



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 06:54 AM UTC

PDB ID : 7ZQ9 / pdb_00007zq9
EMDB ID : EMD-14867
Title : Dimeric PSI of Chlamydomonas reinhardtii at 2.74 Å resolution (symmetry expanded)
Authors : Naschberger, A.; Amunts, A.
Deposited on : 2022-04-29
Resolution : 2.74 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

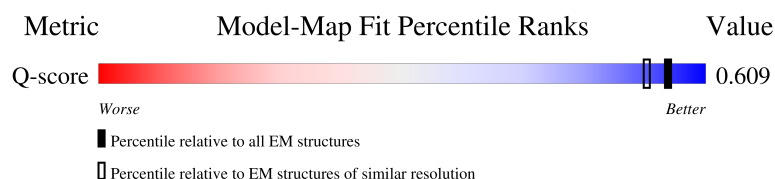
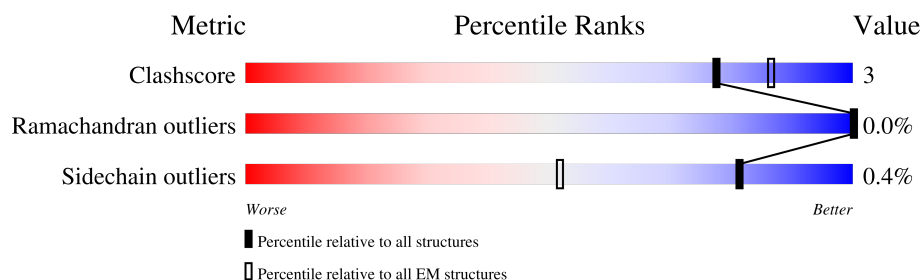
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 2.74 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.



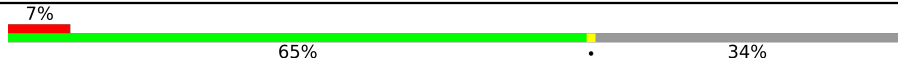
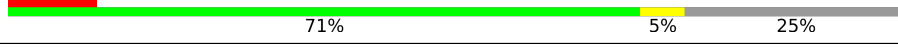
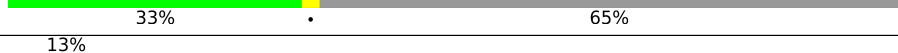
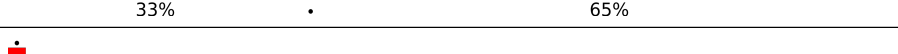
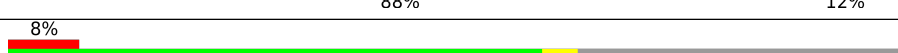
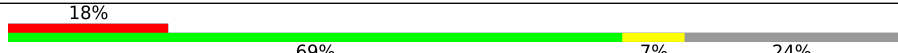
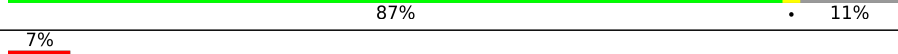
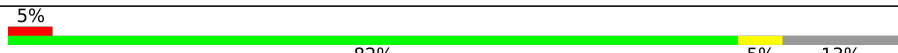
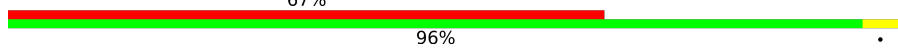
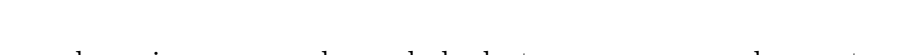
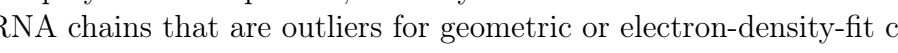
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10492 (2.24 - 3.24)

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

Mol	Chain	Length	Quality of chain
1	A	751	 94% 5%
2	B	735	 95%
3	C	81	 95%
4	D	196	 70% 27%

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Mol	Chain	Length	Quality of chain
5	E	97	
6	F	227	
7	G	126	
8	I	106	
8	I2	106	
9	J	40	
10	L	196	
10	L2	196	
11	K	113	
12	1	228	
12	Z	228	
13	3	298	
14	7	241	
15	8	243	
16	4	264	
17	5	257	
18	6	257	
19	9	213	
19	92	213	
20	B2	180	

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
21	CL0	A	801	X	-	-	-
22	CLA	1	602	X	-	-	-
22	CLA	1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	1	604	X	-	-	-
22	CLA	1	608	X	-	-	-
22	CLA	1	609	X	-	-	-
22	CLA	1	610	X	-	-	-
22	CLA	1	611	X	-	-	-
22	CLA	1	612	X	-	-	-
22	CLA	1	613	X	-	-	-
22	CLA	1	614	X	-	-	-
22	CLA	1	616	X	-	-	-
22	CLA	3	602	X	-	-	-
22	CLA	3	603	X	-	-	-
22	CLA	3	604	X	-	-	-
22	CLA	3	606	X	-	-	-
22	CLA	3	607	X	-	-	-
22	CLA	3	609	X	-	-	-
22	CLA	3	610	X	-	-	-
22	CLA	3	611	X	-	-	-
22	CLA	3	612	X	-	-	-
22	CLA	3	613	X	-	-	-
22	CLA	3	614	X	-	-	-
22	CLA	3	615	X	-	-	-
22	CLA	3	617	X	-	-	-
22	CLA	4	602	X	-	-	-
22	CLA	4	603	X	-	-	-
22	CLA	4	604	X	-	-	-
22	CLA	4	609	X	-	-	-
22	CLA	4	610	X	-	-	-
22	CLA	4	611	X	-	-	-
22	CLA	4	612	X	-	-	-
22	CLA	4	613	X	-	-	-
22	CLA	4	614	X	-	-	-
22	CLA	4	616	X	-	-	-
22	CLA	5	601	X	-	-	-
22	CLA	5	602	X	-	-	-
22	CLA	5	603	X	-	-	-
22	CLA	5	604	X	-	-	-
22	CLA	5	609	X	-	-	-
22	CLA	5	610	X	-	-	-
22	CLA	5	611	X	-	-	-
22	CLA	5	612	X	-	-	-
22	CLA	5	613	X	-	-	-
22	CLA	5	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	5	616	X	-	-	-
22	CLA	5	617	X	-	-	-
22	CLA	5	621	X	-	-	-
22	CLA	6	602	X	-	-	-
22	CLA	6	603	X	-	-	-
22	CLA	6	604	X	-	-	-
22	CLA	6	609	X	-	-	-
22	CLA	6	610	X	-	-	-
22	CLA	6	611	X	-	-	-
22	CLA	6	612	X	-	-	-
22	CLA	6	613	X	-	-	-
22	CLA	6	614	X	-	-	-
22	CLA	6	617	X	-	-	-
22	CLA	6	622	X	-	-	-
22	CLA	7	602	X	-	-	-
22	CLA	7	603	X	-	-	-
22	CLA	7	604	X	-	-	-
22	CLA	7	608	X	-	-	-
22	CLA	7	609	X	-	-	-
22	CLA	7	610	X	-	-	-
22	CLA	7	611	X	-	-	-
22	CLA	7	612	X	-	-	-
22	CLA	7	613	X	-	-	-
22	CLA	7	614	X	-	-	-
22	CLA	7	616	X	-	-	-
22	CLA	7	620	X	-	-	-
22	CLA	8	602	X	-	-	-
22	CLA	8	603	X	-	-	-
22	CLA	8	604	X	-	-	-
22	CLA	8	608	X	-	-	-
22	CLA	8	609	X	-	-	-
22	CLA	8	610	X	-	-	-
22	CLA	8	611	X	-	-	-
22	CLA	8	612	X	-	-	-
22	CLA	8	613	X	-	-	-
22	CLA	8	614	X	-	-	-
22	CLA	8	616	X	-	-	-
22	CLA	9	601	X	-	-	-
22	CLA	9	602	X	-	-	-
22	CLA	9	603	X	-	-	-
22	CLA	9	604	X	-	-	-
22	CLA	9	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	9	610	X	-	-	-
22	CLA	9	611	X	-	-	-
22	CLA	9	612	X	-	-	-
22	CLA	9	613	X	-	-	-
22	CLA	9	614	X	-	-	-
22	CLA	92	601	X	-	-	-
22	CLA	92	602	X	-	-	-
22	CLA	92	603	X	-	-	-
22	CLA	92	604	X	-	-	-
22	CLA	92	609	X	-	-	-
22	CLA	92	610	X	-	-	-
22	CLA	92	611	X	-	-	-
22	CLA	92	612	X	-	-	-
22	CLA	92	613	X	-	-	-
22	CLA	92	614	X	-	-	-
22	CLA	A	802	X	-	-	-
22	CLA	A	803	X	-	-	-
22	CLA	A	804	X	-	-	-
22	CLA	A	805	X	-	-	-
22	CLA	A	806	X	-	-	-
22	CLA	A	807	X	-	-	-
22	CLA	A	808	X	-	-	-
22	CLA	A	809	X	-	-	-
22	CLA	A	810	X	-	-	-
22	CLA	A	811	X	-	-	-
22	CLA	A	812	X	-	-	-
22	CLA	A	813	X	-	-	-
22	CLA	A	814	X	-	-	-
22	CLA	A	815	X	-	-	-
22	CLA	A	816	X	-	-	-
22	CLA	A	817	X	-	-	-
22	CLA	A	818	X	-	-	-
22	CLA	A	819	X	-	-	-
22	CLA	A	820	X	-	-	-
22	CLA	A	821	X	-	-	-
22	CLA	A	822	X	-	-	-
22	CLA	A	823	X	-	-	-
22	CLA	A	824	X	-	-	-
22	CLA	A	825	X	-	-	-
22	CLA	A	826	X	-	-	-
22	CLA	A	827	X	-	-	-
22	CLA	A	828	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	A	829	X	-	-	-
22	CLA	A	830	X	-	-	-
22	CLA	A	831	X	-	-	-
22	CLA	A	832	X	-	-	-
22	CLA	A	833	X	-	-	-
22	CLA	A	834	X	-	-	-
22	CLA	A	835	X	-	-	-
22	CLA	A	836	X	-	-	-
22	CLA	A	837	X	-	-	-
22	CLA	A	838	X	-	-	-
22	CLA	A	839	X	-	-	-
22	CLA	A	840	X	-	-	-
22	CLA	A	841	X	-	-	-
22	CLA	A	842	X	-	-	-
22	CLA	A	843	X	-	-	-
22	CLA	A	845	X	-	-	-
22	CLA	A	854	X	-	-	-
22	CLA	B	802	X	-	-	-
22	CLA	B	803	X	-	-	-
22	CLA	B	804	X	-	-	-
22	CLA	B	805	X	-	-	-
22	CLA	B	806	X	-	-	-
22	CLA	B	807	X	-	-	-
22	CLA	B	808	X	-	-	-
22	CLA	B	809	X	-	-	-
22	CLA	B	810	X	-	-	-
22	CLA	B	811	X	-	-	-
22	CLA	B	812	X	-	-	-
22	CLA	B	813	X	-	-	-
22	CLA	B	814	X	-	-	-
22	CLA	B	815	X	-	-	-
22	CLA	B	816	X	-	-	-
22	CLA	B	817	X	-	-	-
22	CLA	B	818	X	-	-	-
22	CLA	B	819	X	-	-	-
22	CLA	B	820	X	-	-	-
22	CLA	B	821	X	-	-	-
22	CLA	B	822	X	-	-	-
22	CLA	B	823	X	-	-	-
22	CLA	B	824	X	-	-	-
22	CLA	B	825	X	-	-	-
22	CLA	B	826	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	B	827	X	-	-	-
22	CLA	B	828	X	-	-	-
22	CLA	B	829	X	-	-	-
22	CLA	B	830	X	-	-	-
22	CLA	B	831	X	-	-	-
22	CLA	B	832	X	-	-	-
22	CLA	B	833	X	-	-	-
22	CLA	B	834	X	-	-	-
22	CLA	B	835	X	-	-	-
22	CLA	B	836	X	-	-	-
22	CLA	B	837	X	-	-	-
22	CLA	B	838	X	-	-	-
22	CLA	B	839	X	-	-	-
22	CLA	B	840	X	-	-	-
22	CLA	B	841	X	-	-	-
22	CLA	B2	804	X	-	-	-
22	CLA	B2	805	X	-	-	-
22	CLA	B2	806	X	-	-	-
22	CLA	B2	807	X	-	-	-
22	CLA	B2	808	X	-	-	-
22	CLA	B2	809	X	-	-	-
22	CLA	B2	810	X	-	-	-
22	CLA	B2	811	X	-	-	-
22	CLA	B2	812	X	-	-	-
22	CLA	B2	813	X	-	-	-
22	CLA	B2	814	X	-	-	-
22	CLA	B2	815	X	-	-	-
22	CLA	B2	820	X	-	-	-
22	CLA	B2	828	X	-	-	-
22	CLA	B2	829	X	-	-	-
22	CLA	B2	839	X	-	-	-
22	CLA	F	301	X	-	-	-
22	CLA	F	303	X	-	-	-
22	CLA	F	304	X	-	-	-
22	CLA	G	203	X	-	-	-
22	CLA	G	204	X	-	-	-
22	CLA	J	101	X	-	-	-
22	CLA	K	201	X	-	-	-
22	CLA	K	203	X	-	-	-
22	CLA	K	204	X	-	-	-
22	CLA	K	206	X	-	-	-
22	CLA	L	203	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
22	CLA	L	204	X	-	-	-
22	CLA	L2	203	X	-	-	-
22	CLA	L2	204	X	-	-	-
22	CLA	Z	602	X	-	-	-
22	CLA	Z	603	X	-	-	-
22	CLA	Z	604	X	-	-	-
22	CLA	Z	608	X	-	-	-
22	CLA	Z	609	X	-	-	-
22	CLA	Z	610	X	-	-	-
22	CLA	Z	611	X	-	-	-
22	CLA	Z	612	X	-	-	-
22	CLA	Z	613	X	-	-	-
22	CLA	Z	614	X	-	-	-
22	CLA	Z	616	X	-	-	-
31	CHL	1	601	X	-	-	-
31	CHL	1	606	X	-	-	-
31	CHL	1	607	X	-	-	-
31	CHL	3	608	X	-	-	-
31	CHL	4	601	X	-	-	-
31	CHL	4	606	X	-	-	-
31	CHL	4	607	X	-	-	-
31	CHL	4	608	X	-	-	-
31	CHL	4	618	X	-	-	-
31	CHL	5	606	X	-	-	-
31	CHL	5	607	X	-	-	-
31	CHL	5	608	X	-	-	-
31	CHL	5	618	X	-	-	-
31	CHL	6	601	X	-	-	-
31	CHL	6	606	X	-	-	-
31	CHL	6	607	X	-	-	-
31	CHL	6	608	X	-	-	-
31	CHL	6	616	X	-	-	-
31	CHL	6	618	X	-	-	-
31	CHL	7	601	X	-	-	-
31	CHL	7	606	X	-	-	-
31	CHL	7	607	X	-	-	-
31	CHL	8	601	X	-	-	-
31	CHL	8	606	X	-	-	-
31	CHL	8	607	X	-	-	-
31	CHL	9	606	X	-	-	-
31	CHL	9	607	X	-	-	-
31	CHL	92	606	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CHL	92	607	X	-	-	-
31	CHL	Z	601	X	-	-	-
31	CHL	Z	606	X	-	-	-
31	CHL	Z	607	X	-	-	-
32	XAT	1	618	X	-	-	-
32	XAT	5	624	X	-	-	-
33	NEX	6	625	X	-	-	-

2 Entry composition [i](#)

There are 34 unique types of molecules in this entry. The entry contains 113459 atoms, of which 56999 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 10 is a protein called PSI subunit V.

Mol	Chain	Residues	Atoms						AltConf	Trace
10	L	124	Total	C	H	N	O	S	0	0
			1806	586	907	146	164	3		
10	L2	102	Total	C	H	N	O	S	0	0
			1487	487	748	120	130	2		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

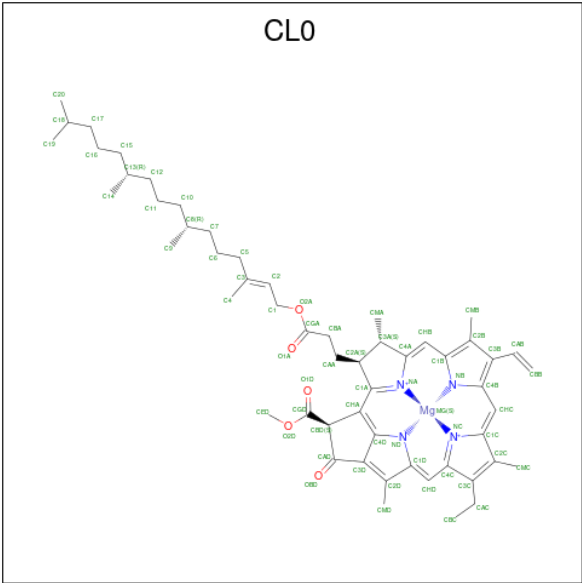
- Molecule 19 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms						AltConf	Trace
19	9	186	Total	C	H	N	O	S	0	0
			2820	918	1400	238	257	7		
19	92	184	Total	C	H	N	O	S	0	0
			2802	913	1392	236	254	7		

- Molecule 20 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

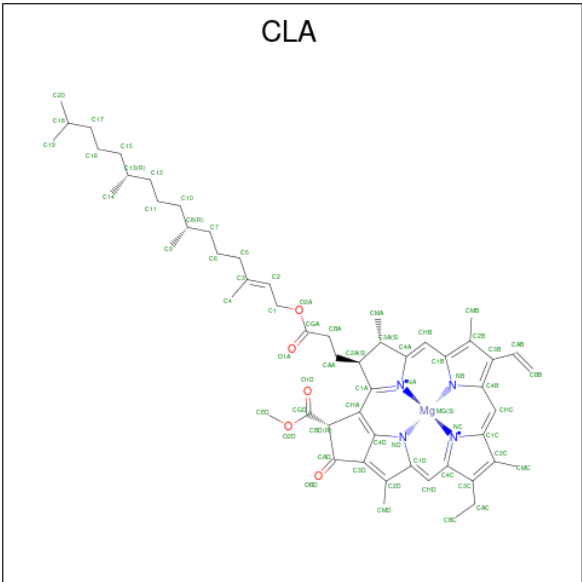
Mol	Chain	Residues	Atoms						AltConf	Trace
20	B2	180	Total	C	H	N	O	S	0	0
			2865	972	1396	247	247	3		

- Molecule 21 is CHLOROPHYLL A ISOMER (CCD ID: CL0) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 22 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



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

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

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

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

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Mol	Chain	Residues	Atoms						AltConf
22	F	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	F	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	G	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	G	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	J	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	L	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	L	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	K	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	1	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	1	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			73	34	31	1	4	3	
22	3	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			122	51	61	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	3	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	7	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			76	35	33	1	4	3	
22	7	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	7	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			125	52	63	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	8	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	Z	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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Mol	Chain	Residues	Atoms						AltConf
22	Z	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	Z	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	Z	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
22	Z	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	Z	1	Total 89	C 40	H 39	Mg 1	N 4	O 5	0
22	Z	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	4	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	4	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	4	1	Total 89	C 40	H 39	Mg 1	N 4	O 5	0
22	4	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	4	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	4	1	Total 119	C 50	H 59	Mg 1	N 4	O 5	0
22	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
22	4	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	4	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
22	4	1	Total 78	C 35	H 33	Mg 1	N 4	O 5	0
22	5	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	5	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	5	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0
22	5	1	Total 104	C 45	H 49	Mg 1	N 4	O 5	0
22	5	1	Total 137	C 55	H 72	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms						AltConf
22	5	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	5	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			113	48	55	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	6	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			79	36	33	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	

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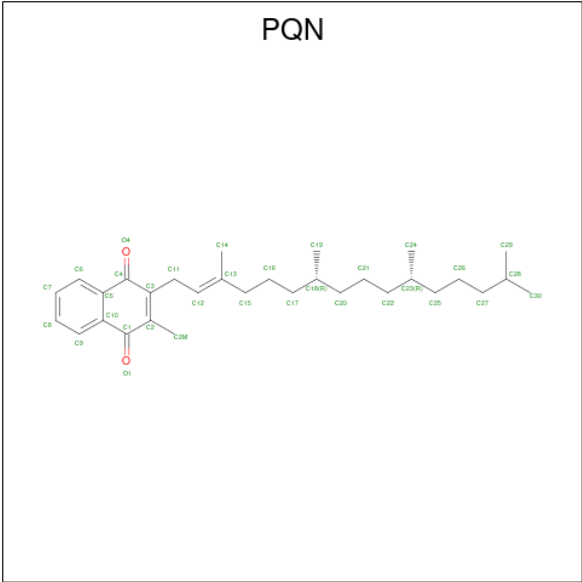
Mol	Chain	Residues	Atoms						AltConf
22	9	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			98	43	45	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			92	41	41	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	9	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			104	45	49	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			95	42	43	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			100	44	46	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			110	47	53	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

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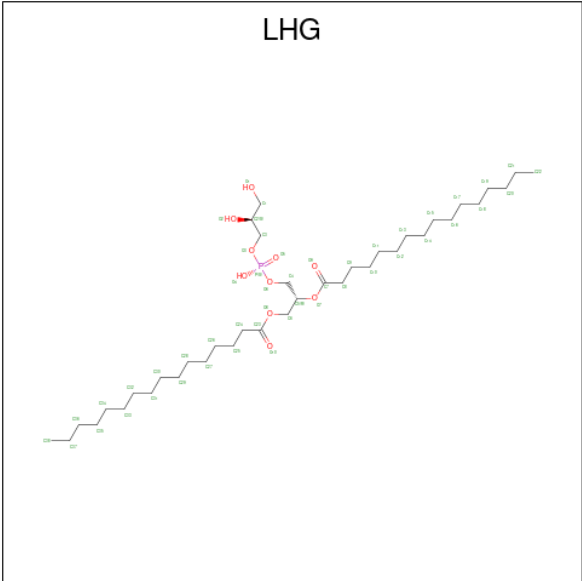
Mol	Chain	Residues	Atoms						AltConf
22	B2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	B2	1	Total	C	H	Mg	N	O	0
			107	46	51	1	4	5	
22	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	L2	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			89	40	39	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			119	50	59	1	4	5	
22	92	1	Total	C	H	Mg	N	O	0
			78	35	33	1	4	5	

- Molecule 23 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by depositor).



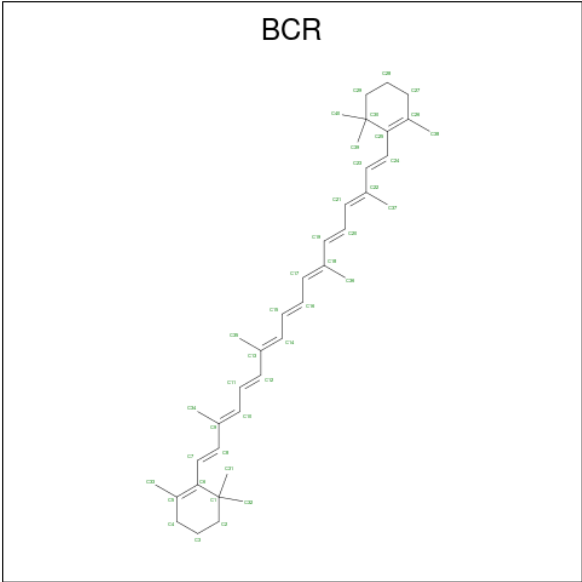
Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	H	O	P	0
			123	38	74	10	1	

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Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	H	O	P	0
			87	27	49	10	1	
24	B	1	Total	C	H	O	P	0
			108	34	63	10	1	
24	1	1	Total	C	H	O	P	0
			87	28	48	10	1	
24	3	1	Total	C	H	O	P	0
			63	20	32	10	1	
24	3	1	Total	C	H	O	P	0
			114	36	67	10	1	
24	7	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	8	1	Total	C	H	O	P	0
			105	33	61	10	1	
24	Z	1	Total	C	H	O	P	0
			87	28	48	10	1	
24	4	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	4	1	Total	C	H	O	P	0
			87	27	49	10	1	
24	5	1	Total	C	H	O	P	0
			81	26	44	10	1	
24	6	1	Total	C	H	O	P	0
			123	38	74	10	1	
24	6	1	Total	C	H	O	P	0
			78	25	42	10	1	
24	9	1	Total	C	H	O	P	0
			96	30	55	10	1	
24	92	1	Total	C	H	O	P	0
			57	18	28	10	1	

- Molecule 25 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	A	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	B	1	Total	C	H	0
			96	40	56	
25	G	1	Total	C	H	0
			96	40	56	
25	I	1	Total	C	H	0
			96	40	56	

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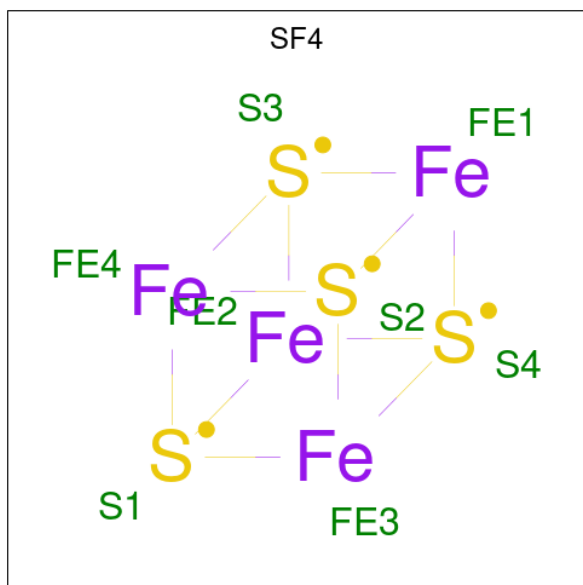
Mol	Chain	Residues	Atoms			AltConf
25	J	1	Total 96	C 40	H 56	0
25	L	1	Total 96	C 40	H 56	0
25	L	1	Total 96	C 40	H 56	0
25	K	1	Total 96	C 40	H 56	0
25	K	1	Total 96	C 40	H 56	0
25	3	1	Total 96	C 40	H 56	0
25	3	1	Total 96	C 40	H 56	0
25	3	1	Total 96	C 40	H 56	0
25	7	1	Total 96	C 40	H 56	0
25	8	1	Total 96	C 40	H 56	0
25	4	1	Total 96	C 40	H 56	0
25	5	1	Total 96	C 40	H 56	0
25	6	1	Total 96	C 40	H 56	0
25	9	1	Total 96	C 40	H 56	0
25	B2	1	Total 47	C 20	H 27	0
25	B2	1	Total 96	C 40	H 56	0
25	B2	1	Total 96	C 40	H 56	0
25	B2	1	Total 34	C 14	H 20	0
25	I2	1	Total 96	C 40	H 56	0
25	L2	1	Total 96	C 40	H 56	0
25	L2	1	Total 96	C 40	H 56	0

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Mol	Chain	Residues	Atoms			AltConf
25	92	1	Total	C	H	0
			96	40	56	

- Molecule 26 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 27 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).

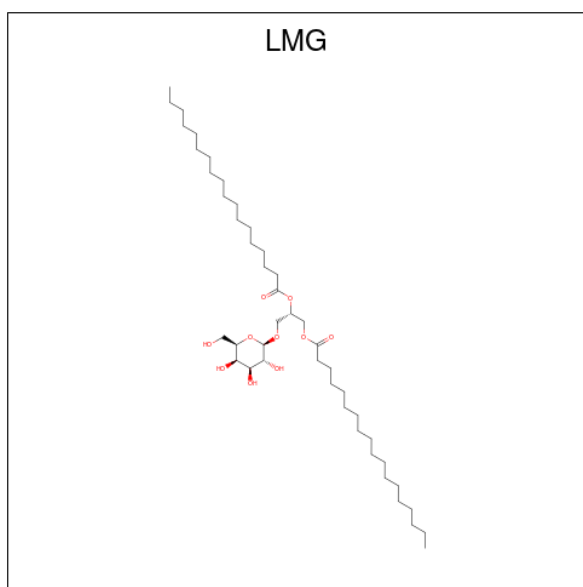


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Mol	Chain	Residues	Atoms				AltConf
27	1	1	Total	C	H	O	0
			59	18	35	6	
27	1	1	Total	C	H	O	0
			59	18	35	6	
27	7	1	Total	C	H	O	0
			69	21	37	11	
27	7	1	Total	C	H	O	0
			50	16	28	6	
27	7	1	Total	C	H	O	0
			54	16	27	11	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	8	1	Total	C	H	O	0
			81	24	46	11	
27	8	1	Total	C	H	O	0
			59	18	35	6	
27	Z	1	Total	C	H	O	0
			66	20	35	11	
27	Z	1	Total	C	H	O	0
			50	16	28	6	
27	4	1	Total	C	H	O	0
			72	22	39	11	
27	4	1	Total	C	H	O	0
			44	14	24	6	
27	5	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			44	14	24	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	6	1	Total	C	H	O	0
			59	18	35	6	
27	9	1	Total	C	H	O	0
			59	18	35	6	
27	92	1	Total	C	H	O	0
			81	24	46	11	

- Molecule 28 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by depositor).



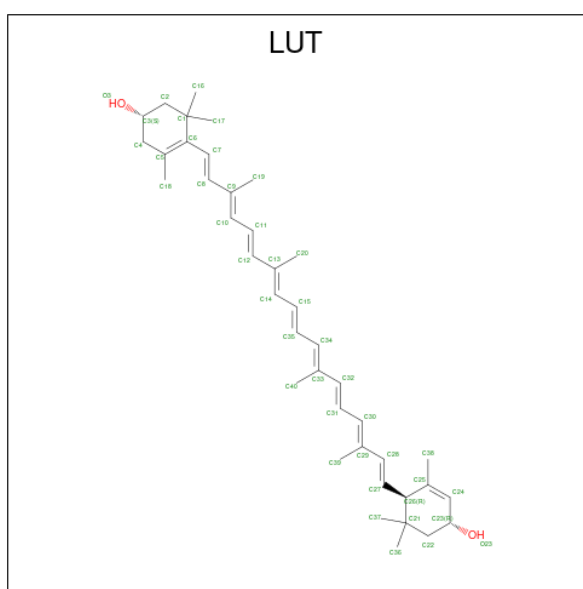
Mol	Chain	Residues	Atoms				AltConf
28	A	1	Total	C	H	O	0
			117	38	69	10	
28	A	1	Total	C	H	O	0
			78	26	42	10	
28	B	1	Total	C	H	O	0
			99	33	56	10	
28	B	1	Total	C	H	O	0
			78	26	42	10	
28	J	1	Total	C	H	O	0
			99	32	57	10	
28	J	1	Total	C	H	O	0
			75	25	40	10	
28	1	1	Total	C	H	O	0
			78	26	42	10	
28	1	1	Total	C	H	O	0
			96	32	54	10	
28	3	1	Total	C	H	O	0
			120	40	75	5	
28	7	1	Total	C	H	O	0
			81	27	44	10	
28	8	1	Total	C	H	O	0
			66	22	34	10	
28	8	1	Total	C	H	O	0
			99	32	57	10	
28	4	1	Total	C	H	O	0
			96	31	55	10	
28	6	1	Total	C	H	O	0
			55	18	35	2	

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Mol	Chain	Residues	Atoms				AltConf
28	9	1	Total	C	H	O	0
			105	34	61	10	
28	B2	1	Total	C	H	O	0
			99	33	56	10	
28	B2	1	Total	C	H	O	0
			63	21	32	10	

- Molecule 29 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$) (labeled as "Ligand of Interest" by depositor).



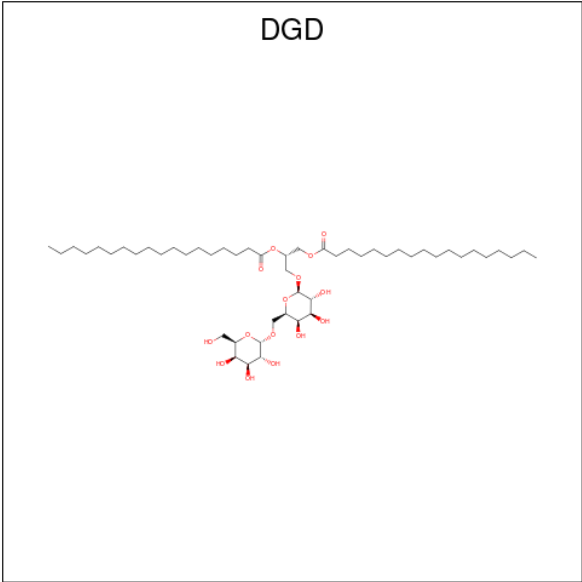
Mol	Chain	Residues	Atoms				AltConf
29	A	1	Total	C	H	O	0
			98	40	56	2	
29	F	1	Total	C	H	O	0
			98	40	56	2	
29	1	1	Total	C	H	O	0
			98	40	56	2	
29	1	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	
29	3	1	Total	C	H	O	0
			98	40	56	2	

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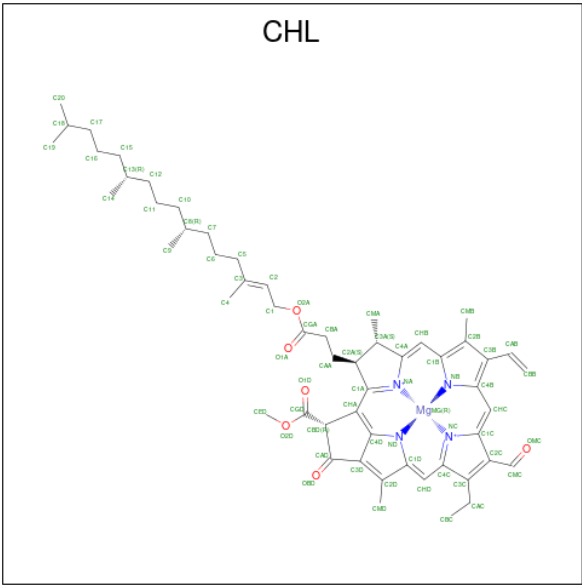
Mol	Chain	Residues	Atoms				AltConf
29	7	1	Total	C	H	O	0
			98	40	56	2	
29	7	1	Total	C	H	O	0
			98	40	56	2	
29	8	1	Total	C	H	O	0
			98	40	56	2	
29	Z	1	Total	C	H	O	0
			98	40	56	2	
29	Z	1	Total	C	H	O	0
			59	25	33	1	
29	4	1	Total	C	H	O	0
			98	40	56	2	
29	5	1	Total	C	H	O	0
			98	40	56	2	
29	5	1	Total	C	H	O	0
			98	40	56	2	
29	6	1	Total	C	H	O	0
			98	40	56	2	
29	9	1	Total	C	H	O	0
			98	40	56	2	
29	9	1	Total	C	H	O	0
			98	40	56	2	
29	92	1	Total	C	H	O	0
			98	40	56	2	
29	92	1	Total	C	H	O	0
			98	40	56	2	

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: C₅₁H₉₆O₁₅) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 31 is CHLOROPHYLL B (CCD ID: CHL) (formula: C₅₅H₇₀MgN₄O₆).



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

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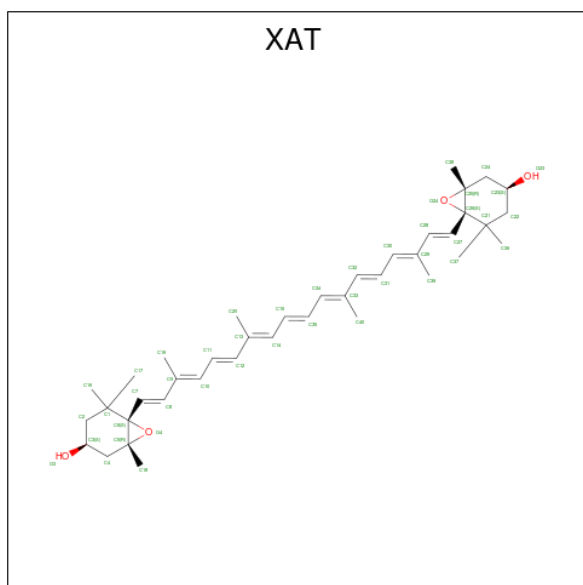
Mol	Chain	Residues	Atoms						AltConf
31	3	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	7	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	7	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	7	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	8	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	Z	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	Z	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	Z	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 103	C 45	H 47	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	4	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	5	1	Total 77	C 35	H 31	Mg 1	N 4	O 6	0
31	5	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	5	1	Total 88	C 40	H 37	Mg 1	N 4	O 6	0
31	5	1	Total 72	C 34	H 29	Mg 1	N 4	O 4	0
31	6	1	Total 136	C 55	H 70	Mg 1	N 4	O 6	0
31	6	1	Total 109	C 47	H 51	Mg 1	N 4	O 6	0

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Mol	Chain	Residues	Atoms						AltConf
31	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			136	55	70	1	4	6	
31	6	1	Total	C	H	Mg	N	O	0
			72	34	29	1	4	4	
31	9	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
31	9	1	Total	C	H	Mg	N	O	0
			88	40	37	1	4	6	
31	92	1	Total	C	H	Mg	N	O	0
			69	33	27	1	4	4	
31	92	1	Total	C	H	Mg	N	O	0
			77	35	31	1	4	6	

- Molecule 32 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



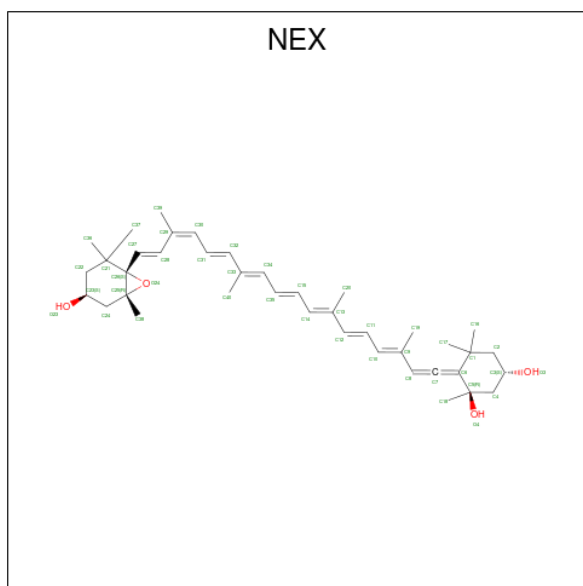
Mol	Chain	Residues	Atoms				AltConf
32	1	1	Total	C	H	O	0
			100	40	56	4	
32	7	1	Total	C	H	O	0
			100	40	56	4	

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Mol	Chain	Residues	Atoms				AltConf
32	8	1	Total	C	H	O	0
			100	40	56	4	
32	Z	1	Total	C	H	O	0
			100	40	56	4	
32	4	1	Total	C	H	O	0
			100	40	56	4	
32	5	1	Total	C	H	O	0
			100	40	56	4	
32	6	1	Total	C	H	O	0
			100	40	56	4	

- Molecule 33 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTADECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (CCD ID: NEX) (formula: C₄₀H₅₆O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
33	5	1	Total	C	H	O	0
			100	40	56	4	
33	6	1	Total	C	H	O	0
			100	40	56	4	

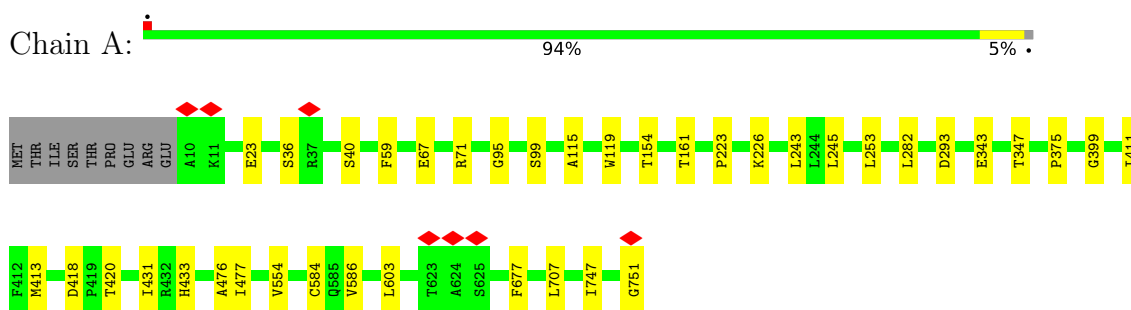
- Molecule 34 is water.

Mol	Chain	Residues	Atoms		AltConf
34	H	11	Total 11	O 11	0
34	H	20	Total 20	O 20	0
34	H	1	Total 1	O 1	0
34	H	1	Total 1	O 1	0
34	H	4	Total 4	O 4	0
34	H	2	Total 2	O 2	0
34	H	7	Total 7	O 7	0
34	H	6	Total 6	O 6	0
34	H	7	Total 7	O 7	0
34	H	7	Total 7	O 7	0
34	H	5	Total 5	O 5	0
34	H	4	Total 4	O 4	0
34	H	7	Total 7	O 7	0
34	H	5	Total 5	O 5	0
34	H	1	Total 1	O 1	0

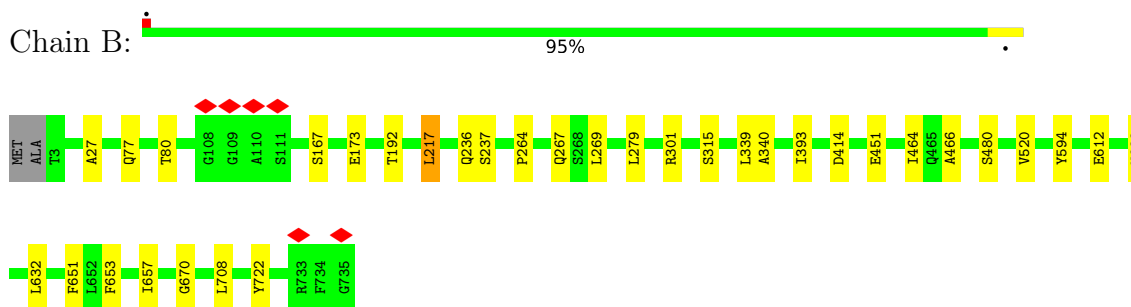
3 Residue-property plots

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

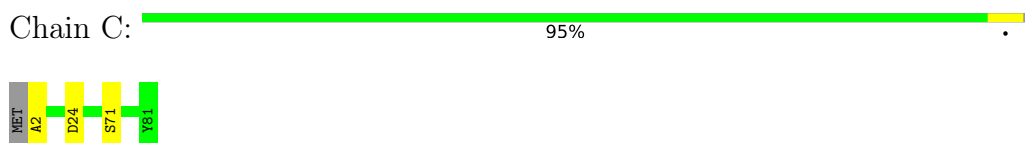
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



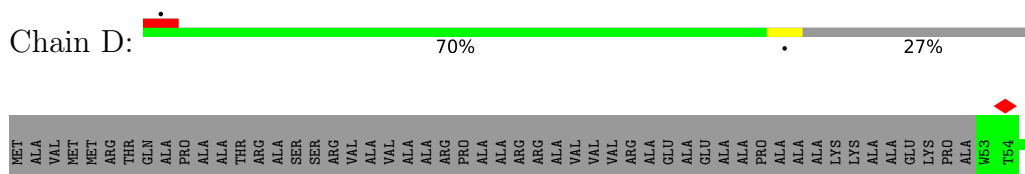
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

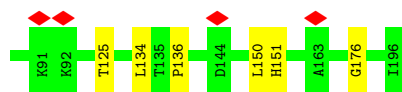


- Molecule 3: Photosystem I iron-sulfur center

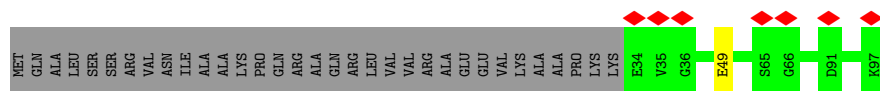


- Molecule 4: Photosystem I reaction center subunit II, chloroplastic

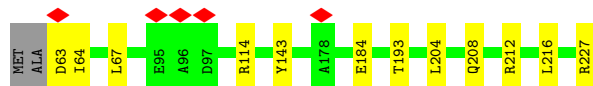
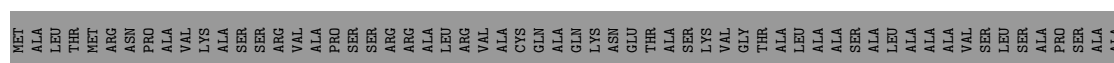




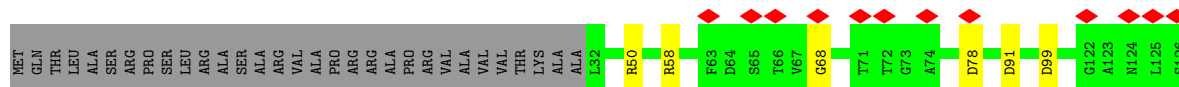
- Molecule 5: Photosystem I reaction center subunit IV, chloroplastic



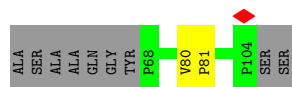
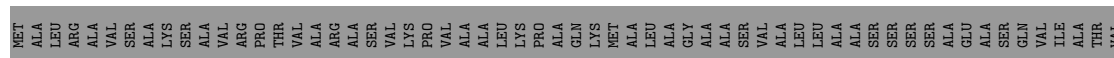
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



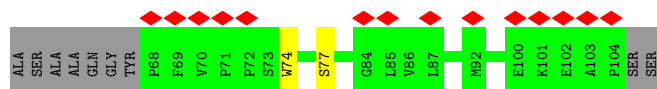
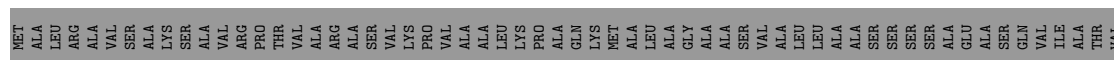
- Molecule 7: Photosystem I reaction center subunit V, chloroplastic



- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 8: Photosystem I reaction center subunit VIII



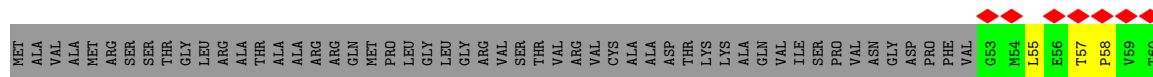
- Molecule 9: Photosystem I reaction center subunit IX

Chain J:  88% 12%



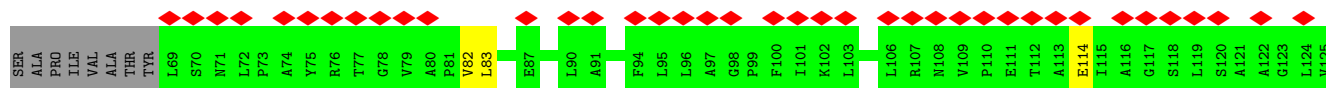
- Molecule 10: PSI subunit V

Chain L:  8% 60% 37%



- Molecule 10: PSI subunit V

Chain L2:  28% 51% 48%



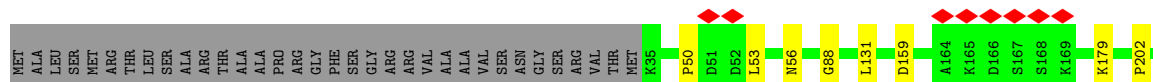
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain K:  18% 69% 7% 24%

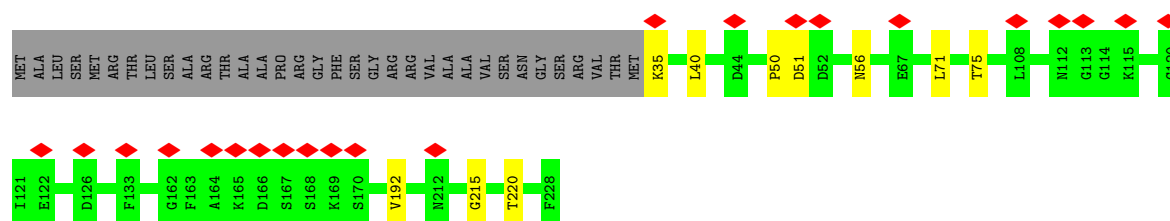
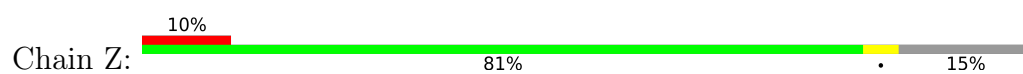


- Molecule 12: Chlorophyll a-b binding protein, chloroplastic

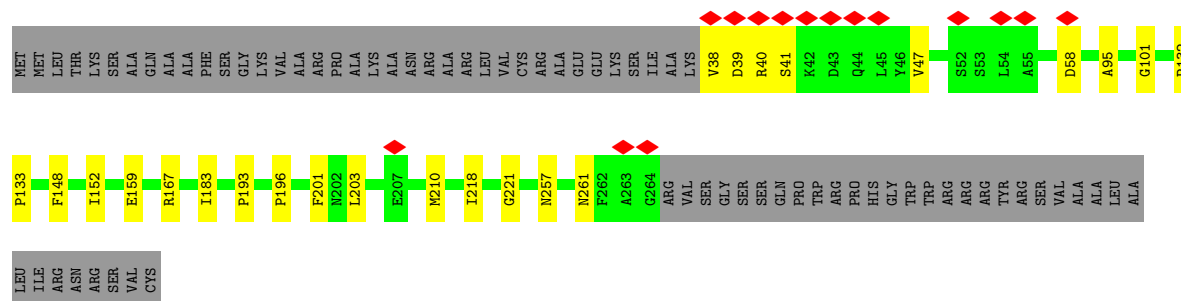
Chain 1:  81% 15%



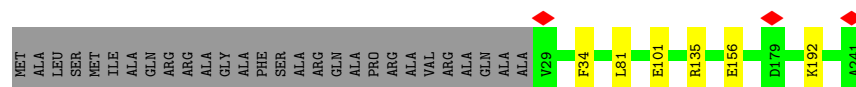
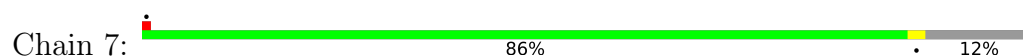
- Molecule 12: Chlorophyll a-b binding protein, chloroplastic



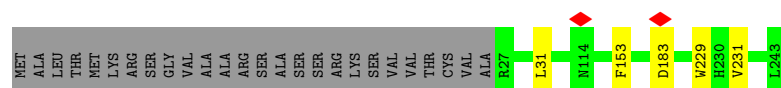
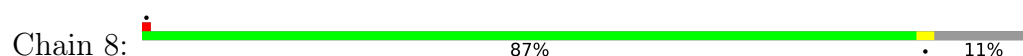
- Molecule 13: Chlorophyll a-b binding protein, chloroplastic



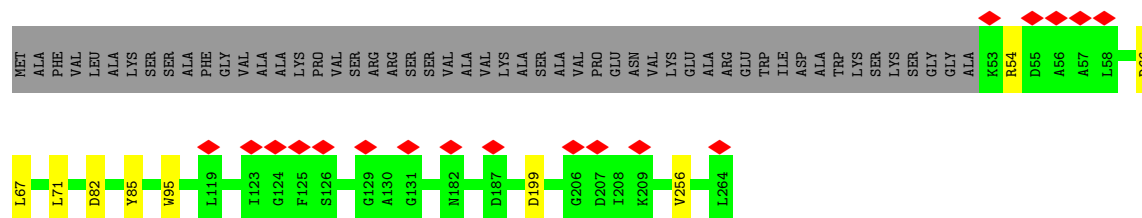
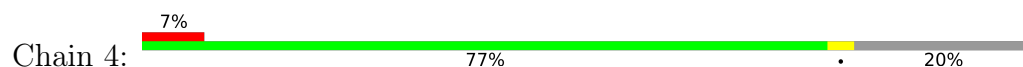
- Molecule 14: Chlorophyll a-b binding protein, chloroplastic



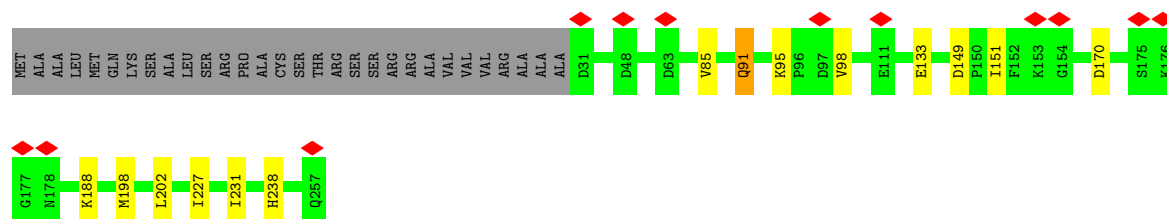
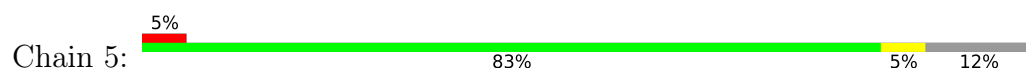
- Molecule 15: Chlorophyll a-b binding protein, chloroplastic



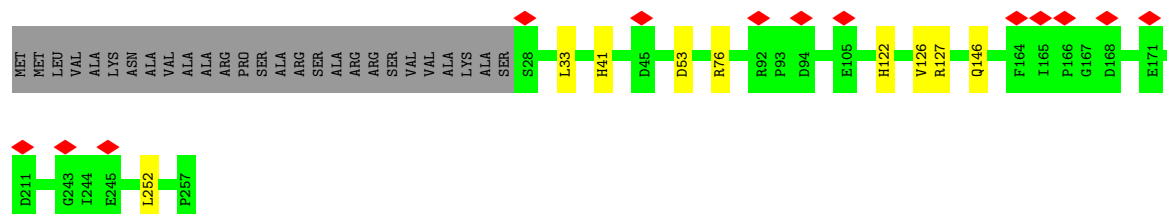
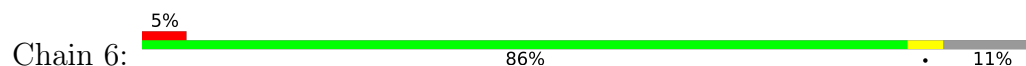
- Molecule 16: Chlorophyll a-b binding protein, chloroplastic (Lhca4)



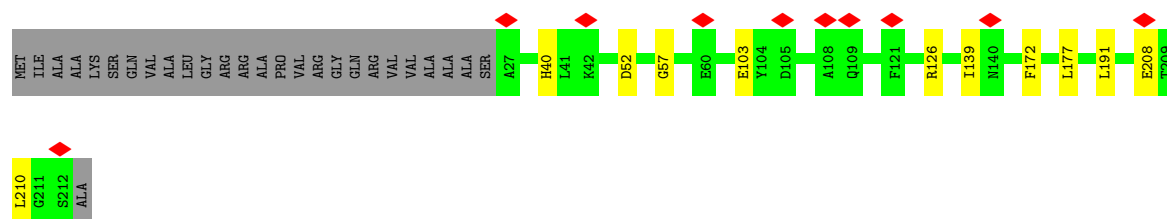
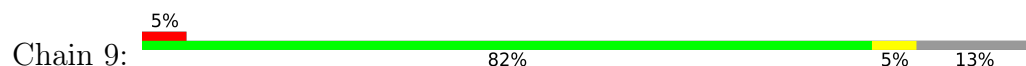
- Molecule 17: Chlorophyll a-b binding protein, chloroplastic



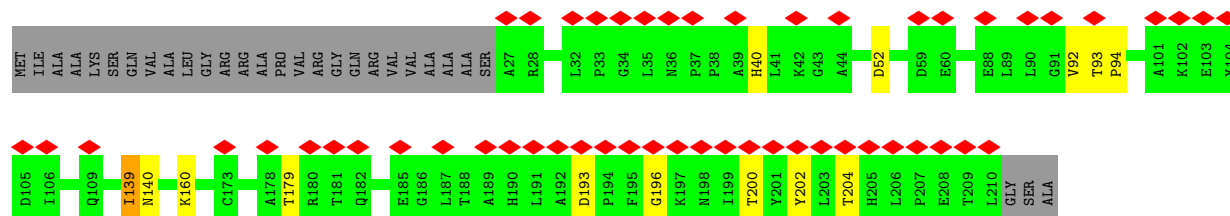
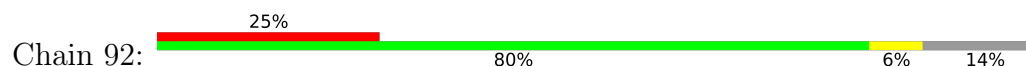
- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



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



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



- Molecule 20: Photosystem I P700 chlorophyll a apoprotein A2





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28346	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.8	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	5000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.175	Depositor
Minimum map value	-0.075	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.031	Depositor
Map size ($\text{\AA}$)	588.0, 588.0, 588.0	wwPDB
Map dimensions	700, 700, 700	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.84, 0.84, 0.84	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.17	0/6021	0.23	0/8208
2	B	0.18	0/6036	0.23	0/8240
3	C	0.16	0/611	0.29	0/826
4	D	0.14	0/1161	0.24	0/1567
5	E	0.15	0/516	0.18	0/700
6	F	0.14	0/1292	0.21	0/1747
7	G	0.15	0/721	0.19	0/980
8	I	0.15	0/293	0.26	0/406
8	I2	0.10	0/293	0.24	0/406
9	J	0.17	0/329	0.23	0/452
10	L	0.15	0/920	0.20	0/1257
10	L2	0.10	0/757	0.17	0/1031
11	K	0.15	0/588	0.18	0/795
12	1	0.15	0/1491	0.21	0/2028
12	Z	0.13	0/1491	0.19	0/2028
13	3	0.16	0/1784	0.24	0/2420
14	7	0.17	0/1702	0.21	0/2310
15	8	0.17	0/1701	0.23	0/2315
16	4	0.13	0/1703	0.20	0/2321
17	5	0.14	0/1830	0.22	0/2492
18	6	0.14	0/1834	0.21	0/2505
19	9	0.14	0/1461	0.21	0/1987
19	92	0.12	0/1451	0.20	0/1974
20	B2	0.09	0/1522	0.19	0/2071
All	All	0.15	0/37508	0.22	0/51066

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5825	5675	5675	26	0
2	B	5824	5576	5577	31	0
3	C	601	582	581	2	0
4	D	1133	1151	1150	4	0
5	E	506	505	504	1	0
6	F	1266	1302	1301	9	0
7	G	706	687	686	4	0
8	I	281	292	292	1	0
8	I2	281	292	292	1	0
9	J	329	328	328	2	0
10	L	899	907	905	7	0
10	L2	739	748	747	2	0
11	K	583	620	620	7	0
12	1	1445	1397	1396	8	0
12	Z	1445	1397	1396	7	0
13	3	1736	1695	1694	15	0
14	7	1650	1590	1589	7	0
15	8	1650	1630	1629	5	0
16	4	1648	1603	1602	7	0
17	5	1775	1747	1746	14	0
18	6	1772	1770	1770	9	0
19	9	1420	1400	1399	10	0
19	92	1410	1392	1391	9	0
20	B2	1469	1396	1395	4	0
21	A	65	72	72	0	0
22	1	639	625	625	5	0
22	3	740	718	718	12	0
22	4	565	534	534	3	0
22	5	740	712	712	10	0
22	6	628	605	605	1	0
22	7	652	598	598	5	0
22	8	614	578	578	4	0
22	9	565	535	535	2	0
22	92	545	505	505	4	0
22	A	2718	2856	2856	28	0
22	B	2463	2580	2580	25	0
22	B2	919	891	891	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	F	175	177	177	1	0
22	G	106	92	92	0	0
22	J	55	49	49	1	0
22	K	196	158	158	3	0
22	L	110	105	105	1	0
22	L2	90	66	66	0	0
22	Z	627	593	593	6	0
23	A	33	46	46	0	0
23	B	33	46	46	0	0
24	1	39	48	48	1	0
24	3	78	99	99	1	0
24	4	87	123	123	1	0
24	5	37	44	44	1	0
24	6	85	116	116	1	0
24	7	49	74	74	1	0
24	8	44	61	61	0	0
24	9	41	55	55	0	0
24	92	29	28	28	1	0
24	A	87	123	123	0	0
24	B	45	63	63	0	0
24	Z	39	48	48	0	0
25	3	120	168	168	7	0
25	4	40	56	56	0	0
25	5	40	56	56	0	0
25	6	40	56	56	2	0
25	7	40	56	56	0	0
25	8	40	56	56	2	0
25	9	40	56	56	2	0
25	92	40	56	56	3	0
25	A	200	280	280	12	0
25	B	280	392	392	11	0
25	B2	114	159	159	6	0
25	G	40	56	56	0	0
25	I	40	56	56	1	0
25	I2	40	56	56	0	0
25	J	40	56	56	1	0
25	K	80	112	112	6	0
25	L	80	112	112	5	0
25	L2	80	112	112	3	0
26	A	8	0	0	0	0
26	C	16	0	0	0	0
27	1	148	201	201	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	4	53	63	63	0	0
27	5	24	35	35	0	0
27	6	92	129	129	1	0
27	7	81	92	92	1	0
27	8	107	151	151	1	0
27	9	24	35	35	1	0
27	92	35	46	46	2	0
27	A	196	262	262	4	0
27	B	35	46	46	3	0
27	G	24	35	35	0	0
27	K	24	35	35	0	0
27	Z	53	63	63	1	0
28	1	78	96	96	0	0
28	3	45	75	75	1	0
28	4	41	55	55	1	0
28	6	20	35	35	0	0
28	7	37	44	44	0	0
28	8	74	91	91	0	0
28	9	44	61	61	1	0
28	A	84	111	111	1	0
28	B	79	98	98	1	0
28	B2	74	88	88	0	0
28	J	77	97	97	2	0
29	1	84	112	112	2	0
29	3	126	168	168	2	0
29	4	42	56	56	1	0
29	5	84	112	112	4	0
29	6	42	56	56	1	0
29	7	84	112	112	4	0
29	8	42	56	56	0	0
29	9	84	112	112	3	0
29	92	84	112	112	0	0
29	A	42	56	56	1	0
29	F	42	56	56	3	0
29	Z	68	89	89	1	0
30	B	59	79	79	1	0
31	1	158	132	132	1	0
31	3	66	70	70	1	0
31	4	300	288	288	3	0
31	5	206	167	167	2	0
31	6	350	327	327	7	0
31	7	158	132	132	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	8	198	210	210	3	0
31	9	93	64	64	0	0
31	92	88	58	58	0	0
31	Z	178	171	171	1	0
32	1	44	56	56	1	0
32	4	44	56	56	0	0
32	5	44	56	56	0	0
32	6	44	56	56	0	0
32	7	44	56	56	0	0
32	8	44	56	56	0	0
32	Z	44	56	56	0	0
33	5	44	56	56	0	0
33	6	44	56	56	1	0
34	H	88	0	0	12	0
All	All	56460	56999	56982	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 324 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)
29:7:624:LUT:H381	29:7:624:LUT:H28	1.51	0.92
27:B:853:LMU:H2O1	27:B:853:LMU:H6'	1.15	0.87
1:A:95:GLY:O	1:A:99:SER:OG	1.94	0.83
17:5:170:ASP:OD1	29:5:620:LUT:O23	1.96	0.82
2:B:301:ARG:NH1	7:G:68:GLY:O	2.15	0.80

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	740/751 (98%)	729 (98%)	11 (2%)	0	100	100
2	B	731/735 (100%)	718 (98%)	13 (2%)	0	100	100
3	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
4	D	142/196 (72%)	138 (97%)	4 (3%)	0	100	100
5	E	62/97 (64%)	61 (98%)	1 (2%)	0	100	100
6	F	163/227 (72%)	162 (99%)	1 (1%)	0	100	100
7	G	93/126 (74%)	93 (100%)	0	0	100	100
8	I	35/106 (33%)	35 (100%)	0	0	100	100
8	I2	35/106 (33%)	34 (97%)	1 (3%)	0	100	100
9	J	38/40 (95%)	37 (97%)	1 (3%)	0	100	100
10	L	120/196 (61%)	117 (98%)	3 (2%)	0	100	100
10	L2	98/196 (50%)	95 (97%)	3 (3%)	0	100	100
11	K	84/113 (74%)	82 (98%)	2 (2%)	0	100	100
12	1	192/228 (84%)	192 (100%)	0	0	100	100
12	Z	192/228 (84%)	189 (98%)	3 (2%)	0	100	100
13	3	225/298 (76%)	218 (97%)	7 (3%)	0	100	100
14	7	211/241 (88%)	210 (100%)	1 (0%)	0	100	100
15	8	215/243 (88%)	213 (99%)	2 (1%)	0	100	100
16	4	210/264 (80%)	207 (99%)	3 (1%)	0	100	100
17	5	225/257 (88%)	220 (98%)	5 (2%)	0	100	100
18	6	228/257 (89%)	225 (99%)	3 (1%)	0	100	100
19	9	184/213 (86%)	179 (97%)	4 (2%)	1 (0%)	24	40
19	92	182/213 (85%)	178 (98%)	3 (2%)	1 (0%)	24	40
20	B2	166/180 (92%)	164 (99%)	2 (1%)	0	100	100
All	All	4649/5592 (83%)	4572 (98%)	75 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	601/610 (98%)	599 (100%)	2 (0%)	86	92
2	B	596/597 (100%)	594 (100%)	2 (0%)	86	92
3	C	69/70 (99%)	69 (100%)	0	100	100
4	D	121/152 (80%)	120 (99%)	1 (1%)	73	83
5	E	55/81 (68%)	55 (100%)	0	100	100
6	F	127/169 (75%)	127 (100%)	0	100	100
7	G	71/94 (76%)	71 (100%)	0	100	100
8	I	31/76 (41%)	31 (100%)	0	100	100
8	I2	31/76 (41%)	31 (100%)	0	100	100
9	J	35/35 (100%)	34 (97%)	1 (3%)	37	59
10	L	90/148 (61%)	89 (99%)	1 (1%)	65	79
10	L2	72/148 (49%)	72 (100%)	0	100	100
11	K	59/80 (74%)	59 (100%)	0	100	100
12	1	137/162 (85%)	137 (100%)	0	100	100
12	Z	137/162 (85%)	137 (100%)	0	100	100
13	3	174/230 (76%)	172 (99%)	2 (1%)	65	79
14	7	164/181 (91%)	164 (100%)	0	100	100
15	8	163/183 (89%)	162 (99%)	1 (1%)	78	87
16	4	166/205 (81%)	166 (100%)	0	100	100
17	5	184/206 (89%)	181 (98%)	3 (2%)	55	72
18	6	184/203 (91%)	184 (100%)	0	100	100
19	9	142/159 (89%)	142 (100%)	0	100	100
19	92	141/159 (89%)	141 (100%)	0	100	100
20	B2	153/153 (100%)	152 (99%)	1 (1%)	76	85
All	All	3703/4339 (85%)	3689 (100%)	14 (0%)	81	90

5 of 14 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
13	3	38	VAL
13	3	218	ILE
20	B2	17	PRO
17	5	202	LEU
17	5	238	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
16	4	166	GLN
18	6	88	GLN
19	92	140	ASN
17	5	257	GLN
2	B	631	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	AME	J	1	9	9,10,11	0.55	0	9,11,13	0.88	1 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	AME	J	1	9	-	3/9/10/12	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	J	1	AME	O-C-CA	-2.57	118.15	124.77

There are no chirality outliers.

All (3) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

397 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	$\# Z > 2$
22	CLA	92	602	19	69,73,73	1.18	5 (7%)	82,113,113	0.85	3 (3%)
28	LMG	1	628	-	42,42,55	0.19	0	50,50,63	0.29	0
30	DGD	B	850	-	60,60,67	0.17	0	74,74,81	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	K	204	-	50,54,73	1.38	5 (10%)	59,90,113	0.99	3 (5%)
22	CLA	L2	203	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)
31	CHL	8	607	34	60,74,74	1.91	10 (16%)	58,114,114	1.11	5 (8%)
27	LMU	K	208	-	24,24,36	0.10	0	29,29,47	0.31	0
22	CLA	B2	814	-	64,68,73	1.22	4 (6%)	76,107,113	0.84	3 (3%)
22	CLA	A	854	34	69,73,73	1.23	5 (7%)	82,113,113	0.79	3 (3%)
24	LHG	6	629	-	35,35,48	0.26	0	38,41,54	0.29	0
22	CLA	A	823	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	3 (3%)
28	LMG	A	860	-	36,36,55	0.20	0	44,44,63	0.24	0
29	LUT	1	617	-	42,43,43	0.28	0	51,60,60	0.42	0
31	CHL	4	606	34	50,64,74	2.16	10 (20%)	46,102,114	1.26	6 (13%)
25	BCR	K	202	-	41,41,41	0.16	0	56,56,56	0.37	0
25	BCR	B	844	-	41,41,41	0.13	0	56,56,56	0.46	0
29	LUT	6	621	-	42,43,43	0.26	0	51,60,60	0.40	0
31	CHL	8	606	34	60,74,74	1.97	10 (16%)	58,114,114	1.08	5 (8%)
22	CLA	B2	805	-	69,73,73	1.16	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	4	611	24	64,68,73	1.24	4 (6%)	76,107,113	0.85	3 (3%)
22	CLA	8	611	24	49,53,73	1.43	5 (10%)	58,89,113	0.98	3 (5%)
22	CLA	Z	611	24	64,68,73	1.22	4 (6%)	76,107,113	0.86	3 (3%)
28	LMG	7	626	-	37,37,55	0.19	0	45,45,63	0.26	0
28	LMG	8	629	-	42,42,55	0.18	0	50,50,63	0.16	0
22	CLA	B2	828	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	8	608	34	54,58,73	1.34	5 (9%)	64,95,113	0.93	2 (3%)
26	SF4	C	102	3	0,12,12	-	-	-	-	-
27	LMU	Z	622	-	32,32,36	0.10	0	43,43,47	0.18	0
22	CLA	7	614	-	47,51,73	1.46	5 (10%)	55,86,113	1.02	4 (7%)
24	LHG	9	622	22	40,40,48	0.25	0	43,46,54	0.29	0
22	CLA	9	612	19	69,73,73	1.16	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	A	822	34	69,73,73	1.18	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	4	616	16	49,53,73	1.40	4 (8%)	58,89,113	0.96	3 (5%)
22	CLA	6	613	34	69,73,73	1.18	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	9	601	19	50,54,73	1.40	4 (8%)	59,90,113	0.98	3 (5%)
25	BCR	I2	172	-	41,41,41	0.12	0	56,56,56	0.32	0
22	CLA	1	613	34	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	7	603	-	56,60,73	1.31	5 (8%)	65,97,113	0.92	3 (4%)
25	BCR	B2	843	-	20,20,41	0.82	1 (5%)	27,27,56	0.25	0
25	BCR	K	207	-	41,41,41	0.14	0	56,56,56	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	3	617	13	50,54,73	1.37	4 (8%)	59,90,113	0.98	2 (3%)
22	CLA	4	609	16	64,68,73	1.25	4 (6%)	76,107,113	0.86	2 (2%)
22	CLA	B	841	24	69,73,73	1.18	5 (7%)	82,113,113	0.84	4 (4%)
33	NEX	5	625	-	40,46,46	0.45	1 (2%)	50,70,70	0.77	4 (8%)
31	CHL	1	601	12	60,74,74	1.95	10 (16%)	58,114,114	1.05	4 (6%)
31	CHL	7	606	34	40,54,74	2.42	10 (25%)	34,90,114	1.41	5 (14%)
25	BCR	A	850	-	41,41,41	0.16	0	56,56,56	0.24	0
22	CLA	A	820	-	69,73,73	1.16	5 (7%)	82,113,113	0.84	3 (3%)
22	CLA	A	843	34	69,73,73	1.17	5 (7%)	82,113,113	0.85	3 (3%)
27	LMU	8	625	-	24,24,36	0.12	0	29,29,47	0.28	0
32	XAT	1	618	-	41,47,47	0.14	0	54,74,74	0.71	1 (1%)
31	CHL	4	607	34	60,74,74	1.97	10 (16%)	58,114,114	1.04	5 (8%)
22	CLA	9	604	19	57,61,73	1.27	5 (8%)	67,98,113	0.90	3 (4%)
22	CLA	A	827	34	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	6	610	18	64,68,73	1.22	5 (7%)	76,107,113	0.85	3 (3%)
31	CHL	8	601	15	60,74,74	1.97	10 (16%)	58,114,114	1.10	4 (6%)
22	CLA	1	610	12	69,73,73	1.17	5 (7%)	82,113,113	0.80	3 (3%)
25	BCR	7	623	-	41,41,41	0.16	0	56,56,56	0.38	0
22	CLA	B	828	-	69,73,73	1.15	5 (7%)	82,113,113	0.80	3 (3%)
31	CHL	4	618	16	40,54,74	2.40	10 (25%)	34,90,114	1.36	5 (14%)
23	PQN	A	844	-	34,34,34	0.32	0	43,45,45	0.44	0
22	CLA	6	622	34	59,63,73	1.29	4 (6%)	70,101,113	0.88	2 (2%)
22	CLA	B	838	-	54,58,73	1.36	4 (7%)	64,95,113	0.92	2 (3%)
22	CLA	6	604	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
25	BCR	8	619	-	41,41,41	0.15	0	56,56,56	0.32	0
22	CLA	8	603	-	69,73,73	1.21	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	A	832	-	59,63,73	1.25	5 (8%)	70,101,113	0.90	2 (2%)
25	BCR	B	846	-	41,41,41	0.13	0	56,56,56	0.35	0
22	CLA	B	817	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
27	LMU	Z	621	-	22,22,36	0.13	0	27,27,47	0.27	0
31	CHL	Z	606	34	40,54,74	2.36	10 (25%)	34,90,114	1.44	5 (14%)
31	CHL	92	606	-	36,50,74	2.52	10 (27%)	29,85,114	1.37	4 (13%)
29	LUT	Z	617	-	42,43,43	0.28	0	51,60,60	0.45	0
28	LMG	4	624	-	41,41,55	0.18	0	49,49,63	0.26	0
29	LUT	A	856	-	42,43,43	0.29	0	51,60,60	0.42	0
22	CLA	92	611	24	69,73,73	1.20	5 (7%)	82,113,113	0.82	2 (2%)
26	SF4	C	101	3	0,12,12	-	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B	819	34	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
22	CLA	3	609	13	65,69,73	1.20	5 (7%)	77,108,113	0.83	2 (2%)
24	LHG	5	623	22	36,36,48	0.26	0	39,42,54	0.29	0
22	CLA	B	805	-	69,73,73	1.14	5 (7%)	82,113,113	0.84	3 (3%)
29	LUT	5	620	-	42,43,43	0.27	0	51,60,60	0.49	0
25	BCR	I	172	-	41,41,41	0.20	0	56,56,56	0.37	0
25	BCR	B	848	-	41,41,41	0.13	0	56,56,56	0.47	0
27	LMU	1	623	-	24,24,36	0.13	0	29,29,47	0.26	0
22	CLA	5	613	17	60,64,73	1.26	5 (8%)	71,102,113	0.88	3 (4%)
22	CLA	B2	820	-	60,64,73	1.25	4 (6%)	71,102,113	0.89	3 (4%)
22	CLA	1	608	34	69,73,73	1.19	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	A	835	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	L2	204	-	49,53,73	1.39	4 (8%)	58,89,113	0.98	3 (5%)
22	CLA	B	821	-	69,73,73	1.21	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	B	810	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	B	834	-	64,68,73	1.23	5 (7%)	76,107,113	0.85	3 (3%)
22	CLA	5	601	17	69,73,73	1.18	4 (5%)	82,113,113	0.84	2 (2%)
25	BCR	A	852	-	41,41,41	0.13	0	56,56,56	0.38	0
22	CLA	A	805	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
22	CLA	B	806	2	69,73,73	1.18	5 (7%)	82,113,113	0.77	2 (2%)
22	CLA	A	815	-	59,63,73	1.28	5 (8%)	70,101,113	0.88	2 (2%)
25	BCR	A	851	-	41,41,41	0.15	0	56,56,56	0.33	0
25	BCR	G	205	-	41,41,41	0.15	0	56,56,56	0.31	0
22	CLA	8	604	34	64,68,73	1.24	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	Z	604	34	61,65,73	1.25	5 (8%)	72,103,113	0.88	3 (4%)
22	CLA	Z	602	12	64,68,73	1.24	5 (7%)	76,107,113	0.88	3 (3%)
22	CLA	3	614	-	49,53,73	1.40	5 (10%)	58,89,113	0.97	3 (5%)
22	CLA	7	602	14	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	3	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.80	2 (2%)
27	LMU	B	853	-	36,36,36	0.12	0	47,47,47	0.70	2 (4%)
24	LHG	1	620	22	38,38,48	0.28	0	41,44,54	0.31	0
29	LUT	F	305	-	42,43,43	0.39	0	51,60,60	0.88	2 (3%)
22	CLA	B	820	-	60,64,73	1.28	5 (8%)	71,102,113	0.86	2 (2%)
25	BCR	B	843	-	41,41,41	0.17	0	56,56,56	0.32	0
26	SF4	A	853	1,2	0,12,12	-	-	-	-	-
22	CLA	8	616	15	49,53,73	1.38	5 (10%)	58,89,113	0.97	3 (5%)
22	CLA	B	808	-	69,73,73	1.15	5 (7%)	82,113,113	0.81	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	604	34	59,63,73	1.29	5 (8%)	70,101,113	0.89	3 (4%)
27	LMU	1	622	-	19,19,36	0.13	0	24,24,47	0.30	0
22	CLA	6	609	18	59,63,73	1.26	5 (8%)	70,101,113	0.92	4 (5%)
22	CLA	92	603	19	49,53,73	1.40	5 (10%)	58,89,113	0.98	3 (5%)
29	LUT	3	621	-	42,43,43	0.31	0	51,60,60	0.40	0
22	CLA	1	609	12	69,73,73	1.17	5 (7%)	82,113,113	0.83	2 (2%)
25	BCR	B2	845	-	41,41,41	0.14	0	56,56,56	0.32	0
22	CLA	B2	807	-	59,63,73	1.28	4 (6%)	70,101,113	0.87	3 (4%)
28	LMG	J	104	-	35,35,55	0.19	0	43,43,63	0.20	0
22	CLA	A	831	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	92	604	19	54,58,73	1.34	4 (7%)	64,95,113	0.92	3 (4%)
22	CLA	8	609	15	49,53,73	1.42	5 (10%)	58,89,113	0.95	2 (3%)
22	CLA	B	811	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	2 (2%)
27	LMU	A	862	-	20,20,36	0.13	0	25,25,47	0.28	0
25	BCR	B2	848	-	14,14,41	0.38	0	20,20,56	0.32	0
27	LMU	A	865	-	24,24,36	0.12	0	29,29,47	0.46	0
31	CHL	1	607	34	40,54,74	2.42	10 (25%)	34,90,114	1.28	4 (11%)
22	CLA	A	808	-	54,58,73	1.32	5 (9%)	64,95,113	0.90	2 (3%)
24	LHG	3	623	-	46,46,48	0.24	0	49,52,54	0.28	0
22	CLA	3	607	13	59,63,73	1.28	5 (8%)	70,101,113	0.89	3 (4%)
22	CLA	B	840	-	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	J	101	9	59,63,73	1.29	4 (6%)	70,101,113	0.88	2 (2%)
22	CLA	9	613	19	69,73,73	1.17	5 (7%)	82,113,113	0.85	4 (4%)
25	BCR	3	719	-	41,41,41	0.12	0	56,56,56	0.41	0
24	LHG	6	619	22	48,48,48	0.23	0	51,54,54	0.24	0
22	CLA	3	613	13	64,68,73	1.23	5 (7%)	76,107,113	0.84	3 (3%)
28	LMG	8	626	-	32,32,55	0.20	0	40,40,63	0.19	0
22	CLA	K	203	34	64,68,73	1.24	4 (6%)	76,107,113	0.86	3 (3%)
22	CLA	B	818	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	814	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	612	17	49,53,73	1.38	4 (8%)	58,89,113	0.95	2 (3%)
22	CLA	G	203	-	64,68,73	1.23	4 (6%)	76,107,113	0.81	2 (2%)
22	CLA	3	604	34	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
27	LMU	8	624	-	24,24,36	0.13	0	29,29,47	0.27	0
28	LMG	3	722	-	44,44,55	0.20	0	46,46,63	0.26	0
22	CLA	B	832	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	1	611	24	65,69,73	1.22	5 (7%)	77,108,113	0.83	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	6	614	-	54,58,73	1.33	5 (9%)	64,95,113	0.93	3 (4%)
22	CLA	B	807	-	59,63,73	1.31	5 (8%)	70,101,113	0.88	3 (4%)
22	CLA	A	819	-	64,68,73	1.25	5 (7%)	76,107,113	0.87	2 (2%)
22	CLA	B2	839	-	49,53,73	1.42	4 (8%)	58,89,113	1.00	3 (5%)
22	CLA	B	831	-	59,63,73	1.26	5 (8%)	70,101,113	0.86	3 (4%)
25	BCR	L	201	-	41,41,41	0.18	0	56,56,56	0.35	0
22	CLA	6	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	9	610	19	64,68,73	1.22	5 (7%)	76,107,113	0.88	3 (3%)
25	BCR	5	622	-	41,41,41	0.16	0	56,56,56	0.32	0
22	CLA	9	609	19	55,59,73	1.32	5 (9%)	64,96,113	0.92	3 (4%)
22	CLA	6	602	18	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
27	LMU	7	628	-	22,22,36	0.14	0	27,27,47	0.32	0
22	CLA	Z	616	12	64,68,73	1.24	4 (6%)	76,107,113	0.86	3 (3%)
27	LMU	6	632	-	20,20,36	0.15	0	25,25,47	0.25	0
22	CLA	7	616	14	50,54,73	1.38	5 (10%)	59,90,113	0.94	3 (5%)
22	CLA	A	842	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	B	835	34	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
31	CHL	9	606	-	36,50,74	2.54	10 (27%)	29,85,114	1.42	4 (13%)
31	CHL	9	607	34	45,59,74	2.32	10 (22%)	40,96,114	1.22	4 (10%)
25	BCR	B	801	-	41,41,41	0.17	0	56,56,56	0.38	0
25	BCR	92	623	-	41,41,41	0.14	0	56,56,56	0.33	0
27	LMU	7	627	-	33,33,36	0.10	0	44,44,47	0.18	0
25	BCR	A	849	-	41,41,41	0.18	0	56,56,56	0.32	0
24	LHG	A	847	22	37,37,48	0.28	0	40,43,54	0.31	0
31	CHL	6	606	34	52,66,74	2.13	10 (19%)	48,104,114	1.18	5 (10%)
27	LMU	A	864	-	24,24,36	0.11	0	29,29,47	0.31	0
22	CLA	6	611	24	62,66,73	1.26	4 (6%)	73,104,113	0.86	2 (2%)
22	CLA	A	826	34	69,73,73	1.19	4 (5%)	82,113,113	0.81	2 (2%)
22	CLA	B2	810	-	69,73,73	1.18	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	5	621	34	50,54,73	1.42	4 (8%)	59,90,113	1.07	5 (8%)
32	XAT	Z	618	-	41,47,47	0.16	0	54,74,74	0.62	0
22	CLA	7	611	24	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	B2	811	-	58,62,73	1.32	4 (6%)	71,100,113	0.97	4 (5%)
21	CL0	A	801	-	58,73,73	1.50	6 (10%)	60,113,113	1.56	3 (5%)
25	BCR	3	620	-	41,41,41	0.21	0	56,56,56	0.36	0
29	LUT	92	617	-	42,43,43	0.21	0	51,60,60	0.40	0
28	LMG	B2	855	-	31,31,55	0.20	0	39,39,63	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	5	614	-	49,53,73	1.40	4 (8%)	58,89,113	0.96	3 (5%)
24	LHG	4	623	-	37,37,48	0.25	0	40,43,54	0.31	0
22	CLA	3	611	-	69,73,73	1.18	5 (7%)	82,113,113	0.82	3 (3%)
31	CHL	5	606	34	40,54,74	2.39	10 (25%)	34,90,114	1.39	5 (14%)
29	LUT	7	624	-	42,43,43	0.23	0	51,60,60	0.43	0
22	CLA	8	602	15	66,70,73	1.22	5 (7%)	78,109,113	0.85	2 (2%)
22	CLA	7	610	14	69,73,73	1.21	5 (7%)	82,113,113	0.85	3 (3%)
31	CHL	1	606	34	40,54,74	2.42	10 (25%)	34,90,114	1.39	5 (14%)
22	CLA	B2	815	-	61,65,73	1.24	4 (6%)	72,103,113	0.86	3 (4%)
22	CLA	B	822	-	63,67,73	1.22	5 (7%)	74,105,113	0.87	3 (4%)
22	CLA	B	830	-	49,53,73	1.36	5 (10%)	58,89,113	0.97	2 (3%)
22	CLA	4	610	16	64,68,73	1.22	4 (6%)	76,107,113	0.82	2 (2%)
22	CLA	L	203	-	69,73,73	1.17	5 (7%)	82,113,113	0.80	3 (3%)
22	CLA	4	603	16	69,73,73	1.18	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	92	612	19	69,73,73	1.15	4 (5%)	82,113,113	0.81	2 (2%)
22	CLA	Z	608	34	54,58,73	1.35	5 (9%)	64,95,113	0.94	4 (6%)
24	LHG	7	625	22	48,48,48	0.24	0	51,54,54	0.23	0
29	LUT	5	626	-	42,43,43	0.25	0	51,60,60	0.40	0
22	CLA	7	608	34	54,58,73	1.34	5 (9%)	64,95,113	0.90	2 (3%)
29	LUT	3	720	-	42,43,43	0.22	0	51,60,60	0.34	0
31	CHL	6	618	18	37,51,74	2.50	10 (27%)	30,86,114	1.49	5 (16%)
31	CHL	6	616	18	60,74,74	1.98	10 (16%)	58,114,114	1.09	6 (10%)
25	BCR	B	847	-	41,41,41	0.20	0	56,56,56	0.41	0
22	CLA	A	830	-	69,73,73	1.17	5 (7%)	82,113,113	0.81	2 (2%)
25	BCR	L	205	-	41,41,41	0.15	0	56,56,56	0.39	0
22	CLA	1	603	-	61,65,73	1.26	5 (8%)	72,103,113	0.87	2 (2%)
22	CLA	4	613	16	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
27	LMU	92	624	-	36,36,36	0.09	0	47,47,47	0.23	0
22	CLA	B2	809	20	56,60,73	1.33	4 (7%)	65,97,113	0.90	2 (3%)
29	LUT	1	619	-	42,43,43	0.21	0	51,60,60	0.41	0
22	CLA	8	614	-	61,65,73	1.26	5 (8%)	72,103,113	0.86	3 (4%)
22	CLA	B	824	34	69,73,73	1.21	4 (5%)	82,113,113	0.83	2 (2%)
22	CLA	1	604	34	54,58,73	1.34	5 (9%)	64,95,113	0.94	3 (4%)
22	CLA	B2	813	-	69,73,73	1.18	4 (5%)	82,113,113	0.82	3 (3%)
22	CLA	1	602	12	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	B	827	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	2 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	8	612	15	59,63,73	1.24	5 (8%)	70,101,113	0.86	2 (2%)
25	BCR	4	621	-	41,41,41	0.15	0	56,56,56	0.35	0
22	CLA	A	838	-	55,59,73	1.29	5 (9%)	64,96,113	0.93	2 (3%)
22	CLA	3	606	34	46,50,73	1.47	5 (10%)	53,85,113	1.00	2 (3%)
29	LUT	4	619	-	42,43,43	0.27	0	51,60,60	0.49	0
31	CHL	5	618	17	37,51,74	2.50	10 (27%)	30,86,114	1.49	5 (16%)
28	LMG	6	633	-	19,19,55	0.30	0	19,19,63	0.29	0
22	CLA	K	201	11	49,53,73	1.42	4 (8%)	58,89,113	0.98	1 (1%)
28	LMG	A	859	-	48,48,55	0.18	0	56,56,63	0.18	0
22	CLA	Z	609	12	69,73,73	1.21	4 (5%)	82,113,113	0.82	2 (2%)
22	CLA	B	814	-	64,68,73	1.20	5 (7%)	76,107,113	0.86	3 (3%)
22	CLA	K	206	11	49,53,73	1.40	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	A	824	-	49,53,73	1.39	5 (10%)	58,89,113	0.99	3 (5%)
32	XAT	4	620	-	41,47,47	0.13	0	54,74,74	0.69	0
22	CLA	7	609	14	49,53,73	1.43	5 (10%)	58,89,113	0.95	3 (5%)
22	CLA	4	602	16	64,68,73	1.24	5 (7%)	76,107,113	0.84	3 (3%)
27	LMU	6	631	-	24,24,36	0.13	0	29,29,47	0.27	0
22	CLA	Z	613	34	69,73,73	1.17	5 (7%)	82,113,113	0.85	3 (3%)
22	CLA	B2	808	-	49,53,73	1.39	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	7	613	14	69,73,73	1.18	5 (7%)	82,113,113	0.84	2 (2%)
31	CHL	Z	607	34	60,74,74	1.98	10 (16%)	58,114,114	1.09	6 (10%)
22	CLA	B	839	34	69,73,73	1.19	5 (7%)	82,113,113	0.84	2 (2%)
22	CLA	B	815	-	69,73,73	1.17	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	92	610	19	64,68,73	1.23	5 (7%)	76,107,113	0.87	3 (3%)
22	CLA	A	811	-	69,73,73	1.15	5 (7%)	82,113,113	0.82	3 (3%)
31	CHL	7	607	34	40,54,74	2.40	10 (25%)	34,90,114	1.43	5 (14%)
32	XAT	7	622	-	41,47,47	0.15	0	54,74,74	0.62	1 (1%)
22	CLA	5	617	-	69,73,73	1.17	4 (5%)	82,113,113	0.81	3 (3%)
22	CLA	B	825	34	69,73,73	1.16	5 (7%)	82,113,113	0.79	2 (2%)
27	LMU	1	625	-	24,24,36	0.11	0	29,29,47	0.31	0
31	CHL	7	601	14	60,74,74	1.99	10 (16%)	58,114,114	1.05	5 (8%)
22	CLA	A	833	-	69,73,73	1.20	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	602	17	69,73,73	1.18	4 (5%)	82,113,113	0.82	2 (2%)
24	LHG	Z	620	22	38,38,48	0.26	0	41,44,54	0.30	0
22	CLA	9	602	19	64,68,73	1.23	5 (7%)	76,107,113	0.85	3 (3%)
22	CLA	5	616	17	57,61,73	1.29	5 (8%)	67,98,113	0.90	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	A	812	-	69,73,73	1.15	5 (7%)	82,113,113	0.79	3 (3%)
25	BCR	6	623	-	41,41,41	0.18	0	56,56,56	0.34	0
24	LHG	3	721	-	30,30,48	0.26	0	33,36,54	0.36	0
28	LMG	B	854	-	36,36,55	0.19	0	44,44,63	0.17	0
28	LMG	J	103	-	42,42,55	0.18	0	50,50,63	0.39	0
22	CLA	B	803	-	69,73,73	1.19	4 (5%)	82,113,113	0.78	2 (2%)
29	LUT	3	622	-	42,43,43	0.31	0	51,60,60	0.49	0
22	CLA	A	836	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	7	620	34	57,61,73	1.29	4 (7%)	67,98,113	0.90	2 (2%)
22	CLA	9	611	24	69,73,73	1.19	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	5	609	17	69,73,73	1.16	5 (7%)	82,113,113	0.80	3 (3%)
27	LMU	5	627	-	24,24,36	0.11	0	29,29,47	0.25	0
27	LMU	6	628	-	24,24,36	0.12	0	29,29,47	0.30	0
27	LMU	7	629	-	28,28,36	0.10	0	39,39,47	0.27	0
22	CLA	5	611	24	59,63,73	1.26	5 (8%)	70,101,113	0.88	3 (4%)
27	LMU	A	863	-	36,36,36	0.09	0	47,47,47	0.27	0
33	NEX	6	625	-	40,46,46	0.30	0	50,70,70	0.86	4 (8%)
22	CLA	A	845	24	49,53,73	1.39	4 (8%)	58,89,113	0.94	2 (3%)
22	CLA	7	612	14	56,60,73	1.29	5 (8%)	65,97,113	0.89	2 (3%)
29	LUT	7	621	-	42,43,43	0.27	0	51,60,60	0.39	0
27	LMU	9	624	-	24,24,36	0.13	0	29,29,47	0.28	0
32	XAT	8	618	-	41,47,47	0.17	0	54,74,74	0.61	0
22	CLA	A	829	-	69,73,73	1.22	5 (7%)	82,113,113	0.82	3 (3%)
25	BCR	L2	201	-	41,41,41	0.14	0	56,56,56	0.36	0
27	LMU	A	858	-	36,36,36	0.09	0	47,47,47	0.19	0
31	CHL	5	608	34	45,59,74	2.29	10 (22%)	40,96,114	1.33	6 (15%)
27	LMU	4	626	-	20,20,36	0.15	0	25,25,47	0.28	0
27	LMU	1	627	-	22,22,36	0.13	0	27,27,47	0.30	0
27	LMU	A	857	-	35,35,36	0.09	0	46,46,47	0.18	0
25	BCR	J	102	-	41,41,41	0.15	0	56,56,56	0.31	0
22	CLA	5	610	17	64,68,73	1.20	4 (6%)	76,107,113	0.83	2 (2%)
22	CLA	A	839	-	69,73,73	1.17	5 (7%)	82,113,113	0.83	4 (4%)
22	CLA	A	804	-	69,73,73	1.17	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	B	816	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	A	840	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	A	813	-	69,73,73	1.17	5 (7%)	82,113,113	0.86	3 (3%)
22	CLA	Z	612	12	49,53,73	1.36	4 (8%)	58,89,113	0.95	2 (3%)
22	CLA	1	612	12	49,53,73	1.39	4 (8%)	58,89,113	0.97	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	CLA	B2	804	-	49,53,73	1.37	4 (8%)	58,89,113	0.97	3 (5%)
22	CLA	3	602	13	64,68,73	1.22	5 (7%)	76,107,113	0.84	3 (3%)
24	LHG	4	622	22	48,48,48	0.23	0	51,54,54	0.28	0
22	CLA	8	613	15	69,73,73	1.17	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	1	616	12	50,54,73	1.41	5 (10%)	59,90,113	0.97	3 (5%)
22	CLA	B2	806	20	69,73,73	1.16	4 (5%)	82,113,113	0.81	2 (2%)
31	CHL	6	608	34	45,59,74	2.29	10 (22%)	40,96,114	1.29	6 (15%)
22	CLA	9	614	-	49,53,73	1.43	4 (8%)	58,89,113	0.96	3 (5%)
22	CLA	3	615	34	69,73,73	1.20	4 (5%)	82,113,113	0.84	3 (3%)
28	LMG	9	620	22	44,44,55	0.17	0	52,52,63	0.37	0
31	CHL	3	608	34	60,74,74	2.00	10 (16%)	58,114,114	1.12	5 (8%)
22	CLA	A	806	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	3 (3%)
22	CLA	B	833	-	62,66,73	1.22	5 (8%)	73,104,113	0.89	3 (4%)
28	LMG	B	852	-	43,43,55	0.17	0	51,51,63	0.23	0
22	CLA	4	612	16	49,53,73	1.39	4 (8%)	58,89,113	0.96	2 (3%)
31	CHL	4	601	16	60,74,74	1.97	10 (16%)	58,114,114	1.12	5 (8%)
22	CLA	5	603	-	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
25	BCR	B2	844	-	41,41,41	0.14	0	56,56,56	0.30	0
22	CLA	9	603	19,28	59,63,73	1.26	5 (8%)	70,101,113	0.90	4 (5%)
22	CLA	A	821	-	59,63,73	1.28	5 (8%)	70,101,113	0.85	2 (2%)
27	LMU	4	625	-	34,34,36	0.10	0	45,45,47	0.19	0
22	CLA	92	614	-	49,53,73	1.41	4 (8%)	58,89,113	0.98	3 (5%)
22	CLA	4	614	-	59,63,73	1.29	4 (6%)	70,101,113	0.87	2 (2%)
22	CLA	L	204	-	49,53,73	1.40	4 (8%)	58,89,113	0.99	3 (5%)
22	CLA	B	802	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	B	837	-	69,73,73	1.19	5 (7%)	82,113,113	0.82	2 (2%)
22	CLA	A	810	1	69,73,73	1.20	4 (5%)	82,113,113	0.85	2 (2%)
32	XAT	6	624	-	41,47,47	0.14	0	54,74,74	0.65	0
22	CLA	Z	610	12	64,68,73	1.22	5 (7%)	76,107,113	0.84	3 (3%)
22	CLA	92	609	19	49,53,73	1.40	4 (8%)	58,89,113	0.99	2 (3%)
22	CLA	F	304	6	69,73,73	1.17	4 (5%)	82,113,113	0.90	4 (4%)
22	CLA	6	617	-	49,53,73	1.42	4 (8%)	58,89,113	0.96	3 (5%)
29	LUT	9	616	-	42,43,43	0.28	0	51,60,60	0.39	0
24	LHG	B	851	22	44,44,48	0.26	0	47,50,54	0.32	0
22	CLA	Z	614	-	54,58,73	1.32	5 (9%)	64,95,113	0.93	3 (4%)
22	CLA	4	604	34	54,58,73	1.33	5 (9%)	64,95,113	0.93	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CHL	Z	601	12	60,74,74	1.96	10 (16%)	58,114,114	1.10	5 (8%)
31	CHL	6	607	34	60,74,74	1.95	10 (16%)	58,114,114	1.10	5 (8%)
22	CLA	92	613	19	64,68,73	1.21	4 (6%)	76,107,113	0.86	3 (3%)
22	CLA	G	204	7	50,54,73	1.38	4 (8%)	59,90,113	0.96	3 (5%)
22	CLA	A	809	1	69,73,73	1.15	5 (7%)	82,113,113	0.89	4 (4%)
22	CLA	A	802	-	69,73,73	1.16	5 (7%)	82,113,113	0.77	2 (2%)
22	CLA	F	301	34	69,73,73	1.14	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	837	1	61,65,73	1.31	4 (6%)	72,103,113	0.90	3 (4%)
22	CLA	7	604	34	55,59,73	1.29	5 (9%)	64,96,113	0.92	3 (4%)
27	LMU	G	206	-	24,24,36	0.13	0	29,29,47	0.24	0
31	CHL	92	607	-	40,54,74	2.38	10 (25%)	34,90,114	1.33	5 (14%)
22	CLA	B2	829	-	69,73,73	1.17	4 (5%)	82,113,113	0.82	3 (3%)
27	LMU	8	628	-	24,24,36	0.15	0	29,29,47	0.33	0
28	LMG	B2	852	-	43,43,55	0.17	0	51,51,63	0.18	0
22	CLA	A	803	34	69,73,73	1.25	5 (7%)	82,113,113	0.85	4 (4%)
29	LUT	92	616	-	42,43,43	0.26	0	51,60,60	0.34	0
22	CLA	Z	603	-	59,63,73	1.29	5 (8%)	70,101,113	0.86	2 (2%)
22	CLA	3	612	13	50,54,73	1.37	5 (10%)	59,90,113	0.94	3 (5%)
25	BCR	L2	205	-	41,41,41	0.15	0	56,56,56	0.35	0
28	LMG	1	624	-	36,36,55	0.19	0	44,44,63	0.18	0
22	CLA	B	812	-	69,73,73	1.19	5 (7%)	82,113,113	0.83	2 (2%)
22	CLA	B2	812	-	64,68,73	1.19	4 (6%)	76,107,113	0.86	3 (3%)
25	BCR	B	845	-	41,41,41	0.14	0	56,56,56	0.37	0
24	LHG	92	622	22	28,28,48	0.29	0	31,34,54	0.31	0
22	CLA	A	825	-	59,63,73	1.30	5 (8%)	70,101,113	0.89	2 (2%)
22	CLA	A	841	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
27	LMU	8	627	-	36,36,36	0.10	0	47,47,47	0.38	0
22	CLA	B	823	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	3 (3%)
25	BCR	3	718	-	41,41,41	0.17	0	56,56,56	0.35	0
27	LMU	1	621	-	36,36,36	0.10	0	47,47,47	0.29	0
22	CLA	92	601	19	49,53,73	1.38	4 (8%)	58,89,113	0.94	2 (3%)
27	LMU	1	626	-	24,24,36	0.12	0	29,29,47	0.27	0
25	BCR	9	623	-	41,41,41	0.13	0	56,56,56	0.35	0
22	CLA	3	610	13	69,73,73	1.18	5 (7%)	82,113,113	0.83	3 (3%)
29	LUT	Z	619	-	26,26,43	0.38	0	33,35,60	0.38	0
22	CLA	A	828	-	69,73,73	1.18	5 (7%)	82,113,113	0.77	2 (2%)
32	XAT	5	624	-	41,47,47	0.13	0	54,74,74	0.66	0
22	CLA	F	303	34	49,53,73	1.40	5 (10%)	58,89,113	0.98	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CHL	4	608	-	60,74,74	1.99	10 (16%)	58,114,114	1.06	5 (8%)
22	CLA	B	804	-	49,53,73	1.41	4 (8%)	58,89,113	0.94	2 (3%)
22	CLA	A	834	-	69,73,73	1.19	5 (7%)	82,113,113	0.84	3 (3%)
24	LHG	8	620	22	43,43,48	0.27	0	46,49,54	0.27	0
22	CLA	A	818	-	69,73,73	1.16	5 (7%)	82,113,113	0.82	3 (3%)
22	CLA	A	816	-	69,73,73	1.16	4 (5%)	82,113,113	0.83	3 (3%)
22	CLA	A	817	34	59,63,73	1.29	5 (8%)	70,101,113	0.88	2 (2%)
22	CLA	B	813	-	69,73,73	1.16	5 (7%)	82,113,113	0.81	2 (2%)
22	CLA	A	807	1	69,73,73	1.19	5 (7%)	82,113,113	0.78	2 (2%)
29	LUT	9	617	-	42,43,43	0.21	0	51,60,60	0.41	0
27	LMU	A	861	-	24,24,36	0.12	0	29,29,47	0.30	0
31	CHL	5	607	34	60,74,74	2.01	10 (16%)	58,114,114	0.99	4 (6%)
22	CLA	8	610	15	69,73,73	1.16	4 (5%)	82,113,113	0.80	2 (2%)
22	CLA	6	612	18	49,53,73	1.38	4 (8%)	58,89,113	0.97	2 (3%)
22	CLA	B	829	-	69,73,73	1.15	5 (7%)	82,113,113	0.83	2 (2%)
27	LMU	6	630	-	24,24,36	0.14	0	29,29,47	0.28	0
22	CLA	B	809	2	69,73,73	1.19	5 (7%)	82,113,113	0.79	2 (2%)
22	CLA	B	836	-	64,68,73	1.21	5 (7%)	76,107,113	0.87	3 (3%)
23	PQN	B	842	-	34,34,34	0.32	0	43,45,45	0.44	0
31	CHL	6	601	18	60,74,74	1.98	10 (16%)	58,114,114	1.00	4 (6%)
22	CLA	B	826	-	69,73,73	1.16	5 (7%)	82,113,113	0.83	3 (3%)
29	LUT	8	617	-	42,43,43	0.31	0	51,60,60	0.45	0
24	LHG	A	846	-	48,48,48	0.24	0	51,54,54	0.30	0
25	BCR	A	848	-	41,41,41	0.15	0	56,56,56	0.30	0
22	CLA	1	614	-	64,68,73	1.22	5 (7%)	76,107,113	0.87	3 (3%)

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
22	CLA	92	602	19	1/1/20/20	7/39/115/115	-
28	LMG	1	628	-	-	5/37/57/70	0/1/1/1
30	DGD	B	850	-	-	10/48/88/95	0/2/2/2
22	CLA	K	204	-	1/1/15/20	4/17/93/115	-
22	CLA	L2	203	-	1/1/15/20	4/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CHL	8	607	34	3/3/26/26	8/39/137/137	-
27	LMU	K	208	-	-	3/15/35/61	0/1/1/2
22	CLA	B2	814	-	1/1/19/20	3/33/109/115	-
22	CLA	A	854	34	1/1/20/20	1/39/115/115	-
24	LHG	6	629	-	-	10/40/40/53	-
22	CLA	A	823	-	1/1/20/20	6/39/115/115	-
28	LMG	A	860	-	-	6/31/51/70	0/1/1/1
29	LUT	1	617	-	-	2/29/67/67	0/2/2/2
31	CHL	4	606	34	3/3/24/26	1/27/125/137	-
25	BCR	K	202	-	-	2/29/63/63	0/2/2/2
25	BCR	B	844	-	-	0/29/63/63	0/2/2/2
29	LUT	6	621	-	-	2/29/67/67	0/2/2/2
31	CHL	8	606	34	3/3/26/26	2/39/137/137	-
22	CLA	B2	805	-	1/1/20/20	2/39/115/115	-
22	CLA	4	611	24	1/1/19/20	5/33/109/115	-
22	CLA	8	611	24	1/1/15/20	2/15/91/115	-
22	CLA	Z	611	24	1/1/19/20	5/33/109/115	-
28	LMG	7	626	-	-	8/32/52/70	0/1/1/1
28	LMG	8	629	-	-	9/37/57/70	0/1/1/1
22	CLA	B2	828	-	1/1/20/20	6/39/115/115	-
22	CLA	8	608	34	1/1/17/20	2/21/97/115	-
26	SF4	C	102	3	-	-	0/6/5/5
27	LMU	Z	622	-	-	3/17/57/61	0/2/2/2
22	CLA	7	614	-	1/1/14/20	5/13/89/115	-
24	LHG	9	622	22	-	12/45/45/53	-
22	CLA	9	612	19	1/1/20/20	5/39/115/115	-
22	CLA	A	822	34	1/1/20/20	0/39/115/115	-
22	CLA	4	616	16	1/1/15/20	0/15/91/115	-
22	CLA	6	613	34	1/1/20/20	4/39/115/115	-
22	CLA	9	601	19	1/1/15/20	2/17/93/115	-
25	BCR	I2	172	-	-	0/29/63/63	0/2/2/2
22	CLA	1	613	34	1/1/20/20	5/39/115/115	-
22	CLA	7	603	-	1/1/17/20	4/24/100/115	-
25	BCR	B2	843	-	-	0/13/30/63	0/1/1/2
25	BCR	K	207	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	3	617	13	1/1/15/20	2/17/93/115	-
22	CLA	4	609	16	1/1/19/20	6/33/109/115	-
22	CLA	B	841	24	1/1/20/20	8/39/115/115	-
33	NEX	5	625	-	-	2/27/83/83	1/3/3/3
31	CHL	1	601	12	3/3/26/26	8/39/137/137	-
31	CHL	7	606	34	3/3/21/26	2/15/113/137	-
25	BCR	A	850	-	-	0/29/63/63	0/2/2/2
22	CLA	A	820	-	1/1/20/20	6/39/115/115	-
22	CLA	A	843	34	1/1/20/20	7/39/115/115	-
27	LMU	8	625	-	-	2/15/35/61	0/1/1/2
32	XAT	1	618	-	1/1/26/26	0/31/93/93	0/4/4/4
31	CHL	4	607	34	3/3/26/26	1/39/137/137	-
22	CLA	9	604	19	1/1/17/20	0/25/101/115	-
22	CLA	A	827	34	1/1/20/20	2/39/115/115	-
22	CLA	6	610	18	1/1/19/20	0/33/109/115	-
31	CHL	8	601	15	3/3/26/26	7/39/137/137	-
22	CLA	1	610	12	1/1/20/20	2/39/115/115	-
25	BCR	7	623	-	-	2/29/63/63	0/2/2/2
22	CLA	B	828	-	1/1/20/20	4/39/115/115	-
31	CHL	4	618	16	3/3/21/26	0/15/113/137	-
23	PQN	A	844	-	-	3/23/43/43	0/2/2/2
22	CLA	6	622	34	1/1/18/20	2/27/103/115	-
22	CLA	B	838	-	1/1/17/20	1/21/97/115	-
22	CLA	6	604	-	1/1/20/20	2/39/115/115	-
25	BCR	8	619	-	-	4/29/63/63	0/2/2/2
22	CLA	8	603	-	1/1/20/20	5/39/115/115	-
22	CLA	A	832	-	1/1/18/20	0/27/103/115	-
25	BCR	B	846	-	-	2/29/63/63	0/2/2/2
22	CLA	B	817	-	1/1/20/20	8/39/115/115	-
27	LMU	Z	621	-	-	2/13/33/61	0/1/1/2
31	CHL	Z	606	34	3/3/21/26	5/15/113/137	-
31	CHL	92	606	-	3/3/20/26	0/10/108/137	-
29	LUT	Z	617	-	-	2/29/67/67	0/2/2/2
28	LMG	4	624	-	-	6/36/56/70	0/1/1/1
29	LUT	A	856	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	92	611	24	1/1/20/20	4/39/115/115	-
26	SF4	C	101	3	-	-	0/6/5/5
22	CLA	B	819	34	1/1/19/20	5/33/109/115	-
22	CLA	3	609	13	1/1/19/20	2/35/111/115	-
24	LHG	5	623	22	-	11/41/41/53	-
22	CLA	B	805	-	1/1/20/20	8/39/115/115	-
29	LUT	5	620	-	-	2/29/67/67	0/2/2/2
25	BCR	I	172	-	-	0/29/63/63	0/2/2/2
25	BCR	B	848	-	-	2/29/63/63	0/2/2/2
27	LMU	1	623	-	-	1/15/35/61	0/1/1/2
22	CLA	5	613	17	1/1/18/20	4/29/105/115	-
22	CLA	B2	820	-	1/1/18/20	7/29/105/115	-
22	CLA	1	608	34	1/1/20/20	2/39/115/115	-
22	CLA	A	835	-	1/1/20/20	6/39/115/115	-
22	CLA	L2	204	-	1/1/15/20	6/15/91/115	-
22	CLA	B	821	-	1/1/20/20	5/39/115/115	-
22	CLA	B	810	-	1/1/20/20	2/39/115/115	-
22	CLA	B	834	-	1/1/19/20	8/33/109/115	-
22	CLA	5	601	17	1/1/20/20	5/39/115/115	-
25	BCR	A	852	-	-	4/29/63/63	0/2/2/2
22	CLA	A	805	-	1/1/18/20	1/27/103/115	-
22	CLA	B	806	2	1/1/20/20	2/39/115/115	-
22	CLA	A	815	-	1/1/18/20	2/27/103/115	-
25	BCR	A	851	-	-	2/29/63/63	0/2/2/2
25	BCR	G	205	-	-	1/29/63/63	0/2/2/2
22	CLA	8	604	34	1/1/19/20	2/33/109/115	-
22	CLA	Z	604	34	1/1/18/20	2/30/106/115	-
22	CLA	Z	602	12	1/1/19/20	2/33/109/115	-
22	CLA	3	614	-	1/1/15/20	2/15/91/115	-
22	CLA	7	602	14	1/1/20/20	2/39/115/115	-
22	CLA	3	603	-	1/1/20/20	5/39/115/115	-
27	LMU	B	853	-	-	7/21/61/61	0/2/2/2
24	LHG	1	620	22	-	7/43/43/53	-
29	LUT	F	305	-	-	5/29/67/67	0/2/2/2
22	CLA	B	820	-	1/1/18/20	5/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	BCR	B	843	-	-	0/29/63/63	0/2/2/2
26	SF4	A	853	1,2	-	-	0/6/5/5
22	CLA	8	616	15	1/1/15/20	0/15/91/115	-
22	CLA	B	808	-	1/1/20/20	9/39/115/115	-
22	CLA	5	604	34	1/1/18/20	5/27/103/115	-
27	LMU	1	622	-	-	4/10/30/61	0/1/1/2
22	CLA	6	609	18	1/1/18/20	4/27/103/115	-
22	CLA	92	603	19	1/1/15/20	4/15/91/115	-
29	LUT	3	621	-	-	2/29/67/67	0/2/2/2
22	CLA	1	609	12	1/1/20/20	5/39/115/115	-
25	BCR	B2	845	-	-	4/29/63/63	0/2/2/2
22	CLA	B2	807	-	1/1/18/20	2/27/103/115	-
28	LMG	J	104	-	-	8/30/50/70	0/1/1/1
22	CLA	A	831	-	1/1/20/20	2/39/115/115	-
22	CLA	92	604	19	1/1/17/20	4/21/97/115	-
22	CLA	8	609	15	1/1/15/20	0/15/91/115	-
22	CLA	B	811	-	1/1/20/20	7/39/115/115	-
31	CHL	1	607	34	3/3/21/26	2/15/113/137	-
25	BCR	B2	848	-	-	2/5/22/63	0/1/1/2
27	LMU	A	862	-	-	2/11/31/61	0/1/1/2
27	LMU	A	865	-	-	3/15/35/61	0/1/1/2
22	CLA	A	808	-	1/1/17/20	0/21/97/115	-
24	LHG	3	623	-	-	12/51/51/53	-
22	CLA	3	607	13	1/1/18/20	5/27/103/115	-
22	CLA	B	840	-	1/1/20/20	7/39/115/115	-
22	CLA	J	101	9	1/1/18/20	3/27/103/115	-
22	CLA	9	613	19	1/1/20/20	4/39/115/115	-
25	BCR	3	719	-	-	2/29/63/63	0/2/2/2
24	LHG	6	619	22	-	6/53/53/53	-
22	CLA	3	613	13	1/1/19/20	5/33/109/115	-
28	LMG	8	626	-	-	6/27/47/70	0/1/1/1
22	CLA	K	203	34	1/1/19/20	1/33/109/115	-
22	CLA	B	818	-	1/1/20/20	4/39/115/115	-
22	CLA	A	814	-	1/1/20/20	5/39/115/115	-
22	CLA	5	612	17	1/1/15/20	5/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	G	203	-	1/1/19/20	2/33/109/115	-
22	CLA	3	604	34	1/1/20/20	1/39/115/115	-
27	LMU	8	624	-	-	1/15/35/61	0/1/1/2
28	LMG	3	722	-	-	5/46/46/70	-
22	CLA	B	832	-	1/1/20/20	5/39/115/115	-
22	CLA	1	611	24	1/1/19/20	4/35/111/115	-
22	CLA	6	614	-	1/1/17/20	2/21/97/115	-
22	CLA	B	807	-	1/1/18/20	3/27/103/115	-
22	CLA	A	819	-	1/1/19/20	3/33/109/115	-
22	CLA	B2	839	-	1/1/15/20	5/15/91/115	-
22	CLA	B	831	-	1/1/18/20	1/27/103/115	-
25	BCR	L	201	-	-	4/29/63/63	0/2/2/2
22	CLA	6	603	-	1/1/20/20	7/39/115/115	-
22	CLA	9	610	19	1/1/19/20	0/33/109/115	-
25	BCR	5	622	-	-	2/29/63/63	0/2/2/2
22	CLA	9	609	19	1/1/17/20	4/23/99/115	-
22	CLA	6	602	18	1/1/20/20	2/39/115/115	-
27	LMU	7	628	-	-	3/13/33/61	0/1/1/2
22	CLA	Z	616	12	1/1/19/20	4/33/109/115	-
27	LMU	6	632	-	-	3/11/31/61	0/1/1/2
22	CLA	7	616	14	1/1/15/20	3/17/93/115	-
22	CLA	A	842	-	1/1/20/20	3/39/115/115	-
22	CLA	B	835	34	1/1/15/20	2/15/91/115	-
31	CHL	9	606	-	3/3/20/26	0/10/108/137	-
31	CHL	9	607	34	3/3/23/26	1/21/119/137	-
25	BCR	B	801	-	-	0/29/63/63	0/2/2/2
25	BCR	92	623	-	-	4/29/63/63	0/2/2/2
27	LMU	7	627	-	-	2/18/58/61	0/2/2/2
25	BCR	A	849	-	-	0/29/63/63	0/2/2/2
24	LHG	A	847	22	-	4/42/42/53	-
31	CHL	6	606	34	3/3/24/26	2/30/128/137	-
27	LMU	A	864	-	-	2/15/35/61	0/1/1/2
22	CLA	6	611	24	1/1/18/20	4/31/107/115	-
22	CLA	A	826	34	1/1/20/20	7/39/115/115	-
22	CLA	B2	810	-	1/1/20/20	4/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	621	34	1/1/15/20	11/17/93/115	-
32	XAT	Z	618	-	-	0/31/93/93	0/4/4/4
22	CLA	7	611	24	1/1/20/20	7/39/115/115	-
22	CLA	B2	811	-	1/1/17/20	2/25/101/115	-
21	CL0	A	801	-	3/3/25/25	3/37/135/135	-
25	BCR	3	620	-	-	4/29/63/63	0/2/2/2
29	LUT	92	617	-	-	0/29/67/67	0/2/2/2
28	LMG	B2	855	-	-	2/26/46/70	0/1/1/1
22	CLA	5	614	-	1/1/15/20	4/15/91/115	-
24	LHG	4	623	-	-	15/42/42/53	-
22	CLA	3	611	-	1/1/20/20	6/39/115/115	-
31	CHL	5	606	34	3/3/21/26	2/15/113/137	-
29	LUT	7	624	-	-	4/29/67/67	0/2/2/2
22	CLA	8	602	15	1/1/19/20	3/36/112/115	-
22	CLA	7	610	14	1/1/20/20	7/39/115/115	-
31	CHL	1	606	34	3/3/21/26	0/15/113/137	-
22	CLA	B2	815	-	1/1/18/20	4/30/106/115	-
22	CLA	B	822	-	1/1/18/20	3/32/108/115	-
22	CLA	B	830	-	1/1/15/20	0/15/91/115	-
22	CLA	4	610	16	1/1/19/20	3/33/109/115	-
22	CLA	L	203	-	1/1/20/20	6/39/115/115	-
22	CLA	4	603	16	1/1/20/20	7/39/115/115	-
22	CLA	92	612	19	1/1/20/20	7/39/115/115	-
22	CLA	Z	608	34	1/1/17/20	2/21/97/115	-
24	LHG	7	625	22	-	13/53/53/53	-
29	LUT	5	626	-	-	4/29/67/67	0/2/2/2
22	CLA	7	608	34	1/1/17/20	0/21/97/115	-
29	LUT	3	720	-	-	0/29/67/67	0/2/2/2
31	CHL	6	618	18	3/3/20/26	2/12/110/137	-
31	CHL	6	616	18	3/3/26/26	3/39/137/137	-
25	BCR	B	847	-	-	2/29/63/63	0/2/2/2
22	CLA	A	830	-	1/1/20/20	4/39/115/115	-
25	BCR	L	205	-	-	2/29/63/63	0/2/2/2
22	CLA	1	603	-	1/1/18/20	6/30/106/115	-
22	CLA	4	613	16	1/1/20/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	92	624	-	-	1/21/61/61	0/2/2/2
22	CLA	B2	809	20	1/1/17/20	2/24/100/115	-
29	LUT	1	619	-	-	2/29/67/67	0/2/2/2
22	CLA	8	614	-	1/1/18/20	7/30/106/115	-
22	CLA	B	824	34	1/1/20/20	3/39/115/115	-
22	CLA	1	604	34	1/1/17/20	0/21/97/115	-
22	CLA	B2	813	-	1/1/20/20	3/39/115/115	-
22	CLA	1	602	12	1/1/19/20	2/33/109/115	-
22	CLA	B	827	-	1/1/20/20	5/39/115/115	-
22	CLA	8	612	15	1/1/18/20	4/27/103/115	-
25	BCR	4	621	-	-	2/29/63/63	0/2/2/2
22	CLA	A	838	-	1/1/17/20	0/23/99/115	-
22	CLA	3	606	34	1/1/14/20	0/12/88/115	-
29	LUT	4	619	-	-	1/29/67/67	0/2/2/2
31	CHL	5	618	17	3/3/20/26	2/12/110/137	-
28	LMG	6	633	-	-	1/17/17/70	-
22	CLA	K	201	11	1/1/15/20	2/15/91/115	-
28	LMG	A	859	-	-	9/43/63/70	0/1/1/1
22	CLA	Z	609	12	1/1/20/20	8/39/115/115	-
22	CLA	B	814	-	1/1/19/20	3/33/109/115	-
22	CLA	K	206	11	1/1/15/20	4/15/91/115	-
22	CLA	A	824	-	1/1/15/20	4/15/91/115	-
32	XAT	4	620	-	-	0/31/93/93	0/4/4/4
22	CLA	7	609	14	1/1/15/20	1/15/91/115	-
22	CLA	4	602	16	1/1/19/20	2/33/109/115	-
27	LMU	6	631	-	-	4/15/35/61	0/1/1/2
22	CLA	Z	613	34	1/1/20/20	2/39/115/115	-
22	CLA	B2	808	-	1/1/15/20	4/15/91/115	-
22	CLA	7	613	14	1/1/20/20	0/39/115/115	-
31	CHL	Z	607	34	3/3/26/26	4/39/137/137	-
22	CLA	B	839	34	1/1/20/20	5/39/115/115	-
22	CLA	B	815	-	1/1/20/20	4/39/115/115	-
22	CLA	92	610	19	1/1/19/20	0/33/109/115	-
22	CLA	A	811	-	1/1/20/20	4/39/115/115	-
31	CHL	7	607	34	3/3/21/26	0/15/113/137	-
32	XAT	7	622	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	5	617	-	1/1/20/20	5/39/115/115	-
22	CLA	B	825	34	1/1/20/20	2/39/115/115	-
27	LMU	1	625	-	-	5/15/35/61	0/1/1/2
31	CHL	7	601	14	3/3/26/26	4/39/137/137	-
22	CLA	A	833	-	1/1/20/20	1/39/115/115	-
22	CLA	5	602	17	1/1/20/20	1/39/115/115	-
24	LHG	Z	620	22	-	6/43/43/53	-
22	CLA	9	602	19	1/1/19/20	2/33/109/115	-
22	CLA	5	616	17	1/1/17/20	6/25/101/115	-
22	CLA	A	812	-	1/1/20/20	7/39/115/115	-
25	BCR	6	623	-	-	2/29/63/63	0/2/2/2
24	LHG	3	721	-	-	12/35/35/53	-
28	LMG	B	854	-	-	2/31/51/70	0/1/1/1
28	LMG	J	103	-	-	3/37/57/70	0/1/1/1
22	CLA	B	803	-	1/1/20/20	3/39/115/115	-
29	LUT	3	622	-	-	2/29/67/67	0/2/2/2
22	CLA	A	836	-	1/1/20/20	5/39/115/115	-
22	CLA	7	620	34	1/1/17/20	6/25/101/115	-
22	CLA	9	611	24	1/1/20/20	6/39/115/115	-
22	CLA	5	609	17	1/1/20/20	3/39/115/115	-
27	LMU	5	627	-	-	1/15/35/61	0/1/1/2
27	LMU	6	628	-	-	2/15/35/61	0/1/1/2
27	LMU	7	629	-	-	4/13/53/61	0/2/2/2
22	CLA	5	611	24	1/1/18/20	4/27/103/115	-
27	LMU	A	863	-	-	7/21/61/61	0/2/2/2
33	NEX	6	625	-	1/1/25/25	4/27/83/83	0/3/3/3
22	CLA	A	845	24	1/1/15/20	2/15/91/115	-
22	CLA	7	612	14	1/1/17/20	3/24/100/115	-
29	LUT	7	621	-	-	2/29/67/67	0/2/2/2
27	LMU	9	624	-	-	4/15/35/61	0/1/1/2
32	XAT	8	618	-	-	0/31/93/93	0/4/4/4
22	CLA	A	829	-	1/1/20/20	8/39/115/115	-
25	BCR	L2	201	-	-	4/29/63/63	0/2/2/2
27	LMU	A	858	-	-	6/21/61/61	0/2/2/2
31	CHL	5	608	34	3/3/23/26	0/21/119/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	LMU	4	626	-	-	0/11/31/61	0/1/1/2
27	LMU	1	627	-	-	3/13/33/61	0/1/1/2
27	LMU	A	857	-	-	3/20/60/61	0/2/2/2
25	BCR	J	102	-	-	2/29/63/63	0/2/2/2
22	CLA	5	610	17	1/1/19/20	2/33/109/115	-
22	CLA	A	839	-	1/1/20/20	2/39/115/115	-
22	CLA	A	804	-	1/1/20/20	4/39/115/115	-
22	CLA	B	816	-	1/1/20/20	0/39/115/115	-
22	CLA	A	840	-	1/1/20/20	6/39/115/115	-
22	CLA	A	813	-	1/1/20/20	3/39/115/115	-
22	CLA	Z	612	12	1/1/15/20	5/15/91/115	-
22	CLA	1	612	12	1/1/15/20	6/15/91/115	-
22	CLA	B2	804	-	1/1/15/20	2/15/91/115	-
22	CLA	3	602	13	1/1/19/20	2/33/109/115	-
24	LHG	4	622	22	-	13/53/53/53	-
22	CLA	8	613	15	1/1/20/20	7/39/115/115	-
22	CLA	1	616	12	1/1/15/20	2/17/93/115	-
22	CLA	B2	806	20	1/1/20/20	6/39/115/115	-
31	CHL	6	608	34	3/3/23/26	0/21/119/137	-
22	CLA	9	614	-	1/1/15/20	4/15/91/115	-
22	CLA	3	615	34	1/1/20/20	5/39/115/115	-
28	LMG	9	620	22	-	7/39/59/70	0/1/1/1
31	CHL	3	608	34	3/3/26/26	3/39/137/137	-
22	CLA	A	806	-	1/1/20/20	10/39/115/115	-
22	CLA	B	833	-	1/1/18/20	4/31/107/115	-
28	LMG	B	852	-	-	5/38/58/70	0/1/1/1
22	CLA	4	612	16	1/1/15/20	4/15/91/115	-
31	CHL	4	601	16	3/3/26/26	6/39/137/137	-
22	CLA	5	603	-	1/1/20/20	15/39/115/115	-
25	BCR	B2	844	-	-	0/29/63/63	0/2/2/2
22	CLA	9	603	19,28	1/1/18/20	5/27/103/115	-
22	CLA	A	821	-	1/1/18/20	4/27/103/115	-
27	LMU	4	625	-	-	3/19/59/61	0/2/2/2
22	CLA	92	614	-	1/1/15/20	4/15/91/115	-
22	CLA	4	614	-	1/1/18/20	5/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	L	204	-	1/1/15/20	1/15/91/115	-
22	CLA	B	802	-	1/1/20/20	5/39/115/115	-
22	CLA	B	837	-	1/1/20/20	0/39/115/115	-
22	CLA	A	810	1	1/1/20/20	8/39/115/115	-
32	XAT	6	624	-	-	0/31/93/93	0/4/4/4
22	CLA	Z	610	12	1/1/19/20	0/33/109/115	-
22	CLA	92	609	19	1/1/15/20	8/15/91/115	-
22	CLA	F	304	6	1/1/20/20	8/39/115/115	-
22	CLA	6	617	-	1/1/15/20	2/15/91/115	-
29	LUT	9	616	-	-	2/29/67/67	0/2/2/2
24	LHG	B	851	22	-	12/49/49/53	-
22	CLA	Z	614	-	1/1/17/20	0/21/97/115	-
22	CLA	4	604	34	1/1/17/20	1/21/97/115	-
31	CHL	Z	601	12	3/3/26/26	7/39/137/137	-
31	CHL	6	607	34	3/3/26/26	8/39/137/137	-
22	CLA	92	613	19	1/1/19/20	2/33/109/115	-
22	CLA	G	204	7	1/1/15/20	4/17/93/115	-
22	CLA	A	809	1	1/1/20/20	6/39/115/115	-
22	CLA	A	802	-	1/1/20/20	0/39/115/115	-
22	CLA	F	301	34	1/1/20/20	3/39/115/115	-
22	CLA	A	837	1	1/1/18/20	1/30/106/115	-
22	CLA	7	604	34	1/1/17/20	1/23/99/115	-
27	LMU	G	206	-	-	4/15/35/61	0/1/1/2
31	CHL	92	607	-	3/3/21/26	2/15/113/137	-
22	CLA	B2	829	-	1/1/20/20	2/39/115/115	-
27	LMU	8	628	-	-	4/15/35/61	0/1/1/2
28	LMG	B2	852	-	-	3/38/58/70	0/1/1/1
22	CLA	A	803	34	1/1/20/20	2/39/115/115	-
29	LUT	92	616	-	-	2/29/67/67	0/2/2/2
22	CLA	Z	603	-	1/1/18/20	6/27/103/115	-
22	CLA	3	612	13	1/1/15/20	2/17/93/115	-
25	BCR	L2	205	-	-	2/29/63/63	0/2/2/2
28	LMG	1	624	-	-	4/31/51/70	0/1/1/1
22	CLA	B	812	-	1/1/20/20	2/39/115/115	-
22	CLA	B2	812	-	1/1/19/20	3/33/109/115	-
25	BCR	B	845	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	LHG	92	622	22	-	9/33/33/53	-
22	CLA	A	825	-	1/1/18/20	7/27/103/115	-
22	CLA	A	841	-	1/1/20/20	7/39/115/115	-
27	LMU	8	627	-	-	9/21/61/61	0/2/2/2
22	CLA	B	823	-	1/1/20/20	4/39/115/115	-
25	BCR	3	718	-	-	2/29/63/63	0/2/2/2
27	LMU	1	621	-	-	6/21/61/61	0/2/2/2
22	CLA	92	601	19	1/1/15/20	4/15/91/115	-
27	LMU	1	626	-	-	0/15/35/61	0/1/1/2
25	BCR	9	623	-	-	2/29/63/63	0/2/2/2
22	CLA	3	610	13	1/1/20/20	0/39/115/115	-
29	LUT	Z	619	-	-	2/18/37/67	0/1/1/2
22	CLA	A	828	-	1/1/20/20	5/39/115/115	-
32	XAT	5	624	-	1/1/26/26	0/31/93/93	0/4/4/4
22	CLA	F	303	34	1/1/15/20	1/15/91/115	-
31	CHL	4	608	-	3/3/26/26	5/39/137/137	-
22	CLA	B	804	-	1/1/15/20	4/15/91/115	-
22	CLA	A	834	-	1/1/20/20	6/39/115/115	-
24	LHG	8	620	22	-	14/48/48/53	-
22	CLA	A	818	-	1/1/20/20	2/39/115/115	-
22	CLA	A	816	-	1/1/20/20	4/39/115/115	-
22	CLA	A	817	34	1/1/18/20	4/27/103/115	-
22	CLA	B	813	-	1/1/20/20	3/39/115/115	-
22	CLA	A	807	1	1/1/20/20	3/39/115/115	-
29	LUT	9	617	-	-	0/29/67/67	0/2/2/2
27	LMU	A	861	-	-	2/15/35/61	0/1/1/2
31	CHL	5	607	34	3/3/26/26	11/39/137/137	-
22	CLA	8	610	15	1/1/20/20	2/39/115/115	-
22	CLA	6	612	18	1/1/15/20	2/15/91/115	-
22	CLA	B	829	-	1/1/20/20	3/39/115/115	-
27	LMU	6	630	-	-	1/15/35/61	0/1/1/2
22	CLA	B	809	2	1/1/20/20	6/39/115/115	-
22	CLA	B	836	-	1/1/19/20	4/33/109/115	-
23	PQN	B	842	-	-	1/23/43/43	0/2/2/2
31	CHL	6	601	18	3/3/26/26	4/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
22	CLA	B	826	-	1/1/20/20	4/39/115/115	-
29	LUT	8	617	-	-	2/29/67/67	0/2/2/2
24	LHG	A	846	-	-	9/53/53/53	-
25	BCR	A	848	-	-	2/29/63/63	0/2/2/2
22	CLA	1	614	-	1/1/19/20	7/33/109/115	-

The worst 5 of 1385 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Z	601	CHL	MG-NB	-7.46	1.91	2.05
31	6	601	CHL	MG-NB	-7.44	1.91	2.05
31	8	601	CHL	MG-NB	-7.43	1.91	2.05
31	9	607	CHL	MG-NB	-7.43	1.91	2.05
31	4	606	CHL	MG-NB	-7.41	1.91	2.05

The worst 5 of 765 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	A	801	CL0	C1B-CHB-C4A	9.95	127.72	121.32
31	8	601	CHL	C1B-CHB-C4A	5.02	124.55	121.32
31	4	601	CHL	C1B-CHB-C4A	4.98	124.53	121.32
31	3	608	CHL	C1B-CHB-C4A	4.86	124.45	121.32
31	8	607	CHL	C1B-CHB-C4A	4.72	124.36	121.32

5 of 328 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
21	A	801	CL0	ND
21	A	801	CL0	NA
21	A	801	CL0	NC
22	A	802	CLA	ND
22	A	803	CLA	ND

5 of 1439 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	A	806	CLA	CAD-CBD-CGD-O1D
22	A	806	CLA	CAD-CBD-CGD-O2D
22	A	806	CLA	C2-C3-C5-C6
22	A	806	CLA	C4-C3-C5-C6
22	A	809	CLA	CHA-CBD-CGD-O1D

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
33	5	625	NEX	C1-C2-C3-C4-C5-C6

163 monomers are involved in 223 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	92	602	CLA	1	0
30	B	850	DGD	1	0
22	K	204	CLA	1	0
22	A	854	CLA	1	0
22	A	823	CLA	1	0
28	A	860	LMG	1	0
29	1	617	LUT	2	0
31	4	606	CHL	2	0
25	K	202	BCR	3	0
25	B	844	BCR	2	0
29	6	621	LUT	1	0
31	8	606	CHL	2	0
22	B2	828	CLA	4	0
27	Z	622	LMU	1	0
22	A	822	CLA	1	0
22	1	613	CLA	1	0
25	K	207	BCR	3	0
22	4	609	CLA	1	0
22	B	841	CLA	3	0
31	1	601	CHL	1	0
25	A	850	BCR	1	0
22	A	820	CLA	1	0
22	A	843	CLA	3	0
32	1	618	XAT	1	0
31	8	601	CHL	1	0
25	8	619	BCR	2	0
22	8	603	CLA	1	0
22	B	817	CLA	1	0
29	Z	617	LUT	1	0
28	4	624	LMG	1	0
29	A	856	LUT	1	0
22	92	611	CLA	1	0
22	3	609	CLA	1	0
24	5	623	LHG	1	0
29	5	620	LUT	3	0
25	I	172	BCR	1	0
25	B	848	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	B	821	CLA	1	0
22	B	834	CLA	1	0
25	A	852	BCR	4	0
22	B	806	CLA	1	0
25	A	851	BCR	3	0
22	8	604	CLA	1	0
22	3	603	CLA	2	0
27	B	853	LMU	3	0
24	1	620	LHG	1	0
29	F	305	LUT	3	0
25	B	843	BCR	2	0
22	B	808	CLA	1	0
25	B2	845	BCR	2	0
28	J	104	LMG	1	0
22	A	831	CLA	1	0
27	A	862	LMU	2	0
24	3	623	LHG	1	0
22	3	607	CLA	1	0
22	B	840	CLA	2	0
22	J	101	CLA	1	0
25	3	719	BCR	5	0
24	6	619	LHG	1	0
28	3	722	LMG	1	0
22	B	832	CLA	1	0
25	L	201	BCR	1	0
22	6	603	CLA	1	0
22	9	609	CLA	1	0
27	7	628	LMU	1	0
22	Z	616	CLA	2	0
25	B	801	BCR	2	0
25	92	623	BCR	3	0
25	A	849	BCR	2	0
31	6	606	CHL	1	0
22	5	621	CLA	2	0
25	3	620	BCR	1	0
24	4	623	LHG	1	0
22	3	611	CLA	1	0
31	5	606	CHL	1	0
29	7	624	LUT	4	0
22	7	610	CLA	3	0
22	L	203	CLA	1	0
22	Z	608	CLA	1	0

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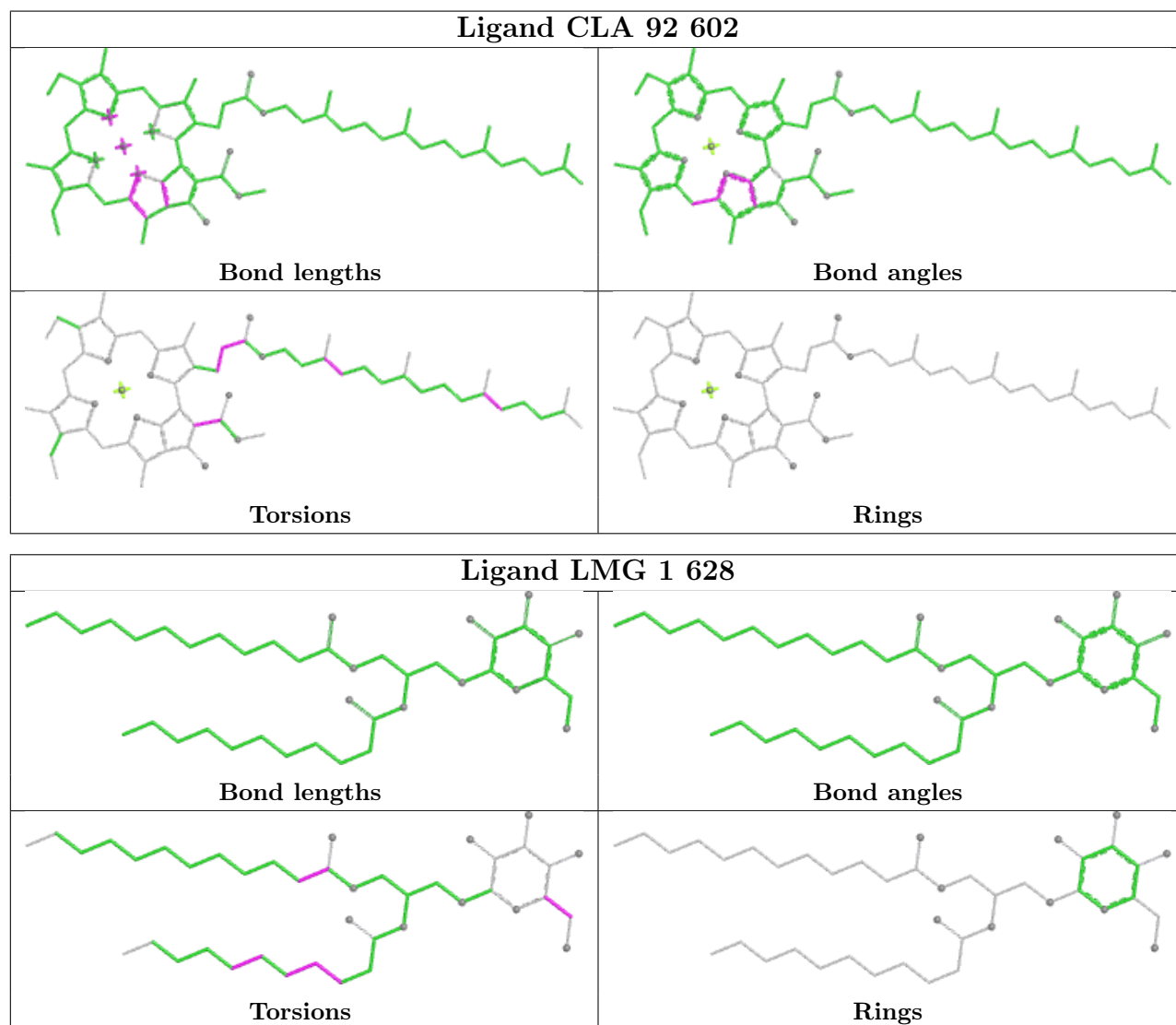
Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	7	625	LHG	1	0
29	5	626	LUT	1	0
22	7	608	CLA	1	0
25	B	847	BCR	1	0
22	A	830	CLA	1	0
25	L	205	BCR	4	0
22	1	603	CLA	3	0
22	4	613	CLA	2	0
27	92	624	LMU	2	0
22	1	602	CLA	1	0
22	B	827	CLA	1	0
22	8	612	CLA	1	0
29	4	619	LUT	1	0
22	K	201	CLA	2	0
22	7	609	CLA	1	0
22	Z	613	CLA	1	0
22	B	839	CLA	2	0
22	A	811	CLA	3	0
22	5	617	CLA	2	0
31	7	601	CHL	3	0
22	A	833	CLA	3	0
22	5	602	CLA	1	0
22	5	616	CLA	3	0
22	A	812	CLA	1	0
25	6	623	BCR	2	0
28	B	854	LMG	1	0
28	J	103	LMG	1	0
29	3	622	LUT	2	0
22	7	620	CLA	1	0
27	6	628	LMU	1	0
27	A	863	LMU	2	0
33	6	625	NEX	1	0
27	9	624	LMU	1	0
22	A	829	CLA	2	0
27	A	858	LMU	1	0
31	5	608	CHL	1	0
27	A	857	LMU	1	0
25	J	102	BCR	1	0
22	A	839	CLA	1	0
22	A	804	CLA	1	0
22	B	816	CLA	2	0
22	A	840	CLA	1	0

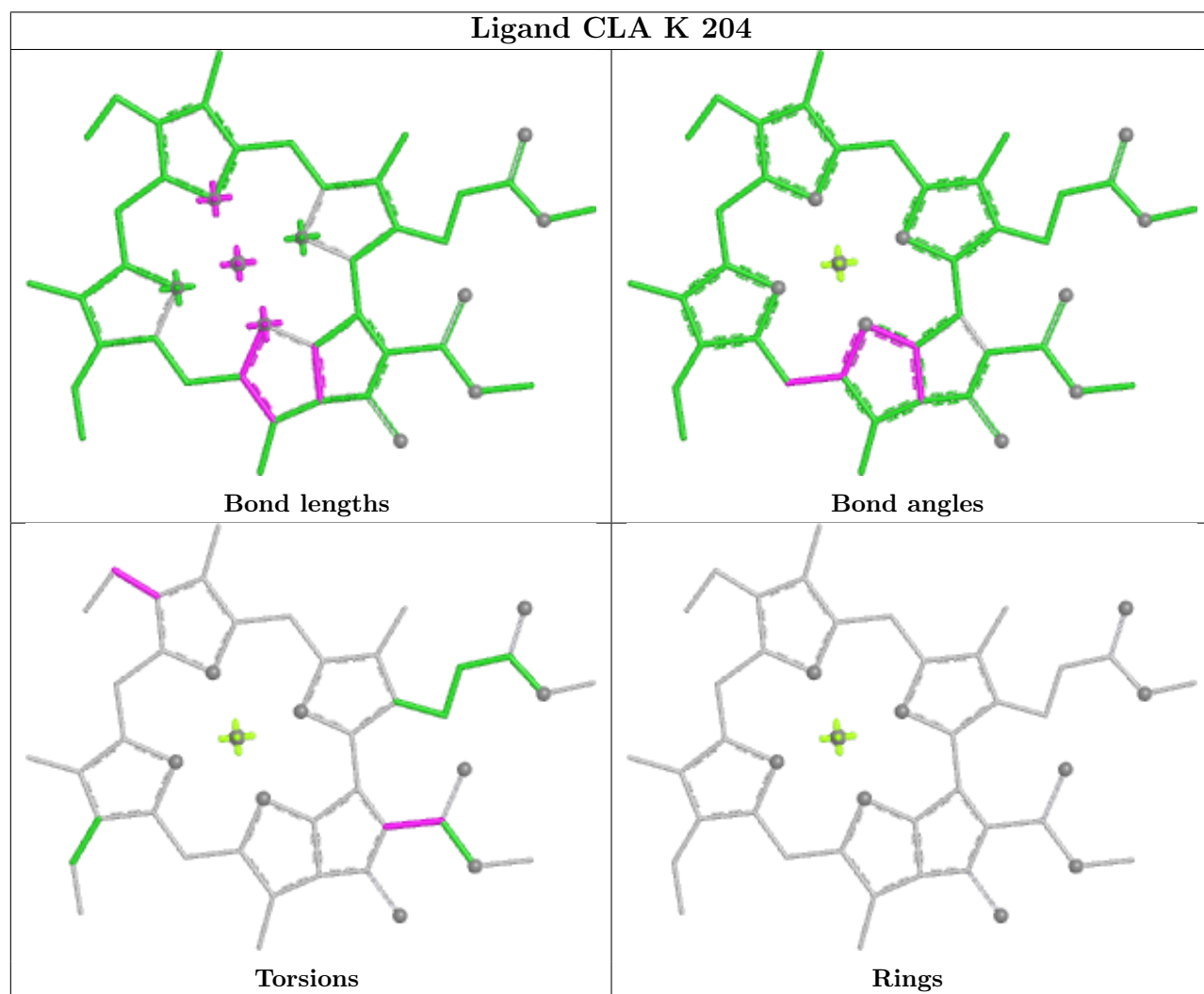
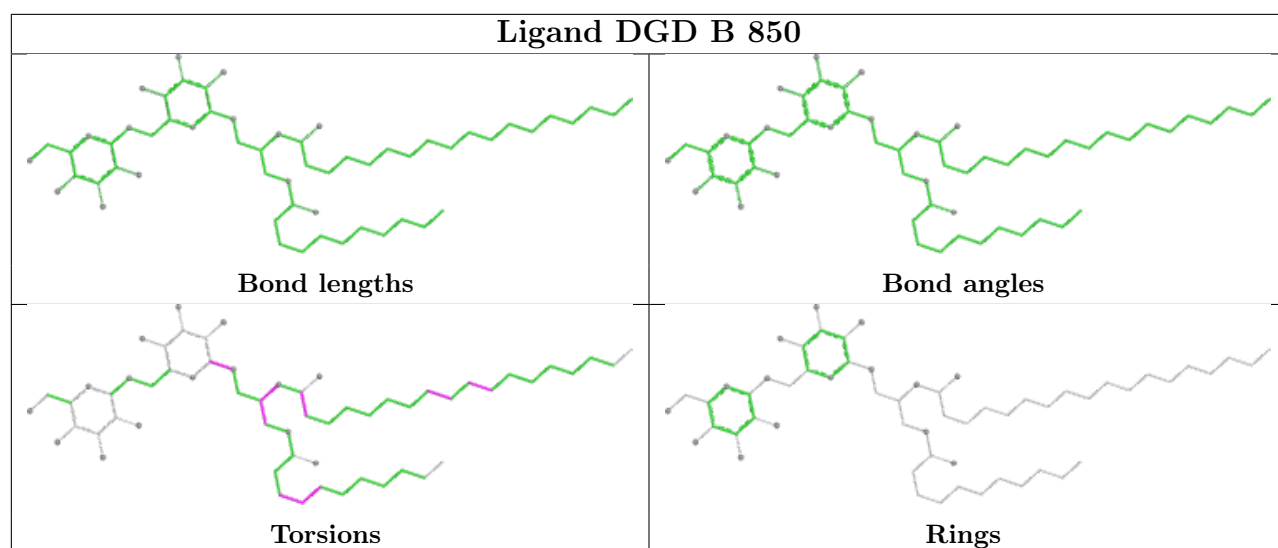
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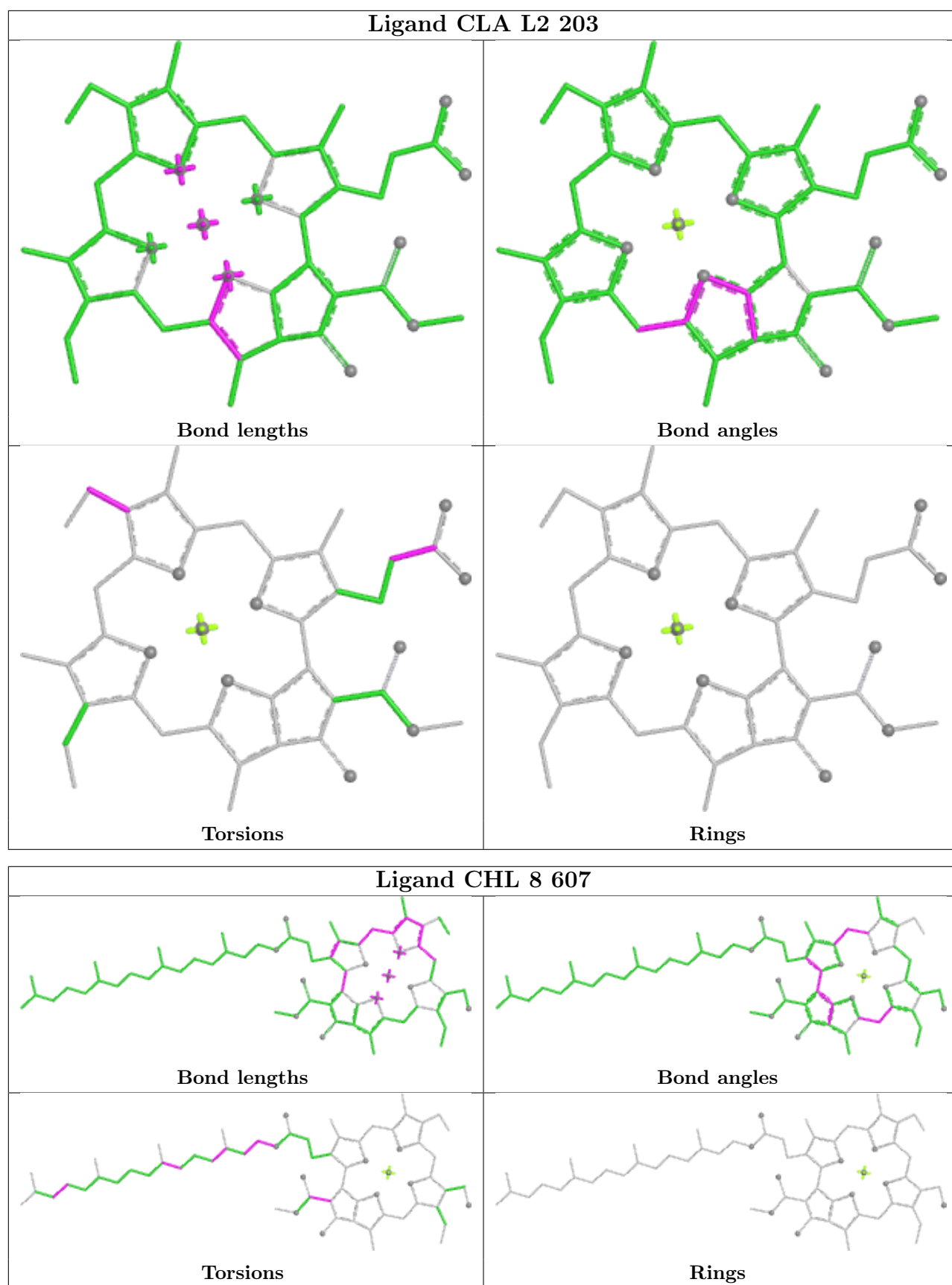
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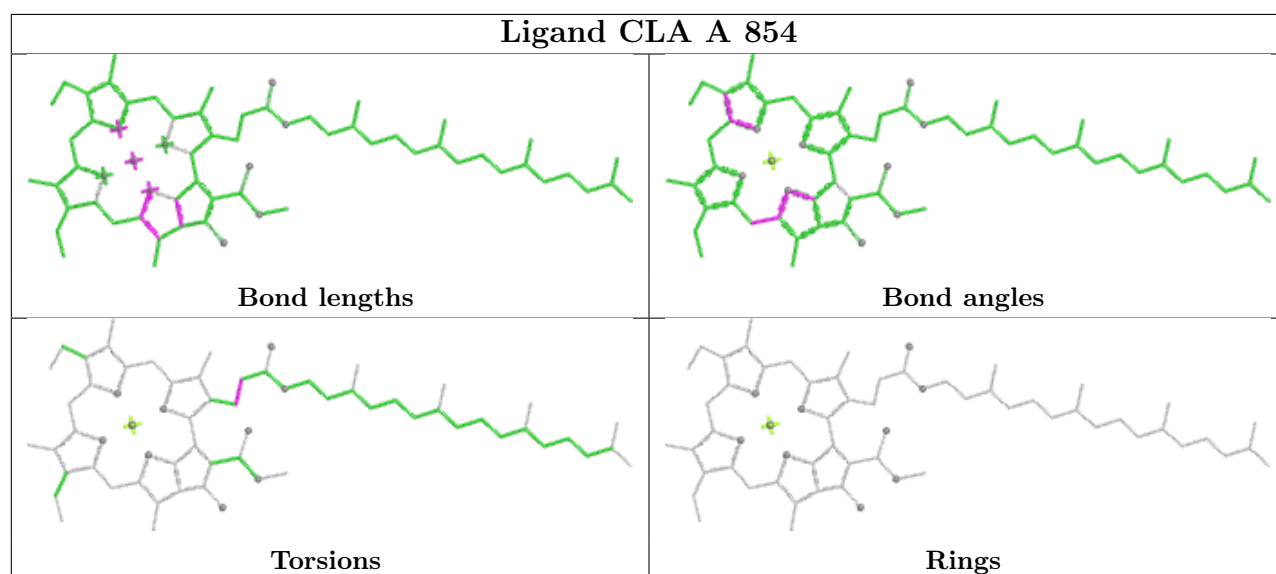
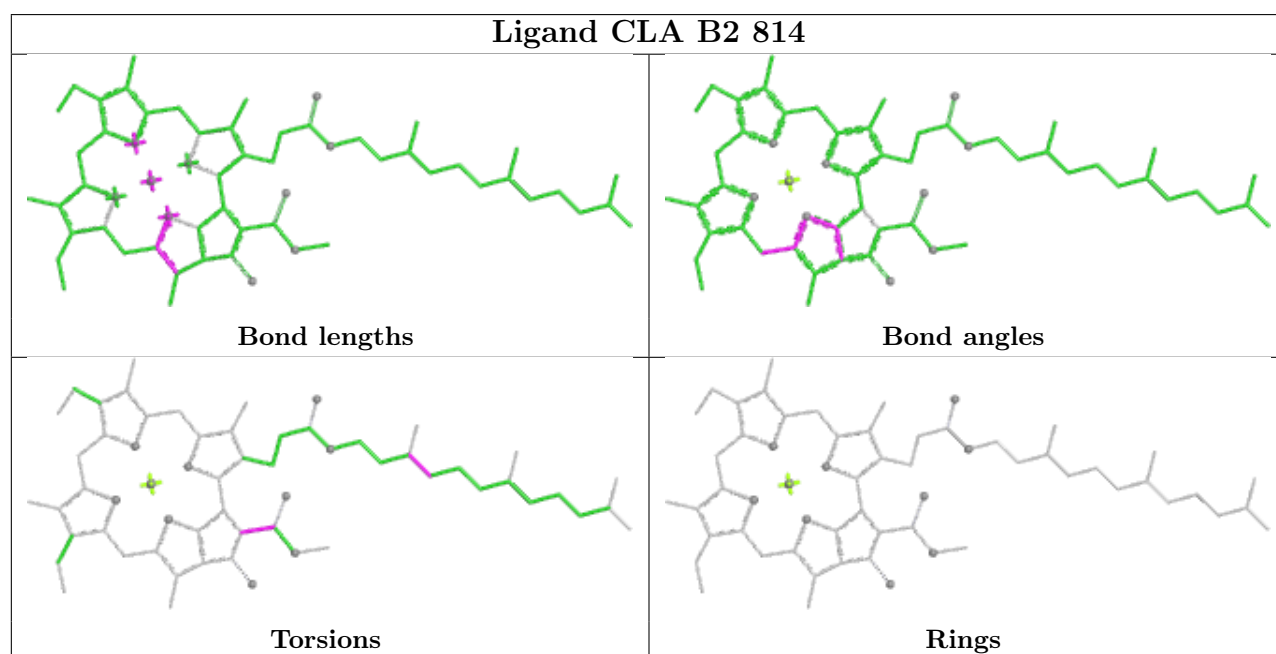
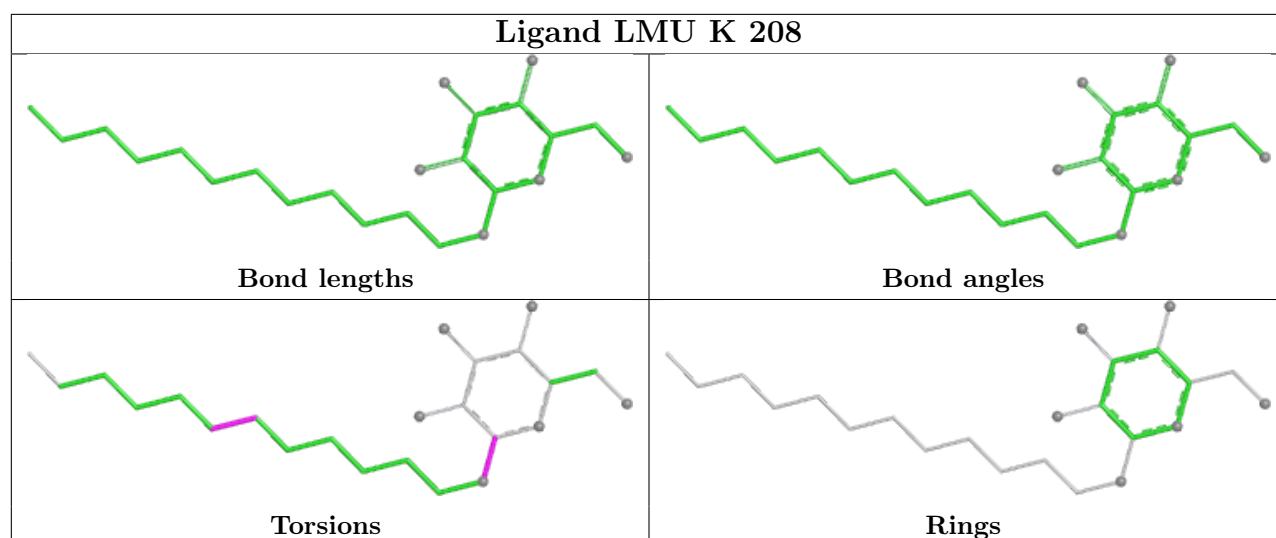
Mol	Chain	Res	Type	Clashes	Symm-Clashes
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22	3	602	CLA	1	0
22	8	613	CLA	1	0
31	6	608	CHL	2	0
22	9	614	CLA	1	0
22	3	615	CLA	5	0
28	9	620	LMG	1	0
31	3	608	CHL	1	0
22	A	806	CLA	1	0
31	4	601	CHL	1	0
22	5	603	CLA	3	0
25	B2	844	BCR	4	0
22	4	614	CLA	1	0
22	B	802	CLA	1	0
22	B	837	CLA	2	0
22	A	810	CLA	1	0
22	F	304	CLA	1	0
29	9	616	LUT	1	0
31	Z	601	CHL	1	0
31	6	607	CHL	1	0
22	92	613	CLA	2	0
22	A	809	CLA	2	0
22	A	802	CLA	2	0
22	B2	829	CLA	1	0
22	A	803	CLA	1	0
22	Z	603	CLA	2	0
25	L2	205	BCR	3	0
25	B	845	BCR	3	0
24	92	622	LHG	1	0
22	A	825	CLA	1	0
27	8	627	LMU	1	0
22	B	823	CLA	1	0
25	3	718	BCR	1	0
25	9	623	BCR	2	0
22	3	610	CLA	2	0
22	A	818	CLA	1	0
22	A	817	CLA	1	0
29	9	617	LUT	2	0
22	B	829	CLA	6	0
22	B	836	CLA	1	0
31	6	601	CHL	3	0
25	A	848	BCR	3	0

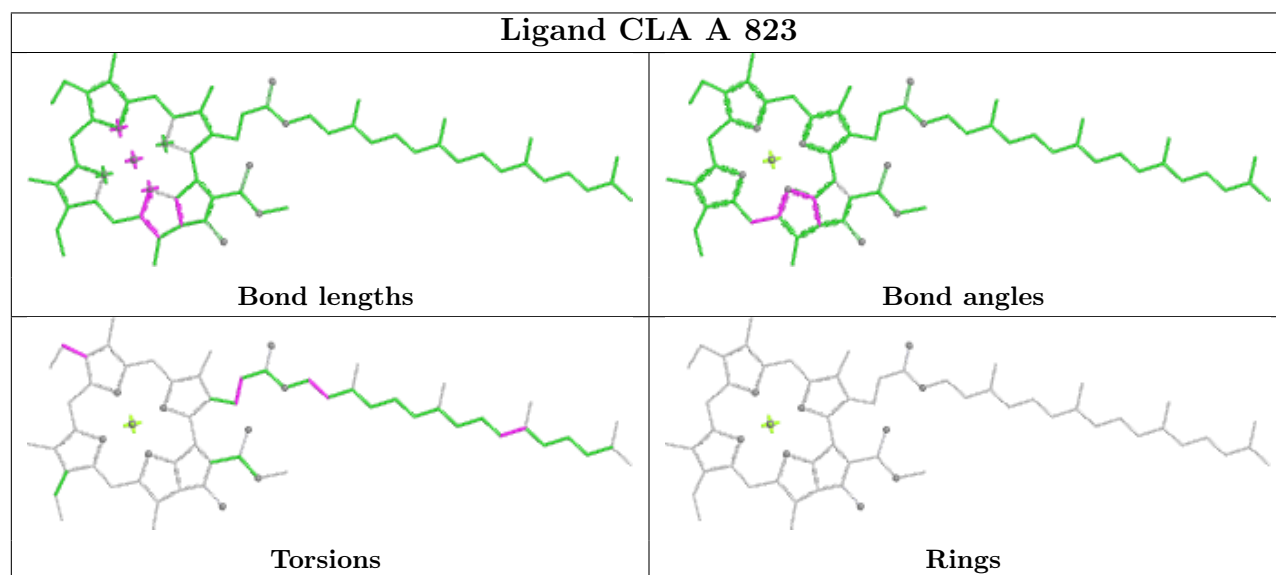
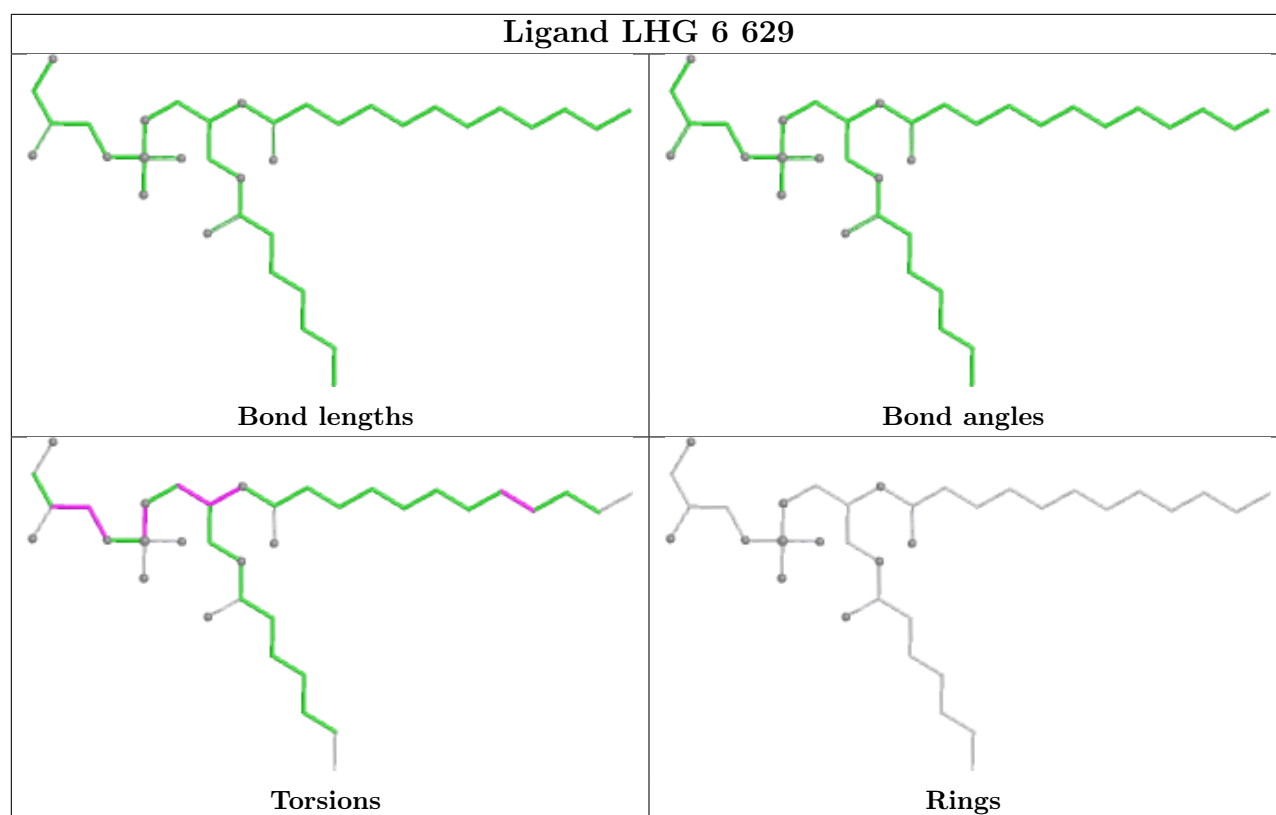
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

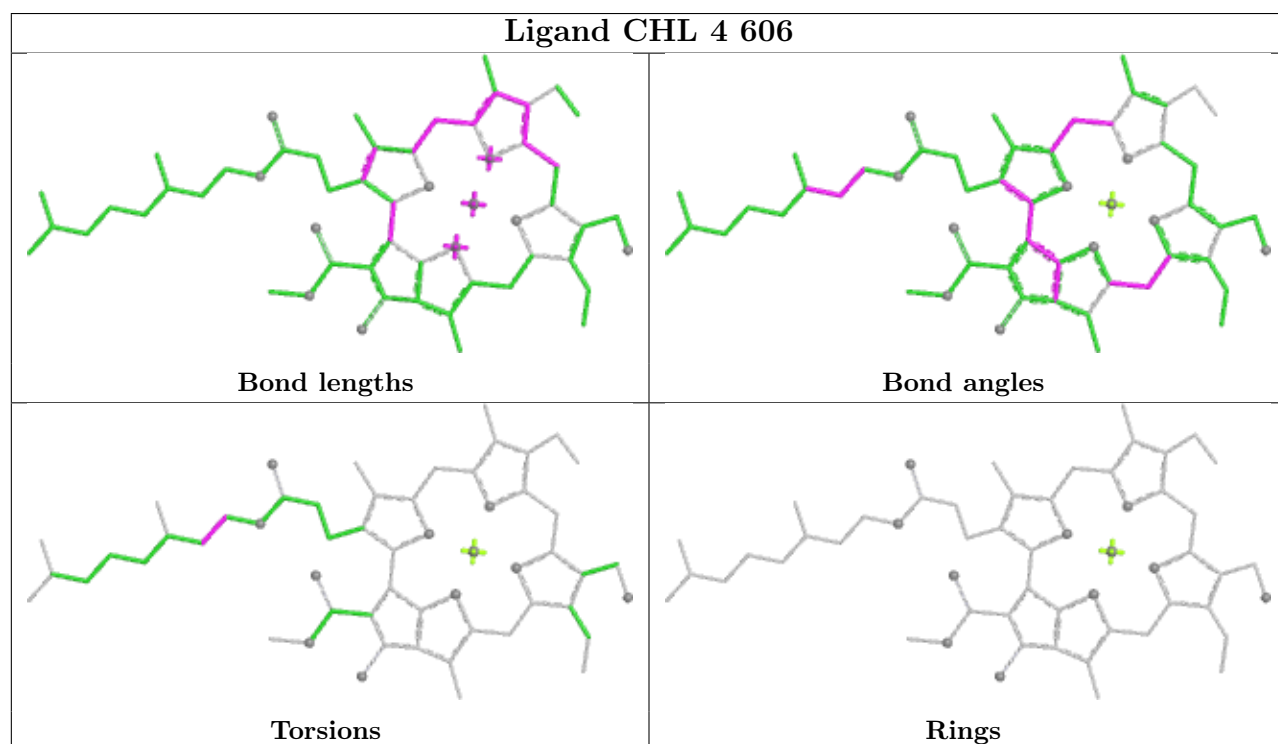
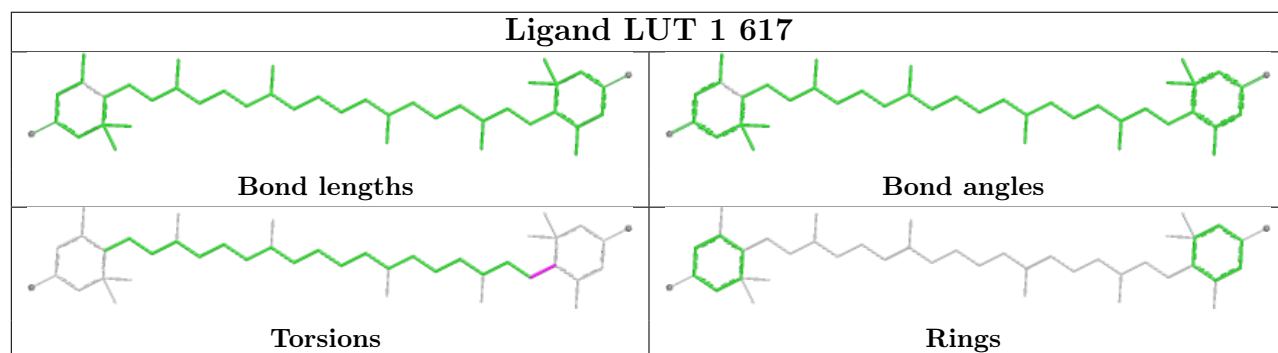
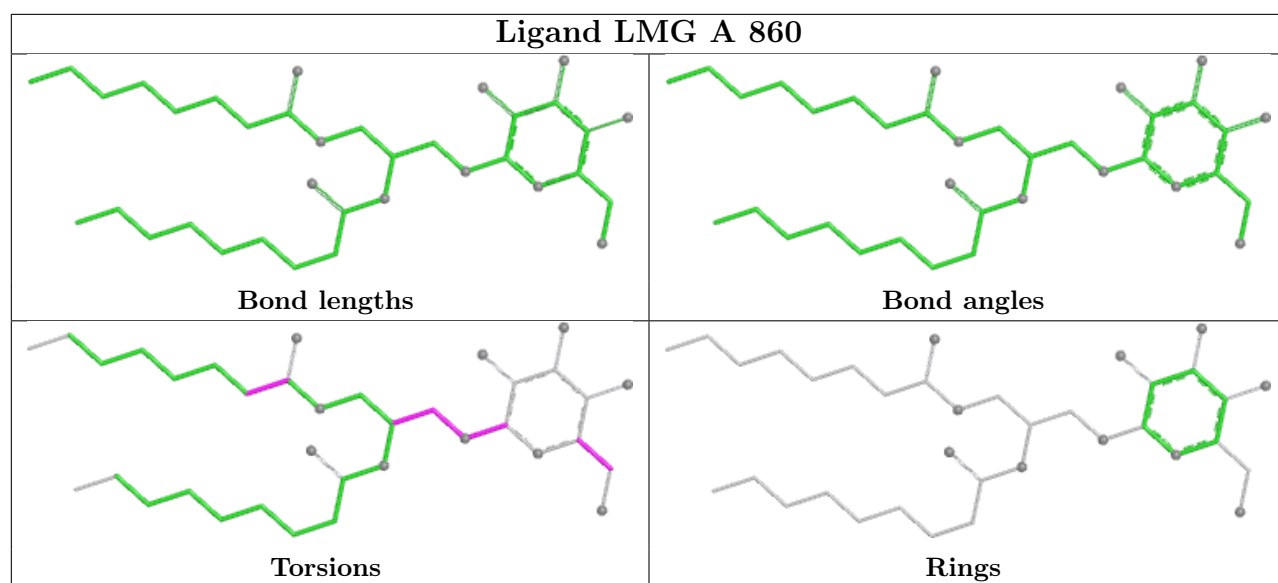


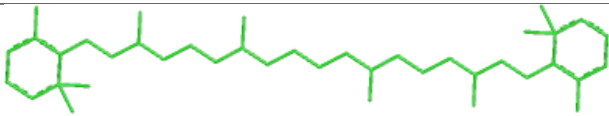
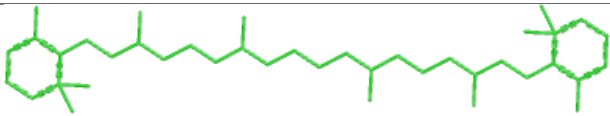
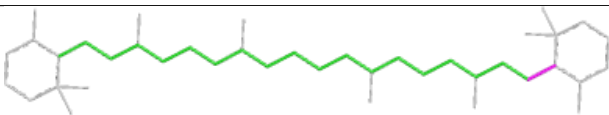
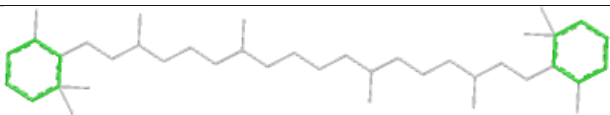


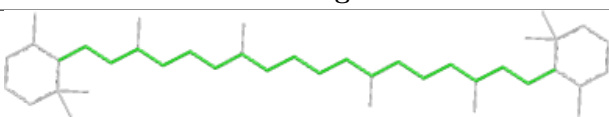
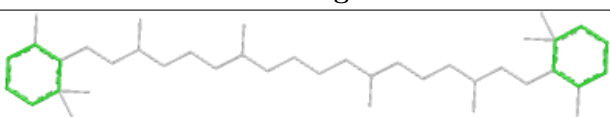


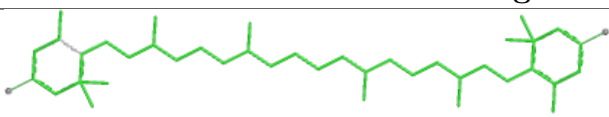
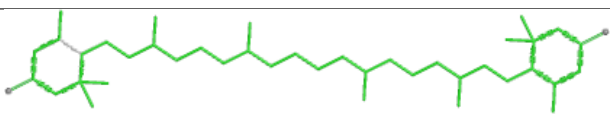
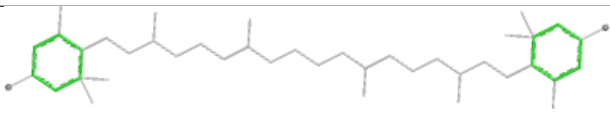


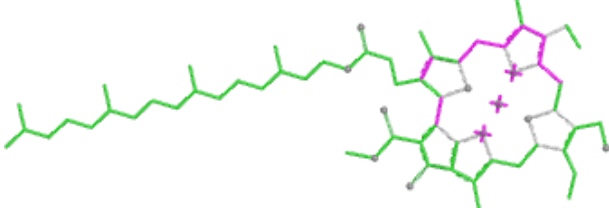
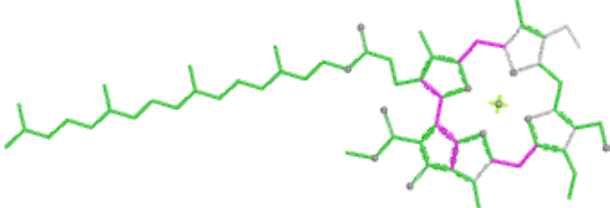
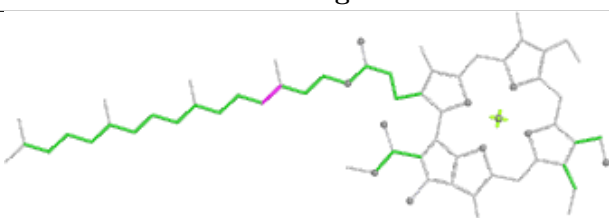
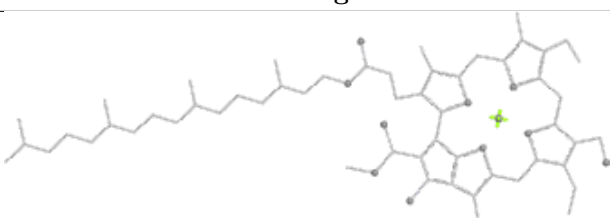


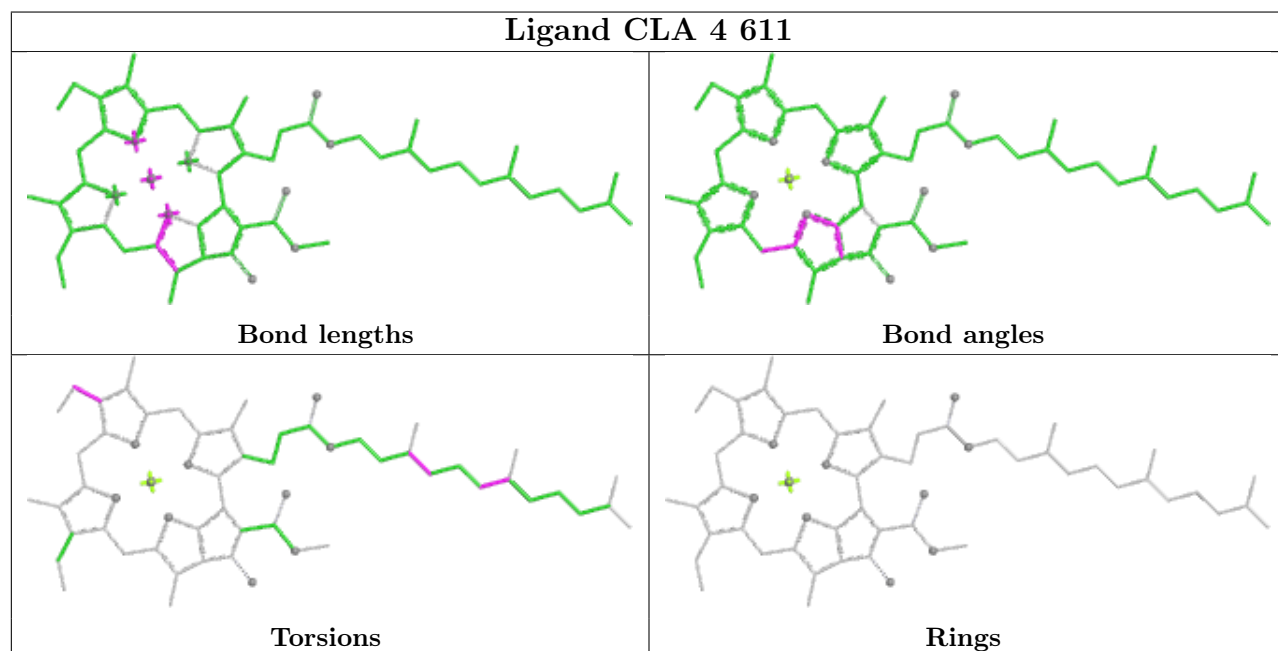
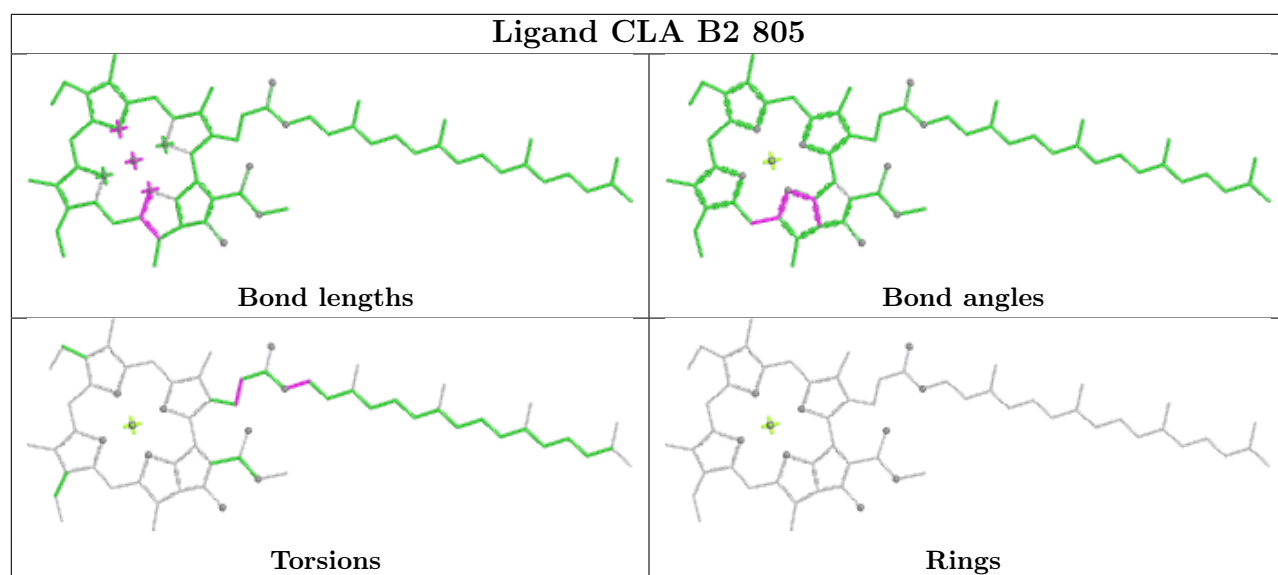


Ligand BCR K 202	
	
Bond lengths	Bond angles
	
Torsions	Rings

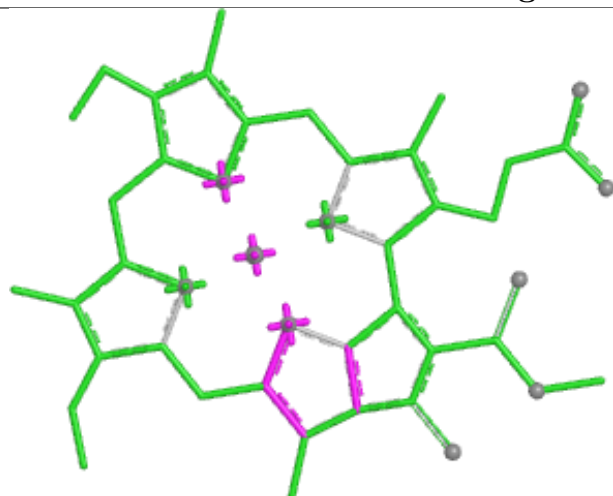
Ligand BCR B 844	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 6 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

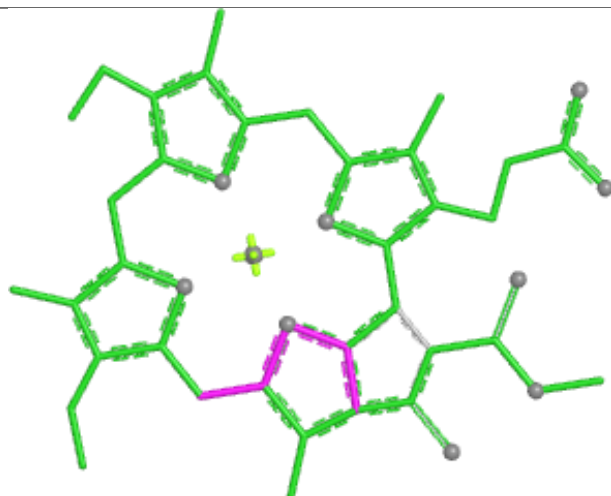
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Bond lengths	Bond angles
	
Torsions	Rings



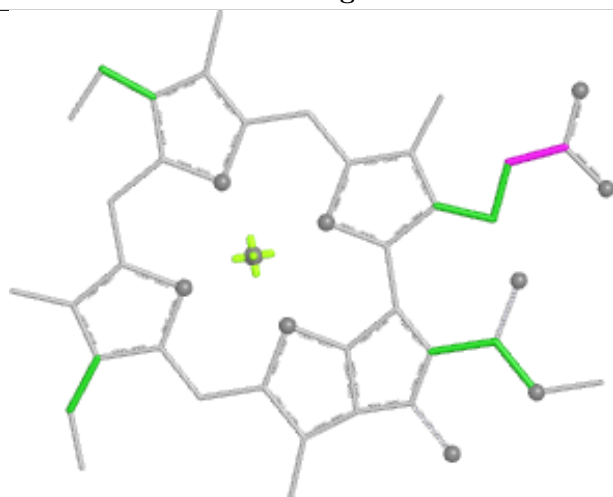
Ligand CLA 8 611



Bond lengths



Bond angles

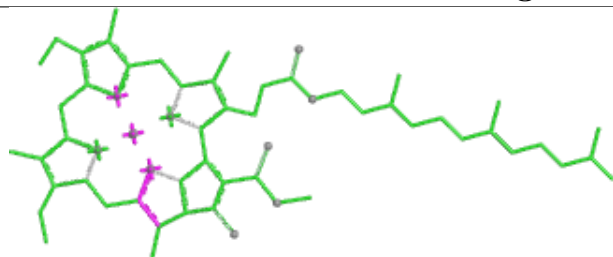


Torsions

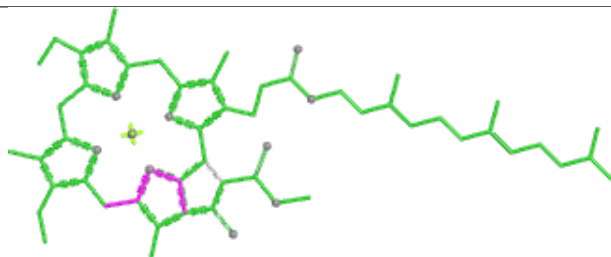


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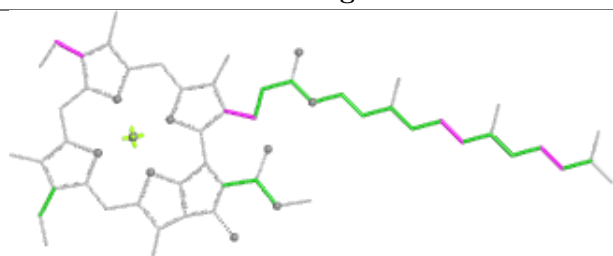
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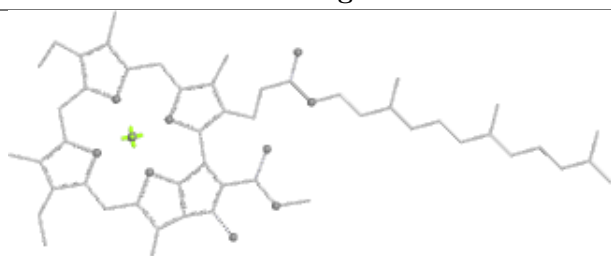
Bond lengths



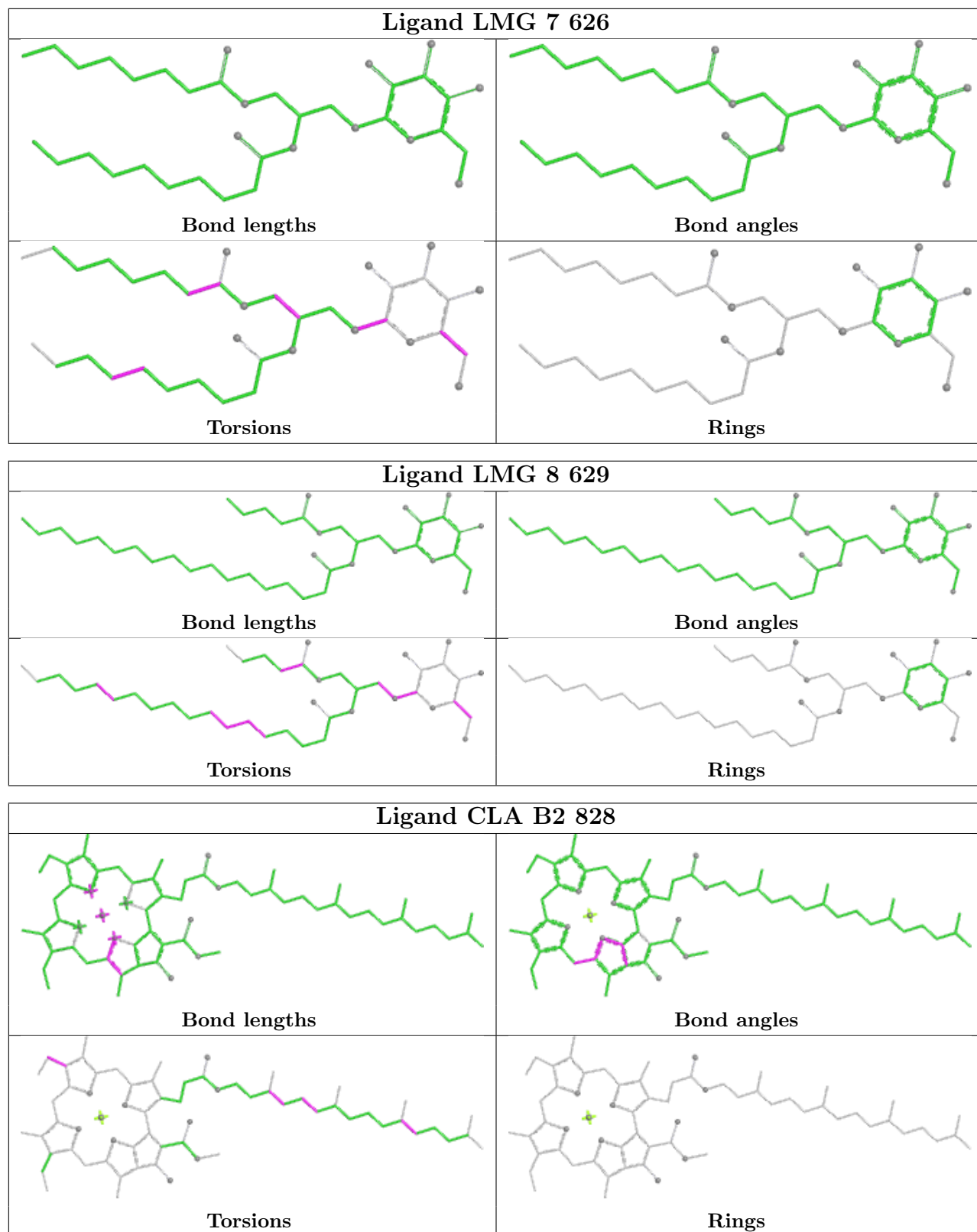
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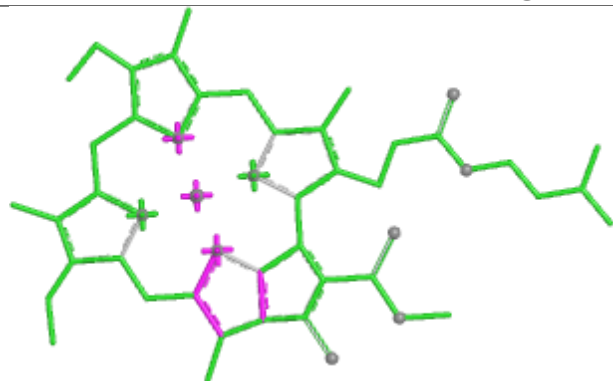
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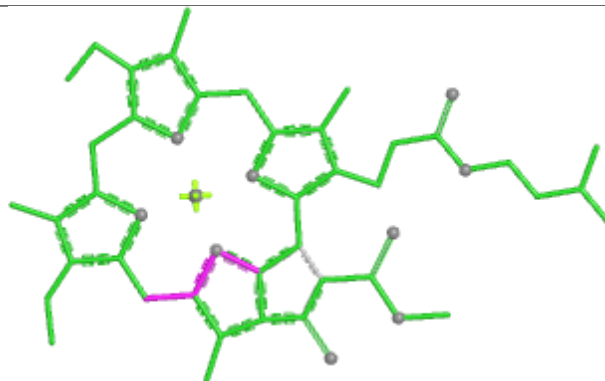
Rings



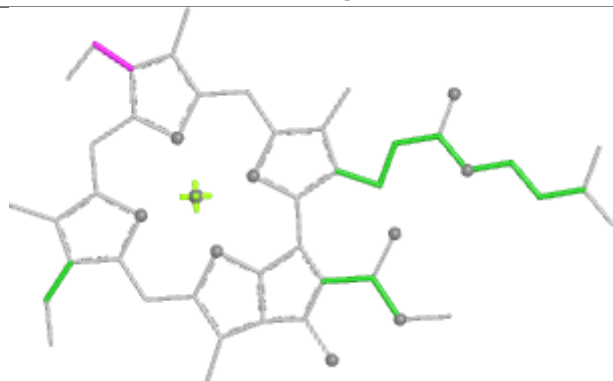
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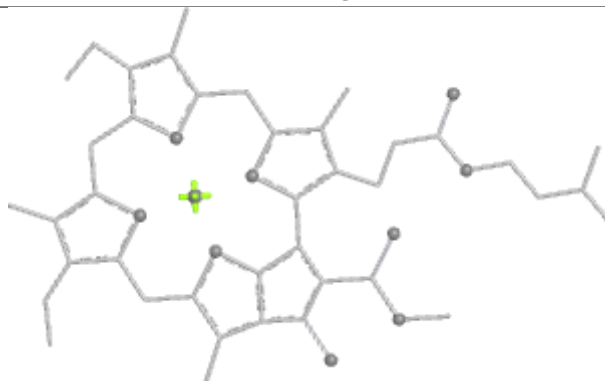
Bond lengths



Bond angles

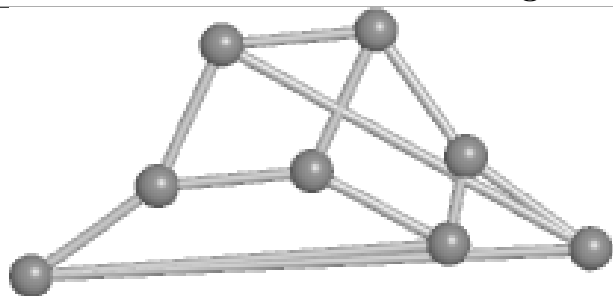


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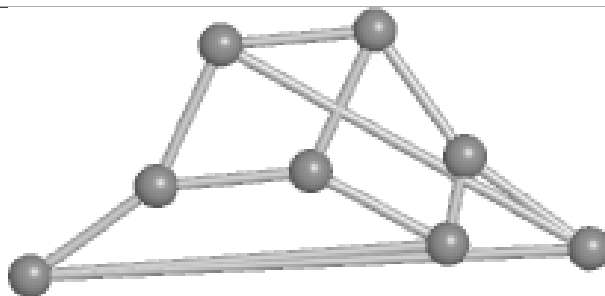


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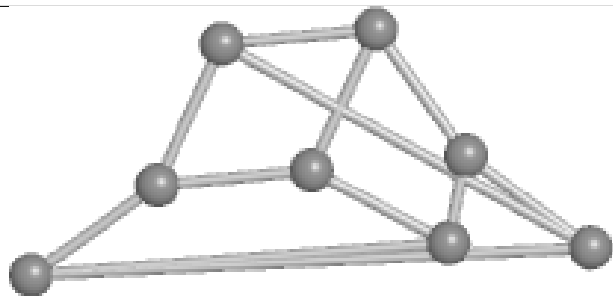
Ligand SF4 C 102



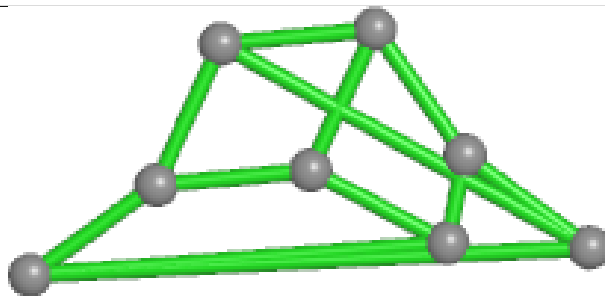
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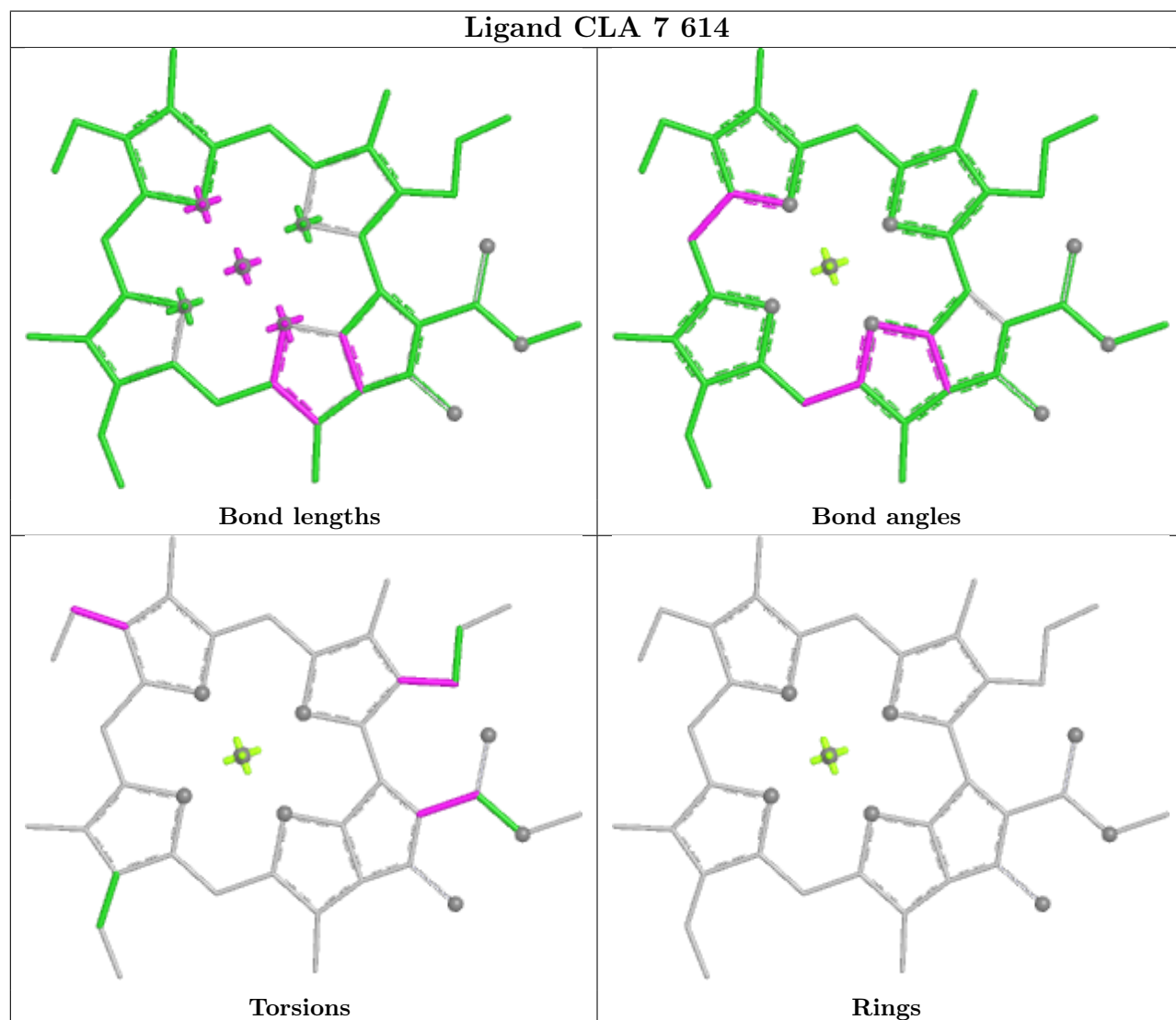
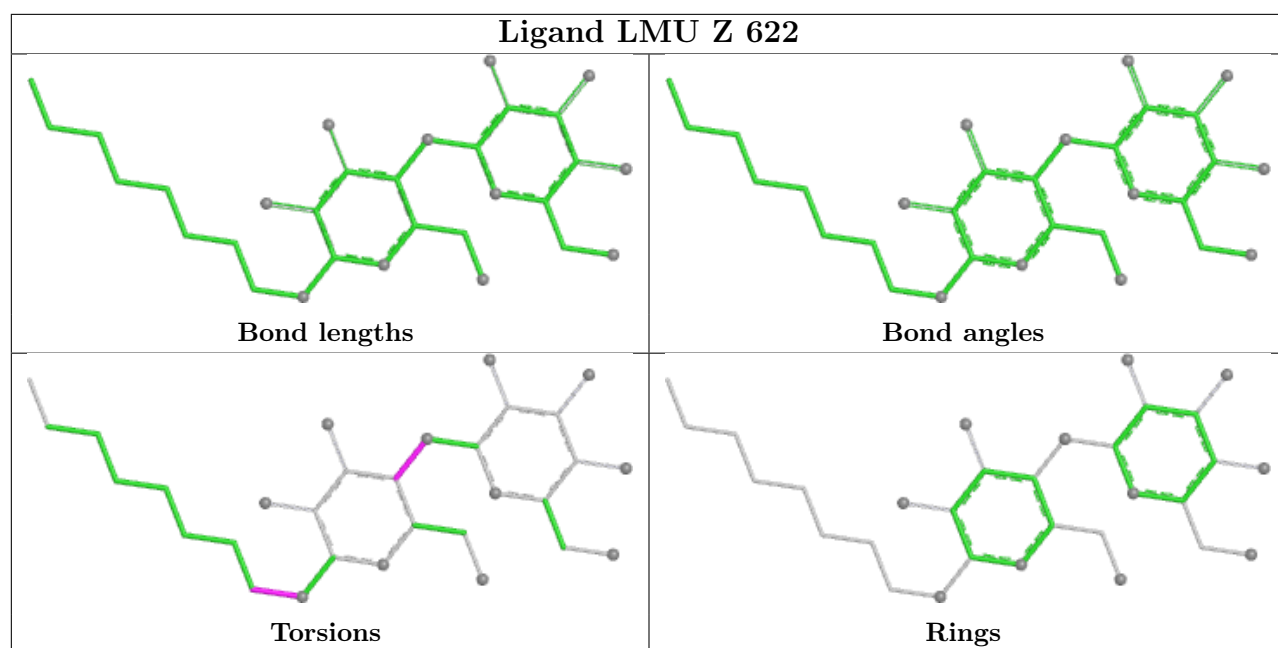
Bond angles

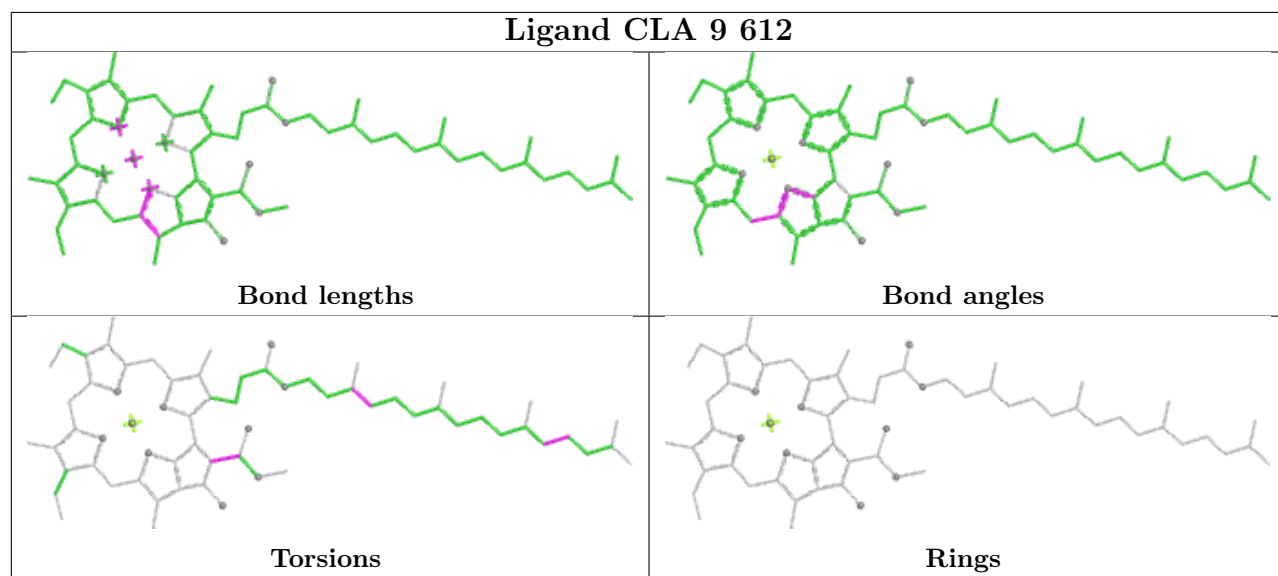
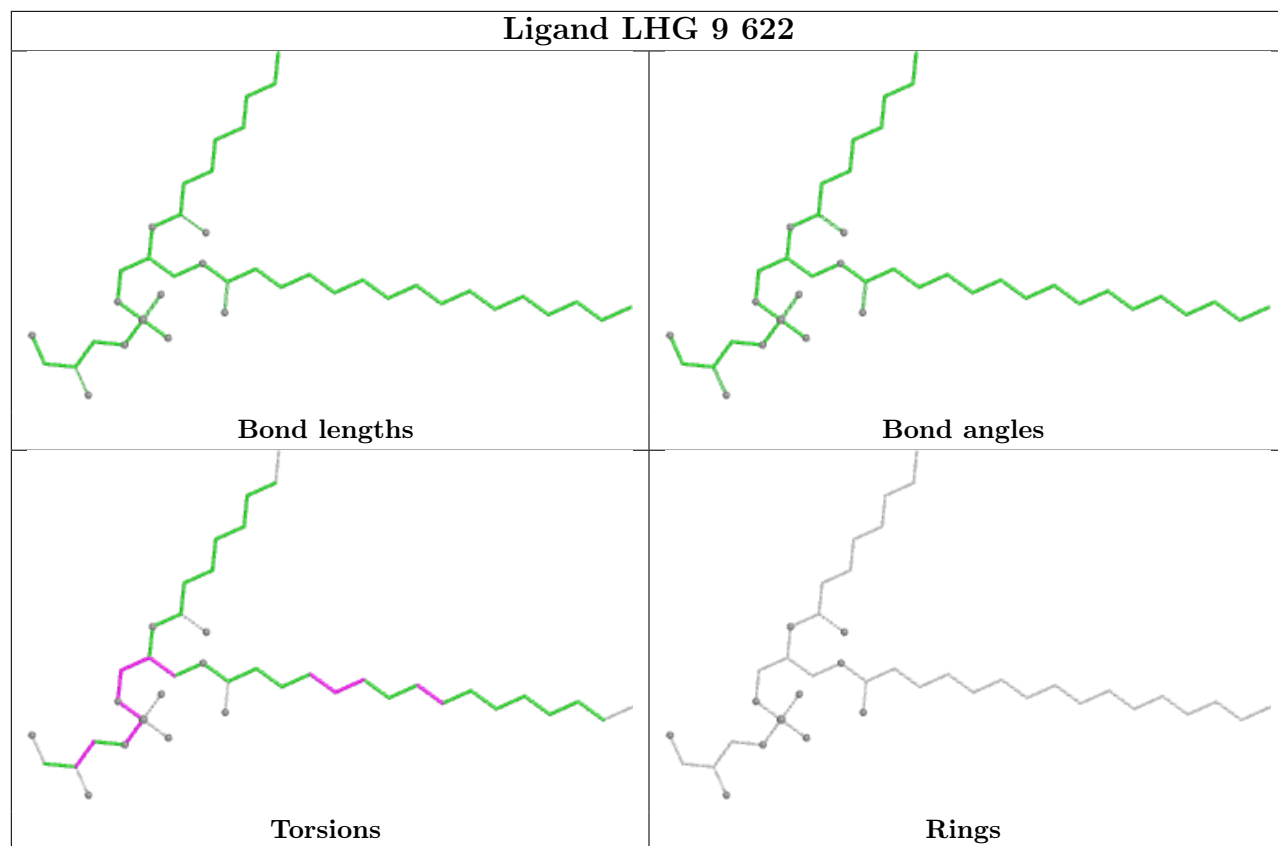


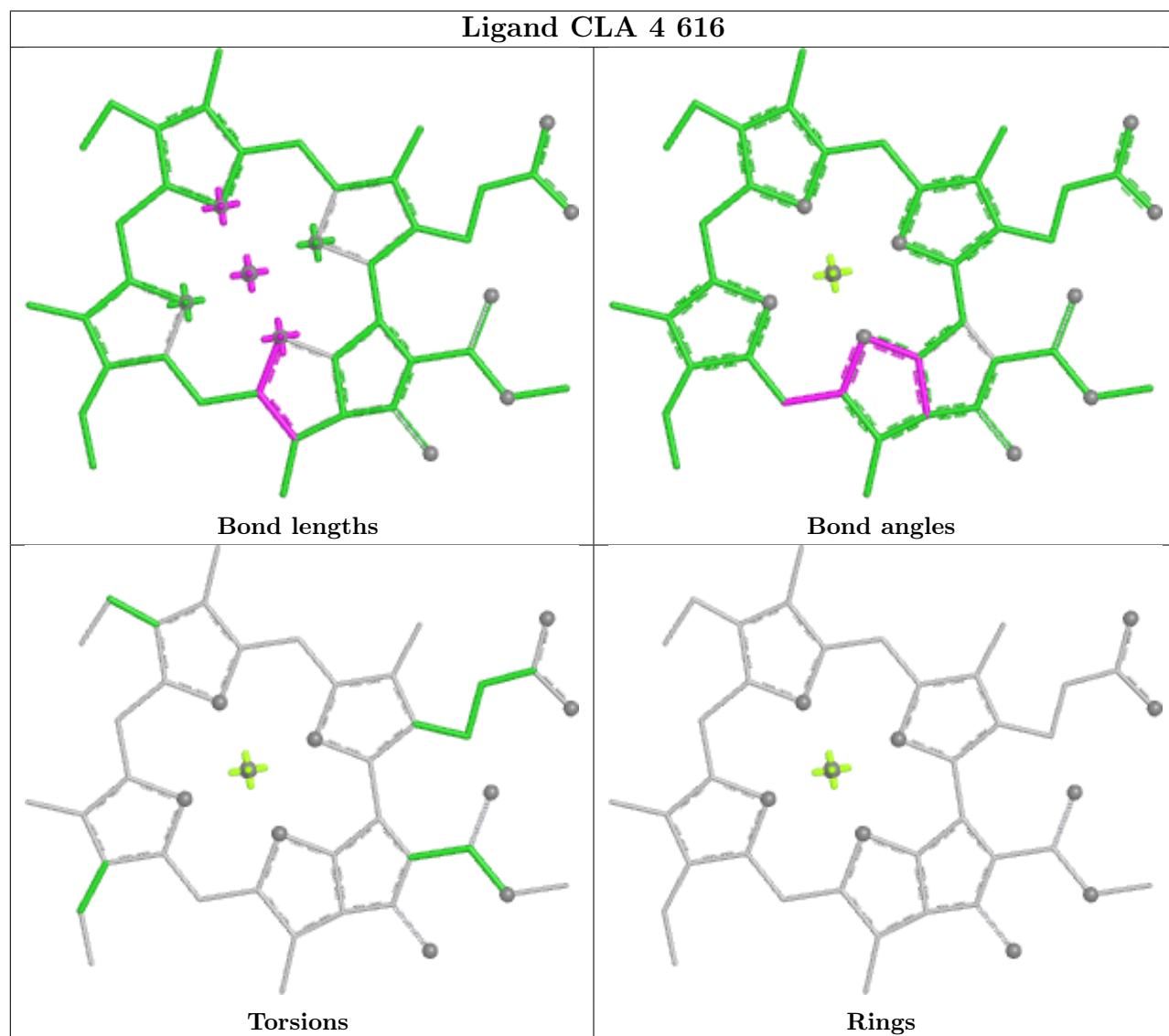
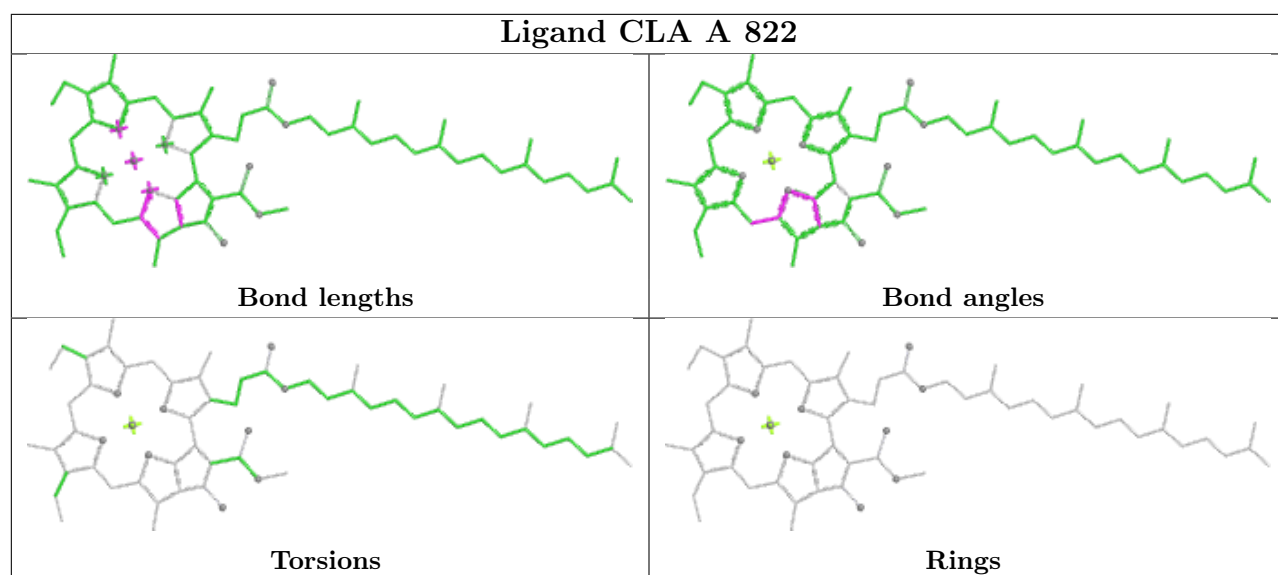
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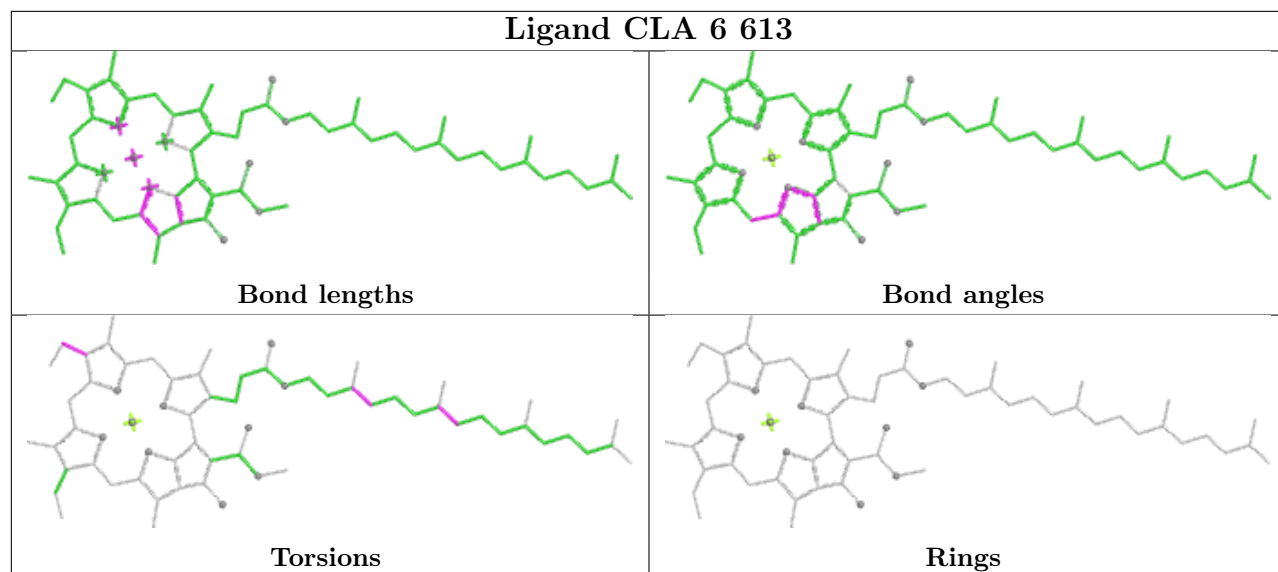
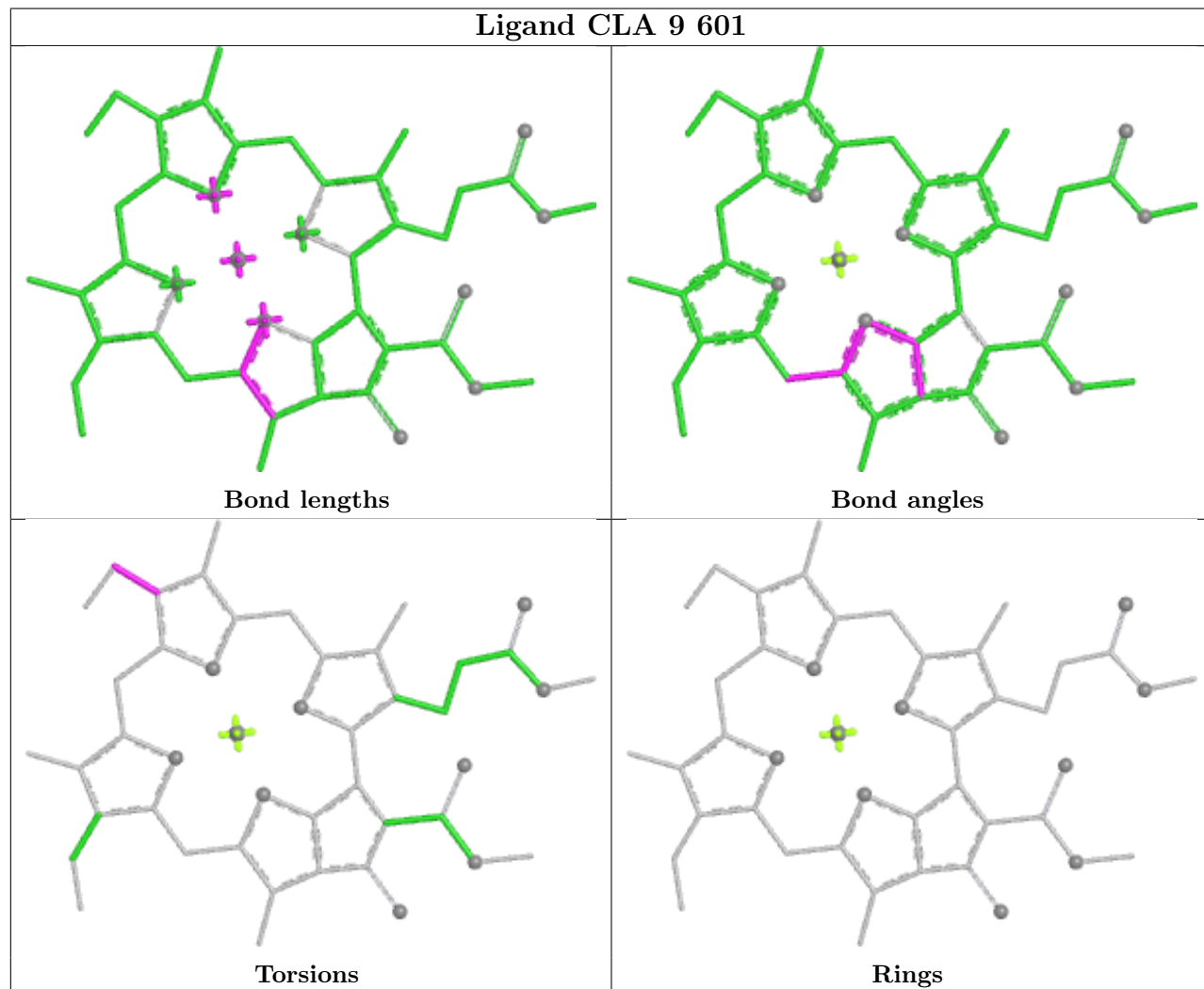


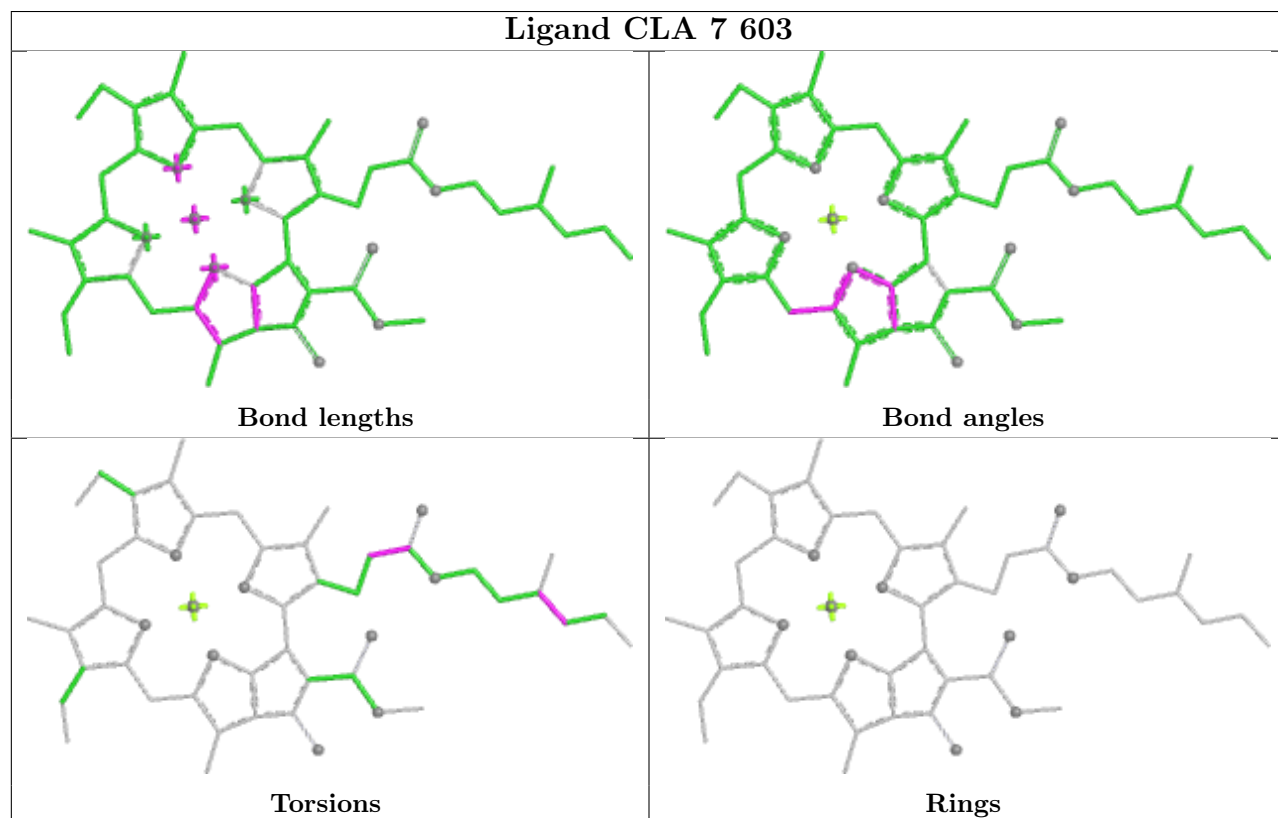
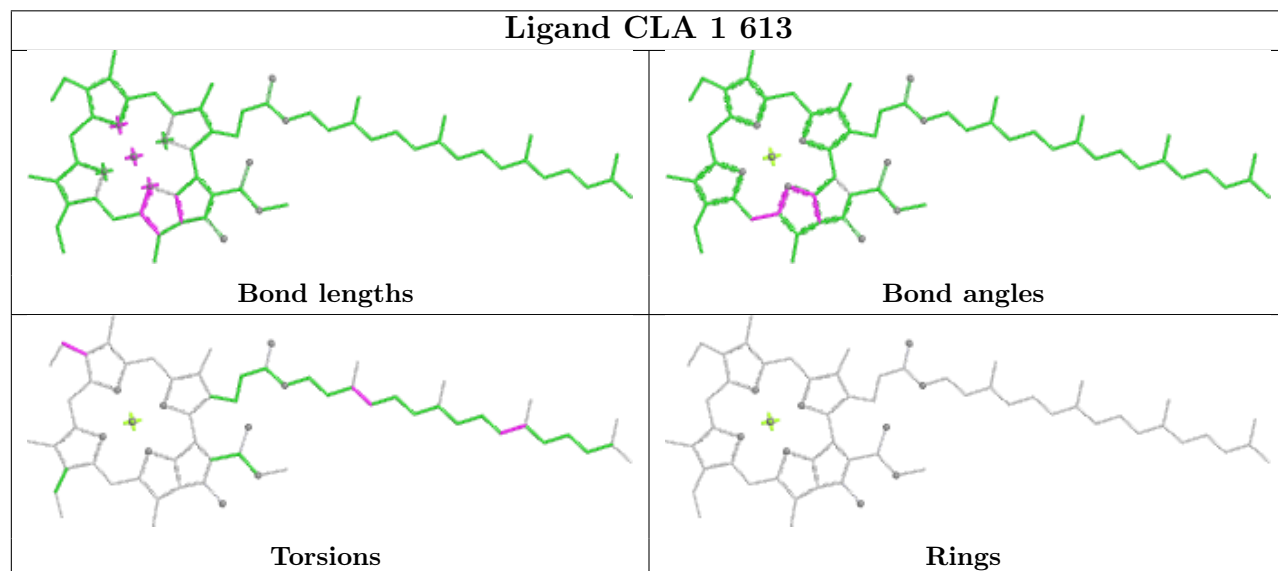
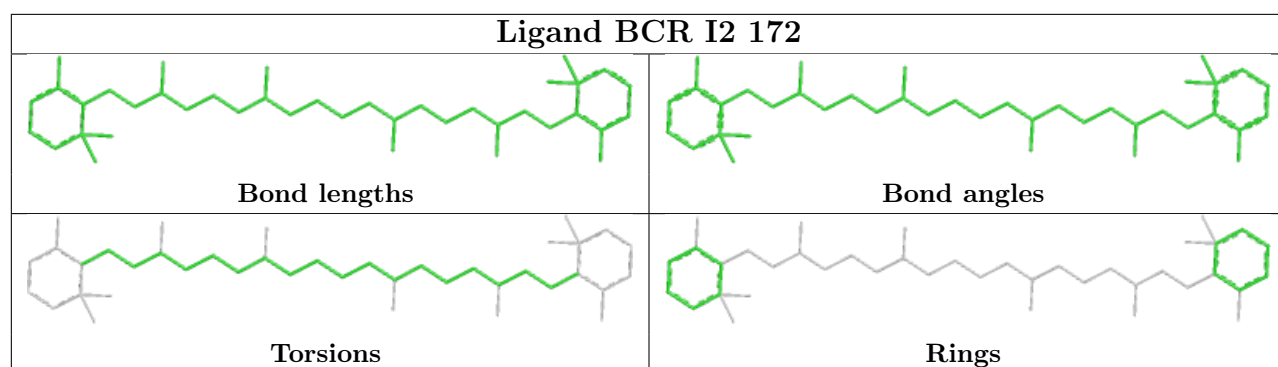
Rings

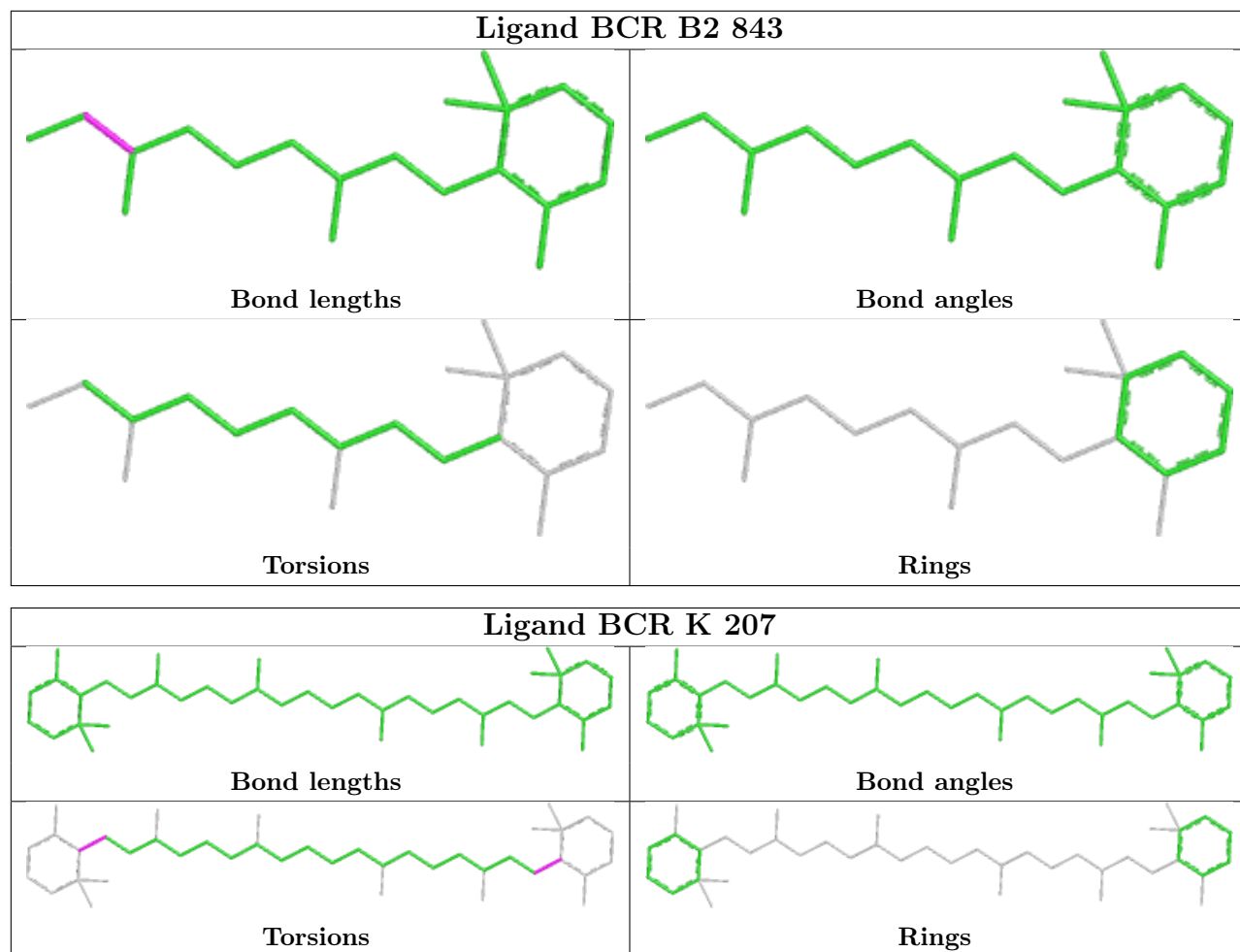




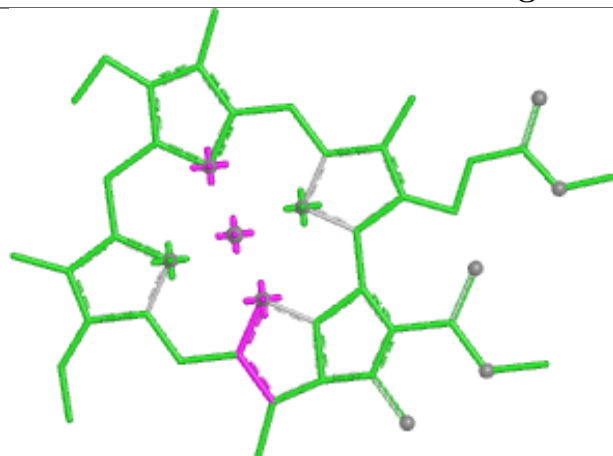


Ligand CLA 6 613**Ligand CLA 9 601**

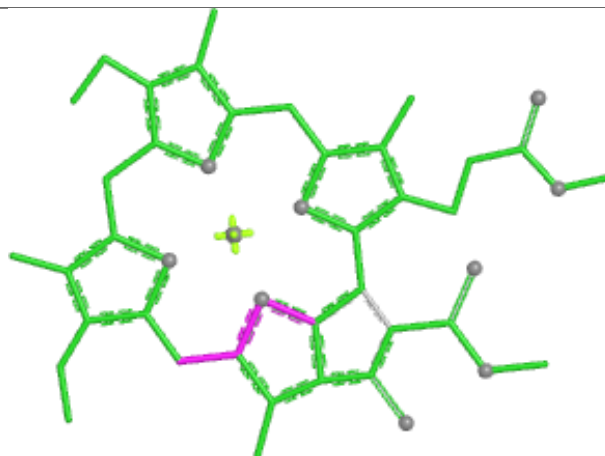




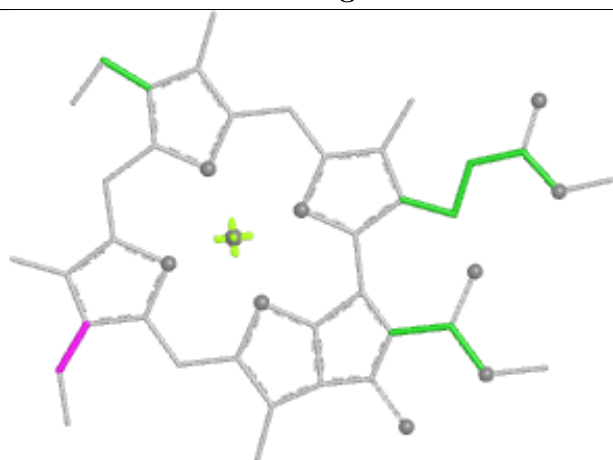
Ligand CLA 3 617



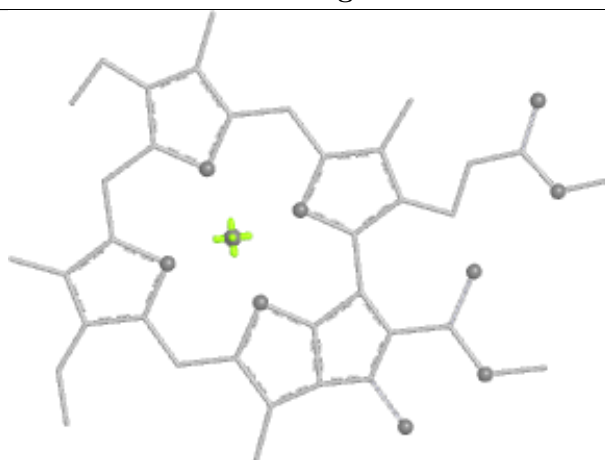
Bond lengths



Bond angles

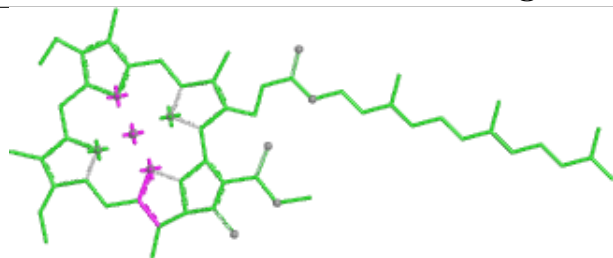


Torsions

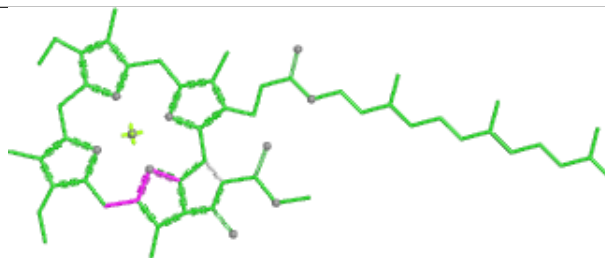


Rings

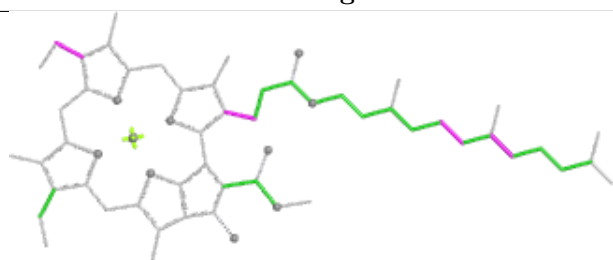
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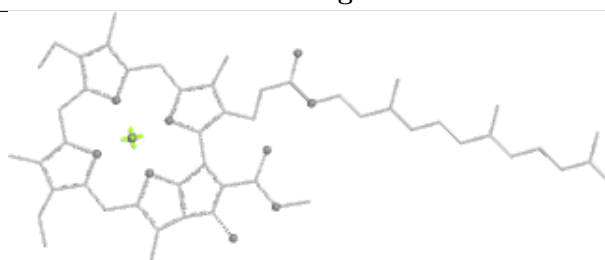
Bond lengths



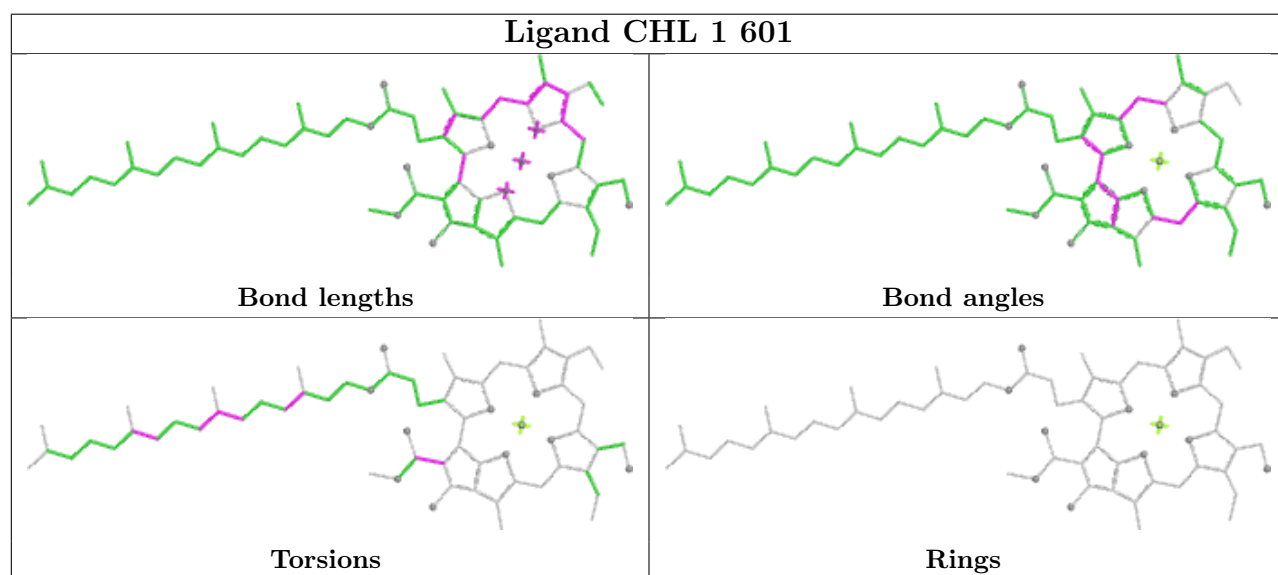
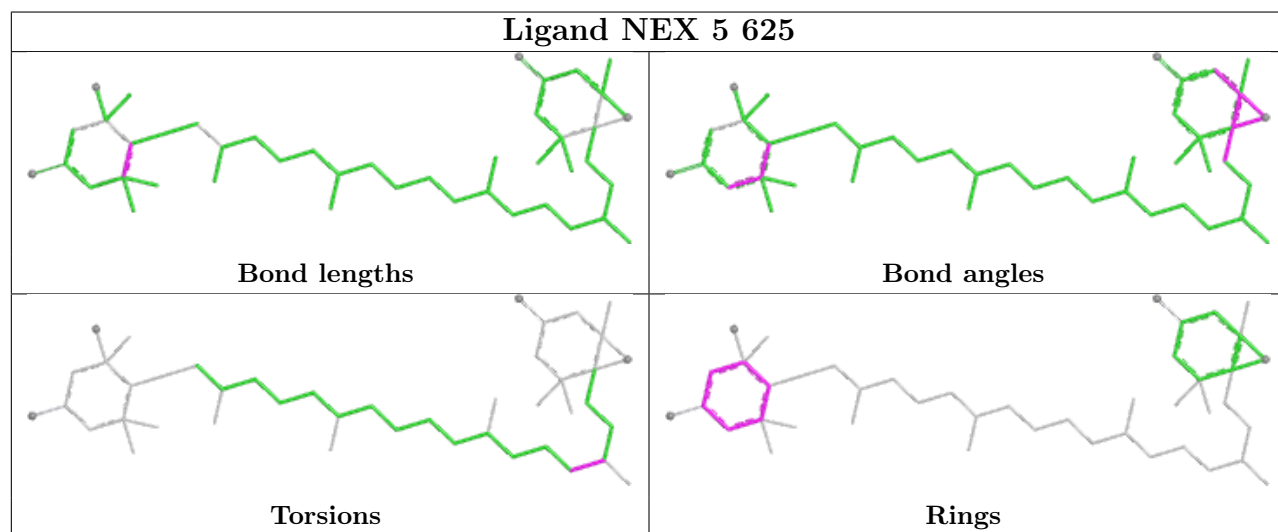
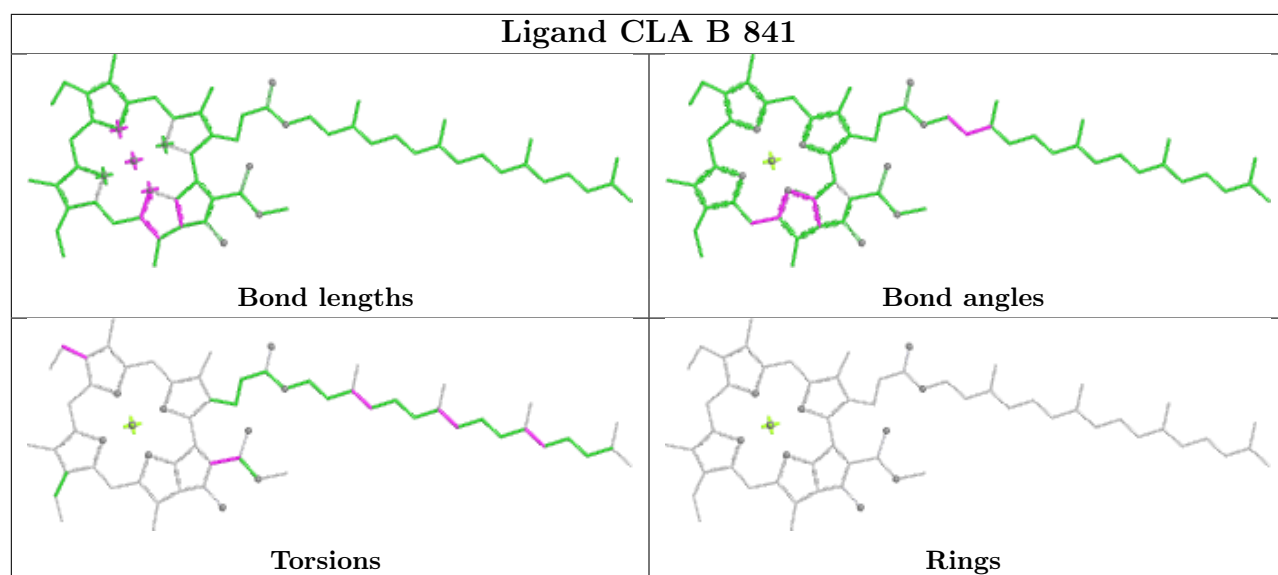
Bond angles



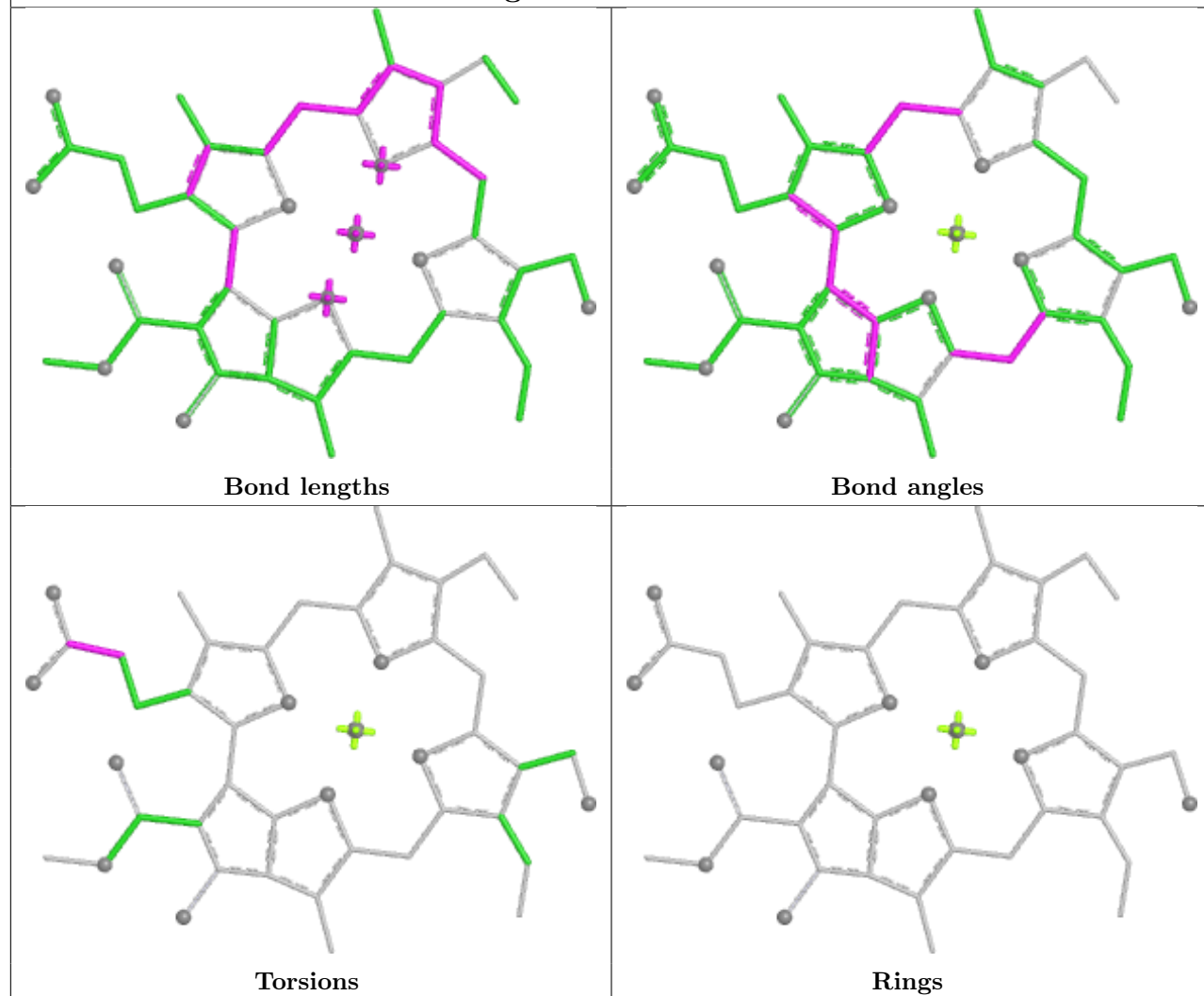
Torsions



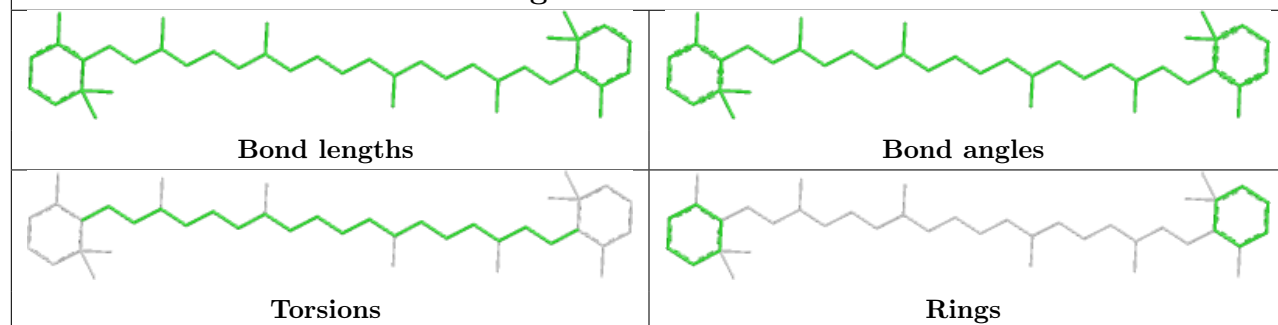
Rings

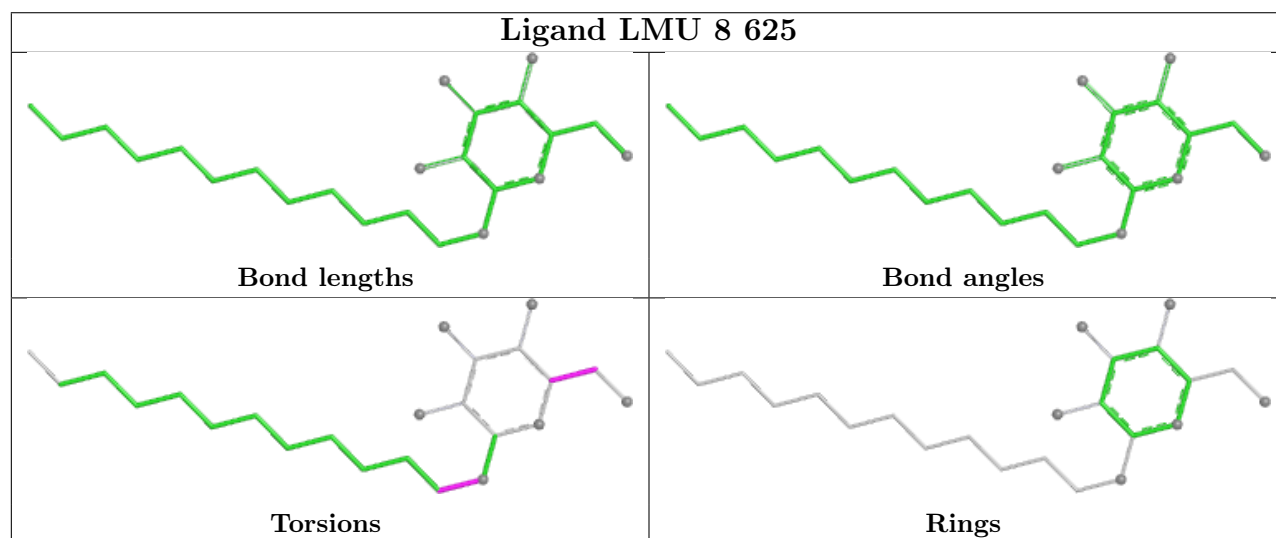
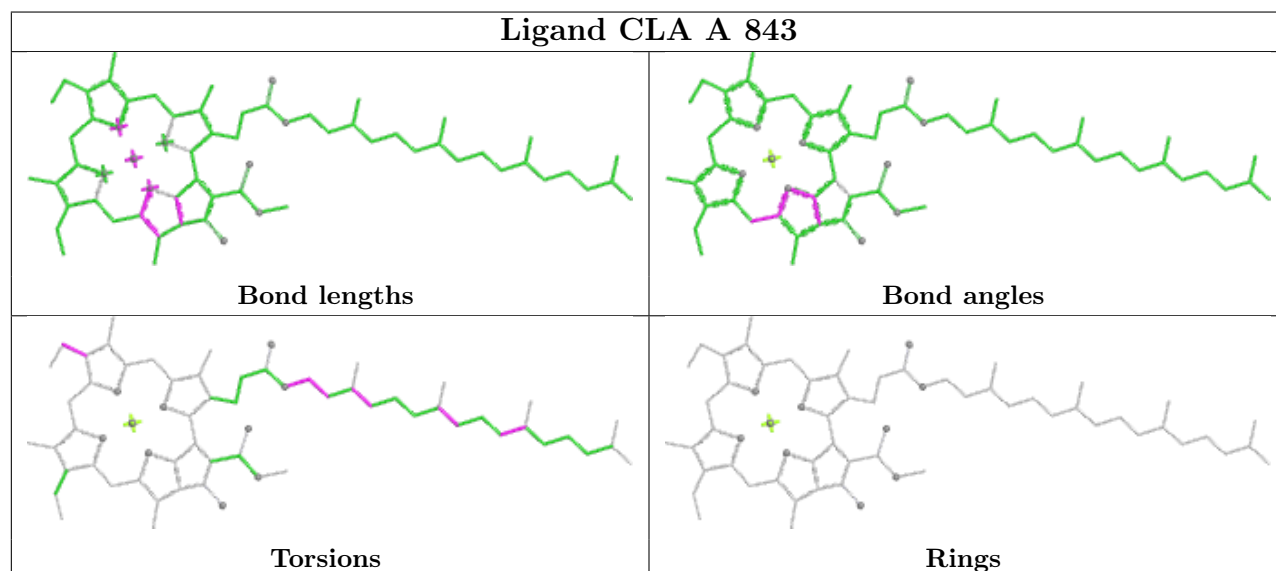
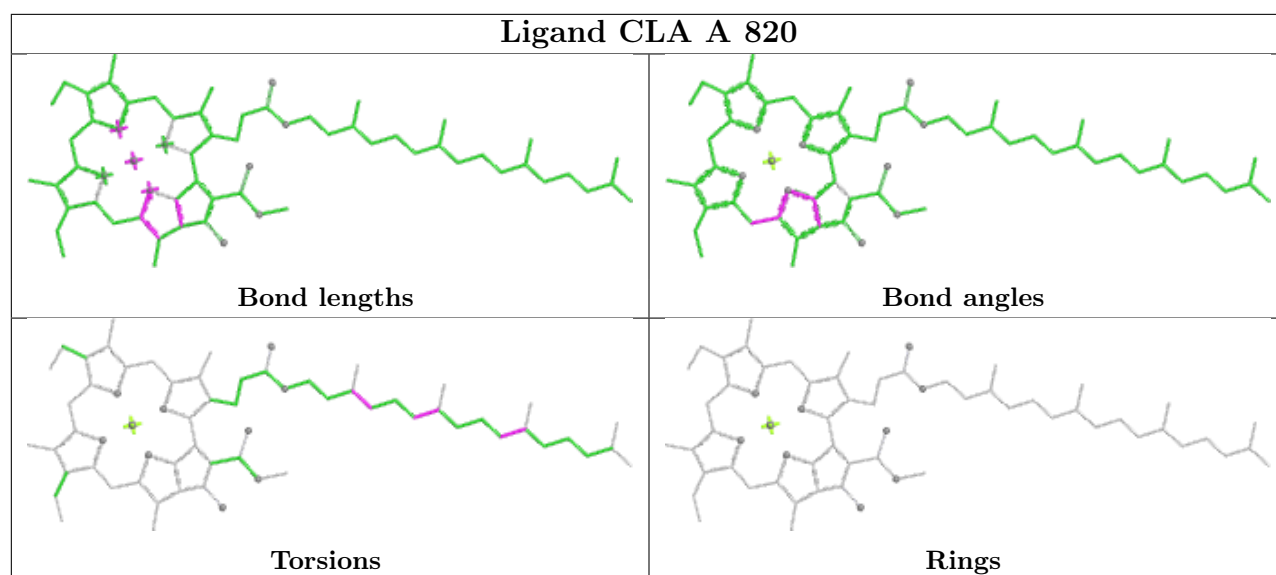


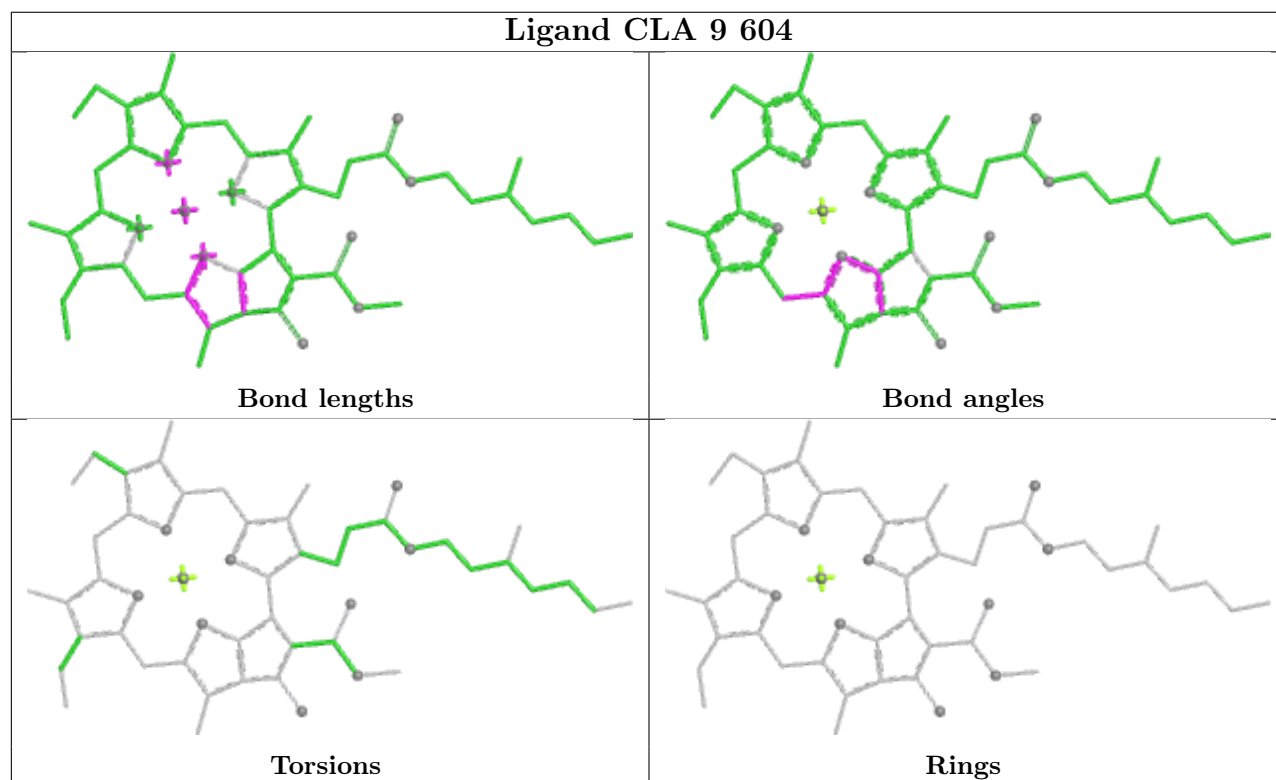
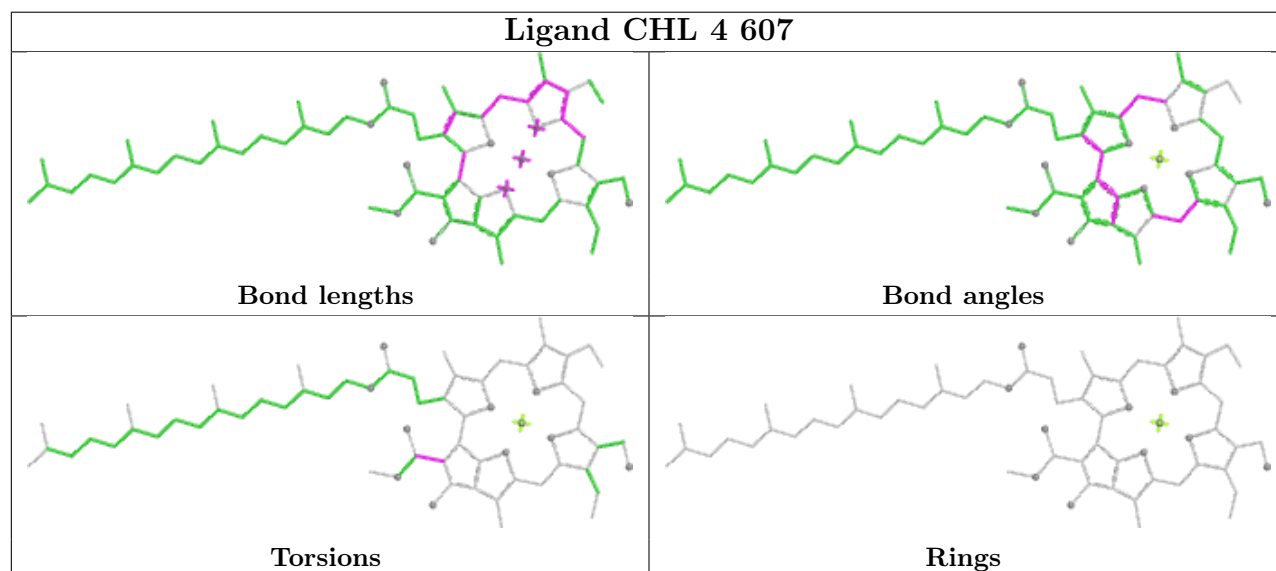
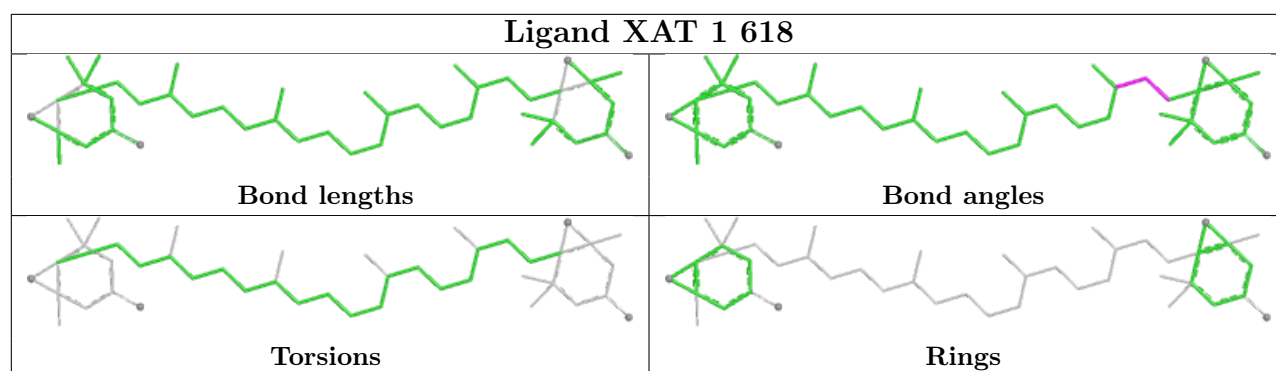
Ligand CHL 7 606

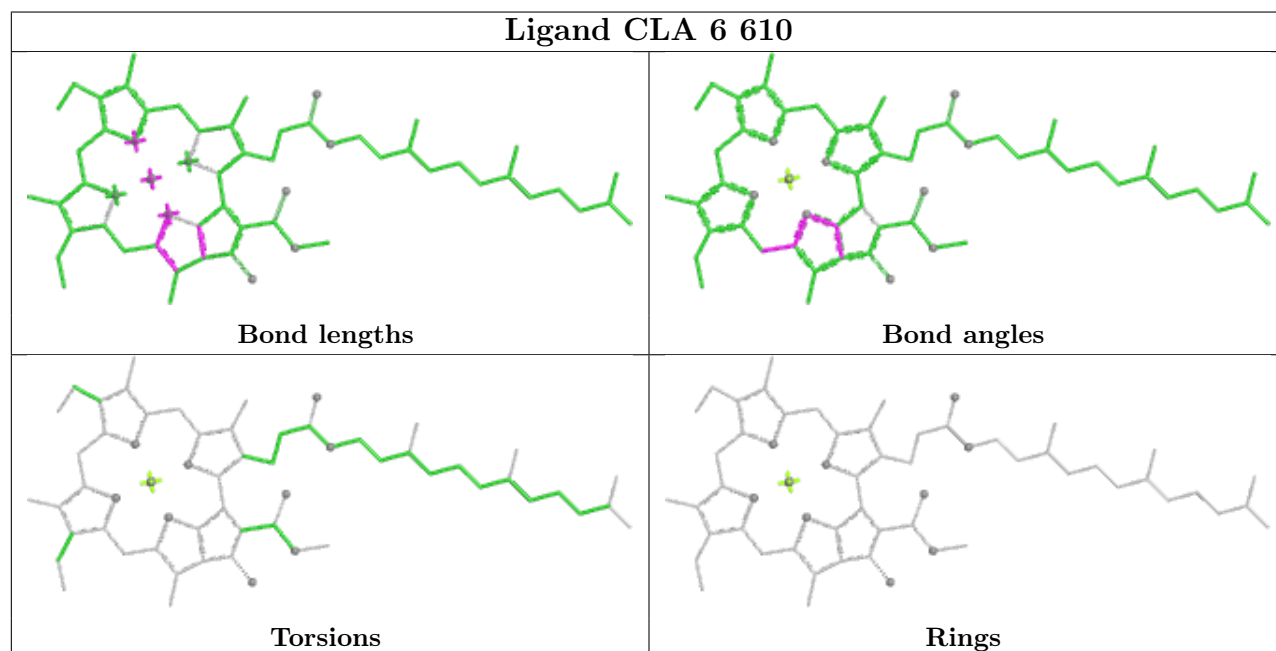
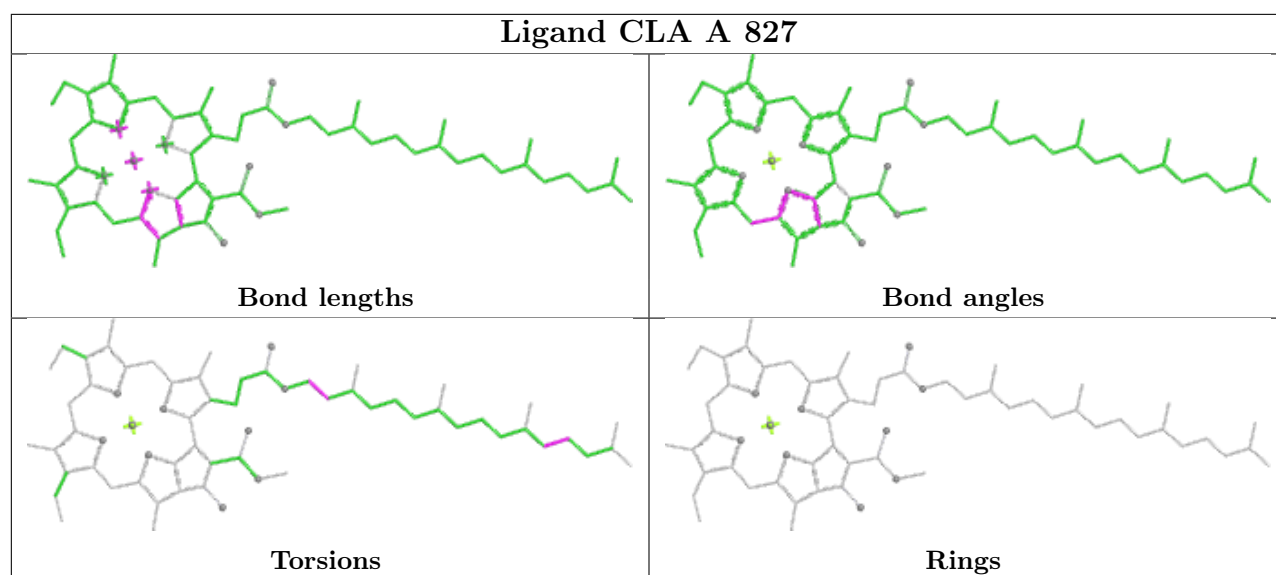


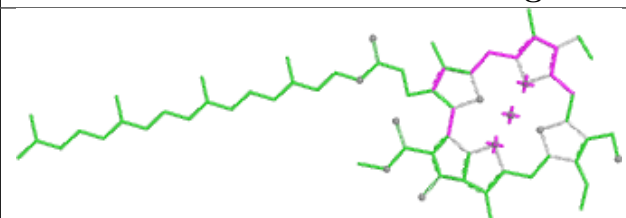
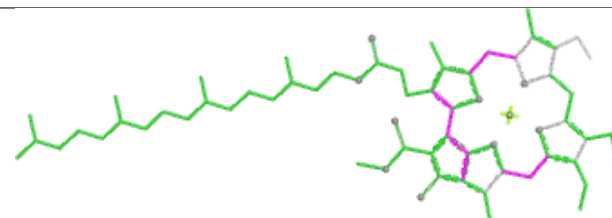
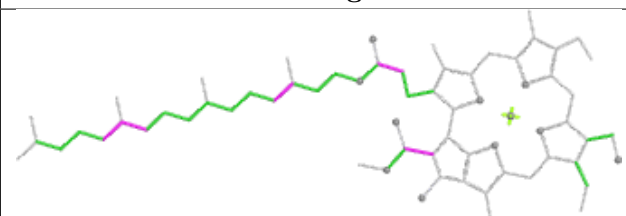
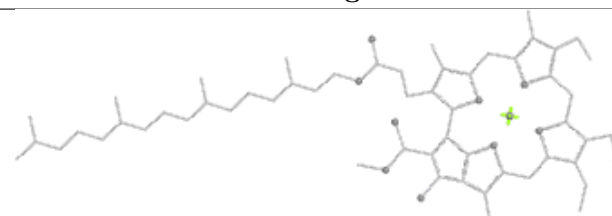
Ligand BCR A 850

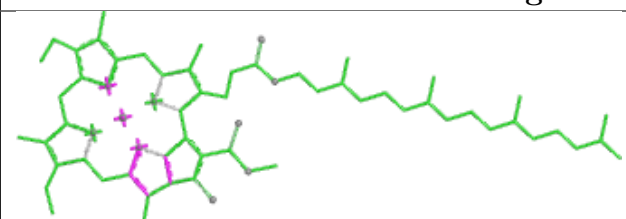
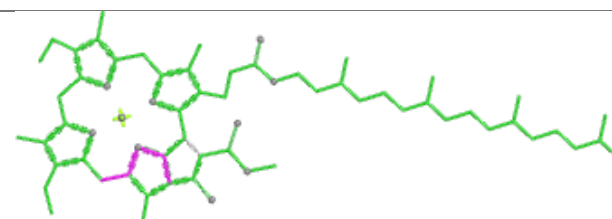
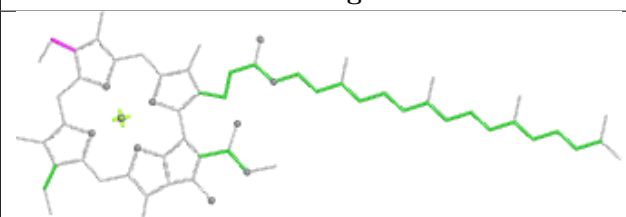
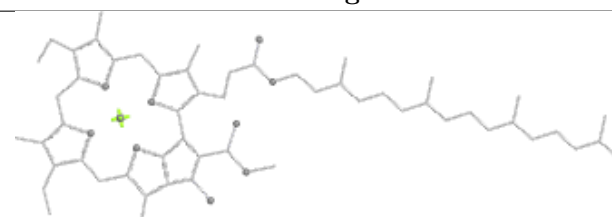


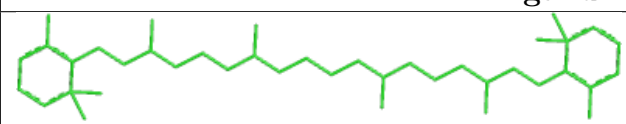
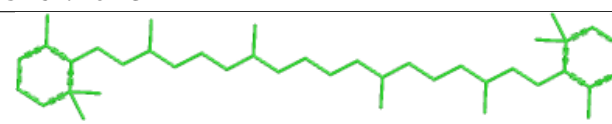
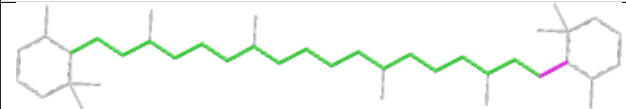
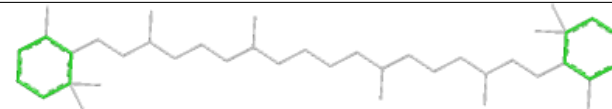


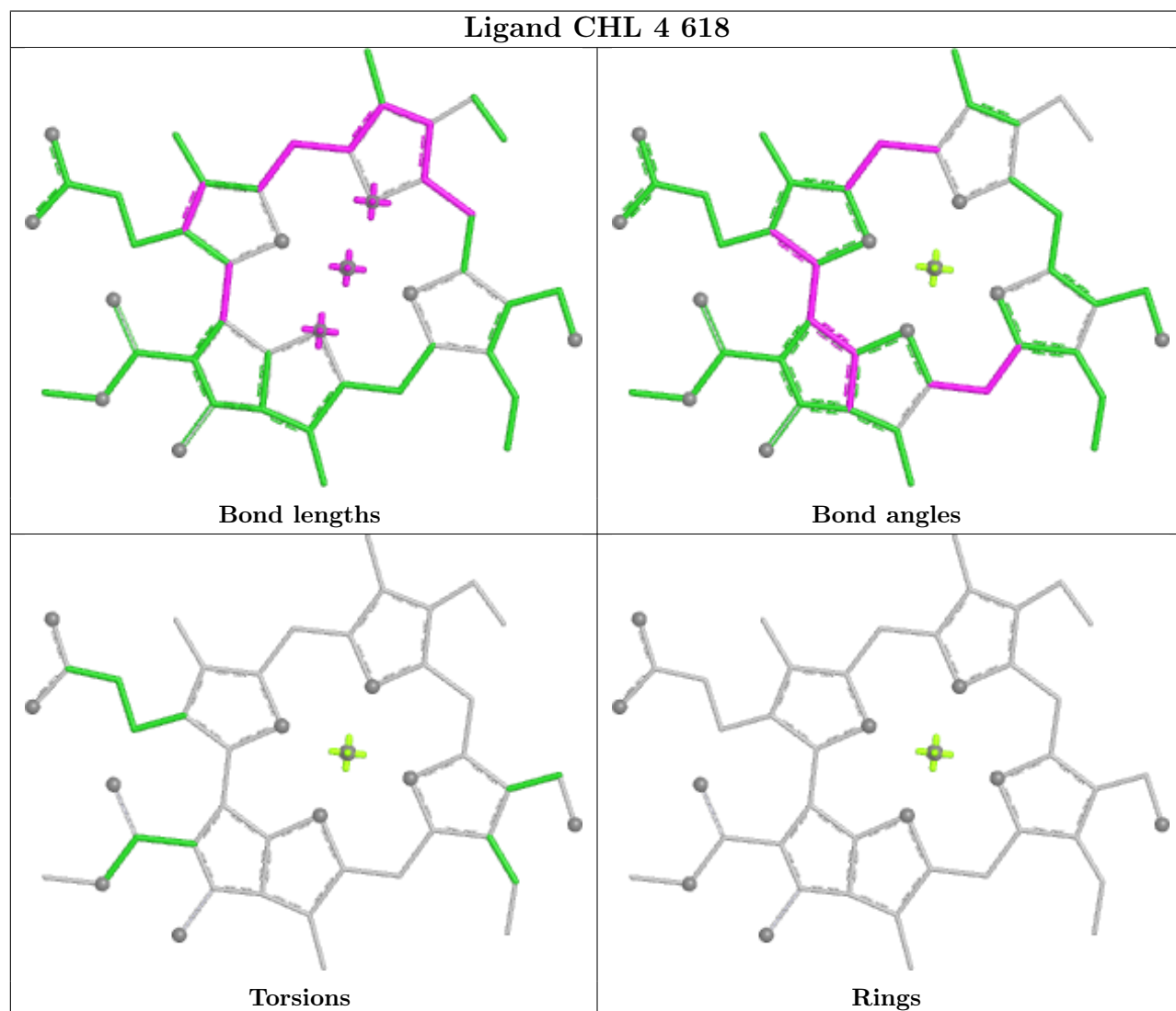
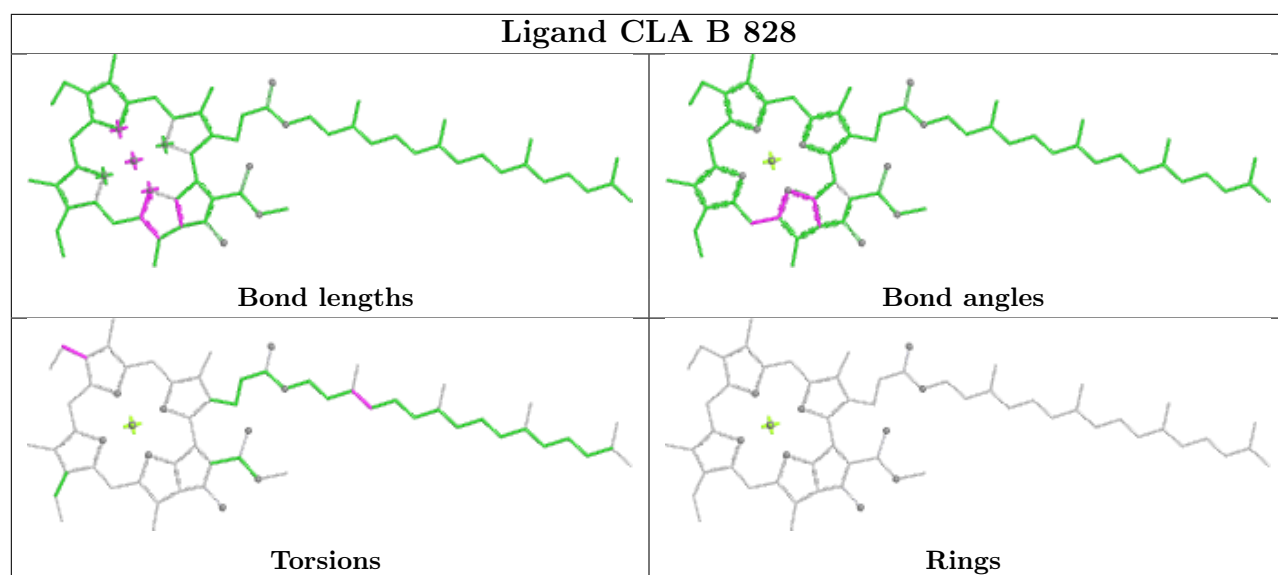


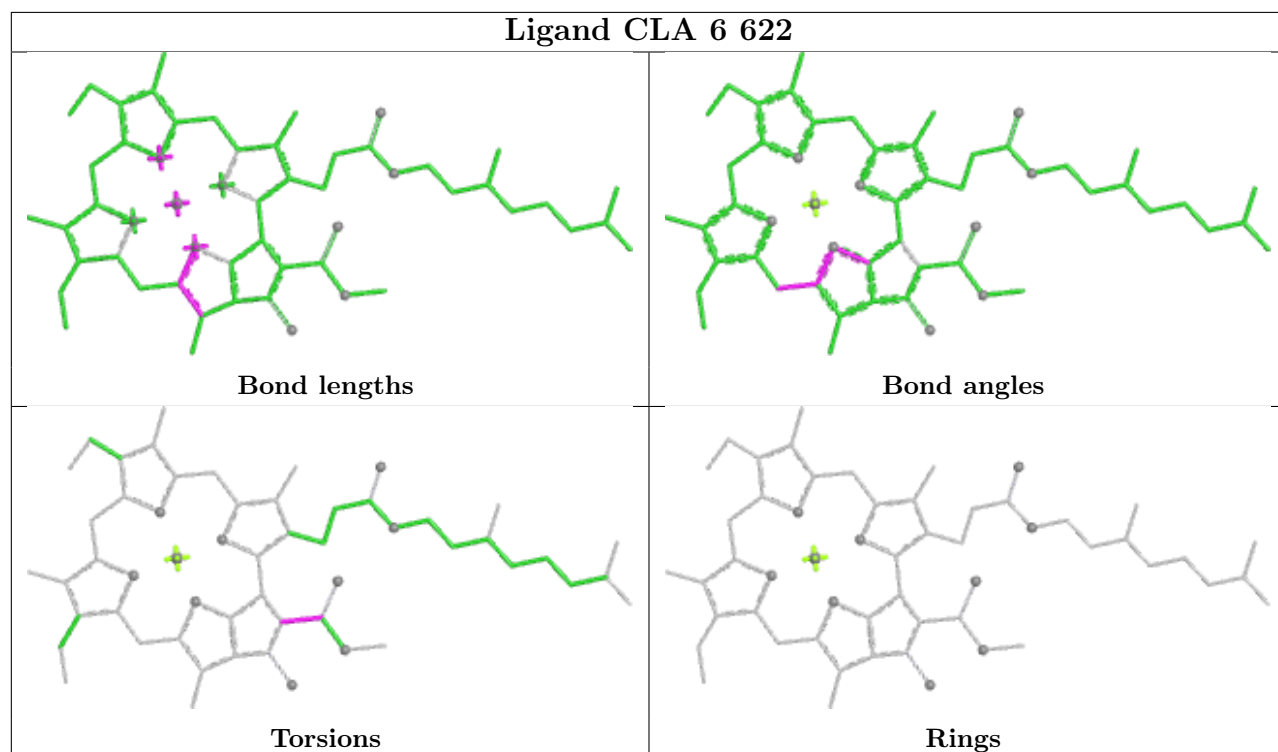
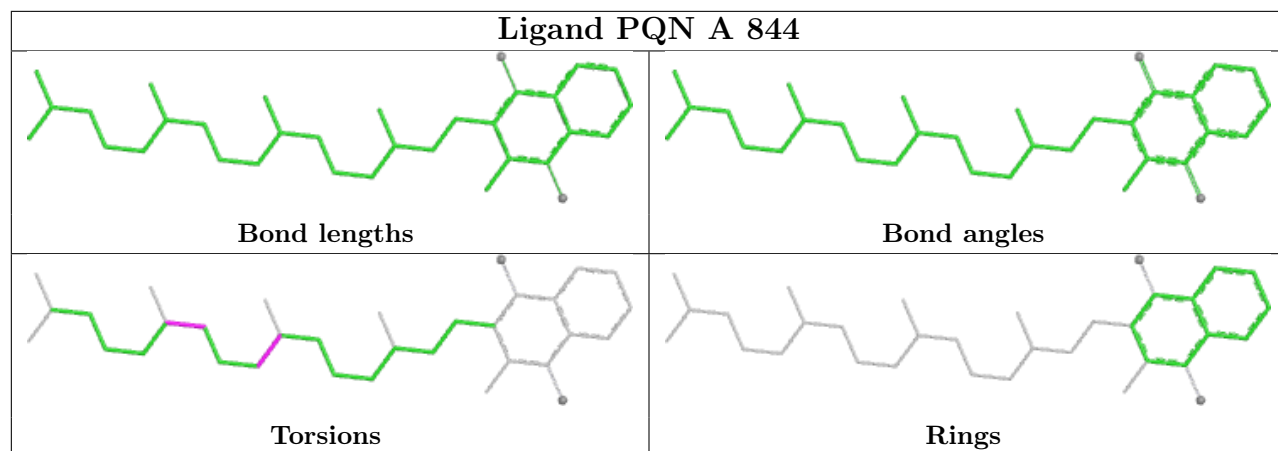


Ligand CHL 8 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

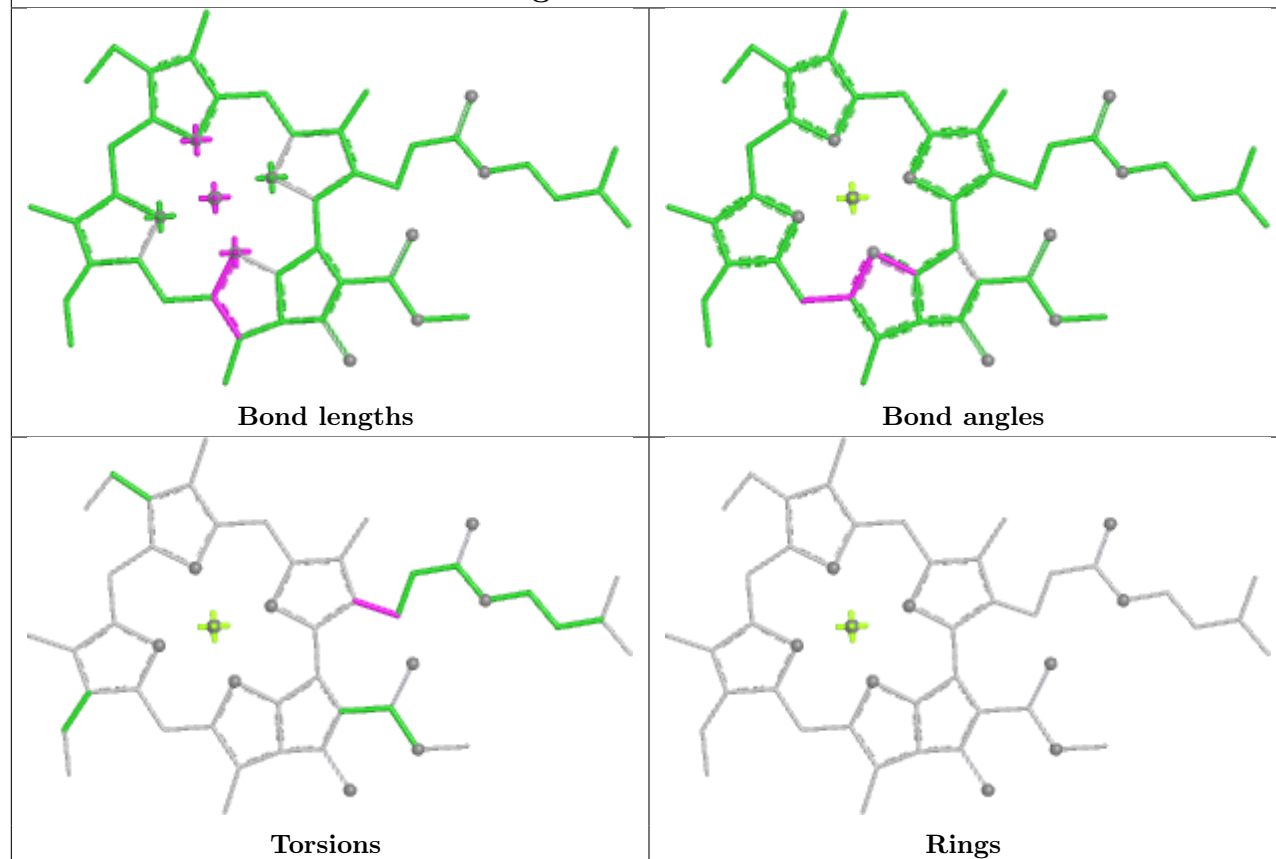
Ligand CLA 1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR 7 623	
	
Bond lengths	Bond angles
	
Torsions	Rings

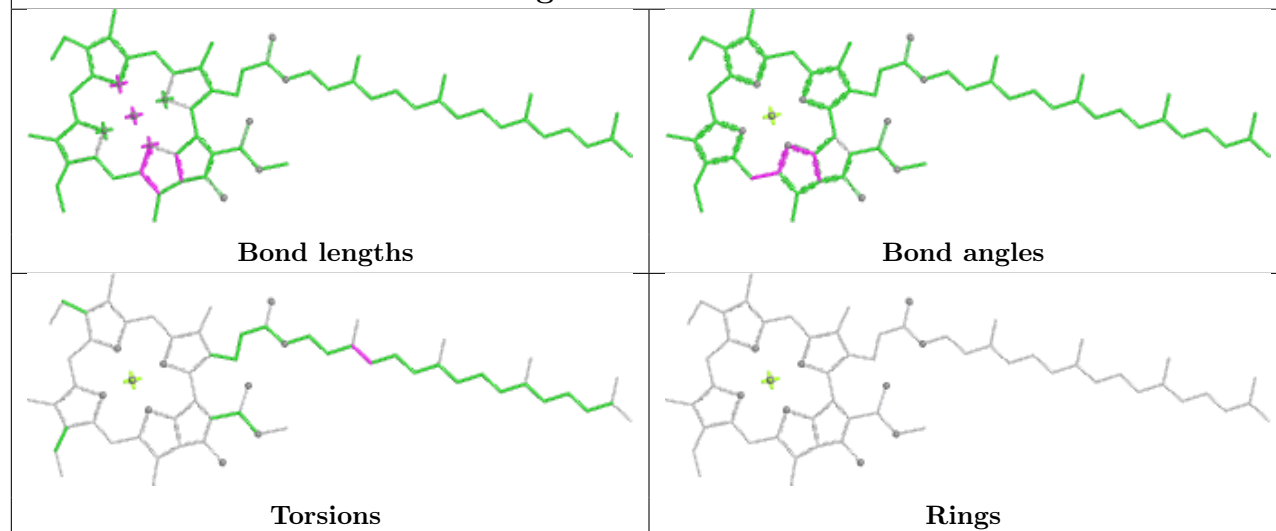


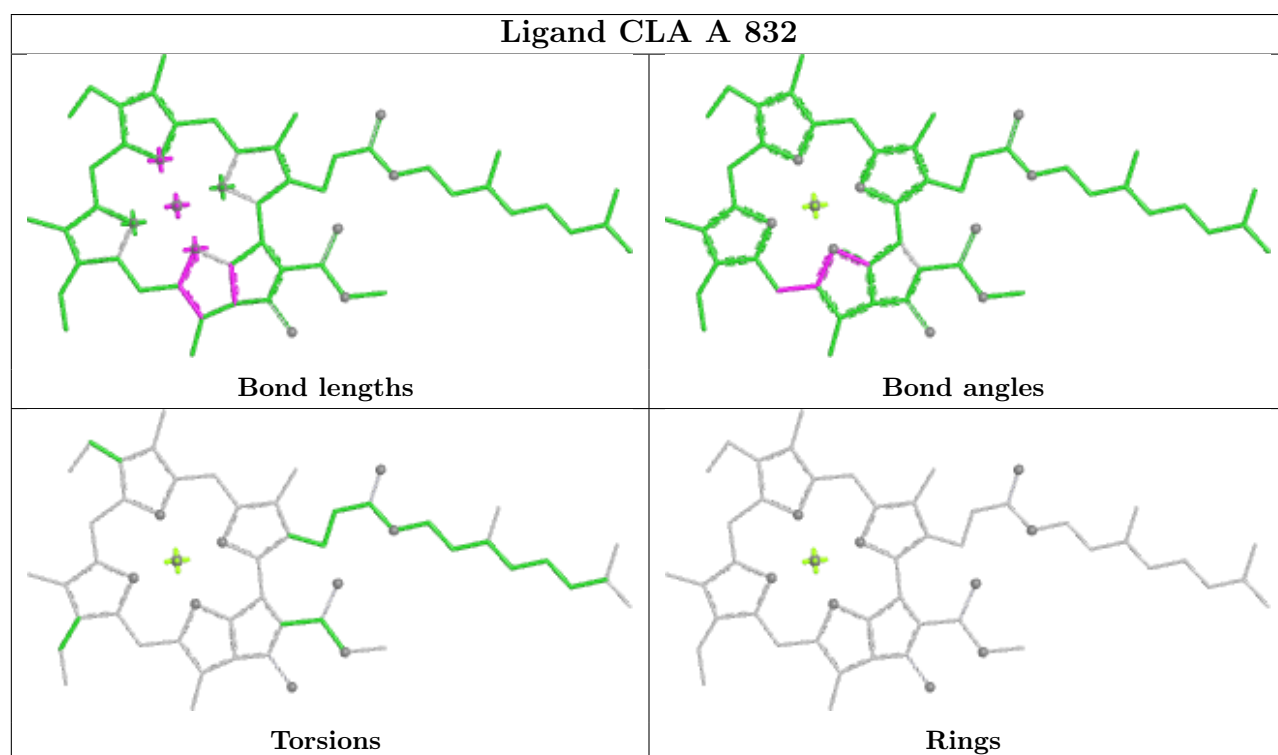
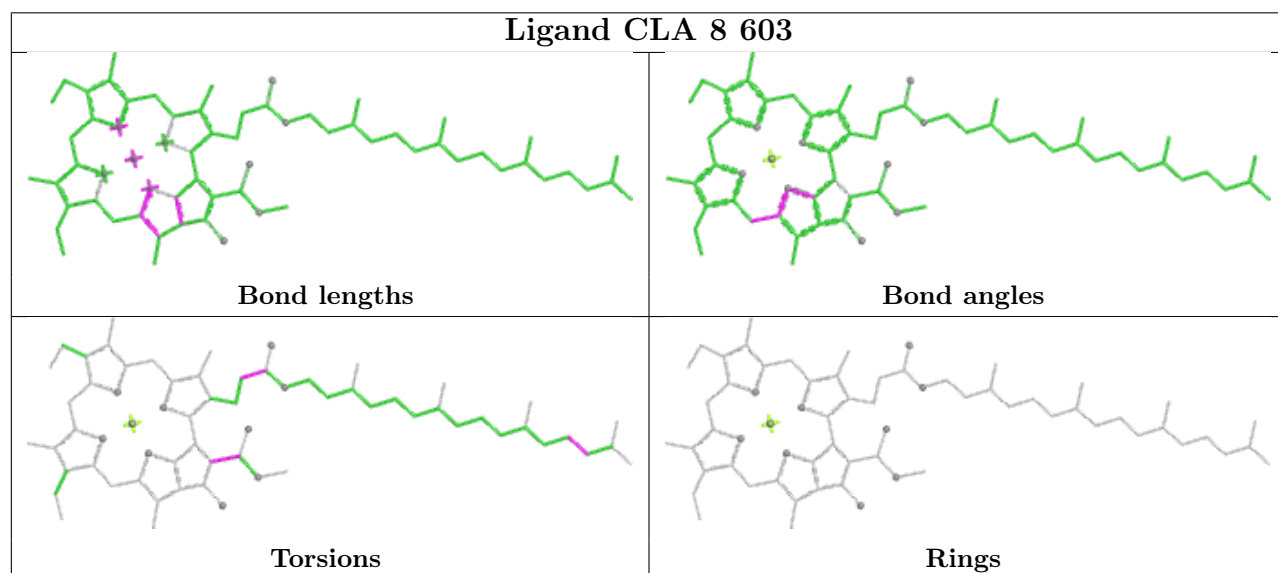
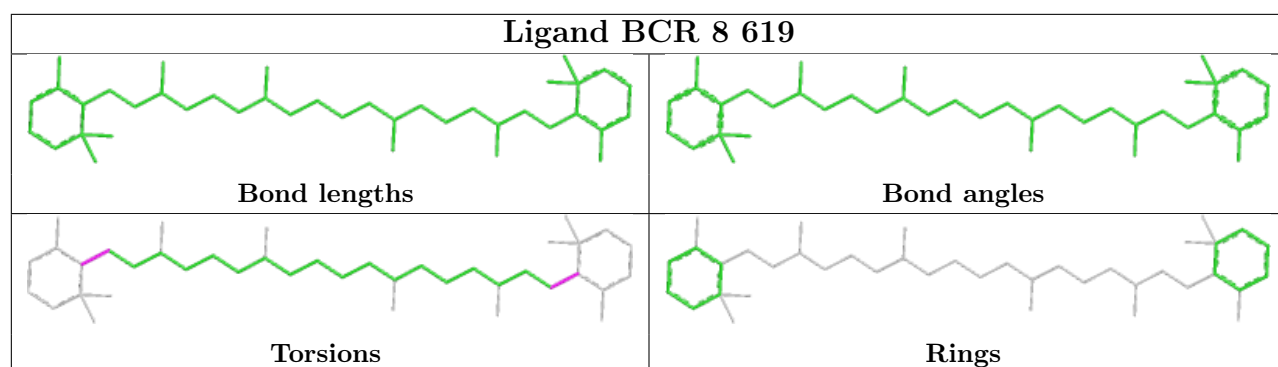


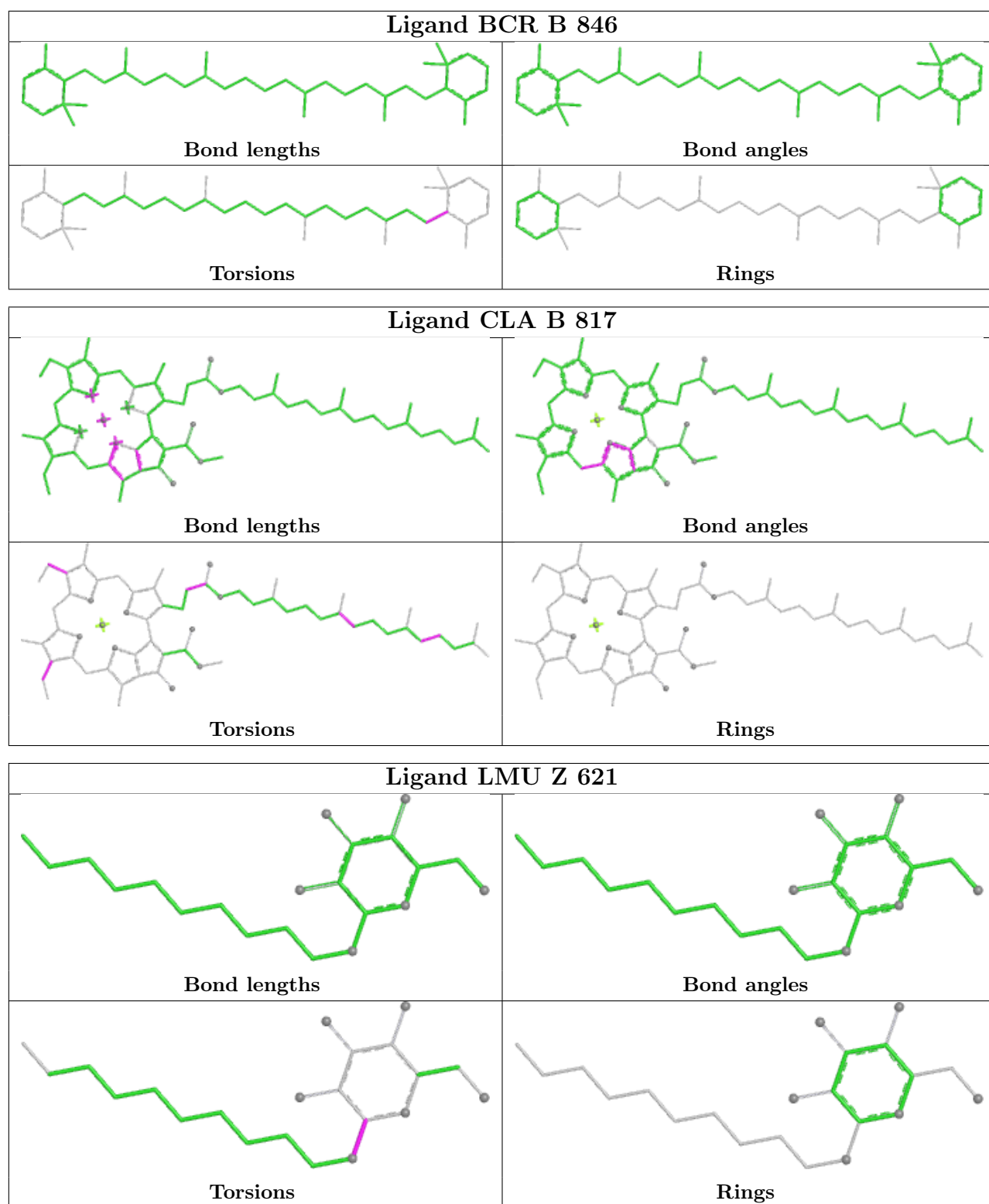
Ligand CLA B 838



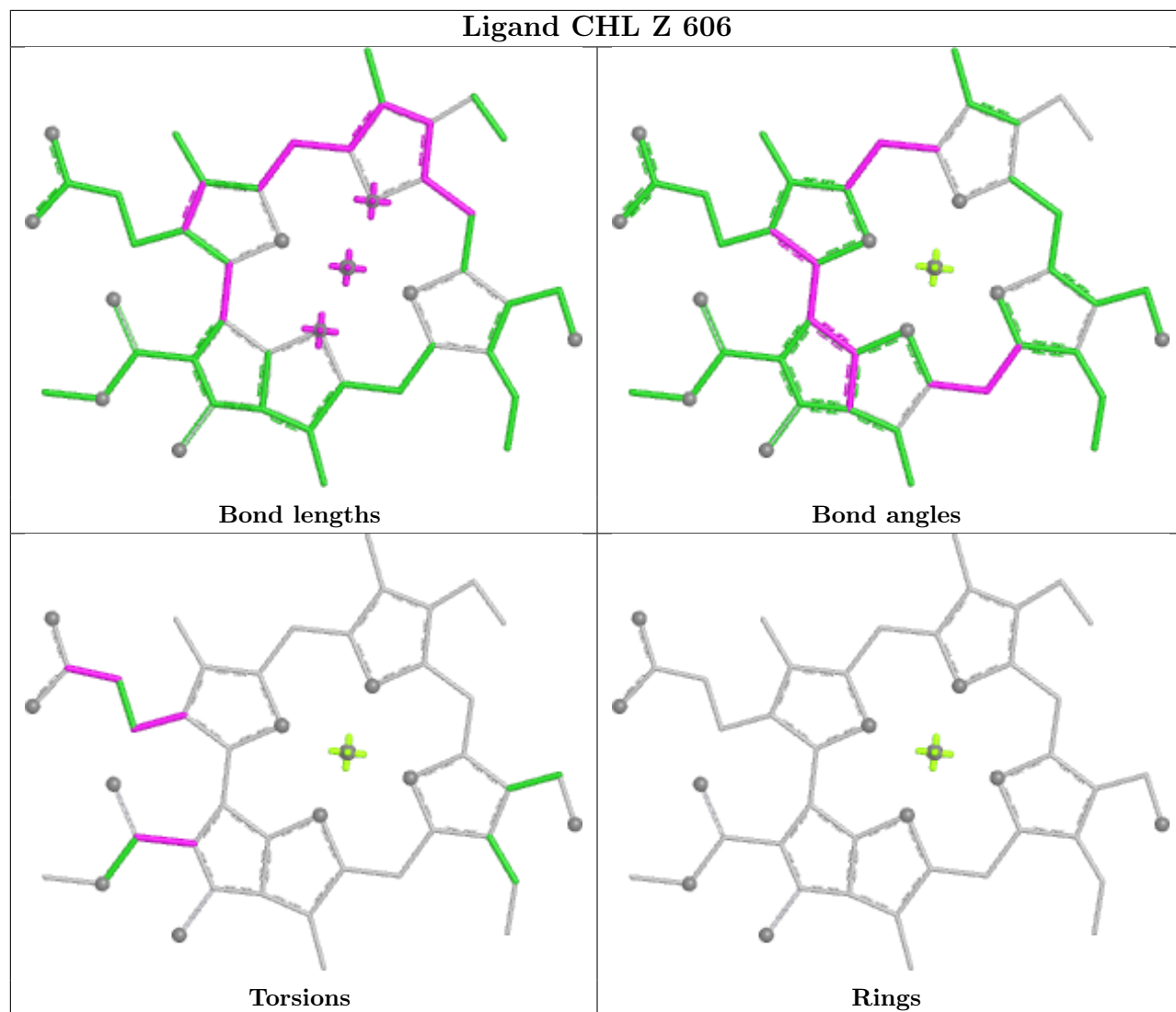
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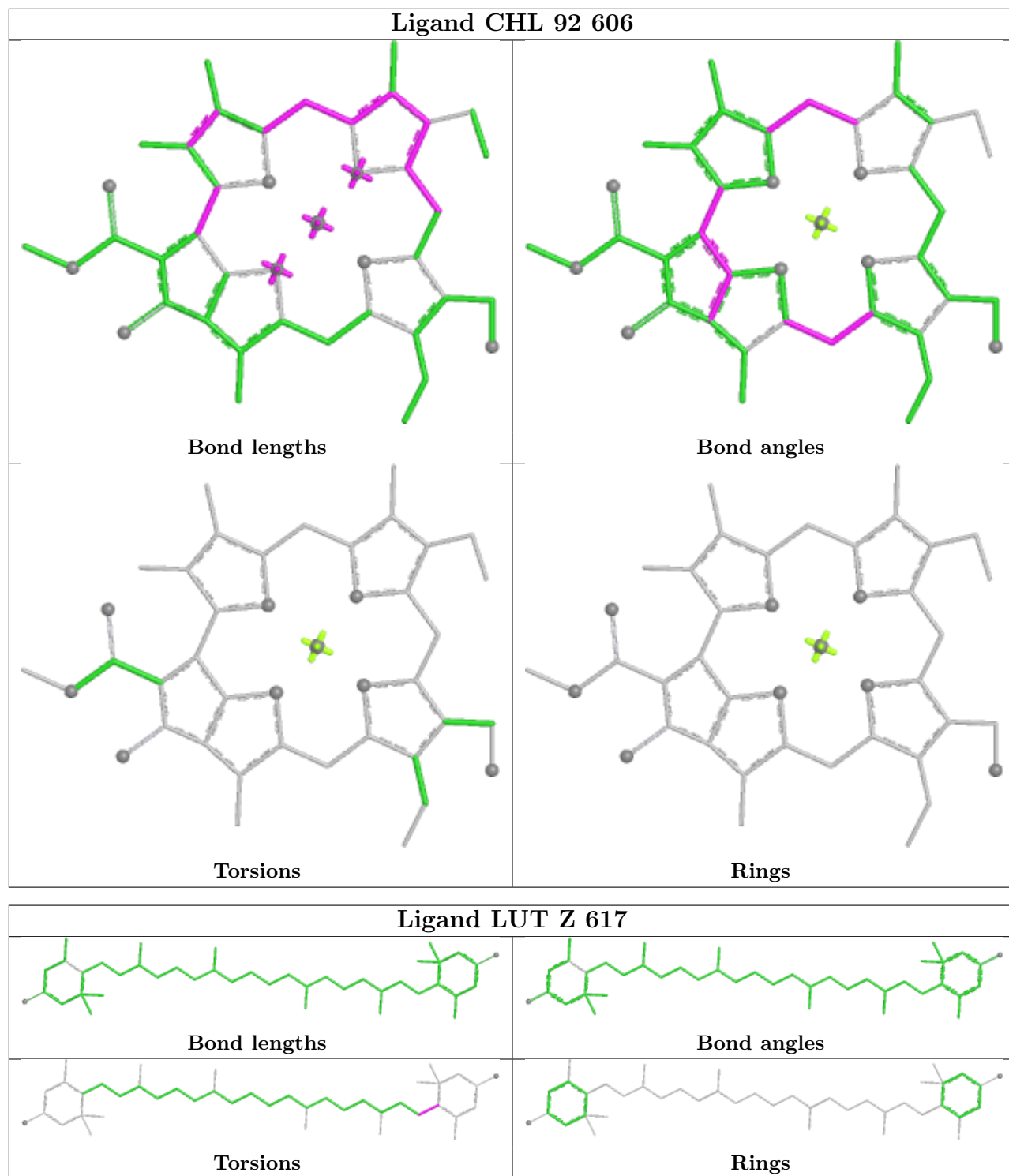


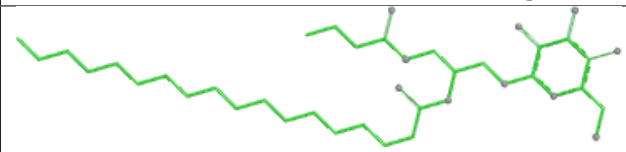
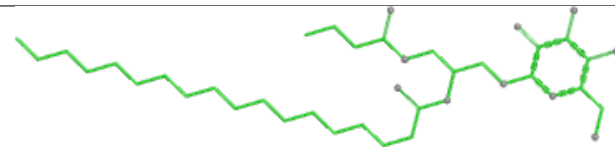
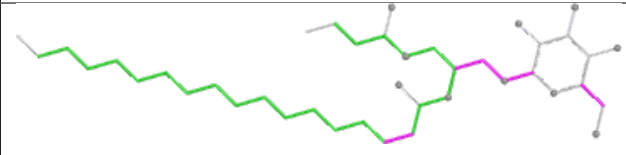
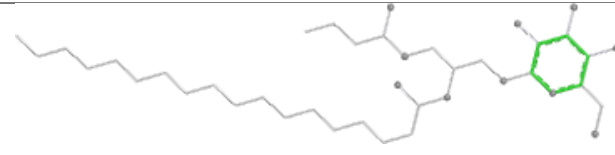


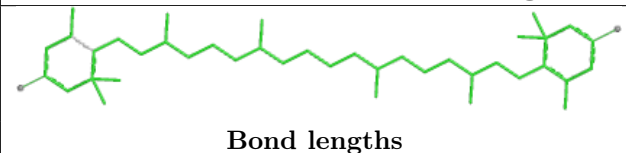
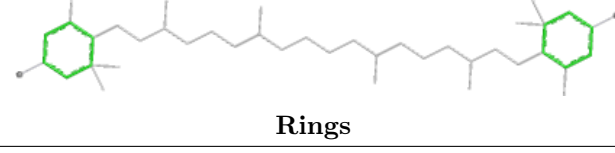


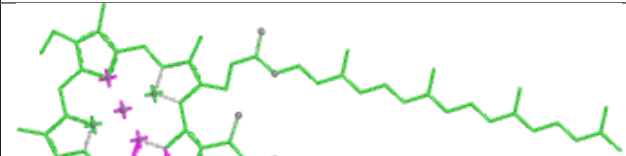
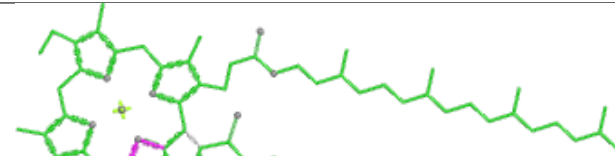
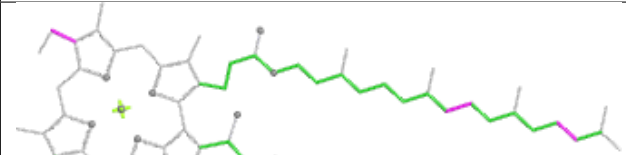
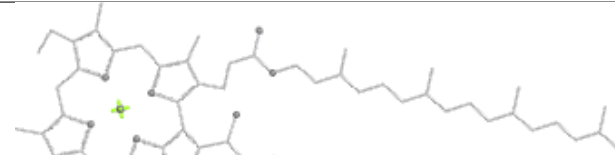
Ligand CHL Z 606

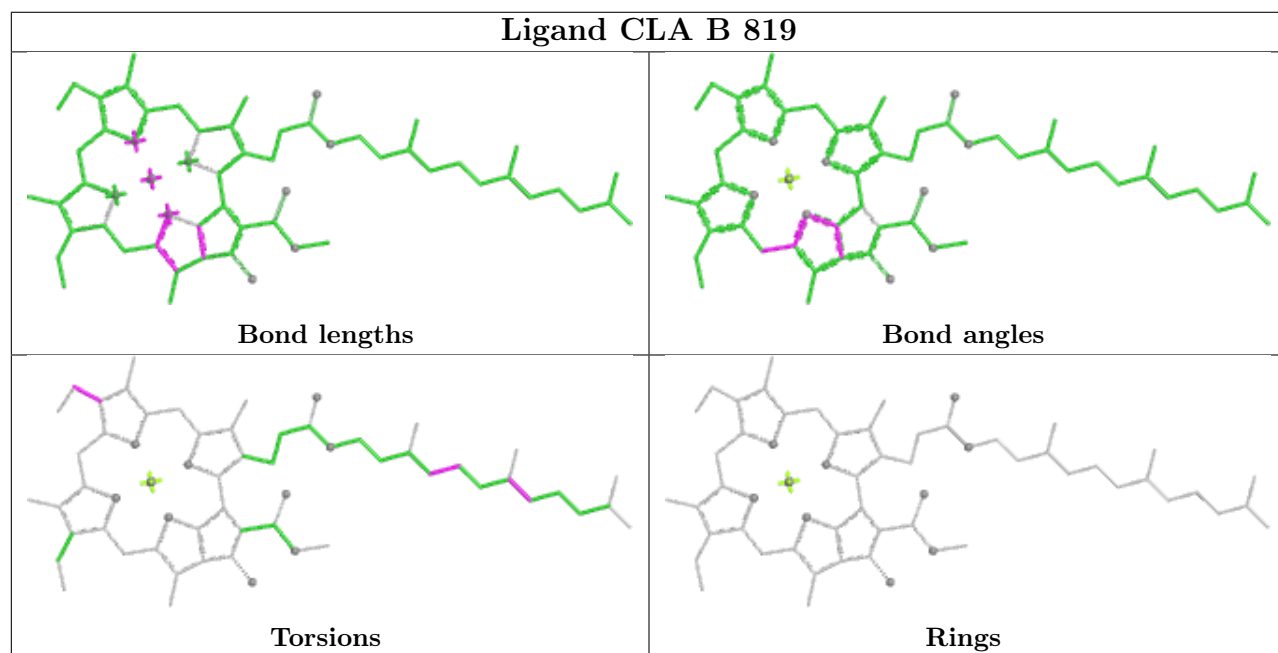
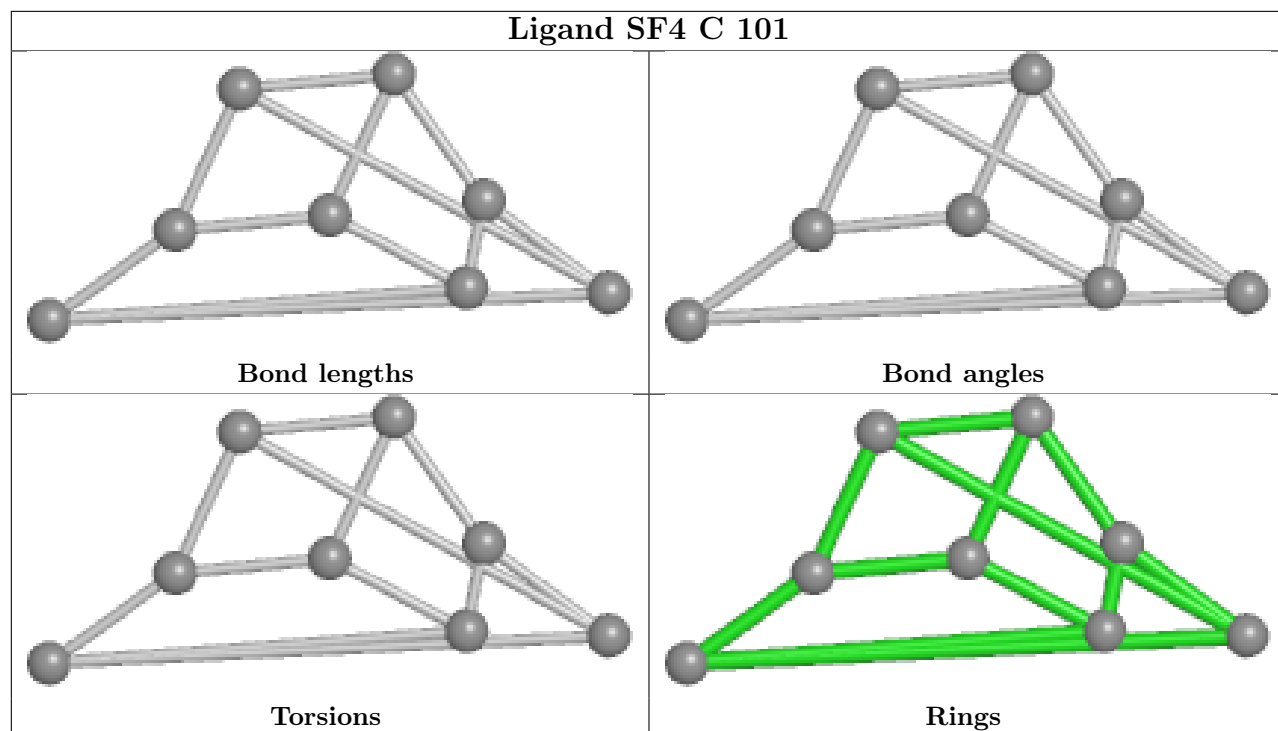


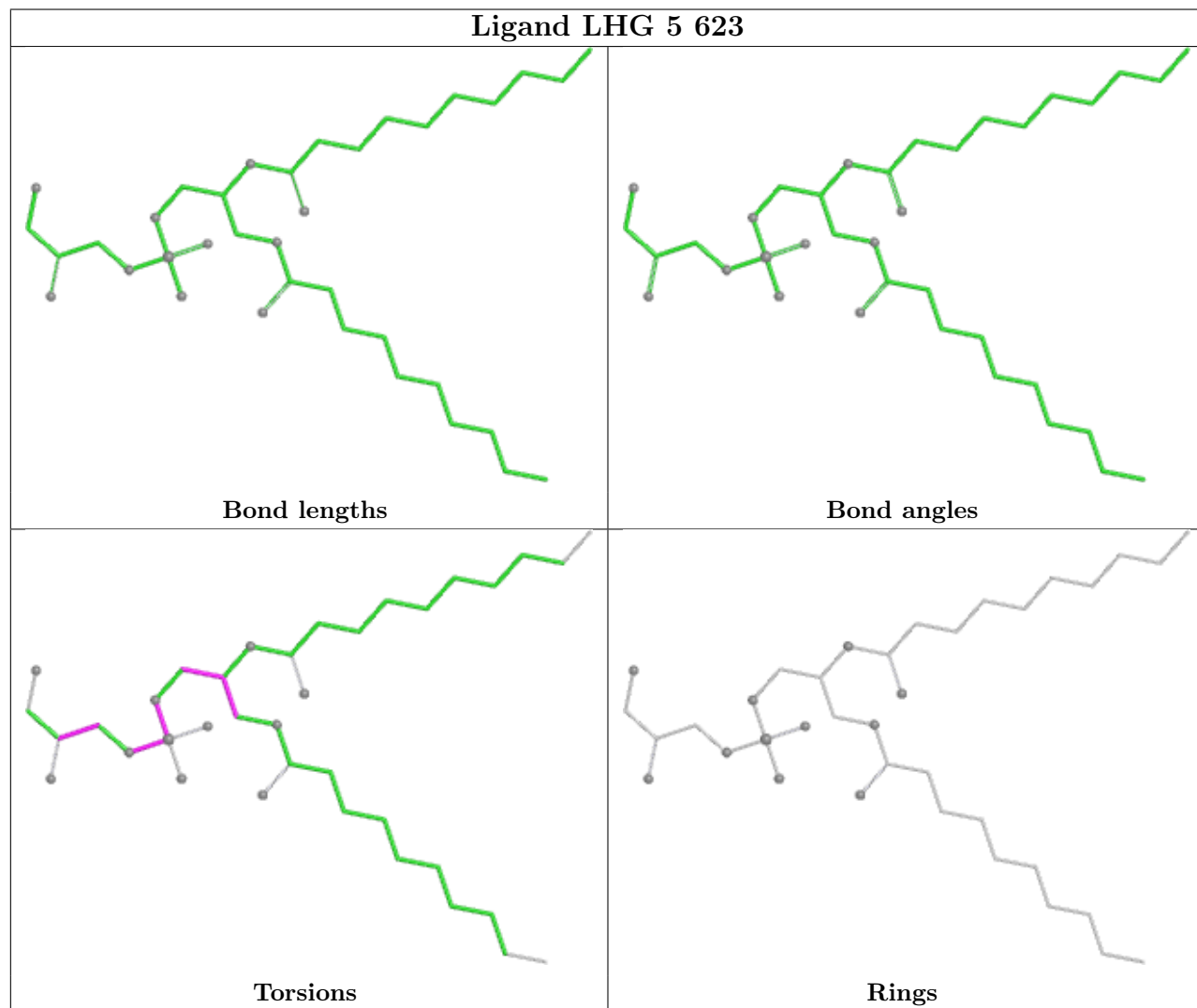
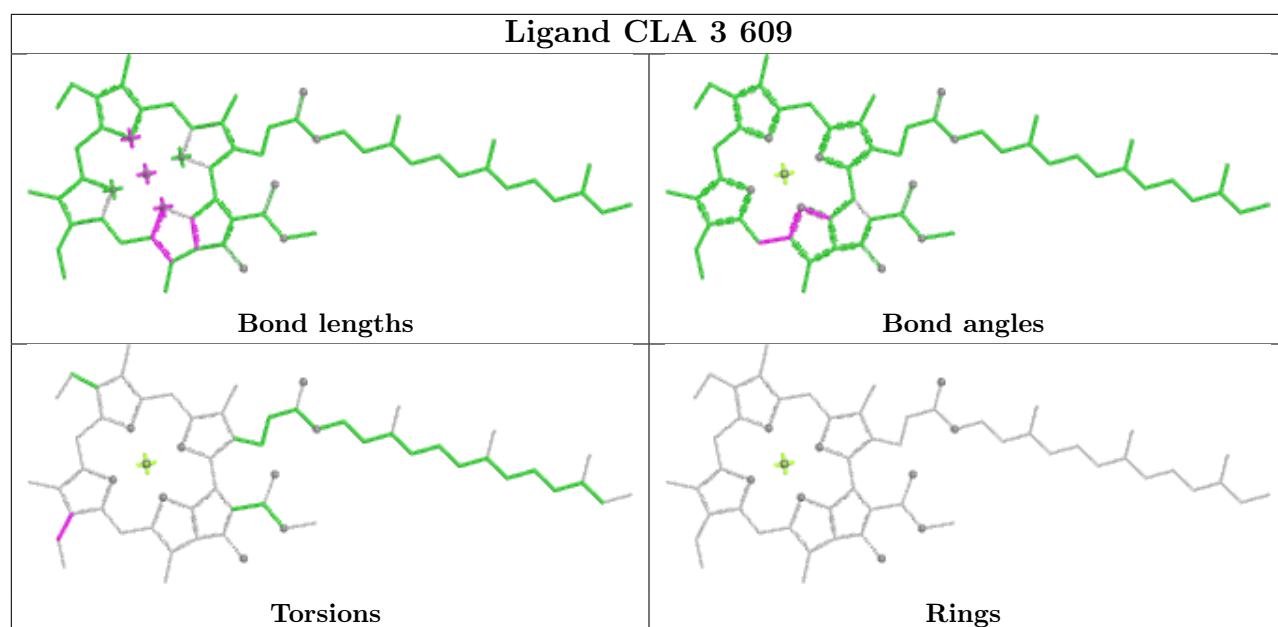


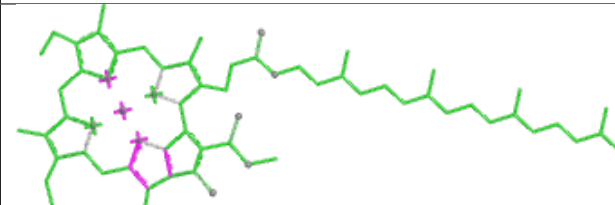
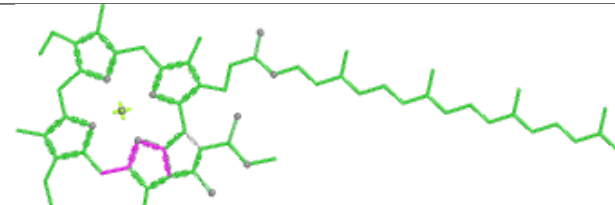
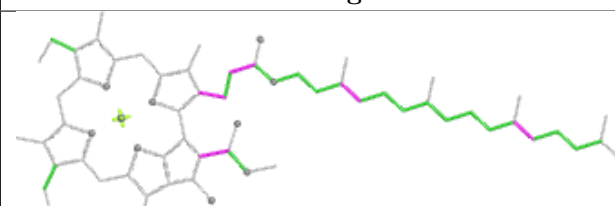
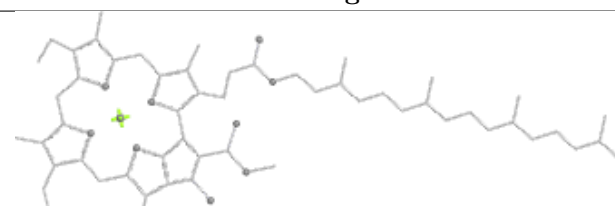
Ligand LMG 4 624	
	
Bond lengths	Bond angles
	
Torsions	Rings

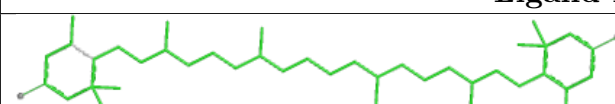
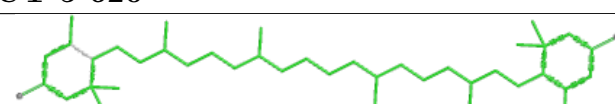
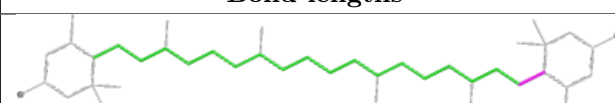
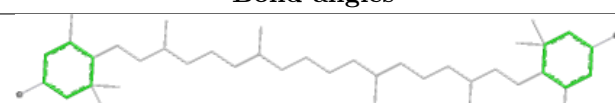
Ligand LUT A 856	
	
Bond lengths	Bond angles
	
Torsions	Rings

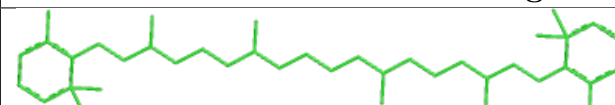
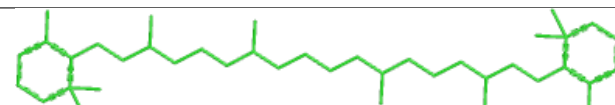
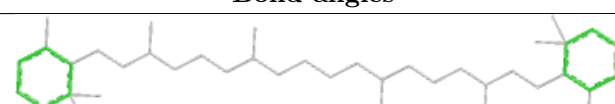
Ligand CLA 92 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

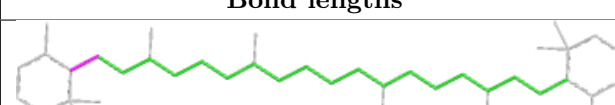
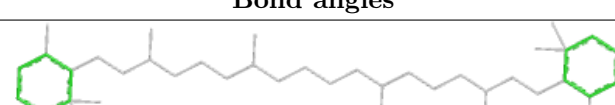


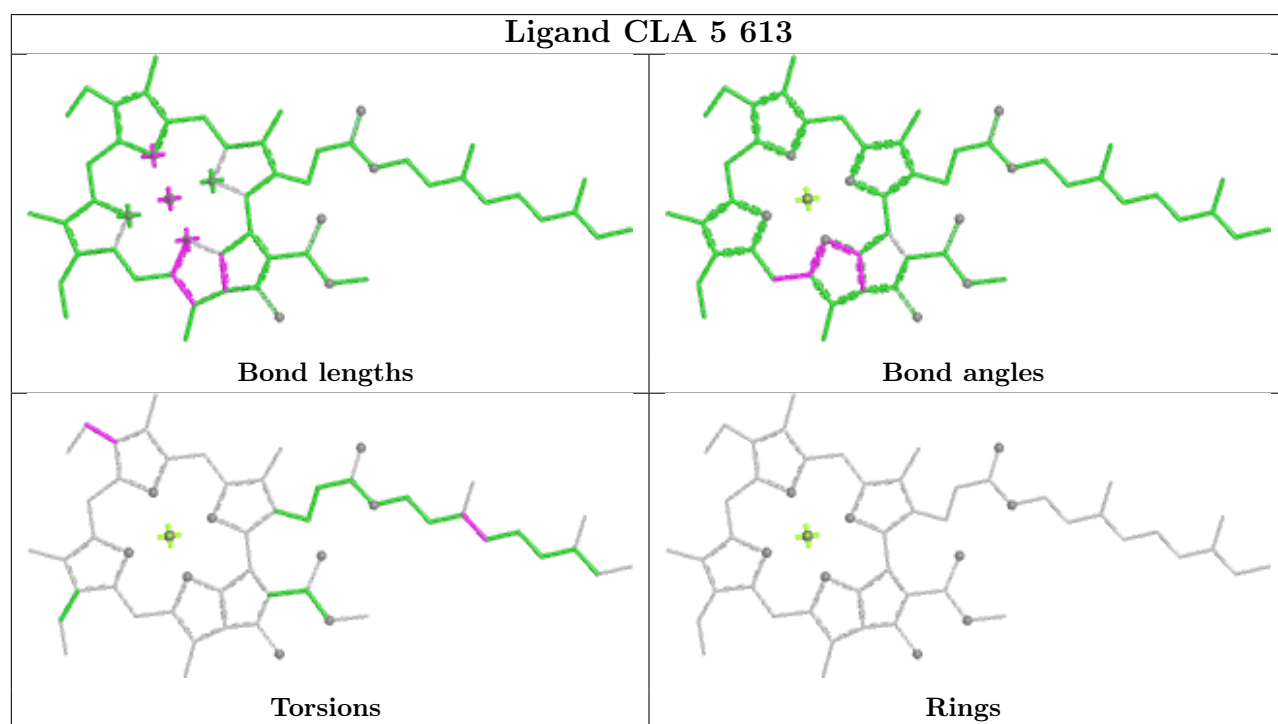
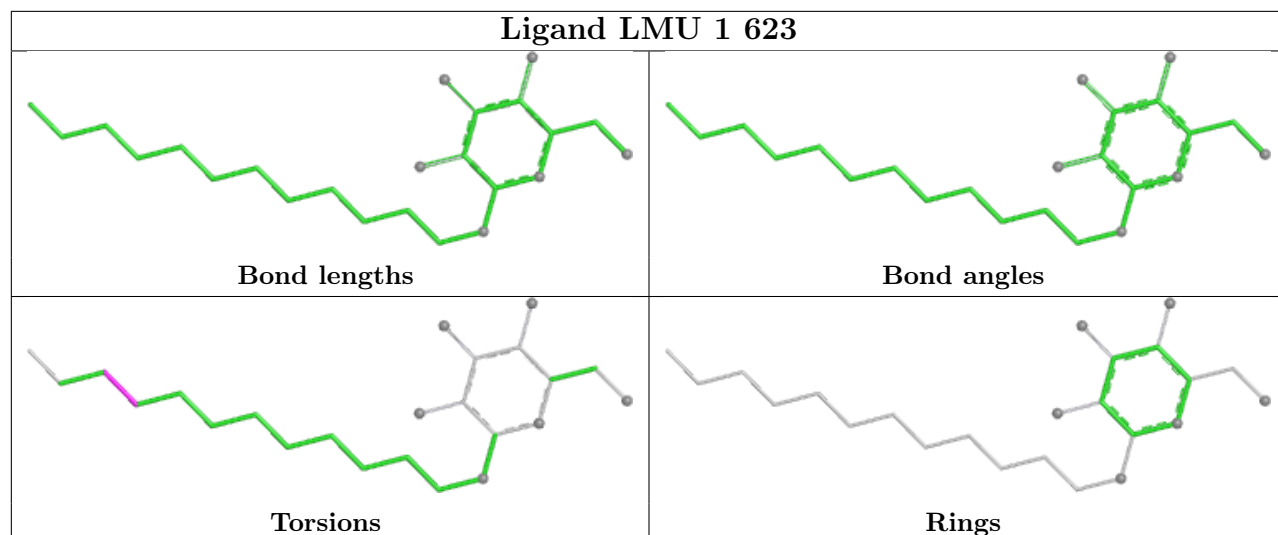


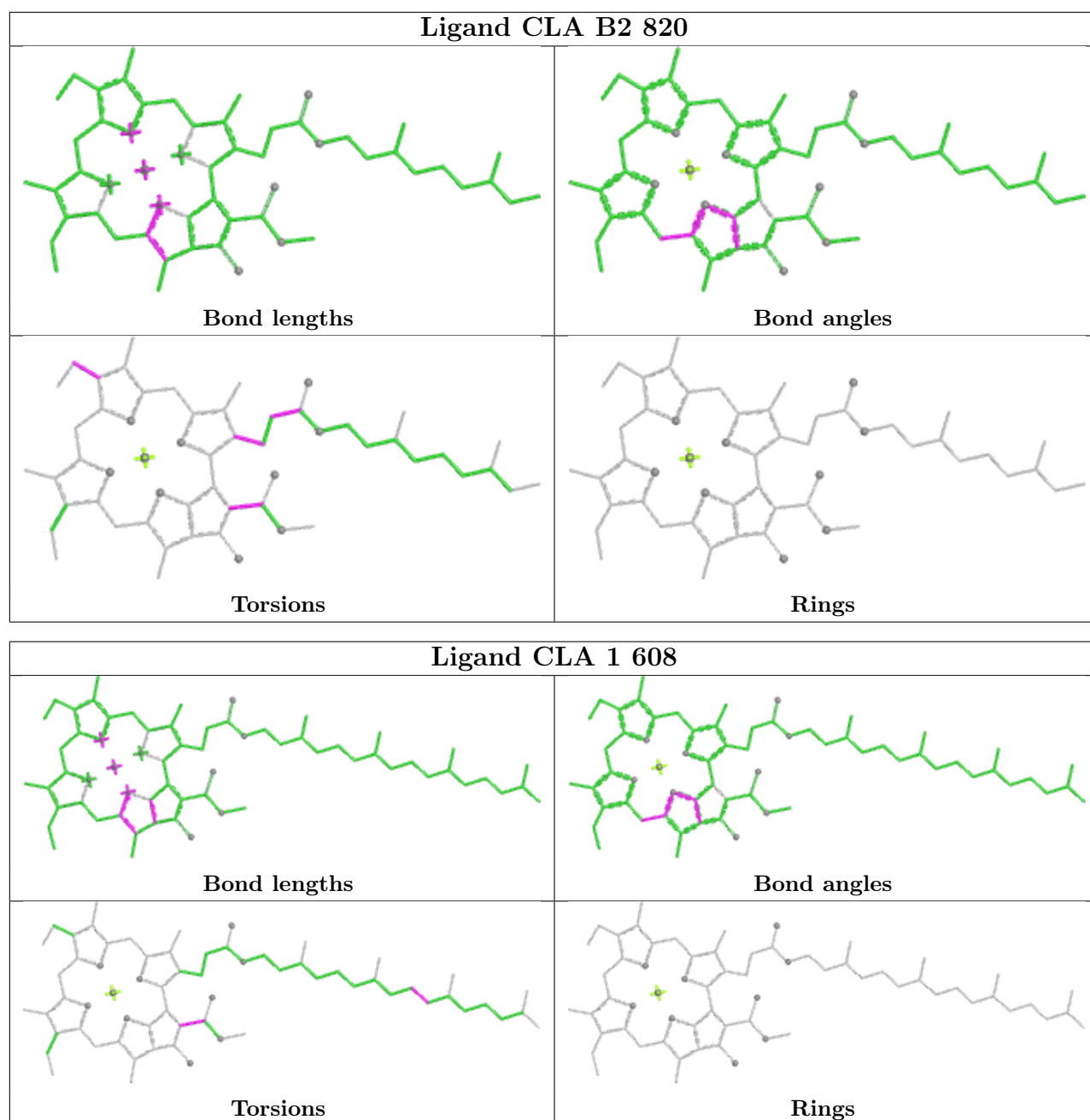
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Bond lengths	Bond angles
	
Torsions	Rings

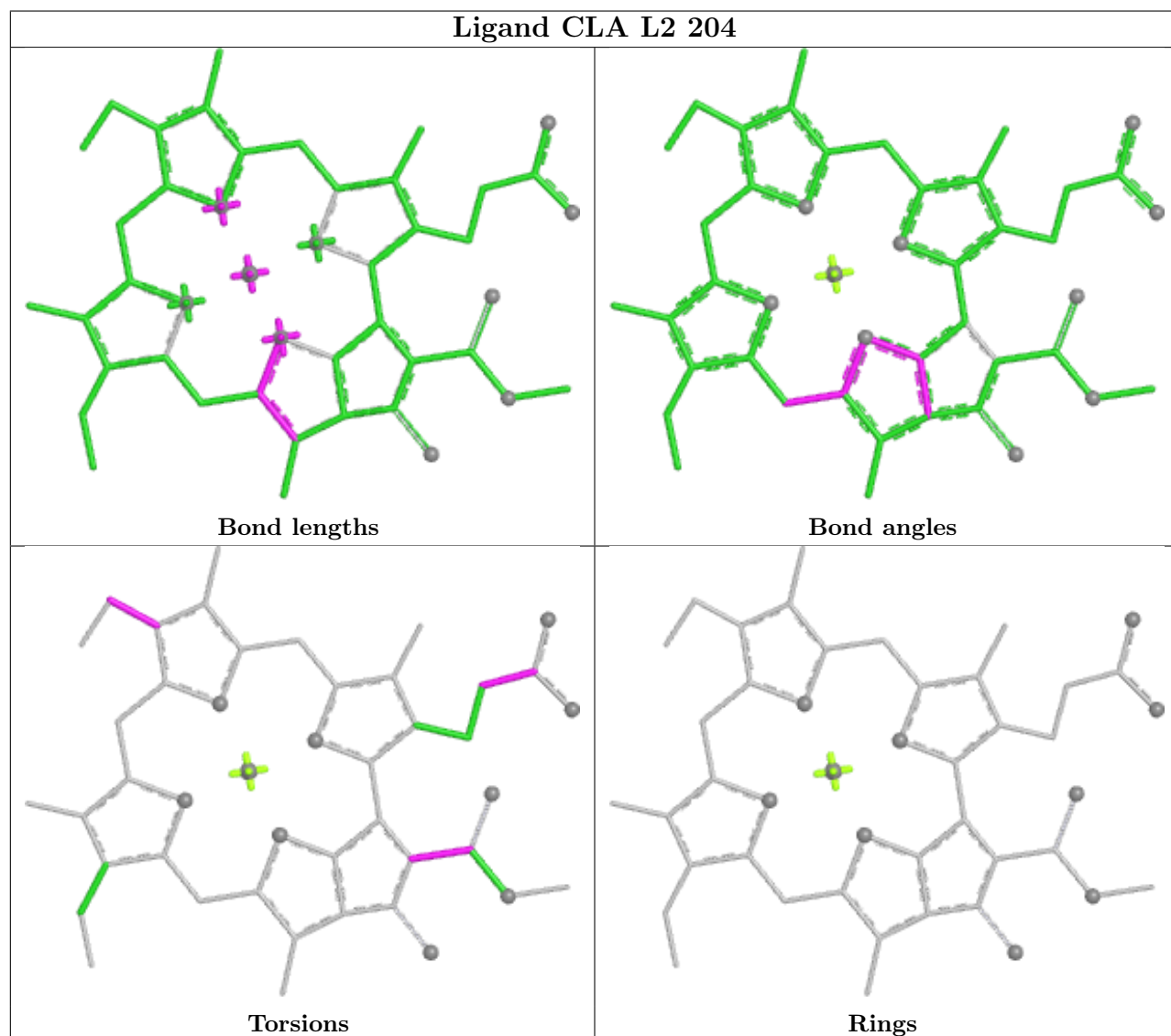
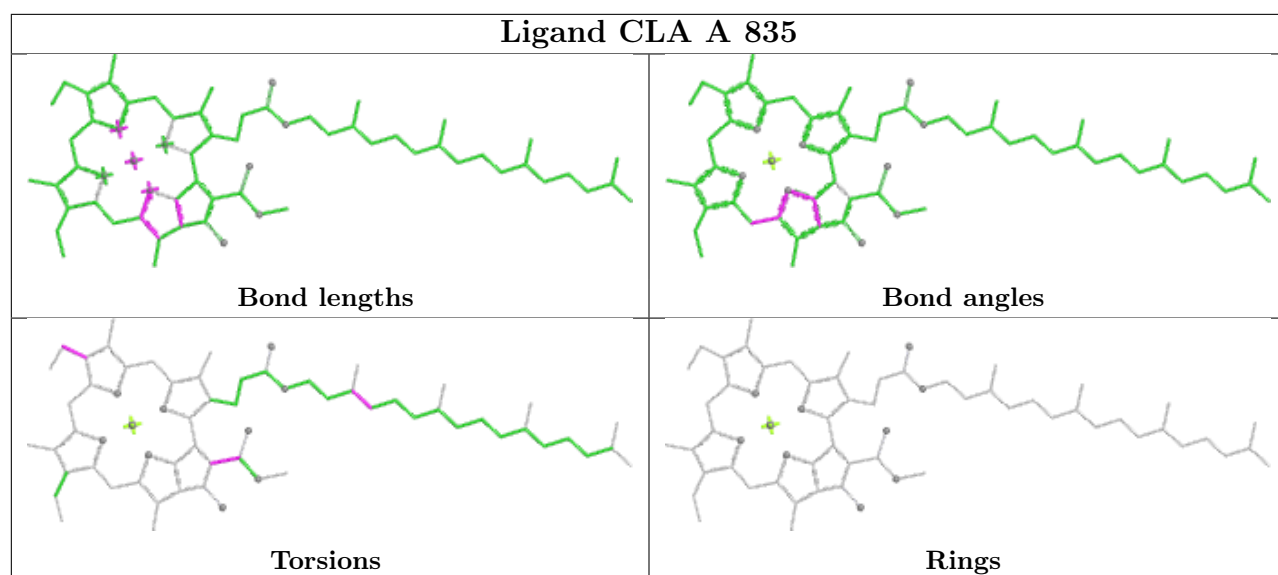
Ligand LUT 5 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

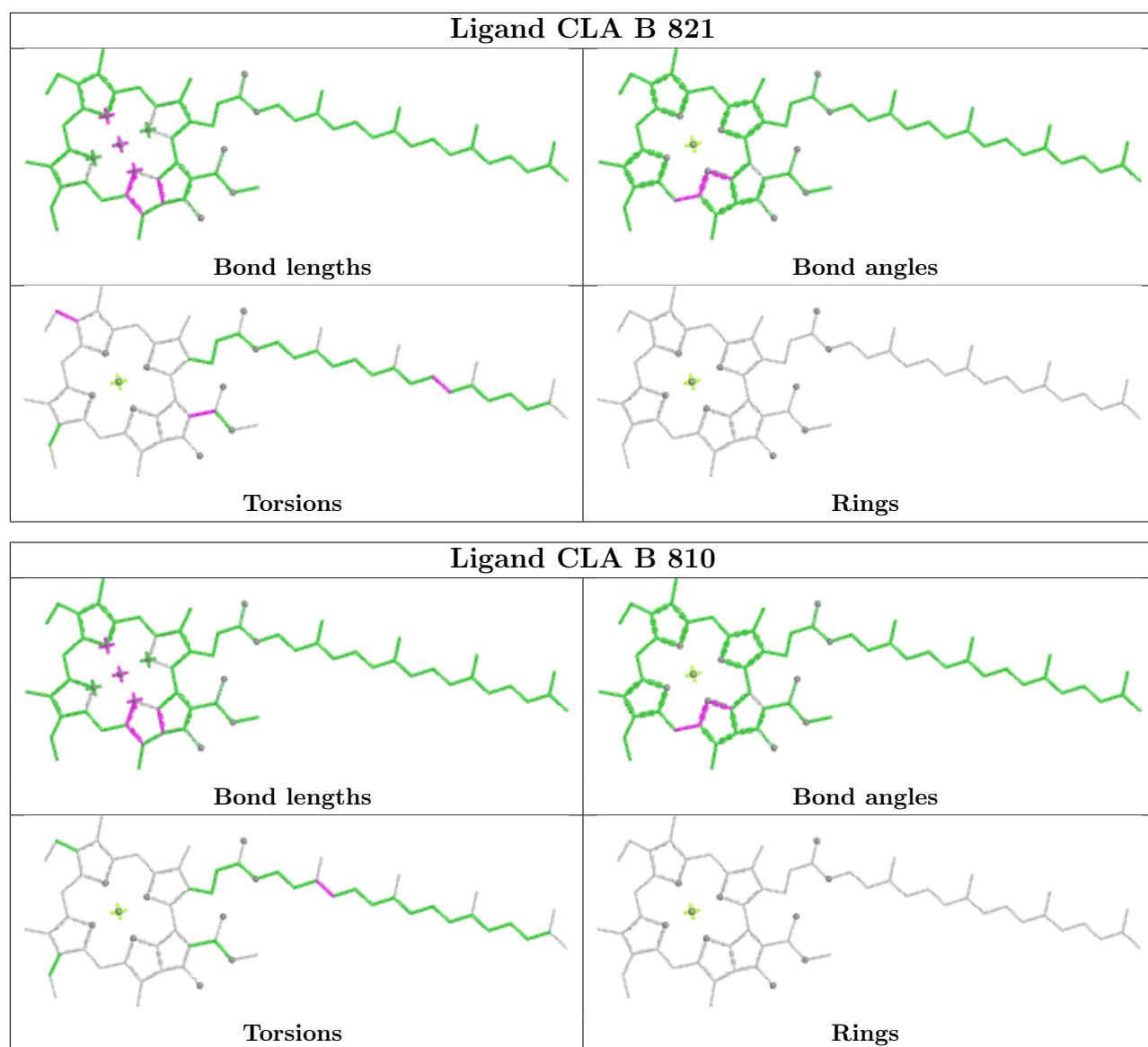
Ligand BCR I 172	
	
Bond lengths	Bond angles
	
Torsions	Rings

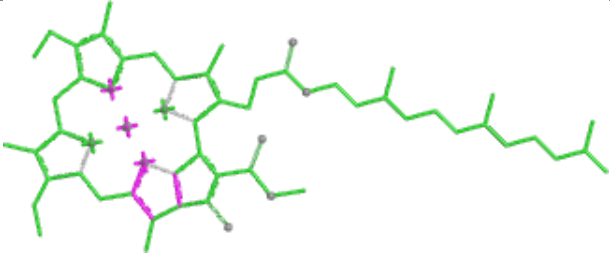
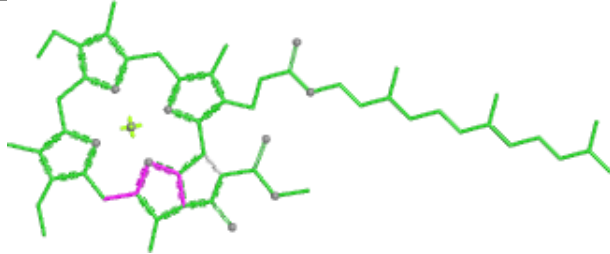
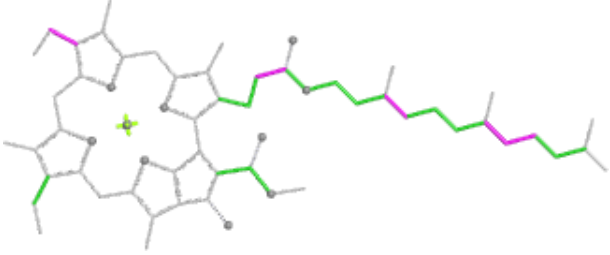
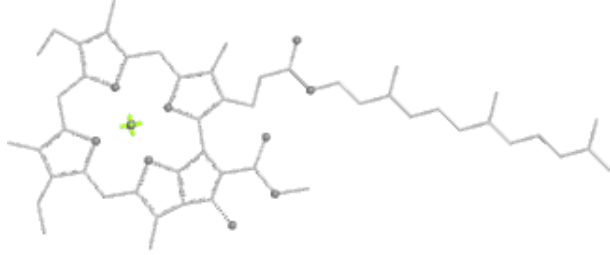
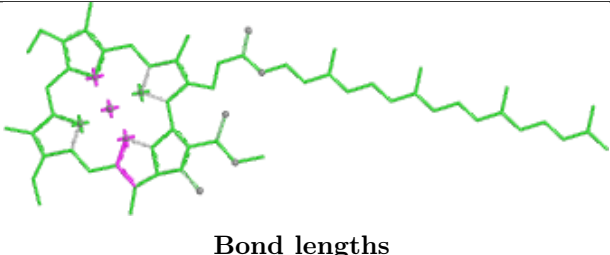
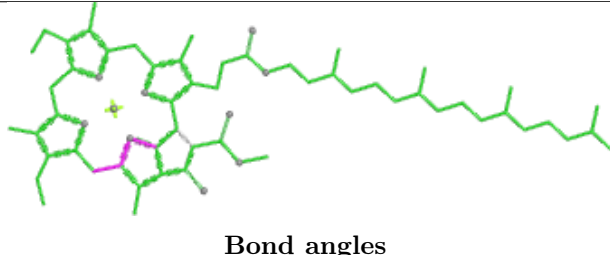
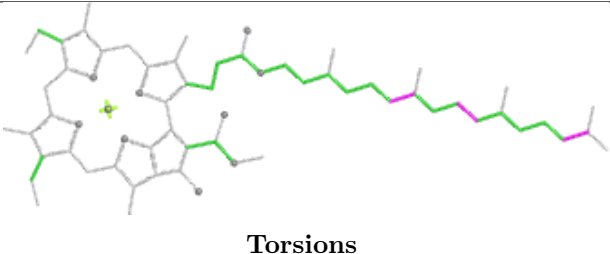
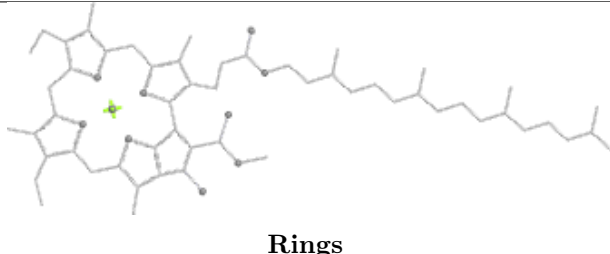
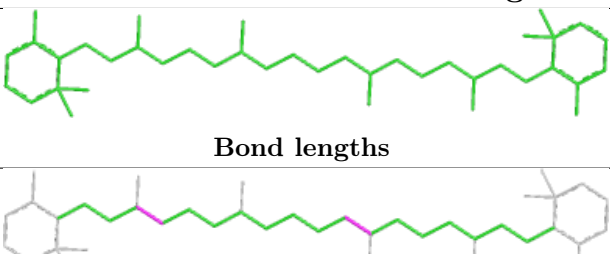
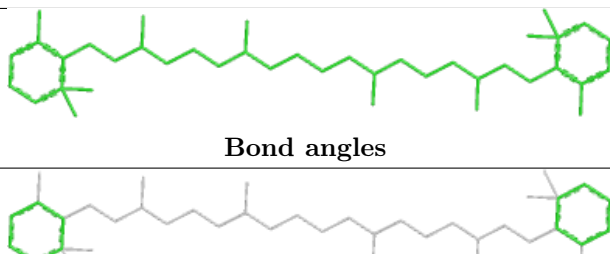
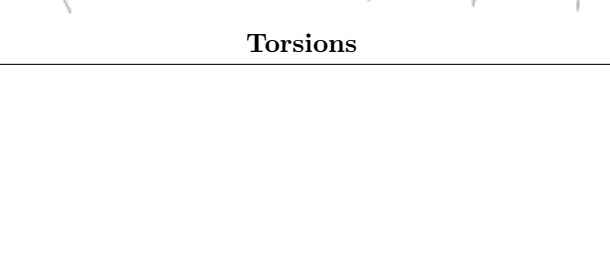
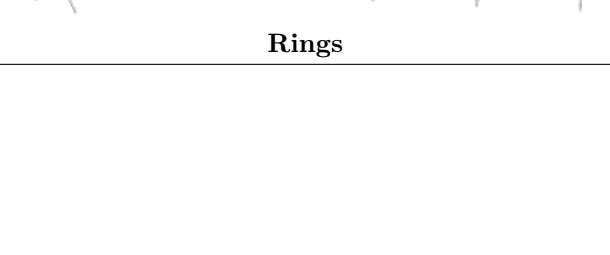
Ligand BCR B 848	
	
Bond lengths	Bond angles
	
Torsions	Rings

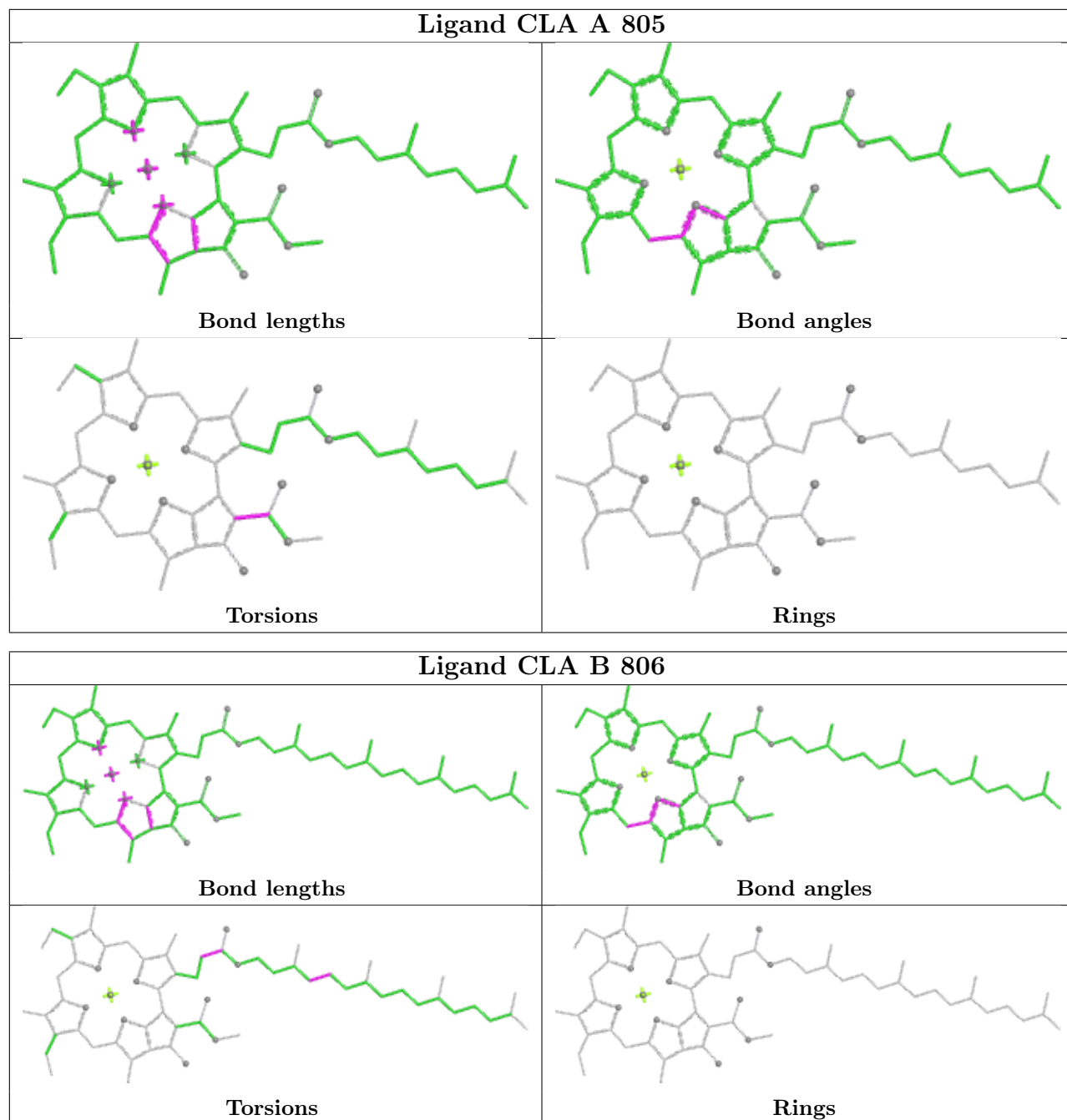


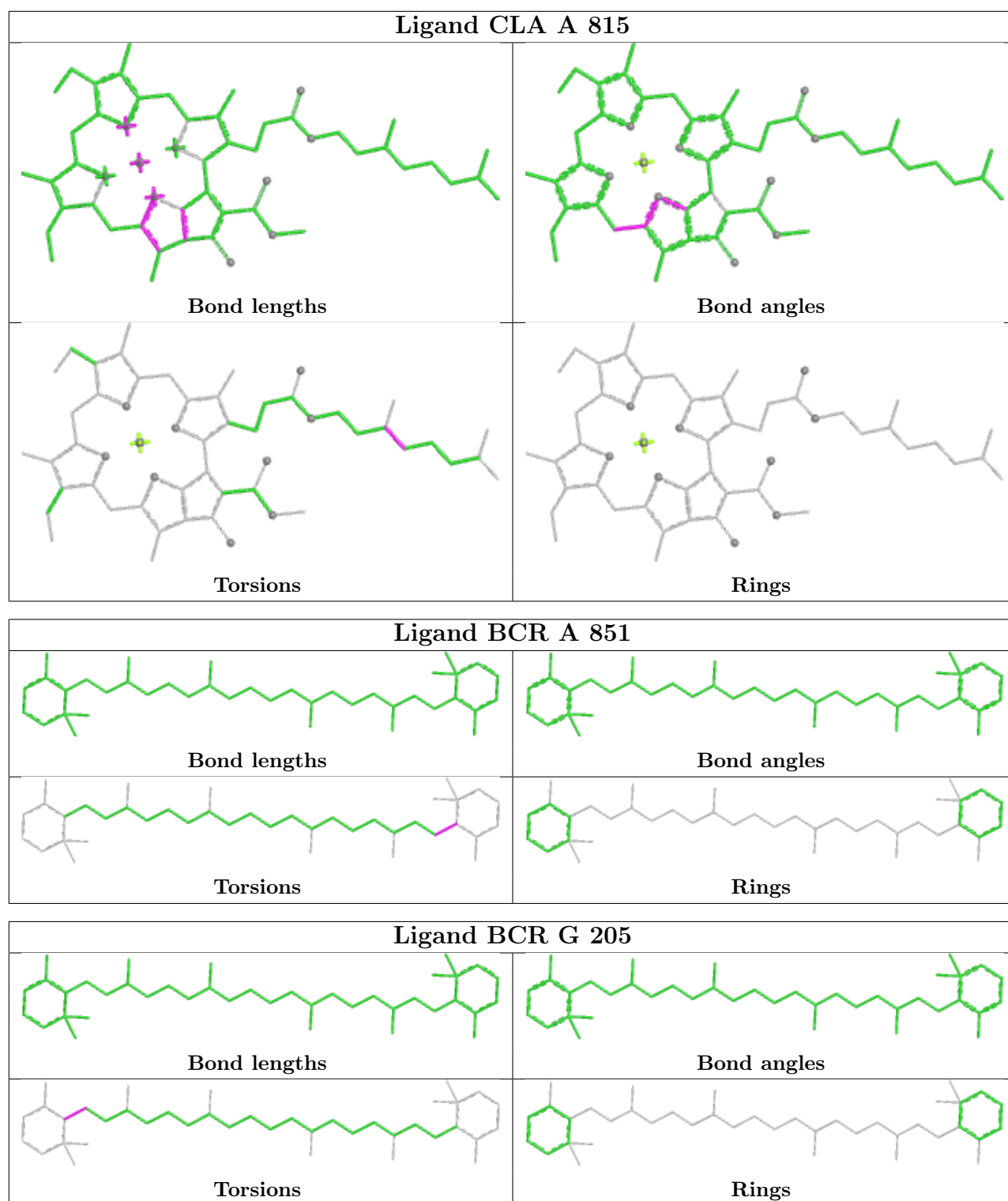


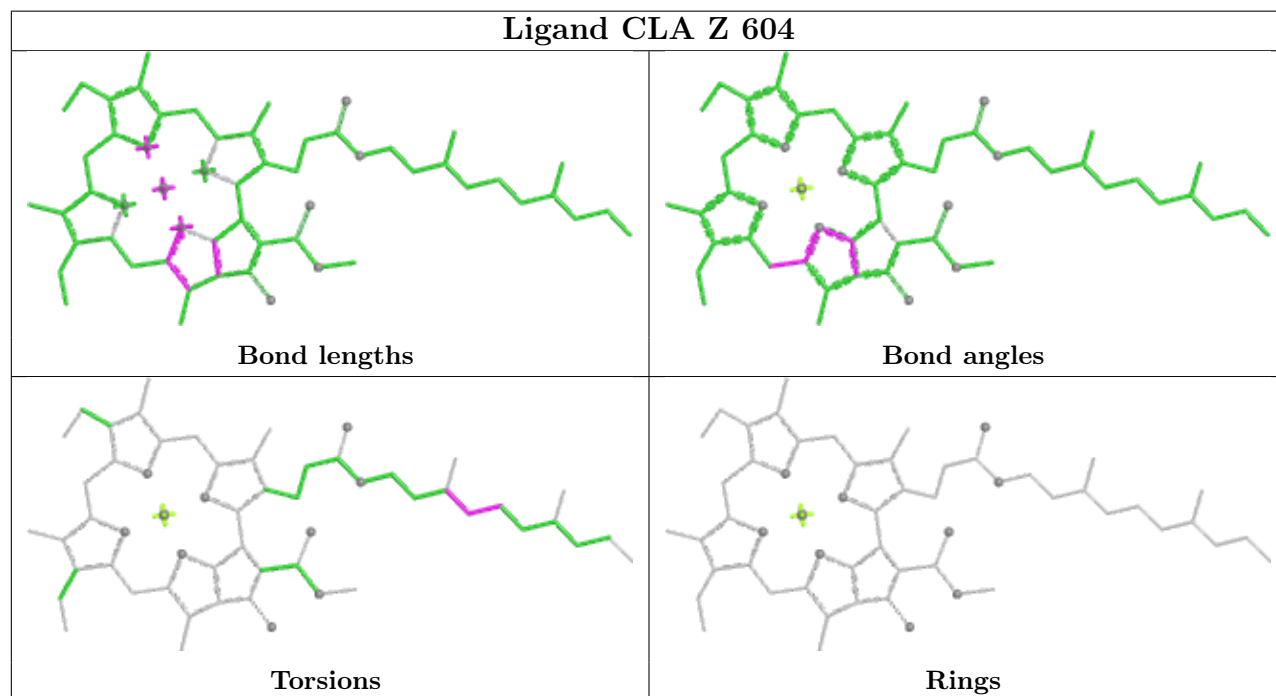
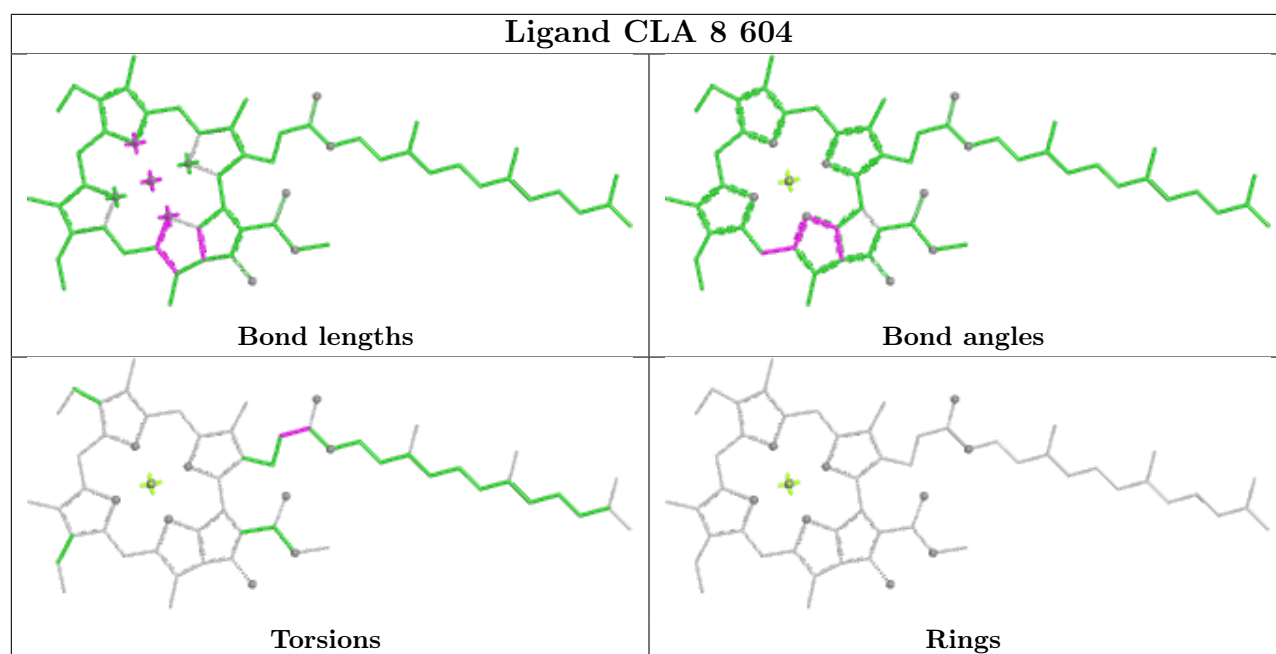




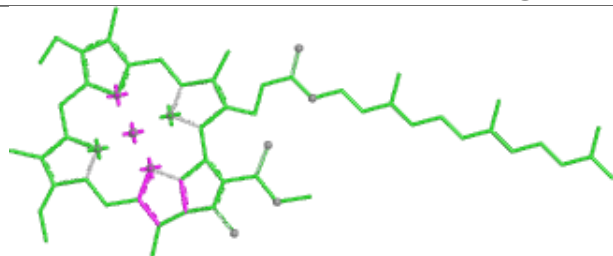
Ligand CLA B 834	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand CLA 5 601	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 852	
 Bond lengths	 Bond angles
 Torsions	 Rings



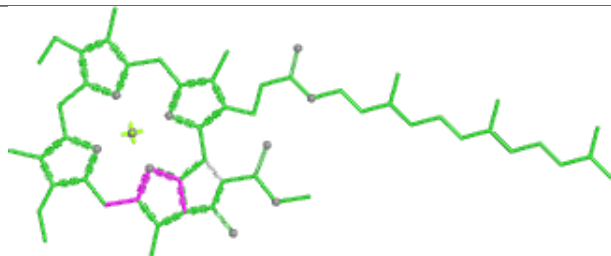




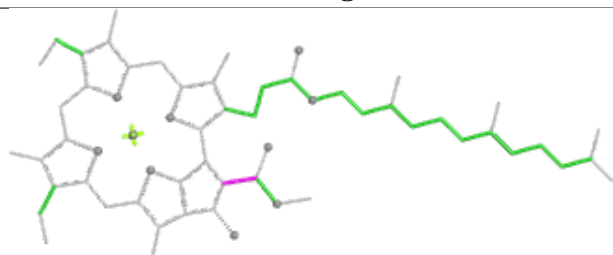
Ligand CLA Z 602



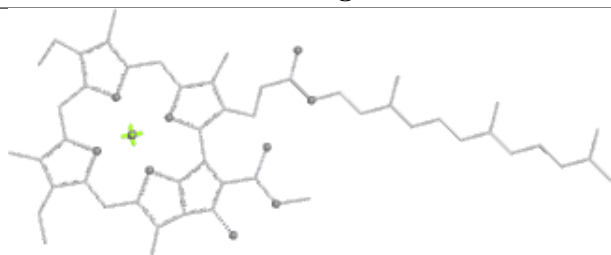
Bond lengths



Bond angles

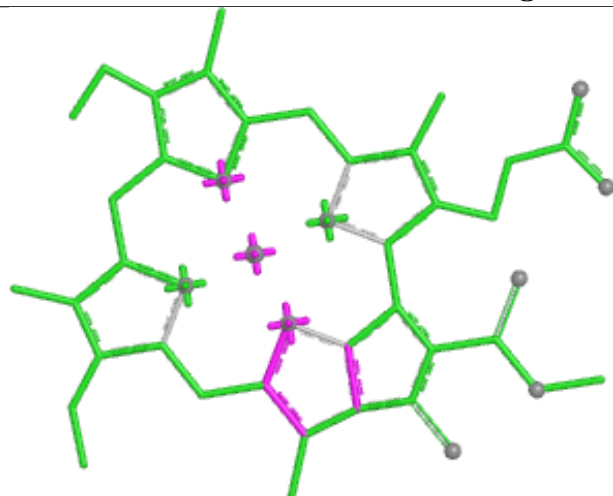


Torsions

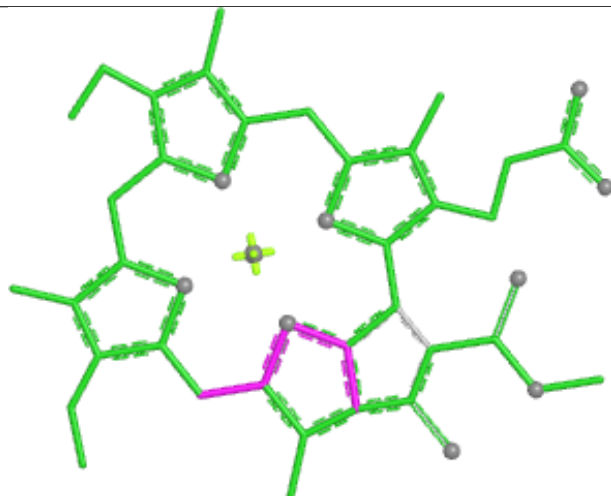


Rings

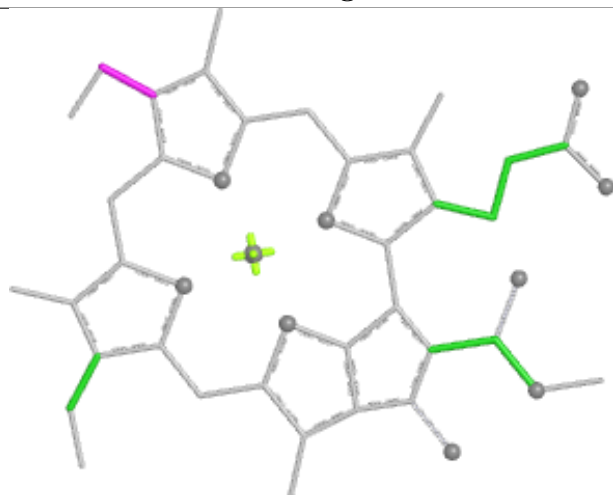
Ligand CLA 3 614



Bond lengths



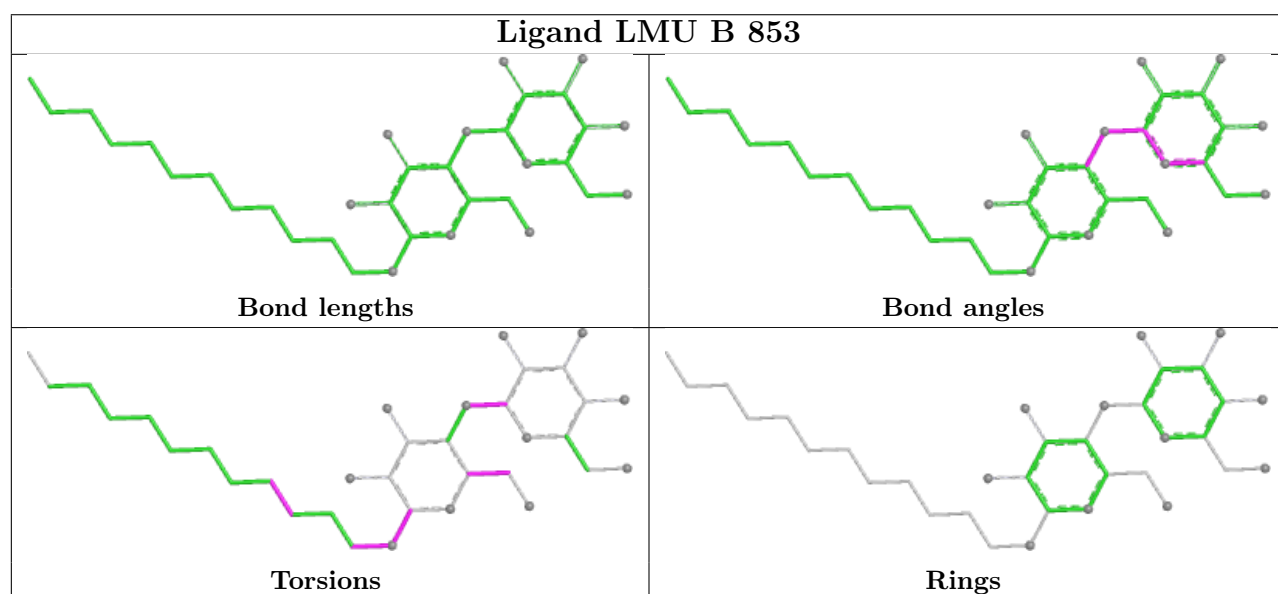
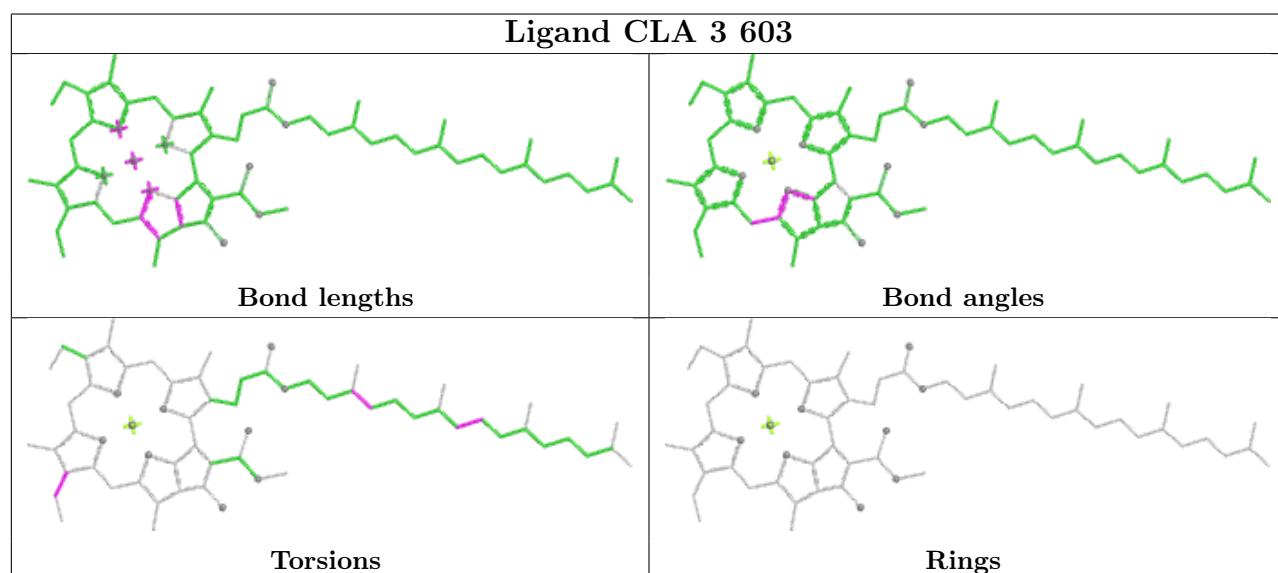
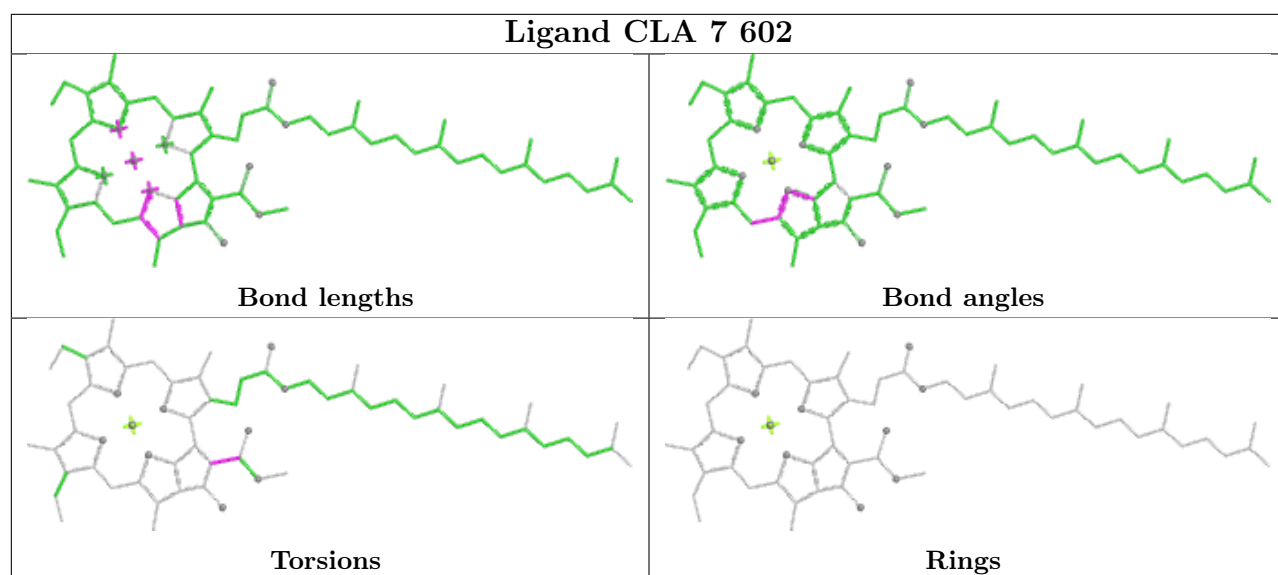
Bond angles

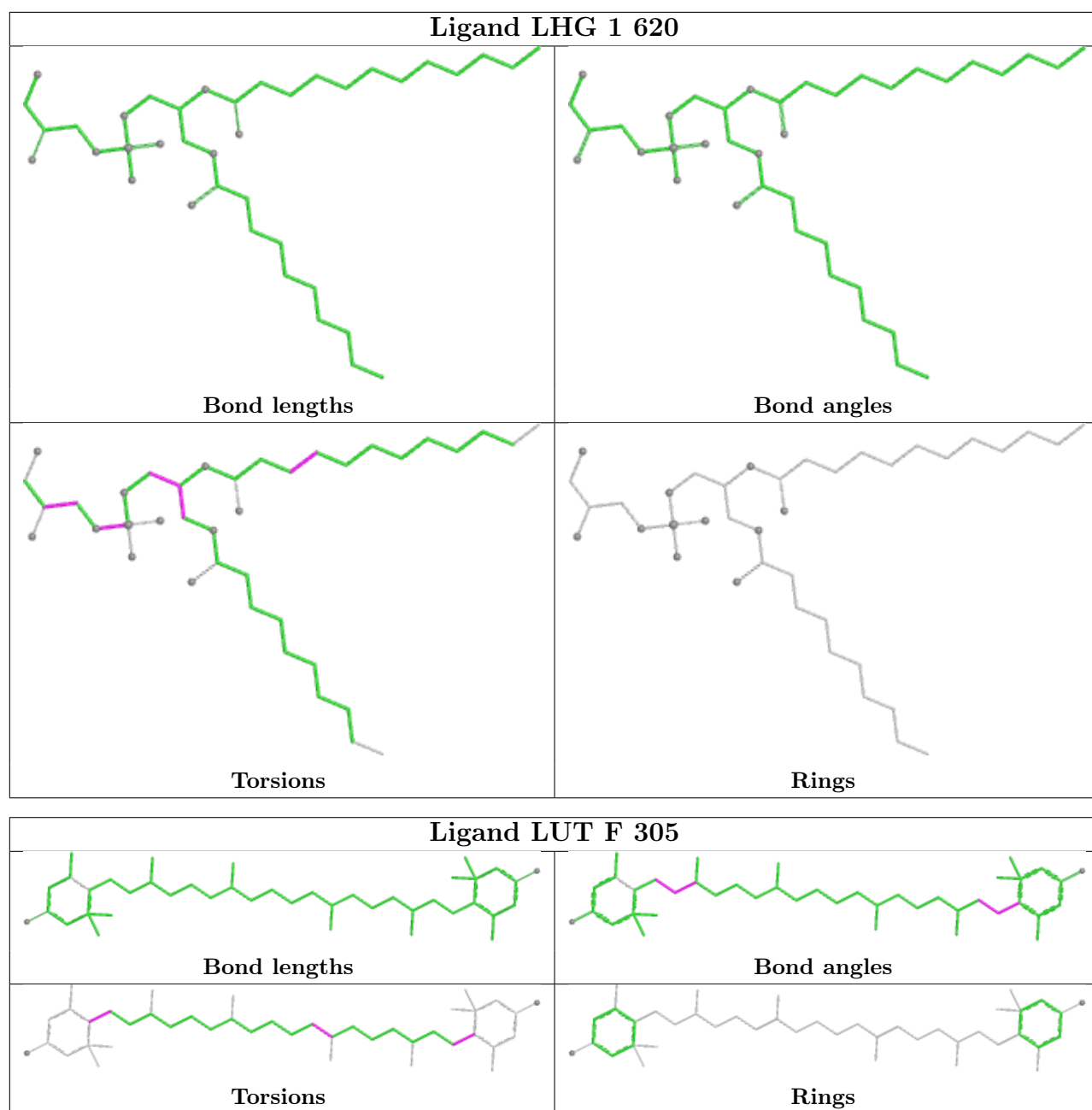


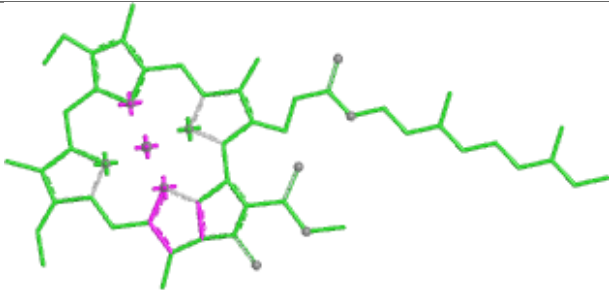
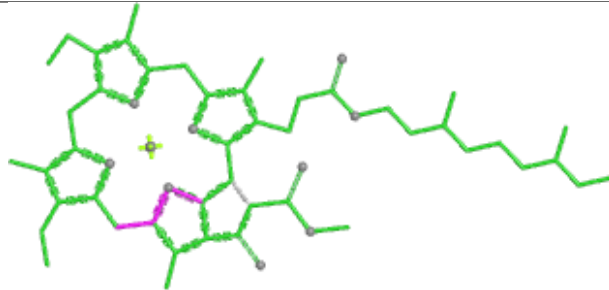
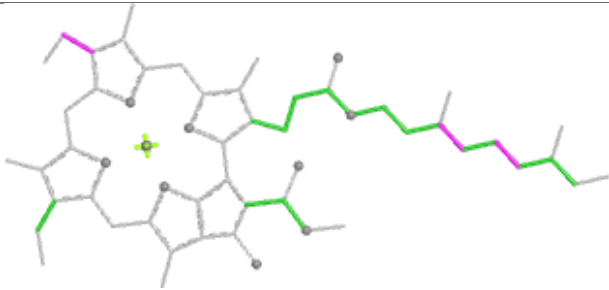
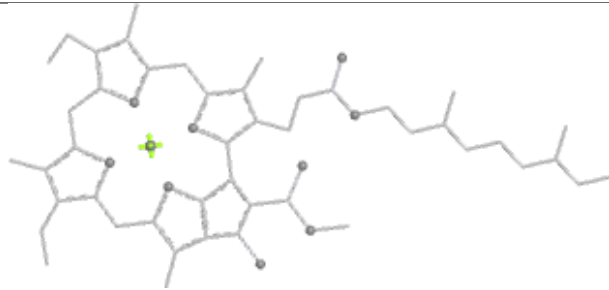
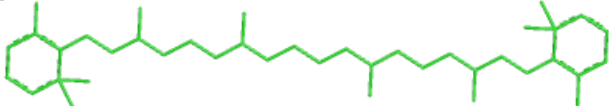
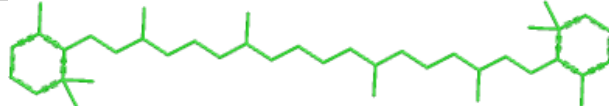
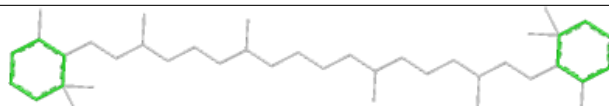
Torsions

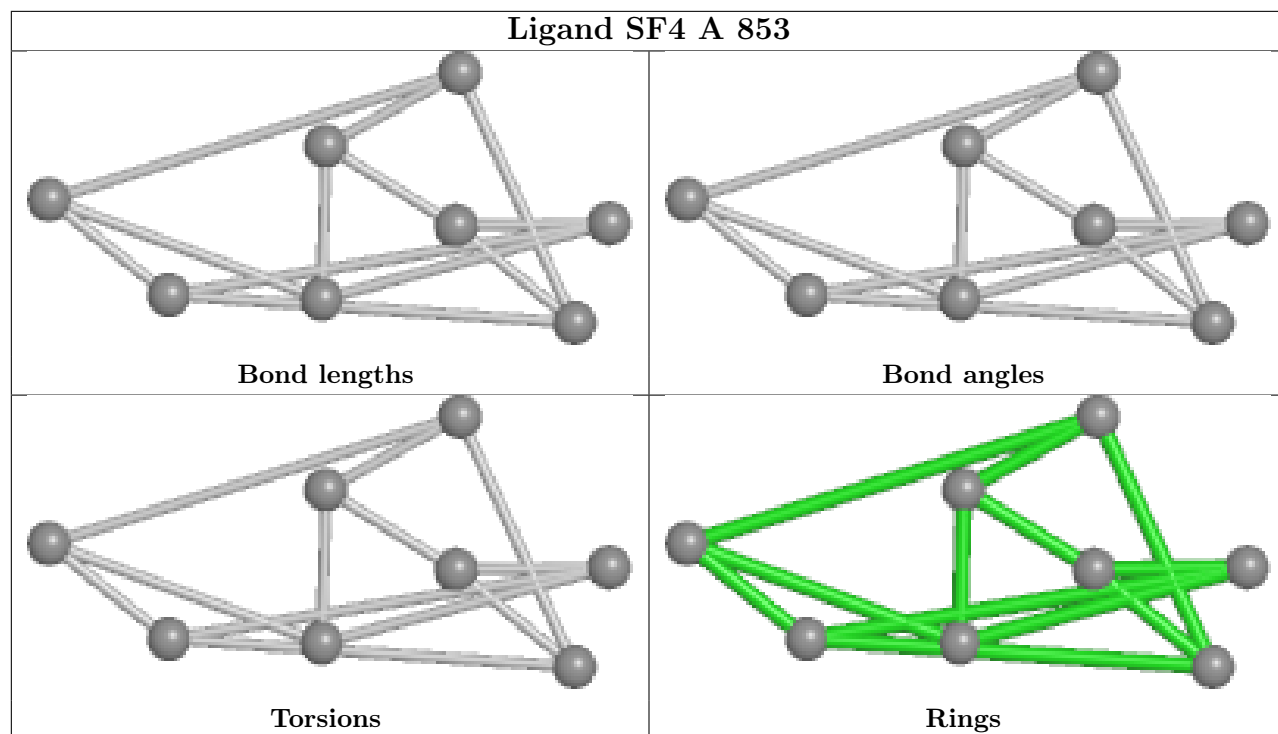


Rings

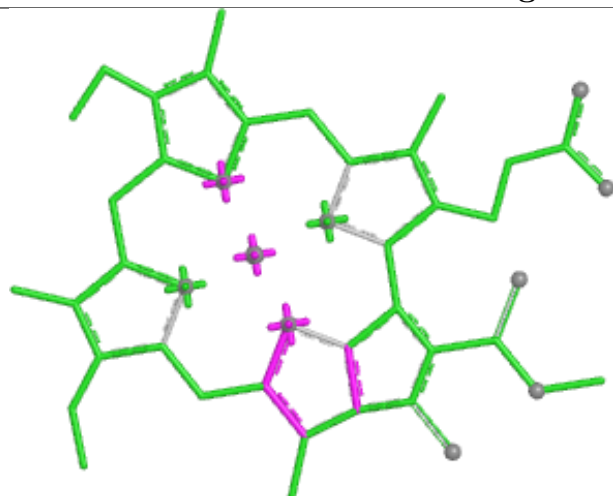




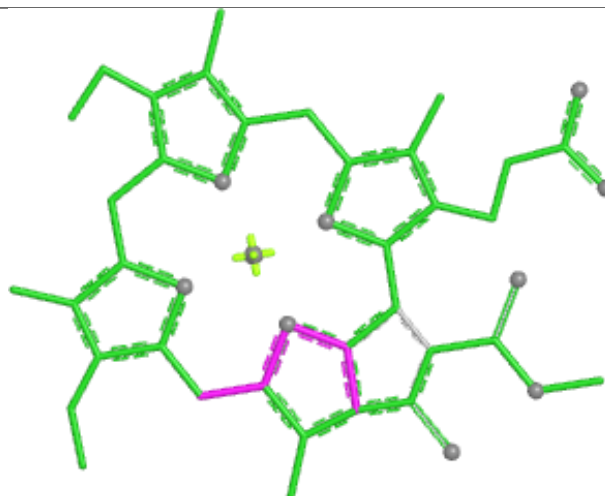
Ligand CLA B 820	
	
Bond lengths	Bond angles
	
Torsions	Rings
Ligand BCR B 843	
	
Bond lengths	Bond angles
	
Torsions	Rings



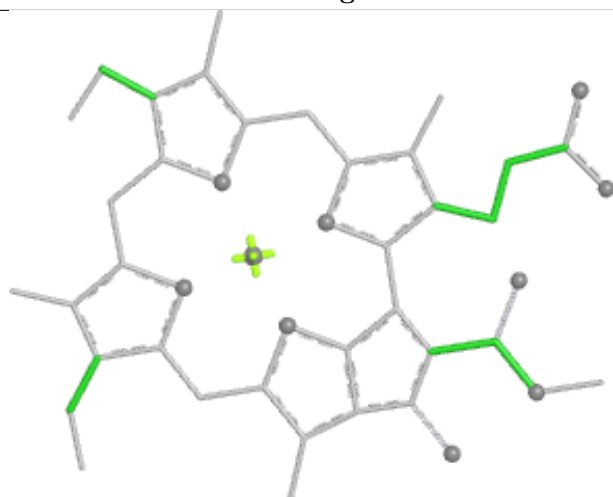
Ligand CLA 8 616



Bond lengths



Bond angles

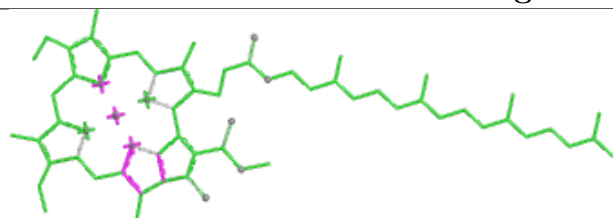


Torsions

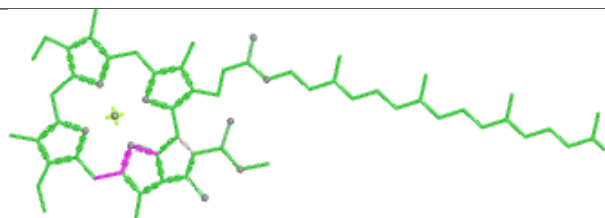


Rings

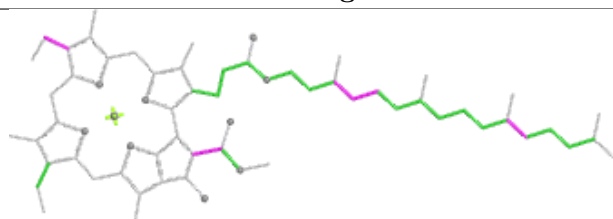
Ligand CLA B 808



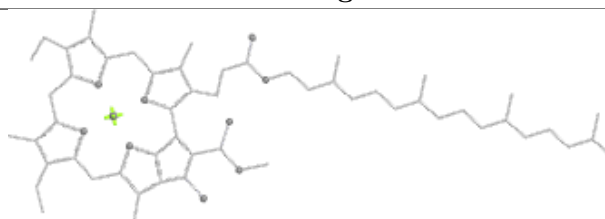
Bond lengths



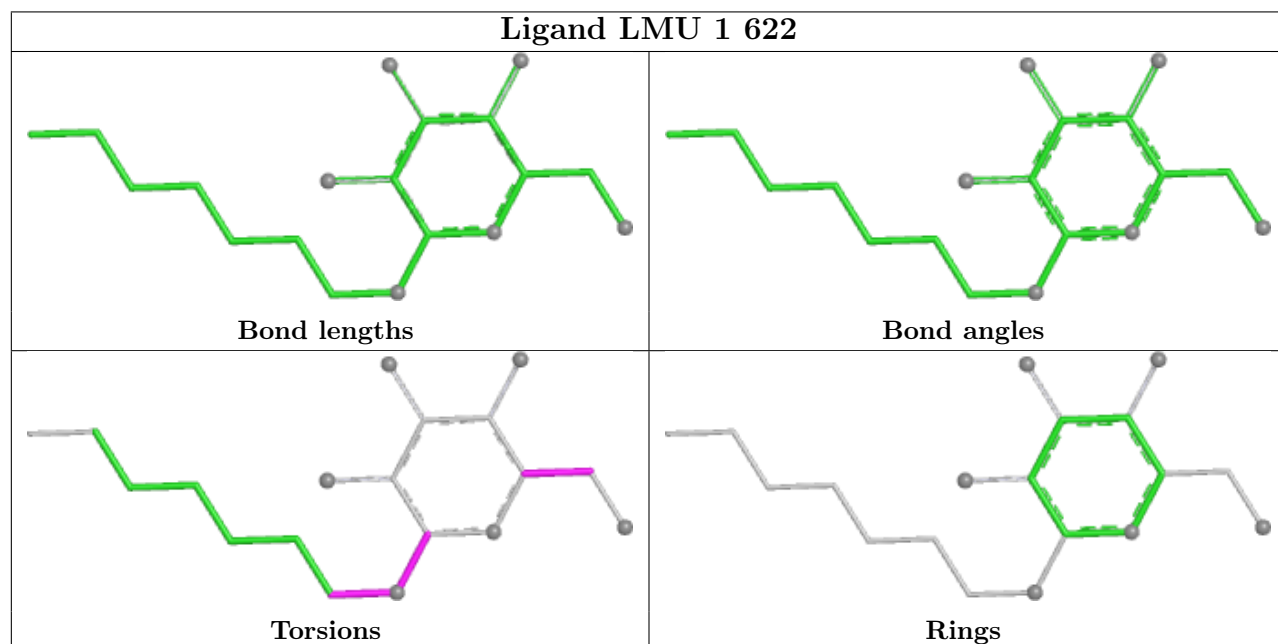
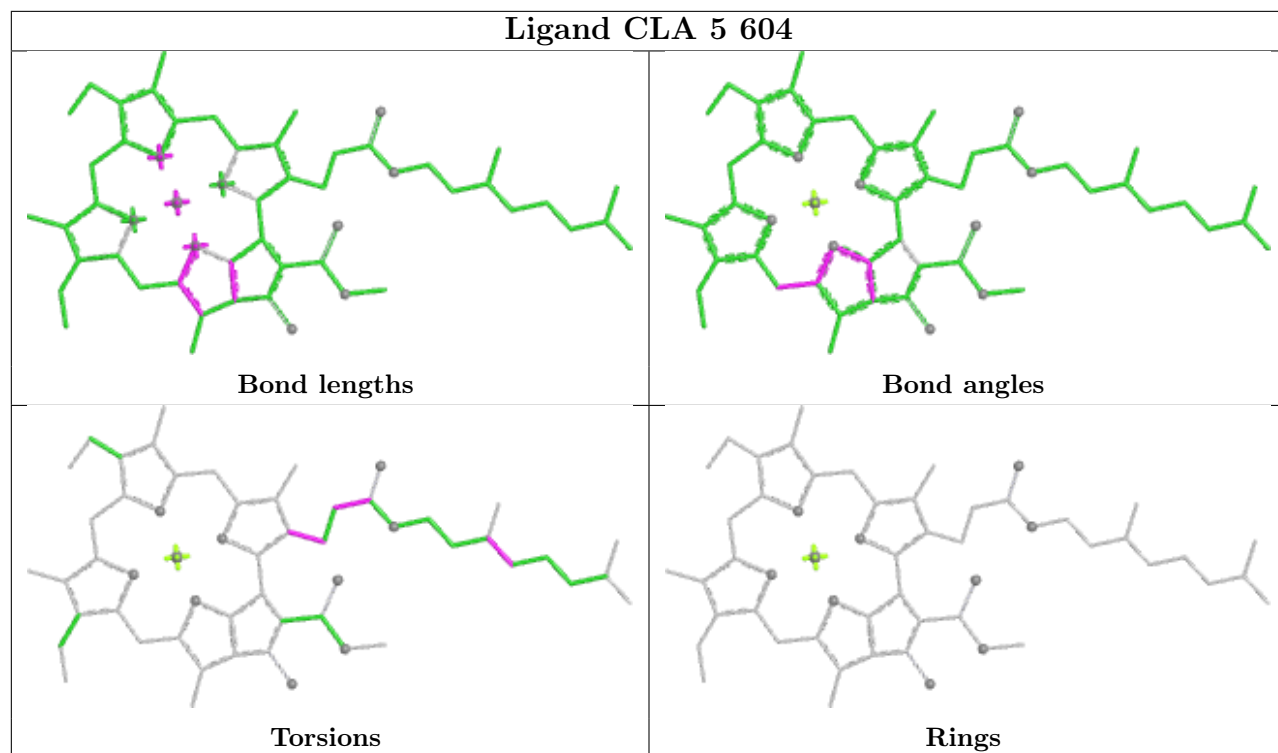
Bond angles

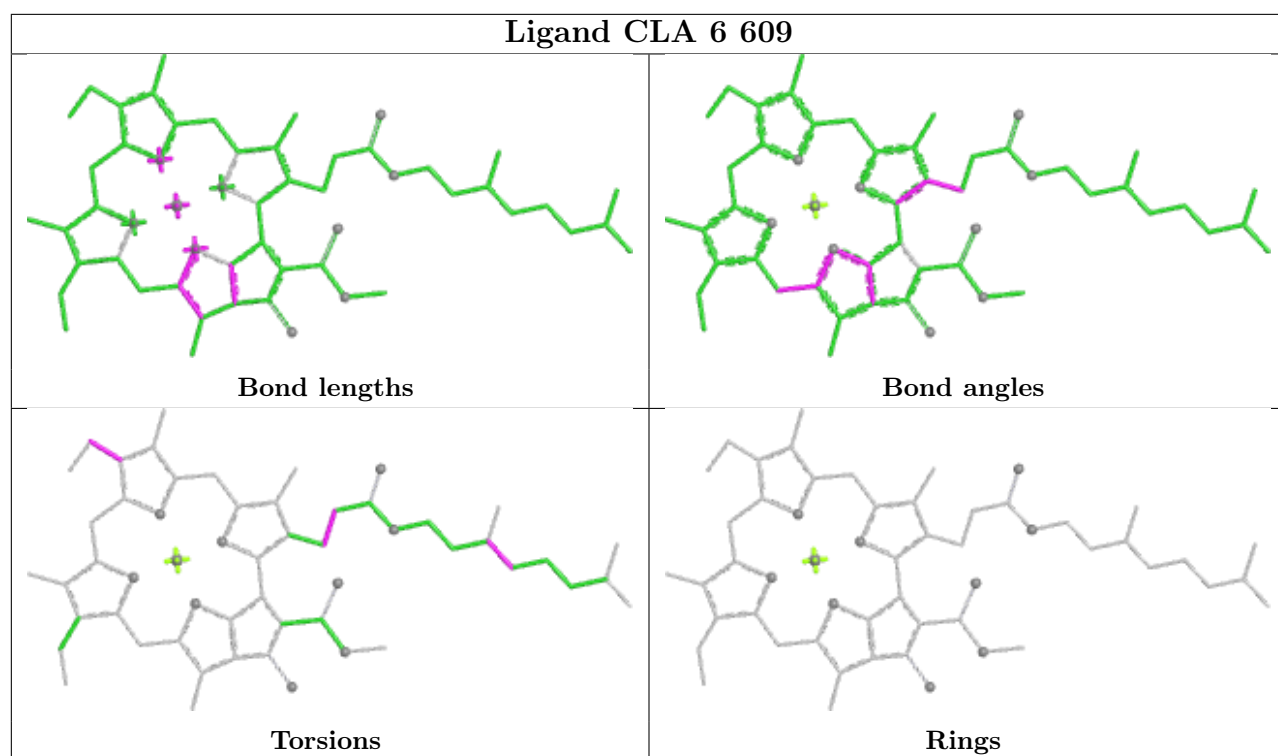


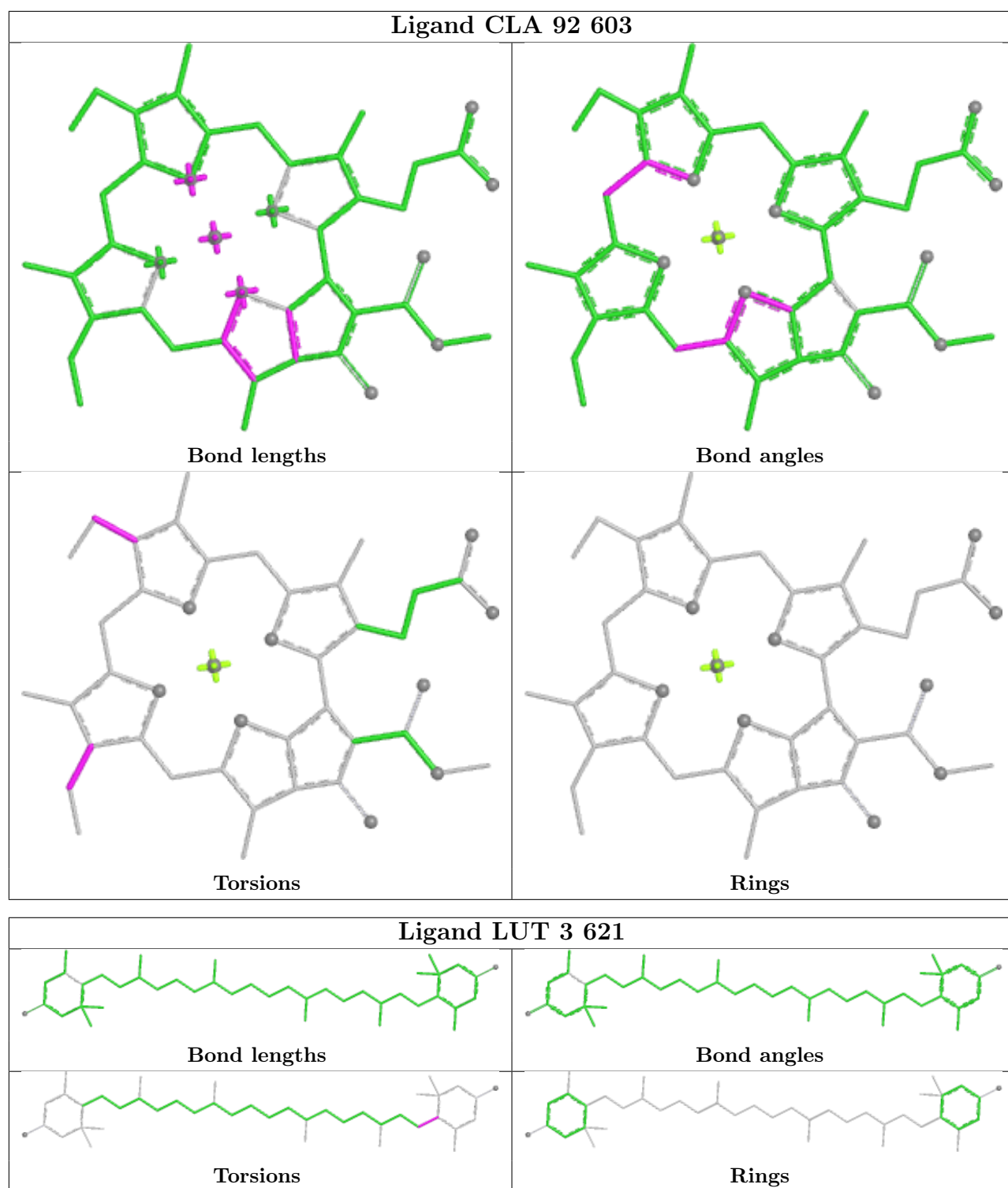
Torsions

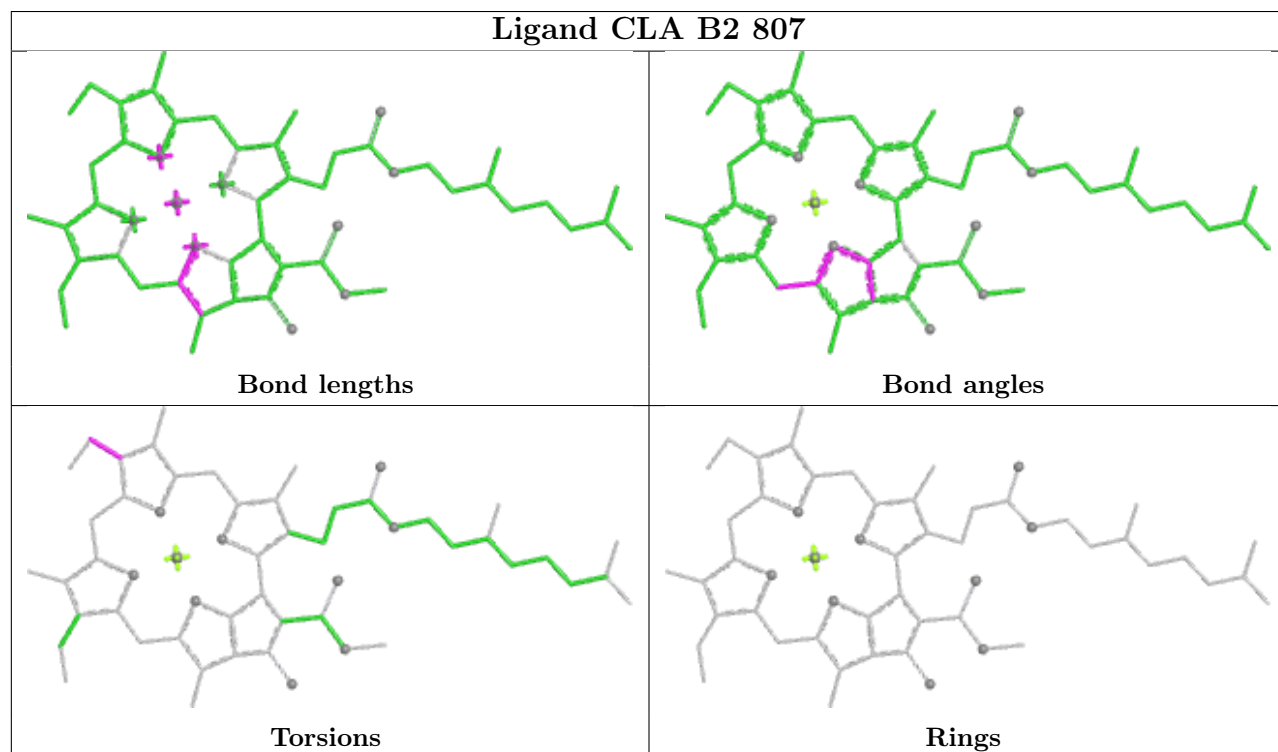
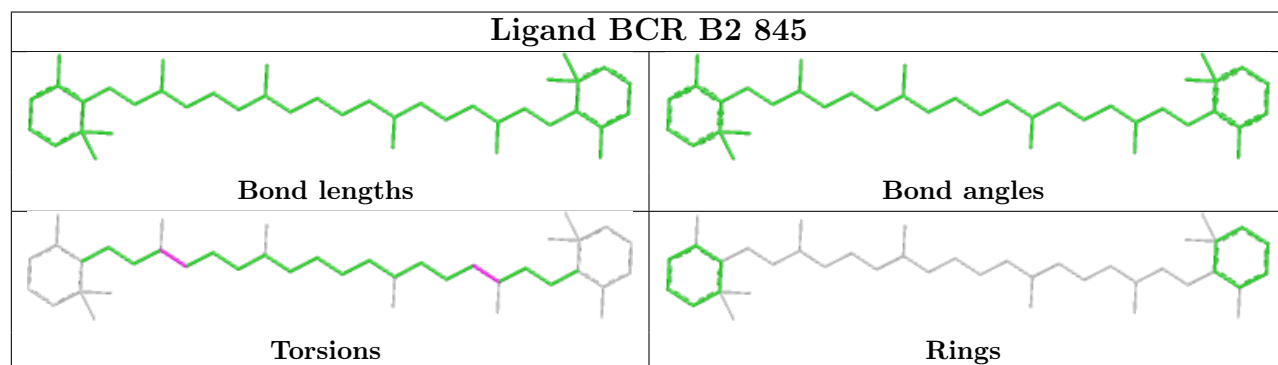
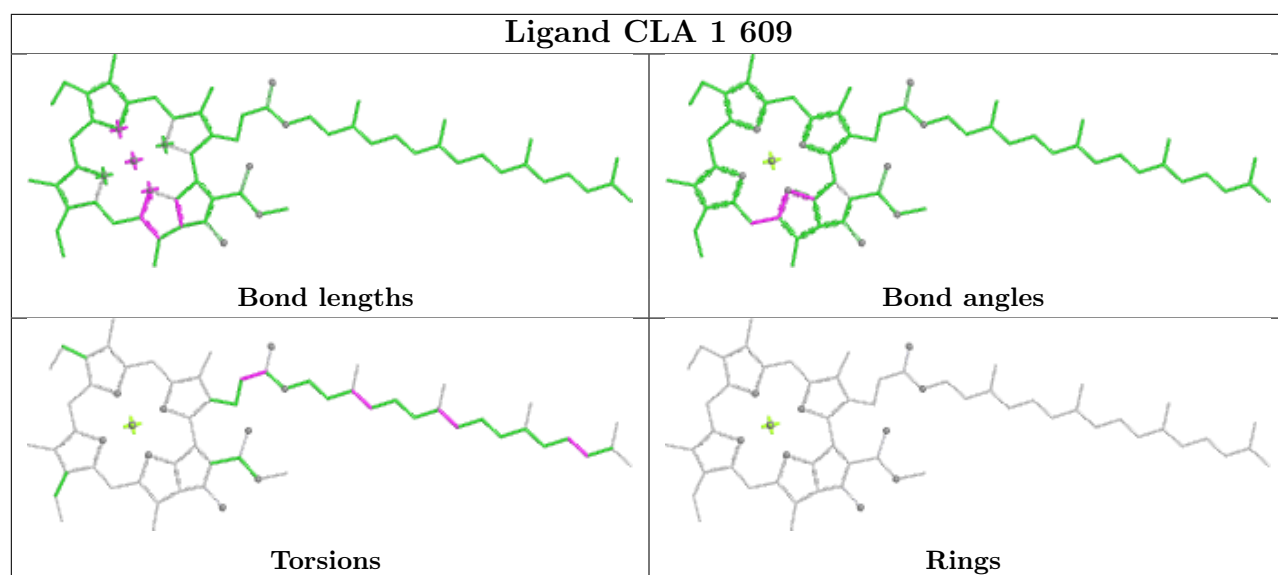


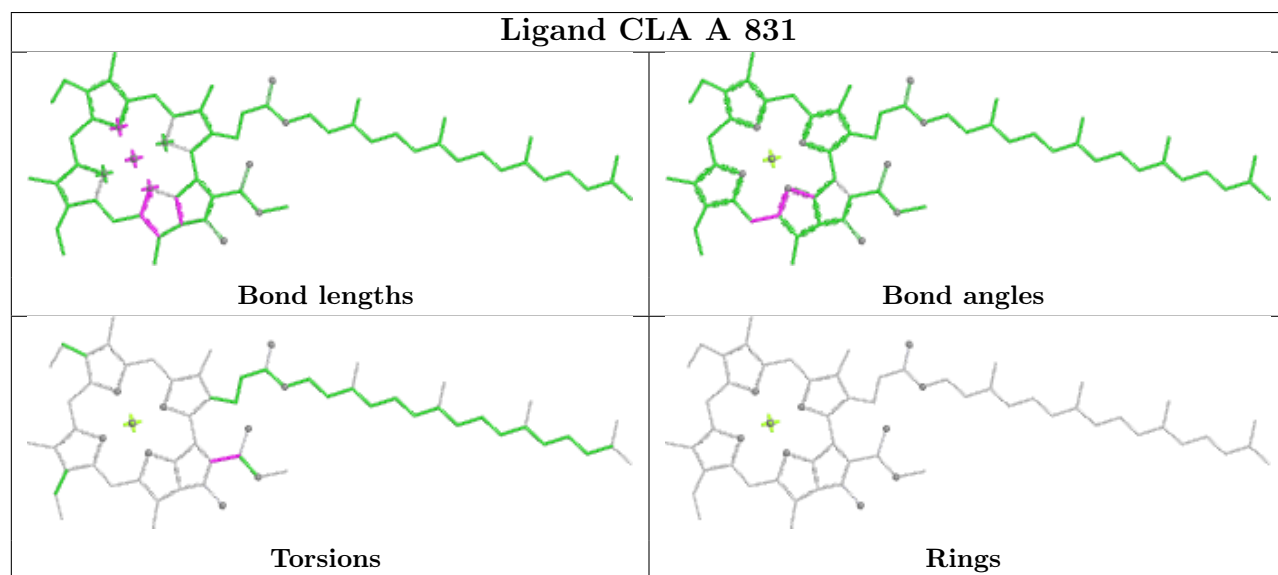
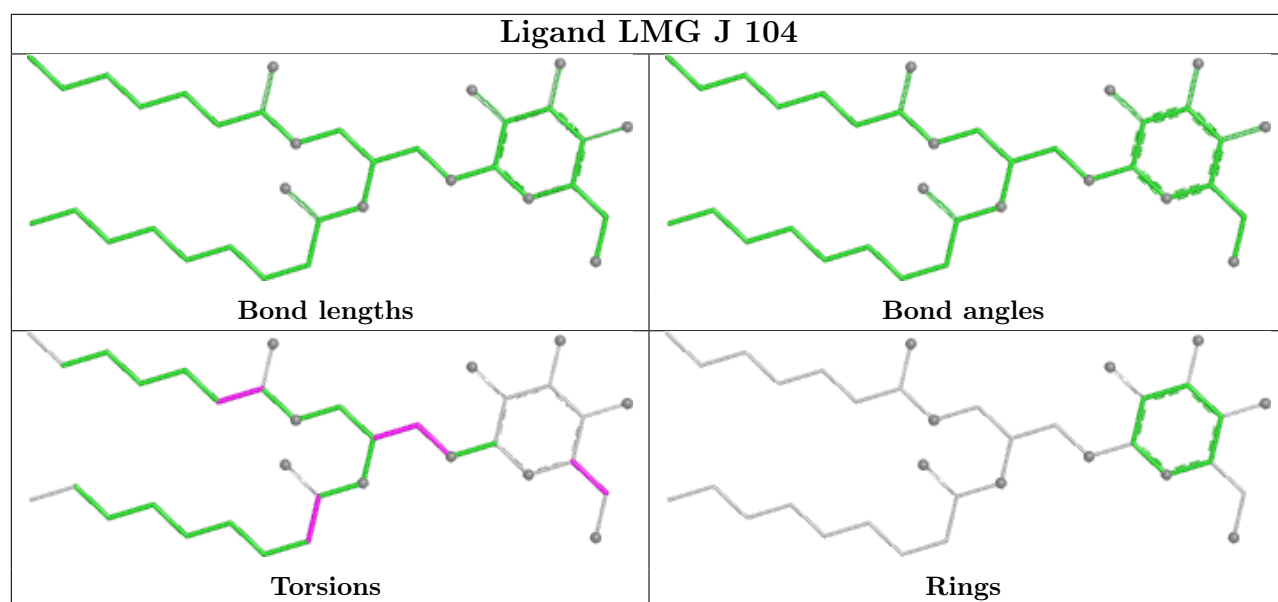
Rings

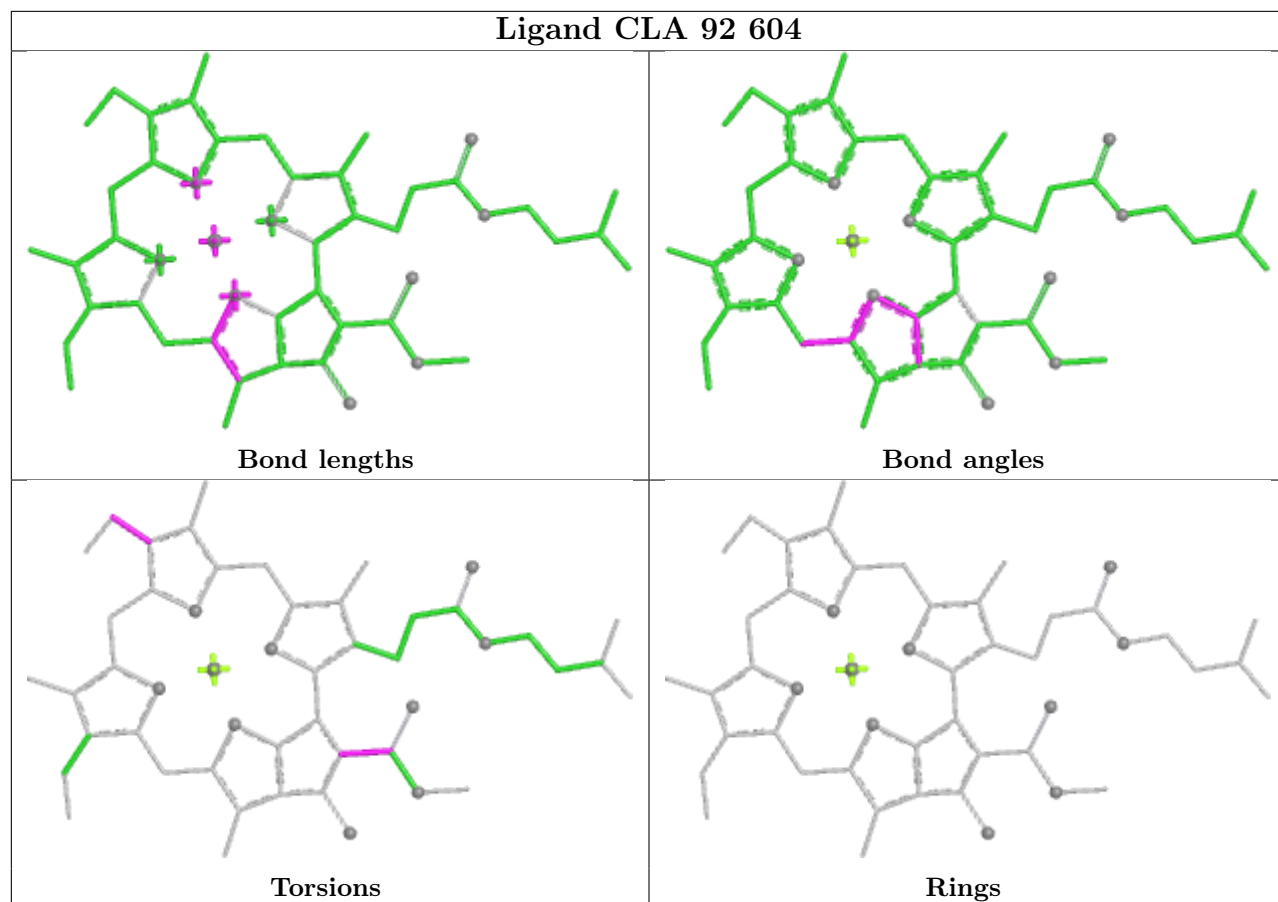




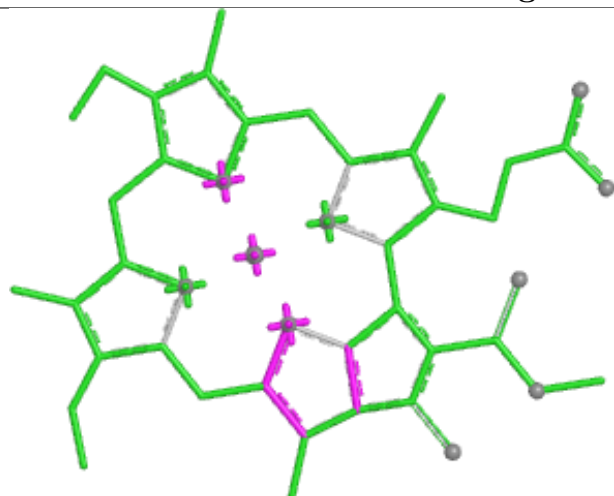




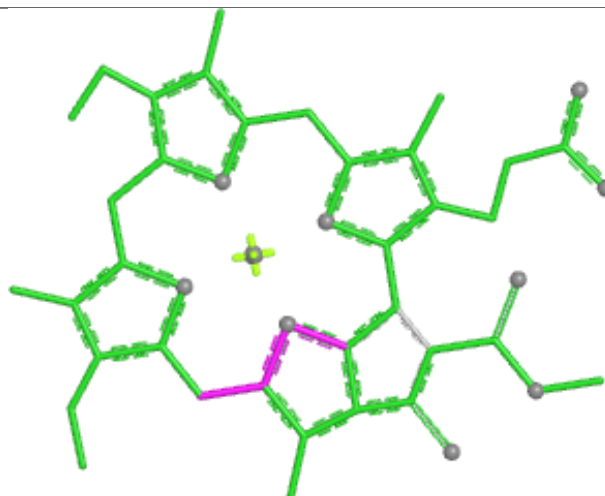




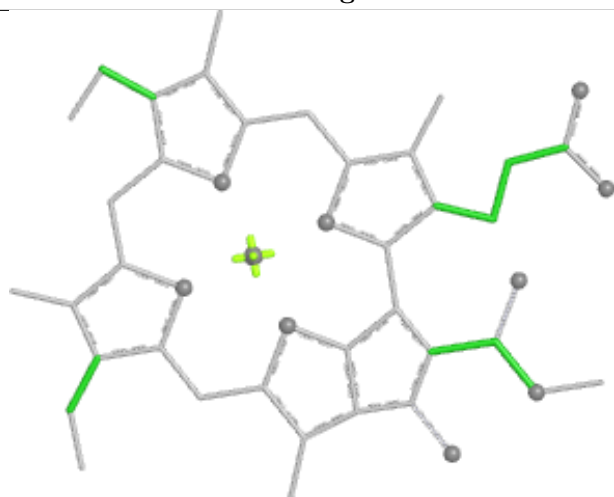
Ligand CLA 8 609



Bond lengths



Bond angles

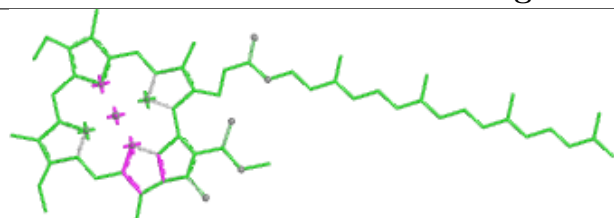


Torsions

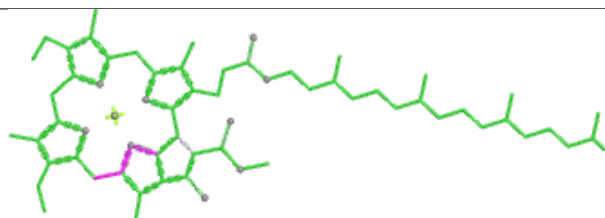


Rings

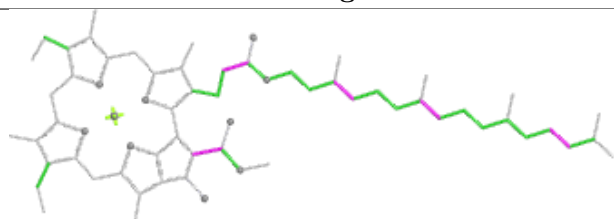
Ligand CLA B 811



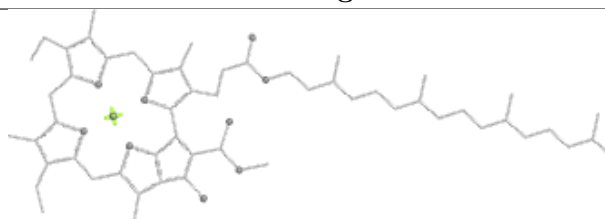
Bond lengths



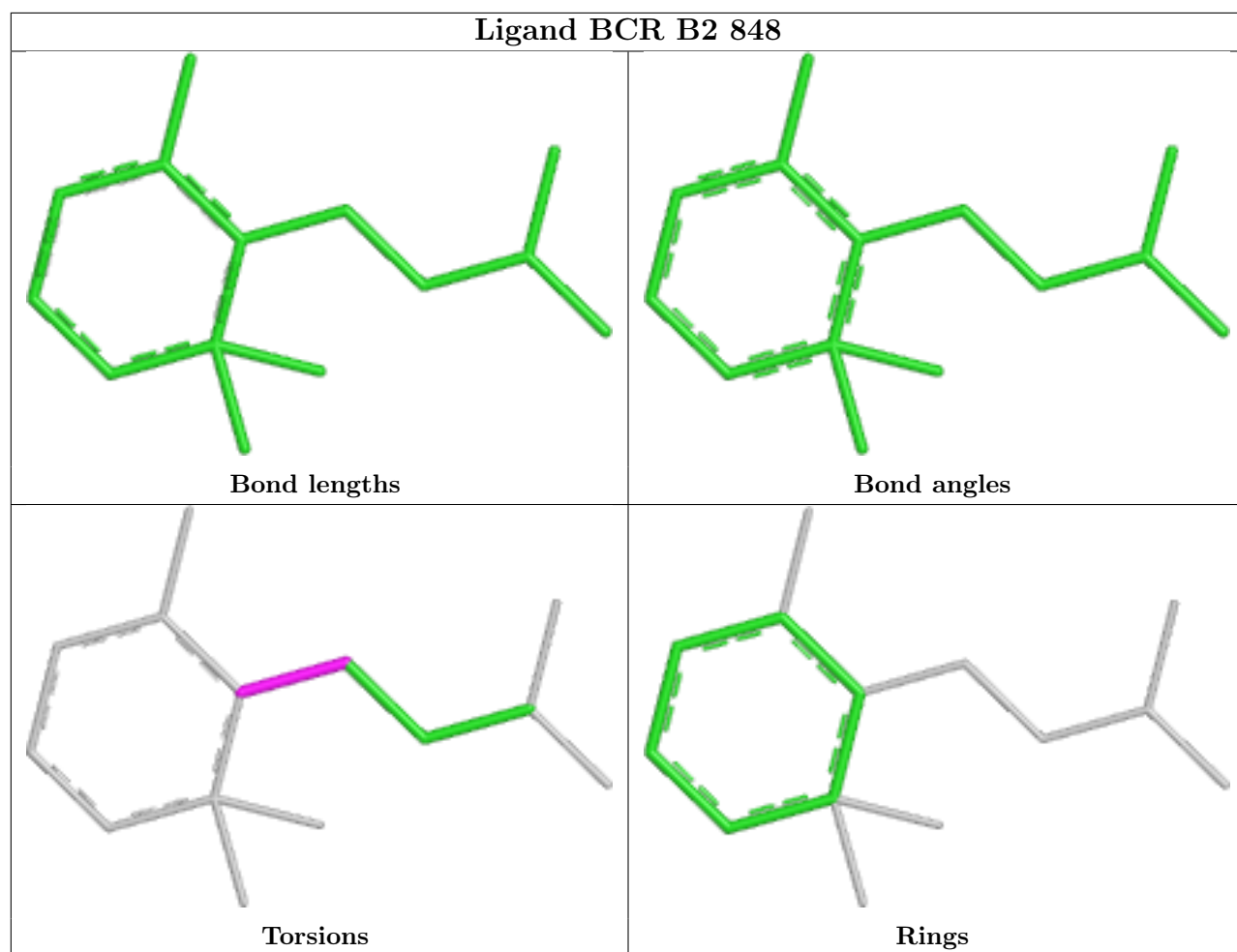
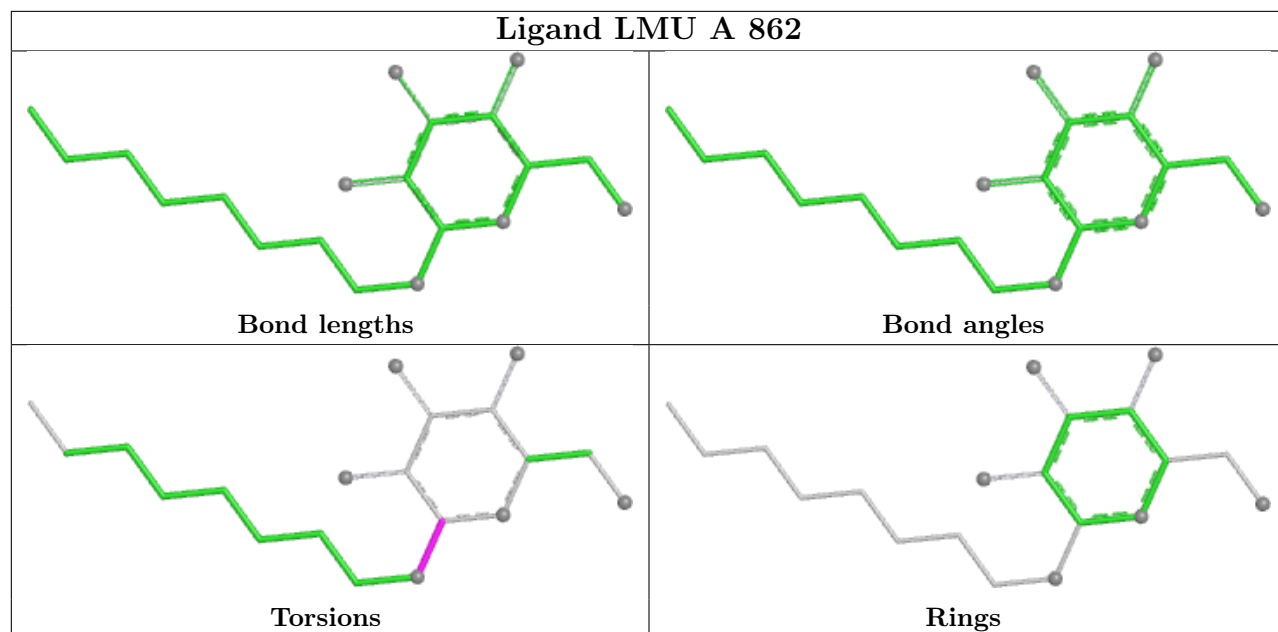
Bond angles

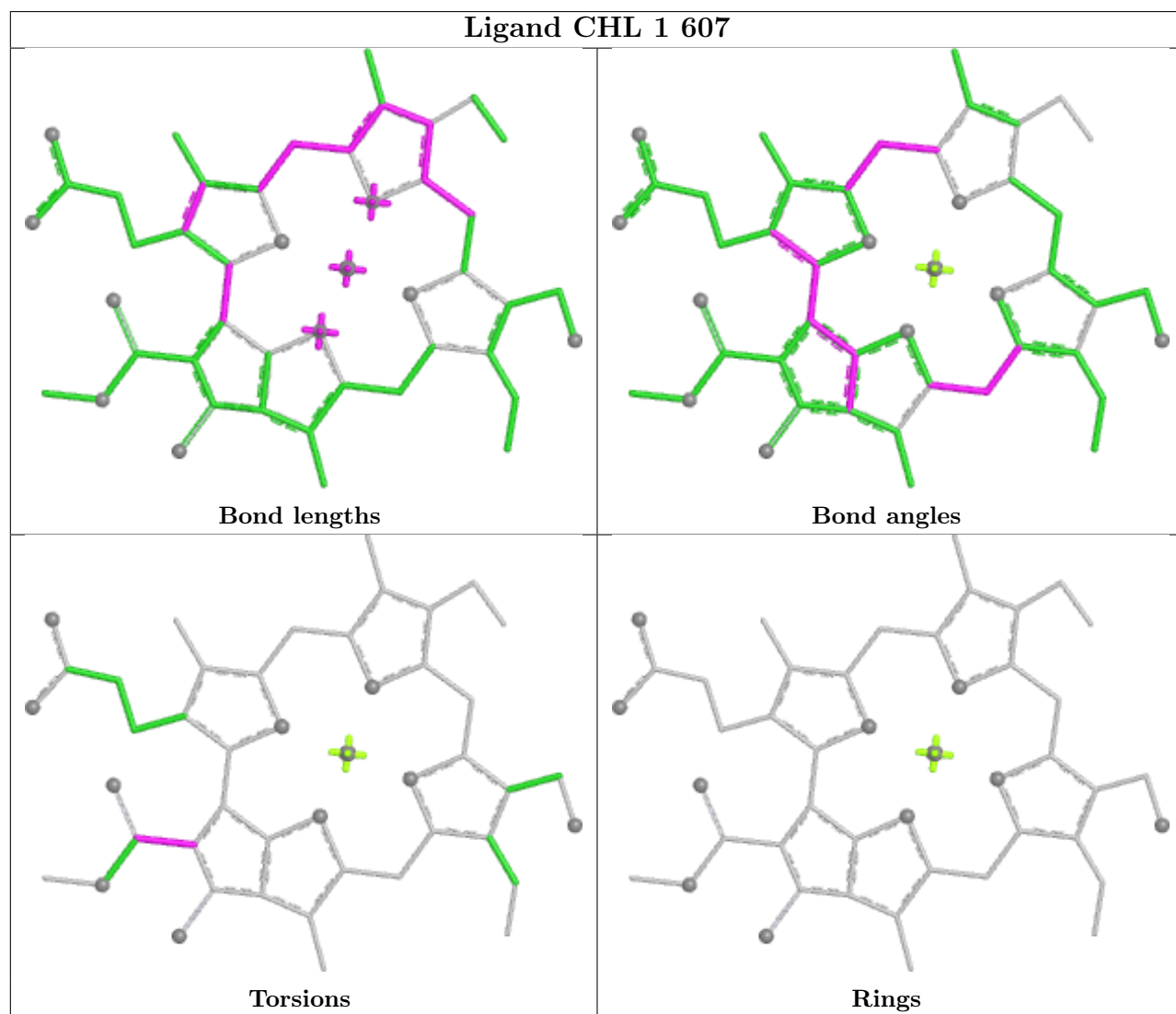
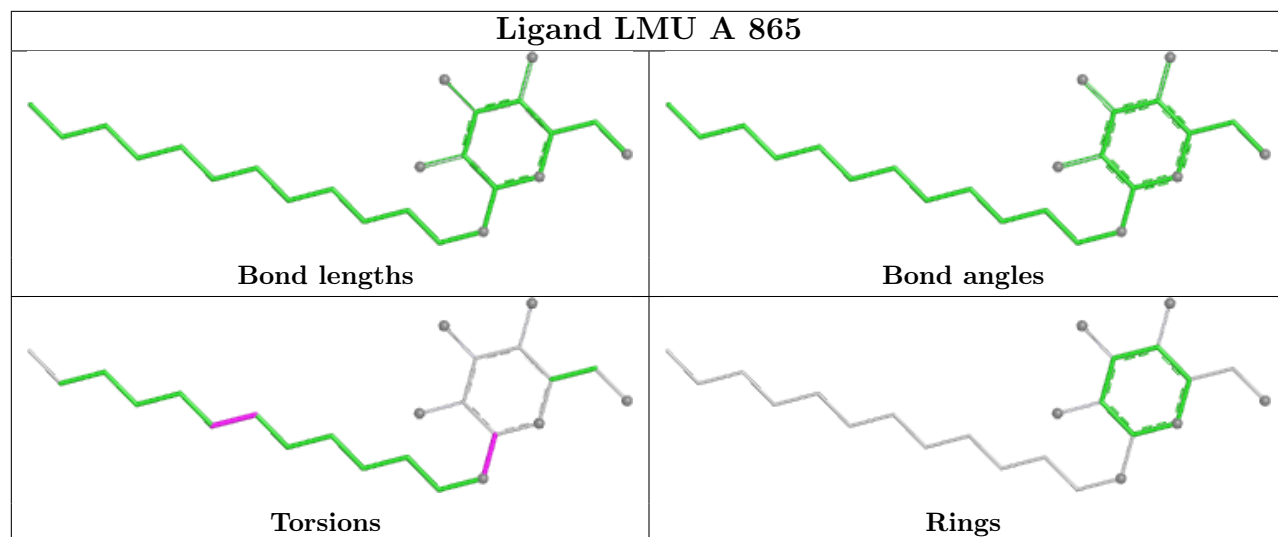


Torsions

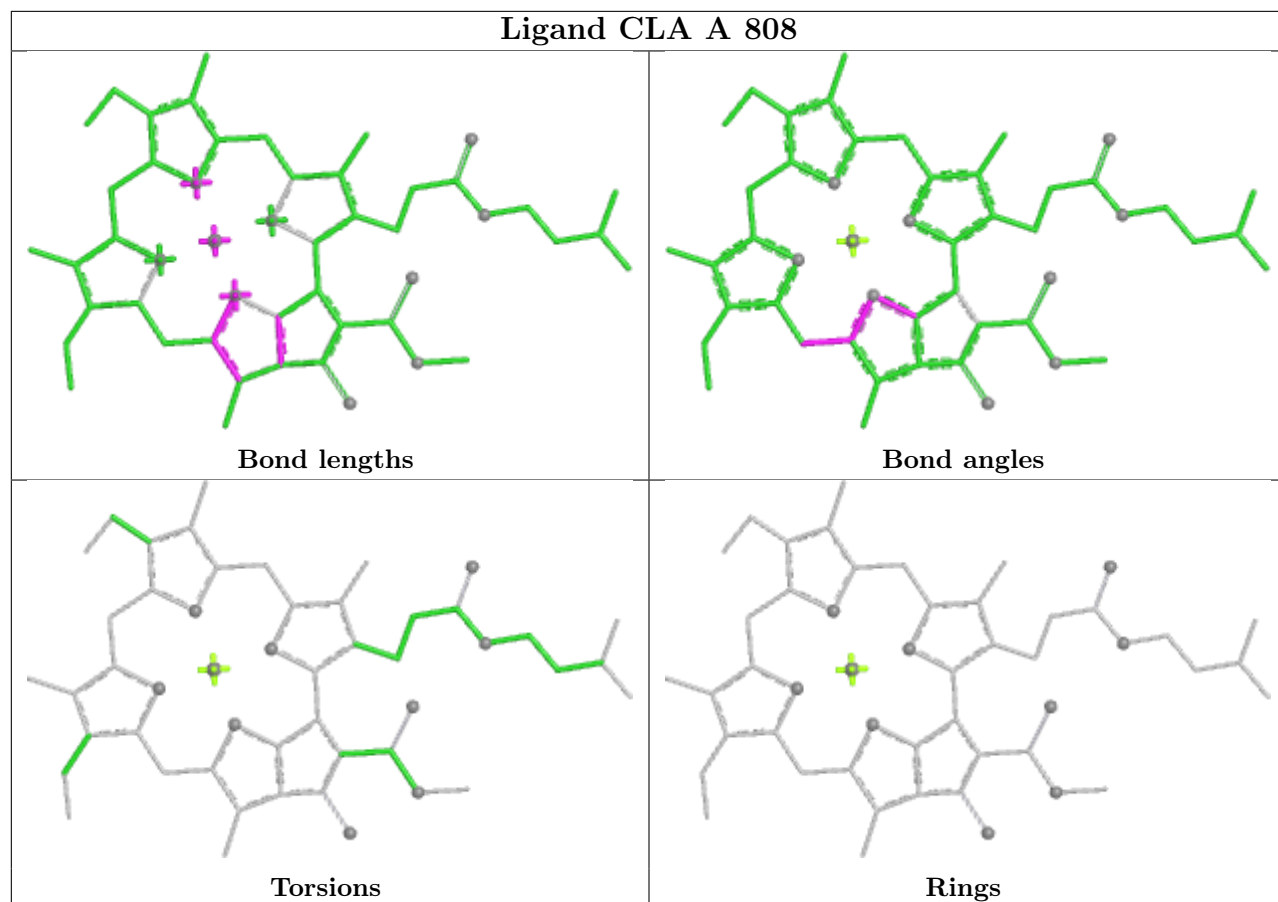


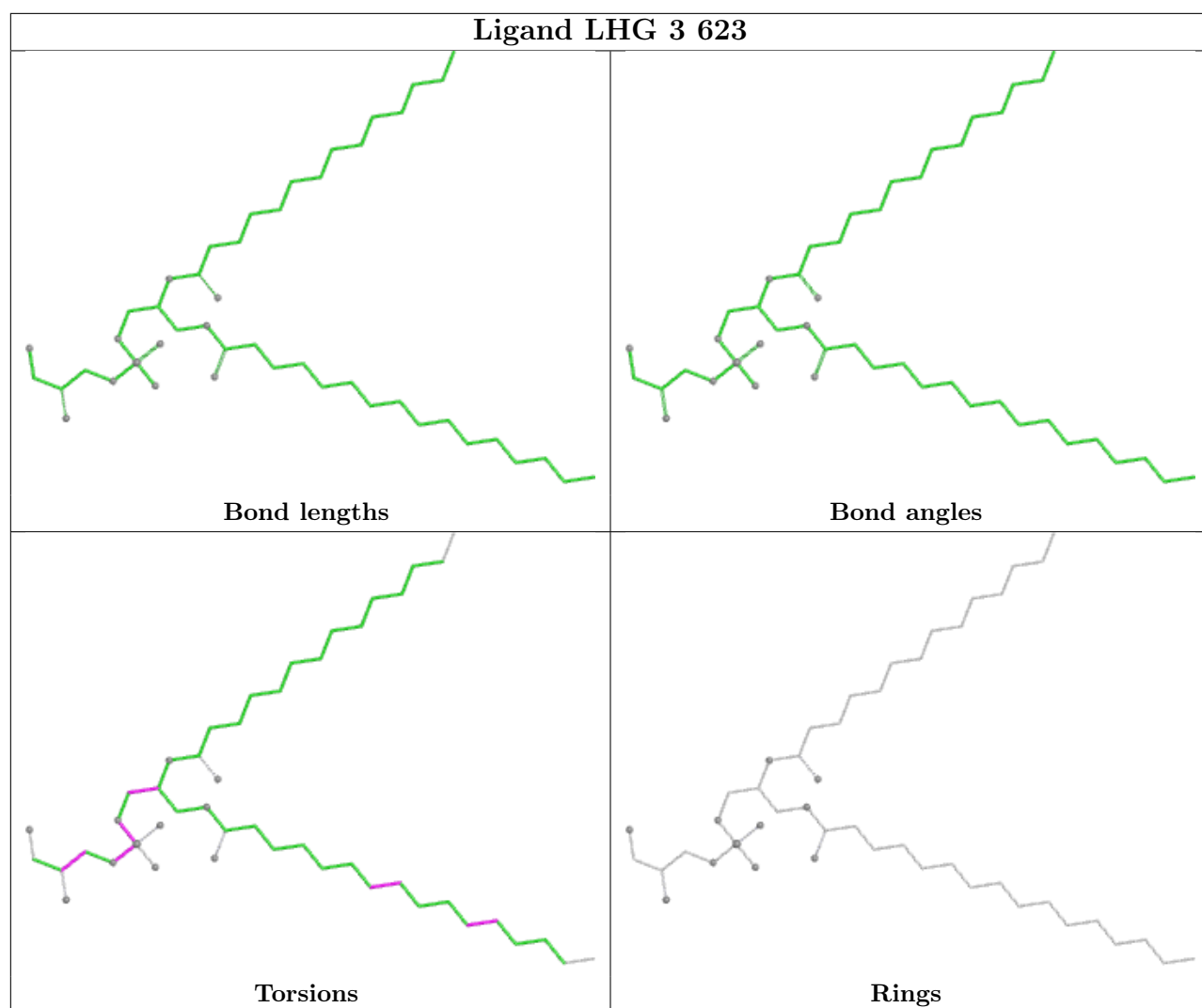
Rings

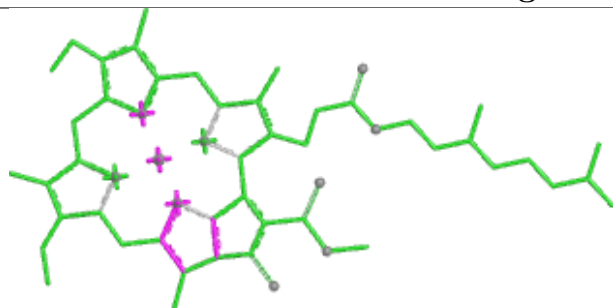
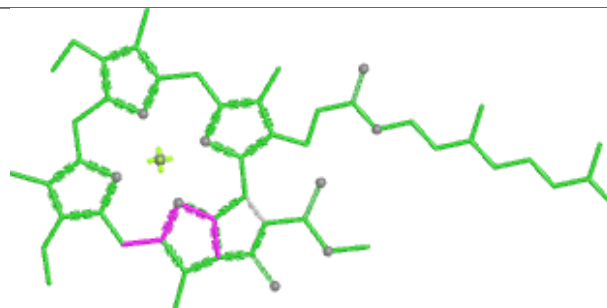
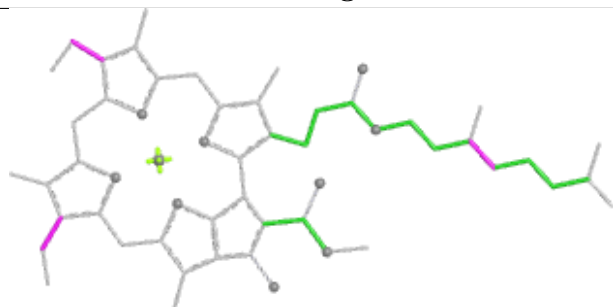
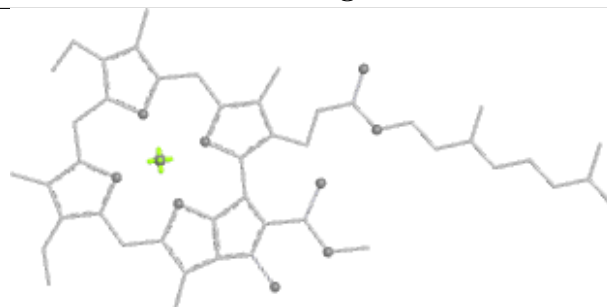
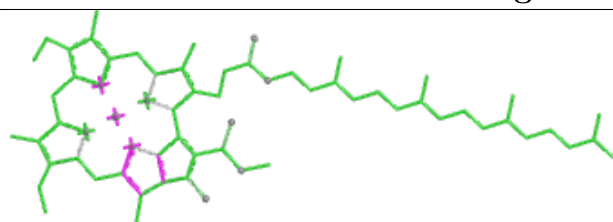
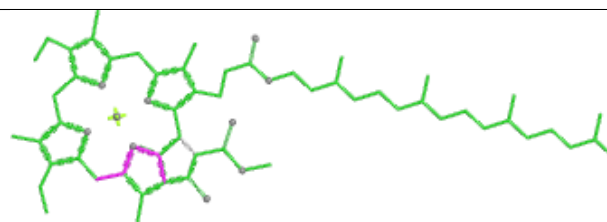
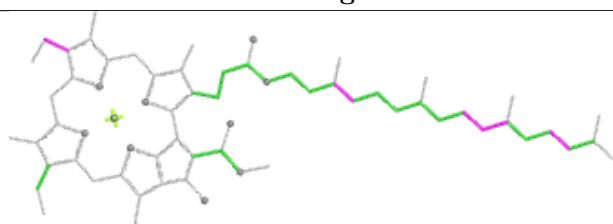
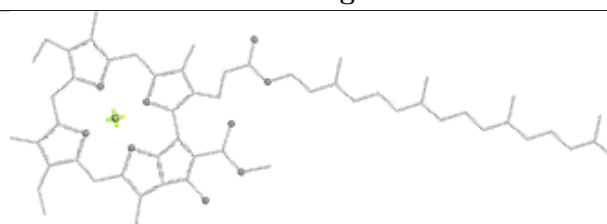




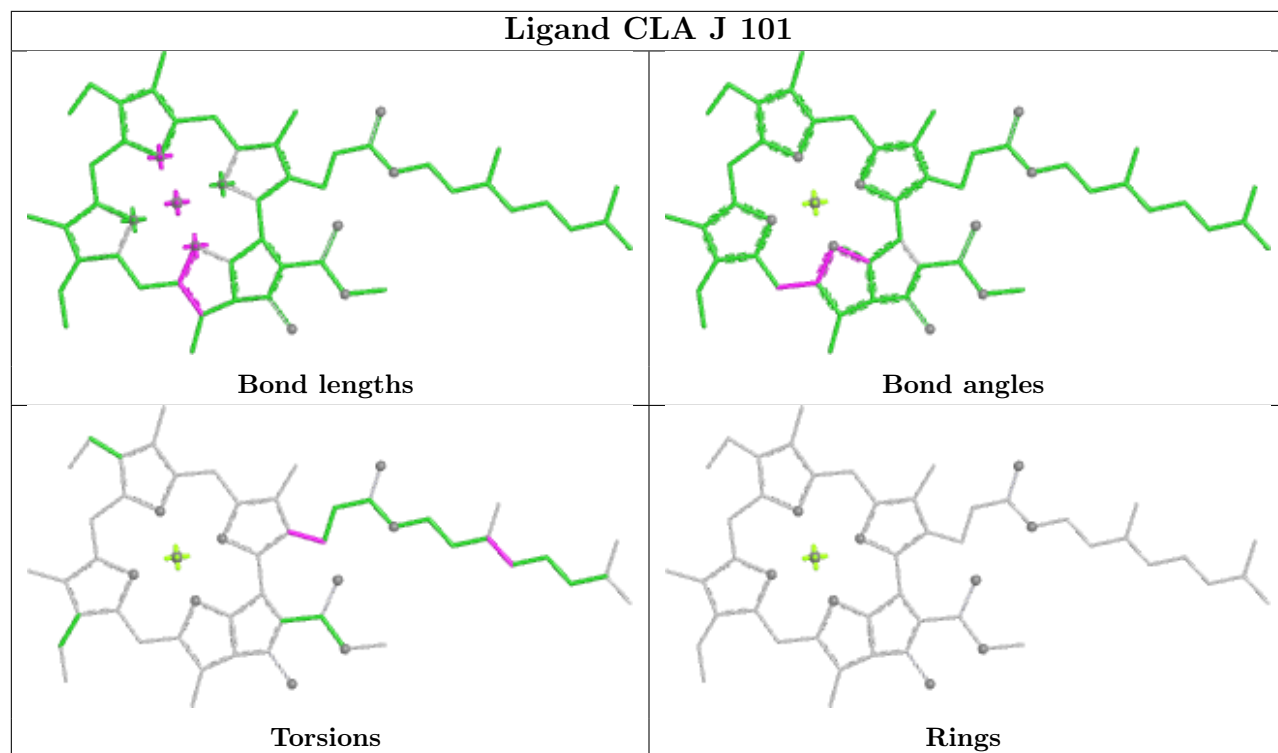
Ligand CLA A 808



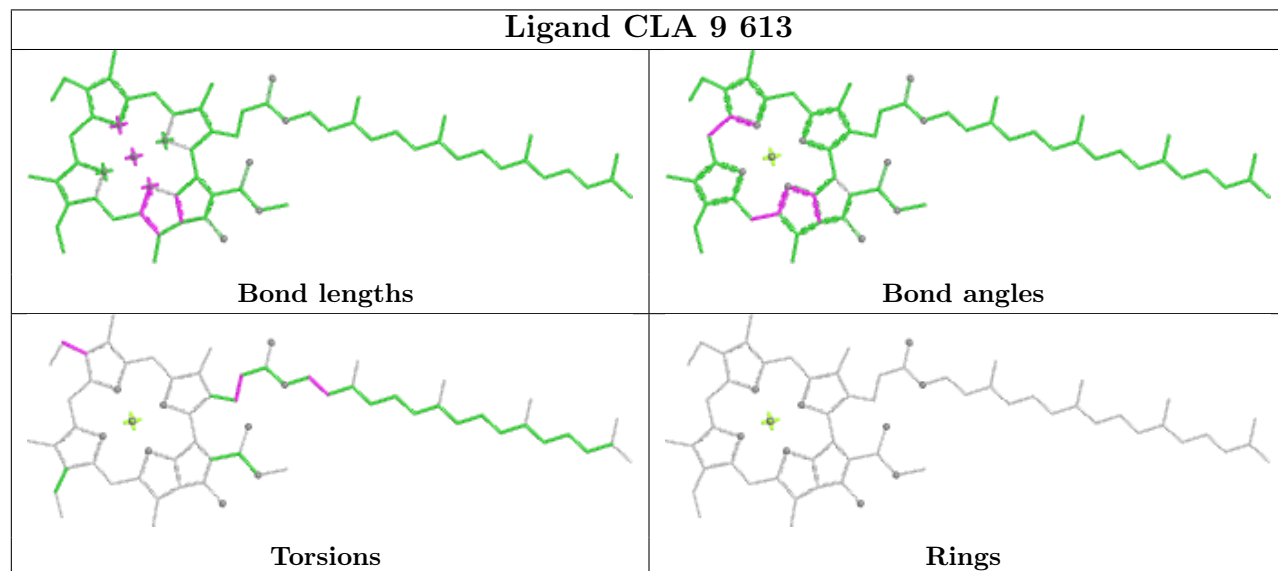


Ligand CLA 3 607**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA B 840****Bond lengths****Bond angles****Torsions****Rings**

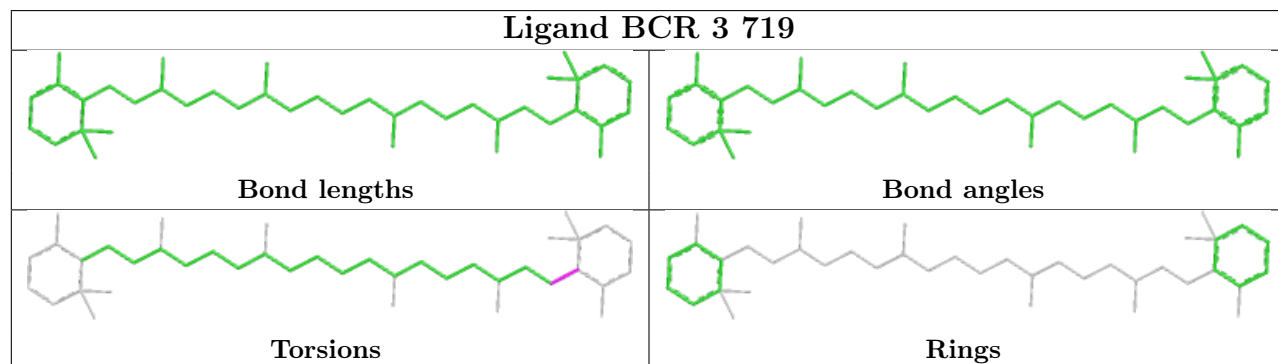
Ligand CLA J 101

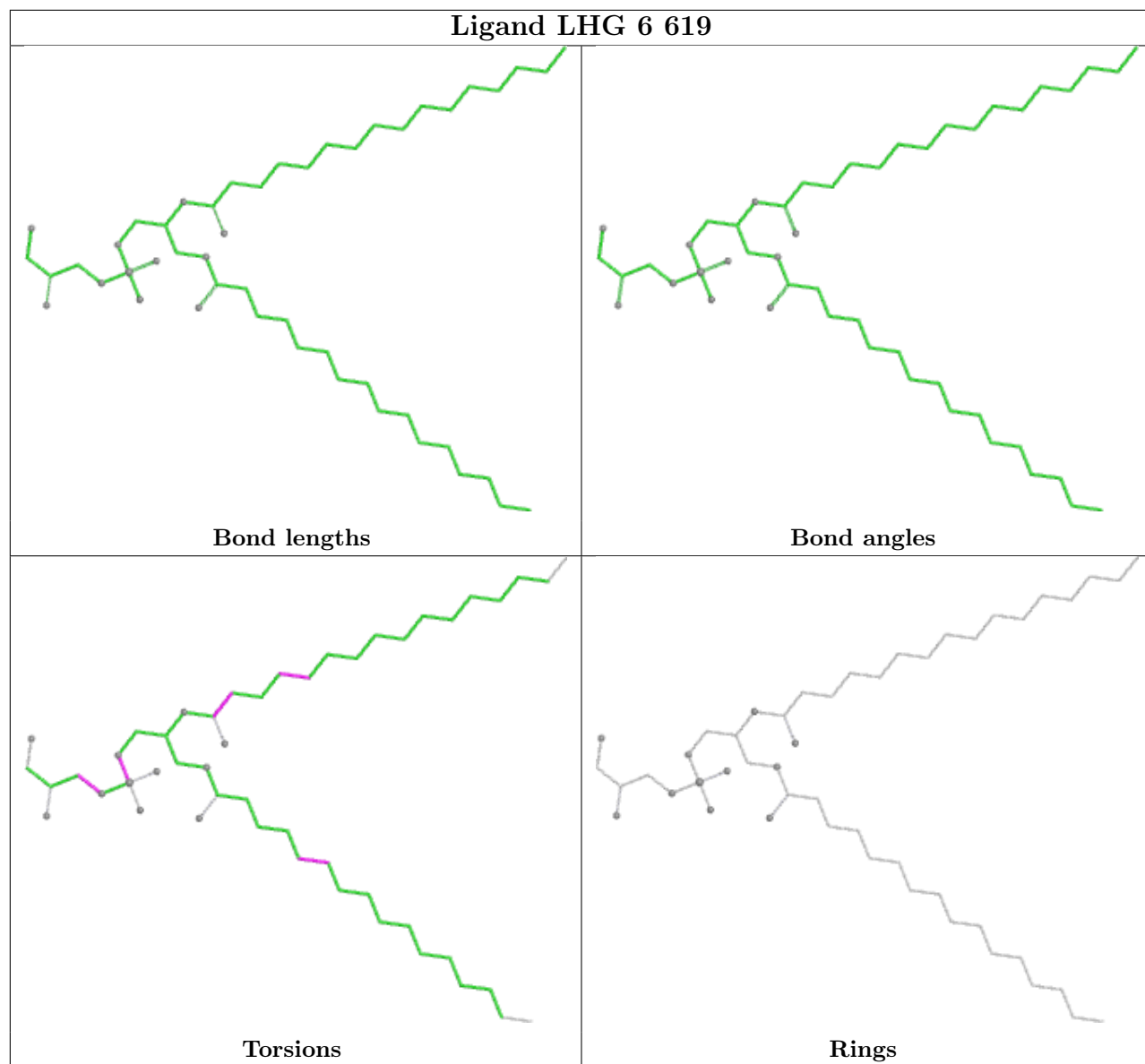


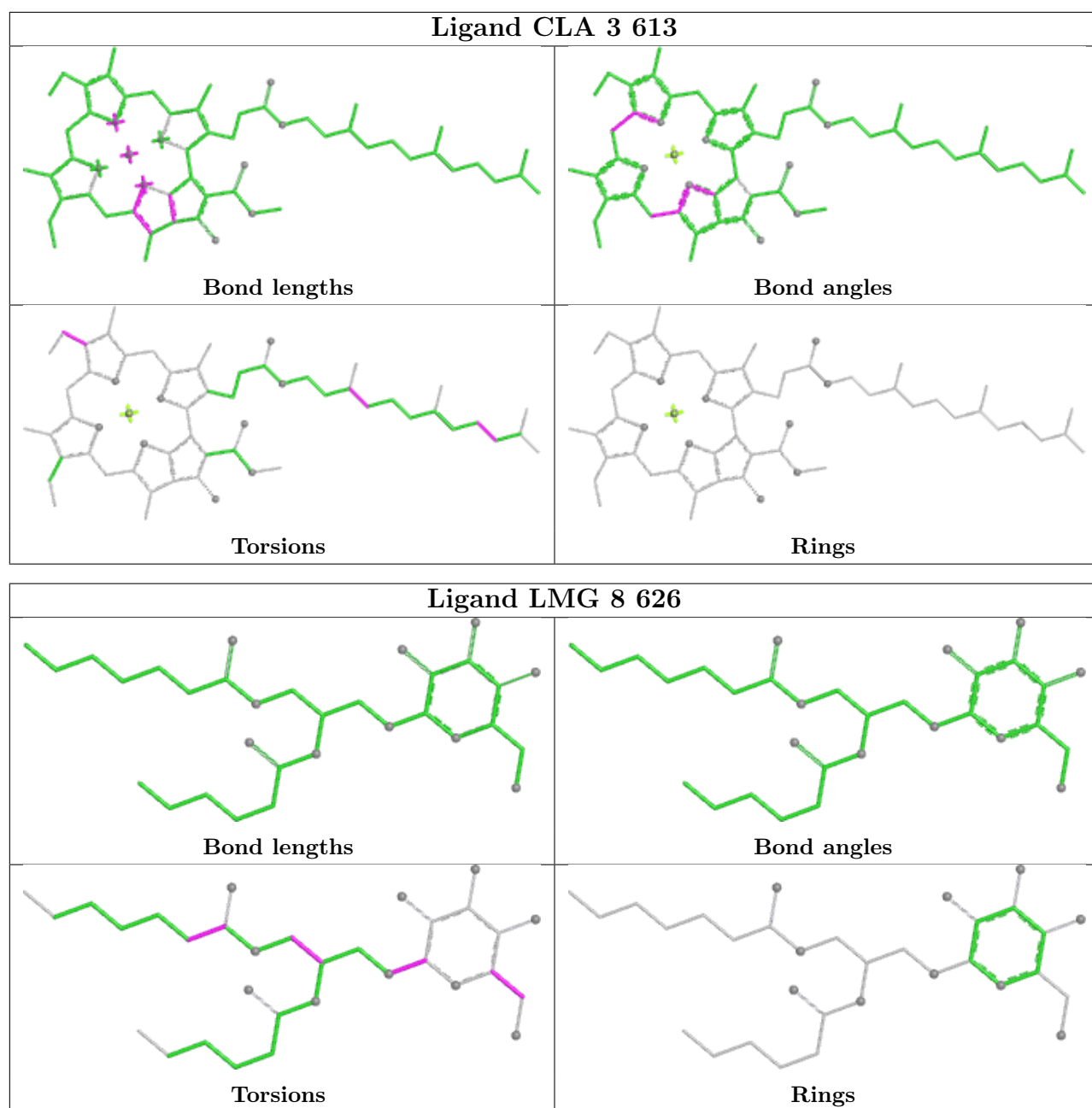
Ligand CLA 9 613

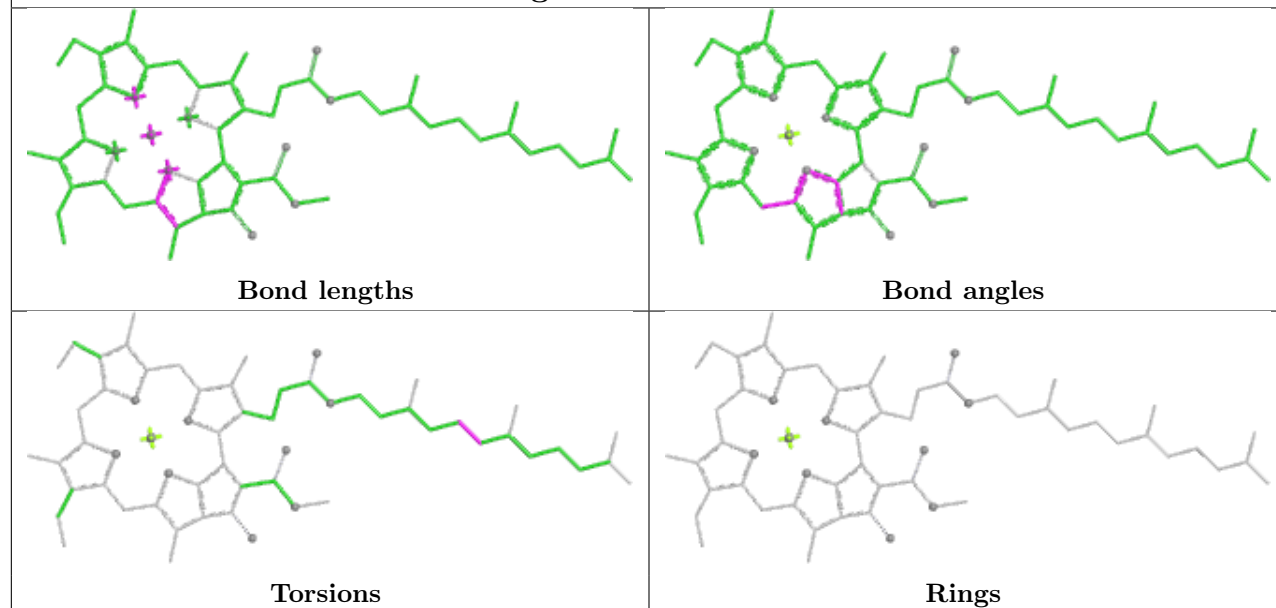
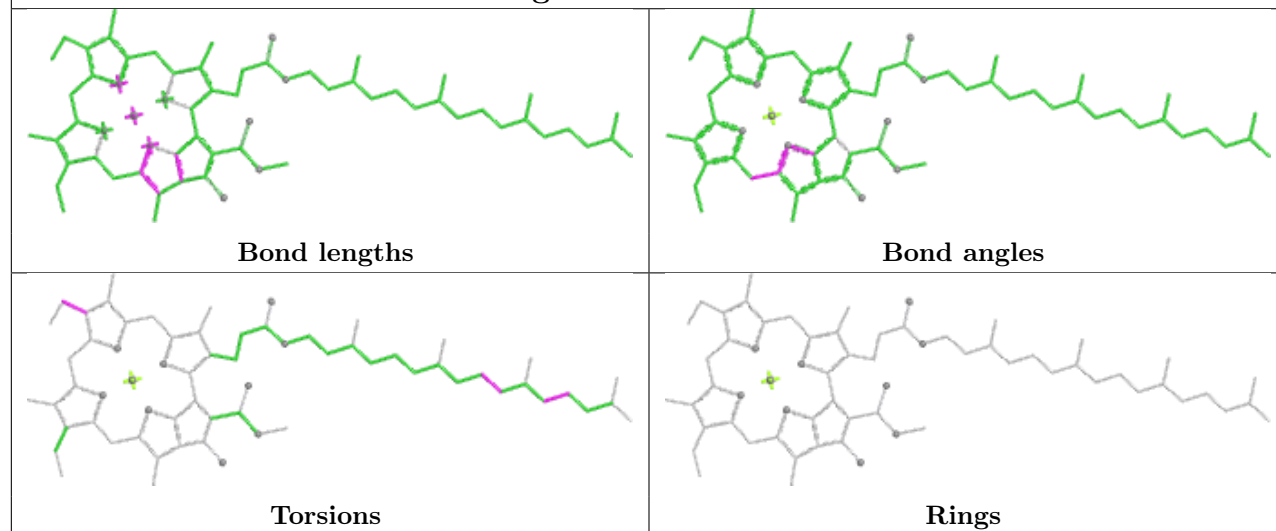


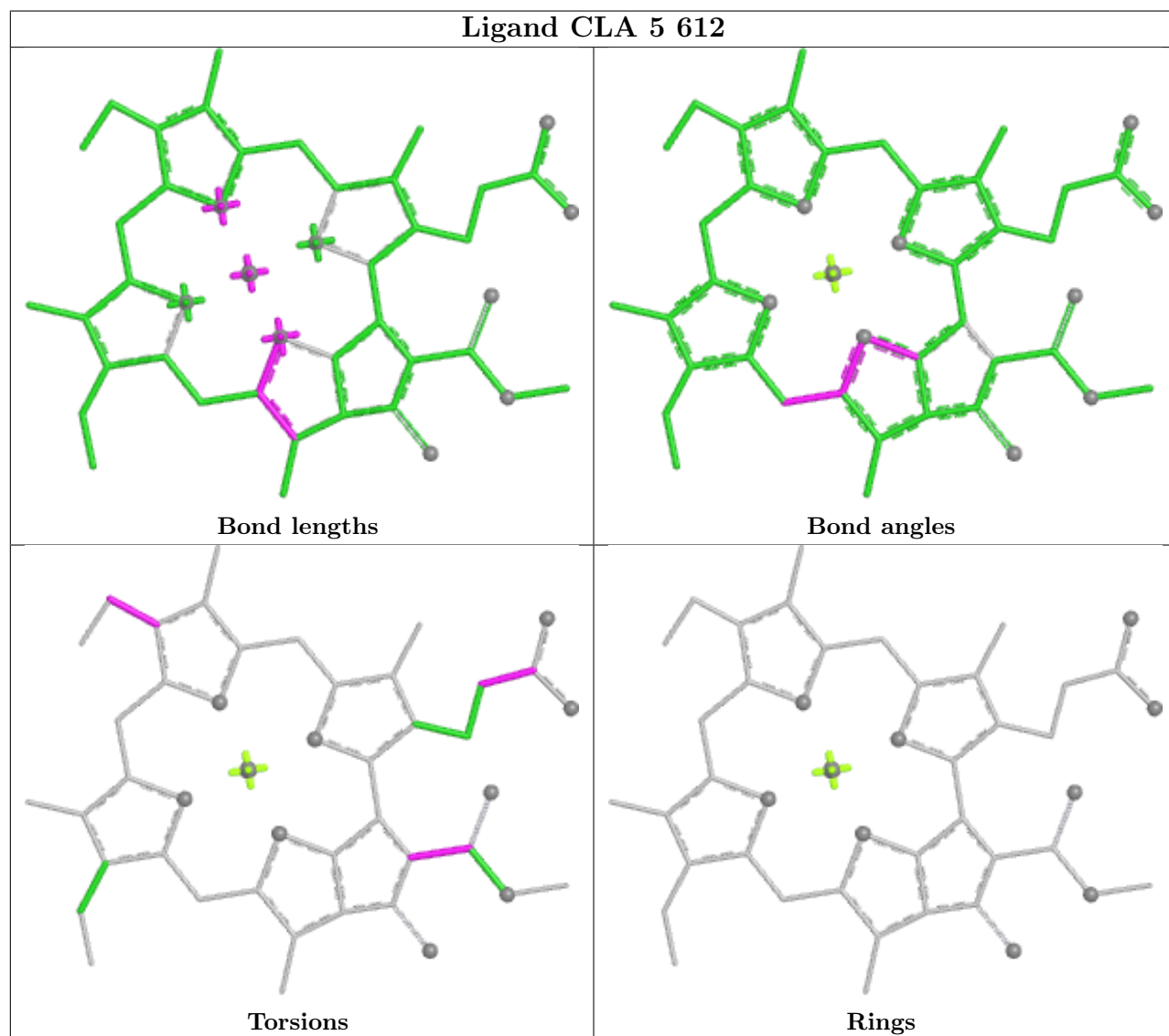
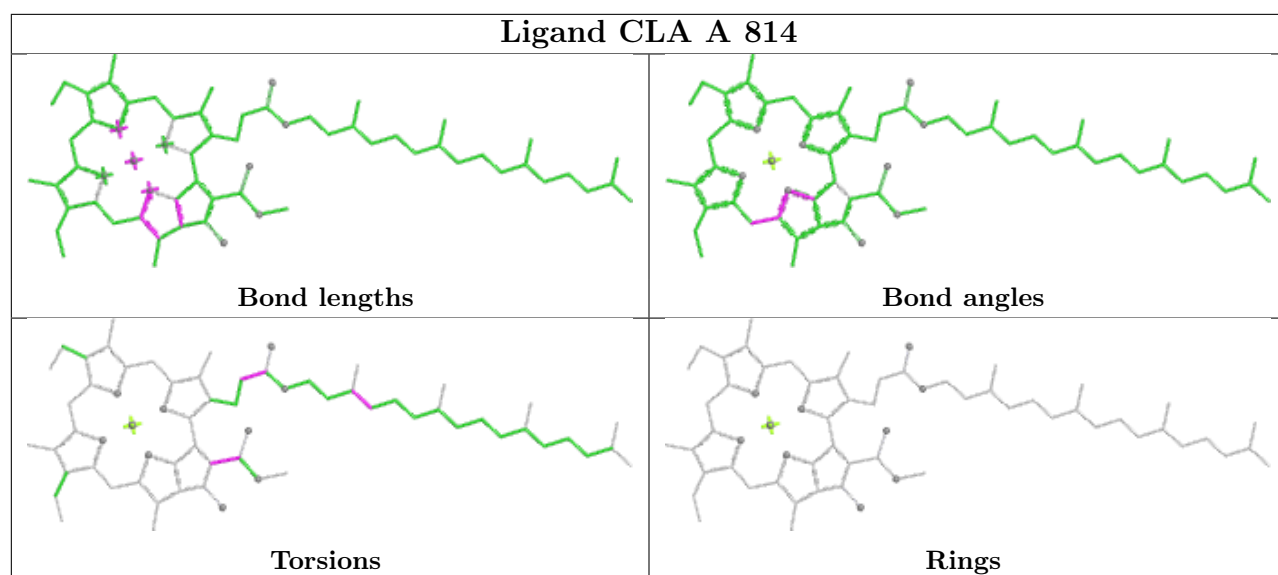
Ligand BCR 3 719



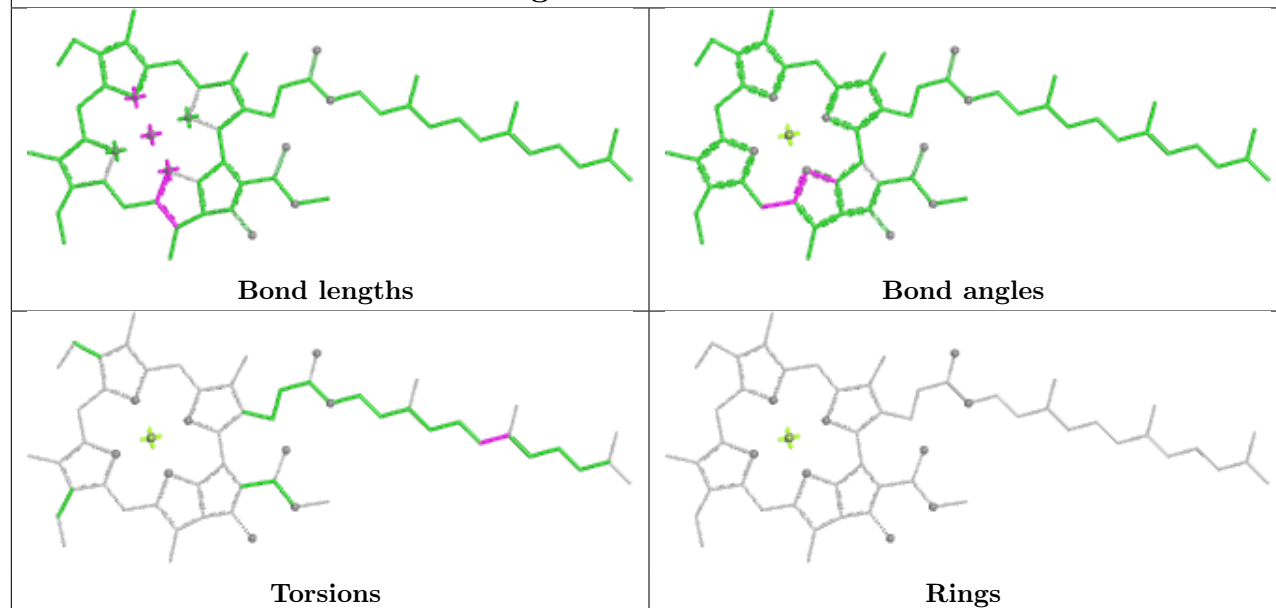




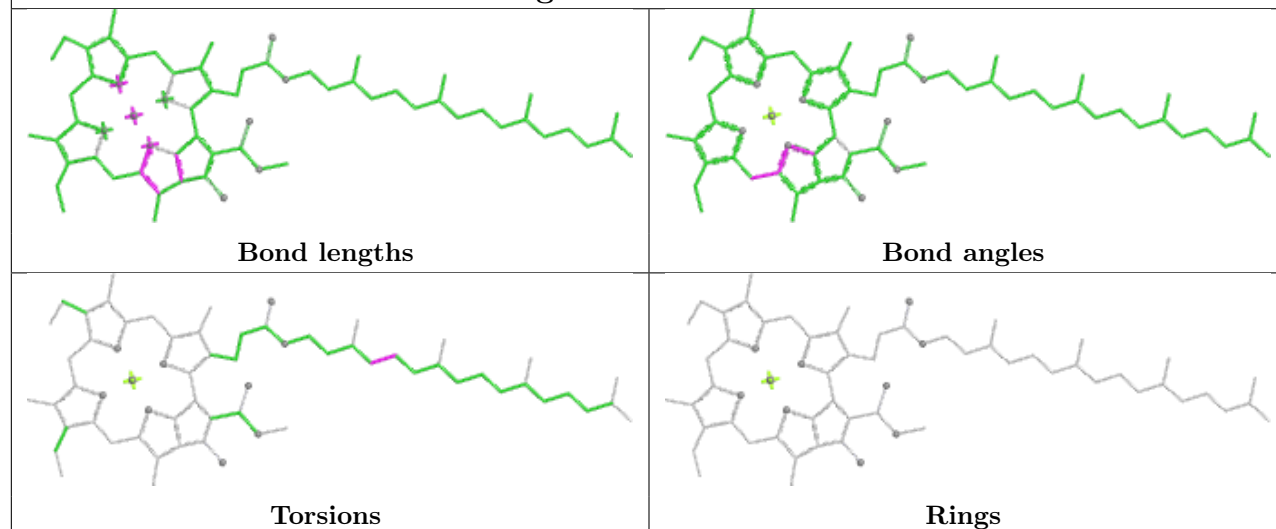
Ligand CLA K 203**Ligand CLA B 818**



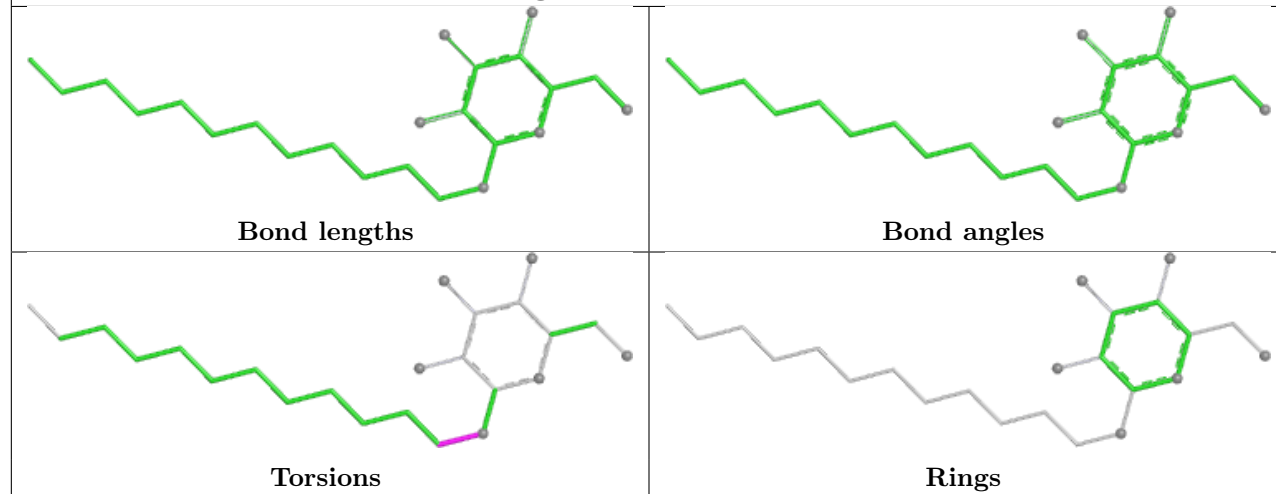
Ligand CLA G 203

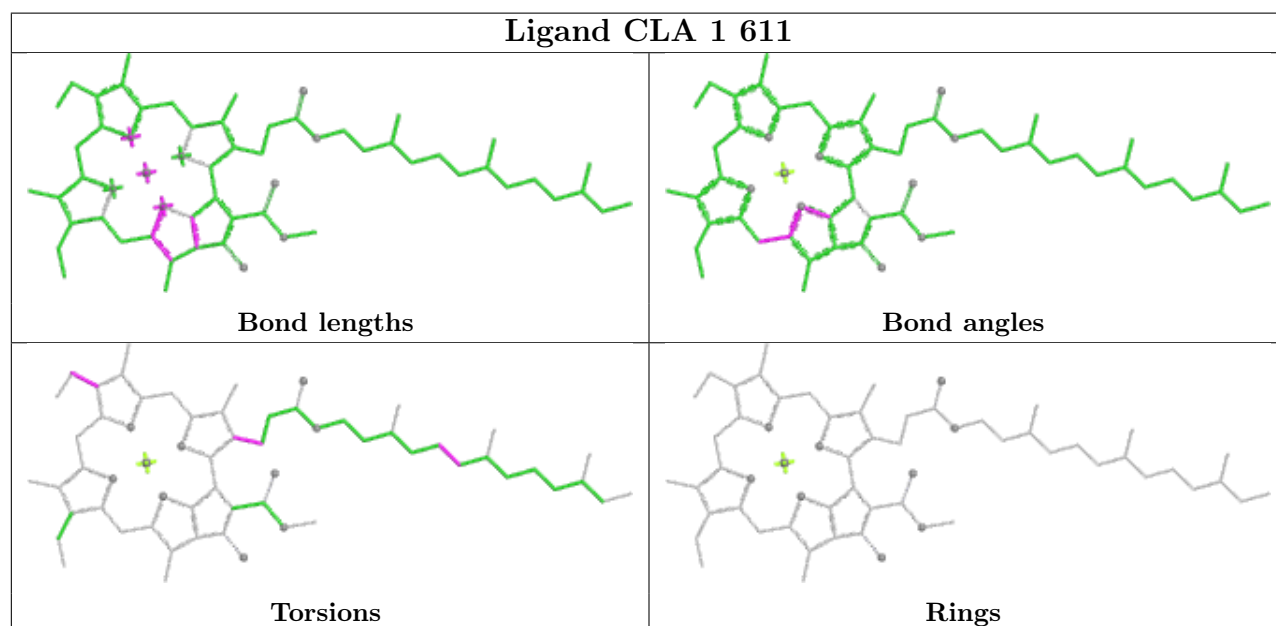
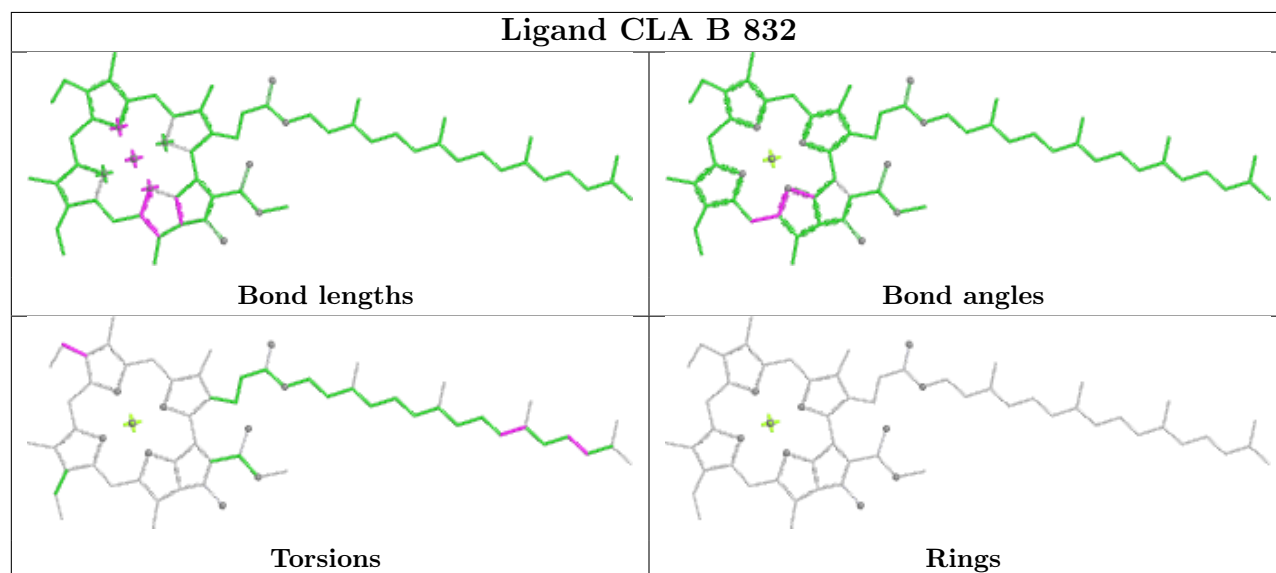
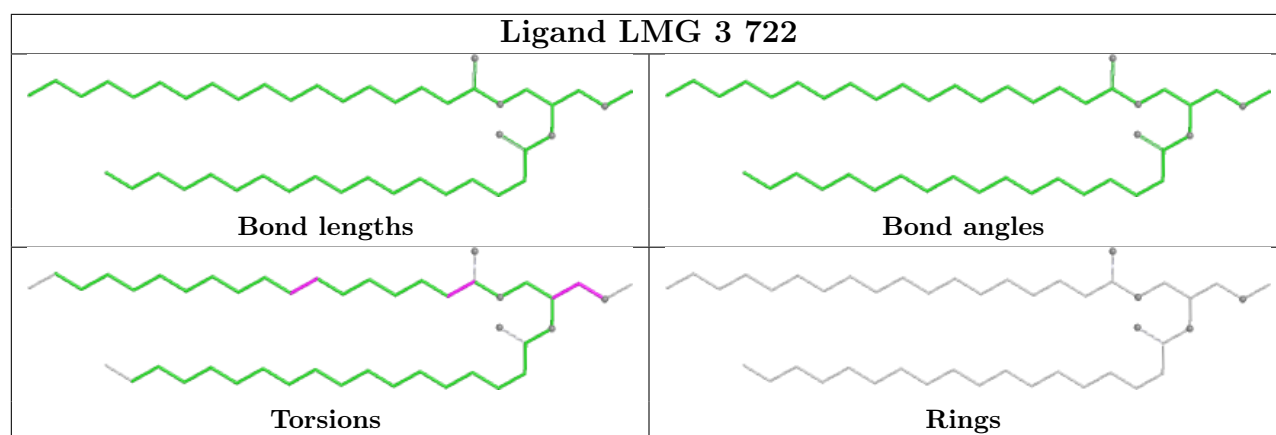


Ligand CLA 3 604

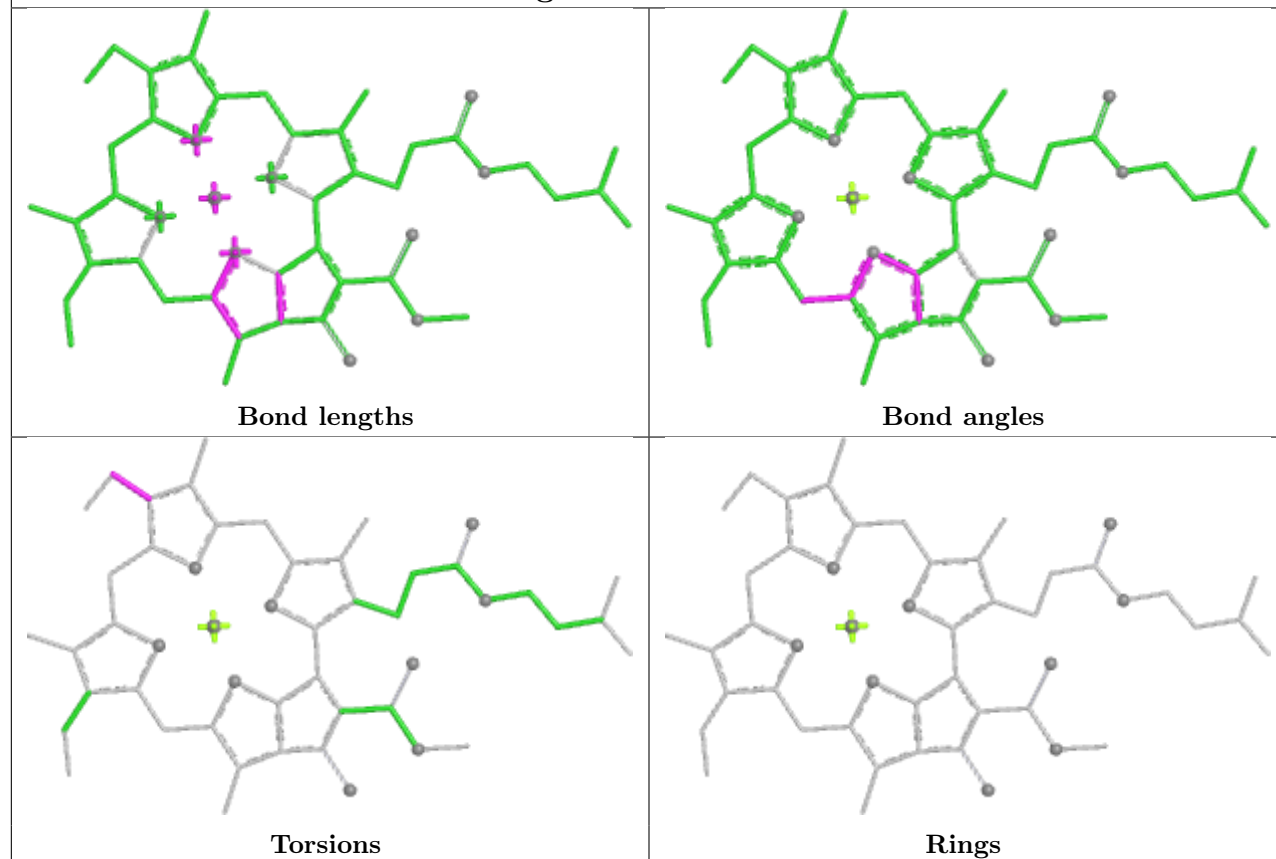


Ligand LMU 8 624

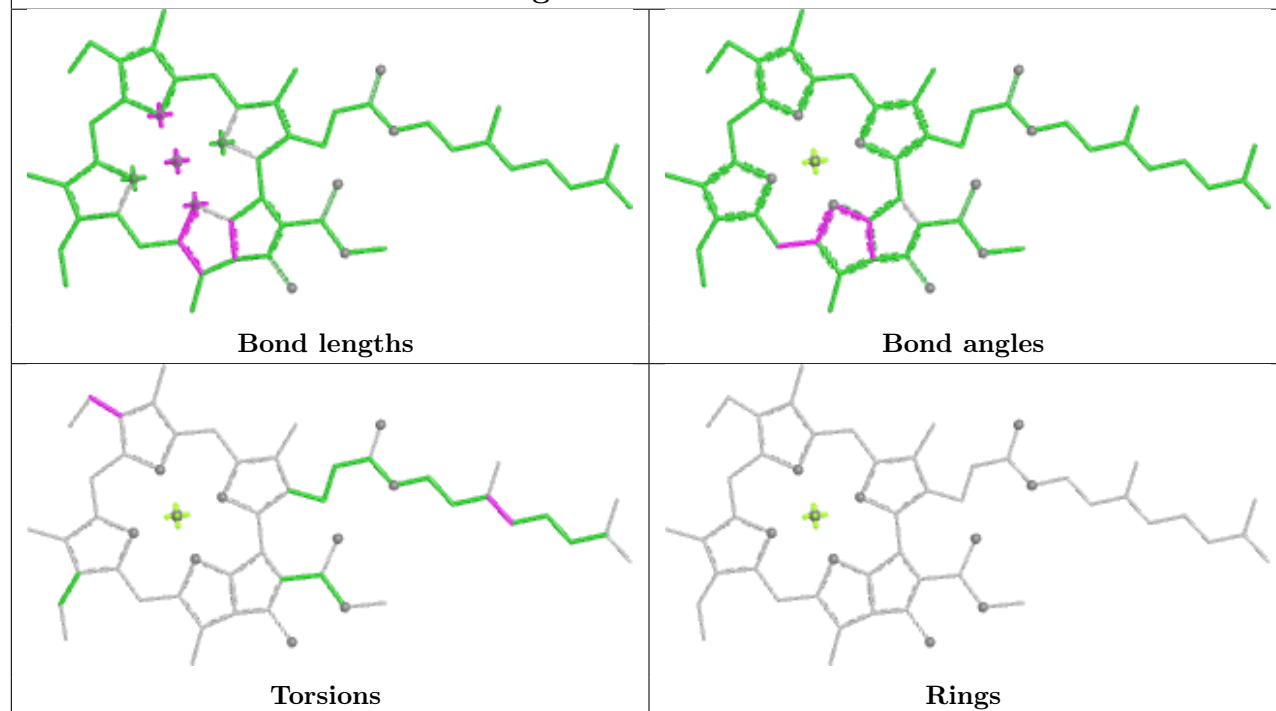


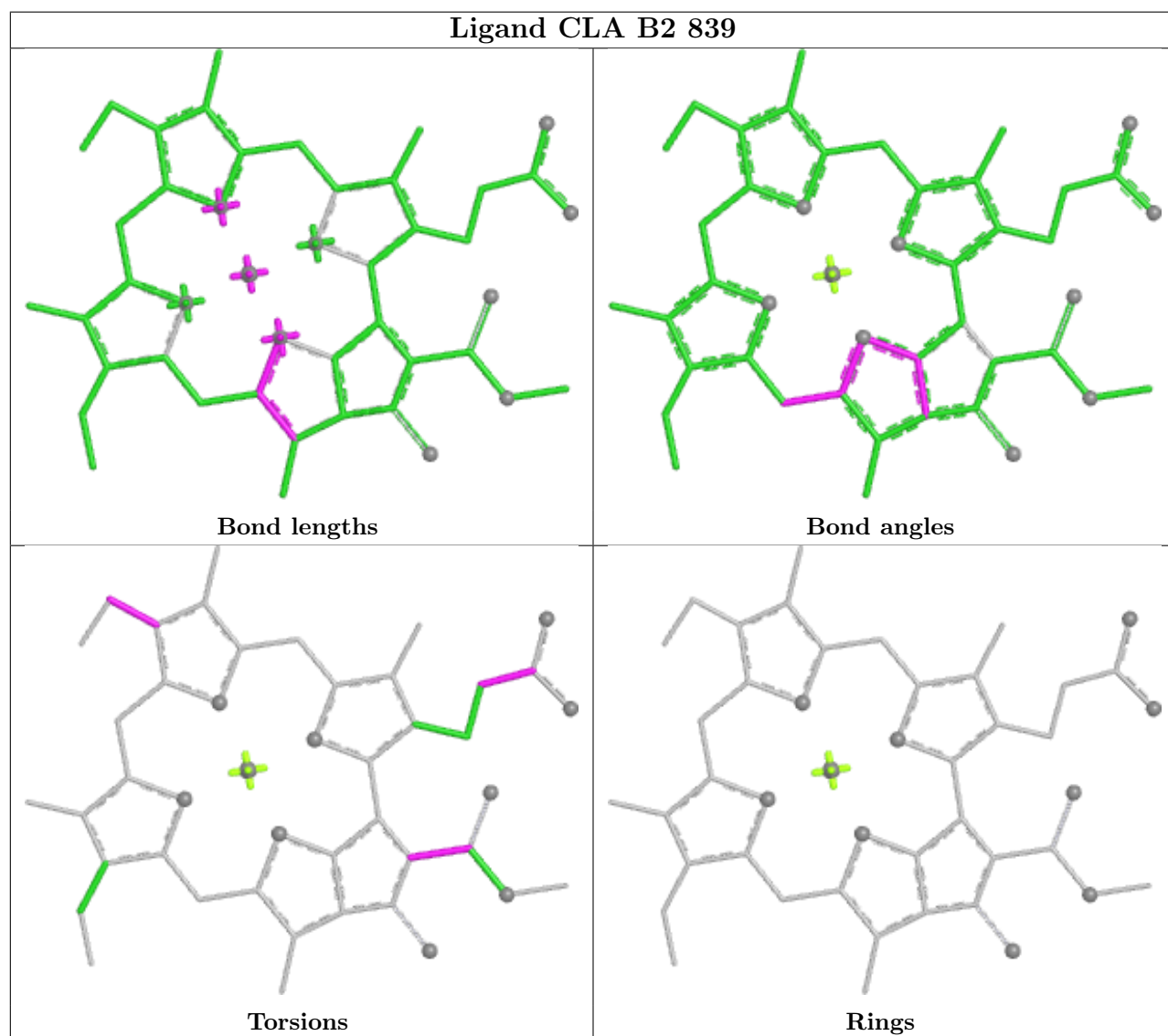
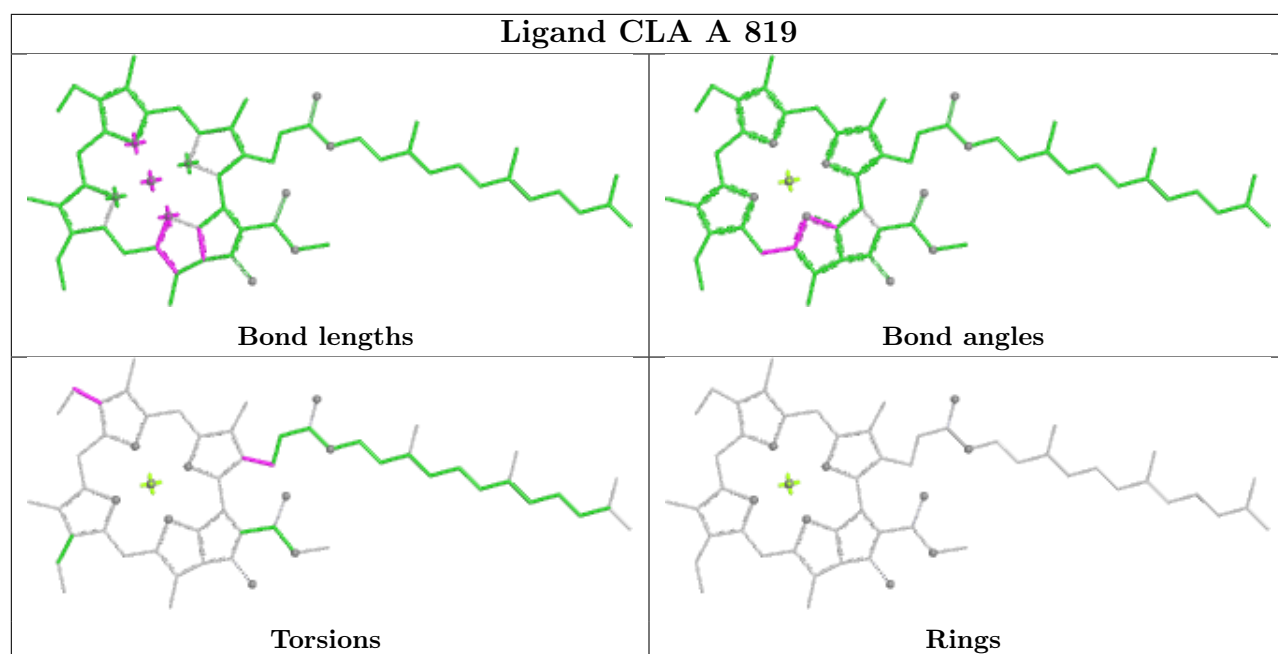


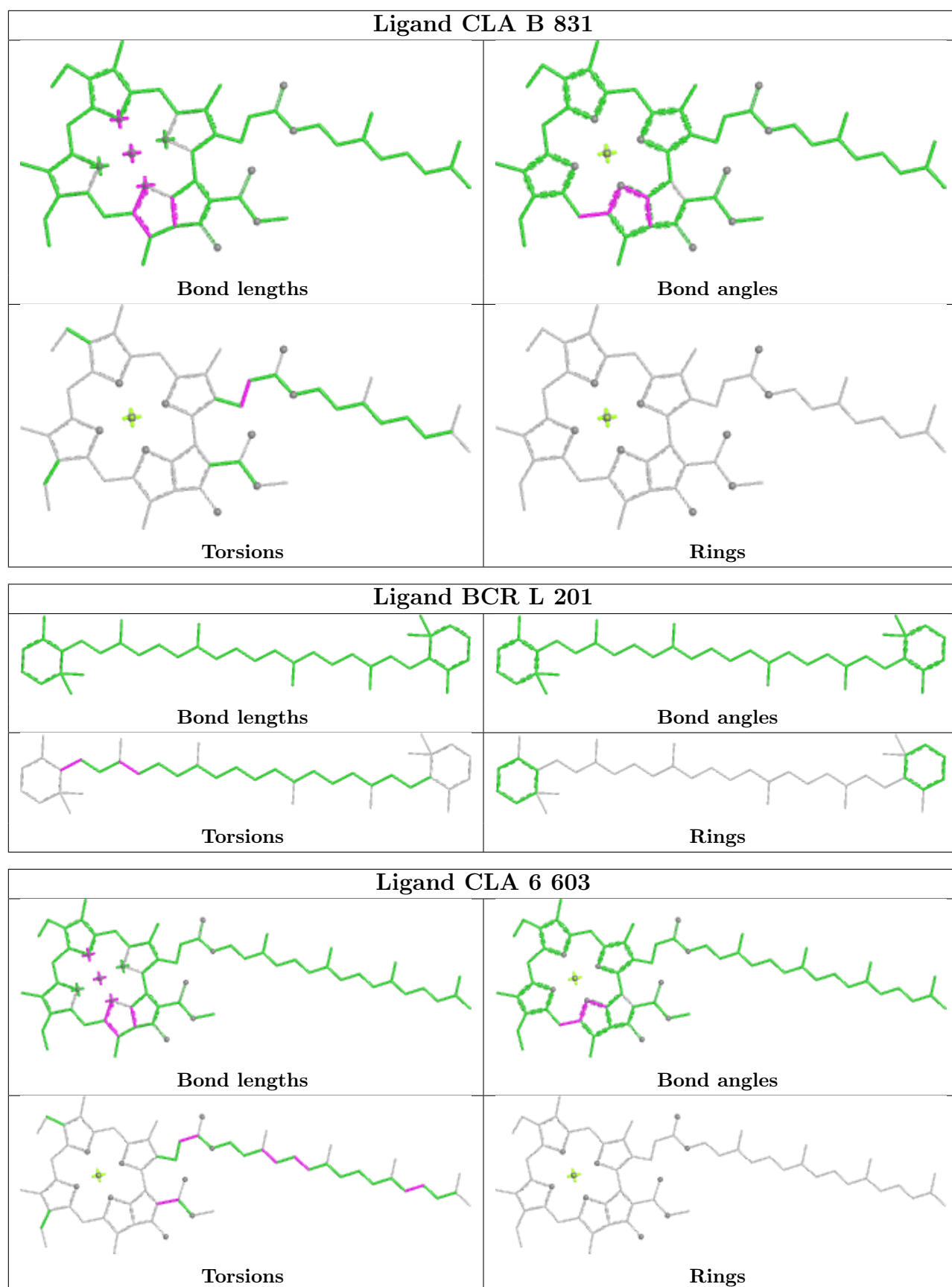
Ligand CLA 6 614

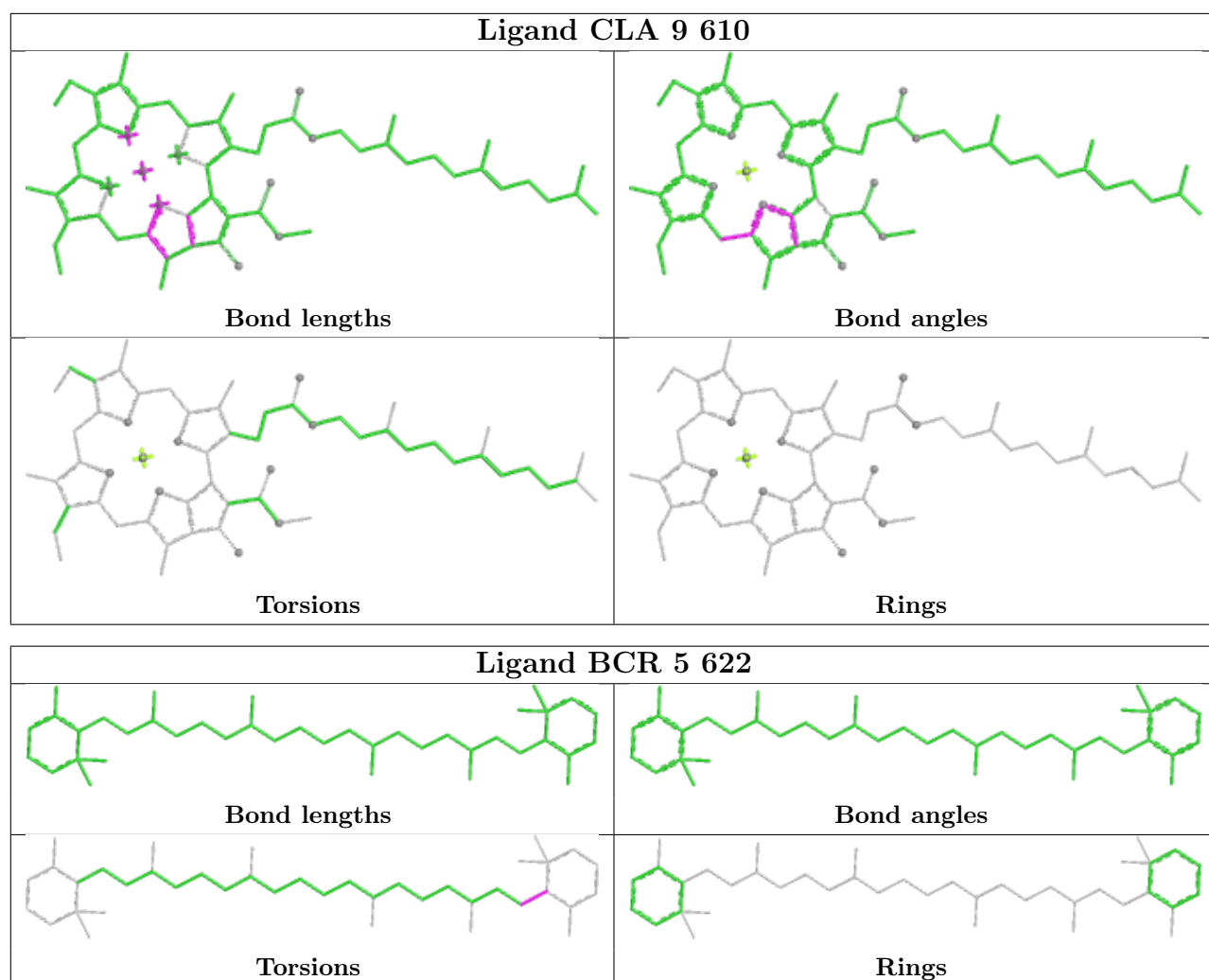


Ligand CLA B 807

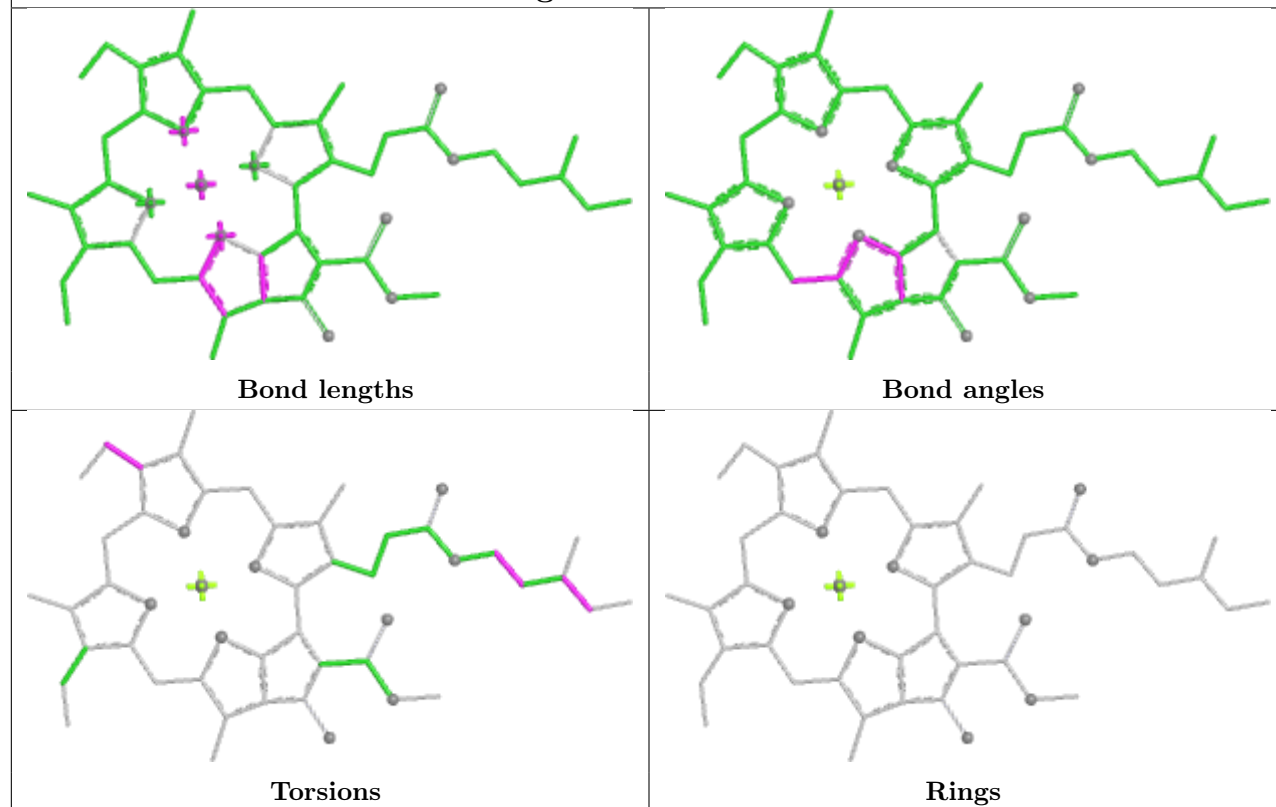




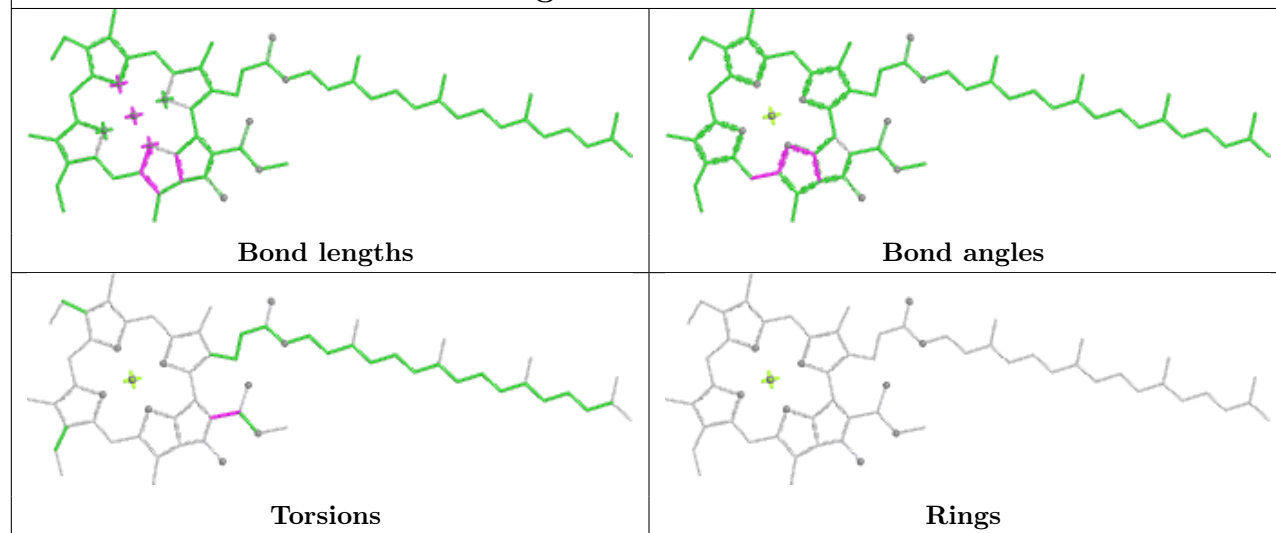


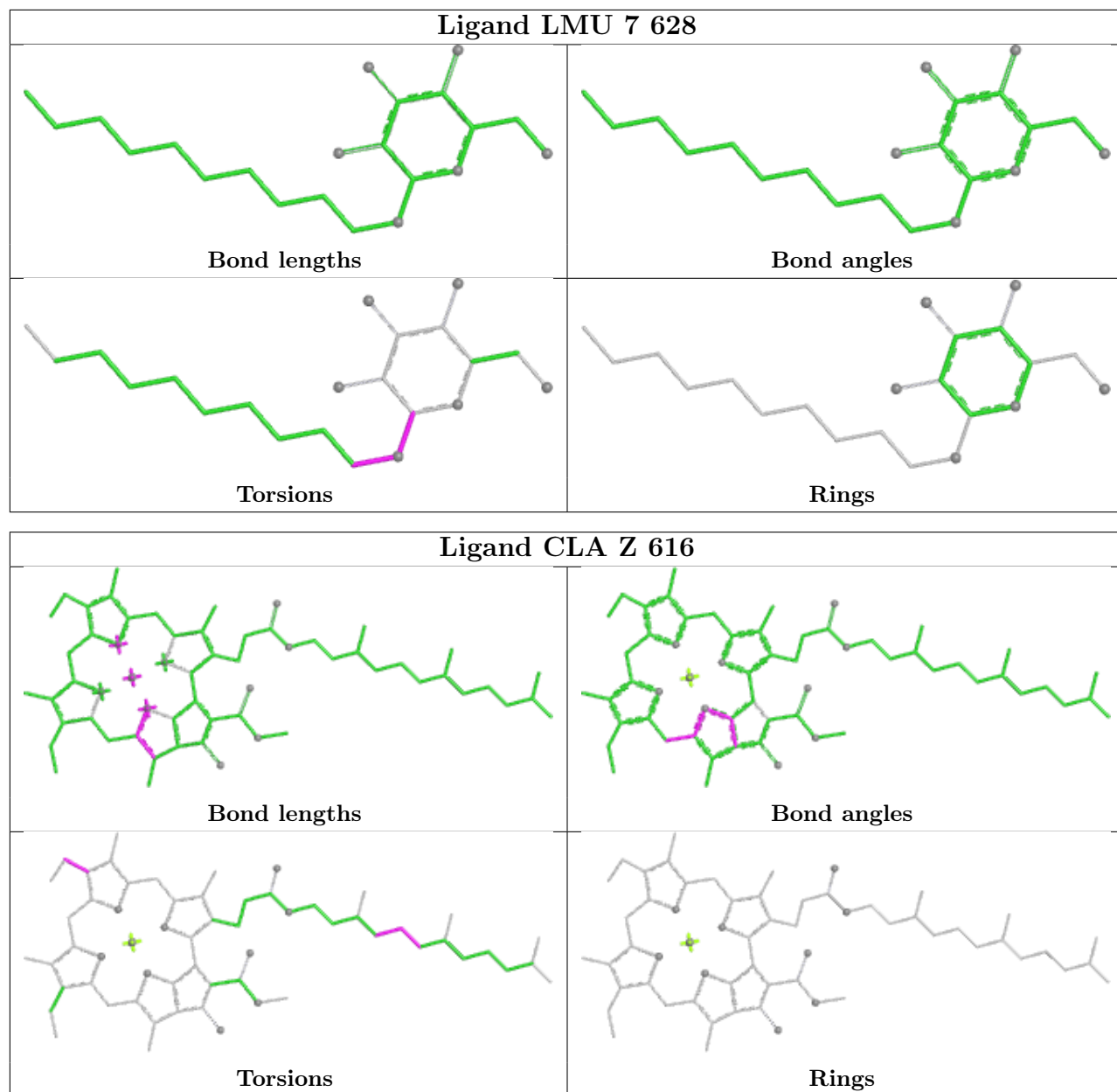


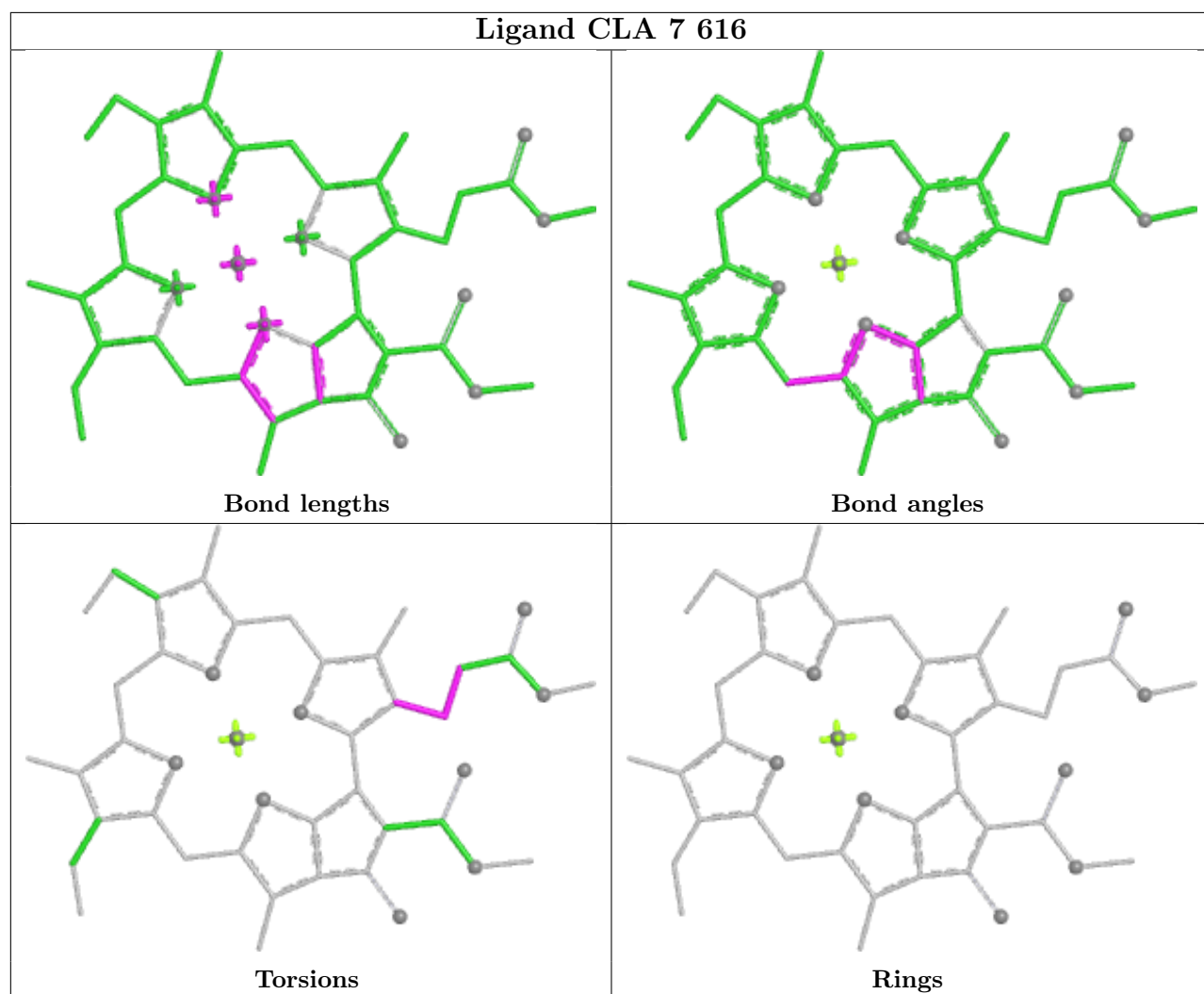
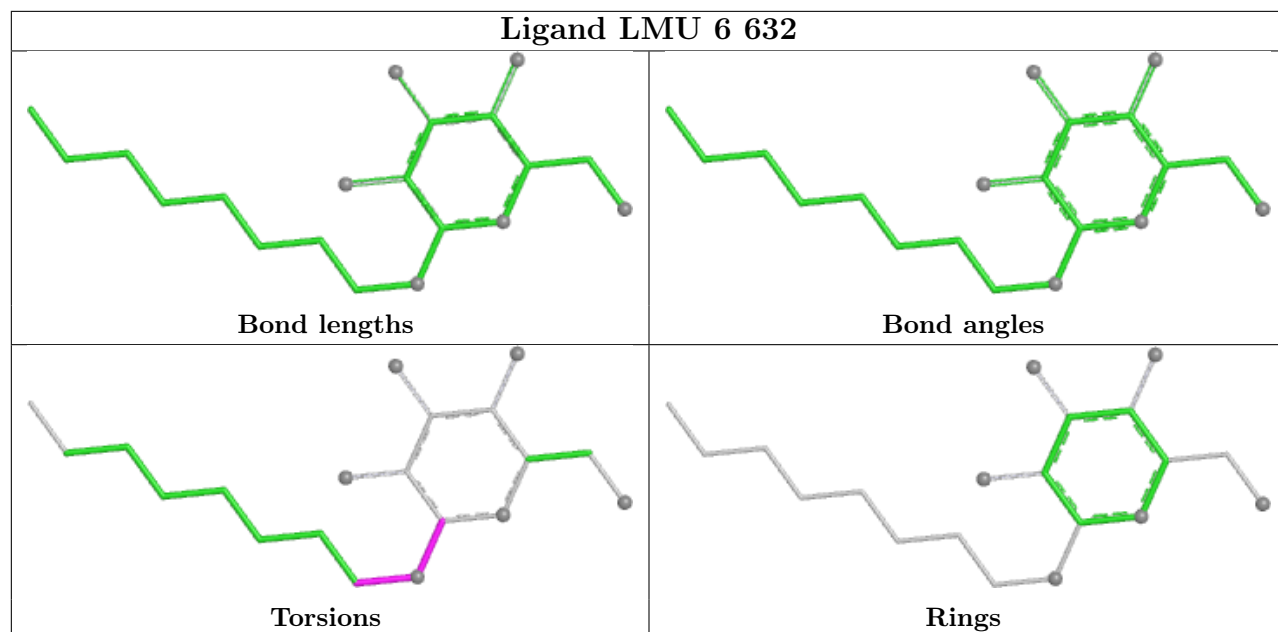
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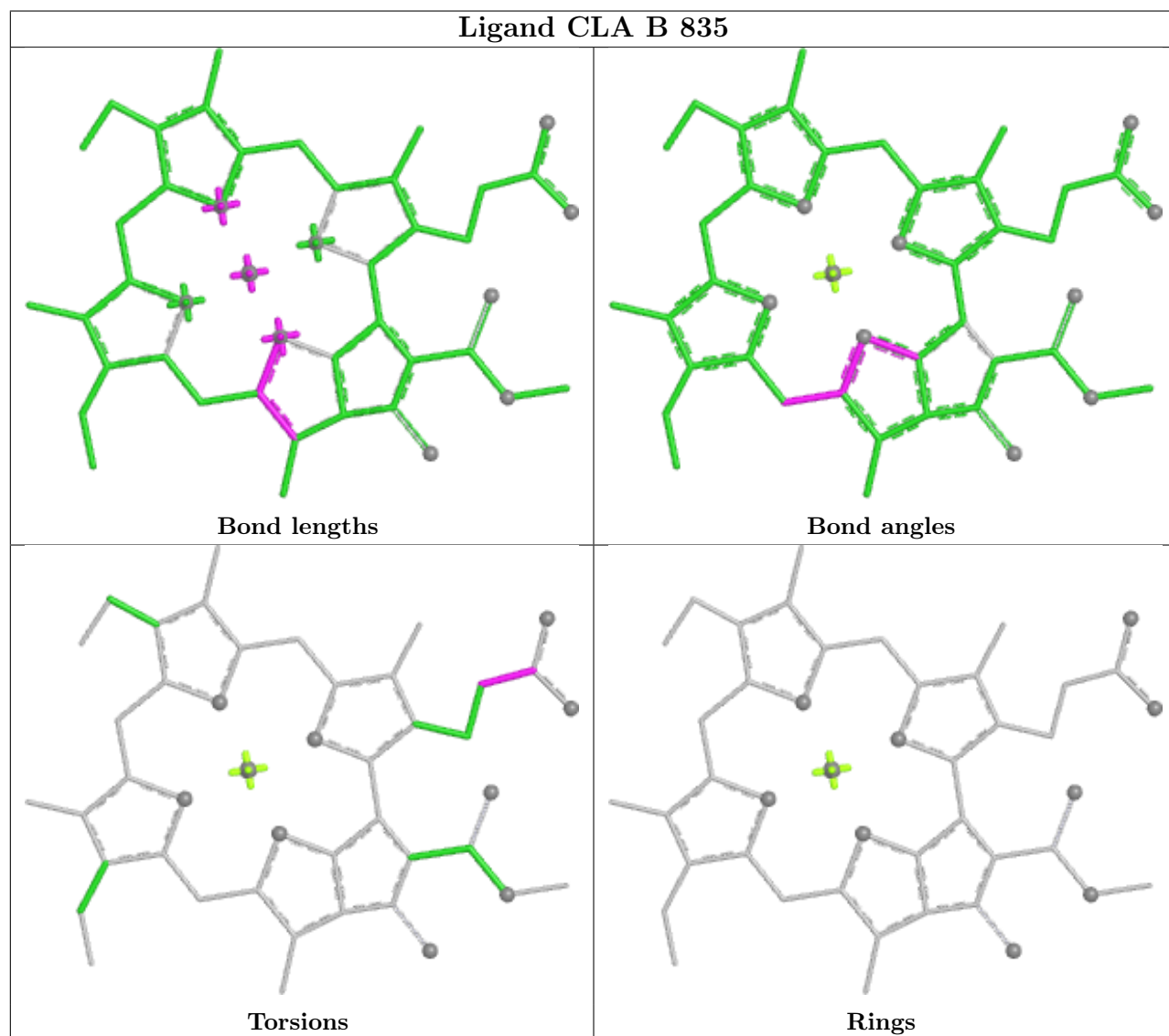
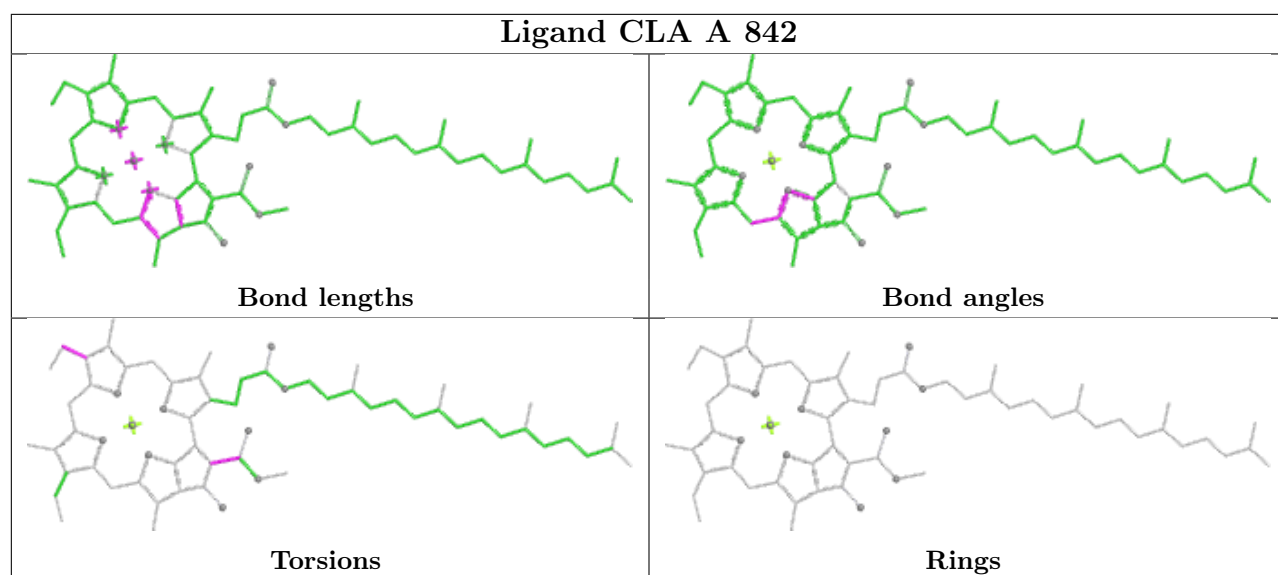


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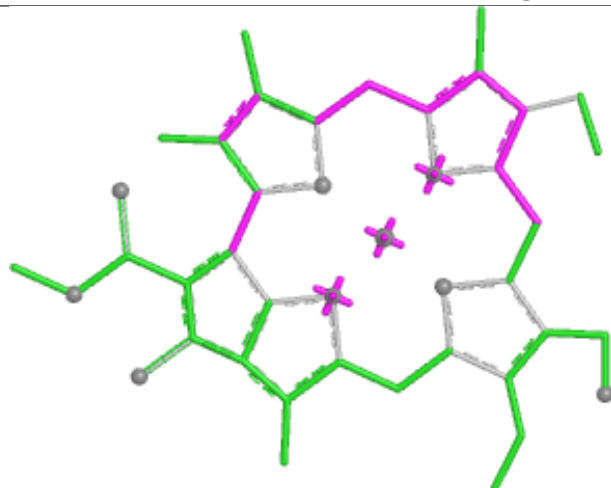




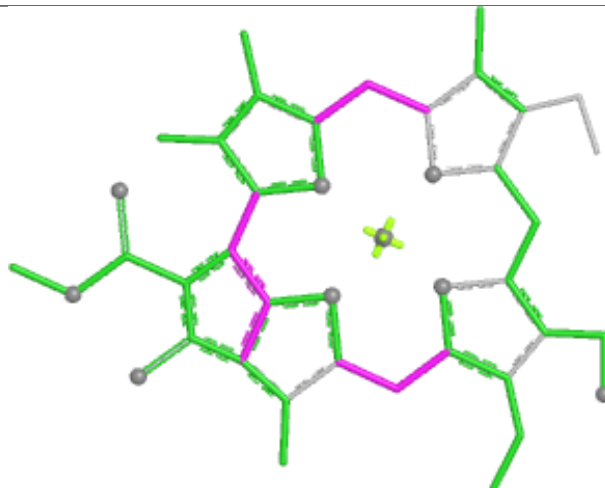




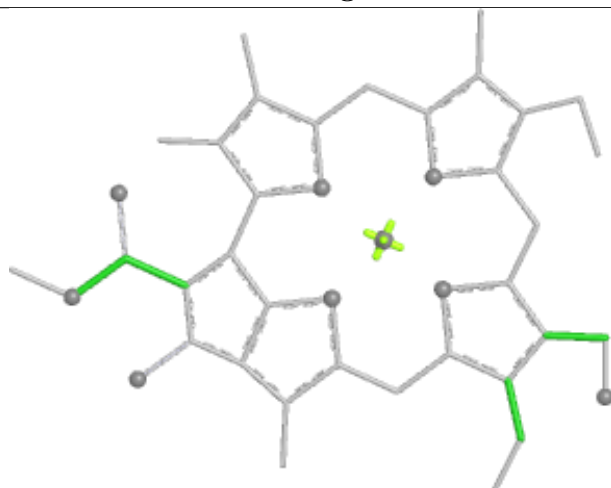
Ligand CHL 9 606



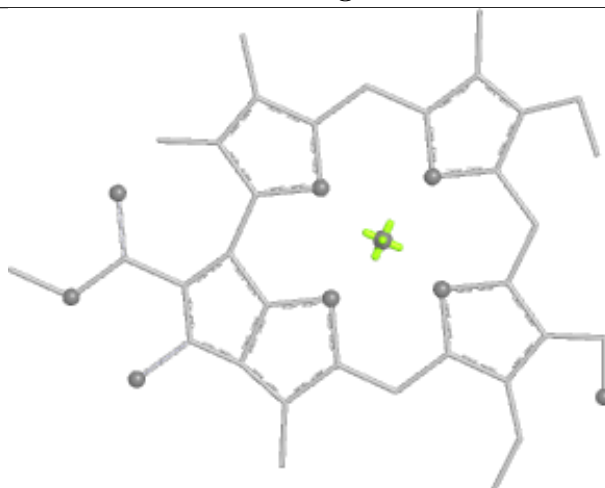
Bond lengths



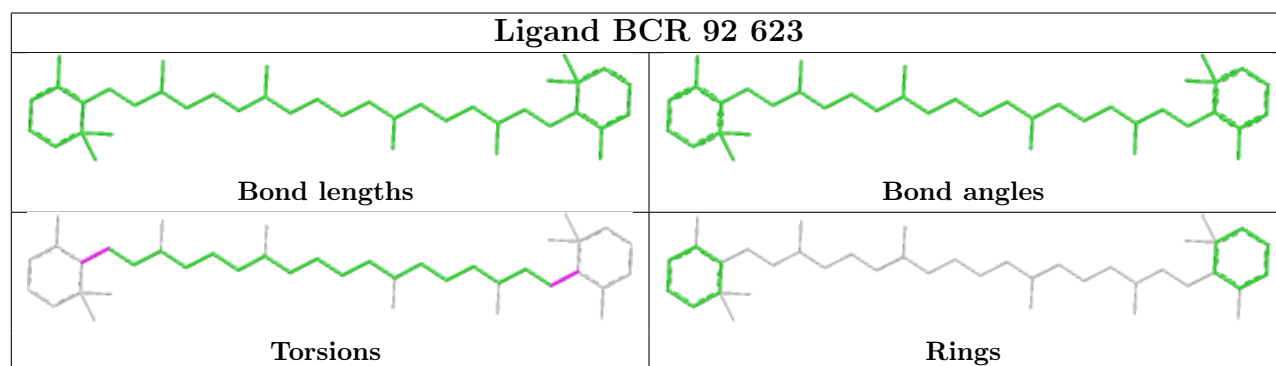
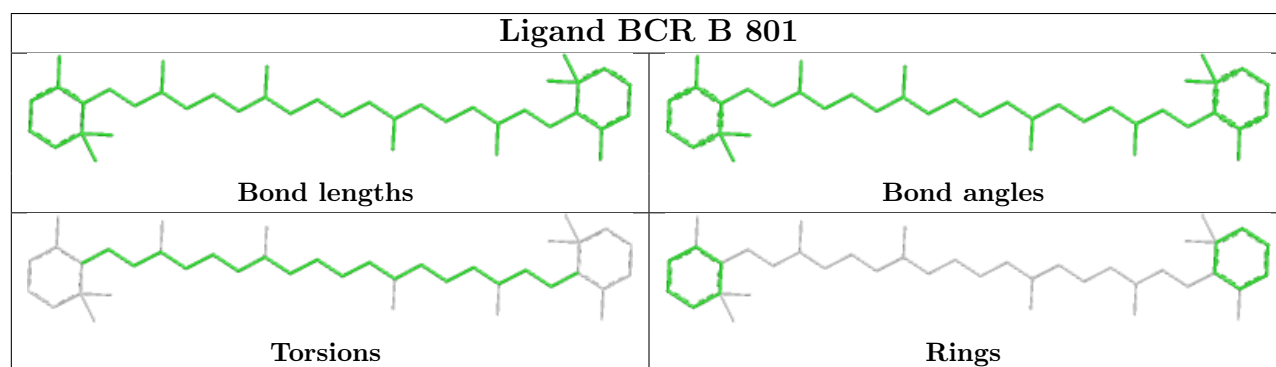
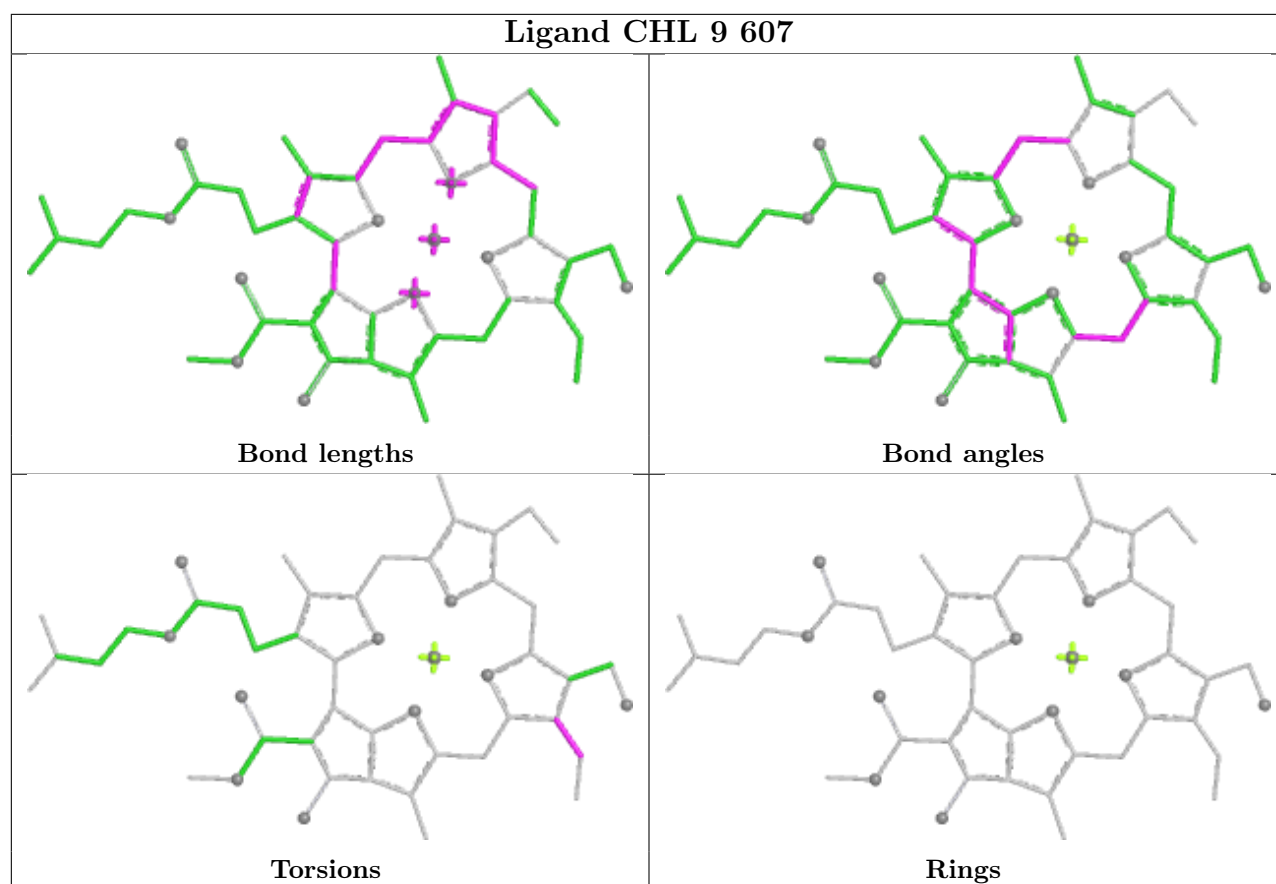
Bond angles

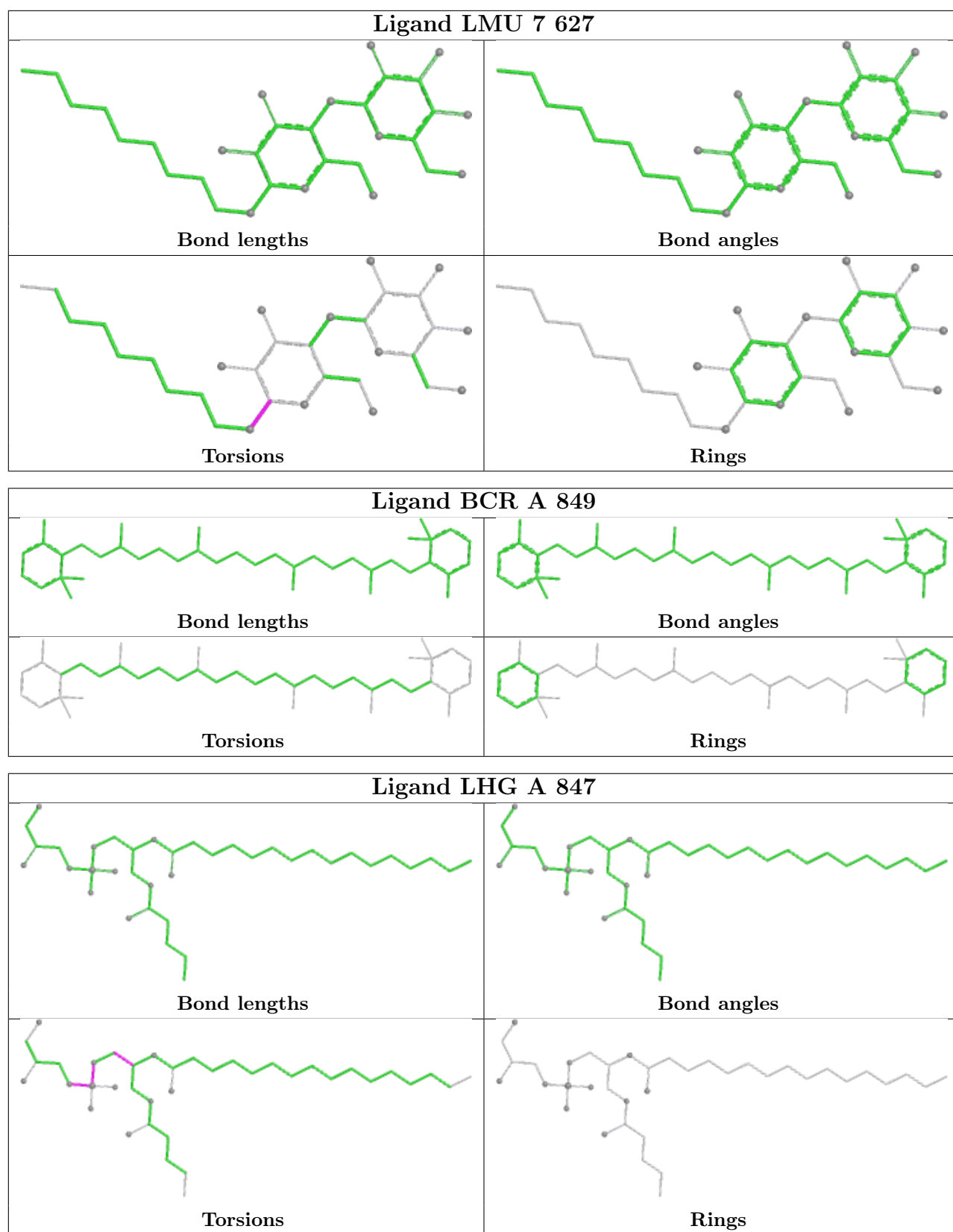


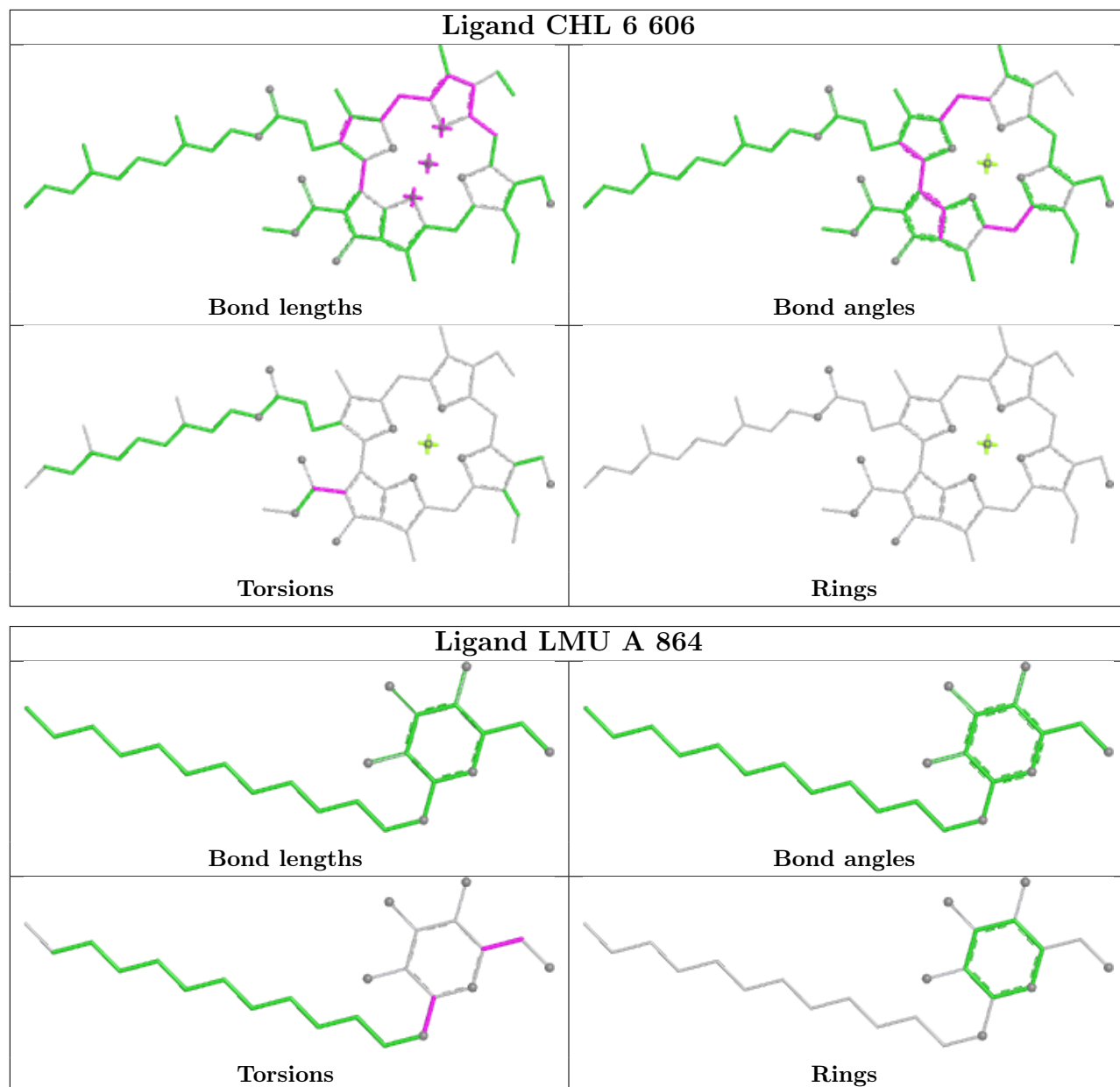
Torsions

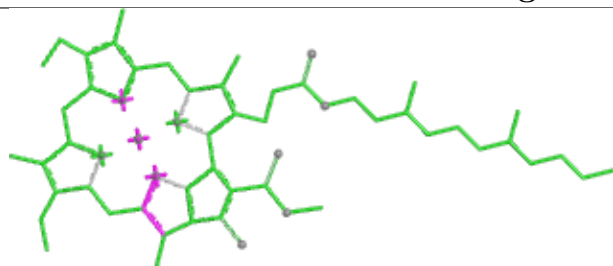


Rings

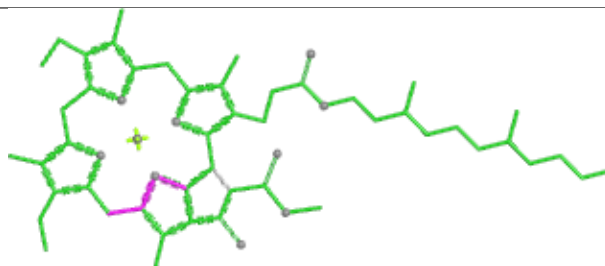




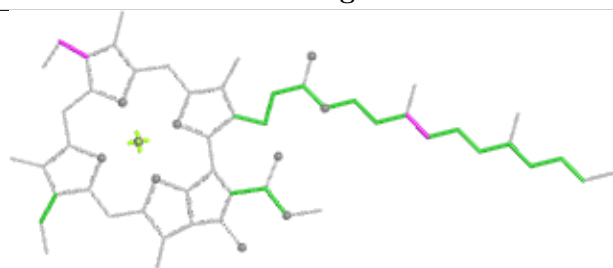


Ligand CLA 6 611

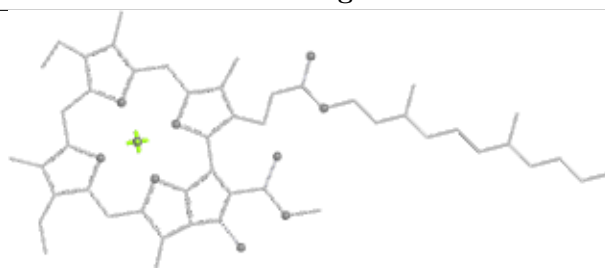
Bond lengths



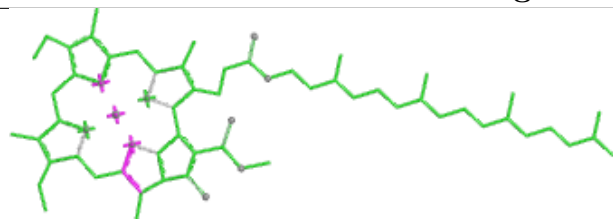
Bond angles



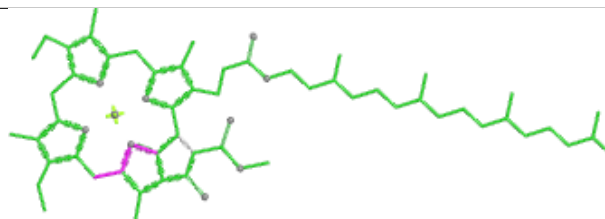
Torsions



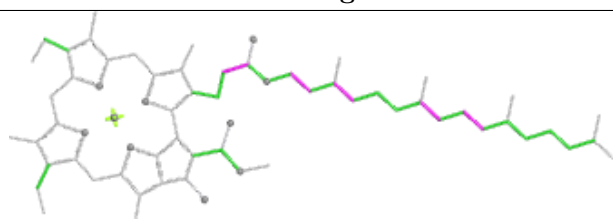
Rings

Ligand CLA A 826

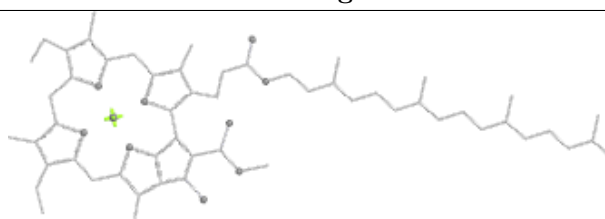
Bond lengths



Bond angles

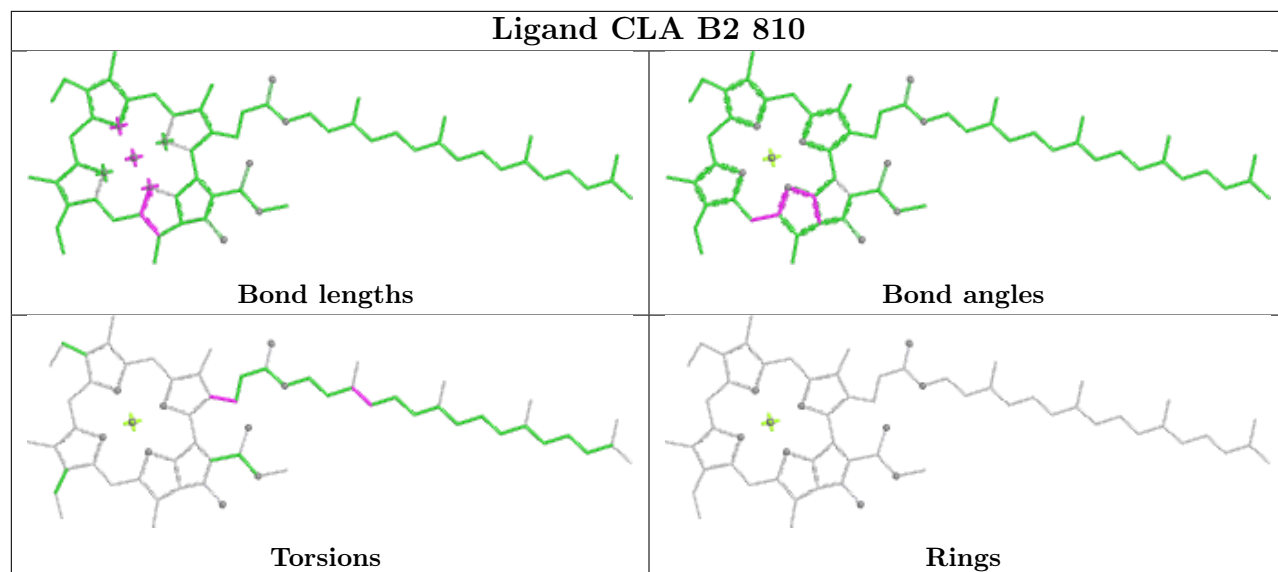


Torsions

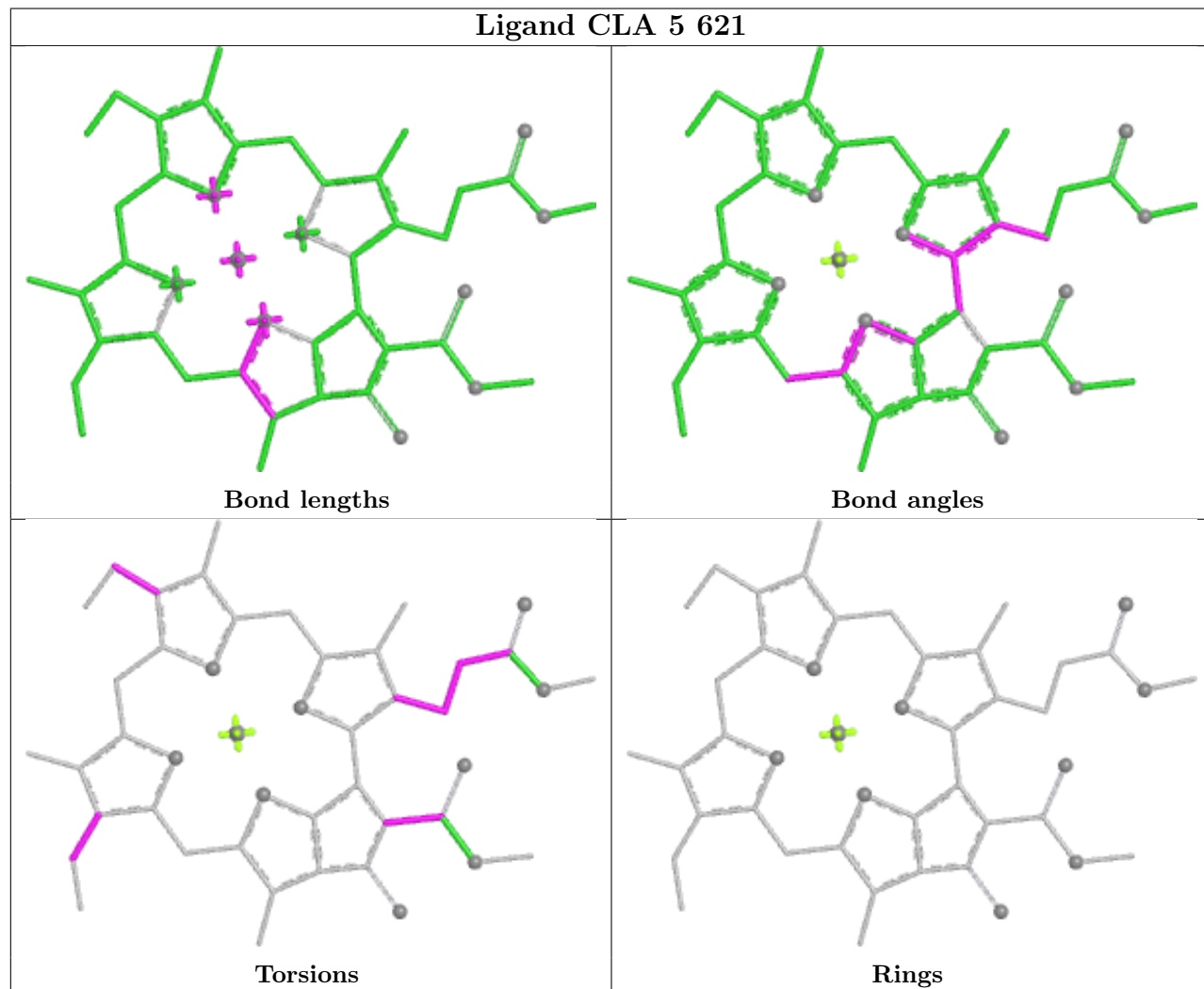


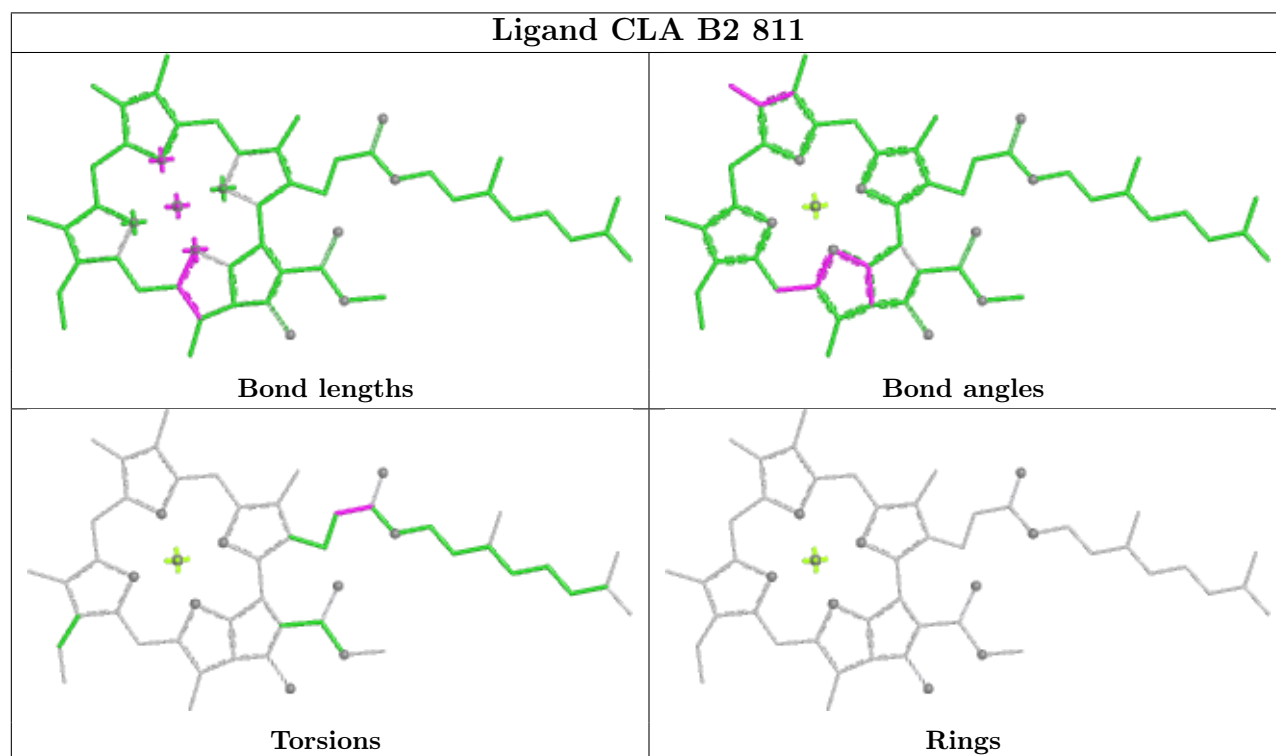
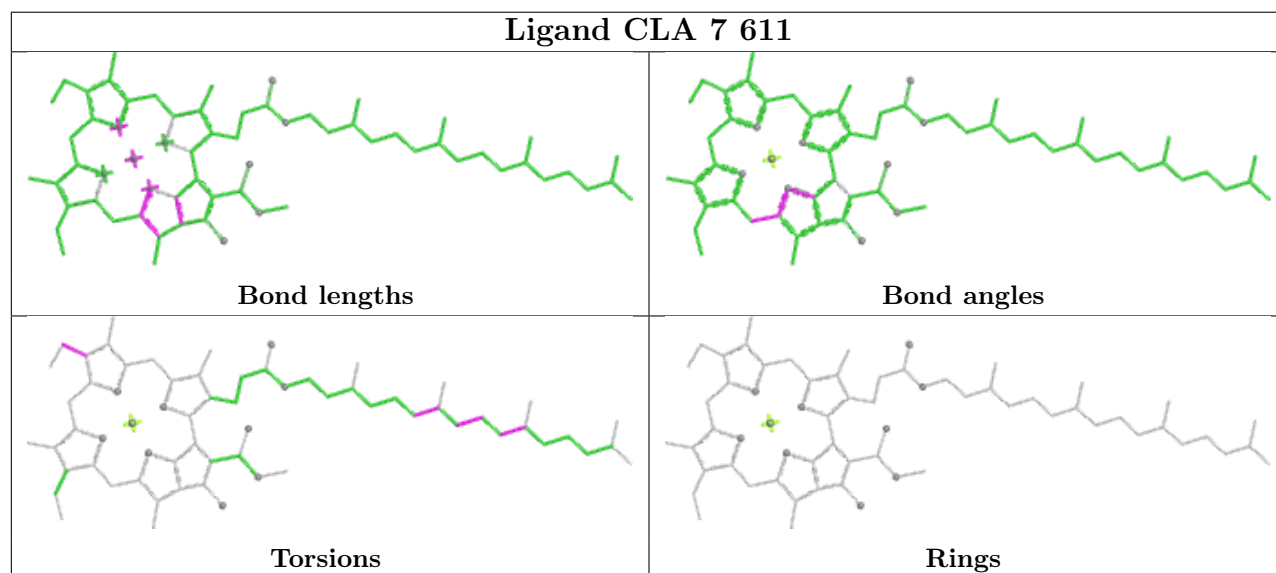
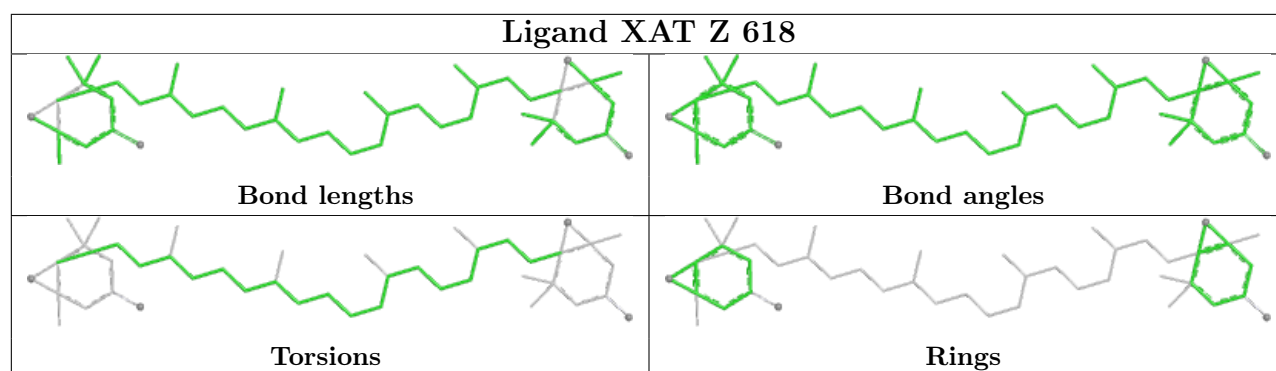
Rings

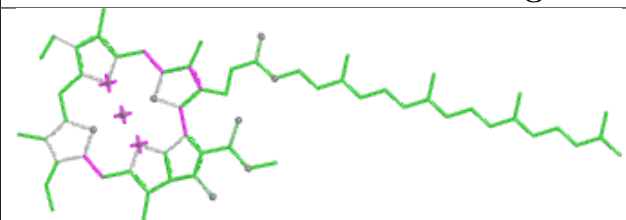
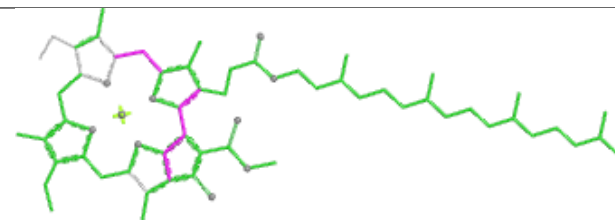
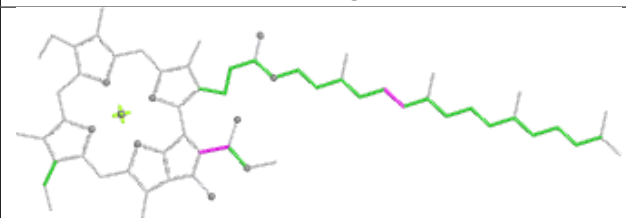
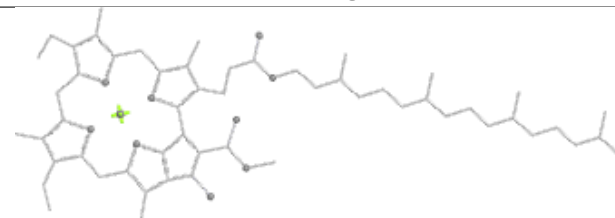
Ligand CLA B2 810

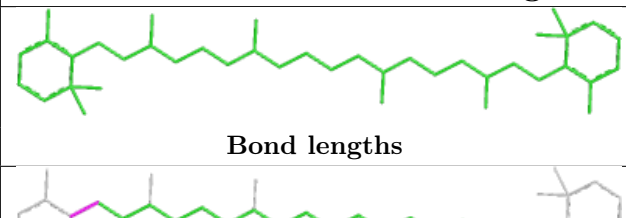
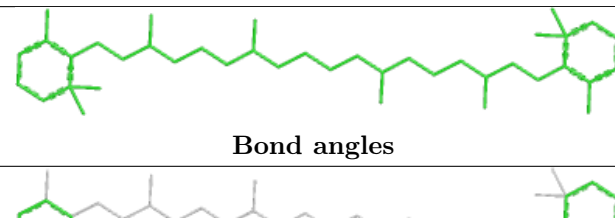
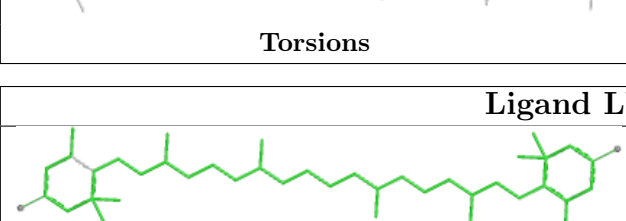
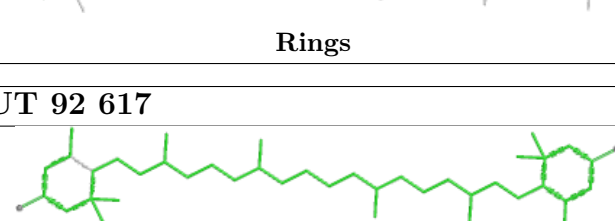


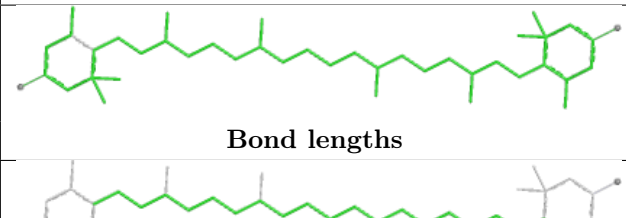
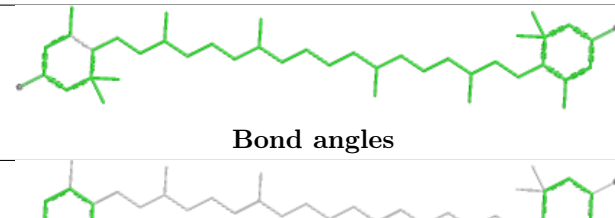
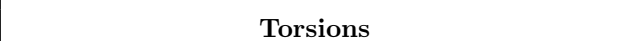
Ligand CLA 5 621

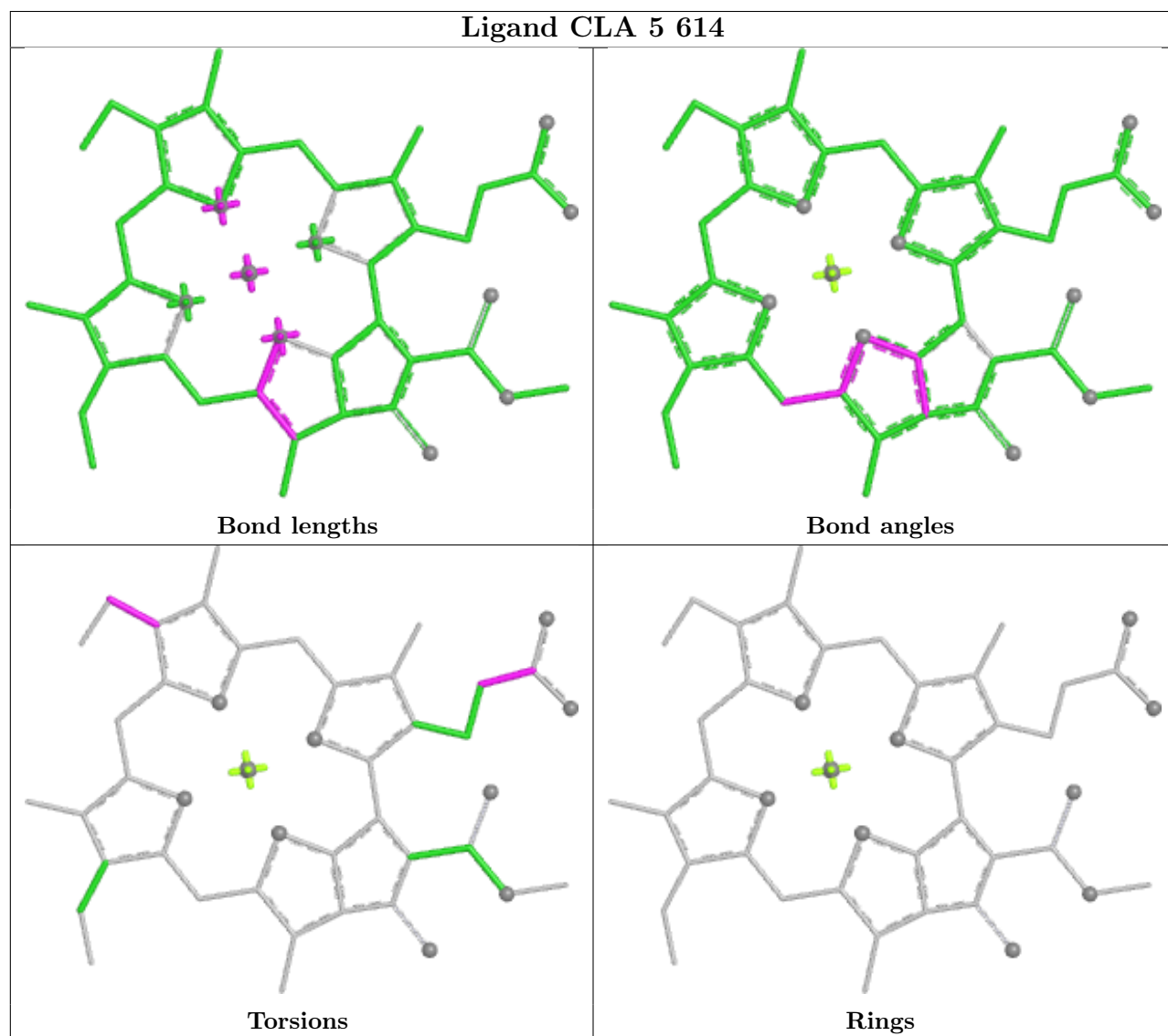
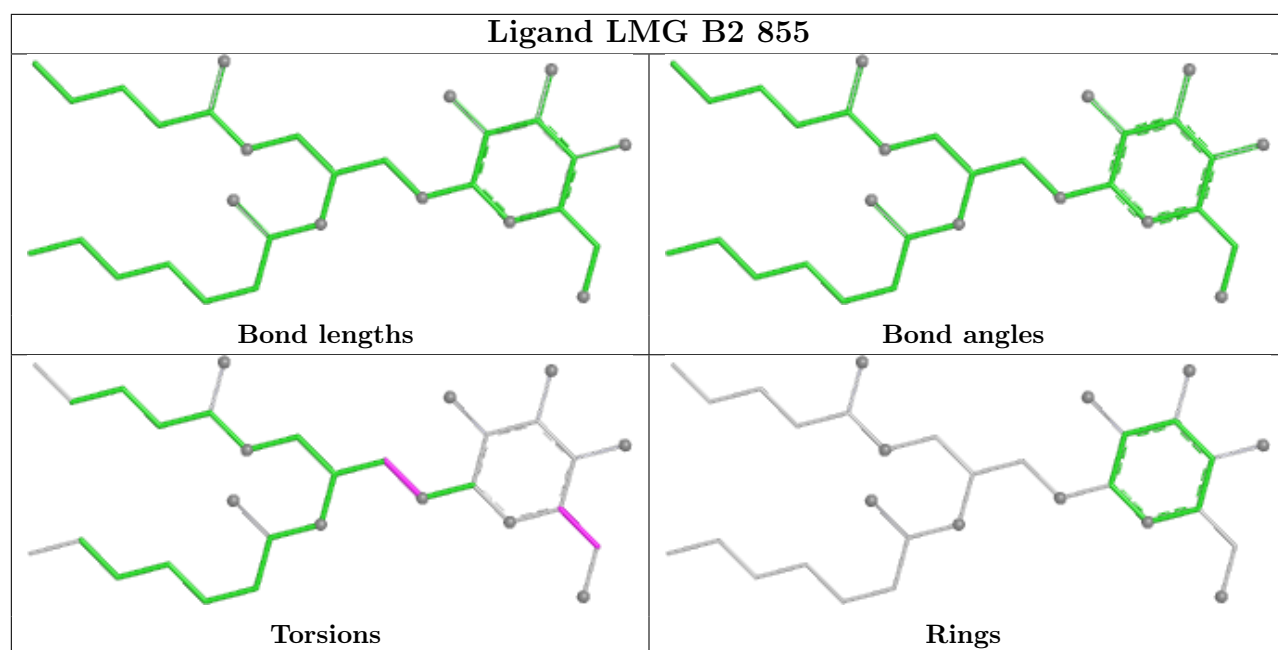


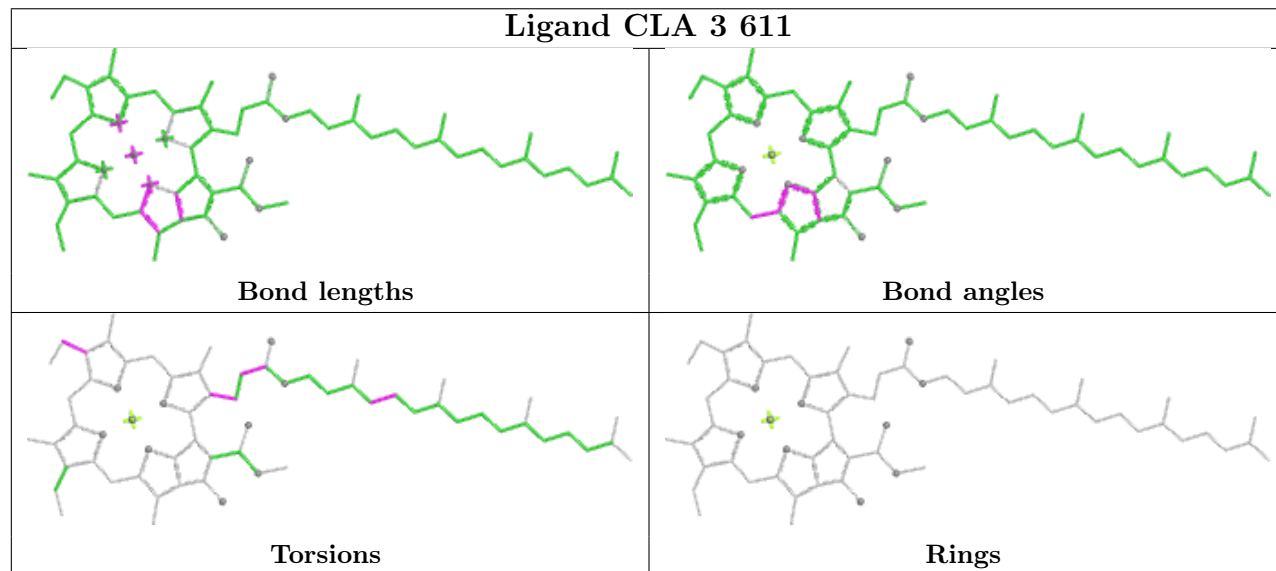
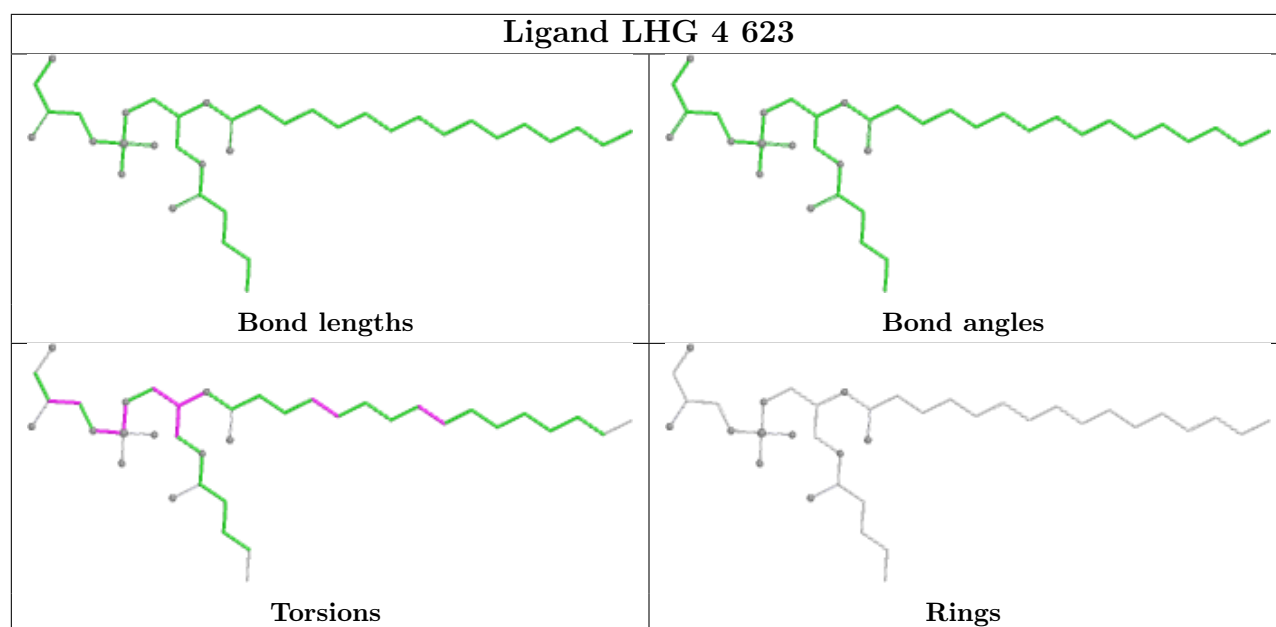


Ligand CL0 A 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

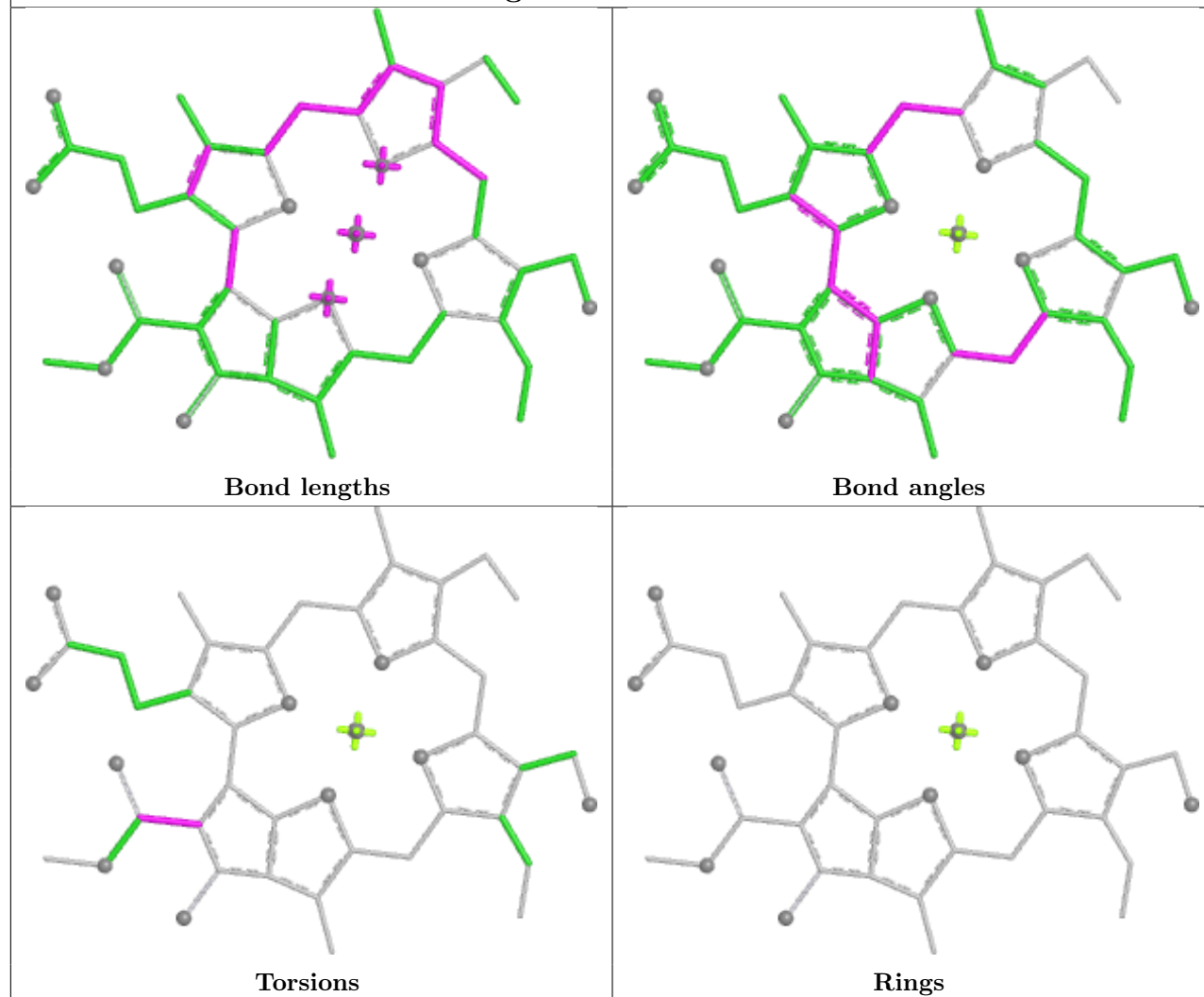
Ligand BCR 3 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT 92 617	
	
Bond lengths	Bond angles
	
Torsions	Rings

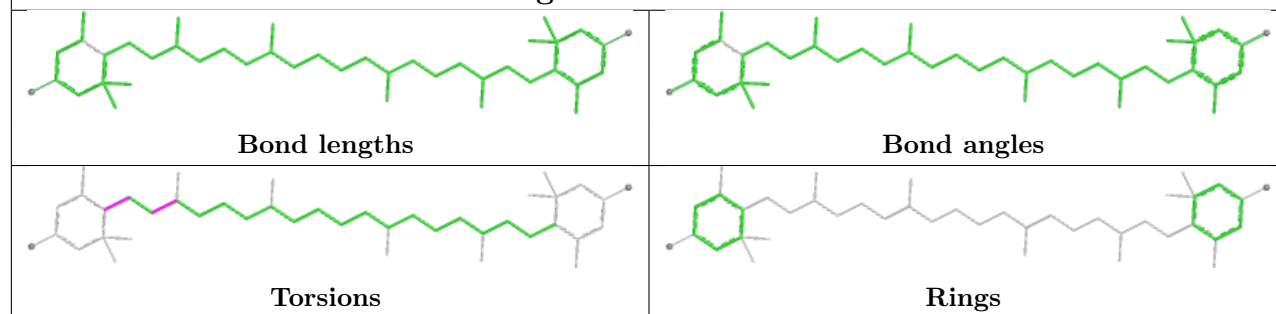


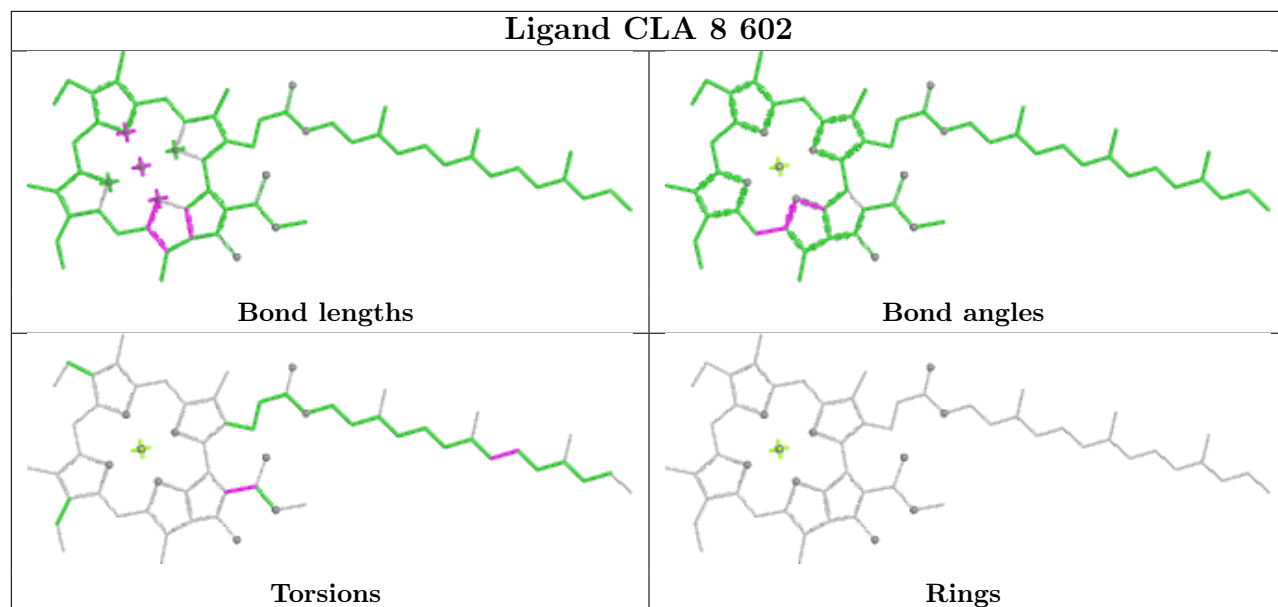
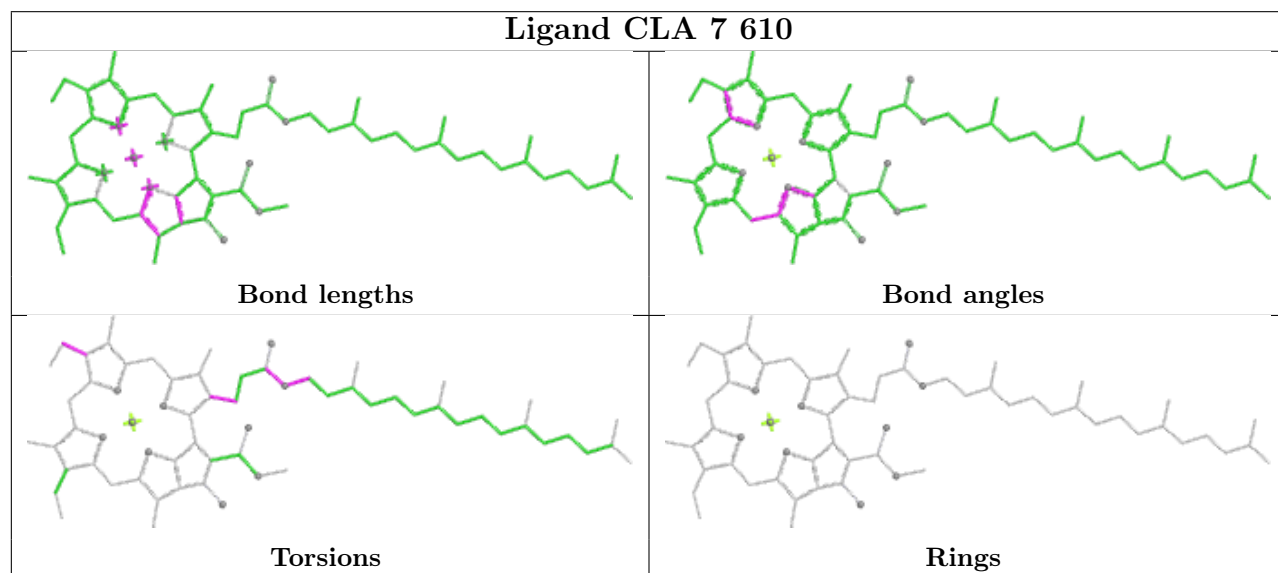


Ligand CHL 5 606

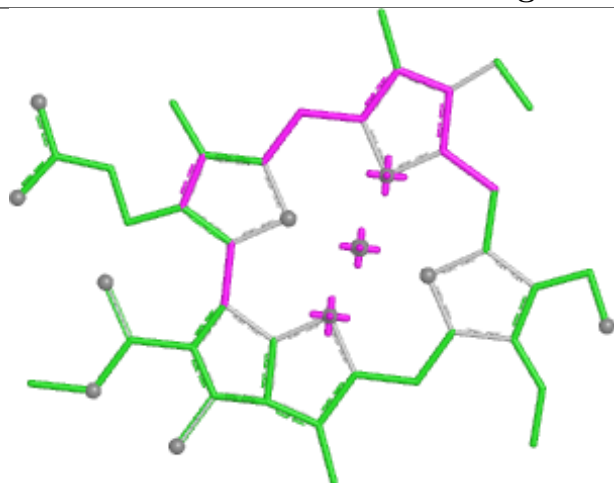


Ligand LUT 7 624

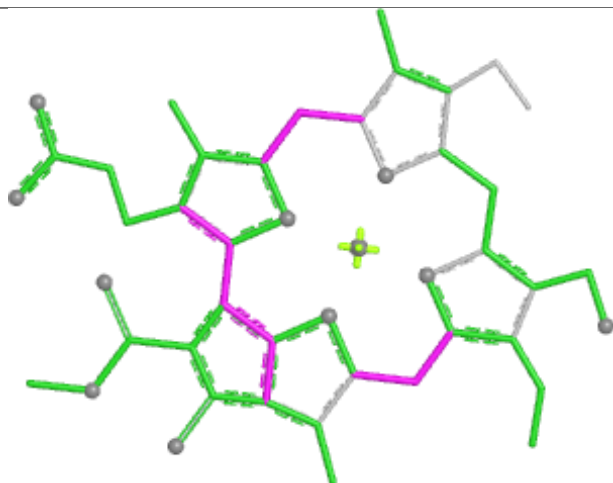


Ligand CLA 8 602**Ligand CLA 7 610**

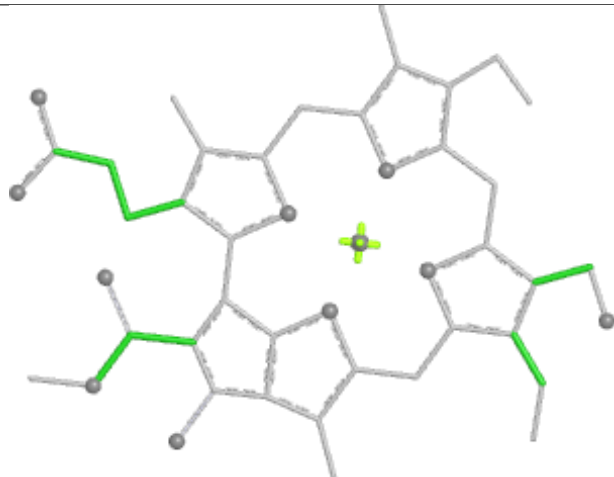
Ligand CHL 1 606



Bond lengths



Bond angles

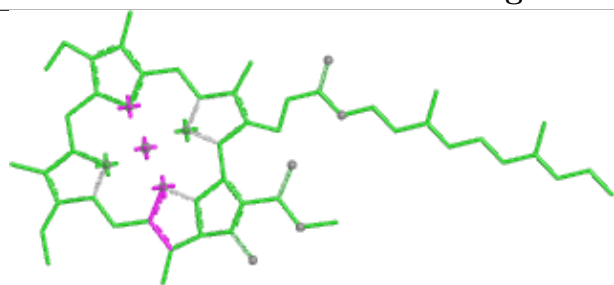


Torsions

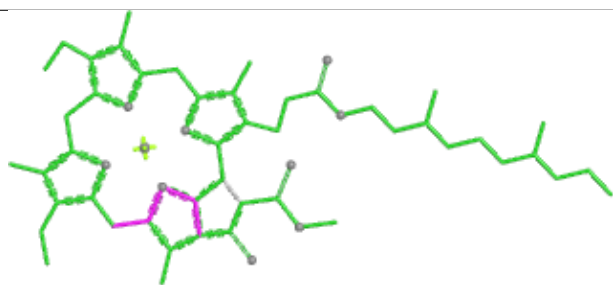


Rings

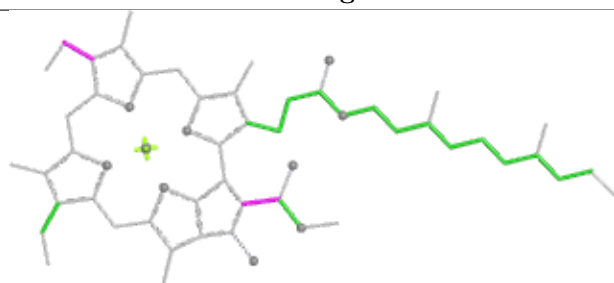
Ligand CLA B2 815



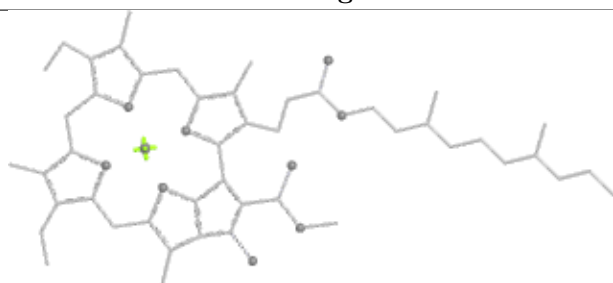
Bond lengths



Bond angles

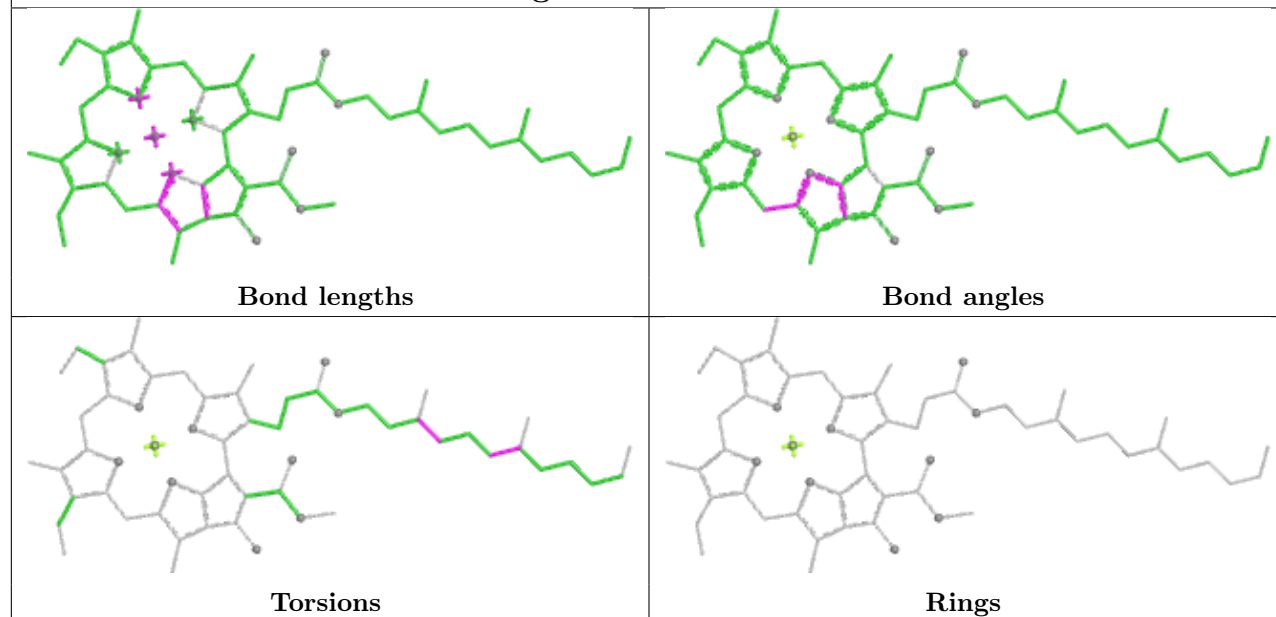


Torsions

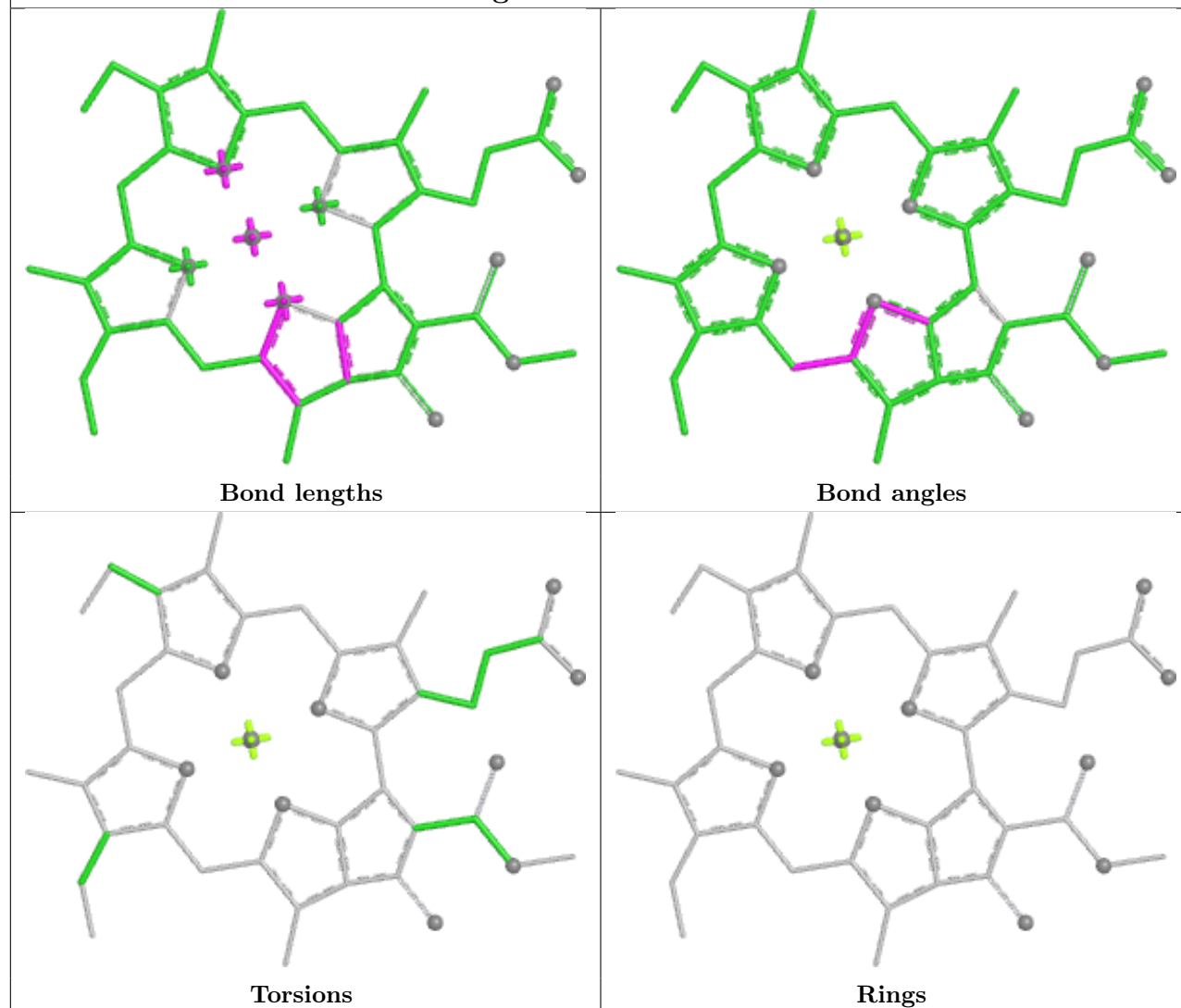


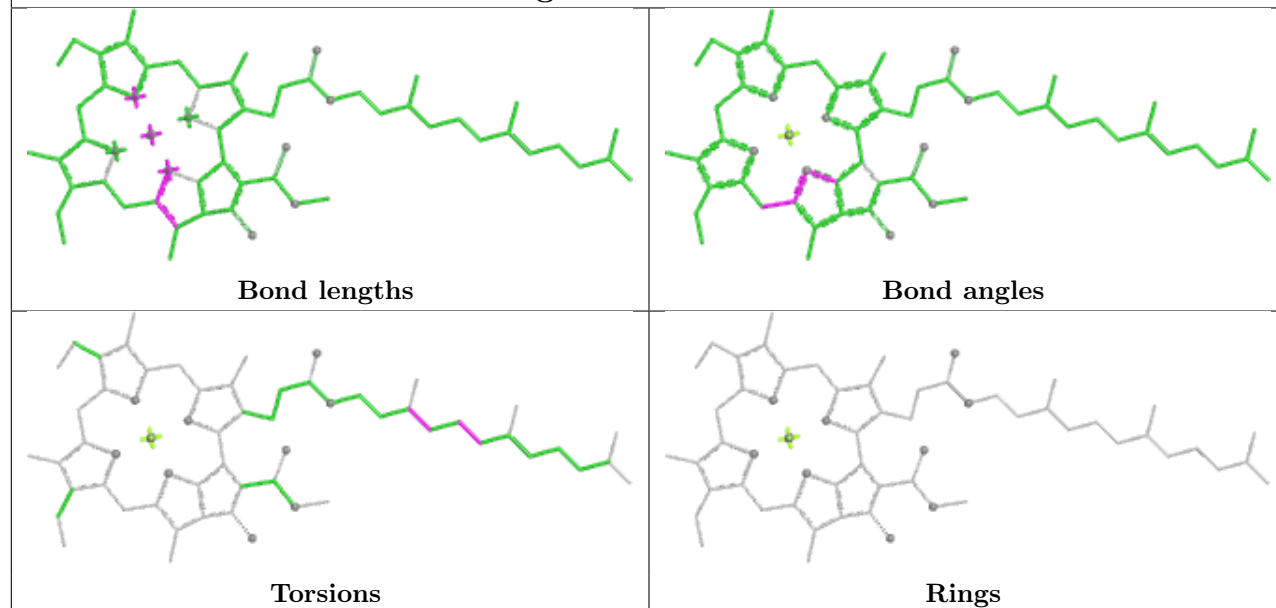
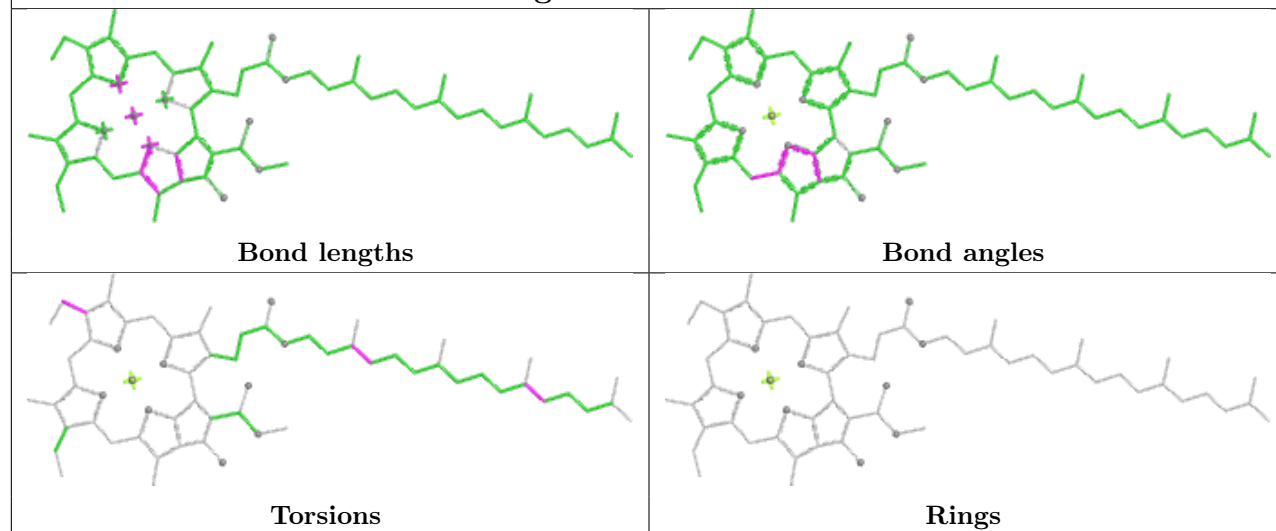
Rings

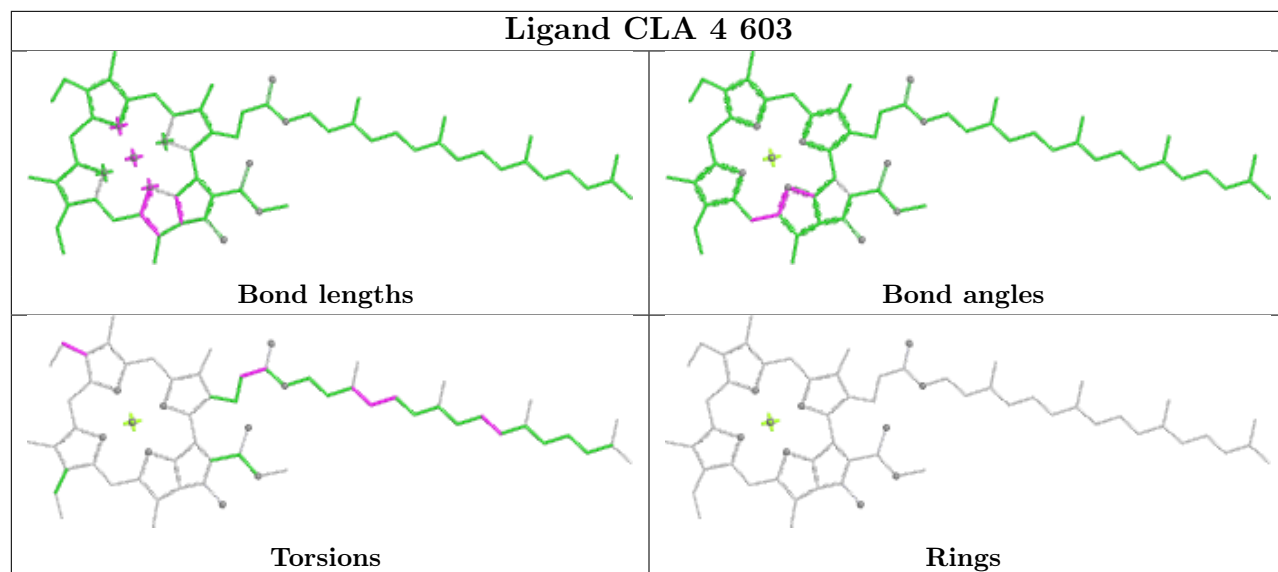
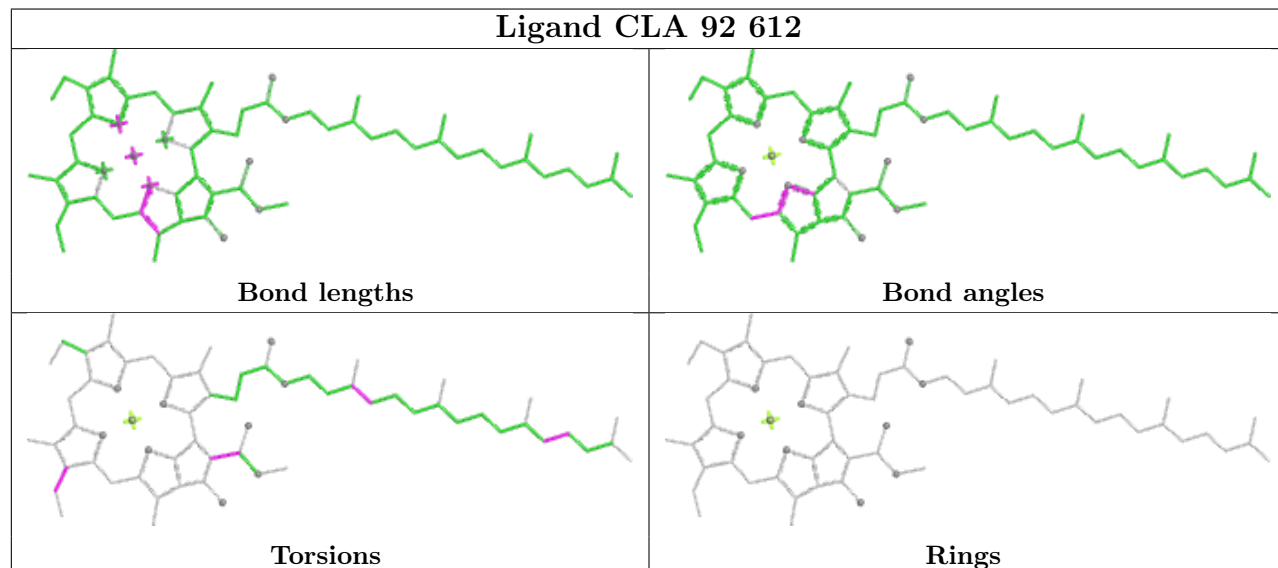
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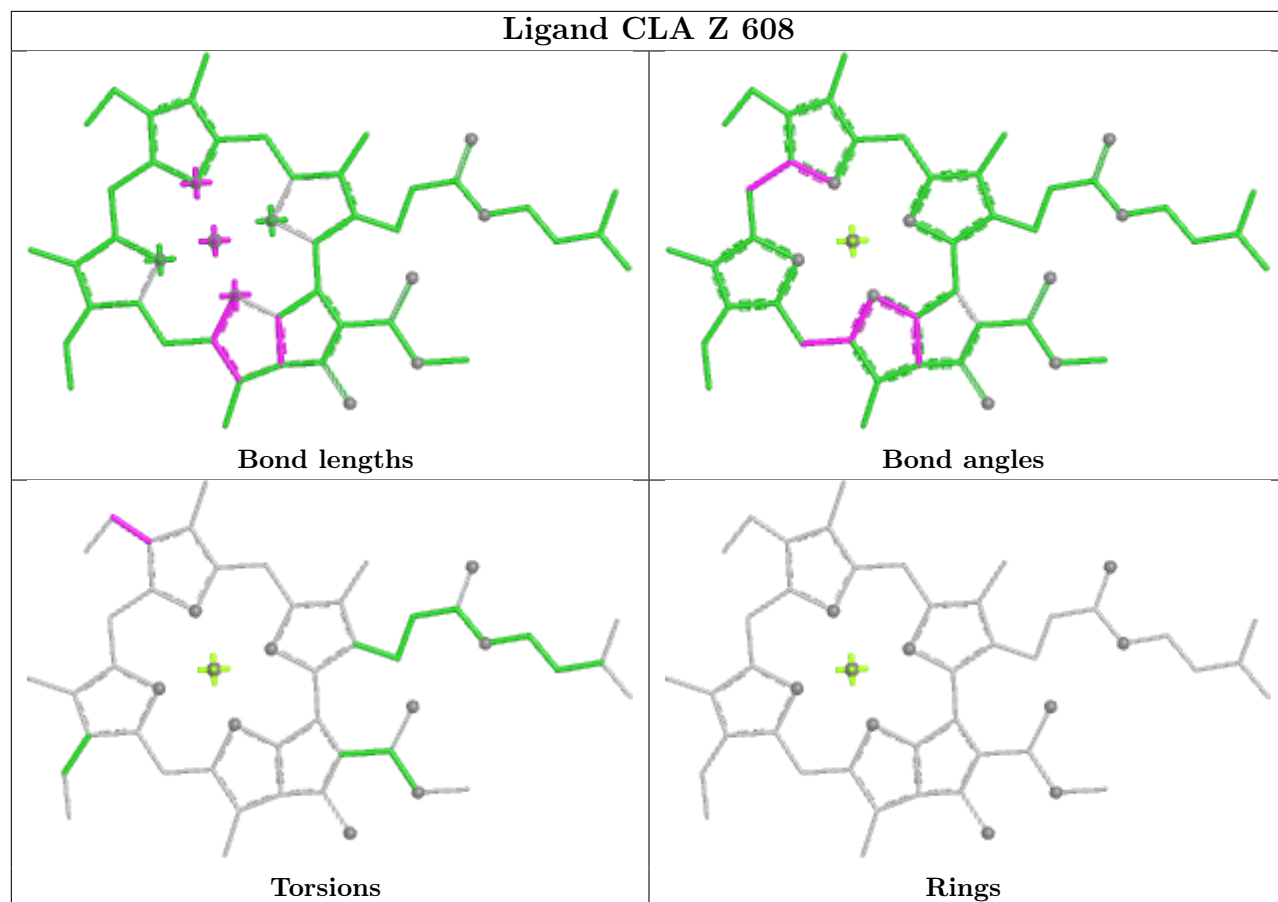
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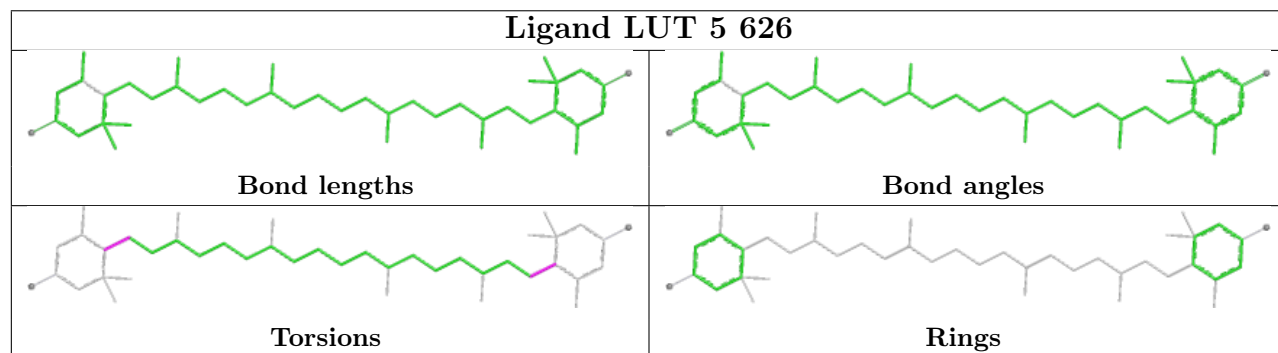
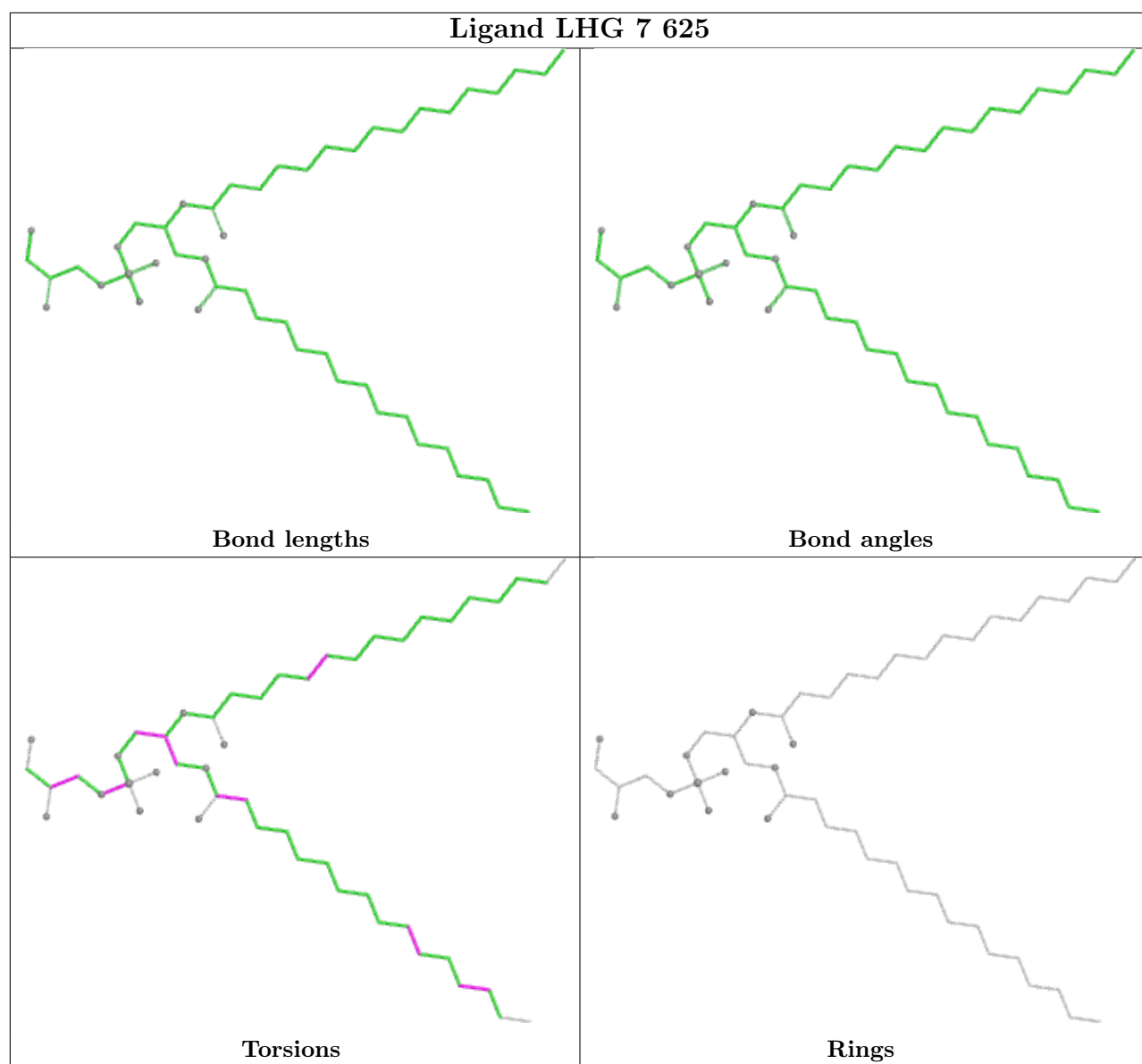


Ligand CLA 4 610**Ligand CLA L 203**

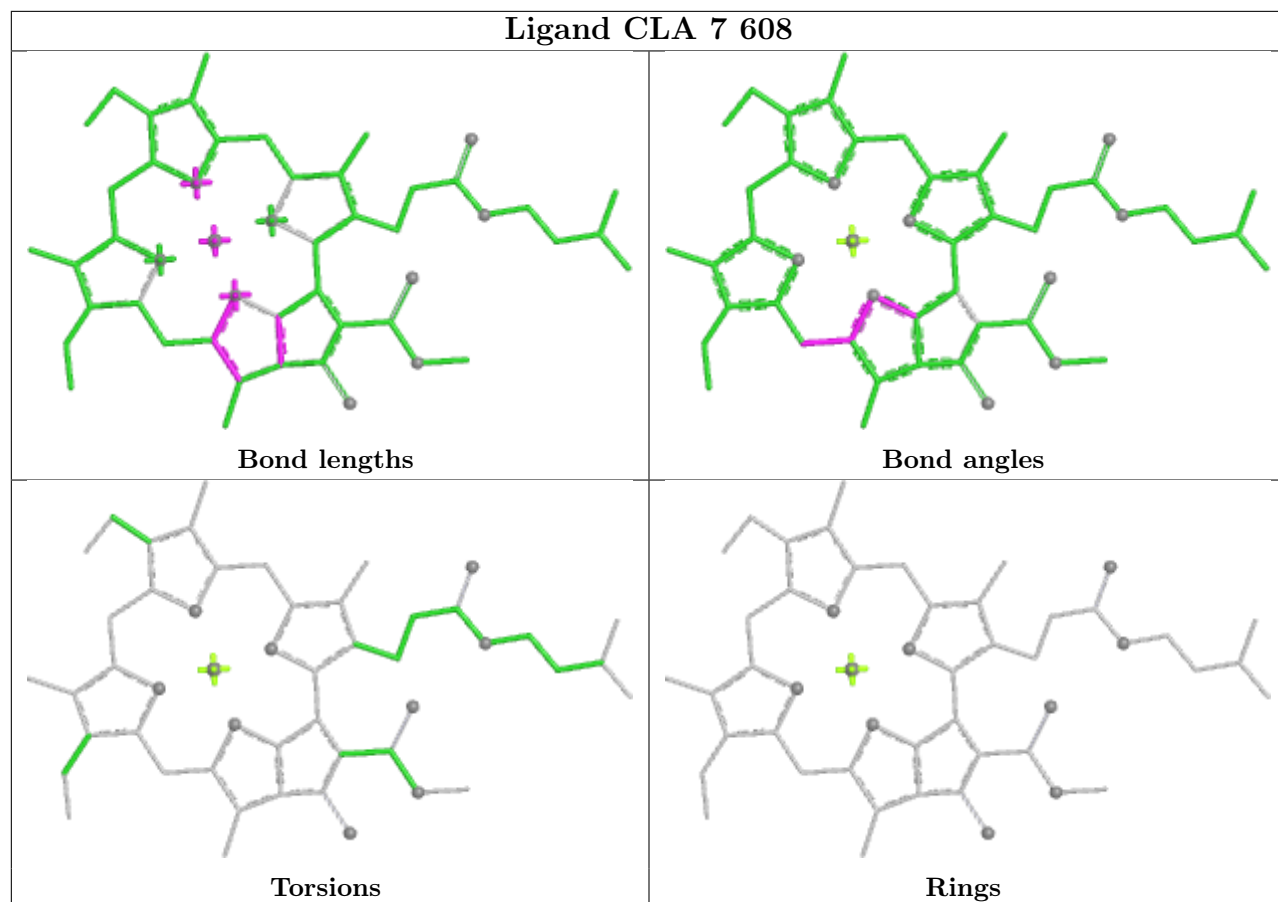
Ligand CLA 4 603**Ligand CLA 92 612**

Ligand CLA Z 608

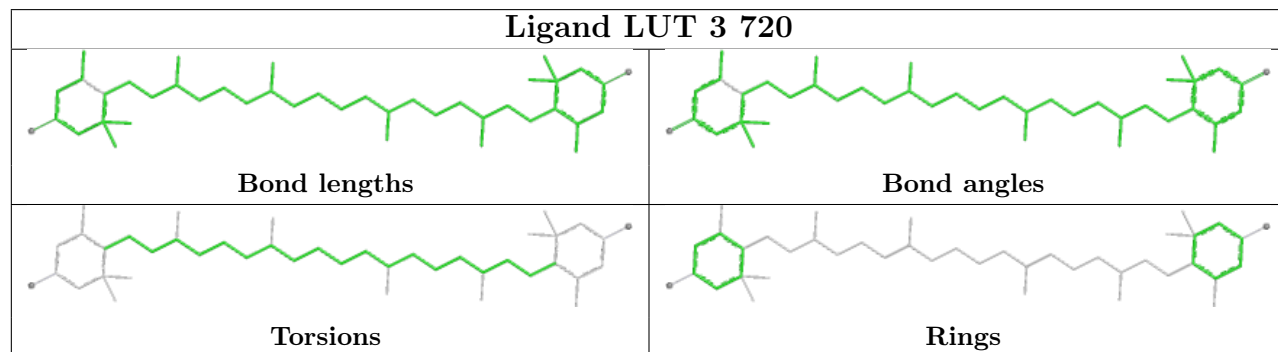




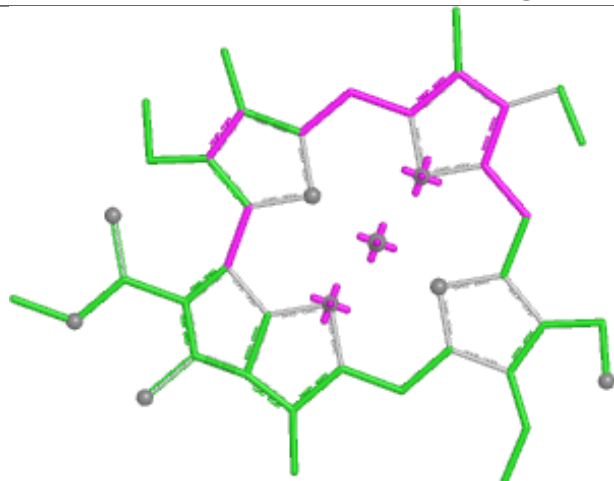
Ligand CLA 7 608



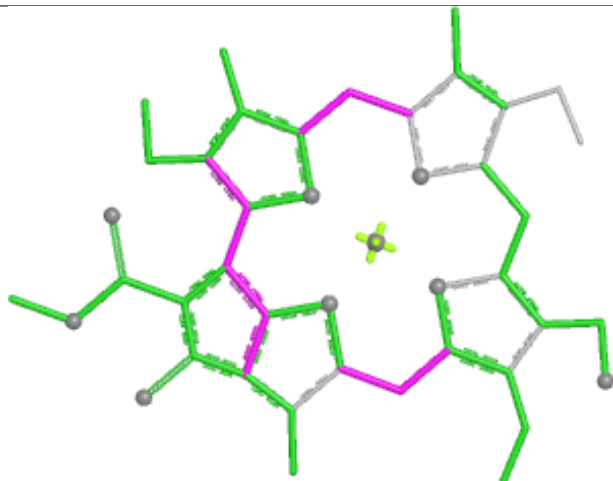
Ligand LUT 3 720



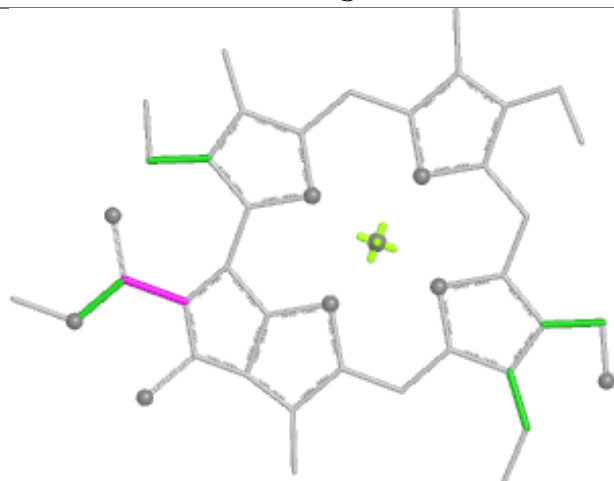
Ligand CHL 6 618



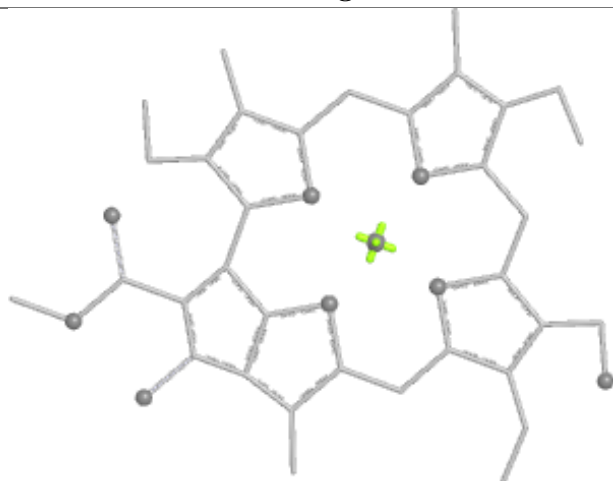
Bond lengths



Bond angles

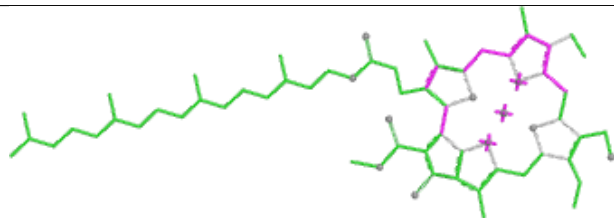


Torsions

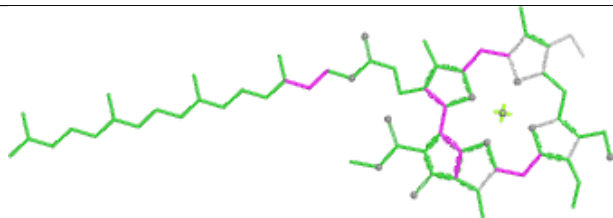


Rings

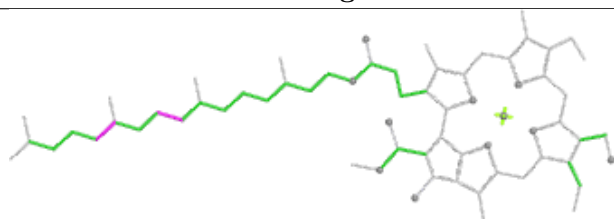
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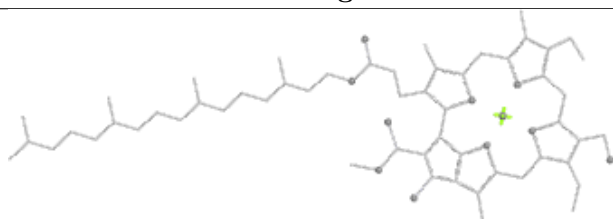
Bond lengths



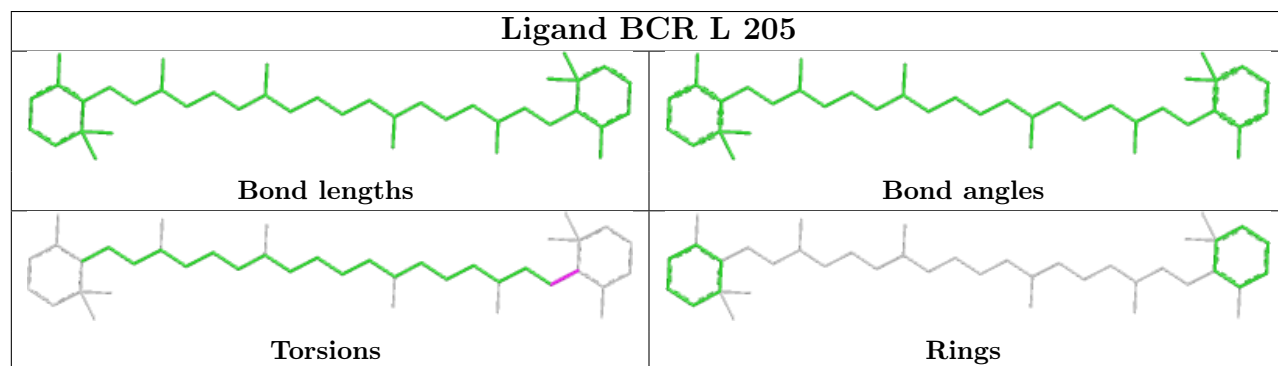
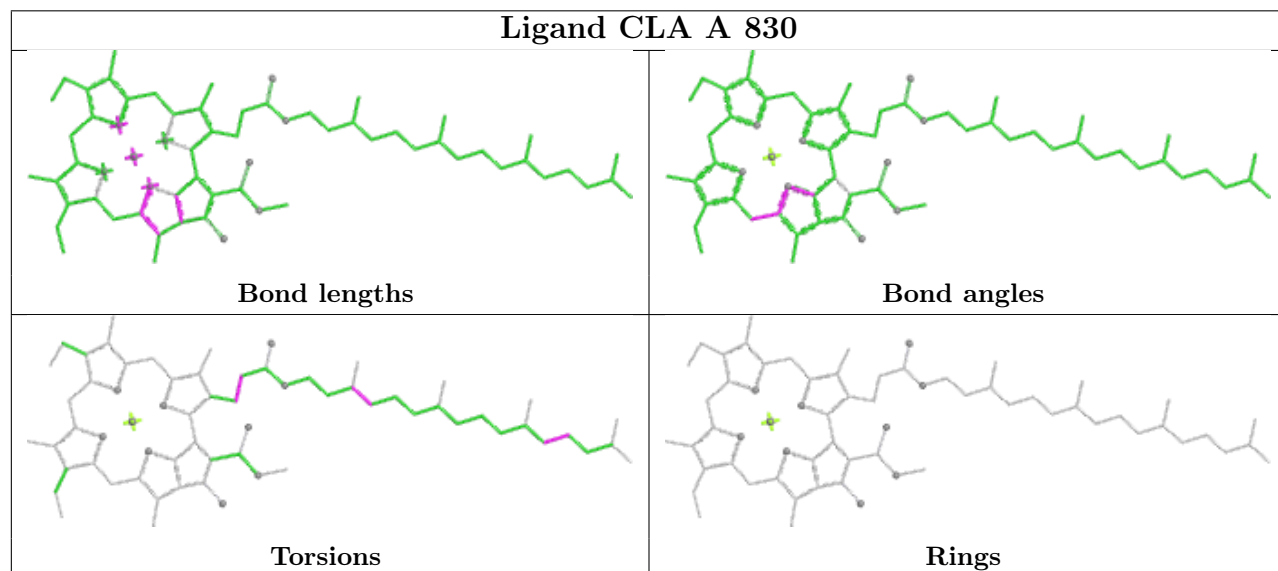
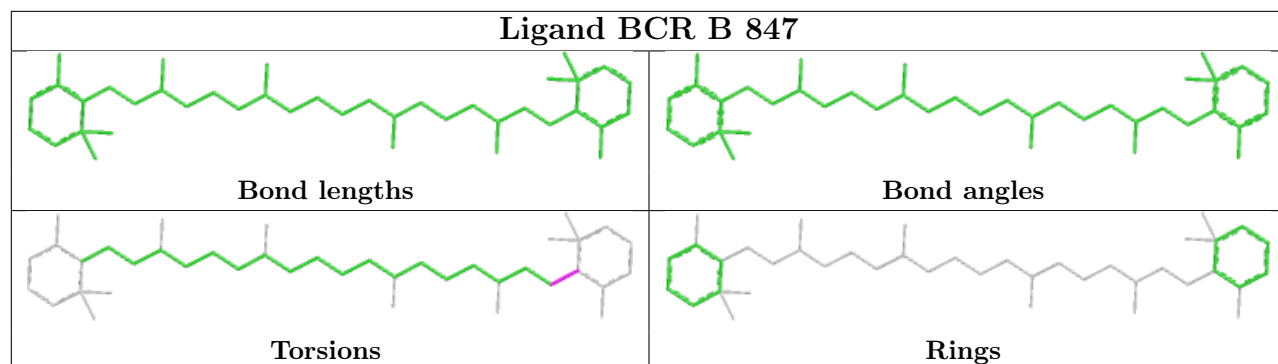
Bond angles

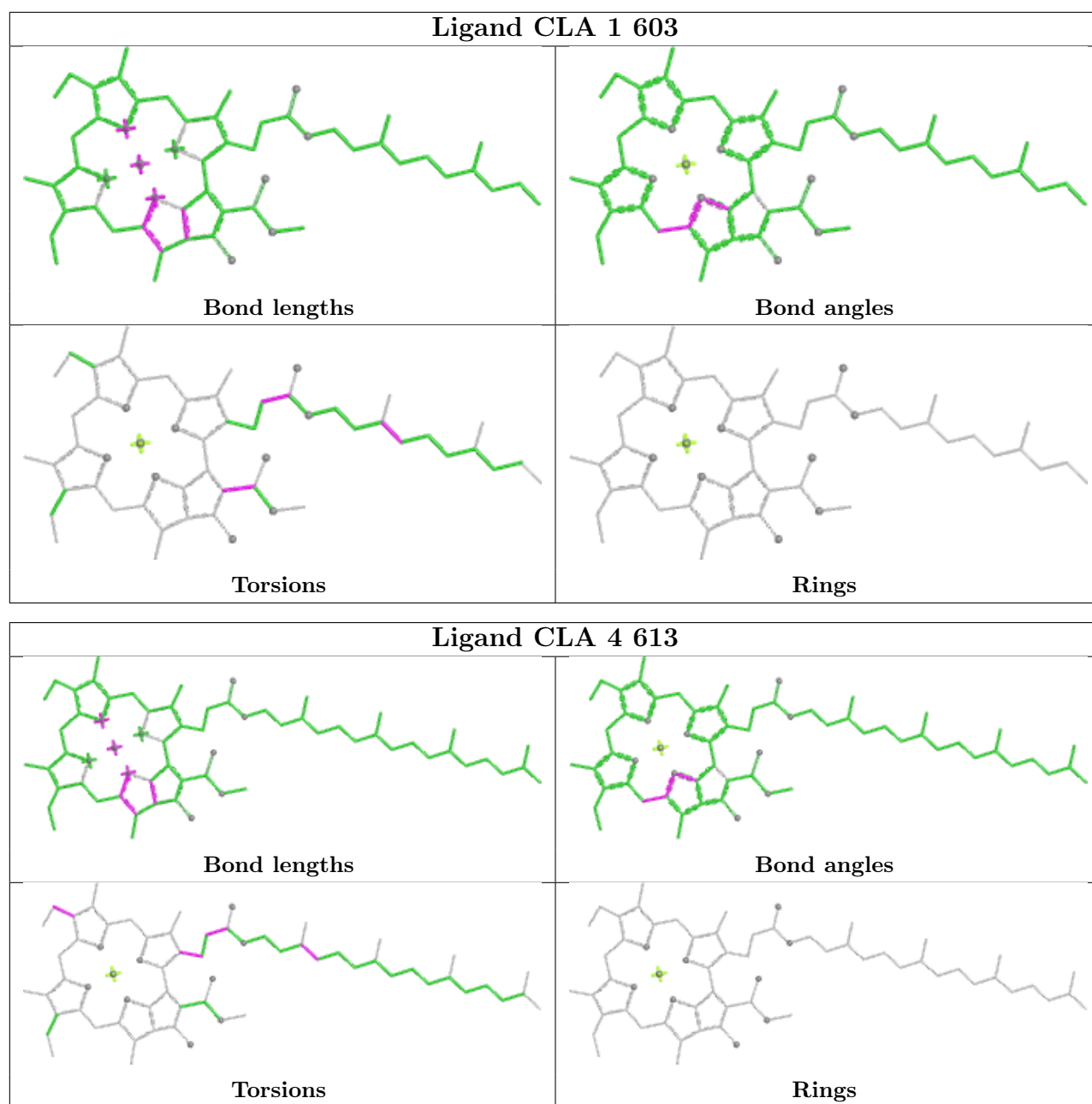


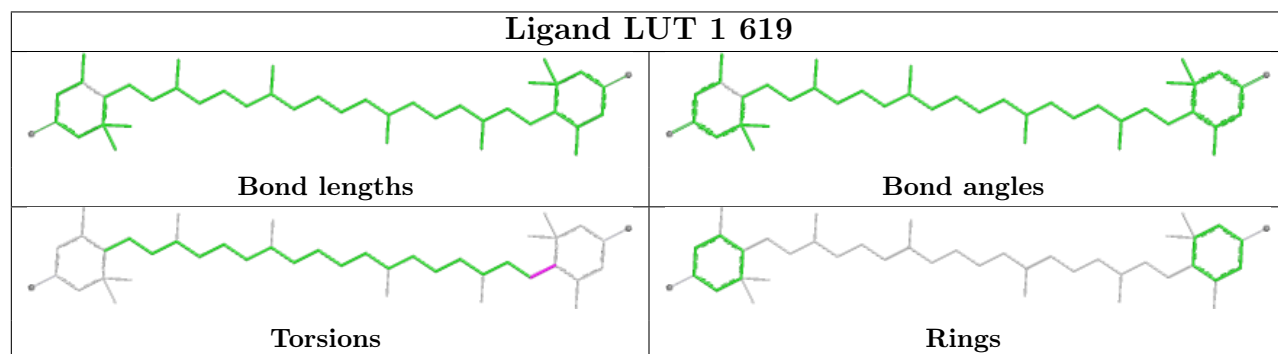
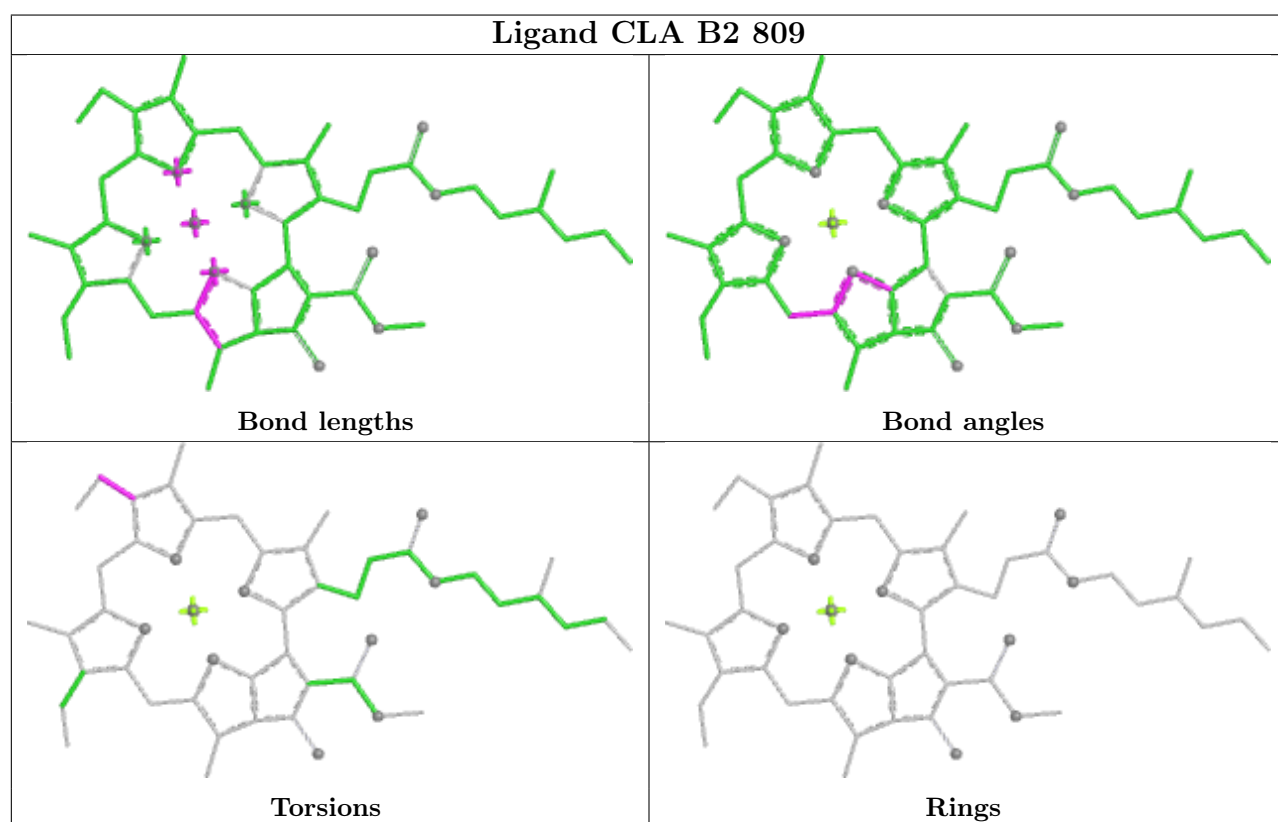
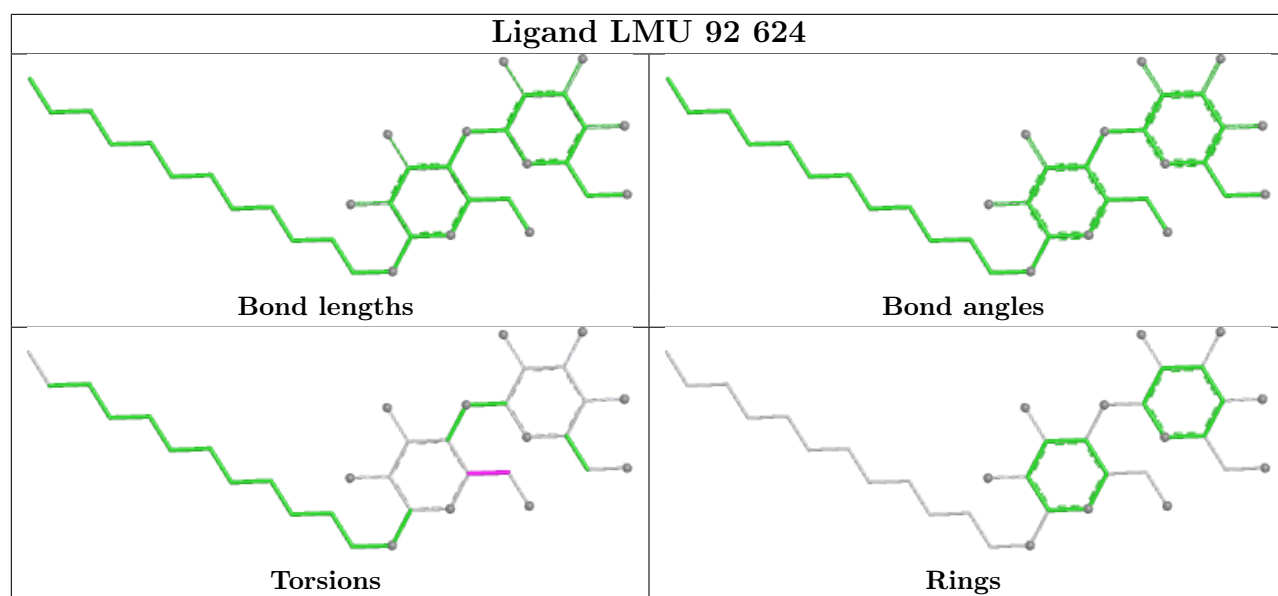
Torsions

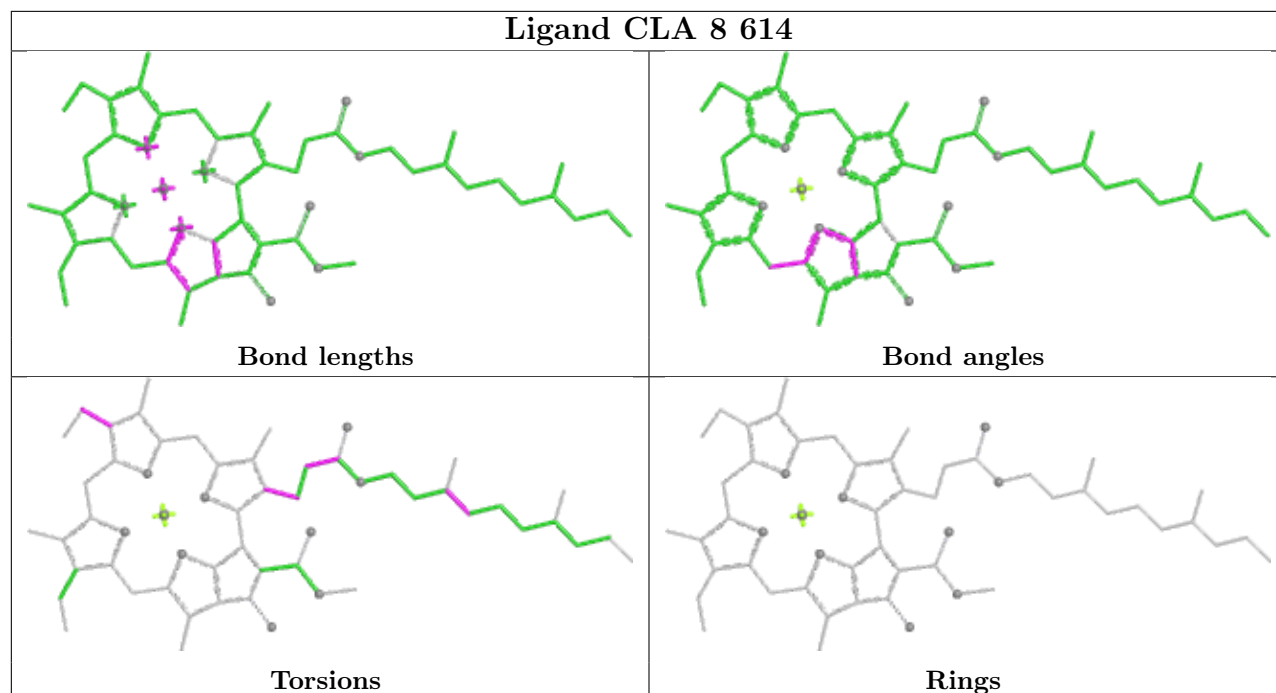
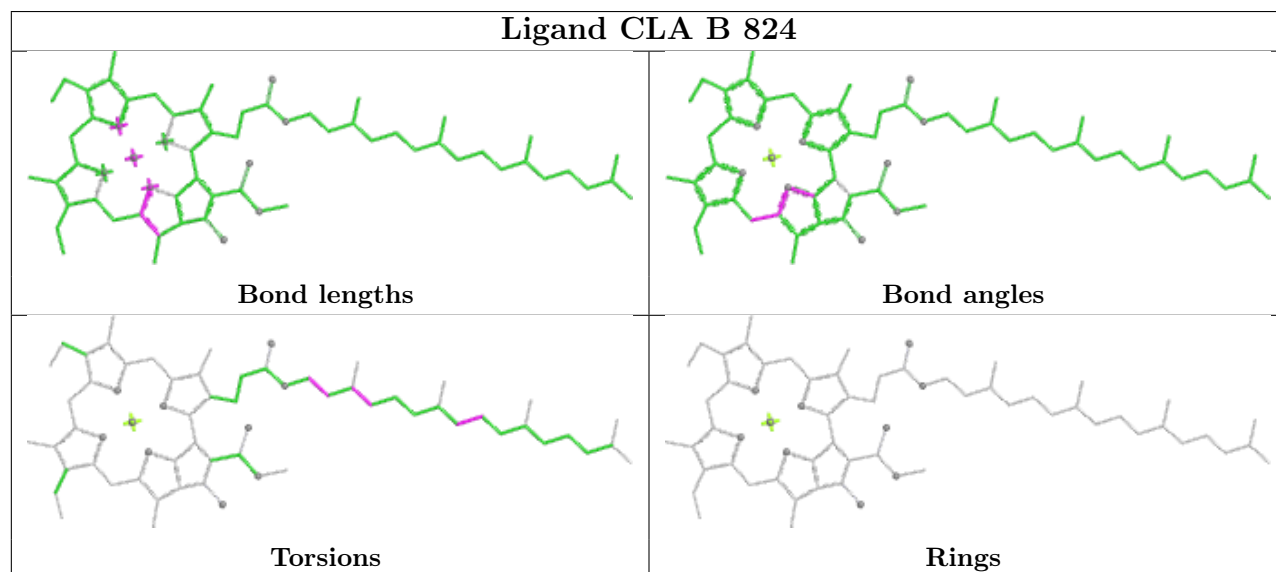


Rings

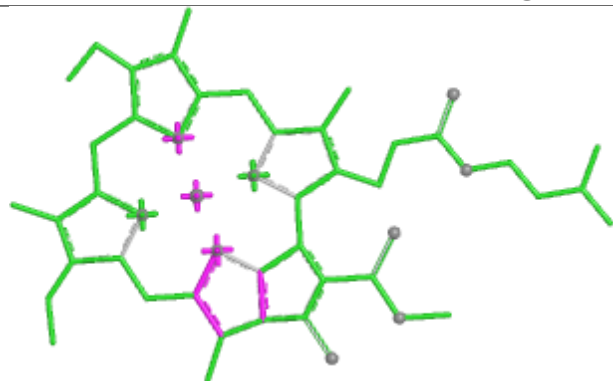




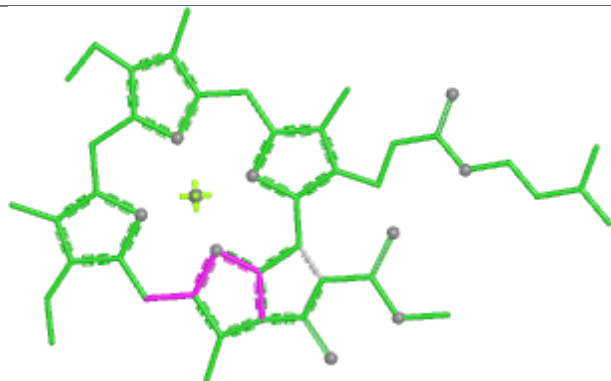


Ligand CLA 8 614**Ligand CLA B 824**

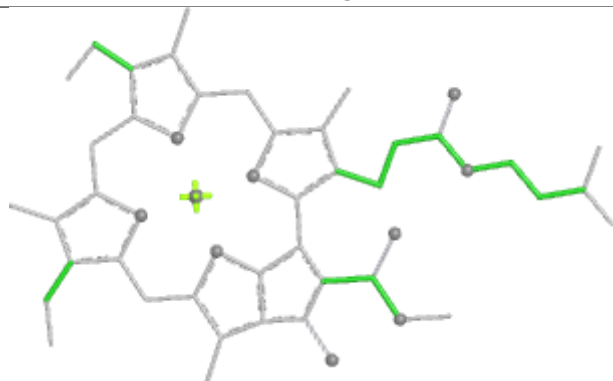
Ligand CLA 1 604



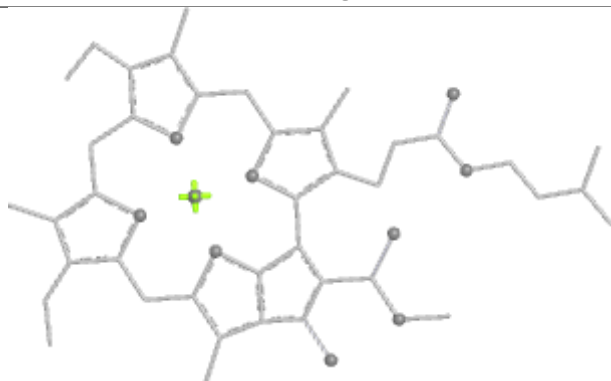
Bond lengths



Bond angles

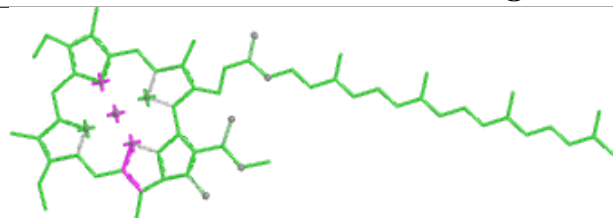


Torsions

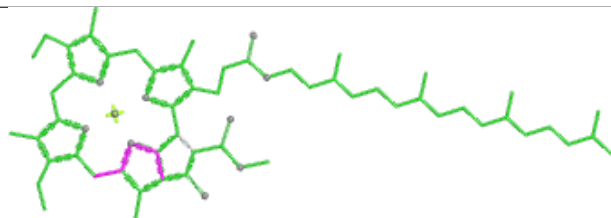


Rings

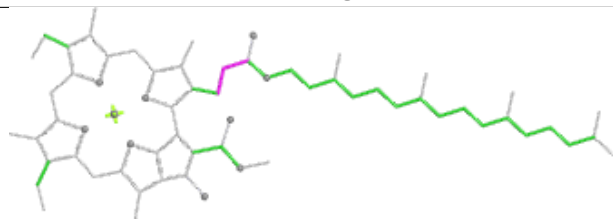
Ligand CLA B2 813



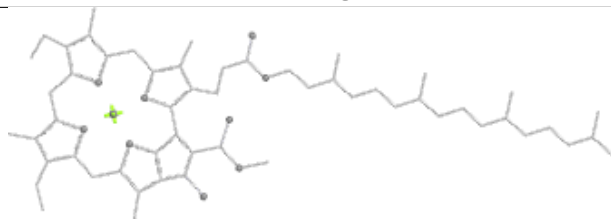
Bond lengths



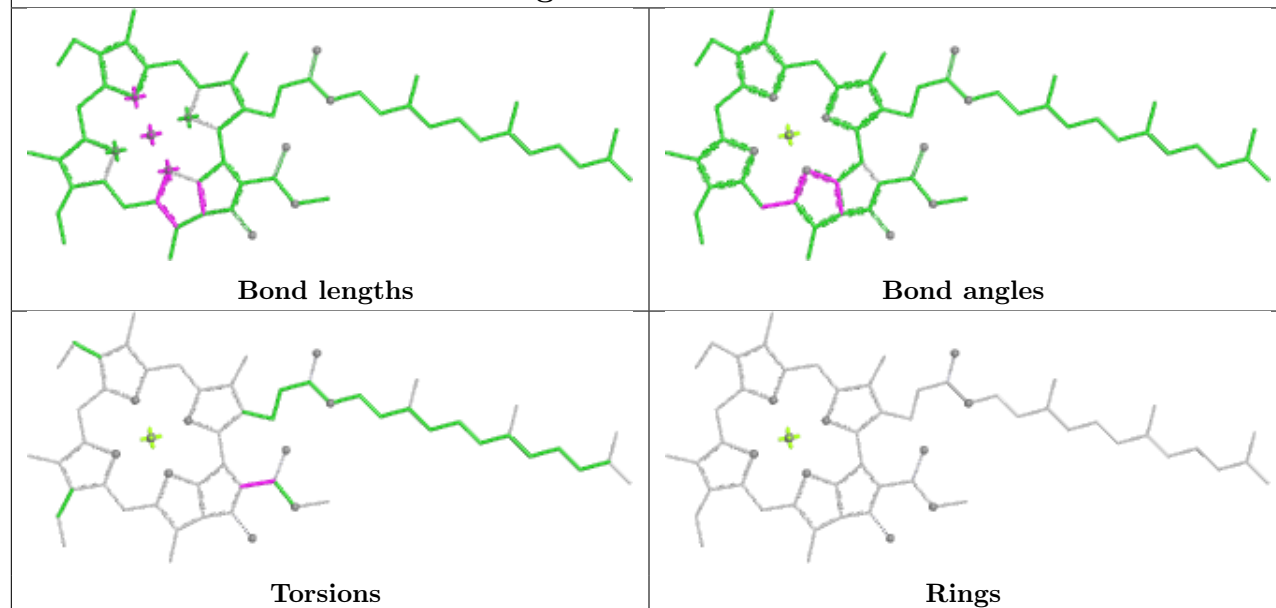
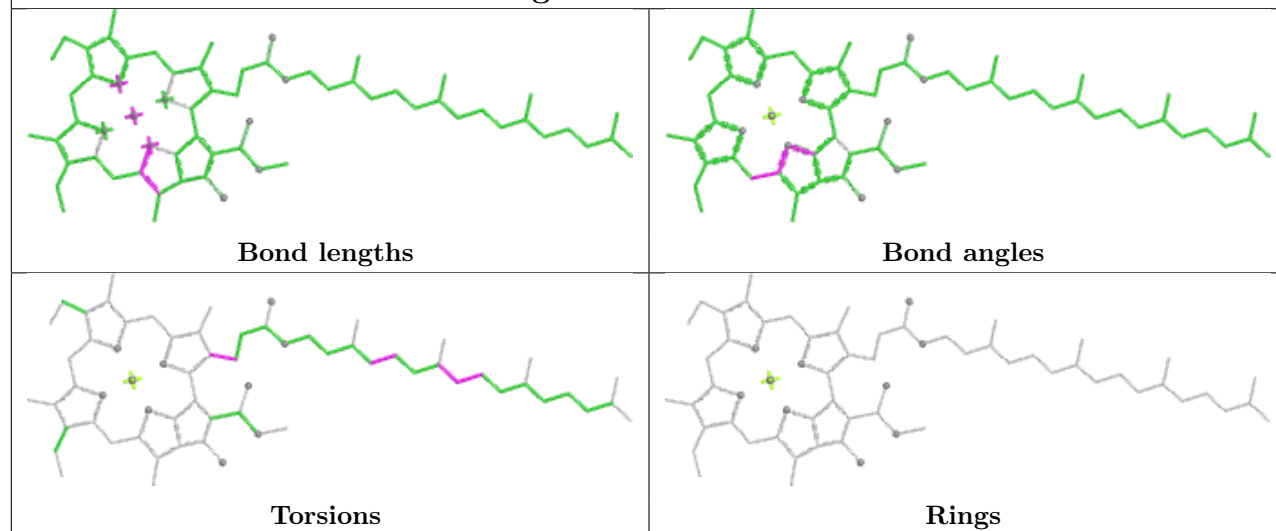
Bond angles

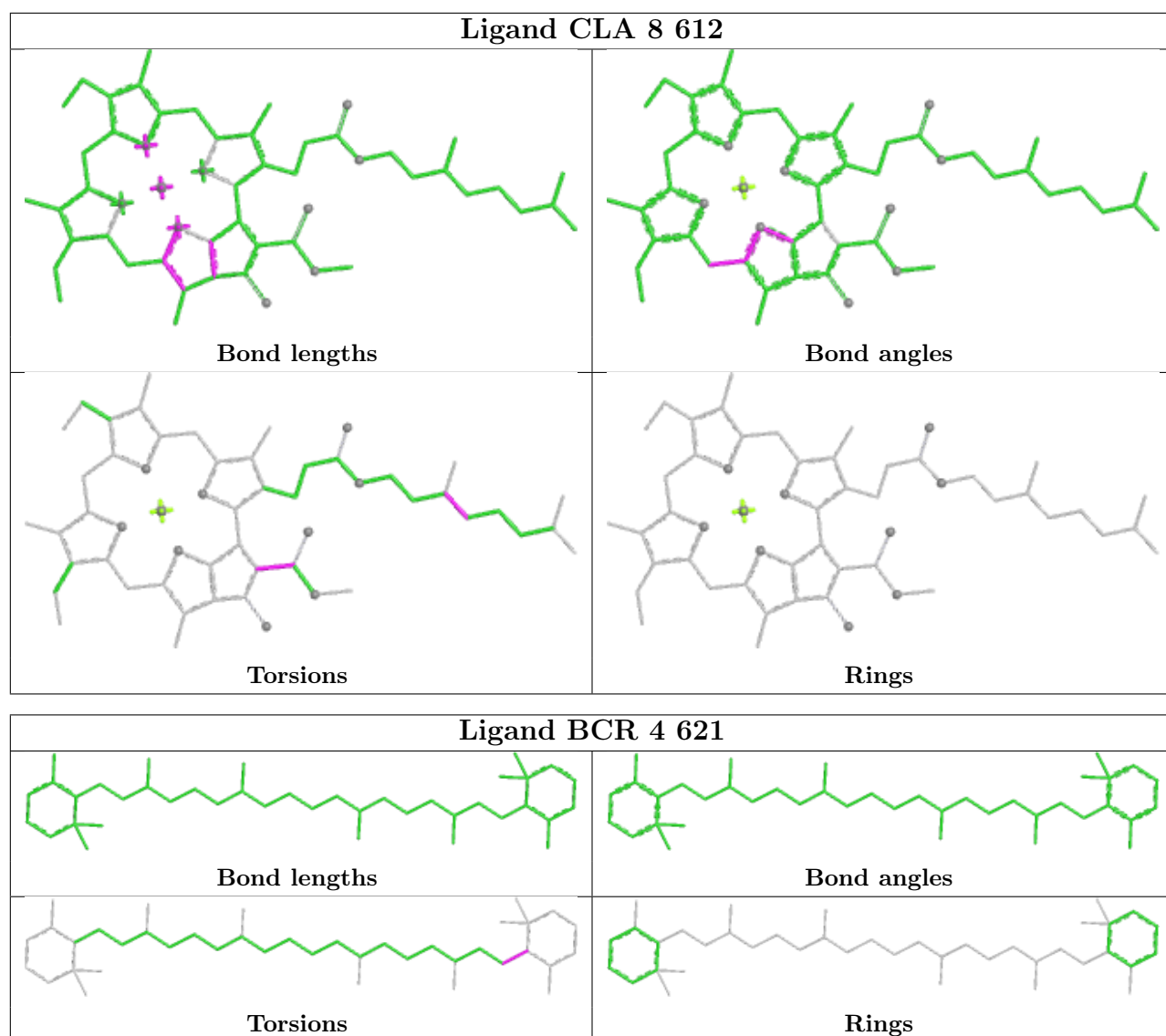


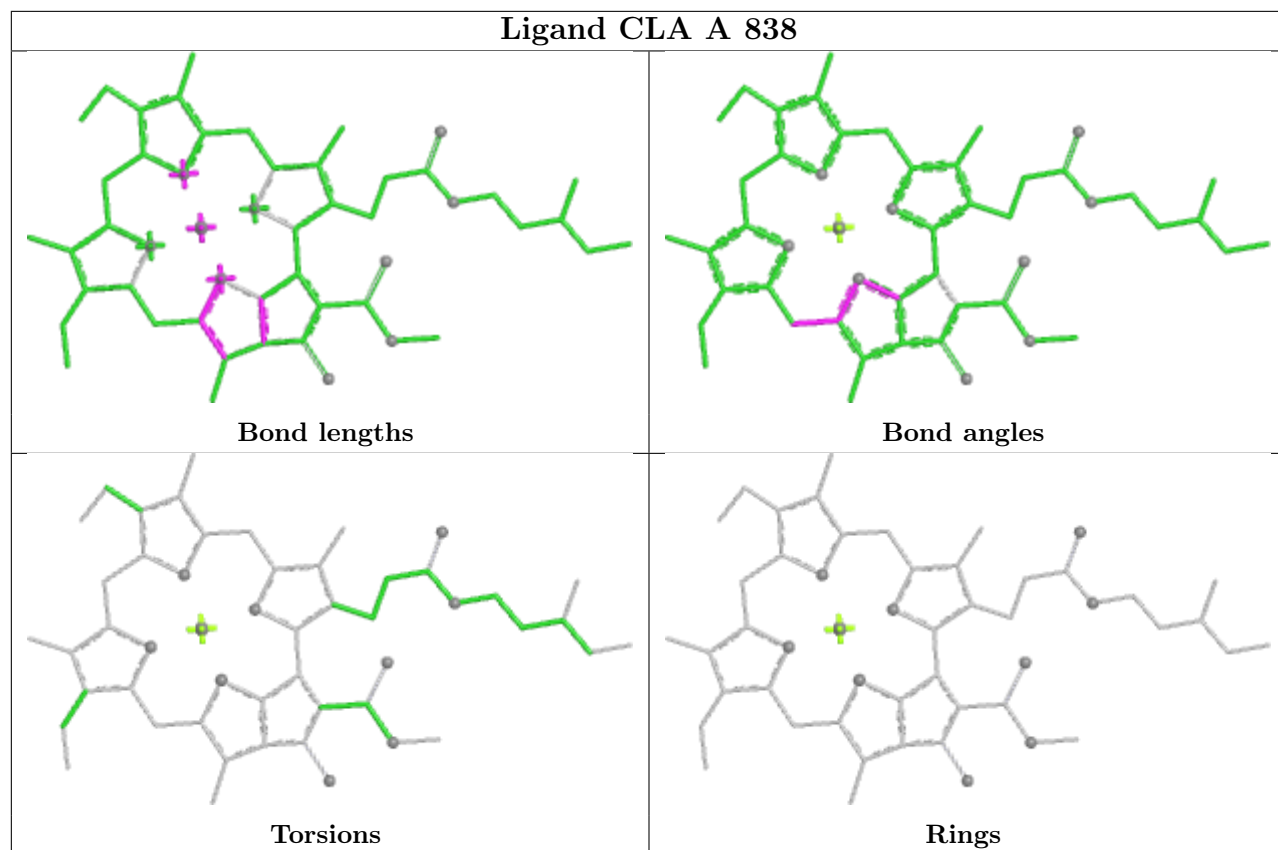
Torsions



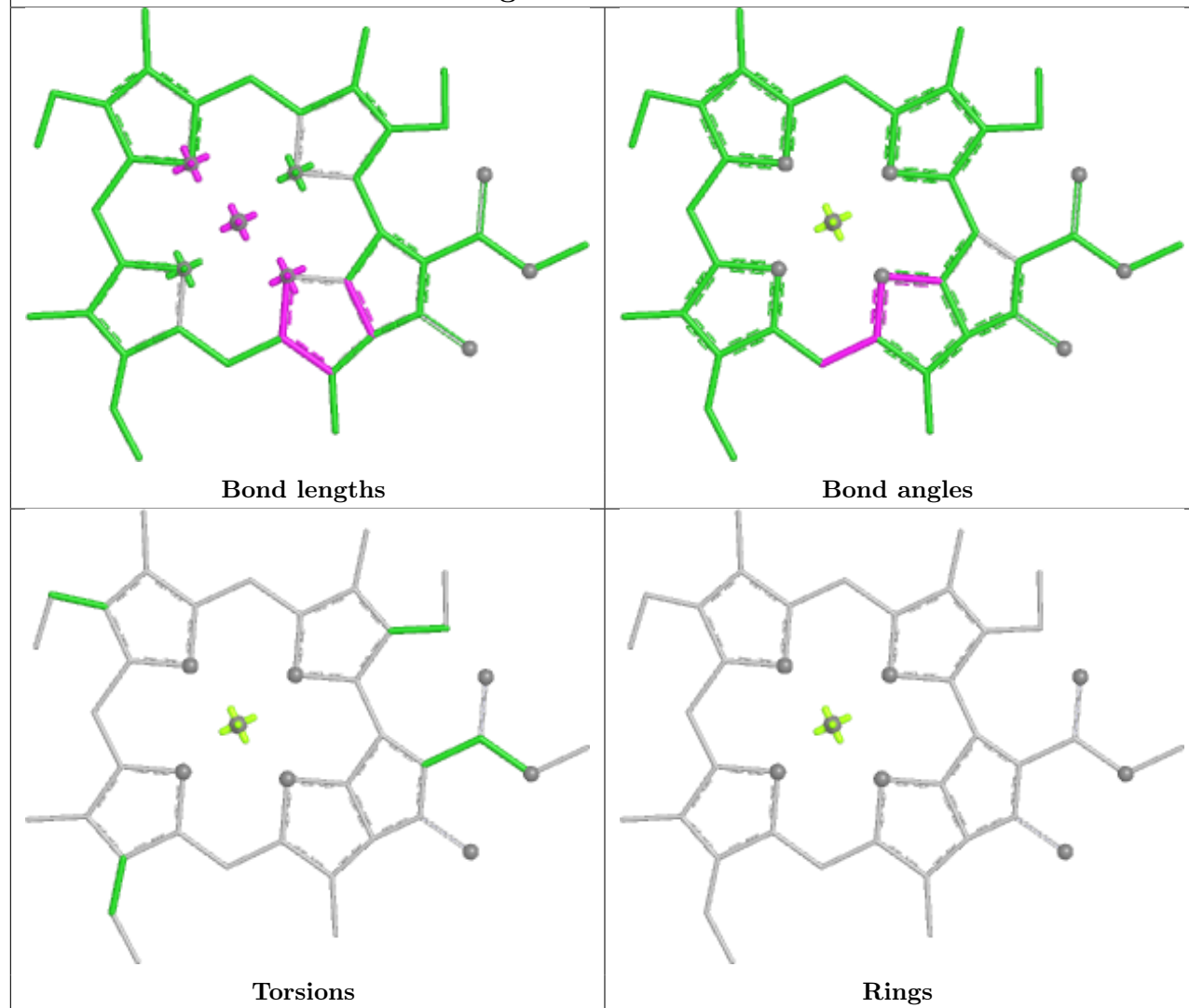
Rings

Ligand CLA 1 602**Ligand CLA B 827**

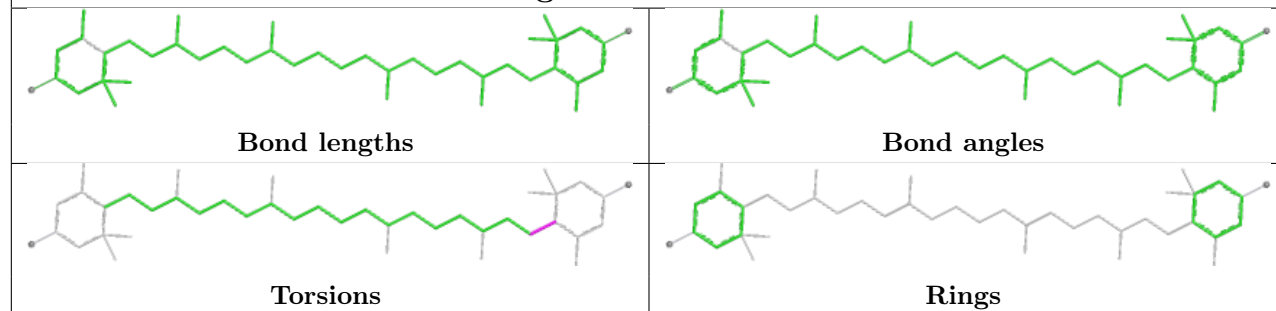


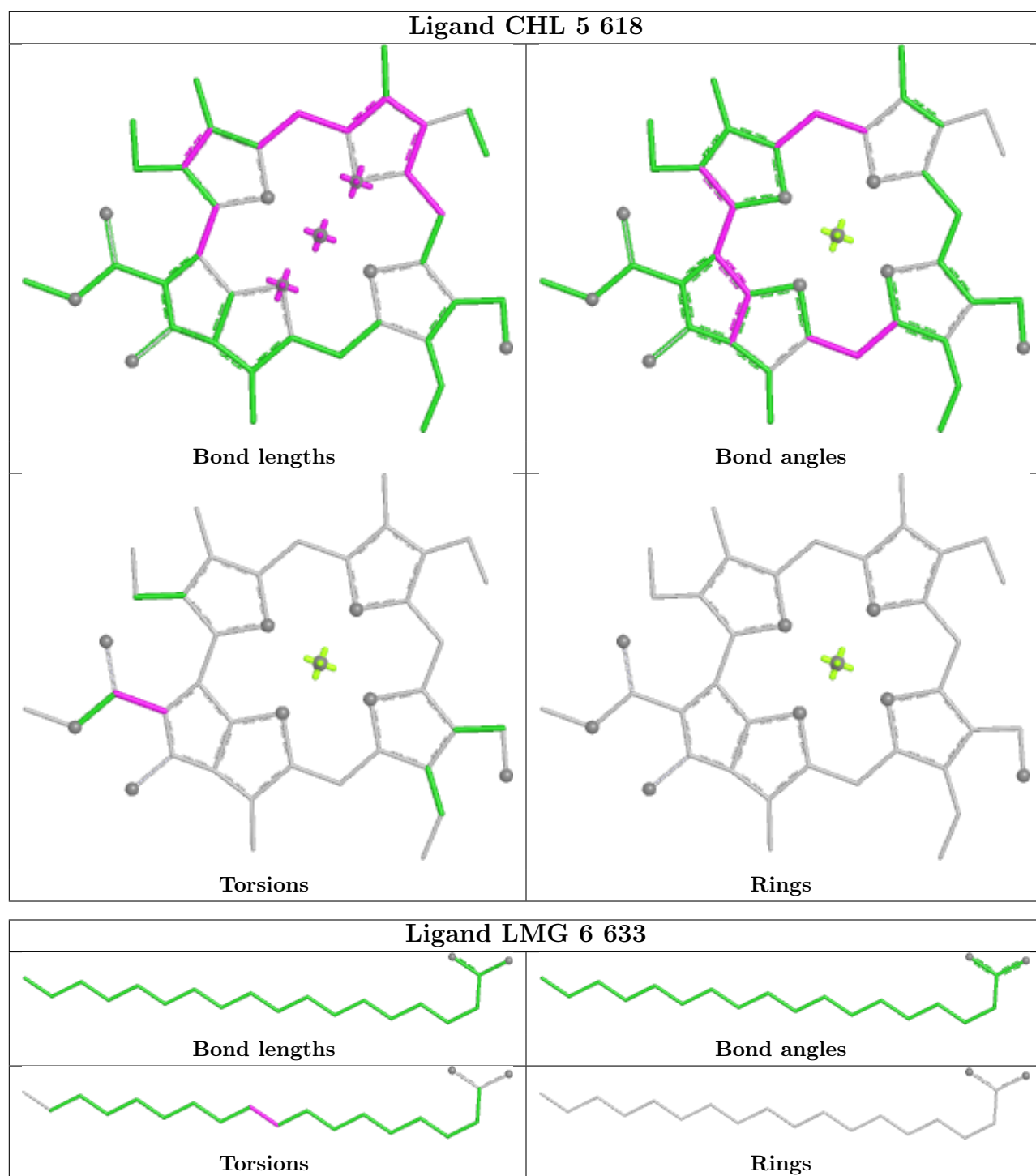


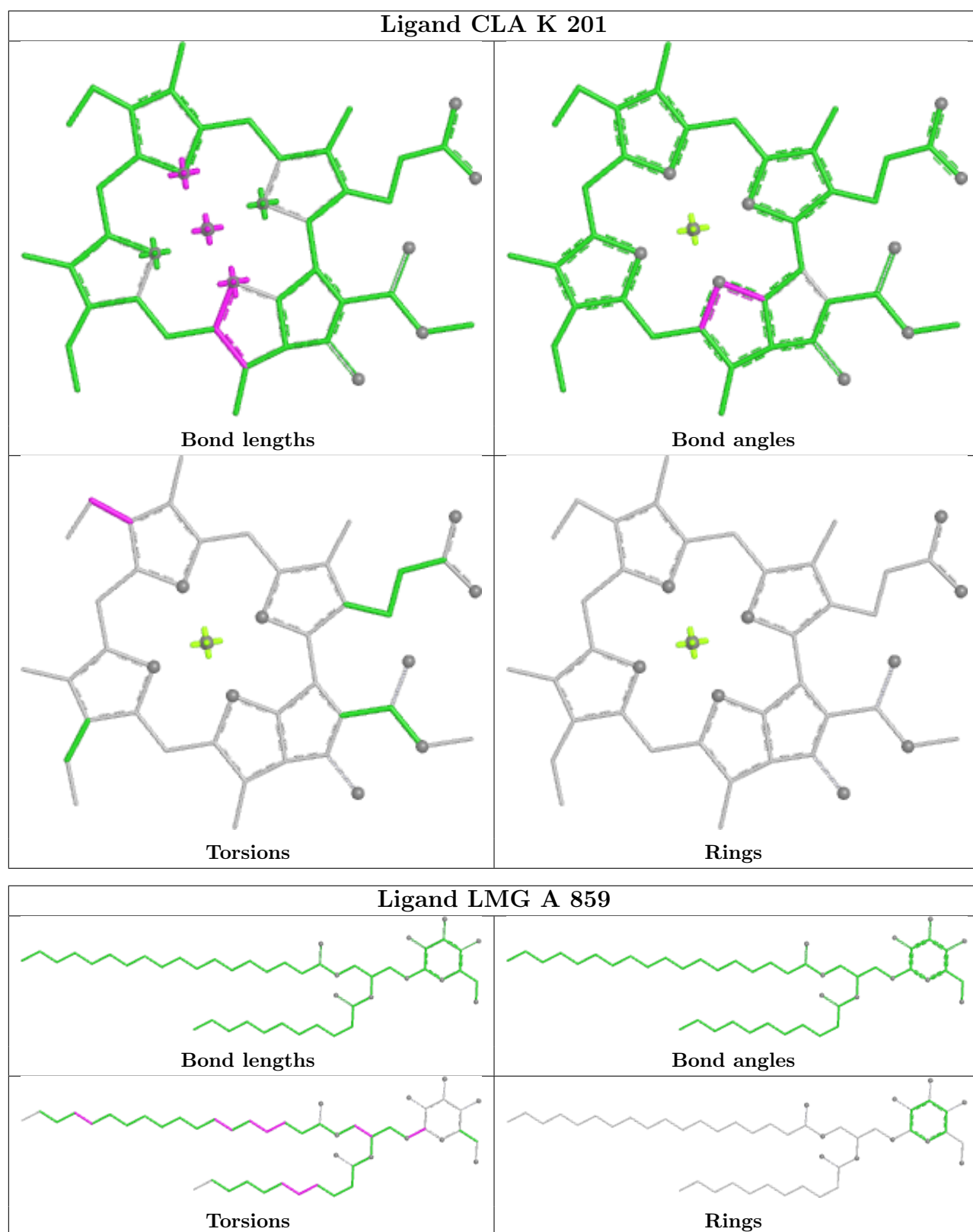
Ligand CLA 3 606

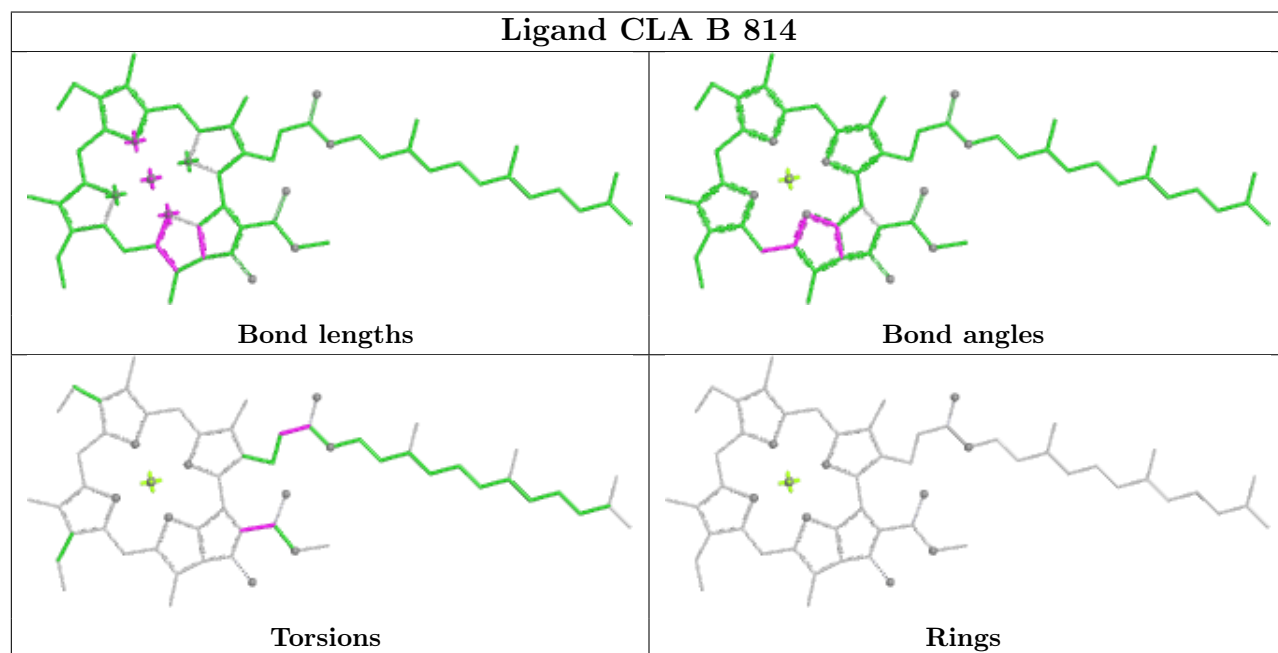
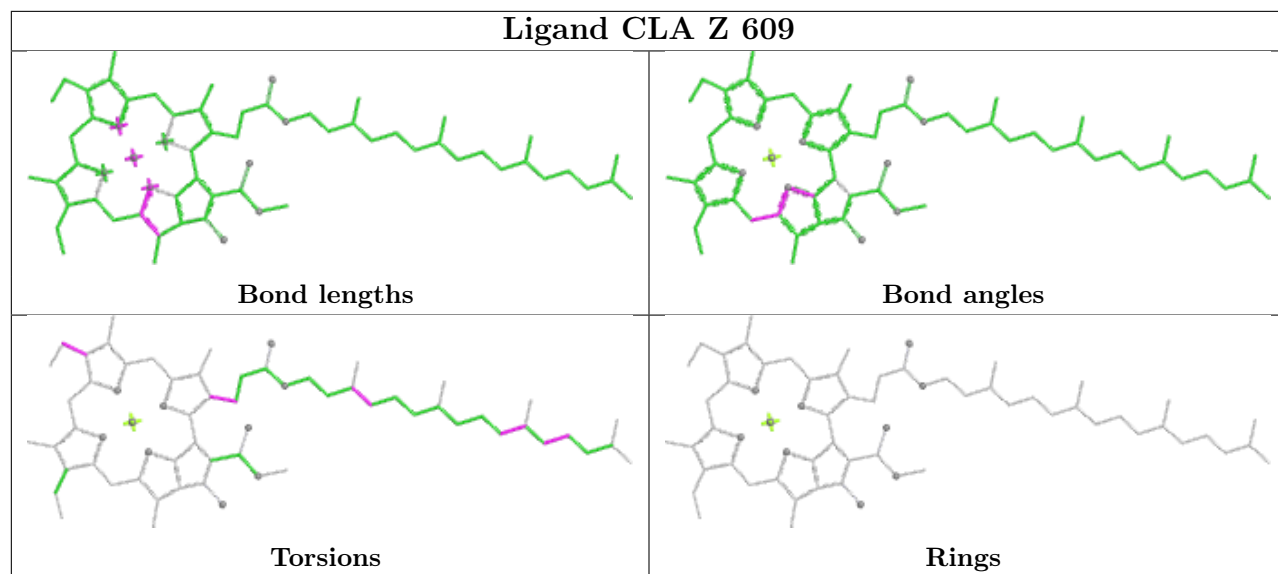


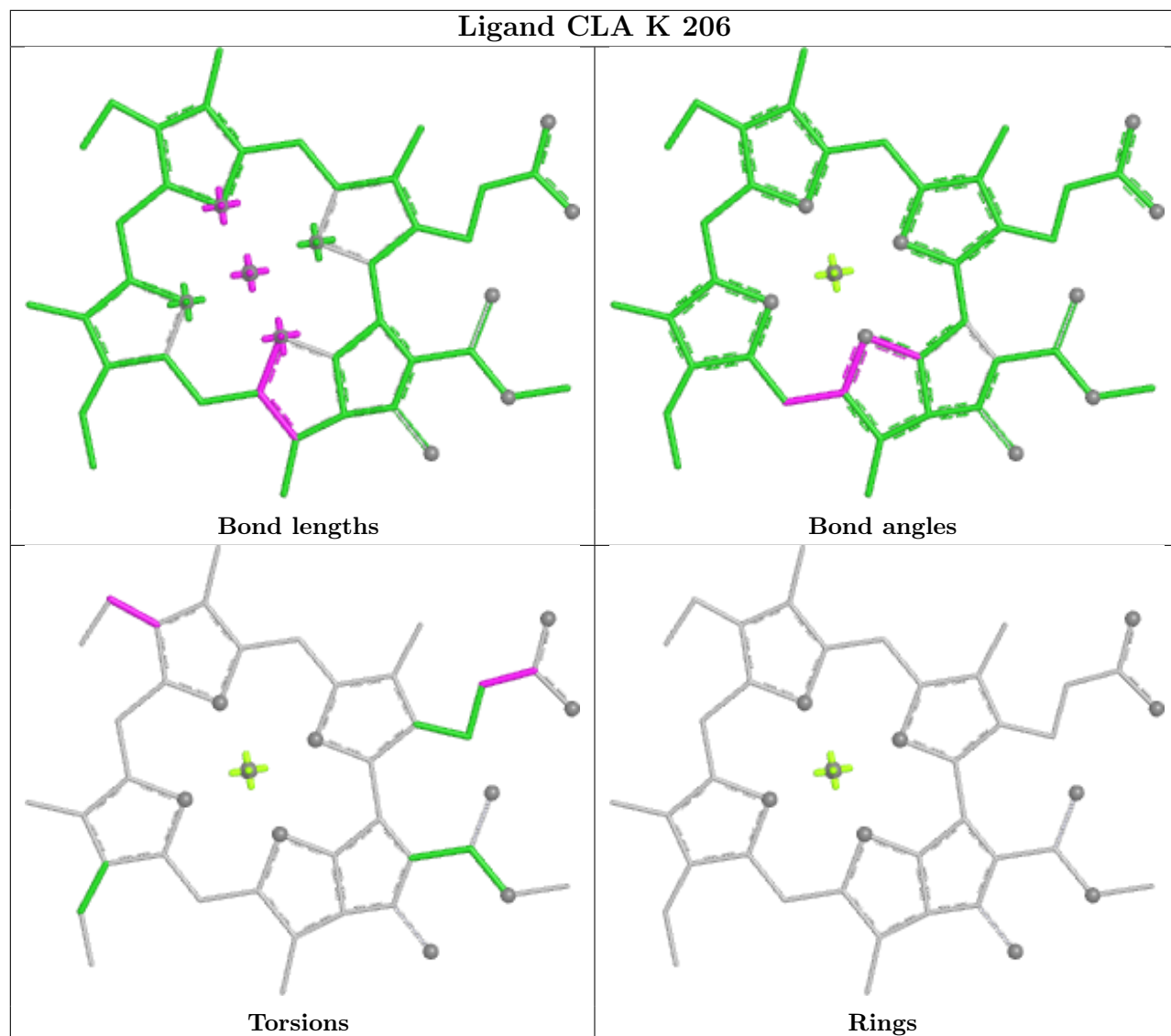
Ligand LUT 4 619

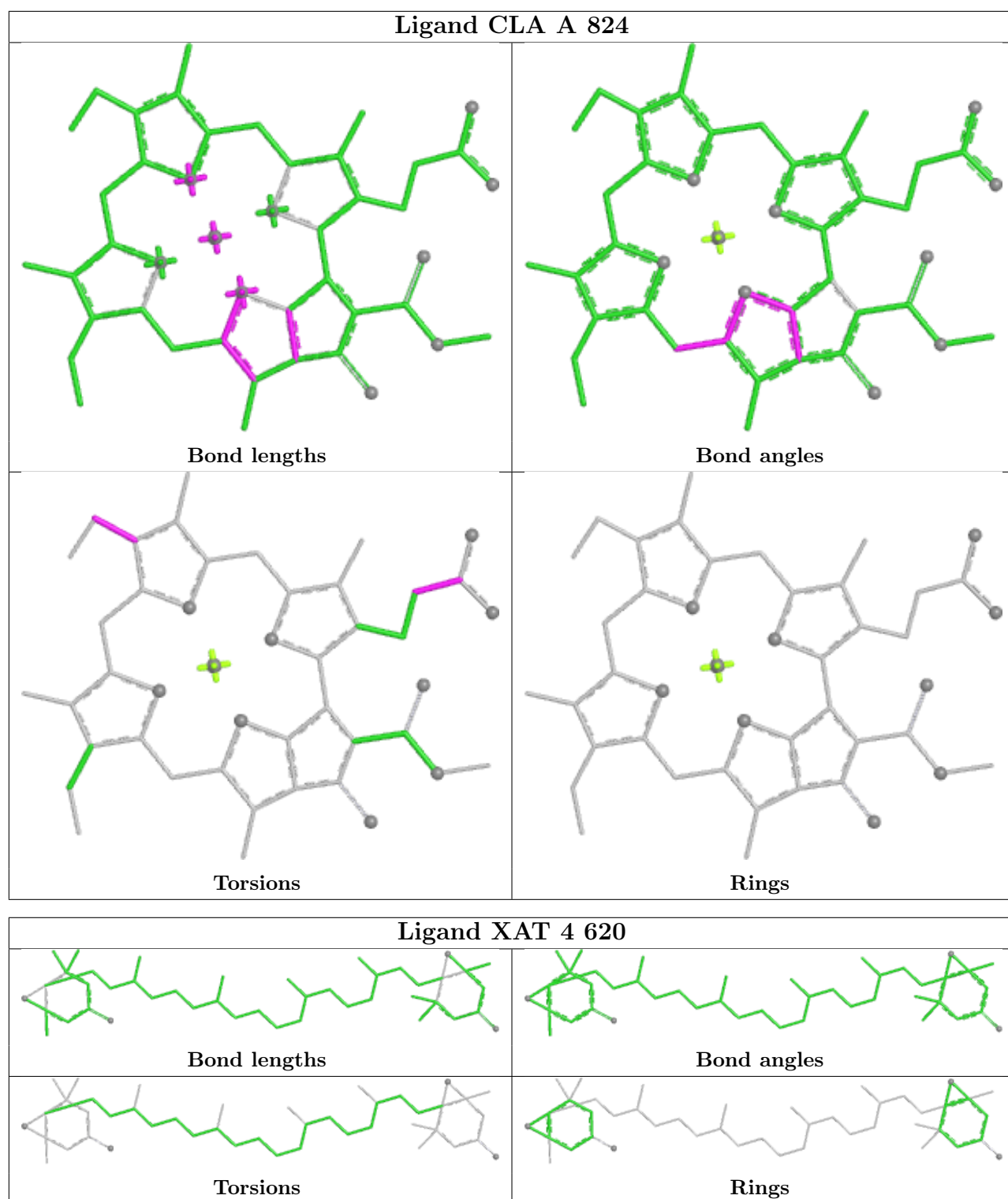




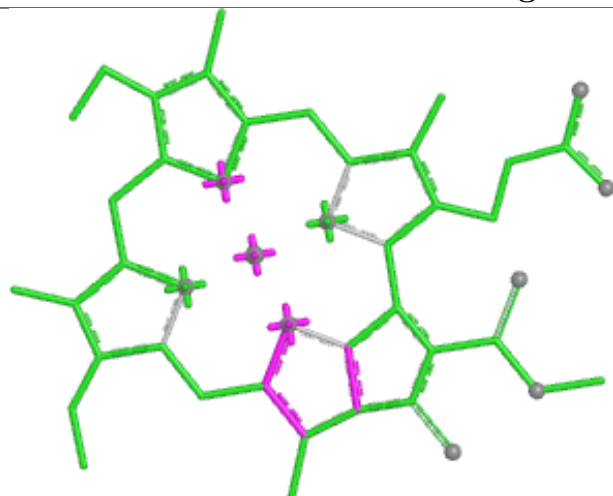




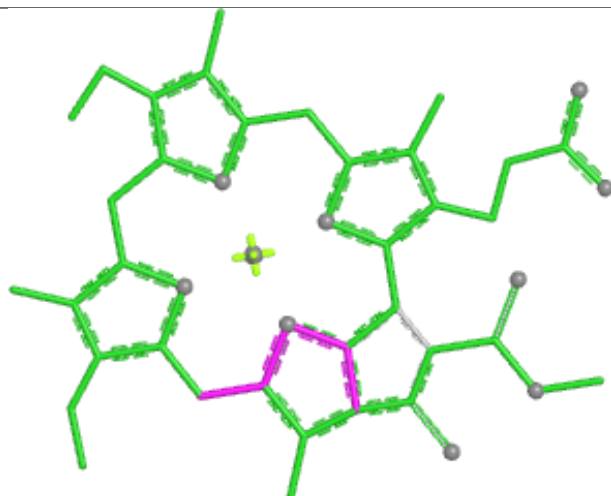




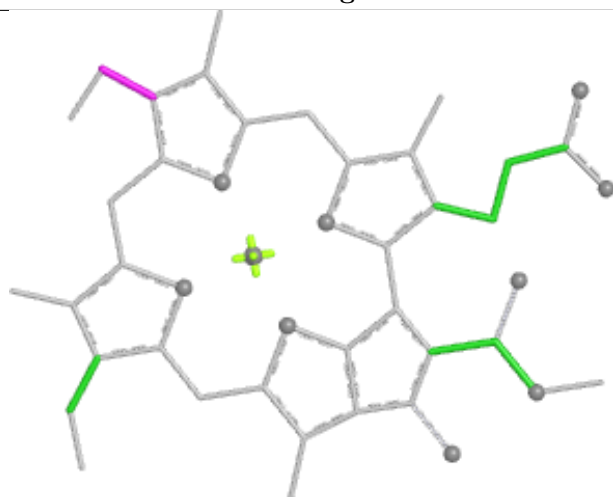
Ligand CLA 7 609



Bond lengths



Bond angles

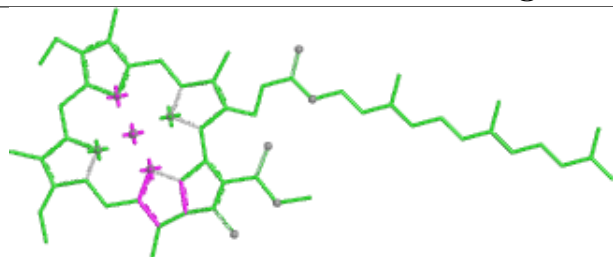


Torsions

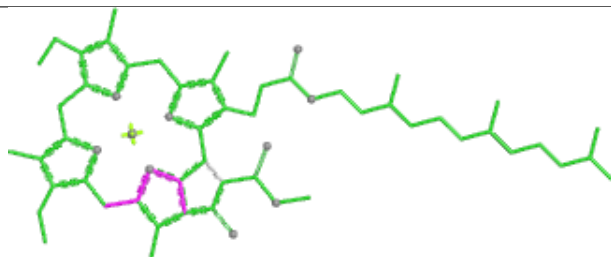


Rings

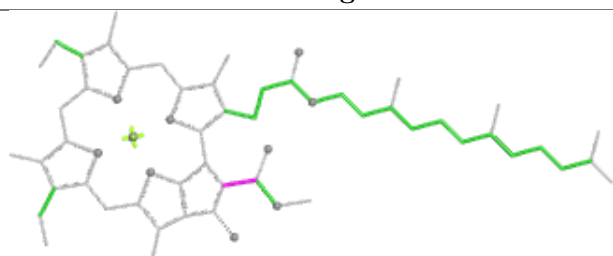
Ligand CLA 4 602



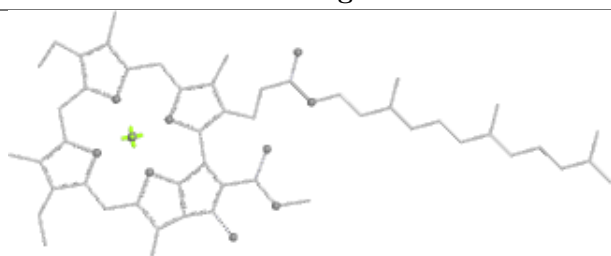
Bond lengths



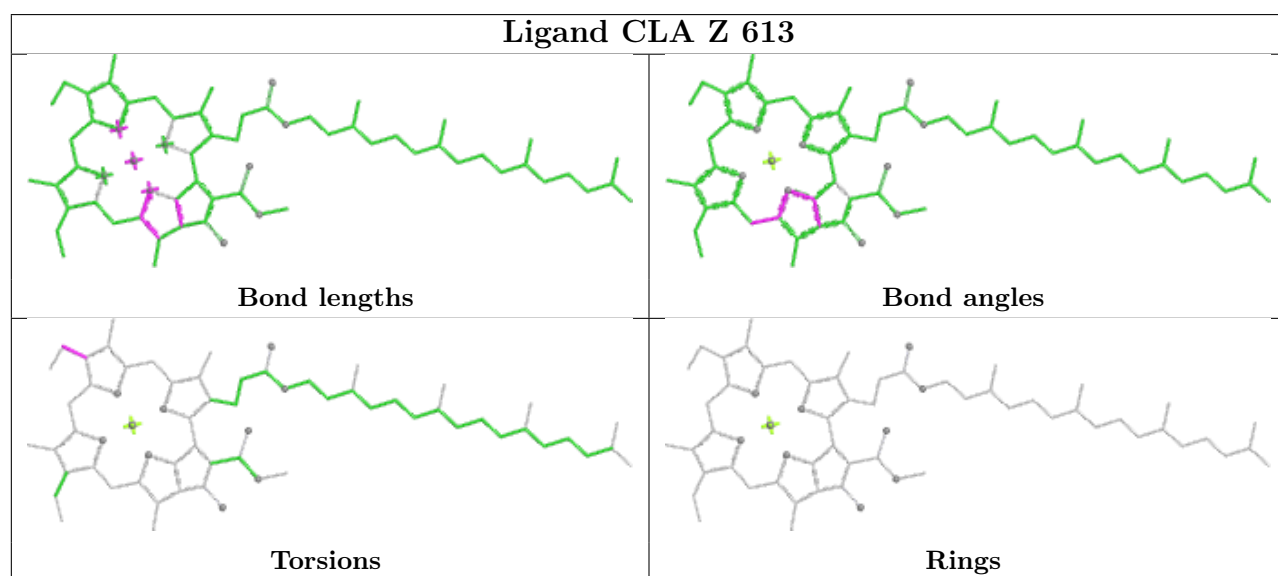
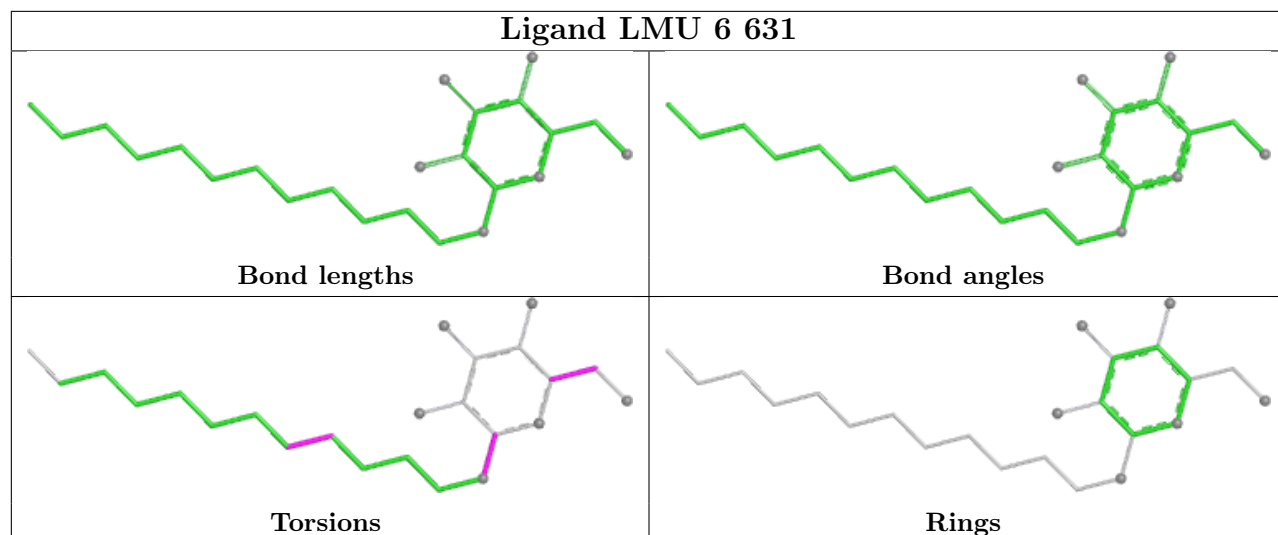
Bond angles



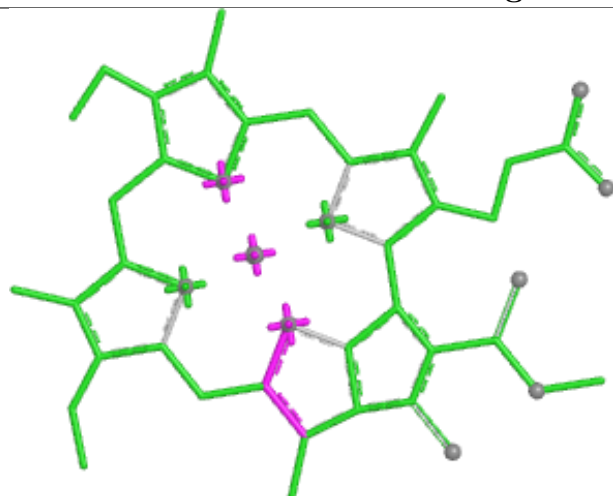
Torsions



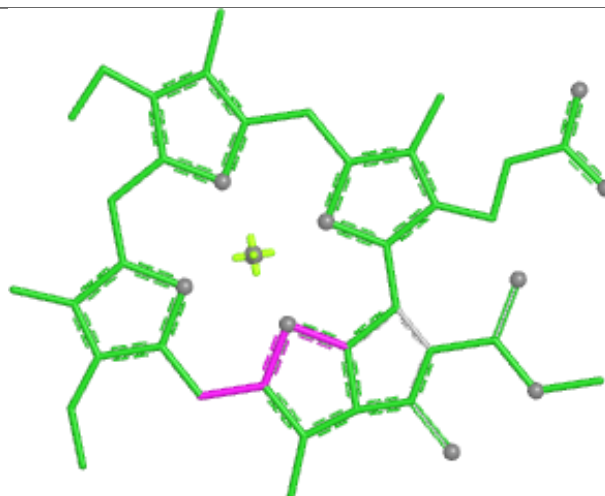
Rings



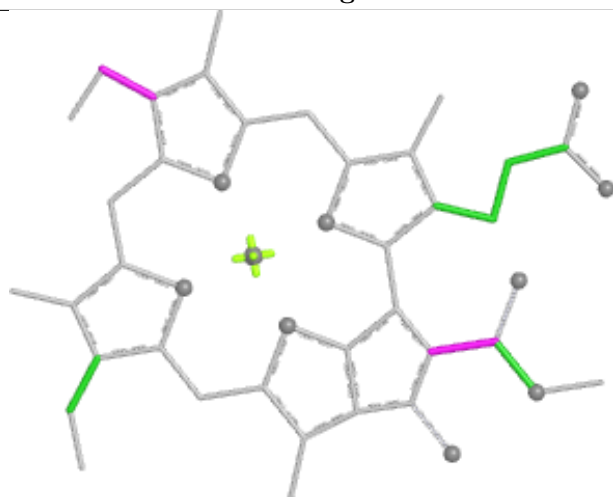
Ligand CLA B2 808



Bond lengths



Bond angles

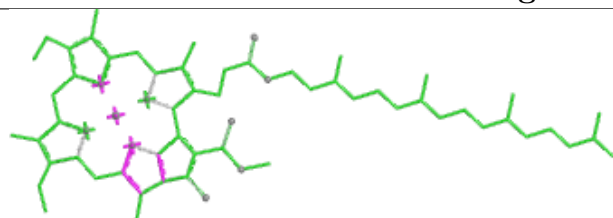


Torsions

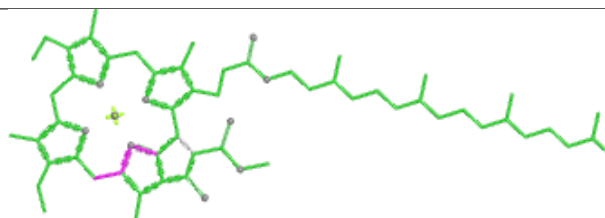


Rings

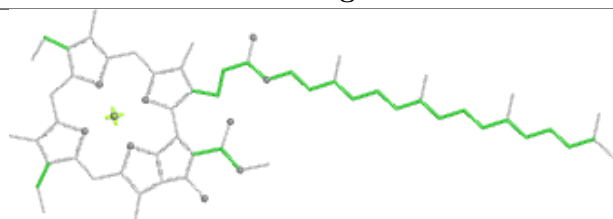
Ligand CLA 7 613



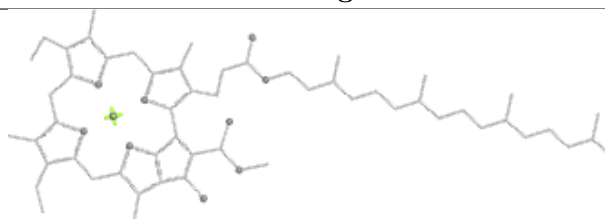
Bond lengths



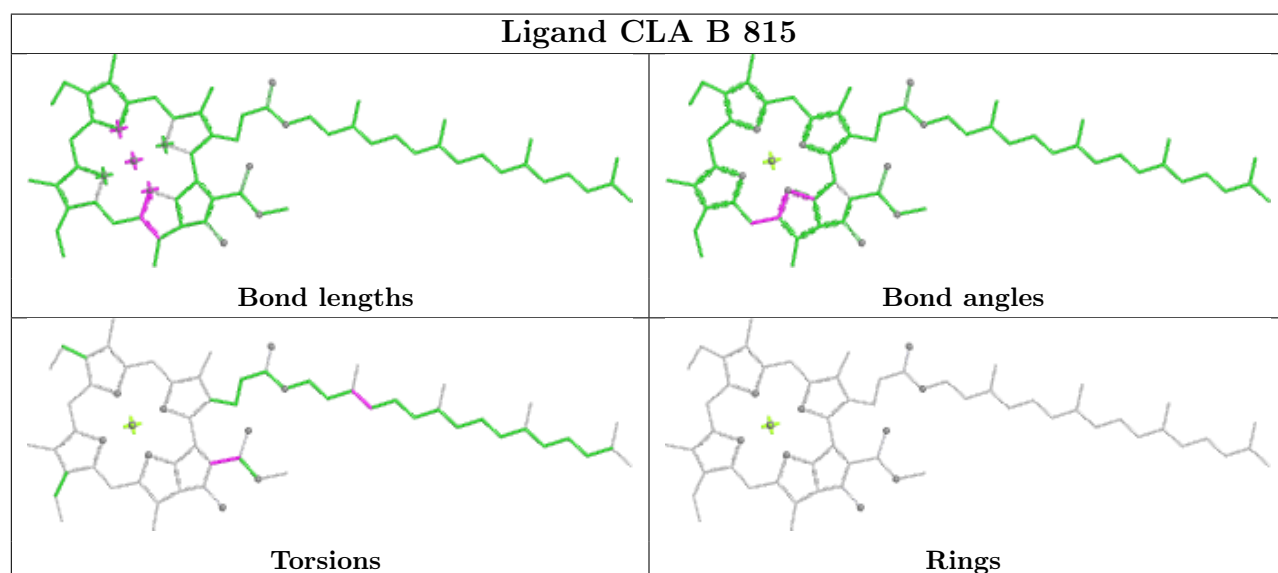
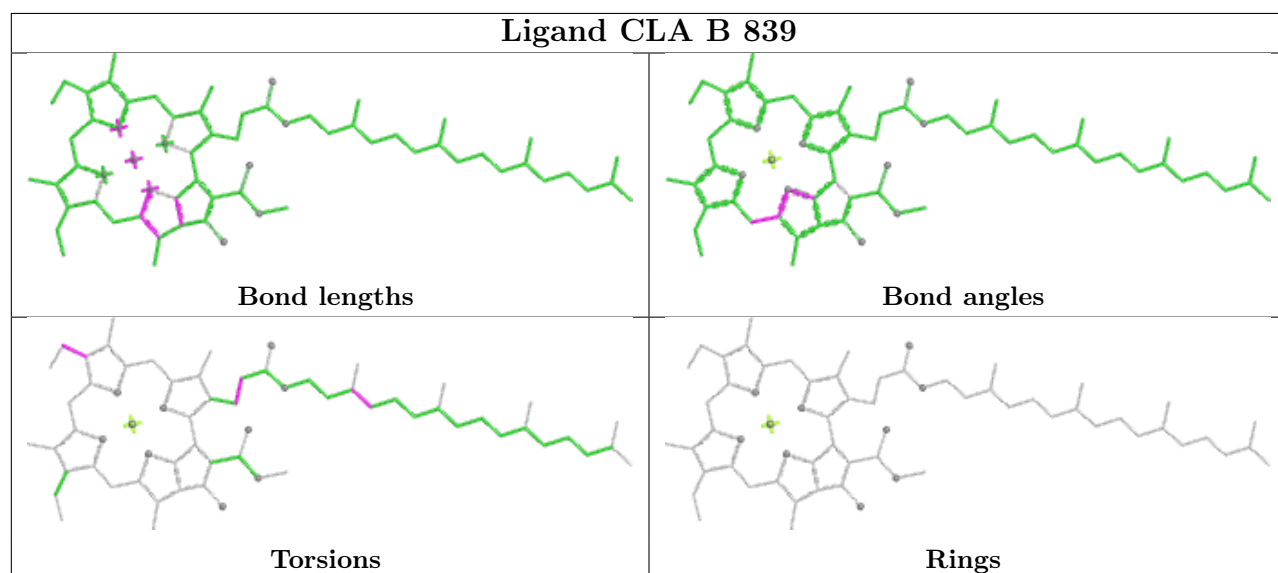
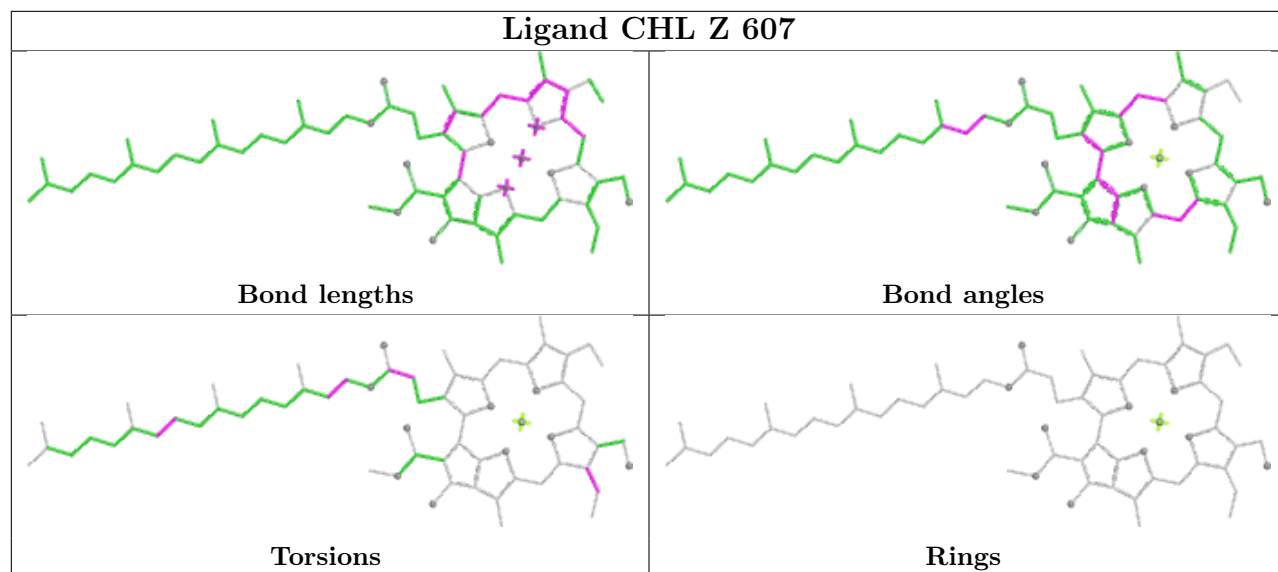
Bond angles

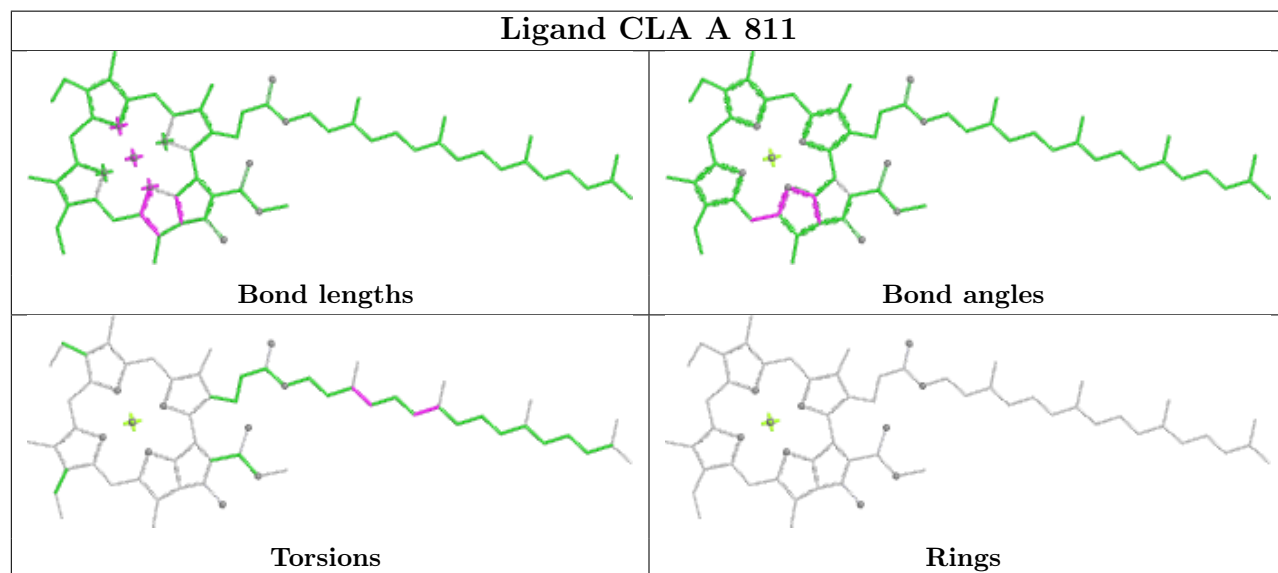
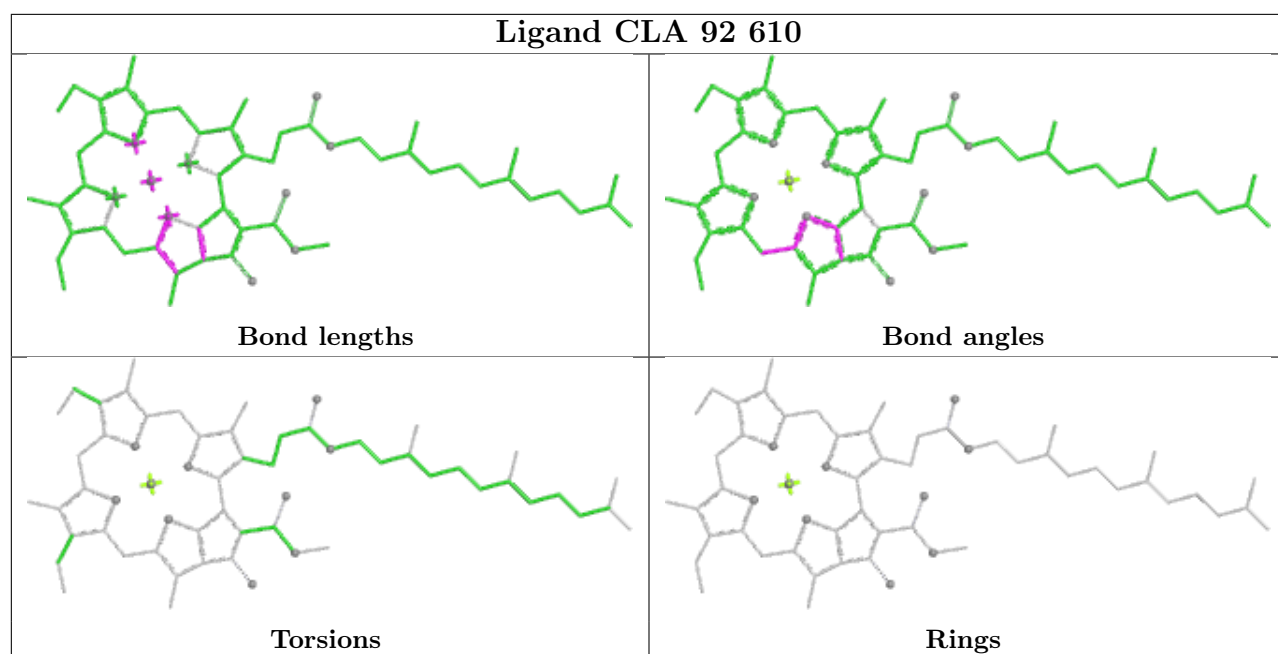


Torsions

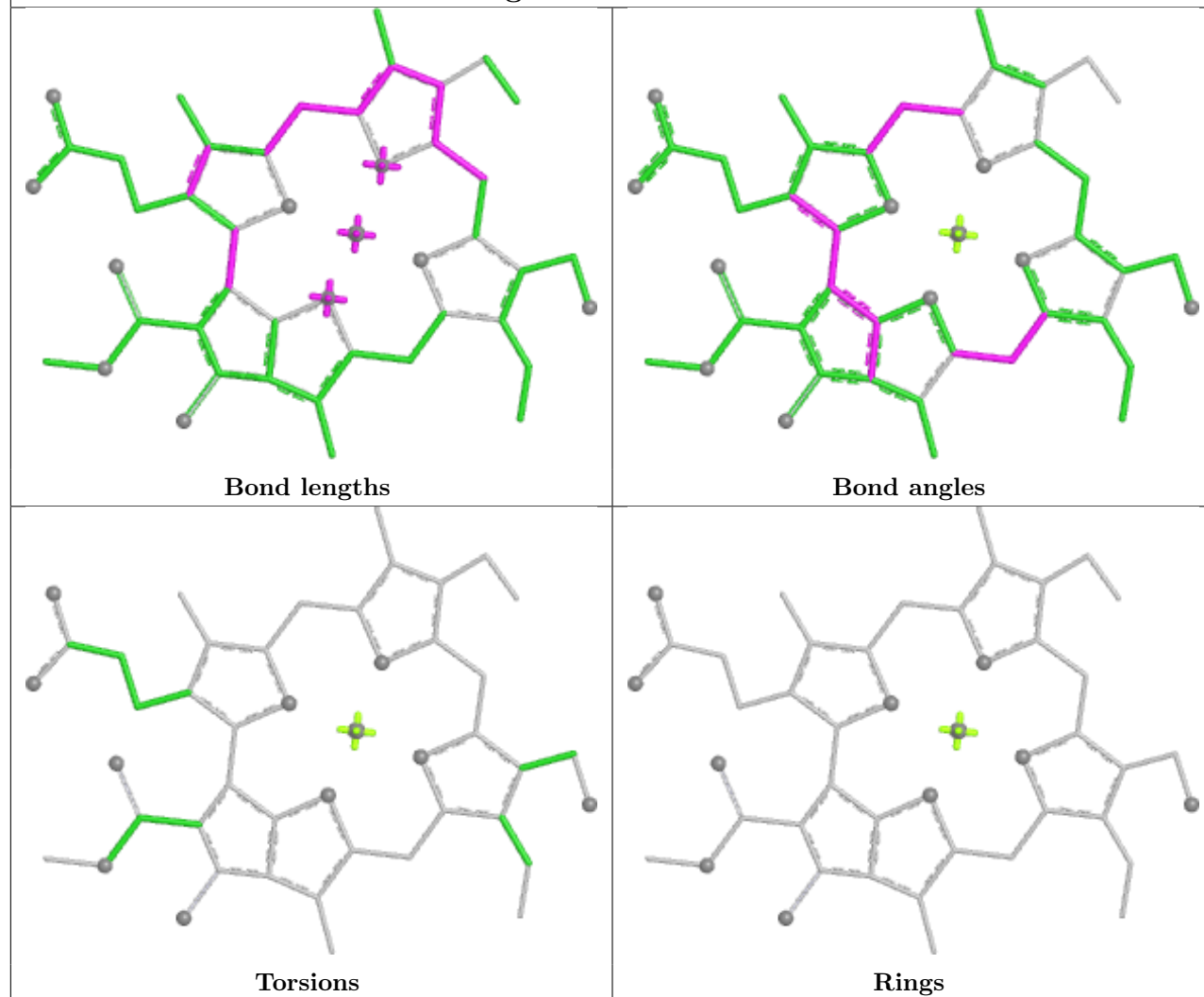


Rings

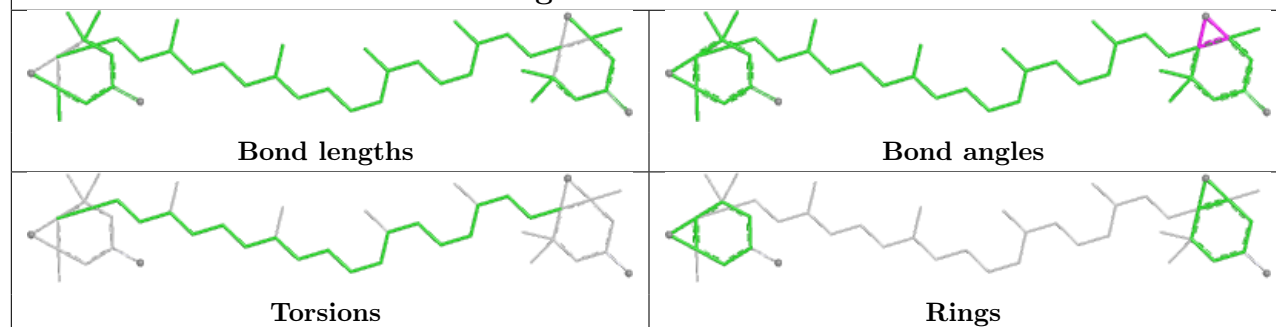


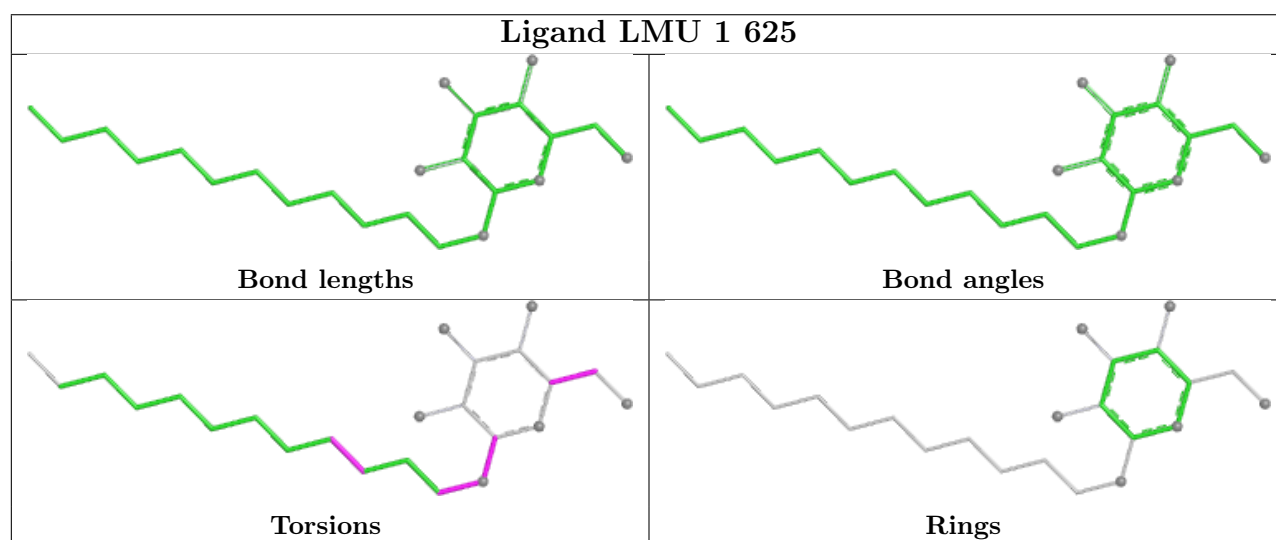
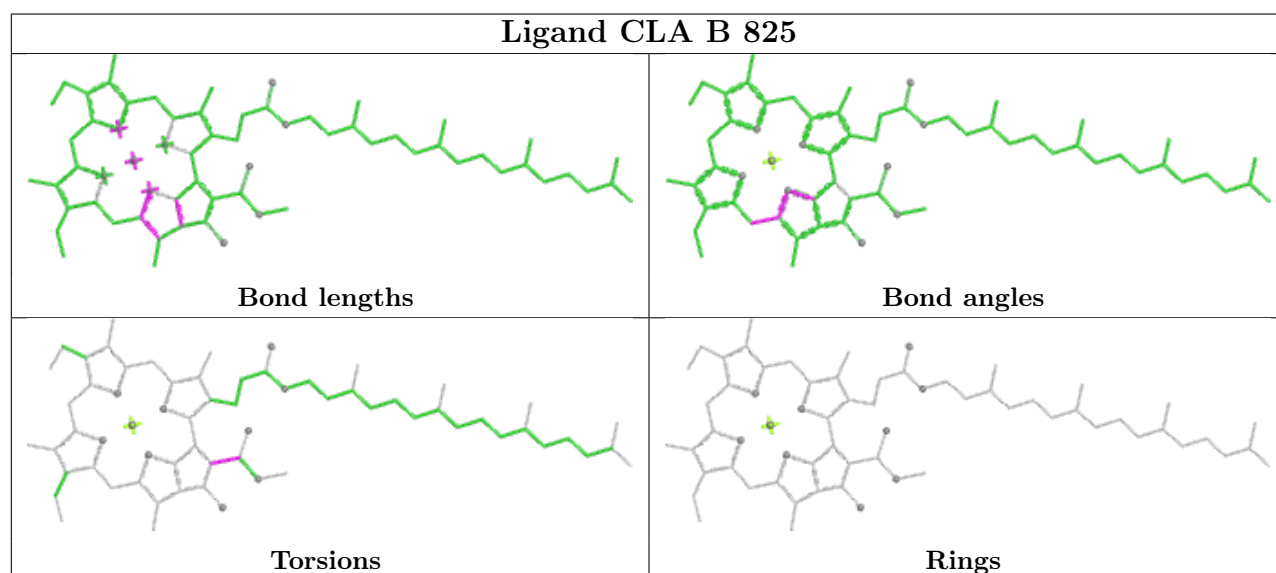
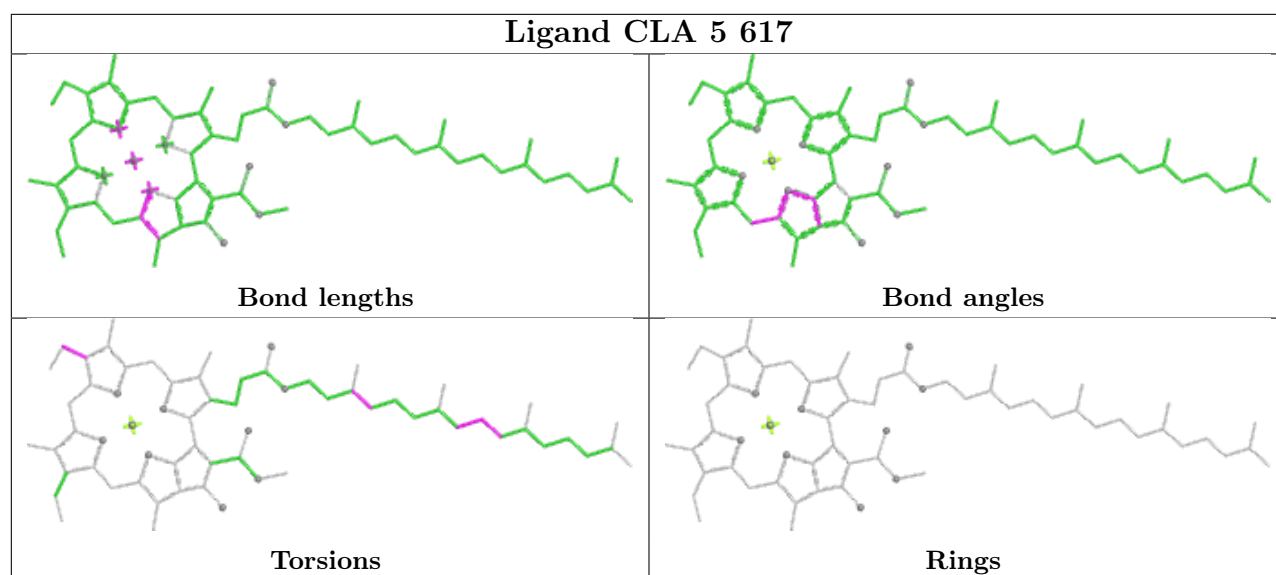


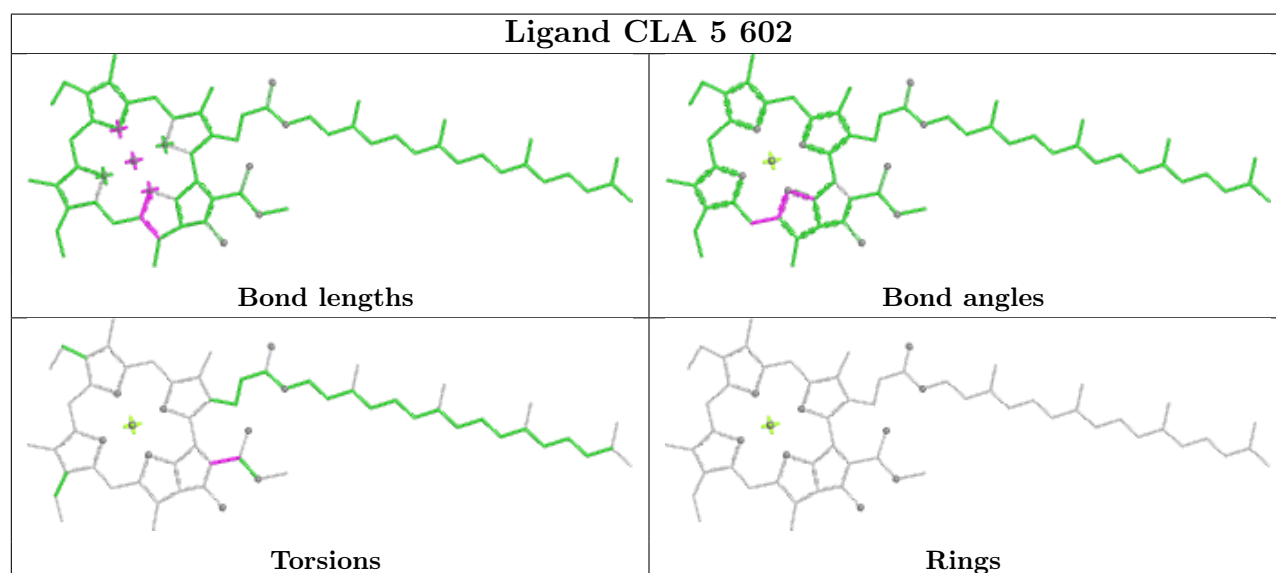
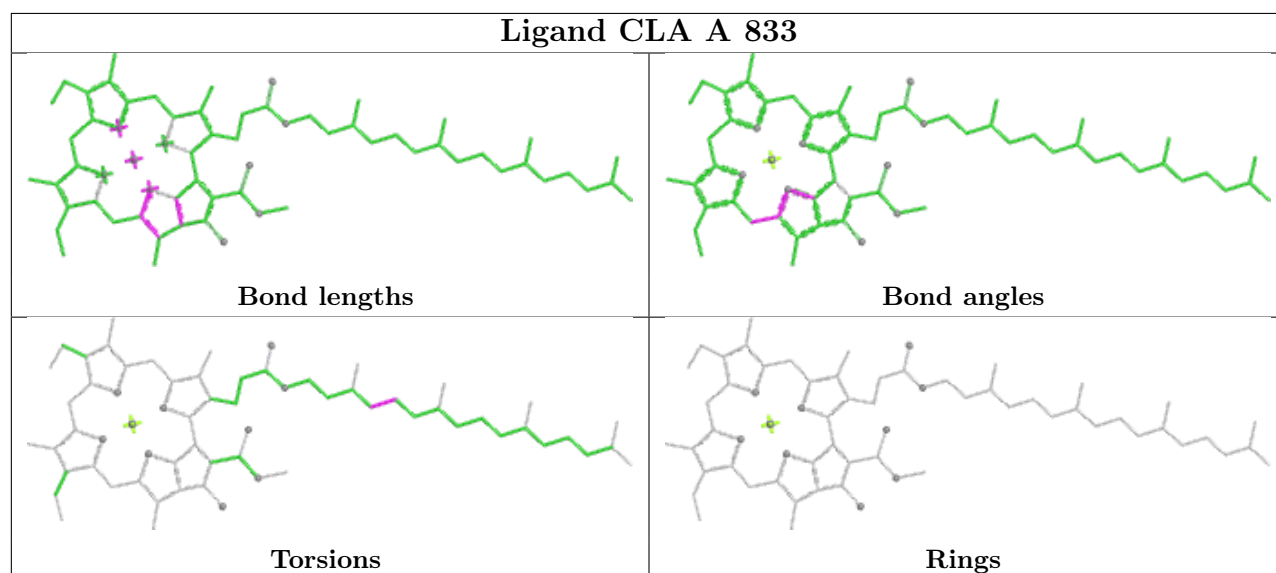
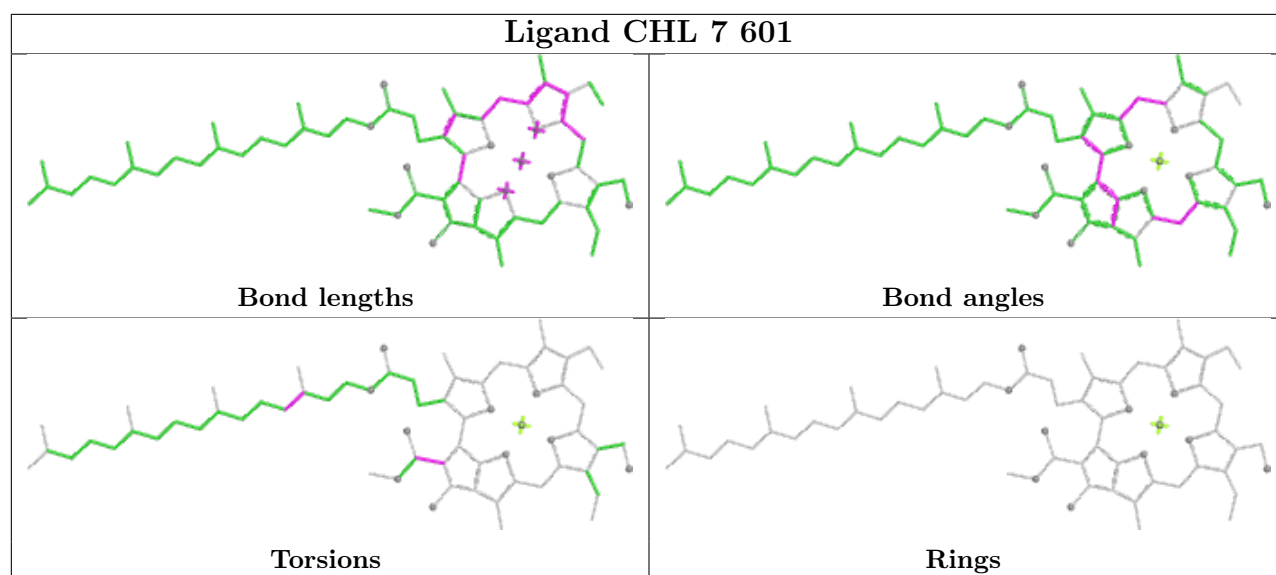
Ligand CHL 7 607

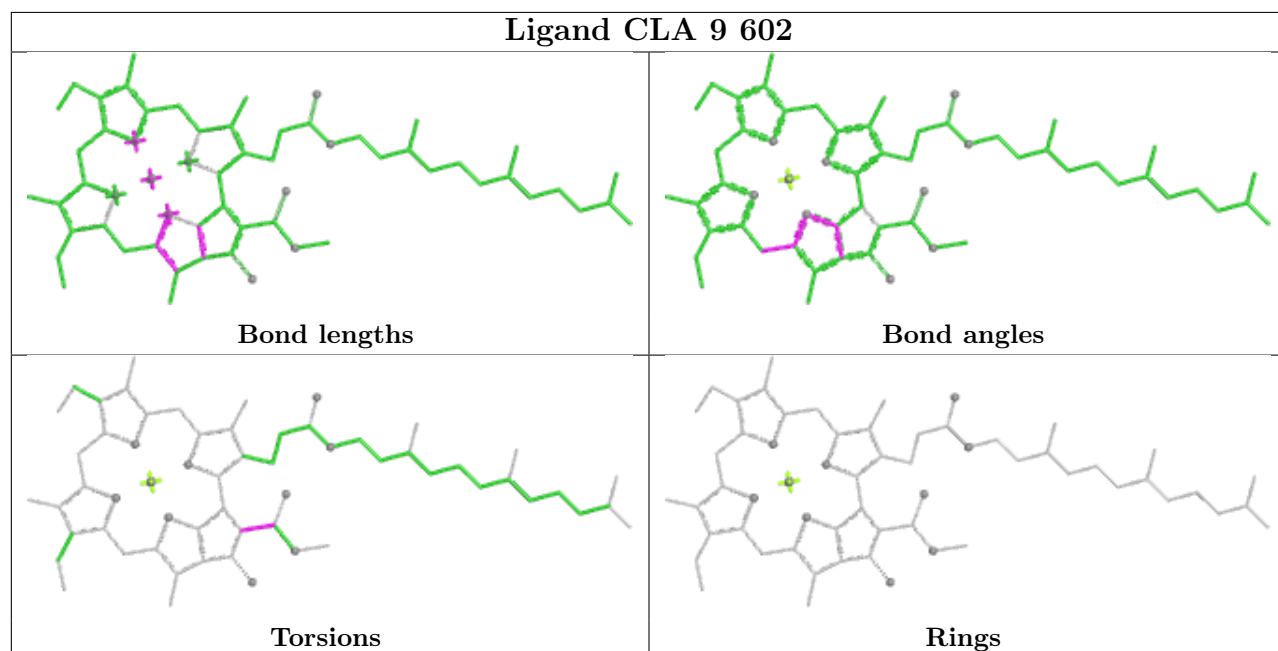
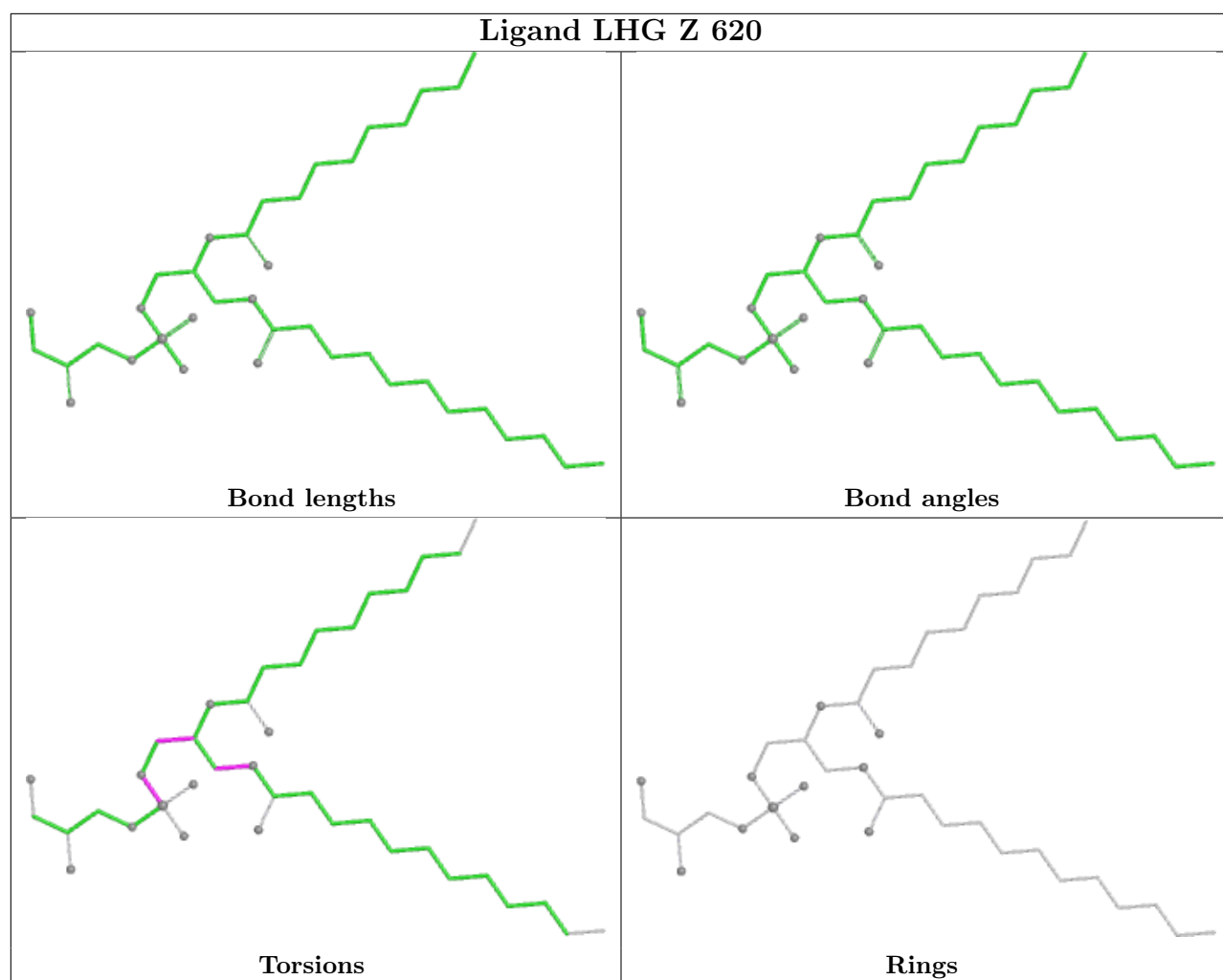


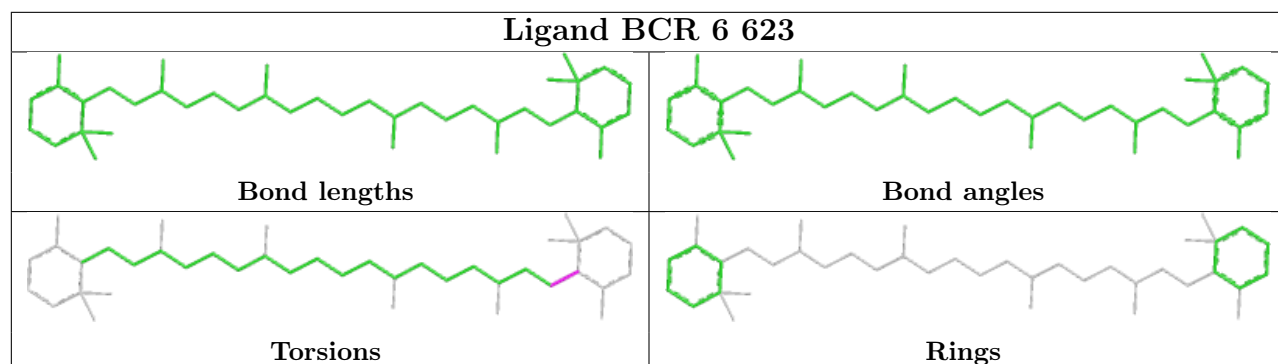
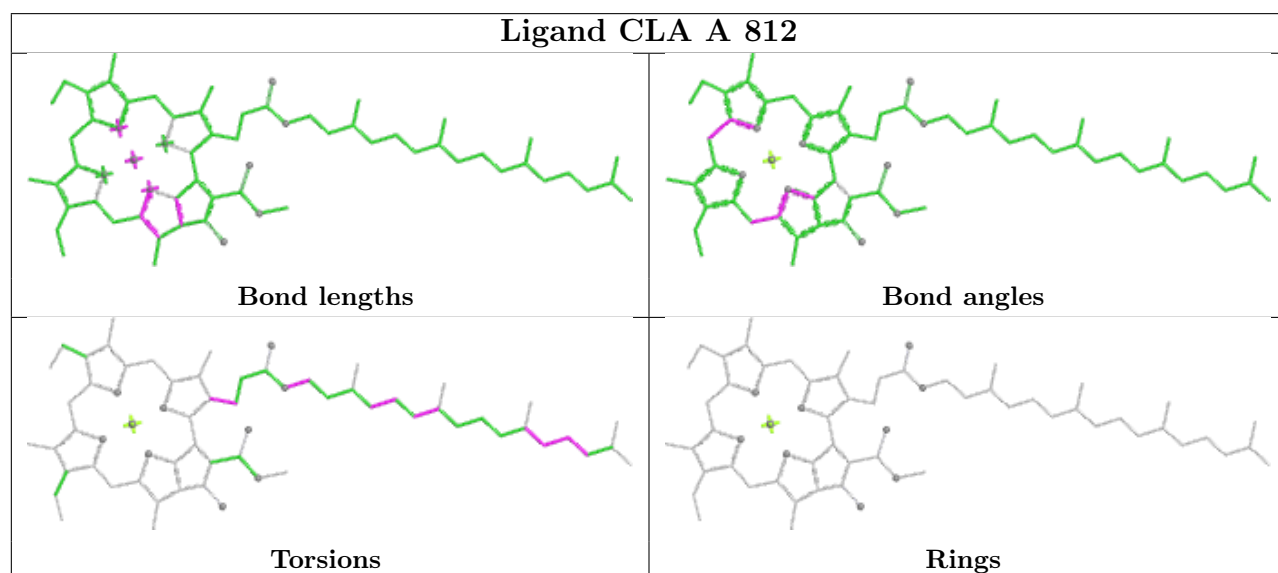
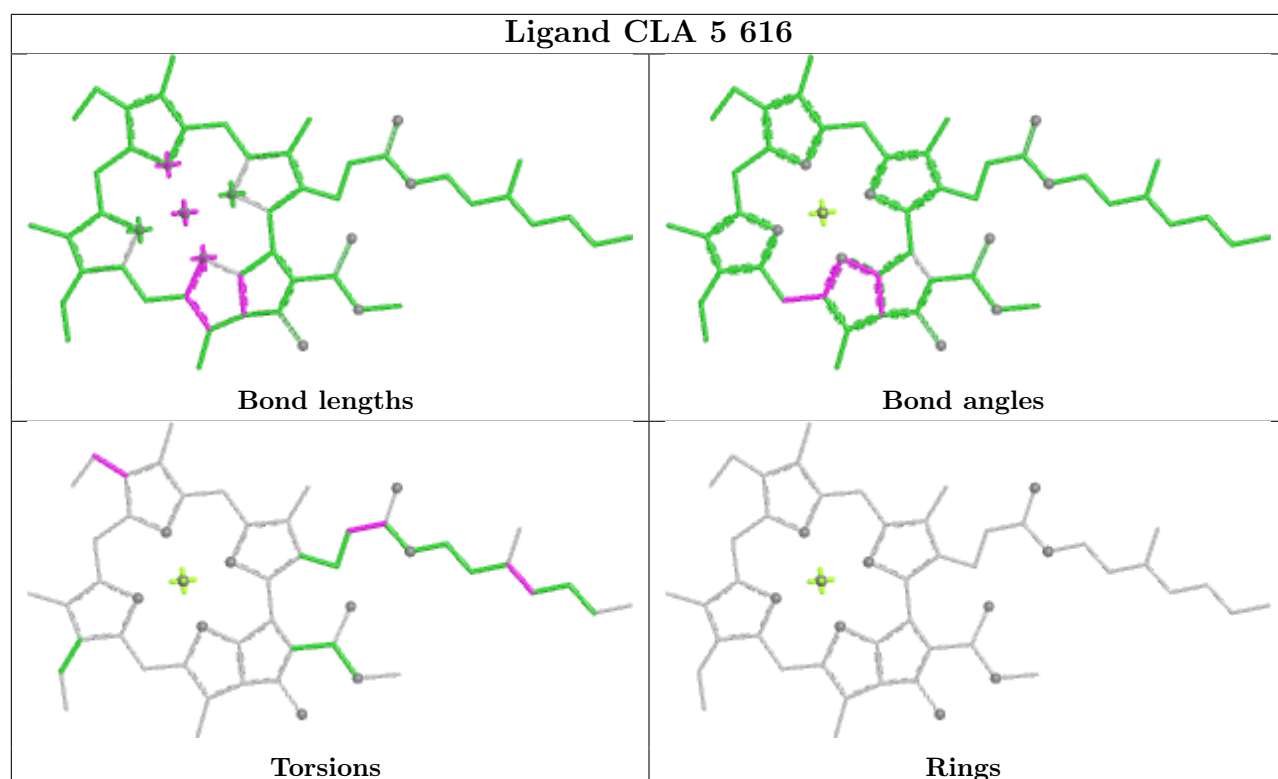
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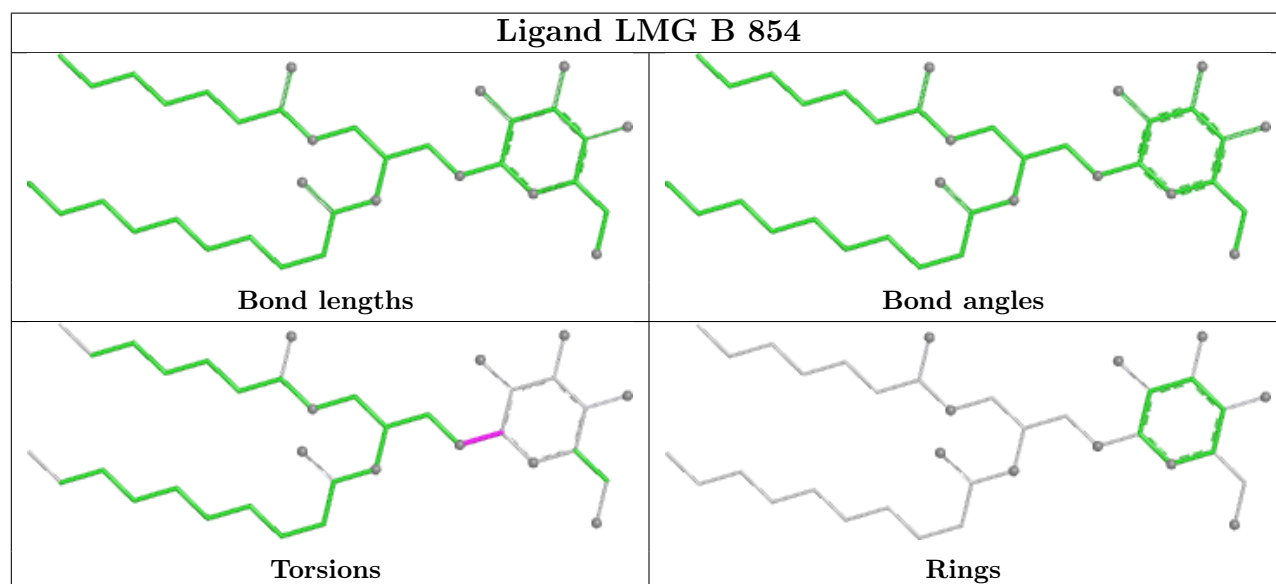
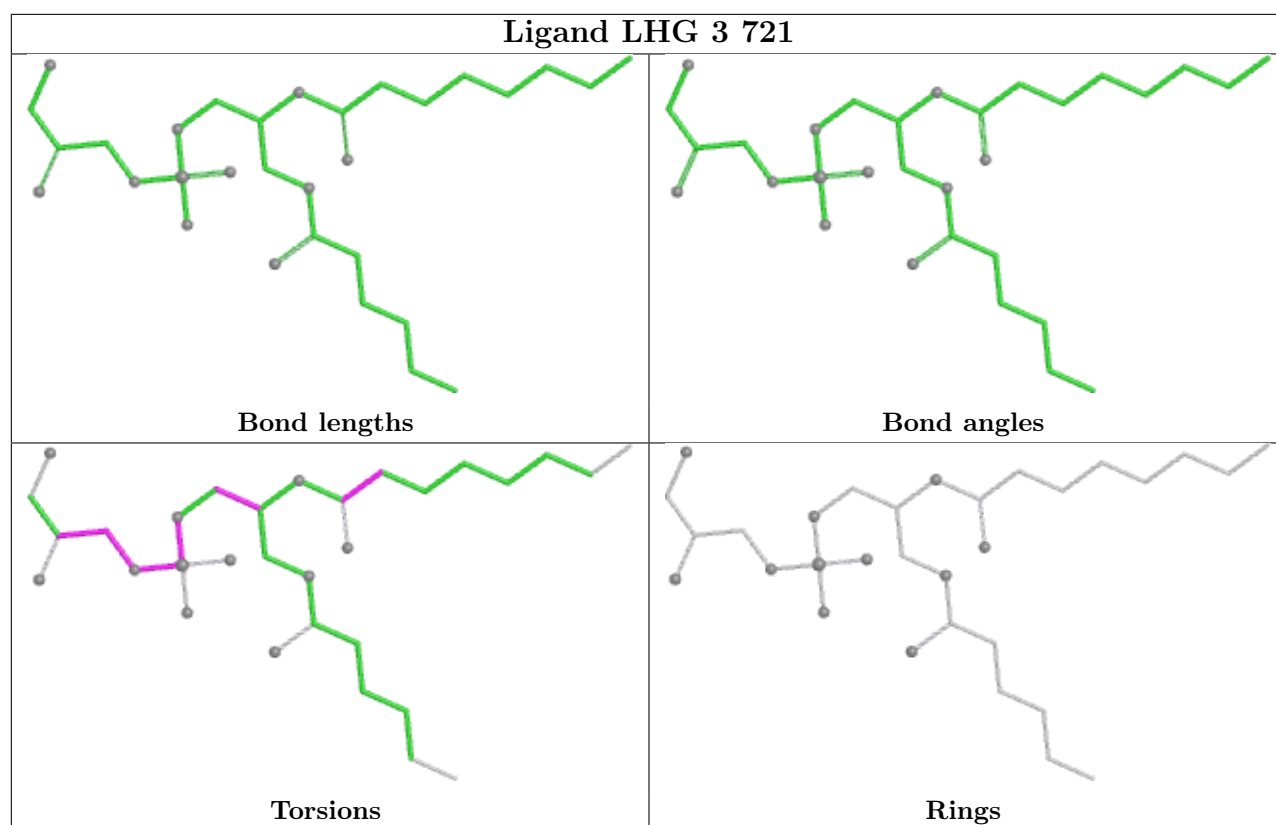


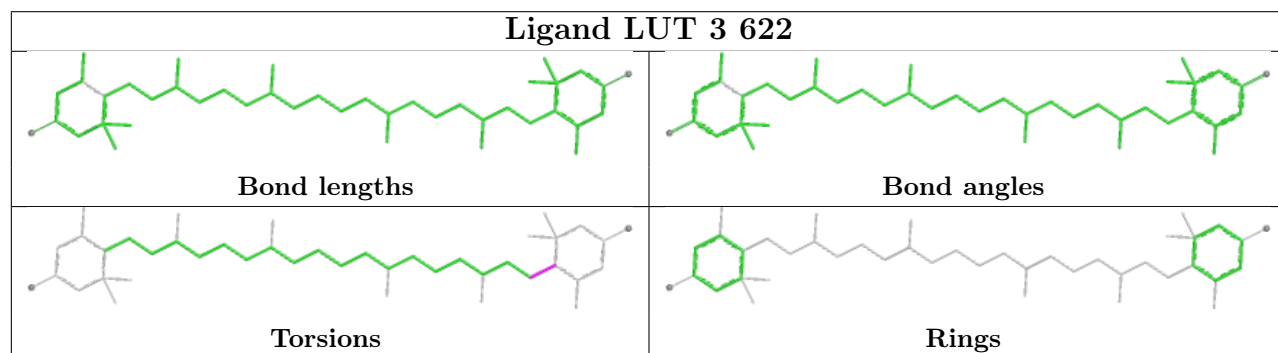
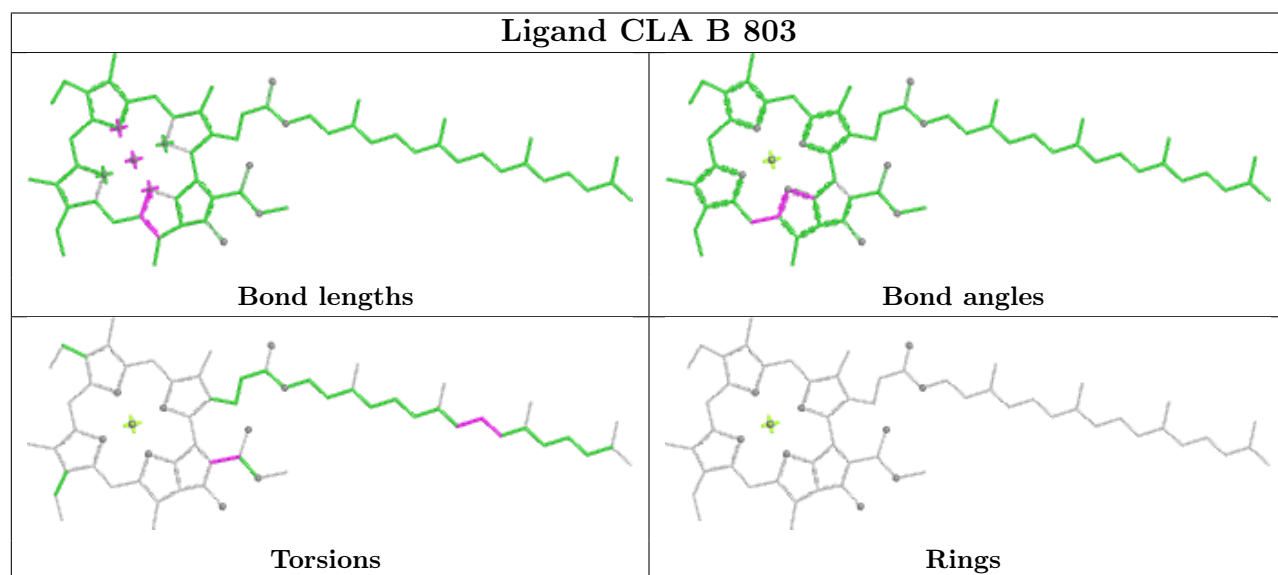
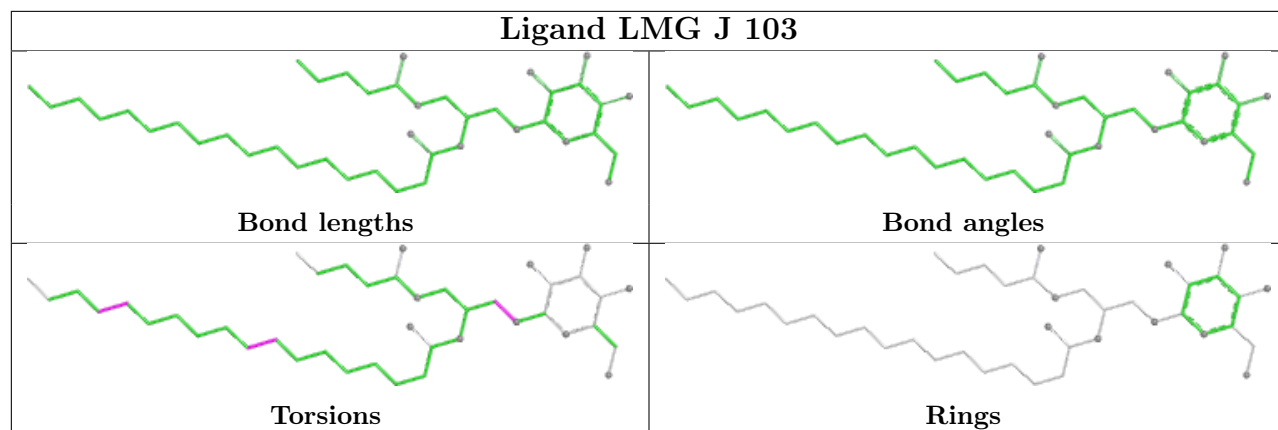


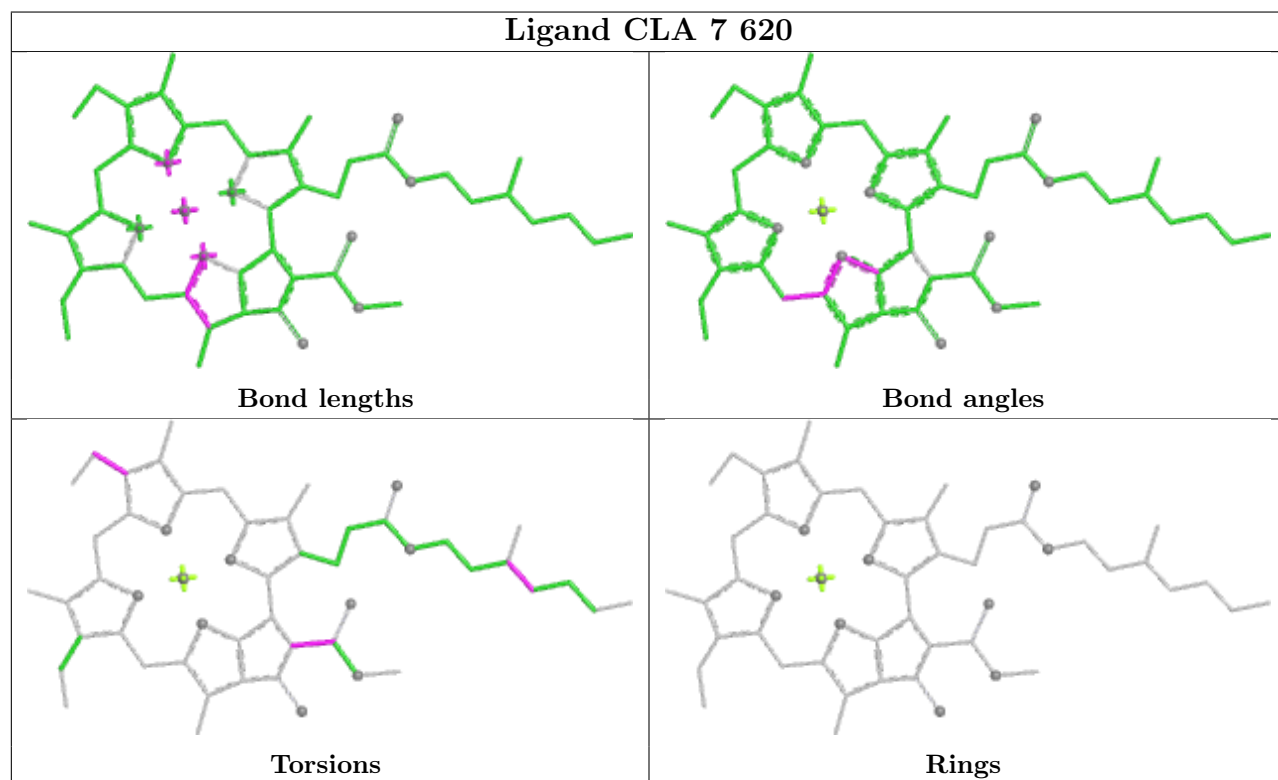
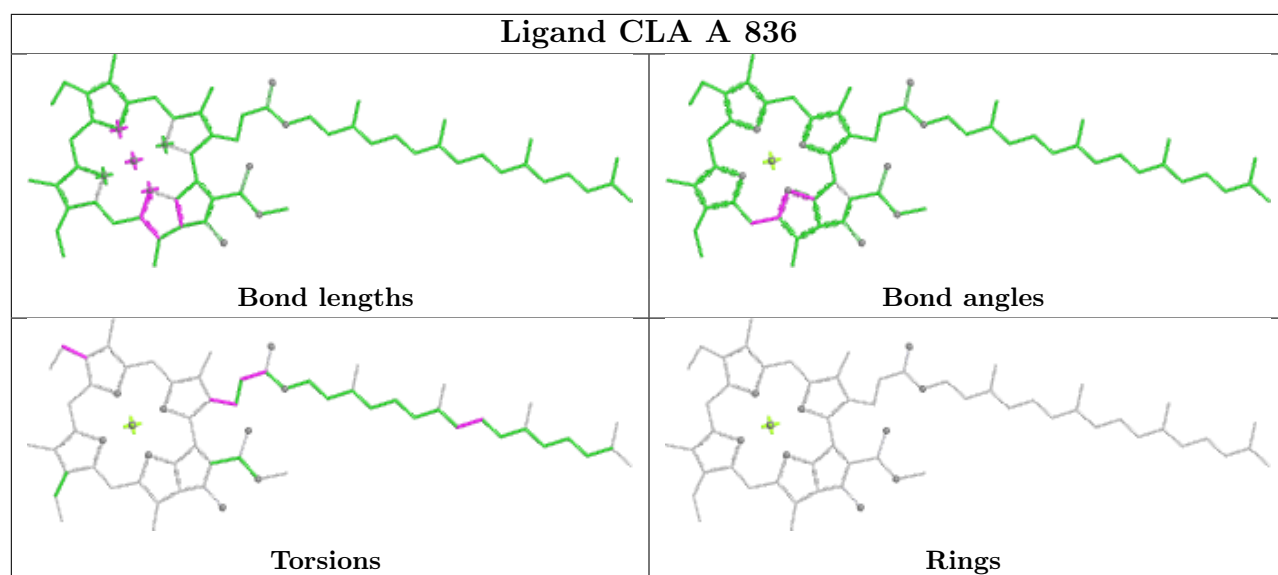


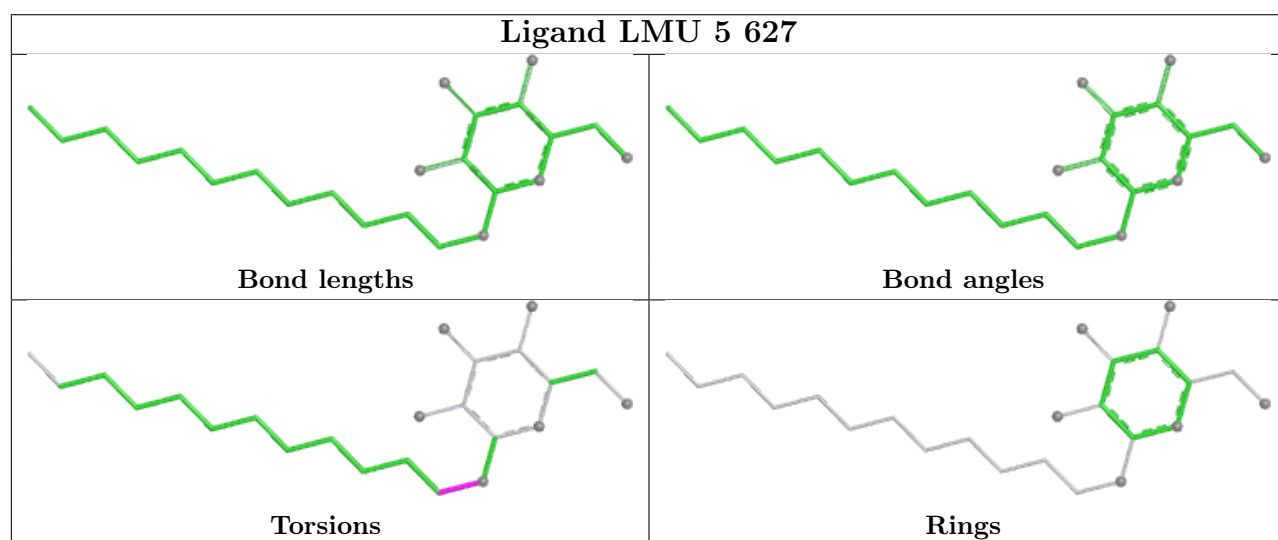
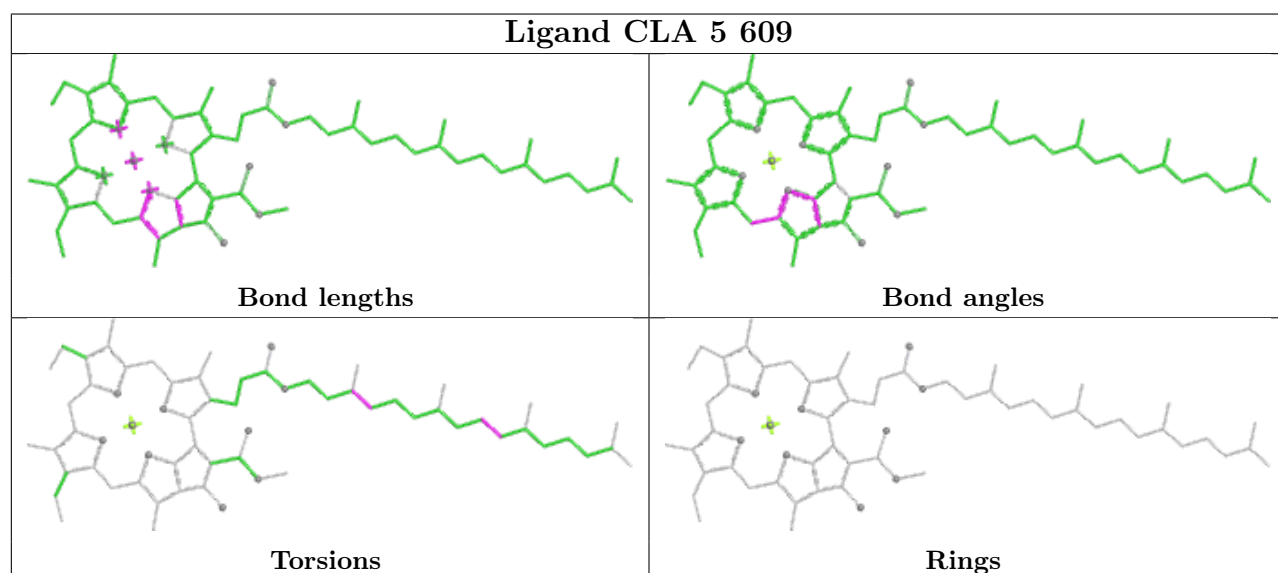
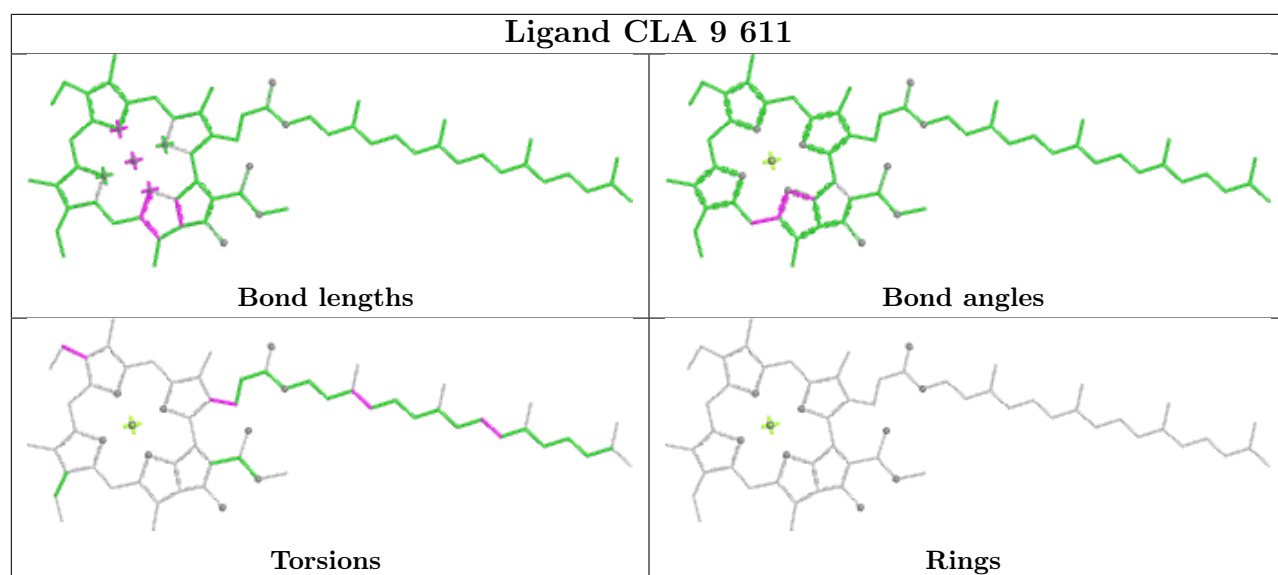


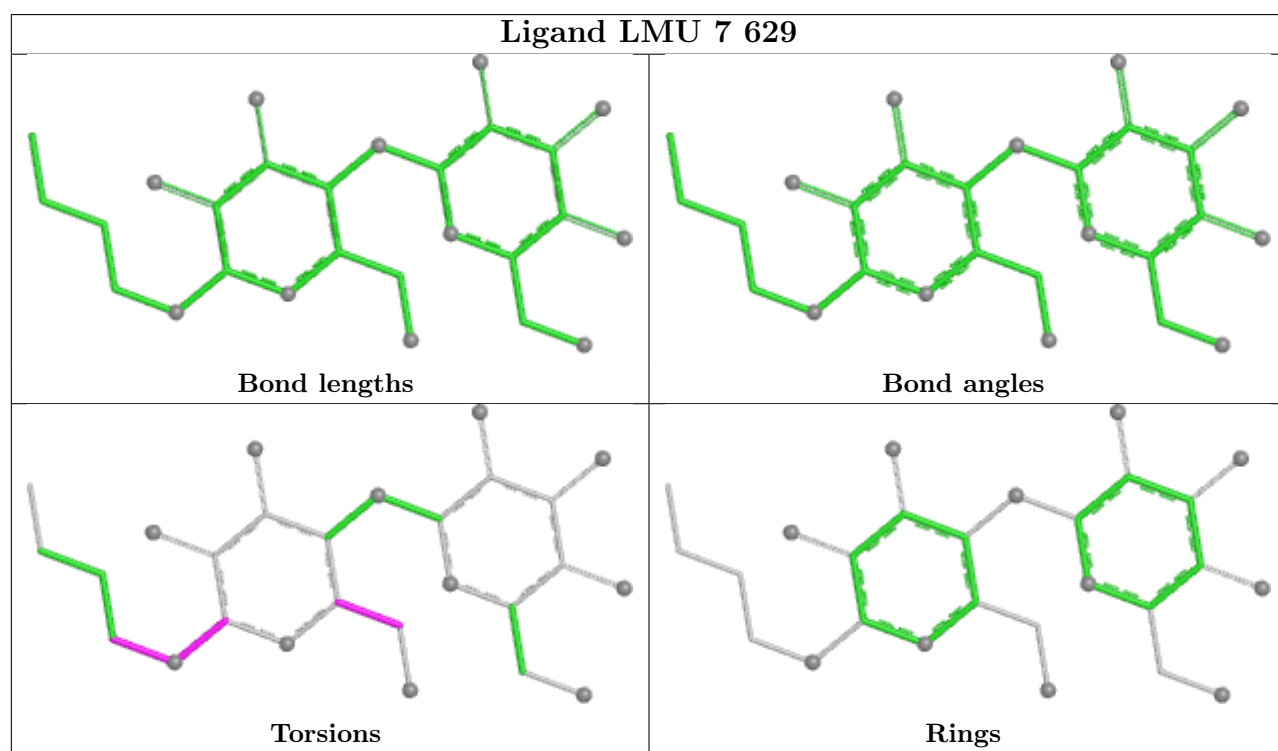
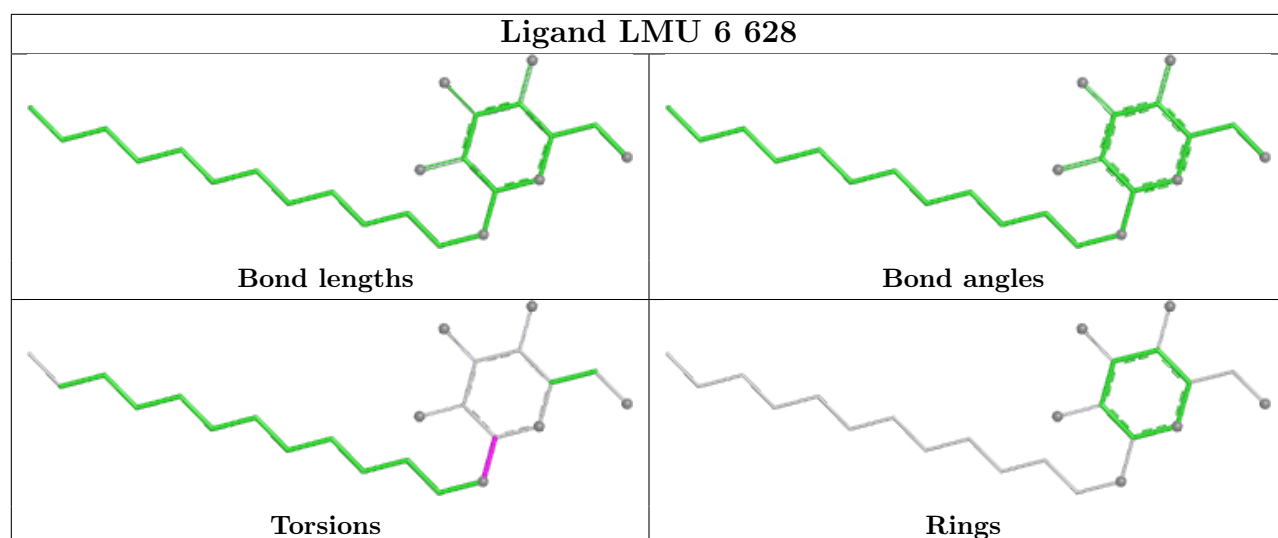


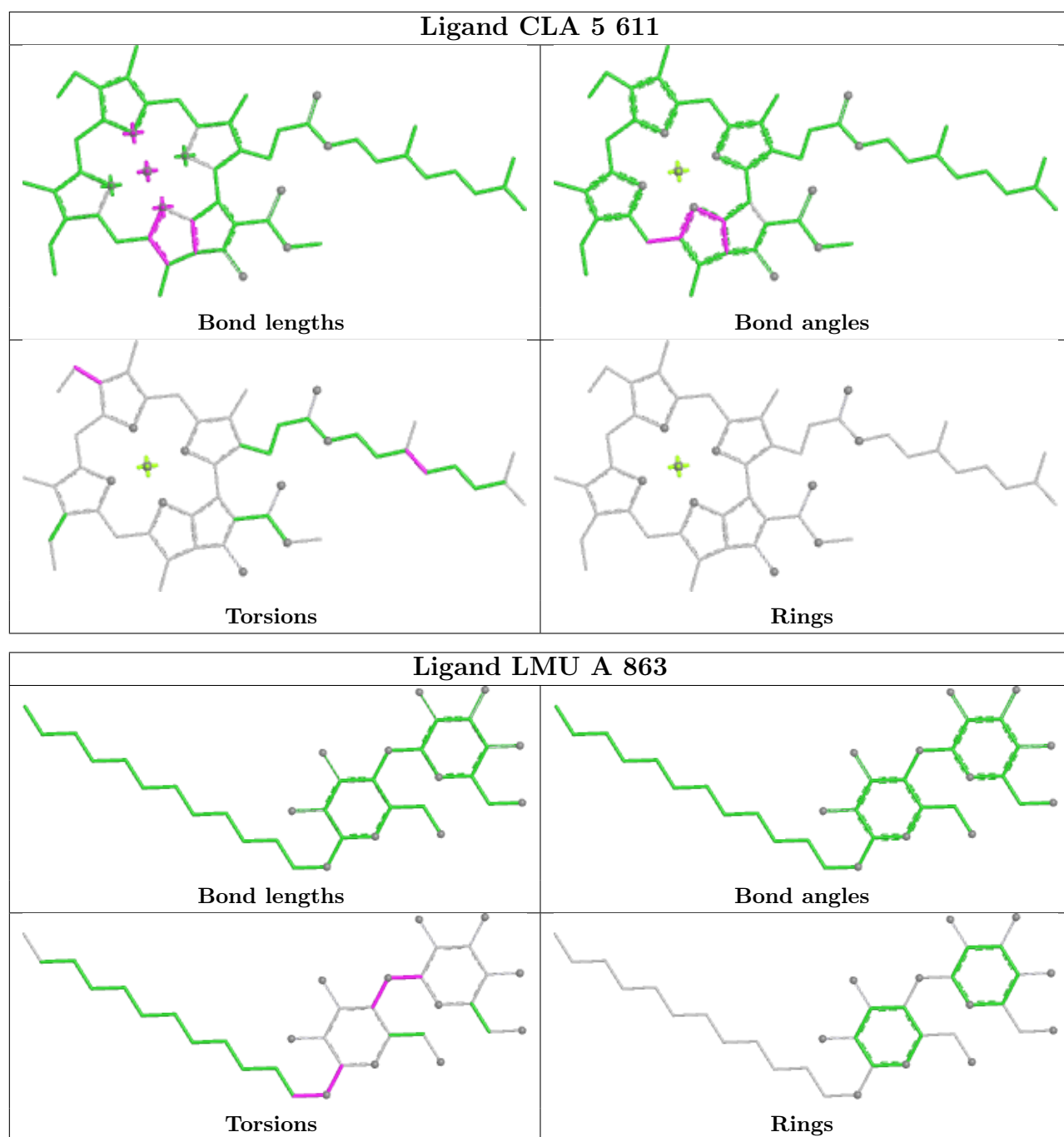


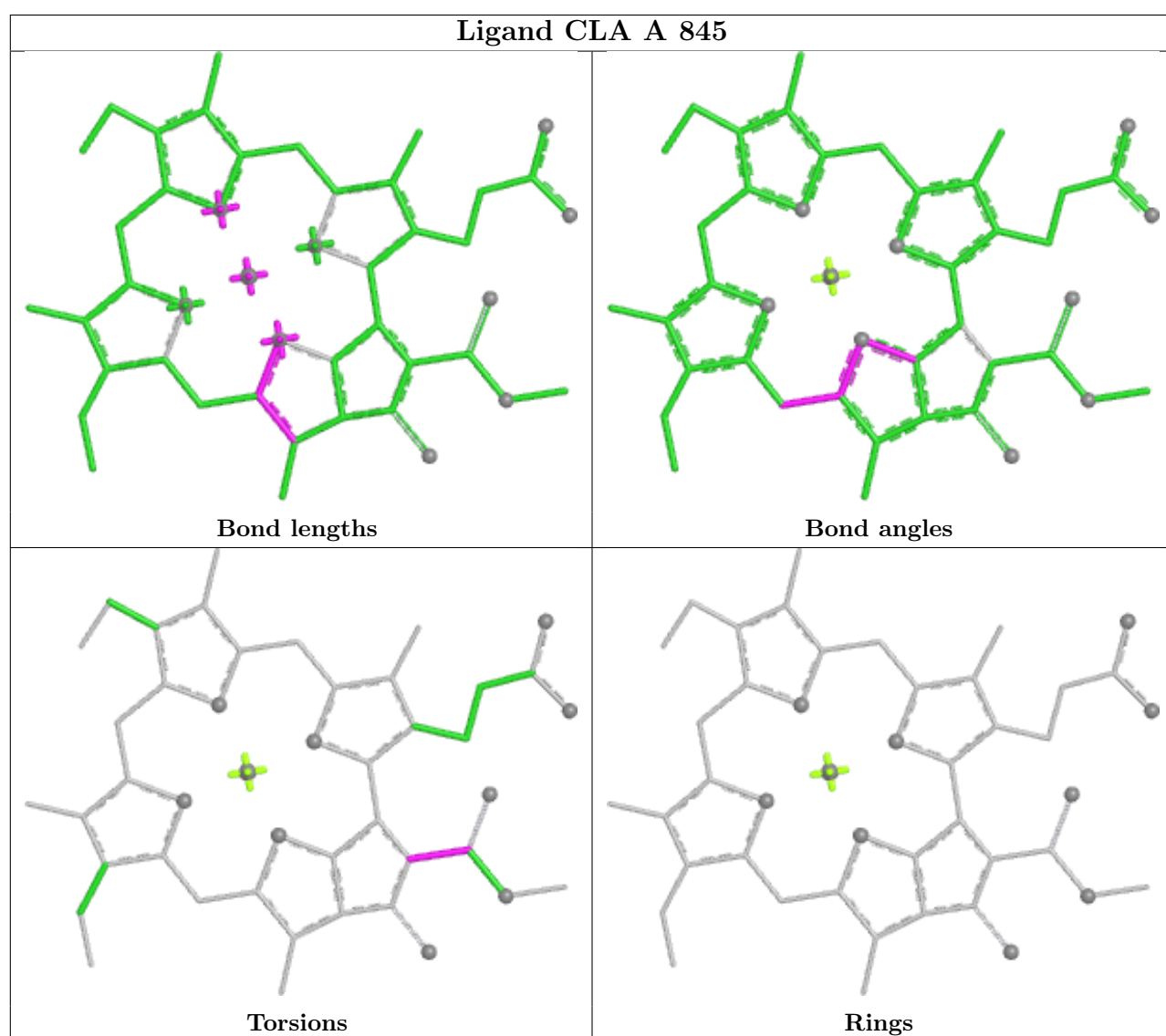
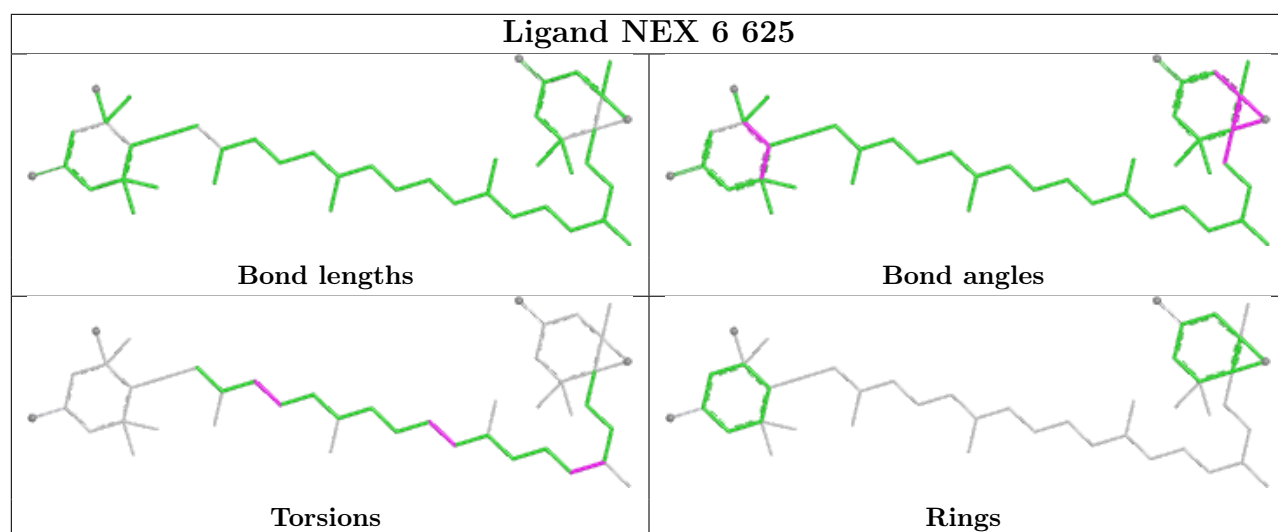


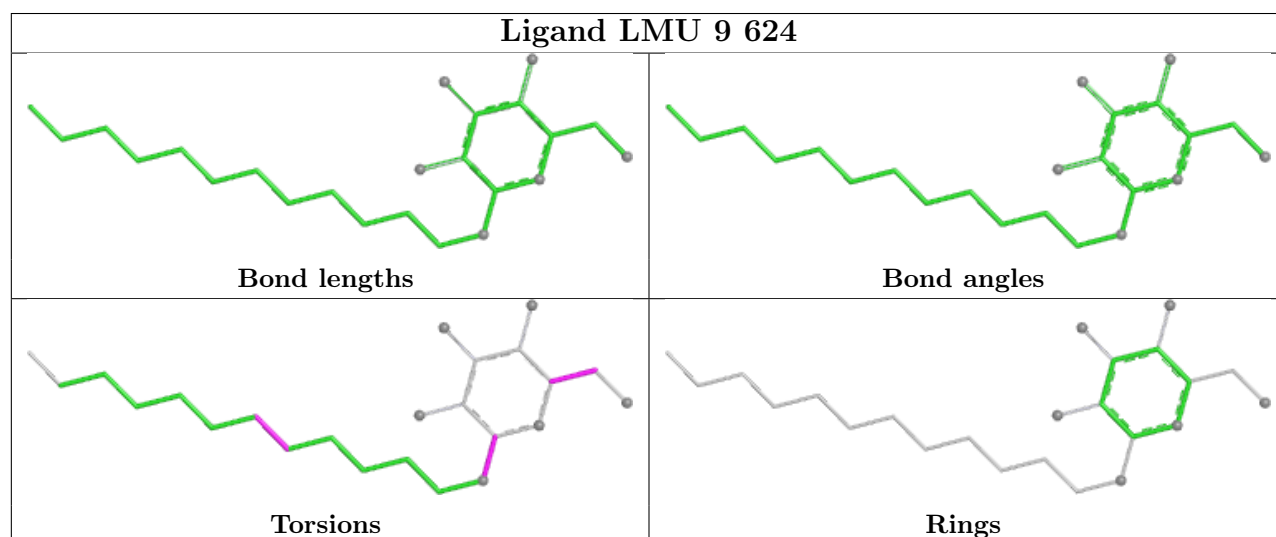
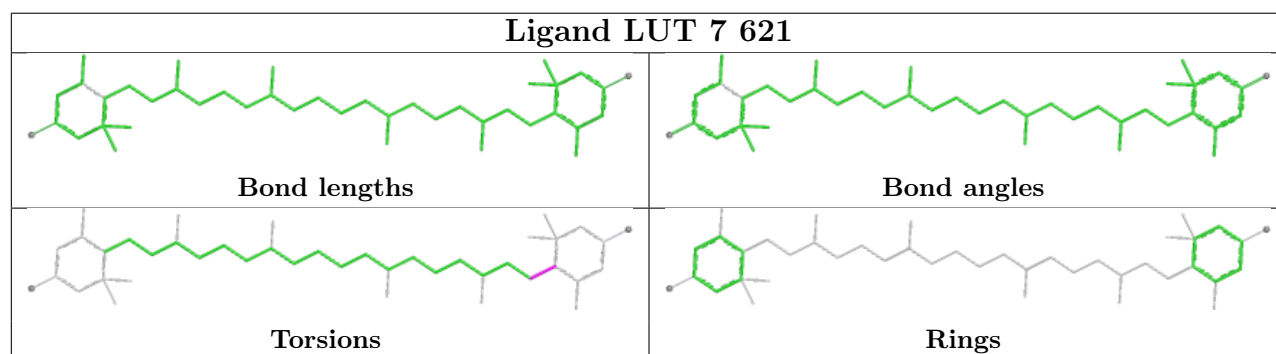
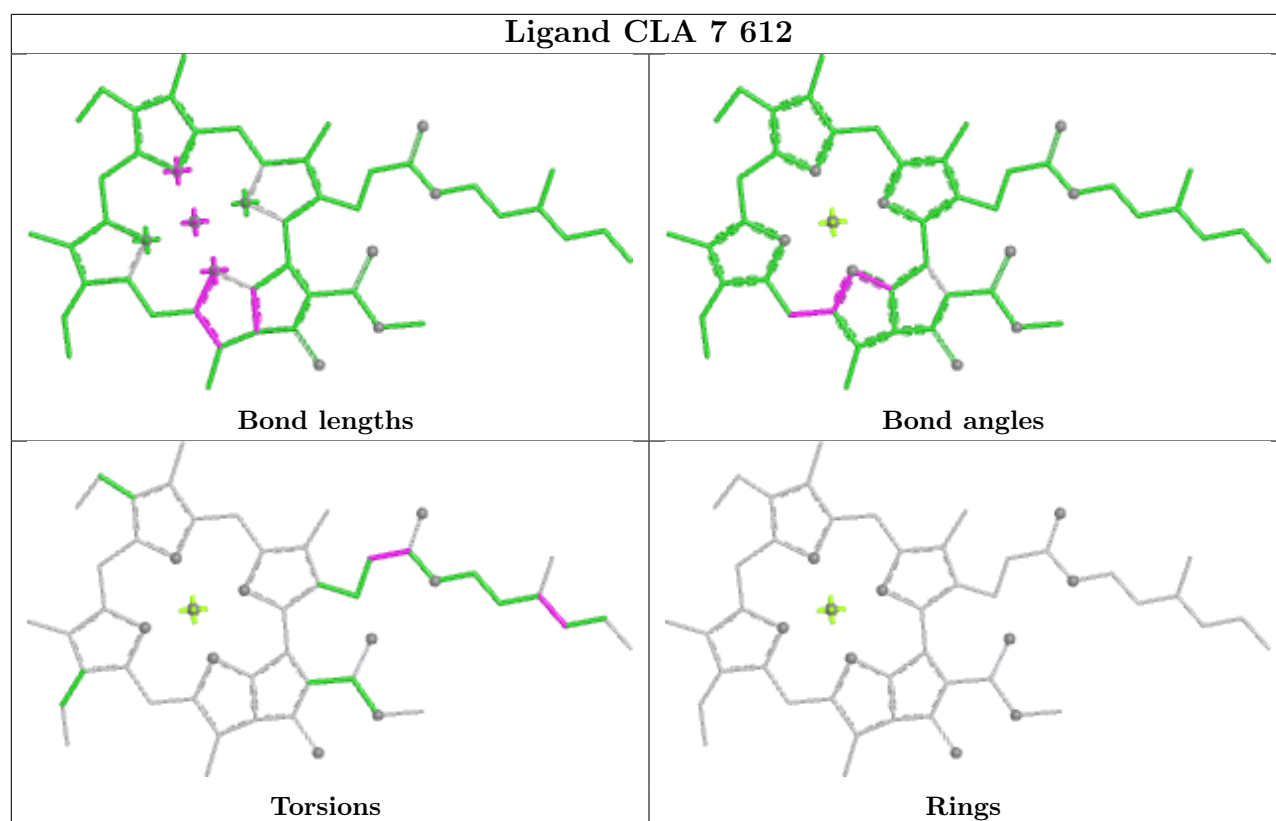


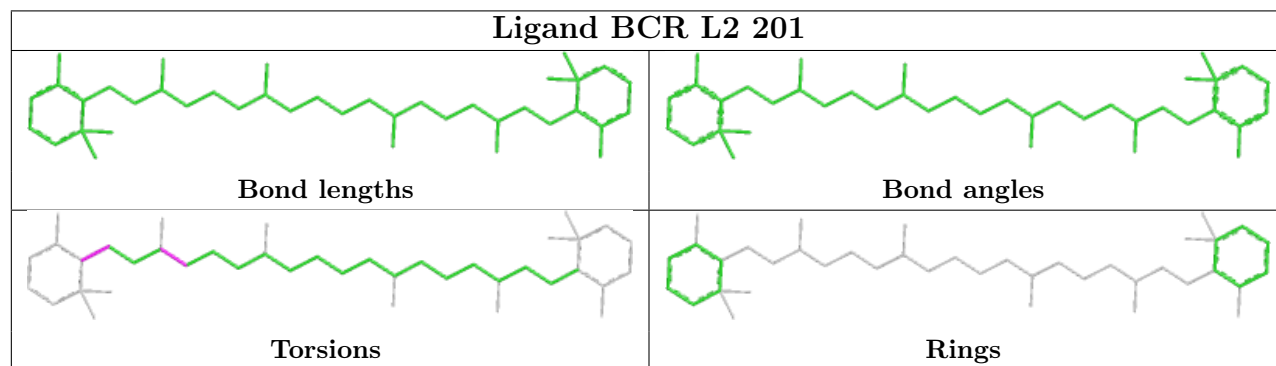
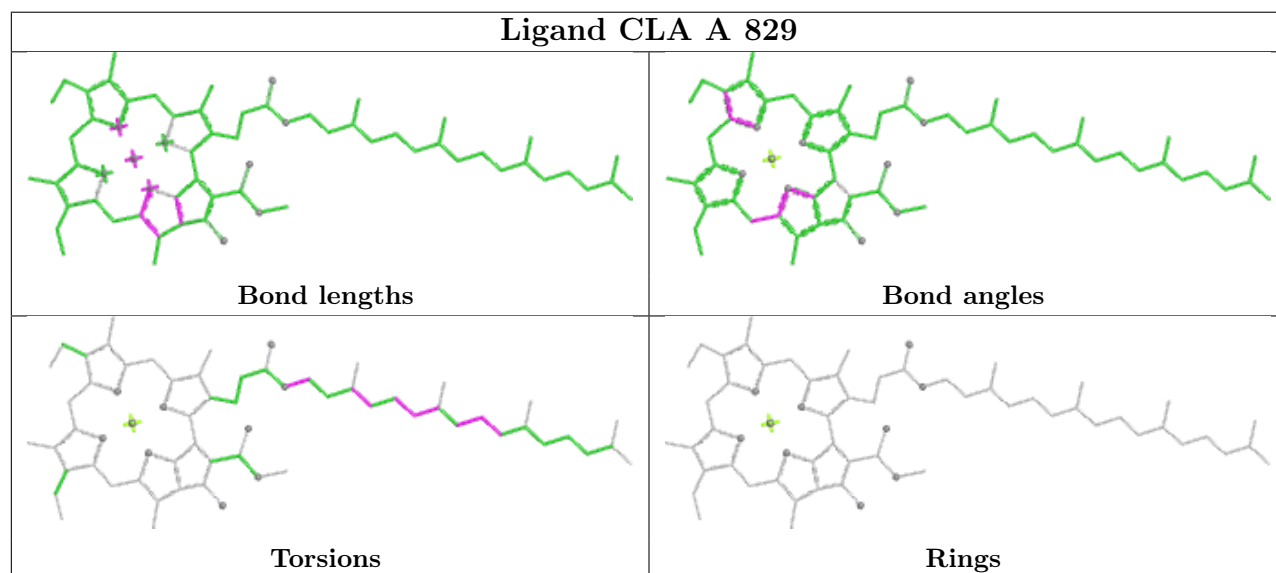
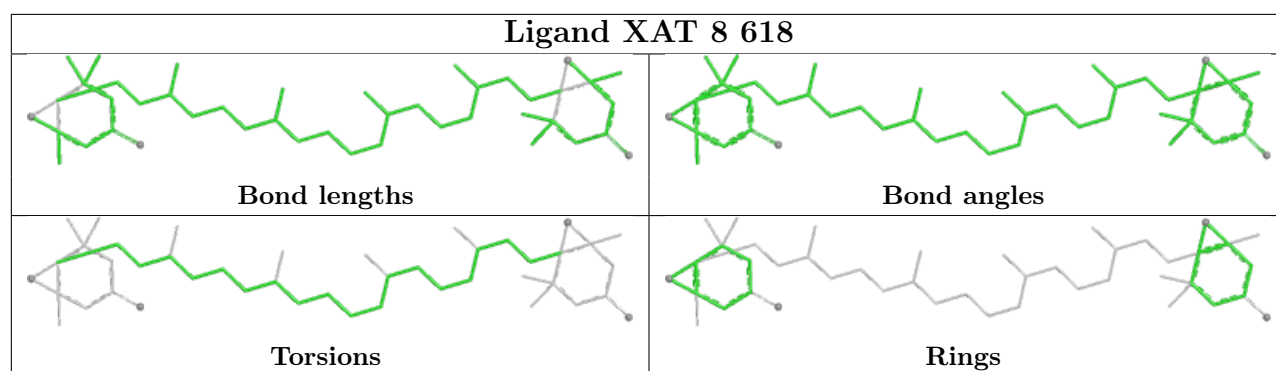


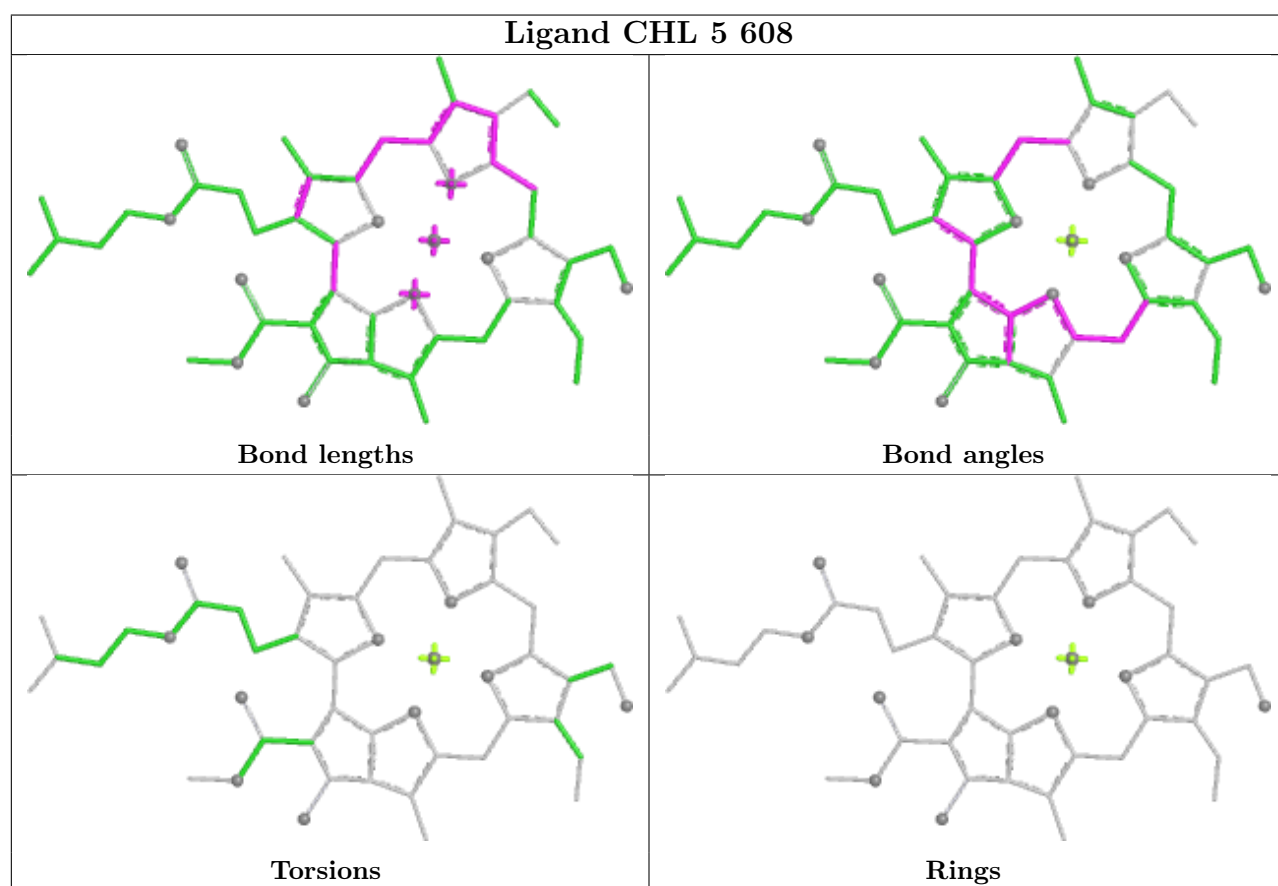
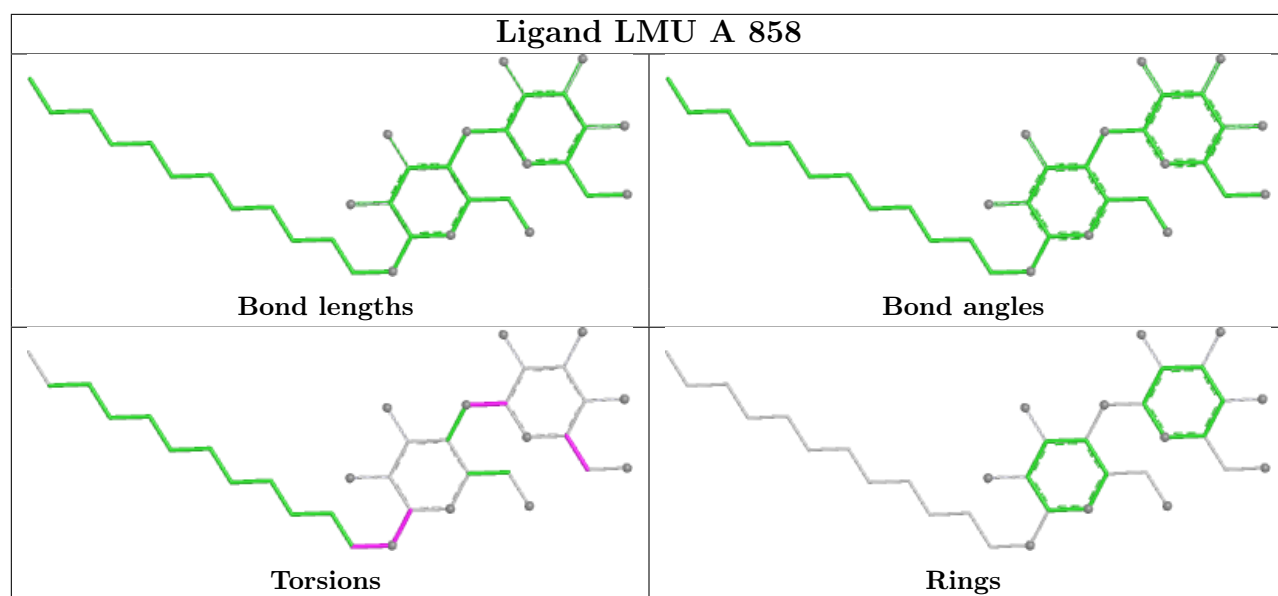


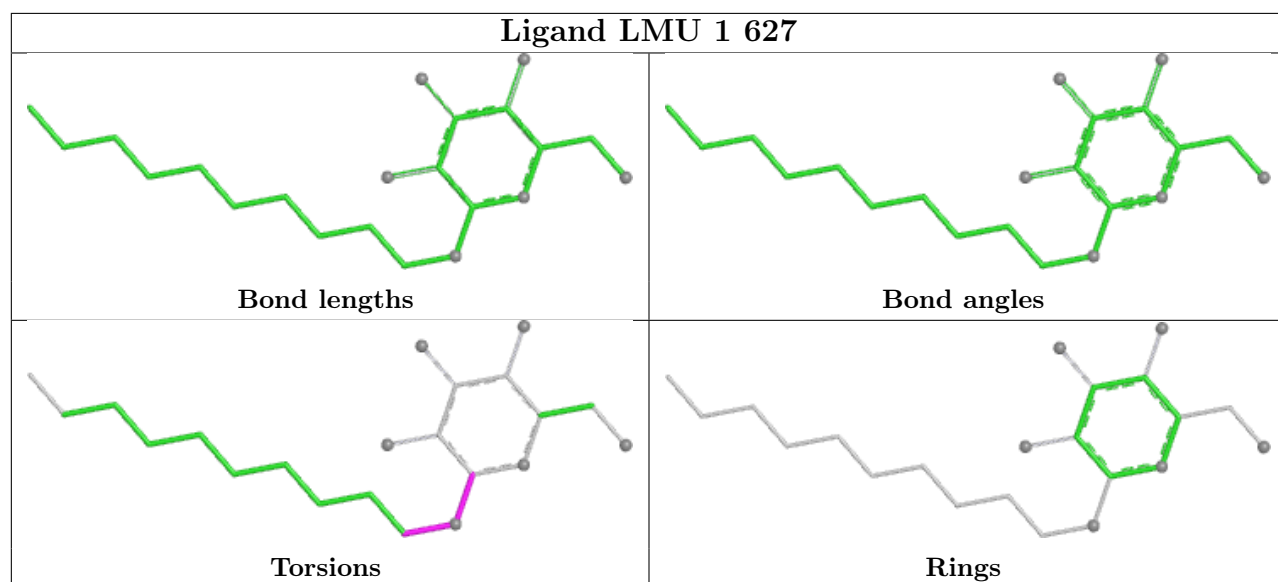
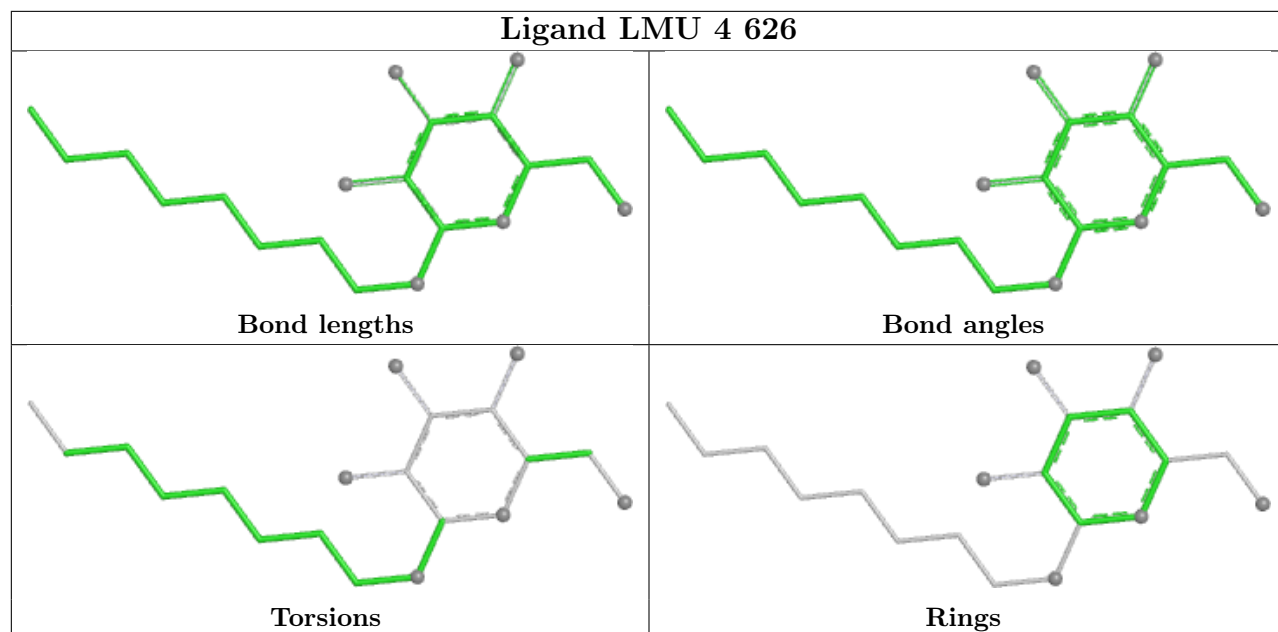


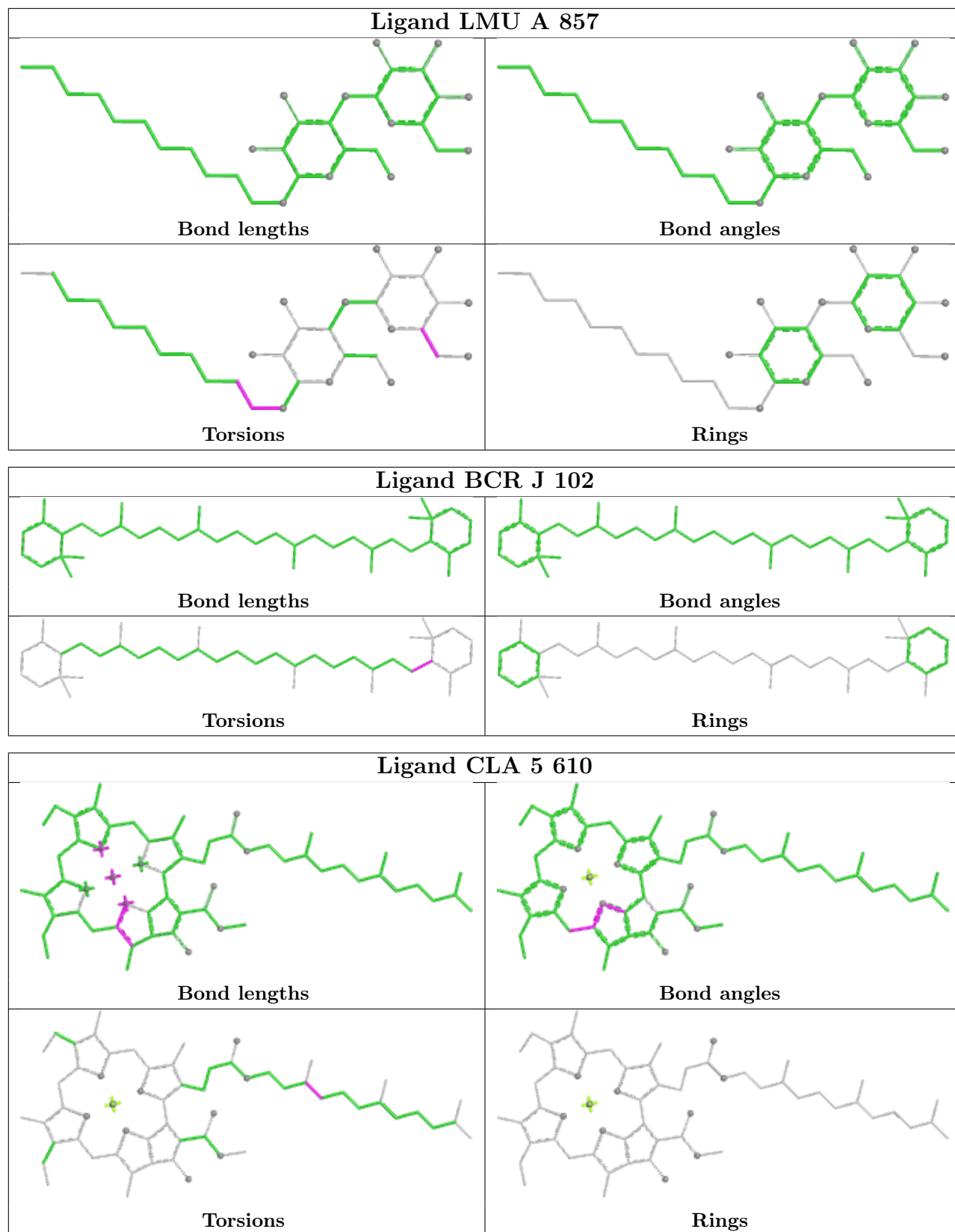


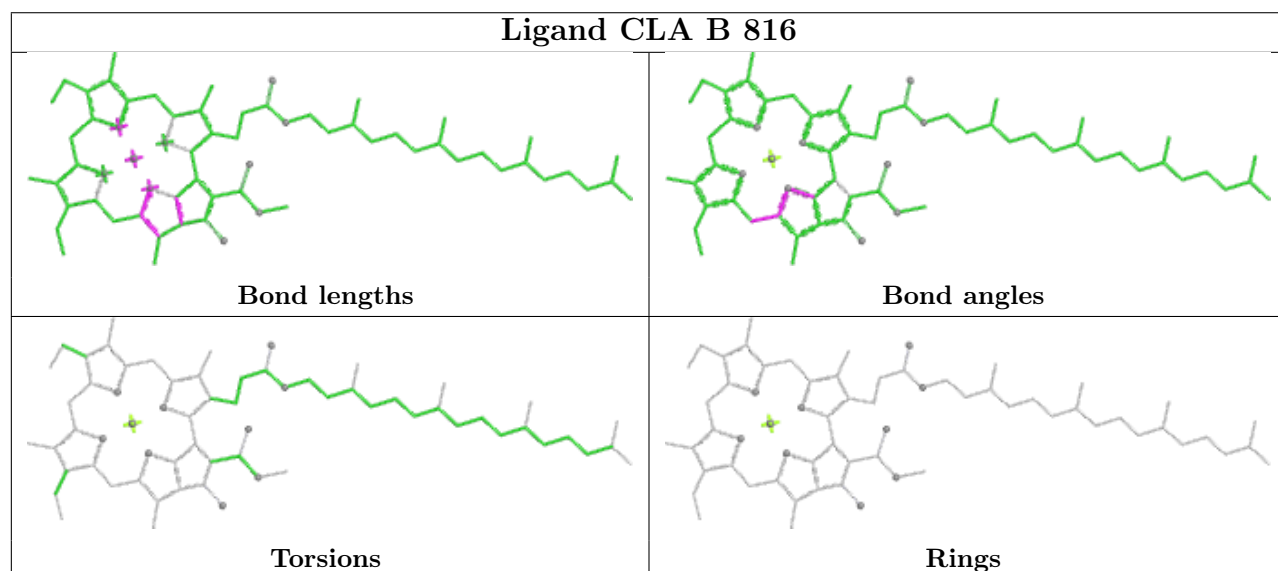
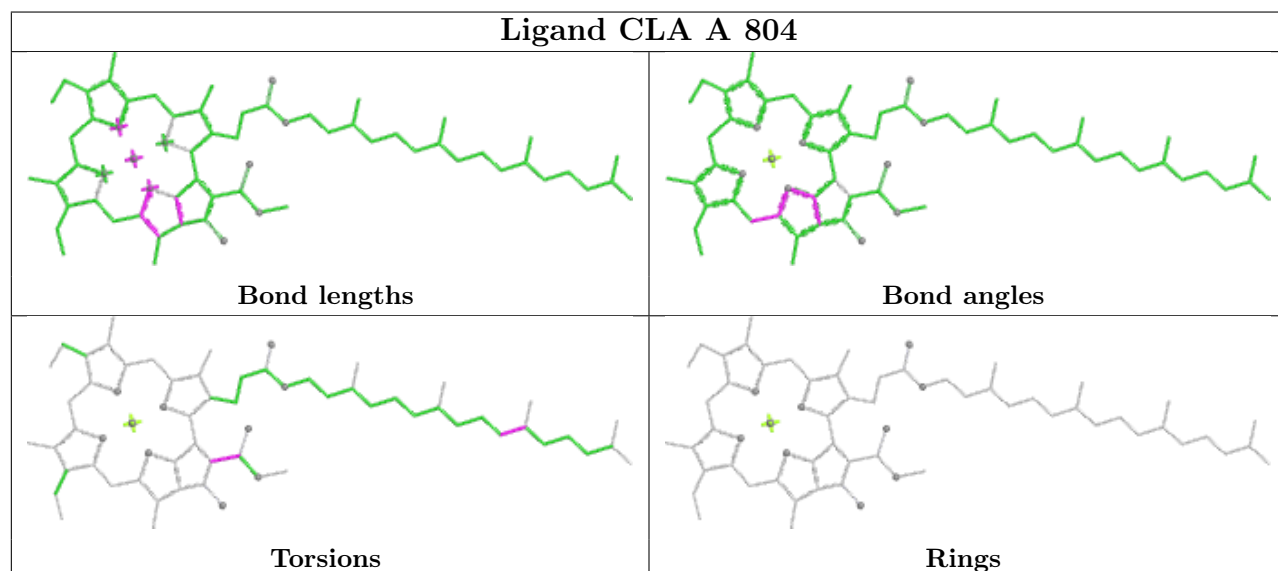
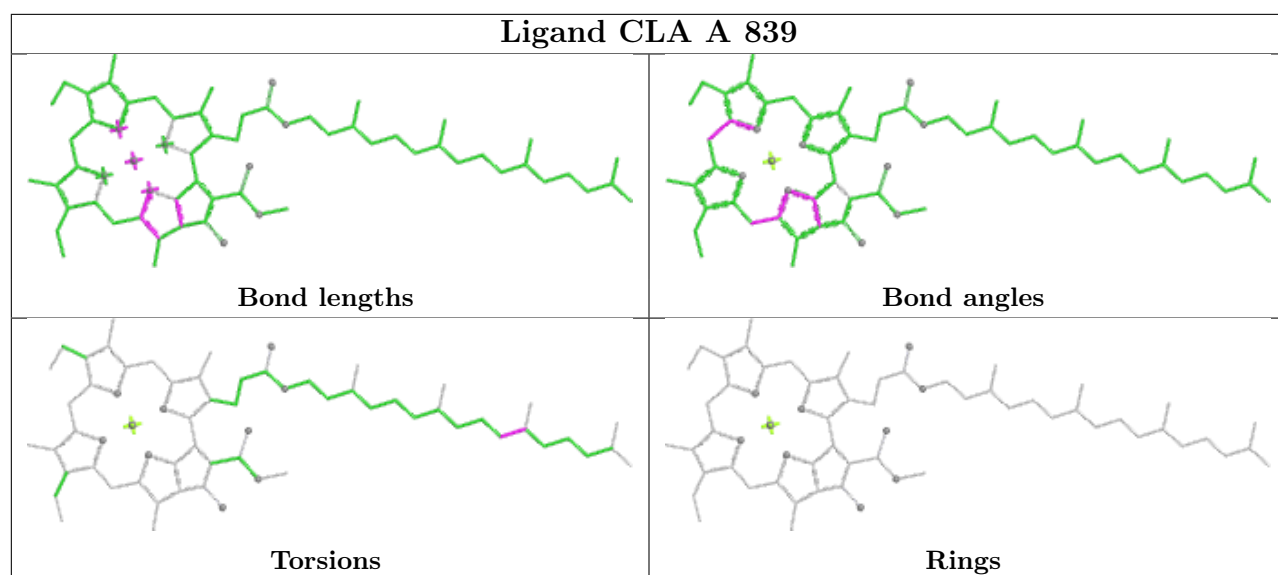


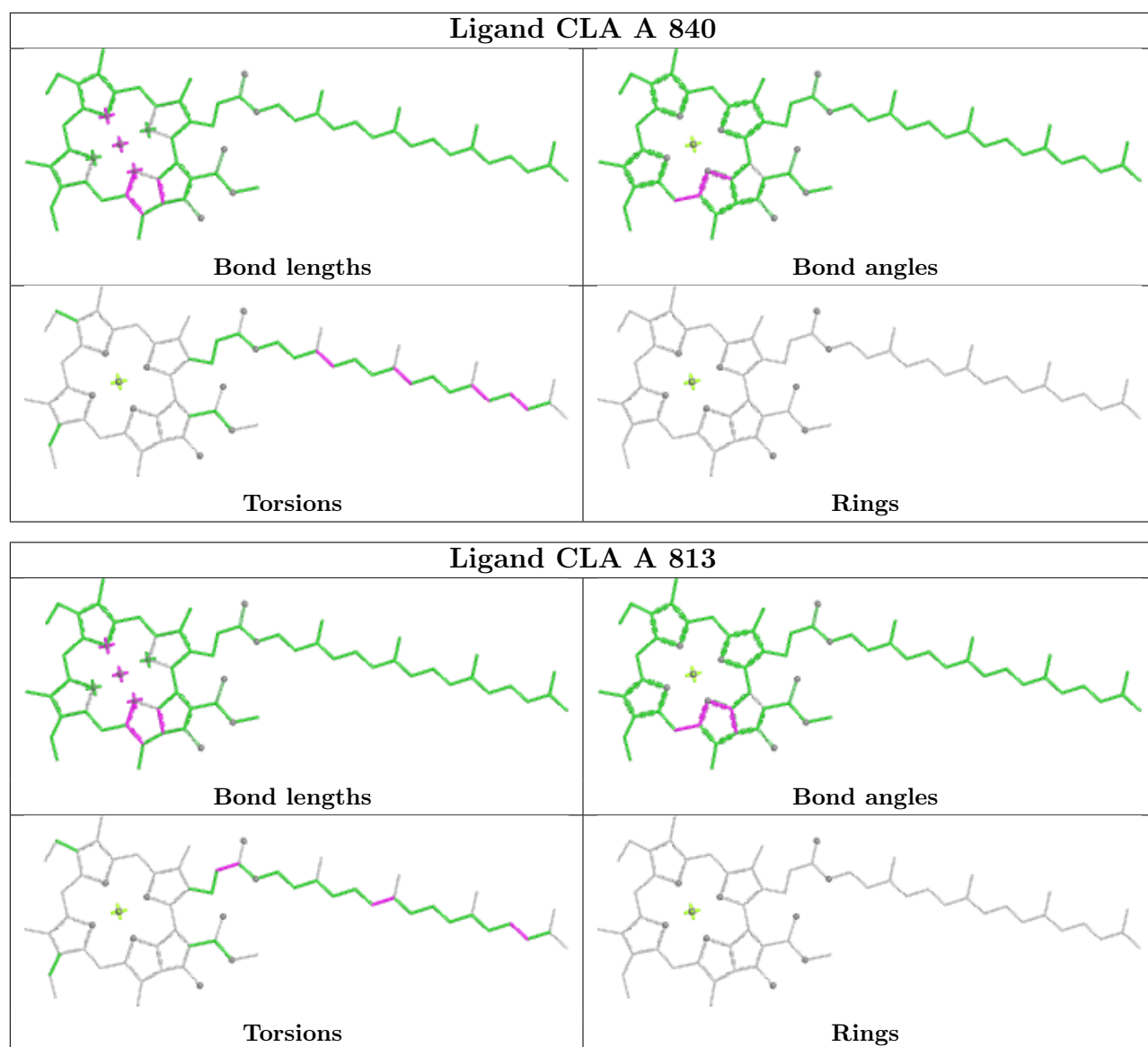




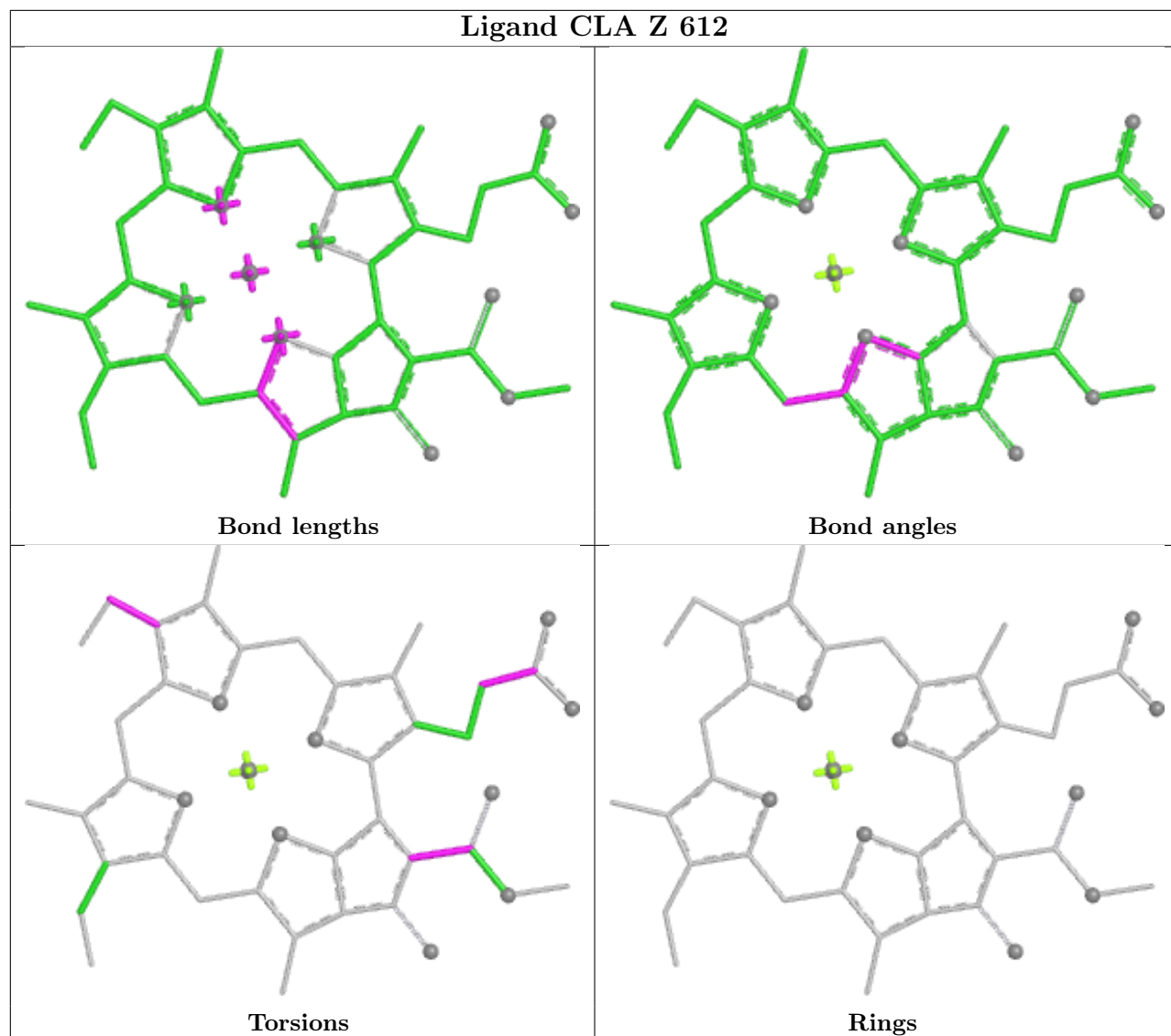




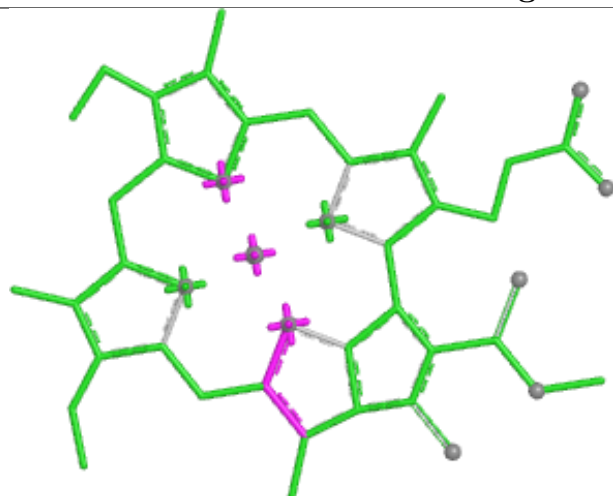




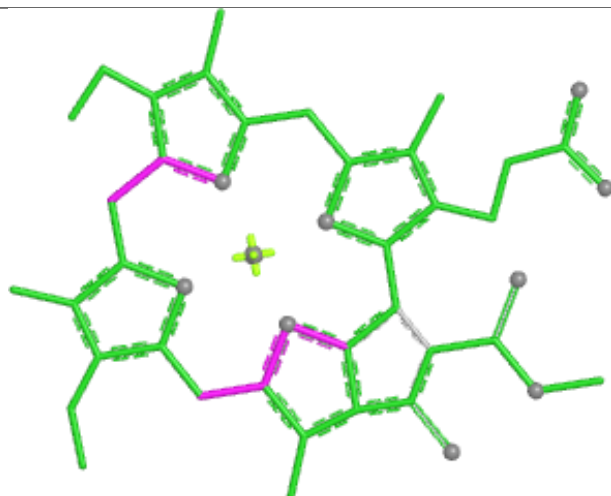
Ligand CLA Z 612



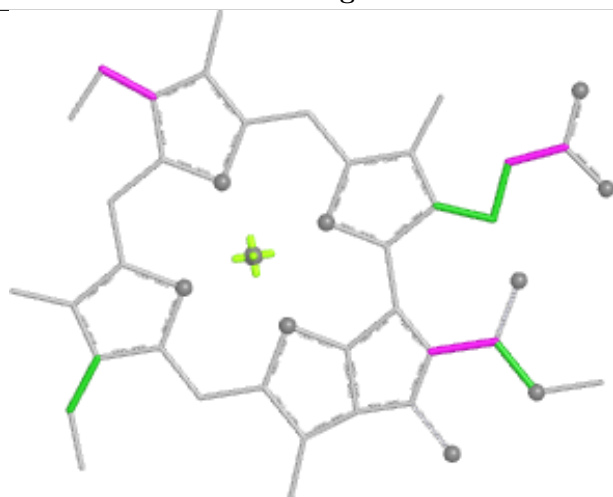
Ligand CLA 1 612



Bond lengths



Bond angles

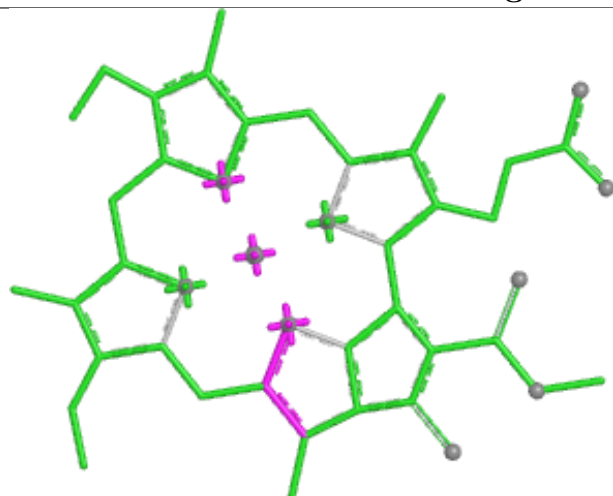


Torsions

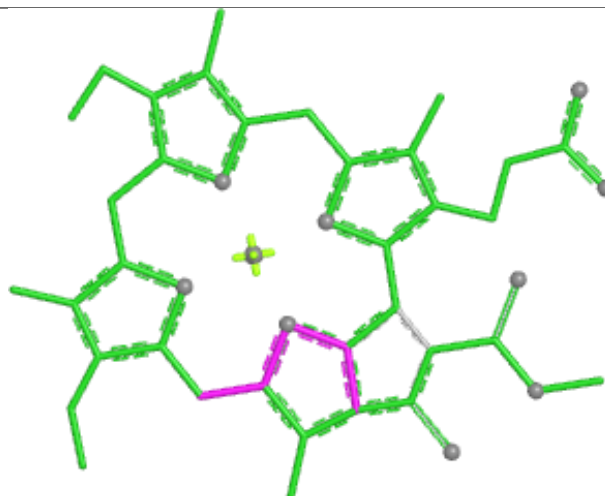


Rings

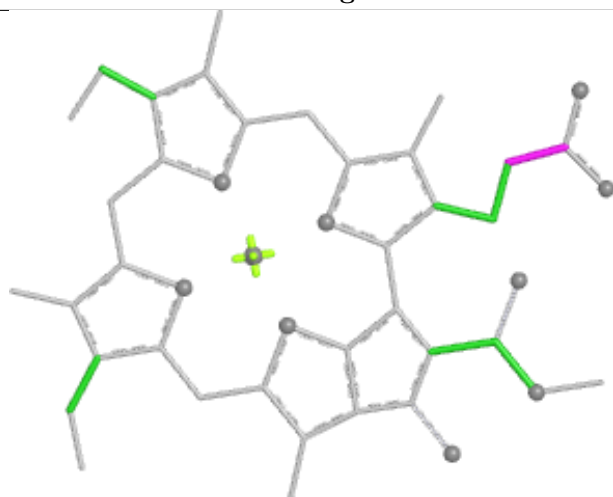
Ligand CLA B2 804



Bond lengths



Bond angles

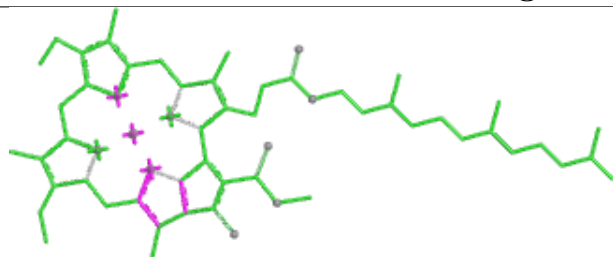


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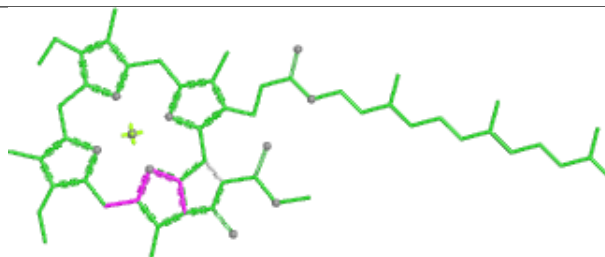


Rings

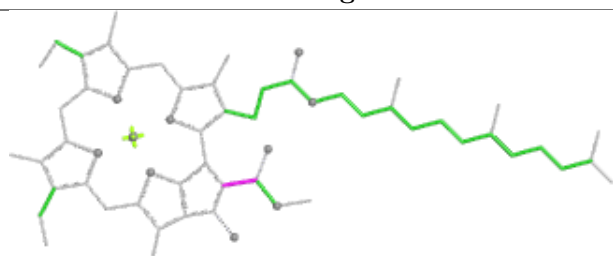
Ligand CLA 3 602



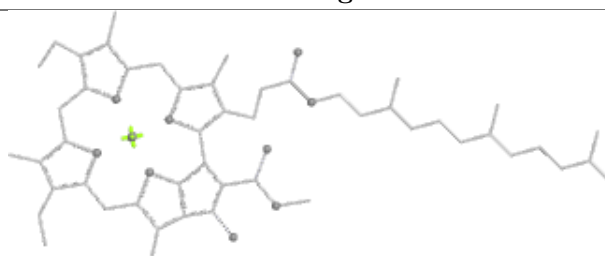
Bond lengths



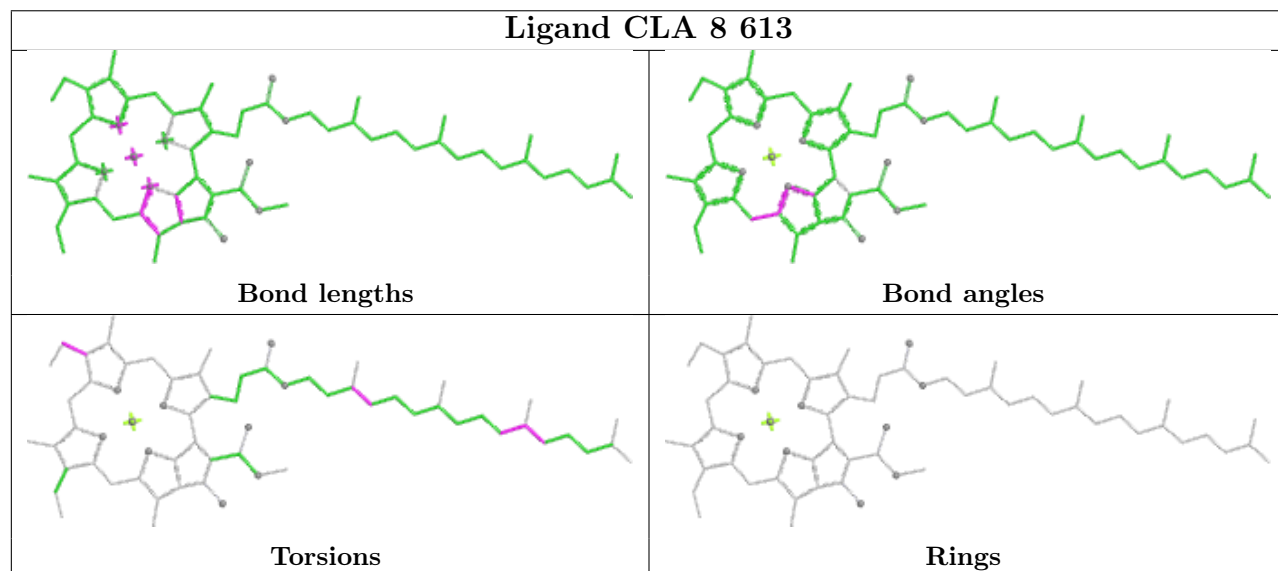
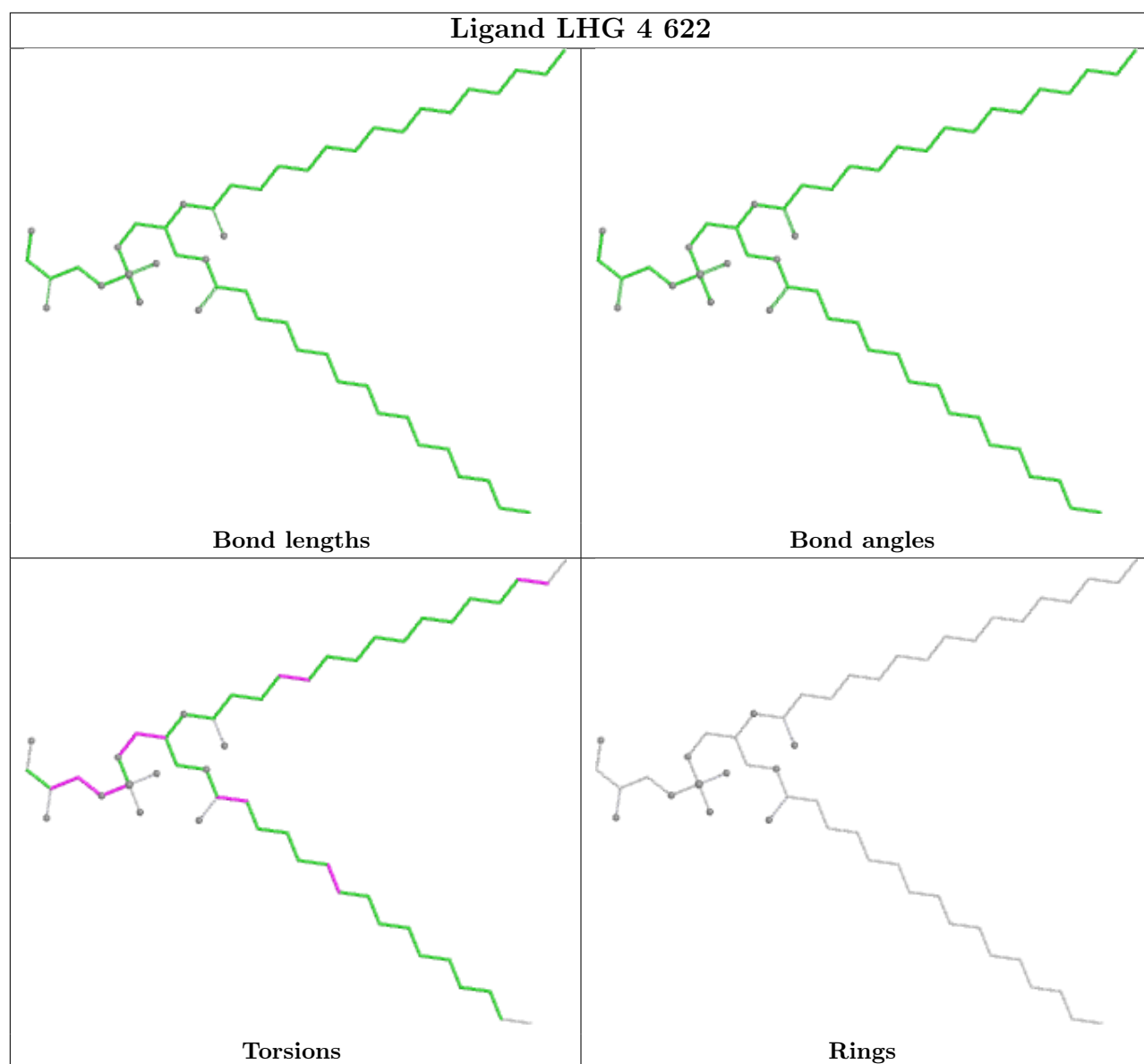
Bond angles



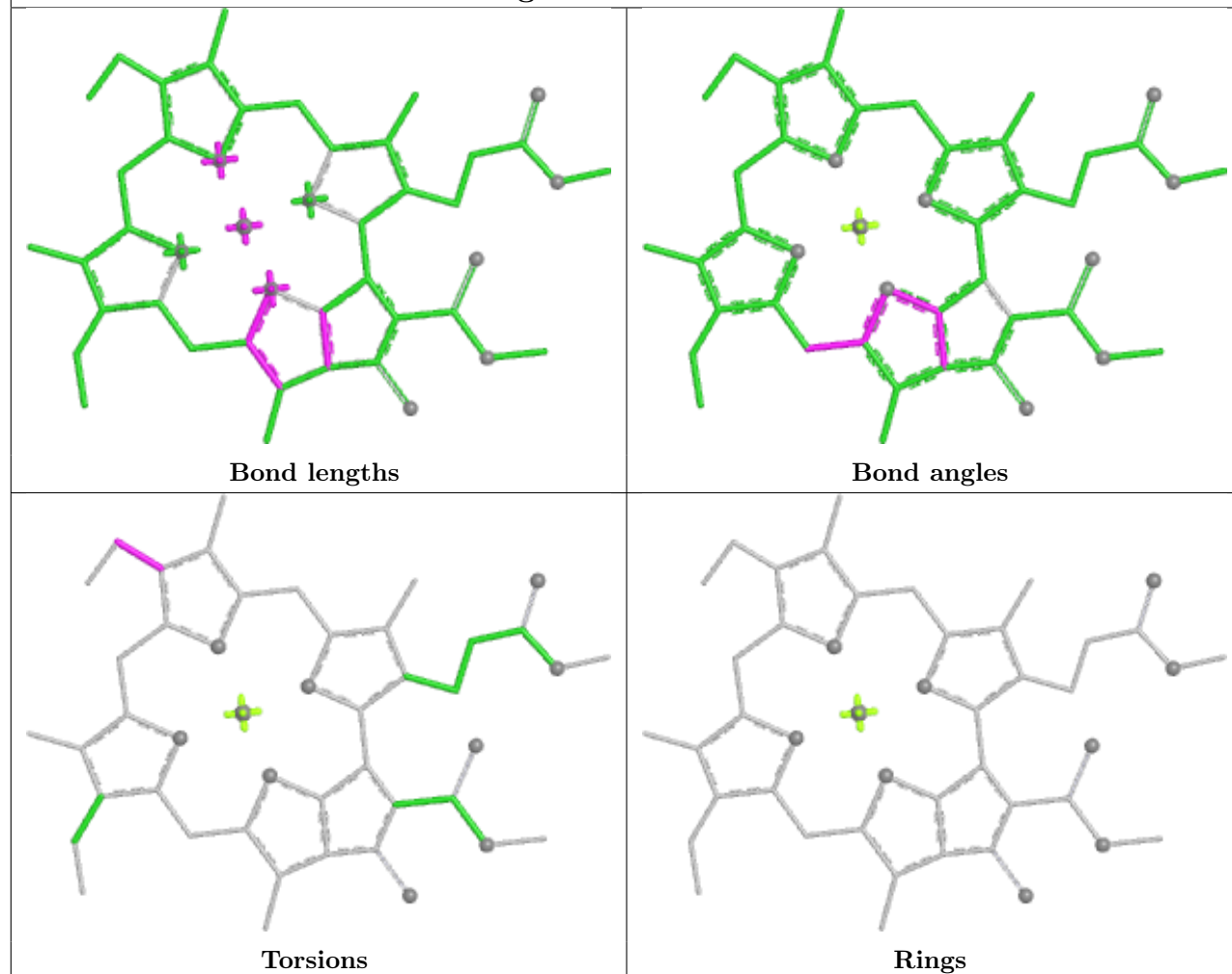
Torsions



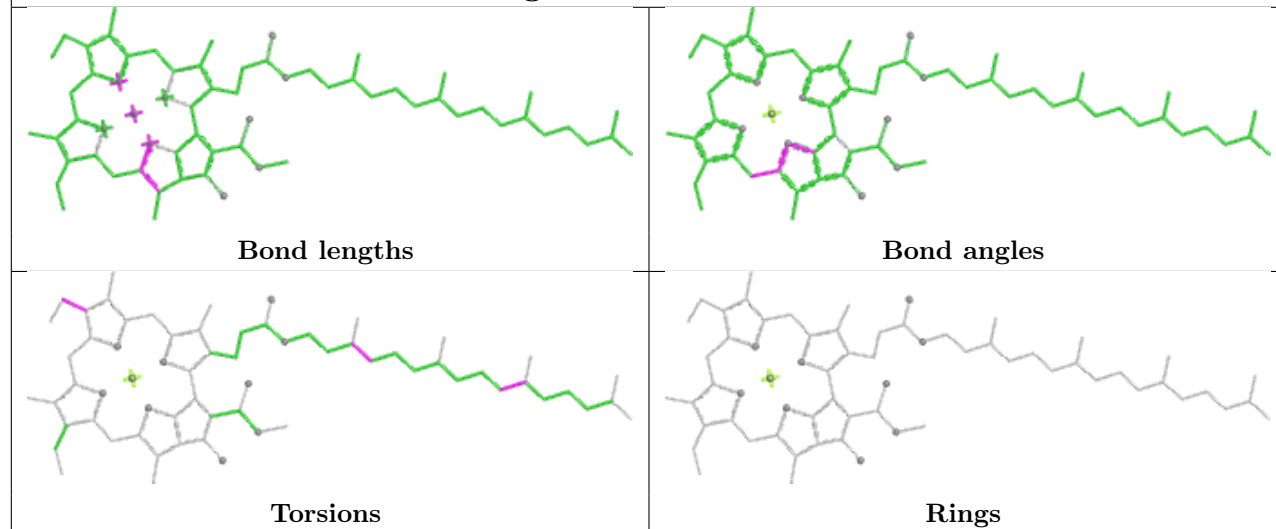
Rings

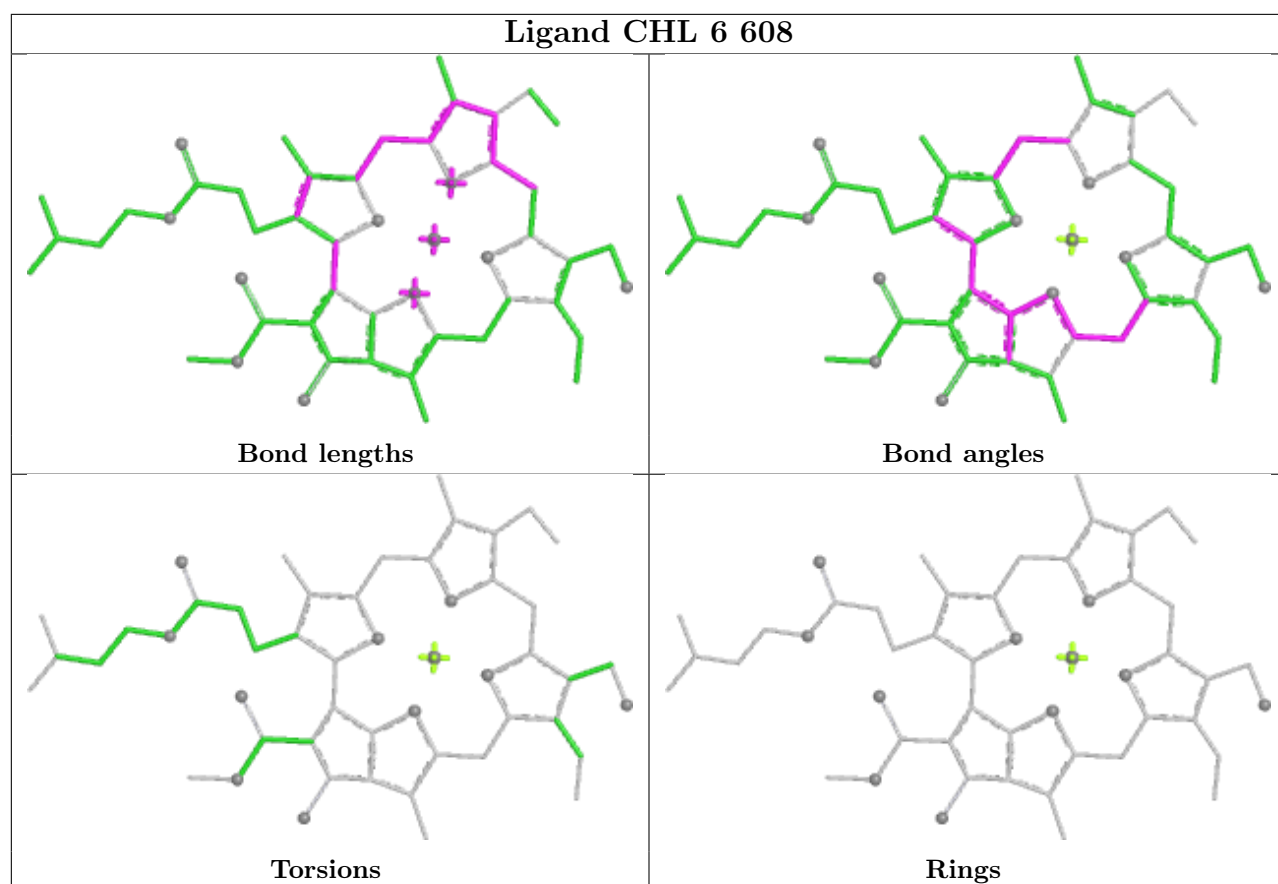


Ligand CLA 1 616

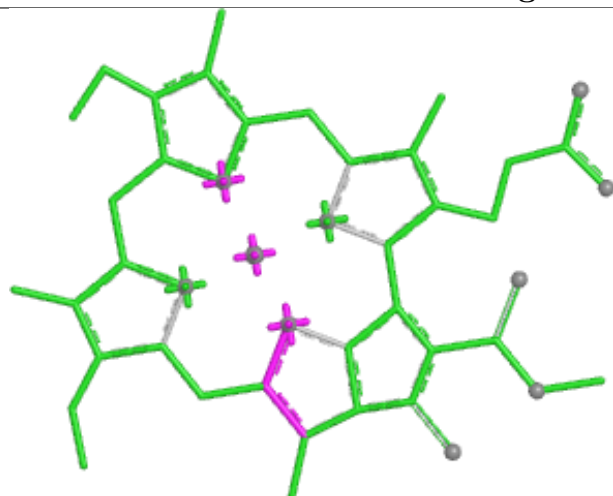


Ligand CLA B2 806

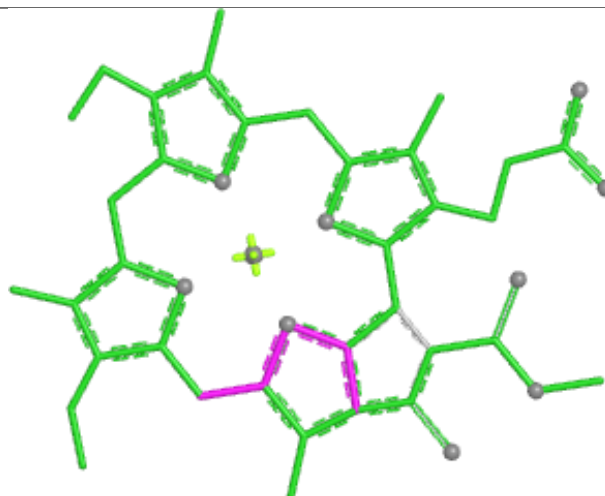




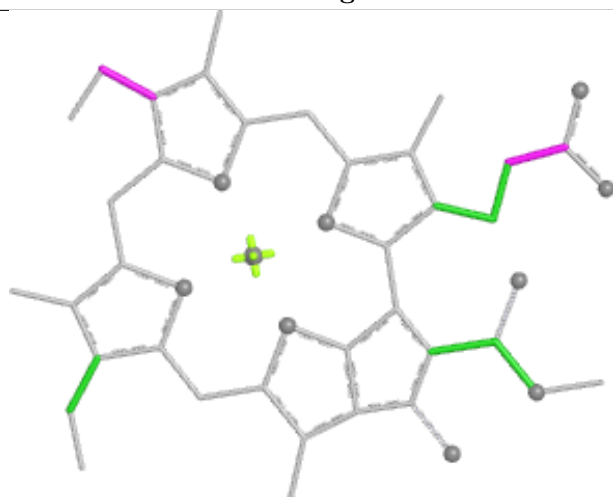
Ligand CLA 9 614



Bond lengths



Bond angles

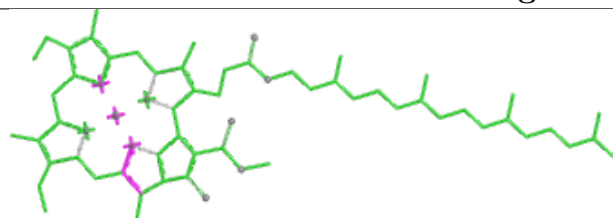


Torsions

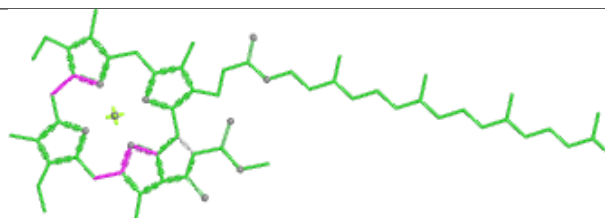


Rings

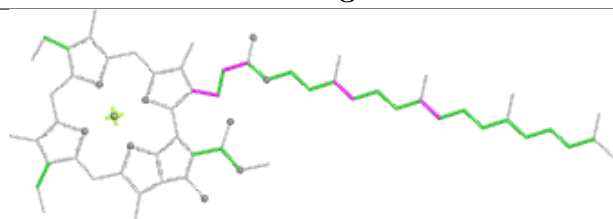
Ligand CLA 3 615



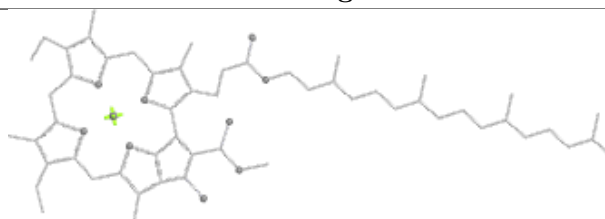
Bond lengths



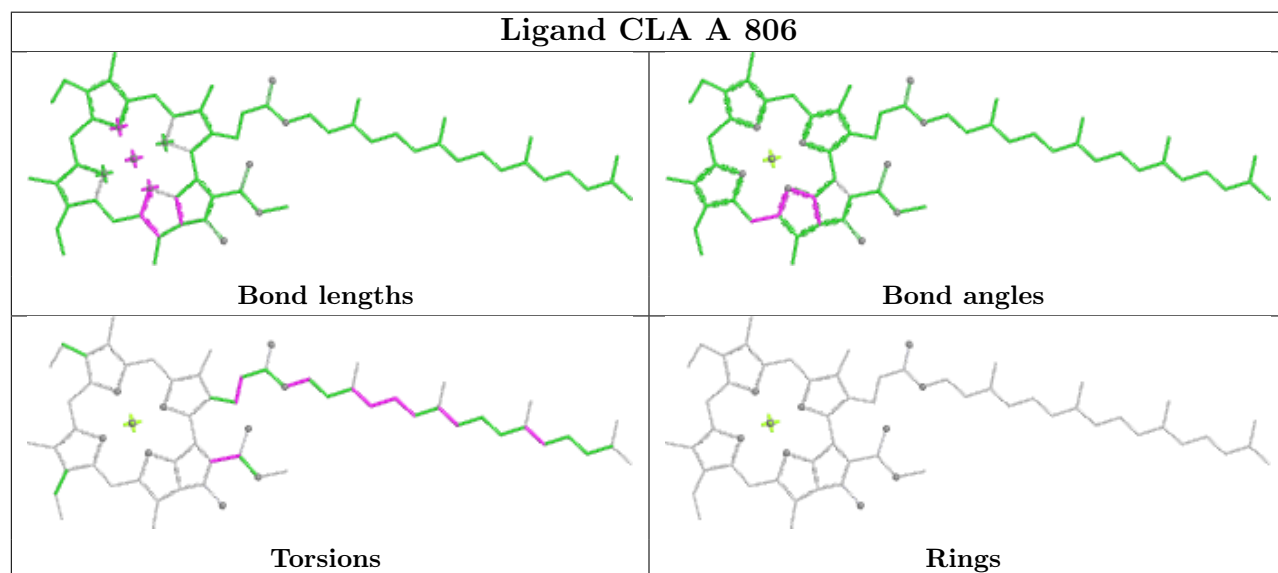
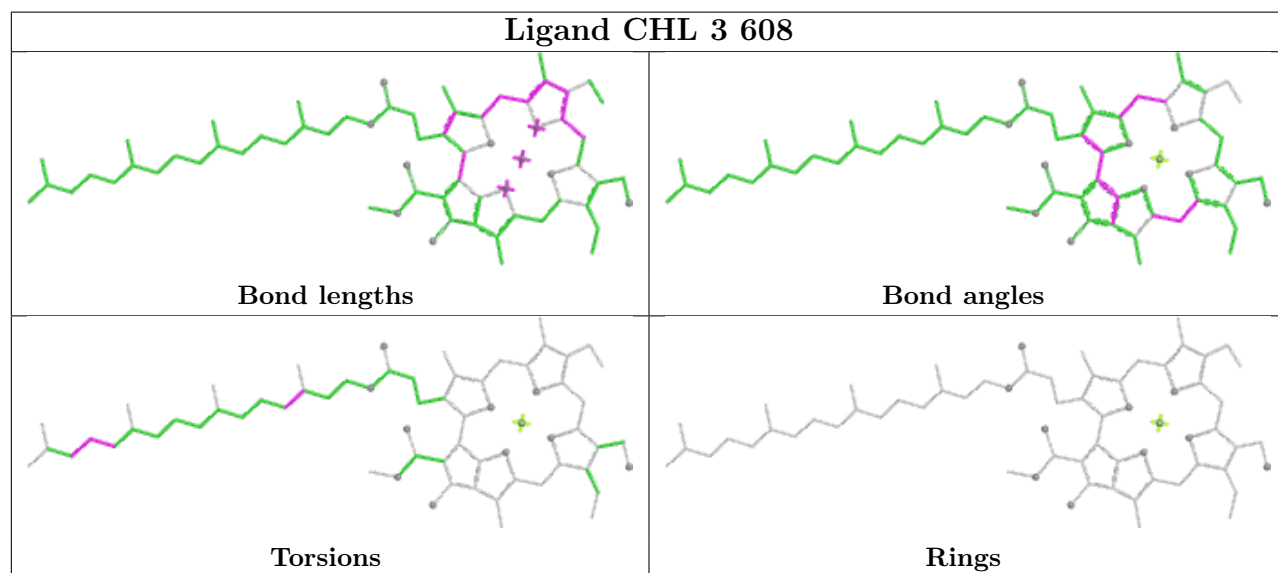
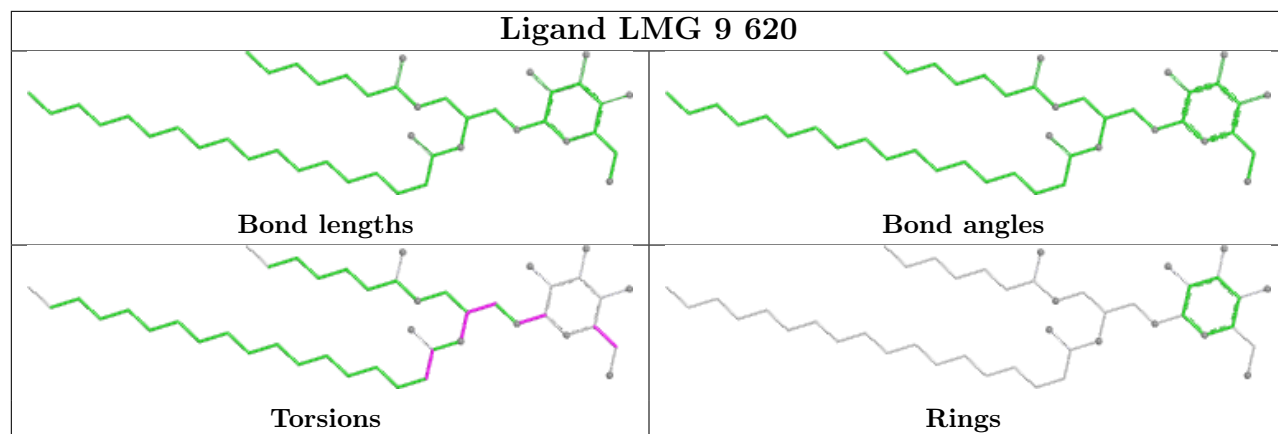
Bond angles

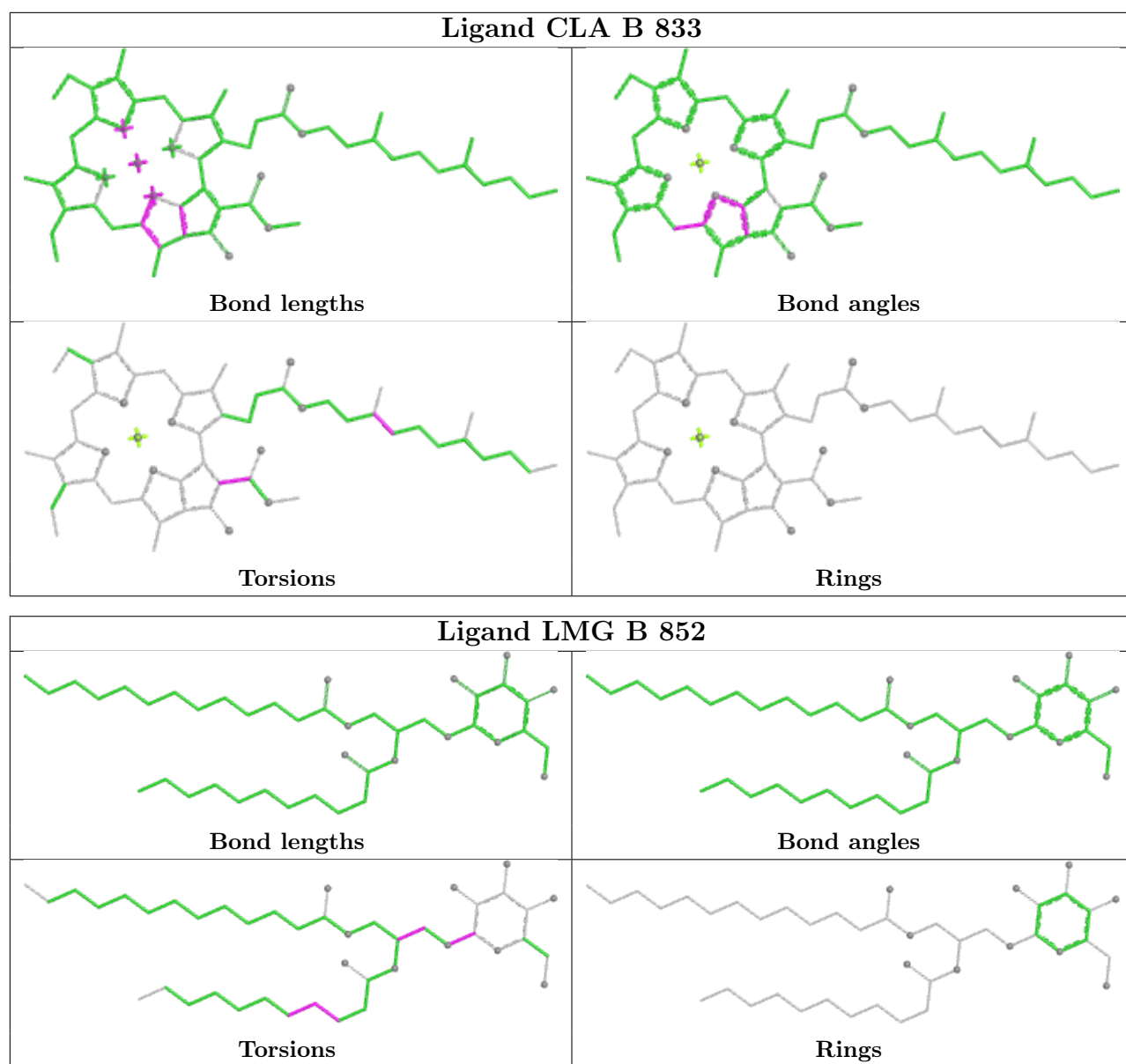


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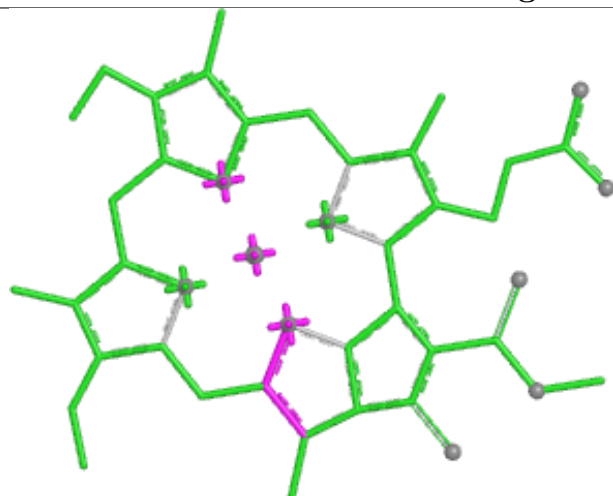


Rings

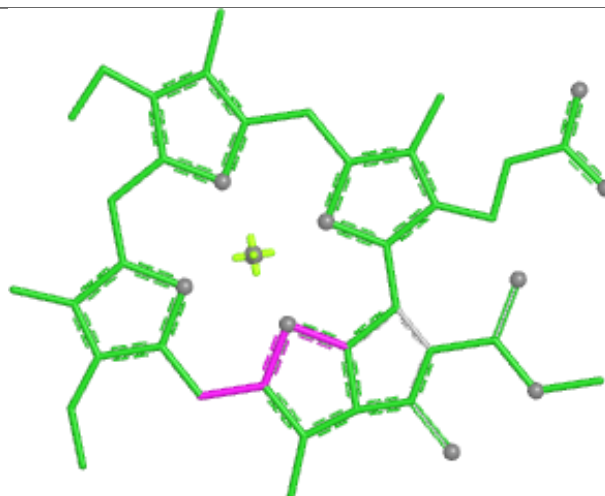




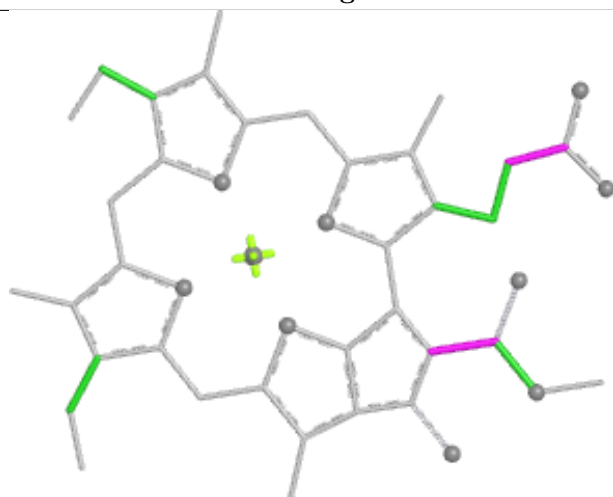
Ligand CLA 4 612



Bond lengths



Bond angles

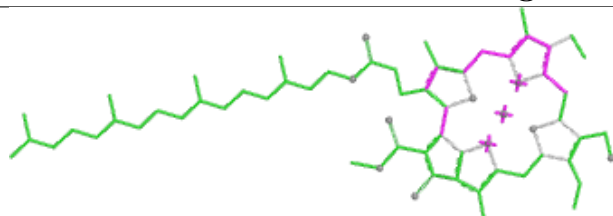


Torsions

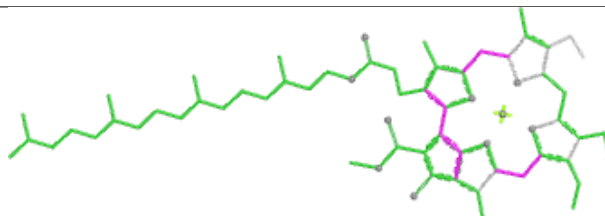


Rings

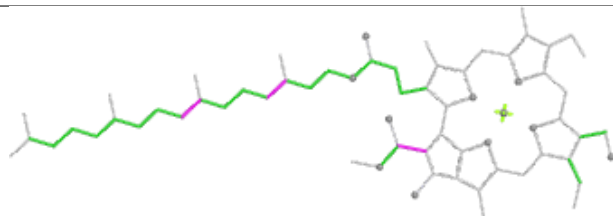
Ligand CHL 4 601



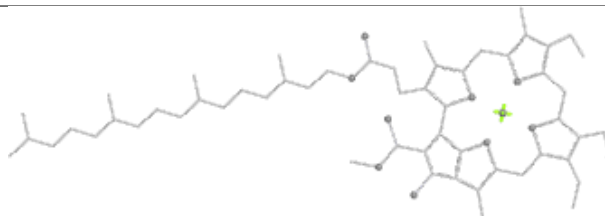
Bond lengths



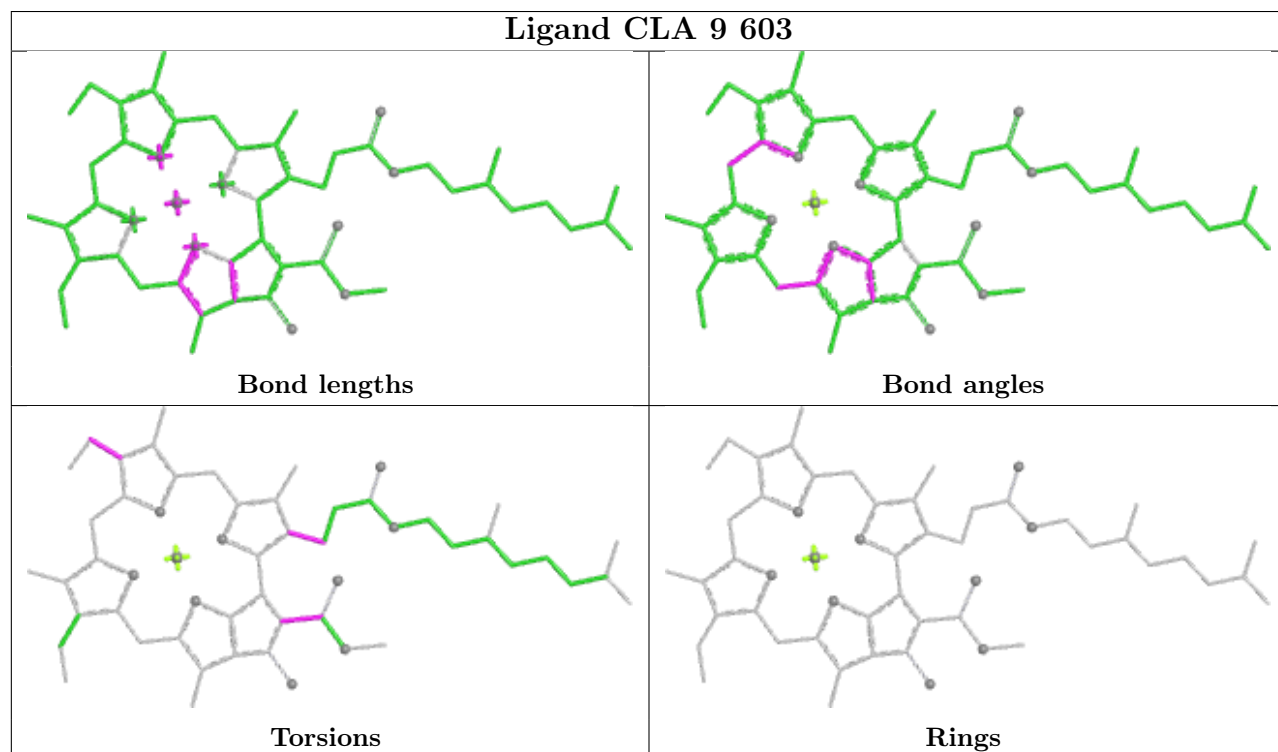
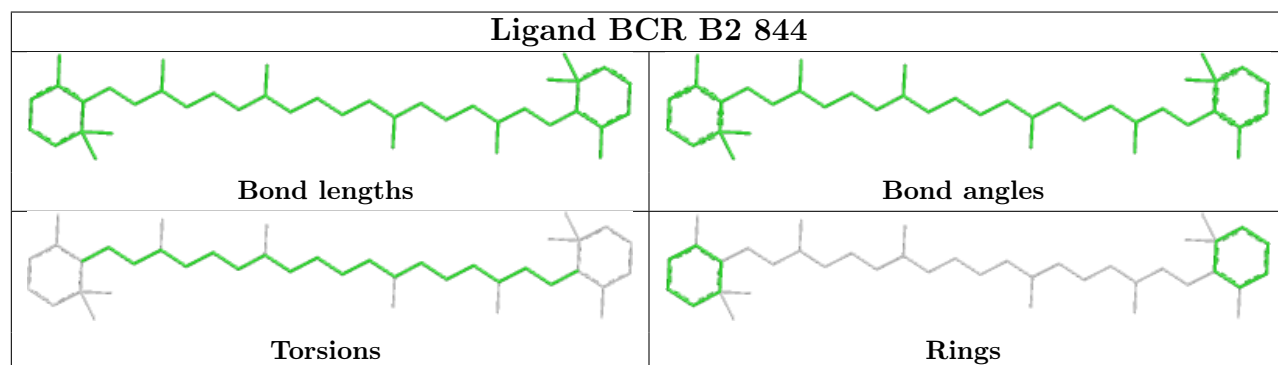
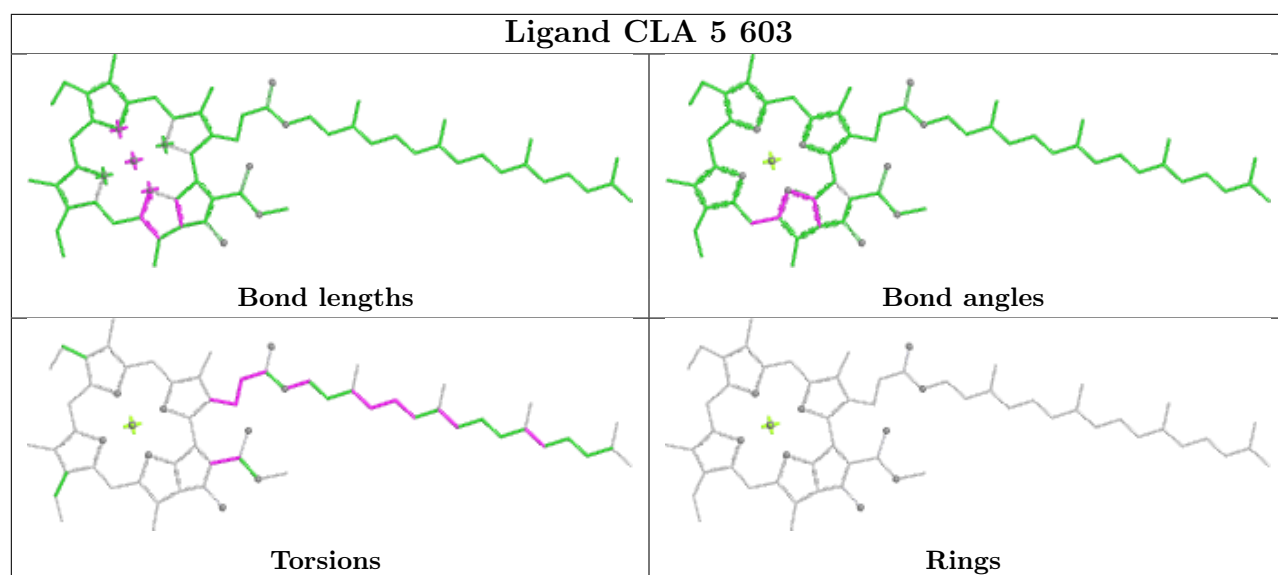
Bond angles

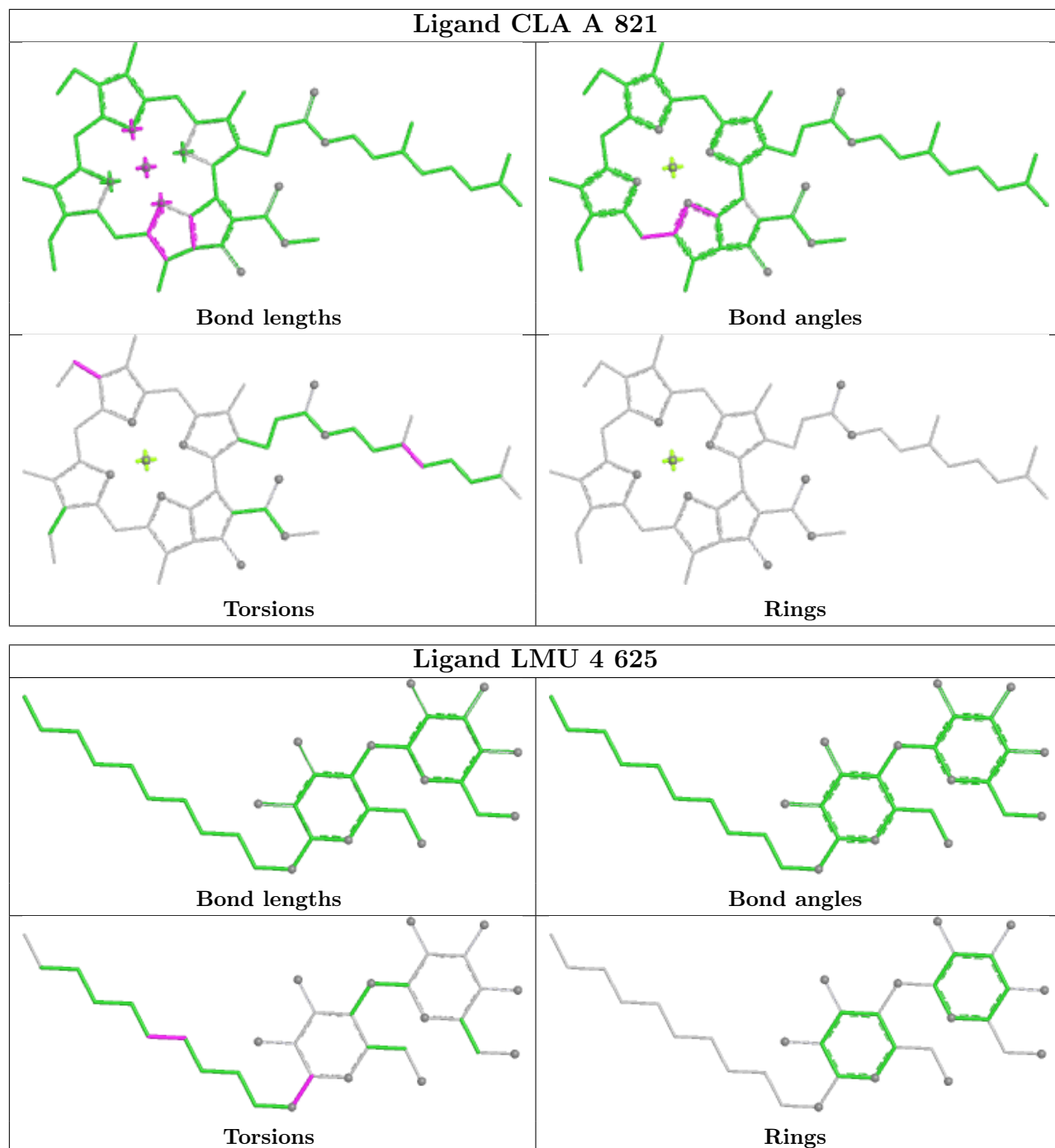


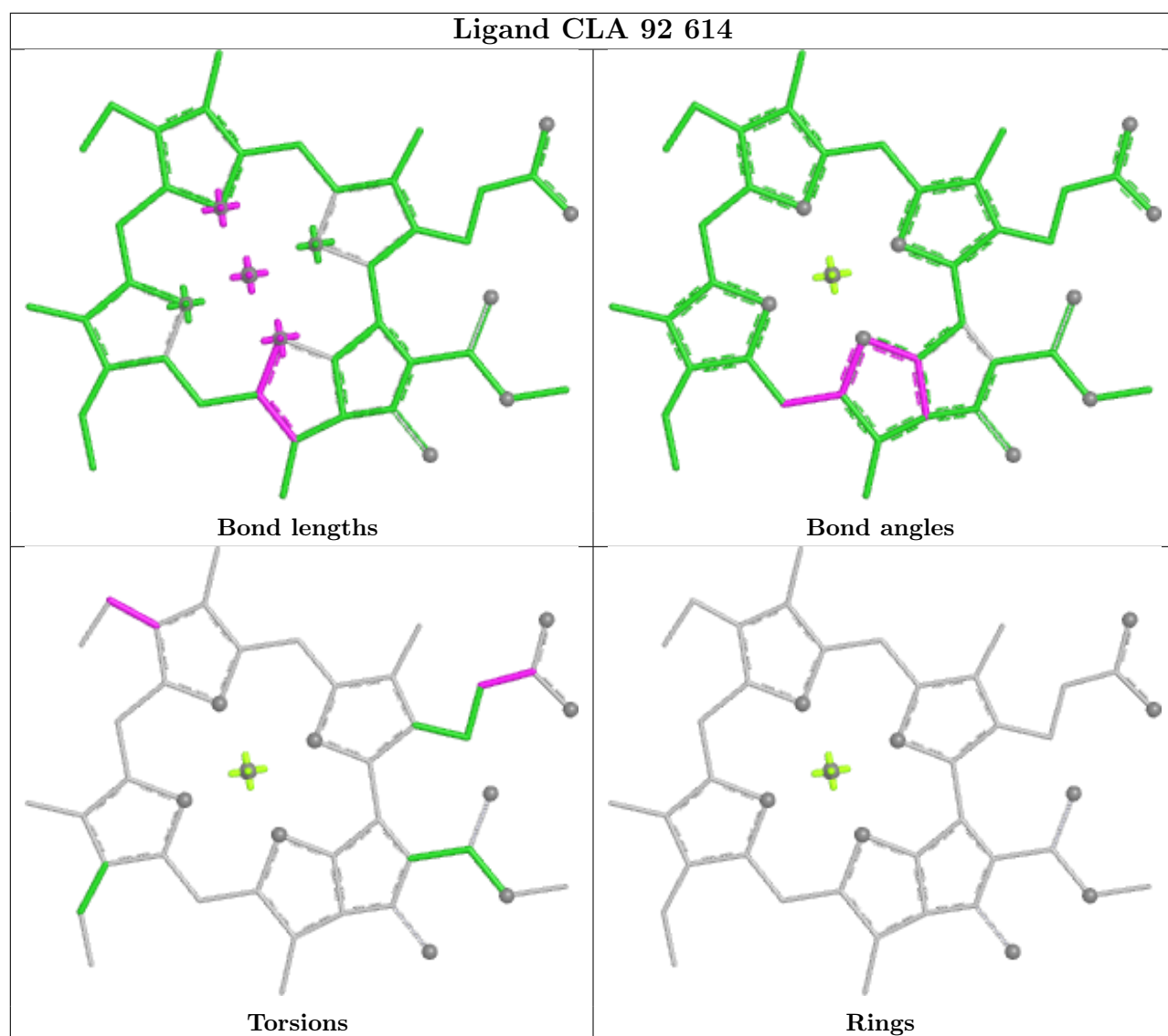
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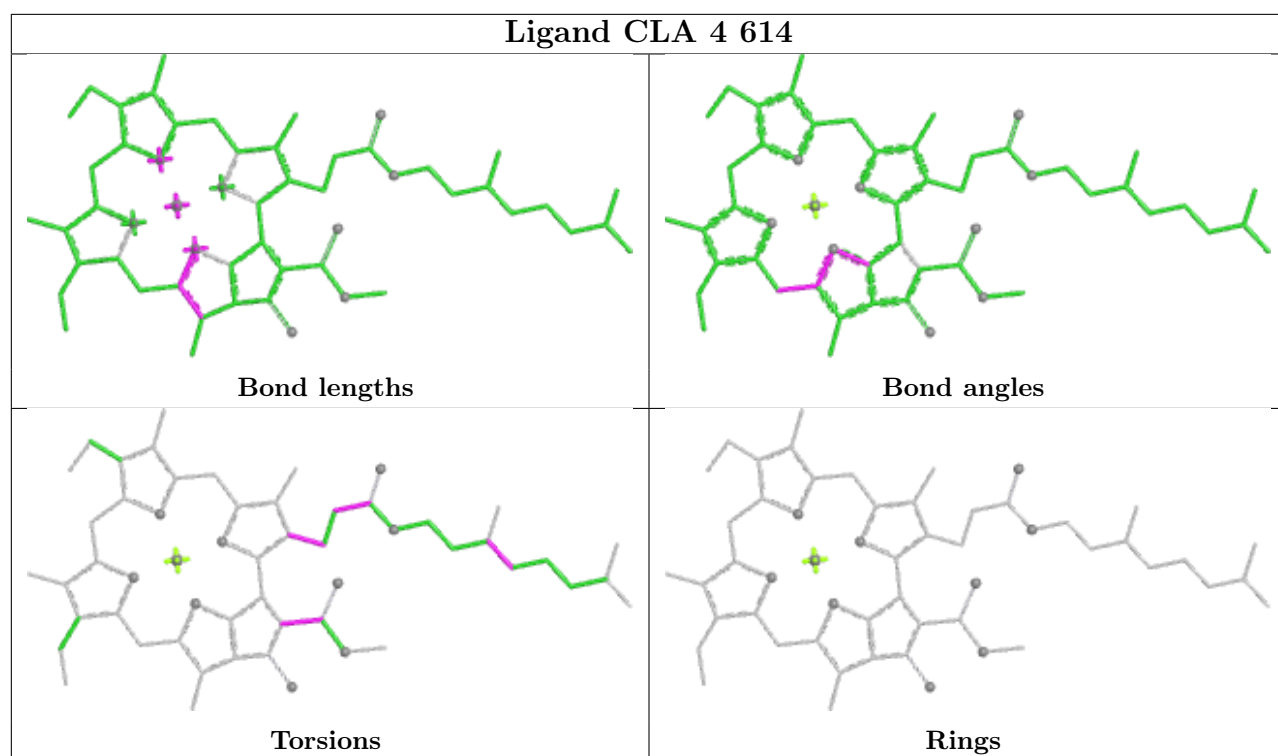


Rings

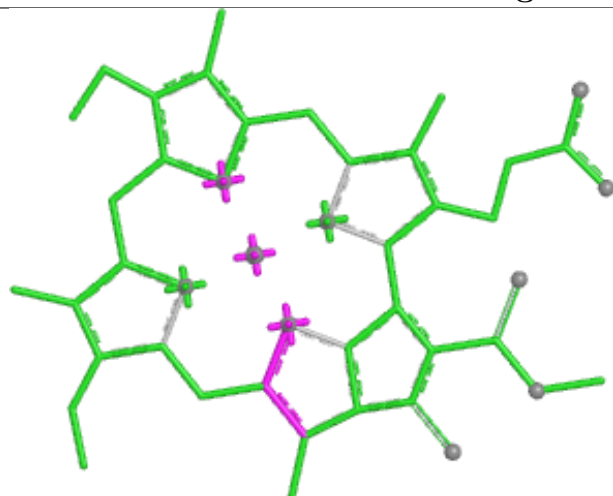




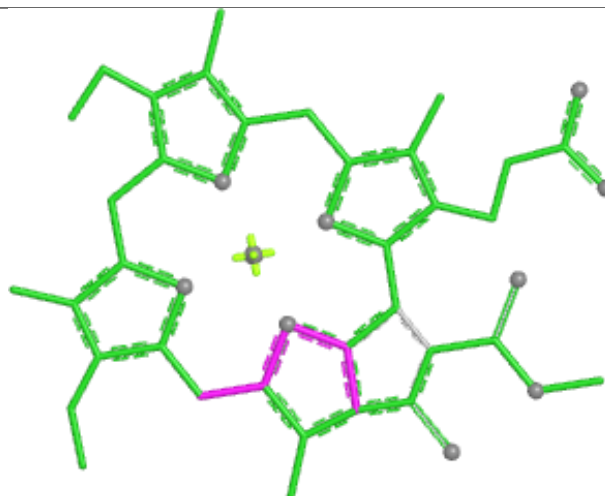




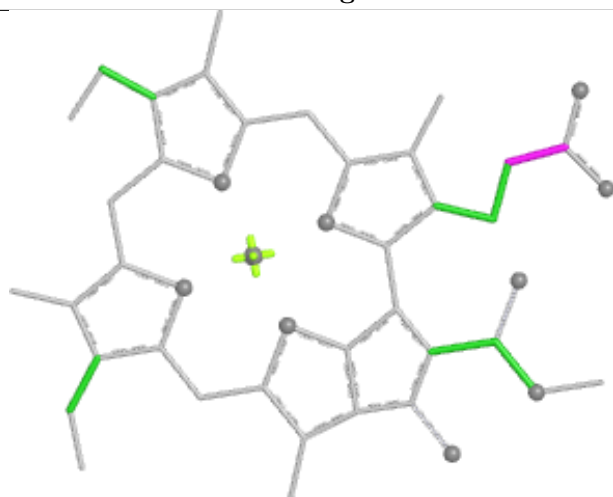
Ligand CLA L 204



Bond lengths



Bond angles

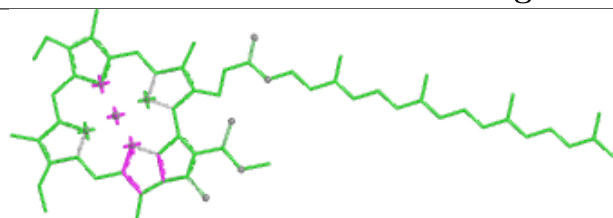


Torsions

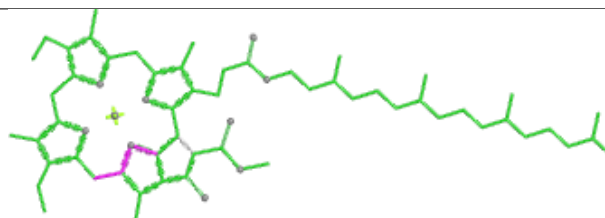


Rings

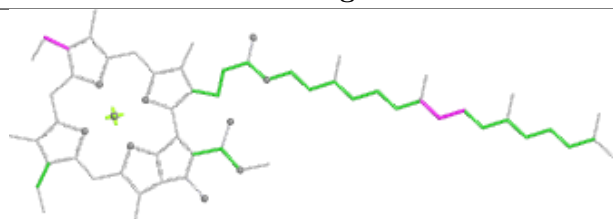
Ligand CLA B 802



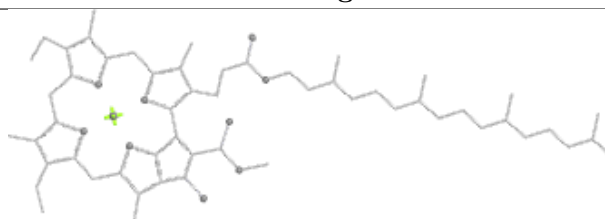
Bond lengths



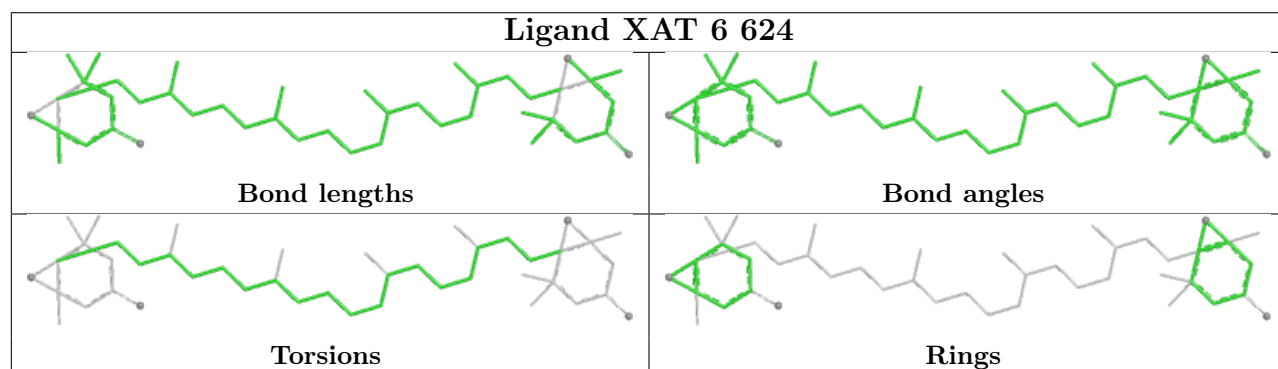
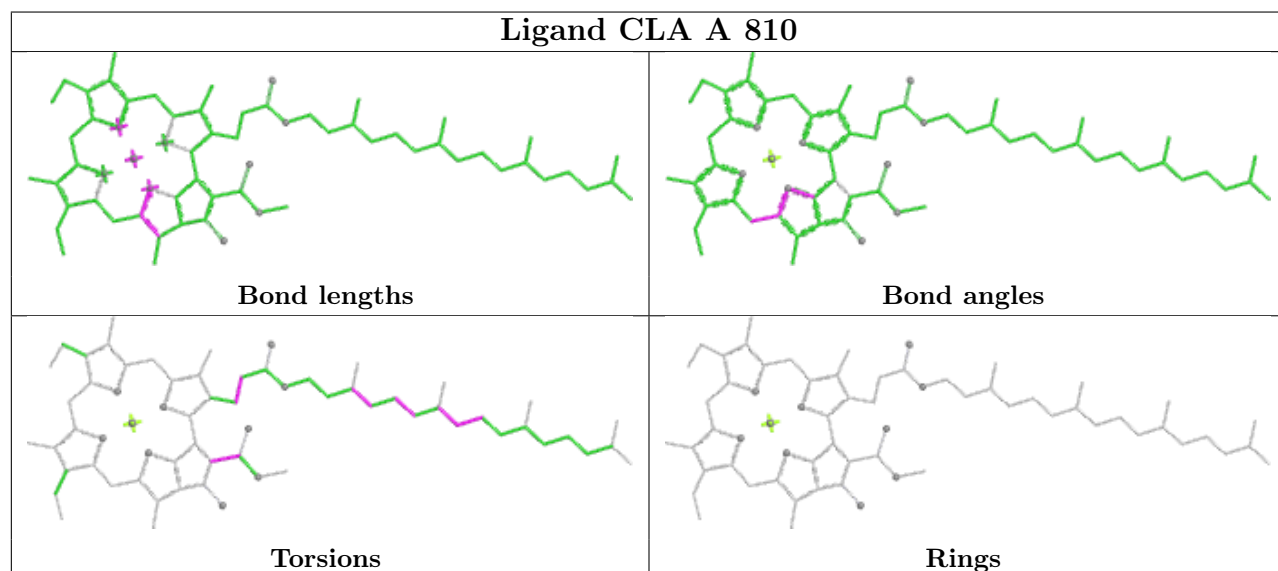
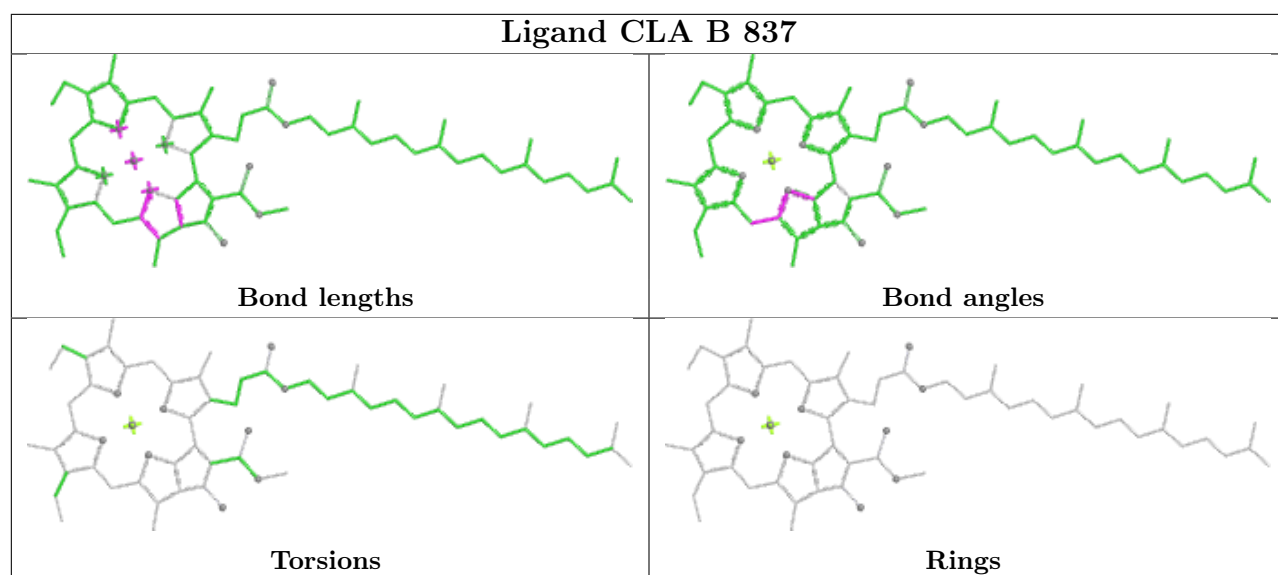
Bond angles



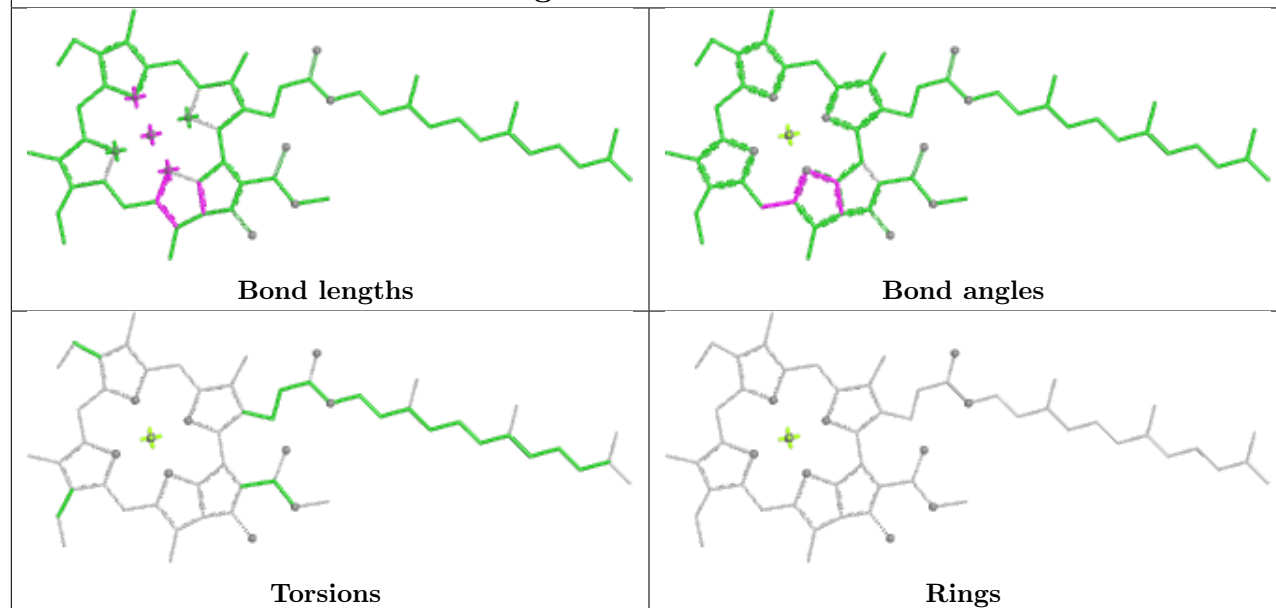
Torsions



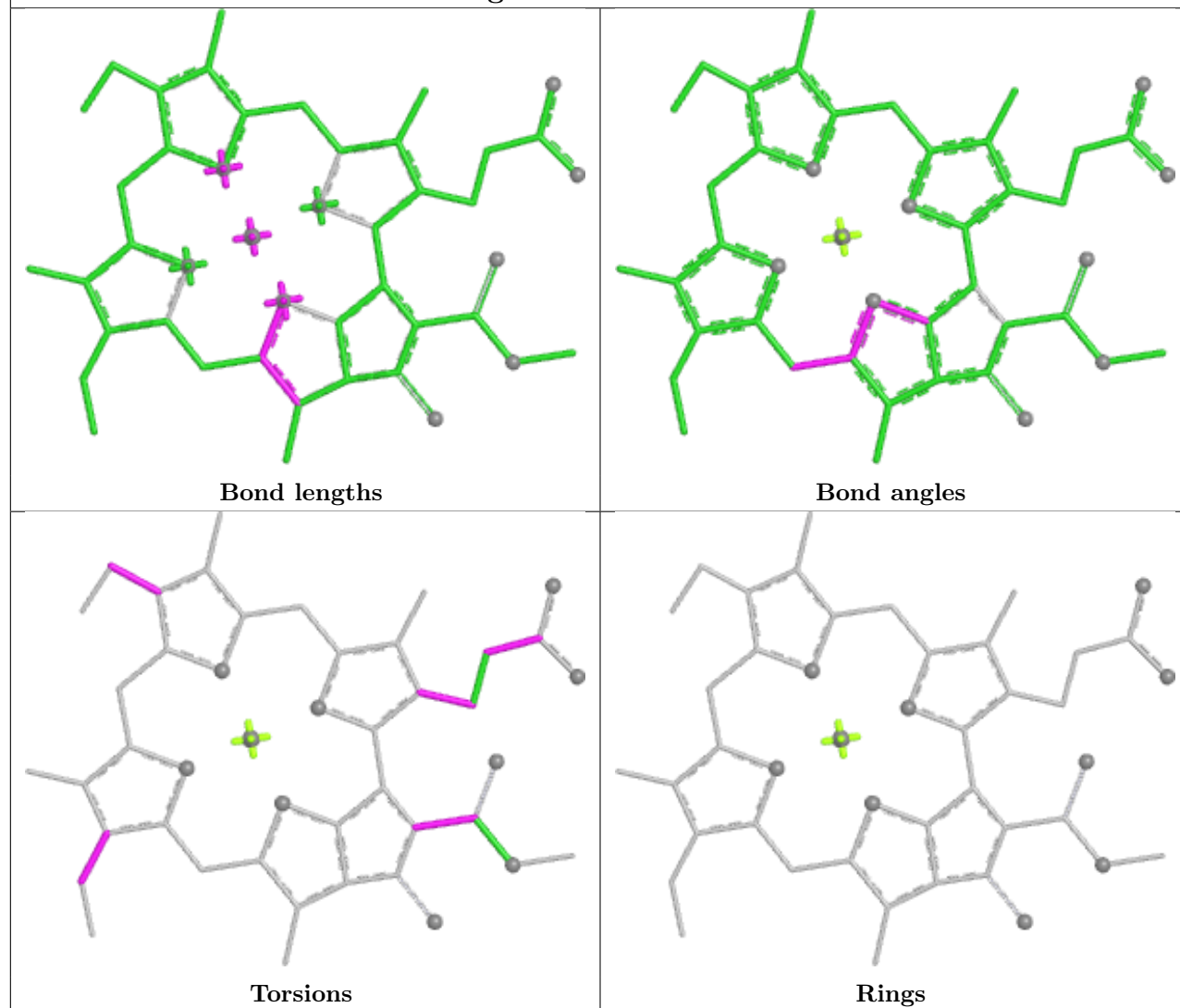
Rings



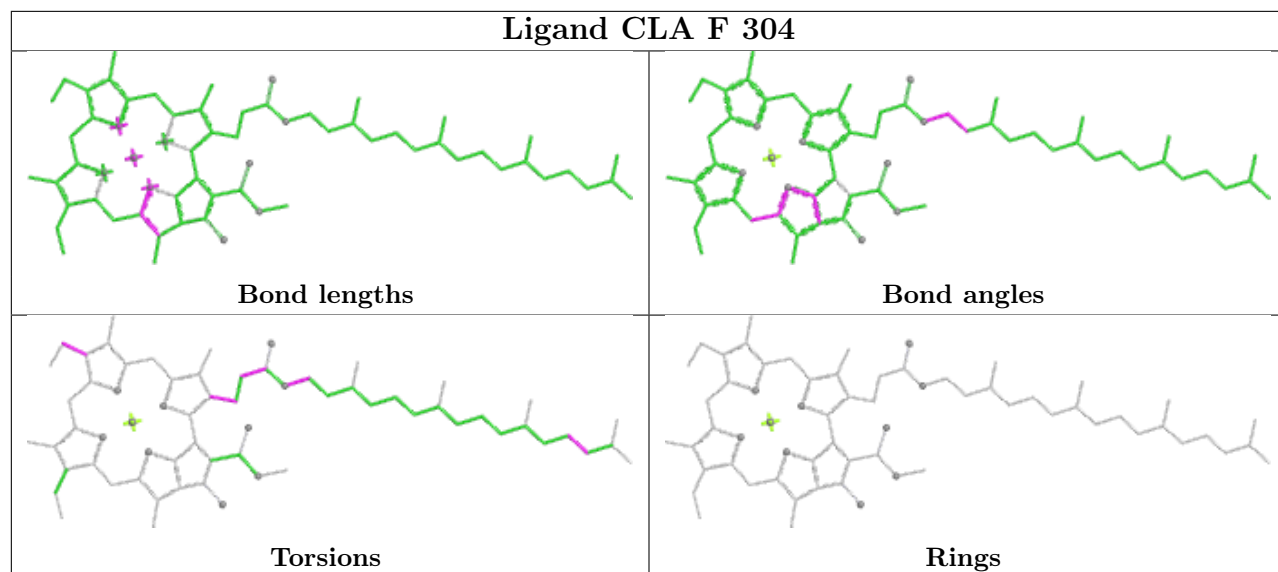
Ligand CLA Z 610



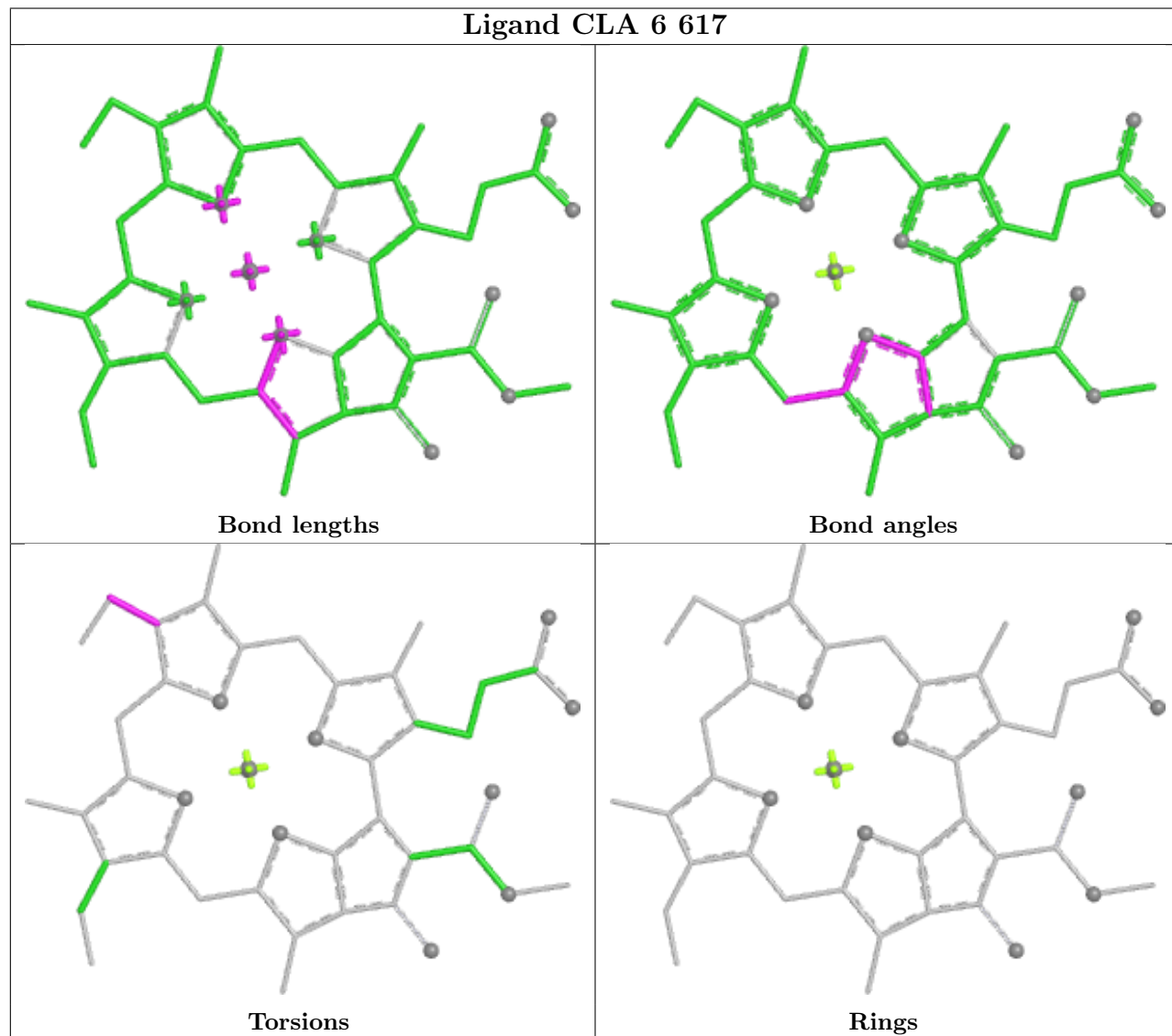
Ligand CLA 92 609

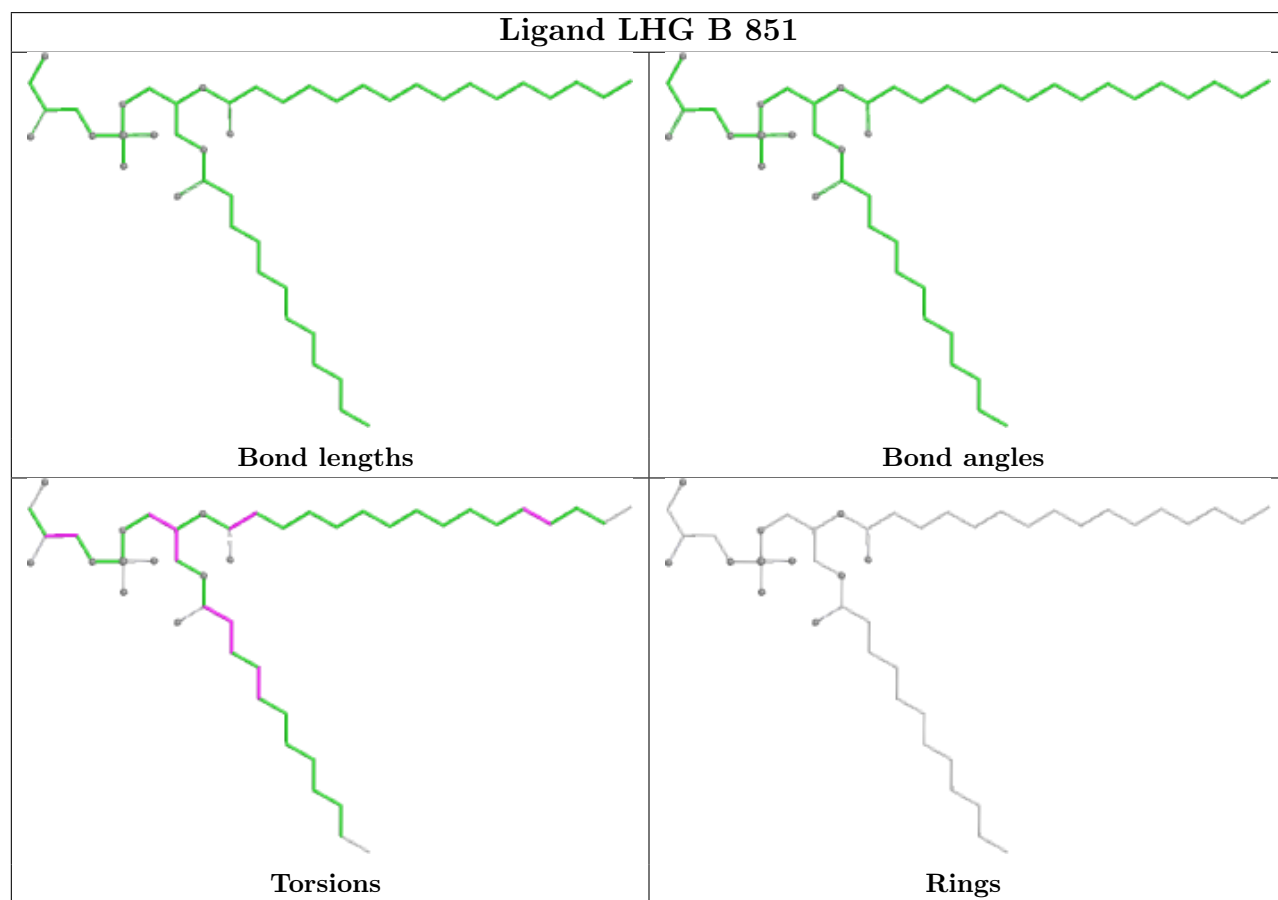
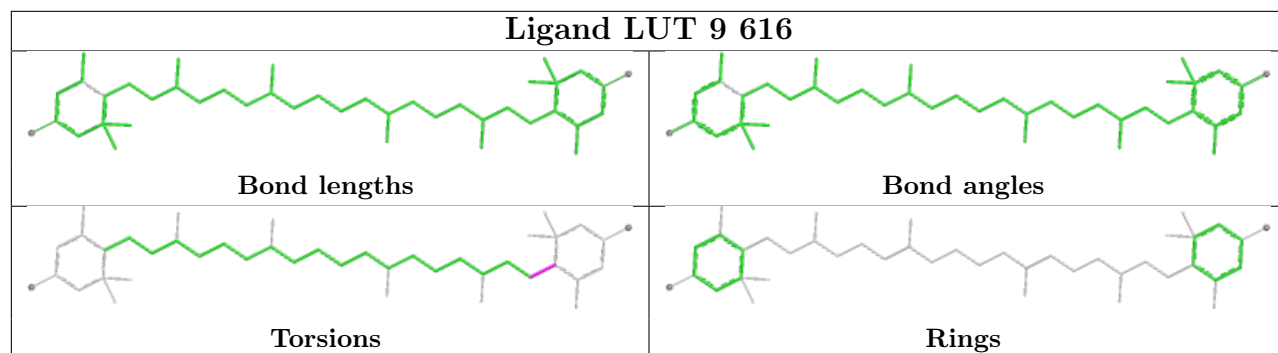


Ligand CLA F 304

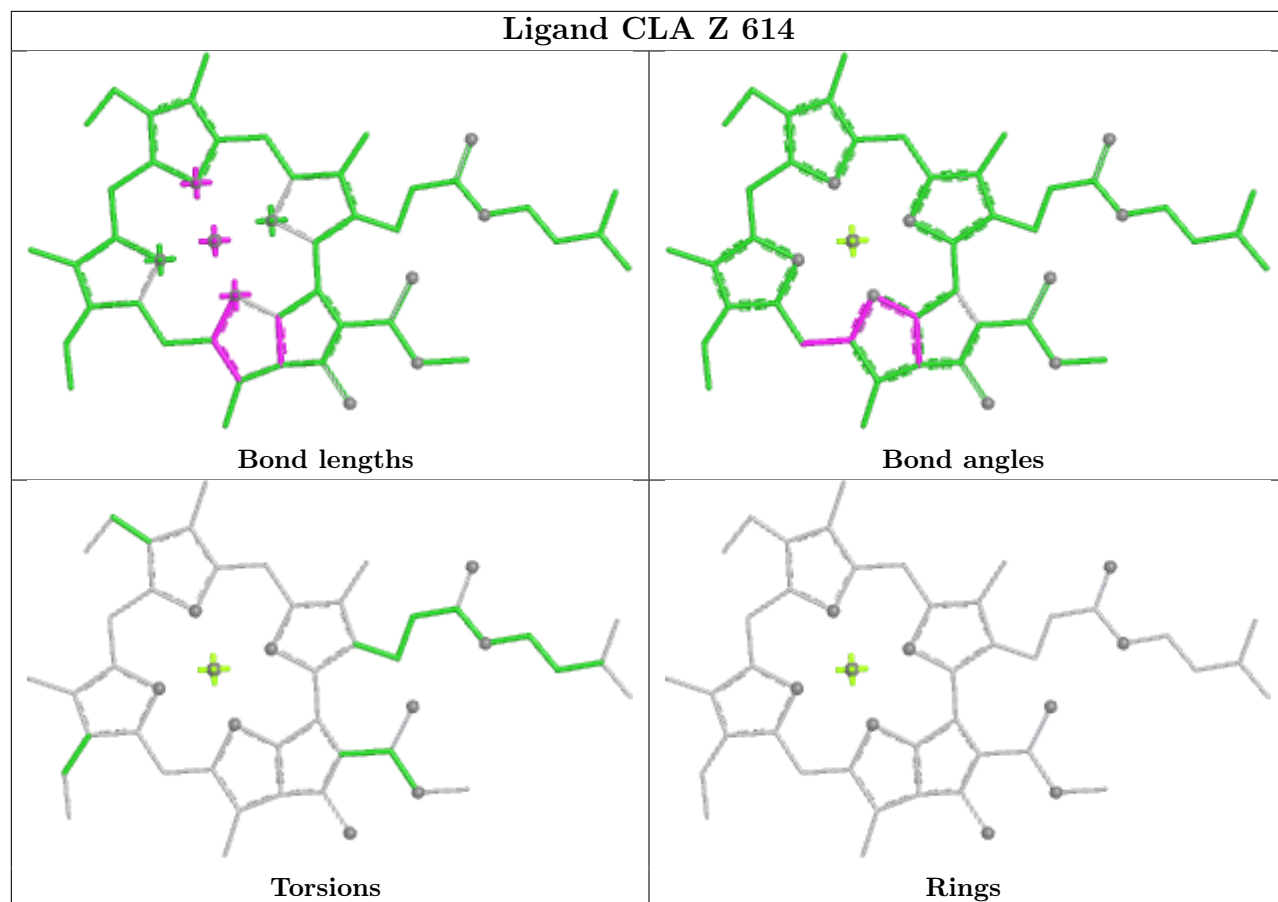


Ligand CLA 6 617

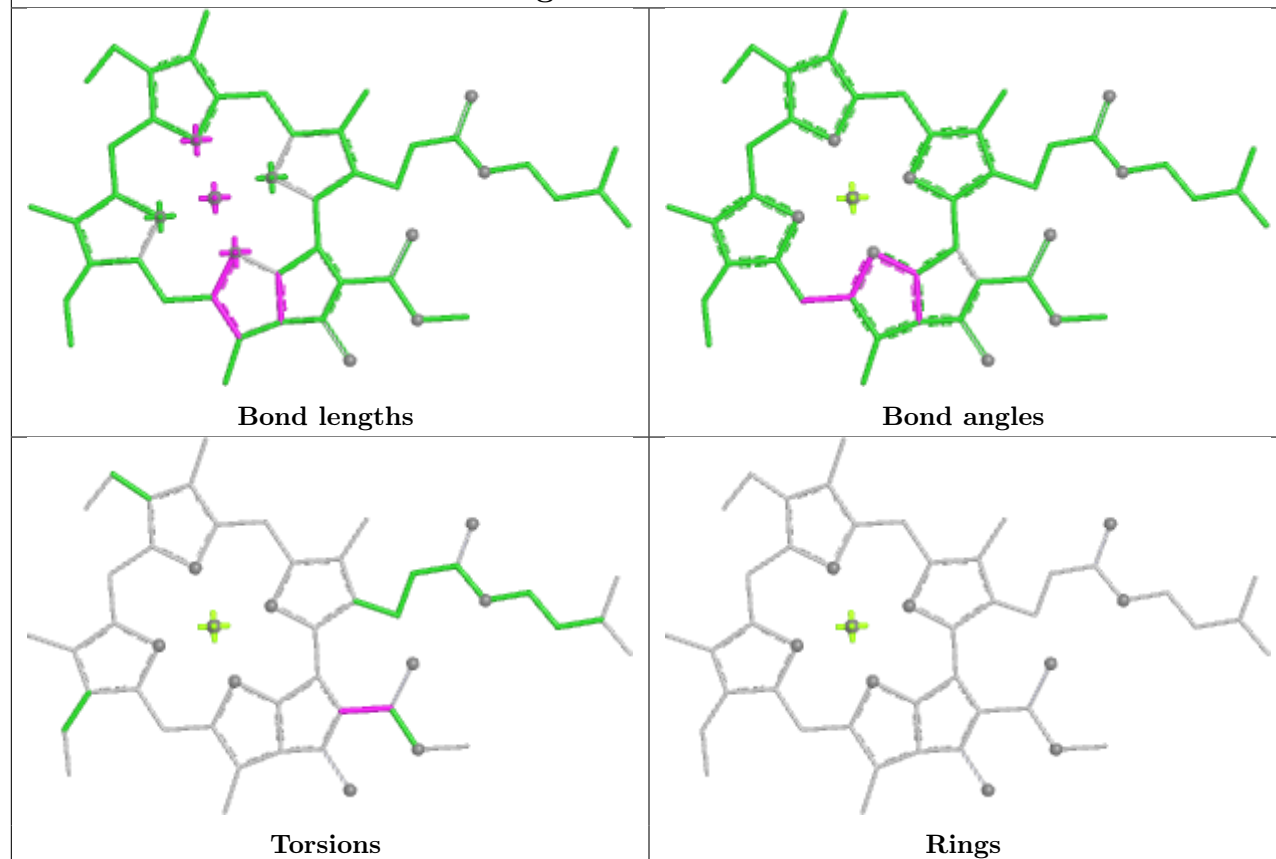




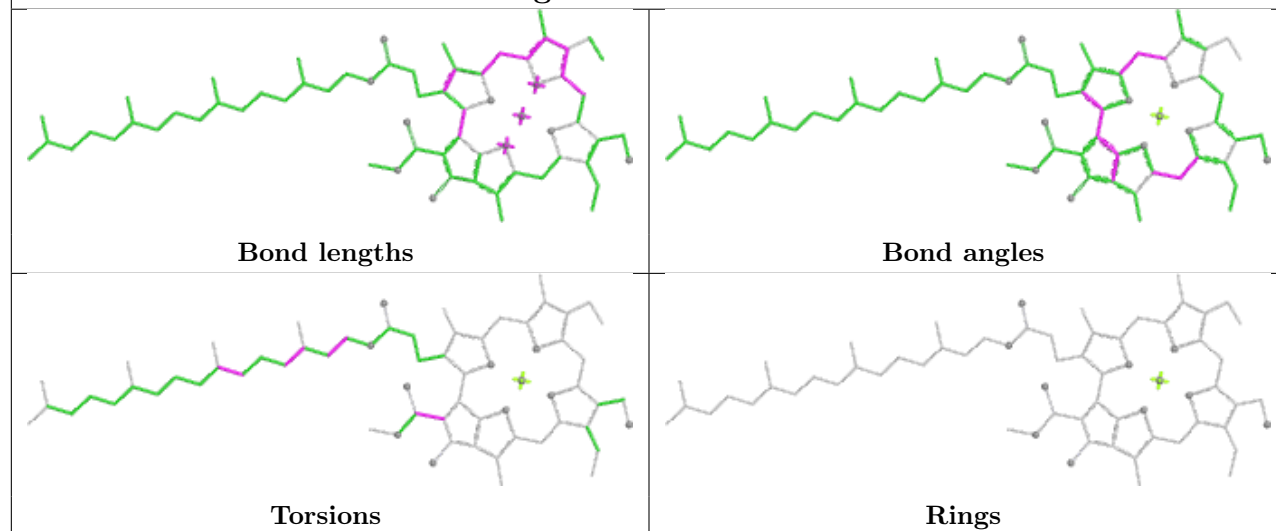
Ligand CLA Z 614

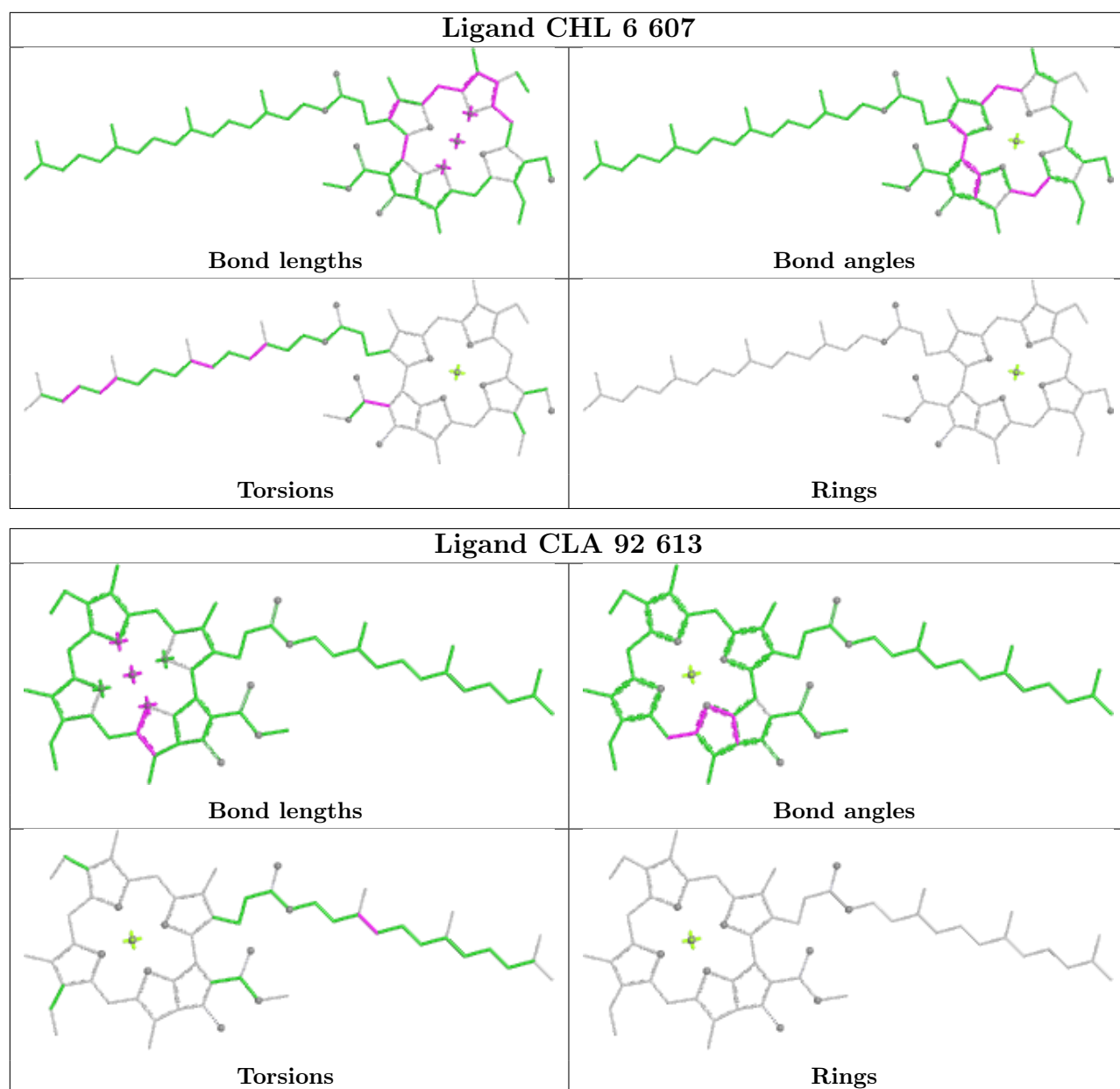


Ligand CLA 4 604

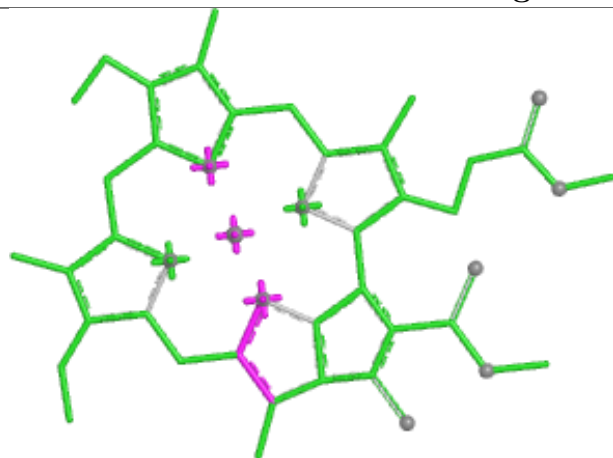


Ligand CHL Z 601

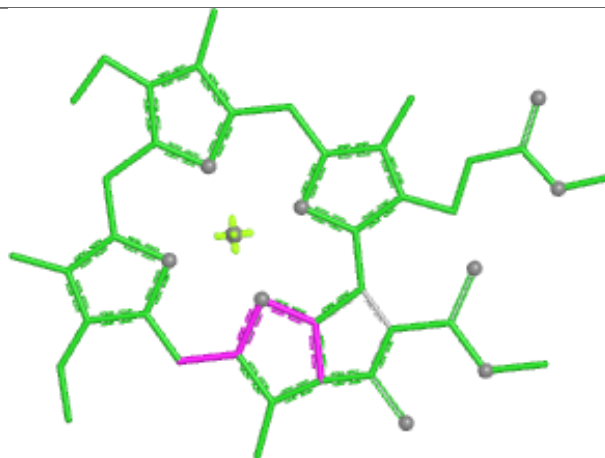




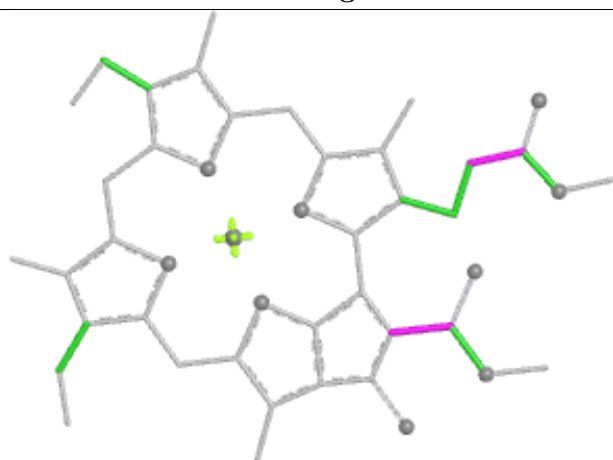
Ligand CLA G 204



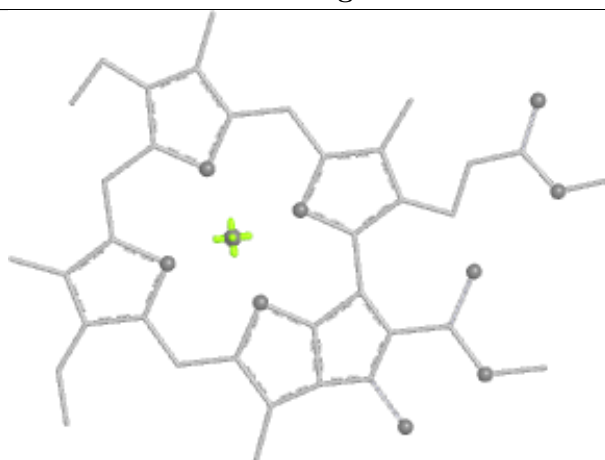
Bond lengths



Bond angles

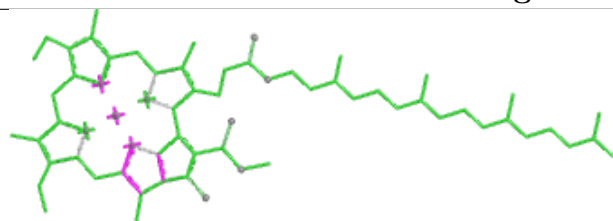


Torsions

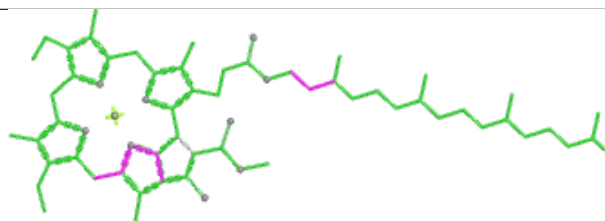


Rings

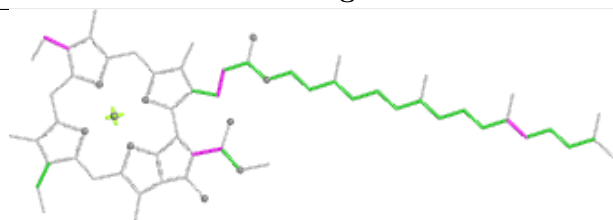
Ligand CLA A 809



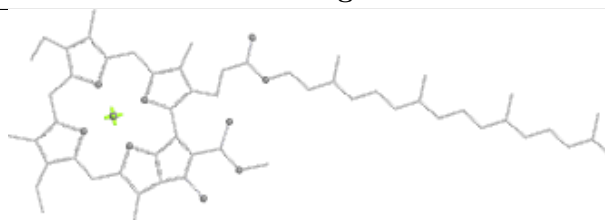
Bond lengths



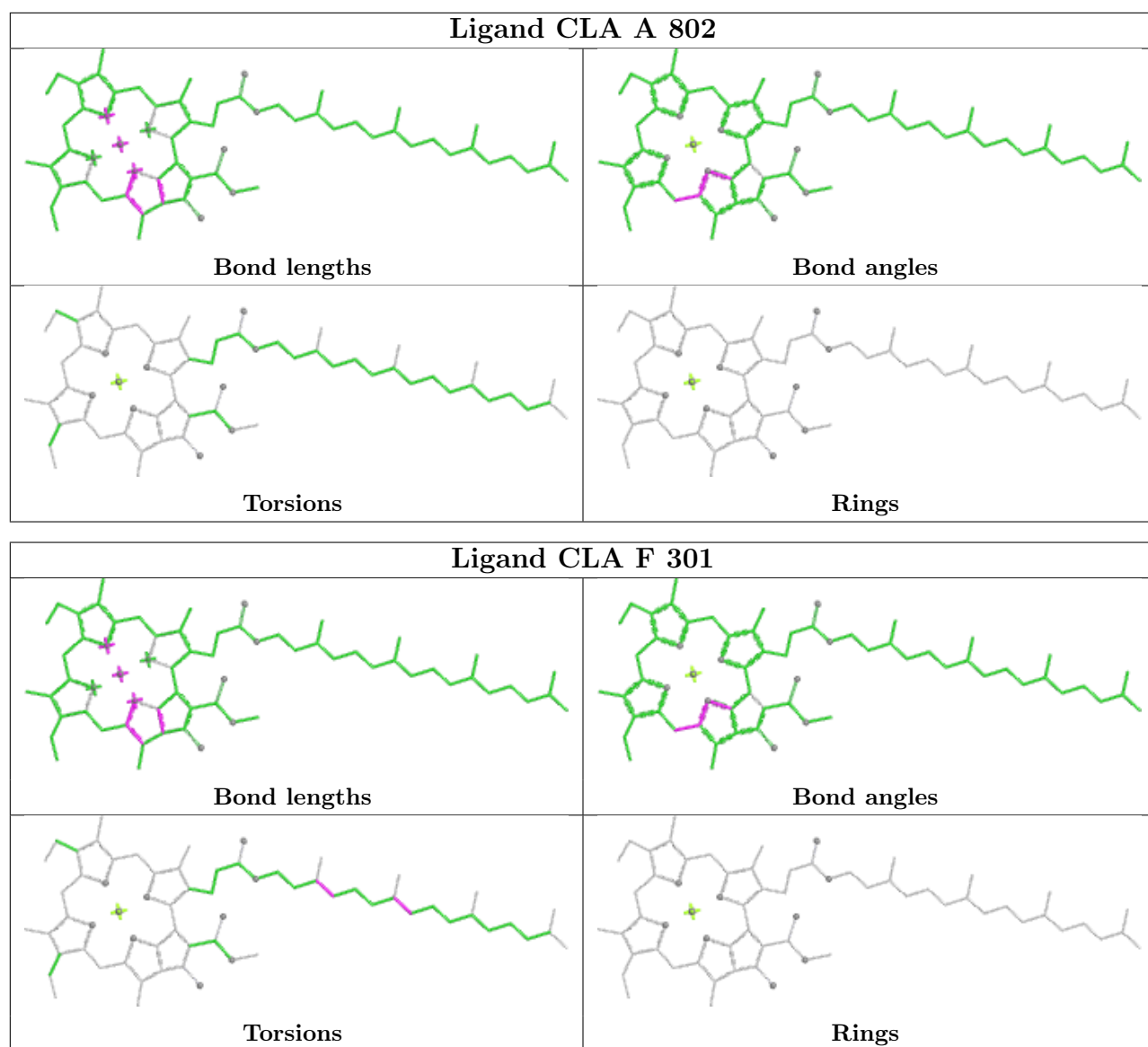
Bond angles



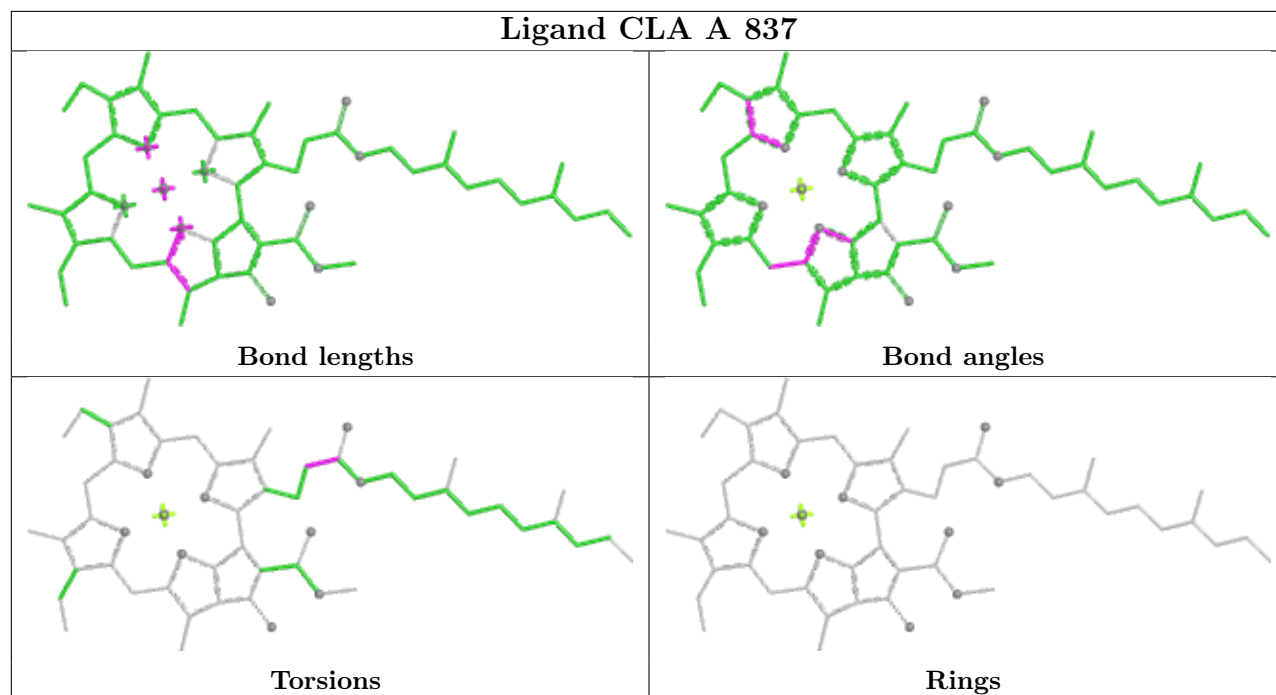
Torsions



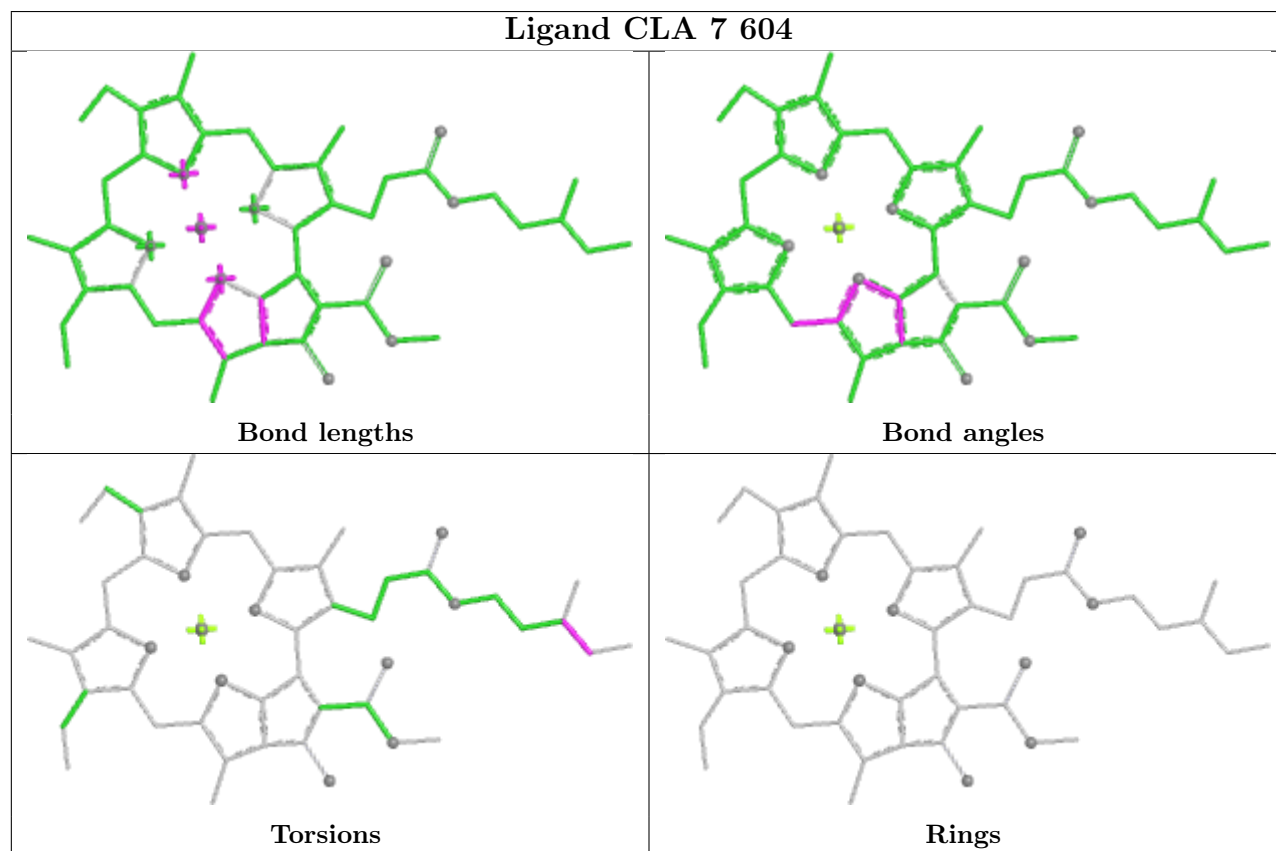
Rings

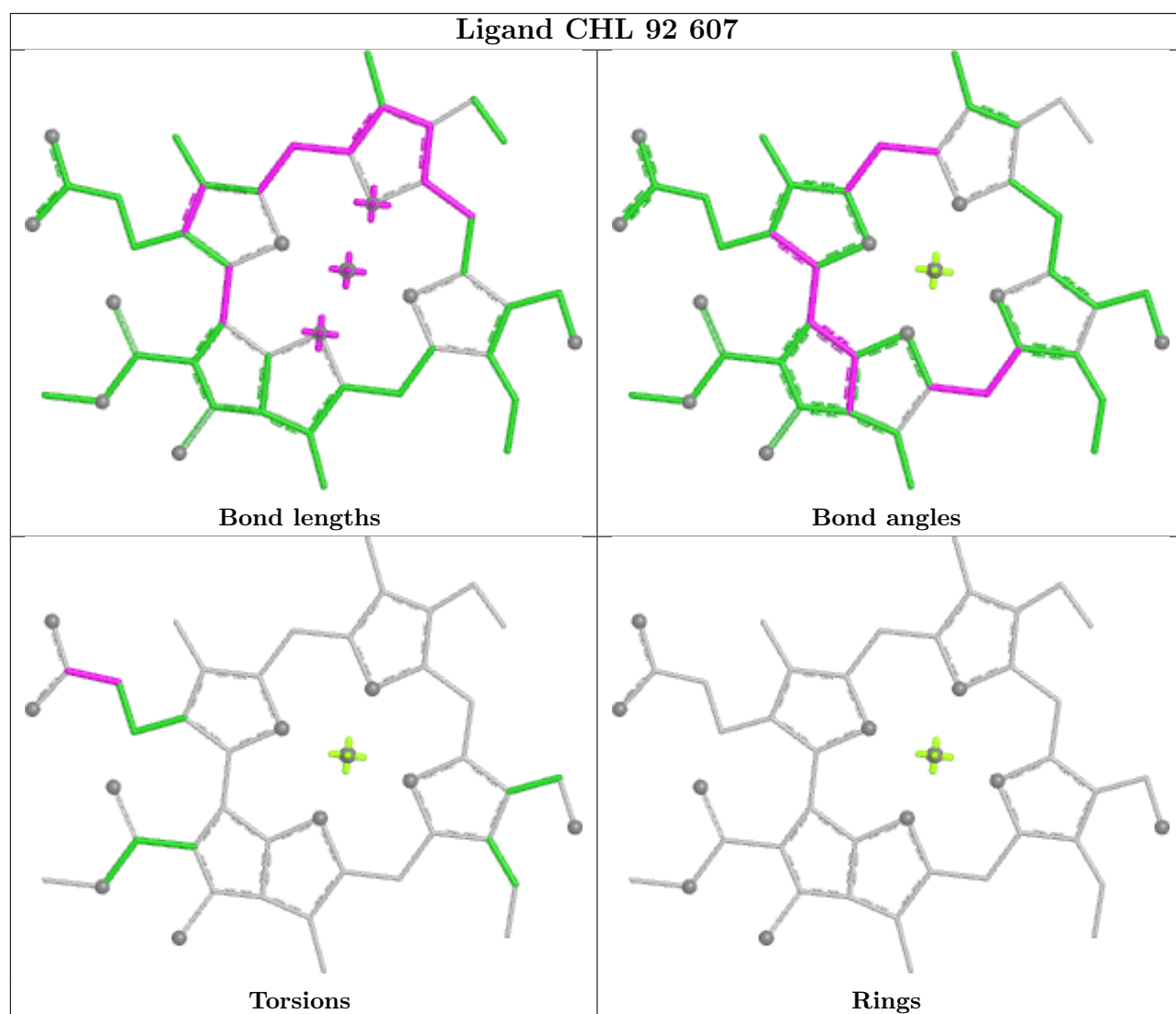
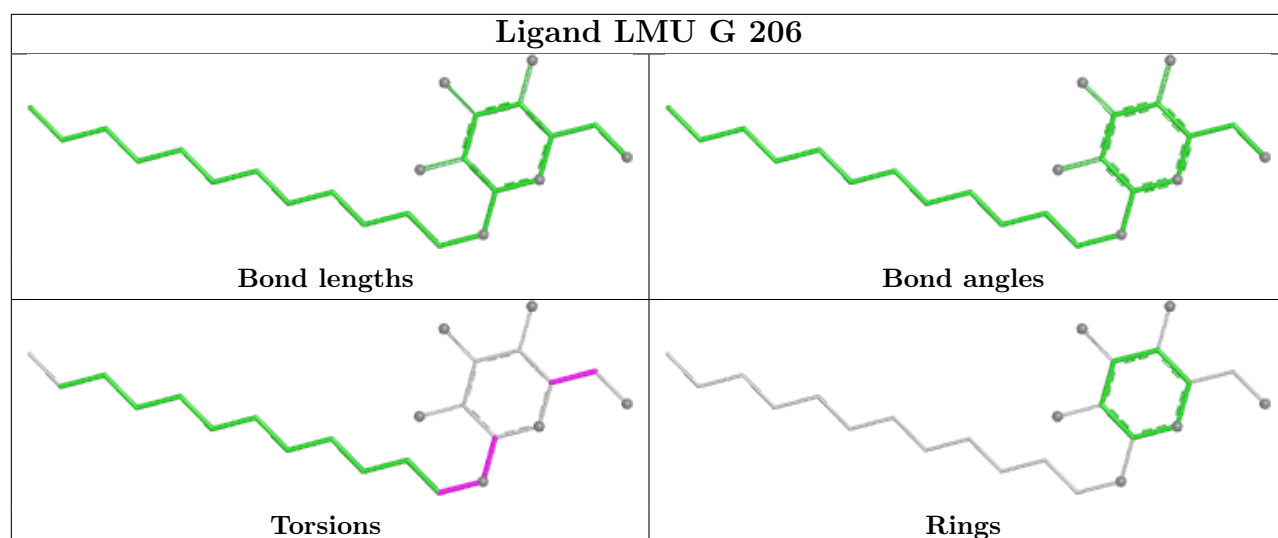


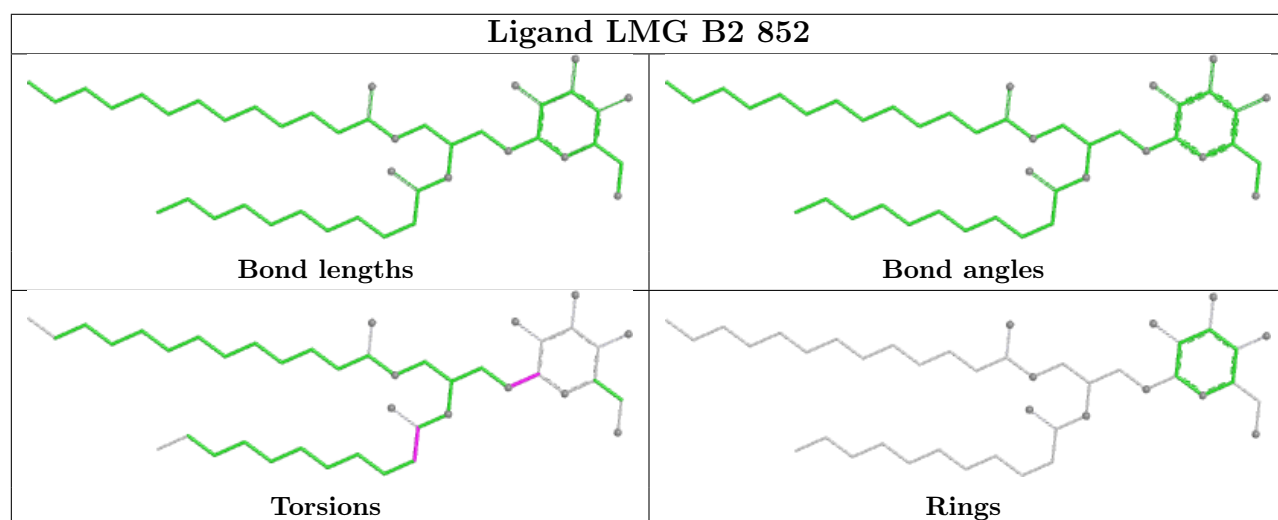
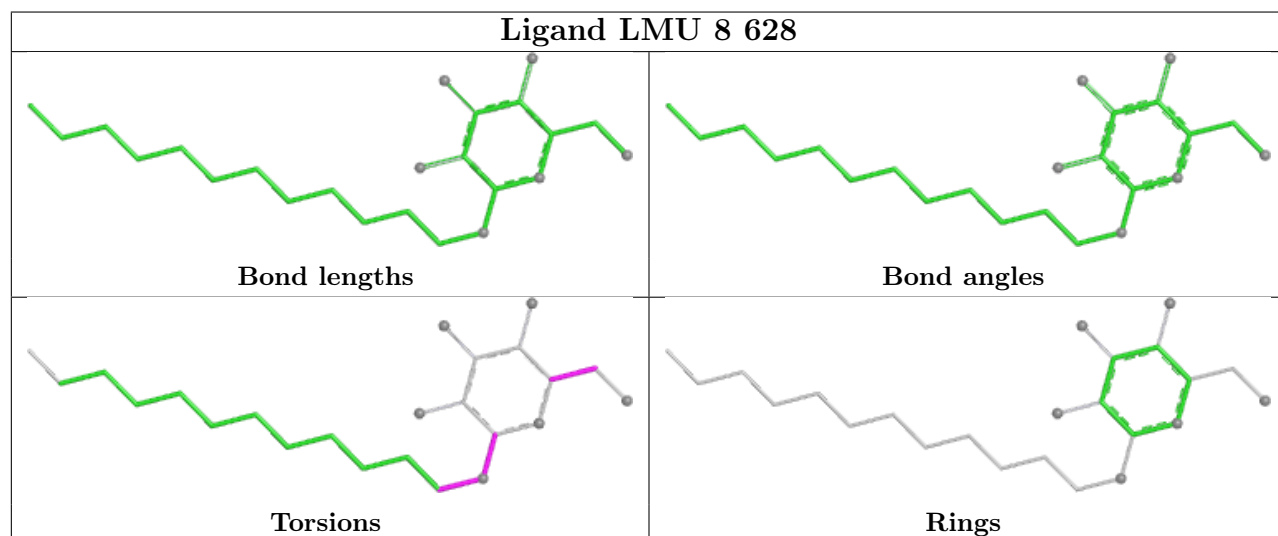
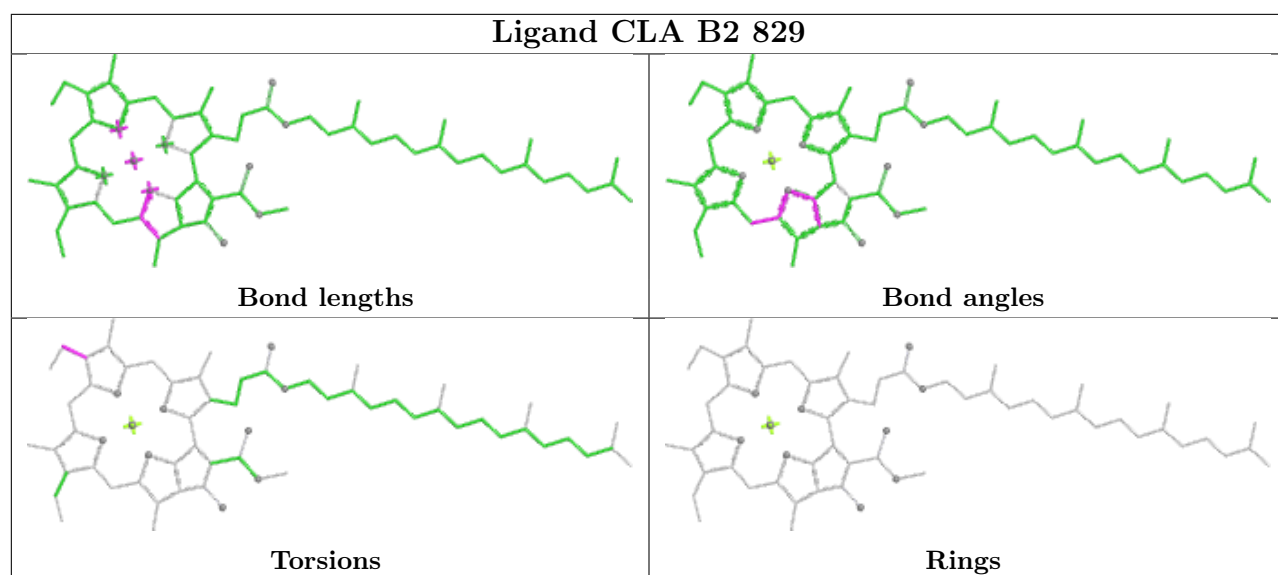
Ligand CLA A 837

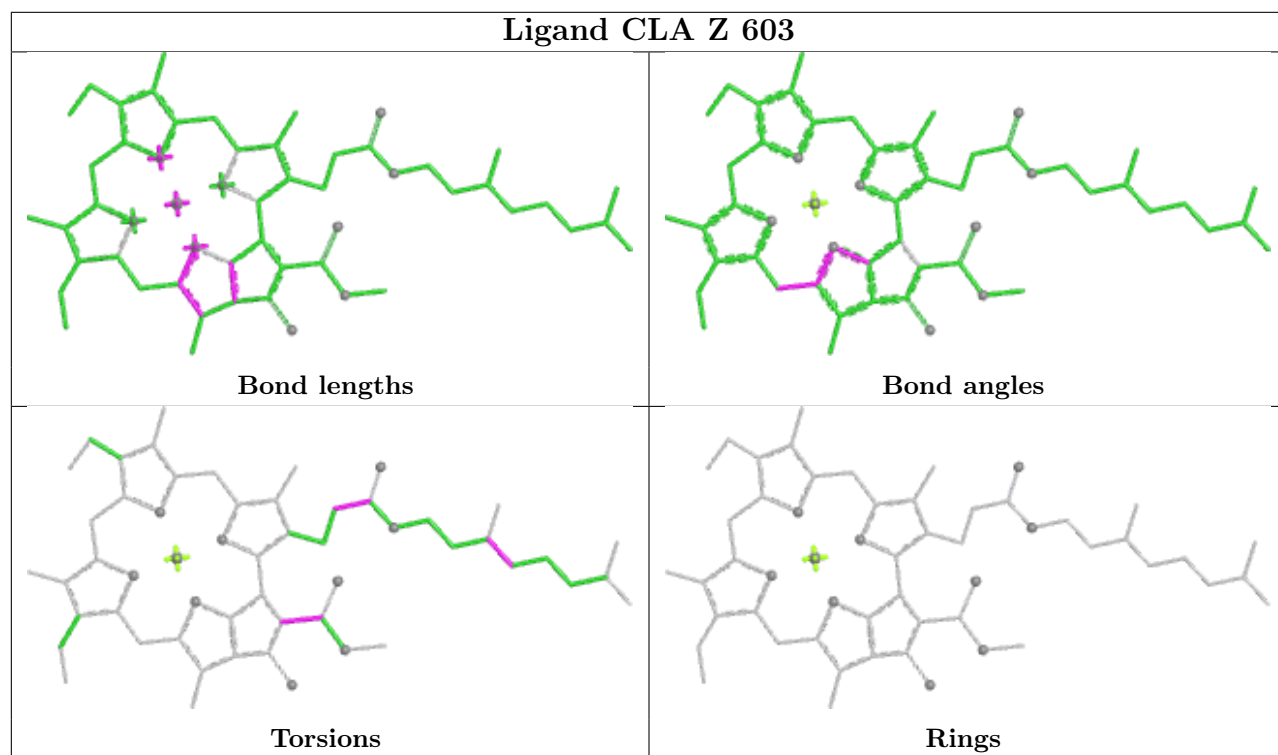
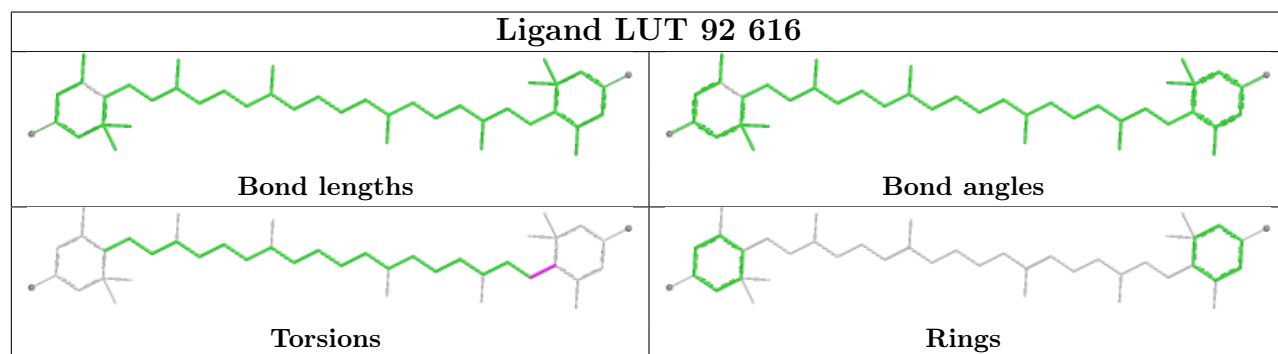
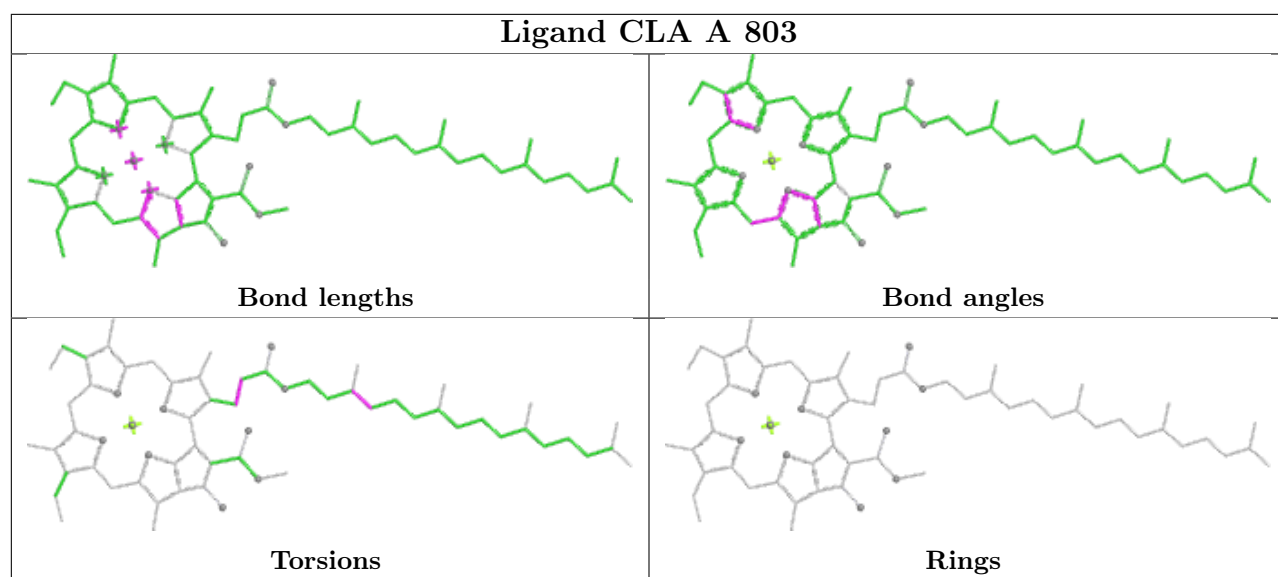


Ligand CLA 7 604

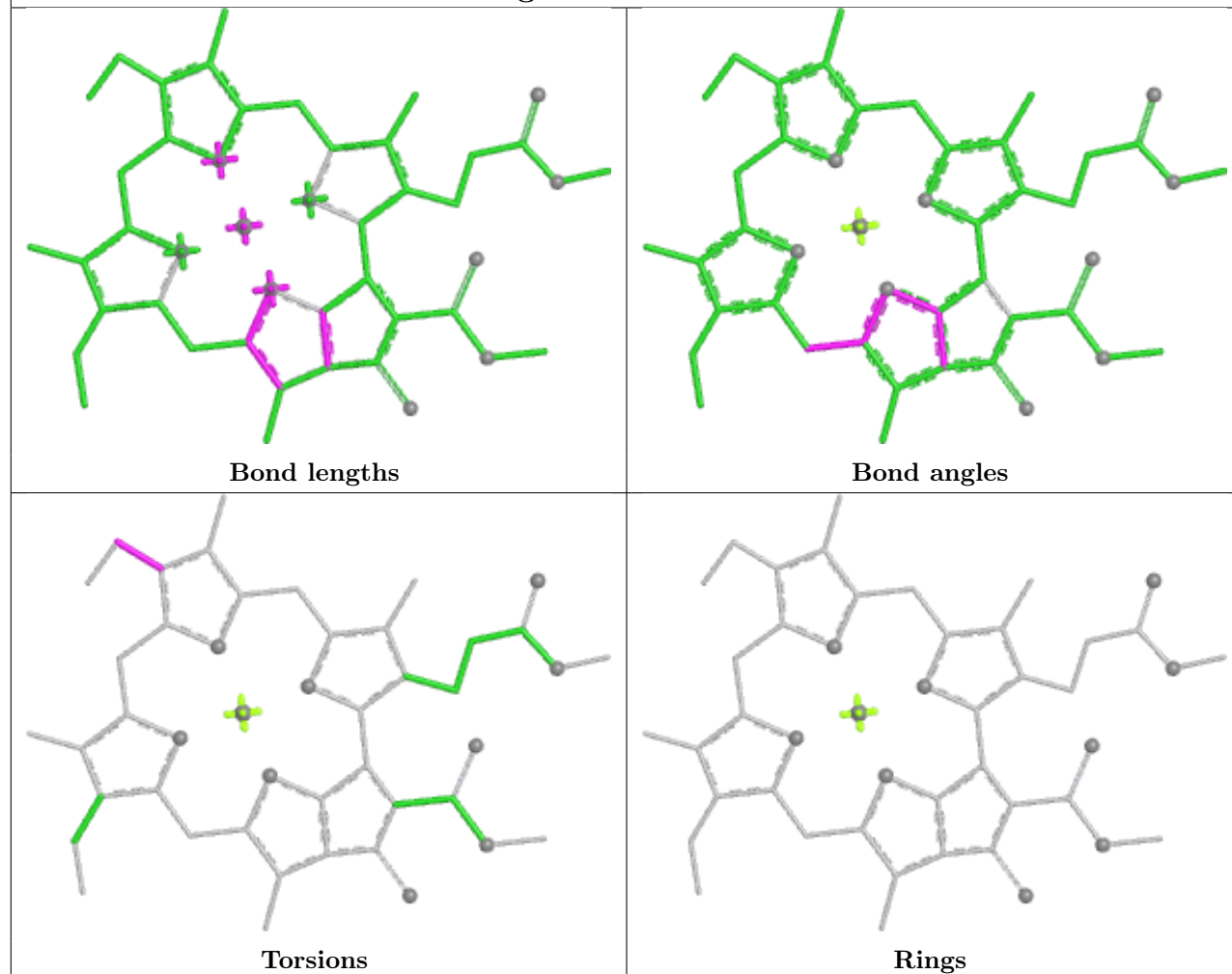




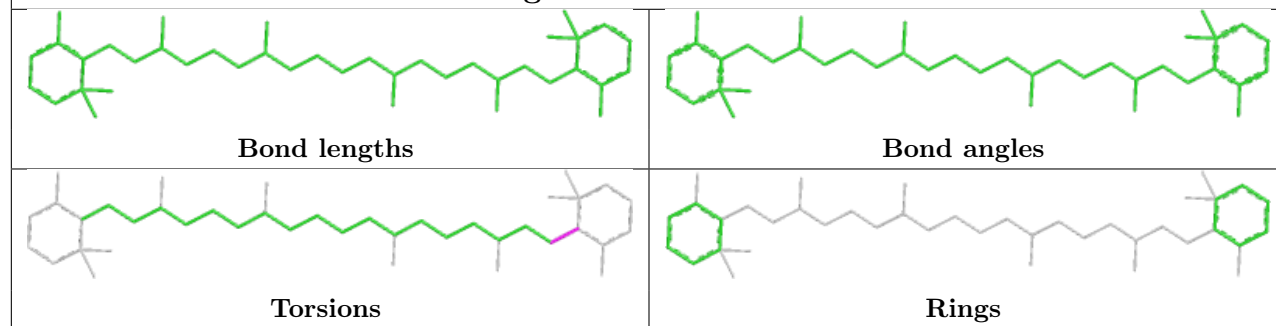


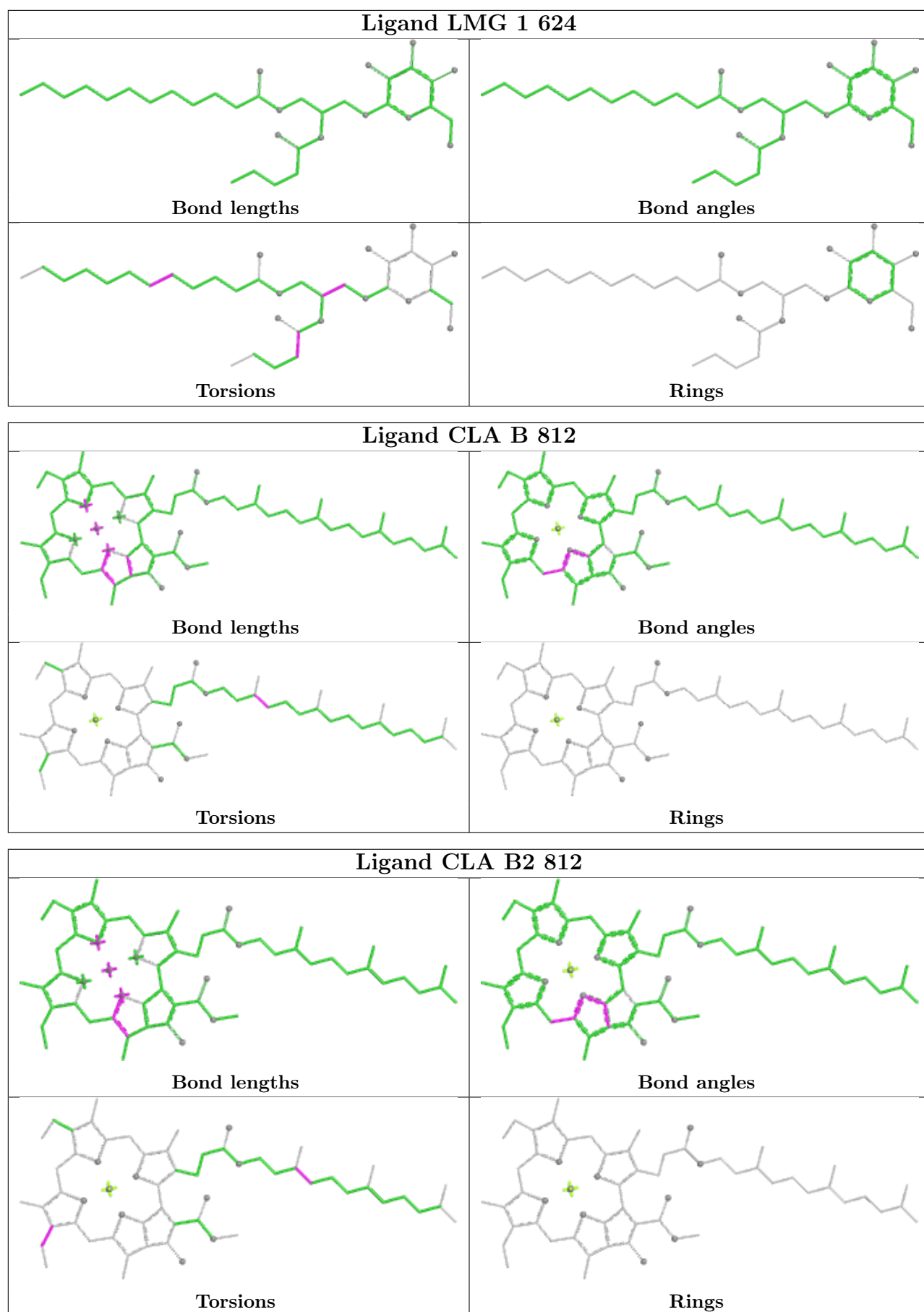


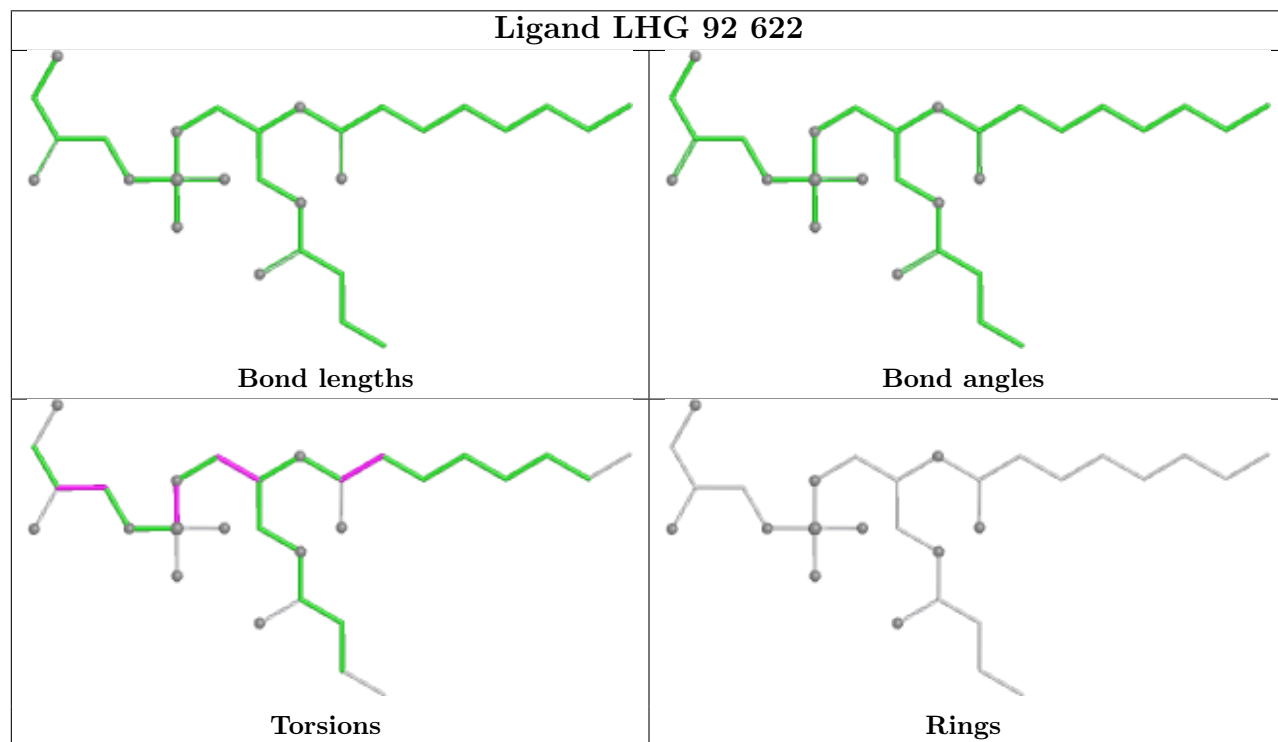
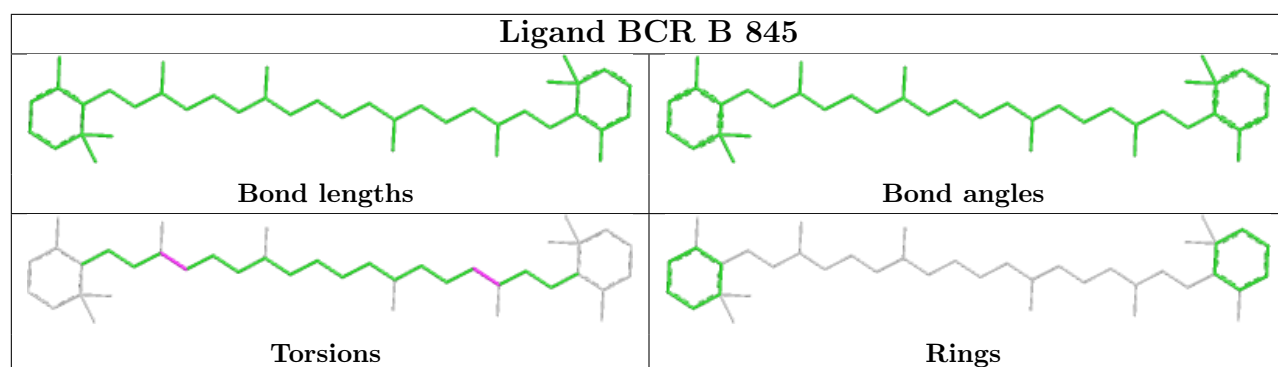
Ligand CLA 3 612

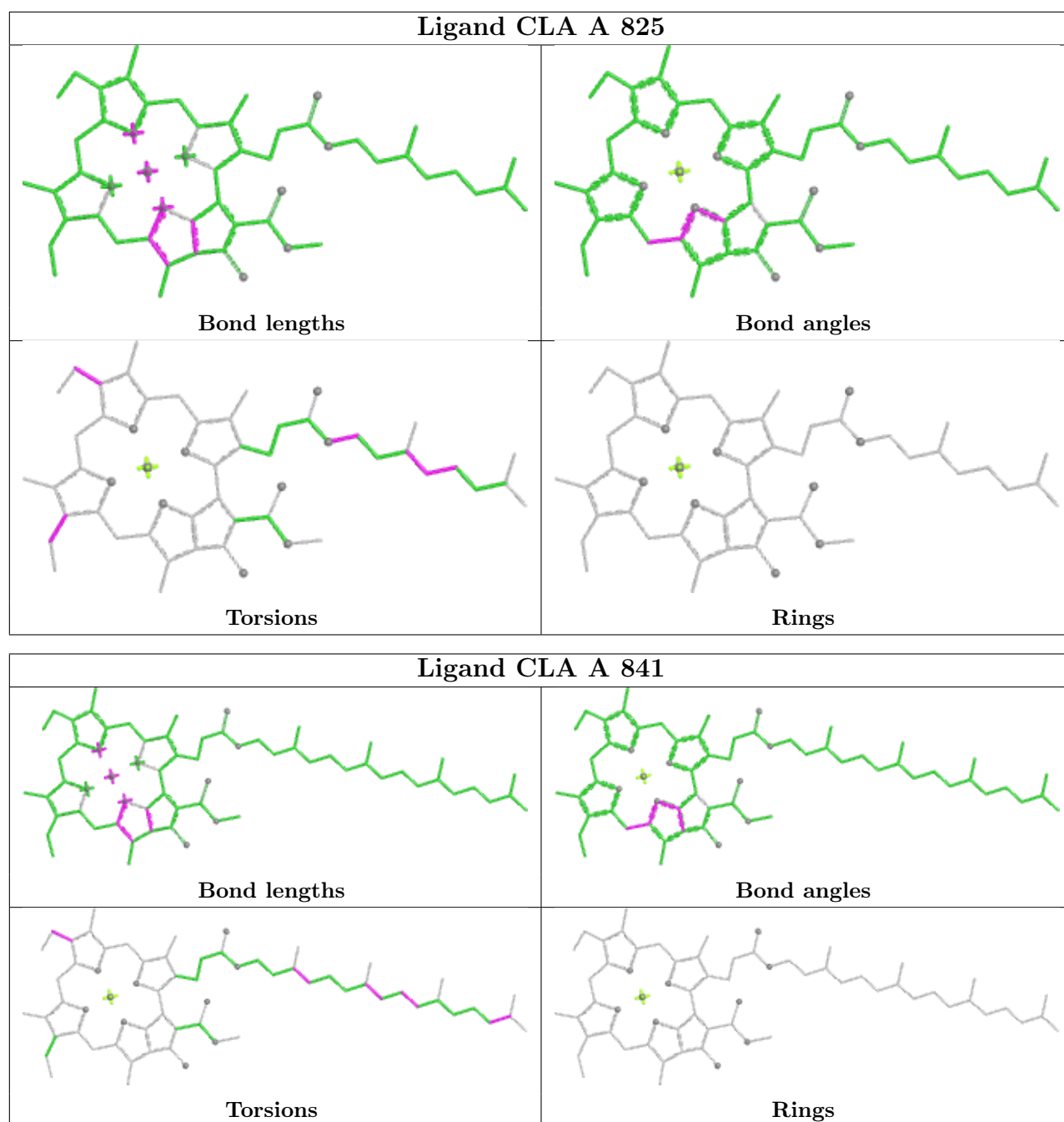


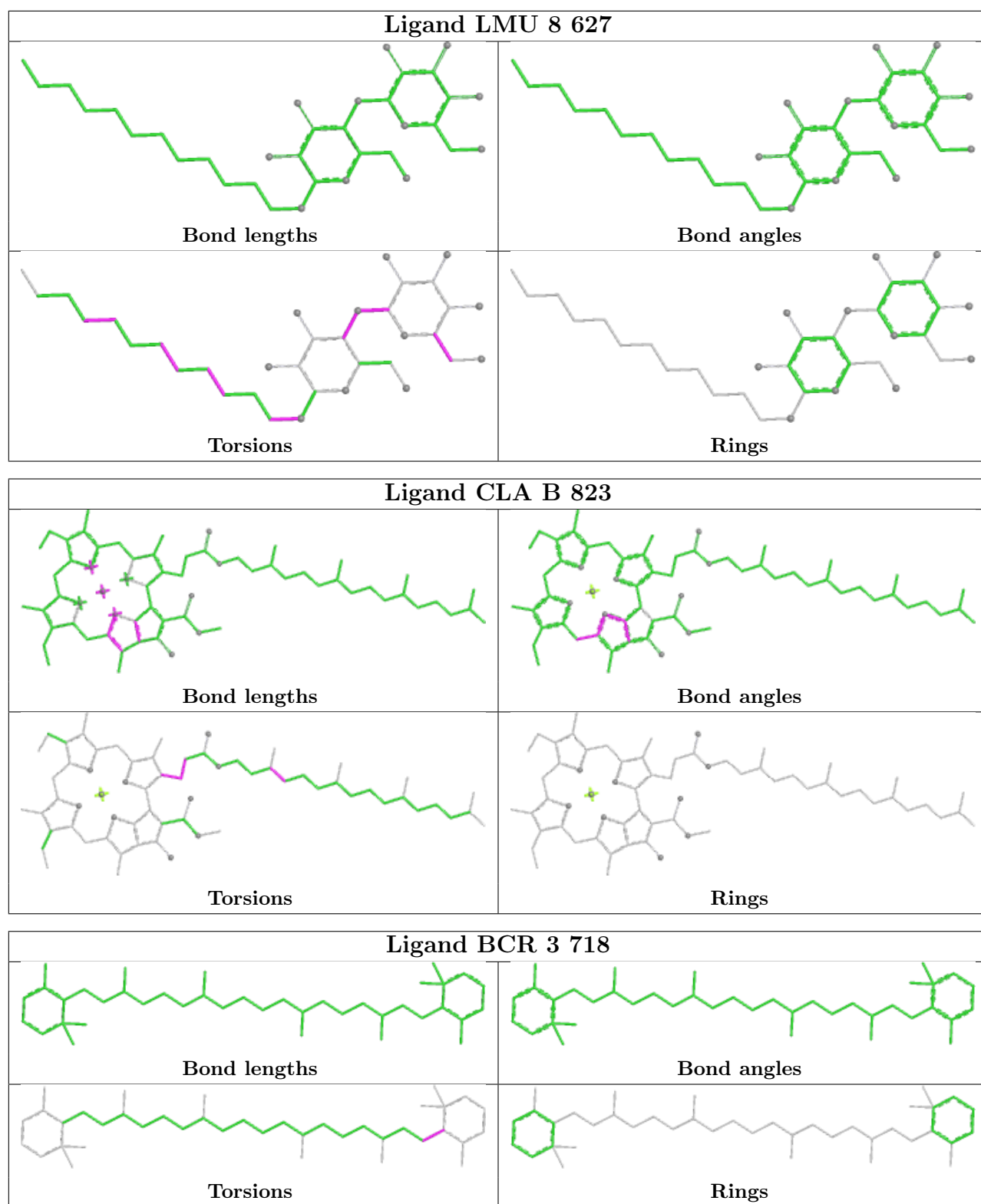
Ligand BCR L2 205

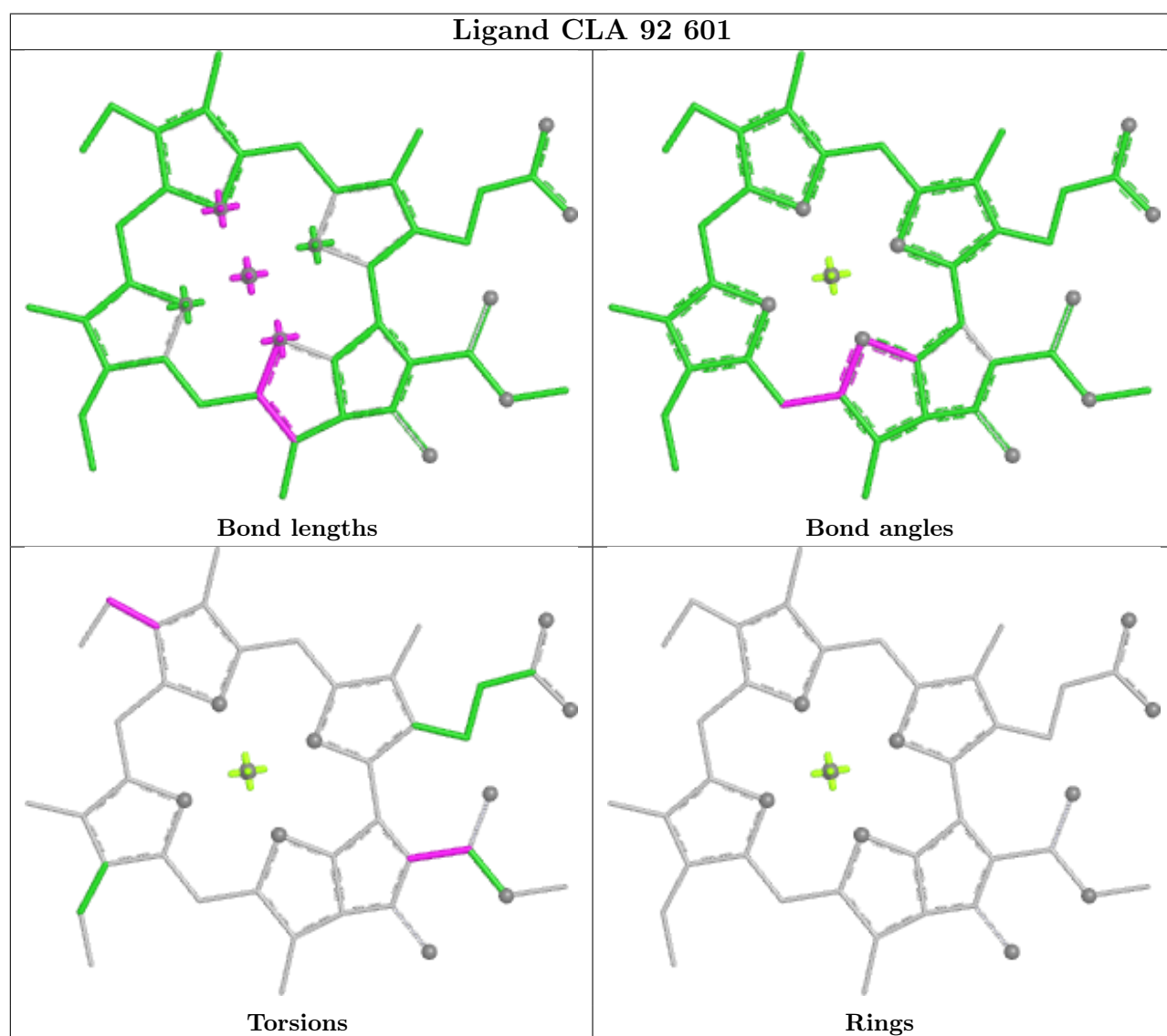
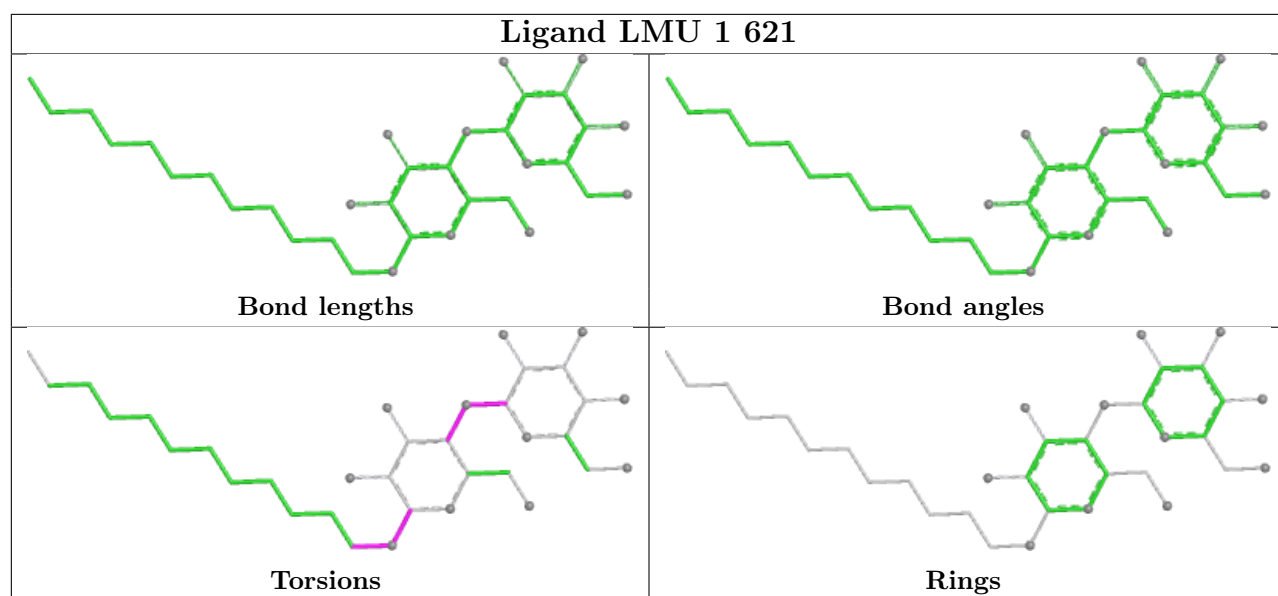


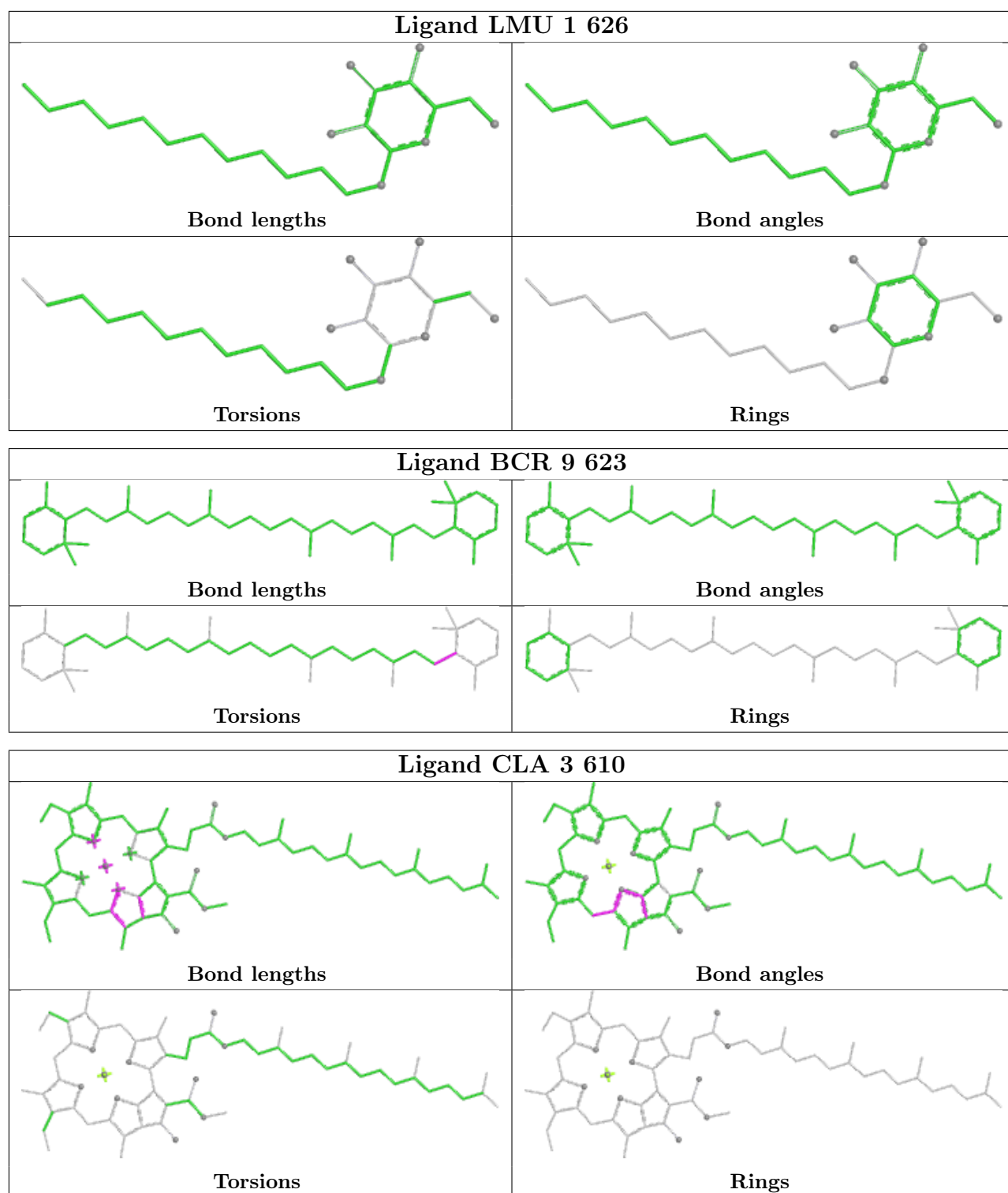




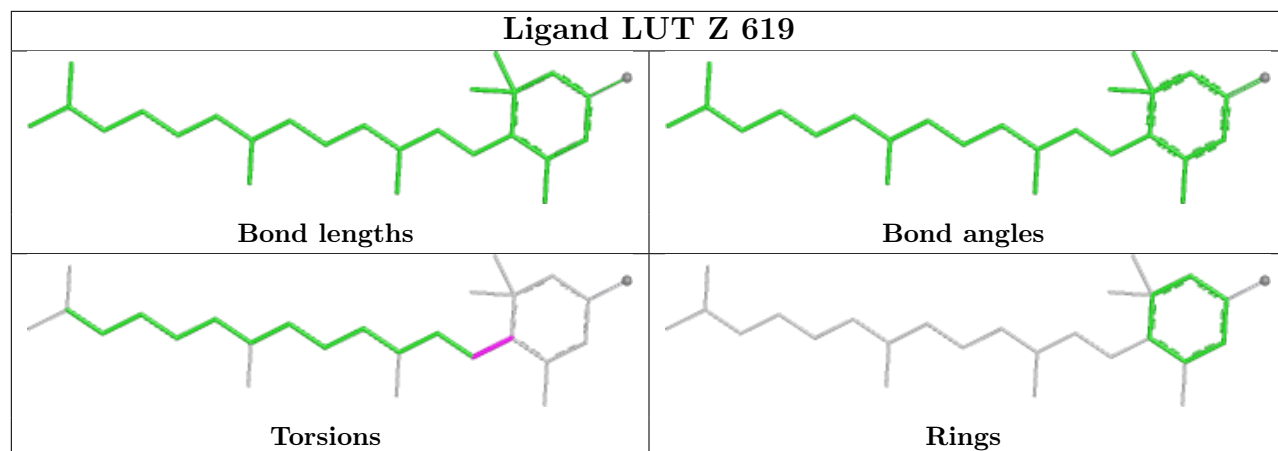




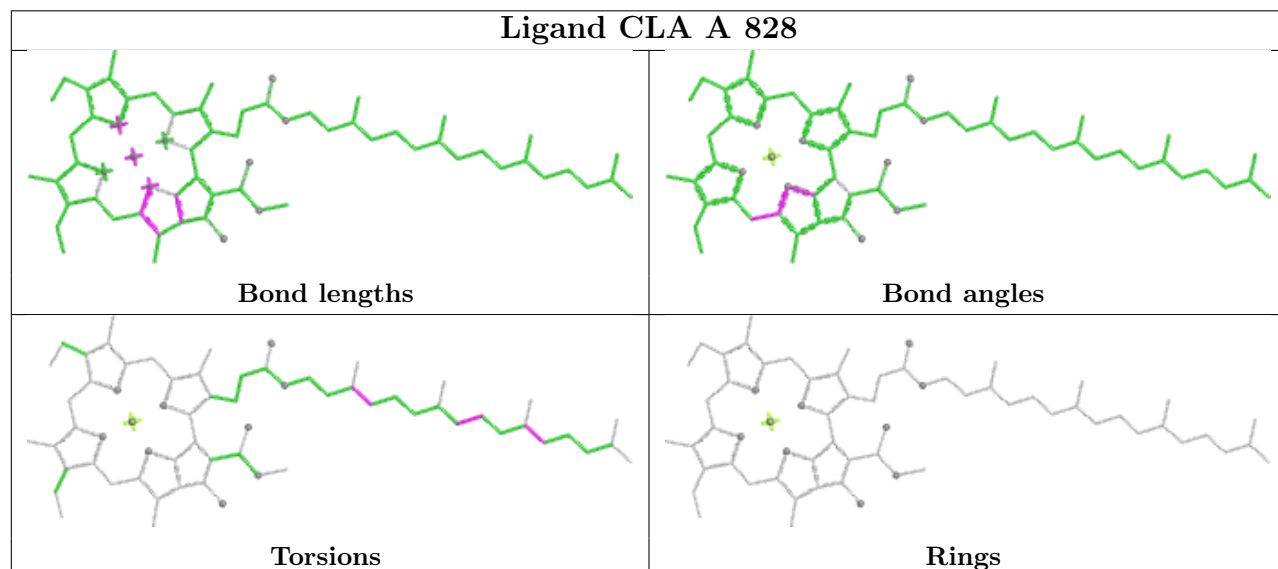




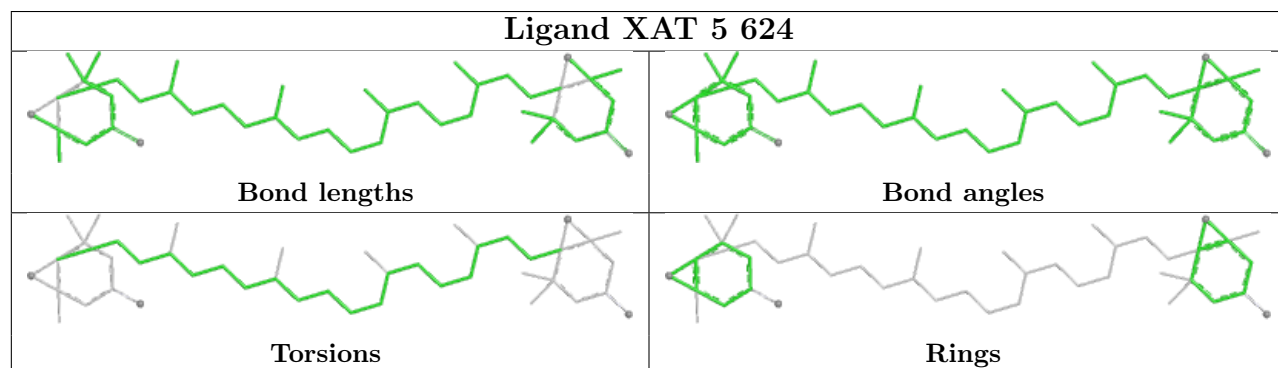
Ligand LUT Z 619

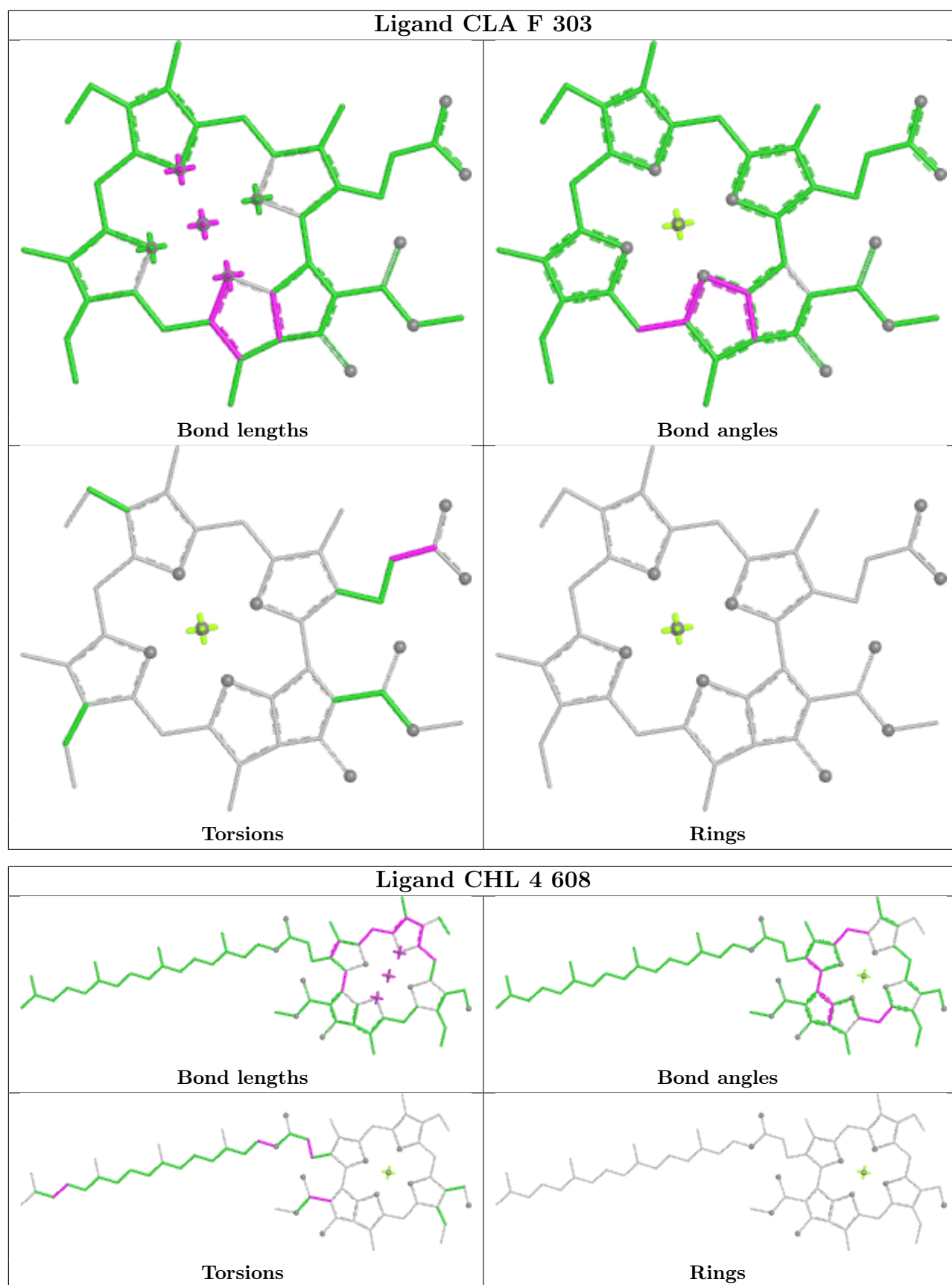


Ligand CLA A 828

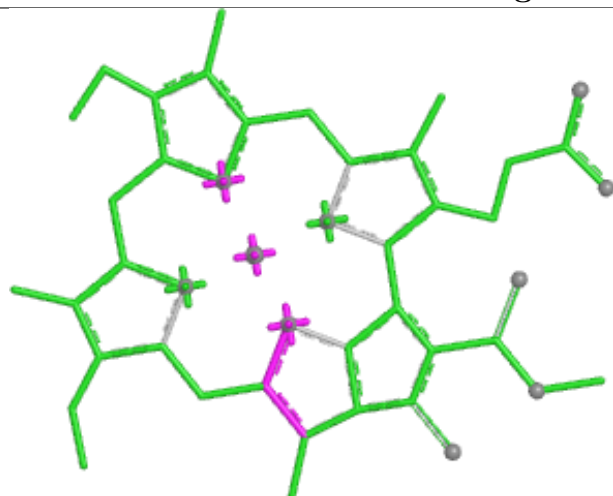


Ligand XAT 5 624

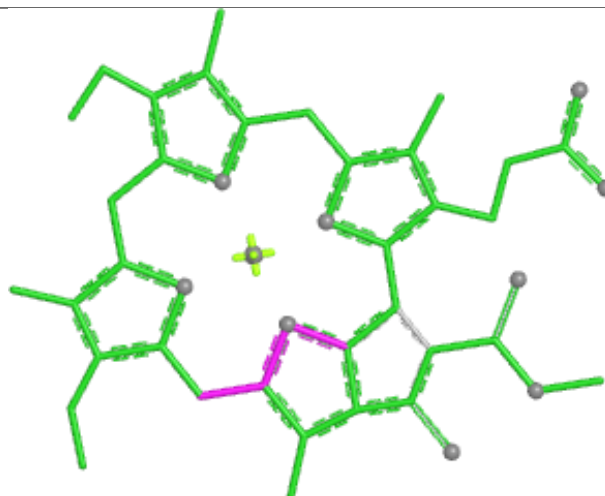




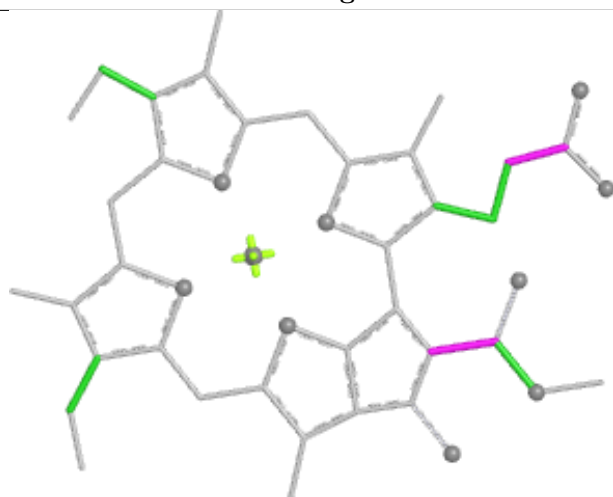
Ligand CLA B 804



Bond lengths



Bond angles

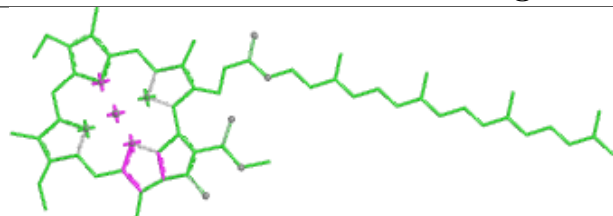


Torsions

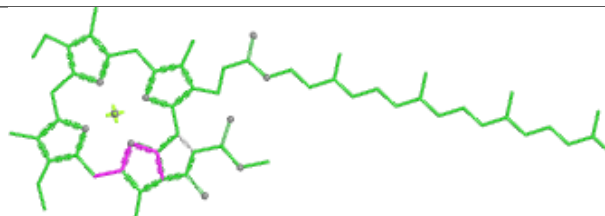


Rings

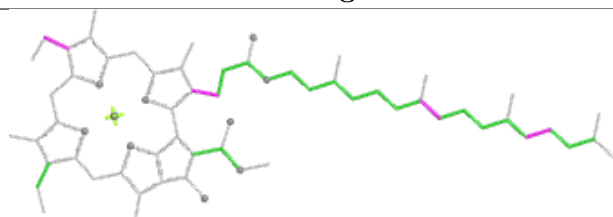
Ligand CLA A 834



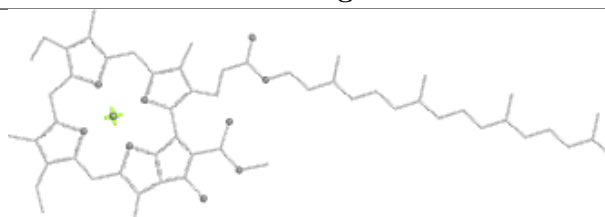
Bond lengths



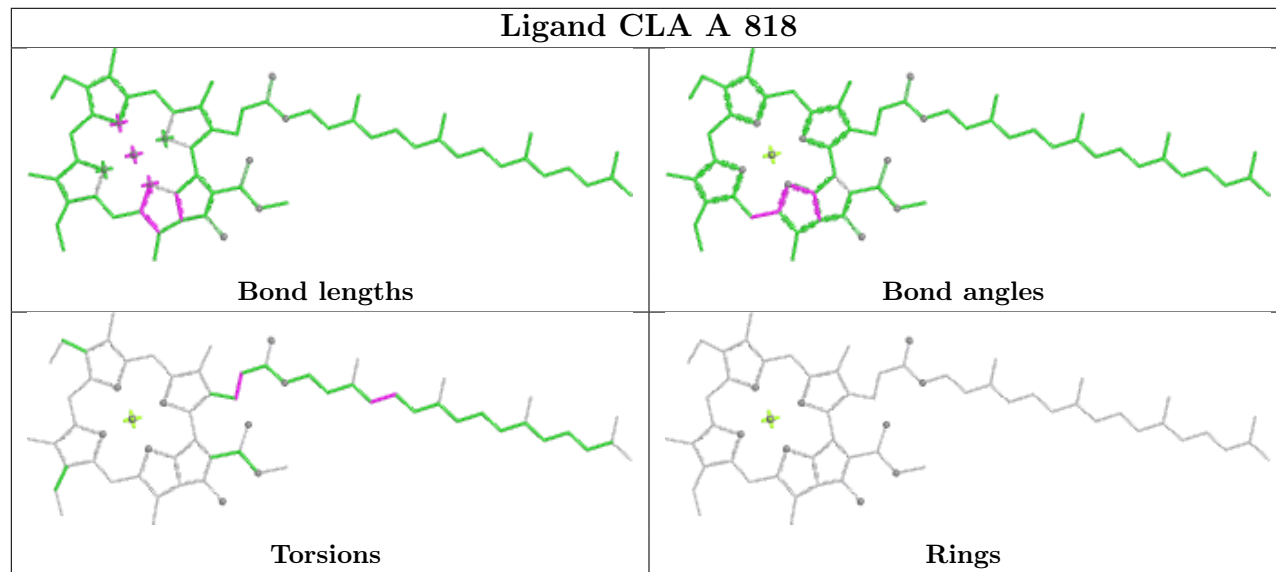
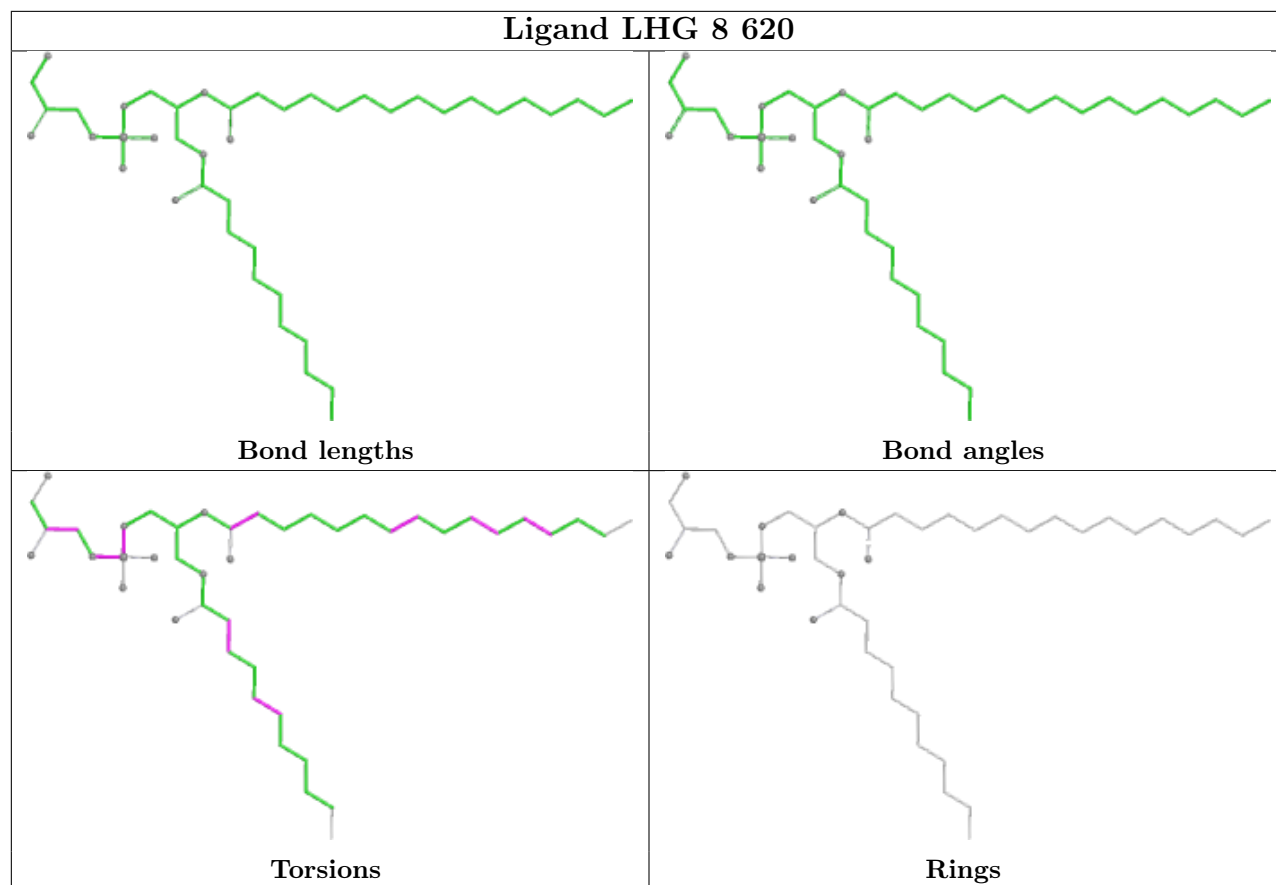
Bond angles

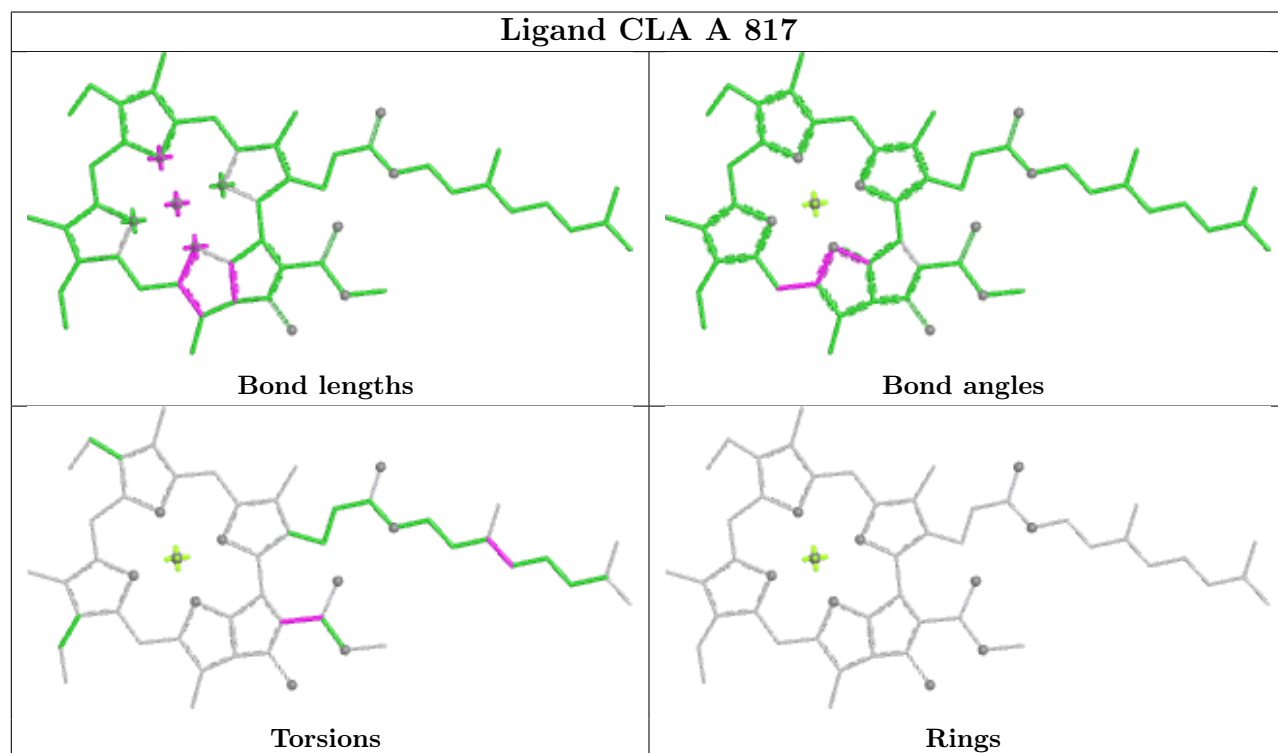
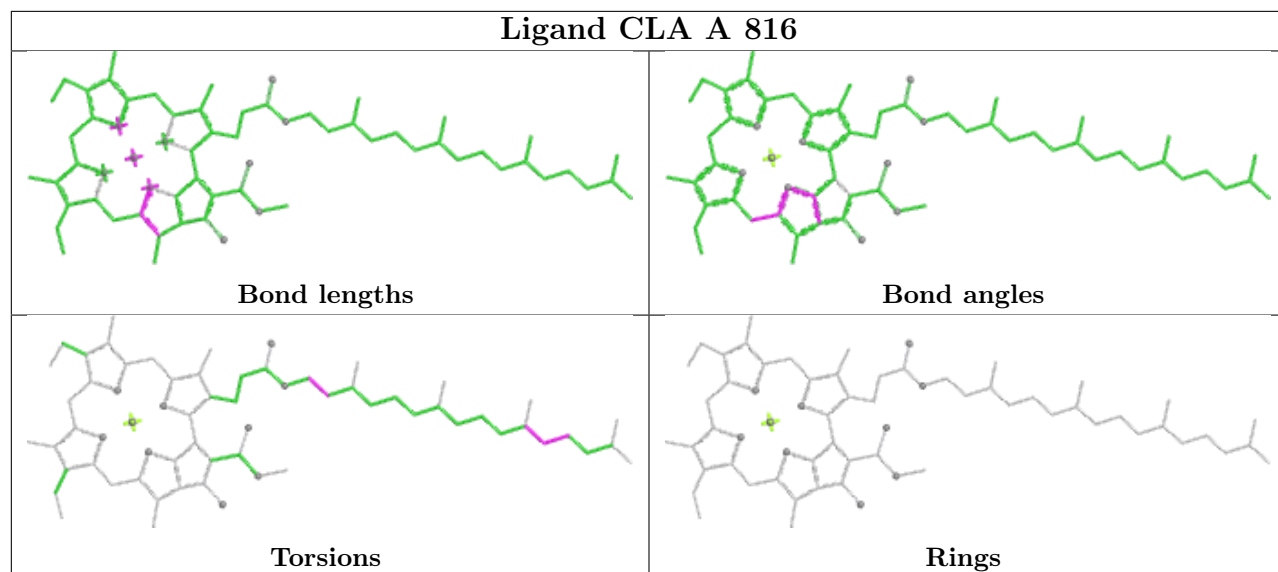


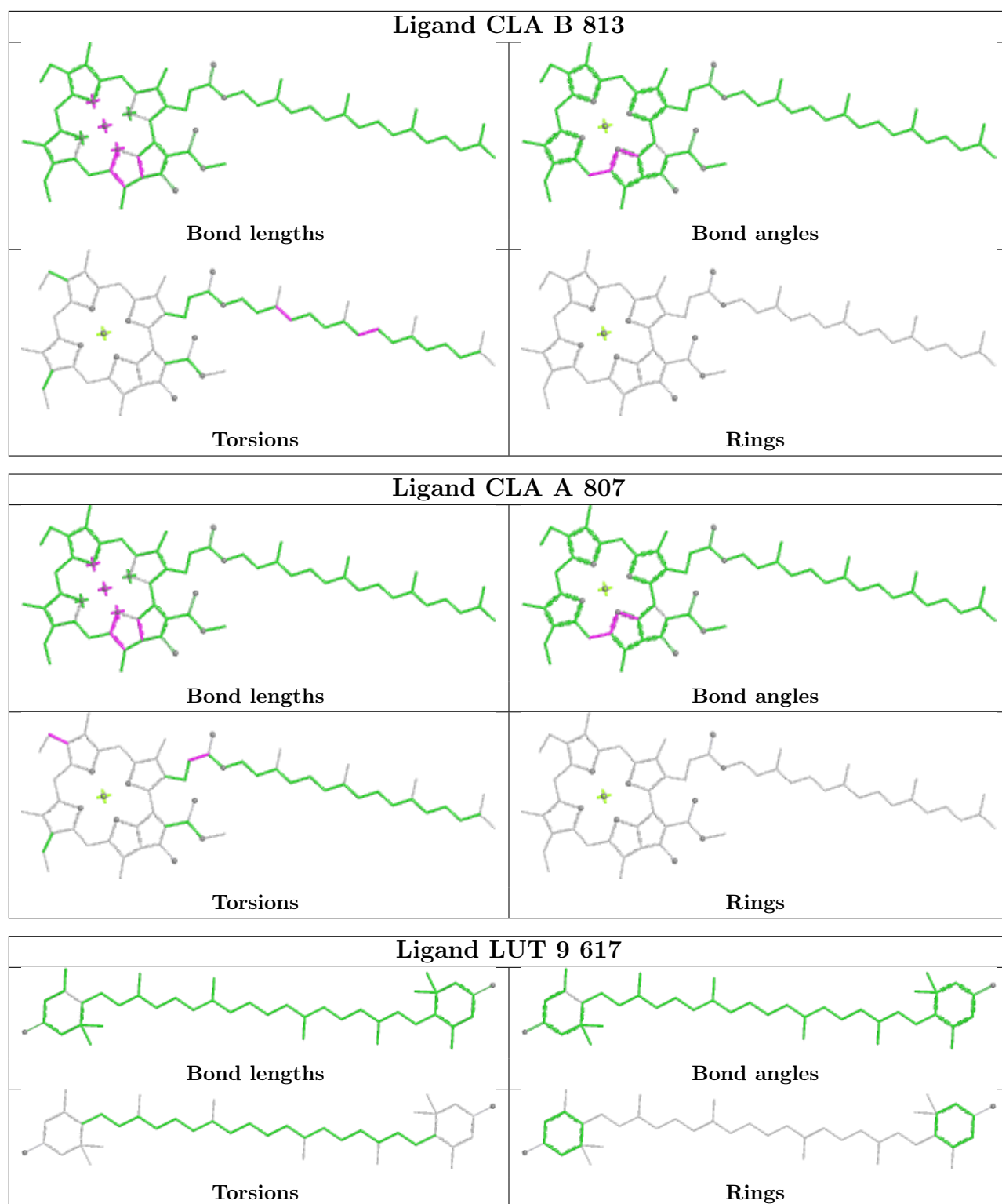
Torsions

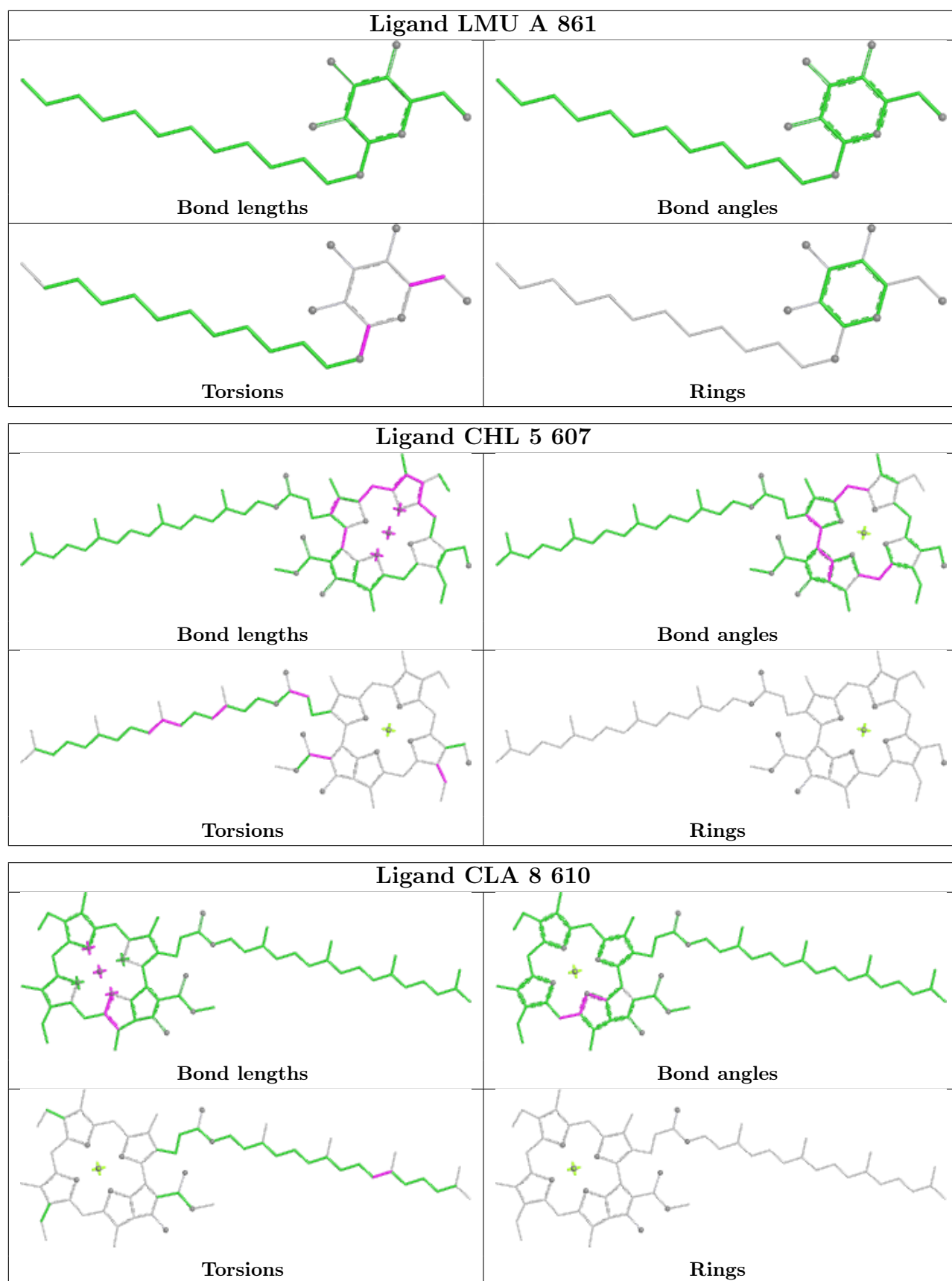


Rings

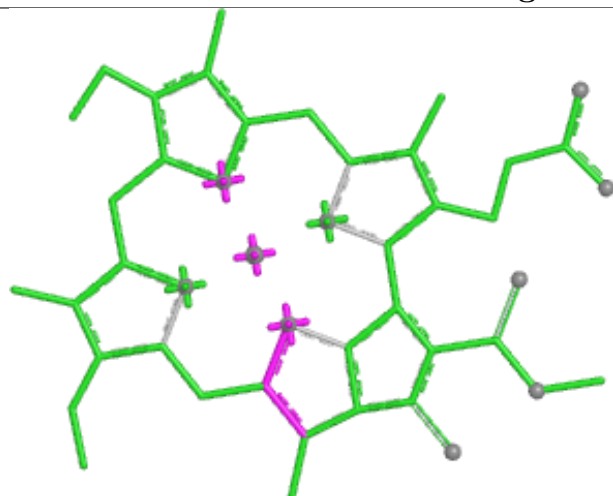




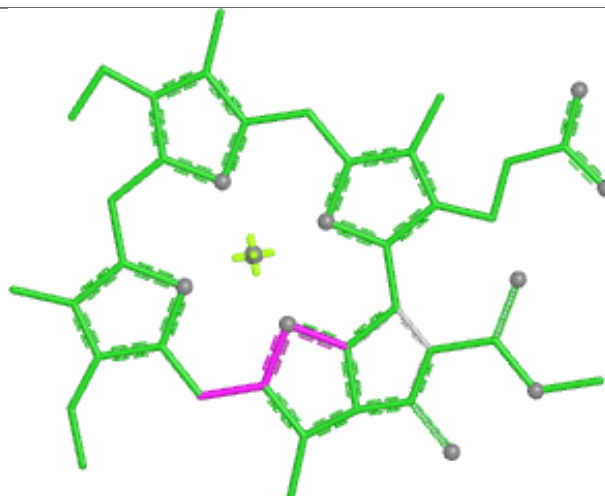




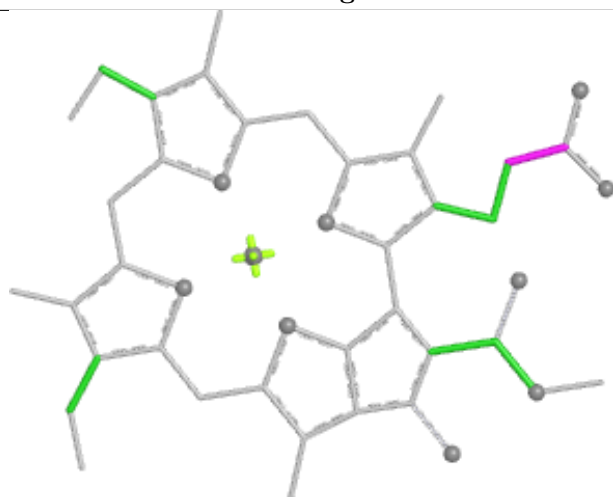
Ligand CLA 6 612



Bond lengths



Bond angles

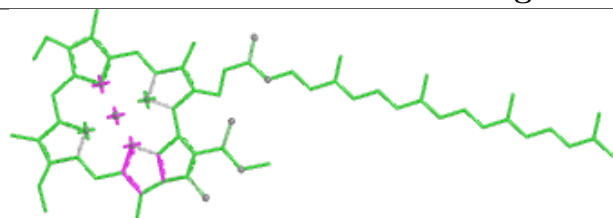


Torsions

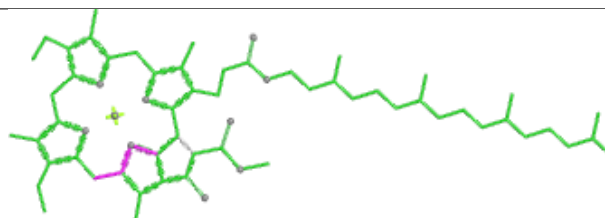


Rings

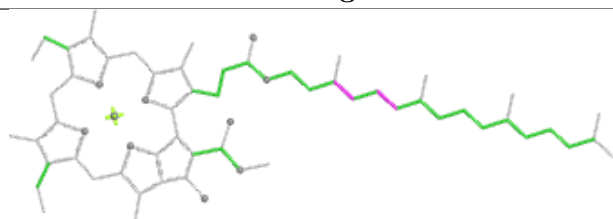
Ligand CLA B 829



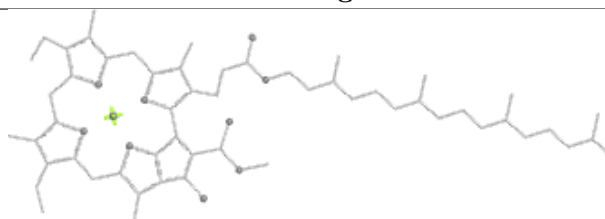
Bond lengths



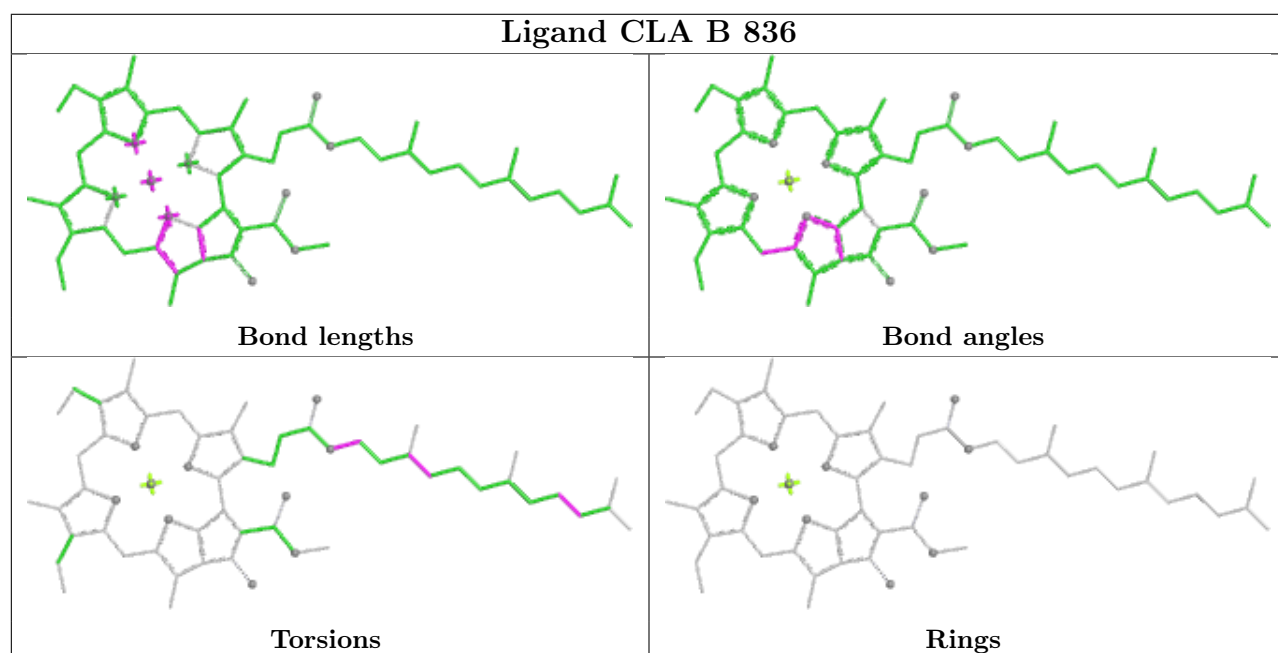
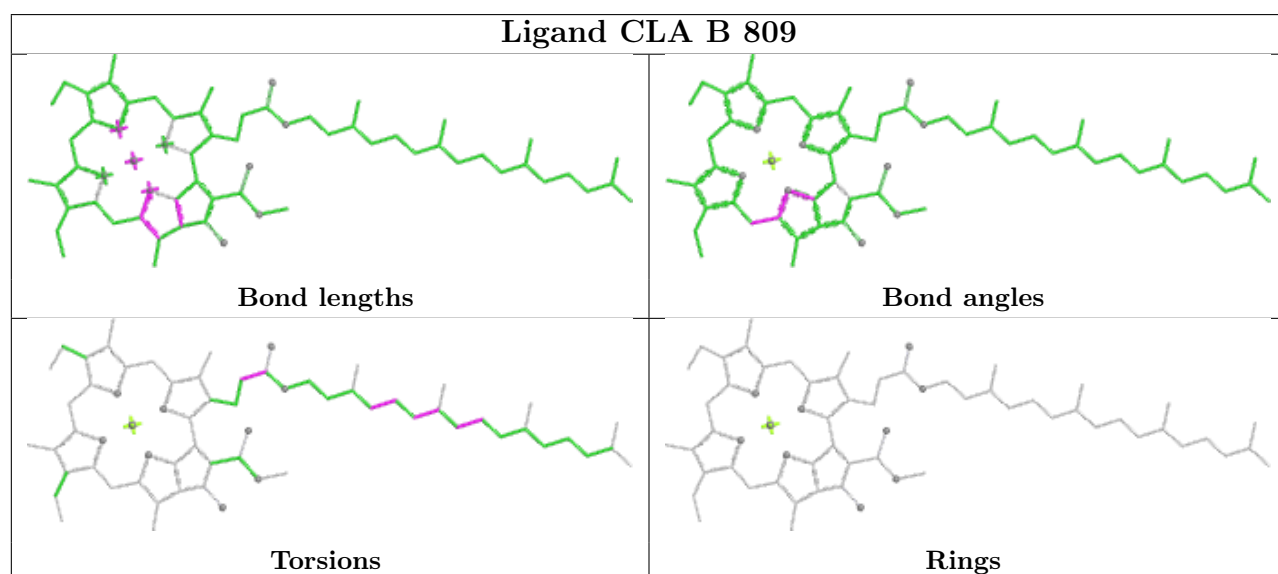
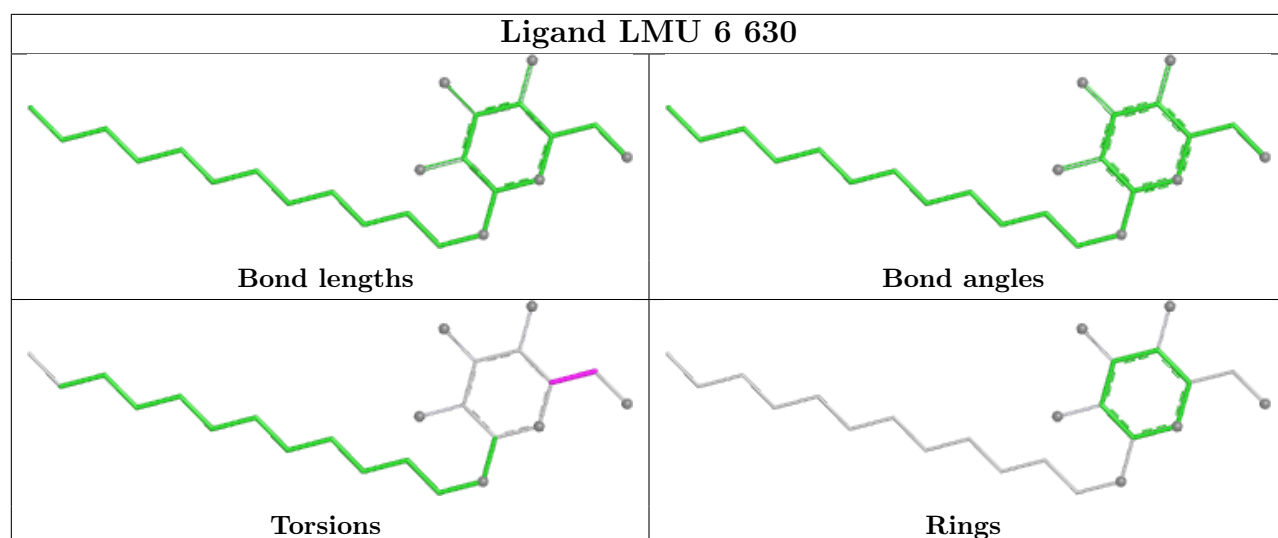
Bond angles

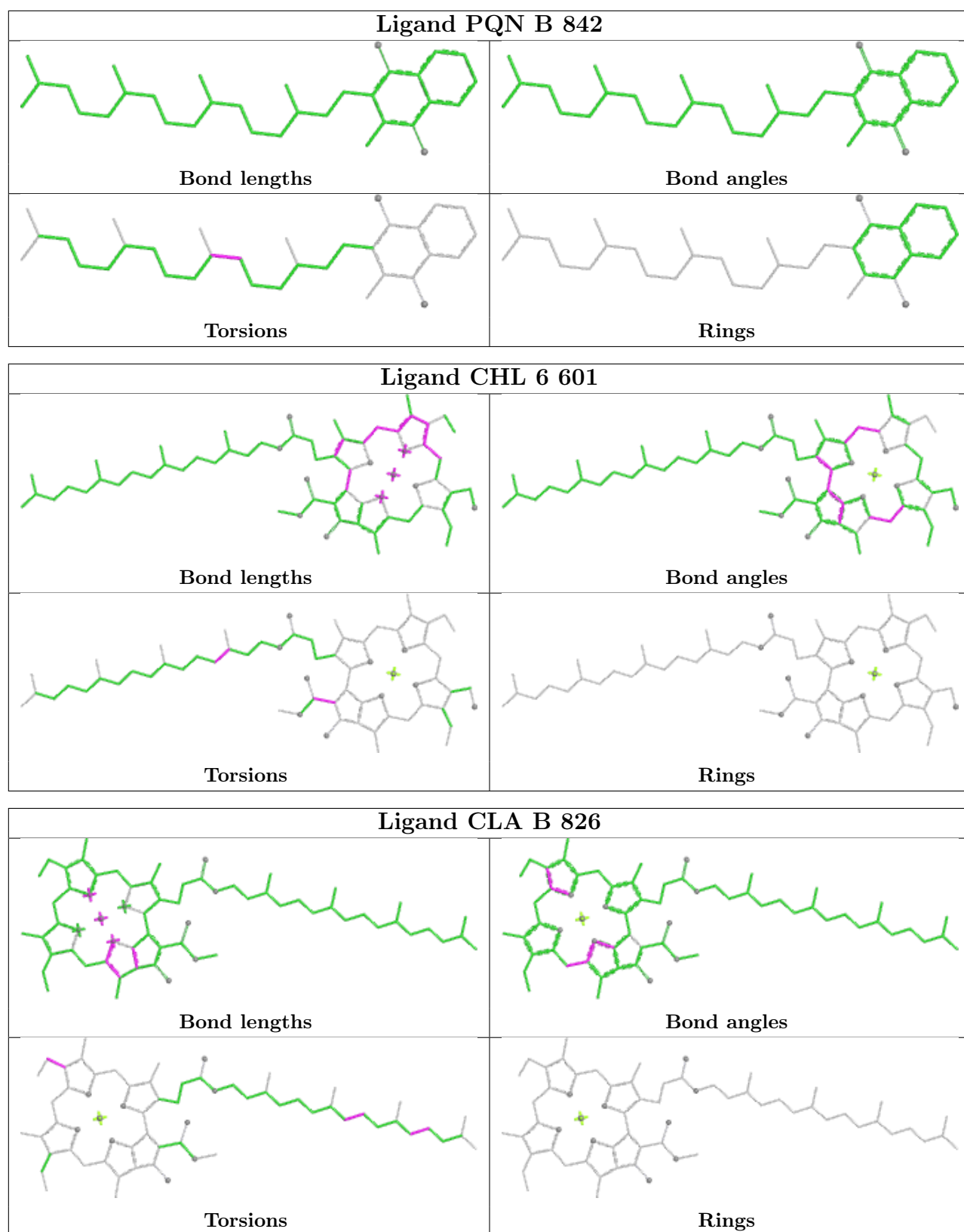


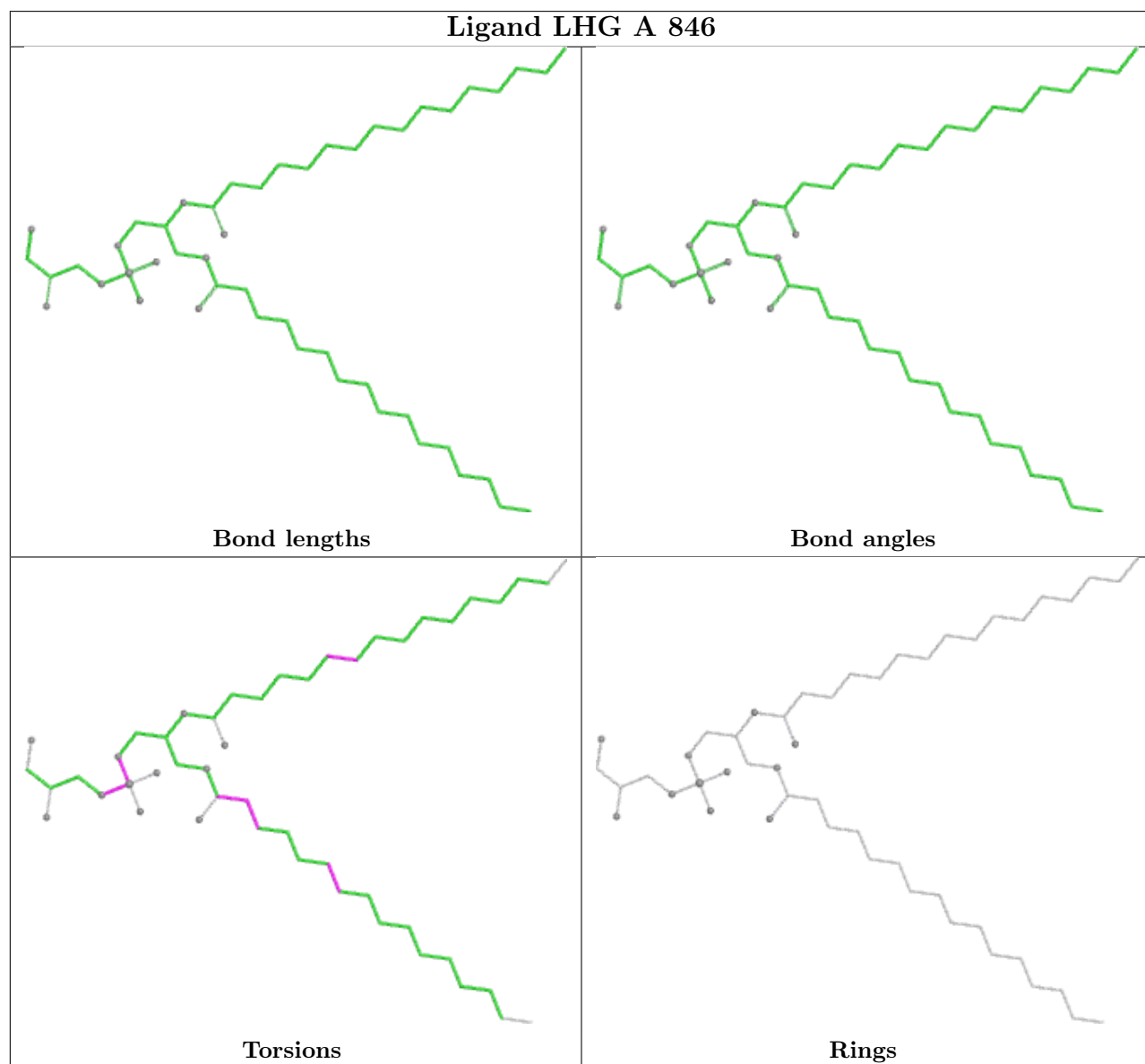
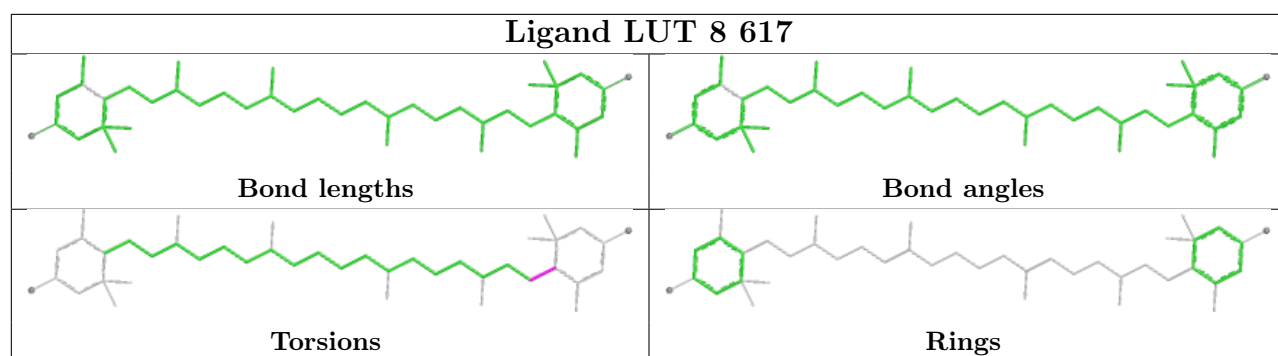
Torsions

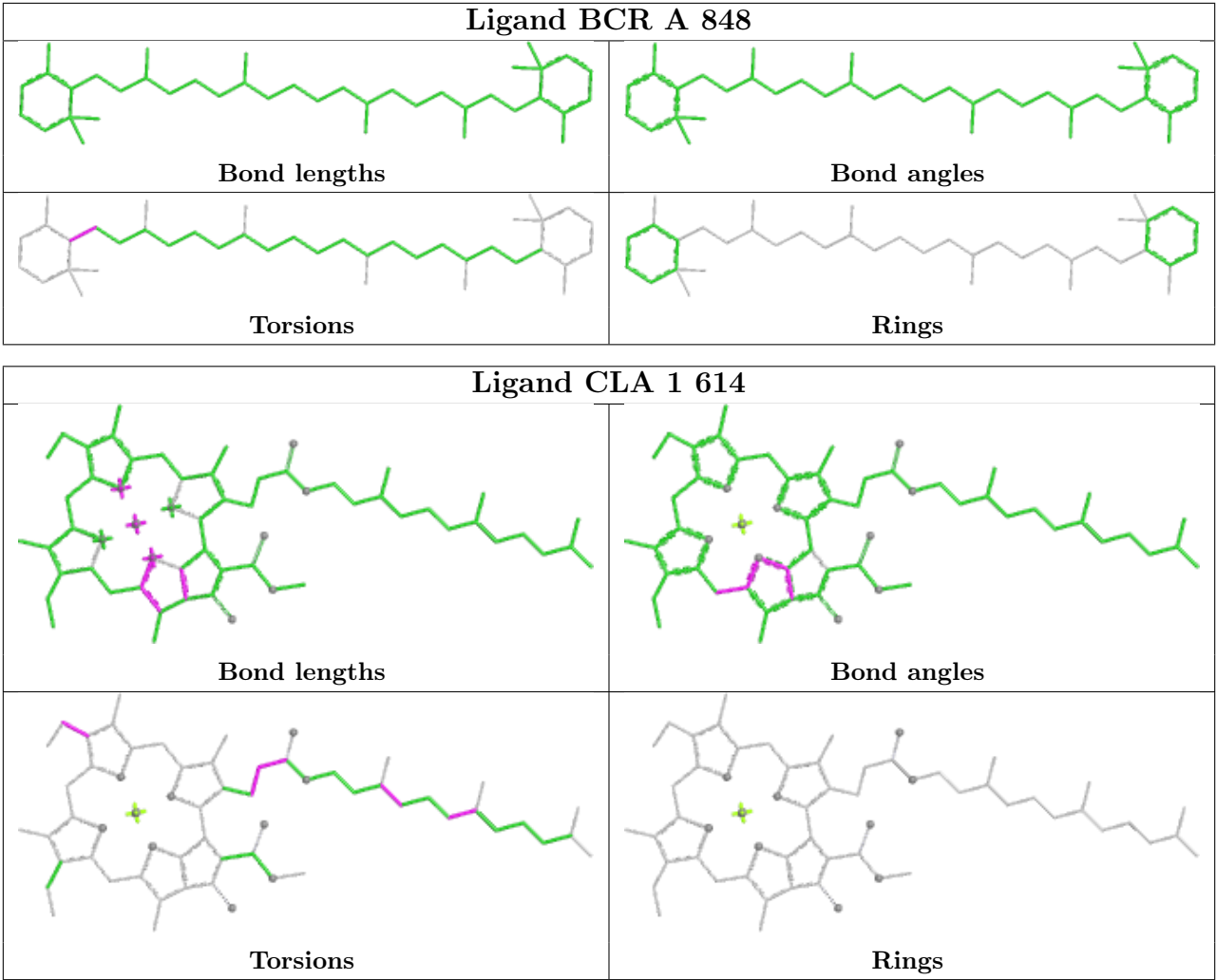


Rings









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
20	B2	6

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B2	218:PRO	C	683:HIS	N	78.76
1	B2	169:PHE	C	191:TRP	N	27.65

Continued on next page...

Continued from previous page...

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B2	115:ASN	C	128:ILE	N	22.89
1	B2	77:GLN	C	88:ILE	N	9.86
1	B2	107:ARG	C	112:GLY	N	7.45

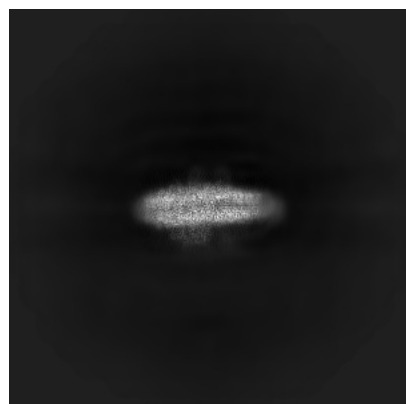
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14867. These allow visual inspection of the internal detail of the map and identification of artifacts.

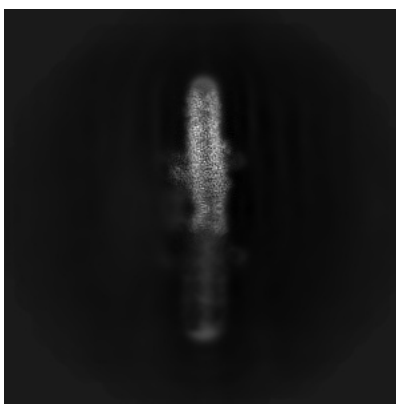
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

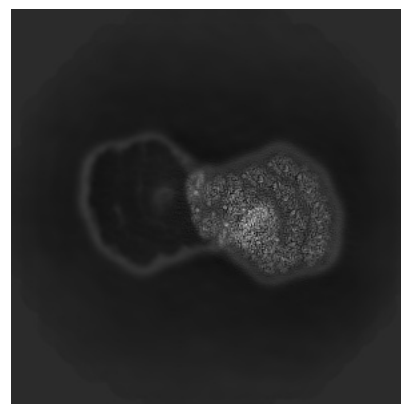
6.1.1 Primary map



X

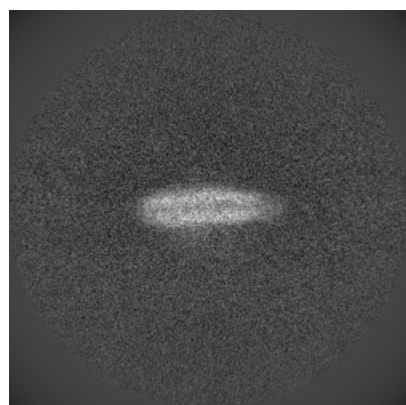


Y

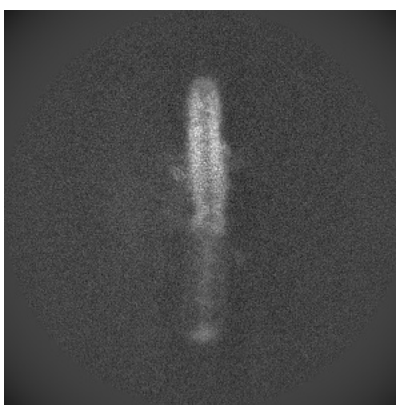


Z

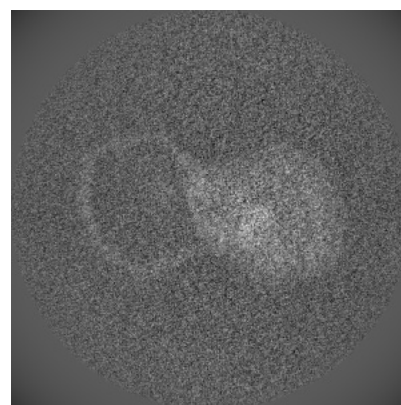
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices [i](#)

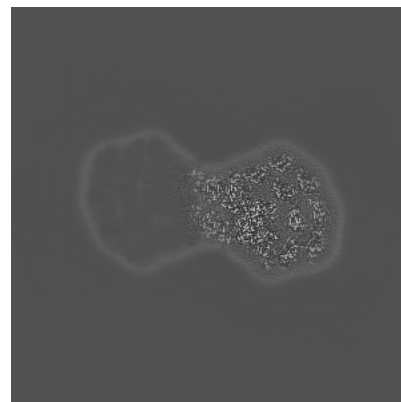
6.2.1 Primary map



X Index: 350

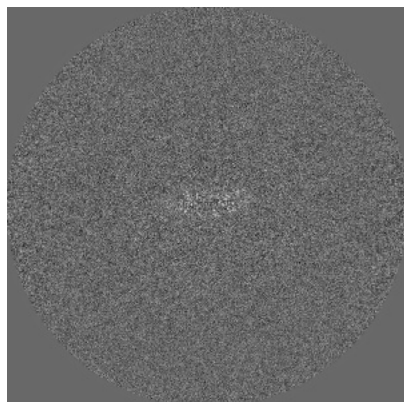


Y Index: 350

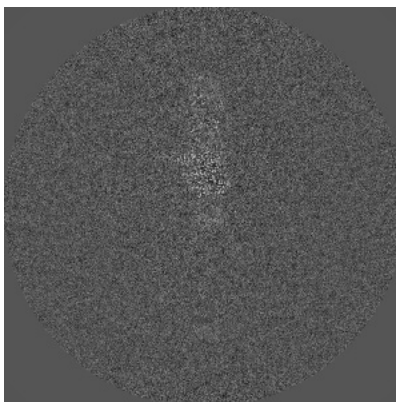


Z Index: 350

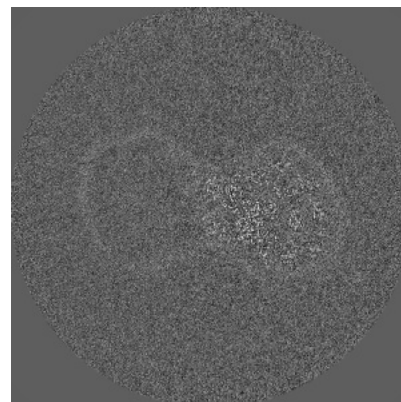
6.2.2 Raw map



X Index: 350



Y Index: 350



Z Index: 350

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

6.3 Largest variance slices [i](#)

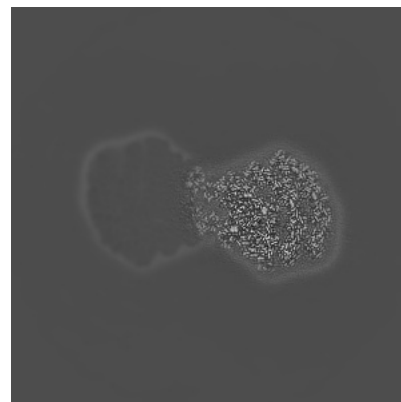
6.3.1 Primary map



X Index: 416

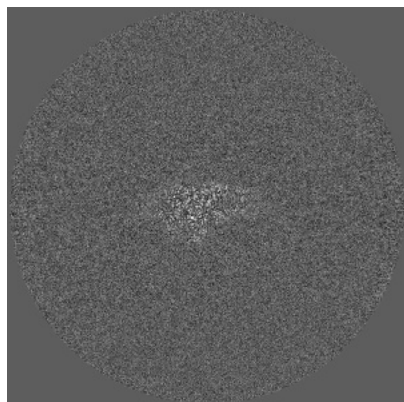


Y Index: 323

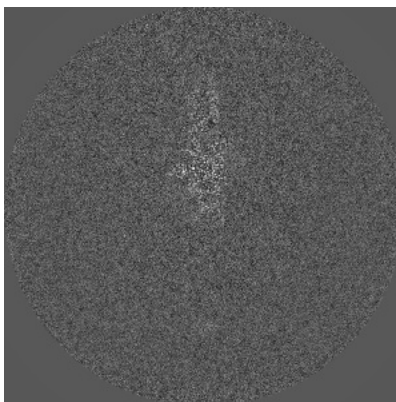


Z Index: 340

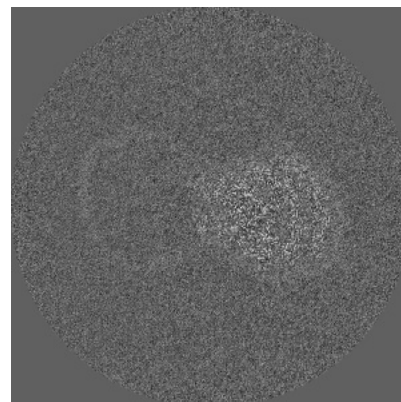
6.3.2 Raw map



X Index: 415



Y Index: 323

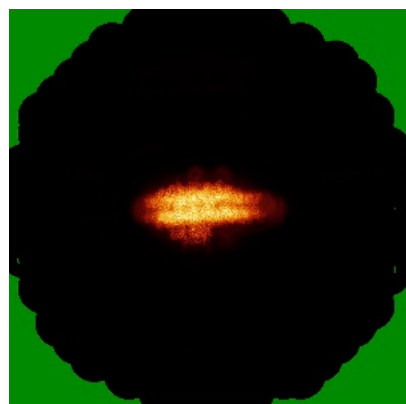


Z Index: 340

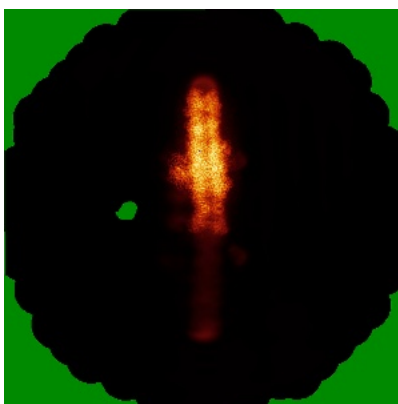
The images above show the largest variance slices of the map in three orthogonal directions.

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

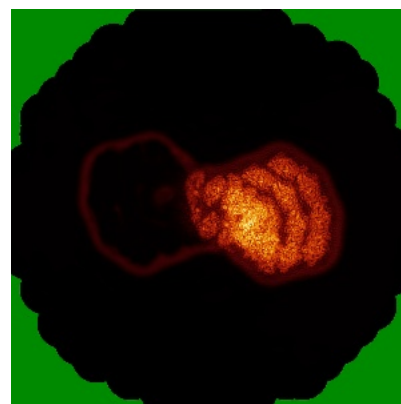
6.4.1 Primary map



X

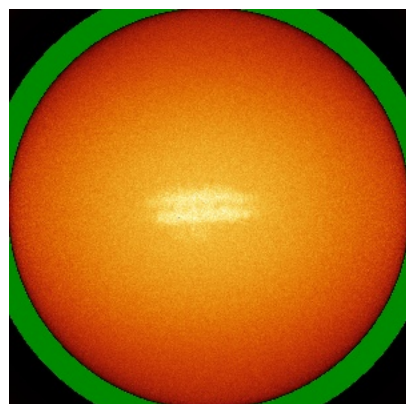


Y

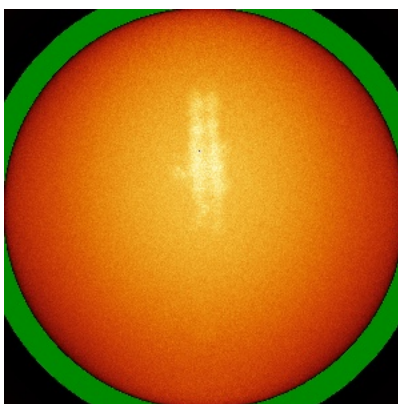


Z

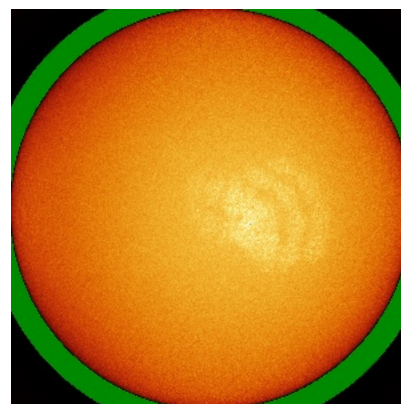
6.4.2 Raw map



X



Y

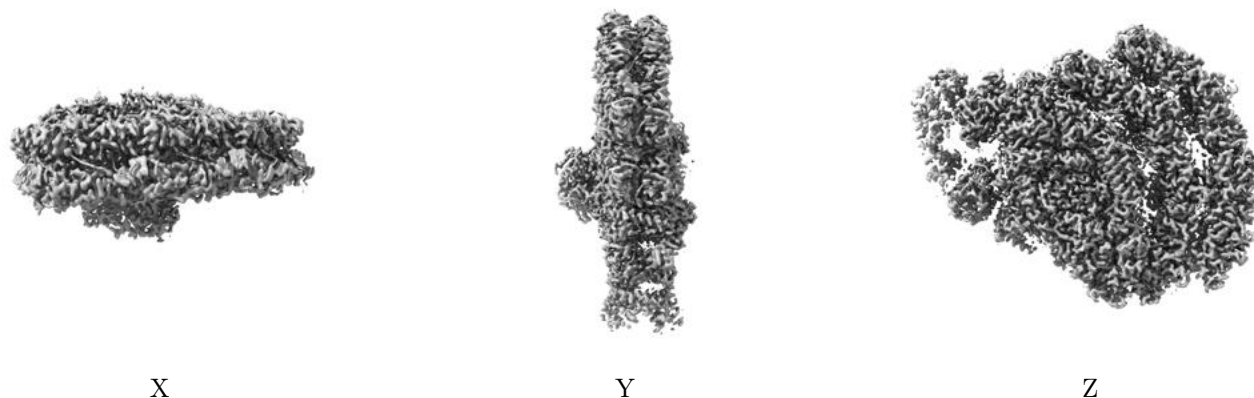


Z

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.

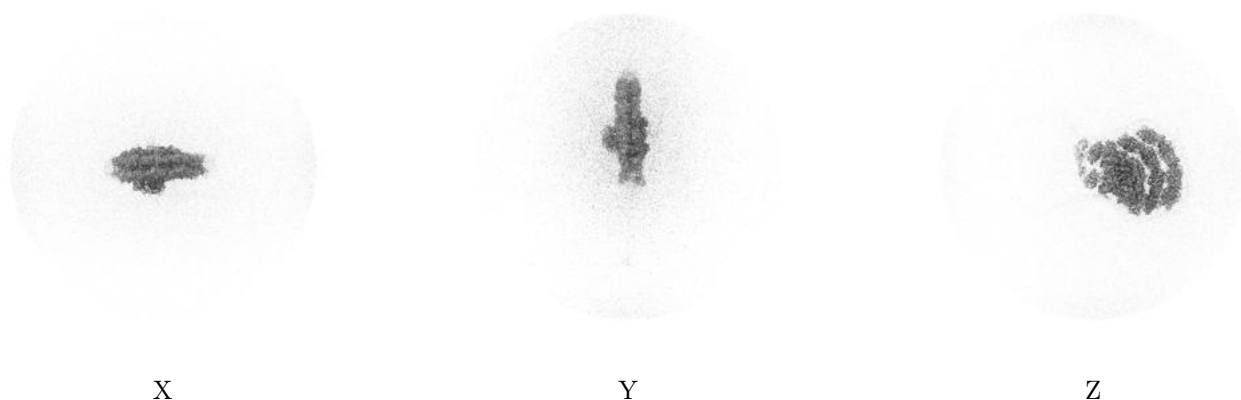
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.031. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

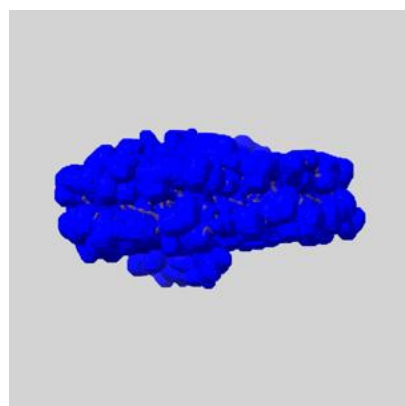
6.6 Mask visualisation [i](#)

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

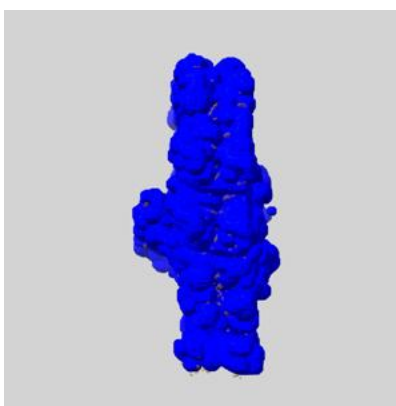
A mask typically either:

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

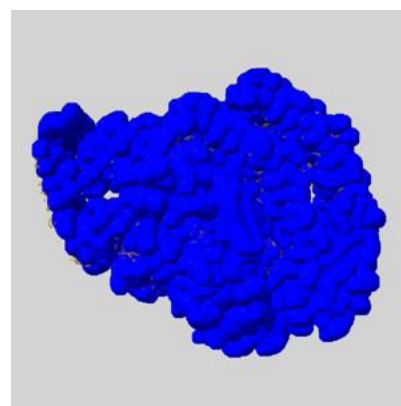
6.6.1 emd_14867_msk_1.map [i](#)



X



Y

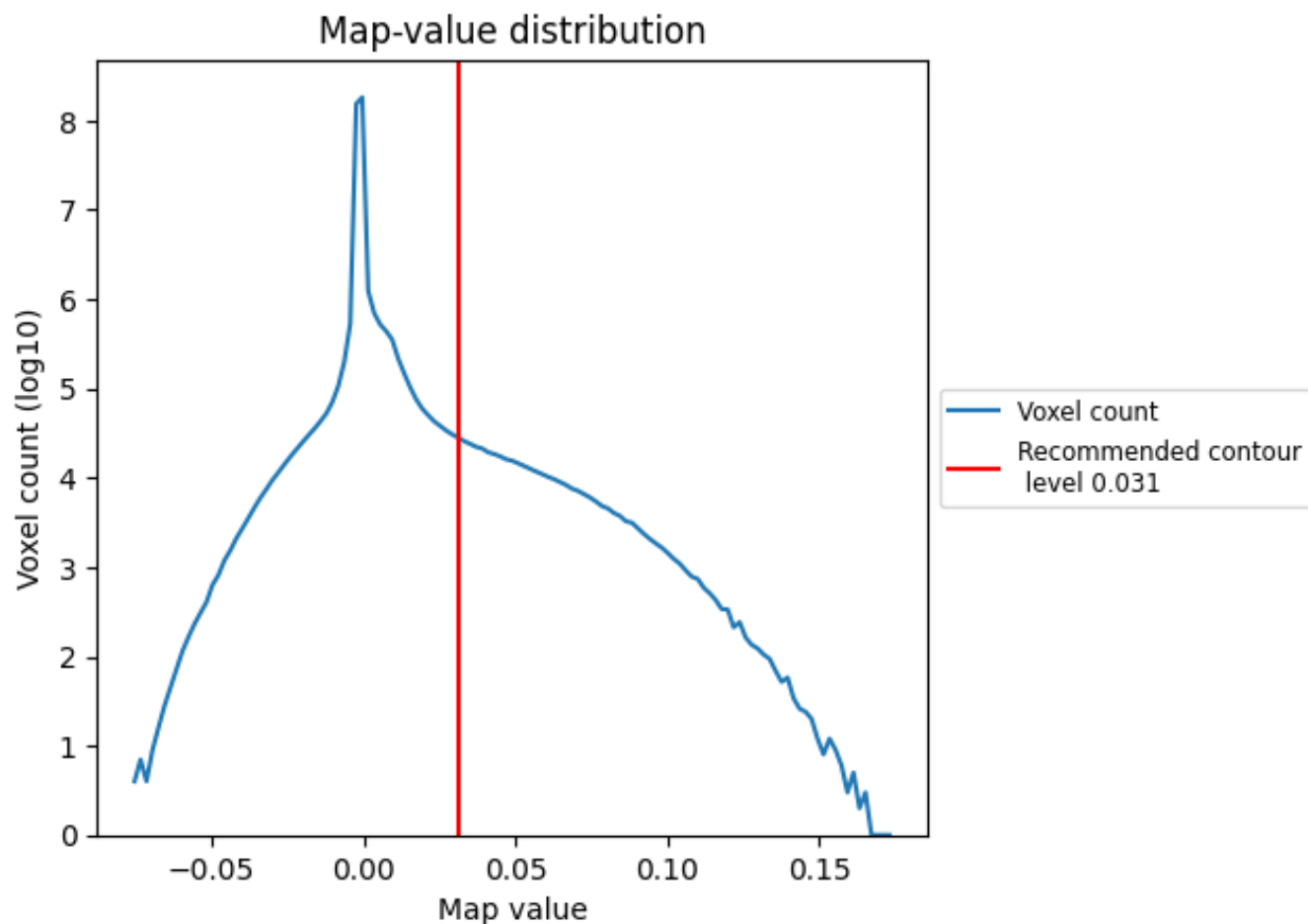


Z

7 Map analysis [i](#)

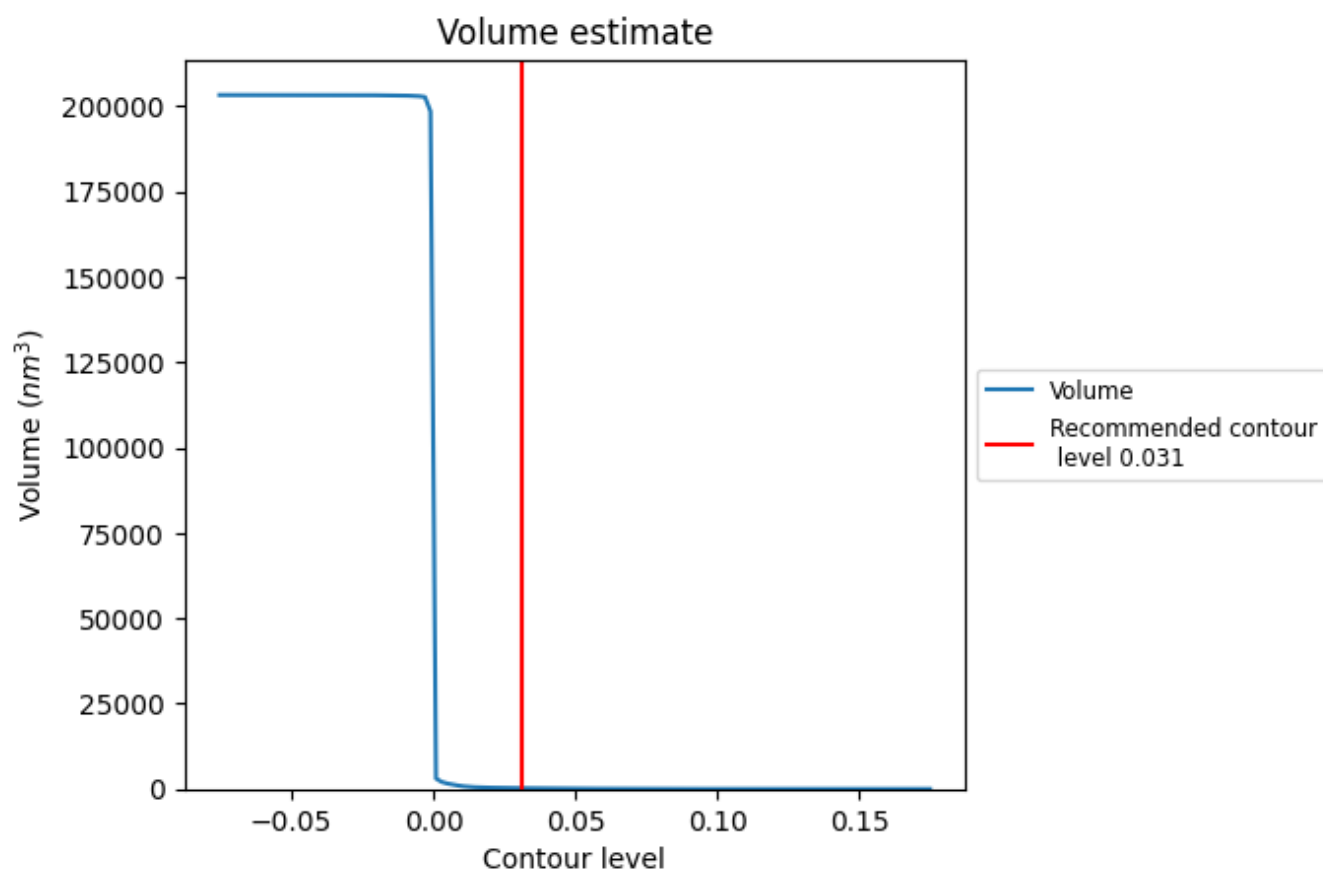
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

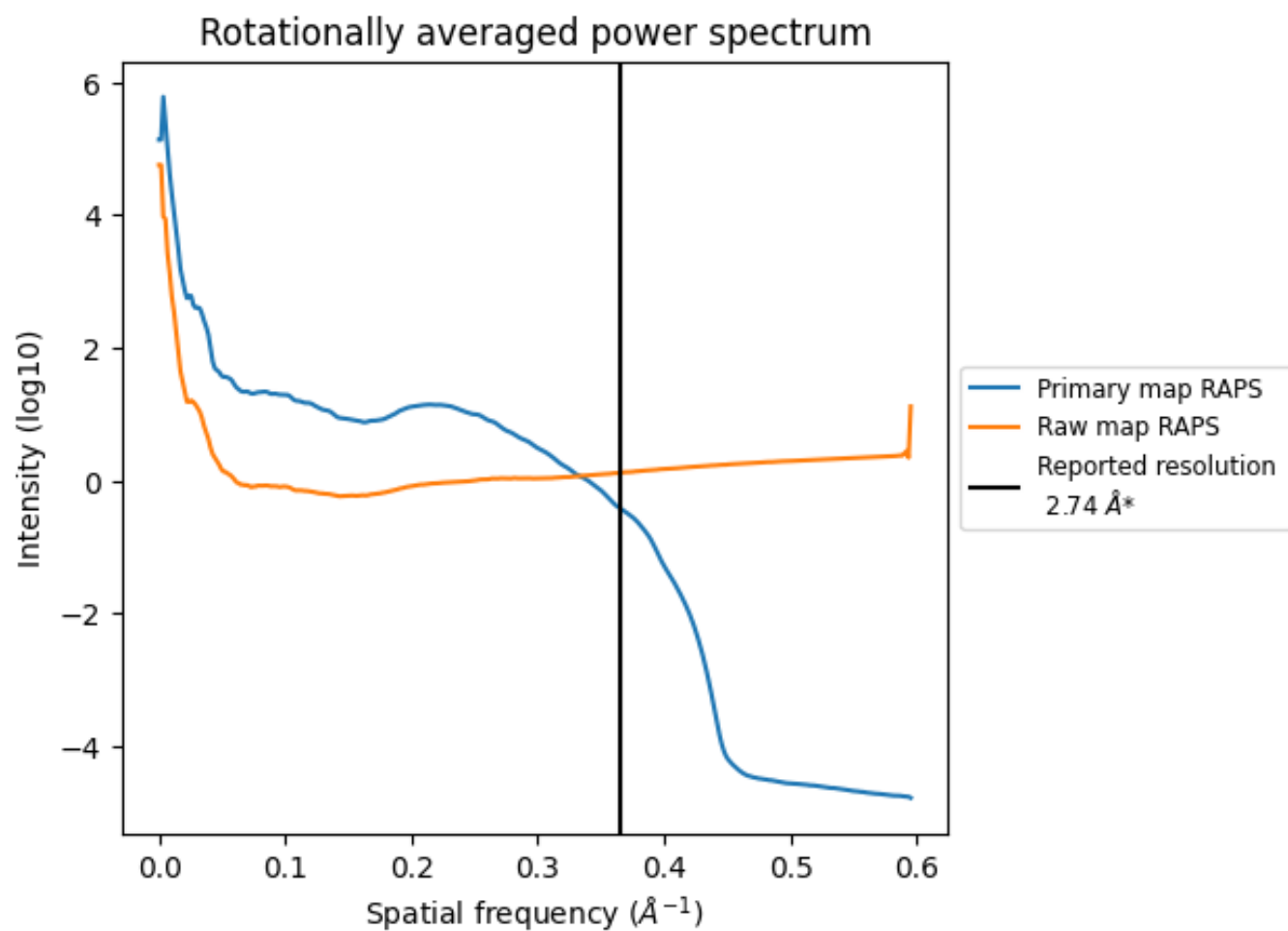
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 231 nm^3 ; this corresponds to an approximate mass of 209 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 ⓘ

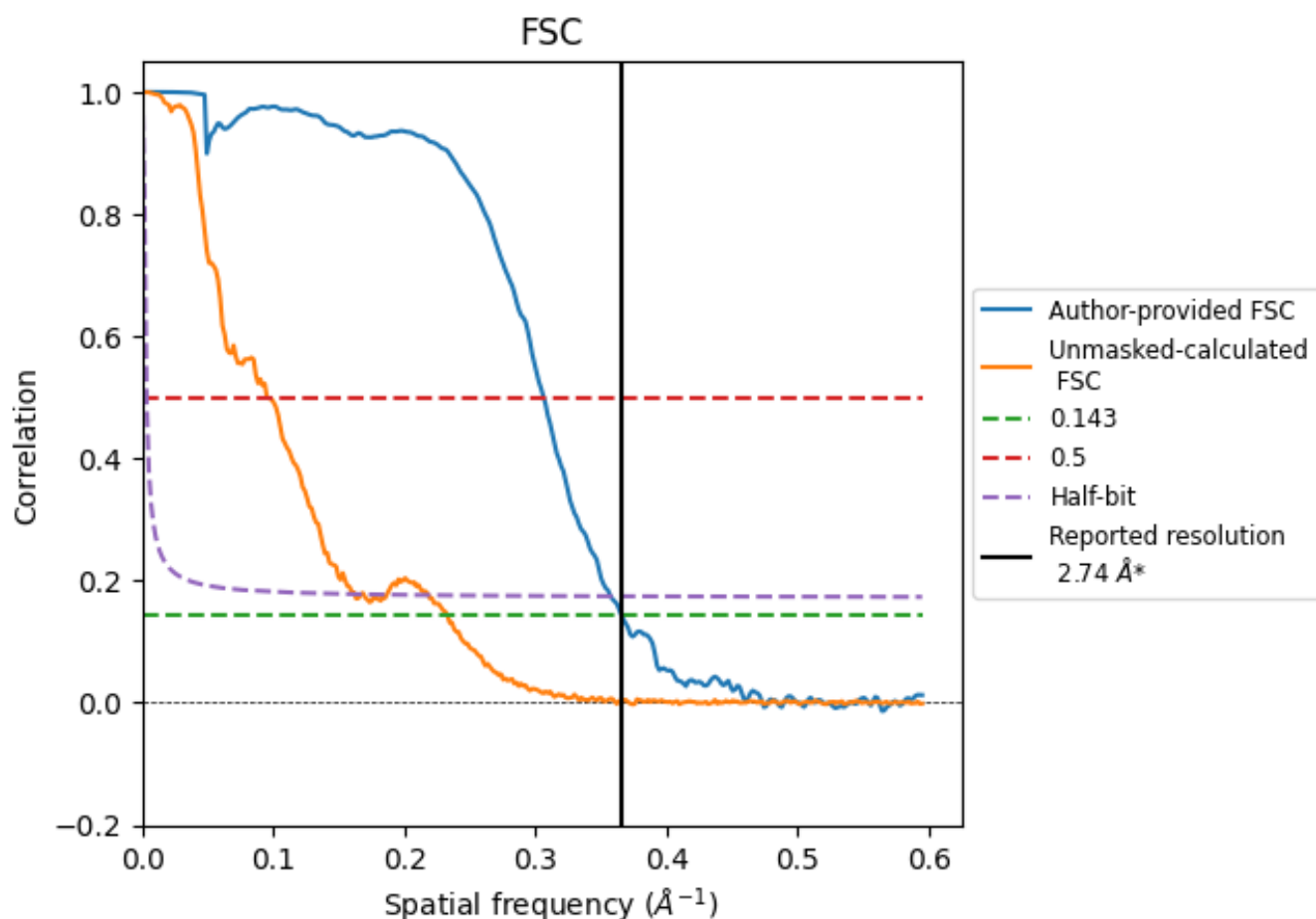


*Reported resolution corresponds to spatial frequency of 0.365 $\text{\AA}^{-1}$

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 0.365 Å⁻¹

8.2 Resolution estimates [i](#)

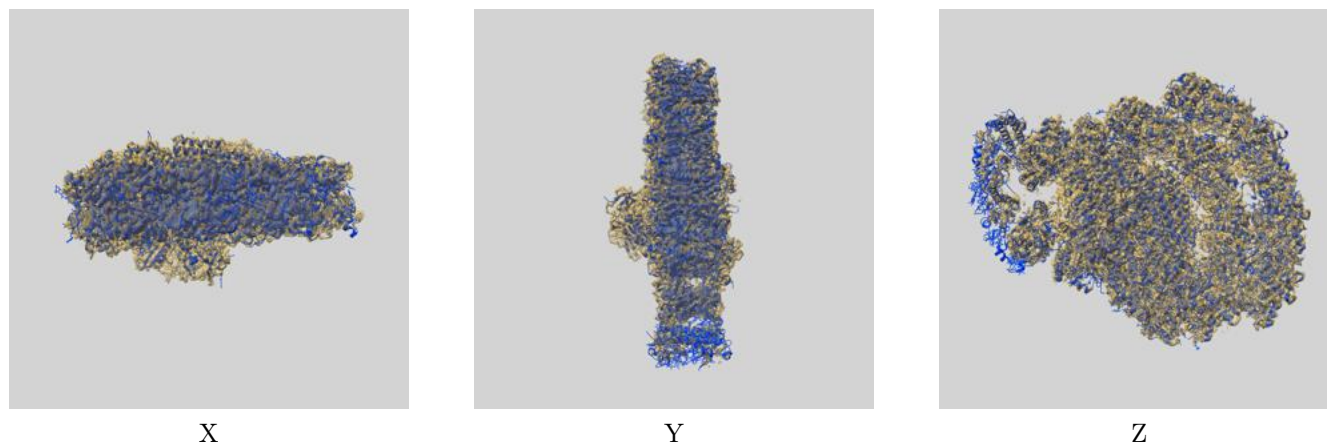
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.74	-	-
Author-provided FSC curve	2.73	3.26	2.80
Unmasked-calculated*	4.30	10.50	6.17

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.30 differs from the reported value 2.74 by more than 10 %

9 Map-model fit [i](#)

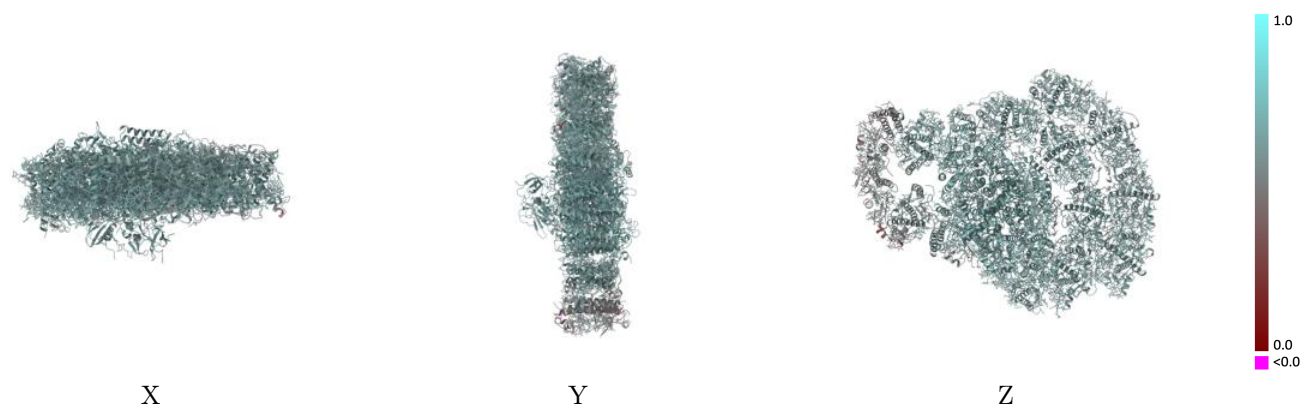
This section contains information regarding the fit between EMDB map EMD-14867 and PDB model 7ZQ9. Per-residue inclusion information can be found in section [3](#) on page [41](#).

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.031 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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

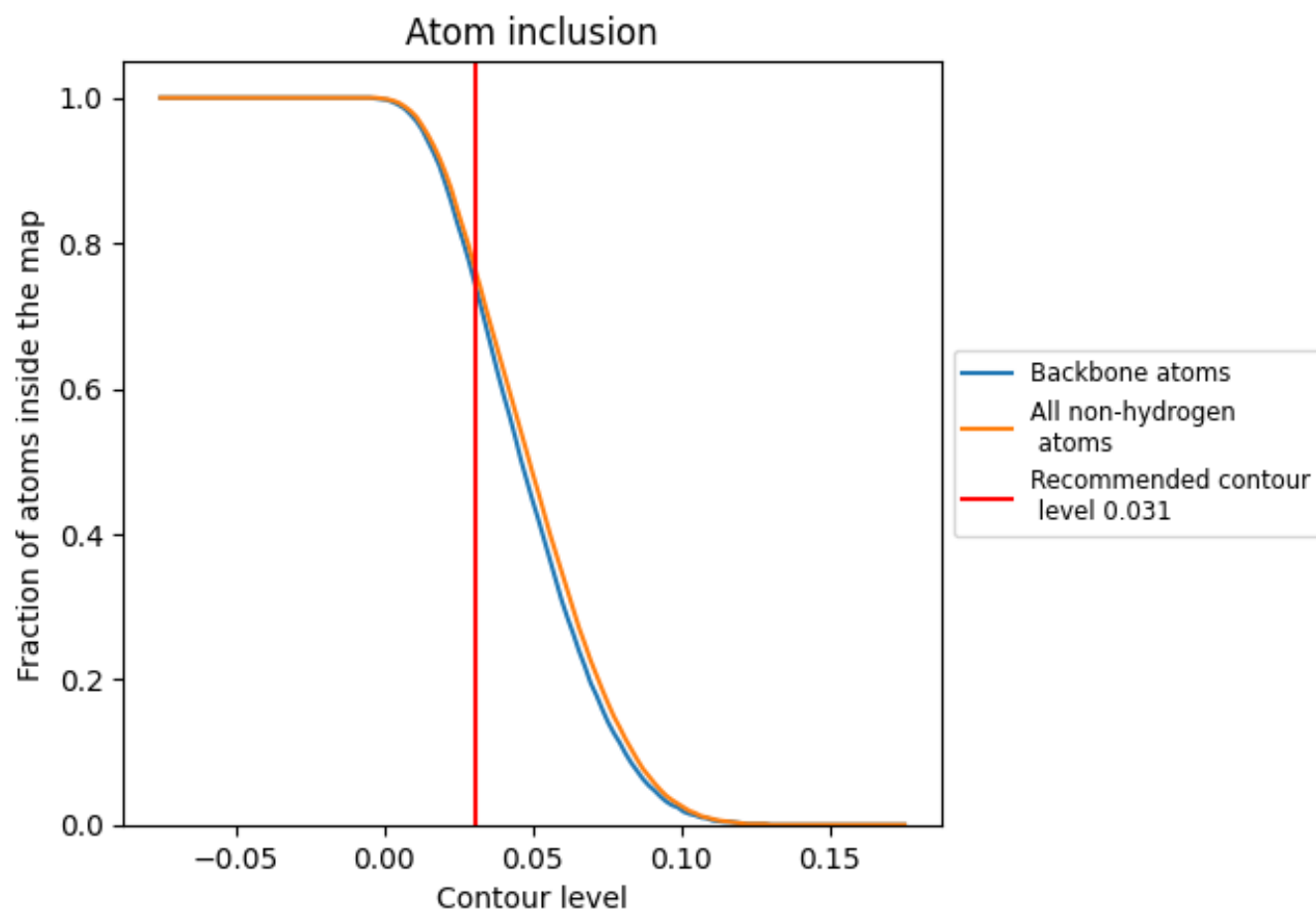


The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 76% 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 (0.031) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7580	0.6090
1	0.7690	0.6100
3	0.7890	0.6130
4	0.6760	0.5800
5	0.7360	0.5940
6	0.6910	0.5870
7	0.8220	0.6170
8	0.8330	0.6210
9	0.7150	0.5960
92	0.5280	0.5380
A	0.8970	0.6530
B	0.9100	0.6580
B2	0.2380	0.4950
C	0.9070	0.6460
D	0.7900	0.6170
E	0.7730	0.6160
F	0.8130	0.6180
G	0.7110	0.6000
I	0.8020	0.6160
I2	0.3950	0.5110
J	0.8420	0.6240
K	0.6190	0.5850
L	0.6650	0.5780
L2	0.3430	0.4920
Z	0.6750	0.5840

1.0

0.0

<0.0