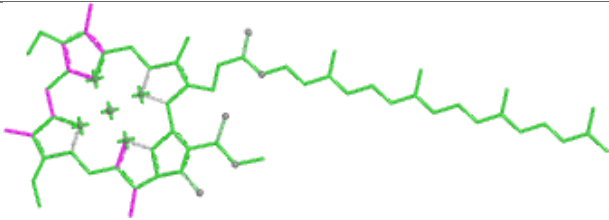
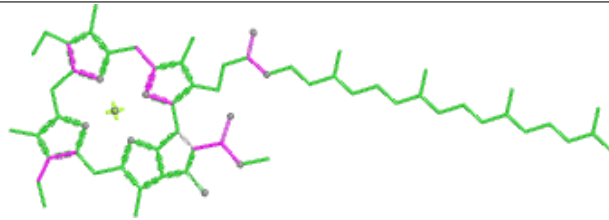
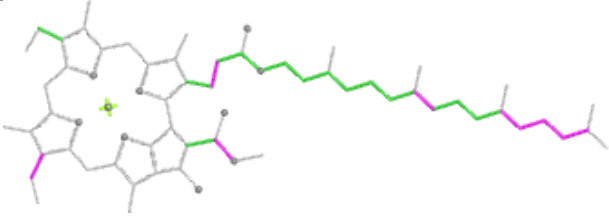
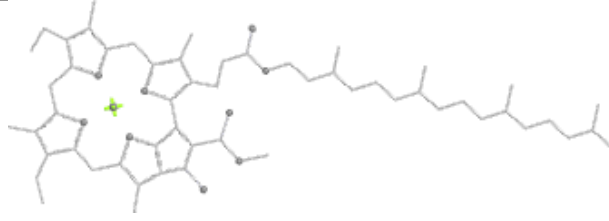


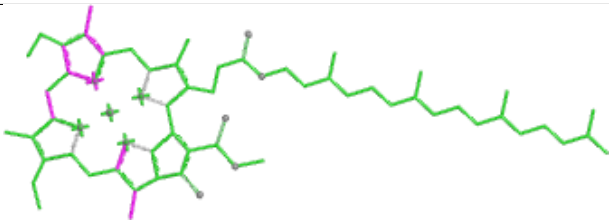
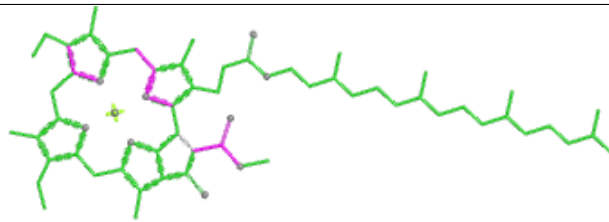
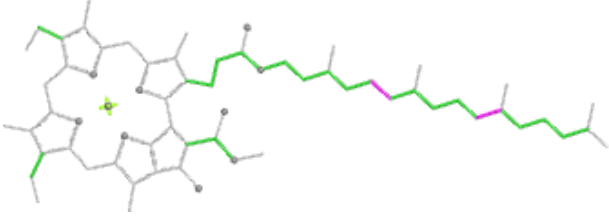
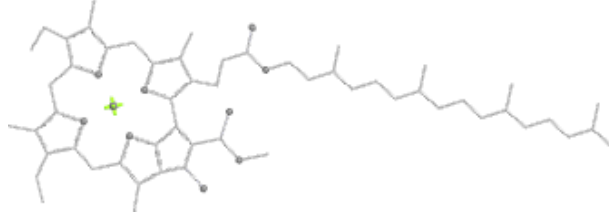


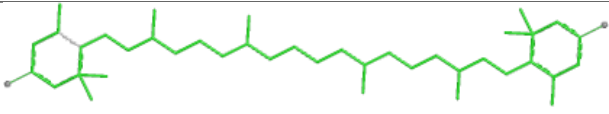
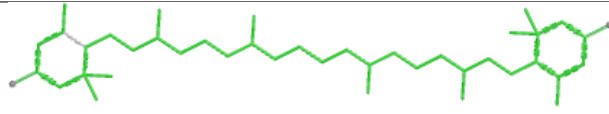
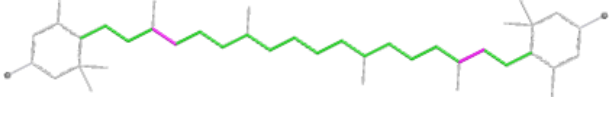
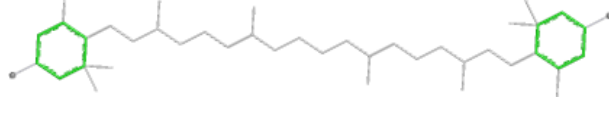
**Ligand CLA 1 313****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 7 602****Bond lengths****Bond angles****Torsions****Rings**

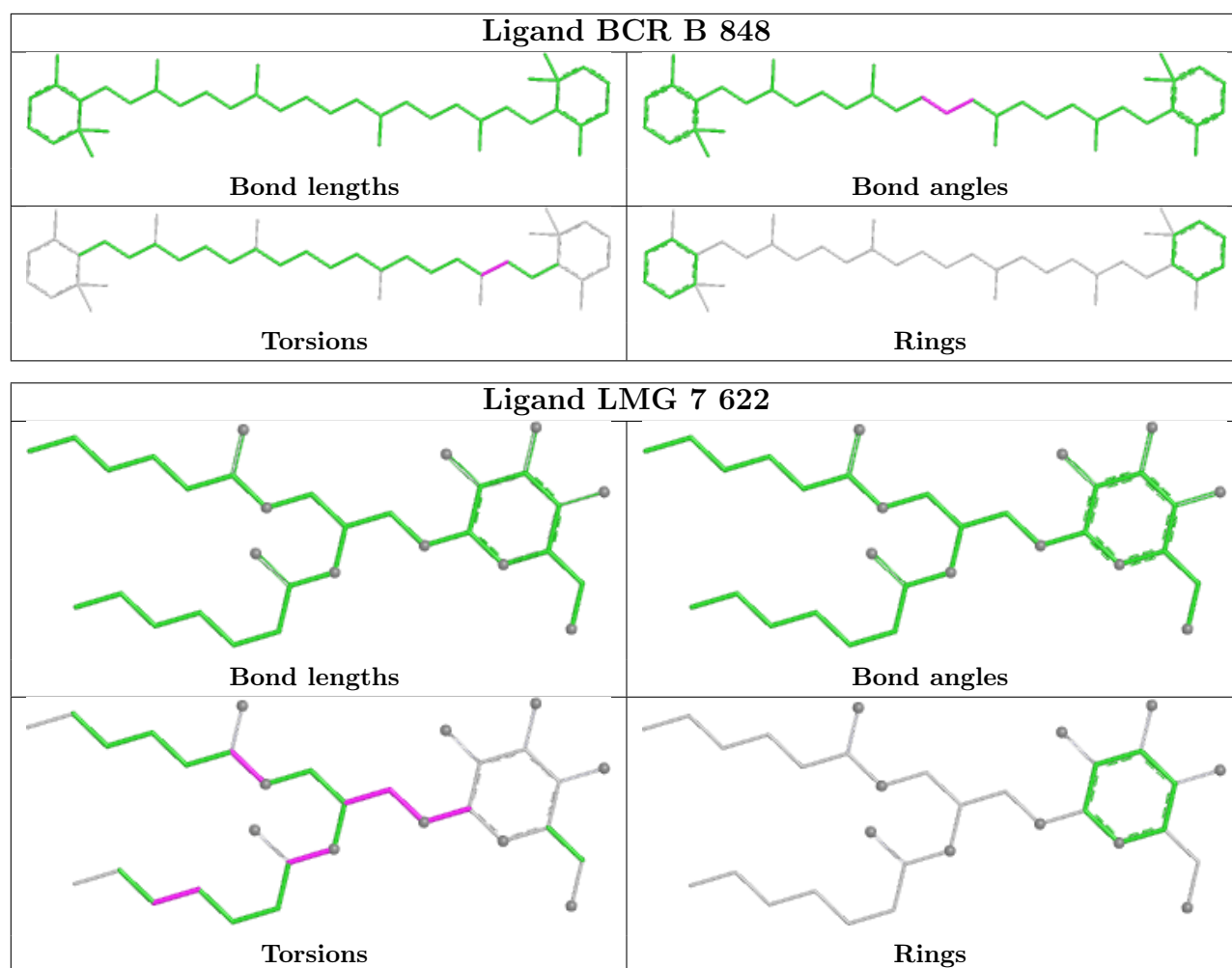


**Ligand CLA B 815****Ligand CLA B 820**

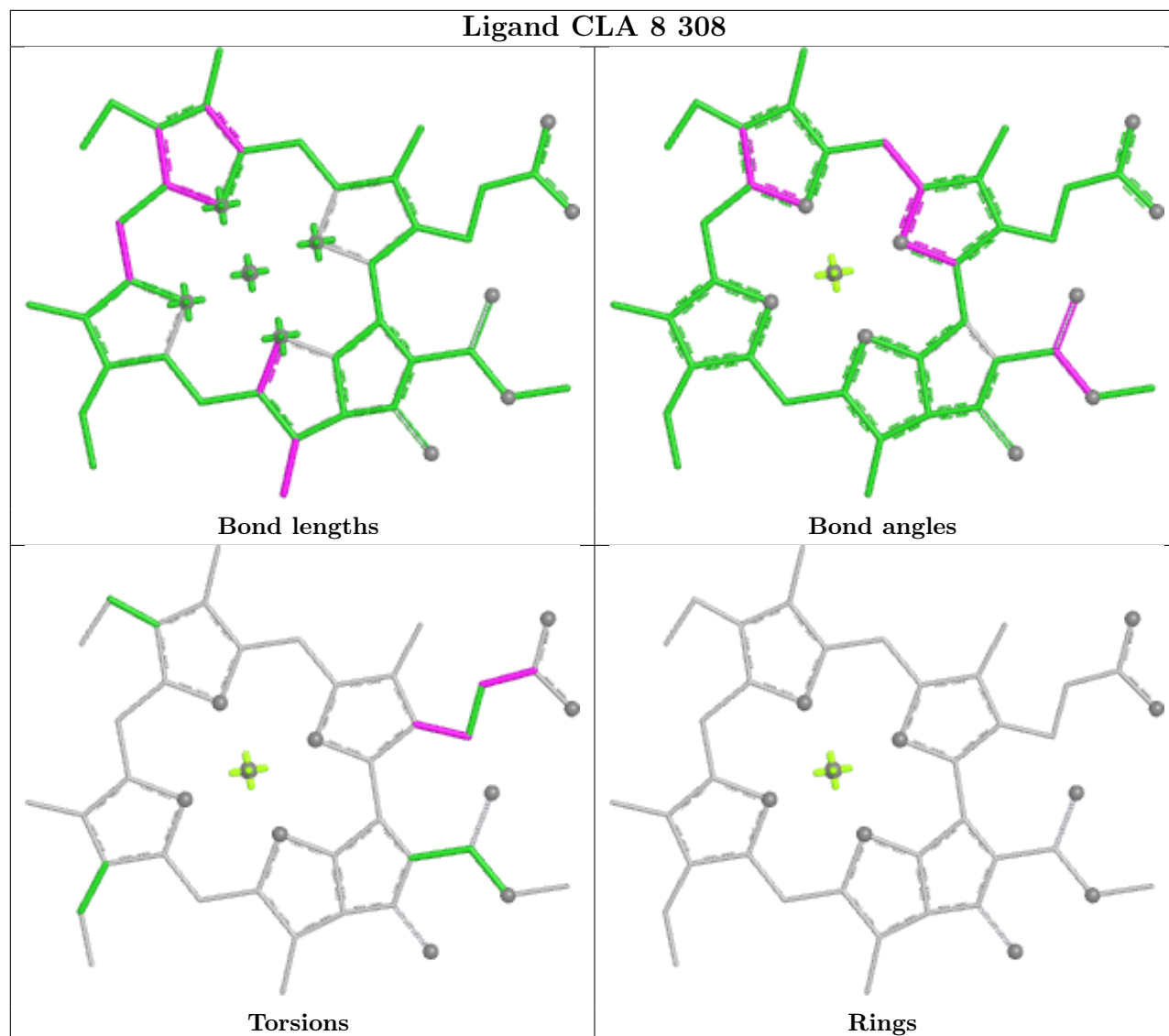
Ligand CLA B 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

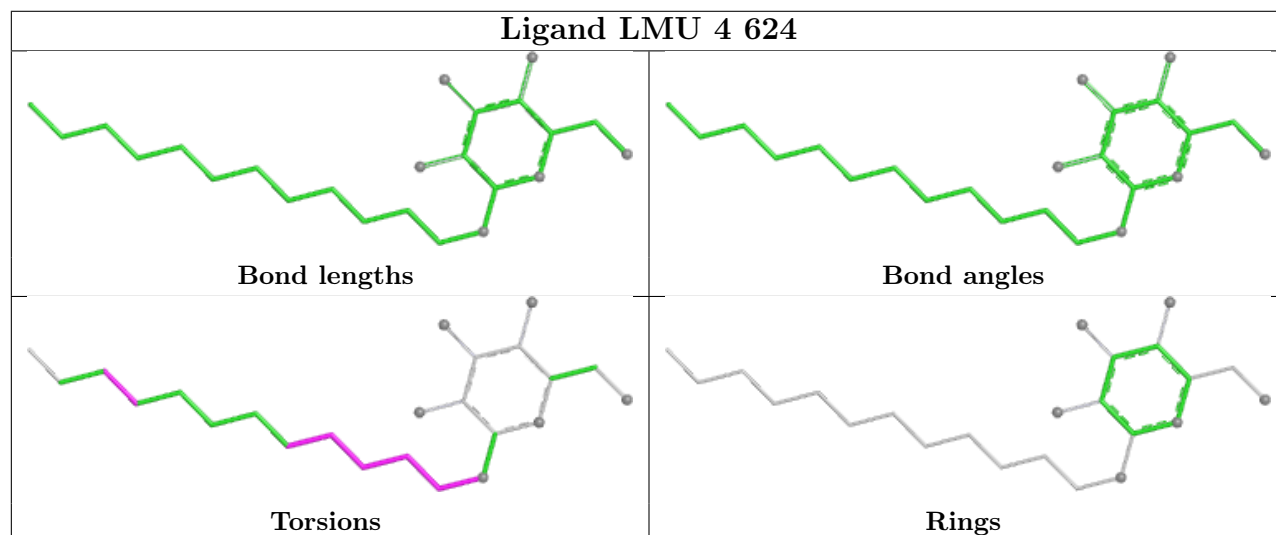
Ligand LUT Z 615	
	
Bond lengths	Bond angles
	
Torsions	Rings

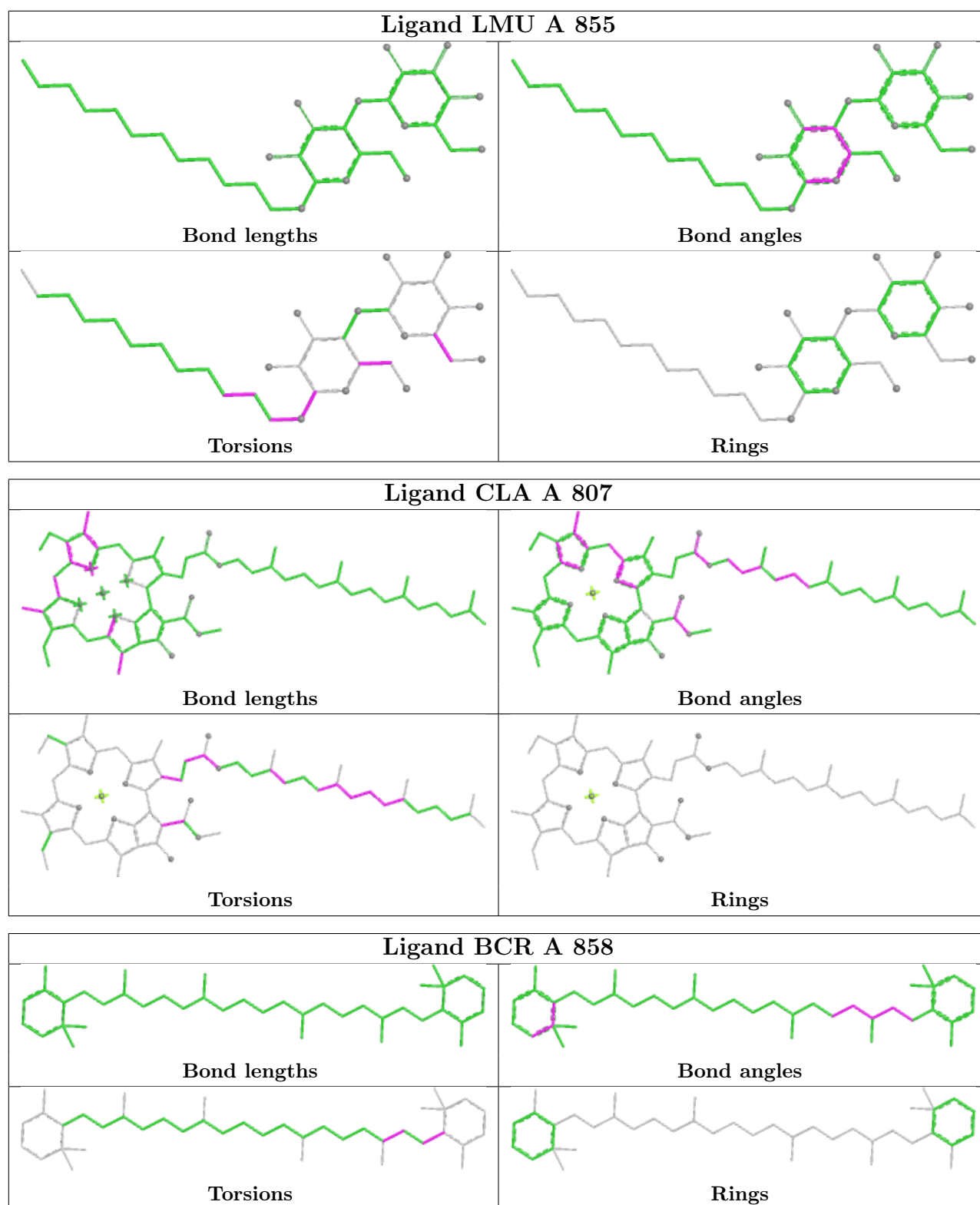


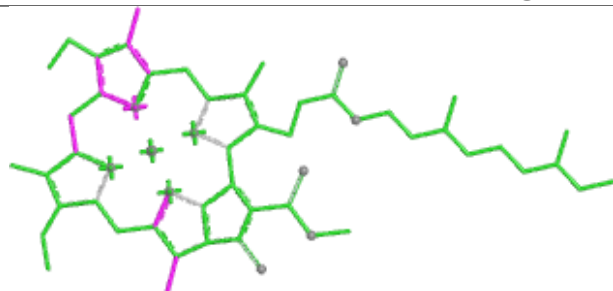
## Ligand CLA 8 308



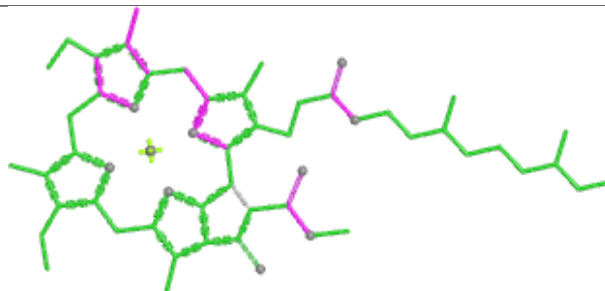
## Ligand LMU 4 624



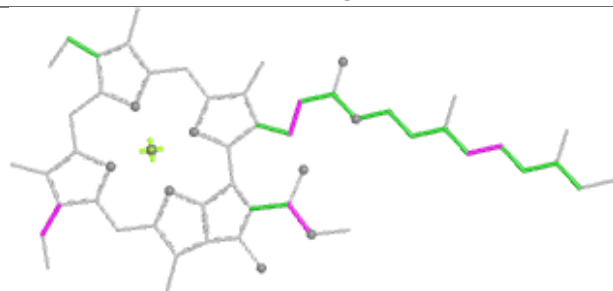


**Ligand CLA 5 313**

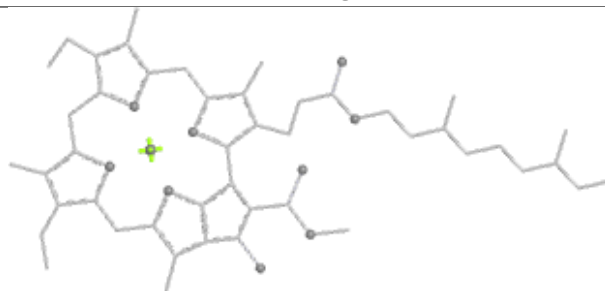
Bond lengths



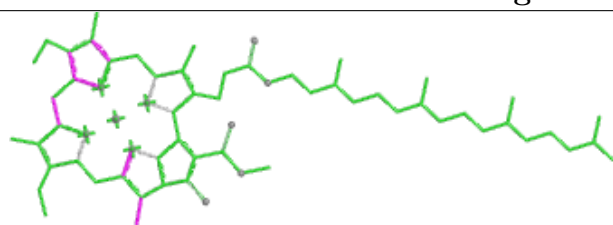
Bond angles



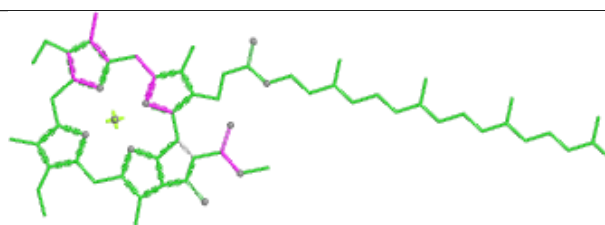
Torsions



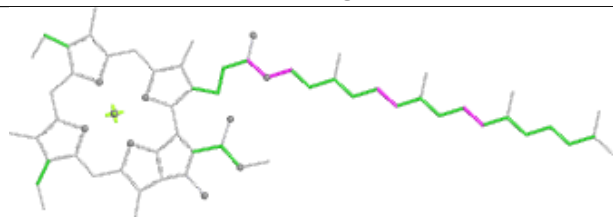
Rings

**Ligand CLA A 834**

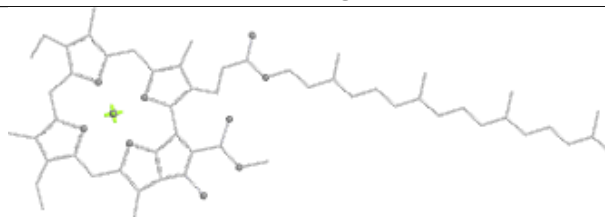
Bond lengths



Bond angles



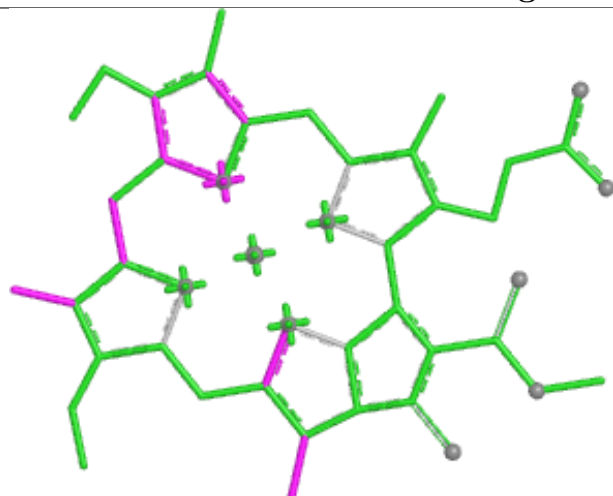
Torsions



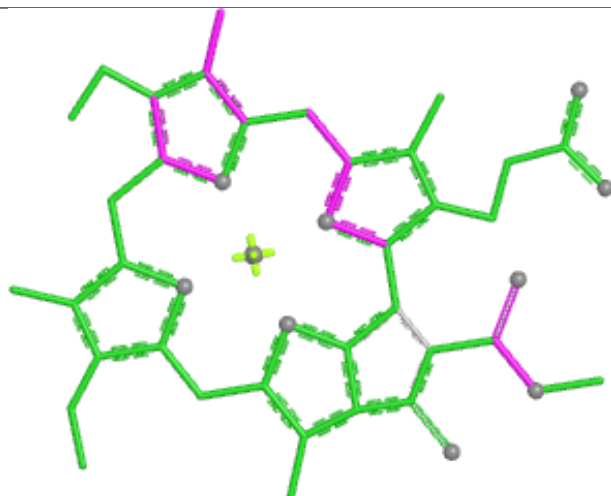
Rings



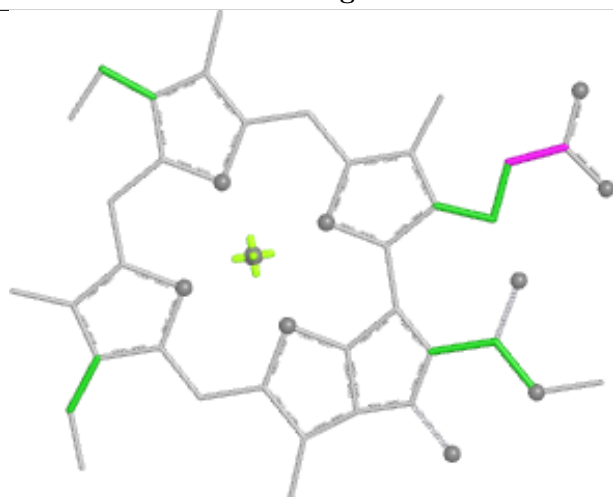
## Ligand CLA 4 611



Bond lengths



Bond angles

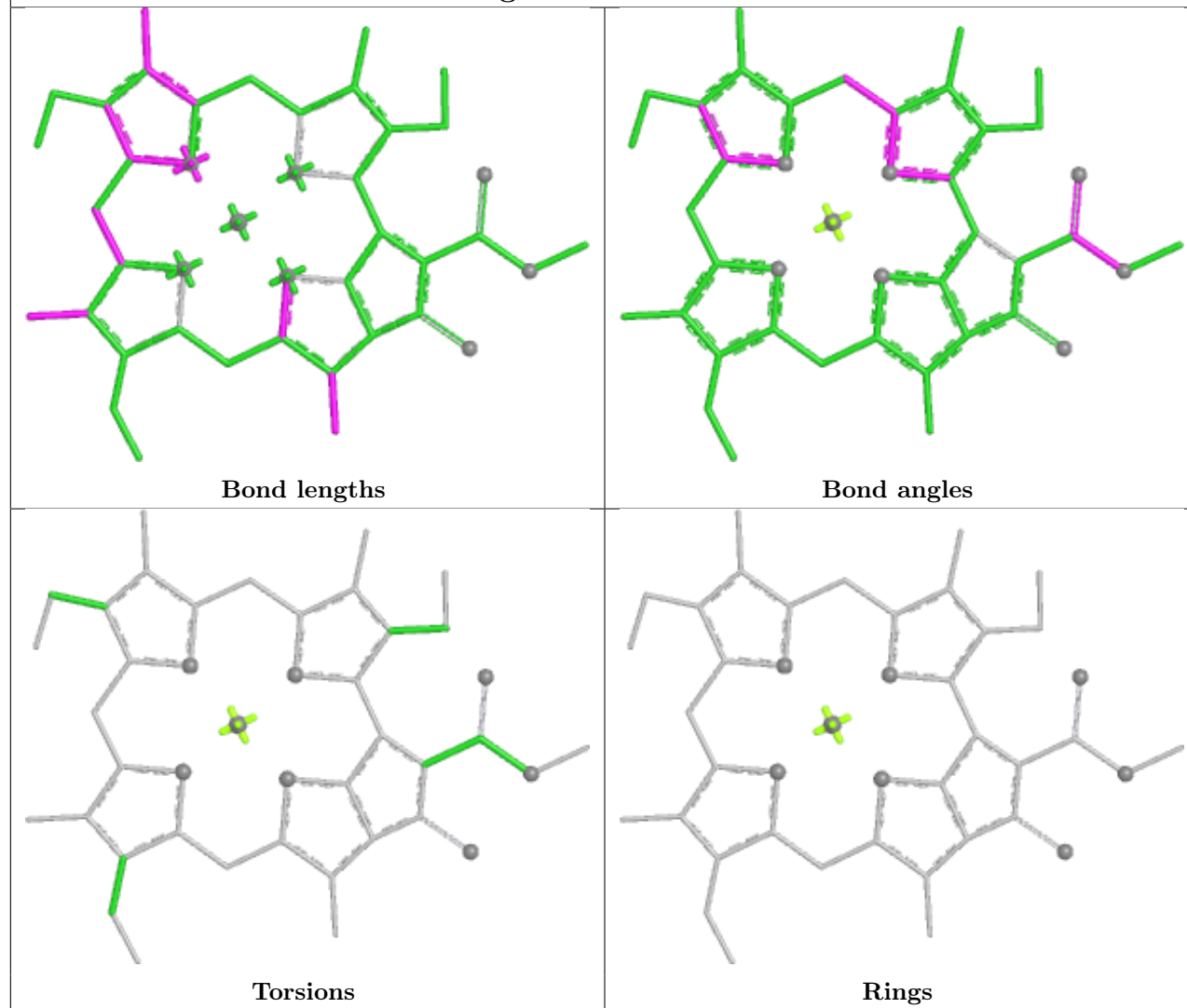


Torsions

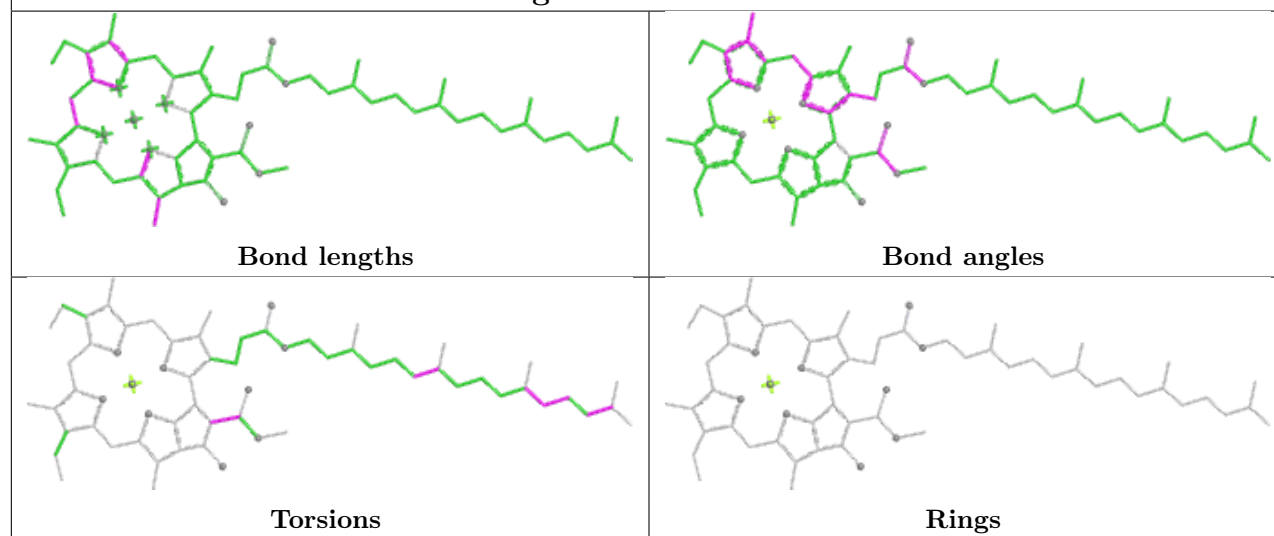


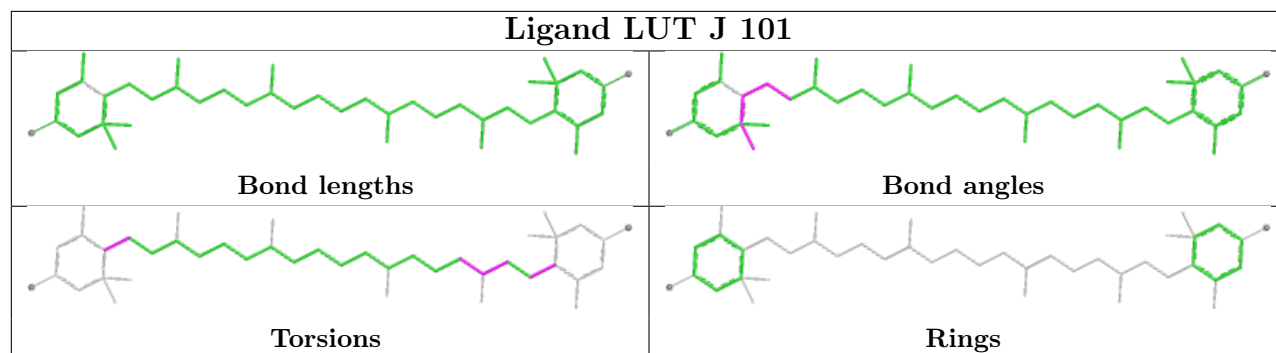
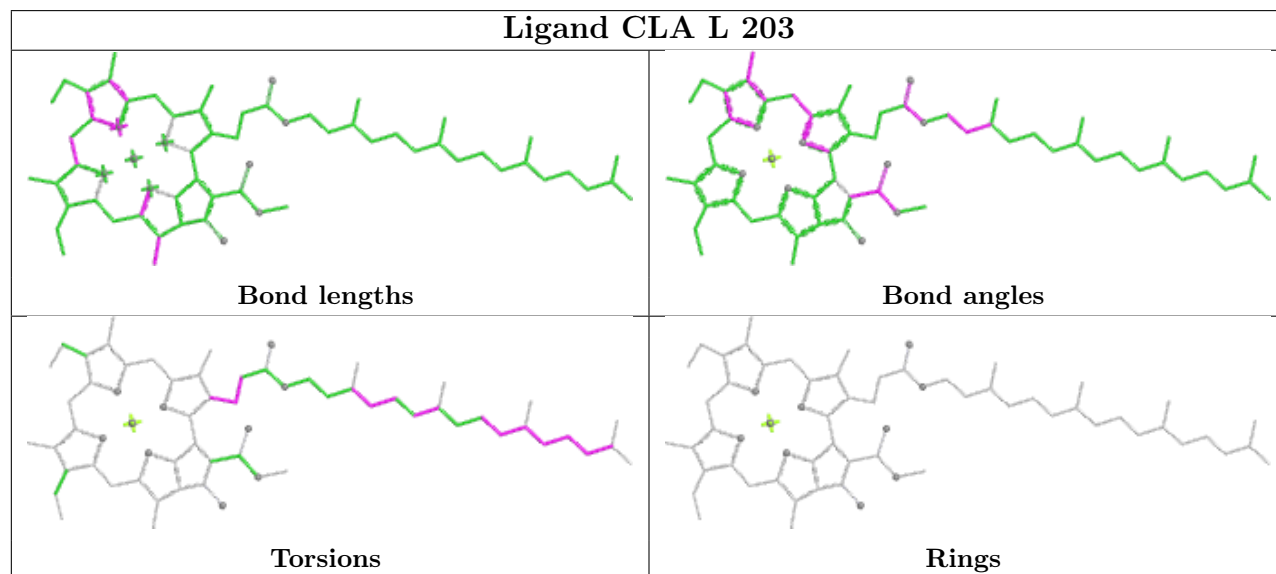
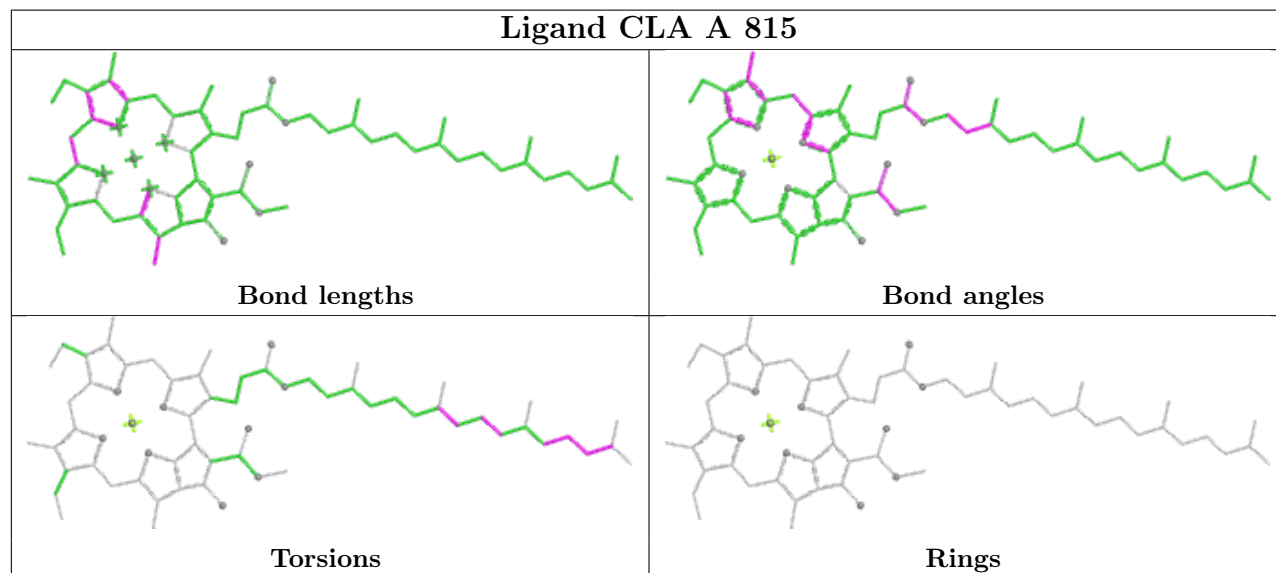
Rings

## Ligand CLA 3 304

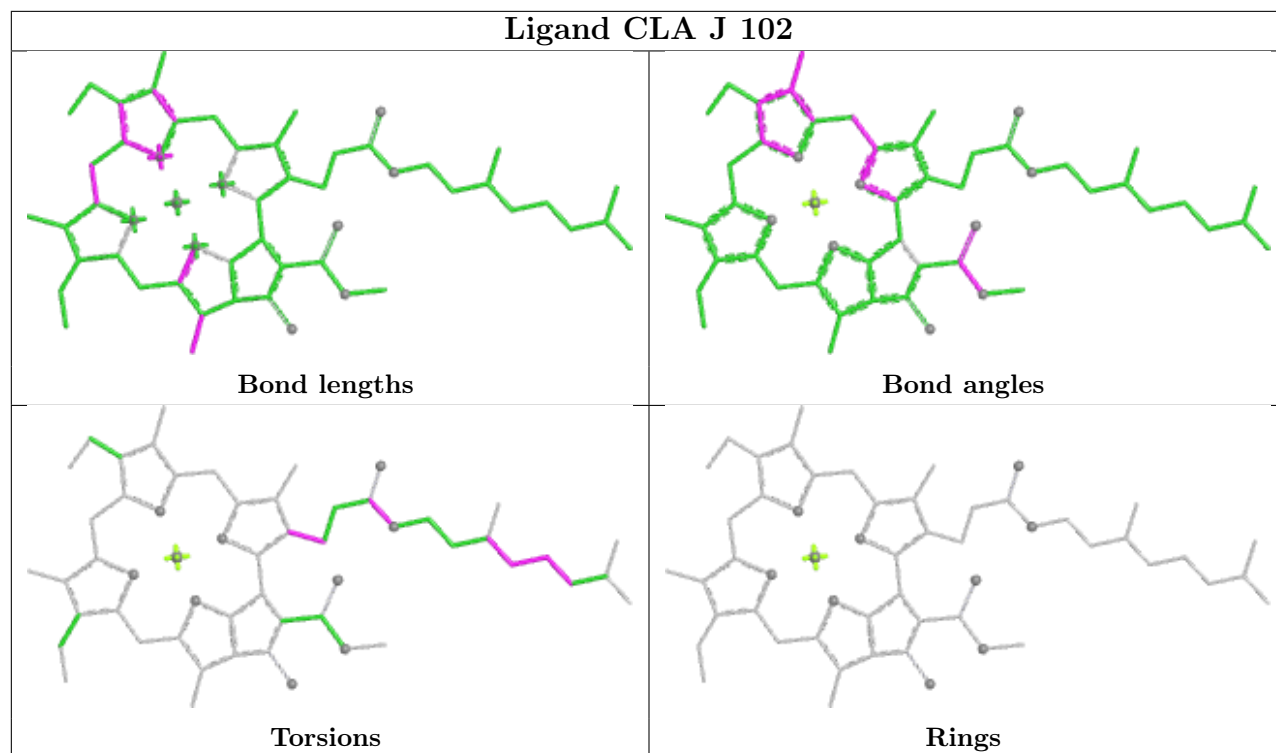


## Ligand CLA B 826

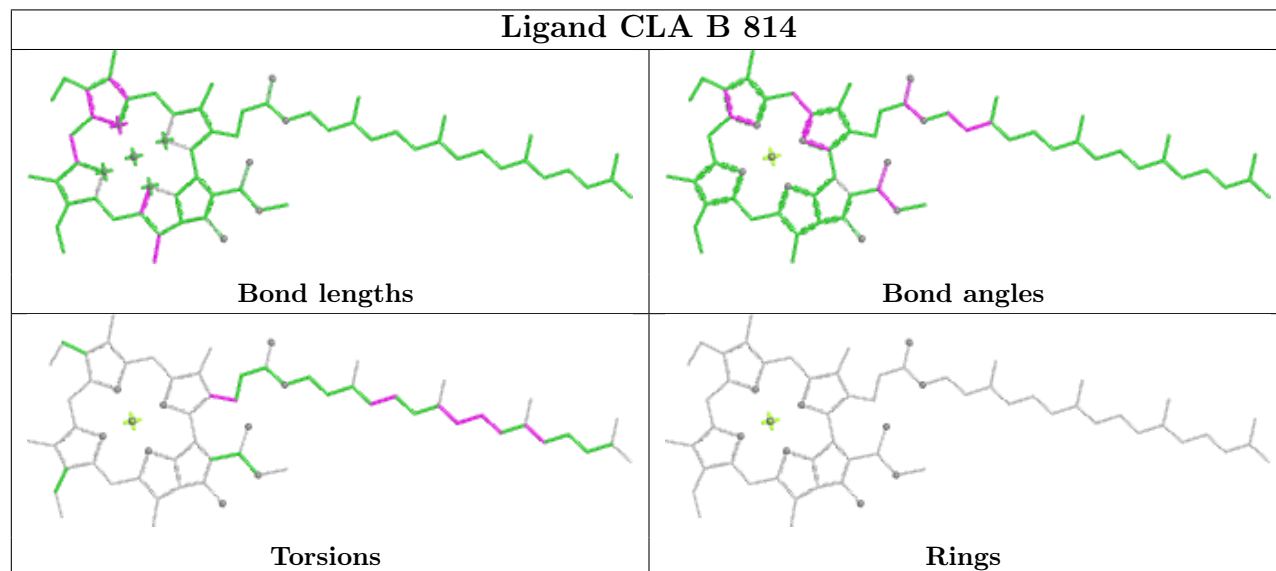


**Ligand LUT J 101****Ligand CLA L 203****Ligand CLA A 815**

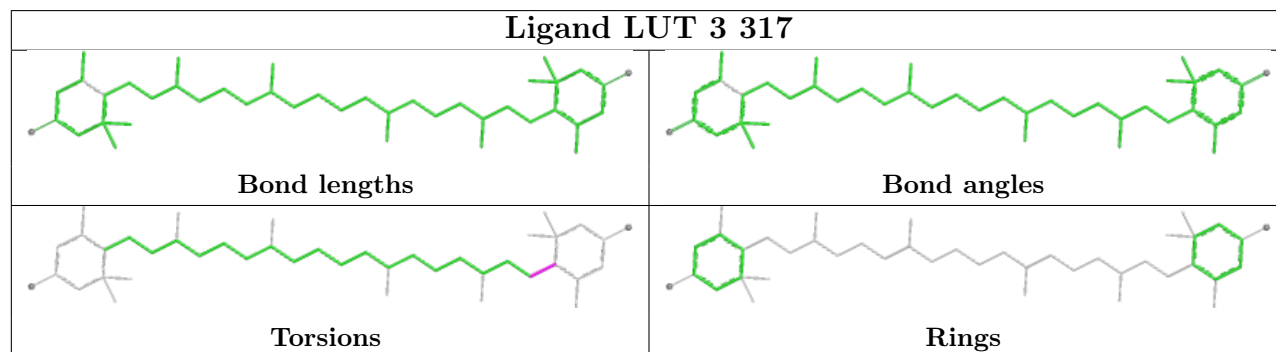
## Ligand CLA J 102

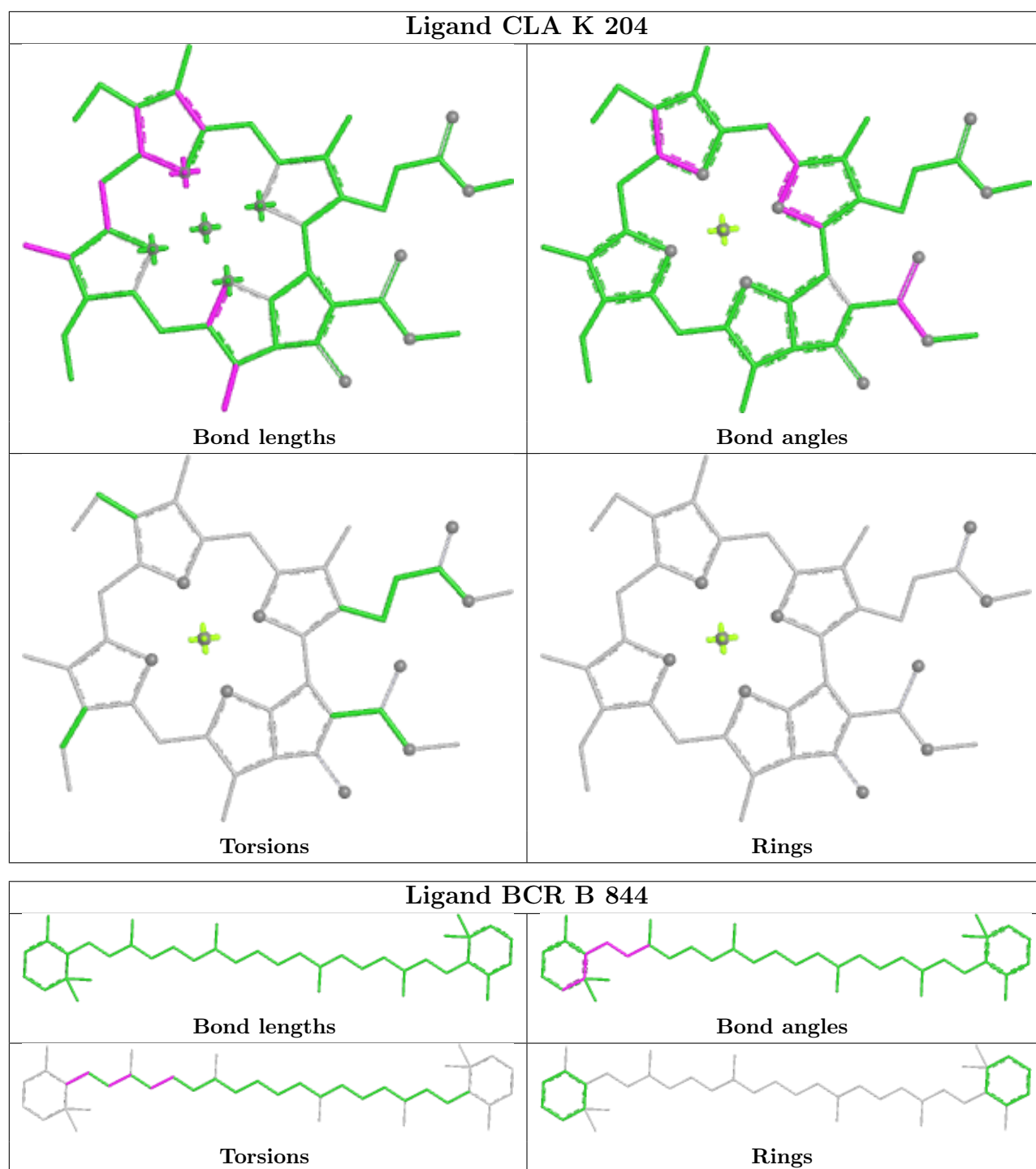


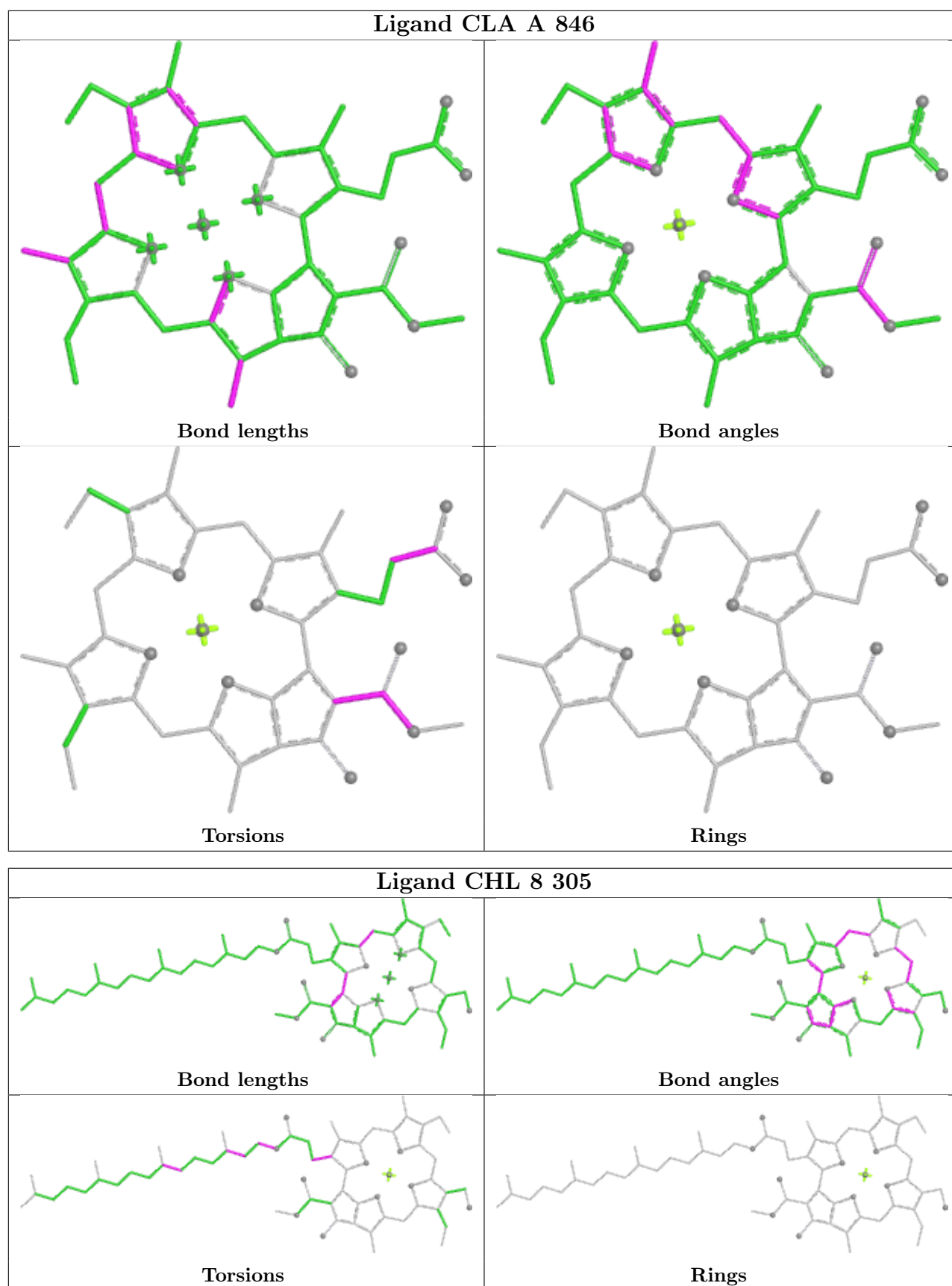
## Ligand CLA B 814

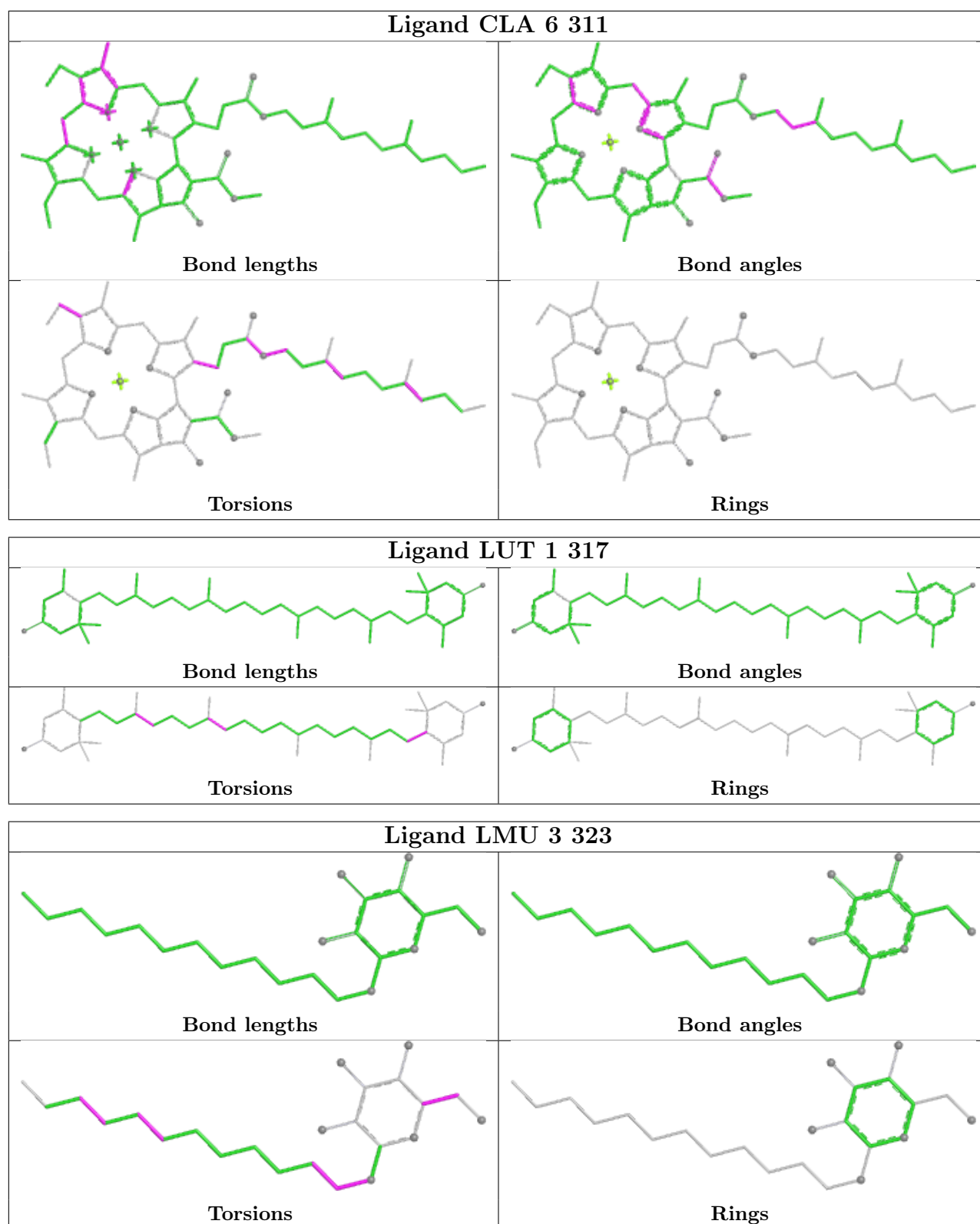


## Ligand LUT 3 317

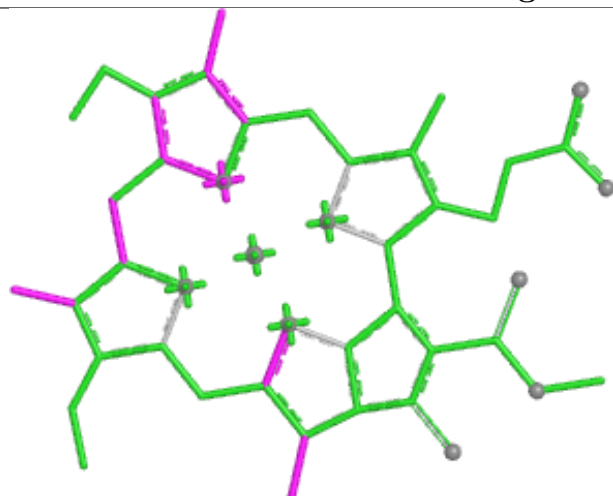








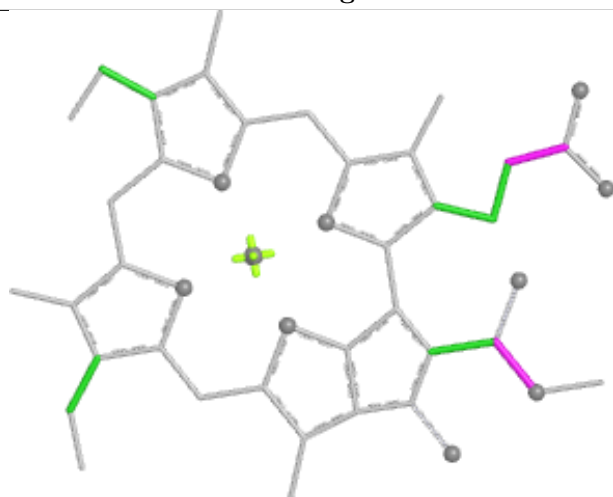
## Ligand CLA 1 311



Bond lengths



Bond angles

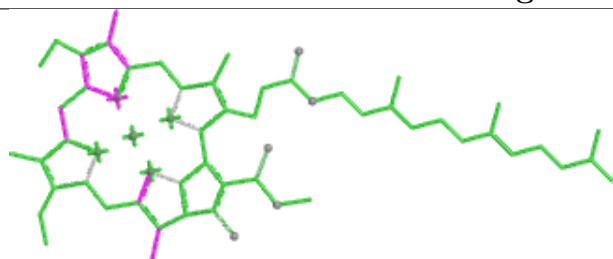


Torsions

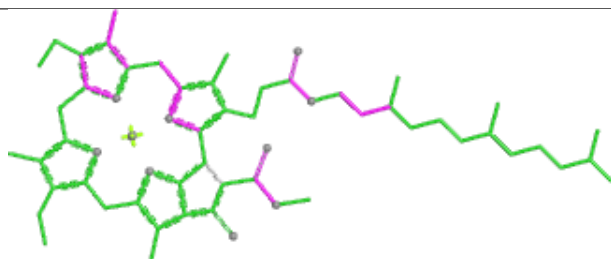


Rings

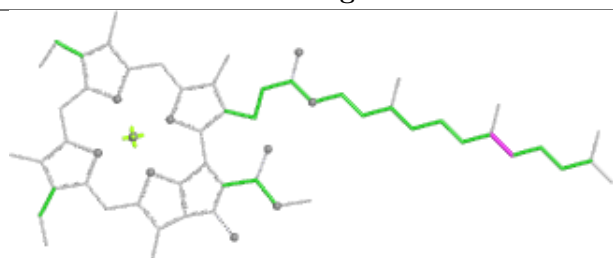
## Ligand CLA Z 609



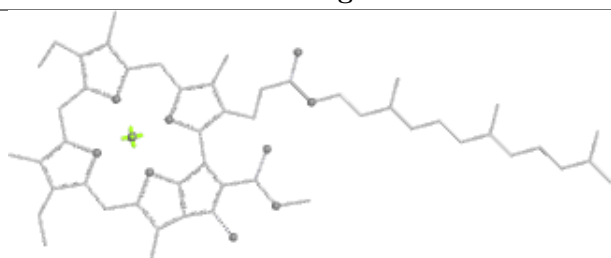
Bond lengths



Bond angles

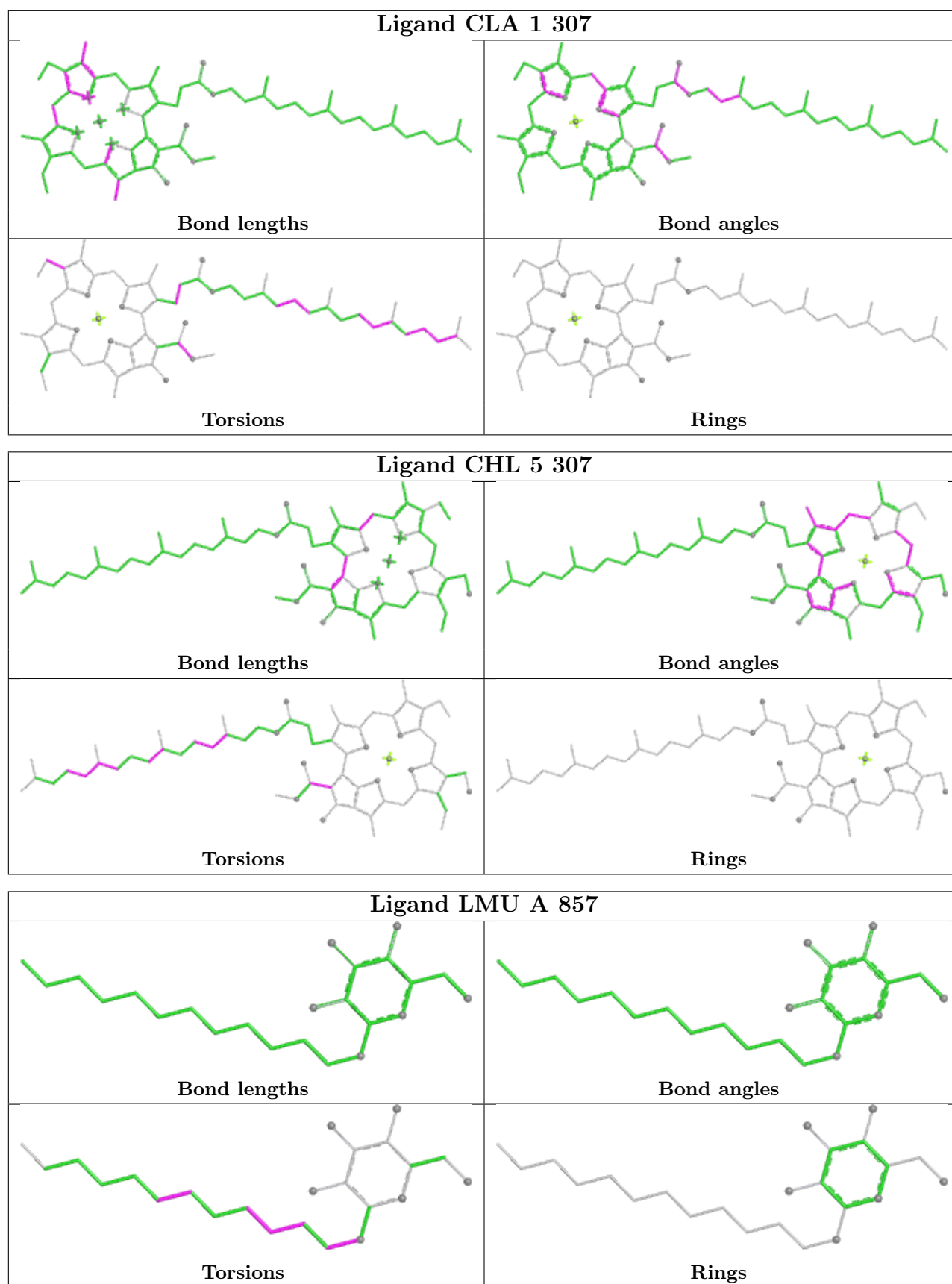


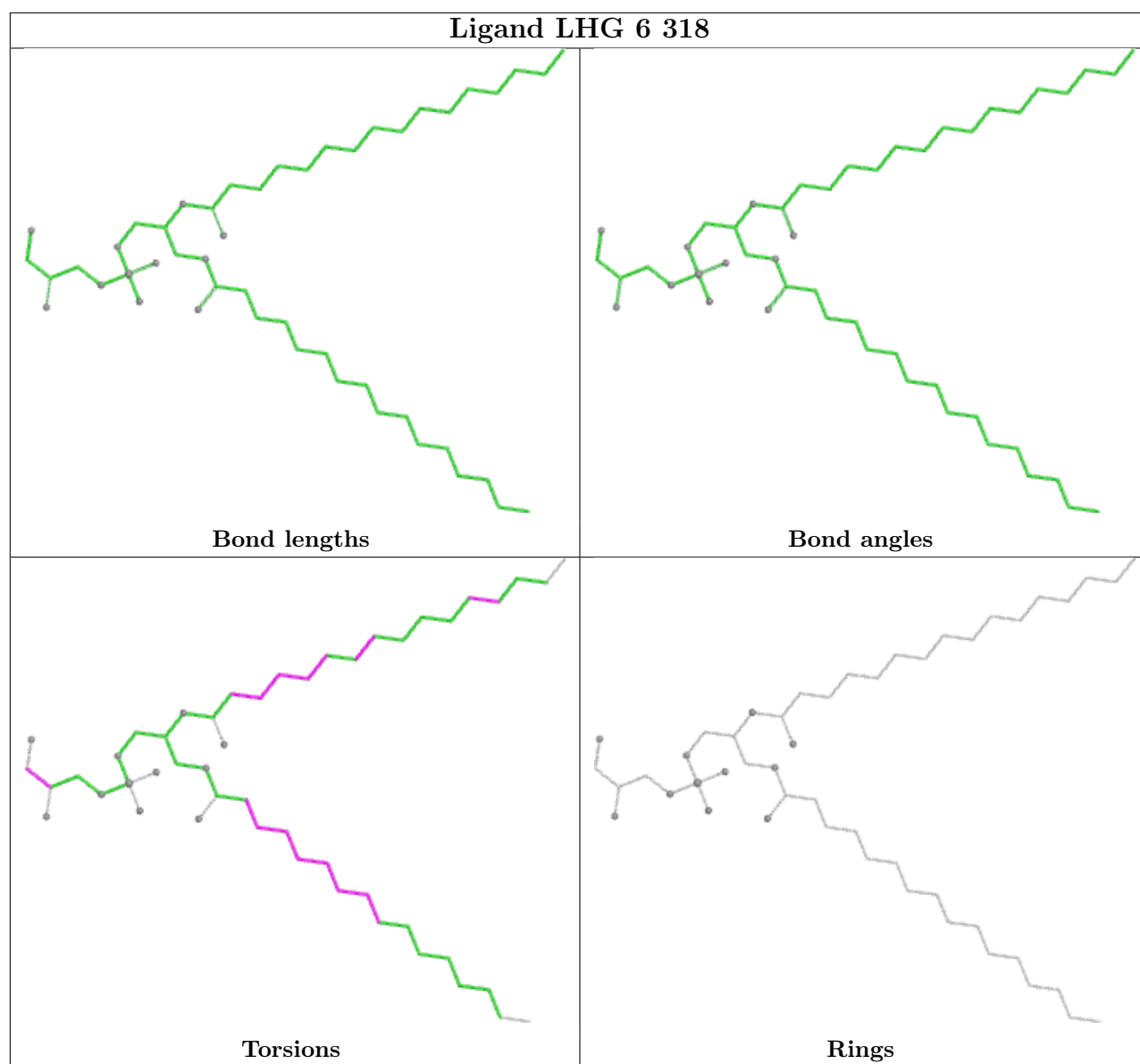
Torsions



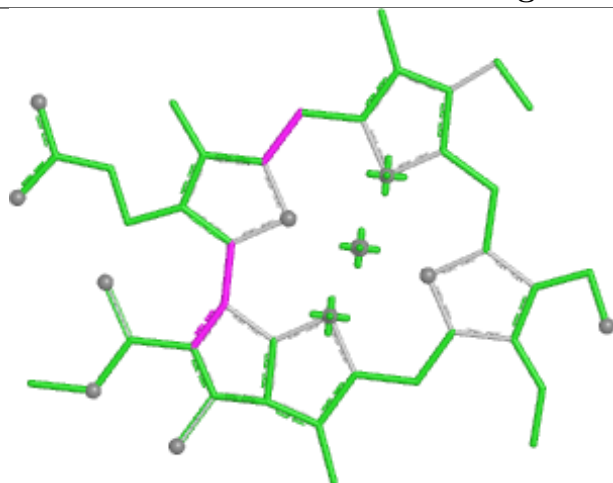
Rings



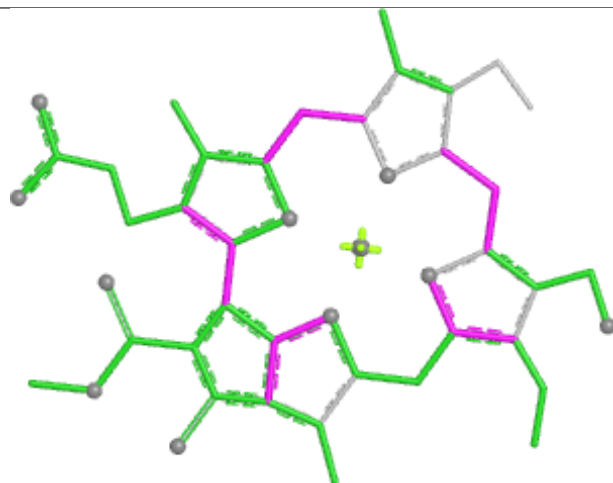




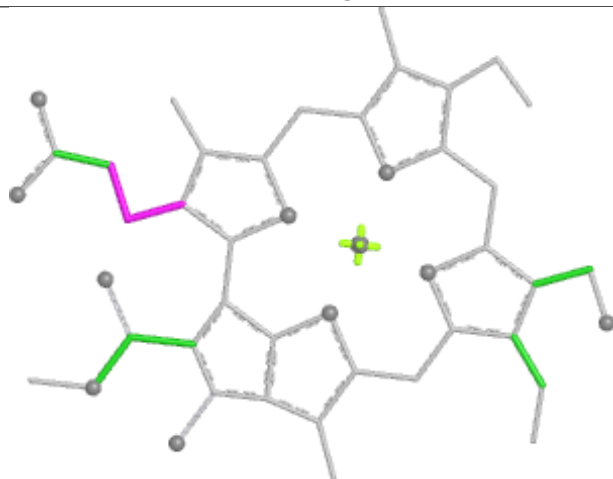
## Ligand CHL 7 606



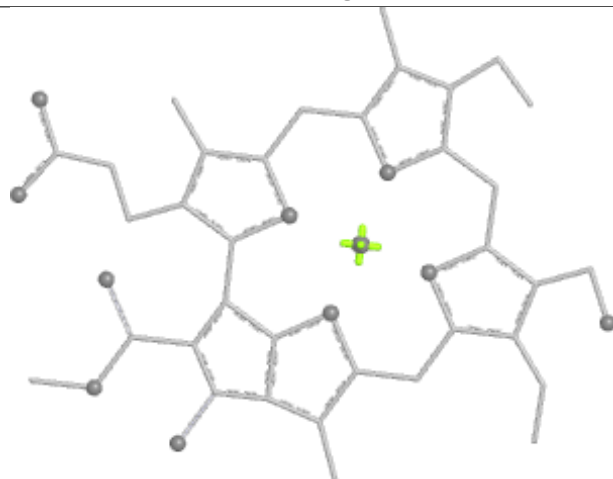
Bond lengths



Bond angles

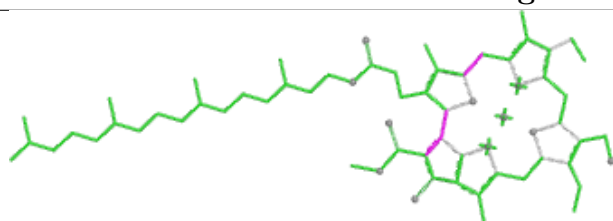


Torsions

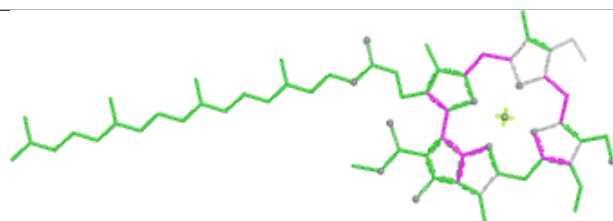


Rings

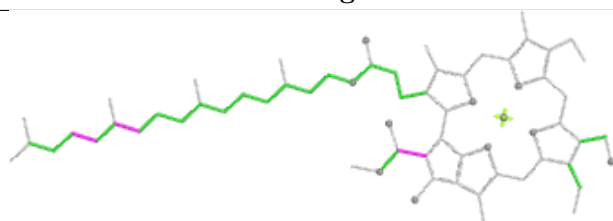
## Ligand CHL 3 306



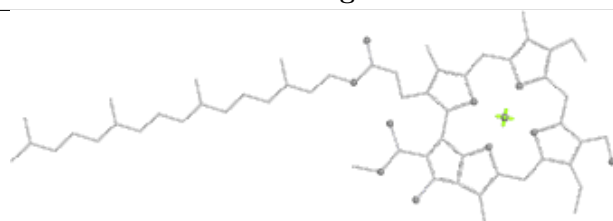
Bond lengths



Bond angles

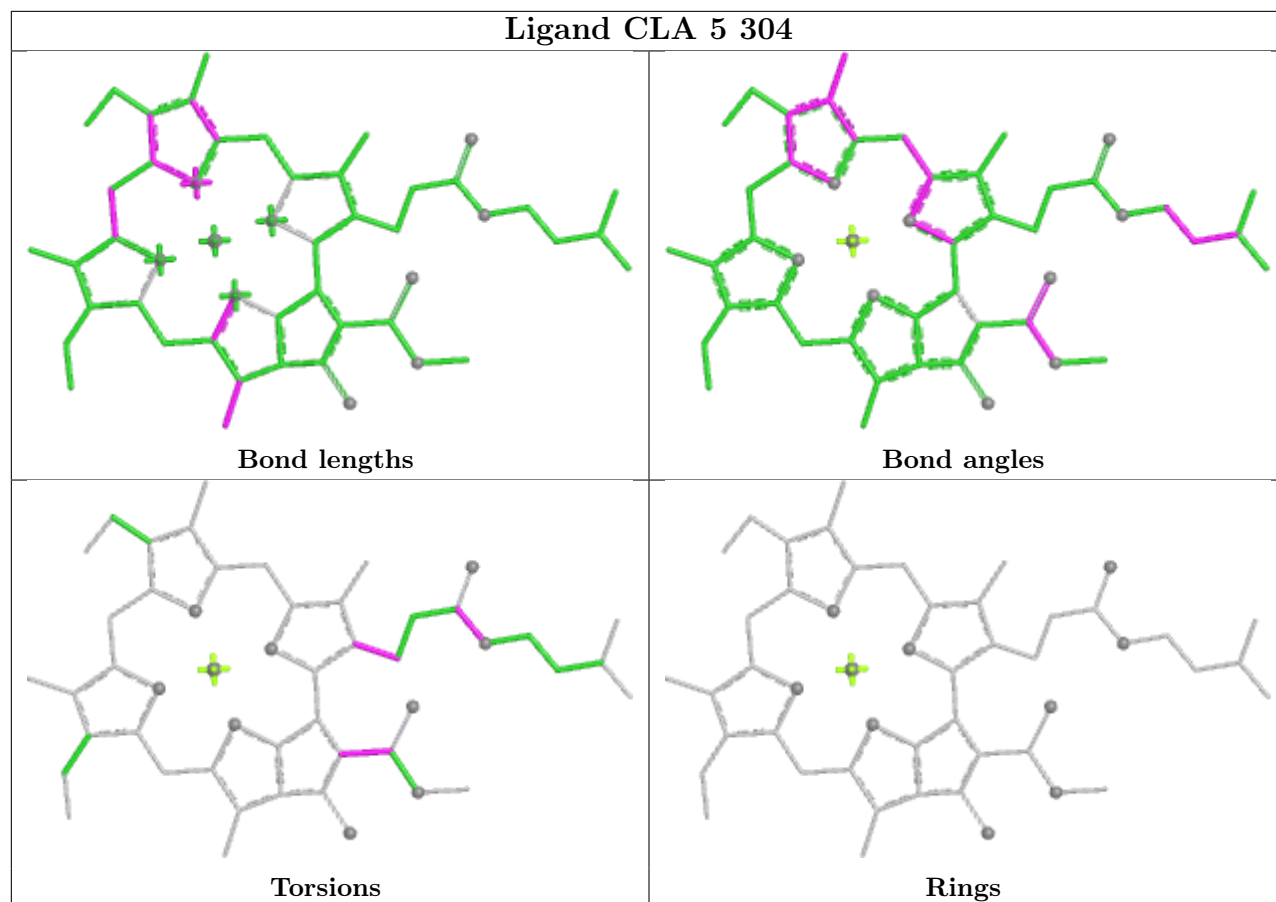


Torsions

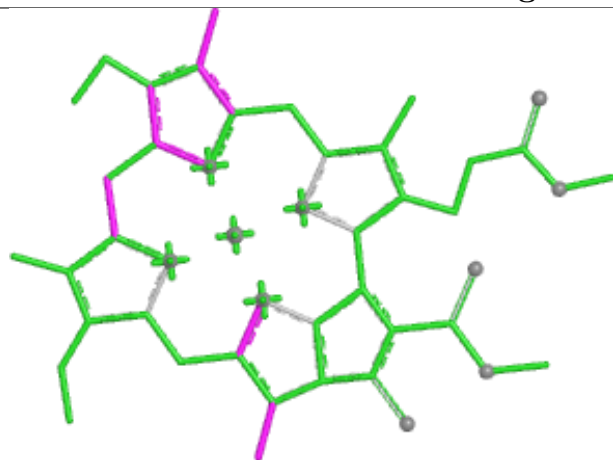


Rings

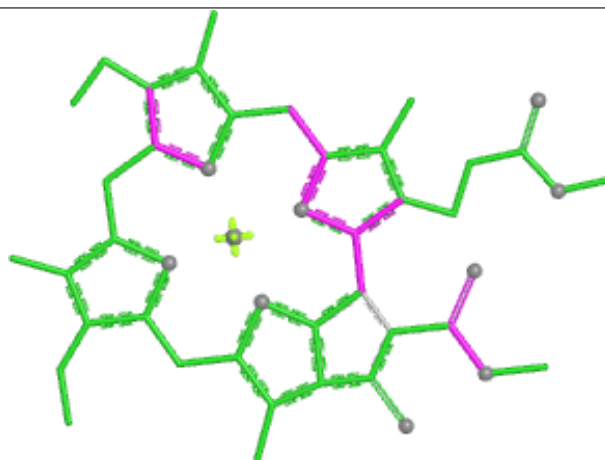
## Ligand CLA 5 304



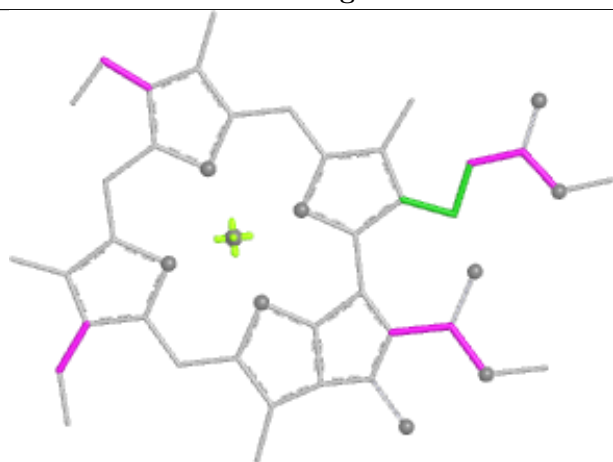
## Ligand CLA 5 319



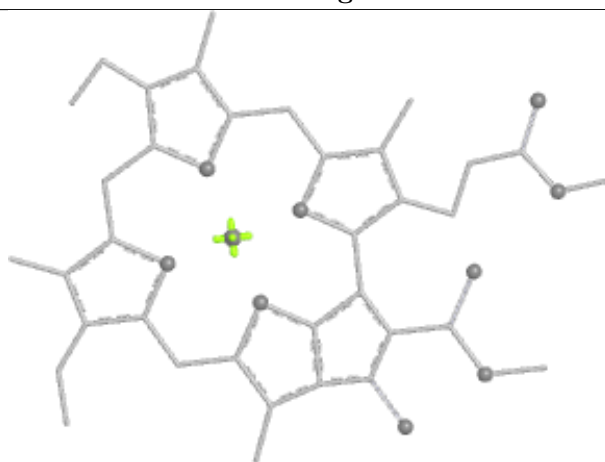
Bond lengths



Bond angles

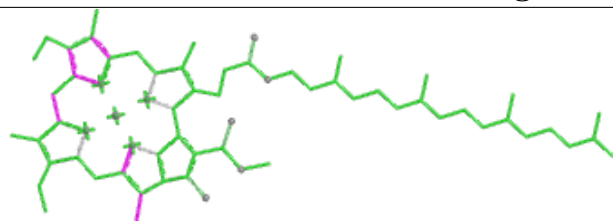


Torsions

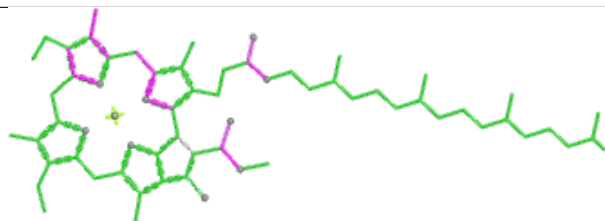


Rings

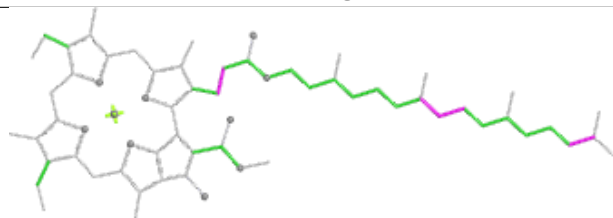
## Ligand CLA A 814



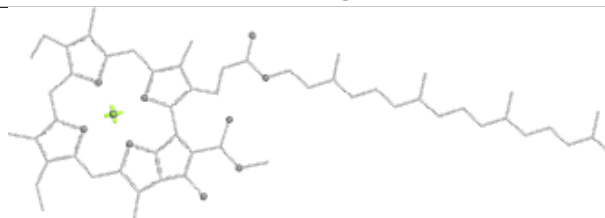
Bond lengths



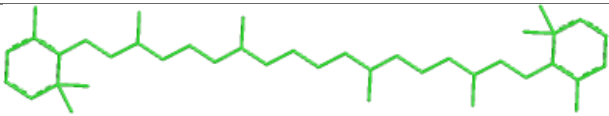
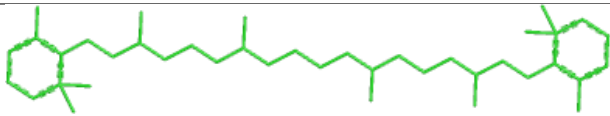
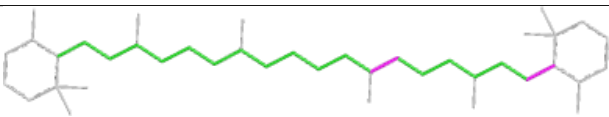
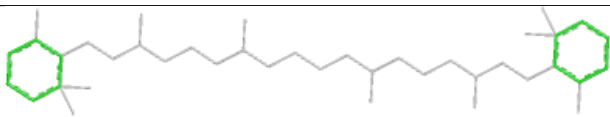
Bond angles

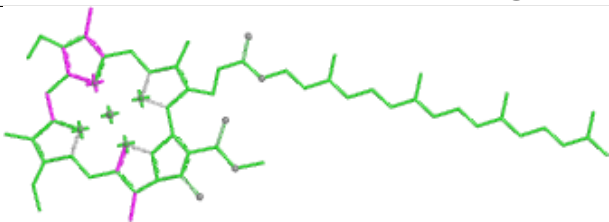
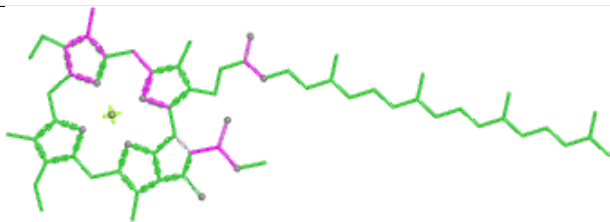
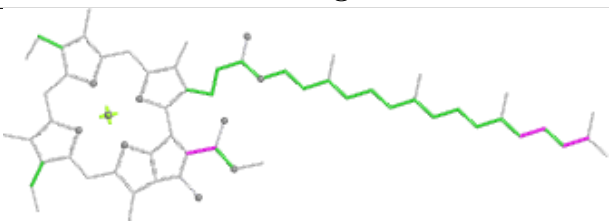
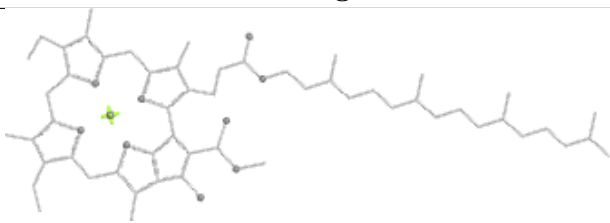


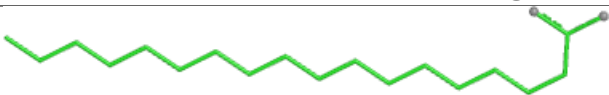
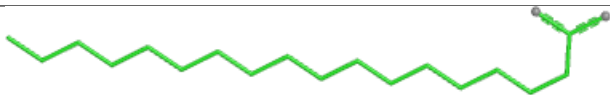

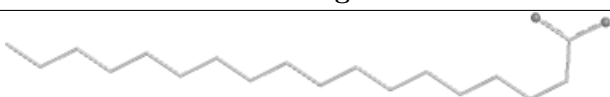
Torsions

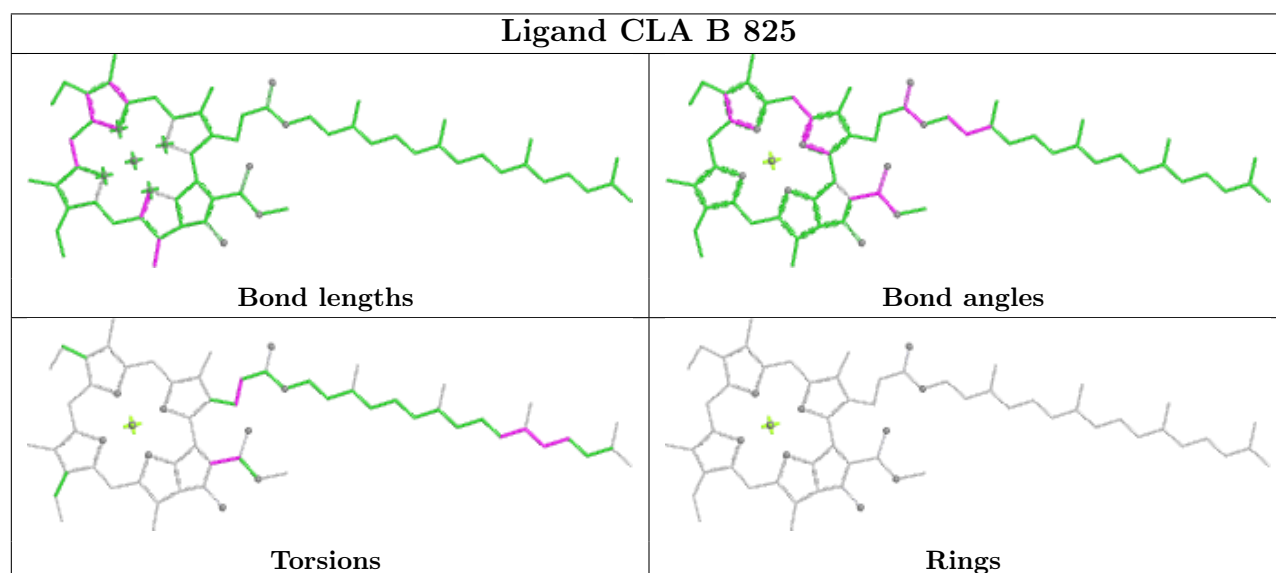
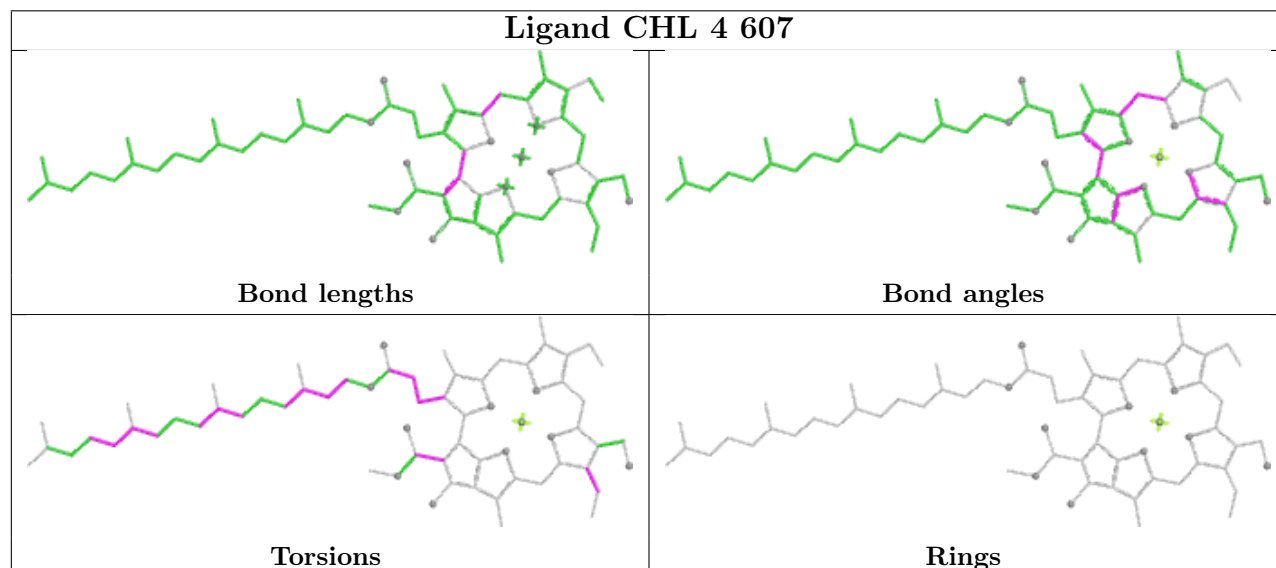
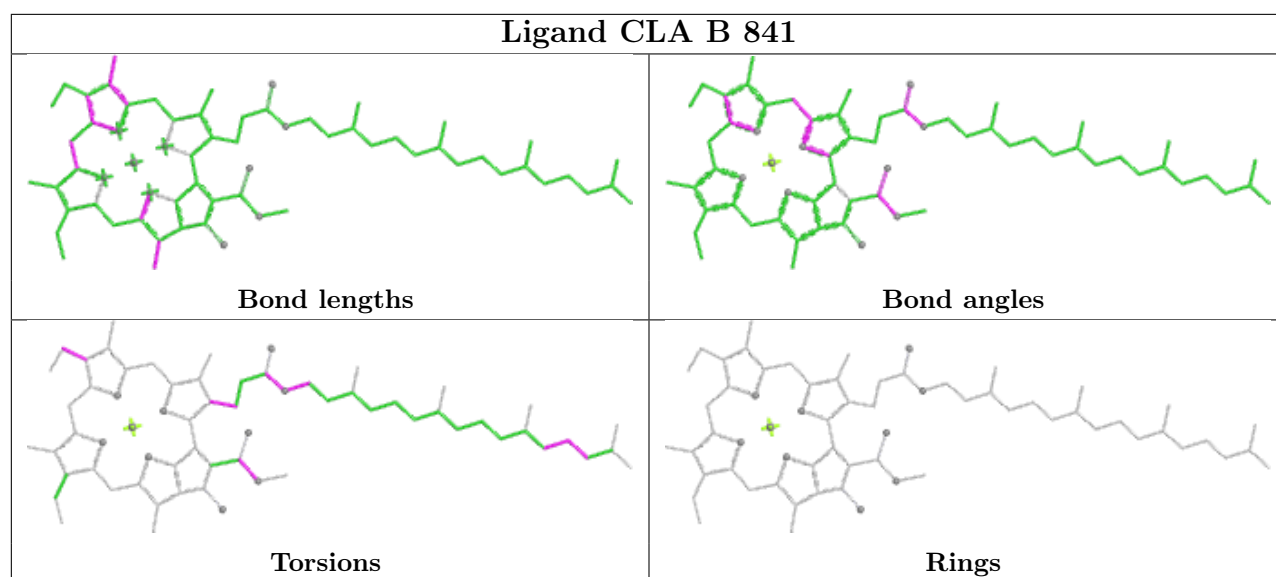


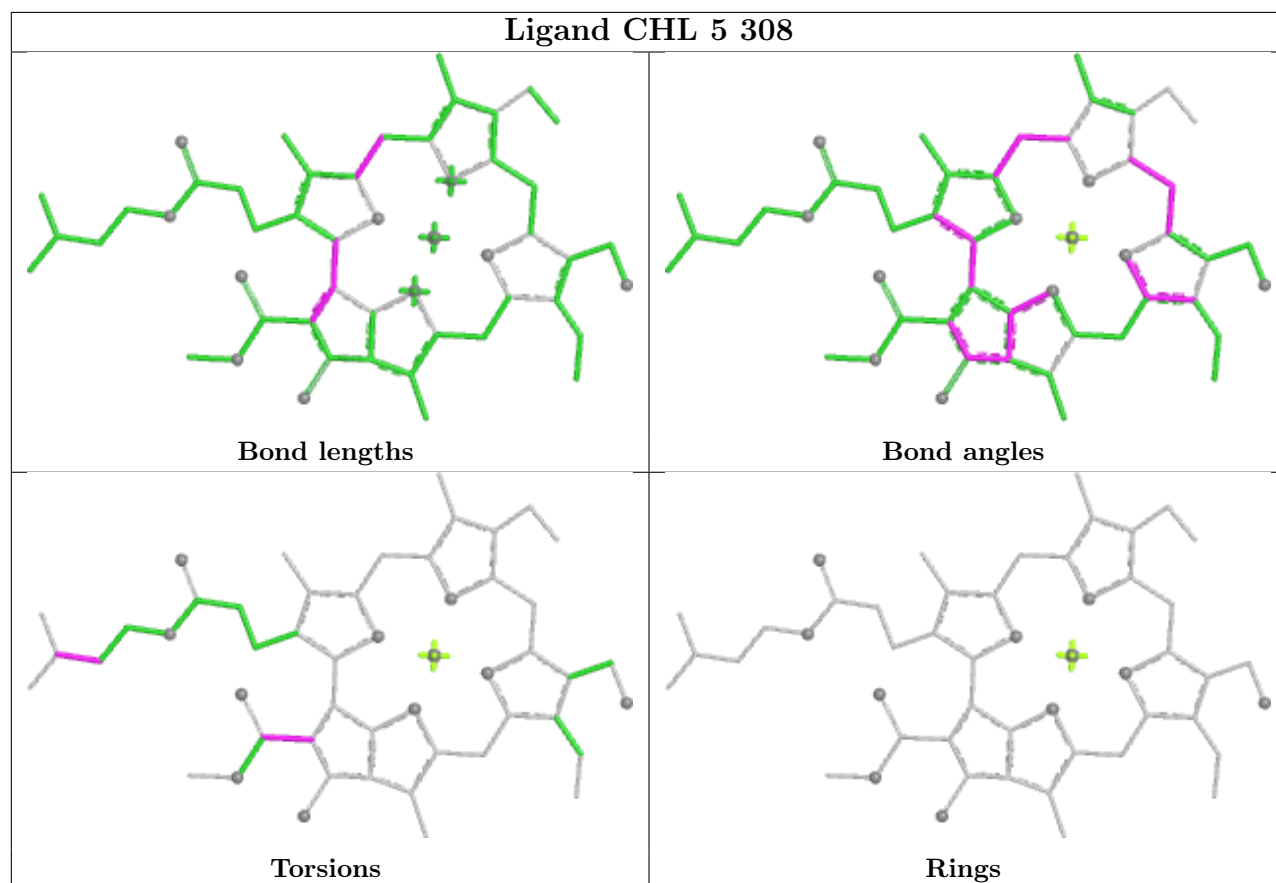
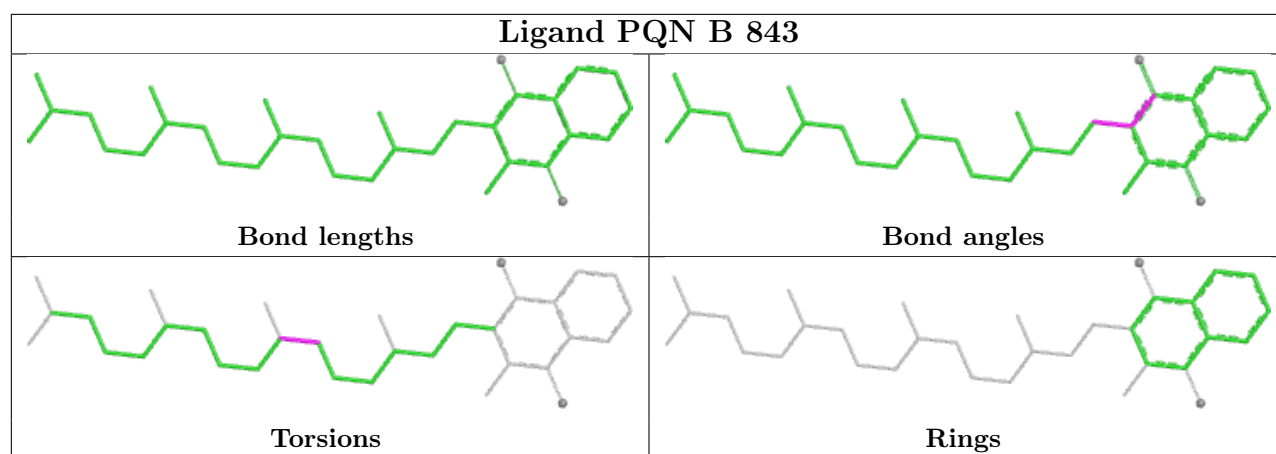
Rings

Ligand BCR J 103	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 805	
	
Bond lengths	Bond angles
	
Torsions	Rings

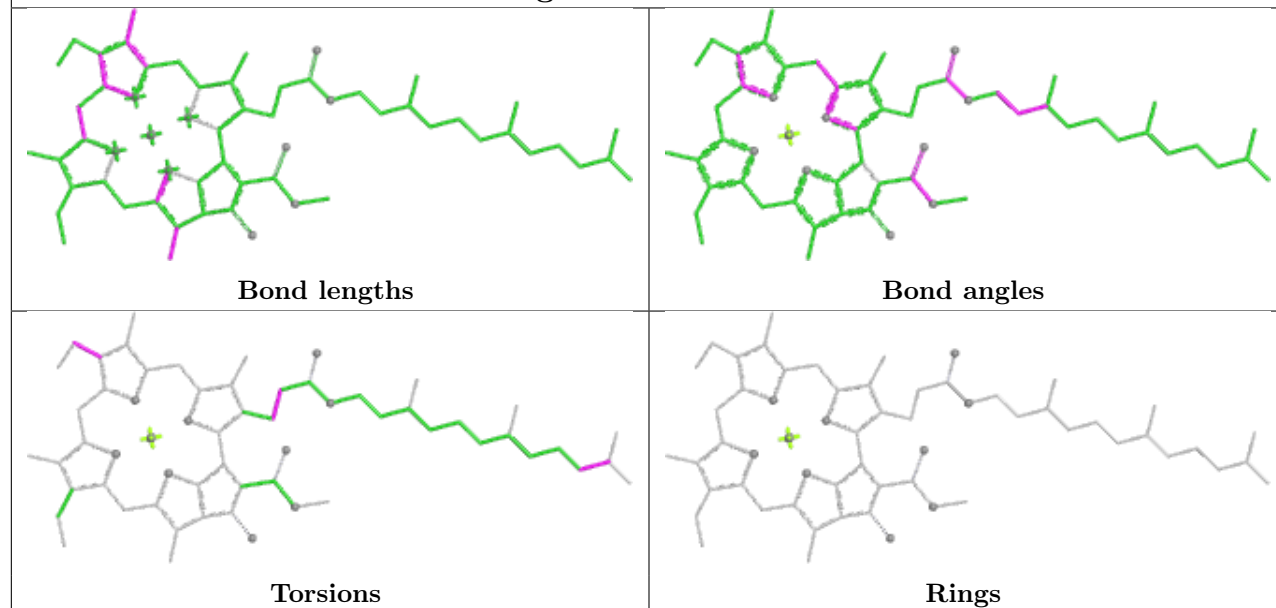
Ligand LMG 6 326	
	
Bond lengths	Bond angles
	
Torsions	Rings



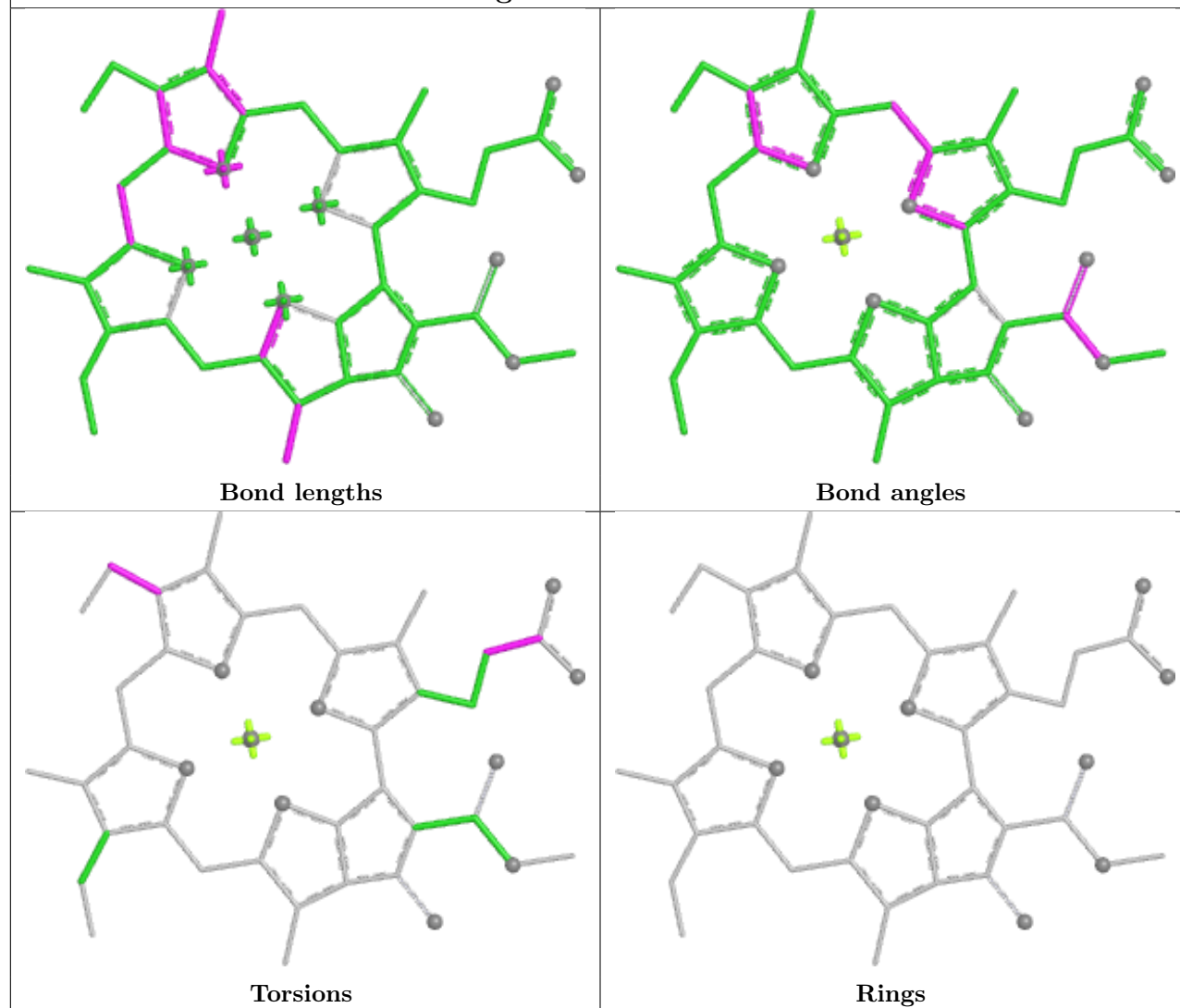


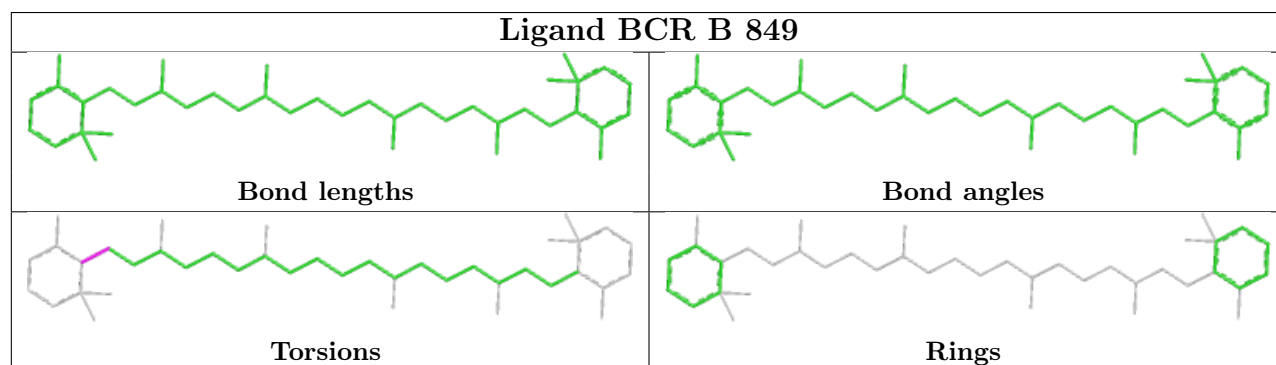
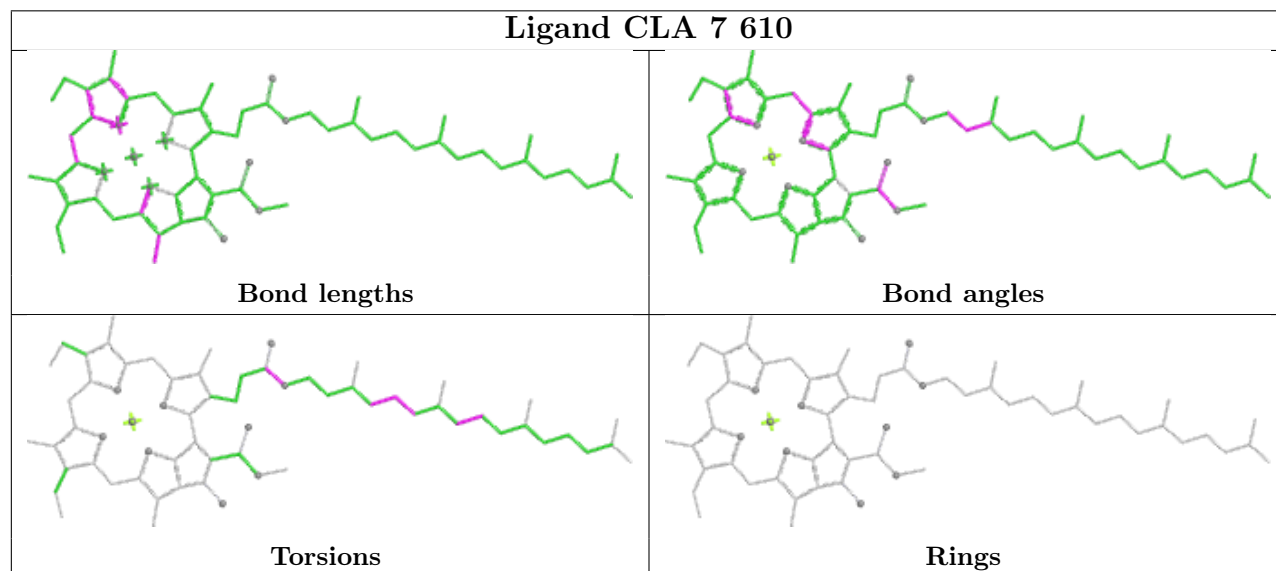
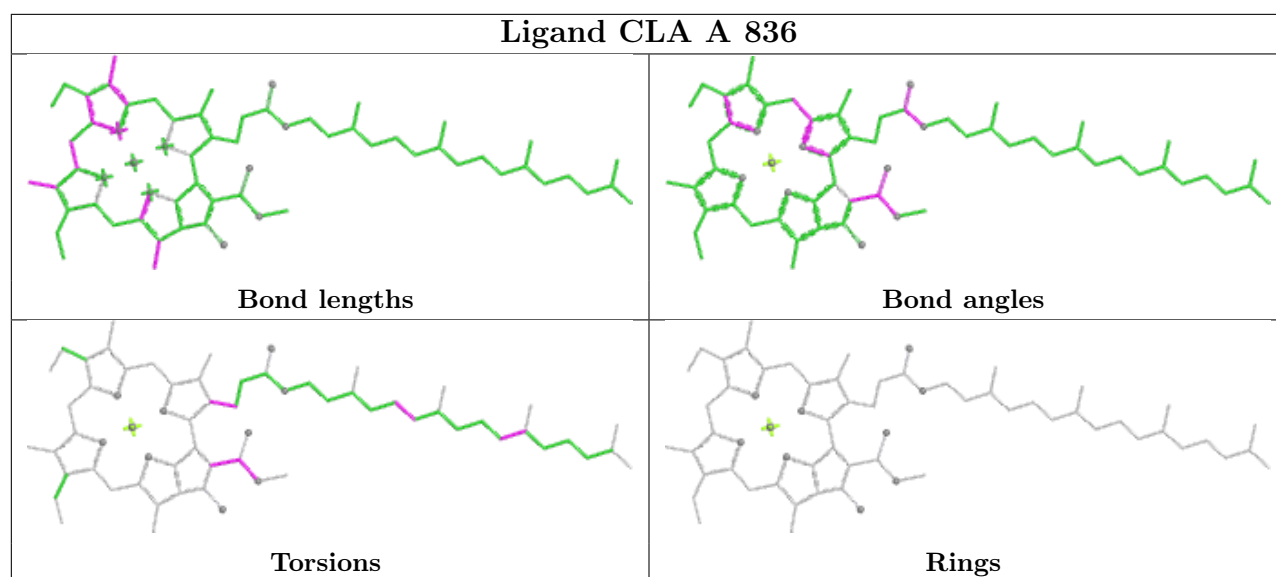


## Ligand CLA 3 311

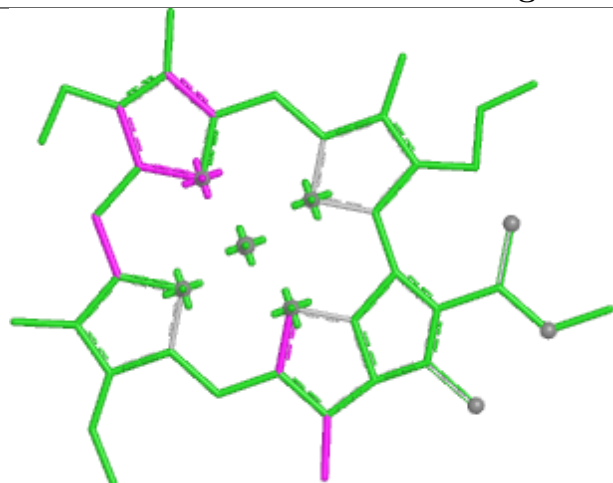


## Ligand CLA 8 310

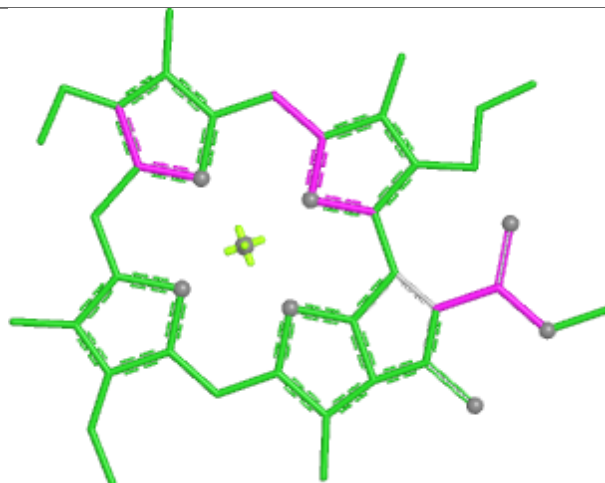




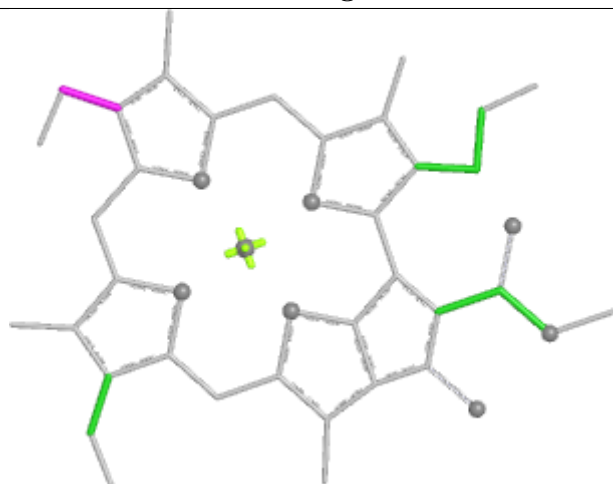
## Ligand CLA 7 613



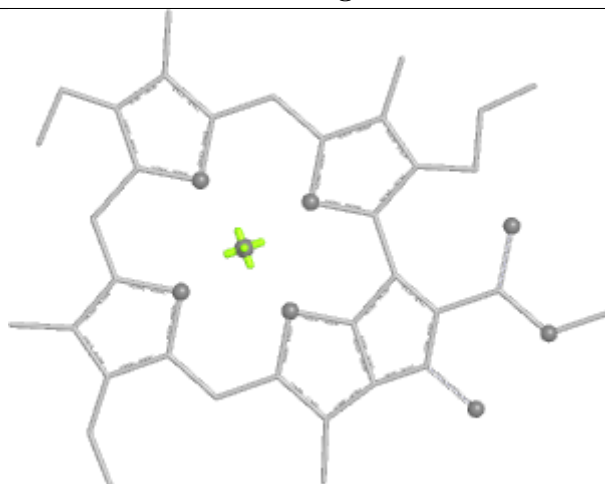
Bond lengths



Bond angles

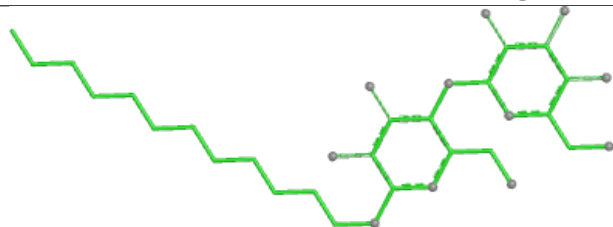


Torsions

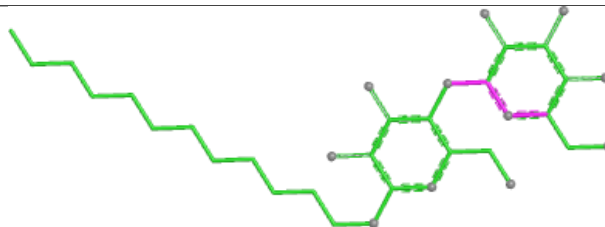


Rings

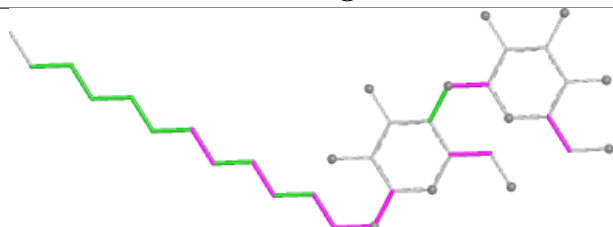
## Ligand LMU 1 301



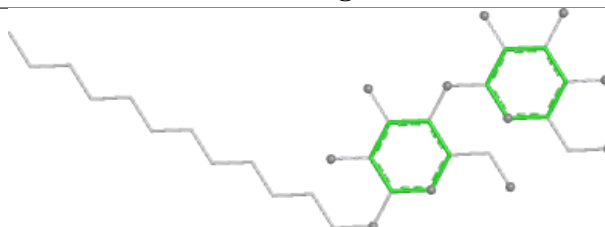
Bond lengths



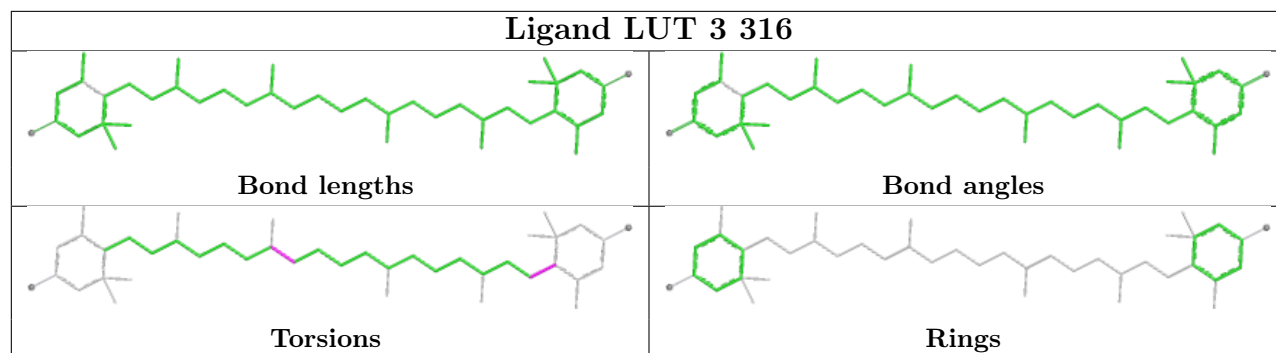
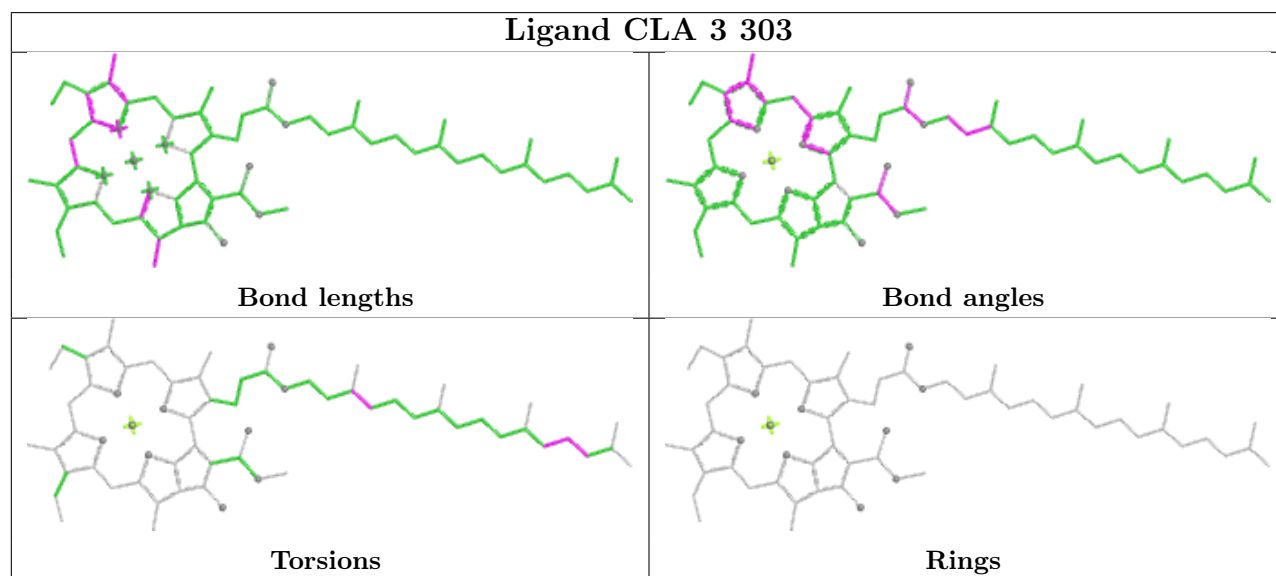
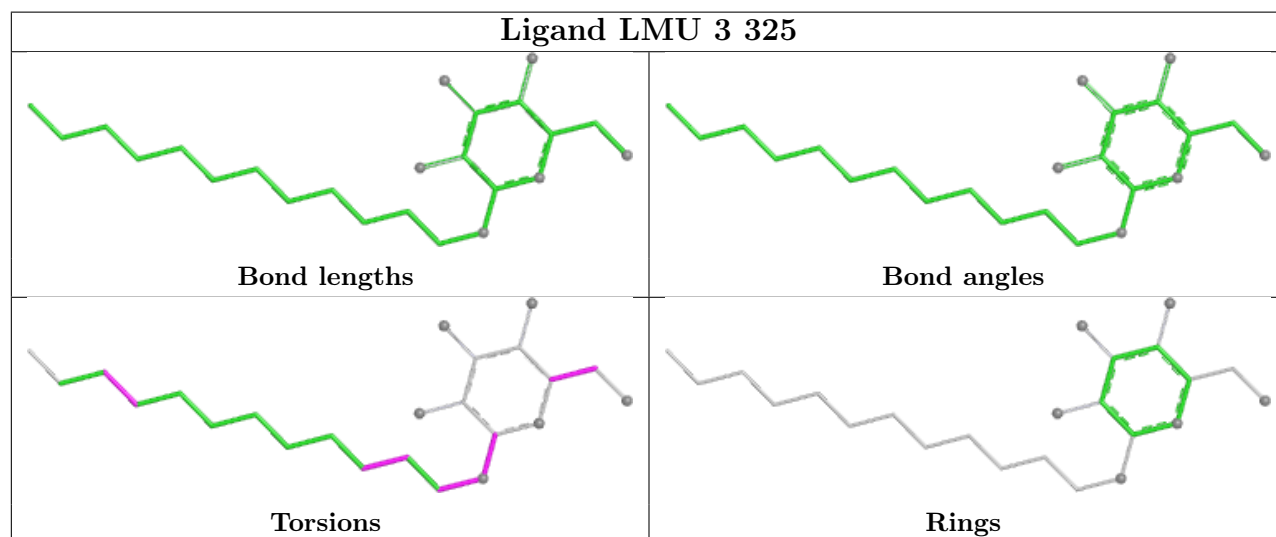
Bond angles

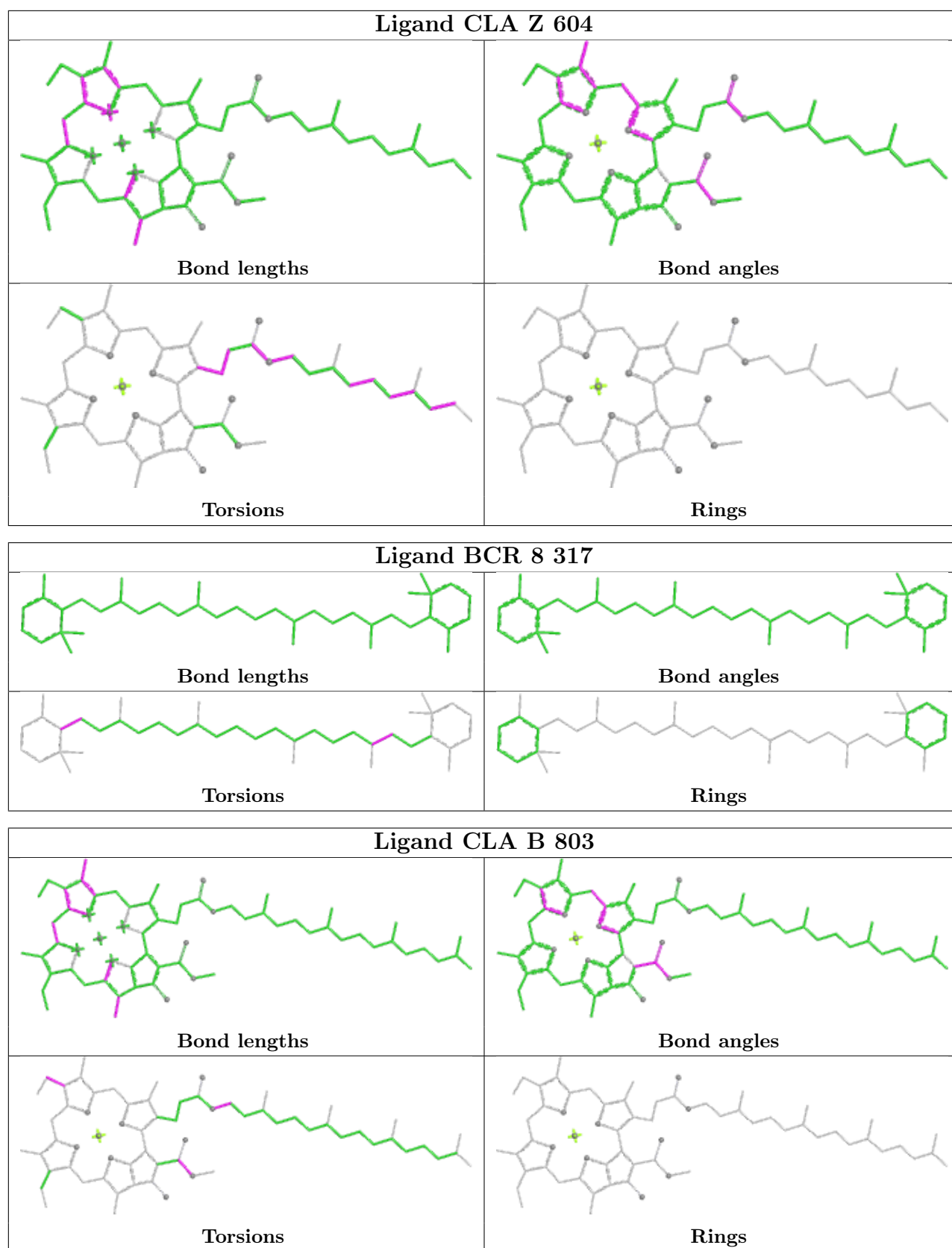


Torsions

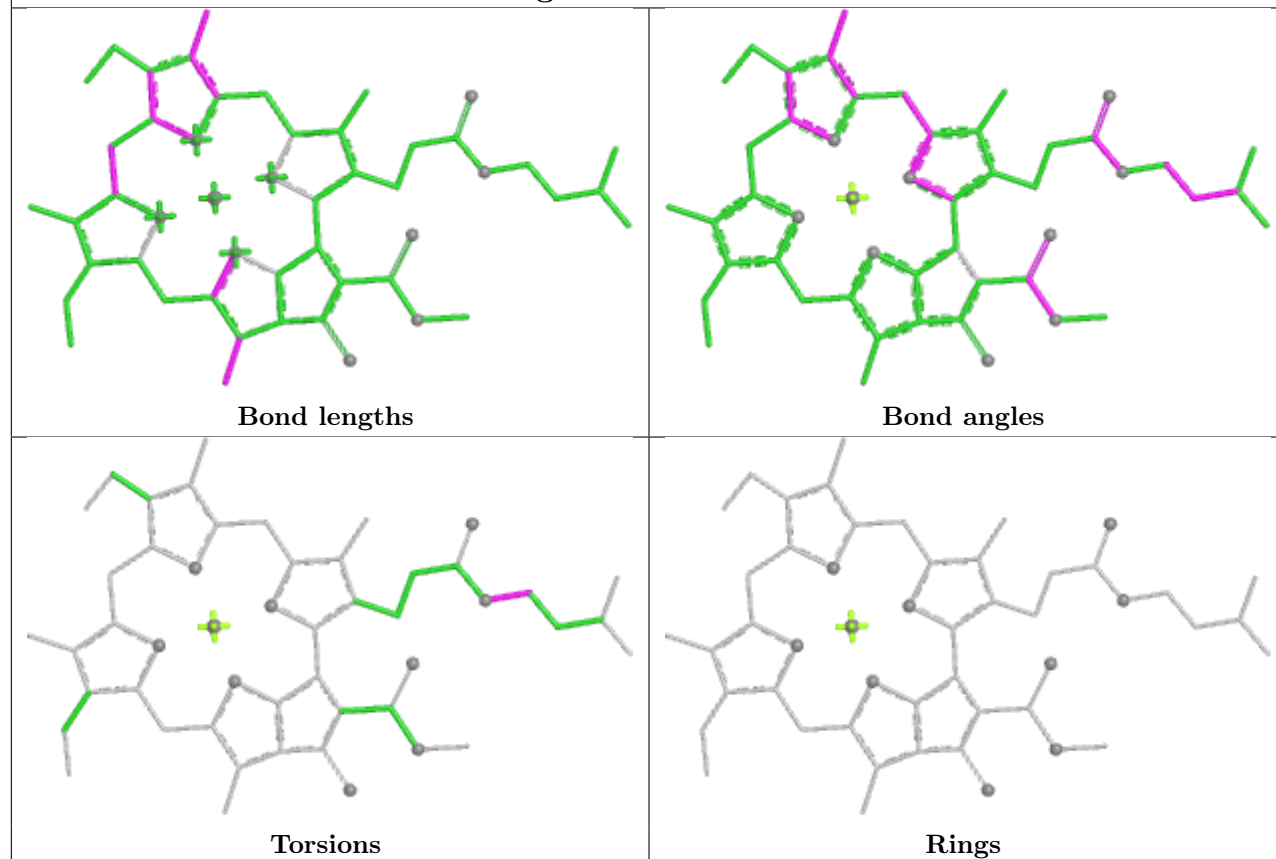


Rings

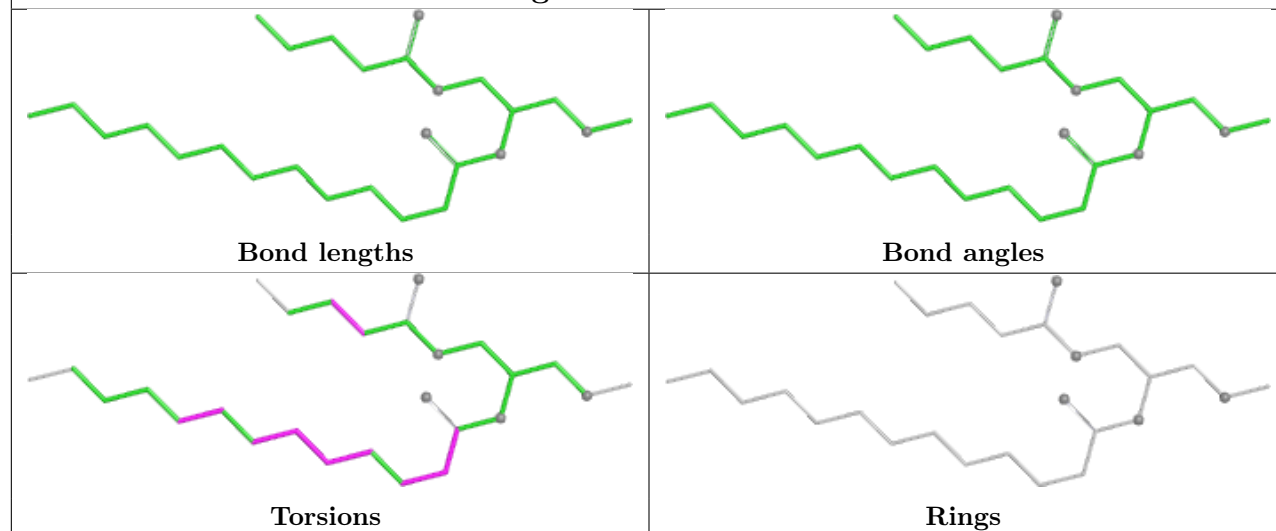
**Ligand LUT 3 316****Ligand CLA 3 303****Ligand LMU 3 325**



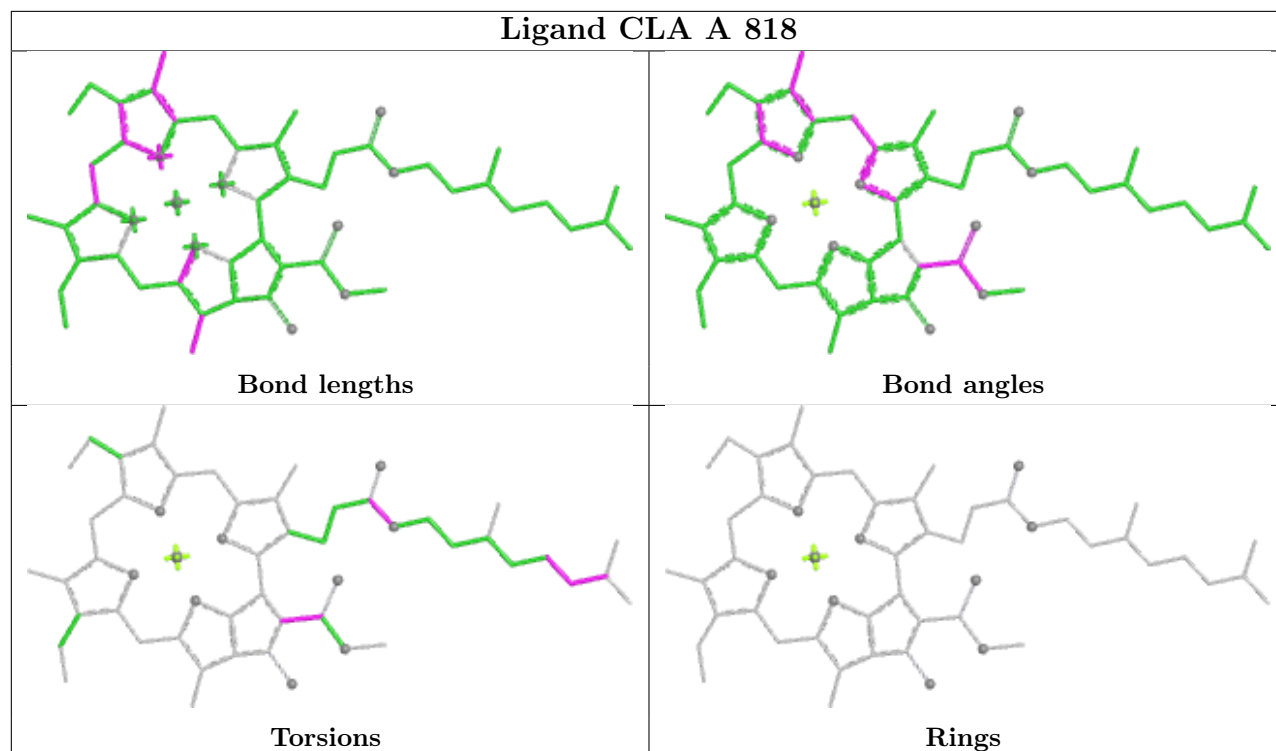
## Ligand CLA 7 607



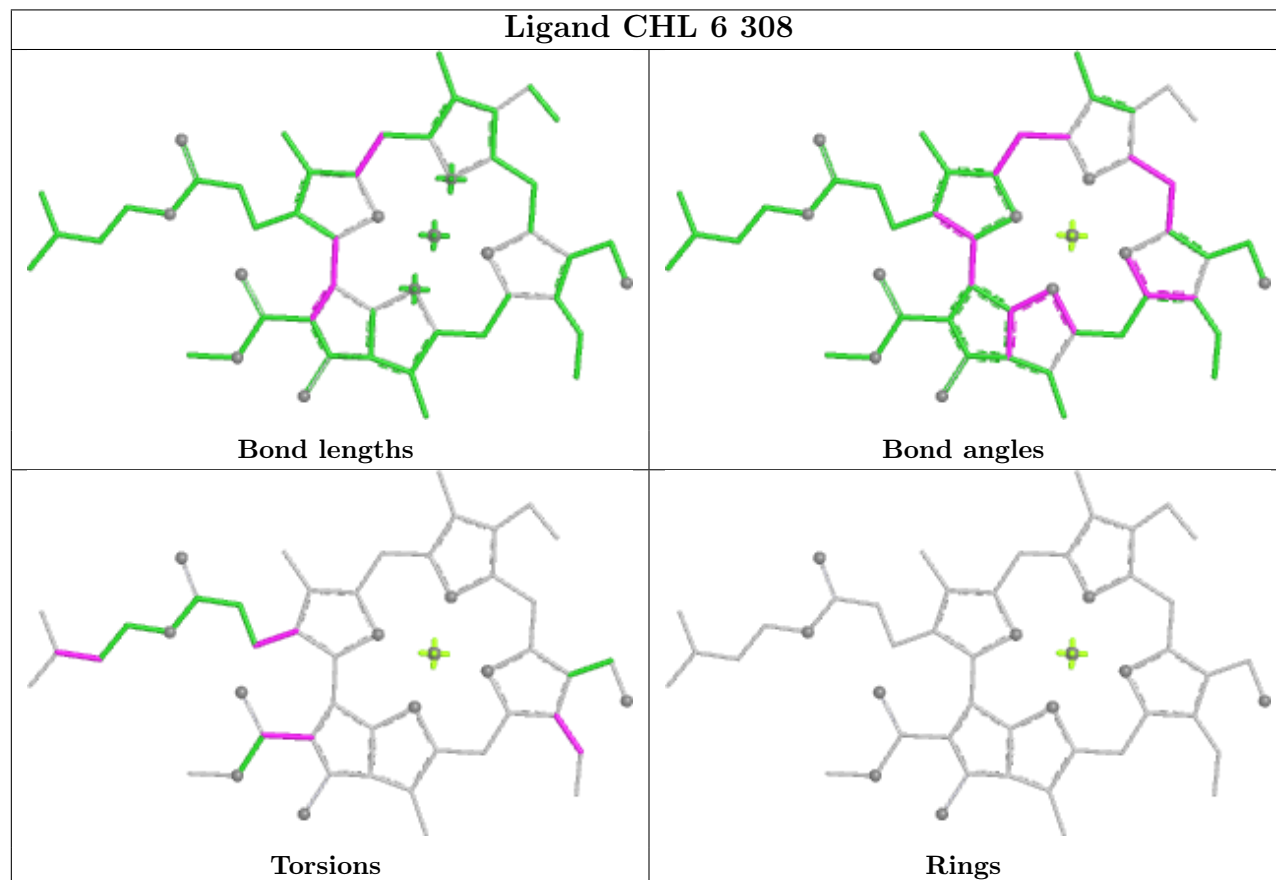
## Ligand LMG 6 301

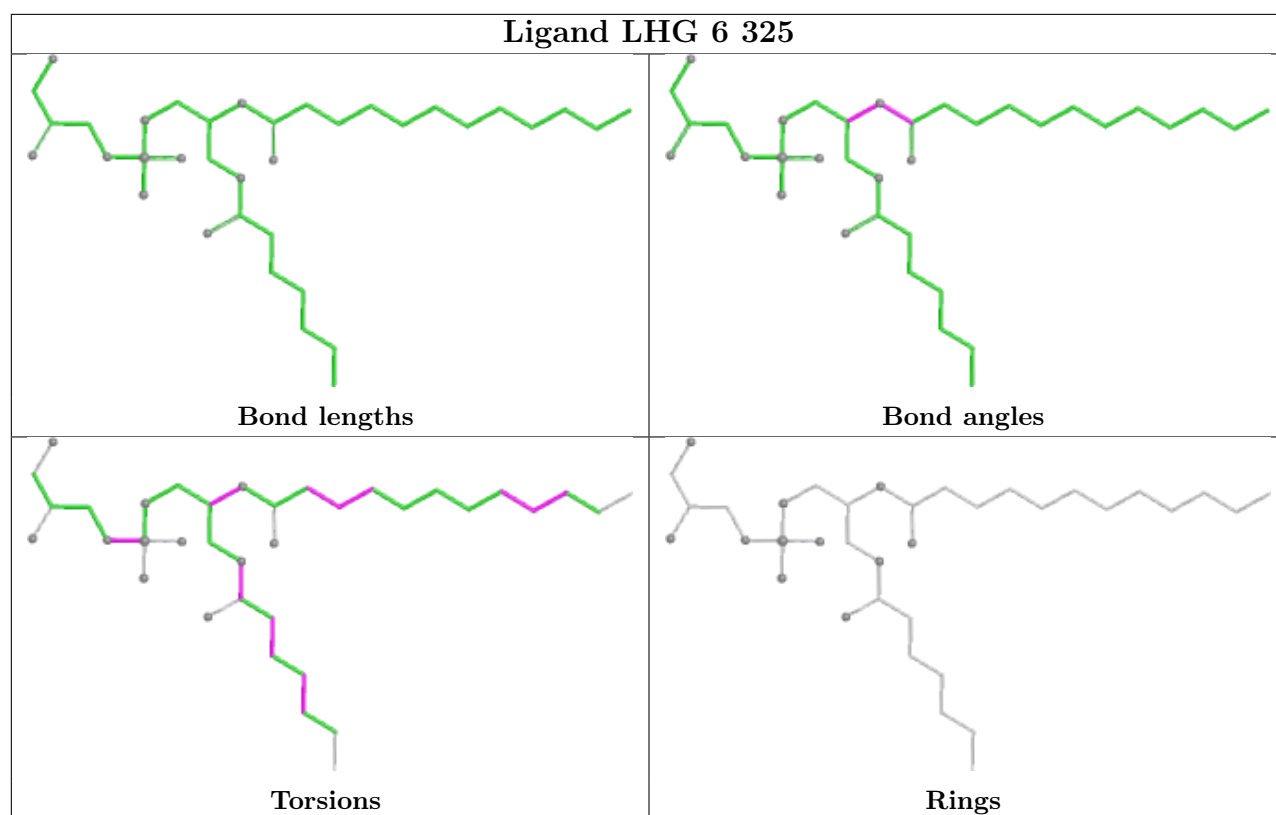


## Ligand CLA A 818



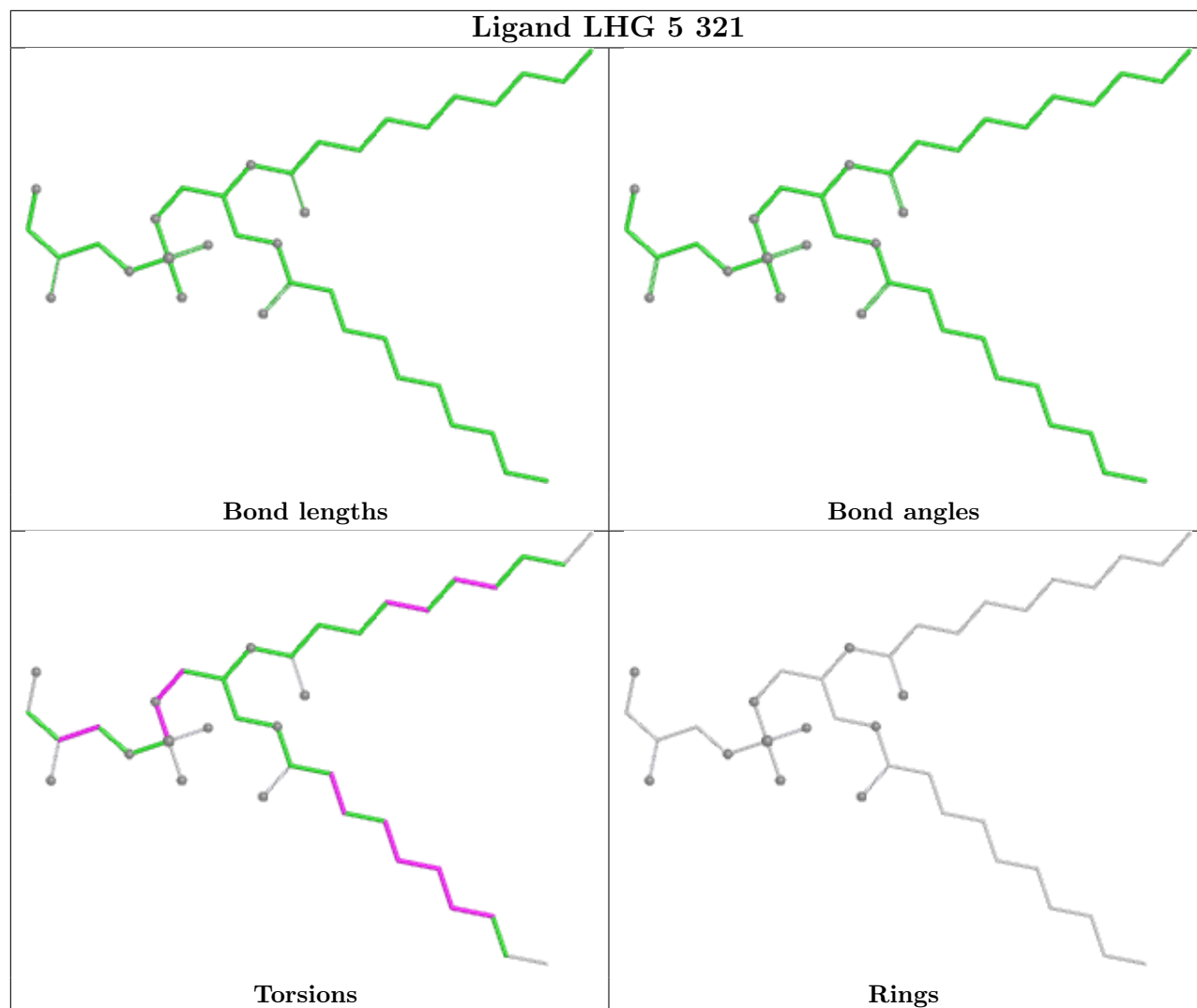
## Ligand CHL 6 308



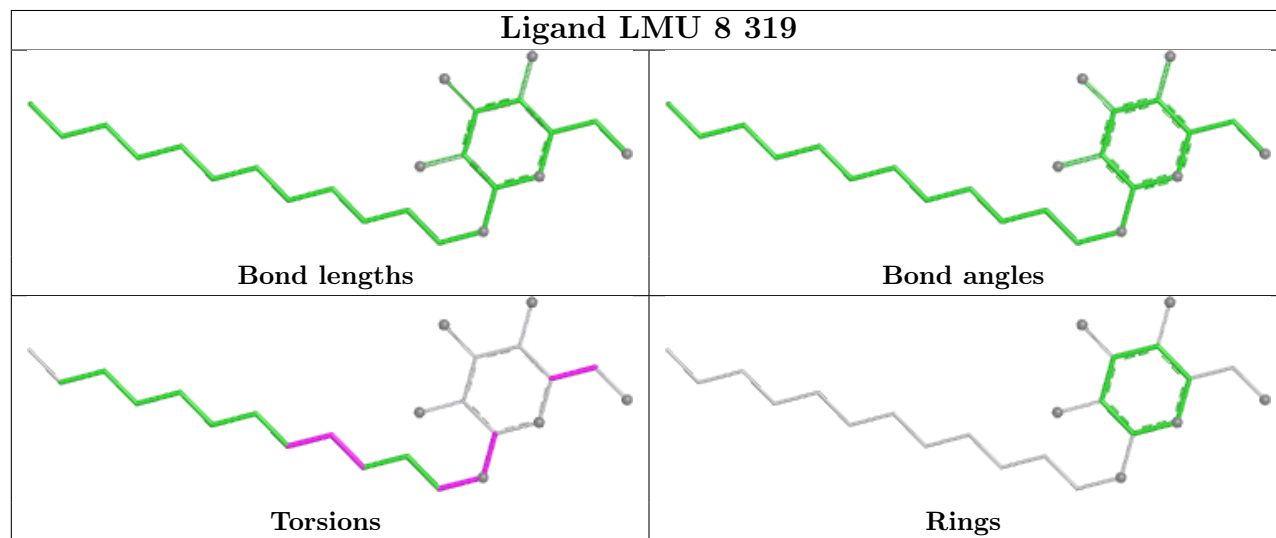


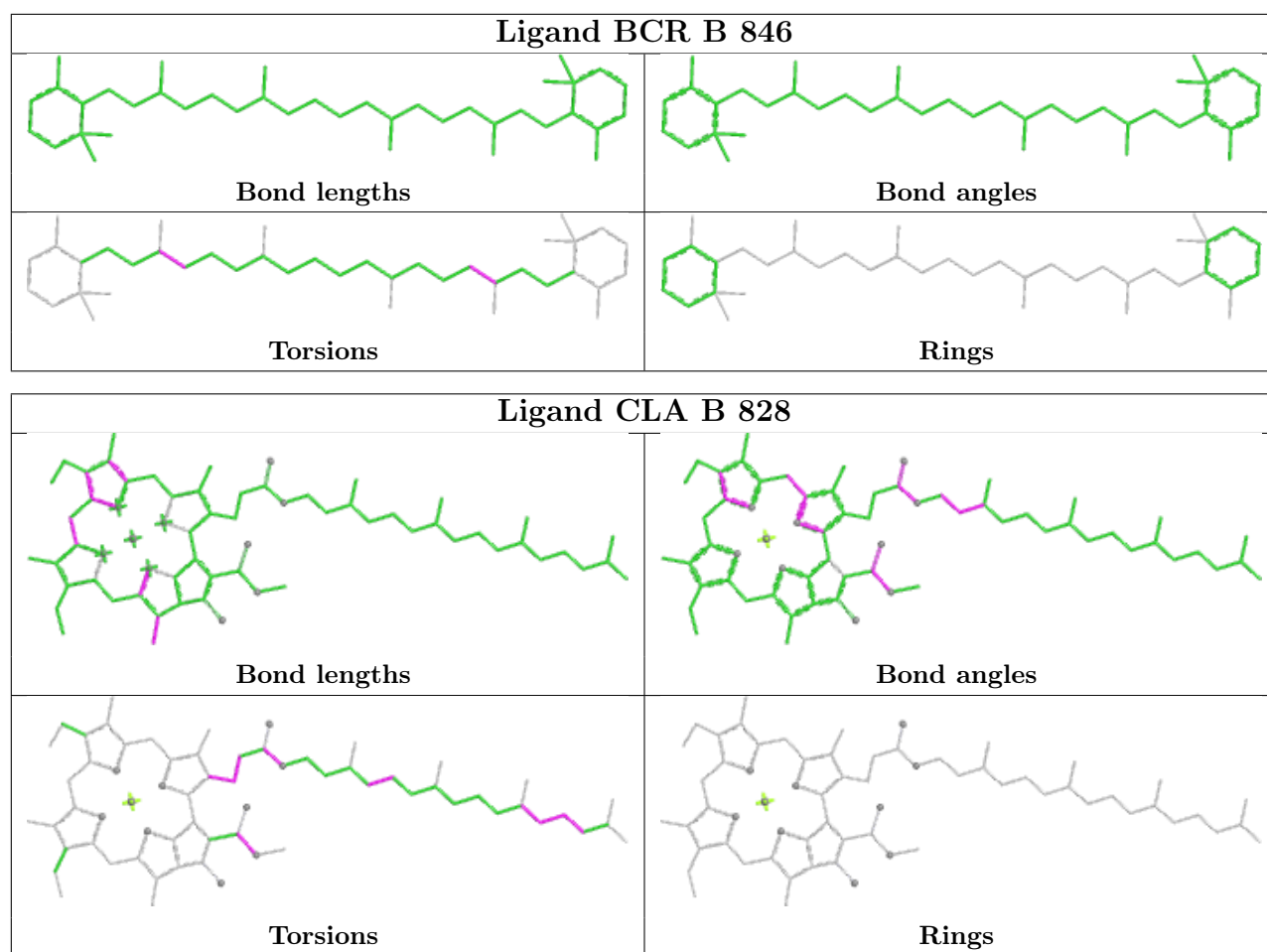


## Ligand LHG 5 321

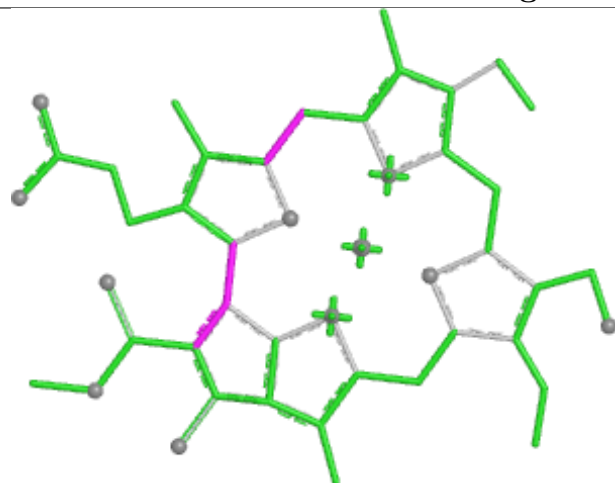


## Ligand LMU 8 319

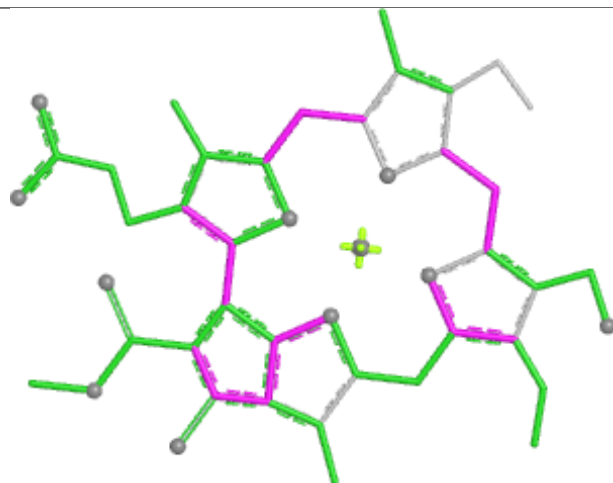




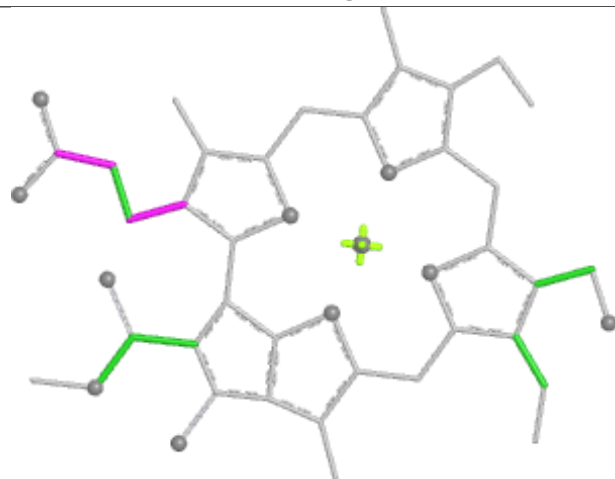
## Ligand CHL 6 306



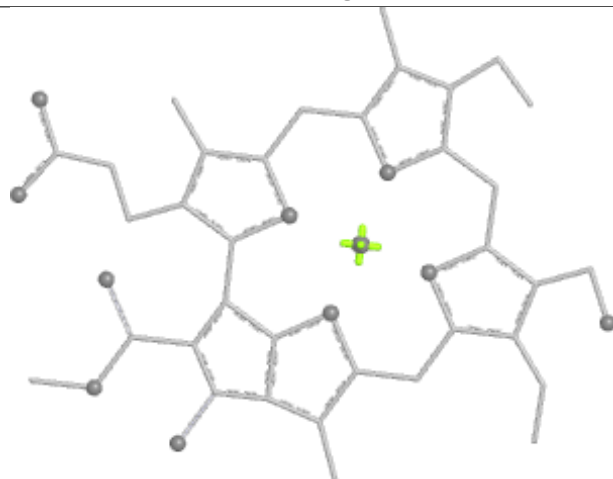
Bond lengths



Bond angles

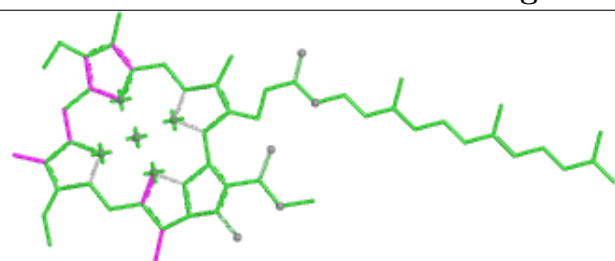


Torsions

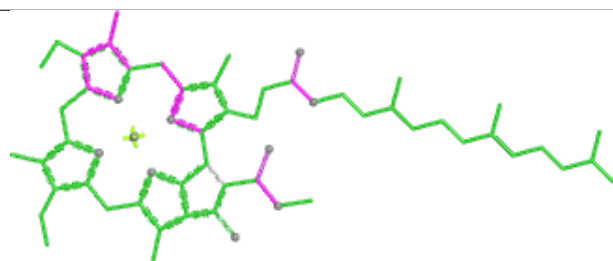


Rings

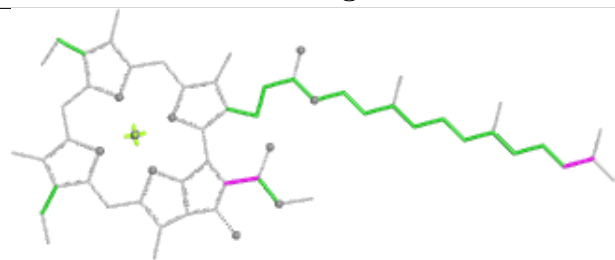
## Ligand CLA 3 301



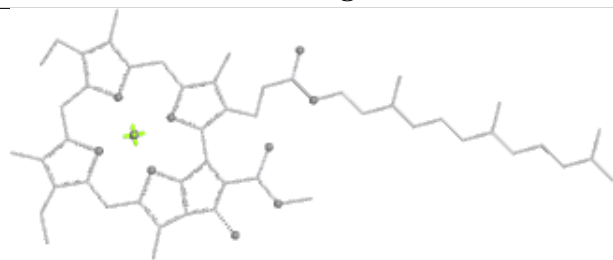
Bond lengths



Bond angles

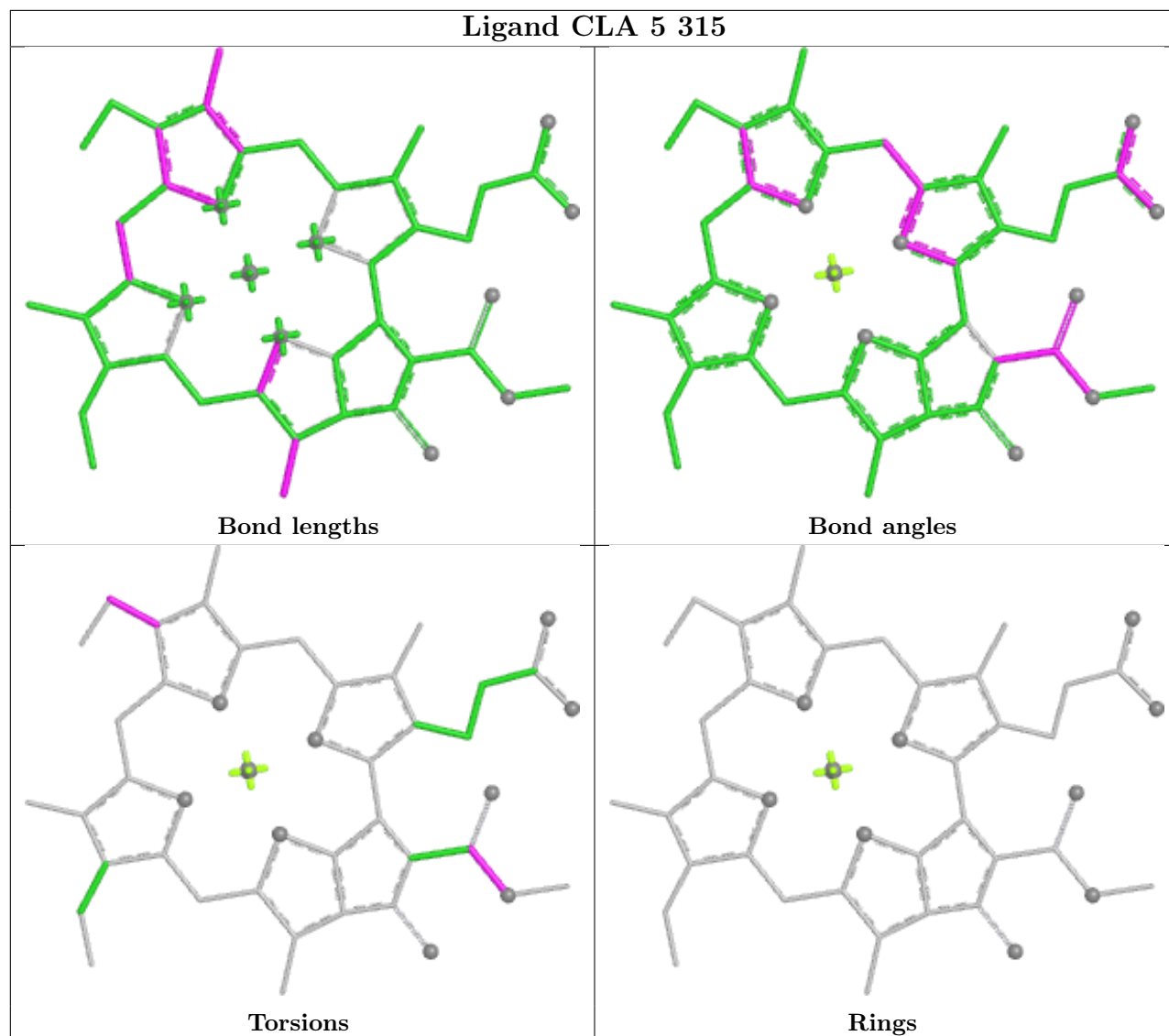


Torsions

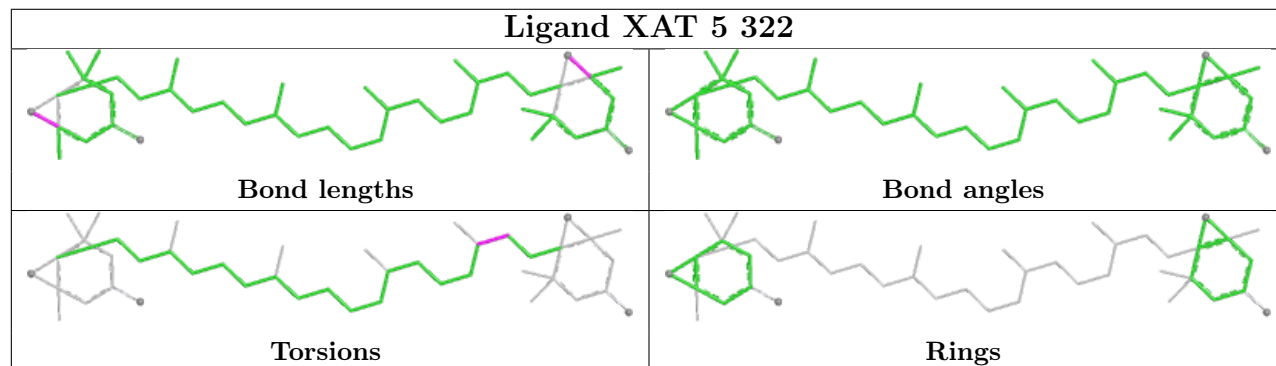


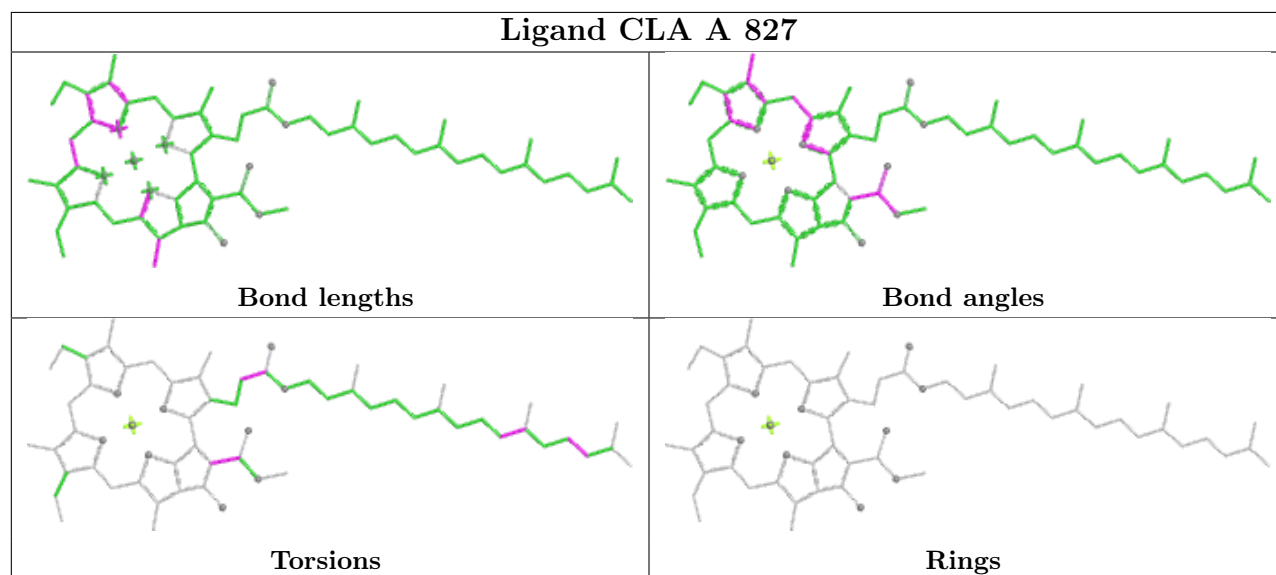
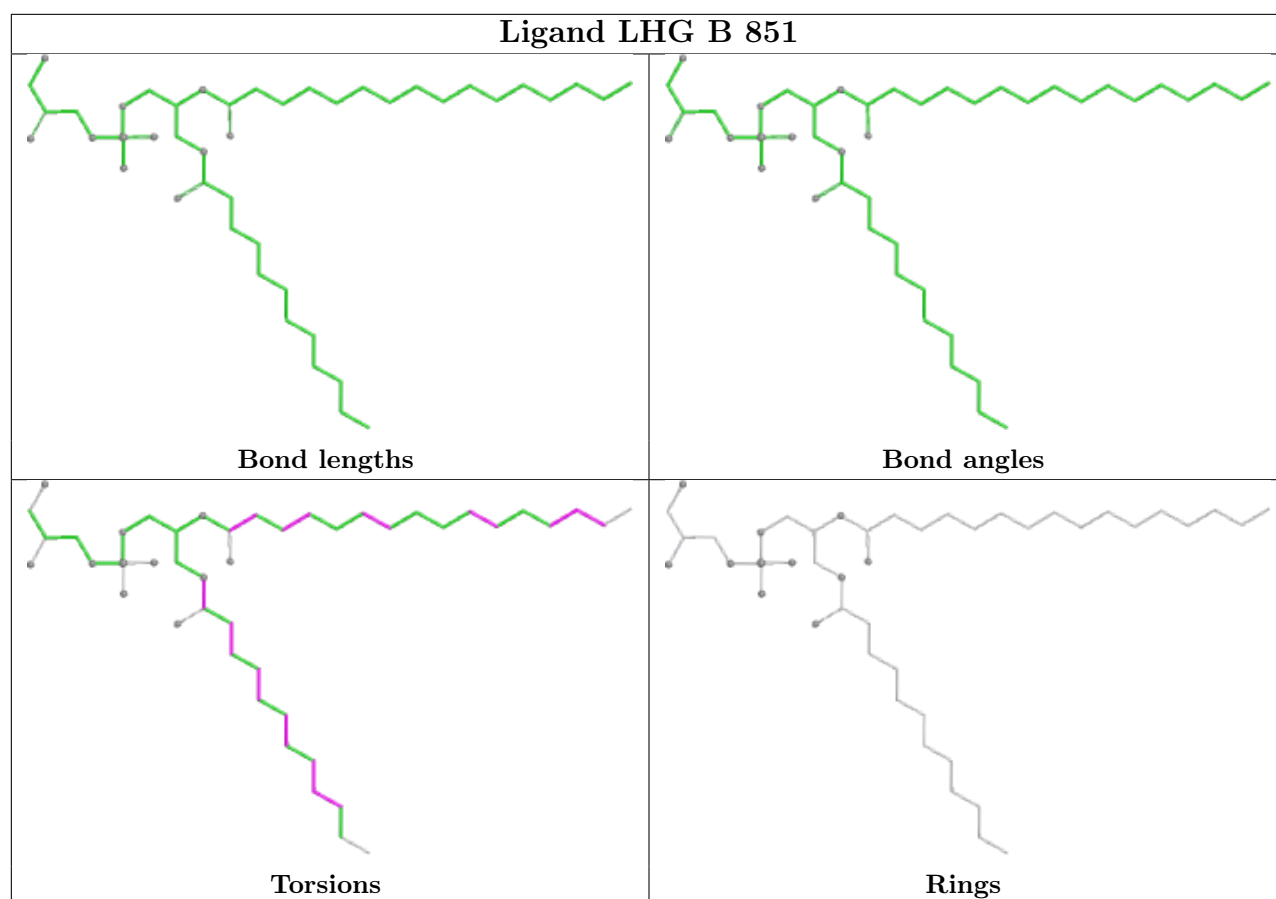
Rings

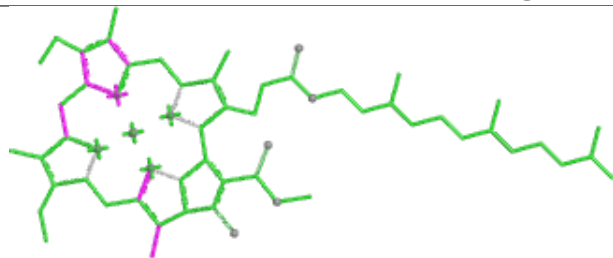
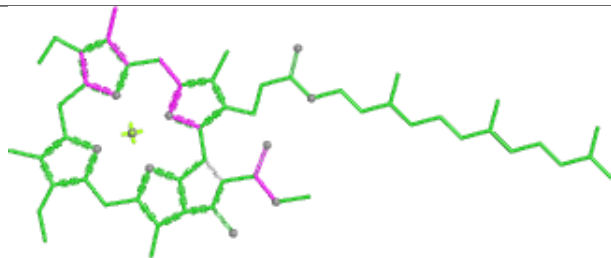
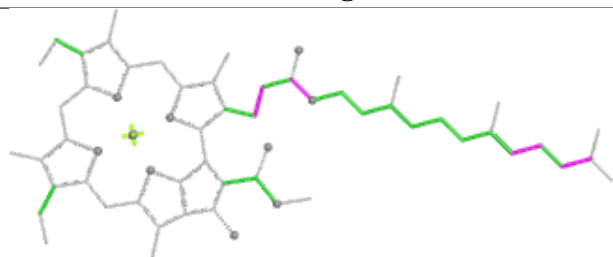
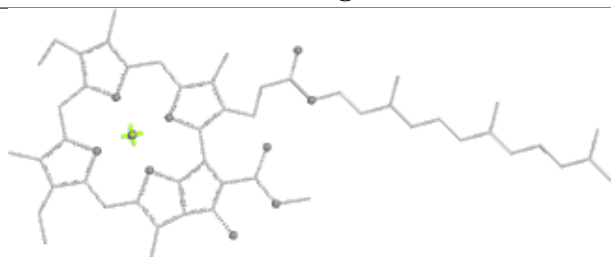
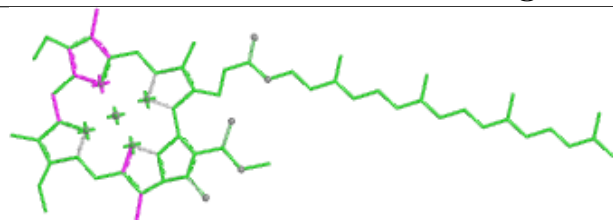
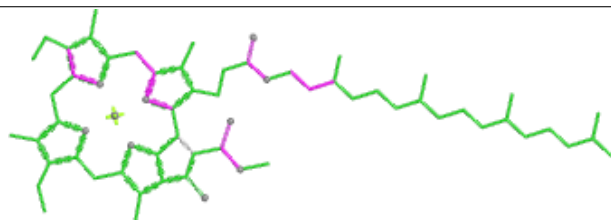
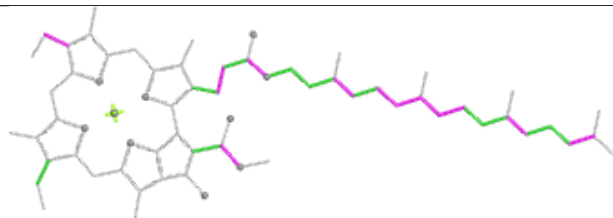
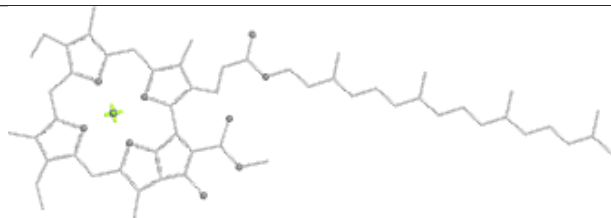
## Ligand CLA 5 315

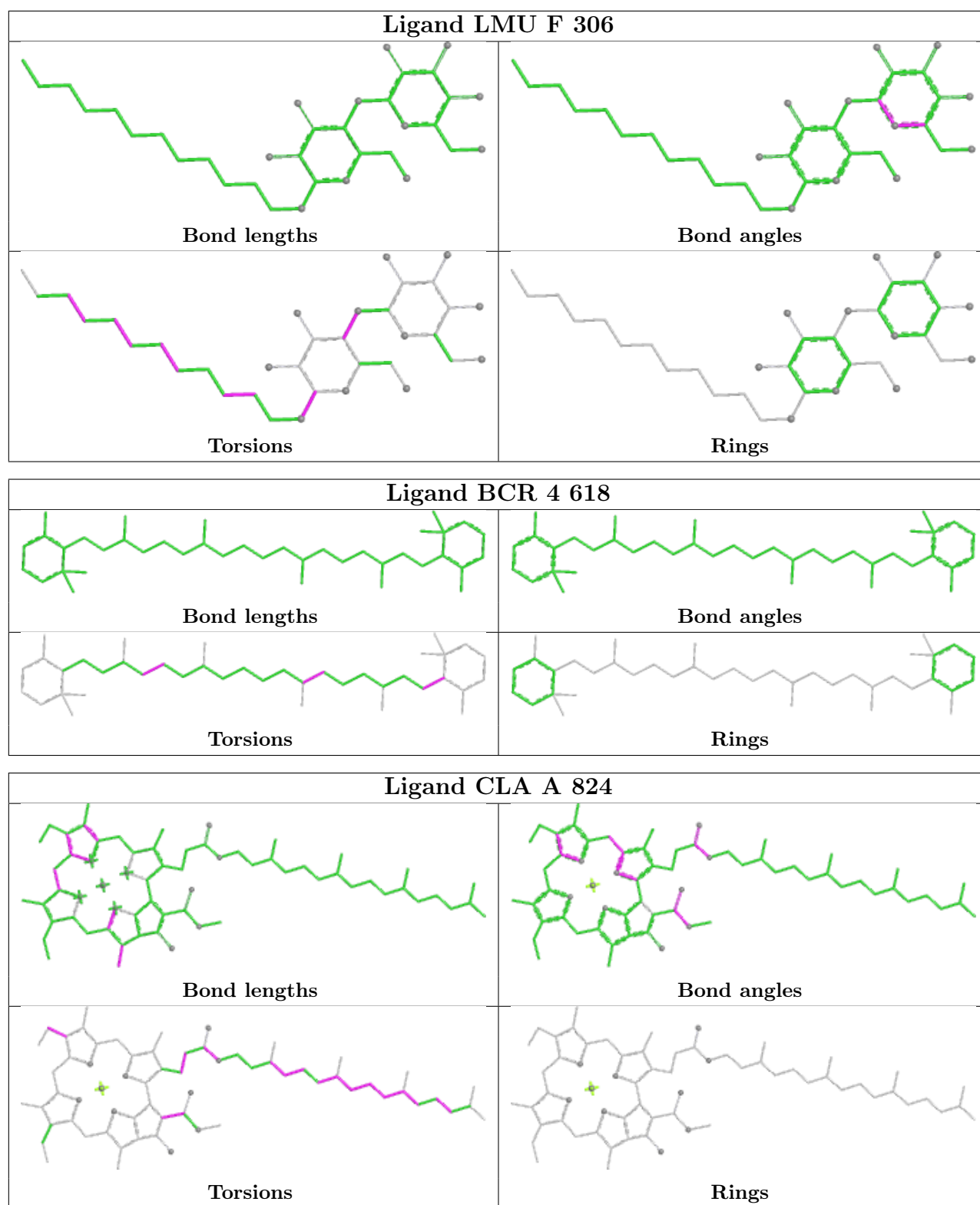


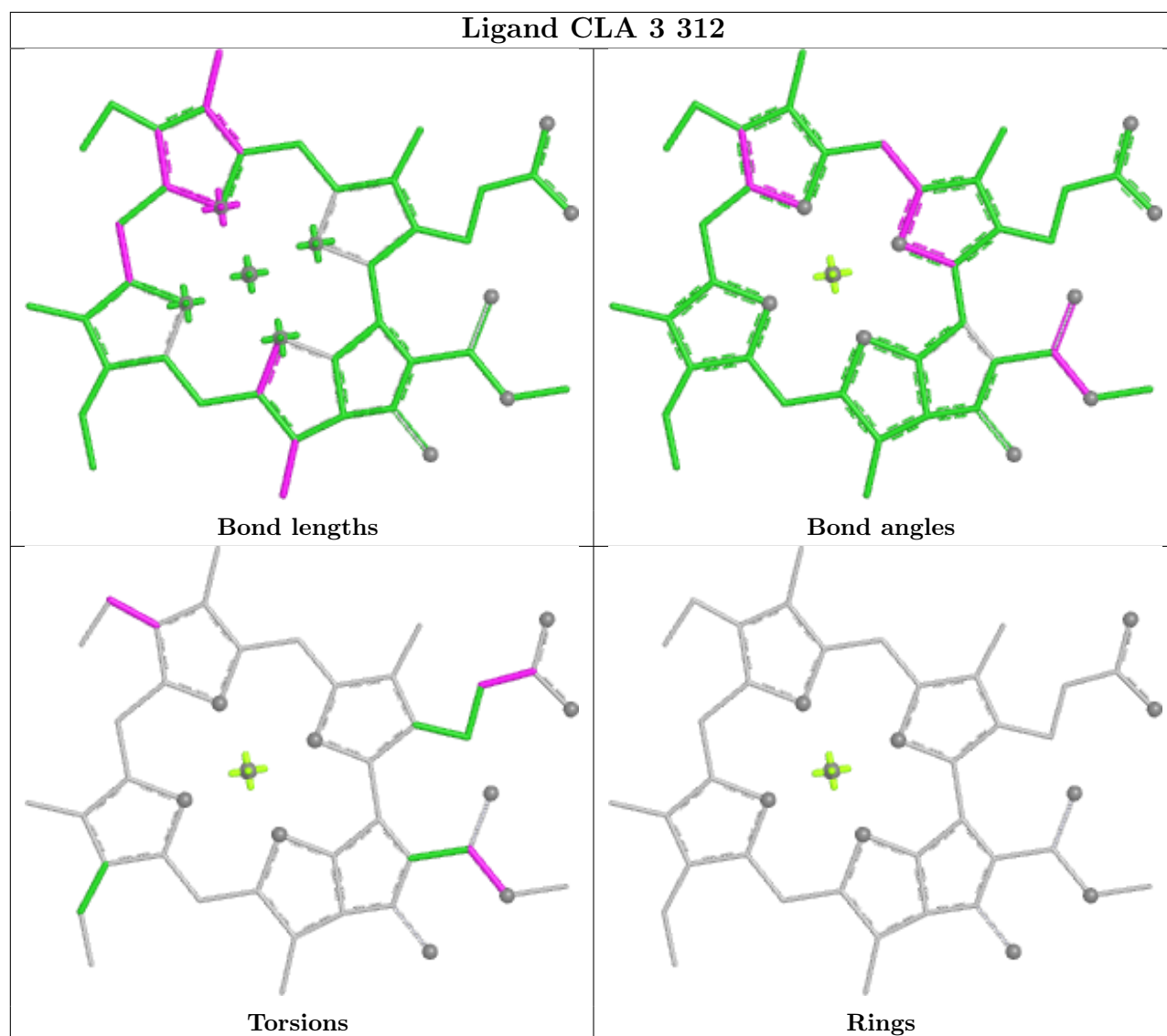
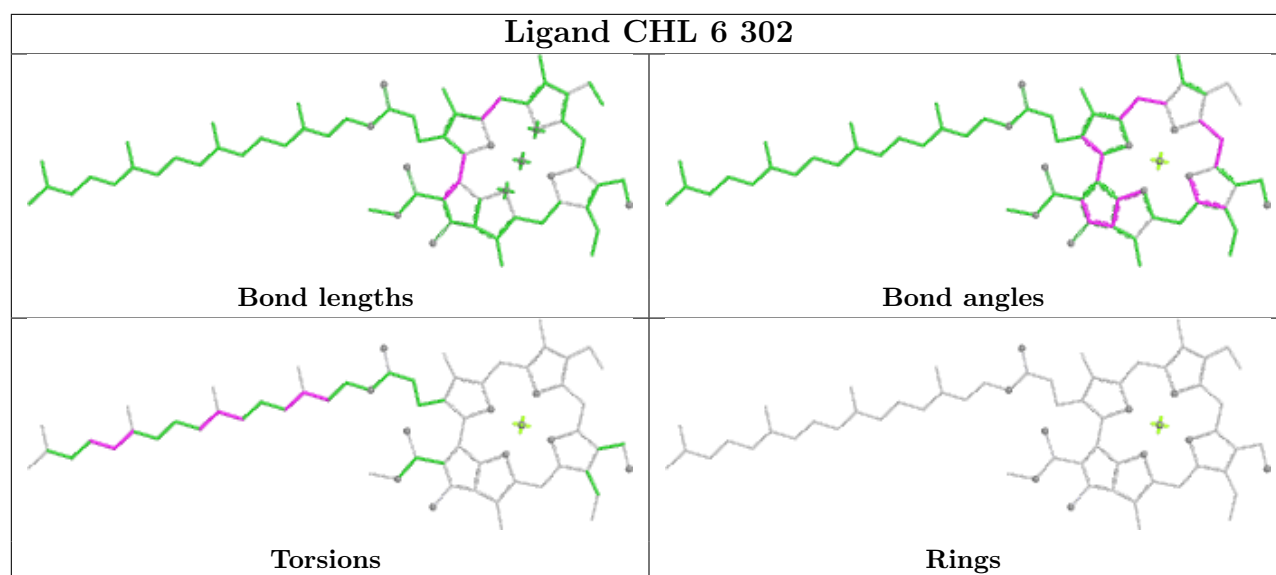
## Ligand XAT 5 322



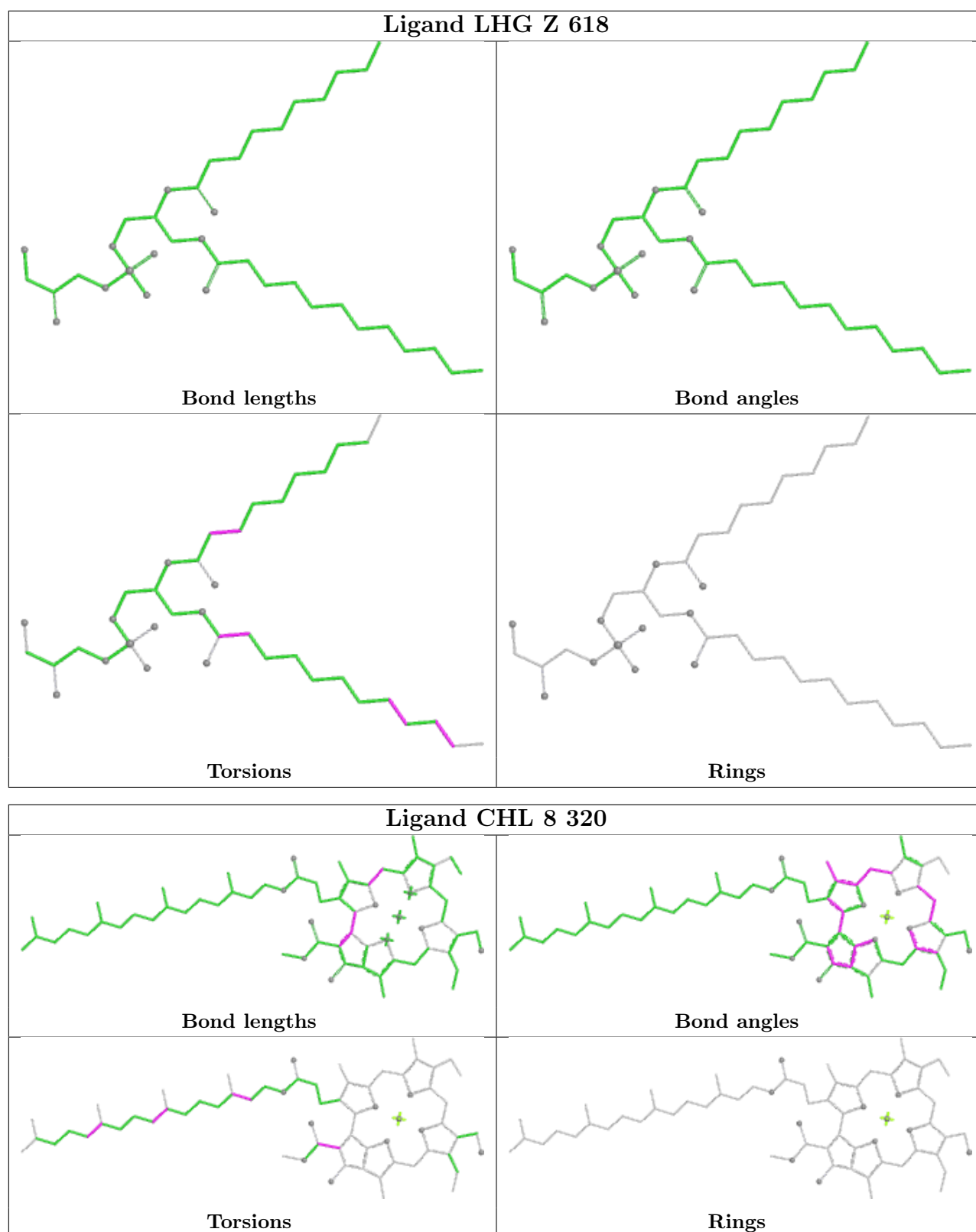


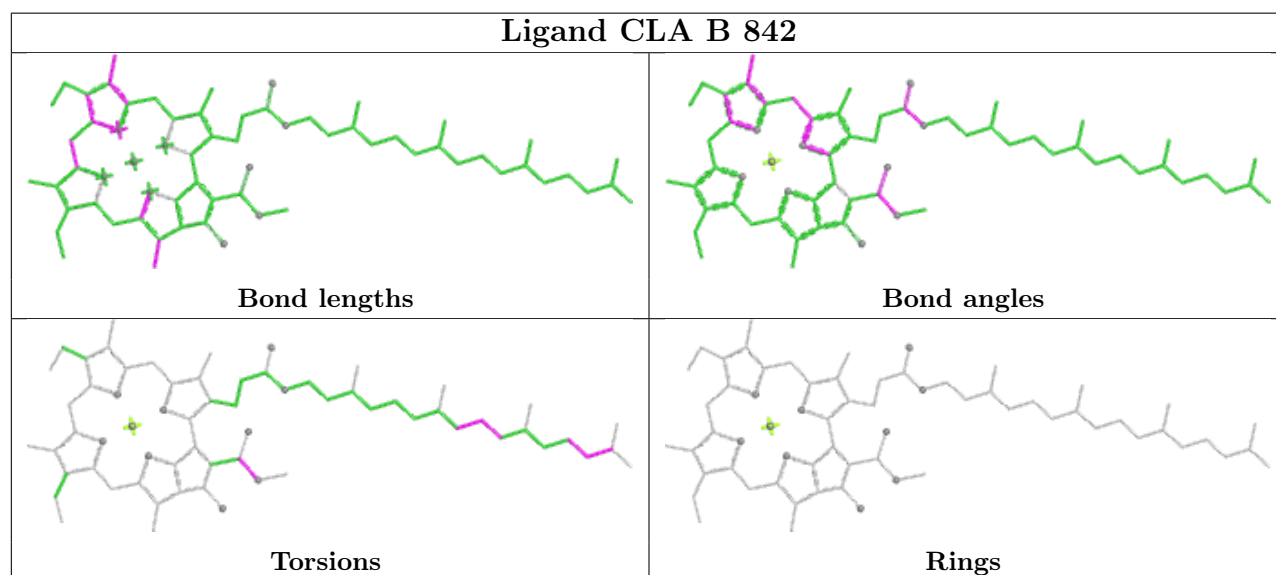
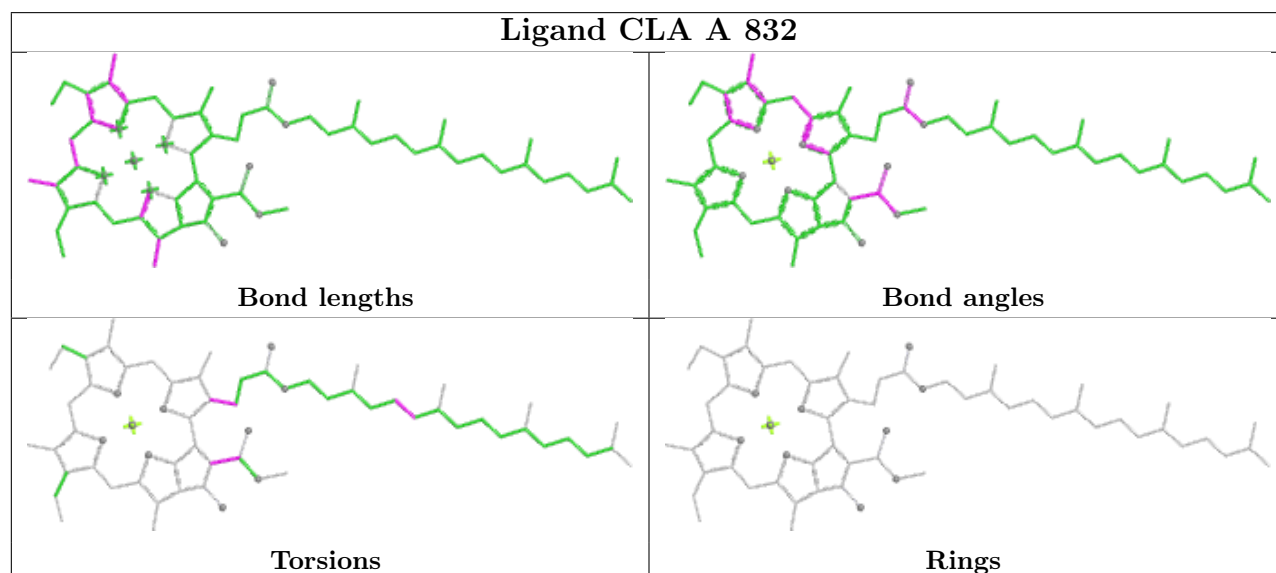
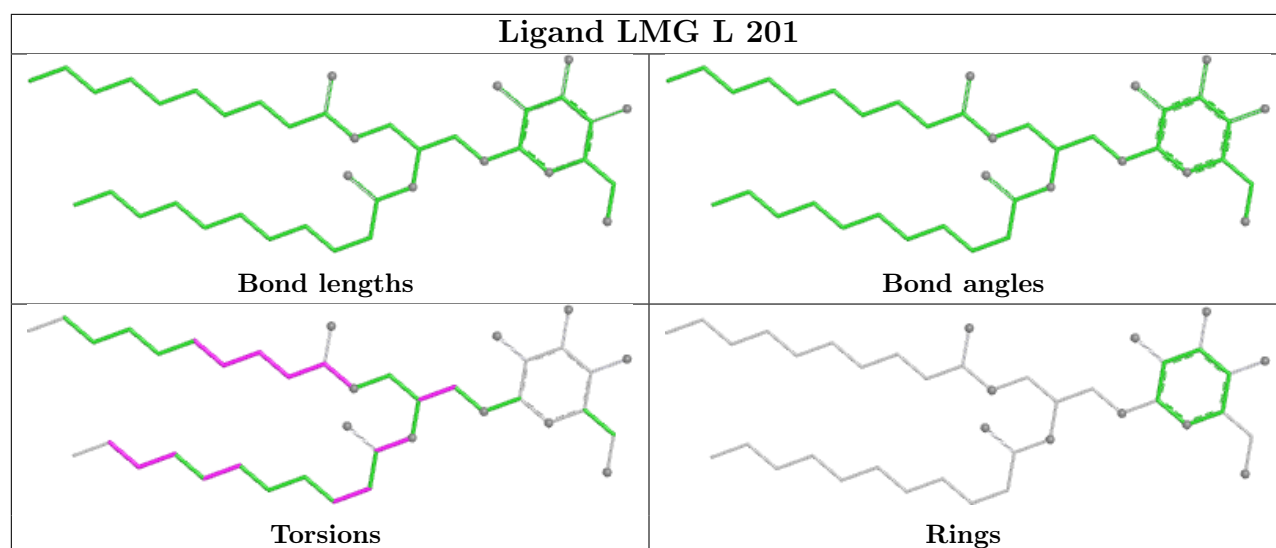
**Ligand CLA 1 302****Bond lengths****Bond angles****Torsions****Rings****Ligand CLA 6 305****Bond lengths****Bond angles****Torsions****Rings**

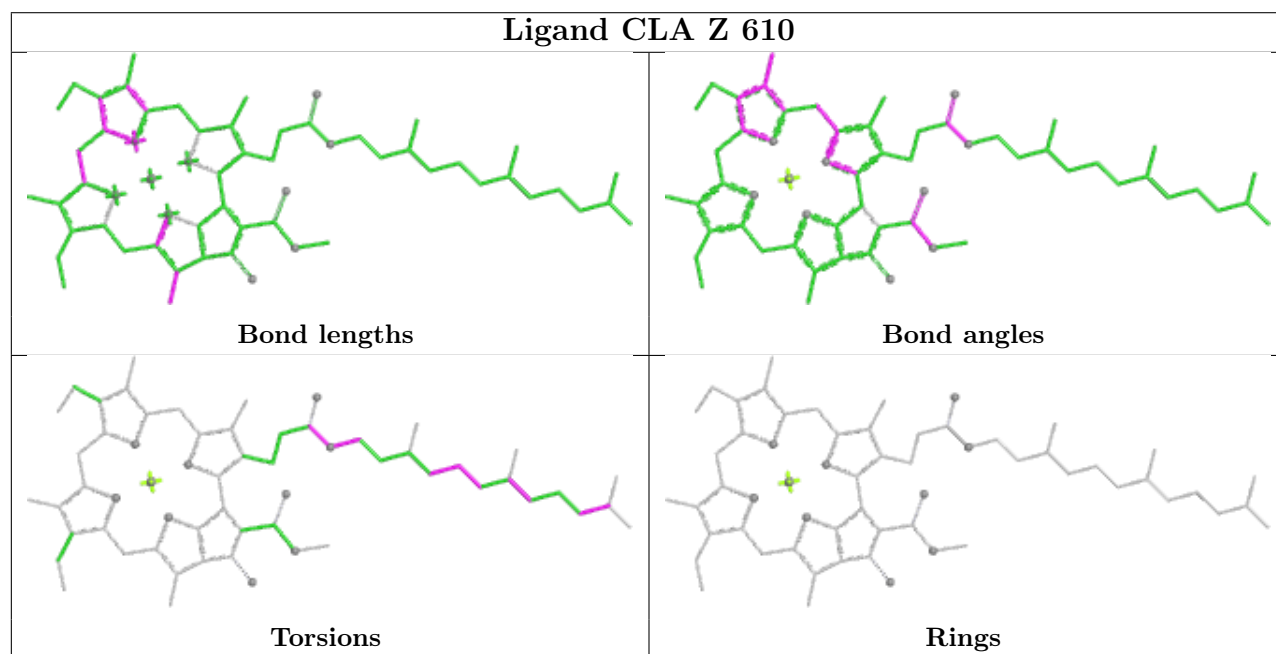
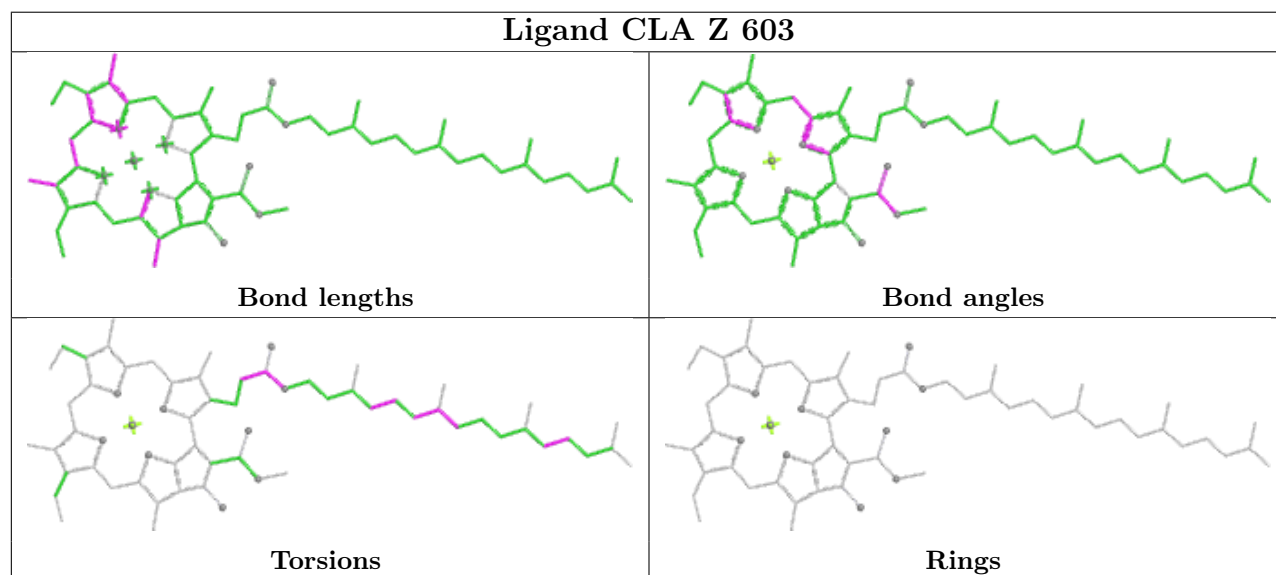
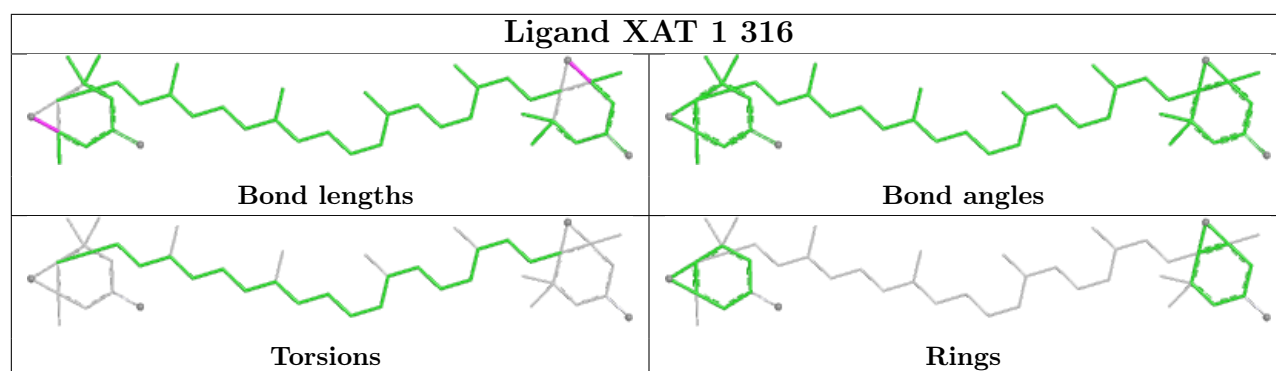




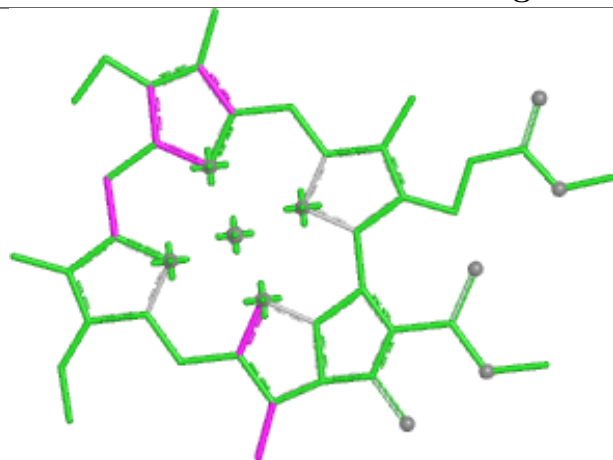




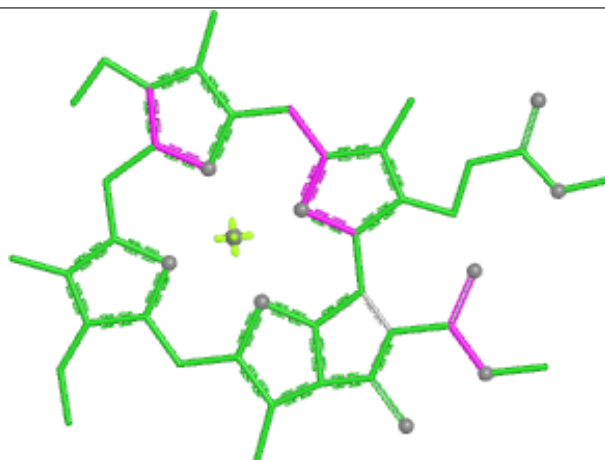




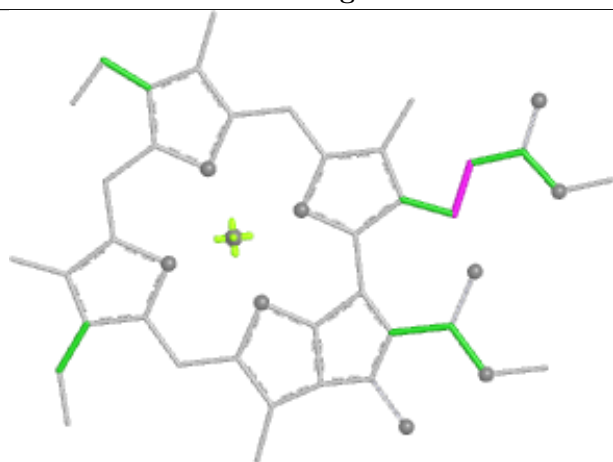
## Ligand CLA G 203



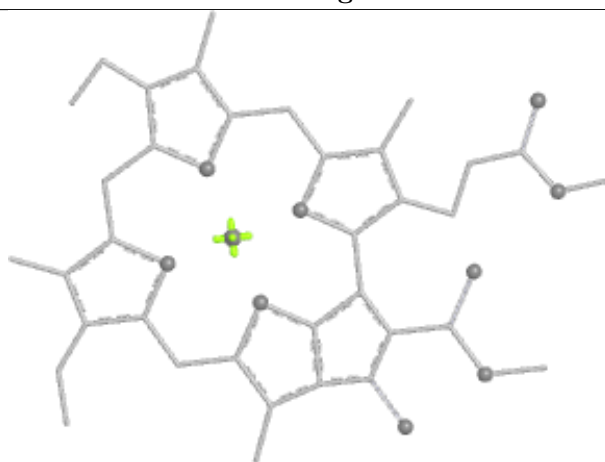
Bond lengths



Bond angles



Torsions



Rings

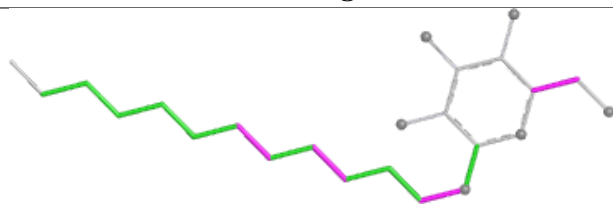
## Ligand LMU 1 321



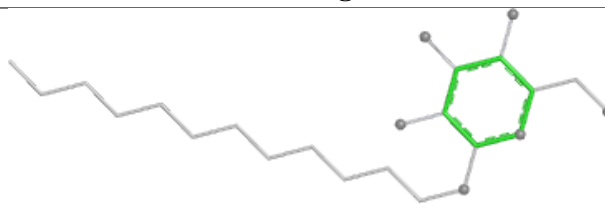
Bond lengths



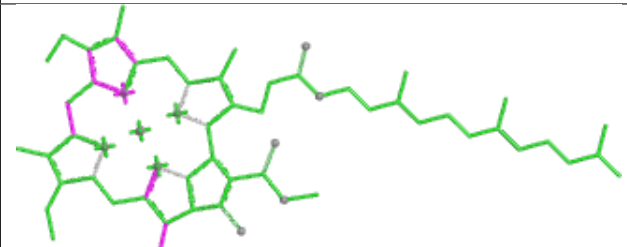
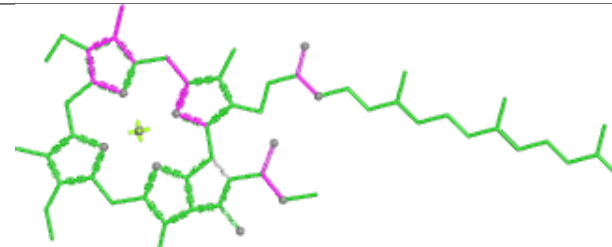
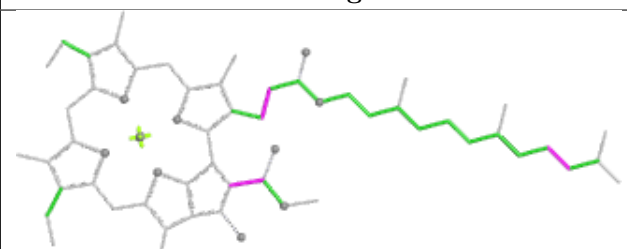
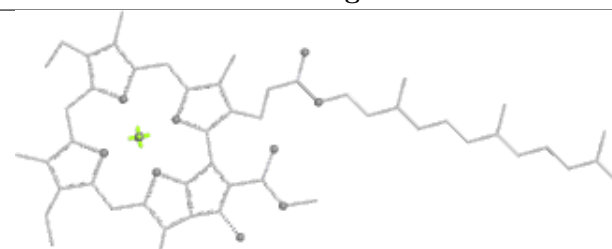
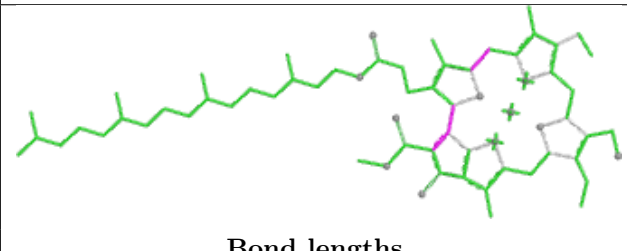
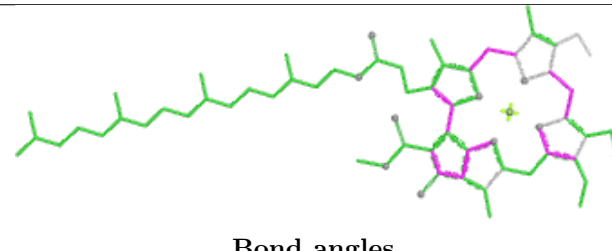
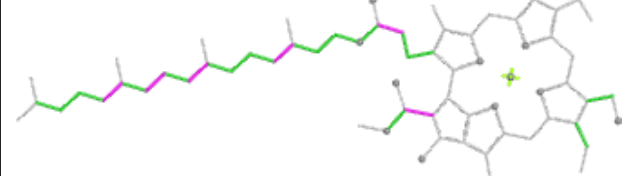
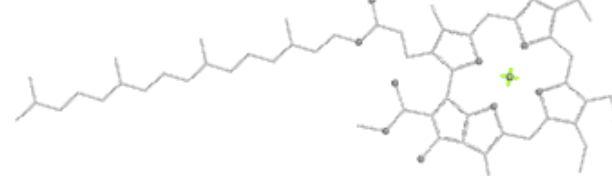
Bond angles

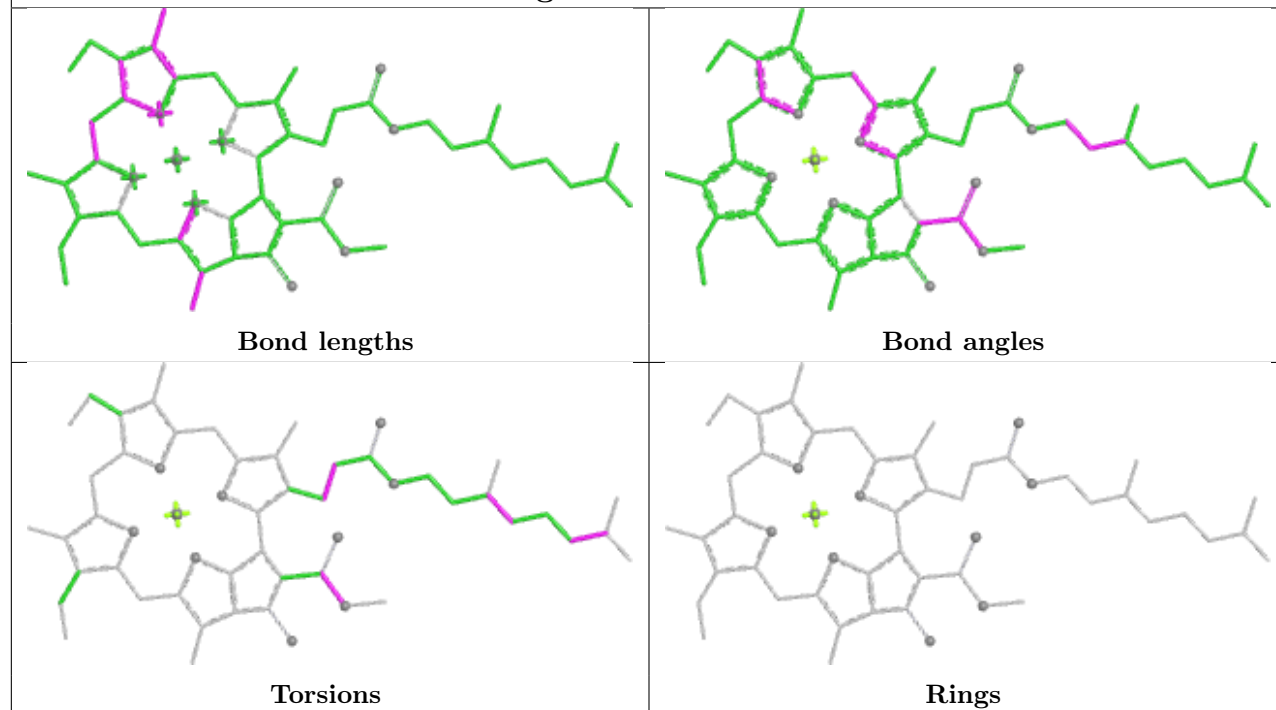
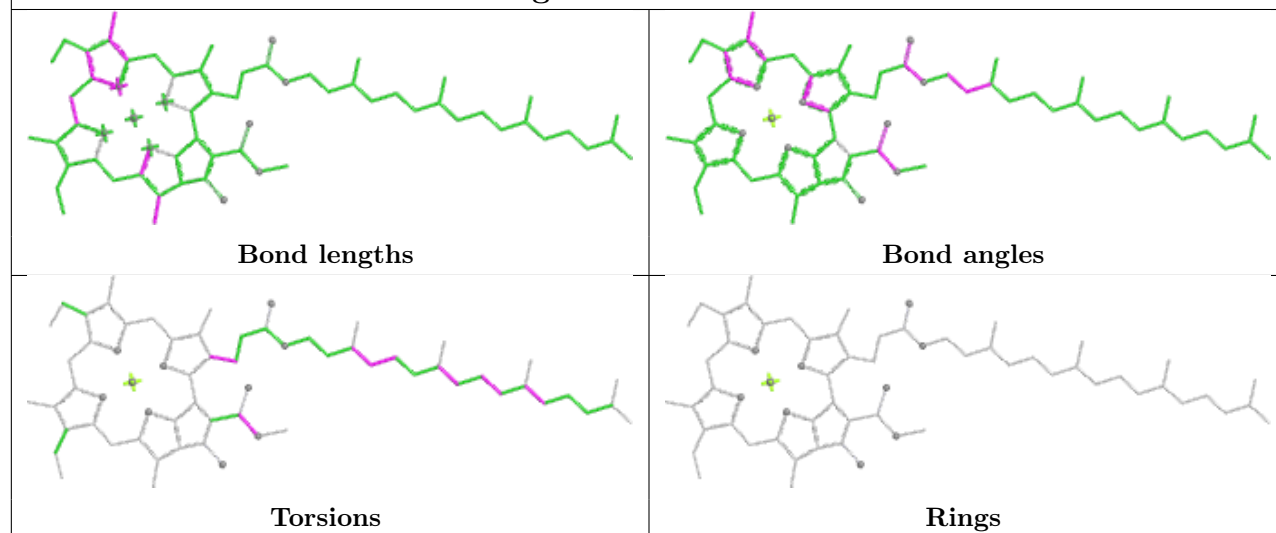


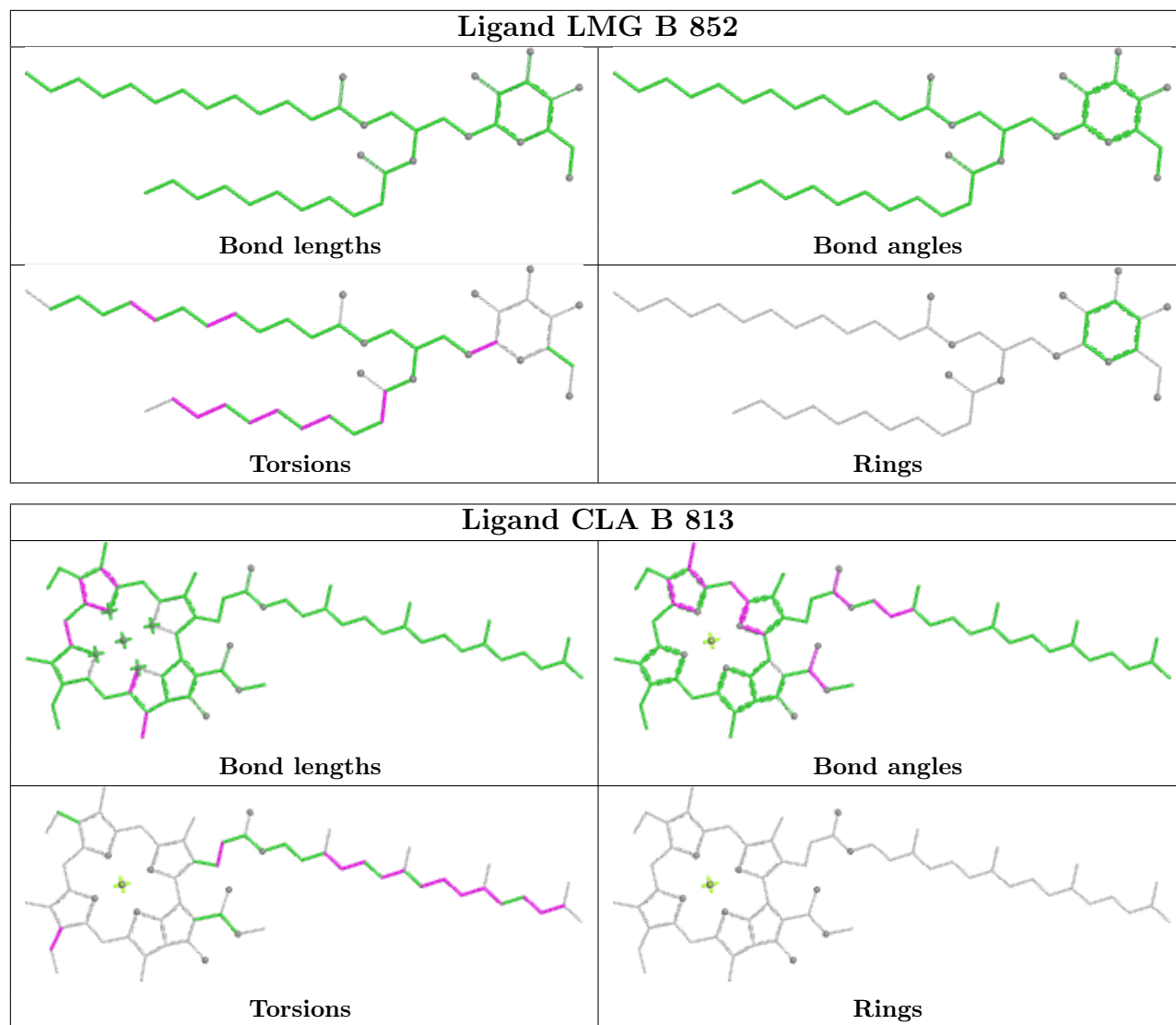
Torsions



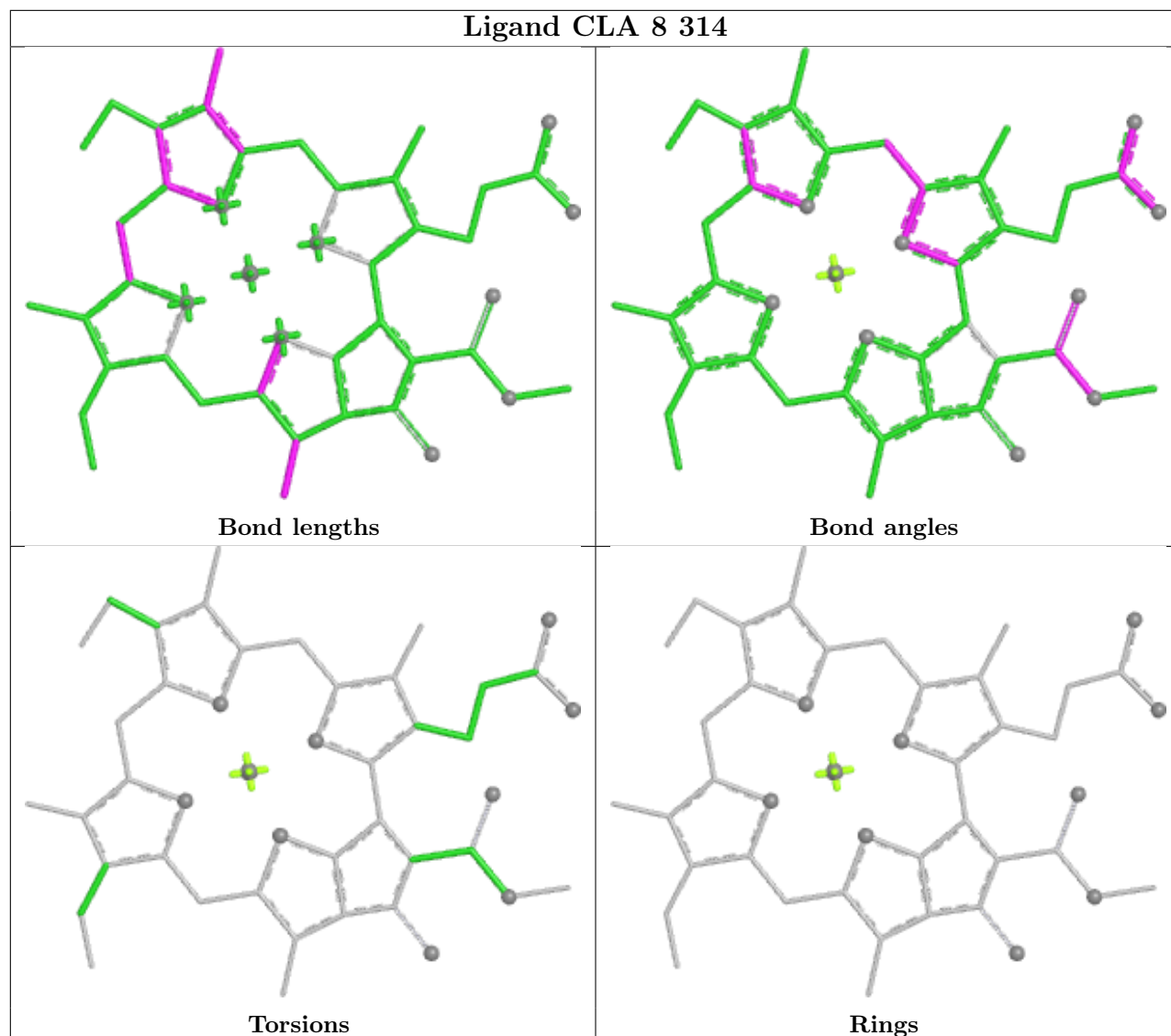
Rings

Ligand CLA 4 602	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand CHL 7 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

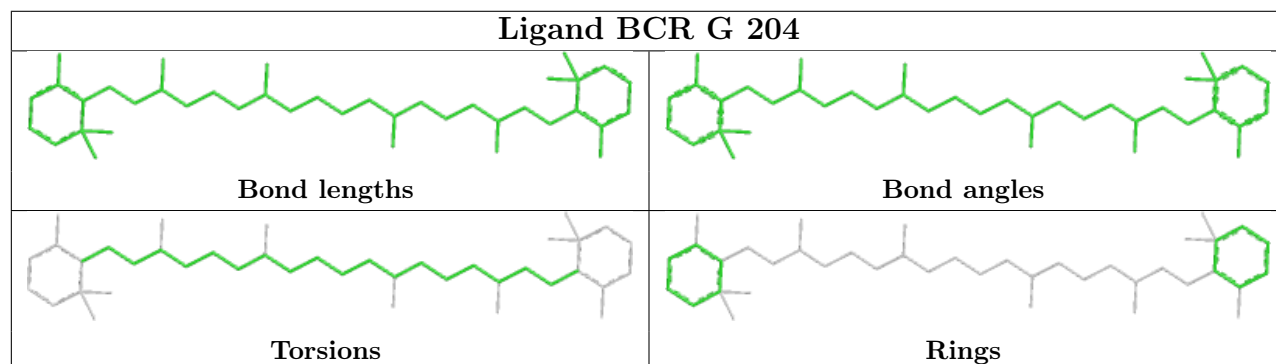
**Ligand CLA 3 309****Ligand CLA B 801**



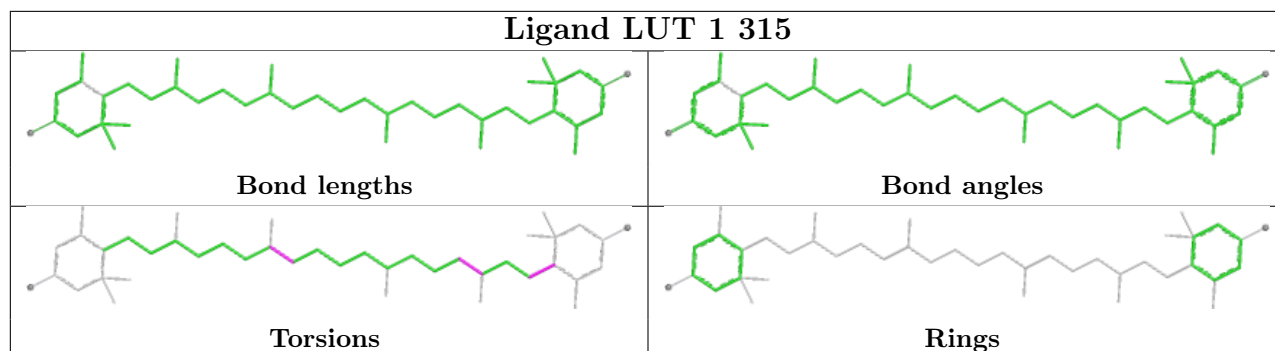
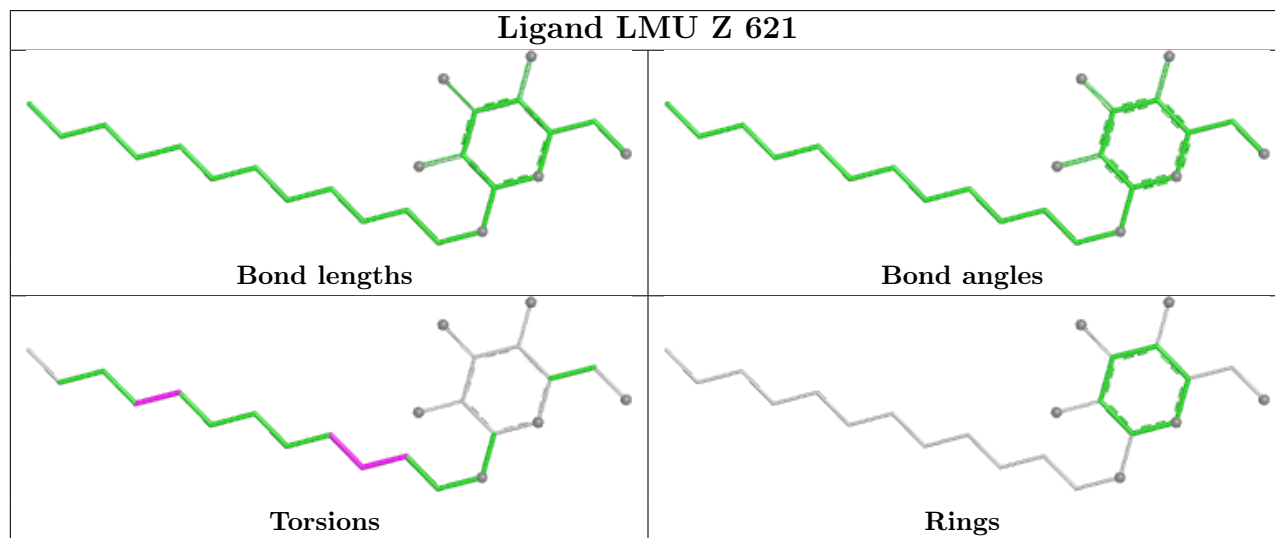
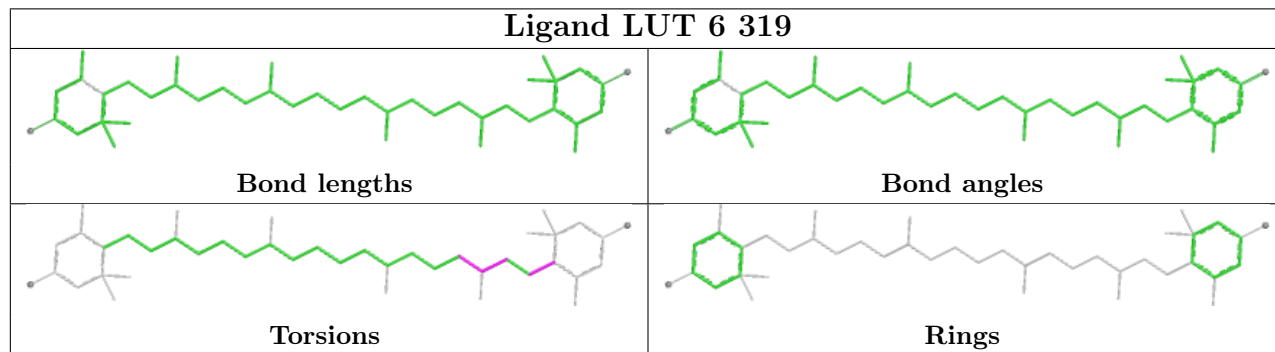
## Ligand CLA 8 314

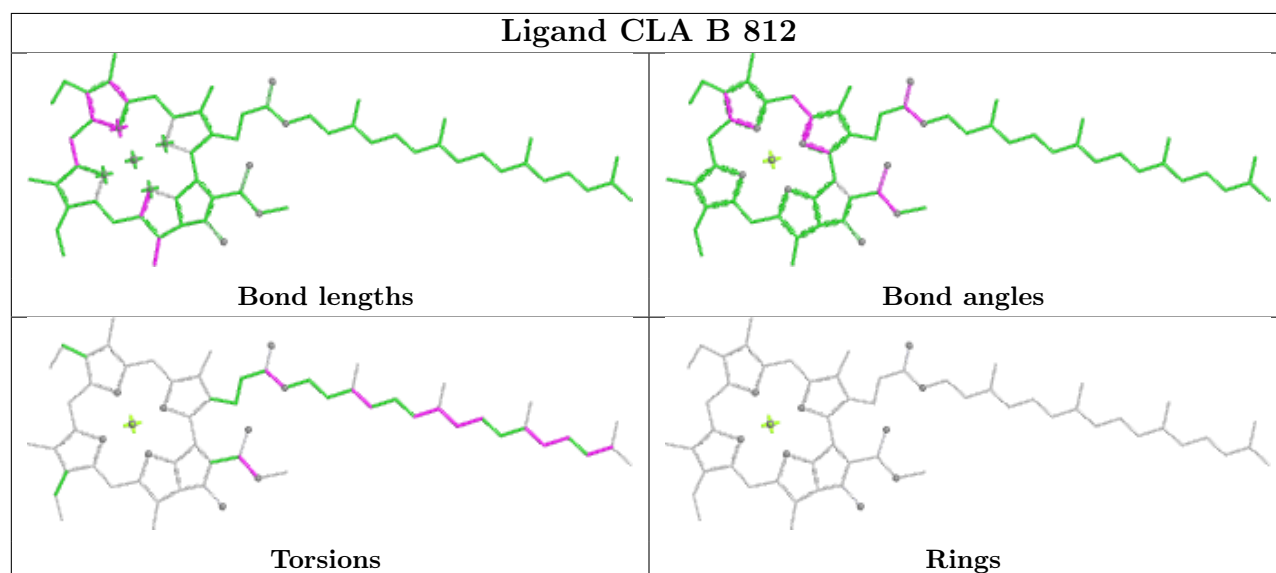
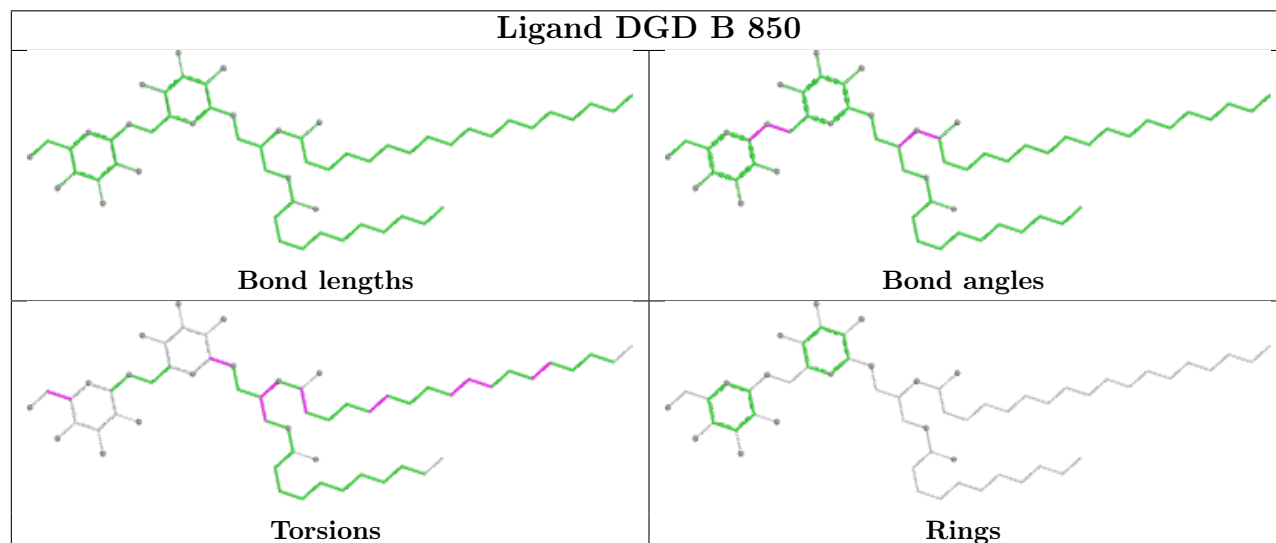
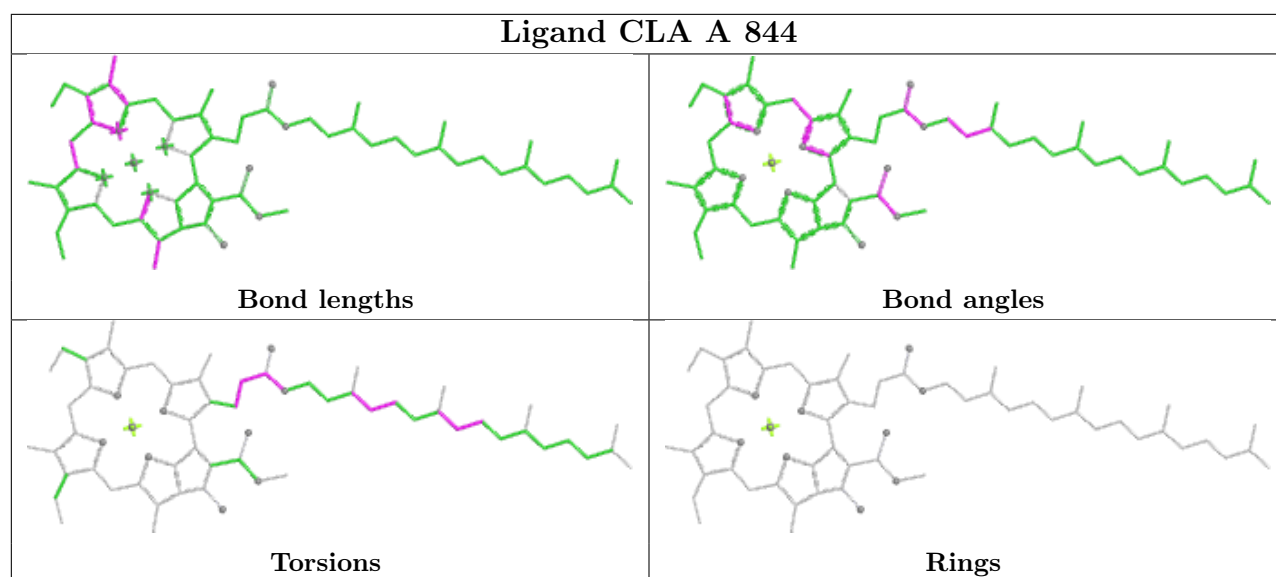


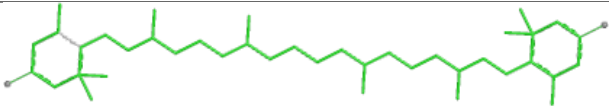
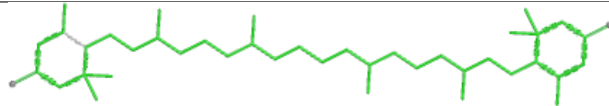
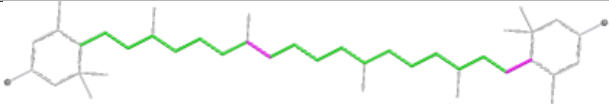
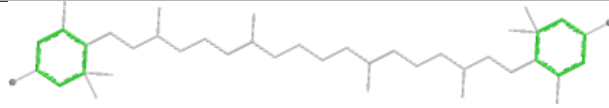
## Ligand BCR G 204

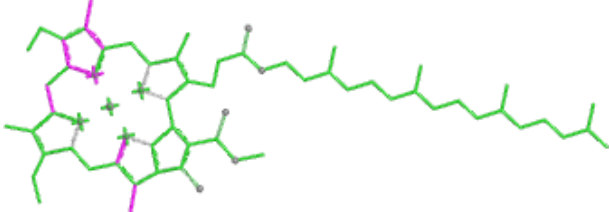
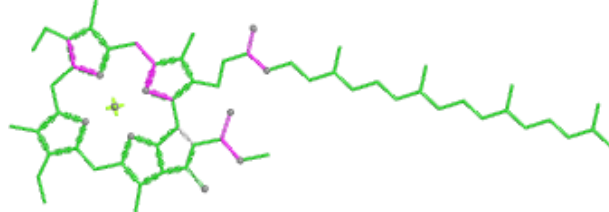
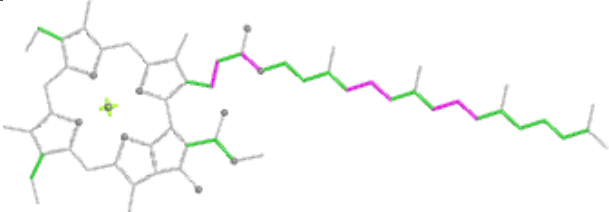
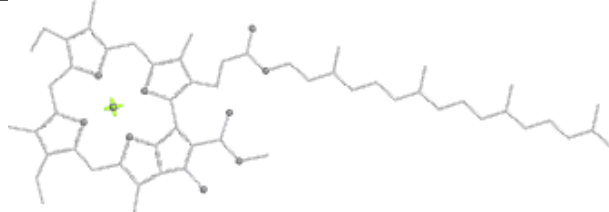


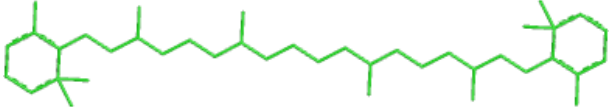
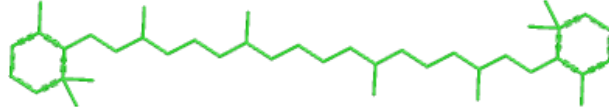
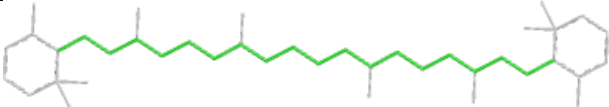
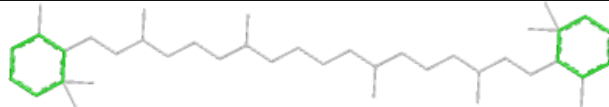


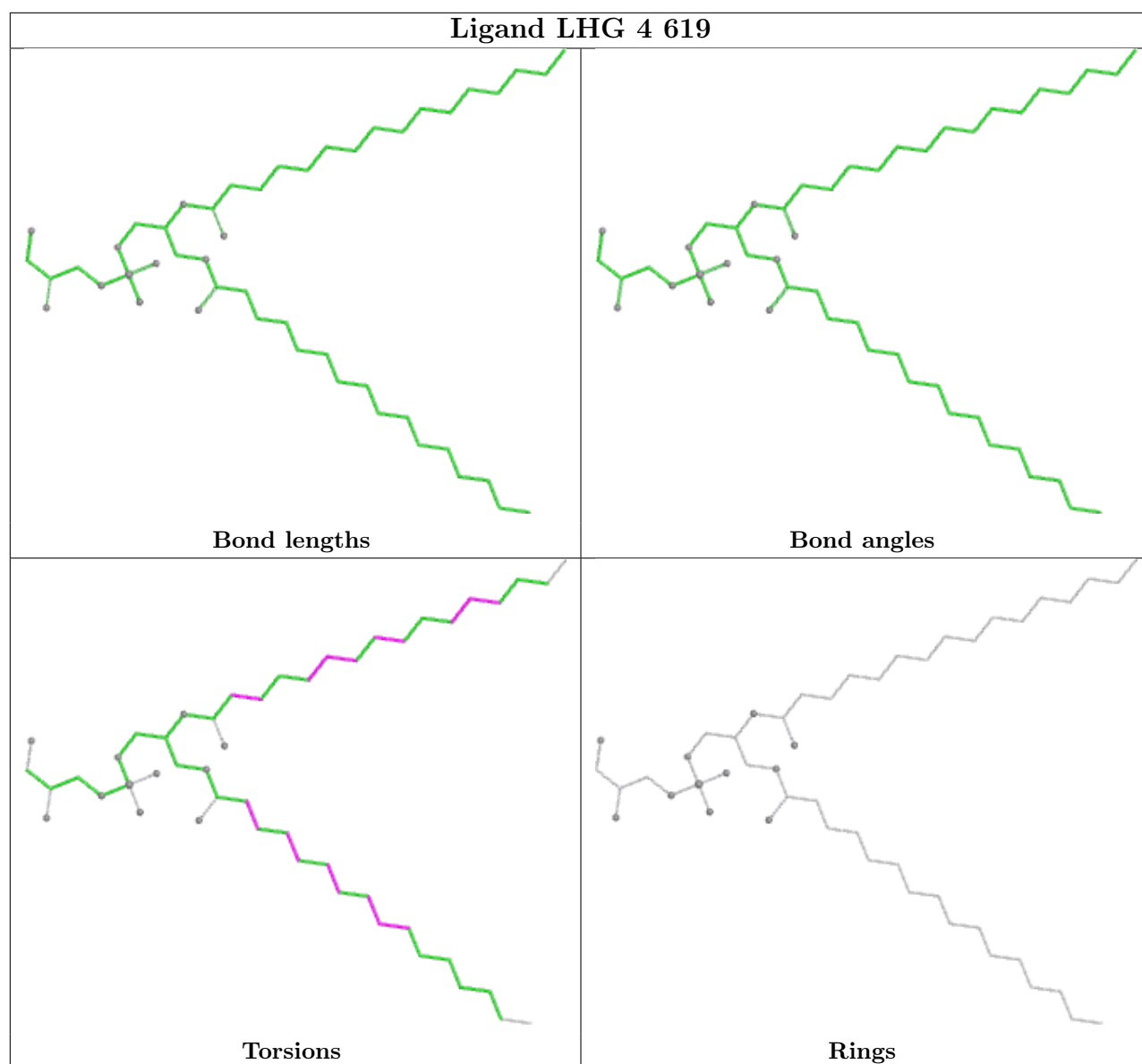
**Ligand LUT 1 315****Ligand LMU Z 621****Ligand LUT 6 319**

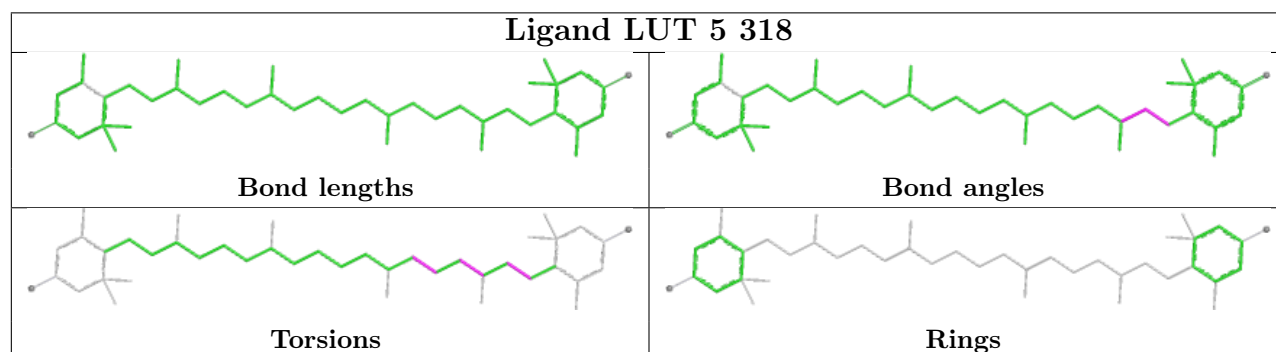
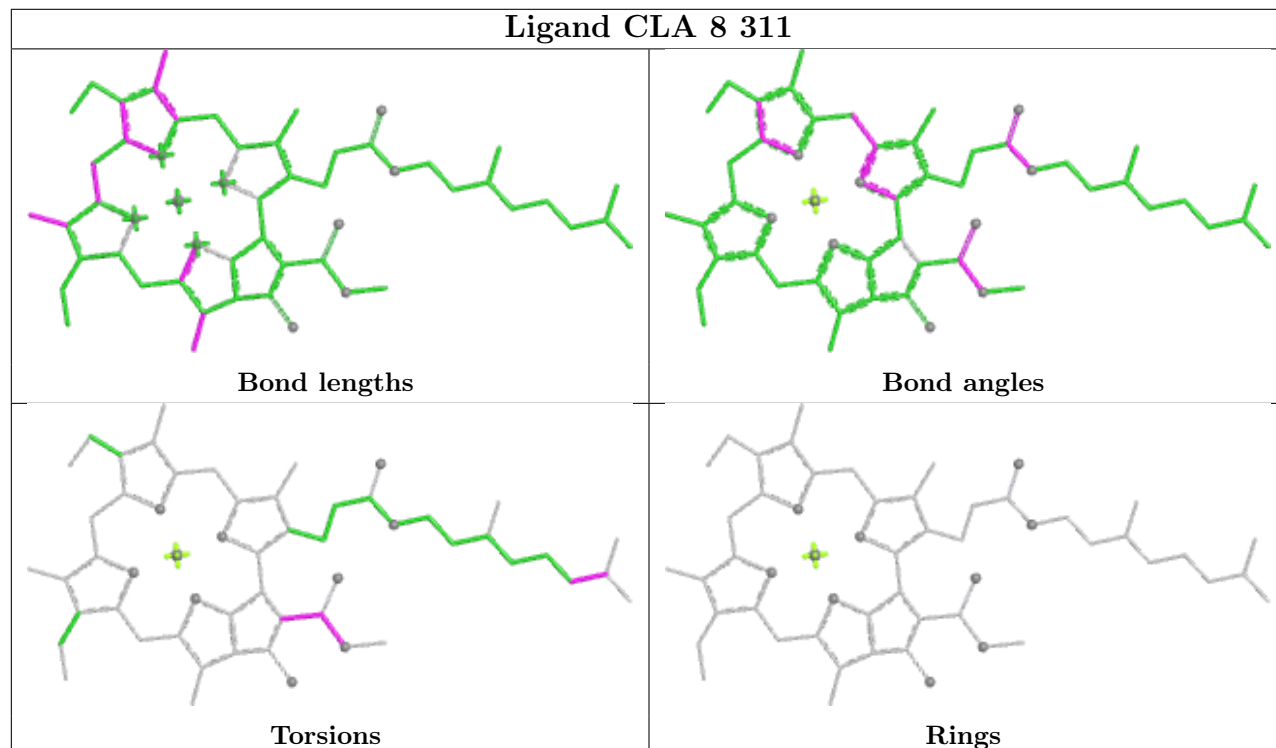
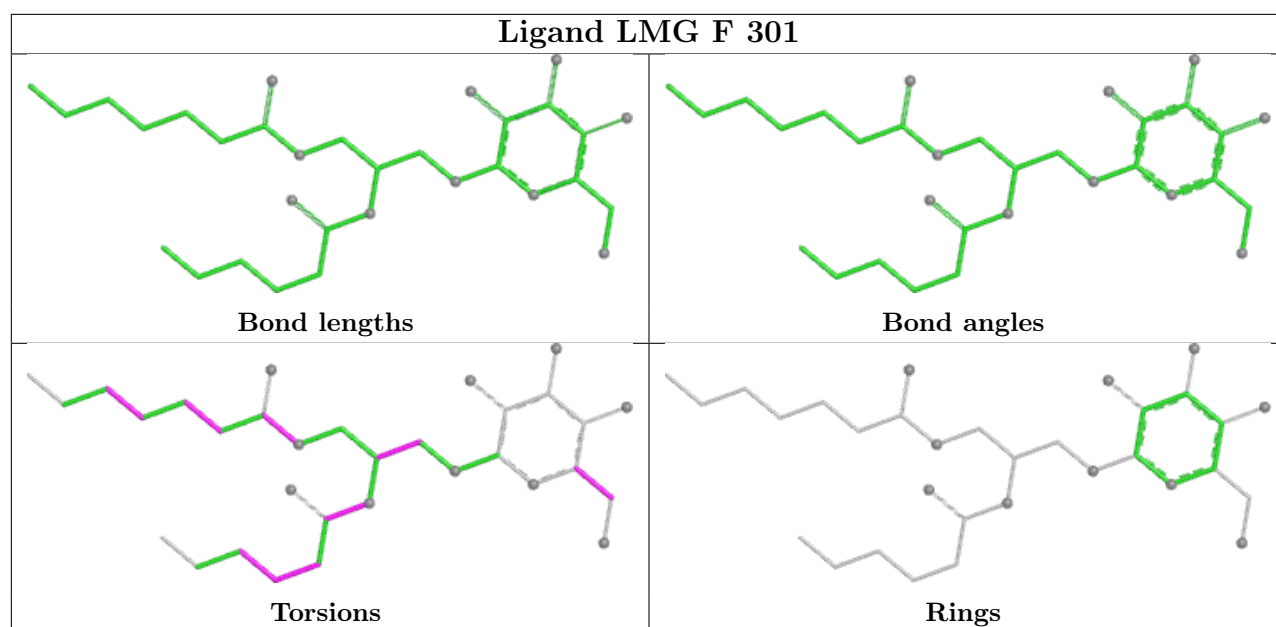


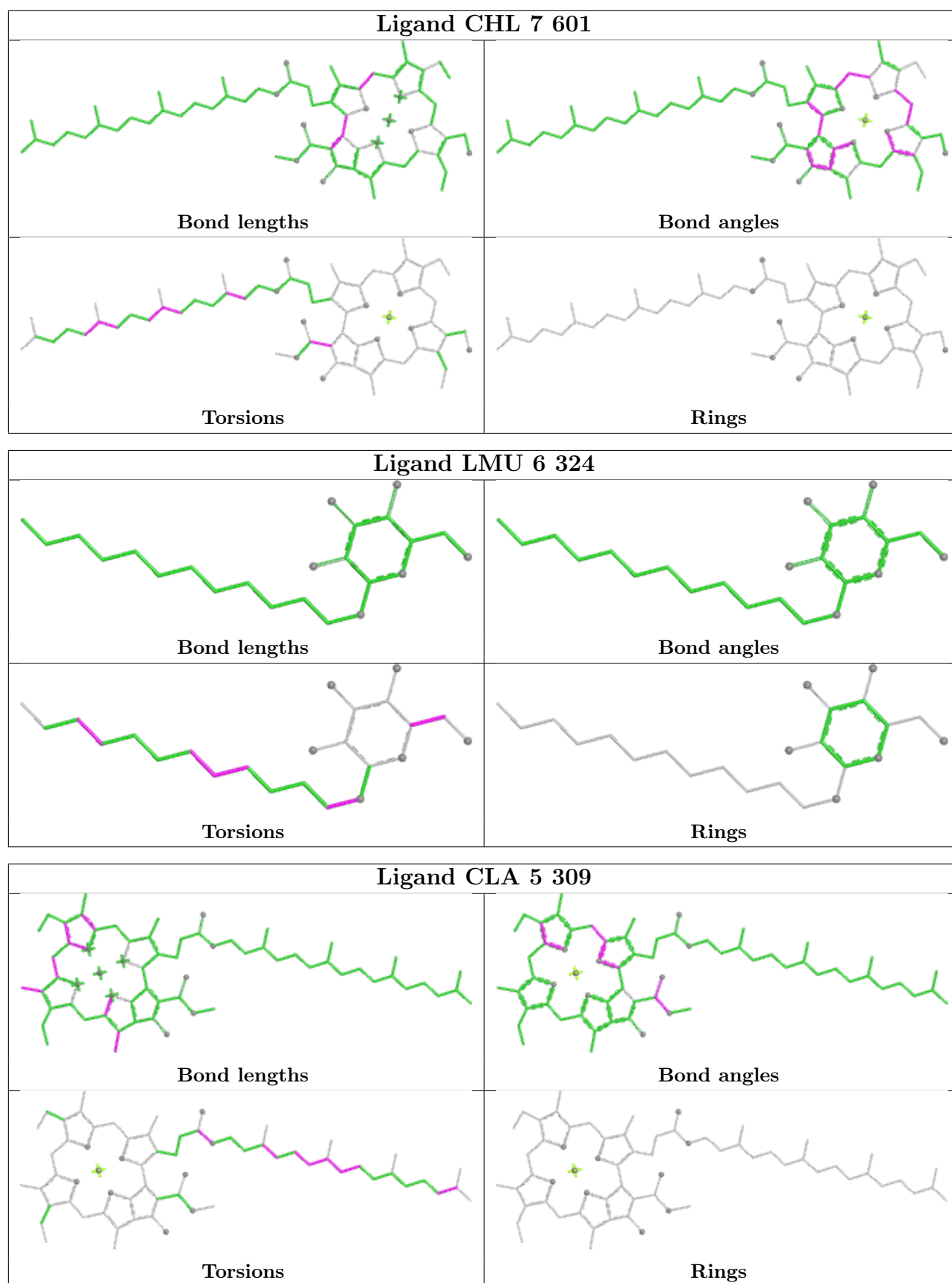
Ligand LUT 4 616	
	Bond lengths
	Bond angles
	Torsions
	Rings

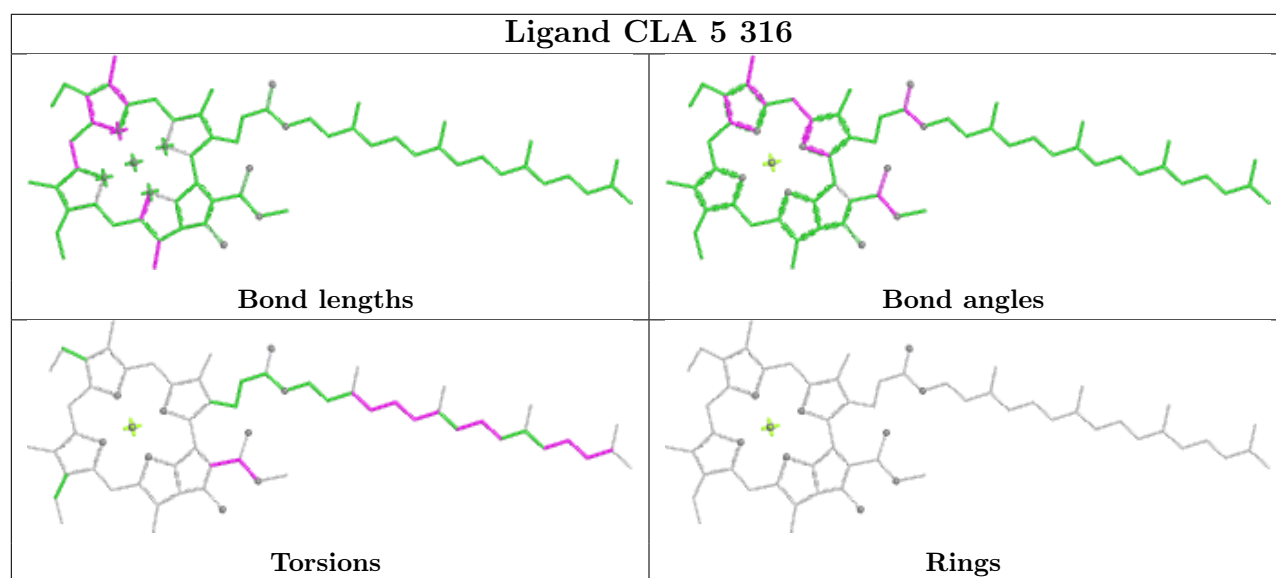
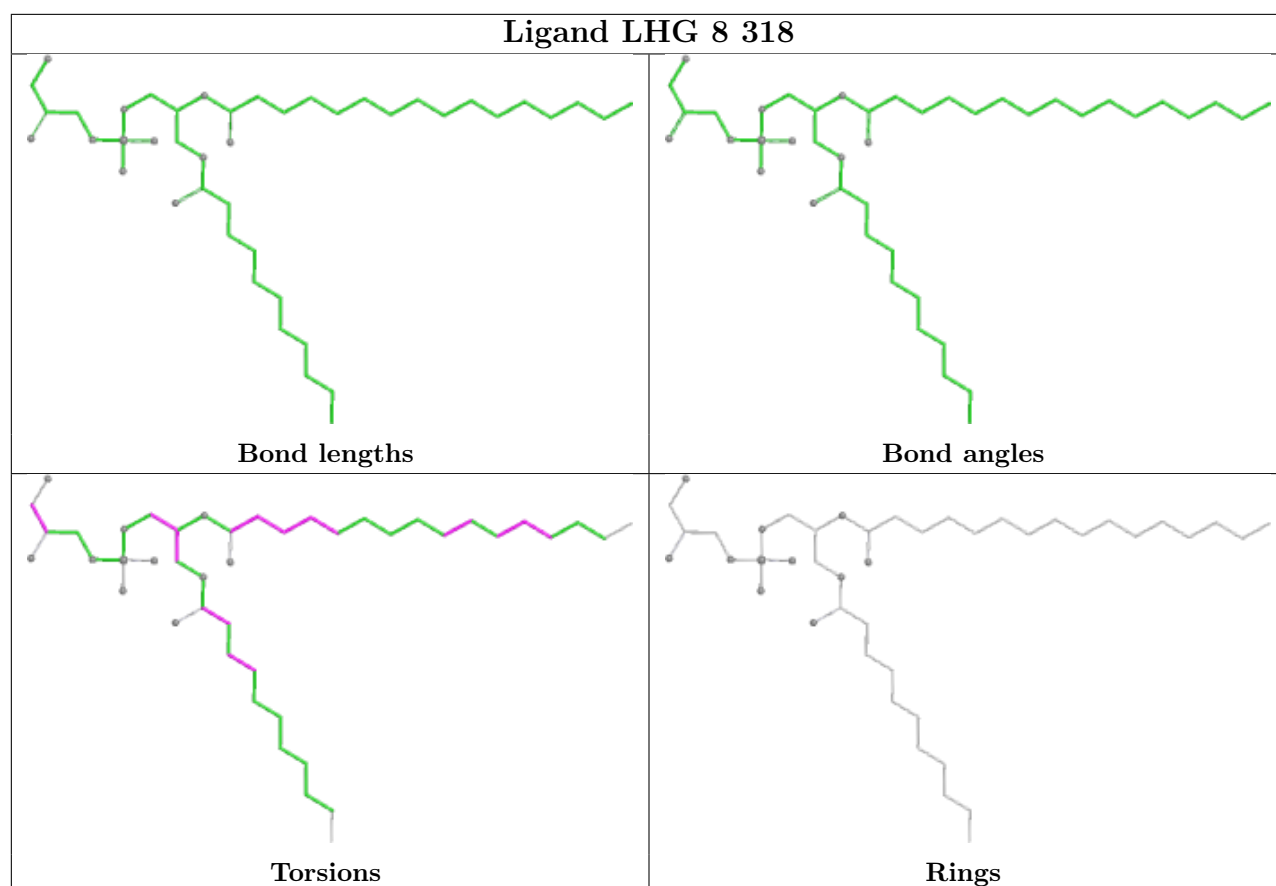
Ligand CLA B 817	
	Bond lengths
	Bond angles
	Torsions
	Rings

Ligand BCR B 847	
	Bond lengths
	Bond angles
	Torsions
	Rings

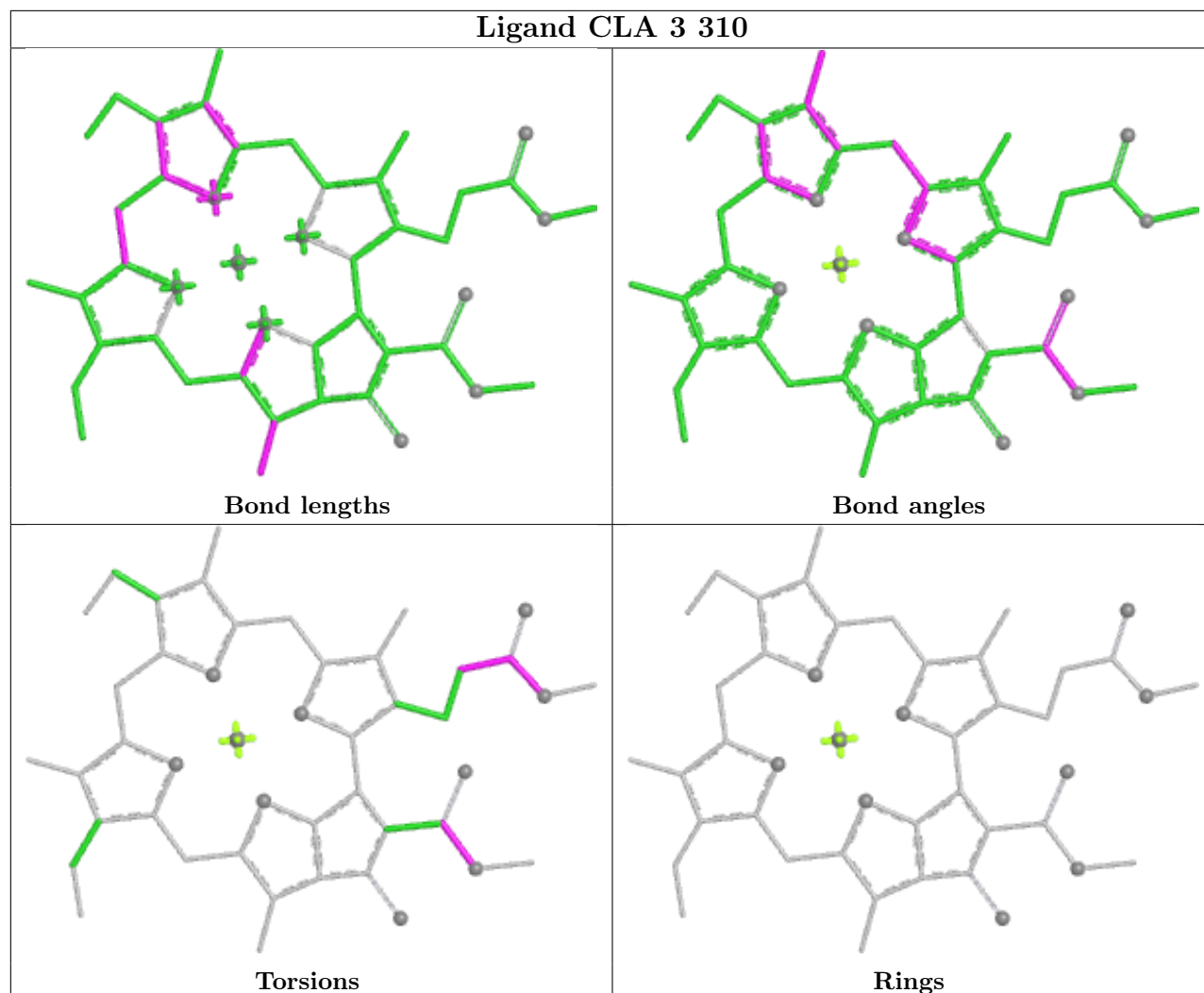






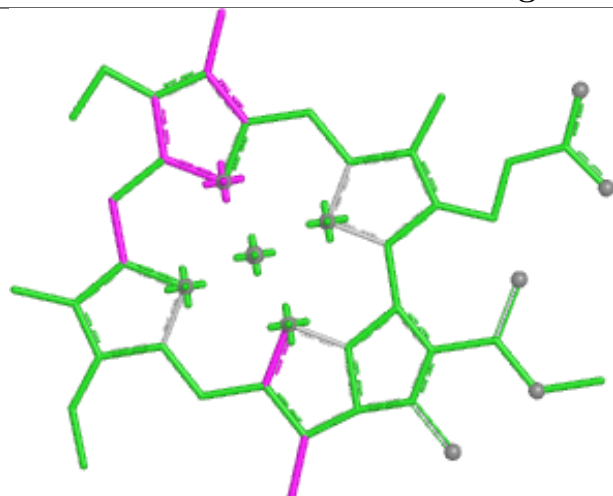


## Ligand CLA 3 310

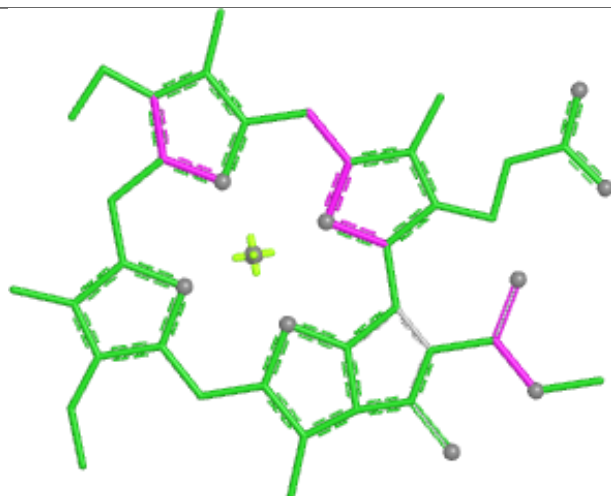




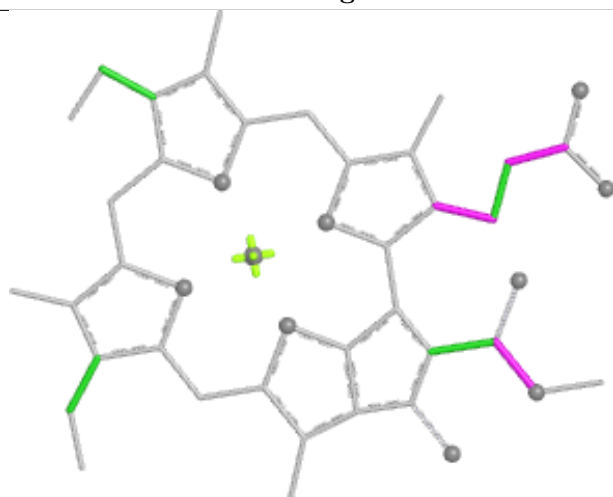
## Ligand CLA 5 314



Bond lengths



Bond angles

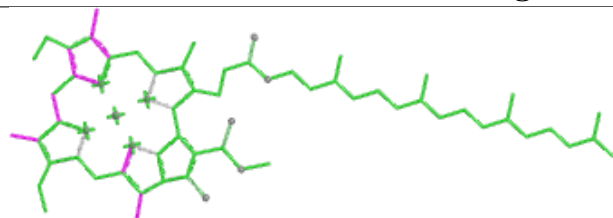


Torsions

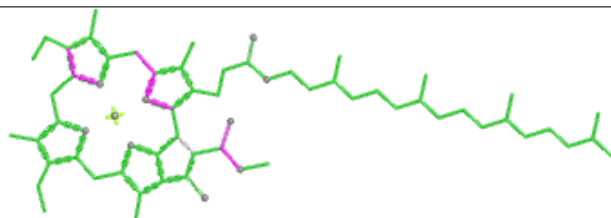


Rings

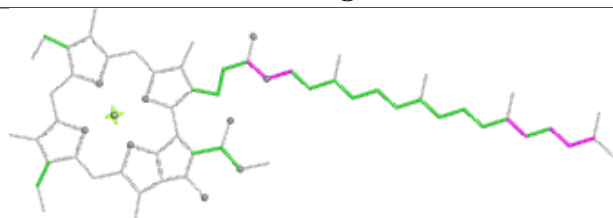
## Ligand CLA A 837



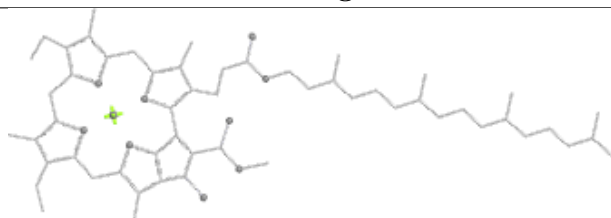
Bond lengths



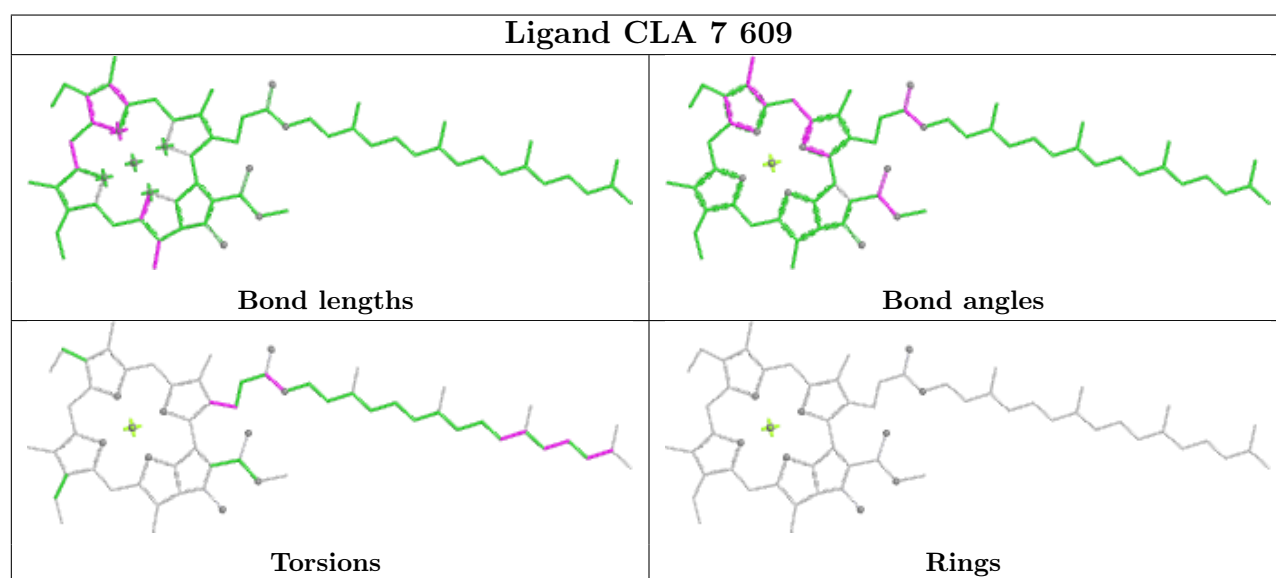
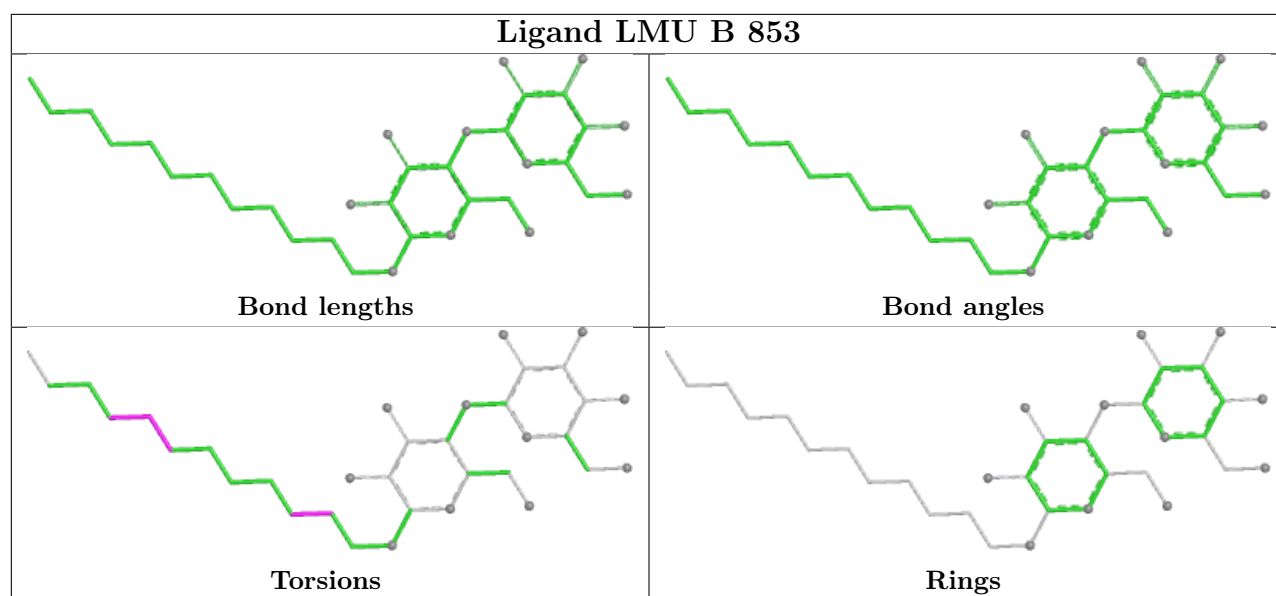
Bond angles



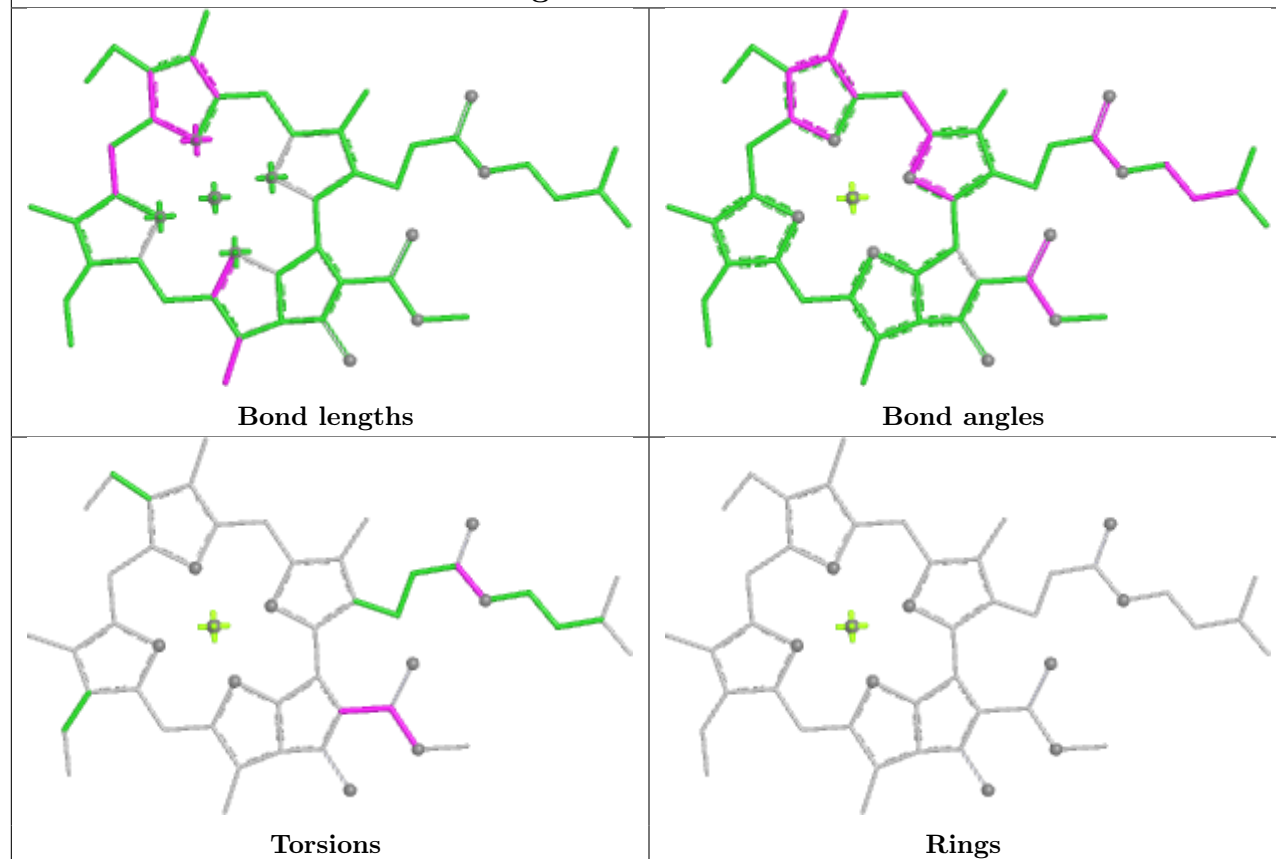
Torsions



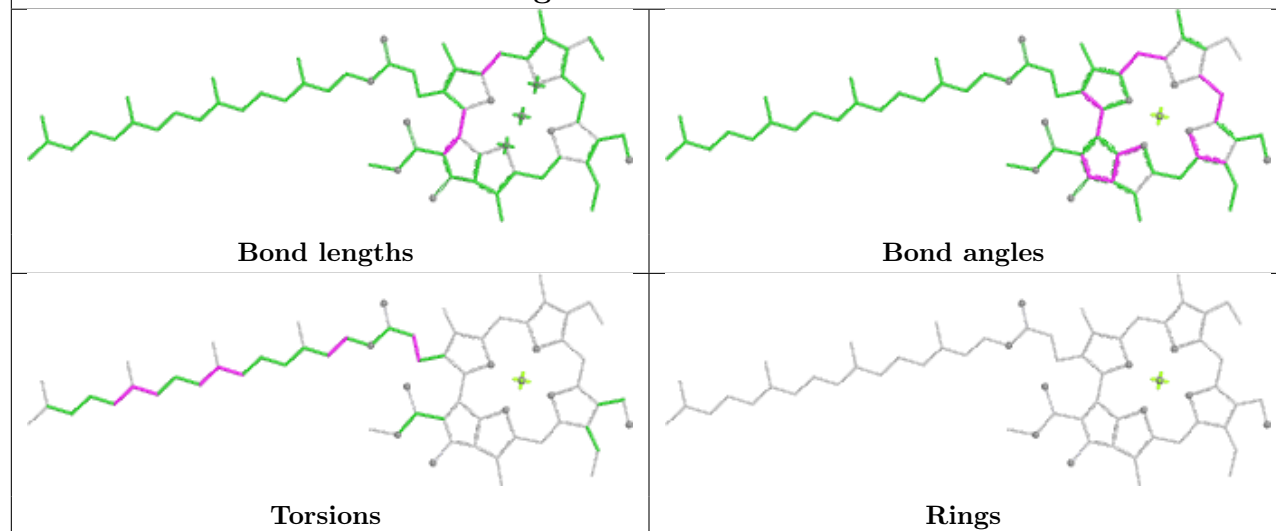
Rings

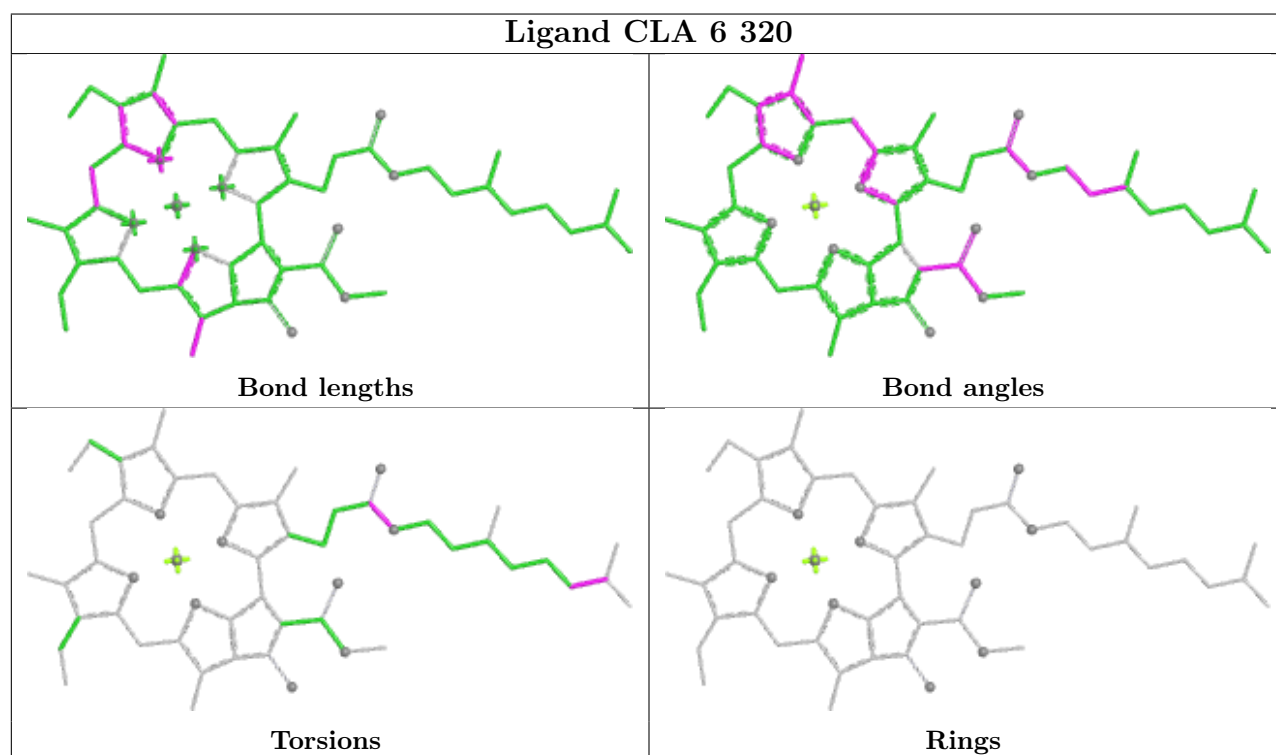
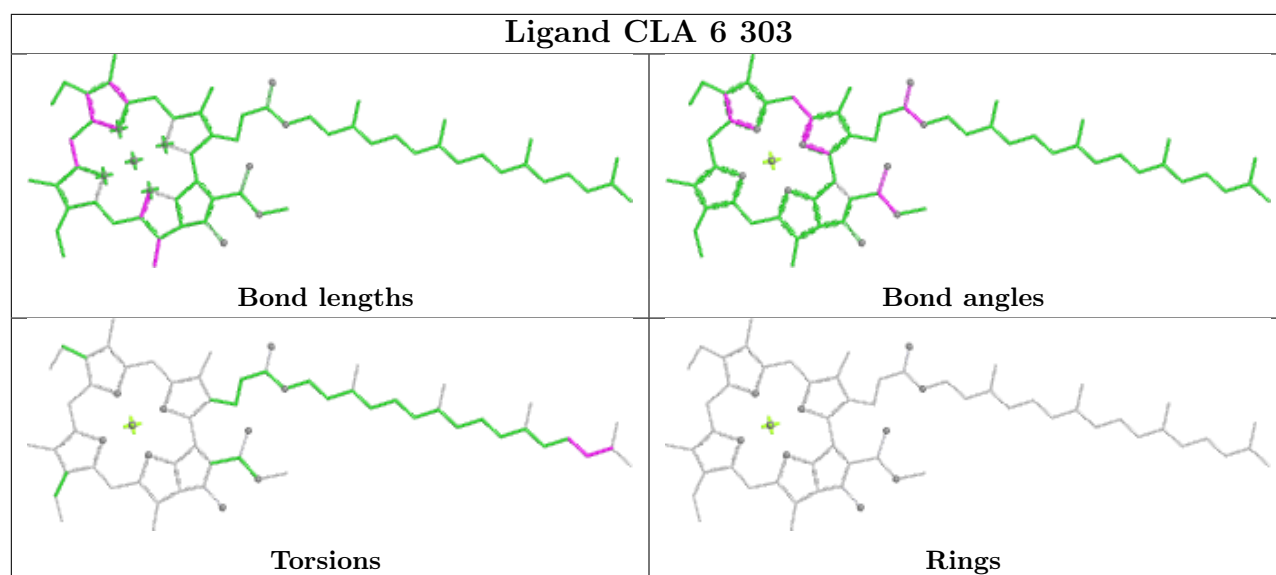


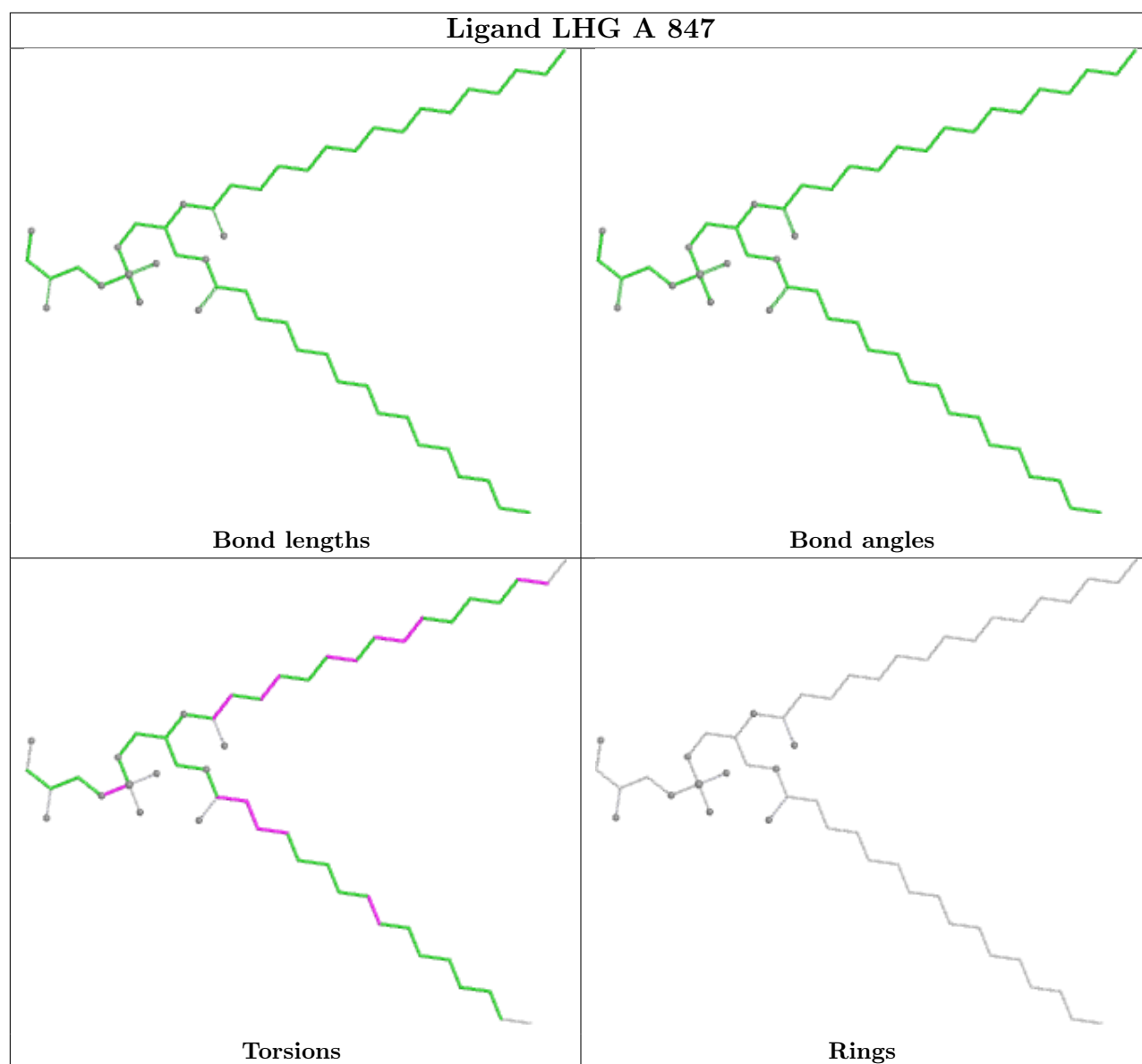
## Ligand CLA A 809

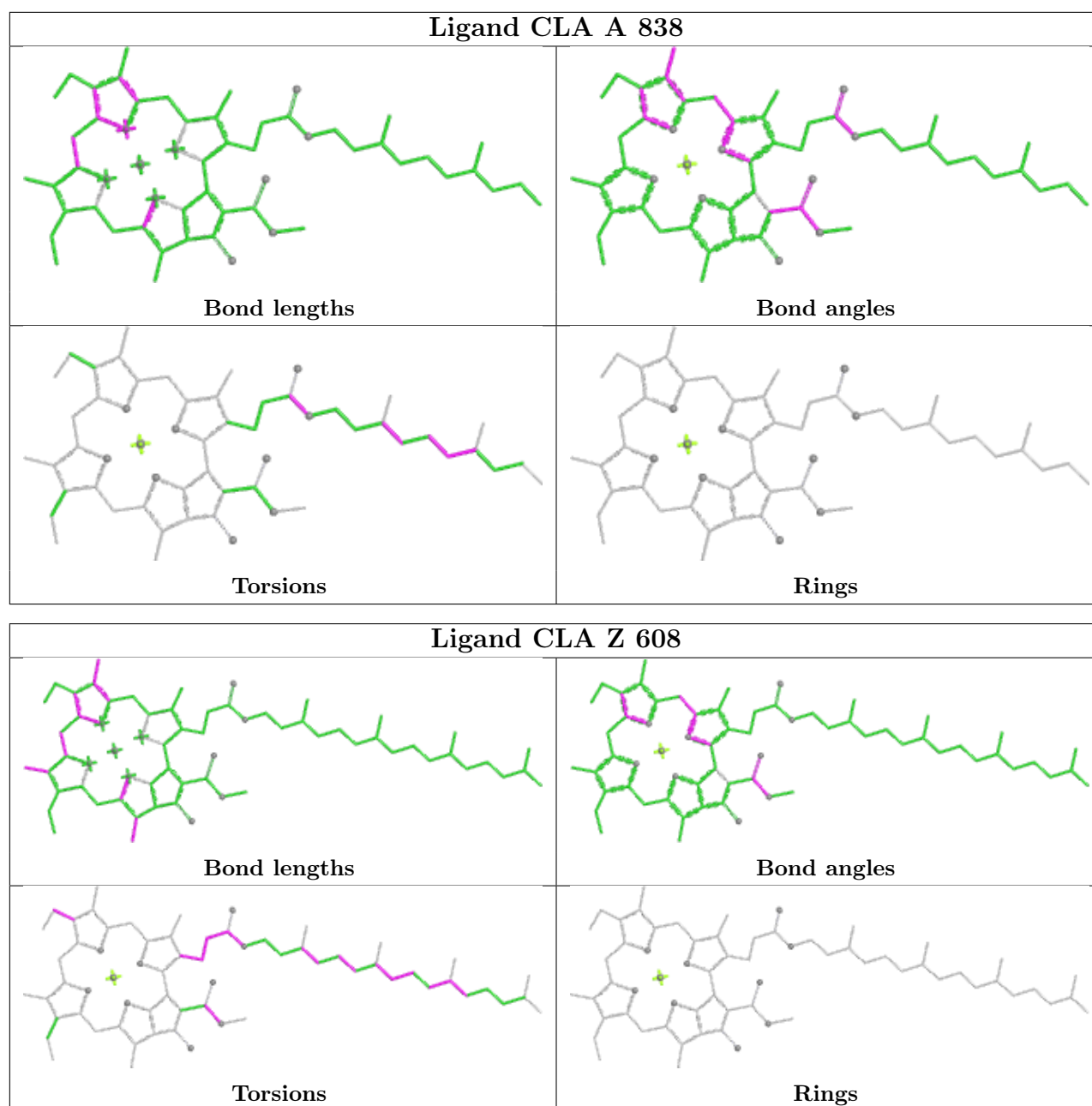


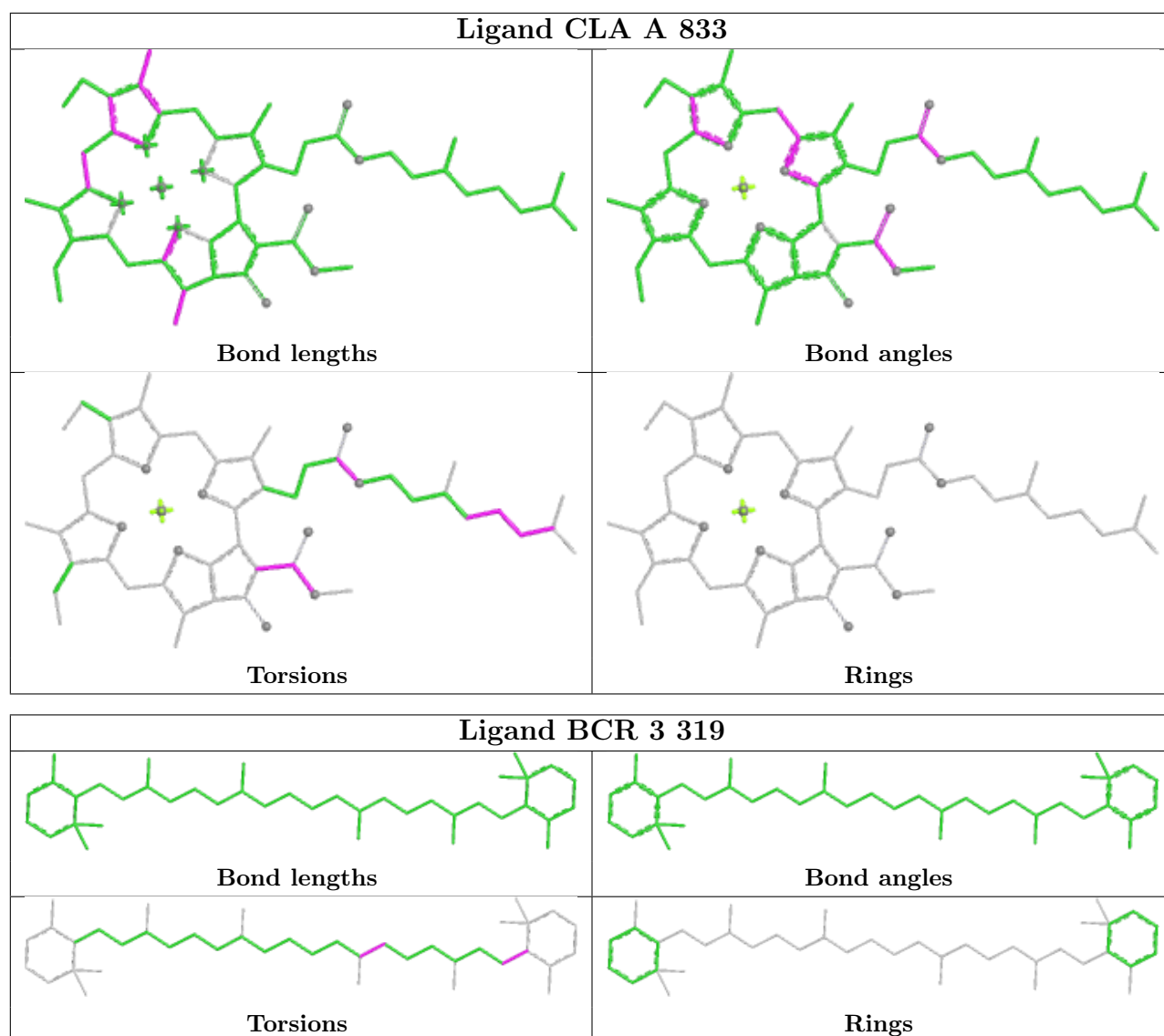
## Ligand CHL Z 601

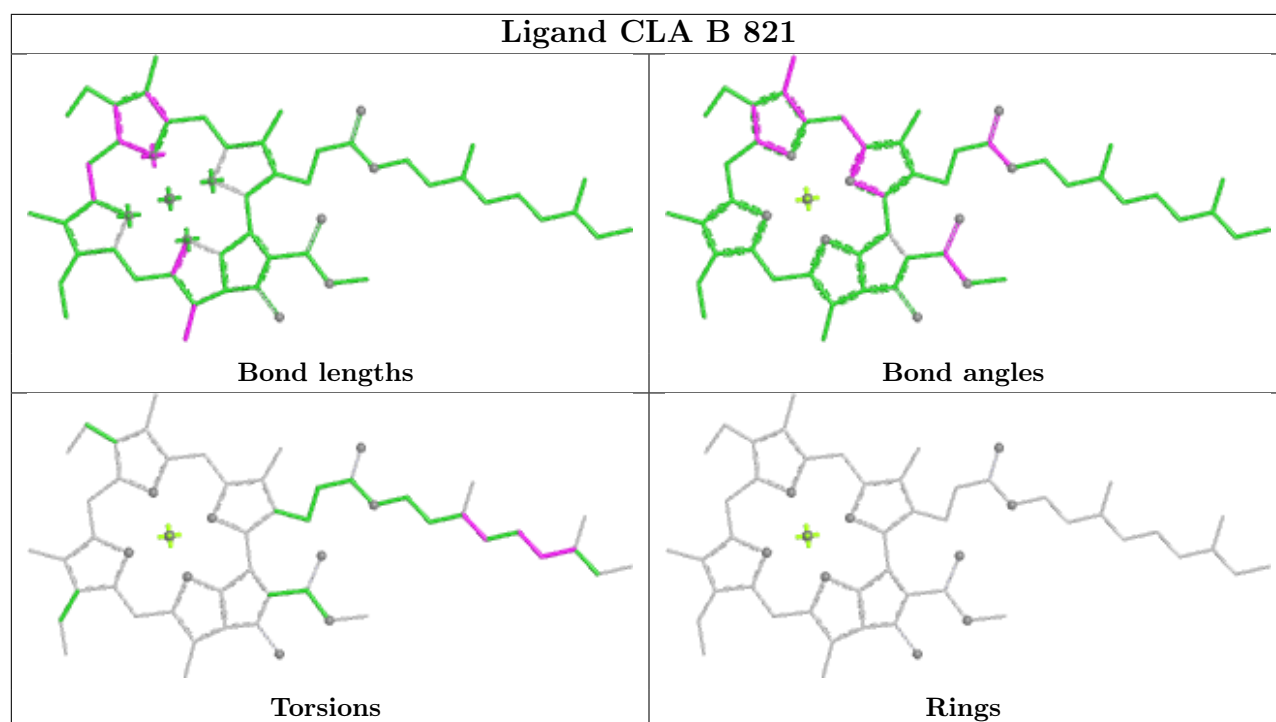






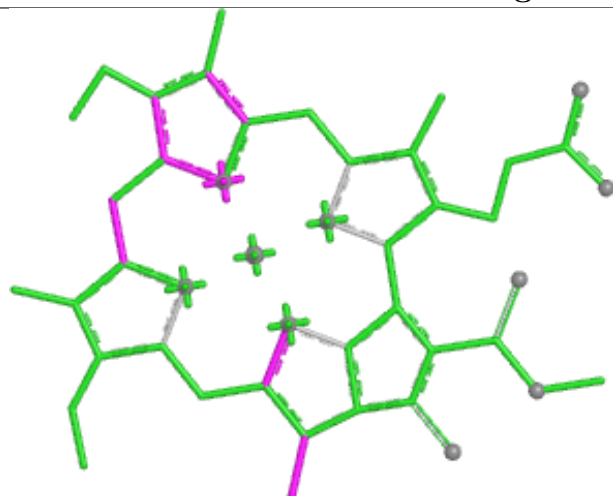




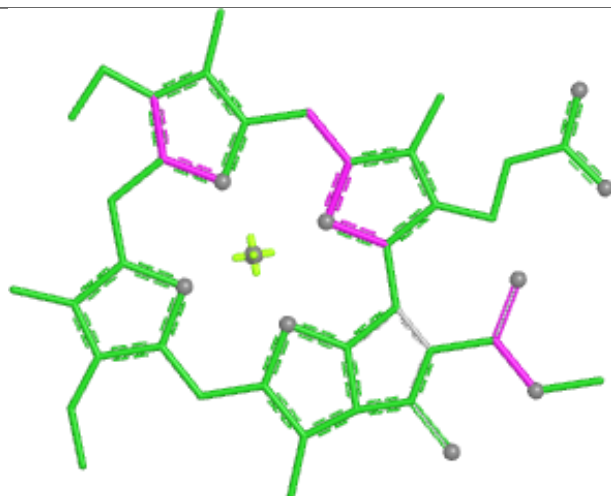




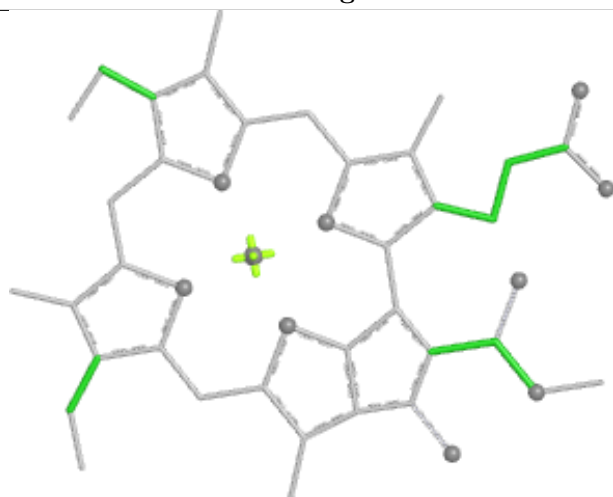
## Ligand CLA B 831



Bond lengths



Bond angles

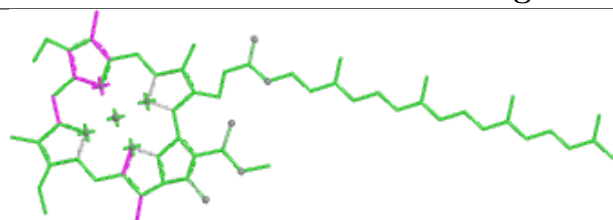


Torsions

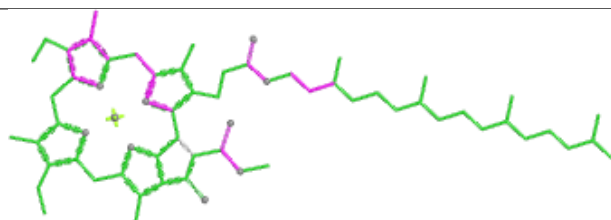


Rings

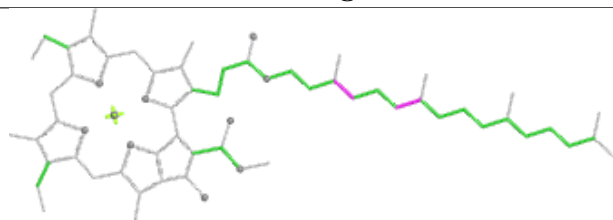
## Ligand CLA A 823



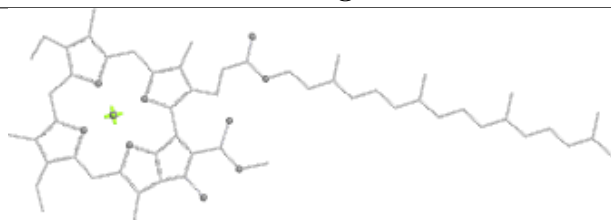
Bond lengths



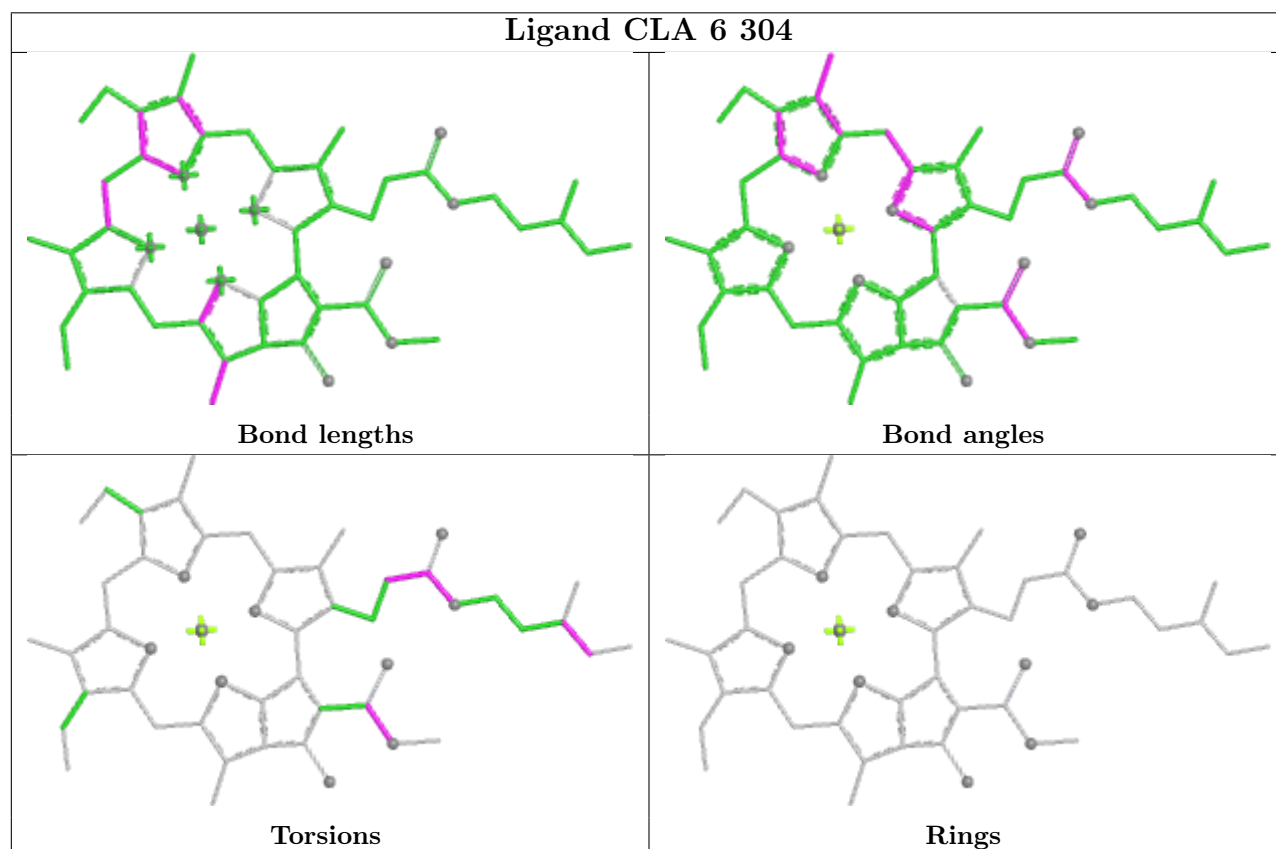
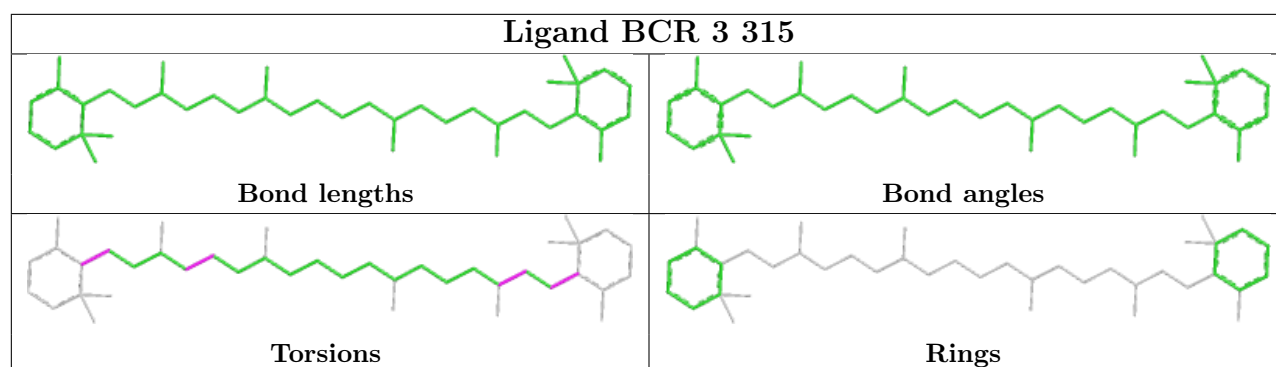
Bond angles

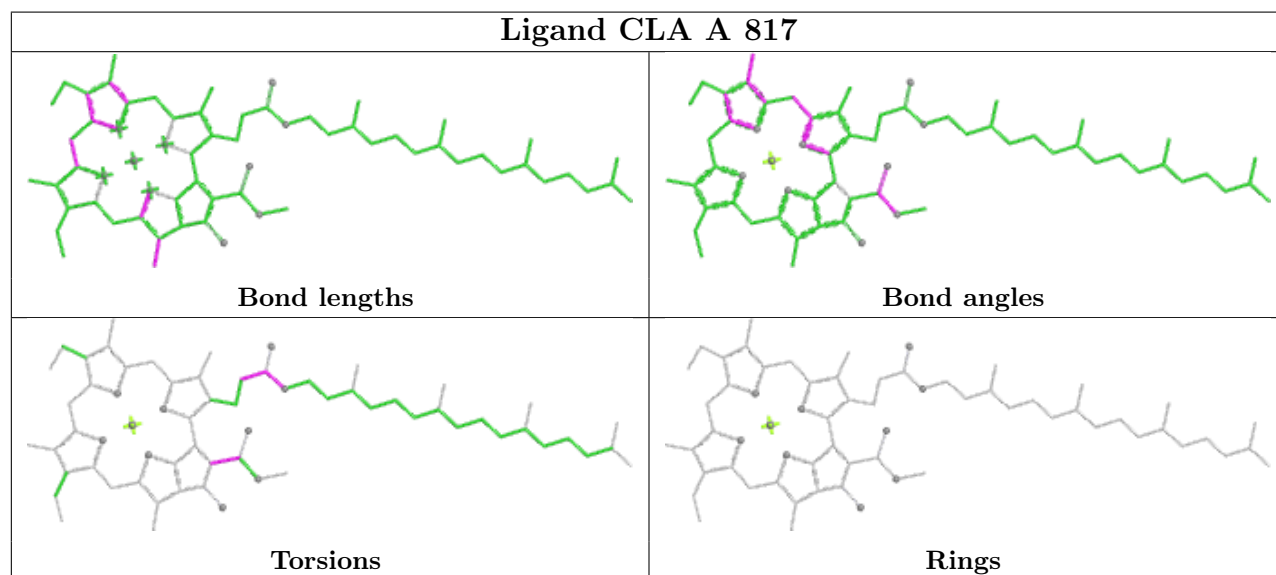
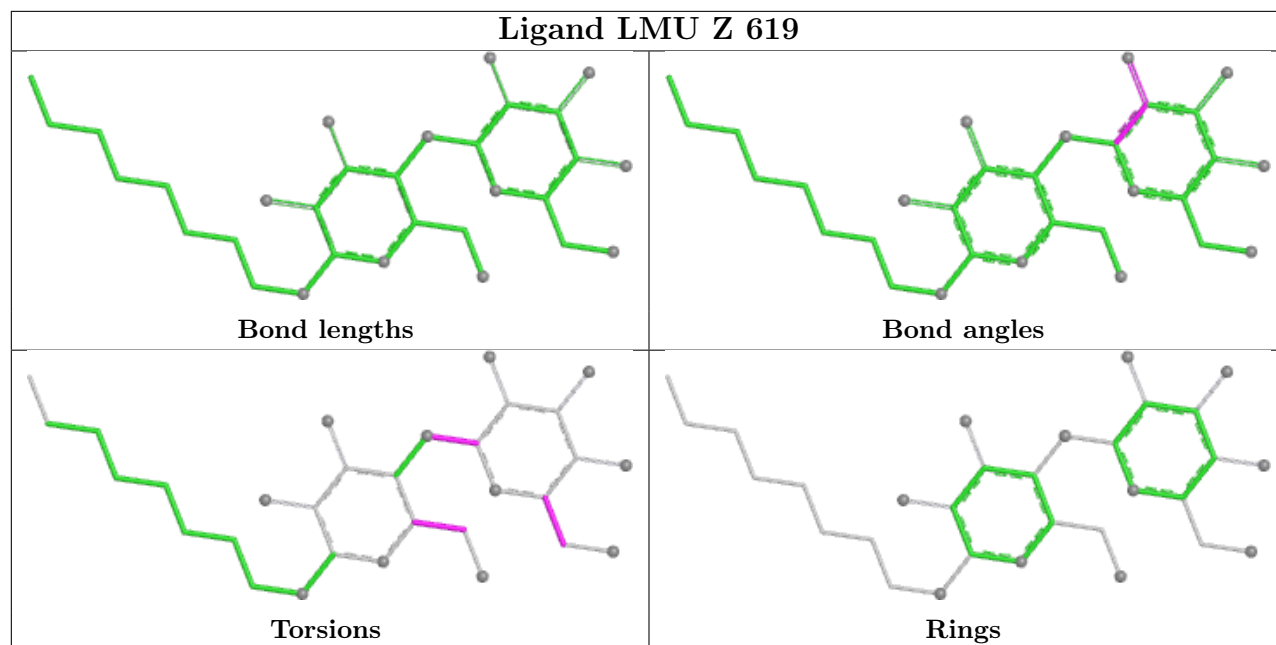


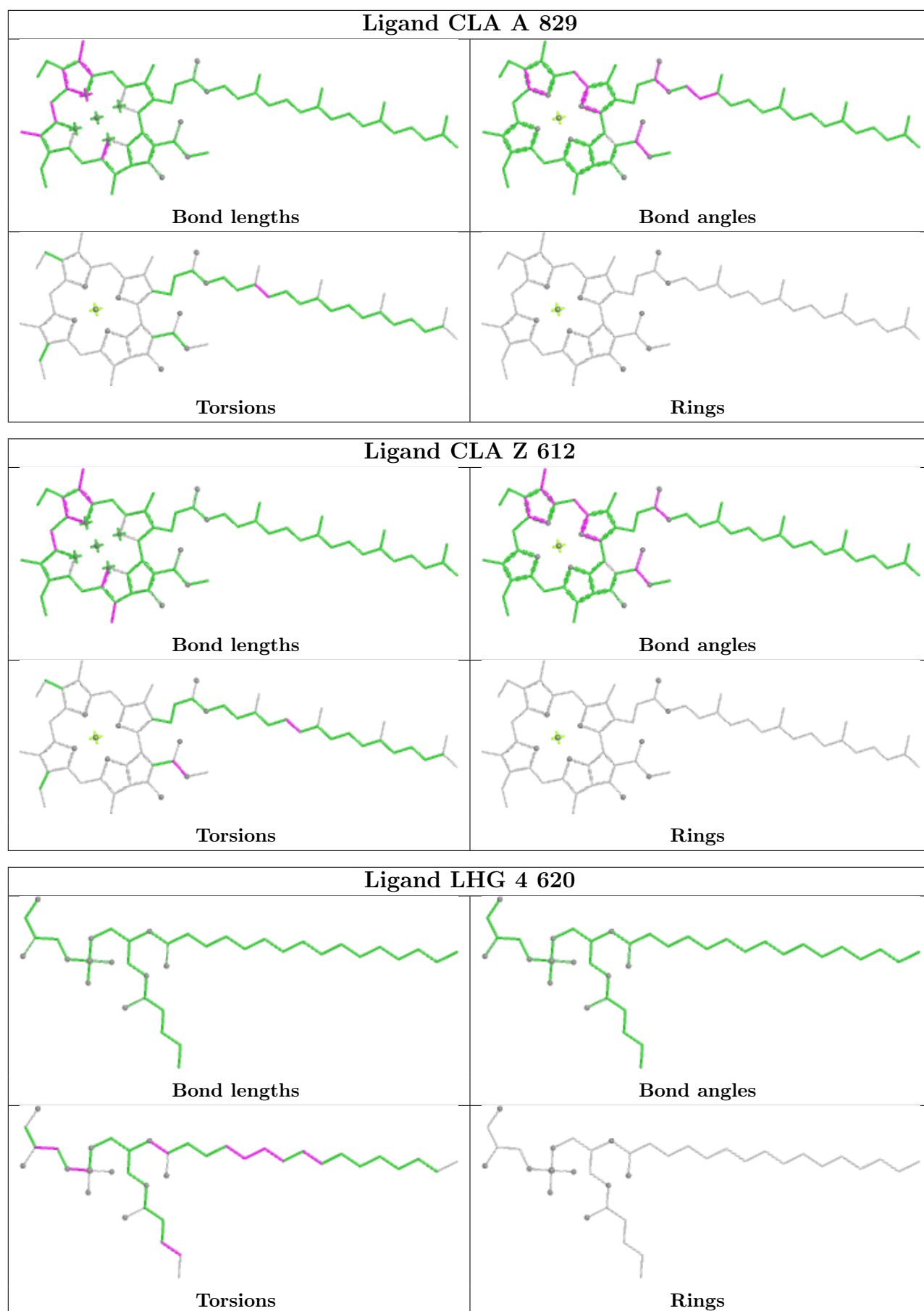
Torsions



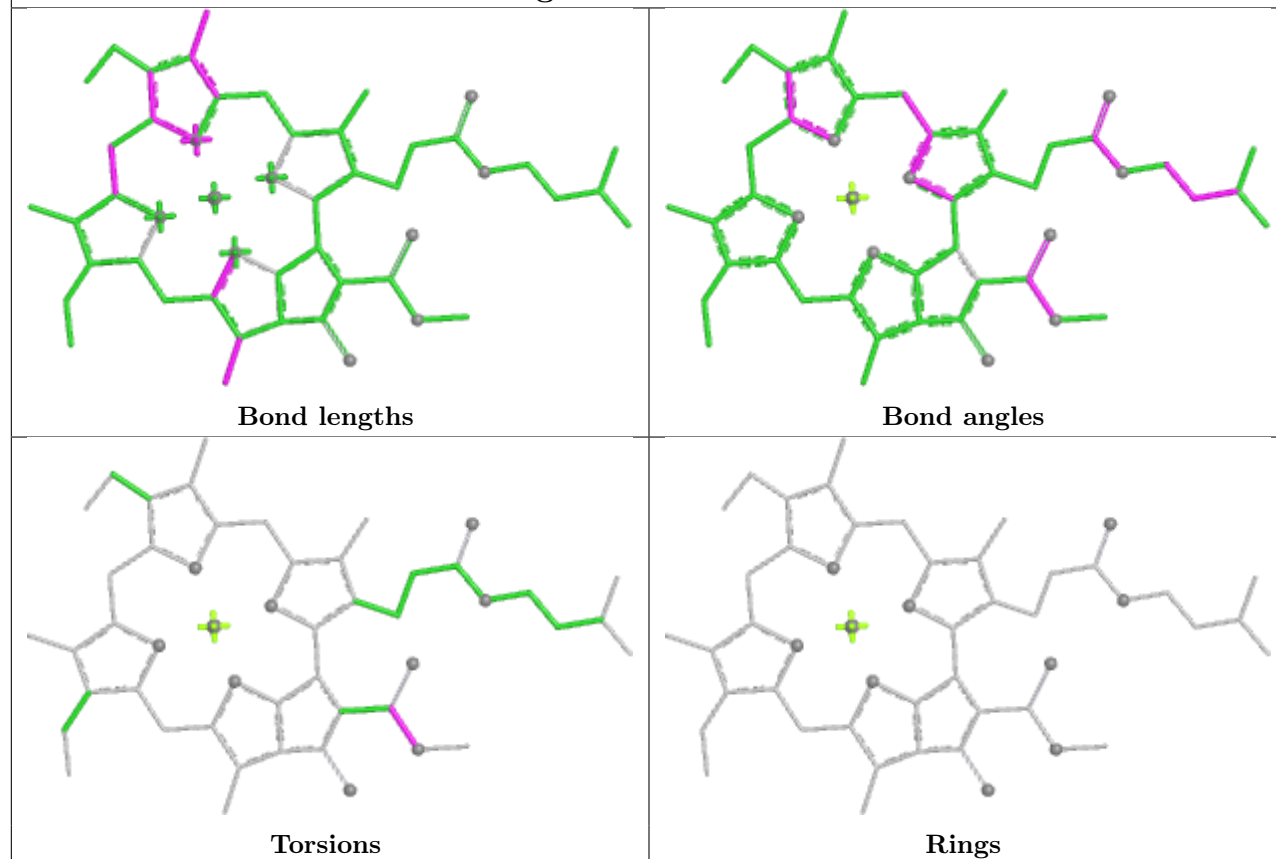
Rings



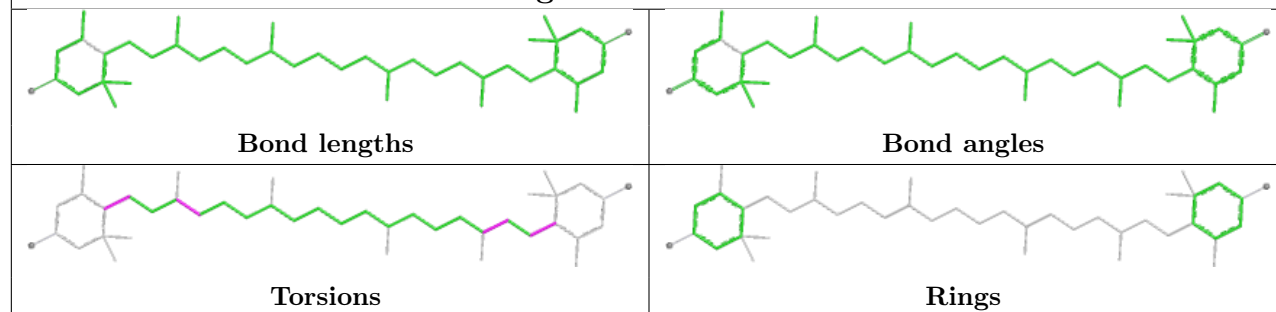


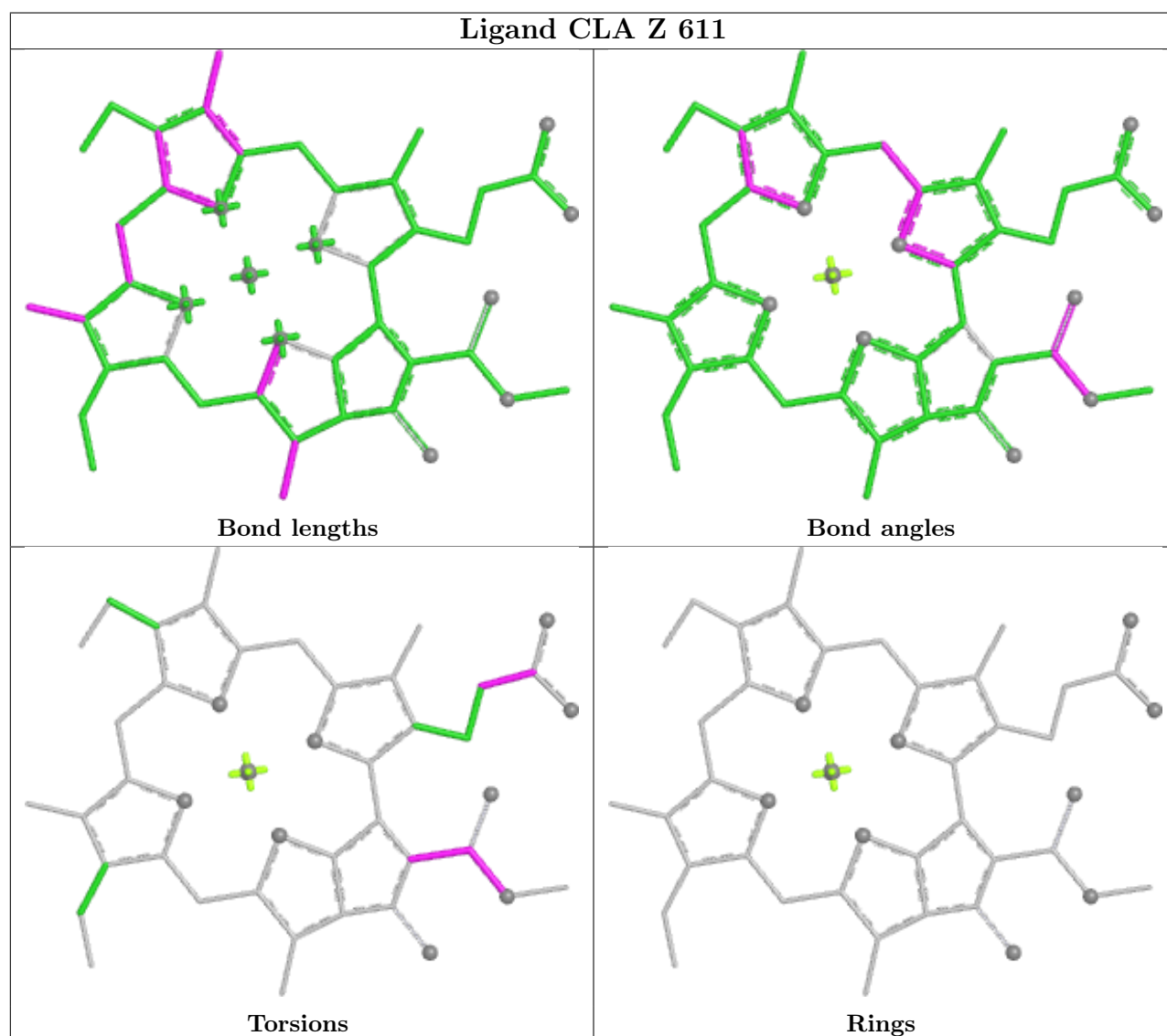
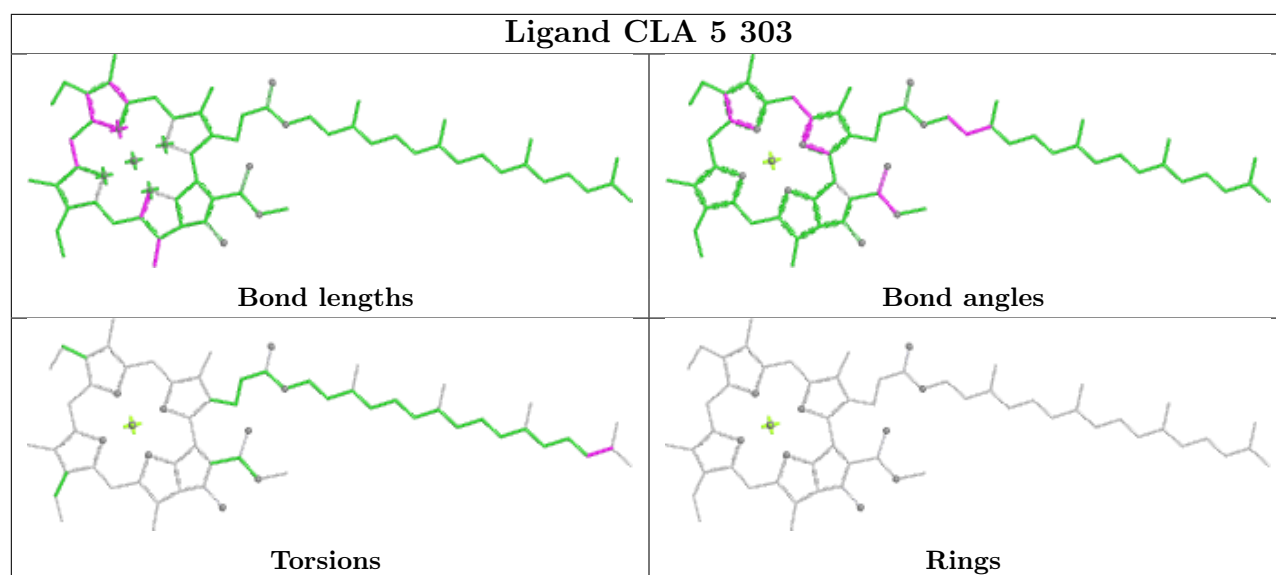


## Ligand CLA 8 307

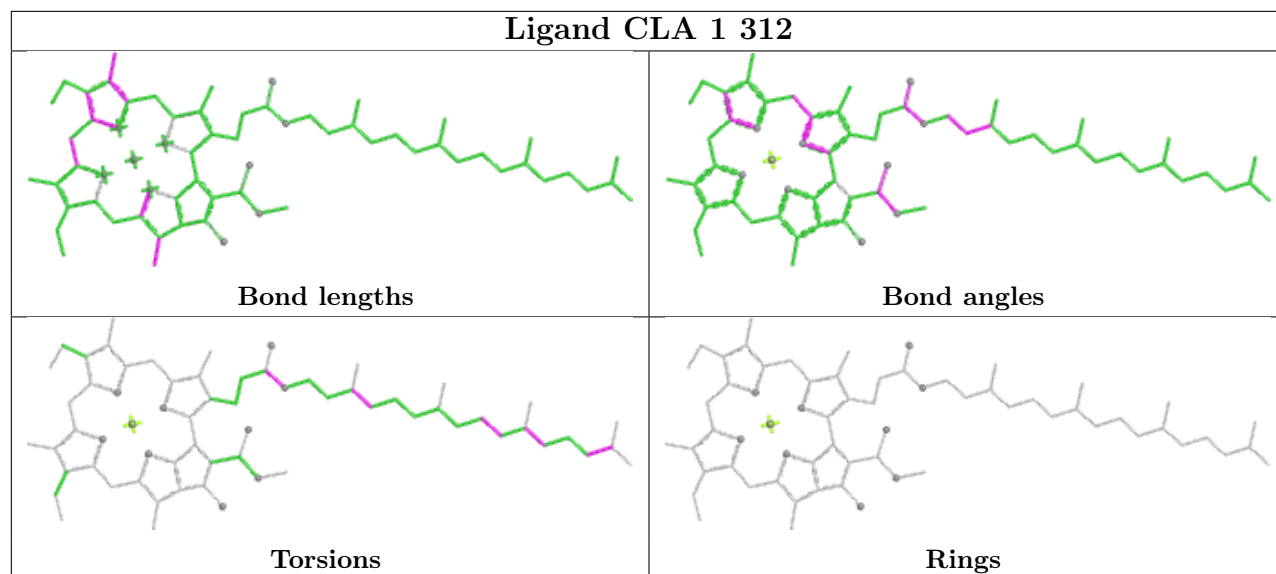


## Ligand LUT 8 301

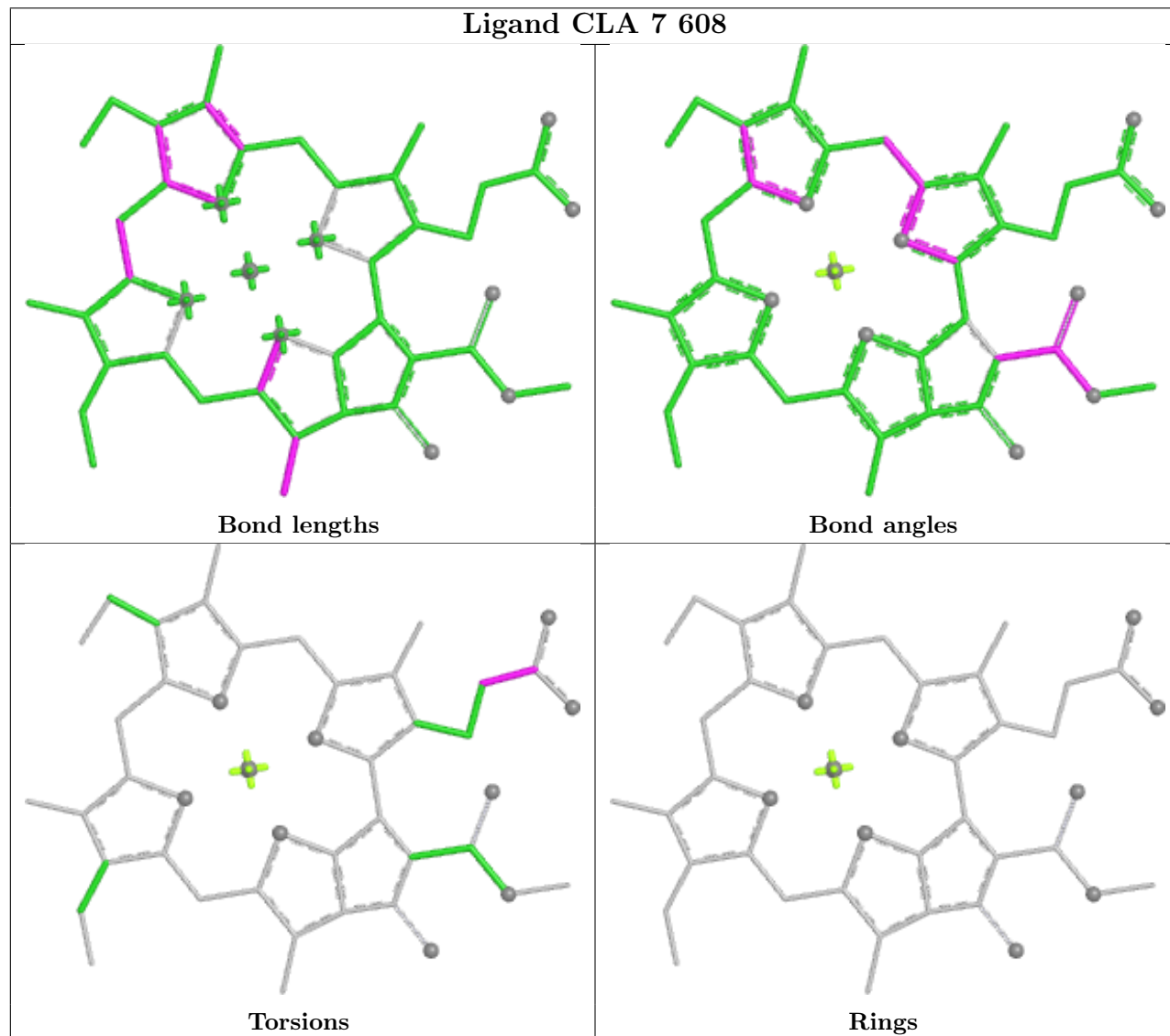




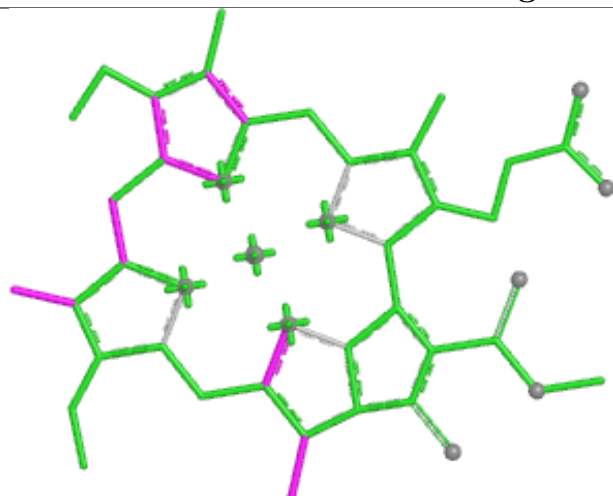
## Ligand CLA 1 312



## Ligand CLA 7 608



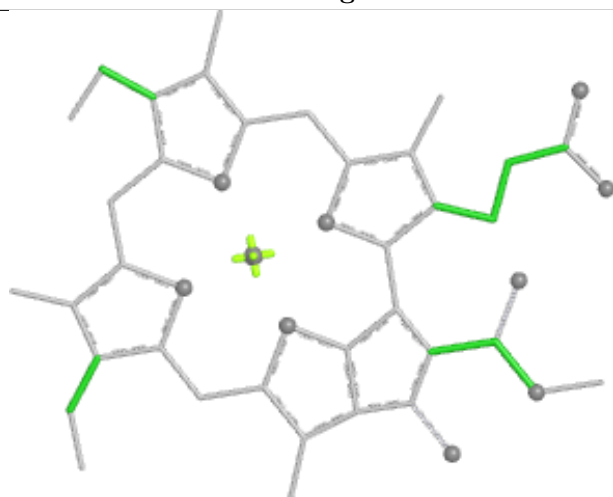
## Ligand CLA 3 314



Bond lengths



Bond angles

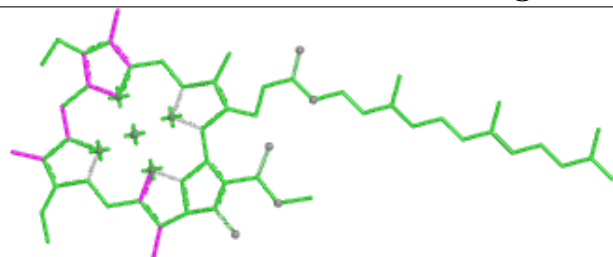


Torsions

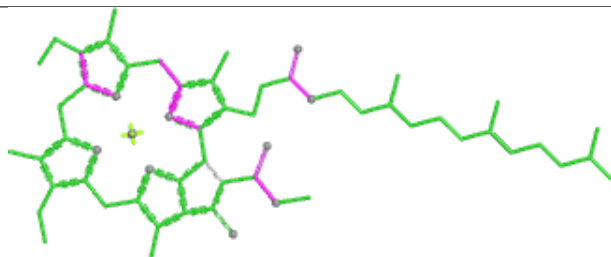


Rings

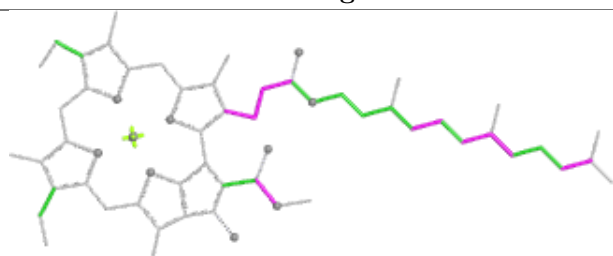
## Ligand CLA A 820



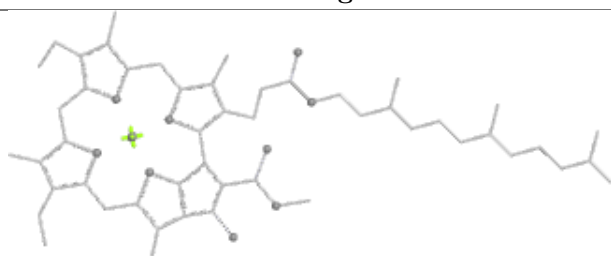
Bond lengths



Bond angles

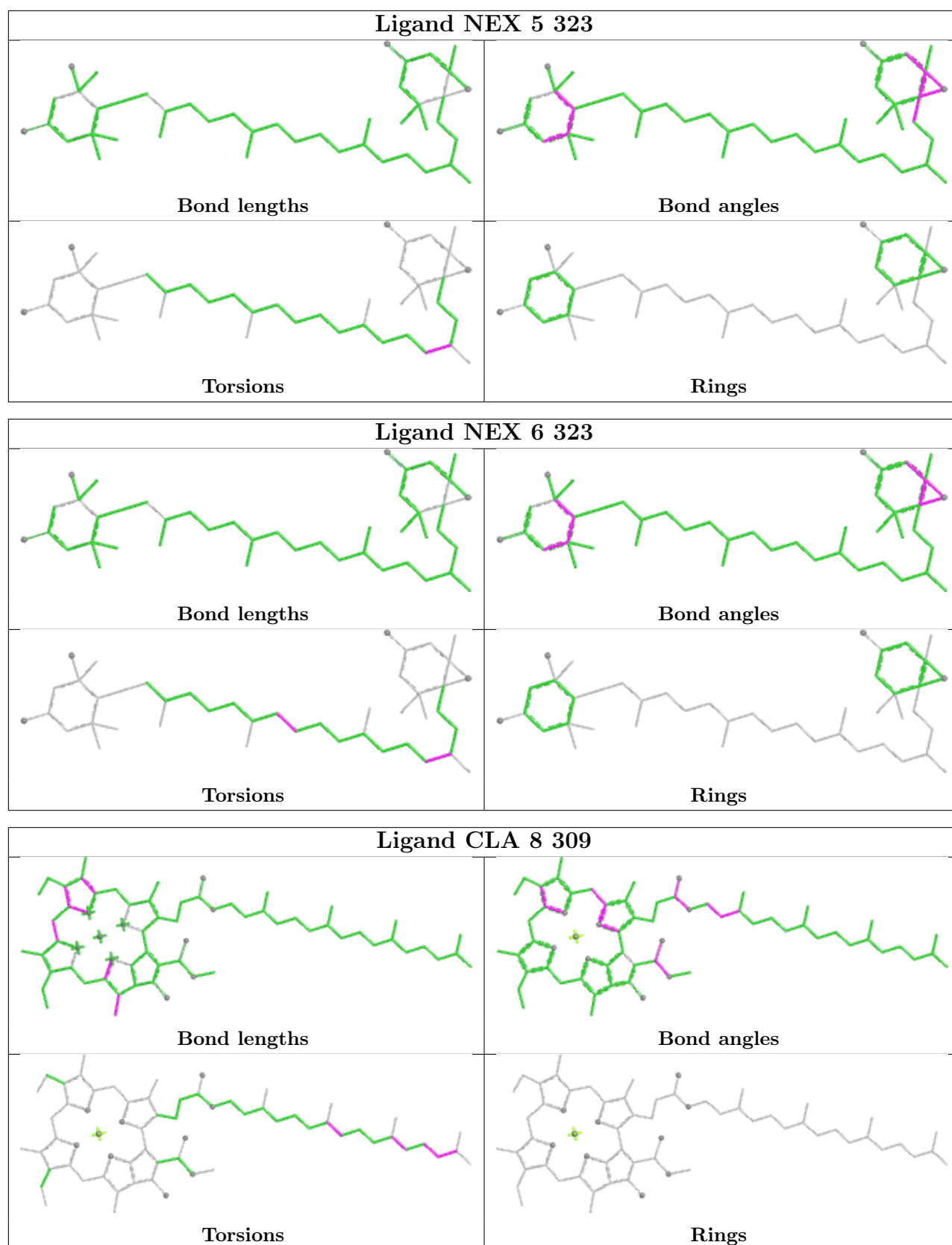


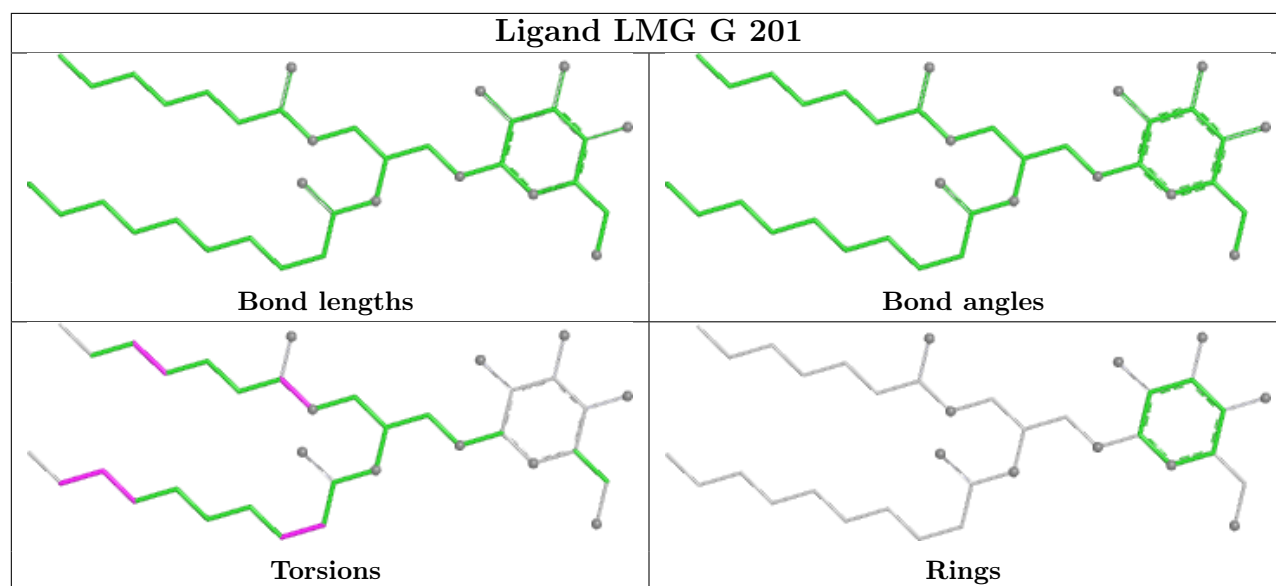
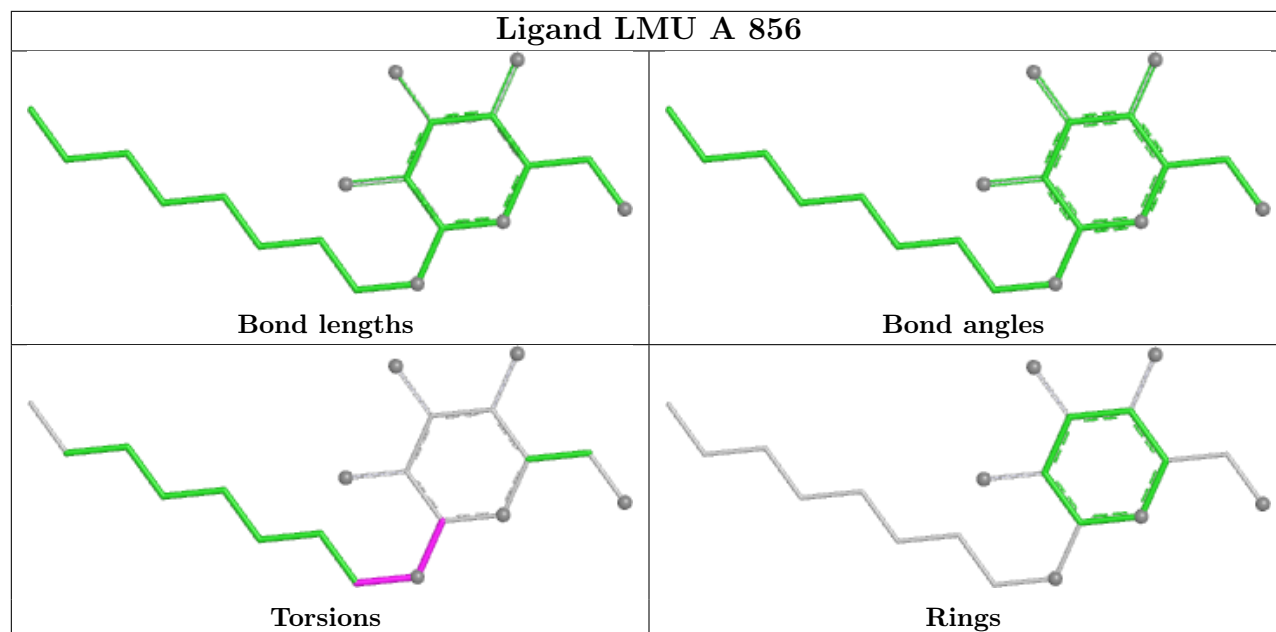
Torsions



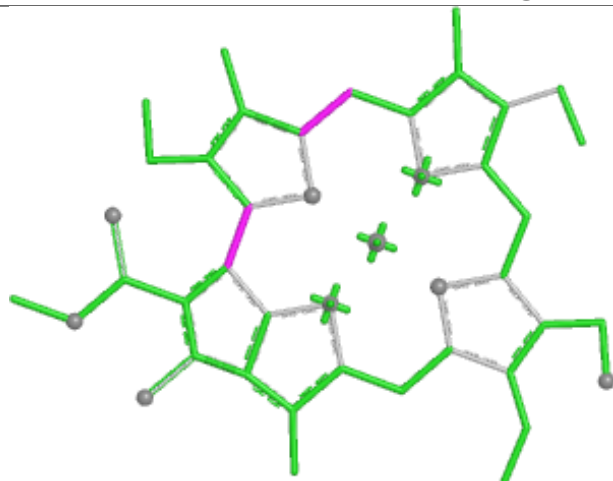
Rings



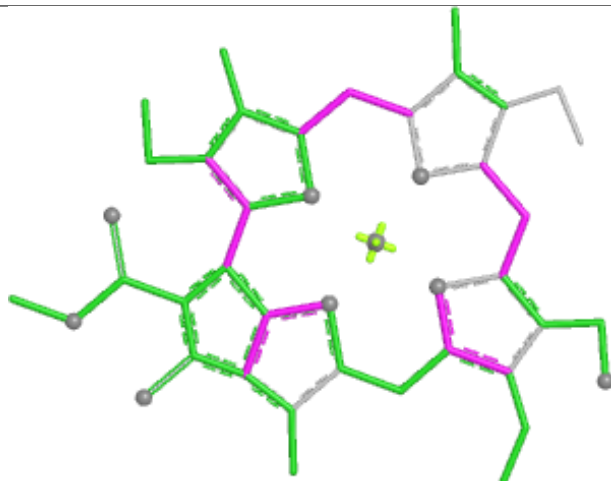




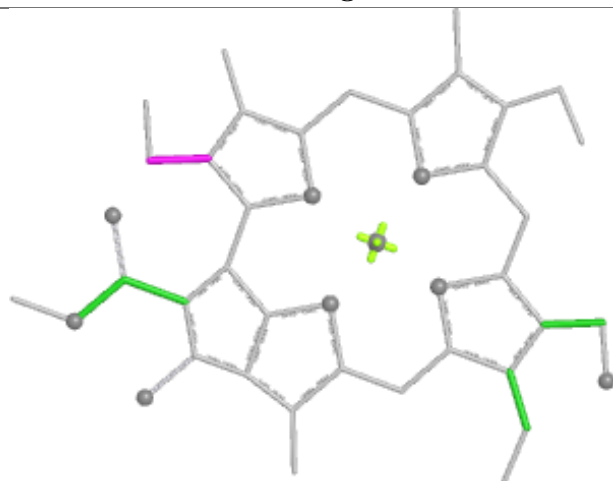
## Ligand CHL 4 606



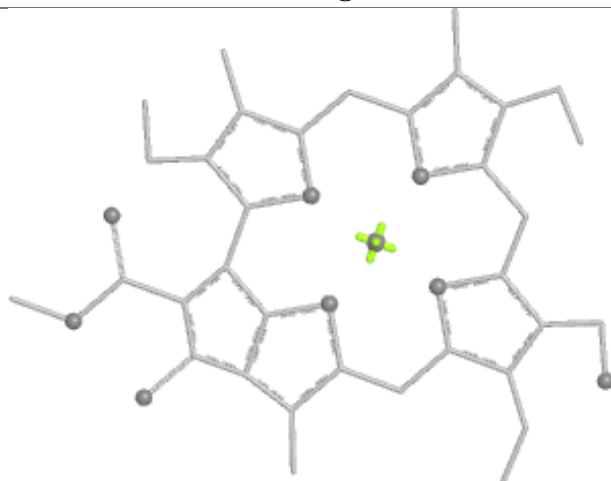
Bond lengths



Bond angles

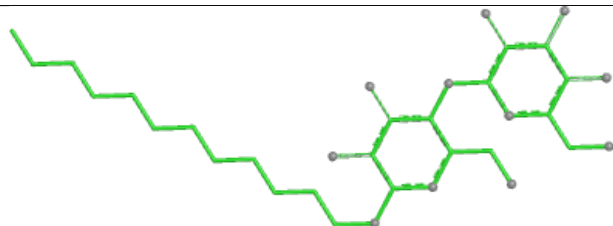


Torsions

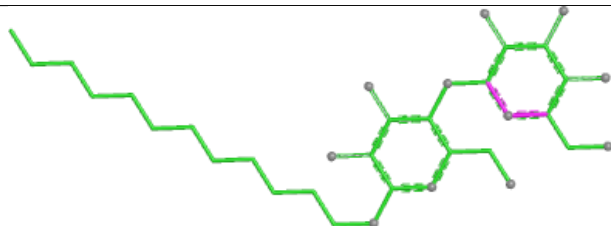


Rings

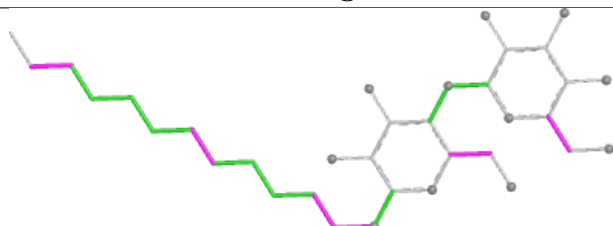
## Ligand LMU 1 319



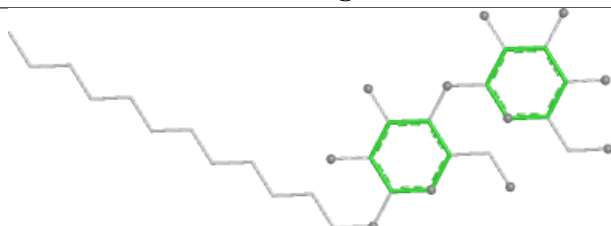
Bond lengths



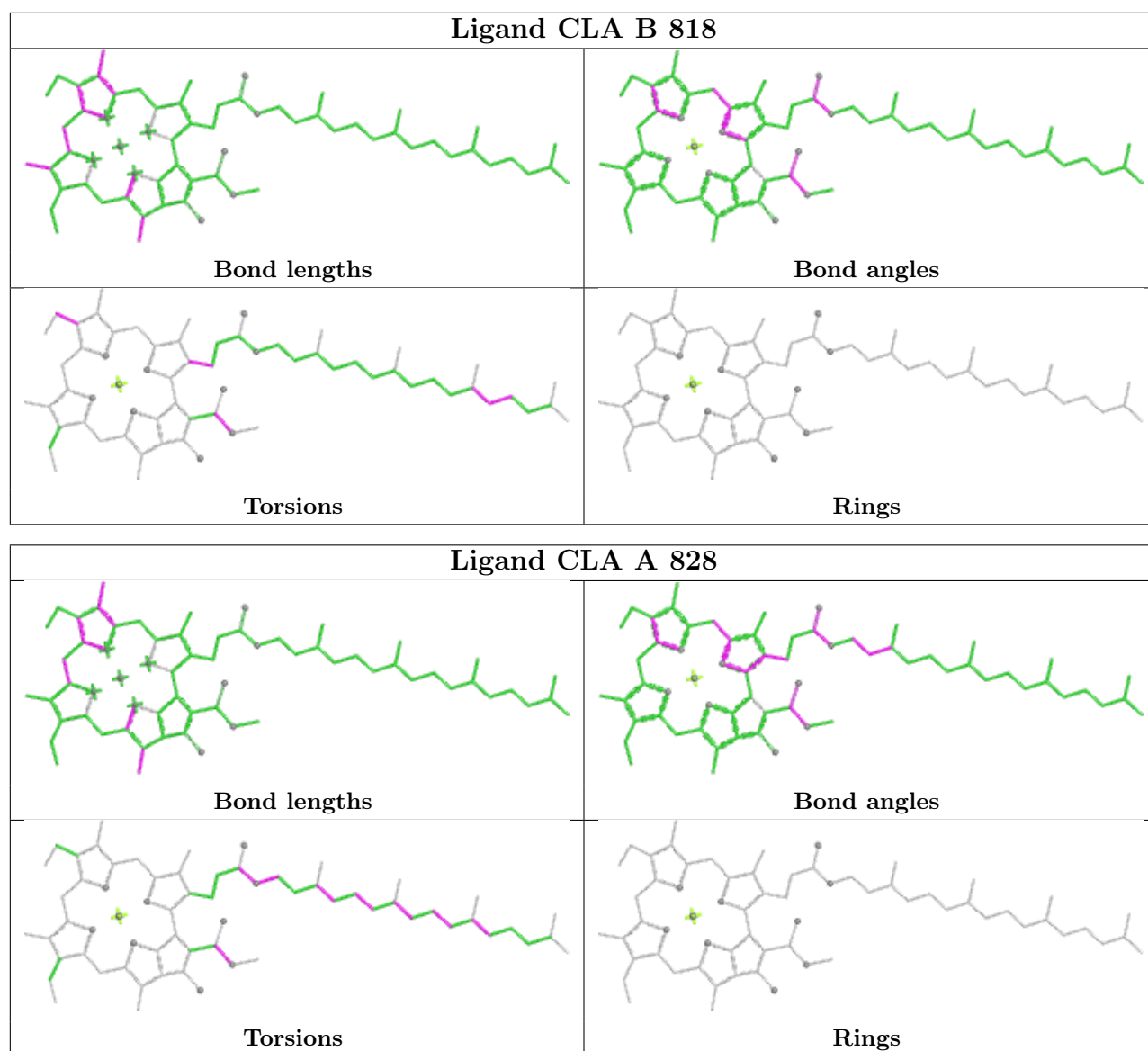
Bond angles

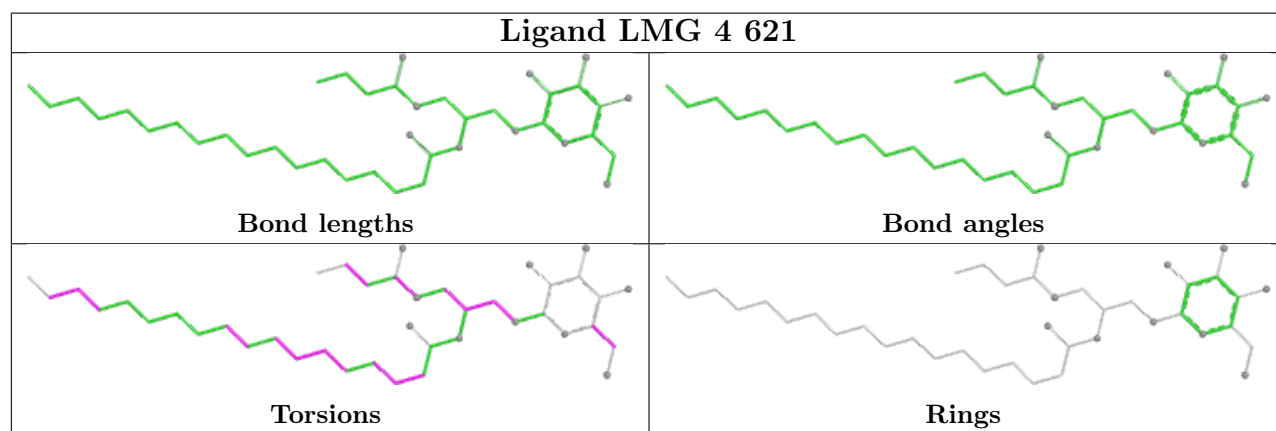
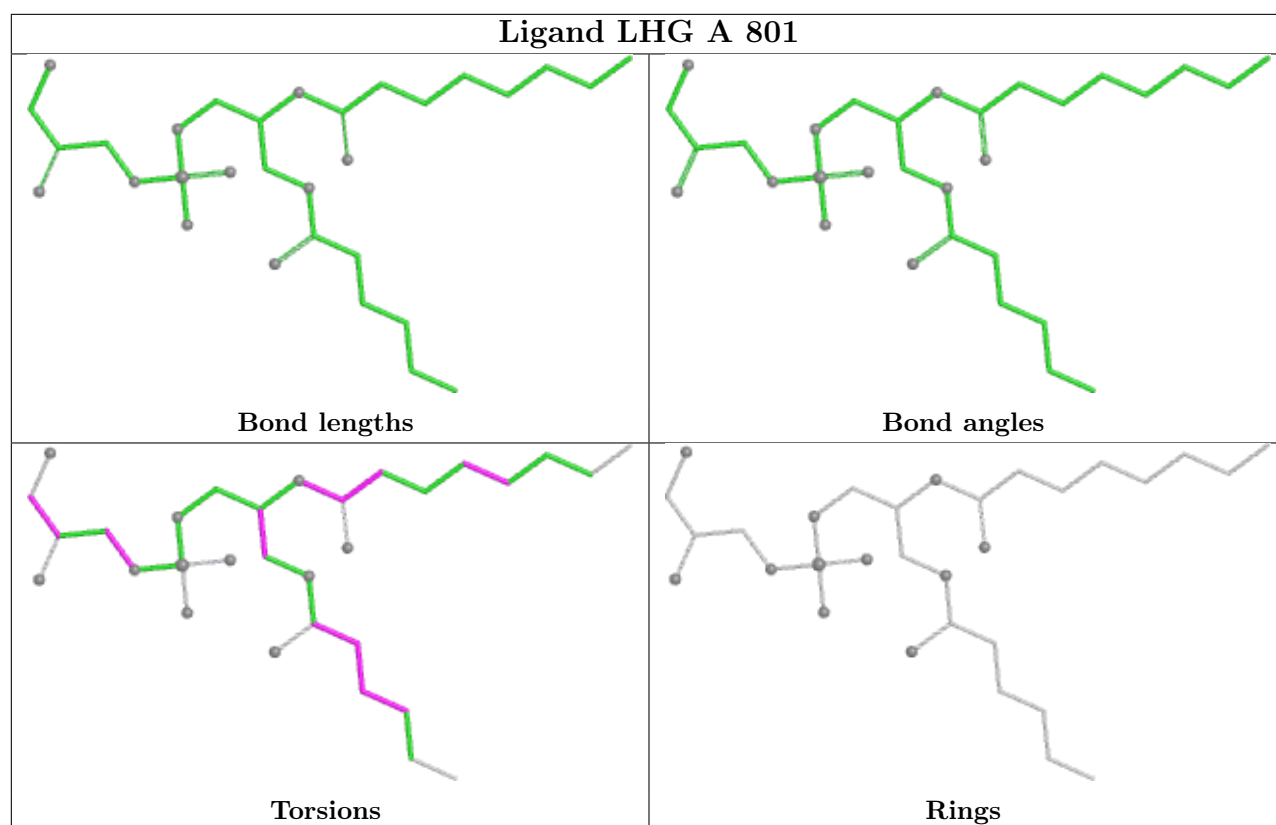


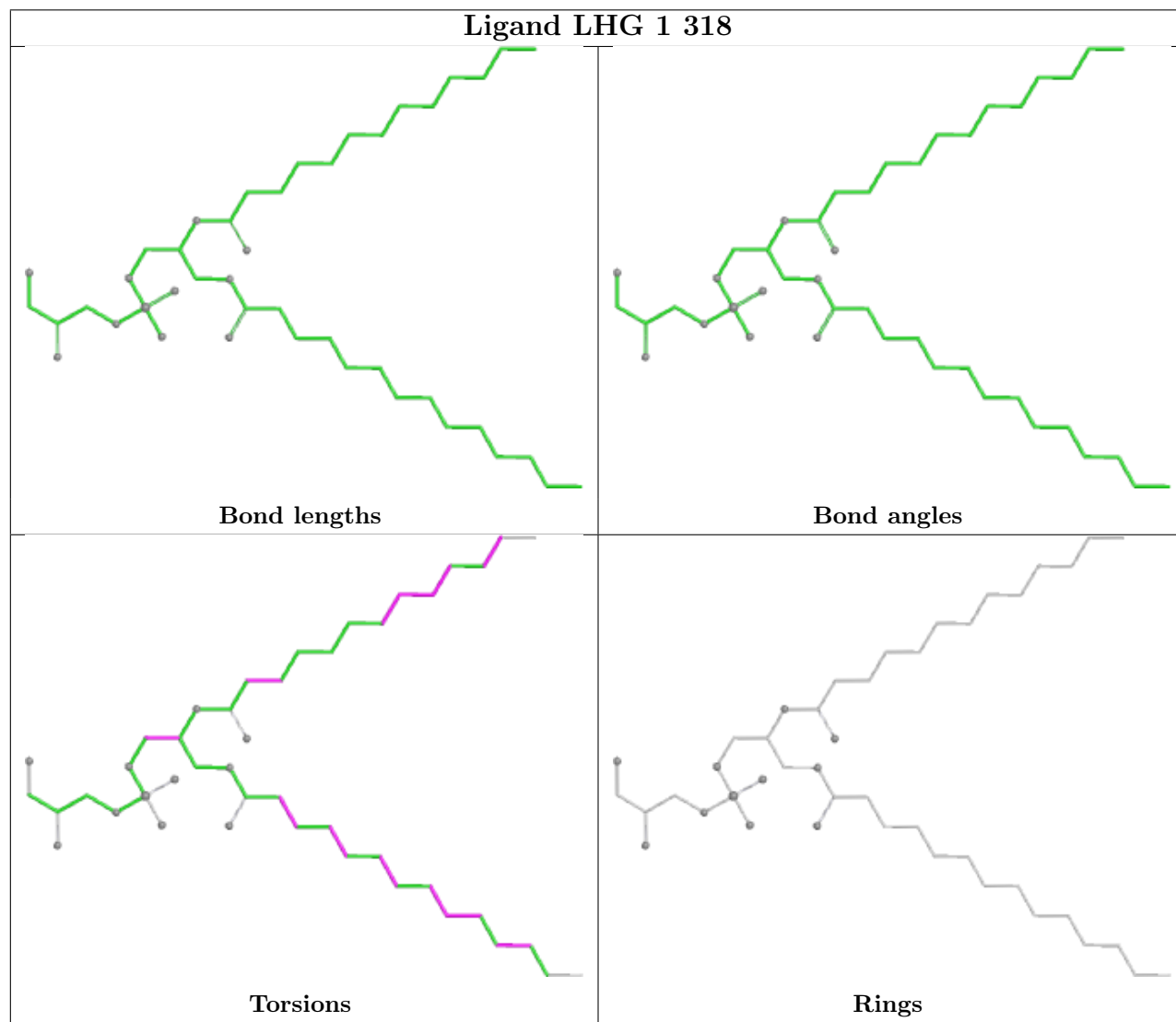
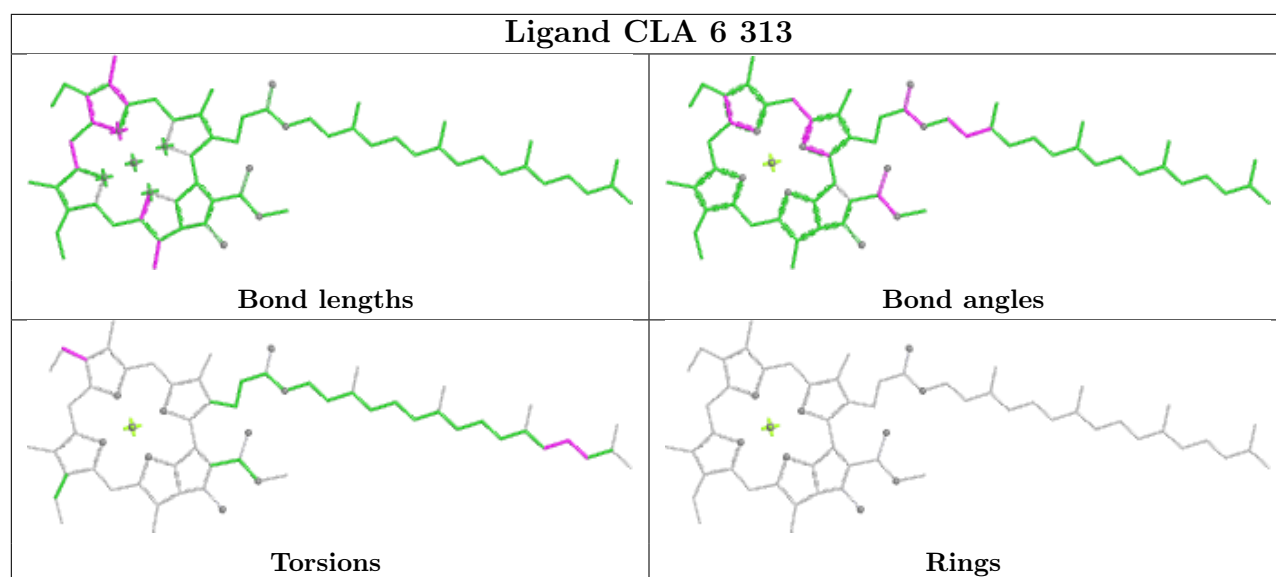
Torsions

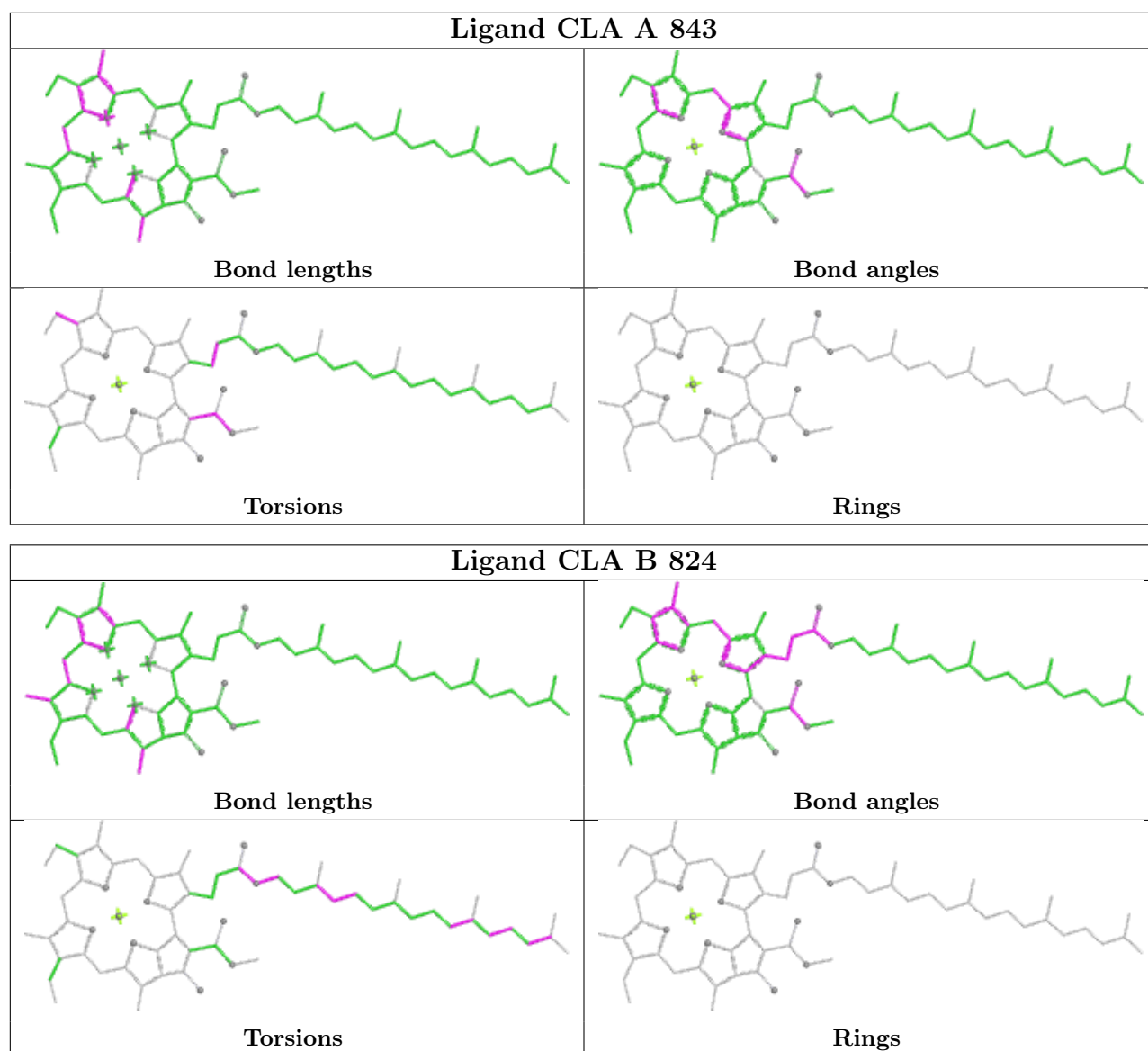


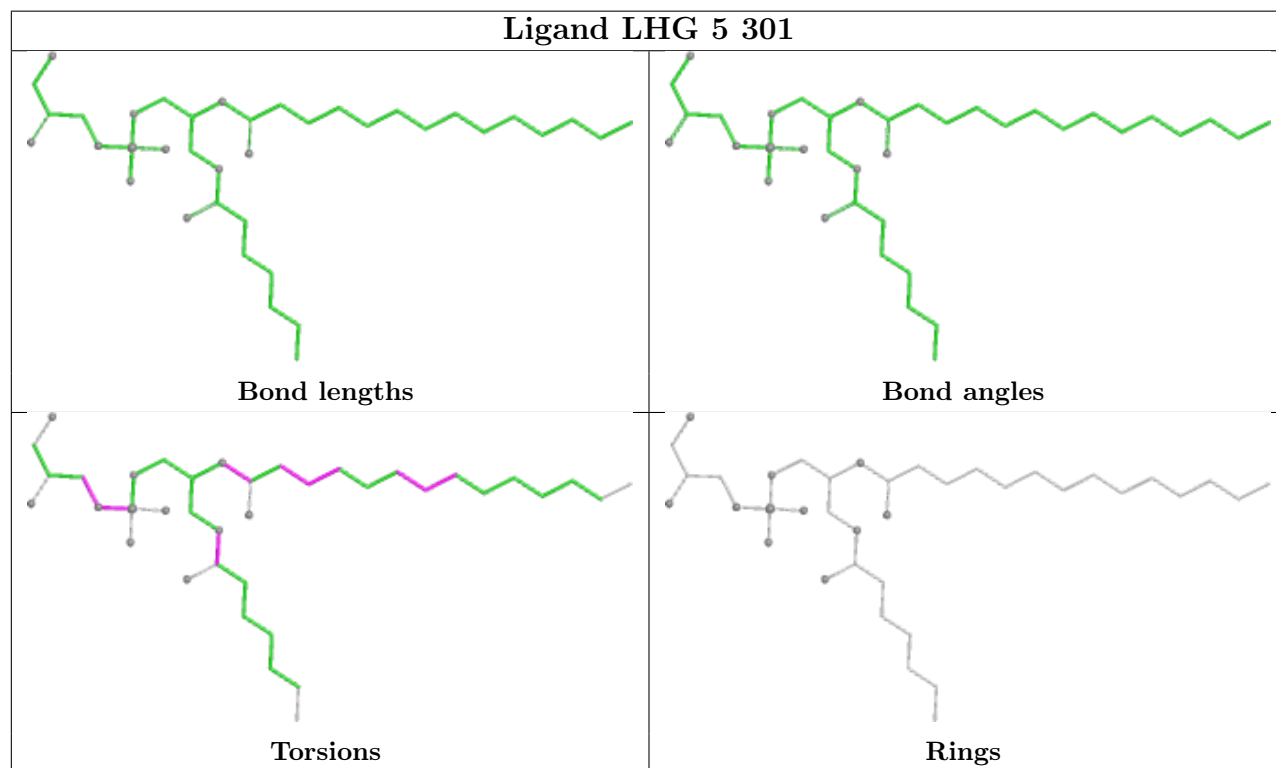
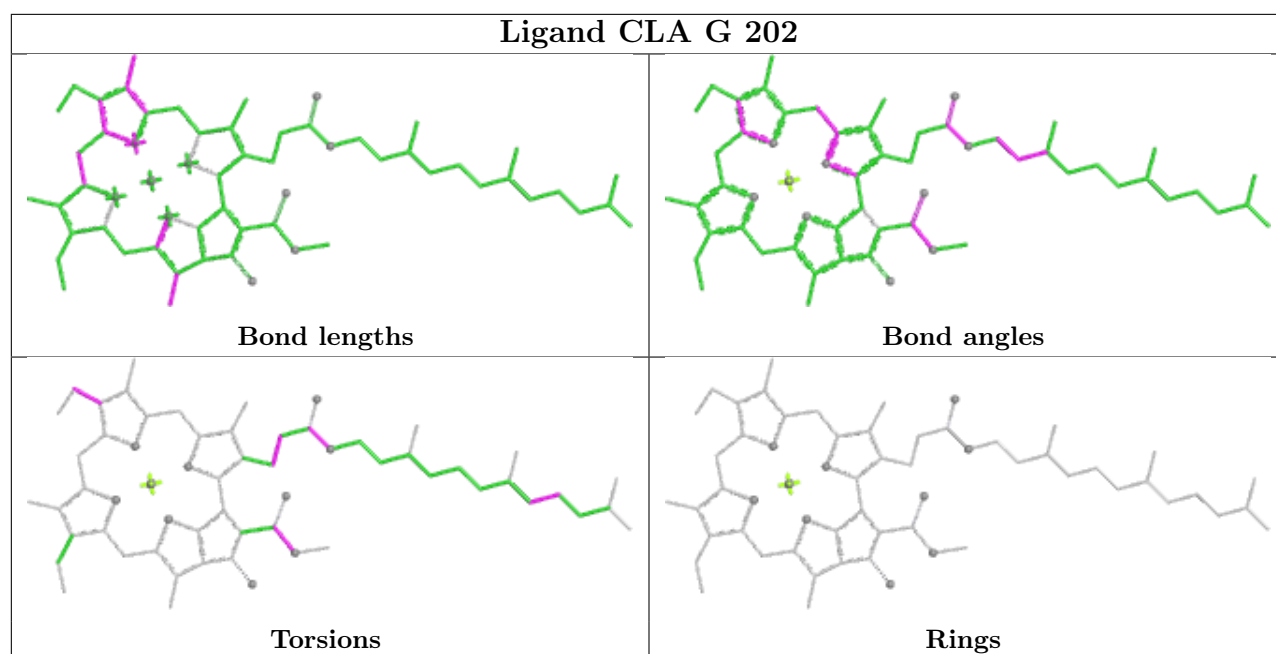
Rings



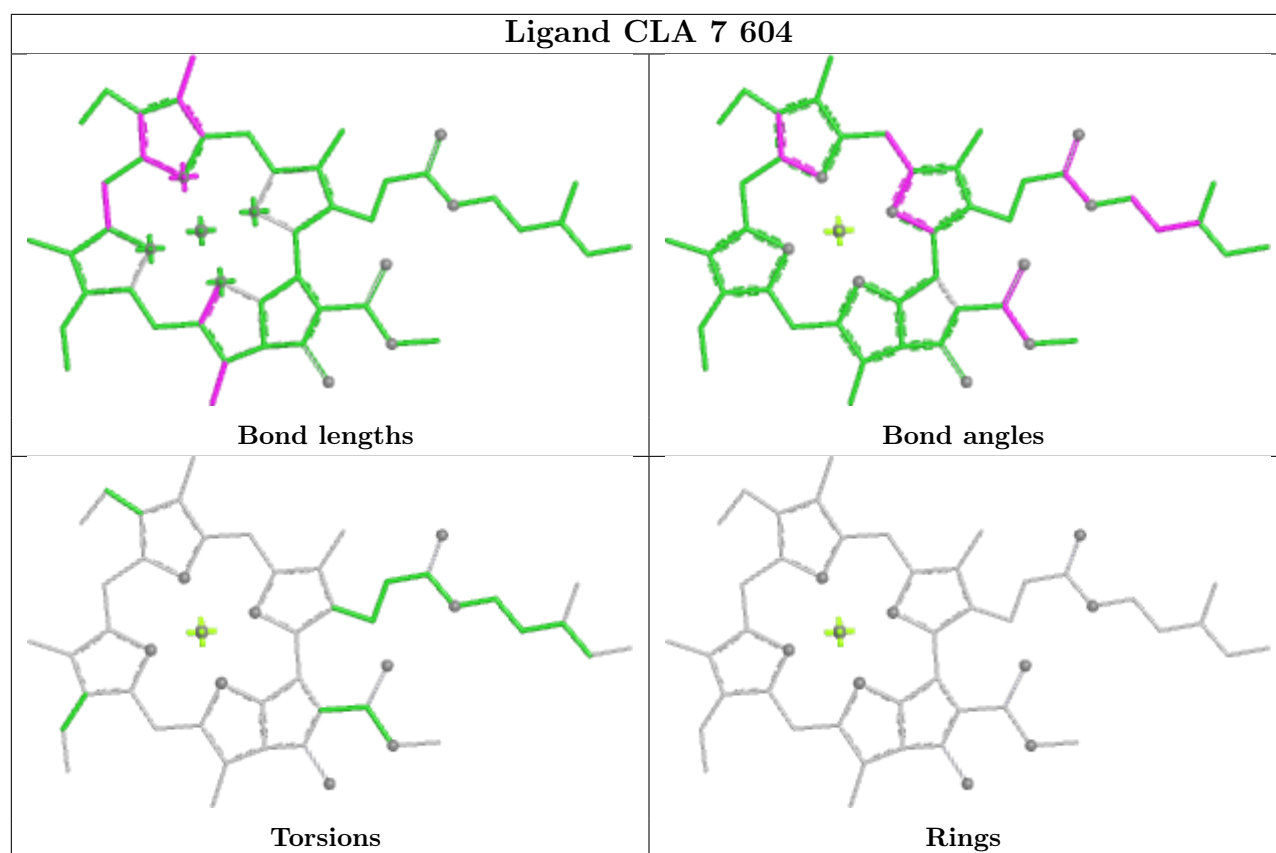




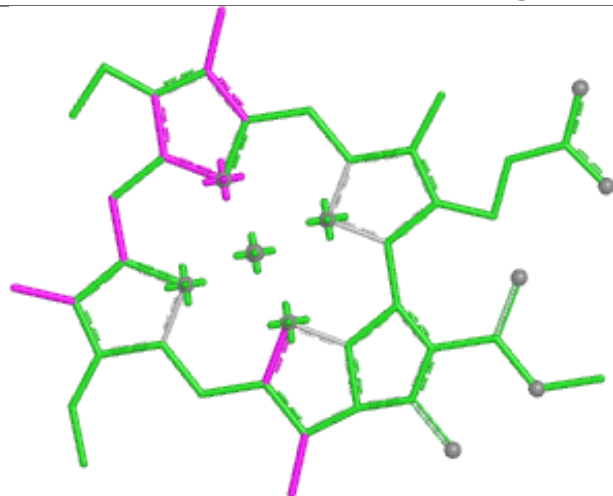




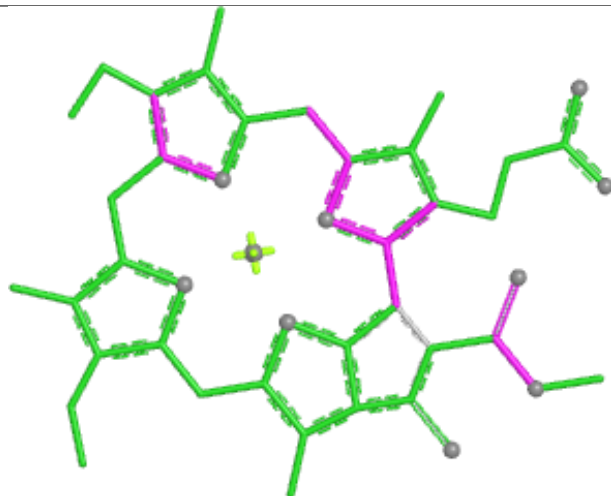




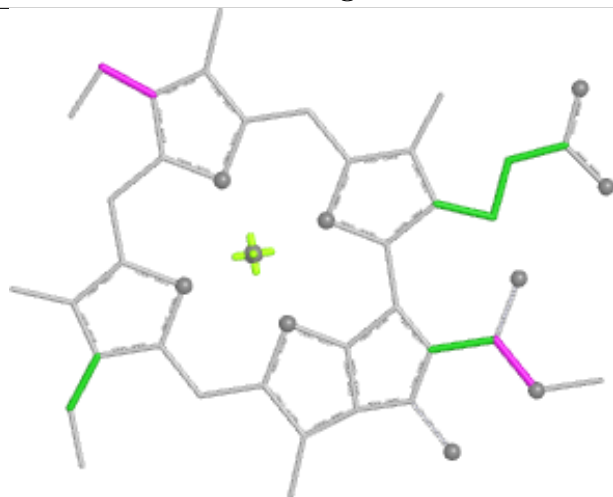
## Ligand CLA K 202



Bond lengths



Bond angles

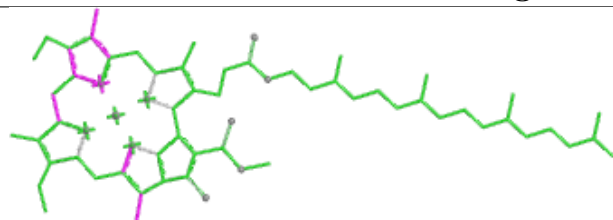


Torsions

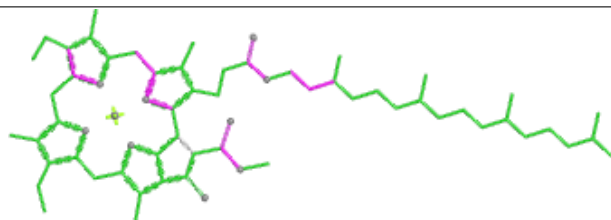


Rings

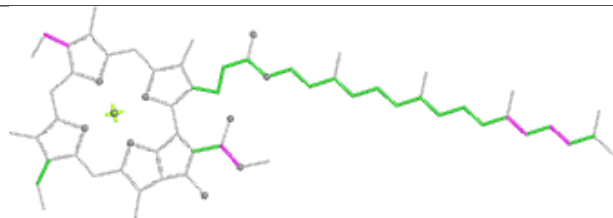
## Ligand CLA A 835



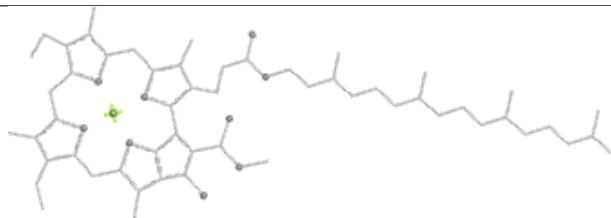
Bond lengths



Bond angles

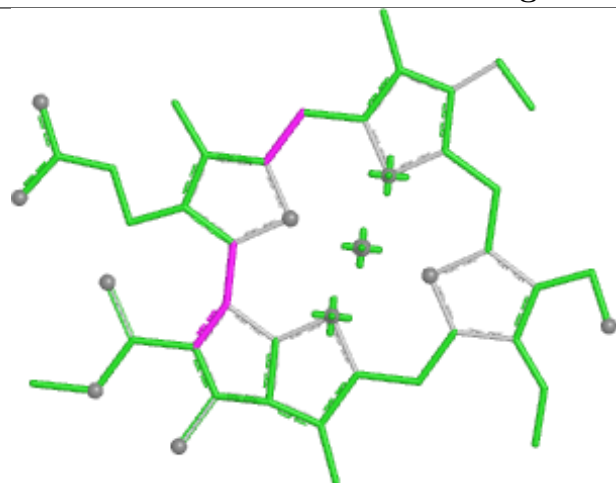


Torsions

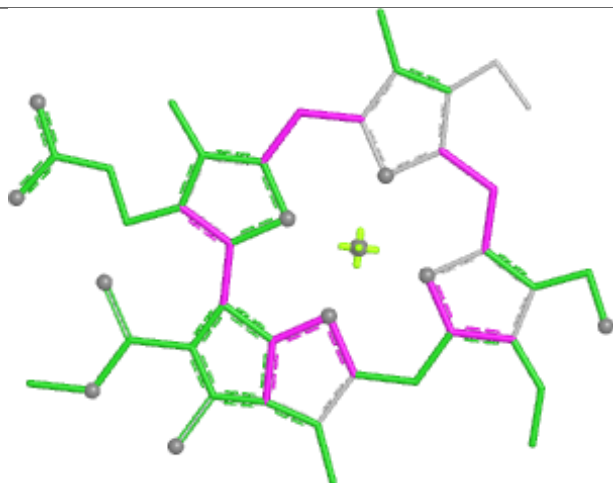


Rings

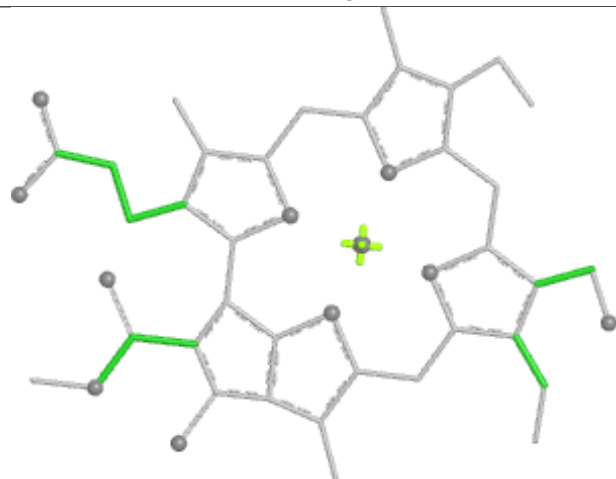
## Ligand CHL 7 605



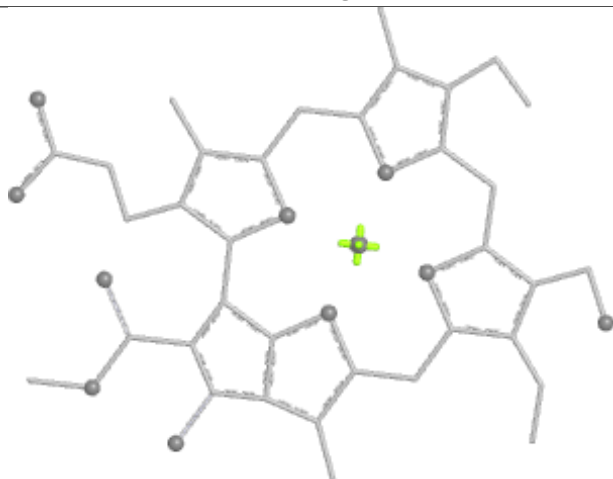
Bond lengths



Bond angles

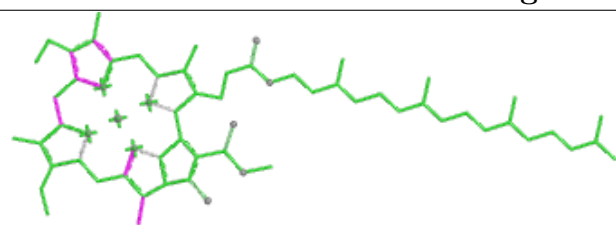


Torsions

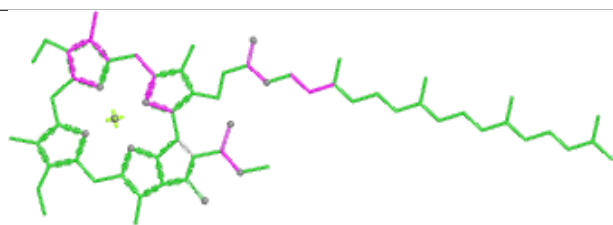


Rings

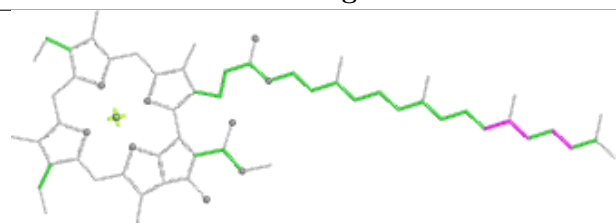
## Ligand CLA 3 308



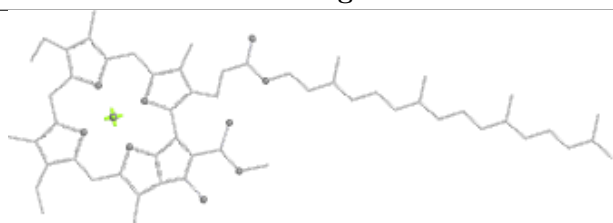
Bond lengths



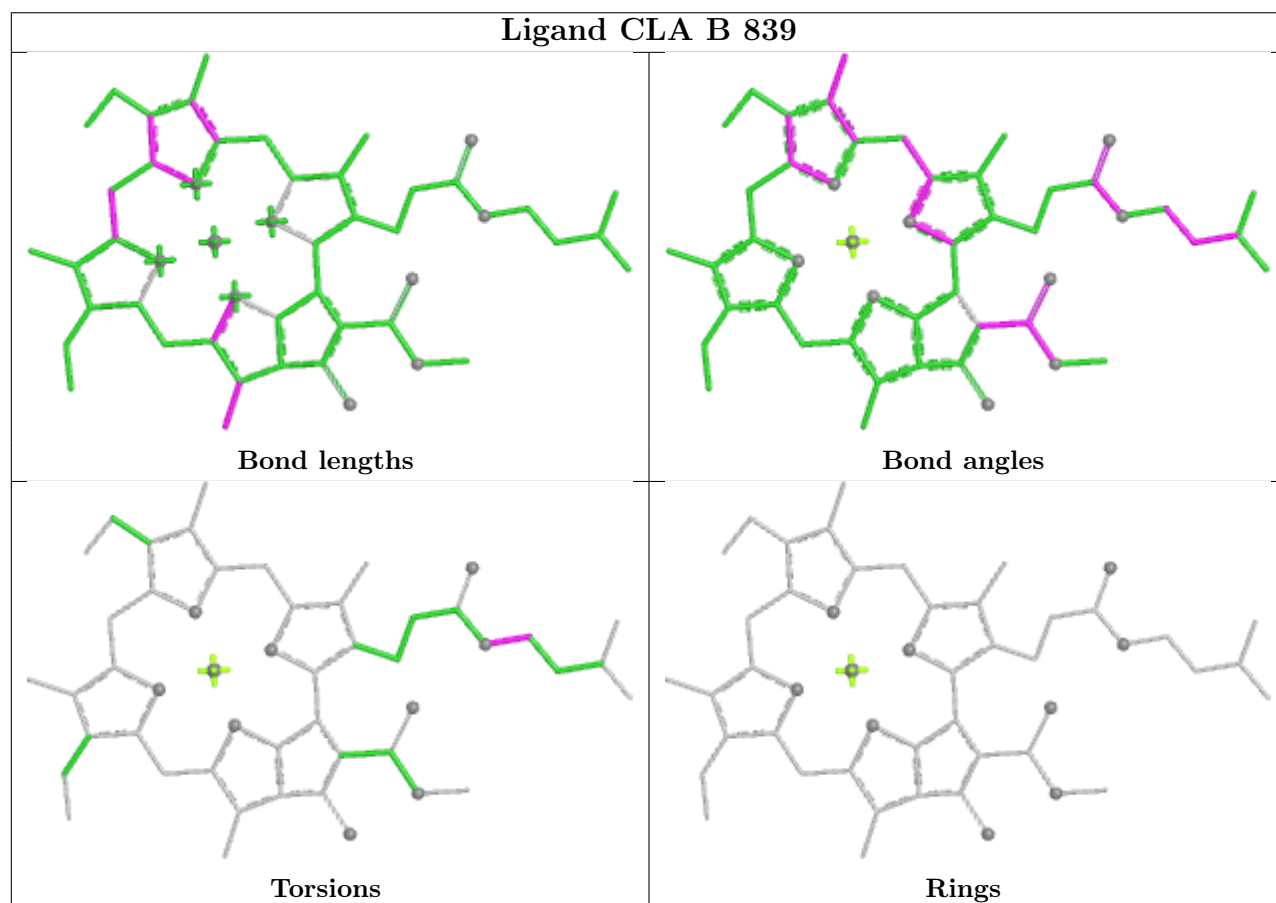
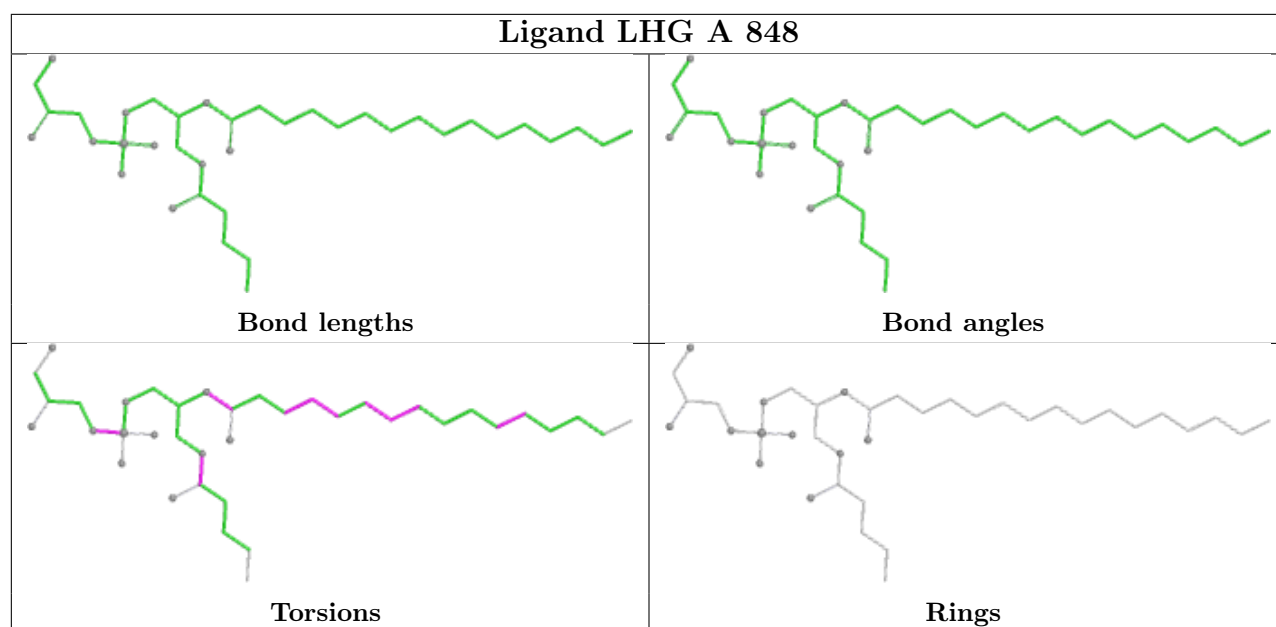
Bond angles



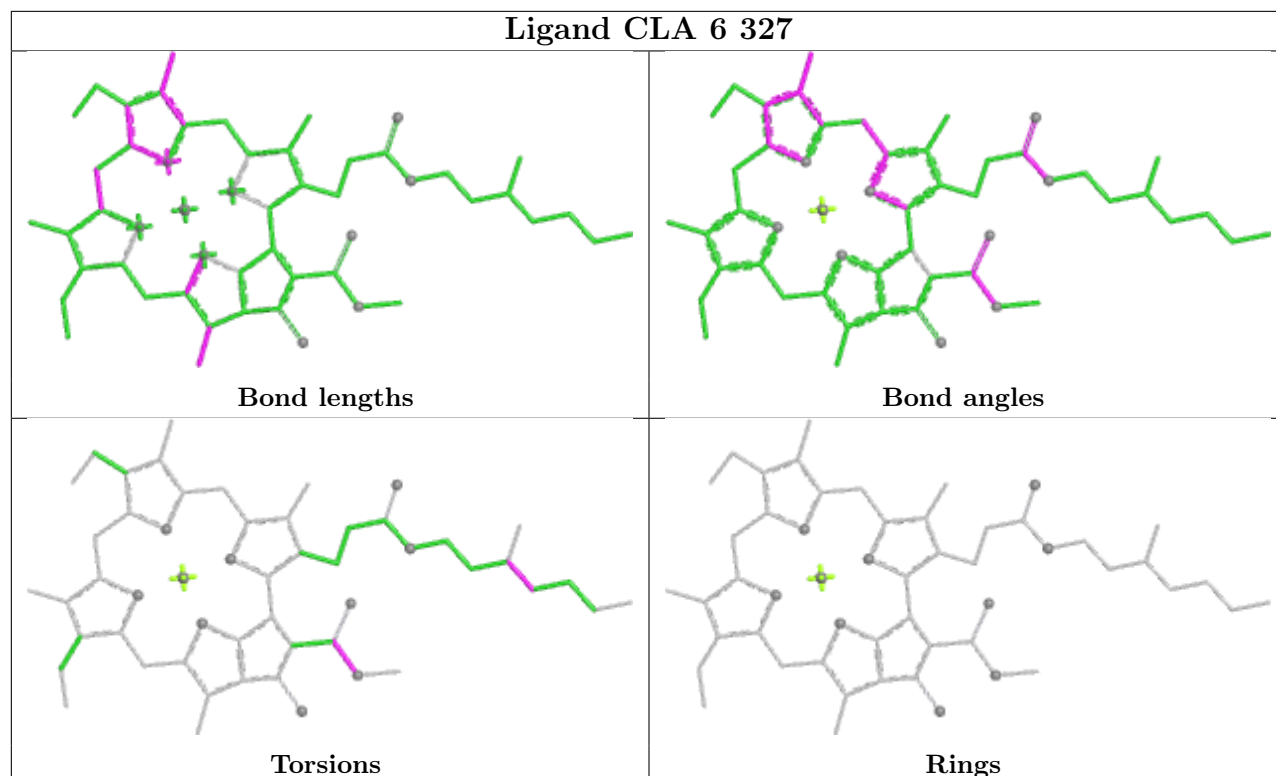
Torsions



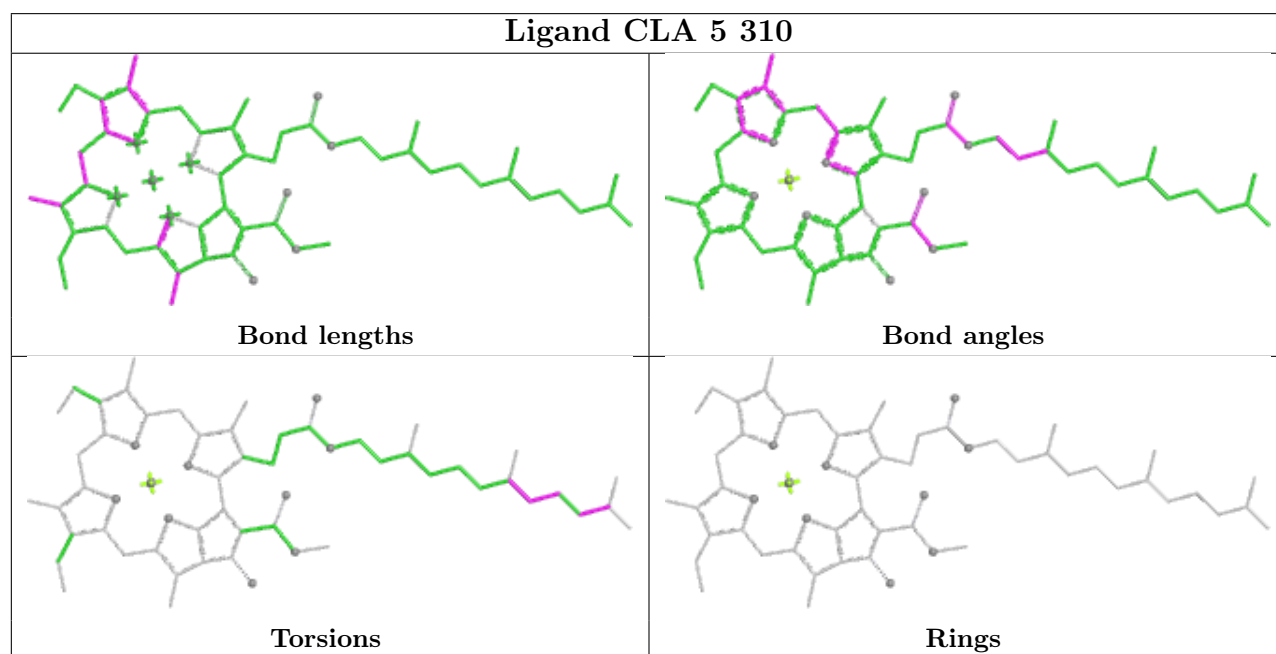
Rings



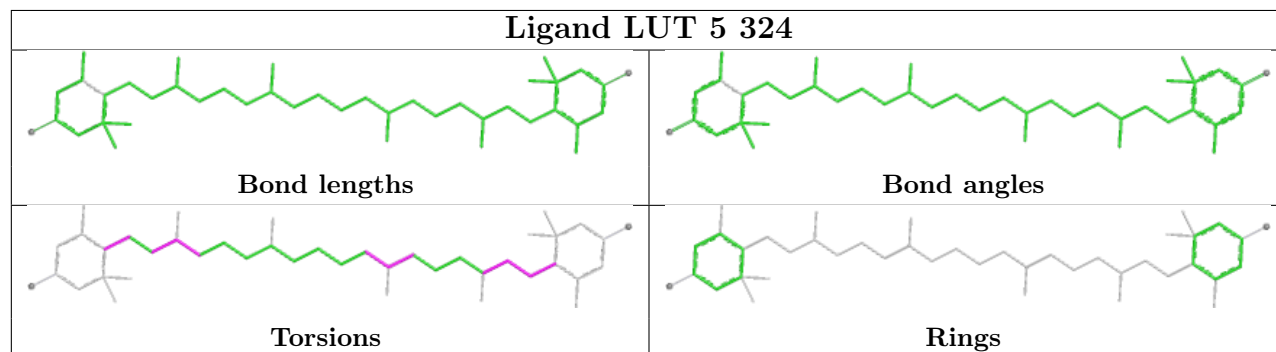
## Ligand CLA 6 327

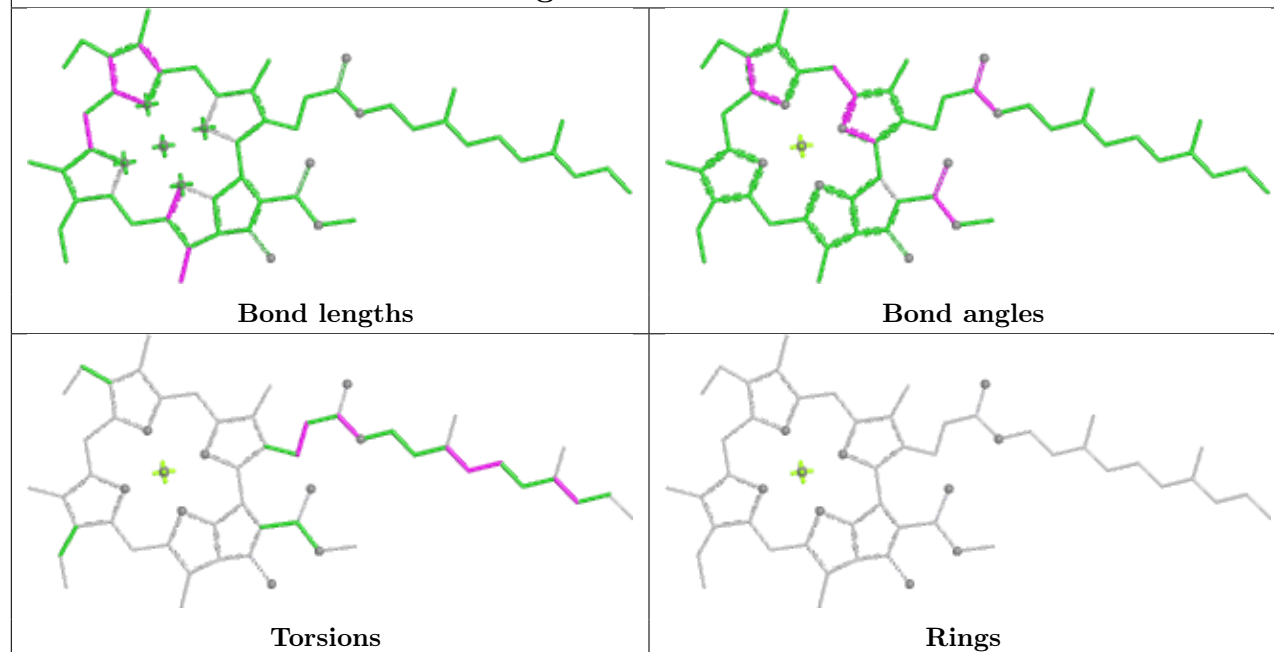
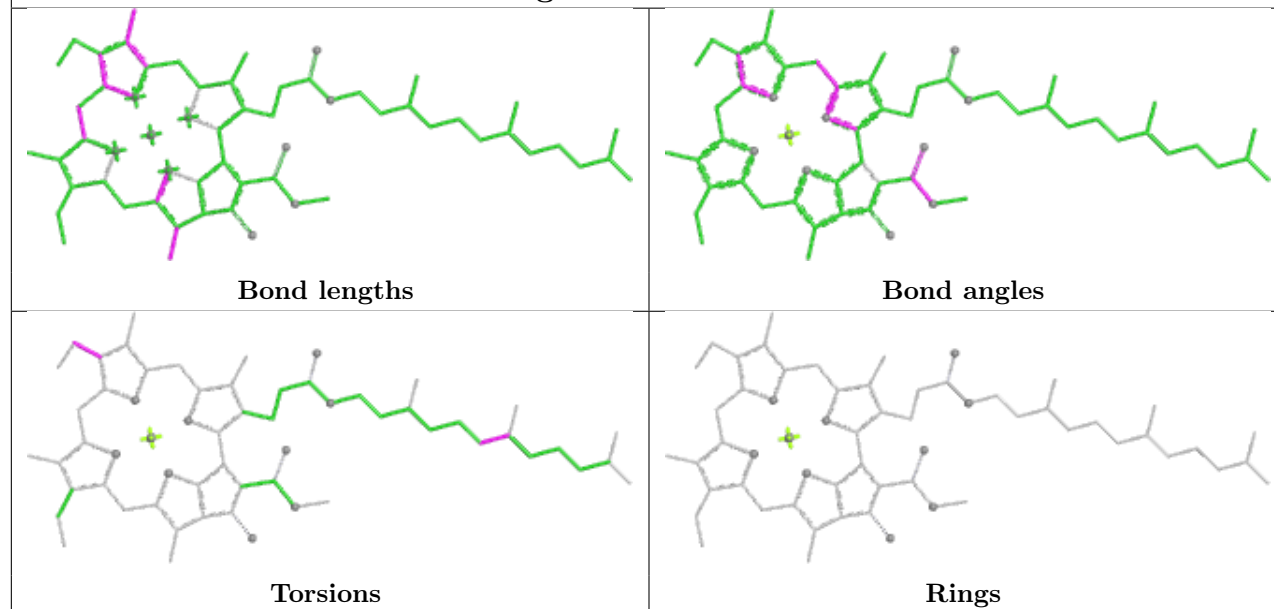


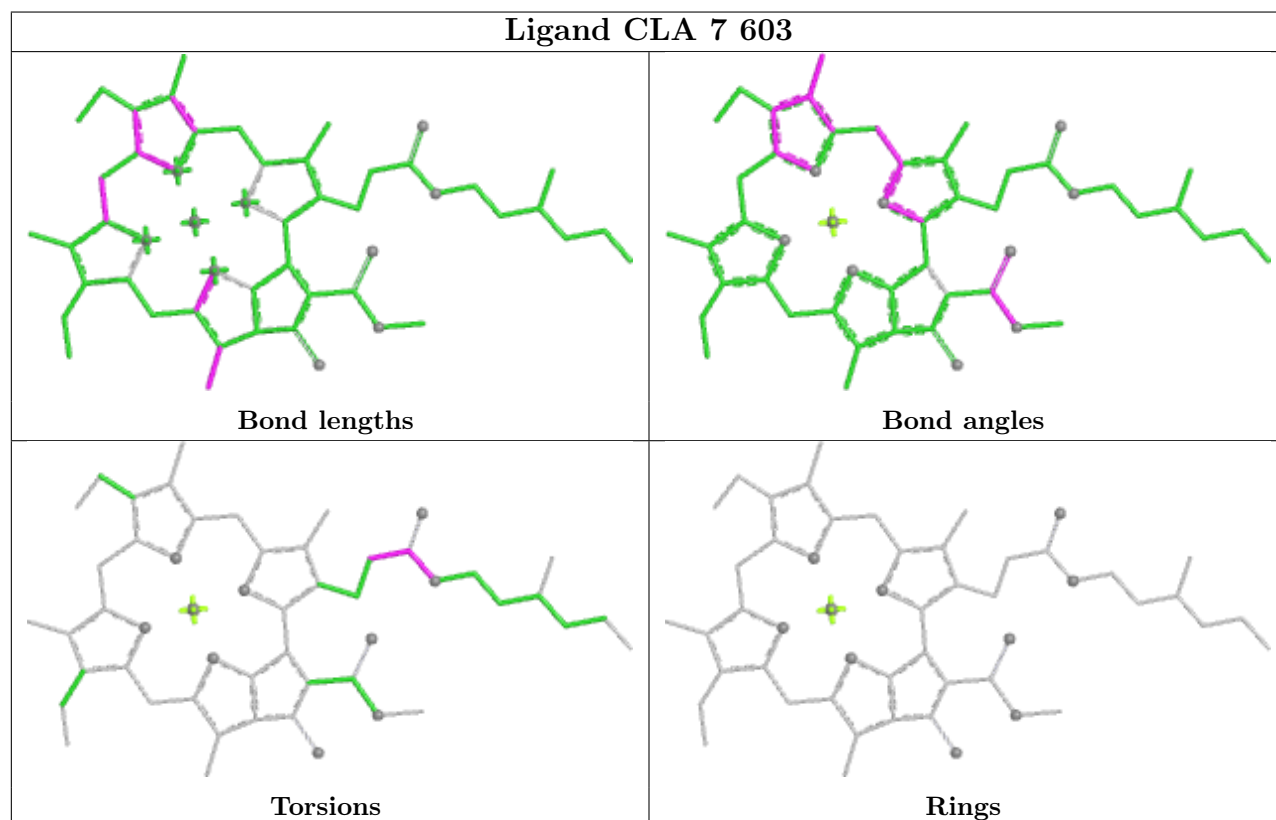
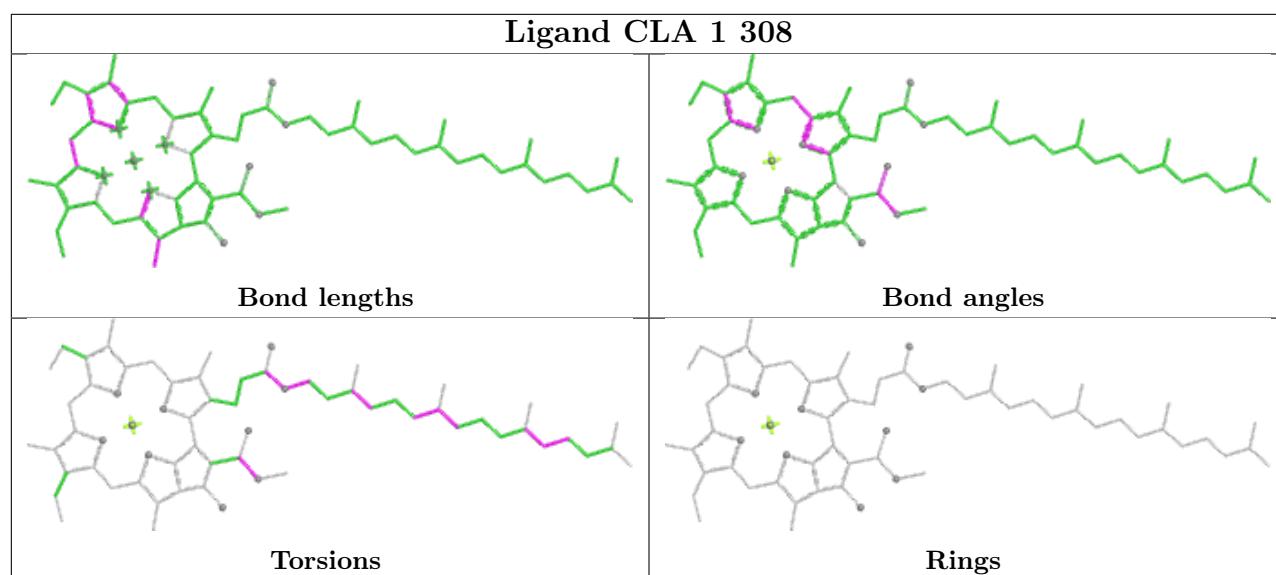
## Ligand CLA 5 310

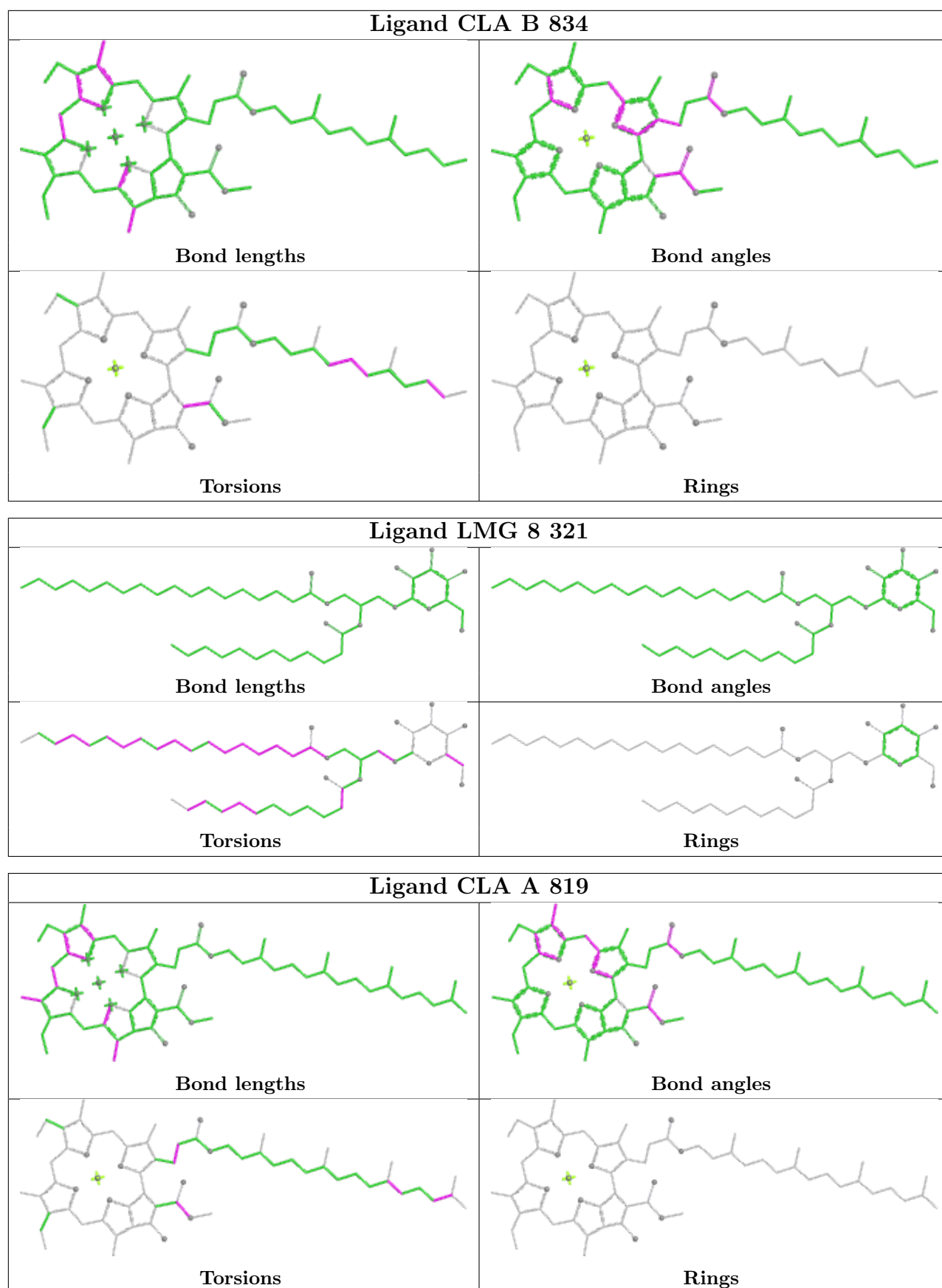


## Ligand LUT 5 324

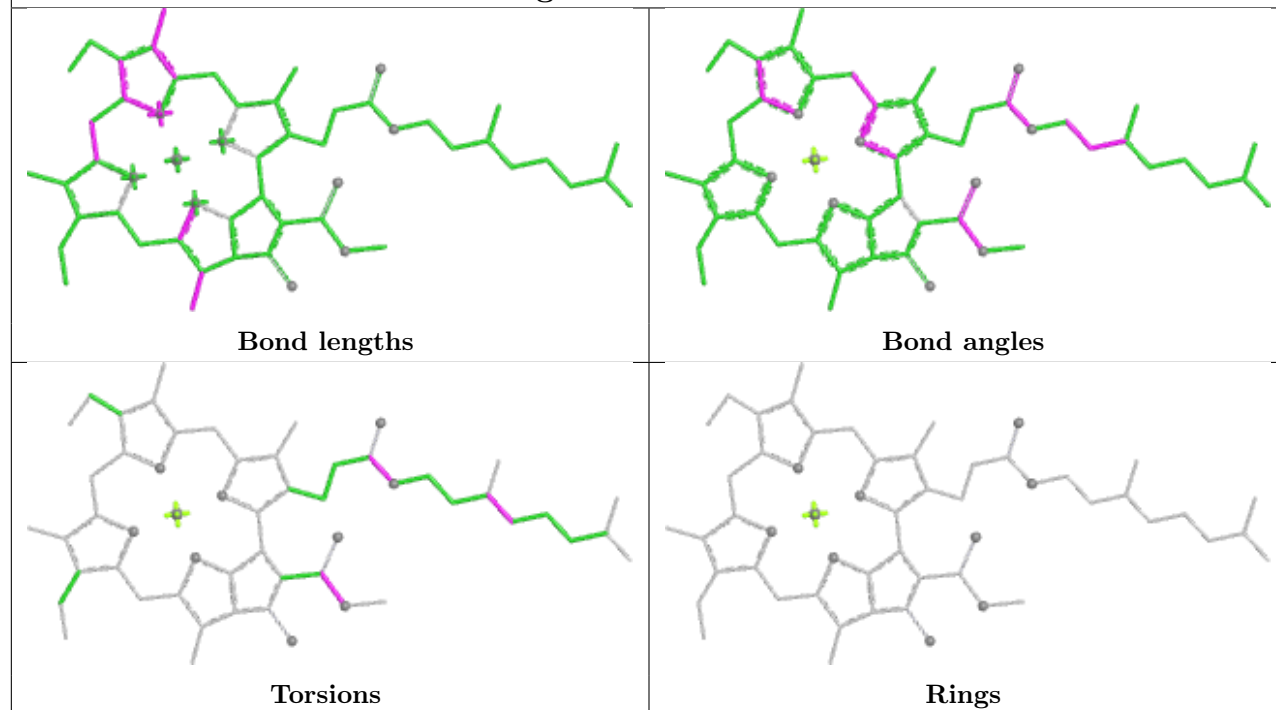
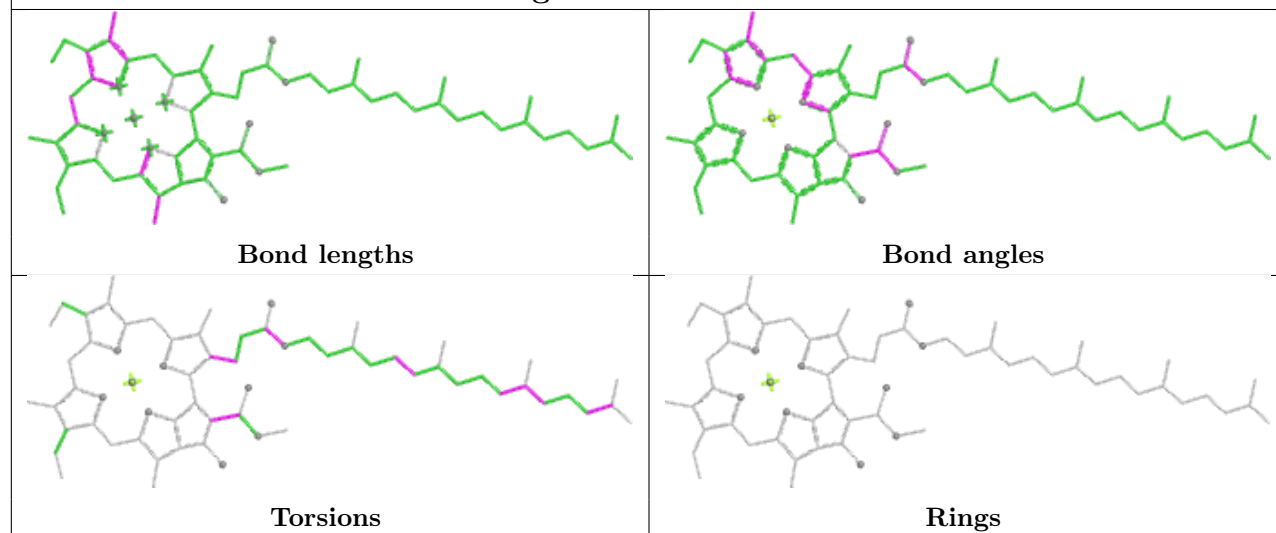
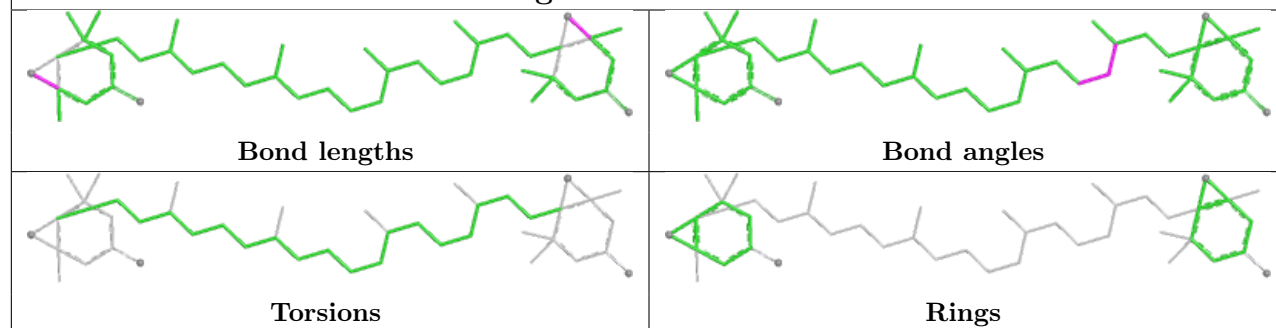


**Ligand CLA 1 303****Ligand CLA 4 610**

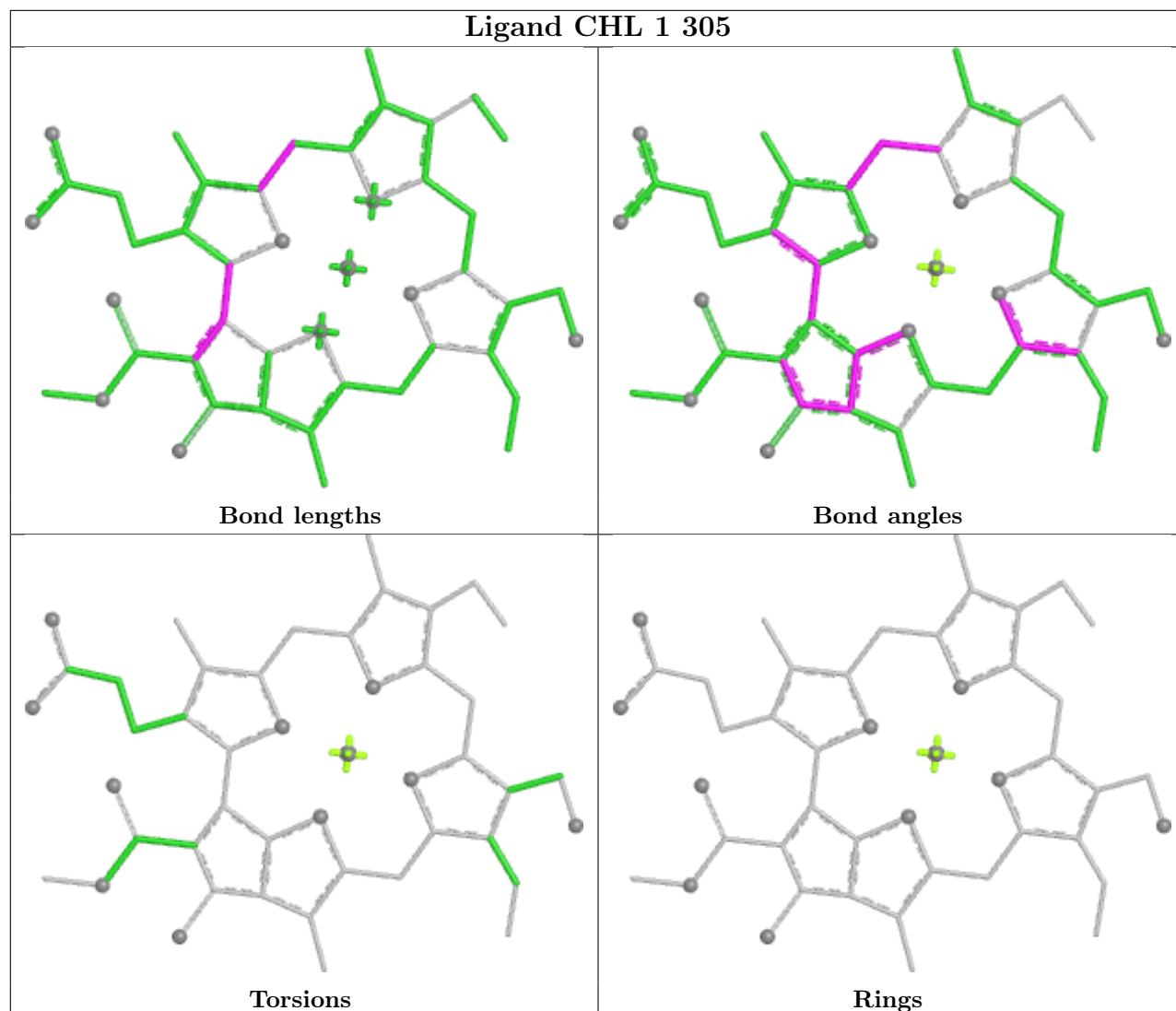


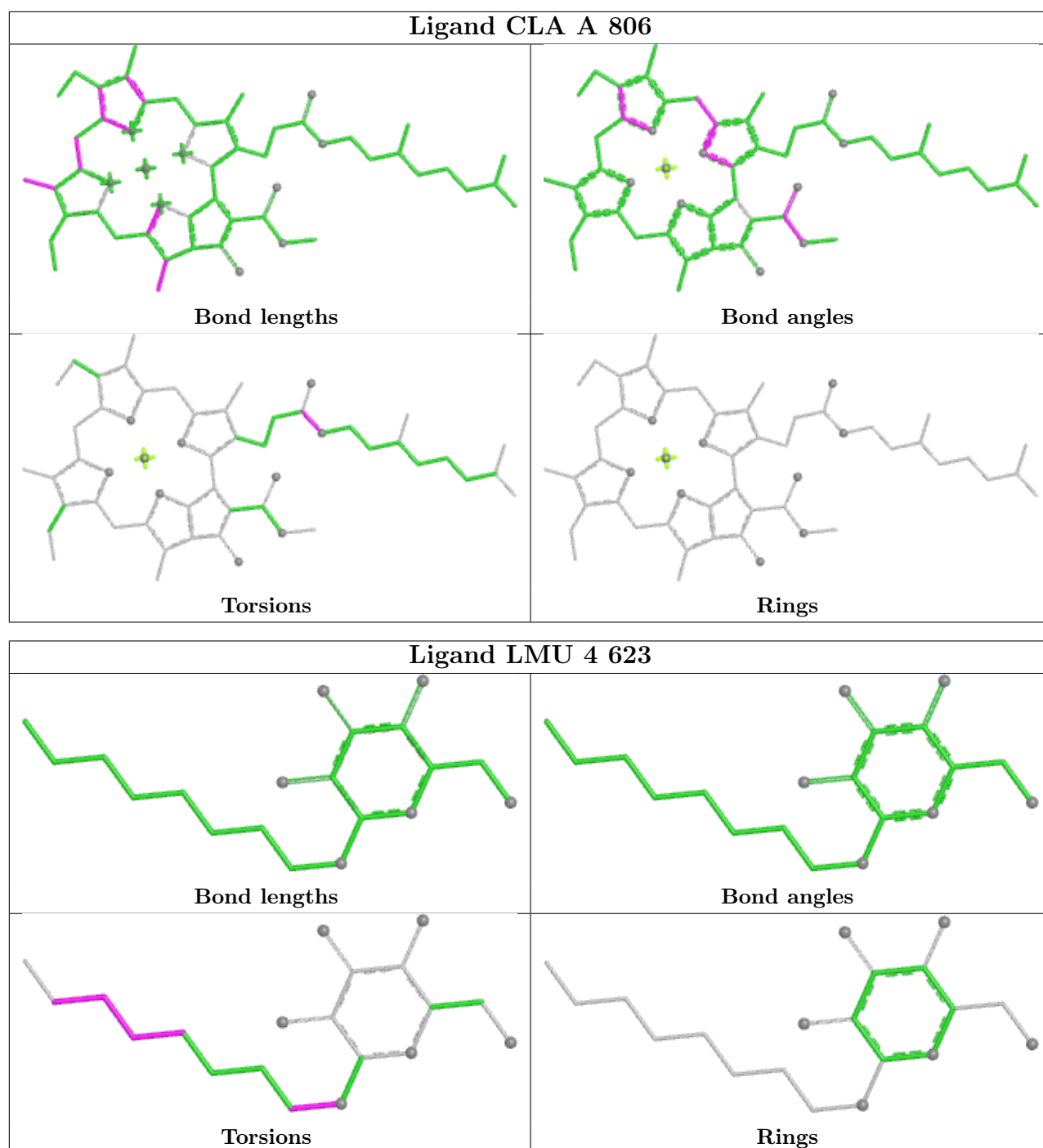




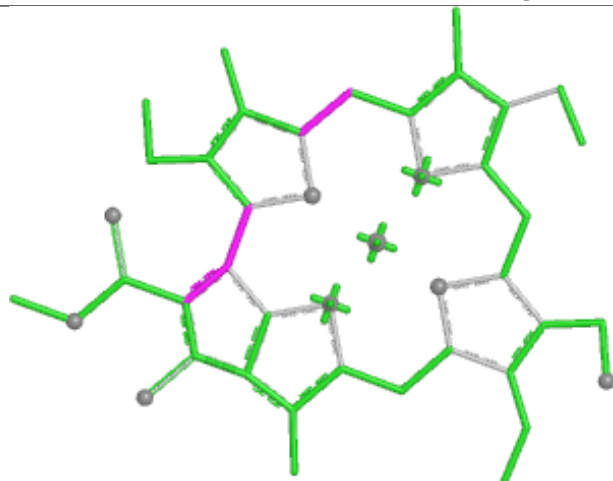
**Ligand CLA 4 613****Ligand CLA B 830****Ligand XAT 4 617**

## Ligand CHL 1 305

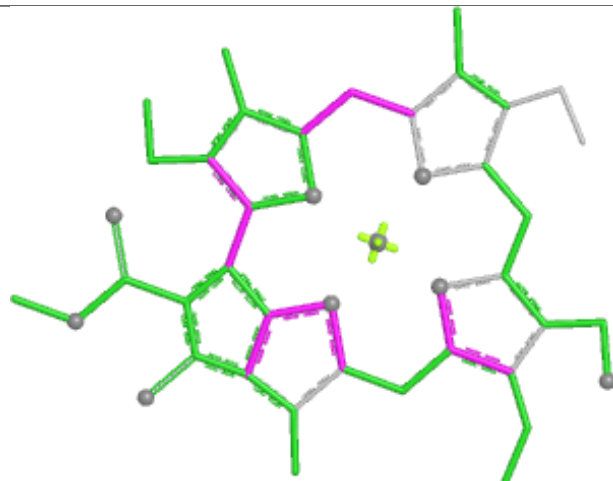




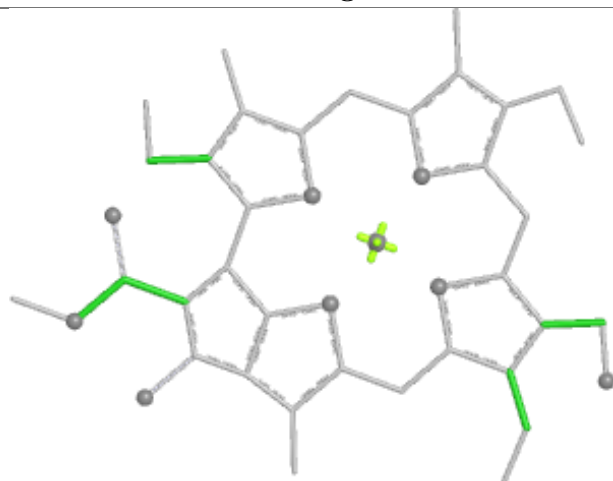
## Ligand CHL 6 317



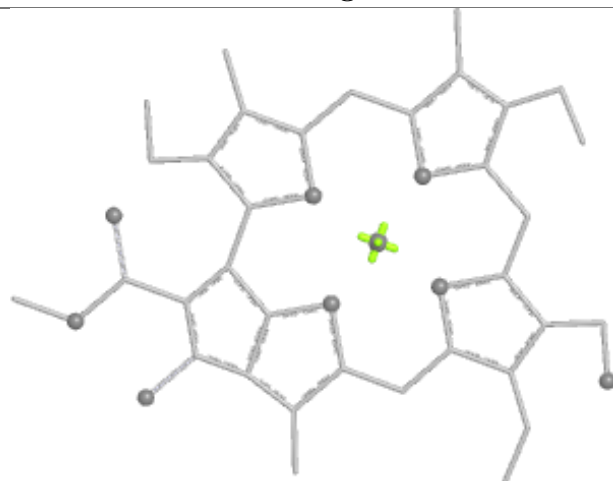
Bond lengths



Bond angles

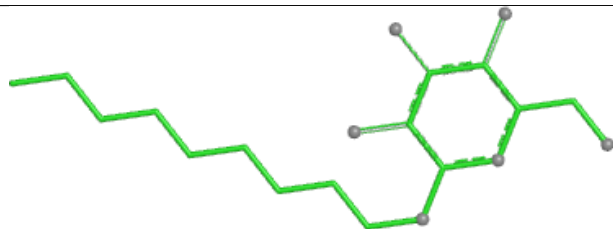


Torsions

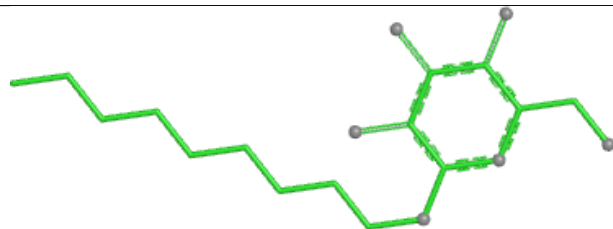


Rings

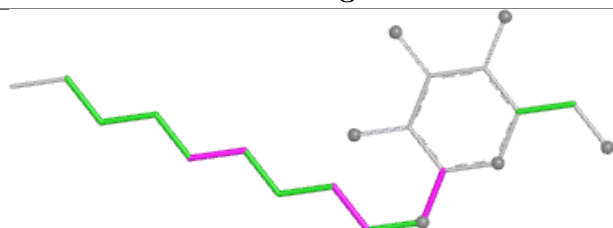
## Ligand LMU 7 619



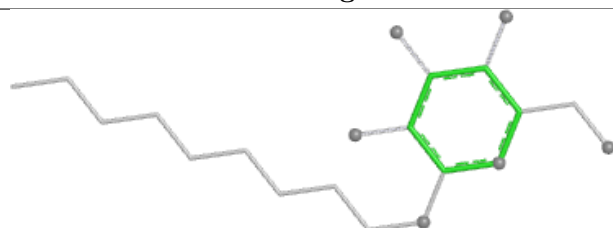
Bond lengths



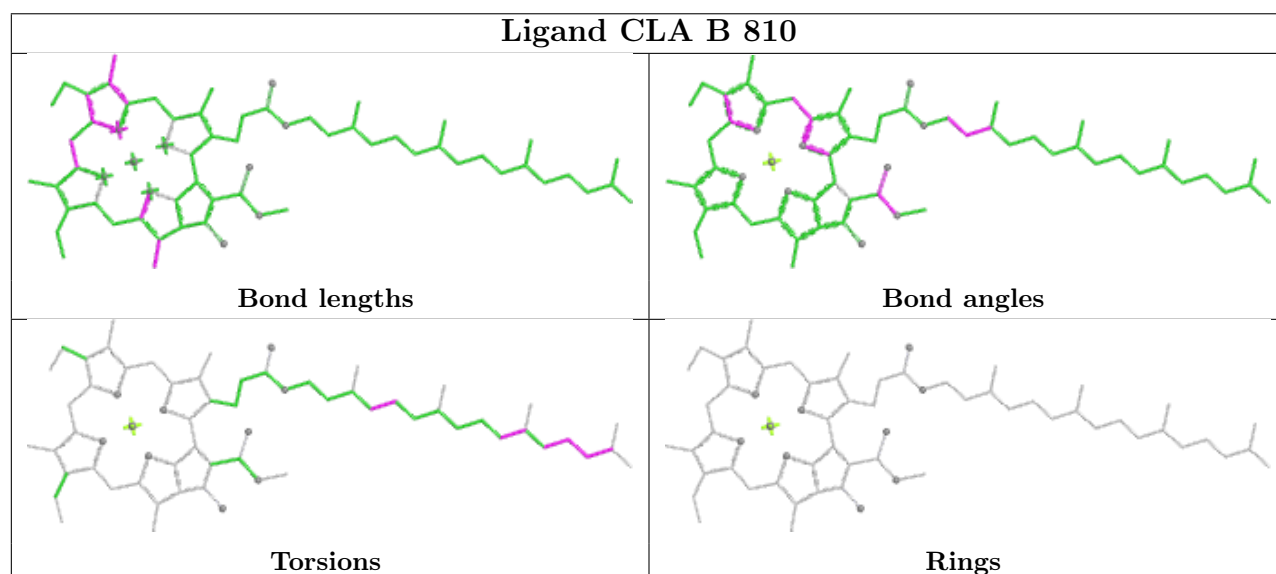
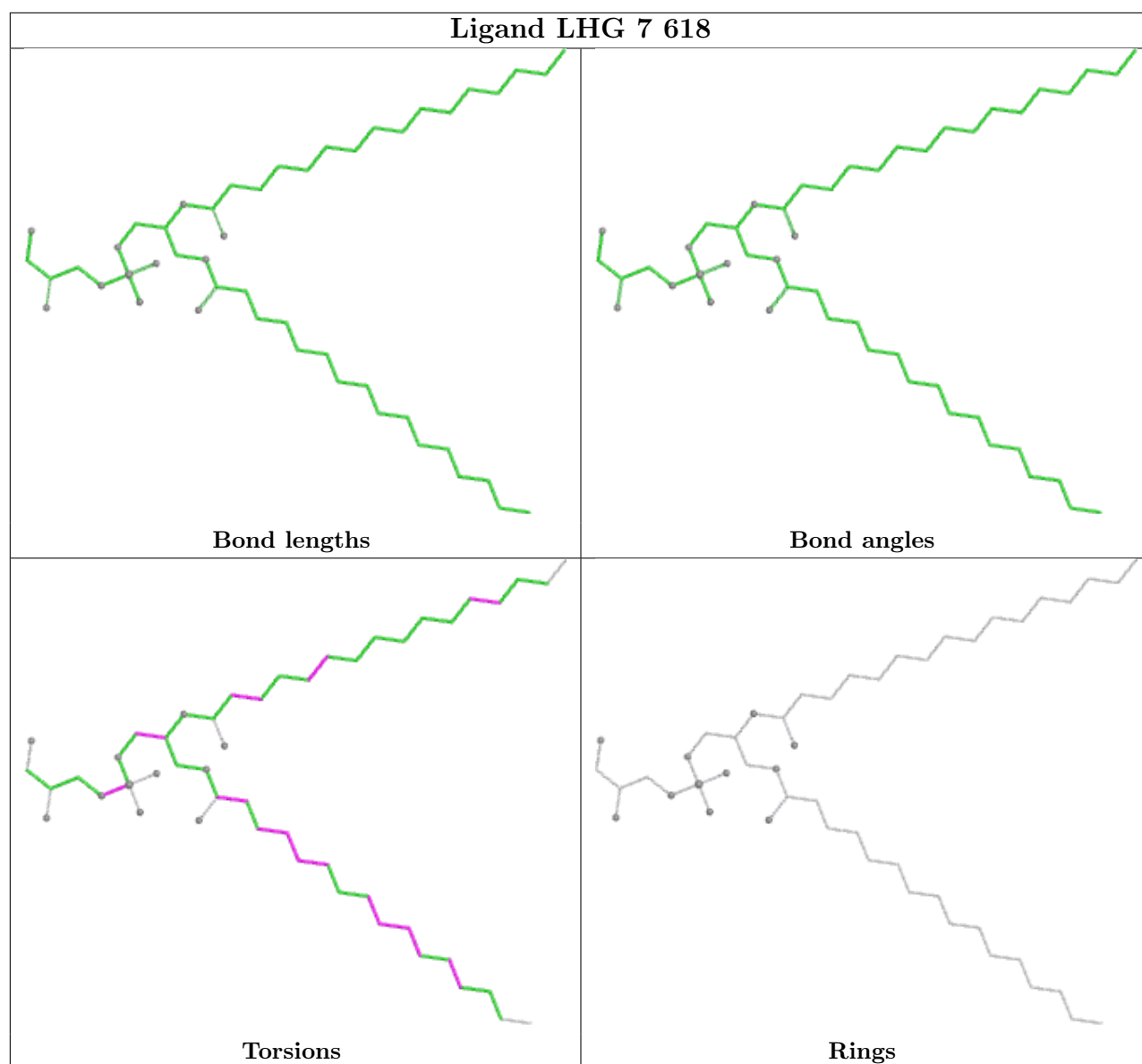
Bond angles



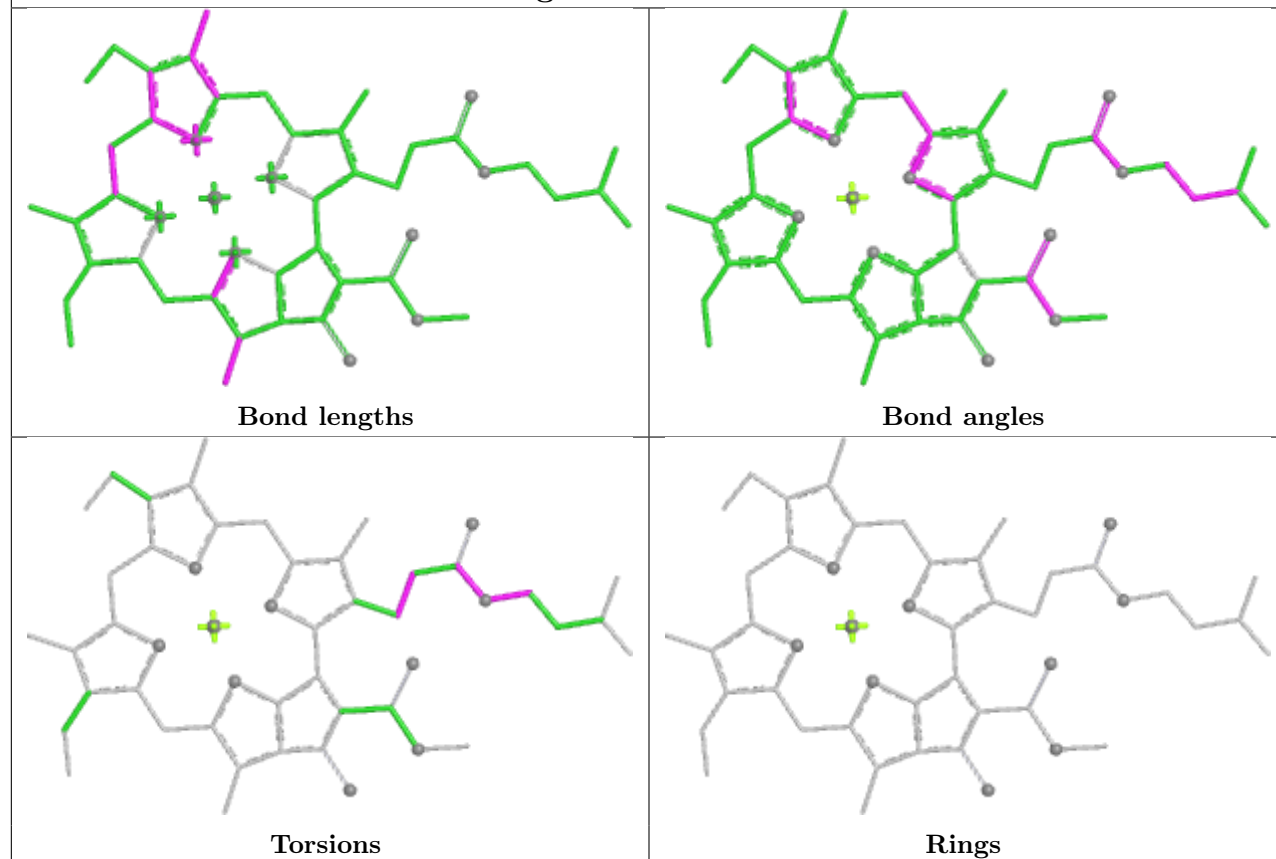
Torsions



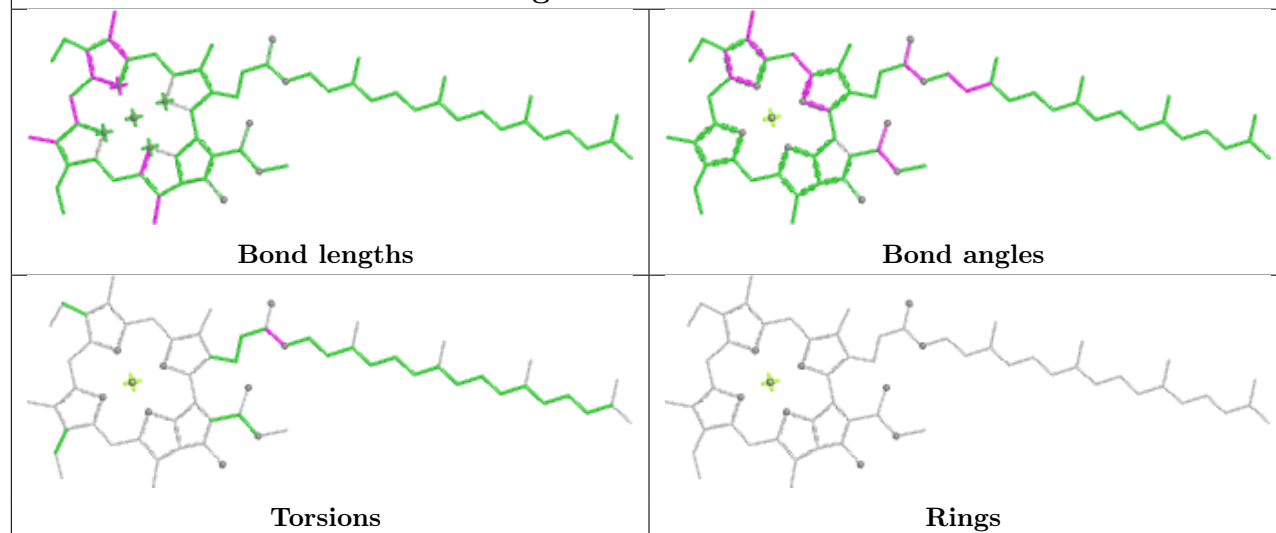
Rings

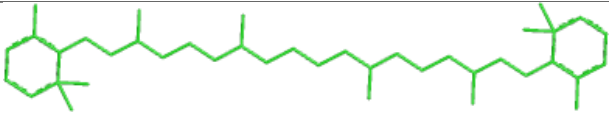
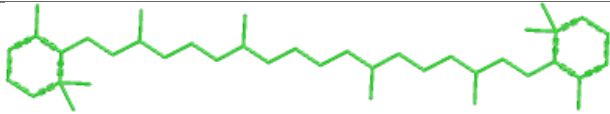
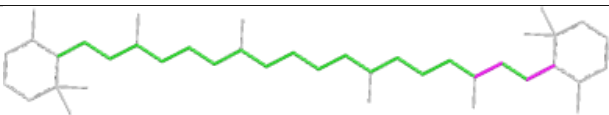
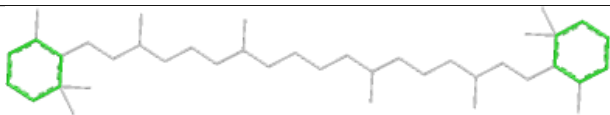


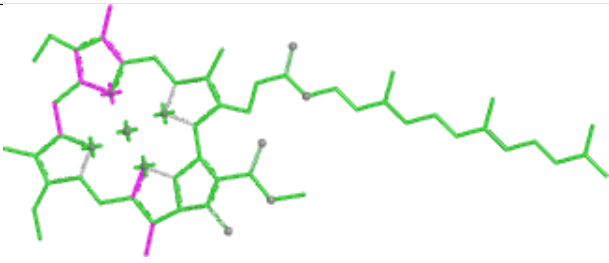
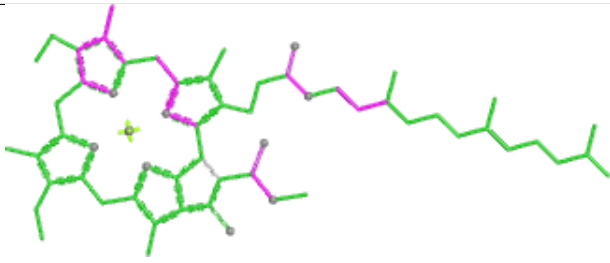
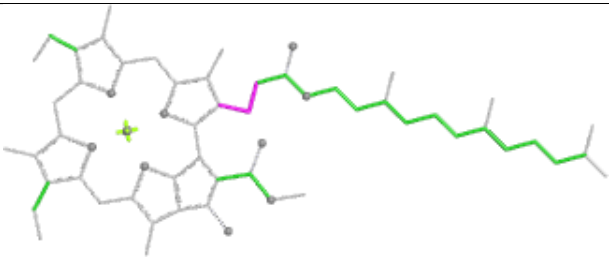
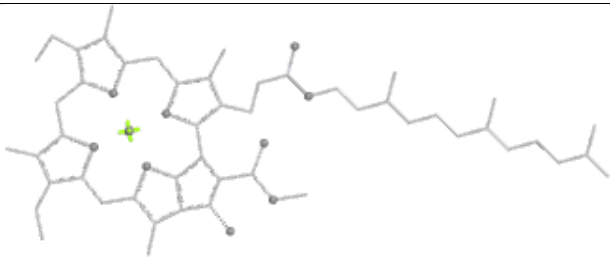
## Ligand CLA 4 604

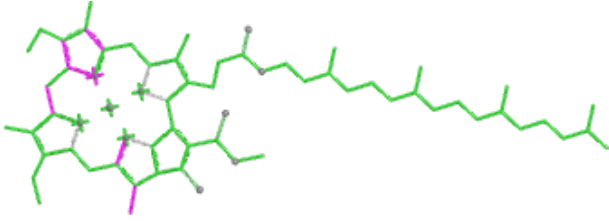
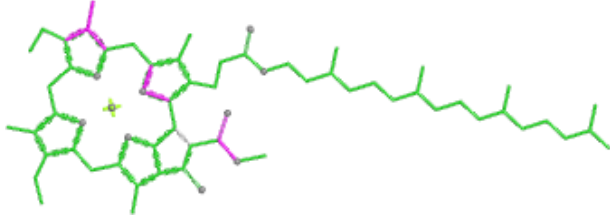
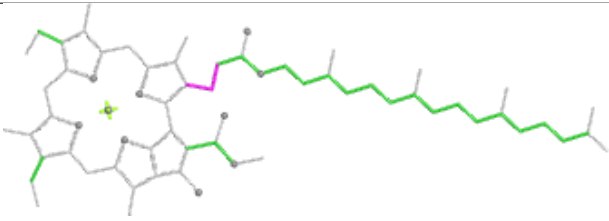
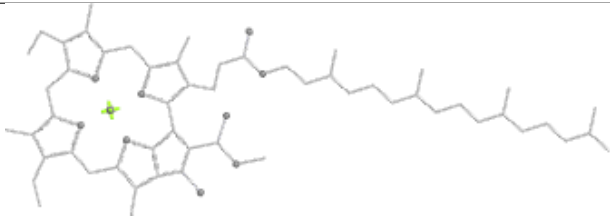


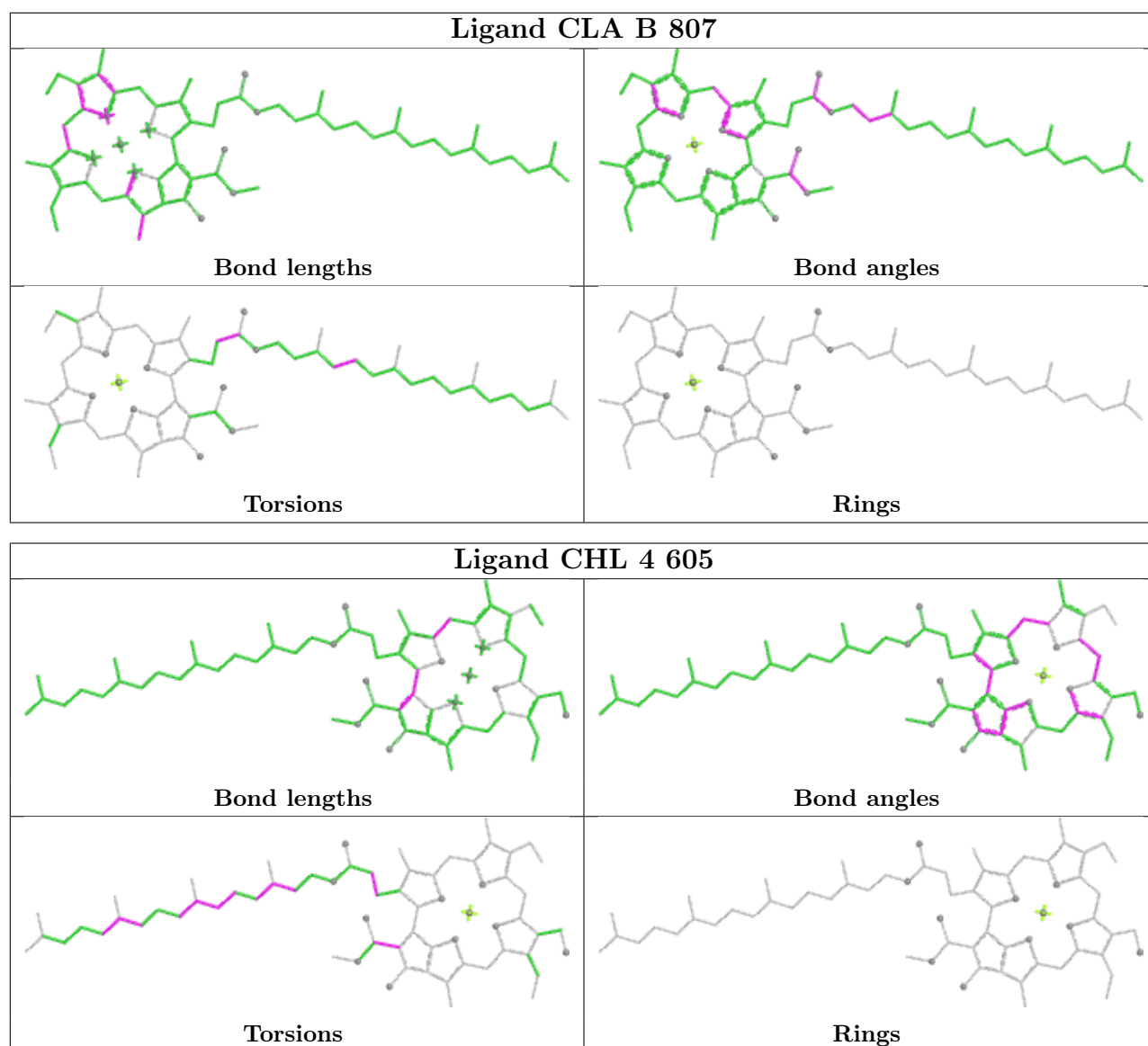
## Ligand CLA B 827



Ligand BCR A 852	
	
Bond lengths	Bond angles
	
Torsions	Rings

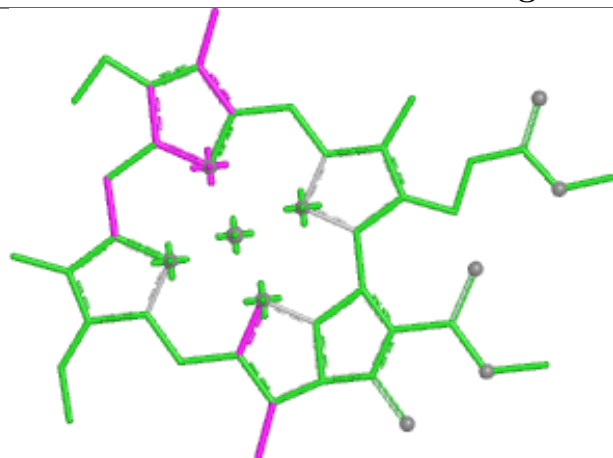
Ligand CLA 6 310	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A 804	
	
Bond lengths	Bond angles
	
Torsions	Rings

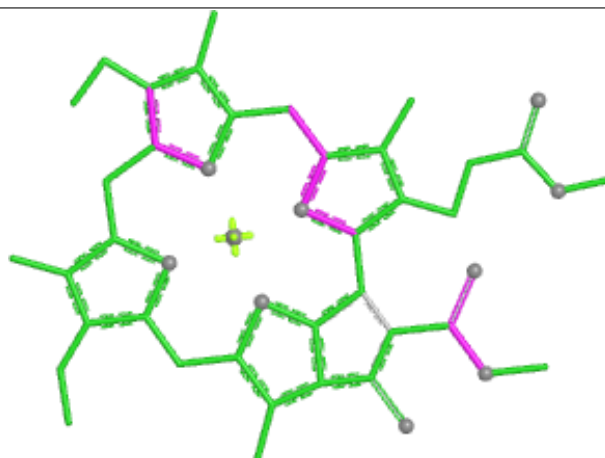




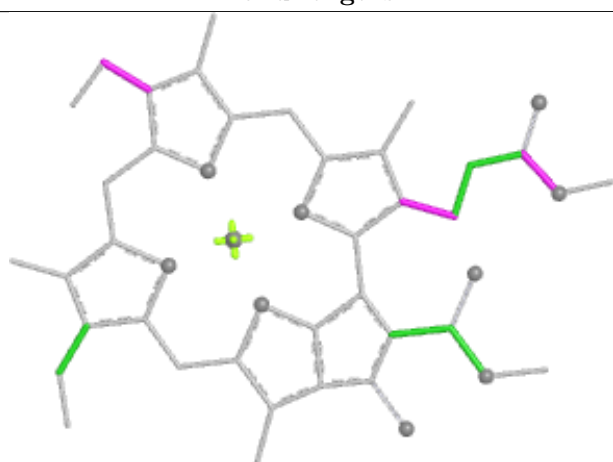
## Ligand CLA 7 614



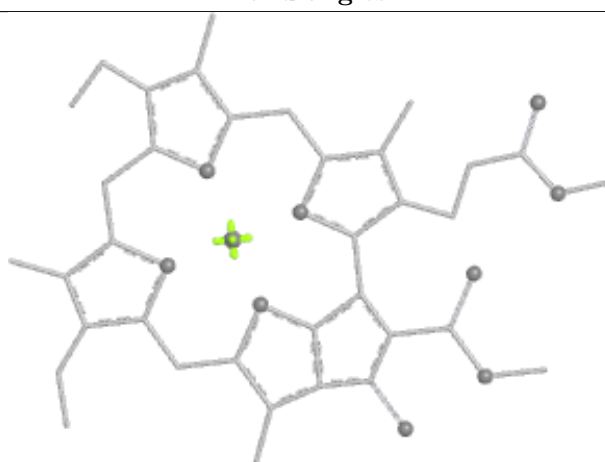
Bond lengths



Bond angles

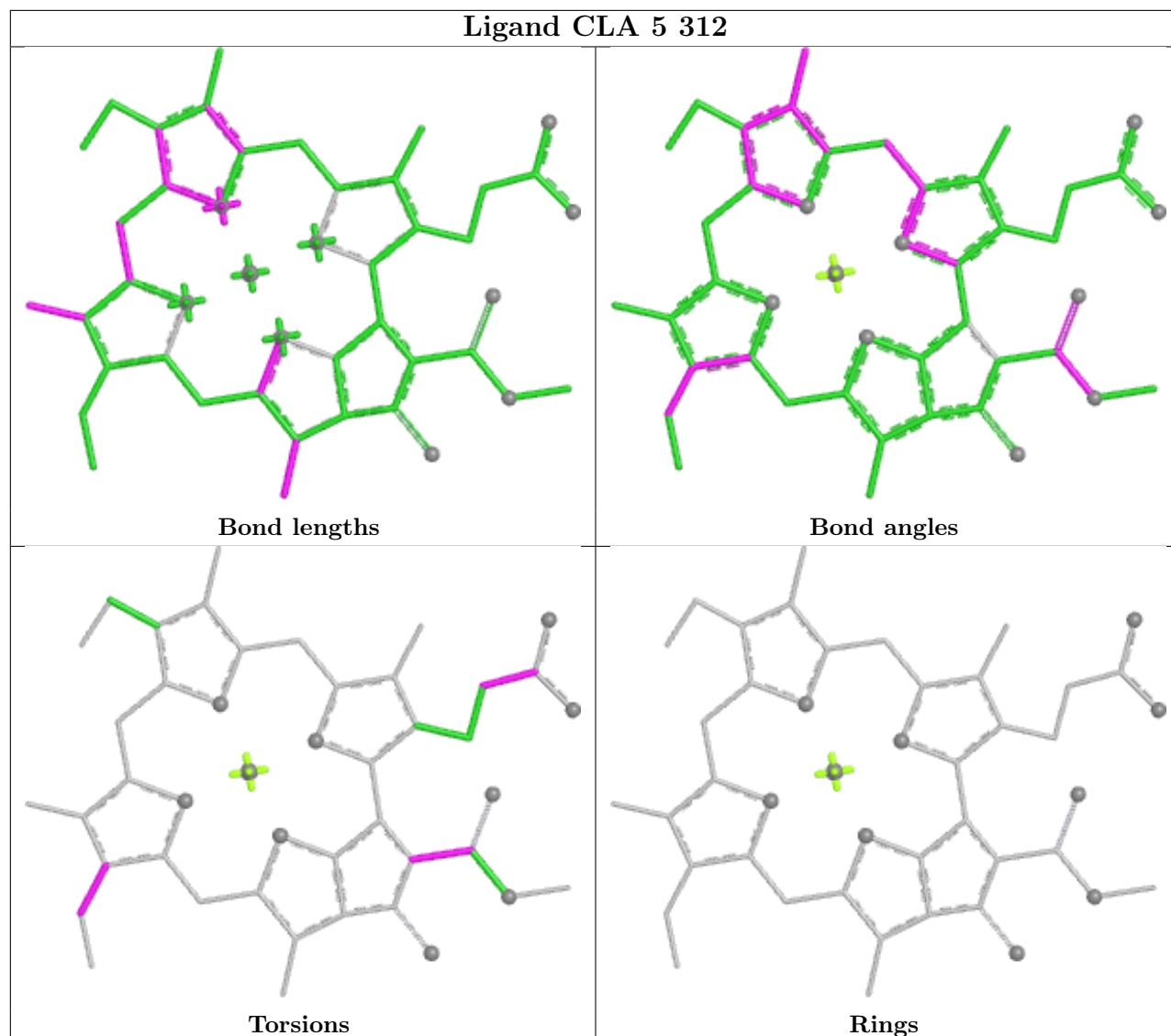


Torsions

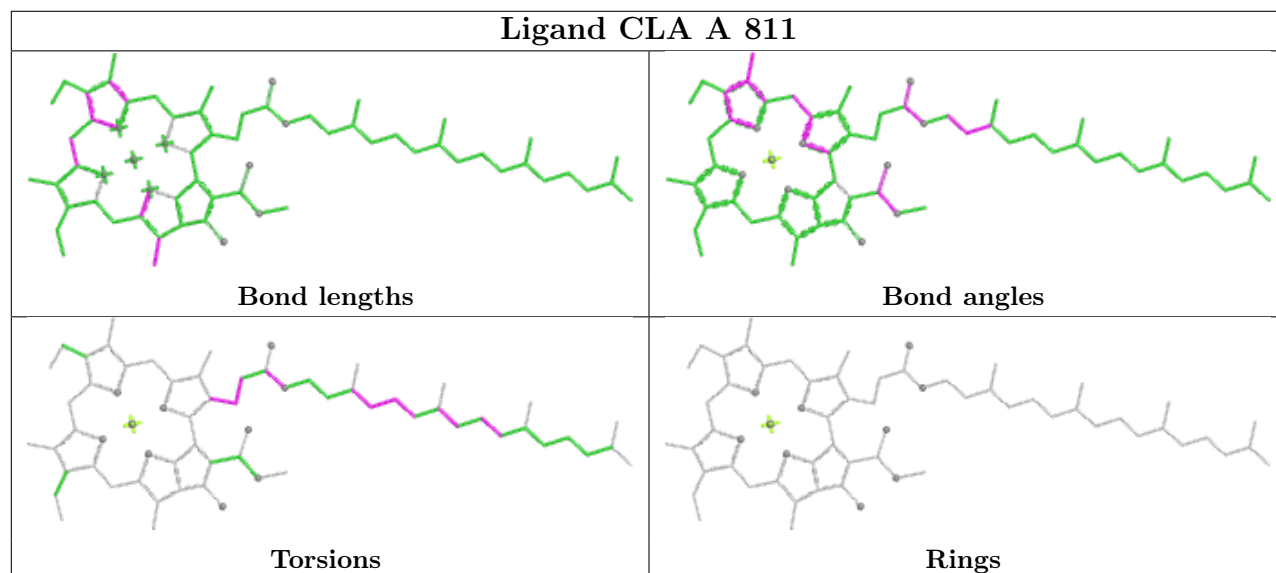


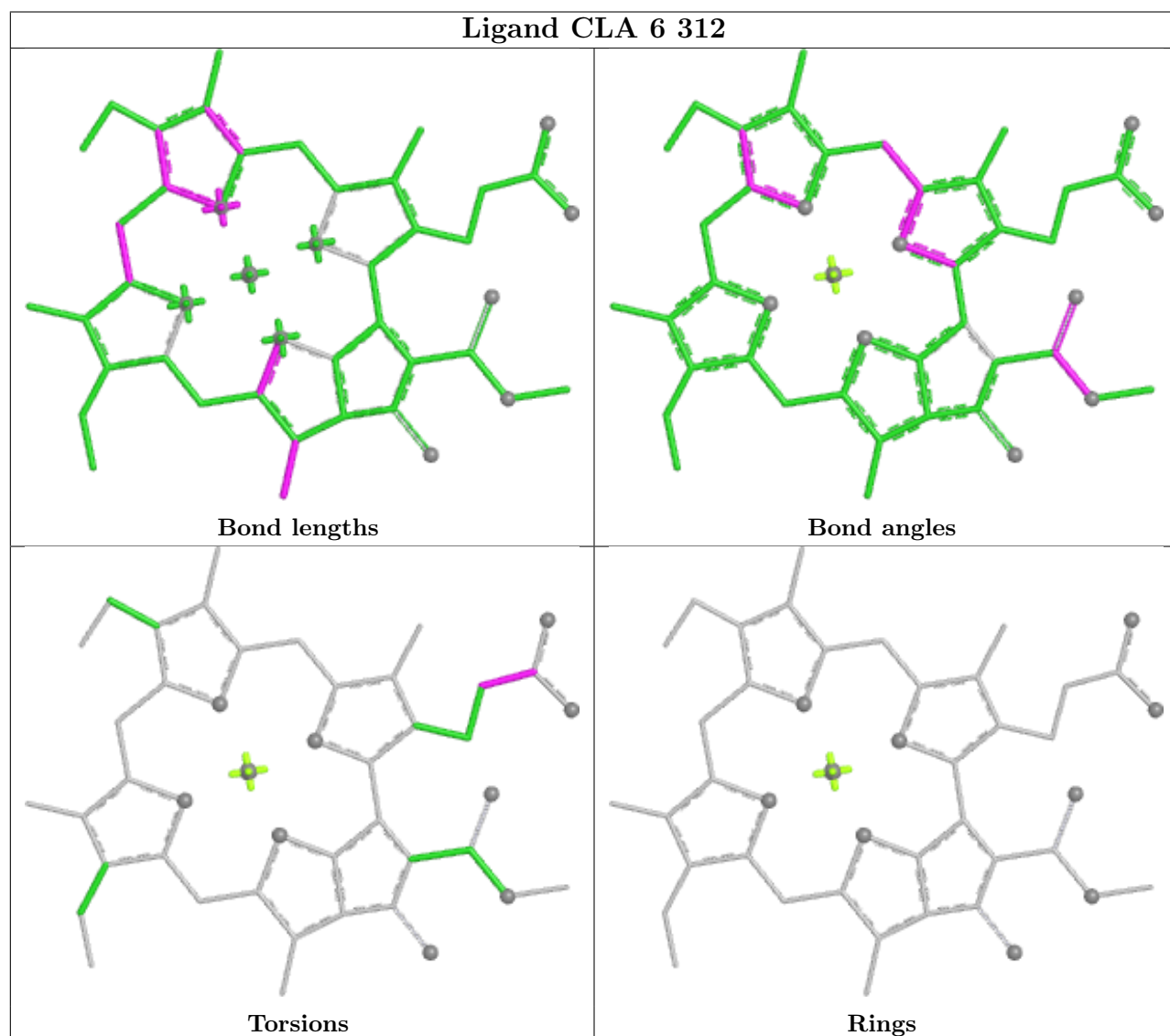
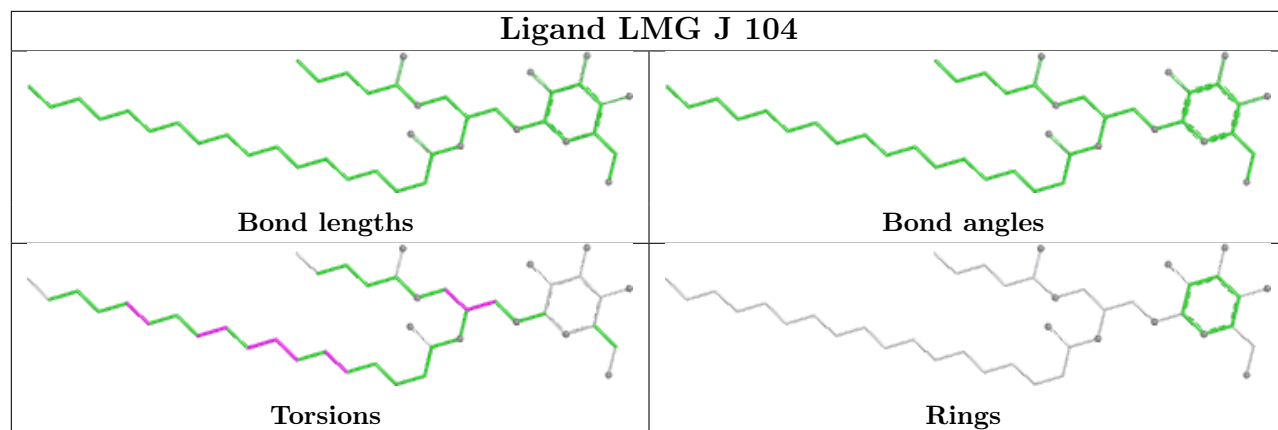
Rings

## Ligand CLA 5 312

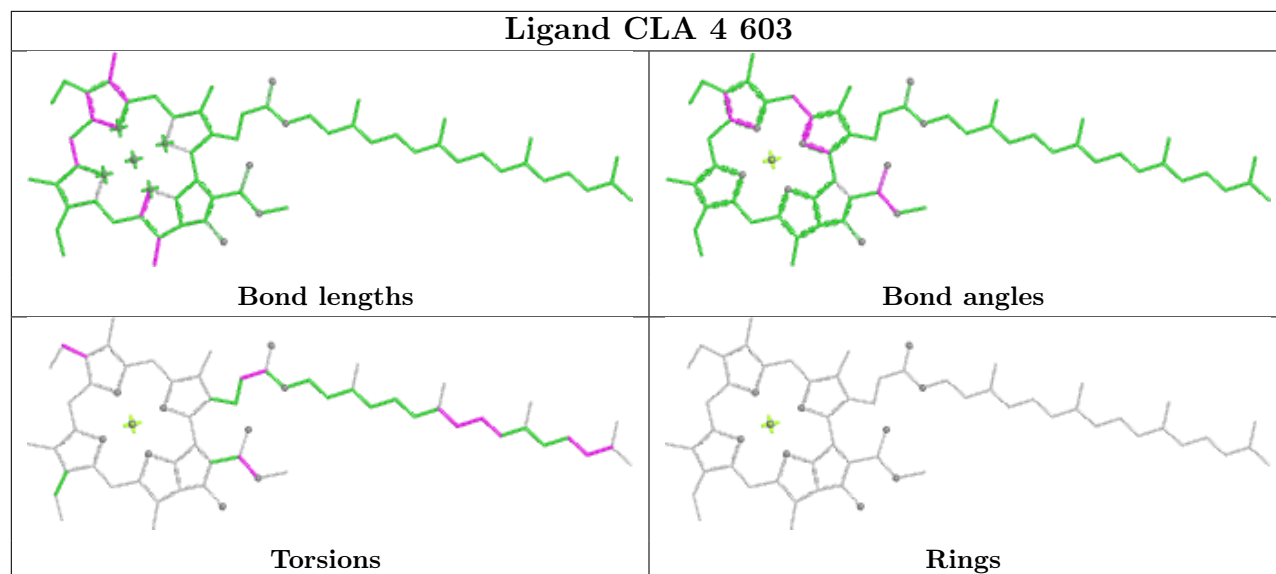


## Ligand CLA A 811

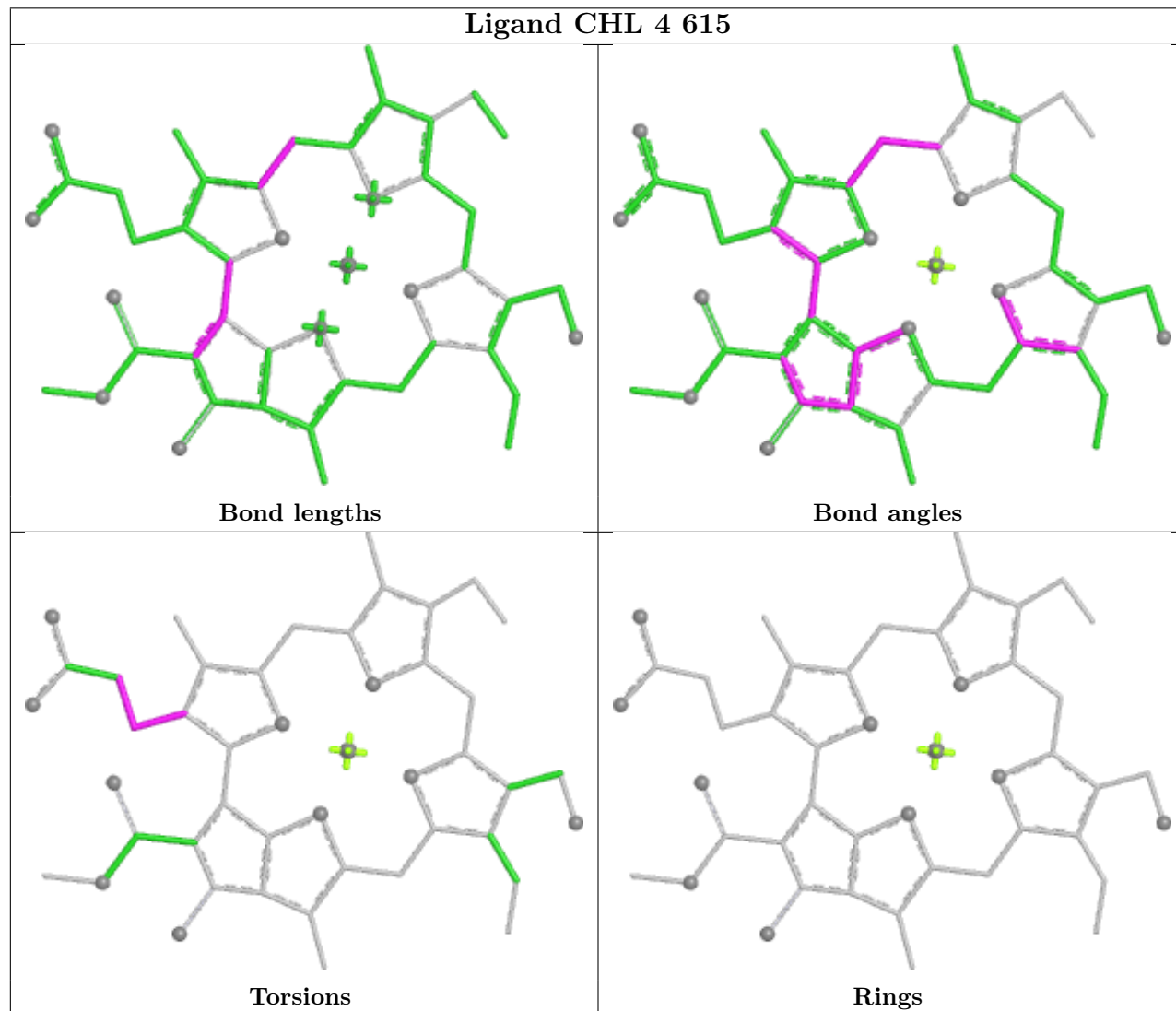


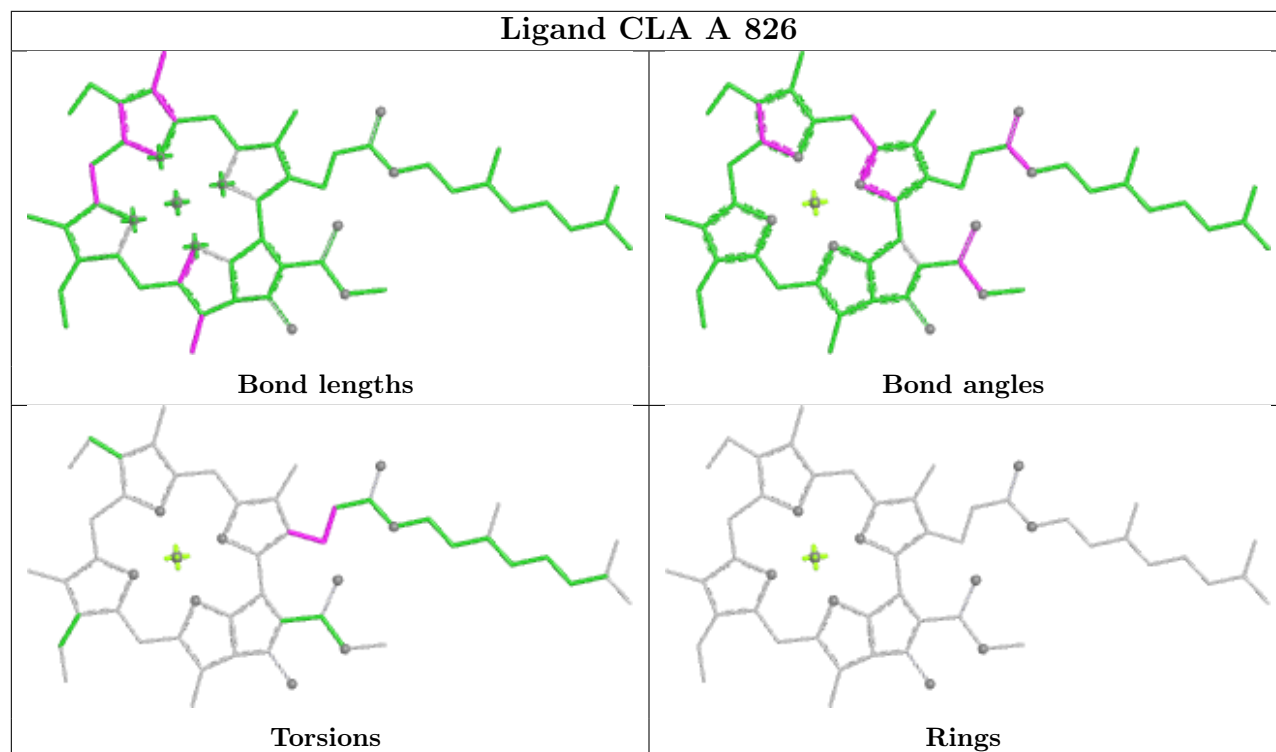
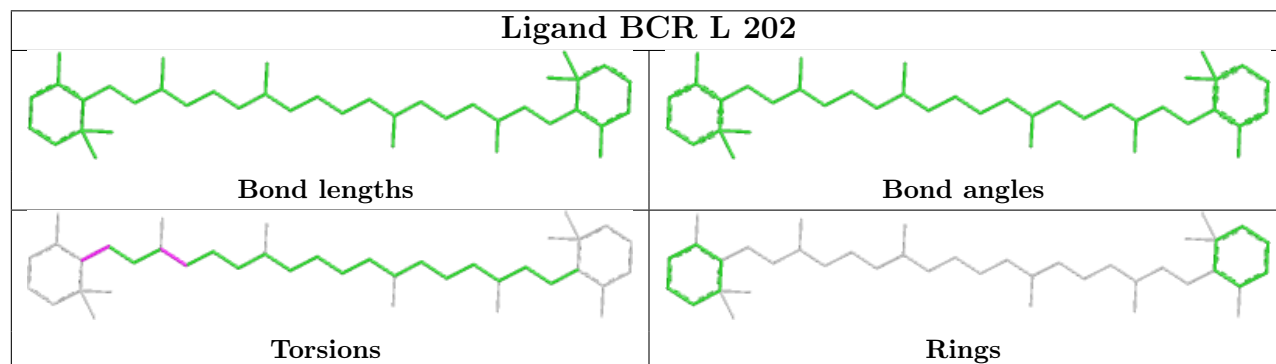
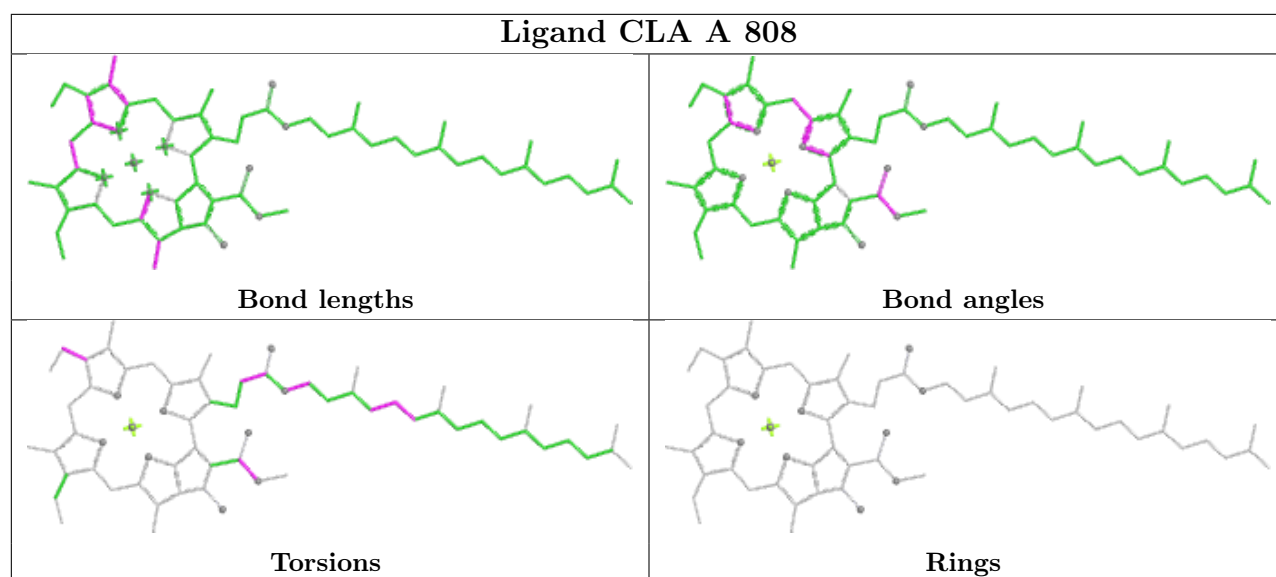


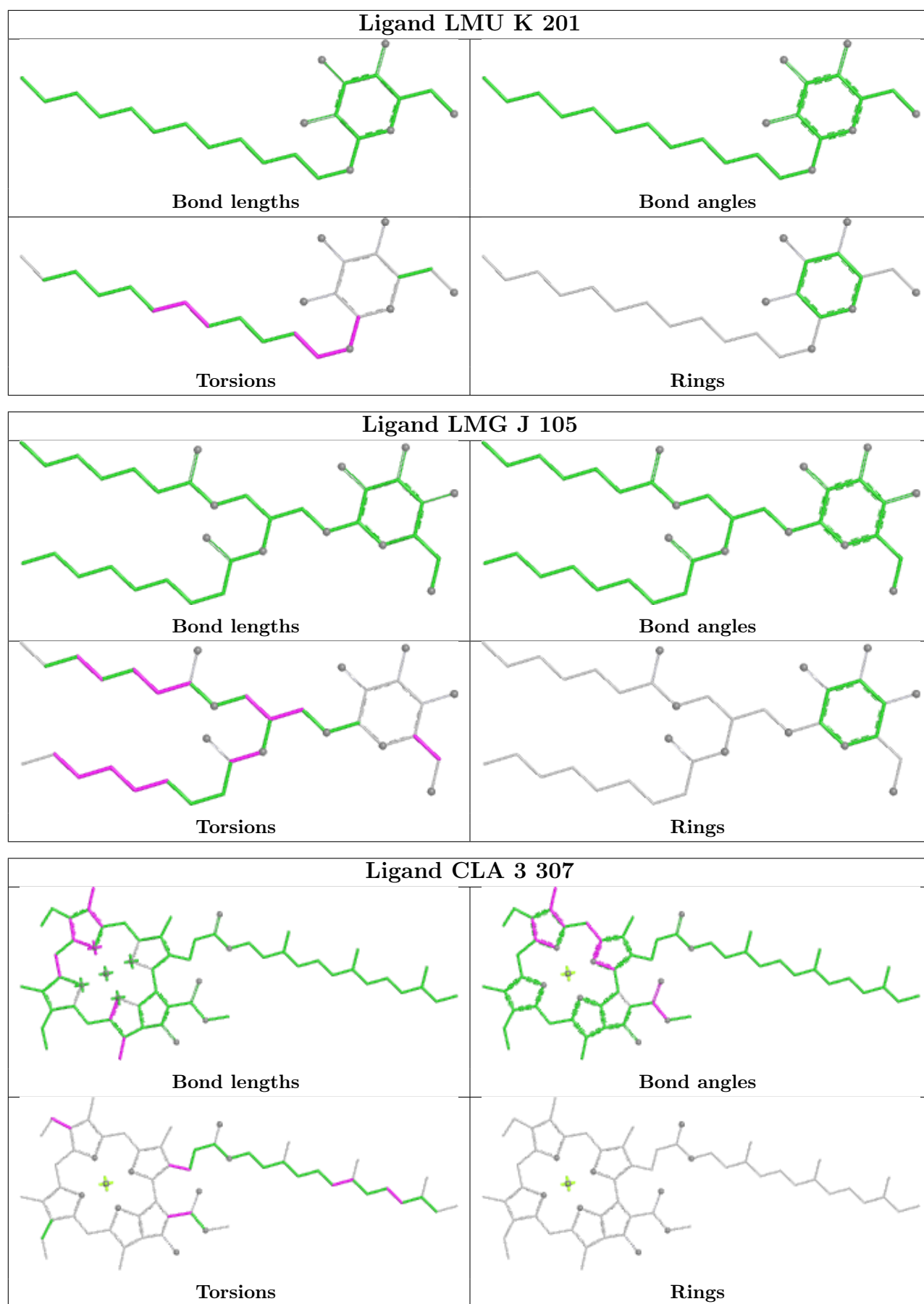
## Ligand CLA 4 603

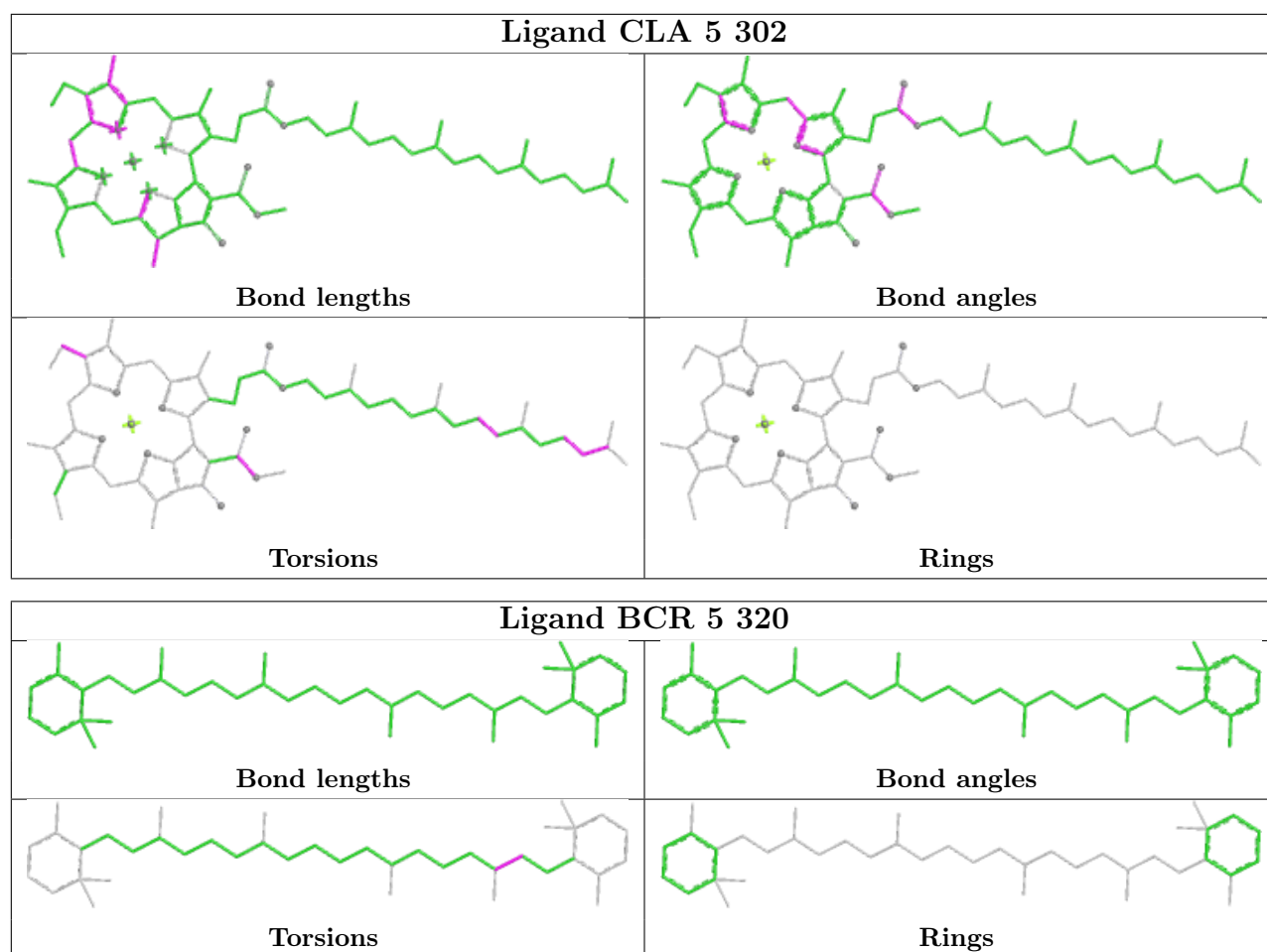


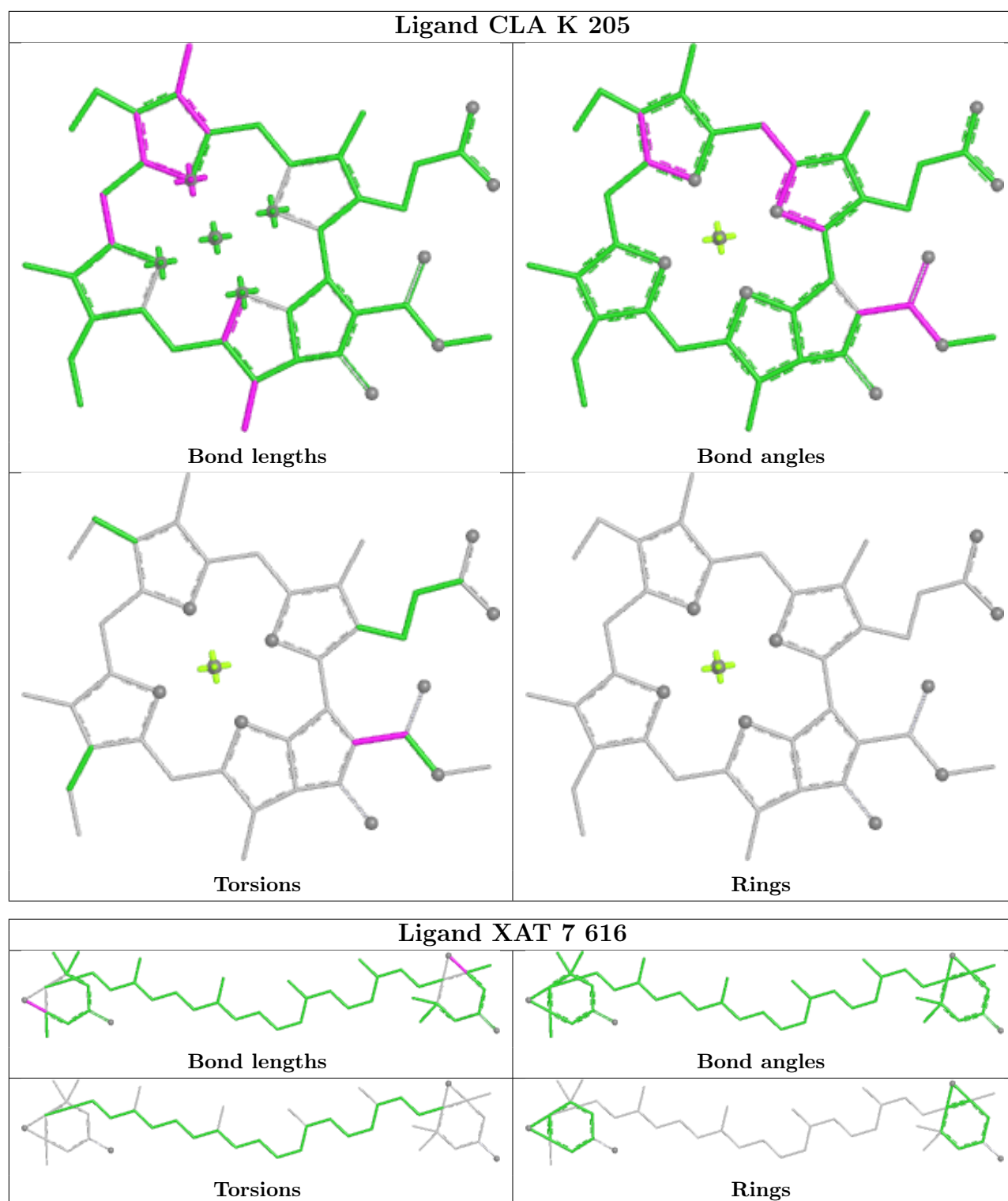
## Ligand CHL 4 615



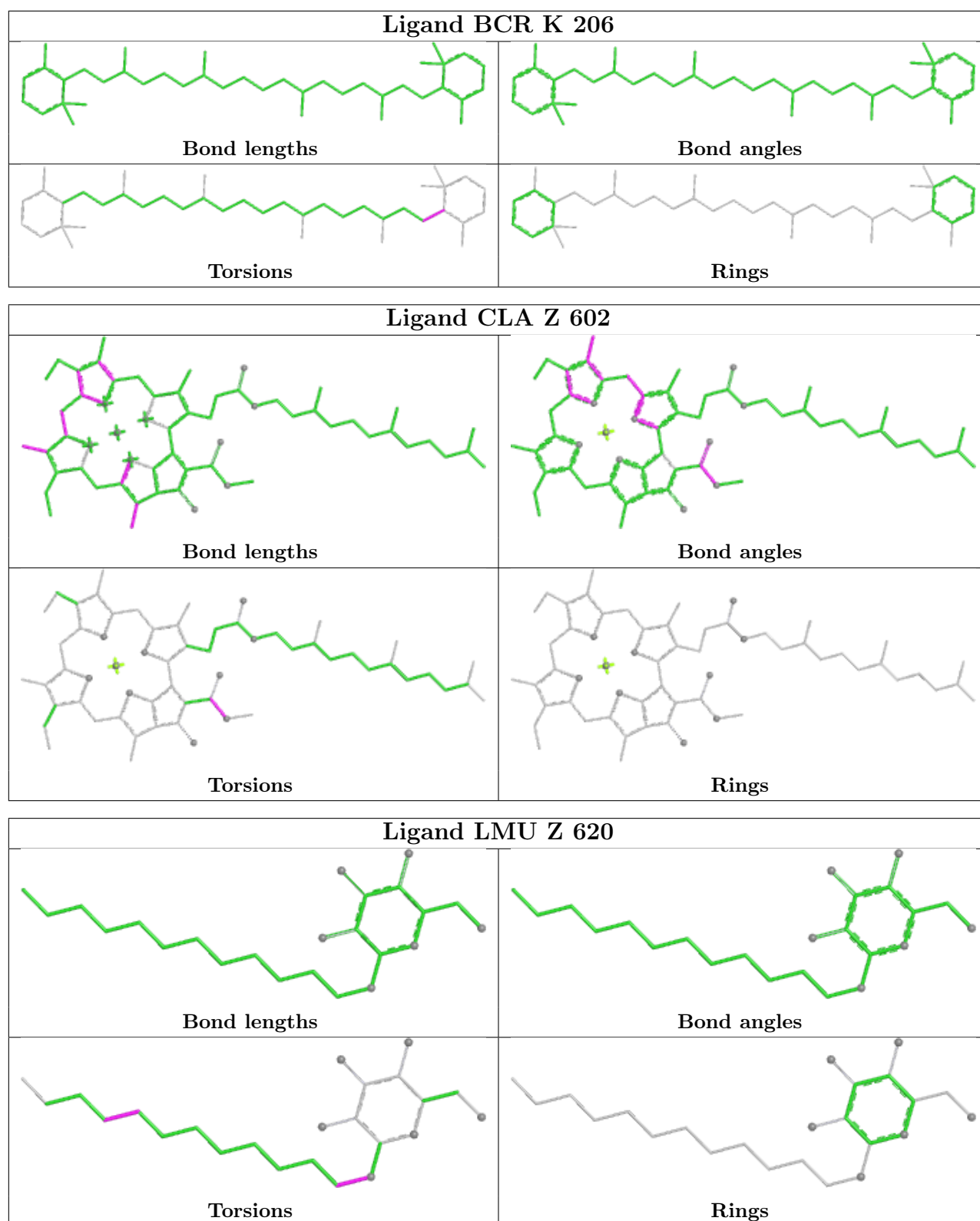


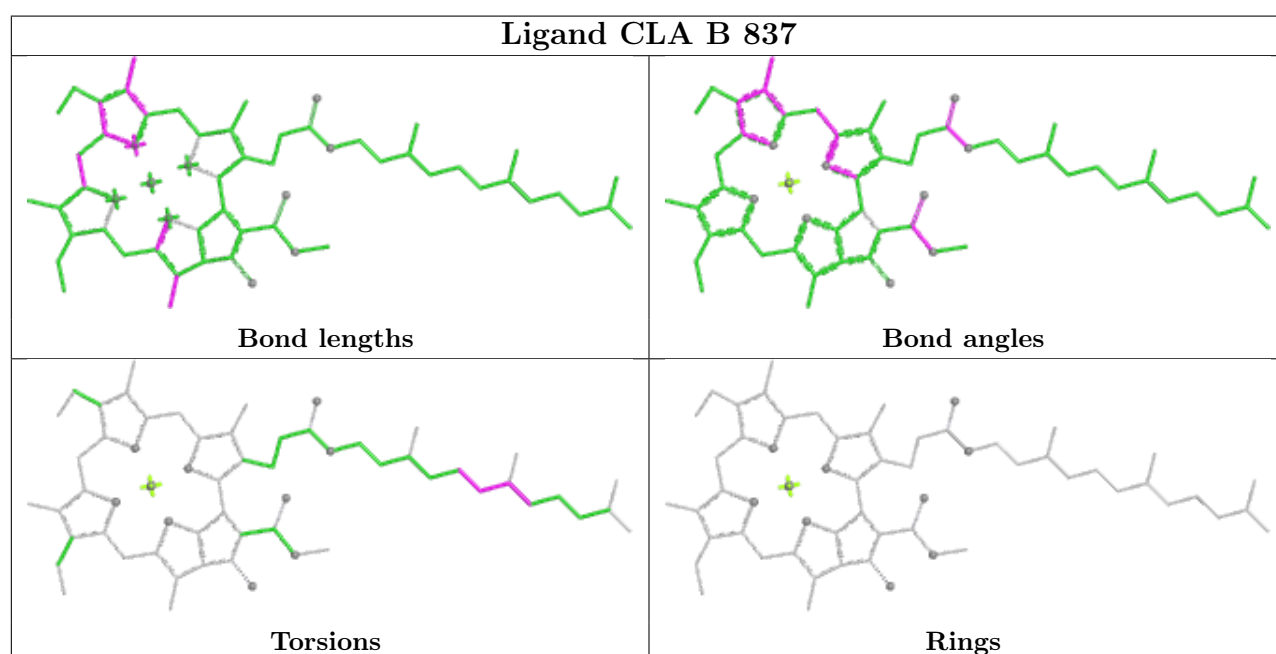
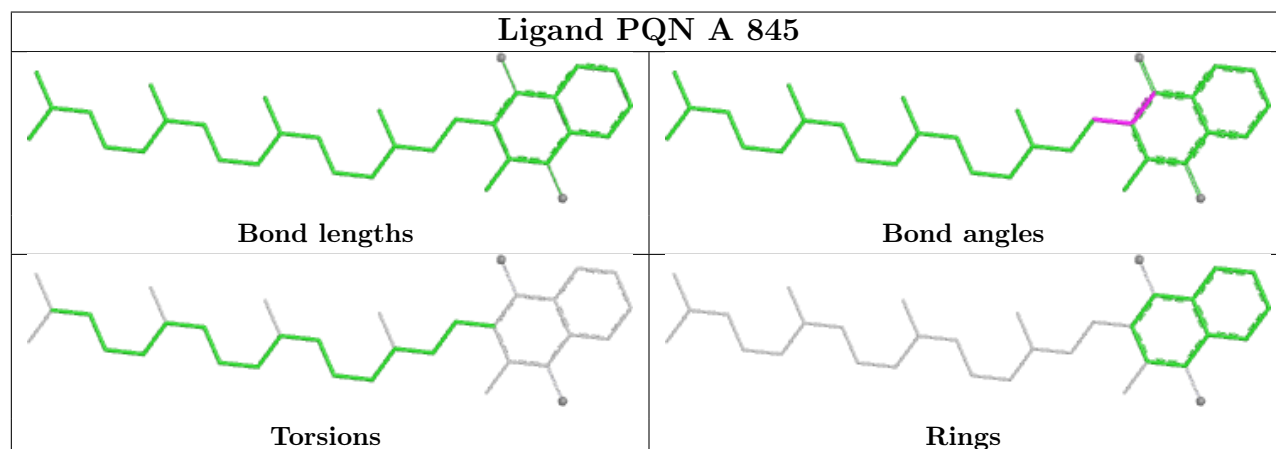
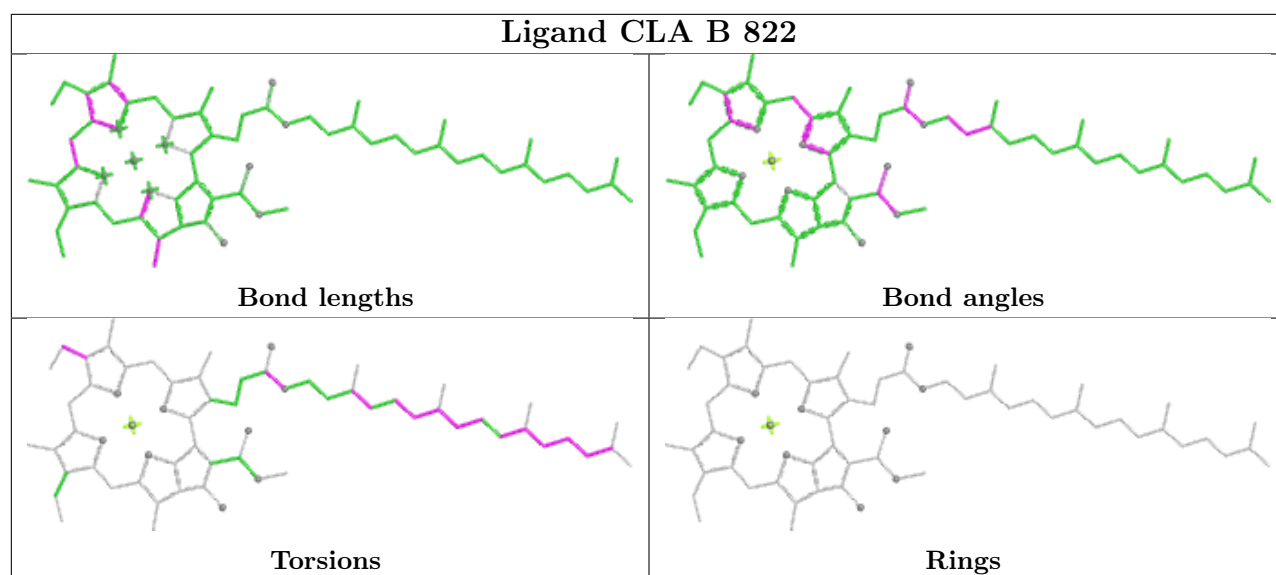


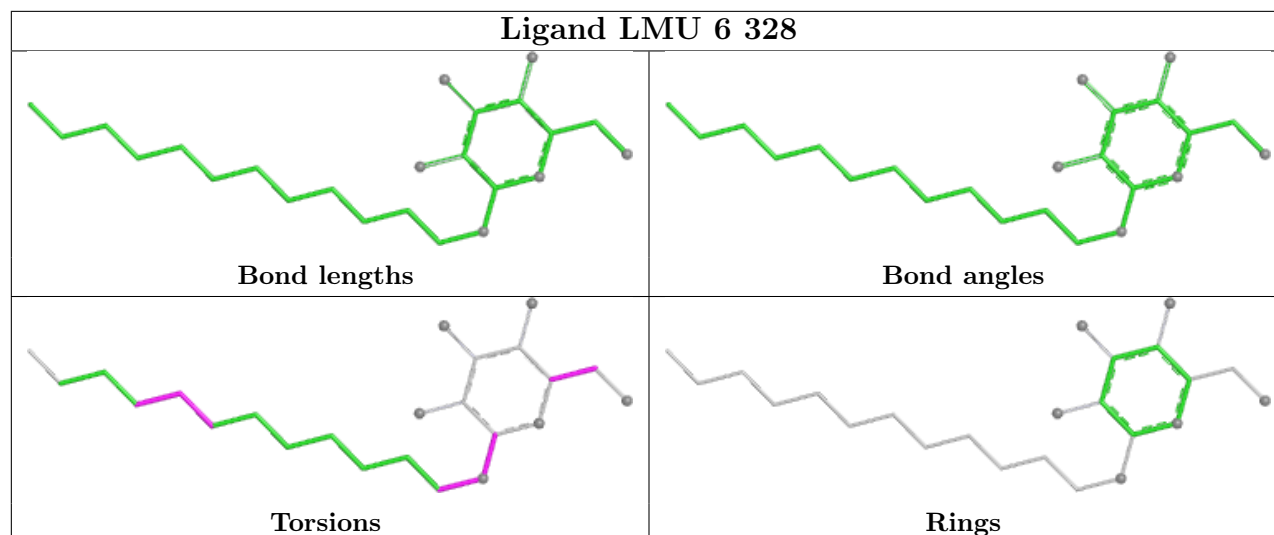












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
18	L	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	142:SER	C	157:ALA	N	10.13

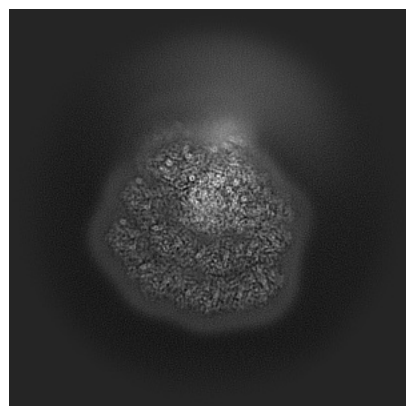
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-54803. These allow visual inspection of the internal detail of the map and identification of artifacts.

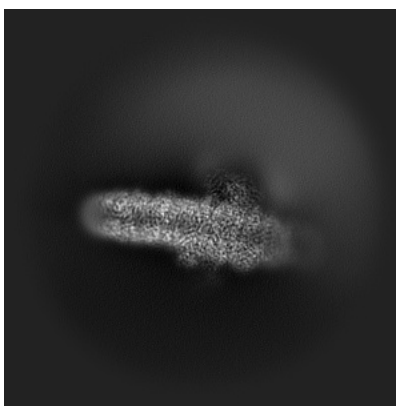
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

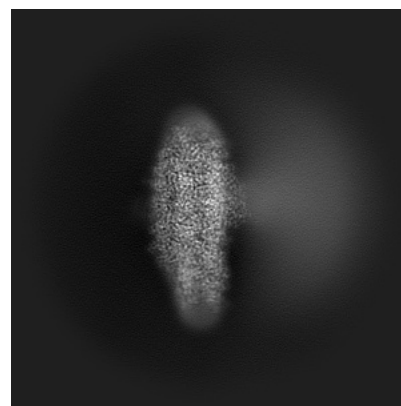
#### 6.1.1 Primary map



X

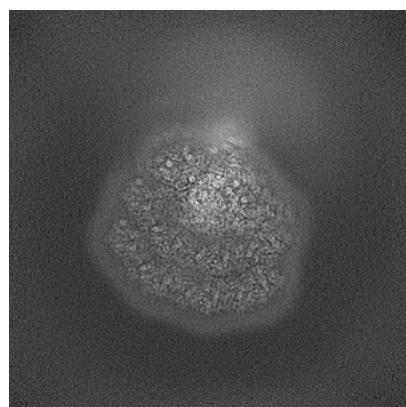


Y

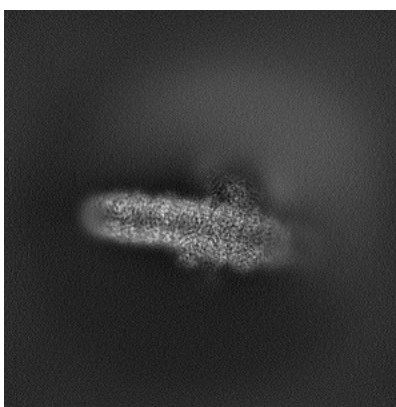


Z

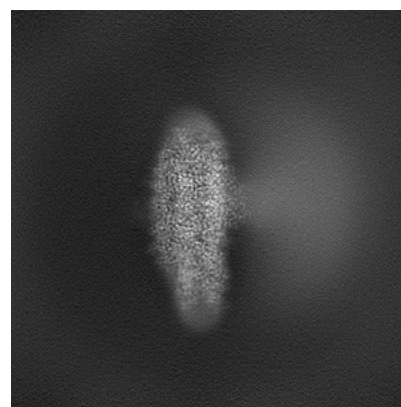
#### 6.1.2 Raw map



X



Y

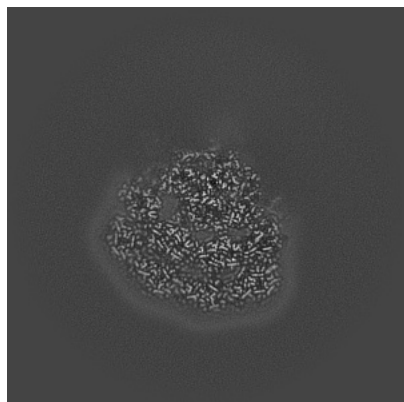


Z

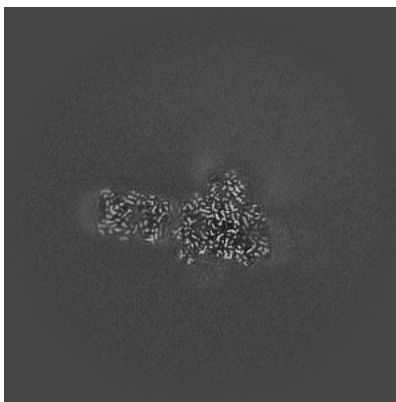
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

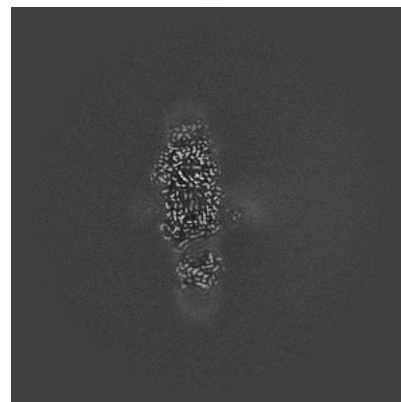
### 6.2.1 Primary map



X Index: 256

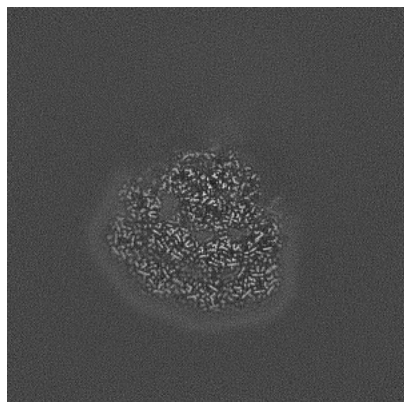


Y Index: 256

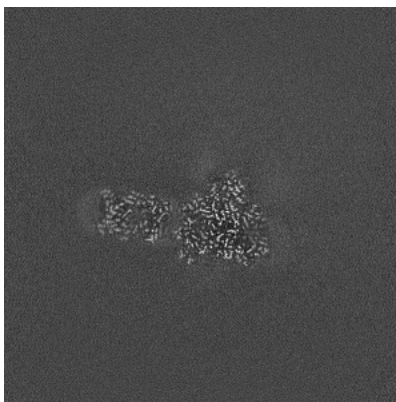


Z Index: 256

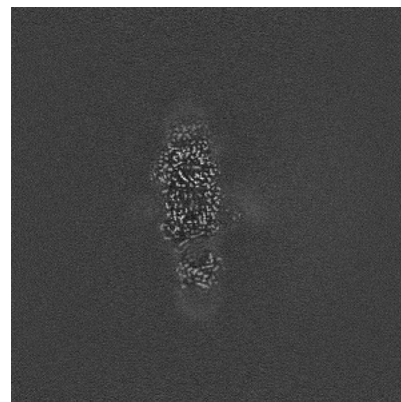
### 6.2.2 Raw map



X Index: 256



Y Index: 256

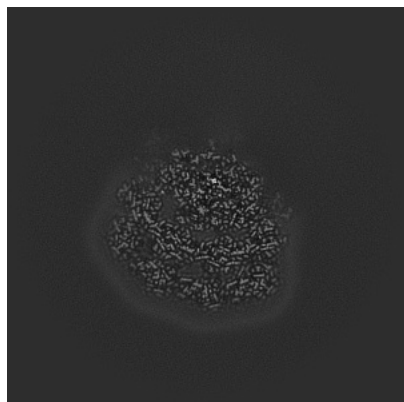


Z Index: 256

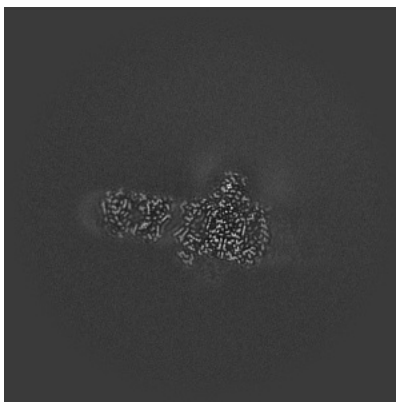
The images above show central slices of the map in three orthogonal directions.

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

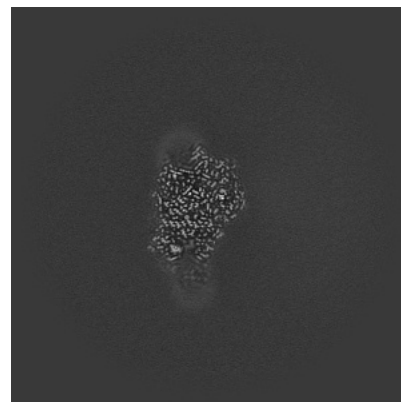
### 6.3.1 Primary map



X Index: 253

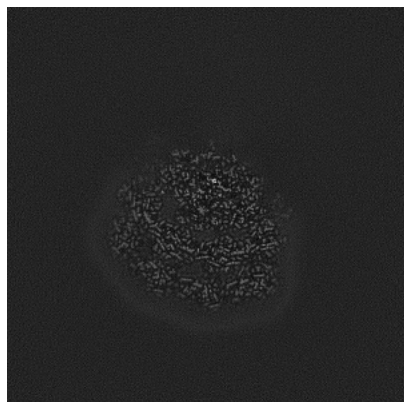


Y Index: 261

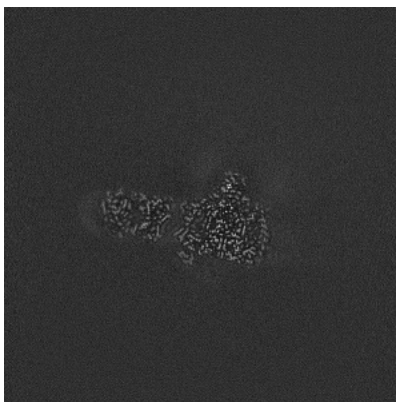


Z Index: 296

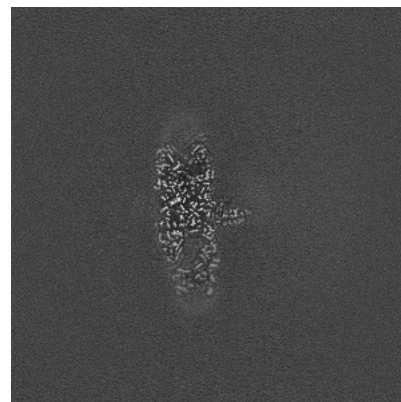
### 6.3.2 Raw map



X Index: 253



Y Index: 261



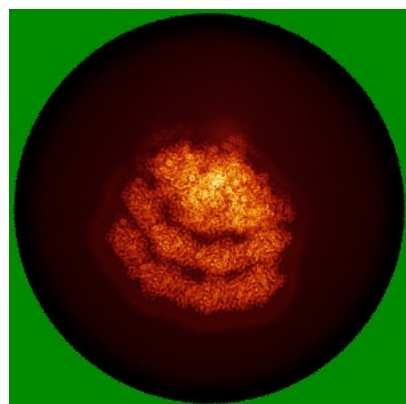
Z Index: 276

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

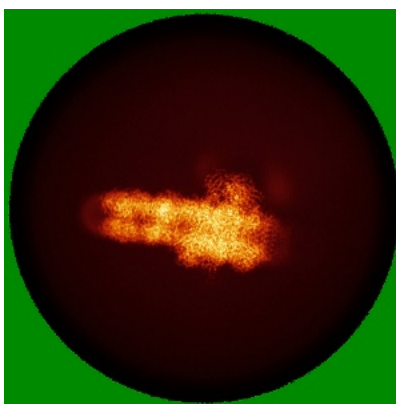


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

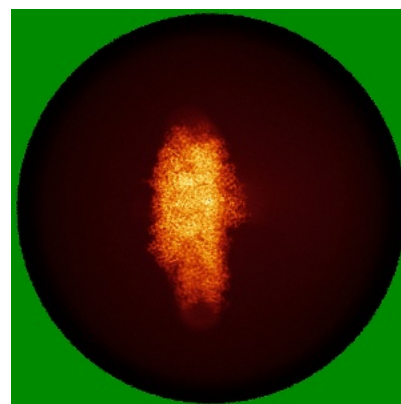
### 6.4.1 Primary map



X

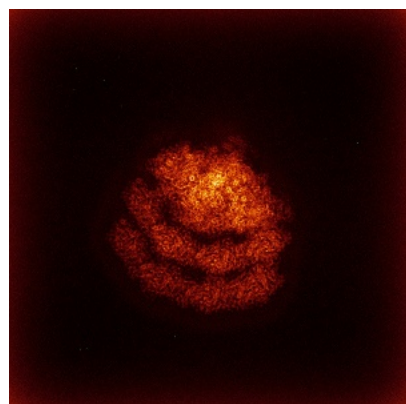


Y

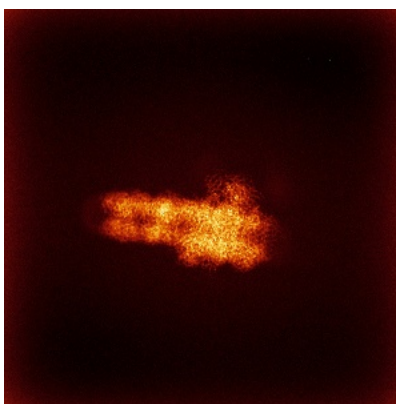


Z

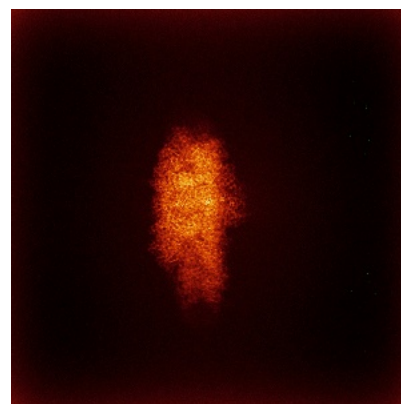
### 6.4.2 Raw map



X



Y

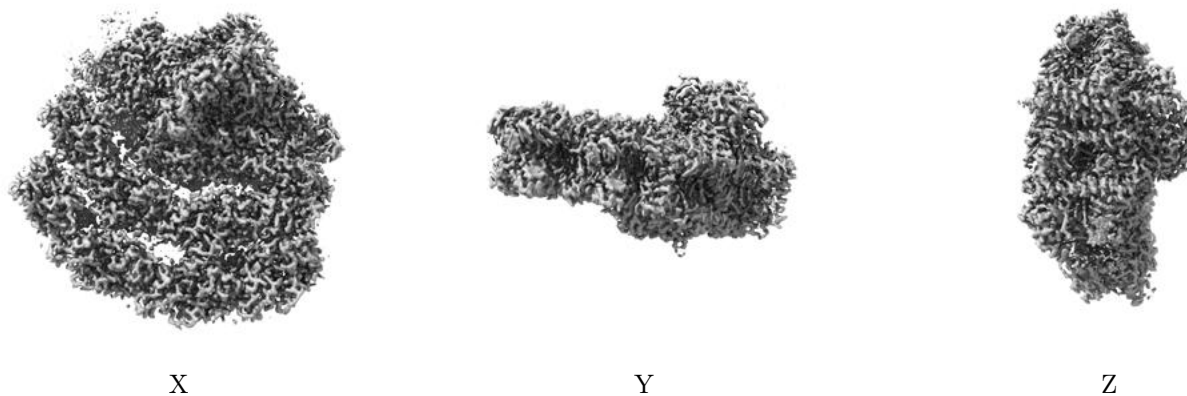


Z

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.

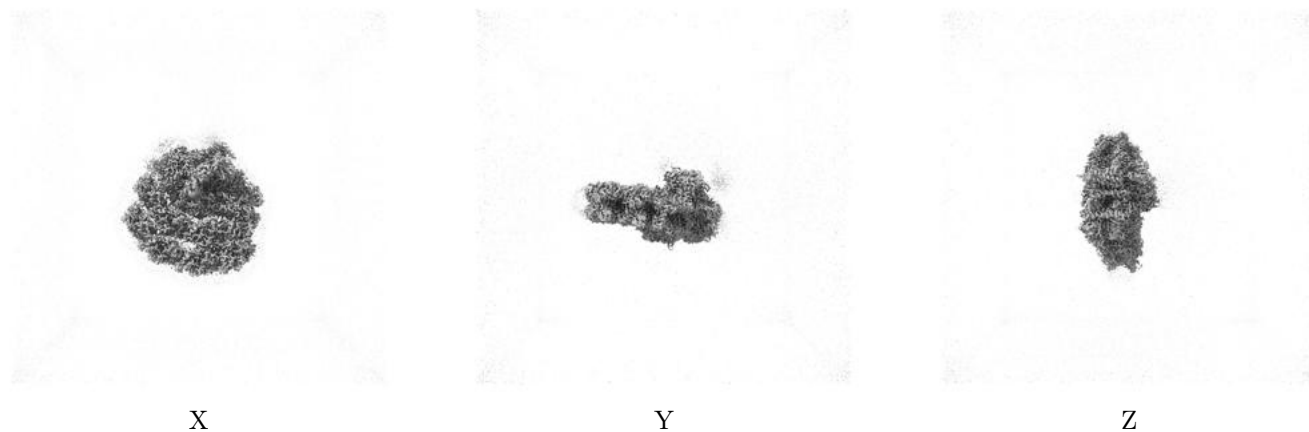
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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](#)

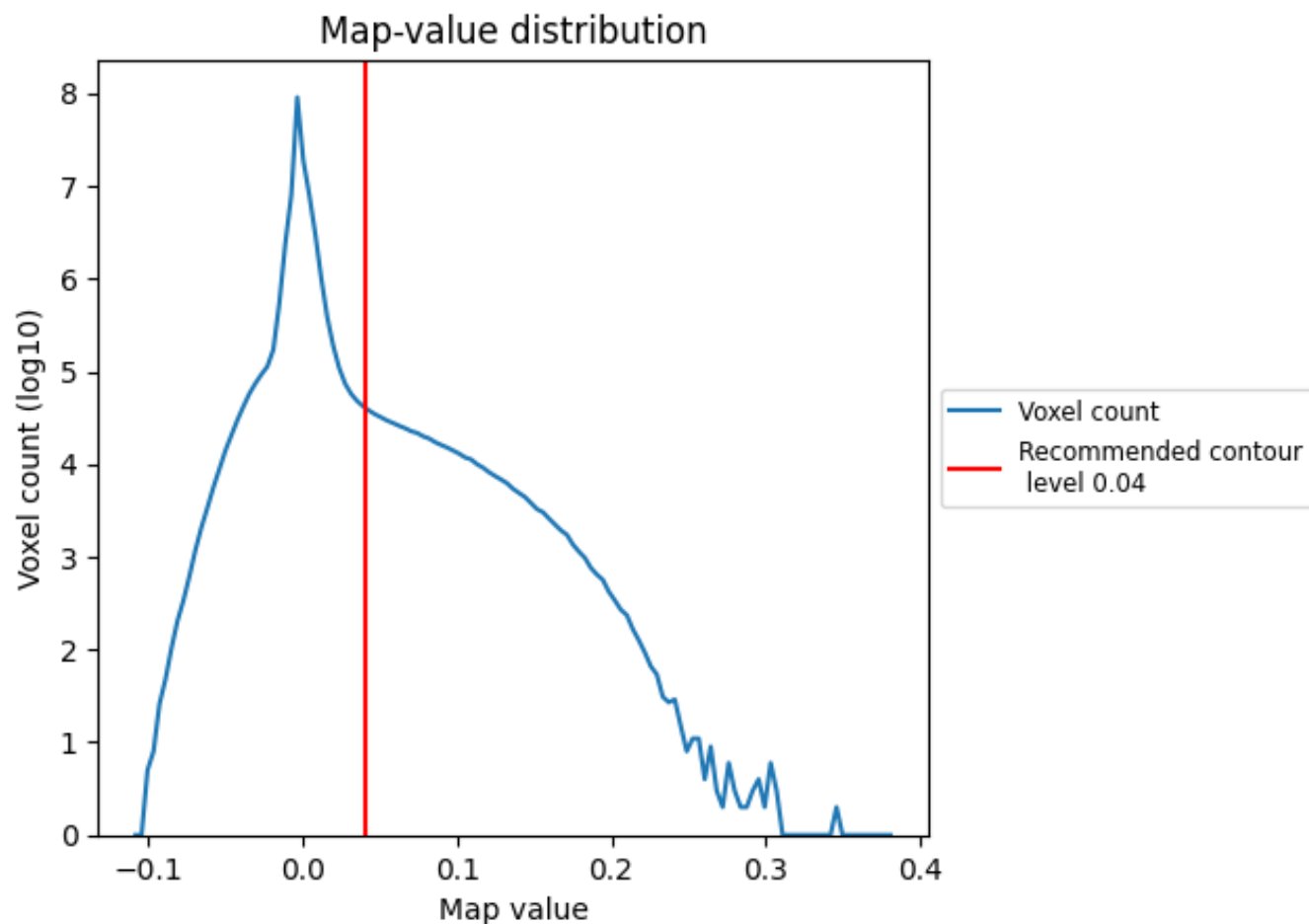
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

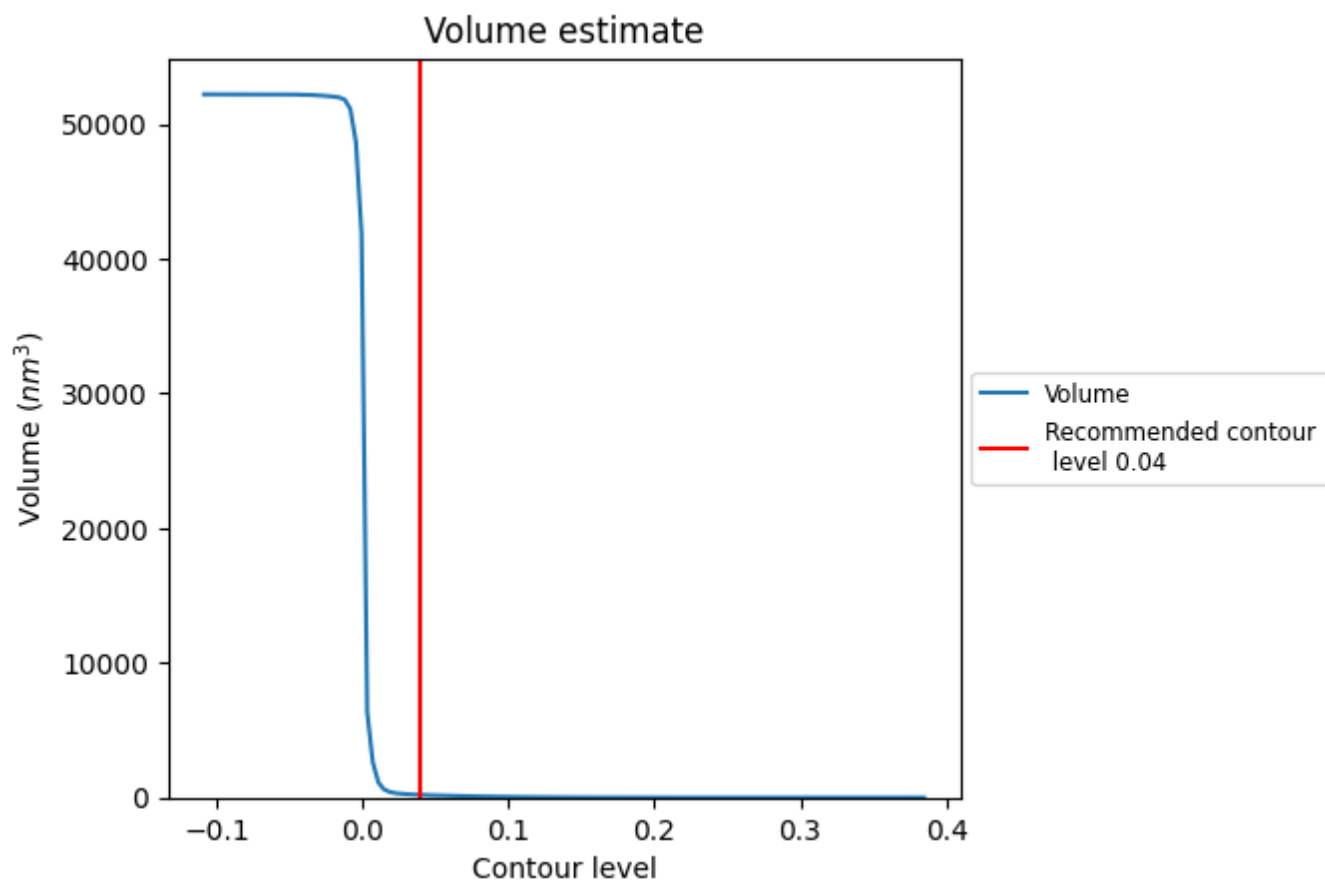
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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

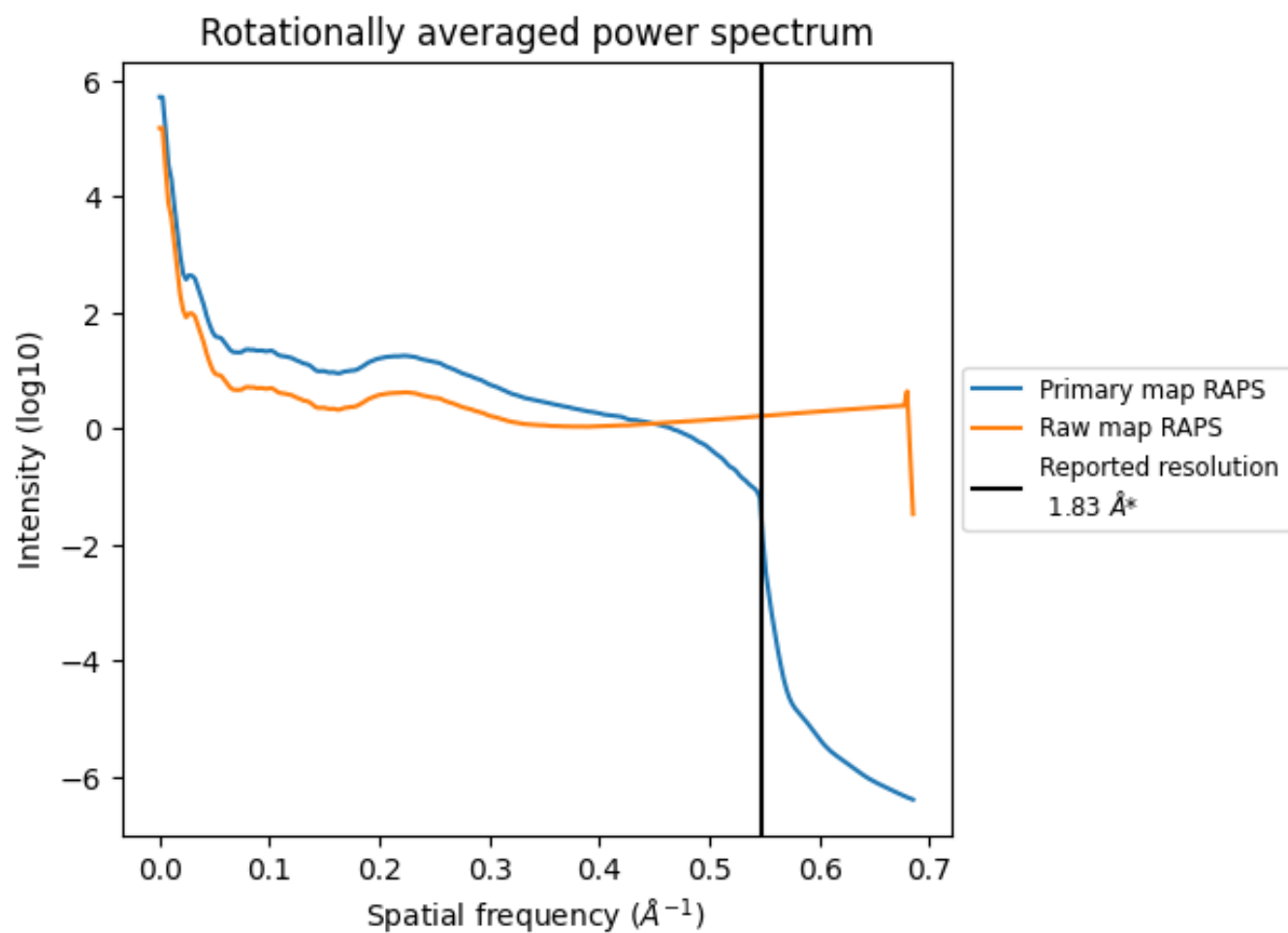
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 200  $\text{nm}^3$ ; this corresponds to an approximate mass of 181 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 ⓘ

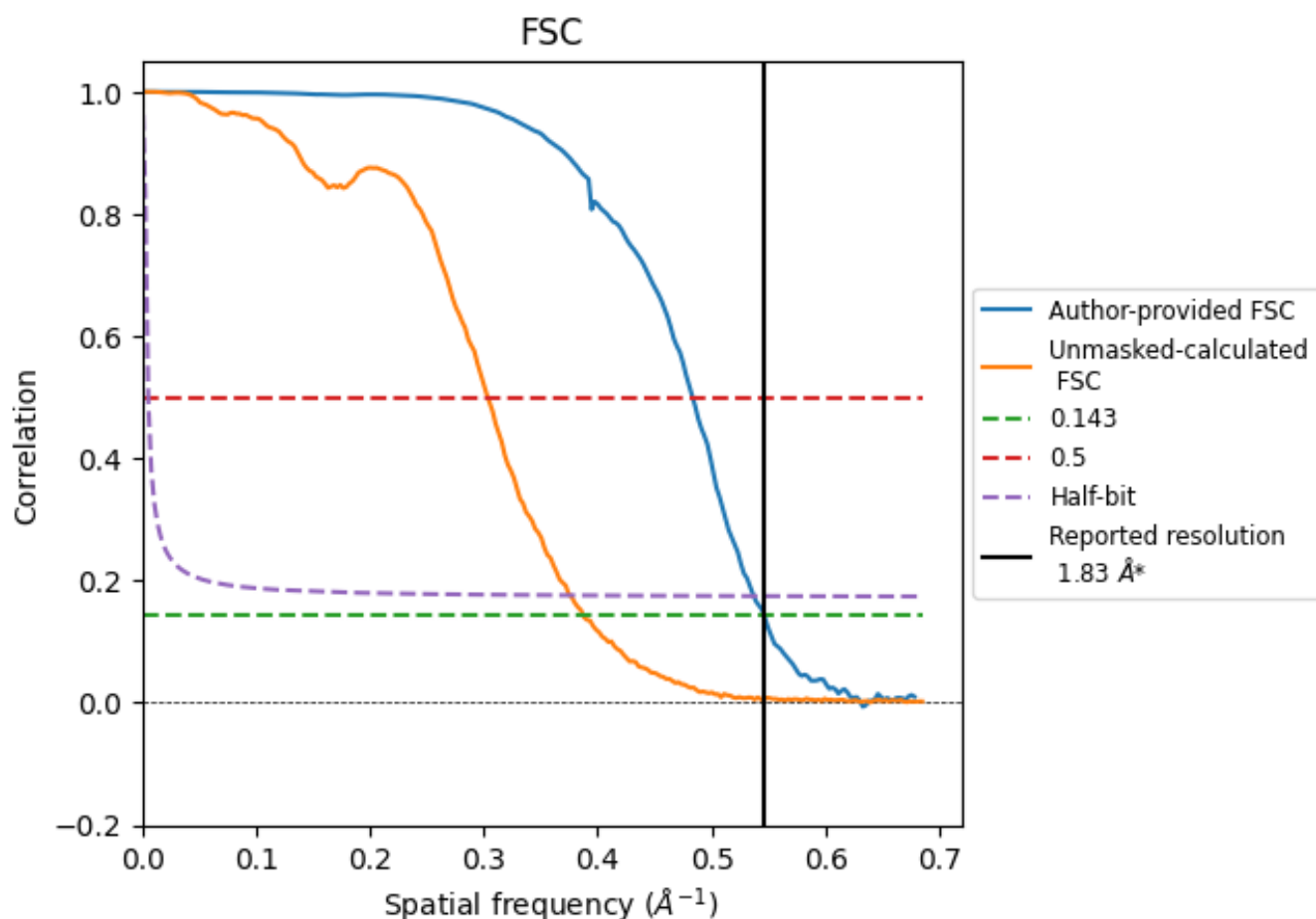


\*Reported resolution corresponds to spatial frequency of 0.546  $\text{\AA}^{-1}$

## 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 0.546 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

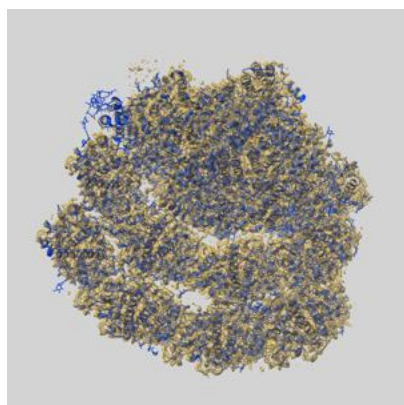
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	1.83	-	-
Author-provided FSC curve	1.83	2.07	1.86
Unmasked-calculated*	2.58	3.30	2.66

\*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 2.58 differs from the reported value 1.83 by more than 10 %

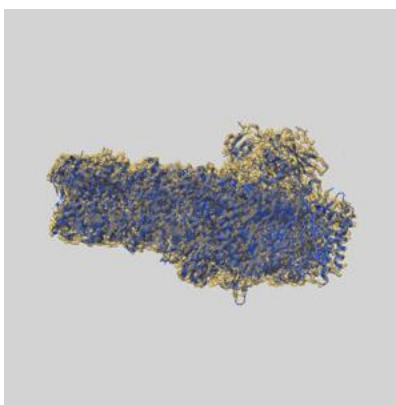
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-54803 and PDB model 9SE6. Per-residue inclusion information can be found in section [3](#) on page [35](#).

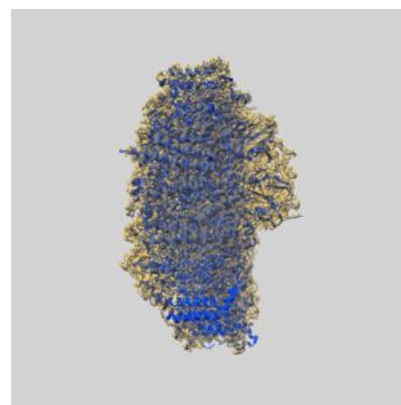
### 9.1 Map-model overlay [i](#)



X



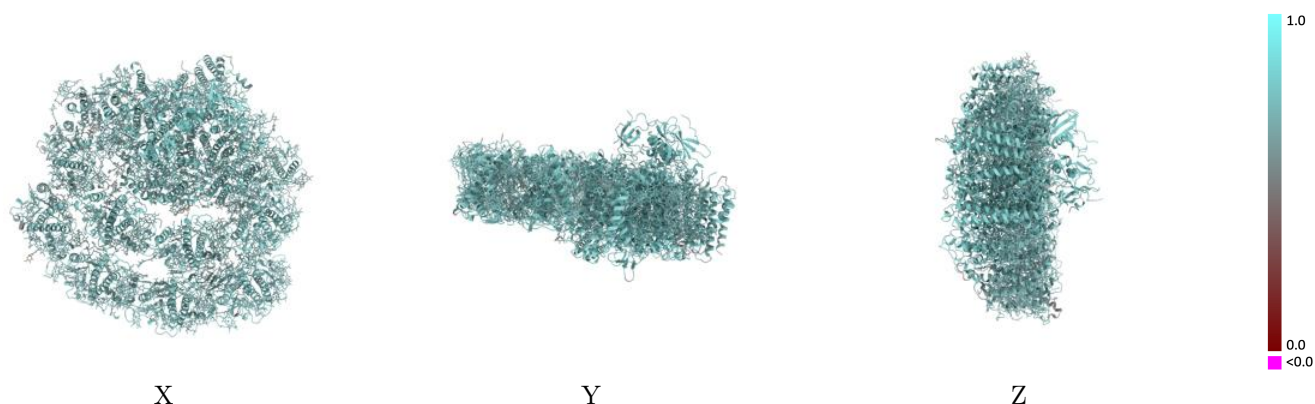
Y



Z

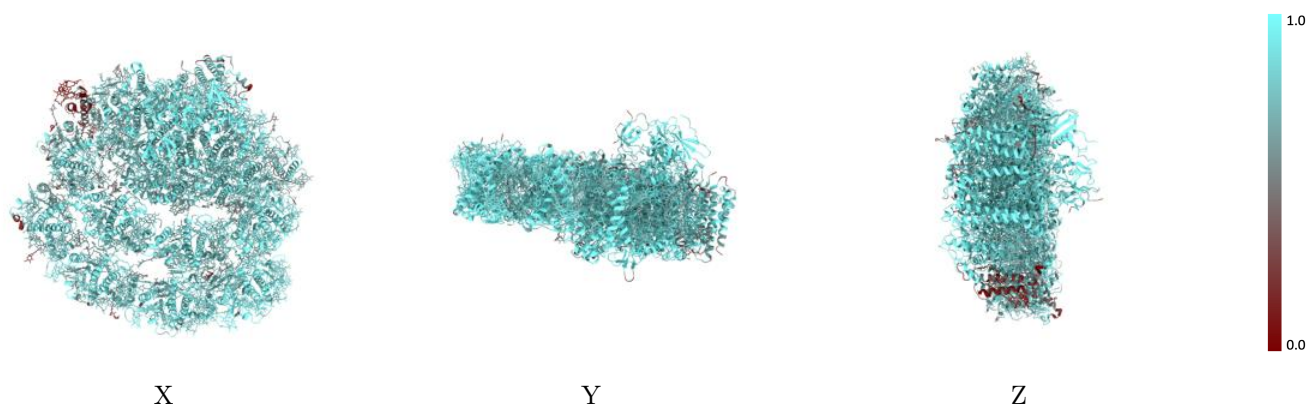
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



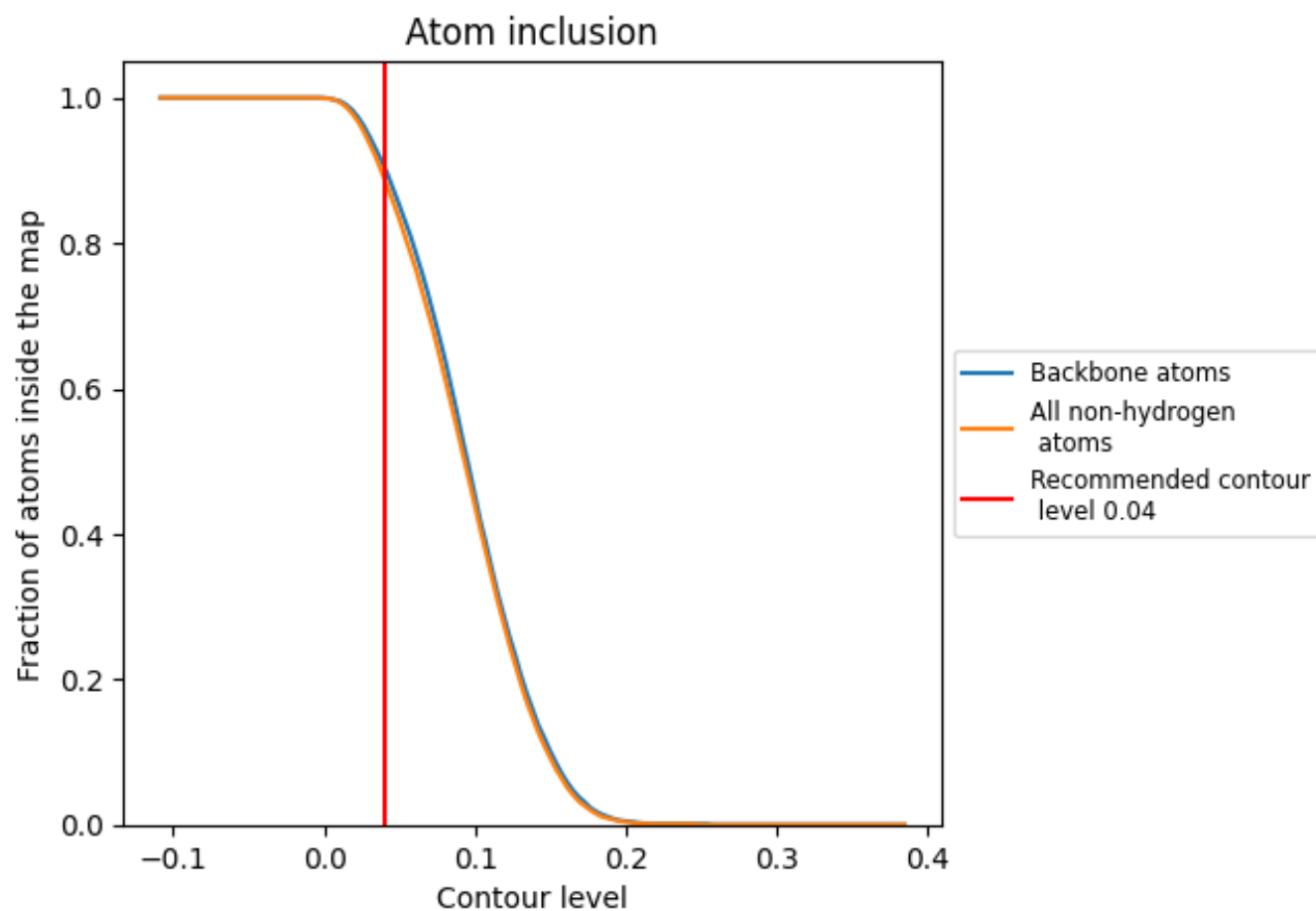
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.04).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 89% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8890	<div></div> 0.7200
1	<div></div> 0.8090	<div></div> 0.6830
3	<div></div> 0.9120	<div></div> 0.7230
4	<div></div> 0.8430	<div></div> 0.6810
5	<div></div> 0.9080	<div></div> 0.7020
6	<div></div> 0.8810	<div></div> 0.6960
7	<div></div> 0.9240	<div></div> 0.7300
8	<div></div> 0.9120	<div></div> 0.7250
A	<div></div> 0.9490	<div></div> 0.7540
B	<div></div> 0.9300	<div></div> 0.7430
C	<div></div> 0.9820	<div></div> 0.7630
D	<div></div> 0.9240	<div></div> 0.7400
E	<div></div> 0.8900	<div></div> 0.7250
F	<div></div> 0.8920	<div></div> 0.7270
G	<div></div> 0.1770	<div></div> 0.6260
I	<div></div> 0.8650	<div></div> 0.7140
J	<div></div> 0.9100	<div></div> 0.7350
K	<div></div> 0.7540	<div></div> 0.6890
L	<div></div> 0.7230	<div></div> 0.6770
Z	<div></div> 0.7830	<div></div> 0.6680

1.0

0.0

<0.0